# Summary

September 27, 2023

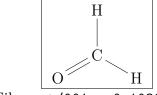
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### 0.1 Loaded Graphs

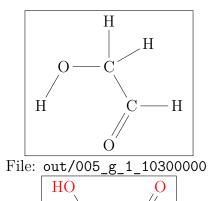
#### 0.1.1 Formaldehyde



File: out/001\_g\_0\_10300000 H<sub>2</sub>C \_\_\_\_O

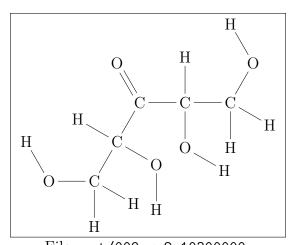
File: out/003\_g\_0\_11310100

#### 0.1.2 Glycolaldehyde



File: out/007\_g\_1\_11310100

#### 0.1.3 random1

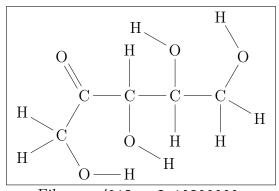


File: out/009\_g\_2\_10300000

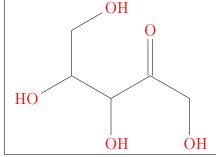
OH
OH
OH
OH

File: out/011\_g\_2\_11310100

#### 0.1.4 random2

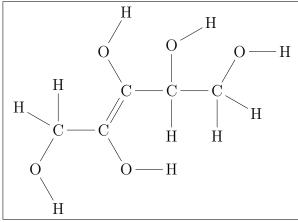


File: out/013\_g\_3\_10300000



File: out/015\_g\_3\_11310100

### 0.1.5 random3



File: out/017\_g\_4\_10300000

OH

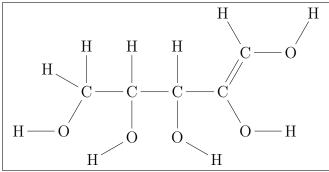
OH

OH

OH

File: out/019\_g\_4\_11310100

#### 0.1.6 random4



File: out/021\_g\_5\_10300000

OH

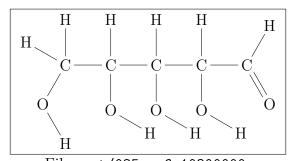
OH

OH

OH

File: out/023\_g\_5\_11310100

#### 0.1.7 random5



File: out/025\_g\_6\_10300000

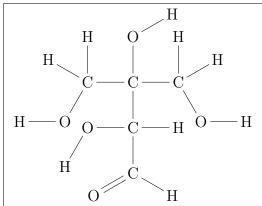
