



UNIVERSITÄT
LEIPZIG

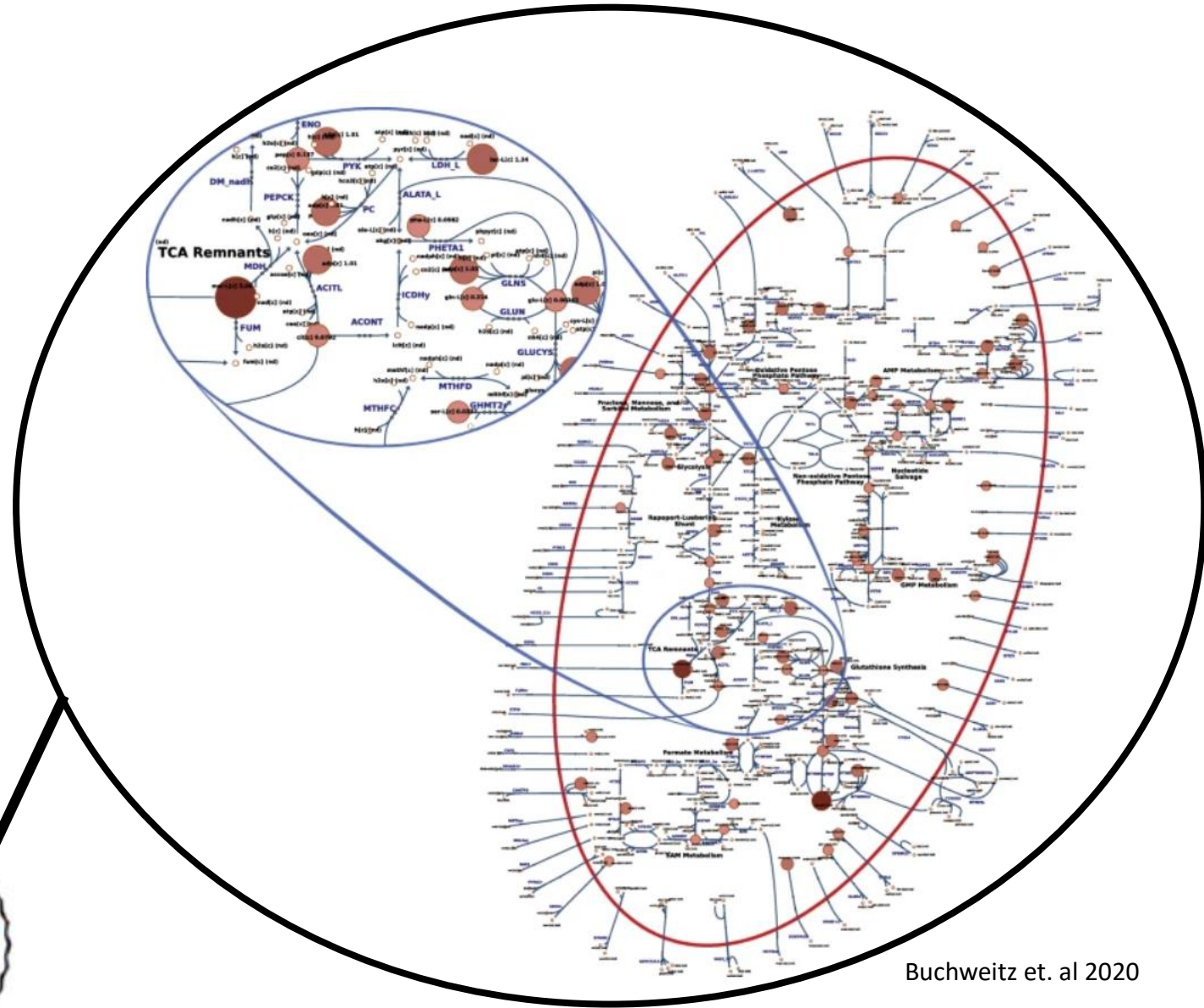
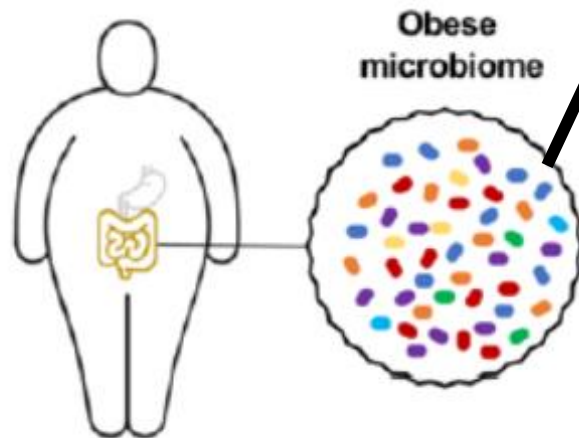
MATOMIC Mathematical Modelling for Microbial Community Induced
Metabolic Diseases

Atom Transition Networks for Atom Tracing

Nora Beier, 14.02.2023

Introduction

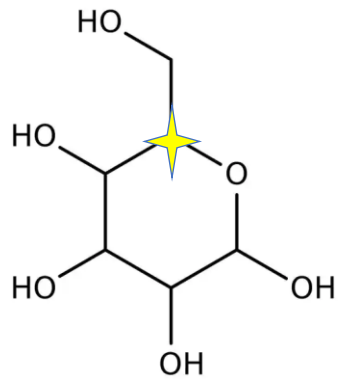
Gut microbial communities influence the host Health condition



Buchweitz et. al 2020

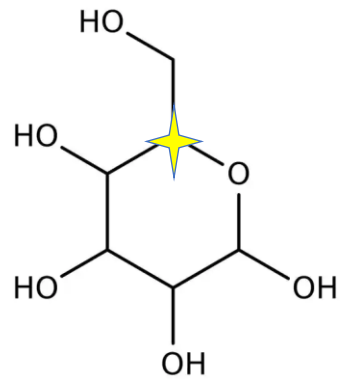
Atom Tracing for isotopic labelling experiments

Isotopic
labelled substrate

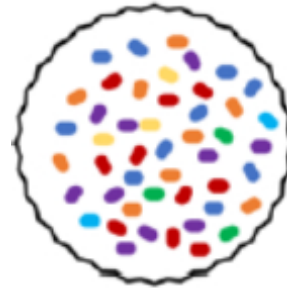


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Isotopic
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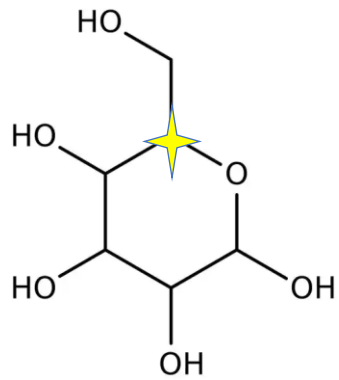


Bacterial culture

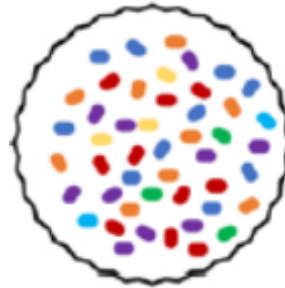


Atom Tracing for isotopic labelling experiments

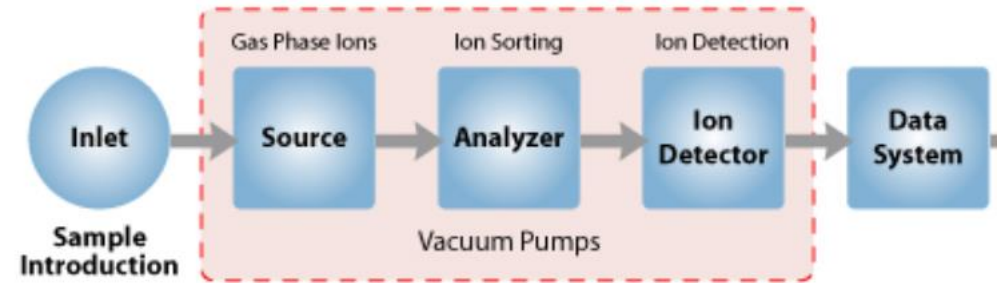
Isotopic
labelled substrate



Bacterial culture

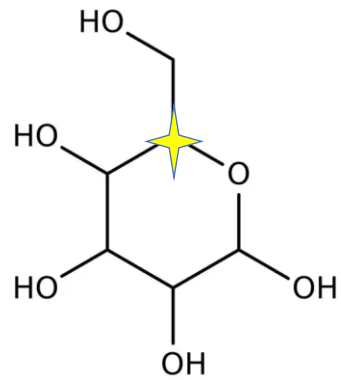


mass-spectrometry Analysis

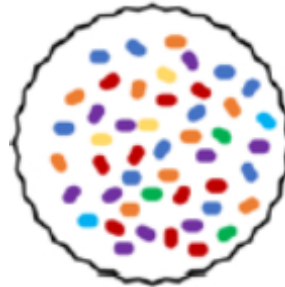


Atom Tracing for isotopic labelling experiments

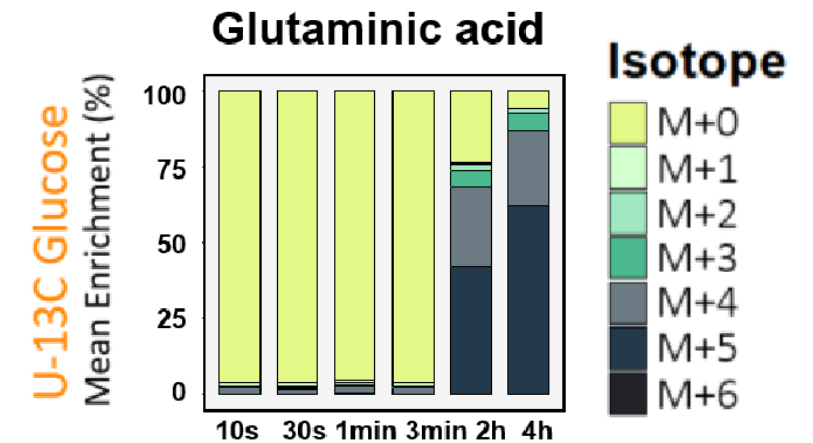
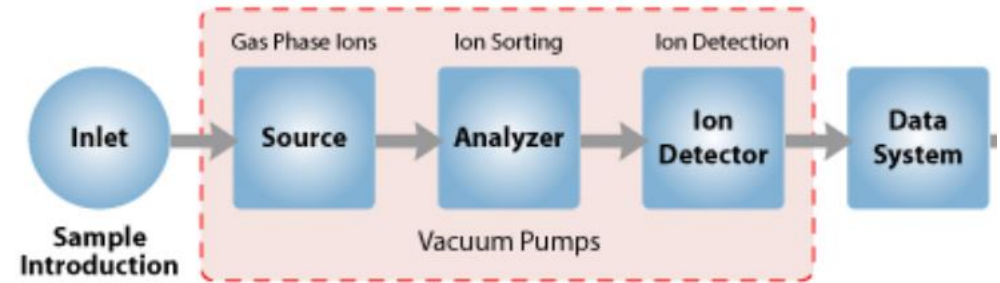
Isotopic
labelled substrate



