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Supporting Information

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Quantum–Chemical Insight into the Reactivity of 5–Bromo–10,20–diaryl–porphyrins towards Nucleophiles

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The mean value of dihedral angles [1]-[2]-[3]-[4] and [1]-[2]-[3]-[4'] (Fig. 1) is selected as a reference for the comparison of orientation of *meso*-amino groups. This mean angle characterizes the orientation of lone pair of nitrogen atom with respect to macrocyclic plane and thus the degree of conjugation of amino-group and porphyrin aromatic system.

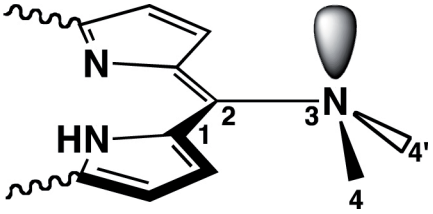

Figure S1. The dihedral angles applied for analysis of respective orientation of the lone pair of the amino-group.

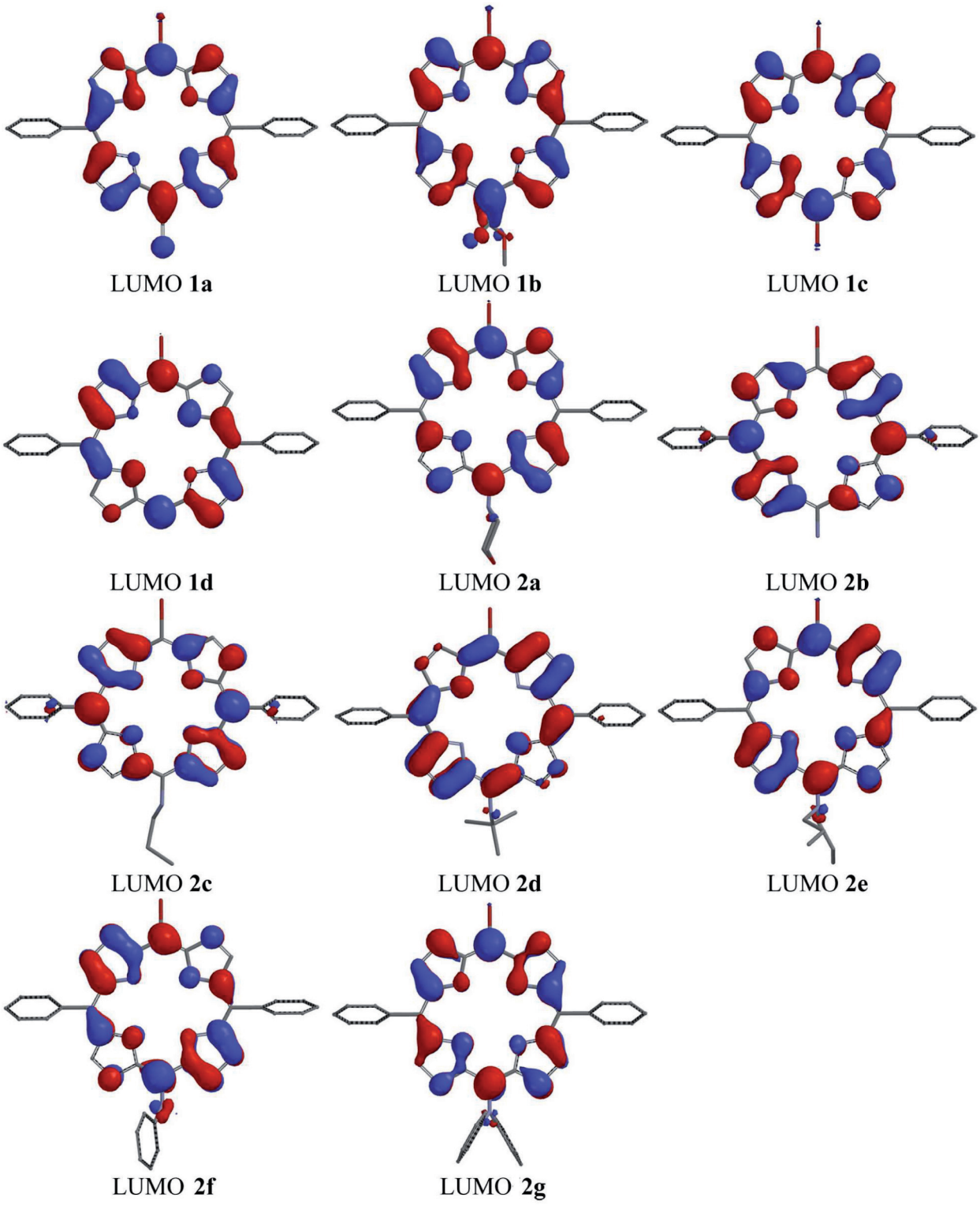

Figure S2. Diagrams of LUMO of investigated compounds **1** and **2**. Protons are omitted for clarity. Red and blue zones of the diagrams correspond to opposite sign of the orbitals.

