Relatório - Exercise (part 1) – implementation of FBA problem - Resultados

1. What is the wild-type production of your group's compound?

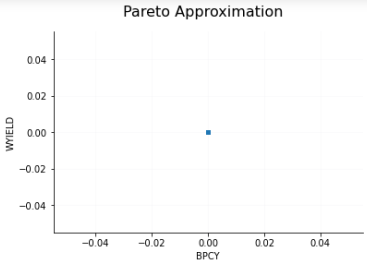
```
A produção de lactato para as condições ambientais de Oxigénio = 0 mmol/gDW/h e Glicose = 15 mmol/gDW/h é: 0.0 mmol/gDW/h.
```

2. What are the maximum compound production capabilities?

```
3  {'R_EX_lac__L_e': [0.0, 1.1141818181817698],
    'R_EX_lac__D_e': [0.0, 12.255999999998616]}
```

3.a. Evaluate if single gene deletions enhance the production of the compound.Rank the mutants obtained according to the compound production capacity and growth performance.

Problema de Otimização de Gene Knockout utilizando MEWpy



Gen	Eval	Worst	Best	Median	Average	Std Dev	Worst	Best	Median	Average	Std Dev
0	100	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
1	200	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
2	300	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
3	400	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
4	500	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
5	600	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
6	700	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
7	800	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
8	900	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
9	1000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
10	1100	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000


```
[[0.0, 0.0];{'G_b3187': 0}, [0.0, 0.0];{'G_b2716': 0}, [0.0, 0.0];{'G_b0754': 0}, [0.0, 0.0];{'G_b0366': 0}, [0.0,
0.0];{'G_b3291': 0}, [0.0, 0.0];{'G_b4485': 0}, [0.0, 0.0];{'G_b3137': 0}, [0.0, 0.0];{'G_b2436': 0}, [0.0, 0.
0];{'G_b2489': 0}, [0.0, 0.0];{'G_b1393': 0}, [0.0, 0.0];{'G_b1492': 0}, [0.0, 0.0];{'G_b0199': 0}, [0.0, 0.0];{'G
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[0.0, 0.0];{'G_b1602': 0}, [0.0, 0.0];{'G_b3266': 0}, [0.0, 0.0];{'G_b3425': 0}, [0.0, 0.0];{'G_b1193': 0}, [0.0,
0.0];{'G_b0417': 0}, [0.0, 0.0];{'G_b3367': 0}, [0.0, 0.0];{'G_b1022': 0}, [0.0, 0.0];{'G_b4090': 0}, [0.0, 0.
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': 0}, [0.0, 0.0];{'G_b3409': 0}, [0.0, 0.0];{'G_b4130': 0}, [0.0, 0.0];{'G_b0154': 0}, [0.0, 0.0];{'G_b1474': 0},
[0.0, 0.0];{'G_b4024': 0}, [0.0, 0.0];{'G_b1394': 0}, [0.0, 0.0];{'G_b1812': 0}, [0.0, 0.0];{'G_b4311': 0}, [0.0,
0.0];{'G_b3713': 0}, [0.0, 0.0];{'G_b1606': 0}, [0.0, 0.0];{'G_b2037': 0}, [0.0, 0.0];{'G_b2418': 0}, [0.0, 0.
0];{'G_b3772': 0}, [0.0, 0.0];{'G_b1329': 0}, [0.0, 0.0];{'G_b3785': 0}, [0.0, 0.0];{'G_b3008': 0}, [0.0, 0.0];{'G
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[0.0, 0.0];{'G_b0590': 0}, [0.0, 0.0];{'G_b4266': 0}, [0.0, 0.0];{'G_b4054': 0}, [0.0, 0.0];{'G_b2320': 0}, [0.0,
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```

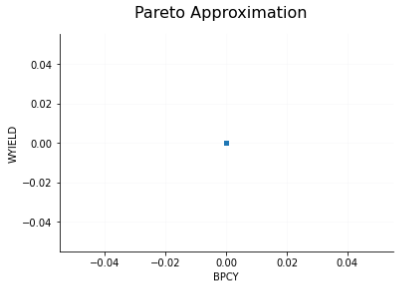
Single Knock Out utilizando utilizando o COBRApy

Primeiros 47 valores de crescimento ordenados	Valores de crescimento diferentes do máximo e viáveis

	ids	growth	status
1482	{b3619}	0.045195	optimal
1463	{b3875}	0.045195	optimal
1459	{b0861}	0.045195	optimal
1457	{b2366}	0.045195	optimal
1456	{b2490}	0.045195	optimal
1455	{b1896}	0.045195	optimal
1454	{b4291}	0.045195	optimal
1453	{b2813}	0.045195	optimal
1465	{b0356}	0.045195	optimal
1483	{b1430}	0.045195	optimal
1484	{b2724}	0.045195	optimal
1466	{b2155}	0.045195	optimal
1467	{b0514}	0.045195	optimal
1468	{b2498}	0.045195	optimal
1469	{b0875}	0.045195	optimal
1470	{b3909}	0.045195	optimal
1461	{b0628}	0.045195	optimal
1471	{b2134}	0.045195	optimal
1472	{b3656}	0.045195	optimal
1473	{b1514}	0.045195	optimal
1475	{b1619}	0.045195	optimal
1476	{b1917}	0.045195	optimal
1477	{b3727}	0.045195	optimal
1478	{b1479}	0.045195	optimal
1479	{b0517}	0.045195	optimal
1480	{b3623}	0.045195	optimal
1493	{b0810}	0.045195	optimal
1495	{b0781}	0.045195	optimal
1496	{b0651}	0.045195	optimal
1497	{b3291}	0.045195	optimal
1498	{b3225}	0.045195	optimal
1494	{b3132}	0.045195	optimal
887	{b0337}	0.045195	optimal
926	{b2224}	0.045195	optimal
908	{b1918}	0.045195	optimal
896	{b1054}	0.045195	optimal
891	{b3032}	0.045195	optimal
892	{b2422}	0.045195	optimal
893	{b2465}	0.045195	optimal
925	{b0655}	0.045195	optimal
894	{b0754}	0.045195	optimal
895	{b0336}	0.045195	optimal
897	{b3073}	0.045195	optimal
906	{b2923}	0.045195	optimal
898	{b1391}	0.045195	optimal
899	{b2255}	0.045195	optimal
901	{b0783}	0.045195	optimal

735	{b3816}	0.044851	optimal
515	{b2529}	0.044612	optimal
1031	{b2528}	0.044612	optimal
843	{b0155}	0.044502	optimal
779	{b2320}	0.044404	optimal
1492	{b1511}	0.044122	optimal
702	{b1517}	0.044122	optimal
961	{b1518}	0.044122	optimal
62	{b0870}	0.044008	optimal
571	{b4384}	0.044004	optimal
1071	{b4383}	0.044004	optimal
1209	{b0474}	0.044004	optimal
1076	{b4208}	0.034107	optimal
721	{b4238}	0.016901	optimal
1440	{b1378}	0.016266	optimal
1283	{b1380}	0.005022	optimal

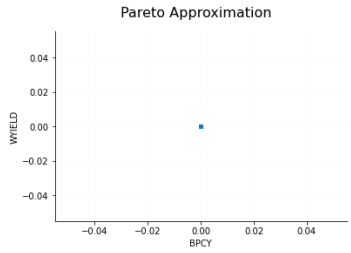
Problema de Otimização de Gene Knockout utilizando MEWpy com Modelo alternativo (IMM904)



Gen	Eval	Worst	Best	Median	Average	Std Dev	Worst	Best	Median	Average	Std Dev
0	100	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
1	200	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
2	300	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
3	400	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
4	500	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
5	600	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
6	700	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
7	800	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
8	900	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
9	1000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
10	1100	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

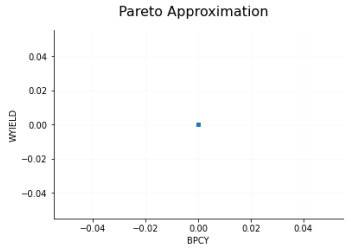
3.b. Determine the best strategy, up to five modifications, to improve the compound production.

Problema de Otimização de Gene Under/Over utilizando MEWpy



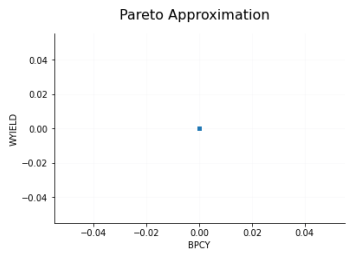

