

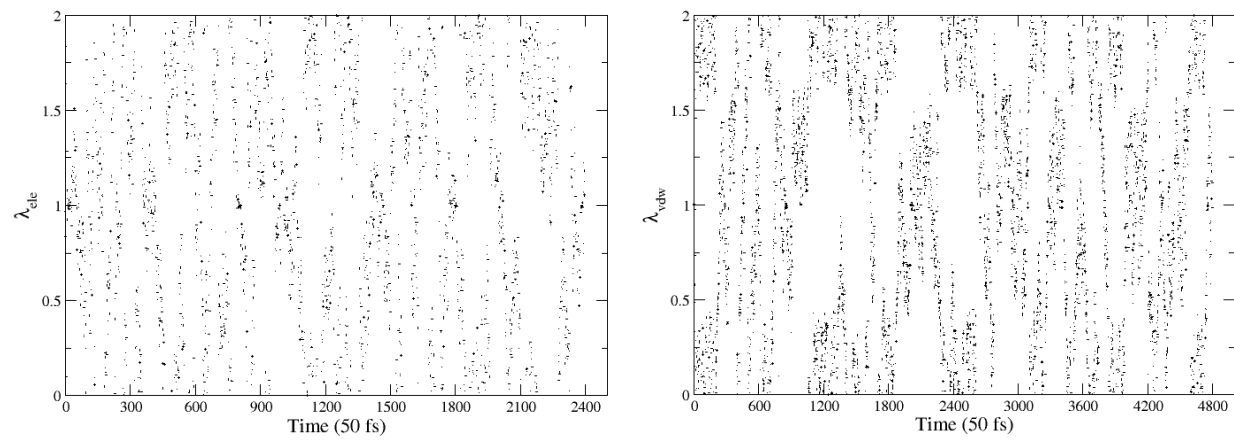
# Supporting Information for “ $\lambda$ -meta dynamics approach to compute absolute solvation free energy”

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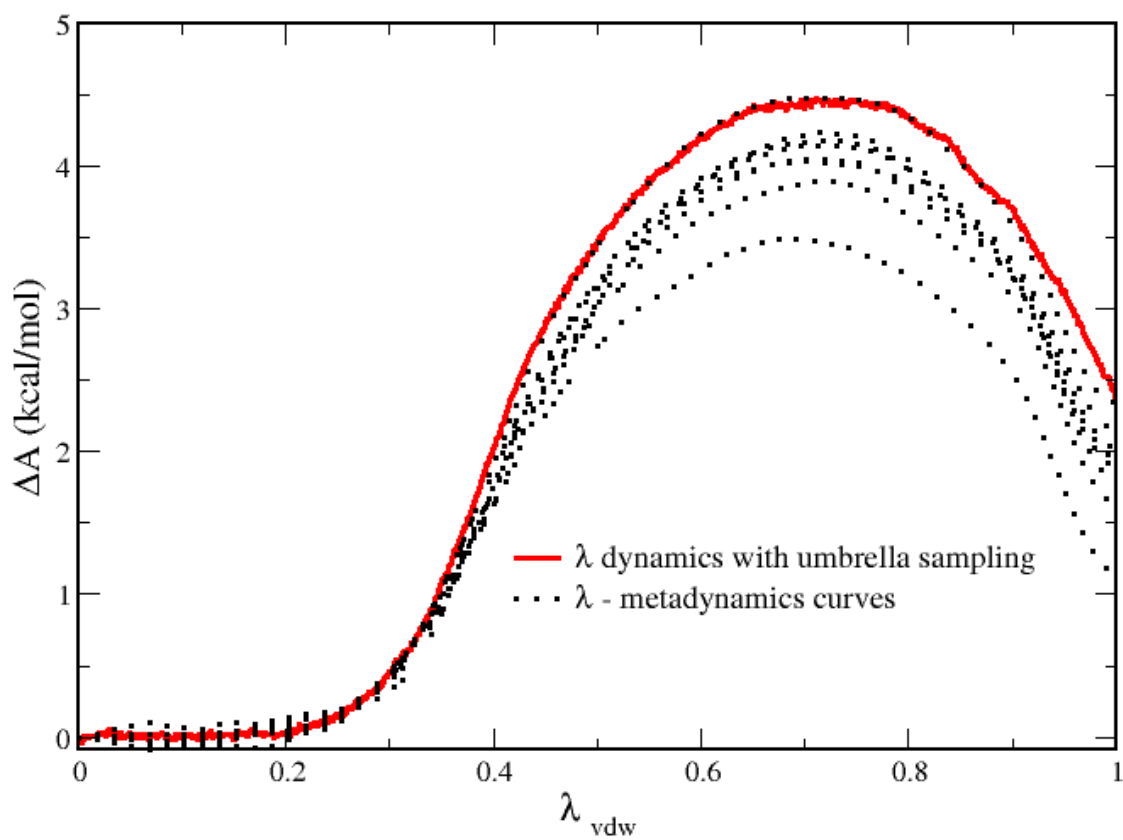
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## I. Supporting figures



**Figure S1.** Trajectories of  $\lambda_{ele}$  and  $\lambda_{vdw}$  during  $\lambda$ -metadynamics for methanol.



**Figure S2.** PMFs of  $\lambda_{vdw}$  from eight independent  $\lambda$ -metadynamics (dashed black lines) and from  $\lambda$  dynamics with umbrella sampling (read solid line) for methanol.

