Decomposition and Evaluation of Graph Transformation Rules

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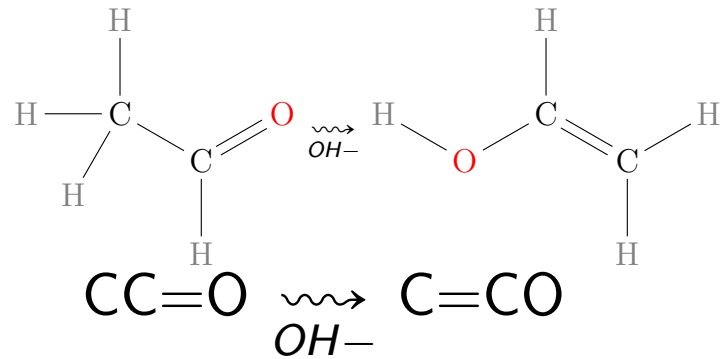
My master

- Systematically find reaction mechanisms
- Elementary steps, using few general graph transformation rules
- Replaceable objective and evaluation function



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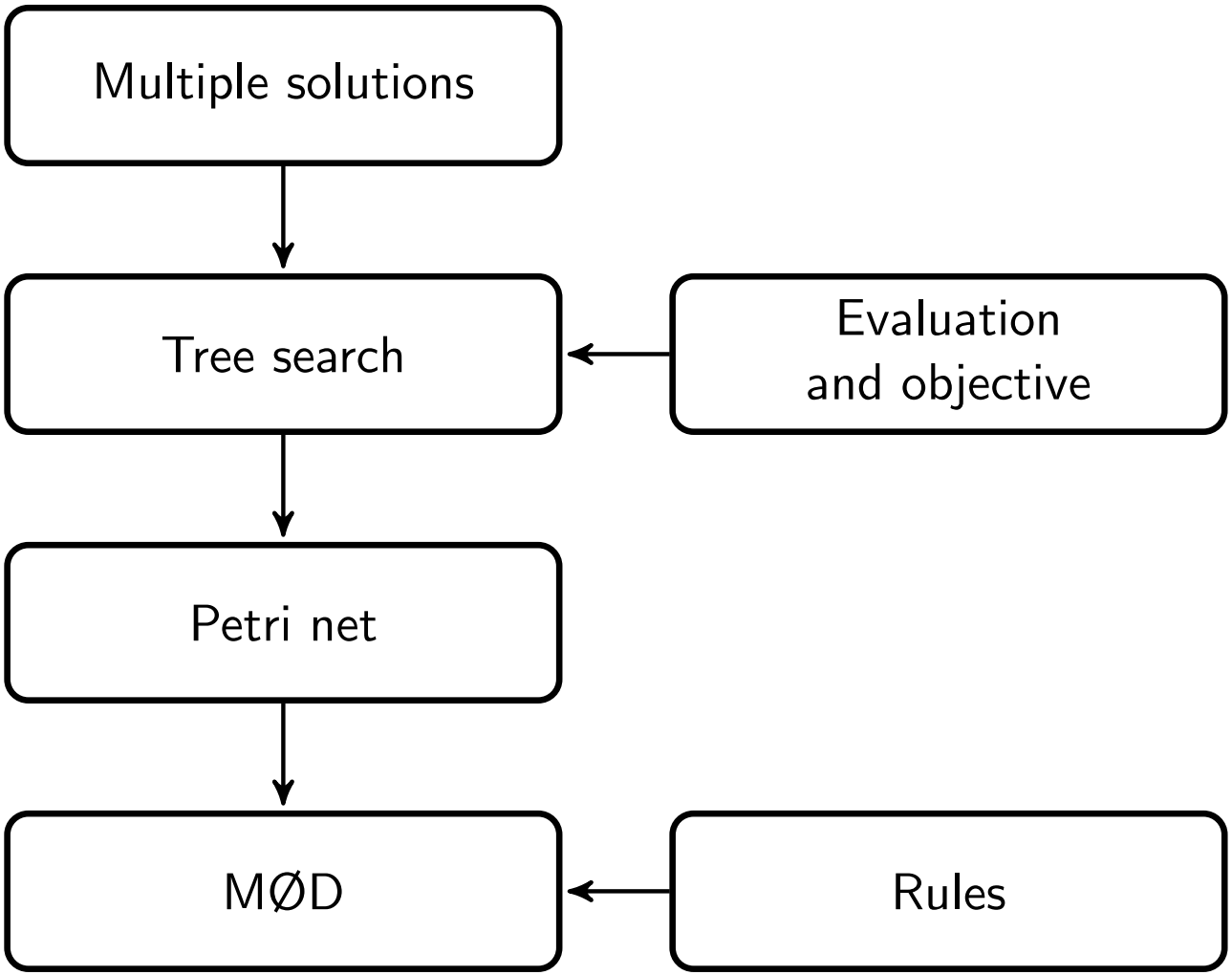
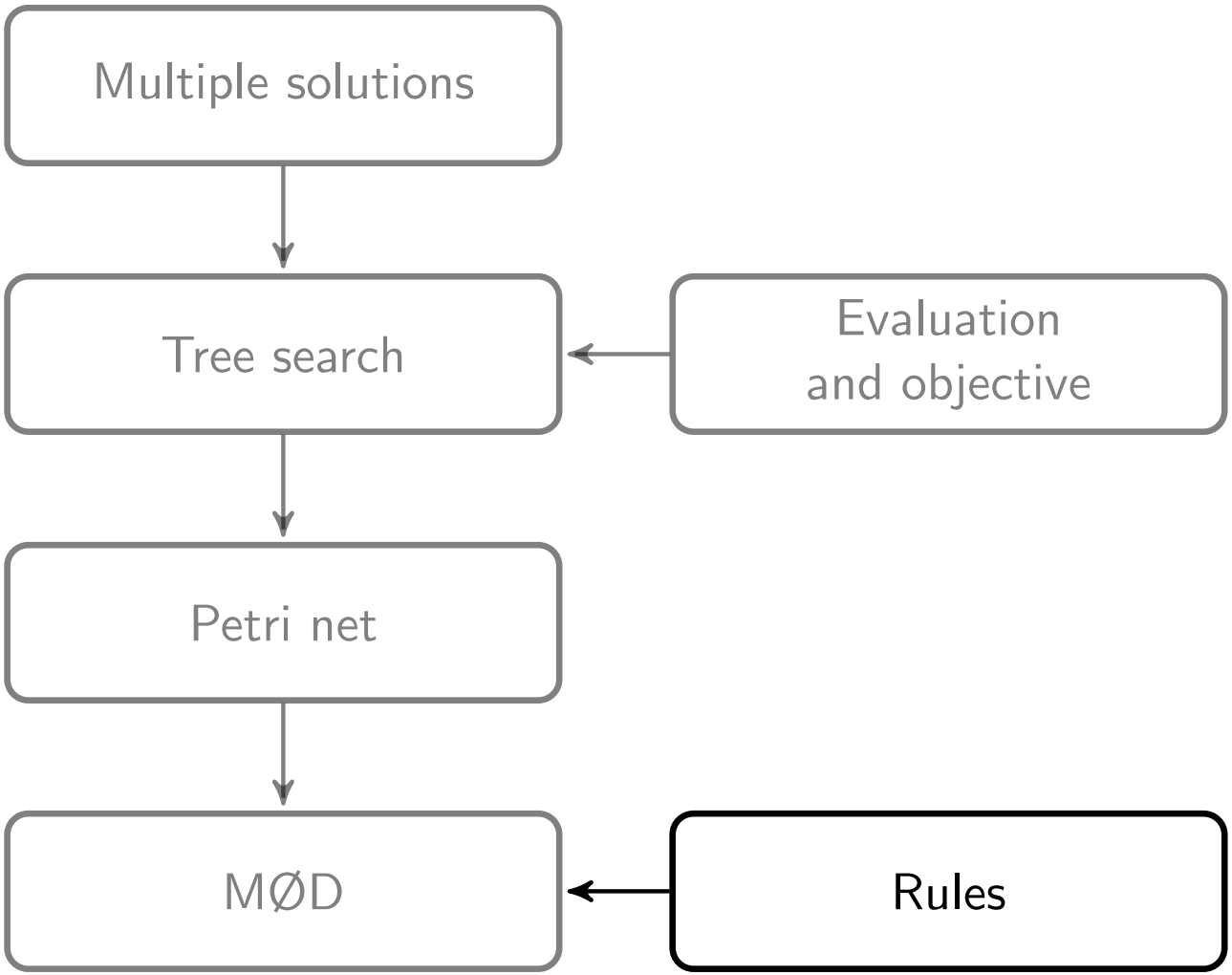

