

D_modelagem_bio_Artigo_02_ver_05

November 21, 2020

1 Artigo 02: Modelagem de dados para quatro atividades enzimáticas: fpase, cmcase, beta-glicosidase e xilanase - conjunto de dados EETA

In [1]: *# criei umas marcações para acesso rápido utilizando @, exemplo @outliers*

1.1 Descrição do que foi feito neste notebook:

- Utilização da base de dados do extrato enzimático EETA durante a fermentação e com desnaturação
- Após PCA trabalhou-se somente com os dados da fermentação, totalizando 81 amostras

1.2 Importação de módulos utilizados durante todo o processamento

```
In [2]: #importação de módulos
        #@import
        import pandas as pd
        import numpy as np
        import time

        #Para plotagens
        import matplotlib.pyplot as plt
        import seaborn as sns

        #Filtro Digital de Savitzky-Golay para suavização dos dados
        from scipy.signal import savgol_filter

        #pré-processamento:

        #Transformação nos dados
        from sklearn.preprocessing import StandardScaler, MinMaxScaler, Normalizer, scale, LabelEncoder
        #Seleção de atributos
        from sklearn.feature_selection import mutual_info_regression, SelectKBest, SelectPercentile

        #particionamento de base de dados para treinamento, validação e teste
        from sklearn.model_selection import train_test_split

        #algoritmos para o aprendizado:
```

```

from sklearn.decomposition import PCA, KernelPCA
from sklearn.linear_model import LinearRegression
from sklearn import svm
from sklearn.cross_decomposition import PLSRegression, PLSSVD
from sklearn.ensemble import RandomForestRegressor
from sklearn.multioutput import MultiOutputRegressor
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.neighbors import KNeighborsRegressor
from sklearn.kernel_ridge import KernelRidge
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import learning_curve
from xgboost import XGBRegressor

#Métricas para avaliação dos algoritmos de aprendizado
from sklearn.model_selection import cross_val_predict
from sklearn.metrics import mean_squared_error, r2_score

import statsmodels.api as sm

import warnings
warnings.filterwarnings("ignore")

%matplotlib inline

```

1.3 FUNÇÕES GERAIS

In [3]: *#@fglobal*

1.3.1 Funções para validação dos modelos multivariados

In [526]: *#@fvalidações*

```

#RMSE
def rmse(ref,pred):
    #recebe como entrada dois vetores dos valores de referência e preditos
    ref = pd.Series(ref)
    pred=pd.Series(pred)
    n=len(ref) #total de amostras
    mse = 0
    for i in range(n):
        mse +=(ref[i]-pred[i])**2
    mse=mse/n
    rmse=np.sqrt(mse)
    return rmse

#bias
def bias(ref,pred):
    ref = pd.Series(ref)
    pred=pd.Series(pred)

```

```

b=0
n = len(ref)
for r, p in zip(ref, pred):
    b += (r-p)
return (b/n)

#SEP
def sep(ref,pred):
    ref = pd.Series(ref)
    pred=pd.Series(pred)
    b = bias(ref,pred)
    sep = 0
    n = len(ref)
    for i in range(n):
        sep +=(ref[i]-pred[i]-b)**2
    sep = np.sqrt(sep/(n-1))
    return sep

#RPIQ
def rpiq(ref, pred):
    ref = pd.Series(ref)
    pred=pd.Series(pred)
    q1 = ref.quantile(0.25)
    q3 = ref.quantile(0.75)
    iq=q3-q1
    rpiq = iq/rmse(ref, pred)
    return rpiq

#RPD
def rpd(ref,pred):
    ref = pd.Series(ref)
    pred=pd.Series(pred)
    rpd = np.std(ref)/rmse(ref,pred)
    return rpd

#RER
def rer(ref,pred):
    ref = pd.Series(ref)
    pred=pd.Series(pred)
    rer = (np.max(ref) -np.min(ref) )/sep(ref,pred)
    return rer

#R2
def getr2(ref,pred):
    r2=r2_score(ref,pred)
    return r2

#MSE
def getmse(ref,pred):
    mse = mean_squared_error(ref,pred)

```

```

        return mse
    #RMSE forma simples de calcular
    def getrmse(ref,pred):
        rmse = np.sqrt(mean_squared_error(ref,pred))
        return rmse

```

1.3.2 Funções de pré-processamento

```

In [5]: #funções gerais de pré-processamento de spectros
        #@fspec
        #MSC(Multiplicative scatter correction)correção do espalhamento multiplicativo de sina
        def msc(input_data, reference=None):
            ''' Perform Multiplicative scatter correction'''
            # mean centre correction
            for i in range(input_data.shape[0]):
                input_data[i,:] -= input_data[i,:].mean()
            # Get the reference spectrum. If not given, estimate it from the mean
            if reference is None:
                # Calculate mean
                ref = np.mean(input_data, axis=0)
            else:
                ref = reference
            # Define a new array and populate it with the corrected data
            data_msc = np.zeros_like(input_data)
            for i in range(input_data.shape[0]):
                # Run regression
                fit = np.polyfit(ref, input_data[i,:], 1, full=True)
                # Apply correction
                data_msc[i,:] = (input_data[i,:] - fit[0][1]) / fit[0][0]
            return (data_msc, ref)

        #Variável normal padrão (SNV) Standard Normal Variate
        def snv(input_data):

            # Define a new array and populate it with the corrected data
            data_snv = np.zeros_like(input_data)
            for i in range(input_data.shape[0]):
                # Apply correction
                data_snv[i,:] = (input_data[i,:] - np.mean(input_data[i,:])) / np.std(input_da
            return data_snv

```

1.3.3 Função teste para correção de espectros

```

In [6]: #@ftestes
        def executePreSpec(dados,wint,wtxt):
            x = dados.loc[:,wtxt].values
            w = wint

```

```

Xmsc = msc(x)[0] # Take the first element of the output tuple
Xsnv = snv(x)
## Plot spectra
plt.figure(figsize=(8,9))
with plt.style.context(('ggplot')):
    ax1 = plt.subplot(311)
    plt.plot(w, x.T)
    plt.title('Original data')
    ax2 = plt.subplot(312)
    plt.plot(w, Xmsc.T)
    plt.ylabel('Absorbance spectra')
    plt.title('MSC')
    ax2 = plt.subplot(313)
    plt.plot(w, Xsnv.T)
    plt.xlabel('Wavelength (nm)')
    plt.title('SNV')
    plt.show()

```

1.3.4 Funções para plotar resultados

In [7]: *#@grafResiduos*

```

def graficoResiduos(modelo, treino_teste, y_c, y_cv, y_p):
    #gráfico de resíduos:
    res_c = treino_teste[2] - y_c #resíduos da calibração
    res_cv = treino_teste[2] - y_cv #resíduos da validação
    res_p = treino_teste[3] - y_p #resíduos da predição
    residuos = [res_c, res_cv, res_p]
    ys = [y_c, y_cv, y_p]
    modelos = ['cal', 'val', 'pred']
    cores = ['b', 'r', 'k']
    cores_ae = ['b', 'g', 'r', 'y']
    fig = plt.figure(figsize=(20,20))
    plt.subplots_adjust(hspace = 0.3, wspace=0.2)
    for i, res, m in zip([0,1,2], residuos, modelos):
        ig = i+1
        for cor, j in zip(cores_ae, [0,1,2,3]):
            ax = fig.add_subplot(4,3,ig)
            ax = sns.residplot(res.iloc[:,j], ys[i][:,j], color=cor, robust=True, label=
            ax.set_title(modelo+' :Resíduos('+m+')')
            ax.set_xlabel('Preditos')
            ax.set_ylabel('Resíduos')
            plt.legend(loc='best')
            ig+=3

```

In [8]: *#@grafHistogramas*

```

def graficoHist(modelo, treino_teste, y_c, y_cv, y_p):
    res_c = treino_teste[2] - y_c #resíduos da calibração
    res_cv = treino_teste[2] - y_cv #resíduos da validação

```

```

res_p = treino_teste[3] - y_p #resíduos da predição
#histograma dos resíduos para verificar se segue uma distribuição normal
#gráfico de resíduos: histograma
residuos = [res_c, res_cv, res_p]
modelos = ['cal', 'val', 'pred']
cores = ['b', 'r', 'k']
cores_ae=['b', 'g', 'r', 'y']
for i,res, m in zip([0,1,2],residuos, modelos):
    fig = plt.figure(figsize=(20,5))
    plt.subplots_adjust(hspace = 0.5, wspace=0.1)

    for cor,j in zip(cores_ae,[0,1,2,3]):
        ax = fig.add_subplot(1,4,j+1)
        ax = sns.distplot(res.iloc[:,j], color=cores_ae[j], kde=False, label=var_ae[j])
        ax.set_title(modelo+' :Histograma dos resíduos('+m+')')

```

In [110]: *#gráfico: reais x preditos - separando calibração validação predição*
#@grafreaispred

```

def graficoReaisPreditosSep(modelo, treino_teste, y_c, y_cv,y_p):
    res_c = treino_teste[2] #variável resposta da calibração
    res_cv = treino_teste[2] #variável resposta da validação
    res_p = treino_teste[3] #variável resposta da predição
    reais= [res_c, res_cv, res_p]
    ys = [y_c, y_cv, y_p]
    modelos = ['cal', 'val', 'pred']
    cores = ['b', 'r', 'k']
    cores_ae=['b', 'g', 'r', 'y']
    mark=['x', '1', '+']
    fig = plt.figure(figsize=(20,20))
    plt.subplots_adjust(hspace = 0.3, wspace=0.2)
    for i,re, m in zip([0,1,2],reais, modelos):
        ig = i+1
        for cor,j in zip(cores_ae,[0,1,2,3]):
            ax = fig.add_subplot(4,3,ig)
            ax.scatter(re.iloc[:,j], ys[i][:,j],marker=mark[i],c=cores[i], edgecolor=cores[i])
            ax.plot(ys[i][:,j], ys[i][:,j], color=cores[i])

            ax.set_title(modelo)
            ax.set_xlabel('Reais')
            ax.set_ylabel('Preditos')
            plt.legend(loc='best')
            ig+=3

```

In [118]: *#gráfico: reais x preditos - juntando cal, val e predição*
#@grafreaispred

```

def graficoReaisPreditos(modelo, treino_teste, y_c, y_cv,y_p):
    res_c = treino_teste[2] #variável resposta da calibração
    res_cv = treino_teste[2] #variável resposta da validação

```

```

res_p = treino_teste[3] #variável resposta da predição
reais= [res_c, res_cv, res_p]
ys = [y_c, y_cv, y_p]
modelos = ['cal', 'val', 'pred']
cores = ['b', 'r', 'k']
cores_ae=['b', 'g', 'r', 'y']
mark=['x', '1', '+']
fig = plt.figure(figsize=(10,30))
plt.subplots_adjust(hspace = 0.3, wspace=0.2)

for i in range(4):
    for j in range(3):
        ax = fig.add_subplot(4,1,i+1)
        ax.scatter(reais[j].iloc[:,i], ys[j][:,i],c=cores[j],marker=mark[j],label=
        if j == 0:
            ax.plot(ys[j][:,i], ys[j][:,i], color=cores[j], label=modelos[j])
        ax.set_title(modelo+'-->'+var_ae[i])
        ax.set_xlabel('Reais')
        ax.set_ylabel('Preditos')
        plt.legend(loc='best')

```

In []:

In [11]: *#@grafTreinamento*

```

def graficoTreinamento(modelo, y_treino, y_c, y_cv):
    #####
    #Gráficos de treinamento e validação cruzada para todas as atividades
    #cria um data frame com os valores reais e preditos na calibração e validação
    df_cv = {}
    for valor in var_ae:
        df_cv[valor] = []
    i=0
    for valor in var_ae:
        df = pd.DataFrame(columns=['reais', 'cal', 'val'], index=y_treino.index)
        df['reais'] = y_treino[valor]
        df['cal'] = pd.DataFrame(y_c[:,i],index= y_treino.index)
        df['val'] = pd.DataFrame(y_cv[:,i],index= y_treino.index)
        i +=1
        df_cv[valor] = df.copy()
    #cria data frame com os valores dos intervalos de medições
    df_cv_inter ={}
    for valor in var_ae:
        df_cv_inter[valor] = []
    for valor in var_ae:
        df_cv_inter[valor] = df_cv[valor].copy()
        df_cv_inter[valor]['inter'] = dados.loc[:, 'inter']
    #ordena valores pelo intervalo

```

```

df_ord_treino = {}
for valor in var_ae:
    df_ord_treino[valor] = []
for valor in var_ae:
    df_ord_treino[valor] = df_cv_inter[valor].sort_values(['inter'])
x = list(df_ord_treino['xilanase']['inter'])

#calculando a média para cada ponto
df_treino_media = {}
for valor in var_ae:
    df_treino_media[valor] = []
for valor in var_ae:
    df_treino_media[valor] = df_ord_treino[valor].groupby('inter').mean()

x = list(df_treino_media['xilanase'].index)
var = ['reais', 'cal', 'val']
tipo = ['ko-', 'bo-', 'ro-']
tipoAE= ['bo-', 'go-', 'ro-', 'yo-']
fig = plt.figure(figsize=(15,5))
j=1
plt.subplots_adjust(hspace = 0.7, wspace=0.5)
for valor in var_ae:
    ax = fig.add_subplot(2,2,j)
    for i in range(3):
        ax.plot(x,df_treino_media[valor][var[i]], tipo[i], label=var[i])
        ax.legend(loc=2)
        ax.set_title('Calibração e validação cruzada:'+modelo+': '+valor)
        ax.set_xlabel('Tempo de fermentação')
        ax.set_ylabel('Atividade enzimática')
        ax.set_xticks(x)
    j+=1

```

In []: *#@grafTreinamento grandes*

```

def graficoTreinamentoG(modelo, y_treino, y_c, y_cv):
    #####
    #Gráficos de treinamento e validação cruzada para todas as atividades
    #cria um data frame com os valores reais e preditos na calibração e validação
    df_cv = {}
    for valor in var_ae:
        df_cv[valor] = []
    i=0
    for valor in var_ae:
        df = pd.DataFrame(columns=['reais', 'cal', 'val'], index=y_treino.index)
        df['reais'] = y_treino[valor]
        df['cal'] = pd.DataFrame(y_c[:,i],index= y_treino.index)
        df['val'] = pd.DataFrame(y_cv[:,i],index= y_treino.index)
        i +=1
        df_cv[valor] = df.copy()

```



```

#cria data frame com os valores dos intervalos de medições
df_cv_inter = {}
for valor in var_ae:
    df_cv_inter[valor] = []
for valor in var_ae:
    df_cv_inter[valor] = df_cv[valor].copy()
    df_cv_inter[valor]['inter'] = dados.loc[:, 'inter']
#ordena valores pelo intervalo
df_ord_treino = {}
for valor in var_ae:
    df_ord_treino[valor] = []
for valor in var_ae:
    df_ord_treino[valor] = df_cv_inter[valor].sort_values(['inter'])
x = list(df_ord_treino['xilanase']['inter'])

#calculando a média para cada ponto
df_treino_media = {}
for valor in var_ae:
    df_treino_media[valor] = []
for valor in var_ae:
    df_treino_media[valor] = df_ord_treino[valor].groupby('inter').mean()

x = list(df_treino_media['xilanase'].index)
var = ['reais', 'cal', 'val']
tipo = ['ko-', 'bo-', 'ro-']
tipoAE = ['bo-', 'go-', 'ro-', 'yo-']
fig = plt.figure(figsize=(15,5))
j=1
plt.subplots_adjust(hspace = 0.7, wspace=0.5)
for valor in var_ae:
    ax = fig.add_subplot(2,2,j)
    for i in range(3):
        ax.plot(x, df_treino_media[valor][var[i]], tipo[i], label=var[i])
        ax.legend(loc=2)
        ax.set_title('Calibração e validação cruzada: '+modelo+' : '+valor)
        ax.set_xlabel('Tempo de fermentação')
        ax.set_ylabel('Atividade enzimática')
        ax.set_xticks(x)
    j+=1

```

```

In [12]: #@grafTeste (predição )
def graficoTeste(modelo, y_teste, y_p):
    #####
    #para todas as atividades
    #cria um data frame com os valores reais e preditos para os dados de teste
    df_pred = {}
    for valor in var_ae:
        df_pred[valor] = []

```

```

i=0
for valor in var_ae:
    df =pd.DataFrame(columns=['reais','preditos'], index= y_teste.index)
    df['reais'] = y_teste[valor]
    df['preditos'] = pd.DataFrame(y_p[:,i],index= y_teste.index)
    i +=1
    df_pred[valor] = df.copy()

#cria data frame com os valores dos intervalos de medições
df_pred_inter = {}
for valor in var_ae:
    df_pred_inter[valor] = []
for valor in var_ae:
    df_pred_inter[valor] = df_pred[valor].copy()
    df_pred_inter[valor]['inter'] = dados.loc[:,'inter']

#ordena valores pelo intervalo
df_ord_teste = {}
for valor in var_ae:
    df_ord_teste[valor] = []
for valor in var_ae:
    df_ord_teste[valor] = df_pred_inter[valor].sort_values(['inter'])

#calculando a média para cada ponto
df_teste_media = {}
for valor in var_ae:
    df_teste_media[valor] = []
for valor in var_ae:
    df_teste_media[valor] = df_ord_teste[valor].groupby('inter').mean()

x = list(df_teste_media['xilanase'].index)
var = ['reais', 'preditos']
tipoAE= ['bo-.', 'go-.','ro-.', 'yo-.']
j = 0
fig = plt.figure(figsize=(15,5))
plt.subplots_adjust(hspace = 0.7, wspace=0.5)
for valor in var_ae:
    ax = fig.add_subplot(2,2,j+1)
    ax.plot(x,df_teste_media[valor][var[0]], 'ko-.', label=var[0])
    ax.plot(x,df_teste_media[valor][var[1]], tipoAE[j], label=var[1])
    j +=1
    ax.legend(loc=2)
    ax.set_title('Validação externa: Modelo '+modelo+'-'+valor)
    ax.set_xlabel('Tempo de fermentação')
    ax.set_ylabel('Atividade enzimática')
    ax.set_xticks(x)

```

In []: *#@grafTeste grande (predição)*

```

def graficoTesteG(modelo, y_teste, y_p):
    #####
    #para todas as atividades
    #cria um data frame com os valores reais e preditos para os dados de teste
    df_pred = {}
    for valor in var_ae:
        df_pred[valor] = []
    i=0
    for valor in var_ae:
        df = pd.DataFrame(columns=['reais', 'preditos'], index= y_teste.index)
        df['reais'] = y_teste[valor]
        df['preditos'] = pd.DataFrame(y_p[:,i], index= y_teste.index)
        i +=1
        df_pred[valor] = df.copy()

    #cria data frame com os valores dos intervalos de medições
    df_pred_inter = {}
    for valor in var_ae:
        df_pred_inter[valor] = []
    for valor in var_ae:
        df_pred_inter[valor] = df_pred[valor].copy()
        df_pred_inter[valor]['inter'] = dados.loc[:, 'inter']

    #ordena valores pelo intervalo
    df_ord_teste = {}
    for valor in var_ae:
        df_ord_teste[valor] = []
    for valor in var_ae:
        df_ord_teste[valor] = df_pred_inter[valor].sort_values(['inter'])

    #calculando a média para cada ponto
    df_teste_media = {}
    for valor in var_ae:
        df_teste_media[valor] = []
    for valor in var_ae:
        df_teste_media[valor] = df_ord_teste[valor].groupby('inter').mean()

    x = list(df_teste_media['xilanase'].index)
    var = ['reais', 'preditos']
    tipoAE= ['bo-.', 'go-.', 'ro-.', 'yo-.']
    j = 0
    fig = plt.figure(figsize=(15,5))
    plt.subplots_adjust(hspace = 0.7, wspace=0.5)
    for valor in var_ae:
        ax = fig.add_subplot(2,2,j+1)
        ax.plot(x, df_teste_media[valor][var[0]], 'ko-.', label=var[0])
        ax.plot(x, df_teste_media[valor][var[1]], tipoAE[j], label=var[1])
        j +=1

```

```

ax.legend(loc=2)
ax.set_title('Validação externa: Modelo '+modelo+':'+valor)
ax.set_xlabel('Tempo de fermentação')
ax.set_ylabel('Atividade enzimática')
ax.set_xticks(x)

```

In []:

1.3.5 Função para calcular intervalo de confiança para a média dos modelos criados:

```

In [13]: #@interConfiança
         #para intervalo de confiança = 95% Z = 1,96
         # a proporção de acertos do modelo será de p +- (valor calculado para intervalo de co
         # seja n o número amostras (neste caso o número de modelos criados, exemplo 40)
         #P(a) = o resultado da proporção de acerto
         #P(e) = proporção de erro
         #p =- intervalo de confiança
         #ic = z*raizquadrada((pa*(1-pa))/n)
         #exemplo:
def calculaIntConf(n,pa):
    z = 1.96
    ic = z*(np.sqrt((pa*(1-pa))/n))
    ic_min = p - ic
    ic_max = pa + ic
    return ic_min, ic_max

```

1.4 Base de dados

```

In [14]: #@data
         #Escolha da base de dados

```

```

In [15]: #base de dados contendo todos os dados
dados= pd.read_excel('A_dados.xlsx',sheet_name='todos')
dados_back = dados.copy()

```

```

In [362]: #@backupdata
          dados = dados_back.copy() #backup da base para uso posterior rápido

```

```

In [13]: #@dadosshape
          dados.shape #tamanho da base dados

```

```

Out[13]: (1451, 713)

```

```

In [16]: #Separar somente as amostras que contenham todas as atividades enzimáticas
dados = dados.loc[(dados['betaglicosidase'].notnull())
                  & (dados['cmcase'].notnull())
                  & (dados['fpase'].notnull())
                  & (dados['xilanase'].notnull())]
resultados = '\nTotal geral de amostras com todas as atividades enzimáticas:'+str(dad
print(resultados)

```

Total geral de amostras com todas as atividades enzimáticas:938

```
In [ ]: #escolha a base de dados que quer trabalhar por extrato enzimático
#dados = pd.read_excel('A_dados.xlsx',sheet_name='celluclast')
#dados = pd.read_excel('A_dados.xlsx',sheet_name='bio')
#dados = pd.read_excel('A_dados.xlsx',sheet_name='celic')
```

```
#dados = dados[(dados['eenz'] == 'celluclast')]
#dados = dados[(dados['eenz'] == 'eeta')]
#dados = dados[(dados['eenz'] == 'ctec2')]
#dados = dados[(dados['eenz'] == 'eeta') & (dados['experimento']=='biof')]
```

```
In [15]: dados = dados[(dados['eenz'] == 'eeta')] #base de dados do extrato EETA exp 1
dados.shape
```

```
Out[15]: (129, 713)
```

```
In [363]: dados = dados[(dados['eenz'] == 'eeta') & (dados['experimento']=='biof')] #base de dados
```

```
In [ ]:
```

```
In [2446]: dadosB1 = dados[(dados['experimento']=='biof')]
dadosB1.shape
#dadosB = dados[(dados['eenz'] == 'eeta') & (dados['experimento']=='bioB')] #fermenta
#dadosE = dados[(dados['eenz'] == 'eeta') & (dados['experimento']=='bioE')] #fermenta
```

```
Out[2446]: (81, 713)
```

```
In [1235]: dadosB2 = dados[dados['experimento']=='bioB'] # eeta de fermentação em bior exp 2
dadosB2.shape
```

```
Out[1235]: (21, 713)
```

```
In [1236]: dadosE = dados[dados['experimento']=='bioE'] # eeta de fermentação em erlemeyer exp2
dadosE.shape
```

```
Out[1236]: (24, 713)
```

```
In [2447]: dadosD1= dados[dados['experimento']=='biod1'] # eeta de desnaturação 1 exp 1
dadosD1.shape
```

```
Out[2447]: (33, 713)
```

```
In [1238]: dadosD2= dados[dados['experimento']=='biod2'] # eeta de desnaturação 2 exp 2
dadosD2.shape
```

```
Out[1238]: (33, 713)
```

```

In [2448]: frames = [dadosB1, dadosD1]
           dados = pd.concat(frames)

In [2441]: dados = dadosB1.copy()

In [31]: dados.shape

Out[31]: (81, 717)

In [ ]:

In [ ]: #Separar somente as amostras que contenham betaglicosidase
        dados = dados.loc[(dados['betaglicosidase'].notnull()) ]
        resultados = '\nTotal geral de amostras para betaglicosidase:'+str(dados.shape[0])

In [ ]: #Separar somente as amostras que contenham cmcase
        dados = dados.loc[(dados['cmcase'].notnull()) ]
        resultados = '\nTotal geral de amostras para cmcase:'+str(dados.shape[0])

In [ ]: #Separar somente as amostras que contenham fpase
        dados = dados.loc[(dados['fpase'].notnull()) ]
        resultados = '\nTotal geral de amostras para fpase:'+str(dados.shape[0])

In [ ]: #Separar somente as amostras que contenham xilanase
        dados = dados.loc[(dados['xilanase'].notnull()) ]
        resultados = '\nTotal geral de amostras para xilanase:'+str(dados.shape[0])

```

1.5 Estatística básica do conjunto de dados: atividade enzimática

```

In [17]: #@statistic

In [18]: dados['betaglicosidase'].describe()

Out[18]: count      81.000000
         mean        1.985255
         std         1.599679
         min         0.030827
         25%         0.382773
         50%         2.164345
         75%         3.596691
         max         4.603719
         Name: betaglicosidase, dtype: float64

In [19]: dados['cmcase'].describe()

Out[19]: count      81.000000
         mean        0.057668
         std         0.035836
         min         0.011206
         25%         0.031505

```

```
50%      0.055725
75%      0.072961
max       0.171262
Name: cmcase, dtype: float64
```

```
In [20]: dados['fpase'].describe()
```

```
Out[20]: count      81.000000
mean       0.044621
std        0.025433
min        0.010442
25%        0.013869
50%        0.052863
75%        0.068121
max        0.091917
Name: fpase, dtype: float64
```

```
In [21]: dados['xilanase'].describe()
```

```
Out[21]: count      81.000000
mean      10.931162
std        6.510726
min         0.072595
25%        8.477247
50%       11.573610
75%       15.397347
max       20.136787
Name: xilanase, dtype: float64
```

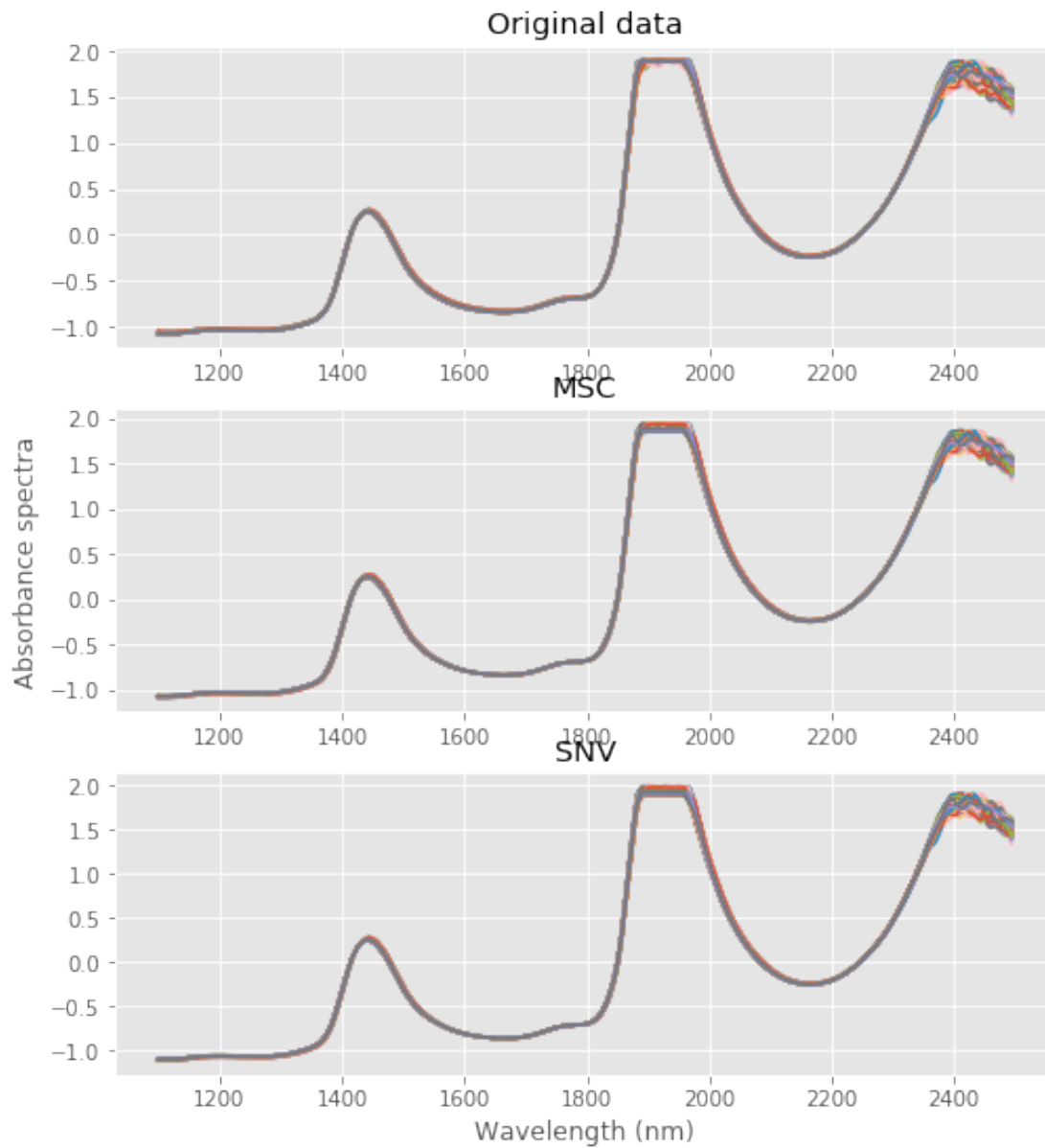
```
In [484]: #verifica quantos são os valores nulos no conjunto de dados por coluna
          #dados.isnull().sum()
```

1.6 imprimindo os espectros:

```
In [364]: #@plotspec
          #criando vetores com os nomes dos atributos apenas para plotagem
```

```
var_abs_int = np.arange(1100,2496,2)
var_abs_txt=[]
for valor in var_abs_int:
    var_abs_txt += [str(valor)+'nm']
var_ae=['betaglicosidase','cmcase','fpase','xilanase']
```

```
In [23]: #teste das correções dos espectros:
          #@testescorreções
          executePreSpec(dados,var_abs_int,var_abs_txt)
```



In []:

In []:

```
In [24]: X=dados.loc[:,var_abs_txt]
         xT= np.transpose(X)
         len(X.columns)
```

Out[24]: 698

In [25]: *#gráfico de dispersão 3 em um*


```

fonte = {'family': 'serif',
        'color': 'black',
        'weight': 'normal',
        'size': 16,
        }

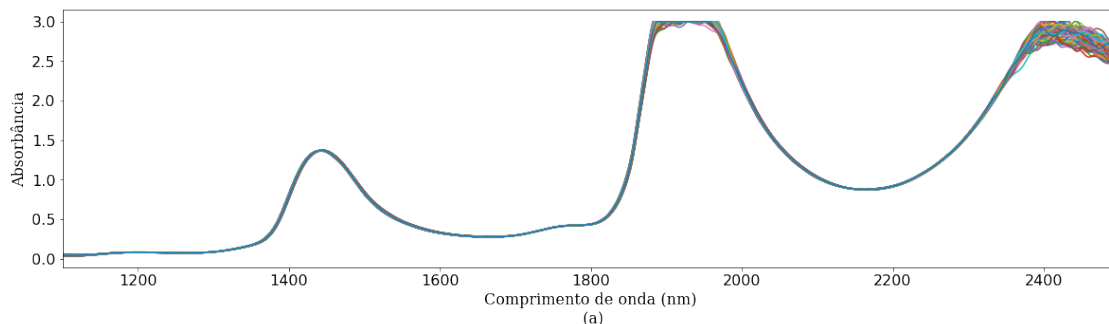
figuras = ['(a)', '(b)', '(c)']
limites = [[1100,2500],[1850,2000], [2300,2500]]
fig, ax = plt.subplots(1, 1, figsize=(20, 5))
plt.subplots_adjust(hspace = 0.5, wspace=0.1)
ax.plot(var_abs_int, xT)
ax.grid(False)
ax.set_xlabel('Comprimento de onda (nm)\n (a)', fontdict=fonte)
ax.set_ylabel('Absorbância', fontdict=fonte)
ax.set_xlim(limites[0][0],limites[0][1])
ax.tick_params(labelsize=16)

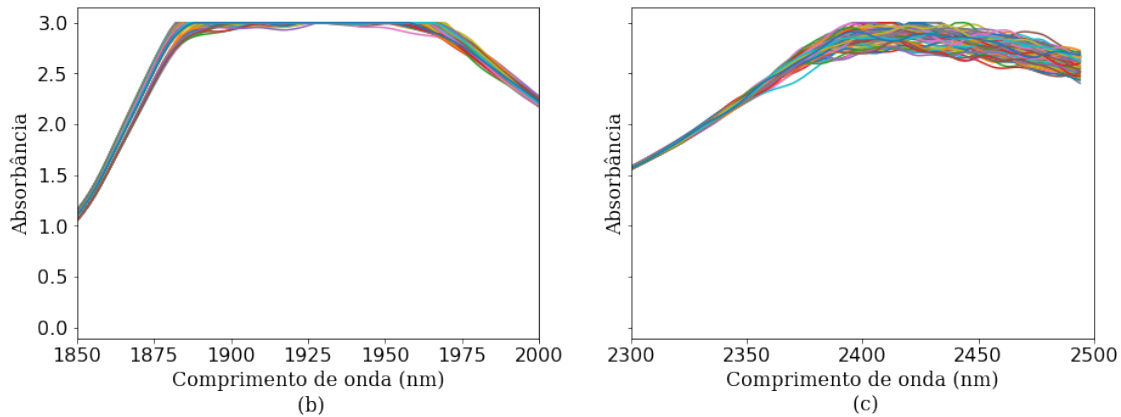
_, [ax1,ax2] = plt.subplots(1, 2, sharey=True, figsize=(15, 5))
ax1.plot(var_abs_int, xT)
ax1.grid(False)
ax1.set_xlabel('Comprimento de onda (nm)\n (b)', fontdict=fonte)
ax1.set_ylabel('Absorbância', fontdict=fonte)
ax1.set_xlim(limites[1][0],limites[1][1])
ax1.tick_params(labelsize=16)

ax2.plot(var_abs_int, xT)
ax2.grid(False)
ax2.set_xlabel('Comprimento de onda (nm)\n (c)', fontdict=fonte)
ax2.set_ylabel('Absorbância', fontdict=fonte)
ax2.set_xlim(limites[2][0],limites[2][1])
ax2.tick_params(labelsize=16)

plt.show()

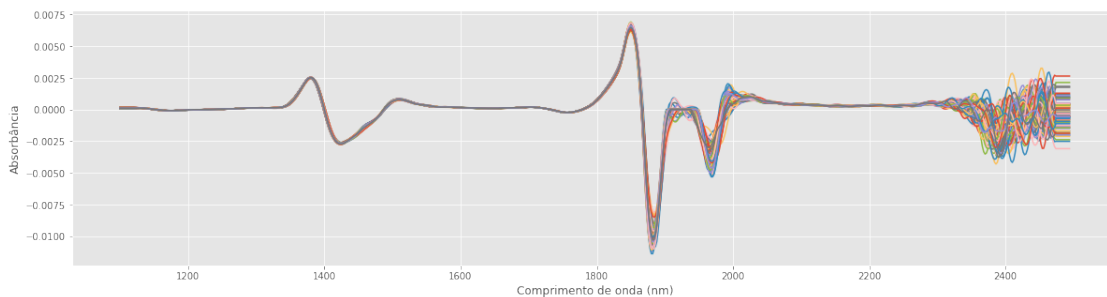
```





In [26]: *#Aplicando 2 derivada para impressão dos espectros:*

```
X=dados.loc[:, '1100nm': '2494nm']
wl = np.arange(1100,2495,2)
X2 = savgol_filter(X,21,polyorder=2, deriv=2)
# Imprimendo gráfico para segunda derivada
plt.figure(figsize=(20,5))
with plt.style.context('ggplot'):
    plt.plot(wl, X2.T)
    plt.xlabel('Comprimento de onda (nm)')
    plt.ylabel('Absorbância')
    plt.show()
```



In []:

```
In [53]: #dados_bio1=dados[dados.loc[:, 'experimento'] != 'biof']
#seleção de dados apenas da desnaturação
```

2 Seleção de atributos relevantes

```
In [19]: #@seleção de atributos
#1ºDefinimos os atributos importantes para determinação da atividade específica e ver
```

```

In [20]: from sklearn.model_selection import train_test_split
         from sklearn.feature_selection import mutual_info_regression, SelectKBest, SelectPerceptron

In [21]: #definindo as variáveis iniciais para o pré-processamento
         var_ae=['betaglicosidase','cmcase','fpase','xilanase']

         #criando um vetor com os nomes das absorbâncias para seleção posterior
         var_abs_int = np.arange(1100,2495,2)
         var_abs_txt=[]
         for valor in var_abs_int:
             var_abs_txt += [str(valor)+'nm']

In [22]: #Definindo os dataFrames iniciais para começar o processamento da seleção de atributos
         #Separando a matriz de dados independentes df_y, da de dados dependentes df_x
         df_x = dados.loc[:,var_abs_txt] #absorbâncias
         df_y = dados.loc[:,var_ae] #AE

In [31]: df_x.head(5)

Out[31]:
           1100nm    1102nm    1104nm    1106nm    1108nm    1110nm    1112nm  \
710  0.034299  0.034316  0.034365  0.034483  0.034698  0.035024  0.035451
711  0.036330  0.036267  0.036176  0.036125  0.036156  0.036290  0.036520
712  0.035881  0.035590  0.035438  0.035454  0.035622  0.035896  0.036219
713  0.035179  0.035056  0.034928  0.034866  0.034919  0.035102  0.035402
714  0.034658  0.034638  0.034605  0.034636  0.034780  0.035040  0.035381

           1114nm    1116nm    1118nm  ...    2476nm    2478nm    2480nm  \
710  0.035942  0.036455  0.036959  ...  2.586343  2.569360  2.558197
711  0.036817  0.037139  0.037451  ...  2.633472  2.631909  2.625733
712  0.036545  0.036860  0.037174  ...  2.610536  2.606123  2.594931
713  0.035788  0.036231  0.036707  ...  2.527729  2.520406  2.514344
714  0.035754  0.036137  0.036536  ...  2.585836  2.576738  2.567044

           2482nm    2484nm    2486nm    2488nm    2490nm    2492nm    2494nm
710  2.549708  2.540445  2.529844  2.520292  2.514482  2.512945  2.513940
711  2.613571  2.595041  2.570789  2.542441  2.512763  2.485513  2.464201
712  2.575879  2.550428  2.522418  2.496677  2.476537  2.461961  2.451295
713  2.507968  2.499267  2.488241  2.477992  2.472582  2.473660  2.479099
714  2.556880  2.546410  2.536578  2.528261  2.521858  2.518125  2.517375

[5 rows x 698 columns]

In [32]: df_y.head(5)

Out[32]:
           betaglicosidase    cmcase    fpase    xilanase
710             0.087354    0.021666    0.012690    0.107064
711             0.087354    0.021666    0.012690    0.107064
712             0.087354    0.021666    0.012690    0.107064
713             0.030827    0.021327    0.011302    0.099591
714             0.030827    0.021327    0.011302    0.099591

```

```
In [24]: #separando o conjunto de dados em treino e teste
x_treino, x_teste, y_treino, y_teste = train_test_split(df_x,df_y,test_size=0.25, ran

# Imprime o tamanho das bases geradas
print('Particionamento para treinamento e teste:\n','X_treino:',x_treino.shape,'Y_tre
```

Particionamento para treinamento e teste:

X_treino: (60, 698) Y_treino: (60, 4) X_teste: (21, 698) Y_teste: (21, 4)

2.1 Seleção de variáveis: método: mutua info regression:

```
In [29]: var_ae=['betaglicosidase','cmcase','fpase','xilanase']
sel_mi={}
for valor in var_ae:
    sel_mi[valor] = mutual_info_regression(x_treino,y_treino.loc[:,valor])
```

```
In [30]: sel_mi_graph = {}
for valor in var_ae:
    sel_mi_graph[valor] = pd.Series(sel_mi[valor])
```

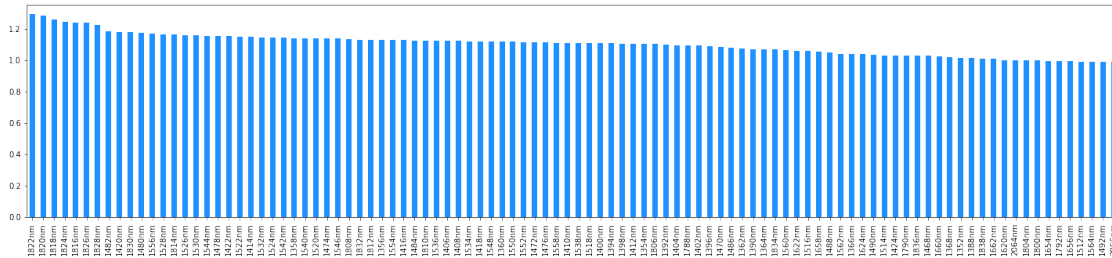
```
In [31]: for valor in var_ae:
    sel_mi_graph[valor].index = x_treino.columns
    sel_mi_graph[valor] = sel_mi_graph[valor].sort_values(ascending=False)
```

```
In [32]: from matplotlib import colors as mcolors
colors = dict(mcolors.BASE_COLORS, **mcolors.CSS4_COLORS)
cores = list(colors.keys())
```

```
In [1398]: #enzima = 'betaglicosidase'
#print('\n Variáveis mais importantes para %s: '%enzima)
#inicio = sel_mi_graph[enzima][sel_mi_graph[enzima]>.8][:20]
#fim = sel_mi_graph[enzima][sel_mi_graph[enzima]<.3][-50:-20]
#juntos = inicio.append(fim)
#juntos[:].plot.bar(figsize=(22,5),color=cores[52:53])
```

```
In [33]: enzima = 'betaglicosidase'
print('\n Variáveis mais importantes para %s: '%enzima)
sel_mi_graph[enzima][:100].plot.bar(figsize=(25,5),color=cores[52:53])
print('-----')
```

Variáveis mais importantes para betaglicosidase:



```
In [34]: print('\n Variáveis MENOS importantes para %s: '%enzima)
temp=sel_mi_graph[enzima][sel_mi_graph[enzima]<.3]
#Lista das variáveis menos importantes
temp.sort_values()[:50].index
```

Variáveis MENOS importantes para betaglicosidase:

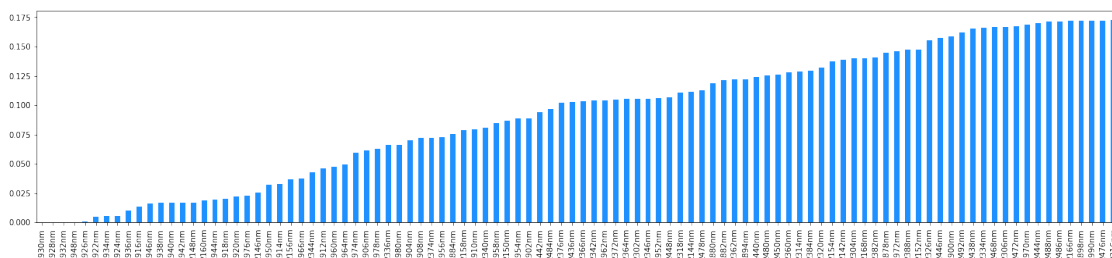
```
Out[34]: Index(['1930nm', '1928nm', '1932nm', '1948nm', '1926nm', '1922nm', '1934nm',
               '1924nm', '1936nm', '1916nm', '1946nm', '1938nm', '1940nm', '1942nm',
               '2148nm', '2160nm', '1944nm', '1918nm', '1920nm', '1976nm', '2146nm',
               '1950nm', '1914nm', '2156nm', '1966nm', '2344nm', '1912nm', '1960nm',
               '1964nm', '1974nm', '1906nm', '1978nm', '2336nm', '1980nm', '1904nm',
               '1908nm', '2374nm', '1956nm', '1884nm', '2158nm', '1910nm', '2340nm',
               '1958nm', '2150nm', '1954nm', '1902nm', '1442nm', '2484nm', '2376nm',
               '2436nm'],
              dtype='object')
```

```
In [ ]:
```

```
In [35]: print('\n Variáveis MENOS importantes para %s: '%enzima)
temp=sel_mi_graph[enzima][sel_mi_graph[enzima]<.3]
#Lista das variáveis menos importantes
temp.sort_values()[:100].plot.bar(figsize=(25,5),color=cores[52:53])
```

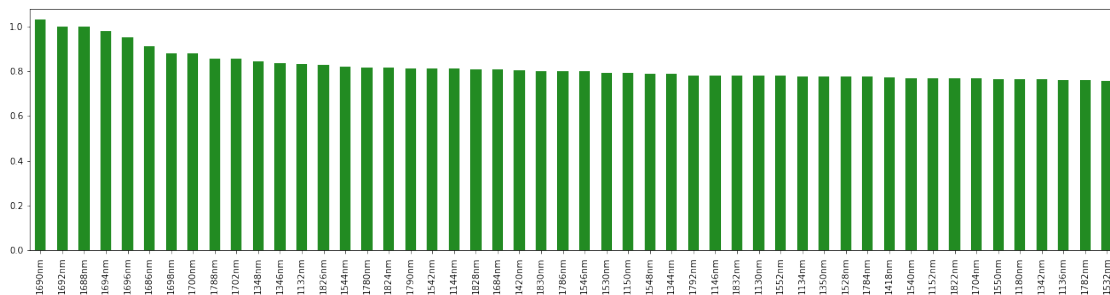
Variáveis MENOS importantes para betaglicosidase:

```
Out[35]: <matplotlib.axes._subplots.AxesSubplot at 0x7fc227b2b128>
```



```
In [36]: enzima = 'cmcase'
print('\n Variáveis mais importantes para %s:'%enzima)
sel_mi_graph[enzima][:50].plot.bar(figsize=(22,5),color=cores[55:56])
print('-----')
```

Variáveis mais importantes para cmcase:



```
In [37]: print('\n Variáveis MENOS importantes para %s:'%enzima)
temp=sel_mi_graph[enzima][sel_mi_graph[enzima]<.3]
#Lista das variáveis menos importantes
temp.sort_values()[:50].index
```

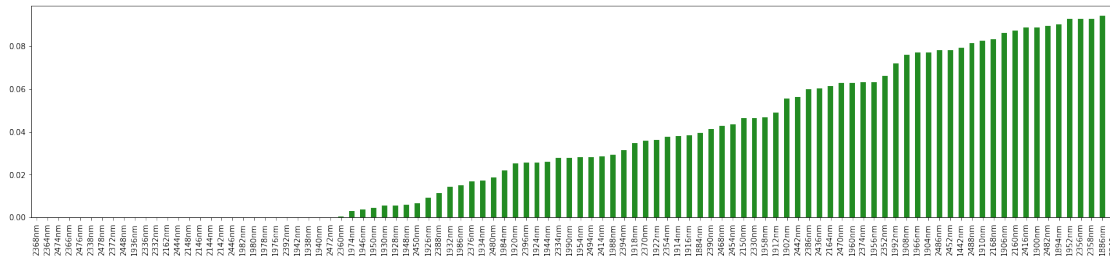
Variáveis MENOS importantes para cmcase:

```
Out[37]: Index(['2368nm', '2364nm', '2474nm', '2366nm', '2476nm', '2338nm', '2478nm',
                '2372nm', '2448nm', '1936nm', '2336nm', '2332nm', '2162nm', '2444nm',
                '2148nm', '2146nm', '2144nm', '2142nm', '2446nm', '1982nm', '1980nm',
                '1978nm', '1976nm', '2392nm', '1942nm', '1938nm', '1940nm', '2472nm',
                '2360nm', '1974nm', '1946nm', '1950nm', '1930nm', '1928nm', '1948nm',
                '2450nm', '1926nm', '2388nm', '1932nm', '1986nm', '2376nm', '1934nm',
                '2480nm', '1984nm', '1920nm', '2396nm', '1924nm', '1944nm', '2334nm',
                '1990nm'],
                dtype='object')
```

```
In [38]: print('\n Variáveis MENOS importantes para %s:'%enzima)
temp=sel_mi_graph[enzima][sel_mi_graph[enzima]<.3]
#Lista das variáveis menos importantes
temp.sort_values()[:100].plot.bar(figsize=(25,5),color=cores[55:56])
```

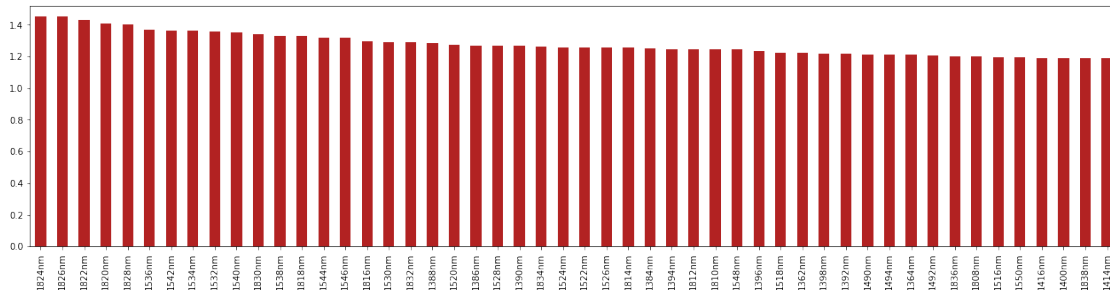
Variáveis MENOS importantes para cmcase:

```
Out[38]: <matplotlib.axes._subplots.AxesSubplot at 0x7fc22650ff28>
```



```
In [39]: enzima = 'fpase'
print('\n Variáveis mais importantes para %s: '%enzima)
sel_mi_graph[enzima][:50].plot.bar(figsize=(22,5),color=cores[53:54])
print('-----')
```

Variáveis mais importantes para fpase:



```
In [40]: print('\n Variáveis MENOS importantes para %s: '%enzima)
temp=sel_mi_graph[enzima][sel_mi_graph[enzima]<.3]
#Lista das variáveis menos importantes
temp.sort_values()[:50].index
```

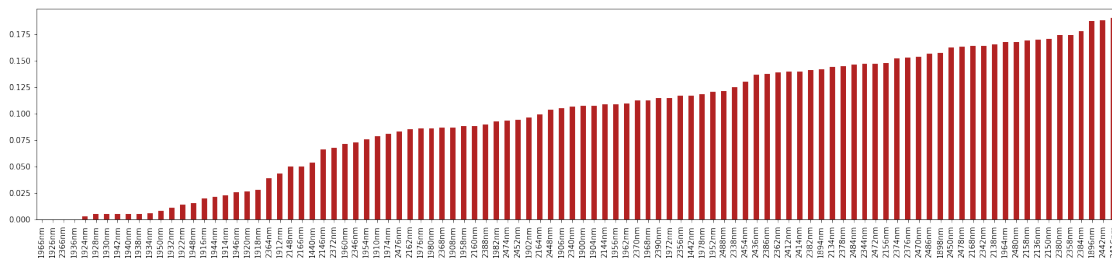
Variáveis MENOS importantes para fpase:

```
Out[40]: Index(['1966nm', '1926nm', '2366nm', '1936nm', '1924nm', '1928nm', '1930nm',
               '1942nm', '1940nm', '1938nm', '1934nm', '1950nm', '1932nm', '1922nm',
               '1948nm', '1916nm', '1944nm', '1914nm', '1946nm', '1920nm', '1918nm',
               '2364nm', '1912nm', '2148nm', '2166nm', '1440nm', '2146nm', '2372nm',
               '1960nm', '2346nm', '1954nm', '1910nm', '1974nm', '2476nm', '2162nm',
               '1976nm', '1980nm', '2368nm', '1908nm', '1958nm', '2160nm', '2388nm',
               '1982nm', '2474nm', '2452nm', '1902nm', '2164nm', '2448nm', '1906nm',
               '2340nm'],
              dtype='object')
```

```
In [41]: print('\n Variáveis MENOS importantes para %s: '%enzima)
temp=sel_mi_graph[enzima][sel_mi_graph[enzima]<.3]
#Lista das variáveis menos importantes
temp.sort_values()[:100].plot.bar(figsize=(25,5),color=cores[53:54])
```

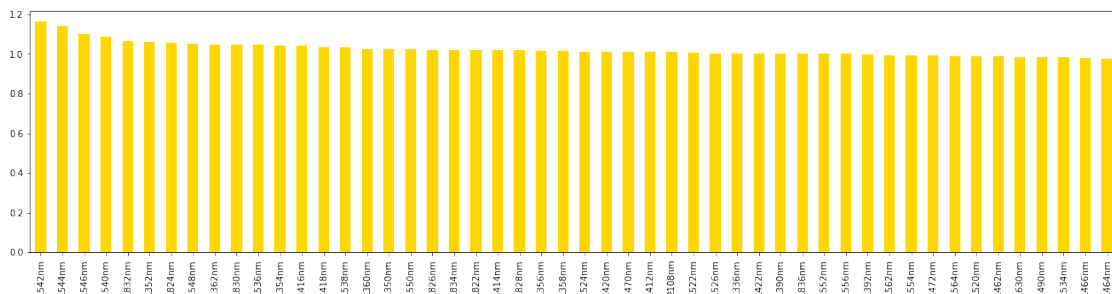
Variáveis MENOS importantes para fpase:

```
Out[41]: <matplotlib.axes._subplots.AxesSubplot at 0x7fc226f9e2b0>
```



```
In [42]: enzima = 'xilanase'
print('\n Variáveis mais importantes para %s: '%enzima)
sel_mi_graph[enzima][:50].plot.bar(figsize=(22,5),color=cores[59:60])
print('-----')
```

Variáveis mais importantes para xilanase:




```
In [43]: print('\n Variáveis MENOS importantes para %s: '%enzima)
temp=sel_mi_graph[enzima][sel_mi_graph[enzima]<.3]
#Lista das variáveis menos importantes
temp.sort_values()[:50].index
```

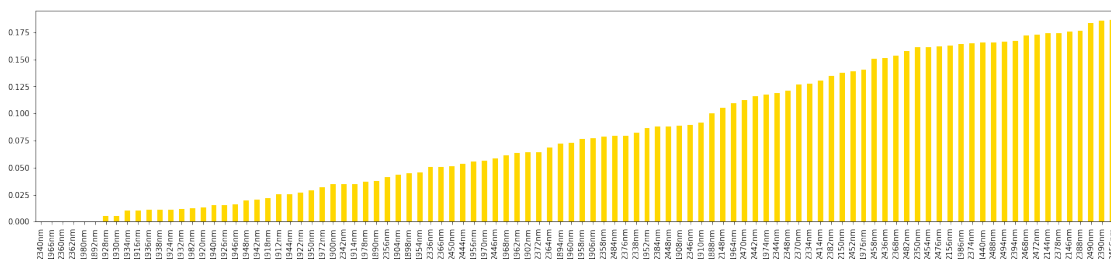
Variáveis MENOS importantes para xilanase:

```
Out[43]: Index(['2340nm', '1966nm', '2360nm', '2362nm', '1980nm', '1892nm', '1928nm',
               '1930nm', '1934nm', '1916nm', '1936nm', '1938nm', '1924nm', '1932nm',
               '1982nm', '1920nm', '1940nm', '1926nm', '1946nm', '1948nm', '1942nm',
               '1918nm', '1912nm', '1944nm', '1922nm', '1950nm', '1972nm', '1900nm',
               '2342nm', '1914nm', '1978nm', '1890nm', '2356nm', '1904nm', '1898nm',
               '1954nm', '2336nm', '2366nm', '2450nm', '2444nm', '1956nm', '1970nm',
               '2446nm', '1968nm', '1962nm', '1902nm', '2372nm', '2364nm', '1894nm',
               '1960nm'],
              dtype='object')
```

```
In [44]: print('\n Variáveis MENOS importantes para %s: '%enzima)
temp=sel_mi_graph[enzima][sel_mi_graph[enzima]<.3]
#Lista das variáveis menos importantes
temp.sort_values()[:100].plot.bar(figsize=(25,5),color=cores[59:60])
```

Variáveis MENOS importantes para xilanase:

```
Out[44]: <matplotlib.axes._subplots.AxesSubplot at 0x7fc227cd99b0>
```



```
In [46]: #verificando o total de variáveis com correlação maior que 0.8 para cada atividade en
var_ae=['betaglicosidase','cmcase','fpase','xilanase']
total={'betaglicosidase':0,'cmcase':0,'fpase':0,'xilanase':0}
for valor in var_ae:
    total[valor]=len(sel_mi_graph[valor][sel_mi_graph[valor]>.7])
```

```

print('Total de variáveis com correlação superior a .8 para cada enzima\n')
for valor in var_ae:
    print(valor,':',total[valor])

```

Total de variáveis com correlação superior a .8 para cada enzima

```

betaglicosidase : 308
cmcase : 105
fpase : 306
xilanase : 277

```

```

In [47]: #verificando o total de variáveis que mais se correlacionam com cada atividade enzim
var_ae=['betaglicosidase','cmcase','fpase','xilanase']
total={'betaglicosidase':0,'cmcase':0,'fpase':0,'xilanase':0}
corr = [0.95,0.7,.95,0.85]
for valor,i in zip(var_ae,[0,1,2,3]):
    total[valor]=len(sel_mi_graph[valor][sel_mi_graph[valor]>corr[i]])
print('Total de variáveis com correlação alta para cada enzima\n')
for valor in var_ae:
    print(valor,':',total[valor])

```

Total de variáveis com correlação alta para cada enzima

```

betaglicosidase : 115
cmcase : 105
fpase : 163
xilanase : 169

```

```

In [ ]: '''
#Exibindo as variáveis mais significativas
var_ae=['betaglicosidase','cmcase','fpase','xilanase']
corr = [1,0.7,1,0.85]
for valor,i in zip(var_ae,[0,1,2,3]):
    print('\nAtributos + significativos para:',valor)
    print(sel_mi_graph[valor][sel_mi_graph[valor]>corr[i]].index[:30])
'''

```

```

In [48]: #Considerando o total de cada atividade, as variáveis mais significativas de cada ati
sel_ = {}
for valor in var_ae:
    sel_[valor] = list(sel_mi_graph[valor].index)
sel_2 = []
for valor in var_ae:
    sel_2 += sel_[valor][:total[valor]]
#elimina repetições:
sel_2 = list(set(sel_2))

print('Total de variáveis significativas sem repetição:',len(sel_2))

```

Total de variáveis significativas sem repetição: 244

```
In [49]: #ordena as variáveis por nome
sel_2.sort()
print('Variáveis mais sigificativas:',sel_2)
```

Variáveis mais sigificativas: ['1128nm', '1130nm', '1132nm', '1134nm', '1136nm', '1138nm', '1140nm']

```
In [ ]:
```

```
In [50]: #renomear as absorbâncias
var_abs_txt = sel_2.copy()
```

3 Outliers

- Após verificar as variáveis mais importantes, vamos utilizá-las para conferir possíveis outliers

```
In [1650]: #2
           #Outliers: realizar teste com o arquivo D_outliers, nesse mesmo diretório
```

```
In [ ]: #amostras 28,30 e 62 que representam os pontos
amostra: descrição exper  temperatura tempoRetirada
28 : bio_p3_t1_2    biof    30    72
30 : bio_p3_t2_1    biof    30    72
62 : bio_p6_t3_3    biof    30   144
```

```
In [1671]: #Resetando o índice dos dados:
dados=dados.reset_index(drop=True)
dados.index
```

```
Out[1671]: RangeIndex(start=0, stop=81, step=1)
```

```
In [2399]: dados_com_outliers = dados_back.copy()
```

```
In [1545]: dados = dados_com_outliers.copy()
```

```
In [1546]: dados = dados[(dados['eenz'] == 'eeta') & (dados['experimento']=='biof')]
```

```
In [1662]: outliers = [28,30,62]
           #removendo as amostras consideradas outliers (testar os algoritmos sem remover outliers)
dados = dados.drop(outliers)
```

```
In [1663]: dados.shape
```

```
Out[1663]: (78, 713)
```

4 Definição das variáveis

variáveis para os processamentos: (antes ou após remoção de outliers, com ou sem seleção de atributos:

```
In [245]: #@var_abs_txt
          #@var_abs_int
          # Opções de definição da variável das absorbâncias

In [246]: #opção 1: Escolha de todos os valores de absorbância (sem nenhuma seleção de atributos)
          var_ae=['betaglicosidase','cmcase','fpase','xilanase']
          #criando vetores com os nomes dos atributos

          #criando um vetor com os nomes das absorbâncias para seleção posterior
          var_abs_int = np.arange(1100,2496,2)
          var_abs_txt=[]
          for valor in var_abs_int:
              var_abs_txt += [str(valor)+'nm']

In [367]: #opção 2: Escolha de algumas absorbâncias e exclusão de outras - duas faixas excluídas
          #variáveis após excluir algumas bandas do espectro
          var_ae=['betaglicosidase','cmcase','fpase','xilanase']
          #criando vetores com os nomes dos atributos

          abs1 = np.arange(1100,1875,2)
          abs2 = np.arange(1974,2351,2)
          var_abs_int = np.concatenate((abs1,abs2),axis=0)
          var_abs_txt=[]
          for valor in var_abs_int:
              var_abs_txt += [str(valor)+'nm']

In [369]: #opção 3: Exclusão da faixa final de ruído, a partir da abs 2350
          #variáveis após excluir algumas bandas do espectro
          var_ae=['betaglicosidase','cmcase','fpase','xilanase']
          #criando vetores com os nomes dos atributos

          var_abs_int = np.arange(1100,2351,2)
          var_abs_txt=[]
          for valor in var_abs_int:
              var_abs_txt += [str(valor)+'nm']

In [371]: #opção 4: Definição das absorbâncias através da seleção de atributos feita previamente
          var_abs_txt = sel_2.copy()
          var_ae=['betaglicosidase','cmcase','fpase','xilanase']
          var_abs_int=[]
          for valor in var_abs_txt:
              var_abs_int += [int(valor[:4])]

In [52]: #Variável para trabalhar no pré-processamento dos espectros
          preProc = {0:'Pré-proc: 0--> Sem pré-processamento',
```

```

1: 'Pré-proc: 1--> Padronização',
2: 'Pré-proc: 2--> Suavização(SavGol) - Par:3,1,1',
3: 'Pré-proc: 3--> Suavização(SavGol) - Par:3,2,1',
4: 'Pré-proc: 4--> Suavização(SavGol) - Par:5,1,1',
5: 'Pré-proc: 5--> Suavização(SavGol) - Par:5,2,1',
6: 'Pré-proc: 6--> Suavização(SavGol) - Par:3,2,2',
7: 'Pré-proc: 7--> Suavização(SavGol) - Par:5,2,2',
8: 'Pré-proc: 8--> Suavização(SavGol) - Par:3,1,1 --> Padronização',
9: 'Pré-proc: 9--> Padronização --> Suavização(SavGol) - Par:3,1,1',
10: 'Pré-proc: 10--> MSC',
11: 'Pré-proc: 11--> SNV'}

```

4.1 Definindo x e y

```

In [53]: #@dfxy
         #Definindo os dataFrames iniciais a partir da base de dados escolhida e pré-processada
         df_x = dados.loc[:,var_abs_txt] #absorbâncias
         df_y = dados.loc[:,var_ae] #AE

```

```

In [54]: df_x.shape

```

```

Out[54]: (81, 244)

```

```

In [118]: #se precisar eliminar colunas com dados nulos
         #dadosb=dados.dropna(axis=1)

```

5 Análise inicial da base de dados e de seu conteúdo através de PCA

```

In [55]: #@pca
         #utilizar o PCA para reduzir as dimensões e poder analisar os dados
         #Para utilizar o PCA é necessário realizar a normalização dos dados (tornar a variância 1)
         #pré-processamento
         scaler = StandardScaler()
         scaler.fit(df_x)
         df_x_scaler = scaler.transform(df_x)
         pca = PCA(n_components=7)
         #treinar o pca com os dados padronizados
         pca.fit(df_x_scaler)
         #Após treinar o pca, agora posso transformar os dados
         x_pca = pca.transform(df_x_scaler)
         print('Dados originais:',df_x.shape,'Pós PCA:', x_pca.shape)

```

```

Dados originais: (81, 244) Pós PCA: (81, 7)

```

```

In [56]: #Exibindo a variância explicada pelas componentes principais
         variancia_explicada = pca.explained_variance_ratio_[0:10]
         # Explicação da variância pelas componentes principais

```

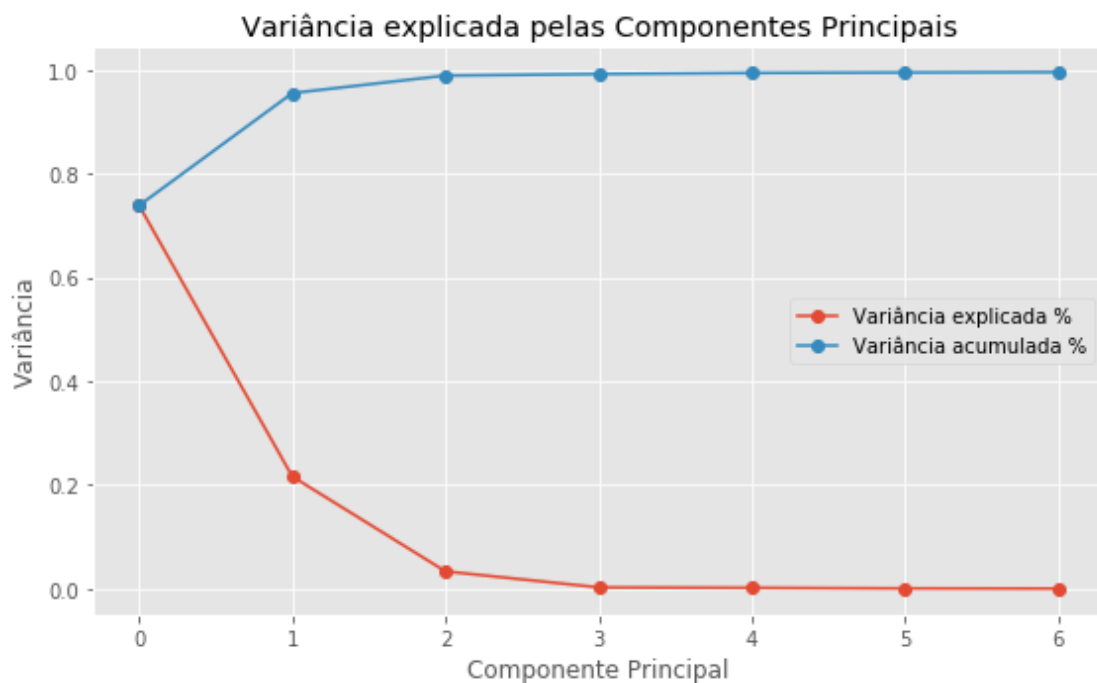
```

with plt.style.context(('ggplot')):
    fig, (ax1) = plt.subplots(nrows=1, ncols=1, figsize=(8,5))
    fig.set_tight_layout(True)

    ax1.plot(variancia_explicada, '-o', label="Variância explicada %")
    ax1.plot(np.cumsum(variancia_explicada), '-o', label = 'Variância acumulada %')
    ax1.set_xlabel("Componente Principal")
    ax1.set_ylabel("Variância")

    ax1.set_title('Variância explicada pelas Componentes Principais')
    plt.legend()
    plt.show()

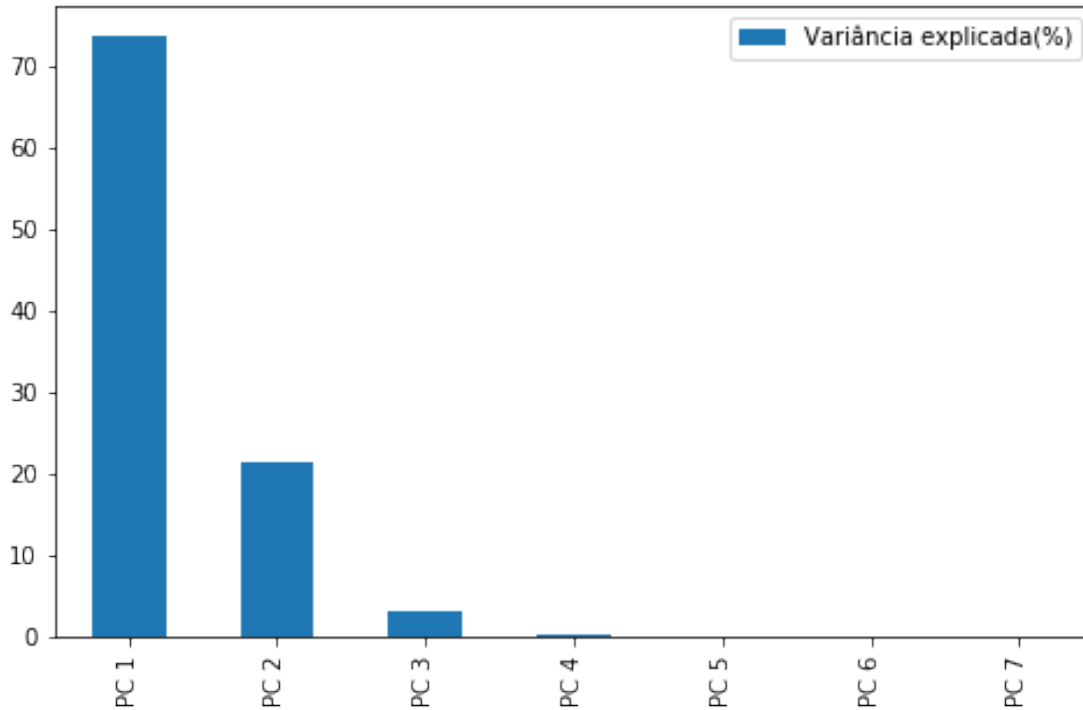
```



```

In [57]: perc = pca.explained_variance_ratio_ * 100
perc = pd.DataFrame(perc, columns=['Variância explicada(%)'], index=['PC %s' % pc for
ax = perc.plot(kind='bar', figsize=(8,5))

```



```
In [58]: texto = ''
perc['Variância acumulada(%)'] = np.cumsum(pca.explained_variance_ratio_[:7])
perc
```

```
Out[58]:
```

	Variância explicada(%)	Variância acumulada(%)
PC 1	73.850533	0.738505
PC 2	21.646207	0.954967
PC 3	3.377077	0.988738
PC 4	0.294734	0.991686
PC 5	0.210249	0.993788
PC 6	0.091238	0.994700
PC 7	0.060917	0.995310

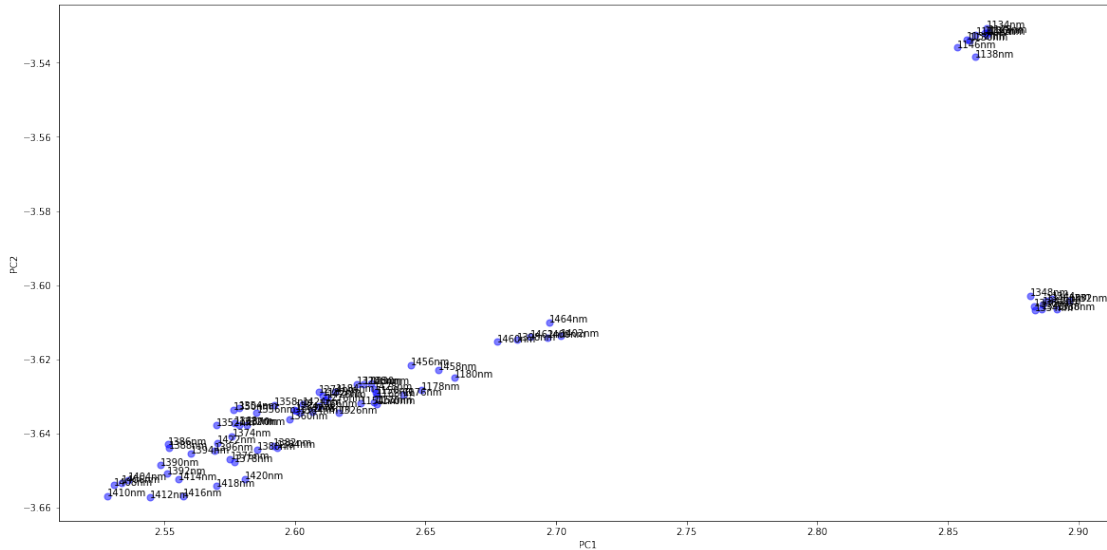
```
In [59]: loadings = pd.DataFrame(pca.components_.T)
loadings.index = ['A %s' % pc for pc in loadings.index + 1]
loadings.columns = ['PC %s' % pc for pc in loadings.columns + 1]
PCs = np.dot(loadings.values.T, df_x.T)
marker = dict(linestyle='none', marker='o', markersize=7, color='blue', alpha=0.5)
```

```
In [60]: fig, ax = plt.subplots(figsize=(20, 10))
ax.plot(PCs[0], PCs[1], label="Scores", **marker)

ax.set_xlabel("PC1")
```

```
ax.set_ylabel("PC2")
```

```
text = [ax.text(x, y, t) for x, y, t in
        zip(PCs[0], PCs[1], df_x.columns)]
```



```
In [73]: PCs.shape, df_x.shape, loadings.shape
```

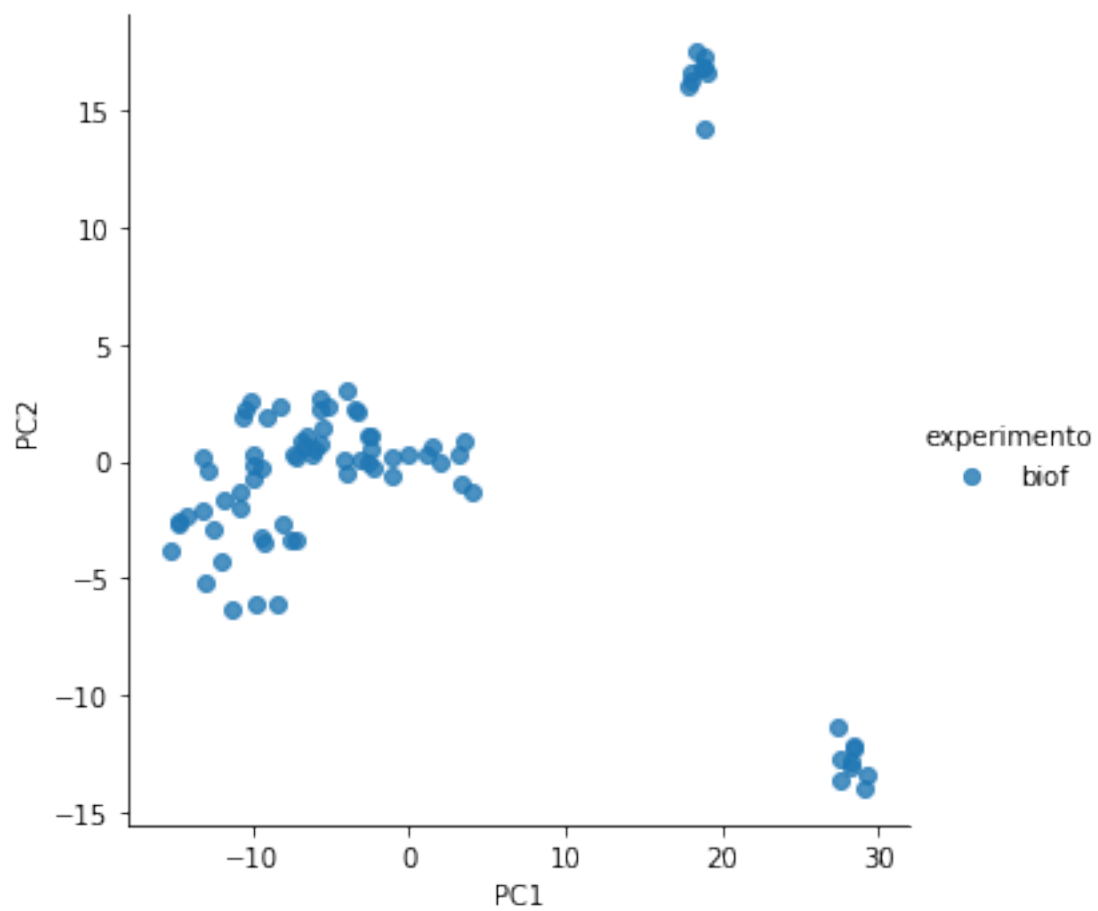
```
Out[73]: ((7, 81), (81, 261), (261, 7))
```

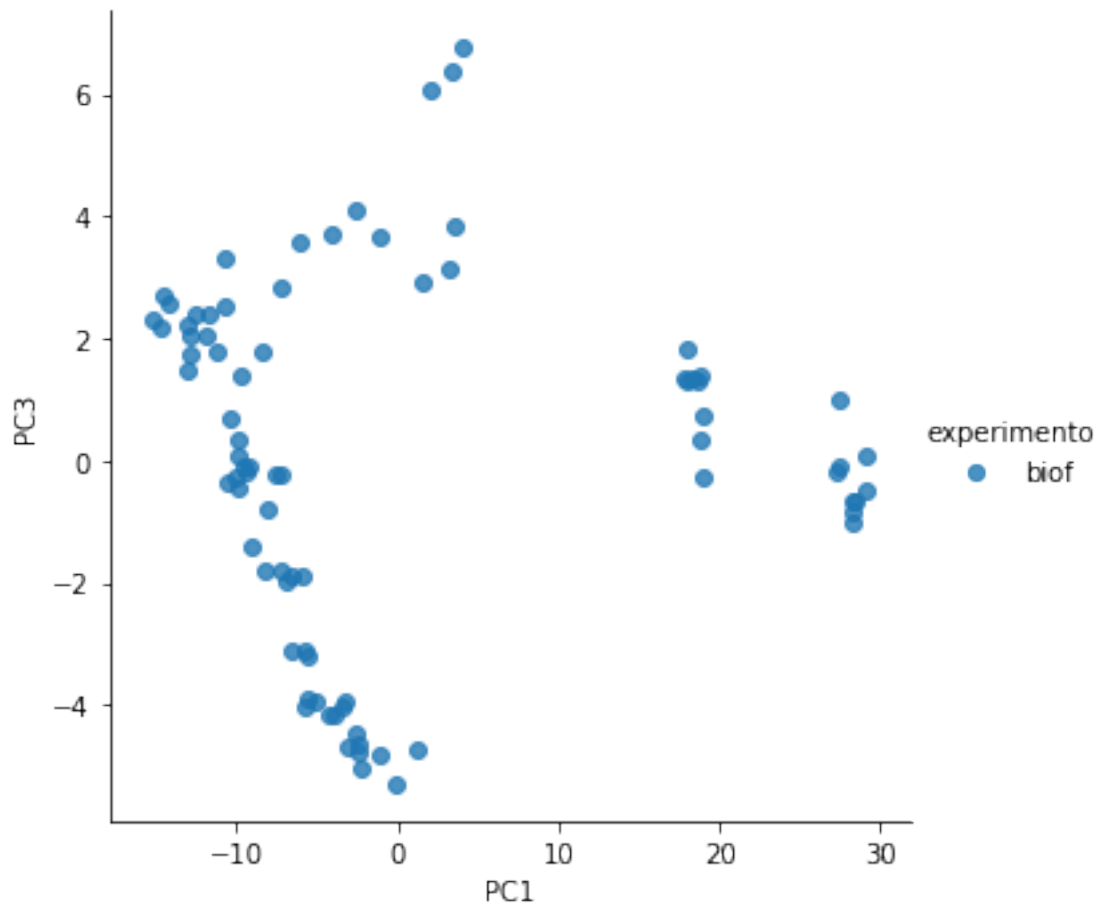
```
In [61]: #dataframes separados por intervalo de tempo, temperatura, experimento e ae  
#servirão para fazer análises gráficas com PCA
```

```
temp_yinter = dados.loc[:, 'inter']  
temp_ye = dados.loc[:, 'eenz']  
temp_yt = dados.loc[:, 'temp']  
temp_yex = dados.loc[:, 'experimento']  
temp_ybeta = dados.loc[:, 'betaglicosidase']  
temp_ycmc = dados.loc[:, 'cmcase']  
temp_yfpase = dados.loc[:, 'fpase']  
temp_yxil = dados.loc[:, 'xilanase']
```

```
In [62]: #configurando paleta de cores
```

```
palettes = ["deep", "muted", "pastel", "bright", "dark", "colorblind"]  
#Desenhando o gráfico dos scores da PC1 com PC2 diferenciando por experimento  
dados_plot = pd.DataFrame(zip(x_pca[:, 0], x_pca[:, 1], temp_yex), columns=["PC1", "PC2",  
sns.lmplot("PC1", "PC2", dados_plot, hue="experimento", fit_reg=False)  
plt.rcParams['figure.figsize']=(20,10)  
  
dados_plot = pd.DataFrame(zip(x_pca[:, 0], x_pca[:, 2], temp_yex), columns=["PC1", "PC3",  
sns.lmplot("PC1", "PC3", dados_plot, hue="experimento", fit_reg=False)  
plt.rcParams['figure.figsize']=(20,10)
```

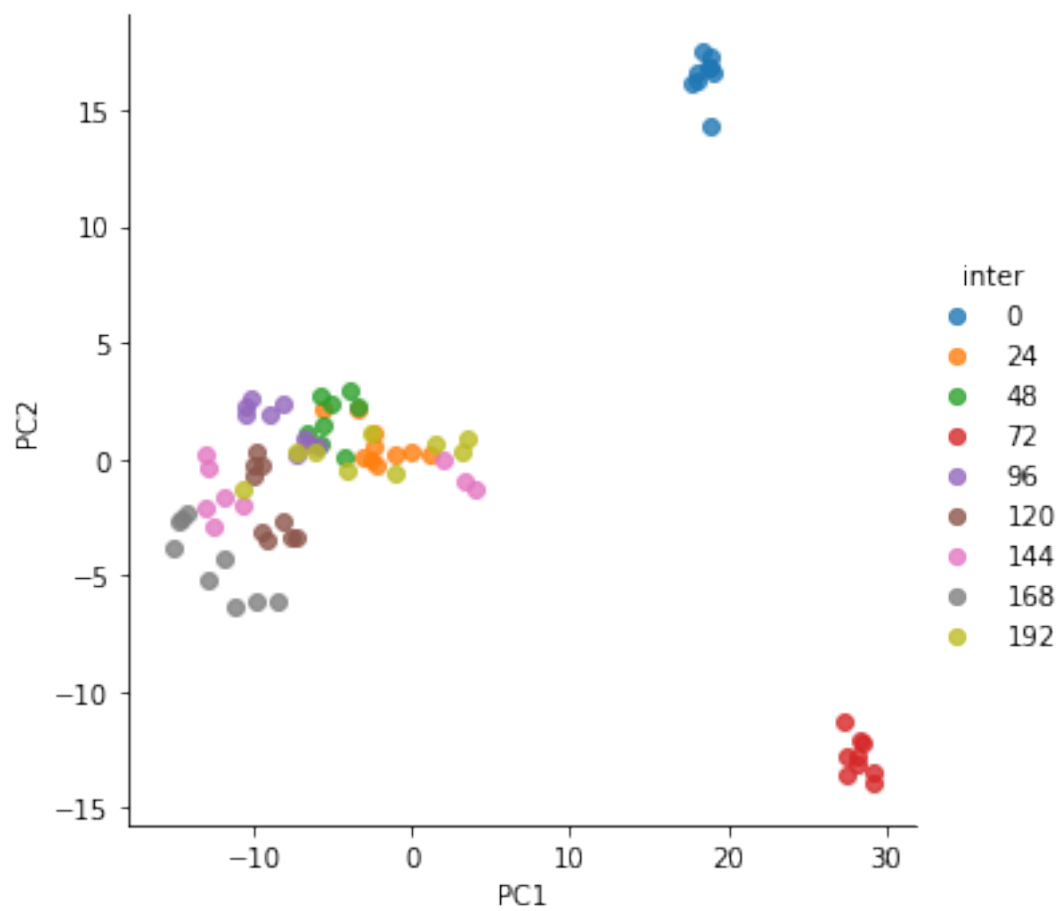



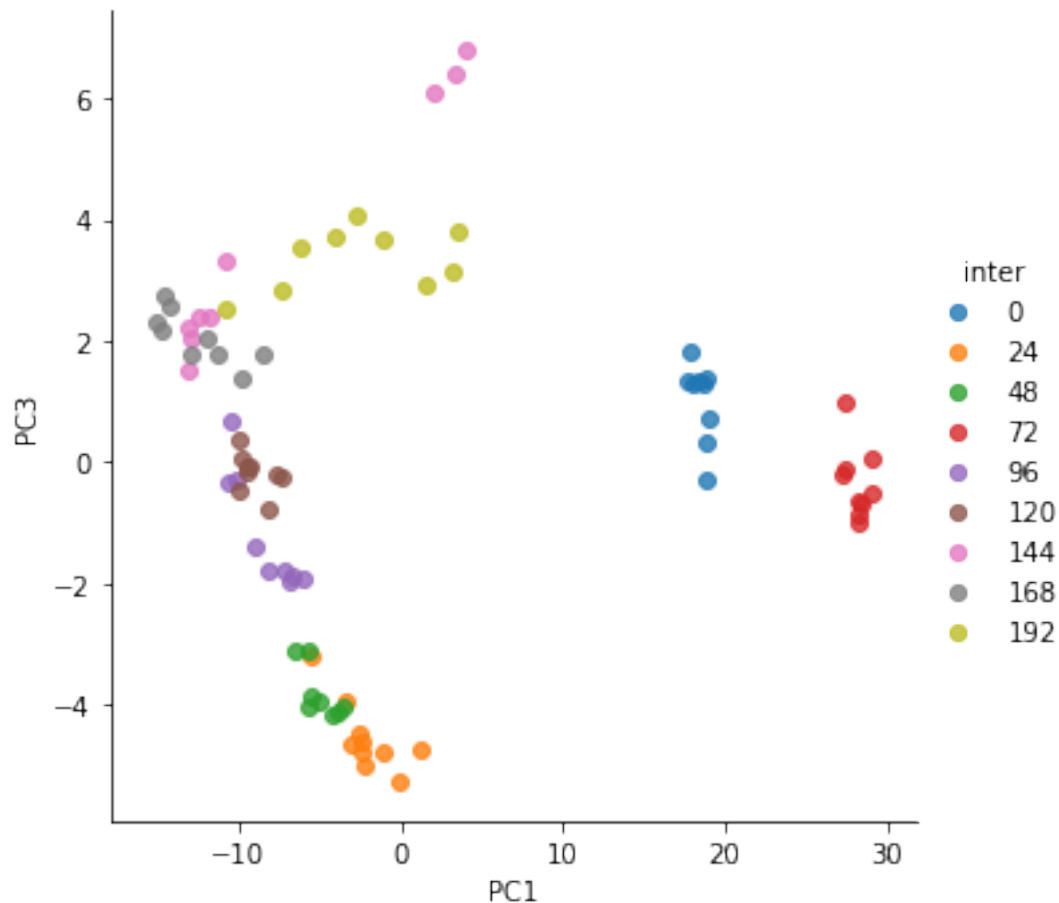


```
In [132]: #Como selecionar amostras partindo dos gráficos gerados.
          #assim dá pra separar as amostras em função da apresentação dada
          #exemplo: biof = dados_plot[(dados_plot['PC2'] > -10) ]
```

```
In [63]: #Desenhando o gráfico dos scores da PC1 com PC2 diferenciando por tempo de fermentação
dados_plot = pd.DataFrame(zip(x_pca[:,0],x_pca[:,1],temp_yinter), columns=["PC1", "PC2"])
sns.lmplot("PC1", "PC2", dados_plot, hue="inter", fit_reg=False)
plt.rcParams['figure.figsize']=(15,10)

dados_plot = pd.DataFrame(zip(x_pca[:,0],x_pca[:,2],temp_yinter), columns=["PC1", "PC3"])
sns.lmplot("PC1", "PC3", dados_plot, hue="inter", fit_reg=False)
plt.rcParams['figure.figsize']=(15,10)
```





In []: *#Após separação de dados dará para selecionar algum conjunto de dados com características*

In [283]: *#verifica quais dados estão separados no biof*
#biof = dados_plot[(dados_plot['PC2'] > -10) & (dados_plot['PC1'] < 0)]

In [284]: *#biof = dados.iloc[list(biof.index)]*

In [1095]: *#Separa os dados do experimento da fermentação e da desnaturação*

```
#biod = dados[ dados['experimento'] == 'biod1']
#biof = dados[ dados['experimento'] == 'biof']
#bioe = dados[ dados['experimento'] == 'bioE']
```

In [1097]: *#biod.shape, biof.shape, bioe.shape*

Out[1097]: ((33, 713), (81, 713), (24, 713))

In [146]: *#Definindo os dataFrames iniciais a partir da base de dados escolhida e pré-processada*
df_x = dados.loc[:,var_abs_txt] #absorbâncias
df_y = dados.loc[:,var_ae]#AE

6 Função de pré-processamento

In [64]: `@preproc`

```
def executaPreproc(preproc, padroniza = False, IC=0):
    #separando o conjunto de dados em treino e teste
    x_treino, x_teste, y_treino, y_teste = train_test_split(df_x, df_y, test_size=0.25,

    #parâmetros para savgol: janela, grau do polinômio, derivada
    par = [3, 1, 1]
    #sem pré-processamento preproc=0
    if preproc == 1:          #preproc=1: padronização (z=(xi-m)/s) SNV
        if padroniza: #padroniza y
            y_treino = StandardScaler().fit_transform(y_treino.values) #treino
            y_teste = StandardScaler().fit_transform(y_teste.values) #teste

            x_treino = StandardScaler().fit_transform(x_treino.values) #treino
            x_teste = StandardScaler().fit_transform(x_teste.values) #teste
    elif preproc in range(2, 8):
        if preproc == 2: #SG:3,1,1
            par=[3, 1, 1]
        elif preproc == 3:
            par=[3, 2, 1]
        elif preproc == 4:
            par=[5, 1, 1]
        elif preproc == 5:
            par=[5, 2, 1]
        elif preproc == 6:
            par=[3, 2, 2]
        elif preproc == 7:
            par=[5, 2, 2]
        x_treino = savgol_filter(x_treino, par[0], polyorder = par[1], deriv=par[2])
        x_teste = savgol_filter(x_teste, par[0], polyorder = par[1], deriv=par[2]) #t
    elif preproc == 8:
        x_treino = savgol_filter(x_treino, par[0], polyorder = par[1], deriv=par[2])
        x_teste = savgol_filter(x_teste, par[0], polyorder = par[1], deriv=par[2]) #t
        x_treino = StandardScaler().fit_transform(x_treino[:, :]) #treino
        x_teste = StandardScaler().fit_transform(x_teste[:, :]) #teste
    elif preproc == 9:
        x_treino = StandardScaler().fit_transform(x_treino.values) #treino
        x_teste = StandardScaler().fit_transform(x_teste.values) #teste
        x_treino = savgol_filter(x_treino, par[0], polyorder = par[1], deriv=par[2])
        x_teste = savgol_filter(x_teste, par[0], polyorder = par[1], deriv=par[2]) #t
    elif preproc == 10:
        x_treino = msc(x_treino.values)[0]
        x_teste = msc(x_teste.values)[0]
    elif preproc == 11:
        x_treino = snv(x_treino.values)
        x_teste = snv(x_teste.values)
```

```

        return (x_treino, x_teste, y_treino, y_teste)

In [65]: def executaPreprocSimples(preproc,x):
        #parâmetros para savgol: janela, grau do polinômio, derivada
        par = [3,1,1]
        if preproc == 1:
            x = StandardScaler().fit_transform(x.values)
        elif preproc in range(2,8):
            if preproc == 2:
                par=[3,1,1]
            elif preproc == 3:
                par=[3,2,1]
            elif preproc == 4:
                par=[5,1,1]
            elif preproc == 5:
                par=[5,2,1]
            elif preproc == 6:
                par=[3,2,2]
            elif preproc == 7:
                par=[5,2,2]
            x= savgol_filter(x_treino, par[0], polyorder = par[1], deriv=par[2])
        elif preproc == 8:
            x = savgol_filter(x, par[0], polyorder = par[1], deriv=par[2])
            x = StandardScaler().fit_transform(x[:,:])
        elif preproc == 9:
            x = StandardScaler().fit_transform(x[:,:])
            x = savgol_filter(x, par[0], polyorder = par[1], deriv=par[2])
        elif preproc == 10:
            x_treino = msc(x_treino.values)[0]
            x_teste = msc(x_teste.values)[0]
        elif preproc == 11:
            x_treino = snv(x_treino.values)
            x_teste = snv(x_teste.values)

        return x

```

7 Modelagem:

7.1 Função geral de modelagem

```

In [66]: #@modelagemCVP executa calibração, validação e predição
def executaCVP(treino_teste, reg):
    x_treino = treino_teste[0].copy()
    x_teste = treino_teste[1].copy()
    y_treino = treino_teste[2].copy()
    y_teste = treino_teste[3].copy()

    # Fit

```

```

reg.fit(x_treino, y_treino)

# Calibração
y_c = reg.predict(x_treino)

# Cross-validation
y_cv = cross_val_predict(reg, x_treino, y_treino, cv=10)

# Predição nos dados de teste
y_p = reg.predict(x_teste)

y = y_treino.copy()

return [reg, treino_teste,y_c,y_cv,y_p]

```

```

In [67]: #@modelagemMetrics
#Retorna tabela de resultados:
def calMetrics(reais, preditos):
    result = {}
    result['BIAS'] = round(bias(reais, preditos),4)
    result['MSE'] = round(getmse(reais, preditos),4)
    result['R2'] = round(getr2(reais, preditos),4)
    result['RER'] = round(rer(reais, preditos),4)
    result['RMSE'] = round(getrmse(reais, preditos),4)
    #result['RMSE'] = rmse(reais, preditos)
    result['RPD'] = round(rpd(reais, preditos),4)
    result['RPIQ'] = round(rpiq(reais, preditos),4)
    result['SEP'] = round(sep(reais, preditos),4)
    return result

```

In []:

```

In [68]: #@modelagemcalvalpred
#exibe resultados para calibração, validação cruzada e predição
def retornaCVP(y,yp):
    #yp contem os valores estimados da calibração, validação e teste
    var = ['cal', 'val', 'pred']
    var_ae=['betaglicosidase', 'cmcase', 'fpase', 'xilanase']
    res_cvp = {}
    for i in range(3):
        if i < 2:
            j=0
        else:
            j=1
        for e,ie in zip(var_ae,[0,1,2,3]):
            reais = y[j].loc[:,e]
            pred = yp[i][:,ie]
            r = pd.Series(calMetrics(reais, pred))

```

```

        if ie == 0:
            res = pd.DataFrame(r, index=r.index, columns=[e])
        else:
            res[e] = r
            res_cvp[var[i]] = res
    return res_cvp

In [69]: #@modelagemResultados
def exhibeResultados(result):
    #recuperando resultados da modelagem
    reg, treino_teste, y_c, y_cv, y_p = result

    #x_treino, x_teste, y_treino, y_teste = treino_teste
    y_ = [treino_teste[2].reset_index(drop=True), treino_teste[3].reset_index(drop=True)]
    yp=[y_c, y_cv, y_p]
    resultados = retornaCVP(y_, yp)
    return resultados

```

7.2 PCA->KNN

```

In [70]: #pcaknn
#função completa para execução do PCA-->KNN:
#A variável preproc determinará o tipo de processamento que será executado (0,1,2,3,4)
def executaPCA_KNN(preproc, nPC, vizinhos, padroniza=False, ic=0):
    #separando o conjunto de dados em treino e teste

    #separando o conjunto de dados em treino e teste
    #x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc, True)
    x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc, padroniza, ic)

    # Roda o PCA e produz uma variável reduzida xRed e seleciona as primeiras componentes
    pca = PCA(n_components=nPC)
    x_treino = pca.fit_transform(x_treino)[:nPC]
    x_teste = pca.fit_transform(x_teste)[:nPC]

    #Passo 2: Aplicar o KNN sobre as componentes selecionadas
    reg = MultiOutputRegressor(KNeighborsRegressor(n_neighbors=vizinhos))
    result = executaCVP([x_treino, x_teste, y_treino, y_teste], reg)

    return result

```

In []:

7.2.1 PCA->KNN: testes

```

In [71]: #pcaknn teste simples
#teste simples:
modelo = 'PCA-KNN:'

```



```

preproc=1
nPC=3
k=1
result = executaPCA_KNN(preproc,nPC,k)
print('Parâmetros do modelo:',modelo,'\n',result[0])

resultados=exibeResultados(result)
'''
for k,v in zip(resultados.keys(),resultados.values()):
    print(k)
    print(v,'\n-----')'''

```

Parâmetros do modelo: PCA-KNN:

```

MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=1, p=2,
weights='uniform'),
n_jobs=None)

```

Out[71]: "\nfor k,v in zip(resultados.keys(),resultados.values()):\n print(k)\n print(v,

In [72]: resultados['cal']

Out[72]:

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

In [73]: resultados['val']

Out[73]:

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0096	0.0012	0.0007	0.2166
MSE	0.0142	0.0002	0.0001	9.6653
R2	0.9945	0.8802	0.9214	0.7825
RER	38.1274	12.0524	11.1603	6.4154
RMSE	0.1193	0.0132	0.0073	3.1089
RPD	13.4932	2.8893	3.5661	2.1442
RPIQ	27.0767	3.3201	6.7580	2.8813
SEP	0.1199	0.0133	0.0073	3.1275

In [74]: resultados['pred']

Out[74]:

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2072	0.0000	0.0011	0.3035

MSE	0.2883	0.0004	0.0000	2.1676
R2	0.8740	0.5105	0.9163	0.9350
RER	7.6223	5.2184	11.0451	13.5731
RMSE	0.5369	0.0187	0.0067	1.4723
RPD	2.8170	1.4293	3.4557	3.9233
RPIQ	5.8368	1.5272	6.1996	2.6361
SEP	0.5075	0.0192	0.0068	1.4762

```
In [86]: #pcaknn teste completo
#pre = preprocessamento, k=número de vizinhos
modelo = 'PCA-KNN:'
print(modelo,':\n')
for nPC in range(3,4):
    print('PC:',nPC)
    for pre in range(12):
        print('Pré-processamento:\n', preProc[pre])
        for k in range(1,4):
            result = executaPCA_KNN(pre,nPC,k)
            print('Vizinhos:', k, '\n')
            print('Parâmetros do modelo:',modelo,'\n',result[0])
            resultados=exibeResultados(result)
            for k,v in zip(resultados.keys(),resultados.values()):
                print(k)
                print(v, '\n-----')
```

PCA-KNN: :

PC: 3

Pré-processamento:

Pré-proc: 0--> Sem pré-processamento

Vizinhos: 1

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=1, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0683	-0.0052	-0.0020	-0.2889
MSE	0.4149	0.0011	0.0002	11.8507
R2	0.8399	0.2175	0.7214	0.7333
RER	7.0795	4.7504	5.9607	5.8001
RMSE	0.6442	0.0338	0.0137	3.4425
RPD	2.4994	1.1305	1.8945	1.9365
RPIQ	5.0155	1.2990	3.5903	2.6021
SEP	0.6459	0.0337	0.0137	3.4593

pred	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.1067	-0.0050	-0.0028	0.0779
MSE	2.3877	0.0017	0.0005	107.6861
R2	-0.0437	-1.3801	0.1496	-2.2276
RER	2.4491	2.3839	3.4480	1.8844
RMSE	1.5452	0.0413	0.0213	10.3772
RPD	0.9788	0.6482	1.0844	0.5566
RPIQ	2.0281	0.6926	1.9454	0.3740
SEP	1.5796	0.0420	0.0216	10.6332

Vizinhos: 2

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='min',
metric_params=None, n_jobs=None, n_neighbors=2, p=2,
weights='uniform'),
n_jobs=None)
```

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0286	-0.0019	-0.0004	-0.0501
MSE	0.0825	0.0002	0.0000	3.1895
R2	0.9682	0.8335	0.9417	0.9282
RER	15.8683	10.2538	12.9209	11.1450
RMSE	0.2872	0.0156	0.0063	1.7859
RPD	5.6059	2.4508	4.1421	3.7326
RPIQ	11.2494	2.8162	7.8496	5.0156
SEP	0.2882	0.0156	0.0063	1.8003

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0230	-0.0009	0.0003	0.0068
MSE	0.2662	0.0009	0.0001	7.9021
R2	0.8973	0.3833	0.7942	0.8222
RER	8.7971	5.2904	6.8656	7.0779
RMSE	0.5160	0.0300	0.0118	2.8111
RPD	3.1203	1.2734	2.2041	2.3714

RPIQ	6.2614	1.4632	4.1770	3.1865
SEP	0.5198	0.0303	0.0119	2.8348

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.1018	-0.0035	-0.0018	0.0351
MSE	2.2594	0.0013	0.0005	105.6213
R2	0.0124	-0.8345	0.1208	-2.1657
RER	2.5174	2.7085	3.3745	1.9027
RMSE	1.5031	0.0362	0.0216	10.2772
RPD	1.0062	0.7383	1.0665	0.5620
RPIQ	2.0849	0.7889	1.9134	0.3776
SEP	1.5367	0.0370	0.0221	10.5310

Vizinhos: 3

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='min',
metric_params=None, n_jobs=None, n_neighbors=3, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0080	-0.0012	-0.0001	0.0195
MSE	0.1214	0.0004	0.0001	3.6356
R2	0.9532	0.7270	0.9096	0.9182
RER	13.0175	7.9644	10.3560	10.4353
RMSE	0.3484	0.0200	0.0078	1.9067
RPD	4.6206	1.9140	3.3256	3.4961
RPIQ	9.2721	2.1994	6.3023	4.6978
SEP	0.3513	0.0201	0.0079	1.9227

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0124	-0.0009	0.0002	0.1412
MSE	0.2257	0.0008	0.0001	8.3712
R2	0.9129	0.4353	0.8376	0.8116
RER	9.5479	5.5291	7.7275	6.8849
RMSE	0.4751	0.0287	0.0105	2.8933
RPD	3.3888	1.3307	2.4812	2.3040
RPIQ	6.8002	1.5291	4.7021	3.0960
SEP	0.4789	0.0289	0.0105	2.9142

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0467	-0.0038	-0.0002	-0.0569
MSE	2.1596	0.0011	0.0004	106.0836
R2	0.0560	-0.5249	0.1766	-2.1795

RER	2.5704	2.9766	3.4745	1.8986
RMSE	1.4696	0.0330	0.0209	10.2997
RPD	1.0292	0.8098	1.1021	0.5608
RPIQ	2.1325	0.8653	1.9771	0.3768
SEP	1.5051	0.0336	0.0215	10.5539

Pré-processamento:

Pré-proc: 1--> Padronização

Vizinhos: 1

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi',
metric_params=None, n_jobs=None, n_neighbors=1, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0096	0.0012	0.0007	0.2166
MSE	0.0142	0.0002	0.0001	9.6653
R2	0.9945	0.8802	0.9214	0.7825
RER	38.1274	12.0524	11.1603	6.4154
RMSE	0.1193	0.0132	0.0073	3.1089
RPD	13.4932	2.8893	3.5661	2.1442
RPIQ	27.0767	3.3201	6.7580	2.8813
SEP	0.1199	0.0133	0.0073	3.1275

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2072	0.0000	0.0011	0.3035
MSE	0.2883	0.0004	0.0000	2.1676
R2	0.8740	0.5105	0.9163	0.9350
RER	7.6223	5.2184	11.0451	13.5731
RMSE	0.5369	0.0187	0.0067	1.4723
RPD	2.8170	1.4293	3.4557	3.9233
RPIQ	5.8368	1.5272	6.1996	2.6361
SEP	0.5075	0.0192	0.0068	1.4762

Vizinhos: 2

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi  
metric_params=None, n_jobs=None, n_neighbors=2, p=2,  
weights='uniform'),  
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0029	0.0011	0.0005	0.1279
MSE	0.0039	0.0001	0.0000	2.4388
R2	0.9985	0.9627	0.9788	0.9451
RER	72.6662	21.7263	21.5544	12.7834
RMSE	0.0625	0.0074	0.0038	1.5617
RPD	25.7729	5.1783	6.8628	4.2687
RPIQ	51.7183	5.9503	13.0055	5.7359
SEP	0.0629	0.0074	0.0038	1.5696

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0136	0.0004	0.0012	0.3212
MSE	0.0912	0.0002	0.0001	5.5528
R2	0.9648	0.8364	0.9217	0.8750
RER	15.0290	10.2694	11.2851	8.5229
RMSE	0.3020	0.0155	0.0073	2.3564
RPD	5.3306	2.4720	3.5746	2.8289
RPIQ	10.6968	2.8406	6.7742	3.8013
SEP	0.3043	0.0156	0.0072	2.3542

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2592	0.0048	0.0031	0.8671
MSE	0.3230	0.0003	0.0001	4.5862
R2	0.8588	0.5572	0.8908	0.8625
RER	7.4638	5.7004	10.4649	9.9861
RMSE	0.5684	0.0178	0.0076	2.1416
RPD	2.6612	1.5027	3.0266	2.6972
RPIQ	5.5139	1.6056	5.4298	1.8123
SEP	0.5183	0.0176	0.0071	2.0065

Vizinhos: 3

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi  
metric_params=None, n_jobs=None, n_neighbors=3, p=2,  
weights='uniform'),  
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0010	0.0001	0.0005	0.1701
MSE	0.0345	0.0001	0.0000	2.4646
R2	0.9867	0.9328	0.9645	0.9445
RER	24.3975	16.0204	16.6032	12.7485
RMSE	0.1859	0.0099	0.0049	1.5699
RPD	8.6621	3.8575	5.3077	4.2462
RPIQ	17.3822	4.4326	10.0585	5.7058
SEP	0.1874	0.0100	0.0049	1.5738

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0123	-0.0001	0.0008	0.1444
MSE	0.1250	0.0003	0.0001	4.7048
R2	0.9518	0.7625	0.9191	0.8941
RER	12.8325	8.5223	11.0096	9.1932
RMSE	0.3536	0.0186	0.0074	2.1690
RPD	4.5534	2.0521	3.5159	3.0733
RPIQ	9.1372	2.3580	6.6630	4.1297
SEP	0.3564	0.0188	0.0074	2.1825

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2597	0.0030	0.0025	0.2548
MSE	0.3279	0.0003	0.0001	5.4755
R2	0.8567	0.6274	0.8907	0.8359
RER	7.3980	6.0822	10.0915	8.4067
RMSE	0.5726	0.0163	0.0076	2.3400
RPD	2.6414	1.6383	3.0249	2.4685
RPIQ	5.4729	1.7505	5.4269	1.6586
SEP	0.5229	0.0165	0.0074	2.3835

Pré-processamento:

Pré-proc: 2--> Suavização(SavGol) - Par:3,1,1
 Vizinhos: 1

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=1, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0

RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0107	0.0031	0.0009	0.3724
MSE	0.3889	0.0012	0.0002	20.7364
R2	0.8500	0.2036	0.7370	0.5334
RER	7.2724	4.6730	6.0856	4.3839
RMSE	0.6236	0.0341	0.0133	4.5537
RPD	2.5817	1.1205	1.9498	1.4639
RPIQ	5.1806	1.2876	3.6951	1.9671
SEP	0.6288	0.0343	0.0134	4.5768

pred				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.1002	-0.0152	-0.0022	-1.0517
MSE	2.4293	0.0019	0.0004	50.4970
R2	-0.0619	-1.6759	0.2326	-0.5135
RER	2.4273	2.3809	3.6204	2.7824
RMSE	1.5586	0.0438	0.0202	7.1061
RPD	0.9704	0.6113	1.1415	0.8128
RPIQ	2.0107	0.6532	2.0479	0.5462
SEP	1.5938	0.0421	0.0206	7.2014

Vizinhos: 2

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=2, p=2,
weights='uniform'),
n_jobs=None)
```

cal				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0078	0.0010	0.0003	-0.0080
MSE	0.0855	0.0003	0.0000	4.1276
R2	0.9670	0.8101	0.9385	0.9071
RER	15.5101	9.5485	12.5720	9.7933
RMSE	0.2925	0.0167	0.0064	2.0316
RPD	5.5048	2.2950	4.0321	3.2812
RPIQ	11.0465	2.6371	7.6411	4.4090
SEP	0.2948	0.0168	0.0065	2.0488

val				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0556	0.0013	-0.0005	0.1404
MSE	0.2905	0.0010	0.0002	13.6131

R2	0.8879	0.3021	0.7729	0.6937
RER	8.4580	4.9754	6.5397	5.3964
RMSE	0.5390	0.0319	0.0124	3.6896
RPD	2.9870	1.1970	2.0982	1.8068
RPIQ	5.9939	1.3755	3.9763	2.4278
SEP	0.5407	0.0322	0.0125	3.7180

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0476	-0.0118	-0.0012	-0.8014
MSE	2.0581	0.0012	0.0004	38.9090
R2	0.1004	-0.6283	0.2541	-0.1662
RER	2.6331	3.0497	3.6565	3.1610
RMSE	1.4346	0.0342	0.0199	6.2377
RPD	1.0543	0.7837	1.1579	0.9260
RPIQ	2.1845	0.8373	2.0773	0.6222
SEP	1.4692	0.0328	0.0204	6.3388

Vizinhos: 3

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='min',
metric_params=None, n_jobs=None, n_neighbors=3, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0177	0.0016	-0.0000	0.1283
MSE	0.0929	0.0004	0.0001	6.2925
R2	0.9642	0.7030	0.9103	0.8584
RER	14.9035	7.6423	10.3963	7.9420
RMSE	0.3048	0.0208	0.0078	2.5085
RPD	5.2825	1.8351	3.3386	2.6575
RPIQ	10.6004	2.1087	6.3269	3.5709
SEP	0.3068	0.0209	0.0078	2.5263

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0203	0.0024	0.0012	0.3106
MSE	0.2890	0.0010	0.0002	13.0411
R2	0.8885	0.3297	0.7763	0.7065
RER	8.4416	5.0870	6.6169	5.5300
RMSE	0.5376	0.0313	0.0123	3.6112
RPD	2.9950	1.2214	2.1145	1.8460
RPIQ	6.0101	1.4035	4.0071	2.4805
SEP	0.5417	0.0315	0.0123	3.6282

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0661	-0.0092	-0.0004	0.0481
MSE	2.1454	0.0011	0.0004	36.6093
R2	0.0622	-0.5973	0.1676	-0.0973
RER	2.5802	3.0011	3.4561	3.2319
RMSE	1.4647	0.0338	0.0211	6.0506
RPD	1.0326	0.7912	1.0961	0.9547
RPIQ	2.1395	0.8454	1.9664	0.6415
SEP	1.4994	0.0334	0.0216	6.1998

Pré-processamento:

Pré-proc: 3--> Suavização(SavGol) - Par:3,2,1
Vizinhos: 1

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=1, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0020	0.0030	0.0007	0.1881
MSE	0.4179	0.0012	0.0002	22.3056
R2	0.8388	0.1966	0.7317	0.4981
RER	7.0148	4.6514	6.0190	4.2161
RMSE	0.6464	0.0343	0.0134	4.7229
RPD	2.4906	1.1157	1.9305	1.4115
RPIQ	4.9979	1.2820	3.6584	1.8966
SEP	0.6519	0.0344	0.0135	4.7590

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.1338	-0.0181	-0.0037	-1.3308
MSE	2.4529	0.0021	0.0005	52.1324
R2	-0.0722	-1.9110	0.1490	-0.5625
RER	2.4194	2.3303	3.4694	2.7555
RMSE	1.5662	0.0457	0.0213	7.2203

RPD	0.9657	0.5861	1.0840	0.8000
RPIQ	2.0010	0.6262	1.9448	0.5375
SEP	1.5990	0.0430	0.0215	7.2718

Vizinhos: 2

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=2, p=2,
weights='uniform'),
n_jobs=None)
```

cal		betaglicosidase	cmcase	fpase	xilanase
BIAS		0.0301	0.0017	0.0005	-0.1111
MSE		0.0870	0.0002	0.0000	4.6371
R2		0.9664	0.8335	0.9459	0.8957
RER		15.4511	10.2391	13.4461	9.2518
RMSE		0.2950	0.0156	0.0060	2.1534
RPD		5.4572	2.4510	4.3001	3.0957
RPIQ		10.9509	2.8165	8.1490	4.1597
SEP		0.2960	0.0156	0.0061	2.1687

val		betaglicosidase	cmcase	fpase	xilanase
BIAS		-0.0212	0.0021	0.0003	0.3755
MSE		0.2694	0.0010	0.0001	13.6283
R2		0.8961	0.3077	0.7932	0.6933
RER		8.7439	5.0023	6.8493	5.4176
RMSE		0.5190	0.0318	0.0118	3.6917
RPD		3.1019	1.2019	2.1989	1.8058
RPIQ		6.2246	1.3811	4.1670	2.4264
SEP		0.5230	0.0320	0.0119	3.7035

pred		betaglicosidase	cmcase	fpase	xilanase
BIAS		-0.0434	-0.0118	-0.0011	-0.8527
MSE		2.0517	0.0011	0.0004	38.8735
R2		0.1031	-0.6046	0.2594	-0.1651
RER		2.6369	3.0760	3.6690	3.1660
RMSE		1.4324	0.0339	0.0199	6.2349
RPD		1.0559	0.7894	1.1620	0.9264
RPIQ		2.1878	0.8435	2.0847	0.6225
SEP		1.4671	0.0326	0.0203	6.3288

Vizinhos: 3

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
```

```
metric_params=None, n_jobs=None, n_neighbors=3, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0141	0.0019	0.0004	0.2101
MSE	0.0794	0.0004	0.0001	6.6343
R2	0.9694	0.7009	0.9182	0.8507
RER	16.1113	7.6259	10.9001	7.7504
RMSE	0.2818	0.0209	0.0074	2.5757
RPD	5.7131	1.8284	3.4956	2.5881
RPIQ	11.4644	2.1010	6.6244	3.4777
SEP	0.2838	0.0210	0.0075	2.5888

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0031	0.0017	0.0011	0.5118
MSE	0.3335	0.0010	0.0001	11.5892
R2	0.8714	0.3050	0.7796	0.7392
RER	7.8527	4.9890	6.6592	5.9117
RMSE	0.5775	0.0319	0.0122	3.4043
RPD	2.7881	1.1995	2.1302	1.9582
RPIQ	5.5948	1.3784	4.0369	2.6313
SEP	0.5823	0.0321	0.0122	3.3940

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0359	-0.0085	0.0003	-0.2913
MSE	1.9372	0.0009	0.0004	27.1032
R2	0.1532	-0.2670	0.2431	0.1877
RER	2.7134	3.3809	3.6239	3.7620
RMSE	1.3918	0.0301	0.0201	5.2061
RPD	1.0867	0.8884	1.1494	1.1095
RPIQ	2.2516	0.9492	2.0621	0.7455
SEP	1.4257	0.0296	0.0206	5.3263

Pré-processamento:

Pré-proc: 4--> Suavização(SavGol) - Par:5,1,1
Vizinhos: 1

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=1, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0

MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0744	0.0027	0.0004	0.3753
MSE	0.4243	0.0013	0.0002	11.7161
R2	0.8363	0.1318	0.7124	0.7364
RER	7.0077	4.4704	5.8087	5.8480
RMSE	0.6513	0.0356	0.0139	3.4229
RPD	2.4718	1.0732	1.8648	1.9475
RPIQ	4.9602	1.2333	3.5339	2.6170
SEP	0.6525	0.0358	0.0140	3.4310

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0436	-0.0125	-0.0026	-1.1770
MSE	2.4032	0.0015	0.0005	38.2635
R2	-0.0505	-1.0992	0.0973	-0.1468
RER	2.4363	2.6628	3.3411	3.2200
RMSE	1.5502	0.0388	0.0219	6.1857
RPD	0.9757	0.6902	1.0525	0.9338
RPIQ	2.0215	0.7375	1.8883	0.6274
SEP	1.5879	0.0376	0.0223	6.2227

Vizinhos: 2

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=2, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0274	0.0009	0.0001	0.0208
MSE	0.0953	0.0003	0.0000	2.0663
R2	0.9632	0.7924	0.9324	0.9535
RER	14.7463	9.1268	11.9735	13.8426
RMSE	0.3087	0.0174	0.0067	1.4375
RPD	5.2149	2.1947	3.8449	4.6374
RPIQ	10.4647	2.5219	7.2864	6.2314
SEP	0.3101	0.0175	0.0068	1.4495

val				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0571	0.0008	-0.0001	0.4992
MSE	0.3285	0.0009	0.0001	7.4153
R2	0.8733	0.3733	0.8063	0.8331
RER	7.9516	5.2482	7.0751	7.4325
RMSE	0.5731	0.0303	0.0114	2.7231
RPD	2.8092	1.2632	2.2720	2.4480
RPIQ	5.6371	1.4516	4.3056	3.2895
SEP	0.5751	0.0305	0.0115	2.6995

pred				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0184	-0.0126	-0.0014	-1.0780
MSE	1.9140	0.0013	0.0004	26.5776
R2	0.1633	-0.8212	0.3209	0.2034
RER	2.7291	2.8860	3.8357	3.8788
RMSE	1.3835	0.0361	0.0190	5.1553
RPD	1.0933	0.7410	1.2135	1.1204
RPIQ	2.2652	0.7917	2.1771	0.7528
SEP	1.4175	0.0347	0.0194	5.1659

Vizinhos: 3

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='min',
metric_params=None, n_jobs=None, n_neighbors=3, p=2,
weights='uniform'),
n_jobs=None)
```

cal				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0113	0.0011	0.0003	0.3020
MSE	0.1017	0.0004	0.0001	3.0499
R2	0.9608	0.7550	0.9243	0.9314
RER	14.2255	8.4031	11.3300	11.5669
RMSE	0.3190	0.0189	0.0071	1.7464
RPD	5.0476	2.0201	3.6343	3.8171
RPIQ	10.1289	2.3213	6.8872	5.1291
SEP	0.3215	0.0190	0.0072	1.7346

val				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0365	0.0001	0.0003	0.0677
MSE	0.2857	0.0009	0.0001	7.8795
R2	0.8898	0.3630	0.8128	0.8227
RER	8.5041	5.2033	7.1980	7.0900
RMSE	0.5345	0.0305	0.0112	2.8070
RPD	3.0123	1.2529	2.3110	2.3748

RPIQ	6.0448	1.4397	4.3795	3.1911
SEP	0.5377	0.0308	0.0113	2.8299

```
-----
pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0084 -0.0079  0.0002  -0.9496
MSE      1.8788  0.0008  0.0004  24.5923
R2       0.1788 -0.1803  0.3234   0.2629
RER      2.7544  3.4918  3.8327   4.0175
RMSE     1.3707  0.0291  0.0190   4.9591
RPD      1.1035  0.9205  1.2157   1.1648
RPIQ     2.2863  0.9835  2.1810   0.7826
SEP      1.4045  0.0287  0.0195   4.9875
-----
```

Pré-processamento:

Pré-proc: 5--> Suavização(SavGol) - Par:5,2,1
 Vizinhos: 1

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=1, p=2,
weights='uniform'),
n_jobs=None)
```

```
cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0      0.0      0.0      0.0
MSE      0.0      0.0      0.0      0.0
R2       1.0      1.0      1.0      1.0
RER      inf      inf      inf      inf
RMSE     0.0      0.0      0.0      0.0
RPD      inf      inf      inf      inf
RPIQ     inf      inf      inf      inf
SEP      0.0      0.0      0.0      0.0
-----
```

```
val
      betaglicosidase  cmcase  fpase  xilanase
BIAS     -0.0778  0.0017 -0.0001   0.4762
MSE      0.2715  0.0013  0.0002  12.2964
R2       0.8953  0.0978  0.7587   0.7233
RER      8.8020  4.3768  6.3396   5.7270
RMSE     0.5210  0.0363  0.0127   3.5066
RPD      3.0901  1.0528  2.0358   1.9010
RPIQ     6.2009  1.2097  3.8580   2.5545
SEP      0.5195  0.0366  0.0129   3.5035
-----
```

```
pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0446 -0.0115 -0.0012  -1.5337
```

MSE	2.1470	0.0014	0.0004	35.4530
R2	0.0615	-0.9445	0.1862	-0.0626
RER	2.5777	2.7509	3.5002	3.3988
RMSE	1.4653	0.0373	0.0208	5.9542
RPD	1.0322	0.7171	1.1085	0.9701
RPIQ	2.1387	0.7662	1.9887	0.6518
SEP	1.5008	0.0364	0.0213	5.8954

Vizinhos: 2

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi',
metric_params=None, n_jobs=None, n_neighbors=2, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0211	-0.0003	-0.0002	0.0547
MSE	0.0584	0.0003	0.0000	2.2442
R2	0.9775	0.7812	0.9384	0.9495
RER	18.8367	8.8797	12.5532	13.2902
RMSE	0.2417	0.0179	0.0064	1.4981
RPD	6.6625	2.1378	4.0292	4.4499
RPIQ	13.3695	2.4565	7.6357	5.9794
SEP	0.2428	0.0180	0.0065	1.5097

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0200	0.0007	0.0003	0.3843
MSE	0.2272	0.0008	0.0001	8.4385
R2	0.9123	0.4395	0.8183	0.8101
RER	9.5210	5.5487	7.3080	6.9099
RMSE	0.4767	0.0286	0.0111	2.9049
RPD	3.3775	1.3357	2.3462	2.2948
RPIQ	6.7775	1.5348	4.4463	3.0836
SEP	0.4803	0.0288	0.0111	2.9037

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0740	-0.0054	0.0004	-0.3423
MSE	1.9385	0.0010	0.0003	44.0594
R2	0.1527	-0.3422	0.3517	-0.3205
RER	2.7155	3.2005	3.9164	2.9499
RMSE	1.3923	0.0310	0.0186	6.6377
RPD	1.0864	0.8632	1.2420	0.8702
RPIQ	2.2509	0.9223	2.2282	0.5847
SEP	1.4247	0.0313	0.0190	6.7926

Vizinhos: 3

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi  
metric_params=None, n_jobs=None, n_neighbors=3, p=2,  
weights='uniform'),  
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0024	0.0017	0.0005	0.2996
MSE	0.0631	0.0004	0.0000	3.9574
R2	0.9757	0.7450	0.9367	0.9109
RER	18.0526	8.2576	12.4123	10.1170
RMSE	0.2512	0.0193	0.0065	1.9893
RPD	6.4092	1.9803	3.9755	3.3510
RPIQ	12.8614	2.2755	7.5338	4.5028
SEP	0.2533	0.0194	0.0066	1.9832

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0482	-0.0001	0.0001	0.0868
MSE	0.2066	0.0008	0.0001	7.2626
R2	0.9203	0.4618	0.8545	0.8366
RER	10.0335	5.6609	8.1640	7.3867
RMSE	0.4545	0.0280	0.0099	2.6949
RPD	3.5423	1.3631	2.6217	2.4736
RPIQ	7.1083	1.5663	4.9683	3.3239
SEP	0.4558	0.0283	0.0100	2.7162

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0034	-0.0058	-0.0001	0.0433
MSE	1.9920	0.0008	0.0004	36.7467
R2	0.1293	-0.1465	0.2983	-0.1014
RER	2.6750	3.4808	3.7635	3.2259
RMSE	1.4114	0.0287	0.0193	6.0619
RPD	1.0717	0.9339	1.1938	0.9529
RPIQ	2.2204	0.9979	2.1417	0.6402
SEP	1.4462	0.0288	0.0198	6.2114

Pré-processamento:

Pré-proc: 6--> Suavização(SavGol) - Par:3,2,2

Vizinhos: 1

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi  
metric_params=None, n_jobs=None, n_neighbors=1, p=2,  
weights='uniform'),
```

```

n_jobs=None)

cal
      betaglicosidase  cmcase  fpase  xylanase
BIAS                0.0      0.0    0.0      0.0
MSE                 0.0      0.0    0.0      0.0
R2                  1.0      1.0    1.0      1.0
RER                 inf      inf    inf      inf
RMSE                0.0      0.0    0.0      0.0
RPD                 inf      inf    inf      inf
RPIQ                inf      inf    inf      inf
SEP                 0.0      0.0    0.0      0.0
-----

val
      betaglicosidase  cmcase  fpase  xylanase
BIAS            -0.0133  0.0043  0.0010   0.5028
MSE              0.4932  0.0011  0.0002  28.9321
R2               0.8097  0.2558  0.6663   0.3489
RER              6.4579  4.8561  5.4026   3.7152
RMSE             0.7023  0.0330  0.0150   5.3789
RPD              2.2925  1.1592  1.7310   1.2393
RPIQ             4.6003  1.3320  3.2805   1.6653
SEP              0.7081  0.0330  0.0151   5.4005
-----

pred
      betaglicosidase  cmcase  fpase  xylanase
BIAS                0.0710 -0.0148 -0.0009  -0.2499
MSE                 2.8458  0.0023  0.0005  62.0605
R2                 -0.2440 -2.1702  0.0814  -0.8601
RER                 2.2400  2.1579  3.2918   2.4834
RMSE                1.6870  0.0477  0.0221   7.8778
RPD                 0.8966  0.5616  1.0434   0.7332
RPIQ                1.8577  0.6001  1.8718   0.4927
SEP                 1.7271  0.0464  0.0227   8.0683
-----

```

Vizinhos: 2

Parâmetros do modelo: PCA-KNN:

```

MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=2, p=2,
weights='uniform'),
n_jobs=None)

```

```

cal
      betaglicosidase  cmcase  fpase  xylanase
BIAS                0.0031  0.0018  0.0004   0.0984
MSE                 0.1211  0.0003  0.0001   7.0691
R2                  0.9533  0.8222  0.9208   0.8409
RER                 13.0318  9.9088 11.0809   7.4884
RMSE                0.3480  0.0161  0.0073   2.6588

```

RPD	4.6267	2.3715	3.5539	2.5072
RPIQ	9.2844	2.7251	6.7350	3.3690
SEP	0.3509	0.0162	0.0074	2.6794

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0140	0.0035	0.0009	0.4724
MSE	0.3635	0.0010	0.0002	18.0852
R2	0.8598	0.3346	0.7277	0.5930
RER	7.5237	5.1229	5.9801	4.7077
RMSE	0.6029	0.0312	0.0135	4.2527
RPD	2.6705	1.2259	1.9165	1.5675
RPIQ	5.3589	1.4087	3.6319	2.1063
SEP	0.6078	0.0312	0.0136	4.2620

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0308	-0.0116	0.0006	-0.0489
MSE	2.6425	0.0013	0.0005	48.1440
R2	-0.1551	-0.8699	0.0783	-0.4430
RER	2.3229	2.8145	3.2850	2.8183
RMSE	1.6256	0.0366	0.0222	6.9386
RPD	0.9304	0.7313	1.0416	0.8325
RPIQ	1.9278	0.7814	1.8687	0.5594
SEP	1.6654	0.0356	0.0227	7.1098

Vizinhos: 3

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=3, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0085	0.0024	0.0007	0.2676
MSE	0.1406	0.0004	0.0001	7.8177
R2	0.9458	0.7200	0.8907	0.8241
RER	12.0978	7.9022	9.4493	7.1487
RMSE	0.3749	0.0202	0.0086	2.7960
RPD	4.2942	1.8897	3.0247	2.3842
RPIQ	8.6171	2.1715	5.7319	3.2037
SEP	0.3780	0.0203	0.0086	2.8067

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0637	0.0030	0.0022	0.3975
MSE	0.3013	0.0010	0.0002	17.5321

R2	0.8838	0.3335	0.7648	0.6055
RER	8.3174	5.1101	6.5181	4.7733
RMSE	0.5489	0.0312	0.0126	4.1871
RPD	2.9331	1.2249	2.0618	1.5921
RPIQ	5.8859	1.4076	3.9072	2.1393
SEP	0.5498	0.0313	0.0125	4.2034

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0682	-0.0074	0.0014	0.2420
MSE	2.2699	0.0010	0.0005	47.8255
R2	0.0078	-0.4119	0.0987	-0.4334
RER	2.5084	3.1593	3.3276	2.8293
RMSE	1.5066	0.0318	0.0219	6.9156
RPD	1.0039	0.8416	1.0533	0.8352
RPIQ	2.0800	0.8992	1.8897	0.5612
SEP	1.5423	0.0317	0.0224	7.0820

Pré-processamento:

Pré-proc: 7--> Suavização(SavGol) - Par:5,2,2

Vizinhos: 1

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=1, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0334	0.0057	0.0012	0.5452
MSE	0.4528	0.0015	0.0002	24.8038
R2	0.8253	-0.0018	0.6915	0.4418
RER	6.7476	4.1961	5.6258	4.0191
RMSE	0.6729	0.0383	0.0144	4.9803
RPD	2.3928	0.9991	1.8006	1.3385
RPIQ	4.8015	1.1481	3.4122	1.7986
SEP	0.6777	0.0381	0.0145	4.9922

```

-----
pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS          -0.0071 -0.0174 -0.0018   0.4328
MSE           2.8469  0.0028  0.0008  122.9413
R2            -0.2444 -2.8411 -0.4318  -2.6848
RER           2.2376  1.9746  2.6403   1.7649
RMSE          1.6873  0.0525  0.0276  11.0879
RPD           0.8964  0.5102  0.8357   0.5209
RPIQ          1.8573  0.5452  1.4993   0.3500
SEP           1.7289  0.0507  0.0282  11.3530
-----

```

Vizinhos: 2

Parâmetros do modelo: PCA-KNN:

```

MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=2, p=2,
weights='uniform'),
n_jobs=None)

```

```

cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS          -0.0128  0.0020  0.0003   0.1457
MSE           0.1080  0.0004  0.0001   5.7237
R2            0.9584  0.7526  0.9257   0.8712
RER          13.8116  8.3958 11.4351   8.3318
RMSE          0.3286  0.0190  0.0071   2.3924
RPD           4.9001  2.0106  3.6689   2.7864
RPIQ          9.8330  2.3103  6.9529   3.7441
SEP           0.3311  0.0191  0.0071   2.4081
-----

```

```

val
      betaglicosidase  cmcase  fpase  xilanase
BIAS          -0.0344  0.0019 -0.0000  -0.1853
MSE           0.3349  0.0013  0.0002  24.2611
R2            0.8708  0.1246  0.7062   0.4541
RER           7.8494  4.4451  5.7454   4.0423
RMSE          0.5787  0.0358  0.0141   4.9256
RPD           2.7820  1.0688  1.8451   1.3534
RPIQ          5.5826  1.2282  3.4965   1.8186
SEP           0.5826  0.0360  0.0142   4.9636
-----

```

```

pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS           0.0787 -0.0097  0.0009   0.4581
MSE           2.5455  0.0015  0.0006  120.5696
R2            -0.1127 -1.0459 -0.0885  -2.6137
RER           2.3692  2.6391  3.0237   1.7824
RMSE          1.5955  0.0383  0.0241  10.9804

```

RPD	0.9480	0.6991	0.9585	0.5260
RPIQ	1.9642	0.7470	1.7196	0.3535
SEP	1.6329	0.0379	0.0247	11.2418

Vizinhos: 3

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=3, p=2,
weights='uniform'),
n_jobs=None)
```

cal		betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0258	0.0008	-0.0001	-0.1766	
MSE	0.1286	0.0005	0.0001	10.4577	
R2	0.9504	0.6267	0.8802	0.7647	
RER	12.6798	6.8014	8.9987	6.1617	
RMSE	0.3586	0.0233	0.0090	3.2338	
RPD	4.4902	1.6368	2.8897	2.0614	
RPIQ	9.0105	1.8808	5.4762	2.7699	
SEP	0.3606	0.0235	0.0091	3.2563	

val		betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0253	0.0017	0.0009	-0.0826	
MSE	0.3971	0.0012	0.0002	22.3174	
R2	0.8468	0.2113	0.6728	0.4978	
RER	7.2015	4.6822	5.4526	4.2123	
RMSE	0.6302	0.0339	0.0148	4.7241	
RPD	2.5548	1.1260	1.7481	1.4111	
RPIQ	5.1267	1.2939	3.3128	1.8961	
SEP	0.6350	0.0342	0.0149	4.7633	

pred		betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1418	-0.0041	0.0026	0.6826	
MSE	2.2594	0.0010	0.0005	102.8705	
R2	0.0124	-0.4423	0.0851	-2.0832	
RER	2.5229	3.0655	3.3184	1.9323	
RMSE	1.5031	0.0321	0.0221	10.1425	
RPD	1.0062	0.8327	1.0455	0.5695	
RPIQ	2.0849	0.8897	1.8757	0.3827	
SEP	1.5334	0.0327	0.0225	10.3694	

Pré-processamento:

Pré-proc: 8--> Suavização(SavGol) - Par:3,1,1 --> Padronização
Vizinhos: 1

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi  
metric_params=None, n_jobs=None, n_neighbors=1, p=2,  
weights='uniform'),  
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0003	0.0010	0.0002	-0.4326
MSE	0.0197	0.0005	0.0001	12.0140
R2	0.9924	0.6812	0.8939	0.7296
RER	32.3031	7.3629	9.5623	5.7855
RMSE	0.1404	0.0216	0.0085	3.4661
RPD	11.4691	1.7711	3.0701	1.9232
RPIQ	23.0150	2.0352	5.8181	2.5843
SEP	0.1416	0.0217	0.0085	3.4680

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.0529	-0.0192	-0.0013	-0.8801
MSE	1.2186	0.0024	0.0004	120.9676
R2	0.4673	-2.3109	0.1684	-2.6256
RER	3.4239	2.1828	3.4637	1.7836
RMSE	1.1039	0.0487	0.0211	10.9985
RPD	1.3701	0.5496	1.0966	0.5252
RPIQ	2.8389	0.5872	1.9673	0.3529
SEP	1.1299	0.0459	0.0215	11.2340

Vizinhos: 2

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi  
metric_params=None, n_jobs=None, n_neighbors=2, p=2,  
weights='uniform'),  
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.0039	0.0008	0.0003	0.0003

MSE	0.0039	0.0001	0.0000	1.4397
R2	0.9985	0.9328	0.9829	0.9676
RER	72.7330	16.0646	23.8724	16.5820
RMSE	0.0625	0.0099	0.0034	1.1999
RPD	25.7722	3.8571	7.6429	5.5558
RPIQ	51.7168	4.4321	14.4838	7.4654
SEP	0.0629	0.0100	0.0034	1.2100

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0032	0.0018	0.0007	0.0780
MSE	0.1061	0.0005	0.0001	6.3640
R2	0.9591	0.6919	0.8960	0.8568
RER	13.9230	7.5091	9.6922	7.8907
RMSE	0.3257	0.0212	0.0084	2.5227
RPD	4.9431	1.8014	3.1007	2.6425
RPIQ	9.9193	2.0700	5.8761	3.5508
SEP	0.3284	0.0213	0.0084	2.5428

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.1726	-0.0243	-0.0032	-0.9978
MSE	1.1647	0.0029	0.0005	119.6625
R2	0.4909	-3.0436	0.0878	-2.5865
RER	3.5439	2.0350	3.3355	1.7951
RMSE	1.0792	0.0538	0.0220	10.9390
RPD	1.4015	0.4973	1.0470	0.5280
RPIQ	2.9038	0.5314	1.8784	0.3548
SEP	1.0916	0.0492	0.0224	11.1624

Vizinhos: 3

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=3, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.0070	0.0002	0.0001	0.0203
MSE	0.0450	0.0002	0.0000	2.8679
R2	0.9826	0.8741	0.9534	0.9355
RER	21.3801	11.7045	14.4334	11.7495
RMSE	0.2122	0.0136	0.0056	1.6935
RPD	7.5868	2.8180	4.6342	3.9364
RPIQ	15.2245	3.2382	8.7821	5.2894
SEP	0.2139	0.0137	0.0056	1.7077

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0039	0.0014	0.0007	0.2323
MSE	0.1883	0.0005	0.0001	6.3119
R2	0.9273	0.6424	0.8797	0.8580
RER	10.4490	6.9581	9.0069	7.9535
RMSE	0.4340	0.0229	0.0090	2.5123
RPD	3.7098	1.6722	2.8832	2.6534
RPIQ	7.4443	1.9215	5.4639	3.5654
SEP	0.4376	0.0230	0.0090	2.5227

pred	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.1906	-0.0229	-0.0035	-0.5386
MSE	1.1173	0.0025	0.0005	118.5787
R2	0.5116	-2.5348	0.1404	-2.5540
RER	3.6313	2.1797	3.4458	1.7979
RMSE	1.0570	0.0503	0.0214	10.8894
RPD	1.4309	0.5319	1.0786	0.5304
RPIQ	2.9648	0.5683	1.9350	0.3564
SEP	1.0653	0.0459	0.0216	11.1446

Pré-processamento:

Pré-proc: 9--> Padronização --> Suavização(SavGol) - Par:3,1,1
Vizinhos: 1

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=1, p=2,
weights='uniform'),
n_jobs=None)
```

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0144	-0.0013	-0.0002	-0.2357
MSE	0.3897	0.0007	0.0002	14.3631
R2	0.8497	0.5524	0.7481	0.6768
RER	7.2661	6.2153	6.2058	5.2600

RMSE	0.6242	0.0256	0.0130	3.7899
RPD	2.5791	1.4947	1.9926	1.7590
RPIQ	5.1755	1.7176	3.7762	2.3635
SEP	0.6293	0.0258	0.0131	3.8145

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2323	-0.0025	0.0022	0.6188
MSE	2.6837	0.0019	0.0008	135.2361
R2	-0.1731	-1.6857	-0.5430	-3.0533
RER	2.3281	2.2316	2.5455	1.6839
RMSE	1.6382	0.0439	0.0287	11.6291
RPD	0.9233	0.6102	0.8050	0.4967
RPIQ	1.9130	0.6520	1.4443	0.3337
SEP	1.6617	0.0449	0.0293	11.8994

Vizinhos: 2

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=2, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0071	-0.0007	0.0000	-0.1297
MSE	0.0974	0.0002	0.0000	3.6026
R2	0.9624	0.8886	0.9358	0.9189
RER	14.5324	12.4625	12.2859	10.5070
RMSE	0.3121	0.0128	0.0066	1.8981
RPD	5.1583	2.9962	3.9455	3.5121
RPIQ	10.3512	3.4429	7.4770	4.7193
SEP	0.3147	0.0128	0.0066	1.9096

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0096	0.0019	0.0006	0.3843
MSE	0.2389	0.0005	0.0001	13.4742
R2	0.9078	0.6313	0.8249	0.6968
RER	9.2790	6.8638	7.4554	5.4502
RMSE	0.4888	0.0232	0.0109	3.6707
RPD	3.2939	1.6469	2.3900	1.8160
RPIQ	6.6098	1.8925	4.5292	2.4403
SEP	0.4928	0.0233	0.0109	3.6814

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2588	-0.0027	0.0012	0.2615

MSE	2.7308	0.0021	0.0008	117.1086
R2	-0.1937	-1.9017	-0.4991	-2.5100
RER	2.3132	2.1470	2.5773	1.8075
RMSE	1.6525	0.0456	0.0283	10.8217
RPD	0.9153	0.5870	0.8167	0.5338
RPIQ	1.8964	0.6272	1.4653	0.3586
SEP	1.6724	0.0466	0.0289	11.0857

Vizinhos: 3

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=3, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0058	0.0011	0.0004	0.1871
MSE	0.1116	0.0002	0.0001	5.5171
R2	0.9569	0.8349	0.9227	0.8758
RER	13.5740	10.2459	11.2185	8.4976
RMSE	0.3341	0.0155	0.0072	2.3489
RPD	4.8187	2.4610	3.5963	2.8381
RPIQ	9.6696	2.8279	6.8153	3.8136
SEP	0.3369	0.0156	0.0073	2.3611

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0052	0.0010	0.0006	0.3598
MSE	0.2221	0.0006	0.0001	11.4925
R2	0.9143	0.5709	0.8410	0.7414
RER	9.6226	6.3451	7.8234	5.9023
RMSE	0.4713	0.0250	0.0103	3.3901
RPD	3.4163	1.5266	2.5077	1.9664
RPIQ	6.8554	1.7542	4.7523	2.6423
SEP	0.4752	0.0252	0.0104	3.3994

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2583	-0.0019	0.0024	0.7161
MSE	2.7718	0.0017	0.0008	117.2306
R2	-0.2116	-1.3442	-0.4850	-2.5136
RER	2.2954	2.3871	2.5962	1.8100
RMSE	1.6649	0.0410	0.0281	10.8273
RPD	0.9085	0.6531	0.8206	0.5335
RPIQ	1.8823	0.6979	1.4722	0.3585
SEP	1.6853	0.0419	0.0287	11.0704

Pré-processamento:

Pré-proc: 10--> MSC

Vizinhos: 1

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='min',
metric_params=None, n_jobs=None, n_neighbors=1, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0441	0.0015	0.0005	0.4163
MSE	0.3109	0.0011	0.0001	11.7836
R2	0.8801	0.2663	0.8216	0.7348
RER	8.1585	4.8539	7.3791	5.8392
RMSE	0.5576	0.0327	0.0110	3.4327
RPD	2.8876	1.1675	2.3674	1.9420
RPIQ	5.7945	1.3415	4.4865	2.6095
SEP	0.5605	0.0330	0.0110	3.4361

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.3177	-0.0004	0.0063	0.0632
MSE	0.8855	0.0015	0.0002	104.1704
R2	0.6129	-1.1150	0.6151	-2.1222
RER	4.2624	2.5106	5.6530	1.9159
RMSE	0.9410	0.0389	0.0143	10.2064
RPD	1.6073	0.6876	1.6118	0.5659
RPIQ	3.3303	0.7347	2.8916	0.3803
SEP	0.9076	0.0399	0.0132	10.4582

Vizinhos: 2

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='min',
metric_params=None, n_jobs=None, n_neighbors=2, p=2,
weights='uniform'),
```

```

n_jobs=None)

cal
      betaglicosidase  cmcase    fpase  xilanase
BIAS          -0.0195 -0.0002  -0.0001   0.1515
MSE           0.0767  0.0003   0.0000   2.7846
R2            0.9704  0.8075   0.9543   0.9373
RER          16.4121  9.4654  14.5643  11.9726
RMSE          0.2770  0.0168   0.0055   1.6687
RPD           5.8127  2.2791   4.6758   3.9948
RPIQ          11.6643  2.6189   8.8610   5.3680
SEP           0.2786  0.0169   0.0056   1.6758
-----

val
      betaglicosidase  cmcase    fpase  xilanase
BIAS          -0.0275 -0.0015  -0.0000   0.3585
MSE           0.2719  0.0009   0.0001   9.4310
R2            0.8951  0.3906   0.8285   0.7878
RER           8.7092  5.3263   7.5195   6.5234
RMSE          0.5214  0.0298   0.0107   3.0710
RPD           3.0879  1.2809   2.4148   2.1707
RPIQ           6.1964  1.4719   4.5762   2.9168
SEP           0.5251  0.0300   0.0108   3.0757
-----

pred
      betaglicosidase  cmcase    fpase  xilanase
BIAS           0.2197 -0.0004   0.0045   0.5657
MSE           0.5141  0.0008   0.0001  96.0282
R2            0.7753 -0.0997   0.7566  -1.8782
RER           5.5313  3.4819   6.9535   1.9988
RMSE          0.7170  0.0281   0.0114   9.7994
RPD           2.1094  0.9536   2.0269   0.5894
RPIQ           4.3706  1.0189   3.6363   0.3961
SEP           0.6994  0.0288   0.0107  10.0246
-----

```

Vizinhos: 3

Parâmetros do modelo: PCA-KNN:

```

MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=3, p=2,
weights='uniform'),
n_jobs=None)

```

```

cal
      betaglicosidase  cmcase    fpase  xilanase
BIAS           0.0075  0.0004   0.0005   0.2439
MSE           0.0998  0.0004   0.0000   4.3591
R2            0.9615  0.7494   0.9347   0.9019
RER          14.3597  8.2986  12.2211   9.5952
RMSE          0.3159  0.0191   0.0066   2.0879

```

RPD	5.0969	1.9977	3.9127	3.1929
RPIQ	10.2280	2.2955	7.4149	4.2903
SEP	0.3185	0.0193	0.0067	2.0911

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0028	-0.0005	0.0004	0.4352
MSE	0.3043	0.0011	0.0001	9.3547
R2	0.8826	0.2690	0.7805	0.7895
RER	8.2211	4.8579	6.6498	6.5720
RMSE	0.5516	0.0327	0.0122	3.0585
RPD	2.9189	1.1696	2.1344	2.1795
RPIQ	5.8572	1.3440	4.0449	2.9287
SEP	0.5562	0.0329	0.0123	3.0530

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2599	-0.0018	0.0041	0.4422
MSE	0.7230	0.0008	0.0002	96.7139
R2	0.6840	-0.0969	0.6958	-1.8987
RER	4.6632	3.4935	6.0382	1.9904
RMSE	0.8503	0.0280	0.0127	9.8343
RPD	1.7788	0.9548	1.8131	0.5874
RPIQ	3.6855	1.0202	3.2528	0.3947
SEP	0.8296	0.0287	0.0123	10.0670

Pré-processamento:

Pré-proc: 11--> SNV

Vizinhos: 1

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=1, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xilanase
--	-----------------	--------	-------	----------

BIAS	-0.0441	0.0015	0.0005	0.4163
MSE	0.3109	0.0011	0.0001	11.7836
R2	0.8801	0.2663	0.8216	0.7348
RER	8.1585	4.8539	7.3791	5.8392
RMSE	0.5576	0.0327	0.0110	3.4327
RPD	2.8876	1.1675	2.3674	1.9420
RPIQ	5.7945	1.3415	4.4865	2.6095
SEP	0.5605	0.0330	0.0110	3.4361

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.3177	-0.0004	0.0063	0.0632
MSE	0.8855	0.0015	0.0002	104.1704
R2	0.6129	-1.1150	0.6151	-2.1222
RER	4.2624	2.5106	5.6530	1.9159
RMSE	0.9410	0.0389	0.0143	10.2064
RPD	1.6073	0.6876	1.6118	0.5659
RPIQ	3.3303	0.7347	2.8916	0.3803
SEP	0.9076	0.0399	0.0132	10.4582

Vizinhos: 2

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=2, p=2,
weights='uniform'),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.0195	-0.0002	-0.0001	0.1515
MSE	0.0767	0.0003	0.0000	2.7846
R2	0.9704	0.8075	0.9543	0.9373
RER	16.4121	9.4654	14.5643	11.9726
RMSE	0.2770	0.0168	0.0055	1.6687
RPD	5.8127	2.2791	4.6758	3.9948
RPIQ	11.6643	2.6189	8.8610	5.3680
SEP	0.2786	0.0169	0.0056	1.6758

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.0274	-0.0014	-0.0002	0.3704
MSE	0.2719	0.0009	0.0001	9.4055
R2	0.8951	0.3913	0.8327	0.7883
RER	8.7092	5.3290	7.6150	6.5354
RMSE	0.5214	0.0298	0.0106	3.0668
RPD	3.0879	1.2817	2.4452	2.1736
RPIQ	6.1965	1.4728	4.6338	2.9208
SEP	0.5251	0.0300	0.0107	3.0701

```

-----
pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.2197 -0.0004  0.0045   0.5657
MSE           0.5141  0.0008  0.0001  96.0282
R2            0.7753 -0.0997  0.7566  -1.8782
RER           5.5313  3.4819  6.9535   1.9988
RMSE          0.7170  0.0281  0.0114   9.7994
RPD           2.1094  0.9536  2.0269   0.5894
RPIQ          4.3706  1.0189  3.6363   0.3961
SEP           0.6994  0.0288  0.0107  10.0246
-----

```

Vizinhos: 3

Parâmetros do modelo: PCA-KNN:

```

MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=3, p=2,
weights='uniform'),
n_jobs=None)

```

```

cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.0075  0.0004  0.0005   0.2439
MSE           0.0998  0.0004  0.0000   4.3591
R2            0.9615  0.7494  0.9347   0.9019
RER          14.3597  8.2986 12.2211   9.5952
RMSE          0.3159  0.0191  0.0066   2.0879
RPD           5.0969  1.9977  3.9127   3.1929
RPIQ         10.2280  2.2955  7.4149   4.2903
SEP           0.3185  0.0193  0.0067   2.0911
-----

```

```

val
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.0028 -0.0005  0.0004   0.4352
MSE           0.3043  0.0011  0.0001   9.3547
R2            0.8826  0.2690  0.7805   0.7895
RER           8.2211  4.8579  6.6498   6.5720
RMSE          0.5516  0.0327  0.0122   3.0585
RPD           2.9189  1.1696  2.1344   2.1795
RPIQ          5.8572  1.3440  4.0449   2.9287
SEP           0.5562  0.0329  0.0123   3.0530
-----

```

```

pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.2362 -0.0033  0.0035   0.3508
MSE           0.7075  0.0009  0.0002  96.6372
R2            0.6907 -0.2368  0.7124  -1.8964
RER           4.6764  3.3035  6.1297   1.9904
RMSE          0.8412  0.0298  0.0124   9.8304

```


RPD	1.7981	0.8992	1.8645	0.5876
RPIQ	3.7256	0.9607	3.3451	0.3948
SEP	0.8273	0.0303	0.0122	10.0668

In []:

```
In [87]: #teste 2 escolhendo o modelo mais otimizado
modelo = 'PCA-KNN:'
maior=[-1,-1,-1,-1]
maiorGerado=[0,0,0,0]
for i in range(100):
    result = executaPCA_KNN(1,3,1,False,i)
    resultados=exibeResultados(result)
    r2 = resultados['pred'].loc[resultados['pred'].index=='R2']
    r = []
    for j in range(4):
        r.append(r2.iloc[:,j][0])
        if r[j]>maior[j]:
            maior[j] = r[j]
            maiorGerado[j]=i
    print('\r%d%% completos'%(i+1), end='')
print('\n','r2:',maior,'\nsemente: b c f x',maiorGerado)
```

100% completos

r2: [0.9924, 0.9748, 0.9842, 0.9846]

semente: b c f x [81, 82, 68, 68]

```
In [96]: #pcaknn teste otimizado
modelo = 'PCA-KNN:'
preproc=1
nPC=3
k=1
gera=82
result = executaPCA_KNN(preproc,nPC,k, False, gera)
print('Parâmetros do modelo:',modelo,'\n',result[0])

resultados=exibeResultados(result)
```

Parâmetros do modelo: PCA-KNN:

```
MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=1, p=2,
weights='uniform'),
n_jobs=None)
```

```
In [97]: resultados['cal']
```

```
Out [97]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

```
In [98]: resultados['val']
```

```
Out [98]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0089	0.0012	0.0007	0.2494
MSE	0.0163	0.0002	0.0001	9.7738
R2	0.9939	0.8773	0.9127	0.7798
RER	35.6397	12.1814	10.5171	6.3845
RMSE	0.1275	0.0131	0.0077	3.1263
RPD	12.7901	2.8547	3.3844	2.1311
RPIQ	25.1981	2.7357	6.3745	2.3266
SEP	0.1283	0.0131	0.0077	3.1426

```
In [99]: resultados['pred']
```

```
Out [99]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.1334	0.0018	-0.0029	-0.2634
MSE	0.1575	0.0000	0.0001	1.5489
R2	0.9265	0.9748	0.8906	0.9552
RER	9.9542	22.3389	9.0440	15.0354
RMSE	0.3968	0.0048	0.0075	1.2446
RPD	3.6892	6.2960	3.0232	4.7269
RPIQ	6.8461	8.1782	5.5096	2.7138
SEP	0.3830	0.0045	0.0071	1.2464

```
In [101]: reg, treino_teste,y_c,y_cv,y_p = result
```

7.2.2 Reais x preditos

```
In [ ]: #pcaknn reaisxpreditos
```

```
In [ ]:
```

```
In [102]: #calibração
```

```
pred=pd.DataFrame(y_c, columns=var_ae)
reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('CALIBRAÇÃO:\n')
reais_pred
```

CALIBRAÇÃO:

```
Out[102]:
```

	betaglicosidase	cmcase	fpase	xylanase	pred: betaglicosidase \
0	0.600960	0.055887	0.011606	20.136787	0.600960
1	2.164345	0.082978	0.052863	18.832405	2.164345
2	0.055433	0.018093	0.010575	0.327476	0.055433
3	0.167115	0.011663	0.010442	0.111691	0.167115
4	0.087354	0.021666	0.012690	0.107064	0.087354
5	0.389996	0.031505	0.028323	14.177685	0.389996
6	0.055433	0.018093	0.010575	0.327476	0.055433
7	2.164345	0.082978	0.052863	18.832405	2.164345
8	3.560973	0.058556	0.056106	10.097754	3.560973
9	3.899420	0.111790	0.061343	10.951244	3.899420
10	4.603719	0.171262	0.091917	16.811540	4.603719
11	0.172414	0.011206	0.012128	0.092439	0.172414
12	3.880348	0.055725	0.069144	11.325589	3.880348
13	0.087354	0.021666	0.012690	0.107064	0.087354
14	2.912307	0.105796	0.074679	14.681307	2.912307
15	2.977361	0.070384	0.056737	10.800176	2.977361
16	4.603719	0.171262	0.091917	16.811540	4.603719
17	0.030827	0.021327	0.011302	0.099591	0.030827
18	3.596691	0.106528	0.085014	13.647554	3.596691
19	0.427951	0.039043	0.033365	13.762416	0.427951
20	0.382773	0.040468	0.030080	12.446105	0.382773
21	3.596691	0.106528	0.085014	13.647554	3.596691
22	2.912307	0.105796	0.074679	14.681307	2.912307
23	0.590459	0.046495	0.026706	18.709464	0.590459
24	3.106775	0.078125	0.054548	11.052574	3.106775
25	2.114992	0.072961	0.050492	18.412714	2.114992
26	0.075936	0.013639	0.013869	0.072595	0.075936
27	0.030827	0.021327	0.011302	0.099591	0.030827
28	3.596691	0.106528	0.085014	13.647554	3.596691
29	3.234247	0.067160	0.054272	8.477247	3.234247
30	3.597384	0.051579	0.073083	15.397347	3.597384
31	3.880348	0.055725	0.069144	11.325589	3.880348
32	3.106775	0.078125	0.054548	11.052574	3.106775
33	0.590459	0.046495	0.026706	18.709464	0.590459
34	3.234247	0.067160	0.054272	8.477247	3.234247
35	0.075936	0.013639	0.013869	0.072595	0.075936
36	2.977361	0.070384	0.056737	10.800176	2.977361
37	3.887630	0.041788	0.060524	11.026731	3.887630
38	3.724300	0.056102	0.068121	11.573610	3.724300
39	0.382773	0.040468	0.030080	12.446105	0.382773
40	3.880348	0.055725	0.069144	11.325589	3.880348
41	0.055433	0.018093	0.010575	0.327476	0.055433
42	0.427951	0.039043	0.033365	13.762416	0.427951

43	0.075936	0.013639	0.013869	0.072595	0.075936
44	3.234247	0.067160	0.054272	8.477247	3.234247
45	0.600960	0.055887	0.011606	20.136787	0.600960
46	3.560973	0.058556	0.056106	10.097754	3.560973
47	0.172414	0.011206	0.012128	0.092439	0.172414
48	4.603719	0.171262	0.091917	16.811540	4.603719
49	3.724300	0.056102	0.068121	11.573610	3.724300
50	0.427951	0.039043	0.033365	13.762416	0.427951
51	3.887630	0.041788	0.060524	11.026731	3.887630
52	2.114992	0.072961	0.050492	18.412714	2.114992
53	0.649142	0.060508	0.025982	18.427379	0.649142
54	2.114992	0.072961	0.050492	18.412714	2.114992
55	0.600960	0.055887	0.011606	20.136787	0.600960
56	0.649142	0.060508	0.025982	18.427379	0.649142
57	3.597384	0.051579	0.073083	15.397347	3.597384
58	3.887630	0.041788	0.060524	11.026731	3.887630
59	0.030827	0.021327	0.011302	0.099591	0.030827

	pred: cmcase	pred: fpase	pred: xylanase
0	0.055887	0.011606	20.136787
1	0.082978	0.052863	18.832405
2	0.018093	0.010575	0.327476
3	0.011663	0.010442	0.111691
4	0.021666	0.012690	0.107064
5	0.031505	0.028323	14.177685
6	0.018093	0.010575	0.327476
7	0.082978	0.052863	18.832405
8	0.058556	0.056106	10.097754
9	0.111790	0.061343	10.951244
10	0.171262	0.091917	16.811540
11	0.011206	0.012128	0.092439
12	0.055725	0.069144	11.325589
13	0.021666	0.012690	0.107064
14	0.105796	0.074679	14.681307
15	0.070384	0.056737	10.800176
16	0.171262	0.091917	16.811540
17	0.021327	0.011302	0.099591
18	0.106528	0.085014	13.647554
19	0.039043	0.033365	13.762416
20	0.040468	0.030080	12.446105
21	0.106528	0.085014	13.647554
22	0.105796	0.074679	14.681307
23	0.046495	0.026706	18.709464
24	0.078125	0.054548	11.052574
25	0.072961	0.050492	18.412714
26	0.013639	0.013869	0.072595
27	0.021327	0.011302	0.099591
28	0.106528	0.085014	13.647554

29	0.067160	0.054272	8.477247
30	0.051579	0.073083	15.397347
31	0.055725	0.069144	11.325589
32	0.078125	0.054548	11.052574
33	0.046495	0.026706	18.709464
34	0.067160	0.054272	8.477247
35	0.013639	0.013869	0.072595
36	0.070384	0.056737	10.800176
37	0.041788	0.060524	11.026731
38	0.056102	0.068121	11.573610
39	0.040468	0.030080	12.446105
40	0.055725	0.069144	11.325589
41	0.018093	0.010575	0.327476
42	0.039043	0.033365	13.762416
43	0.013639	0.013869	0.072595
44	0.067160	0.054272	8.477247
45	0.055887	0.011606	20.136787
46	0.058556	0.056106	10.097754
47	0.011206	0.012128	0.092439
48	0.171262	0.091917	16.811540
49	0.056102	0.068121	11.573610
50	0.039043	0.033365	13.762416
51	0.041788	0.060524	11.026731
52	0.072961	0.050492	18.412714
53	0.060508	0.025982	18.427379
54	0.072961	0.050492	18.412714
55	0.055887	0.011606	20.136787
56	0.060508	0.025982	18.427379
57	0.051579	0.073083	15.397347
58	0.041788	0.060524	11.026731
59	0.021327	0.011302	0.099591

```
In [103]: #validação
pred=pd.DataFrame(y_cv, columns=var_ae)
reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('VALIDAÇÃO CRUZADA:\n')
reais_pred
```

VALIDAÇÃO CRUZADA:

```
Out[103]:      betaglicosidase      cmcase      fpase      xilanase  pred: betaglicosidase \
0          0.600960  0.055887  0.011606  20.136787          0.600960
```

1	2.164345	0.082978	0.052863	18.832405	2.114992
2	0.055433	0.018093	0.010575	0.327476	0.055433
3	0.167115	0.011663	0.010442	0.111691	0.055433
4	0.087354	0.021666	0.012690	0.107064	0.030827
5	0.389996	0.031505	0.028323	14.177685	0.382773
6	0.055433	0.018093	0.010575	0.327476	0.055433
7	2.164345	0.082978	0.052863	18.832405	2.114992
8	3.560973	0.058556	0.056106	10.097754	3.560973
9	3.899420	0.111790	0.061343	10.951244	3.596691
10	4.603719	0.171262	0.091917	16.811540	4.603719
11	0.172414	0.011206	0.012128	0.092439	0.172414
12	3.880348	0.055725	0.069144	11.325589	3.596691
13	0.087354	0.021666	0.012690	0.107064	0.075936
14	2.912307	0.105796	0.074679	14.681307	2.912307
15	2.977361	0.070384	0.056737	10.800176	3.234247
16	4.603719	0.171262	0.091917	16.811540	4.603719
17	0.030827	0.021327	0.011302	0.099591	0.075936
18	3.596691	0.106528	0.085014	13.647554	3.596691
19	0.427951	0.039043	0.033365	13.762416	0.055433
20	0.382773	0.040468	0.030080	12.446105	0.382773
21	3.596691	0.106528	0.085014	13.647554	3.880348
22	2.912307	0.105796	0.074679	14.681307	2.912307
23	0.590459	0.046495	0.026706	18.709464	0.590459
24	3.106775	0.078125	0.054548	11.052574	3.106775
25	2.114992	0.072961	0.050492	18.412714	2.114992
26	0.075936	0.013639	0.013869	0.072595	0.087354
27	0.030827	0.021327	0.011302	0.099591	0.087354
28	3.596691	0.106528	0.085014	13.647554	3.880348
29	3.234247	0.067160	0.054272	8.477247	3.234247
30	3.597384	0.051579	0.073083	15.397347	3.597384
31	3.880348	0.055725	0.069144	11.325589	3.880348
32	3.106775	0.078125	0.054548	11.052574	3.106775
33	0.590459	0.046495	0.026706	18.709464	0.590459
34	3.234247	0.067160	0.054272	8.477247	3.234247
35	0.075936	0.013639	0.013869	0.072595	0.030827
36	2.977361	0.070384	0.056737	10.800176	3.106775
37	3.887630	0.041788	0.060524	11.026731	3.887630
38	3.724300	0.056102	0.068121	11.573610	3.724300
39	0.382773	0.040468	0.030080	12.446105	0.389996
40	3.880348	0.055725	0.069144	11.325589	3.880348
41	0.055433	0.018093	0.010575	0.327476	0.427951
42	0.427951	0.039043	0.033365	13.762416	0.055433
43	0.075936	0.013639	0.013869	0.072595	0.087354
44	3.234247	0.067160	0.054272	8.477247	3.234247
45	0.600960	0.055887	0.011606	20.136787	0.649142
46	3.560973	0.058556	0.056106	10.097754	3.560973
47	0.172414	0.011206	0.012128	0.092439	0.172414
48	4.603719	0.171262	0.091917	16.811540	4.603719

49	3.724300	0.056102	0.068121	11.573610	3.724300
50	0.427951	0.039043	0.033365	13.762416	0.427951
51	3.887630	0.041788	0.060524	11.026731	3.887630
52	2.114992	0.072961	0.050492	18.412714	2.114992
53	0.649142	0.060508	0.025982	18.427379	0.600960
54	2.114992	0.072961	0.050492	18.412714	2.114992
55	0.600960	0.055887	0.011606	20.136787	0.600960
56	0.649142	0.060508	0.025982	18.427379	0.600960
57	3.597384	0.051579	0.073083	15.397347	3.597384
58	3.887630	0.041788	0.060524	11.026731	3.560973
59	0.030827	0.021327	0.011302	0.099591	0.075936

	pred: cmcase	pred: fpase	pred: xilanase
0	0.055887	0.011606	20.136787
1	0.072961	0.050492	18.412714
2	0.018093	0.010575	0.327476
3	0.018093	0.010575	0.327476
4	0.021327	0.011302	0.099591
5	0.040468	0.030080	12.446105
6	0.018093	0.010575	0.327476
7	0.072961	0.050492	18.412714
8	0.058556	0.056106	10.097754
9	0.106528	0.085014	13.647554
10	0.171262	0.091917	16.811540
11	0.011206	0.012128	0.092439
12	0.106528	0.085014	13.647554
13	0.013639	0.013869	0.072595
14	0.105796	0.074679	14.681307
15	0.067160	0.054272	8.477247
16	0.171262	0.091917	16.811540
17	0.013639	0.013869	0.072595
18	0.106528	0.085014	13.647554
19	0.018093	0.010575	0.327476
20	0.040468	0.030080	12.446105
21	0.055725	0.069144	11.325589
22	0.105796	0.074679	14.681307
23	0.046495	0.026706	18.709464
24	0.078125	0.054548	11.052574
25	0.072961	0.050492	18.412714
26	0.021666	0.012690	0.107064
27	0.021666	0.012690	0.107064
28	0.055725	0.069144	11.325589
29	0.067160	0.054272	8.477247
30	0.051579	0.073083	15.397347
31	0.055725	0.069144	11.325589
32	0.078125	0.054548	11.052574
33	0.046495	0.026706	18.709464
34	0.067160	0.054272	8.477247

35	0.021327	0.011302	0.099591
36	0.078125	0.054548	11.052574
37	0.041788	0.060524	11.026731
38	0.056102	0.068121	11.573610
39	0.031505	0.028323	14.177685
40	0.055725	0.069144	11.325589
41	0.039043	0.033365	13.762416
42	0.018093	0.010575	0.327476
43	0.021666	0.012690	0.107064
44	0.067160	0.054272	8.477247
45	0.060508	0.025982	18.427379
46	0.058556	0.056106	10.097754
47	0.011206	0.012128	0.092439
48	0.171262	0.091917	16.811540
49	0.056102	0.068121	11.573610
50	0.039043	0.033365	13.762416
51	0.041788	0.060524	11.026731
52	0.072961	0.050492	18.412714
53	0.055887	0.011606	20.136787
54	0.072961	0.050492	18.412714
55	0.055887	0.011606	20.136787
56	0.055887	0.011606	20.136787
57	0.051579	0.073083	15.397347
58	0.058556	0.056106	10.097754
59	0.013639	0.013869	0.072595

```
In [104]: #predição
pred=pd.DataFrame(y_p, columns=var_ae)
reais = treino_teste[3]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('Predição (validação externa):\n')
reais_pred
```

Predição (validação externa):

```
Out[104]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	3.724300	0.056102	0.068121	11.573610	3.724300
1	0.382773	0.040468	0.030080	12.446105	0.382773
2	2.164345	0.082978	0.052863	18.832405	2.164345
3	0.172414	0.011206	0.012128	0.092439	0.172414
4	2.912307	0.105796	0.074679	14.681307	2.912307
5	3.899420	0.111790	0.061343	10.951244	3.596691
6	3.899420	0.111790	0.061343	10.951244	3.596691

7	0.167115	0.011663	0.010442	0.111691	0.172414
8	0.087354	0.021666	0.012690	0.107064	0.075936
9	0.389996	0.031505	0.028323	14.177685	0.389996
10	3.597384	0.051579	0.073083	15.397347	3.597384
11	2.977361	0.070384	0.056737	10.800176	3.234247
12	0.389996	0.031505	0.028323	14.177685	0.389996
13	3.106775	0.078125	0.054548	11.052574	3.106775
14	2.711042	0.054804	0.068844	13.582877	3.880348
15	2.711042	0.054804	0.068844	13.582877	3.597384
16	2.711042	0.054804	0.068844	13.582877	3.597384
17	0.590459	0.046495	0.026706	18.709464	0.590459
18	3.560973	0.058556	0.056106	10.097754	3.887630
19	0.649142	0.060508	0.025982	18.427379	0.649142
20	0.167115	0.011663	0.010442	0.111691	0.055433

	pred: cmcase	pred: fpase	pred: xilanase
0	0.056102	0.068121	11.573610
1	0.040468	0.030080	12.446105
2	0.082978	0.052863	18.832405
3	0.011206	0.012128	0.092439
4	0.105796	0.074679	14.681307
5	0.106528	0.085014	13.647554
6	0.106528	0.085014	13.647554
7	0.011206	0.012128	0.092439
8	0.013639	0.013869	0.072595
9	0.031505	0.028323	14.177685
10	0.051579	0.073083	15.397347
11	0.067160	0.054272	8.477247
12	0.031505	0.028323	14.177685
13	0.078125	0.054548	11.052574
14	0.055725	0.069144	11.325589
15	0.051579	0.073083	15.397347
16	0.051579	0.073083	15.397347
17	0.046495	0.026706	18.709464
18	0.041788	0.060524	11.026731
19	0.060508	0.025982	18.427379
20	0.018093	0.010575	0.327476

7.2.3 PCA->KNN: Gráficos de desempenho

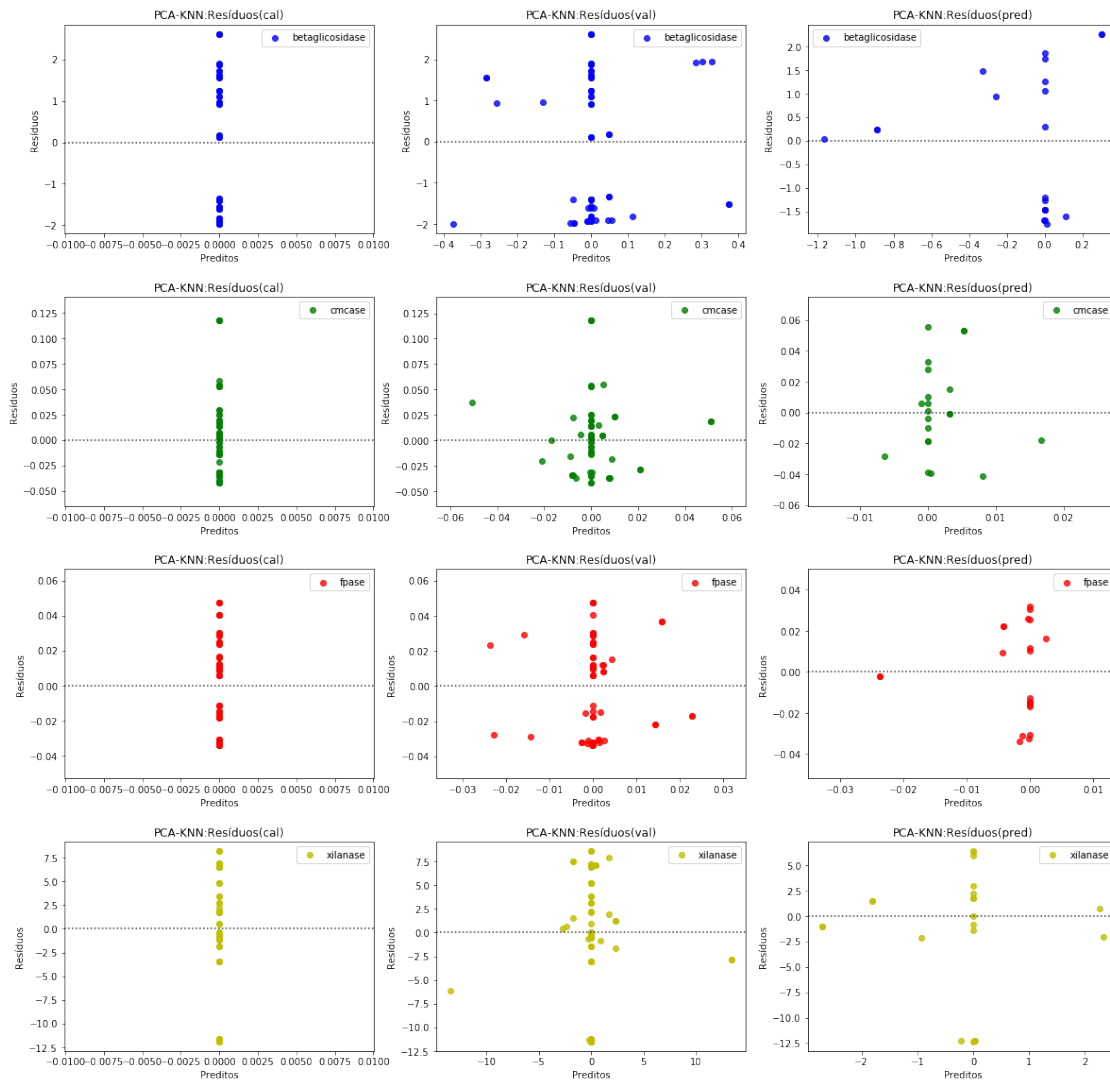
In []:

7.2.4 PCA->KNN: Gráficos dos resíduos

```
In [105]: #@pcaknngraf
          #título para os gráficos
          modelo = 'PCA-KNN'
```

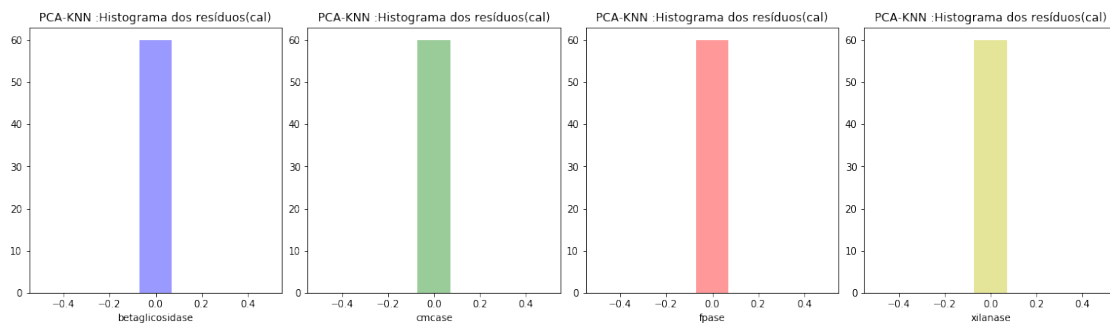
In [106]: *#gráfico dos resíduos*

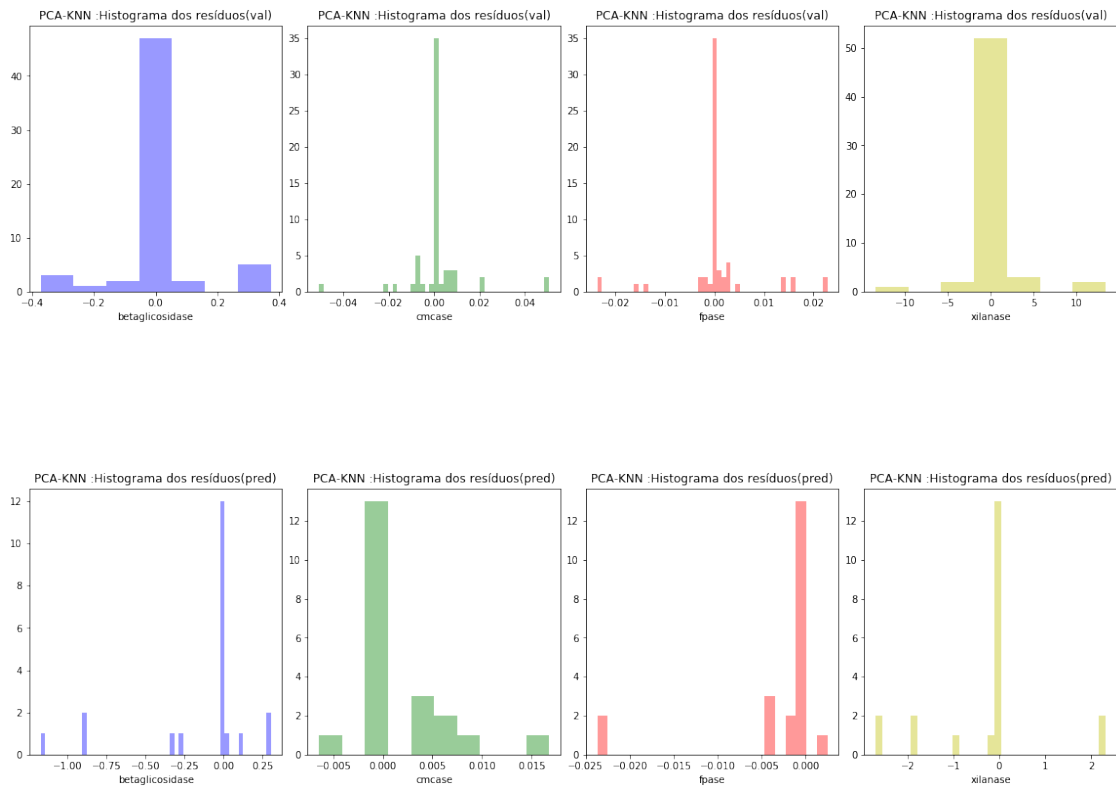
`graficoResiduos(modelo, treino_teste, y_c,y_cv,y_p)`



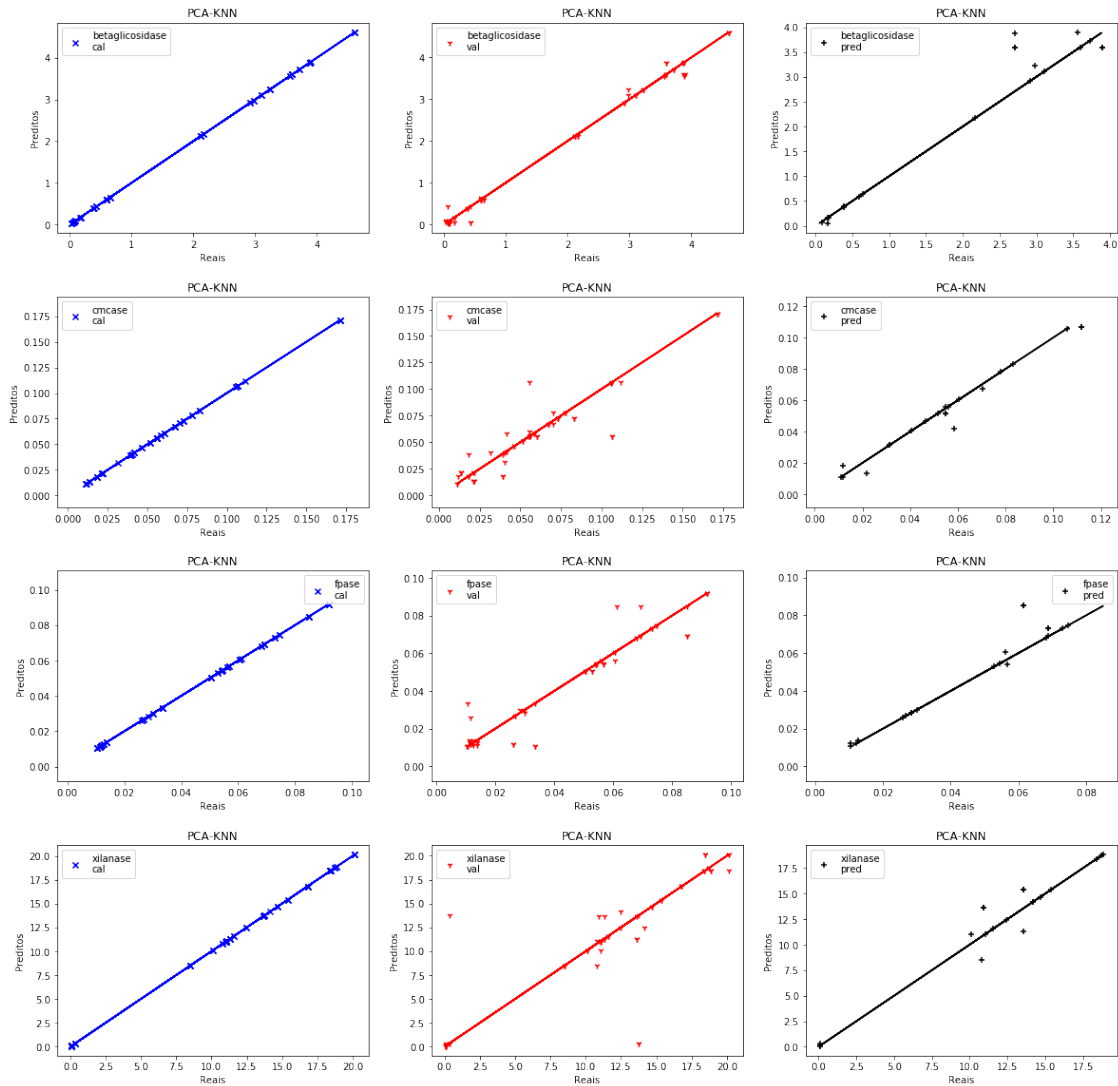
In [107]: *#histograma dos resíduos*

`graficoHist(modelo, treino_teste, y_c,y_cv,y_p)`

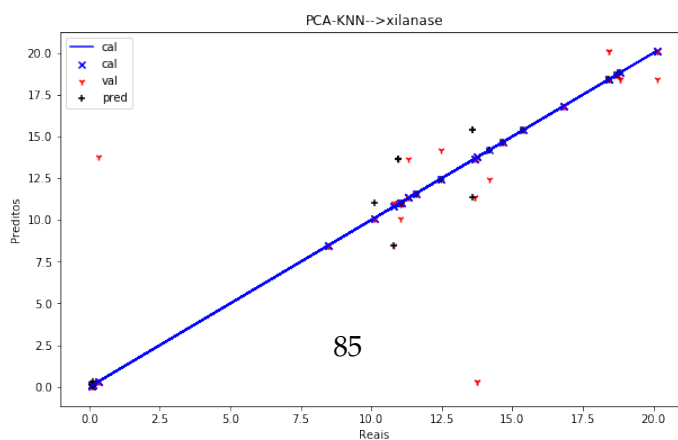
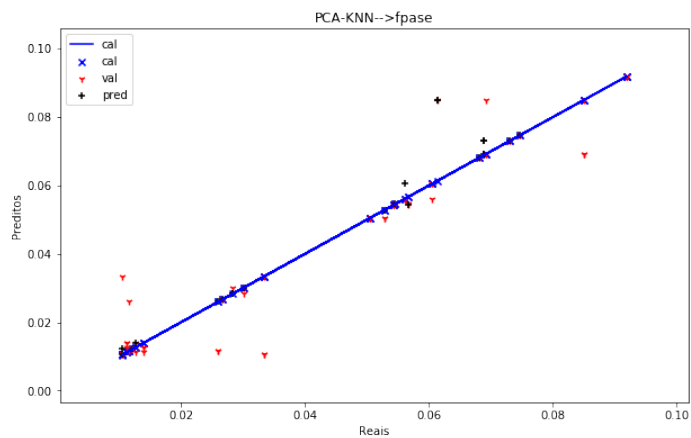
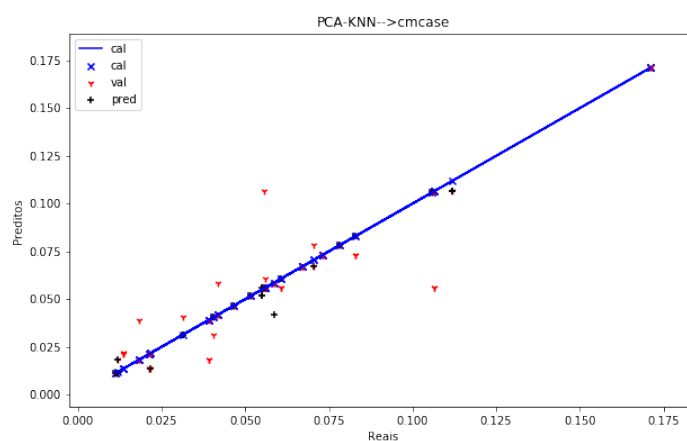
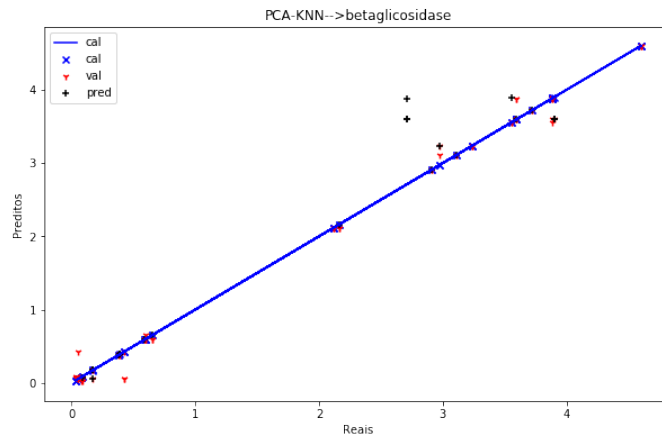




```
In [117]: #gráfico de reais x preditos
          graficoReaisPreditosSep(modelo, treino_teste, y_c,y_cv,y_p)
```

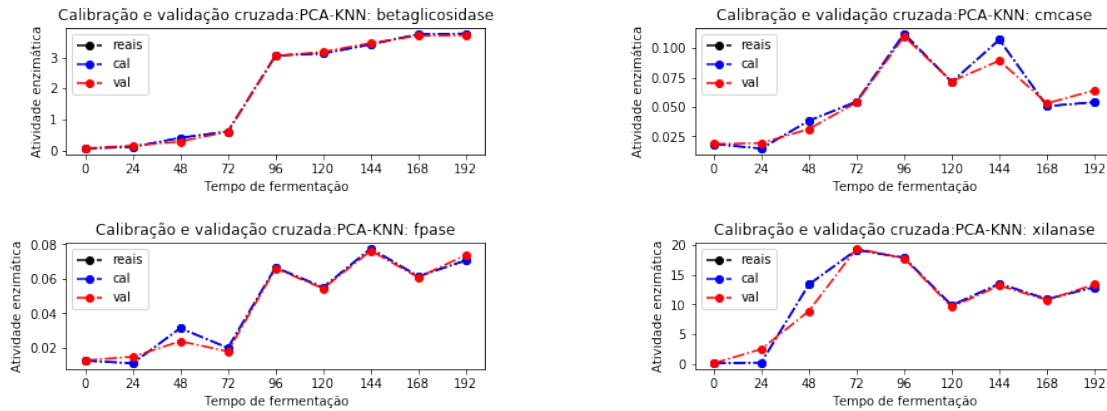


In [119]: *#gráfico de reais x preditos conjuntamente*
graficoReaisPreditos(modelo, treino_teste, y_c,y_cv,y_p)



7.2.5 PCA->KNN: Gráficos: dados de treino

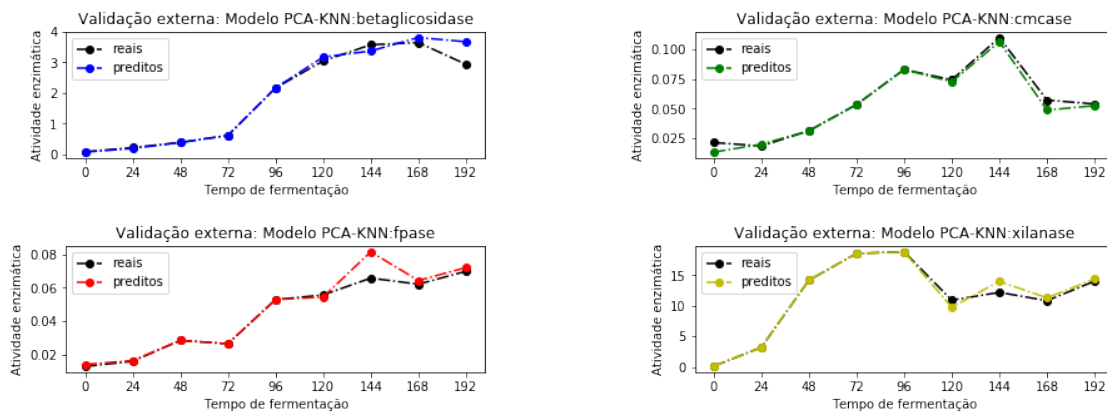
```
In [120]: y_treino = treino_teste[2]  
          graficoTreinamento(modelo, y_treino, y_c,y_cv)
```



```
In [ ]:
```

7.2.6 PCA->KNN: Gráficos de teste

```
In [121]: y_teste = treino_teste[3]  
          graficoTeste(modelo, y_teste, y_p)
```



7.2.7 PCA-knn: teste com base externa: EETA desnaturado

In [120]: `#@testeExterno`

```
#rodando o pcaknn com os dados de treino
modelo = 'PCA-KNN:'
preproc=1
nPC=3
k=1
gera=0
result = executaPCA_KNN(preproc,nPC,k, False, gera)
#print('Parâmetros do modelo:',m,'\n',result[0])

resultados=exibeResultados(result)
reg, treino_teste,y_c,y_cv,y_p = result
```

In [133]: `#buscando base de teste externa`

```
de = dados_back.copy()
de=de[(de['eenz'] == 'eeta')&(de['experimento']=='biod1')&(de['inter']!= 1)&(de['int
#Separar somente as amostras que contenham todas as atividades enzimáticas
de = de.loc[(de['betaglicosidase'].notnull())
            & (de['cmcase'].notnull())
            & (de['fpase'].notnull())
            &(de['xilanase'].notnull())]

de.shape
```

Out[133]: (21, 713)

In [134]: `de.head(5)`

```
Out[134]:
```

		descricao	1100nm	1102nm	1104nm	1106nm	1108nm	\
791	bio_25janp0_1_desn	0.038744	0.038471	0.038295	0.038206	0.038193		
792	bio_25janp0_2_desn	0.038601	0.038637	0.038631	0.038613	0.038621		
793	bio_25janp0_3_desn	0.039642	0.039467	0.039371	0.039322	0.039300		
794	bio_25janp10_1_desn	0.053291	0.051491	0.050285	0.049398	0.048688		
795	bio_25janp10_2_desn	0.053027	0.051663	0.050706	0.049957	0.049301		

		1110nm	1112nm	1114nm	1116nm	...	cmcase	fpase	xilanase	\
791		0.038237	0.038330	0.038481	0.038710	...	0.035	0.051	24.094	
792		0.038688	0.038837	0.039073	0.039391	...	0.035	0.051	24.094	
793		0.039299	0.039333	0.039428	0.039612	...	0.035	0.051	24.094	
794		0.048107	0.047656	0.047341	0.047144	...	0.026	0.005	0.256	
795		0.048693	0.048133	0.047644	0.047249	...	0.026	0.005	0.256	

	proteinas	eenz	temp	dur	inter	proc	experimento
791	NaN	eeta	70	33	0	des	biod1
792	NaN	eeta	70	33	0	des	biod1
793	NaN	eeta	70	33	0	des	biod1
794	NaN	eeta	70	33	30	des	biod1
795	NaN	eeta	70	33	30	des	biod1

[5 rows x 713 columns]

```
In [135]: #Definindo os dataFrames iniciais para começar o processamento
de_x = de.loc[:,var_abs_txt] #absorbências
de_y = de.loc[:,var_ae] #AE
de_inter=pd.DataFrame(de.loc[:,'inter'], columns=['inter'])
#df = dados.loc[:,var_abs_txt+var_ae]

In [136]: de_x.shape,de_y.shape, de_inter.shape

Out[136]: ((21, 244), (21, 4), (21, 1))

In [137]: #executa pré-processamento equivalente ao do modelo de treinamento
x = executaPreprocSimples(1,de_x)
pca = PCA(n_components=3)
x = pca.fit_transform(x)[:,:3]
preditos=reg.predict(x)

In [138]: #para exibir o gráfico
#para todas as atividades
#cria um data frame com os valores reais e preditos para os dados de teste
df_pred = {}
for valor in var_ae:
    df_pred[valor] = []
i=0
for valor in var_ae:
    df =pd.DataFrame(columns=['reais','preditos'], index= de_y.index)
    df['reais'] = de_y[valor]
    df['preditos'] = pd.DataFrame(preditos[:,i],index= de_y.index)
    i +=1
    df_pred[valor] = df.copy()

df_pred_inter = {}
for valor in var_ae:
    df_pred_inter[valor] = []
for valor in var_ae:
    df_pred_inter[valor] = df_pred[valor].copy()
    df_pred_inter[valor]['inter'] = de_inter.loc[:,'inter']

#ordena valores pelo intervalo
df_ord_teste = {}
for valor in var_ae:
    df_ord_teste[valor] = []
for valor in var_ae:
    df_ord_teste[valor] = df_pred_inter[valor].sort_values(['inter'])

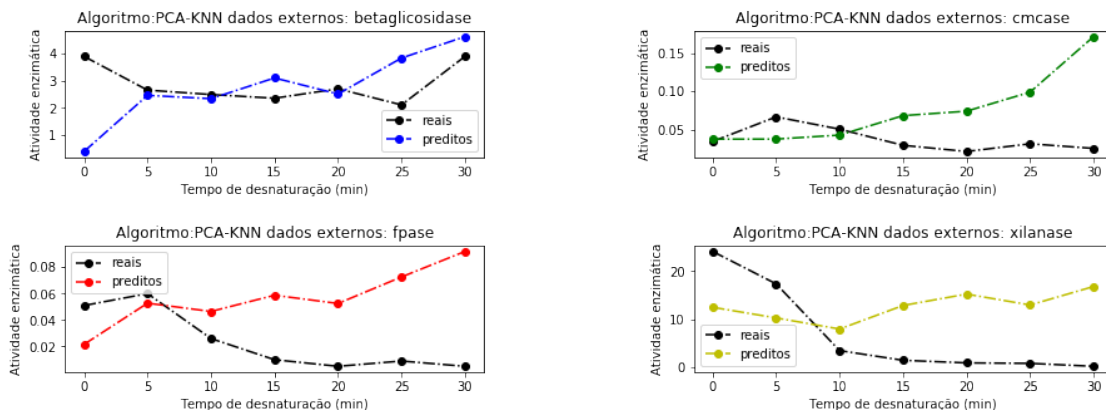
#calculando a média para cada ponto
df_teste_media = {}
```



```

for valor in var_ae:
    df_teste_media[valor] = []
for valor in var_ae:
    df_teste_media[valor] = df_ord_teste[valor].groupby('inter').mean()
x = list(df_teste_media['xilanase'].index)
var = ['reais', 'preditos']
tipoAE= ['bo-.', 'go-.', 'ro-.', 'yo-.']
j = 0
fig = plt.figure(figsize=(15,5))
plt.subplots_adjust(hspace = 0.7, wspace=0.5)
for valor in var_ae:
    ax = fig.add_subplot(2,2,j+1)
    ax.plot(x,df_teste_media[valor][var[0]], 'ko-', label=var[0])
    ax.plot(x,df_teste_media[valor][var[1]], tipoAE[j], label=var[1])
    j +=1
    ax.legend(loc=2)
    ax.set_title('Algoritmo:'+modelo+' dados externos'+': '+valor)
    ax.set_xlabel('Tempo de desnaturação (min)')
    ax.set_ylabel('Atividade enzimática')
    ax.set_xticks(x)
    plt.legend(loc='best')

```



In []:

In []:

7.3 KNN

In [144]: *#knn*

```

#função completa para execução do KNN:
#A variável preproc determinará o tipo de processamento que será executado (0,1,2,3.
from sklearn.neighbors import KNeighborsRegressor
def executaKNN(preproc,k,IC=0):

```

```

#separando o conjunto de dados em treino e teste
x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc,False,IC)

# Cria um objeto de regressão linear
reg = MultiOutputRegressor(KNeighborsRegressor(n_neighbors=k))
#reg = KNeighborsRegressor(n_neighbors=n)

result = executaCVP([x_treino, x_teste, y_treino, y_teste], reg)

return result

```

7.3.1 KNN: testes

```

In [145]: #knn teste simples
          modelo = 'KNN:'
          preproc=1
          k=2
          result = executaKNN(preproc,k)
          print('Parâmetros do modelo:',modelo,'\n',result[0])

          resultados=exibeResultados(result)

```

Parâmetros do modelo: KNN:

```

MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='min',
metric_params=None, n_jobs=None, n_neighbors=2, p=2,
weights='uniform'),
n_jobs=None)

```

In [146]: resultados['cal']

```

Out[146]:
          betaglicosidase  cmcase  fpase  xilanase
BIAS          0.0047    0.0000  0.0001    0.0895
MSE           0.0024    0.0000  0.0000    0.9963
R2            0.9991    0.9871  0.9774    0.9776
RER          92.2512   36.5837  20.7102   20.0136
RMSE          0.0494    0.0043  0.0039    0.9982
RPD          32.6062    8.8090  6.6477    6.6785
RPIQ          65.4306   10.1224  12.5978    8.9741
SEP           0.0496    0.0044  0.0039    1.0025

```

In [147]: resultados['val']

```

Out[147]:
          betaglicosidase  cmcase  fpase  xilanase
BIAS          -0.0077    0.0001  0.0006    0.4719

```

MSE	0.0884	0.0002	0.0000	4.5714
R2	0.9659	0.8450	0.9332	0.8971
RER	15.2592	10.5496	12.0868	9.5409
RMSE	0.2973	0.0150	0.0067	2.1381
RPD	5.4159	2.5402	3.8680	3.1178
RPIQ	10.8681	2.9189	7.3302	4.1895
SEP	0.2997	0.0152	0.0067	2.1030

In [148]: resultados['pred']

Out[148]:

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1428	-0.0012	0.0002	0.1324
MSE	0.1908	0.0002	0.0000	1.9708
R2	0.9166	0.7220	0.9312	0.9409
RER	9.1463	6.9485	12.0272	13.9914
RMSE	0.4368	0.0141	0.0061	1.4039
RPD	3.4630	1.8967	3.8130	4.1145
RPIQ	7.1752	2.0266	6.8406	2.7646
SEP	0.4230	0.0144	0.0062	1.4321

