Summary

October 7, 2024

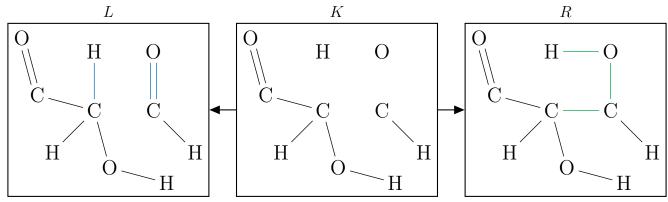
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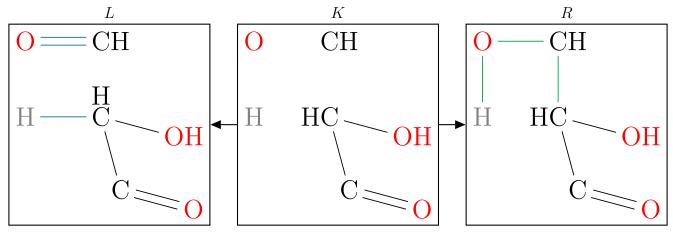
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0.1 Loaded Rules

0.1.1 AL

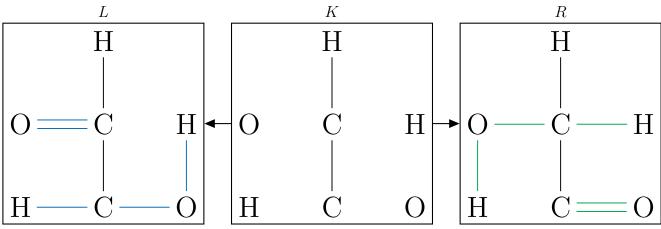


Files: $out/001_r_0_10300000_{L, K, R}$

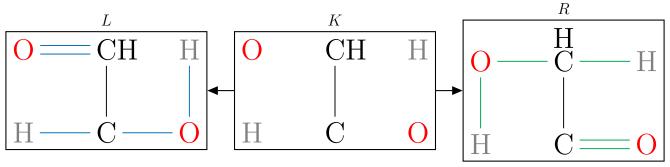


Files: out/003_r_0_11300100_{L, K, R}

0.1.2 AlKe



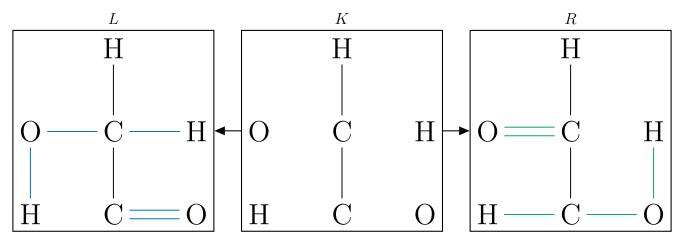
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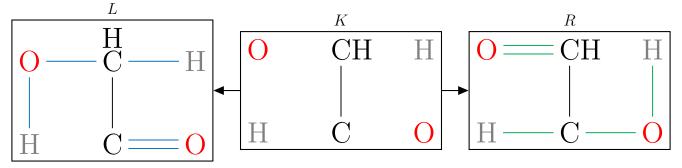
Files: $out/008_r_1_11300100_{L, K, R}$

$$\begin{aligned} |\{e \in \text{outEdges}(1) \mid \\ \text{label}(\text{target}(e)) \in \{\text{`O'}\} \\ \}| &= 1 \end{aligned}$$

0.1.3 KeAl



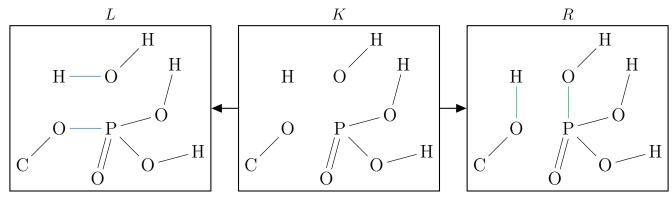
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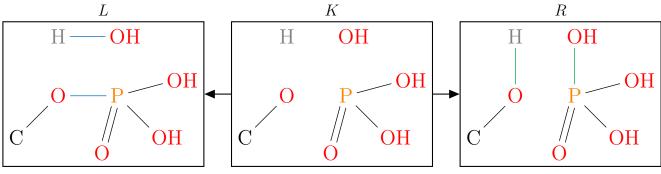
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\begin{aligned} |\{e \in \text{outEdges}(1) \mid \\ \text{label}(\text{target}(e)) \in \{\text{`0'}\} \\ \}| = 1 \end{aligned}
```

0.1.4 PHL

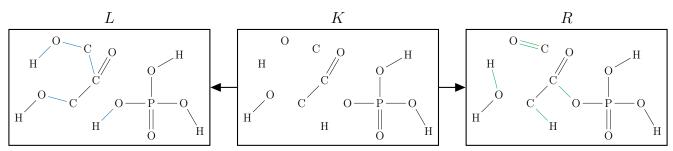


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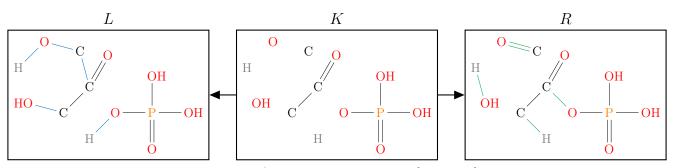


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0.1.5 PKL

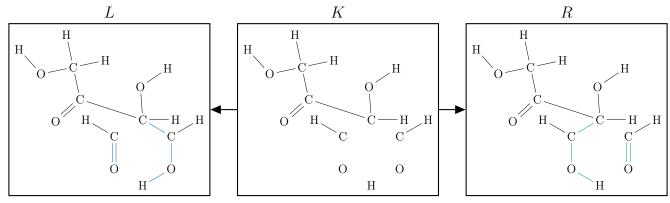


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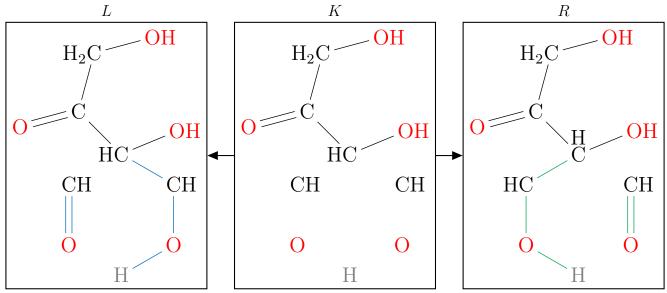


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0.1.6 TAL

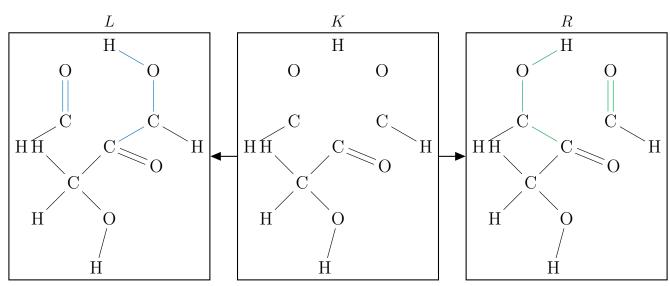


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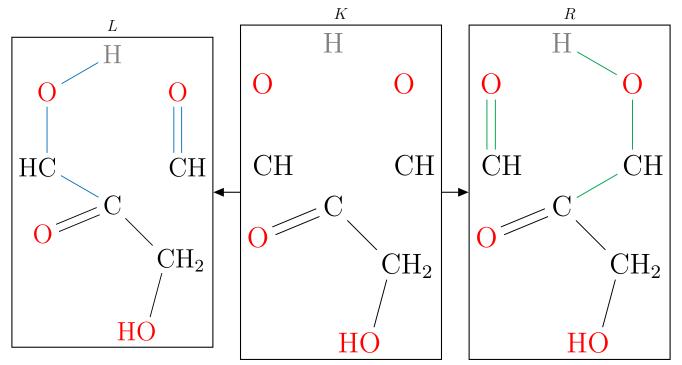


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0.1.7 TKL

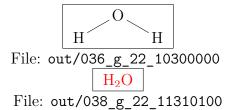


