Anexos - Relatório 1

Anexo 1

```
simul.summary()

Metabolites: 1877
Reactions: 2712
Genes: 1516
```

Anexo 2

```
    Reaction ID  Flux rate
0  EX_lac__L_e        0.0
1  EX_lac__D_e        0.0

    Reaction ID  Flux rate
0    EX_glcn_e        0.0
1   EX_glc__D_e      -10.0
2    EX_glcur_e        0.0
3  EX_2ddglcn_e        0.0
4     EX_glcr_e        0.0
5  EX_glcur1p_e        0.0
6  EX_udpglcur_e       0.0
7   EX_5dglcn_e        0.0
8    EX_2dglc_e        0.0
9  EX_metglcur_e       0.0

                        Reaction ID  Flux rate
0  BIOMASS_Ec_iML1515_core_75p37M    0.876997
1    BIOMASS_Ec_iML1515_WT_75p37M    0.000000

   Reaction ID  Flux rate
0    EX_co2_e  24.003293
1    EX_h2o2_e   0.000000
2    EX_no2_e   0.000000
3    EX_so2_e   0.000000
4     EX_o2_e -22.131763
5    EX_o2s_e   0.000000
```

Anexo 3

```python
const = {'EX_glc__D_e'  : (-15.0, 100000.0),
         'EX_o2_e' : (0,10000)}

print(simul.FVA(reactions=["EX_lac__L_e"], constraints = const))
print(simul.FVA(reactions=["EX_lac__D_e"], constraints = const))

{'EX_lac__L_e': [0.0, 1.114181818181784]}
{'EX_lac__D_e': [0.0, 12.255999999999567]}
```

