Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information: Is Preservation of Symmetry Necessary for Coarse-Graining?

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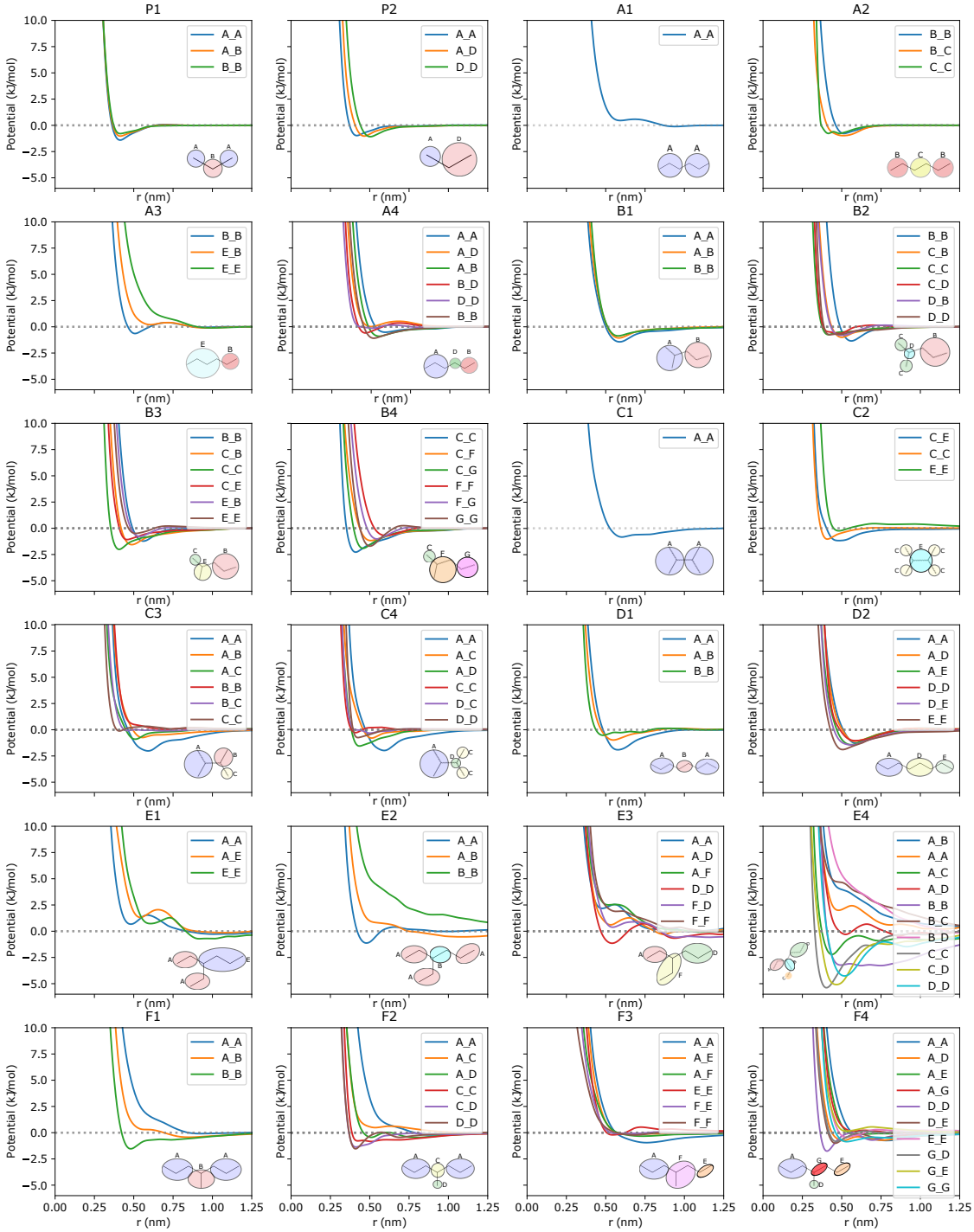

Fig. S1: Potential plots for the 24 mappings for 7 molecules obtained using force matching (FM).

