

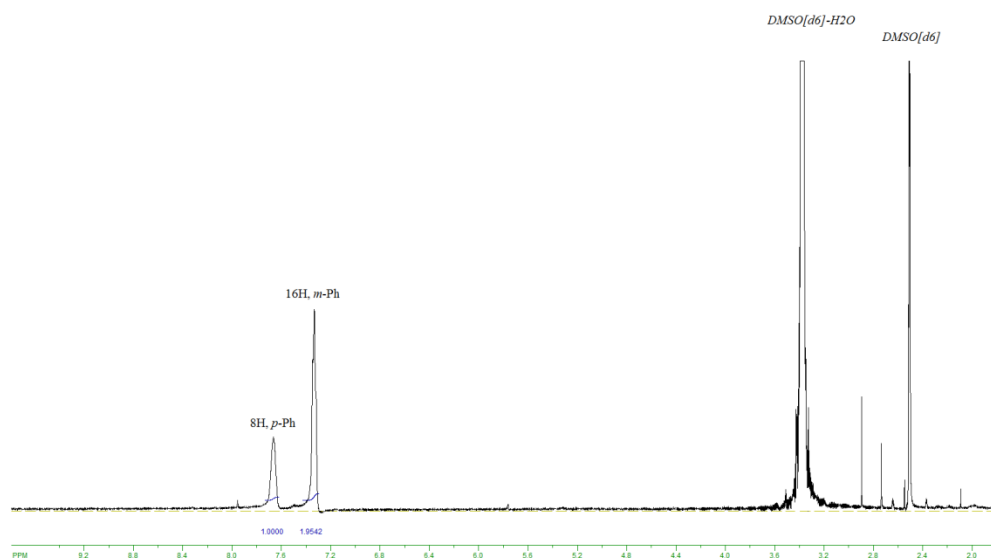
# Supplementary Information

of the article «Synthesis, Structure, and Spectral-Luminescent Properties of Peripherally Fluorinated Mg(II) and Zn(II) Octaphenyltetraazaporphyrins»

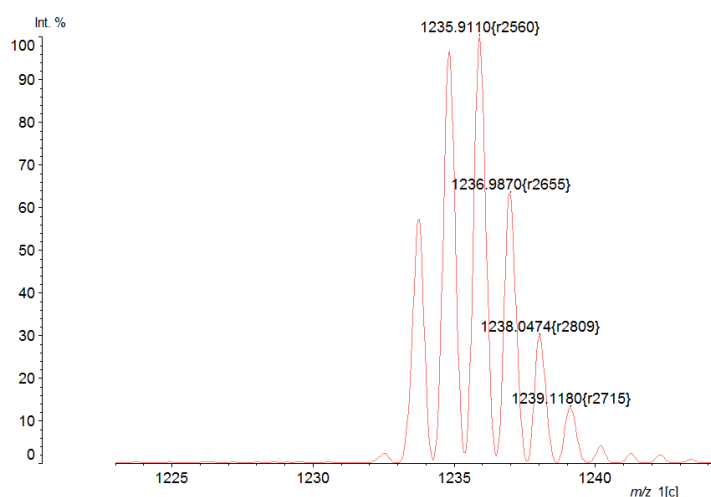
Alexey Rusanov<sup>1,2</sup>, Natalya Chizhova<sup>1</sup> and Nugzar Mamardashvili<sup>1\*</sup>

<sup>1</sup>G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences, Russia, 153045, Ivanovo, Akademicheskaya St. 1, <sup>2</sup>Ivanovo State University of Chemistry and Technology Russia, 153460, Ivanovo, Sheremetevsky Pr. 7