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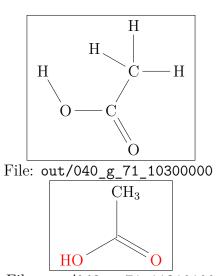


Files: $out/033_r_6_11300100_{L, K, R}$

0.1.8 H_20

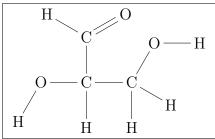


$0.1.9 p_{0,6}$

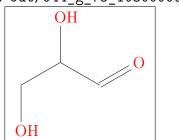


File: out/042_g_71_11310100

$0.1.10 p_{0.7}$

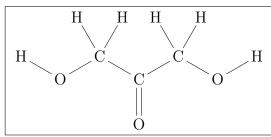


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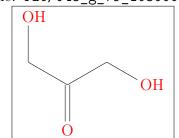


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$0.1.11 p_{0,8}$

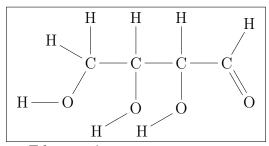


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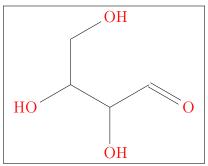


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0.1.12 p_{0,9}

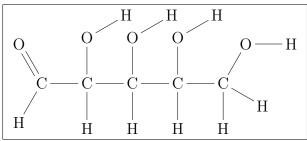


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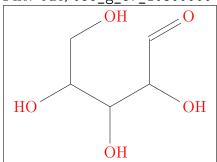


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$0.1.13 p_{0.10}$

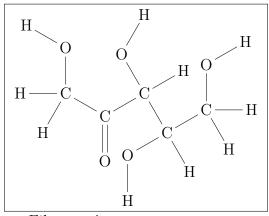


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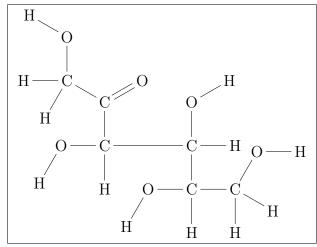
$0.1.14 p_{0,11}$



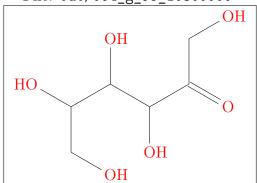
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$0.1.15 p_{0,12}$

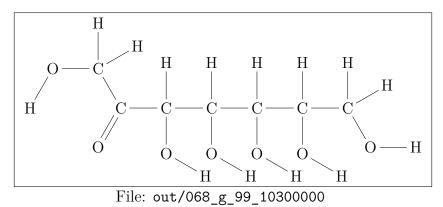


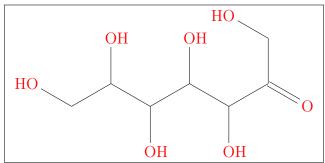
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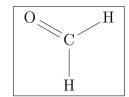
0.1.16 p_{0,13}





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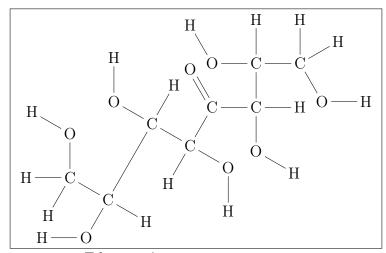
0.1.17 p_{0,17}



File: out/072_g_185_10300000 O === CH₂

File: out/074_g_185_11310100

$0.1.18 p_{0,27}$



File: out/076_g_255_10300000

OH

OH

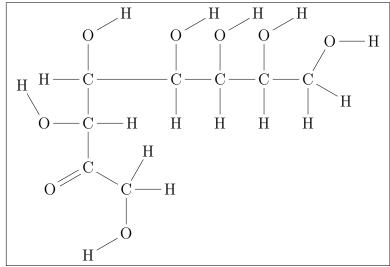
OH

OH

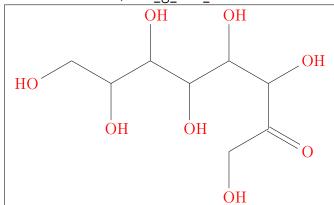
OH

