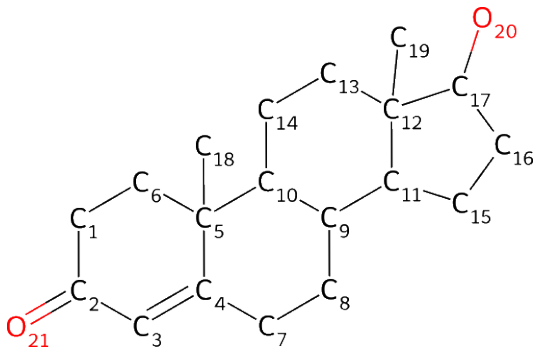
C-oxidation BDE Energy Report for: 292_testosterone-out

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

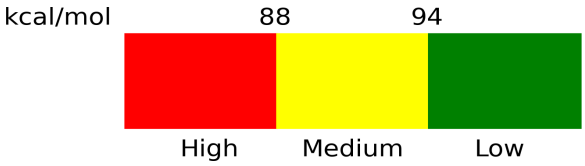


Atom	BDE (kcal/mol)	Propensity
C1	89.85	Moderate
C3	111.16	Low
C6	97.41	Low
C7	80.04	High
C8	98.29	Low
C9	95.6	Low
C10	93.97	Moderate
C11	90.34	Moderate
C13	98.48	Low
C14	95.47	Low
C15	96.59	Low
C16	96.51	Low
C17	91.21	Moderate
C18	100.2	Low
C19	100.48	Low

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.*