Multiple solutions
Tree search
Evaluation
and objective
Petri net
MØD
Rules

My master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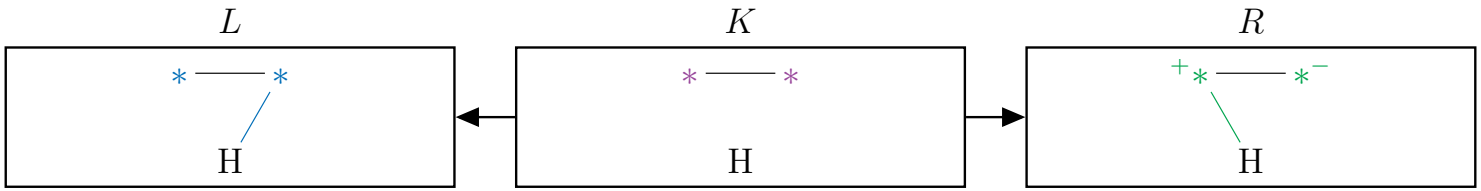
Rules

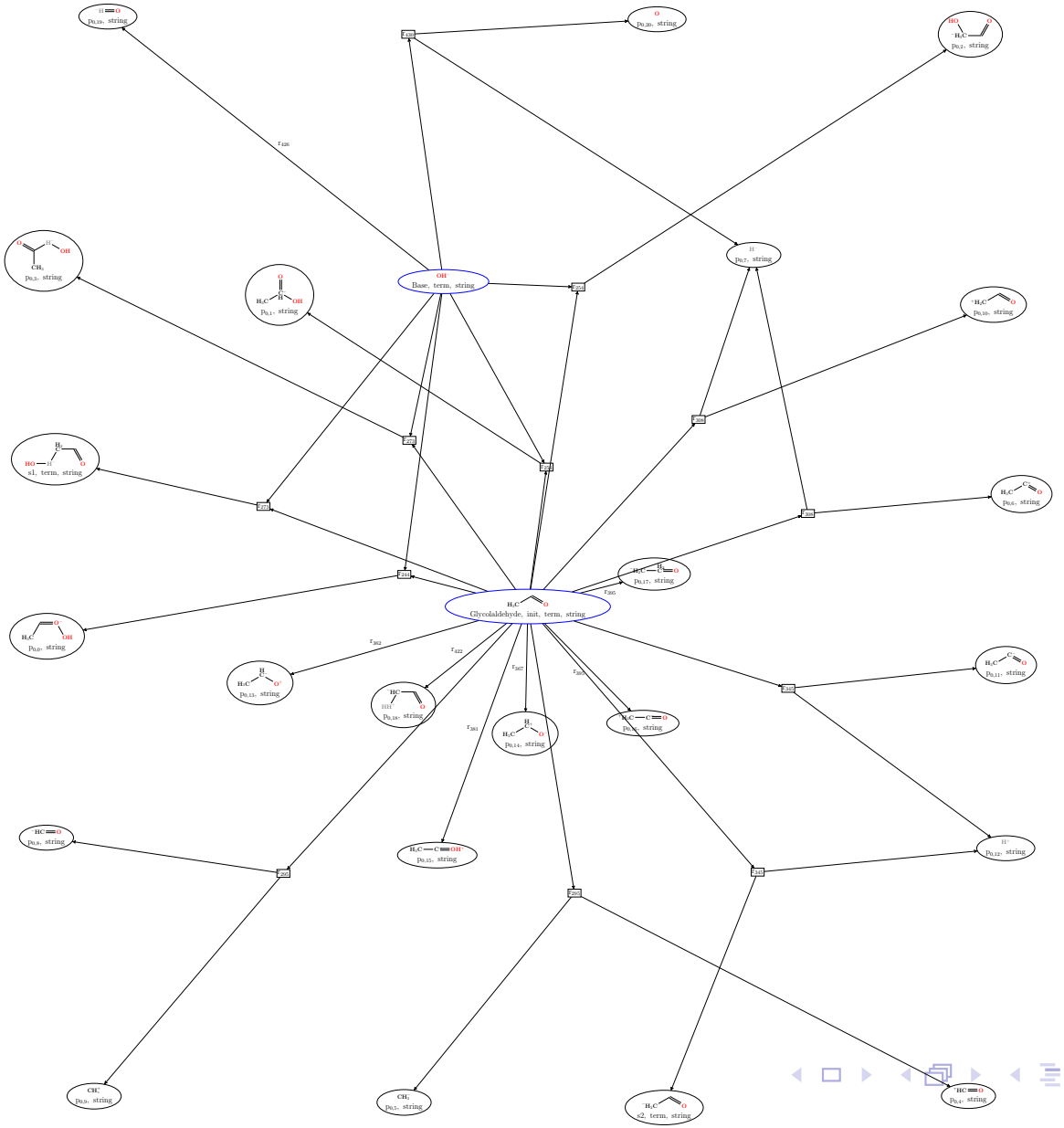
Charge seperation

Hydrogen move



Rules

1 iteration (23 new nodes)



