Supplementary Material for Chemical Communications

SUPPLEMENTARY INFORMATION

Figure-Eight Aromatic Core-modified Octaphyrins With Six *meso* Links: Syntheses and Structural Characterization

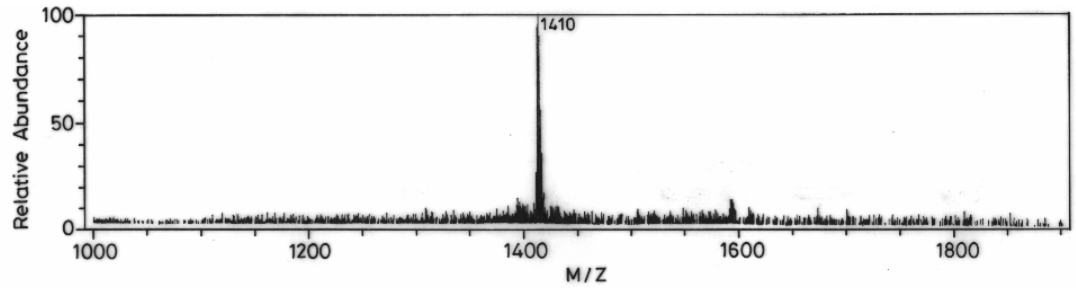
Harapriya Rath, Jeyaraman Sankar, Viswanathan PrabhuRaja, Tavarekere K. Chandrashekar* , Bhawani S. Joshi and Raja Roy

---

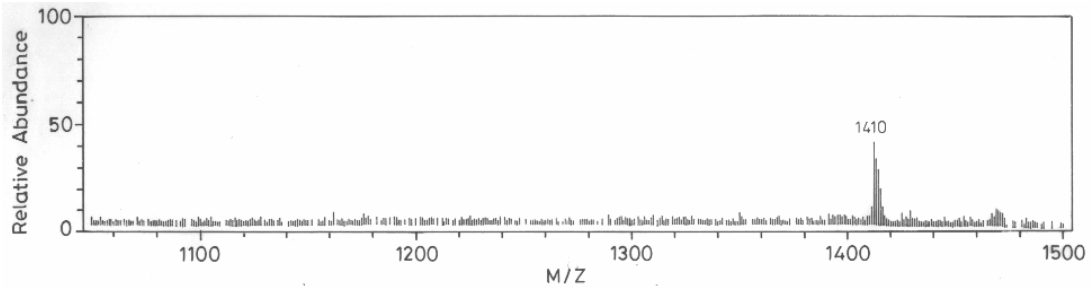
CONTENTS

Supplementary Material for Chemical Communications

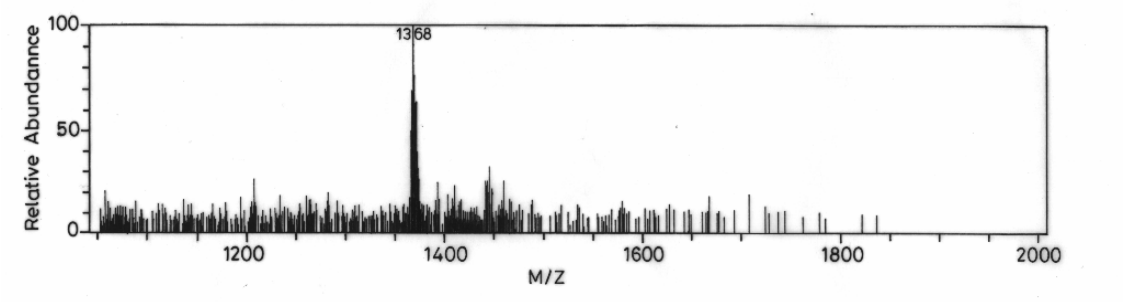
S1-A: FAB-MASS Spectrum of 5:



