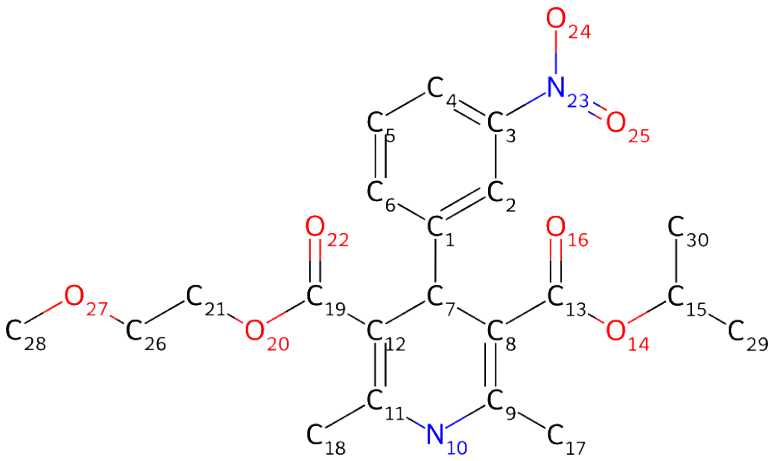
C-oxidation BDE Energy Report for: nimodipine

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

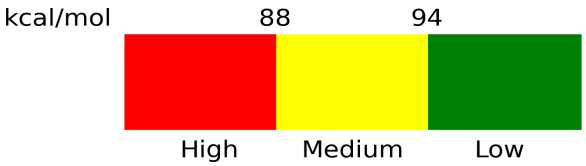


Atom	BDE (kcal/mol)	Propensity	SASA (Å²)
C2	114.47	Low	0.64
C4	114.9	Low	22.84
C5	112.47	Low	30.03
C6	112.22	Low	8.11
C7	81.22	High	5.90
C15	96.19	Low	17.27
C17	87.98	High	26.45
C18	88.14	Moderate	26.65
C21	95.67	Low	20.48
C26	92.38	Moderate	16.09
C28	96.42	Low	26.16
C29	102.68	Low	19.81
C30	102.93	Low	24.12

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.*