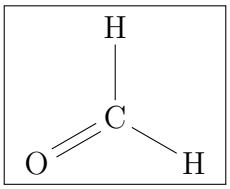
Summary

October 16, 2019

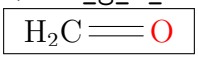
Contents

0.1 Loaded Graphs

0.1.1 `Formaldehyde`

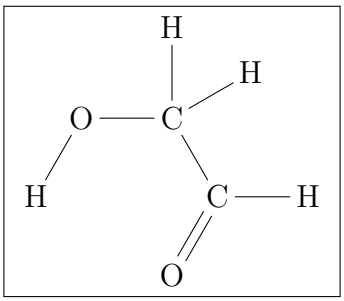


File: `out/000_g_0_10300000`

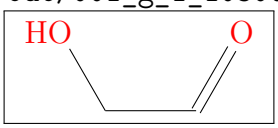


File: `out/000_g_0_11310100`

0.1.2 `Glycolaldehyde`



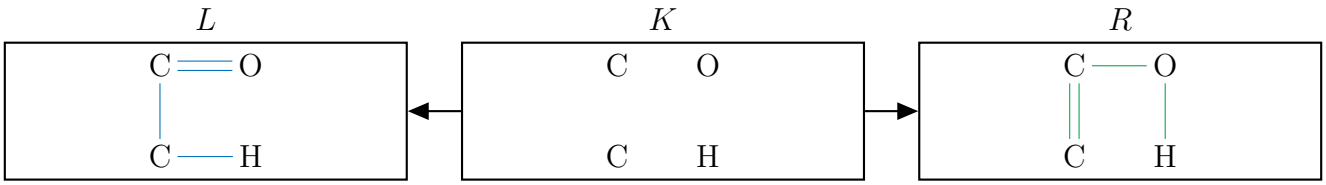
File: `out/001_g_1_10300000`



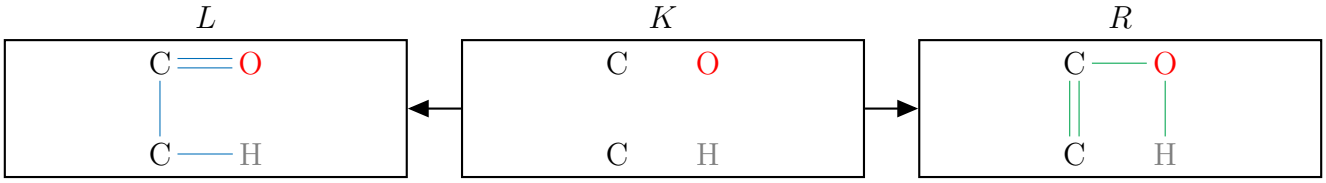
File: `out/001_g_1_11310100`

0.2 Loaded Rules

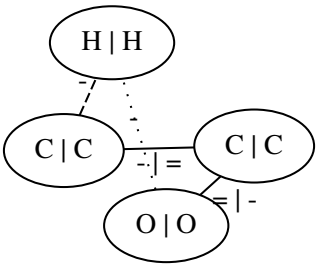
0.2.1 Keto-enol isomerization ->



Files: out/003_r_0_10300000_{L, K, R}



