Supplementary Information

Bis-Resorcin[4]arene-Bridged Porphyrin Conjugates: Synthesis, Fluorescence and Binding studies

Talal F. Al-Azemi,[a]*Mickey Vinodh,[a] and Fatemeh H. Alipour [a]

[a]*Department of Chemistry, Kuwait University, P O Box 5969, Safat 13060, Kuwait.*

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Single crystal X-ray diffraction:

*X-Ray structure of octametoxy-methyl resorcin[4]arene (**RO**):*

Singles crystals of RO suitable for single crystal X-ray diffraction were grown from solvent diffusion method. RO (50mg), dissolved in 1 mL acetone was taken in a small vial with a narrow opening and kept inside a big vial containing 10ml methanol. Methanol was allowed to diffuse into the RO solution slowly and within 5 days suitable single crystals were grown. The single crystal data collections were made on a Rigaku R-AXIS RAPID diffractometer using crystalclear software package at -123 ^{o}C. The structure was solved and refined using the Bruker SHELXTL Software Package (Structure solution program- SHELXS-97 and Refinement program- SHELXL-97[2]).

*X-Ray structure of monobromo-octametoxy-methyl resorcin[4]arene (**ROBr**):*

Singles crystal **ROBr,** suitable for single crystal X-ray diffraction were grown from solvent diffusion method. Monobrominated resorcinarene (**ROBr,** 50 mg), dissolved in 1 mL ethylacetate was taken in a small vial with a narrow opening and kept inside a big vial containing 10ml Hexane. Hexane was allowed to diffuse into the resorcinarene solution slowly and within 10 days suitable single crystals were grown. The single crystal data collections were made on a Rigaku R-AXIS RAPID diffractometer using crystalclear software package at -123 ^{o}C. The structure was solved by direct methods[2] and was expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropic ally. Hydrogen atoms were refined using the riding model. All calculations were performed using the CrystalStructure[3] crystallographic software package except for refinement, which was performed using SHELXL-97[2].

*X-Ray structure of 5-15-di(3-hydroxyphenyl)-10,20-di(4-toluyl)porphyrin **(PT):***

Single crystal of **PT** was grown by slow solvent evaporation of **PT** dissolved in ethylacetate solution. The single crystal data collections were made on a Rigaku R-AXIS RAPID diffractometer using crystalclear software package at -123 ^{o}C. The structure was solved by direct methods[2] and was expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropic ally. Hydrogen atoms were refined

using the riding model. All calculations were performed using the Crystal Structure[3] crystallographic software package except for refinement, which was performed using SHELXL-97[2].

Table S1: Crystal data and experimental parameters of the structural analysis of **RO ROBr** and **PT**.

Compound	RO	ROBr	PT
Crystal Dimension/mm	0.20×0.20×0.20	0.20× 0.20× 0.20	0.35×0.30×0.04
Crystal Shape	Block	Block	Platlet
Formula weight	$C_{64}H_{96}O_8$	$C_{64}H_{95}BrO_8$	$C_{46}H_{34}N_4O_2$
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group(no.)	P 1 21/n 1	P21/n (14)	P21/n (14)
T/^{o}C	-123 (2)	-123 (2)	-123 (2)
a/Å	12.8462(4)	12.9612(8)	10.449(1)
b//Å	25.7060(8)	25.917(2)	8.0623(8)
c/Å	18.2551(13)	18.2147(12)	20.834(2)
α/deg	90	90	90
β/deg	93.941(7)	94.004(7)	100.701(7)
γ/deg	90	90	90
V/ Å^3	6014.0	6103.7(7)	1724.5(3)
Z	4	4	2
μ(MOKα) mm^{-1}	0.070	7.264	0.804
ρ_{calcd}/g cm^{-3}	1.097	1.167	1.299
θ_{max}/deg	50.1	55.0	54.9
Reflections collected	47235	48945	9534
Unique reflections	10607	11022	3898
R_{int}	0.0340	0.0424	0.0479
R (I > 2σ)	0.0499	0.0795	0.0657
R (all data)	0.0708	0.1107	0.0997
R_w(all data)	0.1444	0.2801	0.2450
Peak$_{max}$ (e$^-$/Å3)	0.651	0.65	0.53

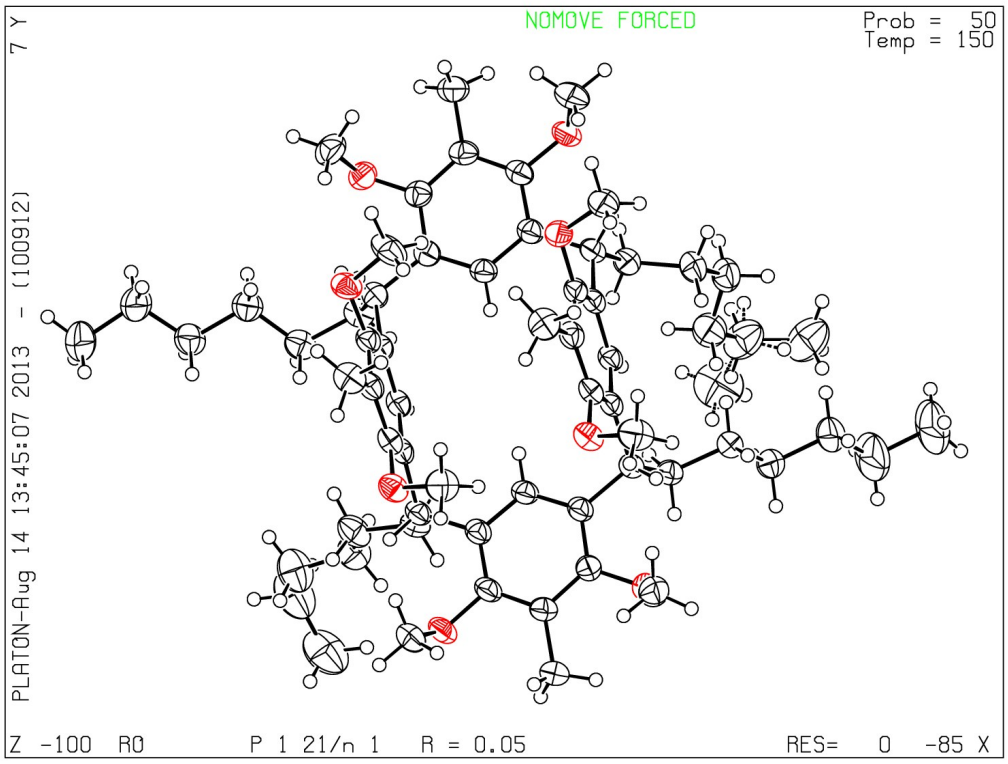


Fig. 1S: Average structures of**RO** obtained from crystal data as a result of disorder of heavy bromine atoms

