

Publications Reported for this Reporting Period

NIH Public Access Compliance	Citation
Complete	Laury ML, Wang Z, Gordon AS, Ponder JW. Absolute binding free energies for the SAMPL6 cucurbit[8]uril host-guest challenge via the AMOEBA polarizable force field. J Comput Aided Mol Des. 2018 Oct;32(10):1087-1095. doi: 10.1007/s10822-018-0147-5. Epub 2018 Oct 15. PubMed PMID: 30324303; PubMed Central PMCID: PMC6240481.