Anexo 4

```python
print(best_val_l)
print(best_val_d)

[]
[('s0001', 6.86)]
```
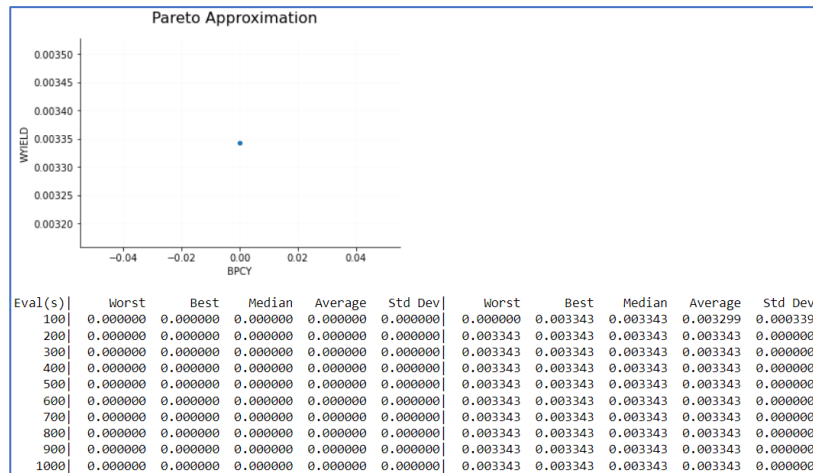
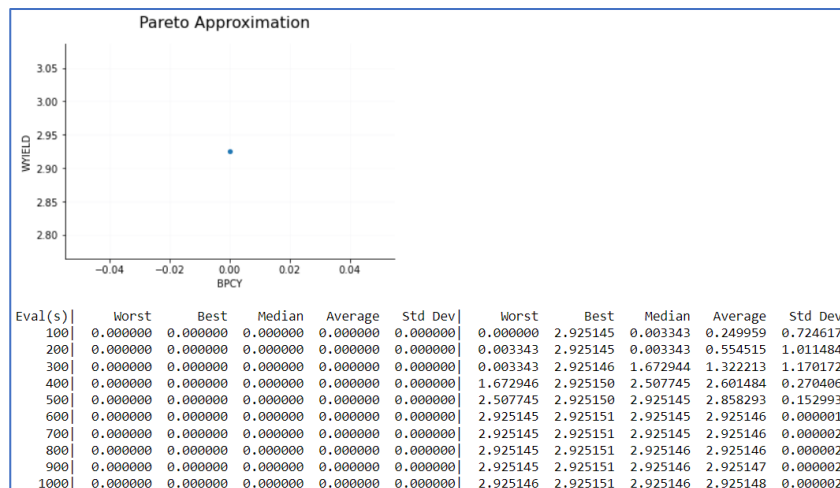## Anexo 5

```python
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"]

0.0
```
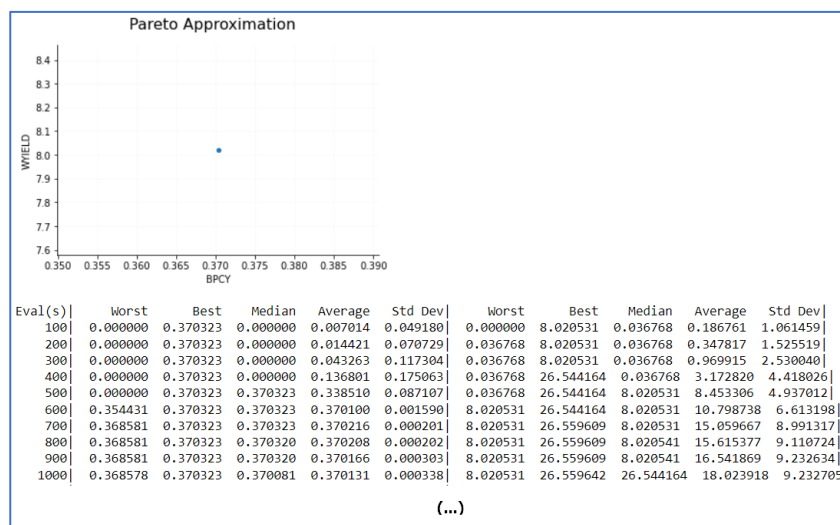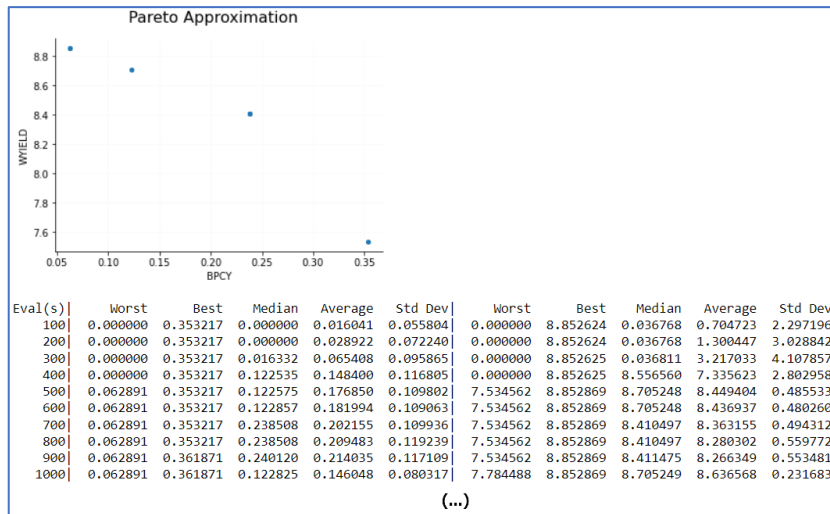
Anexo 6

Pareto Approximation

Eval(s)	Worst	Best	Median	Average	Std Dev	Worst	Best	Median	Average	Std Dev
100	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.003343	0.003343	0.003299	0.000339
200	0.000000	0.000000	0.000000	0.000000	0.000000	0.003343	0.003343	0.003343	0.003343	0.000000
300	0.000000	0.000000	0.000000	0.000000	0.000000	0.003343	0.003343	0.003343	0.003343	0.000000
400	0.000000	0.000000	0.000000	0.000000	0.000000	0.003343	0.003343	0.003343	0.003343	0.000000
500	0.000000	0.000000	0.000000	0.000000	0.000000	0.003343	0.003343	0.003343	0.003343	0.000000
600	0.000000	0.000000	0.000000	0.000000	0.000000	0.003343	0.003343	0.003343	0.003343	0.000000
700	0.000000	0.000000	0.000000	0.000000	0.000000	0.003343	0.003343	0.003343	0.003343	0.000000
800	0.000000	0.000000	0.000000	0.000000	0.000000	0.003343	0.003343	0.003343	0.003343	0.000000
900	0.000000	0.000000	0.000000	0.000000	0.000000	0.003343	0.003343	0.003343	0.003343	0.000000
1000	0.000000	0.000000	0.000000	0.000000	0.000000	0.003343	0.003343	0.003343	0.003343	0.000000

