$[#6X3H1:1] \sim [#6X3:2] (\sim [#6X3H1]) - [#6X3:3] (\sim [#6X3H1]) \sim [#6X3H1:4]$ mol WBOs 155419 molecules 10<sup>5</sup>  $10^{4}$ log(# of molecules) 10<sup>3</sup> 10<sup>2</sup>  $10^{1}$ 10<sup>0</sup> 0.98 1.08 1.00 1.02 1.04 1.06 AM1-WIBERG-ELF10 with Openeye