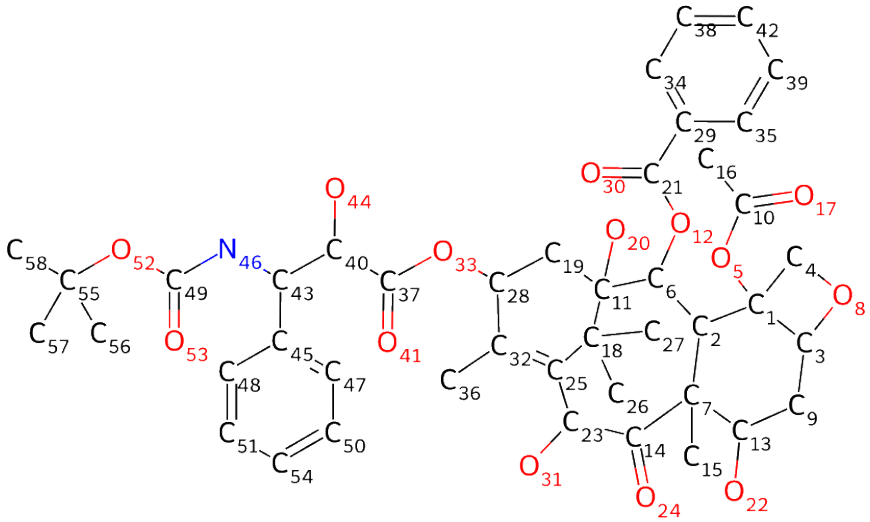
C-oxidation BDE Energy Report for: 118_docetaxel-out

This report covers the results for bond dissociation enthalpies (BDE) and solvent accessible surface area (SASA) calculations performed for 118_docetaxel-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



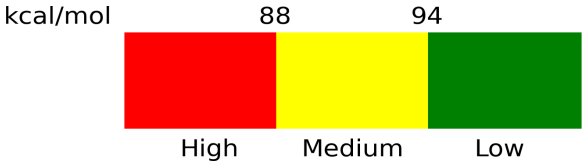
Atom	BDE (kcal/mol)	Propensity	SASA (Å²)
C2	90.15	Moderate	0.00
C3	91.12	Moderate	0.18
C4	94.51	Low	3.18
C6	92.75	Moderate	0.00
C9	96.75	Low	0.67
C13	89.53	Moderate	0.00
C15	101.03	Low	3.85
C16	97.68	Low	2.93
C19	93.81	Moderate	0.00
C23	75.47	High	0.00
C26	99.24	Low	3.90
C27	96.01	Low	3.53

C28	73.66	High	0.00
C34	114.22	Low	3.69
C35	112.92	Low	11.15
C36	84.93	High	3.96
C38	112.56	Low	9.93
C39	112.35	Low	16.26
C40	83.49	High	0.00
C42	112.35	Low	15.78
C43	84.53	High	0.00
C47	112.09	Low	3.54
C50	112.33	Low	13.19
C51	112.15	Low	13.39
C54	112.71	Low	14.75
C56	103.7	Low	4.31
C57	103.7	Low	4.34
C58	103.7	Low	4.40

Missing Sites:

C48.

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.*