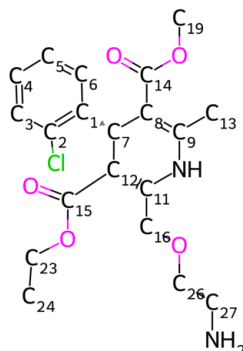


# C-oxidation BDE Energy Report for: amlodipine

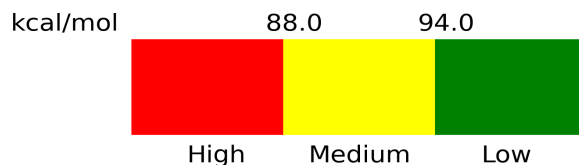
This report covers the results for BDE calculations performed for: amlodipine. Oxidation propensity is established using C-H Bond Dissociation Enthalpies (BDE). The lower the C-H BDE values the higher the propensity for C-oxidation. Details for the DFT calculations and overall workflow are explained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

## Bond Dissociation Energies (kcal/mol)



Atom	BDE (kcal/mol)	Propensity
C3	112.82	Low
C4	112.43	Low
C5	112.42	Low
C6	110.91	Low
C7	77.58	High
C13	88.06	Moderate
C16	84.52	High
C19	97.88	Low
C23	94.92	Low
C24	102.63	Low
C26	94.81	Low
C27	92.63	Moderate

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/amlodipine