Rules

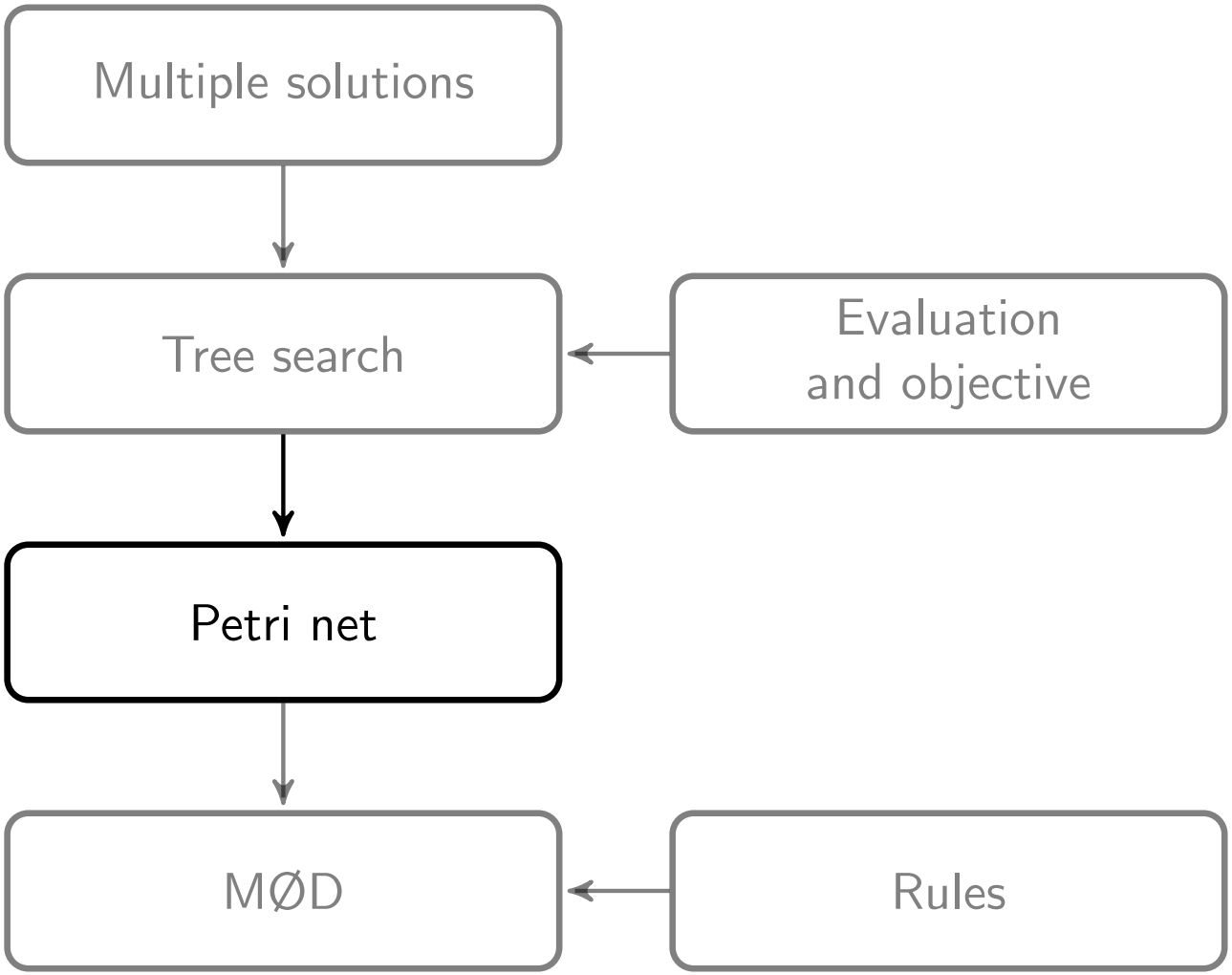
Full reaction network:
100 000+ nodes

Rules

Full reaction network:
100.000+ nodes

Disallow:
Rings of 3 and 4 atoms
C with less then 3 bonds
H with a double bond or H+ with 2 bonds

New reaction network:
40 000 nodes
14 000 them are allowed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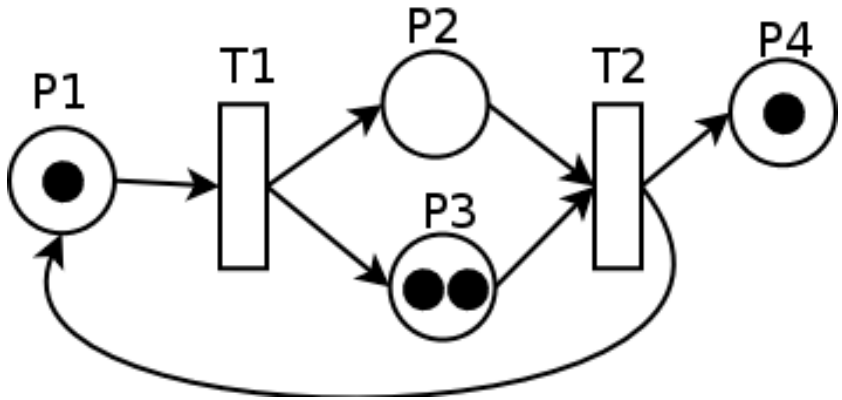
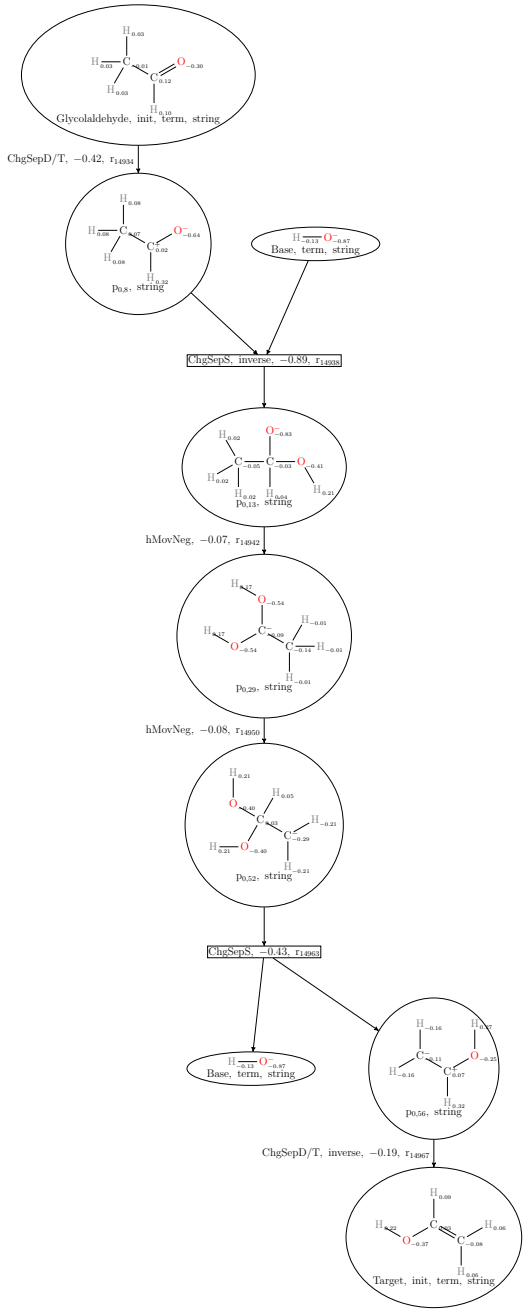
Petri net

