Supplementary Data

On the photodynamic properties of Al, Ga and In hemin complexes . A quantum chemical investigation.

Maciej Spiegel [a], Nino Russo *[b]

On the photophysical properties of Al, Ga and In hemin complexes. A quantum chemical investigation.

Maciej Spiegel [a], Nino Russo *[b]

[a] M. Spiegel

Department of Organic Chemistry and Pharmaceutical Technology, Wroclaw

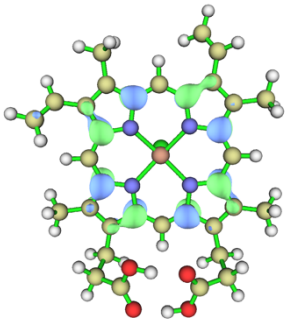
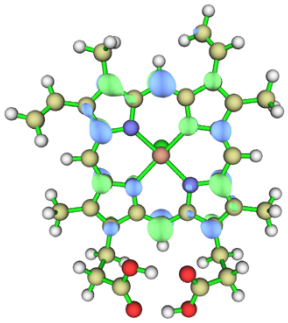
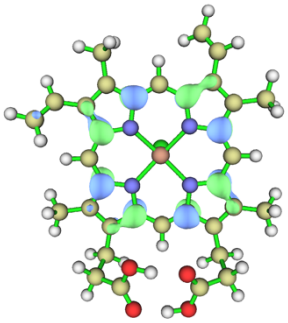
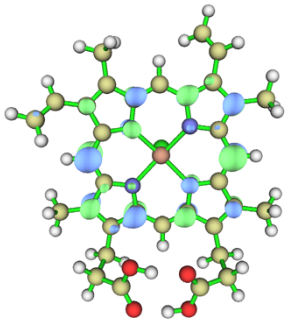
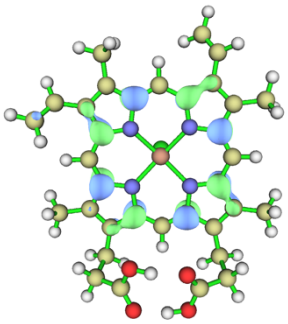
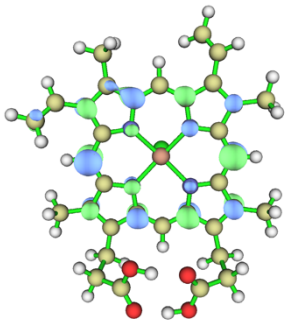
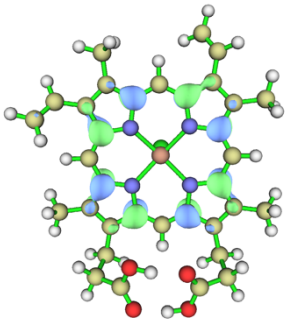
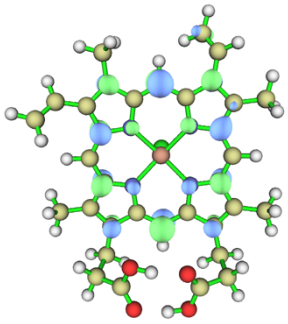
Medical University, Borowska 211 A, 50-556 Wroclaw, Poland