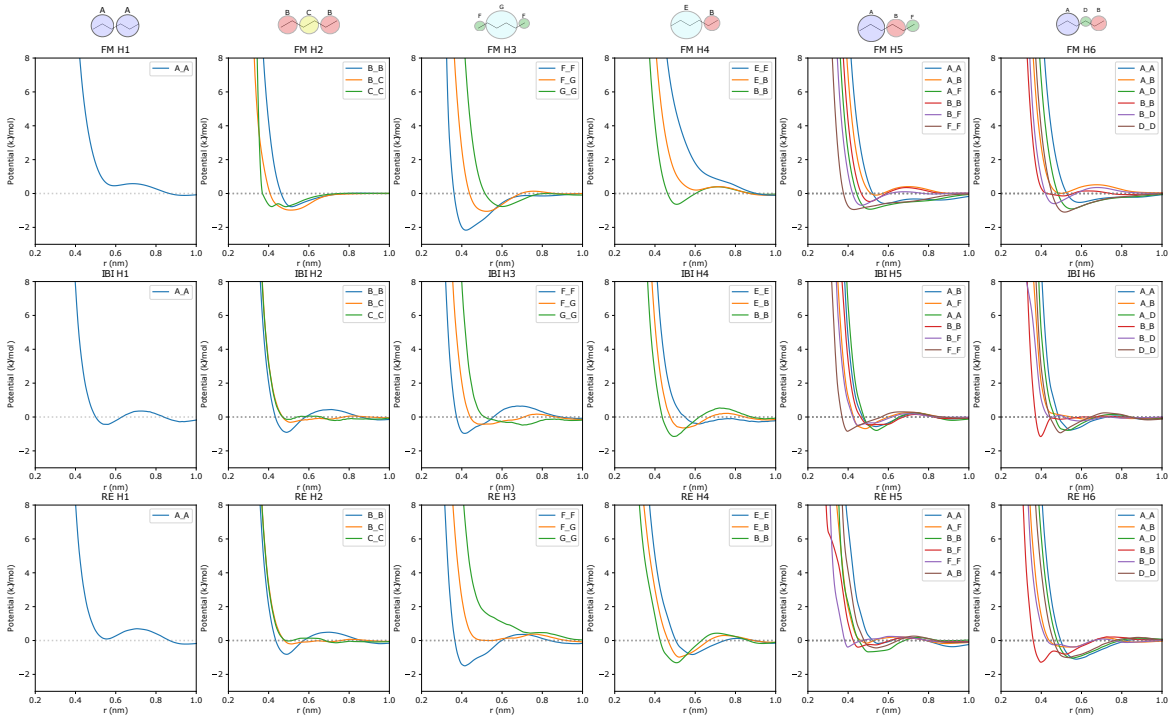

Fig. S2: Potential plots for the 6 hexane mappings obtained using FM, iterative Boltzmann inversion (IBI) and relative entropy (RE).

SI Equilibrium Bond Length and Angle Value Selection

In all the coarse-grained (CG) simulations, the bonds and angles are constrained. The corresponding set values are determined using the equilibrium distributions of the bonds and angles from equilibrated fine-grained (FG) simulation trajectory mapped into the CG coordinates. The equilibrium bond and angle distributions of the CG mappings for all the 7 molecules along with the corresponding set values (indicated using dotted vertical lines) are given in Figures S3 and S4 respectively. The mode values from the bond and angle distributions were set as constraints for all the mappings except H3, H5, B2, C2, E2, E4 and F4 (marked with '$*$' in Figures S3 and S4). Setting the mode values for bonds and angles for those 7 mappings yielded instability of the system owing to large bond rotations. To address this problem, a single molecule, with mapped CG coordinates, was isolated from the equilibrated box and its bond and angle values were used for setting constraints. Using PACKMOL[1], A new box was populated with copies of the isolated molecule such that the box size and the number of molecules were consistent with the original system. The refilled box was allowed to equilibrate for 100ps. The production CG simulation was started with the last frame of the equilibration simulation.