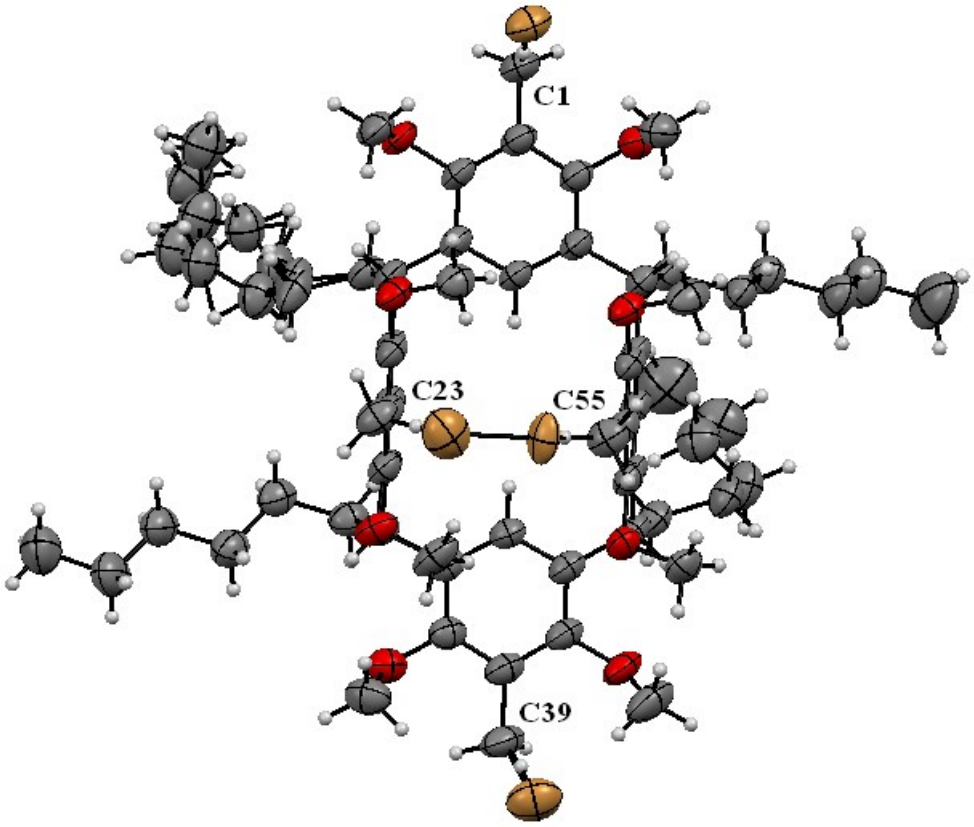
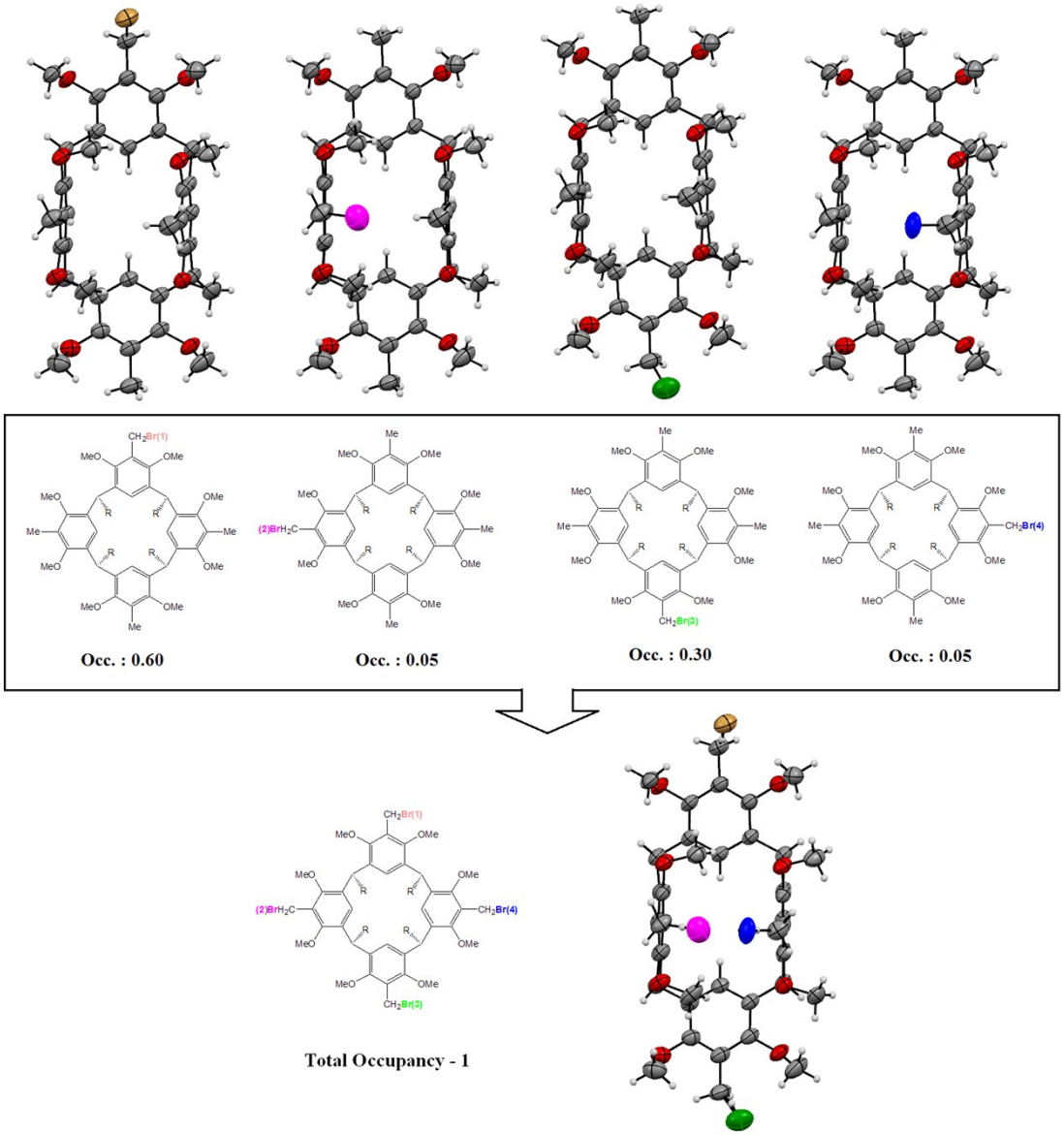


Fig. 2S: Structures of **ROBr** obtained from crystal data as a result of disorder of heavy bromine atoms.



Fig, 3S: Occupancies of bromine atom in the crystal structure of **ROBr** at different sites.

MS spectra of the synthesized functionalized porphyrins:

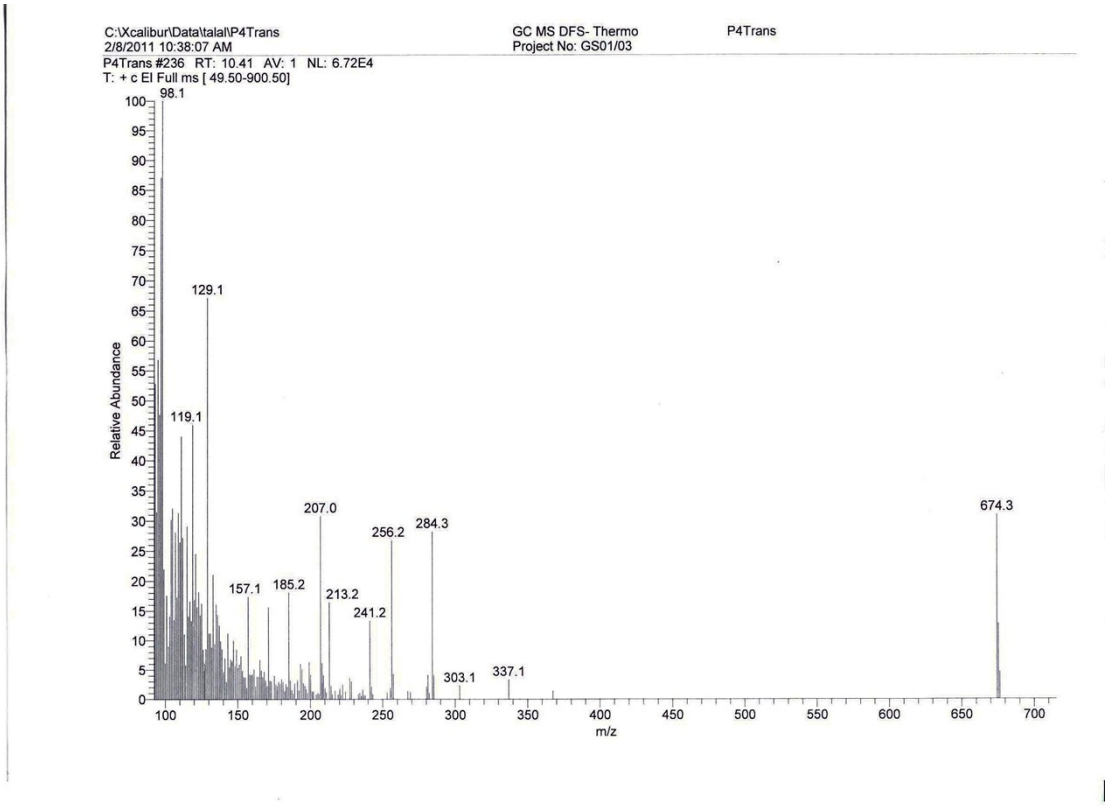


Fig4S: ESI-MS of **PT**

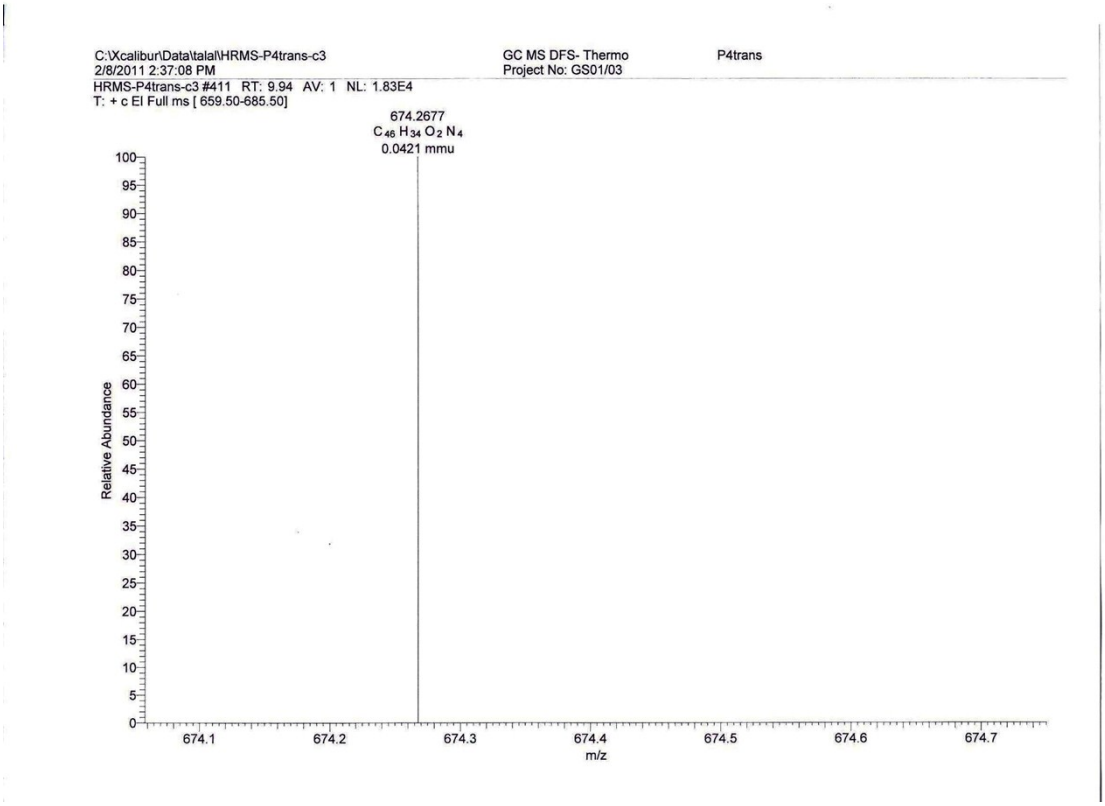


Fig. 5S: HRMS **of PT**

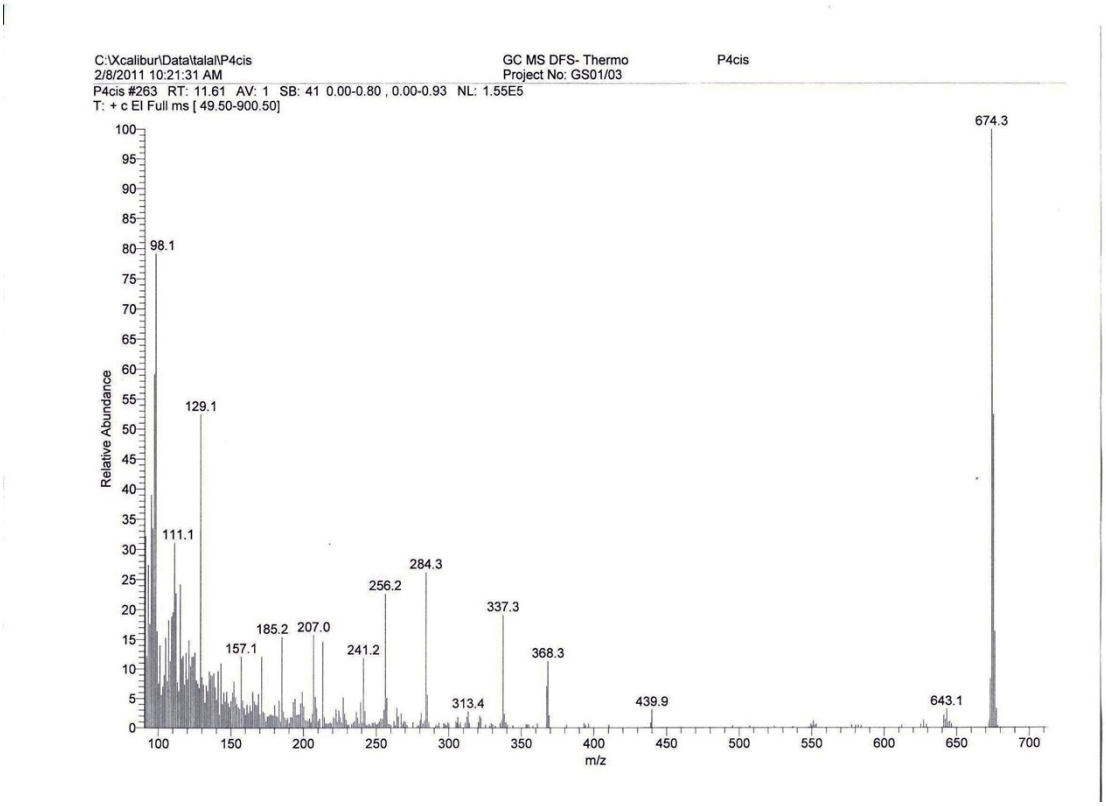


Fig. 6S: ESI-MS of **PC**

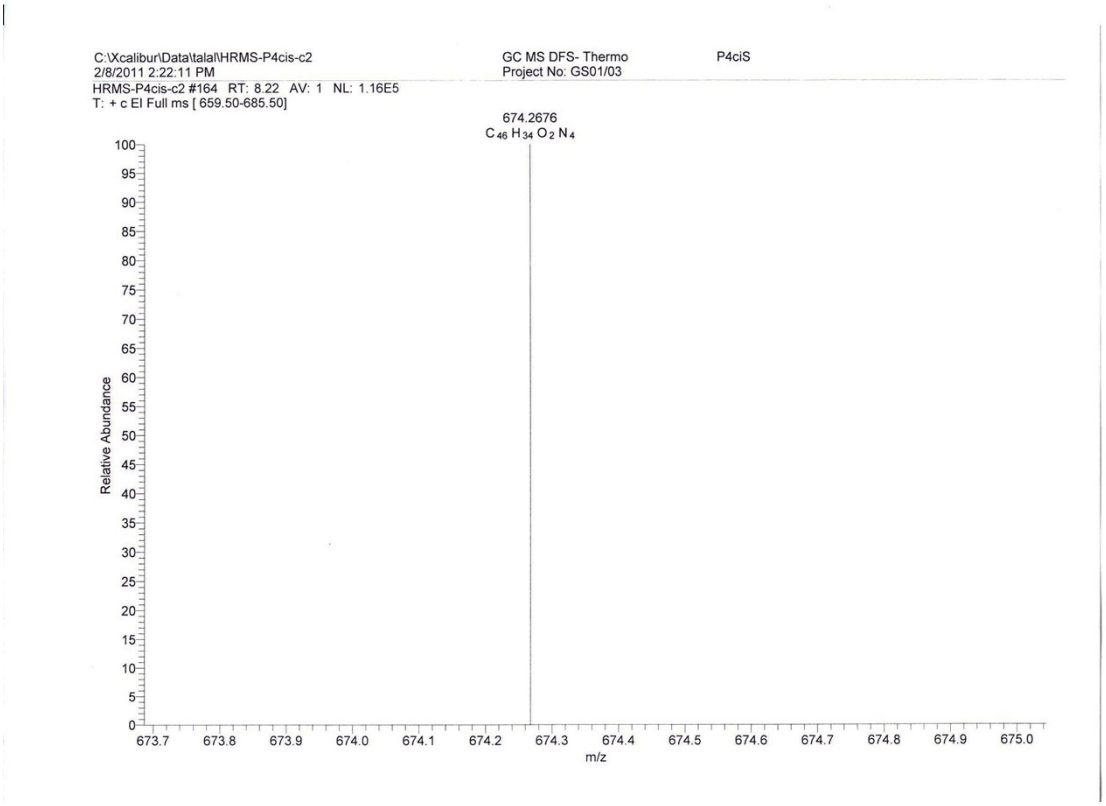


