TACsy

Training Alliance for Computational systems chemistry

A Sensitivity Analysis for Rule-based Systems Chemistry

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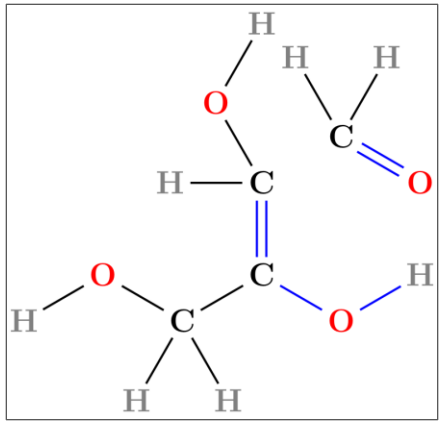

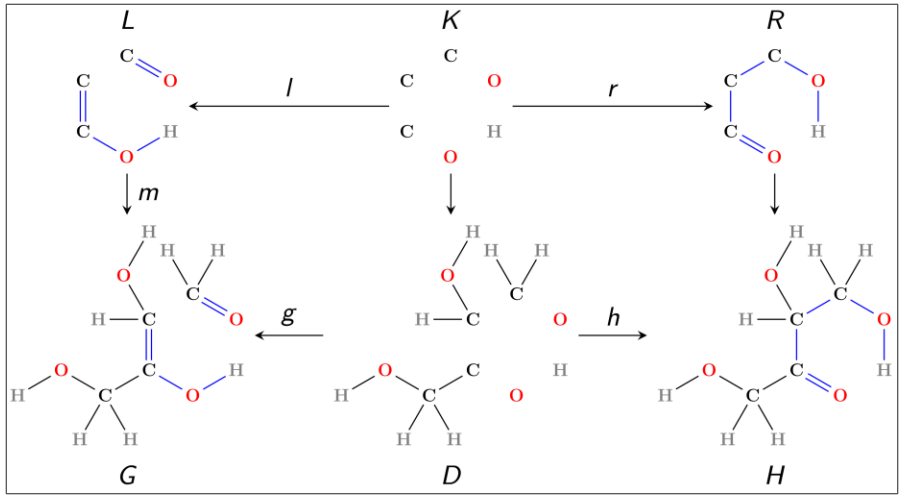

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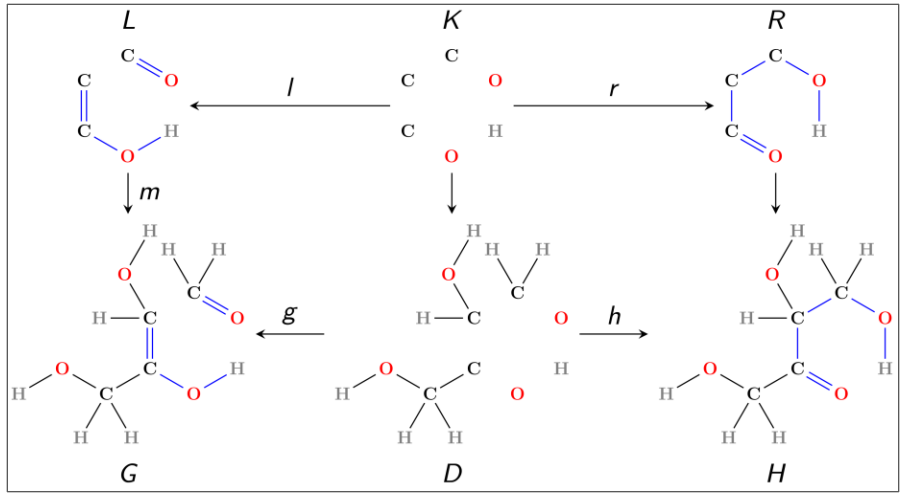