OH

OH

OH

File: out/027\_g\_6\_11310100

#### 0.1.8 random6



File: out/029\_g\_7\_10300000

OH

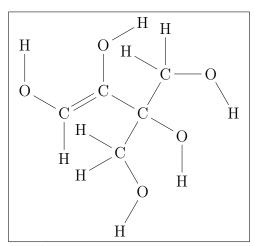
OH

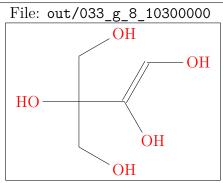
OH

OH

File: out/031\_g\_7\_11310100

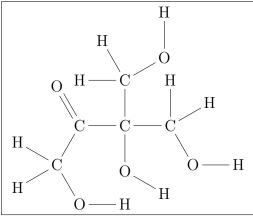
#### 0.1.9 random7





File: out/035\_g\_8\_11310100

#### 0.1.10 random8



File: out/037\_g\_9\_10300000

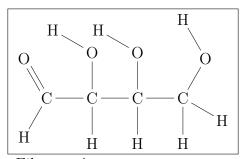
OH

OH

OH

File: out/039\_g\_9\_11310100

### $0.1.11 g_{10}$



File: out/041\_g\_10\_10300000

OH

OH

File: out/043\_g\_10\_11310100

### 0.1.12 g\_{11}

File: out/045\_g\_11\_10300000

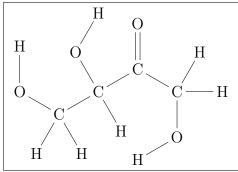
OH

OH

OH

File: out/047\_g\_11\_11310100

## 0.1.13 g\_{12}



File: out/049\_g\_12\_10300000

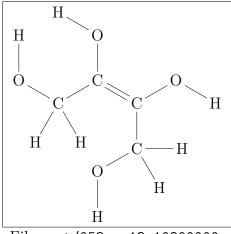
OH

OH

OH

File: out/051\_g\_12\_11310100

### $0.1.14 \ g_{13}$



File: out/053\_g\_13\_10300000

OH

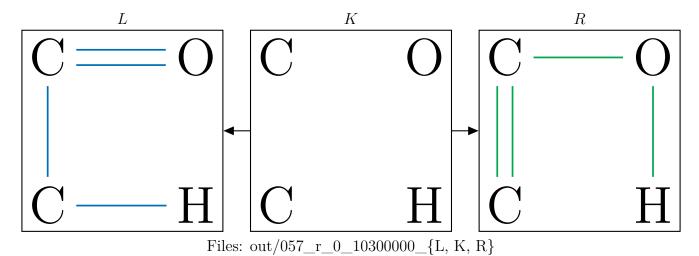
OH

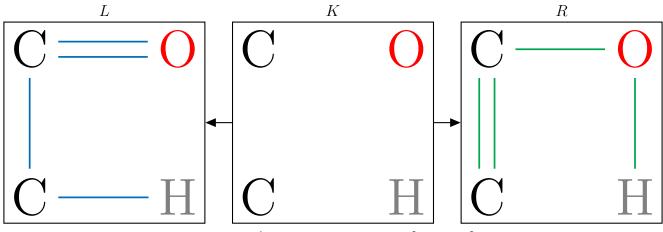
File: out/055\_g\_13\_11310100