Fig. 7S: HRMS **of PC**

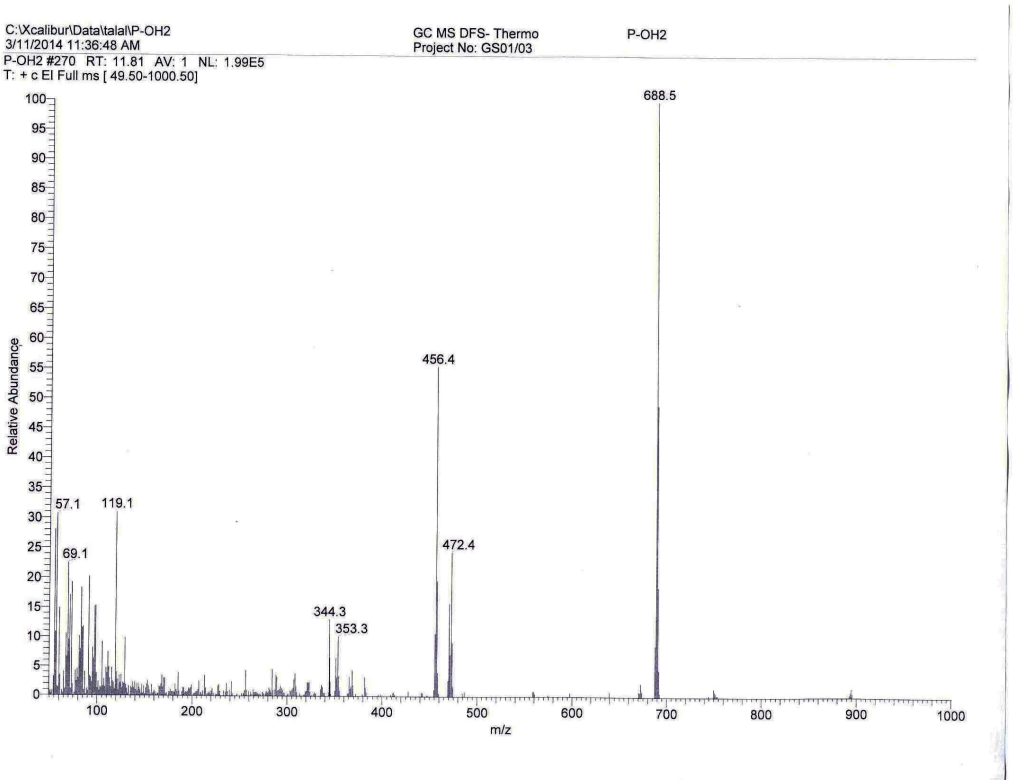


Fig. 8S: ESI-MS of **PH**

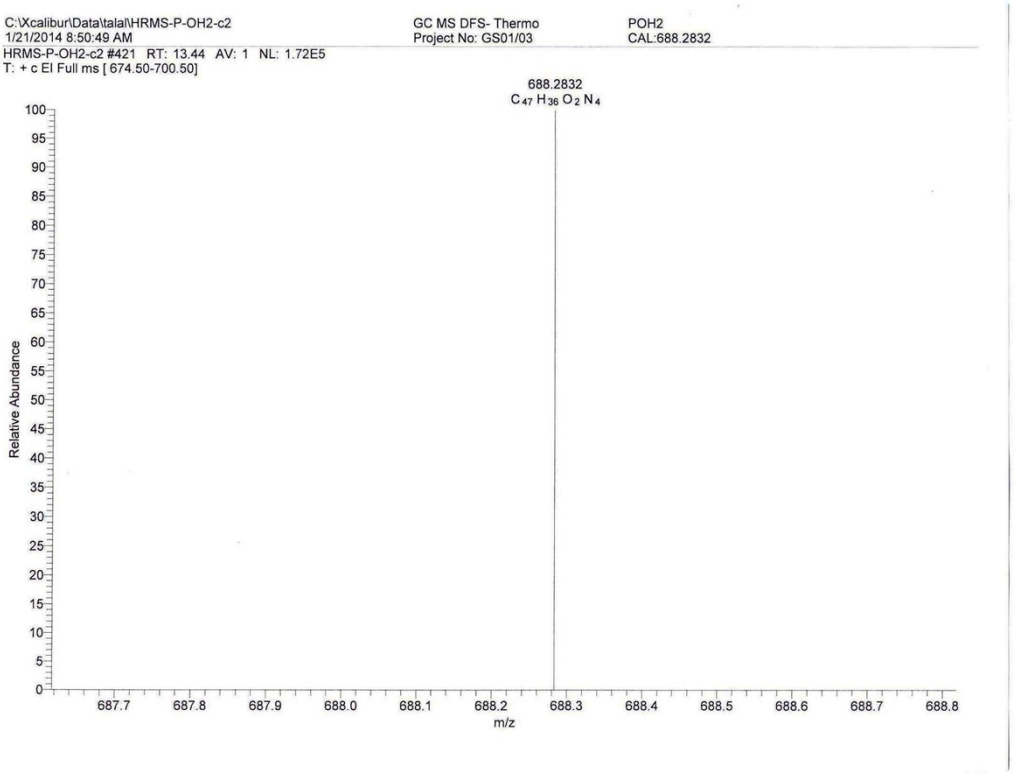


Fig. 9S: HRMS **of PH**

MS spectra of the synthesized Bis-Resorcinarene Bridged Porphyrin Conjugates:

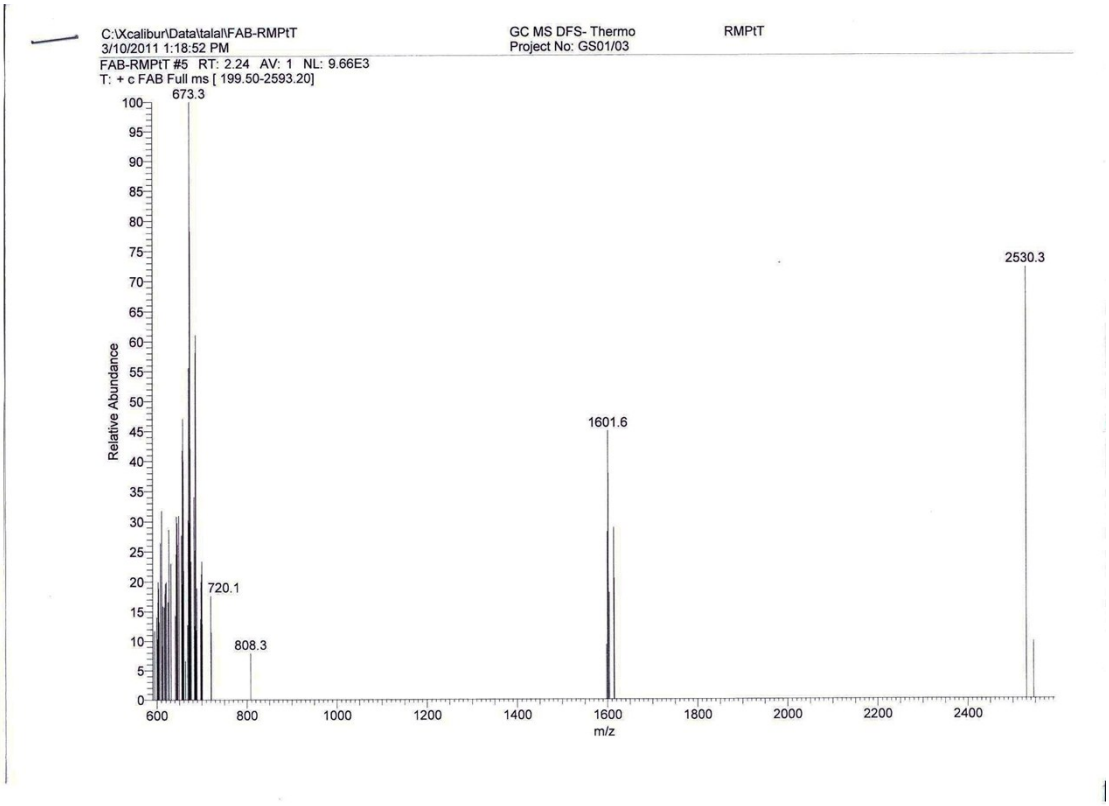


Fig. 10S: FAB-MS of **$(RC)_2PT$**

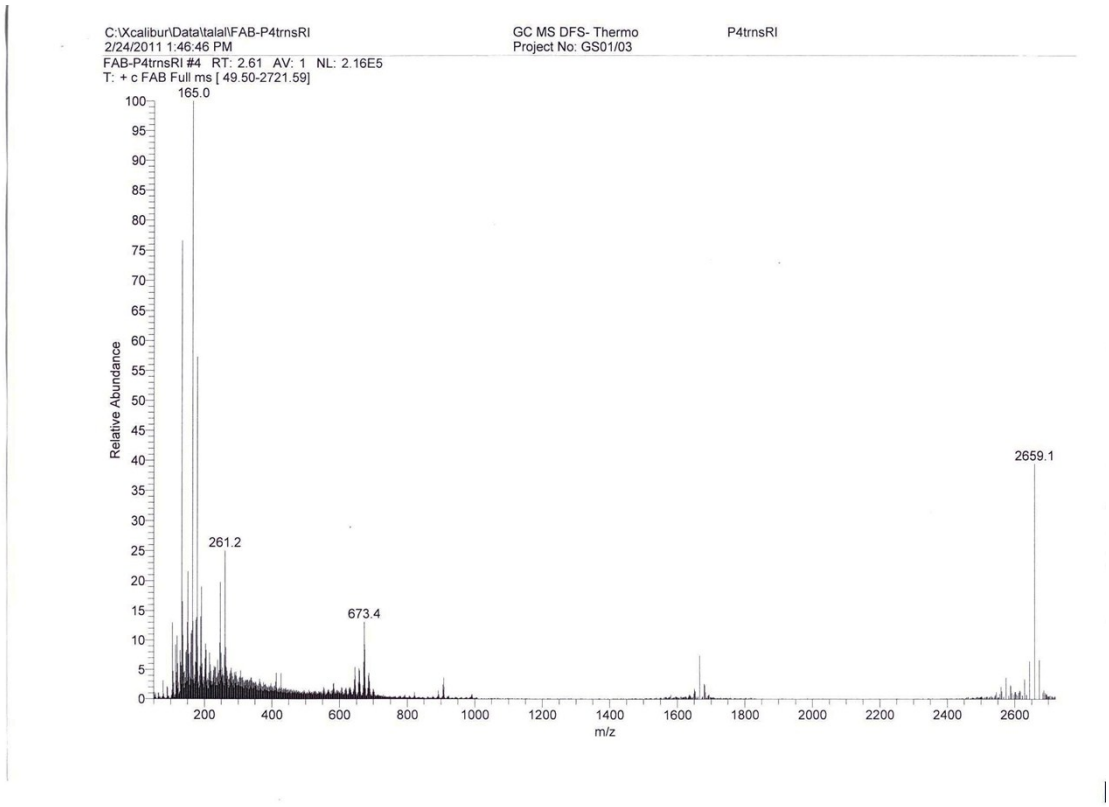


Fig. 11S: FAB-MS of **$(RO)_2PT$**

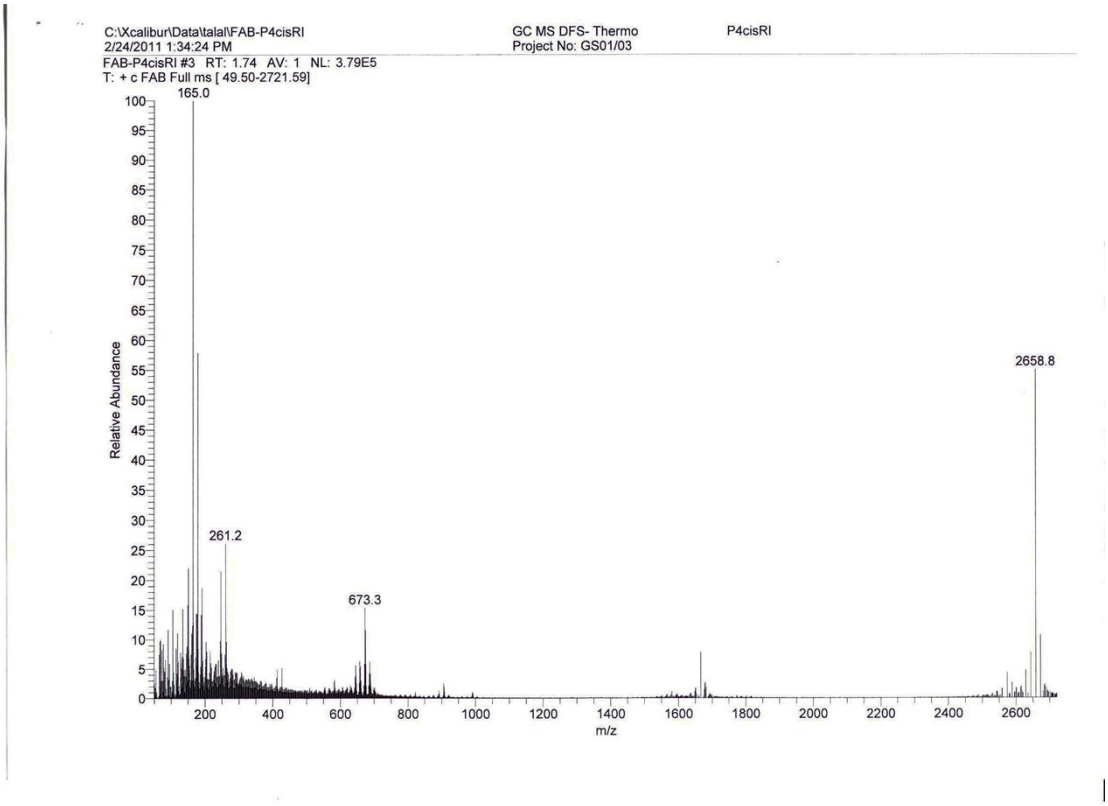


Fig. 12S: FAB-MS of **$(RO)_2PC$**

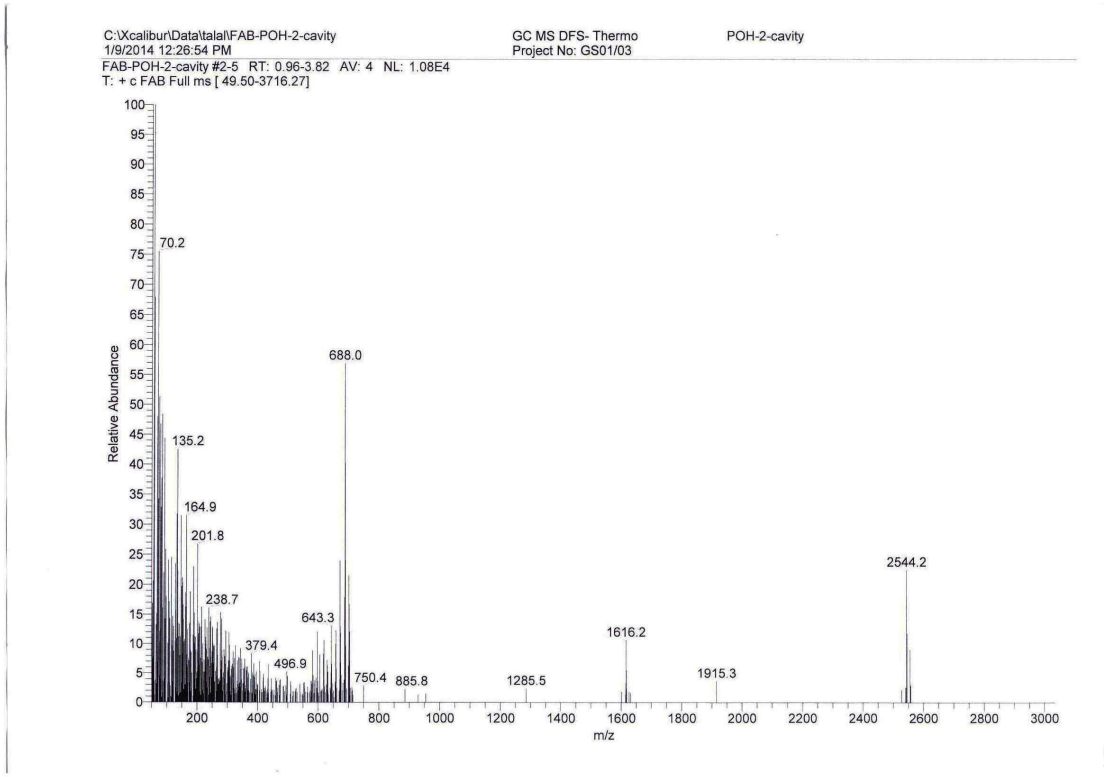


Fig. 13S: FAB-MS of **$(RO)_2PH$**

NMR spectra:

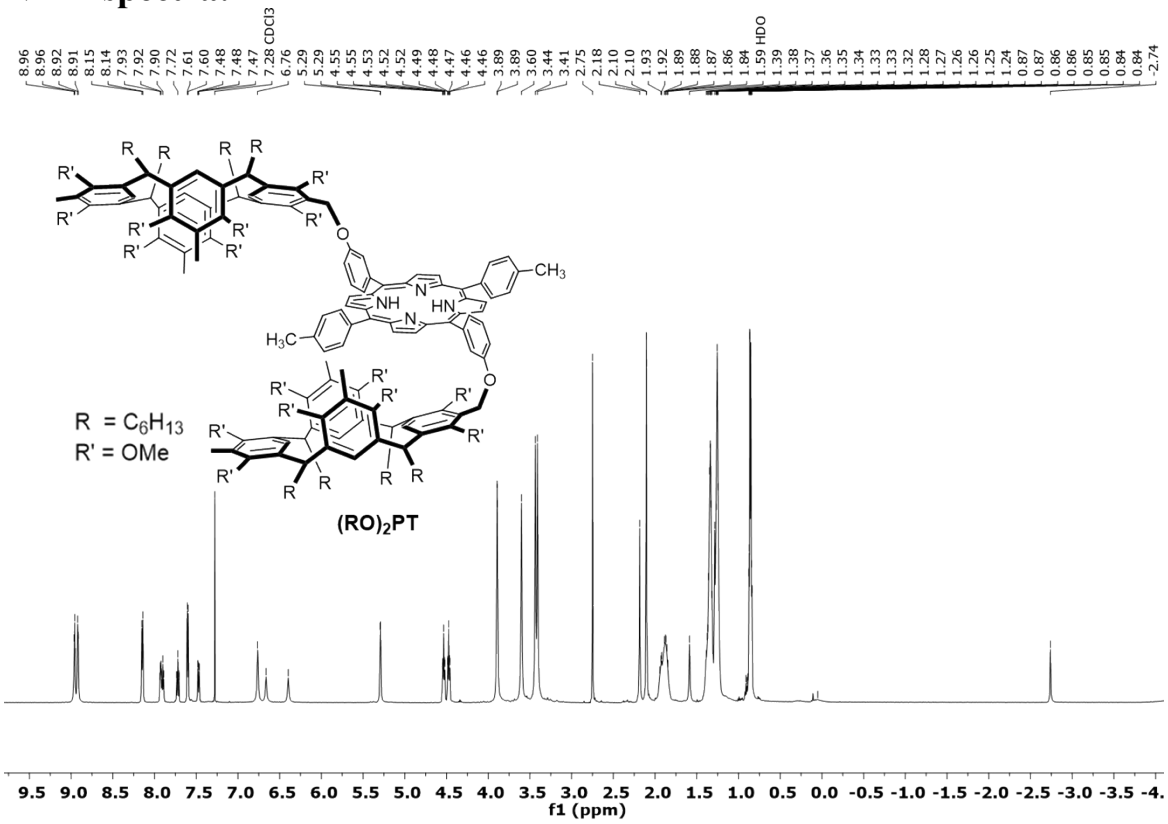


Fig.14S: ^{1}HNMR (600 MHz, $CDCl_3$) spectrum of $(RO)_2PT$.

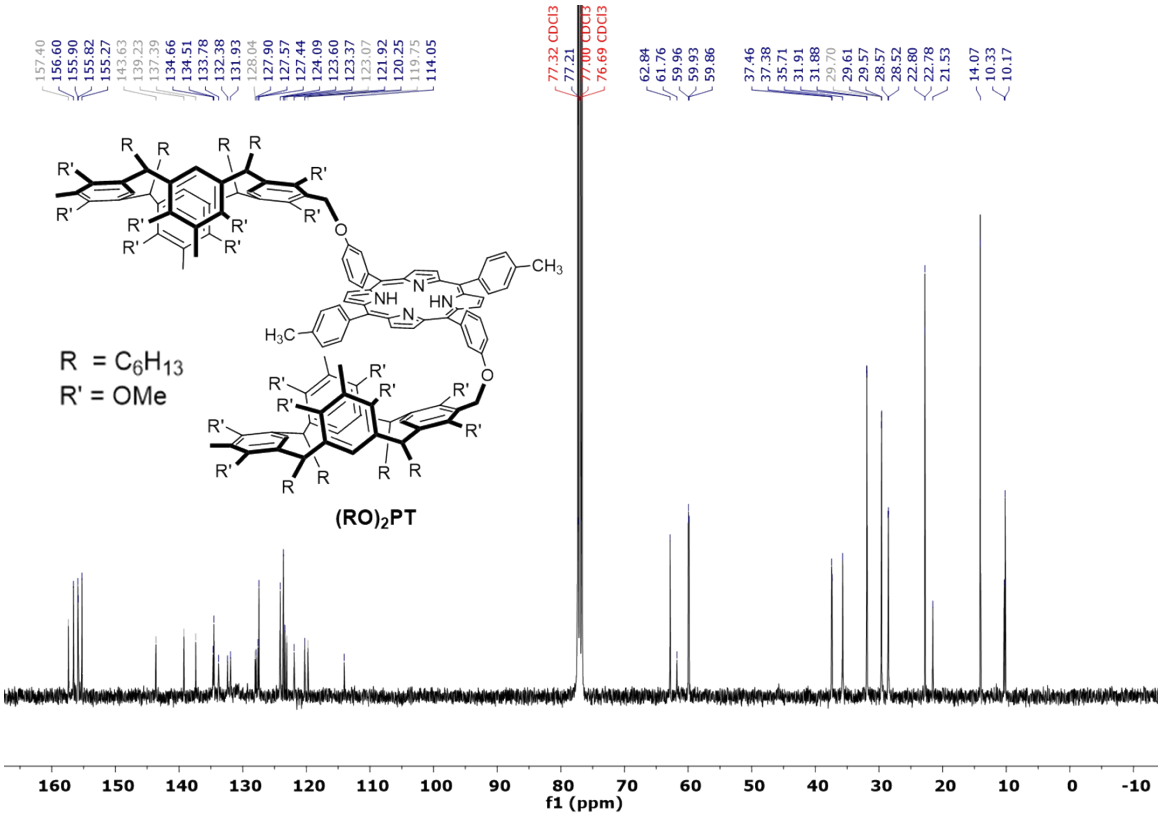


Fig.15S: ^{13}CNMR (150 MHz, $CDCl_3$) spectrum of $(RO)_2PT$.

