

## Supporting Information

# Oxygen Bridged Neutral Annulenes: A Novel Class of Materials for Organic Field-Effect Transistors

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**Cif files of 12a and 12b**

## General Information

$^1\text{H}$  (400 MHz),  $^{13}\text{C}$  (100 MHz) NMR spectra were recorded on a BRUKER AVANCE II 400 NMR Spectrometer and UNITY INOVA-400MHz NMR Spectrometer. Tetramethylsilane (TMS) served as the internal standard (0 ppm for  $^1\text{H}$  and 77.0 ppm for  $^{13}\text{C}$ ) and  $\text{CDCl}_3$  was used as solvent. The following abbreviations were used to express the multiplicities: s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet; br = broad. Data are reported as follows: chemical shifts in ppm ( $\delta$ ), integration, coupling constant J (Hz) and assignment. Mass spectra were recorded on Bruker Daltonics esquire3000\_00037 mass spectrometer and an UPLC-Q-TOF instrument, having SYNAPT mass spectrometer and ACQUITY high performance liquid chromatography (WATERS) with a TDA detector. Elemental analyses were performed with a Thermoelectron FLASH EA1112 CHNS analyzer and were within  $\pm 0.4\%$  of the theoretical values. IR spectrum was recorded on VARIAN 660-IR Fourier-Transform Spectrophotometer in range 400-4000  $\text{cm}^{-1}$  using KBr as medium. UV-Vis spectra were recorded on a SHIMADZU 1601 PC spectrophotometer, with a quartz cuvette (path length, 1 cm) and studies were performed in AR grade DCM. TGA were performed on a SDT Q600 TA instrument with a temp. rise of  $10^\circ\text{C}/\text{minute}$  under nitrogen atmosphere. Electrochemical studies were carried out on CHI 660C Electrochemical Workstation with a conventional three-electrode configuration consisting of platinum working electrode (2 mm diameter), counter electrode and Ag/AgCl as reference electrode. The experiments were carried out on  $10^{-4}\text{M}$  solutions of samples in DCM containing 0.1 M tetrabutylammonium hexafluorophosphate ( $\text{TBAPF}_6$ ) as supporting electrolyte at room temperature. Deoxygenation of the solutions was achieved by bubbling nitrogen for 30 min and the working electrode was cleaned after each run. The cyclic voltammograms were recorded with a scan rate of  $100\text{ mVs}^{-1}$ . All reactions were monitored by thin-layer chromatography carried out on Merck pre-coated TLC plates (silica gel 60 F<sub>254</sub>, 0.25 mm), visualization by using UV (254 nm). Melting points were determined in open capillaries and are uncorrected. Reactions that required anhydrous conditions were carried out under the blanket of deoxygenated (BASF catalyst) anhydrous nitrogen gas in oven/flame dried glassware. The products were purified by flash column chromatography on silica gel 60-120 mesh. All reagents and chemicals were purchased from Sigma-Aldrich. DMF, 1,2-DCE,  $\text{TiCl}_4$ , Pyridine and DCM were purchased locally, dried and distilled prior to use.  $\text{POCl}_3$  was distilled at constant b.p. prior to use. THF and toluene were distilled from sodium/benzophenone (benzophenone ketyl). Anhydrous DCM was stored over fused  $\text{CaCl}_2$  and distilled before use. Zinc dust was activated prior to use using standard (2M HCl and subsequent water washing) methods. DDQ and hydrazine hydrate were purchased from Sigma-Aldrich, and were used as received. All theoretical studies were performed with a GAUSSIAN 09 software package. *Meso*-substituted bisfuran-2-yl methanes were prepared according to literature procedure,<sup>[1]</sup> but by taking the corresponding new aldehydes.

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[1] Tanaka, S.; Tomokuni, H.; J. Heterocyclic Chem., 1991, 28, 991-994.

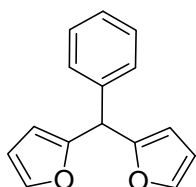
## Experimental Section

The *meso*-phenyl and *meso-p*-tolyl substituted bisfuran-2-ylmethane derivatives (**9**)s were synthesized according to the literature procedure<sup>1</sup>.

### General procedure for the synthesis of the dialdehydes **10a** and **10b**

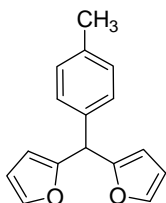
POCl<sub>3</sub> (4.9 g, 32 mmol) was added slowly to N,N'-dimethylformamide (2.6g, 35.6 mmol) maintained below 20°C. To this solution, *meso*-phenyl-2,2'-difurylmethane **9a** (3g, 13.4 mmol) in dry ethylene dichloride (30 ml) was added with stirring over 20 minutes, maintaining the temperature below 20°C. The mixture was left at r.t. for 3 hours, refluxed for 1 hour, cooled and added to a solution of sodium acetate (81 g) in water (120 ml). The mixture was refluxed for 15 minutes, cooled and extracted thoroughly with ethyl acetate. The combined ethyl acetate layers were washed with saturated aqueous sodium bicarbonate solution and then with water. The extract was dried over anhydrous sodium sulfate. The concentrated solution was then chromatographed on silica and the dialdehyde **10a** was isolated as thick red oil (1.6g, 43%). Dialdehyde **10b** was analogously prepared (42%) from *meso-p*-tolyl-2,2'-difurylmethane **9b**.

The characteristic data for **9a**, **9b**, **10a** and **10b** is presented below.



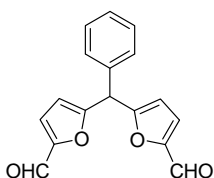
### Phenyl-di(furan-2-yl)methane, **9a**

(Yield = 15%), <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.29-7.35 (4H, m), 7.21-7.27 (3H, m), 6.30-6.31 (2H, m), 6.01-6.02 (2H, m), 5.44 (1H, s); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 154.4, 142.0, 139.4, 128.6, 128.4, 127.2, 110.3, 107.6, 45.0; Anal. Calcd. (%) for C<sub>15</sub>H<sub>12</sub>O<sub>2</sub>: C, 80.35; H, 5.35; Found: C, 80.52; H, 5.42; *m/z* 247 (M<sup>+</sup> + 23).



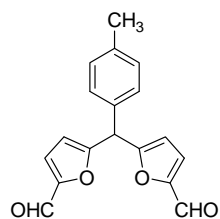
### *p*-Tolyl-di(furan-2-yl)methane, **9b**

(Yield = 16%), <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.31-7.32 (2H, m), 7.08-7.13 (4H, m), 6.26-6.27 (2H, m), 5.99-6.00 (2H, m), 5.40 (1H, s), 2.29 (3H, s); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 154.7, 142.0, 136.9, 129.4, 128.3, 110.4, 107.5, 44.8, 21.2; Anal. Calcd. (%) for C<sub>16</sub>H<sub>14</sub>O<sub>2</sub>: C, 80.67; H, 5.88; Found: C, 81.02; H, 6.11; *m/z* 262 (M<sup>+</sup> + 23).



### Phenyl-di(5-formylfuran-2-yl)methane, **10a**

(Yield = 43%), <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) 9.58 (2H, s), 7.32-7.39 (3H, m), 7.26-7.28 (2H, m), 7.20 (2H, d, J=3.6 Hz), 6.32 (2H, d, J=3.24 Hz), 5.61 (1H, s); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) 177.5, 159.2, 152.6, 136.5, 129.1, 128.8, 128.3, 128.2, 122.2, 111.3, 45.5; UPLC-Q-TOF MS 279 (M<sup>+</sup>, 100%).



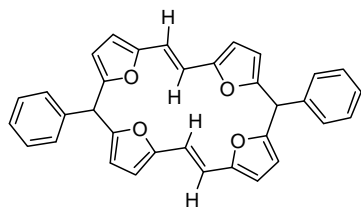
***p*-Tolyl-di(5-formylfuran-2-yl)methane, **10b****

(Yield = 42%),  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) 9.57 (2H, s), 7.19 (2H, d,  $J=3.64$  Hz), 7.16 (4H, s), 6.31 (2H, d,  $J=3.2$ Hz), 5.56 (1H, s), 2.34 (3H, s);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) 177.5, 159.5, 152.6, 138, 133.5, 129.7, 128.2, 122.2, 111.2, 45.2, 21.1; UPLC-Q-TOF MS 293 ( $\text{M}^-$ , 100%).

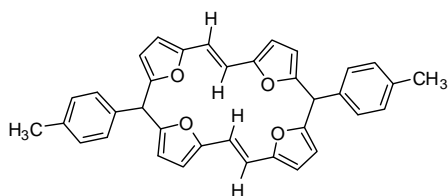
**General procedure for the synthesis of the *meso*-substituted dihydrotetraoxa annulenes **11a** and **11b****

To a stirring suspension of zinc dust (2.4 g, 38 mmol) in 200 ml of THF maintained under nitrogen atmosphere, a solution of 19.6 ml of 1.0 M  $\text{TiCl}_4$  (in  $\text{CH}_2\text{Cl}_2$ ) was added over 20 minutes. The reaction mixture was refluxed for 1 hour, and treated with a solution of dialdehyde **10a** (0.5 g, 1.78 mmol) and pyridine (2.8 g, 35.6 mmol) dissolved in 200 ml of THF. The addition was made using a hypodermic syringe over 40 minutes to the gently refluxing suspension. After refluxing under nitrogen for 18 hours, the reaction was carefully quenched with a solution of aqueous  $\text{K}_2\text{CO}_3$  (10%, 100 ml). The reaction mixture was filtered, and the filtrate was concentrated under reduced pressure and the residue extracted with 300 ml methylene chloride. The extract was washed with water (2 x 50 ml) and dried over anhydrous sodium sulfate. The solvent was evaporated under reduced pressure and the residue was chromatographed (over silica) to isolate the **11a** (67 mg, 15%), m.p.  $>250^\circ\text{C}$ .

Using dialdehyde **10b**, dihydrotetraoxaannulene **11b** was analogously prepared in 13% yield. The characteristic data for **11a** and **11b** is presented below.



**Meso-Phenyldihydrotetraoxa[22]annulene[2,1,2,1] **11a****, (Yield =15%),  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) 7.29-7.44 (10H, m), 7.07 (4H, s), 6.21 (4H, d,  $J=3.2$  Hz), 5.97 (4H, d,  $J=3.2$  Hz), 5.32 (2H, s);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) 153.1, 152.9, 138.3, 128.8, 128.6, 127.5, 116, 109, 106.4, 45; IR (KBr):724, 782, 960, 1014, 1274, 1447, 1500, 1586, 2854, 3021, 3117  $\text{cm}^{-1}$ ; UPLC-Q-TOF MS: 494, 495, 496.

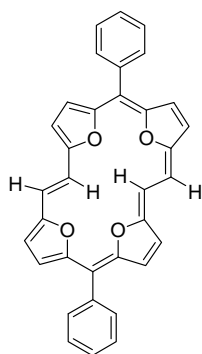


**meso-p-Tolyldihydrotetraoxa[22]annulene[2,1,2,1] **11b****, (Yield = 13%),  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) 7.27-7.31 (4H, m), 7.15-7.18 (4H, m), 7.05 (4H, d,  $J= 4.04$  Hz), 6.20 (4H, d,  $J= 3.2$  Hz), 6.03 (2H, d,  $J= 3.28$  Hz), 5.96 (2H, d,  $J= 3$  Hz), 5.28 (2H, d,  $J= 4.88$  Hz), 2.36 (6H, s);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) 153.3, 153.2, 152.9, 152.8, 137.1, 129.3, 128.6, 128.3, 115.9, 108.9, 106.3, 44.6, 44.4, 21.1; IR (KBr):764, 953, 1012, 1275, 1450, 1500, 1571, 2917, 3010, 3100  $\text{cm}^{-1}$ ; UPLC-Q-TOF MS: 522, 523, 524.

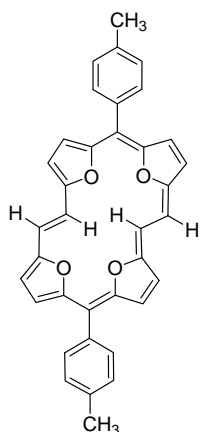
**General procedure for the synthesis of the *meso*-substituted tetraoxa[22]annulenes **12a** and **12b**:**

To a solution of **11a** (0.1g, 0.2 mmol) in 5 ml toluene, was added under nitrogen with stirring, a solution of DDQ (0.114 g, 0.5 mmol) in 5 ml toluene. Shortly after mixing the two solutions, purple precipitates formed and the reaction mixture was stirred for additional 3 h. The purple precipitates were filtered and added to 3 ml of hydrazine hydrate (98%). After boiling for 10 minutes, the solid was filtered, washed with water, and dried. The resulting product was dissolved in methylene chloride and chromatographed on silica (DCM). Evaporation of the purple solution gave 0.06 g (60%) of shining metallic purple **12a** (m.pt. >280 °C).

Using the same procedure, **11b** was oxidized to corresponding **12b** in 42% yield. The characteristic data for **12a** and **12b** is presented below.



**meso-Phenyltetraoxa[22]annulene[2,1,2,1] 12a**, (Yield = 60%),  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ) 10.47 (2H, d,  $J = 14.84$  Hz), 9.72 (2H, d,  $J = 4.32$  Hz), 9.12 (2H, d,  $J = 4.28$  Hz), 9.09 (2H, d,  $J = 4.24$  Hz), 9.01 (2H, d,  $J = 4.24$  Hz), 8.39 (4H, d,  $J = 6.88$  Hz), 7.84 (4H, t,  $J = 7.5$  Hz), 7.75 (2H, t,  $J = 7.52$  Hz), -5.42 (2H, d,  $J = 14.88$  Hz); IR (KBr): 779, 1175, 1299, 1654, 3100  $\text{cm}^{-1}$ ; Anal. Calcd. (%) for  $\text{C}_{34}\text{H}_{22}\text{O}_4$ : C, 82.59; H, 4.45; Found: C, 82.29; H, 4.26; UPLC-Q-TOF MS: 494 (100%).



**Meso-p-Tolyltetraoxa[22]annulene[2,1,2,1] 12b**, (Yield = 42%),  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ) 10.45 (2H, d,  $J = 15.0$  Hz), 9.67 (2H, d,  $J = 5.0$  Hz), 9.10 (4H, m), 8.98 (2H, d,  $J = 5.0$  Hz), 8.27 (4H, d,  $J = 6.80$  Hz), 7.64 (4H, d,  $J = 7.2$  Hz), 2.69 (6H, s), -5.40 (2H, d,  $J = 15$  Hz); IR (KBr): 779, 1176, 1301, 1645, 3100  $\text{cm}^{-1}$ ; Anal. Calcd. (%) for  $\text{C}_{36}\text{H}_{26}\text{O}_4$ : C, 82.76; H, 4.98; Found: C, 82.41; H, 4.99; UPLC-Q-TOF MS: 522 (100%).

Copies of  $^1\text{H}$ ,  $^{13}\text{C}$  NMR, IR and Mass Spectra

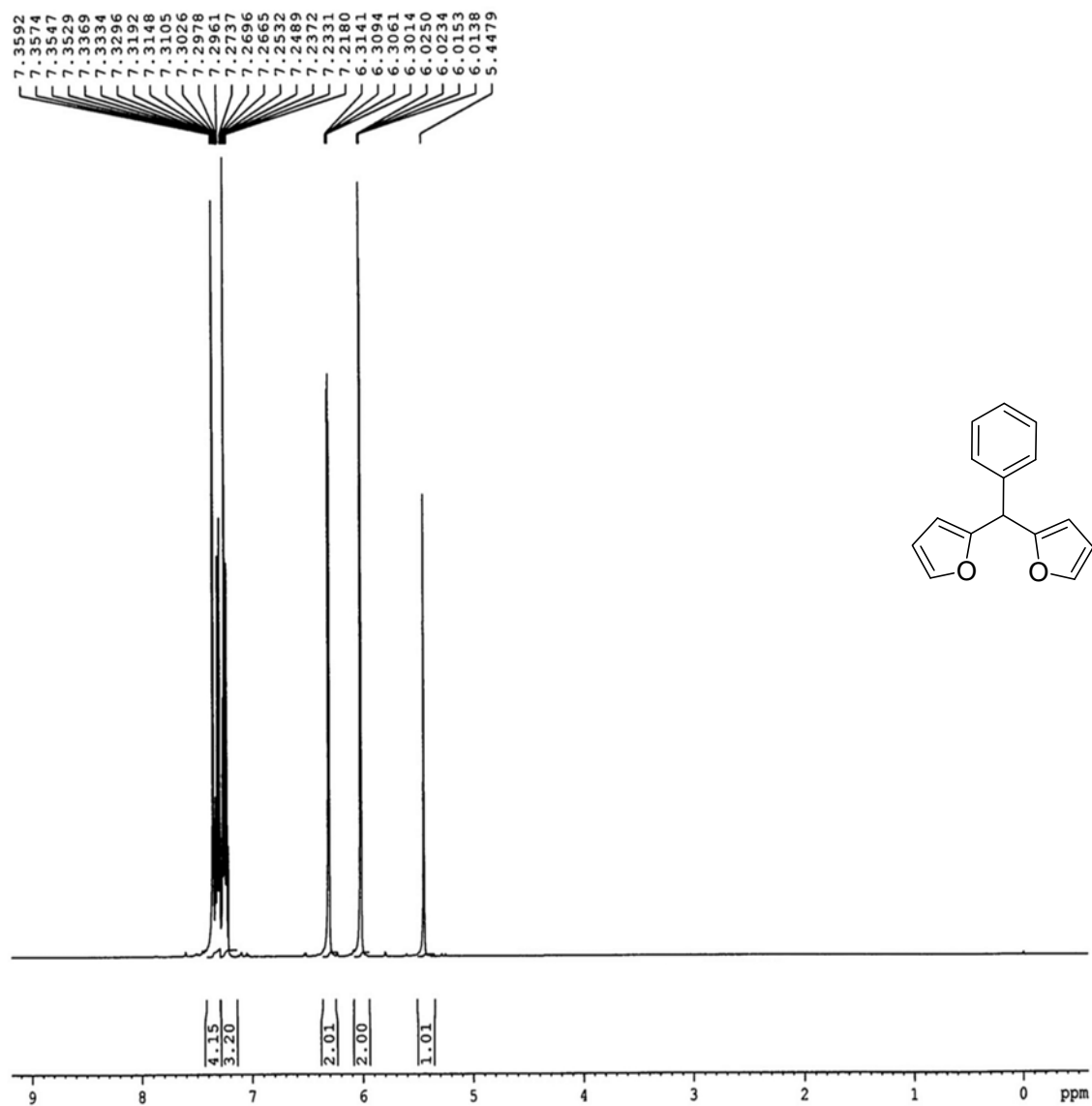


Figure S1 :  $^1\text{H}$  NMR spectrum of 9a.

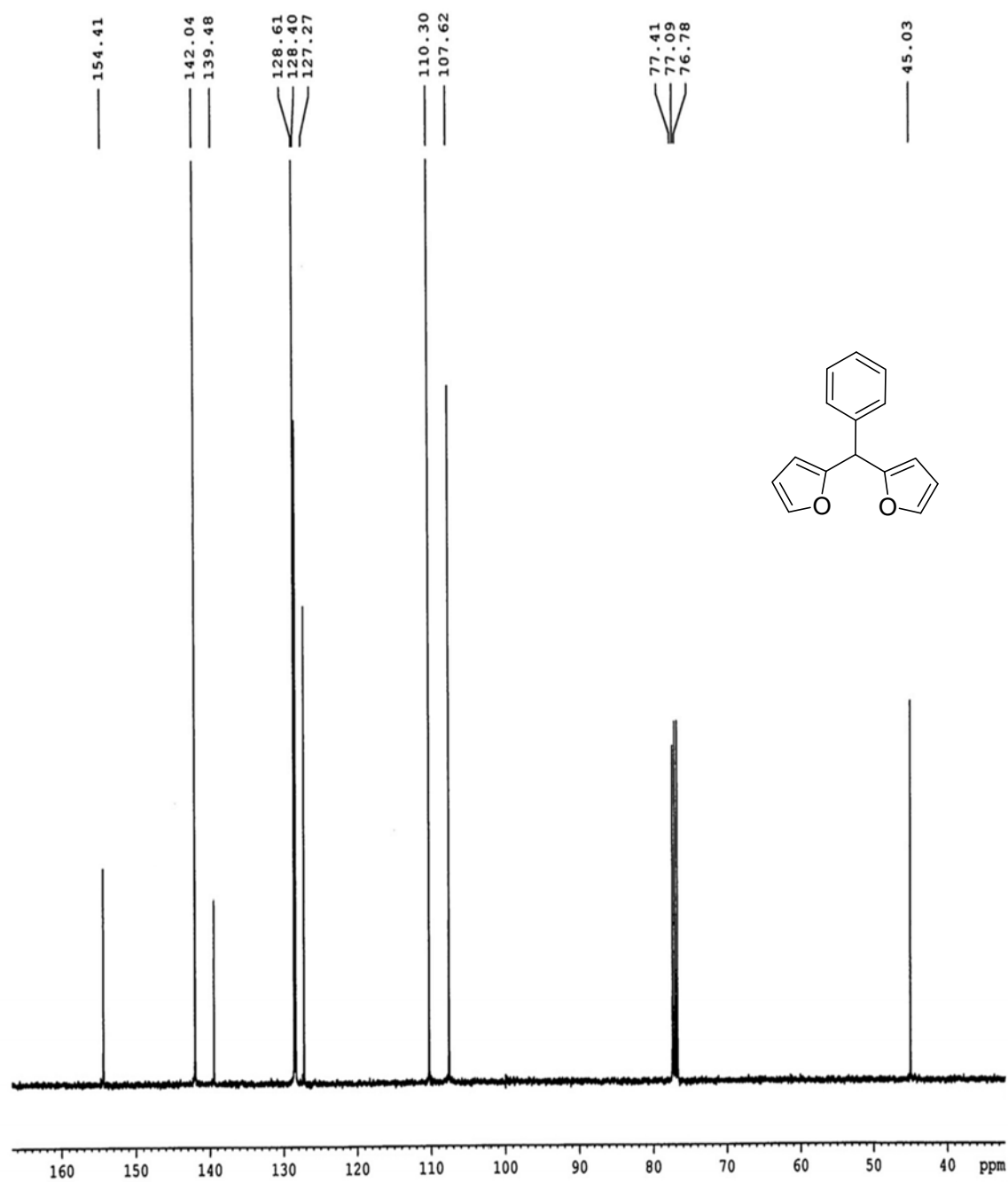


Figure S2:  $^{13}\text{C}$  NMR spectrum of **9a**.

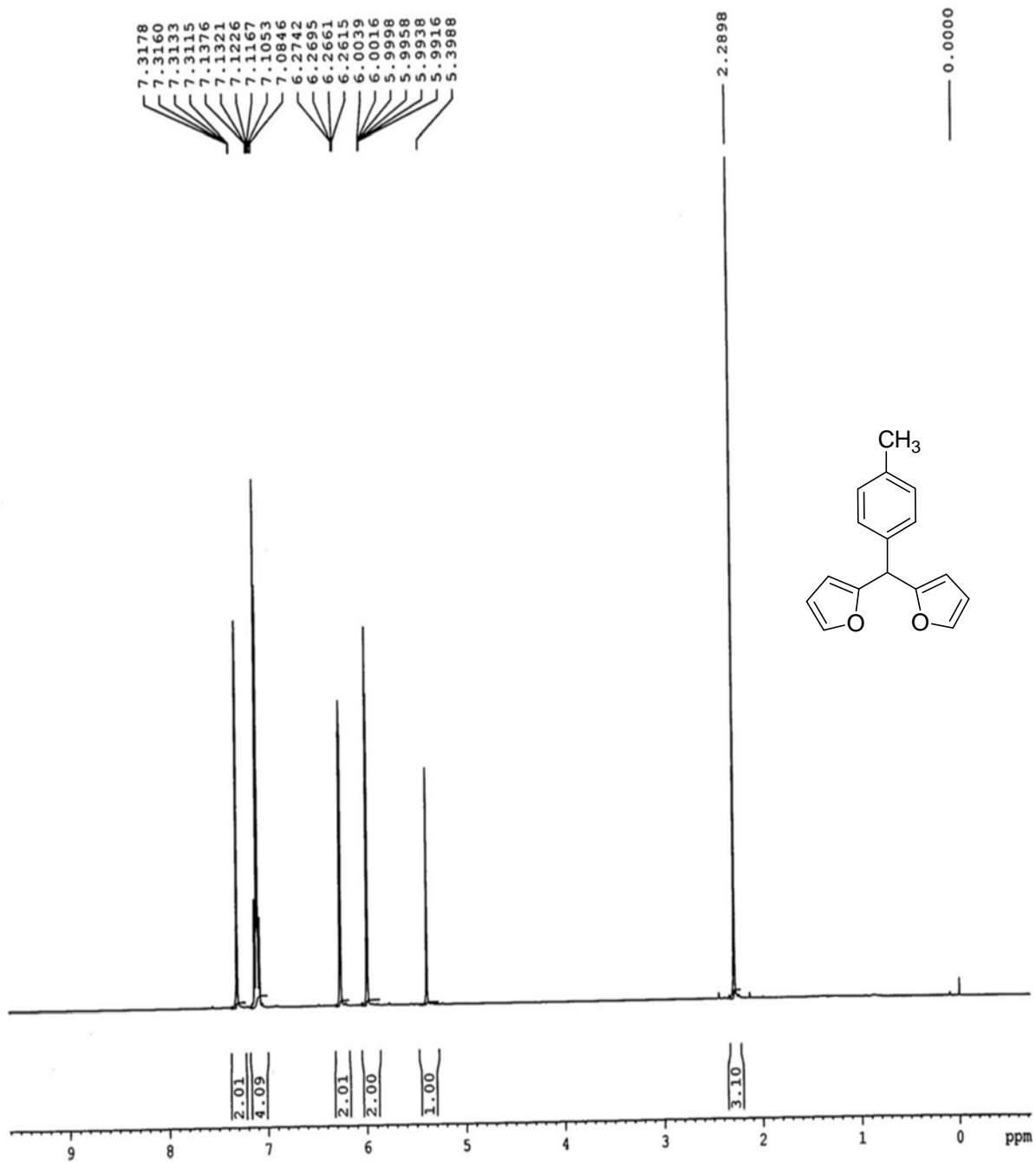


Figure S3:  $^1\text{H}$  NMR spectrum of **9b**.