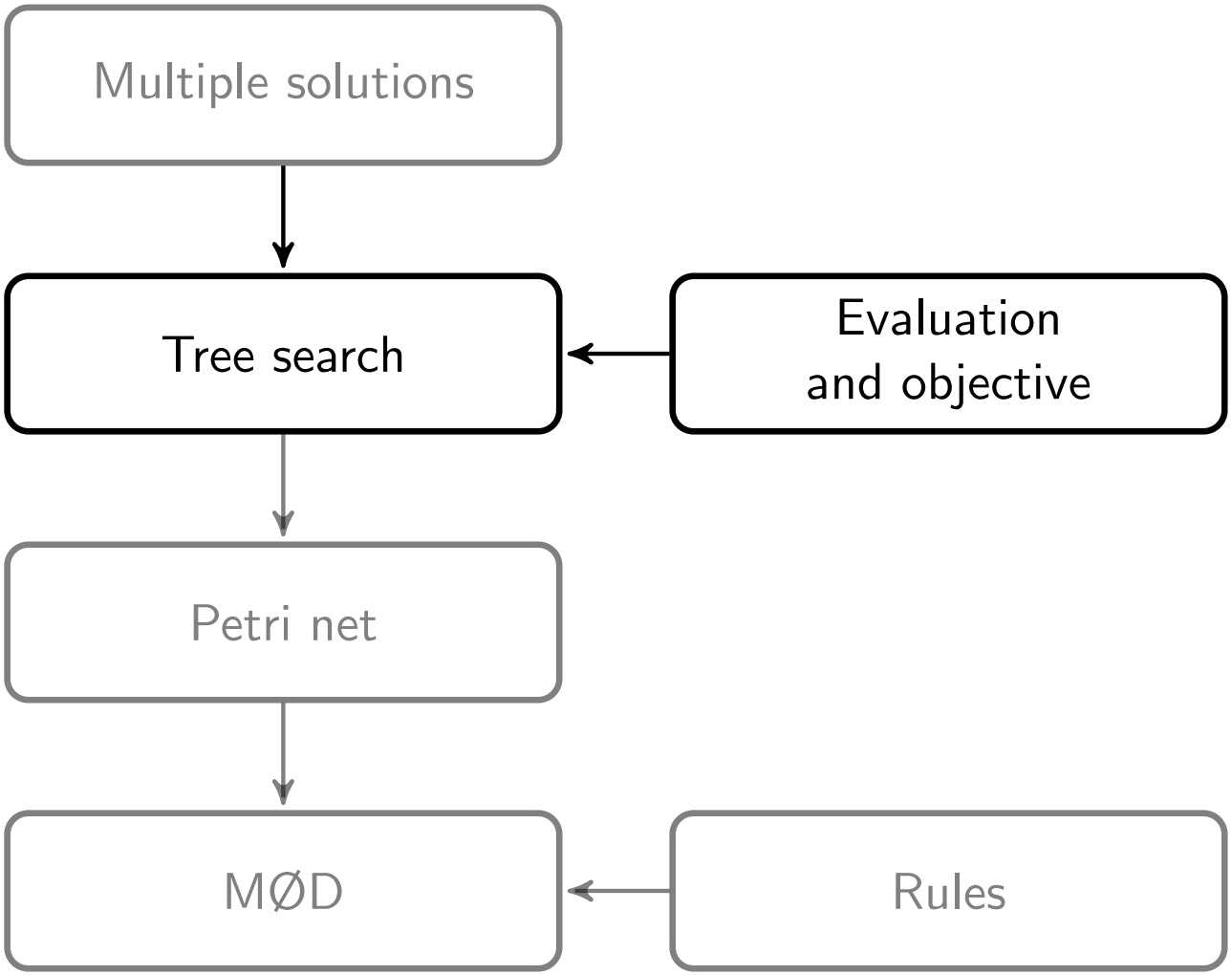


Molecules are places
Rules applied are the transitions
Tokens used to represent current molecules
Markings are different states of the reaction

States: 18 000

Petri net


Glycolaldehyde, init, term, string
ChgSepD/T, −0.42, r14934
p0,8, string
Base, term, string
ChgSepS, inverse, −0.89, r14938
p0,13, string
hMovNeg, −0.07, r14942
p0,29, string
hMovNeg, −0.08, r14950
p0,52, string
ChgSepS, −0.43, r14963
Base, term, string
p0,56, string
ChgSepD/T, inverse, −0.19, r14967
Target, init, term, string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Tree search

Search though markings
Use A*/Dijkstra like search
Evaluation function for edges between markings
Objective function to minimize

