

# Supplementary Material for

## Comparing dimerization free energies and binding modes of small aromatic molecules with different force fields

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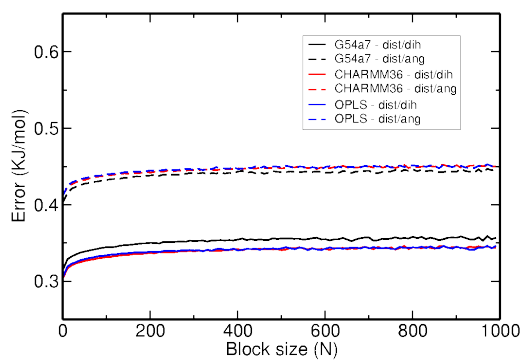
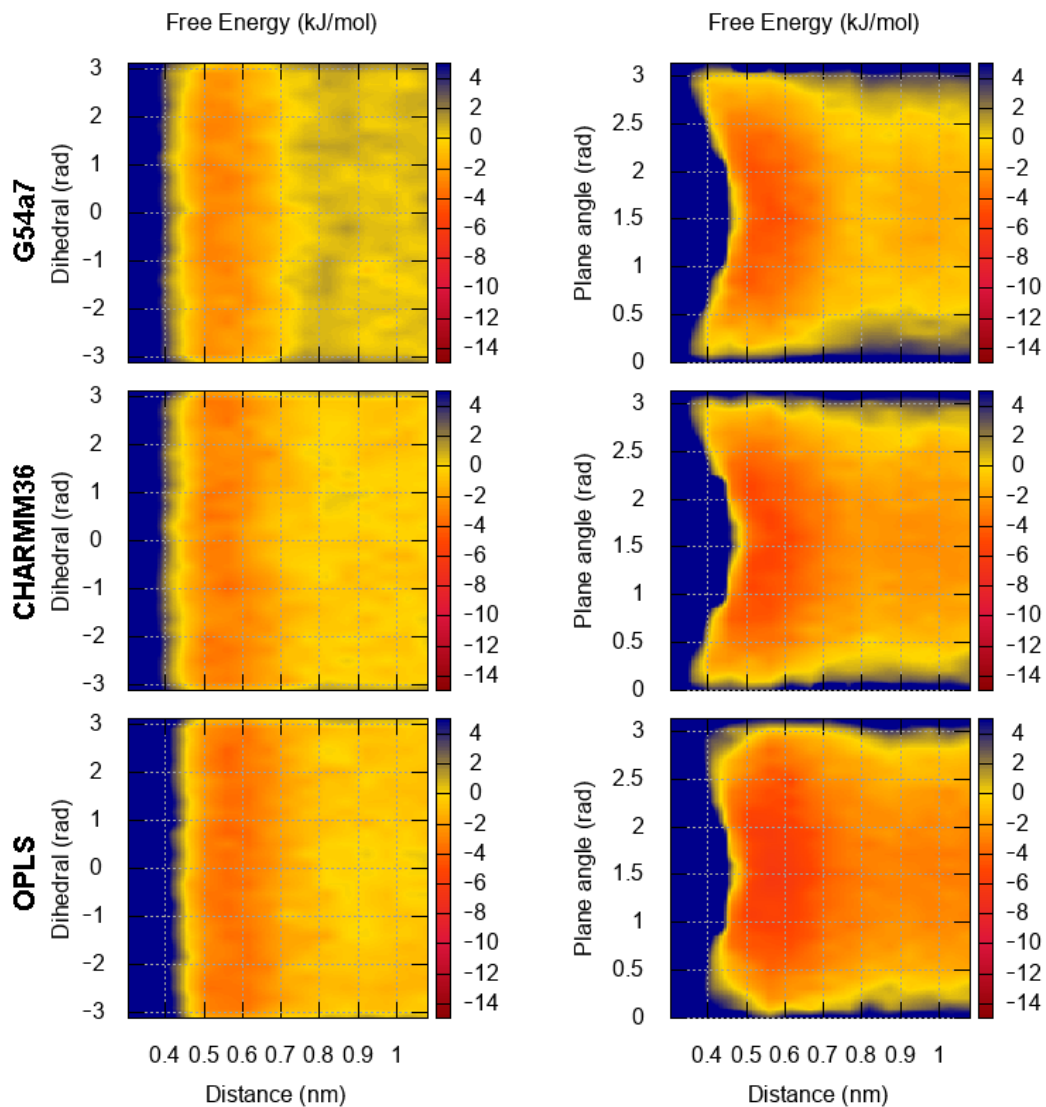