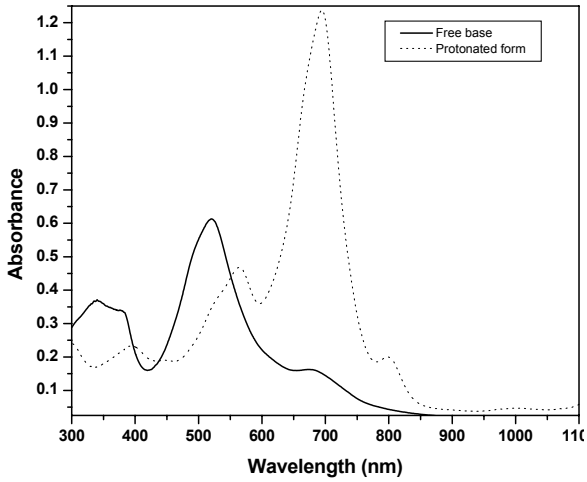
S1-B: FAB-MASS Spectrum of 6:



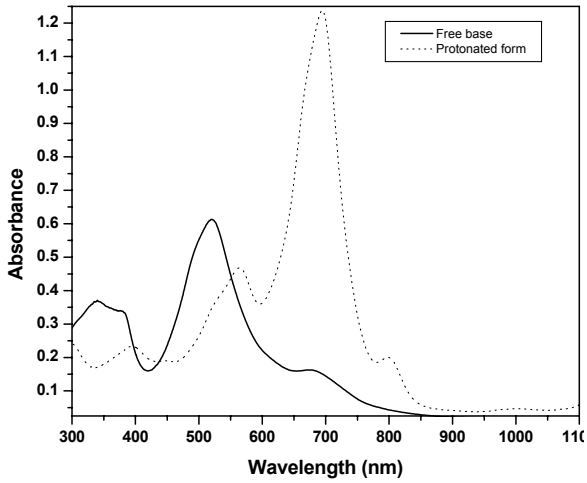
S1-C: FAB-MASS Spectrum of 7:



S2-A: UV - Vis Spectrum of 6:

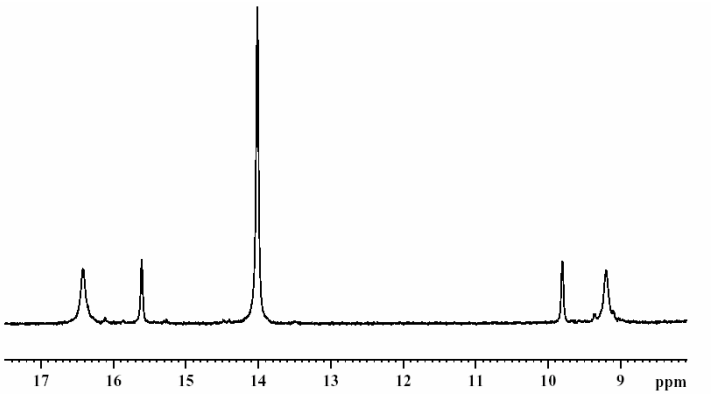


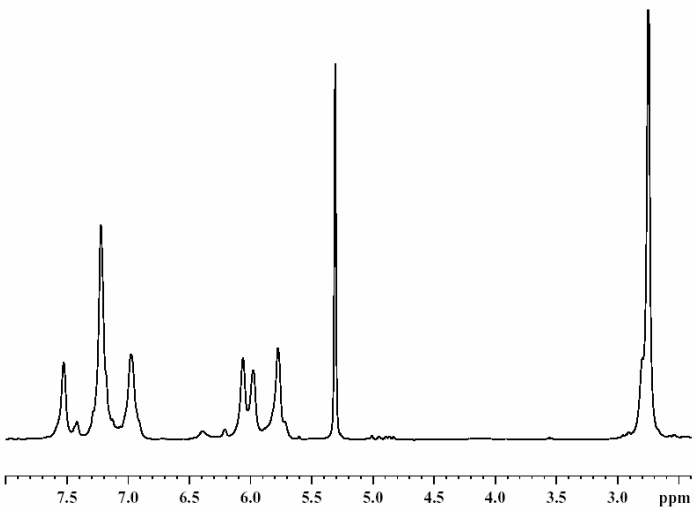
S2-B: UV - Vis Spectrum of 7



Supplementary Material for Chemical Communications

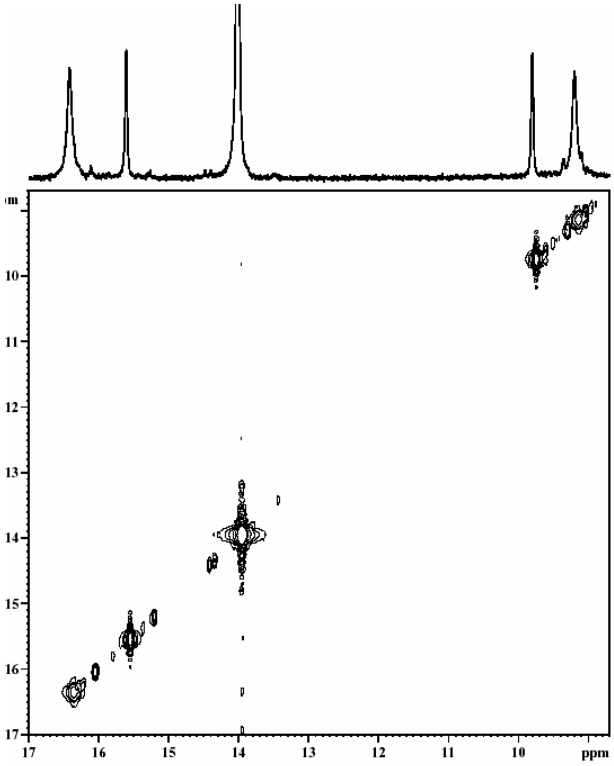
S3: ^{1}H NMR Spectra of 5:





Supplementary Material for Chemical Communications

^{1}H spectrum of free base 5 at 208K in CD_2Cl_2



^{1}H-^{1}H COSY spectrum of free base 5 at 208K in CD_2Cl_2

Supplementary Material for Chemical Communications

S4: Synthetic procedure: Macrocycle 5

In presence of acid catalyst:

In a typical procedure, modified tetrapyrrane **4** (0.6 g, 1.1 mmol) was reacted with pentafluoro benzaldehyde (0.14ml,1.1mmol) in dry dichloromethane (250 mL) and stirred under a nitrogen atmosphere in the absence of light for 15 min. *p*-Tolyl sulphonic acid (0.0452 g, 0.22 mmol)/ methane sulphonic acid (0.007ml, 0.11mmol) was added and stirring continued for 90 min. The reaction mixture was exposed to air, and chloranil (0.2925g, 1.1mmol) was added; the reaction mixture was refluxed for 90 min on a preheated oil bath. The solvent was removed under reduced pressure. Upon purification by column chromatography with alumina (basic, grade III), a pink band eluted with 2:3 dichloromethane/petroleum ether, which on solvent evaporation afforded **5** as a dark green solid [170 mg, 11%].

In absence of acid catalyst:

In a typical procedure, modified tetrapyrrane **4** (0.6 g, 1.1 mmol) was reacted with pentafluoro benzaldehyde (0.14ml,1.1mmol) in dry dichloromethane (10 mL) and stirred under a nitrogen atmosphere in the absence of light for 90 min. The reaction mixture was exposed to air, and DDQ (0.2497g, 1.1mmol) was added along with 2ml of dry toluene. The reaction mixture was allowed to stir for further 90 min. The solvent was removed under reduced pressure. Upon purification by column chromatography with alumina (basic, grade III), a pink band eluted with 2:3 dichloromethane/petroleum ether, which on solvent evaporation afforded **5** as a dark green solid [77 mg, 5%].

Supplementary Material for Chemical Communications