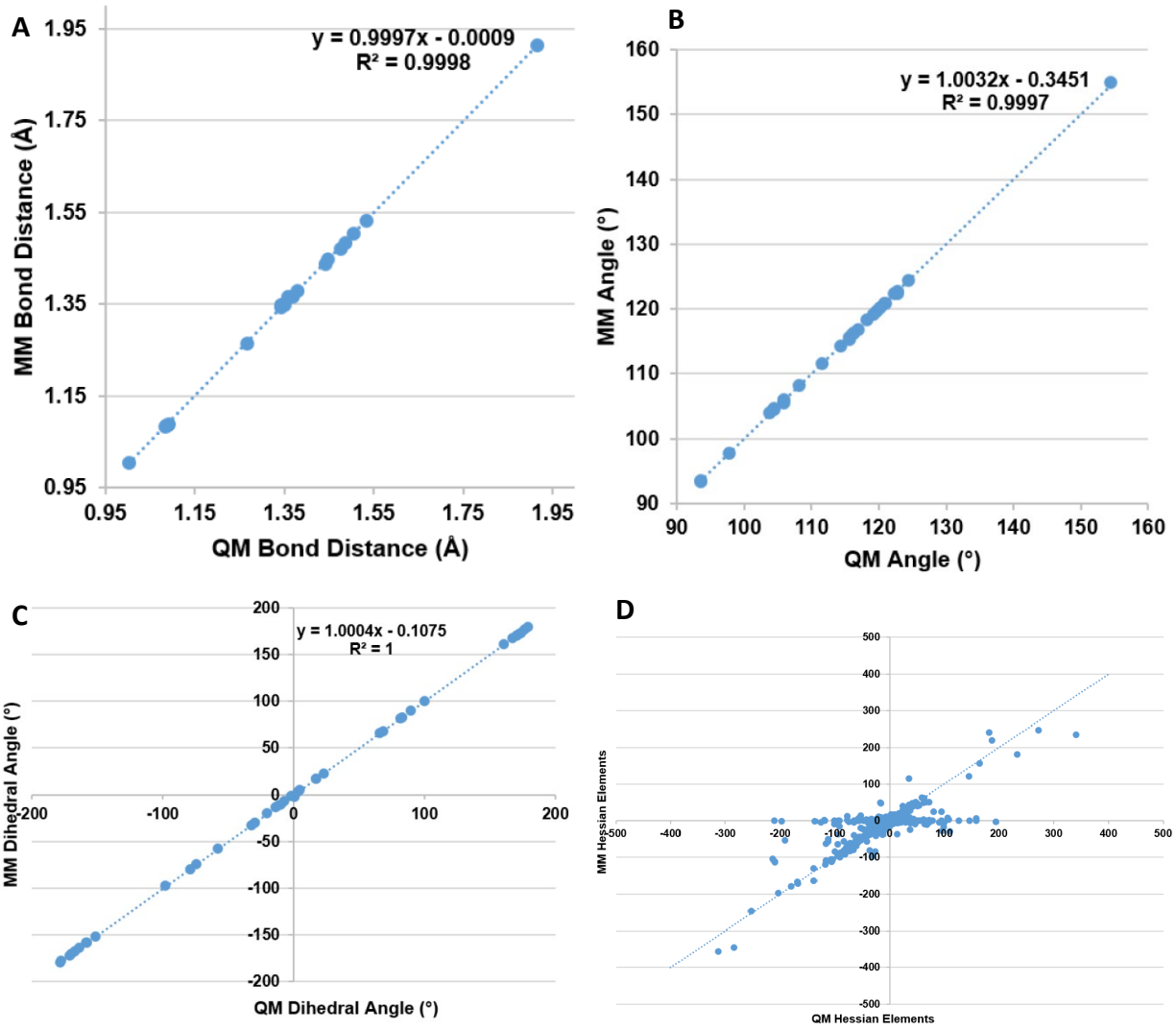
Comparison of bond distances (A), bond angles (B), dihedral angles (C) and Hessian matrix elements (D) from electronic structure calculations and fitted TSFF



Note that there are a significant number of hessian matrix elements that a set to 0 in the optimized TSFF. For details, see [1, 2]

1. Norrby P-O, Liljefors T. Automated molecular mechanics parameterization with simultaneous utilization of experimental and quantum mechanical data. J Comp Chem. 1998;19:1146-66.
2. Limé E, Norrby P-O. Improving the Q2MM method for transition state force field modeling. J Comp Chem. 2015;36:244-50.