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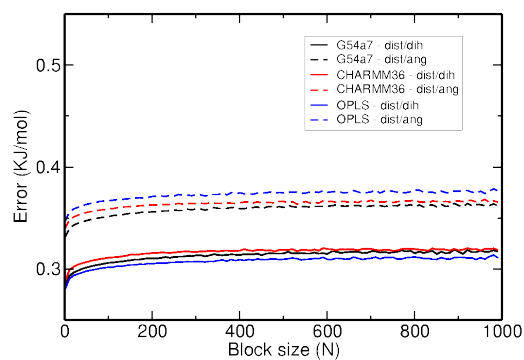
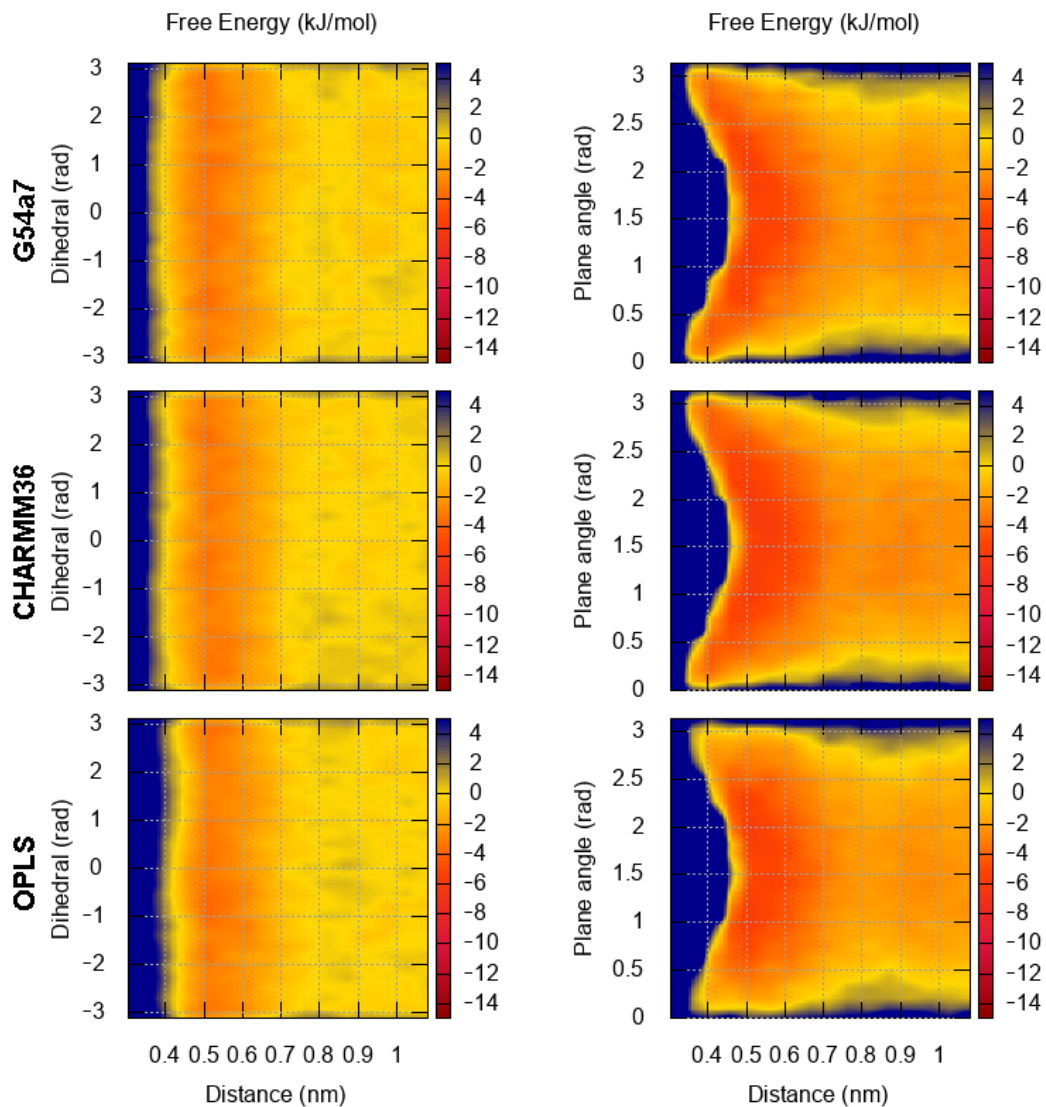
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Name	Molecule ID	Opt. Solvation Free Energy	Simulation time (ns)
Benzene	804	✓	100
Toluene	21	✓	100
Chlorobenzene	3176	✓	150
Phenol	1061	✓	100
Styrene	1266	✓	100
para-Cresol	17	✓	150
