Electronic Supplementary Information:

on/*off* Electrochemical switches based on quinone-bisketals

Noelia Fuentes,[a] Luis Álvarez de Cienfuegos,[a] Andrés Parra,[a] Duane Choquesillo-Lazarte,[b] Juan M. García-Ruiz,[b] M. Luisa Marcos,[c] Elena Buñuel,[d] Maria Ribagorda,[d] M. Carmen Carreño,*[,d] Diego J. Cárdenas,*[,d] and Juan M. Cuerva*[,a]

Departamento de Química Orgánica,[a] Universidad de Granada, Campus Fuentenueva s/n, E-18071 Granada (Spain). Laboratorio de Estudios Cristalográficos IACT,[b] CSIC- Universidad de Granada, 18100, Granada (Spain). Departamento de Química (Módulo 9),[c] y Departamento de Química Orgánica (Módulo 1),[d] Universidad Autónoma de Madrid, c/ Francisco Tomás y Valiente 7, Cantoblanco, E-28049, Madrid (Spain).

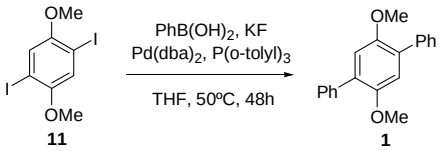
Contents

General details. ^{1}H NMR and ^{13}C NMR spectra were recorded on a NMR Variant 400 L900, Variant 500 L900 and AV-300 Bruker spectrometers in $CDCl_3$, CD_3OD or DMSO-d_6 with tetramethylsilane as an internal standard. Data are reported as follows: chemical shift in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet and m = multiplet) coupling constant (Hz), integration, and interpretation. Peak assignments were made with the aid of DEPT method. Ultraviolet spectra (UV) were obtained on a Helyos α spectrometer. High resolution mass spectra (HRMS) were obtained by electrospray technique using a QSTAR (Applied Biosystems) instrument and by FAB technique using a VG AutoSpec instrument. The following known compounds were isolated as pure samples and showed NMR spectra matching those of the reported compounds: **1**,[1] **2**,[2] **4**,[3] **7**,[4] **11**,[5] **12**,[6] **15**,[7] and **17**.[8]

[1] J. E. Klare, G. S. Tulevski and C. Nuckolls, *Langmuir* 2004, **20**, 10068-10072.
[2] D. Yue, T. Yao and R. C. Larock, *J. Org. Chem.* 2005, **70**, 10292-10296.
[3] N. Sanyal and P. M. Lahti, *Cryst. Growth Des.* 2006, **6**, 1253-1255
[4] A. Palmgren, A. Thorarensen, A. and J. Bäckvall, *J. Org. Chem.* 1998**, 63**, 3764-3768.
[5] S. M. Waybright, C. P. Singleton, K. Wachter, C. J. Murphy and U. H. F. Bunz, *J. Am. Chem. Soc.* 2001, **123**, 1828-1833.
[6] S-H. Hsiao, Y.-H. Chang, *J. Polym. Sci. Part. A: Polym. Chem.* 2004, **42**, 1255-1271.
[7] J. P. Amara and T. M. Swager, *Macromolecules* 2005, **38**, 9091-9094.
[8] H. Tsuji, C. Mitsui, L. Ilies, Y. Sato and E. Nakamura, *J. Am. Chem. Soc.* 2007, **129**, 11902-11903.

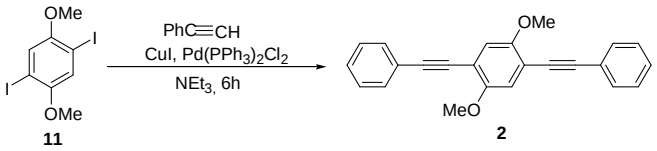
Synthesis of *p*-dialkoxybenzenes (1-8).

Synthesis of compound 1.



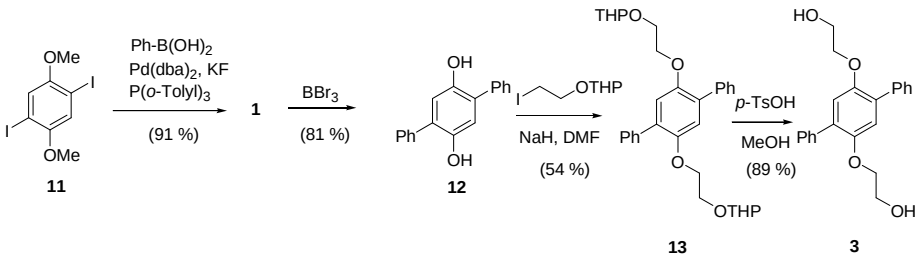
A mixture of phenyl boronic acid (469 mg, 3.84 mmol), 2,5-diiodo-1,4-dimethoxybenzene **11** (500 mg, 1.28 mmol), KF (446 mg, 7.69 mmol), $Pd(dba)_2$ (73 mg, 0.13 mmol) and P(*o*-tolyl)$_3$ (78 mg, 0.26 mmol) in THF (20 mL) was warmed to 55 ºC and stirred for 48 h under argon. The reaction was then diluted with EtOAc, washed with brine, dried over anhydrous Na_2SO_4, and the solvent removed. The residue was submitted to flash chromatography (EtOAc/Hexane: 1/9) to give **1** (340 mg, 91 %) as a white solid.

Synthesis of compound 2.



CuI (7 mg, 0.04 mmol) was added to a solution of Et_3N (6 mL), $Pd(PPh_3)_2Cl_2$ (54 mg, 0.08 mmol), phenyl acetylene (188 mg, 1.85 mmol) and 2,5-diiodo-1,4-dimethoxybenzene **11** (300 mg, 0.77 mmol), stirred for 5 min beforehand under argon. The reaction was allowed to stir at room temperature for 6h and the resulting solution was filtered, washed with 10 % aqueous HCl solution, and extracted with diethyl ether (3 x 10 mL). The combined ether fractions were dried over anhydrous Na_2SO_4, concentrated under vacuum, and the crude product submitted to flash chromatography (EtOAc/Hexane: 1/9) to give **2** (200 mg, 77 %) as a yellow solid.

Synthesis of compound 3.

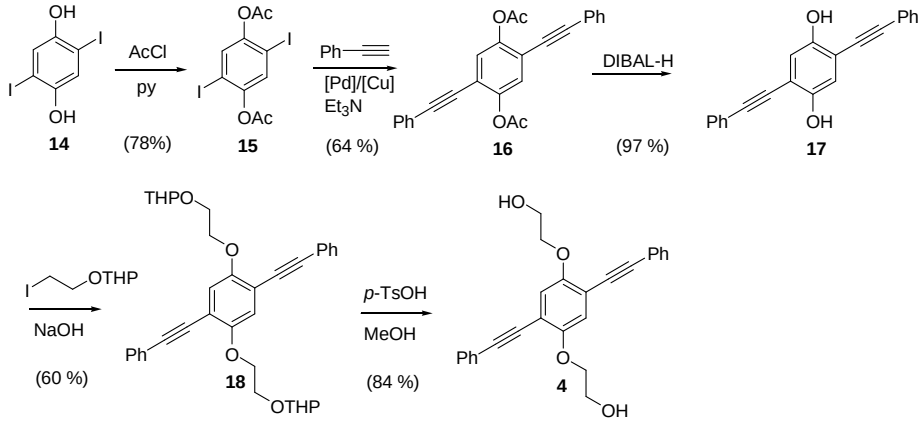


*Synthesis of compound 12***.** A solution of boron tribromide 1M in CH_2Cl_2 (5.48 mL, 5.48 mmol) was slowly added to **1** (530 mg, 1.83 mmol) in dry CH_2Cl_2 (75 mL) at -78 ºC. The reaction mixture was stirred under argon at room temperature for 48 h. Then, water (50 mL) was slowly added, the organic layers were collected, dried over Na_2SO_4 and evaporated to dryness. The residue was purified by column chromatography (EtOAc/Hexane: 3/7) to give **12** (388 mg, 81 %) as a white solid.

Synthesis of compound 13. A sample of $I(CH_2)_2OTHP$[9] (834 mg, 3.26 mmol) was added to a mixture of NaH (178 mg, 4.44 mmol) and hydroquinone **12** (388 mg, 1.49 mmol) in DMF (25 mL). The resulting solution was stirred at room temperature for 12 h and then diluted with EtOAc, washed with 10 % aqueous HCl solution, dried over anhydrous Na_2SO_4, and concentrated. The residue was submitted to flash chromatography (EtOAc/Hexane: 4/6) to give **13** (420 mg, 54 %) as a colourless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 8.4, 1.3 Hz, 4H), 7.42 (t, *J* = 8.4 Hz, 4H), 7.34-7.31 (m, 2H), 7.04 (s, 2H), 4.59 (t, *J* = 3.4 Hz, 2H), 4.12 (t, *J* = 5.0 Hz, 4H), 3.94 (dt, *J* = 11.2, 4.4 Hz, 2H), 3.80-3.76 (m, 2H), 3.69 (dt, *J* = 11.2, 5.2 Hz, 2H), 3.44-3.41 (m, 2H), 1.81-1.75 (m, 2H), 1.68-1.46 (m, 10H); ^{13}C NMR (125 MHz, $CDCl_3$; DEPT) δ 150.4 (C), 138.3 (C), 131.1 (C), 129.6 (CH), 128.0 (CH), 127.0 (CH), 116.8 (CH), 99.0 (CH), 69.2 (CH_2), 66.0 (CH_2), 62.0 (CH_2), 30.6 (CH_2), 25.5 (CH_2), 19.3 (CH_2); HRMS FAB: *m/z* calcd. for $C_{32}H_{38}O_6$ $[M]^+$ 518.2668, found *m/z* 518.2664.

Synthesis of compound 3. *p*-Toluensulfonic acid (46 mg, 0.24 mmol) was added to a solution of THP-derivative **13** (420 mg, 0.81 mmol) in MeOH (20 mL). The resulting mixture was stirred for 2 h, and then diluted with EtOAc, washed with brine, dried over anhydrous Na_2SO_4, and the solvent removed. The residue was submitted to flash chromatography (EtOAc/Hexane: 1/1) to give **3** (274 mg, 89 %) as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.0 Hz, 4H), 7.45 (t, *J* = 8.0 Hz, 4H), 7.37 (t, *J* = 8.0 Hz, 2H), 7.03 (s, 2H), 4.04 (t, *J* = 4.0 Hz, 4H), 3.78 (t, *J* = 4.0 Hz, 4H); ^{13}C NMR (125 MHz, $CDCl_3$; DEPT) δ 150.5 (C), 138.2 (C), 132.1(C), 129.6 (CH), 128.6 (CH), 127.7 (CH), 117.6 (CH), 71.6 (CH_2), 61.7 (CH_2); HRMS ES: *m/z* calcd. for $C_{22}H_{22}O_4Na$ $[M+Na]^+$ 373.1416 , found *m/z* 373.1410.

Synthesis of compound 4.



*Synthesis of compound 15***.** Pyridine (3.2 g, 32 mmol) was added to a solution of 2,5-diiodohydroquinone 14 (2.1 g, 5.29 mmol) in dry CH_2Cl_2 (30 mL). The solution was cooled to 0 ºC and then acetyl chloride (1.7 g, 21.32 mmol) was added. The reaction was stirred for 3 h at room temperature. MeOH (10 mL) was then added and the resulting mixture was stirred for another 5 min, and subsequently the solvent removed. The residue was diluted with EtOAc, washed with brine, dried over anhydrous Na_2SO_4, and concentrated under vacuum. The crude was submitted to flash chromatography (EtOAc/Hexane: 4/6) to give **15** (1.8 g, 78 %) as a brown solid.

[9] It was prepared from $OH(CH_2)_2OTHP$ according to known procedure: J. Garegg and B. Samuelsson, *J. Chem. Soc. Perkin I.* 1980, 2866-2869. $I(CH_2)_2OTHP$ was isolated as pure sample and showed NMR spectra identical to those reported: J. H. Bushweller and P. A. Bartlett, *J. Org. Chem.* 1989, **54**, 2404–2409.

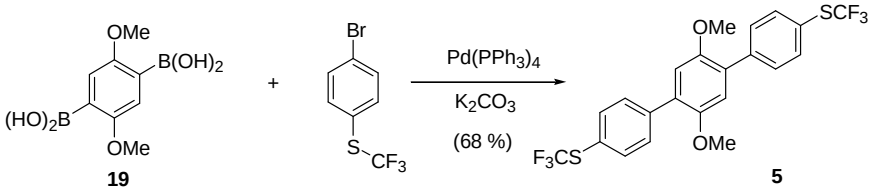
Synthesis of compound 16. CuI (33 mg, 0.17 mmol) was added to a solution of Et_3N (10 mL), $PdCl_2(PPh_3)_2$ (240 mg, 0.34 mmol), phenyl acetylene (840 mg, 8.23 mmol) and and diacetate **15** (1.5 g, 3.43 mmol), stirred for 5 min beforehand under argon. The mixture was allowed to stir at room temperature for 6 h and the resulting solution was diluted with CH_2Cl_2, washed with brine, dried over anhydrous Na_2SO_4 and concentrated under vacuum. Recrystallization from EtOAc gave the diacetate **16** (864 mg, 64 %) as orange needles. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.40 (m, 4H), 7.30-7.28 (m, 6H), 7.19 (s, 2H), 2.30 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$; DEPT) δ 168.5 (C), 148.8 (C), 131.6 (CH), 128.9 (CH), 128.5 (CH), 126.2 (CH), 122.5 (C), 118.5 (C), 96.4 (C), 83.5 (C), 20.7 (CH_3); HRMS ES: *m/z* calcd. for $C_{26}H_{18}O_4Na$ $[M+Na]^+$ 417.1103, found *m/z* 417.1097.

Synthesis of compound 17. DIBAL-H (548 mg, 3.80 mmol) was added dropwise to a deoxigenated solution of **16** (250 mg, 0.63 mmol) in THF (20 mL) under argon at 0 ºC. The mixture was stirred at room temperature for 2 h and, then, diluted with EtOAc, washed with brine, dried over anhydrous Na_2SO_4, and the solvent removed. The residue was submitted to flash chromatography (EtOAc/Hexane: 3/7) to give hydroquinone **17** (190 mg, 97 %) as a yellow solid.

Synthesis of compound 18. Hydroquinone **17** (152 mg, 0.43 mmol) was slowly added to a mixture of NaH (31 mg, 1.29 mmol) and $I(CH_2)_2OTHP$[5] (243 mg, 0.95 mmol) in DMF (25 mL). The resulting solution was stirred at room temperature for 4 h and then diluted with EtOAc, washed with brine, dried over anhydrous Na_2SO_4, and the solvent removed. The residue was submitted to flash chromatography (EtOAc/Hexane: 5/95) to give **18** (420 mg, 54 %) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.53 (m, 4H), 7.35-7.33 (m, 6H), 7.09 (s, 2H), 4.78 (t, J = 2.8 Hz, 2H), 4.24 (t, J = 3.0 Hz, 4H), 4.11-4.06 (m, 2H), 3.94-3.85 (m, 4H), 3.51-3.45 (m, 2H), 1.81-1.74 (m, 2H), 1.73-1.46 (m, 10H); ^{13}C NMR (125 MHz, $CDCl_3$; DEPT) δ 153.7 (C), 131.6 (CH), 128.4 (CH), 128.3 (CH), 123.4 (C), 117.4 (CH), 114.3 (C), 99.0 (CH), 94.9 (C), 85.7 (C), 69.3 (CH_2), 65.8 (CH_2), 61.9 (CH_2), 30.5 (CH_2), 25.4 (CH_2), 19.2 (CH_2); HRMS ES: *m/z* calcd. for $C_{36}H_{38}O_6Na$ $[M+Na]^+$ 589.2566, found *m/z* 589.2560.

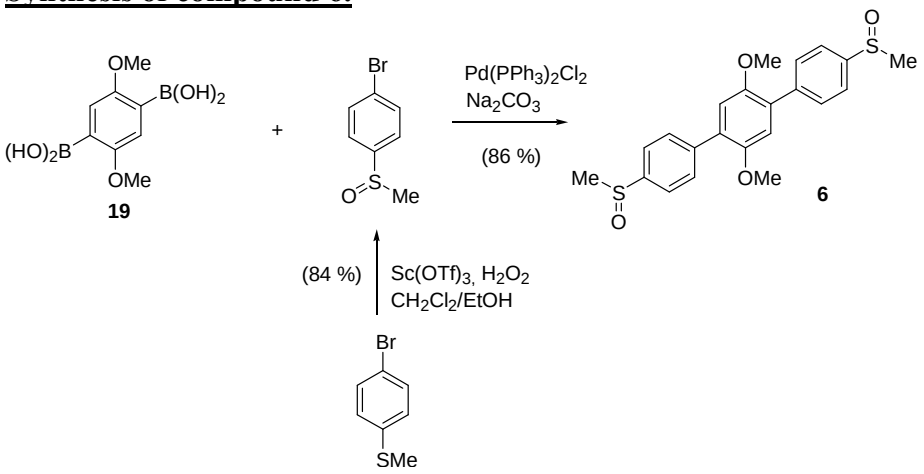
Synthesis of compound 4. *p*-Toluensulfonic acid (14 mg, 0.07 mmol) was added to a solution of THP-derivative **18** (150 mg, 0.25 mmol) in MeOH (15 mL). The resulting mixture was stirred for 2 h, and then diluted with EtOAc, washed with brine, dried over anhydrous Na_2SO_4, and the solvent removed. The residue was submitted to flash chromatography (EtOAc/Hexane: 6/4) to give **4** (87 mg, 84 %) as a yellow solid.

Synthesis of compound 5.



A mixture of 2,5-dimethoxy-1,4-benzenediboronic acid **19**[10] (80 mg, 0.36 mmol), 1-bromo-4-trifluoromethylthiobenzene (232 mg, 0.90 mmol), potassium carbonate (150 mg, 1.08 mmol) and $Pd(PPh_3)_4$ (12 mg, 0.01 mmol) in DMSO (12 mL) was heated at 100 ºC for 72 h under argon. The reaction was partitioned between water and EtOAc, the organic layer was dried over Na_2SO_4, filtrated and concentrated. The residue was submitted to flash chromatography (EtOAc/Hexane: 1/9) to give **5** (121 mg, 68 %) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.8 Hz, 4H), 7.64 (d, J = 8.8 Hz, 4H), 6.97 (s, 2H), 3.81 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$; DEPT) δ 150.7 (C), 140.8 (C), 135.9 (CH), 130.5 (CH), 129.6 (C), 129.6 (q, $^1J_{C\text{-}F}$ = 240 Hz, C), 123.0 (C), 114.5 (CH), 56.4 (CH_3); HRMS FAB: *m/z* calcd. for $C_{22}H_{16}F_6O_2S_2$ $[M]^+$ 490.0496, found *m/z* 490.0502.

Synthesis of compound 6.



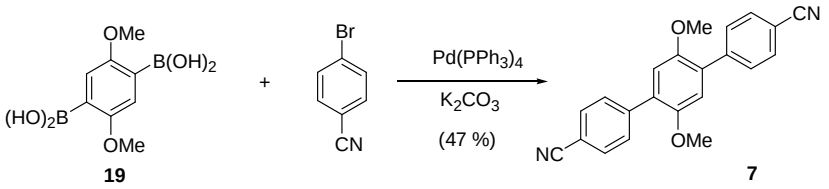
Synthesis of 4-bromophenylmethylsulfoxide. H_2O_2 (30% v/v, 251 mg, 7.39 mmol) was added with stirring to a suspension of $Sc(OTf)_3$ (145 mg, 0.29 mmol) in a mixture of CH_2Cl_2/EtOH (10:1, 1 mL) at room temperature. After 5 min, 4-bromomethylthioanysole (300 mg, 1.49 mmol) was added. The mixture was stirred for 8 h, and then diluted with CH_2Cl_2, washed with water, dried over anhydrous Na_2SO_4, and the solvent removed. The residue was submitted to flash chromatography (MeOH/CH_2Cl_2: 1/49) to give 4-bromophenylmethylsulfoxyde[11] (272 mg, 84 %) as a white solid.

Synthesis of 6. Degassed 1,4-dioxane was added to a mixture of 2,5-dimethoxy-1,4-benzenediboronic acid **19** (215 mg, 0.95 mmol), 4-bromophenylmethylsulfoxyde (543 mg, 2.48 mmol) and $Pd(PPh_3)_2Cl_2$ (67 mg, 0.09 mmol) in a 50 ml round bottom flask under argon atmosphere. The mixture was stirred at 20 °C for 30 min. Degassed aqueous Na_2CO_3 solution (1 M, 3.8 mL) was added and the reaction mixture was heated at reflux under argon for 72 h. Solvent was then removed under vacuum. The residue was submitted to flash chromatography (MeOH/CH_2Cl_2: 1/40) to give **6** (343 mg, 86 %) as a brown solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.5 Hz, 4H), 7.70 (d, J = 8.2 Hz, 4H), 6.98 (s, 2H), 3.81 (s, 6H), 2.78 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$; DEPT) δ 150.7 (C), 144.3 (C), 141.0 (C), 130.4 (CH), 129.6 (C), 123.4 (CH), 114.5

[10] C. Wang, M. Kilitziraki, J. A. H. MacBride, M. R. Bryce, L. E. Horsburgh, A. K. Sheridan, A. P. Monkman and I. D. W. Samuel, *Adv. Mat.* 2000, **12**, 217-222.
[11] M. Matteucci, G. Bhalay and M. Bradley, *Org. Lett.*, 2003, **5**, 235–237.

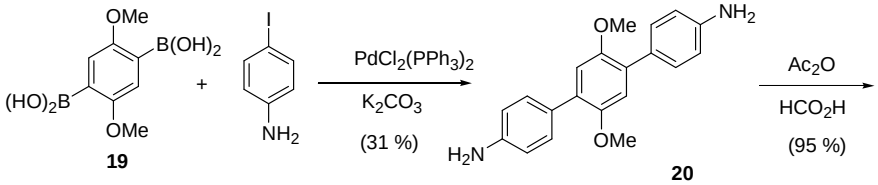
(CH), 56.4 (CH_3), 43.9 (CH_3); HRMS ES: *m/z* calcd. for $C_{22}H_{23}O_4S_2$ $[M+H]^+$ 415.1032, found *m/z* 415.1032.

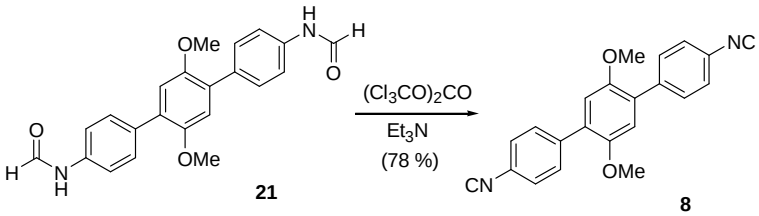
Synthesis of compound 7.



A mixture of 2,5-dimethoxy-1,4-benzenediboronic acid **19** (150 mg, 0.66 mmol), 4-iodobenzonitrile (380.7 mg, 1.66 mmol), K_2CO_3 (275.6 mg, 1.99 mmol) and $Pd(PPh_3)_4$ (22 mg, 0.02 mmol) in degassed DMSO (12 mL) was heated at reflux under argon for 72 h. The reaction was partitioned between water and EtOAc, the organic layer was dried over Na_2SO_4, filtrated and concentrated. The residue was submitted to flash chromatography (EtOAc/Hexane: 4/6) to give **7**[12] (106 mg, 47 %) as a white solid.

Synthesis of compound 8.





Synthesis of 20. Degassed 1,4-dioxane (12 mL) was added to a mixture of 2,5-dimethoxy-1,4-benzenediboronic acid **19** (150 mg, 0.66 mmol), 4-iodoaniline (378.6 mg, 1.73 mmol) and $Pd(PPh_3)_2Cl_2$ (46.6 mg, 0.06 mmol) in a 50 ml round bottom flask under argon atmosphere. The mixture was stirred at 20 °C for 30 min. Degassed aqueous Na_2CO_3 solution (1 M, 2.6 mL) was added and the reaction mixture was heated at reflux under argon for 72 h. Solvent was then removed under vacuum. The residue was submitted to flash chromatography (EtOAc/Hexane: 4/6) to give **20** (66 mg, 31 %) as a brown solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.4 Hz, 4H), 6.93 (s, 2H), 6.75 (d, *J* = 8.4 Hz, 4H), 3.77 (s, 6H); ^{13}C NMR (120 MHz, $CDCl_3$; DEPT) δ 150.7 (C), 145.5 (C), 130.3 (CH), 129.7 (C), 128.6 (C), 114.8 (CH), 114.5 (CH), 56.5 (CH_3); HRMS FAB: *m/z* calcd. for $C_{20}H_{20}N_2O_2$ $[M]^+$ 320.1525, found *m/z* 320.1528.

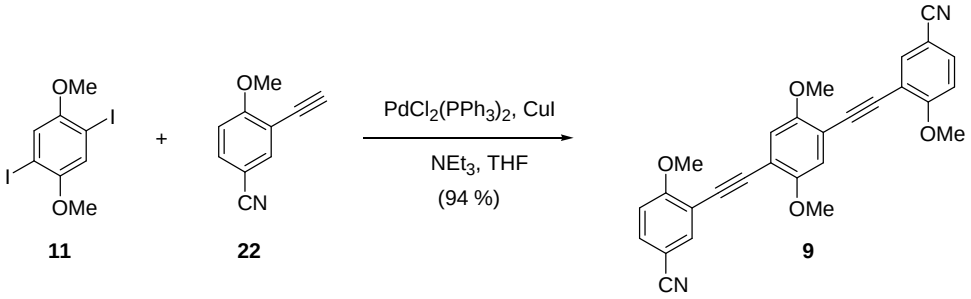
*Synthesis of 21***.** Acetic anhydride (77 mL, 8.14 mmol) was added to an oven-dried round-bottom flask equipped with a reflux condenser under argon. Formic acid (0.24 mL, 6.51 mmol) was then added dropwise. The flask was then heated to 60 °C and

[12] A. Palmgren, A. Thorarensen and J. Bäckvall, *J. Org. Chem.* 1998**, 63**, 3764-3768.

stirred for 30 min before being cooled to -10 °C. A solution of diamine **20** (434 mg, 1.36 mmol) in THF (20 mL) was slowly added to the reaction mixture, which was then allowed to warm to room temperature and stir overnight. Solvent was removed by rotary evaporation and water was added, yielding a white precipitate which was filtered and washed with water. The material was recrystallized from CH_2Cl_2/hexane to afford **21** (485 mg, 95 %) as a grey solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.25 (s, 2H, mayor isomer), 10.19 (d, J =10.8 Hz, 2H, minor isomer), 8.82 (d, J = 11.6 Hz, 1H, minor isomer), 8.29 (s, 1H, mayor isomer), 7.63 (d, J = 8.5 Hz, 4H, mayor isomer), 7.52 (d, J = 8.8 Hz, 4H), 7.24 (d, J = 8.8 Hz, 4H, minor isomer), 6.99 (s, 2H), 3.74 (s, 6H); ^{13}C NMR (100 MHz, DMSO-d_6; DEPT) δ 163.1 (CH, minor isomer), 160.5 (CH, mayor isomer), 151.1 (C), 138.0 (C, minor isomer), 133.9 (C, mayor isomer), 131.1 (CH, minor isomer), 130.6 (CH, mayor isomer), 130.2 (C), 130.1 (C), 119.7 (CH, mayor isomer), 118.0 (CH, minor isomer), 115.2 (CH), 57.12 (CH_3); HRMS FAB: *m/z* calcd. for $C_{22}H_{20}N_2O_4$ $[M]^+$ 376.1423, found *m/z* 376.1429.

Synthesis of compound 8. Compound **21** (100 mg, 0.27 mmol) was added to a Schlenk flask containing triphosgene (200 mg, 0.69 mmol). The flask was sealed, evacuated, and back-filled with Argon. The flask was cooled to 0 °C before the addition of distilled CH_2Cl_2 (5 mL) and Et_3N (4 mL) under positive argon pressure. The solution was stirred overnight at room temperature. The reaction mixture was washed with water, dried over anhydrous Na_2SO_4, and the solvent removed. Purification by flash chromatography (EtOAc/Hexane: 1/9) yielded the desired product **8** (71 mg, 78 %) as a orange solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66-7.56 (m, 4H), 7.44 (d, J = 8.0 Hz, 4H), 6.93 (s, 2H), 3.80 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$; DEPT) δ 164.5 (C), 150.9 (C), 139.6 (C), 130.7 (CH), 129.6 (C), 126.4 (CH), 114.6 (CH), 56.7 (CH_3); HRMS ES: *m/z* calcd. for $C_{22}H_{17}N_2O_2$ $[M+H]^+$ 341.1285, found *m/z* 341.1284.

