# C-oxidation BDE Energy Report for: 073_buprenorphine-out

This report covers the results for BDE calculations performed for: 073_buprenorphine-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
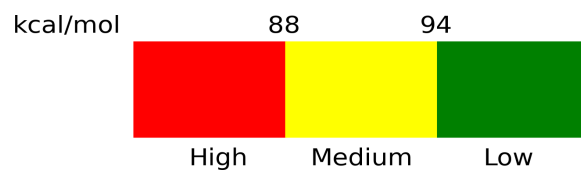
Bond Dissociation Energies (kcal/mol)
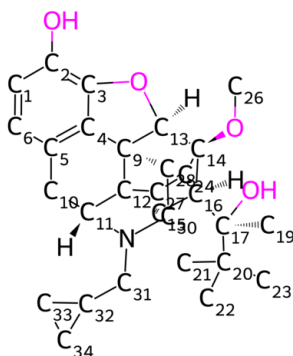
Atom	BDE (kcal/mol)	Propensity
C1	113.99	Low
C6	112.43	Low
C10	83.54	High
C11	97.18	Low
C13	97.72	Low
C15	94.65	Low
C16	83.74	High
C19	100.64	Low
C21	100.95	Low
C22	98.59	Low
C23	98.92	Low
C24	94.02	Low
C26	96.54	Low
C27	94.88	Low
C28	97.46	Low
C30	89.03	Moderate

C31	86.74	High
C32	104.8	Low
C33	106.51	Low
C34	107.83	Low

Risk Scale:

kcal/mol   88   94

High   Medium   Low

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.*