Bacterial culture

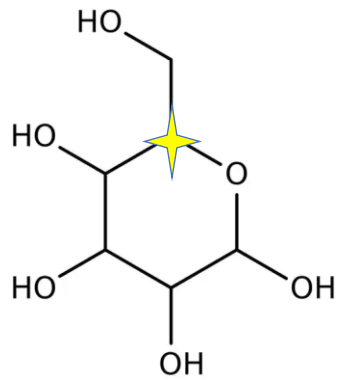


mass-spectrometry Analysis

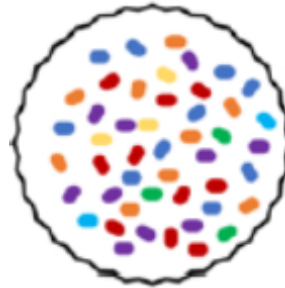


Atom Tracing for isotopic labelling experiments

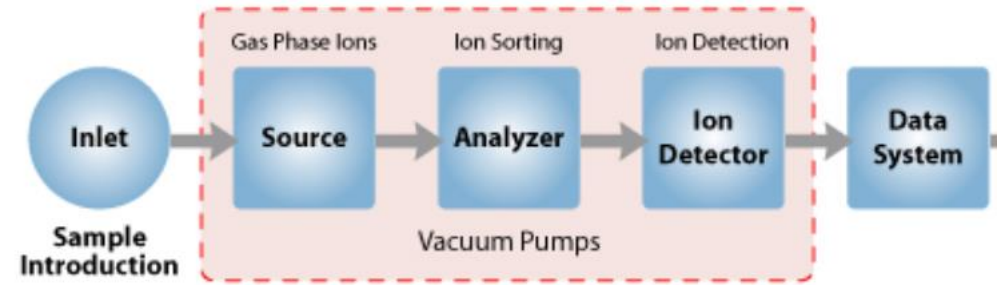
Isotopic
labelled substrate



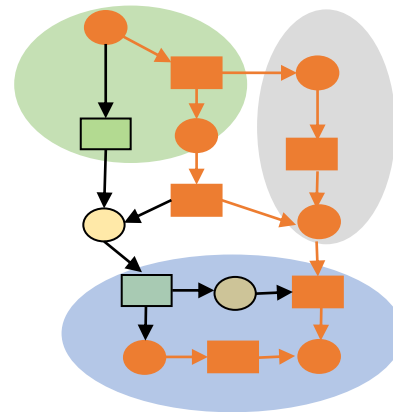
Bacterial culture



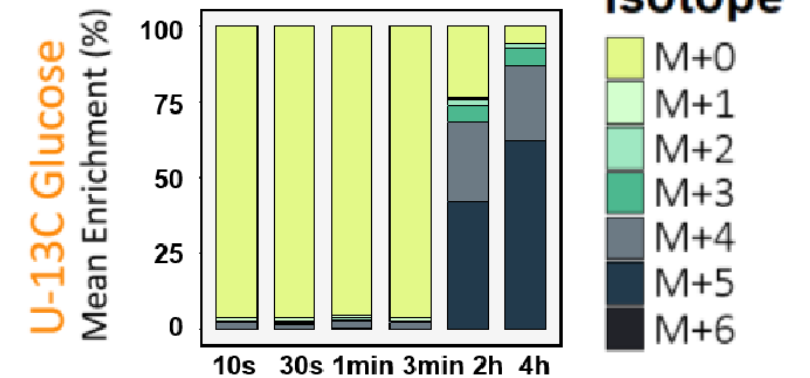
mass-spectrometry Analysis



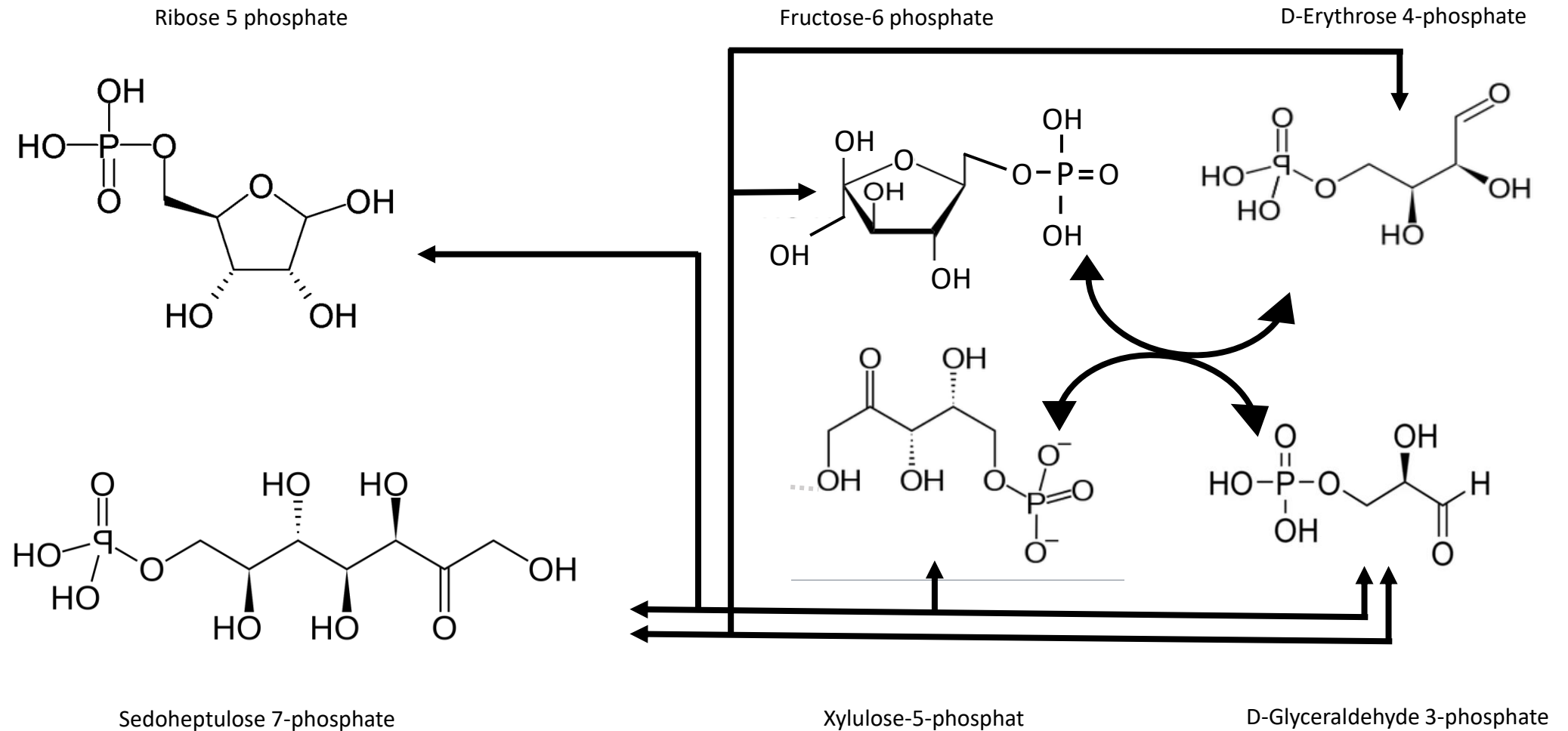
Metabolic Network Analysis



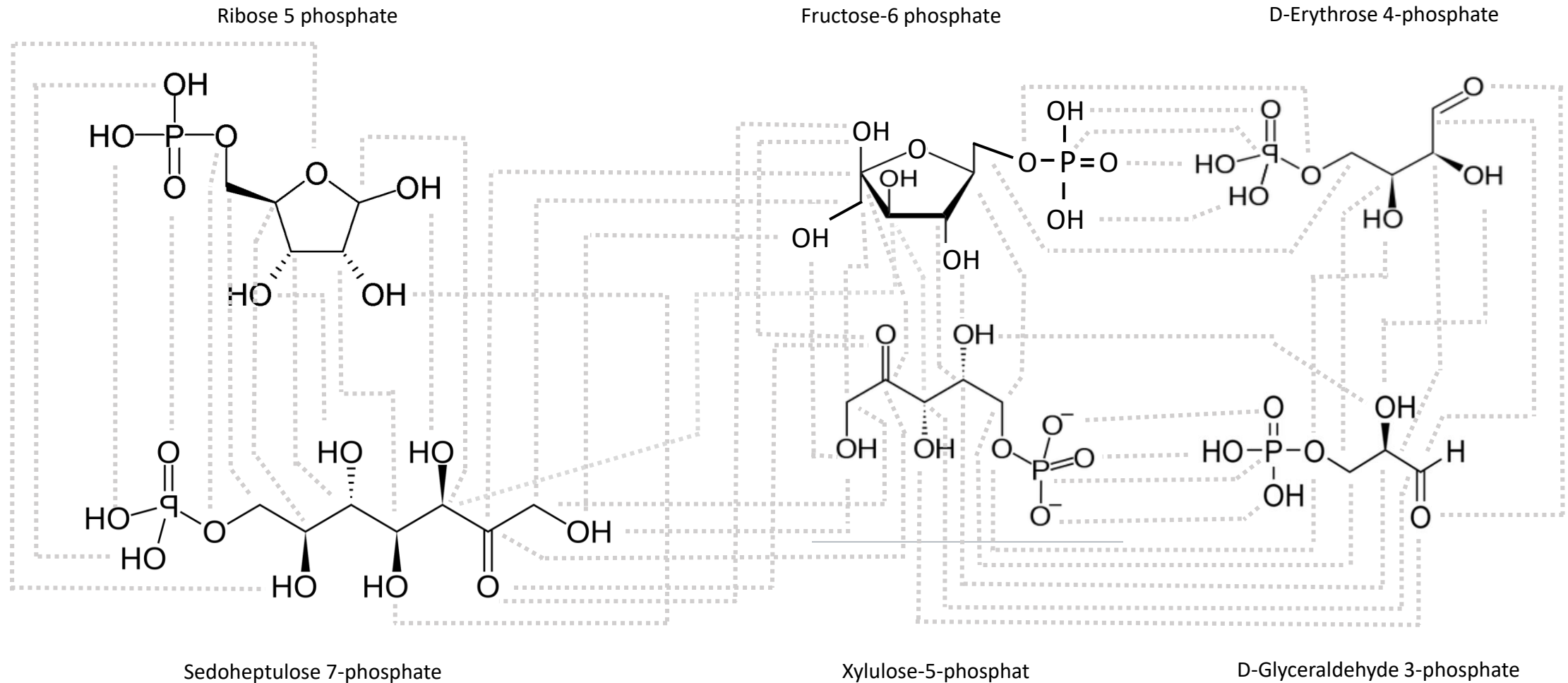
Glutaminic acid



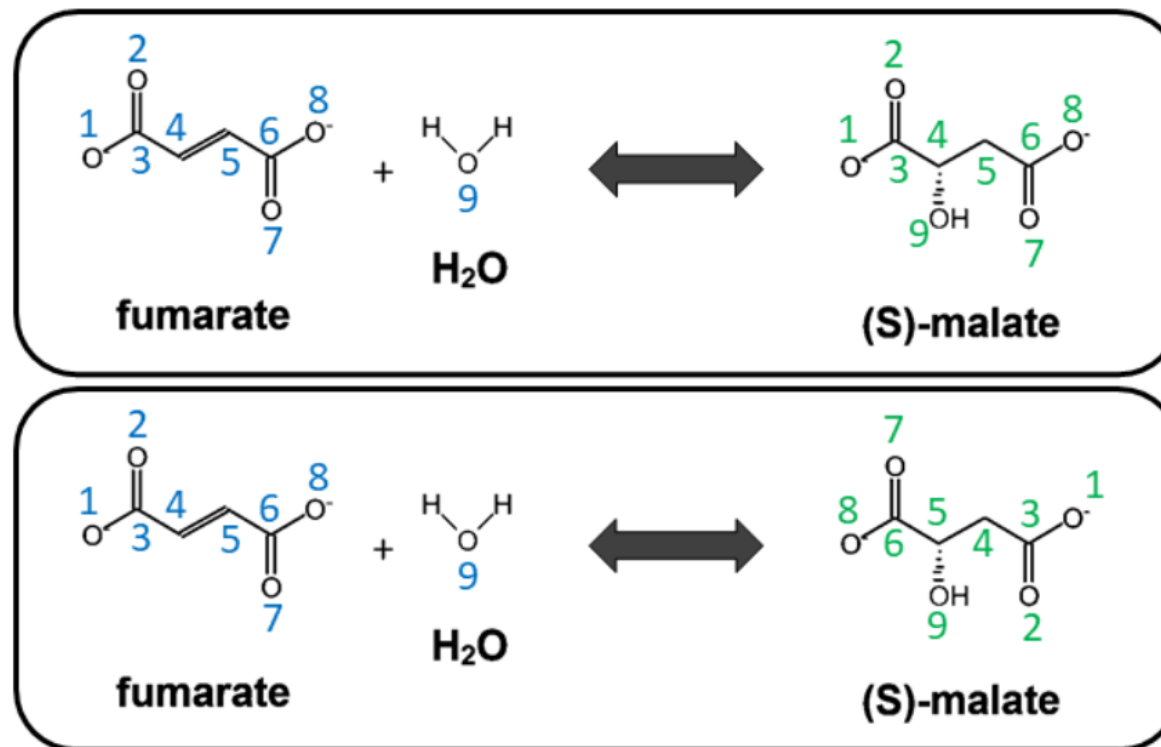
Metabolic Networks vs Atom-Transition Networks



Metabolic Networks vs Atom-Transition Networks

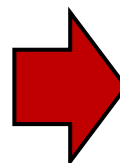


Atom-Atom Mapping



