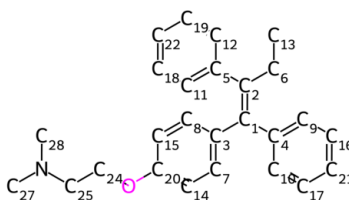


C-oxidation BDE Energy Report for: 280_tamoxifen-out

This report covers the results for BDE calculations performed for: 280_tamoxifen-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

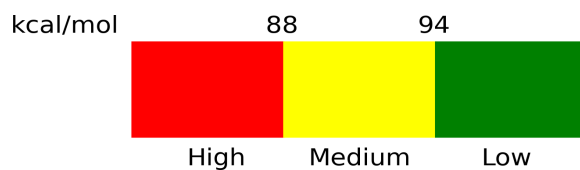
Bond Dissociation Energies (kcal/mol)



Atom	BDE (kcal/mol)	Propensity
C6	78.31	High
C7	110.62	Low
C8	111.97	Low
C9	112.36	Low
C10	111.13	Low
C11	111.83	Low
C12	110.96	Low
C13	101.19	Low
C14	111.6	Low
C15	113.93	Low
C16	111.92	Low
C17	111.92	Low
C18	111.9	Low
C19	111.84	Low
C21	112.43	Low
C22	112.44	Low

C24	93.65	Moderate
C25	89.46	Moderate
C27	93.2	Moderate
C28	92.42	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.*