Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

LOCAL AND MACROCYCLIC (ANTI)AROMATICITY OF PORPHYRINOIDS REVELEAD BY THE TOPOLOGY OF THE INDUCED MAGNETIC FIELD

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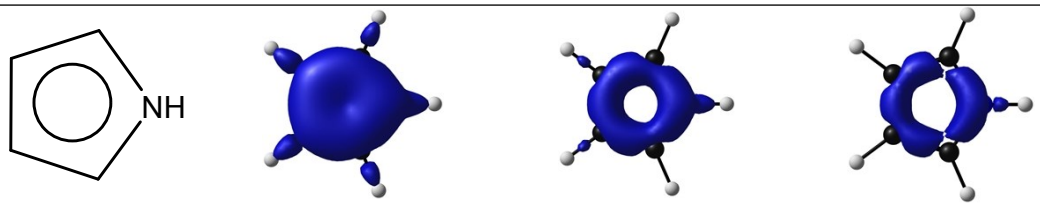
SUPPORTING INFORMATION

Table S1. Strengths of the magnetically induced currents (in nA.T^{-1}) flowing around the macrocyclic ring (macroring), C=C and C-N-C bonds for porphyrin at the B3LYP/6-31g** level.

Rings	Macroring	C-N-C	C=C
NH	27.1	8.5	18.6
N	27.0	14.9	12.0

Fig. S1. B^{ind}_{zz} isosurfaces showing the bifurcation process of pyrrole. Isovalues are shown in parentheses.



Pyrrole (-30 ppm) (-40 ppm) (-45 ppm)

Fig. S2. B^{ind}_{zz} isosurfaces for azafulvene (a) and furan (b) at ± 35 ppm isovalue at the B3LYP/6-31g** level. Global bifurcation values are showed in parenthesis.

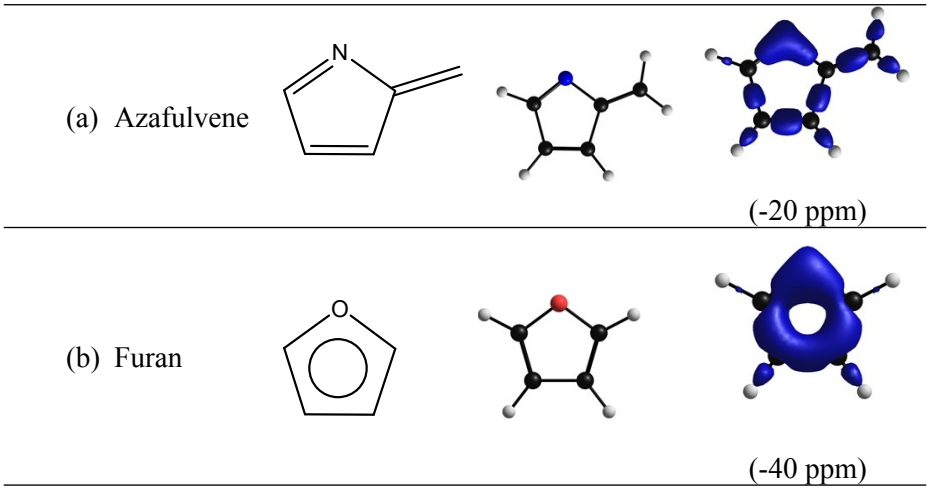


Fig. S3. B^{ind}_{zz} isosurfaces for non-planar porphyrinoids at ± 35, +/- 25 and +/- 10 respectively at B3LYP/6-31g** level. Global bifurcation values are showed in parenthesis.

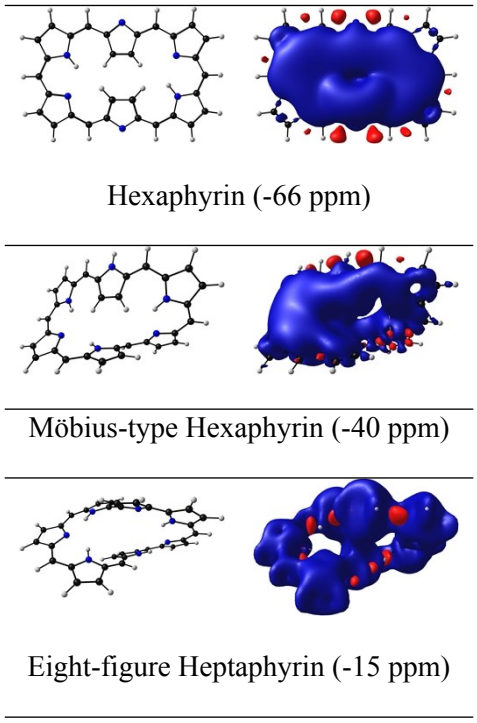


Fig. S4. Ring current strength (in nA.T^{-1}) values for planar aromatic dihydrodideazaporphyrin (*left*) and; the hydrogenated dihydrodideazaporphyrin in *meso*-carbons (*right*).