```
Gen    Eval|     Worst      Best    Median   Average   Std Dev|     Worst      Best    Median   Average   Std Dev|
   0     100|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   1     200|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   2     300|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   3     400|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   4     500|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   5     600|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   6     700|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   7     800|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   8     900|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   9    1000|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
  10    1100|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
[0.0, 0.0];{'G_b0774': 0.125, 'G_b1337': 2, 'G_b1250': 0, 'G_b2487': 16, 'G_b2222': 4}
```

Problema de Otimização de Reaction Under/Over utilizando MEWpy




```
Gen    Eval|     Worst      Best    Median   Average   Std Dev|     Worst      Best    Median   Average   Std Dev|
   0     100|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   1     200|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   2     300|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   3     400|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   4     500|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   5     600|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
[0.0, 0.0];{'R_CDAPPA140': 8, 'R_HG2abcpp': 2, 'R_ARBt2rpp': 0.25, 'R_SHKK': 32, 'R_PLIPA1E181pp': 8}
```

Problema de Otimização de Gene Under/Over utilizando MEWpy




```
Gen    Eval|     Worst      Best    Median   Average   Std Dev|     Worst      Best    Median   Average   Std Dev|
   0     100|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   1     200|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   2     300|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   3     400|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   4     500|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
   5     600|  0.000000  0.000000  0.000000  0.000000  0.000000|  0.000000  0.000000  0.000000  0.000000  0.000000|
[0.0, 0.0];{'G_YLR070C': 0.0625, 'G_YDR342C': 16, 'G_YDR403W': 8, 'G_YGR138C': 0.0625}
```