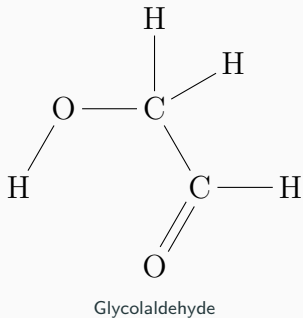
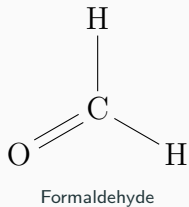
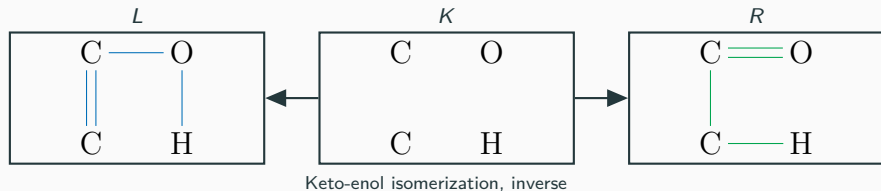
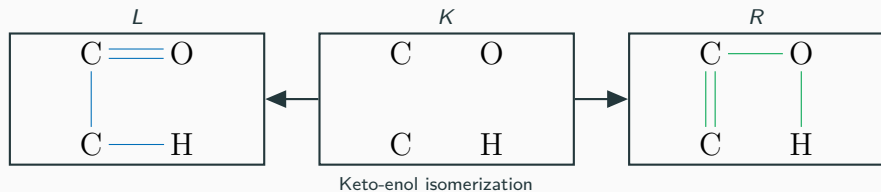


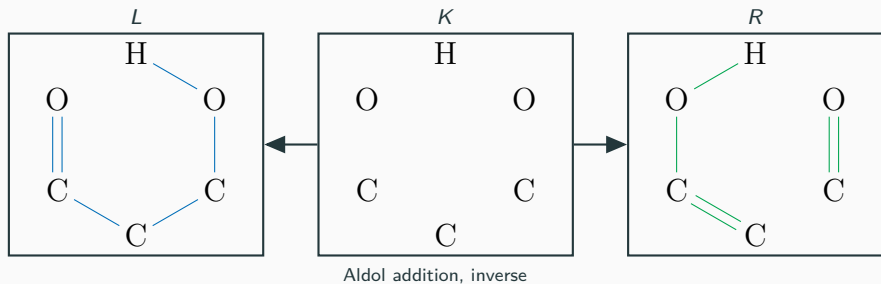
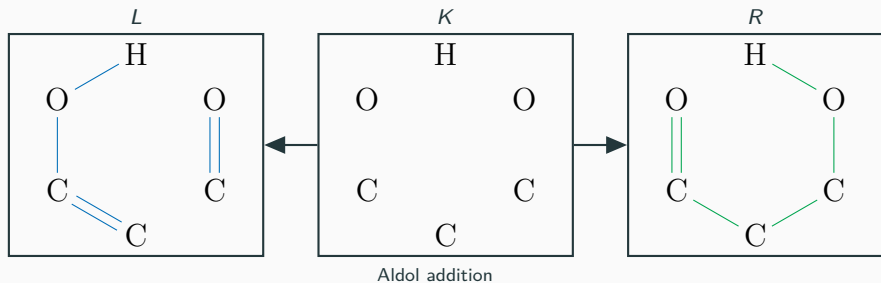
## The Beginning: A look at MØD