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$0.1.19 p_{0,29}$

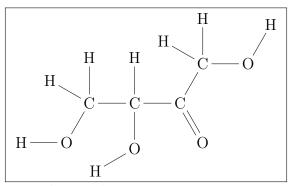


File: out/080_g_272_10300000



File: out/082_g_272_11310100

0.1.20 p_{0,30}



File: out/084_g_274_10300000

OH

OH

OH

File: out/086_g_274_11310100

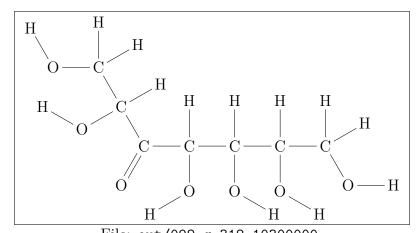
$0.1.21 p_{0,34}$

File: out/088_g_312_10300000

HO
OH
OH

File: out/090_g_312_11310100

0.1.22 p_{0,36}



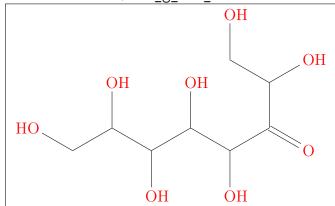
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OH HO
OH
OH
OH
OH

File: out/094_g_318_11310100

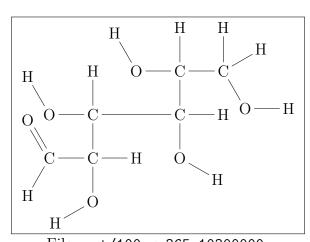
0.1.23 p_{0,37}

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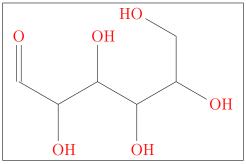


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$0.1.24 p_{0,44}$

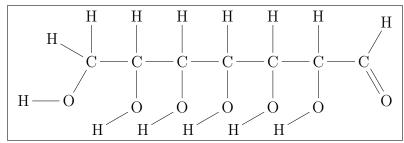


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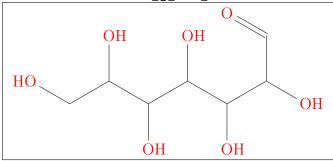


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0.1.25 p_{0,45}

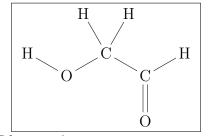


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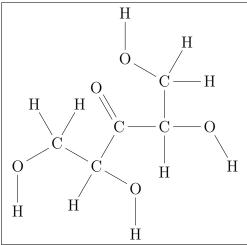
0.1.26 p_{0,47}



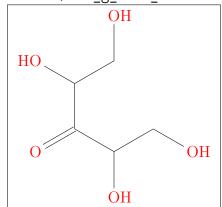
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File: out/110_g_412_11310100

0.1.27 p_{0,56}

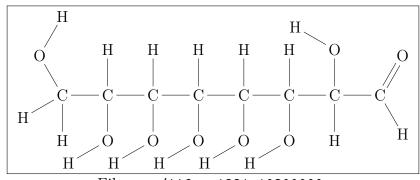


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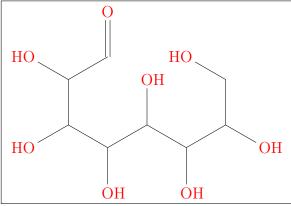


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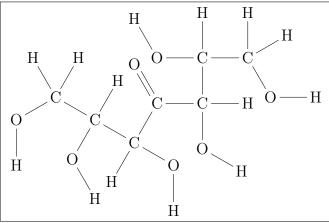
0.1.28 p_{0,57}



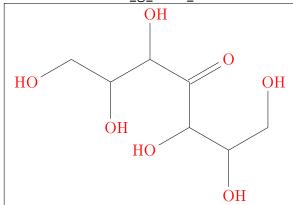
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0.1.29 p_{0,60}

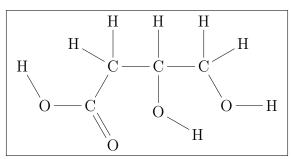


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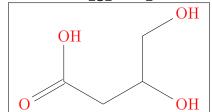