Cyclohexane	17666	✓	100
Naphthalene	820	✓	100
Pyrene	7233	✓	150
Tetracene	33259	✗	150

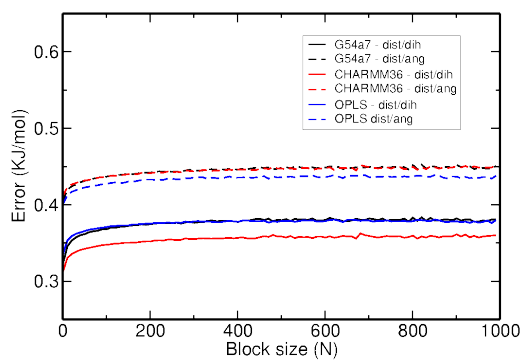
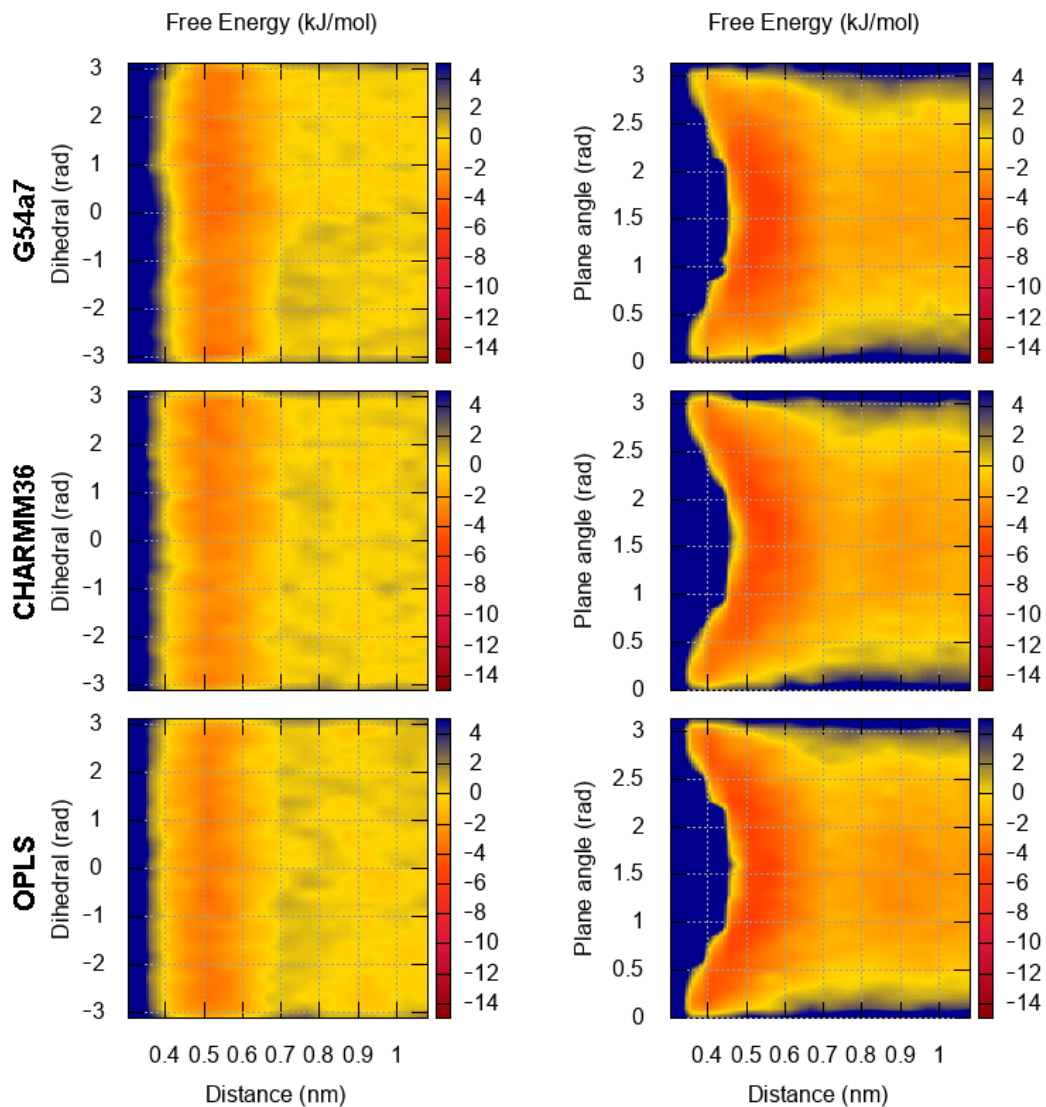
**Table S1:** ATB entries for the topologies used. Most of the parameters have been optimised to reproduce experimental solvation free energies.



