Supporting Information: BAR-based Optimum Adaptive Sampling Regime for Variance Minimization in Alchemical Transformation: The Nonequilibrium Stratification

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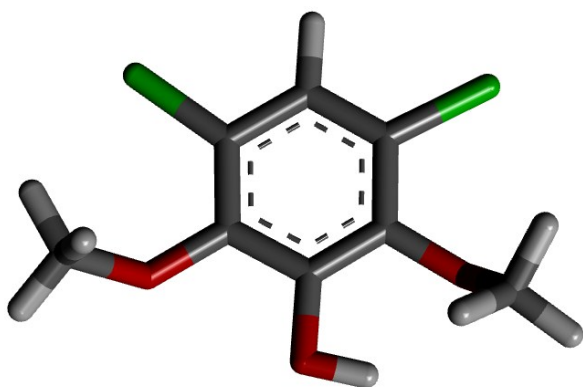[5]Department of Chemistry, New York University, NY, NY 10003, USA

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Figure S1. Structures of molecules simulated in this work.(Red O atom, grey C, white H, green Cl, blue N atom.)
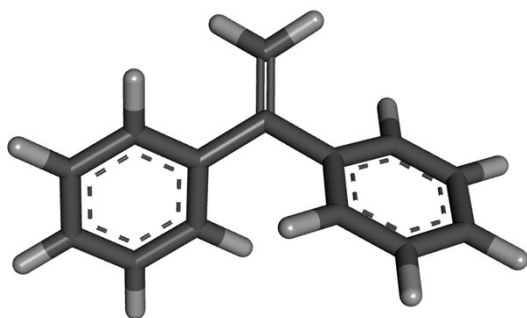
a)SAMPL4-1
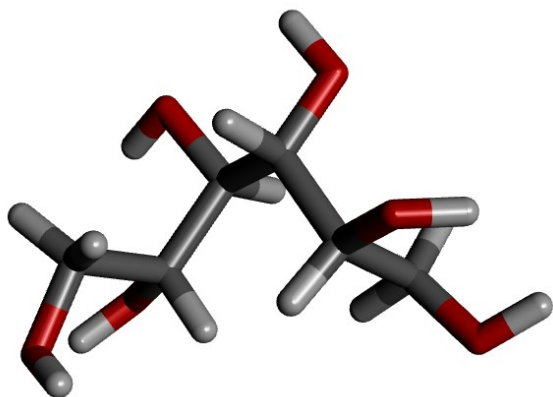
b)SAMPL4-10

c)SAMPL4-20

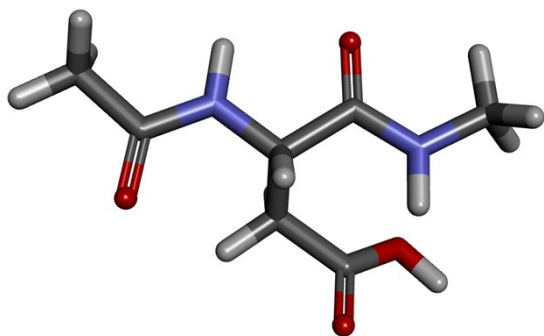d)model compound for ASP to ASH transformation