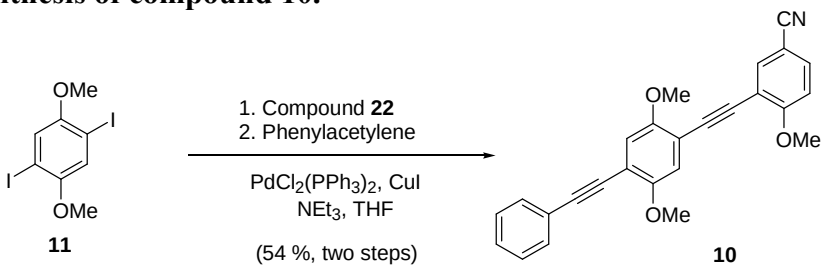
Synthesis of compound 9.



CuI (4.3 mg, 0.02 mmol) was added to a solution of Et_3N (7 mL), $Pd(PPh_3)_2Cl_2$ (10.2 mg, 0.01 mmol), 3-ethynyl-4methoxybenzonitrile (100 mg, 0.64 mmol) and 2,5-diiodo-1,4-dimethoxybenzene **11** (113 mg, 028 mmol) in THF (10 mL), stirred for 5 min beforehand under argon. The reaction was allowed to stir at room temperature for 12 h. Then, the resulting solution was diluted with EtOAc and washed with a NH_4Cl solution. The organic layer was dried over anhydrous Na_2SO_4, concentrated under vacuum and the crude product submitted to flash chromatography (EtOAc/Hexane: 1/9) to give **9** (122 mg, 94 %) as a yellow solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ : 7.80 (d, J = 2.1 Hz, 2H), 7.59 (dd, J = 8.6, 2.1 Hz, 2H), 7.04 (s, 2H), 6.96 (d, J = 8.6 Hz, 2H), 3.99 (s, 6H), 3.92 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$; DEPT) δ : 163.2 (C), 154.5 (C), 137.5 (CH), 134.2 (CH), 118.7 (C), 116.1 (CH), 114.6 (C), 113.8 (C), 111.6 (CH), 104.7 (C), 91.7

(C), 89.5 (C), 56.9 (CH_3), 56.7 (CH_3); HRMS ES: *m/z* calcd. for $C_{28}H_{20}N_2O_4Na$ $[M+Na]^+$ 471.1321, found *m/z* 471.1321.

Synthesis of compound 10.



CuI (14.2 mg, 0.09 mmol) was added to a solution of Et_3N (7 mL), $Pd(PPh_3)_2Cl_2$ (23.4 mg, 0.04 mmol), 3-ethynyl-4methoxybenzonitrile (150 mg, 0.95 mmol) and 2,5-diiodo-1,4-dimethoxybenzene **11** (745.1 mg, 0.77 mmol) in THF (10 mL), stirred for 5 min beforehand under argon. The reaction was allowed to stir at room temperature for 6 h. Then, phenyl acetylene (433 mg, 4.24 mmol) was added and the resulting mixture was allowed to stir at room temperature for another 12h. EtOAc was added and the solution washed with a NH_4Cl solution. The organic layer was dried over anhydrous Na_2SO_4, concentrated under vacuum and the crude product submitted to flash chromatography (EtOAc/Hexane: 4/6) to give **10** (202 mg, 54 %) as a yellow solid. ^1H NMR (400 MHz, $CDCl_3$) δ : 7.79 (d, *J* = 2 Hz, 1H), 7.59-7.55 (m, 3H), 7.37-7.33 (m, 3H), 7.04 (s, 1H), 7.03 (s, 1H), 6.93 (d, *J* = 8.6 Hz, 1H), 3.96 (s, 3H), 3.90 (s, 3H), 3.89 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$; DEPT) δ: 163.1 (C), 154.4 (C), 154.2 (C), 137.3 (CH), 134.1 (CH), 132.0 (CH), 128.7 (CH), 128.6 (CH), 123.4 (C), 118.7 (C), 116.0 (CH), 116.0 (CH), 114.5 (C), 114.4 (C), 113.0 (C), 111.6 (CH), 104.5 (C), 96.5 (C), 92.0 (C), 89.1 (C), 85.8 (C), 56.8 (CH_3), 56.6 (CH_3); HRMS EI: *m/z* calcd. for $C_{26}H_{19}NO_3$ $[M]^+$ 393.1365, found *m/z* 393.1347.

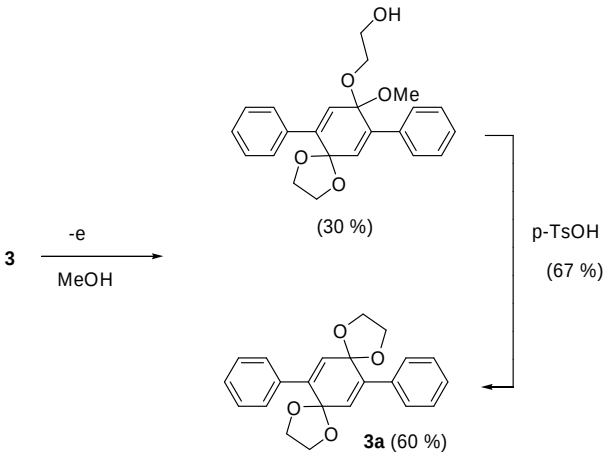
General Procedure for Anodic Oxidation

Electrolysis was carried out in a single cell apparatus in a reagent grade MeOH using a circular platinum gauze anode (5 cm x 5 cm in diameter) 45-mesh, a graphite cathode (9 mm x 40 mm), and an AMEL (model 549) power supply. A solution of the corresponding dimethoxybenzene in MeOH with 1 % KOH was anodically oxidized at 0 °C, under constant current (1 A, 2 V). The reaction was monitored by TLC. The methanolic solution was evaporated under reduced pressure, extracted with EtOAc, washed with brine, dried over $MgSO_4$, filtered, and concentrated under vacuum. Flash chromatography with Et_3N pre-treated silica gel afforded the corresponding quinone bisketals **1a-10a**.

Synthesis of compound 1a. It was prepared by electrolysis of precursor **1** (200 mg, 0.69 mmol) in 150 mL of MeOH with KOH (300 mg, 5.34 mmol), according to previously described general procedure, for 80 min. The compound was purified by flash chromatography (EtOAc/Hexane: 1/9) to give **1a** (219 mg, 87 %) as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78-7.74 (m, 4H), 7.34-7.33 (m, 6H), 6.36 (s, 2H), 3.28 (s, 12H); ^{13}C NMR (75 MHz, $CDCl_3$; DEPT) δ 142.7 (C), 136.7 (C), 131.5 (CH), 128.4 (CH), 128.3 (CH), 128.0 (CH), 97.6 (C), 51.1 (CH_3); HRMS ES: *m/z* calcd. for $C_{22}H_{24}O_4Na$ $[M+Na]^+$ 375.1572, found *m/z* 375.1566.

Synthesis of compound 2a. It was prepared by electrolysis of precursor **2** (200 mg, 0.59 mmol) in 150 mL of MeOH with KOH (300 mg, 5.34 mmol) according to previously described general procedure for 80 min. The compound was purified by flash chromatography (EtOAc/Hexane: 2/98) to give **2a** (174 mg, 74 %) as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.56-7.48 (m, 4H), 7.35-7.25 (m, 6H), 6.45 (s, 2H), 3.40 (s, 12H); ^{13}C NMR (75 MHz, $CDCl_3$; DEPT) δ 137.1 (CH), 131.9 (CH), 128.7 (CH), 128.3 (CH), 127.9 (C), 122.7 (C), 94.7 (C), 92.8 (C), 84.8 (C), 51.4 (CH_3); HRMS ES: *m/z* calcd. for $C_{26}H_{24}O_4Na$ $[M+Na]^+$ 423.1572, found *m/z* 423.1566.

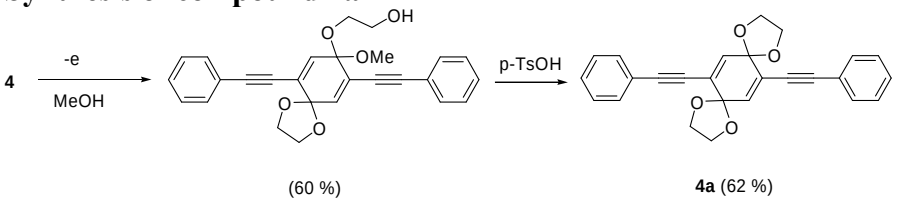
Synthesis of compound 3a.



It was prepared by electrolysis of precursor **3** (220 mg, 0.628 mmol) in 80 mL of MeOH with KOH (632 mg, 11.26 mmol) according to previously described general procedure for 2 h. The compound was purified by flash chromatography (EtOAc/Hexane: 2/8) to give acyclic ketal (80 mg, 30 %) and **3a** (132 mg, 60 %). The acyclic ketal (80 mg, 0.19 mmol) was tread with *p*-toluensulfonic acid (6 mg, 0.03 mmol) in ether to give **3a** (45

mg, 67 %) as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50-7.49 (m, 4H), 7.34-7.32 (m, 6H), 5.92 (s, 2H), 3.97 (m, 4H), 3.70 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$; DEPT) δ 141.1 (C), 138.4 (C), 131.7 (CH), 129.6 (CH), 128.1 (CH), 127.9 (CH), 101.6 (C), 66.0 (CH_2); HRMS FAB: *m/z* calcd. for $C_{22}H_{21}O_4$ $[M+H]^+$ 349.1440, found *m/z* 349.1436.

Synthesis of compound 4a



(60 %) **4a** (62 %)

Compound **4a** was prepared by electrolysis of precursor **4** (80 mg, 0.20 mmol) in 80 mL of MeOH with KOH (632 mg, 11.26 mmol) according to previously described general procedure for 2h. The compound was purified by flash chromatography (EtOAc/Hexane: 2/8) to give acyclic ketal (52 mg, 60 %). This compound (52 mg, 0.12 mmol) was treated with *p*-toluensulfonic acid (4 mg, 0.02 mmol) in ether to give **4a** (29 mg, 62 %) as a yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45-7.43 (m, 4H), 7.33-7.32 (m, 6H), 6.21 (s, 2H), 4.37-4.34 (m, 4H), 4.16-4.13 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$; DEPT) δ 135.7 (CH), 131.7 (CH), 128.7 (CH), 128.5 (CH), 126.3 (C), 122.7 (C), 99.5 (C), 92.3 (C), 85.3 (C), 66.8(CH_2). A good quality mass spectrum for this compound could not be obtained.

Synthesis of compound 5a. Compound **5a** was prepared by electrolysis of precursor **5** (50 mg, 0.10 mmol) in 110 mL of MeOH with KOH (790 mg, 14.08 mmol) according to previously described general procedure for 2h. The compound was purified by flash chromatography (EtOAc/Hexane: 2/98) to give **5a** (51 mg, 90 %) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 8.2 Hz, 4H), 7.66 (d, J = 8.2 H, 4H), 6.45 (s, 2H), 3.30 (s, 12H); ^{13}C NMR (75 MHz, $CDCl_3$; DEPT) δ 141.9 (C), 139.2(C), 136.3(CH), 132.3 (CH), 130.0 (q, $^1J_{C\text{-}F}$ = 260 Hz, C) 129.2 (CH), 124.4 (C), 97.3 (C), 51.3 (CH_3); HRMS ES: *m/z* calcd. for $C_{24}H_{22}F_6O_4S_2Na$ $[M+Na]^+$ 575.0761, found *m/z* 575.0755.

Synthesis of compound 6a. Compound **6a** was prepared by electrolysis of precursor **6** (50 mg, 0.12 mmol) in 80 mL of MeOH with KOH (632 mg. 11.26 mmol) according to previously described general procedure for 3 h. The compound was purified by flash chromatography (MeOH/CH_2Cl_2: 1/40) to give **6a** (42 mg, 72 %) as a white solid. ^{1}H NMR (500 MHz, CD_3OD) δ 8.01 (d, J = 10.0 Hz, 4H), 7.72 (d, J = 10.0 Hz, 4H), 6.57 (s, 2H), 3.30 (s, 12H), 2.83 (s, 6H); ^{13}C NMR (125 MHz, CD_3OD; DEPT) δ 146.7 (C), 144.1 (C), 142.1 (C), 134.5 (CH), 131.3 (CH), 128.6 (CH), 99.4 (C), 52.4 (CH_3), 44.4(CH_3); HRMS ES: *m/z* calcd. for $C_{24}H_{28}O_6S_2Na$ $[M+Na]^+$ 499.1225, found *m/z* 499.1219.

Synthesis of compound 7a. Compound **7a** was prepared by electrolysis of precursor **7** (45 mg, 0.13 mmol) in 300 mL of MeOH with KOH (2.3 g, 42.24 mmol) according to previously described general procedure for 22 h. The compound was purified by flash chromatography (EtOAc/Hexane: 3/7) to give starting **7** (14 mg) and bisketal **7a** (29 mg, 54 %, 87 % bsmr) as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.87 (d, J = 8.1 Hz, 4H), 7.67 (d, J = 8.1 Hz, 4H), 6.47 (s, 2H), 3.29 (s, 12H); ^{13}C NMR (75 MHz, CDCl3; DEPT) δ: 141.5 (C), 141.0 (C), 132.5 (CH), 132.3 (CH), 128.9 (CH), 118.7 (C),

112.5 (C), 97.1 (C), 51.3 (CH_3); HRMS ES: *m/z* calcd. for $C_{24}H_{22}N_2O_4Na$ $[M+Na]^+$ 425.1477, found *m/z* 425.1471.

Synthesis of compound 8a. Compound **8a** was prepared by electrolysis of precursor **8** (37 mg, 0.11 mmol) in 200 mL of MeOH with KOH (1.5 g, 28.16 mmol) according to previously described general procedure for h. The compound was purified by flash chromatography (EtOAc/Hexane: 3/7) to give **8a** (24 mg, 56 %) as a white solid. ^1H NMR (300 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.6 Hz, 4H), 7.39 (d, *J* = 8.6 Hz, 4H), 6.40 (s, 2H), 3.28 (s, 12H); ^{13}C NMR (125 MHz, $CDCl_3$; DEPT) δ 164.9 (C), 141.4 (C), 137.4 (C), 131.7 (CH), 128.9 (CH), 126.2 (CH), 97.0 (C), 51.0 (CH_3), (one carbon signal was not observed); HRMS ES: *m/z* calcd. for $C_{24}H_{22}N_2O_4Na$ $[M+Na]^+$ 425.1477, found *m/z* 425.1471.

Synthesis of compound 9a. Compound **9a** was prepared by electrolysis of **9** (50 mg, 0.11 mmol) in 180 mL of MeOH with 600 mg of KOH (10.7 mmol) according to previously described general procedure [25200 C, 75 % current efficiency]. The compound was purified by flash chromatography (EtOAc/Hexane: 3/7) to give **9a** (32 mg, 57 %), (78% bsmr) as a yellow solid. ^1H NMR (300 MHz, $CDCl_3$) δ : 7.75 (d, *J* = 2.2 Hz, 2H), 7.60 (dd, *J* = 8.6, 2.2 Hz, 2H), 6.93 (d, *J* = 8.6 Hz, 2H), 6.51 (s, 2H), 3.95 (s, 6H), 3.42 (s, 12H); ^{13}C NMR (75 MHz, $CDCl_3$; DEPT) δ : 163.5 (C), 138.0 (CH), 137.6 (CH), 134.5 (CH), 127.7 (C), 118.6 (C), 114.0 (C), 111.7 (CH), 104.5 (C), 94.8 (C), 90.9 (C), 87.2 (C), 56.6 (CH_3), 51.7 (CH_3); HRMS ES: *m/z* calcd. for $C_{30}H_{26}N_2O_6Na$ $[M+Na]^+$ 536.1689, found *m/z* 533.1676.

Synthesis of compound 10a. Compound **10a** was prepared by electrolysis of **10** (80 mg, 0.20 mmol) in 80 mL of MeOH with 600 mg of KOH (10.7 mmol) according to previously described general procedure [7200 C, 100 % current efficiency]. The compound was purified by flash chromatography (EtOAc/Hexane: 2/8) to give **10a** (53 mg, 82 %), as a yellow solid. ^1H NMR (300 MHz, $CDCl_3$) δ : 7.74 (d, *J* = 3.5 Hz, 1H), 7.59 (dd, *J* = 9.2, 3.5 Hz, 1H), 7.53-7.49 (m, 2H), 7.34-7.32 (m,3H), 6.90 (d, *J* = 9.2 Hz, 1H), 6.49 (s, 1H), 6.47 (s, 1H), 3.80 (s, 3H), 3.42 (s, 6H), 3.40 (s,6H); ^{13}C NMR (75 MHz, $CDCl_3$; DEPT) δ: 163.4 (C), 138.2 (CH), 137.6 (CH), 137.3 (CH), 134.5 (CH), 132.2 (CH), 129.0 (CH), 128.6 (CH), 128.0 (C), 127.9 (C), 123.0 (C), 118.6 (C), 114.0 (C), 111.6 (CH), 104.5 (C), 95.0 (C), 94.9 (C), 93.3(C), 90.9 (C), 87.1 (C), 85.0 (C), 56.6 (CH_3), 51.7 (CH_3); HRMS ES: *m/z* calcd. for $C_{28}H_{25}NO_5Na$ $[M+Na]^+$ 478.1630, found *m/z* 478.1625.

COMPUTATIONAL METHODS

Gaussian 03, Revision E.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Calculations were performed with Gaussian 03 at DFT level. The geometries of the structures were optimized using the B3LYP hybrid functional. The 6-31G(d,p) basis set was used for all atoms. Harmonic frequencies were calculated at the same level to characterize the stationary points.

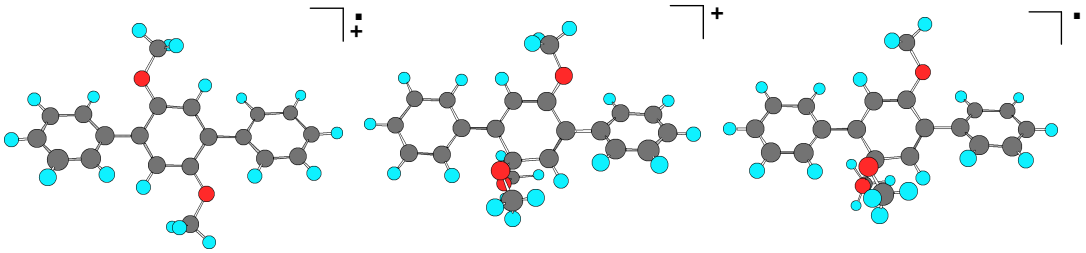
Calculated geometrical parameters of **1**, **2**, **5-10**, **1a-10a** and intermediates **A-C** (see below) can be found in the following Table

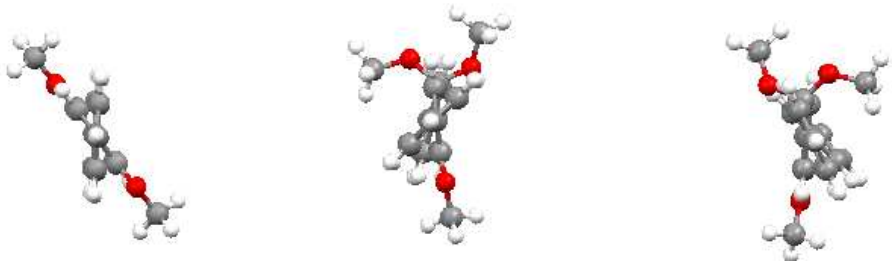
Table S1.

Compound	Length (Å)	Linearity (º)	Torsion Angle (º)
1	13.66	178.6	45.0
1a	13.76	178.8	27.8
3a	13.70	178.8	29.3
2	18.74	179.8	0
2a	18.73	169.1	0.4
4a	18.82	179.6	14.3
5	15.04[a]	178.6	41.5
5a	15.16[a]	179.2	26.5
6	15.09[a]	179.6	40.6
6a	15.18[a]	178.1	26.7
7	16.66	179.1	40.1
7a	16.72	171.6	23.3
8	16.58	179.1	40.0
8a	16.64	171.0	23.3
9	18.75	177.5	5.8
9a	18.80	178.8	0.2
10	18.75	178.4	6.1
10a	18.81	179.0	0.0
A	13.62	179.1	40.0
B	13.67	175.6	53.1, 15.7

C	13.64	170.8	48.0, 24.5

[a] Distances between terminal sulphur atoms.





Compound 1

```
Zero-point correction=                           0.327825
(Hartree/Particle)
 Thermal correction to Energy=                    0.346730
 Thermal correction to Enthalpy=                  0.347674
 Thermal correction to Gibbs Free Energy=         0.279703
 Sum of electronic and zero-point Energies=           -923.080987
 Sum of electronic and thermal Energies=              -923.062082
 Sum of electronic and thermal Enthalpies=            -923.061138
 Sum of electronic and thermal Free Energies=         -923.129109

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -4.935588   -1.204397   -0.826597
    2          6             0       -5.717470   -0.418728    0.021153
    3          6             0       -5.098309    0.513329    0.856798
    4          6             0       -3.712351    0.659718    0.847818
    5          6             0       -2.910682   -0.129142    0.004292
    6          6             0       -3.548400   -1.060296   -0.833773
    7          6             0       -1.426156   -0.032871    0.013209
    8          6             0       -0.735156    1.197246    0.012863
    9          6             0        0.661476    1.209319    0.011297
   10          6             0        1.426153    0.032885    0.013208
   11          6             0        0.735155   -1.197227    0.012875
   12          6             0       -0.661479   -1.209301    0.011303
   13          6             0        2.910677    0.129148    0.004290
   14          6             0        3.548406    1.060292   -0.833780
   15          6             0        4.935594    1.204376   -0.826595
```

16	6	0	5.717462	0.418699	0.021164
17	6	0	5.098289	-0.513354	0.856804
18	6	0	3.712330	-0.659728	0.847814
19	8	0	1.496888	-2.336982	0.004734
20	6	0	0.841253	-3.589845	-0.077094
21	8	0	-1.496880	2.337004	0.004708
22	6	0	-0.841223	3.589861	-0.077076
23	1	0	-5.404968	-1.926142	-1.489485
24	1	0	-6.798222	-0.528325	0.028154
25	1	0	-5.697434	1.128415	1.522749
26	1	0	-3.241882	1.385934	1.500124
27	1	0	-2.949196	-1.661101	-1.511911
28	1	0	1.193368	2.152293	0.030557
29	1	0	-1.193366	-2.152278	0.030565
30	1	0	2.949205	1.661100	-1.511918
31	1	0	5.404996	1.926104	-1.489487
32	1	0	6.798215	0.528290	0.028168
33	1	0	5.697405	-1.128446	1.522757
34	1	0	3.241833	-1.385952	1.500092
35	1	0	1.632478	-4.340812	-0.110269
36	1	0	0.229952	-3.670259	-0.985591
37	1	0	0.204890	-3.777561	0.797954
38	1	0	-1.632438	4.340837	-0.110279
39	1	0	-0.229882	3.670269	-0.985546
40	1	0	-0.204895	3.777560	0.798002

Compound 2

Zero-point correction= 0.347585
(Hartree/Particle)
Thermal correction to Energy= 0.370816
Thermal correction to Enthalpy= 0.371760
Thermal correction to Gibbs Free Energy= 0.290686
Sum of electronic and zero-point Energies= -1075.374235
Sum of electronic and thermal Energies= -1075.351004
Sum of electronic and thermal Enthalpies= -1075.350060
Sum of electronic and thermal Free Energies= -1075.431134

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.605996	1.021928	-0.000124
2	6	0	8.281079	-0.201757	-0.000063
3	6	0	7.553513	-1.394762	0.000000
4	6	0	6.161651	-1.369559	-0.000001
5	6	0	5.470175	-0.140528	-0.000056
6	6	0	6.214576	1.057626	-0.000120
7	6	0	4.047276	-0.104359	-0.000056
8	6	0	2.831373	-0.052441	0.000002
9	6	0	1.413144	-0.018824	0.000044
10	6	0	0.716893	1.216020	0.000093
11	6	0	-0.675187	1.219430	0.000101
12	6	0	-1.413138	0.018891	0.000072
13	6	0	-0.716890	-1.215952	0.000058
14	6	0	0.675190	-1.219363	0.000029
15	6	0	-2.831369	0.052507	0.000048
16	6	0	-4.047272	0.104422	-0.000016
17	6	0	-5.470174	0.140524	-0.000039
18	6	0	-6.161709	1.369521	-0.000159
19	6	0	-7.553574	1.394657	-0.000177

20	6	0	-8.281079	0.201617	-0.000080
21	6	0	-7.605936	-1.022036	0.000036
22	6	0	-6.214515	-1.057668	0.000058
23	8	0	-1.491006	-2.337611	0.000062
24	6	0	-0.844104	-3.599432	-0.000008
25	8	0	1.491001	2.337679	0.000124
26	6	0	0.844093	3.599488	0.000142
27	1	0	8.166864	1.952248	-0.000174
28	1	0	9.366904	-0.225497	-0.000064
29	1	0	8.073304	-2.348635	0.000045
30	1	0	5.594133	-2.294702	0.000042
31	1	0	5.685521	2.005058	-0.000164
32	1	0	-1.228723	2.149438	0.000124
33	1	0	1.228730	-2.149367	-0.000030
34	1	0	-5.594235	2.294691	-0.000236
35	1	0	-8.073409	2.348505	-0.000269
36	1	0	-9.366906	0.225298	-0.000095
37	1	0	-8.166762	-1.952381	0.000113
38	1	0	-5.685410	-2.005072	0.000152
39	1	0	-1.640877	-4.344726	0.000026
40	1	0	-0.221980	-3.736496	0.894020
41	1	0	-0.222091	-3.736456	-0.894119
42	1	0	1.640856	4.344792	0.000157
43	1	0	0.222013	3.736507	0.894210
44	1	0	0.222019	3.736549	-0.893923

Compound 5

Zero-point correction= 0.338927
(Hartree/Particle)
Thermal correction to Energy= 0.368656
Thermal correction to Enthalpy= 0.369600
Thermal correction to Gibbs Free Energy= 0.271844
Sum of electronic and zero-point Energies= -2393.479128
Sum of electronic and thermal Energies= -2393.449399
Sum of electronic and thermal Enthalpies= -2393.448455
Sum of electronic and thermal Free Energies= -2393.546211

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.661528	0.647425	-0.569517
2	6	0	4.925018	1.444199	0.313548
3	6	0	3.554051	1.241725	0.452291
4	6	0	2.885612	0.245720	-0.281264
5	6	0	3.642671	-0.550832	-1.158952
6	6	0	5.011959	-0.350199	-1.307214
7	6	0	1.413587	0.090401	-0.148449
8	6	0	0.782023	-1.168165	-0.049231
9	6	0	-0.605065	-1.235946	0.097285
10	6	0	-1.413594	-0.090267	0.148277
11	6	0	-0.782074	1.168295	0.048919
12	6	0	0.605007	1.236077	-0.097575
13	6	0	-2.885619	-0.245576	0.281256
14	6	0	-3.642324	0.549767	1.160327
15	6	0	-5.011608	0.349098	1.308617
16	6	0	-5.661476	-0.647395	0.569659
17	6	0	-4.925281	-1.443033	-0.314693
18	6	0	-3.554327	-1.240488	-0.453518
19	8	0	-1.591105	2.271440	0.075172

20	6	0	-1.005984	3.551022	-0.104551
21	8	0	1.590979	-2.271371	-0.075714
22	6	0	1.005871	-3.550902	0.104471
23	16	0	7.416547	0.943222	-0.794085
24	6	0	8.083341	-0.257676	0.406504
25	9	0	9.423190	-0.158181	0.374810
26	9	0	7.672270	-0.020872	1.663867
27	9	0	7.749067	-1.527236	0.115195
28	16	0	-7.416482	-0.943217	0.794322
29	6	0	-8.083322	0.257515	-0.406410
30	9	0	-9.423172	0.158102	-0.374576
31	9	0	-7.748935	1.527090	-0.115363
32	9	0	-7.672393	0.020453	-1.663783
33	1	0	5.426593	2.211579	0.893822
34	1	0	2.995723	1.849598	1.157647
35	1	0	3.150963	-1.326818	-1.732712
36	1	0	5.580973	-0.963921	-1.997581
37	1	0	-1.088779	-2.198403	0.206548
38	1	0	1.088663	2.198543	-0.206973
39	1	0	-3.150428	1.324764	1.735287
40	1	0	-5.580380	0.961881	2.000018
41	1	0	-5.427071	-2.209596	-0.895860
42	1	0	-2.996174	-1.847470	-1.159784
43	1	0	-1.831272	4.263864	-0.072925
44	1	0	-0.293544	3.789823	0.695837
45	1	0	-0.497078	3.631302	-1.073583
46	1	0	1.831146	-4.263762	0.072886
47	1	0	0.497143	-3.630899	1.073617
48	1	0	0.293287	-3.789920	-0.695723

