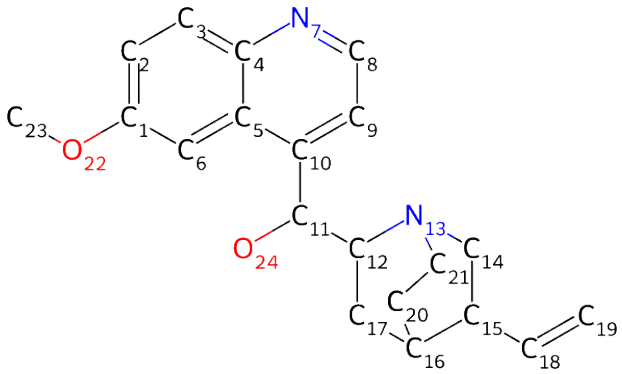
C-oxidation BDE Energy Report for: 245_quinidine-out

This report covers the results for bond dissociation enthalpies (BDE) and solvent accessible surface area (SASA) calculations performed for 245_quinidine-out. Oxidation propensity is established using C-H BDE. The lower the C-H BDE values the higher the propensity for C-oxidation. Details for the density functional theory (DFT) calculations and overall workflow are explained at the end of this document.

BDE and SASA

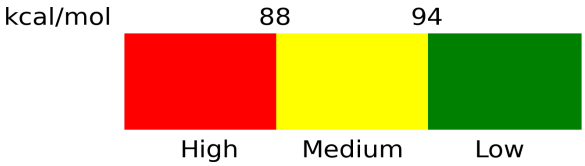


Atom	BDE (kcal/mol)	Propensity	SASA (Å²)
C2	114.14	Low	13.36
C3	114.31	Low	15.67
C6	110.24	Low	4.60
C8	106.1	Low	19.23
C9	112.53	Low	6.97
C11	84.79	High	0.00
C12	93.4	Moderate	0.00
C14	95.77	Low	0.79
C15	79.44	High	0.00
C16	100.2	Low	0.00
C17	96.9	Low	0.35
C18	106.55	Low	4.28
C19	111.15	Low	24.12
C20	97.4	Low	2.04
C21	97.33	Low	2.65
C23	97.37	Low	9.27

Missing Sites:

None

Risk Scale:



Calculation Details

Conformational search calculations were performed only for the base ground state molecule. The lowest energy conformer was selected to generate radicals and run optimization DFT calculations. DFT calculations were performed using Gaussian with B3LYP level of theory and 6-31G(d,p) basis set. The BDE protocol was adapted from: *Lienard, P., Gavartin, J., Boccardi, G., & Meunier, M. (2015). Predicting drug substances autoxidation. Pharmaceutical research, 32, 300-310.*