Different Mapper available:

RXN Mapper (84.5%)
Graphormer (89.5%)



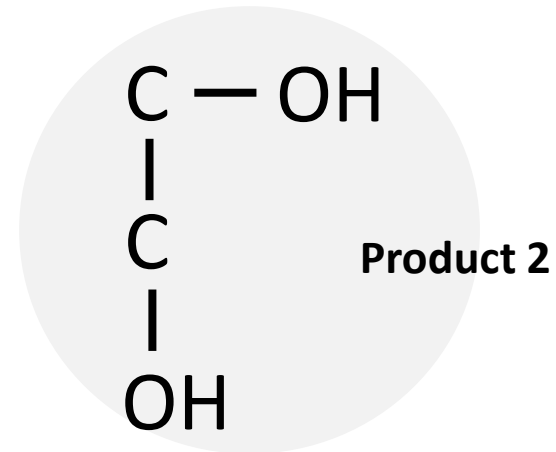
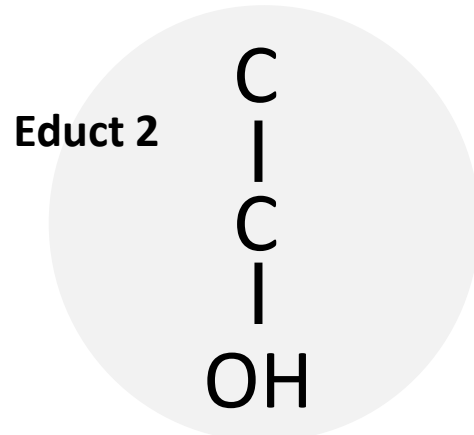
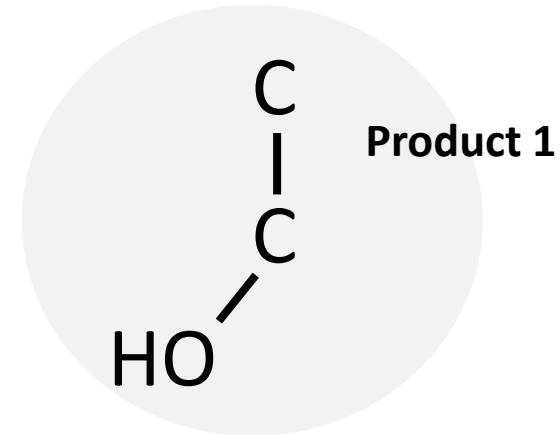
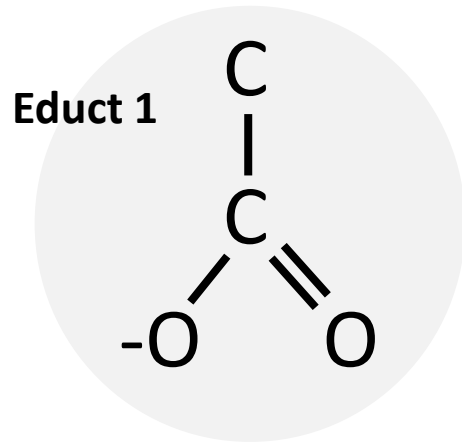
Verification necessary

Marcos: Comparison of Atom Maps

Build ATNs

Educt 1 + Educt 2 = Product 1 + Product 2

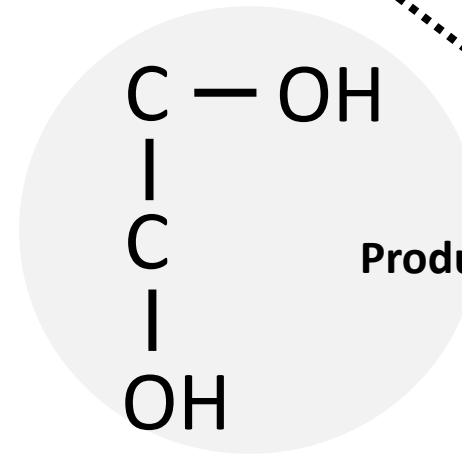
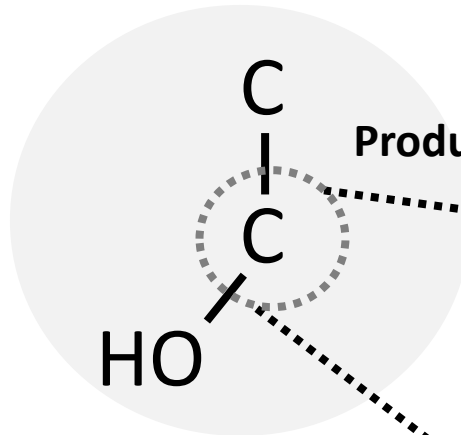
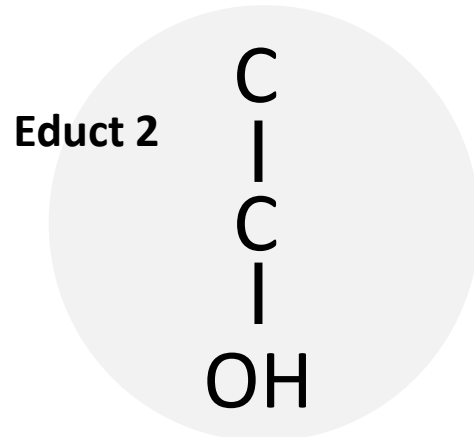
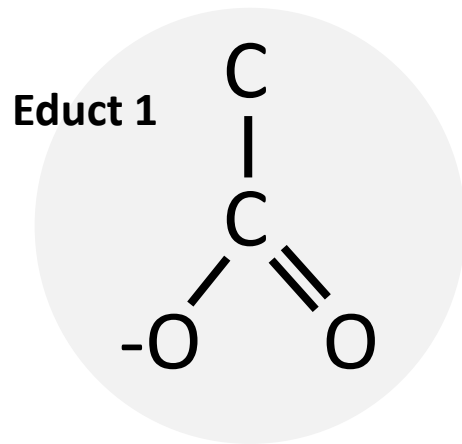
[C:1][C:2](=[O:3])[O-:4].[C:5][C:6][OH:7]>>[C:1][C:2][OH:4].[OH:3][C:5][C:6][OH:7]



Build ATNs

Educt 1 + Educt 2 = Product 1 + Product 2

[C:1][C:2](=[O:3])[O-:4].[C:5][C:6][OH:7]>>[C:1][C:2][OH:4].[OH:3][C:5][C:6][OH:7]

