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

TWO-LEVEL STOCHASTIC SEARCH OF LOW-ENERGY CONFORMERS FOR MOLECULAR SPECTROSCOPY: IMPLEMENTATION AND VALIDATION OF MM AND QM MODELS.

Electronic Supplementary Information

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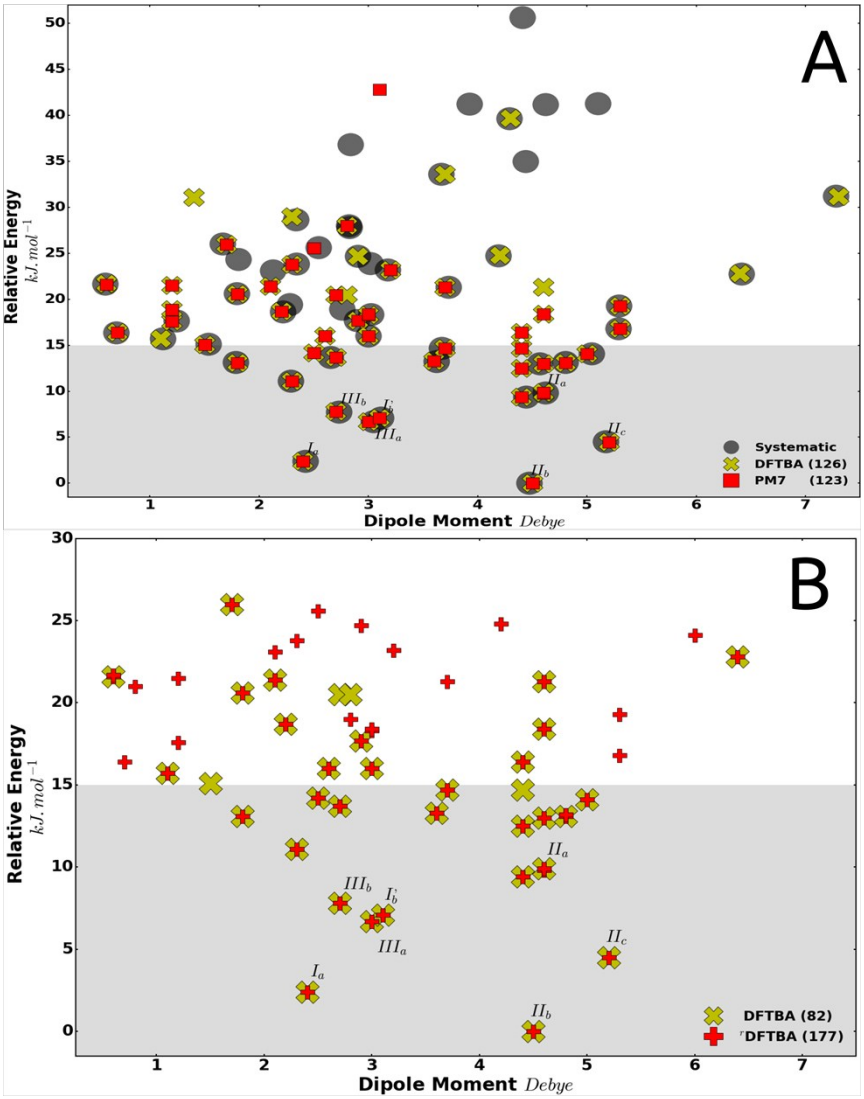

Figure S1. (A) Comparison of L-Thr conformers identified by the cheap schemes and previous systematic approach[2]. Shaded portion highlight the low-lying structures within 15 kJ.mol^{-1}. The values in parenthesis indicate the total number of DFT optimizations. **(B)** L-Thr low-lying structures located with DFTBA model through standard and restarts samplings utilizing the worst conformer. Shading highlights low-lying states

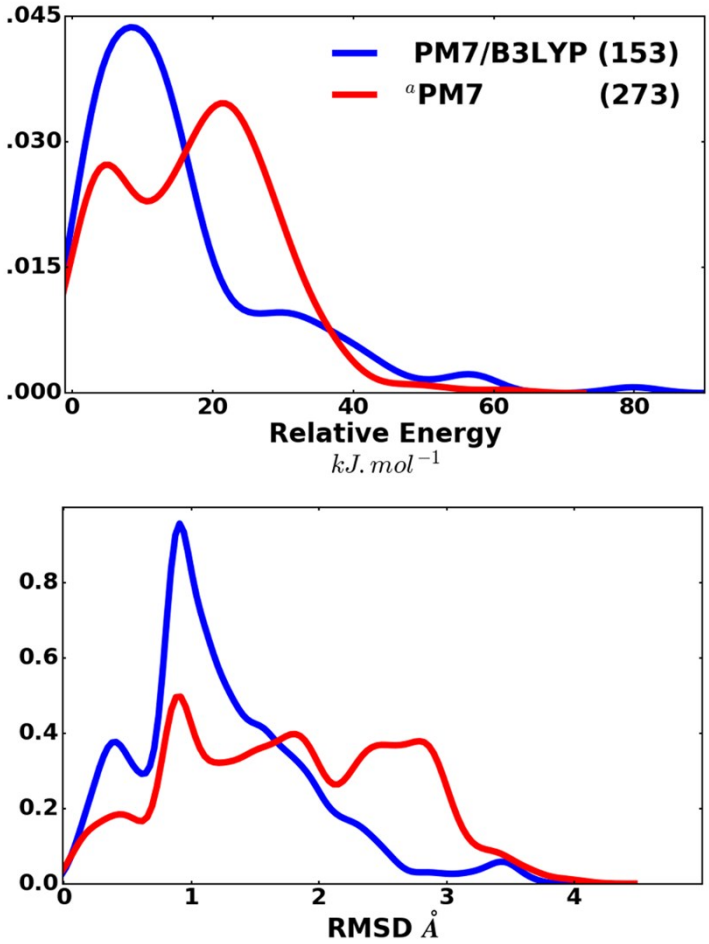

Figure S2. Ferrocene derivative conformer search. Distribution of relative energies and heavy atom RMSD of accepted structures. [a]Sampling without single point estimations. Values in parenthesis indicate population size of accepted structures.