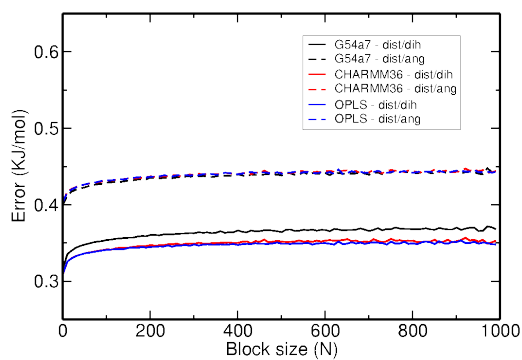
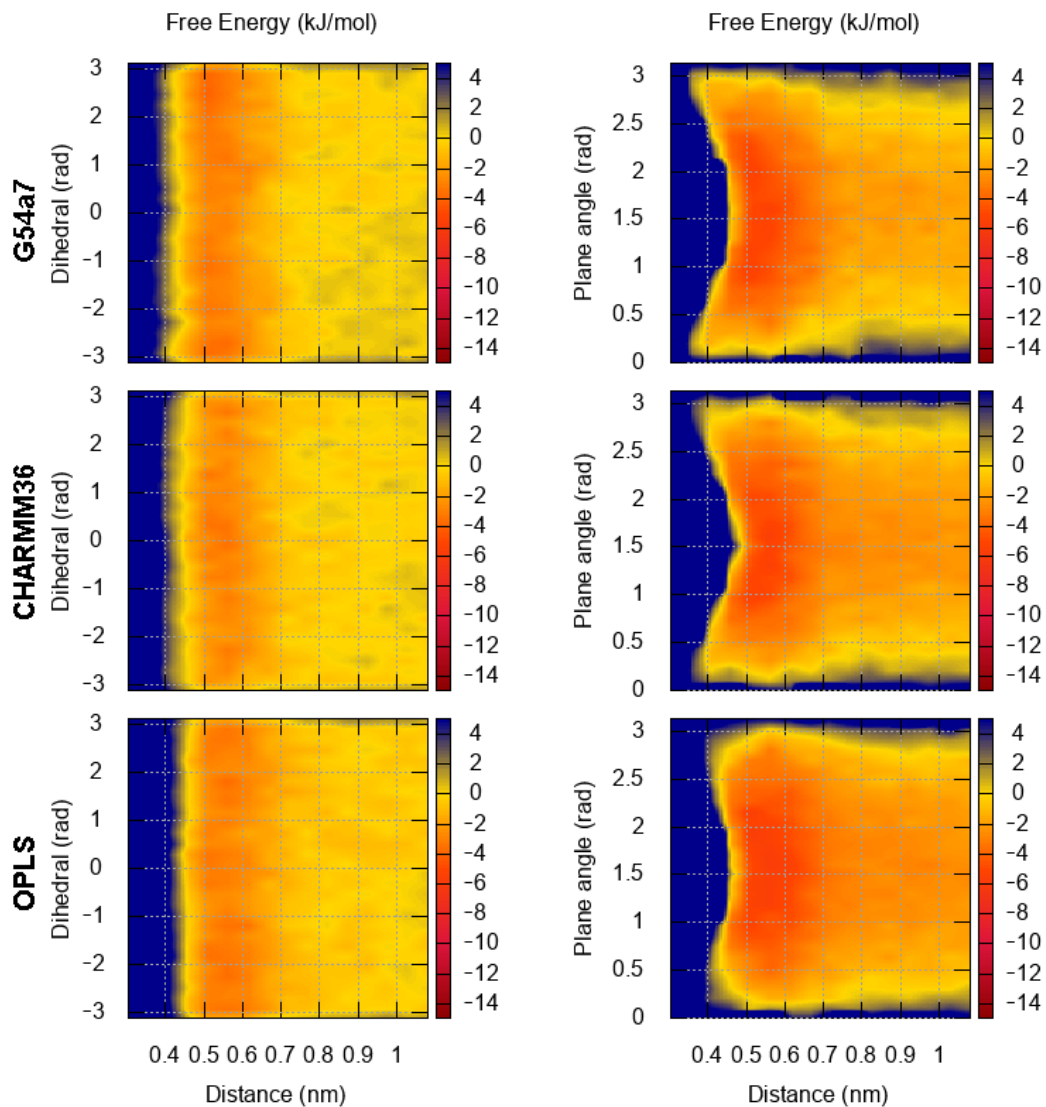
**Figure S1:** FES for the dimerization of toluene (top) and statistical error of the FES calculations as a function of the block size (bottom).



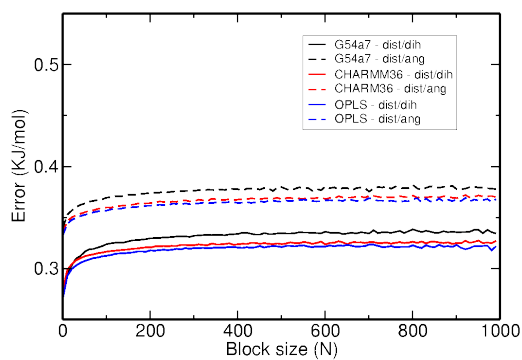
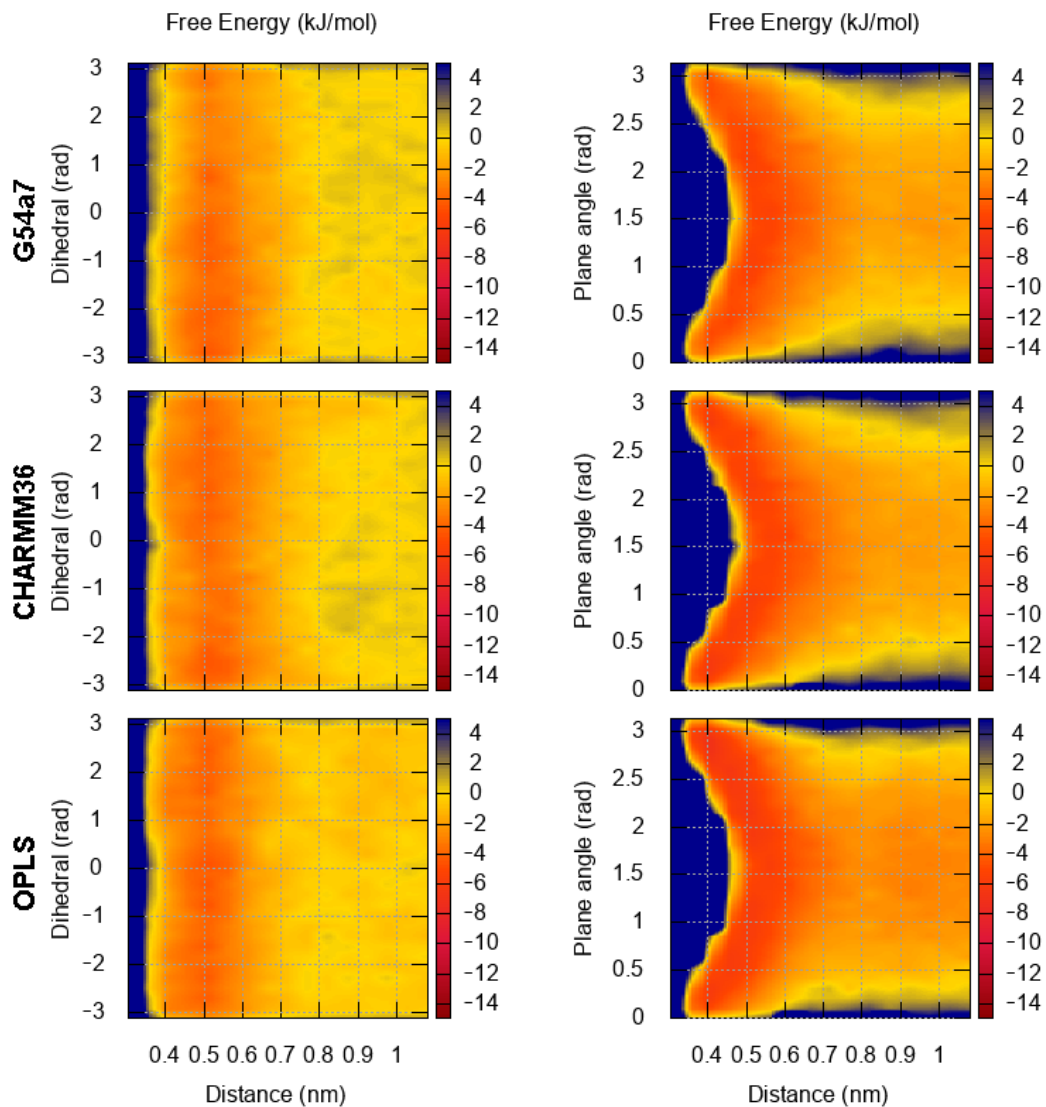