Anexo 7

Pareto Approximation

Eval(s)	Worst	Best	Median	Average	Std Dev	Worst	Best	Median	Average	Std Dev
100	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	2.925145	0.003343	0.249959	0.724617
200	0.000000	0.000000	0.000000	0.000000	0.000000	0.003343	2.925145	0.003343	0.554515	1.011484
300	0.000000	0.000000	0.000000	0.000000	0.000000	0.003343	2.925146	1.672944	1.322213	1.170172
400	0.000000	0.000000	0.000000	0.000000	0.000000	1.672946	2.925150	2.507745	2.601484	0.270406
500	0.000000	0.000000	0.000000	0.000000	0.000000	2.507745	2.925150	2.925145	2.858293	0.152993
600	0.000000	0.000000	0.000000	0.000000	0.000000	2.925145	2.925151	2.925145	2.925146	0.000001
700	0.000000	0.000000	0.000000	0.000000	0.000000	2.925145	2.925151	2.925145	2.925146	0.000002
800	0.000000	0.000000	0.000000	0.000000	0.000000	2.925145	2.925151	2.925146	2.925146	0.000002
900	0.000000	0.000000	0.000000	0.000000	0.000000	2.925145	2.925151	2.925146	2.925147	0.000002
1000	0.000000	0.000000	0.000000	0.000000	0.000000	2.925146	2.925151	2.925146	2.925148	0.000002

Anexo 8

Pareto Approximation

Eval(s)	Worst	Best	Median	Average	Std Dev	Worst	Best	Median	Average	Std Dev
100	0.000000	0.370323	0.000000	0.007014	0.049180	0.000000	8.020531	0.036768	0.186761	1.061459
200	0.000000	0.370323	0.000000	0.014421	0.070729	0.036768	8.020531	0.036768	0.347817	1.525519
300	0.000000	0.370323	0.000000	0.043263	0.117304	0.036768	8.020531	0.036768	0.969915	2.530040
400	0.000000	0.370323	0.000000	0.136801	0.175063	0.036768	26.544164	0.036768	3.172820	4.418026
500	0.000000	0.370323	0.370323	0.338510	0.087107	0.036768	26.544164	8.020531	8.453306	4.937012
600	0.354431	0.370323	0.370323	0.370100	0.001590	8.020531	26.544164	8.020531	10.798738	6.613198
700	0.368581	0.370323	0.370323	0.370216	0.000201	8.020531	26.559609	8.020531	15.059667	8.991317
800	0.368581	0.370323	0.370320	0.370208	0.000202	8.020531	26.559609	8.020541	15.615377	9.110724
900	0.368581	0.370323	0.370320	0.370166	0.000303	8.020531	26.559609	8.020541	16.541869	9.232634
1000	0.368578	0.370323	0.370081	0.370131	0.000338	8.020531	26.559642	26.544164	18.023918	9.232705

(…)

Anexo 9

Eval(s)	Worst	Best	Median	Average	Std Dev	Worst	Best	Median	Average	Std Dev
100	0.000000	0.353217	0.000000	0.016041	0.055804	0.000000	8.852624	0.036768	0.704723	2.297196
200	0.000000	0.353217	0.000000	0.028922	0.072240	0.000000	8.852624	0.036768	1.300447	3.028842
300	0.000000	0.353217	0.016332	0.065408	0.095865	0.000000	8.852625	0.036811	3.217033	4.107857
400	0.000000	0.353217	0.122535	0.148400	0.116805	0.000000	8.852625	8.556560	7.335623	2.802958
500	0.062891	0.353217	0.122575	0.176850	0.109802	7.534562	8.852869	8.705248	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
700	0.062891	0.353217	0.238508	0.202155	0.109936	7.534562	8.852869	8.410497	8.363155	0.494312
800	0.062891	0.353217	0.238508	0.209483	0.119239	7.534562	8.852869	8.410497	8.280302	0.559772
900	0.062891	0.361871	0.240120	0.214035	0.117109	7.534562	8.852869	8.411475	8.266349	0.553481
1000	0.062891	0.361871	0.122825	0.146048	0.080317	7.784488	8.852869	8.705249	8.636568	0.231683

(…)

Anexo 10

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

Anexo 11

```python
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(simul.FVA(reactions=["EX_lac__D_e"], constraints = const))
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]}
```

Anexo 12

```
Gene Reaction Rule:

b2296 or b1849 or b3115

Genes:

b3115 (tdcD)
b1849 (purT)
b2296 (ackA)
```

Anexo 13

```
Gene Reaction Rule:

b0351 or b1241

Genes:

b1241 (adhE)
b0351 (mhpF)
```

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