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$0.1.30 p_{0,61}$



File: out/124_g_1429_10300000



File: out/126_g_1429_11310100

$0.1.31 p_{0,62}$

File: out/128_g_1437_10300000

OH

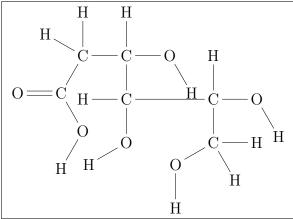
OH

OH

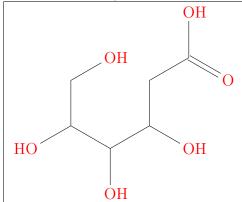
OH

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0.1.32 p_{0,63}

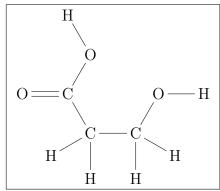


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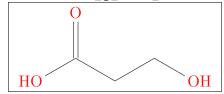


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0.1.33 p_{0,68}

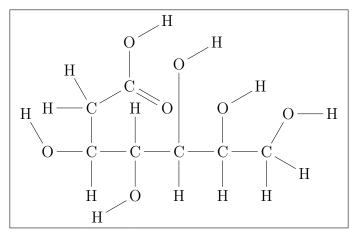


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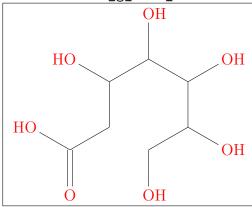


File: out/138_g_2596_11310100

$0.1.34 p_{0,69}$



File: out/140_g_2604_10300000



File: out/142_g_2604_11310100

0.2 Derivation Graph

0.2.1 DG Hyper, dg_0

Figure too large, see out/143_dg_0_11100_coord.pdf

 $File: \ \mathtt{out/279_dg_0_11100}$

$$|V| = 81$$

 $|E| = 414$

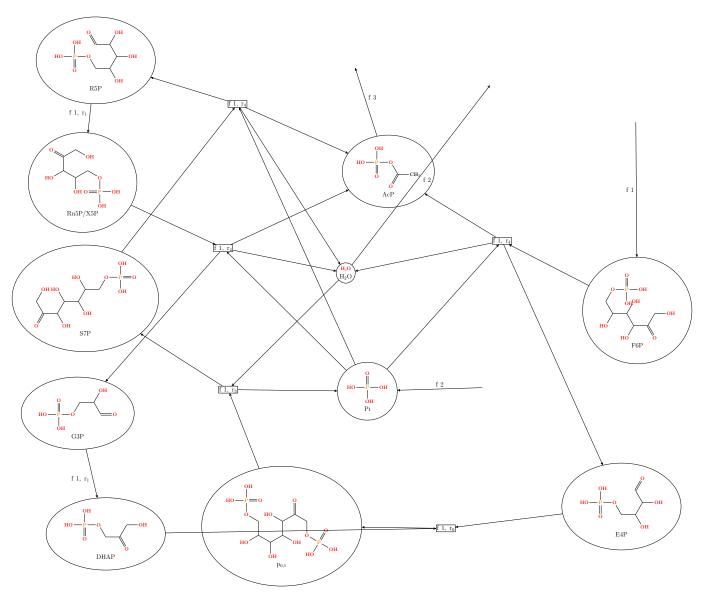
0.3 Enumerated Flows with 7 reactions

0.4 Enumerated Flows with 7 unique reactions

0.4.1 Solution 0

Overall Data

Objective value (integral): 7
Vertex/Graph In Out
AcP 0 3
F6P 1 0
H_20 0 2
Pi 2 0



File: out/284_dg_0_11100_f_0_0_filt

|E| = 7 |P| = 7

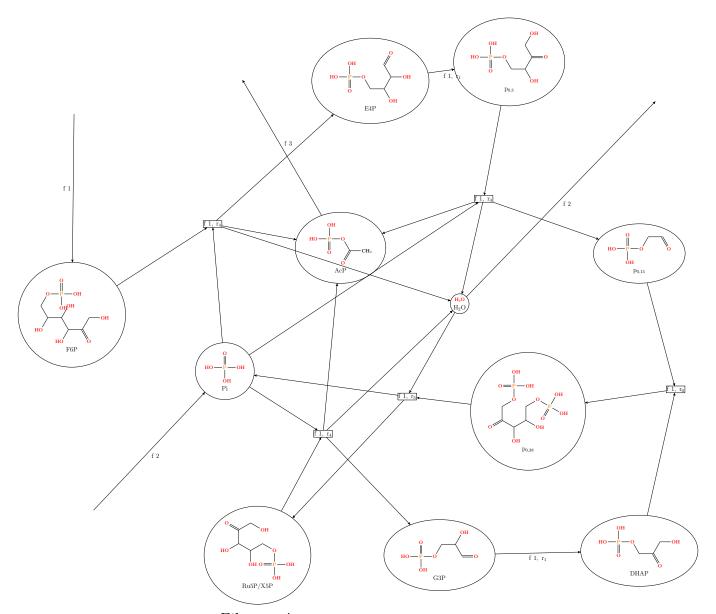
0.4.2 Solution 1

Overall Data

Objective value (integral): 7

Vertex/Graph In Out

AcP 0 3 F6P 1 0 H_2O 0 2 Pi 2 0



File: out/289_dg_0_11100_f_0_1_filt

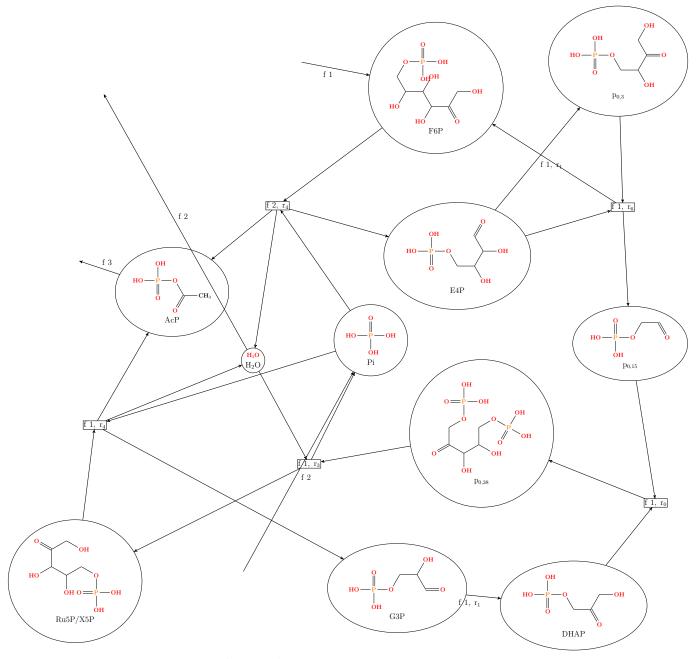
$$|E| = 7 |P| = 7$$

- 0.5 Enumerated Flows with 8 unique reactions
- 0.6 Enumerated Flows with 9 unique reactions
- 0.7 Enumerated Flows with 10 unique reactions