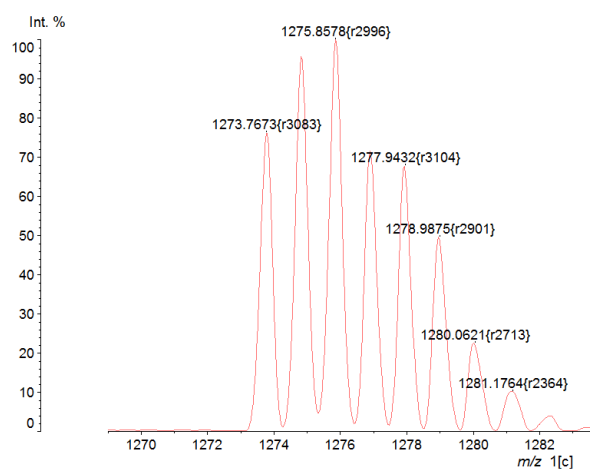
\* Correspondence: [nugzarstrasburg@mail.ru](mailto:nugzarstrasburg@mail.ru); Tel.: +7-9038893456



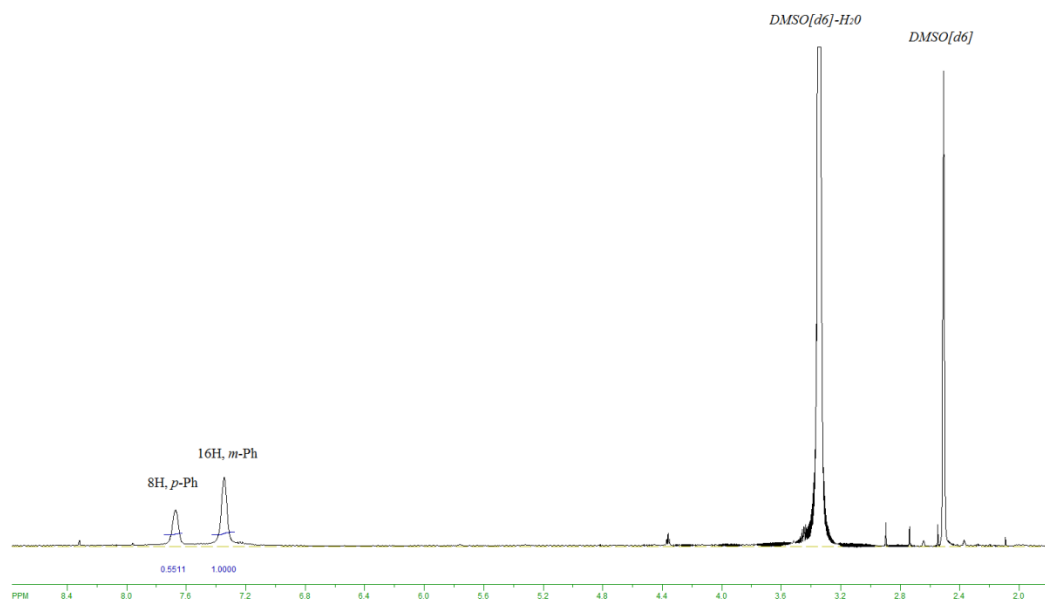
**Figure S1.** <sup>1</sup>H NMR spectrum of the Mg(II)-octa-(2,6-difluorophenyl)tetraazaporphyrin in d<sub>6</sub> DMSO.



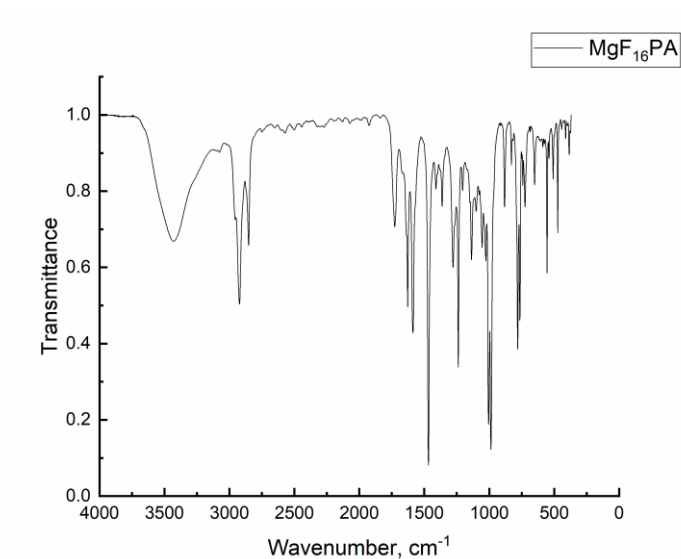
**Figure S2.** The isotopic distribution of the molecular ion peak of Mg(II)-octa-(2,6-difluorophenyl)tetraazaporphyrin.