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## 0.2 Loaded Rules

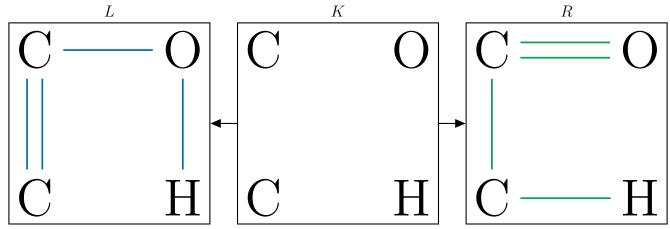
### 0.2.1 Keto-enol isomerization ->



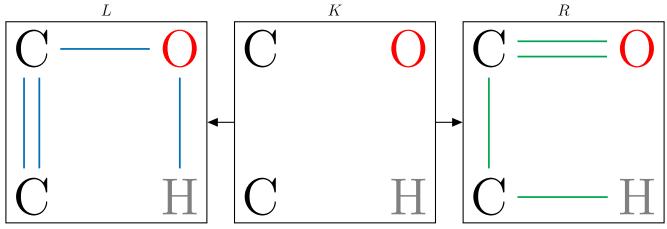


Files: out/059\_r\_0\_11300100\_{L, K, R}

### 0.2.2 Keto-enol isomerization <-

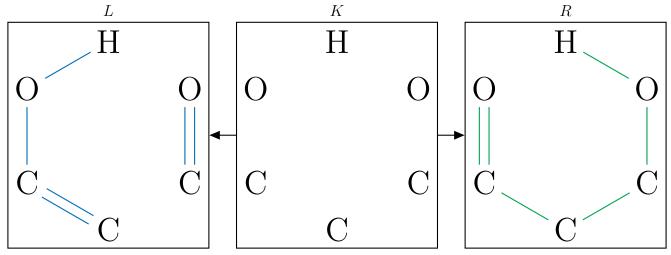


Files: out/062\_r\_1\_10300000\_{L, K, R}

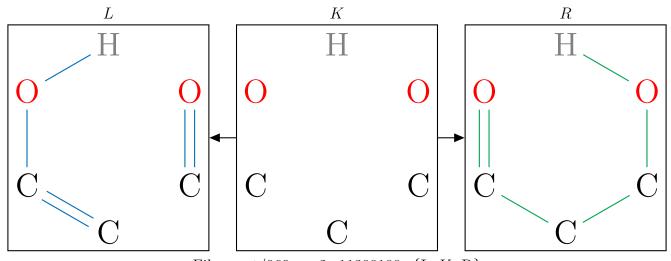


Files: out/064\_r\_1\_11300100\_{L, K, R}

### 0.2.3 Aldol Addition ->

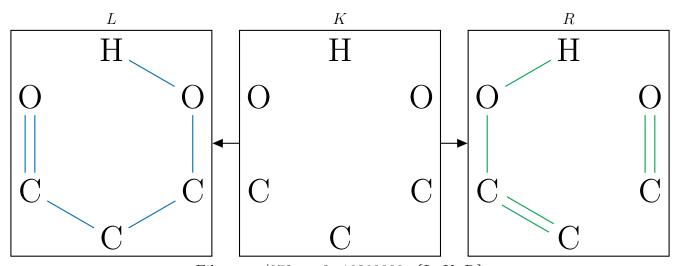


Files:  $out/067_r_2_10300000_{L, K, R}$ 

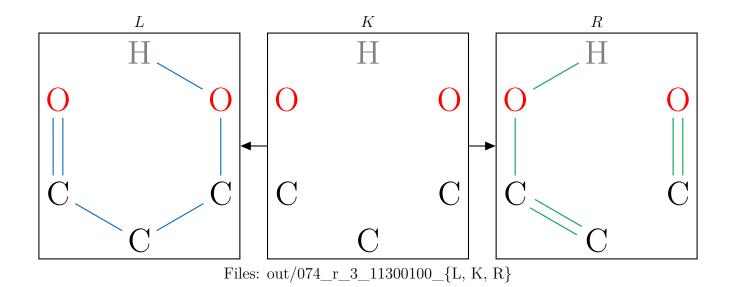


# Files: out/069\_r\_2\_11300100\_{L, K, R}

### 0.2.4 Aldol Addition <-



Files: out/072\_r\_3\_10300000\_{L, K, R}



### 0.2.5 DG Hyper, dg\_0

Figure too large, see out/076\_dg\_0\_11100\_coord.pdf

File: out/205\_dg\_0\_11100

### 0.3 Product Graphs

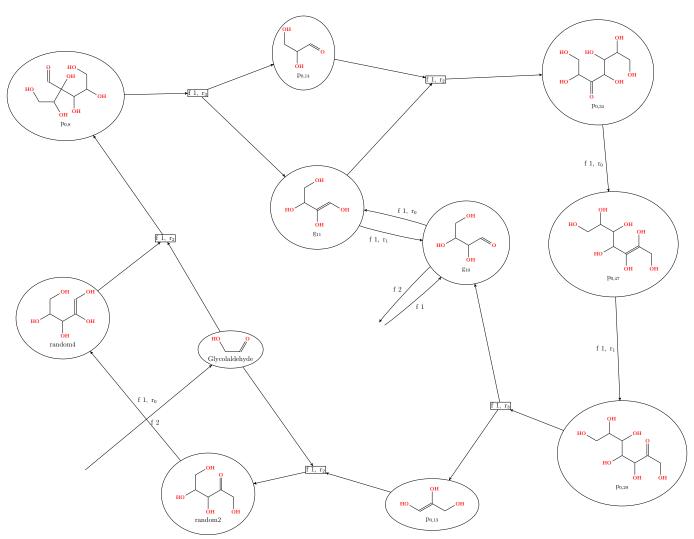
## 0.4 Trying C(C(C(CO)O)O)=O

### 0.5 Flow Solutions, id 0

#### 0.5.1 Solution 0

#### Overall Data

Objective value (integral): 14 Vertex/Graph In Out OA Glycolaldehyde 2 0 0 g\_{10} 1 2 1



