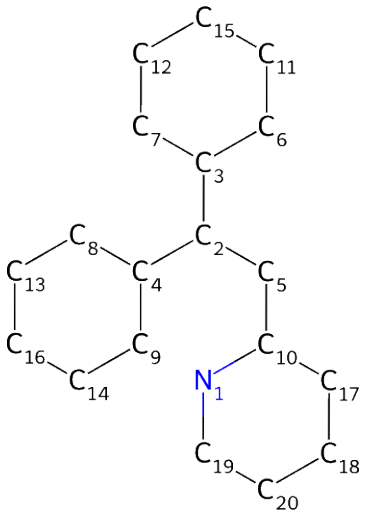
C-oxidation BDE Energy Report for: structure_444-out

This report covers the results for BDE calculations performed for: structure_444-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

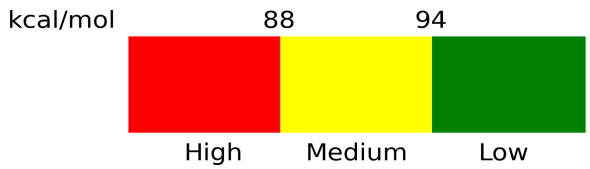
Bond Dissociation Energies (kcal/mol)



Atom	BDE (kcal/mol)	BDE Risk
C2	88.71	Moderate
C3	92.04	Moderate
C4	91.39	Moderate
C5	96.87	Low
C6	97.62	Low
C7	96.38	Low
C8	97.13	Low
C9	97.02	Low
C10	87.43	High
C11	97.66	Low
C12	98.01	Low
C13	97.77	Low
C14	98.09	Low
C15	97.98	Low

C16	97.95	Low
C17	99.44	Low
C18	97.91	Low
C19	90.7	Moderate
C20	99.38	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.*