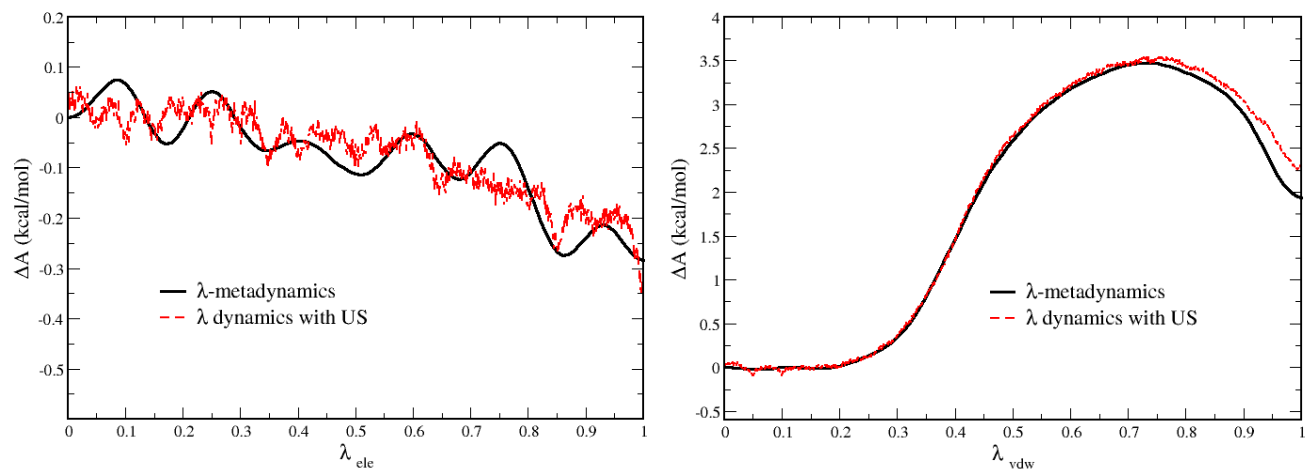


Figure S3. PMFs from  $\lambda$ -metadynamics and umbrella sampling for methane

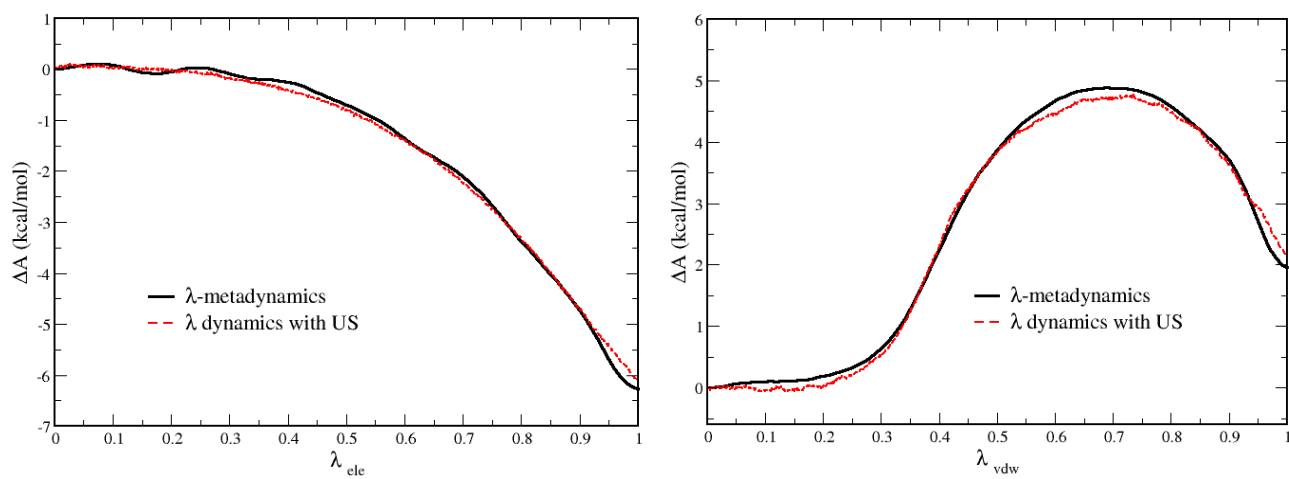


Figure S4. PMFs from  $\lambda$ -metadynamics and umbrella sampling for methylamine