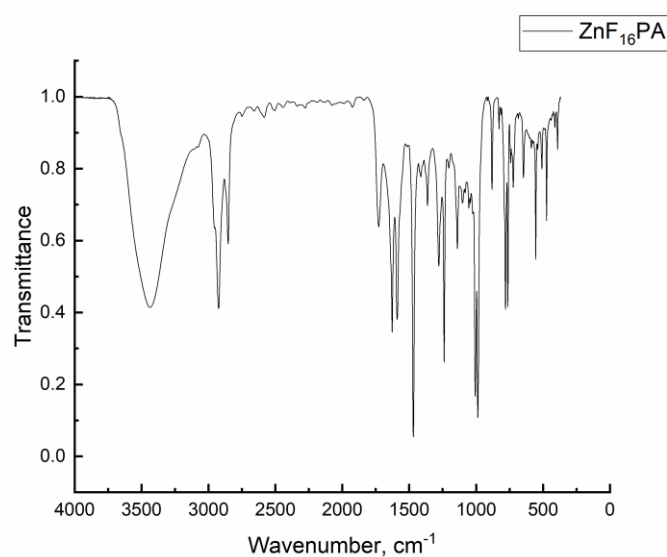
**Figure S3.** The isotopic distribution of the molecular ion peak of Zn(II)-octa-(2,6-difluorophenyl)tetraazaporphyrin.



**Figure S4.** <sup>1</sup>H NMR spectrum of the Zn(II)-octa-(2,6-difluorophenyl)tetraazaporphyrin in *d*<sub>6</sub> DMSO.



**Figure S5.** IR spectrum of the Mg(II)-octa-(2,6-difluorophenyl)tetraazaporphyrin in KBr tablets.

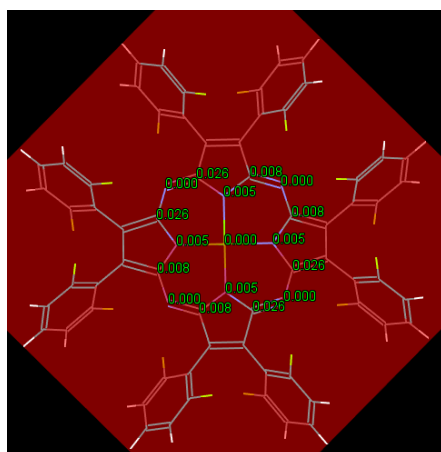


**Figure S6.** IR spectrum of the Zn(II)-octa-(2,6-difluorophenyl)tetraazaporphyrin in KBr tablets.

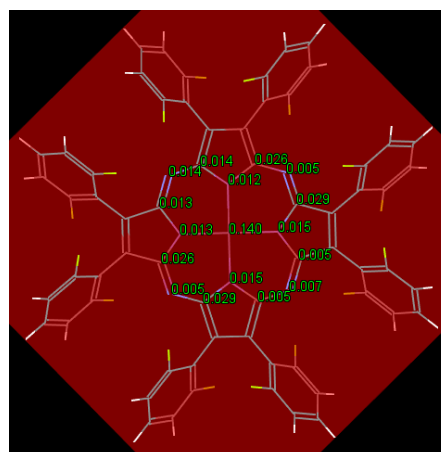
**Table S1.** The values from visualization of the planarity measure and equations of them.