Compound 6

Zero-point correction= 0.391021
(Hartree/Particle)
Thermal correction to Energy= 0.419163
Thermal correction to Enthalpy= 0.420107
Thermal correction to Gibbs Free Energy= 0.329366
Sum of electronic and zero-point Energies= -1948.357255
Sum of electronic and thermal Energies= -1948.329113
Sum of electronic and thermal Enthalpies= -1948.328168
Sum of electronic and thermal Free Energies= -1948.418910

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.718945	-0.152562	-0.170230
2	6	0	4.965170	-0.911190	-1.067003
3	6	0	3.575423	-0.820347	-1.036004
4	6	0	2.923155	0.035110	-0.128147
5	6	0	3.709271	0.805890	0.747815
6	6	0	5.099903	0.715436	0.726132
7	6	0	1.438245	0.086379	-0.095693
8	6	0	0.710307	1.285421	0.052077
9	6	0	-0.682808	1.274420	0.068911
10	6	0	-1.427754	0.090681	-0.047738
11	6	0	-0.699558	-1.108328	-0.193351
12	6	0	0.693354	-1.097526	-0.211246
13	6	0	-2.912950	0.141110	-0.023354
14	6	0	-3.691541	-0.624896	-0.910073
15	6	0	-5.081945	-0.528726	-0.905452
16	6	0	-5.709493	0.326367	-0.002656

17	6	0	-4.961708	1.109092	0.878336
18	6	0	-3.572477	1.006216	0.869991
19	8	0	-1.338159	-2.325296	-0.334101
20	6	0	-1.712822	-2.945335	0.897510
21	8	0	1.348711	2.501505	0.194693
22	6	0	1.720631	3.126846	-1.036207
23	16	0	7.541741	-0.191126	-0.207648
24	8	0	8.029350	0.875020	0.748377
25	6	0	7.728698	-1.806639	0.650704
26	16	0	-7.526544	0.464269	-0.074815
27	8	0	-7.991652	-0.389885	-1.233377
28	6	0	-7.865238	-0.488194	1.461542
29	1	0	5.450101	-1.560280	-1.792320
30	1	0	2.986338	-1.398737	-1.741446
31	1	0	3.223637	1.478993	1.444249
32	1	0	5.721775	1.309373	1.389853
33	1	0	-1.192210	2.228840	0.154863
34	1	0	1.202986	-2.051659	-0.299502
35	1	0	-3.199995	-1.292267	-1.607937
36	1	0	-5.696295	-1.095233	-1.599434
37	1	0	-5.450478	1.792073	1.569192
38	1	0	-2.989052	1.596417	1.570335
39	1	0	-2.189287	-3.892338	0.636277
40	1	0	-0.832430	-3.140571	1.523296
41	1	0	-2.422318	-2.325759	1.459195
42	1	0	2.197579	4.072582	-0.771906
43	1	0	2.429122	2.509696	-1.601413
44	1	0	0.838341	3.324145	-1.658416
45	1	0	8.800429	-1.997642	0.739382
46	1	0	7.252772	-2.594041	0.061227
47	1	0	7.275865	-1.733806	1.641821
48	1	0	-8.950422	-0.526383	1.579223
49	1	0	-7.463551	-1.497129	1.345856
50	1	0	-7.410902	0.017328	2.317096

Compound 7

Zero-point correction= 0.324953
(Hartree/Particle)
Thermal correction to Energy= 0.345922
Thermal correction to Enthalpy= 0.346866
Thermal correction to Gibbs Free Energy= 0.274414
Sum of electronic and zero-point Energies= -1107.553347
Sum of electronic and thermal Energies= -1107.532379
Sum of electronic and thermal Enthalpies= -1107.531434
Sum of electronic and thermal Free Energies= -1107.603886

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.031601	-1.551386	0.000042
2	6	0	-4.994739	-2.952456	-0.000010
3	6	0	-3.744142	-3.589832	-0.000058
4	6	0	-2.577498	-2.839850	-0.000053
5	6	0	-2.583300	-1.425364	-0.000002
6	6	0	-3.855596	-0.809872	0.000046
7	6	0	-1.299726	-0.660778	0.000001
8	6	0	-1.180412	0.754496	0.000032
9	6	0	0.077324	1.355560	0.000031
10	6	0	1.299726	0.660778	-0.000001
11	6	0	1.180412	-0.754496	-0.000032

12	6	0	-0.077324	-1.355560	-0.000031
13	6	0	2.583300	1.425364	0.000002
14	6	0	3.855596	0.809872	-0.000046
15	6	0	5.031601	1.551386	-0.000042
16	6	0	4.994739	2.952456	0.000010
17	6	0	3.744142	3.589832	0.000058
18	6	0	2.577498	2.839850	0.000053
19	8	0	2.322888	-1.507850	-0.000064
20	6	0	2.236809	-2.924713	-0.000042
21	8	0	-2.322888	1.507850	0.000064
22	6	0	-2.236809	2.924713	0.000042
23	6	0	-6.204868	-3.718546	-0.000015
24	7	0	-7.187643	-4.341810	-0.000019
25	6	0	6.204868	3.718546	0.000015
26	7	0	7.187643	4.341810	0.000019
27	1	0	-5.988757	-1.040290	0.000080
28	1	0	-3.691865	-4.673482	-0.000099
29	1	0	-1.647098	-3.392478	-0.000093
30	1	0	-3.927684	0.264734	0.000088
31	1	0	0.102122	2.432630	0.000057
32	1	0	-0.102122	-2.432630	-0.000057
33	1	0	3.927684	-0.264734	-0.000088
34	1	0	5.988757	1.040290	-0.000080
35	1	0	3.691865	4.673482	0.000099
36	1	0	1.647098	3.392478	0.000093
37	1	0	3.267185	-3.283045	-0.000040
38	1	0	1.726145	-3.300230	-0.895540
39	1	0	1.726146	-3.300203	0.895467
40	1	0	-3.267185	3.283045	0.000040
41	1	0	-1.726145	3.300230	0.895540
42	1	0	-1.726146	3.300203	-0.895467

Compound 8

Zero-point correction= 0.322473
(Hartree/Particle)
Thermal correction to Energy= 0.345725
Thermal correction to Enthalpy= 0.346669
Thermal correction to Gibbs Free Energy= 0.268060
Sum of electronic and zero-point Energies= -1107.492021
Sum of electronic and thermal Energies= -1107.468769
Sum of electronic and thermal Enthalpies= -1107.467825
Sum of electronic and thermal Free Energies= -1107.546434

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.072910	0.638643	0.897212
2	6	0	-5.722356	-0.272026	0.053060
3	6	0	-4.976741	-1.081589	-0.812911
4	6	0	-3.590219	-0.975872	-0.825345
5	6	0	-2.916483	-0.071323	0.015185
6	6	0	-3.686306	0.735762	0.873573
7	6	0	-1.432572	-0.012103	0.009618
8	6	0	-0.710047	1.196717	0.090977
9	6	0	0.682846	1.195680	0.075887
10	6	0	1.432544	0.012107	-0.009539
11	6	0	0.710022	-1.196712	-0.090892
12	6	0	-0.682872	-1.195676	-0.075806
13	6	0	2.916454	0.071323	-0.015149

14	6	0	3.686236	-0.735799	-0.873538
15	6	0	5.072840	-0.638698	-0.897231
16	6	0	5.722326	0.271991	-0.053131
17	6	0	4.976752	1.081585	0.812847
18	6	0	3.590229	0.975883	0.825337
19	8	0	1.357643	-2.411492	-0.197985
20	6	0	1.719496	-3.004796	1.051870
21	8	0	-1.357682	2.411491	0.198053
22	6	0	-1.719252	3.004923	-1.051821
23	7	0	-7.103022	-0.369070	0.072122
24	6	0	-8.281547	-0.451540	0.088295
25	7	0	7.102992	0.369020	-0.072248
26	6	0	8.281514	0.451518	-0.088471
27	1	0	-5.661807	1.256288	1.566719
28	1	0	-5.489575	-1.776400	-1.469094
29	1	0	-3.019968	-1.593291	-1.512349
30	1	0	-3.189847	1.443137	1.526282
31	1	0	1.187617	2.155734	0.112814
32	1	0	-1.187634	-2.155733	-0.112734
33	1	0	3.189742	-1.443195	-1.526201
34	1	0	5.661705	-1.256371	-1.566738
35	1	0	5.489619	1.776407	1.468993
36	1	0	3.020010	1.593325	1.512346
37	1	0	2.201192	-3.955656	0.816207
38	1	0	0.832454	-3.188950	1.671089
39	1	0	2.420580	-2.370654	1.607829
40	1	0	-2.200931	3.955796	-0.816177
41	1	0	-0.832083	3.189068	-1.670860
42	1	0	-2.420271	2.370868	-1.607964

Compound 1a

Zero-point correction= 0.414466
(Hartree/Particle)
Thermal correction to Energy= 0.439170
Thermal correction to Enthalpy= 0.440114
Thermal correction to Gibbs Free Energy= 0.360654
Sum of electronic and zero-point Energies= -1153.196494
Sum of electronic and thermal Energies= -1153.171790
Sum of electronic and thermal Enthalpies= -1153.170846
Sum of electronic and thermal Free Energies= -1153.250307

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.961533	-1.593295	0.093744
2	6	0	-5.769849	-0.460772	0.211889
3	6	0	-5.174724	0.799556	0.273347
4	6	0	-3.787134	0.934181	0.230450
5	6	0	-2.957697	-0.199551	0.134716
6	6	0	-3.575861	-1.462523	0.047795
7	6	0	-1.472150	-0.094900	0.109403
8	6	0	-0.820424	1.189550	-0.406903
9	6	0	0.682527	1.097157	-0.535040
10	6	0	1.471800	0.095343	-0.108789
11	6	0	0.819956	-1.189060	0.407800
12	6	0	-0.683015	-1.096758	0.535719
13	6	0	2.957390	0.199462	-0.134838
14	6	0	3.576307	1.462482	-0.053556
15	6	0	4.962008	1.592357	-0.100354
16	6	0	5.769802	0.458953	-0.213680

17	6	0	5.174021	-0.801296	-0.269564
18	6	0	3.786357	-0.935038	-0.225892
19	8	0	1.117008	-2.315626	-0.427239
20	6	0	0.797115	-2.213127	-1.805582
21	8	0	-1.117819	2.315802	0.428483
22	6	0	-0.793459	2.214681	1.805875
23	8	0	1.396780	-1.639241	1.621649
24	6	0	1.311685	-0.760314	2.730287
25	8	0	-1.397303	1.640046	-1.620583
26	6	0	-1.312895	0.761128	-2.729288
27	1	0	-5.410142	-2.580258	0.023044
28	1	0	-6.851148	-0.560092	0.242695
29	1	0	-5.793230	1.689209	0.353377
30	1	0	-3.337133	1.917710	0.267751
31	1	0	-2.965800	-2.351322	-0.079509
32	1	0	1.109164	2.001209	-0.961827
33	1	0	-1.109927	-2.000939	0.961991
34	1	0	2.966979	2.352261	0.070260
35	1	0	5.411076	2.579420	-0.034118
36	1	0	6.851141	0.557628	-0.245092
37	1	0	5.792023	-1.691626	-0.345871
38	1	0	3.335992	-1.918516	-0.259460
39	1	0	1.014278	-3.194665	-2.232620
40	1	0	1.408929	-1.459577	-2.317828
41	1	0	-0.262107	-1.981494	-1.968291
42	1	0	-1.012894	3.195481	2.233441
43	1	0	0.267059	1.986824	1.965408
44	1	0	-1.400997	1.458980	2.320054
45	1	0	1.744299	-1.301420	3.574459
46	1	0	0.273634	-0.497154	2.971874
47	1	0	1.886828	0.161384	2.571724
48	1	0	-1.742328	1.303756	-3.574112
49	1	0	-1.891156	-0.158839	-2.571972
50	1	0	-0.275225	0.494905	-2.969099

Compound 2a

Zero-point correction= 0.433399
(Hartree/Particle)
Thermal correction to Energy= 0.462903
Thermal correction to Enthalpy= 0.463847
Thermal correction to Gibbs Free Energy= 0.368647
Sum of electronic and zero-point Energies= -1305.487752
Sum of electronic and thermal Energies= -1305.458248
Sum of electronic and thermal Enthalpies= -1305.457304
Sum of electronic and thermal Free Energies= -1305.552504

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.564930	-0.868596	-0.480189
2	6	0	-8.203035	0.372722	-0.548684
3	6	0	-7.452018	1.546638	-0.446492
4	6	0	-6.071671	1.484930	-0.276772
5	6	0	-5.418111	0.237737	-0.205705
6	6	0	-6.185177	-0.940783	-0.310106
7	6	0	-4.005770	0.167915	-0.031580
8	6	0	-2.800234	0.102936	0.124214
9	6	0	-1.385743	0.035893	0.265027
10	6	0	-0.731517	-1.346702	0.432325

11	6	0	0.769254	-1.294562	0.277126
12	6	0	1.511278	-0.175377	0.219793
13	6	0	0.868802	1.210684	0.301410
14	6	0	-0.639648	1.157581	0.225651
15	6	0	2.927818	-0.214797	0.109366
16	6	0	4.138003	-0.240984	-0.007467
17	6	0	5.556146	-0.263189	-0.138672
18	6	0	6.284241	0.942063	-0.211180
19	6	0	7.670083	0.919122	-0.340978
20	6	0	8.353115	-0.298594	-0.400562
21	6	0	7.640788	-1.498583	-0.329241
22	6	0	6.254686	-1.486134	-0.199412
23	8	0	1.361089	2.079232	-0.719292
24	6	0	1.127273	1.681129	-2.062126
25	8	0	-1.288257	-2.290175	-0.479136
26	6	0	-1.170803	-1.984773	-1.861357
27	8	0	1.322912	1.746996	1.520402
28	6	0	0.901980	3.071213	1.840614
29	8	0	-0.916506	-1.880571	1.720639
30	6	0	-2.238953	-2.238061	2.126577
31	1	0	-8.144876	-1.783532	-0.559352
32	1	0	-9.279717	0.424987	-0.680957
33	1	0	-7.944086	2.513500	-0.499235
34	1	0	-5.484943	2.394388	-0.196669
35	1	0	-5.685233	-1.902524	-0.256992
36	1	0	1.241044	-2.272344	0.264554
37	1	0	-1.130615	2.120046	0.111924
38	1	0	5.748080	1.884262	-0.162994
39	1	0	8.219974	1.854334	-0.395208
40	1	0	9.434463	-0.312339	-0.501391
41	1	0	8.167635	-2.447437	-0.374277
42	1	0	5.697848	-2.415918	-0.142291
43	1	0	1.517469	2.485465	-2.689642
44	1	0	0.058474	1.549439	-2.277454
45	1	0	1.655823	0.751781	-2.309422
46	1	0	-1.576780	-2.845478	-2.397377
47	1	0	-0.124257	-1.840954	-2.160886
48	1	0	-1.746319	-1.092523	-2.137892
49	1	0	1.501073	3.370326	2.703032
50	1	0	-0.158627	3.107159	2.121785
51	1	0	1.086192	3.762973	1.013340
52	1	0	-2.111443	-2.832838	3.033990
53	1	0	-2.744627	-2.837077	1.364857
54	1	0	-2.845594	-1.356111	2.358172

Compound 3a

Zero-point correction= 0.373219
(Hartree/Particle)
Thermal correction to Energy= 0.394278
Thermal correction to Enthalpy= 0.395222
Thermal correction to Gibbs Free Energy= 0.321608
Sum of electronic and zero-point Energies= -1150.840054
Sum of electronic and thermal Energies= -1150.818995
Sum of electronic and thermal Enthalpies= -1150.818051
Sum of electronic and thermal Free Energies= -1150.891666

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-4.829551	1.660132	-0.850960
2	6	0	-5.667782	1.056877	0.087826
3	6	0	-5.128366	0.174855	1.026634
4	6	0	-3.761805	-0.107074	1.028151
5	6	0	-2.908012	0.495836	0.087986
6	6	0	-3.462474	1.382026	-0.849871
7	6	0	-1.436936	0.253372	0.085595
8	6	0	-0.926198	-1.161045	-0.131080
9	6	0	0.573846	-1.269685	-0.188978
10	6	0	1.437106	-0.253371	-0.085651
11	6	0	0.926362	1.161057	0.131016
12	6	0	-0.573694	1.269698	0.188892
13	6	0	2.908169	-0.495914	-0.088018
14	6	0	3.462379	-1.382857	0.849285
15	6	0	4.829417	-1.661123	0.850419
16	6	0	5.667886	-1.057251	-0.087757
17	6	0	5.128735	-0.174461	-1.025993
18	6	0	3.762209	0.107622	-1.027557
19	8	0	1.448863	1.690035	1.360562
20	6	0	2.382927	2.723687	1.056008
21	8	0	-1.448660	-1.690084	-1.360608
22	6	0	-2.383523	-2.722979	-1.055912
23	8	0	1.420932	2.014879	-0.913444
24	6	0	1.907781	3.211737	-0.308298
25	8	0	-1.420764	-2.014852	0.913423
26	6	0	-1.908490	-3.211378	0.308287
27	1	0	-5.239404	2.344669	-1.588499
28	1	0	-6.732539	1.272618	0.088880
29	1	0	-5.772666	-0.290808	1.767529
30	1	0	-3.341899	-0.782112	1.764612
31	1	0	-2.812195	1.840574	-1.588828
32	1	0	0.940745	-2.283156	-0.330499
33	1	0	-0.940621	2.283166	0.330370
34	1	0	2.811925	-1.841842	1.587816
35	1	0	5.239060	-2.346246	1.587531
36	1	0	6.732621	-1.273092	-0.088774
37	1	0	5.773227	0.291688	-1.766417
38	1	0	3.342508	0.783215	-1.763620
39	1	0	3.404535	2.325877	1.006225
40	1	0	2.325295	3.483422	1.840984
41	1	0	-2.326620	-3.482719	-1.840932
42	1	0	-3.404802	-2.324365	-1.005911
43	1	0	2.703298	3.615170	-0.940516
44	1	0	1.107453	3.959884	-0.215275
45	1	0	-2.704168	-3.614338	0.940608
46	1	0	-1.108634	-3.960010	0.215109

Compound 4a

Zero-point correction= 0.392730
(Hartree/Particle)
Thermal correction to Energy= 0.418227
Thermal correction to Enthalpy= 0.419171
Thermal correction to Gibbs Free Energy= 0.330494
Sum of electronic and zero-point Energies= -1303.130166
Sum of electronic and thermal Energies= -1303.104669
Sum of electronic and thermal Enthalpies= -1303.103725
Sum of electronic and thermal Free Energies= -1303.192402

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-7.691625	-0.684841	-0.267412
2	6	0	-8.307650	0.547197	-0.033353
3	6	0	-7.525021	1.679740	0.205866
4	6	0	-6.136139	1.585760	0.212562
5	6	0	-5.504071	0.347477	-0.021725
6	6	0	-6.303313	-0.788352	-0.262742
7	6	0	-4.082149	0.250907	-0.015347
8	6	0	-2.867143	0.189079	-0.009586
9	6	0	-1.445889	0.126082	-0.009583
10	6	0	-0.813293	-1.258399	0.058970
11	6	0	0.689313	-1.236310	0.056411
12	6	0	1.445941	-0.125902	0.009868
13	6	0	0.813346	1.258584	-0.058432
14	6	0	-0.689262	1.236490	-0.056066
15	6	0	2.867189	-0.188922	0.009675
16	6	0	4.082196	-0.250797	0.014948
17	6	0	5.504101	-0.347581	0.021064
18	6	0	6.303640	0.788771	0.258600
19	6	0	7.691935	0.685033	0.263021
20	6	0	8.307655	-0.547762	0.032160
21	6	0	7.524733	-1.680828	-0.203599
22	6	0	6.135866	-1.586625	-0.210023
23	8	0	1.232519	1.944691	-1.244374
24	6	0	2.143930	2.977894	-0.870020
25	8	0	-1.291537	-2.030157	-1.047404
26	6	0	-1.708132	-3.301245	-0.553804
27	8	0	1.291477	2.030026	1.048240
28	6	0	1.707821	3.301371	0.555042
29	8	0	-1.232332	-1.944167	1.245179
30	6	0	-2.143991	-2.977295	0.871230
31	1	0	-8.295514	-1.567970	-0.455252
32	1	0	-9.390940	0.624335	-0.037842
33	1	0	-7.999013	2.639893	0.388262
34	1	0	-5.525090	2.462966	0.398964
35	1	0	-5.822483	-1.743425	-0.448705
36	1	0	1.156714	-2.215293	0.099089
37	1	0	-1.156672	2.215464	-0.098860
38	1	0	5.823063	1.744455	0.442062
39	1	0	8.296050	1.568579	0.448151
40	1	0	9.390933	-0.625077	0.036442
41	1	0	7.998485	-2.641570	-0.383500
42	1	0	5.524591	-2.464240	-0.393738
43	1	0	3.177826	2.612594	-0.902060
44	1	0	2.025945	3.809233	-1.570658
45	1	0	-2.513357	-3.668593	-1.195585
46	1	0	-0.878627	-4.023136	-0.568442
47	1	0	2.512866	3.668719	1.197043
48	1	0	0.878135	4.023049	0.569765
49	1	0	-2.026057	-3.808479	1.572059
50	1	0	-3.177816	-2.611802	0.903320

Compound 5a

Zero-point correction= 0.425563
(Hartree/Particle)
Thermal correction to Energy= 0.460184
Thermal correction to Enthalpy= 0.461129
Thermal correction to Gibbs Free Energy= 0.355886

Sum of electronic and zero-point Energies= -2623.593288
Sum of electronic and thermal Energies= -2623.558667
Sum of electronic and thermal Enthalpies= -2623.557723
Sum of electronic and thermal Free Energies= -2623.662966

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.997483	-1.108407	-0.852249
2	6	0	5.727205	0.086835	-0.867604
3	6	0	5.062244	1.302567	-0.681263
4	6	0	3.682331	1.329226	-0.487733
5	6	0	2.931596	0.138842	-0.479995
6	6	0	3.622514	-1.077692	-0.645789
7	6	0	1.455147	0.136270	-0.285993
8	6	0	0.805131	1.284822	0.488691
9	6	0	-0.666764	1.074041	0.761054
10	6	0	-1.444578	0.091811	0.273466
11	6	0	-0.794574	-1.055594	-0.503185
12	6	0	0.677708	-0.845956	-0.773792
13	6	0	-2.920095	0.084474	0.474248
14	6	0	-3.612657	1.295456	0.665502
15	6	0	-4.988723	1.318594	0.871238
16	6	0	-5.713507	0.121366	0.883569
17	6	0	-5.044749	-1.091059	0.681849
18	6	0	-3.668927	-1.108284	0.466239
19	8	0	-0.937184	-2.308988	0.174208
20	6	0	-0.457552	-2.398334	1.507759
21	8	0	0.947670	2.537741	-0.189855
22	6	0	0.464201	2.627395	-1.522012
23	8	0	-1.486843	-1.354032	-1.701481
24	6	0	-1.557959	-0.321838	-2.672202
25	8	0	1.497998	1.584179	1.686301
26	6	0	1.569174	0.552264	2.657336
27	1	0	5.508373	-2.055916	-0.984144
28	16	0	7.495879	0.072793	-1.173432
29	1	0	5.626214	2.229560	-0.683175
30	1	0	3.179913	2.274774	-0.331483
31	1	0	3.080654	-2.016577	-0.597019
32	1	0	-1.086297	1.874839	1.364699
33	1	0	1.098458	-1.648796	-1.373916
34	1	0	-3.075127	2.237214	0.625055
35	1	0	-5.504526	2.263576	1.005858
36	16	0	-7.476800	0.156438	1.213730
37	1	0	-5.602571	-2.021066	0.688758
38	1	0	-3.164538	-2.050143	0.295106
39	1	0	-0.596090	-3.441044	1.800477
40	1	0	-1.023493	-1.757560	2.195804
41	1	0	0.607054	-2.146944	1.582747
42	1	0	0.603504	3.669790	-1.815536
43	1	0	-0.600966	2.377677	-1.593756
44	1	0	1.027081	1.985436	-2.211481
45	1	0	-2.066873	-0.757765	-3.533926
46	1	0	-0.563336	0.023136	-2.982798
47	1	0	-2.140032	0.539167	-2.318152
48	1	0	2.077249	0.988685	3.519308
49	1	0	2.151992	-0.308502	2.303905
50	1	0	0.574545	0.206719	2.967307
51	6	0	-8.113852	-0.132907	-0.472082
52	9	0	-7.732339	0.815334	-1.343090

53	9	0	-9.455113	-0.127605	-0.400375
54	9	0	-7.725276	-1.315897	-0.982014
55	6	0	8.084398	-0.434094	0.476513
56	9	0	7.740370	0.434094	1.441488
57	9	0	9.424904	-0.500642	0.424327
58	9	0	7.618482	-1.641276	0.848197

Compound 6a

Zero-point correction= 0.479085
(Hartree/Particle)
Thermal correction to Energy= 0.512487
Thermal correction to Enthalpy= 0.513431
Thermal correction to Gibbs Free Energy= 0.413154
Sum of electronic and zero-point Energies= -2178.476210
Sum of electronic and thermal Energies= -2178.442808
Sum of electronic and thermal Enthalpies= -2178.441864
Sum of electronic and thermal Free Energies= -2178.542141

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.079130	1.182535	-0.035866
2	6	0	-5.771229	-0.016867	-0.182592
3	6	0	-5.083378	-1.221058	-0.335143
4	6	0	-3.690386	-1.229079	-0.319926
5	6	0	-2.963200	-0.029649	-0.179838
6	6	0	-3.686938	1.168601	-0.022840
7	6	0	-1.474365	-0.007007	-0.186464
8	6	0	-0.709674	-1.257853	0.252338
9	6	0	0.783294	-1.048485	0.358715
10	6	0	1.475563	0.036377	-0.030698
11	6	0	0.710826	1.287366	-0.469790
12	6	0	-0.782513	1.078673	-0.574310
13	6	0	2.964567	0.057806	-0.035875
14	6	0	3.687358	-1.142164	-0.185436
15	6	0	5.079497	-1.157012	-0.175067
16	6	0	5.772592	0.041053	-0.021360
17	6	0	5.086236	1.251063	0.083202
18	6	0	3.692979	1.259113	0.080161
19	8	0	0.935605	2.391583	0.415403
20	6	0	0.651439	2.202358	1.792934
21	8	0	-0.932127	-2.362422	-0.632089
22	6	0	-0.647699	-2.172665	-2.010188
23	8	0	1.224086	1.839394	-1.668485
24	6	0	1.168746	1.017786	-2.823366
25	8	0	-1.224590	-1.809575	1.451500
26	6	0	-1.167372	-0.987539	2.605287
27	1	0	-5.644707	2.103583	0.072137
28	16	0	-7.591798	0.050528	-0.250652
29	1	0	-5.623041	-2.156050	-0.466510
30	1	0	-3.155678	-2.164532	-0.420329
31	1	0	-3.154936	2.102208	0.130595
32	1	0	1.292535	-1.934544	0.729118
33	1	0	-1.292009	1.964290	-0.945375
34	1	0	3.155102	-2.075691	-0.337822
35	1	0	5.643937	-2.075862	-0.304996
36	16	0	7.594391	-0.010239	-0.080399
37	1	0	5.627734	2.190833	0.162299
38	1	0	3.159310	2.197266	0.157593
39	1	0	0.806637	3.176259	2.261991
40	1	0	1.325352	1.471968	2.258782

41	1	0	-0.385213	1.888629	1.962927
42	1	0	-0.801702	-3.146751	-2.479077
43	1	0	0.388587	-1.857776	-2.179538
44	1	0	-1.322651	-1.443244	-2.475719
45	1	0	1.538908	1.633228	-3.645620
46	1	0	0.144817	0.696205	-3.052838
47	1	0	1.810055	0.131590	-2.730396
48	1	0	-1.536476	-1.602033	3.428917
49	1	0	-1.807942	-0.100598	2.512638
50	1	0	-0.143130	-0.665767	2.833477
51	8	0	7.989453	-1.442196	-0.367015
52	6	0	7.861202	0.270316	1.717329
53	1	0	7.381615	-0.537156	2.274662
54	1	0	7.449500	1.240984	2.004092
55	1	0	8.940389	0.254235	1.884502
56	8	0	-7.984378	1.509643	-0.176192
57	6	0	-7.885651	-0.672460	1.414494
58	1	0	-7.420643	-0.029611	2.164882
59	1	0	-7.471410	-1.682671	1.455297
60	1	0	-8.967404	-0.702287	1.561949

