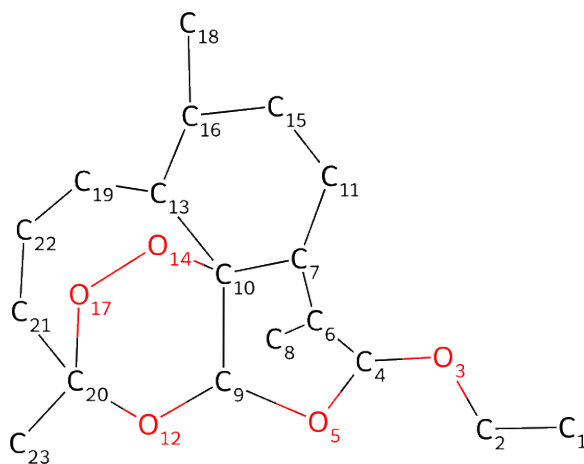


C-oxidation BDE Energy Report for: 063_beta_artheether-out

This report covers the results for bond dissociation enthalpies (BDE) and solvent accessible surface area (SASA) calculations performed for 063_beta_artheether-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	102.64	Low	4.98
C2	95.62	Low	3.56
C4	95.02	Low	14.67
C6	91.43	Moderate	16.83
C7	83.73	High	2.61
C8	99.58	Low	4.23
C9	77.75	High	0.44
C11	98.99	Low	30.80
C13	95.21	Low	2.05
C15	96.76	Low	7.42
C16	93.49	Moderate	12.19
C18	100.61	Low	12.43
C19	93.58	Moderate	87.57
C21	97.05	Low	0.39

C22	94.76	Low	0.38
C23	102.99	Low	3.21

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.*