COMPUTATIONAL VALIDATION OF THE IMPORTANCE OF STEREOCHEMISTRY IN VIRTUAL SCREENING: STEREOCHEMISTRY REARS ITS UGLY HEAD. Wayne C. Guida, Wesley H. Brooks, Kenyon G. Daniel and Shen-Shu Sung, Departments of Chemistry and Oncologic Sciences, University of South Florida, 4202 E. Fowler Ave, CHE 205,Tampa, Florida 33620; High Throughput Screening & Chemistry Core and Drug Discovery Department, H. Lee Moffitt Cancer Center & Research Institute, Tampa, Florida 33612.

Consideration of stereochemistry early in the identification of lead compounds can improve the efficiency and efficacy of the drug discovery process. Proper enumeration of the relevant stereoisomers in general, and enantiomeric pairs in particular, of chiral compounds contained within 3D databases, is crucial if one is to use virtual screening as an effective drug discovery tool. The impact of the neglect of enantiomeric pairs on the virtual screening of compounds against MDM2, which is the product of a proto-oncogene, will be described.