Dihydrodideazaporphyrin

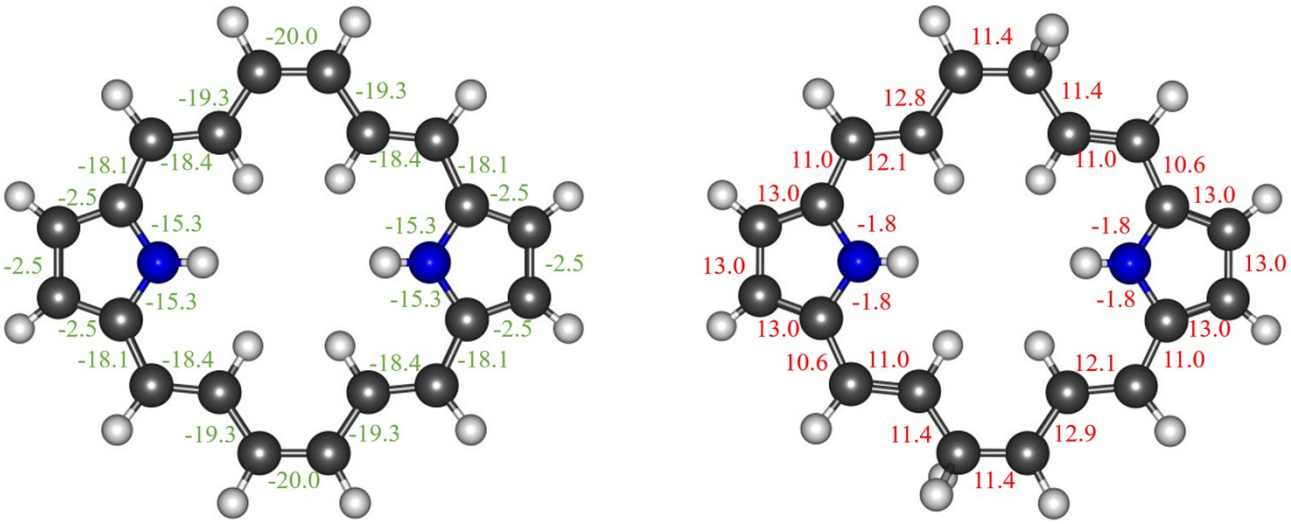
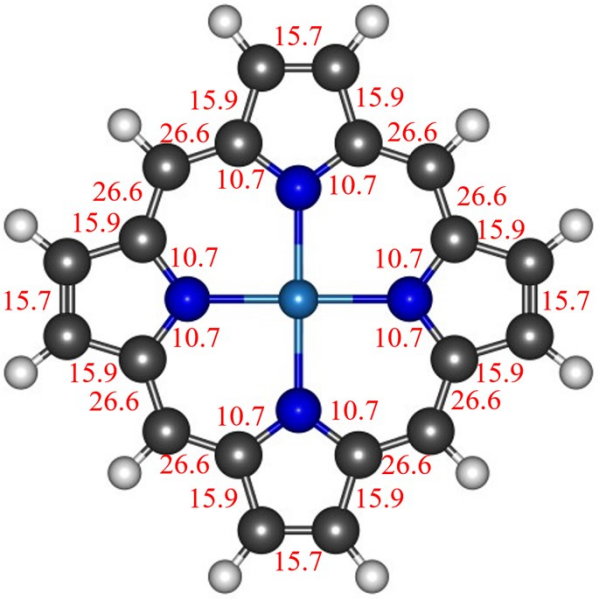
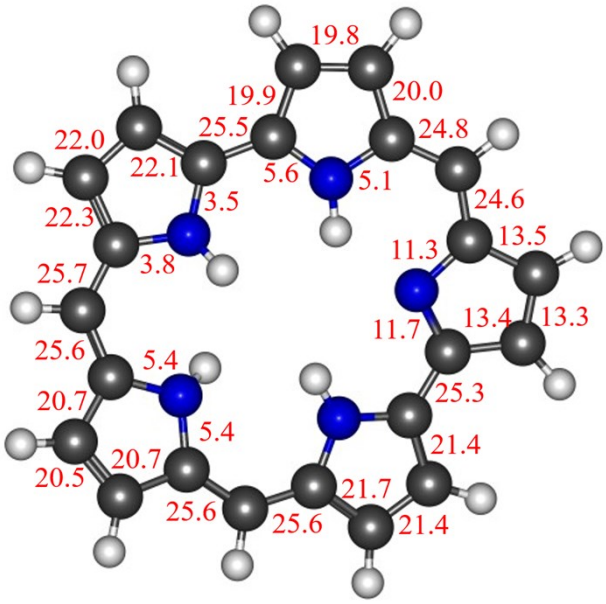