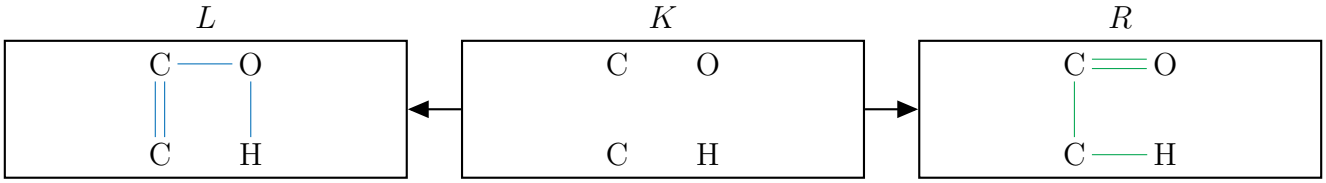
Files: out/004_r_0_11300100_{L, K, R}



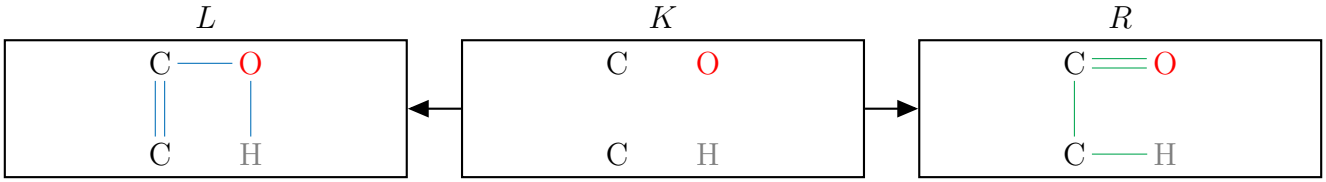
File: out/005_r_0_combined

$$|\{e \in \text{outEdges}(1) \mid \text{label}(\text{target}(e)) \in \{\text{'O'}\}\}| = 1$$

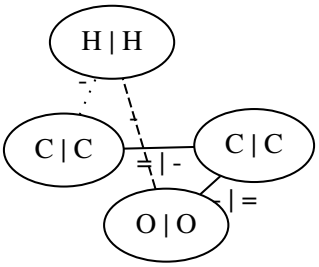
0.2.2 Keto-enol isomerization <-



Files: out/008_r_1_10300000_{L, K, R}



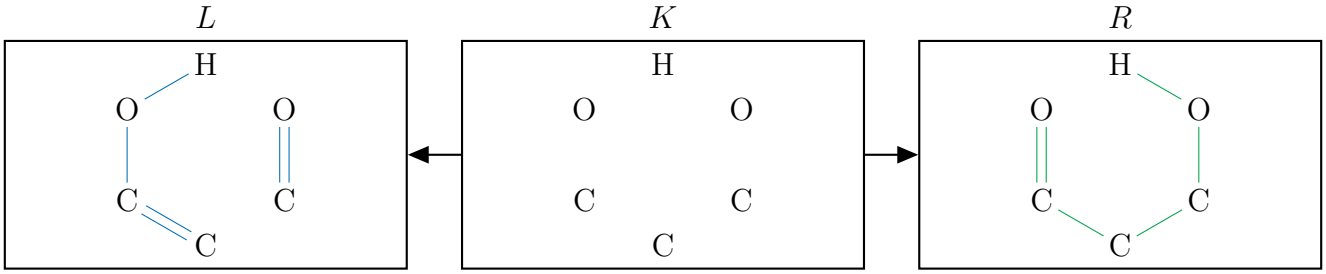
Files: out/009_r_1_11300100_{L, K, R}



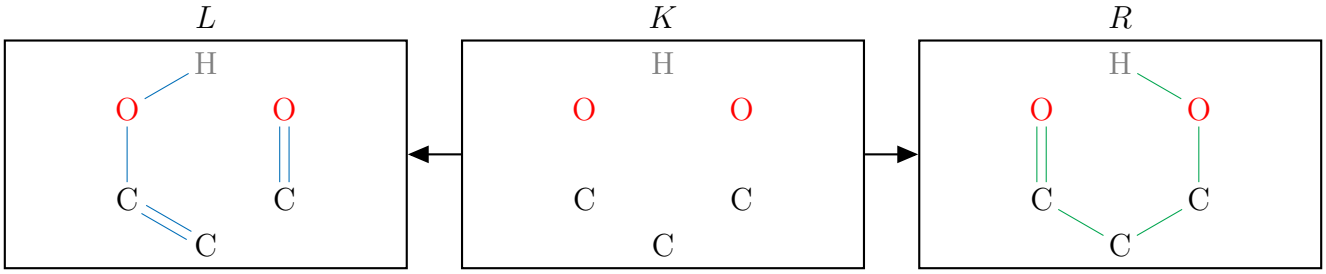
File: out/010_r_1_combined

$$|\{e \in \text{outEdges}(1) \mid \text{label}(\text{target}(e)) \in \{\text{'O'}\}\}| = 1$$