**Figure S2:** FES for the dimerization of chlorobenzene (top) and statistical error of the FES calculations as a function of the block size (bottom).



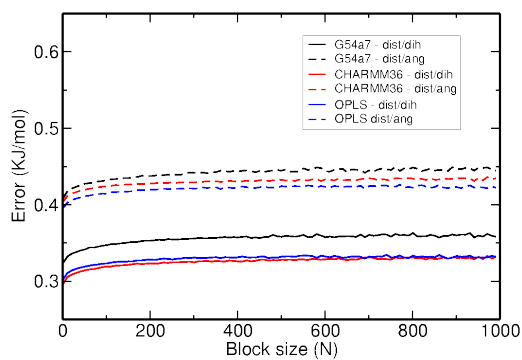
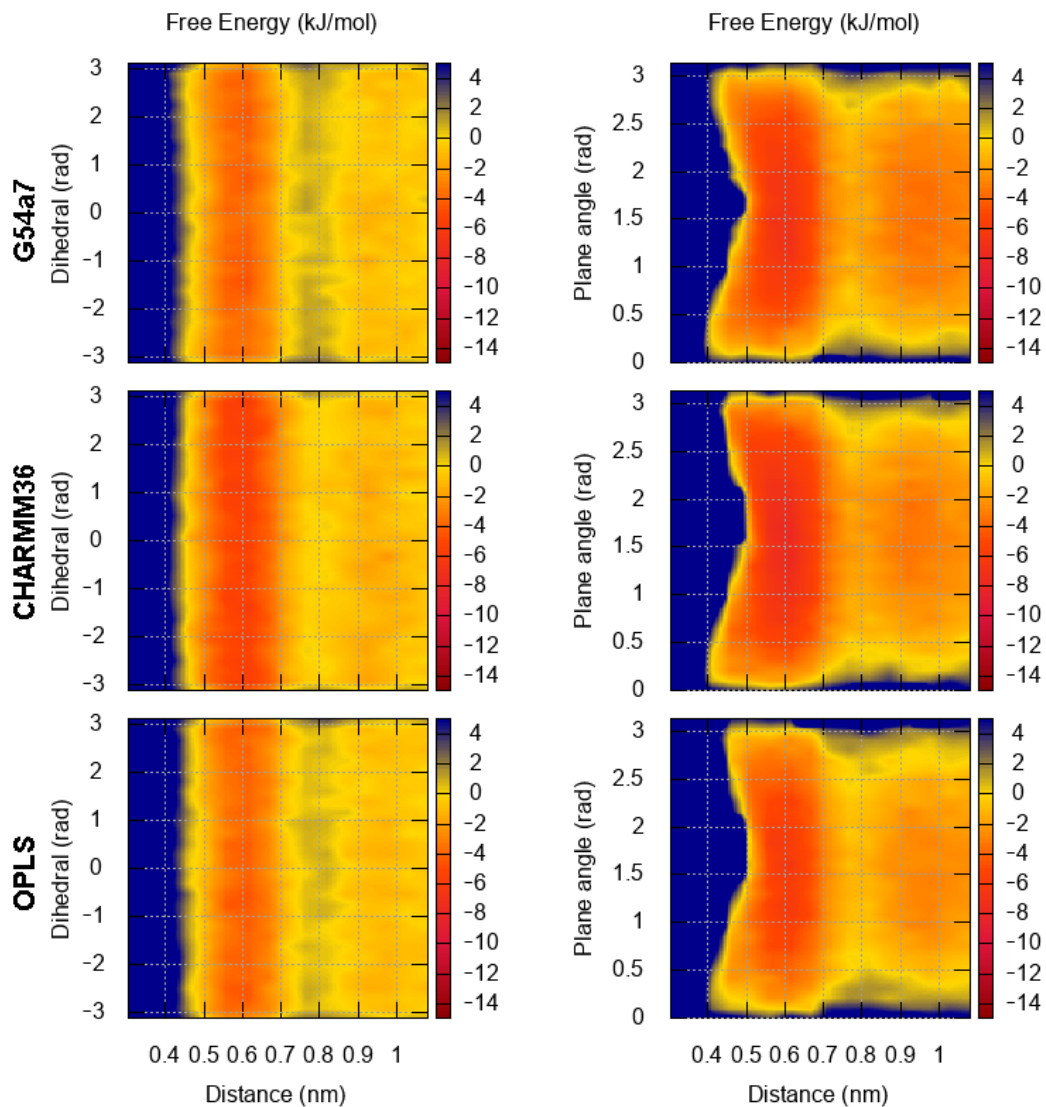
**Figure S3:** FES for the dimerization of phenol (top) and statistical