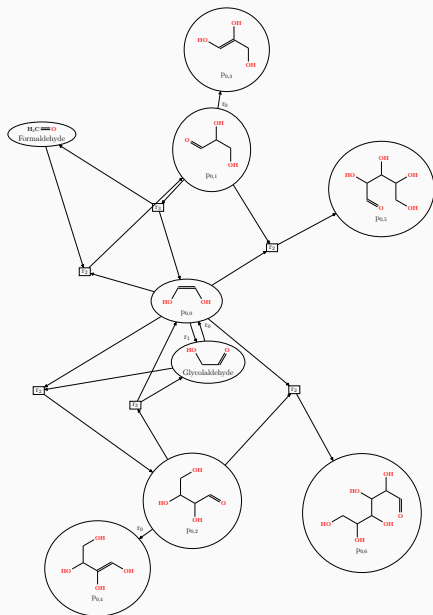
# The Beginning: A look at MØD



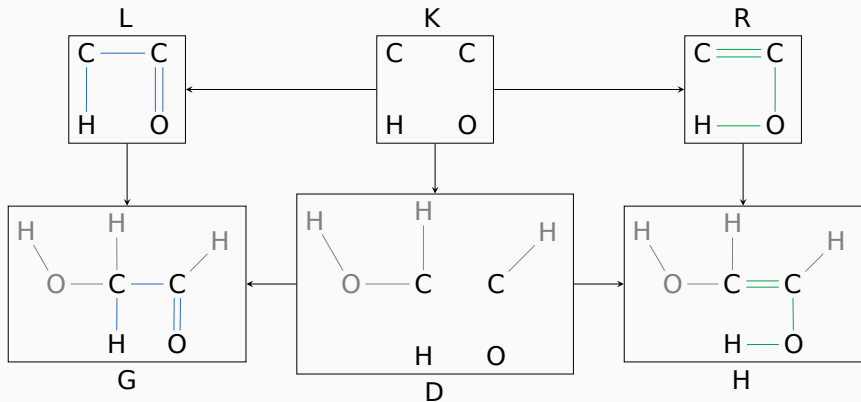
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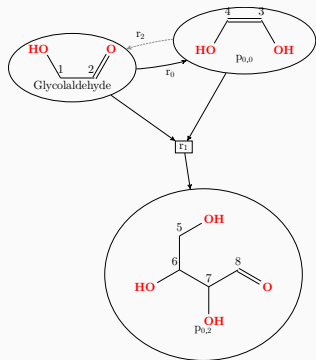
# The Beginning: A look at MØD



# Tracking Atoms Through Reactions

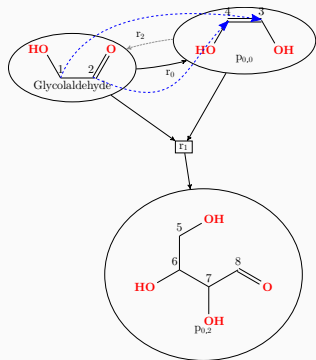


# The Characteristic Semigroup of Reaction Networks



Marc Hellmuth, Daniel Merkle, and **Nikolai Nøjgaard**, *Atom tracking using cayley graphs*, 16th International Symposium on Bioinformatics Research and Applications (accepted) (2020)

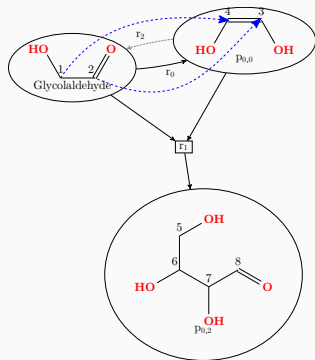
# The Characteristic Semigroup of Reaction Networks



$$s_1 = [3, 4, 3, 4, 5, 6, 7, 8]$$

Marc Hellmuth, Daniel Merkle, and Nikolai Nøjgaard, *Atom tracking using cayley graphs*, 16th International Symposium on Bioinformatics Research and Applications (accepted) (2020)

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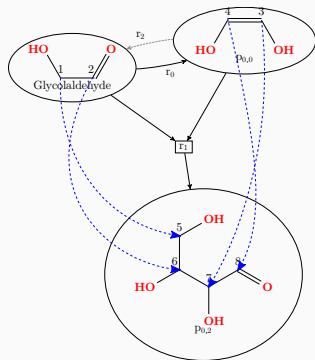
$$s_1 = [3, 4, 3, 4, 5, 6, 7, 8]$$

$$s_2 = [4, 3, 3, 4, 5, 6, 7, 8]$$

Marc Hellmuth, Daniel Merkle, and Nikolai Nøjgaard, *Atom tracking using cayley graphs*, 16th International Symposium on Bioinformatics Research and Applications (accepted) (2020)



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$$s_1 = [3, 4, 3, 4, 5, 6, 7, 8]$$

