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

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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

![Image of SAMPL4-1](image1.png)

b) SAMPL4-10

![Image of SAMPL4-10](image2.png)

c) SAMPL4-20

![Image of SAMPL4-20](image3.png)

d) model compound for ASP to ASH transformation

![Image of model compound](image4.png)
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.
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<th>NCE</th>
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