





Erlotinib, ring bonds, 42 conformations (26, 27) (26, 25)(25, 24)(24, 23)(23, 22)(22, 27)**Bond indices** (20, 19)(20, 8)(8, 9) ----(8, 7) -(7, 6) -(6, 11)(11, 10)(10, 9)(9, 17)(17, 18)H (18, 19)

1.4 Bond order 1.5

1.6

1.2

1.3