```
In [149]: #knn teste completo
#Executa o modelo KNN variando o tipo de processamento e o número de vizinhos
for pre in range(0,12):
    for viz in range(1,7):
        result = executaKNN(pre,viz)
        print('Pe-proc:',pre, '-> vizinhos:', viz,'\n')
        resultados=exibeResultados(result)
        for k,v in zip(resultados.keys(),resultados.values()):
            print(k)
            print(v,'\n-----')
```

Pe-proc: 0 -> vizinhos: 1

```
cal
betaglicosidase  cmcase  fpase  xilanase
BIAS            0.0      0.0    0.0      0.0
MSE             0.0      0.0    0.0      0.0
R2              1.0      1.0    1.0      1.0
RER             inf      inf    inf      inf
RMSE            0.0      0.0    0.0      0.0
RPD             inf      inf    inf      inf
RPIQ            inf      inf    inf      inf
SEP             0.0      0.0    0.0      0.0
-----

val
betaglicosidase  cmcase  fpase  xilanase
BIAS            -0.0801 -0.0021 -0.0007 -0.0832
MSE             0.2587  0.0008  0.0001  2.3003
R2              0.9002  0.4418  0.8391  0.9482
```

RER	9.0288	5.5730	7.7814	13.1381
RMSE	0.5086	0.0286	0.0104	1.5167
RPD	3.1656	1.3384	2.4929	4.3953
RPIQ	6.3524	1.5380	4.7243	5.9060
SEP	0.5065	0.0287	0.0105	1.5272

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1384	-0.0014	0.0026	-0.1545
MSE	0.2253	0.0001	0.0001	3.4676
R2	0.9015	0.9284	0.8740	0.8961
RER	8.3151	13.9228	9.3504	10.5372
RMSE	0.4747	0.0072	0.0082	1.8622
RPD	3.1864	3.7380	2.8177	3.1019
RPIQ	6.6021	3.9940	5.0550	2.0842
SEP	0.4653	0.0072	0.0080	1.9016

Pe-proc: 0 -> vizinhos: 2

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0461	-0.0012	-0.0001	0.0030
MSE	0.0646	0.0002	0.0000	0.5670
R2	0.9751	0.8673	0.9617	0.9872
RER	18.1472	11.4401	15.9167	26.4232
RMSE	0.2541	0.0139	0.0051	0.7530
RPD	6.3363	2.7449	5.1111	8.8530
RPIQ	12.7150	3.1542	9.6858	11.8959
SEP	0.2520	0.0140	0.0051	0.7593

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0192	-0.0005	0.0002	0.0026
MSE	0.2067	0.0008	0.0001	4.2717
R2	0.9203	0.4844	0.8703	0.9039
RER	9.9826	5.7849	8.6495	9.6265
RMSE	0.4547	0.0274	0.0093	2.0668
RPD	3.5411	1.3927	2.7769	3.2253
RPIQ	7.1060	1.6003	5.2624	4.3340
SEP	0.4581	0.0277	0.0094	2.0843

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1377	-0.0013	0.0030	0.0709
MSE	0.2684	0.0001	0.0001	6.1950
R2	0.8827	0.8543	0.9009	0.8143
RER	7.5596	9.6494	11.0324	7.8596
RMSE	0.5181	0.0102	0.0073	2.4890

RPD	2.9196	2.6203	3.1773	2.3207
RPIQ	6.0492	2.7997	5.7002	1.5593
SEP	0.5117	0.0104	0.0068	2.5494

Pe-proc: 0 -> vizinhos: 3

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0367	-0.0002	0.0006	-0.0258
MSE	0.0878	0.0003	0.0000	1.6843
R2	0.9661	0.8102	0.9488	0.9621
RER	15.4216	9.5320	13.8202	15.3340
RMSE	0.2963	0.0167	0.0059	1.2978
RPD	5.4331	2.2951	4.4185	5.1366
RPIQ	10.9026	2.6373	8.3734	6.9022
SEP	0.2965	0.0168	0.0059	1.3085

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0166	-0.0020	-0.0002	0.1073
MSE	0.2359	0.0007	0.0001	4.6864
R2	0.9090	0.5117	0.8431	0.8945
RER	9.3427	5.9595	7.8629	9.2021
RMSE	0.4857	0.0267	0.0103	2.1648
RPD	3.3152	1.4310	2.5246	3.0793
RPIQ	6.6525	1.6444	4.7843	4.1378
SEP	0.4895	0.0269	0.0104	2.1804

pred	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1788	-0.0001	0.0036	0.1265
MSE	0.2534	0.0001	0.0001	7.1622
R2	0.8892	0.8386	0.8756	0.7853
RER	8.0226	9.0892	9.9768	7.3148
RMSE	0.5034	0.0108	0.0081	2.6762
RPD	3.0044	2.4894	2.8356	2.1583
RPIQ	6.2250	2.6598	5.0871	1.4502
SEP	0.4822	0.0110	0.0075	2.7393

Pe-proc: 0 -> vizinhos: 4

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0197	0.0004	0.0004	0.1441
MSE	0.1300	0.0004	0.0001	2.7647
R2	0.9498	0.7171	0.9126	0.9378
RER	12.5945	7.8099	10.5513	12.0113
RMSE	0.3606	0.0203	0.0077	1.6627

RPD	4.4649	1.8802	3.3828	4.0092
RPIQ	8.9598	2.1605	6.4108	5.3873
SEP	0.3631	0.0205	0.0077	1.6704

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0361	-0.0002	0.0009	0.2457
MSE	0.2555	0.0007	0.0001	6.3521
R2	0.9014	0.5111	0.8368	0.8571
RER	8.9936	5.9395	7.7378	7.9321
RMSE	0.5055	0.0267	0.0105	2.5203
RPD	3.1850	1.4301	2.4753	2.6450
RPIQ	6.3913	1.6434	4.6909	3.5541
SEP	0.5085	0.0269	0.0105	2.5295

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1759	0.0010	0.0034	0.0304
MSE	0.2495	0.0001	0.0001	6.6040
R2	0.8910	0.8130	0.9006	0.8021
RER	8.0767	8.4778	11.3406	7.6097
RMSE	0.4995	0.0116	0.0073	2.5698
RPD	3.0283	2.3126	3.1711	2.2477
RPIQ	6.2745	2.4709	5.6890	1.5103
SEP	0.4790	0.0118	0.0066	2.6331

Pe-proc: 0 -> vizinhos: 5

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0250	-0.0006	0.0004	0.0222
MSE	0.1552	0.0004	0.0001	3.7132
R2	0.9401	0.7200	0.9019	0.9164
RER	11.5323	7.8525	9.9549	10.3258
RMSE	0.3940	0.0202	0.0081	1.9270
RPD	4.0863	1.8899	3.1923	3.4594
RPIQ	8.1999	2.1716	6.0496	4.6485
SEP	0.3965	0.0204	0.0082	1.9431

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0499	0.0004	0.0012	0.3994
MSE	0.2594	0.0007	0.0001	7.1218
R2	0.8999	0.5328	0.8460	0.8397
RER	8.9466	6.0766	7.9889	7.5404
RMSE	0.5093	0.0261	0.0102	2.6687
RPD	3.1612	1.4630	2.5484	2.4979
RPIQ	6.3435	1.6811	4.8293	3.3566

SEP	0.5111	0.0263	0.0102	2.6609
-----	--------	--------	--------	--------

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1699	0.0000	0.0030	0.0849
MSE	0.2487	0.0002	0.0001	7.4153
R2	0.8913	0.6970	0.8892	0.7777
RER	8.0517	6.6324	10.2812	7.1844
RMSE	0.4987	0.0147	0.0077	2.7231
RPD	3.0327	1.8166	3.0036	2.1212
RPIQ	6.2836	1.9410	5.3887	1.4253
SEP	0.4805	0.0151	0.0073	2.7890

Pe-proc: 0 -> vizinhos: 6

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0461	0.0001	0.0008	0.0855
MSE	0.1828	0.0005	0.0001	4.4972
R2	0.9295	0.6702	0.8860	0.8988
RER	10.6683	7.2319	9.2628	9.3897
RMSE	0.4276	0.0219	0.0088	2.1207
RPD	3.7656	1.7413	2.9619	3.1435
RPIQ	7.5564	2.0009	5.6131	4.2239
SEP	0.4286	0.0221	0.0088	2.1368

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0984	0.0009	0.0017	0.5366
MSE	0.3030	0.0007	0.0001	11.7240
R2	0.8831	0.5423	0.8289	0.7362
RER	8.3720	6.1418	7.6190	5.8835
RMSE	0.5505	0.0259	0.0107	3.4240
RPD	2.9246	1.4781	2.4172	1.9469
RPIQ	5.8689	1.6984	4.5808	2.6161
SEP	0.5462	0.0261	0.0107	3.4103

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1823	0.0002	0.0030	0.2163
MSE	0.3419	0.0003	0.0001	7.8296
R2	0.8505	0.6083	0.8535	0.7653
RER	6.7953	5.8342	8.7755	7.0093
RMSE	0.5847	0.0167	0.0088	2.7982
RPD	2.5866	1.5978	2.6129	2.0643
RPIQ	5.3594	1.7073	4.6877	1.3870
SEP	0.5693	0.0172	0.0085	2.8587

Pe-proc: 1 -> vizinhos: 1

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0094	0.0000	0.0002	0.1790
MSE	0.0098	0.0001	0.0001	3.9853
R2	0.9962	0.9485	0.9095	0.9103
RER	46.1256	18.2918	10.3551	10.0068
RMSE	0.0988	0.0087	0.0078	1.9963
RPD	16.3031	4.4045	3.3238	3.3393
RPIQ	32.7153	5.0612	6.2989	4.4870
SEP	0.0991	0.0088	0.0079	2.0051

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2184	0.0020	0.0017	0.5338
MSE	0.2957	0.0001	0.0000	3.2066
R2	0.8707	0.8466	0.9164	0.9039
RER	7.5809	9.4999	11.2614	11.4400
RMSE	0.5438	0.0105	0.0067	1.7907
RPD	2.7814	2.5533	3.4589	3.2257
RPIQ	5.7629	2.7282	6.2055	2.1674
SEP	0.5103	0.0105	0.0066	1.7515

Pe-proc: 1 -> vizinhos: 2

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0047	0.0000	0.0001	0.0895
MSE	0.0024	0.0000	0.0000	0.9963
R2	0.9991	0.9871	0.9774	0.9776
RER	92.2512	36.5837	20.7102	20.0136
RMSE	0.0494	0.0043	0.0039	0.9982
RPD	32.6062	8.8090	6.6477	6.6785
RPIQ	65.4306	10.1224	12.5978	8.9741
SEP	0.0496	0.0044	0.0039	1.0025

val				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0077	0.0001	0.0006	0.4719
MSE	0.0884	0.0002	0.0000	4.5714
R2	0.9659	0.8450	0.9332	0.8971
RER	15.2592	10.5496	12.0868	9.5409
RMSE	0.2973	0.0150	0.0067	2.1381
RPD	5.4159	2.5402	3.8680	3.1178
RPIQ	10.8681	2.9189	7.3302	4.1895
SEP	0.2997	0.0152	0.0067	2.1030

pred				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1428	-0.0012	0.0002	0.1324
MSE	0.1908	0.0002	0.0000	1.9708
R2	0.9166	0.7220	0.9312	0.9409
RER	9.1463	6.9485	12.0272	13.9914
RMSE	0.4368	0.0141	0.0061	1.4039
RPD	3.4630	1.8967	3.8130	4.1145
RPIQ	7.1752	2.0266	6.8406	2.7646
SEP	0.4230	0.0144	0.0062	1.4321

Pe-proc: 1 -> vizinhos: 3

cal				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0028	0.0002	0.0002	0.1907
MSE	0.0223	0.0001	0.0000	1.6381
R2	0.9914	0.9456	0.9752	0.9631
RER	30.3695	17.8150	19.7827	15.7208
RMSE	0.1493	0.0089	0.0041	1.2799
RPD	10.7807	4.2885	6.3482	5.2084
RPIQ	21.6336	4.9279	12.0303	6.9987
SEP	0.1506	0.0090	0.0041	1.2763

val				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0071	-0.0010	0.0006	0.2188
MSE	0.1342	0.0003	0.0001	3.1771
R2	0.9482	0.7769	0.9058	0.9285
RER	12.3805	8.8071	10.1678	11.2474
RMSE	0.3663	0.0181	0.0080	1.7824
RPD	4.3948	2.1172	3.2574	3.7399
RPIQ	8.8191	2.4329	6.1731	5.0254
SEP	0.3694	0.0182	0.0080	1.7839

pred				
	betaglicosidase	cmcase	fpase	xilanase

BIAS	0.1670	-0.0011	0.0013	0.2684
MSE	0.1536	0.0001	0.0000	2.9331
R2	0.9328	0.8599	0.9436	0.9121
RER	10.6472	9.8124	13.6673	11.5606
RMSE	0.3919	0.0100	0.0055	1.7126
RPD	3.8590	2.6719	4.2108	3.3727
RPIQ	7.9955	2.8549	7.5543	2.2662
SEP	0.3633	0.0102	0.0055	1.7332

Pe-proc: 1 -> vizinhos: 4

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0005	-0.0006	0.0004	0.1523
MSE	0.0791	0.0002	0.0000	1.7146
R2	0.9695	0.8683	0.9503	0.9614
RER	16.1235	11.4553	14.0007	15.2985
RMSE	0.2812	0.0139	0.0058	1.3094
RPD	5.7246	2.7554	4.4841	5.0909
RPIQ	11.4875	3.1662	8.4978	6.8408
SEP	0.2836	0.0140	0.0058	1.3115

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0407	-0.0003	0.0011	0.2106
MSE	0.1639	0.0004	0.0001	3.3164
R2	0.9368	0.7180	0.8936	0.9254
RER	11.2568	7.8214	9.6224	10.9993
RMSE	0.4049	0.0203	0.0085	1.8211
RPD	3.9765	1.8832	3.0659	3.6605
RPIQ	7.9795	2.1640	5.8101	4.9188
SEP	0.4062	0.0205	0.0085	1.8241

pred	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1913	-0.0015	0.0024	-0.0639
MSE	0.1844	0.0001	0.0000	3.8815
R2	0.9194	0.8015	0.9240	0.8837
RER	9.8201	8.2576	12.3110	9.9306
RMSE	0.4294	0.0119	0.0064	1.9701
RPD	3.5222	2.2445	3.6284	2.9319
RPIQ	7.2979	2.3982	6.5094	1.9700
SEP	0.3939	0.0121	0.0061	2.0177

Pe-proc: 1 -> vizinhos: 5

cal	betaglicosidase	cmcase	fpase	xilanase
-----	-----------------	--------	-------	----------

BIAS	0.0116	-0.0006	0.0005	0.1329
MSE	0.1251	0.0003	0.0000	2.0932
R2	0.9517	0.8015	0.9265	0.9529
RER	12.8268	9.3270	11.5097	13.8104
RMSE	0.3537	0.0170	0.0070	1.4468
RPD	4.5517	2.2444	3.6879	4.6076
RPIQ	9.1338	2.5790	6.9889	6.1913
SEP	0.3565	0.0172	0.0071	1.4528

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0106	-0.0009	0.0001	0.1833
MSE	0.1962	0.0005	0.0001	4.4898
R2	0.9243	0.6627	0.8584	0.8990
RER	10.2394	7.1573	8.2765	9.4251
RMSE	0.4430	0.0222	0.0098	2.1189
RPD	3.6344	1.7218	2.6578	3.1460
RPIQ	7.2932	1.9786	5.0368	4.2274
SEP	0.4466	0.0224	0.0098	2.1288

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1980	-0.0013	0.0024	-0.0978
MSE	0.2334	0.0002	0.0000	4.2655
R2	0.8980	0.6967	0.9180	0.8722
RER	8.5680	6.6568	11.8111	9.4787
RMSE	0.4831	0.0147	0.0066	2.0653
RPD	3.1310	1.8158	3.4917	2.7968
RPIQ	6.4873	1.9401	6.2643	1.8792
SEP	0.4515	0.0150	0.0063	2.1139

Pe-proc: 1 -> vizinhos: 6

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0287	-0.0004	0.0005	-0.0071
MSE	0.1300	0.0004	0.0001	2.9256
R2	0.9499	0.7545	0.9084	0.9342
RER	12.6175	8.3824	10.3112	11.6323
RMSE	0.3605	0.0189	0.0079	1.7104
RPD	4.4656	2.0181	3.3039	3.8974
RPIQ	8.9611	2.3189	6.2611	5.2370
SEP	0.3624	0.0191	0.0079	1.7249

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0421	-0.0012	-0.0009	0.0999
MSE	0.2420	0.0005	0.0001	6.0550

R2	0.9067	0.6529	0.8384	0.8637
RER	9.2523	7.0594	7.7777	8.0923
RMSE	0.4919	0.0225	0.0104	2.4607
RPD	3.2730	1.6975	2.4877	2.7091
RPIQ	6.5679	1.9505	4.7144	3.6402
SEP	0.4942	0.0227	0.0105	2.4794

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1996	-0.0018	0.0025	-0.1620
MSE	0.2380	0.0003	0.0001	4.6801
R2	0.8960	0.5840	0.8979	0.8597
RER	8.4805	5.6916	10.4737	9.0643
RMSE	0.4879	0.0173	0.0074	2.1634
RPD	3.1002	1.5504	3.1295	2.6700
RPIQ	6.4235	1.6566	5.6144	1.7940
SEP	0.4562	0.0176	0.0071	2.2106

Pe-proc: 2 -> vizinhos: 1

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0030	0.0075	0.0024	0.6784
MSE	0.3246	0.0012	0.0001	15.0302
R2	0.8748	0.2100	0.8087	0.6618
RER	7.9593	4.7897	7.2786	5.2124
RMSE	0.5697	0.0340	0.0113	3.8769
RPD	2.8259	1.1251	2.2865	1.7195
RPIQ	5.6707	1.2928	4.3331	2.3105
SEP	0.5745	0.0334	0.0112	3.8493

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1114	-0.0072	0.0020	-0.0047
MSE	0.2319	0.0003	0.0001	4.1462
R2	0.8986	0.5638	0.8466	0.8757
RER	8.0590	6.0535	8.2516	9.6033

RMSE	0.4815	0.0177	0.0090	2.0362
RPD	3.1411	1.5140	2.5532	2.8367
RPIQ	6.5082	1.6177	4.5806	1.9060
SEP	0.4800	0.0165	0.0090	2.0865

Pe-proc: 2 -> vizinhos: 2

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0053	0.0026	0.0009	0.2945
MSE	0.0800	0.0003	0.0000	3.5748
R2	0.9691	0.8139	0.9526	0.9196
RER	16.0308	9.7533	14.5018	10.6532
RMSE	0.2829	0.0165	0.0056	1.8907
RPD	5.6907	2.3181	4.5934	3.5258
RPIQ	11.4195	2.6637	8.7049	4.7377
SEP	0.2853	0.0164	0.0056	1.8834

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0003	0.0027	0.0002	0.2102
MSE	0.3051	0.0010	0.0001	8.3171
R2	0.8823	0.2846	0.8282	0.8128
RER	8.2089	4.9276	7.5141	6.9174
RMSE	0.5524	0.0323	0.0108	2.8839
RPD	2.9146	1.1823	2.4126	2.3115
RPIQ	5.8486	1.3586	4.5720	3.1060
SEP	0.5571	0.0325	0.0108	2.9005

pred	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1568	-0.0046	0.0020	-0.2284
MSE	0.4988	0.0002	0.0001	6.1306
R2	0.7820	0.6669	0.8408	0.8163
RER	5.4824	6.6256	8.0899	7.9313
RMSE	0.7063	0.0154	0.0092	2.4760
RPD	2.1416	1.7327	2.5060	2.3329
RPIQ	4.4372	1.8513	4.4958	1.5675
SEP	0.7056	0.0151	0.0092	2.5263

Pe-proc: 2 -> vizinhos: 3

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0103	0.0020	0.0005	0.1421
MSE	0.1216	0.0005	0.0000	4.1081
R2	0.9531	0.6778	0.9279	0.9076
RER	13.0120	7.3486	11.6298	9.8407

RMSE	0.3487	0.0217	0.0070	2.0268
RPD	4.6178	1.7618	3.7231	3.2890
RPIQ	9.2666	2.0245	7.0556	4.4195
SEP	0.3514	0.0218	0.0070	2.0389

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0364	0.0032	0.0012	0.3930
MSE	0.2410	0.0008	0.0001	10.5107
R2	0.9070	0.4467	0.8222	0.7635
RER	9.2630	5.6186	7.4281	6.1826
RMSE	0.4909	0.0284	0.0109	3.2420
RPD	3.2798	1.3444	2.3715	2.0562
RPIQ	6.5815	1.5448	4.4942	2.7630
SEP	0.4937	0.0285	0.0110	3.2453

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1446	-0.0031	0.0018	0.1591
MSE	0.5039	0.0002	0.0001	6.3190
R2	0.7797	0.6735	0.8523	0.8106
RER	5.4321	6.5235	8.3743	7.7945
RMSE	0.7099	0.0153	0.0089	2.5138
RPD	2.1307	1.7501	2.6021	2.2978
RPIQ	4.4146	1.8699	4.6683	1.5440
SEP	0.7122	0.0153	0.0089	2.5707

Pe-proc: 2 -> vizinhos: 4

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0110	0.0019	0.0004	0.1276
MSE	0.1328	0.0004	0.0001	5.0284
R2	0.9488	0.7039	0.9082	0.8868
RER	12.4481	7.6653	10.2876	8.8871
RMSE	0.3645	0.0208	0.0079	2.2424
RPD	4.4176	1.8376	3.3002	2.9728
RPIQ	8.8648	2.1116	6.2541	3.9946
SEP	0.3674	0.0209	0.0079	2.2577

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0579	0.0027	0.0016	0.2375
MSE	0.2104	0.0007	0.0001	11.3668
R2	0.9188	0.5086	0.8190	0.7442
RER	9.9660	5.9550	7.3975	5.9161
RMSE	0.4587	0.0268	0.0110	3.3715
RPD	3.5101	1.4266	2.3505	1.9772

RPIQ	7.0436	1.6393	4.4545	2.6569
SEP	0.4589	0.0269	0.0110	3.3915

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1020	-0.0027	0.0013	0.0770
MSE	0.4630	0.0002	0.0001	5.6614
R2	0.7976	0.7523	0.8625	0.8303
RER	5.6120	7.4911	8.6036	8.2226
RMSE	0.6804	0.0133	0.0086	2.3794
RPD	2.2229	2.0091	2.6965	2.4276
RPIQ	4.6058	2.1467	4.8377	1.6312
SEP	0.6893	0.0134	0.0087	2.4368

Pe-proc: 2 -> vizinhos: 5

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0356	0.0019	0.0009	0.2396
MSE	0.1441	0.0005	0.0001	6.8696
R2	0.9444	0.6872	0.8879	0.8454
RER	11.9998	7.4546	9.3530	7.6230
RMSE	0.3796	0.0214	0.0087	2.6210
RPD	4.2418	1.7879	2.9868	2.5434
RPIQ	8.5119	2.0545	5.6602	3.4176
SEP	0.3811	0.0215	0.0087	2.6321

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0483	0.0011	0.0010	0.4017
MSE	0.2265	0.0008	0.0001	12.2719
R2	0.9126	0.4413	0.8143	0.7238
RER	9.5769	5.5602	7.2551	5.7173
RMSE	0.4760	0.0286	0.0112	3.5031
RPD	3.3827	1.3378	2.3208	1.9029
RPIQ	6.7880	1.5373	4.3981	2.5570
SEP	0.4775	0.0288	0.0112	3.5094

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1228	-0.0027	0.0020	-0.0499
MSE	0.4396	0.0003	0.0001	8.1084
R2	0.8078	0.5661	0.8714	0.7570
RER	5.7944	5.6068	9.0566	6.8682
RMSE	0.6630	0.0176	0.0083	2.8475
RPD	2.2812	1.5181	2.7882	2.0285
RPIQ	4.7265	1.6221	5.0022	1.3630
SEP	0.6676	0.0179	0.0082	2.9174

Pe-proc: 2 -> vizinhos: 6

```
cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0584  0.0014  0.0011   0.1378
MSE      0.1519  0.0005  0.0001   7.7806
R2       0.9414  0.6430  0.8772   0.8249
RER     11.7675  6.9647  8.9517   7.1416
RMSE     0.3898  0.0228  0.0091   2.7894
RPD      4.1309  1.6737  2.8540   2.3899
RPIQ     8.2894  1.9233  5.4086   3.2113
SEP      0.3886  0.0230  0.0091   2.8095
-----
```

```
val
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0923  0.0022  0.0018   0.7324
MSE      0.2417  0.0008  0.0001  15.8408
R2       0.9067  0.4447  0.7908   0.6435
RER     9.3899  5.5903  6.8897   5.0859
RMSE     0.4917  0.0285  0.0119   3.9800
RPD      3.2746  1.3420  2.1864   1.6749
RPIQ     6.5711  1.5420  4.1435   2.2506
SEP      0.4870  0.0286  0.0118   3.9451
-----
```

```
pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.1053 -0.0028  0.0019   0.0329
MSE      0.3680  0.0004  0.0001   8.3026
R2       0.8391  0.5105  0.8765   0.7512
RER     6.3194  5.2794  9.2168   6.7868
RMSE     0.6066  0.0187  0.0081   2.8814
RPD      2.4932  1.4293  2.8456   2.0046
RPIQ     5.1659  1.5272  5.1051   1.3470
SEP      0.6122  0.0190  0.0081   2.9524
-----
```

Pe-proc: 3 -> vizinhos: 1

```
cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0      0.0    0.0     0.0
MSE      0.0      0.0    0.0     0.0
R2       1.0      1.0    1.0     1.0
RER      inf     inf    inf     inf
RMSE     0.0      0.0    0.0     0.0
RPD      inf     inf    inf     inf
RPIQ     inf     inf    inf     inf
SEP      0.0      0.0    0.0     0.0
```



```

-----
val
      betaglicosidase  cmcase  fpase  xilanase
BIAS      -0.0299  0.0046  0.0012   0.4606
MSE        0.5111  0.0014  0.0002  10.8308
R2         0.8028  0.0399  0.7396   0.7563
RER        6.3487  4.2700  6.1285   6.1057
RMSE       0.7149  0.0374  0.0132   3.2910
RPD        2.2521  1.0206  1.9596   2.0256
RPIQ       4.5193  1.1727  3.7137   2.7218
SEP        0.7203  0.0375  0.0133   3.2861
-----

```

```

pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.1195 -0.0068  0.0019  -0.0284
MSE        0.2324  0.0003  0.0001   4.1063
R2         0.8984  0.5566  0.8447   0.8769
RER        8.0845  5.9381  8.1898   9.6507
RMSE       0.4820  0.0178  0.0091   2.0264
RPD        3.1378  1.5017  2.5375   2.8505
RPIQ       6.5013  1.6045  4.5524   1.9153
SEP        0.4785  0.0169  0.0091   2.0762
-----

```

Pe-proc: 3 -> vizinhos: 2

```

cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0072  0.0021  0.0007   0.1920
MSE        0.1103  0.0003  0.0000   3.2067
R2         0.9575  0.7930  0.9447   0.9278
RER       13.6583  9.1923 13.3321  11.1752
RMSE       0.3321  0.0174  0.0061   1.7907
RPD        4.8482  2.1977  4.2536   3.7227
RPIQ       9.7289  2.5254  8.0609   5.0022
SEP        0.3348  0.0174  0.0061   1.7954
-----

```

```

val
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0228  0.0024  0.0002   0.1635
MSE        0.3325  0.0010  0.0001   7.8319
R2         0.8717  0.2975  0.8202   0.8238
RER        7.8705  4.9691  7.3456   7.1217
RMSE       0.5766  0.0320  0.0110   2.7985
RPD        2.7922  1.1931  2.3584   2.3820
RPIQ       5.6031  1.3710  4.4694   3.2008
SEP        0.5810  0.0322  0.0111   2.8173
-----

```

```

pred

```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1772	-0.0057	0.0019	-0.2233
MSE	0.4933	0.0002	0.0001	6.1031
R2	0.7844	0.7161	0.8399	0.8171
RER	5.5551	7.4763	8.0551	7.9478
RMSE	0.7023	0.0143	0.0092	2.4704
RPD	2.1535	1.8769	2.4990	2.3381
RPIQ	4.4620	2.0054	4.4834	1.5710
SEP	0.6964	0.0134	0.0093	2.5211

Pe-proc: 3 -> vizinhos: 3

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0086	0.0014	0.0003	0.0514
MSE	0.1474	0.0005	0.0001	3.4572
R2	0.9432	0.6717	0.9226	0.9222
RER	11.8158	7.2630	11.2074	10.7047
RMSE	0.3839	0.0219	0.0072	1.8594
RPD	4.1941	1.7454	3.5949	3.5852
RPIQ	8.4163	2.0056	6.8126	4.8176
SEP	0.3870	0.0220	0.0073	1.8743

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0056	0.0018	0.0007	0.3141
MSE	0.2951	0.0009	0.0001	9.9188
R2	0.8862	0.4121	0.8051	0.7768
RER	8.3486	5.4263	7.0658	6.3491
RMSE	0.5432	0.0293	0.0115	3.1494
RPD	2.9640	1.3042	2.2654	2.1167
RPIQ	5.9478	1.4987	4.2931	2.8442
SEP	0.5477	0.0295	0.0115	3.1602

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1624	-0.0023	0.0024	-0.0396
MSE	0.5211	0.0002	0.0001	8.0764
R2	0.7722	0.7109	0.8399	0.7579
RER	5.3678	6.8783	8.1598	6.8814
RMSE	0.7218	0.0144	0.0092	2.8419
RPD	2.0953	1.8600	2.4991	2.0325
RPIQ	4.3414	1.9874	4.4834	1.3657
SEP	0.7207	0.0146	0.0091	2.9118

Pe-proc: 3 -> vizinhos: 4

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0194	0.0018	0.0004	0.1189
MSE	0.1326	0.0004	0.0001	5.0279
R2	0.9489	0.7050	0.9064	0.8869
RER	12.4723	7.6746	10.1937	8.8856
RMSE	0.3641	0.0208	0.0079	2.2423
RPD	4.4220	1.8412	3.2688	2.9729
RPIQ	8.8736	2.1157	6.1947	3.9948
SEP	0.3666	0.0209	0.0080	2.2581

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0382	0.0015	0.0012	0.1546
MSE	0.2475	0.0007	0.0001	10.8026
R2	0.9045	0.4971	0.8106	0.7569
RER	9.1425	5.8651	7.1976	6.0602
RMSE	0.4975	0.0271	0.0113	3.2867
RPD	3.2364	1.4101	2.2981	2.0282
RPIQ	6.4945	1.6203	4.3550	2.7254
SEP	0.5002	0.0273	0.0113	3.3108

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1356	-0.0023	0.0021	0.2011
MSE	0.4607	0.0002	0.0001	9.3055
R2	0.7986	0.7118	0.8379	0.7211
RER	5.6766	6.8892	8.0376	6.4242
RMSE	0.6788	0.0144	0.0093	3.0505
RPD	2.2284	1.8626	2.4841	1.8935
RPIQ	4.6170	1.9901	4.4566	1.2723
SEP	0.6815	0.0145	0.0093	3.1190

Pe-proc: 3 -> vizinhos: 5

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0244	0.0011	0.0007	0.1807
MSE	0.1723	0.0005	0.0001	6.6088
R2	0.9335	0.6752	0.8807	0.8513
RER	10.9448	7.2956	9.0413	7.7586
RMSE	0.4150	0.0218	0.0090	2.5708
RPD	3.8792	1.7545	2.8951	2.5931
RPIQ	7.7843	2.0161	5.4865	3.4844
SEP	0.4178	0.0219	0.0090	2.5860

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0549	0.0005	0.0010	0.3173

MSE	0.2399	0.0008	0.0001	11.9046
R2	0.9075	0.4316	0.8112	0.7321
RER	9.3176	5.5093	7.1932	5.7911
RMSE	0.4898	0.0288	0.0113	3.4503
RPD	3.2873	1.3264	2.3015	1.9321
RPIQ	6.5967	1.5241	4.3616	2.5962
SEP	0.4908	0.0291	0.0113	3.4647

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.1255	-0.0031	0.0019	-0.0605
MSE	0.3892	0.0003	0.0001	7.6539
R2	0.8299	0.5363	0.8728	0.7706
RER	6.1782	5.4386	9.0755	7.0698
RMSE	0.6238	0.0182	0.0082	2.7666
RPD	2.4246	1.4685	2.8034	2.0879
RPIQ	5.0236	1.5691	5.0294	1.4029
SEP	0.6262	0.0184	0.0082	2.8342

Pe-proc: 3 -> vizinhos: 6

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0459	0.0003	0.0008	0.0363
MSE	0.1701	0.0005	0.0001	7.4242
R2	0.9344	0.6314	0.8720	0.8329
RER	11.0628	6.8405	8.7332	7.3028
RMSE	0.4125	0.0232	0.0093	2.7247
RPD	3.9034	1.6470	2.7949	2.4466
RPIQ	7.8329	1.8926	5.2965	3.2875
SEP	0.4134	0.0234	0.0093	2.7475

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0961	0.0021	0.0019	0.7171
MSE	0.2625	0.0008	0.0001	14.6722
R2	0.8987	0.4504	0.8017	0.6698
RER	9.0105	5.6176	7.0894	5.2878
RMSE	0.5124	0.0283	0.0116	3.8304
RPD	3.1424	1.3488	2.2456	1.7403
RPIQ	6.3057	1.5499	4.2555	2.3385
SEP	0.5075	0.0285	0.0115	3.7945

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0860	-0.0035	0.0016	0.0489
MSE	0.3540	0.0004	0.0001	8.1304
R2	0.8452	0.4803	0.8739	0.7563

RER	6.4124	5.1520	9.0428	6.8589
RMSE	0.5950	0.0193	0.0082	2.8514
RPD	2.5420	1.3872	2.8165	2.0258
RPIQ	5.2669	1.4822	5.0530	1.3611
SEP	0.6033	0.0194	0.0082	2.9214

Pe-proc: 4 -> vizinhos: 1

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0891	0.0025	0.0005	0.4774
MSE	0.3817	0.0013	0.0001	6.0952
R2	0.8528	0.1398	0.7882	0.8628
RER	7.4177	4.4892	6.7720	8.2140
RMSE	0.6178	0.0354	0.0119	2.4688
RPD	2.6061	1.0782	2.1726	2.7001
RPIQ	5.2297	1.2390	4.1173	3.6282
SEP	0.6165	0.0357	0.0120	2.4427

pred	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1114	-0.0072	0.0020	-0.0047
MSE	0.2319	0.0003	0.0001	4.1462
R2	0.8986	0.5638	0.8466	0.8757
RER	8.0590	6.0535	8.2516	9.6033
RMSE	0.4815	0.0177	0.0090	2.0362
RPD	3.1411	1.5140	2.5532	2.8367
RPIQ	6.5082	1.6177	4.5806	1.9060
SEP	0.4800	0.0165	0.0090	2.0865

Pe-proc: 4 -> vizinhos: 2

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0465	0.0009	0.0002	0.2412
MSE	0.0956	0.0003	0.0000	1.5284
R2	0.9631	0.7984	0.9473	0.9656

RER	14.8316	9.2611	13.5705	16.4088
RMSE	0.3093	0.0172	0.0060	1.2363
RPD	5.2061	2.2272	4.3552	5.3921
RPIQ	10.4471	2.5593	8.2534	7.2455
SEP	0.3083	0.0173	0.0060	1.2228

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0157	0.0008	0.0001	0.1981
MSE	0.2328	0.0007	0.0001	5.9638
R2	0.9102	0.5225	0.8728	0.8658
RER	9.4025	6.0129	8.7310	8.1742
RMSE	0.4825	0.0264	0.0093	2.4421
RPD	3.3366	1.4471	2.8037	2.7297
RPIQ	6.6954	1.6629	5.3133	3.6680
SEP	0.4863	0.0266	0.0093	2.4546

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1419	-0.0022	0.0023	0.0990
MSE	0.2635	0.0002	0.0001	6.3349
R2	0.8848	0.7733	0.8987	0.8101
RER	7.6523	7.7887	10.4336	7.7751
RMSE	0.5134	0.0127	0.0073	2.5169
RPD	2.9463	2.1002	3.1418	2.2949
RPIQ	6.1045	2.2441	5.6365	1.5420
SEP	0.5055	0.0129	0.0071	2.5771

Pe-proc: 4 -> vizinhos: 3

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0023	0.0004	0.0003	0.0384
MSE	0.0904	0.0003	0.0000	2.3041
R2	0.9651	0.7613	0.9441	0.9482
RER	15.0798	8.5022	13.1855	13.1119
RMSE	0.3007	0.0187	0.0061	1.5179
RPD	5.3539	2.0468	4.2284	4.3917
RPIQ	10.7436	2.3520	8.0131	5.9012
SEP	0.3032	0.0188	0.0062	1.5302

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0039	0.0001	0.0005	0.1377
MSE	0.2497	0.0007	0.0001	6.5949
R2	0.9037	0.5349	0.8497	0.8516
RER	9.0743	6.0895	8.0420	7.7587
RMSE	0.4997	0.0261	0.0101	2.5681

RPD	3.2217	1.4663	2.5796	2.5958
RPIQ	6.4650	1.6849	4.8886	3.4881
SEP	0.5039	0.0263	0.0101	2.5860

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1177	-0.0036	0.0015	0.0856
MSE	0.4194	0.0002	0.0001	7.0223
R2	0.8167	0.6695	0.8551	0.7895
RER	5.9287	6.5331	8.4012	7.3829
RMSE	0.6476	0.0154	0.0088	2.6500
RPD	2.3356	1.7393	2.6266	2.1797
RPIQ	4.8393	1.8584	4.7122	1.4646
SEP	0.6525	0.0153	0.0089	2.7140

Pe-proc: 4 -> vizinhos: 4

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0041	0.0004	0.0001	-0.0469
MSE	0.1144	0.0003	0.0000	3.1258
R2	0.9559	0.7655	0.9317	0.9297
RER	13.4082	8.5772	11.9174	11.2576
RMSE	0.3382	0.0185	0.0068	1.7680
RPD	4.7602	2.0649	3.8268	3.7705
RPIQ	9.5522	2.3727	7.2522	5.0665
SEP	0.3411	0.0187	0.0068	1.7823

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0196	0.0003	0.0009	0.1546
MSE	0.2422	0.0007	0.0001	7.7913
R2	0.9066	0.4956	0.8315	0.8247
RER	9.2219	5.8478	7.6112	7.1389
RMSE	0.4921	0.0271	0.0107	2.7913
RPD	3.2716	1.4080	2.4360	2.3882
RPIQ	6.5651	1.6179	4.6164	3.2091
SEP	0.4959	0.0274	0.0107	2.8105

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1030	-0.0051	0.0012	-0.0131
MSE	0.4603	0.0003	0.0001	8.3332
R2	0.7988	0.5939	0.8417	0.7502
RER	5.6298	6.0008	7.9933	6.7739
RMSE	0.6785	0.0171	0.0092	2.8867
RPD	2.2293	1.5693	2.5135	2.0010
RPIQ	4.6190	1.6768	4.5094	1.3445

SEP	0.6872	0.0167	0.0093	2.9580
-----	--------	--------	--------	--------

Pe-proc: 4 -> vizinhos: 5

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0222	0.0002	0.0006	0.0444
MSE	0.1538	0.0005	0.0001	4.4422
R2	0.9407	0.6889	0.8995	0.9000
RER	11.5824	7.4457	9.8494	9.4421
RMSE	0.3921	0.0213	0.0082	2.1076
RPD	4.1057	1.7927	3.1543	3.1629
RPIQ	8.2389	2.0600	5.9776	4.2500
SEP	0.3948	0.0215	0.0083	2.1250

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0206	0.0001	0.0006	0.4214
MSE	0.2606	0.0008	0.0001	9.0736
R2	0.8995	0.4286	0.8187	0.7958
RER	8.8898	5.4942	7.3258	6.6707
RMSE	0.5105	0.0289	0.0110	3.0122
RPD	3.1537	1.3229	2.3488	2.2130
RPIQ	6.3286	1.5202	4.4511	2.9737
SEP	0.5144	0.0291	0.0111	3.0078

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1019	-0.0032	0.0019	-0.0712
MSE	0.4187	0.0003	0.0001	6.3818
R2	0.8170	0.6249	0.8753	0.8087
RER	5.9083	6.0813	9.1804	7.7436
RMSE	0.6471	0.0164	0.0082	2.5262
RPD	2.3375	1.6327	2.8318	2.2865
RPIQ	4.8431	1.7445	5.0804	1.5363
SEP	0.6548	0.0165	0.0081	2.5876

Pe-proc: 4 -> vizinhos: 6

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0294	-0.0001	0.0006	0.1333
MSE	0.1771	0.0005	0.0001	5.2701
R2	0.9317	0.6473	0.8791	0.8814
RER	10.8006	6.9930	8.9756	8.6816
RMSE	0.4209	0.0227	0.0090	2.2957
RPD	3.8254	1.6838	2.8759	2.9038
RPIQ	7.6764	1.9349	5.4501	3.9019

SEP	0.4234	0.0229	0.0091	2.3111
-----	--------	--------	--------	--------

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0498	0.0011	0.0012	0.6569
MSE	0.2766	0.0009	0.0001	14.0007
R2	0.8933	0.4095	0.7996	0.6849
RER	8.6604	5.4079	6.9939	5.4013
RMSE	0.5260	0.0294	0.0116	3.7418
RPD	3.0610	1.3013	2.2340	1.7816
RPIQ	6.1425	1.4954	4.2335	2.3939
SEP	0.5280	0.0296	0.0116	3.7147

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0929	-0.0026	0.0018	-0.0041
MSE	0.3800	0.0003	0.0001	6.2420
R2	0.8339	0.5895	0.8906	0.8129
RER	6.1953	5.7655	9.8087	7.8267
RMSE	0.6164	0.0171	0.0076	2.4984
RPD	2.4537	1.5607	3.0233	2.3120
RPIQ	5.0838	1.6676	5.4240	1.5534
SEP	0.6244	0.0174	0.0076	2.5601

Pe-proc: 5 -> vizinhos: 1

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0907	0.0041	0.0008	0.5901
MSE	0.1669	0.0009	0.0001	9.7508
R2	0.9356	0.4066	0.8887	0.7806
RER	11.3830	5.4446	9.3783	6.4886
RMSE	0.4086	0.0294	0.0087	3.1226
RPD	3.9407	1.2981	2.9973	2.1348
RPIQ	7.9078	1.4916	5.6800	2.8686
SEP	0.4017	0.0294	0.0087	3.0922

```

pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.1049 -0.0050  0.0011   0.0331
MSE      0.2318  0.0002  0.0001   4.0488
R2      0.8987  0.7491  0.8659   0.8787
RER      8.0341  7.8678  8.6846   9.7194
RMSE     0.4815  0.0134  0.0085   2.0122
RPD      3.1413  1.9965  2.7305   2.8707
RPIQ     6.5086  2.1332  4.8987   1.9288
SEP      0.4815  0.0127  0.0086   2.0616
-----

```

Pe-proc: 5 -> vizinhos: 2

```

cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS     -0.0444  0.0013  0.0003   0.2720
MSE      0.0406  0.0002  0.0000   2.2369
R2      0.9843  0.8709  0.9744   0.9497
RER     23.0593 11.6069 19.5024  13.5286
RMSE     0.2016  0.0137  0.0042   1.4956
RPD      7.9862  2.7827  6.2450   4.4571
RPIQ    16.0258  3.1976 11.8347   5.9891
SEP      0.1983  0.0138  0.0042   1.4831
-----

```

```

val
      betaglicosidase  cmcase  fpase  xilanase
BIAS     -0.0268  0.0004  0.0001   0.2777
MSE      0.2245  0.0007  0.0001   8.7387
R2      0.9134  0.5088  0.8632   0.8034
RER      9.5852  5.9264  8.4204   6.7604
RMSE     0.4738  0.0268  0.0096   2.9561
RPD      3.3977  1.4269  2.7039   2.2550
RPIQ     6.8182  1.6396  5.1240   3.0302
SEP      0.4771  0.0270  0.0097   2.9679
-----

```

```

pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.1037 -0.0052  0.0014  -0.0804
MSE      0.3025  0.0003  0.0001   6.2604
R2      0.8678  0.6184  0.8762   0.8124
RER      6.9894  6.2284  9.0987   7.8192
RMSE     0.5500  0.0165  0.0081   2.5021
RPD      2.7499  1.6188  2.8423   2.3086
RPIQ     5.6976  1.7297  5.0992   1.5512
SEP      0.5535  0.0161  0.0082   2.5626
-----

```

Pe-proc: 5 -> vizinhos: 3

cal				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0153	0.0007	0.0003	0.1680
MSE	0.0834	0.0003	0.0000	3.3258
R2	0.9678	0.7669	0.9476	0.9252
RER	15.7219	8.6080	13.6224	10.9566
RMSE	0.2888	0.0185	0.0059	1.8237
RPD	5.5742	2.0711	4.3685	3.6554
RPIQ	11.1857	2.3799	8.2786	4.9118
SEP	0.2909	0.0186	0.0060	1.8312

val				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0100	0.0011	0.0008	0.2003
MSE	0.1563	0.0006	0.0001	7.5614
R2	0.9397	0.5630	0.8696	0.8298
RER	11.4725	6.2884	8.6534	7.2548
RMSE	0.3954	0.0253	0.0094	2.7498
RPD	4.0720	1.5127	2.7694	2.4242
RPIQ	8.1712	1.7382	5.2481	3.2575
SEP	0.3986	0.0255	0.0094	2.7656

pred				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0967	-0.0022	0.0012	0.1098
MSE	0.2511	0.0002	0.0001	7.2852
R2	0.8902	0.7165	0.9040	0.7816
RER	7.6785	6.9397	10.3342	7.2507
RMSE	0.5011	0.0142	0.0072	2.6991
RPD	3.0184	1.8782	3.2282	2.1400
RPIQ	6.2539	2.0068	5.7915	1.4379
SEP	0.5038	0.0144	0.0072	2.7635

Pe-proc: 5 -> vizinhos: 4

cal				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0095	0.0001	0.0001	0.0502
MSE	0.1004	0.0004	0.0000	3.6553
R2	0.9613	0.7556	0.9279	0.9177
RER	14.3203	8.4008	11.5962	10.4102
RMSE	0.3168	0.0189	0.0070	1.9119
RPD	5.0821	2.0228	3.7235	3.4867
RPIQ	10.1983	2.3244	7.0563	4.6852
SEP	0.3193	0.0191	0.0070	1.9274

val				
	betaglicosidase	cmcase	fpase	xilanase

BIAS	0.0193	0.0011	0.0009	0.2668
MSE	0.2068	0.0008	0.0001	10.1966
R2	0.9202	0.4827	0.8325	0.7705
RER	9.9799	5.7791	7.6393	6.2527
RMSE	0.4548	0.0275	0.0106	3.1932
RPD	3.5401	1.3904	2.4436	2.0876
RPIQ	7.1040	1.5977	4.6308	2.8052
SEP	0.4582	0.0277	0.0107	3.2089

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0831	-0.0038	0.0011	0.0353
MSE	0.3971	0.0002	0.0001	9.2500
R2	0.8264	0.6679	0.8452	0.7228
RER	6.0438	6.5395	8.0682	6.4298
RMSE	0.6302	0.0154	0.0091	3.0414
RPD	2.4001	1.7352	2.5416	1.8992
RPIQ	4.9730	1.8541	4.5597	1.2761
SEP	0.6401	0.0153	0.0092	3.1163

Pe-proc: 5 -> vizinhos: 5

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0230	0.0007	0.0006	0.0437
MSE	0.1116	0.0004	0.0001	5.3344
R2	0.9570	0.7014	0.9062	0.8800
RER	13.6090	7.6048	10.1975	8.6161
RMSE	0.3340	0.0209	0.0079	2.3096
RPD	4.8204	1.8301	3.2649	2.8863
RPIQ	9.6731	2.1029	6.1872	3.8784
SEP	0.3360	0.0210	0.0080	2.3287

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0494	0.0015	0.0012	0.5617
MSE	0.2097	0.0008	0.0001	10.5386
R2	0.9191	0.4621	0.8257	0.7628
RER	9.9617	5.6713	7.5014	6.2227
RMSE	0.4579	0.0280	0.0108	3.2463
RPD	3.5163	1.3635	2.3949	2.0535
RPIQ	7.0560	1.5668	4.5386	2.7593
SEP	0.4590	0.0282	0.0109	3.2243

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0867	-0.0024	0.0019	0.1805
MSE	0.4574	0.0003	0.0001	7.8818

R2	0.8001	0.6146	0.8555	0.7638
RER	5.6290	5.9432	8.4913	6.9796
RMSE	0.6763	0.0166	0.0088	2.8074
RPD	2.2365	1.6108	2.6310	2.0575
RPIQ	4.6339	1.7211	4.7202	1.3824
SEP	0.6873	0.0168	0.0088	2.8708

Pe-proc: 5 -> vizinhos: 6

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0353	0.0007	0.0007	0.1908
MSE	0.1535	0.0005	0.0001	6.2155
R2	0.9408	0.6503	0.8819	0.8601
RER	11.6198	7.0268	9.0918	8.0041
RMSE	0.3918	0.0226	0.0089	2.4931
RPD	4.1088	1.6911	2.9098	2.6739
RPIQ	8.2451	1.9432	5.5143	3.5929
SEP	0.3935	0.0228	0.0090	2.5068

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0422	0.0009	0.0012	0.7451
MSE	0.2753	0.0008	0.0001	13.5583
R2	0.8938	0.4218	0.8059	0.6949
RER	8.6702	5.4646	7.1089	5.5176
RMSE	0.5247	0.0291	0.0114	3.6822
RPD	3.0684	1.3152	2.2695	1.8104
RPIQ	6.1573	1.5112	4.3010	2.4327
SEP	0.5274	0.0293	0.0115	3.6364

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0831	-0.0027	0.0015	-0.0308
MSE	0.4104	0.0003	0.0001	6.4009
R2	0.8206	0.5545	0.8728	0.8082
RER	5.9437	5.5347	8.9841	7.7295
RMSE	0.6406	0.0179	0.0082	2.5300
RPD	2.3611	1.4982	2.8039	2.2831
RPIQ	4.8921	1.6008	5.0303	1.5340
SEP	0.6509	0.0181	0.0083	2.5923

Pe-proc: 6 -> vizinhos: 1

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0

R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0005	0.0076	0.0019	0.6161
MSE	0.4496	0.0012	0.0002	27.4000
R2	0.8266	0.1561	0.7239	0.3834
RER	6.7632	4.6307	5.9817	3.8276
RMSE	0.6705	0.0351	0.0136	5.2345
RPD	2.4013	1.0886	1.9031	1.2735
RPIQ	4.8186	1.2509	3.6066	1.7113
SEP	0.6761	0.0346	0.0136	5.2420

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2276	-0.0034	0.0037	0.3275
MSE	1.2413	0.0003	0.0002	6.4925
R2	0.4574	0.5206	0.6343	0.8054
RER	3.4616	5.3659	5.4078	7.7385
RMSE	1.1141	0.0185	0.0140	2.5480
RPD	1.3576	1.4443	1.6537	2.2669
RPIQ	2.8128	1.5432	2.9668	1.5232
SEP	1.1176	0.0187	0.0138	2.5893

Pe-proc: 6 -> vizinhos: 2

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0021	0.0030	0.0007	0.2005
MSE	0.1043	0.0003	0.0000	6.4654
R2	0.9597	0.7955	0.9307	0.8545
RER	14.0386	9.3227	11.8804	7.8493
RMSE	0.3230	0.0173	0.0068	2.5427
RPD	4.9843	2.2116	3.7977	2.6217
RPIQ	10.0019	2.5413	7.1970	3.5228
SEP	0.3257	0.0172	0.0069	2.5562

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0028	0.0046	0.0008	0.4458
MSE	0.3846	0.0011	0.0002	17.2070
R2	0.8516	0.2170	0.7229	0.6128
RER	7.3122	4.7381	5.9253	4.8244

RMSE	0.6202	0.0338	0.0137	4.1481
RPD	2.5961	1.1301	1.8999	1.6070
RPIQ	5.2097	1.2986	3.6004	2.1594
SEP	0.6254	0.0338	0.0138	4.1589

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2076	-0.0038	0.0029	0.0787
MSE	0.7237	0.0003	0.0001	7.4641
R2	0.6837	0.6147	0.7758	0.7763
RER	4.5764	6.0424	6.9109	7.1603
RMSE	0.8507	0.0166	0.0109	2.7321
RPD	1.7780	1.6110	2.1117	2.1142
RPIQ	3.6839	1.7213	3.7886	1.4206
SEP	0.8453	0.0166	0.0108	2.7984

Pe-proc: 6 -> vizinhos: 3

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0107	0.0030	0.0006	0.2352
MSE	0.1516	0.0005	0.0001	7.3820
R2	0.9415	0.6724	0.8944	0.8339
RER	11.6493	7.3270	9.6083	7.3505
RMSE	0.3894	0.0219	0.0084	2.7170
RPD	4.1345	1.7473	3.0773	2.4535
RPIQ	8.2967	2.0078	5.8318	3.2969
SEP	0.3925	0.0218	0.0085	2.7296

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0834	0.0043	0.0021	0.2343
MSE	0.2973	0.0010	0.0002	17.3294
R2	0.8853	0.3178	0.7586	0.6100
RER	8.4152	5.0747	6.4256	4.7871
RMSE	0.5453	0.0316	0.0127	4.1629
RPD	2.9526	1.2107	2.0352	1.6014
RPIQ	5.9250	1.3912	3.8569	2.1518
SEP	0.5434	0.0315	0.0127	4.1913

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1812	-0.0004	0.0028	0.1363
MSE	0.4965	0.0002	0.0001	9.2905
R2	0.7830	0.7626	0.8473	0.7215
RER	5.5442	7.4982	8.4993	6.4218
RMSE	0.7047	0.0130	0.0090	3.0480
RPD	2.1465	2.0526	2.5588	1.8951

RPIQ	4.4473	2.1931	4.5905	1.2733
SEP	0.6978	0.0134	0.0088	3.1202

Pe-proc: 6 -> vizinhos: 4

cal				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0427	0.0025	0.0011	0.0891
MSE	0.1651	0.0006	0.0001	9.6292
R2	0.9363	0.6167	0.8694	0.7833
RER	11.2215	6.7467	8.6774	6.4144
RMSE	0.4064	0.0237	0.0094	3.1031
RPD	3.9621	1.6152	2.7666	2.1482
RPIQ	7.9507	1.8561	5.2429	2.8867
SEP	0.4075	0.0237	0.0094	3.1280

val				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0850	0.0035	0.0023	0.3530
MSE	0.2787	0.0009	0.0002	17.4368
R2	0.8925	0.3744	0.7712	0.6076
RER	8.7028	5.2857	6.6293	4.7819
RMSE	0.5279	0.0302	0.0124	4.1757
RPD	3.0496	1.2643	2.0907	1.5964
RPIQ	6.1197	1.4528	3.9620	2.1451
SEP	0.5255	0.0303	0.0123	4.1959

pred				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1981	0.0011	0.0029	0.2475
MSE	0.4348	0.0002	0.0001	9.9593
R2	0.8099	0.6636	0.8298	0.7015
RER	6.0029	6.3102	8.0270	6.2154
RMSE	0.6594	0.0155	0.0095	3.1558
RPD	2.2939	1.7242	2.4237	1.8303
RPIQ	4.7527	1.8422	4.3482	1.2298
SEP	0.6445	0.0159	0.0093	3.2238

Pe-proc: 6 -> vizinhos: 5

cal				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0728	0.0028	0.0017	0.1113
MSE	0.1703	0.0006	0.0001	10.1883
R2	0.9343	0.6120	0.8635	0.7707
RER	11.1645	6.7145	8.5661	6.2371
RMSE	0.4126	0.0238	0.0096	3.1919
RPD	3.9017	1.6053	2.7063	2.0885

RPIQ	7.8295	1.8447	5.1287	2.8063
SEP	0.4096	0.0238	0.0095	3.2169

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0506	0.0006	0.0011	0.0498
MSE	0.2534	0.0008	0.0001	20.0564
R2	0.9022	0.4631	0.7784	0.5487
RER	9.0541	5.6690	6.6408	4.4430
RMSE	0.5034	0.0280	0.0122	4.4784
RPD	3.1984	1.3647	2.1242	1.4885
RPIQ	6.4181	1.5682	4.0256	2.0001
SEP	0.5051	0.0282	0.0123	4.5160

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1849	-0.0007	0.0028	0.0999
MSE	0.5816	0.0003	0.0001	10.7044
R2	0.7458	0.5519	0.7996	0.6792
RER	5.1025	5.4586	7.3182	5.9795
RMSE	0.7627	0.0179	0.0103	3.2718
RPD	1.9832	1.4939	2.2337	1.7655
RPIQ	4.1091	1.5962	4.0073	1.1863
SEP	0.7582	0.0183	0.0102	3.3510

Pe-proc: 6 -> vizinhos: 6

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0516	0.0010	0.0011	-0.1230
MSE	0.1903	0.0006	0.0001	12.6266
R2	0.9266	0.6081	0.8459	0.7159
RER	10.4695	6.6393	7.9793	5.6026
RMSE	0.4362	0.0239	0.0102	3.5534
RPD	3.6911	1.5974	2.5471	1.8760
RPIQ	7.4068	1.8356	4.8269	2.5208
SEP	0.4368	0.0241	0.0102	3.5812

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0943	0.0016	0.0017	0.1004
MSE	0.2931	0.0008	0.0002	25.0514
R2	0.8869	0.4411	0.7625	0.4363
RER	8.5056	5.5634	6.4464	3.9760
RMSE	0.5414	0.0286	0.0126	5.0051
RPD	2.9737	1.3376	2.0519	1.3319
RPIQ	5.9674	1.5370	3.8885	1.7897
SEP	0.5376	0.0288	0.0126	5.0464

```

-----
pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.1767 -0.0015  0.0025  -0.2386
MSE           0.6313  0.0004  0.0001   9.2822
R2            0.7240  0.4418  0.8038   0.7218
RER           4.8734  4.9006  7.3454   6.4380
RMSE          0.7946  0.0200  0.0102   3.0467
RPD           1.9036  1.3385  2.2576   1.8959
RPIQ          3.9441  1.4302  4.0502   1.2739
SEP           0.7938  0.0204  0.0102   3.1123
-----

```

Pe-proc: 7 -> vizinhos: 1

```

cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.0      0.0    0.0     0.0
MSE           0.0      0.0    0.0     0.0
R2            1.0      1.0    1.0     1.0
RER           inf      inf    inf     inf
RMSE          0.0      0.0    0.0     0.0
RPD           inf      inf    inf     inf
RPIQ          inf      inf    inf     inf
SEP           0.0      0.0    0.0     0.0
-----

```

```

val
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.0398  0.0090  0.0020   0.1858
MSE           0.4520  0.0013  0.0002  24.8868
R2            0.8256  0.1272  0.7415   0.4400
RER           6.7567  4.5921  6.1954   3.9911
RMSE          0.6723  0.0357  0.0132   4.9887
RPD           2.3948  1.0704  1.9670   1.3363
RPIQ          4.8055  1.2300  3.7275   1.7956
SEP           0.6768  0.0349  0.0132   5.0273
-----

```

```

pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.2020 -0.0048  0.0016   0.0569
MSE           1.4322  0.0006  0.0002   1.7281
R2            0.3739  0.2303  0.5603   0.9482
RER           3.2006  4.2525  4.7790  14.8890
RMSE          1.1968  0.0235  0.0153   1.3146
RPD           1.2638  1.1399  1.5081   4.3940
RPIQ          2.6186  1.2179  2.7057   2.9524
SEP           1.2087  0.0235  0.0156   1.3458
-----

```

Pe-proc: 7 -> vizinhos: 2

cal				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0083	0.0031	0.0006	0.0078
MSE	0.1000	0.0003	0.0000	5.9493
R2	0.9614	0.7963	0.9376	0.8661
RER	14.3456	9.3523	12.5149	8.1572
RMSE	0.3162	0.0172	0.0065	2.4391
RPD	5.0916	2.2159	4.0027	2.7330
RPIQ	10.2174	2.5463	7.5855	3.6724
SEP	0.3188	0.0171	0.0065	2.4597

val				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0158	0.0038	0.0005	0.0393
MSE	0.3209	0.0012	0.0002	19.8016
R2	0.8762	0.1702	0.7313	0.5544
RER	8.0075	4.5862	6.0111	4.4713
RMSE	0.5665	0.0348	0.0134	4.4499
RPD	2.8420	1.0978	1.9293	1.4981
RPIQ	5.7029	1.2614	3.6561	2.0130
SEP	0.5711	0.0349	0.0136	4.4873

pred				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1788	-0.0043	0.0027	-0.3850
MSE	0.7366	0.0002	0.0001	4.7290
R2	0.6780	0.7767	0.7944	0.8583
RER	4.4975	8.2171	7.2020	9.1363
RMSE	0.8583	0.0126	0.0105	2.1746
RPD	1.7623	2.1163	2.2055	2.6562
RPIQ	3.6514	2.2613	3.9567	1.7847
SEP	0.8602	0.0122	0.0104	2.1931

Pe-proc: 7 -> vizinhos: 3

cal				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0023	0.0021	0.0002	-0.1337
MSE	0.1265	0.0005	0.0001	8.3817
R2	0.9512	0.6460	0.8921	0.8114
RER	12.7513	7.0095	9.4833	6.8797
RMSE	0.3556	0.0227	0.0085	2.8951
RPD	4.5272	1.6806	3.0445	2.3026
RPIQ	9.0848	1.9312	5.7695	3.0940
SEP	0.3586	0.0228	0.0086	2.9164

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0480	0.0039	0.0013	0.1376
MSE	0.3654	0.0010	0.0002	18.6132
R2	0.8590	0.2981	0.7166	0.5811
RER	7.5257	4.9941	5.8776	4.6141
RMSE	0.6045	0.0320	0.0138	4.3143
RPD	2.6636	1.1936	1.8786	1.5451
RPIQ	5.3450	1.3715	3.5600	2.0762
SEP	0.6076	0.0320	0.0139	4.3485

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2071	-0.0022	0.0025	-0.2338
MSE	0.5169	0.0002	0.0001	5.0636
R2	0.7741	0.7649	0.8620	0.8482
RER	5.4839	7.6370	8.8786	8.7371
RMSE	0.7189	0.0130	0.0086	2.2502
RPD	2.1038	2.0623	2.6921	2.5669
RPIQ	4.3590	2.2036	4.8297	1.7248
SEP	0.7055	0.0131	0.0084	2.2933

Pe-proc: 7 -> vizinhos: 4

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0341	0.0031	0.0010	0.0795
MSE	0.1952	0.0006	0.0001	10.4431
R2	0.9247	0.6106	0.8469	0.7650
RER	10.2943	6.7137	7.9948	6.1587
RMSE	0.4418	0.0238	0.0102	3.2316
RPD	3.6441	1.6026	2.5555	2.0628
RPIQ	7.3126	1.8415	4.8430	2.7719
SEP	0.4442	0.0238	0.0102	3.2579

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0946	0.0029	0.0019	0.0377
MSE	0.3111	0.0009	0.0002	18.6755
R2	0.8800	0.3596	0.7609	0.5797
RER	8.2491	5.2138	6.4382	4.6042
RMSE	0.5578	0.0306	0.0127	4.3215
RPD	2.8864	1.2496	2.0452	1.5426
RPIQ	5.7921	1.4359	3.8759	2.0728
SEP	0.5544	0.0307	0.0127	4.3578

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2150	0.0004	0.0029	-0.0861

MSE	0.4747	0.0002	0.0001	5.8143
R2	0.7925	0.7619	0.8557	0.8257
RER	5.7677	7.4860	8.7827	8.1146
RMSE	0.6890	0.0131	0.0088	2.4113
RPD	2.1953	2.0496	2.6325	2.3955
RPIQ	4.5485	2.1899	4.7229	1.6096
SEP	0.6707	0.0134	0.0085	2.4693

Pe-proc: 7 -> vizinhos: 5

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0530	0.0021	0.0012	-0.0867
MSE	0.1958	0.0006	0.0001	10.8083
R2	0.9245	0.6023	0.8535	0.7568
RER	10.3226	6.6115	8.1957	6.0540
RMSE	0.4425	0.0241	0.0099	3.2876
RPD	3.6387	1.5858	2.6128	2.0277
RPIQ	7.3017	1.8222	4.9515	2.7246
SEP	0.4430	0.0242	0.0099	3.3142

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0667	0.0012	0.0012	-0.0494
MSE	0.2723	0.0009	0.0001	19.2200
R2	0.8950	0.4081	0.7855	0.5675
RER	8.7619	5.4027	6.7583	4.5386
RMSE	0.5218	0.0294	0.0120	4.3841
RPD	3.0854	1.2998	2.1592	1.5206
RPIQ	6.1913	1.4935	4.0919	2.0432
SEP	0.5219	0.0296	0.0121	4.4208

pred	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2241	-0.0001	0.0032	-0.1904
MSE	0.5863	0.0003	0.0001	7.9643
R2	0.7437	0.6057	0.8260	0.7613
RER	5.1563	5.8149	8.0151	6.9448
RMSE	0.7657	0.0168	0.0096	2.8221
RPD	1.9753	1.5926	2.3975	2.0468
RPIQ	4.0926	1.7017	4.3013	1.3753
SEP	0.7503	0.0172	0.0093	2.8852

Pe-proc: 7 -> vizinhos: 6

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0677	0.0008	0.0010	-0.1947

MSE	0.1872	0.0006	0.0001	12.3779
R2	0.9278	0.6114	0.8551	0.7215
RER	10.6123	6.6665	8.2233	5.6639
RMSE	0.4326	0.0238	0.0099	3.5182
RPD	3.7214	1.6042	2.6274	1.8948
RPIQ	7.4678	1.8434	4.9792	2.5460
SEP	0.4309	0.0240	0.0099	3.5425

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.1000	0.0016	0.0017	-0.0196
MSE	0.2949	0.0008	0.0002	24.6630
R2	0.8862	0.4305	0.7746	0.4450
RER	8.4959	5.5116	6.6245	4.0064
RMSE	0.5430	0.0288	0.0123	4.9662
RPD	2.9648	1.3252	2.1061	1.3423
RPIQ	5.9495	1.5227	3.9912	1.8037
SEP	0.5382	0.0290	0.0123	5.0081

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.1834	-0.0017	0.0024	-0.4320
MSE	0.5460	0.0004	0.0001	12.0481
R2	0.7614	0.4597	0.8322	0.6389
RER	5.2746	4.9866	7.9554	5.6777
RMSE	0.7389	0.0197	0.0095	3.4710
RPD	2.0470	1.3605	2.4412	1.6641
RPIQ	4.2413	1.4537	4.3797	1.1181
SEP	0.7334	0.0201	0.0094	3.5291

Pe-proc: 8 -> vizinhos: 1

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.0050	0.0003	-0.0006	-0.1393
MSE	0.0533	0.0001	0.0000	0.9427
R2	0.9794	0.9175	0.9609	0.9788

RER	19.6504	14.4611	15.8526	20.7061
RMSE	0.2308	0.0110	0.0051	0.9709
RPD	6.9751	3.4808	5.0571	6.8658
RPIQ	13.9970	3.9998	9.5835	9.2257
SEP	0.2327	0.0111	0.0051	0.9690

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0738	-0.0052	-0.0000	-0.0211
MSE	0.0446	0.0007	0.0001	2.3190
R2	0.9805	0.0782	0.8832	0.9305
RER	19.0755	3.8824	9.2230	12.8421
RMSE	0.2112	0.0257	0.0079	1.5228
RPD	7.1602	1.0415	2.9255	3.7931
RPIQ	14.8355	1.1129	5.2485	2.5487
SEP	0.2028	0.0258	0.0081	1.5603

Pe-proc: 8 -> vizinhos: 2

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0127	-0.0002	-0.0001	-0.0484
MSE	0.0094	0.0000	0.0000	0.2053
R2	0.9964	0.9840	0.9937	0.9954
RER	47.1484	32.8715	39.4519	44.1648
RMSE	0.0970	0.0048	0.0021	0.4531
RPD	16.5952	7.9055	12.6415	14.7125
RPIQ	33.3015	9.0841	23.9566	19.7696
SEP	0.0970	0.0049	0.0021	0.4543

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0290	0.0018	-0.0000	0.0886
MSE	0.1341	0.0002	0.0000	1.2463
R2	0.9483	0.8307	0.9478	0.9720
RER	12.4211	10.1588	13.6276	17.8787
RMSE	0.3662	0.0157	0.0059	1.1164
RPD	4.3962	2.4301	4.3763	5.9713
RPIQ	8.8218	2.7924	8.2935	8.0238
SEP	0.3682	0.0158	0.0060	1.1222

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0012	-0.0040	-0.0002	-0.2257
MSE	0.0577	0.0002	0.0000	1.1859
R2	0.9748	0.7363	0.9211	0.9645
RER	15.7152	7.4340	11.2283	18.3550
RMSE	0.2402	0.0137	0.0065	1.0890

RPD	6.2958	1.9475	3.5600	5.3042
RPIQ	13.0446	2.0809	6.3868	3.5640
SEP	0.2462	0.0135	0.0066	1.0916

Pe-proc: 8 -> vizinhos: 3

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0102	0.0007	-0.0000	0.0189
MSE	0.0702	0.0001	0.0000	0.6123
R2	0.9729	0.9203	0.9685	0.9862
RER	17.1301	14.7457	17.5491	25.4343
RMSE	0.2649	0.0108	0.0046	0.7825
RPD	6.0775	3.5429	5.6356	8.5192
RPIQ	12.1956	4.0712	10.6799	11.4475
SEP	0.2670	0.0109	0.0046	0.7889

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0004	0.0014	0.0007	0.2108
MSE	0.2489	0.0004	0.0001	2.0489
R2	0.9040	0.7200	0.8978	0.9539
RER	9.0891	7.8674	9.7779	14.0531
RMSE	0.4989	0.0202	0.0083	1.4314
RPD	3.2271	1.8898	3.1279	4.6571
RPIQ	6.4757	2.1716	5.9276	6.2579
SEP	0.5031	0.0203	0.0083	1.4277

pred	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0680	-0.0063	-0.0008	-0.1099
MSE	0.1323	0.0003	0.0001	1.3465
R2	0.9422	0.6285	0.8748	0.9596
RER	10.5645	6.5016	8.9570	16.9275
RMSE	0.3638	0.0163	0.0082	1.1604
RPD	4.1577	1.6406	2.8259	4.9778
RPIQ	8.6146	1.7530	5.0698	3.3447
SEP	0.3662	0.0154	0.0083	1.1837

Pe-proc: 8 -> vizinhos: 4

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0103	0.0009	0.0002	0.1399
MSE	0.1367	0.0002	0.0000	1.1190
R2	0.9473	0.8538	0.9440	0.9748
RER	12.2714	10.8788	13.1740	18.9750
RMSE	0.3697	0.0146	0.0061	1.0578

RPD	4.3553	2.6151	4.2272	6.3017
RPIQ	8.7397	3.0050	8.0109	8.4677
SEP	0.3726	0.0147	0.0062	1.0574

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0151	0.0001	0.0005	0.0973
MSE	0.2504	0.0005	0.0001	1.6152
R2	0.9034	0.6775	0.8882	0.9637
RER	9.0654	7.3135	9.3302	15.7013
RMSE	0.5004	0.0217	0.0087	1.2709
RPD	3.2172	1.7610	2.9905	5.2452
RPIQ	6.4559	2.0236	5.6672	7.0481
SEP	0.5044	0.0219	0.0087	1.2779

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0609	-0.0066	-0.0009	-0.0417
MSE	0.1720	0.0003	0.0001	1.1582
R2	0.9248	0.6282	0.8887	0.9653
RER	9.2035	6.5507	9.5198	18.1833
RMSE	0.4147	0.0163	0.0077	1.0762
RPD	3.6472	1.6400	2.9979	5.3672
RPIQ	7.5568	1.7523	5.3784	3.6063
SEP	0.4203	0.0153	0.0078	1.1020

Pe-proc: 8 -> vizinhos: 5

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0123	0.0001	0.0002	0.0819
MSE	0.1693	0.0003	0.0000	0.9891
R2	0.9347	0.7987	0.9287	0.9777
RER	11.0254	9.2554	11.6679	20.0735
RMSE	0.4115	0.0171	0.0069	0.9945
RPD	3.9128	2.2286	3.7450	6.7028
RPIQ	7.8518	2.5608	7.0971	9.0066
SEP	0.4148	0.0173	0.0070	0.9995

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0451	-0.0013	0.0000	0.2775
MSE	0.2743	0.0006	0.0001	3.4424
R2	0.8942	0.6201	0.8687	0.9225
RER	8.6911	6.7483	8.5950	10.8455
RMSE	0.5237	0.0236	0.0094	1.8554
RPD	3.0743	1.6225	2.7602	3.5929
RPIQ	6.1691	1.8644	5.2307	4.8279

SEP	0.5262	0.0237	0.0095	1.8500
-----	--------	--------	--------	--------

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.1343	-0.0108	-0.0024	-0.3295
MSE	0.1874	0.0004	0.0001	1.4679
R2	0.9181	0.4034	0.8760	0.9560
RER	9.1731	5.5479	9.3821	16.7718
RMSE	0.4329	0.0207	0.0081	1.2116
RPD	3.4938	1.2947	2.8395	4.7675
RPIQ	7.2389	1.3834	5.0942	3.2034
SEP	0.4217	0.0180	0.0079	1.1947

Pe-proc: 8 -> vizinhos: 6

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0209	-0.0006	0.0003	0.0675
MSE	0.1777	0.0004	0.0001	1.7472
R2	0.9314	0.7457	0.9136	0.9607
RER	10.7697	8.2384	10.6018	15.0717
RMSE	0.4216	0.0193	0.0076	1.3218
RPD	3.8190	1.9829	3.4013	5.0432
RPIQ	7.6636	2.2785	6.4457	6.7766
SEP	0.4246	0.0194	0.0077	1.3312

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0568	-0.0025	-0.0004	0.1565
MSE	0.2374	0.0006	0.0001	5.6901
R2	0.9084	0.5767	0.8657	0.8720
RER	9.3705	6.4144	8.5056	8.3589
RMSE	0.4872	0.0249	0.0095	2.3854
RPD	3.3043	1.5370	2.7284	2.7946
RPIQ	6.6307	1.7661	5.1706	3.7552
SEP	0.4880	0.0250	0.0096	2.4003

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.1452	-0.0105	-0.0025	-0.3587
MSE	0.2360	0.0005	0.0001	2.0874
R2	0.8968	0.3139	0.8653	0.9374
RER	8.1439	5.0116	9.0026	13.9718
RMSE	0.4858	0.0222	0.0085	1.4448
RPD	3.1135	1.2073	2.7251	3.9979
RPIQ	6.4510	1.2899	4.8889	2.6863
SEP	0.4750	0.0200	0.0083	1.4341

Pe-proc: 9 -> vizinhos: 1

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0017	-0.0019	-0.0005	-0.2244
MSE	0.1344	0.0002	0.0001	3.3446
R2	0.9481	0.8636	0.8930	0.9247
RER	12.3677	11.3457	9.5337	10.9621
RMSE	0.3667	0.0141	0.0085	1.8288
RPD	4.3911	2.7073	3.0573	3.6451
RPIQ	8.8116	3.1109	5.7939	4.8980
SEP	0.3697	0.0141	0.0085	1.8303

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0680	-0.0025	0.0012	0.1893
MSE	0.0898	0.0003	0.0000	1.1488
R2	0.9607	0.6241	0.9348	0.9656
RER	12.9355	6.0256	12.6103	18.5355
RMSE	0.2997	0.0164	0.0059	1.0718
RPD	5.0472	1.6311	3.9169	5.3892
RPIQ	10.4576	1.7428	7.0272	3.6211
SEP	0.2991	0.0166	0.0059	1.0810

Pe-proc: 9 -> vizinhos: 2

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0010	-0.0009	-0.0002	-0.0992
MSE	0.0336	0.0000	0.0000	0.8431
R2	0.9870	0.9660	0.9732	0.9810
RER	24.7505	22.7198	19.0317	21.7958
RMSE	0.1832	0.0070	0.0042	0.9182
RPD	8.7875	5.4261	6.1051	7.2599
RPIQ	17.6338	6.2351	11.5696	9.7552
SEP	0.1848	0.0070	0.0043	0.9206

val				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0082	-0.0000	0.0002	0.0322
MSE	0.1175	0.0002	0.0000	1.4895
R2	0.9547	0.8837	0.9351	0.9665
RER	13.2328	12.1803	12.2273	16.3081
RMSE	0.3428	0.0130	0.0066	1.2205
RPD	4.6969	2.9329	3.9242	5.4621
RPIQ	9.4253	3.3702	7.4367	7.3395
SEP	0.3456	0.0131	0.0067	1.2303

pred				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1095	0.0005	0.0024	-0.0669
MSE	0.1290	0.0002	0.0000	1.0406
R2	0.9436	0.7540	0.9576	0.9688
RER	11.0369	7.3669	17.6403	19.2104
RMSE	0.3592	0.0133	0.0048	1.0201
RPD	4.2113	2.0160	4.8593	5.6624
RPIQ	8.7255	2.1541	8.7178	3.8047
SEP	0.3505	0.0136	0.0042	1.0430

Pe-proc: 9 -> vizinhos: 3

cal				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0003	-0.0005	0.0001	-0.0115
MSE	0.0504	0.0001	0.0000	0.5819
R2	0.9805	0.9516	0.9706	0.9869
RER	20.1943	18.8982	18.1831	26.0851
RMSE	0.2245	0.0084	0.0044	0.7628
RPD	7.1699	4.5434	5.8367	8.7388
RPIQ	14.3879	5.2208	11.0611	11.7425
SEP	0.2264	0.0085	0.0045	0.7692

val				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0267	0.0010	0.0002	0.1696
MSE	0.1693	0.0003	0.0001	1.8949
R2	0.9347	0.7939	0.9213	0.9574
RER	11.0429	9.1633	11.1020	14.5648
RMSE	0.4115	0.0173	0.0073	1.3765
RPD	3.9125	2.2030	3.5635	4.8427
RPIQ	7.8511	2.5314	6.7531	6.5073
SEP	0.4141	0.0175	0.0073	1.3776

pred				
	betaglicosidase	cmcase	fpase	xilanase

BIAS	0.1239	0.0005	0.0020	0.0353
MSE	0.1374	0.0001	0.0000	1.0980
R2	0.9400	0.8466	0.9514	0.9671
RER	10.8084	9.3317	15.5752	18.6717
RMSE	0.3706	0.0105	0.0051	1.0479
RPD	4.0809	2.5529	4.5351	5.5124
RPIQ	8.4555	2.7277	8.1361	3.7038
SEP	0.3579	0.0107	0.0048	1.0731

Pe-proc: 9 -> vizinhos: 4

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0087	0.0008	0.0002	0.0314
MSE	0.0763	0.0001	0.0000	0.7401
R2	0.9706	0.9110	0.9579	0.9833
RER	16.4286	13.9524	15.1856	23.1428
RMSE	0.2762	0.0114	0.0053	0.8603
RPD	5.8301	3.3520	4.8739	7.7488
RPIQ	11.6991	3.8517	9.2364	10.4122
SEP	0.2783	0.0115	0.0054	0.8670

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0339	-0.0009	-0.0001	-0.0762
MSE	0.2054	0.0004	0.0001	3.2827
R2	0.9208	0.7536	0.8924	0.9261
RER	10.0336	8.3767	9.4942	10.9911
RMSE	0.4532	0.0190	0.0085	1.8118
RPD	3.5524	2.0145	3.0485	3.6793
RPIQ	7.1286	2.3149	5.7772	4.9439
SEP	0.4558	0.0191	0.0086	1.8255

pred	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1291	-0.0002	0.0019	0.0765
MSE	0.1210	0.0001	0.0000	0.8725
R2	0.9471	0.8927	0.9513	0.9738
RER	11.6866	11.1495	15.3321	21.0044
RMSE	0.3479	0.0088	0.0051	0.9341
RPD	4.3478	3.0532	4.5313	6.1837
RPIQ	9.0085	3.2623	8.1294	4.1550
SEP	0.3310	0.0090	0.0049	0.9540

Pe-proc: 9 -> vizinhos: 5

cal	betaglicosidase	cmcase	fpase	xilanase
-----	-----------------	--------	-------	----------

BIAS	-0.0250	0.0001	0.0002	-0.0435
MSE	0.1262	0.0002	0.0000	2.0622
R2	0.9513	0.8440	0.9338	0.9536
RER	12.7947	10.5148	12.1101	13.8615
RMSE	0.3553	0.0151	0.0067	1.4360
RPD	4.5315	2.5318	3.8866	4.6421
RPIQ	9.0933	2.9093	7.3654	6.2378
SEP	0.3574	0.0152	0.0067	1.4475

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0085	-0.0003	-0.0000	0.1289
MSE	0.2179	0.0004	0.0001	4.1902
R2	0.9160	0.6954	0.8853	0.9057
RER	9.7170	7.5259	9.1945	9.7391
RMSE	0.4667	0.0211	0.0088	2.0470
RPD	3.4494	1.8120	2.9527	3.2566
RPIQ	6.9219	2.0822	5.5955	4.3759
SEP	0.4706	0.0213	0.0089	2.0602

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1498	-0.0000	0.0022	0.0243
MSE	0.1106	0.0001	0.0000	1.3034
R2	0.9516	0.8586	0.9302	0.9609
RER	12.7121	9.7098	12.8233	17.1320
RMSE	0.3326	0.0101	0.0061	1.1417
RPD	4.5474	2.6594	3.7844	5.0595
RPIQ	9.4219	2.8415	6.7894	3.3996
SEP	0.3043	0.0103	0.0058	1.1696

Pe-proc: 9 -> vizinhos: 6

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0171	-0.0004	-0.0001	-0.1517
MSE	0.1442	0.0003	0.0001	2.5852
R2	0.9444	0.8129	0.9234	0.9418
RER	11.9539	9.6041	11.2528	12.4298
RMSE	0.3797	0.0165	0.0072	1.6079
RPD	4.2399	2.3118	3.6131	4.1460
RPIQ	8.5082	2.6565	6.8471	5.5711
SEP	0.3825	0.0167	0.0072	1.6142

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0063	-0.0003	0.0000	0.3042
MSE	0.2413	0.0005	0.0001	7.4142

R2	0.9069	0.6448	0.8689	0.8332
RER	9.2325	6.9692	8.6007	7.3530
RMSE	0.4912	0.0228	0.0094	2.7229
RPD	3.2777	1.6780	2.7620	2.4482
RPIQ	6.5773	1.9281	5.2342	3.2897
SEP	0.4953	0.0230	0.0095	2.7287

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.1165	-0.0008	0.0019	-0.0344
MSE	0.1119	0.0001	0.0000	2.2952
R2	0.9511	0.8358	0.9270	0.9312
RER	12.0384	9.0329	12.2580	12.9105
RMSE	0.3346	0.0108	0.0062	1.5150
RPD	4.5210	2.4675	3.7015	3.8127
RPIQ	9.3673	2.6365	6.6407	2.5618
SEP	0.3214	0.0111	0.0061	1.5520

Pe-proc: 10 -> vizinhos: 1

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.0904	0.0015	-0.0004	0.0339
MSE	0.2546	0.0010	0.0001	2.2943
R2	0.9018	0.3415	0.8529	0.9484
RER	9.1339	5.1238	8.1248	13.1389
RMSE	0.5046	0.0310	0.0100	1.5147
RPD	3.1905	1.2323	2.6072	4.4010
RPIQ	6.4024	1.4161	4.9408	5.9138
SEP	0.5007	0.0312	0.0100	1.5271

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0563	-0.0055	0.0008	-0.4424
MSE	0.3523	0.0005	0.0001	5.1492
R2	0.8460	0.2474	0.7614	0.8457
RER	6.3893	4.3336	6.4709	8.7859

RMSE	0.5936	0.0232	0.0113	2.2692
RPD	2.5482	1.1527	2.0474	2.5455
RPIQ	5.2797	1.2317	3.6732	1.7104
SEP	0.6055	0.0231	0.0115	2.2806

Pe-proc: 10 -> vizinhos: 2

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0432	-0.0003	-0.0006	-0.0177
MSE	0.0638	0.0003	0.0000	0.6074
R2	0.9754	0.8249	0.9621	0.9863
RER	18.2212	9.9270	16.0924	25.5359
RMSE	0.2526	0.0160	0.0051	0.7794
RPD	6.3741	2.3900	5.1361	8.5535
RPIQ	12.7908	2.7463	9.7333	11.4936
SEP	0.2510	0.0161	0.0051	0.7857

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0182	0.0014	0.0008	0.2169
MSE	0.2230	0.0007	0.0001	4.8418
R2	0.9140	0.5182	0.8776	0.8910
RER	9.6087	5.9921	8.9313	9.0863
RMSE	0.4723	0.0265	0.0091	2.2004
RPD	3.4090	1.4407	2.8581	3.0295
RPIQ	6.8408	1.6555	5.4163	4.0708
SEP	0.4759	0.0267	0.0091	2.2082

pred	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1003	-0.0024	0.0023	-0.1194
MSE	0.3019	0.0004	0.0001	6.8397
R2	0.8680	0.5077	0.8263	0.7950
RER	6.9888	5.2456	7.8001	7.4848
RMSE	0.5494	0.0188	0.0096	2.6153
RPD	2.7529	1.4253	2.3997	2.2086
RPIQ	5.7038	1.5229	4.3052	1.4840
SEP	0.5535	0.0191	0.0096	2.6771

Pe-proc: 10 -> vizinhos: 3

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0243	0.0019	0.0008	0.1738
MSE	0.0958	0.0003	0.0000	2.1861
R2	0.9630	0.8000	0.9508	0.9508
RER	14.6936	9.3454	14.1879	13.5506

RMSE	0.3096	0.0171	0.0058	1.4786
RPD	5.2009	2.2358	4.5082	4.5086
RPIQ	10.4365	2.5692	8.5434	6.0583
SEP	0.3112	0.0171	0.0057	1.4807

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0260	-0.0002	0.0006	0.3267
MSE	0.2608	0.0009	0.0001	6.4255
R2	0.8994	0.4004	0.8258	0.8554
RER	8.8903	5.3633	7.4728	7.9151
RMSE	0.5107	0.0296	0.0108	2.5348
RPD	3.1524	1.2914	2.3961	2.6298
RPIQ	6.3259	1.4839	4.5408	3.5338
SEP	0.5144	0.0298	0.0109	2.5349

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1369	-0.0043	0.0026	-0.0430
MSE	0.2716	0.0004	0.0001	7.6962
R2	0.8813	0.4835	0.8196	0.7693
RER	7.5079	5.2121	7.7001	7.0495
RMSE	0.5212	0.0192	0.0098	2.7742
RPD	2.9022	1.3914	2.3542	2.0821
RPIQ	6.0132	1.4867	4.2236	1.3990
SEP	0.5153	0.0192	0.0097	2.8424

Pe-proc: 10 -> vizinhos: 4

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0246	0.0006	0.0006	0.2346
MSE	0.1453	0.0005	0.0001	3.4823
R2	0.9439	0.6881	0.9081	0.9216
RER	11.9210	7.4388	10.2988	10.7472
RMSE	0.3812	0.0213	0.0079	1.8661
RPD	4.2237	1.7905	3.2988	3.5723
RPIQ	8.4757	2.0574	6.2514	4.8001
SEP	0.3836	0.0215	0.0079	1.8669

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0156	-0.0013	0.0006	0.2843
MSE	0.2742	0.0009	0.0001	7.2421
R2	0.8942	0.4034	0.8116	0.8370
RER	8.6641	5.3819	7.1836	7.4349
RMSE	0.5236	0.0295	0.0113	2.6911
RPD	3.0748	1.2947	2.3041	2.4771

RPIQ	6.1702	1.4877	4.3665	3.3286
SEP	0.5278	0.0297	0.0113	2.6986

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1630	-0.0037	0.0025	-0.0513
MSE	0.3664	0.0003	0.0001	9.6633
R2	0.8398	0.5241	0.8422	0.7104
RER	6.4764	5.4011	8.2620	6.2913
RMSE	0.6053	0.0185	0.0092	3.1086
RPD	2.4988	1.4495	2.5176	1.8581
RPIQ	5.1773	1.5488	4.5166	1.2485
SEP	0.5973	0.0185	0.0090	3.1849

Pe-proc: 10 -> vizinhos: 5

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0208	-0.0006	0.0004	0.1916
MSE	0.1791	0.0005	0.0001	4.9187
R2	0.9309	0.6251	0.8758	0.8893
RER	10.7267	6.7848	8.8418	9.0048
RMSE	0.4233	0.0234	0.0091	2.2178
RPD	3.8039	1.6331	2.8371	3.0058
RPIQ	7.6332	1.8766	5.3765	4.0389
SEP	0.4263	0.0236	0.0092	2.2282

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0398	0.0008	0.0012	0.5678
MSE	0.3049	0.0008	0.0001	8.9645
R2	0.8824	0.4337	0.7993	0.7983
RER	8.2335	5.5211	6.9862	6.7680
RMSE	0.5522	0.0288	0.0116	2.9941
RPD	2.9157	1.3289	2.2324	2.2265
RPIQ	5.8509	1.5270	4.2305	2.9917
SEP	0.5554	0.0290	0.0117	2.9646

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2084	-0.0017	0.0034	-0.0015
MSE	0.4908	0.0003	0.0001	6.9199
R2	0.7855	0.5366	0.8327	0.7926
RER	5.6446	5.3877	8.2548	7.4335
RMSE	0.7006	0.0182	0.0094	2.6306
RPD	2.1590	1.4691	2.4446	2.1958
RPIQ	4.4733	1.5697	4.3857	1.4754
SEP	0.6854	0.0186	0.0090	2.6955

Pe-proc: 10 -> vizinhos: 6

```
cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0258  0.0000  0.0006   0.1765
MSE      0.2003  0.0006  0.0001   5.4865
R2      0.9227  0.6224  0.8658   0.8765
RER     10.1495  6.7586  8.5203   8.5184
RMSE     0.4475  0.0235  0.0095   2.3423
RPD      3.5976  1.6274  2.7301   2.8460
RPIQ     7.2192  1.8700  5.1737   3.8242
SEP      0.4506  0.0237  0.0096   2.3554
-----
```

```
val
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0863  0.0009  0.0017   0.7170
MSE      0.3209  0.0008  0.0001  13.3653
R2      0.8762  0.4493  0.7926   0.6992
RER      8.0995  5.5990  6.9136   5.5501
RMSE     0.5665  0.0284  0.0118   3.6559
RPD      2.8422  1.3476  2.1958   1.8234
RPIQ     5.7033  1.5485  4.1612   2.4502
SEP      0.5646  0.0286  0.0118   3.6151
-----
```

```
pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.1746 -0.0020  0.0028   0.0198
MSE      0.4907  0.0005  0.0001   8.0562
R2      0.7855  0.3439  0.8106   0.7585
RER      5.5653  4.5278  7.5348   6.8895
RMSE     0.7005  0.0217  0.0100   2.8383
RPD      2.1593  1.2346  2.2977   2.0351
RPIQ     4.4739  1.3191  4.1223   1.3674
SEP      0.6951  0.0221  0.0099   2.9084
-----
```

Pe-proc: 11 -> vizinhos: 1

```
cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0      0.0      0.0      0.0
MSE      0.0      0.0      0.0      0.0
R2      1.0      1.0      1.0      1.0
RER      inf     inf     inf     inf
RMSE     0.0      0.0      0.0      0.0
RPD      inf     inf     inf     inf
RPIQ     inf     inf     inf     inf
SEP      0.0      0.0      0.0      0.0
```

```

-----
val
      betaglicosidase  cmcase  fpase  xilanase
BIAS      -0.0904  0.0015 -0.0004   0.0339
MSE        0.2546  0.0010  0.0001   2.2943
R2         0.9018  0.3415  0.8529   0.9484
RER        9.1339  5.1238  8.1248  13.1389
RMSE       0.5046  0.0310  0.0100   1.5147
RPD        3.1905  1.2323  2.6072   4.4010
RPIQ       6.4024  1.4161  4.9408   5.9138
SEP        0.5007  0.0312  0.0100   1.5271
-----

```

```

pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0563 -0.0055  0.0008  -0.4424
MSE       0.3523  0.0005  0.0001   5.1492
R2        0.8460  0.2474  0.7614   0.8457
RER       6.3893  4.3336  6.4709   8.7859
RMSE      0.5936  0.0232  0.0113   2.2692
RPD       2.5482  1.1527  2.0474   2.5455
RPIQ      5.2797  1.2317  3.6732   1.7104
SEP       0.6055  0.0231  0.0115   2.2806
-----

```

Pe-proc: 11 -> vizinhos: 2

```

cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS      -0.0432 -0.0003 -0.0006  -0.0177
MSE       0.0638  0.0003  0.0000   0.6074
R2        0.9754  0.8249  0.9621   0.9863
RER      18.2212  9.9270 16.0924  25.5359
RMSE      0.2526  0.0160  0.0051   0.7794
RPD       6.3741  2.3900  5.1361   8.5535
RPIQ     12.7908  2.7463  9.7333  11.4936
SEP       0.2510  0.0161  0.0051   0.7857
-----

```

```

val
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0182  0.0014  0.0008   0.2169
MSE       0.2230  0.0007  0.0001   4.8418
R2        0.9140  0.5182  0.8776   0.8910
RER       9.6087  5.9921  8.9313   9.0863
RMSE      0.4723  0.0265  0.0091   2.2004
RPD       3.4090  1.4407  2.8581   3.0295
RPIQ      6.8408  1.6555  5.4163   4.0708
SEP       0.4759  0.0267  0.0091   2.2082
-----

```

```

pred

```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1003	-0.0024	0.0023	-0.1194
MSE	0.3019	0.0004	0.0001	6.8397
R2	0.8680	0.5077	0.8263	0.7950
RER	6.9888	5.2456	7.8001	7.4848
RMSE	0.5494	0.0188	0.0096	2.6153
RPD	2.7529	1.4253	2.3997	2.2086
RPIQ	5.7038	1.5229	4.3052	1.4840
SEP	0.5535	0.0191	0.0096	2.6771

Pe-proc: 11 -> vizinhos: 3

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0243	0.0019	0.0008	0.1738
MSE	0.0958	0.0003	0.0000	2.1861
R2	0.9630	0.8000	0.9508	0.9508
RER	14.6936	9.3454	14.1879	13.5506
RMSE	0.3096	0.0171	0.0058	1.4786
RPD	5.2009	2.2358	4.5082	4.5086
RPIQ	10.4365	2.5692	8.5434	6.0583
SEP	0.3112	0.0171	0.0057	1.4807

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0260	-0.0002	0.0006	0.3267
MSE	0.2608	0.0009	0.0001	6.4255
R2	0.8994	0.4004	0.8258	0.8554
RER	8.8903	5.3633	7.4728	7.9151
RMSE	0.5107	0.0296	0.0108	2.5348
RPD	3.1524	1.2914	2.3961	2.6298
RPIQ	6.3259	1.4839	4.5408	3.5338
SEP	0.5144	0.0298	0.0109	2.5349

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1369	-0.0043	0.0026	-0.0430
MSE	0.2716	0.0004	0.0001	7.6962
R2	0.8813	0.4835	0.8196	0.7693
RER	7.5079	5.2121	7.7001	7.0495
RMSE	0.5212	0.0192	0.0098	2.7742
RPD	2.9022	1.3914	2.3542	2.0821
RPIQ	6.0132	1.4867	4.2236	1.3990
SEP	0.5153	0.0192	0.0097	2.8424

Pe-proc: 11 -> vizinhos: 4

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0246	0.0006	0.0006	0.2346
MSE	0.1453	0.0005	0.0001	3.4823
R2	0.9439	0.6881	0.9081	0.9216
RER	11.9210	7.4388	10.2988	10.7472
RMSE	0.3812	0.0213	0.0079	1.8661
RPD	4.2237	1.7905	3.2988	3.5723
RPIQ	8.4757	2.0574	6.2514	4.8001
SEP	0.3836	0.0215	0.0079	1.8669

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0156	-0.0013	0.0006	0.2843
MSE	0.2742	0.0009	0.0001	7.2421
R2	0.8942	0.4034	0.8116	0.8370
RER	8.6641	5.3819	7.1836	7.4349
RMSE	0.5236	0.0295	0.0113	2.6911
RPD	3.0748	1.2947	2.3041	2.4771
RPIQ	6.1702	1.4877	4.3665	3.3286
SEP	0.5278	0.0297	0.0113	2.6986

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1630	-0.0037	0.0025	-0.0513
MSE	0.3664	0.0003	0.0001	9.6633
R2	0.8398	0.5241	0.8422	0.7104
RER	6.4764	5.4011	8.2620	6.2913
RMSE	0.6053	0.0185	0.0092	3.1086
RPD	2.4988	1.4495	2.5176	1.8581
RPIQ	5.1773	1.5488	4.5166	1.2485
SEP	0.5973	0.0185	0.0090	3.1849

Pe-proc: 11 -> vizinhos: 5

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0208	-0.0006	0.0004	0.1916
MSE	0.1791	0.0005	0.0001	4.9187
R2	0.9309	0.6251	0.8758	0.8893
RER	10.7267	6.7848	8.8418	9.0048
RMSE	0.4233	0.0234	0.0091	2.2178
RPD	3.8039	1.6331	2.8371	3.0058
RPIQ	7.6332	1.8766	5.3765	4.0389
SEP	0.4263	0.0236	0.0092	2.2282

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0398	0.0008	0.0012	0.5678

MSE	0.3049	0.0008	0.0001	8.9645
R2	0.8824	0.4337	0.7993	0.7983
RER	8.2335	5.5211	6.9862	6.7680
RMSE	0.5522	0.0288	0.0116	2.9941
RPD	2.9157	1.3289	2.2324	2.2265
RPIQ	5.8509	1.5270	4.2305	2.9917
SEP	0.5554	0.0290	0.0117	2.9646

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2084	-0.0017	0.0034	-0.0015
MSE	0.4908	0.0003	0.0001	6.9199
R2	0.7855	0.5366	0.8327	0.7926
RER	5.6446	5.3877	8.2548	7.4335
RMSE	0.7006	0.0182	0.0094	2.6306
RPD	2.1590	1.4691	2.4446	2.1958
RPIQ	4.4733	1.5697	4.3857	1.4754
SEP	0.6854	0.0186	0.0090	2.6955

Pe-proc: 11 -> vizinhos: 6

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0258	0.0000	0.0006	0.1765
MSE	0.2003	0.0006	0.0001	5.4865
R2	0.9227	0.6224	0.8658	0.8765
RER	10.1495	6.7586	8.5203	8.5184
RMSE	0.4475	0.0235	0.0095	2.3423
RPD	3.5976	1.6274	2.7301	2.8460
RPIQ	7.2192	1.8700	5.1737	3.8242
SEP	0.4506	0.0237	0.0096	2.3554

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0863	0.0009	0.0017	0.7170
MSE	0.3209	0.0008	0.0001	13.3653
R2	0.8762	0.4493	0.7926	0.6992
RER	8.0995	5.5990	6.9136	5.5501
RMSE	0.5665	0.0284	0.0118	3.6559
RPD	2.8422	1.3476	2.1958	1.8234
RPIQ	5.7033	1.5485	4.1612	2.4502
SEP	0.5646	0.0286	0.0118	3.6151

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1746	-0.0020	0.0028	0.0198
MSE	0.4907	0.0005	0.0001	8.0562
R2	0.7855	0.3439	0.8106	0.7585

RER	5.5653	4.5278	7.5348	6.8895
RMSE	0.7005	0.0217	0.0100	2.8383
RPD	2.1593	1.2346	2.2977	2.0351
RPIQ	4.4739	1.3191	4.1223	1.3674
SEP	0.6951	0.0221	0.0099	2.9084

