Supplementary Material (ESI) for Dalton Transactions

Supporting Information (2 pages) for the manuscript:

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Bioorganometallic Chemistry 18: A Theoretical DFT Study on the Mechanism of a Novel, Regioselective, Intramolecular N-π Rearrangement of Cis and Trans-η^1-N-Cp*Rh-Hydroxytamoxifen Complexes to their η^6 Derivatives; Potential Breast Cancer Pharmaceuticals, and Fluorescent Probes

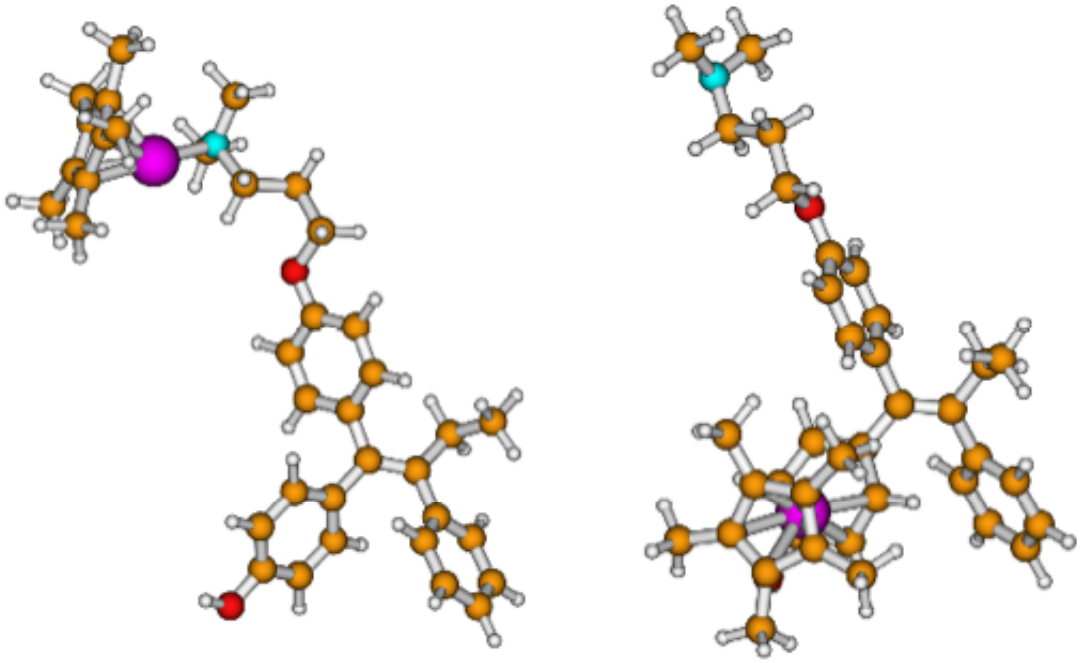

Figure 1S. Optimized geometries of $[\eta^1$-N-Cp*Rh$]^{2+}$ (left) and $[\eta^6$-Cp*Rh$]^{2+}$ (right) dications in the *trans* configuration.

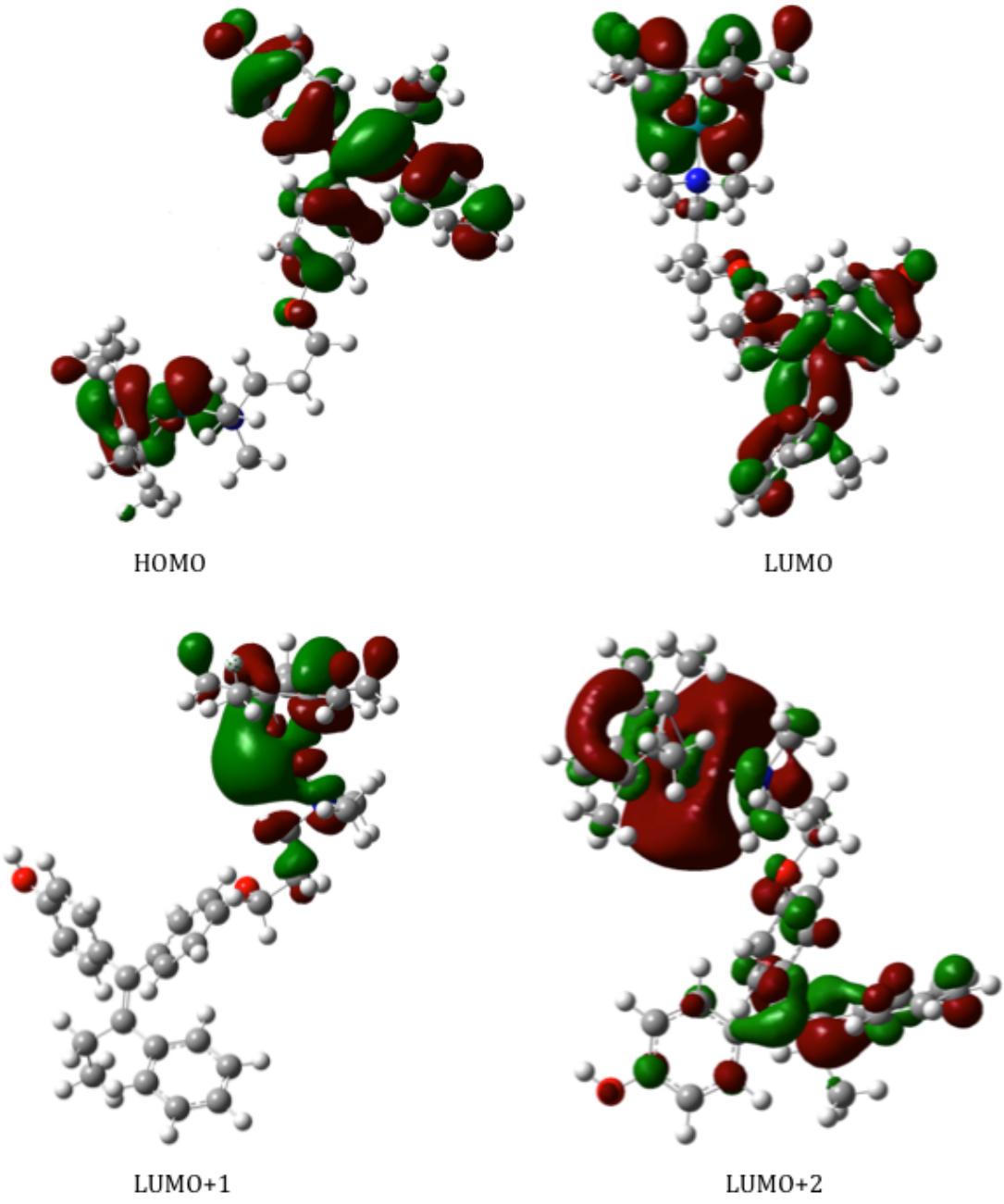

Figure 2S. Density maps of the frontier orbitals in the *cis* [η^1-N-Cp*Rh]$^{2+}$ complex.