Supplementary material

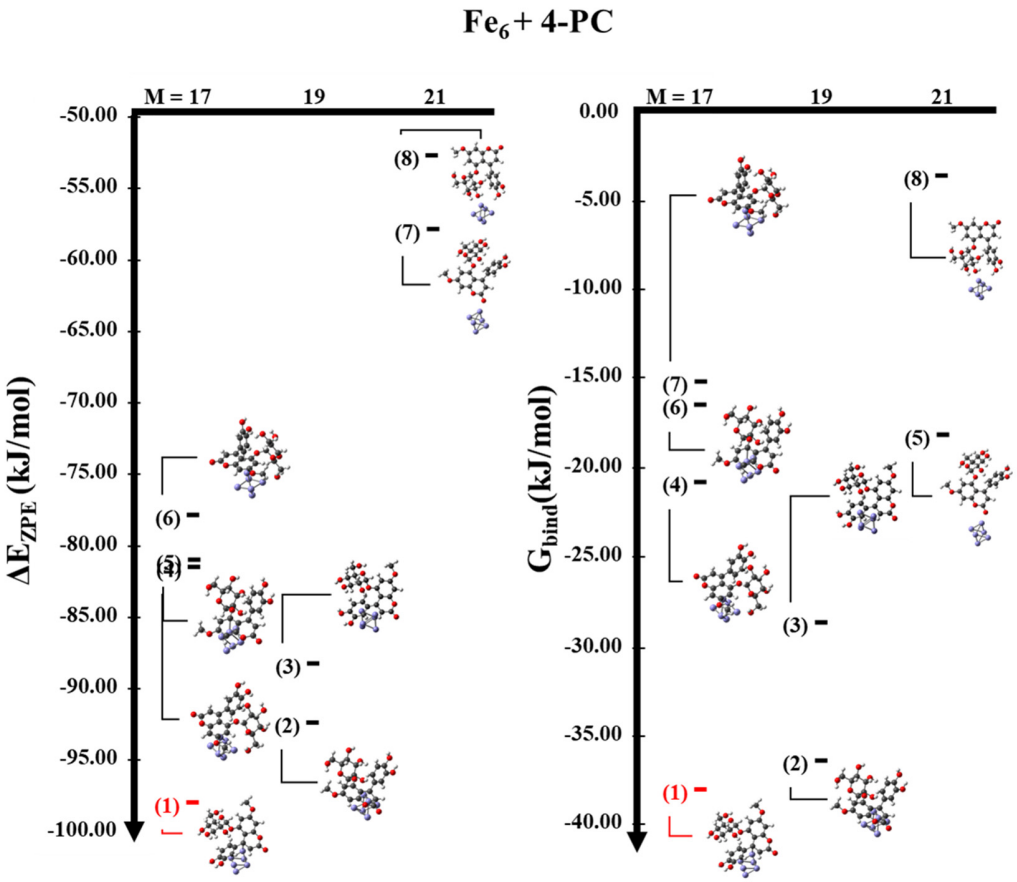

Figure S1. Optimized structures of 4-PC corrosion inhibitor molecule interacting with the Fe_6 cluster at the BPW91-D2/6–311 ++ G (2d,2p) level as function of the ZPE-corrected relative energy ΔE_{ZPE} and G_{bind}.