 $File: \ \mathtt{out/209\_dg\_0\_11100\_f\_0\_0\_filt}$ 

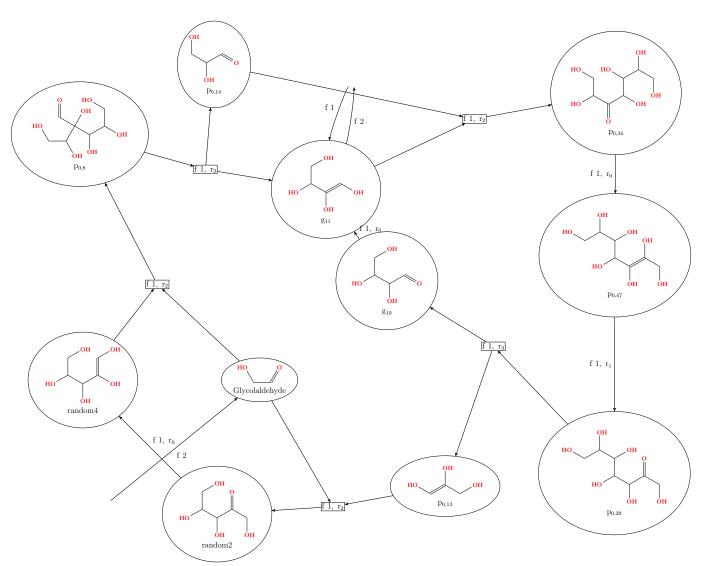
# 0.6 Trying C(O)=C(C(CO)O)O

# 0.7 Flow Solutions, id 1

#### 0.7.1 Solution 0

#### Overall Data

Objective value (integral): 13 Vertex/Graph In Out OA Glycolaldehyde 2 0 0 g\_{11} 1 2 1



 $File: \ \mathtt{out/213\_dg\_0\_11100\_f\_1\_0\_filt}$ 

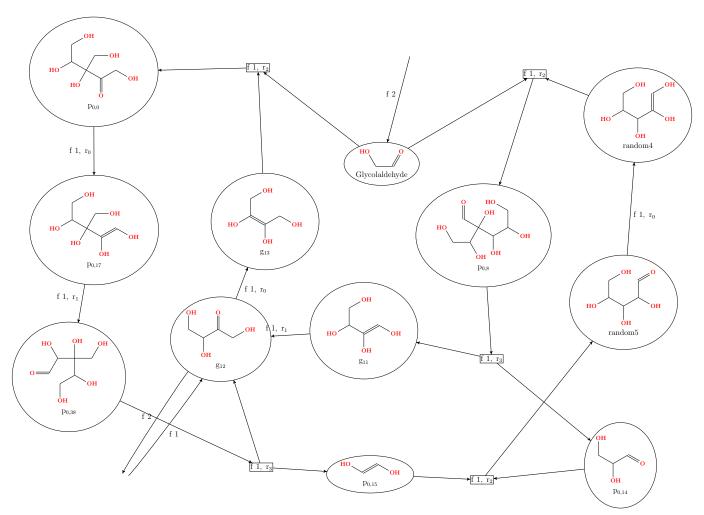
# 0.8 Trying C(CO)(C(CO)O)=O

## 0.9 Flow Solutions, id 2

#### 0.9.1 Solution 0

#### Overall Data

Objective value (integral): 14 Vertex/Graph In Out OA Glycolaldehyde 2 0 0 g\_{12} 1 2 1