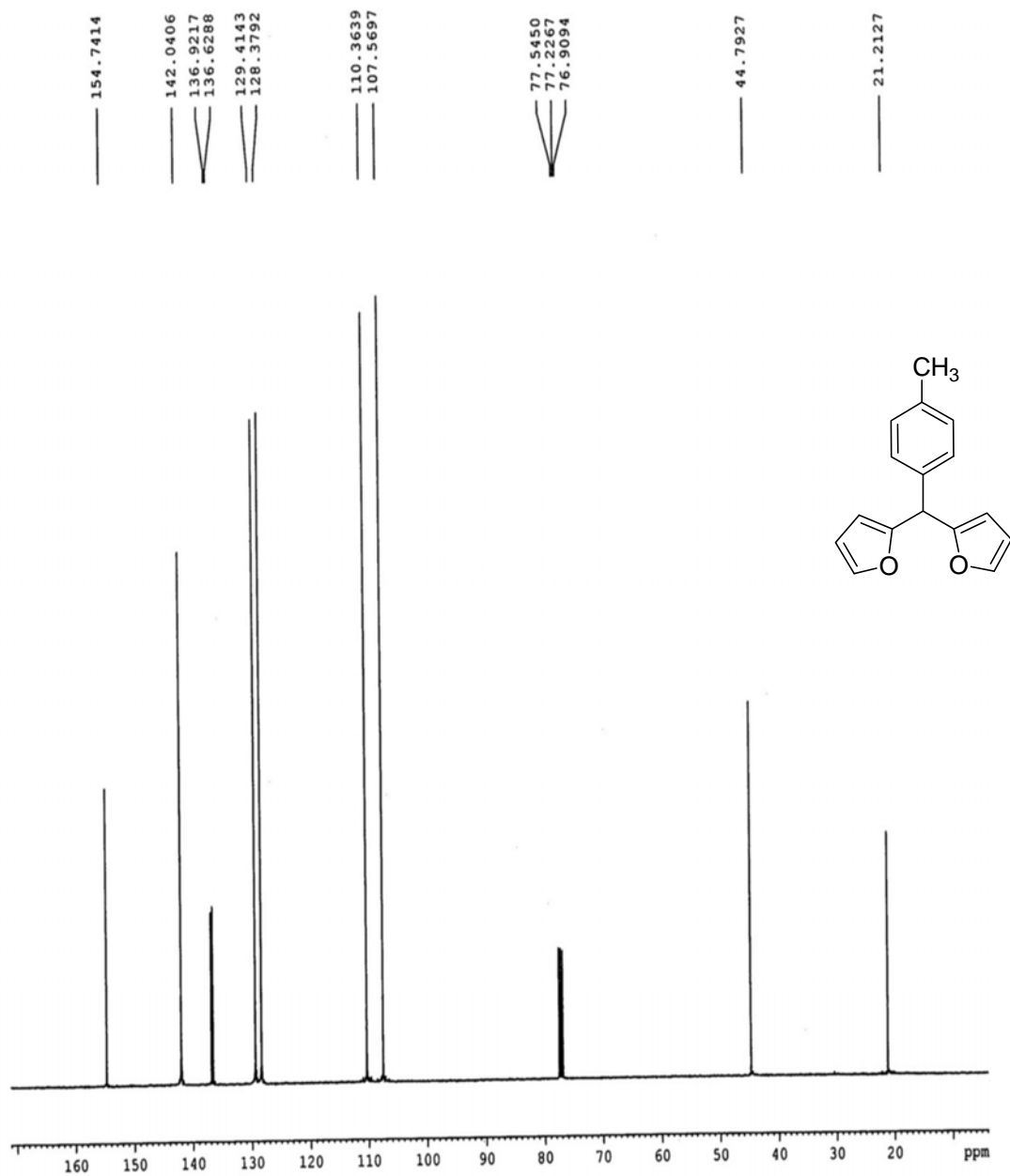


Figure S4:  $^{13}\text{C}$  NMR spectrum of **9b**.

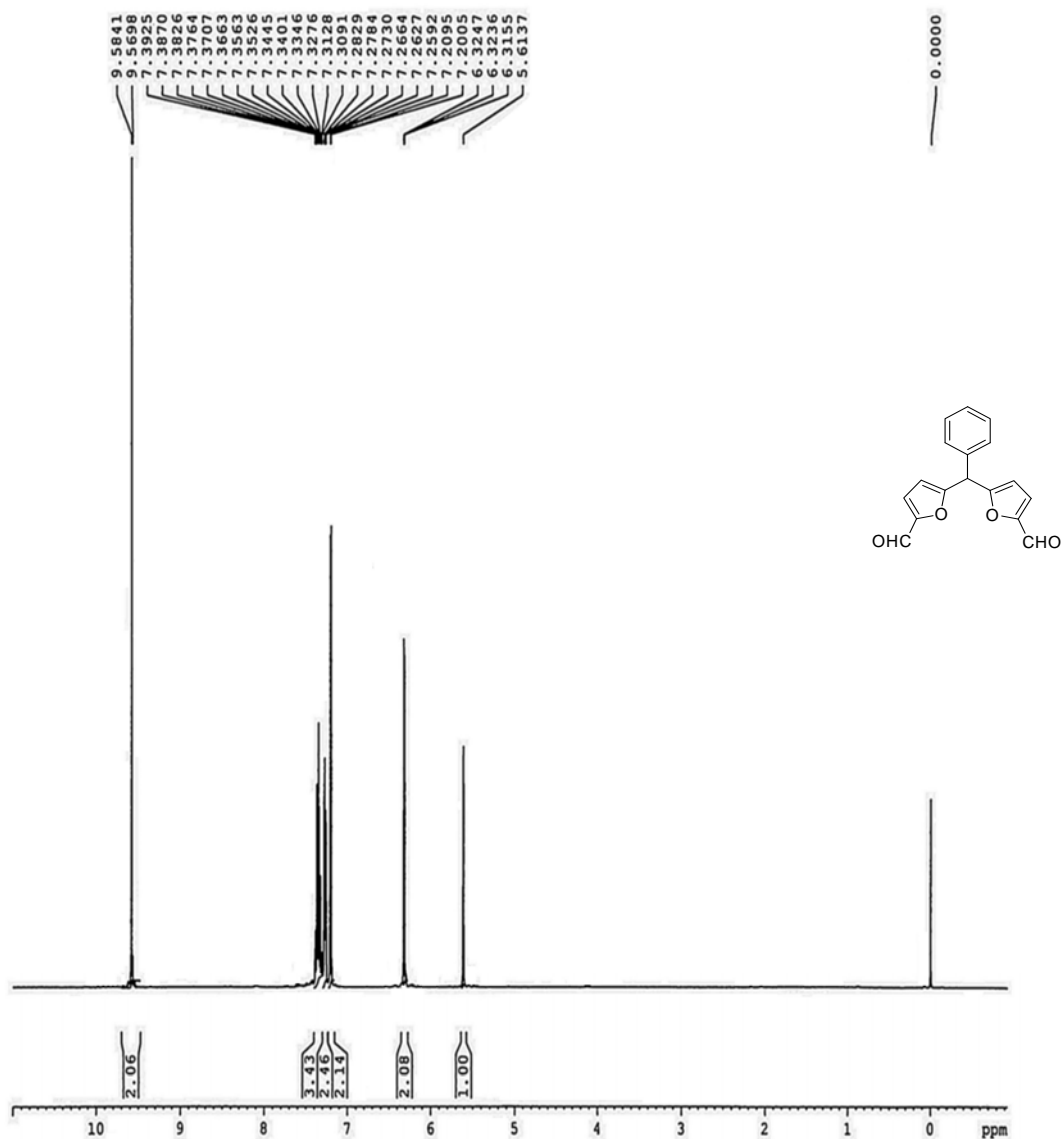


Figure S5 :  $^1\text{H}$  NMR spectrum of **10a**.

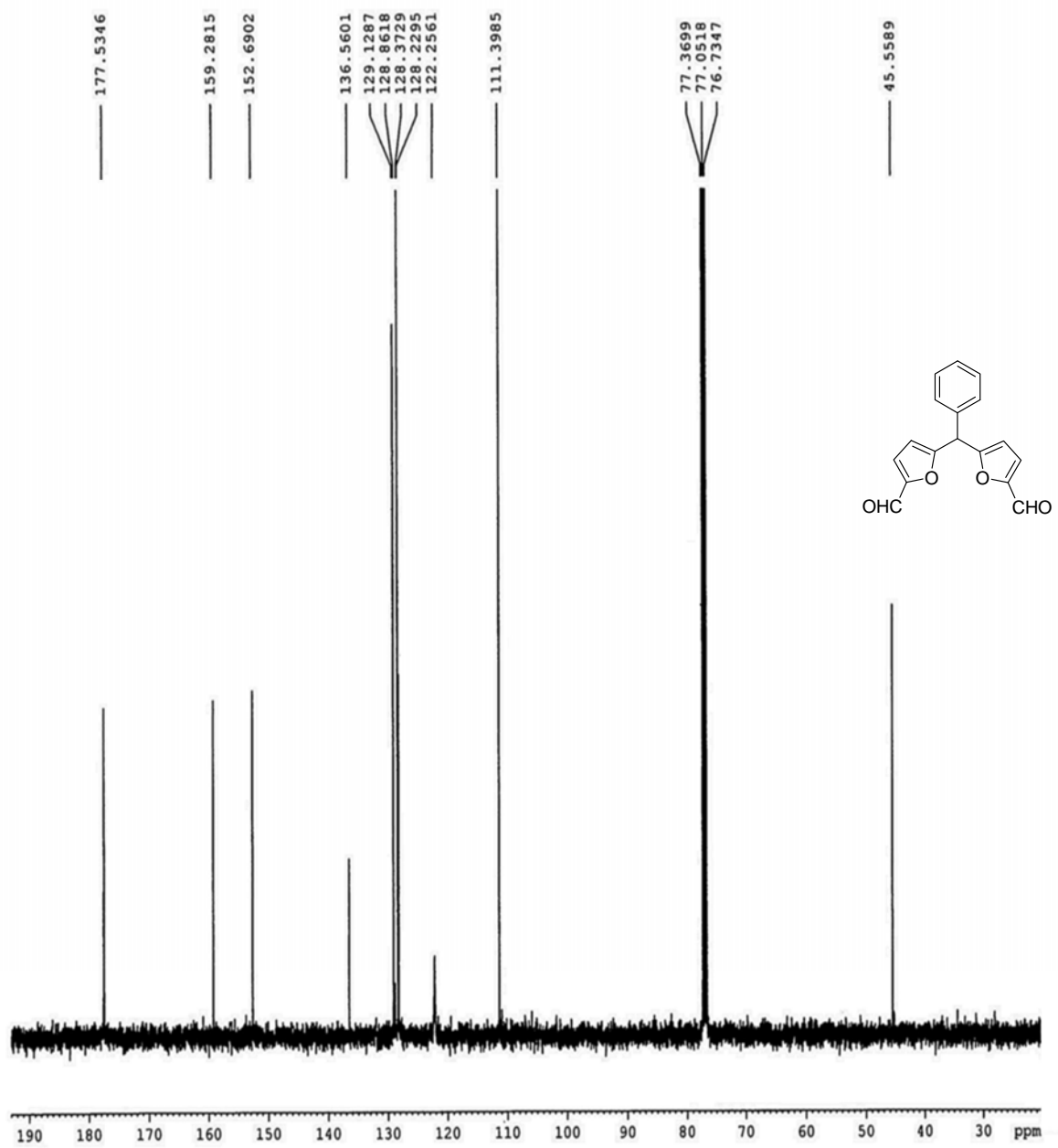
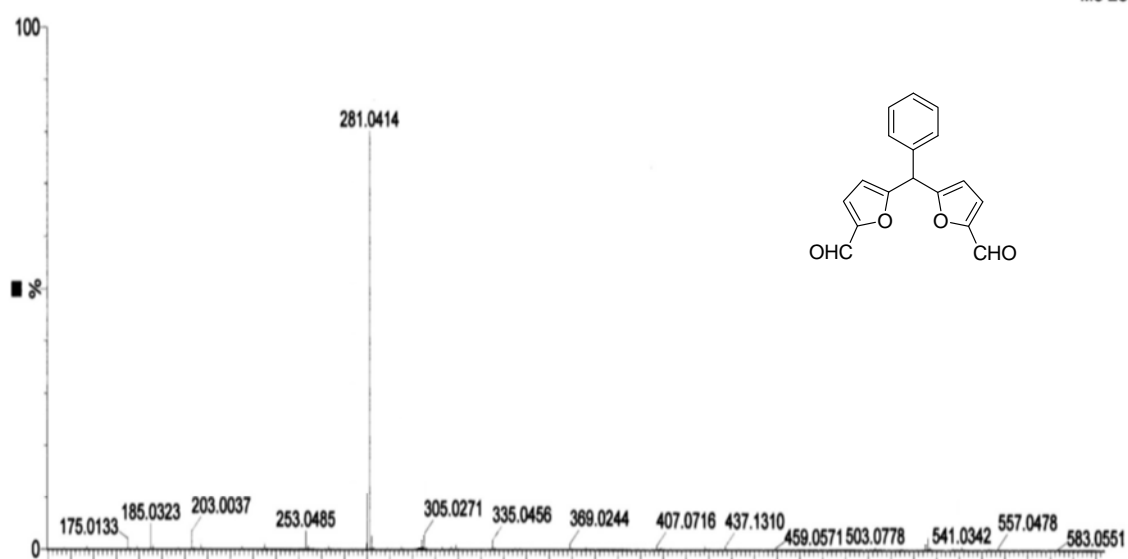


Figure S6:  $^{13}\text{C}$  NMR spectrum of **10a**.

MS ES+



MS0021 20 (1.343) Cm (19:23)

MS ES-

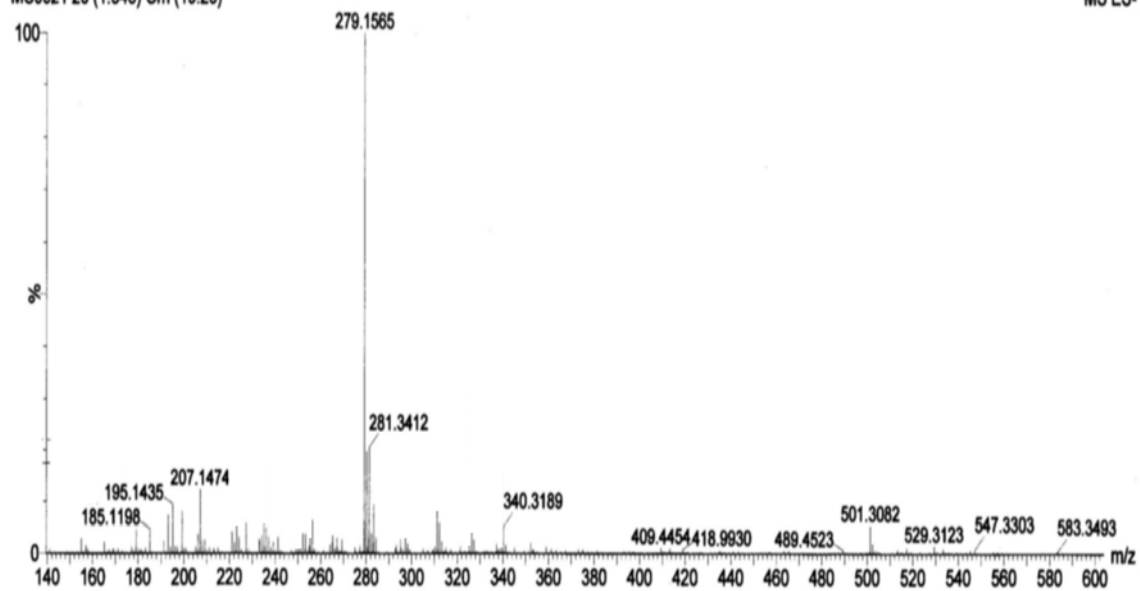


Figure S7: Mass spectrum of 10a.

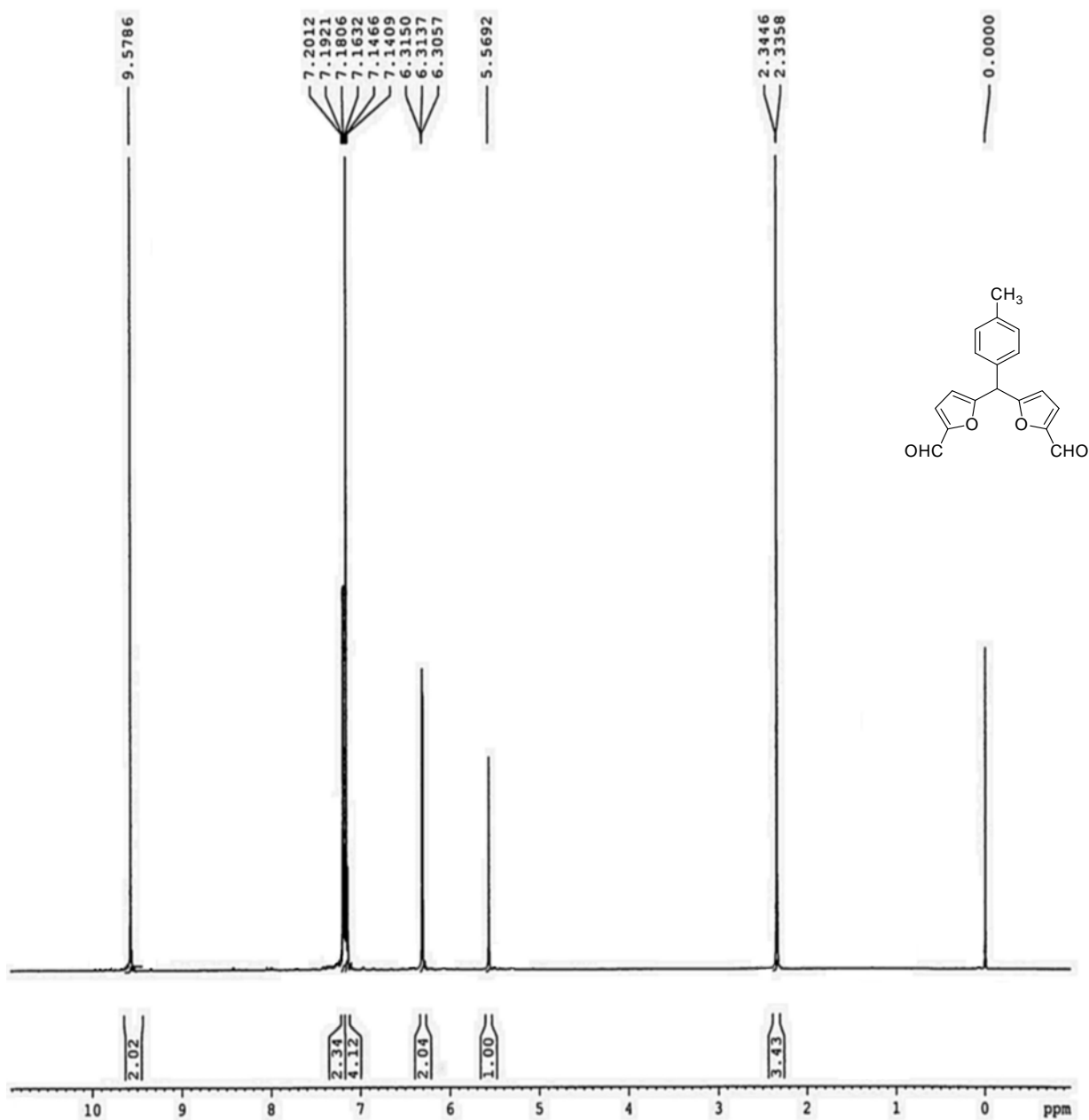


Figure S8 : <sup>1</sup>H NMR spectrum of **10b**.

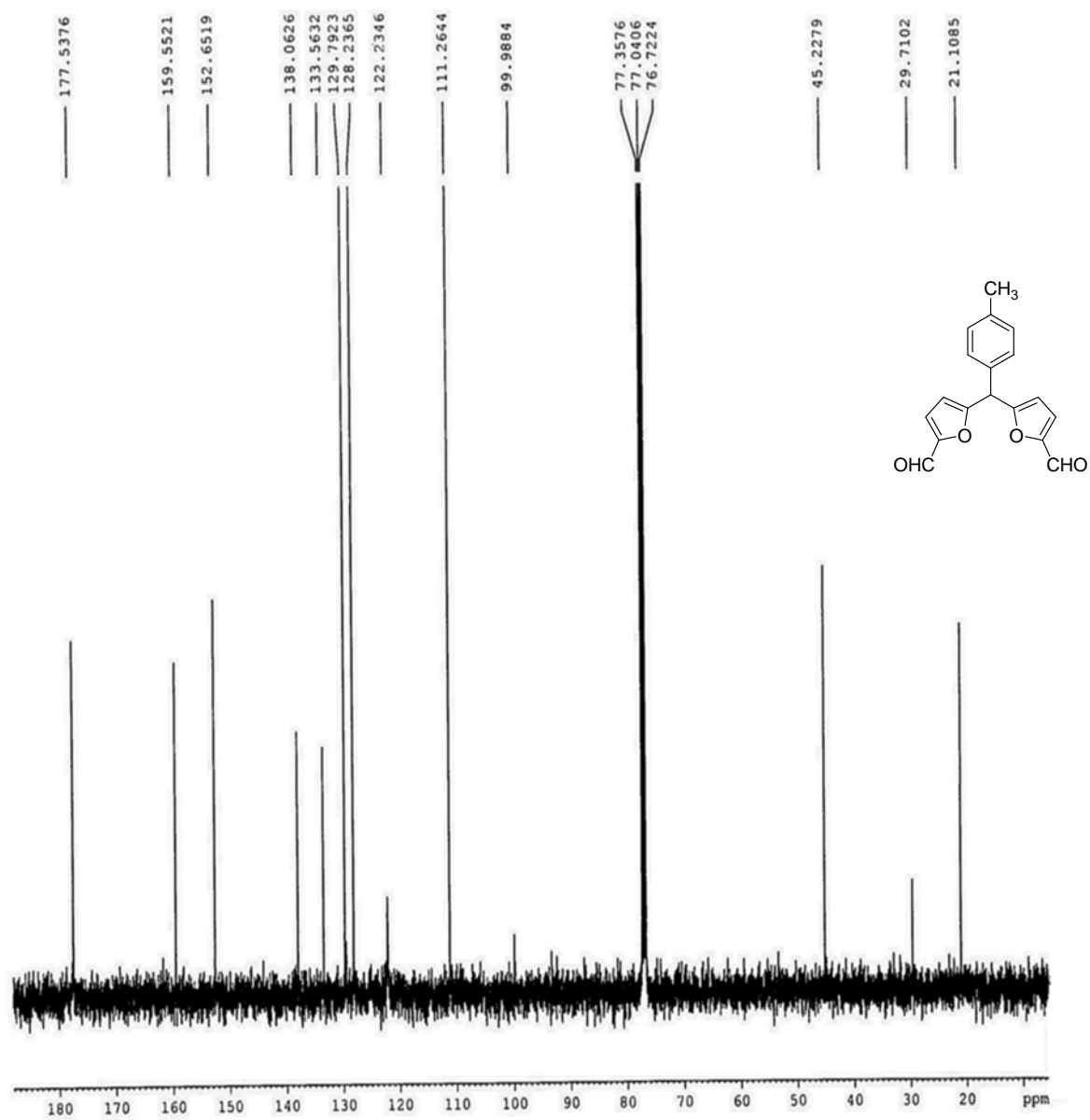


Figure S9:  $^{13}\text{C}$  NMR spectrum of **10b**.

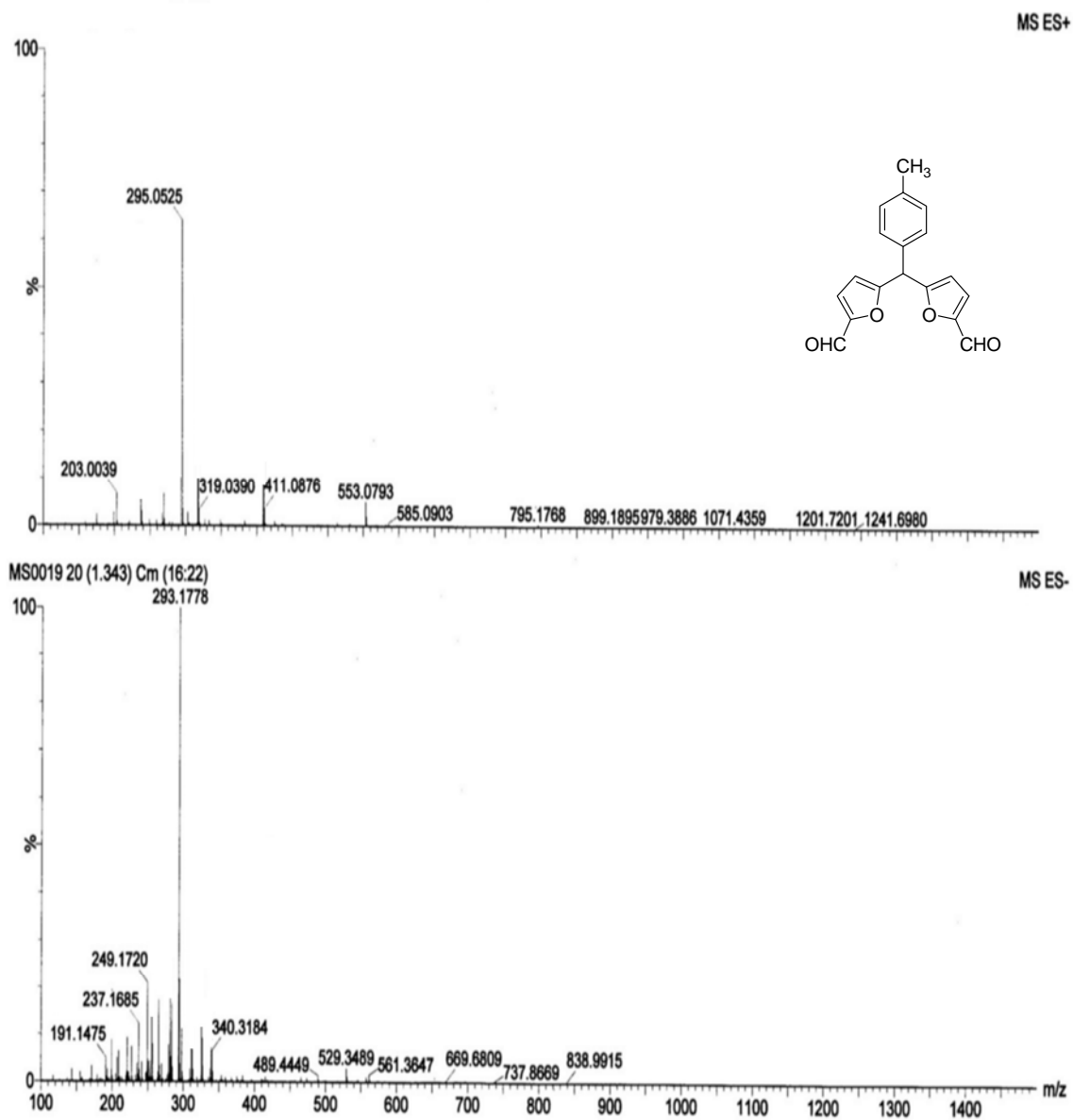


Figure S10: Mass spectrum of 10b.