[b] N. Russo

Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, I-

87136 Rende (CS), Italy

Supplementary Data

S_1		81.3% →	
S_2		55.8% →	
T_1		81.3% →	
T_2		79.5% →	
T_3			

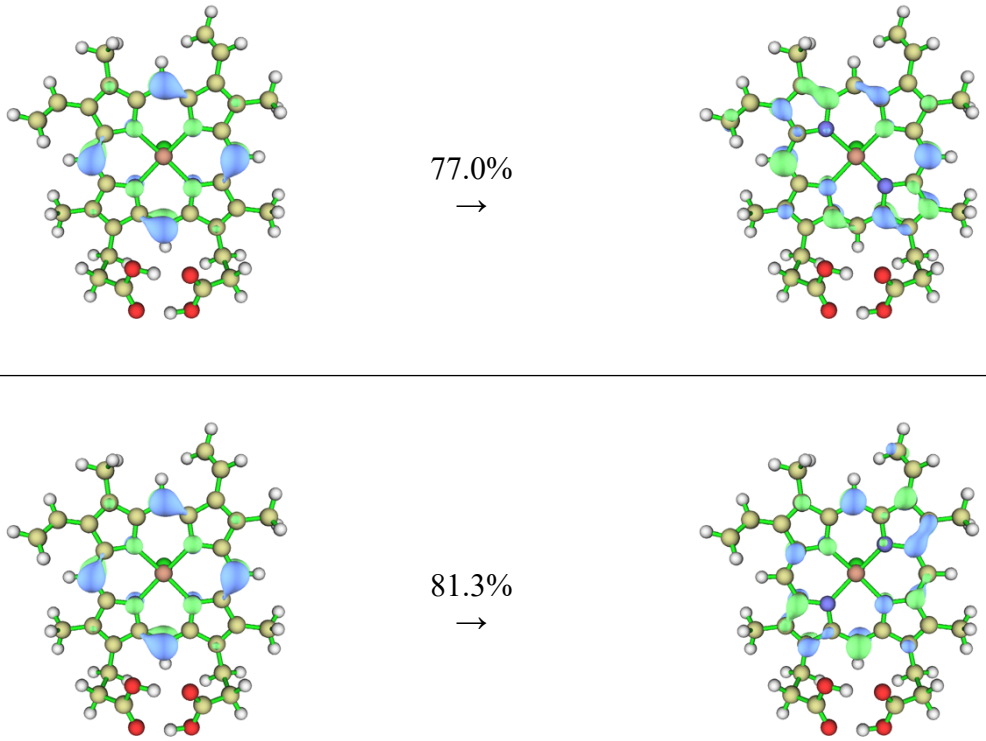
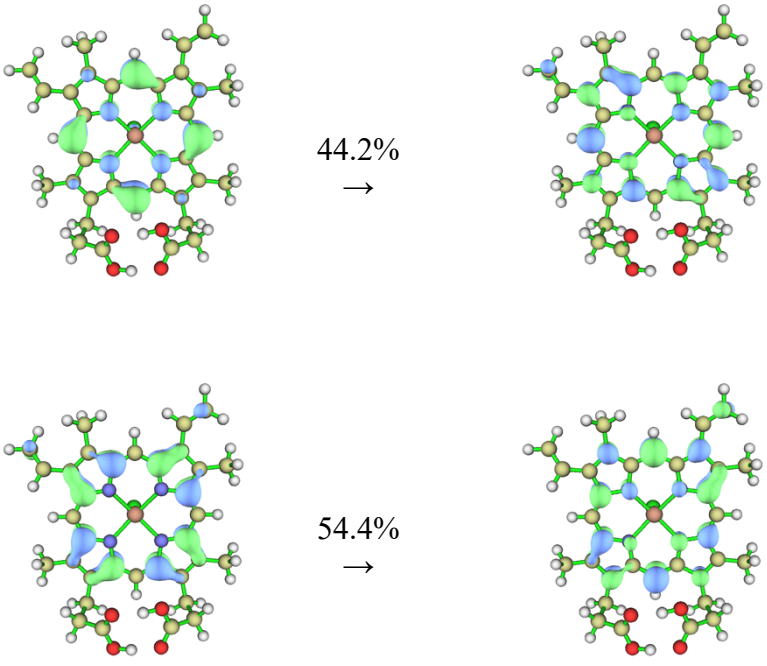
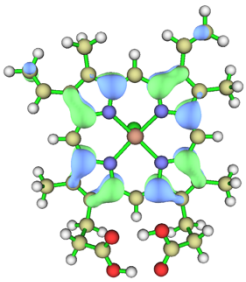
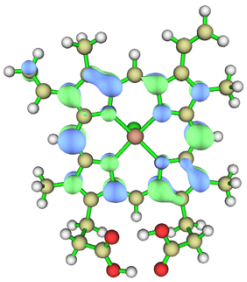
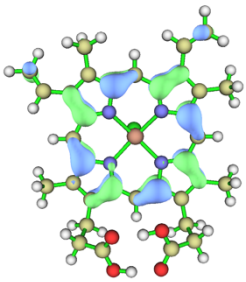
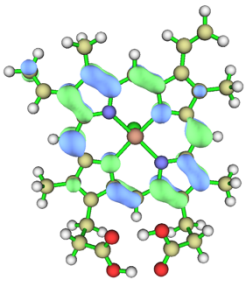
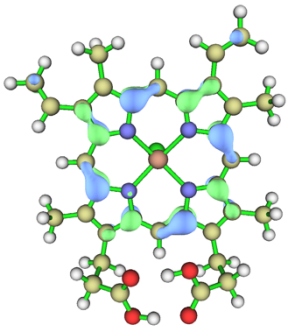
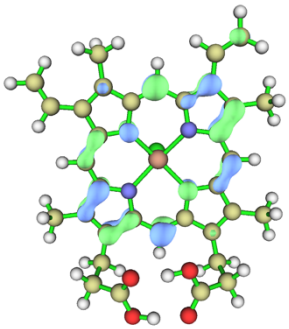
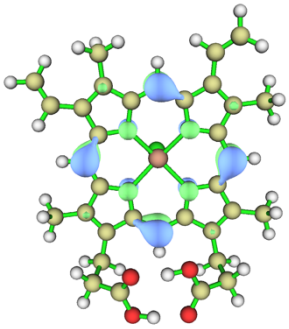
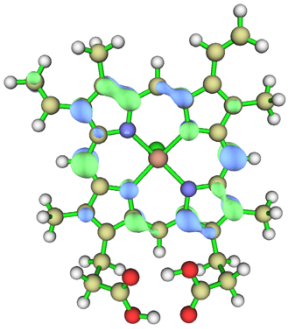