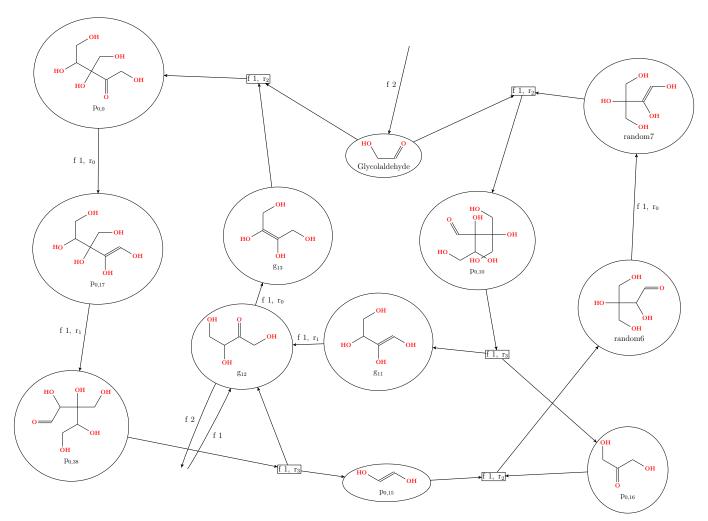


File: out/217\_dg\_0\_11100\_f\_2\_0\_filt

#### 0.9.2 Solution 1

#### Overall Data

Objective value (integral): 14

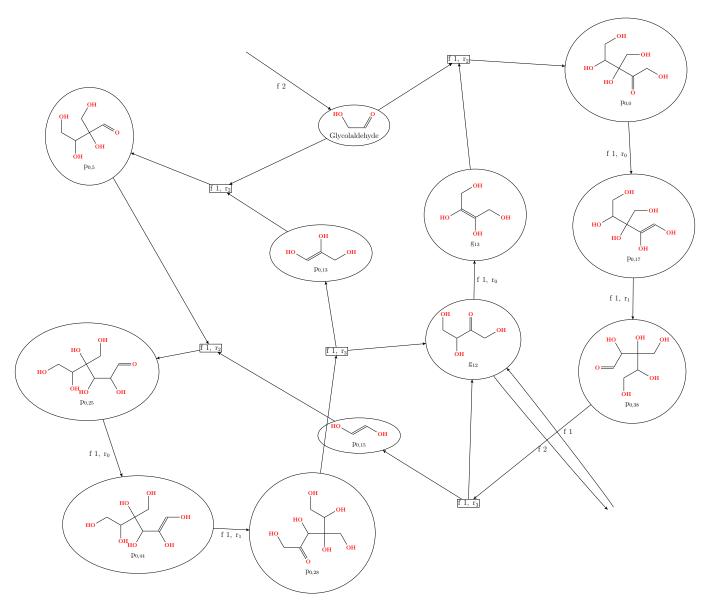


 $File: \ \mathtt{out/220\_dg\_0\_11100\_f\_2\_1\_filt}$ 

### 0.9.3 Solution 2

#### Overall Data

Objective value (integral): 14 Vertex/Graph In Out OA Glycolaldehyde 2 0 0 g 12 1 1 2 1



File: out/223\_dg\_0\_11100\_f\_2\_2\_filt

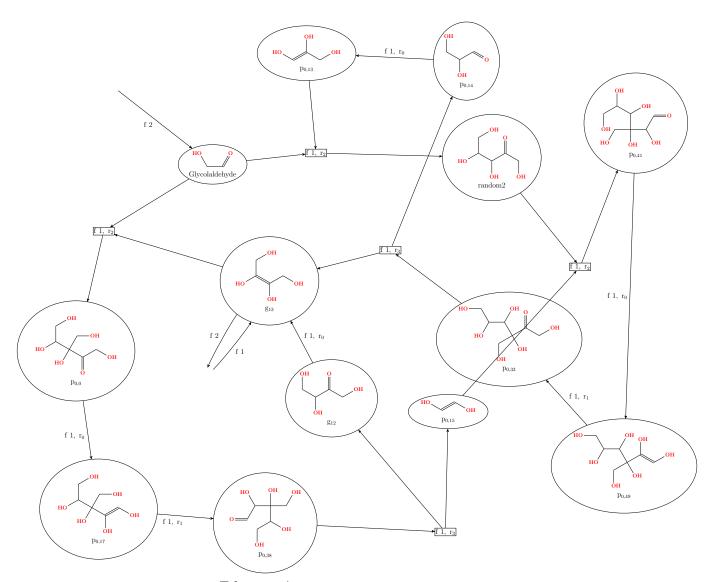
# 0.10 Trying C(CO)(O)=C(CO)O

## 0.11 Flow Solutions, id 3

#### 0.11.1 Solution 0

#### Overall Data

Objective value (integral): 15 Vertex/Graph In Out OA Glycolaldehyde 2 0 0 g\_{13} 1 2 1