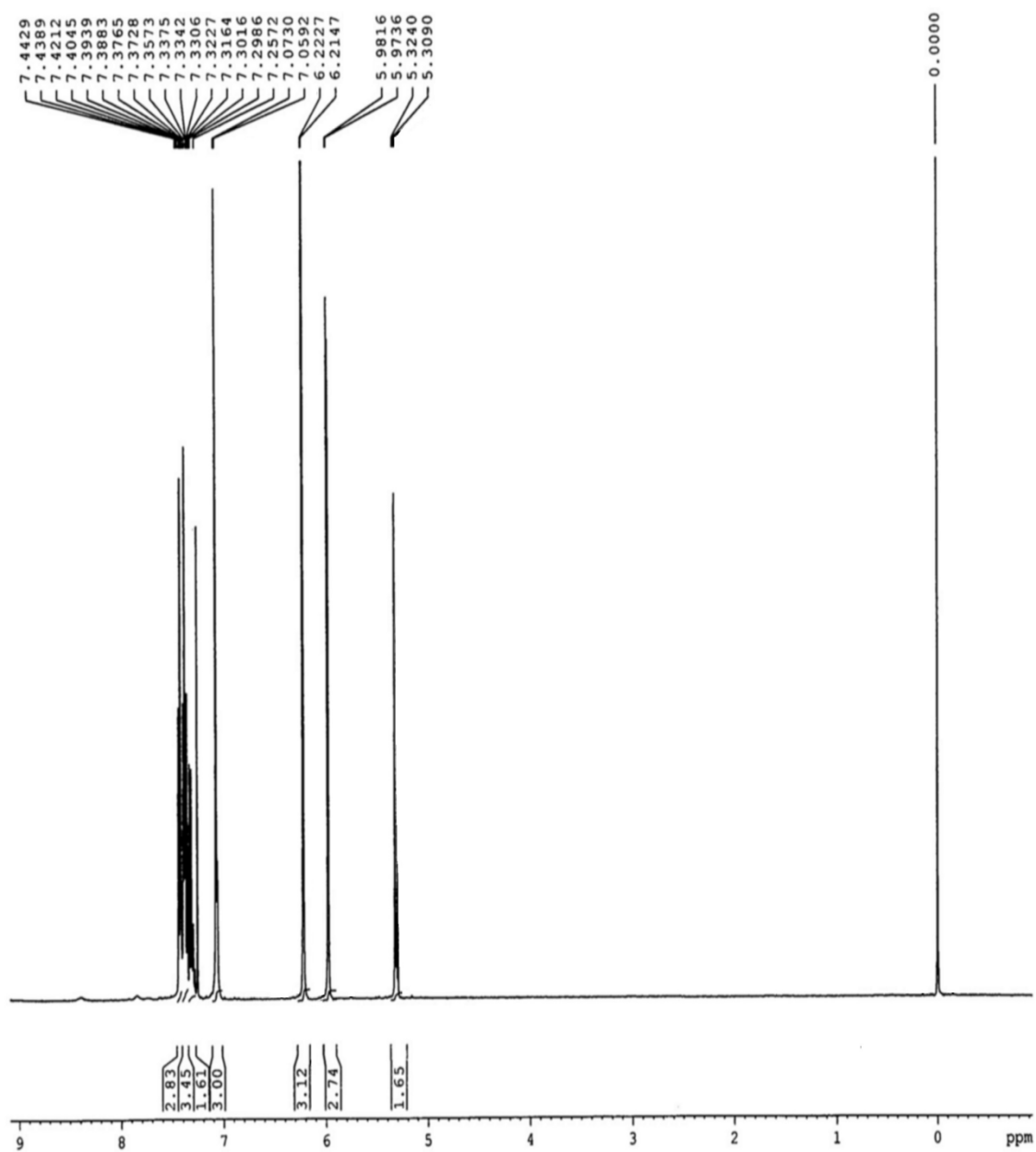


Figure S11 :  $^1\text{H}$  NMR spectrum of 11a.





MSE+

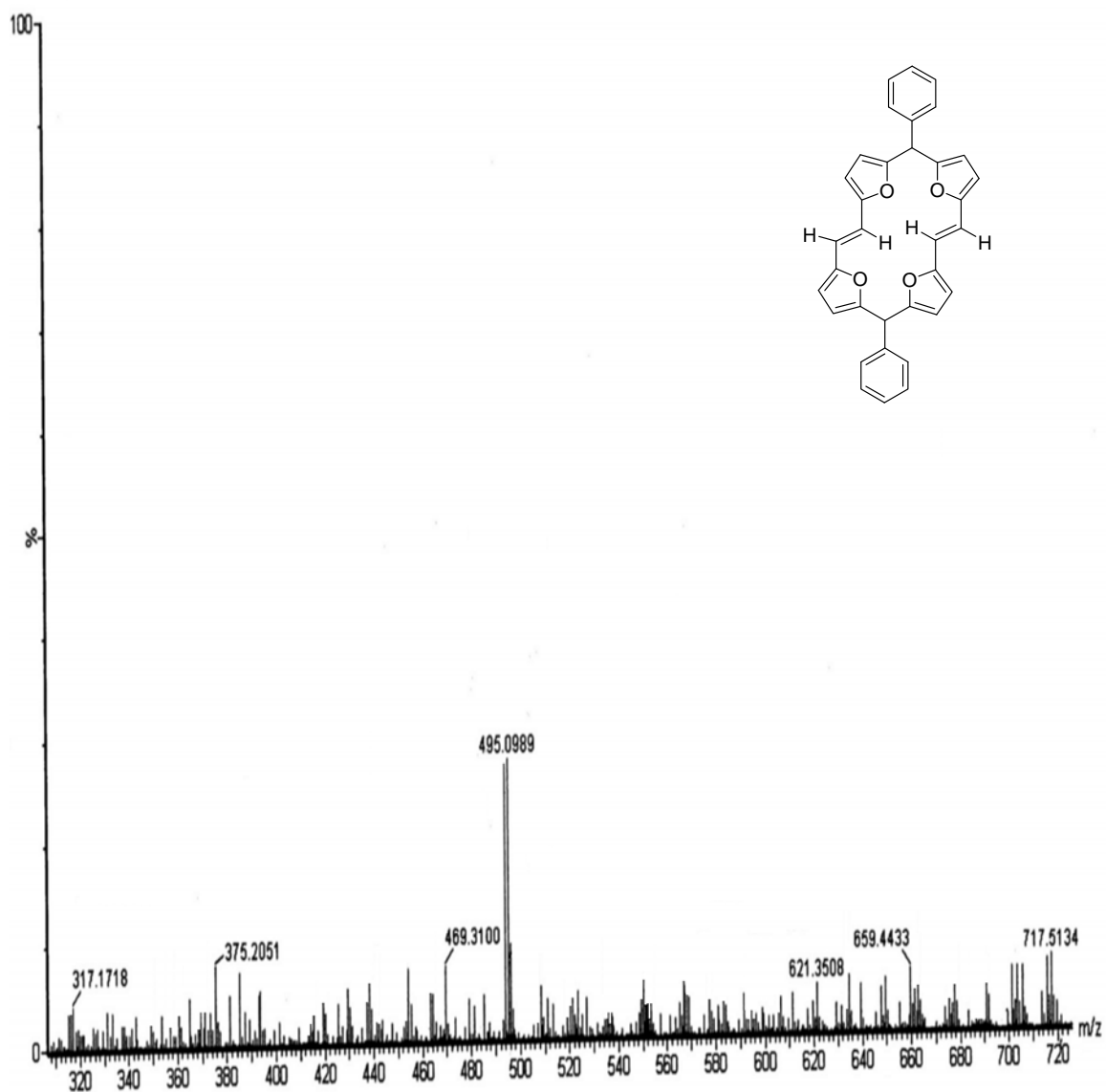
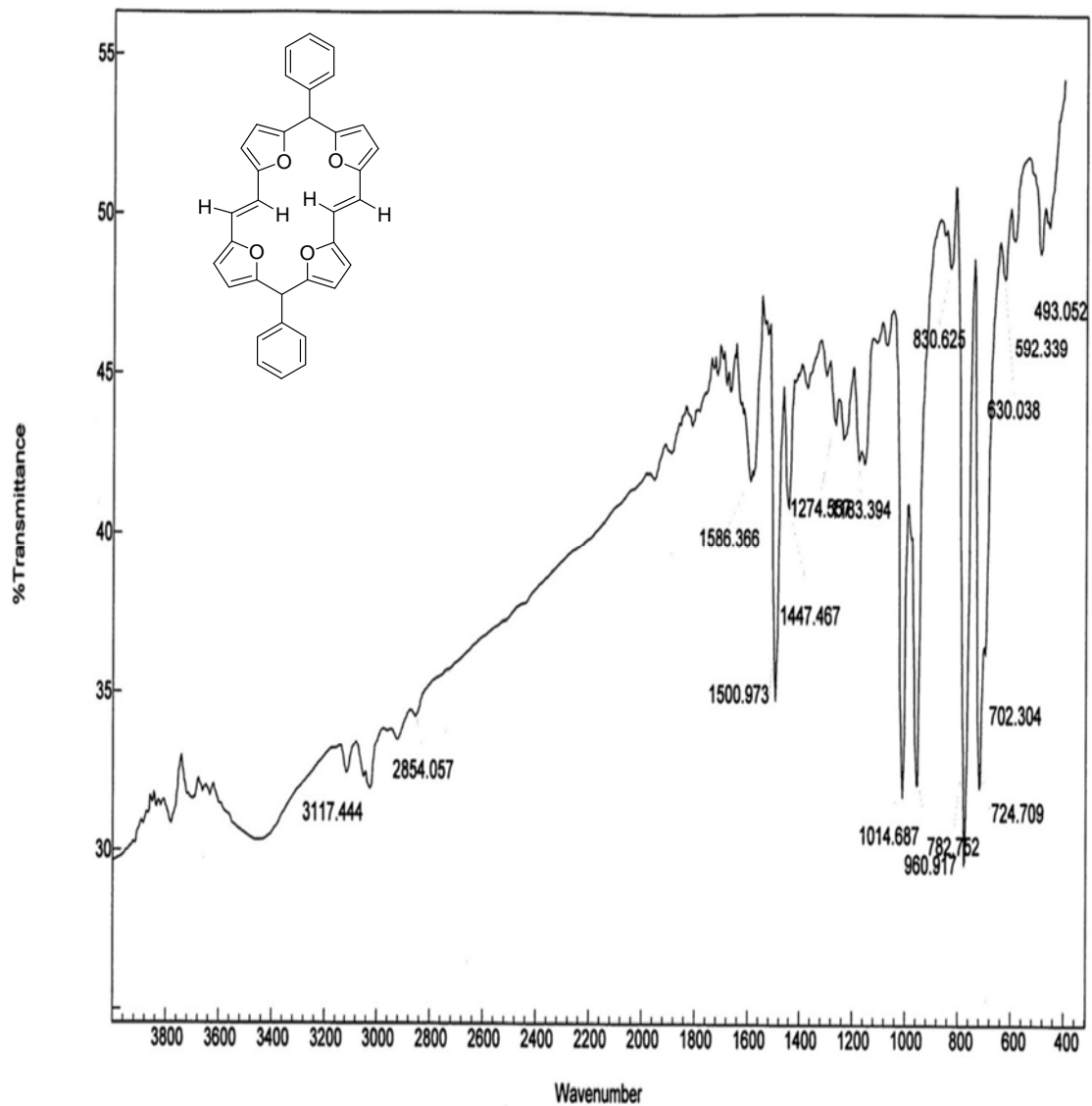
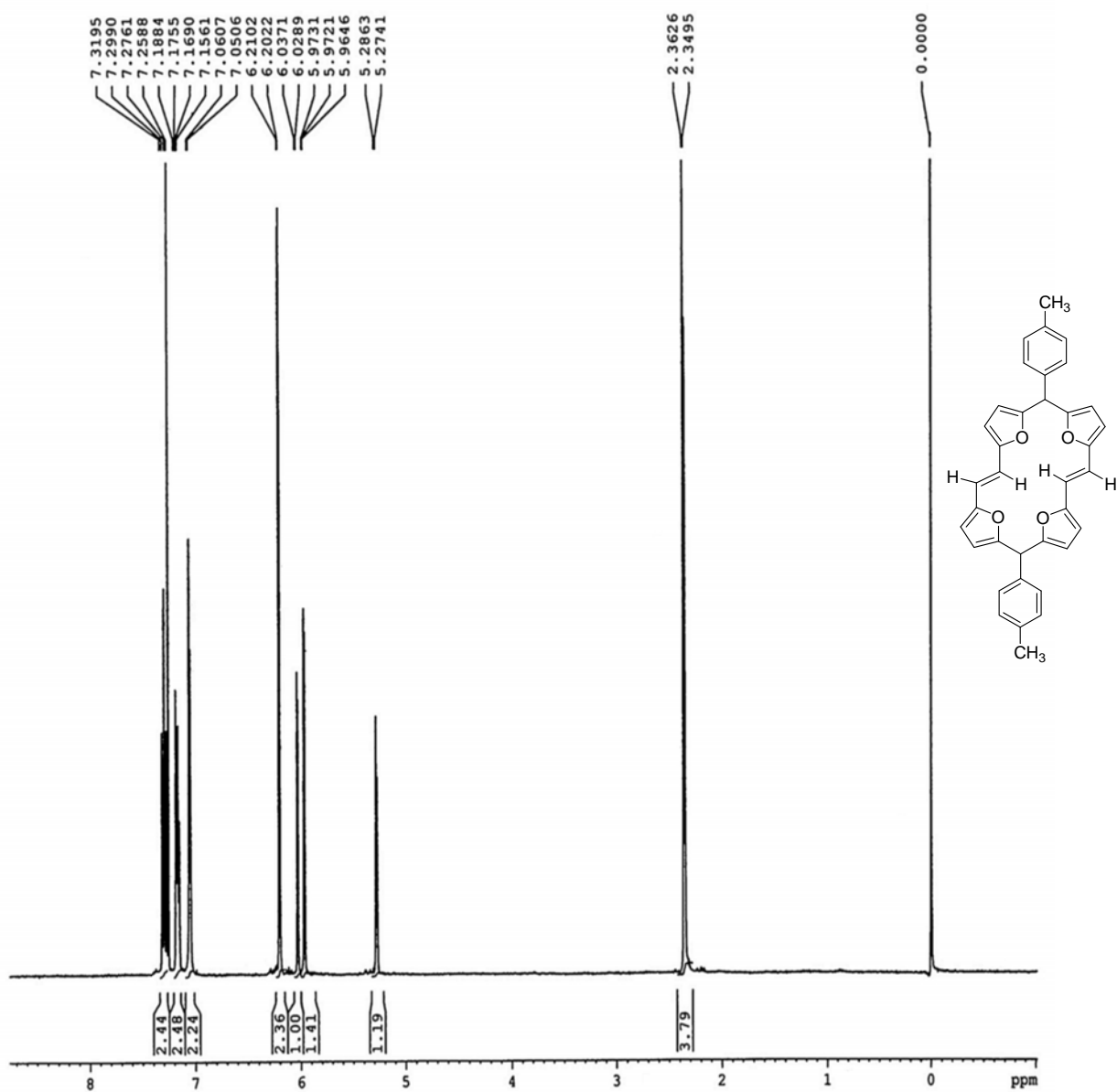


Figure S13: Mass spectrum of **11a**.



**Figure S14:** IR spectrum of **11a**.



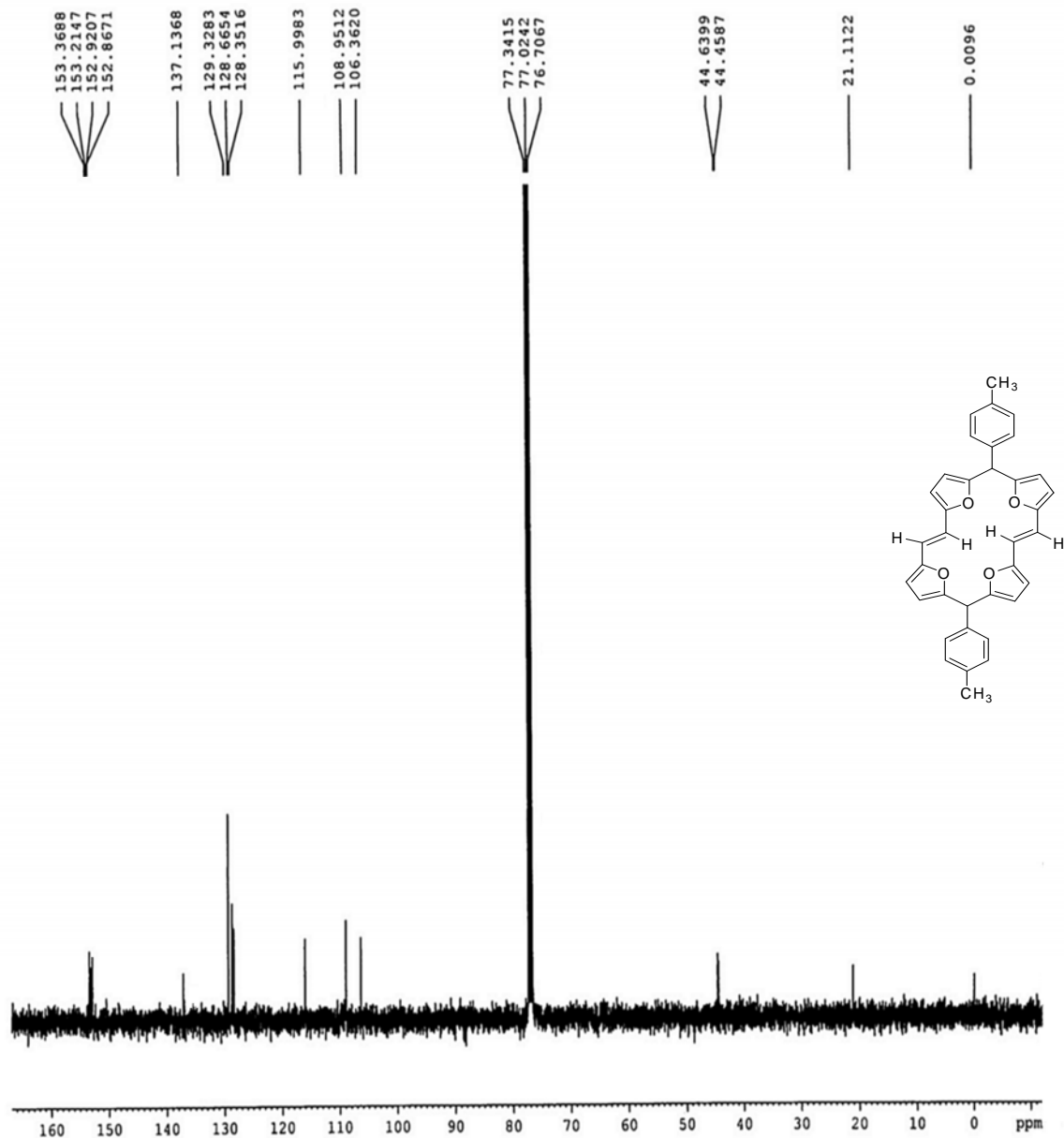


Figure S16:  $^{13}\text{C}$  NMR spectrum of **11b**.

MS ES+

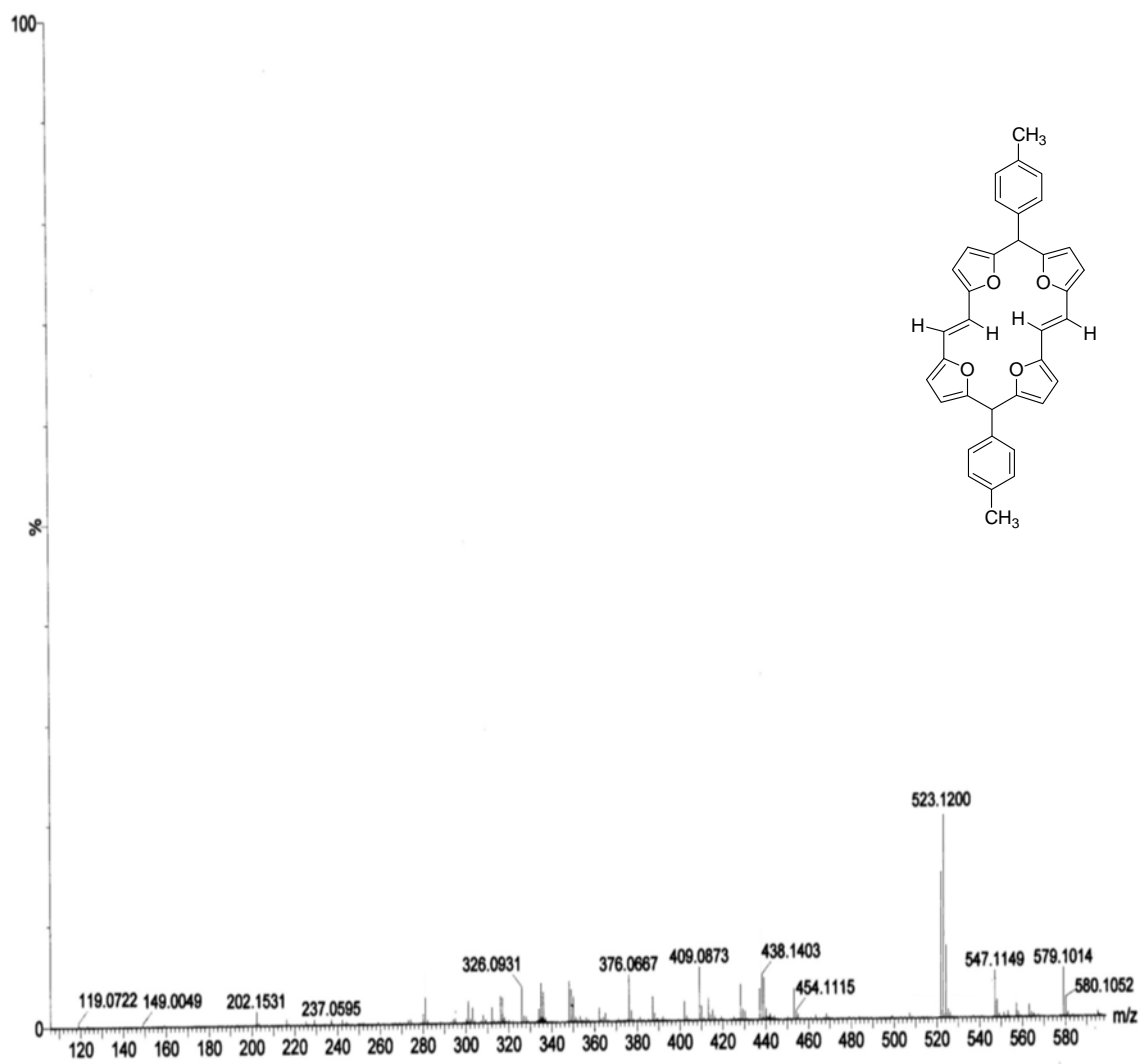
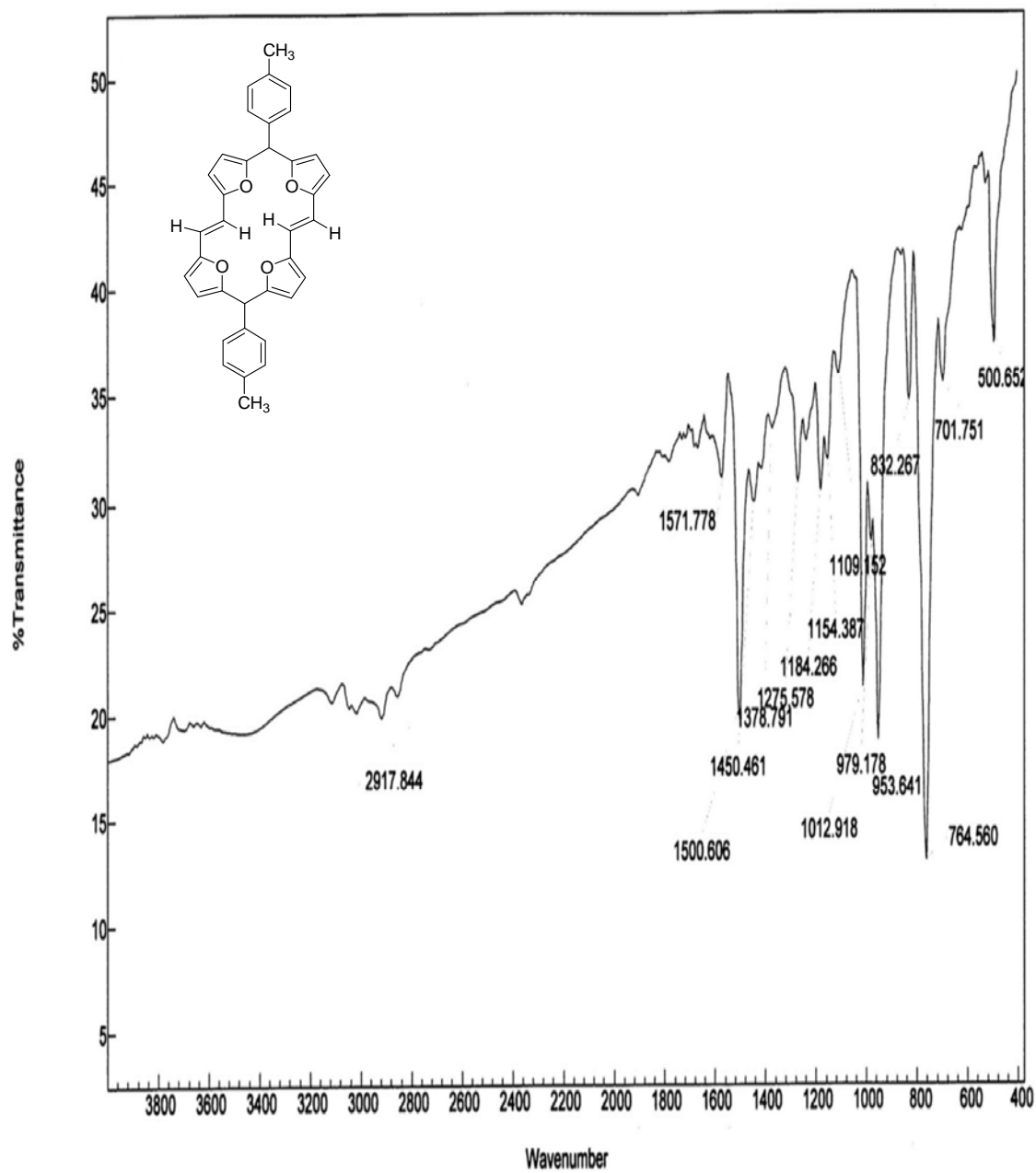
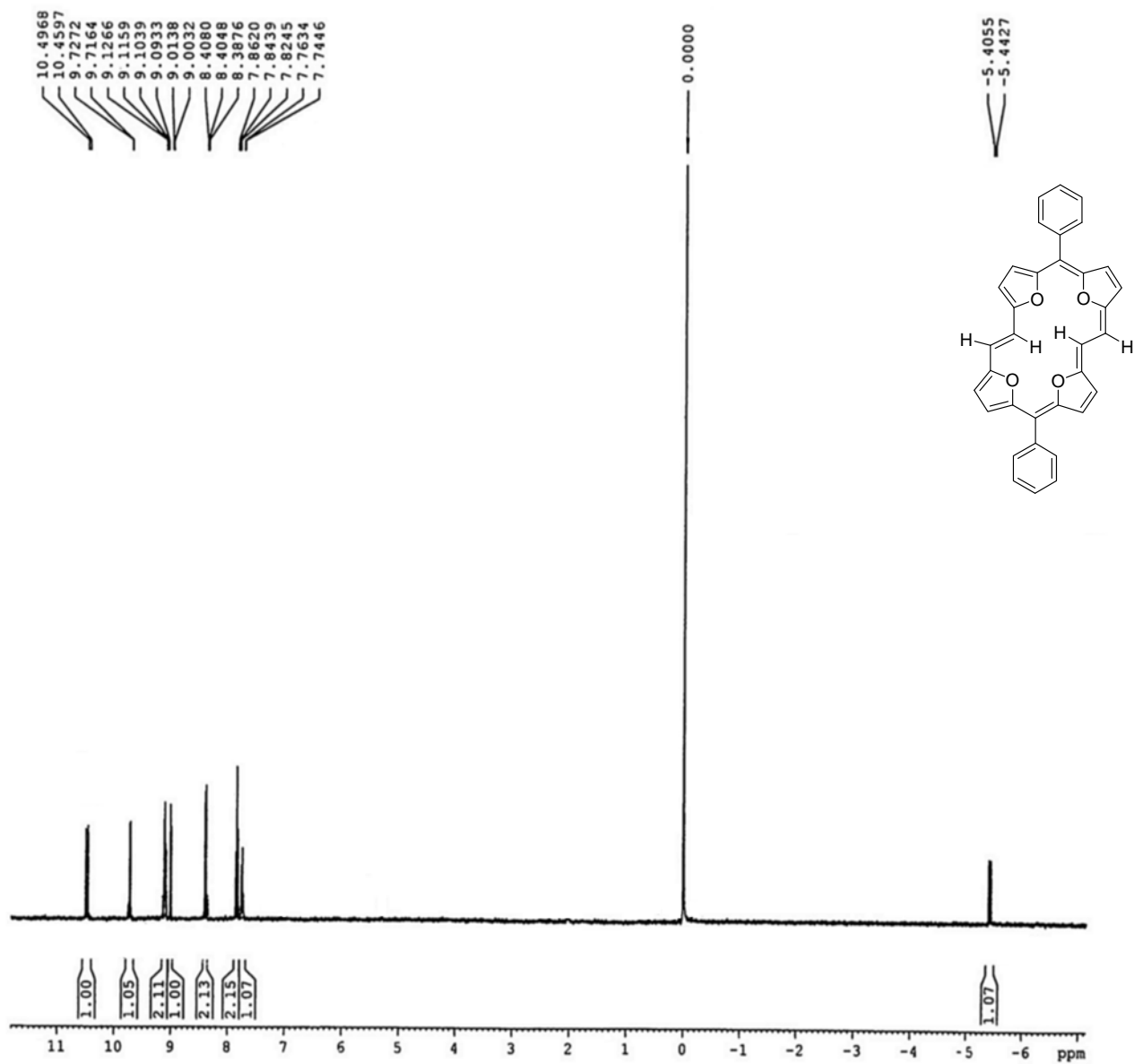


Figure S17: Mass spectrum of **11b**.



