ANEXO – PROJETO QUIMIOMETRIA COM PYTHON

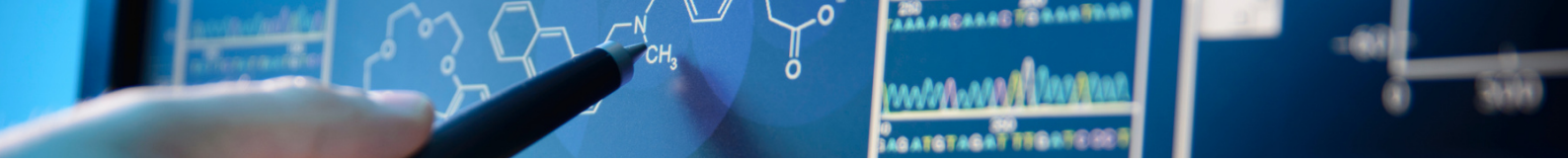
Este arquivo tem por objetivo possibilitar a comparação dos resultados obtidos nos softwares OriginLab e PLS toolbox Solo com aqueles obtidos no projeto com Python.

Software utilizado:

OriginPro 2021b (trial)

Solo 8.9 Demo

Autora: Caroline S. de Oliveira



OriginPro 2021b (trial)

ONEWAY ANOVA

TABELA DE RESULTADO

ANOVAOneWay (12/08/2021 14:49:35)

Notes

Input Data

Descriptive Statistics

	N Analysis	N Missing	Mean	Standard Deviation	SE of Mean
Caju A	10	0	38,9	2,62805	0,83106
Caju B	10	0	41,64	5,49832	1,73872
Caju C	10	0	75,05	6,11451	1,93358
Caju D	10	0	101,39	3,54634	1,12145
Caju E	10	0	65,44	43,87184	13,87349

Análise descritiva dos dados

ANOVA

Overall ANOVA

	DF	Sum of Squares	Mean Square	F Value	Prob>F
Model	4	26509,9652	6627,4913	16,47122	2,2135E-8
Error	45	18106,562	402,36804		
Total	49	44616,5272			

Null Hypothesis: The means of all levels are equal.
Alternative Hypothesis: The means of one or more levels are different.
At the 0.05 level, the population means are significantly different.

Resultado ANOVA

Fit Statistics

R-Square	Coeff Var	Root MSE	Data Mean
0,59417	0,31107	20,05911	64,484

Means Comparisons

Tukey Test

	MeanDiff	SEM	q Value	Prob	Alpha	Sig	LCL	UCL
Caju B Caju A	2,74	8,97071	0,43196	0,99804	0,05	0	-22,74982	28,22982
Caju C Caju A	36,15	8,97071	5,69897	0,0019	0,05	1	10,66018	61,63982
Caju C Caju B	33,41	8,97071	5,26702	0,00471	0,05	1	7,92018	58,89982
Caju D Caju A	62,49	8,97071	9,85142	1,04408E-7	0,05	1	37,00018	87,97982
Caju D Caju B	59,75	8,97071	9,41946	3,13044E-7	0,05	1	34,26018	85,23982
Caju D Caju C	26,34	8,97071	4,15245	0,03969	0,05	1	0,85018	51,82982
Caju E Caju A	26,54	8,97071	4,18398	0,03756	0,05	1	1,05018	52,02982
Caju E Caju B	23,8	8,97071	3,75202	0,07761	0,05	0	-1,68982	49,28982
Caju E Caju C	-9,61	8,97071	1,515	0,82015	0,05	0	-35,09982	15,87982
Caju E Caju D	-35,95	8,97071	5,66744	0,00203	0,05	1	-61,43982	-10,46018

Teste Tukey - comparação de médias

Grouping Letters Table

Sig equals 1 indicates that the difference of the means is significant at the 0,05 level.
Sig equals 0 indicates that the difference of the means is not significant at the 0,05 level.

Grouping Letters Table

Tukey Test

	Mean	Groups			
Caju D	101,39	A			
Caju C	75,05		B		
Caju E	65,44		B	C	
Caju B	41,64			C	D
Caju A	38,9				D

Means that do not share a letter are significantly different.