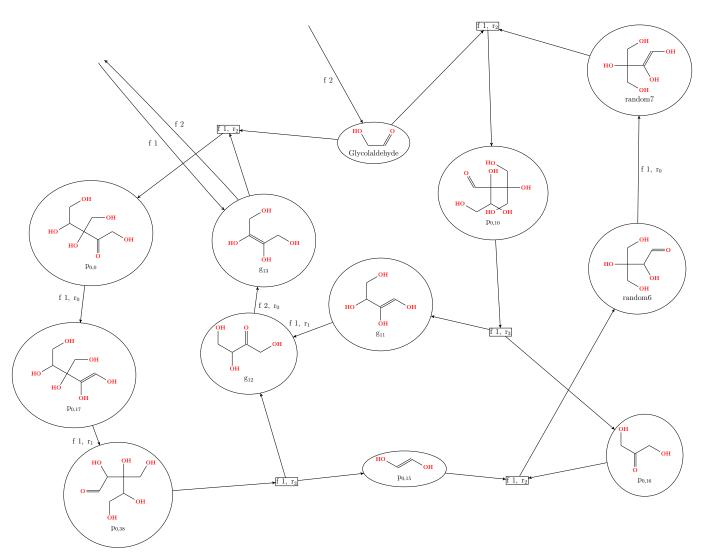
 $File: \ \mathtt{out/227\_dg\_0\_11100\_f\_3\_0\_filt}$ 

#### 0.11.2 Solution 1

#### Overall Data

Objective value (integral): 15

Vertex/Graph In Out OA Glycolaldehyde 2 0 0 g\_{13} 1 2 1

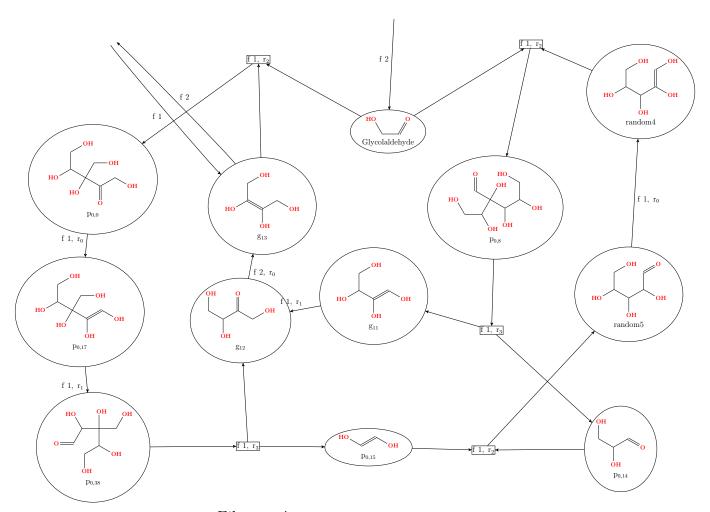


 $File: \ \mathtt{out/230\_dg\_0\_11100\_f\_3\_1\_filt}$ 

### 0.11.3 Solution 2

#### Overall Data

Objective value (integral): 15 Vertex/Graph In Out OA Glycolaldehyde 2 0 0 g\_{13} 1 2 1

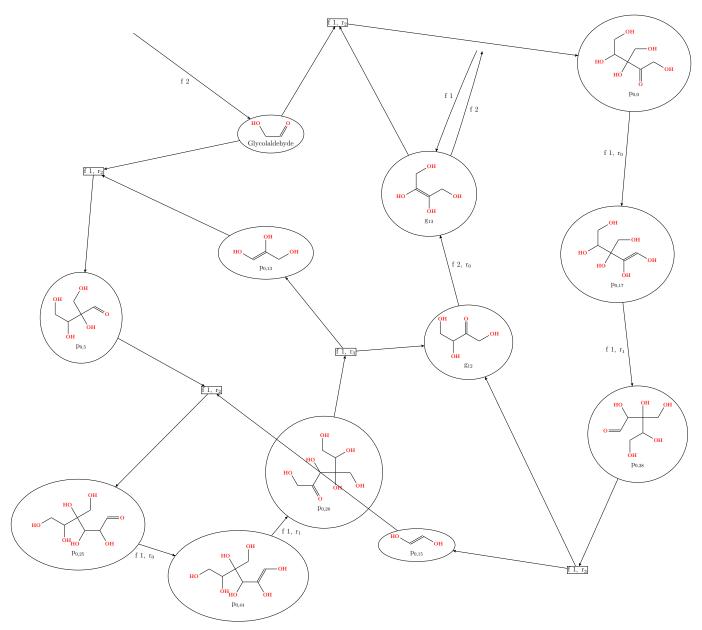


File:  $out/233_dg_0_11100_f_3_2_filt$ 

#### 0.11.4 Solution 3

#### Overall Data

Objective value (integral): 15 Vertex/Graph In Out OA Glycolaldehyde 2 0 0 g\_{13} 1 2 1