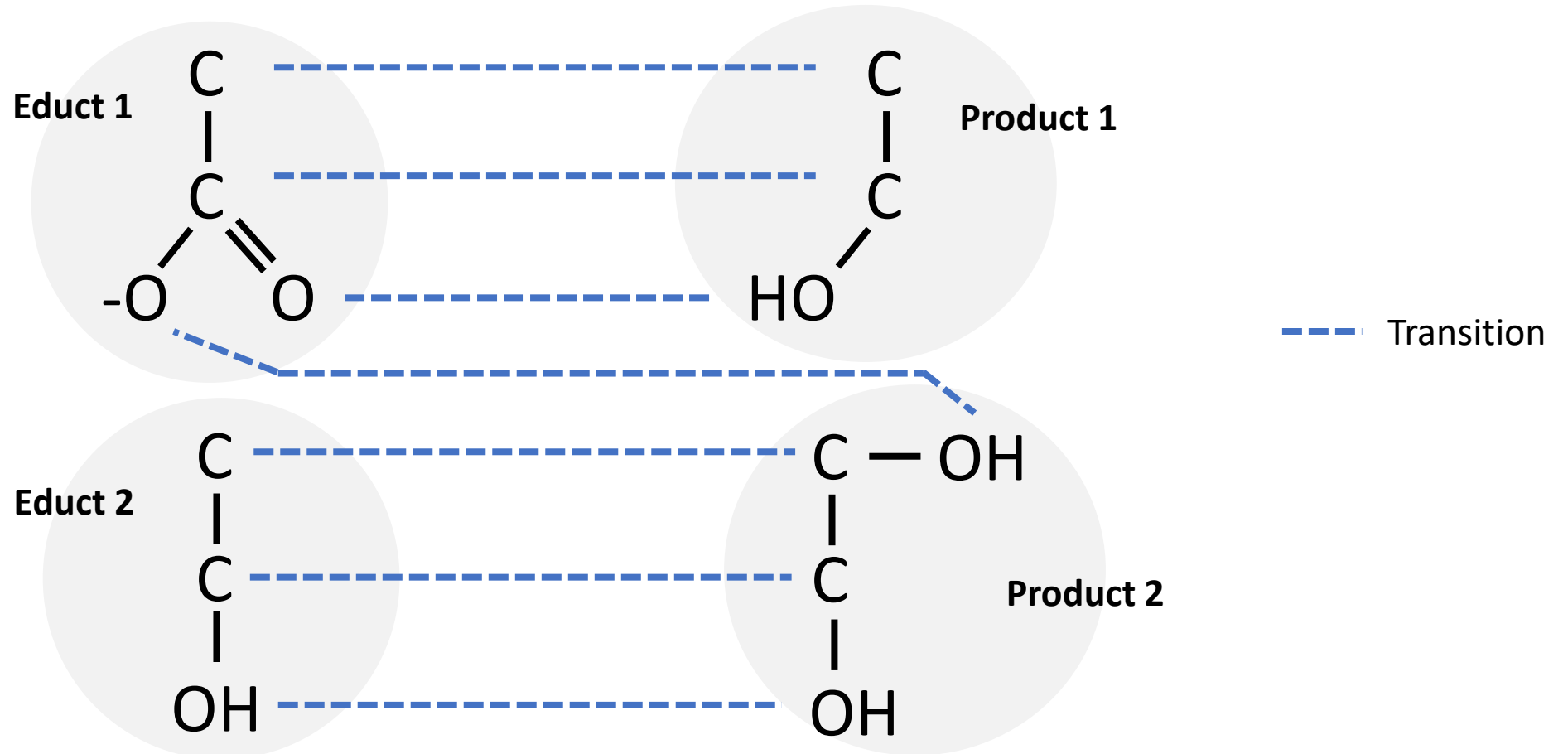


- Label
- Charge
- H count
- aromatic
- Element
- Compound Name

Build ATNs

Educt 1 + Educt 2 = Product 1 + Product 2

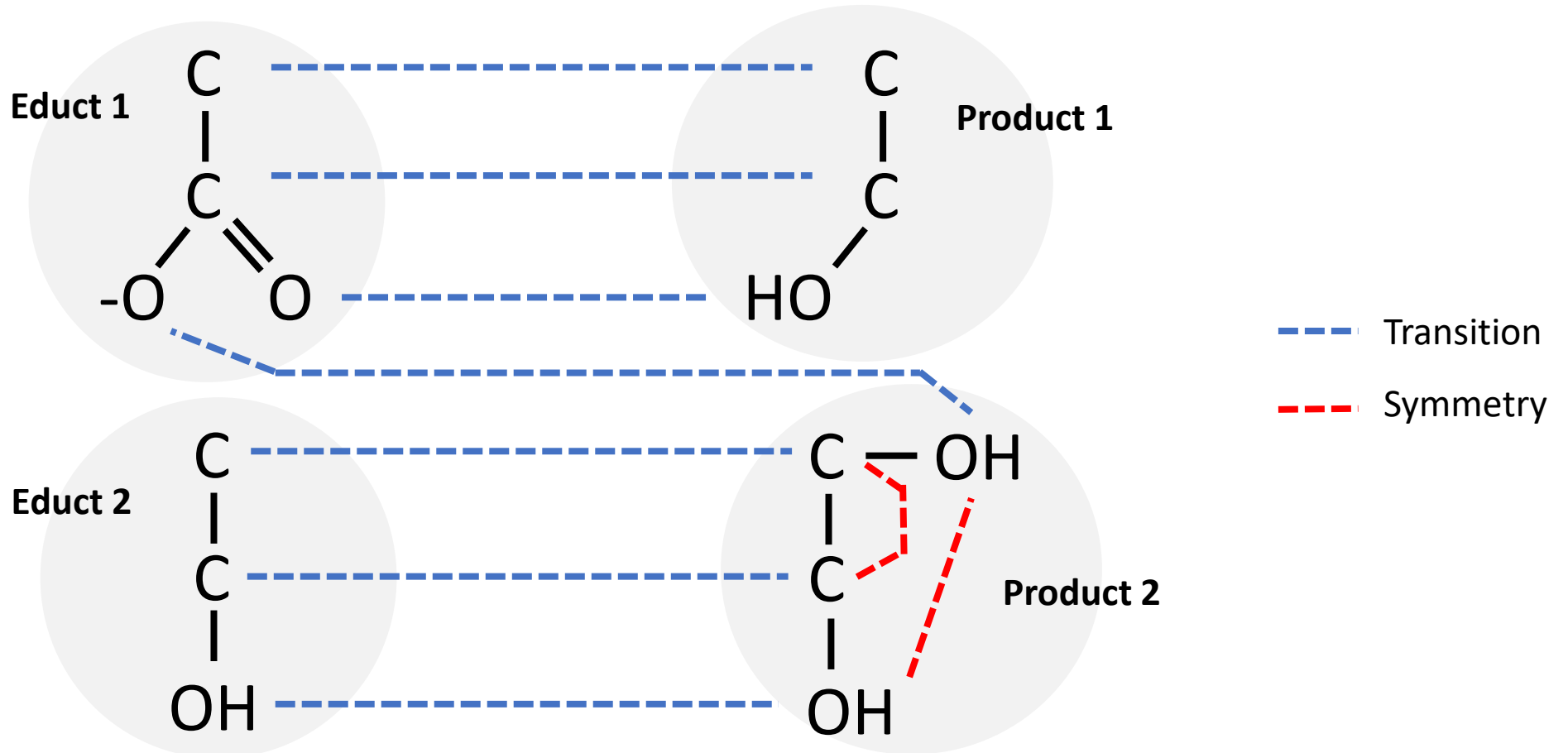
[C:1][C:2](=[O:3])[O-:4].[C:5][C:6][OH:7]>>[C:1][C:2][OH:4].[OH:3][C:5][C:6][OH:7]



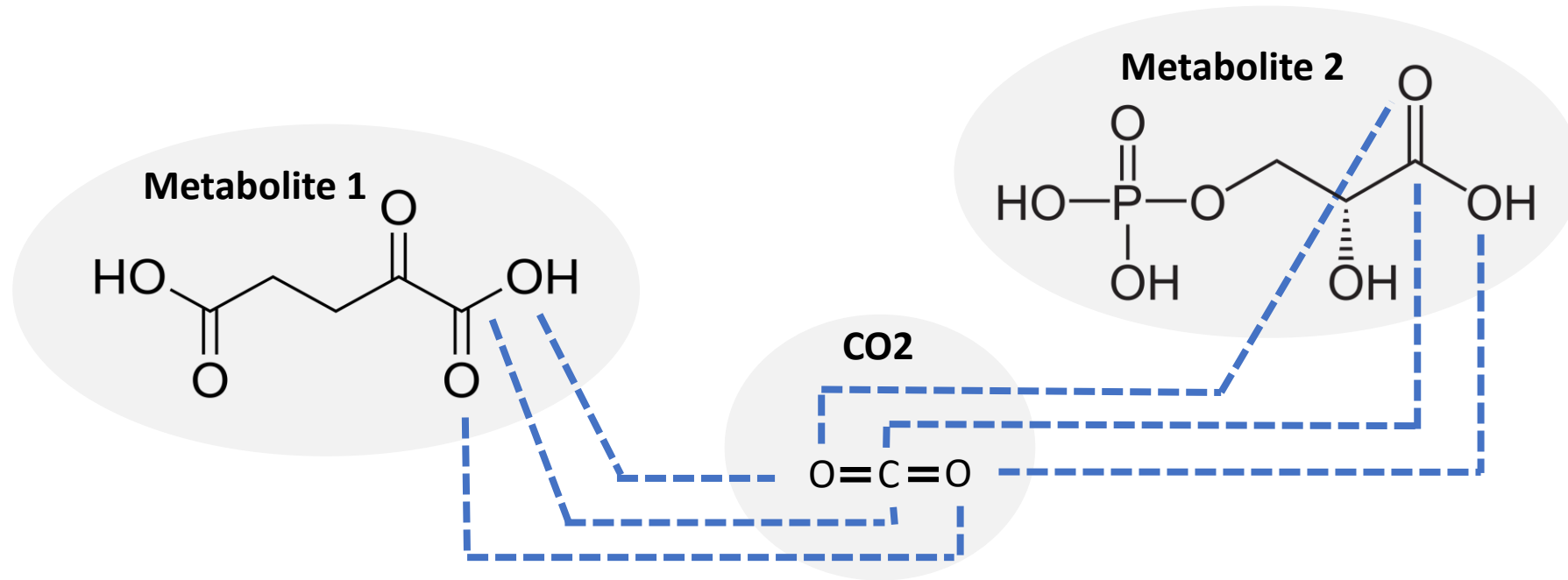
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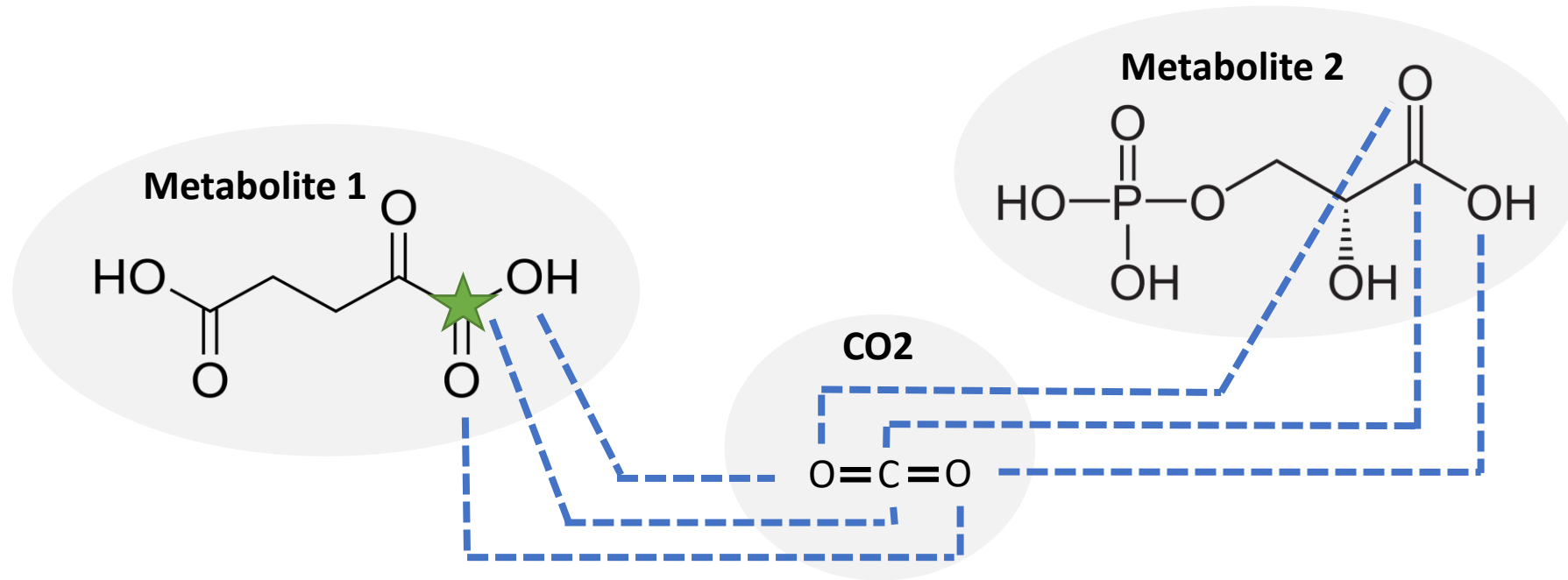
[C:1][C:2](=[O:3])[O-:4].[C:5][C:6][OH:7]>>[C:1][C:2][OH:4].[OH:3][C:5][C:6][OH:7]