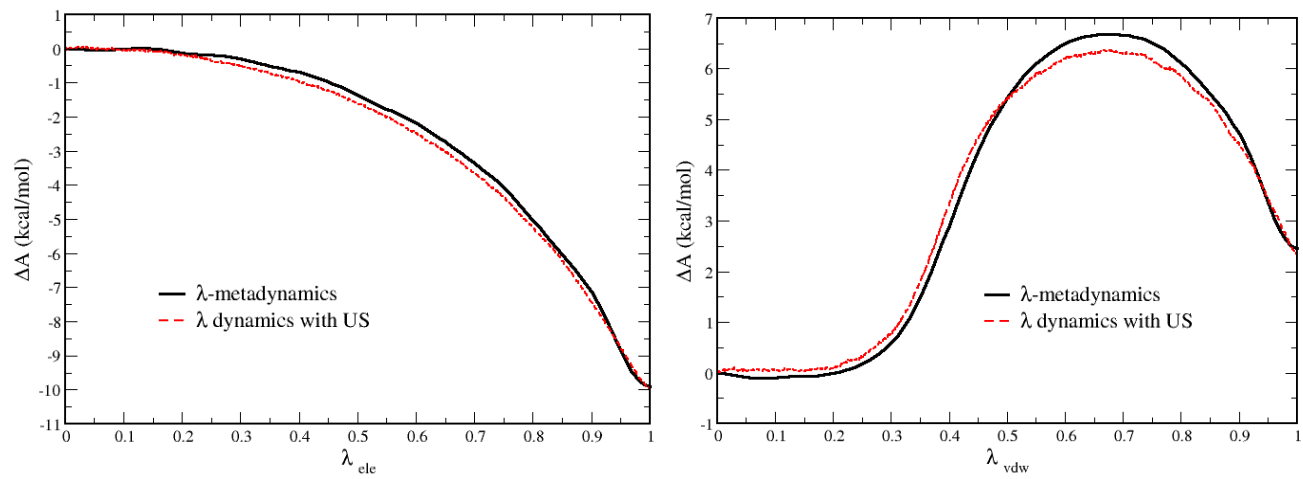


Figure S5. PMFs from  $\lambda$ -metadynamics and umbrella sampling for acetamide

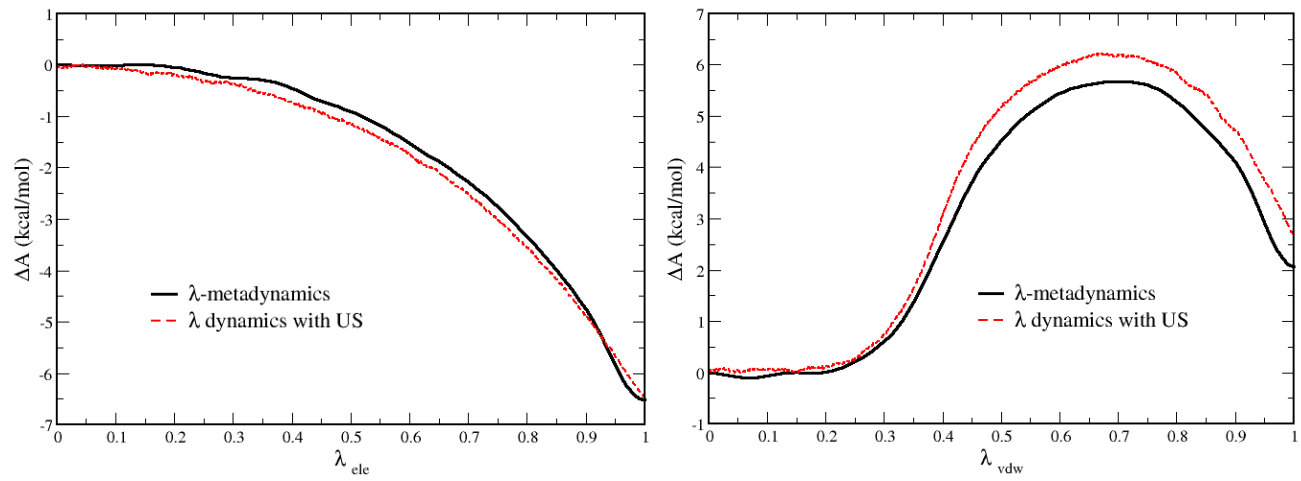


Figure S6. PMFs from  $\lambda$ -metadynamics and umbrella sampling for acetic acid