Figure S1. Natural transition orbitals of the relevant excitations of Al-Hemin. (isoval= 0.05)



		54.8% →	
T_1		68.1% →	
T_2		68.1% →	
T_3		64.6% →	
T_4			

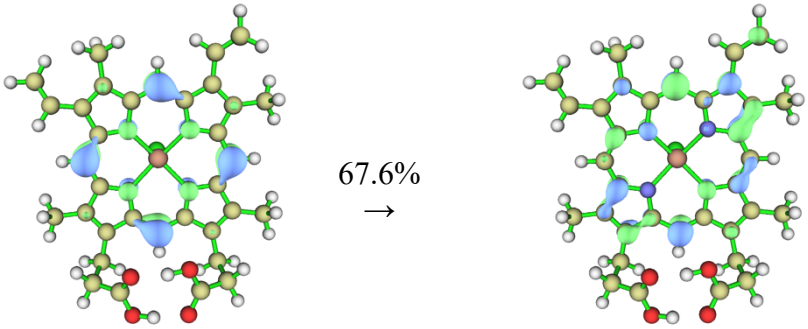
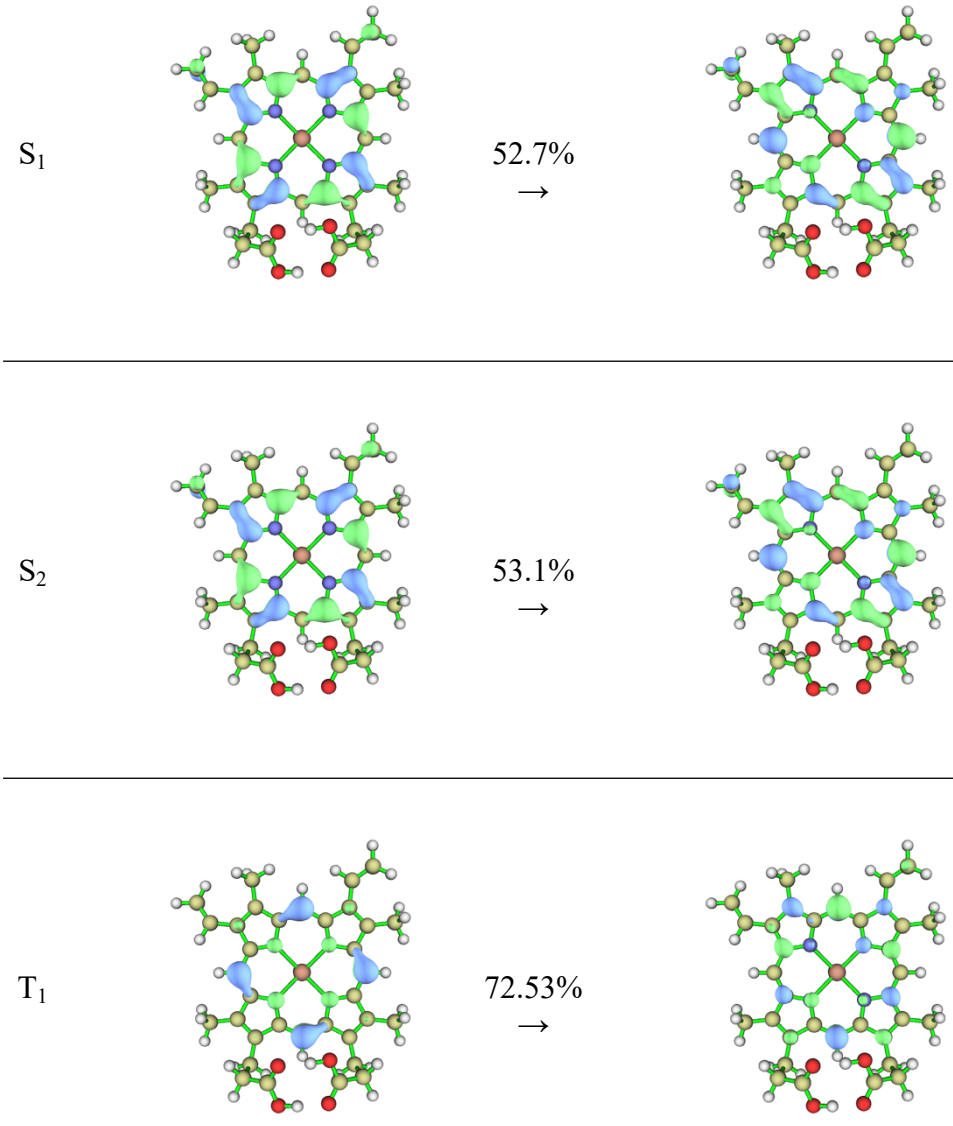