Fig. S5. Ring current strength (in nA.T^{-1}) values for planar aromatic porphyrinoids (See Fig 4 in manuscript)

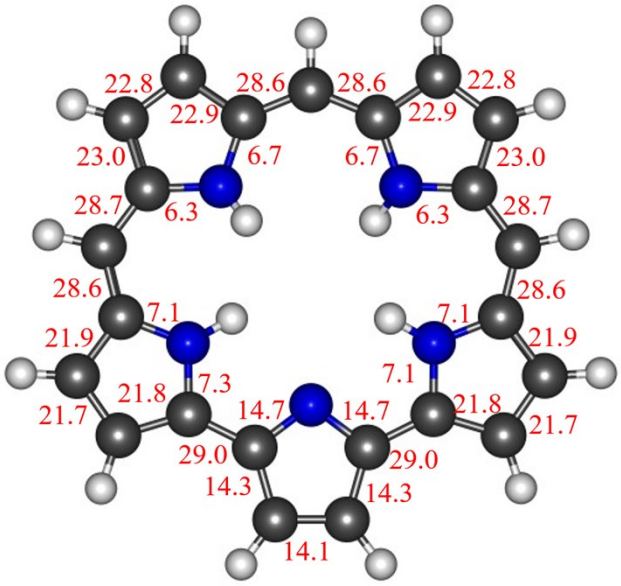
Zn-Porphyrin



Smaragdyrin



Isosmaragdyrin



Pentaphyrin

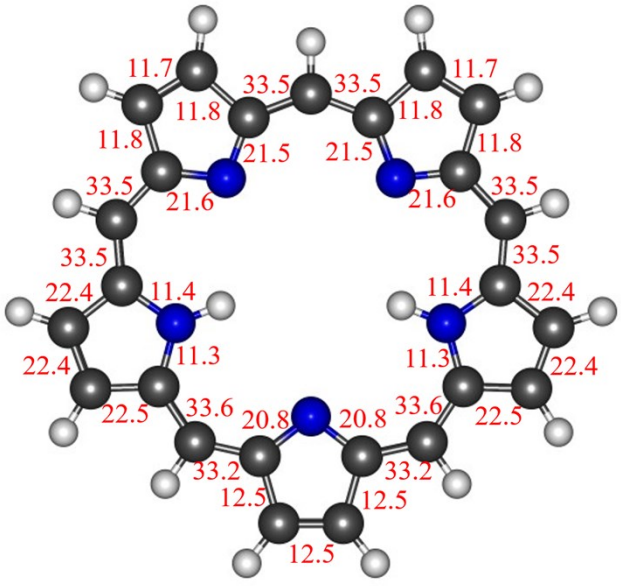
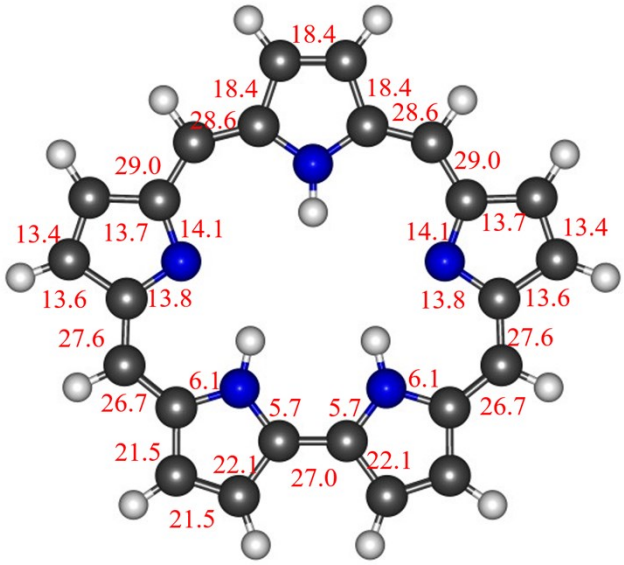


Fig. S6. (Continue) Ring current strength (in $nA.T^{-1}$) values for planar aromatic porphyrinoids (See Fig 4 in manuscript).