error of the FES calculations as a function of the block size (bottom).



**Figure S4:** FES for the dimerization of styrene (top) and statistical error of the FES calculations as a function of the block size (bottom).

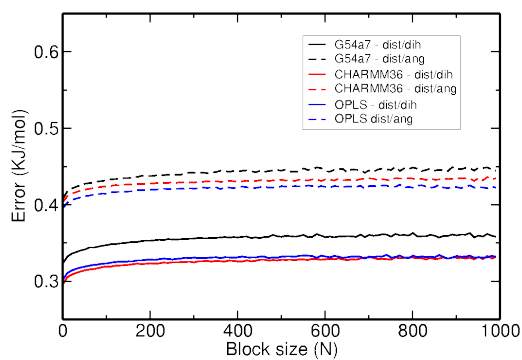
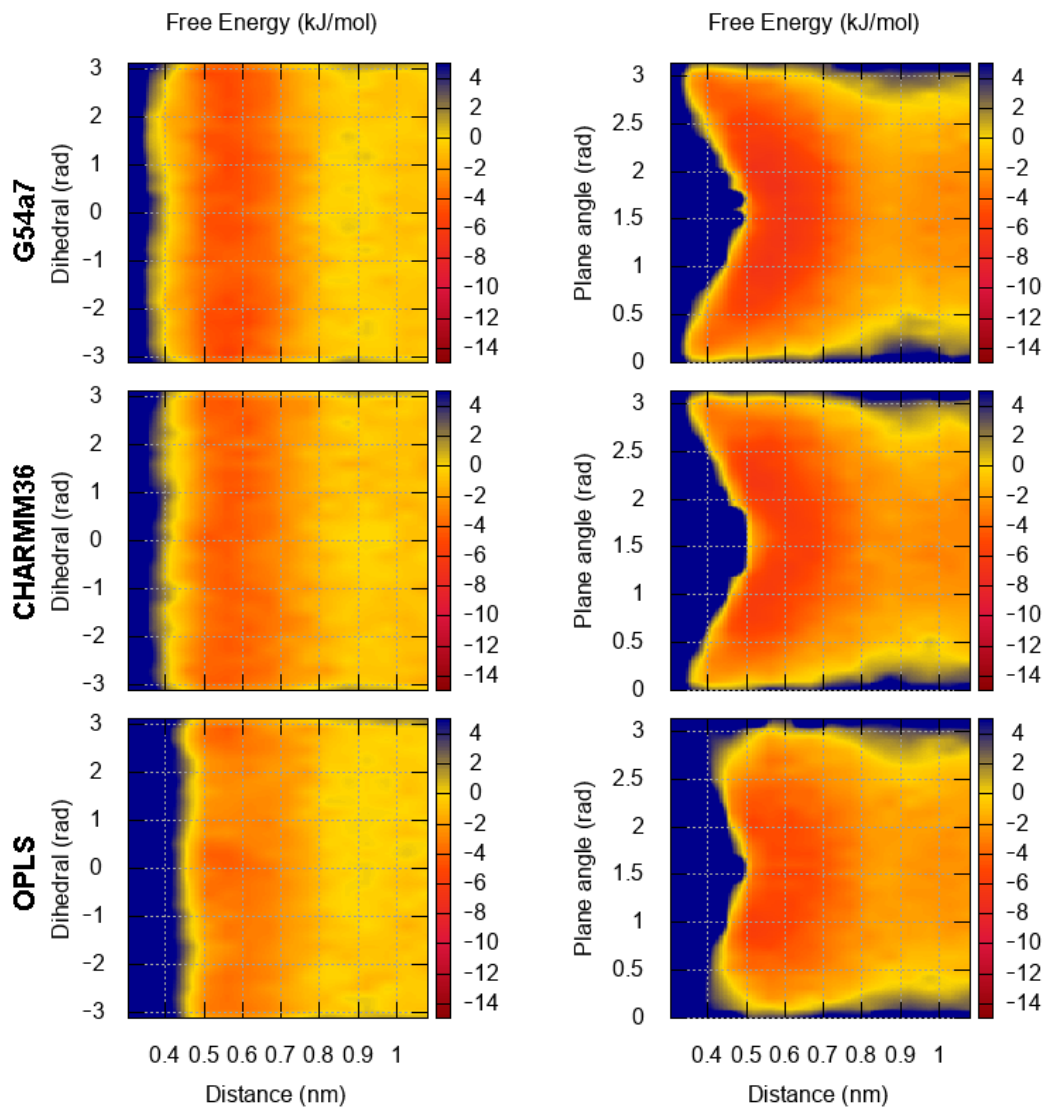


