**Supplementary Information**

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Figure S1: Root mean square fluctuation plots calculate for every subunit from the last 40 ns of the trajectories. The boundaries for domain III and I are indicated by the red line. In Oxy-HCN, domain III and I are largely flexible, where as domain II is stable. This could be because of the presence of oxygen bound in the metal centre in domain II. In Deoxy-HCN, domain II also displays fluctuations (in three subunits) along with domain III and I.