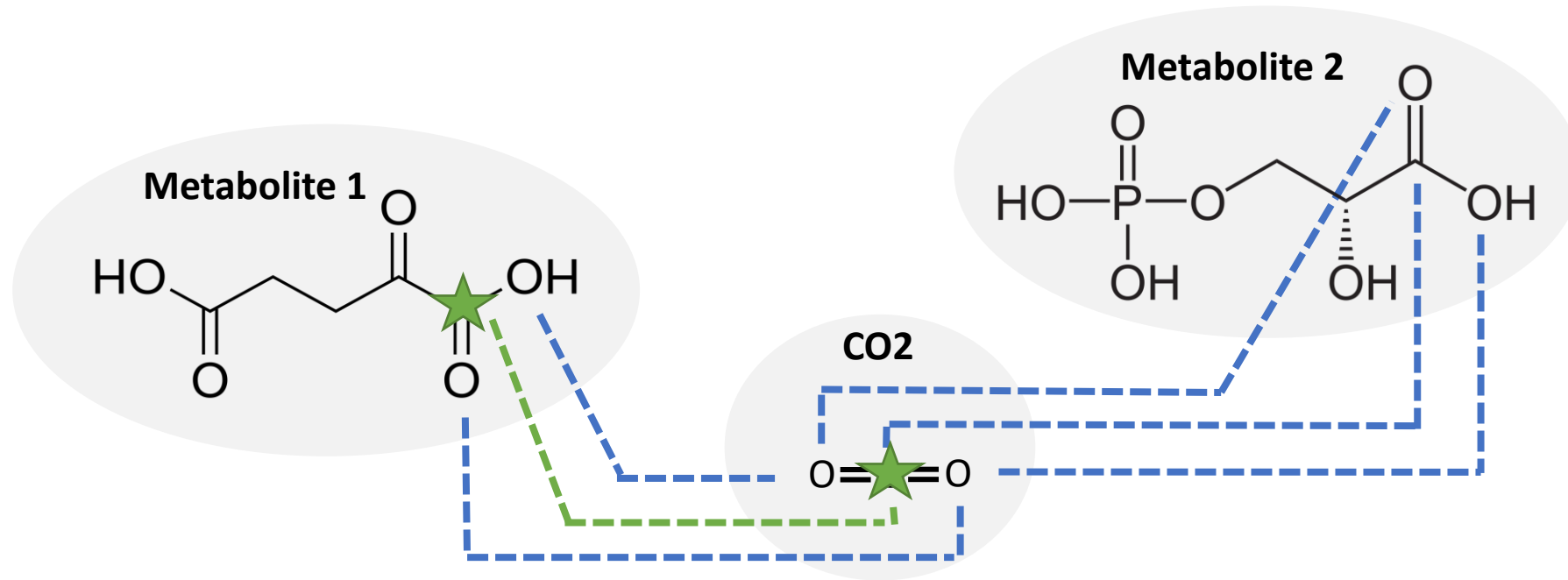
Build ATNs – high concentrated molecules



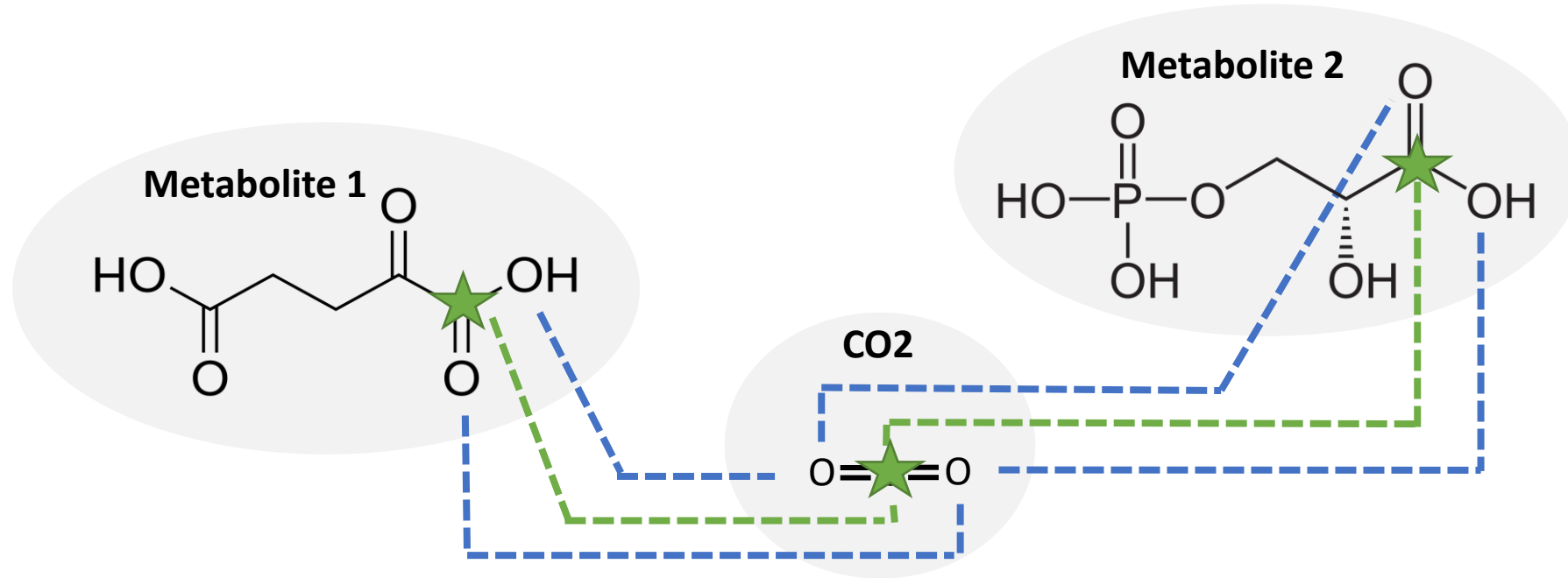
Build ATNs – high concentrated molecules



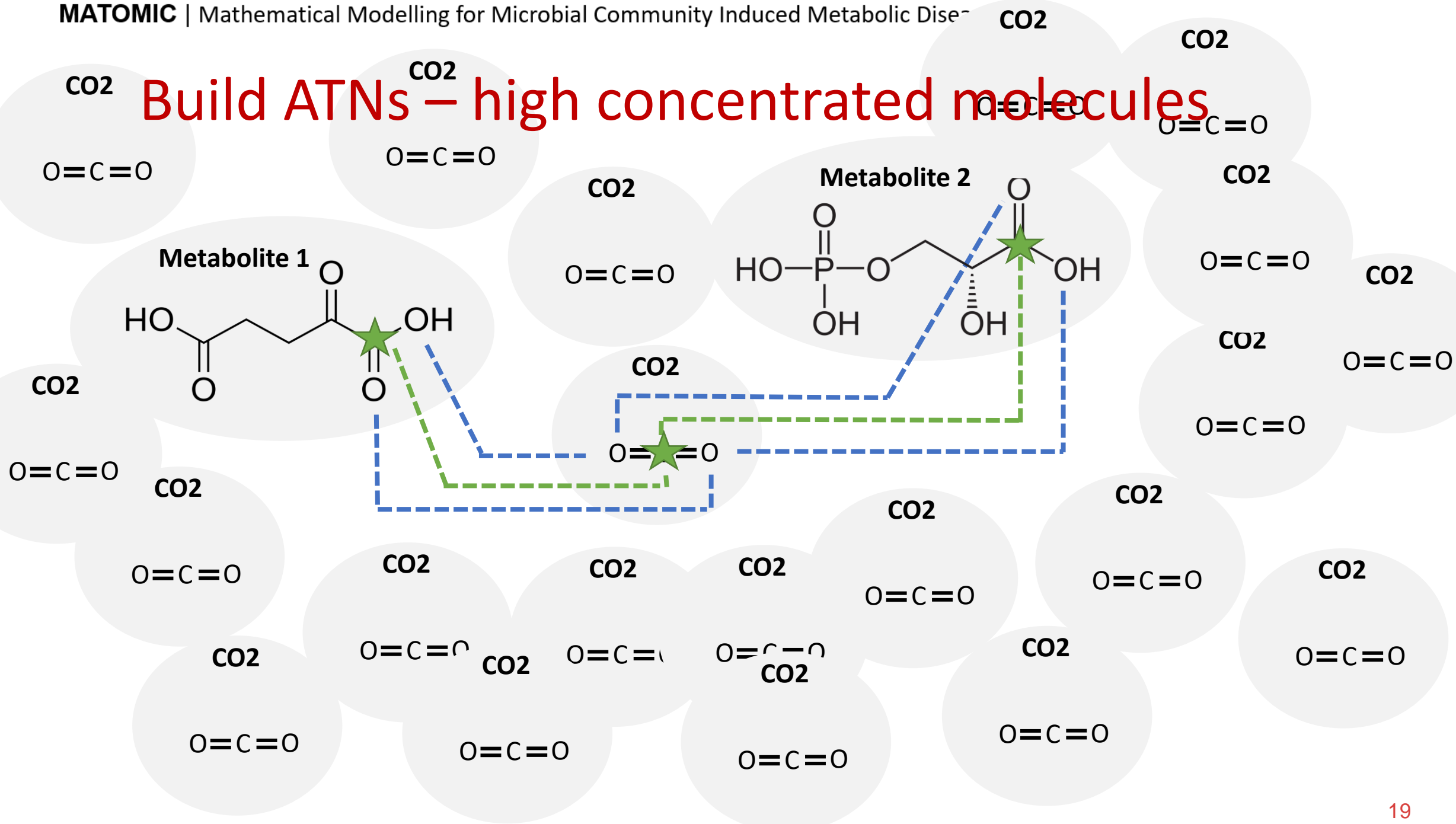
Build ATNs – high concentrated molecules



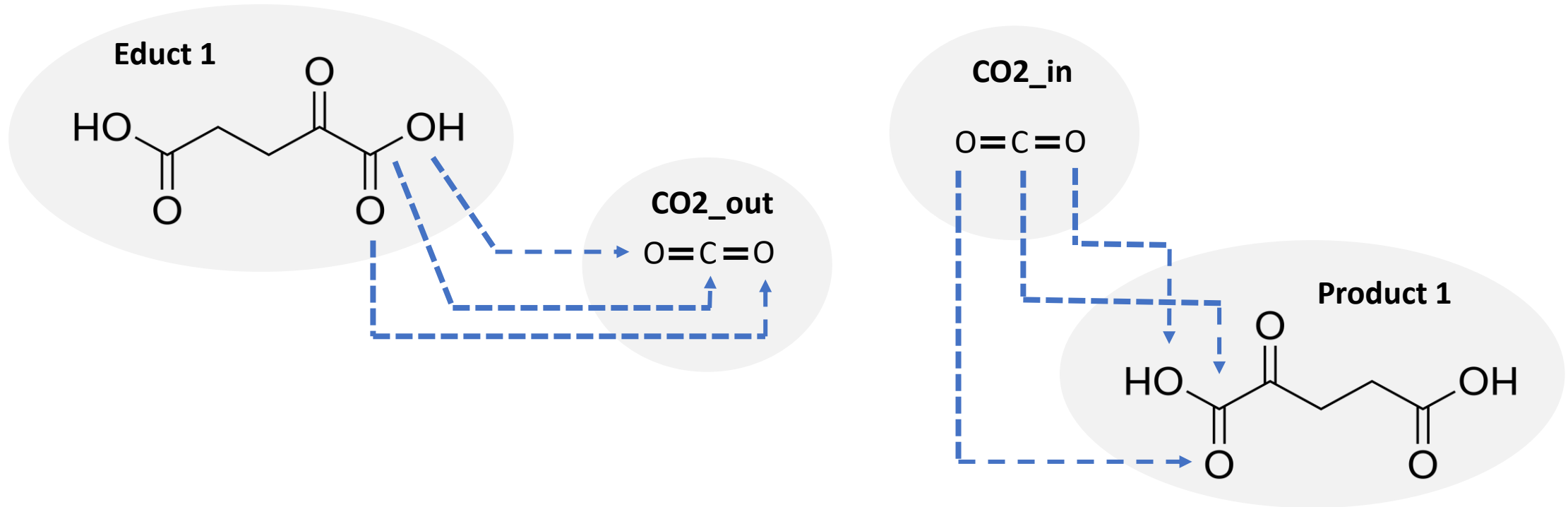
Build ATNs – high concentrated molecules



