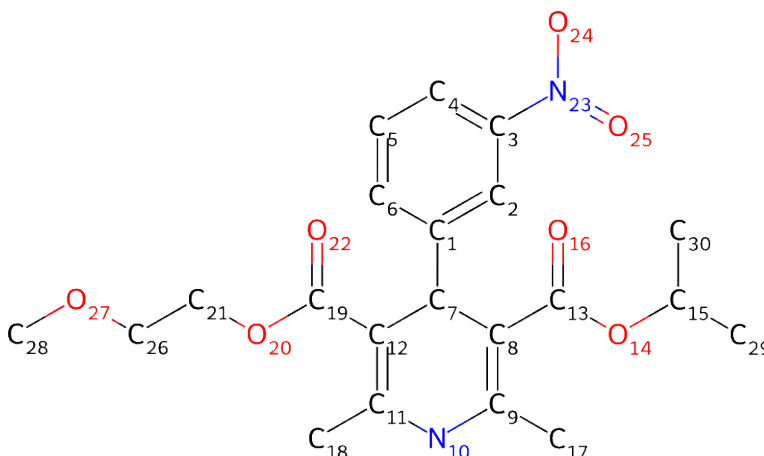


C-oxidation BDE Energy Report for: nimodipine

This report covers the results for bond dissociation enthalpies (BDE) and solvent accessible surface area (SASA) calculations performed for nimodipine. Oxidation propensity is established using C-H BDE. The lower the C-H BDE values the higher the propensity for C-oxidation. Details for the density functional theory (DFT) calculations and overall workflow are explained at the end of this document.

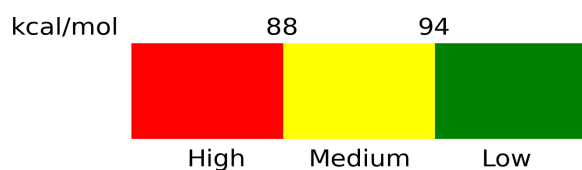
BDE and SASA



Atom	BDE (kcal/mol)	Propensity	SASA (Å ²)
C2	114.47	Low	0.18
C4	114.9	Low	8.87
C5	112.47	Low	7.83
C6	112.22	Low	1.35
C7	81.22	High	0.00
C15	96.19	Low	0.00
C17	87.98	High	7.80
C18	88.14	Moderate	7.78
C21	95.67	Low	0.83
C26	92.38	Moderate	1.14
C28	96.42	Low	8.52
C29	102.68	Low	4.59
C30	102.93	Low	5.78

Missing Sites:

None

Risk Scale:**Calculation Details**

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.*