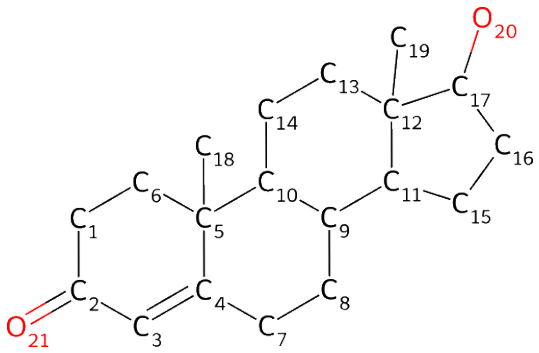
C-oxidation BDE Energy Report for: 292_testosterone-out

This report covers the results for bond dissociation enthalpies (BDE) and solvent accessible surface area (SASA) calculations performed for 292_testosterone-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

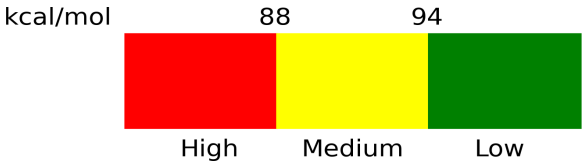


Atom	BDE (kcal/mol)	Propensity	SASA (Å²)
C1	89.85	Moderate	24.27
C3	111.16	Low	23.71
C6	97.41	Low	15.25
C7	80.04	High	20.78
C8	98.29	Low	16.15
C9	95.6	Low	2.32
C10	93.97	Moderate	3.85
C11	90.34	Moderate	7.27
C13	98.48	Low	18.80
C14	95.47	Low	10.34
C15	96.59	Low	18.01
C16	96.51	Low	26.40
C17	91.21	Moderate	17.02
C18	100.2	Low	17.08
C19	100.48	Low	15.70

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.*