Supplementary Material (ESI) for Chemical Communications

Electronic Supplementary Information 3

A Facile and Versatile Preparation of Bilindiones and Biladienones from Tetraarylporphyrins

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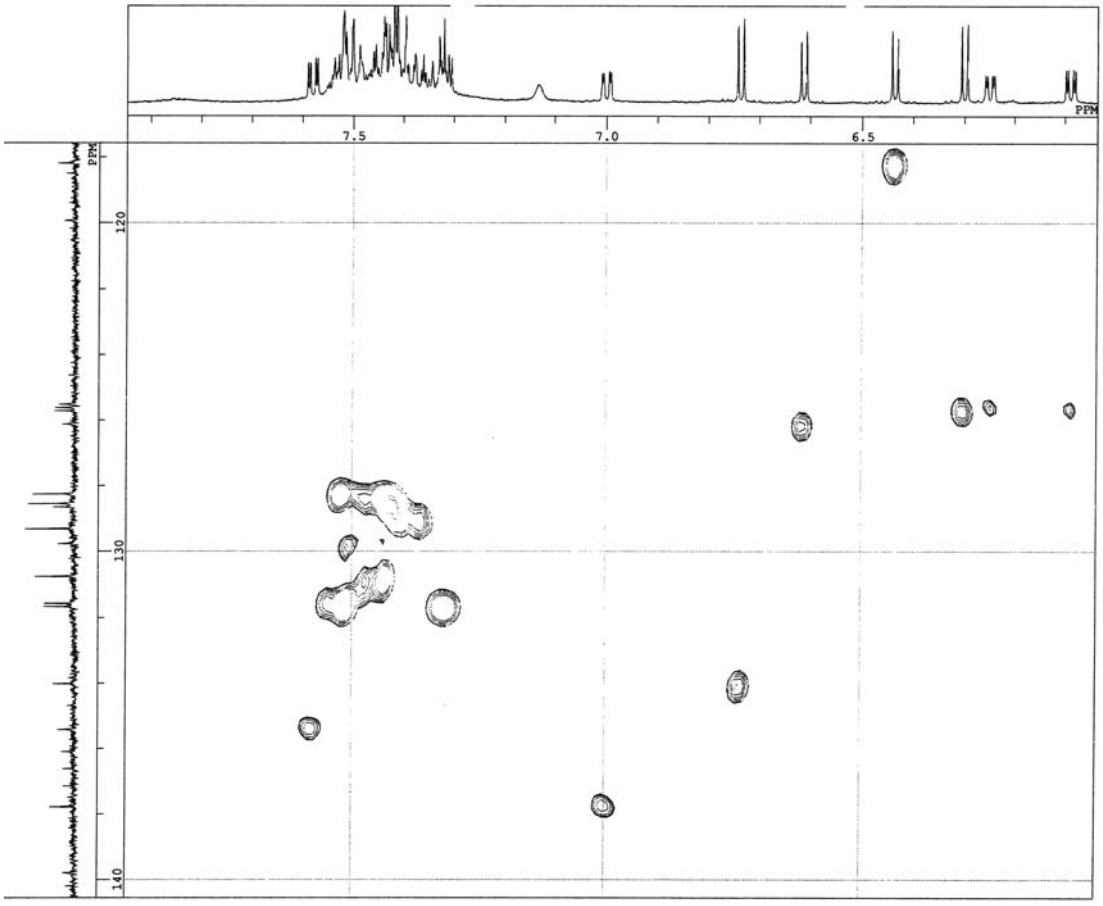

Figure S12. NOESY of **4** (CD_2Cl_2). HMQC of **4** (CD_2Cl_2)