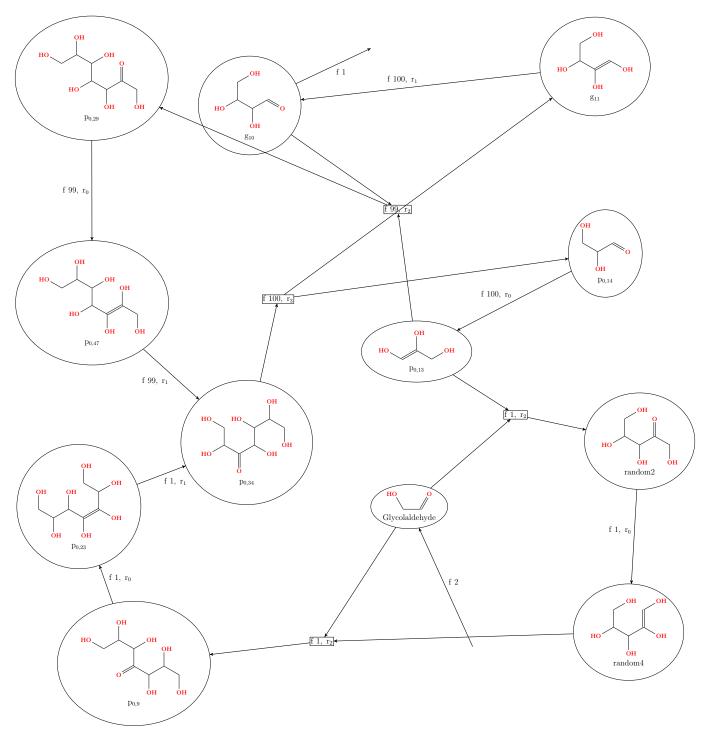
File: out/236\_dg\_0\_11100\_f\_3\_3\_filt

## 0.12 Flow Solutions, id 4

#### 0.12.1 Solution 0

#### Overall Data

Objective value (integral): -1
Vertex/Graph In Out
Glycolaldehyde 2 0
g\_{10} 0 1