Compound 7a

Zero-point correction= 0.411653
(Hartree/Particle)
Thermal correction to Energy= 0.440080
Thermal correction to Enthalpy= 0.441024
Thermal correction to Gibbs Free Energy= 0.352339
Sum of electronic and zero-point Energies= -1337.677344
Sum of electronic and thermal Energies= -1337.648918
Sum of electronic and thermal Enthalpies= -1337.647974
Sum of electronic and thermal Free Energies= -1337.736659

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.162452	0.898182	0.281103
2	6	0	-5.771419	-0.247734	-0.253238
3	6	0	-4.966985	-1.320295	-0.673794
4	6	0	-3.586830	-1.241139	-0.549122
5	6	0	-2.959727	-0.109260	0.011080
6	6	0	-3.779096	0.966459	0.407126
7	6	0	-1.476744	-0.066748	0.145973
8	6	0	-0.771081	1.290888	0.199855
9	6	0	0.737380	1.188929	0.193958
10	6	0	1.476736	0.066942	0.145786
11	6	0	0.771051	-1.290661	0.200499
12	6	0	-0.737421	-1.188727	0.194844
13	6	0	2.959726	0.109349	0.010854
14	6	0	3.778987	-0.966443	0.406966
15	6	0	5.162341	-0.898400	0.280847
16	6	0	5.771467	0.247371	-0.253614
17	6	0	4.967158	1.320002	-0.674245
18	6	0	3.587004	1.241076	-0.549485
19	6	0	-7.196985	-0.319357	-0.383006
20	7	0	-8.354220	-0.379321	-0.487722
21	6	0	7.197045	0.318789	-0.383351
22	7	0	8.354335	0.378899	-0.487362
23	8	0	1.184008	-2.143869	-0.856761
24	6	0	1.010464	-1.662839	-2.181386

25	8	0	1.183143	-2.077416	1.316356
26	6	0	0.946404	-1.554966	2.614487
27	8	0	-1.182985	2.078168	1.315426
28	6	0	-0.945931	1.556409	2.613775
29	8	0	-1.184328	2.143547	-0.857694
30	6	0	-1.011000	1.661890	-2.182121
31	1	0	-5.778060	1.734211	0.596003
32	1	0	-5.428333	-2.200947	-1.107934
33	1	0	-2.986221	-2.066495	-0.915467
34	1	0	-3.322669	1.859335	0.812164
35	1	0	1.204470	2.170147	0.209906
36	1	0	-1.204546	-2.169912	0.211475
37	1	0	3.322476	-1.859206	0.812154
38	1	0	5.777828	-1.734517	0.595748
39	1	0	5.428591	2.200566	-1.108467
40	1	0	2.986564	2.066531	-0.915888
41	1	0	1.316866	-2.481137	-2.835702
42	1	0	1.640716	-0.789171	-2.390467
43	1	0	-0.034761	-1.407544	-2.396878
44	1	0	1.283845	-2.326421	3.309348
45	1	0	1.517037	-0.636073	2.800539
46	1	0	-0.117393	-1.358372	2.792456
47	1	0	-1.283247	2.328222	3.308299
48	1	0	-1.516492	0.637595	2.800444
49	1	0	0.117912	1.359933	2.791606
50	1	0	-1.317656	2.479822	-2.836776
51	1	0	0.034207	1.406613	-2.397713
52	1	0	-1.641194	0.788042	-2.390632

Compound 8a

Zero-point correction= 0.410248
(Hartree/Particle)
Thermal correction to Energy= 0.438925
Thermal correction to Enthalpy= 0.439870
Thermal correction to Gibbs Free Energy= 0.350881
Sum of electronic and zero-point Energies= -1337.610153
Sum of electronic and thermal Energies= -1337.581475
Sum of electronic and thermal Enthalpies= -1337.580531
Sum of electronic and thermal Free Energies= -1337.669520

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.165402	0.893532	0.277905
2	6	0	-5.764048	-0.252915	-0.256556
3	6	0	-4.966886	-1.325677	-0.677336
4	6	0	-3.586539	-1.243902	-0.550318
5	6	0	-2.959524	-0.112574	0.010177
6	6	0	-3.781787	0.961356	0.404795
7	6	0	-1.477093	-0.069146	0.146613
8	6	0	-0.772819	1.289177	0.200164
9	6	0	0.735472	1.189796	0.195780
10	6	0	1.477093	0.069216	0.146463
11	6	0	0.772823	-1.289082	0.200670
12	6	0	-0.735468	-1.189704	0.196378
13	6	0	2.959517	0.112573	0.009945
14	6	0	3.781781	-0.961191	0.405015
15	6	0	5.165391	-0.893445	0.278037
16	6	0	5.764034	0.252757	-0.256953

17	6	0	4.966868	1.325334	-0.678200
18	6	0	3.586526	1.243638	-0.551087
19	7	0	-7.140101	-0.323446	-0.383677
20	6	0	-8.315223	-0.384972	-0.491143
21	7	0	7.140084	0.323219	-0.384144
22	6	0	8.315234	0.384933	-0.491198
23	8	0	1.187416	-2.142144	-0.856807
24	6	0	1.013108	-1.660053	-2.180505
25	8	0	1.187571	-2.076058	1.316392
26	6	0	0.952192	-1.552452	2.613888
27	8	0	-1.187460	2.076635	1.315584
28	6	0	-0.951933	1.553607	2.613287
29	8	0	-1.187508	2.141782	-0.857644
30	6	0	-1.013336	1.659113	-2.181147
31	1	0	-5.789702	1.723985	0.589444
32	1	0	-5.435417	-2.201993	-1.111829
33	1	0	-2.985830	-2.069536	-0.916089
34	1	0	-3.327667	1.855182	0.810459
35	1	0	1.201327	2.171635	0.212684
36	1	0	-1.201322	-2.171535	0.213739
37	1	0	3.327664	-1.854825	0.811104
38	1	0	5.789691	-1.723768	0.589924
39	1	0	5.435394	2.201445	-1.113112
40	1	0	2.985816	2.069115	-0.917209
41	1	0	1.319069	-2.477625	-2.836116
42	1	0	1.643212	-0.786090	-2.388994
43	1	0	-0.032283	-1.404425	-2.395070
44	1	0	1.288647	-2.323776	3.309535
45	1	0	1.524224	-0.634166	2.799070
46	1	0	-0.111241	-1.353824	2.792006
47	1	0	-1.288308	2.325240	3.308629
48	1	0	-1.523944	0.635403	2.798941
49	1	0	0.111520	1.355057	2.791371
50	1	0	-1.319351	2.476402	-2.837085
51	1	0	0.032031	1.403377	-2.395705
52	1	0	-1.643472	0.785066	-2.389194

Compound 9

Zero-point correction= 0.408457
(Hartree/Particle)
Thermal correction to Energy= 0.441234
Thermal correction to Enthalpy= 0.442178
Thermal correction to Gibbs Free Energy= 0.337888
Sum of electronic and zero-point Energies= -1488.824377
Sum of electronic and thermal Energies= -1488.791600
Sum of electronic and thermal Enthalpies= -1488.790656
Sum of electronic and thermal Free Energies= -1488.894946

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.615237	1.168186	0.044387
2	6	0	-1.376276	-0.015158	-0.035282
3	6	0	-0.691509	-1.254555	-0.094206
4	6	0	0.697093	-1.285979	-0.076652

5	6	0	1.457699	-0.102553	0.004523
6	6	0	0.773252	1.136634	0.062472
7	8	0	1.465095	2.322475	0.092031
8	6	0	1.971386	2.698725	1.375862
9	8	0	-1.380490	-2.441348	-0.124479
10	6	0	-1.906116	-2.807994	-1.404230
11	6	0	2.877130	-0.157720	-0.006273
12	6	0	-2.794829	0.043656	-0.024168
13	6	0	-4.008115	0.129938	-0.013943
14	6	0	4.091359	-0.237569	-0.022969
15	6	0	5.512147	-0.281080	-0.066349
16	6	0	-5.426750	0.195970	0.004208
17	6	0	6.222452	-1.505101	0.036309
18	6	0	7.615109	-1.519916	-0.076040
19	6	0	8.327097	-0.342981	-0.274675
20	6	0	7.639377	0.880956	-0.357830
21	6	0	6.242993	0.904537	-0.258460
22	6	0	-6.093828	1.453199	-0.025819
23	6	0	-7.492920	1.503237	-0.010319
24	6	0	-8.238177	0.328546	0.033773
25	6	0	-7.596373	-0.919330	0.064423
26	6	0	-6.194992	-0.974248	0.050065
27	8	0	-5.291236	2.539537	-0.068814
28	6	0	-5.885085	3.832805	-0.103206
29	6	0	-8.364534	-2.127428	0.109088
30	7	0	-8.990772	-3.107578	0.143947
31	8	0	5.576977	-2.700063	0.181834
32	6	0	4.966955	-2.944252	1.456249
33	6	0	8.363335	2.103291	-0.551321
34	7	0	8.953687	3.093947	-0.704667
35	1	0	-1.116512	2.128594	0.088087
36	1	0	1.196363	-2.247237	-0.126484
37	1	0	2.480960	3.653952	1.236375
38	1	0	1.155517	2.823664	2.099260
39	1	0	2.684600	1.959705	1.758200
40	1	0	-2.415123	-3.763264	-1.263303
41	1	0	-1.100242	-2.929952	-2.139087
42	1	0	-2.622713	-2.064927	-1.771198
43	1	0	8.122961	-2.476035	-0.008333
44	1	0	9.408244	-0.360417	-0.359098
45	1	0	5.709430	1.844304	-0.344244
46	1	0	-8.009061	2.454854	-0.032978
47	1	0	-9.321767	0.375602	0.044888
48	1	0	-5.689725	-1.932825	0.077119
49	1	0	-5.054777	4.538572	-0.135629
50	1	0	-6.508020	3.963973	-0.996003
51	1	0	-6.487254	4.021038	0.793658
52	1	0	4.496007	-3.925509	1.380862
53	1	0	5.724615	-2.963631	2.249252
54	1	0	4.207462	-2.192743	1.691431

Compound 9a

```
 Zero-point correction=                           0.495893
(Hartree/Particle)
 Thermal correction to Energy=                    0.534241
 Thermal correction to Enthalpy=                  0.535185
 Thermal correction to Gibbs Free Energy=         0.419918
 Sum of electronic and zero-point Energies=          -1718.947304
```

Sum of electronic and thermal Energies= -1718.908956
Sum of electronic and thermal Enthalpies= -1718.908011
Sum of electronic and thermal Free Energies= -1719.023279

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.698792	1.231285	0.005530
2	6	0	-1.447844	0.109822	0.005866
3	6	0	-0.811044	-1.286559	0.005713
4	6	0	0.698508	-1.237028	0.004406
5	6	0	1.447589	-0.115585	0.003439
6	6	0	0.810772	1.280860	0.004052
7	8	0	1.276310	2.063487	-1.081688
8	6	0	1.038957	1.568167	-2.389576
9	8	0	-1.278613	-2.069463	-1.078963
10	6	0	-1.043847	-1.574301	-2.387379
11	6	0	2.868031	-0.160604	0.001611
12	6	0	-2.868283	0.155149	0.006695
13	6	0	-4.083601	0.183962	0.002506
14	6	0	4.083438	-0.185756	-0.000336
15	6	0	5.504061	-0.179254	-0.002148
16	6	0	-5.504226	0.180669	-0.000616
17	6	0	6.236127	-1.399447	-0.003633
18	6	0	7.636236	-1.374906	-0.005477
19	6	0	8.316961	-0.161058	-0.005889
20	6	0	7.609812	1.051606	-0.004463
21	6	0	6.207337	1.032012	-0.002593
22	6	0	-6.233420	1.402593	-0.002839
23	6	0	-7.633569	1.381373	-0.006066
24	6	0	-8.317166	0.169137	-0.007112
25	6	0	-7.612888	-1.045192	-0.004972
26	6	0	-6.210383	-1.028927	-0.001743
27	8	0	-5.486923	2.529270	-0.001582
28	6	0	-6.145996	3.790819	-0.003418
29	6	0	-8.321435	-2.290142	-0.006040
30	7	0	-8.902563	-3.298275	-0.006929
31	8	0	5.492340	-2.527915	-0.003149
32	6	0	6.154504	-3.787837	-0.004536
33	6	0	8.315411	2.298224	-0.004920
34	7	0	8.894187	3.307711	-0.005362
35	1	0	-1.171353	2.210012	0.005986
36	6	0	-1.039189	-1.573697	2.399410
37	1	0	1.430415	2.328288	-3.068616
38	1	0	1.565499	0.623504	-2.576288
39	1	0	-0.030056	1.426583	-2.593924
40	1	0	-1.436655	-2.334507	-3.065550
41	1	0	0.024764	-1.432726	-2.593845
42	1	0	-1.570745	-0.629642	-2.573151
43	1	0	8.202636	-2.297833	-0.006618
44	1	0	9.401622	-0.149623	-0.007340
45	1	0	5.648952	1.961183	-0.001484
46	1	0	-8.197779	2.305641	-0.007754
47	1	0	-9.401848	0.160275	-0.009599
48	1	0	-5.654220	-1.959427	-0.000042
49	1	0	-5.352859	4.538837	-0.001733
50	1	0	-6.764022	3.918615	-0.900145
51	1	0	-6.768216	3.919022	0.890342
52	1	0	5.363202	-4.537806	-0.003763
53	1	0	6.773732	-3.913966	-0.900670

54	1	0	6.776158	-3.914665	0.889816
55	8	0	1.278661	2.063442	1.088821
56	6	0	1.043301	1.568517	2.397220
57	1	0	1.437089	2.328192	3.075415
58	1	0	1.568966	0.623166	2.582945
59	1	0	-0.025491	1.428297	2.603707
60	8	0	-1.277044	-2.068828	1.091548
61	1	0	1.171048	-2.215770	0.003931
62	1	0	0.029978	-1.433367	2.603828
63	1	0	-1.431609	-2.333296	3.078477
64	1	0	-1.564585	-0.628378	2.586048

Compound 10

Zero-point correction= 0.377194
(Hartree/Particle)
Thermal correction to Energy= 0.405545
Thermal correction to Enthalpy= 0.406489
Thermal correction to Gibbs Free Energy= 0.312380
Sum of electronic and zero-point Energies= -1282.093751
Sum of electronic and thermal Energies= -1282.065400
Sum of electronic and thermal Enthalpies= -1282.064456
Sum of electronic and thermal Free Energies= -1282.158565

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.553031	-1.275571	0.022842
2	6	0	-2.323508	-0.097252	-0.039894
3	6	0	-1.645379	1.146856	-0.084260
4	6	0	-0.257096	1.187163	-0.067010
5	6	0	0.511980	0.008239	-0.000966
6	6	0	-0.164638	-1.235474	0.040238
7	8	0	0.535252	-2.417140	0.053389
8	6	0	1.037235	-2.810956	1.333393
9	8	0	-2.338889	2.331944	-0.100566
10	6	0	-2.889803	2.697059	-1.369692
11	6	0	1.931035	0.072846	-0.010604
12	6	0	-3.742128	-0.164421	-0.026483
13	6	0	-4.956204	-0.249379	-0.013081
14	6	0	3.144751	0.161374	-0.025117
15	6	0	4.565233	0.214632	-0.066109
16	6	0	-6.377378	-0.339163	0.008112
17	6	0	5.268157	1.441044	0.057379
18	6	0	6.660785	1.466367	-0.053266
19	6	0	7.380467	0.297436	-0.270473
20	6	0	6.700332	-0.929134	-0.374231
21	6	0	5.303988	-0.963000	-0.276725
22	6	0	-7.017991	-1.592554	-0.073608
23	6	0	-8.407439	-1.673977	-0.053835
24	6	0	-9.180478	-0.514274	0.047115
25	6	0	-8.555266	0.732822	0.129257
26	6	0	-7.166547	0.824954	0.110376
27	1	0	-6.414160	-2.490808	-0.152681
28	1	0	-9.152473	1.636508	0.209193
29	8	0	4.616108	2.630197	0.221795
30	6	0	3.996967	2.847287	1.496588
31	6	0	7.432393	-2.143452	-0.586776

32	7	0	8.029992	-3.127263	-0.755487
33	1	0	-2.046149	-2.240756	0.054339
34	1	0	0.235268	2.152514	-0.105577
35	1	0	1.553133	-3.760903	1.181457
36	1	0	1.744192	-2.073872	1.731089
37	1	0	0.218708	-2.952283	2.050775
38	1	0	-3.398532	3.651125	-1.218778
39	1	0	-3.611459	1.952732	-1.723229
40	1	0	-2.098088	2.822076	-2.119482
41	1	0	7.162424	2.424472	0.030869
42	1	0	8.461568	0.322969	-0.353406
43	1	0	4.776343	-1.904524	-0.378386
44	1	0	-8.889441	-2.645190	-0.117710
45	1	0	-10.264268	-0.582069	0.062249
46	1	0	-6.676533	1.790886	0.177483
47	1	0	3.522966	3.828216	1.437170
48	1	0	3.238687	2.088836	1.712314
49	1	0	4.749474	2.854064	2.294754

Compound 10a

Zero-point correction= 0.464668
(Hartree/Particle)
Thermal correction to Energy= 0.498568
Thermal correction to Enthalpy= 0.499512
Thermal correction to Gibbs Free Energy= 0.394768
Sum of electronic and zero-point Energies= -1512.216689
Sum of electronic and thermal Energies= -1512.182788
Sum of electronic and thermal Enthalpies= -1512.181844
Sum of electronic and thermal Free Energies= -1512.286588

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.131783	1.152303	-0.000245
2	6	0	-0.623414	0.035130	0.000115
3	6	0	0.006367	-1.364351	0.000542
4	6	0	1.515871	-1.322047	0.000409
5	6	0	2.272763	-0.205528	0.000016
6	6	0	1.641690	1.193898	-0.000388
7	8	0	2.109022	1.975922	-1.086201
8	6	0	1.884060	1.472754	-2.393116
9	8	0	-0.466288	-2.144608	-1.084282
10	6	0	-0.223552	-1.653428	-2.392441
11	6	0	3.693156	-0.254715	-0.000098
12	6	0	-2.043668	0.089125	0.000172
13	6	0	-3.258836	0.124060	-0.000098
14	6	0	4.909479	-0.272856	-0.000281
15	6	0	6.333802	-0.280516	-0.000443
16	6	0	-4.679450	0.129907	0.000084
17	6	0	7.048134	-1.495695	-0.000164
18	6	0	8.440268	-1.491700	-0.000345
19	6	0	9.141345	-0.282929	-0.000804
20	6	0	8.442063	0.927048	-0.001082
21	6	0	7.050073	0.934021	-0.000908
22	6	0	-5.400710	1.356541	0.000092

23	6	0	-6.800896	1.344813	0.000300
24	6	0	-7.492717	0.137206	0.000478
25	6	0	-6.796494	-1.081696	0.000452
26	6	0	-5.393816	-1.074853	0.000250
27	8	0	-4.646681	2.478461	-0.000084
28	6	0	-5.297415	3.744032	-0.000048
29	6	0	-7.513747	-2.321643	0.000634
30	7	0	-8.102586	-3.325303	0.000782
31	1	0	6.499320	-2.432008	0.000190
32	1	0	-0.335219	2.133699	-0.000525
33	6	0	-0.222954	-1.651792	2.393766
34	1	0	2.272283	2.233513	-3.073450
35	1	0	2.420664	0.532471	-2.572427
36	1	0	0.817590	1.320376	-2.603269
37	1	0	-0.617548	-2.412763	-3.070952
38	1	0	0.846573	-1.517655	-2.594767
39	1	0	-0.744729	-0.706253	-2.582275
40	1	0	8.980454	-2.433981	-0.000136
41	1	0	10.227422	-0.283938	-0.000951
42	1	0	6.500265	1.869547	-0.001131
43	1	0	-7.358896	2.272854	0.000326
44	1	0	-8.577437	0.135602	0.000637
45	1	0	-4.843873	-2.009041	0.000223
46	1	0	-4.499451	4.486951	-0.000215
47	1	0	-5.916943	3.876244	-0.895154
48	1	0	-5.916653	3.876339	0.895246
49	8	0	2.109251	1.976646	1.084804
50	6	0	1.884517	1.474413	2.392120
51	1	0	2.273024	2.235582	3.071833
52	1	0	2.421016	0.534170	2.571957
53	1	0	0.818075	1.322356	2.602653
54	8	0	-0.466084	-2.143844	1.086008
55	1	0	1.981878	-2.303983	0.000685
56	1	0	0.847238	-1.515907	2.595660
57	1	0	-0.616768	-2.410657	3.072908
58	1	0	-0.744041	-0.704471	2.583116
59	1	0	8.983866	1.868431	-0.001433

Intermediate A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.758087	0.004241	0.027006
2	6	0	-0.468977	0.018110	1.070367
3	6	0	0.221928	0.040389	3.782881
4	6	0	-0.525604	-1.155535	1.813514
5	6	0	-0.080280	1.233170	1.679120
6	6	0	0.258709	1.220964	3.051766
7	6	0	-0.176095	-1.151939	3.167602
8	1	0	-0.846596	-2.076917	1.337405
9	1	0	0.597783	2.135332	3.529313
10	1	0	-0.211584	-2.073535	3.740780
11	1	0	0.509440	0.044466	4.829747
12	6	0	-0.070522	2.505528	0.947422
13	6	0	-0.051324	5.025547	-0.460333
14	6	0	-0.483586	3.681390	1.575345
15	6	0	0.378522	2.615950	-0.427930
16	6	0	0.361692	3.849678	-1.088271
17	6	0	-0.500487	4.915110	0.914984

18	1	0	-0.862300	3.613516	2.586364
19	1	0	0.740439	3.917557	-2.099278
20	6	0	-0.041416	6.297933	-1.191977
21	6	0	0.054740	8.683083	-2.680355
22	6	0	0.347470	7.512904	-0.583172
23	6	0	-0.380421	6.310243	-2.564619
24	6	0	-0.343472	7.490844	-3.295683
25	6	0	0.404266	8.686573	-1.326272
26	1	0	0.636610	7.526685	0.460183
27	1	0	-0.719632	5.395941	-3.042191
28	1	0	-0.630994	7.486862	-4.342545
29	1	0	0.725409	9.607885	-0.850134
30	1	0	0.090363	9.604697	-3.253495
31	8	0	0.852025	1.496923	-0.973436
32	8	0	-0.974133	6.034111	1.460419
33	6	0	1.368421	1.493562	-2.315337
34	1	0	0.591229	1.784509	-3.028963
35	1	0	1.678278	0.465775	-2.498511
36	1	0	2.230362	2.163321	-2.393037
37	6	0	-1.490832	6.037432	2.802205
38	1	0	-1.801108	7.065125	2.985194
39	1	0	-0.713662	5.746880	3.516020
40	1	0	-2.352519	5.367338	2.879812

Zero-point correction= 0.329294
(Hartree/Particle)
Thermal correction to Energy= 0.348223
Thermal correction to Enthalpy= 0.349167
Thermal correction to Gibbs Free Energy= 0.280939
Sum of electronic and zero-point Energies= -922.815224
Sum of electronic and thermal Energies= -922.796295
Sum of electronic and thermal Enthalpies= -922.795351
Sum of electronic and thermal Free Energies= -922.863578

Intermediate B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.196584	2.477535	3.359192
2	6	0	0.188643	1.539446	2.814985
3	6	0	0.056329	-0.904692	1.469152
4	6	0	0.176757	0.357035	3.535976
5	6	0	0.133976	1.533312	1.394489
6	6	0	0.051174	0.276832	0.737857
7	6	0	0.118645	-0.872193	2.864480
8	1	0	0.203771	0.384707	4.620703
9	1	0	0.011122	0.240910	-0.339985
10	1	0	0.113022	-1.798643	3.431216
11	1	0	0.008770	-1.856039	0.948802
12	6	0	0.154980	2.781729	0.654390
13	6	0	-0.272891	2.800151	-0.830724
14	6	0	0.569404	3.968493	1.227377
15	1	0	0.974791	3.962173	2.229646
16	6	0	0.524560	5.201081	0.541095
17	6	0	-0.030919	5.339012	-0.804748
18	8	0	0.987187	6.314125	1.055483

19	6	0	1.626023	6.364190	2.351868
20	1	0	2.497493	5.704900	2.367000
21	1	0	0.913439	6.091615	3.134816
22	1	0	1.934683	7.401401	2.468509
23	8	0	0.760822	2.105049	-1.482877
24	8	0	-1.470735	2.082943	-1.040310
25	6	0	-2.660584	2.599088	-0.435377
26	1	0	-2.879444	3.620329	-0.769902
27	1	0	-2.594394	2.579468	0.659679
28	1	0	-3.465526	1.936676	-0.755605
29	6	0	0.669012	1.960896	-2.914018
30	1	0	1.367251	1.160811	-3.162863
31	1	0	0.979823	2.877890	-3.425765
32	1	0	-0.341692	1.676264	-3.216466
33	6	0	-0.122640	6.662834	-1.476442
34	6	0	-0.377009	9.105302	-2.833307
35	6	0	0.376380	6.809298	-2.780550
36	6	0	-0.747933	7.758074	-0.857804
37	6	0	-0.877154	8.968407	-1.535887
38	6	0	0.251367	8.024229	-3.453550
39	1	0	0.883956	5.975979	-3.259137
40	1	0	-1.150634	7.660718	0.145782
41	1	0	-1.372265	9.805039	-1.051910
42	1	0	0.649799	8.126533	-4.458503
43	1	0	-0.474770	10.051686	-3.356757
44	6	0	-0.407982	4.192032	-1.411173
45	1	0	-0.823079	4.228068	-2.413914

Zero-point correction=	0.372740
(Hartree/Particle)	
Thermal correction to Energy=	0.394866
Thermal correction to Enthalpy=	0.395810
Thermal correction to Gibbs Free Energy=	0.320968
Sum of electronic and zero-point Energies=	-1037.869967
Sum of electronic and thermal Energies=	-1037.847841
Sum of electronic and thermal Enthalpies=	-1037.846897
Sum of electronic and thermal Free Energies=	-1037.921739

Intermediate C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.137370	2.545193	3.291001
2	6	0	-0.026997	1.587604	2.790558
3	6	0	0.131952	-0.888993	1.539308
4	6	0	-0.074150	0.422239	3.550277
5	6	0	0.116237	1.547413	1.384478
6	6	0	0.182483	0.273928	0.775212
7	6	0	0.008050	-0.826549	2.929556
8	1	0	-0.190558	0.489570	4.629089
9	1	0	0.294188	0.212810	-0.298659
10	1	0	-0.032332	-1.737685	3.520493
11	1	0	0.194798	-1.854213	1.043036
12	6	0	0.185335	2.793603	0.606858
13	6	0	-0.220016	2.805919	-0.862485
14	6	0	0.639940	3.972367	1.183341