```
In [150]: #Executa o modelo KNN variando os pre-proc mais efetivos
for pre in [1,8,9]:
    for viz in range(1,4):
        result = executaKNN(pre,viz,0)
        print('Pe-proc:',pre, '-> vizinhos:', viz,'\n')
        resultados=exibeResultados(result)
        for k,v in zip(resultados.keys(),resultados.values()):
            print(k)
            print(v,'\n-----')
```

Pe-proc: 1 -> vizinhos: 1

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0094	0.0000	0.0002	0.1790
MSE	0.0098	0.0001	0.0001	3.9853
R2	0.9962	0.9485	0.9095	0.9103
RER	46.1256	18.2918	10.3551	10.0068
RMSE	0.0988	0.0087	0.0078	1.9963
RPD	16.3031	4.4045	3.3238	3.3393
RPIQ	32.7153	5.0612	6.2989	4.4870
SEP	0.0991	0.0088	0.0079	2.0051

pred	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2184	0.0020	0.0017	0.5338
MSE	0.2957	0.0001	0.0000	3.2066
R2	0.8707	0.8466	0.9164	0.9039
RER	7.5809	9.4999	11.2614	11.4400

RMSE	0.5438	0.0105	0.0067	1.7907
RPD	2.7814	2.5533	3.4589	3.2257
RPIQ	5.7629	2.7282	6.2055	2.1674
SEP	0.5103	0.0105	0.0066	1.7515

Pe-proc: 1 -> vizinhos: 2

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0047	0.0000	0.0001	0.0895
MSE	0.0024	0.0000	0.0000	0.9963
R2	0.9991	0.9871	0.9774	0.9776
RER	92.2512	36.5837	20.7102	20.0136
RMSE	0.0494	0.0043	0.0039	0.9982
RPD	32.6062	8.8090	6.6477	6.6785
RPIQ	65.4306	10.1224	12.5978	8.9741
SEP	0.0496	0.0044	0.0039	1.0025

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0077	0.0001	0.0006	0.4719
MSE	0.0884	0.0002	0.0000	4.5714
R2	0.9659	0.8450	0.9332	0.8971
RER	15.2592	10.5496	12.0868	9.5409
RMSE	0.2973	0.0150	0.0067	2.1381
RPD	5.4159	2.5402	3.8680	3.1178
RPIQ	10.8681	2.9189	7.3302	4.1895
SEP	0.2997	0.0152	0.0067	2.1030

pred	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1428	-0.0012	0.0002	0.1324
MSE	0.1908	0.0002	0.0000	1.9708
R2	0.9166	0.7220	0.9312	0.9409
RER	9.1463	6.9485	12.0272	13.9914
RMSE	0.4368	0.0141	0.0061	1.4039
RPD	3.4630	1.8967	3.8130	4.1145
RPIQ	7.1752	2.0266	6.8406	2.7646
SEP	0.4230	0.0144	0.0062	1.4321

Pe-proc: 1 -> vizinhos: 3

cal	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0028	0.0002	0.0002	0.1907
MSE	0.0223	0.0001	0.0000	1.6381
R2	0.9914	0.9456	0.9752	0.9631
RER	30.3695	17.8150	19.7827	15.7208

RMSE	0.1493	0.0089	0.0041	1.2799
RPD	10.7807	4.2885	6.3482	5.2084
RPIQ	21.6336	4.9279	12.0303	6.9987
SEP	0.1506	0.0090	0.0041	1.2763

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0071	-0.0010	0.0006	0.2188
MSE	0.1342	0.0003	0.0001	3.1771
R2	0.9482	0.7769	0.9058	0.9285
RER	12.3805	8.8071	10.1678	11.2474
RMSE	0.3663	0.0181	0.0080	1.7824
RPD	4.3948	2.1172	3.2574	3.7399
RPIQ	8.8191	2.4329	6.1731	5.0254
SEP	0.3694	0.0182	0.0080	1.7839

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1670	-0.0011	0.0013	0.2684
MSE	0.1536	0.0001	0.0000	2.9331
R2	0.9328	0.8599	0.9436	0.9121
RER	10.6472	9.8124	13.6673	11.5606
RMSE	0.3919	0.0100	0.0055	1.7126
RPD	3.8590	2.6719	4.2108	3.3727
RPIQ	7.9955	2.8549	7.5543	2.2662
SEP	0.3633	0.0102	0.0055	1.7332

Pe-proc: 8 -> vizinhos: 1

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0050	0.0003	-0.0006	-0.1393
MSE	0.0533	0.0001	0.0000	0.9427
R2	0.9794	0.9175	0.9609	0.9788
RER	19.6504	14.4611	15.8526	20.7061
RMSE	0.2308	0.0110	0.0051	0.9709
RPD	6.9751	3.4808	5.0571	6.8658

RPIQ	13.9970	3.9998	9.5835	9.2257
SEP	0.2327	0.0111	0.0051	0.9690

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0738	-0.0052	-0.0000	-0.0211
MSE	0.0446	0.0007	0.0001	2.3190
R2	0.9805	0.0782	0.8832	0.9305
RER	19.0755	3.8824	9.2230	12.8421
RMSE	0.2112	0.0257	0.0079	1.5228
RPD	7.1602	1.0415	2.9255	3.7931
RPIQ	14.8355	1.1129	5.2485	2.5487
SEP	0.2028	0.0258	0.0081	1.5603

Pe-proc: 8 -> vizinhos: 2

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0127	-0.0002	-0.0001	-0.0484
MSE	0.0094	0.0000	0.0000	0.2053
R2	0.9964	0.9840	0.9937	0.9954
RER	47.1484	32.8715	39.4519	44.1648
RMSE	0.0970	0.0048	0.0021	0.4531
RPD	16.5952	7.9055	12.6415	14.7125
RPIQ	33.3015	9.0841	23.9566	19.7696
SEP	0.0970	0.0049	0.0021	0.4543

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0290	0.0018	-0.0000	0.0886
MSE	0.1341	0.0002	0.0000	1.2463
R2	0.9483	0.8307	0.9478	0.9720
RER	12.4211	10.1588	13.6276	17.8787
RMSE	0.3662	0.0157	0.0059	1.1164
RPD	4.3962	2.4301	4.3763	5.9713
RPIQ	8.8218	2.7924	8.2935	8.0238
SEP	0.3682	0.0158	0.0060	1.1222

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0012	-0.0040	-0.0002	-0.2257
MSE	0.0577	0.0002	0.0000	1.1859
R2	0.9748	0.7363	0.9211	0.9645
RER	15.7152	7.4340	11.2283	18.3550
RMSE	0.2402	0.0137	0.0065	1.0890
RPD	6.2958	1.9475	3.5600	5.3042
RPIQ	13.0446	2.0809	6.3868	3.5640
SEP	0.2462	0.0135	0.0066	1.0916

Pe-proc: 8 -> vizinhos: 3

```
cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS      -0.0102    0.0007  -0.0000    0.0189
MSE        0.0702    0.0001  0.0000    0.6123
R2         0.9729    0.9203  0.9685    0.9862
RER       17.1301   14.7457  17.5491   25.4343
RMSE       0.2649    0.0108  0.0046    0.7825
RPD        6.0775    3.5429  5.6356    8.5192
RPIQ      12.1956    4.0712  10.6799   11.4475
SEP        0.2670    0.0109  0.0046    0.7889
-----
```

```
val
      betaglicosidase  cmcase  fpase  xilanase
BIAS      -0.0004    0.0014  0.0007    0.2108
MSE        0.2489    0.0004  0.0001    2.0489
R2         0.9040    0.7200  0.8978    0.9539
RER       9.0891    7.8674  9.7779   14.0531
RMSE       0.4989    0.0202  0.0083    1.4314
RPD        3.2271    1.8898  3.1279    4.6571
RPIQ       6.4757    2.1716  5.9276    6.2579
SEP        0.5031    0.0203  0.0083    1.4277
-----
```

```
pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      -0.0680  -0.0063  -0.0008   -0.1099
MSE        0.1323    0.0003  0.0001    1.3465
R2         0.9422    0.6285  0.8748    0.9596
RER      10.5645    6.5016  8.9570   16.9275
RMSE       0.3638    0.0163  0.0082    1.1604
RPD        4.1577    1.6406  2.8259    4.9778
RPIQ       8.6146    1.7530  5.0698    3.3447
SEP        0.3662    0.0154  0.0083    1.1837
-----
```

Pe-proc: 9 -> vizinhos: 1

```
cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS           0.0       0.0    0.0       0.0
MSE           0.0       0.0    0.0       0.0
R2            1.0       1.0    1.0       1.0
RER           inf       inf    inf       inf
RMSE          0.0       0.0    0.0       0.0
RPD           inf       inf    inf       inf
RPIQ          inf       inf    inf       inf
SEP           0.0       0.0    0.0       0.0
```

```
-----
val
      betaglicosidase  cmcase  fpase  xilanase
BIAS      -0.0017  -0.0019  -0.0005  -0.2244
MSE        0.1344   0.0002   0.0001   3.3446
R2         0.9481   0.8636   0.8930   0.9247
RER        12.3677  11.3457   9.5337  10.9621
RMSE       0.3667   0.0141   0.0085   1.8288
RPD        4.3911   2.7073   3.0573   3.6451
RPIQ       8.8116   3.1109   5.7939   4.8980
SEP        0.3697   0.0141   0.0085   1.8303
-----
```

```
pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0680 -0.0025   0.0012   0.1893
MSE       0.0898  0.0003   0.0000   1.1488
R2        0.9607  0.6241   0.9348   0.9656
RER       12.9355  6.0256  12.6103  18.5355
RMSE      0.2997  0.0164   0.0059   1.0718
RPD       5.0472  1.6311   3.9169   5.3892
RPIQ     10.4576  1.7428   7.0272   3.6211
SEP       0.2991  0.0166   0.0059   1.0810
-----
```

Pe-proc: 9 -> vizinhos: 2

```
cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS      -0.0010  -0.0009  -0.0002  -0.0992
MSE       0.0336   0.0000   0.0000   0.8431
R2        0.9870   0.9660   0.9732   0.9810
RER       24.7505  22.7198  19.0317  21.7958
RMSE      0.1832   0.0070   0.0042   0.9182
RPD       8.7875   5.4261   6.1051   7.2599
RPIQ     17.6338   6.2351  11.5696   9.7552
SEP       0.1848   0.0070   0.0043   0.9206
-----
```

```
val
      betaglicosidase  cmcase  fpase  xilanase
BIAS      -0.0082  -0.0000   0.0002   0.0322
MSE       0.1175   0.0002   0.0000   1.4895
R2        0.9547   0.8837   0.9351   0.9665
RER       13.2328  12.1803  12.2273  16.3081
RMSE      0.3428   0.0130   0.0066   1.2205
RPD       4.6969   2.9329   3.9242   5.4621
RPIQ      9.4253   3.3702   7.4367   7.3395
SEP       0.3456   0.0131   0.0067   1.2303
-----
```

```
pred
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1095	0.0005	0.0024	-0.0669
MSE	0.1290	0.0002	0.0000	1.0406
R2	0.9436	0.7540	0.9576	0.9688
RER	11.0369	7.3669	17.6403	19.2104
RMSE	0.3592	0.0133	0.0048	1.0201
RPD	4.2113	2.0160	4.8593	5.6624
RPIQ	8.7255	2.1541	8.7178	3.8047
SEP	0.3505	0.0136	0.0042	1.0430

Pe-proc: 9 -> vizinhos: 3

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0003	-0.0005	0.0001	-0.0115
MSE	0.0504	0.0001	0.0000	0.5819
R2	0.9805	0.9516	0.9706	0.9869
RER	20.1943	18.8982	18.1831	26.0851
RMSE	0.2245	0.0084	0.0044	0.7628
RPD	7.1699	4.5434	5.8367	8.7388
RPIQ	14.3879	5.2208	11.0611	11.7425
SEP	0.2264	0.0085	0.0045	0.7692

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0267	0.0010	0.0002	0.1696
MSE	0.1693	0.0003	0.0001	1.8949
R2	0.9347	0.7939	0.9213	0.9574
RER	11.0429	9.1633	11.1020	14.5648
RMSE	0.4115	0.0173	0.0073	1.3765
RPD	3.9125	2.2030	3.5635	4.8427
RPIQ	7.8511	2.5314	6.7531	6.5073
SEP	0.4141	0.0175	0.0073	1.3776

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1239	0.0005	0.0020	0.0353
MSE	0.1374	0.0001	0.0000	1.0980
R2	0.9400	0.8466	0.9514	0.9671
RER	10.8084	9.3317	15.5752	18.6717
RMSE	0.3706	0.0105	0.0051	1.0479
RPD	4.0809	2.5529	4.5351	5.5124
RPIQ	8.4555	2.7277	8.1361	3.7038
SEP	0.3579	0.0107	0.0048	1.0731

In [151]: #teste 2 escolhendo o modelo otimizado

```

#knn otimizado
maior=[-1,-1,-1,-1]
maiorGerado=[0,0,0,0]
for i in range(100):
    result = executaKNN(8,1,i)
    resultados=exibeResultados(result)
    r2 = resultados['pred'].loc[resultados['pred'].index=='R2']
    r = []
    for j in range(4):
        r.append(r2.iloc[:,j][0])
        if r[j]>maior[j]:
            maior[j] = r[j]
            maiorGerado[j]=i
    print('\r%d%% completos'%(i+1), end='')
print('\n','r2:',maior,'\nsemente: b c f x',maiorGerado)

```

```

100% completos
r2: [0.9995, 0.989, 0.9971, 0.9947]
semente: b c f x [3, 97, 97, 58]

```

```

In [152]: #knn teste otimizado
#@knnnotimizado
preproc=8
k=1
gera=97
result = executaKNN(preproc,k, gera)
print('Parâmetros do modelo:',modelo,'\n',result[0])

resultados=exibeResultados(result)

```

Parâmetros do modelo: KNN:

```

MultiOutputRegressor(estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='mi
metric_params=None, n_jobs=None, n_neighbors=1, p=2,
weights='uniform'),
n_jobs=None)

```

```

In [153]: resultados['cal']

```

```

Out[153]:

```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0	0.0	0.0	0.0
MSE	0.0	0.0	0.0	0.0
R2	1.0	1.0	1.0	1.0
RER	inf	inf	inf	inf
RMSE	0.0	0.0	0.0	0.0
RPD	inf	inf	inf	inf
RPIQ	inf	inf	inf	inf
SEP	0.0	0.0	0.0	0.0

```
In [154]: resultados['val']
```

```
Out[154]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0111	-0.0007	0.0002	0.1509
MSE	0.0267	0.0001	0.0000	3.1988
R2	0.9893	0.9132	0.9499	0.9221
RER	27.8374	15.8531	14.7244	11.1643
RMSE	0.1633	0.0100	0.0055	1.7885
RPD	9.6868	3.3938	4.4655	3.5822
RPIQ	19.6510	3.1864	6.7482	3.3873
SEP	0.1643	0.0101	0.0055	1.7972

```
In [155]: resultados['pred']
```

```
Out[155]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0361	0.0000	0.0002	0.3710
MSE	0.0078	0.0000	0.0000	0.8402
R2	0.9970	0.9890	0.9971	0.9800
RER	54.9529	37.4766	54.3996	23.3597
RMSE	0.0885	0.0042	0.0015	0.9167
RPD	18.2265	9.5431	18.5294	7.0753
RPIQ	33.2335	13.5846	37.2916	14.5312
SEP	0.0828	0.0043	0.0015	0.8589

```
In [156]: #variáveis para geração de gráficos e testes  
reg, treino_teste, y_c, y_cv, y_p = result
```

7.3.2 Reais x preditos

```
In [157]: #knn reaisxpreditos  
#calibração  
pred=pd.DataFrame(y_c, columns=var_ae)  
reais = treino_teste[2]  
reais=reais.reset_index(drop=True)  
reais_pred=reais.copy()  
for var in var_ae:  
    reais_pred['pred: '+var]=pred.loc[:,var]  
print('CALIBRAÇÃO:\n')  
round(reais_pred,4)
```

CALIBRAÇÃO:

```
Out[157]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	0.0874	0.0217	0.0127	0.1071	0.0874
1	0.3828	0.0405	0.0301	12.4461	0.3828
2	0.0308	0.0213	0.0113	0.0996	0.0308
3	3.5610	0.0586	0.0561	10.0978	3.5610

4	2.1150	0.0730	0.0505	18.4127	2.1150
5	3.5974	0.0516	0.0731	15.3973	3.5974
6	0.0874	0.0217	0.0127	0.1071	0.0874
7	3.8803	0.0557	0.0691	11.3256	3.8803
8	0.0759	0.0136	0.0139	0.0726	0.0759
9	0.3900	0.0315	0.0283	14.1777	0.3900
10	3.8994	0.1118	0.0613	10.9512	3.8994
11	0.4280	0.0390	0.0334	13.7624	0.4280
12	0.5905	0.0465	0.0267	18.7095	0.5905
13	0.3900	0.0315	0.0283	14.1777	0.3900
14	3.2342	0.0672	0.0543	8.4772	3.2342
15	0.5905	0.0465	0.0267	18.7095	0.5905
16	0.1724	0.0112	0.0121	0.0924	0.1724
17	0.6010	0.0559	0.0116	20.1368	0.6010
18	0.6010	0.0559	0.0116	20.1368	0.6010
19	0.0554	0.0181	0.0106	0.3275	0.0554
20	0.1724	0.0112	0.0121	0.0924	0.1724
21	2.9774	0.0704	0.0567	10.8002	2.9774
22	2.1643	0.0830	0.0529	18.8324	2.1643
23	2.9123	0.1058	0.0747	14.6813	2.9123
24	4.6037	0.1713	0.0919	16.8115	4.6037
25	3.8876	0.0418	0.0605	11.0267	3.8876
26	3.5967	0.1065	0.0850	13.6476	3.5967
27	0.3828	0.0405	0.0301	12.4461	0.3828
28	3.5610	0.0586	0.0561	10.0978	3.5610
29	0.1671	0.0117	0.0104	0.1117	0.1671
30	3.1068	0.0781	0.0545	11.0526	3.1068
31	2.1643	0.0830	0.0529	18.8324	2.1643
32	4.6037	0.1713	0.0919	16.8115	4.6037
33	3.5610	0.0586	0.0561	10.0978	3.5610
34	2.1150	0.0730	0.0505	18.4127	2.1150
35	3.5967	0.1065	0.0850	13.6476	3.5967
36	0.4280	0.0390	0.0334	13.7624	0.4280
37	3.8994	0.1118	0.0613	10.9512	3.8994
38	2.1643	0.0830	0.0529	18.8324	2.1643
39	0.0308	0.0213	0.0113	0.0996	0.0308
40	3.8876	0.0418	0.0605	11.0267	3.8876
41	2.1150	0.0730	0.0505	18.4127	2.1150
42	0.4280	0.0390	0.0334	13.7624	0.4280
43	2.9123	0.1058	0.0747	14.6813	2.9123
44	0.1724	0.0112	0.0121	0.0924	0.1724
45	2.7110	0.0548	0.0688	13.5829	2.7110
46	0.1671	0.0117	0.0104	0.1117	0.1671
47	3.5974	0.0516	0.0731	15.3973	3.5974
48	3.7243	0.0561	0.0681	11.5736	3.7243
49	3.8803	0.0557	0.0691	11.3256	3.8803
50	0.6491	0.0605	0.0260	18.4274	0.6491
51	0.3828	0.0405	0.0301	12.4461	0.3828

52	0.0308	0.0213	0.0113	0.0996	0.0308
53	3.7243	0.0561	0.0681	11.5736	3.7243
54	3.5974	0.0516	0.0731	15.3973	3.5974
55	0.6491	0.0605	0.0260	18.4274	0.6491
56	3.7243	0.0561	0.0681	11.5736	3.7243
57	3.2342	0.0672	0.0543	8.4772	3.2342
58	3.2342	0.0672	0.0543	8.4772	3.2342
59	0.5905	0.0465	0.0267	18.7095	0.5905

	pred: cmcase	pred: fpase	pred: xilanasase
0	0.0217	0.0127	0.1071
1	0.0405	0.0301	12.4461
2	0.0213	0.0113	0.0996
3	0.0586	0.0561	10.0978
4	0.0730	0.0505	18.4127
5	0.0516	0.0731	15.3973
6	0.0217	0.0127	0.1071
7	0.0557	0.0691	11.3256
8	0.0136	0.0139	0.0726
9	0.0315	0.0283	14.1777
10	0.1118	0.0613	10.9512
11	0.0390	0.0334	13.7624
12	0.0465	0.0267	18.7095
13	0.0315	0.0283	14.1777
14	0.0672	0.0543	8.4772
15	0.0465	0.0267	18.7095
16	0.0112	0.0121	0.0924
17	0.0559	0.0116	20.1368
18	0.0559	0.0116	20.1368
19	0.0181	0.0106	0.3275
20	0.0112	0.0121	0.0924
21	0.0704	0.0567	10.8002
22	0.0830	0.0529	18.8324
23	0.1058	0.0747	14.6813
24	0.1713	0.0919	16.8115
25	0.0418	0.0605	11.0267
26	0.1065	0.0850	13.6476
27	0.0405	0.0301	12.4461
28	0.0586	0.0561	10.0978
29	0.0117	0.0104	0.1117
30	0.0781	0.0545	11.0526
31	0.0830	0.0529	18.8324
32	0.1713	0.0919	16.8115
33	0.0586	0.0561	10.0978
34	0.0730	0.0505	18.4127
35	0.1065	0.0850	13.6476
36	0.0390	0.0334	13.7624
37	0.1118	0.0613	10.9512

38	0.0830	0.0529	18.8324
39	0.0213	0.0113	0.0996
40	0.0418	0.0605	11.0267
41	0.0730	0.0505	18.4127
42	0.0390	0.0334	13.7624
43	0.1058	0.0747	14.6813
44	0.0112	0.0121	0.0924
45	0.0548	0.0688	13.5829
46	0.0117	0.0104	0.1117
47	0.0516	0.0731	15.3973
48	0.0561	0.0681	11.5736
49	0.0557	0.0691	11.3256
50	0.0605	0.0260	18.4274
51	0.0405	0.0301	12.4461
52	0.0213	0.0113	0.0996
53	0.0561	0.0681	11.5736
54	0.0516	0.0731	15.3973
55	0.0605	0.0260	18.4274
56	0.0561	0.0681	11.5736
57	0.0672	0.0543	8.4772
58	0.0672	0.0543	8.4772
59	0.0465	0.0267	18.7095

```
In [158]: #validação
pred=pd.DataFrame(y_cv, columns=var_ae)
reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('VALIDAÇÃO CRUZADA:\n')
round(reais_pred,4)
```

VALIDAÇÃO CRUZADA:

```
Out [158]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	0.0874	0.0217	0.0127	0.1071	0.0874
1	0.3828	0.0405	0.0301	12.4461	0.0554
2	0.0308	0.0213	0.0113	0.0996	0.0308
3	3.5610	0.0586	0.0561	10.0978	3.8876
4	2.1150	0.0730	0.0505	18.4127	2.1643
5	3.5974	0.0516	0.0731	15.3973	3.5974
6	0.0874	0.0217	0.0127	0.1071	0.0308
7	3.8803	0.0557	0.0691	11.3256	3.8803
8	0.0759	0.0136	0.0139	0.0726	0.0308
9	0.3900	0.0315	0.0283	14.1777	0.3828

10	3.8994	0.1118	0.0613	10.9512	3.8994
11	0.4280	0.0390	0.0334	13.7624	0.4280
12	0.5905	0.0465	0.0267	18.7095	0.6491
13	0.3900	0.0315	0.0283	14.1777	0.3828
14	3.2342	0.0672	0.0543	8.4772	3.2342
15	0.5905	0.0465	0.0267	18.7095	0.6010
16	0.1724	0.0112	0.0121	0.0924	0.1724
17	0.6010	0.0559	0.0116	20.1368	0.5905
18	0.6010	0.0559	0.0116	20.1368	0.6491
19	0.0554	0.0181	0.0106	0.3275	0.1671
20	0.1724	0.0112	0.0121	0.0924	0.1671
21	2.9774	0.0704	0.0567	10.8002	3.2342
22	2.1643	0.0830	0.0529	18.8324	2.1643
23	2.9123	0.1058	0.0747	14.6813	2.9123
24	4.6037	0.1713	0.0919	16.8115	4.6037
25	3.8876	0.0418	0.0605	11.0267	3.5610
26	3.5967	0.1065	0.0850	13.6476	3.5967
27	0.3828	0.0405	0.0301	12.4461	0.3900
28	3.5610	0.0586	0.0561	10.0978	3.5610
29	0.1671	0.0117	0.0104	0.1117	0.0554
30	3.1068	0.0781	0.0545	11.0526	2.9774
31	2.1643	0.0830	0.0529	18.8324	2.1643
32	4.6037	0.1713	0.0919	16.8115	4.6037
33	3.5610	0.0586	0.0561	10.0978	3.8876
34	2.1150	0.0730	0.0505	18.4127	2.1150
35	3.5967	0.1065	0.0850	13.6476	3.5967
36	0.4280	0.0390	0.0334	13.7624	0.4280
37	3.8994	0.1118	0.0613	10.9512	3.8994
38	2.1643	0.0830	0.0529	18.8324	2.1643
39	0.0308	0.0213	0.0113	0.0996	0.0308
40	3.8876	0.0418	0.0605	11.0267	3.5610
41	2.1150	0.0730	0.0505	18.4127	2.1643
42	0.4280	0.0390	0.0334	13.7624	0.4280
43	2.9123	0.1058	0.0747	14.6813	2.9123
44	0.1724	0.0112	0.0121	0.0924	0.1671
45	2.7110	0.0548	0.0688	13.5829	3.5974
46	0.1671	0.0117	0.0104	0.1117	0.0554
47	3.5974	0.0516	0.0731	15.3973	3.5974
48	3.7243	0.0561	0.0681	11.5736	3.5967
49	3.8803	0.0557	0.0691	11.3256	3.8803
50	0.6491	0.0605	0.0260	18.4274	0.6010
51	0.3828	0.0405	0.0301	12.4461	0.3900
52	0.0308	0.0213	0.0113	0.0996	0.0759
53	3.7243	0.0561	0.0681	11.5736	3.8876
54	3.5974	0.0516	0.0731	15.3973	3.5974
55	0.6491	0.0605	0.0260	18.4274	0.6491
56	3.7243	0.0561	0.0681	11.5736	3.8876
57	3.2342	0.0672	0.0543	8.4772	3.2342

58	3.2342	0.0672	0.0543	8.4772	2.9774
59	0.5905	0.0465	0.0267	18.7095	0.6491

	pred: cmcase	pred: fpase	pred: xylanase
0	0.0217	0.0127	0.1071
1	0.0181	0.0106	0.3275
2	0.0213	0.0113	0.0996
3	0.0418	0.0605	11.0267
4	0.0830	0.0529	18.8324
5	0.0516	0.0731	15.3973
6	0.0213	0.0113	0.0996
7	0.0557	0.0691	11.3256
8	0.0213	0.0113	0.0996
9	0.0405	0.0301	12.4461
10	0.1118	0.0613	10.9512
11	0.0390	0.0334	13.7624
12	0.0605	0.0260	18.4274
13	0.0405	0.0301	12.4461
14	0.0672	0.0543	8.4772
15	0.0559	0.0116	20.1368
16	0.0112	0.0121	0.0924
17	0.0465	0.0267	18.7095
18	0.0605	0.0260	18.4274
19	0.0117	0.0104	0.1117
20	0.0117	0.0104	0.1117
21	0.0672	0.0543	8.4772
22	0.0830	0.0529	18.8324
23	0.1058	0.0747	14.6813
24	0.1713	0.0919	16.8115
25	0.0586	0.0561	10.0978
26	0.1065	0.0850	13.6476
27	0.0315	0.0283	14.1777
28	0.0586	0.0561	10.0978
29	0.0181	0.0106	0.3275
30	0.0704	0.0567	10.8002
31	0.0830	0.0529	18.8324
32	0.1713	0.0919	16.8115
33	0.0418	0.0605	11.0267
34	0.0730	0.0505	18.4127
35	0.1065	0.0850	13.6476
36	0.0390	0.0334	13.7624
37	0.1118	0.0613	10.9512
38	0.0830	0.0529	18.8324
39	0.0213	0.0113	0.0996
40	0.0586	0.0561	10.0978
41	0.0830	0.0529	18.8324
42	0.0390	0.0334	13.7624
43	0.1058	0.0747	14.6813

44	0.0117	0.0104	0.1117
45	0.0516	0.0731	15.3973
46	0.0181	0.0106	0.3275
47	0.0516	0.0731	15.3973
48	0.1065	0.0850	13.6476
49	0.0557	0.0691	11.3256
50	0.0559	0.0116	20.1368
51	0.0315	0.0283	14.1777
52	0.0136	0.0139	0.0726
53	0.0418	0.0605	11.0267
54	0.0516	0.0731	15.3973
55	0.0605	0.0260	18.4274
56	0.0418	0.0605	11.0267
57	0.0672	0.0543	8.4772
58	0.0704	0.0567	10.8002
59	0.0605	0.0260	18.4274

```
In [159]: #predição
pred=pd.DataFrame(y_p, columns=var_ae)
reais = treino_teste[3]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('Predição (validação externa):\n')
round(reais_pred,4)
```

Predição (validação externa):

```
Out[159]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	0.3900	0.0315	0.0283	14.1777	0.4280
1	3.8803	0.0557	0.0691	11.3256	3.8803
2	0.6491	0.0605	0.0260	18.4274	0.6491
3	3.5967	0.1065	0.0850	13.6476	3.5967
4	3.8994	0.1118	0.0613	10.9512	3.8994
5	2.7110	0.0548	0.0688	13.5829	2.7110
6	4.6037	0.1713	0.0919	16.8115	4.6037
7	2.9123	0.1058	0.0747	14.6813	2.9123
8	3.8876	0.0418	0.0605	11.0267	3.8876
9	0.0554	0.0181	0.0106	0.3275	0.0554
10	0.1671	0.0117	0.0104	0.1117	0.1671
11	2.7110	0.0548	0.0688	13.5829	2.7110
12	0.0874	0.0217	0.0127	0.1071	0.0874
13	2.9774	0.0704	0.0567	10.8002	3.2342
14	3.1068	0.0781	0.0545	11.0526	3.2342
15	0.0759	0.0136	0.0139	0.0726	0.0308

16	3.1068	0.0781	0.0545	11.0526	3.1068
17	2.9774	0.0704	0.0567	10.8002	3.2342
18	0.0759	0.0136	0.0139	0.0726	0.0874
19	0.6010	0.0559	0.0116	20.1368	0.6010
20	0.0554	0.0181	0.0106	0.3275	0.1671

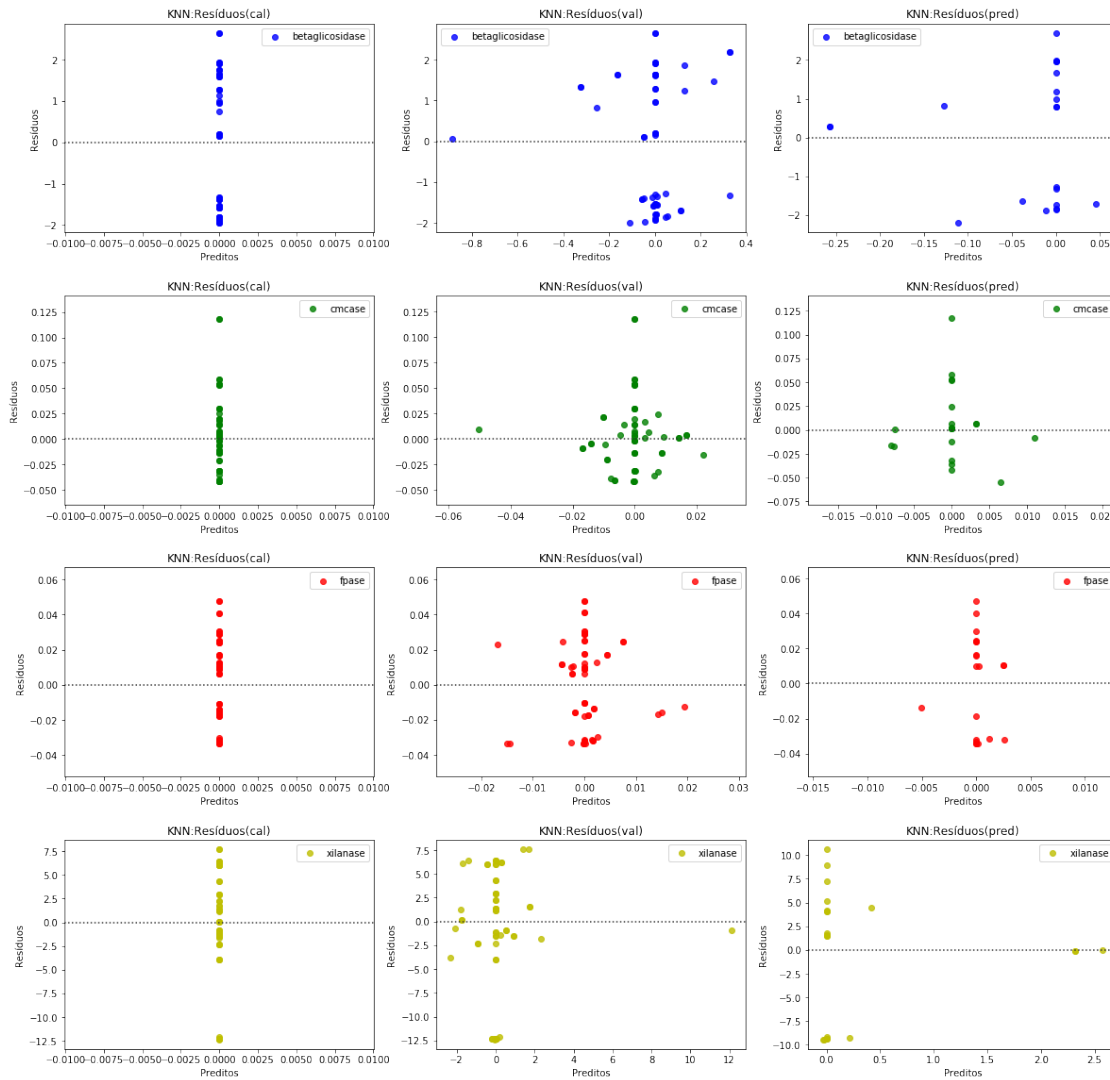
	pred: cmcase	pred: fpase	pred: xilanas
0	0.0390	0.0334	13.7624
1	0.0557	0.0691	11.3256
2	0.0605	0.0260	18.4274
3	0.1065	0.0850	13.6476
4	0.1118	0.0613	10.9512
5	0.0548	0.0688	13.5829
6	0.1713	0.0919	16.8115
7	0.1058	0.0747	14.6813
8	0.0418	0.0605	11.0267
9	0.0181	0.0106	0.3275
10	0.0117	0.0104	0.1117
11	0.0548	0.0688	13.5829
12	0.0217	0.0127	0.1071
13	0.0672	0.0543	8.4772
14	0.0672	0.0543	8.4772
15	0.0213	0.0113	0.0996
16	0.0781	0.0545	11.0526
17	0.0672	0.0543	8.4772
18	0.0217	0.0127	0.1071
19	0.0559	0.0116	20.1368
20	0.0117	0.0104	0.1117

7.3.3 KNN: Gráficos dos resíduos

```
In [162]: #knnGraf
```

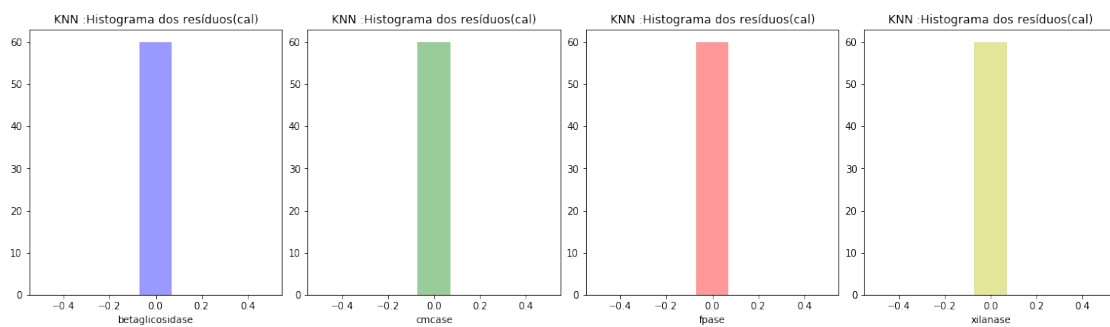
```
In [160]: #título para os gráficos
          modelo = 'KNN'
```

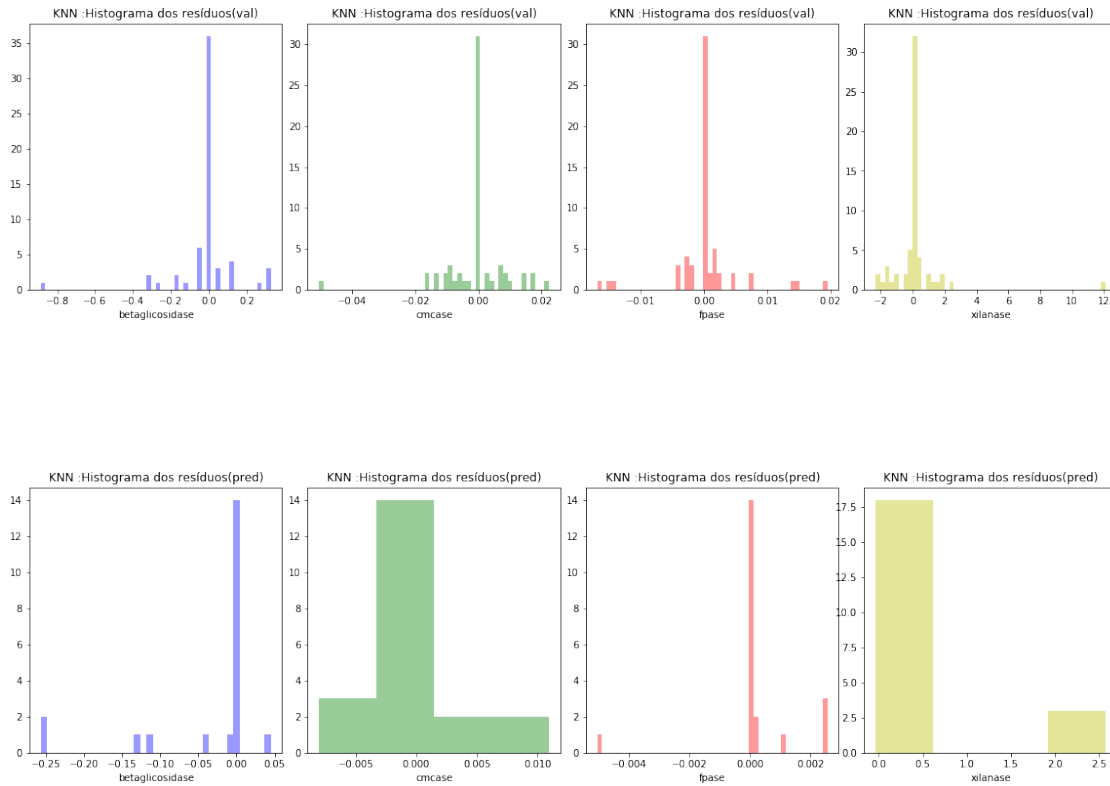
```
In [161]: #gráfico dos resíduos
          graficoResiduos(modelo, treino_teste, y_c,y_cv,y_p)
```



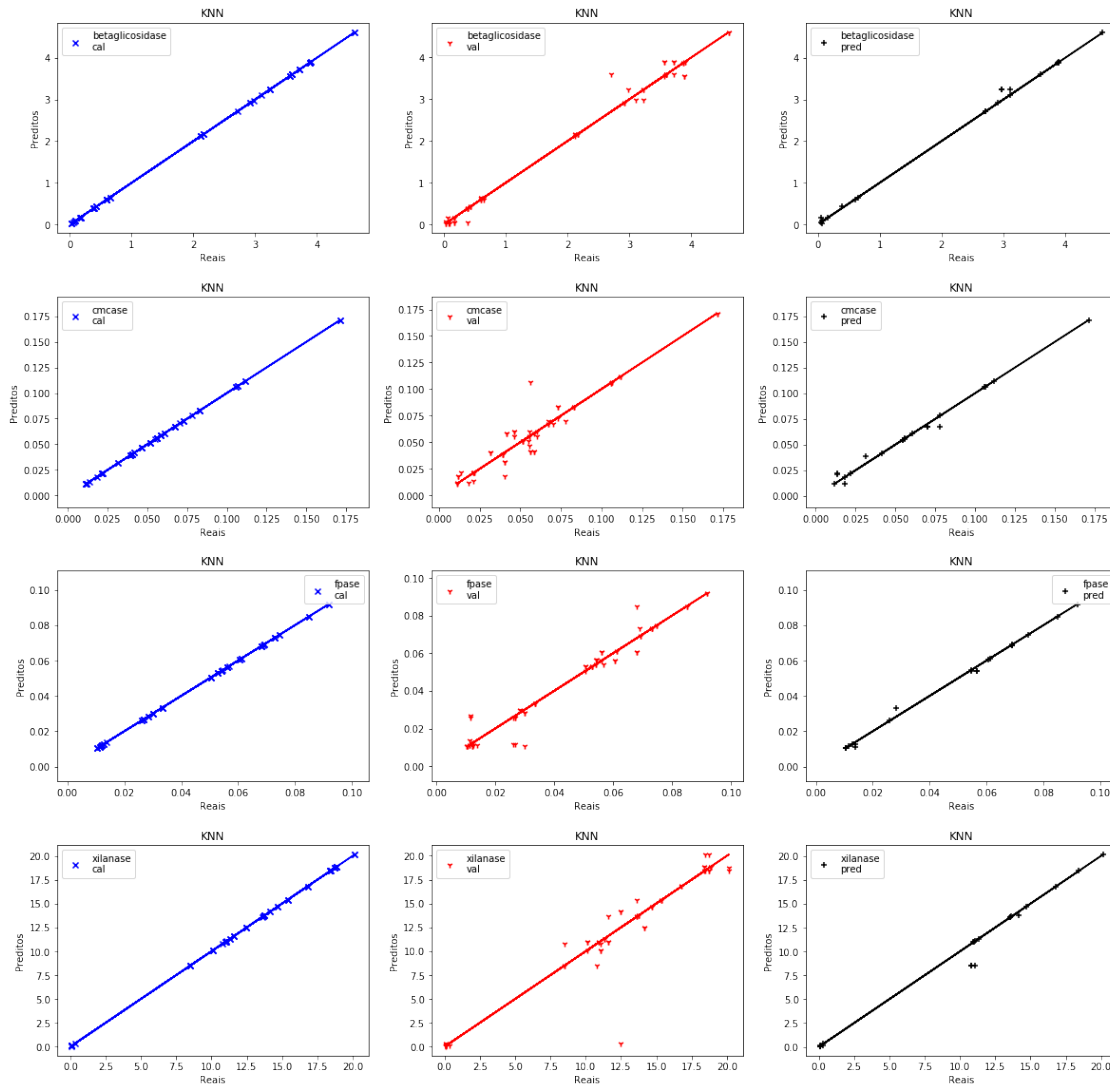
In [162]: *#histograma dos resíduos*

`graficoHist(modelo, treino_teste, y_c,y_cv,y_p)`

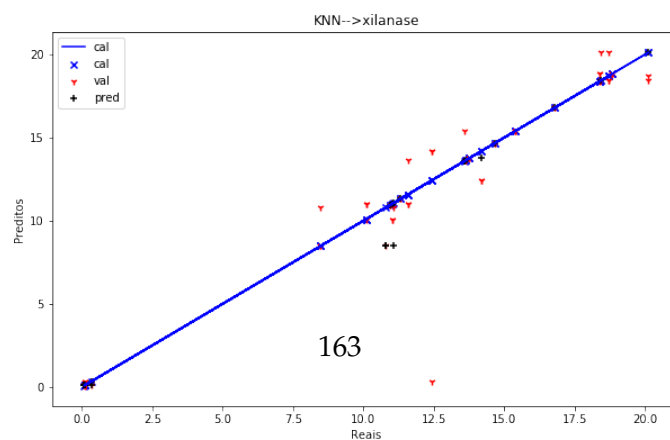
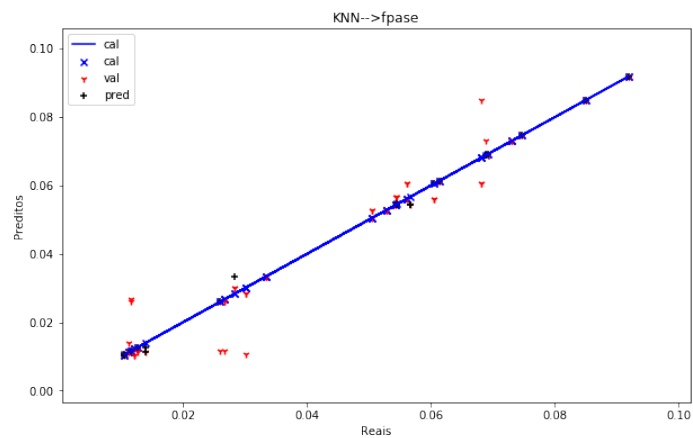
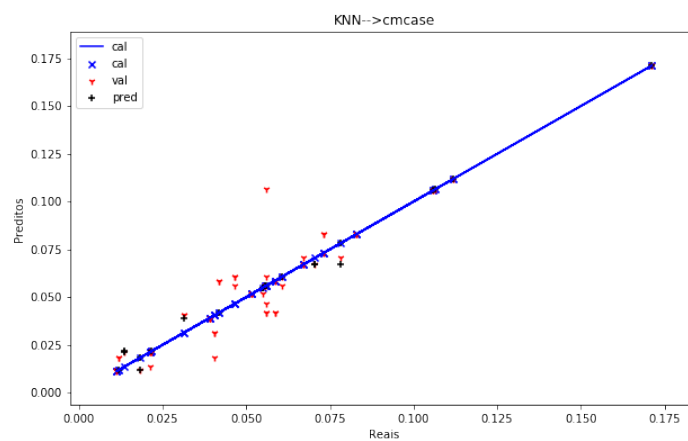
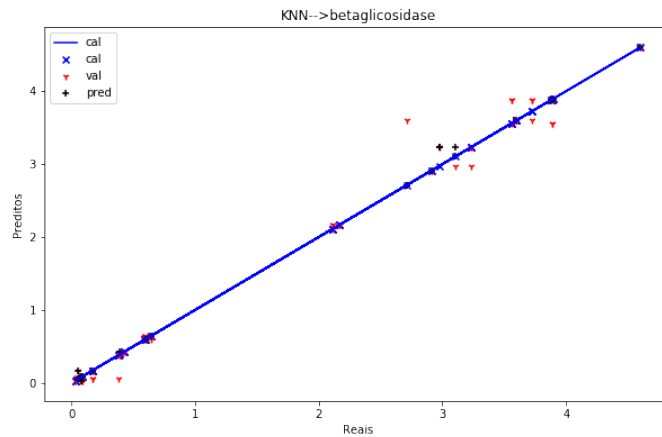




In [163]: *#grafico de reais x preditos*
graficoReaisPreditosSep(modelo, treino_teste, y_c,y_cv,y_p)

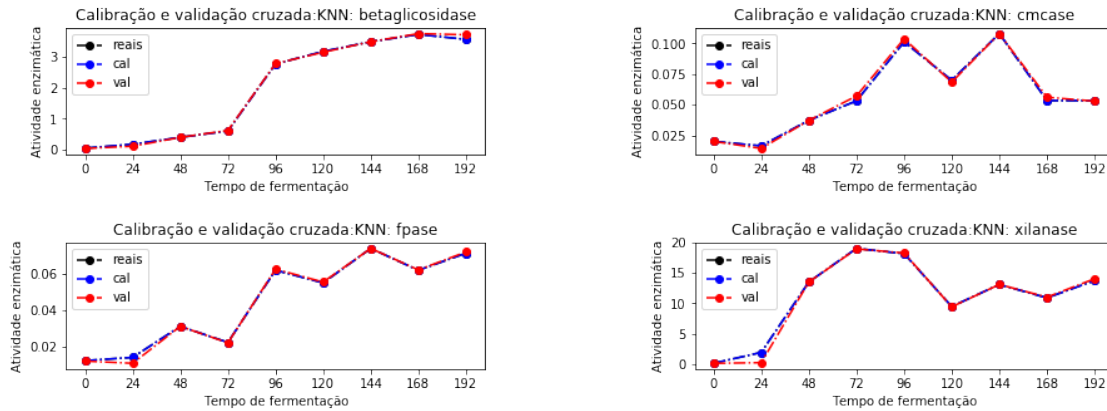


In [164]: *#grafico de reais x preditos conjuntamente*
 graficoReaisPreditos(modelo, treino_teste, y_c,y_cv,y_p)



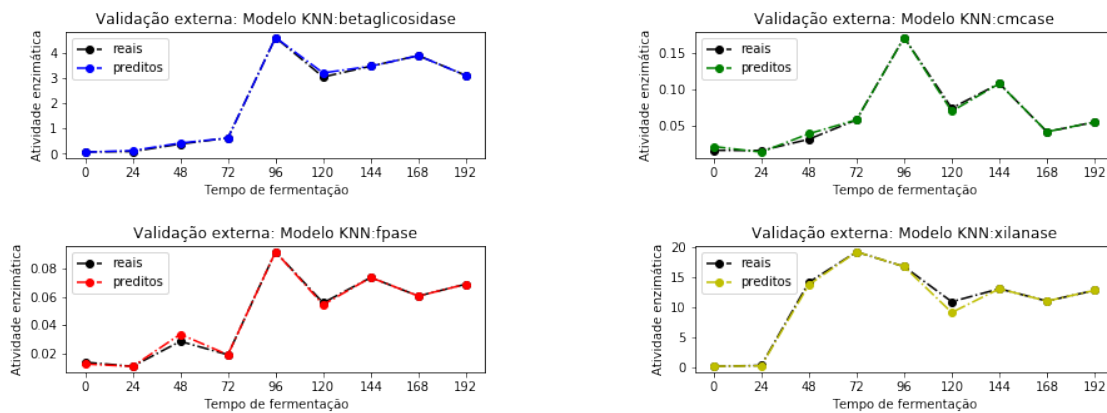
7.3.4 KNN: Gráficos: dados de treino

```
In [165]: y_treino = treino_teste[2]
          graficoTreinamento(modelo, y_treino, y_c,y_cv)
```



7.3.5 KNN:Gráficos de teste

```
In [166]: y_teste = treino_teste[3]
          graficoTeste(modelo, y_teste, y_p)
```



In []:

7.3.6 knn: teste com base externa: EETA desnaturado

In []:

```
In [120]: #@testeExterno
#rodando o knn com os dados de treino
modelo = 'KNN:'
preproc=8
k=1
gera=97
result = executaKNN(preproc,k, gera)
print('Parâmetros do modelo:',modelo,'\n',result[0])

resultados=exibeResultados(result)
```

```
In [182]: de = dados_back.copy()
de=de[(de['eenz'] == 'eeta')]
```

```
In [200]: de = dados_back.copy()
de=de[(de['experimento'] == 'bioB')&(de['inter']!= 120)]
```

In []:

```
In [176]: #buscando base de teste externa
de = dados_back.copy()
de=de[(de['eenz'] == 'eeta')&(de['experimento']=='biod1')&(de['inter']!= 1)&(de['int
#Separar somente as amostras que contenham todas as atividades enzimáticas
de = de.loc[(de['betaglicosidase'].notnull())
            & (de['cmcase'].notnull())
            & (de['fpase'].notnull())
            &(de['xilanase'].notnull())]

de.shape
```

Out[176]: (12, 713)

In [177]: de.head(5)

```
Out[177]:
```

		descricao	1100nm	1102nm	1104nm	1106nm	1108nm	\		
791	bio_25janp0_1_desn		0.038744	0.038471	0.038295	0.038206	0.038193			
792	bio_25janp0_2_desn		0.038601	0.038637	0.038631	0.038613	0.038621			
793	bio_25janp0_3_desn		0.039642	0.039467	0.039371	0.039322	0.039300			
809	bio_25janp5_1_desn		0.048341	0.046943	0.046041	0.045418	0.044937			
810	bio_25janp5_2_desn		0.048823	0.047629	0.046772	0.046076	0.045451			
		1110nm	1112nm	1114nm	1116nm	...	cmcase	fpase	xilanase	\
791	0.038237	0.038330	0.038481	0.038710	...	0.035	0.051	24.094000		
792	0.038688	0.038837	0.039073	0.039391	...	0.035	0.051	24.094000		
793	0.039299	0.039333	0.039428	0.039612	...	0.035	0.051	24.094000		
809	0.044537	0.044219	0.044010	0.043935	...	0.067	0.060	17.361999		

```
810  0.044883  0.044408  0.044065  0.043873  ...   0.067  0.060  17.361999
```

```

      proteínas  eenz  temp  dur  inter  proc  experimento
791         NaN  eeta   70   33     0   des         biod1
792         NaN  eeta   70   33     0   des         biod1
793         NaN  eeta   70   33     0   des         biod1
809         NaN  eeta   70   33     5   des         biod1
810         NaN  eeta   70   33     5   des         biod1

```

```
[5 rows x 713 columns]
```

```

In [201]: #Definindo os dataFrames iniciais para começar o processamento
de_x = de.loc[:,var_abs_txt] #absorbâncias
de_y = de.loc[:,var_ae] #AE
de_inter=pd.DataFrame(de.loc[:, 'inter'], columns=['inter'])
#df = dados.loc[:,var_abs_txt+var_ae]

```

```
In [197]: de_x.shape, de_y.shape, de_inter.shape
```

```
Out[197]: ((21, 244), (21, 4), (21, 1))
```

```

In [202]: #executa pré-processamento equivalente ao do modelo de treinamento
x = executaPreprocSimples(8, de_x)
preditos=reg.predict(x)

```

```

In [203]: #para exibir o gráfico
#para todas as atividades
#cria um data frame com os valores reais e preditos para os dados de teste
df_pred = {}
for valor in var_ae:
    df_pred[valor] = []
i=0
for valor in var_ae:
    df =pd.DataFrame(columns=['reais','preditos'], index= de_y.index)
    df['reais'] = de_y[valor]
    df['preditos'] = pd.DataFrame(preditos[:,i],index= de_y.index)
    i +=1
    df_pred[valor] = df.copy()

df_pred_inter = {}
for valor in var_ae:
    df_pred_inter[valor] = []
for valor in var_ae:
    df_pred_inter[valor] = df_pred[valor].copy()
    df_pred_inter[valor]['inter'] = de_inter.loc[:, 'inter']

#ordena valores pelo intervalo
df_ord_teste = {}
for valor in var_ae:

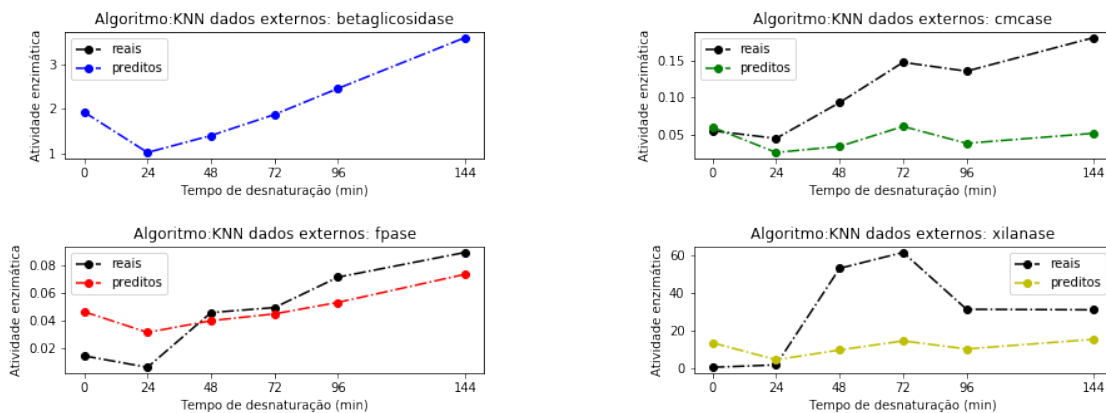
```

```

df_ord_teste[valor] = []
for valor in var_ae:
    df_ord_teste[valor] = df_pred_inter[valor].sort_values(['inter'])

#calculando a média para cada ponto
df_teste_media = {}
for valor in var_ae:
    df_teste_media[valor] = []
for valor in var_ae:
    df_teste_media[valor] = df_ord_teste[valor].groupby('inter').mean()
x = list(df_teste_media['xilanase'].index)
var = ['reais', 'preditos']
tipoAE= ['bo-.', 'go-.', 'ro-.', 'yo-.']
j = 0
fig = plt.figure(figsize=(15,5))
plt.subplots_adjust(hspace = 0.7, wspace=0.5)
for valor in var_ae:
    ax = fig.add_subplot(2,2,j+1)
    ax.plot(x,df_teste_media[valor][var[0]], 'ko-.', label=var[0])
    ax.plot(x,df_teste_media[valor][var[1]], tipoAE[j], label=var[1])
    j +=1
    ax.legend(loc=2)
    ax.set_title('Algoritmo:KNN dados externos: '+valor)
    ax.set_xlabel('Tempo de desnaturação (min)')
    ax.set_ylabel('Atividade enzimática')
    ax.set_xticks(x)
    plt.legend(loc='best')

```



In []:

7.4 GBR: Gradient Boost Regressor

In [204]: *#gbr*
#função completa para execução do GBR

```
def executaGBR(preproc=1, varLoss='ls',n_est=100,IC=0):
    #separando o conjunto de dados em treino e teste
    x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc,False,IC)

    reg = MultiOutputRegressor(GradientBoostingRegressor(n_estimators=n_est,
                                                            learning_rate=0.1,
                                                            max_depth=2,
                                                            random_state=0, lo

    #reg=MultiOutputRegressor(xgb.XGBRegressor())
    result = executaCVP([x_treino, x_teste, y_treino, y_teste], reg)

    return result
```

```
In [205]: #função completa para execução do GBR com PCA
#A variável preproc determinará o tipo de processamento que será executado (0,1,2,3)
def executaPCA_GBR(preproc, varLoss,nPC=3,n_est=100, IC=0):
    #separando o conjunto de dados em treino e teste
    x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc,False, IC)

    reg = MultiOutputRegressor(GradientBoostingRegressor(n_estimators=n_est,
                                                            learning_rate=0.1,
                                                            max_depth=8,
                                                            random_state=IC, 1

    # Roda o PCA e produz uma variável reduzida xRed e seleciona as primeiras componen
    pca = PCA(n_components=nPC)
    x_treino = pca.fit_transform(x_treino)[:,:nPC]
    x_teste = pca.fit_transform(x_teste)[:,:nPC]

    result = executaCVP([x_treino, x_teste, y_treino, y_teste], reg)

    return result
```

```
In [ ]:
```

7.4.1 GBR testes

```
In [206]: warnings.filterwarnings("ignore")
#GBR teste simples
modelo = 'GBR:'
result = executaGBR(preproc=1, varLoss='ls',n_est=50, IC=0)
print('Parâmetros do modelo:',modelo,'\n',result[0])
```



```

resultados=exibeResultados(result)

for k,v in zip(resultados.keys(),resultados.values()):
    print(k)
    print(v, '\n-----')

```

Parâmetros do modelo: GBR:

```

MultiOutputRegressor(estimator=GradientBoostingRegressor(alpha=0.9, criterion='friedman_mse',
    learning_rate=0.1, loss='ls', max_depth=2, max_features=None,
    max_leaf_nodes=None, min_impurity_decrease=0.0,
    min_impurity_split=None, min_samples_leaf=1,
    min_samplerate=0, subsample=1.0, tol=0.0001,
    validation_fraction=0.1, verbose=0, warm_start=False),
    n_jobs=None)

```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	-0.0000	-0.0000
MSE	0.0117	0.0000	0.0000	0.2776
R2	0.9955	0.9884	0.9906	0.9938
RER	41.9128	38.6300	32.1644	37.7645
RMSE	0.1082	0.0041	0.0025	0.5269
RPD	14.8811	9.3018	10.3292	12.6529
RPIQ	29.8617	10.6886	19.5746	17.0020
SEP	0.1091	0.0041	0.0025	0.5313

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0593	0.0003	0.0004	0.1746
MSE	0.2927	0.0004	0.0001	10.1305
R2	0.8871	0.7397	0.8459	0.7720
RER	8.4321	8.1411	7.9393	6.2605
RMSE	0.5410	0.0195	0.0102	3.1828
RPD	2.9758	1.9601	2.5473	2.0944
RPIQ	5.9715	2.2523	4.8273	2.8143
SEP	0.5423	0.0197	0.0103	3.2049

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1788	0.0011	0.0009	0.6419
MSE	0.2562	0.0002	0.0000	9.7073
R2	0.8880	0.7296	0.9156	0.7091
RER	7.9732	7.0435	10.9411	6.4137
RMSE	0.5061	0.0139	0.0067	3.1157
RPD	2.9883	1.9230	3.4414	1.8539
RPIQ	6.1917	2.0547	6.1740	1.2457
SEP	0.4852	0.0142	0.0068	3.1241

```
In [265]: #gbrtestes
#Executa o modelo GBR variando o tipo de processamento e o parâmetro loss
loss_valores = ['ls', 'huber']
for k, v in preProc.items():
    print( 'GBR:\n\t'+v)
    for var in loss_valores:
        print('\n>>>>\tLoss:'+var)
        result = executaGBR(k, var)
        #print('Parâmetros do modelo:',modelo,'\n',result[0])

    resultados=exibeResultados(result)

    for k,v in zip(resultados.keys(),resultados.values()):
        print(k)
        print(v, '\n-----')
```

GBR:

Pré-proc: 0--> Sem pré-processamento

>>>> Loss:ls

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	0.0000
MSE	0.0008	0.0000	0.0000	0.0205
R2	0.9997	0.9994	0.9988	0.9995
RER	162.2013	166.3827	88.5660	138.8733
RMSE	0.0280	0.0010	0.0009	0.1433
RPD	57.5892	40.0636	28.4418	46.5292
RPIQ	115.5638	46.0367	53.8995	62.5224
SEP	0.0282	0.0010	0.0009	0.1445

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0811	0.0009	0.0005	0.2056
MSE	0.3181	0.0002	0.0001	8.7746
R2	0.8773	0.8295	0.8459	0.8025
RER	8.1246	10.0728	7.9415	6.7330
RMSE	0.5640	0.0158	0.0102	2.9622
RPD	2.8546	2.4216	2.5472	2.2504
RPIQ	5.7284	2.7827	4.8271	3.0240
SEP	0.5628	0.0159	0.0103	2.9800

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0540	-0.0018	0.0003	-0.5277
MSE	0.1073	0.0002	0.0001	10.6345
R2	0.9531	0.7778	0.8973	0.6813
RER	11.6859	7.8285	9.8457	6.0764

RMSE	0.3275	0.0126	0.0074	3.2611
RPD	4.6177	2.1213	3.1203	1.7713
RPIQ	9.5677	2.2666	5.5980	1.1901
SEP	0.3310	0.0128	0.0076	3.2975

>>>> Loss:huber

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0273	0.0007	-0.0001	-0.0173
MSE	0.0248	0.0000	0.0000	0.0623
R2	0.9904	0.9907	0.9943	0.9986
RER	29.2515	43.7062	41.0991	79.9341
RMSE	0.1574	0.0037	0.0020	0.2495
RPD	10.2283	10.3473	13.1877	26.7176
RPIQ	20.5250	11.8900	24.9917	35.9011
SEP	0.1563	0.0037	0.0020	0.2510

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0923	0.0012	0.0009	0.1613
MSE	0.4197	0.0004	0.0001	9.0826
R2	0.8381	0.7516	0.8286	0.7956
RER	7.0719	8.3485	7.5465	6.6113
RMSE	0.6478	0.0190	0.0107	3.0137
RPD	2.4852	2.0064	2.4152	2.2119
RPIQ	4.9871	2.3056	4.5770	2.9722
SEP	0.6466	0.0192	0.0108	3.0348

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0240	0.0004	0.0008	-0.5162
MSE	0.1376	0.0002	0.0001	12.1076
R2	0.9398	0.6969	0.8927	0.6371
RER	10.1972	6.6346	9.6739	5.6826
RMSE	0.3710	0.0147	0.0076	3.4796
RPD	4.0767	1.8165	3.0532	1.6600
RPIQ	8.4467	1.9409	5.4776	1.1154
SEP	0.3794	0.0151	0.0077	3.5261

GBR:

Pré-proc: 1--> Padronização

>>>> Loss:ls

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	0.0000
MSE	0.0008	0.0000	0.0000	0.0205

R2	0.9997	0.9994	0.9988	0.9995
RER	162.2013	166.3827	88.5660	138.8733
RMSE	0.0280	0.0010	0.0009	0.1433
RPD	57.5892	40.0636	28.4418	46.5292
RPIQ	115.5638	46.0367	53.8995	62.5224
SEP	0.0282	0.0010	0.0009	0.1445

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0766	0.0009	0.0005	0.1676
MSE	0.3206	0.0002	0.0001	8.4179
R2	0.8763	0.8295	0.8458	0.8106
RER	8.0826	10.0728	7.9399	6.8690
RMSE	0.5662	0.0158	0.0102	2.9014
RPD	2.8433	2.4216	2.5465	2.2976
RPIQ	5.7056	2.7827	4.8259	3.0874
SEP	0.5658	0.0159	0.0103	2.9210

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2500	0.0043	0.0013	0.7394
MSE	0.3043	0.0002	0.0000	8.7367
R2	0.8670	0.7462	0.9092	0.7381
RER	7.6768	7.6562	10.6481	6.8328
RMSE	0.5517	0.0135	0.0070	2.9558
RPD	2.7417	1.9849	3.3189	1.9542
RPIQ	5.6807	2.1208	5.9543	1.3131
SEP	0.5039	0.0131	0.0070	2.9325

>>>> Loss:huber

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0273	0.0007	-0.0001	-0.0173
MSE	0.0248	0.0000	0.0000	0.0623
R2	0.9904	0.9907	0.9943	0.9986
RER	29.2515	43.7062	41.0991	79.9341
RMSE	0.1574	0.0037	0.0020	0.2495
RPD	10.2283	10.3473	13.1877	26.7176
RPIQ	20.5250	11.8900	24.9917	35.9011
SEP	0.1563	0.0037	0.0020	0.2510

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0923	0.0012	0.0009	0.1613
MSE	0.4197	0.0004	0.0001	9.0826
R2	0.8381	0.7516	0.8286	0.7956
RER	7.0719	8.3485	7.5465	6.6113

RMSE	0.6478	0.0190	0.0107	3.0137
RPD	2.4852	2.0064	2.4152	2.2119
RPIQ	4.9871	2.3056	4.5770	2.9722
SEP	0.6466	0.0192	0.0108	3.0348

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0240	0.0004	0.0008	-0.5162
MSE	0.1376	0.0002	0.0001	12.1076
R2	0.9398	0.6969	0.8927	0.6371
RER	10.1972	6.6346	9.6739	5.6826
RMSE	0.3710	0.0147	0.0076	3.4796
RPD	4.0767	1.8165	3.0532	1.6600
RPIQ	8.4467	1.9409	5.4776	1.1154
SEP	0.3794	0.0151	0.0077	3.5261

GBR:

Pré-proc: 2--> Suavização(SavGol) - Par:3,1,1

>>>> Loss:ls

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	-0.0000
MSE	0.0003	0.0000	0.0000	0.0048
R2	0.9999	0.9996	0.9998	0.9999
RER	253.8873	198.7059	247.9922	286.0580
RMSE	0.0179	0.0008	0.0003	0.0696
RPD	90.1421	47.8467	79.6395	95.8431
RPIQ	180.8875	54.9802	150.9231	128.7867
SEP	0.0180	0.0008	0.0003	0.0701

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0131	-0.0017	-0.0001	-0.1607
MSE	0.4643	0.0009	0.0001	3.7155
R2	0.8209	0.3591	0.7982	0.9164
RER	6.6564	5.1956	6.9324	10.3581
RMSE	0.6814	0.0306	0.0117	1.9276
RPD	2.3629	1.2491	2.2262	3.4584
RPIQ	4.7416	1.4354	4.2189	4.6471
SEP	0.6870	0.0308	0.0118	1.9371

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0934	-0.0067	-0.0002	0.0972
MSE	0.1864	0.0003	0.0001	1.7510
R2	0.9185	0.5497	0.8930	0.9475
RER	8.9560	5.8697	9.6397	14.8176

RMSE	0.4318	0.0180	0.0076	1.3232
RPD	3.5031	1.4902	3.0567	4.3652
RPIQ	7.2583	1.5922	5.4838	2.9331
SEP	0.4320	0.0171	0.0077	1.3523

>>>> Loss:huber

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0273	0.0007	-0.0001	-0.0173
MSE	0.0248	0.0000	0.0000	0.0623
R2	0.9904	0.9907	0.9943	0.9986
RER	29.2515	43.7062	41.0991	79.9341
RMSE	0.1574	0.0037	0.0020	0.2495
RPD	10.2283	10.3473	13.1877	26.7176
RPIQ	20.5250	11.8900	24.9917	35.9011
SEP	0.1563	0.0037	0.0020	0.2510

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0923	0.0012	0.0009	0.1613
MSE	0.4197	0.0004	0.0001	9.0826
R2	0.8381	0.7516	0.8286	0.7956
RER	7.0719	8.3485	7.5465	6.6113
RMSE	0.6478	0.0190	0.0107	3.0137
RPD	2.4852	2.0064	2.4152	2.2119
RPIQ	4.9871	2.3056	4.5770	2.9722
SEP	0.6466	0.0192	0.0108	3.0348

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0240	0.0004	0.0008	-0.5162
MSE	0.1376	0.0002	0.0001	12.1076
R2	0.9398	0.6969	0.8927	0.6371
RER	10.1972	6.6346	9.6739	5.6826
RMSE	0.3710	0.0147	0.0076	3.4796
RPD	4.0767	1.8165	3.0532	1.6600
RPIQ	8.4467	1.9409	5.4776	1.1154
SEP	0.3794	0.0151	0.0077	3.5261

GBR:

Pré-proc: 3--> Suavização(SavGol) - Par:3,2,1

>>>> Loss:ls

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	-0.0000
MSE	0.0003	0.0000	0.0000	0.0048

R2	0.9999	0.9996	0.9998	0.9999
RER	253.8873	198.7059	247.9922	286.0580
RMSE	0.0179	0.0008	0.0003	0.0696
RPD	90.1421	47.8467	79.6395	95.8431
RPIQ	180.8875	54.9802	150.9231	128.7867
SEP	0.0180	0.0008	0.0003	0.0701

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.0338	-0.0018	-0.0000	-0.1611
MSE	0.4882	0.0010	0.0001	3.7160
R2	0.8117	0.3479	0.7988	0.9164
RER	6.4976	5.1518	6.9428	10.3575
RMSE	0.6987	0.0309	0.0116	1.9277
RPD	2.3043	1.2384	2.2296	3.4581
RPIQ	4.6239	1.4230	4.2252	4.6468
SEP	0.7038	0.0311	0.0117	1.9372

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0934	-0.0067	-0.0002	0.0972
MSE	0.1864	0.0003	0.0001	1.7510
R2	0.9185	0.5497	0.8930	0.9475
RER	8.9560	5.8697	9.6397	14.8176
RMSE	0.4318	0.0180	0.0076	1.3232
RPD	3.5031	1.4902	3.0567	4.3652
RPIQ	7.2583	1.5922	5.4838	2.9331
SEP	0.4320	0.0171	0.0077	1.3523

>>>> Loss:huber

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0273	0.0007	-0.0001	-0.0173
MSE	0.0248	0.0000	0.0000	0.0623
R2	0.9904	0.9907	0.9943	0.9986
RER	29.2515	43.7062	41.0991	79.9341
RMSE	0.1574	0.0037	0.0020	0.2495
RPD	10.2283	10.3473	13.1877	26.7176
RPIQ	20.5250	11.8900	24.9917	35.9011
SEP	0.1563	0.0037	0.0020	0.2510

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0923	0.0012	0.0009	0.1613
MSE	0.4197	0.0004	0.0001	9.0826
R2	0.8381	0.7516	0.8286	0.7956
RER	7.0719	8.3485	7.5465	6.6113

RMSE	0.6478	0.0190	0.0107	3.0137
RPD	2.4852	2.0064	2.4152	2.2119
RPIQ	4.9871	2.3056	4.5770	2.9722
SEP	0.6466	0.0192	0.0108	3.0348

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0240	0.0004	0.0008	-0.5162
MSE	0.1376	0.0002	0.0001	12.1076
R2	0.9398	0.6969	0.8927	0.6371
RER	10.1972	6.6346	9.6739	5.6826
RMSE	0.3710	0.0147	0.0076	3.4796
RPD	4.0767	1.8165	3.0532	1.6600
RPIQ	8.4467	1.9409	5.4776	1.1154
SEP	0.3794	0.0151	0.0077	3.5261

GBR:

Pré-proc: 4--> Suavização(SavGol) - Par:5,1,1

>>>>

Loss:ls

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0000	-0.0000	-0.0000	0.0000
MSE	0.0004	0.0000	0.0000	0.0058
R2	0.9998	0.9996	0.9998	0.9999
RER	225.8325	204.9318	211.1547	262.1284
RMSE	0.0201	0.0008	0.0004	0.0759
RPD	80.1813	49.3459	67.8096	87.8256
RPIQ	160.8992	56.7029	128.5045	118.0133
SEP	0.0202	0.0008	0.0004	0.0765

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0184	-0.0024	-0.0012	-0.0669
MSE	0.5071	0.0010	0.0002	6.4002
R2	0.8044	0.2918	0.7581	0.8560
RER	6.3703	4.9487	6.3573	7.8673
RMSE	0.7121	0.0322	0.0128	2.5299
RPD	2.2610	1.1883	2.0331	2.6350
RPIQ	4.5371	1.3655	3.8528	3.5407
SEP	0.7179	0.0323	0.0128	2.5503

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0151	-0.0086	-0.0011	-0.1565
MSE	0.2357	0.0004	0.0001	1.8650
R2	0.8970	0.4347	0.8559	0.9441
RER	7.7799	5.3670	8.3726	14.4137

RMSE	0.4855	0.0201	0.0088	1.3656
RPD	3.1153	1.3301	2.6342	4.2297
RPIQ	6.4548	1.4211	4.7259	2.8420
SEP	0.4973	0.0187	0.0089	1.3901

>>>> Loss:huber

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0273	0.0007	-0.0001	-0.0173
MSE	0.0248	0.0000	0.0000	0.0623
R2	0.9904	0.9907	0.9943	0.9986
RER	29.2515	43.7062	41.0991	79.9341
RMSE	0.1574	0.0037	0.0020	0.2495
RPD	10.2283	10.3473	13.1877	26.7176
RPIQ	20.5250	11.8900	24.9917	35.9011
SEP	0.1563	0.0037	0.0020	0.2510

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0923	0.0012	0.0009	0.1613
MSE	0.4197	0.0004	0.0001	9.0826
R2	0.8381	0.7516	0.8286	0.7956
RER	7.0719	8.3485	7.5465	6.6113
RMSE	0.6478	0.0190	0.0107	3.0137
RPD	2.4852	2.0064	2.4152	2.2119
RPIQ	4.9871	2.3056	4.5770	2.9722
SEP	0.6466	0.0192	0.0108	3.0348

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0240	0.0004	0.0008	-0.5162
MSE	0.1376	0.0002	0.0001	12.1076
R2	0.9398	0.6969	0.8927	0.6371
RER	10.1972	6.6346	9.6739	5.6826
RMSE	0.3710	0.0147	0.0076	3.4796
RPD	4.0767	1.8165	3.0532	1.6600
RPIQ	8.4467	1.9409	5.4776	1.1154
SEP	0.3794	0.0151	0.0077	3.5261

GBR:

Pré-proc: 5--> Suavização(SavGol) - Par:5,2,1

>>>> Loss:ls

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0000	-0.0000	-0.0000	0.0000
MSE	0.0004	0.0000	0.0000	0.0058

R2	0.9998	0.9996	0.9998	0.9999
RER	225.8325	204.9318	211.1547	262.1284
RMSE	0.0201	0.0008	0.0004	0.0759
RPD	80.1813	49.3459	67.8096	87.8256
RPIQ	160.8992	56.7029	128.5045	118.0133
SEP	0.0202	0.0008	0.0004	0.0765

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.0185	-0.0023	-0.0011	-0.0791
MSE	0.5069	0.0010	0.0002	6.2896
R2	0.8044	0.2921	0.7603	0.8585
RER	6.3712	4.9489	6.3852	7.9373
RMSE	0.7120	0.0322	0.0127	2.5079
RPD	2.2613	1.1886	2.0426	2.6581
RPIQ	4.5377	1.3658	3.8710	3.5717
SEP	0.7177	0.0323	0.0128	2.5278

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0156	-0.0086	-0.0011	-0.1557
MSE	0.2357	0.0004	0.0001	1.8674
R2	0.8970	0.4352	0.8559	0.9440
RER	7.7807	5.3696	8.3726	14.4032
RMSE	0.4855	0.0201	0.0088	1.3665
RPD	3.1155	1.3306	2.6342	4.2269
RPIQ	6.4552	1.4217	4.7259	2.8401
SEP	0.4972	0.0186	0.0089	1.3912

>>>> Loss:huber

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0273	0.0007	-0.0001	-0.0173
MSE	0.0248	0.0000	0.0000	0.0623
R2	0.9904	0.9907	0.9943	0.9986
RER	29.2515	43.7062	41.0991	79.9341
RMSE	0.1574	0.0037	0.0020	0.2495
RPD	10.2283	10.3473	13.1877	26.7176
RPIQ	20.5250	11.8900	24.9917	35.9011
SEP	0.1563	0.0037	0.0020	0.2510

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0923	0.0012	0.0009	0.1613
MSE	0.4197	0.0004	0.0001	9.0826
R2	0.8381	0.7516	0.8286	0.7956
RER	7.0719	8.3485	7.5465	6.6113

RMSE	0.6478	0.0190	0.0107	3.0137
RPD	2.4852	2.0064	2.4152	2.2119
RPIQ	4.9871	2.3056	4.5770	2.9722
SEP	0.6466	0.0192	0.0108	3.0348

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0240	0.0004	0.0008	-0.5162
MSE	0.1376	0.0002	0.0001	12.1076
R2	0.9398	0.6969	0.8927	0.6371
RER	10.1972	6.6346	9.6739	5.6826
RMSE	0.3710	0.0147	0.0076	3.4796
RPD	4.0767	1.8165	3.0532	1.6600
RPIQ	8.4467	1.9409	5.4776	1.1154
SEP	0.3794	0.0151	0.0077	3.5261

GBR:

Pré-proc: 6--> Suavização(SavGol) - Par:3,2,2

>>>> Loss:ls

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0000	-0.0000	-0.0000	-0.0000
MSE	0.0002	0.0000	0.0000	0.0044
R2	0.9999	0.9998	0.9998	0.9999
RER	346.1287	288.2835	210.1594	298.5123
RMSE	0.0131	0.0006	0.0004	0.0667
RPD	122.8922	69.4162	67.4900	100.0159
RPIQ	246.6068	79.7656	127.8988	134.3937
SEP	0.0132	0.0006	0.0004	0.0672

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0052	-0.0018	-0.0011	-0.0348
MSE	0.5992	0.0010	0.0003	12.1086
R2	0.7688	0.3276	0.5906	0.7275
RER	5.8582	5.0727	4.8772	5.7180
RMSE	0.7741	0.0313	0.0166	3.4797
RPD	2.0799	1.2195	1.5630	1.9157
RPIQ	4.1737	1.4014	2.9619	2.5742
SEP	0.7806	0.0316	0.0167	3.5089

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0008	-0.0051	0.0010	0.0562
MSE	0.2972	0.0007	0.0001	3.1512
R2	0.8701	0.0383	0.8970	0.9056
RER	6.9249	3.7945	9.9116	11.0210

RMSE	0.5452	0.0262	0.0074	1.7752
RPD	2.7743	1.0197	3.1163	3.2539
RPIQ	5.7482	1.0896	5.5908	2.1863
SEP	0.5586	0.0264	0.0075	1.8181

>>>> Loss:huber

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0273	0.0007	-0.0001	-0.0173
MSE	0.0248	0.0000	0.0000	0.0623
R2	0.9904	0.9907	0.9943	0.9986
RER	29.2515	43.7062	41.0991	79.9341
RMSE	0.1574	0.0037	0.0020	0.2495
RPD	10.2283	10.3473	13.1877	26.7176
RPIQ	20.5250	11.8900	24.9917	35.9011
SEP	0.1563	0.0037	0.0020	0.2510

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0923	0.0012	0.0009	0.1613
MSE	0.4197	0.0004	0.0001	9.0826
R2	0.8381	0.7516	0.8286	0.7956
RER	7.0719	8.3485	7.5465	6.6113
RMSE	0.6478	0.0190	0.0107	3.0137
RPD	2.4852	2.0064	2.4152	2.2119
RPIQ	4.9871	2.3056	4.5770	2.9722
SEP	0.6466	0.0192	0.0108	3.0348

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0240	0.0004	0.0008	-0.5162
MSE	0.1376	0.0002	0.0001	12.1076
R2	0.9398	0.6969	0.8927	0.6371
RER	10.1972	6.6346	9.6739	5.6826
RMSE	0.3710	0.0147	0.0076	3.4796
RPD	4.0767	1.8165	3.0532	1.6600
RPIQ	8.4467	1.9409	5.4776	1.1154
SEP	0.3794	0.0151	0.0077	3.5261

GBR:

Pré-proc: 7--> Suavização(SavGol) - Par:5,2,2

>>>> Loss:ls

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0000	0.0000	0.0000	0.0000
MSE	0.0002	0.0000	0.0000	0.0037

R2	0.9999	0.9998	0.9999	0.9999
RER	320.9316	265.9956	257.5927	327.7130
RMSE	0.0141	0.0006	0.0003	0.0607
RPD	113.9460	64.0495	82.7226	109.7995
RPIQ	228.6545	73.5987	156.7657	147.5402
SEP	0.0142	0.0006	0.0003	0.0612

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.0127	-0.0013	-0.0013	-0.3191
MSE	0.6419	0.0008	0.0002	12.3065
R2	0.7523	0.4285	0.6438	0.7231
RER	5.6604	5.4992	5.2364	5.6952
RMSE	0.8012	0.0289	0.0155	3.5081
RPD	2.0095	1.3227	1.6754	1.9003
RPIQ	4.0324	1.5199	3.1751	2.5534
SEP	0.8079	0.0291	0.0156	3.5230

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0447	-0.0048	0.0022	0.4076
MSE	0.1939	0.0006	0.0001	13.3001
R2	0.9152	0.2010	0.8643	0.6014
RER	8.6177	4.1694	8.8538	5.3956
RMSE	0.4404	0.0239	0.0085	3.6469
RPD	3.4346	1.1187	2.7145	1.5839
RPIQ	7.1164	1.1953	4.8699	1.0642
SEP	0.4489	0.0240	0.0084	3.7136

>>>> Loss:huber

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0273	0.0007	-0.0001	-0.0173
MSE	0.0248	0.0000	0.0000	0.0623
R2	0.9904	0.9907	0.9943	0.9986
RER	29.2515	43.7062	41.0991	79.9341
RMSE	0.1574	0.0037	0.0020	0.2495
RPD	10.2283	10.3473	13.1877	26.7176
RPIQ	20.5250	11.8900	24.9917	35.9011
SEP	0.1563	0.0037	0.0020	0.2510

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0923	0.0012	0.0009	0.1613
MSE	0.4197	0.0004	0.0001	9.0826
R2	0.8381	0.7516	0.8286	0.7956
RER	7.0719	8.3485	7.5465	6.6113

RMSE	0.6478	0.0190	0.0107	3.0137
RPD	2.4852	2.0064	2.4152	2.2119
RPIQ	4.9871	2.3056	4.5770	2.9722
SEP	0.6466	0.0192	0.0108	3.0348

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0240	0.0004	0.0008	-0.5162
MSE	0.1376	0.0002	0.0001	12.1076
R2	0.9398	0.6969	0.8927	0.6371
RER	10.1972	6.6346	9.6739	5.6826
RMSE	0.3710	0.0147	0.0076	3.4796
RPD	4.0767	1.8165	3.0532	1.6600
RPIQ	8.4467	1.9409	5.4776	1.1154
SEP	0.3794	0.0151	0.0077	3.5261

GBR:

Pré-proc: 8--> Suavização(SavGol) - Par:3,1,1 --> Padronização

>>>> Loss:ls

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	-0.0000
MSE	0.0003	0.0000	0.0000	0.0046
R2	0.9999	0.9995	0.9998	0.9999
RER	253.8873	182.0917	247.9922	292.3582
RMSE	0.0179	0.0009	0.0003	0.0681
RPD	90.1421	43.8462	79.6395	97.9540
RPIQ	180.8875	50.3832	150.9231	131.6231
SEP	0.0180	0.0009	0.0003	0.0686

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0140	-0.0018	-0.0001	-0.1725
MSE	0.4639	0.0009	0.0001	3.7185
R2	0.8210	0.3586	0.7997	0.9163
RER	6.6592	5.1947	6.9571	10.3594
RMSE	0.6811	0.0306	0.0116	1.9283
RPD	2.3638	1.2487	2.2341	3.4570
RPIQ	4.7435	1.4348	4.2338	4.6452
SEP	0.6867	0.0308	0.0117	1.9368

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.3391	-0.0021	0.0003	-0.1416
MSE	0.3710	0.0002	0.0001	1.6388
R2	0.8378	0.6819	0.8970	0.9509
RER	7.4612	6.5349	9.8330	15.3690

RMSE	0.6091	0.0151	0.0074	1.2802
RPD	2.4831	1.7731	3.1160	4.5121
RPIQ	5.1449	1.8945	5.5902	3.0317
SEP	0.5185	0.0153	0.0076	1.3037

>>>> Loss:huber

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0273	0.0007	-0.0001	-0.0173
MSE	0.0248	0.0000	0.0000	0.0623
R2	0.9904	0.9907	0.9943	0.9986
RER	29.2515	43.7062	41.0991	79.9341
RMSE	0.1574	0.0037	0.0020	0.2495
RPD	10.2283	10.3473	13.1877	26.7176
RPIQ	20.5250	11.8900	24.9917	35.9011
SEP	0.1563	0.0037	0.0020	0.2510

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0923	0.0012	0.0009	0.1613
MSE	0.4197	0.0004	0.0001	9.0826
R2	0.8381	0.7516	0.8286	0.7956
RER	7.0719	8.3485	7.5465	6.6113
RMSE	0.6478	0.0190	0.0107	3.0137
RPD	2.4852	2.0064	2.4152	2.2119
RPIQ	4.9871	2.3056	4.5770	2.9722
SEP	0.6466	0.0192	0.0108	3.0348

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0240	0.0004	0.0008	-0.5162
MSE	0.1376	0.0002	0.0001	12.1076
R2	0.9398	0.6969	0.8927	0.6371
RER	10.1972	6.6346	9.6739	5.6826
RMSE	0.3710	0.0147	0.0076	3.4796
RPD	4.0767	1.8165	3.0532	1.6600
RPIQ	8.4467	1.9409	5.4776	1.1154
SEP	0.3794	0.0151	0.0077	3.5261

GBR:

Pré-proc: 9--> Padronização --> Suavização(SavGol) - Par:3,1,1

>>>> Loss:ls

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	-0.0000
MSE	0.0001	0.0000	0.0000	0.0028

R2	0.9999	0.9999	0.9999	0.9999
RER	371.0931	361.0752	258.5299	378.7833
RMSE	0.0122	0.0004	0.0003	0.0525
RPD	131.7558	86.9439	83.0236	126.9105
RPIQ	264.3932	99.9064	157.3361	170.5327
SEP	0.0123	0.0004	0.0003	0.0530

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0929	0.0011	-0.0000	-0.0988
MSE	0.4645	0.0005	0.0002	2.5208
R2	0.8208	0.6260	0.7744	0.9433
RER	6.7160	6.7993	6.5558	12.5559
RMSE	0.6816	0.0234	0.0123	1.5877
RPD	2.3622	1.6353	2.1053	4.1987
RPIQ	4.7402	1.8791	3.9897	5.6419
SEP	0.6809	0.0235	0.0124	1.5980

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.3107	-0.0033	0.0060	0.0800
MSE	0.4168	0.0003	0.0001	2.2466
R2	0.8178	0.5233	0.7936	0.9327
RER	6.6715	5.3770	8.4578	13.0646
RMSE	0.6456	0.0185	0.0105	1.4989
RPD	2.3429	1.4484	2.2009	3.8537
RPIQ	4.8544	1.5476	3.9486	2.5894
SEP	0.5799	0.0186	0.0088	1.5337

>>>> Loss:huber

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0273	0.0007	-0.0001	-0.0173
MSE	0.0248	0.0000	0.0000	0.0623
R2	0.9904	0.9907	0.9943	0.9986
RER	29.2515	43.7062	41.0991	79.9341
RMSE	0.1574	0.0037	0.0020	0.2495
RPD	10.2283	10.3473	13.1877	26.7176
RPIQ	20.5250	11.8900	24.9917	35.9011
SEP	0.1563	0.0037	0.0020	0.2510

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0923	0.0012	0.0009	0.1613
MSE	0.4197	0.0004	0.0001	9.0826
R2	0.8381	0.7516	0.8286	0.7956
RER	7.0719	8.3485	7.5465	6.6113

RMSE	0.6478	0.0190	0.0107	3.0137
RPD	2.4852	2.0064	2.4152	2.2119
RPIQ	4.9871	2.3056	4.5770	2.9722
SEP	0.6466	0.0192	0.0108	3.0348

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0240	0.0004	0.0008	-0.5162
MSE	0.1376	0.0002	0.0001	12.1076
R2	0.9398	0.6969	0.8927	0.6371
RER	10.1972	6.6346	9.6739	5.6826
RMSE	0.3710	0.0147	0.0076	3.4796
RPD	4.0767	1.8165	3.0532	1.6600
RPIQ	8.4467	1.9409	5.4776	1.1154
SEP	0.3794	0.0151	0.0077	3.5261

GBR:

Pré-proc: 10--> MSC

>>>> Loss:ls

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0000	0.0000	0.0000	0.0000
MSE	0.0006	0.0000	0.0000	0.0168
R2	0.9998	0.9988	0.9993	0.9996
RER	178.3727	118.3719	120.4463	153.3848
RMSE	0.0254	0.0013	0.0007	0.1297
RPD	63.3308	28.5030	38.6798	51.3912
RPIQ	127.0855	32.7525	73.3012	69.0556
SEP	0.0256	0.0014	0.0007	0.1308

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0047	0.0011	0.0000	0.0179
MSE	0.2532	0.0004	0.0001	5.2695
R2	0.9023	0.7288	0.8263	0.8814
RER	9.0129	7.9881	7.4720	8.6677
RMSE	0.5031	0.0199	0.0108	2.2955
RPD	3.1999	1.9204	2.3995	2.9040
RPIQ	6.4211	2.2067	4.5473	3.9022
SEP	0.5074	0.0200	0.0109	2.3148

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0133	0.0029	0.0004	0.8100
MSE	0.1251	0.0001	0.0001	7.6196
R2	0.9453	0.8414	0.8922	0.7716
RER	10.6837	9.5252	9.6153	7.4102

RMSE	0.3536	0.0107	0.0076	2.7604
RPD	4.2772	2.5108	3.0455	2.0925
RPIQ	8.8621	2.6827	5.4638	1.4060
SEP	0.3621	0.0105	0.0078	2.7040

>>>> Loss:huber

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0273	0.0007	-0.0001	-0.0173
MSE	0.0248	0.0000	0.0000	0.0623
R2	0.9904	0.9907	0.9943	0.9986
RER	29.2515	43.7062	41.0991	79.9341
RMSE	0.1574	0.0037	0.0020	0.2495
RPD	10.2283	10.3473	13.1877	26.7176
RPIQ	20.5250	11.8900	24.9917	35.9011
SEP	0.1563	0.0037	0.0020	0.2510

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0923	0.0012	0.0009	0.1613
MSE	0.4197	0.0004	0.0001	9.0826
R2	0.8381	0.7516	0.8286	0.7956
RER	7.0719	8.3485	7.5465	6.6113
RMSE	0.6478	0.0190	0.0107	3.0137
RPD	2.4852	2.0064	2.4152	2.2119
RPIQ	4.9871	2.3056	4.5770	2.9722
SEP	0.6466	0.0192	0.0108	3.0348

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0240	0.0004	0.0008	-0.5162
MSE	0.1376	0.0002	0.0001	12.1076
R2	0.9398	0.6969	0.8927	0.6371
RER	10.1972	6.6346	9.6739	5.6826
RMSE	0.3710	0.0147	0.0076	3.4796
RPD	4.0767	1.8165	3.0532	1.6600
RPIQ	8.4467	1.9409	5.4776	1.1154
SEP	0.3794	0.0151	0.0077	3.5261

GBR:

Pré-proc: 11--> SNV

>>>> Loss:ls

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0000	-0.0000	-0.0000	0.0000
MSE	0.0007	0.0000	0.0000	0.0206

R2	0.9997	0.9988	0.9995	0.9995
RER	177.4806	121.0902	141.1196	138.5058
RMSE	0.0255	0.0013	0.0006	0.1436
RPD	63.0141	29.1575	45.3187	46.4061
RPIQ	126.4498	33.5046	85.8825	62.3569
SEP	0.0258	0.0013	0.0006	0.1449

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0214	0.0006	0.0002	-0.0408
MSE	0.2468	0.0004	0.0001	4.9014
R2	0.9048	0.7383	0.8410	0.8897
RER	9.1368	8.1222	7.8117	8.9884
RMSE	0.4968	0.0195	0.0103	2.2139
RPD	3.2410	1.9549	2.5081	3.0110
RPIQ	6.5036	2.2463	4.7530	4.0460
SEP	0.5005	0.0197	0.0104	2.2322

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0461	0.0002	-0.0016	0.5261
MSE	0.2023	0.0002	0.0000	3.8457
R2	0.9116	0.7598	0.9088	0.8847
RER	8.4382	7.4506	10.7116	10.3509
RMSE	0.4498	0.0131	0.0070	1.9610
RPD	3.3628	2.0403	3.3111	2.9455
RPIQ	6.9676	2.1801	5.9402	1.9791
SEP	0.4585	0.0134	0.0070	1.9358

>>>> Loss:huber

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0273	0.0007	-0.0001	-0.0173
MSE	0.0248	0.0000	0.0000	0.0623
R2	0.9904	0.9907	0.9943	0.9986
RER	29.2515	43.7062	41.0991	79.9341
RMSE	0.1574	0.0037	0.0020	0.2495
RPD	10.2283	10.3473	13.1877	26.7176
RPIQ	20.5250	11.8900	24.9917	35.9011
SEP	0.1563	0.0037	0.0020	0.2510

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0923	0.0012	0.0009	0.1613
MSE	0.4197	0.0004	0.0001	9.0826
R2	0.8381	0.7516	0.8286	0.7956
RER	7.0719	8.3485	7.5465	6.6113

RMSE	0.6478	0.0190	0.0107	3.0137
RPD	2.4852	2.0064	2.4152	2.2119
RPIQ	4.9871	2.3056	4.5770	2.9722
SEP	0.6466	0.0192	0.0108	3.0348

```
-----
pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0240  0.0004  0.0008  -0.5162
MSE      0.1376  0.0002  0.0001  12.1076
R2      0.9398  0.6969  0.8927   0.6371
RER     10.1972  6.6346  9.6739   5.6826
RMSE     0.3710  0.0147  0.0076   3.4796
RPD      4.0767  1.8165  3.0532   1.6600
RPIQ     8.4467  1.9409  5.4776   1.1154
SEP      0.3794  0.0151  0.0077   3.5261
-----
```

In []:

```
In [856]: #gbrtestes - loss = huber
          #Executa o modelo GBR variando o tipo de processamento
          for i in [0,1,2,3,4,5,9]:
              print( 'GBR:\n\t'+preProc[i])
              result = executaGBR(k, 'huber')

          resultados=exibeResultados(result)

          for k,v in zip(resultados.keys(),resultados.values()):
              print(k)
              print(v,'\n-----')
```

GBR:

Pré-proc: 0--> Sem pré-processamento

cal				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0044	0.0003	0.0001	0.0215
MSE	0.0018	0.0000	0.0000	0.0315
R2	0.9993	0.9966	0.9974	0.9993
RER	106.2526	72.4298	61.7355	112.8940
RMSE	0.0429	0.0022	0.0013	0.1775
RPD	37.5249	17.2717	19.7707	37.5476
RPIQ	75.3009	19.8467	37.4671	50.4535
SEP	0.0430	0.0022	0.0013	0.1777

