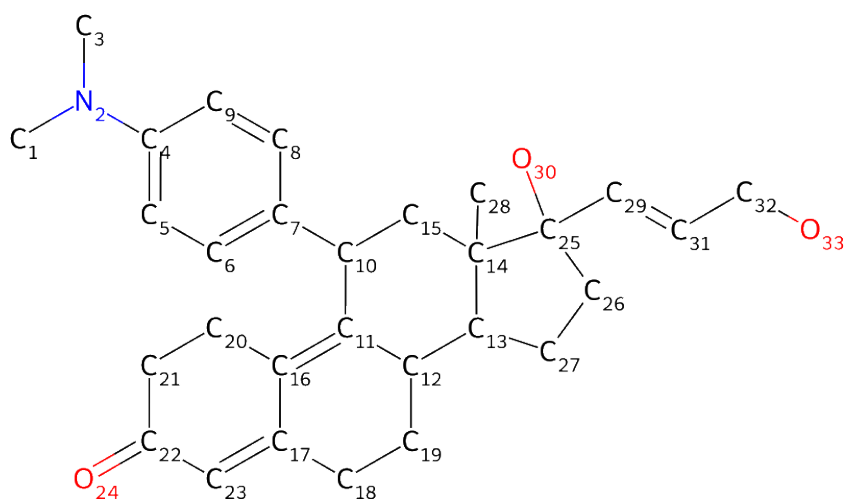


# C-oxidation BDE Energy Report for: 182\_lilopristone-out

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



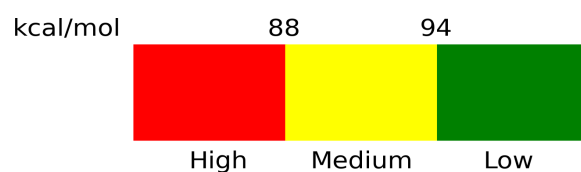
Atom	BDE (kcal/mol)	Propensity
C1	90.21	Moderate
C3	90.13	Moderate
C5	110.33	Low
C6	110.09	Low
C8	109.98	Low
C9	110.2	Low
C10	71.4	High
C12	74.51	High
C13	90.31	Moderate
C15	95.45	Low
C18	83.89	High
C19	98.16	Low
C20	82.78	High

C21	88.57	Moderate
C23	112.26	Low
C26	95.47	Low
C27	96.28	Low
C28	99.66	Low
C29	105.91	Low
C31	108.12	Low
C32	77.55	High

### **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.*