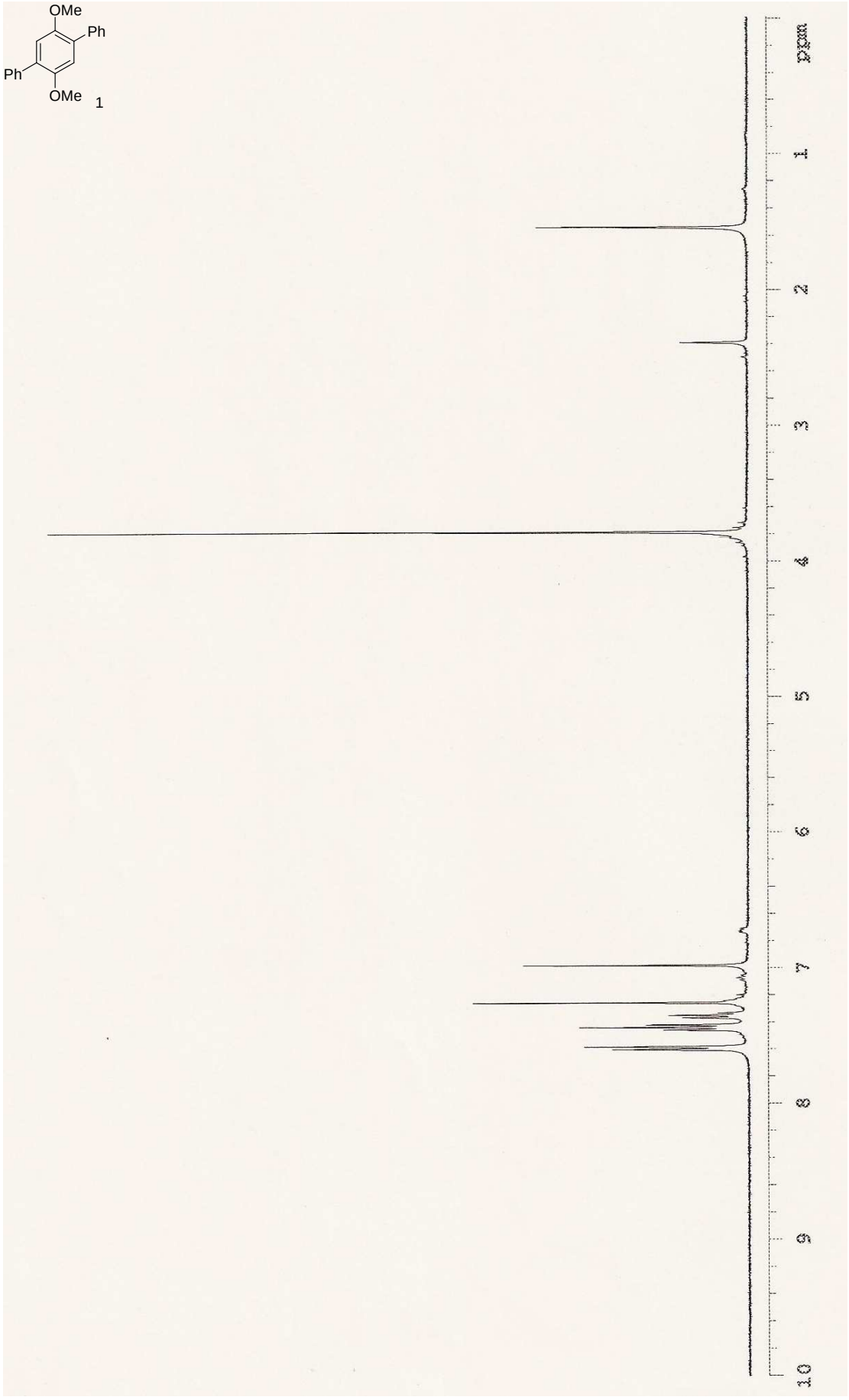
15	1	0	1.044706	3.924750	2.187233
16	6	0	0.616163	5.211293	0.527827
17	6	0	0.030832	5.338847	-0.786323
18	8	0	1.125383	6.355133	1.059197
19	6	0	1.771399	6.305158	2.322771
20	1	0	2.620908	5.611118	2.309317
21	1	0	1.076006	6.011901	3.119803
22	1	0	2.130775	7.318207	2.511387
23	8	0	0.813417	2.105112	-1.555232
24	8	0	-1.407494	2.041416	-1.109006
25	6	0	-2.587917	2.507114	-0.475189
26	1	0	-2.834858	3.537350	-0.767045
27	1	0	-2.507607	2.460855	0.619154
28	1	0	-3.390673	1.840693	-0.801153
29	6	0	0.682375	1.998830	-2.970714
30	1	0	1.448648	1.286144	-3.285782
31	1	0	0.869059	2.958400	-3.471117
32	1	0	-0.305033	1.622811	-3.257746
33	6	0	-0.120210	6.663054	-1.452915
34	6	0	-0.494941	9.115280	-2.790847
35	6	0	0.241193	6.811810	-2.801711
36	6	0	-0.666580	7.771362	-0.783732
37	6	0	-0.854584	8.982601	-1.447425
38	6	0	0.055452	8.024844	-3.465632
39	1	0	0.688107	5.971167	-3.325088
40	1	0	-0.950970	7.678635	0.258943
41	1	0	-1.286215	9.825666	-0.914009
42	1	0	0.347887	8.118397	-4.508303
43	1	0	-0.638927	10.061856	-3.305027
44	6	0	-0.393119	4.201916	-1.406512
45	1	0	-0.884631	4.269771	-2.372264

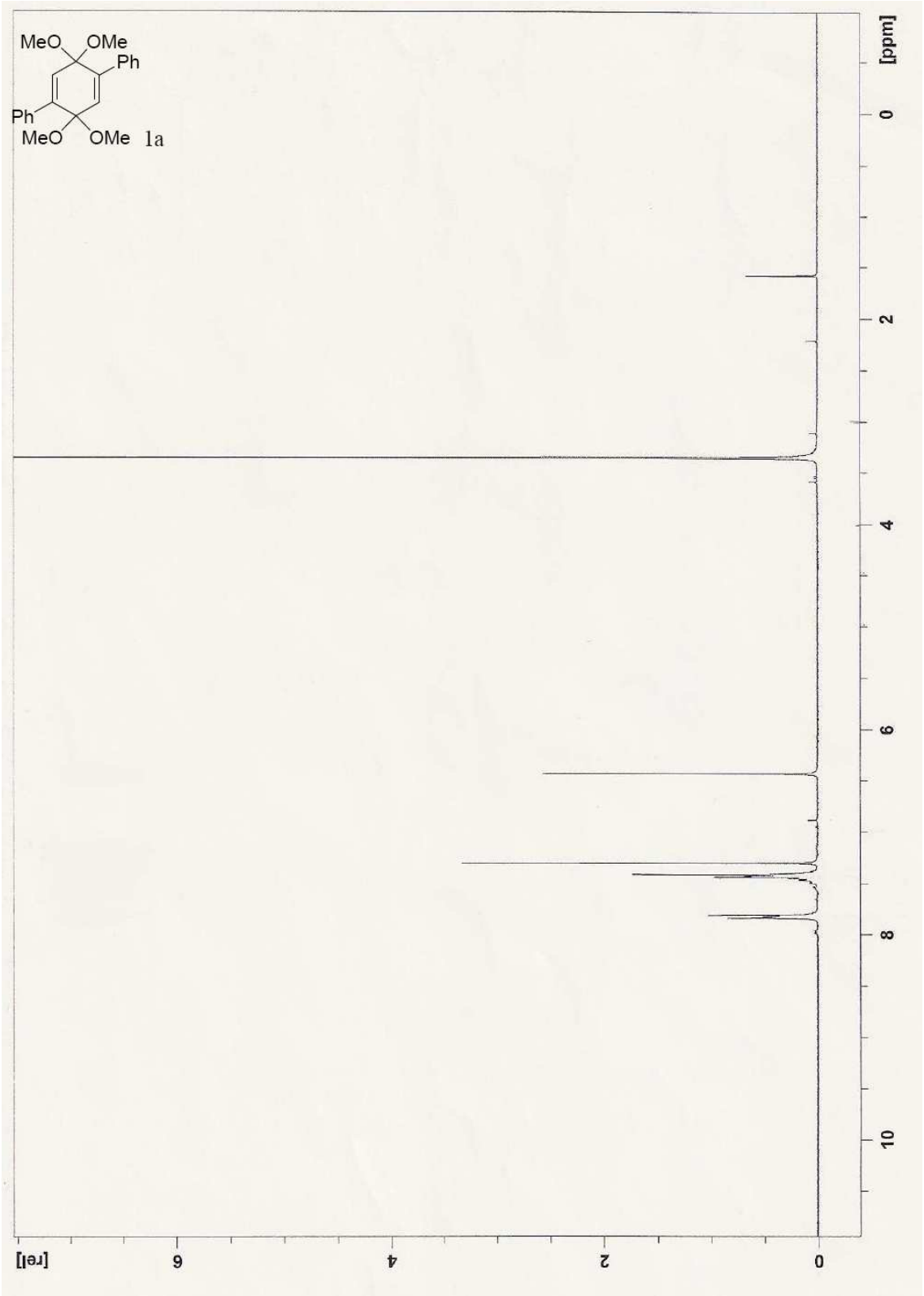
Zero-point correction=	0.370260
(Hartree/Particle)	
Thermal correction to Energy=	0.392314
Thermal correction to Enthalpy=	0.393258
Thermal correction to Gibbs Free Energy=	0.318035
Sum of electronic and zero-point Energies=	-1038.078649
Sum of electronic and thermal Energies=	-1038.056595
Sum of electronic and thermal Enthalpies=	-1038.055651
Sum of electronic and thermal Free Energies=	-1038.130875

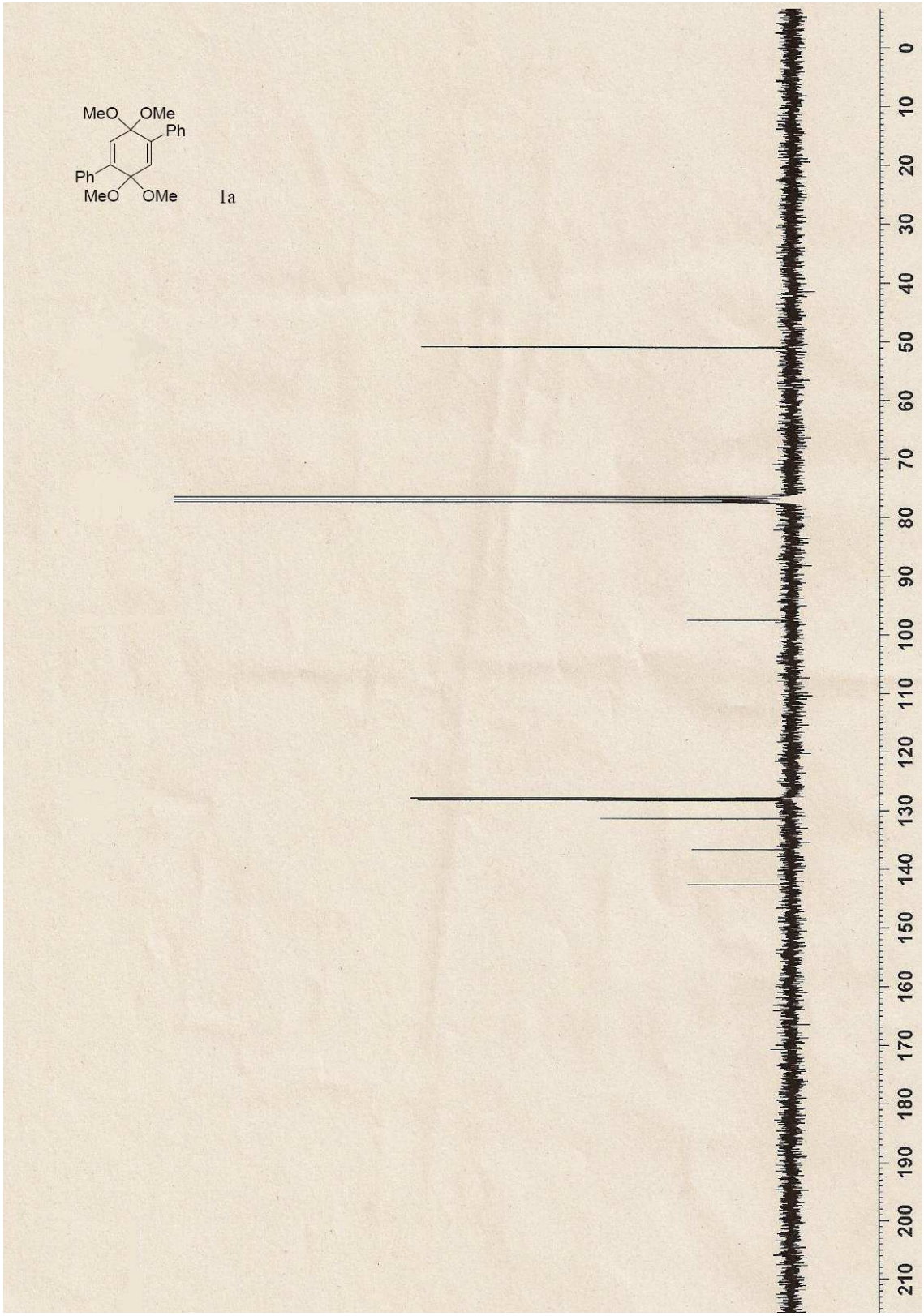
X-ray Structure Determinations. Crystals of **1**, **1a**, **2a**, **3a**, **5** and **5a** were grown from ethyl acetate (**1**, **1a**), diethyl ether (**2a**), toluene (**3a**), dichloromethane (**5**) and isopropanol (**5a**) saturated solutions under slow evaporation at room temperature. Measured crystals were prepared under inert conditions immersed in perfluoropolyether as protecting oil for manipulation. Suitable crystals were mounted on MiTeGen Micromounts™ and these samples were used for data collection. Data were collected with Bruker X8 Proteum (**1**, **1a**, **5**), Bruker SMART CCD 1000 (**2**) diffractometers, whereas those of **2a**, **3a** and **5a** were collected at the ESRF synchrotron BM16 beamline (Grenoble, France). The data were processed with SAINT (**2**),[13] APEX2 (**1**, **1a**, **5**),[14] and HKL2000 programs (**2a**, **3a**, **5a**).[15] The structures were solved by direct methods,[16] which revealed the position of all non-hydrogen atoms. These atoms were refined on F^2 by a full-matrix least-squares procedure using anisotropic displacement parameters.[17] All hydrogen atoms were located in difference Fourier maps and included as fixed contributions riding on attached atoms with isotropic thermal displacement parameters 1.2 times those of the respective atom. Crystal data for **1**: $C_{20}H_{18}O_2$, M = 290.34, Monoclinic, $P2_1/n$, a = 5.8194(3)º, b = 18.0195(8), c = 7.6388(3), β = 100.028(2)º, V = 788.79(6), Z = 2, measured reflections = 6521, independent = 1275, parameters = 101, R_1 = 0.0479, wR_2 = 0.1258, S = 1.029. Crystal data for **1a**: $C_{22}H_{24}O_4$, M = 352.41, Monoclinic, $P2_1/n$, a = 6.4349(7) º, b = 17.3703(19), c = 8.4716(9), β = 110.133(3)º, V = 889.06(17), Z = 2, measured reflections = 8382, independent = 1463, parameters = 120, R_1 = 0.0404, wR_2 = 0.0983, S = 1.066. Crystal data for **2a**: $C_{26}H_{24}O_4$, M = 400.45, Triclinic, P-1, a = 10.786(2)º, b = 12.3380(18), c = 16.619(3), α = 87.87(2), β = 80.36(3), γ = 86.62(3), V = 2175(6), Z = 4, measured reflections = 41742, independent = 7243, parameters = 549, R_1 = 0.0506, wR_2 = 0.1421, S = 1.011. Crystal data for **3a**: $C_{22}H_{20}O_4$, M = 348.38, Monoclinic, $P2_1/n$, a = 10.222(2)º, b = 7.6590(15), c = 22.493(5), β = 102.11(3)º, V = 1721.8(6), Z = 4, measured reflections = 11346, independent = 2986, parameters = 236, R_1 = 0.0748, wR_2 = 0.2534, S = 1.152. Crystal data for **5**: $C_{22}H_{16}F_6O_2S_2$, M = 490.47, Triclinic, P-1, a = 6.9878(7)º, b = 8.8208(9), c = 10.2906(11), α = 93.730(5), β = 109.110(6)º, γ = 112.219(5), V = 541.74(10), Z = 1, measured reflections = 6834, independent = 1771, parameters = 146, R_1 = 0.0595, wR_2 = 0.1647, S = 1.094. Crystal for **5a**: $C_{24}H_{22}F_6O_4S_2$, M = 552.54, Monoclinic, $P2_1/n$, a = 13.639(3)º, b = 6.3760(13), c = 27.642(6), β = 94.69(3)º, V = 2395.8 (8), Z = 4, measured reflections = 40748, independent = 3963, parameters = 329, R_1 = 0.0527, wR_2 = 0.1473, S = 1.092. Crystallographic data (excluding structure factors) for the structures of compounds **1**, **1a**, **2a**, **3a**, **5**, and **5a** reported in this paper have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-750177 (**1**), 750178 (**1a**), 750180 (**2a**), 750181 (**3a**), 750182 (**5**), and 750183 (**5a**). Copies of the data can be obtained free of charge at http://www.ccdc.cam.ac.uk/products/csd/request/.

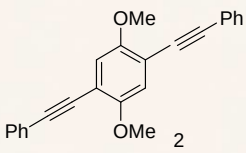
[13] Bruker, SMART and SAINT. Area Detector Control Integration Software, Bruker Analytical X-ray Instruments, Inc., Madison, Wisconsin (1999).
[14] Bruker, APEX2 Software, Bruker AXS Inc. V2009, Madison, Wisconsin, USA (2009).
[15] Z. Otwinowski and W. Minor, Methods in Enzymology, Volume 276: Macromolecular Crystallography, part A, 307-326, 1997, C.W. Carter, Jr. & R. M. Sweet, Eds., Academic Press (New York).
[16] Sheldrick. G. M. *Acta Crystallogr*. **1990**, *46A*, 467.
[17] G. M. Sheldrick. SHELXL-97, Program for the Refinement of Crystal Structures, University of Göttingen, Germany (1997).

Copies of ^{1}H and ^{13}C NMR spectra of new compounds.

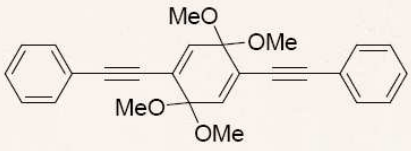



MeO
OMe
Ph
Ph
MeO
OMe
1a
[ppm]
0
2
4
6
8
10
[rel]
0
2
4
6

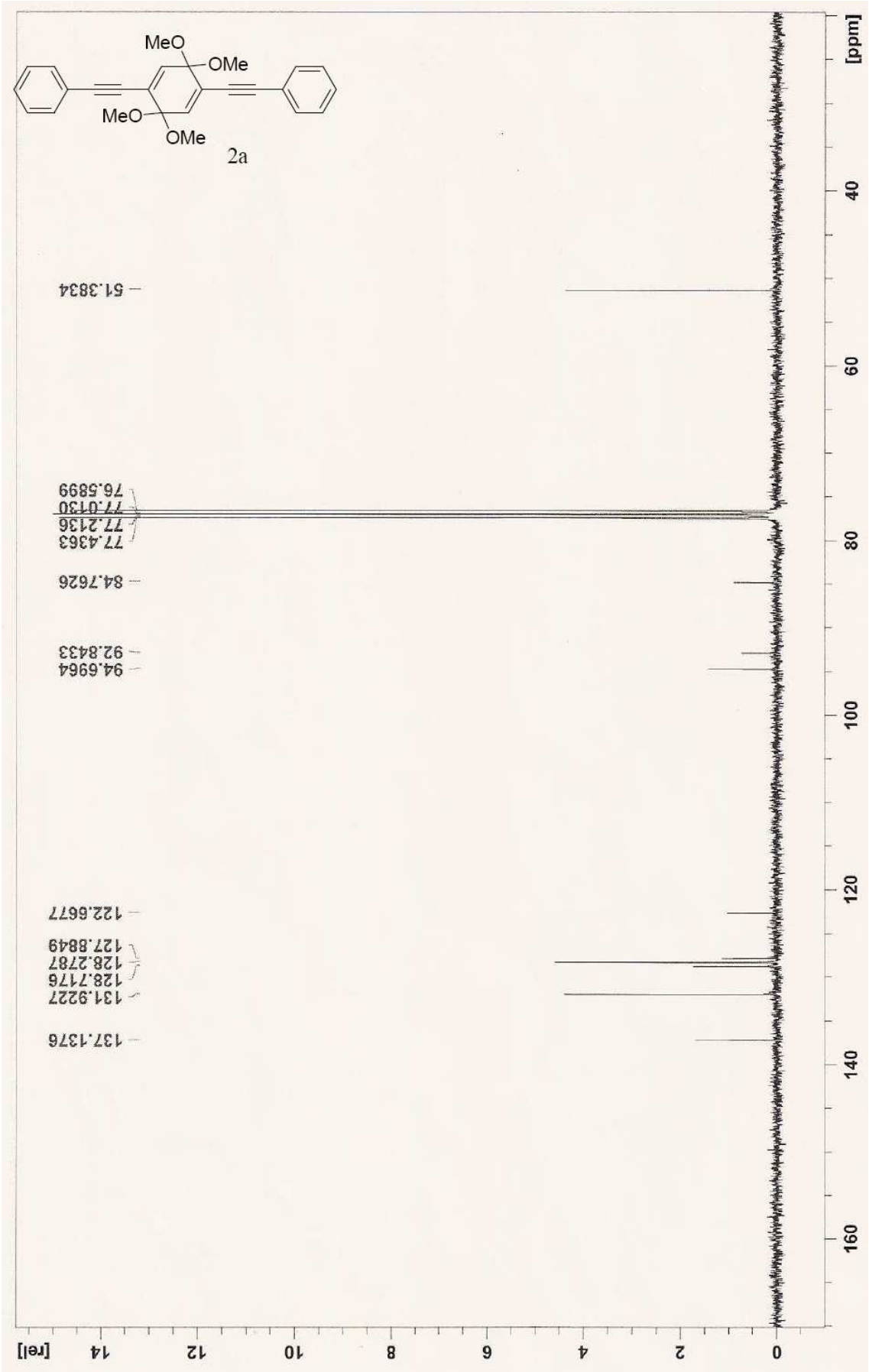

MeO
OMe
Ph
Ph
MeO
OMe
1a
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210

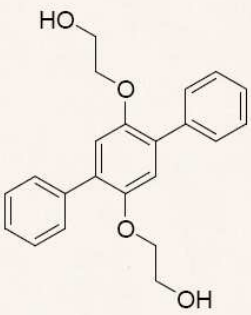


2

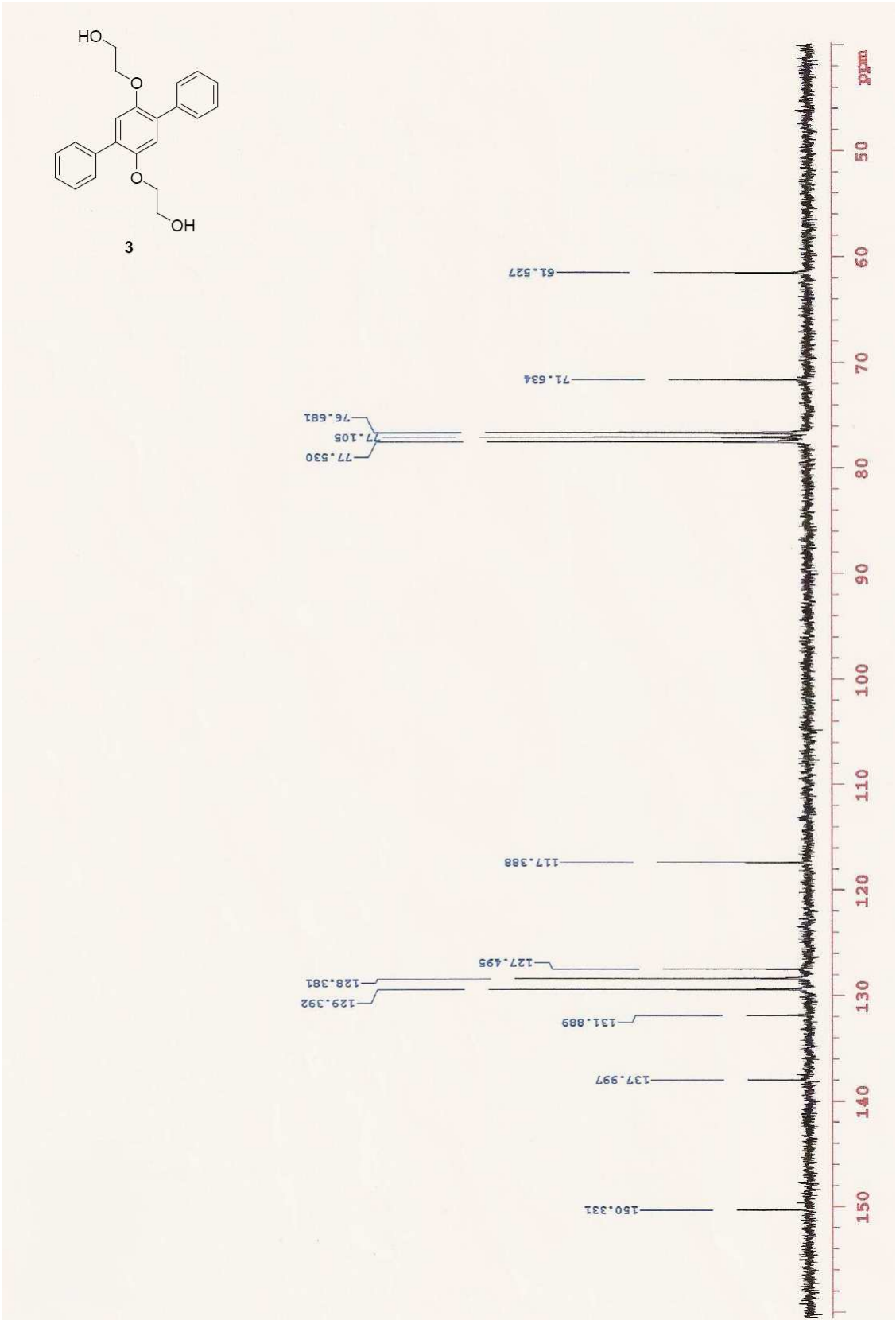


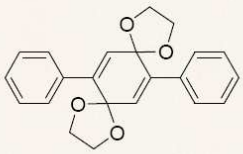
2a


MeO
OMe
MeO
OMe
2a
51.3834
76.5899
77.0130
77.2136
77.4363
84.7626
92.8433
94.6964
122.6677
127.8849
128.2787
128.7176
131.9227
137.1376
[ppm]
[rel]



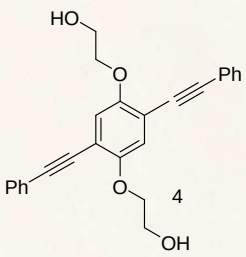
3


HO
O
O
OH
3
61.527
71.634
76.681
77.105
77.530
117.388
127.495
128.381
129.392
131.889
137.997
150.331
ppm
50
60
70
80
90
100
110
120
130
140
150