**Figure S5:** FES for the dimerization of para-cresol (top) and statistical error of the FES calculations as a function of the block size (bottom).

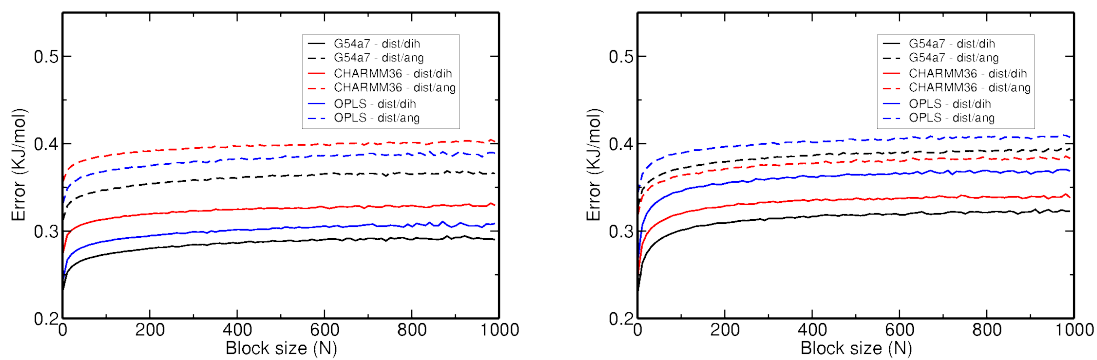


**Figure S6:** FES for the dimerization of cyclohexane (top) and statistical error of the FES calculations as a function of the block size (bottom).





**Figure S7:** FES for the dimerization of naphthalene (top) and statistical error of the FES calculations as a function of the block size (bottom).



**Figure S8:** Statistical error of the FES calculations as a function of the block size for pyrene and anthracene, respectively.