**Figure S18:** IR spectrum of **11b**.





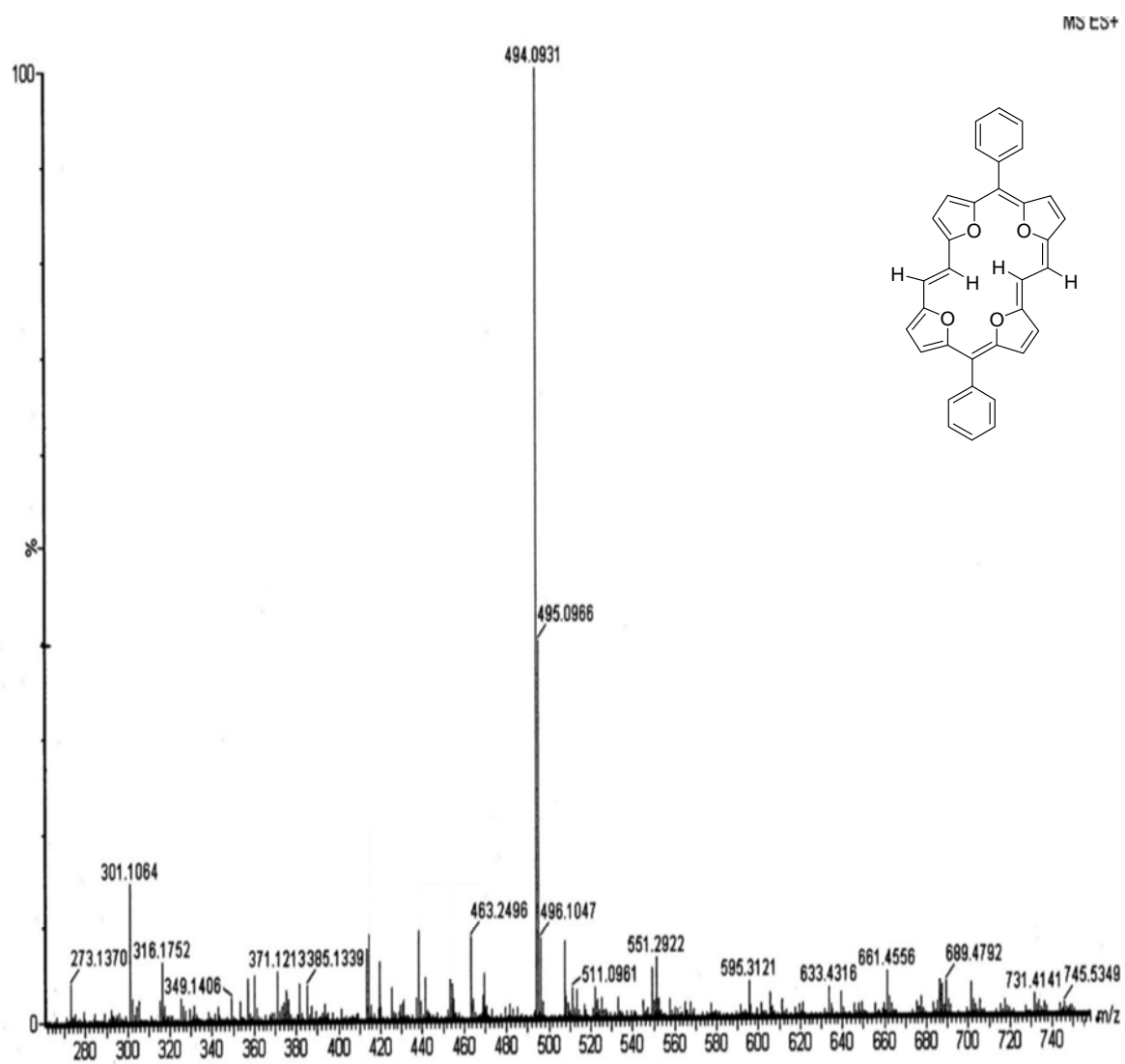


Figure S20: Mass spectrum of 12a.

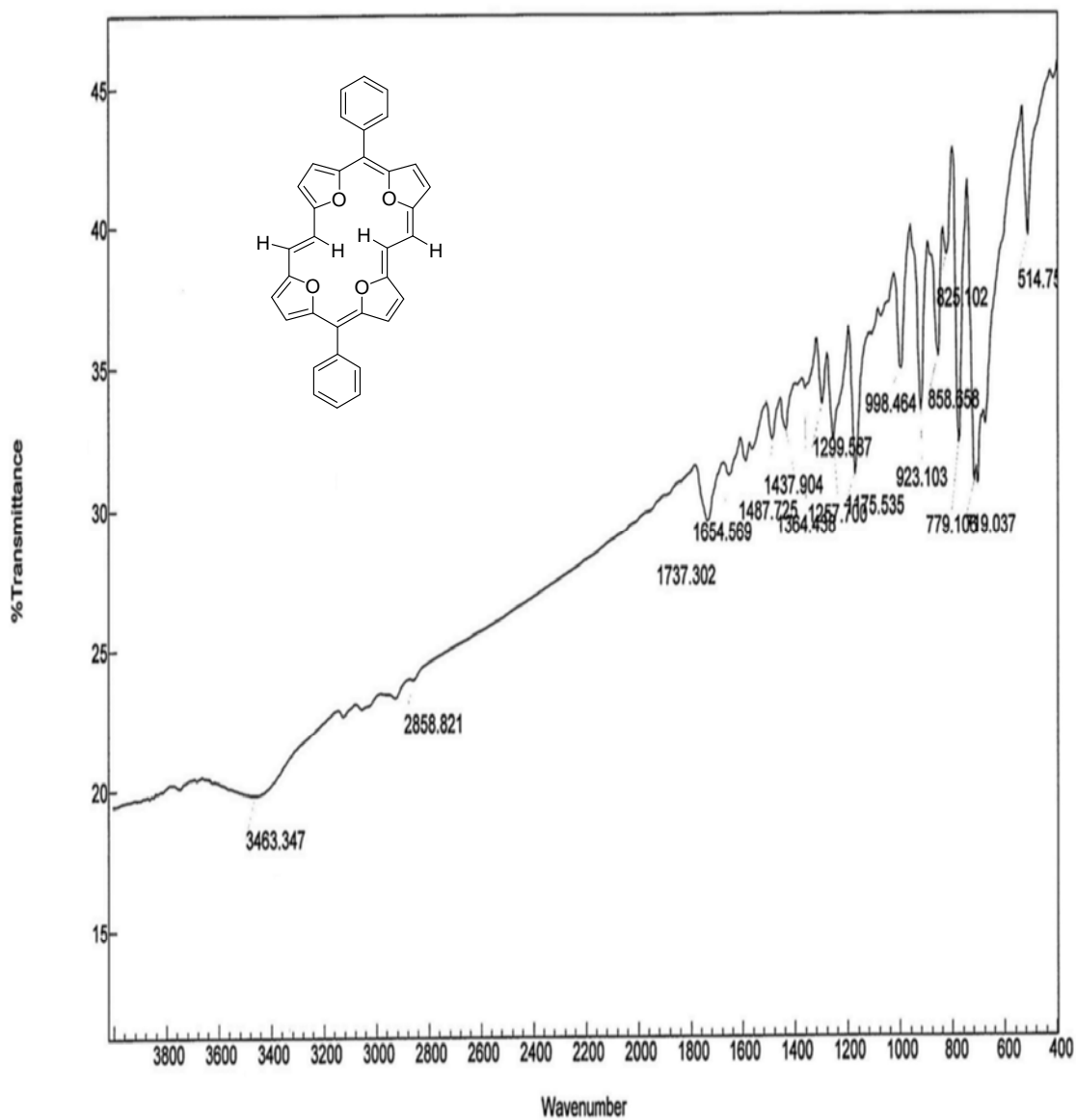
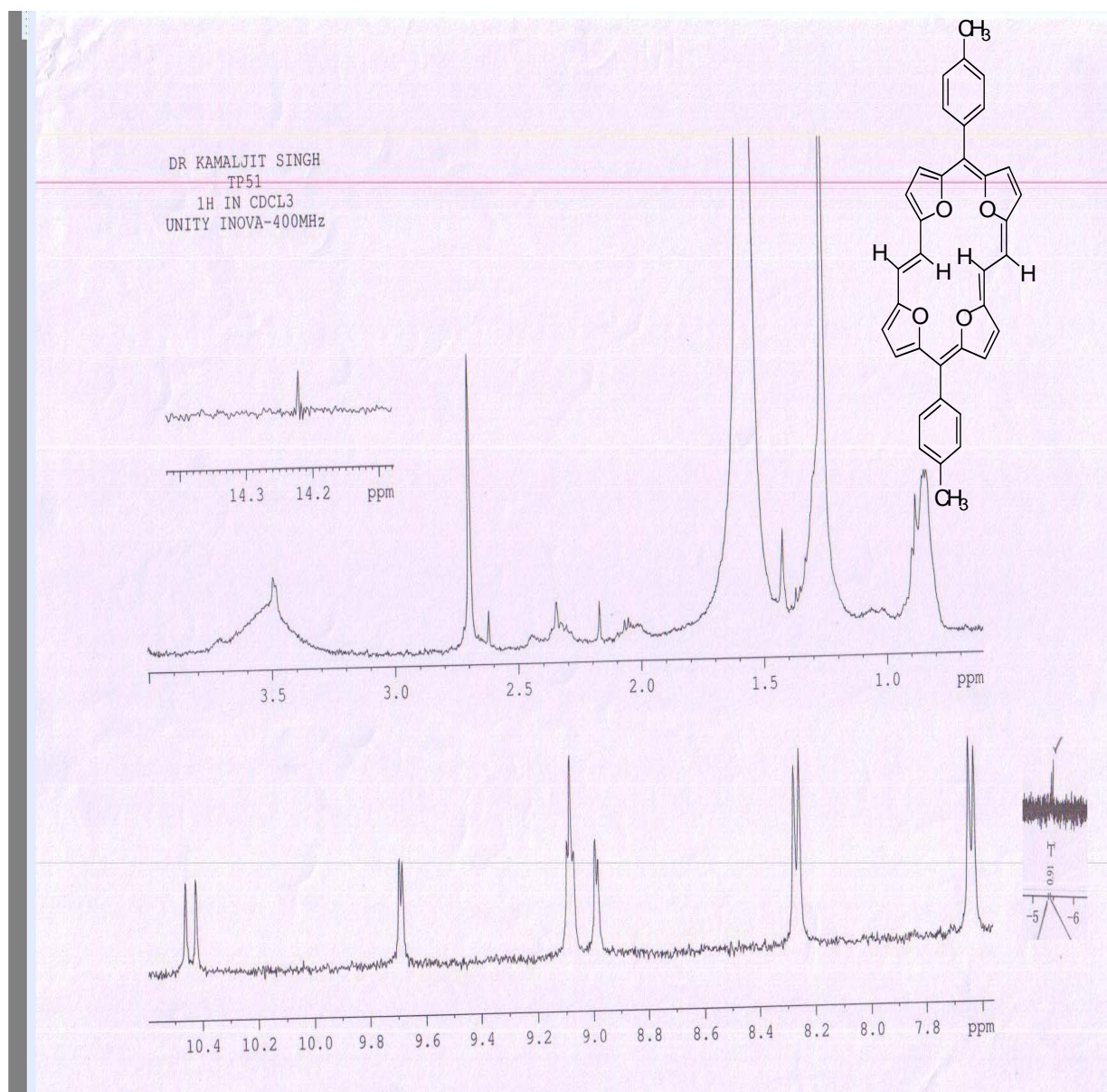
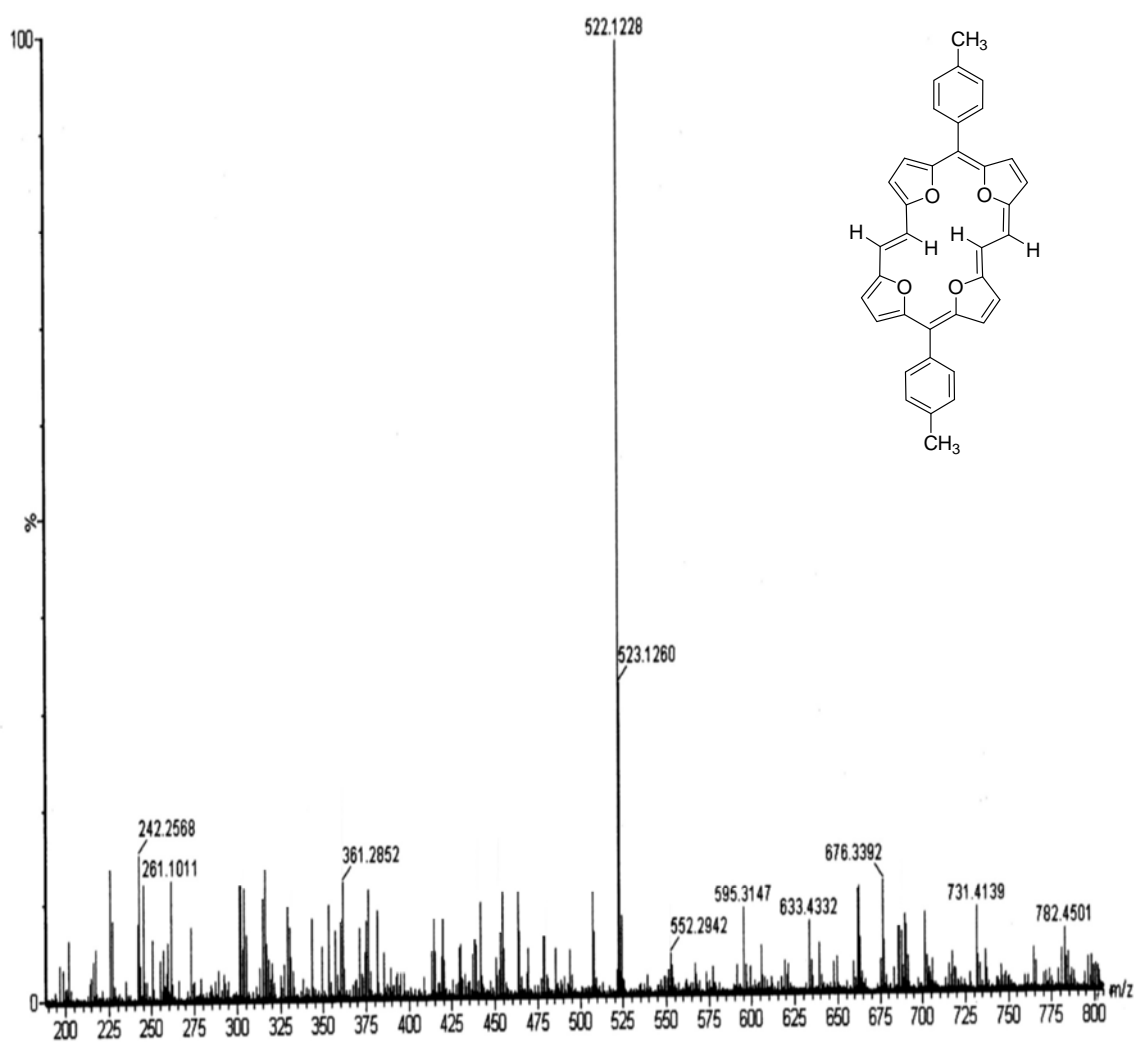


Figure S21: IR spectrum of 12a.



**Figure S22 :**  $^1\text{H}$  NMR spectrum of **12b** (Due to extremely low solubility of **12b** in most of the deuterated solvents, its  $^1\text{H}$  NMR spectra was obtained with great difficulty).

MS ES+



**Figure S23:** Mass spectrum of **12b**.

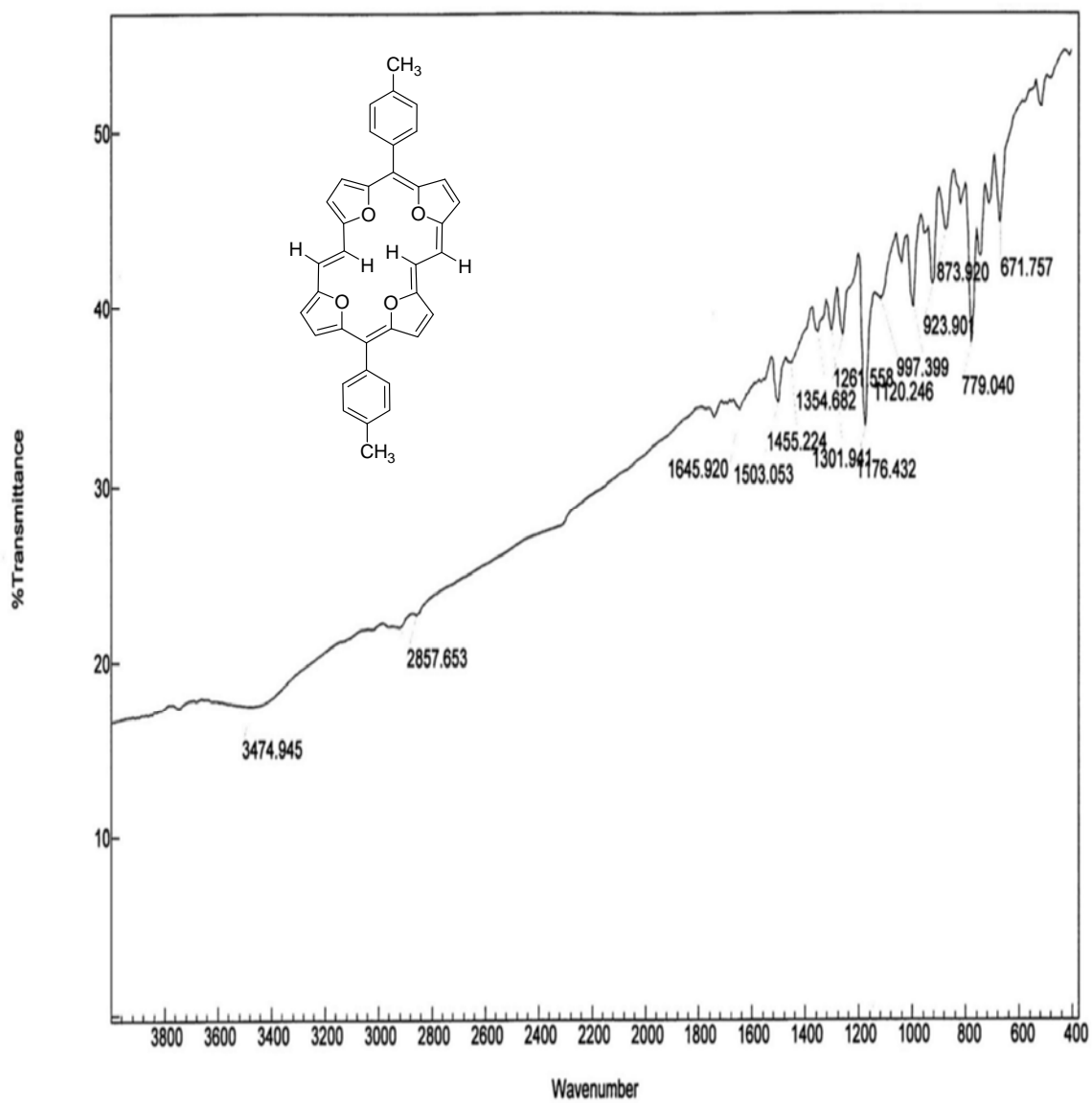


Figure S24: IR spectrum of 12b.

**Table S1.**  $^1\text{H}$  NMR (400 MHz) data of **11a/12a** and **11b/12b** ( $\text{CDCl}_3$ , TMS int.). Chemical shifts ( $\delta$ ) and coupling constants  $J$  [Hz] (Scheme 1).