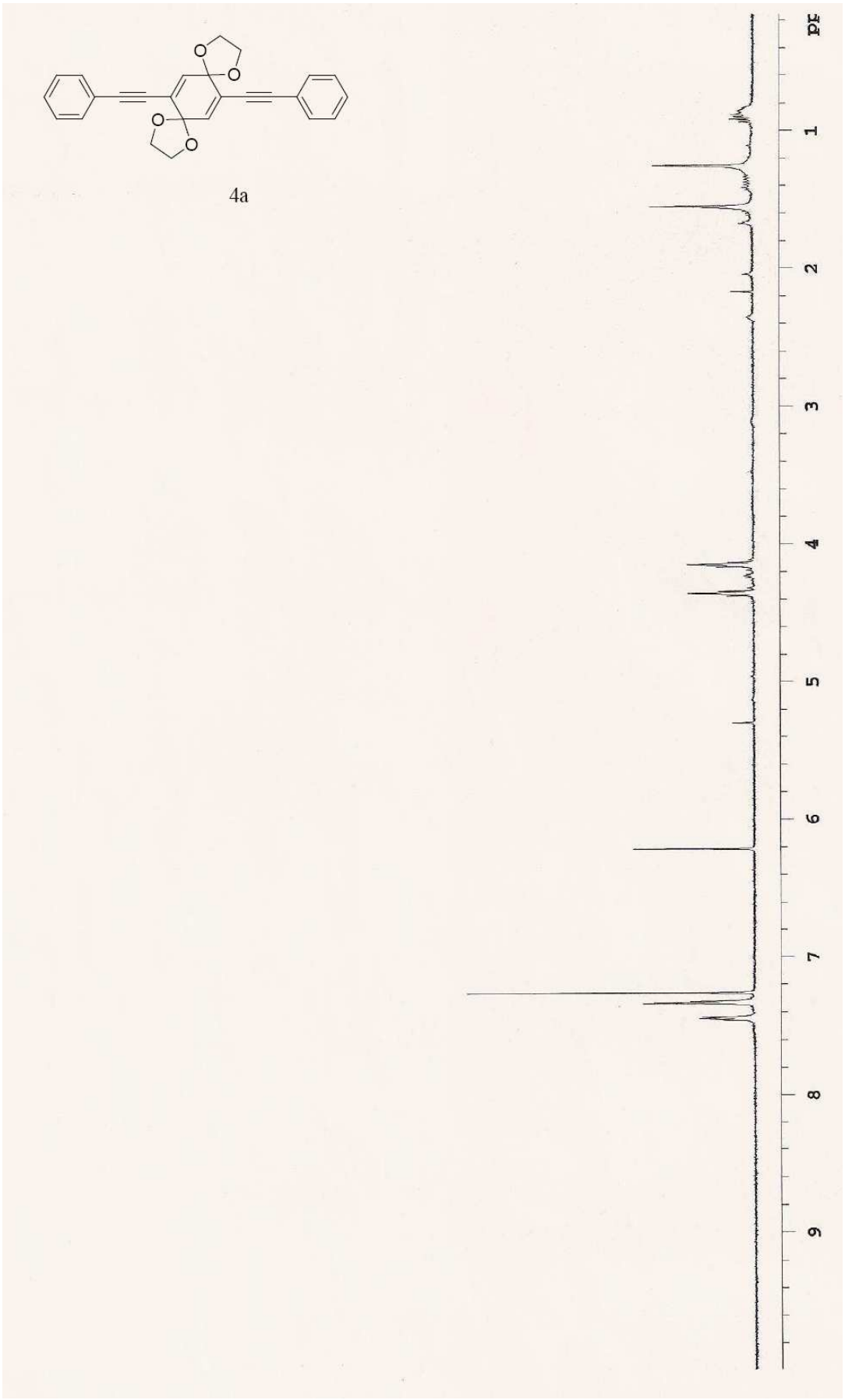


3a

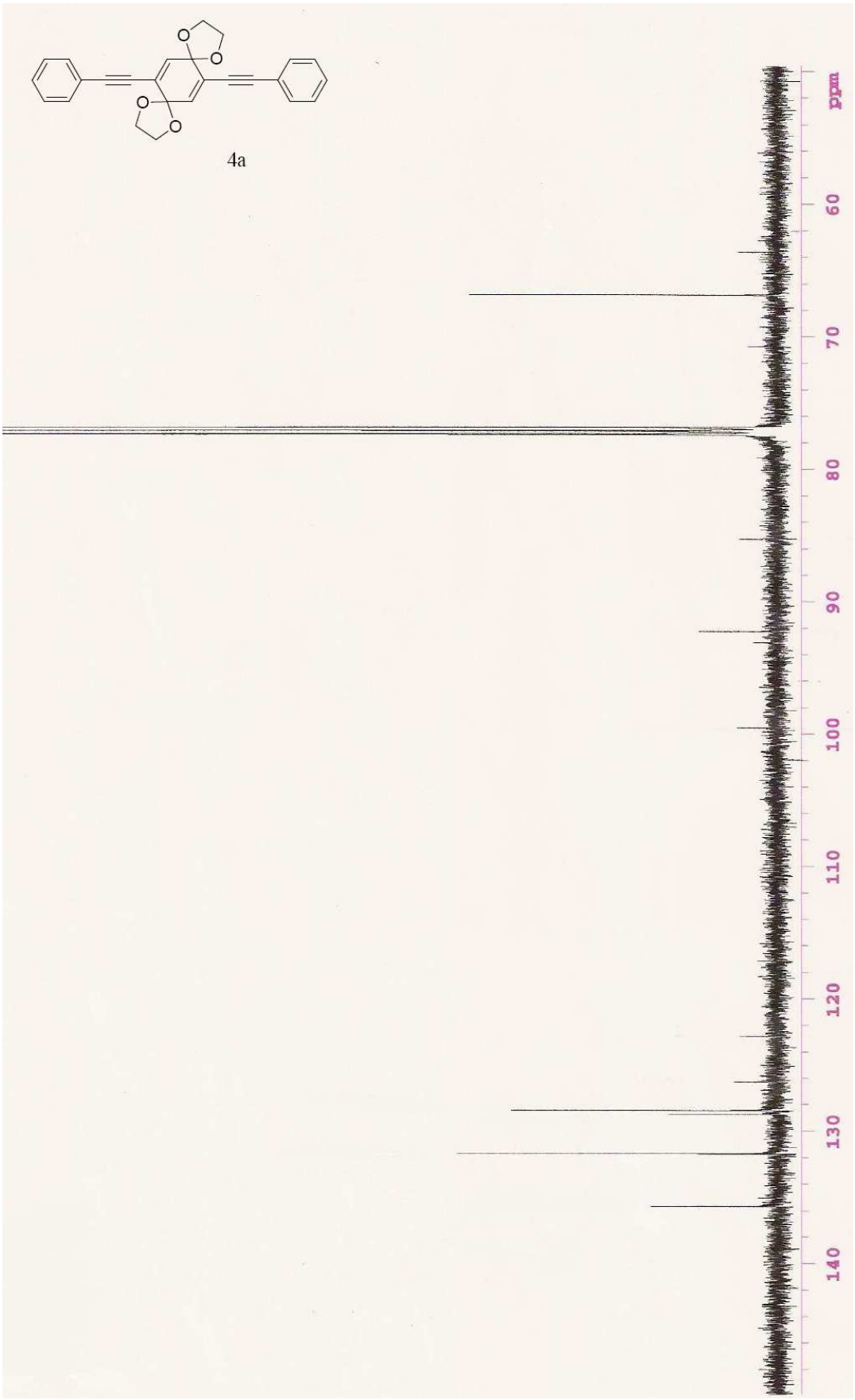

3a
[ppm]
0
50
100
150
200
[rel]
0
2
4
6
8
10
12
14


HO
O
Ph
Ph
O
4
OH

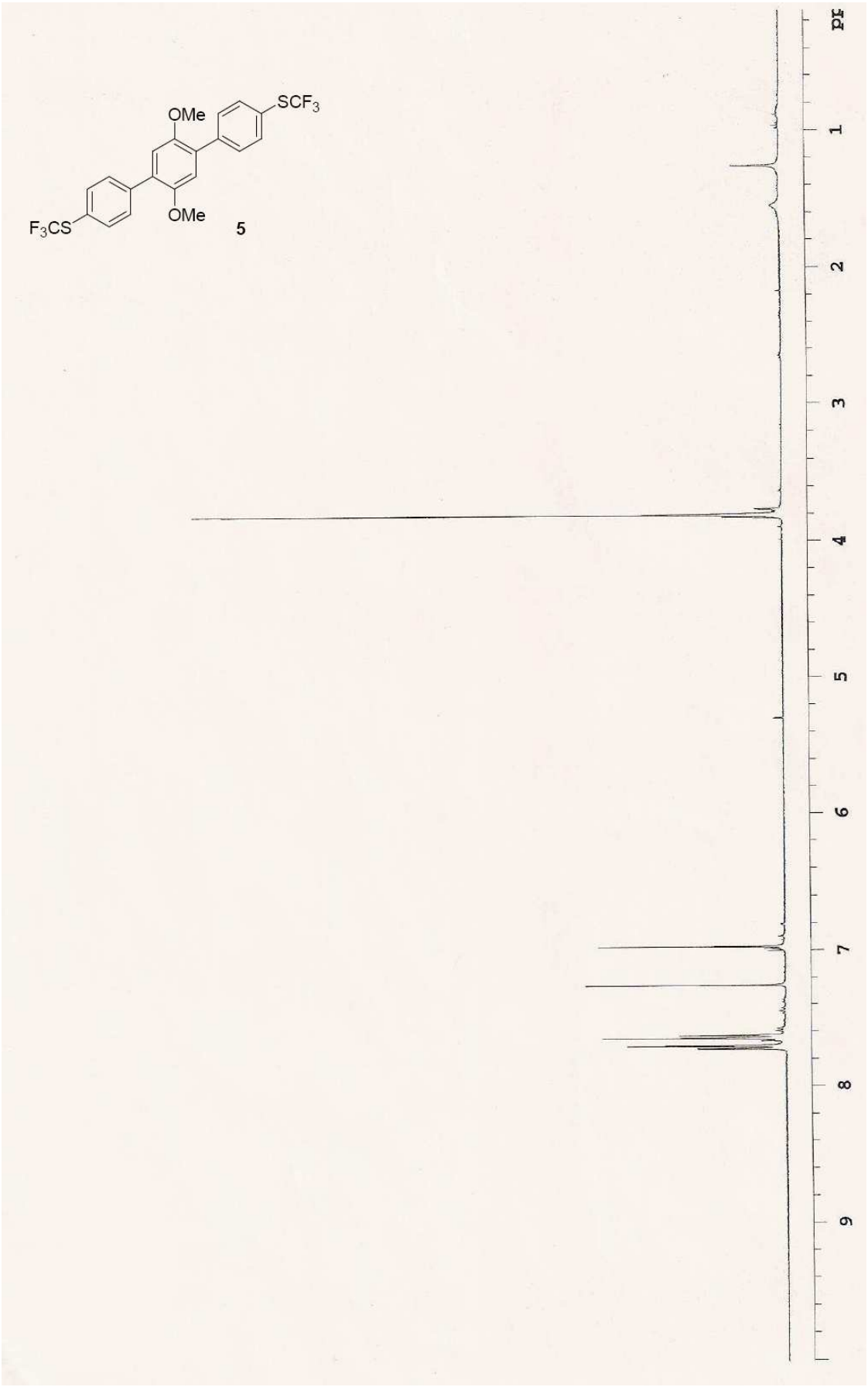
ppm
1
2
3
4
5
6
7
8
9

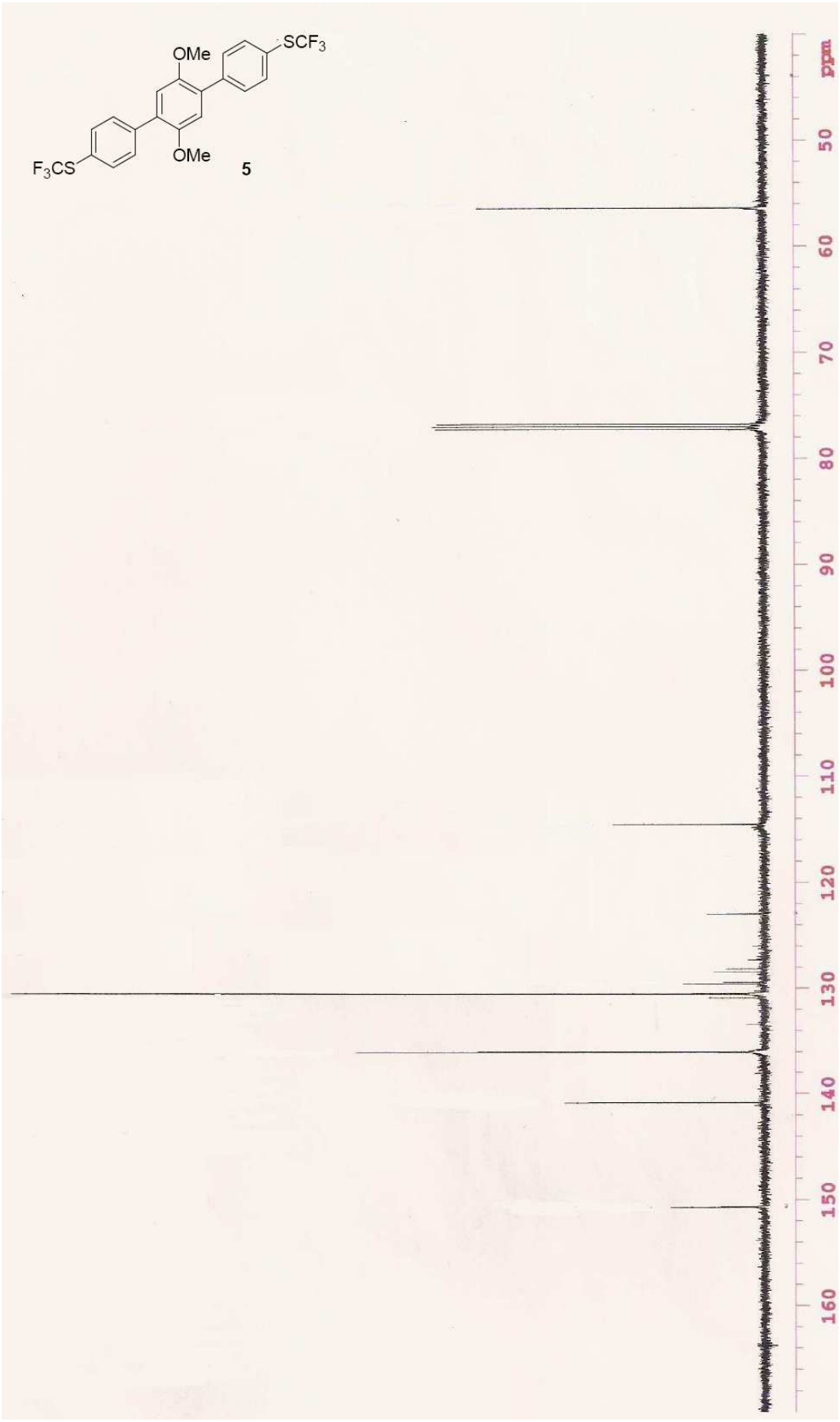


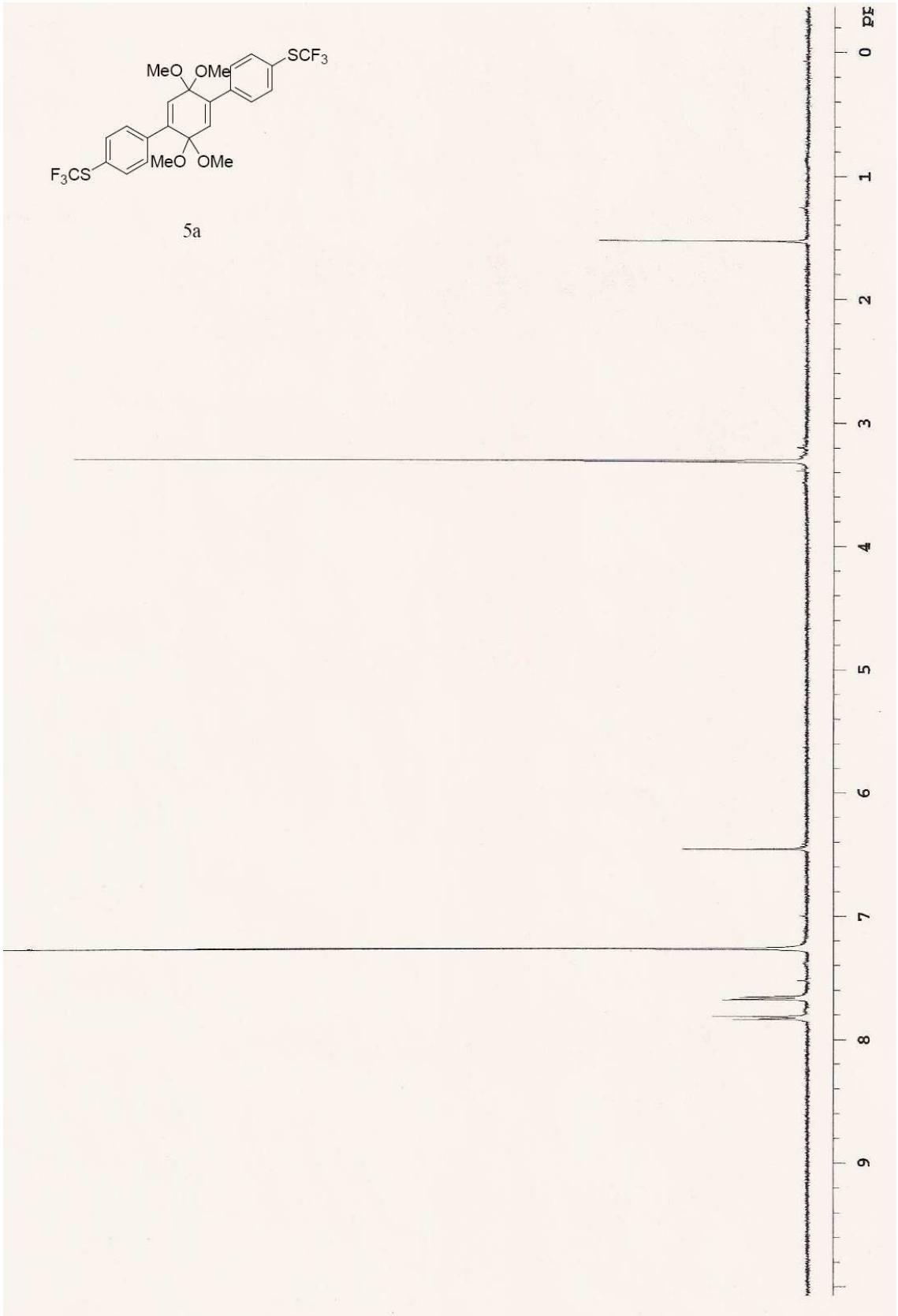
4a

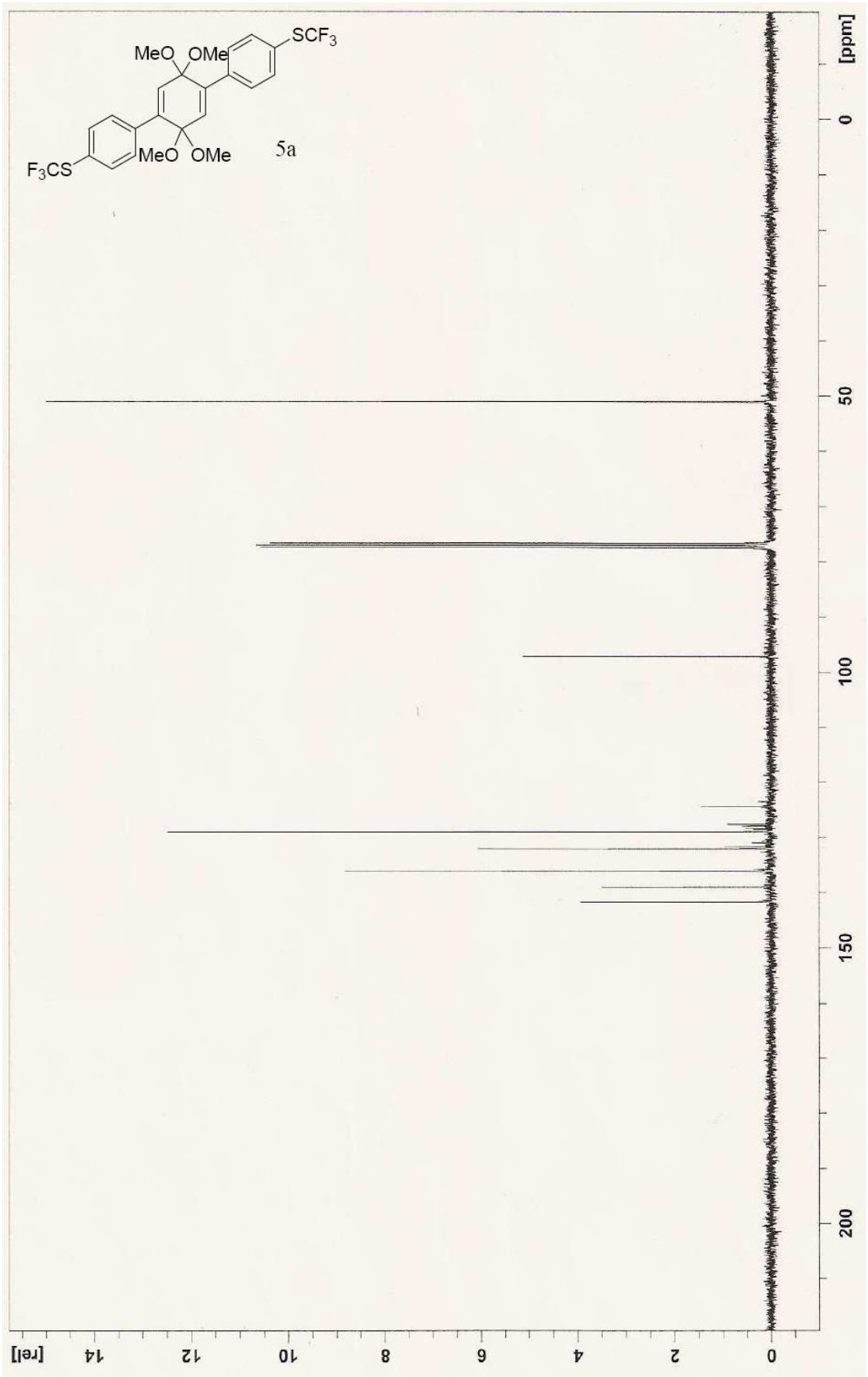


4a

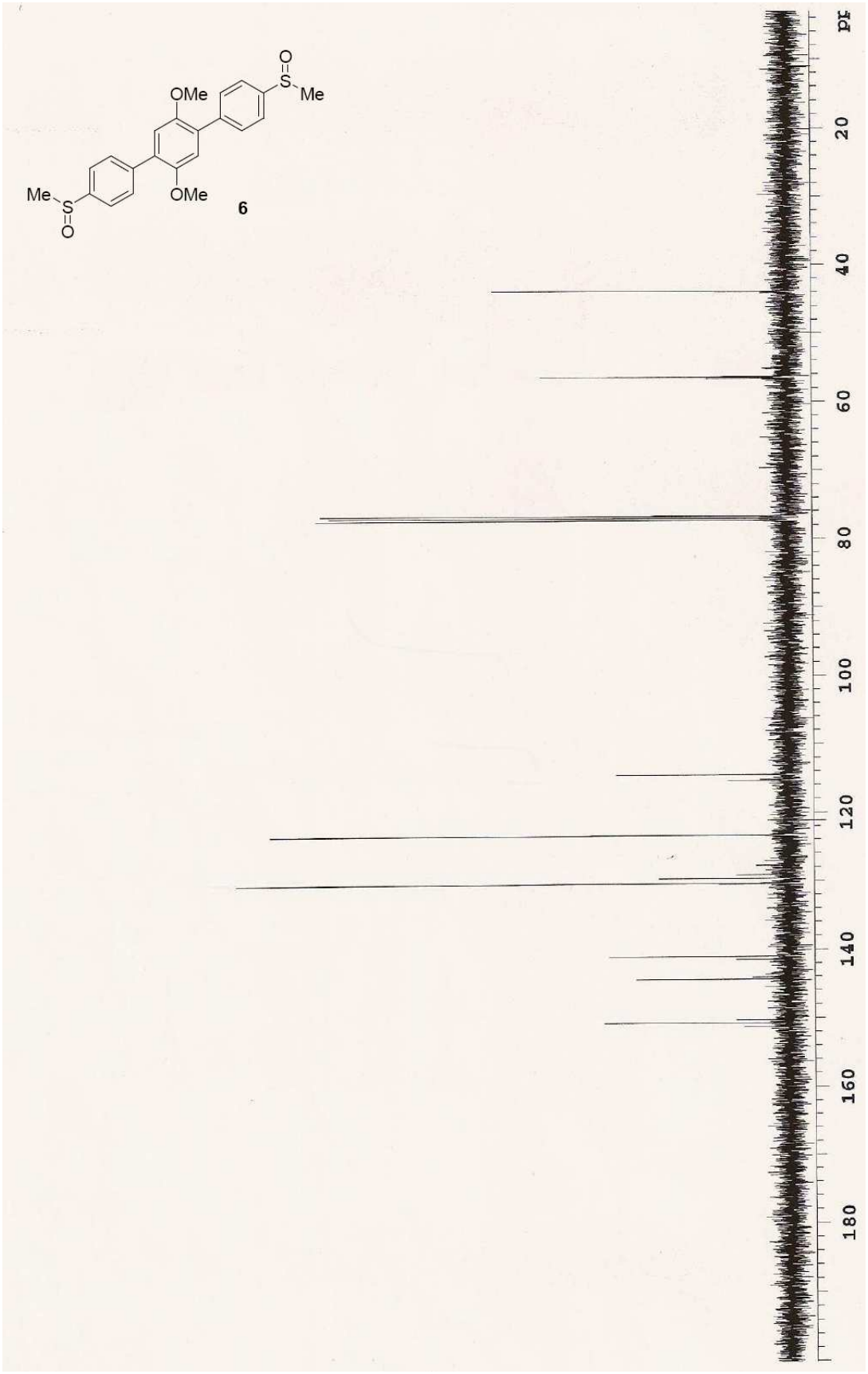

OMe
SCF3
F3CS
OMe
5
ppm
1
2
3
4
5
6
7
8
9

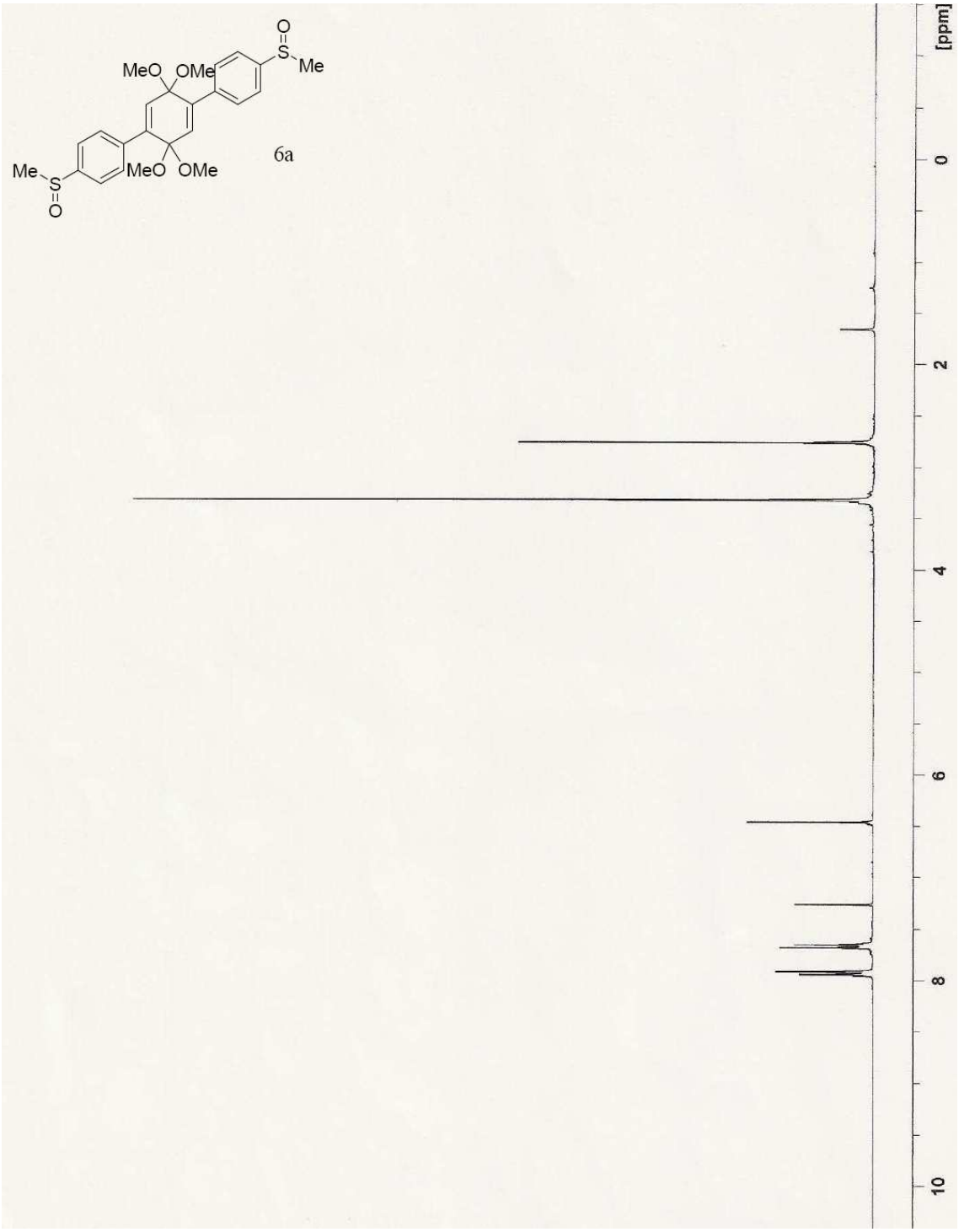

OMe
SCF3
F3CS
OMe
5
ppm
50
60
70
80
90
100
110
120
130
140
150
160

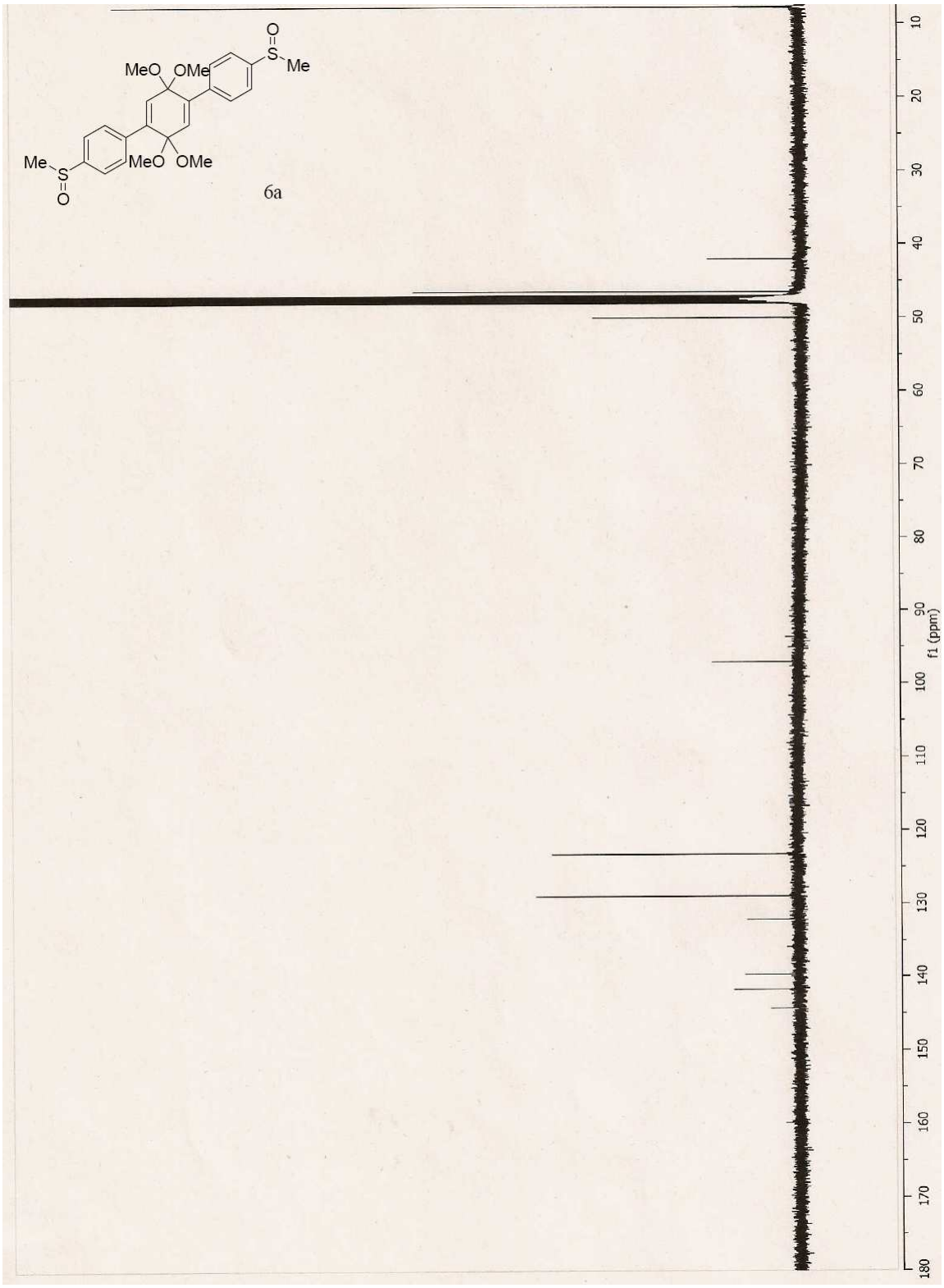

MeO
OMe
SCF3
F3CS
MeO
OMe
5a
ppm
0
1
2
3
4
5
6
7
8
9

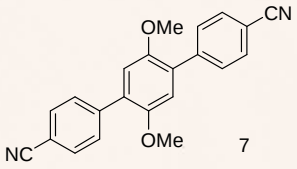

MeO
OMe
SCF3
MeO
OMe
F3CS
5a
[ppm]
0
50
100
150
200
[rel]
0
2
4
6
8
10
12
14


OMe
S
O
