

Prints (Relatório 1)

simul.summary()
Metabolites: 1877
Reactions: 2712
Genes: 1516

#1

```
Reaction ID Flux rate
  EX_lac__L_e
1 EX_lac__D_e
    Reaction ID Flux rate
      EX_glcn_e
   EX_glc__D_e
EX_glcur_e
                     0.0
  EX_2ddglcn_e
                     0.0
      EX_glcr_e
  EX_glcur1p_e
6 EX_udpglcur_e
                     0.0
   EX_5dglcn_e
EX_2dglc_e
                     0.0
                     0.0
9 EX_metglcur_e
Reaction ID Flux rate
    EX_co2_e 24.003293
             0.000000
   EX h2o2 e
   EX_no2_e 0.000000
    EX so2 e
              0.000000
    EX_o2_e -22.131763
    EX_02s_e 0.000000
```

#2

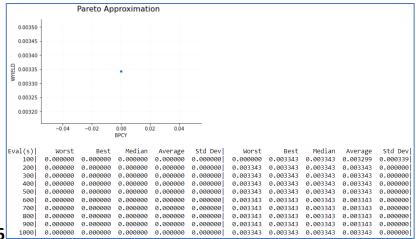
```
print(best_val_1)
print(best_val_d)

[[
[('s0001', 6.86)]
```

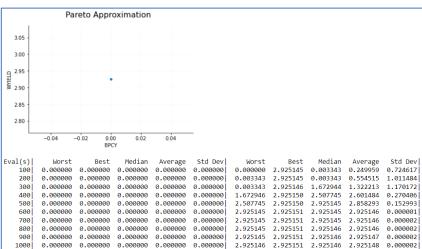
```
from mewpy.problems import GKOProblem
problem = GKOProblem(model, [])
c = problem.solution_to_constraints({"s0001":0})
result = simul.simulate(method="pFBA", constraints = c)
result.fluxes["BIOMASS_Ec_iML1515_core_75p37M"]
#5
```

Biologia de Sistemas – Mestrado em Bioinformática (2021/2022)

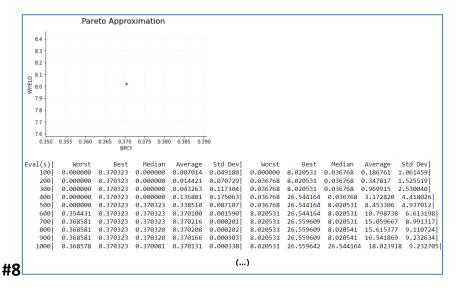




#6



#7





```
Pareto Approximation
            8.8
           8.6
            8.4
         MIEID
8.2
            8.0
           7.8
            7.6
        Eval(s)|
100|
                                                    Median
                                                                              Std Dev
                                                                                                                          Median
                          Worst
                                                                Average
                                                                                                Worst
                                                                                                         8.852624
                      0.000000
                                  0.353217
                                                 0.000000
                                                              0.016041
                                                                            0.055804
                                                                                            0.000000
                                                                                                                       0.036768
                                                                                                                                     0.704723
                                                                                                                                                   2.297196
                                  0.353217
0.353217
                                                              0.028922
0.065408
0.148400
                                                                                                         8.852624
8.852625
                                                                                                                       0.036768
0.036811
                                                                                                                                     1.300447
3.217033
7.335623
             200 İ
                      0.000000
                                                 0.000000
                                                                            0.072240
                                                                                            0.000000
                                                                                                                                                   3.028842
                      0.000000
                                                                            0.095865
0.116805
                                                 0.122535
                      0.000000 0.353217
0.062891 0.353217
                                                                                                          8.852625
                                                                                                                       8.556560
8.705248
                                                 0.122575
                                                                            0.109802
             500
                                                               0.176850
                                                                                            7.534562
                                                                                                         8.852869
                                                                                                                                      8.449404
                                                                                                                                                   0.485533
             600
                      0.062891 0.353217
                                                 0.122857
                                                              0.181994
                                                                            0.109063
                                                                                            7.534562
                                                                                                         8.852869
                                                                                                                       8,705248
                                                                                                                                     8,436937
                                                                                                                                                   0.480260
                      0.062891
0.062891
0.062891
                                  0.353217
0.353217
0.353217
0.361871
                                                0.238508
0.238508
0.240120
                                                              0.202155
0.209483
0.214035
                                                                            0.109936
0.119239
0.117109
                                                                                            7.534562
7.534562
7.534562
                                                                                                         8.852869
8.852869
8.852869
                                                                                                                       8.410497
8.410497
8.411475
                                                                                                                                                   0.494312
0.559772
0.553481
                                                                                                                                     8.363155
8.280302
                                                                                                                                     8.266349
                     0.062891 0.361871 0.122825 0.146048
                                                                            0.080317
                                                                                            7.784488 8.852869
                                                                                                                       8.705249
                                                                                                                                    8.636568
                                                                                                                                                  0.231683
                                                                                      (...)
#9
```

#10 [0.3700803194305872, 26.544171601337318];{'ACKr': 0, 'ACALD': 0}

```
const = {"ACKr":(0,0), "ACALD":(0,0), 'EX_glc_D_e' : (-15.0, 100000.0), 'EX_o2_e' : (0,10000)}
result = simul.simulate(method="pFBA", constraints = const)

print(result.find("EX_lac_D_e"))
print()
print()
print()
print()
print()
print()
print(result.find("BIOMASS_Ec_iML1515_core_75p37M"))
print()
print(simul.FVA(reactions=["BIOMASS_Ec_iML1515_core_75p37M"], constraints = const))

Reaction ID Flux rate
0 EX_lac_D_e 26.668039
{'EX_lac_D_e': [11.570203860940747, 27.230339294122086]}

Reaction ID Flux rate
0 BIOMASS_Ec_iML1515_core_75p37M 0.208159
{'BIOMASS_Ec_iML1515_core_75p37M': [0.18734351937956611, 0.20815946597729315]}
```

Gene Reaction Rule: b2296 or b1849 or b3115 Genes: b3115 (tdcD) b1849 (purT) b2296 (ackA)

Gene Reaction Rule: b0351 or b1241 Genes: b1241 (adhE) b0351 (mhpF)

Trabalho realizado por:

- André Silva (PG)
- Nuno Duarte (PG)
- Roberto Bullitta (PG45474)
- Rute Castro (PG)
- Vânia Miguel (PG45971)