```
-----
val
      betaglicosidase  cmcase  fpase  xilanase
```

BIAS	0.0243	0.0012	-0.0003	0.1046
MSE	0.5057	0.0005	0.0002	11.2580
R2	0.8049	0.6398	0.7696	0.7467
RER	6.3802	6.9295	6.4888	5.9327
RMSE	0.7112	0.0229	0.0125	3.3553
RPD	2.2639	1.6662	2.0834	1.9868
RPIQ	4.5430	1.9146	3.9481	2.6697
SEP	0.7167	0.0231	0.0126	3.3820

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0236	0.0013	-0.0000	-0.5516
MSE	0.3050	0.0003	0.0001	12.0135
R2	0.8667	0.5753	0.8262	0.6399
RER	6.8424	5.6190	7.5624	5.7145
RMSE	0.5523	0.0174	0.0096	3.4660
RPD	2.7387	1.5345	2.3988	1.6665
RPIQ	5.6745	1.6396	4.3036	1.1198
SEP	0.5654	0.0178	0.0099	3.5064

GBR:

Pré-proc: 1--> Padronização

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0044	0.0003	0.0001	0.0215
MSE	0.0018	0.0000	0.0000	0.0315
R2	0.9993	0.9966	0.9974	0.9993
RER	106.2526	72.4298	61.7355	112.8940
RMSE	0.0429	0.0022	0.0013	0.1775
RPD	37.5249	17.2717	19.7707	37.5476
RPIQ	75.3009	19.8467	37.4671	50.4535
SEP	0.0430	0.0022	0.0013	0.1777

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0243	0.0012	-0.0003	0.1046
MSE	0.5057	0.0005	0.0002	11.2580
R2	0.8049	0.6398	0.7696	0.7467
RER	6.3802	6.9295	6.4888	5.9327
RMSE	0.7112	0.0229	0.0125	3.3553
RPD	2.2639	1.6662	2.0834	1.9868
RPIQ	4.5430	1.9146	3.9481	2.6697
SEP	0.7167	0.0231	0.0126	3.3820

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0236	0.0013	-0.0000	-0.5516
MSE	0.3050	0.0003	0.0001	12.0135

R2	0.8667	0.5753	0.8262	0.6399
RER	6.8424	5.6190	7.5624	5.7145
RMSE	0.5523	0.0174	0.0096	3.4660
RPD	2.7387	1.5345	2.3988	1.6665
RPIQ	5.6745	1.6396	4.3036	1.1198
SEP	0.5654	0.0178	0.0099	3.5064

GBR:

Pré-proc: 2--> Suavização(SavGol) - Par:3,1,1

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0044	0.0003	0.0001	0.0215
MSE	0.0018	0.0000	0.0000	0.0315
R2	0.9993	0.9966	0.9974	0.9993
RER	106.2526	72.4298	61.7355	112.8940
RMSE	0.0429	0.0022	0.0013	0.1775
RPD	37.5249	17.2717	19.7707	37.5476
RPIQ	75.3009	19.8467	37.4671	50.4535
SEP	0.0430	0.0022	0.0013	0.1777

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0243	0.0012	-0.0003	0.1046
MSE	0.5057	0.0005	0.0002	11.2580
R2	0.8049	0.6398	0.7696	0.7467
RER	6.3802	6.9295	6.4888	5.9327
RMSE	0.7112	0.0229	0.0125	3.3553
RPD	2.2639	1.6662	2.0834	1.9868
RPIQ	4.5430	1.9146	3.9481	2.6697
SEP	0.7167	0.0231	0.0126	3.3820

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0236	0.0013	-0.0000	-0.5516
MSE	0.3050	0.0003	0.0001	12.0135
R2	0.8667	0.5753	0.8262	0.6399
RER	6.8424	5.6190	7.5624	5.7145
RMSE	0.5523	0.0174	0.0096	3.4660
RPD	2.7387	1.5345	2.3988	1.6665
RPIQ	5.6745	1.6396	4.3036	1.1198
SEP	0.5654	0.0178	0.0099	3.5064

GBR:

Pré-proc: 3--> Suavização(SavGol) - Par:3,2,1

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0044	0.0003	0.0001	0.0215
MSE	0.0018	0.0000	0.0000	0.0315

R2	0.9993	0.9966	0.9974	0.9993
RER	106.2526	72.4298	61.7355	112.8940
RMSE	0.0429	0.0022	0.0013	0.1775
RPD	37.5249	17.2717	19.7707	37.5476
RPIQ	75.3009	19.8467	37.4671	50.4535
SEP	0.0430	0.0022	0.0013	0.1777

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0243	0.0012	-0.0003	0.1046
MSE	0.5057	0.0005	0.0002	11.2580
R2	0.8049	0.6398	0.7696	0.7467
RER	6.3802	6.9295	6.4888	5.9327
RMSE	0.7112	0.0229	0.0125	3.3553
RPD	2.2639	1.6662	2.0834	1.9868
RPIQ	4.5430	1.9146	3.9481	2.6697
SEP	0.7167	0.0231	0.0126	3.3820

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0236	0.0013	-0.0000	-0.5516
MSE	0.3050	0.0003	0.0001	12.0135
R2	0.8667	0.5753	0.8262	0.6399
RER	6.8424	5.6190	7.5624	5.7145
RMSE	0.5523	0.0174	0.0096	3.4660
RPD	2.7387	1.5345	2.3988	1.6665
RPIQ	5.6745	1.6396	4.3036	1.1198
SEP	0.5654	0.0178	0.0099	3.5064

GBR:

Pré-proc: 4--> Suavização(SavGol) - Par:5,1,1

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0044	0.0003	0.0001	0.0215
MSE	0.0018	0.0000	0.0000	0.0315
R2	0.9993	0.9966	0.9974	0.9993
RER	106.2526	72.4298	61.7355	112.8940
RMSE	0.0429	0.0022	0.0013	0.1775
RPD	37.5249	17.2717	19.7707	37.5476
RPIQ	75.3009	19.8467	37.4671	50.4535
SEP	0.0430	0.0022	0.0013	0.1777

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0243	0.0012	-0.0003	0.1046
MSE	0.5057	0.0005	0.0002	11.2580
R2	0.8049	0.6398	0.7696	0.7467
RER	6.3802	6.9295	6.4888	5.9327

RMSE	0.7112	0.0229	0.0125	3.3553
RPD	2.2639	1.6662	2.0834	1.9868
RPIQ	4.5430	1.9146	3.9481	2.6697
SEP	0.7167	0.0231	0.0126	3.3820

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0236	0.0013	-0.0000	-0.5516
MSE	0.3050	0.0003	0.0001	12.0135
R2	0.8667	0.5753	0.8262	0.6399
RER	6.8424	5.6190	7.5624	5.7145
RMSE	0.5523	0.0174	0.0096	3.4660
RPD	2.7387	1.5345	2.3988	1.6665
RPIQ	5.6745	1.6396	4.3036	1.1198
SEP	0.5654	0.0178	0.0099	3.5064

GBR:

Pré-proc: 5--> Suavização(SavGol) - Par:5,2,1

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0044	0.0003	0.0001	0.0215
MSE	0.0018	0.0000	0.0000	0.0315
R2	0.9993	0.9966	0.9974	0.9993
RER	106.2526	72.4298	61.7355	112.8940
RMSE	0.0429	0.0022	0.0013	0.1775
RPD	37.5249	17.2717	19.7707	37.5476
RPIQ	75.3009	19.8467	37.4671	50.4535
SEP	0.0430	0.0022	0.0013	0.1777

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0243	0.0012	-0.0003	0.1046
MSE	0.5057	0.0005	0.0002	11.2580
R2	0.8049	0.6398	0.7696	0.7467
RER	6.3802	6.9295	6.4888	5.9327
RMSE	0.7112	0.0229	0.0125	3.3553
RPD	2.2639	1.6662	2.0834	1.9868
RPIQ	4.5430	1.9146	3.9481	2.6697
SEP	0.7167	0.0231	0.0126	3.3820

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0236	0.0013	-0.0000	-0.5516
MSE	0.3050	0.0003	0.0001	12.0135
R2	0.8667	0.5753	0.8262	0.6399
RER	6.8424	5.6190	7.5624	5.7145
RMSE	0.5523	0.0174	0.0096	3.4660
RPD	2.7387	1.5345	2.3988	1.6665

RPIQ	5.6745	1.6396	4.3036	1.1198
SEP	0.5654	0.0178	0.0099	3.5064

GBR:

Pré-proc: 9--> Padronização --> Suavização(SavGol) - Par:3,1,1

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0044	0.0003	0.0001	0.0215
MSE	0.0018	0.0000	0.0000	0.0315
R2	0.9993	0.9966	0.9974	0.9993
RER	106.2526	72.4298	61.7355	112.8940
RMSE	0.0429	0.0022	0.0013	0.1775
RPD	37.5249	17.2717	19.7707	37.5476
RPIQ	75.3009	19.8467	37.4671	50.4535
SEP	0.0430	0.0022	0.0013	0.1777

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0243	0.0012	-0.0003	0.1046
MSE	0.5057	0.0005	0.0002	11.2580
R2	0.8049	0.6398	0.7696	0.7467
RER	6.3802	6.9295	6.4888	5.9327
RMSE	0.7112	0.0229	0.0125	3.3553
RPD	2.2639	1.6662	2.0834	1.9868
RPIQ	4.5430	1.9146	3.9481	2.6697
SEP	0.7167	0.0231	0.0126	3.3820

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0236	0.0013	-0.0000	-0.5516
MSE	0.3050	0.0003	0.0001	12.0135
R2	0.8667	0.5753	0.8262	0.6399
RER	6.8424	5.6190	7.5624	5.7145
RMSE	0.5523	0.0174	0.0096	3.4660
RPD	2.7387	1.5345	2.3988	1.6665
RPIQ	5.6745	1.6396	4.3036	1.1198
SEP	0.5654	0.0178	0.0099	3.5064

```
In [292]: #teste 2 escolhendo o modelo mais otimizado
          #gbrotimizado
          maior=[-1,-1,-1,-1]
          maiorGerado=[0,0,0,0]
          for i in range(100):
              result = executaGBR(10,'ls',n_est=50,IC=i)
              resultados=exibeResultados(result)
              r2 = resultados['pred'].loc[resultados['pred'].index=='R2']
```

```

r = []
for j in range(4):
    r.append(r2.iloc[:,j][0])
    if r[j]>maior[j]:
        maior[j] = r[j]
        maiorGerado[j]=i
print('\r%d%% completos'%(i+1), end='')
print('\n', 'r2:', maior, '\nsemente: b c f x', maiorGerado)

```

2% completos

```

-----

KeyboardInterrupt                                Traceback (most recent call last)

<ipython-input-292-2397fb9368bc> in <module>
      4 maiorGerado=[0,0,0,0]
      5 for i in range(100):
----> 6     result = executaGBR(1,'ls',n_est=50,IC=i)
      7     resultados=exibeResultados(result)
      8     r2 = resultados['pred'].loc[resultados['pred'].index=='R2']

<ipython-input-262-174a9f08601e> in executaGBR(preproc, varLoss, n_est, IC)
     13
     14     #reg=MultiOutputRegressor(xgb.XGBRegressor())
--> 15     result = executaCVP([x_treino, x_teste, y_treino, y_teste], reg)
     16
     17     return result

<ipython-input-79-c2df78e37ac6> in executaCVP(treino_teste, reg)
     13
     14     # Cross-validation
--> 15     y_cv = cross_val_predict(reg, x_treino, y_treino, cv=10)
     16
     17     # Predição nos dados de teste

~/anaconda3/lib/python3.7/site-packages/sklearn/model_selection/_validation.py in cross
775     prediction_blocks = parallel(delayed(_fit_and_predict)(
776         clone(estimator), X, y, train, test, verbose, fit_params, method)
--> 777         for train, test in cv.split(X, y, groups))
778
779     # Concatenate the predictions

```

```

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/parallel.py in __call__
918         self._iterating = self._original_iterator is not None
919
--> 920         while self.dispatch_one_batch(iterator):
921             pass
922

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/parallel.py in dispatch_one_batch
757         return False
758     else:
--> 759         self._dispatch(tasks)
760         return True
761

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/parallel.py in _dispatch_one_batch
714         with self._lock:
715             job_idx = len(self._jobs)
--> 716             job = self._backend.apply_async(batch, callback=cb)
717             # A job can complete so quickly than its callback is
718             # called before we get here, causing self._jobs to

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/_parallel_backends.py
180     def apply_async(self, func, callback=None):
181         """Schedule a func to be run"""
--> 182         result = ImmediateResult(func)
183         if callback:
184             callback(result)

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/_parallel_backends.py
547         # Don't delay the application, to avoid keeping the input
548         # arguments in memory
--> 549         self.results = batch()
550
551     def get(self):

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/parallel.py in __call__
223         with parallel_backend(self._backend, n_jobs=self._n_jobs):
224             return [func(*args, **kwargs)
--> 225                     for func, args, kwargs in self.items]
226
227     def __len__(self):

```

```

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/parallel.py in <listcomp>
223         with parallel_backend(self._backend, n_jobs=self._n_jobs):
224             return [func(*args, **kwargs)
--> 225                     for func, args, kwargs in self.items]
226
227     def __len__(self):

~/anaconda3/lib/python3.7/site-packages/sklearn/model_selection/_validation.py in _fit_estimator
848         estimator.fit(X_train, **fit_params)
849     else:
--> 850         estimator.fit(X_train, y_train, **fit_params)
851     func = getattr(estimator, method)
852     predictions = func(X_test)

~/anaconda3/lib/python3.7/site-packages/sklearn/multioutput.py in fit(self, X, y, sample_weight)
167         delayed(_fit_estimator)(
168             self.estimator, X, y[:, i], sample_weight)
--> 169         for i in range(y.shape[1]))
170     return self
171

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/parallel.py in __call__
915         # remaining jobs.
916         self._iterating = False
--> 917         if self.dispatch_one_batch(iterator):
918             self._iterating = self._original_iterator is not None
919

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/parallel.py in dispatch_one_batch
757         return False
758     else:
--> 759         self._dispatch(tasks)
760         return True
761

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/parallel.py in _dispatch_one_batch
714         with self._lock:
715             job_idx = len(self._jobs)
--> 716             job = self._backend.apply_async(batch, callback=cb)
717             # A job can complete so quickly than its callback is
718             # called before we get here, causing self._jobs to

```

```

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/_parallel_backends.py
180     def apply_async(self, func, callback=None):
181         """Schedule a func to be run"""
--> 182         result = ImmediateResult(func)
183         if callback:
184             callback(result)

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/_parallel_backends.py
547         # Don't delay the application, to avoid keeping the input
548         # arguments in memory
--> 549         self.results = batch()
550
551     def get(self):

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/parallel.py in __call__
223         with parallel_backend(self._backend, n_jobs=self._n_jobs):
224             return [func(*args, **kwargs)
--> 225                     for func, args, kwargs in self.items]
226
227     def __len__(self):

~/anaconda3/lib/python3.7/site-packages/sklearn/externals/joblib/parallel.py in <listcomp>
223         with parallel_backend(self._backend, n_jobs=self._n_jobs):
224             return [func(*args, **kwargs)
--> 225                     for func, args, kwargs in self.items]
226
227     def __len__(self):

~/anaconda3/lib/python3.7/site-packages/sklearn/multioutput.py in _fit_estimator(estimator, X, y, sample_weight)
38         estimator.fit(X, y, sample_weight=sample_weight)
39     else:
---> 40         estimator.fit(X, y)
41     return estimator
42

~/anaconda3/lib/python3.7/site-packages/sklearn/ensemble/gradient_boosting.py in fit(self, X, y, sample_weight, stage, monitor, X_idx_sorted)
1463         n_stages = self._fit_stages(X, y, y_pred, sample_weight, self._rng,
1464                                     X_val, y_val, sample_weight_val,
-> 1465                                     begin_at_stage, monitor, X_idx_sorted)
1466
1467         # change shape of arrays after fit (early-stopping or additional ests)

```

```

~/anaconda3/lib/python3.7/site-packages/sklearn/ensemble/gradient_boosting.py in _fit_
1540         else:
1541             # no need to fancy index w/ no subsampling
-> 1542             self.train_score_[i] = loss_(y, y_pred, sample_weight)
1543
1544             if self.verbose > 0:

~/anaconda3/lib/python3.7/site-packages/sklearn/ensemble/gradient_boosting.py in __call__
453         return np.mean((y - pred.ravel()) ** 2.0)
454     else:
-> 455         return (1.0 / sample_weight.sum() *
456                 np.sum(sample_weight * ((y - pred.ravel()) ** 2.0)))
457

~/anaconda3/lib/python3.7/site-packages/numpy/core/_methods.py in _sum(a, axis, dtype,
34 def _sum(a, axis=None, dtype=None, out=None, keepdims=False,
35         initial=_NoValue):
---> 36     return umr_sum(a, axis, dtype, out, keepdims, initial)
37
38 def _prod(a, axis=None, dtype=None, out=None, keepdims=False,

```

KeyboardInterrupt:

In [207]: *#gbrtestes -otimizado*

```

modelo= 'GBR:'
result = executaGBR(preproc=10,varLoss = 'ls', n_est=70, IC=0)
print('Parâmetros do modelo:',modelo,'\n',result[0])

resultados=exibeResultados(result)
for k,v in zip(resultados.keys(),resultados.values()):
    print(k)
    print(v,'\n-----')
```

Parâmetros do modelo: GBR:

```

MultiOutputRegressor(estimator=GradientBoostingRegressor(alpha=0.9, criterion='friedman_mse',
learning_rate=0.1, loss='ls', max_depth=2, max_features=None,
max_leaf_nodes=None, min_impurity_decrease=0.0,
min_impurity_split=None, min_samples_leaf=1,
min_sampl...ate=0, subsample=1.0, tol=0.0001,
validation_fraction=0.1, verbose=0, warm_start=False),
n_jobs=None)

cal
betaglicosidase    cmcase    fpase    xilanas
BIAS              -0.0000   -0.0000   0.0000   0.0000
```

MSE	0.0026	0.0000	0.0000	0.0811
R2	0.9990	0.9942	0.9975	0.9982
RER	88.1374	54.7326	62.7219	69.8766
RMSE	0.0514	0.0029	0.0013	0.2847
RPD	31.2930	13.1791	20.1423	23.4120
RPIQ	62.7954	15.1440	38.1713	31.4593
SEP	0.0519	0.0029	0.0013	0.2871

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0286	0.0001	0.0002	-0.1108
MSE	0.2839	0.0004	0.0001	8.9485
R2	0.8905	0.6928	0.8202	0.7986
RER	8.5229	7.4934	7.3457	6.6557
RMSE	0.5328	0.0212	0.0110	2.9914
RPD	3.0217	1.8043	2.3585	2.2285
RPIQ	6.0636	2.0733	4.4696	2.9944
SEP	0.5365	0.0214	0.0111	3.0146

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0237	-0.0026	0.0002	0.6358
MSE	0.1246	0.0001	0.0000	4.2426
R2	0.9455	0.8732	0.9199	0.8728
RER	10.7189	10.6424	11.1412	9.9808
RMSE	0.3530	0.0095	0.0065	2.0598
RPD	4.2846	2.8083	3.5325	2.8043
RPIQ	8.8774	3.0006	6.3374	1.8843
SEP	0.3609	0.0094	0.0067	2.0076

In [208]: resultados['cal']

Out[208]:

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0000	-0.0000	0.0000	0.0000
MSE	0.0026	0.0000	0.0000	0.0811
R2	0.9990	0.9942	0.9975	0.9982
RER	88.1374	54.7326	62.7219	69.8766
RMSE	0.0514	0.0029	0.0013	0.2847
RPD	31.2930	13.1791	20.1423	23.4120
RPIQ	62.7954	15.1440	38.1713	31.4593
SEP	0.0519	0.0029	0.0013	0.2871

In [209]: resultados['val']

Out[209]:

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0286	0.0001	0.0002	-0.1108
MSE	0.2839	0.0004	0.0001	8.9485

R2	0.8905	0.6928	0.8202	0.7986
RER	8.5229	7.4934	7.3457	6.6557
RMSE	0.5328	0.0212	0.0110	2.9914
RPD	3.0217	1.8043	2.3585	2.2285
RPIQ	6.0636	2.0733	4.4696	2.9944
SEP	0.5365	0.0214	0.0111	3.0146

In [210]: resultados['pred']

Out [210]:

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0237	-0.0026	0.0002	0.6358
MSE	0.1246	0.0001	0.0000	4.2426
R2	0.9455	0.8732	0.9199	0.8728
RER	10.7189	10.6424	11.1412	9.9808
RMSE	0.3530	0.0095	0.0065	2.0598
RPD	4.2846	2.8083	3.5325	2.8043
RPIQ	8.8774	3.0006	6.3374	1.8843
SEP	0.3609	0.0094	0.0067	2.0076

In [211]: reg, treino_teste, y_c, y_cv, y_p = result

7.4.2 Reais x preditos

In []:

```
In [212]: #knn reaisxpreditos
#calibração
pred=pd.DataFrame(y_c, columns=var_ae)
reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('CALIBRAÇÃO:\n')
round(reais_pred,4)
```

CALIBRAÇÃO:

Out [212]:

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	0.0759	0.0136	0.0139	0.0726	0.0842
1	2.7110	0.0548	0.0688	13.5829	2.7650
2	3.5974	0.0516	0.0731	15.3973	3.5304
3	2.1643	0.0830	0.0529	18.8324	2.2567
4	2.1150	0.0730	0.0505	18.4127	2.1618
5	0.0308	0.0213	0.0113	0.0996	0.0842
6	3.8803	0.0557	0.0691	11.3256	3.8664
7	0.1724	0.0112	0.0121	0.0924	0.1451

8	3.5610	0.0586	0.0561	10.0978	3.6089
9	0.0759	0.0136	0.0139	0.0726	0.0842
10	0.0759	0.0136	0.0139	0.0726	0.0842
11	3.5967	0.1065	0.0850	13.6476	3.5774
12	4.6037	0.1713	0.0919	16.8115	4.5525
13	3.8994	0.1118	0.0613	10.9512	3.8303
14	0.5905	0.0465	0.0267	18.7095	0.5975
15	0.6491	0.0605	0.0260	18.4274	0.6255
16	0.0554	0.0181	0.0106	0.3275	0.1530
17	3.8994	0.1118	0.0613	10.9512	3.8927
18	0.3900	0.0315	0.0283	14.1777	0.4320
19	0.0554	0.0181	0.0106	0.3275	0.0853
20	0.6010	0.0559	0.0116	20.1368	0.6236
21	3.1068	0.0781	0.0545	11.0526	3.1340
22	3.5974	0.0516	0.0731	15.3973	3.4154
23	0.0874	0.0217	0.0127	0.1071	0.0842
24	0.6010	0.0559	0.0116	20.1368	0.6151
25	3.8876	0.0418	0.0605	11.0267	3.8451
26	0.1671	0.0117	0.0104	0.1117	0.1451
27	3.2342	0.0672	0.0543	8.4772	3.1608
28	0.3828	0.0405	0.0301	12.4461	0.3405
29	0.6491	0.0605	0.0260	18.4274	0.6077
30	2.9123	0.1058	0.0747	14.6813	2.9927
31	2.9774	0.0704	0.0567	10.8002	3.0276
32	0.4280	0.0390	0.0334	13.7624	0.4248
33	0.5905	0.0465	0.0267	18.7095	0.5975
34	0.3828	0.0405	0.0301	12.4461	0.3786
35	0.0874	0.0217	0.0127	0.1071	0.0893
36	3.5974	0.0516	0.0731	15.3973	3.5286
37	0.1724	0.0112	0.0121	0.0924	0.2083
38	0.0308	0.0213	0.0113	0.0996	0.0762
39	2.9123	0.1058	0.0747	14.6813	2.9101
40	0.1724	0.0112	0.0121	0.0924	0.1888
41	3.2342	0.0672	0.0543	8.4772	3.1980
42	0.3828	0.0405	0.0301	12.4461	0.3692
43	2.7110	0.0548	0.0688	13.5829	2.7618
44	0.4280	0.0390	0.0334	13.7624	0.3684
45	4.6037	0.1713	0.0919	16.8115	4.5630
46	3.1068	0.0781	0.0545	11.0526	3.1064
47	2.1643	0.0830	0.0529	18.8324	2.2282
48	3.5610	0.0586	0.0561	10.0978	3.6089
49	3.5967	0.1065	0.0850	13.6476	3.6030
50	0.1671	0.0117	0.0104	0.1117	0.1573
51	3.7243	0.0561	0.0681	11.5736	3.7685
52	4.6037	0.1713	0.0919	16.8115	4.4551
53	0.3900	0.0315	0.0283	14.1777	0.3836
54	0.0554	0.0181	0.0106	0.3275	0.0841
55	2.7110	0.0548	0.0688	13.5829	2.7699

56	3.8876	0.0418	0.0605	11.0267	3.8635
57	3.5610	0.0586	0.0561	10.0978	3.6089
58	3.1068	0.0781	0.0545	11.0526	3.1221
59	2.1150	0.0730	0.0505	18.4127	2.0571

	pred: cmcase	pred: fpase	pred: xilanas
0	0.0162	0.0135	0.1813
1	0.0600	0.0690	13.7835
2	0.0521	0.0719	15.3426
3	0.0797	0.0555	18.3500
4	0.0750	0.0522	18.1319
5	0.0201	0.0122	0.1813
6	0.0585	0.0687	11.1866
7	0.0127	0.0121	0.0730
8	0.0591	0.0571	10.4273
9	0.0162	0.0143	0.1813
10	0.0162	0.0135	0.1813
11	0.1050	0.0828	13.2378
12	0.1683	0.0908	16.7338
13	0.1095	0.0606	10.9158
14	0.0482	0.0260	18.5409
15	0.0588	0.0256	18.3451
16	0.0188	0.0114	0.5440
17	0.1108	0.0629	11.3793
18	0.0343	0.0282	14.5046
19	0.0191	0.0116	0.6505
20	0.0548	0.0132	19.7091
21	0.0750	0.0562	11.3890
22	0.0522	0.0704	14.8566
23	0.0203	0.0133	0.1813
24	0.0524	0.0130	19.7091
25	0.0462	0.0617	10.9710
26	0.0144	0.0112	0.3398
27	0.0668	0.0561	8.8393
28	0.0398	0.0292	12.5054
29	0.0574	0.0263	18.2930
30	0.1027	0.0748	14.7998
31	0.0719	0.0569	10.7558
32	0.0350	0.0328	13.6834
33	0.0459	0.0243	18.5409
34	0.0404	0.0298	12.5634
35	0.0201	0.0131	0.1813
36	0.0510	0.0711	15.3426
37	0.0137	0.0122	0.6369
38	0.0201	0.0127	0.1813
39	0.1027	0.0748	14.7998
40	0.0124	0.0118	-0.0173
41	0.0651	0.0536	9.0941

42	0.0377	0.0292	12.5589
43	0.0597	0.0697	13.7835
44	0.0362	0.0306	13.3166
45	0.1658	0.0901	16.7527
46	0.0751	0.0537	10.9624
47	0.0884	0.0544	18.5075
48	0.0597	0.0560	10.1367
49	0.1068	0.0839	13.2336
50	0.0160	0.0113	0.1770
51	0.0585	0.0677	11.8061
52	0.1621	0.0881	16.0129
53	0.0323	0.0288	13.8046
54	0.0237	0.0120	0.6811
55	0.0531	0.0695	13.7835
56	0.0466	0.0594	10.9047
57	0.0571	0.0583	10.6223
58	0.0773	0.0545	11.0751
59	0.0747	0.0509	18.1175

```
In [213]: #validação
pred=pd.DataFrame(y_cv, columns=var_ae)
reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('VALIDAÇÃO CRUZADA:\n')
round(reais_pred,4)
```

VALIDAÇÃO CRUZADA:

```
Out [213]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	0.0759	0.0136	0.0139	0.0726	0.1211
1	2.7110	0.0548	0.0688	13.5829	2.8842
2	3.5974	0.0516	0.0731	15.3973	3.1145
3	2.1643	0.0830	0.0529	18.8324	3.2741
4	2.1150	0.0730	0.0505	18.4127	2.9946
5	0.0308	0.0213	0.0113	0.0996	0.1211
6	3.8803	0.0557	0.0691	11.3256	3.2937
7	0.1724	0.0112	0.0121	0.0924	0.1134
8	3.5610	0.0586	0.0561	10.0978	3.6671
9	0.0759	0.0136	0.0139	0.0726	0.0989
10	0.0759	0.0136	0.0139	0.0726	0.0989
11	3.5967	0.1065	0.0850	13.6476	3.2823
12	4.6037	0.1713	0.0919	16.8115	3.7451
13	3.8994	0.1118	0.0613	10.9512	3.6977

14	0.5905	0.0465	0.0267	18.7095	0.6328
15	0.6491	0.0605	0.0260	18.4274	0.6389
16	0.0554	0.0181	0.0106	0.3275	0.2903
17	3.8994	0.1118	0.0613	10.9512	3.8506
18	0.3900	0.0315	0.0283	14.1777	0.6707
19	0.0554	0.0181	0.0106	0.3275	0.3132
20	0.6010	0.0559	0.0116	20.1368	0.6293
21	3.1068	0.0781	0.0545	11.0526	3.6581
22	3.5974	0.0516	0.0731	15.3973	2.7571
23	0.0874	0.0217	0.0127	0.1071	0.0989
24	0.6010	0.0559	0.0116	20.1368	0.5356
25	3.8876	0.0418	0.0605	11.0267	3.7519
26	0.1671	0.0117	0.0104	0.1117	0.1259
27	3.2342	0.0672	0.0543	8.4772	2.9644
28	0.3828	0.0405	0.0301	12.4461	0.2510
29	0.6491	0.0605	0.0260	18.4274	0.6302
30	2.9123	0.1058	0.0747	14.6813	3.3932
31	2.9774	0.0704	0.0567	10.8002	3.4245
32	0.4280	0.0390	0.0334	13.7624	0.2265
33	0.5905	0.0465	0.0267	18.7095	0.6129
34	0.3828	0.0405	0.0301	12.4461	0.4137
35	0.0874	0.0217	0.0127	0.1071	0.0891
36	3.5974	0.0516	0.0731	15.3973	1.0866
37	0.1724	0.0112	0.0121	0.0924	0.1727
38	0.0308	0.0213	0.0113	0.0996	0.0903
39	2.9123	0.1058	0.0747	14.6813	3.1205
40	0.1724	0.0112	0.0121	0.0924	0.2210
41	3.2342	0.0672	0.0543	8.4772	2.3833
42	0.3828	0.0405	0.0301	12.4461	0.3105
43	2.7110	0.0548	0.0688	13.5829	2.9921
44	0.4280	0.0390	0.0334	13.7624	0.1845
45	4.6037	0.1713	0.0919	16.8115	3.4261
46	3.1068	0.0781	0.0545	11.0526	3.0751
47	2.1643	0.0830	0.0529	18.8324	3.5023
48	3.5610	0.0586	0.0561	10.0978	3.5940
49	3.5967	0.1065	0.0850	13.6476	3.8319
50	0.1671	0.0117	0.0104	0.1117	0.1072
51	3.7243	0.0561	0.0681	11.5736	3.6813
52	4.6037	0.1713	0.0919	16.8115	3.7868
53	0.3900	0.0315	0.0283	14.1777	0.3315
54	0.0554	0.0181	0.0106	0.3275	0.2871
55	2.7110	0.0548	0.0688	13.5829	2.9456
56	3.8876	0.0418	0.0605	11.0267	3.7546
57	3.5610	0.0586	0.0561	10.0978	3.6636
58	3.1068	0.0781	0.0545	11.0526	3.6300
59	2.1150	0.0730	0.0505	18.4127	2.5303

pred: cmcase pred: fpase pred: xylanase

0	0.0168	0.0132	0.3268
1	0.0623	0.0674	14.1170
2	0.0587	0.0694	16.1787
3	0.1267	0.0758	14.8227
4	0.1284	0.0689	17.3826
5	0.0195	0.0132	0.2490
6	0.0738	0.0655	10.8753
7	0.0205	0.0121	0.0662
8	0.0818	0.0641	11.3133
9	0.0220	0.0172	0.2344
10	0.0200	0.0132	0.2344
11	0.0919	0.0757	11.5832
12	0.1129	0.0671	15.3246
13	0.0847	0.0644	11.5080
14	0.0514	0.0188	19.2991
15	0.0555	0.0161	18.3954
16	0.0186	0.0140	13.5152
17	0.0630	0.0765	12.0132
18	0.0358	0.0286	12.5698
19	0.0268	0.0217	3.2567
20	0.0569	0.0254	18.9700
21	0.0674	0.0636	12.9748
22	0.0476	0.0628	13.3761
23	0.0201	0.0125	0.1634
24	0.0308	0.0217	14.1637
25	0.0592	0.0638	11.4497
26	0.0178	0.0127	2.0365
27	0.0634	0.0610	11.9396
28	0.0363	0.0261	8.3807
29	0.0510	0.0275	18.9869
30	0.0992	0.0756	15.2841
31	0.0733	0.0611	10.1500
32	0.0314	0.0313	12.2067
33	0.0491	0.0195	18.3408
34	0.0404	0.0275	13.2205
35	0.0198	0.0134	0.1959
36	0.0450	0.0328	15.3175
37	0.0253	0.0126	2.4953
38	0.0185	0.0166	0.2003
39	0.0953	0.0745	14.7753
40	0.0228	0.0112	1.0173
41	0.0643	0.0483	15.8813
42	0.0364	0.0277	12.3573
43	0.0672	0.0719	13.8974
44	0.0229	0.0184	8.2062
45	0.1482	0.0787	13.8089
46	0.0704	0.0540	10.7192
47	0.1295	0.0769	15.5499

48	0.0620	0.0558	10.2997
49	0.1057	0.0670	11.3014
50	0.0214	0.0158	4.4761
51	0.0652	0.0636	12.4043
52	0.0817	0.0592	11.8804
53	0.0423	0.0280	10.8189
54	0.0336	0.0177	8.1432
55	0.0608	0.0712	14.7639
56	0.0545	0.0574	10.7350
57	0.0558	0.0642	11.0311
58	0.0853	0.0613	11.7639
59	0.0726	0.0606	16.1656

```
In [214]: #predição
pred=pd.DataFrame(y_p, columns=var_ae)
reais = treino_teste[3]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('Predição (validação externa):\n')
round(reais_pred,4)
```

Predição (validação externa):

```
Out[214]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	0.3900	0.0315	0.0283	14.1777	0.2856
1	0.6491	0.0605	0.0260	18.4274	0.6028
2	2.9123	0.1058	0.0747	14.6813	3.1864
3	0.1671	0.0117	0.0104	0.1117	0.2185
4	3.7243	0.0561	0.0681	11.5736	3.6123
5	3.8803	0.0557	0.0691	11.3256	2.8666
6	0.6010	0.0559	0.0116	20.1368	0.5975
7	3.8994	0.1118	0.0613	10.9512	3.8396
8	3.2342	0.0672	0.0543	8.4772	3.1042
9	0.4280	0.0390	0.0334	13.7624	0.2783
10	2.9774	0.0704	0.0567	10.8002	3.3334
11	2.1150	0.0730	0.0505	18.4127	2.0944
12	2.9774	0.0704	0.0567	10.8002	3.6650
13	0.5905	0.0465	0.0267	18.7095	0.6255
14	3.8803	0.0557	0.0691	11.3256	3.0827
15	0.0874	0.0217	0.0127	0.1071	0.0842
16	3.5967	0.1065	0.0850	13.6476	3.7993
17	3.8876	0.0418	0.0605	11.0267	3.6952
18	2.1643	0.0830	0.0529	18.8324	2.4910
19	0.0308	0.0213	0.0113	0.0996	0.1145

20	3.7243	0.0561	0.0681	11.5736	3.8416
----	--------	--------	--------	---------	--------

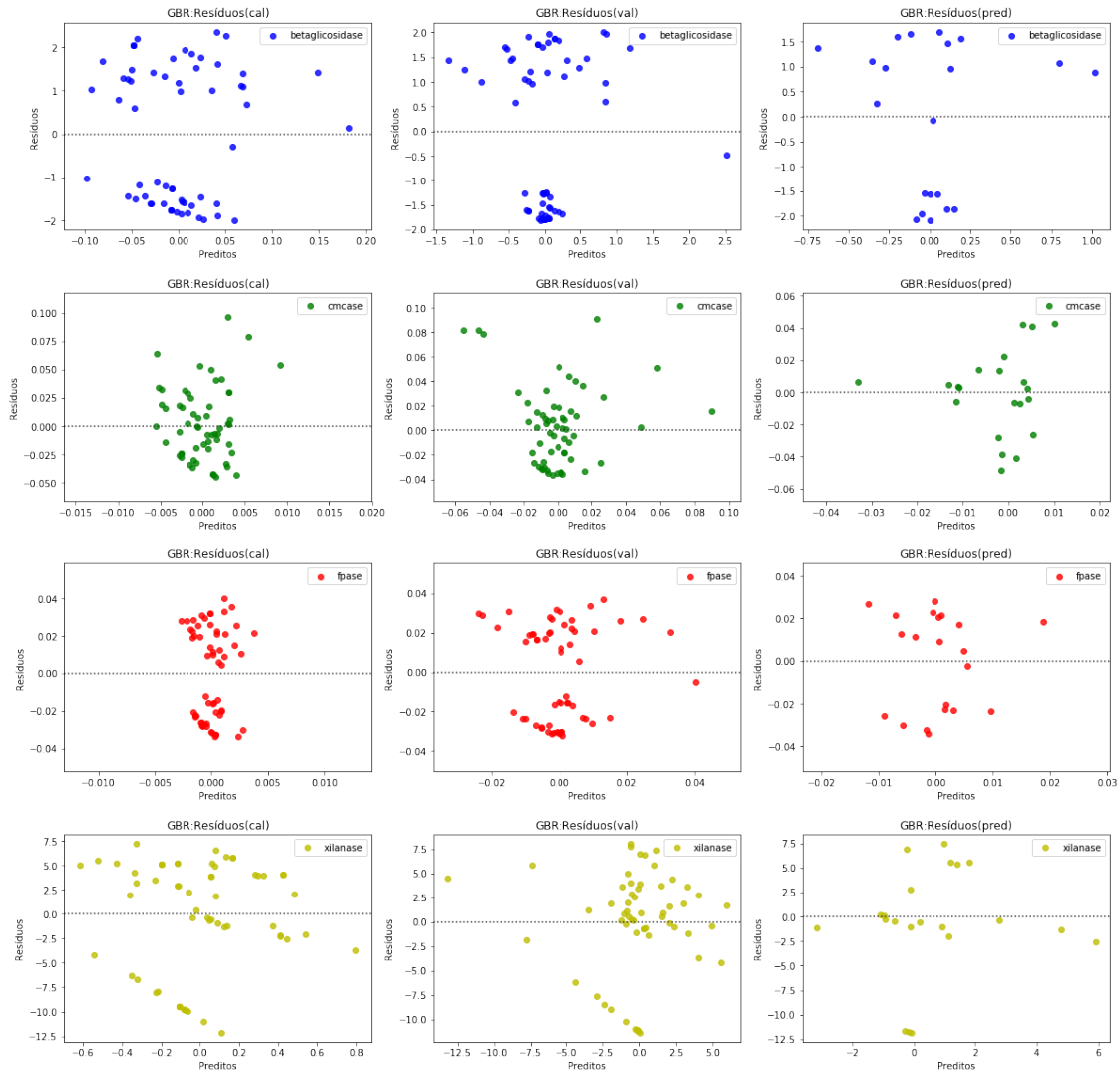
	pred: cmcase	pred: fpase	pred: xilase
0	0.0337	0.0265	9.3818
1	0.0561	0.0244	17.2181
2	0.1027	0.0748	14.7998
3	0.0133	0.0163	0.4034
4	0.0672	0.0676	11.3799
5	0.0688	0.0697	12.4162
6	0.0546	0.0206	19.1675
7	0.1018	0.0731	11.8792
8	0.0630	0.0579	11.6378
9	0.0337	0.0238	7.8443
10	0.0770	0.0561	10.9070
11	0.0750	0.0449	17.0003
12	0.0671	0.0519	9.6762
13	0.0580	0.0237	18.9442
14	0.0665	0.0682	12.2814
15	0.0201	0.0143	0.1813
16	0.1014	0.0661	10.8735
17	0.0747	0.0677	11.6667
18	0.0840	0.0589	17.0333
19	0.0228	0.0127	0.2780
20	0.0536	0.0641	10.6382

In []:

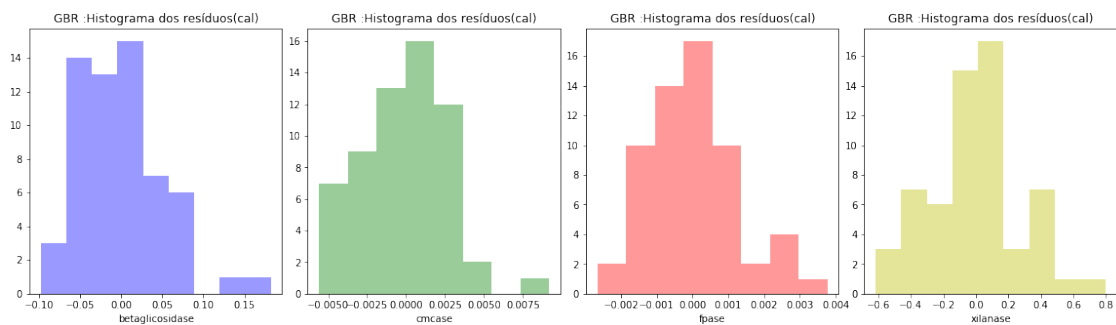
7.4.3 GBR: Gráficos de resíduos - histograma - reais x preditos

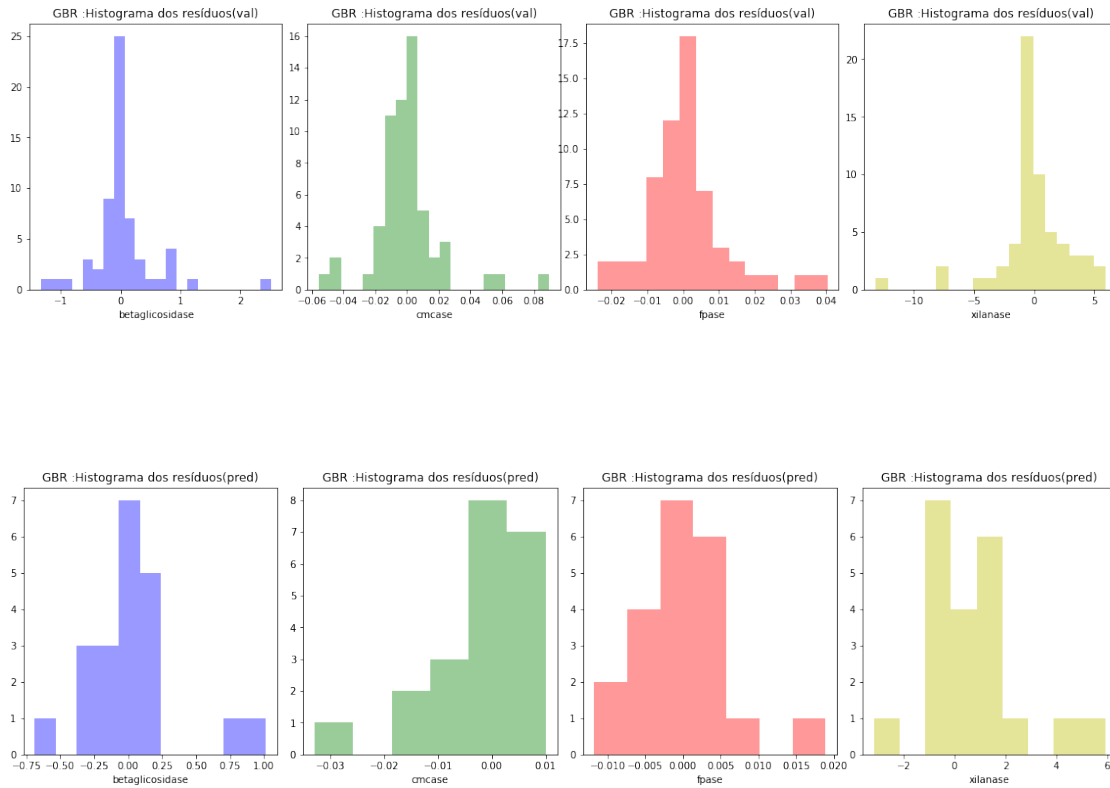
```
In [215]: #título para os gráficos
          modelo = 'GBR'
```

```
In [216]: #gráfico dos resíduos
          #@gbrgraf
          graficoResiduos(modelo, treino_teste, y_c,y_cv,y_p)
```

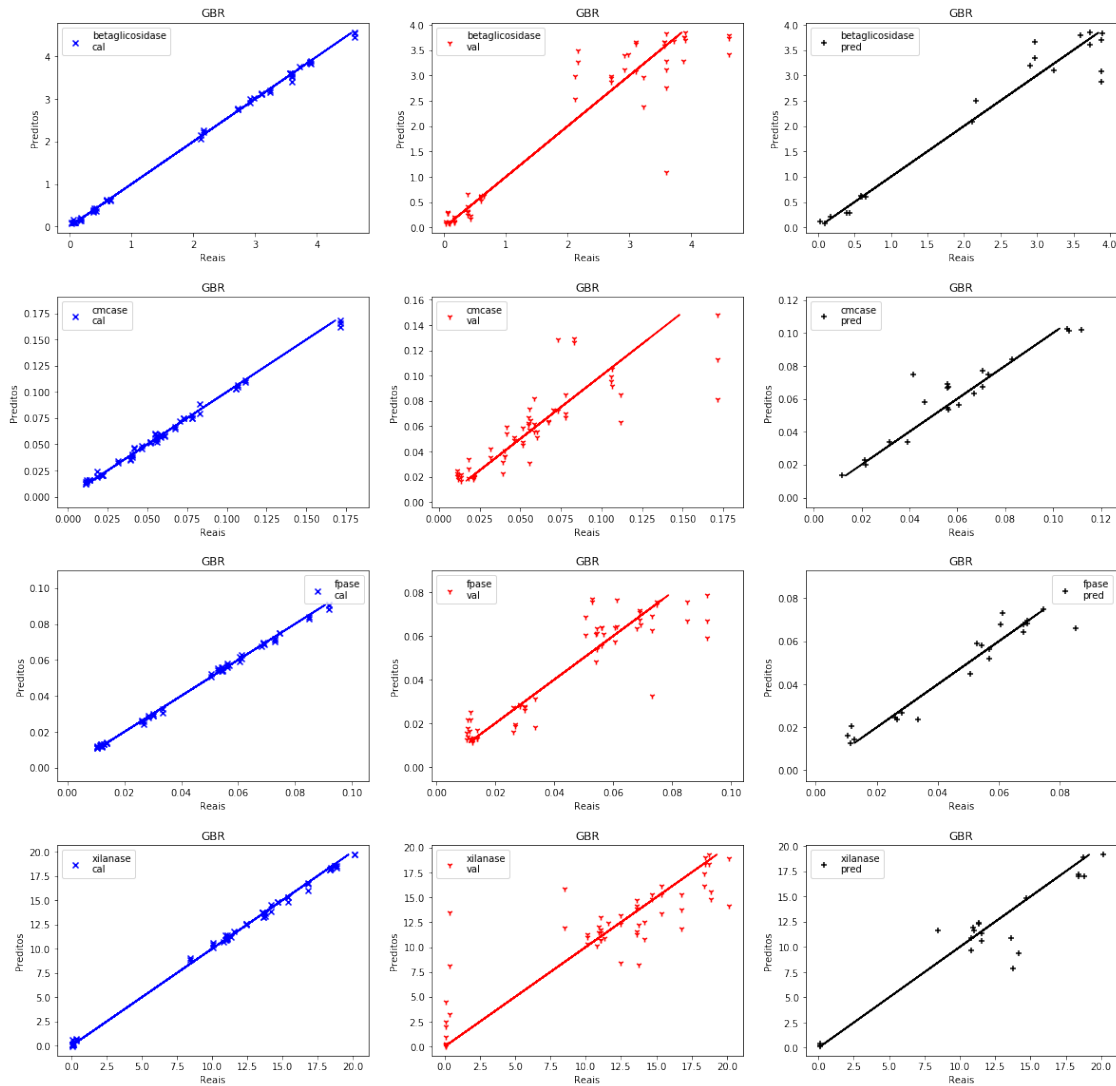


In [217]: *#histograma dos resíduos*
 graficoHist(modelo, treino_teste, y_c,y_cv,y_p)

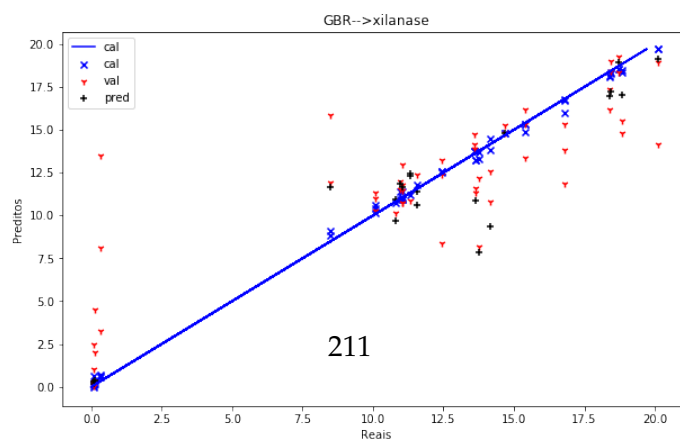
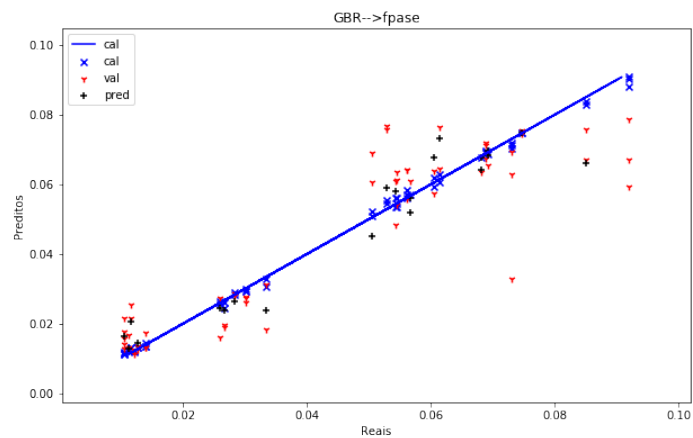
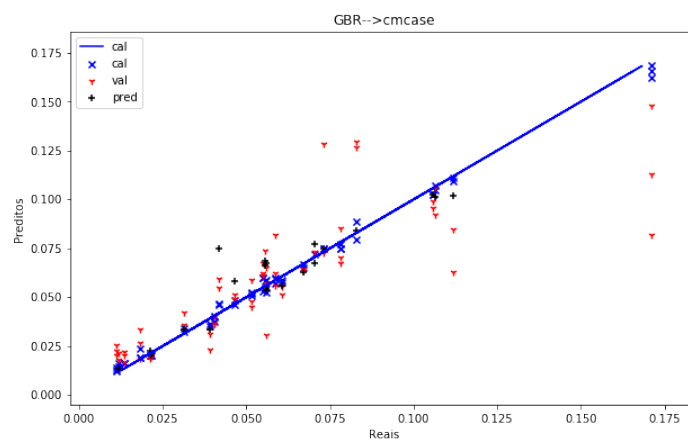
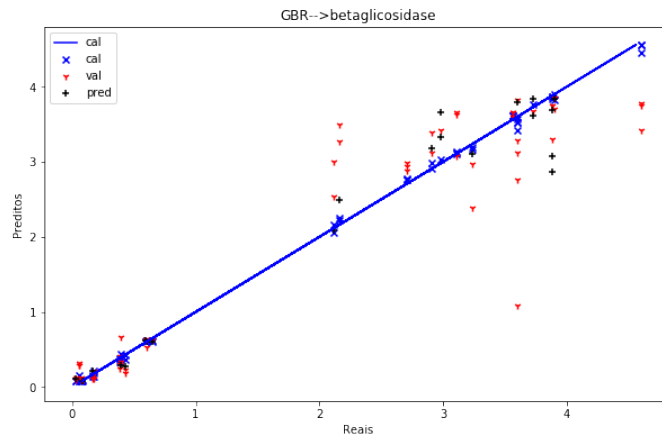




In [218]: *#graico de reais x preditos*
graficoReaisPreditosSep(modelo, treino_teste, y_c,y_cv,y_p)

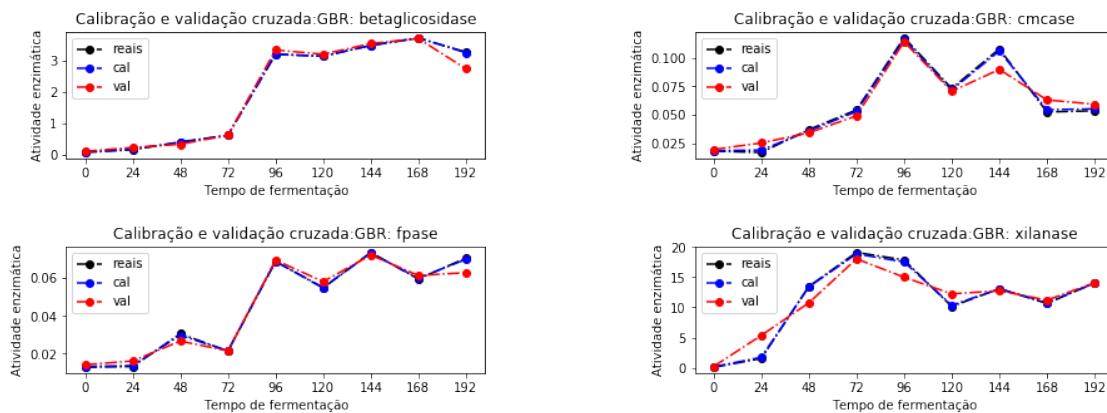


In [219]: *#gráfico de reais x preditos conjuntamente*
`graficoReaisPreditos(modelo, treino_teste, y_c,y_cv,y_p)`



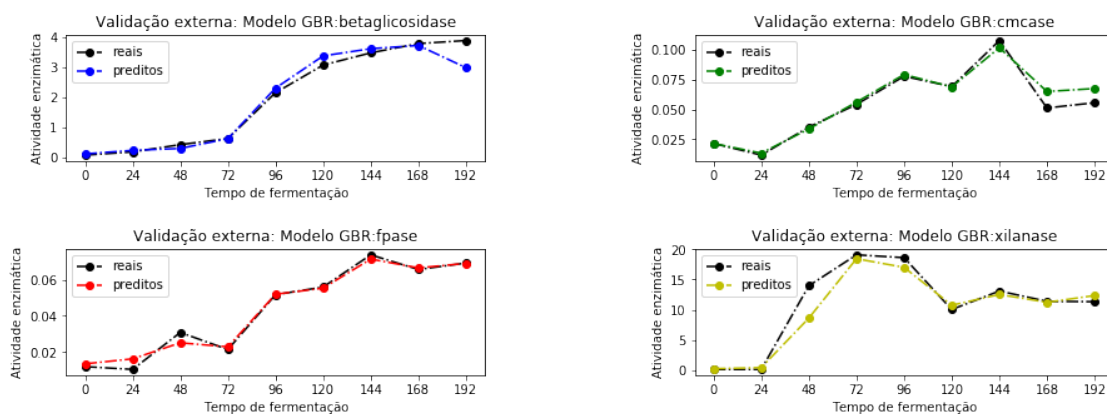
7.4.4 GBR: Gráficos: dados de treino

```
In [220]: y_treino = treino_teste[2]
          graficoTreinamento(modelo, y_treino, y_c,y_cv)
```



7.4.5 GBR: Gráficos de teste

```
In [221]: y_teste = treino_teste[3]
          graficoTeste(modelo, y_teste, y_p)
```



```
In [ ]:
```

7.4.6 GBR: teste com base externa: EETA desnaturado

In []:

```
In [120]: #@gbrtesteExterno
```

```
modelo = 'GBR:'
result = executaGBR(preproc=10,varLoss = 'ls', n_est=70, IC=0)
print('Parâmetros do modelo:',modelo,'\n',result[0])

resultados=exibeResultados(result)
```

```
In [222]: de = dados_back.copy()
de=de[(de['eenz'] == 'eeta')]
```

```
In [223]: de = dados_back.copy()
de=de[(de['experimento'] == 'bioB')&(de['inter']!= 120)]
```

In []:

```
In [176]: #buscando base de teste externa
```

```
de = dados_back.copy()
de=de[(de['eenz'] == 'eeta')&(de['experimento']=='biod1')&(de['inter']!= 1)&(de['int
#Separar somente as amostras que contenham todas as atividades enzimáticas
de = de.loc[(de['betaglicosidase'].notnull())
            & (de['cmcase'].notnull())
            & (de['fpase'].notnull())
            &(de['xilanase'].notnull())]

de.shape
```

```
Out[176]: (12, 713)
```

```
In [177]: de.head(5)
```

```
Out[177]:
```

		descricao	1100nm	1102nm	1104nm	1106nm	1108nm	\
791	bio_25janp0_1_desn		0.038744	0.038471	0.038295	0.038206	0.038193	
792	bio_25janp0_2_desn		0.038601	0.038637	0.038631	0.038613	0.038621	
793	bio_25janp0_3_desn		0.039642	0.039467	0.039371	0.039322	0.039300	
809	bio_25janp5_1_desn		0.048341	0.046943	0.046041	0.045418	0.044937	
810	bio_25janp5_2_desn		0.048823	0.047629	0.046772	0.046076	0.045451	

		1110nm	1112nm	1114nm	1116nm	...	cmcase	fpase	xilanase	\
791		0.038237	0.038330	0.038481	0.038710	...	0.035	0.051	24.094000	
792		0.038688	0.038837	0.039073	0.039391	...	0.035	0.051	24.094000	
793		0.039299	0.039333	0.039428	0.039612	...	0.035	0.051	24.094000	
809		0.044537	0.044219	0.044010	0.043935	...	0.067	0.060	17.361999	
810		0.044883	0.044408	0.044065	0.043873	...	0.067	0.060	17.361999	

	proteinas	eenz	temp	dur	inter	proc	experimento
791	NaN	eeta	70	33	0	des	biod1

792	NaN	eeta	70	33	0	des	biod1
793	NaN	eeta	70	33	0	des	biod1
809	NaN	eeta	70	33	5	des	biod1
810	NaN	eeta	70	33	5	des	biod1

[5 rows x 713 columns]

```
In [224]: #Definindo os dataFrames iniciais para começar o processamento
de_x = de.loc[:,var_abs_txt] #absorbâncias
de_y = de.loc[:,var_ae] #AE
de_inter=pd.DataFrame(de.loc[:,'inter'], columns=['inter'])
#df = dados.loc[:,var_abs_txt+var_ae]

In [197]: de_x.shape,de_y.shape, de_inter.shape

Out[197]: ((21, 244), (21, 4), (21, 1))

In [227]: #executa pré-processamento equivalente ao do modelo de treinamento
x = executaPreprocSimples(1,de_x)
preditos=reg.predict(x)

In [228]: #para exibir o gráfico
#para todas as atividades
#cria um data frame com os valores reais e preditos para os dados de teste
df_pred = {}
for valor in var_ae:
    df_pred[valor] = []
i=0
for valor in var_ae:
    df =pd.DataFrame(columns=['reais','preditos'], index= de_y.index)
    df['reais'] = de_y[valor]
    df['preditos'] = pd.DataFrame(preditos[:,i],index= de_y.index)
    i +=1
    df_pred[valor] = df.copy()

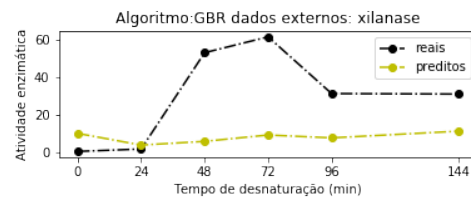
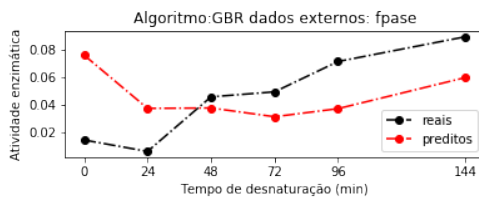
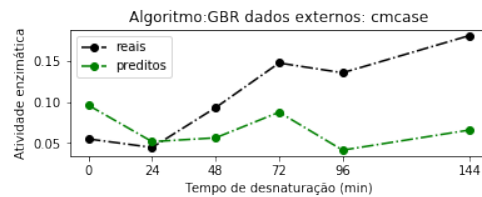
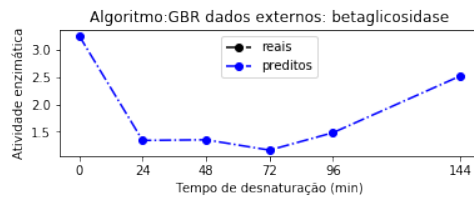
df_pred_inter = {}
for valor in var_ae:
    df_pred_inter[valor] = []
for valor in var_ae:
    df_pred_inter[valor] = df_pred[valor].copy()
    df_pred_inter[valor]['inter'] = de_inter.loc[:,'inter']

#ordena valores pelo intervalo
df_ord_teste = {}
for valor in var_ae:
    df_ord_teste[valor] = []
for valor in var_ae:
    df_ord_teste[valor] = df_pred_inter[valor].sort_values(['inter'])
```

```

#calculando a média para cada ponto
df_teste_media = {}
for valor in var_ae:
    df_teste_media[valor] = []
for valor in var_ae:
    df_teste_media[valor] = df_ord_teste[valor].groupby('inter').mean()
x = list(df_teste_media['xilanase'].index)
var = ['reais', 'preditos']
tipoAE= ['bo-.', 'go-.', 'ro-.', 'yo-.']
j = 0
fig = plt.figure(figsize=(15,5))
plt.subplots_adjust(hspace = 0.7, wspace=0.5)
for valor in var_ae:
    ax = fig.add_subplot(2,2,j+1)
    ax.plot(x,df_teste_media[valor][var[0]], 'ko-.', label=var[0])
    ax.plot(x,df_teste_media[valor][var[1]], tipoAE[j], label=var[1])
    j +=1
    ax.legend(loc=2)
    ax.set_title('Algoritmo:'+modelo+' dados externos'+': '+valor)
    ax.set_xlabel('Tempo de desnaturação (min)')
    ax.set_ylabel('Atividade enzimática')
    ax.set_xticks(x)
    plt.legend(loc='best')

```



7.5 PLS

7.5.1 PLS: função completa

In [229]: `#pls`

`#função completa para execução do PLS:`

`#A variável preproc determinará o tipo de processamento que será executado (0,1,2,3,4)`

`def executaPLS(preproc,IC=0):`

`#separando o conjunto de dados em treino e teste`

```

x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc,False,IC)

#Calcula o número de componentes ideal para o PLS
mse = []
component = np.arange(1, 20)
for i in component:
    pls = PLSRegression(n_components=i)
    # Fit
    pls.fit(x_treino, y_treino)
    # Prediction
    Y_pred = pls.predict(x_teste)

    mse_p = mean_squared_error(y_teste, Y_pred)
    mse.append(mse_p)

    comp = 100*(i+1)/20
    # Truque para atualizar o progresso do processamento na mesma linha
    print("\r%d%% completed " % comp, end='')

# Calcula e imprime a posição do menor valor de MSE
msemin = np.argmin(mse)
print("Sugestão para o número de variáveis latentes: ", msemin+1)

with plt.style.context(('ggplot')):
    plt.plot(component, np.array(mse), '-v', color = 'blue', mfc='blue')
    plt.plot(component[msemin], np.array(mse)[msemin], 'P', ms=10, mfc='red')
    plt.xlabel('Numero de componentes para o PLS')
    plt.ylabel('MSE')
    plt.title('PLS')
    plt.xlim(xmin=-1)

    plt.show()

# Roda o PLS e produz uma variável reduzida xRed e seleciona as primeiras componentes
pls = PLSRegression(n_components=msemin+1)

result = executaCVP([x_treino, x_teste, y_treino, y_teste], pls)

dic = {'result':result,'min':msemin+1}
return dic

```

```

In [230]: #função completa para execução do PLS:
#A variável preproc determinará o tipo de processamento que será executado (0,1,2,3,
def executaPLSResumida(preproc=1, nPC=3, padroniza=False, max=500,IC=0):

```



```

#separando o conjunto de dados em treino e teste
x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc,padroniza,IC)

#Calcula o número de componentes ideal para o PLS
component = nPC

# Roda o PLS e produz uma variável reduzida xRed e seleciona as primeiras compo
pls = PLSRegression(n_components=nPC, max_iter=max)

result = executaCVP([x_treino, x_teste, y_treino, y_teste], pls)

return result

```

7.5.2 PLS: testes

```

In [231]: preK = list(preProc.keys())
          preV = list(preProc.values())

```

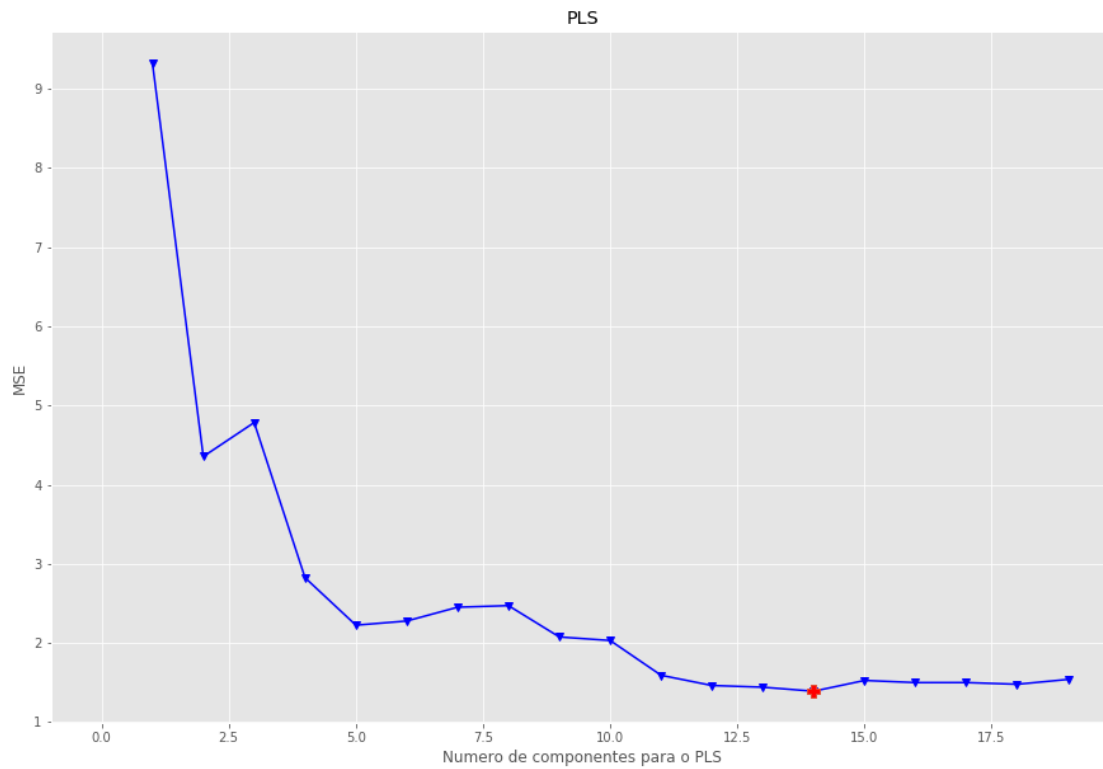
```

In [232]: nVL = []
          for k in preK:
              print(preProc[k])
              dic = executaPLS(k)
              nVL.append(dic['min'])

```

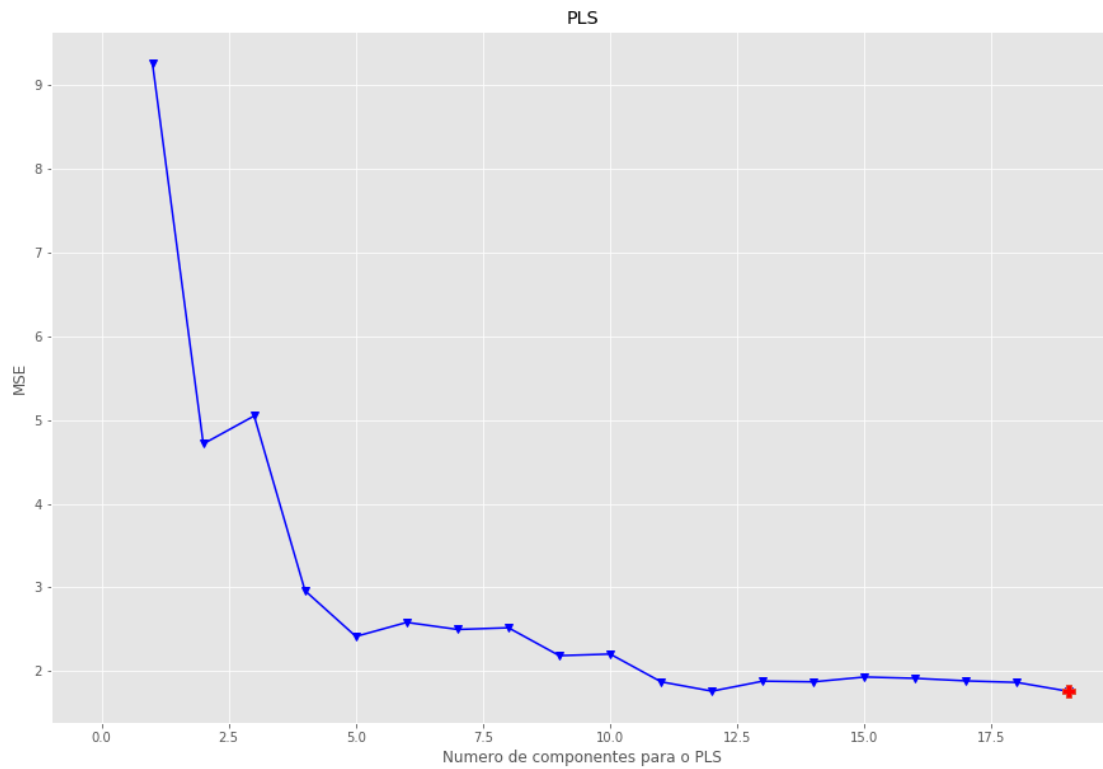
Pré-proc: 0--> Sem pré-processamento

100% completed Sugestão para o número de variáveis latentes: 14

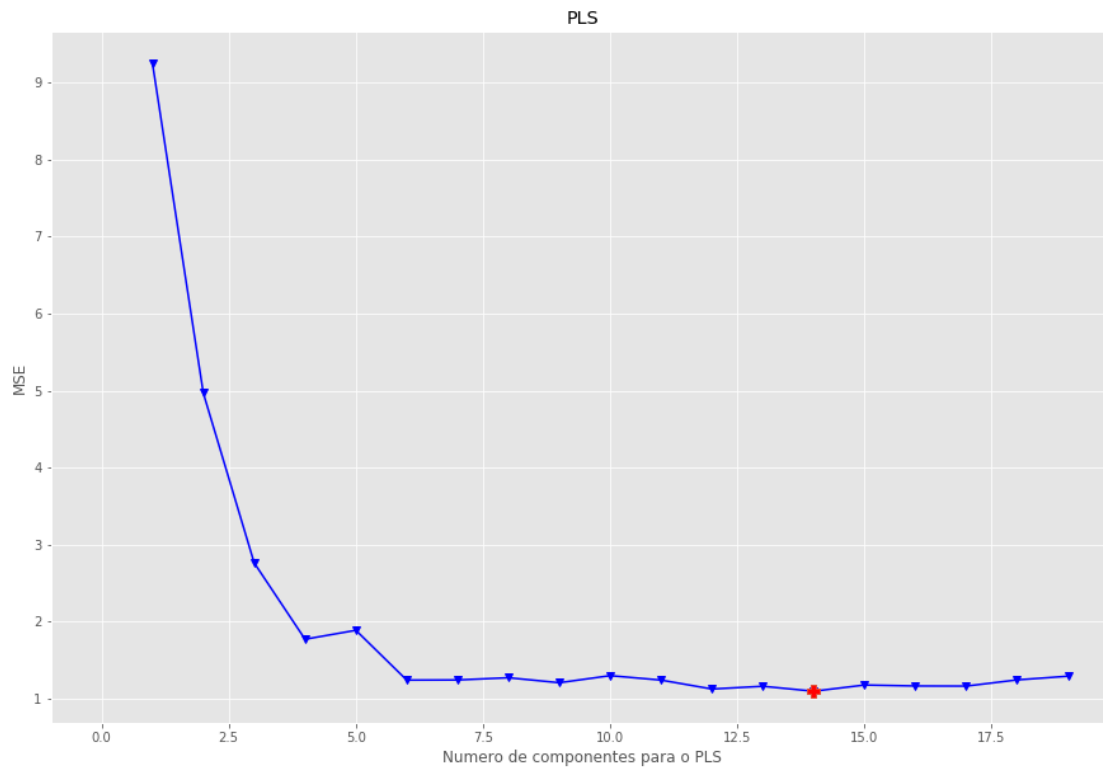


Pré-proc: 1--> Padronização

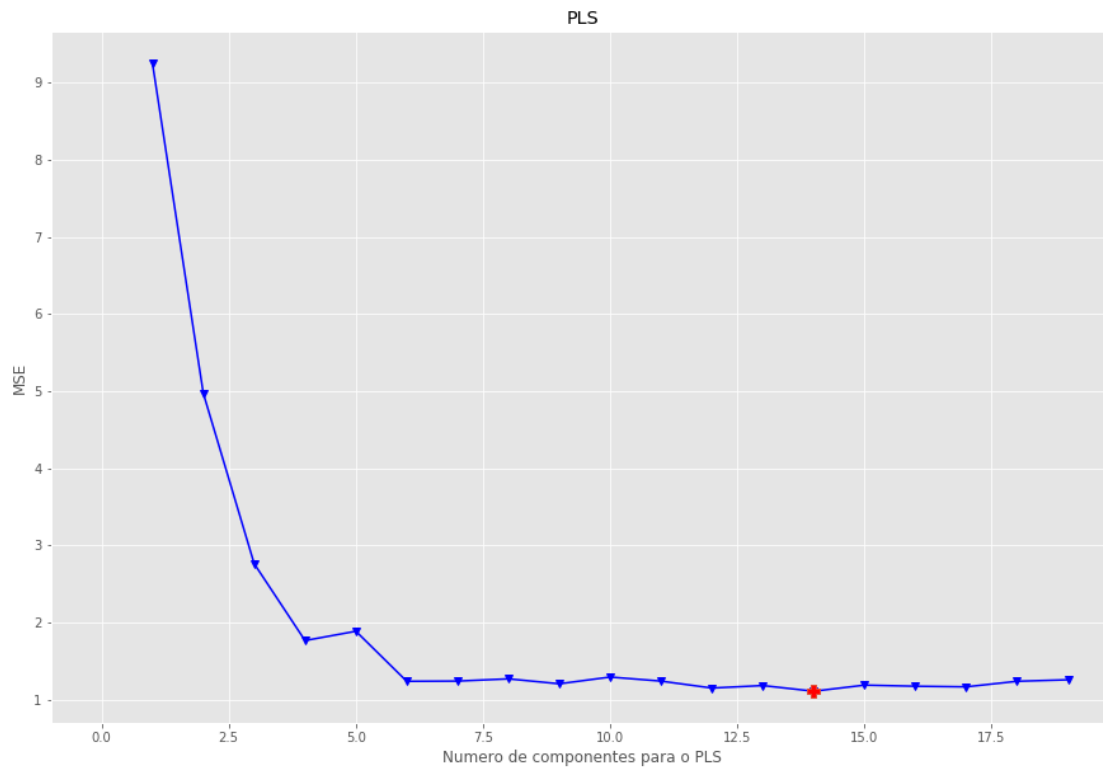
100% completed Sugestão para o número de variáveis latentes: 19



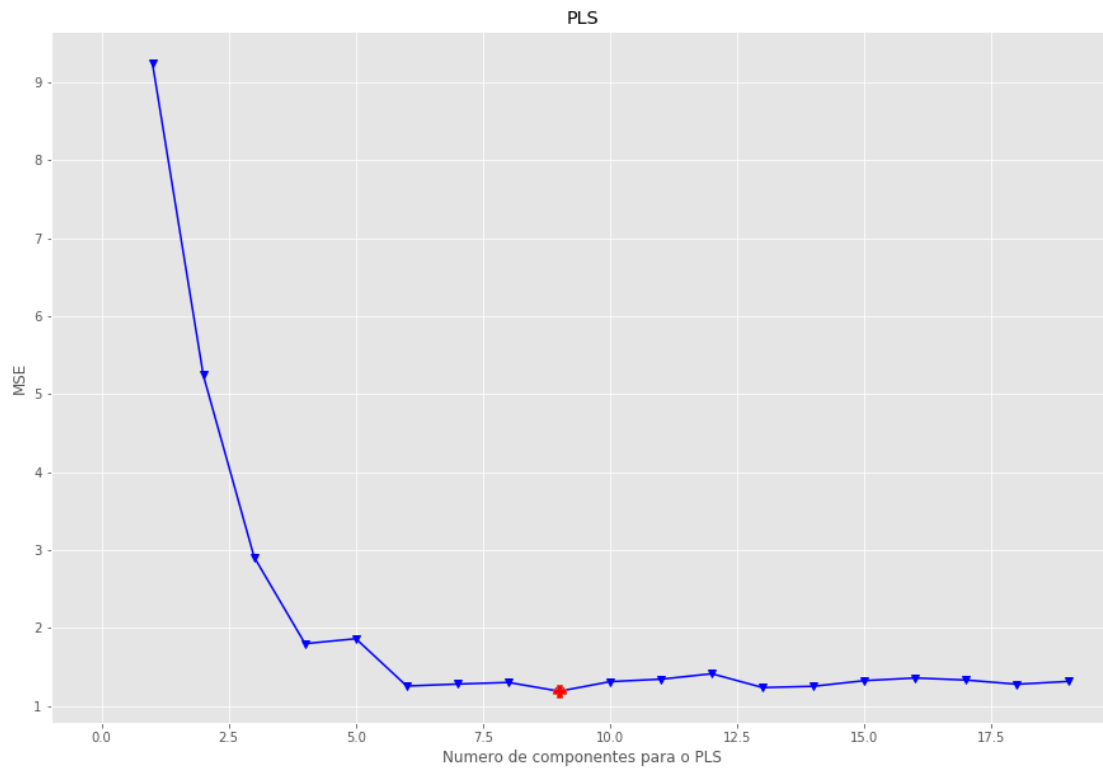
Pré-proc: 2--> Suavização(SavGol) - Par:3,1,1
100% completed Sugestão para o número de variáveis latentes: 14



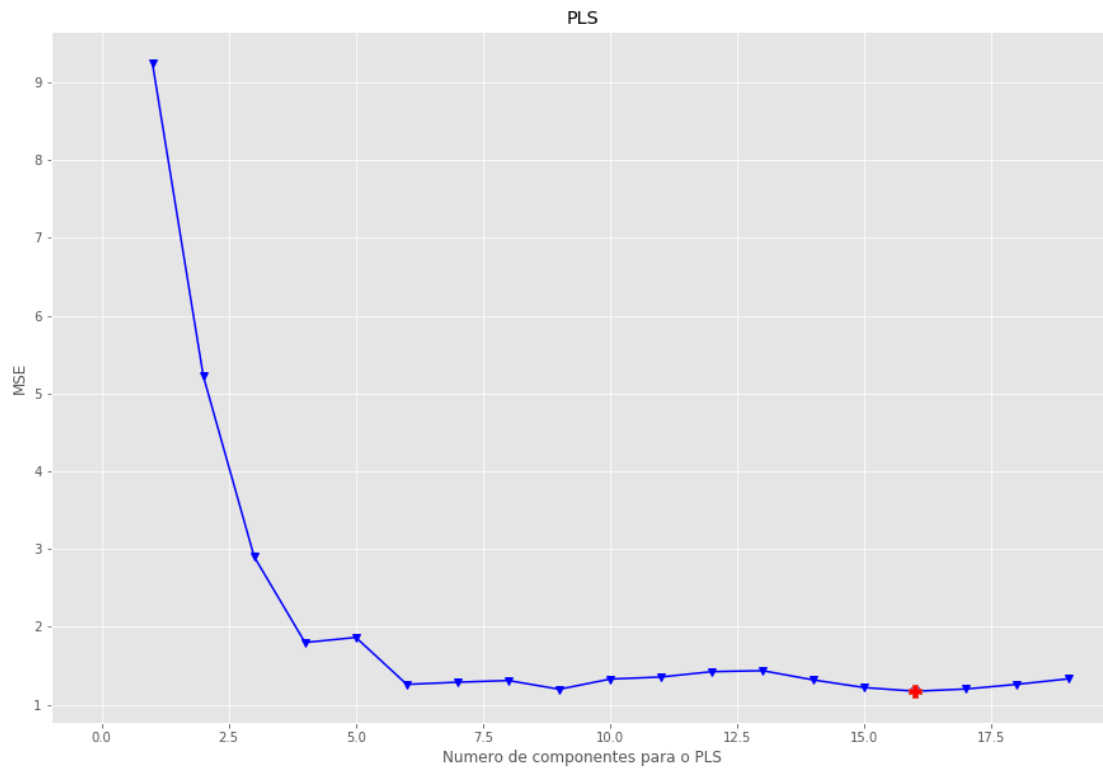
Pré-proc: 3--> Suavização(SavGol) - Par:3,2,1
100% completed Sugestão para o número de variáveis latentes: 14



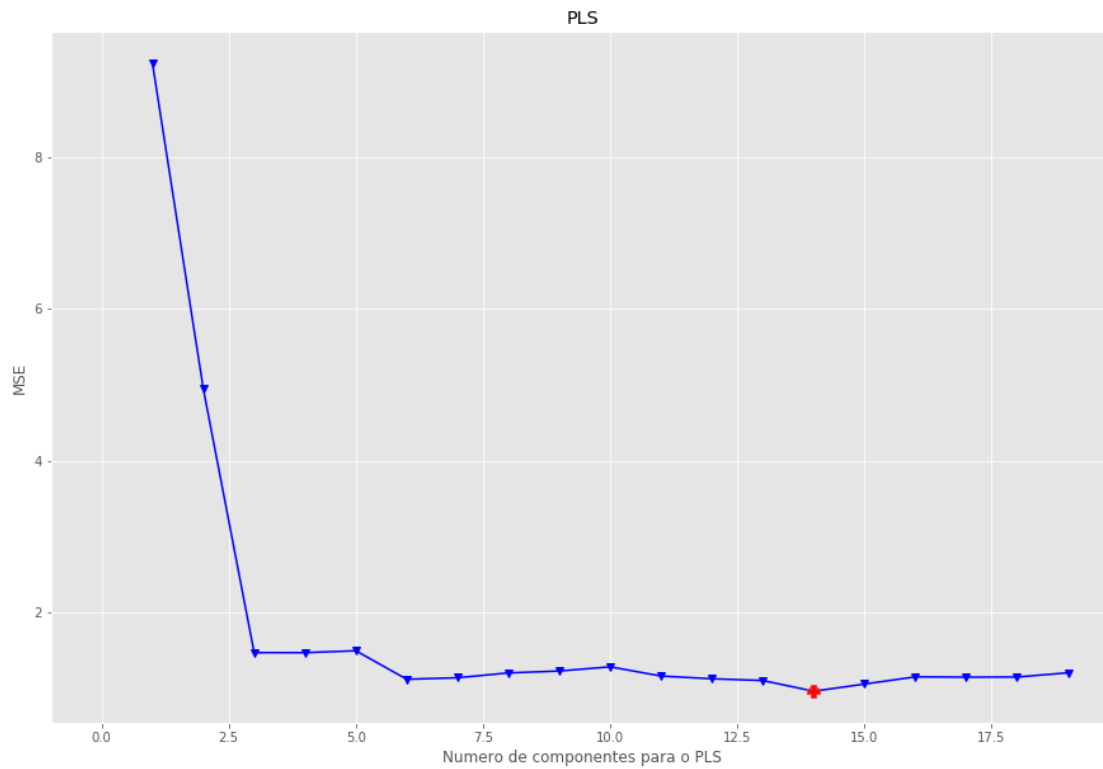
Pré-proc: 4--> Suavização(SavGol) - Par:5,1,1
100% completed Sugestão para o número de variáveis latentes: 9



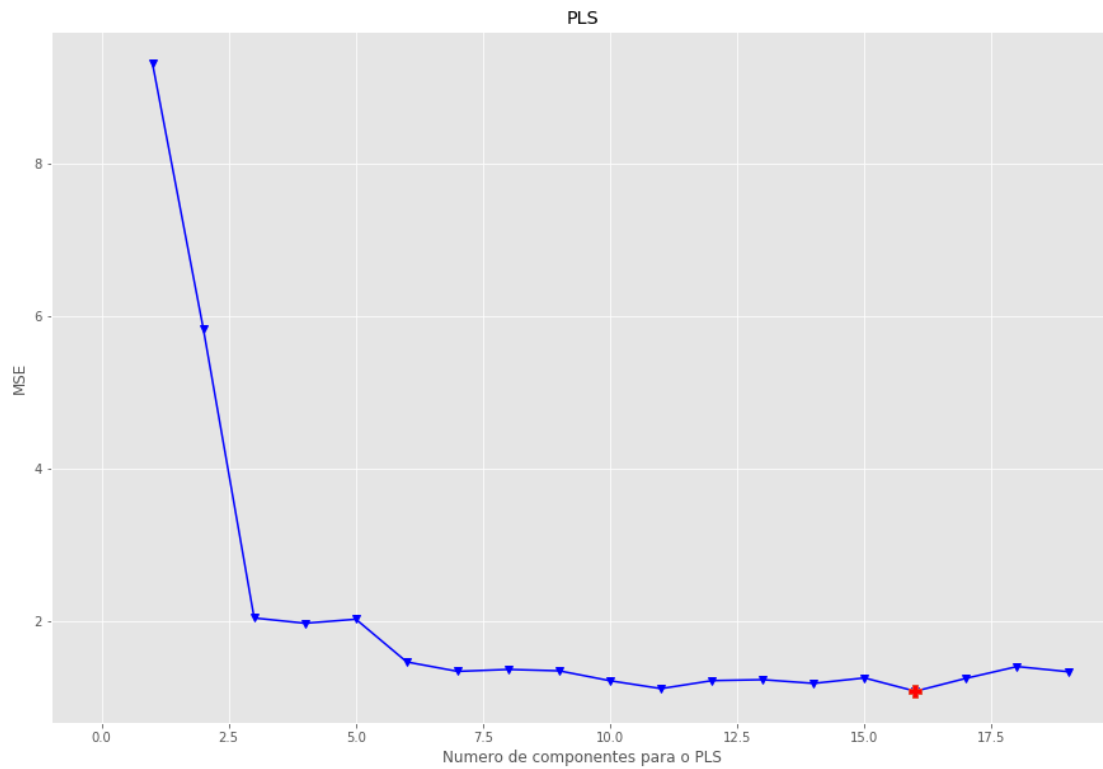
Pré-proc: 5--> Suavização(SavGol) - Par:5,2,1
100% completed Sugestão para o número de variáveis latentes: 16



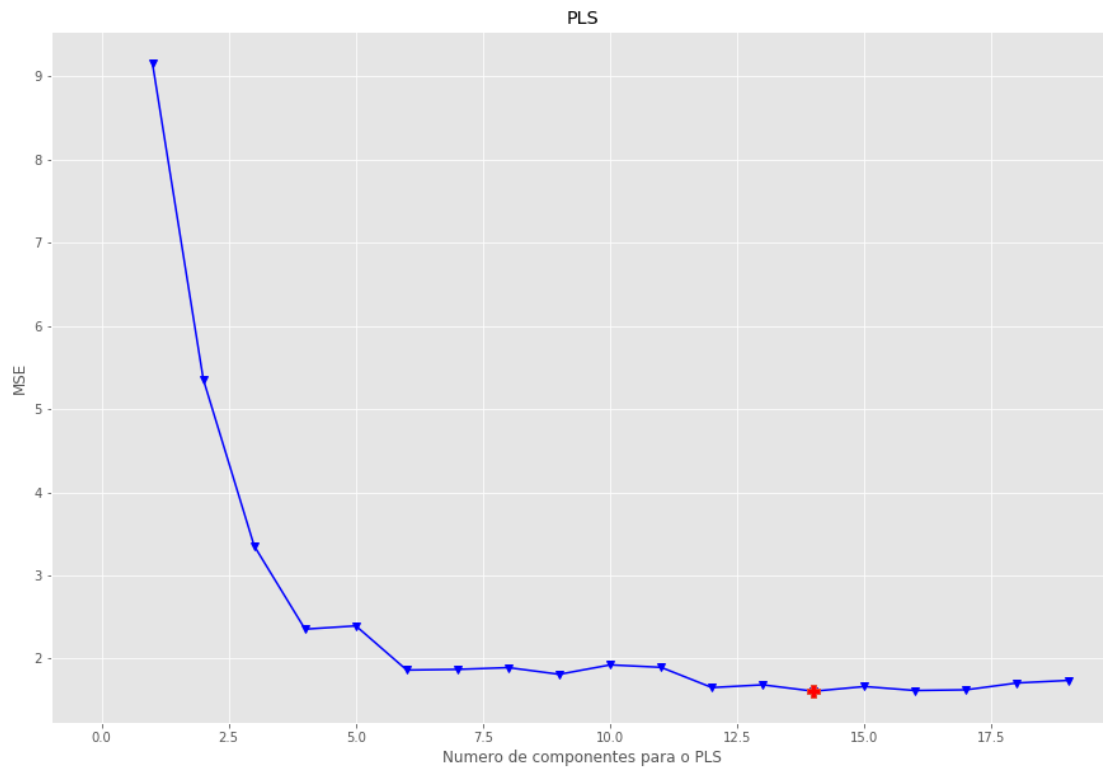
Pré-proc: 6--> Suavização(SavGol) - Par:3,2,2
100% completed Sugestão para o número de variáveis latentes: 14



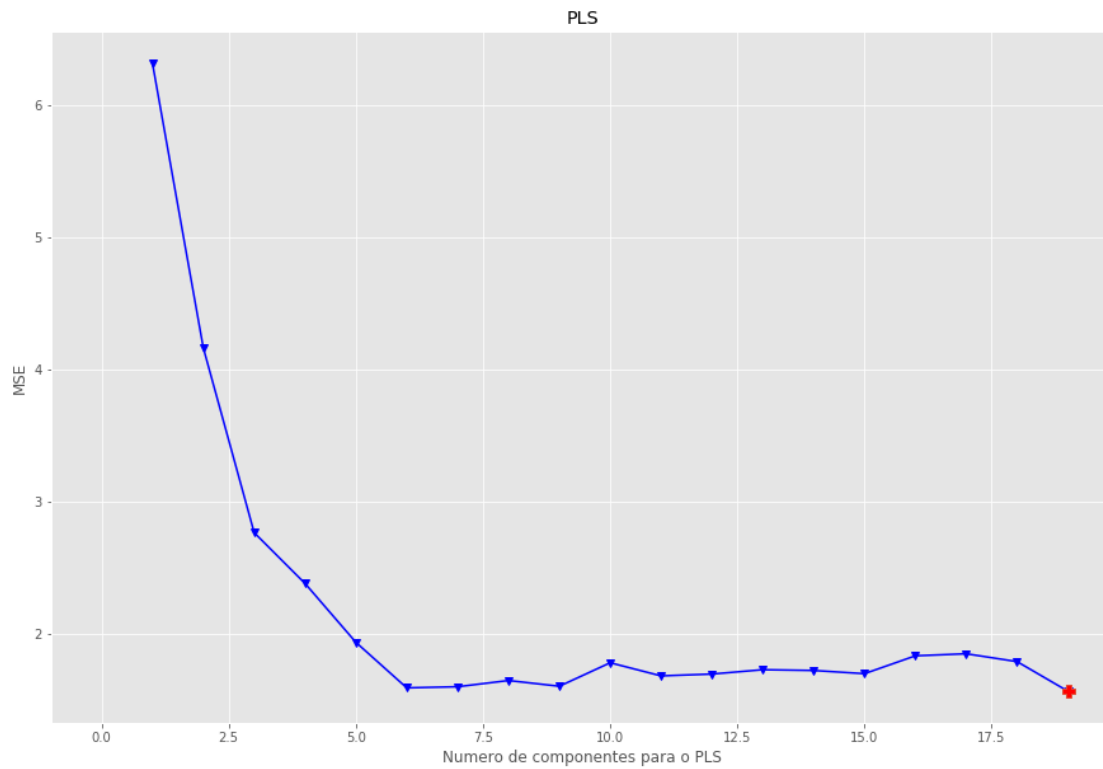
Pré-proc: 7--> Suavização(SavGol) - Par:5,2,2
100% completed Sugestão para o número de variáveis latentes: 16



Pré-proc: 8--> Suavização(SavGol) - Par:3,1,1 --> Padronização
100% completed Sugestão para o número de variáveis latentes: 14

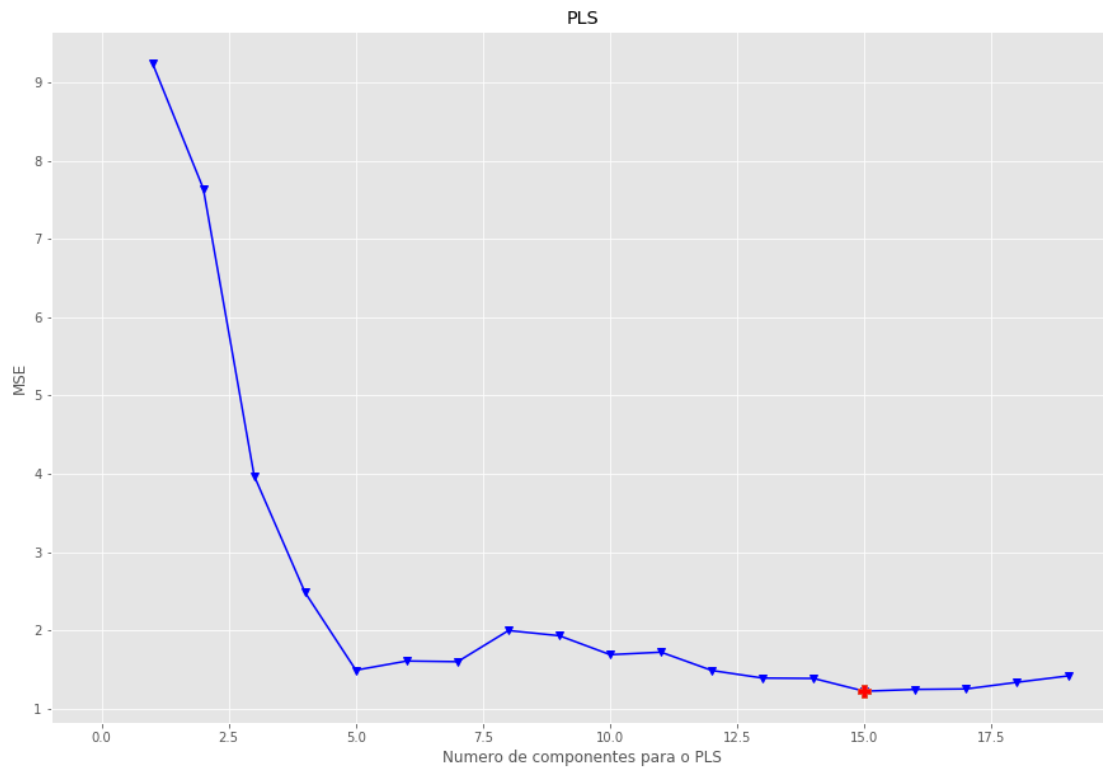


Pré-proc: 9--> Padronização --> Suavização(SavGol) - Par:3,1,1
100% completed Sugestão para o número de variáveis latentes: 19



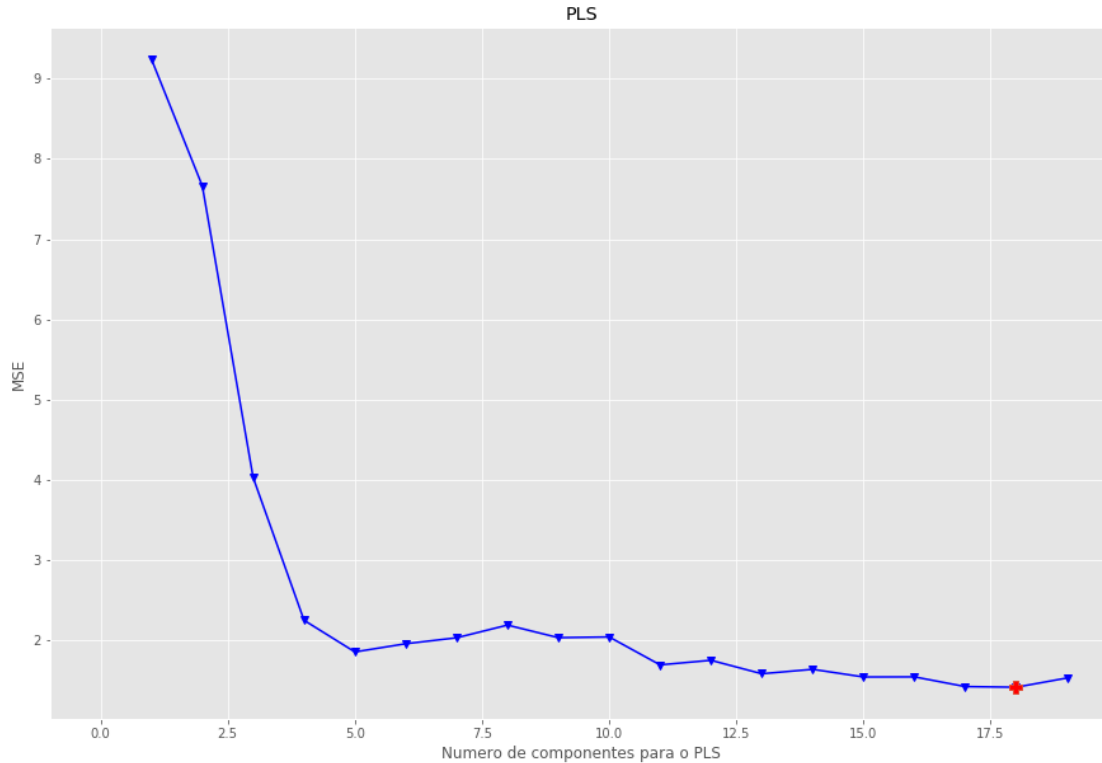
Pré-proc: 10--> MSC

100% completed Sugestão para o número de variáveis latentes: 15



Pré-proc: 11--> SNV

100% completed Sugestão para o número de variáveis latentes: 18



In []:

```
In [233]: #pls teste simples
for k in range(12):
    print(preProc[k])
    result = executaPLSResumida(k,nVL[k])
    print('Parâmetros do modelo:',modelo,'\n',result[0])

    resultados=exibeResultados(result)

    for k,v in zip(resultados.keys(),resultados.values()):
        print(k)
        print(v,'\n-----')
```

Pré-proc: 0--> Sem pré-processamento

Parâmetros do modelo: GBR

PLSRegression(copy=True, max_iter=500, n_components=14, scale=True, tol=1e-06)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	0.0000
MSE	0.1021	0.0001	0.0000	1.7928

R2	0.9606	0.9241	0.9523	0.9597
RER	14.1950	15.0714	14.2649	14.8595
RMSE	0.3195	0.0105	0.0057	1.3390
RPD	5.0399	3.6291	4.5810	4.9786
RPIQ	10.1135	4.1701	8.6813	6.6899
SEP	0.3221	0.0106	0.0057	1.3503

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0692	-0.0034	-0.0012	-0.1523
MSE	0.7906	0.0013	0.0002	8.1842
R2	0.6950	0.1395	0.6730	0.8158
RER	5.1153	4.4979	5.4647	6.9647
RMSE	0.8892	0.0355	0.0148	2.8608
RPD	1.8107	1.0780	1.7487	2.3302
RPIQ	3.6335	1.2388	3.3139	3.1311
SEP	0.8940	0.0356	0.0149	2.8809

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0047	-0.0064	-0.0007	-0.2553
MSE	0.3252	0.0006	0.0001	5.2361
R2	0.8578	0.1025	0.9059	0.8431
RER	6.6202	3.9823	10.3224	8.5992
RMSE	0.5703	0.0254	0.0071	2.2883
RPD	2.6522	1.0555	3.2605	2.5243
RPIQ	5.4951	1.1278	5.8495	1.6961
SEP	0.5844	0.0251	0.0072	2.3301

Pré-proc: 1--> Padronização

Parâmetros do modelo: GBR

PLSRegression(copy=True, max_iter=500, n_components=19, scale=True, tol=1e-06)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	-0.0000
MSE	0.0680	0.0001	0.0000	1.1409
R2	0.9738	0.9401	0.9703	0.9743
RER	17.3874	16.9680	18.0621	18.6273
RMSE	0.2608	0.0094	0.0045	1.0681
RPD	6.1734	4.0857	5.8004	6.2410
RPIQ	12.3880	4.6949	10.9922	8.3862
SEP	0.2630	0.0094	0.0045	1.0771

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0835	-0.0034	-0.0016	-0.1970
MSE	0.9436	0.0014	0.0003	8.1806
R2	0.6360	0.0096	0.6087	0.8159

RER	4.6855	4.1903	5.0012	6.9729
RMSE	0.9714	0.0380	0.0162	2.8602
RPD	1.6574	1.0048	1.5986	2.3307
RPIQ	3.3259	1.1547	3.0295	3.1318
SEP	0.9760	0.0382	0.0163	2.8775

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.5926	0.0005	0.0001	6.4537
R2	0.7410	0.3438	0.8502	0.8066
RER	5.2417	4.5257	8.7433	8.8361
RMSE	0.7698	0.0217	0.0089	2.5404
RPD	1.9648	1.2345	2.5833	2.2737
RPIQ	4.0709	1.3190	4.6346	1.5278
SEP	0.7380	0.0221	0.0085	2.2677

Pré-proc: 2--> Suavização(SavGol) - Par:3,1,1

Parâmetros do modelo: GBR

PLSRegression(copy=True, max_iter=500, n_components=14, scale=True, tol=1e-06)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0000	-0.0000	-0.0000	-0.0000
MSE	0.0703	0.0001	0.0000	1.3597
R2	0.9729	0.9470	0.9778	0.9694
RER	17.1059	18.0449	20.9004	17.0630
RMSE	0.2651	0.0088	0.0039	1.1660
RPD	6.0734	4.3451	6.7119	5.7169
RPIQ	12.1875	4.9929	12.7196	7.6820
SEP	0.2673	0.0089	0.0039	1.1759

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0117	-0.0001	-0.0001	-0.0405
MSE	0.6547	0.0013	0.0002	4.1292
R2	0.7474	0.1300	0.7265	0.9071
RER	5.6049	4.4524	5.9541	9.7933
RMSE	0.8091	0.0356	0.0136	2.0320
RPD	1.9898	1.0721	1.9120	3.2806
RPIQ	3.9929	1.2319	3.6234	4.4082
SEP	0.8159	0.0359	0.0137	2.0488

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0476	-0.0079	-0.0017	-0.5789
MSE	0.5911	0.0010	0.0002	3.7863
R2	0.7416	-0.3751	0.6727	0.8865
RER	4.9198	3.2175	5.5595	10.5260

RMSE	0.7689	0.0314	0.0132	1.9458
RPD	1.9672	0.8528	1.7480	2.9685
RPIQ	4.0760	0.9112	3.1361	1.9946
SEP	0.7863	0.0311	0.0134	1.9036

Pré-proc: 3--> Suavização(SavGol) - Par:3,2,1

Parâmetros do modelo: GBR

PLSRegression(copy=True, max_iter=500, n_components=14, scale=True, tol=1e-06)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0000	-0.0000	-0.0000	-0.0000
MSE	0.0702	0.0001	0.0000	1.3631
R2	0.9729	0.9469	0.9780	0.9693
RER	17.1162	18.0149	20.9802	17.0415
RMSE	0.2649	0.0088	0.0039	1.1675
RPD	6.0771	4.3378	6.7375	5.7097
RPIQ	12.1948	4.9846	12.7681	7.6723
SEP	0.2672	0.0089	0.0039	1.1774

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0102	-0.0001	-0.0001	-0.0369
MSE	0.6606	0.0013	0.0002	4.1126
R2	0.7452	0.1142	0.7220	0.9075
RER	5.5798	4.4126	5.9060	9.8127
RMSE	0.8127	0.0360	0.0137	2.0280
RPD	1.9809	1.0625	1.8966	3.2872
RPIQ	3.9752	1.2209	3.5942	4.4170
SEP	0.8195	0.0363	0.0138	2.0447

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0440	-0.0078	-0.0017	-0.5617
MSE	0.5879	0.0010	0.0002	3.8413
R2	0.7430	-0.3634	0.6683	0.8849
RER	4.9322	3.2281	5.5193	10.4140
RMSE	0.7667	0.0313	0.0133	1.9599
RPD	1.9727	0.8564	1.7364	2.9472
RPIQ	4.0873	0.9151	3.1151	1.9802
SEP	0.7844	0.0310	0.0135	1.9241

Pré-proc: 4--> Suavização(SavGol) - Par:5,1,1

Parâmetros do modelo: GBR

PLSRegression(copy=True, max_iter=500, n_components=9, scale=True, tol=1e-06)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	0.0000
MSE	0.1664	0.0002	0.0000	1.9230

R2	0.9358	0.8896	0.9360	0.9567
RER	11.1161	12.4974	12.3086	14.3477
RMSE	0.4079	0.0127	0.0066	1.3867
RPD	3.9467	3.0093	3.9527	4.8072
RPIQ	7.9199	3.4579	7.4908	6.4595
SEP	0.4114	0.0128	0.0066	1.3984

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0216	-0.0005	-0.0001	-0.0801
MSE	0.4449	0.0008	0.0001	4.4694
R2	0.8284	0.4691	0.8101	0.8994
RER	6.8019	5.7004	7.1450	9.4181
RMSE	0.6670	0.0278	0.0113	2.1141
RPD	2.4137	1.3724	2.2945	3.1532
RPIQ	4.8436	1.5770	4.3482	4.2371
SEP	0.6723	0.0281	0.0114	2.1304

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0121	-0.0068	-0.0026	-0.3616
MSE	0.2217	0.0006	0.0001	4.5401
R2	0.9031	0.1393	0.8277	0.8639
RER	8.0206	4.0919	7.9003	9.3123
RMSE	0.4709	0.0248	0.0096	2.1308
RPD	3.2122	1.0779	2.4088	2.7109
RPIQ	6.6555	1.1517	4.3214	1.8215
SEP	0.4823	0.0245	0.0094	2.1517

Pré-proc: 5--> Suavização(SavGol) - Par:5,2,1

Parâmetros do modelo: GBR

PLSRegression(copy=True, max_iter=500, n_components=16, scale=True, tol=1e-06)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	-0.0000
MSE	0.0608	0.0001	0.0000	1.3326
R2	0.9766	0.9434	0.9723	0.9700
RER	18.3933	17.4490	18.7198	17.2352
RMSE	0.2465	0.0091	0.0043	1.1544
RPD	6.5305	4.2016	6.0116	5.7746
RPIQ	13.1047	4.8280	11.3925	7.7595
SEP	0.2486	0.0092	0.0044	1.1641

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0599	-0.0018	-0.0007	-0.0735
MSE	0.8499	0.0014	0.0002	4.8414
R2	0.6721	0.0348	0.6719	0.8911

RER	4.9292	4.2322	5.4412	9.0475
RMSE	0.9219	0.0375	0.0149	2.2003
RPD	1.7464	1.0179	1.7457	3.0297
RPIQ	3.5045	1.1696	3.3083	4.0710
SEP	0.9277	0.0378	0.0150	2.2176

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0170	-0.0060	-0.0011	-0.4520
MSE	0.7337	0.0011	0.0001	3.9572
R2	0.6793	-0.4715	0.7208	0.8814
RER	4.4085	3.0630	5.9890	10.0940
RMSE	0.8565	0.0325	0.0122	1.9893
RPD	1.7658	0.8244	1.8926	2.9037
RPIQ	3.6587	0.8808	3.3955	1.9510
SEP	0.8775	0.0327	0.0125	1.9851

Pré-proc: 6--> Suavização(SavGol) - Par:3,2,2

Parâmetros do modelo: GBR

PLSRegression(copy=True, max_iter=500, n_components=14, scale=True, tol=1e-06)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	0.0000
MSE	0.0631	0.0000	0.0000	1.0163
R2	0.9757	0.9691	0.9863	0.9771
RER	18.0545	23.6367	26.5880	19.7364
RMSE	0.2512	0.0067	0.0030	1.0081
RPD	6.4102	5.6915	8.5384	6.6126
RPIQ	12.8633	6.5401	16.1809	8.8855
SEP	0.2533	0.0068	0.0031	1.0166

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0437	-0.0009	-0.0008	0.0150
MSE	1.1272	0.0014	0.0002	3.7725
R2	0.5652	0.0432	0.6584	0.9151
RER	4.2748	4.2468	5.3350	10.2440
RMSE	1.0617	0.0374	0.0152	1.9423
RPD	1.5165	1.0223	1.7111	3.4321
RPIQ	3.0431	1.1748	3.2426	4.6118
SEP	1.0697	0.0377	0.0153	1.9586

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0104	-0.0076	-0.0007	-0.3155
MSE	0.3439	0.0005	0.0001	3.5157
R2	0.8497	0.3010	0.8257	0.8946
RER	6.4385	4.6442	7.5719	10.5797

RMSE	0.5865	0.0224	0.0096	1.8750
RPD	2.5790	1.1961	2.3954	3.0806
RPIQ	5.3436	1.2780	4.2975	2.0699
SEP	0.6009	0.0216	0.0098	1.8939

Pré-proc: 7--> Suavização(SavGol) - Par:5,2,2

Parâmetros do modelo: GBR

PLSRegression(copy=True, max_iter=500, n_components=16, scale=True, tol=1e-06)

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0000	-0.0000	-0.0000	0.0000
MSE	0.0727	0.0000	0.0000	0.8754
R2	0.9720	0.9787	0.9862	0.9803
RER	16.8233	28.4786	26.4701	21.2650
RMSE	0.2695	0.0056	0.0031	0.9356
RPD	5.9731	6.8574	8.5005	7.1248
RPIQ	11.9861	7.8798	16.1092	9.5737
SEP	0.2718	0.0056	0.0031	0.9435

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0179	-0.0018	-0.0012	0.0159
MSE	1.1725	0.0015	0.0002	4.0060
R2	0.5477	0.0004	0.6542	0.9099
RER	4.1884	4.1584	5.3108	9.9411
RMSE	1.0828	0.0382	0.0153	2.0015
RPD	1.4869	1.0002	1.7006	3.3306
RPIQ	2.9837	1.1493	3.2228	4.4754
SEP	1.0918	0.0385	0.0153	2.0183

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0363	-0.0052	-0.0015	-0.5257
MSE	0.3931	0.0006	0.0001	3.9192
R2	0.8282	0.1100	0.8140	0.8825
RER	6.0315	3.9564	7.3913	10.2452
RMSE	0.6270	0.0252	0.0100	1.9797
RPD	2.4123	1.0600	2.3185	2.9177
RPIQ	4.9982	1.1326	4.1594	1.9605
SEP	0.6414	0.0253	0.0101	1.9558

Pré-proc: 8--> Suavização(SavGol) - Par:3,1,1 --> Padronização

Parâmetros do modelo: GBR

PLSRegression(copy=True, max_iter=500, n_components=14, scale=True, tol=1e-06)

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	-0.0000
MSE	0.0703	0.0001	0.0000	1.3597

R2	0.9729	0.9470	0.9778	0.9694
RER	17.1059	18.0449	20.9004	17.0630
RMSE	0.2651	0.0088	0.0039	1.1660
RPD	6.0734	4.3451	6.7119	5.7169
RPIQ	12.1875	4.9929	12.7196	7.6820
SEP	0.2673	0.0089	0.0039	1.1759

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0117	-0.0001	-0.0001	-0.0405
MSE	0.6547	0.0013	0.0002	4.1292
R2	0.7474	0.1300	0.7265	0.9071
RER	5.6049	4.4524	5.9541	9.7933
RMSE	0.8091	0.0356	0.0136	2.0320
RPD	1.9898	1.0721	1.9120	3.2806
RPIQ	3.9929	1.2319	3.6234	4.4082
SEP	0.8159	0.0359	0.0137	2.0488

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.6202	0.0009	0.0002	5.8079
R2	0.7289	-0.2653	0.6820	0.8259
RER	5.1078	3.2526	5.7733	9.4834
RMSE	0.7875	0.0301	0.0130	2.4100
RPD	1.9206	0.8890	1.7733	2.3968
RPIQ	3.9795	0.9499	3.1814	1.6105
SEP	0.7574	0.0308	0.0129	2.1129

Pré-proc: 9--> Padronização --> Suavização(SavGol) - Par:3,1,1

Parâmetros do modelo: GBR

PLSRegression(copy=True, max_iter=500, n_components=19, scale=True, tol=1e-06)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	-0.0000
MSE	0.0463	0.0000	0.0000	0.5370
R2	0.9821	0.9827	0.9874	0.9879
RER	21.0687	31.5941	27.7436	27.1520
RMSE	0.2152	0.0050	0.0029	0.7328
RPD	7.4804	7.6076	8.9095	9.0972
RPIQ	15.0109	8.7418	16.8842	12.2242
SEP	0.2170	0.0051	0.0029	0.7390

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0581	-0.0036	-0.0013	-0.0467
MSE	0.9566	0.0012	0.0002	7.5550
R2	0.6310	0.1501	0.6649	0.8300

RER	4.6445	4.5279	5.3982	7.2396
RMSE	0.9781	0.0352	0.0150	2.7486
RPD	1.6461	1.0847	1.7275	2.4253
RPIQ	3.3032	1.2464	3.2738	3.2589
SEP	0.9846	0.0353	0.0151	2.7714

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.6674	0.0006	0.0001	5.5917
R2	0.7083	0.2089	0.7520	0.8324
RER	4.9004	4.1188	6.5999	9.7341
RMSE	0.8169	0.0238	0.0115	2.3647
RPD	1.8514	1.1243	2.0080	2.4427
RPIQ	3.8361	1.2013	3.6025	1.6413
SEP	0.7894	0.0243	0.0113	2.0584

Pré-proc: 10--> MSC

Parâmetros do modelo: GBR

PLSRegression(copy=True, max_iter=500, n_components=15, scale=True, tol=1e-06)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	-0.0000
MSE	0.1029	0.0001	0.0000	1.4056
R2	0.9603	0.9216	0.9517	0.9684
RER	14.1389	14.8337	14.1761	16.7821
RMSE	0.3207	0.0107	0.0057	1.1856
RPD	5.0200	3.5718	4.5525	5.6228
RPIQ	10.0736	4.1044	8.6273	7.5555
SEP	0.3234	0.0108	0.0057	1.1956

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0023	-0.0017	-0.0008	-0.0049
MSE	0.8116	0.0013	0.0003	7.6776
R2	0.6869	0.1289	0.6226	0.8272
RER	5.0334	4.4547	5.0743	7.1806
RMSE	0.9009	0.0357	0.0159	2.7709
RPD	1.7871	1.0714	1.6277	2.4058
RPIQ	3.5861	1.2312	3.0847	3.2328
SEP	0.9085	0.0359	0.0161	2.7942

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1868	0.0059	0.0004	-0.0446
MSE	0.3956	0.0008	0.0001	4.5029
R2	0.8271	-0.1165	0.8328	0.8650
RER	6.2861	3.5341	7.7158	9.2171

RMSE	0.6290	0.0283	0.0094	2.1220
RPD	2.4047	0.9464	2.4455	2.7221
RPIQ	4.9825	1.0112	4.3873	1.8290
SEP	0.6154	0.0283	0.0097	2.1739

Pré-proc: 11--> SNV

Parâmetros do modelo: GBR

PLSRegression(copy=True, max_iter=500, n_components=18, scale=True, tol=1e-06)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0000	-0.0000	-0.0000	-0.0000
MSE	0.0761	0.0001	0.0000	1.2599
R2	0.9706	0.9372	0.9660	0.9716
RER	16.4337	16.5672	16.8799	17.7259
RMSE	0.2759	0.0096	0.0048	1.1224
RPD	5.8348	3.9892	5.4208	5.9390
RPIQ	11.7086	4.5840	10.2728	7.9804
SEP	0.2783	0.0097	0.0048	1.1319

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0319	-0.0018	-0.0010	-0.1068
MSE	0.8851	0.0015	0.0003	8.0277
R2	0.6585	-0.0189	0.5868	0.8194
RER	4.8226	4.1189	4.8533	7.0272
RMSE	0.9408	0.0386	0.0167	2.8333
RPD	1.7113	0.9907	1.5557	2.3528
RPIQ	3.4340	1.1384	2.9481	3.1615
SEP	0.9482	0.0389	0.0168	2.8552

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0550	-0.0083	-0.0022	-0.8890
MSE	0.4785	0.0010	0.0001	5.2000
R2	0.7908	-0.3686	0.7608	0.8441
RER	5.4749	3.2381	6.5673	9.3119
RMSE	0.6918	0.0313	0.0113	2.2804
RPD	2.1865	0.8548	2.0446	2.5330
RPIQ	4.5302	0.9133	3.6680	1.7020
SEP	0.7066	0.0309	0.0114	2.1518

In [261]: #pls otimizado

maior=[-1,-1,-1,-1]

maiorGerado=[0,0,0,0]

for i in range(100):

result = executaPLSResumida(preproc=9,nPC=6,IC=i)

```

resultados=exibeResultados(result)
r2 = resultados['pred'].loc[resultados['pred'].index=='R2']
r = []
for j in range(4):
    r.append(r2.iloc[:,j][0])
    if r[j]>maior[j]:
        maior[j] = r[j]
        maiorGerado[j]=i
print('\r%d%% completos'%(i+1), end='')
print('\n','r2:',maior,'\nsemente: b c f x',maiorGerado)

```

100% completos

r2: [0.9285, 0.844, 0.9411, 0.8928]

semente: b c f x [96, 96, 27, 88]

```

In [264]: #PLS teste otimizado
          modelo = 'PLS:'
          result = executaPLSResumida(preproc=9,nPC=6,IC=88)
          print('Parâmetros do modelo:',modelo,'\n',result[0])

          resultados=exibeResultados(result)

```

Parâmetros do modelo: PLS:

PLSRegression(copy=True, max_iter=500, n_components=6, scale=True, tol=1e-06)

In []:

```
In [265]: resultados['cal']
```

```

Out[265]:
          betaglicosidase  cmcase  fpase  xilanase
BIAS                0.0000  0.0000  0.0000  0.0000
MSE                 0.2632  0.0002  0.0000  3.8078
R2                  0.8926  0.8392  0.9244  0.9034
RER                 8.8395 11.3778 12.2213 10.1961
RMSE                0.5130  0.0139  0.0066  1.9514
RPD                 3.0519  2.4939  3.6360  3.2170
RPIQ                6.1813  2.5665  5.3489  2.9235
SEP                 0.5173  0.0141  0.0067  1.9678

```

```
In [266]: resultados['val']
```

```

Out[266]:
          betaglicosidase  cmcase  fpase  xilanase
BIAS                -0.0292  0.0000 -0.0001 -0.0759
MSE                 0.4224  0.0005  0.0001  7.9623
R2                  0.8277  0.5467  0.8312  0.7980
RER                 6.9846  6.7767  8.1806  7.0536
RMSE                0.6499  0.0234  0.0099  2.8218

```

RPD	2.4091	1.4854	2.4337	2.2247
RPIQ	4.8792	1.5286	3.5802	2.0217
SEP	0.6547	0.0236	0.0100	2.8445

In [267]: resultados['pred']

```
Out[267]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0655	-0.0041	0.0002	-0.8397
MSE	0.4054	0.0005	0.0001	5.1866
R2	0.8521	0.6823	0.8386	0.8928
RER	7.0083	7.4870	6.9417	9.2494
RMSE	0.6367	0.0213	0.0115	2.2774
RPD	2.6006	1.7740	2.4895	3.0537
RPIQ	5.3780	1.8272	4.7992	5.8488
SEP	0.6490	0.0214	0.0117	2.1692

In [268]: reg, treino_teste,y_c,y_cv,y_p = result

7.5.3 Reais x preditos

In []:

```
In [269]: #pls reaisxpreditos
#calibração
pred=pd.DataFrame(y_c, columns=var_ae)
reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('CALIBRAÇÃO:\n')
round(reais_pred,4)
```

CALIBRAÇÃO:

```
Out[269]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	2.9123	0.1058	0.0747	14.6813	3.8214
1	0.1724	0.0112	0.0121	0.0924	0.1393
2	3.5610	0.0586	0.0561	10.0978	3.2643
3	3.8876	0.0418	0.0605	11.0267	3.0345
4	0.3900	0.0315	0.0283	14.1777	0.7269
5	3.8994	0.1118	0.0613	10.9512	3.5483
6	0.3828	0.0405	0.0301	12.4461	1.0102
7	0.4280	0.0390	0.0334	13.7624	0.8989
8	3.2342	0.0672	0.0543	8.4772	2.9166
9	3.2342	0.0672	0.0543	8.4772	3.0917
10	0.5905	0.0465	0.0267	18.7095	0.3204

11	3.5610	0.0586	0.0561	10.0978	3.4985
12	2.7110	0.0548	0.0688	13.5829	3.3673
13	2.9123	0.1058	0.0747	14.6813	3.9315
14	3.8803	0.0557	0.0691	11.3256	3.4247
15	0.0874	0.0217	0.0127	0.1071	0.0194
16	4.6037	0.1713	0.0919	16.8115	3.2953
17	3.5967	0.1065	0.0850	13.6476	3.6088
18	3.5974	0.0516	0.0731	15.3973	2.8590
19	3.8994	0.1118	0.0613	10.9512	3.3366
20	0.4280	0.0390	0.0334	13.7624	0.5887
21	0.6491	0.0605	0.0260	18.4274	0.1827
22	2.1643	0.0830	0.0529	18.8324	2.3864
23	2.9774	0.0704	0.0567	10.8002	3.0298
24	0.3900	0.0315	0.0283	14.1777	0.7196
25	3.1068	0.0781	0.0545	11.0526	3.1532
26	3.2342	0.0672	0.0543	8.4772	3.3141
27	3.1068	0.0781	0.0545	11.0526	4.0406
28	2.1150	0.0730	0.0505	18.4127	2.3251
29	3.8876	0.0418	0.0605	11.0267	3.8726
30	0.4280	0.0390	0.0334	13.7624	0.8937
31	0.6010	0.0559	0.0116	20.1368	0.3691
32	0.0308	0.0213	0.0113	0.0996	-0.5633
33	0.3900	0.0315	0.0283	14.1777	0.5584
34	3.8994	0.1118	0.0613	10.9512	3.5846
35	0.0308	0.0213	0.0113	0.0996	-0.2979
36	3.5974	0.0516	0.0731	15.3973	3.1041
37	0.1724	0.0112	0.0121	0.0924	0.4933
38	4.6037	0.1713	0.0919	16.8115	3.3030
39	0.0554	0.0181	0.0106	0.3275	0.3272
40	3.5610	0.0586	0.0561	10.0978	2.9645
41	2.1150	0.0730	0.0505	18.4127	2.0591
42	0.1671	0.0117	0.0104	0.1117	0.5123
43	2.1643	0.0830	0.0529	18.8324	2.3466
44	0.0874	0.0217	0.0127	0.1071	-0.2098
45	0.1671	0.0117	0.0104	0.1117	0.4715
46	0.6491	0.0605	0.0260	18.4274	1.0077
47	0.0554	0.0181	0.0106	0.3275	0.3213
48	2.1643	0.0830	0.0529	18.8324	2.6048
49	0.0759	0.0136	0.0139	0.0726	0.3375
50	3.7243	0.0561	0.0681	11.5736	3.5883
51	0.0308	0.0213	0.0113	0.0996	-0.0415
52	0.5905	0.0465	0.0267	18.7095	0.5261
53	2.9774	0.0704	0.0567	10.8002	3.2048
54	3.7243	0.0561	0.0681	11.5736	3.6554
55	2.9123	0.1058	0.0747	14.6813	4.3779
56	0.3828	0.0405	0.0301	12.4461	0.6095
57	2.9774	0.0704	0.0567	10.8002	3.3127
58	3.5974	0.0516	0.0731	15.3973	2.6333

59	0.6010	0.0559	0.0116	20.1368	0.3535
----	--------	--------	--------	---------	--------

	pred: cmcase	pred: fpase	pred: xilanas
0	0.1020	0.0803	17.7207
1	0.0030	0.0123	4.1802
2	0.0655	0.0587	10.1505
3	0.0487	0.0551	10.2297
4	0.0352	0.0286	11.2409
5	0.0864	0.0608	10.7614
6	0.0655	0.0333	11.4552
7	0.0366	0.0365	15.6710
8	0.0640	0.0537	10.2543
9	0.0550	0.0501	7.8096
10	0.0492	0.0173	16.6244
11	0.0725	0.0621	9.6499
12	0.0397	0.0653	10.0835
13	0.1076	0.0801	17.0320
14	0.0613	0.0733	14.5177
15	0.0222	0.0126	-1.9118
16	0.1292	0.0720	16.6398
17	0.0965	0.0686	14.8018
18	0.0528	0.0661	11.9090
19	0.0877	0.0641	12.3962
20	0.0283	0.0275	12.3715
21	0.0323	0.0181	19.9946
22	0.0865	0.0549	16.3689
23	0.0637	0.0528	10.2671
24	0.0224	0.0323	13.1210
25	0.0746	0.0584	10.2417
26	0.0592	0.0573	10.4433
27	0.0965	0.0657	8.8219
28	0.0938	0.0560	17.3986
29	0.0676	0.0654	10.0831
30	0.0417	0.0366	14.4444
31	0.0538	0.0172	17.5207
32	0.0073	0.0048	0.0463
33	0.0402	0.0300	13.5200
34	0.1066	0.0694	14.2009
35	0.0067	0.0104	0.8062
36	0.0694	0.0727	16.5136
37	0.0029	0.0138	1.3975
38	0.1366	0.0714	17.0071
39	0.0249	0.0123	3.7113
40	0.0604	0.0542	10.7490
41	0.0833	0.0517	17.6029
42	0.0165	0.0147	2.5171
43	0.0908	0.0562	15.6838
44	0.0204	0.0103	1.2630

45	0.0140	0.0132	1.9317
46	0.0678	0.0274	18.7992
47	0.0257	0.0102	0.7598
48	0.1016	0.0607	16.9353
49	0.0423	0.0217	0.7383
50	0.0622	0.0614	11.4376
51	0.0208	0.0088	-2.3918
52	0.0585	0.0233	18.7798
53	0.0642	0.0547	8.2196
54	0.0715	0.0655	13.8324
55	0.1223	0.0893	18.0468
56	0.0356	0.0349	13.5284
57	0.0679	0.0560	8.0459
58	0.0405	0.0619	11.9782
59	0.0616	0.0209	20.9789

```
In [270]: #validação
pred=pd.DataFrame(y_cv, columns=var_ae)
reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('VALIDAÇÃO CRUZADA:\n')
round(reais_pred,4)
```

VALIDAÇÃO CRUZADA:

```
Out[270]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	2.9123	0.1058	0.0747	14.6813	3.7481
1	0.1724	0.0112	0.0121	0.0924	0.2700
2	3.5610	0.0586	0.0561	10.0978	3.1872
3	3.8876	0.0418	0.0605	11.0267	2.9298
4	0.3900	0.0315	0.0283	14.1777	0.7955
5	3.8994	0.1118	0.0613	10.9512	3.3279
6	0.3828	0.0405	0.0301	12.4461	0.9848
7	0.4280	0.0390	0.0334	13.7624	1.2943
8	3.2342	0.0672	0.0543	8.4772	2.8837
9	3.2342	0.0672	0.0543	8.4772	3.0828
10	0.5905	0.0465	0.0267	18.7095	0.2113
11	3.5610	0.0586	0.0561	10.0978	3.4435
12	2.7110	0.0548	0.0688	13.5829	3.7146
13	2.9123	0.1058	0.0747	14.6813	3.9168
14	3.8803	0.0557	0.0691	11.3256	3.6428
15	0.0874	0.0217	0.0127	0.1071	-0.0387
16	4.6037	0.1713	0.0919	16.8115	2.6067

17	3.5967	0.1065	0.0850	13.6476	3.4998
18	3.5974	0.0516	0.0731	15.3973	2.6632
19	3.8994	0.1118	0.0613	10.9512	3.0558
20	0.4280	0.0390	0.0334	13.7624	0.6297
21	0.6491	0.0605	0.0260	18.4274	0.1813
22	2.1643	0.0830	0.0529	18.8324	2.3272
23	2.9774	0.0704	0.0567	10.8002	3.0467
24	0.3900	0.0315	0.0283	14.1777	0.7722
25	3.1068	0.0781	0.0545	11.0526	3.2339
26	3.2342	0.0672	0.0543	8.4772	3.3278
27	3.1068	0.0781	0.0545	11.0526	4.1550
28	2.1150	0.0730	0.0505	18.4127	2.5194
29	3.8876	0.0418	0.0605	11.0267	4.1670
30	0.4280	0.0390	0.0334	13.7624	1.0420
31	0.6010	0.0559	0.0116	20.1368	0.2622
32	0.0308	0.0213	0.0113	0.0996	-0.7108
33	0.3900	0.0315	0.0283	14.1777	0.7662
34	3.8994	0.1118	0.0613	10.9512	3.4625
35	0.0308	0.0213	0.0113	0.0996	-0.4031
36	3.5974	0.0516	0.0731	15.3973	3.1961
37	0.1724	0.0112	0.0121	0.0924	0.5902
38	4.6037	0.1713	0.0919	16.8115	2.8636
39	0.0554	0.0181	0.0106	0.3275	0.5225
40	3.5610	0.0586	0.0561	10.0978	2.7380
41	2.1150	0.0730	0.0505	18.4127	1.9138
42	0.1671	0.0117	0.0104	0.1117	0.7734
43	2.1643	0.0830	0.0529	18.8324	2.5791
44	0.0874	0.0217	0.0127	0.1071	-0.0031
45	0.1671	0.0117	0.0104	0.1117	0.5628
46	0.6491	0.0605	0.0260	18.4274	1.2739
47	0.0554	0.0181	0.0106	0.3275	0.5789
48	2.1643	0.0830	0.0529	18.8324	2.6801
49	0.0759	0.0136	0.0139	0.0726	0.7224
50	3.7243	0.0561	0.0681	11.5736	3.6148
51	0.0308	0.0213	0.0113	0.0996	0.1466
52	0.5905	0.0465	0.0267	18.7095	0.5719
53	2.9774	0.0704	0.0567	10.8002	3.1506
54	3.7243	0.0561	0.0681	11.5736	3.8263
55	2.9123	0.1058	0.0747	14.6813	4.6103
56	0.3828	0.0405	0.0301	12.4461	0.5613
57	2.9774	0.0704	0.0567	10.8002	3.3061
58	3.5974	0.0516	0.0731	15.3973	2.5053
59	0.6010	0.0559	0.0116	20.1368	0.6035

	pred: cmcase	pred: fpase	pred: xilanase
0	0.0993	0.0797	17.7481
1	0.0127	0.0163	5.5262
2	0.0680	0.0588	10.7406

3	0.0506	0.0544	10.8856
4	0.0390	0.0294	10.6353
5	0.0757	0.0579	10.4413
6	0.0697	0.0321	9.9340
7	0.0499	0.0418	16.4096
8	0.0633	0.0547	11.3639
9	0.0570	0.0517	8.8693
10	0.0488	0.0151	16.2627
11	0.0755	0.0624	9.8816
12	0.0442	0.0663	9.4530
13	0.0964	0.0757	16.3526
14	0.0695	0.0756	15.6745
15	0.0135	0.0104	-2.6979
16	0.0847	0.0564	13.7521
17	0.0935	0.0651	14.8465
18	0.0461	0.0605	9.5041
19	0.0729	0.0596	11.5075
20	0.0207	0.0246	11.0298
21	0.0239	0.0161	20.1709
22	0.0777	0.0513	14.7566
23	0.0674	0.0556	11.4508
24	0.0207	0.0309	11.2771
25	0.0768	0.0597	10.0049
26	0.0718	0.0619	12.2963
27	0.1107	0.0714	11.1125
28	0.1046	0.0586	17.0058
29	0.0913	0.0728	11.2950
30	0.0456	0.0372	14.2582
31	0.0459	0.0180	16.8377
32	0.0001	0.0032	0.3463
33	0.0459	0.0311	12.9543
34	0.1010	0.0689	14.3866
35	0.0009	0.0097	1.5643
36	0.0649	0.0706	15.9679
37	0.0077	0.0172	3.1658
38	0.0956	0.0575	14.5240
39	0.0187	0.0126	5.2641
40	0.0613	0.0546	11.9438
41	0.0829	0.0491	16.1411
42	0.0180	0.0181	5.0120
43	0.0816	0.0543	14.3836
44	0.0275	0.0134	1.9581
45	0.0137	0.0144	3.8457
46	0.0809	0.0332	19.8841
47	0.0185	0.0119	3.9915
48	0.0999	0.0601	15.5334
49	0.0699	0.0311	2.5330
50	0.0735	0.0635	12.3967

51	0.0321	0.0126	-2.5216
52	0.0555	0.0229	18.0360
53	0.0672	0.0540	8.0839
54	0.0885	0.0698	15.3646
55	0.1265	0.0927	18.2229
56	0.0351	0.0337	12.5227
57	0.0648	0.0532	7.4691
58	0.0327	0.0569	10.1703
59	0.0708	0.0287	21.7540

```
In [271]: #predição
pred=pd.DataFrame(y_p, columns=var_ae)
reais = treino_teste[3]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('Predição (validação externa):\n')
round(reais_pred,4)
```

Predição (validação externa):

```
Out[271]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	0.0759	0.0136	0.0139	0.0726	0.5366
1	3.1068	0.0781	0.0545	11.0526	2.7022
2	2.7110	0.0548	0.0688	13.5829	3.0688
3	0.0874	0.0217	0.0127	0.1071	0.3929
4	3.5967	0.1065	0.0850	13.6476	3.4683
5	0.5905	0.0465	0.0267	18.7095	0.9007
6	3.8876	0.0418	0.0605	11.0267	3.2234
7	0.0554	0.0181	0.0106	0.3275	0.7837
8	3.5967	0.1065	0.0850	13.6476	3.7437
9	4.6037	0.1713	0.0919	16.8115	2.6450
10	0.6010	0.0559	0.0116	20.1368	1.0917
11	2.7110	0.0548	0.0688	13.5829	3.4077
12	0.1671	0.0117	0.0104	0.1117	0.8997
13	0.0759	0.0136	0.0139	0.0726	0.0298
14	3.8803	0.0557	0.0691	11.3256	3.5026
15	3.8803	0.0557	0.0691	11.3256	3.4498
16	3.7243	0.0561	0.0681	11.5736	3.1854
17	0.3828	0.0405	0.0301	12.4461	0.9498
18	0.6491	0.0605	0.0260	18.4274	1.2749
19	2.1150	0.0730	0.0505	18.4127	2.0120
20	0.1724	0.0112	0.0121	0.0924	0.7782

pred: cmcase pred: fpase pred: xilanase

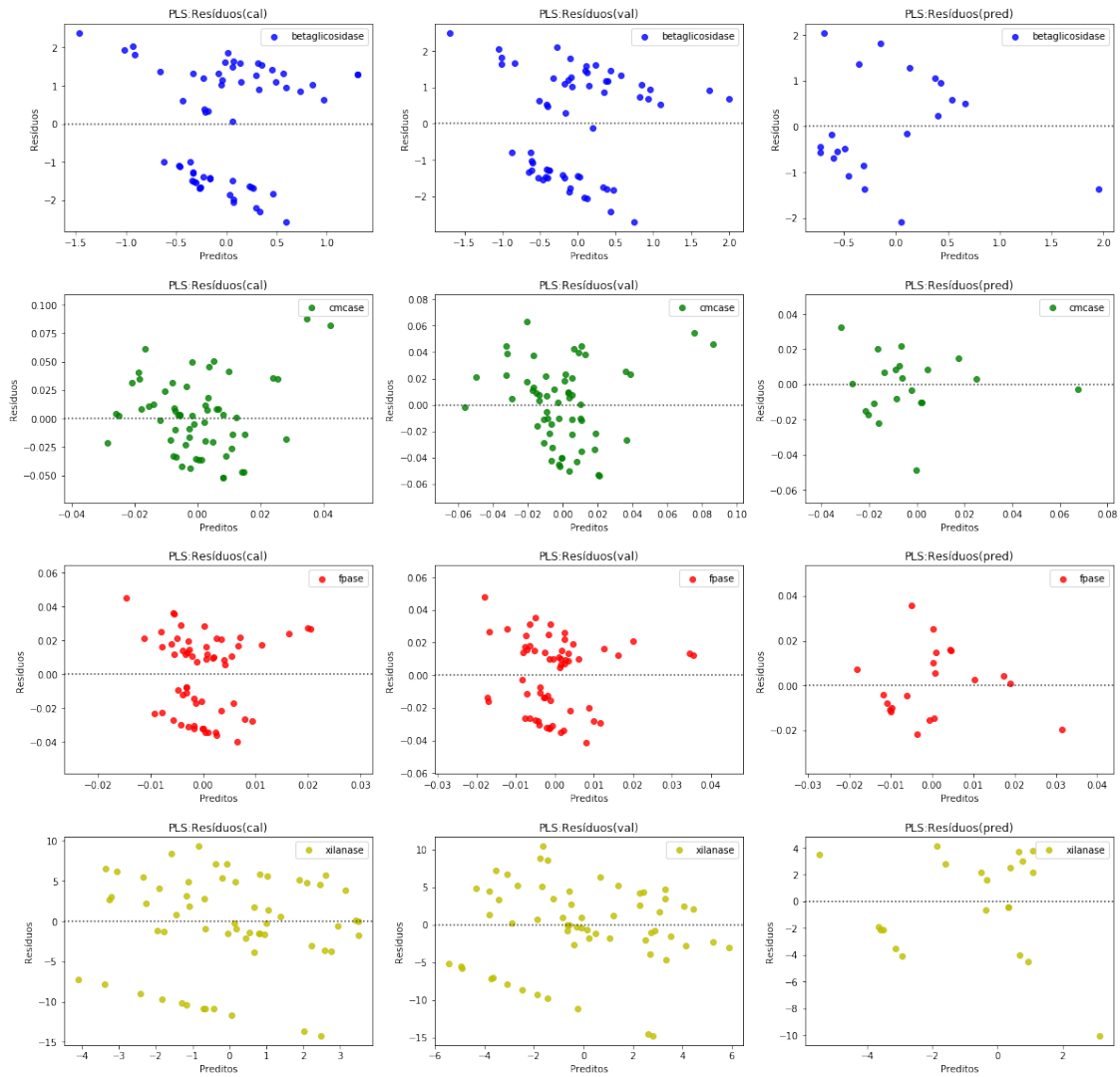
0	0.0297	0.0257	3.6883
1	0.0737	0.0542	10.3767
2	0.0531	0.0643	13.2612
3	0.0396	0.0224	3.0439
4	0.0815	0.0662	14.1599
5	0.0602	0.0273	18.0556
6	0.0736	0.0595	12.6235
7	0.0451	0.0209	3.8442
8	0.0889	0.0677	13.9890
9	0.1036	0.0604	16.4068
10	0.0536	0.0298	19.0451
11	0.0714	0.0737	13.2519
12	0.0332	0.0203	3.7816
13	0.0137	0.0175	3.2135
14	0.0617	0.0690	11.6889
15	0.0578	0.0648	10.3925
16	0.0649	0.0579	13.4350
17	0.0488	0.0295	9.3082
18	0.0679	0.0321	17.3536
19	0.0795	0.0498	17.6314
20	0.0317	0.0231	5.5752

In []:

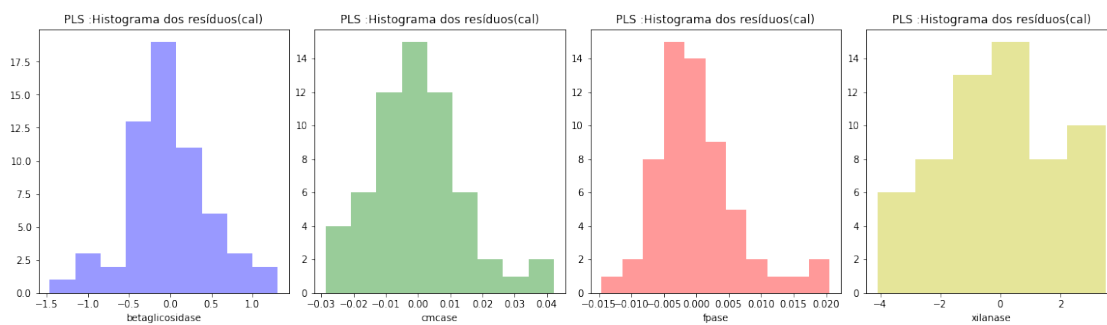
7.5.4 PLS: Gráficos de resíduos - histograma - reais x preditos

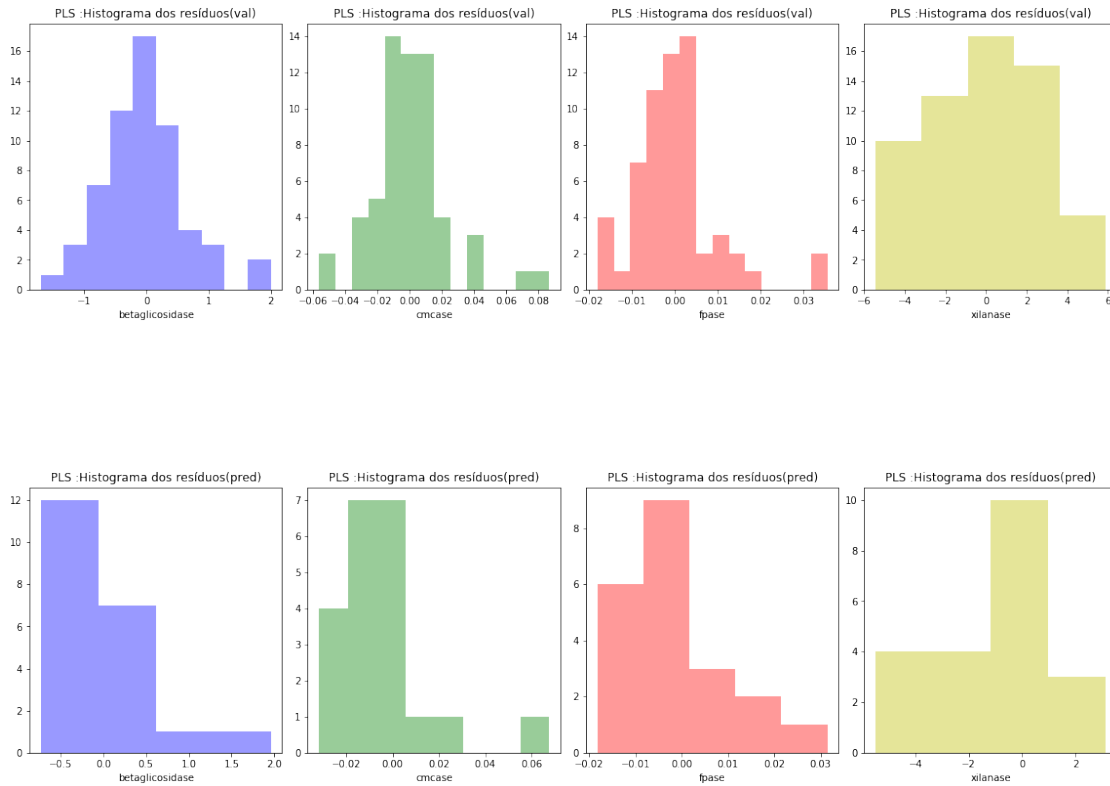
```
In [272]: #título para os gráficos
          modelo = 'PLS'
```

```
In [273]: #gráfico dos resíduos
          graficoResiduos(modelo, treino_teste, y_c,y_cv,y_p)
```

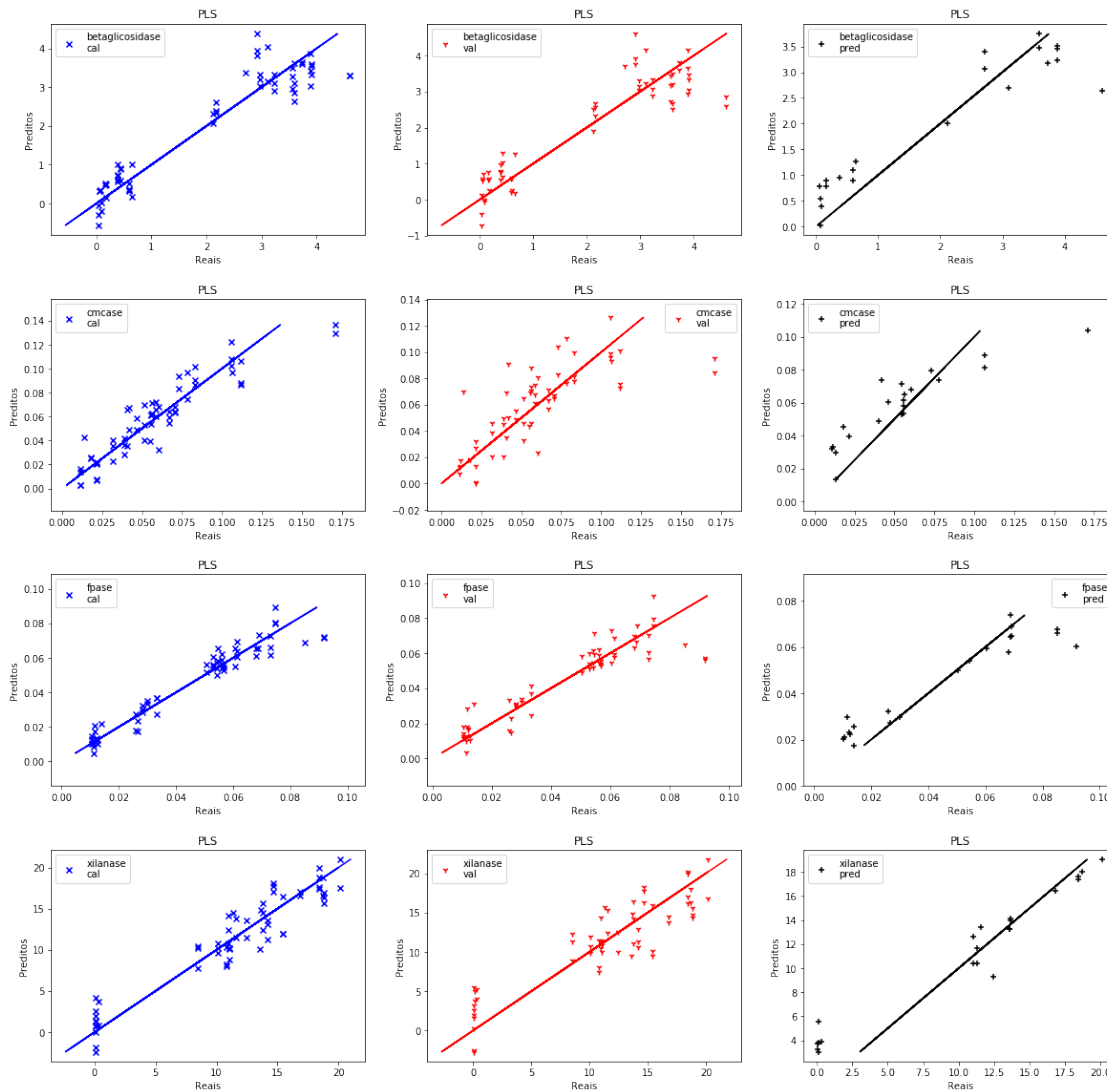


In [274]: *#histograma dos resíduos*
`graficoHist(modelo, treino_teste, y_c,y_cv,y_p)`

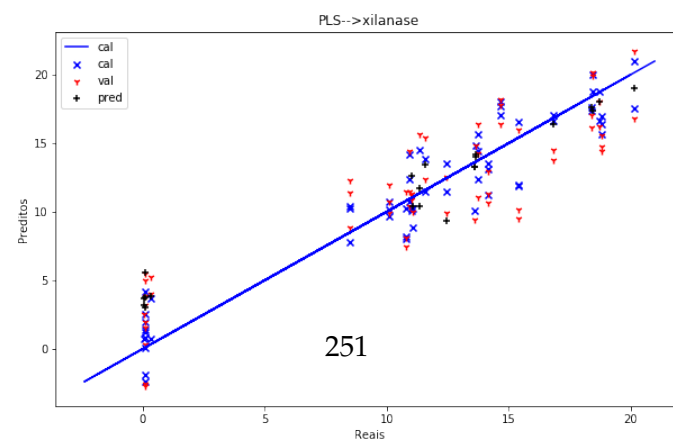
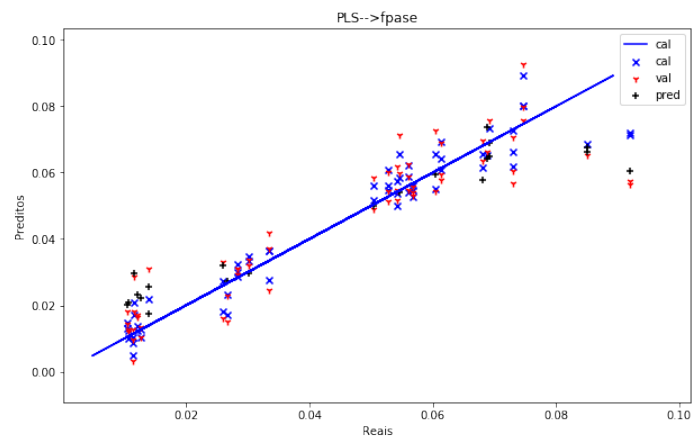
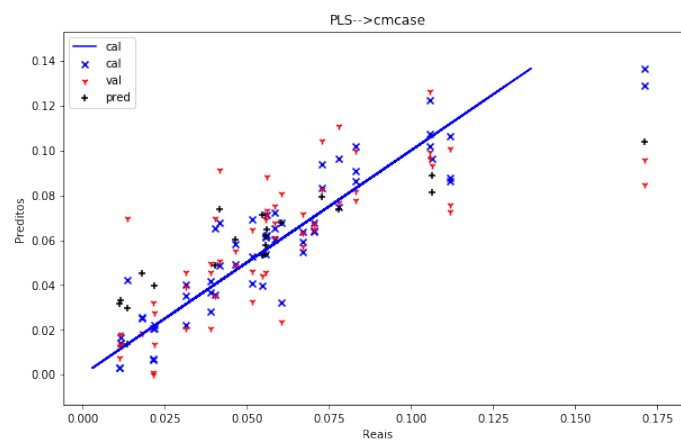
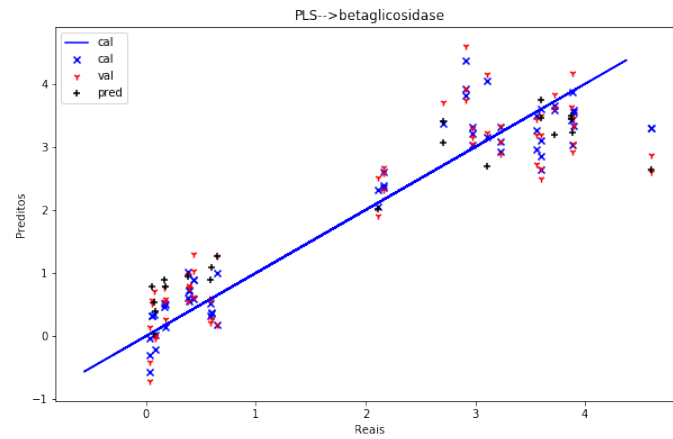




In [275]: *#graico de reais x preditos*
graficoReaisPreditosSep(modelo, treino_teste, y_c,y_cv,y_p)

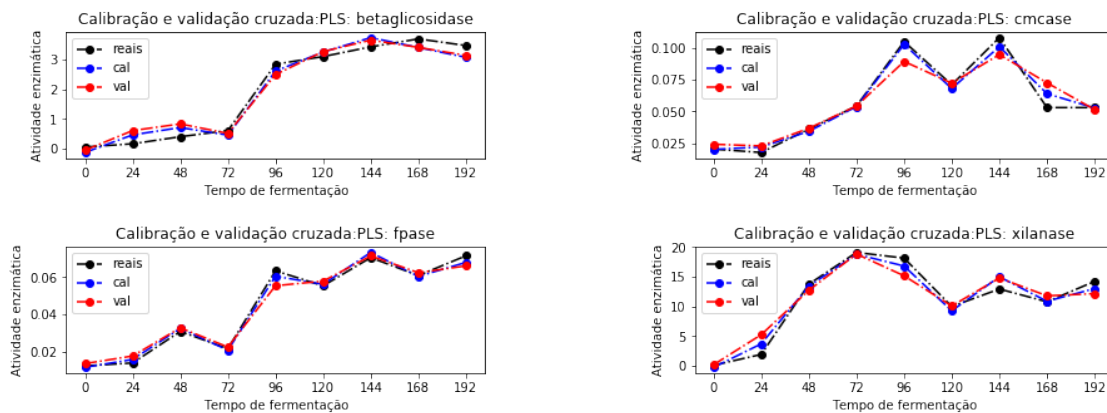


In [276]: *#gráfico de reais x preditos conjuntamente*
`graficoReaisPreditos(modelo, treino_teste, y_c,y_cv,y_p)`



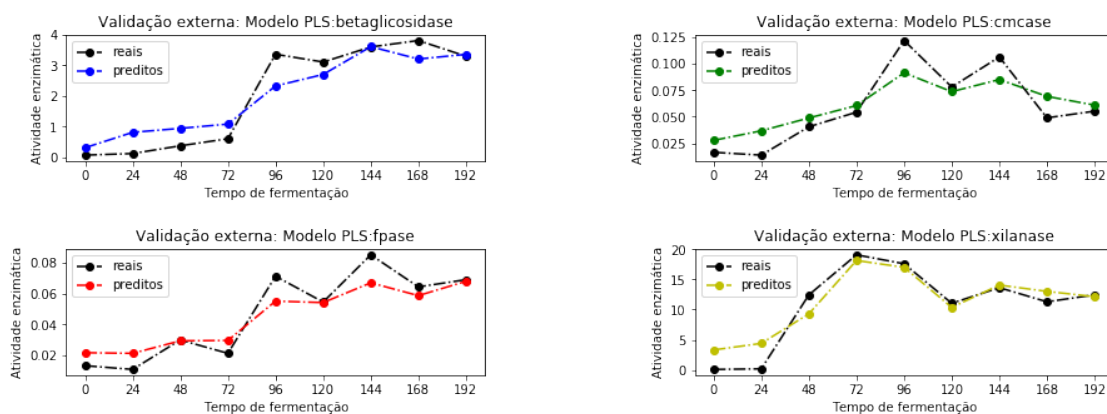
7.5.5 PLS: Gráficos: dados de treino

```
In [277]: y_treino = treino_teste[2]  
          graficoTreinamento(modelo, y_treino, y_c,y_cv)
```



7.5.6 PLS: Gráficos de teste

```
In [278]: y_teste = treino_teste[3]  
          graficoTeste(modelo, y_teste, y_p)
```



```
In [ ]:
```

```
In [ ]:
```

7.6 Ridge: Quadrados mínimos lineares

```
In [279]: #ridge
          #função completa para execução do Ridge:
          from sklearn.linear_model import Ridge
          def executaRidge(preproc, IC=0):
              x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc, False, IC)

              reg = Ridge(alpha = 1.0, solver = 'auto', max_iter=1000)
              #reg = Ridge(alpha=1.0, copy_X=True, fit_intercept=False, max_iter=1000,
                  # normalize=False, random_state=0, solver='auto', tol=0.001)

              result = executaCVP([x_treino, x_teste, y_treino, y_teste], reg)

              return result
```

```
In [280]: #PCA_Ridge
          from sklearn.linear_model import Ridge
          def executaPCA_Ridge(preproc, nPC=4, IC=0):
              x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc, False, IC)

              reg = Ridge(alpha = 1.0, solver = 'auto', max_iter=500)

              # Roda o PCA e produz uma variável reduzida xRed e seleciona as primeiras componentes
              pca = PCA(n_components=nPC)
              x_treino = pca.fit_transform(x_treino)[:,:nPC]
              x_teste = pca.fit_transform(x_teste)[:,:nPC]

              result = executaCVP([x_treino, x_teste, y_treino, y_teste], reg)

              return result
```

```
In [ ]:
```

7.6.1 Ridge: testes

```
In [281]: #ridge teste simples
          modelo = 'Ridge'
          for k in range(12):
              print(preProc[k])
              result = executaRidge(k)
              print('Parâmetros do modelo:', modelo, '\n', result[0])
```

```
resultados=exibeResultados(result)
```

```
for k,v in zip(resultados.keys(),resultados.values()):  
    print(k)  
    print(v,'\n-----')
```

Pré-proc: 0--> Sem pré-processamento

Parâmetros do modelo: Ridge

```
Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,  
      normalize=False, random_state=None, solver='auto', tol=0.001)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0000	0.0000	-0.0000	-0.0000
MSE	1.8488	0.0013	0.0005	42.6472
R2	0.2867	0.1175	0.2580	0.0403
RER	3.3350	4.4208	3.6151	3.0467
RMSE	1.3597	0.0359	0.0223	6.5305
RPD	1.1841	1.0645	1.1609	1.0208
RPIQ	2.3761	1.2232	2.2001	1.3717
SEP	1.3712	0.0362	0.0225	6.5856

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0002	0.0000	-0.0000	-0.0078
MSE	1.9109	0.0014	0.0005	46.1708
R2	0.2628	0.0705	0.2326	-0.0390
RER	3.2803	4.3076	3.5548	2.9281
RMSE	1.3824	0.0368	0.0227	6.7949
RPD	1.1647	1.0372	1.1416	0.9811
RPIQ	2.3371	1.1919	2.1633	1.3183
SEP	1.3940	0.0372	0.0229	6.8523

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2621	0.0018	0.0031	1.2118
MSE	1.4226	0.0006	0.0003	33.9507
R2	0.3781	0.1353	0.3906	-0.0176
RER	3.2446	3.9366	4.0996	3.4310
RMSE	1.1927	0.0249	0.0180	5.8267
RPD	1.2681	1.0754	1.2810	0.9913
RPIQ	2.6274	1.1490	2.2982	0.6661
SEP	1.1923	0.0254	0.0182	5.8401

Pré-proc: 1--> Padronização

Parâmetros do modelo: Ridge

```
Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,  
      normalize=False, random_state=None, solver='auto', tol=0.001)
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	-0.0000
MSE	0.1480	0.0002	0.0000	2.4702
R2	0.9429	0.8511	0.9354	0.9444
RER	11.7890	10.7634	12.2553	12.6592
RMSE	0.3846	0.0147	0.0066	1.5717
RPD	4.1857	2.5917	3.9356	4.2414
RPIQ	8.3993	2.9782	7.4583	5.6993
SEP	0.3879	0.0149	0.0066	1.5850

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0017	-0.0006	-0.0002	0.0131
MSE	0.4481	0.0007	0.0001	7.2265
R2	0.8271	0.5412	0.8192	0.8374
RER	6.7740	6.1329	7.3238	7.4014
RMSE	0.6694	0.0259	0.0110	2.6882
RPD	2.4051	1.4763	2.3515	2.4798
RPIQ	4.8263	1.6964	4.4562	3.3321
SEP	0.6751	0.0261	0.0111	2.7109

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.2690	0.0002	0.0000	7.0322
R2	0.8824	0.6982	0.9341	0.7892
RER	8.5457	6.7054	14.6860	8.3563
RMSE	0.5187	0.0147	0.0059	2.6518
RPD	2.9161	1.8202	3.8950	2.1782
RPIQ	6.0421	1.9448	6.9878	1.4636
SEP	0.4527	0.0149	0.0051	2.3979

Pré-proc: 2--> Suavização(SavGol) - Par:3,1,1

Parâmetros do modelo: Ridge

Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,
normalize=False, random_state=None, solver='auto', tol=0.001)

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	0.0000
MSE	2.4863	0.0014	0.0006	44.3058
R2	0.0408	0.0165	0.0365	0.0030
RER	2.8758	4.1877	3.1724	2.9891
RMSE	1.5768	0.0379	0.0255	6.6563
RPD	1.0211	1.0084	1.0188	1.0015
RPIQ	2.0489	1.1587	1.9307	1.3457
SEP	1.5901	0.0382	0.0257	6.7124

```

val
      betaglicosidase  cmcase  fpase  xilanase
BIAS      -0.0004 -0.0000 -0.0000  -0.0013
MSE        2.5491  0.0015  0.0007   45.9664
R2          0.0166 -0.0223  0.0105  -0.0344
RER         2.8402  4.1074  3.1304   2.9346
RMSE        1.5966  0.0386  0.0258   6.7799
RPD          1.0084  0.9890  1.0053   0.9832
RPIQ         2.0236  1.1365  1.9051   1.3212
SEP          1.6101  0.0390  0.0260   6.8371
-----

pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.2720  0.0020  0.0033   1.2467
MSE           2.2313  0.0007  0.0005  34.8779
R2            0.0246  0.0193  0.0374  -0.0454
RER           2.5704  3.6970  3.2468   3.3874
RMSE          1.4938  0.0265  0.0226   5.9057
RPD           1.0125  1.0098  1.0192   0.9781
RPIQ          2.0979  1.0789  1.8285   0.6572
SEP           1.5051  0.0271  0.0230   5.9152
-----

Pré-proc: 3--> Suavização(SavGol) - Par:3,2,1
Parâmetros do modelo: Ridge
Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,
      normalize=False, random_state=None, solver='auto', tol=0.001)
cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.0000  0.0000  0.0000   0.0000
MSE           2.4865  0.0014  0.0006  44.3074
R2            0.0407  0.0165  0.0364   0.0029
RER           2.8757  4.1876  3.1723   2.9891
RMSE          1.5769  0.0379  0.0255   6.6564
RPD           1.0210  1.0083  1.0187   1.0015
RPIQ          2.0489  1.1587  1.9306   1.3457
SEP           1.5902  0.0382  0.0257   6.7126
-----

val
      betaglicosidase  cmcase  fpase  xilanase
BIAS      -0.0004 -0.0000 -0.0000  -0.0013
MSE        2.5493  0.0015  0.0007   45.9677
R2          0.0165 -0.0224  0.0104  -0.0344
RER         2.8401  4.1073  3.1303   2.9346
RMSE        1.5966  0.0386  0.0258   6.7799
RPD          1.0084  0.9890  1.0052   0.9832
RPIQ         2.0235  1.1365  1.9050   1.3212
SEP          1.6101  0.0390  0.0260   6.8372
-----

```



```

pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.2721  0.0020  0.0033   1.2468
MSE      2.2314  0.0007  0.0005  34.8798
R2       0.0246  0.0193  0.0373  -0.0454
RER      2.5703  3.6969  3.2468   3.3873
RMSE     1.4938  0.0265  0.0226   5.9059
RPD      1.0125  1.0098  1.0192   0.9780
RPIQ     2.0979  1.0789  1.8285   0.6572
SEP      1.5051  0.0271  0.0230   5.9154
-----

Pré-proc: 4--> Suavização(SavGol) - Par:5,1,1
Parâmetros do modelo: Ridge
      Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,
      normalize=False, random_state=None, solver='auto', tol=0.001)
cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0000  0.0000  0.0000   0.0000
MSE      2.5339  0.0014  0.0007  44.3618
R2       0.0225  0.0091  0.0201   0.0017
RER      2.8487  4.1720  3.1458   2.9872
RMSE     1.5918  0.0380  0.0257   6.6605
RPD      1.0114  1.0046  1.0102   1.0009
RPIQ     2.0296  1.1543  1.9144   1.3449
SEP      1.6053  0.0384  0.0259   6.7167
-----

val
      betaglicosidase  cmcase  fpase  xilanase
BIAS     -0.0002 -0.0000 -0.0000  -0.0008
MSE      2.5934  0.0015  0.0007  45.9221
R2      -0.0005 -0.0288 -0.0048  -0.0334
RER      2.8158  4.0944  3.1065   2.9360
RMSE     1.6104  0.0388  0.0260   6.7766
RPD      0.9998  0.9859  0.9976   0.9837
RPIQ     2.0062  1.1329  1.8906   1.3218
SEP      1.6240  0.0391  0.0262   6.8338
-----

pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.2717  0.0020  0.0033   1.2469
MSE      2.2897  0.0007  0.0005  34.8960
R2      -0.0009  0.0083  0.0117  -0.0459
RER      2.5362  3.6763  3.2034   3.3865
RMSE     1.5132  0.0267  0.0229   5.9073
RPD      0.9996  1.0042  1.0059   0.9778
RPIQ     2.0710  1.0730  1.8046   0.6570
SEP      1.5253  0.0272  0.0233   5.9168
-----

```

Pré-proc: 5--> Suavização(SavGol) - Par:5,2,1

Parâmetros do modelo: Ridge

Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,
normalize=False, random_state=None, solver='auto', tol=0.001)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	0.0000
MSE	2.5317	0.0014	0.0007	44.3512
R2	0.0233	0.0095	0.0210	0.0020
RER	2.8500	4.1729	3.1471	2.9876
RMSE	1.5911	0.0380	0.0257	6.6597
RPD	1.0119	1.0048	1.0107	1.0010
RPIQ	2.0305	1.1546	1.9153	1.3450
SEP	1.6046	0.0384	0.0259	6.7159

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0002	-0.0000	-0.0000	-0.0008
MSE	2.5913	0.0015	0.0007	45.9151
R2	0.0003	-0.0284	-0.0040	-0.0332
RER	2.8170	4.0952	3.1077	2.9363
RMSE	1.6098	0.0388	0.0260	6.7761
RPD	1.0002	0.9861	0.9980	0.9838
RPIQ	2.0070	1.1331	1.8913	1.3219
SEP	1.6233	0.0391	0.0262	6.8332

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2716	0.0020	0.0032	1.2466
MSE	2.2874	0.0007	0.0005	34.8866
R2	0.0001	0.0090	0.0128	-0.0456
RER	2.5375	3.6775	3.2052	3.3869
RMSE	1.5124	0.0266	0.0229	5.9065
RPD	1.0001	1.0045	1.0064	0.9779
RPIQ	2.0721	1.0733	1.8056	0.6571
SEP	1.5246	0.0272	0.0233	5.9160

Pré-proc: 6--> Suavização(SavGol) - Par:3,2,2

Parâmetros do modelo: Ridge

Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,
normalize=False, random_state=None, solver='auto', tol=0.001)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	-0.0000
MSE	2.2720	0.0014	0.0006	44.0701
R2	0.1235	0.0497	0.1101	0.0083
RER	3.0084	4.2603	3.3009	2.9971
RMSE	1.5073	0.0373	0.0245	6.6385

RPD	1.0681	1.0258	1.0601	1.0042
RPIQ	2.1434	1.1788	2.0089	1.3493
SEP	1.5200	0.0376	0.0247	6.6946

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0010	-0.0000	-0.0000	-0.0037
MSE	2.3436	0.0014	0.0006	46.2447
R2	0.0959	0.0074	0.0812	-0.0406
RER	2.9621	4.1685	3.2486	2.9258
RMSE	1.5309	0.0381	0.0249	6.8003
RPD	1.0517	1.0037	1.0432	0.9803
RPIQ	2.1104	1.1534	1.9770	1.3172
SEP	1.5438	0.0384	0.0251	6.8577

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2739	0.0020	0.0033	1.2464
MSE	1.9660	0.0007	0.0005	34.8291
R2	0.1406	0.0658	0.1543	-0.0439
RER	2.7455	3.7887	3.4698	3.3898
RMSE	1.4021	0.0259	0.0212	5.9016
RPD	1.0787	1.0346	1.0874	0.9787
RPIQ	2.2350	1.1055	1.9508	0.6576
SEP	1.4091	0.0264	0.0215	5.9110

Pré-proc: 7--> Suavização(SavGol) - Par:5,2,2

Parâmetros do modelo: Ridge

Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,
normalize=False, random_state=None, solver='auto', tol=0.001)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	0.0000
MSE	2.5483	0.0015	0.0007	44.3918
R2	0.0169	0.0068	0.0150	0.0010
RER	2.8406	4.1671	3.1376	2.9862
RMSE	1.5963	0.0381	0.0257	6.6627
RPD	1.0086	1.0034	1.0076	1.0005
RPIQ	2.0239	1.1530	1.9095	1.3444
SEP	1.6098	0.0384	0.0260	6.7189

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0002	-0.0000	-0.0000	-0.0005
MSE	2.6067	0.0015	0.0007	45.9239
R2	-0.0056	-0.0308	-0.0095	-0.0334
RER	2.8086	4.0904	3.0993	2.9360
RMSE	1.6145	0.0388	0.0261	6.7767

RPD	0.9972	0.9849	0.9953	0.9837
RPIQ	2.0011	1.1318	1.8862	1.3218
SEP	1.6281	0.0391	0.0263	6.8339

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2721	0.0020	0.0033	1.2475
MSE	2.3077	0.0007	0.0005	34.9081
R2	-0.0087	0.0048	0.0038	-0.0463
RER	2.5261	3.6698	3.1906	3.3860
RMSE	1.5191	0.0267	0.0230	5.9083
RPD	0.9957	1.0024	1.0019	0.9776
RPIQ	2.0629	1.0711	1.7975	0.6569
SEP	1.5315	0.0273	0.0234	5.9177

Pré-proc: 8--> Suavização(SavGol) - Par:3,1,1 --> Padronização

Parâmetros do modelo: Ridge

Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,
normalize=False, random_state=None, solver='auto', tol=0.001)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	-0.0000	0.0000
MSE	0.0150	0.0000	0.0000	0.1586
R2	0.9942	0.9846	0.9953	0.9964
RER	36.9829	33.4712	45.4088	49.9618
RMSE	0.1226	0.0047	0.0018	0.3982
RPD	13.1307	8.0596	14.5825	16.7396
RPIQ	26.3492	9.2612	27.6349	22.4934
SEP	0.1236	0.0048	0.0018	0.4016

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0171	-0.0015	-0.0002	-0.0633
MSE	0.8004	0.0014	0.0002	8.4701
R2	0.6912	0.0236	0.7529	0.8094
RER	5.0697	4.2060	6.2648	6.8380
RMSE	0.8946	0.0378	0.0129	2.9103
RPD	1.7996	1.0120	2.0116	2.2905
RPIQ	3.6113	1.1629	3.8121	3.0778
SEP	0.9020	0.0381	0.0130	2.9342

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.7096	0.0011	0.0002	7.5434
R2	0.6898	-0.5340	0.5768	0.7739
RER	4.7349	2.9530	4.9636	7.9916
RMSE	0.8424	0.0331	0.0150	2.7465

RPD	1.7955	0.8074	1.5372	2.1031
RPIQ	3.7202	0.8627	2.7577	1.4131
SEP	0.8170	0.0339	0.0150	2.5073

Pré-proc: 9--> Padronização --> Suavização(SavGol) - Par:3,1,1

Parâmetros do modelo: Ridge

Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,
normalize=False, random_state=None, solver='auto', tol=0.001)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	0.0000
MSE	0.2721	0.0004	0.0001	8.0294
R2	0.8950	0.7370	0.8853	0.8193
RER	8.6933	8.0983	9.1947	7.0215
RMSE	0.5216	0.0196	0.0088	2.8336
RPD	3.0865	1.9500	2.9528	2.3525
RPIQ	6.1937	2.2407	5.5957	3.1612
SEP	0.5260	0.0198	0.0089	2.8575

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0041	-0.0002	0.0000	0.0250
MSE	0.4004	0.0006	0.0001	12.2481
R2	0.8455	0.5986	0.8289	0.7244
RER	7.1662	6.5553	7.5279	5.6852
RMSE	0.6328	0.0242	0.0107	3.4997
RPD	2.5443	1.5784	2.4175	1.9048
RPIQ	5.1056	1.8138	4.5813	2.5595
SEP	0.6381	0.0244	0.0108	3.5292

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.3178	0.0003	0.0000	7.8721
R2	0.8611	0.5771	0.9093	0.7641
RER	7.6438	5.6500	11.8433	7.7809
RMSE	0.5637	0.0174	0.0070	2.8057
RPD	2.6830	1.5377	3.3206	2.0587
RPIQ	5.5591	1.6430	5.9573	1.3833
SEP	0.5061	0.0177	0.0063	2.5752

Pré-proc: 10--> MSC

Parâmetros do modelo: Ridge

Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,
normalize=False, random_state=None, solver='auto', tol=0.001)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0000	0.0000	0.0000	0.0000

MSE	1.8558	0.0013	0.0005	43.1838
R2	0.2841	0.1162	0.2553	0.0282
RER	3.3287	4.4174	3.6085	3.0277
RMSE	1.3623	0.0359	0.0224	6.5714
RPD	1.1818	1.0637	1.1588	1.0144
RPIQ	2.3716	1.2223	2.1960	1.3631
SEP	1.3738	0.0362	0.0226	6.6269

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0004	0.0000	-0.0000	-0.0071
MSE	1.9162	0.0014	0.0005	46.6670
R2	0.2608	0.0699	0.2307	-0.0502
RER	3.2759	4.3061	3.5503	2.9125
RMSE	1.3843	0.0369	0.0228	6.8313
RPD	1.1631	1.0369	1.1401	0.9758
RPIQ	2.3339	1.1915	2.1606	1.3112
SEP	1.3959	0.0372	0.0229	6.8890

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.2625	0.0018	0.0031	1.2261
MSE	1.4272	0.0006	0.0003	34.7320
R2	0.3761	0.1334	0.3887	-0.0410
RER	3.2394	3.9324	4.0931	3.3922
RMSE	1.1946	0.0249	0.0180	5.8934
RPD	1.2661	1.0742	1.2790	0.9801
RPIQ	2.6232	1.1478	2.2946	0.6586
SEP	1.1942	0.0255	0.0182	5.9068

Pré-proc: 11--> SNV

Parâmetros do modelo: Ridge

Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,
normalize=False, random_state=None, solver='auto', tol=0.001)

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.0000	-0.0000	0.0000	0.0000
MSE	1.5435	0.0012	0.0004	40.2486
R2	0.4045	0.1745	0.3727	0.0943
RER	3.6499	4.5710	3.9315	3.1362
RMSE	1.2424	0.0347	0.0205	6.3442
RPD	1.2959	1.1007	1.2626	1.0508
RPIQ	2.6005	1.2648	2.3926	1.4119
SEP	1.2529	0.0350	0.0207	6.3977

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0054	0.0001	0.0000	-0.0055

MSE	1.5946	0.0013	0.0004	45.3442
R2	0.3848	0.1202	0.3506	-0.0204
RER	3.5911	4.4277	3.8641	2.9547
RMSE	1.2628	0.0358	0.0209	6.7338
RPD	1.2750	1.0661	1.2409	0.9900
RPIQ	2.5585	1.2251	2.3516	1.3302
SEP	1.2734	0.0361	0.0211	6.7906

pred	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.2341	0.0013	0.0026	1.1260
MSE	1.0568	0.0006	0.0002	33.1372
R2	0.5381	0.1627	0.5554	0.0068
RER	3.7716	3.9960	4.7988	3.4638
RMSE	1.0280	0.0245	0.0154	5.7565
RPD	1.4713	1.0928	1.4997	1.0034
RPIQ	3.0485	1.1677	2.6906	0.6742
SEP	1.0257	0.0251	0.0155	5.7847

In []:

```
In [290]: #ridge otimizando
maior=[-1,-1,-1,-1]
maiorGerado=[0,0,0,0]
for i in range(100):
    result = executaRidge(preproc=9,IC=i)
    resultados=exibeResultados(result)
    r2 = resultados['pred'].iloc[resultados['pred'].index=='R2']
    r = []
    for j in range(4):
        r.append(r2.iloc[:,j][0])
        if r[j]>maior[j]:
            maior[j] = r[j]
            maiorGerado[j]=i
    print('\r%d%% completos'%(i+1), end='')
print('\n','r2:',maior,'\nsemente: b c f x',maiorGerado)
```

100% completos

r2: [0.933, 0.7899, 0.9492, 0.8236]
semente: b c f x [96, 33, 59, 93]

```
In [300]: #ridge teste otimizado
modelo = 'Ridge:'
result = result = executaRidge(preproc=1,IC=96)
print('Parâmetros do modelo:',modelo,'\n',result[0])
```

```
resultados=exibeResultados(result)
```

Parâmetros do modelo: Ridge:

```
Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=1000,  
      normalize=False, random_state=None, solver='auto', tol=0.001)
```

```
In [301]: resultados['cal']
```

```
Out[301]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	0.0000
MSE	0.1397	0.0002	0.0000	2.7195
R2	0.9464	0.8456	0.9367	0.9330
RER	12.1304	10.6456	12.5074	12.0651
RMSE	0.3738	0.0149	0.0065	1.6491
RPD	4.3185	2.5450	3.9750	3.8628
RPIQ	8.5975	2.4879	6.6355	3.2137
SEP	0.3770	0.0150	0.0065	1.6630

```
In [302]: resultados['val']
```

```
Out[302]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0717	-0.0023	-0.0012	-0.1831
MSE	0.4807	0.0008	0.0002	9.0522
R2	0.8156	0.4742	0.7705	0.7769
RER	6.5759	5.7894	6.6005	6.6252
RMSE	0.6933	0.0275	0.0123	3.0087
RPD	2.3285	1.3791	2.0873	2.1172
RPIQ	4.6357	1.3482	3.4844	1.7614
SEP	0.6954	0.0276	0.0123	3.0285

```
In [303]: resultados['pred']
```

```
Out[303]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0255	-0.0043	-0.0051	-0.6730
MSE	0.1345	0.0002	0.0001	8.6340
R2	0.9416	0.6973	0.8920	0.8090
RER	10.3177	6.7185	12.3468	6.8390
RMSE	0.3668	0.0152	0.0078	2.9384
RPD	4.1364	1.8176	3.0428	2.2883
RPIQ	7.7542	2.5545	5.7302	1.9400
SEP	0.3749	0.0150	0.0060	2.9309

```
In [287]: reg, treino_teste,y_c,y_cv,y_p = result
```

7.6.2 Reais x preditos

```
In [ ]:
```



```
In [288]: #ridge reaisxpreditos
#calibração
pred=pd.DataFrame(y_c, columns=var_ae)
reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('CALIBRAÇÃO:\n')
round(reais_pred,4)
```

CALIBRAÇÃO:

```
Out [288]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	3.5610	0.0586	0.0561	10.0978	3.5881
1	0.4280	0.0390	0.0334	13.7624	0.5481
2	3.2342	0.0672	0.0543	8.4772	3.1771
3	0.0308	0.0213	0.0113	0.0996	0.1249
4	3.8994	0.1118	0.0613	10.9512	3.7519
5	0.5905	0.0465	0.0267	18.7095	0.5751
6	0.1724	0.0112	0.0121	0.0924	0.1611
7	0.6010	0.0559	0.0116	20.1368	0.5630
8	2.1643	0.0830	0.0529	18.8324	2.0584
9	0.0759	0.0136	0.0139	0.0726	0.0987
10	3.2342	0.0672	0.0543	8.4772	3.2756
11	0.1671	0.0117	0.0104	0.1117	0.0636
12	3.5610	0.0586	0.0561	10.0978	3.5582
13	2.9123	0.1058	0.0747	14.6813	2.9890
14	3.8994	0.1118	0.0613	10.9512	3.9198
15	0.6491	0.0605	0.0260	18.4274	0.6166
16	0.4280	0.0390	0.0334	13.7624	0.4082
17	0.6491	0.0605	0.0260	18.4274	0.7623
18	2.9123	0.1058	0.0747	14.6813	3.0716
19	0.6491	0.0605	0.0260	18.4274	0.6488
20	2.1150	0.0730	0.0505	18.4127	2.1569
21	0.6010	0.0559	0.0116	20.1368	0.5785
22	0.0308	0.0213	0.0113	0.0996	-0.0142
23	0.0874	0.0217	0.0127	0.1071	0.0243
24	0.0554	0.0181	0.0106	0.3275	0.0697
25	0.1724	0.0112	0.0121	0.0924	0.2656
26	3.8876	0.0418	0.0605	11.0267	3.8068
27	3.8803	0.0557	0.0691	11.3256	3.8549
28	2.7110	0.0548	0.0688	13.5829	2.8608
29	0.1671	0.0117	0.0104	0.1117	0.1130
30	3.1068	0.0781	0.0545	11.0526	3.1491
31	2.1643	0.0830	0.0529	18.8324	2.1813

32	2.9123	0.1058	0.0747	14.6813	2.8563
33	3.7243	0.0561	0.0681	11.5736	3.6938
34	3.7243	0.0561	0.0681	11.5736	3.6235
35	0.1724	0.0112	0.0121	0.0924	0.1320
36	0.1671	0.0117	0.0104	0.1117	0.3047
37	3.1068	0.0781	0.0545	11.0526	3.1119
38	0.4280	0.0390	0.0334	13.7624	0.3843
39	0.3828	0.0405	0.0301	12.4461	0.5113
40	3.5967	0.1065	0.0850	13.6476	3.5080
41	3.5974	0.0516	0.0731	15.3973	3.4035
42	3.8876	0.0418	0.0605	11.0267	3.9966
43	0.0874	0.0217	0.0127	0.1071	0.0493
44	0.3828	0.0405	0.0301	12.4461	0.3660
45	0.3900	0.0315	0.0283	14.1777	0.4816
46	3.2342	0.0672	0.0543	8.4772	3.2270
47	2.7110	0.0548	0.0688	13.5829	2.8335
48	3.1068	0.0781	0.0545	11.0526	3.1146
49	2.9774	0.0704	0.0567	10.8002	2.9776
50	2.7110	0.0548	0.0688	13.5829	2.7560
51	0.6010	0.0559	0.0116	20.1368	0.5538
52	3.5967	0.1065	0.0850	13.6476	3.4913
53	0.5905	0.0465	0.0267	18.7095	0.6265
54	3.8876	0.0418	0.0605	11.0267	3.8281
55	3.8803	0.0557	0.0691	11.3256	3.9146
56	3.5610	0.0586	0.0561	10.0978	3.6822
57	3.5974	0.0516	0.0731	15.3973	3.4187
58	3.8994	0.1118	0.0613	10.9512	3.8893
59	2.1150	0.0730	0.0505	18.4127	2.0844

	pred: cmcase	pred: fpase	pred: xilanasase
0	0.0583	0.0572	10.4331
1	0.0402	0.0352	13.3737
2	0.0669	0.0532	8.7153
3	0.0224	0.0132	0.4890
4	0.1085	0.0607	11.5572
5	0.0467	0.0260	18.8218
6	0.0104	0.0118	0.4643
7	0.0542	0.0131	19.9112
8	0.0788	0.0518	18.4892
9	0.0146	0.0134	-0.0519
10	0.0678	0.0545	9.1554
11	0.0118	0.0094	-0.0077
12	0.0608	0.0560	9.9075
13	0.1070	0.0759	14.7834
14	0.1087	0.0636	11.0802
15	0.0601	0.0257	18.6998
16	0.0407	0.0335	13.4667
17	0.0629	0.0262	18.4974

18	0.1060	0.0764	15.5142
19	0.0617	0.0252	18.1648
20	0.0750	0.0513	18.9235
21	0.0549	0.0127	19.6684
22	0.0206	0.0110	0.1451
23	0.0201	0.0120	-0.2672
24	0.0179	0.0090	-0.0332
25	0.0102	0.0146	0.5020
26	0.0407	0.0610	10.9940
27	0.0558	0.0706	11.4905
28	0.0566	0.0705	13.5932
29	0.0117	0.0115	0.6665
30	0.0783	0.0551	11.0083
31	0.0830	0.0513	18.7269
32	0.1044	0.0750	14.5205
33	0.0553	0.0668	11.3838
34	0.0557	0.0672	11.3848
35	0.0110	0.0116	0.1544
36	0.0147	0.0117	0.3379
37	0.0777	0.0548	10.5206
38	0.0386	0.0325	13.7500
39	0.0387	0.0321	12.6872
40	0.1048	0.0809	13.2737
41	0.0532	0.0695	15.2103
42	0.0439	0.0631	11.4994
43	0.0217	0.0121	0.2652
44	0.0423	0.0282	12.3080
45	0.0329	0.0288	14.0894
46	0.0668	0.0541	8.2403
47	0.0548	0.0687	13.3620
48	0.0773	0.0549	10.8107
49	0.0702	0.0559	10.6723
50	0.0552	0.0699	13.7140
51	0.0537	0.0130	20.2777
52	0.1059	0.0840	13.6035
53	0.0474	0.0249	18.8764
54	0.0430	0.0581	10.5484
55	0.0566	0.0697	11.2855
56	0.0595	0.0574	10.3474
57	0.0496	0.0705	15.0372
58	0.1124	0.0615	10.6508
59	0.0740	0.0505	17.9884

```
In [1062]: #validação
pred=pd.DataFrame(y_cv, columns=var_ae)
reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
```

```

for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('VALIDAÇÃO CRUZADA:\n')
round(reais_pred,4)

```

VALIDAÇÃO CRUZADA:

```

Out[1062]:
    betaglicosidase  cmcase  fpase  xilanas  pred: betaglicosidase \
0      3.2342  0.0672  0.0543    8.4772      2.7566
1      0.3900  0.0315  0.0283   14.1777      0.5290
2      2.9123  0.1058  0.0747   14.6813      3.7219
3      0.0554  0.0181  0.0106    0.3275      0.8852
4      2.1150  0.0730  0.0505   18.4127      3.6636
5      3.8994  0.1118  0.0613   10.9512      3.2920
6      3.2342  0.0672  0.0543    8.4772      2.8189
7      3.5610  0.0586  0.0561   10.0978      4.0764
8      3.5610  0.0586  0.0561   10.0978      4.0725
9      0.0308  0.0213  0.0113    0.0996     -0.3955
10     2.9774  0.0704  0.0567   10.8002      3.0278
11     0.1671  0.0117  0.0104    0.1117     -0.8059
12     0.5905  0.0465  0.0267   18.7095      0.7814
13     3.1068  0.0781  0.0545   11.0526      2.2134
14     3.8994  0.1118  0.0613   10.9512      3.7650
15     3.5974  0.0516  0.0731   15.3973      3.3843
16     3.8803  0.0557  0.0691   11.3256      5.1440
17     0.3900  0.0315  0.0283   14.1777      1.5222
18     3.1068  0.0781  0.0545   11.0526      3.2246
19     2.7110  0.0548  0.0688   13.5829      2.7880
20     3.7243  0.0561  0.0681   11.5736      3.4571
21     0.0874  0.0217  0.0127    0.1071     -0.4743
22     0.0759  0.0136  0.0139    0.0726     -0.4536
23     3.8803  0.0557  0.0691   11.3256      1.9551
24     3.1068  0.0781  0.0545   11.0526      3.5281
25     0.6491  0.0605  0.0260   18.4274      1.0689
26     2.1150  0.0730  0.0505   18.4127      2.9760
27     0.5905  0.0465  0.0267   18.7095      0.2367
28     3.5967  0.1065  0.0850   13.6476      3.8621
29     0.4280  0.0390  0.0334   13.7624      1.7822
30     0.0554  0.0181  0.0106    0.3275      1.1182
31     3.5967  0.1065  0.0850   13.6476      3.5195
32     2.9123  0.1058  0.0747   14.6813      3.0683
33     3.5974  0.0516  0.0731   15.3973      3.0922
34     0.1671  0.0117  0.0104    0.1117      0.3451
35     3.8876  0.0418  0.0605   11.0267      3.4058
36     0.6491  0.0605  0.0260   18.4274      0.6689
37     0.3828  0.0405  0.0301   12.4461      0.9434

```

38	3.5967	0.1065	0.0850	13.6476	2.8730
39	2.1150	0.0730	0.0505	18.4127	2.4629
40	0.0759	0.0136	0.0139	0.0726	0.6554
41	0.1671	0.0117	0.0104	0.1117	0.5818
42	0.4280	0.0390	0.0334	13.7624	1.2096
43	4.6037	0.1713	0.0919	16.8115	3.3256
44	3.5610	0.0586	0.0561	10.0978	4.6518
45	0.6010	0.0559	0.0116	20.1368	0.4559
46	0.1724	0.0112	0.0121	0.0924	0.8868
47	0.3828	0.0405	0.0301	12.4461	0.3780
48	3.8876	0.0418	0.0605	11.0267	3.8076
49	4.6037	0.1713	0.0919	16.8115	2.3752
50	0.1724	0.0112	0.0121	0.0924	0.7466
51	0.5905	0.0465	0.0267	18.7095	-0.5143
52	0.0759	0.0136	0.0139	0.0726	0.1369
53	0.0554	0.0181	0.0106	0.3275	0.3721
54	0.6010	0.0559	0.0116	20.1368	0.4253
55	2.9774	0.0704	0.0567	10.8002	2.2812
56	3.2342	0.0672	0.0543	8.4772	2.8617
57	3.8994	0.1118	0.0613	10.9512	3.9422
58	4.6037	0.1713	0.0919	16.8115	3.1092
59	3.8876	0.0418	0.0605	11.0267	3.6437

	pred: cmcase	pred: fpase	pred: xylanase
0	0.0786	0.0532	10.0562
1	0.0312	0.0363	12.9190
2	0.1265	0.0846	17.2933
3	0.0398	0.0198	1.2053
4	0.1349	0.0801	17.0182
5	0.0976	0.0659	12.3488
6	0.0610	0.0557	10.8357
7	0.0838	0.0678	9.9625
8	0.0834	0.0733	14.0152
9	0.0158	0.0142	3.5474
10	0.0756	0.0567	9.8368
11	-0.0283	-0.0066	-1.7008
12	0.0610	0.0237	16.7722
13	0.0465	0.0459	8.2737
14	0.1035	0.0719	11.8600
15	0.0782	0.0730	13.8236
16	0.1158	0.0974	13.6220
17	0.0716	0.0475	12.2041
18	0.0734	0.0519	10.8048
19	0.0365	0.0600	14.0569
20	0.0559	0.0557	9.7247
21	0.0190	0.0054	0.4906
22	0.0175	0.0167	2.0716
23	0.0017	0.0387	12.8641

24	0.0679	0.0567	8.9414
25	0.0518	0.0363	19.6025
26	0.1095	0.0666	18.3039
27	0.0260	0.0193	16.3504
28	0.0972	0.0807	15.6563
29	0.0708	0.0506	15.9381
30	0.0657	0.0391	5.5658
31	0.0946	0.0739	12.9094
32	0.1013	0.0657	14.4651
33	0.0762	0.0629	12.6993
34	0.0195	0.0127	1.9269
35	0.0308	0.0562	9.4914
36	0.0389	0.0210	18.2921
37	0.0768	0.0375	13.8217
38	0.0530	0.0568	8.4924
39	0.0998	0.0542	15.2207
40	0.0399	0.0170	4.6293
41	0.0321	0.0197	2.3301
42	0.0467	0.0391	12.9040
43	0.0990	0.0679	14.6186
44	0.1011	0.0773	13.5619
45	0.0662	0.0193	18.4559
46	0.0208	0.0213	1.6656
47	0.0066	0.0168	9.4741
48	0.0641	0.0673	13.1468
49	0.0676	0.0474	14.3957
50	0.0227	0.0151	3.0936
51	0.0042	0.0127	15.5359
52	-0.0205	0.0154	1.6439
53	0.0098	0.0137	0.2191
54	0.0376	0.0189	19.7825
55	0.0506	0.0425	7.6911
56	0.0676	0.0524	11.6093
57	0.1208	0.0775	10.4444
58	0.1028	0.0600	14.4810
59	0.0569	0.0582	11.2700

```
In [1063]: #predição
pred=pd.DataFrame(y_p, columns=var_ae)
reais = treino_teste[3]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('Predição (validação externa):\n')
round(reais_pred,4)
```

Predição (validação externa):

```

Out[1063]:
    betaglicosidase  cmcase  fpase  xilanase  pred: betaglicosidase  \
0      3.5974  0.0516  0.0731  15.3973      3.9585
1      3.8803  0.0557  0.0691  11.3256      3.7439
2      3.7243  0.0561  0.0681  11.5736      3.8461
3      2.1643  0.0830  0.0529  18.8324      3.9182
4      0.6491  0.0605  0.0260  18.4274      0.2357
5      0.3900  0.0315  0.0283  14.1777      1.0511
6      2.1643  0.0830  0.0529  18.8324      3.0518
7      0.0874  0.0217  0.0127   0.1071      0.6861
8      2.9123  0.1058  0.0747  14.6813      3.2884
9      0.0308  0.0213  0.0113   0.0996     -0.8406
10     0.3828  0.0405  0.0301  12.4461      1.5538
11     0.4280  0.0390  0.0334  13.7624      0.9922
12     0.0308  0.0213  0.0113   0.0996      0.1783
13     0.1724  0.0112  0.0121   0.0924      0.1588
14     3.7243  0.0561  0.0681  11.5736      4.9058
15     0.0874  0.0217  0.0127   0.1071      0.6000
16     2.9774  0.0704  0.0567  10.8002      2.5004
17     2.1643  0.0830  0.0529  18.8324      2.3034
18     2.7110  0.0548  0.0688  13.5829      4.0600
19     2.7110  0.0548  0.0688  13.5829      2.7219
20     0.6010  0.0559  0.0116  20.1368      0.9115

    pred: cmcase  pred: fpase  pred: xilanase
0      0.0823      0.0809      15.6671
1      0.0581      0.0611      10.6501
2      0.0733      0.0748      12.5182
3      0.1324      0.0732      13.5936
4      0.0320      0.0175      15.3187
5      0.0563      0.0357      10.1028
6      0.0938      0.0614      14.3134
7      0.0356      0.0105       1.1984
8      0.1211      0.0817      18.4668
9     -0.0294     -0.0094     -1.2611
10     0.0949      0.0472      11.1344
11     0.0605      0.0457      13.3416
12     0.0334      0.0198       6.5912
13     0.0106      0.0115       4.2335
14     0.1278      0.0859      13.8037
15     0.0044      0.0095       2.9197
16     0.0562      0.0432       7.7705
17     0.0633      0.0407      13.6693
18     0.0821      0.0807      12.8034
19     0.0115      0.0532      12.0130
20     0.0573      0.0266      17.5853

```