- 0.8 Enumerated Flows with 11 unique reactions
- 0.9 Enumerated Flows with 8 reactions
- 0.10 Enumerated Flows with 7 unique reactions

0.10.1 Solution 5

Overall Data

Objective value (integral): 8
Vertex/Graph In Out
AcP 0 3
F6P 1 0
H_20 0 2
Pi 2 0



 $File: \ \mathtt{out/294_dg_0_11100_f_0_5_filt}$

$$|E| = 7 |P| = 8$$

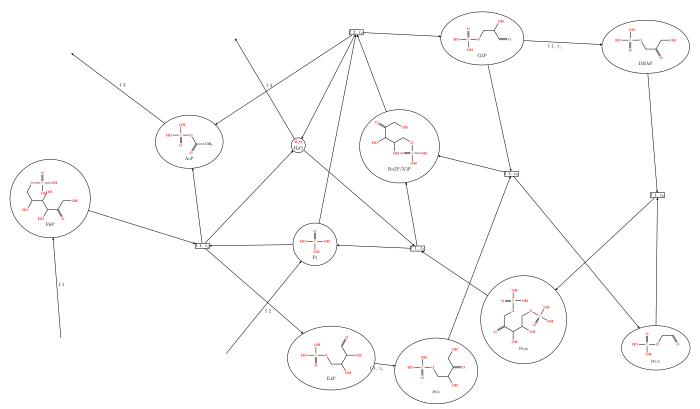
0.10.2 Solution 7

Overall Data

Objective value (integral): 8

Vertex/Graph In Out

AcP 0 3 F6P 1 0 H_2O 0 2 Pi 2 0



 $File: \ \mathtt{out/299_dg_0_11100_f_0_7_filt}$

$$|E| = 7 |P| = 8$$

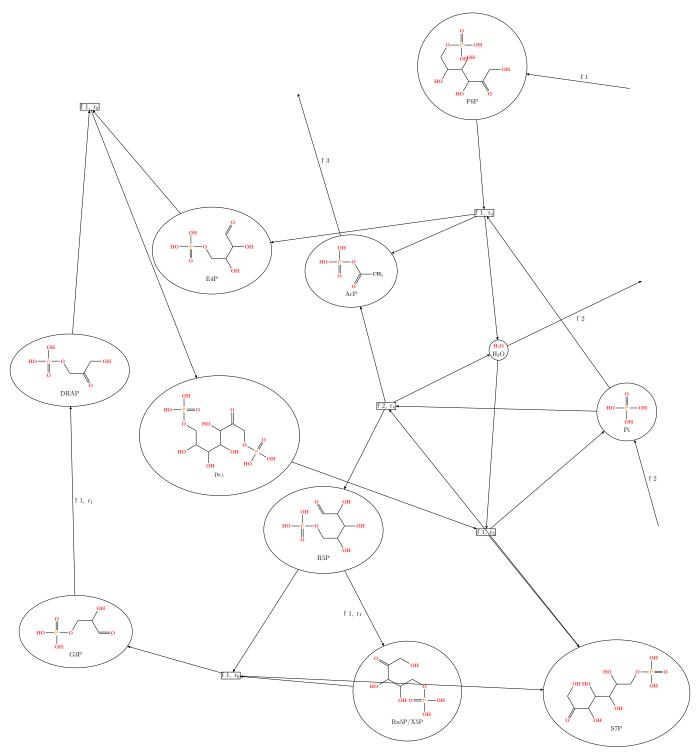
0.10.3 Solution 8

Overall Data

Objective value (integral): 8

Vertex/Graph In Out

AcP 0 3 F6P 1 0 H_20 0 2 Pi 2 0



File: out/304_dg_0_11100_f_0_8_filt

|E| = 7 |P| = 8

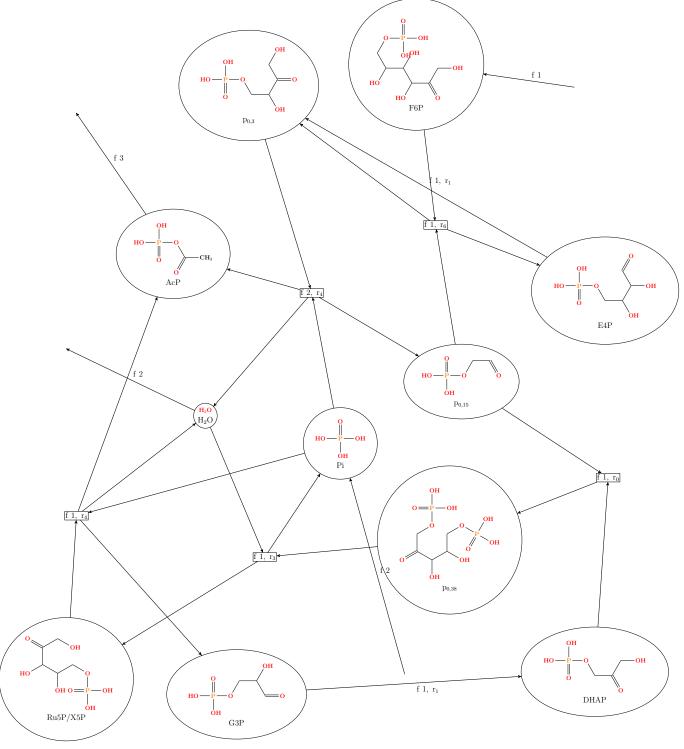
0.10.4 Solution 9

Overall Data

Objective value (integral): 8

Vertex/Graph In Out

AcP	0	3
F6P	1	0
H_20	0	2
Pi	2	0



 $File: \ \mathtt{out/309_dg_0_11100_f_0_9_filt}$

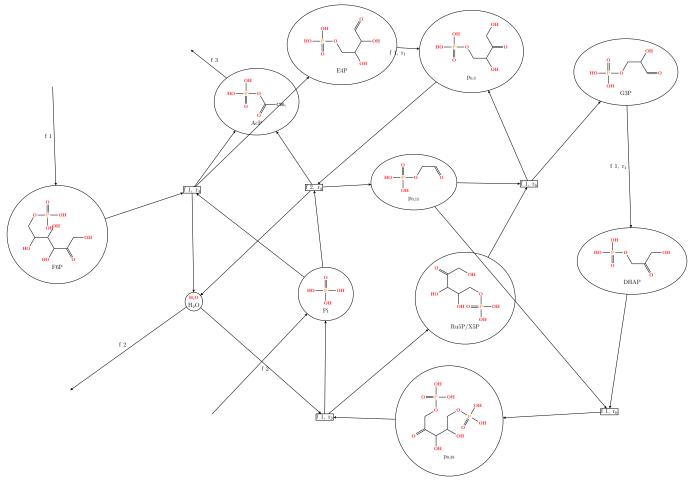
$$|E| = 7 |P| = 8$$

0.10.5 Solution 10

Overall Data

Objective value (integral): 8
Vertex/Graph In Out
AcP 0 3
F6P 1 0
H_20 0 2
Pi 2 0

Filtered Graph



 $File: \ \mathtt{out/314_dg_0_11100_f_0_10_filt}$

$$|E| = 7 |P| = 8$$

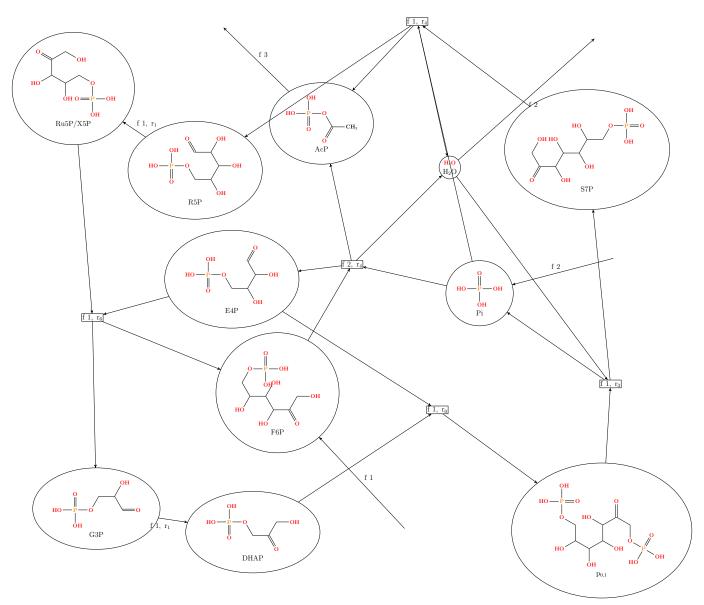
0.10.6 Solution 11

Overall Data

Objective value (integral): 8

Vertex/Graph In Out AcP 0 3 F6P 1 0 H_20 0 2

Pi 2 0



File: out/319_dg_0_11100_f_0_11_filt

|E| = 7 |P| = 8

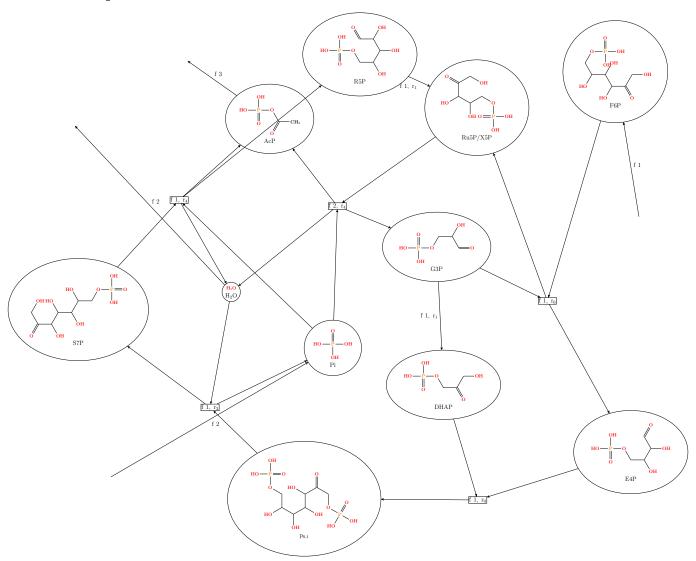
0.10.7 Solution 12

Overall Data

Objective value (integral): 8

Vertex/Graph In Out

AcP 0 3 F6P 1 0 H_20 0 2 Pi 2 0



 $File: \verb"out/324_dg_0_11100_f_0_12_filt"$

|E| = 7 |P| = 8

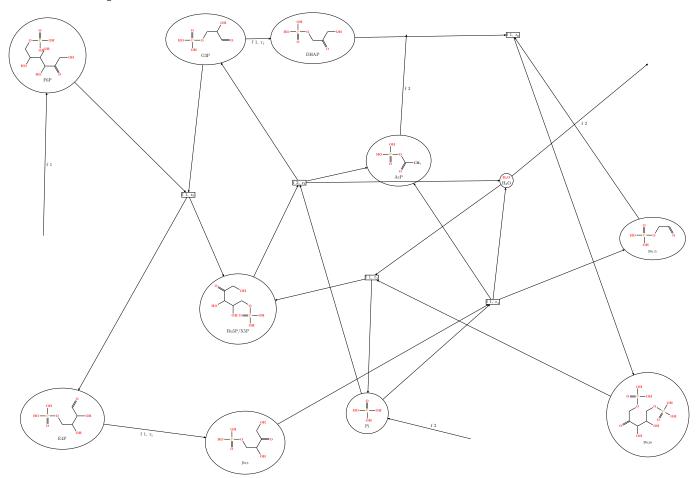
0.10.8 Solution 14