Tabela de agrupamento das amostras por letras

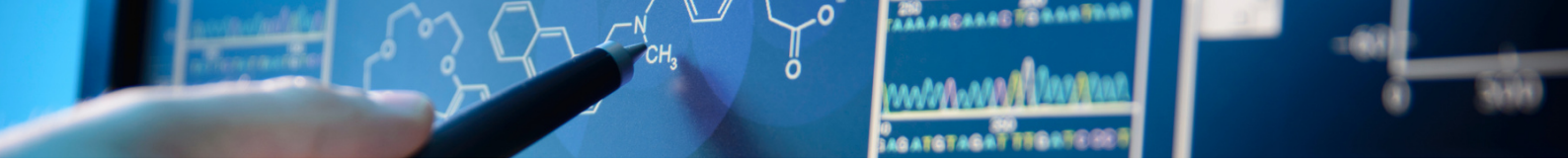
Homogeneity of Variance Test

Levene's Test(Absolute Deviations)

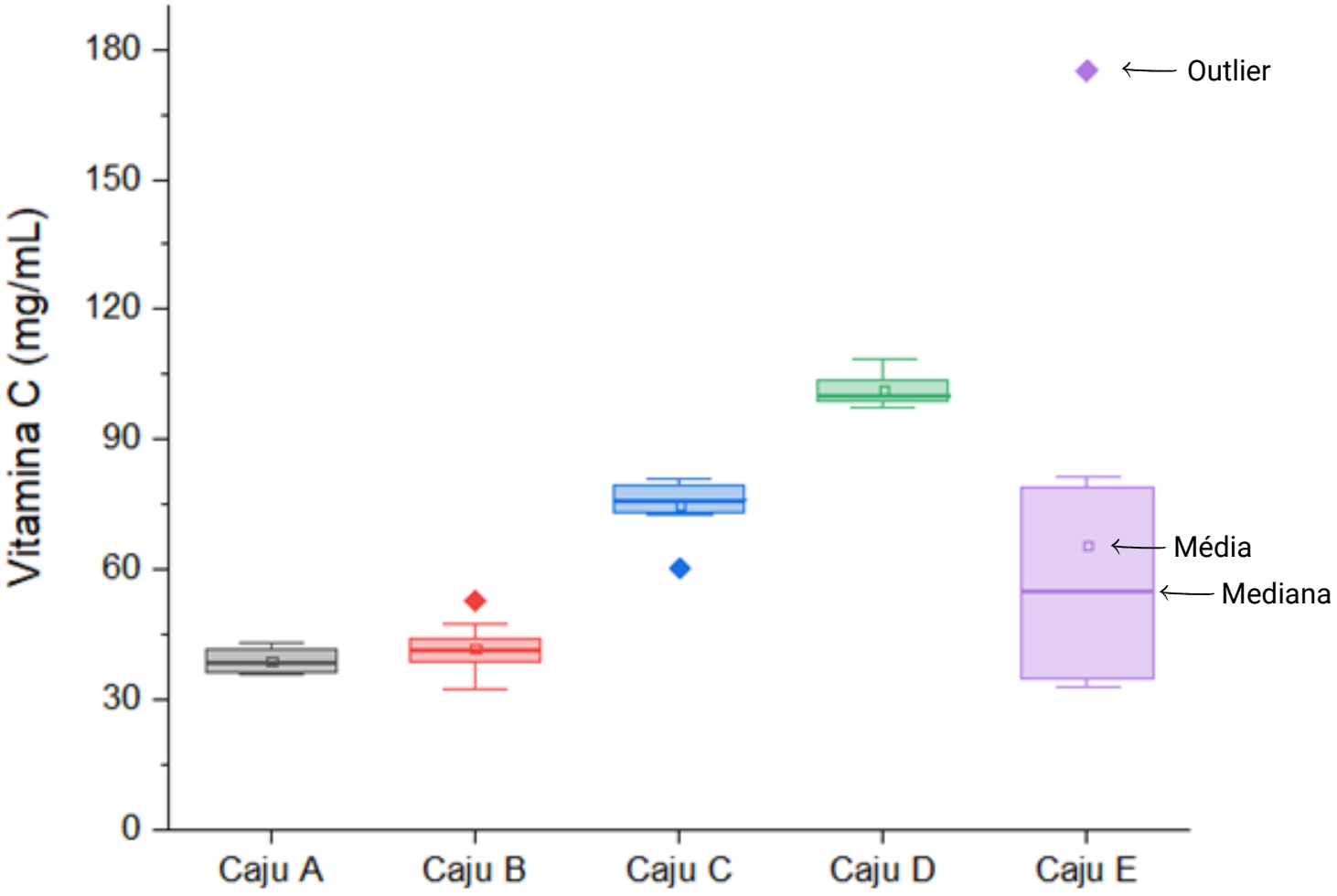
	DF	Sum of Squares	Mean Square	F Value	Prob>F
Model	4	6104,60163	1526,15041	8,42878	3,65426E-5
Error	45	8147,89156	181,06426		