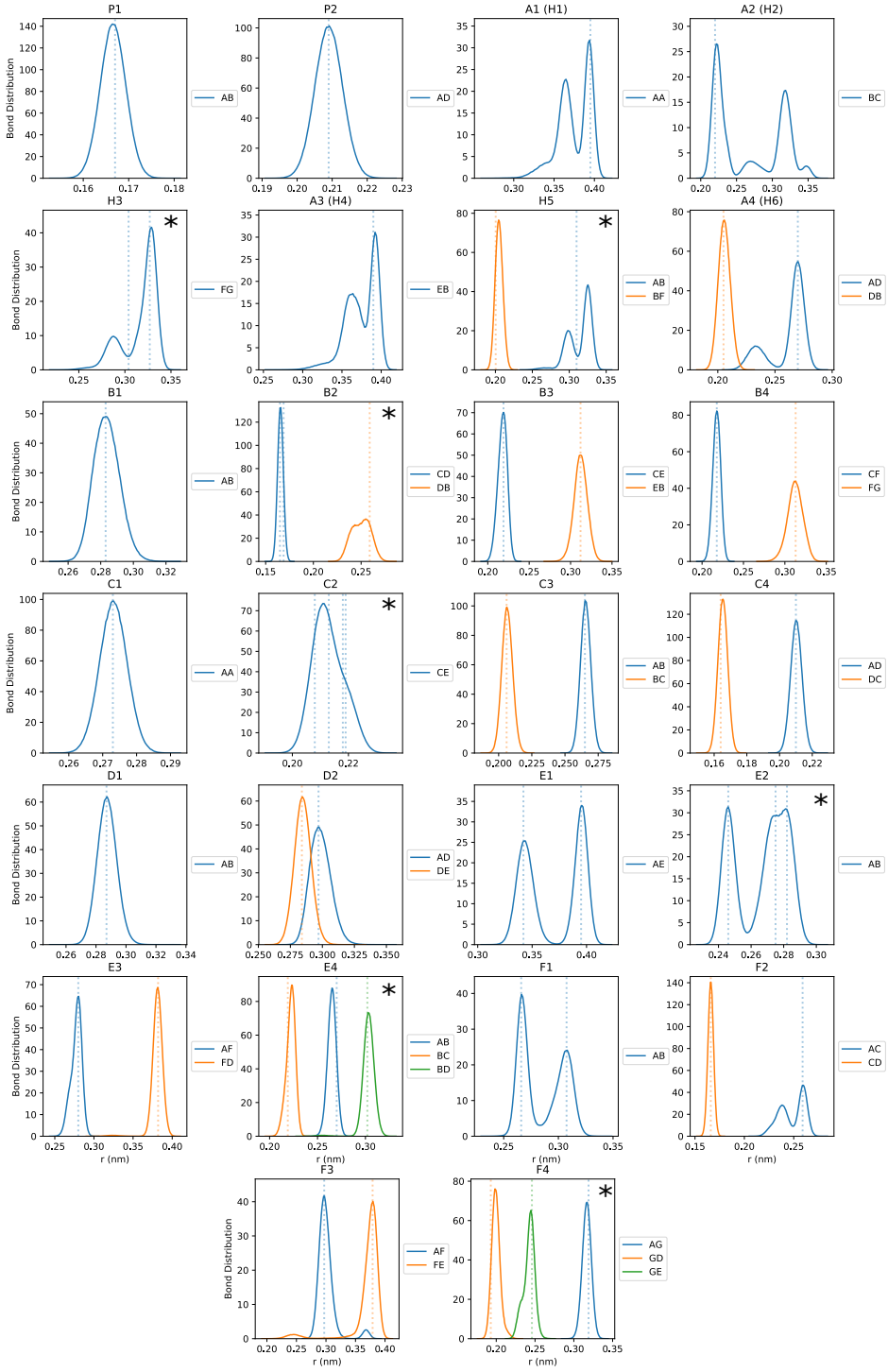

Fig. S3: Equilibrium bond distribution from reference mapped trajectory. The bond values used for CG topology constraints are marked by the dotted vertical lines. For the mappings marked with '$*$', the method for selecting the bond length for CG simulation is described in section SI.