Atom	Values for MgF <sub>16</sub> PA (1)	Values for ZnF <sub>16</sub> PA (2)	Equation 2/1
Metal-ion	0.000	0.140	0.140 (div. by 0)
N	0.005	0.012	2.4
	0.005	0.015	3
	0.005	0.015	3
	0.005	0.013	2.6
Na	0.000	0.014	0.014 (div. by 0)
	0.000	0.005	0.005(div. by 0)

	0.000 0.000	0.007 0.005	0.007(div. by 0) 0.005(div. by 0)
C	0.026; 0.008 0.008; 0.026 0.026; 0.008 0.008; 0.026	0.014; 0.026 0.029; 0.005 0.005; 0.029 0.026; 0.013	0.5; 3.25 3.6; 0.2 0.2; 3.6 3.2; 0.5

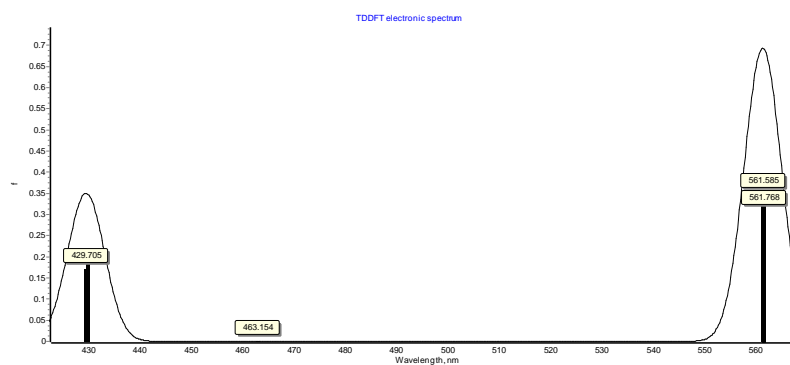


MgF<sub>16</sub>PA

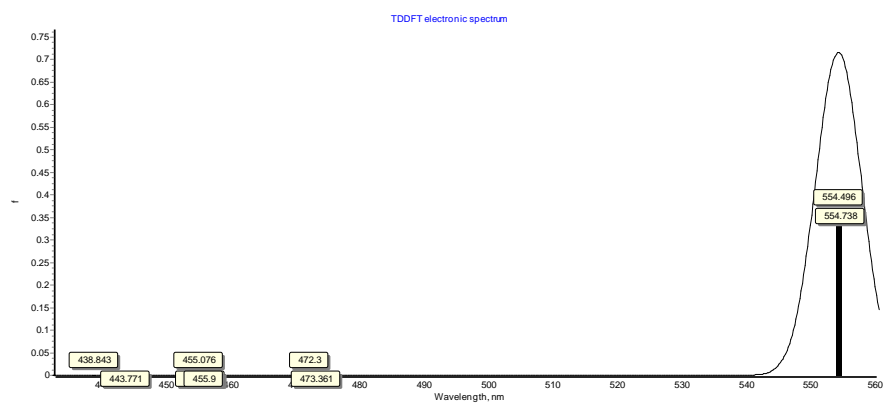


ZnF<sub>16</sub>PA

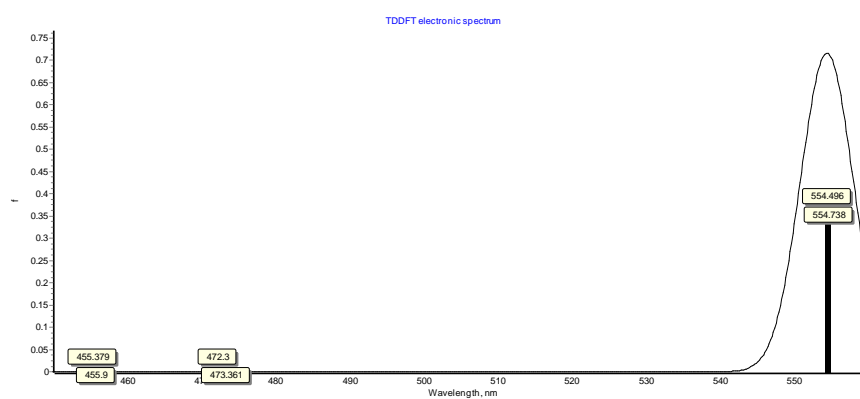
**Figure S7.** Visualization of the planarity measure of the Mg(II)-octa-(2,6-difluorophenyl)tetraazaporphyrin and Zn(II)-octa-(2,6-difluorophenyl)tetraazaporphyrin.



