Novel Mechanism of Heme Degradation to Biliverdin Studied by QM/MM and QM Calculations

Fatemeh Sadat Alavi[a],MahinGheidi[a], Mansour Zahedi[a,*], Nasser Safari[a,*], Ulf Ryde[b]

[a]Department of Chemistry, Faculty of Sciences, ShahidBeheshti University, G.C., Evin, 19839-6313, Tehran, Iran, [b]Department of Theoretical Chemistry, Lund University, Chemical Centre, P.O. Box 124,
SE-221 00 Lund, Sweden

Corresponding Authors

[*]E-mail: m-zahedi@sbu.ac.ir , Phone: +98-21-29902889.

n-safari@sbu.ac.ir, Phone: +98-21-29902886.

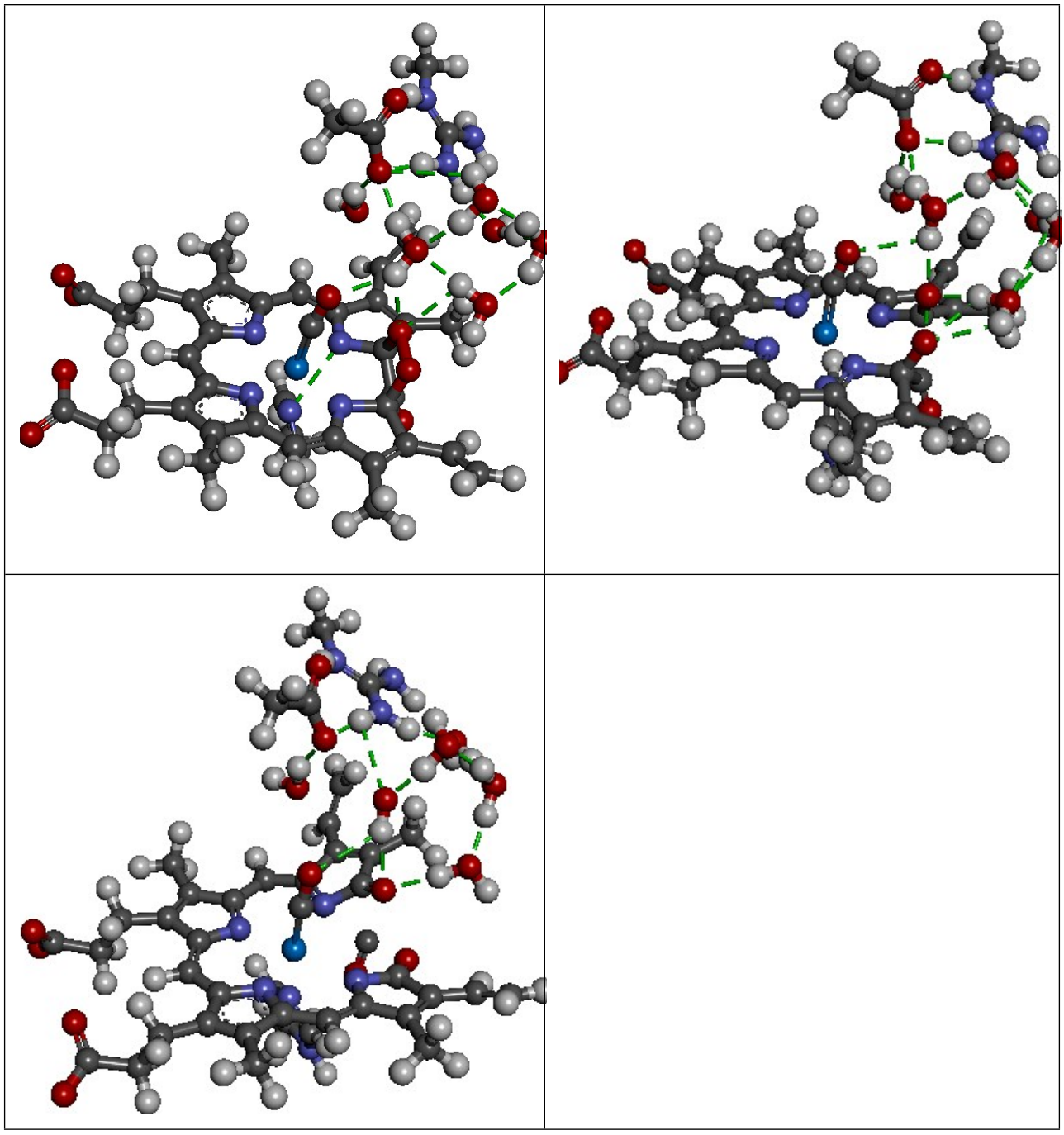

Figure S1: QM/MM optimized structure of the various intermediates For CO ligand

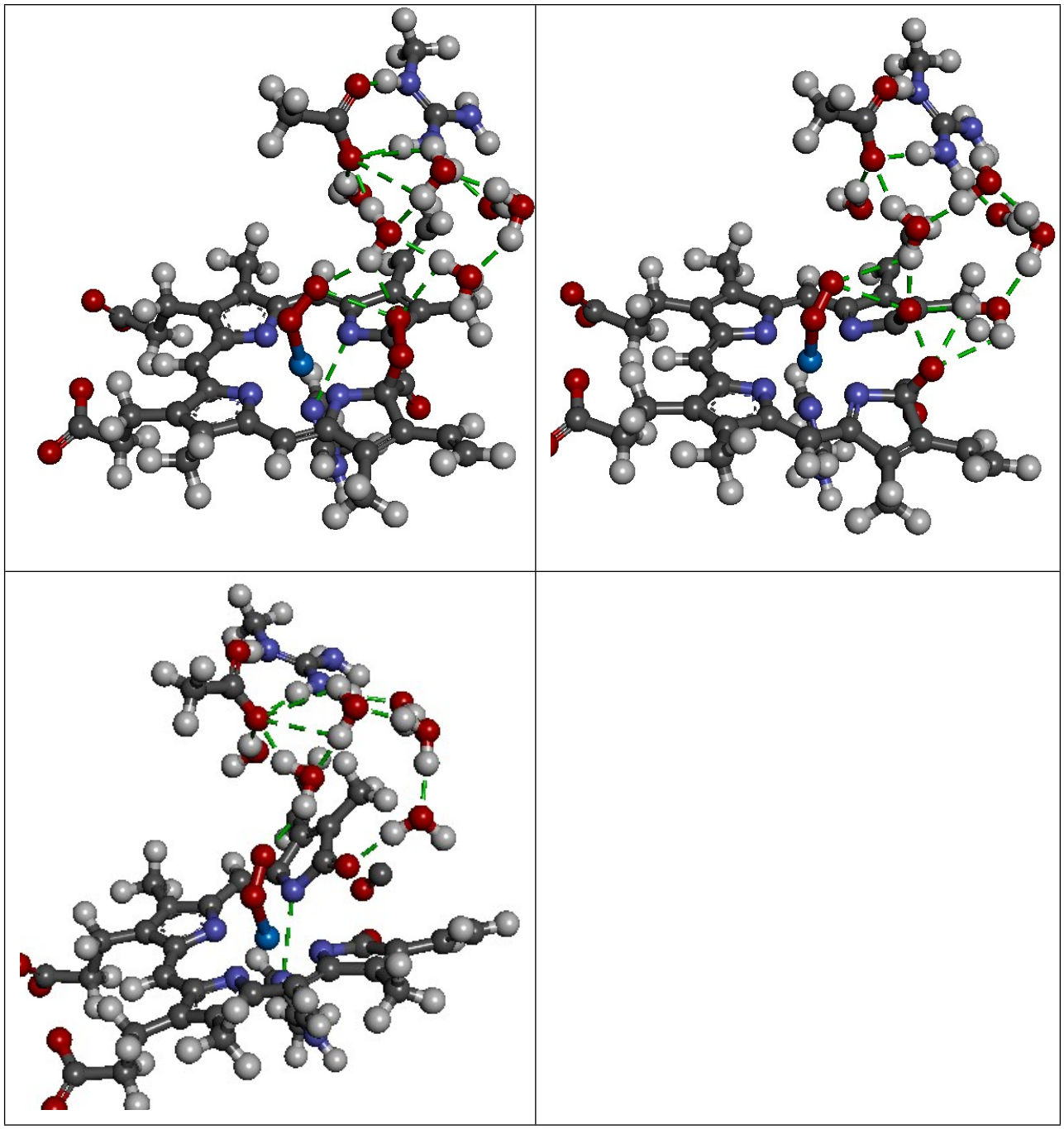

Figure S2: QM/MM optimized structure of the various intermediates For O_2 ligand

Table S1: Relative energies (kcal/mol), obtained with different methods and basis sets for the QM/MM calculations with the H_2O ligand. The various energies are defined in Eqns. 2 and 3, except that $E_{MM} = E_{MM12} - E_{MM1}$.

Method	**QM/MM**	**QM+ptch**			**Big-QM**					E_{tot}
DFT	**TPSS**	**TPSS**	**TPSS**	**TPSS**	**B3LYP**	**TPSS**	E_{disp}	E_{MM}	E_{bq}	
Basis	**SV**	**SV**	**TZ**	**QZ**	**TZ**	**SV**				
1	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**
Ts1	**3.4**	**3.9**	**4.6**	**4.8**	**6.2**	**7.1**	**-0.6**	**-0.1**	**6.4**	**8.9**
2	**-60.0**	**-58.5**	**-62.0**	**-63.2**	**-71.0**	**-61.1**	**1.6**	**-0.5**	**-59.9**	**-73.6**