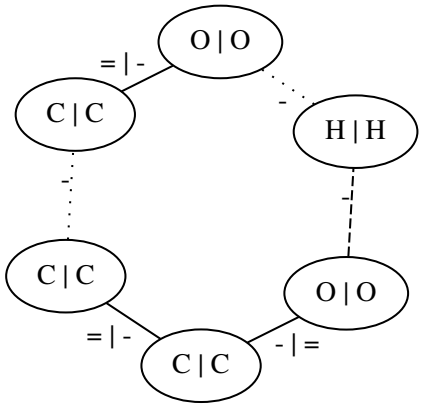
0.2.3 Aldol Addition ->



Files: out/013_r_2_10300000_{L, K, R}



Files: out/014_r_2_11300100_{L, K, R}

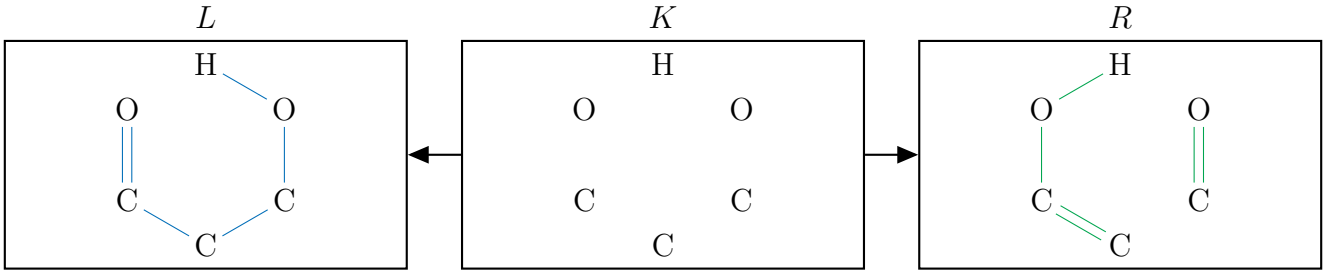


File: out/015_r_2_combined

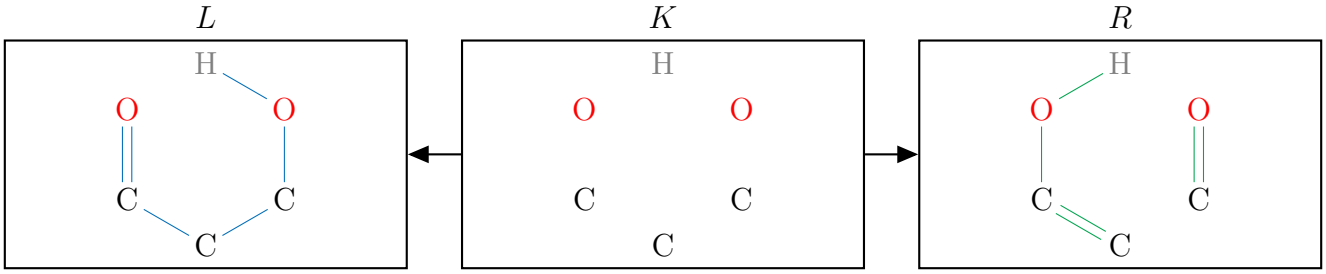
$$|\{e \in \text{outEdges}(1) \mid \text{label}(\text{target}(e)) \in \{\text{'O'}\}\}| = 1$$

$$|\{e \in \text{outEdges}(5) \mid \text{label}(\text{target}(e)) \in \{\text{`O'}\}\}| = 1$$