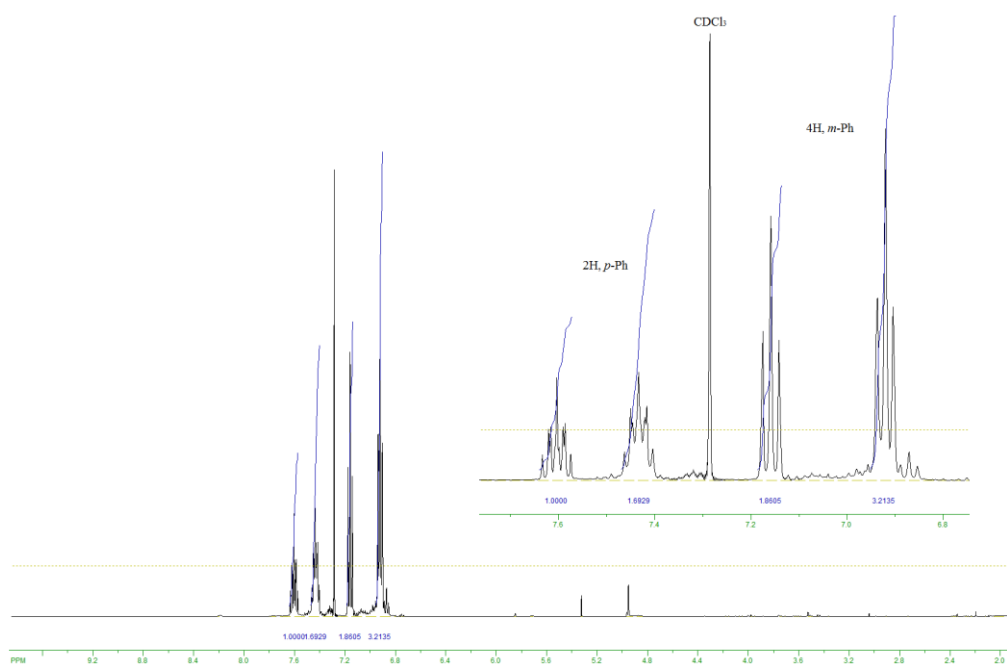
**Figure S8.** Predicted UV-Vis spectrum of the Mg(II)-octa-(2,6-difluorophenyl)tetraazaporphyrin with nstate=10 and root=1 parameters.



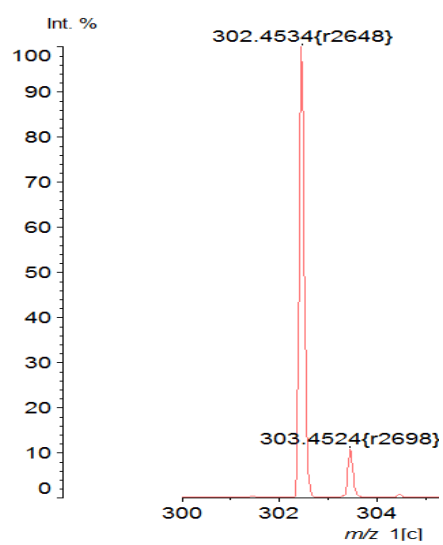
**Figure S9.** Predicted UV-Vis spectrum of the Zn(II)-octa-(2,6-difluorophenyl)tetraazaporphyrin with nstate=10 и root=1 parameters.



**Figure S10.** Predicted UV-Vis spectrum of the Zn(II)-octa-(2,6-difluorophenyl)tetraazaporphyrin with nstate=6 и root=20 parameters.



**Figure S11.**  $^1\text{H}$  NMR spectrum of the di-(2,6-difluorophenyl)maleindinitrile in  $\text{CDCl}_3$ .



**Figure S12.** Mass-spectrum of the di-(2,6-difluorophenyl)maleindinitrile.