Me
Me
S
O
OMe
6
ppm
1
2
3
4
5
6
7
8
9

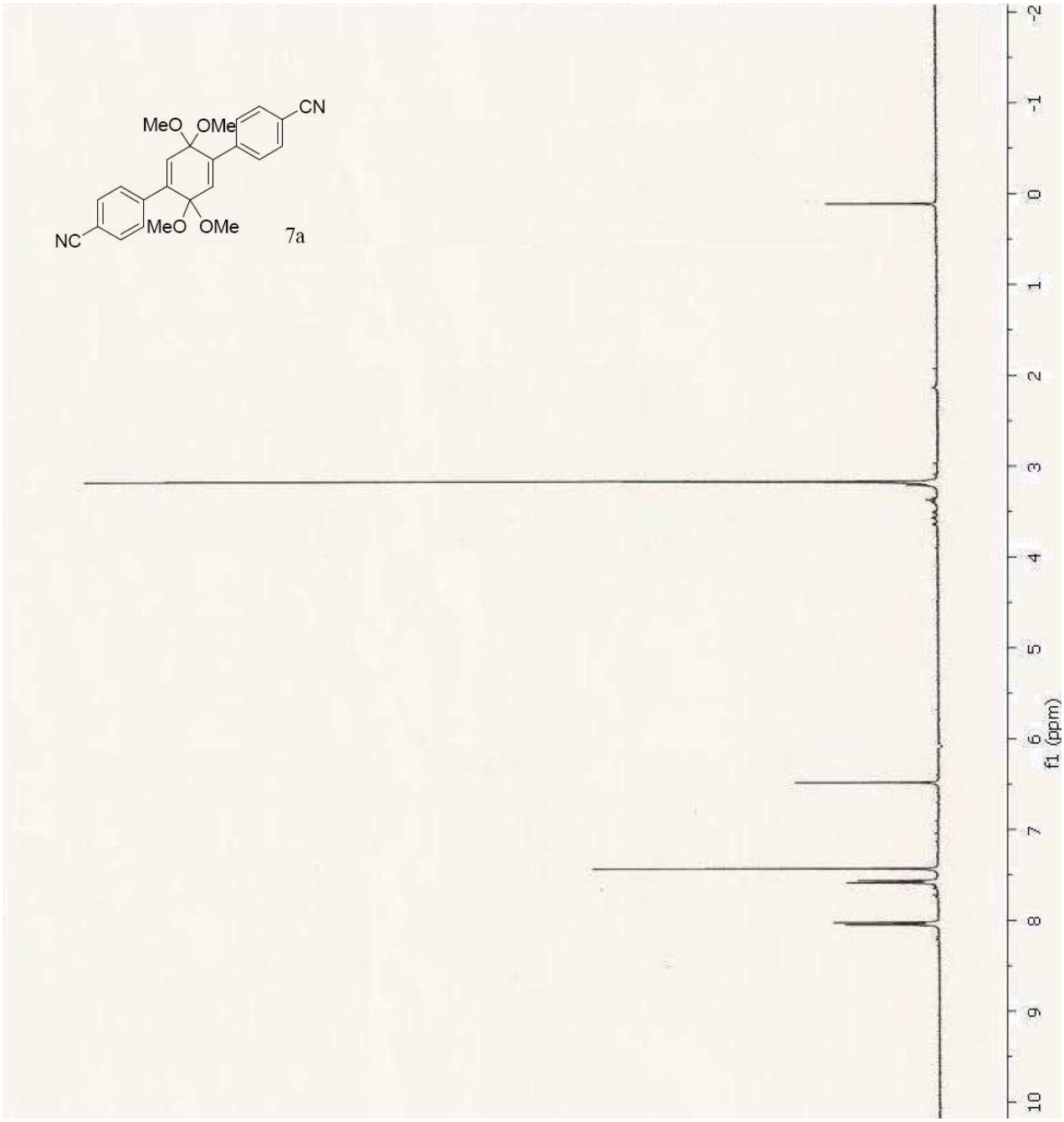

OMe
O
S
Me
Me
S
O
OMe
6
ppm
20
40
60
80
100
120
140
160
180

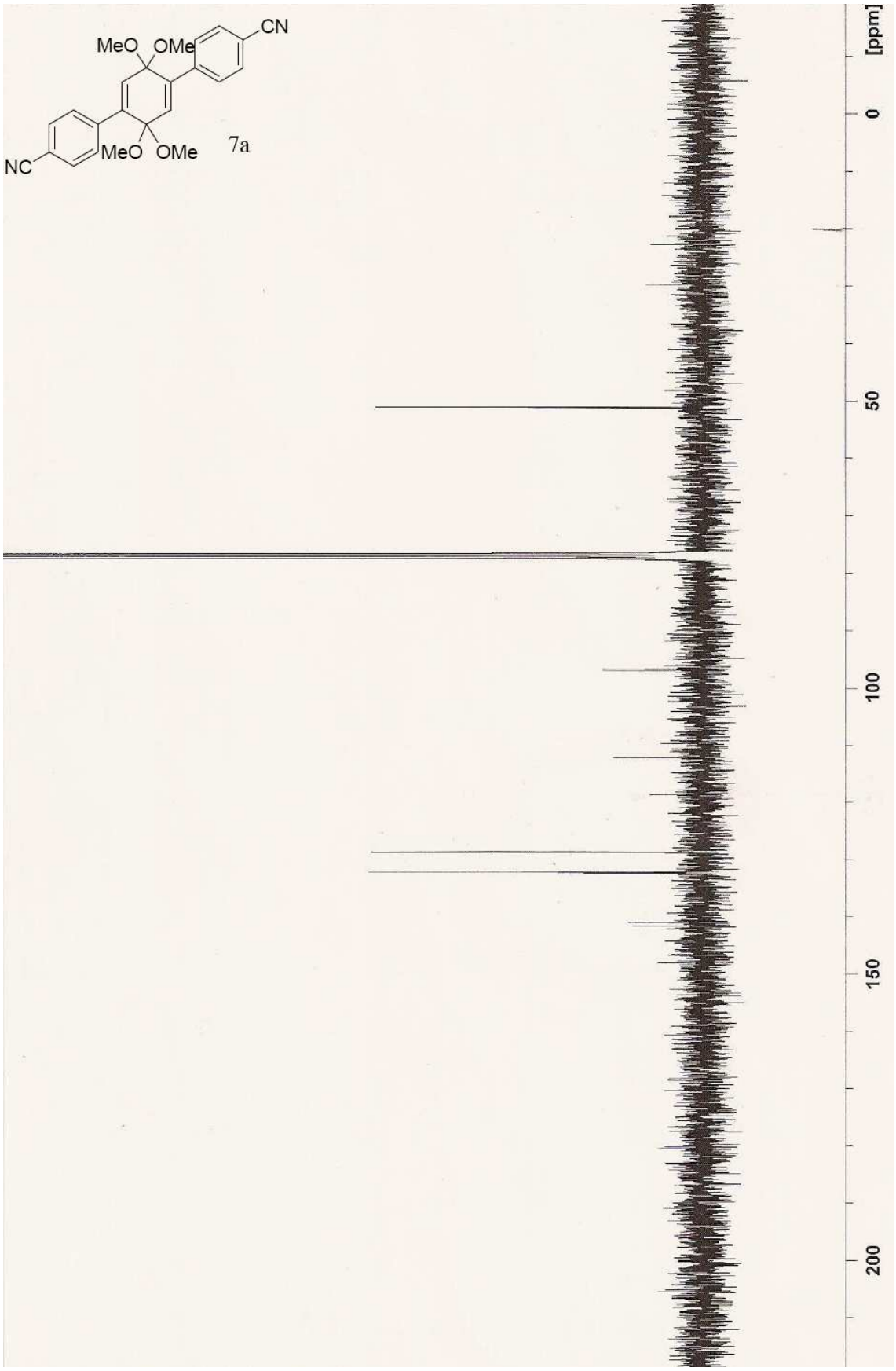

MeO
OMe
S
O
Me
6a
Me
S
O
MeO
OMe
[ppm]
0
2
4
6
8
10

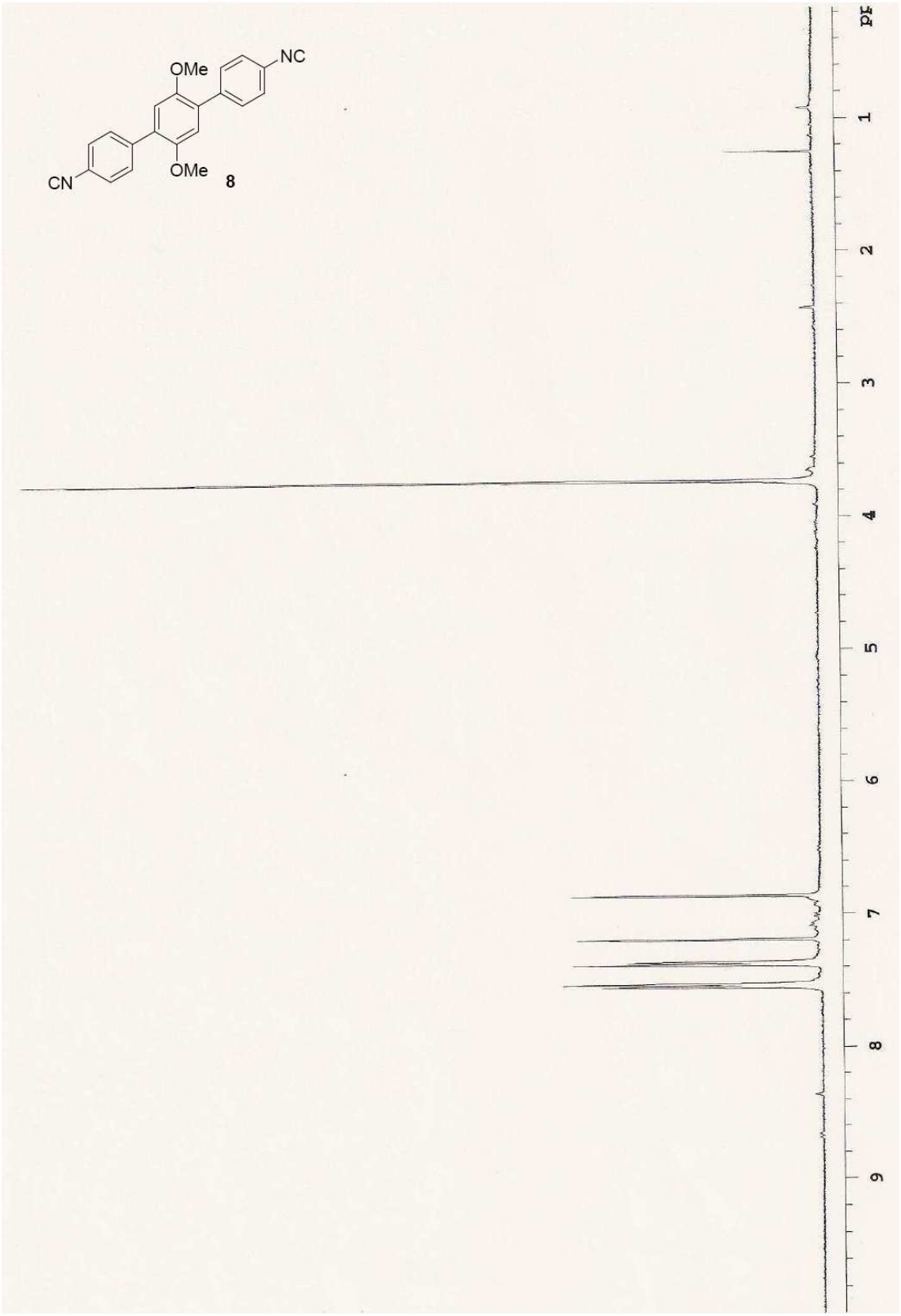

MeO
OMe
O
S
Me
Me
S
O
MeO
OMe
6a
f1 (ppm)

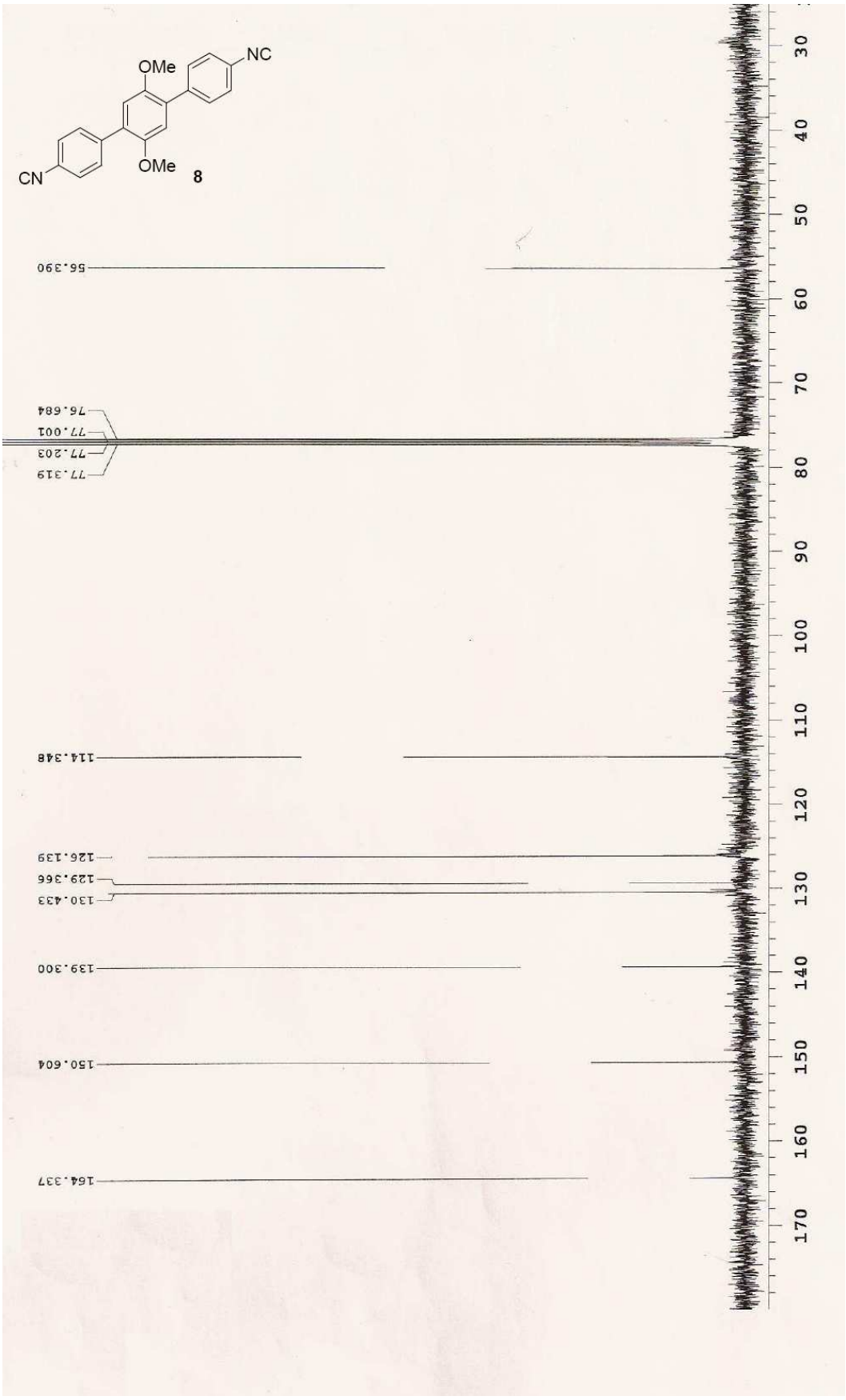


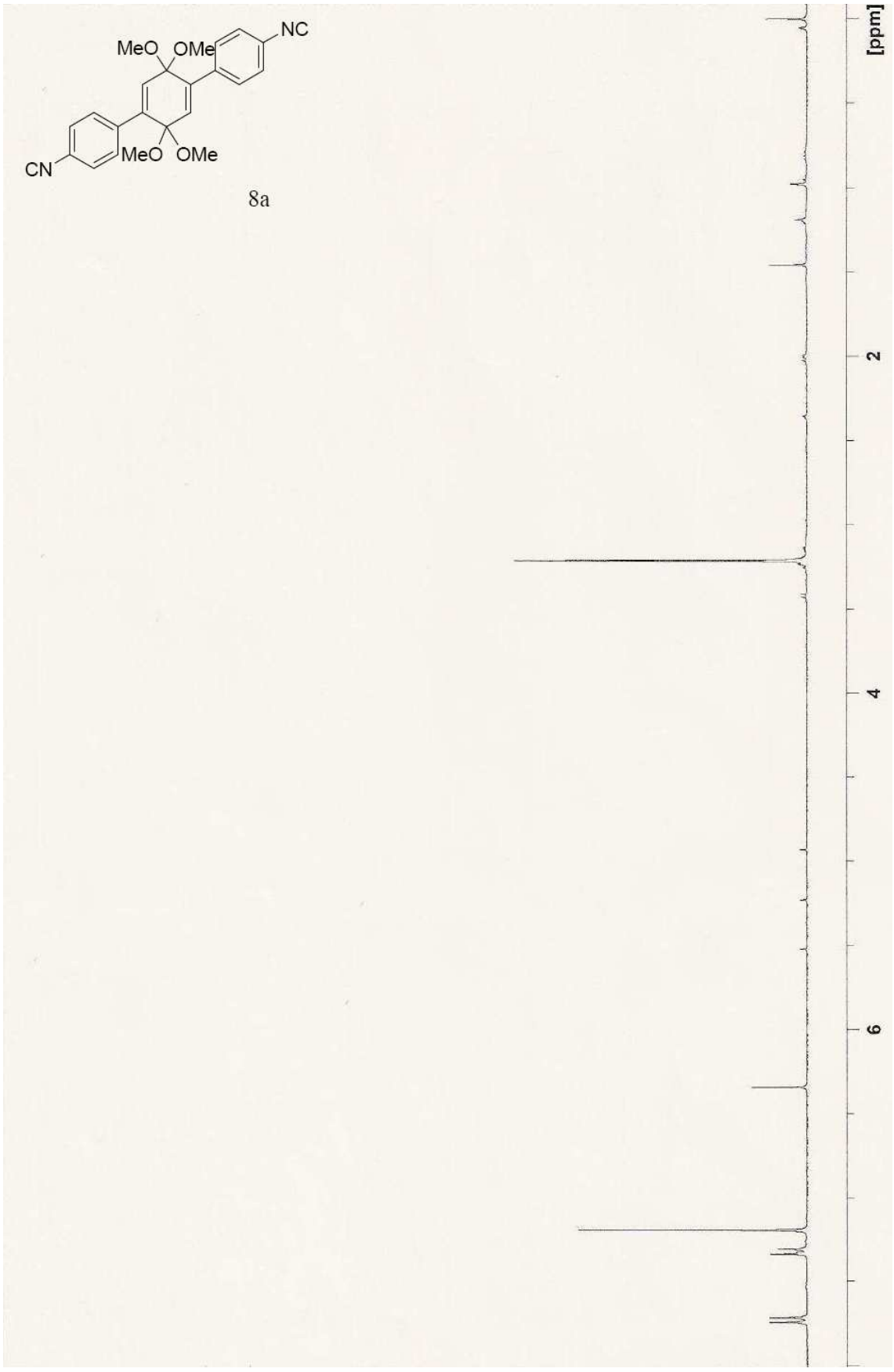
7


CN
MeO
OMe
MeO
OMe
NC
7a
f1 (ppm)

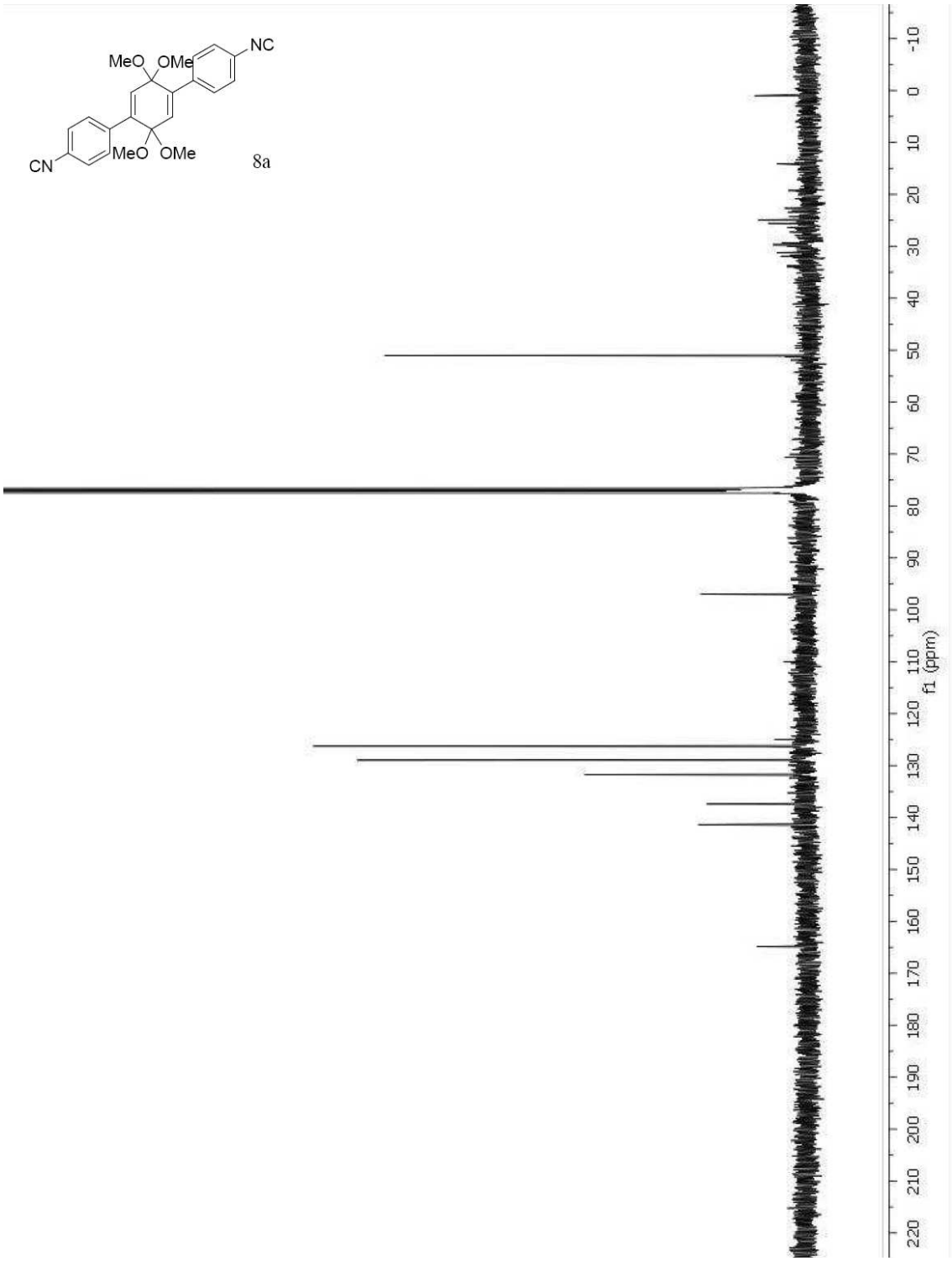

MeO
OMe
CN
NC
MeO
OMe
7a
[ppm]
0
50
100
150
200

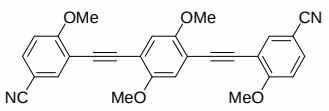

NC
OMe
OMe
CN
8
ppm
1
2
3
4
5
6
7
8
9


OMe
NC
OMe
CN
8
56.390
76.684
77.001
77.203
77.319
114.348
126.139
129.366
130.433
139.300
150.604
164.337
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170