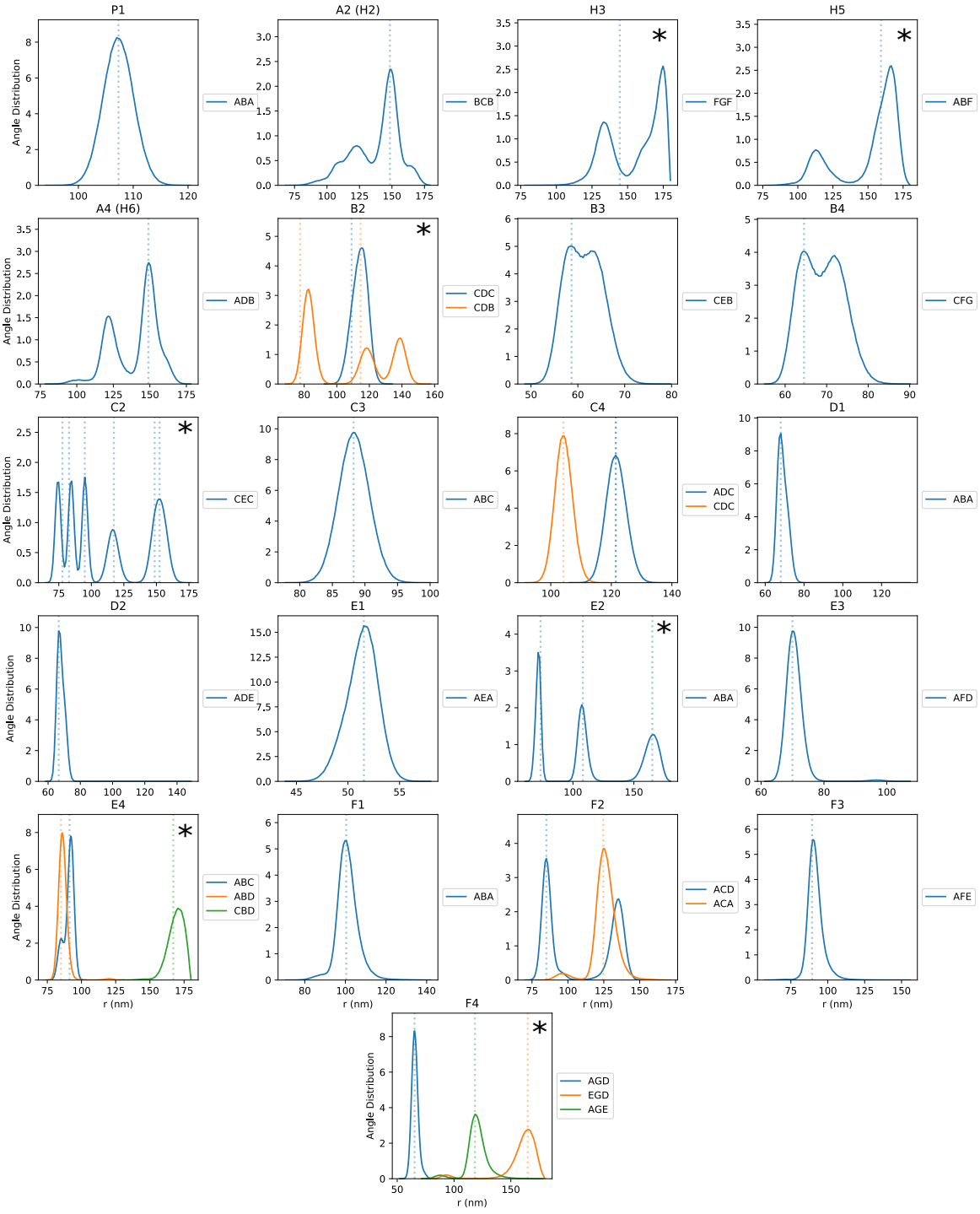

Fig. S4: Equilibrium angle distribution from reference mapped trajectory. The angle values used for CG topology constraints are marked by the dotted vertical lines. For the mappings marked with '$*$', the method for selecting the angle value for CG simulation is described in section SI.