Sapphyrin



Ozaphyrin

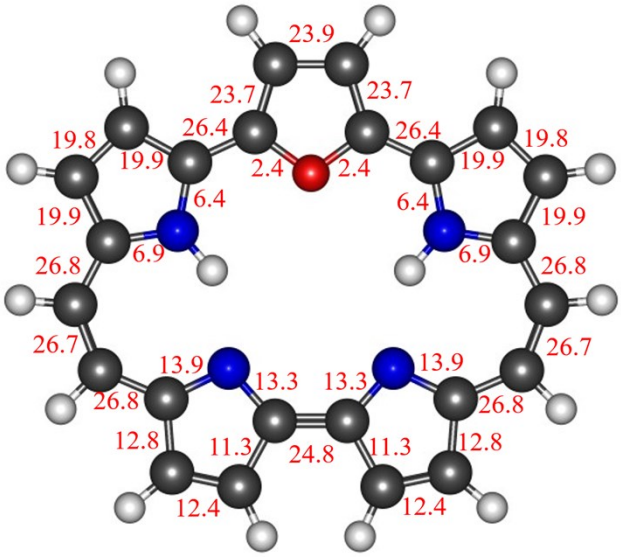
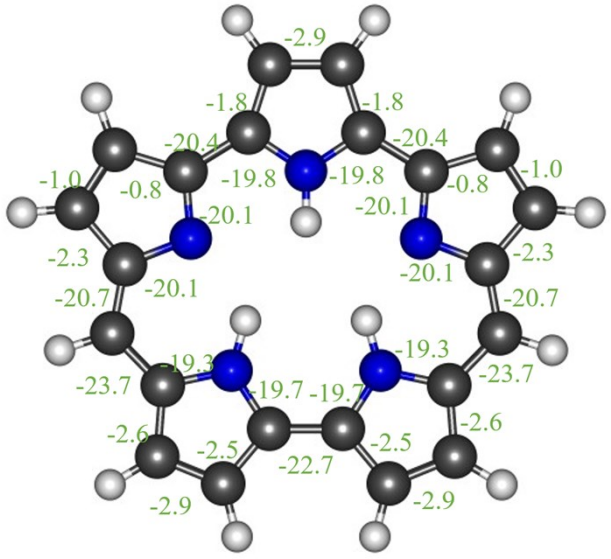
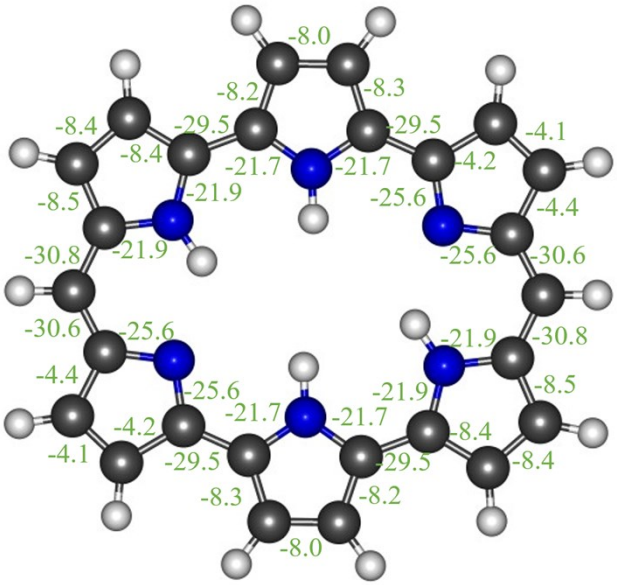


Fig. S7. Ring current strength (in $nA.T^{-1}$) values for antiaromatic porphyrinoids (See Fig 3 and 5 in manuscript)

Orangarin



Amethyrin



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