$\delta$ /ppm ( $J$ /Hz)	<b>11a</b>	<b>11b</b>	<b>12a</b>	<b>12b</b>
H2/H8	6.22 ( $J_{2,3}$ 3.2)	6.21 ( $J_{2,3}$ 3.2)	9.72/9.12 ( $J_{2,3}$ 4.32)	9.67/9.10 ( $J_{2,3}$ 5.0)
H3/H7	5.97 ( $J_{7,8}$ 3.2)	5.96/6.02 ( $J_{7,8}$ 3.2)	9.01/9.09 ( $J_{7,8}$ 4.24)	9.10/8.98 ( $J_{7,8}$ 5.0)
H10/H11	7.07 <sup>[a]</sup>	7.05/7.06 <sup>[a]</sup>	10.46/-5.42 ( $J_{10,11}$ 14.84)	10.42/-5.40 ( $J_{10,11}$ 15.0)

[a] singlet

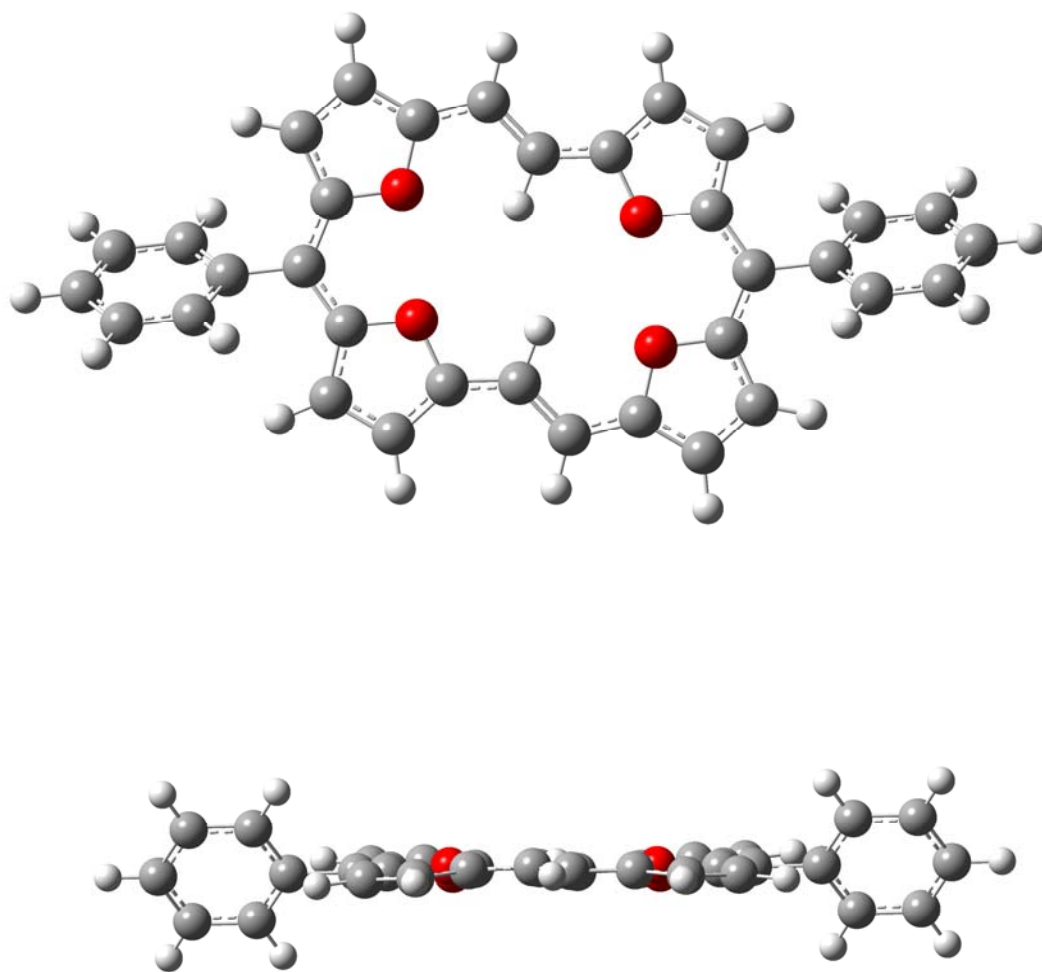
## Theoretical Calculations

### Computational methods

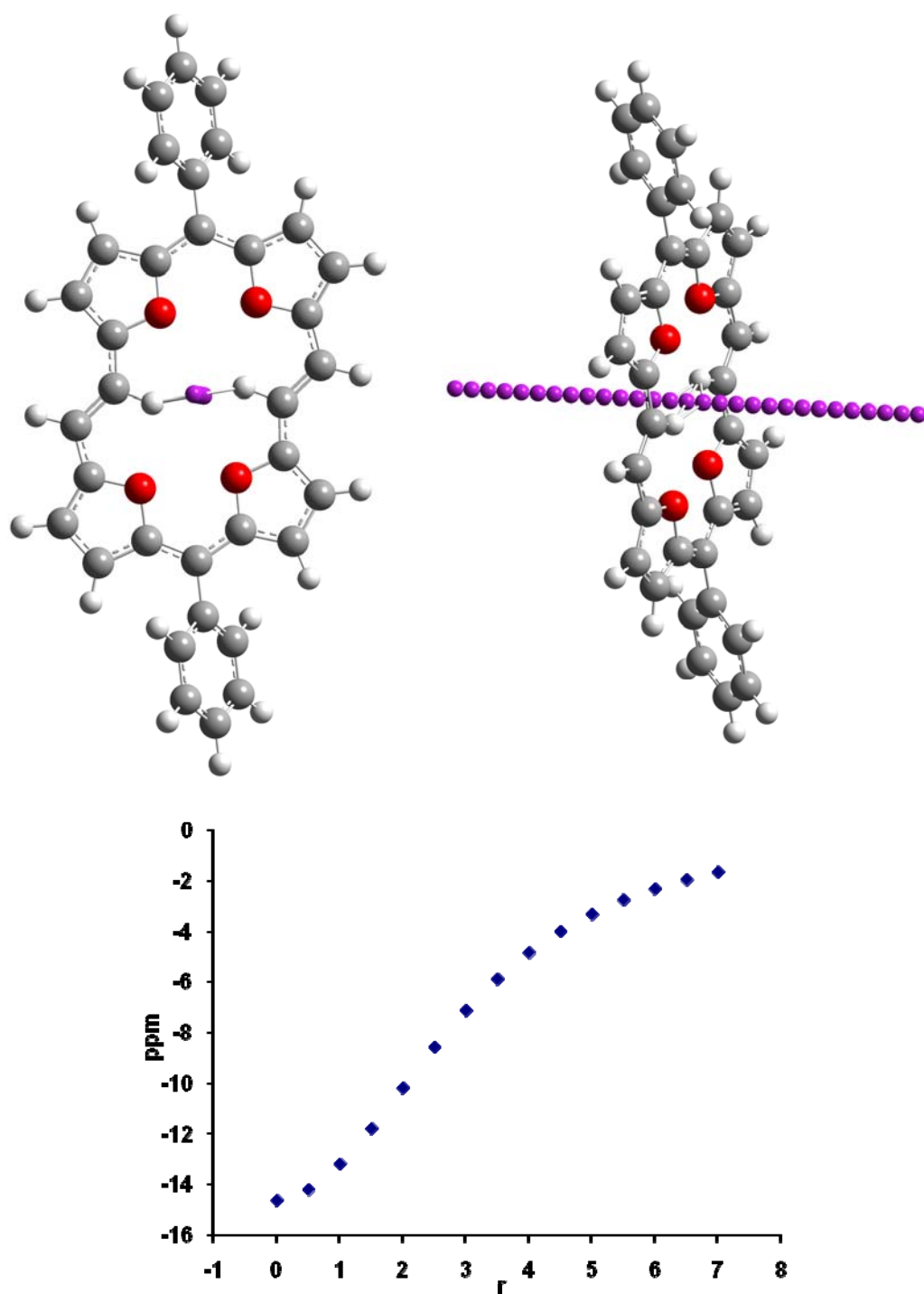
All the calculations were performed at the density functional theory (DFT) level with the B3LYP functional, the gradient correction of the exchange functional by Becke and the correlation functional by Lee, Yang and Parr. The 6-311G(d) split valence plus polarization basis set was used in Gaussian 09 program.<sup>[2],[3]</sup> The results were analyzed and visualized on Gauss View 5.0.9.

<sup>[2]</sup> Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, W. H. G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, Jr., J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2010.

<sup>[3]</sup> Details including the references for the DFT method and basis set can be found online at the homepage of Gaussian, Inc.; <http://www.gaussian.com/>

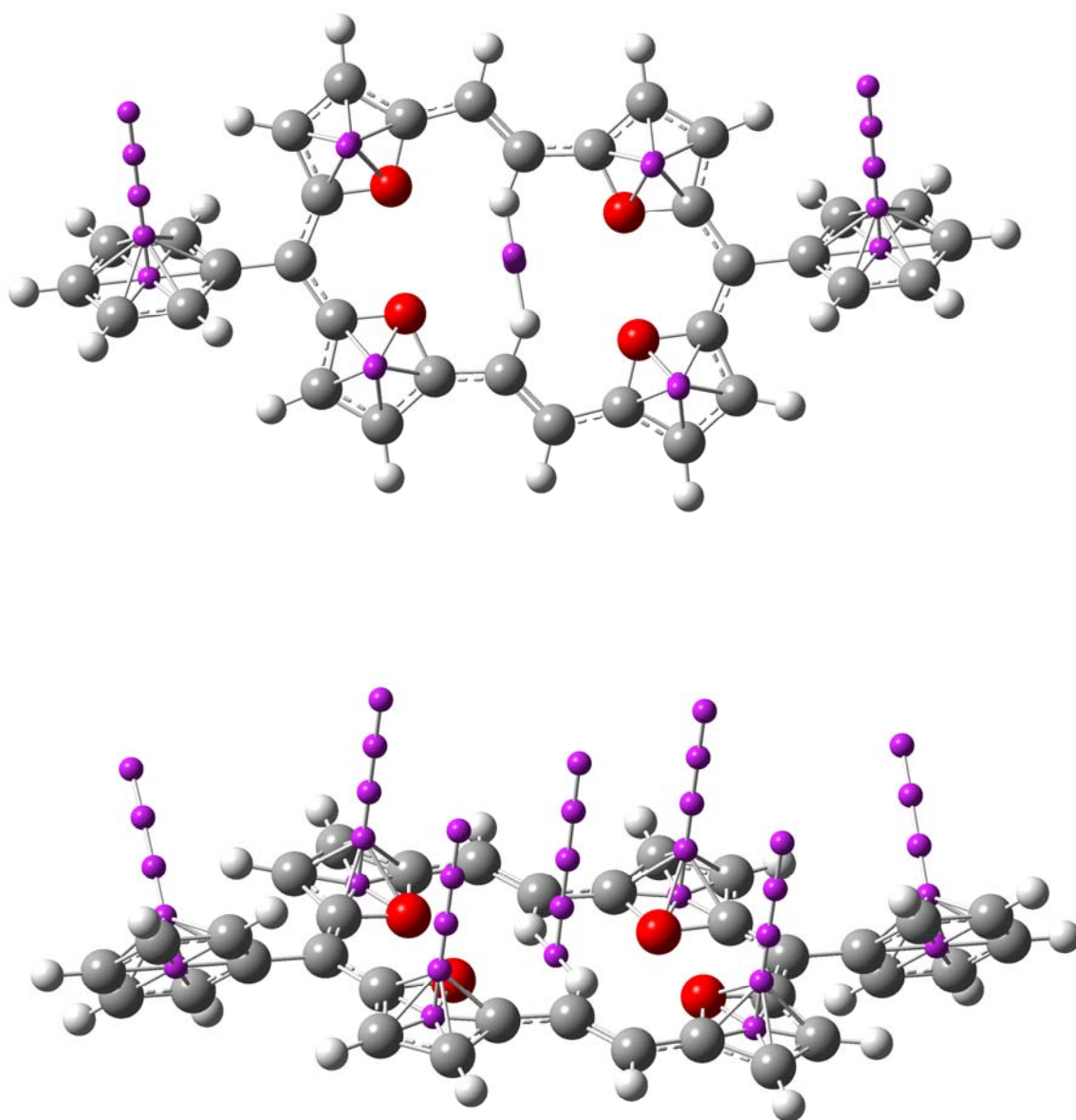


**Figure S25:** Energy minimized structure of **12a** by DFT method at B3LYP/6-311G(d) level using the Gaussian09 program (Top and side views shown above).

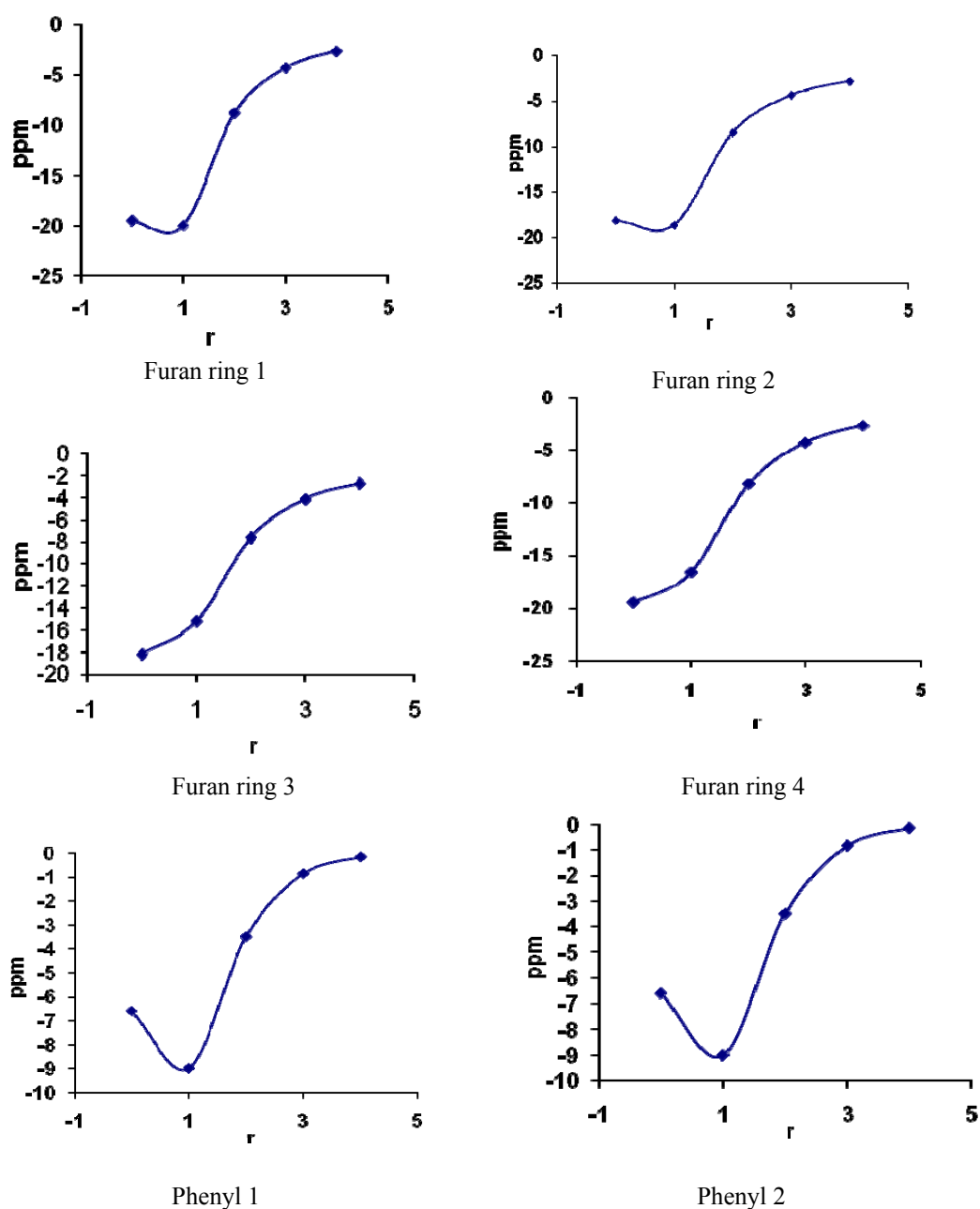


**Figure S26:** The ghost (Bq) atoms were placed (0.5 Å interval) in the centre of the molecule (in purple). The -ve NICS values clearly indicate the aromaticity of **12a**. NICS is maximum at 0 Å and decreases as the distance of the ghost atom is increased in 0.5 Å intervals.



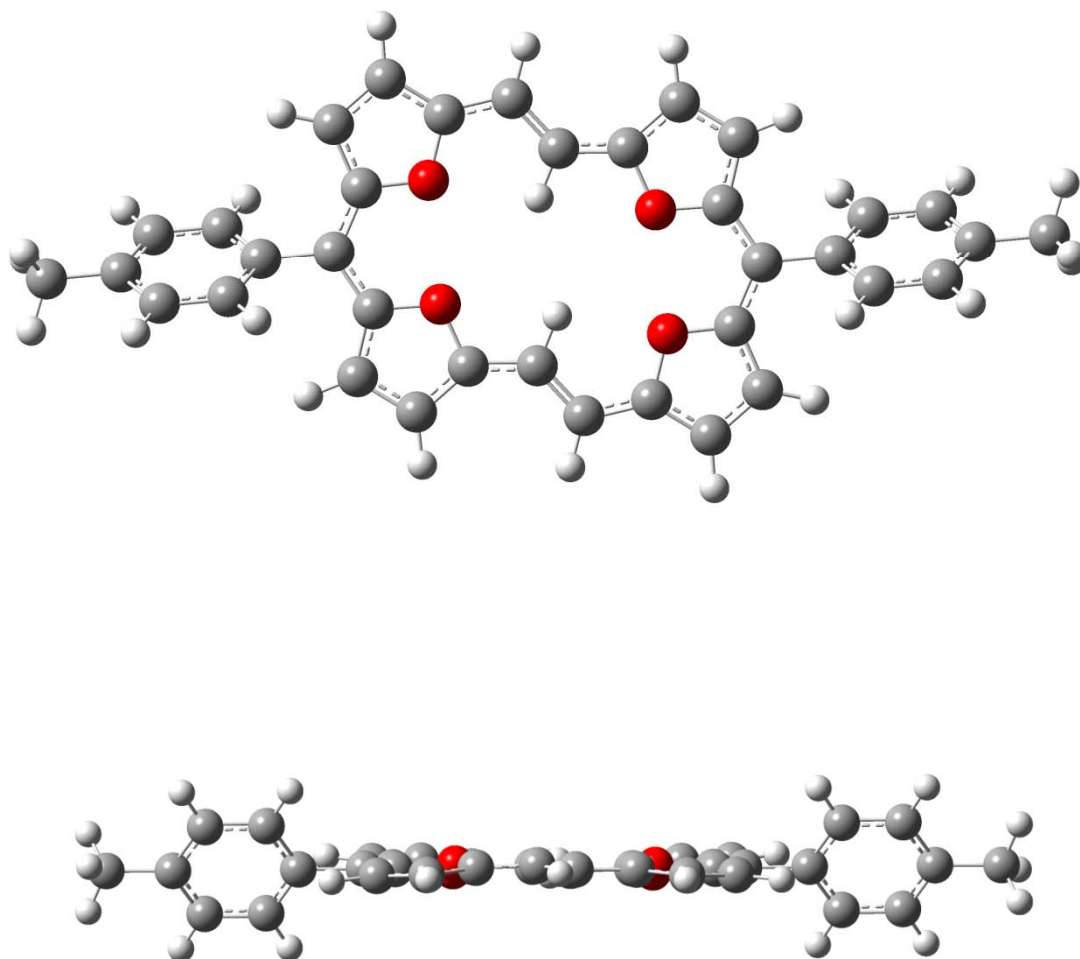


**Figure S27:** Calculation of NICS values for all individual rings in **12a**. The calculation was performed by placing ghost atoms at 1 Å intervals. The NICS vs.  $r$  (distance from centre in Å) graphs are shown on the next page (Figure S28).

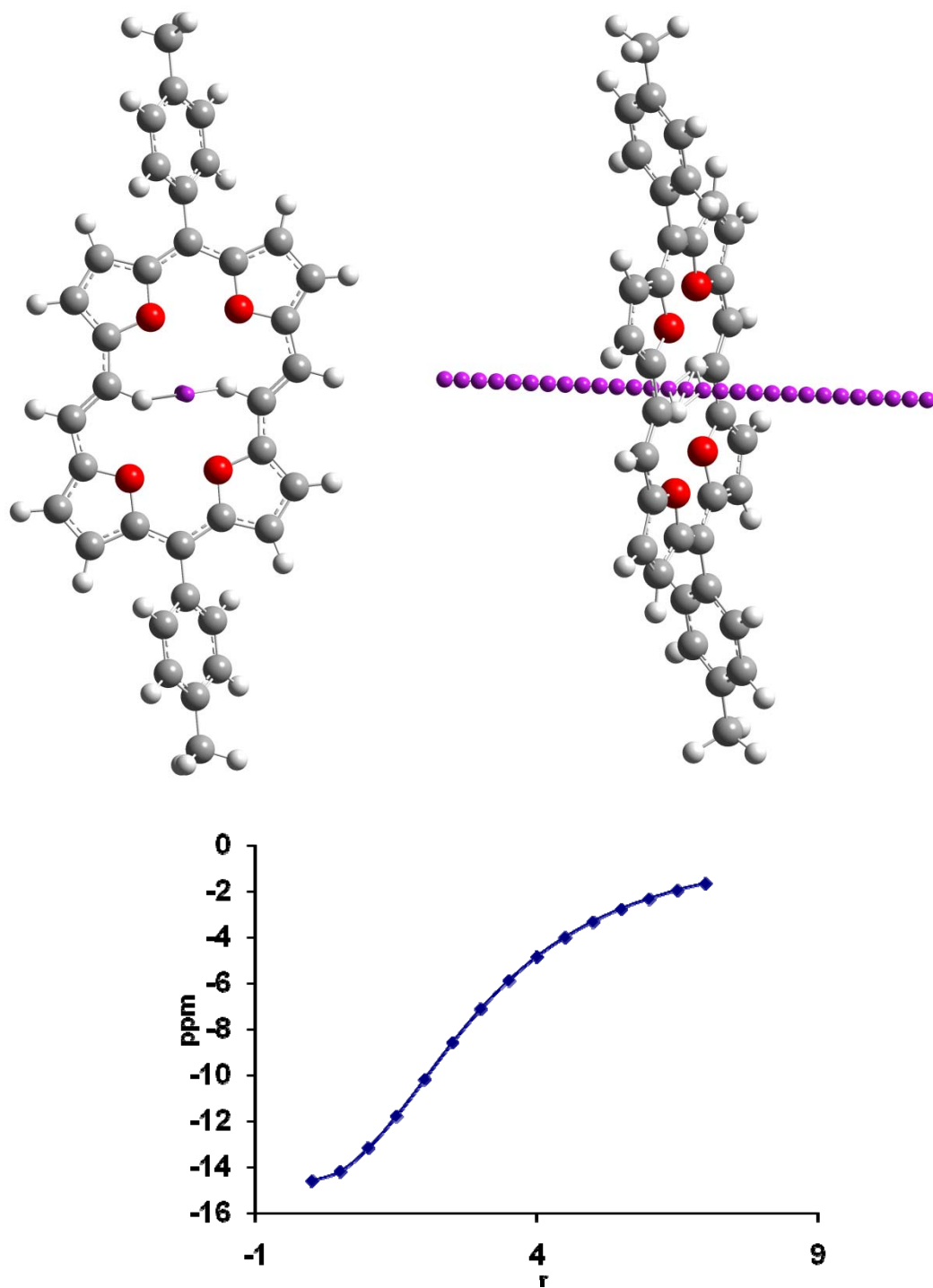


**Figure S28:** As shown above, a set of two furan rings of **12a** (attached to one of the trans double bond) are showing a dip at 1 Å in the calculated NICS values. The behavior of two furan rings is also different from an isolated furan ring (which shows no dip at 1 Å).<sup>[4]</sup> This is also clear from the X-Ray structure. Further, phenyl rings are showing the normal behavior like benzene but with decreased NICS values.

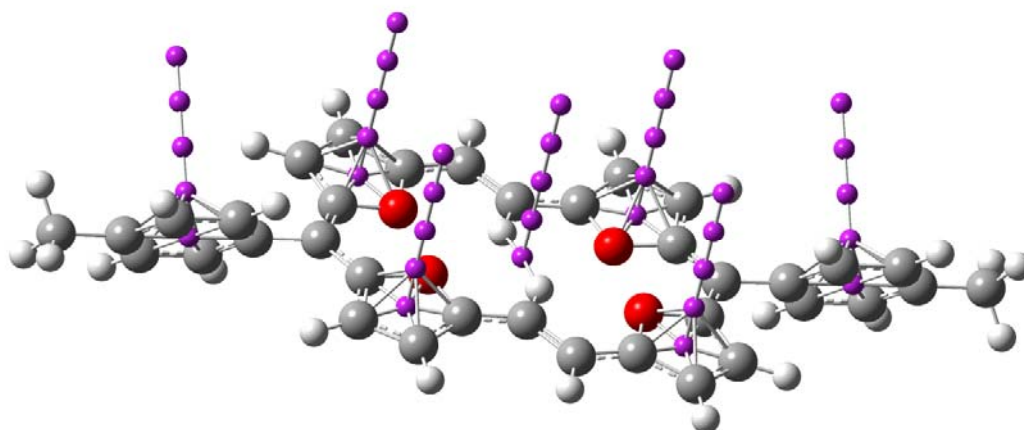
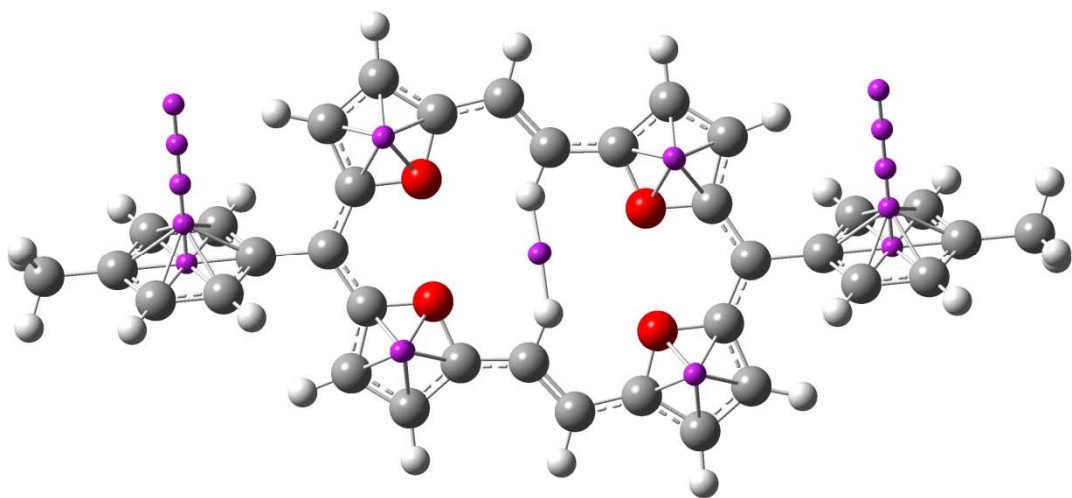
[4] A. Stanger, *J. Org. Chem.* **2006**, *71*, 883-893.



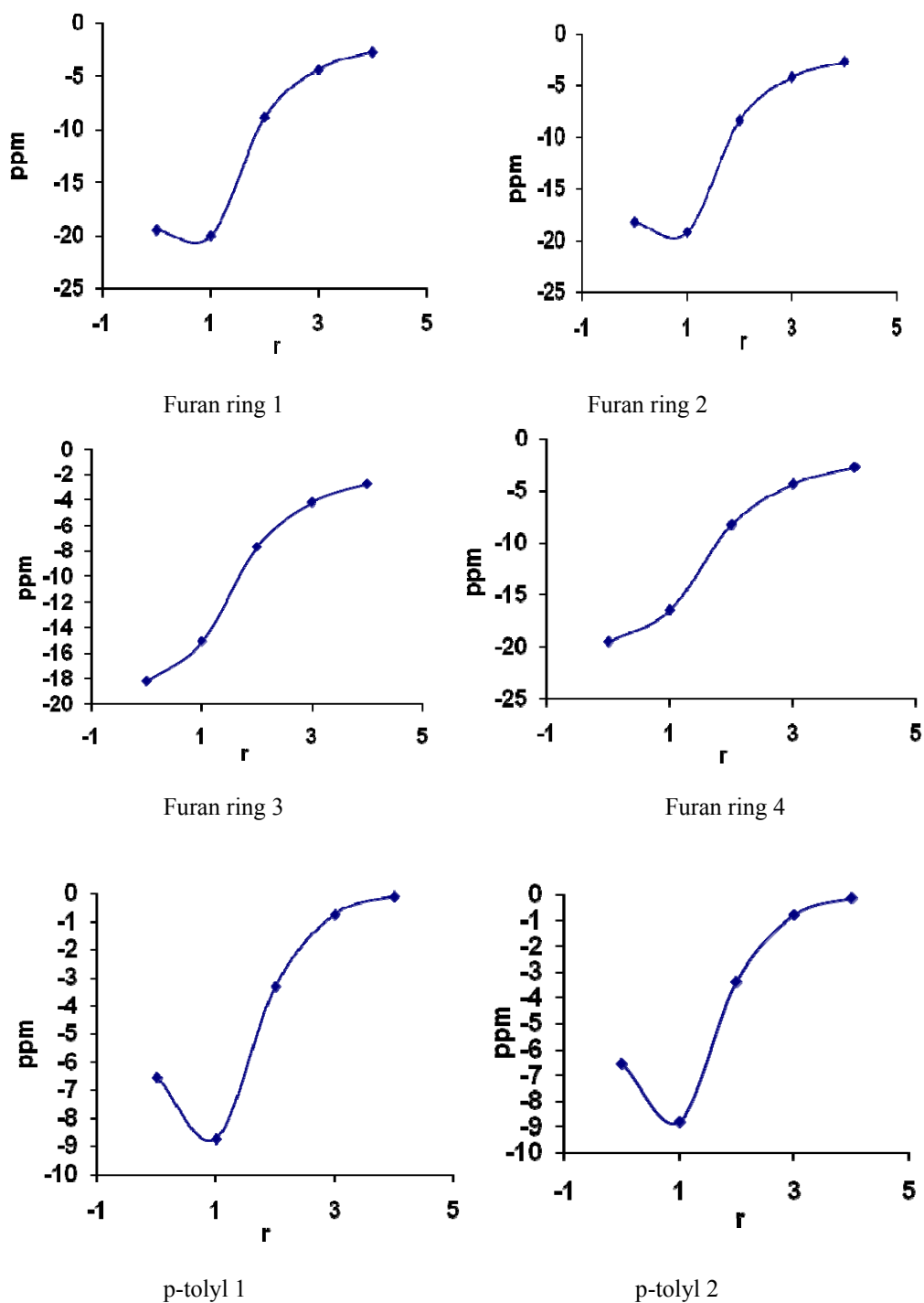
**Figure S29:** Energy minimized structure of **12b** by DFT method at B3LYP/6-311G(d) level using the Gaussian09 software package (Top and side views).



