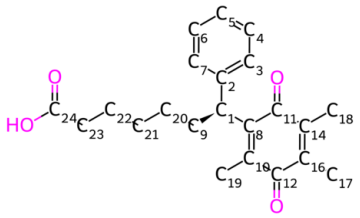
C-oxidation BDE Energy Report for: 271_seratrodast-out

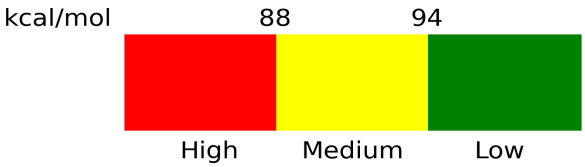
This report covers the results for BDE calculations performed for: 271_seratrodast-out. Oxidation propensity is established using C-H Bond Dissociation Enthalpies (BDE). The lower the C-H BDE values the higher the propensity for C-oxidation. Details for the DFT calculations and overall workflow are explained at the end of this document

Bond Dissociation Energies (kcal/mol)



Atom	BDE (kcal/mol)	Propensity
C3	111.13	Low
C4	112.0	Low
C6	111.87	Low
C7	111.42	Low
C9	97.78	Low
C17	83.08	High
C18	82.64	High
C20	95.57	Low
C21	96.47	Low
C22	98.66	Low
C23	91.63	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.*