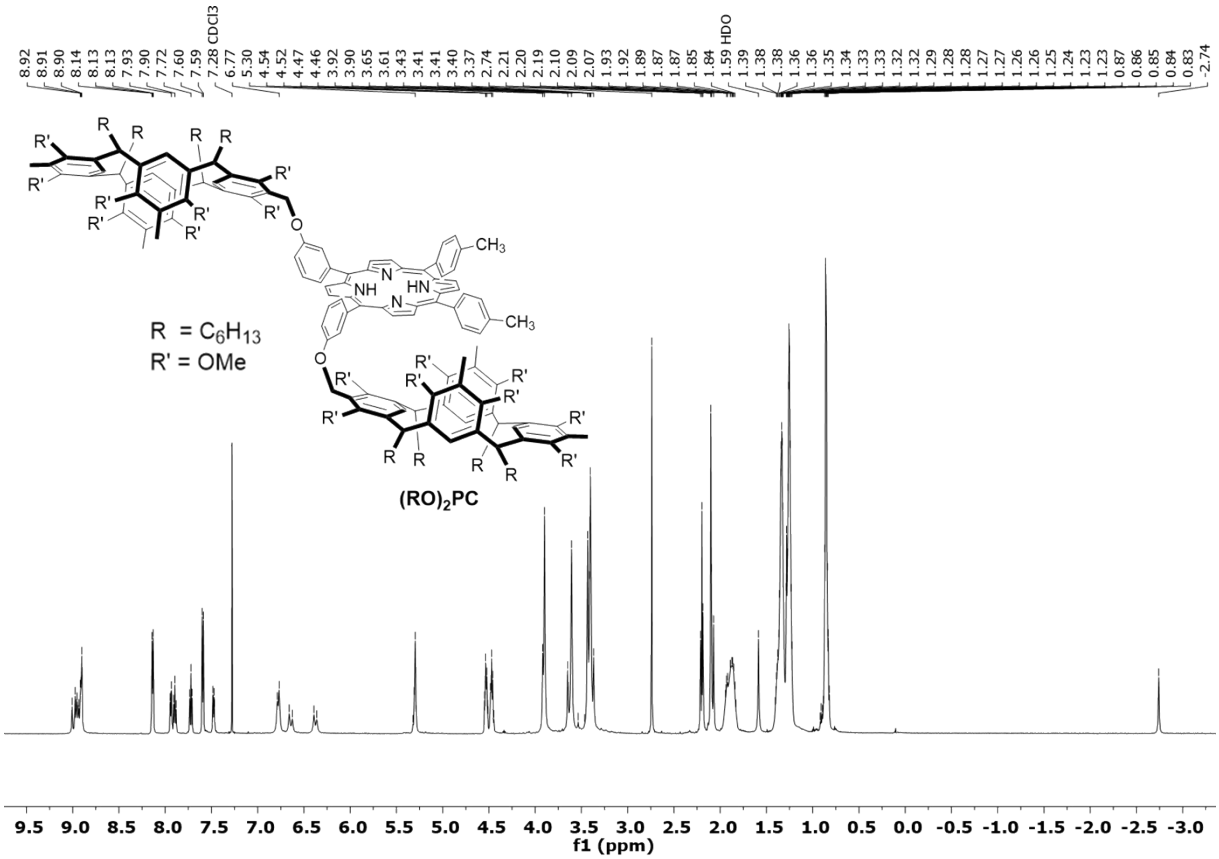


Fig.16S: ^{1}HNMR (600 MHz, $CDCl_3$) spectrum of $(RO)_2PC$.

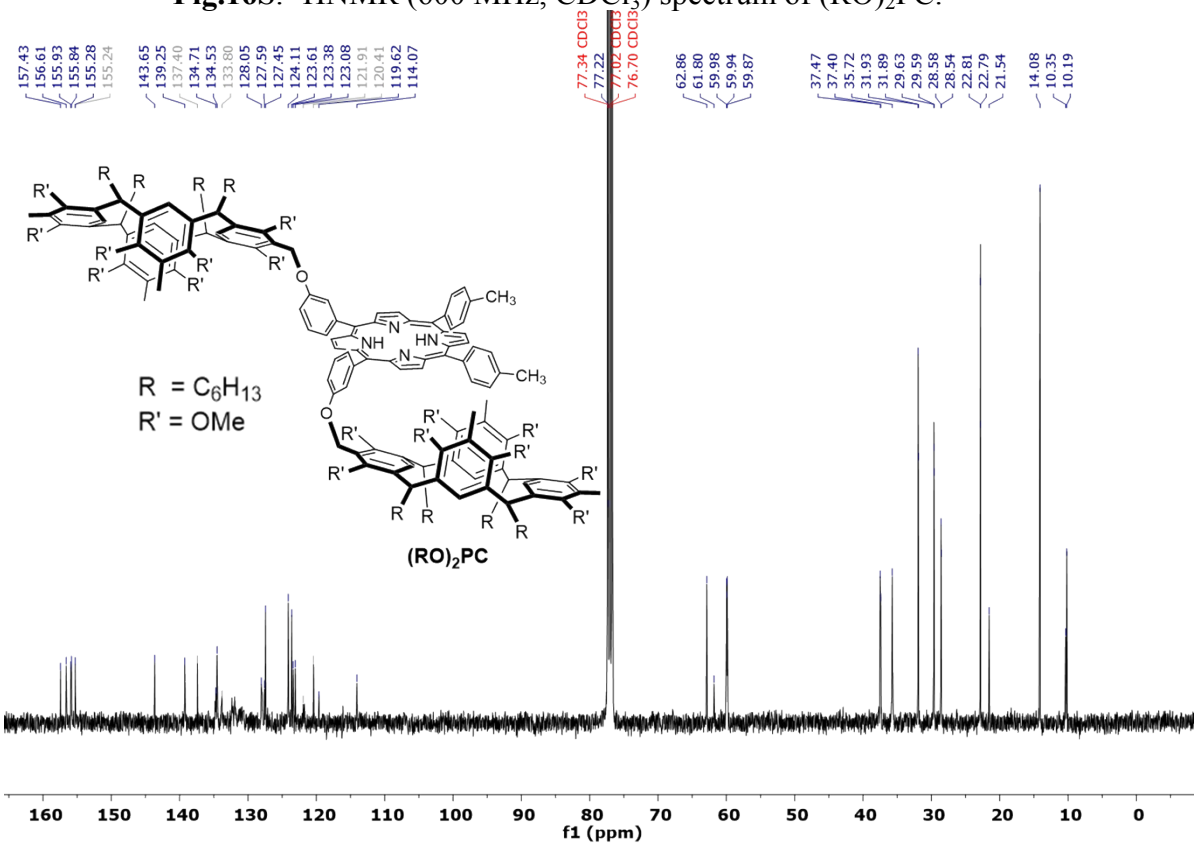


Fig.17S: ^{1}HNMR (600 MHz, $CDCl_3$) spectrum of $(RO)_2PC$.

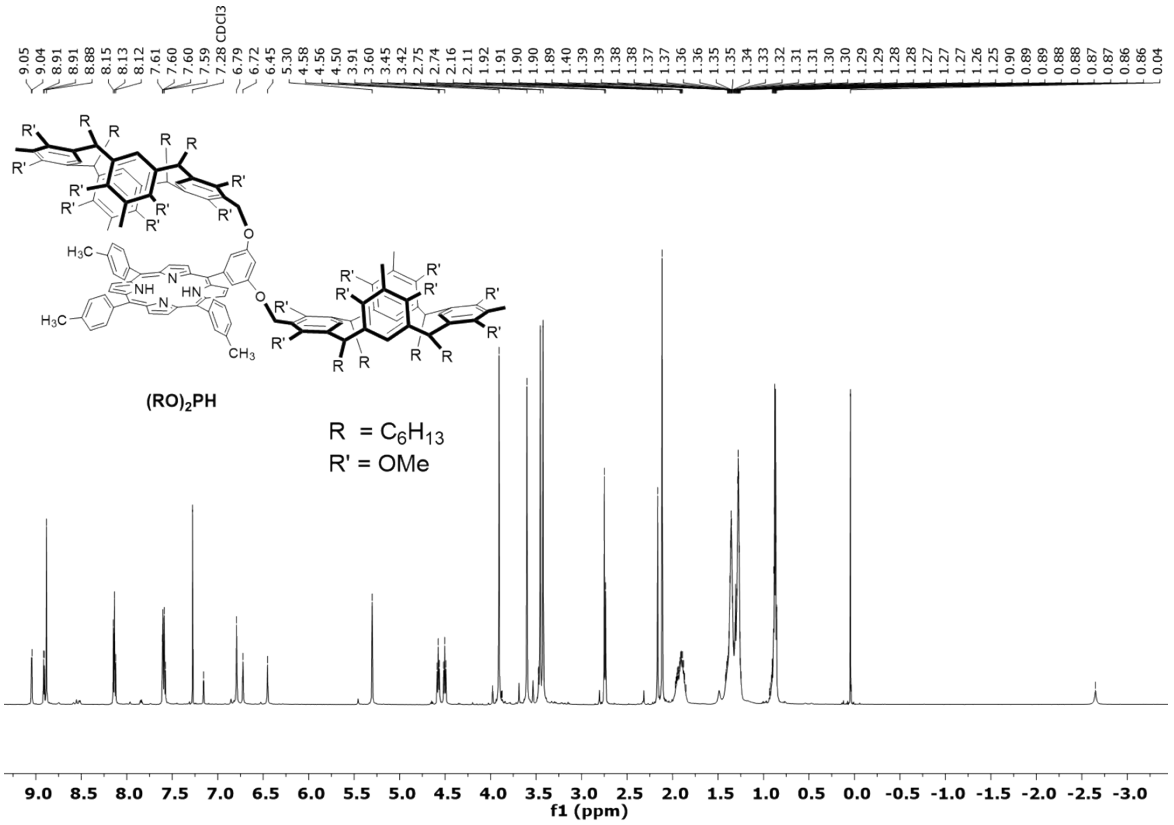


Fig.18S: ^{1}HNMR (600 MHz, $CDCl_3$) spectrum of $(RO)_2PH$.

