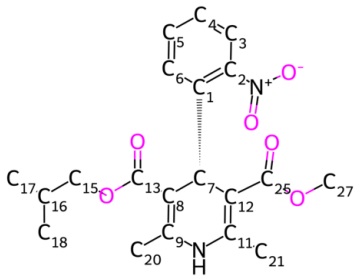
C-oxidation BDE Energy Report for: nisoldipine

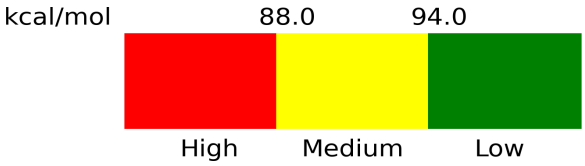
This report covers the results for BDE calculations performed for: nisoldipine. Oxudation propensity is established using C-H Bond Dissociation Enthalpies (BDE). The lower the C-H BDE values the higher the propensity for C-oxidation. Details for the DFT calculations and overall workflow are explained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

Bond Dissociation Energies (kcal/mol)



Atom	BDE (kcal/mol)	Propensity
C3	113.77	Low
C4	112.98	Low
C5	112.45	Low
C6	112.73	Low
C7	72.77	High
C15	96.49	Low
C16	93.6	Moderate
C17	102.55	Low
C18	102.24	Low
C20	88.91	Moderate
C21	88.43	Moderate
C27	98.04	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/nisoldipine