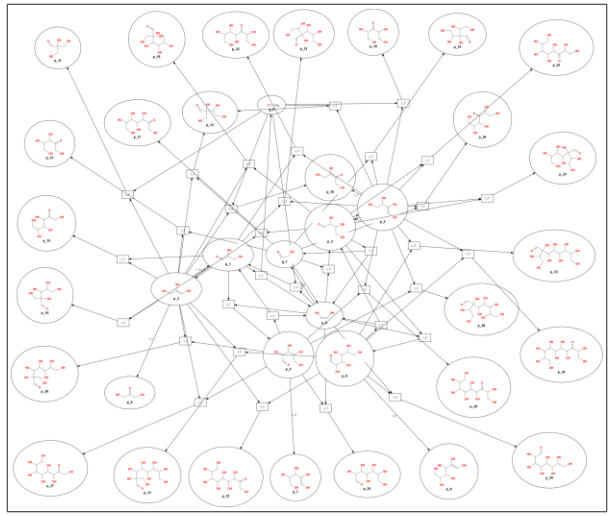

Derivation graph

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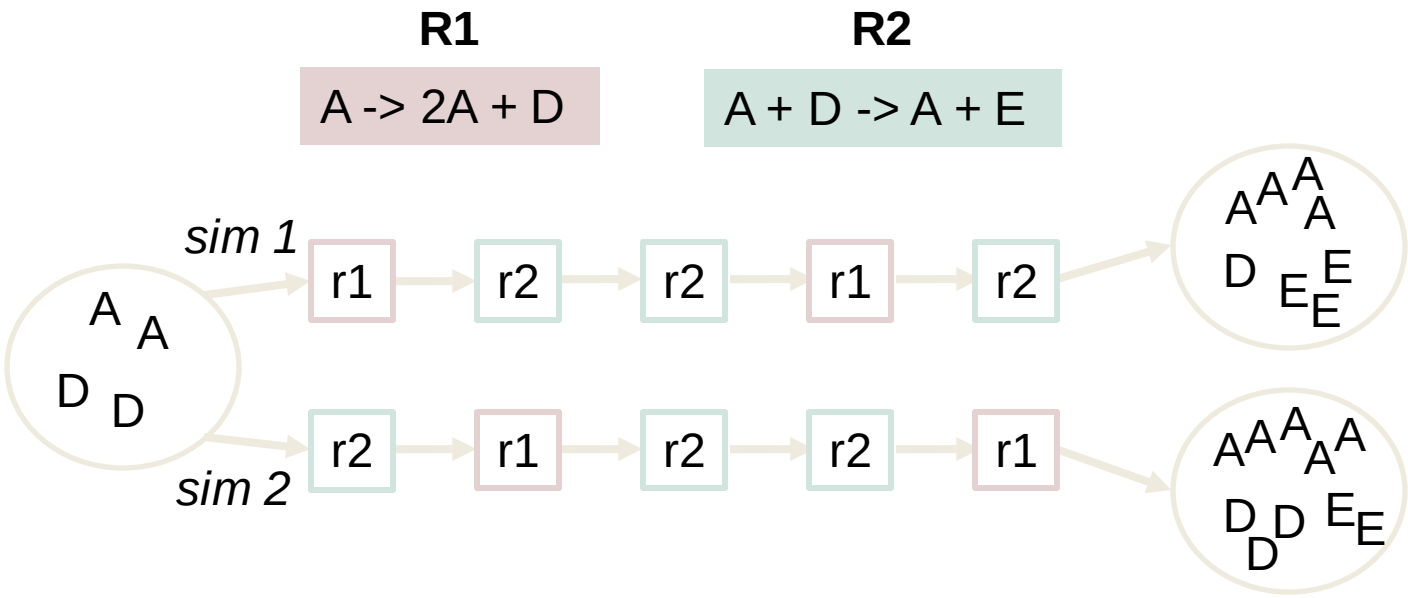

