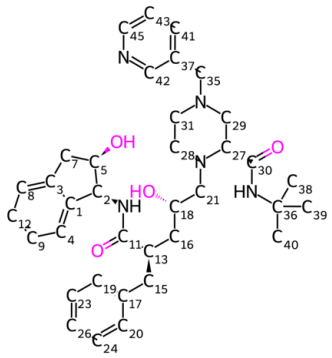
C-oxidation BDE Energy Report for: 167_indinavir-out

This report covers the results for BDE calculations performed for: 167_indinavir-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

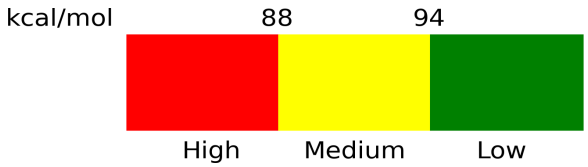
Bond Dissociation Energies (kcal/mol)



Atom	BDE (kcal/mol)	Propensity
C2	78.25	High
C4	113.23	Low
C5	90.92	Moderate
C7	85.0	High
C8	112.29	Low
C9	112.21	Low
C12	112.19	Low
C13	89.57	Moderate
C15	86.61	High
C16	98.43	Low
C18	88.62	Moderate
C19	111.67	Low
C20	112.82	Low
C21	90.12	Moderate
C23	111.87	Low
C24	111.86	Low

C26	112.27	Low
C27	87.38	High
C28	89.62	Moderate
C29	91.76	Moderate
C31	90.97	Moderate
C35	80.75	High
C38	102.9	Low
C39	102.95	Low
C40	102.79	Low
C41	112.5	Low
C42	106.04	Low
C43	112.43	Low
C45	107.06	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.*