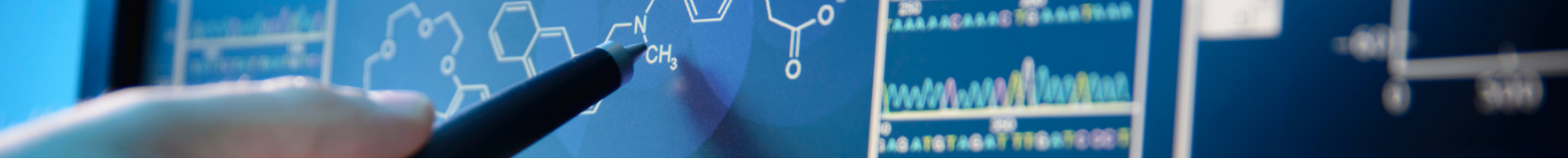
At the 0.05 level, the population variances are significantly different.

Teste levene - avaliação da homogenidade da variância



BOXPLOT - ONEWAY ANOVA





TWOWAY ANOVA

TABELA DE RESULTADO

ANOVATwoWay (12/08/2021 16:00:55)

Notes

Input Data

Descriptive Statistics

Sabor

	N	Mean	SD	SEM	Variance	Missing	NonMissing
Doce	12	2,25833	1,03876	0,29986	1,07902	0	12
Acido	12	6,59167	0,82181	0,23724	0,67538	0	12

Peso

	N	Mean	SD	SEM	Variance	Missing	NonMissing
30g	8	4,275	2,51836	0,89038	6,34214	0	8
50g	8	4,9375	2,11588	0,74808	4,47696	0	8
100g	8	4,0625	2,74899	0,97192	7,55696	0	8

Overall

N	Mean	SD	SEM	Variance	Missing	NonMissing
24	4,425	2,39533	0,48894	5,73761	0	24

Interaction

		N	Mean	SD	SEM	Variance	Missing	NonMissing
Doce	30g	4	2,05	1,06615	0,53307	1,13667	0	4
	50g	4	3,175	0,79739	0,3987	0,63583	0	4
	100g	4	1,55	0,58023	0,29011	0,33667	0	4
Acido	30g	4	6,5	0,67823	0,33912	0,46	0	4
	50g	4	6,7	1,23558	0,61779	1,52667	0	4
	100g	4	6,575	0,68007	0,34004	0,4625	0	4

Análise descritiva dos dados

Dados de adstringência (variável dependente) classificados pelo **sabor** (Fator A)

Dados de adstringência classificados pelo **peso** (Fator B)

Todos os dados de adstringência

Interações sabor:peso

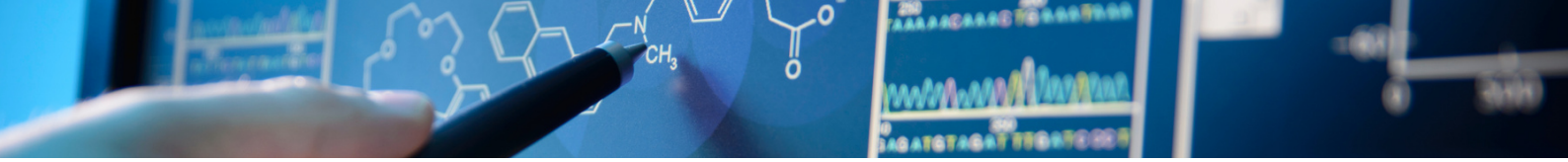


TABELA DE RESULTADO

ANOVATwoWay (12/08/2021 16:00:55)