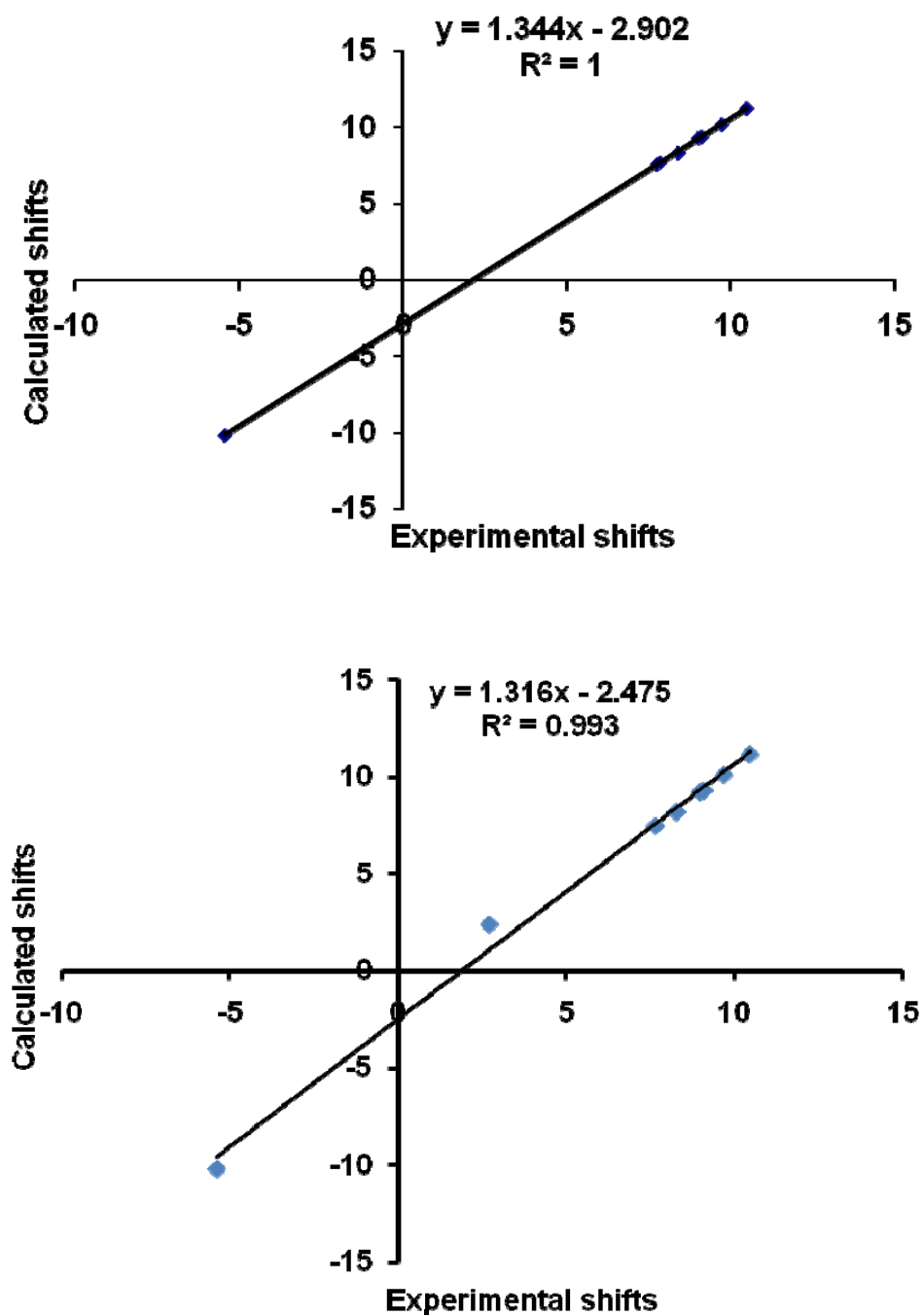
**Figure S30:** The ghost (Bq) atoms were placed at the centre of the molecule (in purple) at successive distances of 0.5 Å to probe the aromaticity. The -ve values of NICS clearly displays the aromaticity of **12b**. At centre NICS is maximum and it goes on decreasing as we move farther from the centre



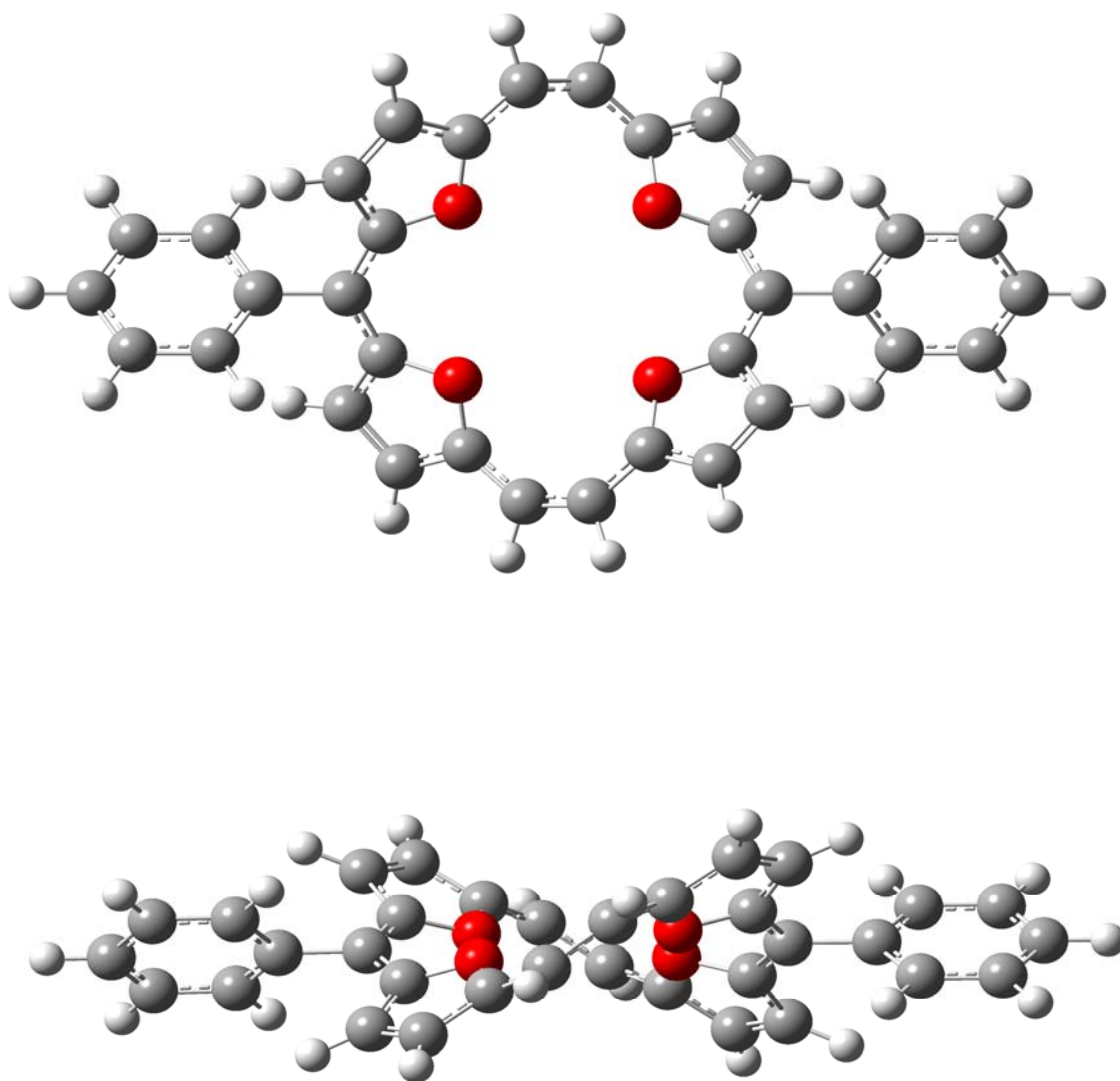
**Figure S31:** When Ghost atoms were placed at the centre of all the individual rings of **12b** with interval of 1 Å, the resulting NICS vs.  $r$  (distance from centre in Å) graphs are shown on the next page (Figure S32).



**Figure S32:** Similar to **12a**, as shown above, the two of the furan rings of **12b** (neighboring to the trans double bond) are showing a dip in the NICS (aromaticity) value at 1 Å, and remaining two are not showing. Also the behavior is different from the normal single furan ring alone (which shows no dip at 1 Å). The X-Ray structure corroborates this observation. *p*-Tolyl rings are showing the normal behavior like toluene but with decreased NICS values.

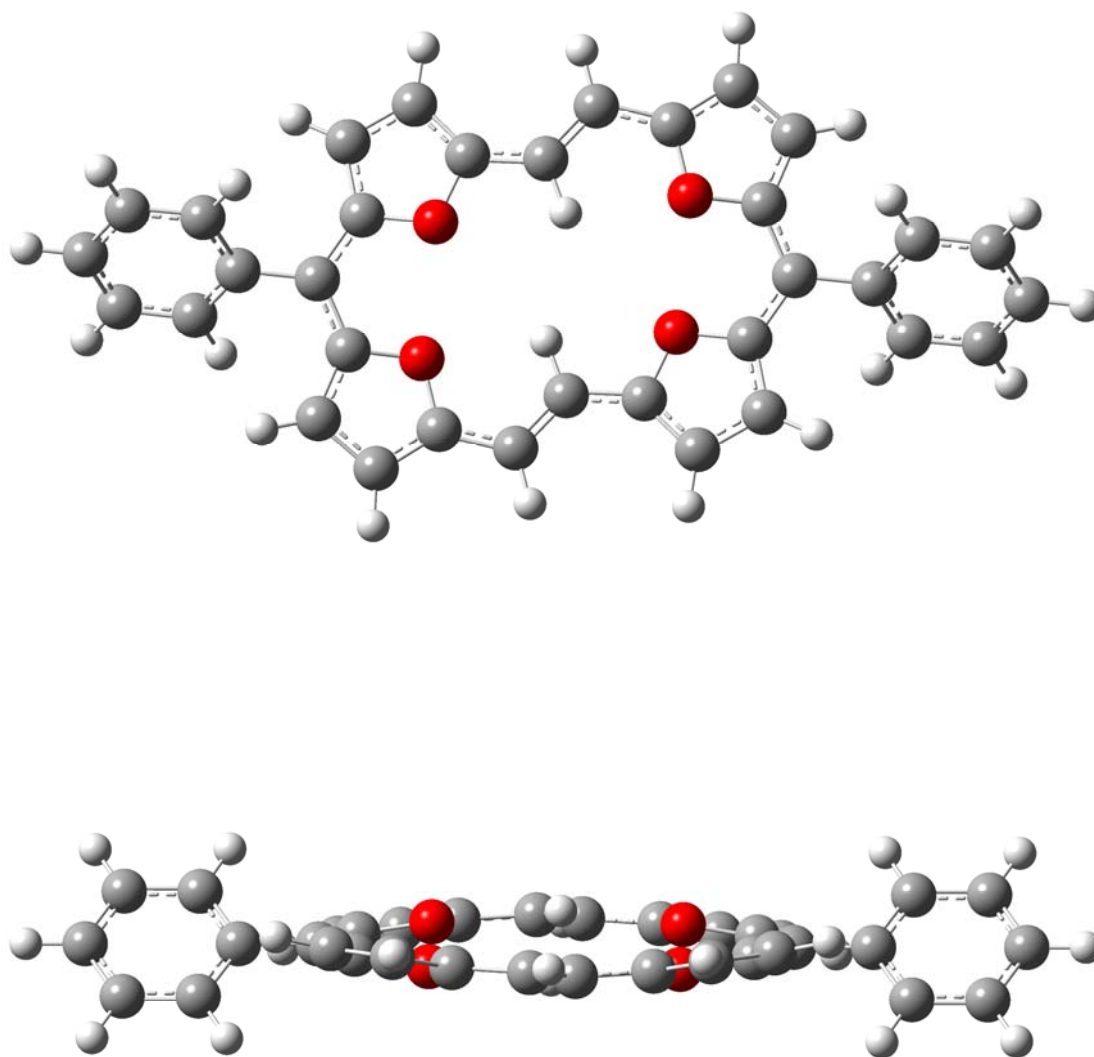


**Figure S33:** Shows the correlation between the  $^1\text{H}$  experimental chemical shifts (ppm) and the calculated chemical shifts (using DFT method and B3LYP/6-311G(d) level) of **12a** (Upper) and **12b** (lower).

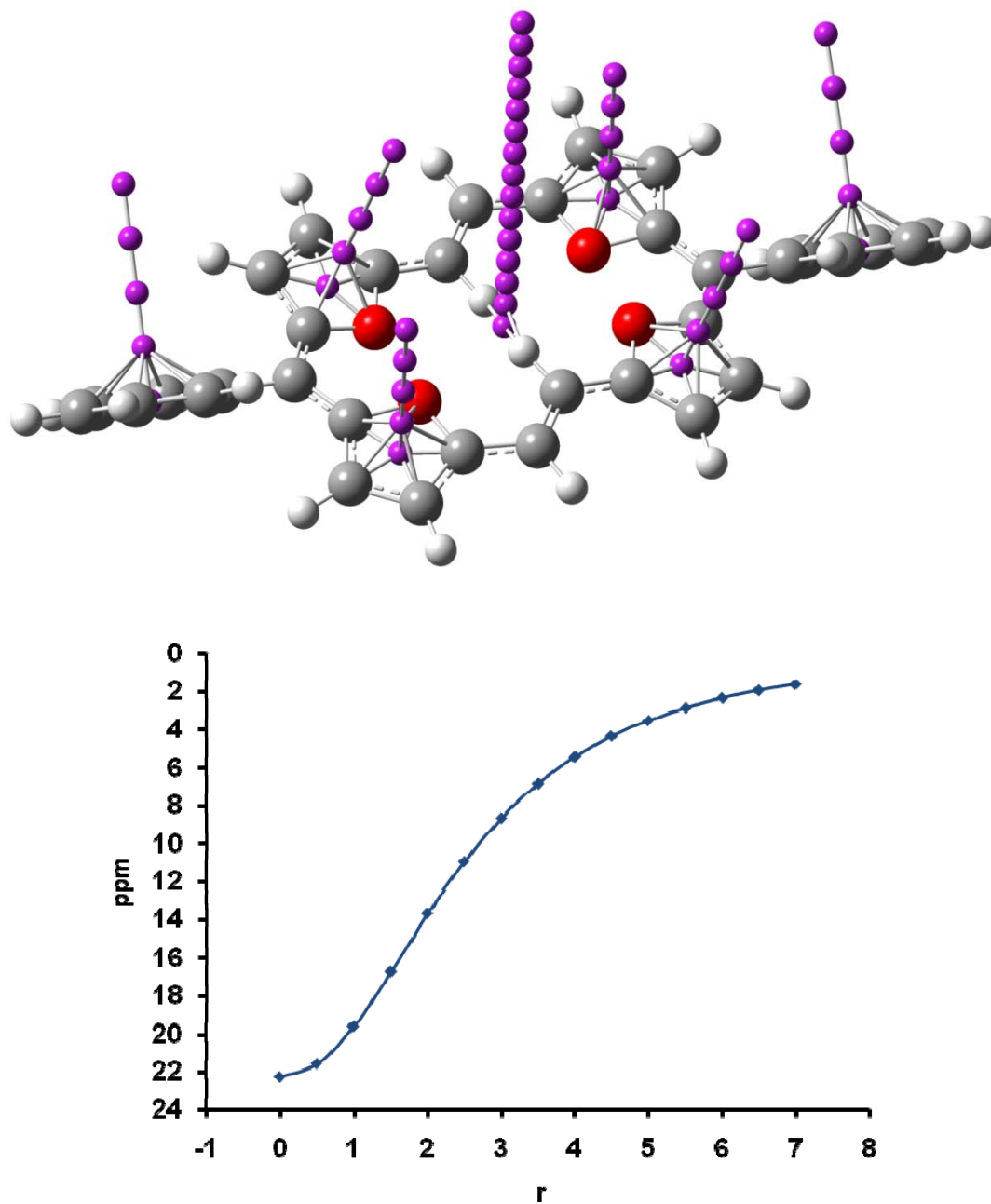


**Figure S34:** Optimized structure of **12a** with *cis, cis* geometry at the two ethylenic links. Top view (upper) and the side view (lower). The side view indicates the loss of planarity due to *cis* configuration of the two double bonds.

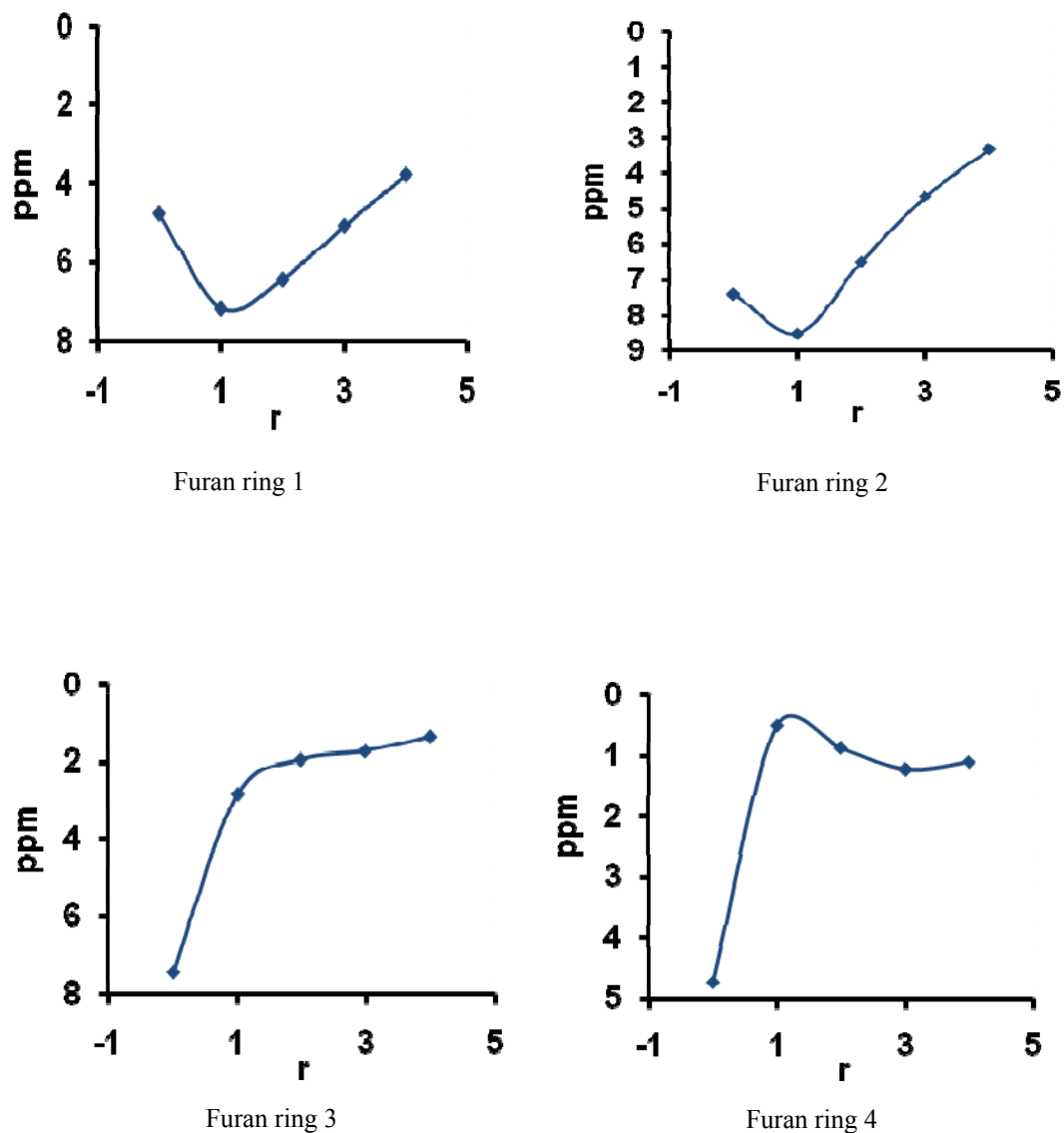




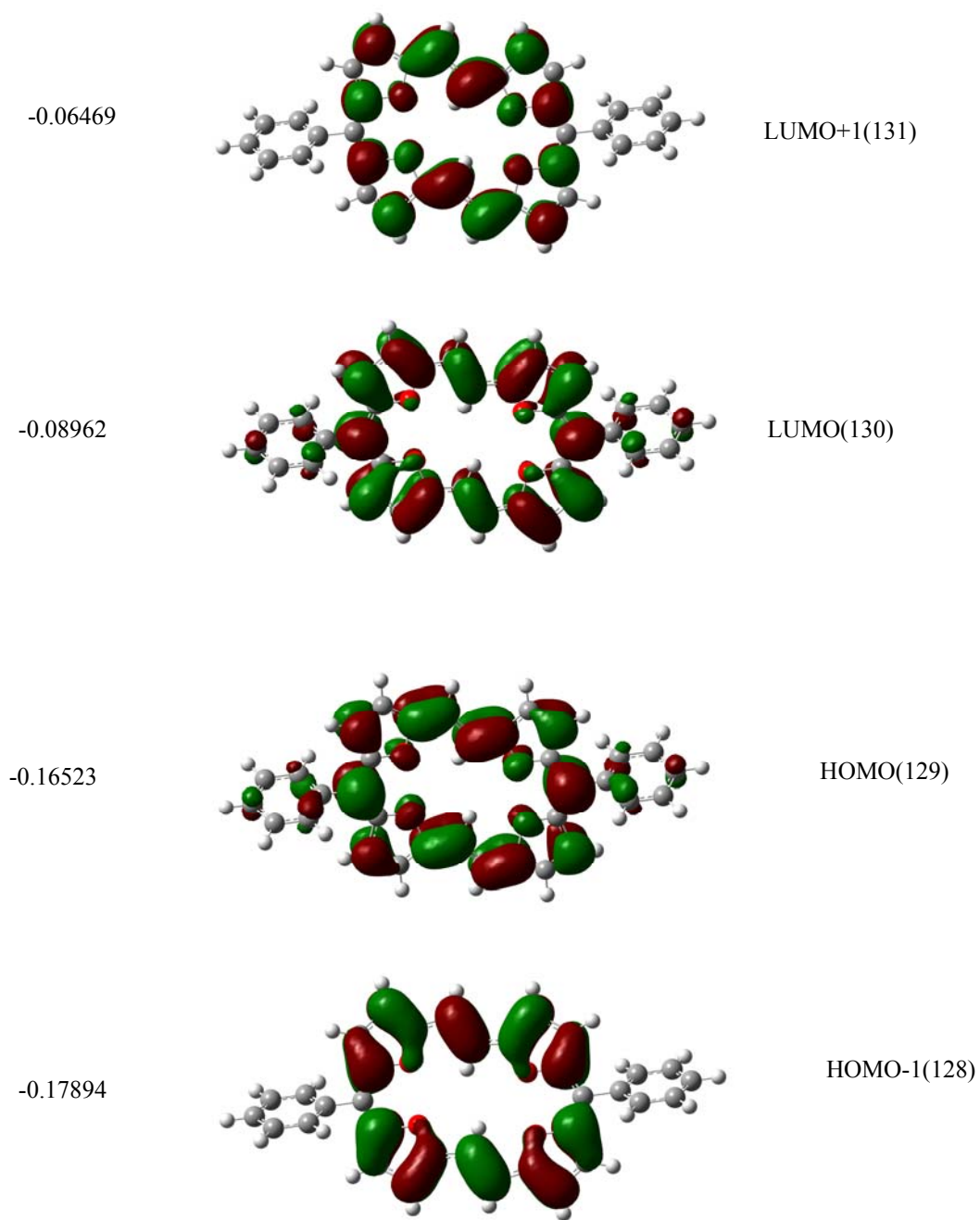
**Figure S35:** Energy minimized structure of antiaromatic dication **13a**. Upper (top view), lower (side view).



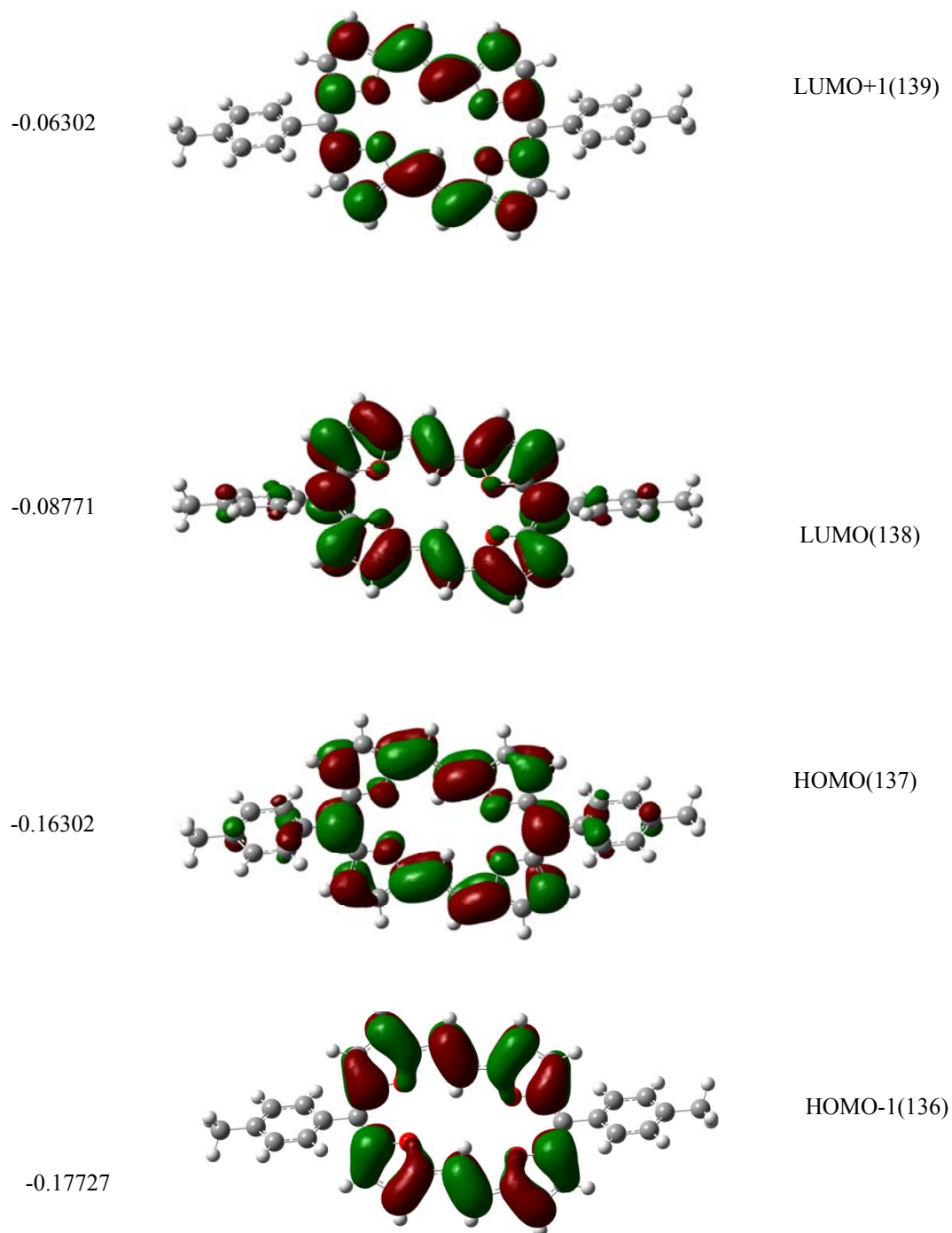
**Figure S36:** Placement of the ghost atoms (at 1 Å intervals) at the centre of all the individual rings as well as the main ring of **13a** (anti aromatic). The +ve NICS values (NICS 1 = 19.59) indicates the antiaromatic behaviour of the dication **13a**. The resulting NICS vs. r (distance from centre in Å) graph is also shown for the main centre of the **13a**. The graphs for the four furan rings are shown (Figure S37). The phenyl groups were showing almost the normal behavior like benzene, so there graphs are not shown.