Figure S2. Dependence of a)simulation time, b) number of works, c) TDV in each state on the order of magnitude of GOCE criteria, the number of iteration for the ASP example from different viewpoints.
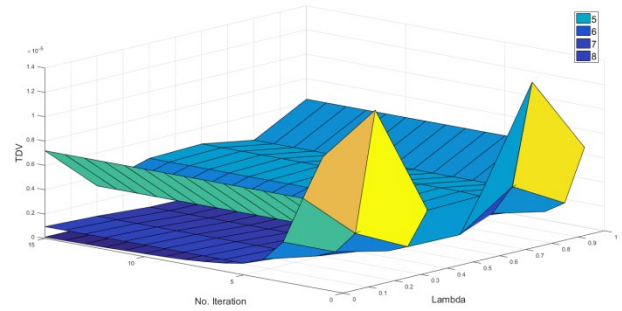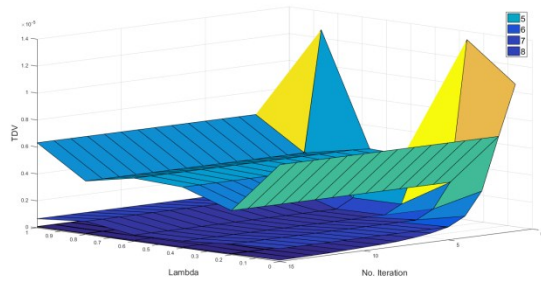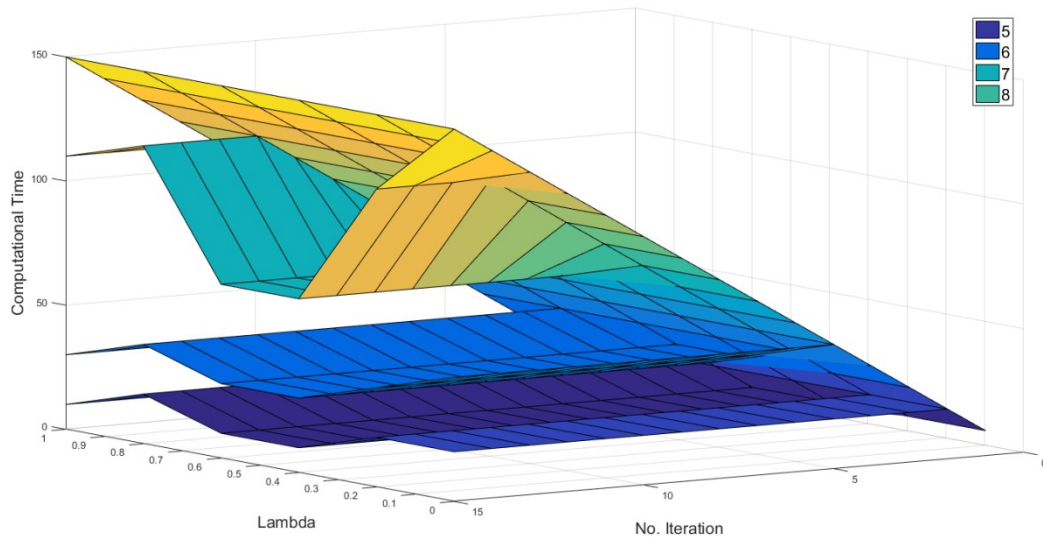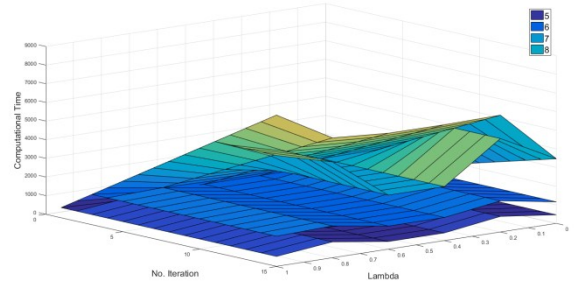

a)

b)

c)
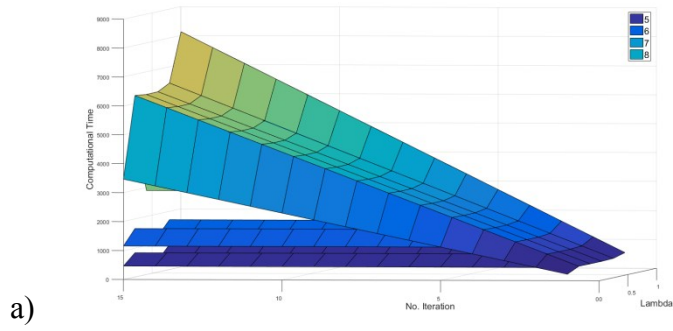
Table S1. Absolute % errors.

Absolute % error	LTL	GOCE	NCE
TIP3P	2.06%	2.27%	4.04%
SAMPL4-1	0.00%	1.03%	0.79%
SAMPL4-10	6.45%	6.32%	4.86%
SAMPL4-20	3.57%	4.68%	10.48%
Aspartate	0.00%	0.34%	0.49%