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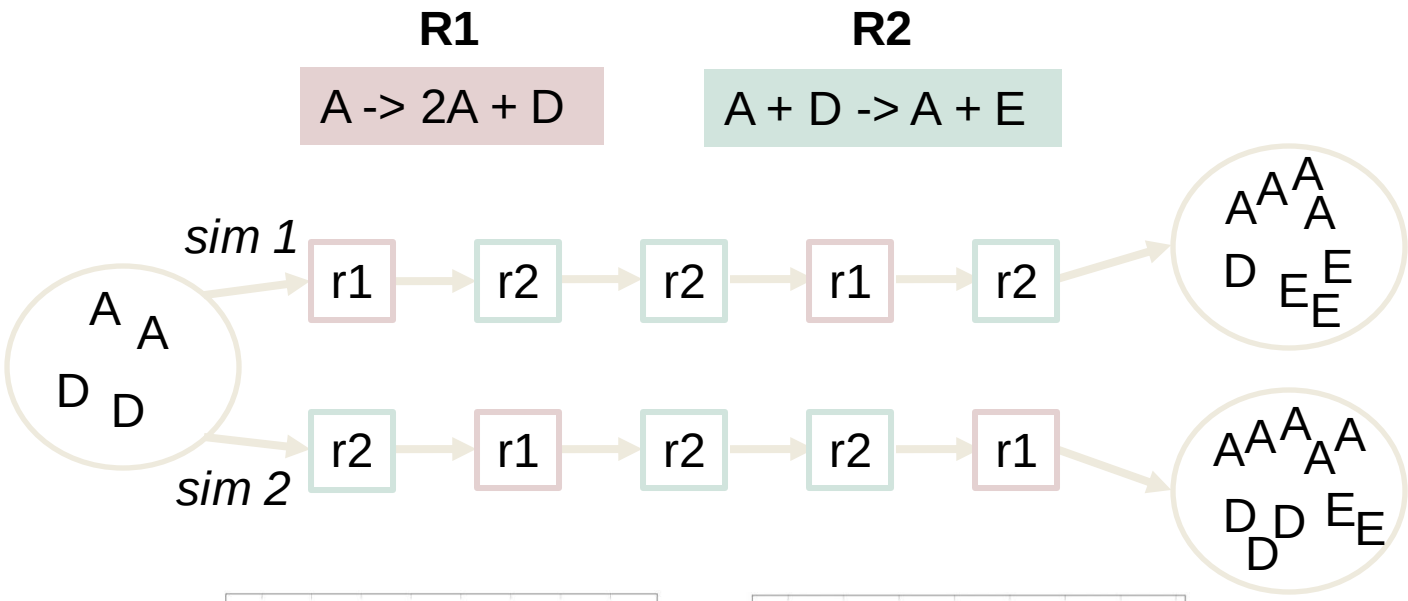

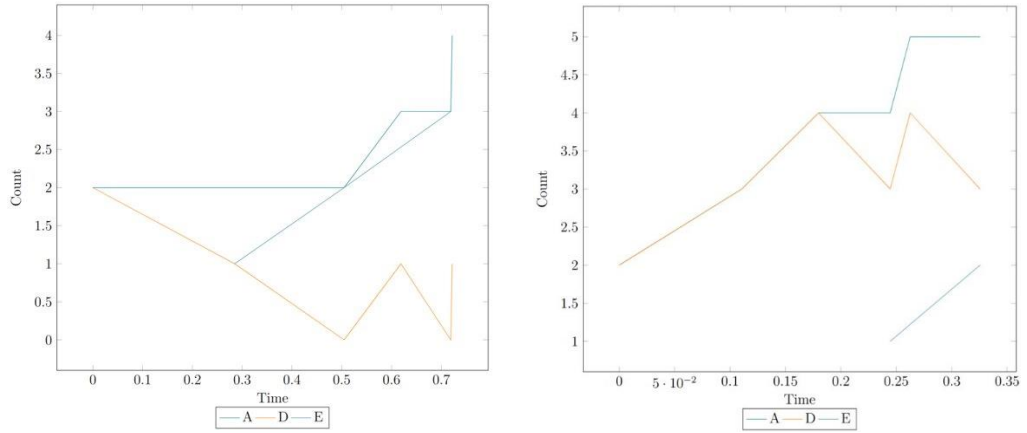

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Current work

Sensitivity Analysis for reaction rate constants

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How changes in the input variables of a model impact the output?

