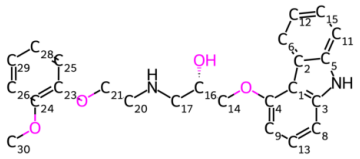
C-oxidation BDE Energy Report for: carvedilol

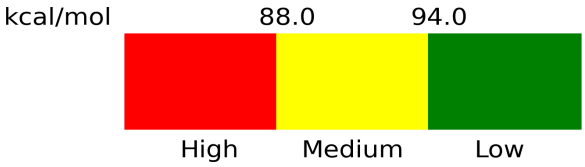
This report covers the results for BDE calculations performed for: carvedilol. Oxudation propensity is established using C-H Bond Dissociation Enthalpies (BDE). The lower the C-H BDE values the higher the propensity for C-oxidation. Details for the DFT calculations and overall workflow are explained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

Bond Dissociation Energies (kcal/mol)



Atom	BDE (kcal/mol)	Propensity
C6	113.0	Low
C8	114.37	Low
C9	112.36	Low
C11	113.19	Low
C12	112.75	Low
C13	112.13	Low
C14	95.37	Low
C15	112.39	Low
C16	88.98	Moderate
C17	92.9	Moderate
C20	97.15	Low
C21	95.12	Low
C25	112.79	Low
C26	111.61	Low
C28	113.0	Low
C29	112.42	Low
C30	97.71	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.*

Output files: /home/wanjiach/carvedilol