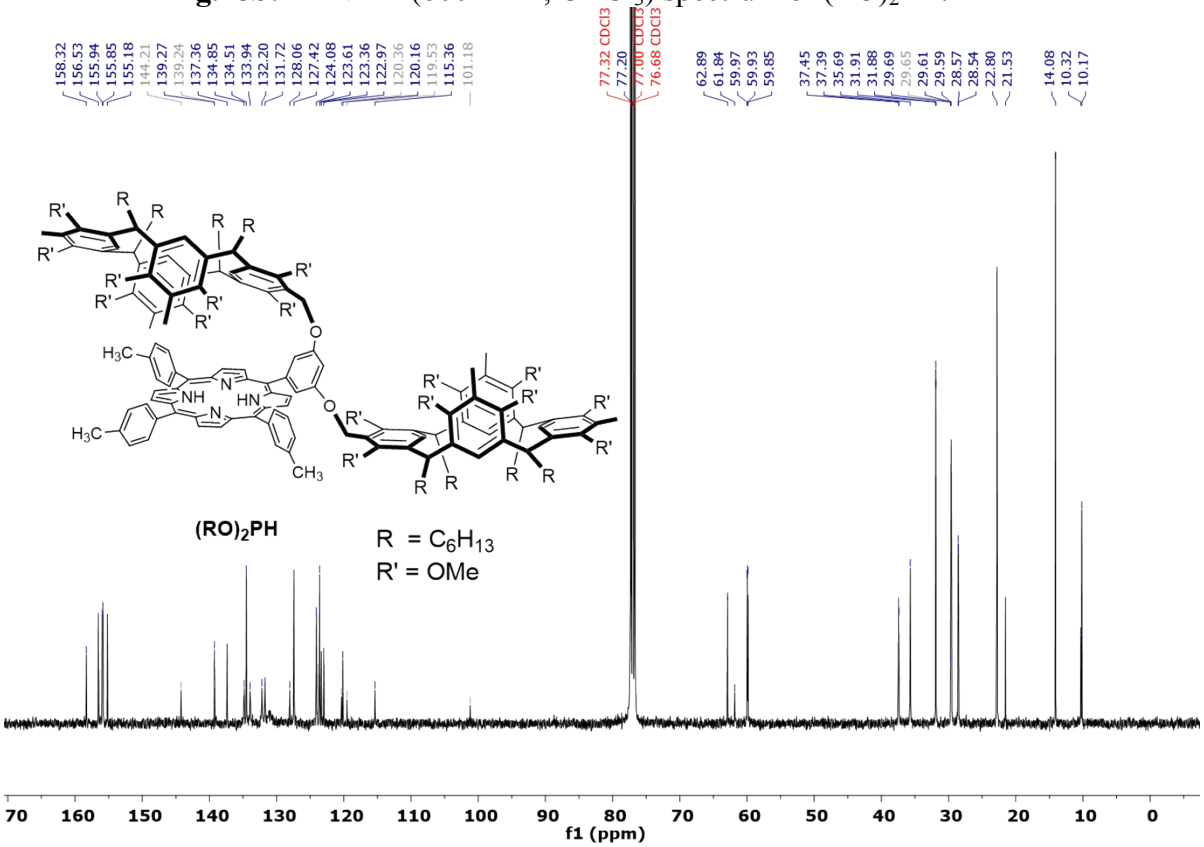


Fig.19S: ^{1}HNMR (600 MHz, $CDCl_3$) spectrum of $(RO)_2PH$.

Various temperatures ^{1}HNMR spectra of RO:

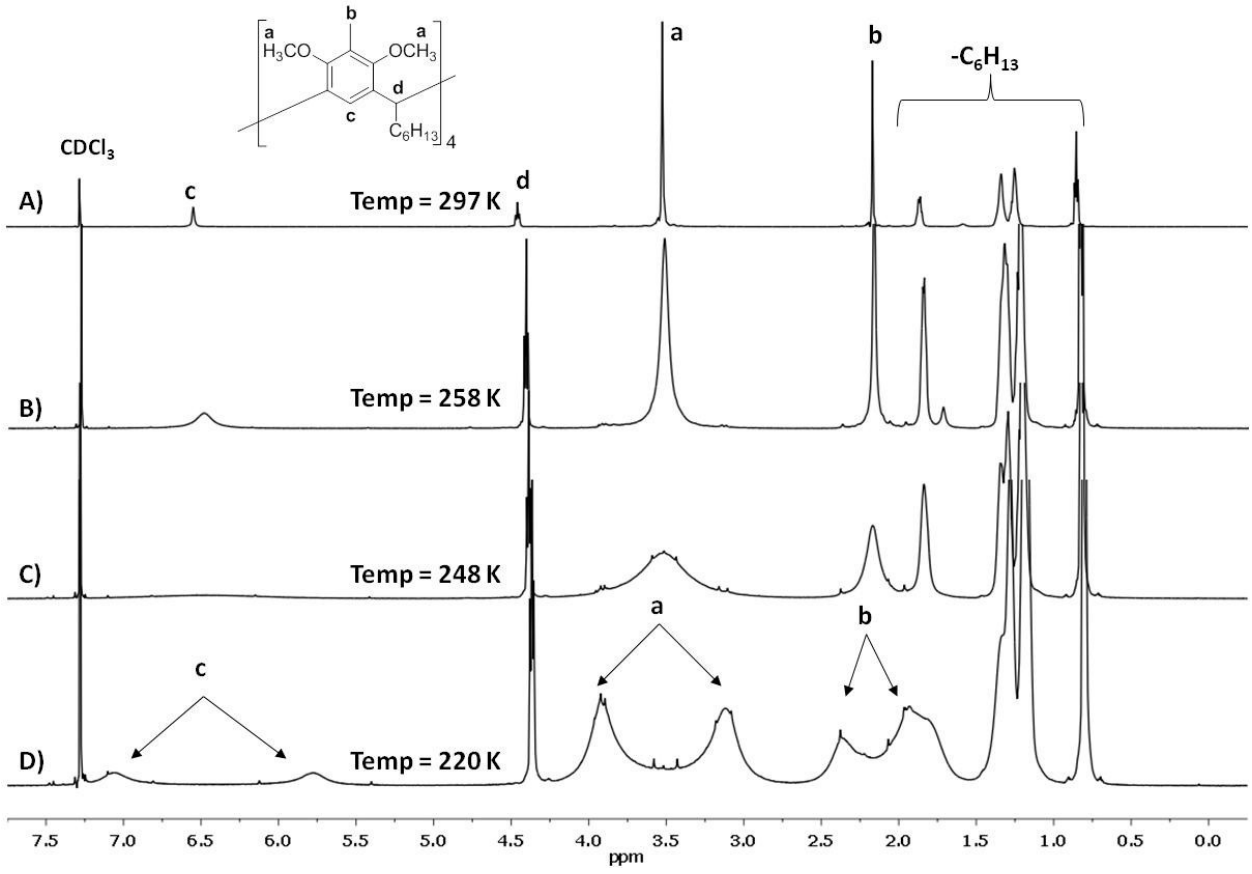


Fig. 20S: ^{1}HNMR (600MHz, $CDCl_3$) spectra of **RO** recorded at various temperatures.

References

1. T. F. Al-Azemi, M. Vinodh, Tetrahedron 2011, 67, 2585-2590.
2. SHELX97: G. M. Sheldrick, Acta Cryst. 2008, A64, 112-122.
3. CrystalStructure 4.0: Crystal Structure Analysis Package, Rigaku Corporation (2000-2010). Tokyo 196-8666, Japan.