File: out/240\_dg\_0\_11100\_f\_4\_0\_filt

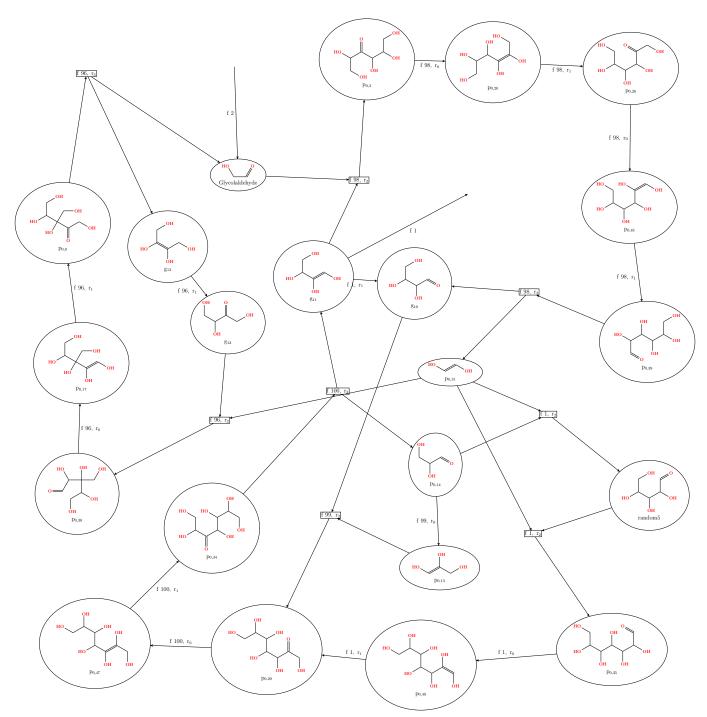
# 0.13 Flow Solutions, id 5

#### 0.13.1 Solution 0

#### Overall Data

Objective value (integral): -1

Vertex/Graph In Out Glycolaldehyde 2 0



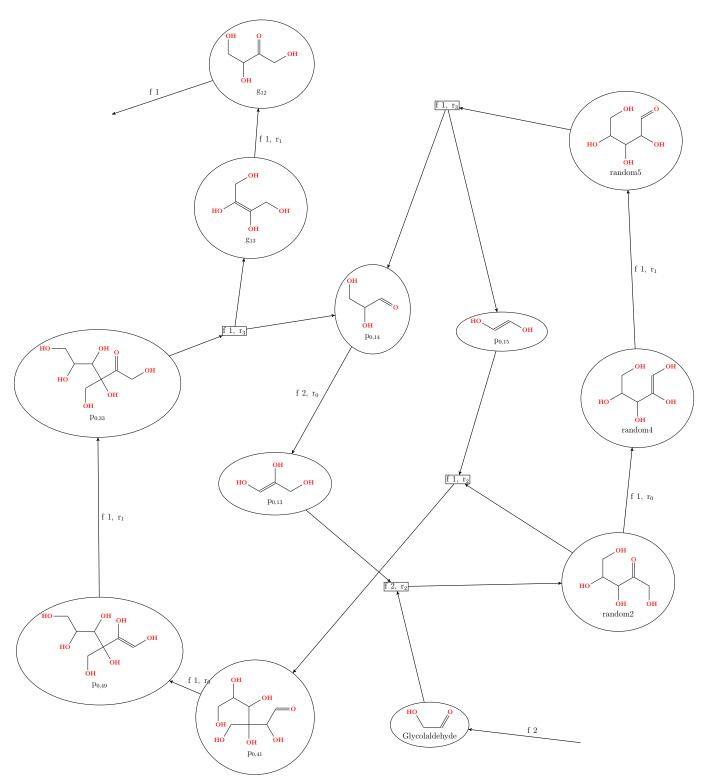
File: out/244\_dg\_0\_11100\_f\_5\_0\_filt

# 0.14 Flow Solutions, id 6

#### 0.14.1 Solution 0

#### Overall Data

Objective value (integral): -1 Vertex/Graph In Out



 $File: \ \mathtt{out/248\_dg\_0\_11100\_f\_6\_0\_filt}$ 

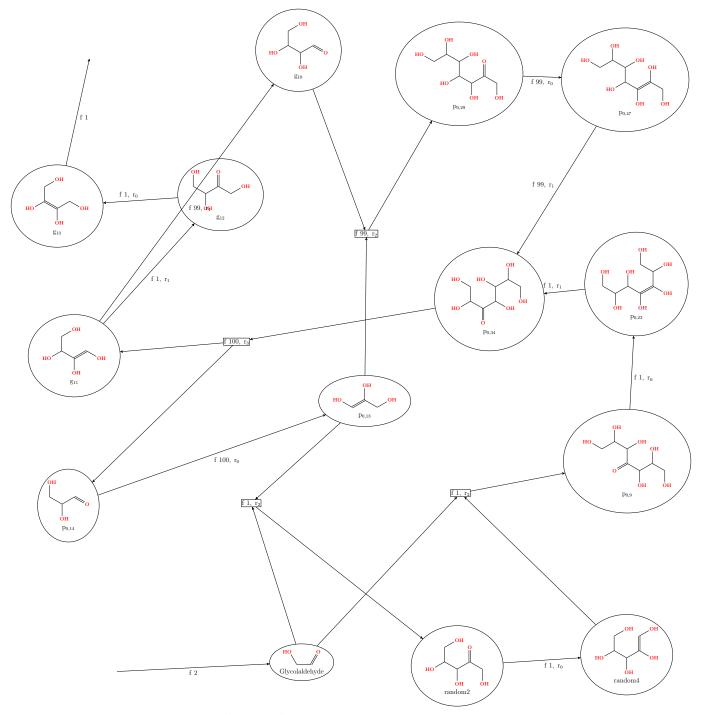
### 0.15 Flow Solutions, id 7

#### 0.15.1 Solution 0

#### Overall Data

Objective value (integral): -1 Vertex/Graph In Out Glycolaldehyde 2 0 g\_{13} 0 1

#### Filtered Graph



File: out/252\_dg\_0\_11100\_f\_7\_0\_filt