**Figure S37:** Here two furan rings are showing a dip in the +ve (antiaromatic) NICS values at a distance of 1 Å from the centre, compared to the other two furan rings. The latter two furan rings are also slightly non-equivalent as indicated by their NICS vs.  $r$  graphs. Normal furan is aromatic (-ve NICS), but antiaromatic ring current of **13a** made the NICS values of the furan rings as +ve.



**Figure S38:** HOMO-LUMO and their neighbouring energy levels for **12a** are shown along with their energies (left) in a.u.. HOMO- LUMO levels are showing high degree of delocalisation on the  $[22\pi]$  annulene ring periphery. The energy of HOMO = -0.16523 a.u. and that of LUMO = -0.08962 a.u. .



**Figure S39:** HOMO-LUMO and their neighbouring energy levels for **12b** are shown along with their energies (left) in a.u.. HOMO- LUMO levels are showing high degree of delocalisation on the  $[22\pi]$  annulene ring periphery. The energy of HOMO = -0.16302 and that of LUMO = -0.08771

### Cartesian coordinates

**Table S2:** Cartesian coordinates of **12a**

SCF Done: E (RB3LYP) = -1610.02038082 A.U. after 16 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	2.438434	-1.518581	0.025317
2	8	0	2.158495	0.996299	-0.085623
3	6	0	2.138711	-2.848425	-0.099328
4	6	0	0.777373	-3.194926	-0.098275
5	1	0	0.522511	-4.243348	-0.214006
6	6	0	3.345356	-3.548389	-0.245659
7	1	0	3.439082	-4.617494	-0.370613
8	6	0	4.376148	-2.614806	-0.223015
9	1	0	5.431843	-2.807876	-0.333945
10	6	0	3.792332	-1.342068	-0.058220
11	6	0	4.321883	-0.039498	-0.009936
12	6	0	5.800766	0.127811	0.002880
13	6	0	6.586573	-0.482782	0.991756
14	1	0	6.102421	-1.067850	1.766469
15	6	0	7.970148	-0.327109	1.002022
16	1	0	8.558480	-0.802817	1.780452
17	6	0	8.597114	0.445198	0.026029
18	1	0	9.675430	0.567589	0.035094
19	6	0	7.829287	1.058784	-0.961803
20	1	0	8.308680	1.655524	-1.731508
21	6	0	6.446137	0.900124	-0.974557
22	1	0	5.856248	1.362560	-1.758798
23	6	0	3.512820	1.113054	0.025094
24	6	0	3.808952	2.482636	0.200145
25	1	0	4.797415	2.895155	0.331332
26	6	0	2.606590	3.176933	0.201043
27	1	0	2.473847	4.241659	0.326725
28	6	0	1.576124	2.238939	0.029677
29	6	0	0.180582	2.204704	-0.015807
30	1	0	-0.203733	1.198024	-0.137220
31	8	0	-2.438434	1.518581	-0.025319
32	8	0	-2.158495	-0.996299	0.085621
33	6	0	-2.138712	2.848425	0.099326
34	6	0	-0.777373	3.194926	0.098272

35	1	0	-0.522510	4.243352	0.214006
36	6	0	-3.345356	3.548389	0.245656
37	1	0	-3.439083	4.617494	0.370610
38	6	0	-4.376148	2.614806	0.223013
39	1	0	-5.431846	2.807877	0.333941
40	6	0	-3.792333	1.342069	0.058218
41	6	0	-4.321883	0.039498	0.009936
42	6	0	-5.800766	-0.127812	-0.002878
43	6	0	-6.586574	0.482783	-0.991754
44	1	0	-6.102425	1.067850	-1.766463
45	6	0	-7.970148	0.327110	-1.002019
46	1	0	-8.558481	0.802820	-1.780448
47	6	0	-8.597115	-0.445199	-0.026026
48	1	0	-9.675424	-0.567589	-0.035091
49	6	0	-7.829286	-1.058787	0.961804
50	1	0	-8.308675	-1.655524	1.731504
51	6	0	-6.446136	-0.900126	0.974558
52	1	0	-5.856247	-1.362564	1.758797
53	6	0	-3.512820	-1.113054	-0.025092
54	6	0	-3.808951	-2.482637	-0.200141
55	1	0	-4.797412	-2.895155	-0.331324
56	6	0	-2.606590	-3.176932	-0.201041
57	1	0	-2.473847	-4.241658	-0.326720
58	6	0	-1.576124	-2.238938	-0.029678
59	6	0	-0.180581	-2.204703	0.015805
60	1	0	0.203734	-1.198023	0.137216

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**Table S3:** Cartesian coordinates of **12b**

SCF Done: E (RB3LYP) = -1688.67114151 A.U. after 17 cycles.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	2.414409	-1.557390	0.027290
2	8	0	2.174728	0.961509	-0.092596
3	6	0	2.092811	-2.881945	-0.098366
4	6	0	3.287505	-3.601093	-0.249496
5	1	0	3.363467	-4.671338	-0.376416
6	6	0	4.333321	-2.684205	-0.229116
7	1	0	5.385331	-2.893757	-0.344116
8	6	0	3.770846	-1.402405	-0.060957
9	6	0	4.321963	-0.108601	-0.012886
10	6	0	3.530594	1.056366	0.022474
11	6	0	3.847749	2.420654	0.201333
12	1	0	4.842236	2.816839	0.336665
13	6	0	2.656494	3.133991	0.200737
14	1	0	2.540217	4.200296	0.329019
15	6	0	1.611775	2.212827	0.024594
16	6	0	0.215820	2.200979	-0.022012
17	1	0	-0.184695	1.200873	-0.145841
18	6	0	-0.725959	3.206263	0.095088
19	1	0	-0.453898	4.250190	0.212762
20	6	0	5.802576	0.034824	-0.000009
21	6	0	6.584292	-0.593342	0.978133
22	1	0	6.098044	-1.178124	1.751930
23	6	0	7.970072	-0.456637	0.986183
24	1	0	8.546876	-0.949818	1.763755
25	6	0	8.629292	0.311964	0.023572
26	6	0	10.131920	0.451417	0.020428
27	1	0	10.575077	0.044189	0.931646
28	1	0	10.438301	1.498536	-0.059491
29	1	0	10.579110	-0.078606	-0.827305
30	6	0	7.847993	0.941856	-0.952189
31	1	0	8.330968	1.541889	-1.719039
32	6	0	6.464829	0.805908	-0.967673
33	1	0	5.886118	1.288513	-1.748286
34	8	0	-2.414409	1.557393	-0.027304
35	8	0	-2.174727	-0.961505	0.092582



36	6	0	-2.092812	2.881948	0.098350
37	6	0	-3.287506	3.601096	0.249479
38	1	0	-3.363468	4.671341	0.376397
39	6	0	-4.333322	2.684207	0.229100
40	1	0	-5.385332	2.893760	0.344099
41	6	0	-3.770846	1.402408	0.060945
42	6	0	-4.321963	0.108603	0.012880
43	6	0	-3.530594	-1.056364	-0.022477
44	6	0	-3.847751	-2.420653	-0.201323
45	1	0	-4.842239	-2.816839	-0.336643
46	6	0	-2.656496	-3.133990	-0.200731
47	1	0	-2.540220	-4.200295	-0.329004
48	6	0	-1.611775	-2.212824	-0.024603
49	6	0	-0.215821	-2.200976	0.021996
50	1	0	0.184695	-1.200869	0.145819
51	6	0	0.725959	-3.206260	-0.095102
52	1	0	0.453897	-4.250188	-0.212772
53	6	0	-5.802576	-0.034822	0.000012
54	6	0	-6.584296	0.593325	-0.978135
55	1	0	-6.098053	1.178096	-1.751944
56	6	0	-7.970077	0.456619	-0.986177
57	1	0	-8.546886	0.949786	-1.763753
58	6	0	-8.629291	-0.311966	-0.023548
59	6	0	-10.131917	-0.451445	-0.020406
60	1	0	-10.575105	-0.043938	-0.931483
61	1	0	-10.438275	-1.498597	0.059188
62	1	0	-10.579094	0.078295	0.827509
63	6	0	-7.847986	-0.941835	0.952223
64	1	0	-8.330957	-1.541851	1.719090
65	6	0	-6.464823	-0.805887	0.967697
66	1	0	-5.886107	-1.288474	1.748317

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**Table S4:** Cartesian coordinates of **12a (Cis configuration)**:

SCF Done: E(RB3LYP) = -1609.97021900 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.560190	3.759211	-0.371480
2	6	0	1.527620	2.833502	-0.763689
3	6	0	2.658224	3.134540	-1.543579
4	1	0	2.796620	4.051692	-2.097524
5	6	0	3.539219	2.083637	-1.422047
6	1	0	4.515320	1.984555	-1.869319
7	6	0	2.942518	1.131842	-0.573509
8	6	0	3.547597	0.003568	-0.003047
9	6	0	5.045856	0.001987	-0.016204
10	6	0	5.758108	-1.032540	-0.640515
11	1	0	5.209932	-1.833090	-1.125580
12	6	0	7.150287	-1.033108	-0.657005
13	1	0	7.682466	-1.837246	-1.155547
14	6	0	7.858559	-0.002279	-0.041641
15	1	0	8.943903	-0.003882	-0.051465
16	1	0	0.842763	4.756850	-0.700039
17	6	0	0.569206	-3.753207	0.432655
18	6	0	1.539048	-2.822255	0.806052
19	6	0	2.679398	-3.115680	1.574577
20	1	0	2.824773	-4.027276	2.135844
21	6	0	3.559726	-2.067147	1.429390
22	1	0	4.542099	-1.964194	1.861844
23	6	0	2.951469	-1.122959	0.580862
24	6	0	5.772361	1.034240	0.595325
25	1	0	5.235573	1.836380	1.090384
26	6	0	7.164623	1.030590	0.586526
27	1	0	7.708184	1.833029	1.075437
28	1	0	0.853048	-4.745939	0.774614
29	6	0	-0.560194	-3.759207	-0.371509
30	6	0	-1.527623	-2.833492	-0.763709
31	6	0	-2.658232	-3.134522	-1.543595
32	1	0	-2.796631	-4.051668	-2.097549
33	6	0	-3.539227	-2.083622	-1.422044
34	1	0	-4.515333	-1.984536	-1.869306
35	6	0	-2.942520	-1.131834	-0.573503

36	6	0	-3.547596	-0.003567	-0.003023
37	6	0	-5.045855	-0.001989	-0.016164
38	6	0	-5.772351	-1.034242	0.595375
39	1	0	-5.235554	-1.836379	1.090430
40	6	0	-7.164612	-1.030596	0.586592
41	1	0	-7.708165	-1.833035	1.075512
42	6	0	-7.858558	0.002270	-0.041569
43	1	0	-8.943902	0.003870	-0.051381
44	1	0	-0.842773	-4.756845	-0.700066
45	6	0	-0.569207	3.753207	0.432688
46	6	0	-1.539045	2.822251	0.806086
47	6	0	-2.679391	3.115669	1.574620
48	1	0	-2.824763	4.027260	2.135896
49	6	0	-3.559720	2.067138	1.429428
50	1	0	-4.542091	1.964182	1.861885
51	6	0	-2.951467	1.122956	0.580890
52	6	0	-5.758117	1.032535	-0.640469
53	1	0	-5.209948	1.833086	-1.125542
54	6	0	-7.150296	1.033099	-0.656944
55	1	0	-7.682482	1.837235	-1.155481
56	1	0	-0.853052	4.745938	0.774646
57	8	0	-1.680346	-1.573512	-0.233431
58	8	0	1.685025	-1.567674	0.261377
59	8	0	1.680346	1.573517	-0.233424
60	8	0	-1.685024	1.567674	0.261402

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**Table S5:** Cartesian coordinates of **13a**:

SCF Done: E(RB3LYP) = -1609.49784641 A.U. after 17 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-2.450962	-1.489983	-0.141256
2	8	0	-2.198629	1.008503	0.261604
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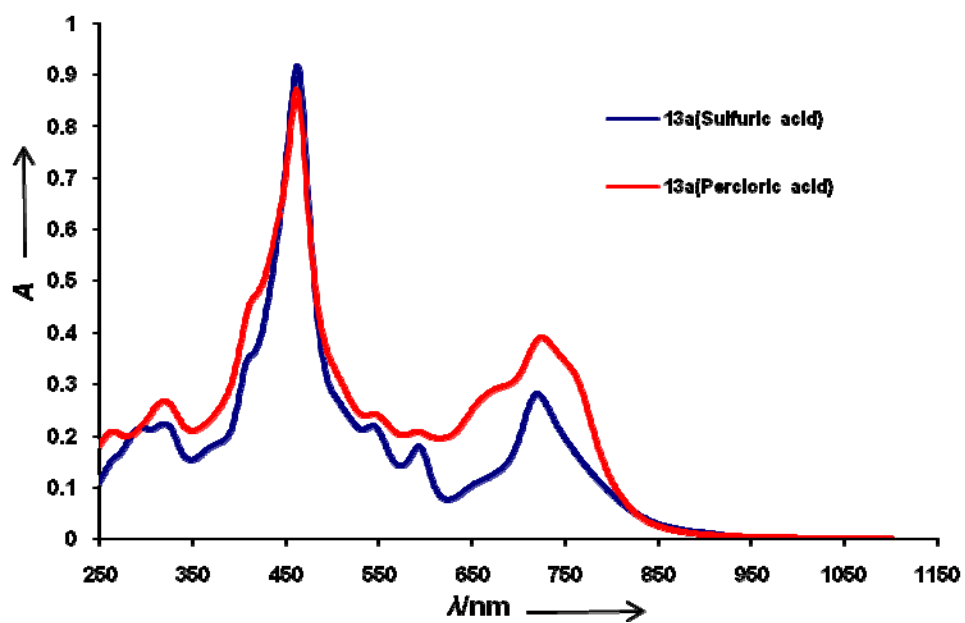


Figure S40: UV-Vis. spectra of **13a** in H<sub>2</sub>SO<sub>4</sub> and HClO<sub>4</sub>.

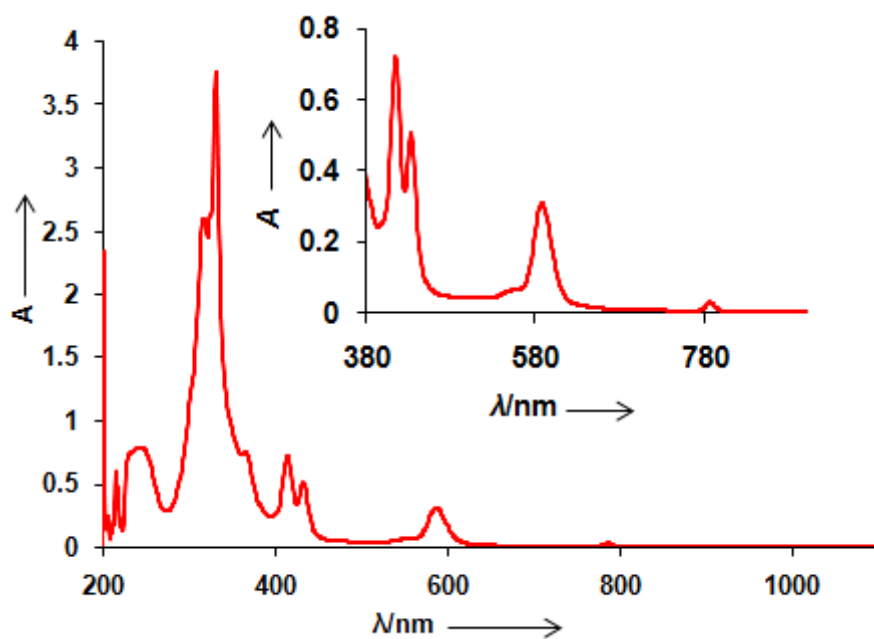


Figure S41: Partial auto-oxidation of **11a** to **12a** (UV-Vis. spectra is showing the presence of both the **11a** as well as traces of **12a**)

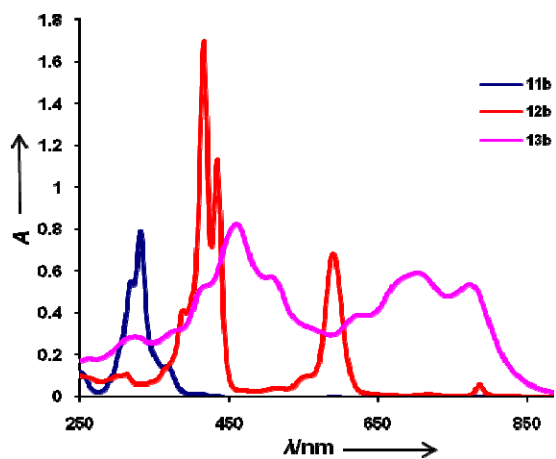


Figure S42a: UV-Vis. spectra of **11b** (DCM), **12b** (DCM) and **13b** (HClO<sub>4</sub>).

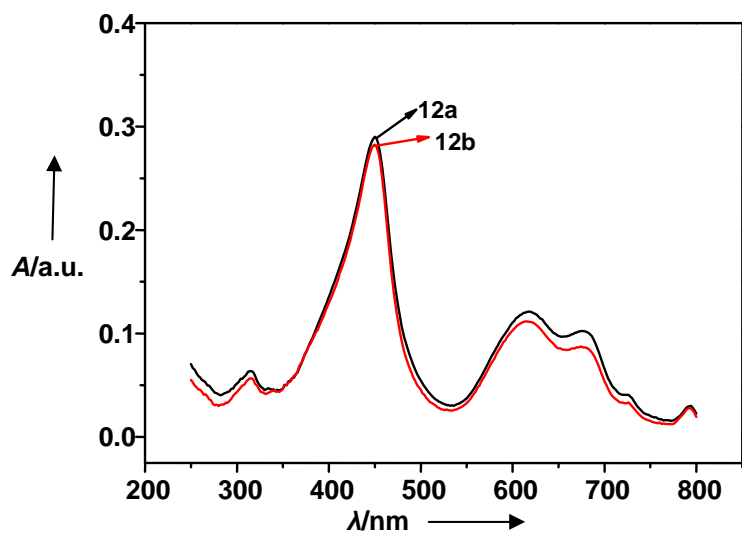


Figure S42b: Normalized UV-vis absorption spectra of thin films of **12a** and **12b** at room temperature.

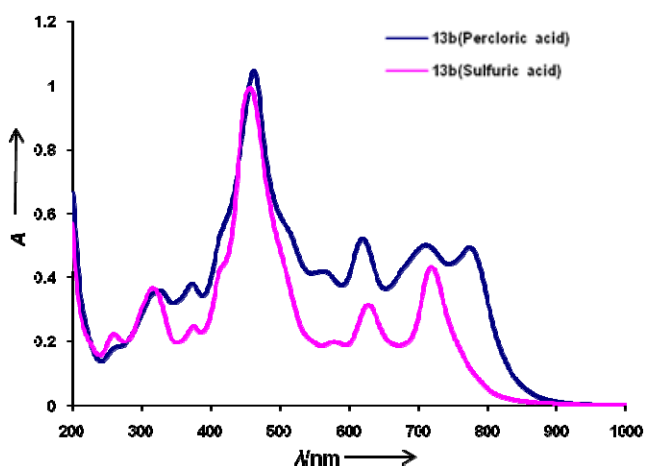
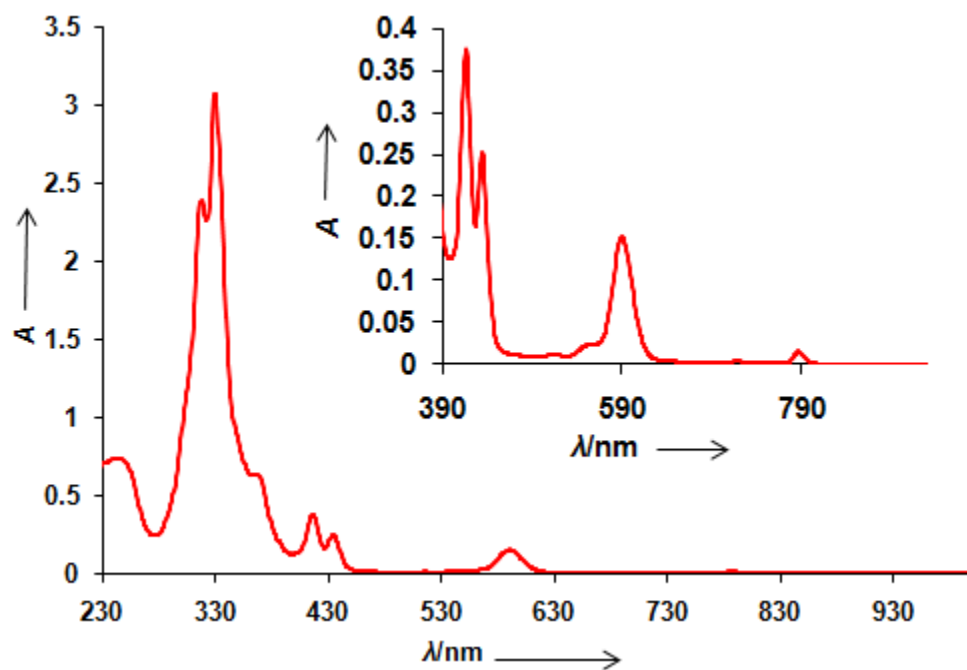
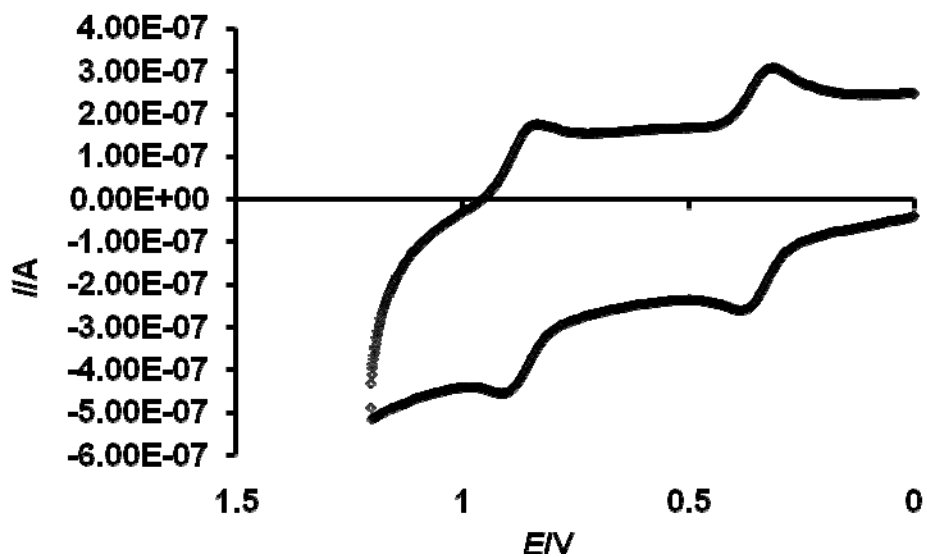


Figure S43: UV-Vis. spectra of **13b** in H<sub>2</sub>SO<sub>4</sub> and HClO<sub>4</sub>.

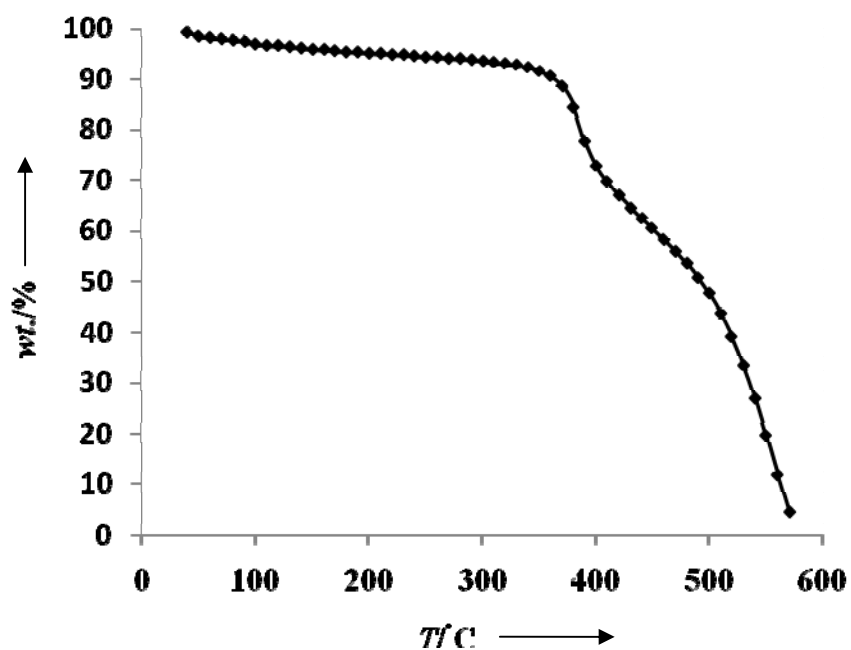


**Figure S44:** Partial auto-oxidation of **11b** to **12b** (UV-Vis. spectra is showing the presence of both the **11b** as well as traces of **12b**)

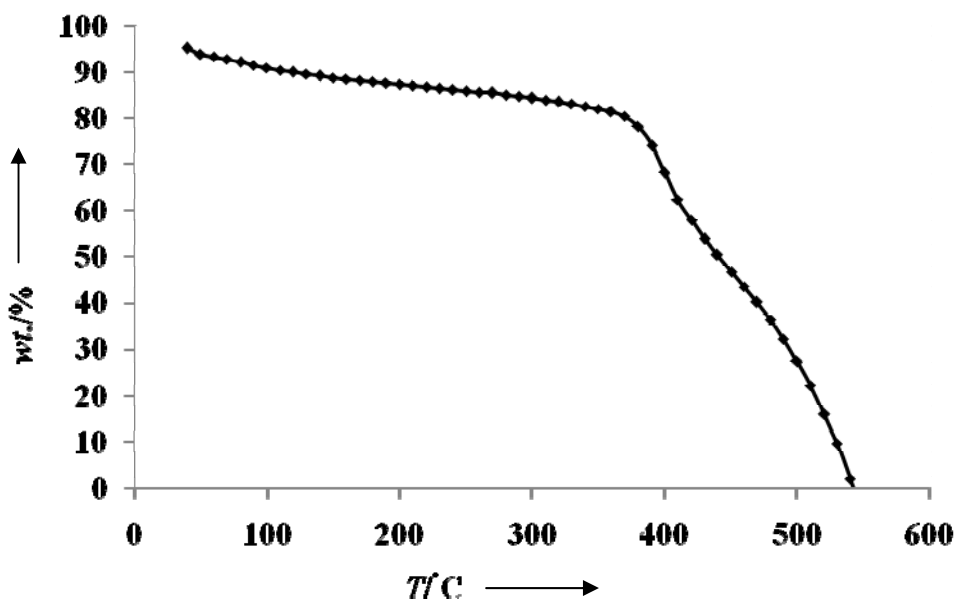




**Figure S45:** Cyclic voltammogram (CV) for **12b** (DCM, electrolyte TBAPF<sub>6</sub>; working electrode: Pt; ref. electrode: Ag/AgCl; Scan rate 100 mV s<sup>-1</sup>).



