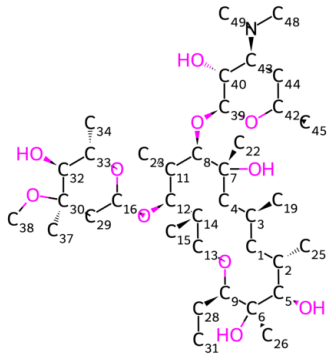
C-oxidation BDE Energy Report for: 130_erythromycin-out

This report covers the results for BDE calculations performed for: 130_erythromycin-out. Oxidation propensity is established using C-H Bond Dissociation Enthalpies (BDE). The lower the C-H BDE values the higher the propensity for C-oxidation. Details for the DFT calculations and overall workflow are explained at the end of this document

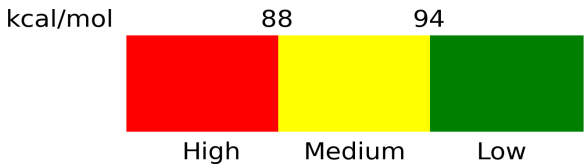
Bond Dissociation Energies (kcal/mol)



Atom	BDE (kcal/mol)	Propensity
C1	94.79	Low
C2	93.6	Moderate
C3	87.6	High
C4	93.23	Moderate
C5	90.89	Moderate
C8	88.23	Moderate
C9	95.45	Low
C11	89.46	Moderate
C12	93.88	Moderate
C13	91.39	Moderate
C14	92.67	Moderate
C15	101.32	Low
C16	89.38	Moderate
C19	98.2	Low
C22	99.74	Low
C23	101.21	Low

C25	98.24	Low
C26	100.66	Low
C28	96.8	Low
C29	99.91	Low
C31	100.4	Low
C32	89.96	Moderate
C33	87.46	High
C34	99.2	Low
C37	99.7	Low
C38	96.42	Low
C39	93.42	Moderate
C40	91.66	Moderate
C42	92.93	Moderate
C43	92.07	Moderate
C44	99.57	Low
C45	102.88	Low
C48	92.8	Moderate
C49	92.81	Moderate

Risk Scale:



Calculation details and output files

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.*