Overall Data

Objective value (integral): 8

Vertex/Graph In Out

AcP 0 3 F6P 1 0 H_20 0 2 Pi 2 0



 $File: \ {\tt out/329_dg_0_11100_f_0_14_filt}$

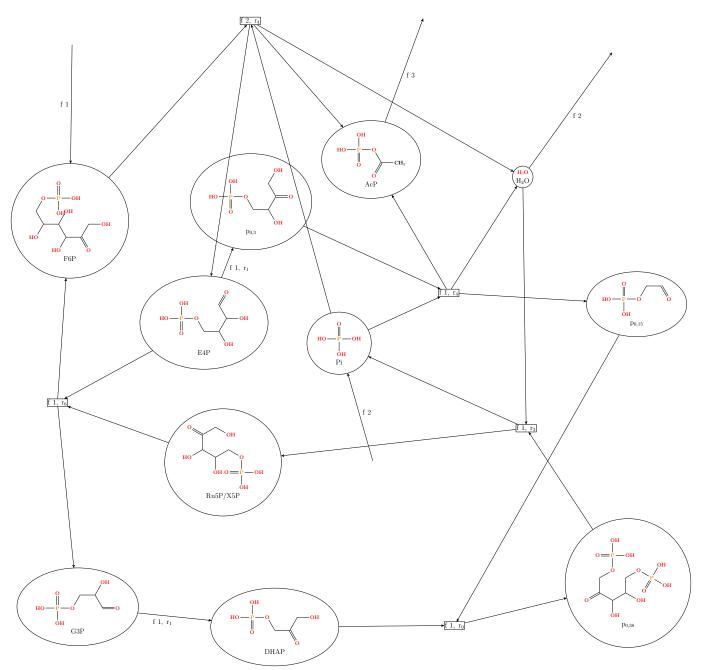
$$|E| = 7 |P| = 8$$

0.10.9 Solution 17

Overall Data

Objective value (integral): 8

Vertex/Graph In Out AcP 0 3 F6P 1 0 H_2O 0 2 Pi 2 0



File: $out/334_dg_0_11100_f_0_17_filt$

$$|E| = 7 |P| = 8$$

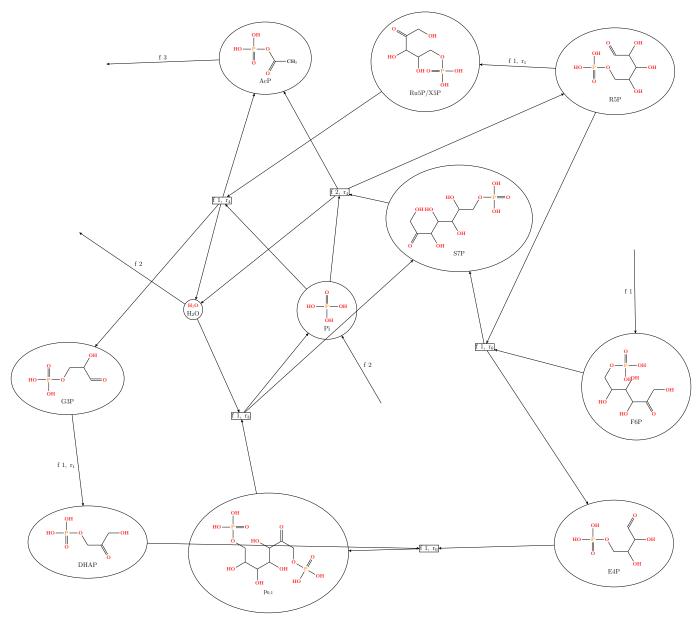
0.10.10 Solution 21

Overall Data

Objective value (integral): 8

Vertex/Graph In Out

AcP 0 3 F6P 1 0 H_20 0 2 Pi 2 0



File: $out/339_dg_0_11100_f_0_21_filt$

$$|E| = 7 |P| = 8$$

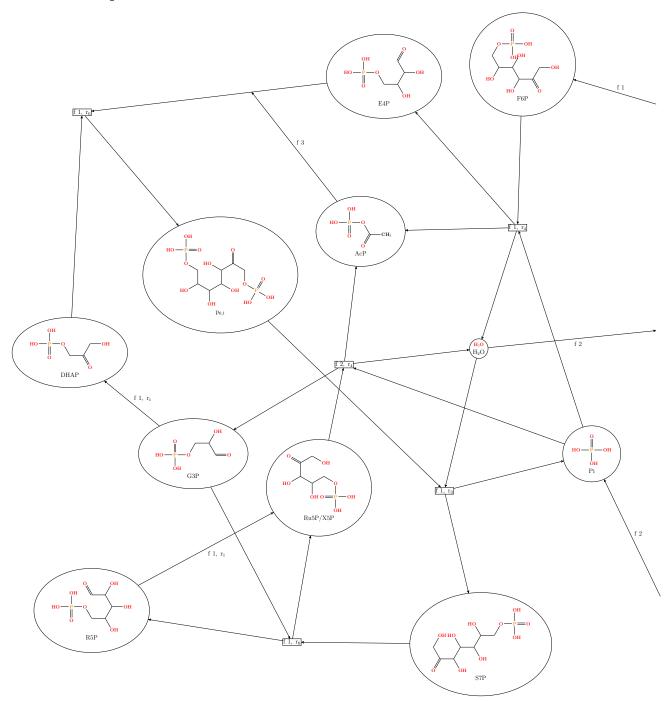
0.10.11 Solution 31

Overall Data

Objective value (integral): 8

Vertex/Graph In Out

AcP 0 3 F6P 1 0 H_20 0 2 Pi 2 0



 $File: \ {\tt out/344_dg_0_11100_f_0_31_filt}$

$$|E| = 7 |P| = 8$$

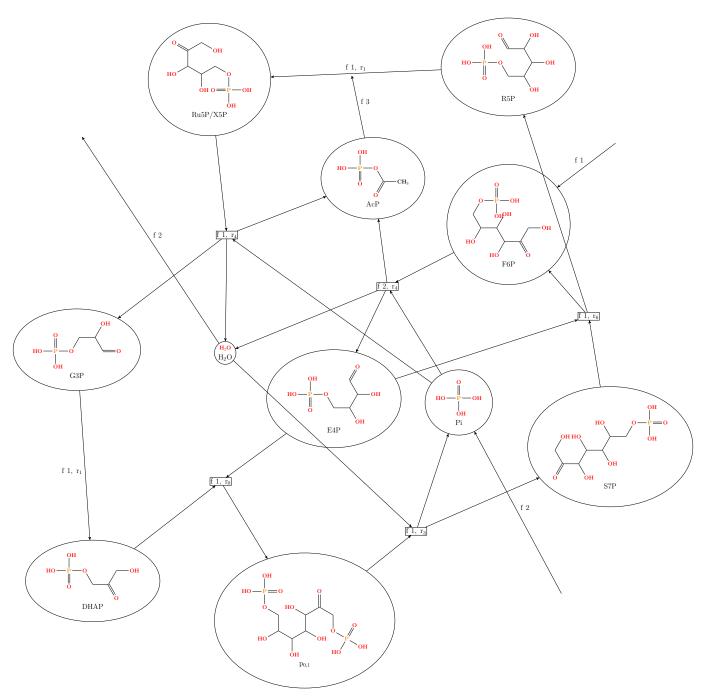
0.10.12 Solution 32

Overall Data

Objective value (integral): 8

Vertex/Graph In Out AcP 0 3 F6P 1 0

H_20 0 2 Pi 2 0



File: out/349_dg_0_11100_f_0_32_filt

|E| = 7 |P| = 8

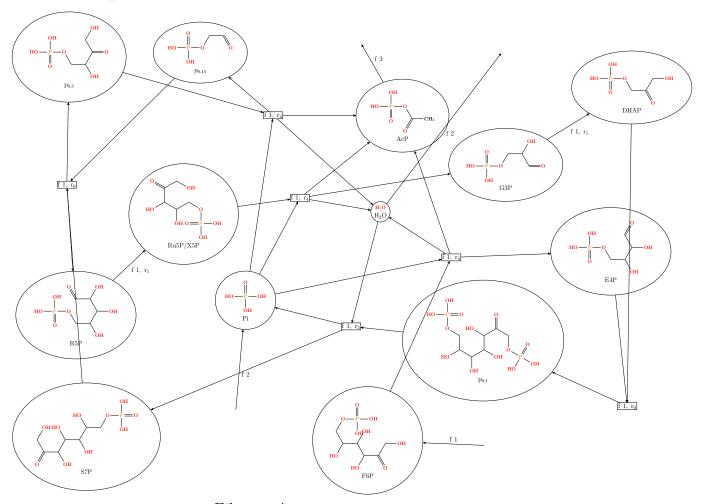
0.11 Enumerated Flows with 8 unique reactions

0.11.1 Solution 2

Overall Data

Objective value (integral): 8
Vertex/Graph In Out
AcP 0 3

F6P	1	0
H_20	0	2
Pi	2	0



File: out/354_dg_0_11100_f_0_2_filt

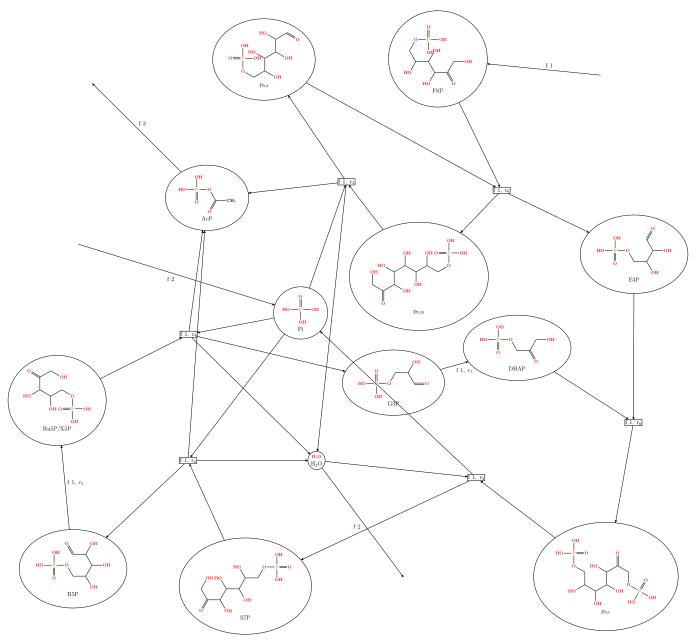
|E| = 8 |P| = 8

0.11.2 Solution 3

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



File: $out/359_dg_0_11100_f_0_3_filt$

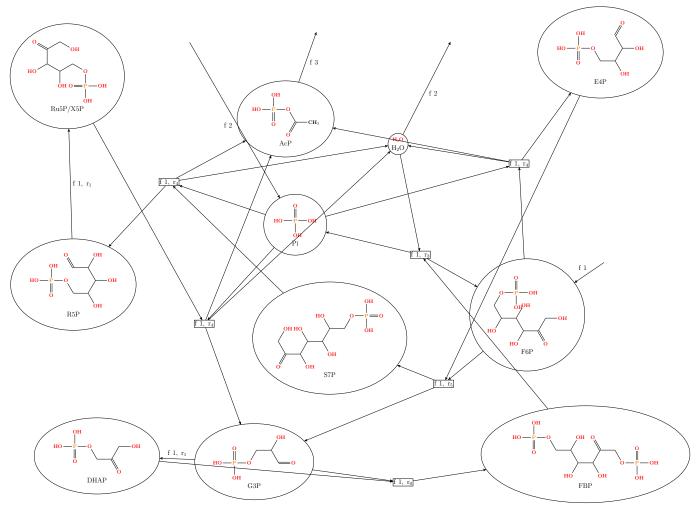
$$|E| = 8 |P| = 8$$

0.11.3 Solution 4

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



File: out/364_dg_0_11100_f_0_4_filt

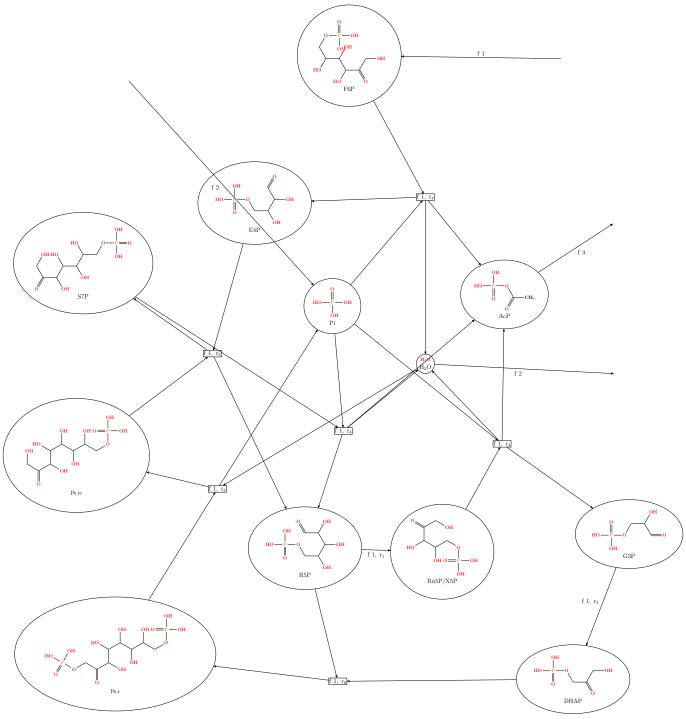
$$|E| = 8 |P| = 8$$

0.11.4 Solution 6