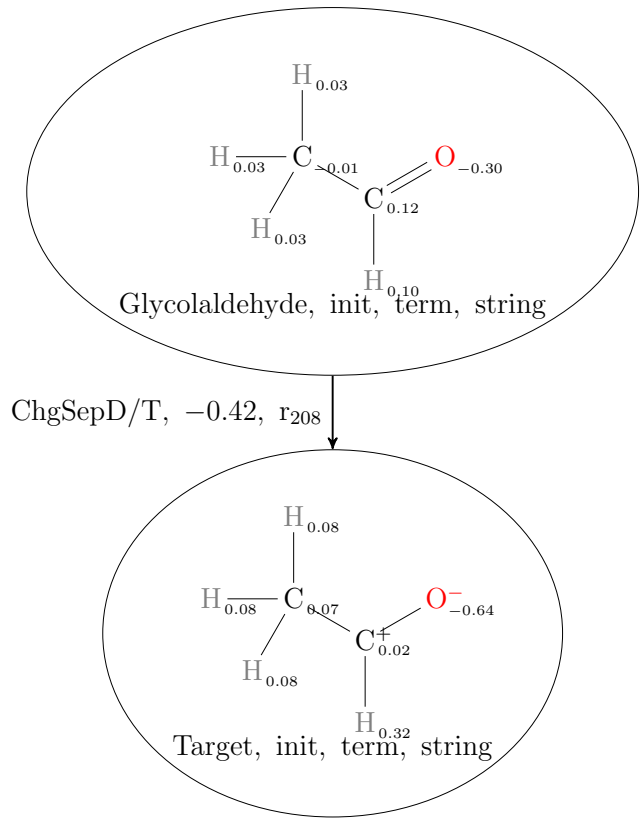
Objective and Evaluation

Partial charge

Use libary to calculate Gasteiger charges
Calculate difference between atoms

atom gaining electron − atom giving electron

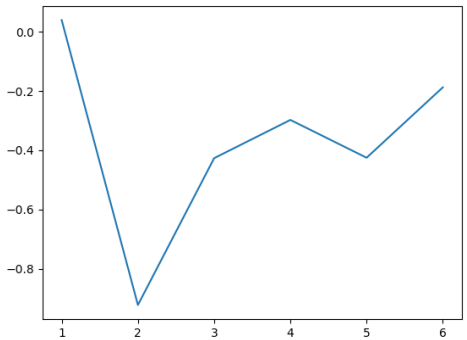
$-0.30 - 0.12 = -0.42$



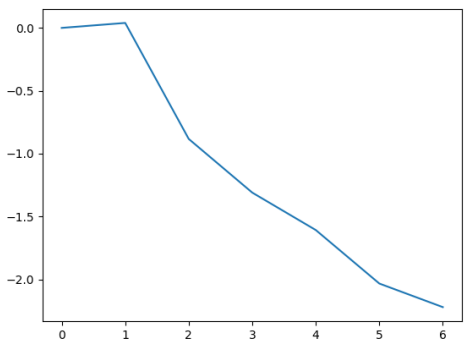
Objective and Evaluation

Partial charge

Min sum

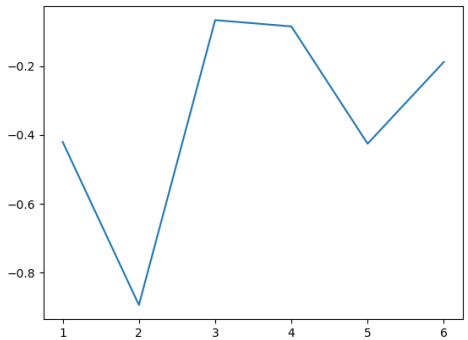


Edge weights

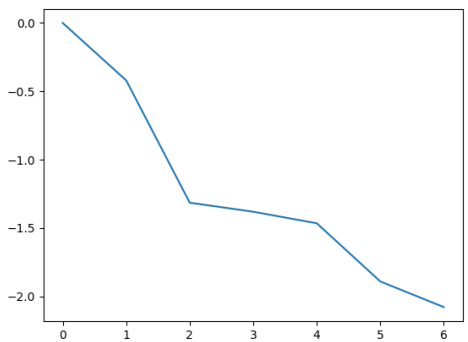


Cumulative weights

Min maximum

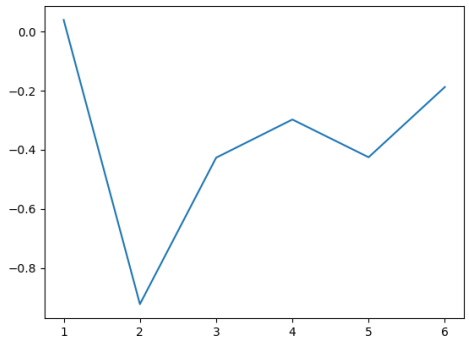


Edge weights



Cumulative weights

Min #sign changes



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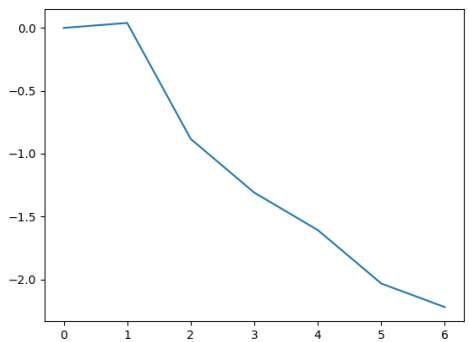

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Objective and Evaluation

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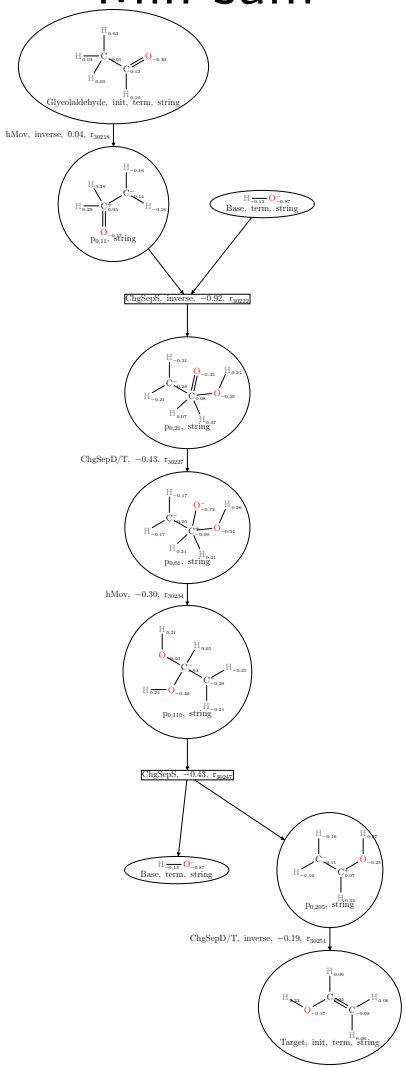
Min sum



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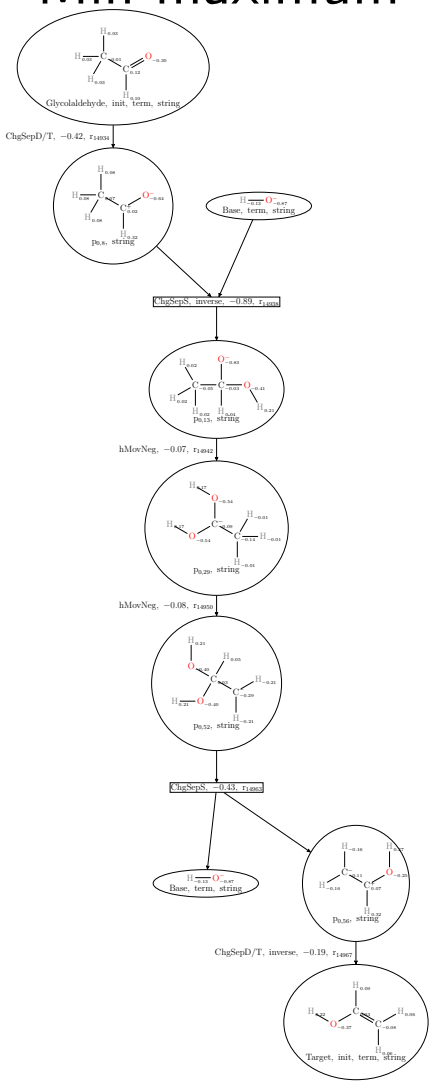

