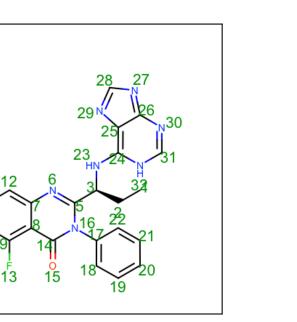
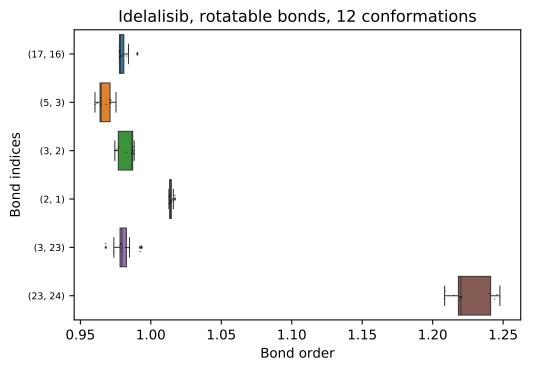


Standard Deviation





## Idelalisib, ring bonds, 12 conformations (20, 19)(20, 21)(21, 22)(22, 17)(17, 18)(18, 19)1 (16, 5)(16, 14)(14, 8)(8, 9)**Bond indices** (8, 7)(7, 12)(12, 11)(11, 10)(10, 9)(7, 6)(6, 5)(24, 32)H (24, 25)(25, 26)(25, 29)(29, 28)(28, 27)(27, 26)(26, 30)(30, 31)

(31, 32)1.8 1.0 1.2 1.3 1.4 1.5 1.6 1.7 Bond order