





Dasatinib, ring bonds, 163 conformations (29, 30)(29, 28)(28, 27)(27, 26)(26, 31) -(31, 30)(2, 3)(2, 1)(1, 5)**Bond indices** (5, 4)(4, 3)(7, 12)(7, 8) -(8, 9)(9, 10) -(10, 11)(11, 12)(14, 15) -(14, 19)(19, 18) -(18, 17) -(17, 16) -(16, 15)1.2 1.5 1.7 1.0 1.1 1.4 1.6

Bond order