- Notes
- Input Data
- Descriptive Statistics
- ANOVA
  - Overall ANOVA

	DF	Sum of Squares	Mean Square	F Value	P Value
Sabor	1	112,66667	112,66667	148,29982	3,98085E-10
Peso	2	3,3325	1,66625	2,19324	0,14047
Interaction	2	2,29083	1,14542	1,50768	0,2481
Model	5	118,29	23,658	31,14033	2,93483E-8
Error	18	13,675	0,75972		
Corrected Total	23	131,965			

At the 0.05 level, the population means of **Sabor** are **significantly** different.
At the 0.05 level, the population means of **Peso** are **not significantly** different.
At the 0.05 level, the interaction between **Sabor** and **Peso** is **not significant**.

Resultado ANOVA

  - Means Comparisons
    - Bonferroni Test
      - Sabor

	MeanDiff	SEM	t Value	Prob	Alpha	Sig	LCL	UCL
Acido Doce	4,33333	0,35584	12,17784	3,98085E-10	0,05	1	3,58575	5,08092

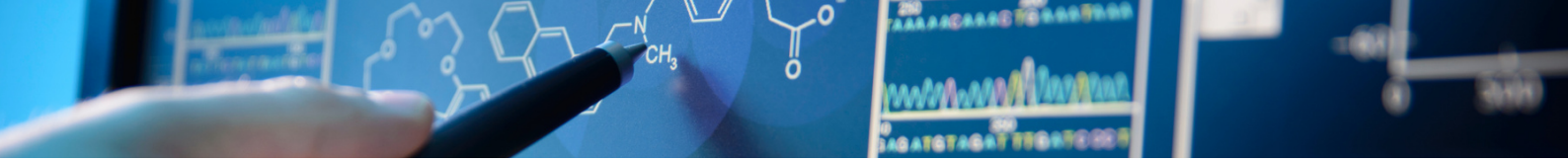
      - Peso

	MeanDiff	SEM	t Value	Prob	Alpha	Sig	LCL	UCL
50g 30g	0,6625	0,43581	1,52016	0,43753	0,05	0	-0,48767	1,81267
100g 30g	-0,2125	0,43581	-0,4876	1	0,05	0	-1,36267	0,93767
100g 50g	-0,875	0,43581	-2,00775	0,17976	0,05	0	-2,02517	0,27517

      - Interactions

Sabor	Peso	Sabor	Peso	MeanDiff	SEM	t Value	Prob	Alpha	Sig	LCL
Doce	50g	Doce	30g	1,125	0,61633	1,82532	1	0,05	0	-0,9584
Doce	100g	Doce	30g	-0,5	0,61633	-0,81126	1	0,05	0	-2,5834
Doce	100g	Doce	50g	-1,625	0,61633	-2,63658	0,25136	0,05	0	-3,7084
Acido	30g	Doce	30g	4,45	0,61633	7,22017	1,53396E-5	0,05	1	2,3665
Acido	30g	Doce	50g	3,325	0,61633	5,39485	5,9733E-4	0,05	1	1,2415
Acido	30g	Doce	100g	4,95	0,61633	8,03143	3,47628E-6	0,05	1	2,8665
Acido	50g	Doce	30g	4,65	0,61633	7,54467	8,38212E-6	0,05	1	2,5665
Acido	50g	Doce	50g	3,525	0,61633	5,71935	3,01869E-4	0,05	1	1,4415
Acido	50g	Doce	100g	5,15	0,61633	8,35593	1,96684E-6	0,05	1	3,0665
Acido	50g	Acido	30g	0,2	0,61633	0,3245	1	0,05	0	-1,8834
Acido	100g	Doce	30g	4,525	0,61633	7,34186	1,22087E-5	0,05	1	2,4415
Acido	100g	Doce	50g	3,4	0,61633	5,51654	4,61773E-4	0,05	1	1,3165
Acido	100g	Doce	100g	5,025	0,61633	8,15312	2,80329E-6	0,05	1	2,9415
Acido	100g	Acido	30g	0,075	0,61633	0,12169	1	0,05	0	-2,0084
Acido	100g	Acido	50g	-0,125	0,61633	-0,20281	1	0,05	0	-2,2084