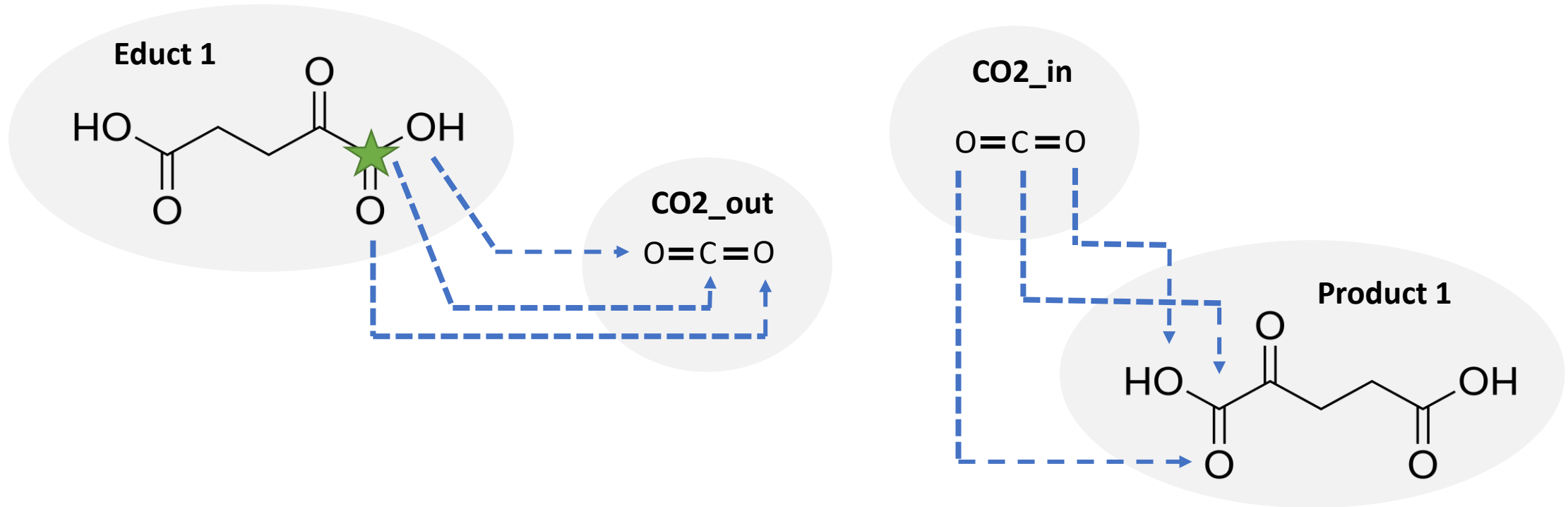
Build ATNs – high concentrated molecules



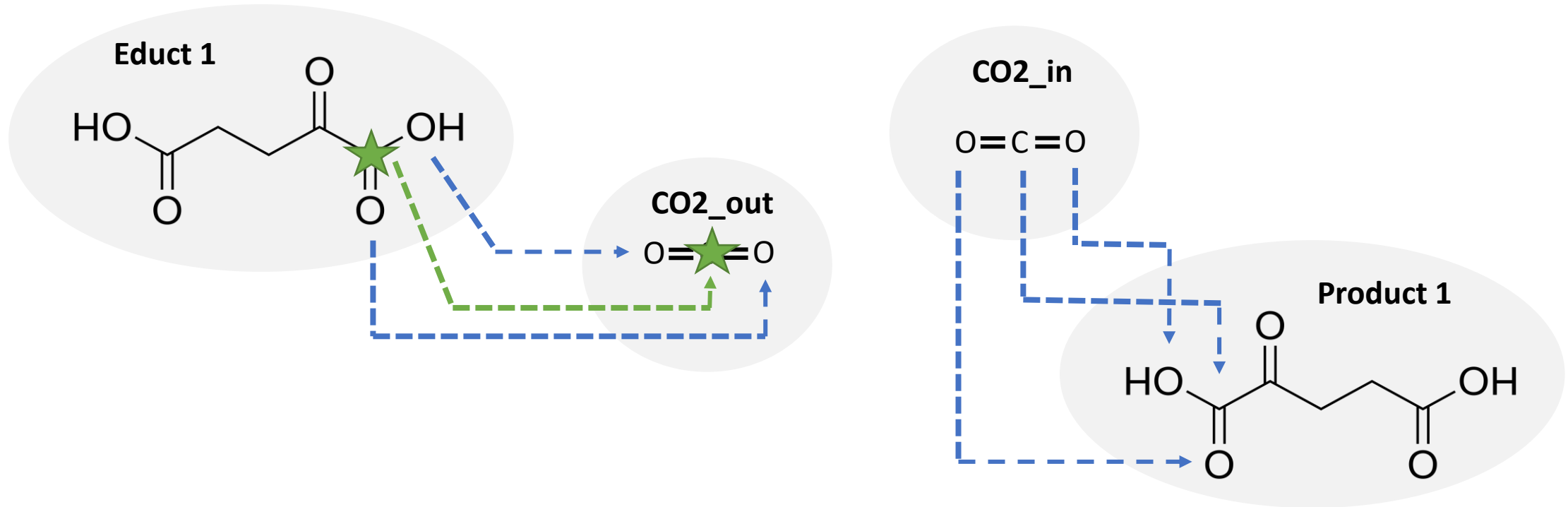
Build ATNs – high concentrated molecules