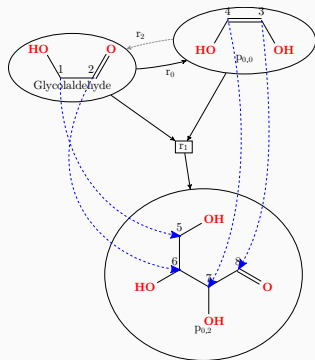
$$s_2 = [4, 3, 3, 4, 5, 6, 7, 8]$$

$$s_3 = [5, 6, 7, 8, 5, 6, 7, 8]$$

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Marc Hellmuth, Daniel Merkle, and Nikolai Nøjgaard, *Atom tracking using cayley graphs*, 16th International Symposium on Bioinformatics Research and Applications (accepted) (2020)

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$$s_1 = [3, 4, 3, 4, 5, 6, 7, 8]$$

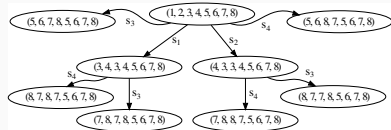
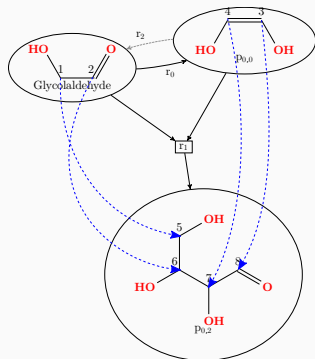
$$s_2 = [4, 3, 3, 4, 5, 6, 7, 8]$$

$$s_3 = [5, 6, 7, 8, 5, 6, 7, 8]$$

$$s_4 = [5, 6, 8, 7, 5, 6, 7, 8]$$

Marc Hellmuth, Daniel Merkle, and Nikolai Nøjgaard, *Atom tracking using cayley graphs*, 16th International Symposium on Bioinformatics Research and Applications (accepted) (2020)

# The Characteristic Semigroup of Reaction Networks



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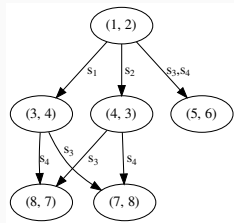
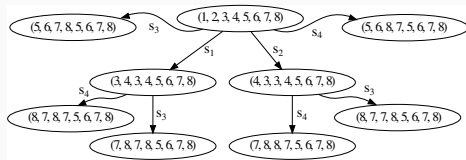
$$s_2 = [4, 3, 3, 4, 5, 6, 7, 8]$$

$$s_3 = [5, 6, 7, 8, 5, 6, 7, 8]$$

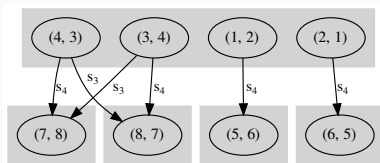
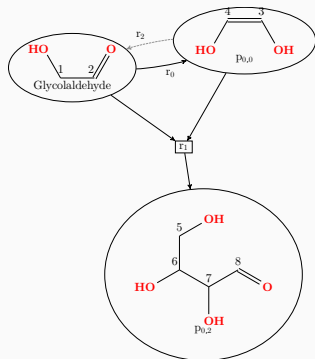
$$s_4 = [5, 6, 8, 7, 5, 6, 7, 8]$$

Marc Hellmuth, Daniel Merkle, and Nikolai Nøjgaard, *Atom tracking using cayley graphs*, 16th International Symposium on Bioinformatics Research and Applications (accepted) (2020)

