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Supplemental Information for:

Computational Investigations of Two Iron and α–ketoglutarate–Dependent Family Enzymes: Structural and Electronic Level Insights

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Methodology for the QM/MM ALKBH2 and ALKBH3 Calculations

QM/MM single point calculations were performed for each critical point structure (reactant, transition state and product) for ALKBH2 and ALKBH3. The ωB97XD functional, and the 6-31G(d,p) basis set were used for the atoms in the QM region. The pseudo-bond approach was used for the bonds that bridge the QM and MM regions.[1] A modified version of the AMBER ff99SB force field including the parameters of the damaged bases was used to model the alkylated double and single stranded substrate and reactive site for ALKBH2 and ALKBH3 MM regions, respectively. The TiP3P force field was used to model the MM water molecules. Gaussian16 and TINKER8 software packages were used with LICHEM 1.1.[2–5]

For the QM single point calculations, the ωB97XD functional, 6-31G(d,p) basis set and the pseudo-bond approach for the cleaved bonds between the QM and the MM regions was used; each QM cluster was embedded in the electrostatic field produced by the MM region (ALKBH2/ALKBH3 + water). Mulliken spin densities for Fe were extracted from the Gaussian16 output file and the electron densities from the formatted check point file employing the Multiwfn 3.8 software package.[6]

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