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



 $File: \verb"out/369_dg_0_11100_f_0_6_filt"$

$$|E| = 8 |P| = 8$$

0.11.5 Solution 13

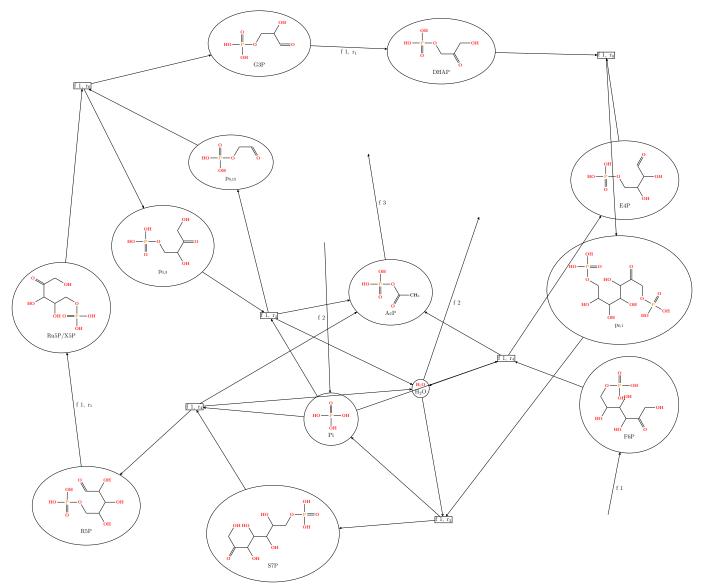
Overall Data

Objective value (integral): 8

Vertex/Graph In Out

AcP 0 3 F6P 1 0 H_20 0 2 Pi 2 0

Filtered Graph



File: out/374_dg_0_11100_f_0_13_filt

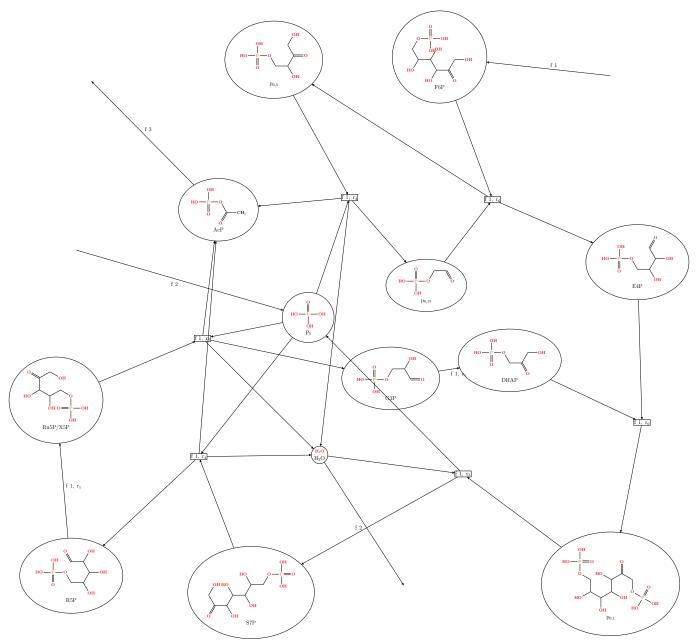
|E| = 8 |P| = 8

0.11.6 Solution 15

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



 $File: \ {\tt out/379_dg_0_11100_f_0_15_filt}$

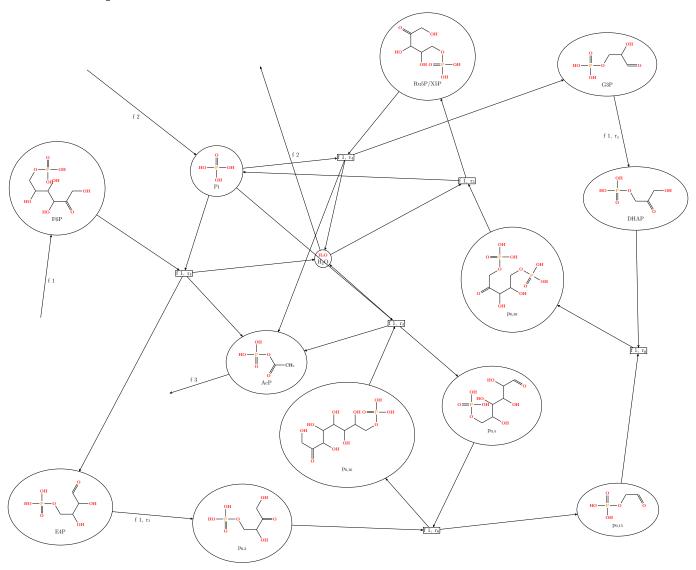
|E| = 8 |P| = 8

0.11.7 Solution 16

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



File: out/384_dg_0_11100_f_0_16_filt

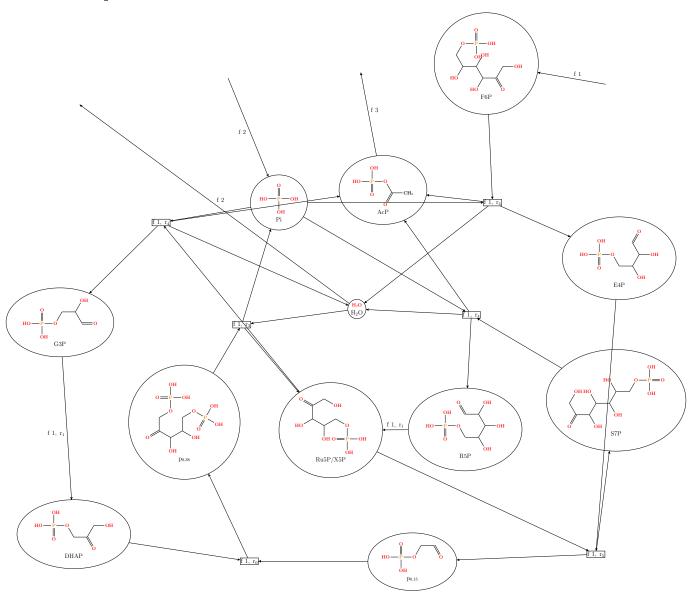
|E| = 8 |P| = 8

0.11.8 Solution 18

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



File: $out/389_dg_0_11100_f_0_18_filt$

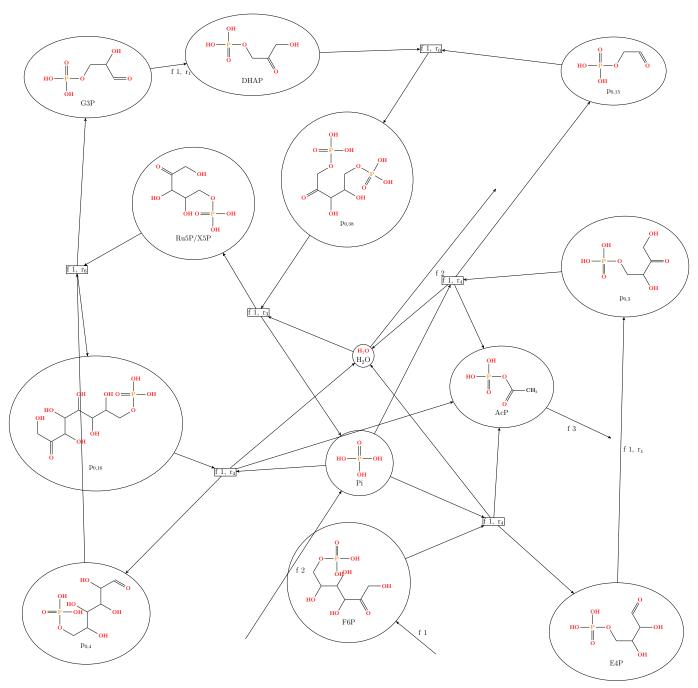
|E| = 8 |P| = 8

0.11.9 Solution 19

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



 $File: \ {\tt out/394_dg_0_11100_f_0_19_filt}$

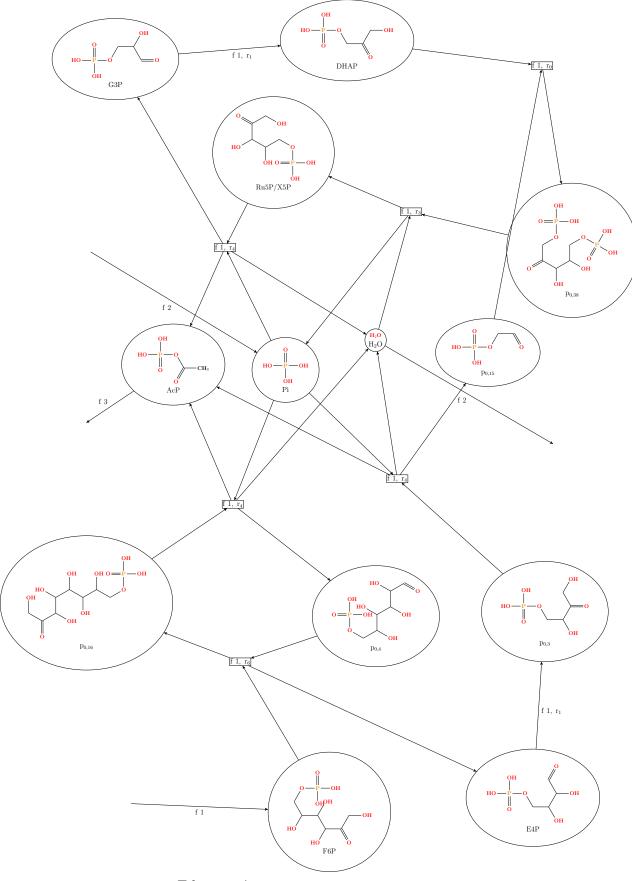
|E| = 8 |P| = 8

0.11.10 Solution 20

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



 $File: \ {\tt out/399_dg_0_11100_f_0_20_filt}$

|E| = 8 |P| = 8

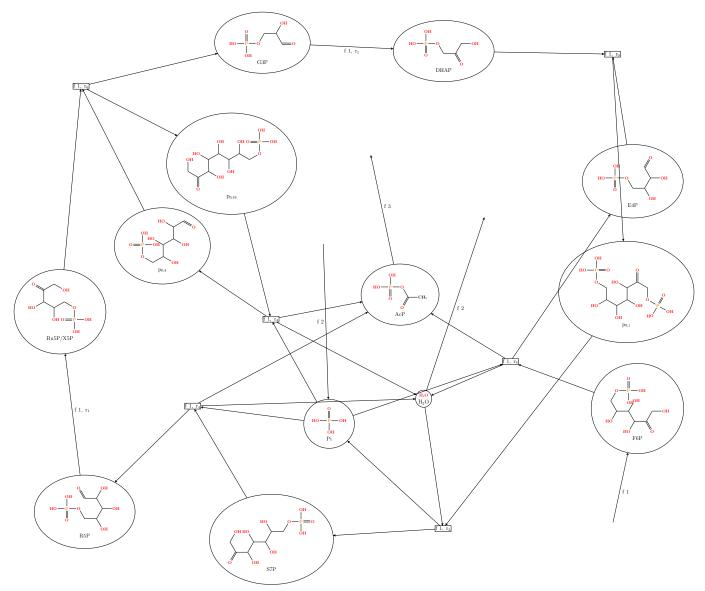
0.11.11 Solution 22

Overall Data

Objective value (integral): 8

Vertex/Graph In Out AcP 0 3 F6P 1 0 H_2O 0 2 Pi 2 0

Filtered Graph



 $File: \ out/404_dg_0_11100_f_0_22_filt$

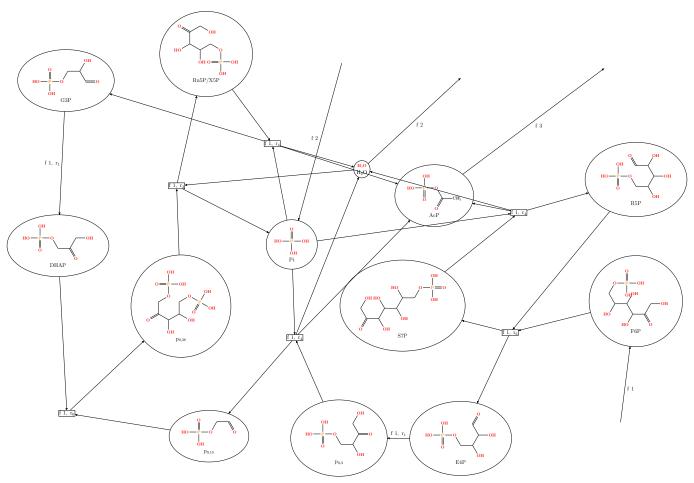
$$|E| = 8 |P| = 8$$

0.11.12 Solution 23

Overall Data

Objective value (integral): 8

Vertex/Graph	In	Out
AcP	0	3
F6P	1	0
H_20	0	2
Pi	2	0



 $File: \ {\tt out/409_dg_0_11100_f_0_23_filt}$

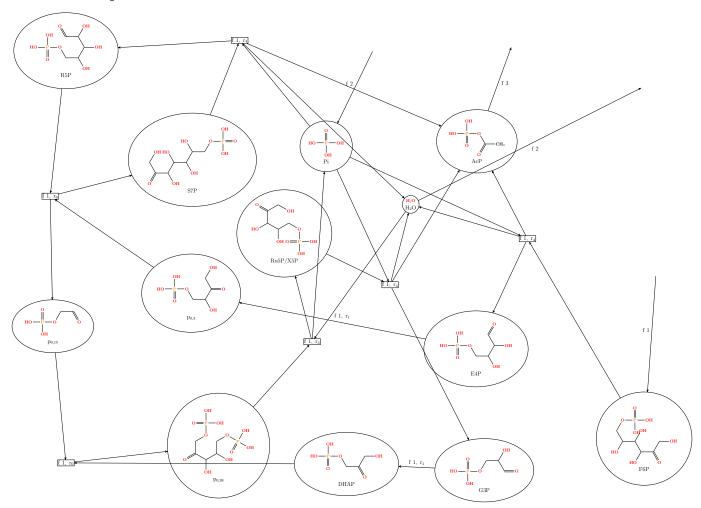