# The Projected Cayley Graph



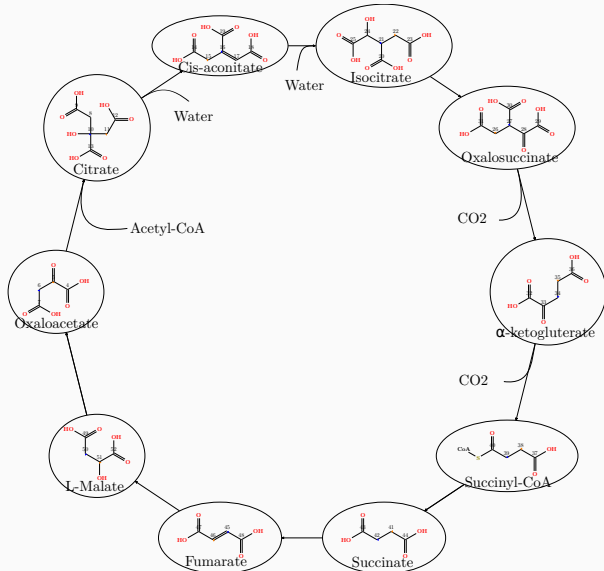
# Reversible Eventtraces



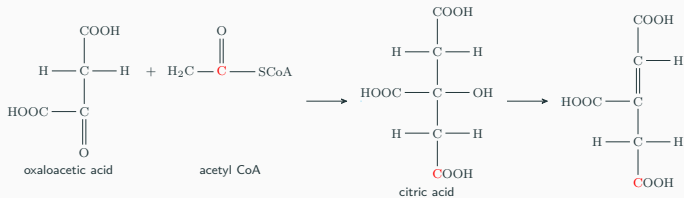
## Natural Subsystems

The natural subsystems of a characteristic semigroup is the set of equivalence classes induced by the  $\mathcal{R}$ -relation.

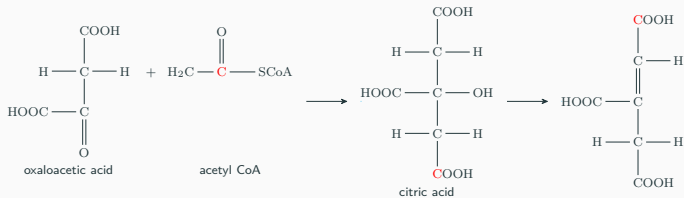
# The TCA Cycle



# Stereochemistry in Citrate

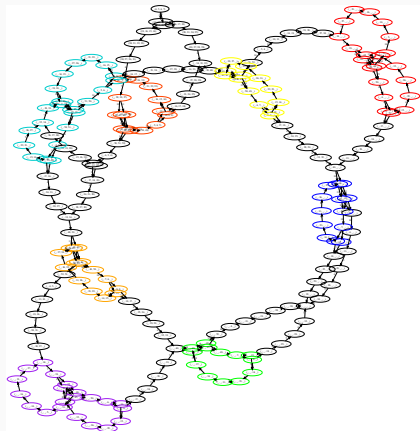
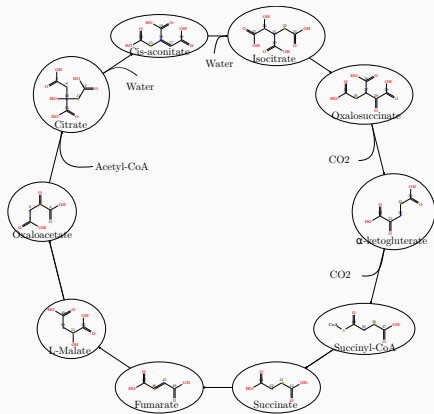
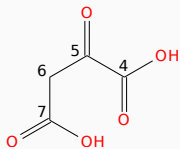


Correct Mechanism



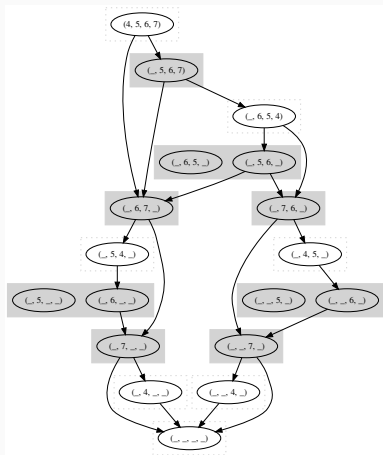
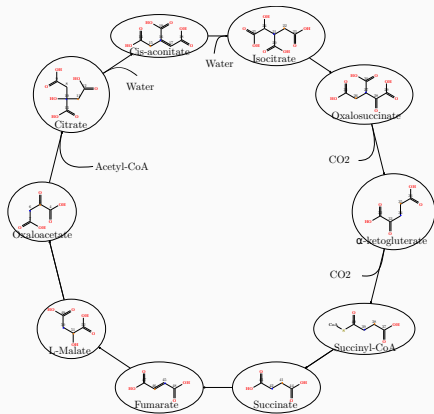
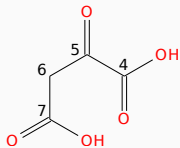
Wrong Mechanism