One-at-a-Time (OAT)

- Change one input variable at a time, keeping others constant.

Derivative-Based Local Methods

- Take partial derivatives of the output with respect to each input.

Regression Analysis

- Fit a linear regression to the model response.

Variance-Based Methods

- Decompose output variance into contributions from input variables and interactions.

Current work

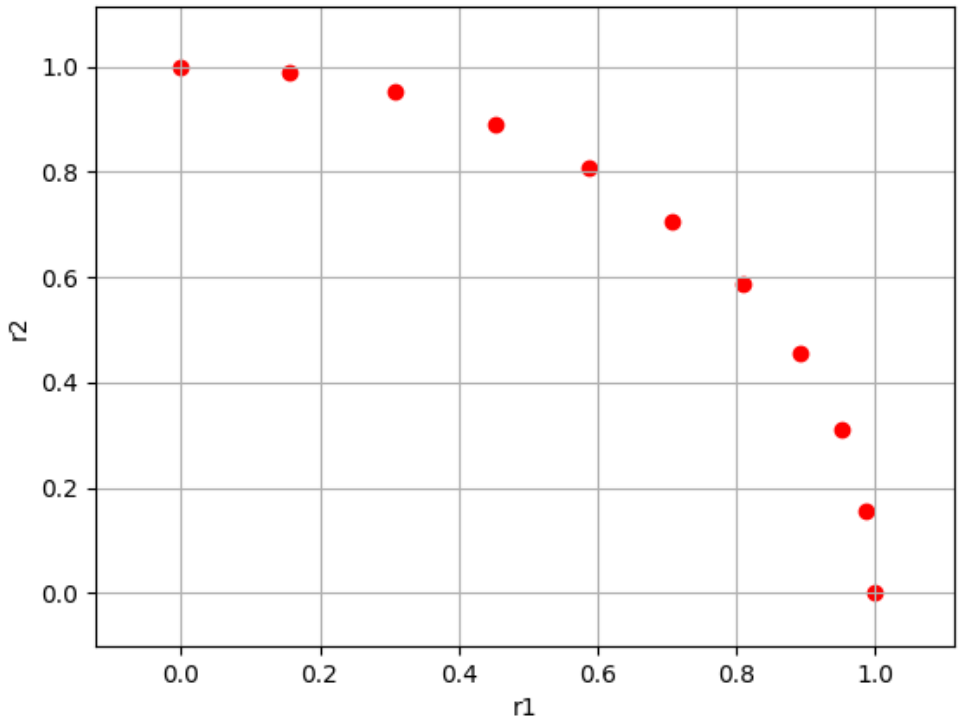
Sensitivity Analysis for reaction rate constants

R1	R2
A -> 2A + D	A + 4D -> E

Initial state: A x10

How sensitive is the time until two E molecules are present at the same time w.r.t the reaction rate constants?