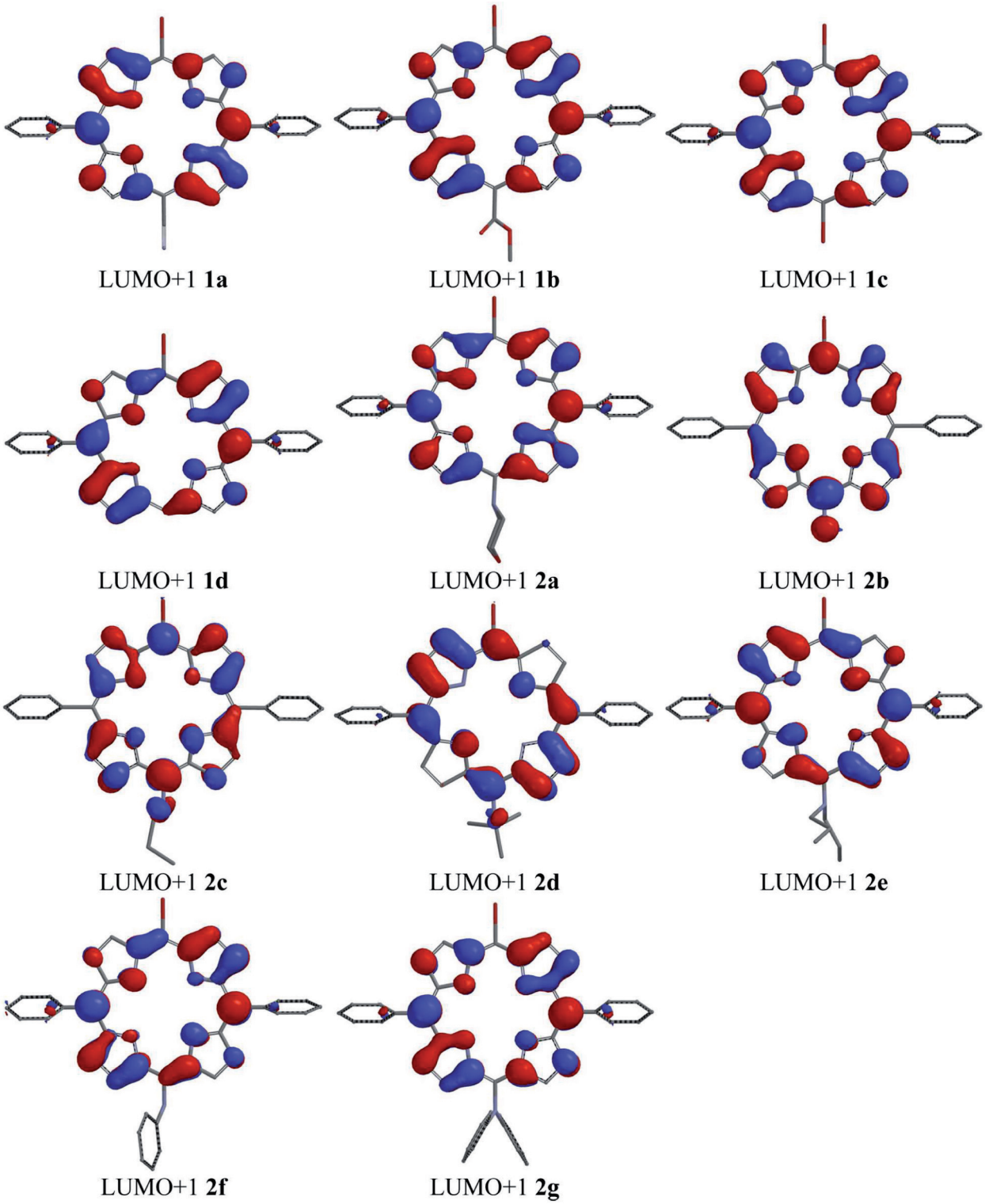

Figure S3. Diagrams of LUMO+1 of investigated compounds **1** and **2**. Protons are omitted for clarity. Red and blue zones of the diagrams correspond to opposite sign of the orbitals.