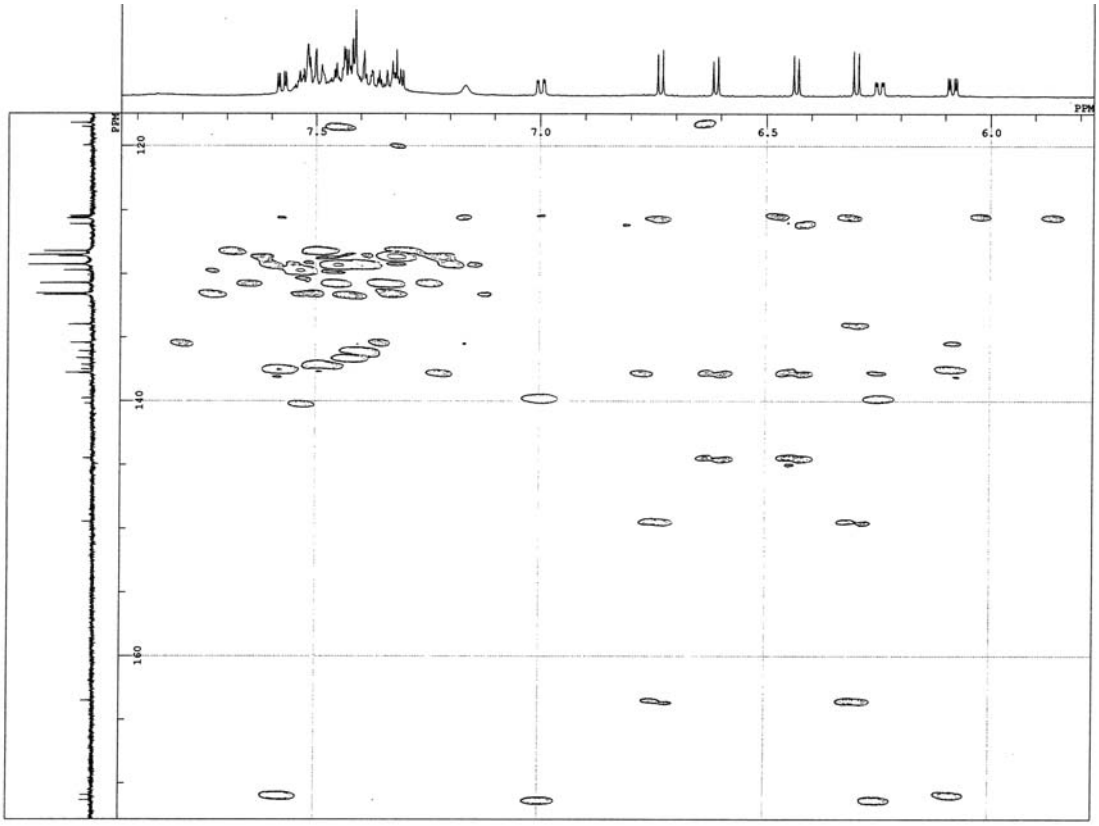

Figure S13. HMBC of **4** (CD_2Cl_2). H-2 and H-3 showed correlation with a carbonyl resonance at 170.9 ppm. Therefore a signal at 170.9 ppm can be assigned to C-1.

H-17 and H-18 showed correlation with a carbonyl resonance at 171.3 ppm. Therefore a signal at 171.3 ppm can be assigned to C-19.

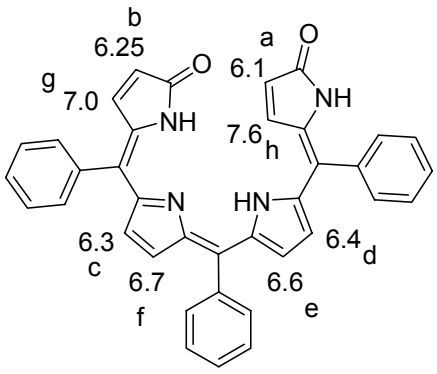

Table S3. β-protons and NH protons in the ^{1}H NMR spectra of **3** and **4**

Protons	δ, ppm (multiplicity)		
	3	**4**	$\Delta\delta$ (**3** – **4**)
H-2	6.21 (d)	6.09 (dd)	+0.12
H-3	7.00 (d)	7.58 (dd)	-0.58
H-7	6.51 (d)	6.43 (d)	+0.08
H-8	6.75 (d)	6.61 (d)	+0.14
H-12	6.75 (d)	6.74 (d)	+0.01
H-13	6.51 (d)	6.30 (d)	+0.21
H-17	7.00 (d)	7.00 (dd)	0.00
H-18	6.21 (d)	6.25 (dd)	-0.04
NH (A)	8.14	7.10	+1.04
NH (D)	8.14	9.11	-0.97
		(NOE with H-3)	
NH (B+C)	12.0	12.35	-0.35

