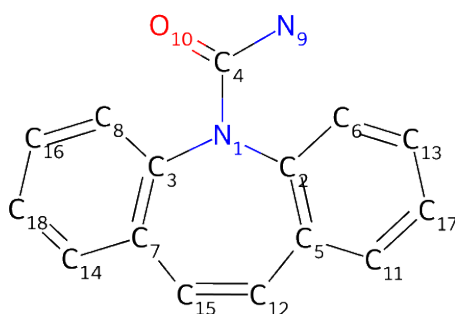


C-oxidation BDE Energy Report for: 015_CARBAMAZEPINE-out

This report covers the results for bond dissociation enthalpies (BDE) and solvent accessible surface area (SASA) calculations performed for 015_CARBAMAZEPINE-out. 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
C6	113.23	Low
C8	113.26	Low
C11	112.24	Low
C12	108.04	Low
C13	112.49	Low
C14	112.23	Low
C15	107.48	Low
C16	112.43	Low
C17	112.65	Low
C18	112.62	Low

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.*