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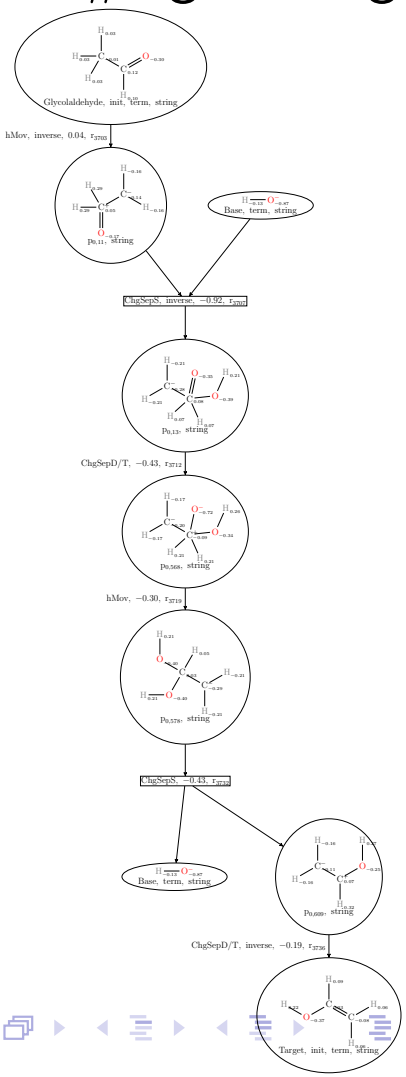


Objective and Evaluation

Energy

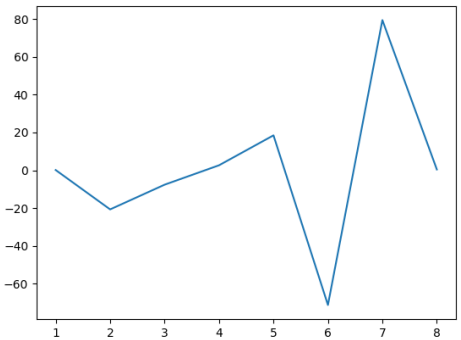
Use libary to calculate energy using force field (Merck Molecular Force Field)
Calculate difference in total energy

Some molecules could not be embedded to 3D

Objective and Evaluation

Energy

Min sum



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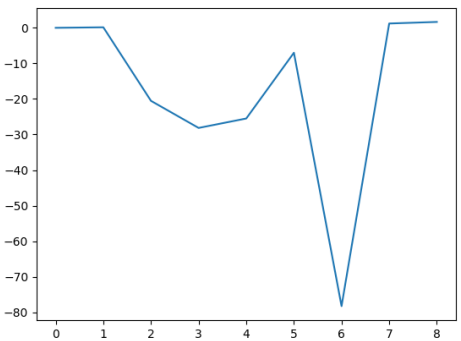

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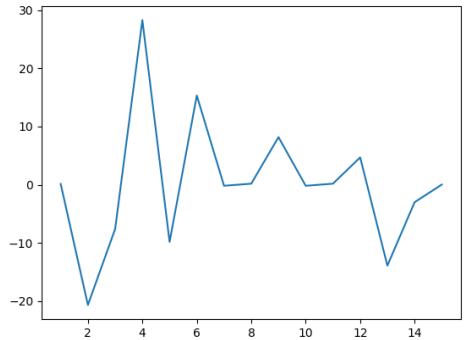
Min maximum



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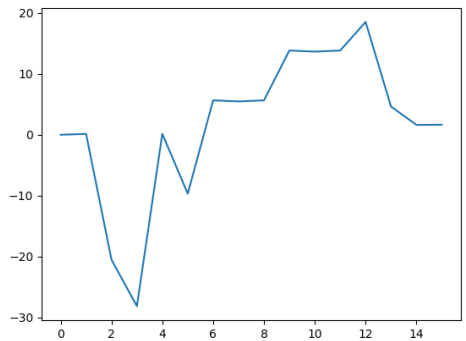

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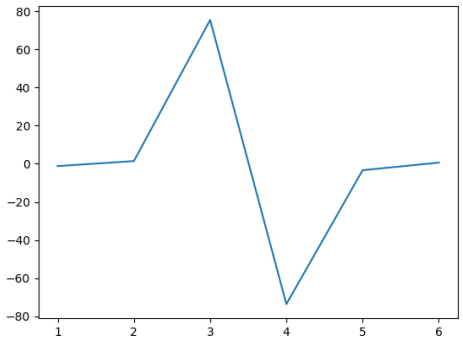

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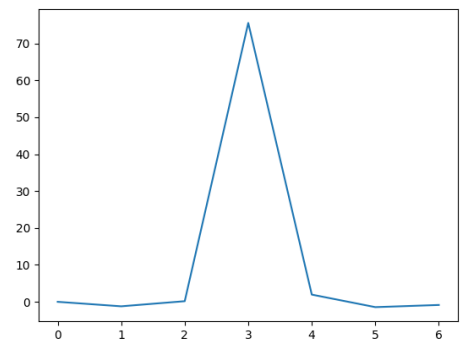
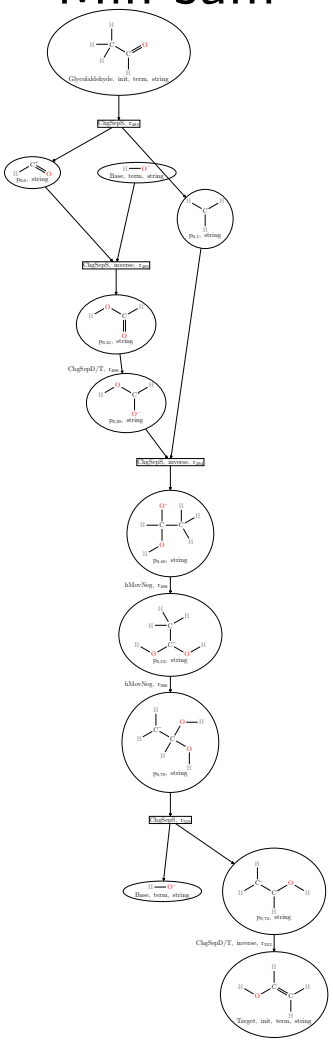