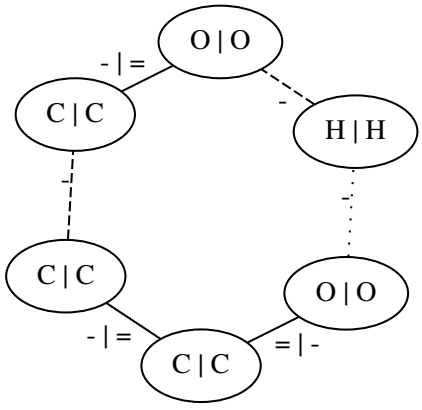
0.2.4 Aldol Addition <-



Files: out/018_r_3_10300000_{L, K, R}



Files: out/019_r_3_11300100_{L, K, R}

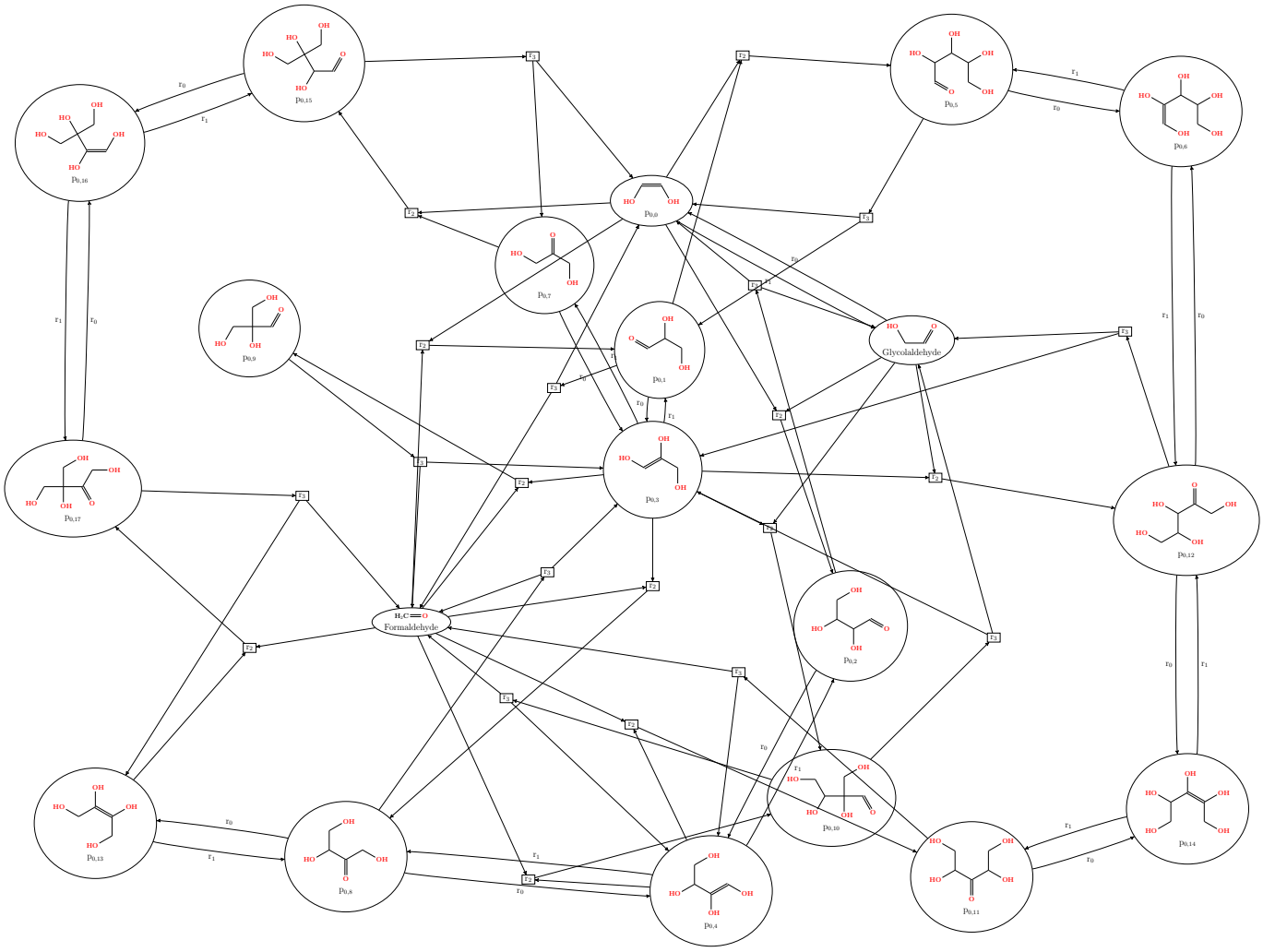


File: out/020_r_3_combined

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

$$|\{e \in \text{outEdges}(5) \mid \text{label}(\text{target}(e)) \in \{\text{'O'}\}\}| = 1$$