Table S4. C-13 signals assigned by HMQC of **3** and **4**

Protons	δ, ppm (multiplicity)		
	3	**4**	$\Delta\delta$ (**3** – **4**)
C-1	171.4	171.3	+0.1
C-2	124.4	125.6	-1.2
C-3	138.2	135.4	+2.8
C-4	138.9	137.5	+1.4
C-6	153.8	144.5	+9.3
C-7	121.8	118.2	+3.6
C-8	130.3	126.1	+4.2
C-9	143.7	137.8	+5.9
C-11	143.7	149.5	-5.8
C-12	130.3	134.0	-3.7
C-13	121.8	125.7	-3.9
C-14	153.8	163.5	-9.7
C-16	138.9	139.8	-0.9
C-17	138.2	137.8	+0.4
C-18	124.4	125.5	-1.1
C-19	171.4	170.9	+0.5

C-5, C-10 and C-15 carbons were not assigned since no correlation was observed for these signals in the HMBC spectrum.

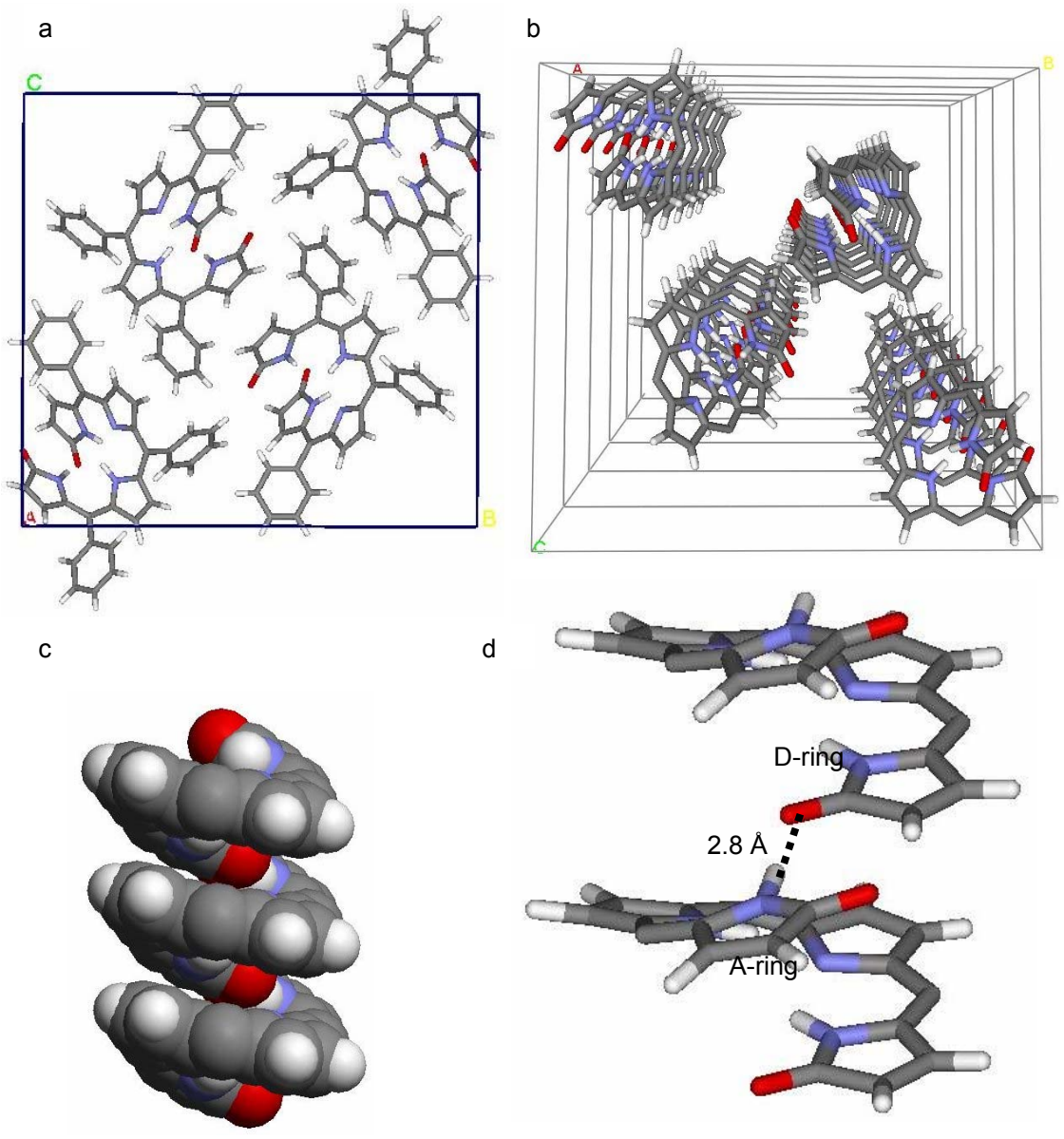

Figure S14. (a) Unit cell packing for **3**. The view is drawn looking down the *a*-axis. (b) Perspective view of **3** along the *a*-axis. (c) Structure of spiral column made up of helical molecule. (d) A dotted line indicates the intermolecular hydrogen bond. The distance between the nitrogen atom of the A ring and the oxygen atom of the carbonyl group of the D ring of the adjacent molecule is 2.8 Å. Except for (a), the phenyl groups are omitted for clarity.

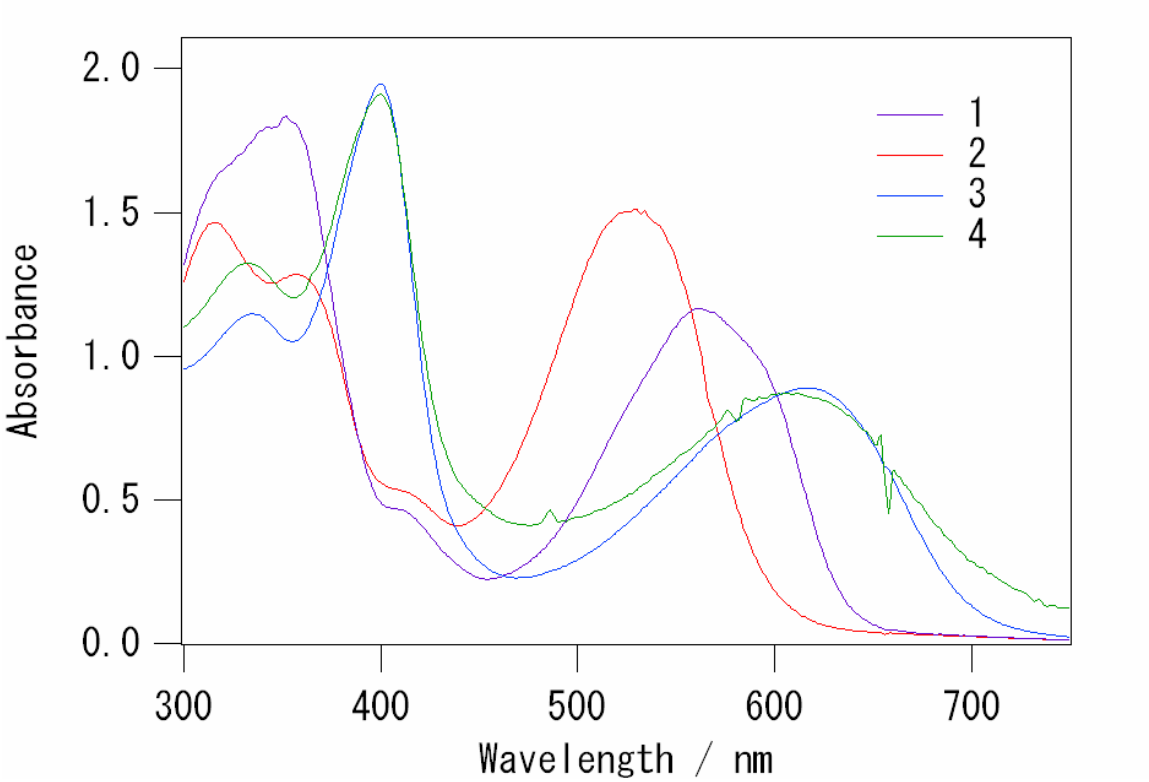

Figure S15. UV-visible absorption spectra of **1-4** in $CHCl_3$.