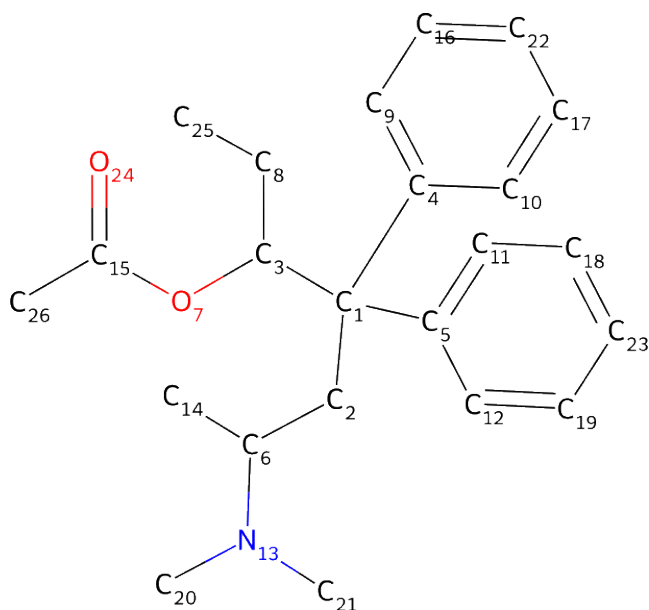


# C-oxidation BDE Energy Report for: 178\_laam-out

This report covers the results for bond dissociation enthalpies (BDE) and solvent accessible surface area (SASA) calculations performed for 178\_laam-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



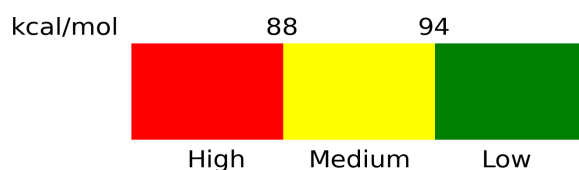
Atom	BDE (kcal/mol)	Propensity	SASA (Å <sup>2</sup> )
C2	94.53	Low	1.92
C3	94.84	Low	0.92
C6	88.11	Moderate	1.45
C8	96.63	Low	10.30
C9	109.08	Low	6.39
C10	110.81	Low	4.75
C11	110.09	Low	5.09
C12	109.64	Low	5.66
C14	99.86	Low	17.91
C16	112.09	Low	34.79
C17	111.98	Low	34.36
C18	111.89	Low	32.66
C19	111.88	Low	34.19

C20	90.29	Moderate	19.68
C21	90.15	Moderate	19.67
C22	112.67	Low	35.99
C23	112.52	Low	35.99
C25	100.89	Low	23.70
C26	97.27	Low	27.89

### 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.*