$$|E| = 8 |P| = 8$$

0.11.13 Solution 24

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



 $File: \ {\tt out/414_dg_0_11100_f_0_24_filt}$

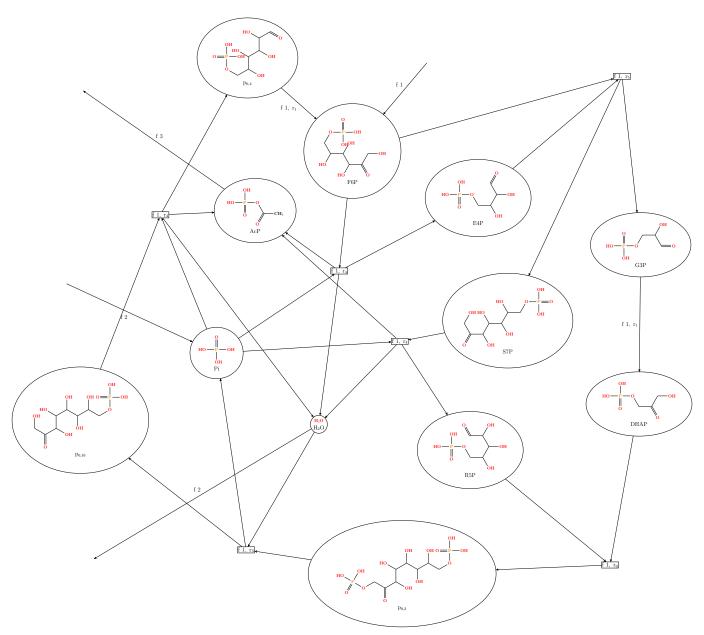
$$|E| = 8 |P| = 8$$

0.11.14 Solution 25

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



 $File: \ {\tt out/419_dg_0_11100_f_0_25_filt}$

|E| = 8 |P| = 8

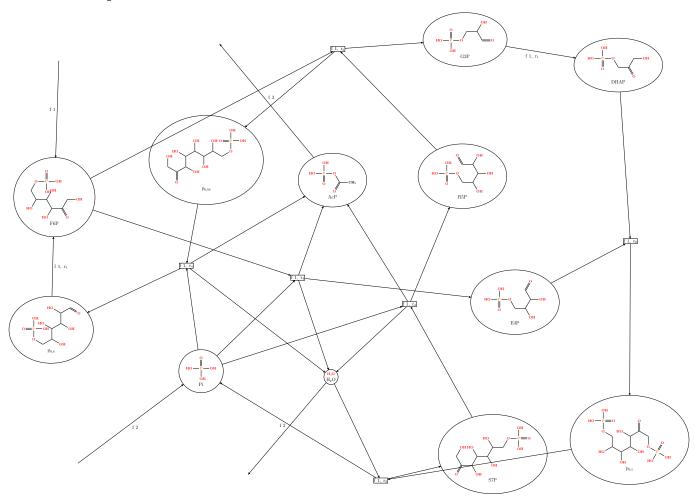
0.11.15 Solution 26

Overall Data

Objective value (integral): 8

Vertex/Graph In Out AcP 0 3 F6P 1 0 H_20 0 2

Pi 2 0



 $File: \ {\tt out/424_dg_0_11100_f_0_26_filt}$

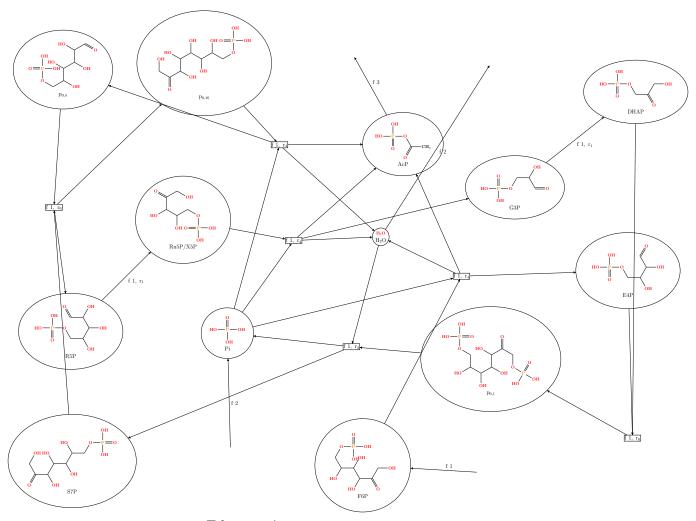
$$|E| = 8 |P| = 8$$

0.11.16 Solution 27

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



File: out/429_dg_0_11100_f_0_27_filt

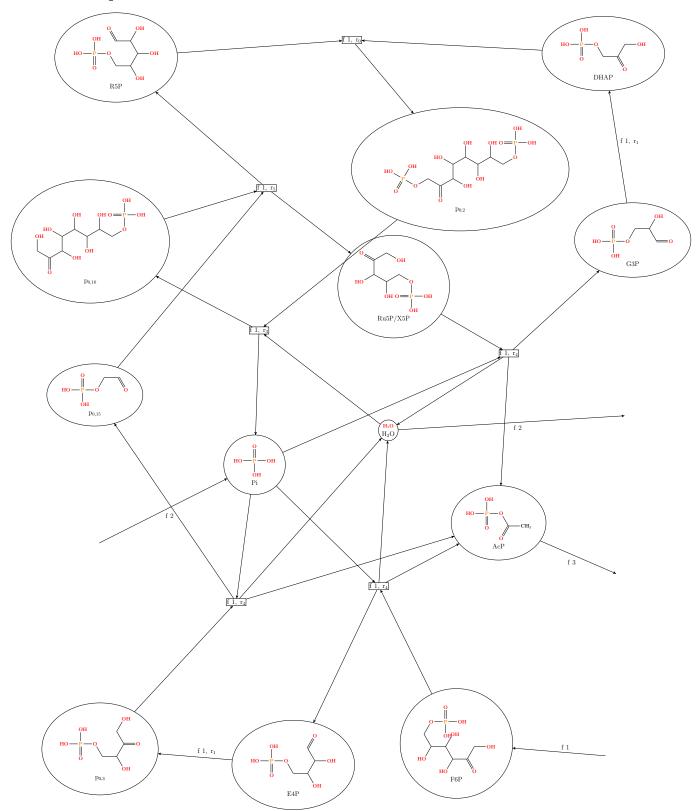
|E| = 8 |P| = 8

0.11.17 Solution 28

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



 $File: \ {\tt out/434_dg_0_11100_f_0_28_filt}$

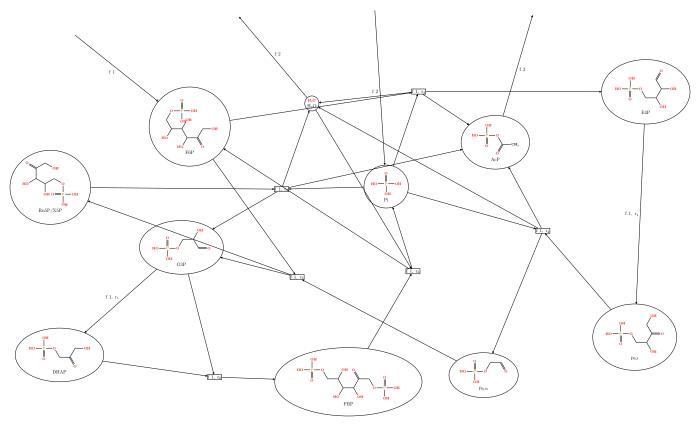
$$|E| = 8 |P| = 8$$

0.11.18 Solution 29

Overall Data

Objective value (integral): 8
Vertex/Graph In Out
AcP 0 3
F6P 1 0
H_20 0 2
Pi 2 0

Filtered Graph



 $File: \ {\tt out/439_dg_0_11100_f_0_29_filt}$

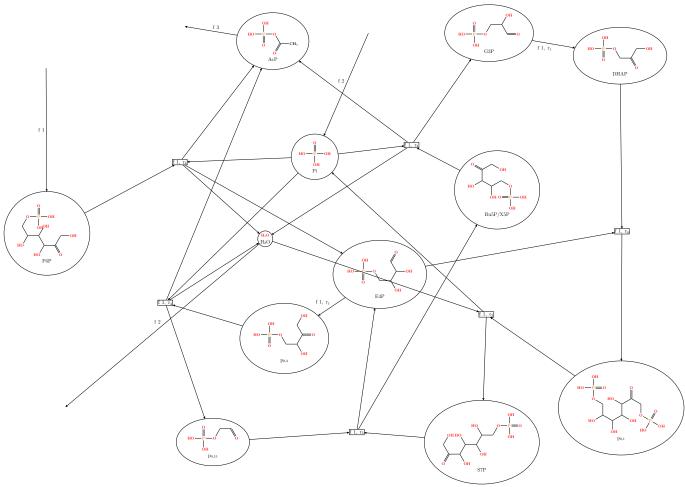
|E| = 8 |P| = 8

0.11.19 Solution 30

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



 $File: \ {\tt out/444_dg_0_11100_f_0_30_filt}$

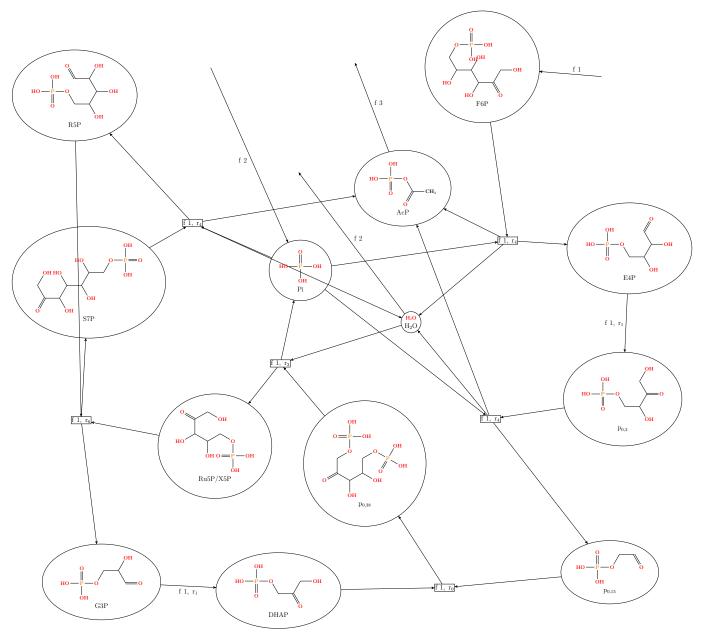
$$|E| = 8 |P| = 8$$

0.11.20 Solution 33

Overall Data

Objective value (integral): 8

Vertex/Graph In Out



 $File: \ {\tt out/449_dg_0_11100_f_0_33_filt}$

|E| = 8 |P| = 8

- 0.12 Enumerated Flows with 9 unique reactions
- 0.13 Enumerated Flows with 10 unique reactions
- 0.14 Enumerated Flows with 11 unique reactions