0.2.5 DG Hyper, `dg_0`



File: `out/041_dg_0_11100`

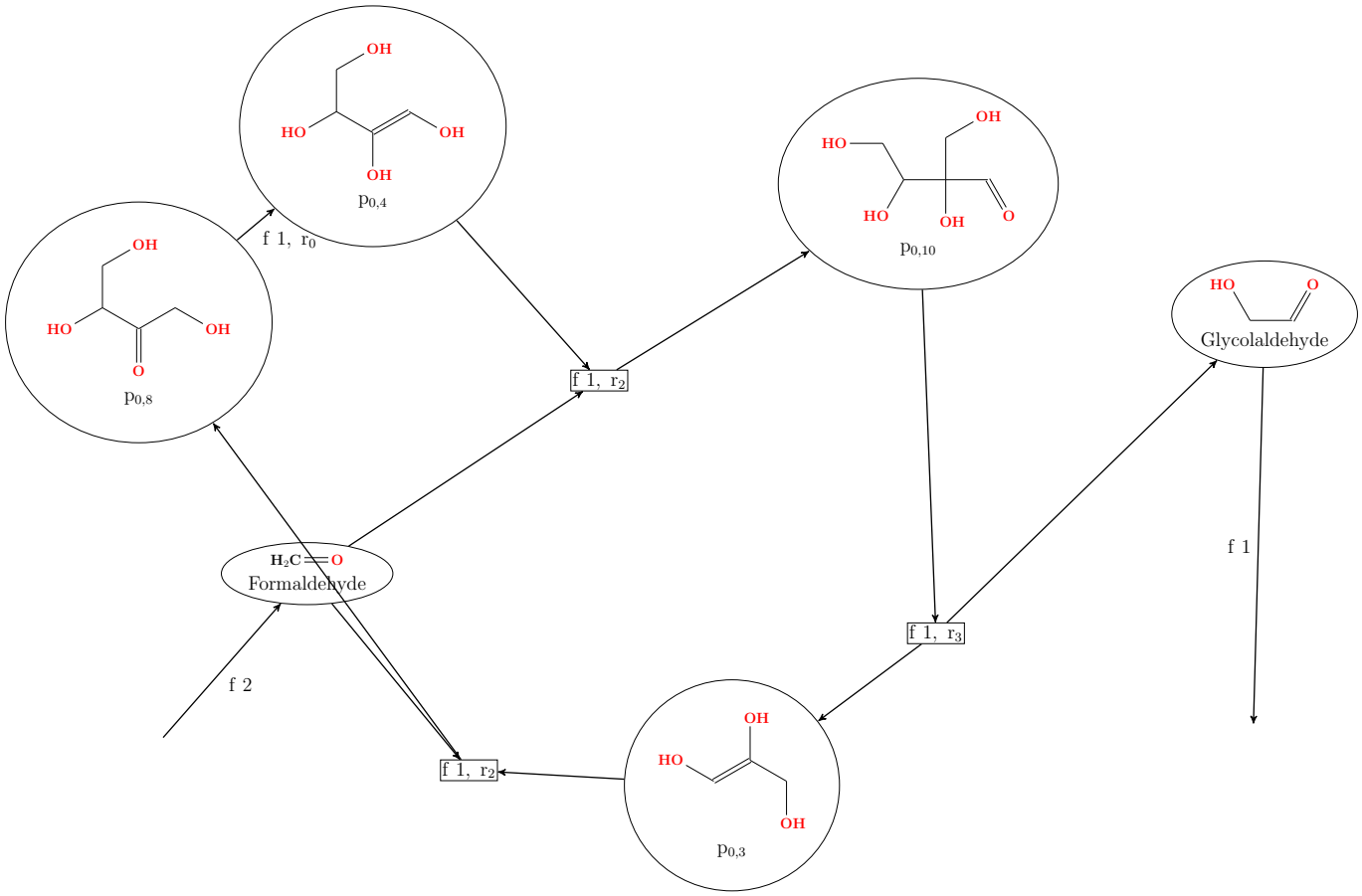
0.3 Flow Solutions, id 0

0.3.1 Solution 0

Overall Data

```
Solution 0 from flow model 0
Objective value: 6
Formaldehyde: inFlow = 2 outFlow = 0 isInCycle = false
Glycolaldehyde: inFlow = 0 outFlow = 1 isInCycle = false
```