**Figure S46:** TGA Analysis of **12a** under N<sub>2</sub> with temperature rise of 10 °C per minute. Thus **12a** is highly stable as it is having a high thermal decomposition temp. of about 374 °C.



**Figure S47:** TGA Analysis of **12b** under N<sub>2</sub> with temperature rise of 10 °C per minute. Thus **12b** is highly stable as it is having a high onset thermal decomposition temp. of about 380 °C.

### X-Ray Diffraction Analysis of 12a:

Single crystals of **12a** suitable for an X-Ray crystal structure determination were grown in a dark, quiet and undisturbed place from dry DCM with a toluene layer upon it (2 weeks).

**Table S6:** The crystallographic data for **12a**.

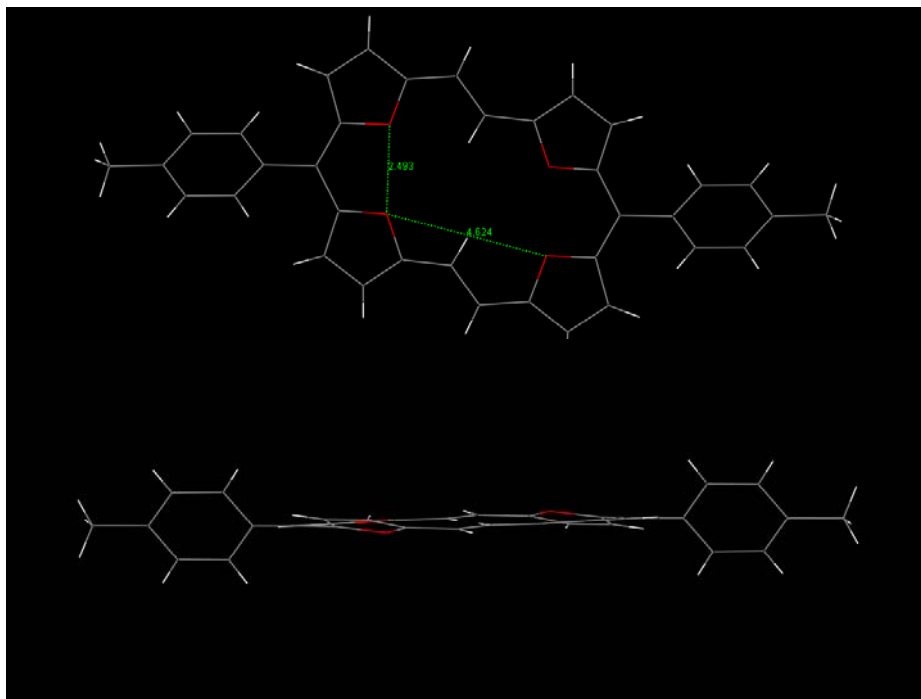
Empirical formula	C <sub>34</sub> H <sub>22</sub> O <sub>4</sub>
Formula weight	494.52
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 13.091(3) Å    alpha = 90 deg. b = 9.1718(12) Å    beta = 107.03(2) deg. c = 10.744(2) Å    gamma = 90 deg.
Volume	1233.5(4) Å <sup>3</sup>
Z, Calculated density	2, 1.331 Mg/m <sup>3</sup>
Absorption coefficient	0.087 mm <sup>-1</sup>
F(000)	516
Crystal size	0.34 x 0.32 x 0.28 mm
Theta range for data collection	3.66 to 25.00 deg.
Limiting indices	-15<=h<=11, -10<=k<=10, -12<=l<=12
Reflections collected / unique	8079 / 2158 [R(int) = 0.0495]
Completeness to theta = 25.00	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9761 and 0.9711
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	2158 / 0 / 172
Goodness-of-fit on F <sup>2</sup>	0.852
Final R indices [I>2sigma(I)]	R1 = 0.0356, wR2 = 0.0723
R indices (all data)	R1 = 0.0641, wR2 = 0.0781
Largest diff. peak and hole	0.100 and -0.149 e.Å <sup>-3</sup>

The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 825048). The data can be obtained free of charge via the Internet at [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).

### X-Ray Diffraction Analysis of **12b**:

Single crystals of **12b** suitable for an X-Ray crystal structure determination were grown in a dark, quiet and undisturbed place from o-dichlorobenzene (10 days).

A)



B)

**Figure S48:** Crystal structure of **12b** (a) molecular structure showing distances between oxygen atoms in the crystal. (b) Side view .

**Table S7:** The crystallographic data for **12b**.

---

Empirical formula	C <sub>36</sub> H <sub>26</sub> O <sub>4</sub>
Formula weight	522.57
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P b c a
Unit cell dimensions	a = 34.541(2) Å    alpha = 90 deg. b = 9.5379(7) Å    beta = 90 deg. c = 7.8246(6) Å    gamma = 90 deg.
Volume	2577.8(3) Å <sup>3</sup>
Z, Calculated density	4, 1.347 Mg/m <sup>3</sup>
Absorption coefficient	0.087 mm <sup>-1</sup>
F(000)	1096
Crystal size	0.21 x 0.17 x 0.13 mm
Theta range for data collection	3.42 to 25.00 deg.
Limiting indices	-41 ≤ h ≤ 41, -10 ≤ k ≤ 11, -9 ≤ l ≤ 9
Reflections collected / unique	17815 / 2270 [R(int) = 0.0975]
Completeness to theta = 25.00	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9888 and 0.9820
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	2270 / 0 / 182
Goodness-of-fit on F <sup>2</sup>	0.813
Final R indices [I > 2 sigma(I)]	R1 = 0.0418, wR2 = 0.0776
R indices (all data)	R1 = 0.1091, wR2 = 0.0872
Largest diff. peak and hole	0.149 and -0.122 e.Å <sup>-3</sup>

---

The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 825049). The data can be obtained free of charge via the Internet at [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).

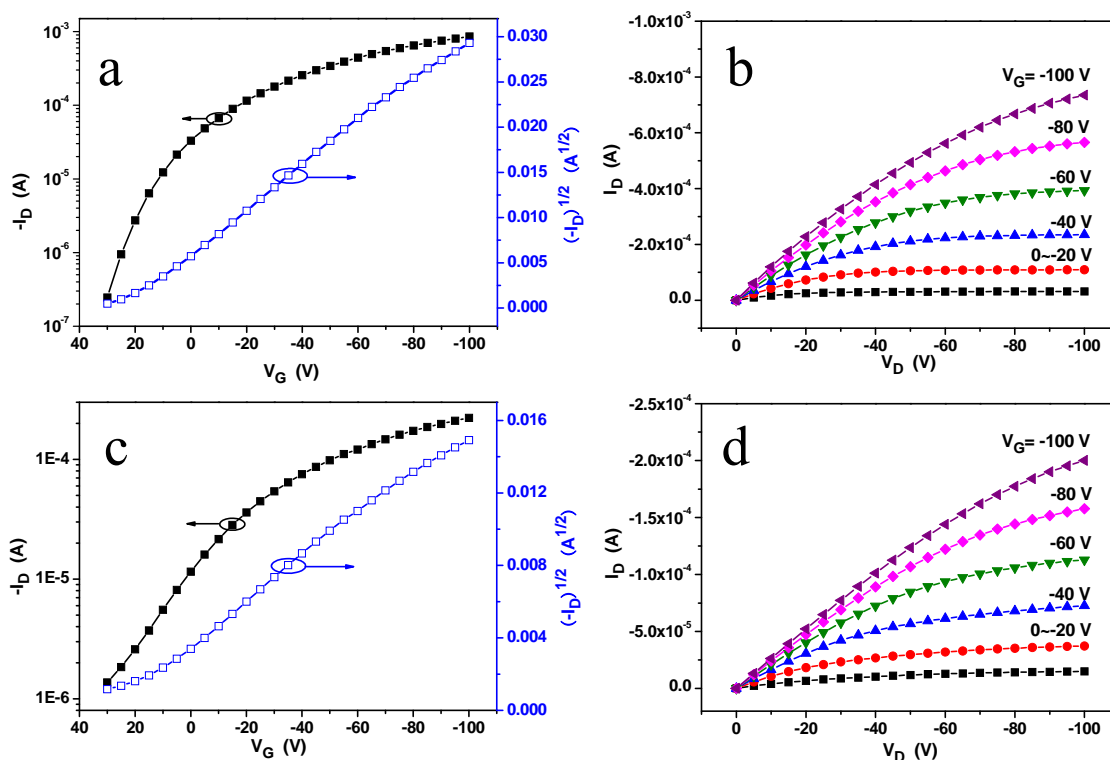
## Thin film transistors of compounds **12a** and **12b**.

### Experimental details

OFET devices were fabricated in the top-contact device configuration. The substrate was heavily doped, n-type Si gate electrode with a 500 nm thick SiO<sub>2</sub> layer as the gate dielectric. The gate dielectric was treated with octadecyltrichlorosilane (OTS) or PMMA (Polymethyl methacrylate) by vapour deposition method. Subsequently, organic semiconductors were deposited on the substrate by thermal evaporation under a pressure of  $8 \times 10^{-4}$  Pa at a deposition rate gradually increased from  $0.1 \text{ \AA s}^{-1}$  to  $0.4 \text{ \AA s}^{-1}$  at the first 20 nm and then maintained  $0.5 \text{ \AA s}^{-1}$  until the thickness of the film was 50 nm. The deposition rate and film thickness were monitored by a quartz crystal microbalance (ULVAC CRTM-6000). Finally, 20 nm thick gold source and drain electrode were deposited through a shadow mask. The channel length (*L*) and width (*W*) were 0.11 mm and 5.30 mm, respectively. The FET characteristics were measured at room temperature in air using Keithley 4200 SCS. Atomic force microscopy (AFM) measurements were carried out with a Nanoscope IIIa instrument (Digital Instruments) operating in tapping mode. UV-Vis spectra were recorded on a JASCO V-570 spectrometer.

### FET characteristics

Top contact OFETs based on the thin films were fabricated. The results are summarized in Table 1 of the manuscript. Here, the mobilities ( $\mu$ ) were calculated in the saturation regime by the following equation:  $I_D = \mu C_i (W/2L)(V_G - V_T)^2$ , where  $I_D$  is the drain current,  $\mu$  is the field-effect mobility,  $C_i$  is the gate dielectric capacitance,  $W$  and  $L$  are the channel width and length, respectively,  $V_T$  is the threshold voltage. **12a** deposited at 60 °C exhibited the best OFET performance ( $0.4 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ). The FET characteristics of **12a** and **12b** are shown below.



**Figure S49.** Transfer and output characteristics of devices based on **12a** (a and b, respectively) and **12b** (c and d, respectively) with OTS treated SiO<sub>2</sub>/Si ( $T_s = 60 \text{ }^\circ\text{C}$ ) substrate.

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O2 0.0559(7) 0.0372(6) 0.0587(6) 0.0072(5) 0.0224(5) 0.0099(5)  
C1 0.0510(10) 0.0330(7) 0.0502(9) 0.0041(7) 0.0071(8) 0.0079(7)  
C2 0.0537(10) 0.0362(8) 0.0523(9) 0.0056(7) 0.0112(8) 0.0107(7)  
C3 0.0602(11) 0.0401(8) 0.0624(10) 0.0109(8) 0.0138(9) 0.0059(8)  
C4 0.0572(11) 0.0493(9) 0.0569(9) 0.0103(8) 0.0155(8) -0.0012(8)  
C5 0.0466(10) 0.0459(9) 0.0431(8) 0.0028(7) 0.0111(7) 0.0001(7)  
C6 0.0448(9) 0.0466(8) 0.0436(8) 0.0000(7) 0.0098(7) 0.0010(7)  
C7 0.0458(10) 0.0466(8) 0.0504(9) -0.0017(7) 0.0120(7) -0.0004(7)  
C8 0.0520(10) 0.0631(10) 0.0535(10) 0.0051(8) 0.0140(8) -0.0030(8)  
C9 0.0705(14) 0.0747(12) 0.0610(11) 0.0027(9) 0.0254(10) -0.0099(10)  
C10 0.0650(14) 0.0770(12) 0.0884(15) -0.0142(11) 0.0395(12) -0.0167(10)  
C11 0.0460(11) 0.1065(16) 0.0839(14) -0.0066(12) 0.0153(10) 0.0010(11)  
C12 0.0523(12) 0.0951(13) 0.0577(10) 0.0020(10) 0.0111(9) 0.0059(10)  
C13 0.0437(9) 0.0470(8) 0.0456(9) -0.0003(7) 0.0140(7) 0.0052(7)  
C14 0.0566(11) 0.0522(9) 0.0740(11) 0.0054(8) 0.0274(9) 0.0147(8)  
C15 0.0623(12) 0.0441(8) 0.0759(12) 0.0077(8) 0.0241(9) 0.0157(9)  
C16 0.0547(11) 0.0368(8) 0.0517(9) 0.0056(7) 0.0128(8) 0.0090(7)  
C17 0.0523(10) 0.0396(8) 0.0531(9) 0.0028(7) 0.0149(8) 0.0102(7)

\_geom\_special\_details

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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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O1 C1 1.3709(16) . ?  
O2 C13 1.3669(16) . ?  
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C1 C3 1.379(2) . ?  
C1 C2 1.3859(19) . ?  
C2 C17 1.3676(18) 3\_556 ?  
C2 H2 0.9300 . ?  
C3 C4 1.376(2) . ?  
C3 H3 0.9300 . ?  
C4 C5 1.3895(19) . ?  
C4 H4 0.9300 . ?  
C5 C6 1.3986(19) . ?  
C6 C13 1.3976(18) . ?  
C6 C7 1.481(2) . ?  
C7 C8 1.381(2) . ?  
C7 C12 1.382(2) . ?

C8 C9 1.377(2) . ?  
C8 H8 0.9300 . ?  
C9 C10 1.360(2) . ?  
C9 H9 0.9300 . ?  
C10 C11 1.370(2) . ?  
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C11 H11 0.9300 . ?  
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C13 C14 1.3858(19) . ?  
C14 C15 1.367(2) . ?  
C14 H14 0.9300 . ?  
C15 C16 1.382(2) . ?  
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C3 C1 C2 137.17(13) . . ?  
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C3 C4 C5 107.69(14) . . ?  
C3 C4 H4 126.2 . . ?  
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O1 C5 C4 107.36(13) . . ?  
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C8 C7 C6 121.51(14) . . ?  
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C9 C8 C7 120.59(16) . . ?  
C9 C8 H8 119.7 . . ?  
C7 C8 H8 119.7 . . ?  
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C9 C10 C11 119.98(17) . . ?  
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C11 C12 H12 119.3 . . ?  
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O2 C13 C14 107.15(13) . . ?  
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C14 C13 C6 132.90(14) . . ?  
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O2 C16 C15 107.28(12) . . ?  
O2 C16 C17 113.24(12) . . ?  
C15 C16 C17 139.43(14) . . ?  
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O1 C5 C6 C13 -0.3(2) . . . . ?  
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C13 C6 C7 C12 -55.9(2) . . . . ?  
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C6 C7 C8 C9 -175.86(14) . . . . ?  
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O2 C13 C14 C15 0.54(18) . . . . ?  
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C14 C15 C16 O2 -1.15(18) . . . . ?  
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Version 1.171.31.7 (release 18-10-2006 CrysAlis171 .NET)
(compiled Oct 18 2006,16:28:17)
Empirical absorption correction using spherical harmonics,
implemented in SCALE3 ABSPACK scaling algorithm.
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 $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is
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C3 C 0.60330(8) 1.3413(3) 0.7026(3) 0.0481(7) Uani 1 1 d ...
H3 H 0.6269 1.3773 0.7392 0.058 Uiso 1 1 calc R ..
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C5 C 0.61897(7) 1.0840(3) 0.6348(3) 0.0392(6) Uani 1 1 d ...
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C7 C 0.62073(7) 0.8280(3) 0.5285(3) 0.0468(7) Uani 1 1 d ...
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C8 C 0.59161(8) 0.7389(3) 0.4786(3) 0.0474(7) Uani 1 1 d ...
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C4 0.0328(16) 0.0448(17) 0.0474(16) 0.0022(14) -0.0049(12) -0.0004(14)  
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C7 0.0358(15) 0.0517(18) 0.0528(16) -0.0041(13) 0.0020(13) 0.0027(14)  
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C15 0.0370(17) 0.0469(18) 0.0491(17) -0.0070(13) -0.0024(13) -0.0024(14)  
C16 0.0412(18) 0.068(2) 0.073(2) -0.0073(15) -0.0065(14) -0.0018(14)  
C17 0.0429(18) 0.0516(18) 0.0480(15) 0.0055(14) -0.0079(13) 0.0028(14)  
C18 0.0427(18) 0.0507(17) 0.0509(16) 0.0077(14) -0.0011(13) -0.0024(14)

\_geom\_special\_details

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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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loop\_

\_geom\_bond\_atom\_site\_label\_1  
\_geom\_bond\_atom\_site\_label\_2  
\_geom\_bond\_distance  
\_geom\_bond\_site\_symmetry\_2  
\_geom\_bond\_publ\_flag

O1 C4 1.378(3) . ?  
O1 C1 1.380(3) . ?  
O2 C6 1.376(2) . ?  
O2 C9 1.387(2) . ?  
C1 C2 1.376(3) . ?  
C1 C11 1.403(3) 5\_676 ?  
C2 C3 1.376(3) . ?  
C2 H2 0.9300 . ?

C3 C4 1.390(3) . ?  
C3 H3 0.9300 . ?  
C4 C5 1.389(3) . ?  
C5 C6 1.411(3) . ?  
C5 C12 1.482(3) . ?  
C6 C7 1.393(3) . ?  
C7 C8 1.373(3) . ?  
C7 H7 0.9300 . ?  
C8 C9 1.375(3) . ?  
C8 H8 0.9300 . ?  
C9 C10 1.389(3) . ?  
C10 C11 1.366(3) . ?  
C10 H10 0.9300 . ?  
C11 C1 1.403(3) 5\_676 ?  
C11 H11 0.9300 . ?  
C12 C18 1.386(3) . ?  
C12 C13 1.391(3) . ?  
C13 C14 1.383(3) . ?  
C13 H13 0.9300 . ?  
C14 C15 1.380(3) . ?  
C14 H14 0.9300 . ?  
C15 C17 1.379(3) . ?  
C15 C16 1.509(3) . ?  
C16 H16A 0.9600 . ?  
C16 H16B 0.9600 . ?  
C16 H16C 0.9600 . ?  
C17 C18 1.379(3) . ?  
C17 H17 0.9300 . ?  
C18 H18 0.9300 . ?

loop\_

\_geom\_angle\_atom\_site\_label\_1  
\_geom\_angle\_atom\_site\_label\_2  
\_geom\_angle\_atom\_site\_label\_3  
\_geom\_angle  
\_geom\_angle\_site\_symmetry\_1  
\_geom\_angle\_site\_symmetry\_3  
\_geom\_angle\_publ\_flag  
C4 O1 C1 108.70(19) . . ?  
C6 O2 C9 108.90(18) . . ?  
C2 C1 O1 107.8(2) . . ?  
C2 C1 C11 137.5(3) . 5\_676 ?  
O1 C1 C11 114.6(2) . 5\_676 ?  
C1 C2 C3 108.1(2) . . ?  
C1 C2 H2 126.0 . . ?  
C3 C2 H2 126.0 . . ?  
C2 C3 C4 108.4(2) . . ?  
C2 C3 H3 125.8 . . ?  
C4 C3 H3 125.8 . . ?  
O1 C4 C5 117.9(2) . . ?  
O1 C4 C3 107.0(2) . . ?  
C5 C4 C3 135.1(2) . . ?  
C4 C5 C6 123.4(2) . . ?  
C4 C5 C12 119.4(2) . . ?  
C6 C5 C12 117.2(2) . . ?  
O2 C6 C7 106.9(2) . . ?  
O2 C6 C5 119.0(2) . . ?  
C7 C6 C5 133.9(2) . . ?  
C8 C7 C6 108.2(2) . . ?  
C8 C7 H7 125.9 . . ?  
C6 C7 H7 125.9 . . ?  
C7 C8 C9 108.6(2) . . ?

C7 C8 H8 125.7 . . ?  
C9 C8 H8 125.7 . . ?  
C8 C9 O2 107.3(2) . . ?  
C8 C9 C10 139.5(2) . . ?  
O2 C9 C10 113.0(2) . . ?  
C11 C10 C9 130.5(2) . . ?  
C11 C10 H10 114.8 . . ?  
C9 C10 H10 114.8 . . ?  
C10 C11 C1 121.0(2) . 5\_676 ?  
C10 C11 H11 119.5 . . ?  
C1 C11 H11 119.5 5\_676 . ?  
C18 C12 C13 117.0(2) . . ?  
C18 C12 C5 121.0(2) . . ?  
C13 C12 C5 122.0(2) . . ?  
C14 C13 C12 120.8(2) . . ?  
C14 C13 H13 119.6 . . ?  
C12 C13 H13 119.6 . . ?  
C15 C14 C13 121.9(2) . . ?  
C15 C14 H14 119.0 . . ?  
C13 C14 H14 119.0 . . ?  
C17 C15 C14 117.2(2) . . ?  
C17 C15 C16 120.6(2) . . ?  
C14 C15 C16 122.2(2) . . ?  
C15 C16 H16A 109.5 . . ?  
C15 C16 H16B 109.5 . . ?  
H16A C16 H16B 109.5 . . ?  
C15 C16 H16C 109.5 . . ?  
H16A C16 H16C 109.5 . . ?  
H16B C16 H16C 109.5 . . ?  
C15 C17 C18 121.4(2) . . ?  
C15 C17 H17 119.3 . . ?  
C18 C17 H17 119.3 . . ?  
C17 C18 C12 121.6(2) . . ?  
C17 C18 H18 119.2 . . ?  
C12 C18 H18 119.2 . . ?

loop\_

\_geom\_torsion\_atom\_site\_label\_1  
\_geom\_torsion\_atom\_site\_label\_2  
\_geom\_torsion\_atom\_site\_label\_3  
\_geom\_torsion\_atom\_site\_label\_4  
\_geom\_torsion  
\_geom\_torsion\_site\_symmetry\_1  
\_geom\_torsion\_site\_symmetry\_2  
\_geom\_torsion\_site\_symmetry\_3  
\_geom\_torsion\_site\_symmetry\_4  
\_geom\_torsion\_publ\_flag  
C4 O1 C1 C2 0.2(2) . . . . ?  
C4 O1 C1 C11 -177.6(2) . . . 5\_676 ?  
O1 C1 C2 C3 0.2(3) . . . . ?  
C11 C1 C2 C3 177.3(3) 5\_676 . . . ?  
C1 C2 C3 C4 -0.5(3) . . . . ?  
C1 O1 C4 C5 179.32(19) . . . . ?  
C1 O1 C4 C3 -0.5(2) . . . . ?  
C2 C3 C4 O1 0.6(3) . . . . ?  
C2 C3 C4 C5 -179.1(2) . . . . ?  
O1 C4 C5 C6 -2.7(3) . . . . ?  
C3 C4 C5 C6 177.1(3) . . . . ?  
O1 C4 C5 C12 175.59(19) . . . . ?  
C3 C4 C5 C12 -4.7(4) . . . . ?  
C9 O2 C6 C7 -1.3(3) . . . . ?  
C9 O2 C6 C5 174.87(19) . . . . ?

C4 C5 C6 O2 -9.2(3) . . . . ?  
C12 C5 C6 O2 172.5(2) . . . . ?  
C4 C5 C6 C7 165.8(2) . . . . ?  
C12 C5 C6 C7 -12.5(4) . . . . ?  
O2 C6 C7 C8 1.2(3) . . . . ?  
C5 C6 C7 C8 -174.2(2) . . . . ?  
C6 C7 C8 C9 -0.6(3) . . . . ?  
C7 C8 C9 O2 -0.2(3) . . . . ?  
C7 C8 C9 C10 173.6(3) . . . . ?  
C6 O2 C9 C8 1.0(2) . . . . ?  
C6 O2 C9 C10 -174.66(18) . . . . ?  
C8 C9 C10 C11 5.9(5) . . . . ?  
O2 C9 C10 C11 179.5(2) . . . . ?  
C9 C10 C11 C1 -175.5(2) . . . . 5\_676 ?  
C4 C5 C12 C18 132.0(2) . . . . ?  
C6 C5 C12 C18 -49.6(3) . . . . ?  
C4 C5 C12 C13 -47.9(3) . . . . ?  
C6 C5 C12 C13 130.4(2) . . . . ?  
C18 C12 C13 C14 0.5(3) . . . . ?  
C5 C12 C13 C14 -179.6(2) . . . . ?  
C12 C13 C14 C15 1.0(4) . . . . ?  
C13 C14 C15 C17 -1.5(3) . . . . ?  
C13 C14 C15 C16 178.5(2) . . . . ?  
C14 C15 C17 C18 0.6(4) . . . . ?  
C16 C15 C17 C18 -179.5(2) . . . . ?  
C15 C17 C18 C12 1.0(4) . . . . ?  
C13 C12 C18 C17 -1.5(4) . . . . ?  
C5 C12 C18 C17 178.6(2) . . . . ?

\_diffn\_measured\_fraction\_theta\_max 0.998  
\_diffn\_reflns\_theta\_full 25.00  
\_diffn\_measured\_fraction\_theta\_full 0.998  
\_refine\_diff\_density\_max 0.149  
\_refine\_diff\_density\_min -0.122  
\_refine\_diff\_density\_rms 0.032