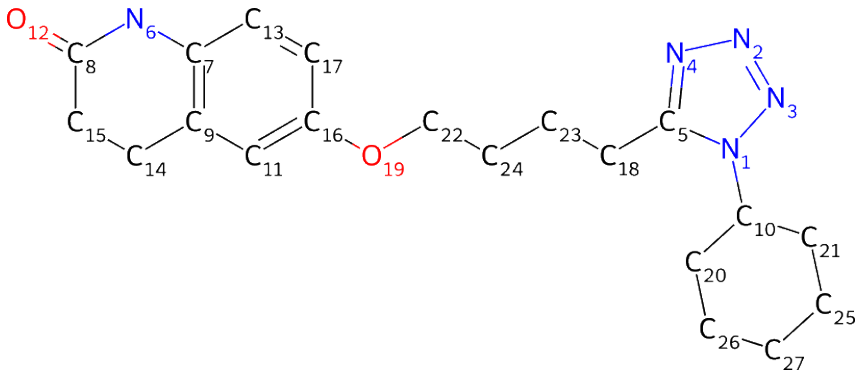
C-oxidation BDE Energy Report for: structure_083-out

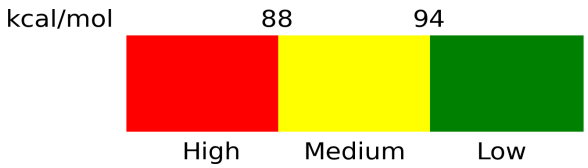
This report covers the results for BDE calculations performed for: structure_083-out. Oxidation propensity is established using C-H Bond Dissociation Enthalpies (BDE). The lower the C-H BDE values the higher the propensity for C-oxidation. Details for the DFT calculations and overall workflow are explained at the end of this document

Bond Dissociation Energies (kcal/mol)



Atom	BDE (kcal/mol)	BDE Risk
C10	93.86	Moderate
C11	113.85	Low
C13	112.99	Low
C14	84.0	High
C15	91.58	Moderate
C17	112.37	Low
C18	87.78	High
C20	98.99	Low
C21	99.05	Low
C22	93.2	Moderate
C23	97.87	Low
C24	98.73	Low
C25	97.96	Low
C26	97.61	Low
C27	98.32	Low

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.*