# C-oxidation BDE Energy Report for: 063_beta_arteether-out

This report covers the results for BDE calculations performed for: 063_beta_arteether-out. Oxidation propensity is established using C-H Bond Dissociation Enthalpies (BDE). The lower the C-H BDE values the higher the propensity for C-oxidation. Details for the DFT calculations and overall workflow are explained at the end of this document

## Bond Dissociation Energies (kcal/mol)
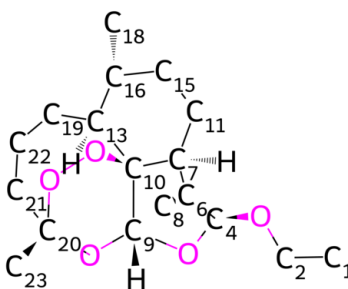


| Atom | BDE (kcal/mol) | Propensity |
|------|----------------|------------|
| C1 | 102.64 | Low |
| C2 | 95.62 | Low |
| C4 | 95.02 | Low |
| C6 | 91.43 | Moderate |
| C7 | 83.73 | High |
| C8 | 99.58 | Low |
| C9 | 77.75 | High |
| C11 | 98.99 | Low |
| C13 | 95.21 | Low |
| C15 | 96.76 | Low |
| C16 | 93.49 | Moderate |
| C18 | 100.61 | Low |
| C19 | 93.58 | Moderate |
| C21 | 97.05 | Low |
| C22 | 94.76 | Low |
| C23 | 102.99 | Low |

Risk Scale:

kcal/mol          88          94



High        Medium        Low
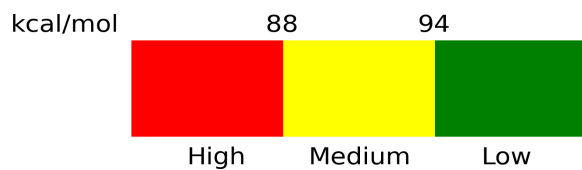
## Calculation details and output files

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.*