Cumulative weights

Objective and Evaluation

Energy

Min sum



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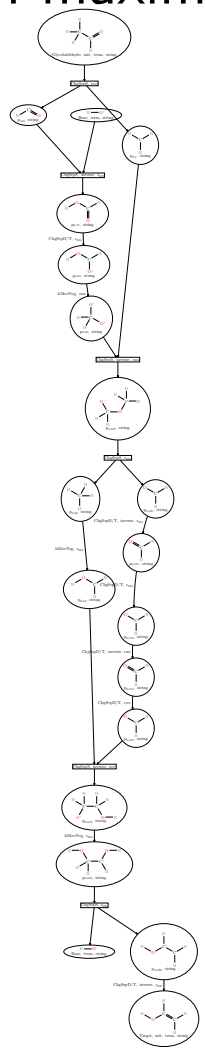

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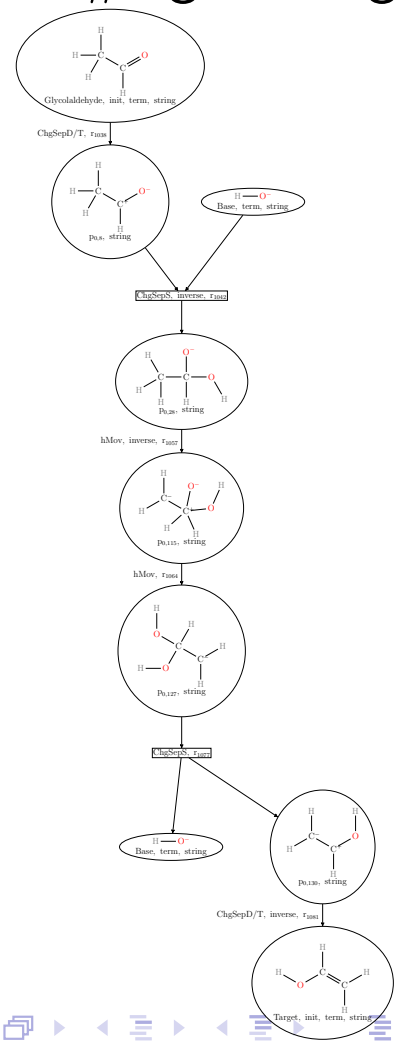