```
In [ ]:
```

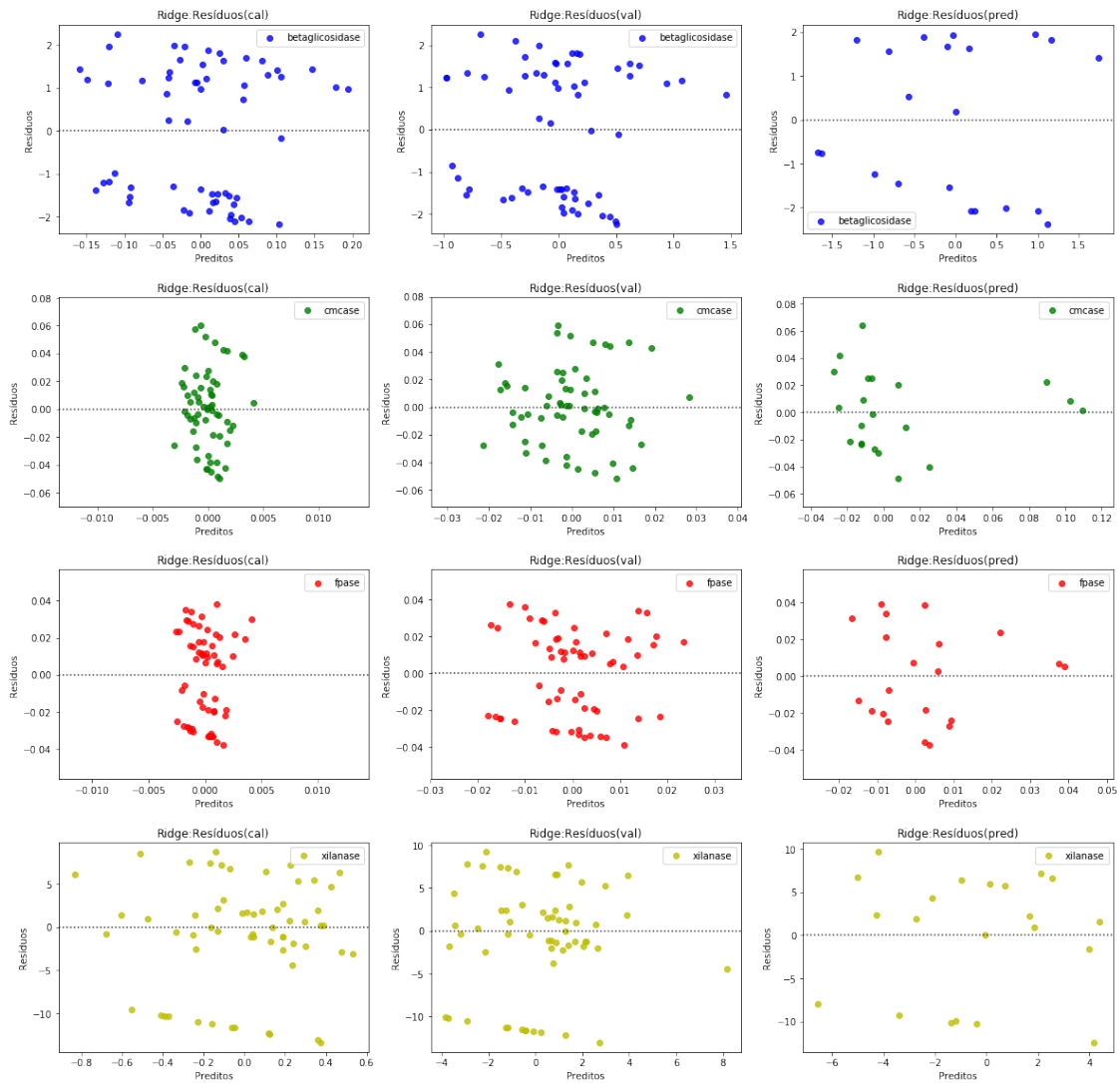
7.6.3 Ridge: Gráficos de resíduos - histograma - reais x preditos

```
In [304]: #título para os gráficos
```

```
modelo = 'Ridge'
```

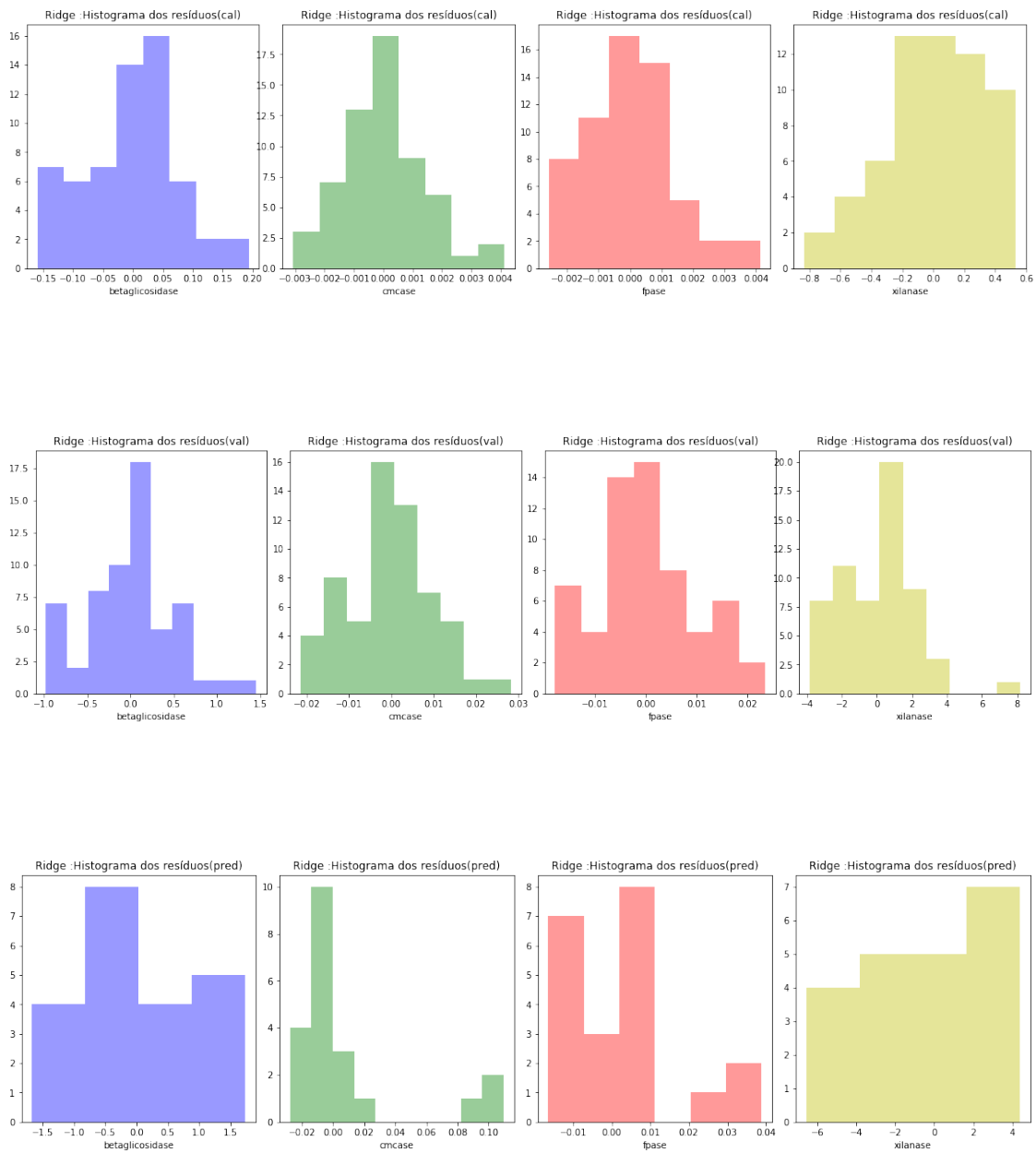
```
In [305]: #gráfico dos resíduos
```

```
graficoResiduos(modelo, treino_teste, y_c,y_cv,y_p)
```

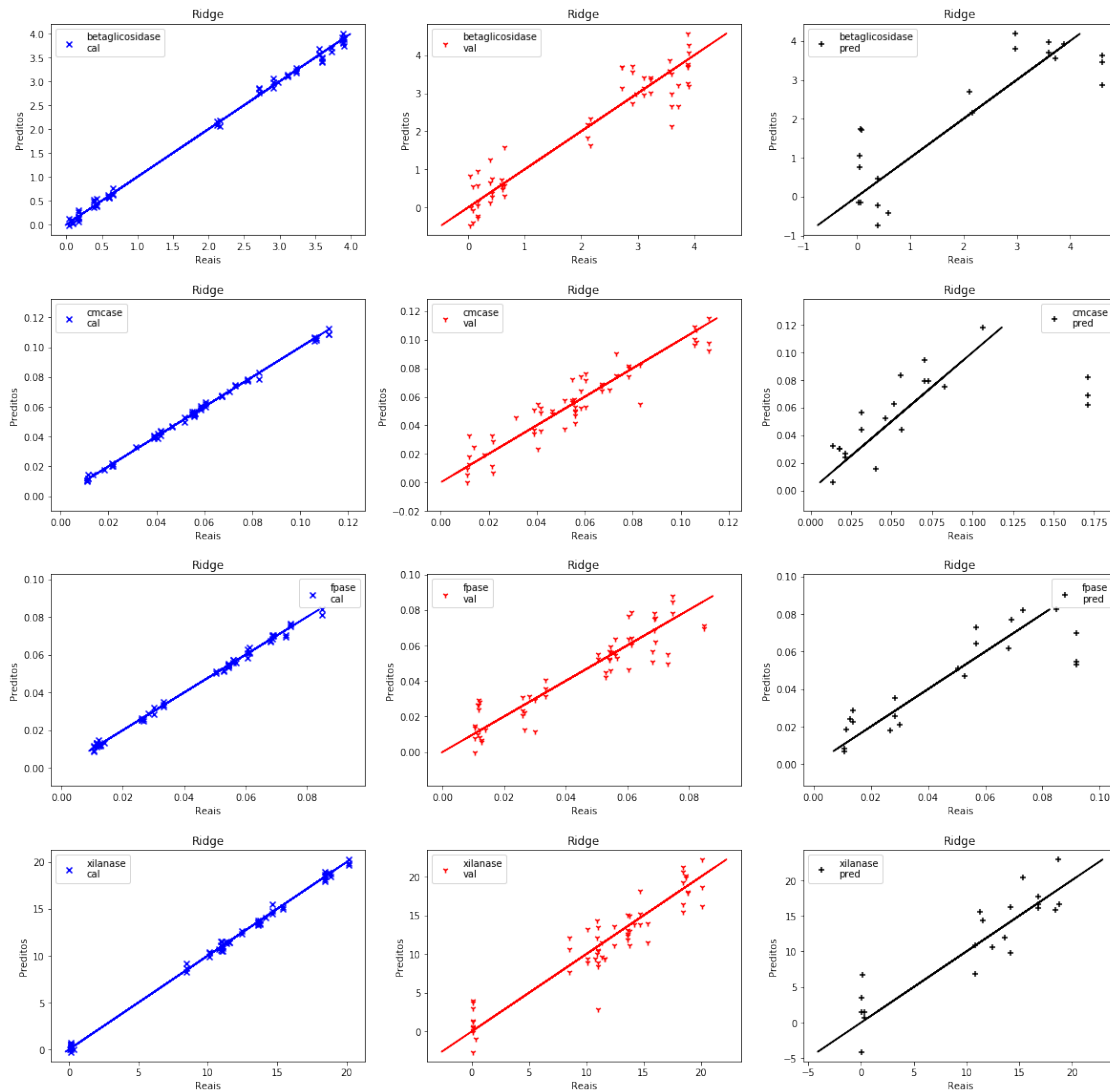


```
In [306]: #histograma dos resíduos
```

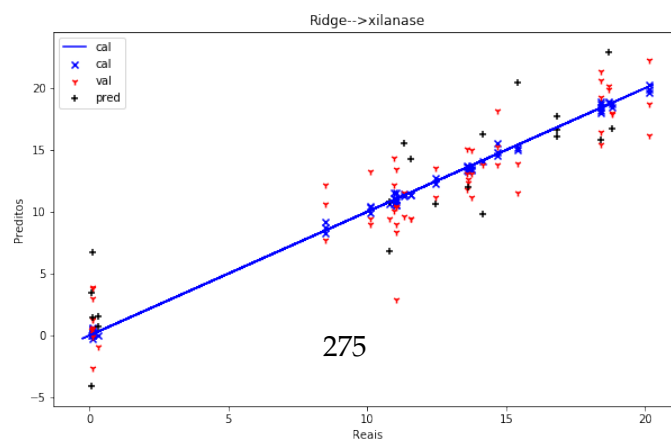
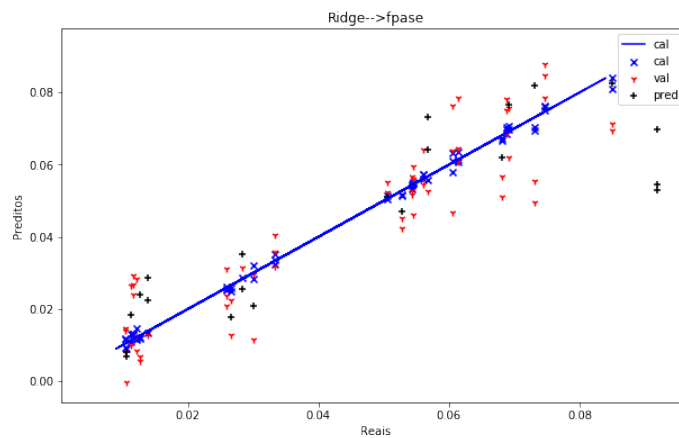
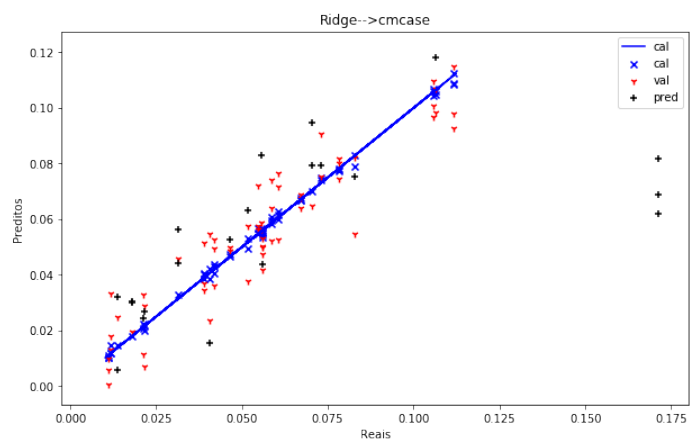
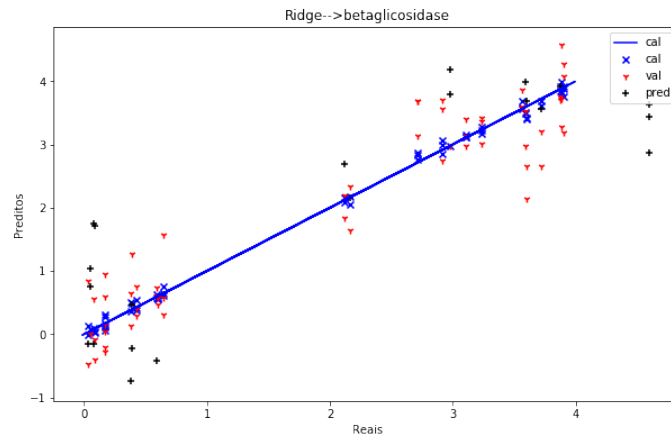
```
graficoHist(modelo, treino_teste, y_c,y_cv,y_p)
```

In [308]: *#graico de reais x preditos*
graficoReaisPreditosSep(modelo, treino_teste, y_c,y_cv,y_p)

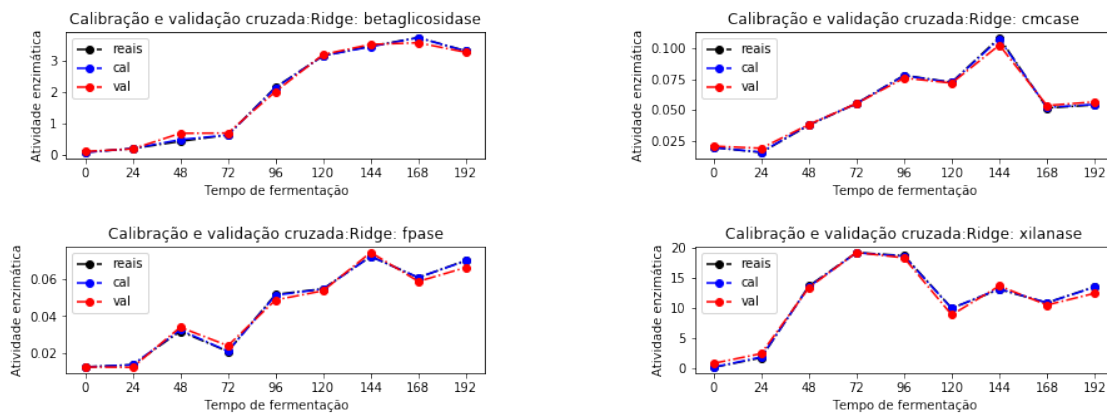


In [309]: *#gráfico de reais x preditos*
`graficoReaisPreditos(modelo, treino_teste, y_c,y_cv,y_p)`



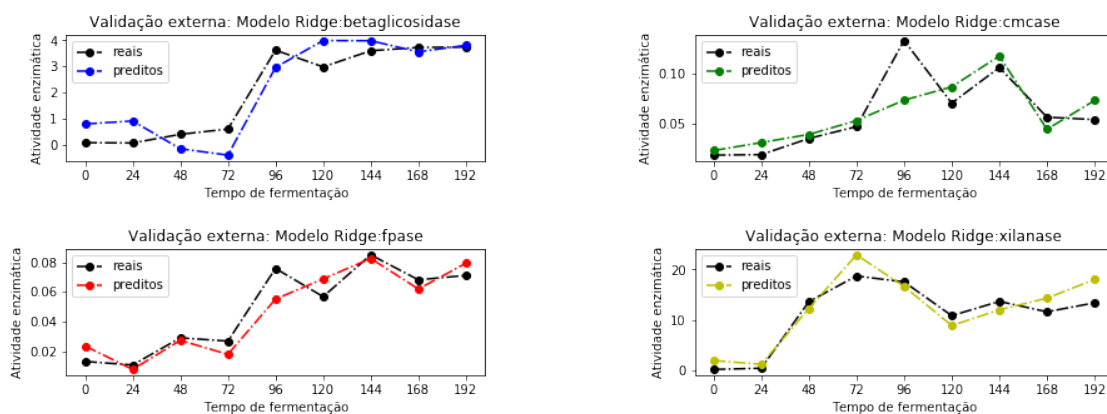
7.6.4 Ridge: Gráficos: dados de treino

```
In [310]: y_treino = treino_teste[2]
          graficoTreinamento(modelo, y_treino, y_c,y_cv)
```



7.6.5 Ridge: Gráficos de teste

```
In [311]: y_teste = treino_teste[3]
          graficoTeste(modelo, y_teste, y_p)
```



```
In [ ]:
```

7.7 Kernel Ridge: Quadrados mínimos lineares com kernel

```
In [417]: #kernelRidge
def executaKernelRidge(preproc=1, teste=1, k='linear', IC=0):
    #separando o conjunto de dados em treino e teste
    x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc,False, IC)

    if teste == 1:
        reg = GridSearchCV(estimator=KernelRidge(), cv=5,
                           param_grid={"kernel":['rbf','linear','poly'],
                                         "alpha": [1e0, 0.1, 1e-2, 1e-3],
                                         "gamma": [.1,.2,0,1,2,3,4,5,10],
                                         "degree": [1,2,3]
                                       })

    elif teste==2:
        #kernel otimizado
        reg = KernelRidge(alpha=1, coef0=1, degree=3, gamma=None, kernel='linear')
    else:
        reg = KernelRidge(kernel = k,alpha = 1.0)

    result = executaCVP([x_treino, x_teste, y_treino, y_teste], reg)

    return result
```

In []:

7.7.1 Kernel Ridge: testes

```
In [418]: #Kernelridge teste para um tipo de pré-processamento
modelo = 'Kernel Ridge'
result = executaKernelRidge(preproc=1,teste=0,k='rbf')
print('Parâmetros do modelo:',modelo,'\n',result[0])

resultados=exibeResultados(result)

for k,v in zip(resultados.keys(),resultados.values()):
    print(k)
    print(v,'\n-----')
```

Parâmetros do modelo: Kernel Ridge

KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='rbf',
kernel_params=None)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0746	0.0026	0.0018	0.5125

MSE	0.3211	0.0005	0.0001	10.0646
R2	0.8761	0.6869	0.8493	0.7735
RER	8.0723	7.4792	8.1520	6.3550
RMSE	0.5667	0.0214	0.0101	3.1725
RPD	2.8411	1.7871	2.5759	2.1013
RPIQ	5.7012	2.0536	4.8815	2.8235
SEP	0.5665	0.0214	0.0100	3.1572

val	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1062	0.0037	0.0026	0.7122
MSE	0.4064	0.0006	0.0001	12.8413
R2	0.8432	0.5871	0.8040	0.7110
RER	7.2142	6.5384	7.2158	5.6652
RMSE	0.6375	0.0246	0.0115	3.5835
RPD	2.5256	1.5562	2.2590	1.8603
RPIQ	5.0680	1.7882	4.2809	2.4997
SEP	0.6339	0.0245	0.0113	3.5416

pred	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2721	-0.0000	0.0032	0.6347
MSE	0.2047	0.0003	0.0001	11.4232
R2	0.9105	0.6006	0.9035	0.6576
RER	10.4462	5.7775	11.3776	5.8904
RMSE	0.4524	0.0169	0.0072	3.3798
RPD	3.3432	1.5824	3.2192	1.7090
RPIQ	6.9269	1.6908	5.7755	1.1483
SEP	0.3703	0.0173	0.0066	3.4017

```
In [419]: #Kernelridge teste pré-proc
          modelo = 'Kernel Ridge'
          for k in range(12):
              print(preProc[k])
              result = executaKernelRidge(k, teste=0, k='poly')
              print('Parâmetros do modelo:',modelo,'\n',result[0])

          resultados=exibeResultados(result)

          for k,v in zip(resultados.keys(),resultados.values()):
              print(k)
              print(v,'\n-----')
```

Pré-proc: 0--> Sem pré-processamento

Parâmetros do modelo: Kernel Ridge

KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='poly',

```

        kernel_params=None)
cal
      betaglicosidase  cmcase  fpase  xylanase
BIAS          0.0112  0.0003  0.0003   0.0561
MSE           2.5384  0.0014  0.0007  44.2665
R2            0.0207  0.0084  0.0182   0.0039
RER           2.8463  4.1707  3.1428   2.9905
RMSE          1.5932  0.0381  0.0257   6.6533
RPD           1.0105  1.0042  1.0092   1.0019
RPIQ          2.0278  1.1539  1.9125   1.3463
SEP           1.6066  0.0384  0.0259   6.7092
-----

```

```

val
      betaglicosidase  cmcase  fpase  xylanase
BIAS          0.0122  0.0004  0.0003   0.0622
MSE           2.5973  0.0015  0.0007  45.8021
R2           -0.0020 -0.0290 -0.0066  -0.0307
RER           2.8138  4.0941  3.1039   2.9400
RMSE          1.6116  0.0388  0.0260   6.7677
RPD           0.9990  0.9858  0.9967   0.9850
RPIQ          2.0047  1.1328  1.8889   1.3236
SEP           1.6252  0.0391  0.0262   6.8245
-----

```

```

pred
      betaglicosidase  cmcase  fpase  xylanase
BIAS          0.2823  0.0023  0.0035   1.3013
MSE           2.2997  0.0007  0.0005  34.8800
R2           -0.0052  0.0060  0.0066  -0.0454
RER           2.5338  3.6754  3.2001   3.3944
RMSE          1.5165  0.0267  0.0230   5.9059
RPD           0.9974  1.0030  1.0033   0.9780
RPIQ          2.0665  1.0717  1.8000   0.6572
SEP           1.5268  0.0272  0.0233   5.9030
-----

```

Pré-proc: 1--> Padronização

Parâmetros do modelo: Kernel Ridge

```

KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='poly',
            kernel_params=None)

```

```

cal
      betaglicosidase  cmcase  fpase  xylanase
BIAS          0.0275  0.0007  0.0007   0.1500
MSE           0.2663  0.0003  0.0001   7.6581
R2            0.8973  0.8142  0.8929   0.8277
RER           8.8003  9.6439  9.5470   7.2003
RMSE          0.5160  0.0165  0.0085   2.7673
RPD           3.1201  2.3201  3.0551   2.4089
RPIQ          6.2610  2.6660  5.7897   3.2369
SEP           0.5196  0.0166  0.0085   2.7866

```

```

-----
val
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0423  0.0013  0.0011  0.2109
MSE      0.3560  0.0004  0.0001  9.8822
R2      0.8627  0.7282  0.8506  0.7776
RER      7.6194  7.9826  8.1029  6.3434
RMSE     0.5966  0.0199  0.0100  3.1436
RPD      2.6984  1.9181  2.5868  2.1206
RPIQ     5.4149  2.2041  4.9021  2.8495
SEP      0.6002  0.0201  0.0101  3.1630
-----

```

```

pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.2499 -0.0007  0.0024  0.6597
MSE      0.3023  0.0002  0.0001  9.9897
R2      0.8679  0.6771  0.8777  0.7006
RER      7.7092  6.4320  9.4363  6.3261
RMSE     0.5498  0.0152  0.0081  3.1606
RPD      2.7509  1.7597  2.8589  1.8275
RPIQ     5.6998  1.8802  5.1290  1.2280
SEP      0.5018  0.0156  0.0079  3.1674
-----

```

Pré-proc: 2--> Suavização(SavGol) - Par:3,1,1

Parâmetros do modelo: Kernel Ridge

```

KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='poly',
             kernel_params=None)

```

```

cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0314  0.0009  0.0007  0.1737
MSE      2.5918  0.0015  0.0007  44.4675
R2      0.0001 -0.0004 -0.0003 -0.0007
RER      2.8172  4.1533  3.1146  2.9847
RMSE     1.6099  0.0382  0.0259  6.6684
RPD      1.0001  0.9998  0.9998  0.9997
RPIQ     2.0068  1.1489  1.8948  1.3433
SEP      1.6232  0.0385  0.0262  6.7224
-----

```

```

val
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.0348  0.0010  0.0008  0.1926
MSE      2.6460  0.0015  0.0007  45.8931
R2     -0.0208 -0.0366 -0.0235 -0.0327
RER      2.7884  4.0805  3.0795  2.9382
RMSE     1.6266  0.0389  0.0262  6.7744
RPD      0.9898  0.9822  0.9885  0.9840
RPIQ     1.9862  1.1286  1.8732  1.3223
SEP      1.6400  0.0392  0.0265  6.8288

```



```

-----
pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.3031  0.0029  0.0040    1.4212
MSE           2.3780  0.0007  0.0005   35.3839
R2            -0.0395 -0.0114 -0.0289   -0.0605
RER           2.4970  3.6515  3.1536    3.3853
RMSE          1.5421  0.0269  0.0234    5.9484
RPD           0.9808  0.9943  0.9859    0.9710
RPIQ          2.0322  1.0624  1.7687    0.6525
SEP           1.5493  0.0274  0.0236    5.9188
-----

```

Pré-proc: 3--> Suavização(SavGol) - Par:3,2,1

Parâmetros do modelo: Kernel Ridge

```

KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='poly',
             kernel_params=None)

```

```

cal
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.0314  0.0009  0.0007    0.1737
MSE           2.5918  0.0015  0.0007   44.4676
R2            0.0001 -0.0004 -0.0003   -0.0007
RER           2.8172  4.1533  3.1146    2.9847
RMSE          1.6099  0.0382  0.0259    6.6684
RPD           1.0001  0.9998  0.9998    0.9997
RPIQ          2.0068  1.1488  1.8948    1.3433
SEP           1.6232  0.0385  0.0262    6.7224
-----

```

```

val
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.0348  0.0010  0.0008    0.1926
MSE           2.6460  0.0015  0.0007   45.8931
R2            -0.0208 -0.0366 -0.0235   -0.0327
RER           2.7884  4.0804  3.0795    2.9381
RMSE          1.6266  0.0389  0.0262    6.7744
RPD           0.9898  0.9822  0.9885    0.9840
RPIQ          1.9862  1.1286  1.8732    1.3223
SEP           1.6400  0.0392  0.0265    6.8289
-----

```

```

pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.3031  0.0029  0.0040    1.4212
MSE           2.3780  0.0007  0.0005   35.3839
R2            -0.0395 -0.0114 -0.0289   -0.0605
RER           2.4970  3.6515  3.1536    3.3853
RMSE          1.5421  0.0269  0.0234    5.9484
RPD           0.9808  0.9943  0.9859    0.9710
RPIQ          2.0322  1.0624  1.7687    0.6525
SEP           1.5493  0.0274  0.0236    5.9188

```

Pré-proc: 4--> Suavização(SavGol) - Par:5,1,1

Parâmetros do modelo: Kernel Ridge

KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='poly',
kernel_params=None)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0314	0.0009	0.0007	0.1737
MSE	2.5924	0.0015	0.0007	44.4680
R2	-0.0001	-0.0005	-0.0005	-0.0007
RER	2.8169	4.1532	3.1143	2.9847
RMSE	1.6101	0.0382	0.0260	6.6684
RPD	0.9999	0.9997	0.9997	0.9997
RPIQ	2.0066	1.1488	1.8946	1.3433
SEP	1.6234	0.0385	0.0262	6.7224

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0348	0.0010	0.0008	0.1926
MSE	2.6465	0.0015	0.0007	45.8921
R2	-0.0210	-0.0367	-0.0236	-0.0327
RER	2.7881	4.0803	3.0792	2.9382
RMSE	1.6268	0.0389	0.0263	6.7744
RPD	0.9897	0.9822	0.9884	0.9840
RPIQ	1.9860	1.1286	1.8731	1.3223
SEP	1.6402	0.0392	0.0265	6.8288

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.3031	0.0029	0.0040	1.4212
MSE	2.3787	0.0007	0.0005	35.3841
R2	-0.0398	-0.0116	-0.0292	-0.0605
RER	2.4965	3.6513	3.1531	3.3853
RMSE	1.5423	0.0269	0.0234	5.9485
RPD	0.9807	0.9943	0.9857	0.9710
RPIQ	2.0319	1.0624	1.7684	0.6525
SEP	1.5496	0.0274	0.0237	5.9188

Pré-proc: 5--> Suavização(SavGol) - Par:5,2,1

Parâmetros do modelo: Kernel Ridge

KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='poly',
kernel_params=None)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0314	0.0009	0.0007	0.1737
MSE	2.5924	0.0015	0.0007	44.4678
R2	-0.0001	-0.0005	-0.0005	-0.0007
RER	2.8169	4.1532	3.1143	2.9847

RMSE	1.6101	0.0382	0.0260	6.6684
RPD	0.9999	0.9998	0.9997	0.9997
RPIQ	2.0066	1.1488	1.8946	1.3433
SEP	1.6234	0.0385	0.0262	6.7224

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0348	0.0010	0.0008	0.1926
MSE	2.6465	0.0015	0.0007	45.8920
R2	-0.0210	-0.0367	-0.0236	-0.0327
RER	2.7881	4.0803	3.0792	2.9382
RMSE	1.6268	0.0389	0.0262	6.7744
RPD	0.9897	0.9822	0.9884	0.9840
RPIQ	1.9860	1.1286	1.8731	1.3223
SEP	1.6402	0.0392	0.0265	6.8288

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.3031	0.0029	0.0040	1.4212
MSE	2.3787	0.0007	0.0005	35.3840
R2	-0.0398	-0.0116	-0.0292	-0.0605
RER	2.4966	3.6513	3.1531	3.3853
RMSE	1.5423	0.0269	0.0234	5.9484
RPD	0.9807	0.9943	0.9857	0.9710
RPIQ	2.0319	1.0624	1.7684	0.6525
SEP	1.5496	0.0274	0.0237	5.9188

Pré-proc: 6--> Suavização(SavGol) - Par:3,2,2

Parâmetros do modelo: Kernel Ridge

KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='poly',
kernel_params=None)

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0315	0.0009	0.0007	0.1738
MSE	2.5881	0.0015	0.0007	44.4653
R2	0.0016	0.0001	0.0009	-0.0006
RER	2.8192	4.1544	3.1165	2.9848
RMSE	1.6088	0.0382	0.0259	6.6682
RPD	1.0008	1.0000	1.0004	0.9997
RPIQ	2.0082	1.1491	1.8959	1.3433
SEP	1.6220	0.0385	0.0261	6.7222

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0349	0.0010	0.0008	0.1927
MSE	2.6426	0.0015	0.0007	45.8995
R2	-0.0195	-0.0362	-0.0224	-0.0329
RER	2.7901	4.0813	3.0811	2.9379

RMSE	1.6256	0.0389	0.0262	6.7749
RPD	0.9904	0.9824	0.9890	0.9840
RPIQ	1.9874	1.1289	1.8742	1.3222
SEP	1.6390	0.0392	0.0264	6.8293

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.3033	0.0029	0.0040	1.4213
MSE	2.3735	0.0007	0.0005	35.3834
R2	-0.0375	-0.0107	-0.0270	-0.0605
RER	2.4994	3.6530	3.1565	3.3854
RMSE	1.5406	0.0269	0.0234	5.9484
RPD	0.9818	0.9947	0.9867	0.9711
RPIQ	2.0341	1.0628	1.7703	0.6525
SEP	1.5478	0.0274	0.0236	5.9187

Pré-proc: 7--> Suavização(SavGol) - Par:5,2,2

Parâmetros do modelo: Kernel Ridge

KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='poly',
kernel_params=None)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0314	0.0009	0.0007	0.1739
MSE	2.5926	0.0015	0.0007	44.4683
R2	-0.0002	-0.0005	-0.0006	-0.0007
RER	2.8168	4.1531	3.1142	2.9847
RMSE	1.6102	0.0382	0.0260	6.6685
RPD	0.9999	0.9997	0.9997	0.9997
RPIQ	2.0065	1.1488	1.8945	1.3433
SEP	1.6234	0.0385	0.0262	6.7224

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0348	0.0010	0.0008	0.1928
MSE	2.6467	0.0015	0.0007	45.8920
R2	-0.0210	-0.0367	-0.0237	-0.0327
RER	2.7880	4.0803	3.0791	2.9382
RMSE	1.6269	0.0389	0.0263	6.7744
RPD	0.9896	0.9821	0.9884	0.9840
RPIQ	1.9859	1.1286	1.8730	1.3223
SEP	1.6402	0.0392	0.0265	6.8288

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.3031	0.0029	0.0040	1.4214
MSE	2.3790	0.0007	0.0005	35.3848
R2	-0.0399	-0.0116	-0.0293	-0.0606
RER	2.4964	3.6512	3.1529	3.3853

RMSE	1.5424	0.0269	0.0234	5.9485
RPD	0.9806	0.9942	0.9857	0.9710
RPIQ	2.0318	1.0623	1.7683	0.6525
SEP	1.5497	0.0274	0.0237	5.9188

Pré-proc: 8--> Suavização(SavGol) - Par:3,1,1 --> Padronização

Parâmetros do modelo: Kernel Ridge

KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='poly',
kernel_params=None)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0240	0.0007	0.0006	0.1338
MSE	0.0791	0.0001	0.0000	1.3324
R2	0.9695	0.9032	0.9604	0.9700
RER	16.1833	13.3664	15.7532	17.3539
RMSE	0.2812	0.0119	0.0052	1.1543
RPD	5.7249	3.2135	5.0235	5.7752
RPIQ	11.4882	3.6926	9.5199	7.7602
SEP	0.2826	0.0120	0.0052	1.1562

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0288	0.0010	0.0010	0.2443
MSE	0.2690	0.0005	0.0001	4.5476
R2	0.8962	0.6527	0.8628	0.8977
RER	8.7568	7.0537	8.4547	9.3918
RMSE	0.5186	0.0225	0.0096	2.1325
RPD	3.1043	1.6968	2.6997	3.1260
RPIQ	6.2294	1.9497	5.1161	4.2005
SEP	0.5222	0.0227	0.0096	2.1364

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2332	0.0008	0.0035	1.2750
MSE	0.2565	0.0003	0.0001	6.8844
R2	0.8879	0.6147	0.8794	0.7937
RER	8.3977	5.8889	10.1183	8.5271
RMSE	0.5065	0.0166	0.0080	2.6238
RPD	2.9864	1.6110	2.8800	2.2015
RPIQ	6.1877	1.7213	5.1668	1.4792
SEP	0.4607	0.0170	0.0074	2.3498

Pré-proc: 9--> Padronização --> Suavização(SavGol) - Par:3,1,1

Parâmetros do modelo: Kernel Ridge

KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='poly',
kernel_params=None)

cal

	betaglicosidase	cmcase	fpase	xilanase
--	-----------------	--------	-------	----------

BIAS	0.0312	0.0009	0.0007	0.1735
MSE	1.0702	0.0010	0.0003	27.9892
R2	0.5871	0.3192	0.5598	0.3702
RER	4.3853	5.0355	4.6973	3.7628
RMSE	1.0345	0.0315	0.0172	5.2905
RPD	1.5563	1.2120	1.5072	1.2600
RPIQ	3.1230	1.3927	2.8562	1.6931
SEP	1.0428	0.0318	0.0173	5.3323

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0373	0.0011	0.0008	0.2083
MSE	1.1445	0.0011	0.0003	32.5103
R2	0.5585	0.2580	0.5264	0.2684
RER	4.2413	4.8239	4.5294	3.4918
RMSE	1.0698	0.0329	0.0179	5.7018
RPD	1.5050	1.1609	1.4531	1.1691
RPIQ	3.0200	1.3340	2.7537	1.5710
SEP	1.0782	0.0332	0.0180	5.7461

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.3043	0.0029	0.0040	1.3915
MSE	0.8689	0.0004	0.0002	22.0750
R2	0.6202	0.3850	0.6663	0.3384
RER	4.2850	4.6997	5.7173	4.3574
RMSE	0.9322	0.0210	0.0133	4.6984
RPD	1.6226	1.2752	1.7312	1.2294
RPIQ	3.3619	1.3625	3.1058	0.8261
SEP	0.9028	0.0213	0.0130	4.5984

Pré-proc: 10--> MSC

Parâmetros do modelo: Kernel Ridge

KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='poly',
kernel_params=None)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0217	0.0006	0.0005	0.1201
MSE	2.5574	0.0015	0.0007	44.4069
R2	0.0134	0.0052	0.0118	0.0007
RER	2.8359	4.1644	3.1330	2.9862
RMSE	1.5992	0.0381	0.0258	6.6639
RPD	1.0068	1.0026	1.0060	1.0004
RPIQ	2.0203	1.1521	1.9064	1.3442
SEP	1.6125	0.0384	0.0260	6.7190

val

	betaglicosidase	cmcase	fpase	xilanase
--	-----------------	--------	-------	----------

BIAS	0.0239	0.0007	0.0005	0.1329
MSE	2.6145	0.0015	0.0007	45.9006
R2	-0.0086	-0.0318	-0.0123	-0.0329
RER	2.8048	4.0892	3.0956	2.9373
RMSE	1.6169	0.0388	0.0261	6.7750
RPD	0.9957	0.9845	0.9939	0.9839
RPIQ	1.9981	1.1313	1.8835	1.3221
SEP	1.6304	0.0391	0.0263	6.8309

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.2934	0.0026	0.0037	1.3686
MSE	2.3302	0.0007	0.0005	35.2267
R2	-0.0186	-0.0013	-0.0074	-0.0558
RER	2.5202	3.6661	3.1829	3.3859
RMSE	1.5265	0.0268	0.0232	5.9352
RPD	0.9908	0.9993	0.9963	0.9732
RPIQ	2.0529	1.0678	1.7875	0.6539
SEP	1.5350	0.0273	0.0234	5.9179

Pré-proc: 11--> SNV

Parâmetros do modelo: Kernel Ridge

KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='poly',
kernel_params=None)

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0038	0.0001	0.0001	0.0217
MSE	2.1077	0.0013	0.0006	43.7359
R2	0.1869	0.0760	0.1677	0.0158
RER	3.1235	4.3204	3.4134	3.0085
RMSE	1.4518	0.0367	0.0237	6.6133
RPD	1.1090	1.0403	1.0962	1.0080
RPIQ	2.2254	1.1954	2.0773	1.3545
SEP	1.4640	0.0370	0.0239	6.6691

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.0034	0.0001	0.0001	0.0192
MSE	2.1805	0.0014	0.0006	46.2875
R2	0.1588	0.0320	0.1386	-0.0416
RER	3.0709	4.2210	3.3550	2.9244
RMSE	1.4767	0.0376	0.0241	6.8035
RPD	1.0903	1.0164	1.0774	0.9798
RPIQ	2.1879	1.1679	2.0418	1.3166
SEP	1.4891	0.0379	0.0243	6.8609

pred

	betaglicosidase	cmcase	fpase	xylanase
--	-----------------	--------	-------	----------

BIAS	0.2712	0.0020	0.0033	1.2609
MSE	1.7547	0.0006	0.0004	34.8529
R2	0.2330	0.0967	0.2453	-0.0446
RER	2.9117	3.8535	3.6782	3.3905
RMSE	1.3247	0.0254	0.0201	5.9036
RPD	1.1418	1.0522	1.1511	0.9784
RPIQ	2.3658	1.1242	2.0652	0.6574
SEP	1.3286	0.0260	0.0203	5.9098

```
In [446]: '''#kernel ridge teste otimização automática
          modelo = 'Kernel Ridge:'
          result = result = executaKernelRidge(preproc=8, teste=1)
          print('Parâmetros do modelo:',modelo,'\n',result[0])'''
```

```
Out[446]: "#kernel ridge teste otimização automática\nmodelo = 'Kernel Ridge:'\nresult = result[0]"
```

```
In [ ]:
```

```
In [442]: #Kernel ridge otimizando
          maior=[-1,-1,-1,-1]
          maiorGerado=[0,0,0,0]
          for i in range(100):
              result = executaKernelRidge(preproc=8,k='poly',teste=0,IC=i)
              resultados=exibeResultados(result)
              r2 = resultados['val'].loc[resultados['val'].index=='R2']
              r = []
              for j in range(4):
                  r.append(r2.iloc[:,j][0])
                  if r[j]>maior[j]:
                      maior[j] = r[j]
                      maiorGerado[j]=i
              print('\r%d%% completos'%(i+1), end='')
          print('\n','r2:',maior,'\nsemente: b c f x',maiorGerado)
```

```
100% completos
```

```
r2: [0.9437, 0.8271, 0.9216, 0.8986]
```

```
semente: b c f x [24, 84, 24, 76]
```

```
In [447]: #kernel ridge teste otimizado
          modelo = 'Kernel Ridge:'
          result = result = executaKernelRidge(preproc=8,k='poly', teste=0, IC=56)
          print('Parâmetros do modelo:',modelo,'\n',result[0])

          resultados=exibeResultados(result)
```

```
Parâmetros do modelo: Kernel Ridge:
```

```
KernelRidge(alpha=1.0, coef0=1, degree=3, gamma=None, kernel='poly',
```



```
kernel_params=None)
```

```
In [448]: resultados['cal']
```

```
Out[448]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0245	0.0007	0.0006	0.1413
MSE	0.0825	0.0001	0.0000	1.4646
R2	0.9690	0.9000	0.9597	0.9667
RER	15.8429	13.1642	15.3841	16.5537
RMSE	0.2873	0.0121	0.0053	1.2102
RPD	5.6778	3.1623	4.9823	5.4793
RPIQ	11.1878	3.4326	9.5206	5.7181
SEP	0.2886	0.0122	0.0053	1.2121

```
In [449]: resultados['val']
```

```
Out[449]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0310	0.0006	0.0010	0.2688
MSE	0.2967	0.0005	0.0001	5.4717
R2	0.8885	0.6565	0.8451	0.8756
RER	8.3391	7.0926	7.8231	8.5625
RMSE	0.5447	0.0224	0.0104	2.3392
RPD	2.9946	1.7061	2.5405	2.8348
RPIQ	5.9008	1.8520	4.8545	2.9584
SEP	0.5484	0.0226	0.0104	2.3433

```
In [450]: resultados['pred']
```

```
Out[450]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2648	-0.0009	0.0047	0.1868
MSE	0.2019	0.0001	0.0000	2.6085
R2	0.9035	0.8348	0.9225	0.9272
RER	10.3998	8.7855	16.6667	11.4120
RMSE	0.4493	0.0109	0.0060	1.6151
RPD	3.2192	2.4601	3.5921	3.7072
RPIQ	5.8841	2.6145	6.8680	2.0912
SEP	0.3720	0.0112	0.0038	1.6439

```
In [451]: reg, treino_teste,y_c,y_cv,y_p = result
```

7.7.2 Kernel Ridge Reais x preditos

```
In [ ]:
```

```
In [452]: #kernelridge reaisxpreditos  
#calibração  
pred=pd.DataFrame(y_c, columns=var_ae)  
reais = treino_teste[2]
```

```

reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('CALIBRAÇÃO:\n')
round(reais_pred,4)

```

CALIBRAÇÃO:

```

Out[452]:

```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	0.3900	0.0315	0.0283	14.1777	0.5021
1	3.2342	0.0672	0.0543	8.4772	2.7688
2	0.4280	0.0390	0.0334	13.7624	0.6112
3	0.0874	0.0217	0.0127	0.1071	0.0625
4	3.8803	0.0557	0.0691	11.3256	3.7916
5	0.0308	0.0213	0.0113	0.0996	0.0209
6	2.9123	0.1058	0.0747	14.6813	3.0441
7	3.8803	0.0557	0.0691	11.3256	3.4825
8	3.5967	0.1065	0.0850	13.6476	3.4087
9	3.5610	0.0586	0.0561	10.0978	3.6376
10	0.3828	0.0405	0.0301	12.4461	0.7303
11	3.8994	0.1118	0.0613	10.9512	3.7574
12	3.5974	0.0516	0.0731	15.3973	3.1709
13	3.5967	0.1065	0.0850	13.6476	3.3682
14	2.9774	0.0704	0.0567	10.8002	2.7724
15	2.1150	0.0730	0.0505	18.4127	2.4117
16	3.1068	0.0781	0.0545	11.0526	3.0945
17	3.7243	0.0561	0.0681	11.5736	3.8878
18	0.1724	0.0112	0.0121	0.0924	0.1687
19	3.1068	0.0781	0.0545	11.0526	3.3321
20	2.9123	0.1058	0.0747	14.6813	2.7780
21	2.7110	0.0548	0.0688	13.5829	2.9889
22	4.6037	0.1713	0.0919	16.8115	3.6685
23	0.6010	0.0559	0.0116	20.1368	0.5797
24	0.6491	0.0605	0.0260	18.4274	0.7064
25	0.0759	0.0136	0.0139	0.0726	0.1178
26	0.6010	0.0559	0.0116	20.1368	0.5716
27	2.1150	0.0730	0.0505	18.4127	1.9887
28	4.6037	0.1713	0.0919	16.8115	3.5363
29	0.3828	0.0405	0.0301	12.4461	0.5992
30	0.1671	0.0117	0.0104	0.1117	0.0477
31	0.1724	0.0112	0.0121	0.0924	0.3475
32	0.0874	0.0217	0.0127	0.1071	0.0905
33	3.8876	0.0418	0.0605	11.0267	3.8359
34	0.0874	0.0217	0.0127	0.1071	0.0783
35	2.1643	0.0830	0.0529	18.8324	2.4876

36	0.0308	0.0213	0.0113	0.0996	0.0464
37	0.3828	0.0405	0.0301	12.4461	0.3004
38	0.4280	0.0390	0.0334	13.7624	0.6030
39	3.5610	0.0586	0.0561	10.0978	3.8253
40	3.5974	0.0516	0.0731	15.3973	3.2185
41	3.5974	0.0516	0.0731	15.3973	3.2735
42	3.2342	0.0672	0.0543	8.4772	3.0616
43	4.6037	0.1713	0.0919	16.8115	3.8892
44	0.6491	0.0605	0.0260	18.4274	0.6693
45	0.6010	0.0559	0.0116	20.1368	0.6538
46	0.0554	0.0181	0.0106	0.3275	0.1590
47	0.5905	0.0465	0.0267	18.7095	0.5460
48	0.0554	0.0181	0.0106	0.3275	0.2499
49	2.1150	0.0730	0.0505	18.4127	2.3113
50	3.8876	0.0418	0.0605	11.0267	4.2246
51	0.1671	0.0117	0.0104	0.1117	0.3934
52	0.4280	0.0390	0.0334	13.7624	0.4934
53	3.8994	0.1118	0.0613	10.9512	3.5127
54	3.5967	0.1065	0.0850	13.6476	3.7716
55	0.3900	0.0315	0.0283	14.1777	0.6305
56	0.1671	0.0117	0.0104	0.1117	0.2467
57	0.5905	0.0465	0.0267	18.7095	0.6035
58	3.5610	0.0586	0.0561	10.0978	3.8848
59	0.1724	0.0112	0.0121	0.0924	0.3792

	pred: cmcase	pred: fpase	pred: xylanase
0	0.0358	0.0295	13.1636
1	0.0601	0.0513	9.6166
2	0.0376	0.0333	13.7578
3	0.0210	0.0122	-0.1315
4	0.0545	0.0682	11.0808
5	0.0221	0.0114	0.2018
6	0.0970	0.0747	14.7453
7	0.0568	0.0653	11.8312
8	0.1020	0.0781	13.9566
9	0.0710	0.0609	11.0380
10	0.0488	0.0317	10.9457
11	0.0997	0.0643	11.9974
12	0.0524	0.0664	13.8288
13	0.0895	0.0742	12.7442
14	0.0654	0.0522	9.7030
15	0.0898	0.0562	15.5076
16	0.0774	0.0550	10.8939
17	0.0700	0.0686	12.1581
18	0.0112	0.0134	2.0498
19	0.0845	0.0584	10.2185
20	0.0946	0.0715	14.2981
21	0.0563	0.0680	13.4355

22	0.1254	0.0732	15.0536
23	0.0547	0.0127	19.7178
24	0.0619	0.0259	18.8120
25	0.0148	0.0144	0.3381
26	0.0557	0.0123	19.7357
27	0.0737	0.0504	16.0170
28	0.1245	0.0711	15.1773
29	0.0393	0.0302	12.1769
30	0.0110	0.0108	1.2493
31	0.0140	0.0153	1.9442
32	0.0212	0.0125	0.2159
33	0.0543	0.0621	10.7609
34	0.0210	0.0125	0.0713
35	0.0852	0.0552	15.1297
36	0.0209	0.0116	0.2169
37	0.0328	0.0258	10.6310
38	0.0407	0.0324	12.7099
39	0.0697	0.0617	10.9106
40	0.0586	0.0694	14.5313
41	0.0475	0.0670	13.7611
42	0.0629	0.0559	10.7091
43	0.1342	0.0771	16.1876
44	0.0606	0.0259	18.5388
45	0.0563	0.0142	20.3425
46	0.0209	0.0121	0.9181
47	0.0462	0.0243	18.5193
48	0.0216	0.0132	1.5375
49	0.0813	0.0549	16.4330
50	0.0627	0.0673	11.6176
51	0.0230	0.0153	1.7044
52	0.0396	0.0335	13.7315
53	0.1005	0.0638	12.4541
54	0.1047	0.0809	13.5939
55	0.0437	0.0325	13.1555
56	0.0210	0.0148	2.1064
57	0.0469	0.0259	18.7276
58	0.0656	0.0605	9.8822
59	0.0191	0.0155	1.6065

In [453]: *#validação*

```

pred=pd.DataFrame(y_cv, columns=var_ae)
reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('VALIDAÇÃO CRUZADA:\n')
round(reais_pred,4)

```

VALIDAÇÃO CRUZADA:

```
Out [453]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	0.3900	0.0315	0.0283	14.1777	0.5538
1	3.2342	0.0672	0.0543	8.4772	2.4443
2	0.4280	0.0390	0.0334	13.7624	0.7470
3	0.0874	0.0217	0.0127	0.1071	-0.0693
4	3.8803	0.0557	0.0691	11.3256	3.6697
5	0.0308	0.0213	0.0113	0.0996	-0.0692
6	2.9123	0.1058	0.0747	14.6813	3.2937
7	3.8803	0.0557	0.0691	11.3256	2.9865
8	3.5967	0.1065	0.0850	13.6476	3.2192
9	3.5610	0.0586	0.0561	10.0978	3.7176
10	0.3828	0.0405	0.0301	12.4461	1.0146
11	3.8994	0.1118	0.0613	10.9512	3.5715
12	3.5974	0.0516	0.0731	15.3973	2.8356
13	3.5967	0.1065	0.0850	13.6476	3.2139
14	2.9774	0.0704	0.0567	10.8002	2.6279
15	2.1150	0.0730	0.0505	18.4127	2.5276
16	3.1068	0.0781	0.0545	11.0526	3.0130
17	3.7243	0.0561	0.0681	11.5736	4.1159
18	0.1724	0.0112	0.0121	0.0924	0.1156
19	3.1068	0.0781	0.0545	11.0526	3.7718
20	2.9123	0.1058	0.0747	14.6813	2.5723
21	2.7110	0.0548	0.0688	13.5829	3.3072
22	4.6037	0.1713	0.0919	16.8115	3.0169
23	0.6010	0.0559	0.0116	20.1368	0.5093
24	0.6491	0.0605	0.0260	18.4274	0.9635
25	0.0759	0.0136	0.0139	0.0726	0.4261
26	0.6010	0.0559	0.0116	20.1368	0.3836
27	2.1150	0.0730	0.0505	18.4127	1.8283
28	4.6037	0.1713	0.0919	16.8115	2.7383
29	0.3828	0.0405	0.0301	12.4461	0.7808
30	0.1671	0.0117	0.0104	0.1117	0.0315
31	0.1724	0.0112	0.0121	0.0924	0.4980
32	0.0874	0.0217	0.0127	0.1071	0.1216
33	3.8876	0.0418	0.0605	11.0267	3.8165
34	0.0874	0.0217	0.0127	0.1071	0.0397
35	2.1643	0.0830	0.0529	18.8324	2.6498
36	0.0308	0.0213	0.0113	0.0996	0.1222
37	0.3828	0.0405	0.0301	12.4461	0.2583
38	0.4280	0.0390	0.0334	13.7624	0.7028
39	3.5610	0.0586	0.0561	10.0978	4.2666
40	3.5974	0.0516	0.0731	15.3973	2.7693
41	3.5974	0.0516	0.0731	15.3973	2.7100
42	3.2342	0.0672	0.0543	8.4772	2.9982

43	4.6037	0.1713	0.0919	16.8115	3.3017
44	0.6491	0.0605	0.0260	18.4274	0.7775
45	0.6010	0.0559	0.0116	20.1368	0.8896
46	0.0554	0.0181	0.0106	0.3275	0.1905
47	0.5905	0.0465	0.0267	18.7095	0.3623
48	0.0554	0.0181	0.0106	0.3275	0.4497
49	2.1150	0.0730	0.0505	18.4127	2.4416
50	3.8876	0.0418	0.0605	11.0267	4.6758
51	0.1671	0.0117	0.0104	0.1117	0.5762
52	0.4280	0.0390	0.0334	13.7624	0.5005
53	3.8994	0.1118	0.0613	10.9512	3.3615
54	3.5967	0.1065	0.0850	13.6476	3.9356
55	0.3900	0.0315	0.0283	14.1777	0.7772
56	0.1671	0.0117	0.0104	0.1117	0.3754
57	0.5905	0.0465	0.0267	18.7095	0.7083
58	3.5610	0.0586	0.0561	10.0978	4.3096
59	0.1724	0.0112	0.0121	0.0924	0.5584

	pred: cmcase	pred: fpase	pred: xylanase
0	0.0380	0.0300	12.5300
1	0.0554	0.0493	10.2977
2	0.0371	0.0333	13.6356
3	0.0185	0.0099	-1.2029
4	0.0526	0.0670	10.8676
5	0.0272	0.0115	0.7839
6	0.0848	0.0748	14.6521
7	0.0577	0.0610	12.4970
8	0.0971	0.0718	14.4716
9	0.0862	0.0664	12.2672
10	0.0548	0.0331	9.7544
11	0.0888	0.0660	13.0206
12	0.0533	0.0610	12.2795
13	0.0782	0.0665	11.4841
14	0.0626	0.0491	8.8968
15	0.0977	0.0576	13.4284
16	0.0751	0.0528	9.7981
17	0.0890	0.0697	12.9094
18	0.0095	0.0136	3.5437
19	0.0973	0.0658	8.4274
20	0.0763	0.0656	13.8361
21	0.0601	0.0685	13.2940
22	0.0943	0.0606	13.9293
23	0.0501	0.0232	16.3710
24	0.0688	0.0265	20.3161
25	0.0239	0.0181	2.1763
26	0.0551	0.0175	16.8263
27	0.0704	0.0486	14.3366
28	0.0900	0.0558	13.7746

29	0.0382	0.0303	11.8880
30	0.0117	0.0120	2.3647
31	0.0168	0.0184	3.4541
32	0.0177	0.0112	1.1698
33	0.0662	0.0639	10.3049
34	0.0173	0.0114	-0.1552
35	0.0875	0.0568	13.6121
36	0.0183	0.0128	0.7728
37	0.0257	0.0221	8.9164
38	0.0417	0.0314	11.9548
39	0.0854	0.0705	12.2131
40	0.0618	0.0635	13.1318
41	0.0451	0.0579	11.4224
42	0.0630	0.0582	12.3399
43	0.1031	0.0645	15.5147
44	0.0600	0.0236	19.2084
45	0.0582	0.0240	21.1449
46	0.0204	0.0122	1.3585
47	0.0456	0.0116	17.6606
48	0.0274	0.0174	2.8679
49	0.0863	0.0577	15.4788
50	0.0926	0.0778	12.7775
51	0.0314	0.0197	3.1935
52	0.0376	0.0324	13.2533
53	0.0977	0.0667	13.6277
54	0.1031	0.0774	13.4304
55	0.0518	0.0351	12.4869
56	0.0309	0.0197	3.8605
57	0.0500	0.0191	18.8331
58	0.0751	0.0663	9.9688
59	0.0265	0.0188	3.0580

```
In [454]: #predição
pred=pd.DataFrame(y_p, columns=var_ae)
reais = treino_teste[3]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('Predição (validação externa):\n')
round(reais_pred,4)
```

Predição (validação externa):

```
Out[454]:      betaglicosidase  cmcase  fpase  xilanase  pred: betaglicosidase \
0           0.0308  0.0213  0.0113   0.0996          -0.1972
```

1	3.7243	0.0561	0.0681	11.5736	2.8025
2	3.8803	0.0557	0.0691	11.3256	3.6194
3	2.1643	0.0830	0.0529	18.8324	2.4051
4	2.7110	0.0548	0.0688	13.5829	2.9089
5	3.8876	0.0418	0.0605	11.0267	3.0409
6	0.5905	0.0465	0.0267	18.7095	0.4276
7	0.0759	0.0136	0.0139	0.0726	-0.0297
8	0.3900	0.0315	0.0283	14.1777	0.2595
9	2.9123	0.1058	0.0747	14.6813	2.8832
10	3.8994	0.1118	0.0613	10.9512	2.9944
11	0.6491	0.0605	0.0260	18.4274	0.7428
12	0.0759	0.0136	0.0139	0.0726	-0.0023
13	3.2342	0.0672	0.0543	8.4772	2.6033
14	3.7243	0.0561	0.0681	11.5736	3.1701
15	2.1643	0.0830	0.0529	18.8324	2.0472
16	2.9774	0.0704	0.0567	10.8002	2.5775
17	0.0554	0.0181	0.0106	0.3275	0.0659
18	2.9774	0.0704	0.0567	10.8002	2.5788
19	3.1068	0.0781	0.0545	11.0526	2.4539
20	2.7110	0.0548	0.0688	13.5829	3.0309

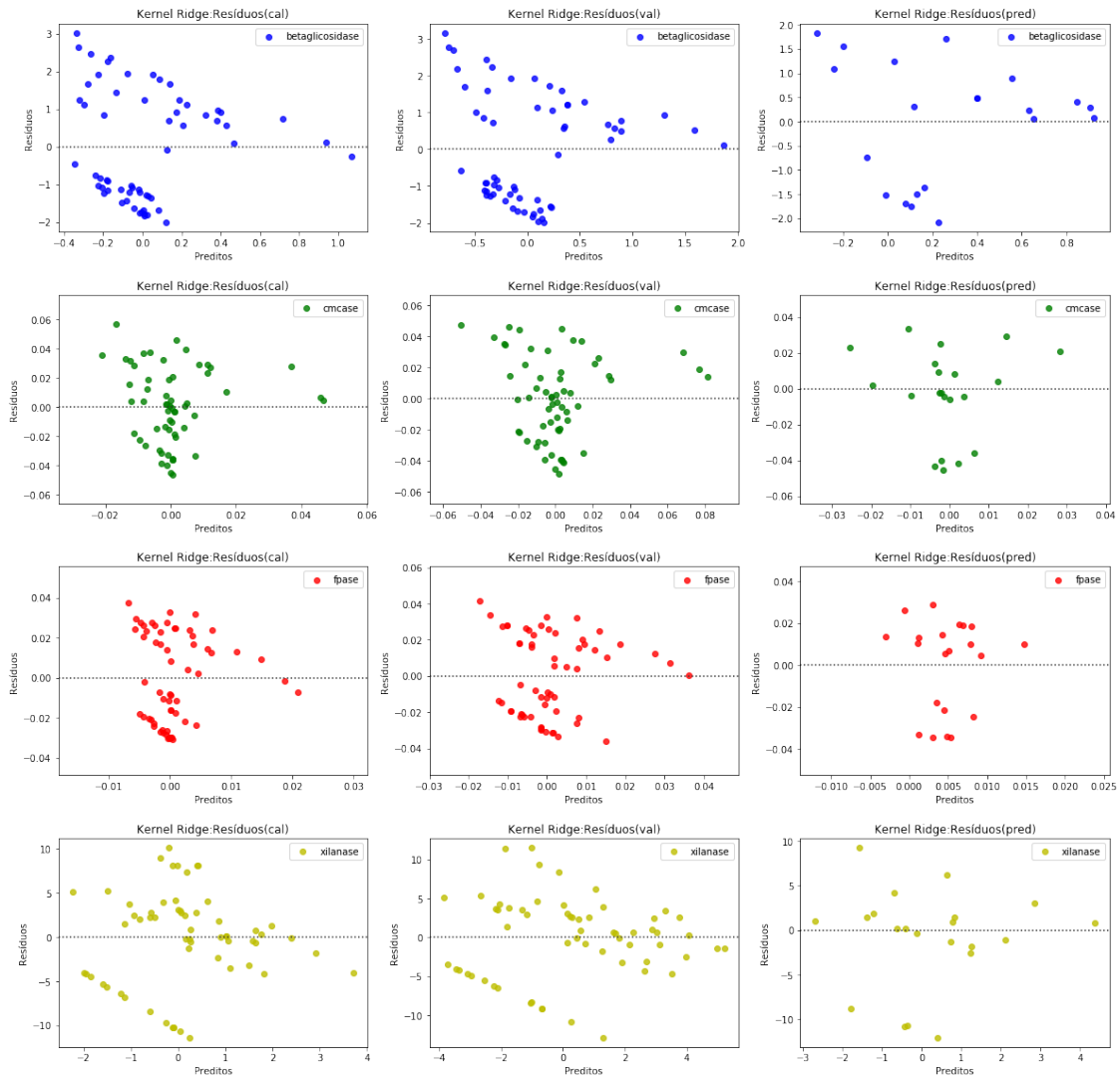
	pred: cmcase	pred: fpase	pred: xilanase
0	0.0192	0.0083	-0.3109
1	0.0581	0.0533	10.3151
2	0.0582	0.0612	10.6024
3	0.0934	0.0559	15.9930
4	0.0562	0.0619	11.4738
5	0.0614	0.0527	11.1532
6	0.0562	0.0185	18.0793
7	0.0152	0.0091	0.4958
8	0.0251	0.0248	13.3550
9	0.0913	0.0716	15.3628
10	0.0835	0.0571	12.3306
11	0.0567	0.0215	19.9909
12	0.0173	0.0085	1.8523
13	0.0699	0.0532	11.1732
14	0.0815	0.0687	12.7851
15	0.0854	0.0483	14.4511
16	0.0690	0.0475	9.5789
17	0.0202	0.0094	0.6866
18	0.0742	0.0556	11.4286
19	0.0658	0.0495	11.4676
20	0.0548	0.0625	12.7919

In []:

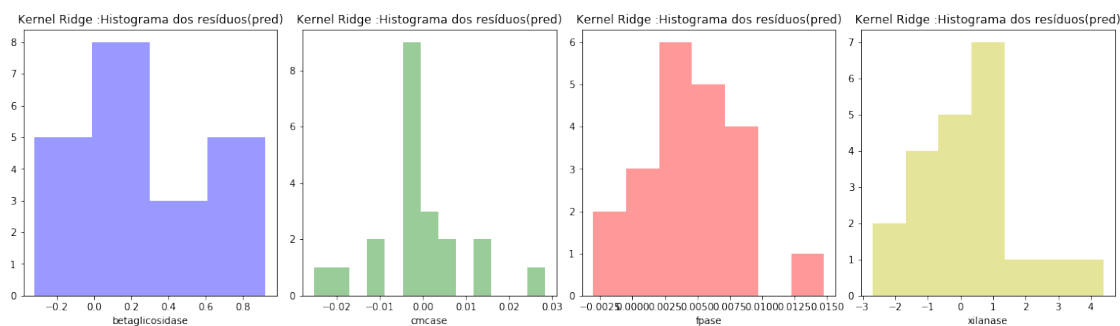
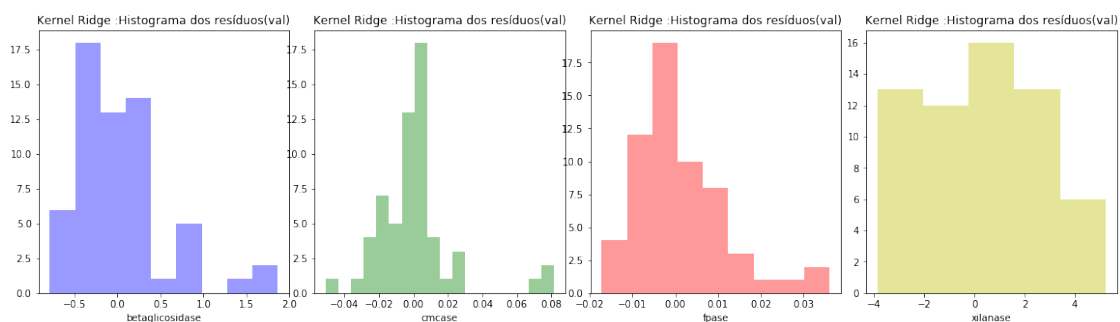
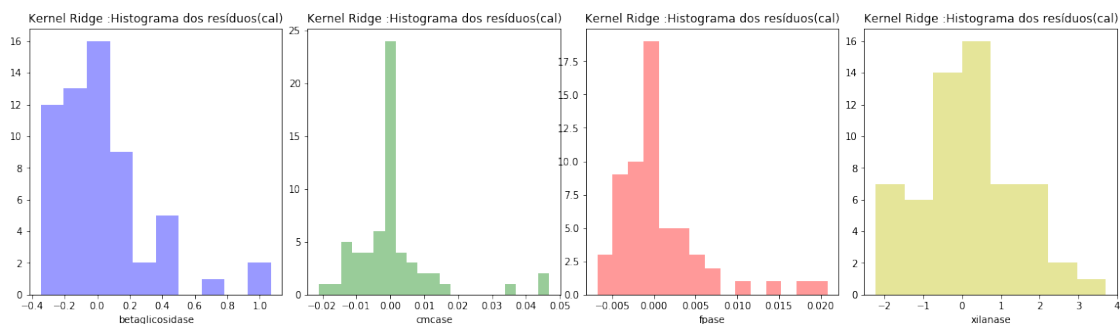
7.8 Kernel Ridge: Gráficos de resíduos - histograma - reais x preditos

```
In [455]: #título para os gráficos  
modelo = 'Kernel Ridge'
```

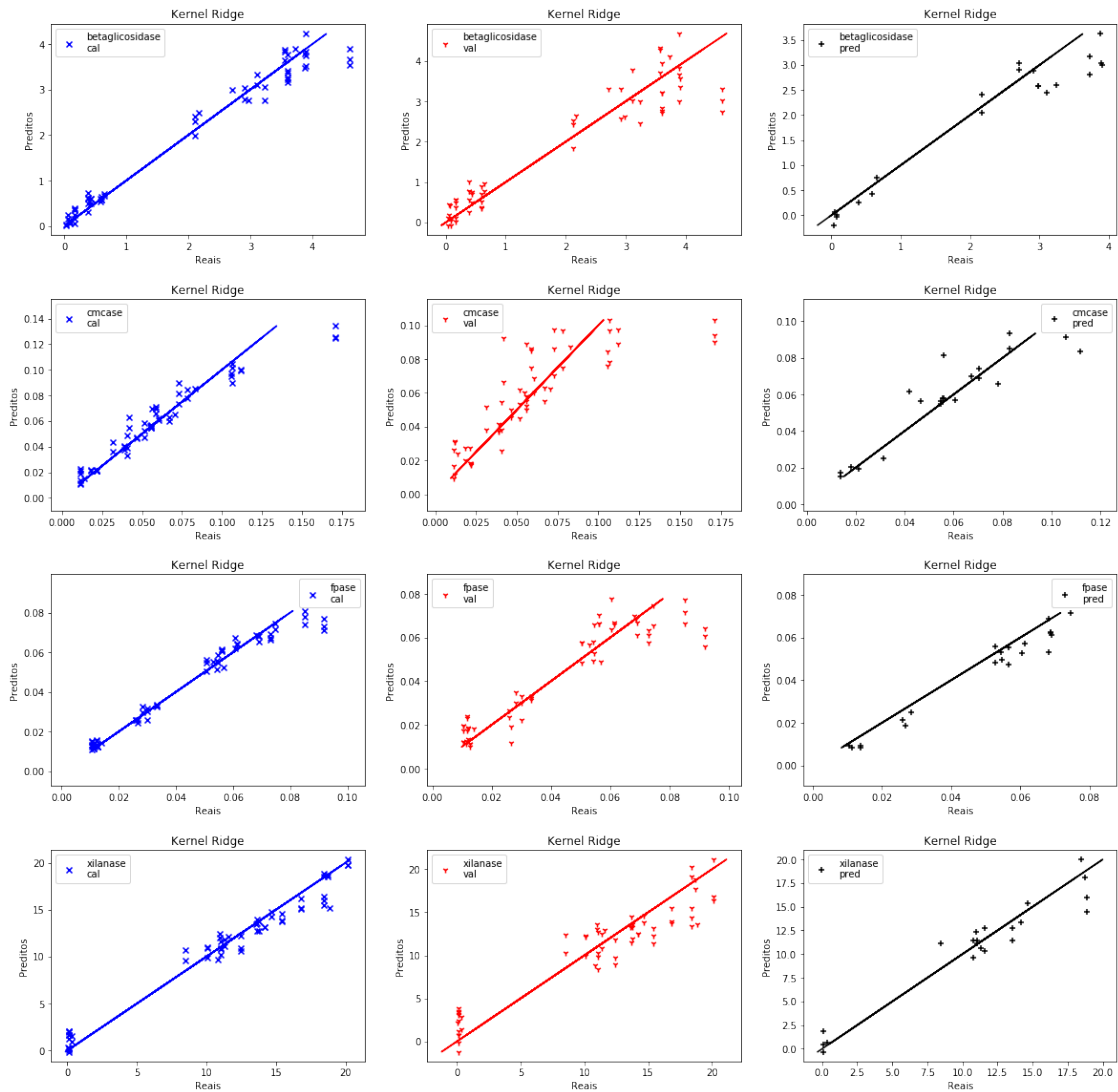
```
In [456]: #gráfico dos resíduos  
graficoResiduos(modelo, treino_teste, y_c,y_cv,y_p)
```



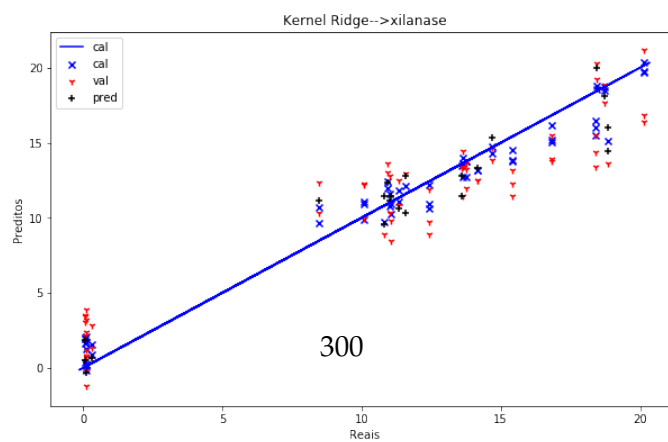
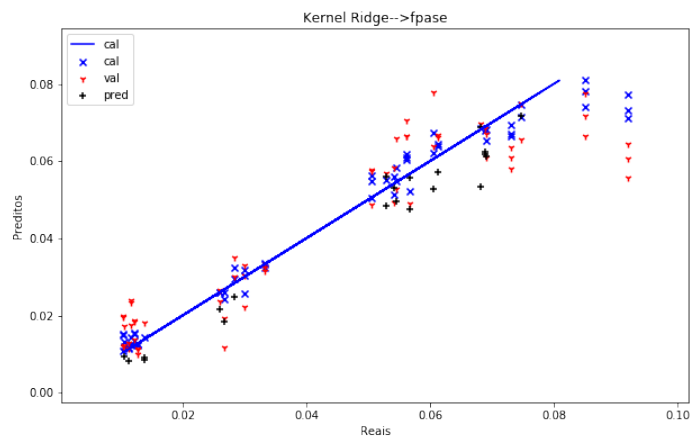
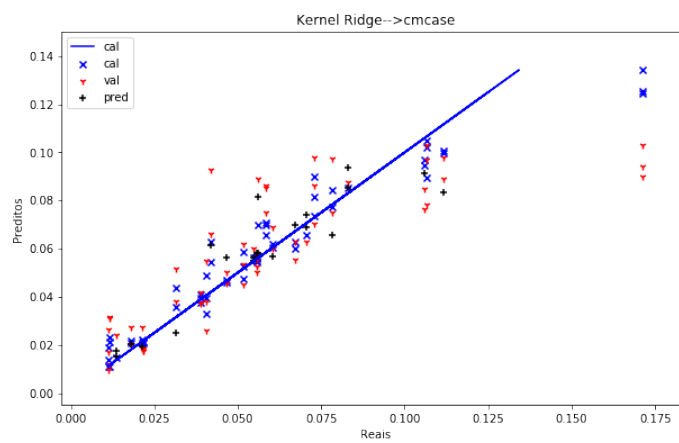
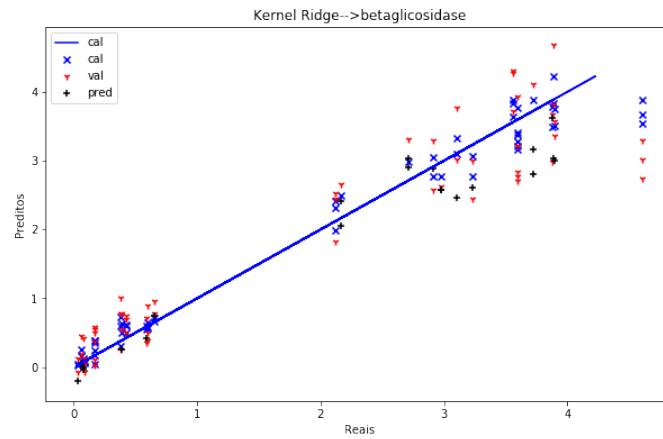
```
In [457]: #histograma dos resíduos  
graficoHist(modelo, treino_teste, y_c,y_cv,y_p)
```



In [458]: *#graico de reais x preditos*
 graficoReaisPreditosSep(modelo, treino_teste, y_c,y_cv,y_p)

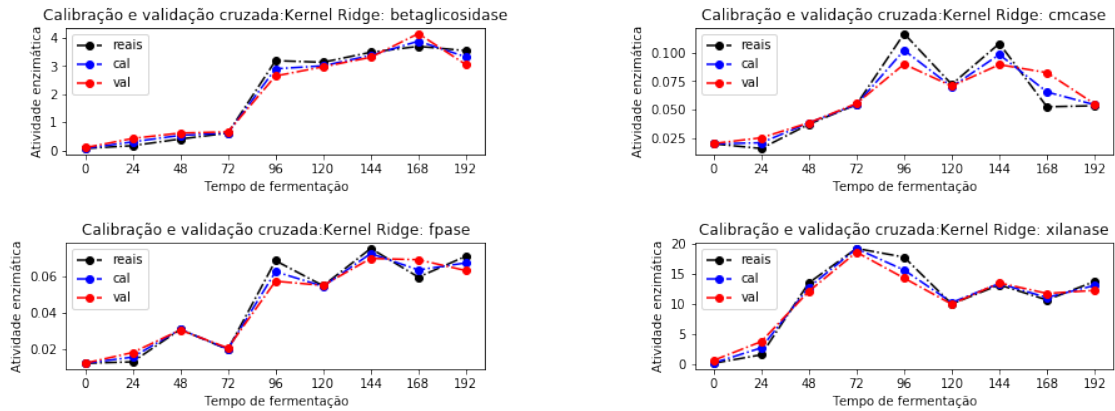


In [459]: *#gráfico de reais x preditos*
`graficoReaisPreditos(modelo, treino_teste, y_c,y_cv,y_p)`



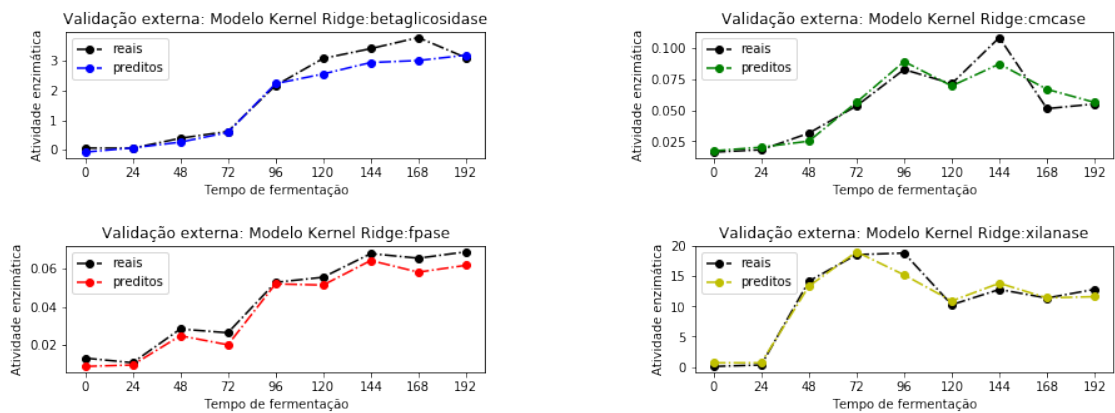
7.8.1 Kernel Ridge: Gráficos: dados de treino

```
In [460]: y_treino = treino_teste[2]  
          graficoTreinamento(modelo, y_treino, y_c,y_cv)
```



7.8.2 Kernel Ridge: Gráficos de teste

```
In [461]: y_teste = treino_teste[3]  
          graficoTeste(modelo, y_teste, y_p)
```



```
In [ ]:
```

7.9 PCR:

7.9.1 PCR: função completa

```
In [350]: #pcr função completa para execução do PCR:
          #A variável preproc determinará o tipo de processamento que será executado (0,1,2,3,4)
          def executaPCR(preproc=0, nPC=3, padroniza=False,IC=0):
              #separando o conjunto de dados em treino e teste

              #separando o conjunto de dados em treino e teste
              #x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc,True)
              x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc,padroniza, IC)

              # Roda o PCA e produz uma variável reduzida e seleciona as primeiras componentes
              pca = PCA(n_components=nPC)
              x_treino = pca.fit_transform(x_treino)[:,:nPC]
              x_teste = pca.fit_transform(x_teste)[:,:nPC]

              #Passo 2: Aplicar a regressão sobre as componentes selecionadas
              reg = MultiOutputRegressor(LinearRegression())
              result = executaCVP([x_treino, x_teste, y_treino, y_teste], reg)

              return result
```

7.9.2 PCR: testes

```
In [374]: #pcr teste diversificado
          for npc in range(2,5):
              for k in [1,10,11]:
                  print('\nNº Componentes principais:',npc,'\n',preProc[k])
                  result = executaPCR(k,npc)
                  print('Parâmetros do modelo:',modelo,'\n',result[0])
                  resultados=exibeResultados(result)

                  for k,v in zip(resultados.keys(),resultados.values()):
                      print(k)
                      print(v,'\n-----')
```

Nº Componentes principais: 2

Pré-proc: 1--> Padronização

Parâmetros do modelo: PCR

MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	0.0000
MSE	1.4714	0.0012	0.0004	27.1550
R2	0.4323	0.1969	0.3770	0.3889
RER	3.7383	4.6342	3.9452	3.8181
RMSE	1.2130	0.0342	0.0205	5.2110
RPD	1.3273	1.1159	1.2670	1.2792
RPIQ	2.6634	1.2823	2.4010	1.7190
SEP	1.2233	0.0345	0.0207	5.2550

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0159	0.0003	0.0001	0.0216
MSE	1.5158	0.0012	0.0004	29.0220
R2	0.4152	0.1492	0.3615	0.3469
RER	3.6835	4.5026	3.8970	3.6933
RMSE	1.2312	0.0353	0.0207	5.3872
RPD	1.3077	1.0842	1.2515	1.2374
RPIQ	2.6242	1.2458	2.3716	1.6627
SEP	1.2415	0.0355	0.0209	5.4326

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.9857	0.0006	0.0002	18.6716
R2	0.5691	0.1840	0.5657	0.4404
RER	3.9536	4.0551	4.8970	4.7266
RMSE	0.9928	0.0242	0.0152	4.3211
RPD	1.5234	1.1070	1.5175	1.3368
RPIQ	3.1564	1.1828	2.7224	0.8982
SEP	0.9785	0.0247	0.0152	4.2392

Nº Componentes principais: 2

Pré-proc: 10--> MSC

Parâmetros do modelo: PCR

MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	0.0000
MSE	0.6192	0.0009	0.0002	27.4644
R2	0.7611	0.3641	0.7569	0.3820
RER	5.7626	5.2081	6.3157	3.7965
RMSE	0.7869	0.0305	0.0128	5.2407
RPD	2.0460	1.2541	2.0282	1.2720
RPIQ	4.1057	1.4410	3.8436	1.7092

SEP	0.7935	0.0307	0.0129	5.2849
-----	--------	--------	--------	--------

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0056	0.0001	0.0000	-0.0091
MSE	0.6628	0.0010	0.0002	31.7760
R2	0.7443	0.3046	0.7365	0.2849
RER	5.5699	4.9802	6.0661	3.5296
RMSE	0.8142	0.0319	0.0133	5.6370
RPD	1.9775	1.1992	1.9480	1.1826
RPIQ	3.9683	1.3780	3.6917	1.5891
SEP	0.8210	0.0321	0.0134	5.6846

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.4112	0.0004	0.0001	27.6224
R2	0.8203	0.4604	0.8689	0.1721
RER	6.4999	4.9951	9.4510	3.8300
RMSE	0.6413	0.0197	0.0084	5.2557
RPD	2.3587	1.3613	2.7618	1.0990
RPIQ	4.8870	1.4545	4.9549	0.7385
SEP	0.5952	0.0200	0.0079	5.2316

Nº Componentes principais: 2

Pré-proc: 11--> SNV

Parâmetros do modelo: PCR

MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None, normalize=False),
n_jobs=None)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	-0.0000
MSE	0.6185	0.0009	0.0002	27.4867
R2	0.7614	0.3642	0.7572	0.3815
RER	5.7661	5.2082	6.3193	3.7950
RMSE	0.7864	0.0305	0.0128	5.2428
RPD	2.0473	1.2541	2.0293	1.2715
RPIQ	4.1082	1.4411	3.8458	1.7085
SEP	0.7931	0.0307	0.0129	5.2870

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0055	0.0001	0.0000	-0.0092
MSE	0.6620	0.0010	0.0002	31.8042
R2	0.7446	0.3046	0.7368	0.2843
RER	5.5735	4.9802	6.0697	3.5280

RMSE	0.8136	0.0319	0.0133	5.6395
RPD	1.9788	1.1992	1.9492	1.1821
RPIQ	3.9709	1.3780	3.6939	1.5884
SEP	0.8205	0.0321	0.0134	5.6871

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.4085	0.0004	0.0001	27.7094
R2	0.8214	0.4601	0.8700	0.1695
RER	6.5262	4.9937	9.4968	3.8237
RMSE	0.6391	0.0197	0.0083	5.2640
RPD	2.3665	1.3609	2.7732	1.0973
RPIQ	4.9032	1.4541	4.9752	0.7373
SEP	0.5928	0.0201	0.0079	5.2403

Nº Componentes principais: 3

Pré-proc: 1--> Padronização

Parâmetros do modelo: PCR

MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None, normalize=False),
n_jobs=None)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	0.0000
MSE	0.4190	0.0009	0.0001	23.4084
R2	0.8383	0.3707	0.7914	0.4732
RER	7.0052	5.2353	6.8177	4.1123
RMSE	0.6473	0.0303	0.0119	4.8382
RPD	2.4872	1.2606	2.1894	1.3778
RPIQ	4.9910	1.4486	4.1491	1.8514
SEP	0.6528	0.0306	0.0120	4.8791

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0012	-0.0000	-0.0001	-0.0041
MSE	0.4434	0.0010	0.0002	26.5326
R2	0.8289	0.3002	0.7732	0.4029
RER	6.8100	4.9646	6.5383	3.8626
RMSE	0.6659	0.0320	0.0124	5.1510
RPD	2.4179	1.1954	2.0996	1.2942
RPIQ	4.8519	1.3737	3.9789	1.7390
SEP	0.6715	0.0322	0.0125	5.1945

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475

MSE	0.2394	0.0004	0.0001	21.6585
R2	0.8954	0.3786	0.8699	0.3509
RER	9.2796	4.6517	9.4950	4.3613
RMSE	0.4892	0.0211	0.0083	4.6539
RPD	3.0915	1.2686	2.7727	1.2412
RPIQ	6.4054	1.3554	4.9744	0.8340
SEP	0.4169	0.0215	0.0079	4.5943

Nº Componentes principais: 3

Pré-proc: 10--> MSC

Parâmetros do modelo: PCR

```
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	0.0000
MSE	0.5031	0.0009	0.0001	19.1226
R2	0.8059	0.3641	0.7886	0.5697
RER	6.3934	5.2081	6.7730	4.5499
RMSE	0.7093	0.0305	0.0119	4.3729
RPD	2.2700	1.2541	2.1750	1.5244
RPIQ	4.5551	1.4410	4.1219	2.0484
SEP	0.7153	0.0307	0.0120	4.4098

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0057	0.0001	0.0000	0.0308
MSE	0.5302	0.0010	0.0002	21.0894
R2	0.7955	0.2949	0.7710	0.5254
RER	6.2280	4.9459	6.5072	4.3326
RMSE	0.7281	0.0321	0.0124	4.5923
RPD	2.2112	1.1909	2.0897	1.4516
RPIQ	4.4371	1.3685	3.9601	1.9506
SEP	0.7342	0.0324	0.0125	4.6310

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.8286	0.0004	0.0001	58.5228
R2	0.6378	0.4600	0.7299	-0.7540
RER	4.3456	4.9933	6.3018	2.5908
RMSE	0.9103	0.0197	0.0120	7.6500
RPD	1.6616	1.3608	1.9242	0.7551
RPIQ	3.4427	1.4540	3.4521	0.5073
SEP	0.8902	0.0201	0.0118	7.7340

Nº Componentes principais: 3

Pré-proc: 11--> SNV

Parâmetros do modelo: PCR

```
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	0.0000
MSE	0.5024	0.0009	0.0001	19.1423
R2	0.8062	0.3642	0.7886	0.5692
RER	6.3978	5.2082	6.7723	4.5475
RMSE	0.7088	0.0305	0.0119	4.3752
RPD	2.2715	1.2541	2.1748	1.5236
RPIQ	4.5582	1.4411	4.1215	2.0473
SEP	0.7148	0.0307	0.0120	4.4121

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0056	0.0001	0.0000	0.0309
MSE	0.5294	0.0010	0.0002	21.1146
R2	0.7958	0.2949	0.7710	0.5249
RER	6.2327	4.9458	6.5069	4.3300
RMSE	0.7276	0.0321	0.0124	4.5951
RPD	2.2128	1.1909	2.0896	1.4507
RPIQ	4.4405	1.3685	3.9599	1.9494
SEP	0.7337	0.0324	0.0125	4.6337

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.8238	0.0004	0.0001	58.6777
R2	0.6399	0.4597	0.7328	-0.7587
RER	4.3597	4.9921	6.3389	2.5873
RMSE	0.9076	0.0197	0.0119	7.6601
RPD	1.6665	1.3605	1.9347	0.7541
RPIQ	3.4528	1.4537	3.4709	0.5067
SEP	0.8874	0.0201	0.0118	7.7445

Nº Componentes principais: 4

Pré-proc: 1--> Padronização

Parâmetros do modelo: PCR

```
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	-0.0000	0.0000	0.0000
MSE	0.3553	0.0007	0.0001	22.4714
R2	0.8629	0.5058	0.7948	0.4943
RER	7.6075	5.9078	6.8745	4.1972
RMSE	0.5961	0.0269	0.0118	4.7404
RPD	2.7010	1.4225	2.2077	1.4063
RPIQ	5.4201	1.6346	4.1837	1.8896
SEP	0.6011	0.0271	0.0119	4.7804

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0063	-0.0000	0.0000	0.0034
MSE	0.4034	0.0009	0.0002	25.9827
R2	0.8444	0.4136	0.7655	0.4153
RER	7.1398	5.4233	6.4307	3.9033
RMSE	0.6352	0.0293	0.0126	5.0973
RPD	2.5348	1.3059	2.0652	1.3078
RPIQ	5.0866	1.5006	3.9136	1.7573
SEP	0.6405	0.0295	0.0127	5.1403

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.2651	0.0009	0.0001	26.7170
R2	0.8841	-0.3256	0.8434	0.1992
RER	8.6321	3.1775	8.5242	3.8984
RMSE	0.5149	0.0308	0.0091	5.1688
RPD	2.9374	0.8685	2.5269	1.1175
RPIQ	6.0862	0.9280	4.5334	0.7509
SEP	0.4482	0.0315	0.0087	5.1399

Nº Componentes principais: 4

Pré-proc: 10--> MSC

Parâmetros do modelo: PCR

```
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
```

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	0.0000
MSE	0.4549	0.0008	0.0001	18.9031
R2	0.8245	0.4514	0.8287	0.5746
RER	6.7236	5.6070	7.5226	4.5762
RMSE	0.6744	0.0283	0.0107	4.3478
RPD	2.3872	1.3501	2.4158	1.5332
RPIQ	4.7903	1.5514	4.5781	2.0603

SEP	0.6801	0.0285	0.0108	4.3845
-----	--------	--------	--------	--------

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0219	0.0007	0.0002	0.0395
MSE	0.5997	0.0010	0.0001	21.7903
R2	0.7687	0.2955	0.7842	0.5097
RER	5.8581	4.9489	6.7047	4.2624
RMSE	0.7744	0.0321	0.0121	4.6680
RPD	2.0791	1.1914	2.1528	1.4281
RPIQ	4.1721	1.3690	4.0797	1.9189
SEP	0.7806	0.0323	0.0122	4.7072

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.8332	0.0002	0.0001	58.0784
R2	0.6358	0.6766	0.7568	-0.7407
RER	4.3325	6.4744	6.6705	2.6010
RMSE	0.9128	0.0152	0.0114	7.6209
RPD	1.6570	1.7586	2.0278	0.7579
RPIQ	3.4332	1.8790	3.6380	0.5093
SEP	0.8929	0.0155	0.0112	7.7038

Nº Componentes principais: 4

Pré-proc: 11--> SNV

Parâmetros do modelo: PCR

MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	0.0000
MSE	0.4587	0.0008	0.0001	18.9723
R2	0.8230	0.4435	0.8278	0.5731
RER	6.6954	5.5672	7.5039	4.5678
RMSE	0.6773	0.0285	0.0108	4.3557
RPD	2.3772	1.3405	2.4098	1.5304
RPIQ	4.7703	1.5404	4.5667	2.0565
SEP	0.6830	0.0287	0.0109	4.3925

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0219	0.0007	0.0002	0.0392
MSE	0.6015	0.0010	0.0001	21.9112
R2	0.7680	0.2852	0.7837	0.5069
RER	5.8493	4.9133	6.6961	4.2506

RMSE	0.7755	0.0323	0.0121	4.6809
RPD	2.0760	1.1828	2.1500	1.4241
RPIQ	4.1658	1.3592	4.0745	1.9136
SEP	0.7818	0.0326	0.0122	4.7203

```
-----
```

pred				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.8275	0.0002	0.0001	58.2782
R2	0.6383	0.6701	0.7598	-0.7467
RER	4.3487	6.4088	6.7154	2.5964
RMSE	0.9097	0.0154	0.0113	7.6340
RPD	1.6627	1.7410	2.0403	0.7566
RPIQ	3.4449	1.8602	3.6604	0.5084
SEP	0.8896	0.0156	0.0111	7.7174

```
-----
```

```
In [384]: #pcr teste simples
          modelo = 'PCR'
          result = executaPCR(preproc=10,nPC=4)
          print('Parâmetros do modelo:',modelo,'\n',result[0])

          resultados=exibeResultados(result)

          for k,v in zip(resultados.keys(),resultados.values()):
              print(k)
              print(v,'\n-----')
```

Parâmetros do modelo: PCR

```
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
```

cal				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	0.0000
MSE	0.4549	0.0008	0.0001	18.9031
R2	0.8245	0.4514	0.8287	0.5746
RER	6.7236	5.6070	7.5226	4.5762
RMSE	0.6744	0.0283	0.0107	4.3478
RPD	2.3872	1.3501	2.4158	1.5332
RPIQ	4.7903	1.5514	4.5781	2.0603
SEP	0.6801	0.0285	0.0108	4.3845

```
-----
```

val				
	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0219	0.0007	0.0002	0.0395
MSE	0.5997	0.0010	0.0001	21.7903

R2	0.7687	0.2955	0.7842	0.5097
RER	5.8581	4.9489	6.7047	4.2624
RMSE	0.7744	0.0321	0.0121	4.6680
RPD	2.0791	1.1914	2.1528	1.4281
RPIQ	4.1721	1.3690	4.0797	1.9189
SEP	0.7806	0.0323	0.0122	4.7072

```
-----
pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS      0.2717  0.0020  0.0033   1.2475
MSE      0.8332  0.0002  0.0001  58.0784
R2      0.6358  0.6766  0.7568  -0.7407
RER      4.3325  6.4744  6.6705   2.6010
RMSE      0.9128  0.0152  0.0114   7.6209
RPD      1.6570  1.7586  2.0278   0.7579
RPIQ      3.4332  1.8790  3.6380   0.5093
SEP      0.8929  0.0155  0.0112   7.7038
-----
```

In []:

```
In [385]: #pcr otimizando
maior=[-1,-1,-1,-1]
maiorGerado=[0,0,0,0]
for i in range(100):
    result = executaPCR(preproc=10, nPC=4, IC=i)
    resultados=exibeResultados(result)
    r2 = resultados['val'].loc[resultados['val'].index=='R2']
    r = []
    for j in range(4):
        r.append(r2.iloc[:,j][0])
        if r[j]>maior[j]:
            maior[j] = r[j]
            maiorGerado[j]=i
    print('\r%d%% completos'%(i+1), end='')
print('\n', 'r2:', maior, '\nsemente: b c f x', maiorGerado)
```

100% completos

r2: [0.889, 0.5887, 0.9224, 0.6119]
semente: b c f x [76, 24, 24, 24]

```
In [408]: #PCr teste otimizado
modelo = 'PCR:'
result = result = executaPCR(preproc=1,nPC=4,IC=24)
print('Parâmetros do modelo:',modelo,'\n',result[0])

resultados=exibeResultados(result)
```

Parâmetros do modelo: PCR:

```
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
```

In [409]: resultados['cal']

```
Out[409]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0000	0.0000	0.0000	0.0000
MSE	0.1920	0.0003	0.0001	16.3422
R2	0.9189	0.5715	0.8987	0.6021
RER	8.7551	5.4434	9.6236	4.9217
RMSE	0.4382	0.0183	0.0077	4.0426
RPD	3.5123	1.5277	3.1412	1.5853
RPIQ	7.2533	2.1218	6.3989	1.5347
SEP	0.4419	0.0185	0.0077	4.0767

In [410]: resultados['val']

```
Out[410]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0159	0.0002	-0.0000	-0.0163
MSE	0.2300	0.0004	0.0001	19.3822
R2	0.9029	0.5136	0.8804	0.5281
RER	8.0039	5.1093	8.8571	4.5193
RMSE	0.4796	0.0195	0.0083	4.4025
RPD	3.2091	1.4338	2.8910	1.4557
RPIQ	6.6273	1.9914	5.8891	1.4092
SEP	0.4833	0.0197	0.0084	4.4396

In [411]: resultados['pred']

```
Out[411]:
```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2201	0.0172	0.0038	1.4274
MSE	1.3604	0.0018	0.0002	30.4087
R2	0.5382	0.2525	0.6844	0.2866
RER	3.8752	4.0015	5.1953	3.6725
RMSE	1.1664	0.0427	0.0158	5.5144
RPD	1.4715	1.1566	1.7802	1.1839
RPIQ	2.8587	1.0300	2.6712	1.2175
SEP	1.1737	0.0400	0.0157	5.4580

In [390]: reg, treino_teste,y_c,y_cv,y_p = result

7.9.3 Reais x preditos

In []:


```
In [391]: #ridge reaisxpreditos
#calibração
pred=pd.DataFrame(y_c, columns=var_ae)
reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('CALIBRAÇÃO:\n')
round(reais_pred,4)
```