Sample reaction rate constants from hypersphere

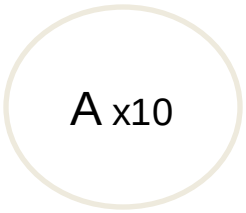


Current work

Sensitivity Analysis for reaction rate constants

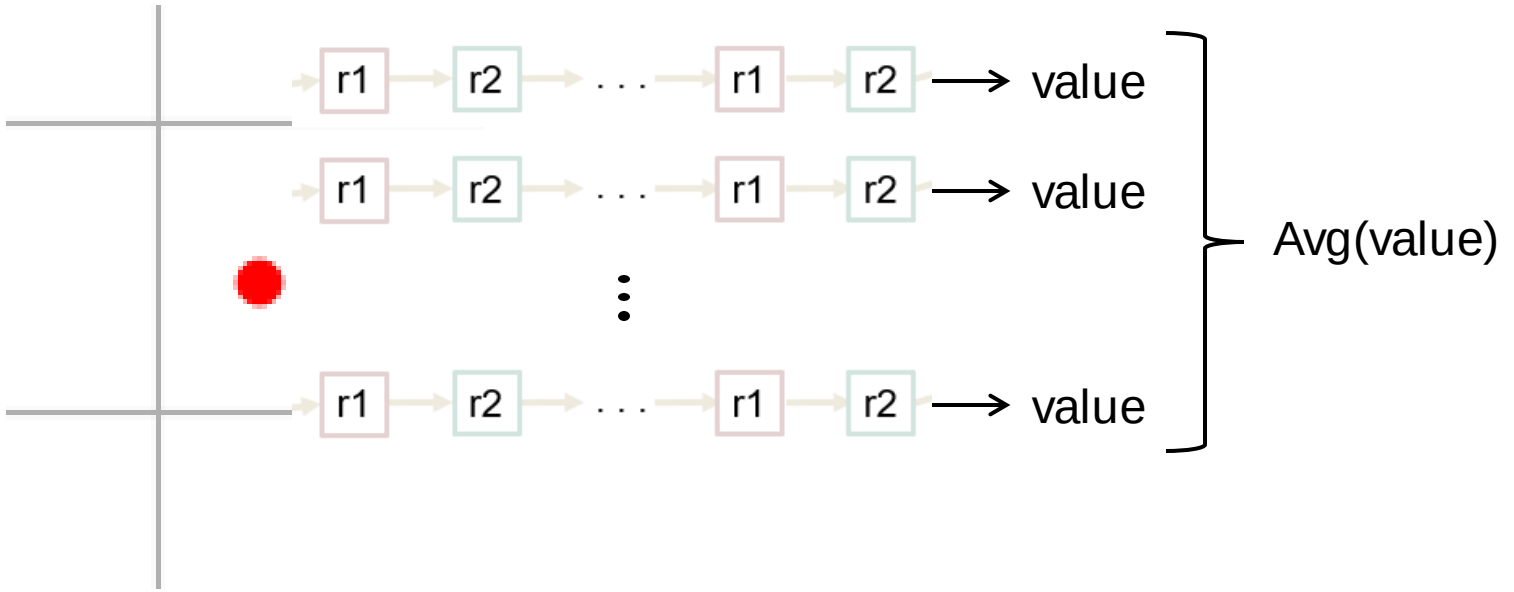
R1	R2
A -> 2A + D	A + 4D -> E

Initial state



How sensitive is the time until two E molecules are present at the same time w.r.t the reaction rate constants?

Run several simulations for each point



Current work

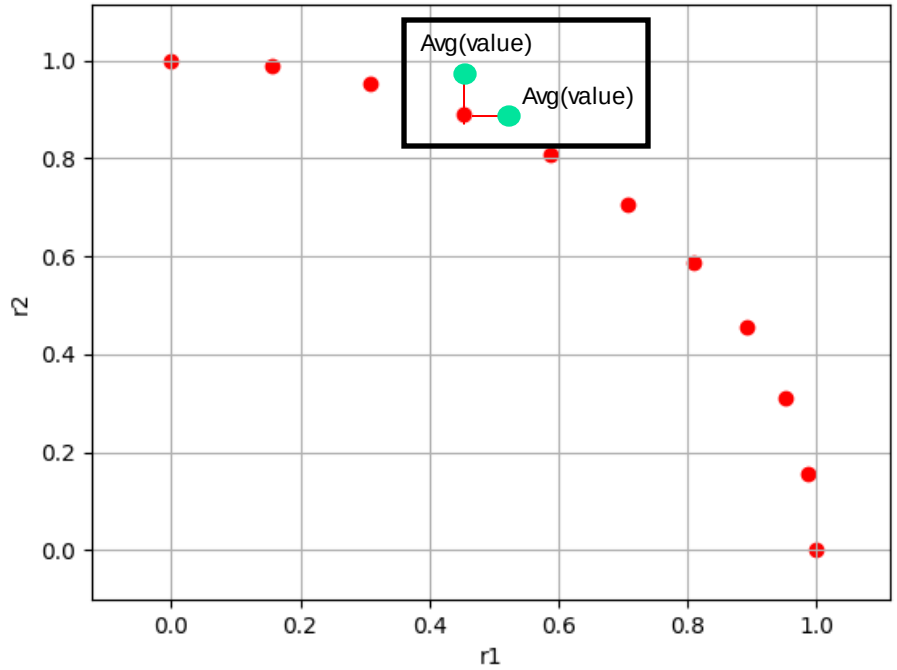
Sensitivity Analysis for reaction rate constants