Figure S2. Natural transition orbitals of the relevant excitations of Ga-Hemin. (isoval= 0.05)



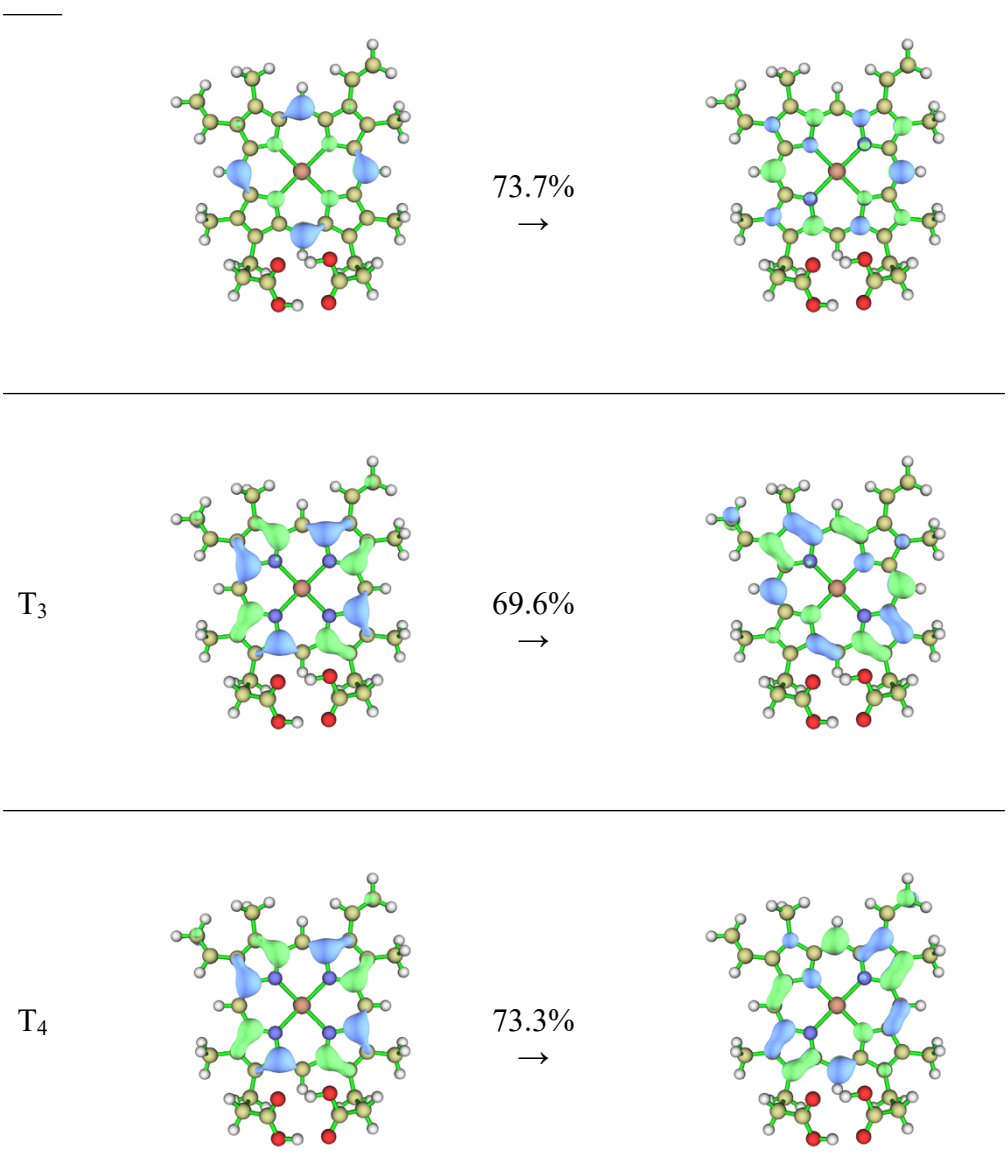


Figure S3. Natural transition orbitals of the relevant excitations of In-Hemin. (isoval= 0.05)