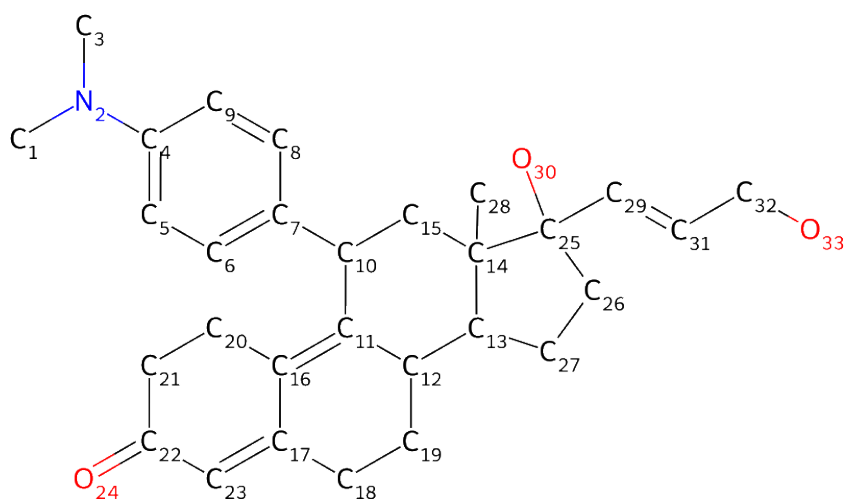


C-oxidation BDE Energy Report for: 182_lilopristone-out

This report covers the results for bond dissociation enthalpies (BDE) and solvent accessible surface area (SASA) calculations performed for 182_lilopristone-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



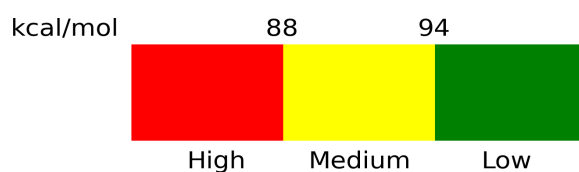
Atom	BDE (kcal/mol)	Propensity	SASA (Å ²)
C1	90.21	Moderate	0.00
C3	90.13	Moderate	0.00
C5	110.33	Low	0.01
C6	110.09	Low	0.00
C8	109.98	Low	0.31
C9	110.2	Low	0.55
C10	71.4	High	0.49
C12	74.51	High	0.16
C13	90.31	Moderate	1.15
C15	95.45	Low	0.22
C18	83.89	High	10.03
C19	98.16	Low	8.99
C20	82.78	High	5.47

C21	88.57	Moderate	5.47
C23	112.26	Low	13.84
C26	95.47	Low	7.51
C27	96.28	Low	1.41
C28	99.66	Low	2.43
C29	105.91	Low	0.92
C31	108.12	Low	11.42
C32	77.55	High	9.17

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.*