$[#6X3H1:1] \sim [#6X3:2] (\sim [#6X3H1]) - [#6X3:3] (\sim [#6X3H1]) \sim [#6X3H1:4]$ mol protomer WBOs 155419 molecules 10⁵ 163865 conformers 10⁴ log(# of molecules) 10³ 10² 10^{1} 10⁰ 1.1 1.0 1.2 1.3 1.4 1.5

AM1-WIBERG-ELF10 with Openeye