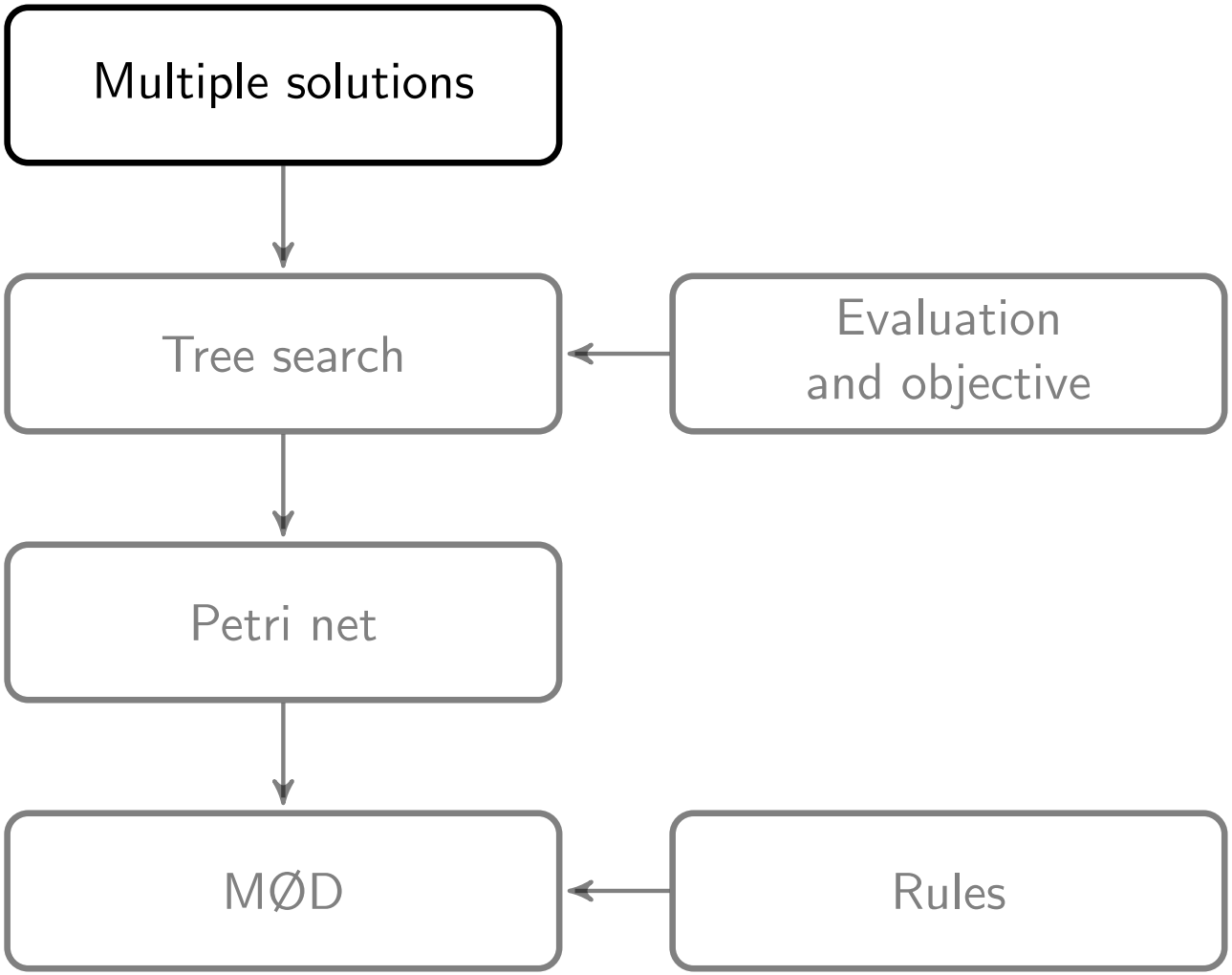
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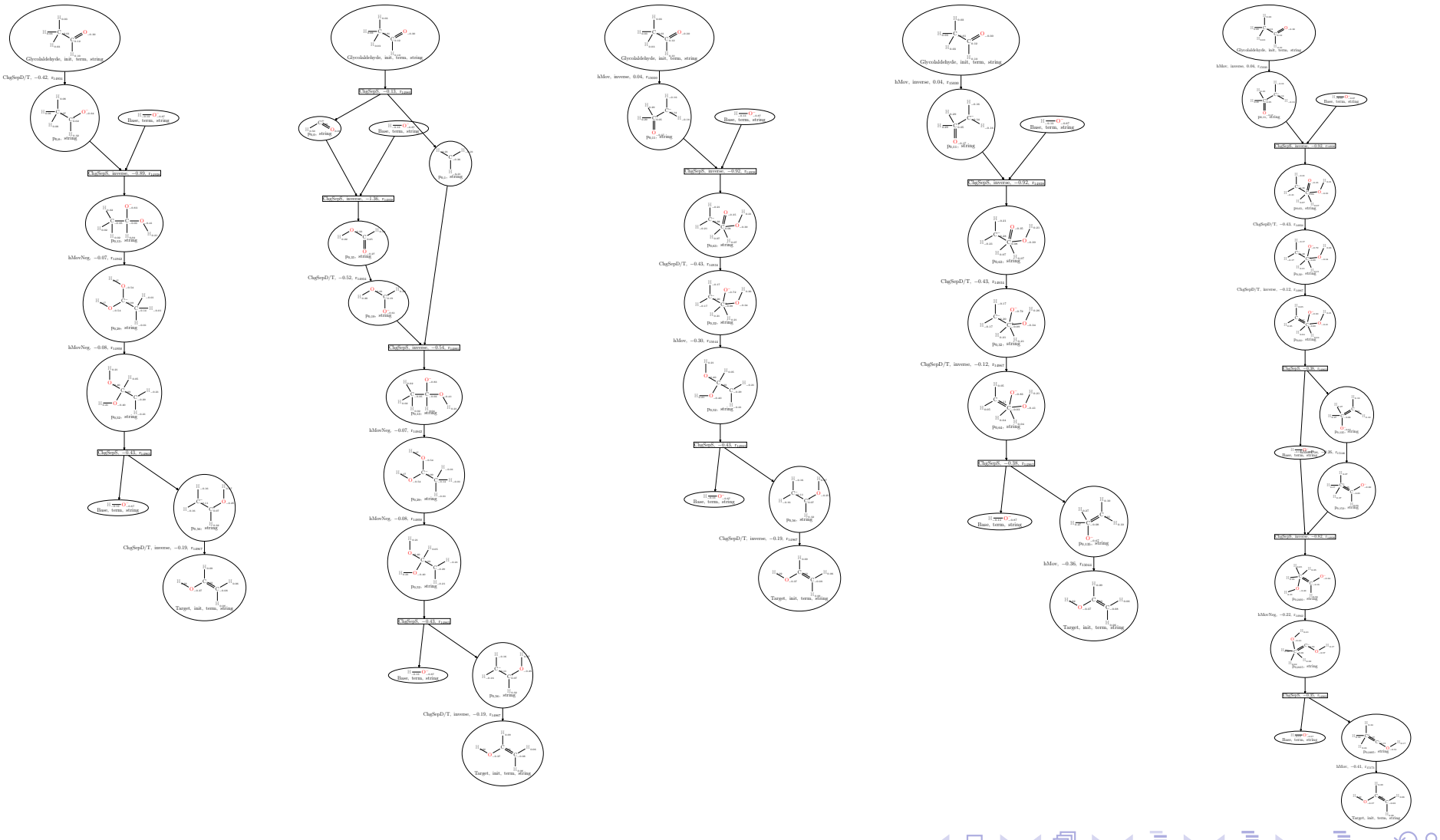
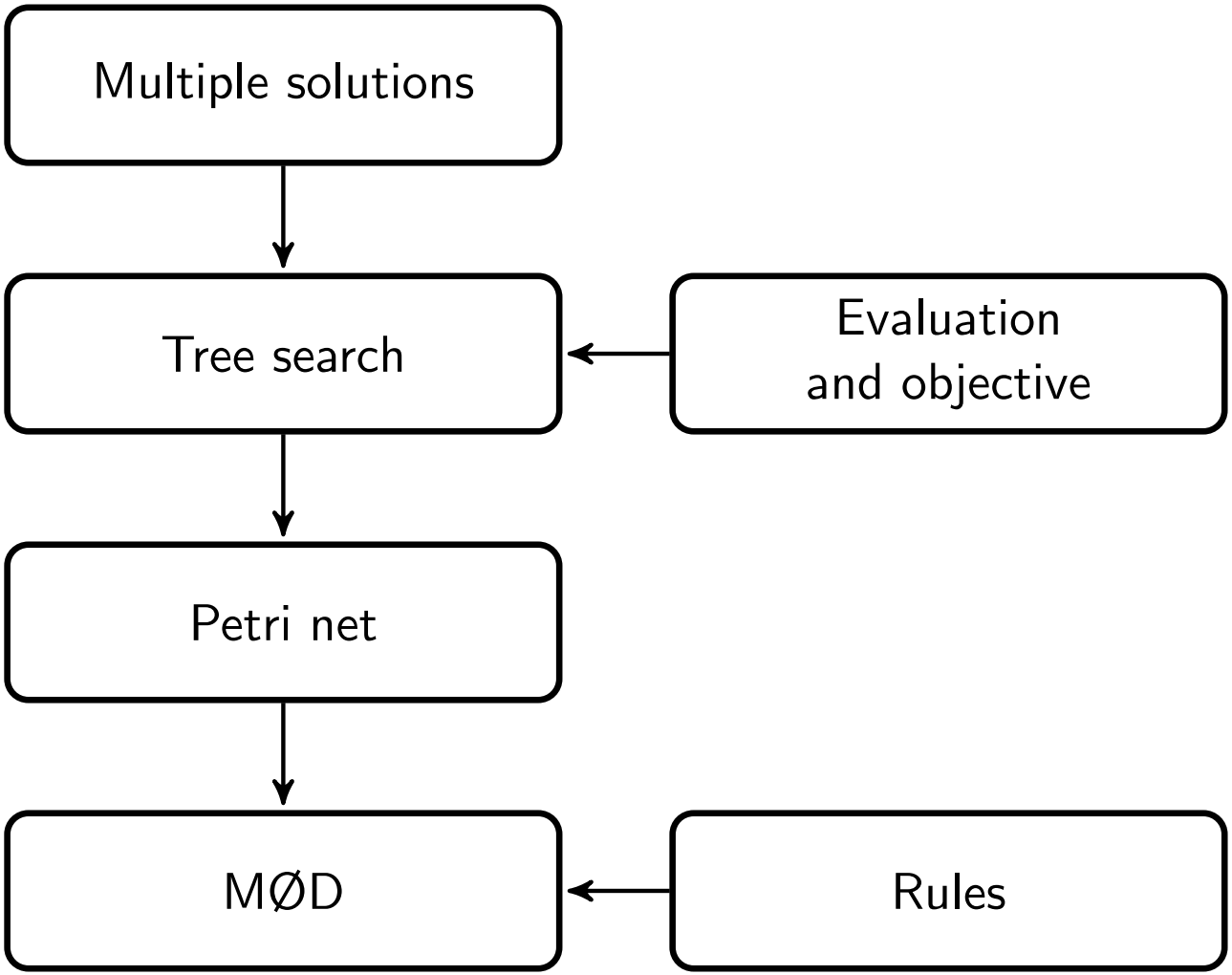
Multiple solutions

Partial charge, Min maximum

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