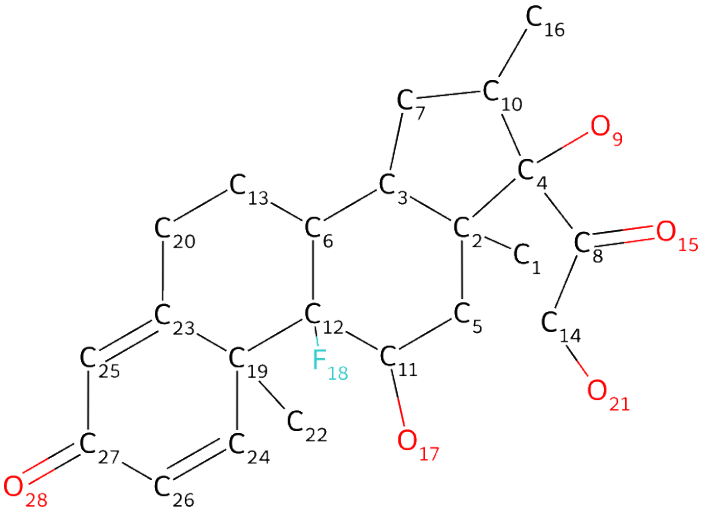
C-oxidation BDE Energy Report for: 107_dexamethasone-out

This report covers the results for bond dissociation enthalpies (BDE) and solvent accessible surface area (SASA) calculations performed for 107_dexamethasone-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



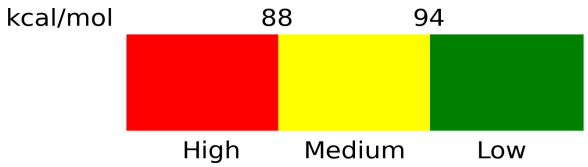
Atom	BDE (kcal/mol)	Propensity
C1	100.05	Low
C3	87.23	High
C5	97.89	Low
C6	96.59	Low
C7	96.69	Low
C10	91.36	Moderate
C11	90.23	Moderate
C13	97.8	Low
C14	75.33	High
C16	99.12	Low
C20	82.62	High
C22	99.77	Low
C24	106.7	Low

C25	112.36	Low
C26	112.38	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.*