Build ATNs – high concentrated molecules

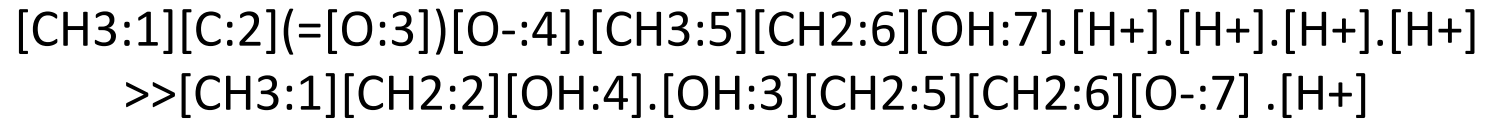


Build ATNs – high concentrated molecules

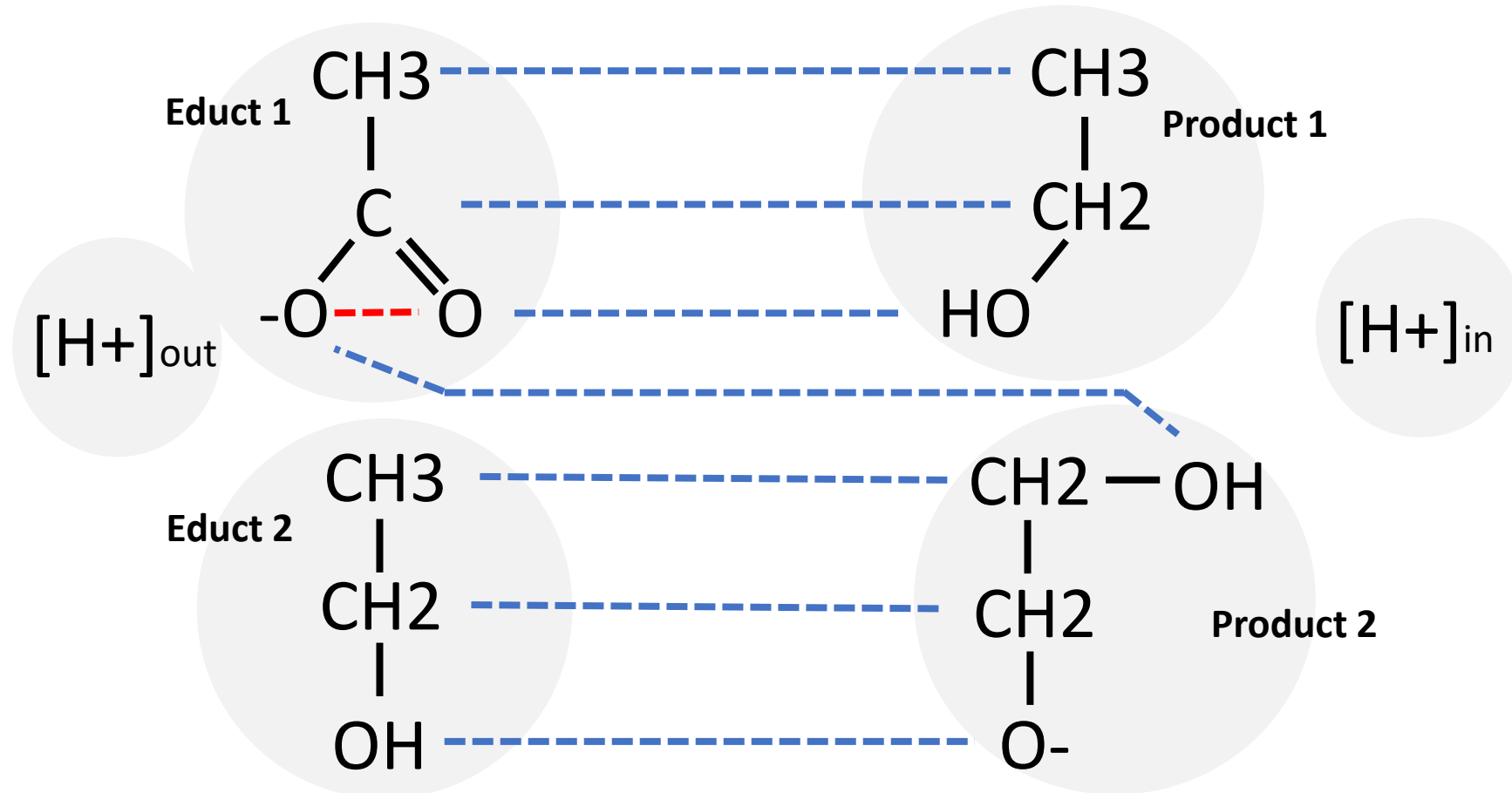


Build ATNs - Hydrogens

Educt 1 + Educt 2 = Product 1 + Product 2

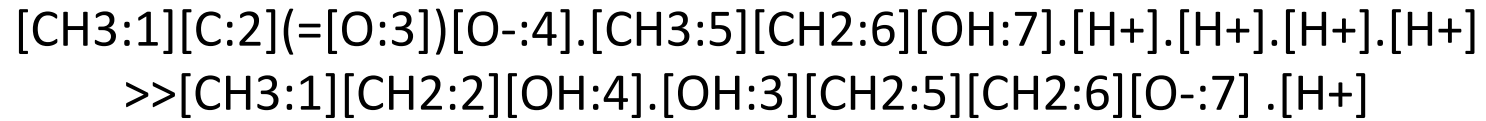


--- Symmetry
 --- Transition

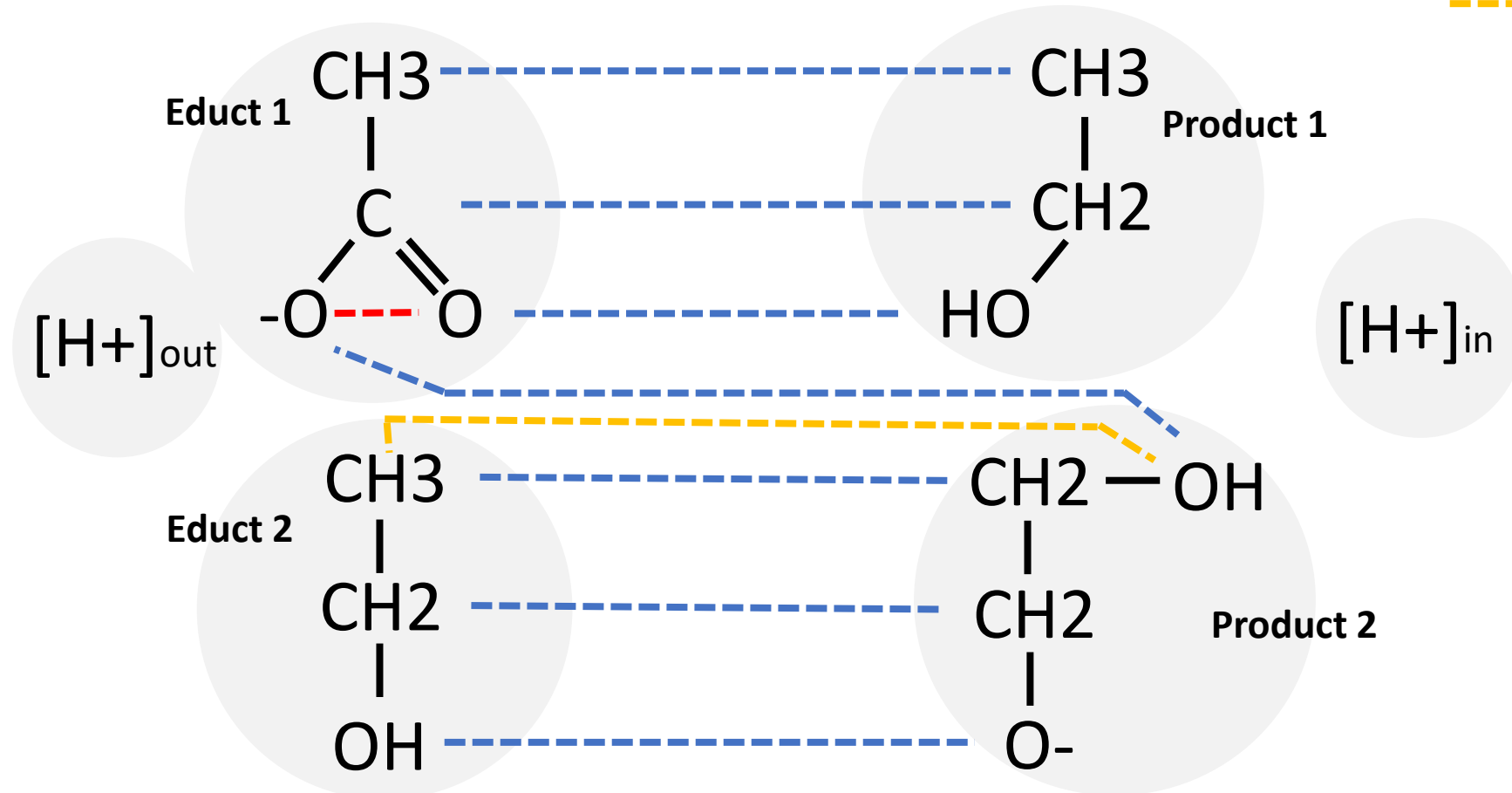


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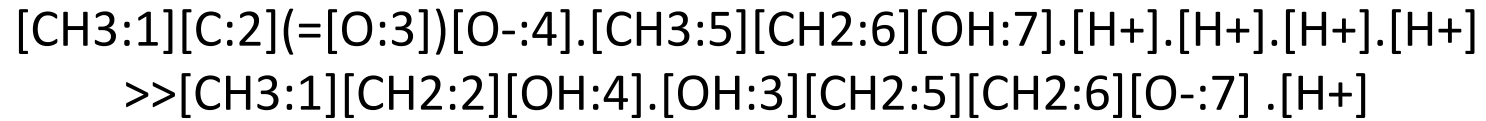


- Symmetry
- Transition
- Hydrogen Reaction

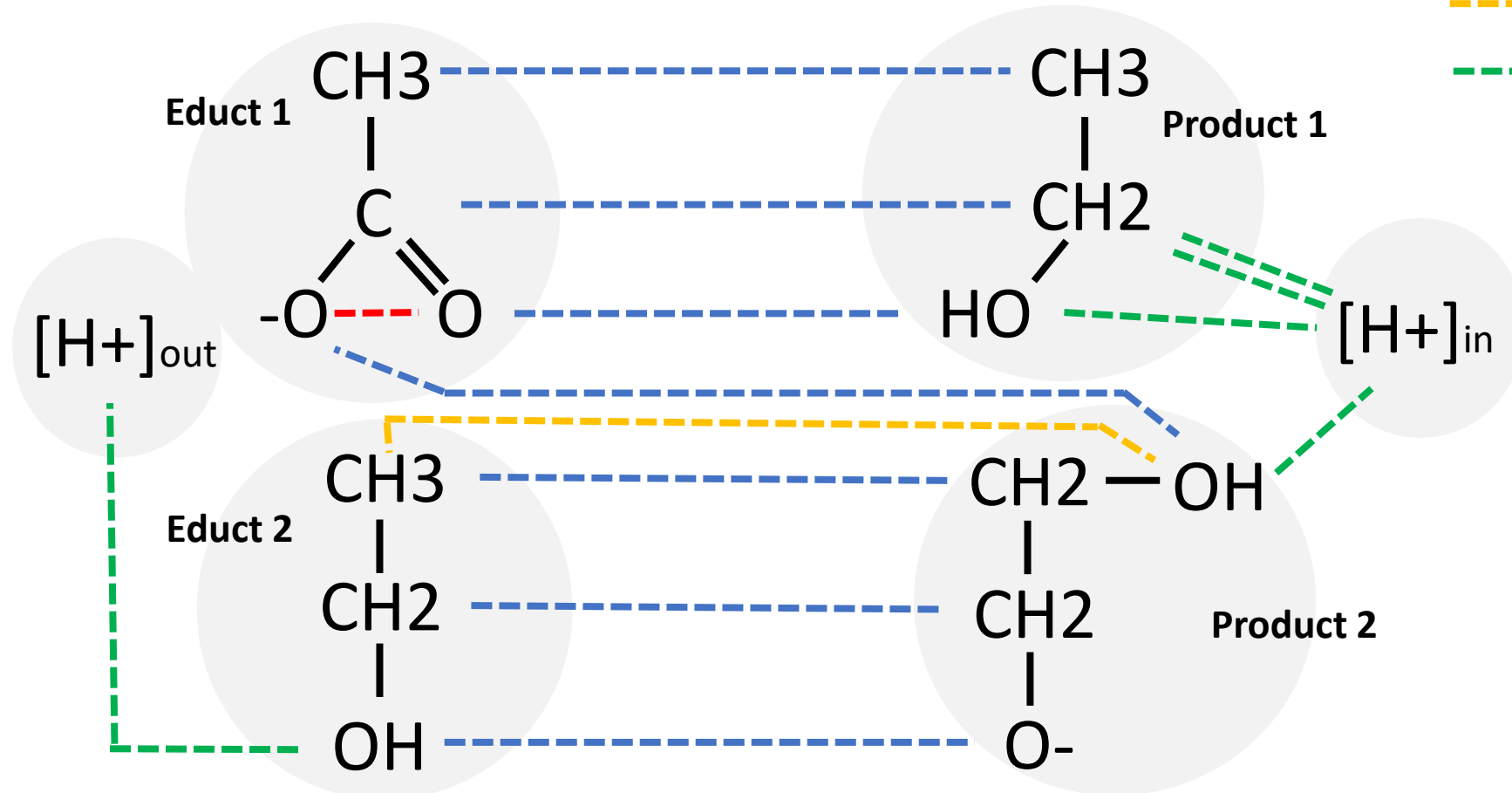


Build ATNs - Hydrogens

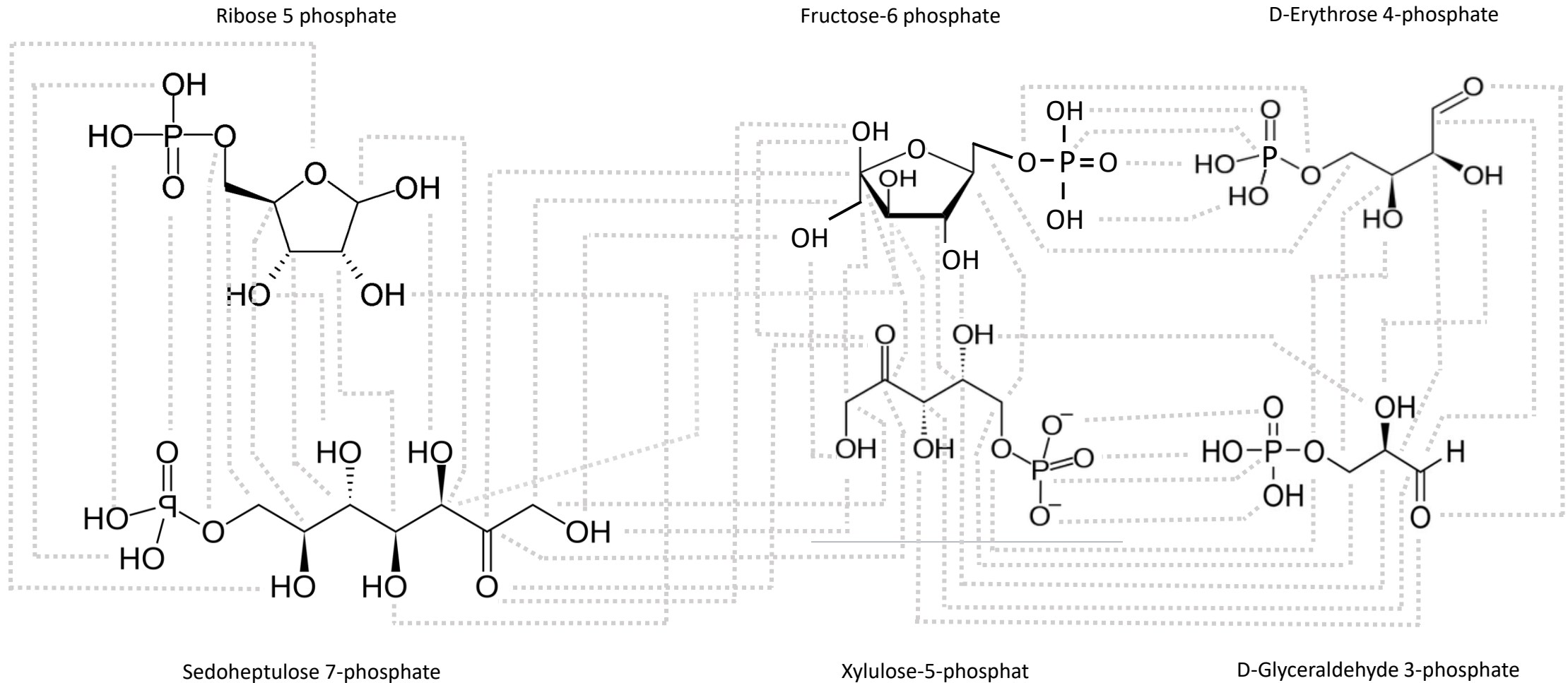
Educt 1 + Educt 2 = Product 1 + Product 2