CALIBRAÇÃO:

```
Out [391]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	3.5967	0.1065	0.0850	13.6476	3.9144
1	0.4280	0.0390	0.0334	13.7624	0.6673
2	0.0759	0.0136	0.0139	0.0726	0.2257
3	3.8876	0.0418	0.0605	11.0267	3.8933
4	0.6010	0.0559	0.0116	20.1368	0.5951
5	3.1068	0.0781	0.0545	11.0526	2.7369
6	2.1150	0.0730	0.0505	18.4127	1.7882
7	2.1643	0.0830	0.0529	18.8324	1.7528
8	2.9774	0.0704	0.0567	10.8002	2.9361
9	3.8803	0.0557	0.0691	11.3256	3.1934
10	3.5974	0.0516	0.0731	15.3973	2.6009
11	0.3900	0.0315	0.0283	14.1777	0.9024
12	0.6010	0.0559	0.0116	20.1368	0.5468
13	0.0874	0.0217	0.0127	0.1071	0.1108
14	0.3900	0.0315	0.0283	14.1777	0.8960
15	2.9774	0.0704	0.0567	10.8002	2.6872
16	2.9774	0.0704	0.0567	10.8002	3.0056
17	0.3828	0.0405	0.0301	12.4461	0.7124
18	0.0308	0.0213	0.0113	0.0996	-0.0610
19	3.7243	0.0561	0.0681	11.5736	3.6104
20	2.1643	0.0830	0.0529	18.8324	1.8977
21	3.2342	0.0672	0.0543	8.4772	2.5644
22	2.9123	0.1058	0.0747	14.6813	3.6457
23	3.8803	0.0557	0.0691	11.3256	3.3255
24	3.5974	0.0516	0.0731	15.3973	2.4499
25	3.2342	0.0672	0.0543	8.4772	2.7236
26	3.5967	0.1065	0.0850	13.6476	4.0044
27	0.6491	0.0605	0.0260	18.4274	0.7946
28	3.8876	0.0418	0.0605	11.0267	4.1390
29	3.8876	0.0418	0.0605	11.0267	3.8556
30	0.0554	0.0181	0.0106	0.3275	0.3115
31	3.7243	0.0561	0.0681	11.5736	3.7439

32	3.1068	0.0781	0.0545	11.0526	2.8587
33	3.8994	0.1118	0.0613	10.9512	3.4454
34	3.5610	0.0586	0.0561	10.0978	4.0652
35	3.1068	0.0781	0.0545	11.0526	2.6236
36	2.9123	0.1058	0.0747	14.6813	3.7953
37	2.7110	0.0548	0.0688	13.5829	3.1525
38	3.5974	0.0516	0.0731	15.3973	2.4601
39	0.0759	0.0136	0.0139	0.0726	-0.0427
40	3.8994	0.1118	0.0613	10.9512	3.6364
41	2.9123	0.1058	0.0747	14.6813	3.6092
42	2.7110	0.0548	0.0688	13.5829	3.2801
43	0.5905	0.0465	0.0267	18.7095	0.4155
44	0.1671	0.0117	0.0104	0.1117	0.4406
45	0.0874	0.0217	0.0127	0.1071	0.0899
46	0.6491	0.0605	0.0260	18.4274	0.7626
47	0.5905	0.0465	0.0267	18.7095	0.7045
48	0.4280	0.0390	0.0334	13.7624	0.4906
49	0.0759	0.0136	0.0139	0.0726	0.0485
50	0.3828	0.0405	0.0301	12.4461	1.1024
51	0.1724	0.0112	0.0121	0.0924	0.2232
52	0.0554	0.0181	0.0106	0.3275	0.4861
53	0.0308	0.0213	0.0113	0.0996	0.1084
54	0.0874	0.0217	0.0127	0.1071	0.4634
55	2.7110	0.0548	0.0688	13.5829	3.0620
56	0.1724	0.0112	0.0121	0.0924	0.0896
57	3.5610	0.0586	0.0561	10.0978	4.0785
58	0.0308	0.0213	0.0113	0.0996	-0.3030
59	0.5905	0.0465	0.0267	18.7095	0.3739

	pred: cmcase	pred: fpase	pred: xilanasase
0	0.0815	0.0698	12.9017
1	0.0311	0.0240	7.5637
2	0.0258	0.0170	1.4690
3	0.0824	0.0691	14.0033
4	0.0523	0.0223	19.0296
5	0.0624	0.0528	10.1335
6	0.0498	0.0375	9.1156
7	0.0458	0.0403	8.3580
8	0.0688	0.0536	12.0997
9	0.0665	0.0684	12.1598
10	0.0597	0.0635	12.6936
11	0.0346	0.0277	8.4924
12	0.0521	0.0181	17.7923
13	0.0232	0.0166	1.2924
14	0.0341	0.0278	8.1244
15	0.0631	0.0501	10.3577
16	0.0704	0.0529	11.7750
17	0.0301	0.0268	7.6876

18	0.0257	0.0062	1.2834
19	0.0800	0.0645	14.4076
20	0.0507	0.0400	9.4180
21	0.0630	0.0481	11.3832
22	0.0771	0.0782	14.7323
23	0.0687	0.0711	12.5448
24	0.0578	0.0607	12.7439
25	0.0660	0.0510	12.0914
26	0.0823	0.0729	12.9071
27	0.0556	0.0241	18.7932
28	0.0843	0.0733	13.4534
29	0.0817	0.0687	13.5769
30	0.0249	0.0225	8.4072
31	0.0801	0.0697	14.9847
32	0.0646	0.0545	10.5219
33	0.0720	0.0635	10.7450
34	0.0827	0.0722	12.6083
35	0.0607	0.0521	10.4775
36	0.0805	0.0793	15.0232
37	0.0662	0.0705	12.4939
38	0.0570	0.0610	12.4353
39	0.0225	0.0115	0.7778
40	0.0752	0.0668	11.3393
41	0.0760	0.0767	13.9761
42	0.0693	0.0705	13.0905
43	0.0476	0.0212	18.0517
44	0.0276	0.0235	8.9069
45	0.0235	0.0156	1.1004
46	0.0532	0.0266	19.1215
47	0.0522	0.0232	17.4766
48	0.0263	0.0247	7.4010
49	0.0219	0.0157	0.7279
50	0.0371	0.0304	7.8915
51	0.0246	0.0212	8.9533
52	0.0288	0.0239	9.0358
53	0.0240	0.0152	1.0314
54	0.0306	0.0178	1.2782
55	0.0671	0.0672	13.1341
56	0.0235	0.0190	8.9192
57	0.0819	0.0746	13.0489
58	0.0170	0.0100	0.4503
59	0.0471	0.0201	17.8709

```
In [392]: #validação
pred=pd.DataFrame(y_cv, columns=var_ae)
reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
```

```

for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('VALIDAÇÃO CRUZADA:\n')
round(reais_pred,4)

```

VALIDAÇÃO CRUZADA:

```

Out[392]:
    betaglicosidase  cmcase  fpase  xilanase  pred: betaglicosidase  \
0          3.5967  0.1065  0.0850   13.6476          3.9194
1          0.4280  0.0390  0.0334   13.7624          0.6755
2          0.0759  0.0136  0.0139    0.0726          0.2414
3          3.8876  0.0418  0.0605   11.0267          3.8973
4          0.6010  0.0559  0.0116   20.1368          0.5957
5          3.1068  0.0781  0.0545   11.0526          2.7439
6          2.1150  0.0730  0.0505   18.4127          1.8063
7          2.1643  0.0830  0.0529   18.8324          1.7314
8          2.9774  0.0704  0.0567   10.8002          2.9511
9          3.8803  0.0557  0.0691   11.3256          3.0660
10         3.5974  0.0516  0.0731   15.3973          2.4312
11         0.3900  0.0315  0.0283   14.1777          0.8987
12         0.6010  0.0559  0.0116   20.1368          0.5243
13         0.0874  0.0217  0.0127    0.1071          0.1201
14         0.3900  0.0315  0.0283   14.1777          0.9519
15         2.9774  0.0704  0.0567   10.8002          2.6929
16         2.9774  0.0704  0.0567   10.8002          2.9973
17         0.3828  0.0405  0.0301   12.4461          0.7767
18         0.0308  0.0213  0.0113    0.0996         -0.1248
19         3.7243  0.0561  0.0681   11.5736          3.5535
20         2.1643  0.0830  0.0529   18.8324          1.8317
21         3.2342  0.0672  0.0543    8.4772          2.4899
22         2.9123  0.1058  0.0747   14.6813          3.7339
23         3.8803  0.0557  0.0691   11.3256          3.3671
24         3.5974  0.0516  0.0731   15.3973          2.3456
25         3.2342  0.0672  0.0543    8.4772          2.7577
26         3.5967  0.1065  0.0850   13.6476          4.0194
27         0.6491  0.0605  0.0260   18.4274          0.8096
28         3.8876  0.0418  0.0605   11.0267          4.1690
29         3.8876  0.0418  0.0605   11.0267          3.8889
30         0.0554  0.0181  0.0106    0.3275          0.3196
31         3.7243  0.0561  0.0681   11.5736          3.7234
32         3.1068  0.0781  0.0545   11.0526          2.8362
33         3.8994  0.1118  0.0613   10.9512          3.4188
34         3.5610  0.0586  0.0561   10.0978          4.0346
35         3.1068  0.0781  0.0545   11.0526          2.6053
36         2.9123  0.1058  0.0747   14.6813          3.9839
37         2.7110  0.0548  0.0688   13.5829          3.2878

```

38	3.5974	0.0516	0.0731	15.3973	2.5795
39	0.0759	0.0136	0.0139	0.0726	-0.0494
40	3.8994	0.1118	0.0613	10.9512	3.6722
41	2.9123	0.1058	0.0747	14.6813	3.7832
42	2.7110	0.0548	0.0688	13.5829	3.3226
43	0.5905	0.0465	0.0267	18.7095	0.4357
44	0.1671	0.0117	0.0104	0.1117	0.4732
45	0.0874	0.0217	0.0127	0.1071	0.0911
46	0.6491	0.0605	0.0260	18.4274	0.7839
47	0.5905	0.0465	0.0267	18.7095	0.7144
48	0.4280	0.0390	0.0334	13.7624	0.6243
49	0.0759	0.0136	0.0139	0.0726	0.0659
50	0.3828	0.0405	0.0301	12.4461	1.2022
51	0.1724	0.0112	0.0121	0.0924	0.3661
52	0.0554	0.0181	0.0106	0.3275	0.6180
53	0.0308	0.0213	0.0113	0.0996	0.1181
54	0.0874	0.0217	0.0127	0.1071	0.4797
55	2.7110	0.0548	0.0688	13.5829	3.0934
56	0.1724	0.0112	0.0121	0.0924	0.0488
57	3.5610	0.0586	0.0561	10.0978	4.1331
58	0.0308	0.0213	0.0113	0.0996	-0.3073
59	0.5905	0.0465	0.0267	18.7095	0.3276

	pred: cmcase	pred: fpase	pred: xilaname
0	0.0819	0.0692	13.0371
1	0.0305	0.0234	7.1446
2	0.0265	0.0171	1.5346
3	0.0827	0.0685	14.0920
4	0.0522	0.0243	18.8623
5	0.0625	0.0521	10.0839
6	0.0471	0.0365	8.1531
7	0.0437	0.0391	7.2935
8	0.0664	0.0527	11.4217
9	0.0673	0.0674	11.7655
10	0.0621	0.0626	12.6091
11	0.0319	0.0263	7.1509
12	0.0515	0.0191	17.4928
13	0.0233	0.0171	1.3482
14	0.0333	0.0272	7.3280
15	0.0625	0.0495	10.0911
16	0.0697	0.0523	11.5917
17	0.0293	0.0262	6.8447
18	0.0268	0.0043	1.3038
19	0.0804	0.0634	14.4687
20	0.0509	0.0388	9.2701
21	0.0636	0.0467	11.3192
22	0.0750	0.0798	15.0009
23	0.0670	0.0720	12.6289

24	0.0575	0.0592	12.3409
25	0.0693	0.0517	12.6093
26	0.0866	0.0733	13.3789
27	0.0555	0.0238	18.9971
28	0.0892	0.0741	14.0524
29	0.0863	0.0694	14.1703
30	0.0248	0.0233	9.2347
31	0.0797	0.0707	15.2390
32	0.0637	0.0556	10.7942
33	0.0711	0.0646	10.9573
34	0.0818	0.0733	12.7309
35	0.0599	0.0531	10.8255
36	0.0717	0.0792	14.3955
37	0.0594	0.0702	11.8836
38	0.0512	0.0605	11.8105
39	0.0232	0.0113	0.9014
40	0.0718	0.0672	11.3005
41	0.0678	0.0765	13.3557
42	0.0704	0.0707	13.1576
43	0.0478	0.0198	18.0196
44	0.0293	0.0247	9.8033
45	0.0237	0.0158	1.1448
46	0.0534	0.0250	19.0169
47	0.0520	0.0216	17.2911
48	0.0277	0.0265	8.5087
49	0.0232	0.0164	0.8168
50	0.0380	0.0317	8.6154
51	0.0261	0.0232	10.1996
52	0.0300	0.0257	10.1467
53	0.0252	0.0158	1.0303
54	0.0311	0.0183	1.2603
55	0.0687	0.0676	13.2759
56	0.0243	0.0190	9.7927
57	0.0835	0.0757	13.0319
58	0.0174	0.0103	0.7363
59	0.0472	0.0189	17.9780

```
In [393]: #predição
pred=pd.DataFrame(y_p, columns=var_ae)
reais = treino_teste[3]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('Predição (validação externa):\n')
round(reais_pred,4)
```

Predição (validação externa):

```

Out[393]:
    betaglicosidase  cmcase  fpase  xilanasase  pred: betaglicosidase  \
0          2.1643  0.0830  0.0529   18.8324          2.8688
1          3.5610  0.0586  0.0561   10.0978          2.7516
2          0.1671  0.0117  0.0104    0.1117          0.5042
3          3.8994  0.1118  0.0613   10.9512          3.0944
4          4.6037  0.1713  0.0919   16.8115          3.9320
5          0.4280  0.0390  0.0334   13.7624          0.9046
6          0.3900  0.0315  0.0283   14.1777          1.6797
7          3.5967  0.1065  0.0850   13.6476          3.4253
8          0.6010  0.0559  0.0116   20.1368         -1.4185
9          0.1671  0.0117  0.0104    0.1117          0.9426
10         3.8803  0.0557  0.0691   11.3256          3.4190
11         0.6491  0.0605  0.0260   18.4274         -0.5173
12         2.1150  0.0730  0.0505   18.4127          2.1520
13         3.7243  0.0561  0.0681   11.5736          1.4824
14         0.1724  0.0112  0.0121    0.0924          0.5743
15         4.6037  0.1713  0.0919   16.8115          3.4638
16         3.2342  0.0672  0.0543    8.4772          1.4197
17         0.3828  0.0405  0.0301   12.4461          2.3244
18         4.6037  0.1713  0.0919   16.8115          3.4534
19         2.1150  0.0730  0.0505   18.4127          2.2057
20         0.0554  0.0181  0.0106    0.3275          1.8299

    pred: cmcase  pred: fpase  pred: xilanasase
0          0.0620          0.0627          11.2042
1          0.0678          0.0493          13.6731
2          0.0290          0.0224           6.0890
3          0.0716          0.0587          14.5006
4          0.0815          0.0726          12.4542
5          0.0343          0.0294           7.1377
6          0.0465          0.0388           7.8813
7          0.0762          0.0654          14.8739
8          0.0185         -0.0028          11.1867
9          0.0377          0.0238           5.5414
10         0.0803          0.0565          13.3037
11         0.0355          0.0046          12.0289
12         0.0496          0.0578          11.4825
13         0.0489          0.0384          14.7737
14         0.0312          0.0213           5.1490
15         0.0718          0.0699          12.0975
16         0.0440          0.0408          12.6059
17         0.0573          0.0448           7.1027
18         0.0715          0.0698          11.8626
19         0.0509          0.0569          11.0232
20         0.0513          0.0352           5.8110

```

```
In [ ]:
```

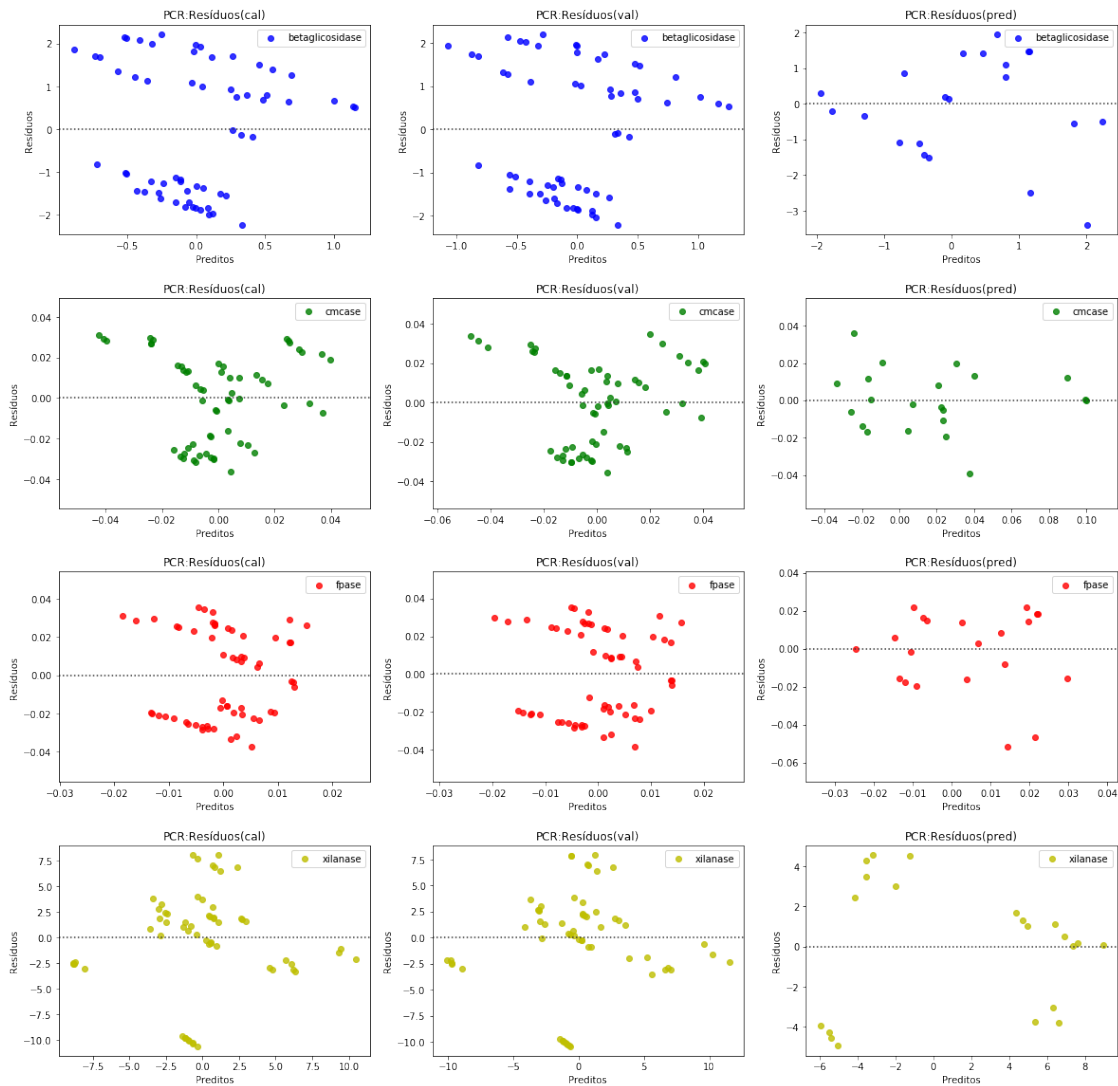
7.9.4 PCR: Gráficos de resíduos - histograma - reais x preditos

```
In [412]: #título para os gráficos
```

```
modelo = 'PCR'
```

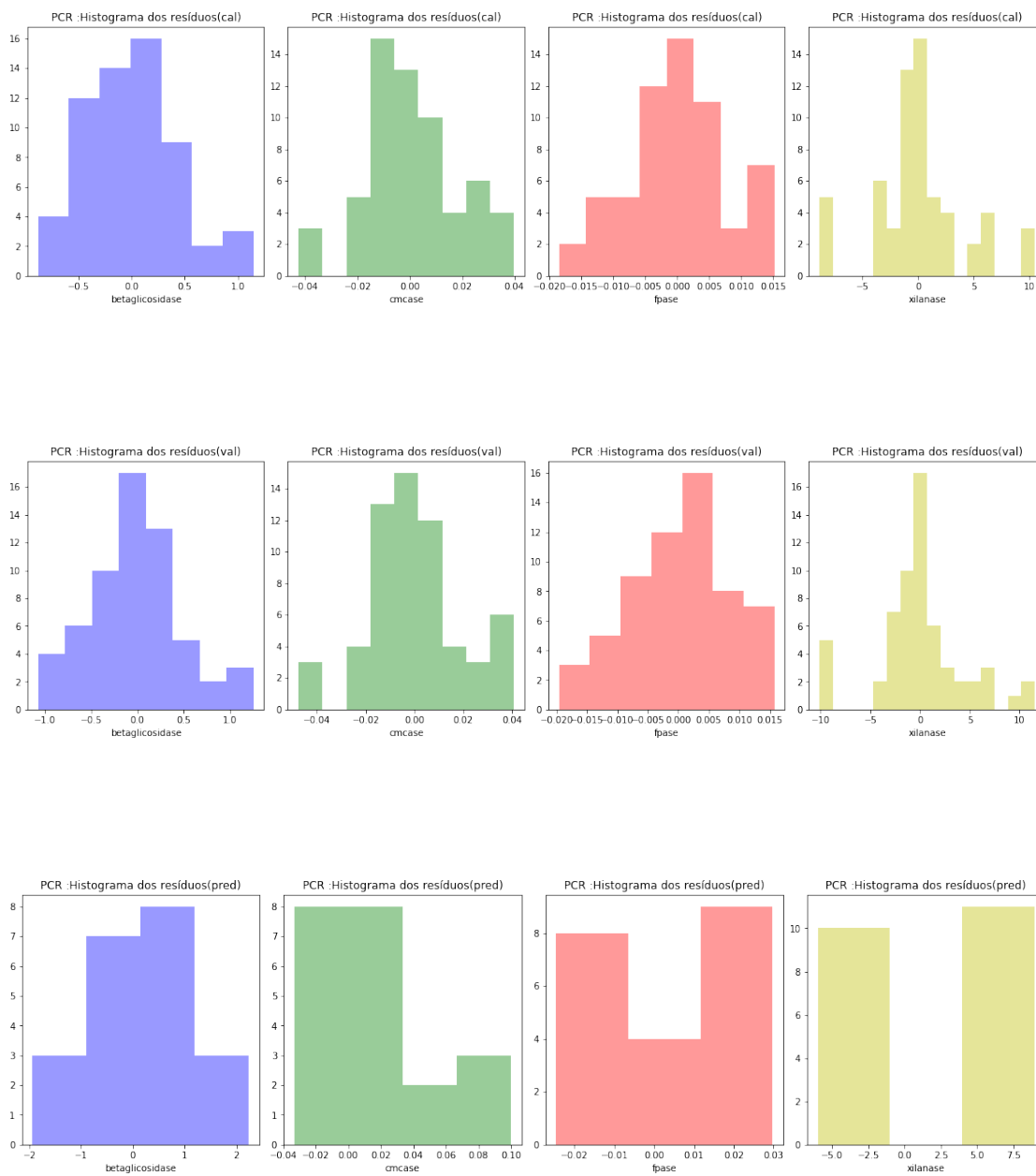
```
In [395]: #gráfico dos resíduos
```

```
graficoResiduos(modelo, treino_teste, y_c,y_cv,y_p)
```

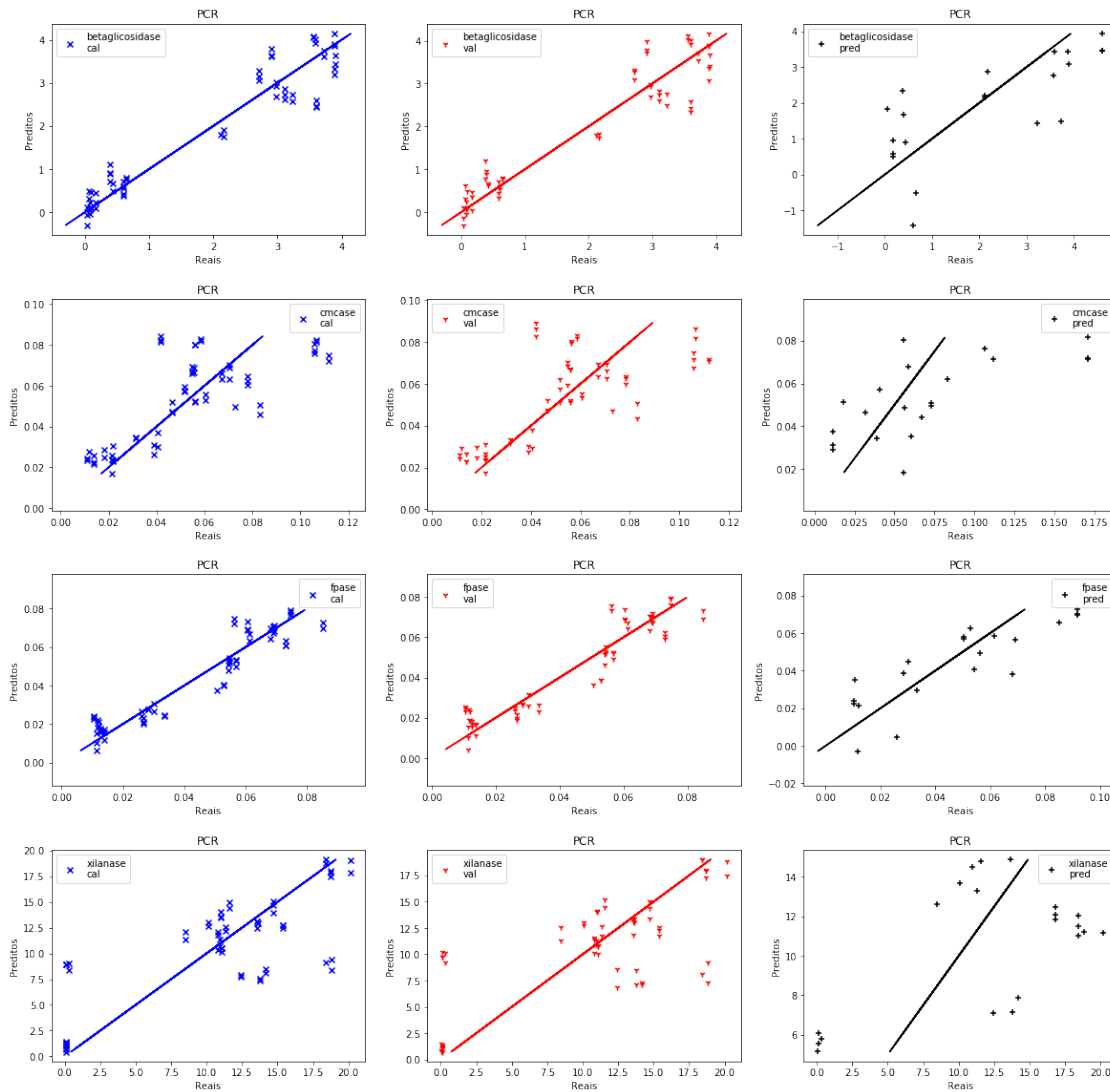


```
In [396]: #histograma dos resíduos
```

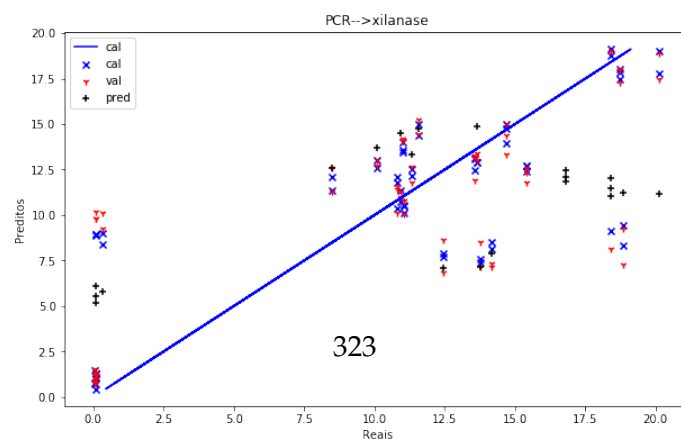
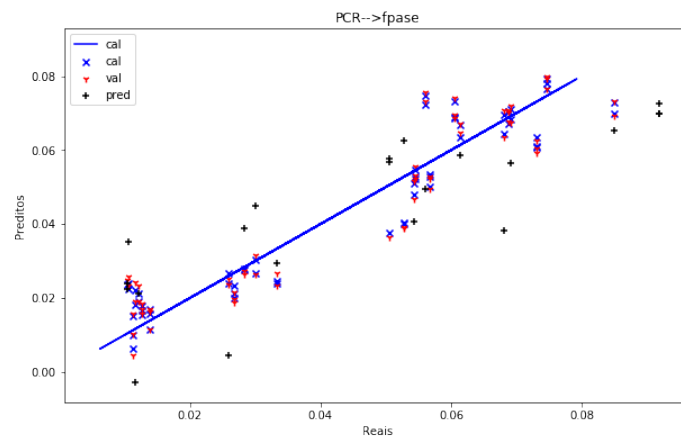
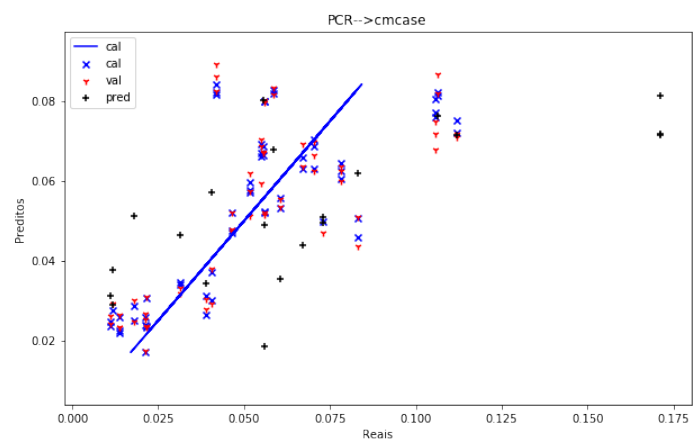
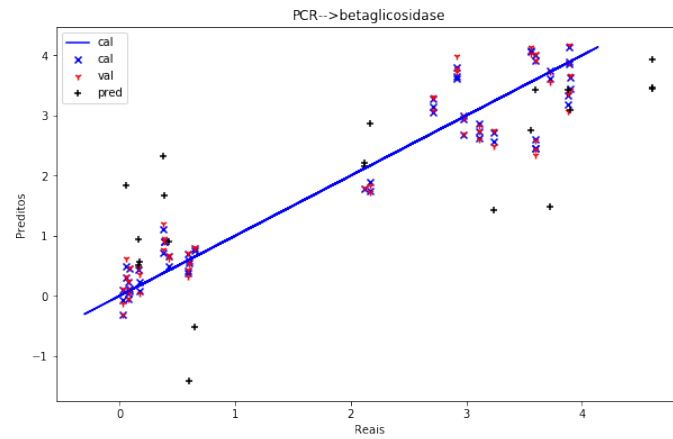
```
graficoHist(modelo, treino_teste, y_c,y_cv,y_p)
```

In [397]: *#graico de reais x preditos*
graficoReaisPreditosSep(modelo, treino_teste, y_c,y_cv,y_p)

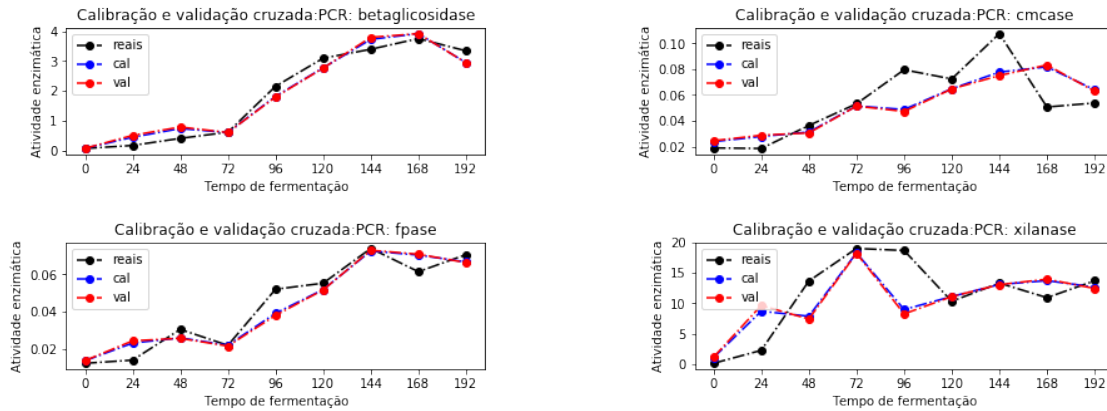


In [398]: *#gráfico de reais x preditos*
`graficoReaisPreditos(modelo, treino_teste, y_c,y_cv,y_p)`



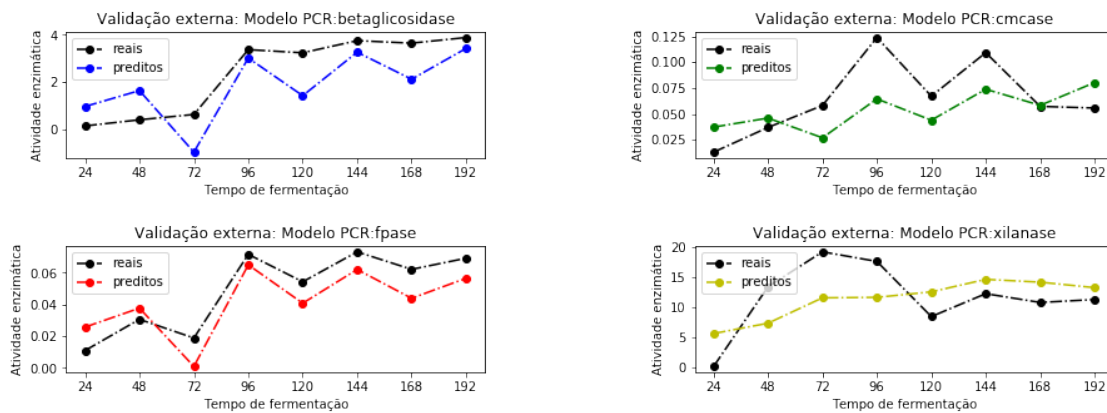
7.9.5 PCR: Gráficos: dados de treino

```
In [399]: y_treino = treino_teste[2]
          graficoTreinamento(modelo, y_treino, y_c,y_cv)
```



7.9.6 PCR: Gráficos de teste

```
In [400]: y_teste = treino_teste[3]
          graficoTeste(modelo, y_teste, y_p)
```



```
In [ ]:
```

7.10 Kernel PCA:

7.10.1 Kernel PCA: função completa

```
In [463]: #kernelpca
          #função completa para execução do Kernel PCA:
          #A variável preproc determinará o tipo de processamento que será executado (0,1,2,3,4)
          def executaKPCA(preproc=1, nPC=3, tk='linear', ic=0):
              #separando o conjunto de dados em treino e teste
              x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc,False,ic)

              # Define um objeto Kernel PCA
              kpca = KernelPCA(n_components=nPC, kernel =tk)

              x_treino = kpca.fit_transform(x_treino)[:,:nPC]
              x_teste = kpca.fit_transform(x_teste)[:,:nPC]

              #Passo 2: Aplicar a regressão sobre as componentes selecionadas

              # Cria um objeto de regressão linear
              reg = LinearRegression()

              result = executaCVP([x_treino, x_teste, y_treino, y_teste], reg)

              return result
```

```
In [ ]:
```

7.10.2 Kernel PCA: testes

```
In [472]: list(np.arange(1,10))
```

```
Out[472]: [1, 2, 3, 4, 5, 6, 7, 8, 9]
```

```
In [477]: #kernelpca otimização parte 1
          varKernel = ['linear','poly','rbf','sigmoid','cosine', 'precomputed']
          for pre, valor in zip(preProc.keys(), preProc.values()):
              maior=[-100,-100,-100,-100]
              #maiorGerado=[0,0,0,0]
              componentes=[0,0,0,0]
              tipokernel=['0','0','0','0']
              print(valor)
              for cp, k in zip(list(np.arange(2,7)),varKernel):
                  result = executaKPCA(pre,cp,k)
                  resultados=exibeResultados(result)
                  r2 = resultados['pred'].loc[resultados['pred'].index=='R2']
```

```

r = []
for j in range(4):
    r.append(r2.iloc[:,j][0])
    if r[j]>maior[j]:
        maior[j] = r[j]
        componentes[j]=cp
        tipokernel[j]=k
    print('\r%d%% completos'%(i+1), end='')
print('\n', 'r2 ( b c f x ):', maior, '\ncomponentes:', componentes, '\nKernel:', tipokernel)
print('-----')

```

Pré-proc: 0--> Sem pré-processamento

100% completos

r2 (b c f x): [-1.0111, -0.3975, -1.0074, 0.4296]

componentes: [6, 3, 3, 6]

Kernel: ['cosine', 'poly', 'poly', 'cosine']

Pré-proc: 1--> Padronização

100% completos

r2 (b c f x): [-0.1511, -0.118, -0.5021, 0.4803]

componentes: [5, 3, 3, 2]

Kernel: ['sigmoid', 'poly', 'poly', 'linear']

Pré-proc: 2--> Suavização(SavGol) - Par:3,1,1

100% completos

r2 (b c f x): [-0.9054, -0.2866, -0.8782, 0.5751]

componentes: [4, 2, 3, 3]

Kernel: ['rbf', 'linear', 'poly', 'poly']

Pré-proc: 3--> Suavização(SavGol) - Par:3,2,1

100% completos

r2 (b c f x): [-0.9508, -0.2835, -0.8917, 0.1019]

componentes: [2, 2, 2, 2]

Kernel: ['linear', 'linear', 'linear', 'linear']

Pré-proc: 4--> Suavização(SavGol) - Par:5,1,1

100% completos

r2 (b c f x): [-0.9255, -0.2854, -0.8937, 0.5553]

componentes: [3, 3, 2, 5]

Kernel: ['poly', 'poly', 'linear', 'sigmoid']

Pré-proc: 5--> Suavização(SavGol) - Par:5,2,1

100% completos

r2 (b c f x): [-0.9642, -0.3205, -0.9162, 0.5923]

componentes: [3, 2, 3, 4]

Kernel: ['poly', 'linear', 'poly', 'rbf']

Pré-proc: 6--> Suavização(SavGol) - Par:3,2,2

```

100% completos
r2 ( b c f x ): [-0.9394, -0.2614, -0.8863, 0.5186]
componentes: [4, 2, 2, 3]
Kernel: ['rbf', 'linear', 'linear', 'poly']
-----
Pré-proc: 7--> Suavização(SavGol) - Par:5,2,2
100% completos
r2 ( b c f x ): [-0.9081, -0.2953, -0.8684, 0.0025]
componentes: [3, 2, 6, 2]
Kernel: ['poly', 'linear', 'cosine', 'linear']
-----
Pré-proc: 8--> Suavização(SavGol) - Par:3,1,1 --> Padronização
100% completos
r2 ( b c f x ): [0.7717, 0.318, 0.812, 0.5661]
componentes: [6, 4, 6, 3]
Kernel: ['cosine', 'rbf', 'cosine', 'poly']
-----
Pré-proc: 9--> Padronização --> Suavização(SavGol) - Par:3,1,1
100% completos
r2 ( b c f x ): [-0.5692, -0.406, -0.454, 0.4754]
componentes: [6, 6, 6, 3]
Kernel: ['cosine', 'cosine', 'cosine', 'poly']
-----
Pré-proc: 10--> MSC
100% completos
r2 ( b c f x ): [-1.0092, -0.1452, -0.9513, 0.537]
componentes: [6, 4, 4, 4]
Kernel: ['cosine', 'rbf', 'rbf', 'rbf']
-----
Pré-proc: 11--> SNV
100% completos
r2 ( b c f x ): [-1.0092, -0.315, -0.9612, 0.5252]
componentes: [6, 6, 6, 4]
Kernel: ['cosine', 'cosine', 'cosine', 'rbf']
-----

```

```

In [485]: #kernelpca otimizado
maior=[-1,-1,-1,-1]
maiorGerado=[0,0,0,0]
componentes=[0,0,0,0]
tipokernel=[0,0,0,0]
for i in range(100):
    result = executaKPCA(8,6,'cosine',ic=i)
    resultados=exibeResultados(result)
    r2 = resultados['pred'].loc[resultados['pred'].index=='R2']
    r = []
    for j in range(4):

```

```

        r.append(r2.iloc[:,j][0])
        if r[j]>maior[j]:
            maior[j] = r[j]
            maiorGerado[j]=i
        print('\r%d%% completos'%(i+1), end='')
    print('\n','r2:',maior,'\nsemente: b c f x',maiorGerado)

```

100% completos

r2: [0.8357, 0.4321, 0.812, 0.6554]

semente: b c f x [3, 3, 0, 99]

7.11 MLR: função completa

In [488]: *#mlr*

#função completa para execução do MLR:

#A variável preproc determinará o tipo de processamento que será executado (0,1,2,3)

```
def executaMLR(preproc=1, param=False, IC=0):
```

```
    x_treino, x_teste, y_treino, y_teste = executaPreproc(preproc,param, IC)
```

```
    # Cria um objeto de regressão linear
```

```
    reg = MultiOutputRegressor(LinearRegression())
```

```
    #reg = LinearRegression()
```

```
    result = executaCVP([x_treino, x_teste, y_treino, y_teste], reg)
```

```
    return result
```

In []:

7.11.1 MLR: testes

In [492]: *#mlr teste variando o tipo de préprocessamento*

```
modelo = 'MLR'
```

```
for k in range(12):
```

```
    result = executaMLR(k)
```

```
    print('Parâmetros do modelo:',modelo,'\n',result[0])
```

```
    print(preProc[k])
```

```
    resultados=exibeResultados(result)
```

```
    for k,v in zip(resultados.keys(),resultados.values()):
```

```
        print(k)
```

```
        print(v, '\n-----')
```


Parâmetros do modelo: MLR

```
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
```

Pré-proc: 0--> Sem pré-processamento

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.000000e+00	-0.000000e+00	-0.000000e+00	-0.000000e+00
MSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
R2	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00
RER	1.202202e+13	2.121951e+13	2.319521e+13	1.322362e+13
RMSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
RPD	4.102941e+12	3.515776e+12	3.693259e+12	2.942458e+12
RPIQ	8.233336e+12	4.039945e+12	6.999012e+12	3.953850e+12
SEP	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.1185	-0.0062	-0.0021	-0.2357
MSE	2.1371	0.0024	0.0005	26.0872
R2	0.1755	-0.6595	0.2662	0.4130
RER	3.1121	3.2496	3.6517	3.8996
RMSE	1.4619	0.0492	0.0222	5.1076
RPD	1.1013	0.7763	1.1674	1.3052
RPIQ	2.2100	0.8920	2.2123	1.7538
SEP	1.4694	0.0493	0.0223	5.1452

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1405	-0.0029	-0.0002	-1.6487
MSE	1.6246	0.0017	0.0003	24.7716
R2	0.2899	-1.3610	0.4254	0.2575
RER	2.9802	2.3821	4.1591	4.1639
RMSE	1.2746	0.0411	0.0175	4.9771
RPD	1.1867	0.6508	1.3192	1.1606
RPIQ	2.4587	0.6954	2.3668	0.7798
SEP	1.2981	0.0420	0.0179	4.8121

Parâmetros do modelo: MLR

```
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
```

Pré-proc: 1--> Padronização

cal

	betaglicosidase	cmcase	fpase	xilanase
--	-----------------	--------	-------	----------

BIAS	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
MSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
R2	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00
RER	6.800688e+14	4.526928e+14	4.110847e+14	6.558143e+14
RMSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
RPD	2.366379e+14	1.081845e+14	1.311649e+14	2.196618e+14
RPIQ	4.748593e+14	1.243138e+14	2.485676e+14	2.951648e+14
SEP	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

val

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.0780	-0.0065	-0.0021	-0.1366
MSE	2.0661	0.0030	0.0005	15.9284
R2	0.2029	-1.0661	0.2294	0.6416
RER	3.1594	2.9098	3.5623	4.9882
RMSE	1.4374	0.0549	0.0228	3.9910
RPD	1.1201	0.6957	1.1392	1.6703
RPIQ	2.2477	0.7994	2.1589	2.2444
SEP	1.4474	0.0550	0.0229	4.0224

pred

	betaglicosidase	cmcase	fpase	xylanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	1.1990	0.0013	0.0003	10.4273
R2	0.4759	-0.8452	0.4432	0.6875
RER	3.5593	2.6917	4.3022	6.5653
RMSE	1.0950	0.0364	0.0172	3.2291
RPD	1.3813	0.7362	1.3402	1.7888
RPIQ	2.8620	0.7866	2.4043	1.2019
SEP	1.0869	0.0372	0.0173	3.0520

Parâmetros do modelo: MLR

```
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
```

Pré-proc: 2--> Suavização(SavGol) - Par:3,1,1

cal

	betaglicosidase	cmcase	fpase	xylanase
BIAS	-0.000000e+00	-0.000000e+00	0.000000e+00	0.000000e+00
MSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
R2	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00
RER	2.695019e+14	1.326921e+14	1.733544e+14	1.673703e+14
RMSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
RPD	9.072785e+13	2.059369e+13	5.380210e+13	5.521952e+13
RPIQ	1.820628e+14	2.366401e+13	1.019592e+14	7.419978e+13
SEP	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0327	-0.0019	-0.0003	0.0858
MSE	1.5328	0.0019	0.0003	11.0058
R2	0.4087	-0.3024	0.5823	0.7523
RER	3.6640	3.6427	4.8190	5.9994
RMSE	1.2381	0.0436	0.0168	3.3175
RPD	1.3004	0.8763	1.5472	2.0094
RPIQ	2.6096	1.0069	2.9322	2.7001
SEP	1.2481	0.0439	0.0169	3.3444

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0118	-0.0111	-0.0031	-0.8088
MSE	1.3159	0.0016	0.0003	18.4350
R2	0.4248	-1.2669	0.4373	0.4475
RER	3.2913	2.5224	4.2714	4.6373
RMSE	1.1471	0.0403	0.0173	4.2936
RPD	1.3185	0.6642	1.3330	1.3453
RPIQ	2.7319	0.7097	2.3915	0.9039
SEP	1.1754	0.0397	0.0175	4.3209

Parâmetros do modelo: MLR

```
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
```

Pré-proc: 3--> Suavização(SavGol) - Par:3,2,1

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.000000e+00	-0.000000e+00	-0.000000e+00	-0.000000e+00
MSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
R2	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00
RER	1.700436e+14	2.121728e+14	1.725312e+14	7.711008e+13
RMSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
RPD	2.665665e+13	1.877961e+13	2.428191e+13	2.448223e+13
RPIQ	5.349167e+13	2.157948e+13	4.601611e+13	3.289735e+13
SEP	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0487	-0.0025	-0.0006	0.0845
MSE	1.6235	0.0020	0.0003	11.9939
R2	0.3737	-0.3381	0.5804	0.7301
RER	3.5615	3.5958	4.8102	5.7467
RMSE	1.2742	0.0442	0.0168	3.4632
RPD	1.2636	0.8645	1.5437	1.9249
RPIQ	2.5356	0.9934	2.9255	2.5865
SEP	1.2840	0.0445	0.0169	3.4914

```

pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.0059 -0.0108 -0.0030  -0.7660
MSE           1.4455  0.0017  0.0003  17.9537
R2            0.3681 -1.4003  0.3658   0.4619
RER           3.1401  2.4407  4.0120   4.6922
RMSE          1.2023  0.0415  0.0184   4.2372
RPD           1.2580  0.6455  1.2557   1.3632
RPIQ          2.6065  0.6897  2.2528   0.9160
SEP           1.2320  0.0410  0.0186   4.2703

```

Parâmetros do modelo: MLR

```

MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
      normalize=False),
      n_jobs=None)

```

Pré-proc: 4--> Suavização(SavGol) - Par:5,1,1

```

cal
      betaglicosidase      cmcase      fpase      xilanase
BIAS    0.000000e+00  0.000000e+00  0.000000e+00 -0.000000e+00
MSE     0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
R2      1.000000e+00  1.000000e+00  1.000000e+00  1.000000e+00
RER     1.816994e+14  1.223372e+14  1.520139e+14  9.357697e+13
RMSE    0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
RPD     4.354183e+13  2.804671e+13  4.672324e+13  1.847156e+13
RPIQ    8.737501e+13  3.222822e+13  8.854415e+13  2.482068e+13
SEP     0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00

```

```

-----
val
      betaglicosidase  cmcase  fpase  xilanase
BIAS        -0.0117 -0.0018 -0.0002   0.0310
MSE         1.6534  0.0024  0.0003  15.1575
R2          0.3622 -0.6207  0.4822   0.6589
RER         3.5268  3.2645  4.3277   5.1106
RMSE        1.2858  0.0487  0.0187   3.8933
RPD         1.2521  0.7855  1.3897   1.7122
RPIQ        2.5126  0.9026  2.6336   2.3008
SEP         1.2966  0.0490  0.0188   3.9260

```

```

-----
pred
      betaglicosidase  cmcase  fpase  xilanase
BIAS          0.0396 -0.0069 -0.0018  -1.1166
MSE           1.1436  0.0019  0.0003  18.1708
R2            0.5001 -1.6803  0.4719   0.4554
RER           3.5328  2.2579  4.3625   4.7533
RMSE          1.0694  0.0438  0.0168   4.2627
RPD           1.4144  0.6108  1.3760   1.3550
RPIQ          2.9305  0.6526  2.4687   0.9105
SEP           1.0950  0.0443  0.0171   4.2155

```

Parâmetros do modelo: MLR

MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)

Pré-proc: 5--> Suavização(SavGol) - Par:5,2,1

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.000000e+00	0.000000e+00	-0.000000e+00	0.000000e+00
MSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
R2	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00
RER	1.046809e+14	9.442676e+13	1.075018e+14	8.139318e+13
RMSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
RPD	3.557583e+13	2.177382e+13	3.081820e+13	2.219513e+13
RPIQ	7.138972e+13	2.502009e+13	5.840288e+13	2.982412e+13
SEP	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0091	-0.0020	-0.0002	0.0632
MSE	1.6209	0.0023	0.0003	15.1408
R2	0.3747	-0.5822	0.5444	0.6593
RER	3.5619	3.3045	4.6138	5.1139
RMSE	1.2731	0.0481	0.0175	3.8911
RPD	1.2646	0.7950	1.4816	1.7132
RPIQ	2.5377	0.9135	2.8077	2.3021
SEP	1.2839	0.0484	0.0177	3.9234

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0318	-0.0078	-0.0023	-1.0163
MSE	1.1616	0.0018	0.0003	19.5155
R2	0.4923	-1.5662	0.4531	0.4151
RER	3.5045	2.3177	4.3018	4.5484
RMSE	1.0778	0.0429	0.0171	4.4176
RPD	1.4034	0.6243	1.3523	1.3075
RPIQ	2.9077	0.6670	2.4260	0.8786
SEP	1.1039	0.0432	0.0173	4.4053

Parâmetros do modelo: MLR

MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)

Pré-proc: 6--> Suavização(SavGol) - Par:3,2,2

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.000000e+00	-0.000000e+00	0.000000e+00	-0.000000e+00
MSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

R2	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00
RER	3.362364e+13	3.808769e+13	1.462532e+14	9.206800e+12
RMSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
RPD	1.192057e+13	9.169837e+12	4.693576e+13	3.084670e+12
RPIQ	2.392090e+13	1.053697e+13	8.894691e+13	4.144944e+12
SEP	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0248	0.0000	0.0000	-0.1134
MSE	1.6344	0.0013	0.0002	8.9963
R2	0.3695	0.0789	0.6488	0.7976
RER	3.5477	4.3273	5.2543	6.6382
RMSE	1.2784	0.0367	0.0154	2.9994
RPD	1.2594	1.0420	1.6873	2.2225
RPIQ	2.5271	1.1973	3.1976	2.9865
SEP	1.2890	0.0370	0.0155	3.0225

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.3053	-0.0087	-0.0009	-0.7585
MSE	1.4479	0.0013	0.0002	9.9103
R2	0.3671	-0.7858	0.5833	0.7030
RER	3.2437	2.8176	4.8925	6.4001
RMSE	1.2033	0.0358	0.0149	3.1481
RPD	1.2570	0.7483	1.5492	1.8348
RPIQ	2.6044	0.7996	2.7793	1.2329
SEP	1.1926	0.0355	0.0152	3.1308

Parâmetros do modelo: MLR

```
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
```

Pré-proc: 7--> Suavização(SavGol) - Par:5,2,2

cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.000000e+00	-0.000000e+00	-0.000000e+00	0.000000e+00
MSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
R2	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00
RER	1.459637e+14	1.823414e+14	1.628253e+14	6.058897e+13
RMSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
RPD	4.283784e+13	3.993911e+13	3.095618e+13	2.021847e+13
RPIQ	8.596233e+13	4.589366e+13	5.866436e+13	2.716803e+13
SEP	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0325	-0.0003	-0.0003	-0.0049

MSE	1.8618	0.0013	0.0002	10.1653
R2	0.2818	0.0894	0.6679	0.7712
RER	3.3243	4.3523	5.4046	6.2404
RMSE	1.3645	0.0365	0.0150	3.1883
RPD	1.1800	1.0479	1.7353	2.0908
RPIQ	2.3678	1.2042	3.2885	2.8095
SEP	1.3756	0.0368	0.0151	3.2152

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.1300	-0.0103	-0.0024	-0.5518
MSE	1.4919	0.0016	0.0003	8.0378
R2	0.3479	-1.2649	0.4450	0.7591
RER	3.1086	2.5093	4.2749	7.0317
RMSE	1.2214	0.0403	0.0172	2.8351
RPD	1.2383	0.6645	1.3424	2.0374
RPIQ	2.5657	0.7100	2.4083	1.3690
SEP	1.2445	0.0399	0.0174	2.8495

Parâmetros do modelo: MLR

```
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
```

Pré-proc: 8--> Suavização(SavGol) - Par:3,1,1 --> Padronização

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.000000e+00	-0.000000e+00	0.000000e+00	0.000000e+00
MSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
R2	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00
RER	2.217617e+14	3.665744e+14	2.265991e+14	1.557064e+14
RMSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
RPD	7.873503e+13	8.826638e+13	7.276927e+13	5.216770e+13
RPIQ	1.579969e+14	1.014261e+14	1.379034e+14	7.009898e+13
SEP	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0332	-0.0015	-0.0002	-0.0988
MSE	1.2457	0.0020	0.0002	11.8730
R2	0.5194	-0.3390	0.6670	0.7328
RER	4.0647	3.5909	5.3969	5.7766
RMSE	1.1161	0.0442	0.0150	3.4457
RPD	1.4425	0.8642	1.7330	1.9346
RPIQ	2.8947	0.9930	3.2841	2.5996
SEP	1.1250	0.0446	0.0151	3.4734

pred

	betaglicosidase	cmcase	fpase	xilanase
--	-----------------	--------	-------	----------

BIAS	0.2717	0.0020	0.0033	1.2475
MSE	1.2857	0.0022	0.0004	12.7801
R2	0.4380	-2.0220	0.3208	0.6170
RER	3.4296	2.1021	3.8823	5.8368
RMSE	1.1339	0.0465	0.0190	3.5749
RPD	1.3339	0.5752	1.2134	1.6158
RPIQ	2.7638	0.6146	2.1768	1.0857
SEP	1.1280	0.0476	0.0192	3.4329

Parâmetros do modelo: MLR

```
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
```

Pré-proc: 9--> Padronização --> Suavização(SavGol) - Par:3,1,1
cal

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.000000e+00	-0.000000e+00	-0.000000e+00	0.000000e+00
MSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
R2	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00
RER	1.903093e+14	3.223956e+14	2.262365e+14	1.339276e+14
RMSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
RPD	6.756762e+13	7.762723e+13	7.265259e+13	4.487099e+13
RPIQ	1.355874e+14	8.920072e+13	1.376823e+14	6.029421e+13
SEP	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0549	0.0008	0.0004	-0.0822
MSE	1.0247	0.0015	0.0002	7.2409
R2	0.6047	-0.0175	0.7315	0.8371
RER	4.4863	4.1178	6.0115	7.3974
RMSE	1.0123	0.0386	0.0134	2.6909
RPD	1.5905	0.9913	1.9297	2.4773
RPIQ	3.1917	1.1391	3.6570	3.3288
SEP	1.0193	0.0389	0.0136	2.7123

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2717	0.0020	0.0033	1.2475
MSE	0.8614	0.0008	0.0002	8.8997
R2	0.6235	-0.0605	0.6082	0.7333
RER	4.2543	3.5543	5.1687	7.2159
RMSE	0.9281	0.0276	0.0145	2.9832
RPD	1.6297	0.9710	1.5975	1.9362
RPIQ	3.3766	1.0375	2.8660	1.3010
SEP	0.9093	0.0282	0.0144	2.7768

Parâmetros do modelo: MLR


```

MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
Pré-proc: 10--> MSC
cal

```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.000000e+00	-0.000000e+00	-0.000000e+00	-0.000000e+00
MSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
R2	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00
RER	2.276586e+13	2.454436e+13	3.431683e+13	1.742426e+13
RMSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
RPD	4.834615e+12	5.424839e+12	6.283970e+12	5.301441e+12
RPIQ	9.701580e+12	6.233631e+12	1.190861e+13	7.123671e+12
SEP	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

```

val

```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0724	-0.0044	-0.0013	-0.0570
MSE	1.9601	0.0026	0.0004	26.6340
R2	0.2438	-0.7598	0.3464	0.4007
RER	3.2432	3.1426	3.8588	3.8555
RMSE	1.4000	0.0507	0.0210	5.1608
RPD	1.1500	0.7538	1.2369	1.2917
RPIQ	2.3076	0.8662	2.3440	1.7357
SEP	1.4100	0.0509	0.0211	5.2041

```

pred

```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.0425	-0.0032	-0.0009	-0.8596
MSE	1.8029	0.0026	0.0005	22.3971
R2	0.2119	-2.6152	0.1386	0.3287
RER	2.8131	1.9239	3.3999	4.2018
RMSE	1.3427	0.0509	0.0214	4.7326
RPD	1.1264	0.5259	1.0775	1.2205
RPIQ	2.3339	0.5620	1.9330	0.8201
SEP	1.3752	0.0520	0.0219	4.7688

```

Parâmetros do modelo: MLR
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)
Pré-proc: 11--> SNV
cal

```

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.000000e+00	-0.000000e+00	0.000000e+00	0.000000e+00
MSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
R2	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00
RER	1.947256e+13	2.462721e+13	3.027246e+13	1.618386e+13

RMSE	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
RPD	6.898540e+12	5.545776e+12	8.157628e+12	3.563288e+12
RPIQ	1.384324e+13	6.372600e+12	1.545934e+13	4.788074e+12
SEP	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

val

	betaglicosidase	cmcase	fpase	xilanase
BIAS	-0.0376	-0.0037	-0.0008	-0.1003
MSE	1.8997	0.0027	0.0004	27.8267
R2	0.2671	-0.8665	0.3379	0.3738
RER	3.2913	3.0477	3.8298	3.7724
RMSE	1.3783	0.0522	0.0211	5.2751
RPD	1.1681	0.7320	1.2290	1.2637
RPIQ	2.3441	0.8411	2.3290	1.6981
SEP	1.3894	0.0525	0.0213	5.3187

pred

	betaglicosidase	cmcase	fpase	xilanase
BIAS	0.2682	0.0029	0.0019	-1.3114
MSE	1.8245	0.0026	0.0005	23.3250
R2	0.2025	-2.5903	0.0350	0.3009
RER	2.8518	1.9299	3.2201	4.2069
RMSE	1.3508	0.0507	0.0227	4.8296
RPD	1.1198	0.5278	1.0180	1.1960
RPIQ	2.3201	0.5639	1.8263	0.8036
SEP	1.3565	0.0519	0.0232	4.7629

In [510]: #MLR otimizado

```

maior=[-1,-1,-1,-1]
maiorGerado=[0,0,0,0]
for i in range(100):
    result = executaMLR(preproc=10,IC=i)
    resultados=exibeResultados(result)
    r2 = resultados['pred'].loc[resultados['pred'].index=='R2']
    r = []
    for j in range(4):
        r.append(r2.iloc[:,j][0])
        if r[j]>maior[j]:
            maior[j] = r[j]
            maiorGerado[j]=i
    print('\r%d%% completos'%(i+1), end='')
print('\n', 'r2:', maior, '\nsemente: b c f x', maiorGerado)

```

100% completos

r2: [0.8007, 0.2856, 0.7779, 0.8061]
semente: b c f x [60, 84, 60, 58]

```

In [511]: #MLR teste otimizado
          modelo = 'MLR:'
          result = executaMLR(preproc=10,IC=60)
          print('Parâmetros do modelo:',modelo,'\n',result[0])

          resultados=exibeResultados(result)

Parâmetros do modelo: MLR:
MultiOutputRegressor(estimator=LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
normalize=False),
n_jobs=None)

In [ ]:

In [512]: resultados['cal']

Out[512]:
          betaglicosidase      cmcase      fpase      xilanase
BIAS      -0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
MSE        0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
R2          1.000000e+00  1.000000e+00  1.000000e+00  1.000000e+00
RER        3.393416e+13  2.812467e+13  3.794781e+13  4.552278e+13
RMSE        0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
RPD         9.934017e+12  5.236136e+12  1.192271e+13  7.192764e+12
RPIQ        2.024224e+13  4.882883e+12  1.964092e+13  7.031981e+12
SEP         0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00

In [513]: resultados['val']

Out[513]:
          betaglicosidase  cmcase  fpase  xilanase
BIAS           0.0128 -0.0002 -0.0005  -0.1889
MSE            0.9650  0.0021  0.0004   10.5681
R2             0.6010 -0.6036  0.4440    0.7205
RER            4.6166  3.4236  4.2674    6.1307
RMSE           0.9823  0.0464  0.0189    3.2509
RPD            1.5831  0.7897  1.3412    1.8914
RPIQ           3.2258  0.7364  2.2094    1.8492
SEP            0.9905  0.0468  0.0191    3.2728

In [514]: resultados['pred']

Out[514]:
          betaglicosidase  cmcase  fpase  xilanase
BIAS          -0.0148 -0.0033  0.0012    0.7844
MSE            0.5523  0.0012  0.0001   19.1697
R2             0.8007 -0.3268  0.7779    0.5015
RER            5.0810  2.8679  5.4943    4.1585
RMSE           0.7432  0.0342  0.0112    4.3783
RPD            2.2401  0.8682  2.1218    1.4163
RPIQ           4.5667  1.1446  4.2755    2.5612
SEP            0.7614  0.0349  0.0114    4.4138

In [515]: reg, treino_teste,y_c,y_cv,y_p = result

```

7.11.2 Reais x preditos

In []:

```
In [516]: #pls reaisxpreditos
#calibração
pred=pd.DataFrame(y_c, columns=var_ae)
reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('CALIBRAÇÃO:\n')
round(reais_pred,4)
```

CALIBRAÇÃO:

```
Out [516]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	0.0308	0.0213	0.0113	0.0996	0.0308
1	0.4280	0.0390	0.0334	13.7624	0.4280
2	2.9774	0.0704	0.0567	10.8002	2.9774
3	3.8876	0.0418	0.0605	11.0267	3.8876
4	3.2342	0.0672	0.0543	8.4772	3.2342
5	0.4280	0.0390	0.0334	13.7624	0.4280
6	0.5905	0.0465	0.0267	18.7095	0.5905
7	2.1643	0.0830	0.0529	18.8324	2.1643
8	2.9123	0.1058	0.0747	14.6813	2.9123
9	0.0759	0.0136	0.0139	0.0726	0.0759
10	3.5967	0.1065	0.0850	13.6476	3.5967
11	3.8803	0.0557	0.0691	11.3256	3.8803
12	0.4280	0.0390	0.0334	13.7624	0.4280
13	3.5967	0.1065	0.0850	13.6476	3.5967
14	0.0554	0.0181	0.0106	0.3275	0.0554
15	0.3828	0.0405	0.0301	12.4461	0.3828
16	2.9774	0.0704	0.0567	10.8002	2.9774
17	0.1724	0.0112	0.0121	0.0924	0.1724
18	3.2342	0.0672	0.0543	8.4772	3.2342
19	0.3828	0.0405	0.0301	12.4461	0.3828
20	0.0554	0.0181	0.0106	0.3275	0.0554
21	0.6010	0.0559	0.0116	20.1368	0.6010
22	0.0759	0.0136	0.0139	0.0726	0.0759
23	3.7243	0.0561	0.0681	11.5736	3.7243
24	4.6037	0.1713	0.0919	16.8115	4.6037
25	0.0874	0.0217	0.0127	0.1071	0.0874
26	3.5974	0.0516	0.0731	15.3973	3.5974
27	0.6491	0.0605	0.0260	18.4274	0.6491
28	2.9123	0.1058	0.0747	14.6813	2.9123

29	2.1643	0.0830	0.0529	18.8324	2.1643
30	0.6491	0.0605	0.0260	18.4274	0.6491
31	0.3900	0.0315	0.0283	14.1777	0.3900
32	3.5610	0.0586	0.0561	10.0978	3.5610
33	0.6010	0.0559	0.0116	20.1368	0.6010
34	2.7110	0.0548	0.0688	13.5829	2.7110
35	4.6037	0.1713	0.0919	16.8115	4.6037
36	3.1068	0.0781	0.0545	11.0526	3.1068
37	3.5967	0.1065	0.0850	13.6476	3.5967
38	0.3900	0.0315	0.0283	14.1777	0.3900
39	2.1150	0.0730	0.0505	18.4127	2.1150
40	3.5974	0.0516	0.0731	15.3973	3.5974
41	4.6037	0.1713	0.0919	16.8115	4.6037
42	2.1150	0.0730	0.0505	18.4127	2.1150
43	3.1068	0.0781	0.0545	11.0526	3.1068
44	0.6010	0.0559	0.0116	20.1368	0.6010
45	2.9123	0.1058	0.0747	14.6813	2.9123
46	3.8876	0.0418	0.0605	11.0267	3.8876
47	3.8994	0.1118	0.0613	10.9512	3.8994
48	3.7243	0.0561	0.0681	11.5736	3.7243
49	2.1150	0.0730	0.0505	18.4127	2.1150
50	2.1643	0.0830	0.0529	18.8324	2.1643
51	0.5905	0.0465	0.0267	18.7095	0.5905
52	0.5905	0.0465	0.0267	18.7095	0.5905
53	0.1724	0.0112	0.0121	0.0924	0.1724
54	3.8803	0.0557	0.0691	11.3256	3.8803
55	0.1724	0.0112	0.0121	0.0924	0.1724
56	0.0554	0.0181	0.0106	0.3275	0.0554
57	3.7243	0.0561	0.0681	11.5736	3.7243
58	3.5610	0.0586	0.0561	10.0978	3.5610
59	2.7110	0.0548	0.0688	13.5829	2.7110

	pred: cmcase	pred: fpase	pred: xilanas
0	0.0213	0.0113	0.0996
1	0.0390	0.0334	13.7624
2	0.0704	0.0567	10.8002
3	0.0418	0.0605	11.0267
4	0.0672	0.0543	8.4772
5	0.0390	0.0334	13.7624
6	0.0465	0.0267	18.7095
7	0.0830	0.0529	18.8324
8	0.1058	0.0747	14.6813
9	0.0136	0.0139	0.0726
10	0.1065	0.0850	13.6476
11	0.0557	0.0691	11.3256
12	0.0390	0.0334	13.7624
13	0.1065	0.0850	13.6476
14	0.0181	0.0106	0.3275

15	0.0405	0.0301	12.4461
16	0.0704	0.0567	10.8002
17	0.0112	0.0121	0.0924
18	0.0672	0.0543	8.4772
19	0.0405	0.0301	12.4461
20	0.0181	0.0106	0.3275
21	0.0559	0.0116	20.1368
22	0.0136	0.0139	0.0726
23	0.0561	0.0681	11.5736
24	0.1713	0.0919	16.8115
25	0.0217	0.0127	0.1071
26	0.0516	0.0731	15.3973
27	0.0605	0.0260	18.4274
28	0.1058	0.0747	14.6813
29	0.0830	0.0529	18.8324
30	0.0605	0.0260	18.4274
31	0.0315	0.0283	14.1777
32	0.0586	0.0561	10.0978
33	0.0559	0.0116	20.1368
34	0.0548	0.0688	13.5829
35	0.1713	0.0919	16.8115
36	0.0781	0.0545	11.0526
37	0.1065	0.0850	13.6476
38	0.0315	0.0283	14.1777
39	0.0730	0.0505	18.4127
40	0.0516	0.0731	15.3973
41	0.1713	0.0919	16.8115
42	0.0730	0.0505	18.4127
43	0.0781	0.0545	11.0526
44	0.0559	0.0116	20.1368
45	0.1058	0.0747	14.6813
46	0.0418	0.0605	11.0267
47	0.1118	0.0613	10.9512
48	0.0561	0.0681	11.5736
49	0.0730	0.0505	18.4127
50	0.0830	0.0529	18.8324
51	0.0465	0.0267	18.7095
52	0.0465	0.0267	18.7095
53	0.0112	0.0121	0.0924
54	0.0557	0.0691	11.3256
55	0.0112	0.0121	0.0924
56	0.0181	0.0106	0.3275
57	0.0561	0.0681	11.5736
58	0.0586	0.0561	10.0978
59	0.0548	0.0688	13.5829

```
In [517]: #validação
pred=pd.DataFrame(y_cv, columns=var_ae)
```

```

reais = treino_teste[2]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('VALIDAÇÃO CRUZADA:\n')
round(reais_pred,4)

```

VALIDAÇÃO CRUZADA:

```

Out[517]:

```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	0.0308	0.0213	0.0113	0.0996	-1.5392
1	0.4280	0.0390	0.0334	13.7624	0.2104
2	2.9774	0.0704	0.0567	10.8002	2.6949
3	3.8876	0.0418	0.0605	11.0267	4.7097
4	3.2342	0.0672	0.0543	8.4772	3.0431
5	0.4280	0.0390	0.0334	13.7624	0.0316
6	0.5905	0.0465	0.0267	18.7095	0.6350
7	2.1643	0.0830	0.0529	18.8324	2.3328
8	2.9123	0.1058	0.0747	14.6813	4.8602
9	0.0759	0.0136	0.0139	0.0726	1.1080
10	3.5967	0.1065	0.0850	13.6476	3.8294
11	3.8803	0.0557	0.0691	11.3256	3.8496
12	0.4280	0.0390	0.0334	13.7624	-0.3343
13	3.5967	0.1065	0.0850	13.6476	3.3986
14	0.0554	0.0181	0.0106	0.3275	0.6942
15	0.3828	0.0405	0.0301	12.4461	1.3775
16	2.9774	0.0704	0.0567	10.8002	3.4682
17	0.1724	0.0112	0.0121	0.0924	0.7942
18	3.2342	0.0672	0.0543	8.4772	3.1599
19	0.3828	0.0405	0.0301	12.4461	2.4283
20	0.0554	0.0181	0.0106	0.3275	0.7261
21	0.6010	0.0559	0.0116	20.1368	-0.1234
22	0.0759	0.0136	0.0139	0.0726	-0.5575
23	3.7243	0.0561	0.0681	11.5736	4.5961
24	4.6037	0.1713	0.0919	16.8115	3.6170
25	0.0874	0.0217	0.0127	0.1071	0.7436
26	3.5974	0.0516	0.0731	15.3973	2.8426
27	0.6491	0.0605	0.0260	18.4274	1.1814
28	2.9123	0.1058	0.0747	14.6813	0.9617
29	2.1643	0.0830	0.0529	18.8324	2.9507
30	0.6491	0.0605	0.0260	18.4274	0.9715
31	0.3900	0.0315	0.0283	14.1777	0.9101
32	3.5610	0.0586	0.0561	10.0978	5.7842
33	0.6010	0.0559	0.0116	20.1368	-0.7111
34	2.7110	0.0548	0.0688	13.5829	2.7305

35	4.6037	0.1713	0.0919	16.8115	3.0005
36	3.1068	0.0781	0.0545	11.0526	2.6007
37	3.5967	0.1065	0.0850	13.6476	2.7718
38	0.3900	0.0315	0.0283	14.1777	0.8109
39	2.1150	0.0730	0.0505	18.4127	2.1791
40	3.5974	0.0516	0.0731	15.3973	1.8483
41	4.6037	0.1713	0.0919	16.8115	3.3998
42	2.1150	0.0730	0.0505	18.4127	3.0887
43	3.1068	0.0781	0.0545	11.0526	2.9226
44	0.6010	0.0559	0.0116	20.1368	0.9911
45	2.9123	0.1058	0.0747	14.6813	4.2881
46	3.8876	0.0418	0.0605	11.0267	4.0625
47	3.8994	0.1118	0.0613	10.9512	2.1067
48	3.7243	0.0561	0.0681	11.5736	4.0639
49	2.1150	0.0730	0.0505	18.4127	2.8273
50	2.1643	0.0830	0.0529	18.8324	2.4900
51	0.5905	0.0465	0.0267	18.7095	2.1122
52	0.5905	0.0465	0.0267	18.7095	-0.2673
53	0.1724	0.0112	0.0121	0.0924	-1.5336
54	3.8803	0.0557	0.0691	11.3256	3.6609
55	0.1724	0.0112	0.0121	0.0924	-0.0780
56	0.0554	0.0181	0.0106	0.3275	-1.6289
57	3.7243	0.0561	0.0681	11.5736	5.0127
58	3.5610	0.0586	0.0561	10.0978	2.6242
59	2.7110	0.0548	0.0688	13.5829	2.3151

	pred: cmcase	pred: fpase	pred: xylanase
0	-0.0400	-0.0075	2.7169
1	0.0116	0.0306	13.7627
2	0.0646	0.0668	14.9106
3	0.1165	0.0822	14.8748
4	0.0873	0.0682	10.2581
5	-0.0124	0.0101	19.0705
6	0.0861	0.0226	18.4600
7	0.0981	0.0552	20.7258
8	0.1583	0.1183	16.6304
9	0.0152	0.0132	-2.6451
10	0.1201	0.0857	16.1051
11	0.0329	0.0580	10.6738
12	-0.0159	0.0062	10.7902
13	0.1174	0.0857	11.0503
14	0.0460	0.0337	3.4767
15	0.0906	0.0317	14.6239
16	0.0782	0.0426	8.7090
17	-0.0689	-0.0013	-1.6165
18	0.0306	0.0364	9.7421
19	0.1055	0.0581	15.4124
20	0.0108	0.0048	-1.7043

21	0.0074	-0.0021	17.9971
22	0.0894	0.0477	-0.9813
23	0.0944	0.0846	15.0645
24	0.0560	0.0491	14.2364
25	0.0250	0.0306	6.3309
26	0.0404	0.0465	16.1896
27	0.1068	0.0246	19.9189
28	0.0449	0.0527	14.3118
29	0.1553	0.0820	16.8579
30	0.0025	0.0206	20.0996
31	0.0448	0.0362	11.8457
32	0.1165	0.0877	16.0185
33	0.0467	0.0230	14.1990
34	0.0139	0.0532	13.6166
35	0.0714	0.0647	19.2712
36	0.0666	0.0531	5.5784
37	0.0808	0.0727	10.3060
38	0.0328	0.0350	5.7832
39	0.0474	0.0618	22.6312
40	0.0209	0.0675	11.0916
41	0.1104	0.0566	13.2198
42	0.1444	0.0777	17.8680
43	0.1013	0.0722	9.4992
44	0.1165	0.0461	18.5049
45	0.1339	0.0963	17.1222
46	0.0252	0.0610	8.0711
47	0.0419	0.0436	12.6679
48	0.0465	0.0641	10.3048
49	0.1105	0.0613	18.1324
50	0.0828	0.0468	18.4518
51	0.1214	0.0370	28.1990
52	0.0502	0.0123	19.4218
53	-0.0128	-0.0026	-1.4521
54	0.0543	0.0788	10.3867
55	0.0349	0.0179	5.4093
56	0.0019	-0.0094	4.7472
57	0.1503	0.0945	9.3315
58	0.0387	0.0363	8.8053
59	0.0659	0.0689	12.1369

```
In [518]: #predição
pred=pd.DataFrame(y_p, columns=var_ae)
reais = treino_teste[3]
reais=reais.reset_index(drop=True)
reais_pred=reais.copy()
for var in var_ae:
    reais_pred['pred: '+var]=pred.loc[:,var]
print('Predição (validação externa):\n')
```

```
round(reais_pred,4)
```

Predição (validação externa):

```
Out [518]:
```

	betaglicosidase	cmcase	fpase	xilanase	pred: betaglicosidase \
0	0.1671	0.0117	0.0104	0.1117	-0.6753
1	2.9774	0.0704	0.0567	10.8002	3.6595
2	3.5610	0.0586	0.0561	10.0978	4.5673
3	0.1671	0.0117	0.0104	0.1117	0.7090
4	3.2342	0.0672	0.0543	8.4772	2.1132
5	0.0308	0.0213	0.0113	0.0996	-0.3576
6	3.8803	0.0557	0.0691	11.3256	4.2026
7	0.3900	0.0315	0.0283	14.1777	0.6878
8	0.6491	0.0605	0.0260	18.4274	0.9045
9	2.7110	0.0548	0.0688	13.5829	3.9102
10	3.5974	0.0516	0.0731	15.3973	2.7498
11	0.0874	0.0217	0.0127	0.1071	-0.2337
12	3.1068	0.0781	0.0545	11.0526	2.0880
13	3.8876	0.0418	0.0605	11.0267	3.8741
14	3.8994	0.1118	0.0613	10.9512	3.9079
15	0.0308	0.0213	0.0113	0.0996	-0.9366
16	0.0759	0.0136	0.0139	0.0726	0.9339
17	0.1671	0.0117	0.0104	0.1117	0.1183
18	3.8994	0.1118	0.0613	10.9512	3.0880
19	0.0874	0.0217	0.0127	0.1071	1.4245
20	0.3828	0.0405	0.0301	12.4461	0.5657

	pred: cmcase	pred: fpase	pred: xilanase
0	0.0390	0.0084	-3.2716
1	0.1491	0.0544	7.3234
2	0.0342	0.0602	8.2259
3	0.0491	0.0271	-1.1774
4	0.0213	0.0421	12.2540
5	-0.0008	0.0145	0.8137
6	0.0865	0.0863	18.9238
7	0.0313	0.0115	8.1411
8	0.0808	0.0267	22.8094
9	0.0336	0.0737	14.4259
10	0.0636	0.0651	12.2027
11	-0.0083	0.0054	-1.7303
12	0.0595	0.0397	3.9879
13	0.0440	0.0580	9.9002
14	0.1320	0.0718	7.0167
15	-0.0330	-0.0089	1.3154
16	0.0254	0.0139	-8.1283
17	-0.0120	0.0071	2.9564

18	0.1317	0.0731	14.5338
19	0.0921	0.0271	6.2279
20	0.0190	0.0115	6.3112

In []:

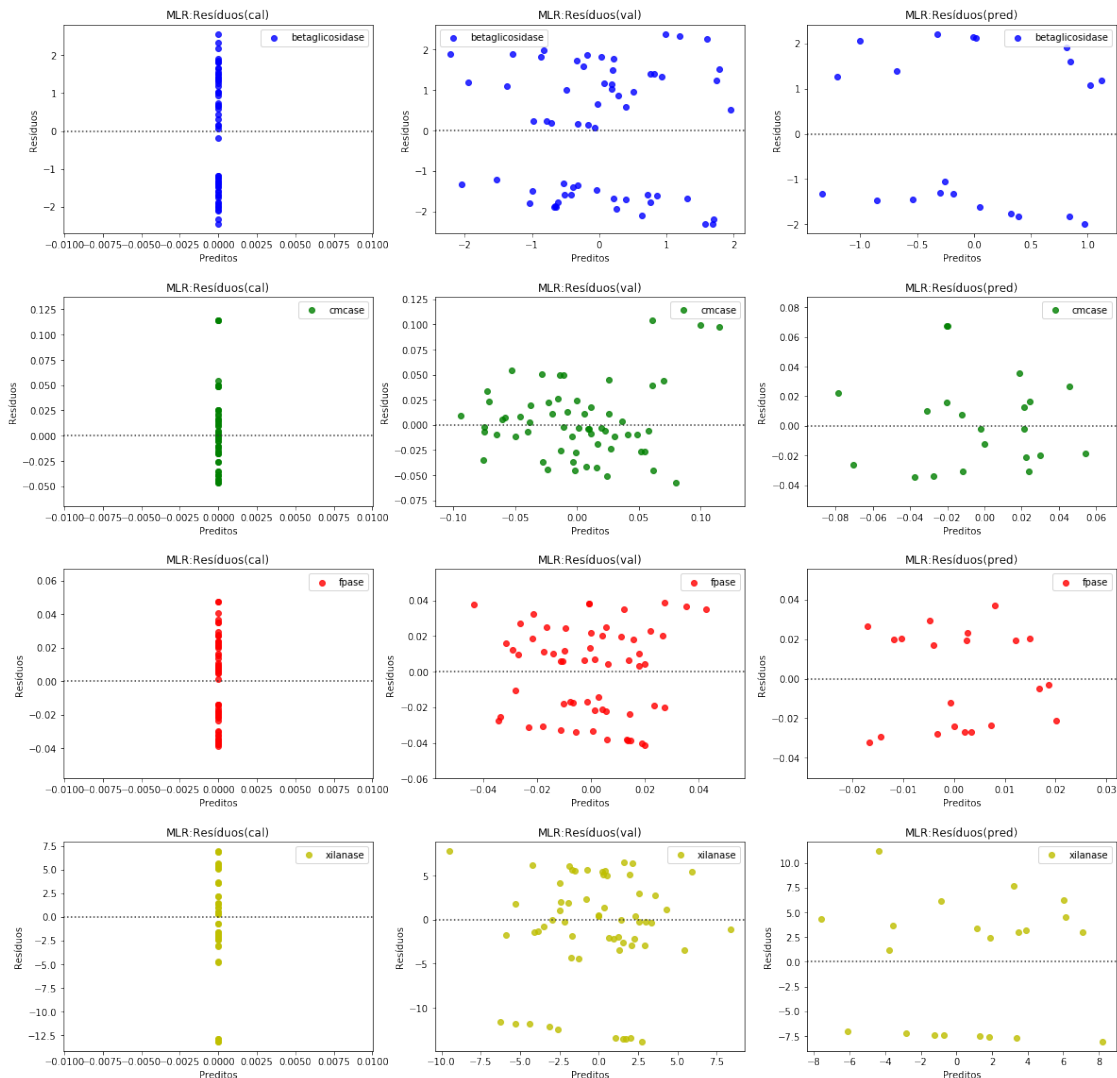
7.11.3 MLR: Gráficos de resíduos - histograma - reais x preditos

In [519]: *#título para os gráficos*

modelo = 'MLR'

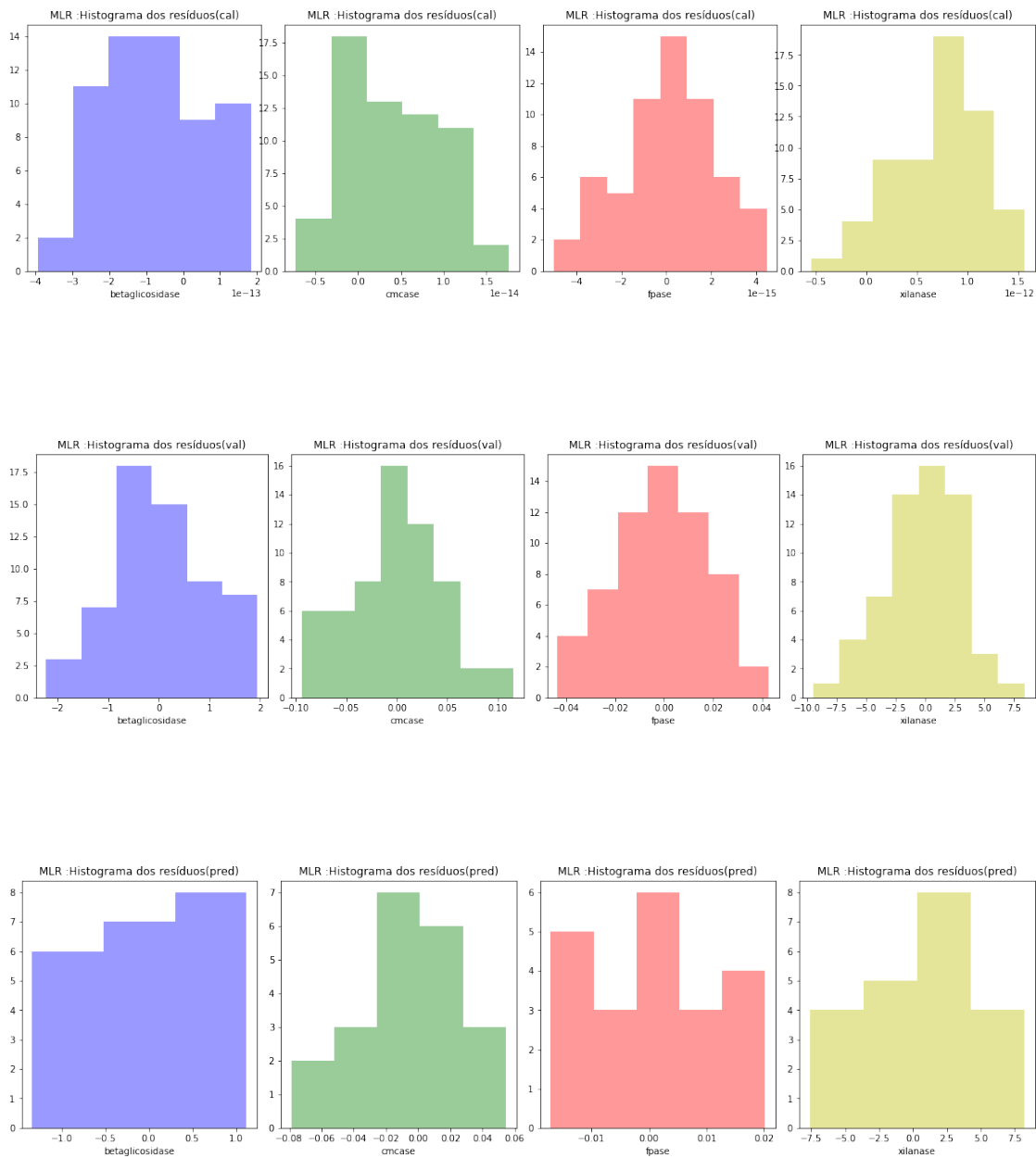
In [520]: *#gráfico dos resíduos*

graficoResiduos(modelo, treino_teste, y_c,y_cv,y_p)

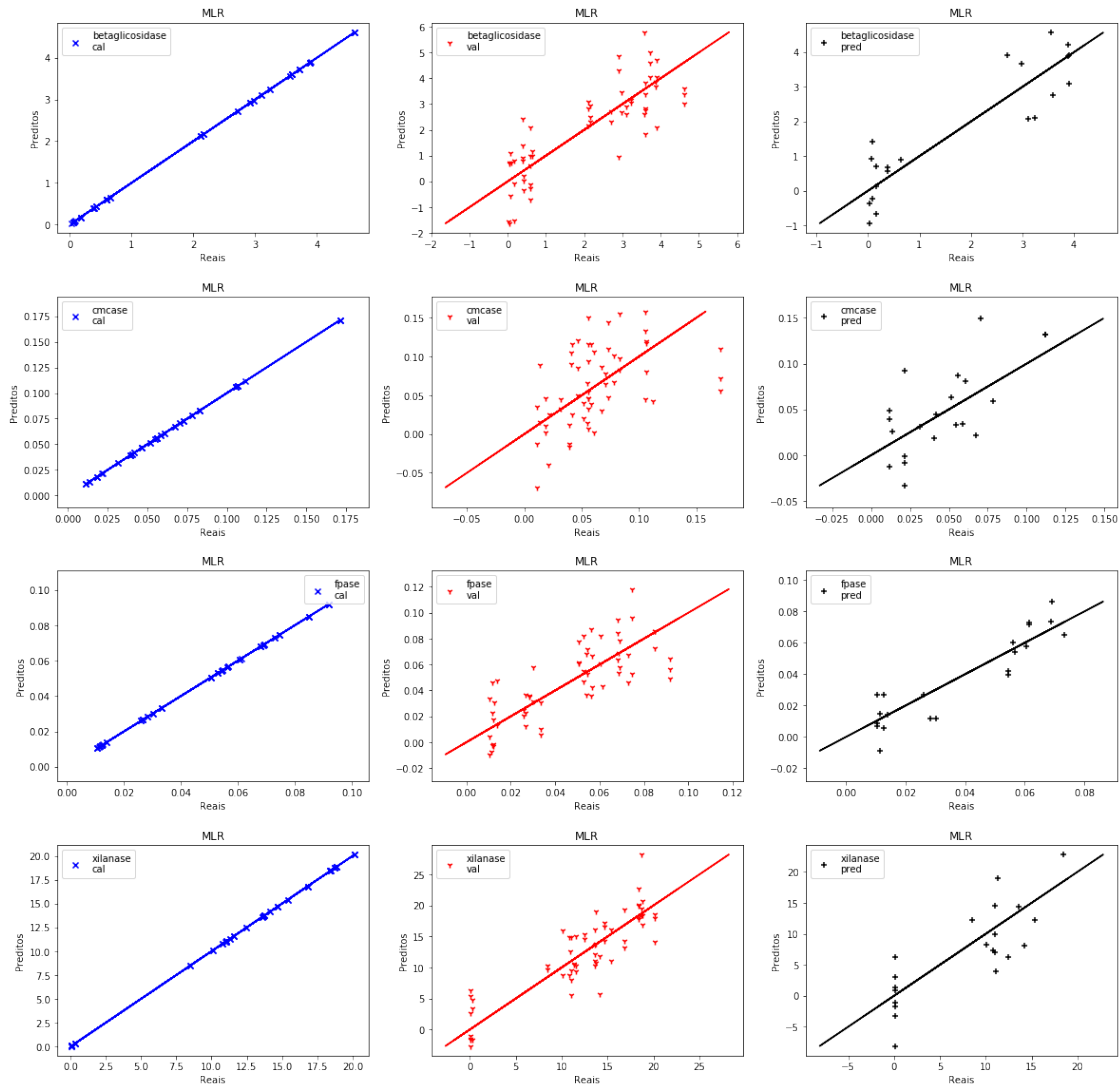


In [521]: *#histograma dos resíduos*

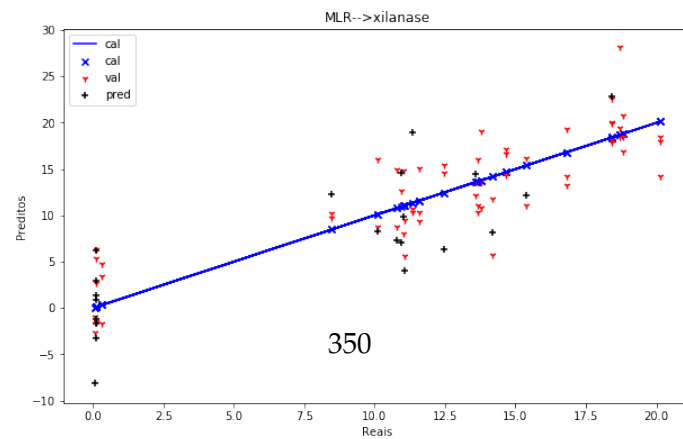
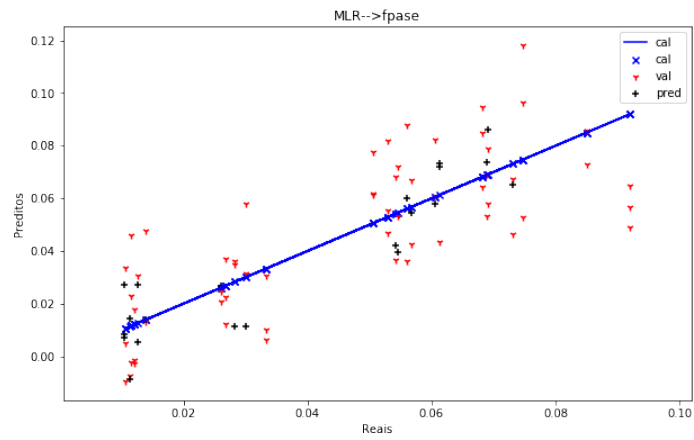
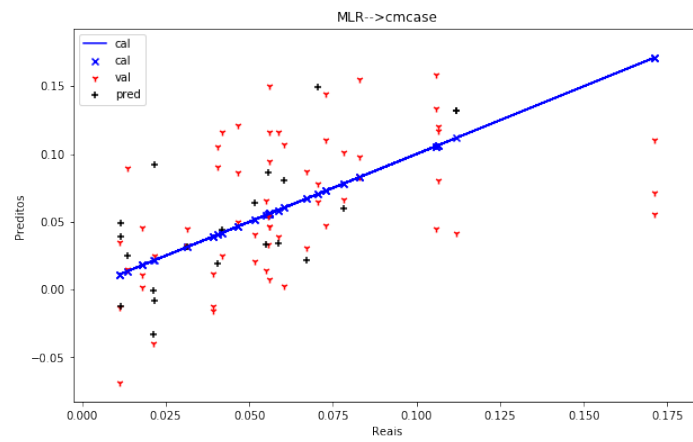
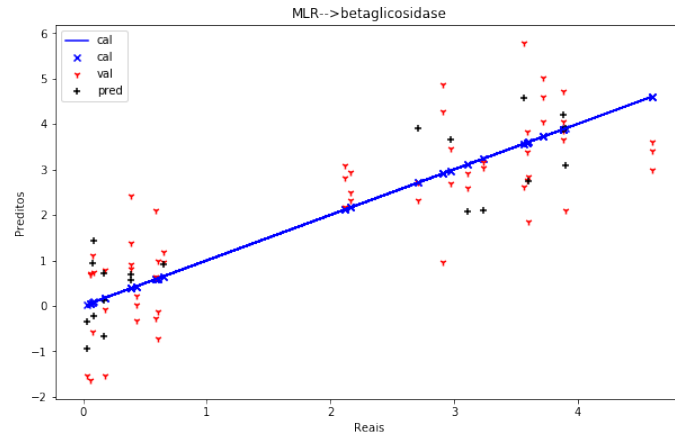
graficoHist(modelo, treino_teste, y_c,y_cv,y_p)



In [522]: *#graico de reais x preditos*
 graficoReaisPreditosSep(modelo, treino_teste, y_c,y_cv,y_p)

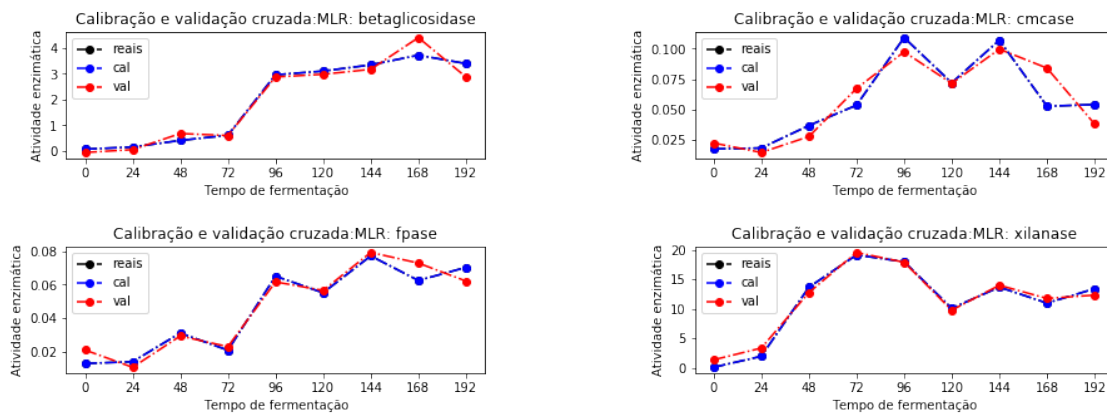


In [523]: *#gráfico de reais x preditos conjuntamente*
`graficoReaisPreditos(modelo, treino_teste, y_c,y_cv,y_p)`



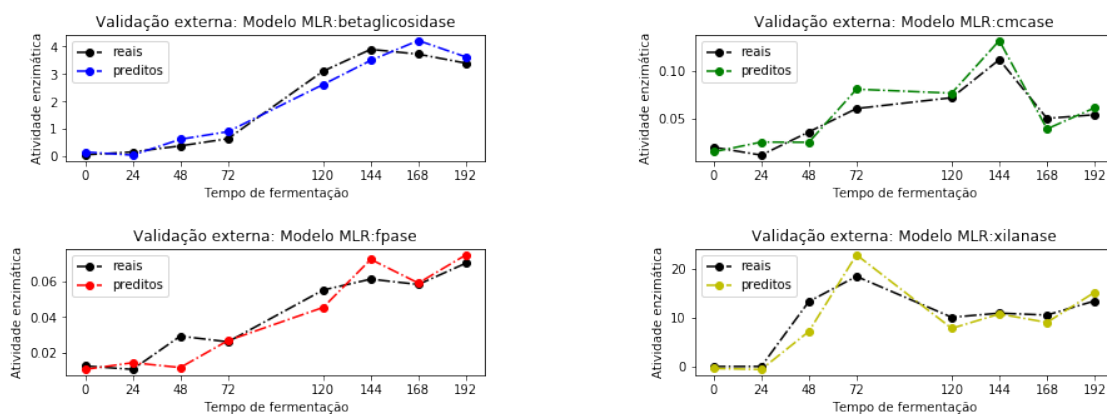
7.11.4 MLR: Gráficos: dados de treino

```
In [524]: y_treino = treino_teste[2]
          graficoTreinamento(modelo, y_treino, y_c,y_cv)
```



7.11.5 MLR: Gráficos de teste

```
In [525]: y_teste = treino_teste[3]
          graficoTeste(modelo, y_teste, y_p)
```



In []:

8 CONFIGURAÇÕES GERAIS:

In [725]: `#@config`

```
#Formatação de fonte nos gráficos
plt.rc('font', size=SMALL_SIZE)           # controls default text sizes
plt.rc('axes', titlesize=SMALL_SIZE)       # fontsize of the axes title
plt.rc('axes', labelsiz=SMALL_SIZE)        # fontsize of the x and y labels
plt.rc('xtick', labelsiz=SMALL_SIZE)       # fontsize of the tick labels
plt.rc('ytick', labelsiz=SMALL_SIZE)       # fontsize of the tick labels
plt.rc('legend', fontsize=SMALL_SIZE)      # legend fontsize
plt.rc('figure', titlesize=BIGGER_SIZE)    # fontsize of the figure title
fig.tight_layout() #melhorando a visualização dos gráficos sobrepostos mas muda a f
plt.subplots_adjust(hspace = .5)#ajusta altura entre um gráfico e outro
```

9 Referências

.....incluir ref ##### Referência para cálculo das medidas: RMSE, RPD e RPIQ - Prediction of Soil-Available Potassium Content with Visible Near-Infrared Ray Spectroscopy of Different Pre-treatment Transformations by the Boosting Algorithms

Referência para cálculo de todas as medidas estatísticas : RMSEP, precisão, bias

- ESTADO DA ARTE DE FIGURAS DE MÉRITO EM CALIBRAÇÃO MULTIVARIADA (Quim. Nova, Vol. 32, No. 5, 1278-1287, 2009)

RMSEP, SEP, bias, RPD:

- ANÁLISE MULTIVARIADA DE IMAGENS NA QUÍMICA: UM EXPERIMENTO PARA DETERMINAÇÃO DO pH DE ÁGUAS POTÁVEIS