Filtered Graph



File: `out/045_dg_0_11100_f_0_0_filt`

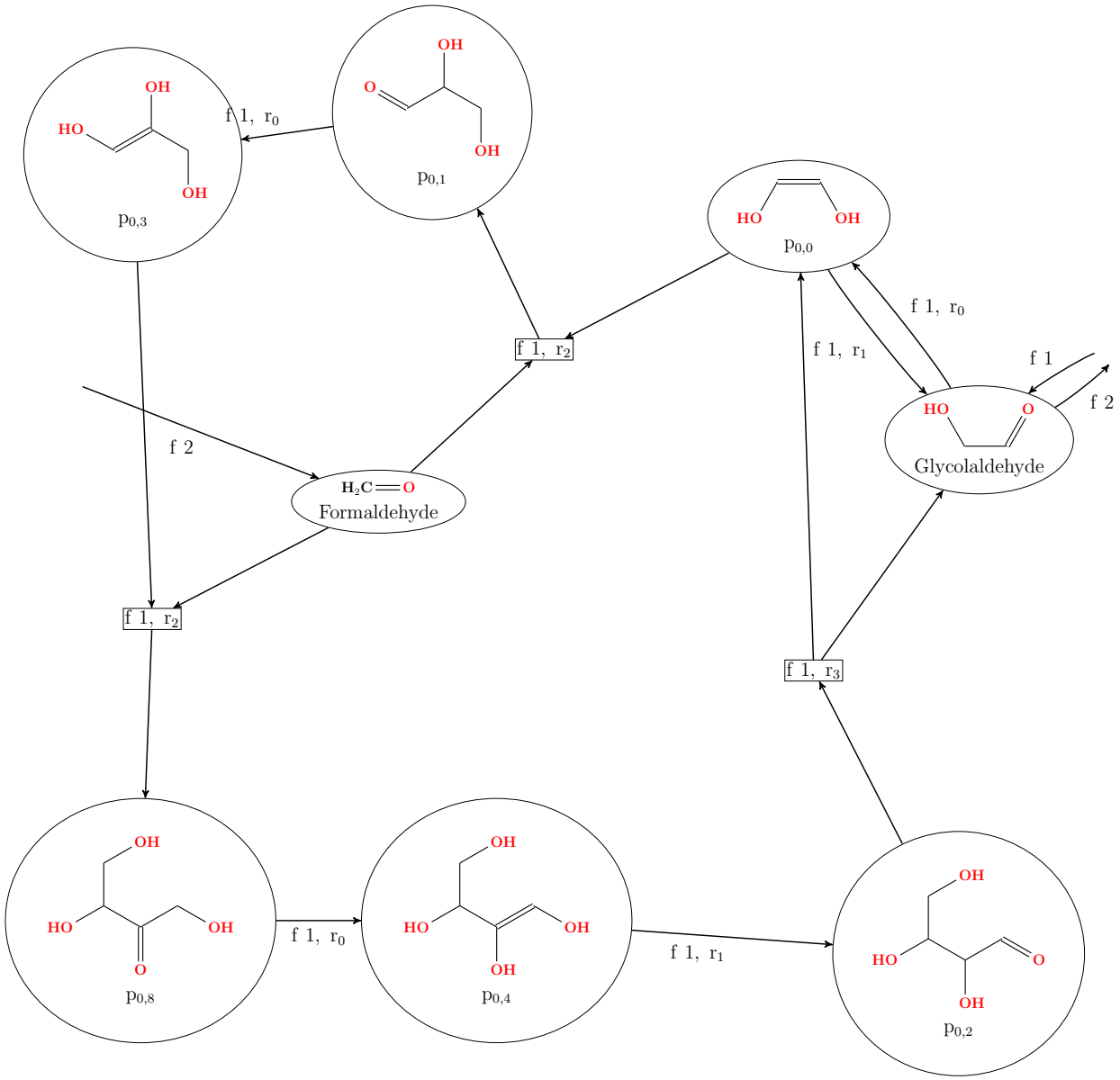
0.4 Flow Solutions, id 1

0.4.1 Solution 0

Overall Data

```
Solution 0 from flow model 1
Objective value: 12
Formaldehyde: inFlow = 2 outFlow = 0 isOverallAutocata = 0 isInCycle = false
Glycolaldehyde: inFlow = 1 outFlow = 2 isOverallAutocata = 1 isInCycle = true
```

Filtered Graph



File: `out/049_dg_0_11100_f_1_0_filt`