# Carbon Trajectories and Cayley Graphs

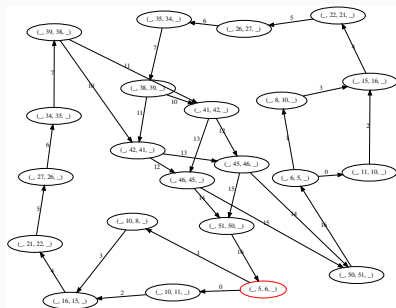
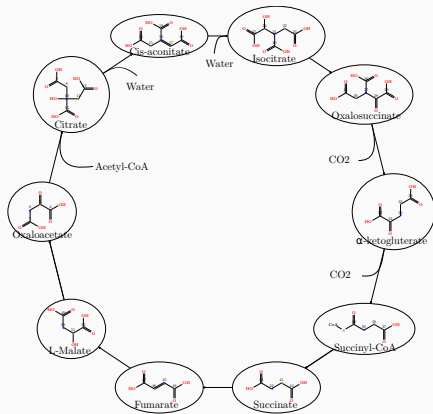
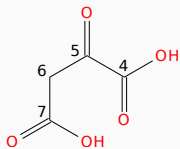




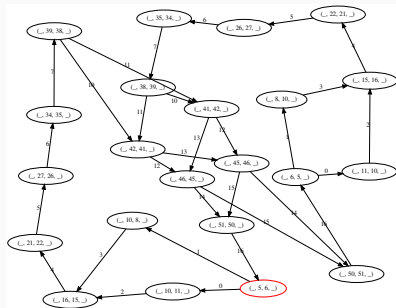
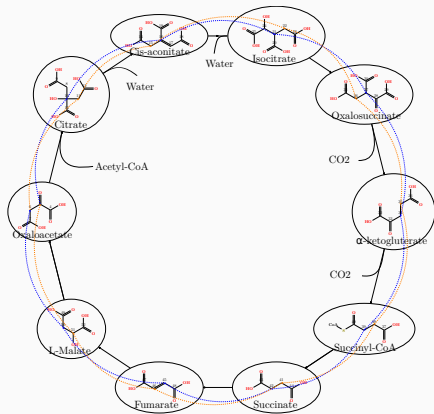
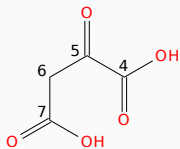
# Carbon Trajectories and Cayley Graphs



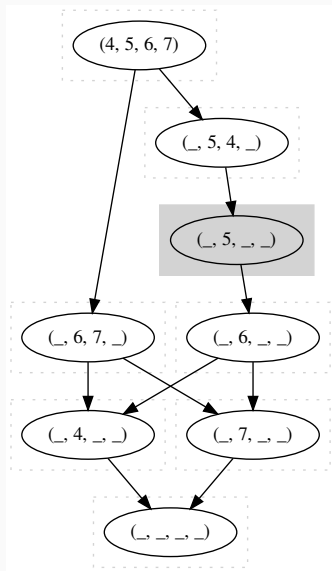
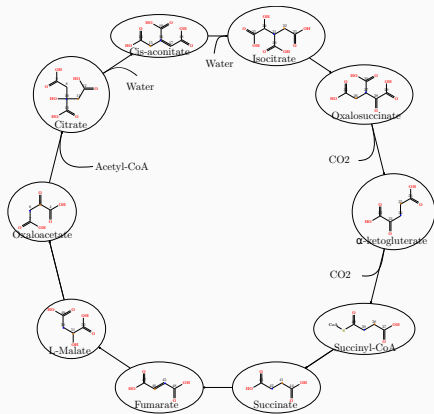
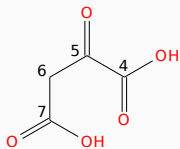
# Carbon Trajectories and Cayley Graphs



# Carbon Trajectories and Cayley Graphs



# Carbon Trajectories and Cayley Graphs



## Summary

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- Using it we can track the trajectories of select atoms in relation to each other.
- Allows for relatively easy modifications to account for e.g. stereochemistry.