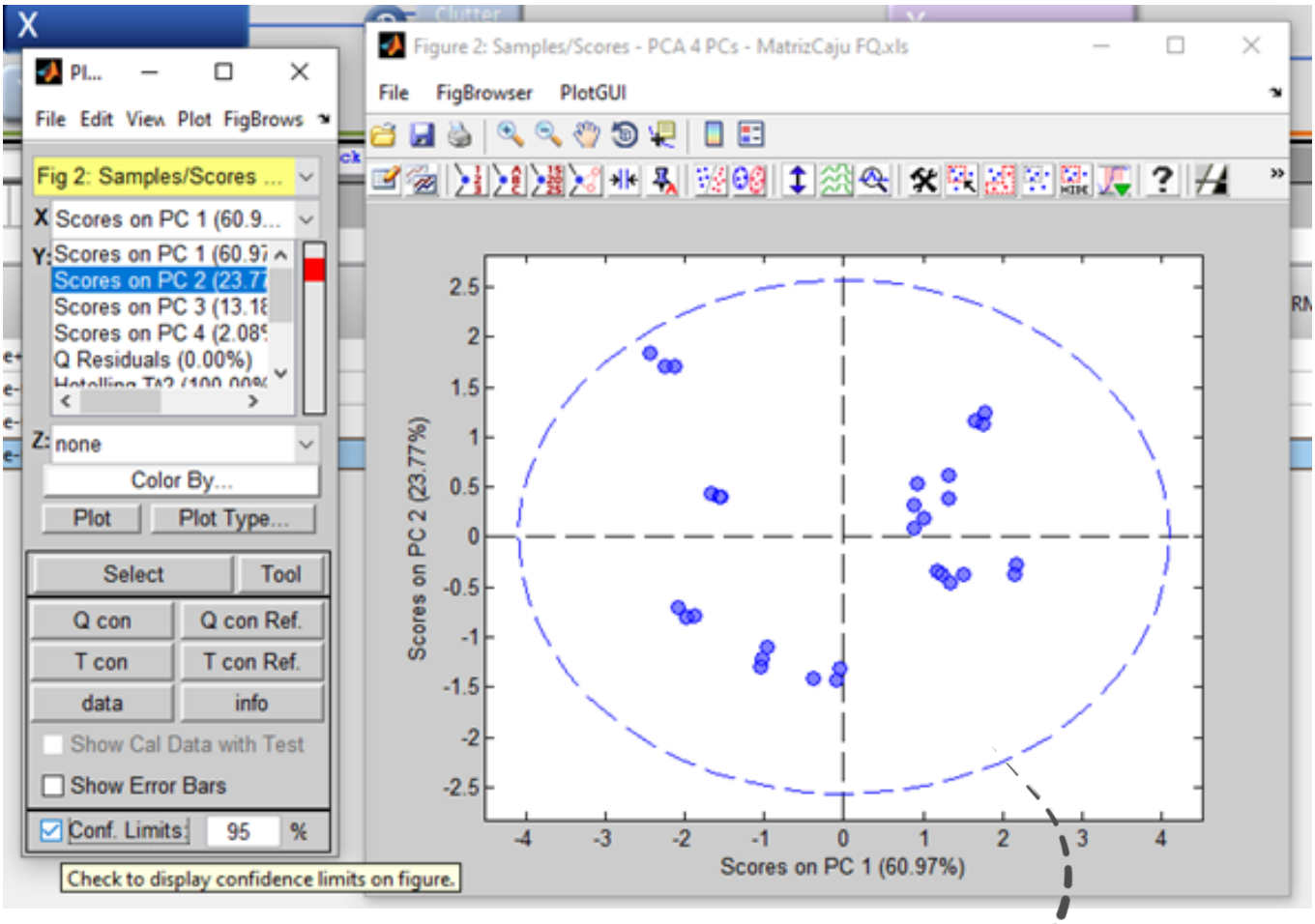
Teste Bonferroni



Solo 8.9 Demo

PCA

Algoritmo: Singular Value Decomposition (svd)
Autoescalado
n° de componentes = 4
Distribuição normal
Limite de confiança – 95%



Linha pontilhada indica o limite de confiança de 95%.

