# 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
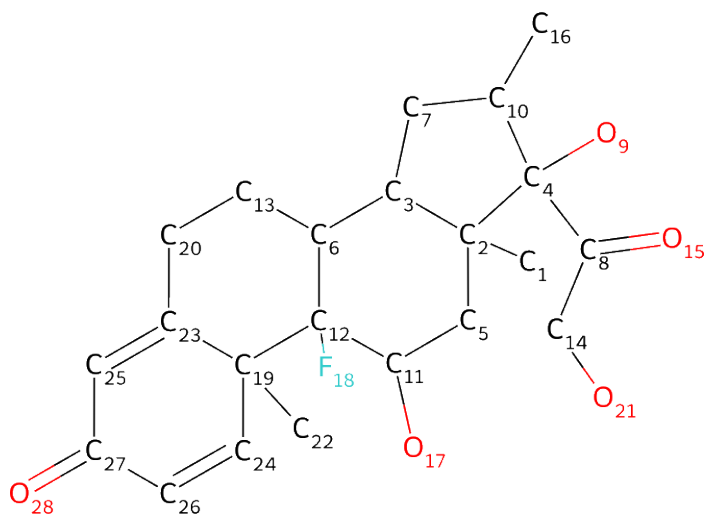
Atom	BDE (kcal/mol)	Propensity	SASA (Å²)
C1	100.05	Low	11.66
C3	87.23	High	2.38
C5	97.89	Low	9.94
C6	96.59	Low	2.26
C7	96.69	Low	13.44
C10	91.36	Moderate	7.58
C11	90.23	Moderate	13.20
C13	97.8	Low	15.29
C14	75.33	High	19.39
C16	99.12	Low	25.06
C20	82.62	High	20.57
C22	99.77	Low	17.80
C24	106.7	Low	14.03

C25	112.36	Low	23.49
C26	112.38	Low	32.89

Missing Sites:

None

Risk Scale:

kcal/mol   88   94

| High | Medium | Low |

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.*