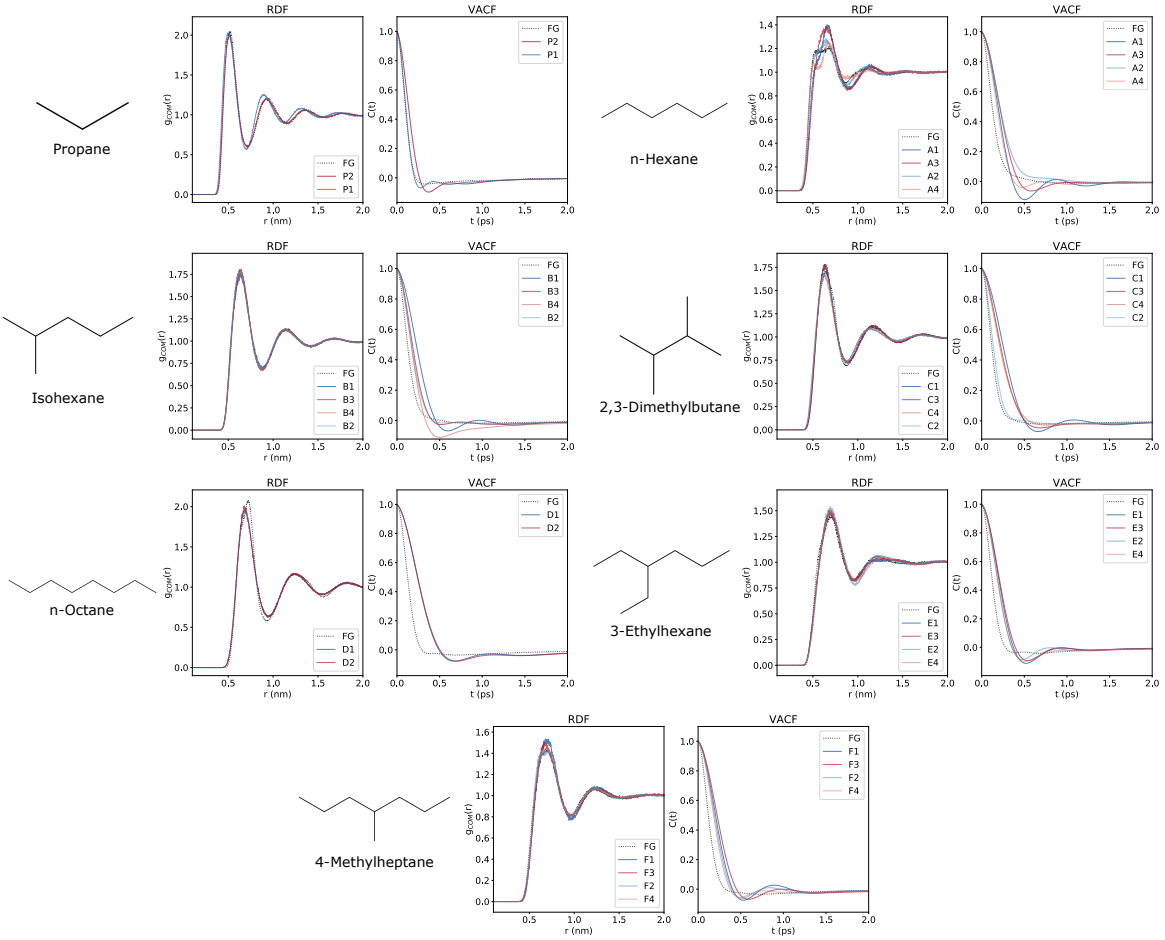

Fig. S5: Center of mass radial distribution function (COM-RDF) and velocity auto-correlation function (VACF) plots for the 24 mappings for 7 molecules along with the reference fine-grain (FG) plots. The symmetric and the asymmetric mappings are indicated by different shades of blue and red respectively. For each molecule, the mappings are arranged in the order of increasing resolution from top to bottom in the figure legend.