R1	R2
A -> 2A + D	A + 4D -> E

Initial state: A x10

How sensitive is the time until two E molecules are present at the same time w.r.t the reaction rate constants?

Repeat for neighboring points



Current work

Sensitivity Analysis for reaction rate constants

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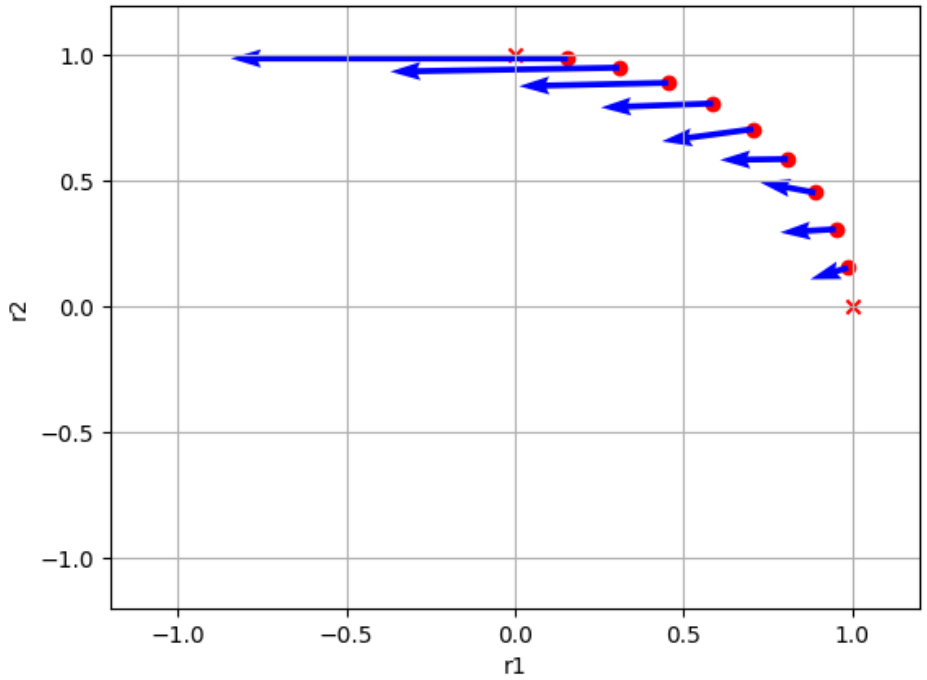
R1	R2
A -> 2A + D	A + 4D -> E

Initial state: A x10

How sensitive is the time until two E molecules are present at the same time w.r.t the reaction rate constants?

Calculate vector field using forward differences

$$\frac{f(x+h)-f(x)}{h}$$



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Formose process on
an early Earth as
seen by DALL·E

