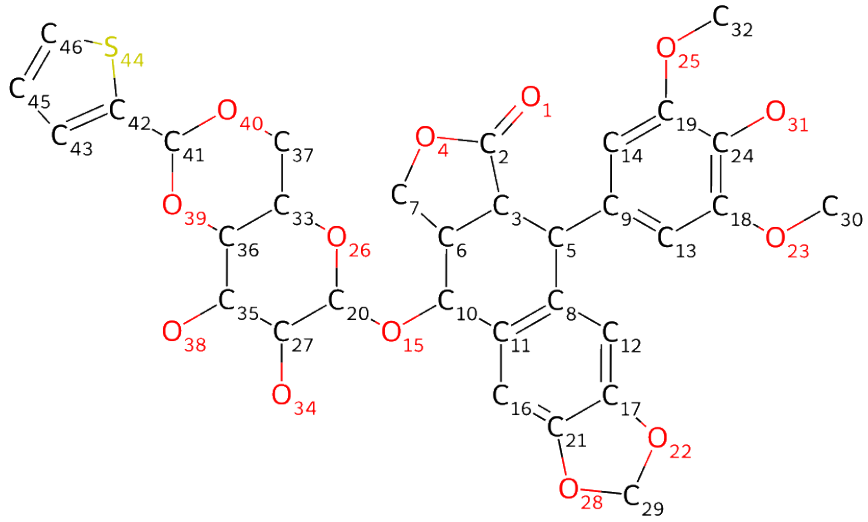
C-oxidation BDE Energy Report for: 285_teniposide-out

This report covers the results for bond dissociation enthalpies (BDE) and solvent accessible surface area (SASA) calculations performed for 285_teniposide-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



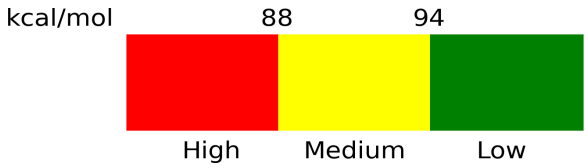
Atom	BDE (kcal/mol)	Propensity	SASA (Å²)
C3	85.55	High	0.00
C5	81.31	High	0.00
C6	96.1	Low	0.00
C7	97.72	Low	2.58
C10	83.16	High	0.00
C12	115.03	Low	7.12
C13	112.27	Low	0.10
C14	111.74	Low	0.10
C16	113.71	Low	3.89
C20	93.62	Moderate	0.06
C27	93.2	Moderate	0.00
C29	91.11	Moderate	5.28

C30	96.56	Low	10.25
C32	96.72	Low	10.25
C33	94.85	Low	0.00
C35	93.57	Moderate	0.00
C36	95.03	Low	0.00
C37	96.69	Low	2.26
C41	81.03	High	0.07
C43	115.34	Low	12.86
C45	115.47	Low	18.12
C46	117.7	Low	18.38

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.*