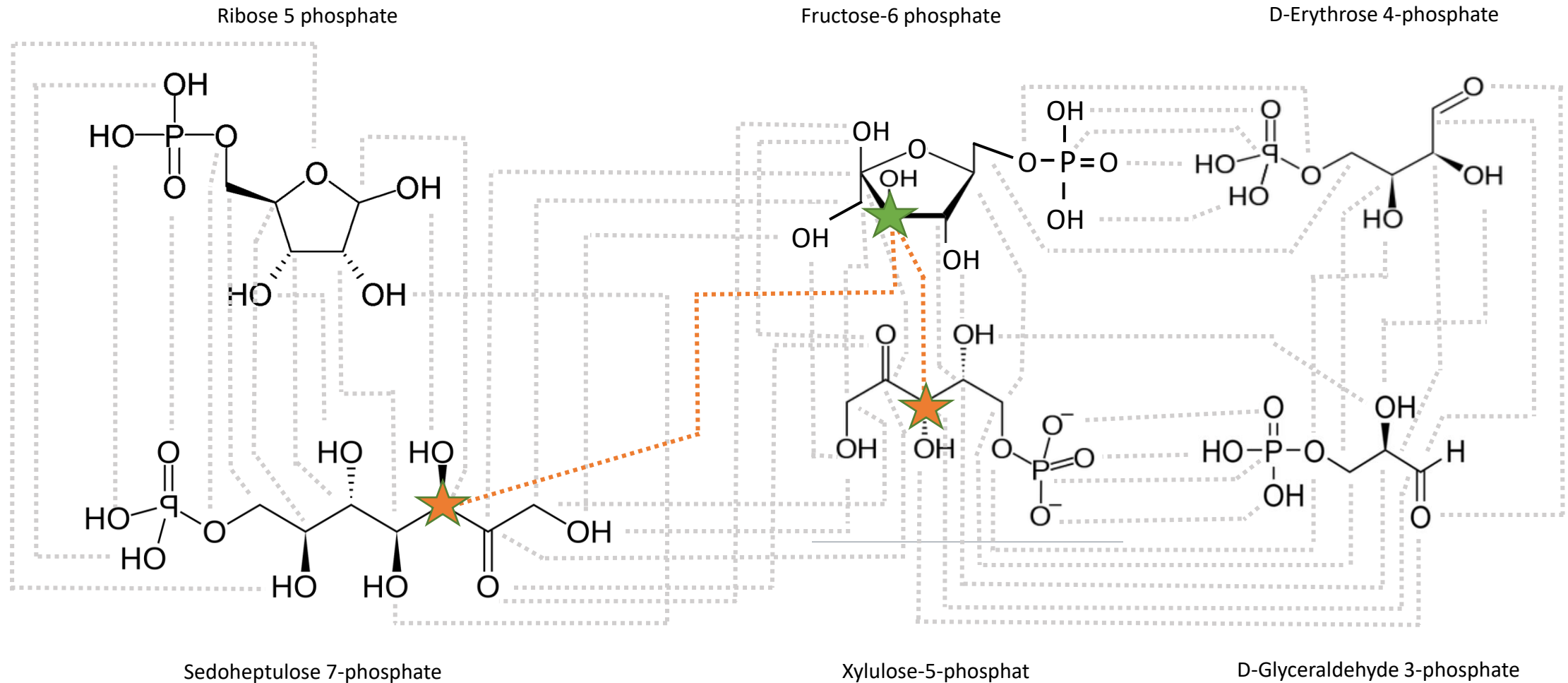
- Symmetry
- Transition
- Hydrogen Reaction
- Hydrogen free



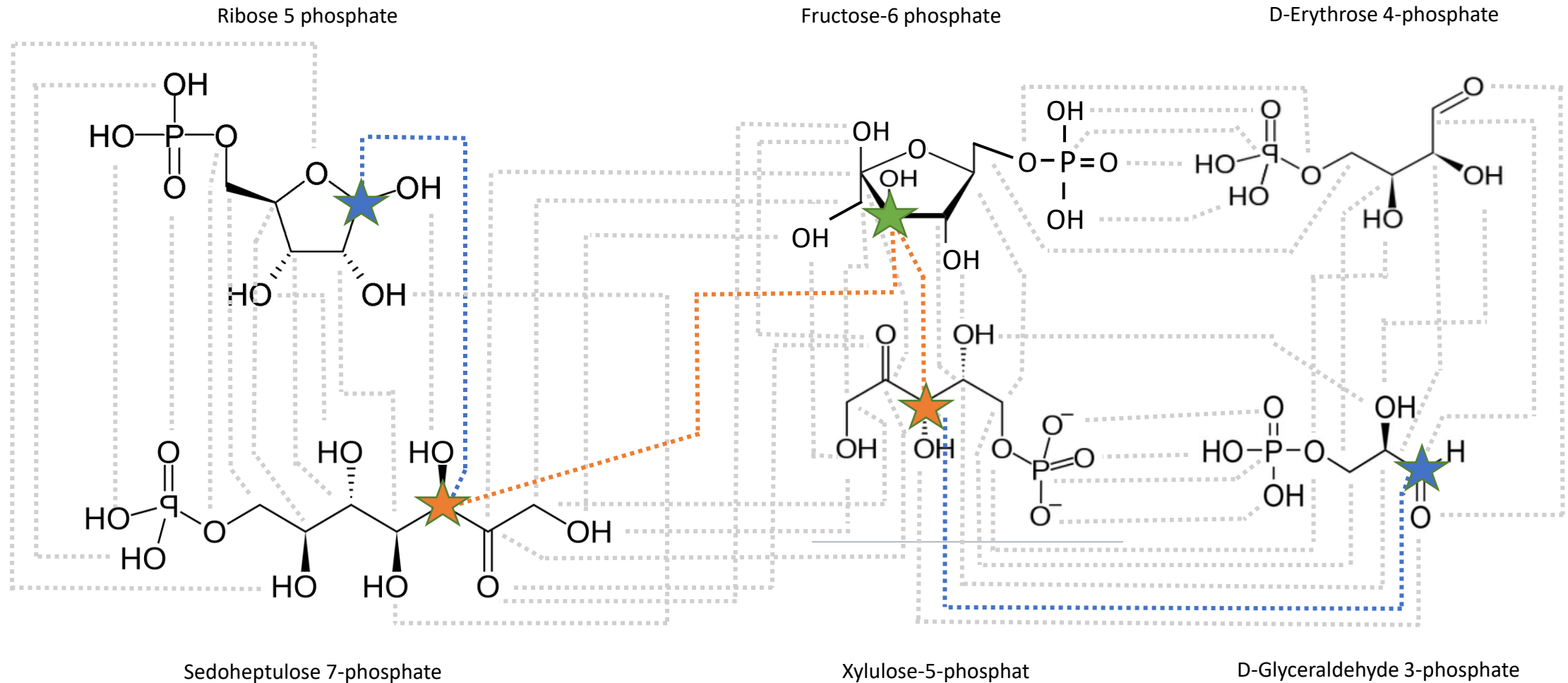
BFS* to Trace Isotope Markers



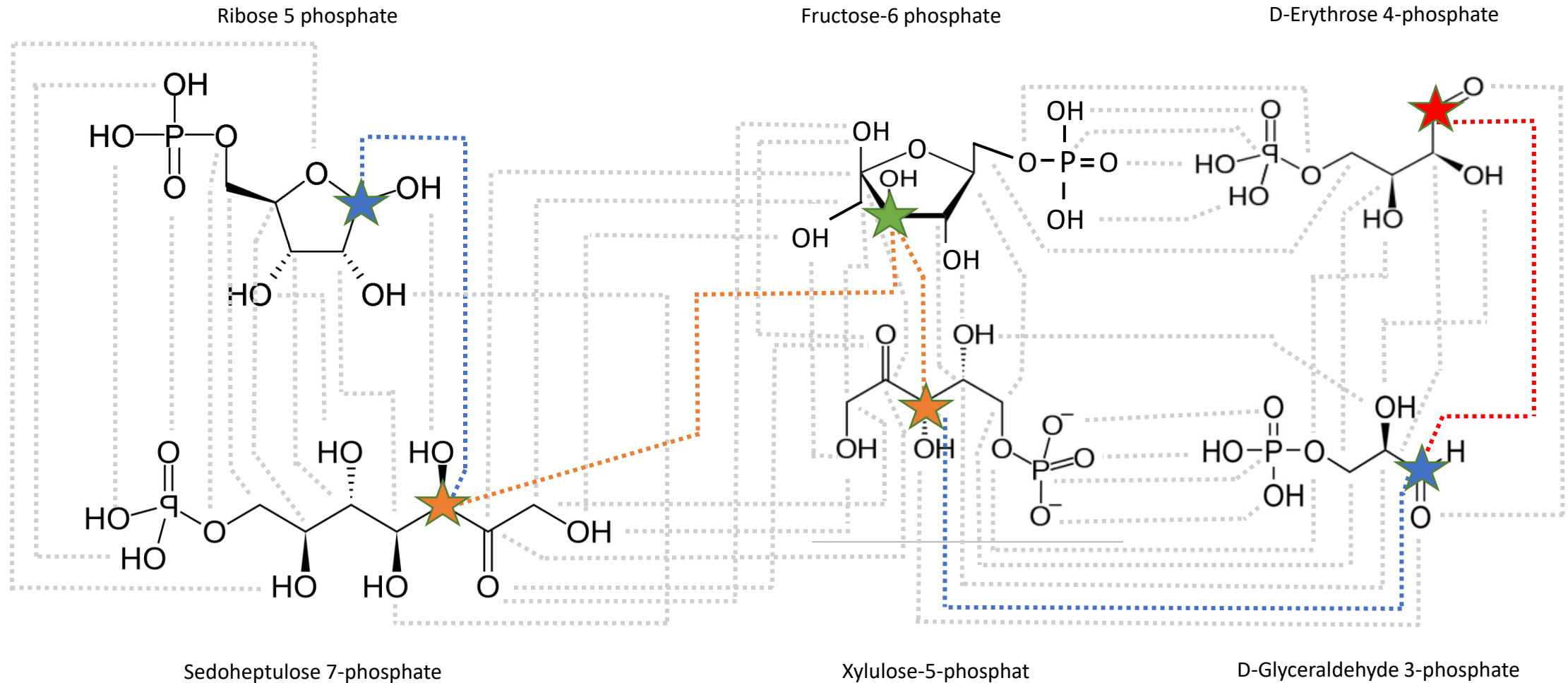
BFS to Trace Isotope Markers



BFS to Trace Isotope Markers



BFS to Trace Isotope Markers



Thank you for the attention