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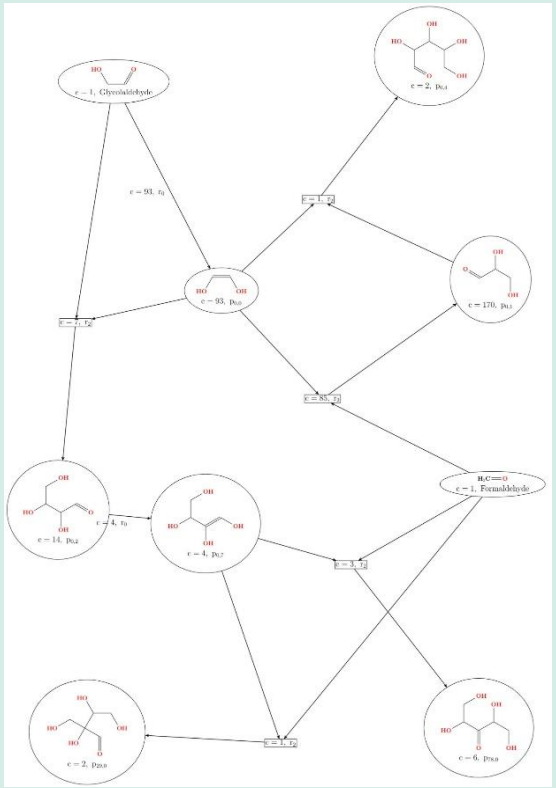
Formose + borate

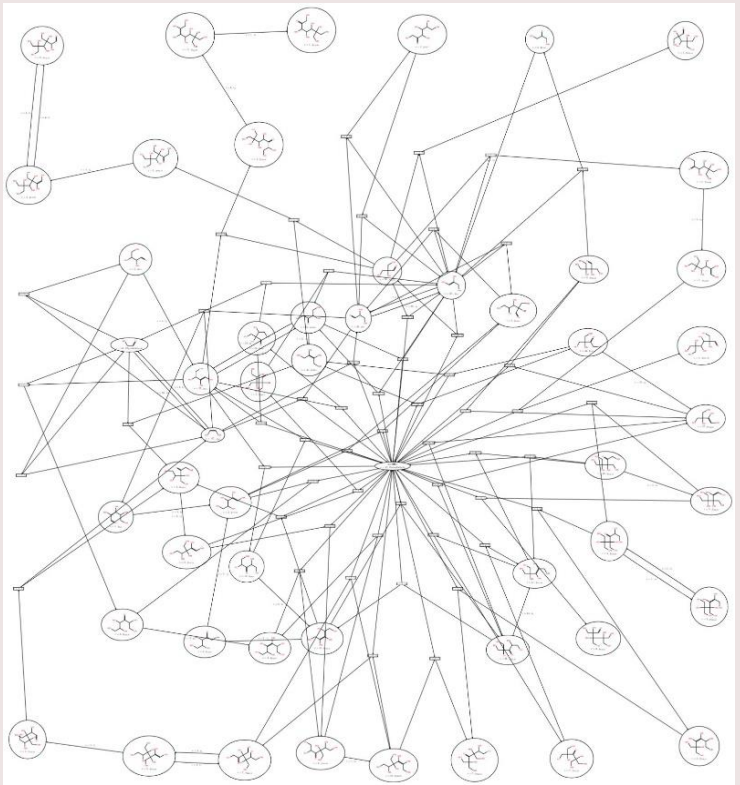
- Kim, H. J., Ricardo, A., Illangkoon, H. I., Kim, M. J., Carrigan, M. A., Frye, F., & Benner, S. A. (2011). **Synthesis of carbohydrates in mineral-guided prebiotic cycles.** *Journal of the American Chemical Society*, *133*(24), 9457-9468.

- Andersen, J. L., Flamm, C., Merkle, D., & Stadler, P. F. (2014). **Generic strategies for chemical space exploration.** *International journal of computational biology and drug design, 7(2-3), 225-258.*

With borate



Without borate



Current work

Sensitivity Analysis for reaction rate constants

With borate

		Average	Std Dev
	Size of DG	38.7	7.83
	Unique pentoses in DG	7.05	0.86
Final state of the simulation	Total amount pentoses	7.65	1.98
	Unique pentoses	2.8	0.81
	Carbons in pentoses	38.25	9.91

Without borate

		Average	Std Dev
	Size of DG	95.8	9.28
	Unique pentoses in DG	7.75	0.89
Final state of the simulation	Total amount pentoses	12	3.29
	Unique pentoses	2.8	0.6
	Carbons in pentoses	60	16.43

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Thank you!

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