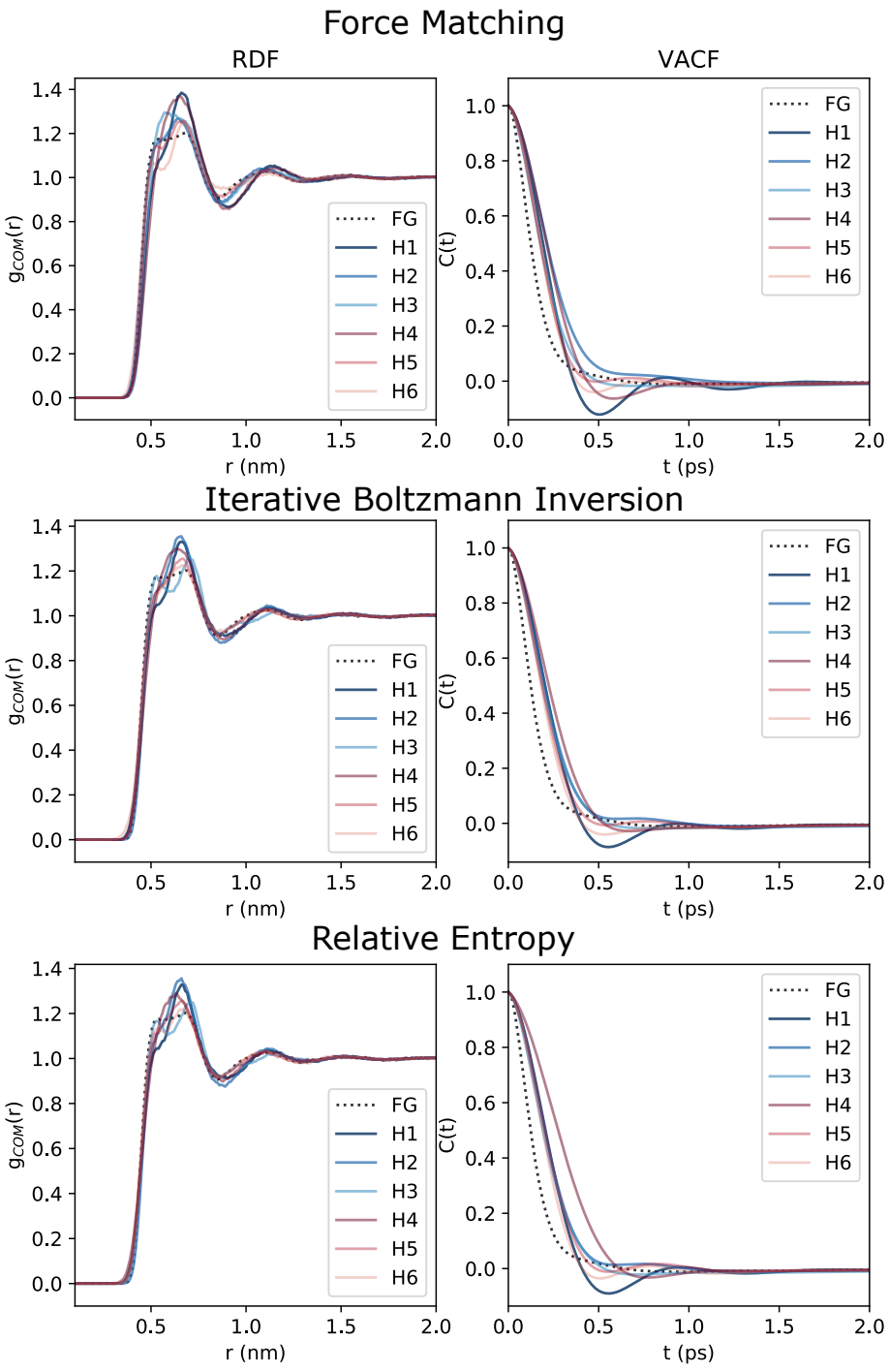

Fig. S6: Comparison of COM-RDF and VACF plots for the 6 hexane mappings for force-matching (FM), iterative Boltzmann inversion (IBI) and relative entropy (RE) along with the reference FG plots. The symmetric and the asymmetric mappings are indicated by different shades of blue and red respectively.

References

[1] L. Martínez, R. Andrade, E. G. Birgin and J. M. Martínez, *J. Comput. Chem.*, 2009, **30**, 2157–2164.