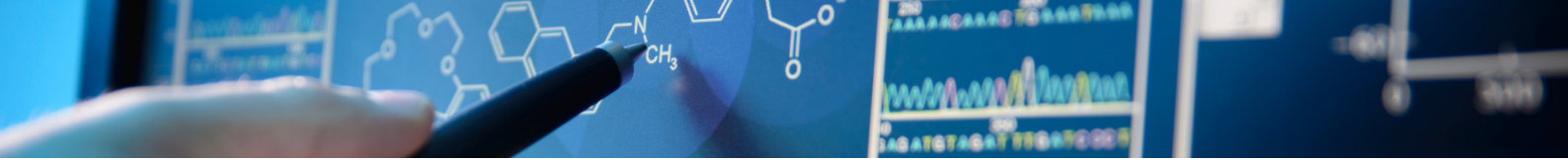


GRÁFICO DE SCORES

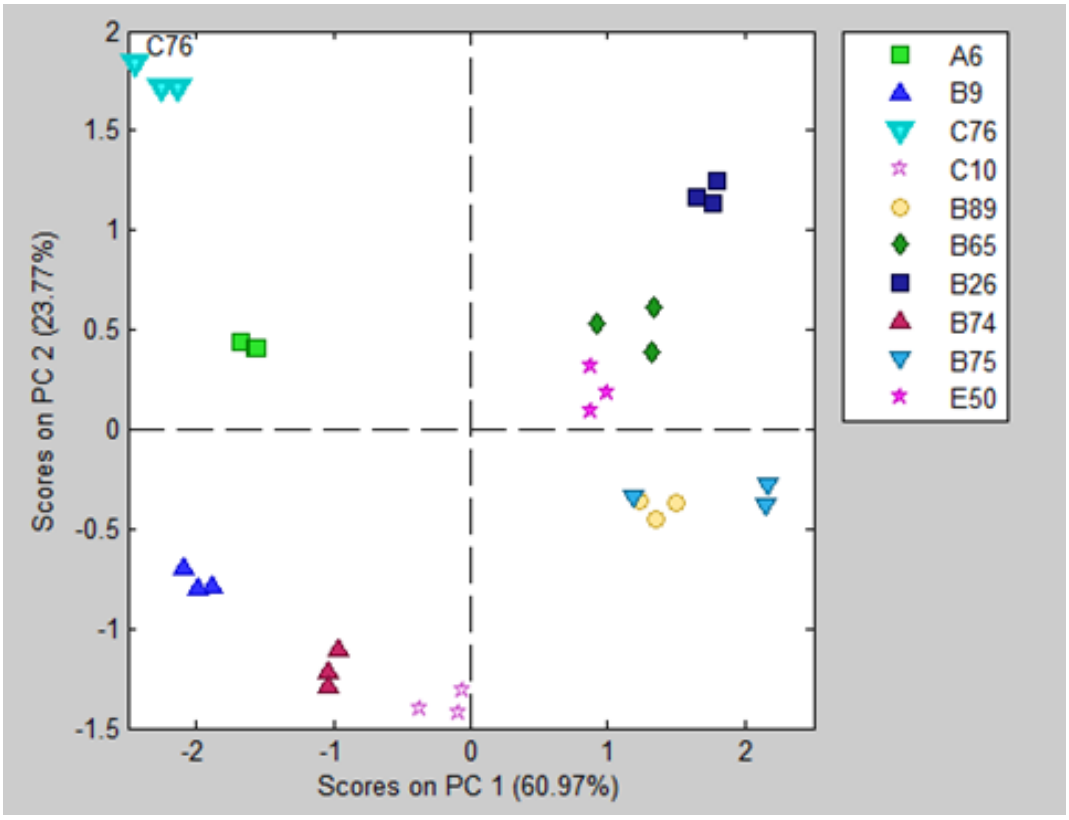


GRÁFICO DE LOADINGS