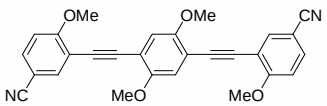


8a

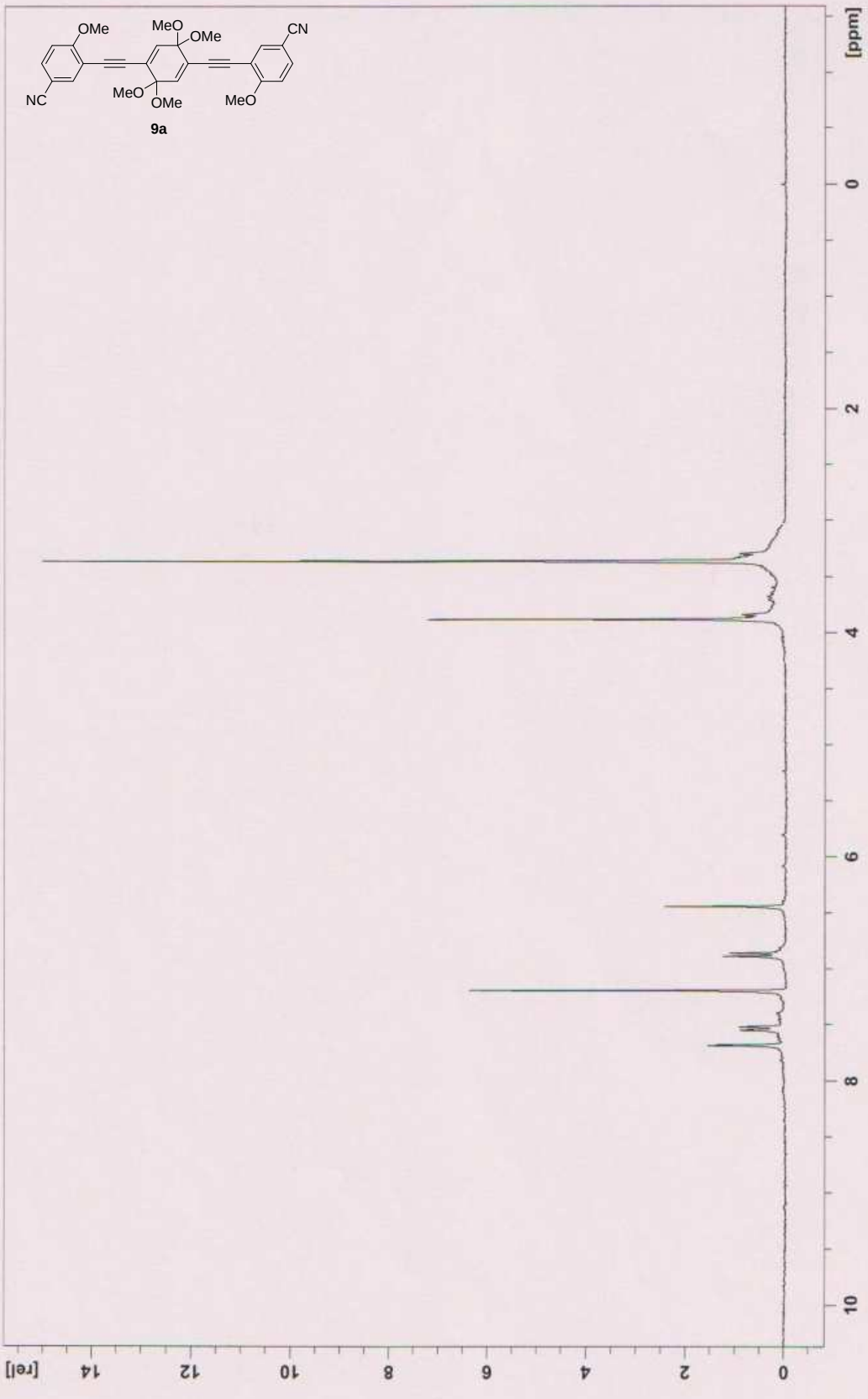

MeO
OMe
NC
MeO
OMe
CN
8a
f1 (ppm)



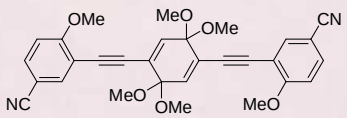
9



9

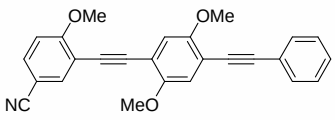


9a

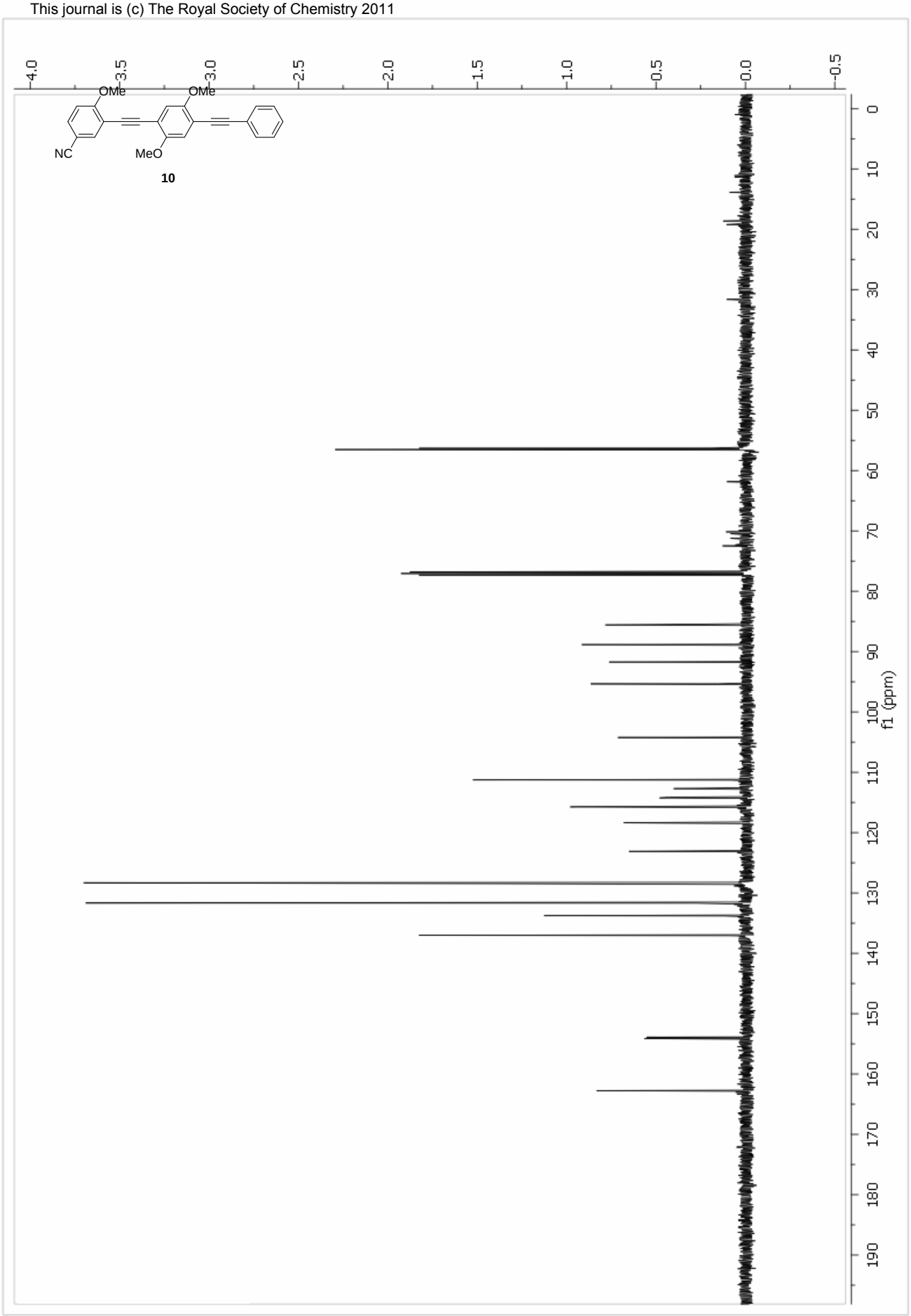

OMe
MeO
OMe
CN
NC
MeO
OMe
MeO

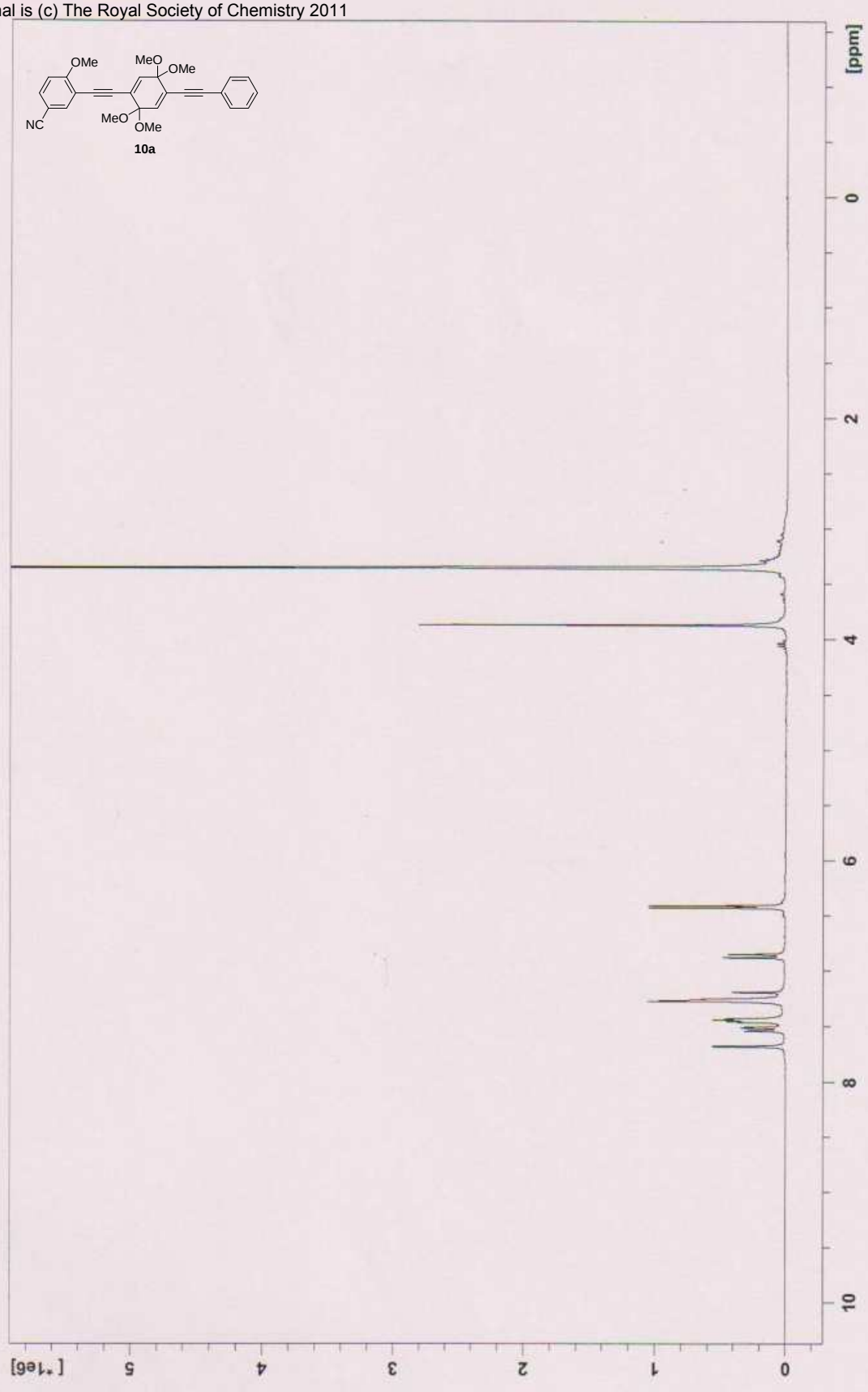
9a

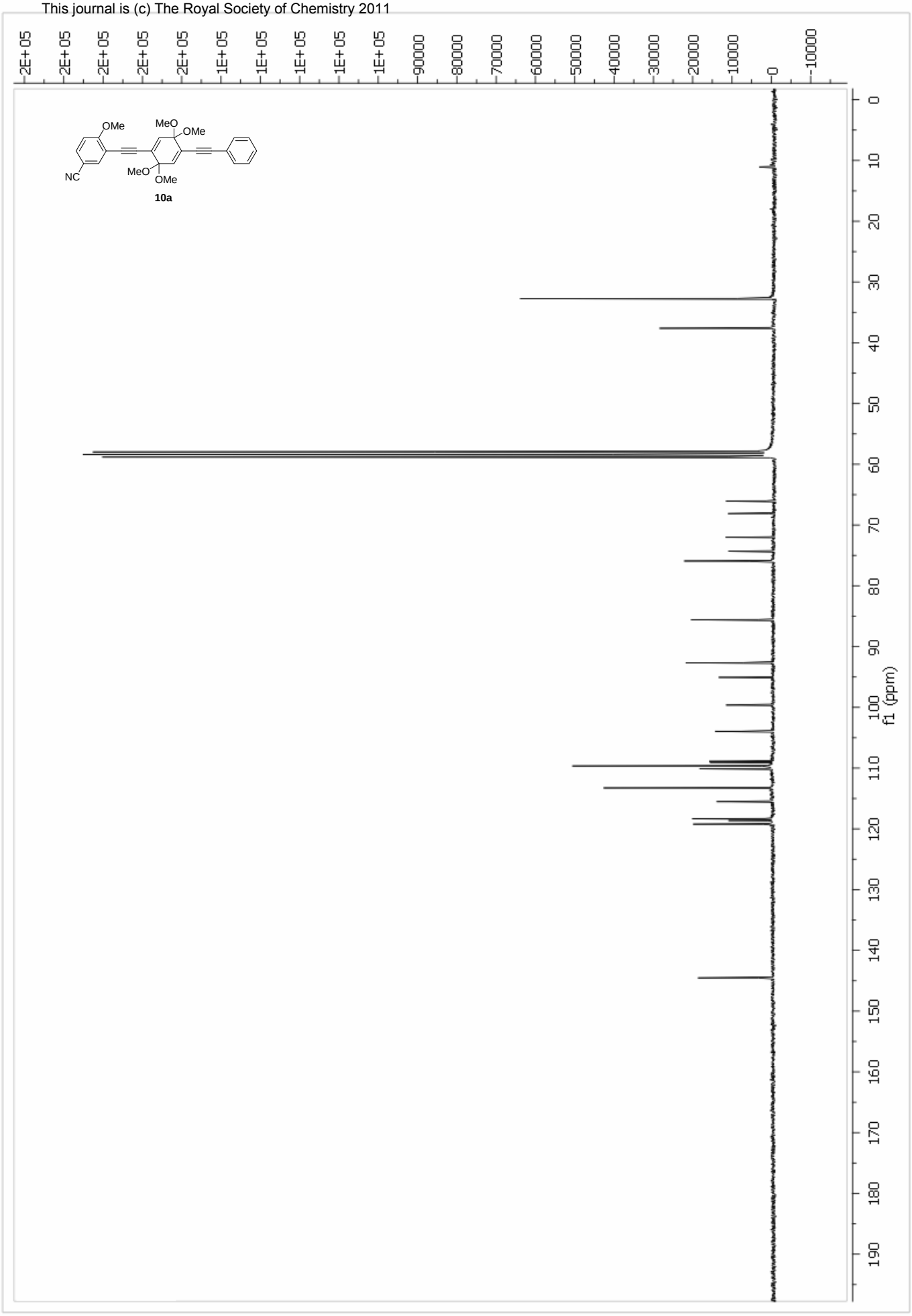
[ppm]
0
50
100
150
200
100.0000
[rel]
-0.0
0.2
0.4
0.6
0.8
1.0
1.2



10


OMe
OMe
NC
MeO
10
f1 (ppm)


OMe
MeO
OMe
NC
MeO
OMe
10a
[ppm]
0
2
4
6
8
10
[*1e6]
5
4
3
2
1
0


OMe
MeO
OMe
MeO
OMe
NC
10a
f1 (ppm)

Copies UV-vis spectra of compounds 1, 2, 5-10 and 1a-10a

UV-vis spectra were recorded using a Helyos α spectrometer at T = 298 K.

Concentrations of 0.0001 M in CH_2Cl_2 were used.

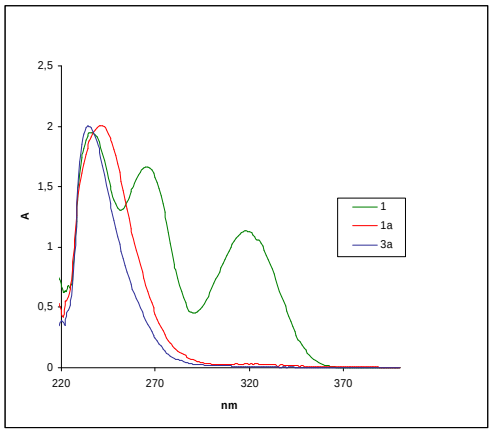


Figure S1. UV-*vis* spectra of compounds **1** (green), **1a** (red) and **3a** (blue).

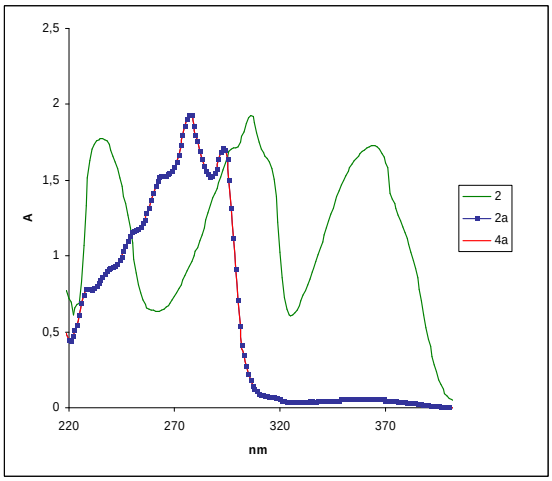


Figure S2. UV-*vis* spectra of compounds **2** (green), **2a** (blue) and **4a** (red).

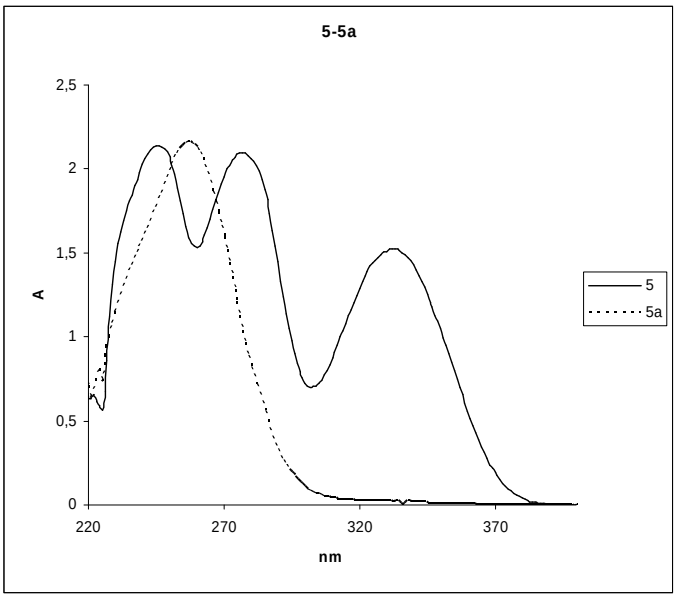


Figure S3. Uv-*vis* spectra of compounds **5** and **5a**

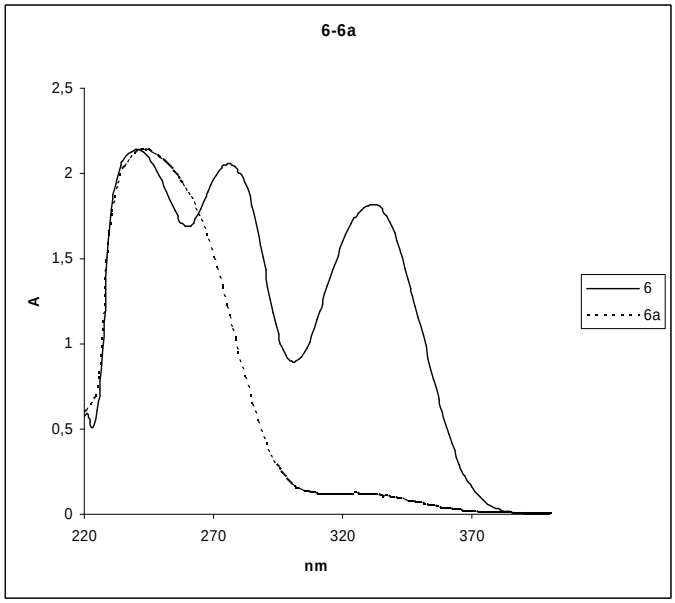


Figure S4. Uv-*vis* spectra of compounds **6** and **6a**

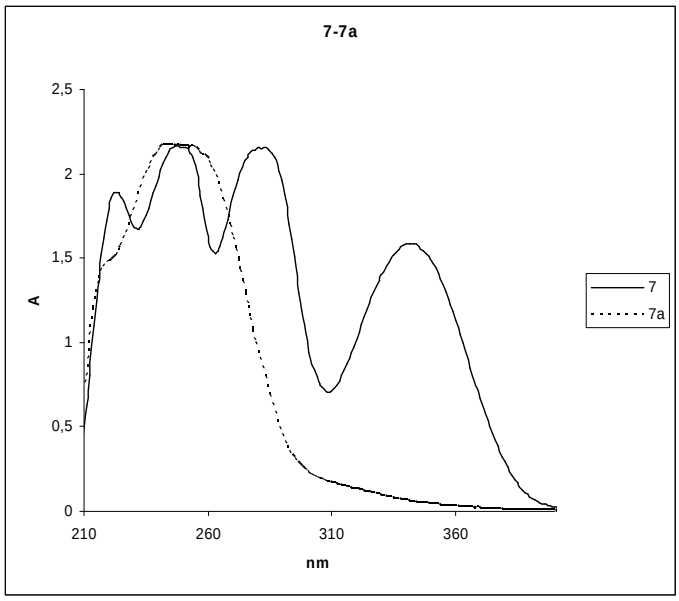


Figure S5. Uv-*vis* spectra of compounds **7** and **7a**

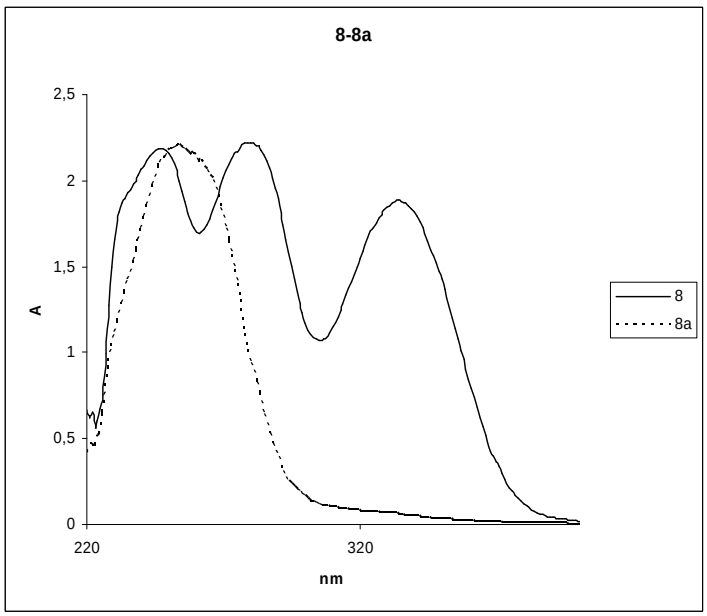


Figure S6. Uv-*vis* spectra of compounds **8** and **8a**

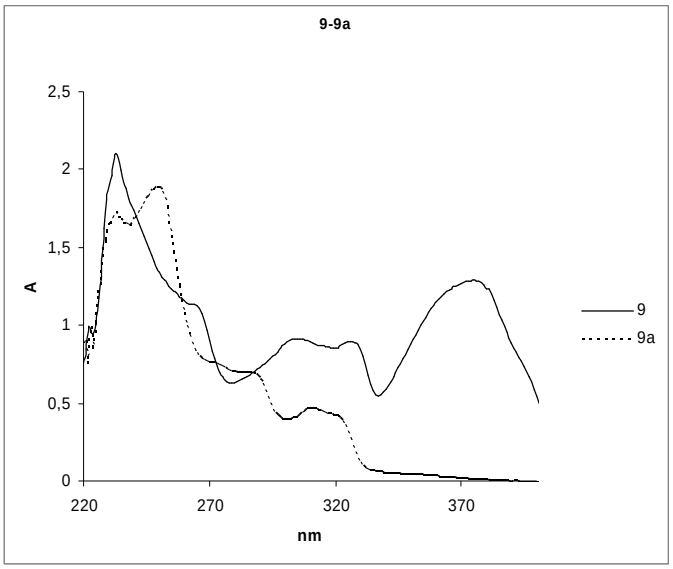


Figure S7. Uv-*vis* spectra of compounds **9** and **9a**

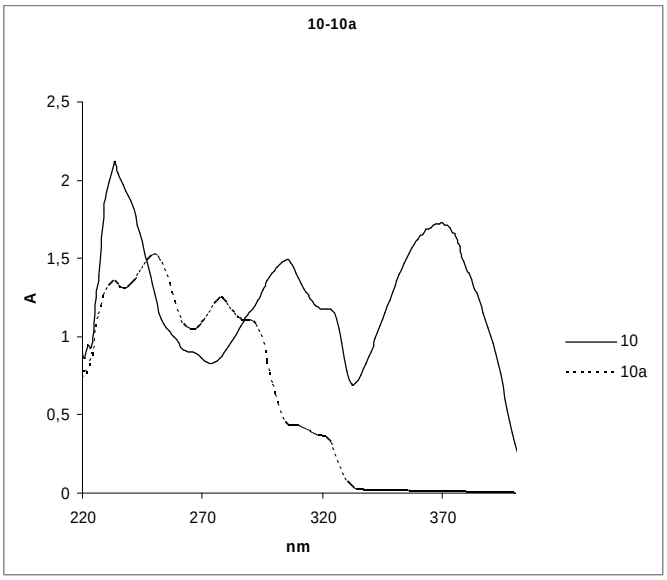


Figure S8. Uv-*vis* spectra of compounds **10** and **10a**

Table S2. HOMO-LUMO optical gaps for compounds **1-10**

Compound	UV-vis λ_{max} (nm)	Gap (eV)
1	318	3.92
1a	241	5.18
2	364	3.43
2a	293	4.26
3	314	3.97
3a	234	5.34
4	358	3.48
4a	293	4.26
5	333	3.75
5a	257	4.86
6	331	3.77
6a	242	5.16
7	343	3.64
7a	257	4.86
8	337	3.70
8a	254	4.91
9	375	3.33
9a	250	4.99
10	370	3.37
10a	278	4.49

Cyclic voltammetry

Electrochemical cyclic and square-wave voltammetry (CV and SWV, respectively) measurements were carried out with an Ecochemie PGSTAT30 electrochemistry system in a three electrode cell under nitrogen atmosphere in anhydrous deoxygenated acetonitrile containing 0.15 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) as supporting electrolyte. Polycrystalline Pt was used as working electrode; the counter electrode was a Pt gauze and the reference electrode was a silver wire quasi-reference electrode. Ferrocene (Fc) was added after a series of experiments and used as internal standard; all potentials in this work are referred to the Fc^+/Fc couple.

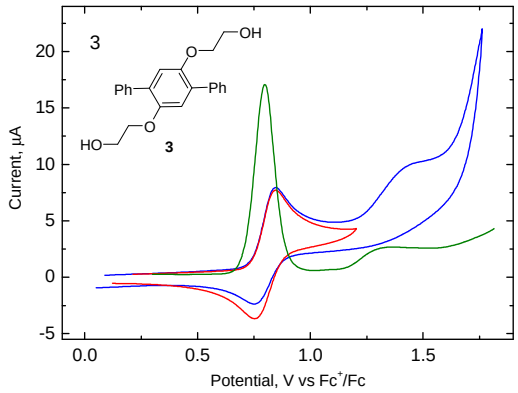


Figure S9. Cyclic and square wave voltammograms for the oxidation of a solution of **3** in acetonitrile containing 0.15 M $TBAPF_6$ at 25°C on a Pt working electrode. CV: v = 0.1 Vs^{-1} with different positive switching potentials (blue and red). SWV: scan increment = 2 mV, SW amplitude = 25 mV, frequency = 15 Hz (green).

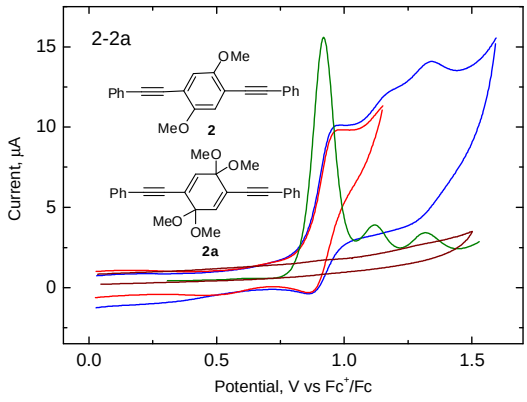


Figure S10. Cyclic and square wave voltammograms for the oxidation of a solution of **2** in acetonitrile containing 0.15 M $TBAPF_6$ at 25°C on a Pt working electrode. CV: v = 0.1 Vs^{-1} with different positive switching potentials (blue and red). SWV: scan increment = 2 mV, SW amplitude = 25 mV, frequency = 15 Hz (green). CV of a solution of **2a** is also shown (brown).

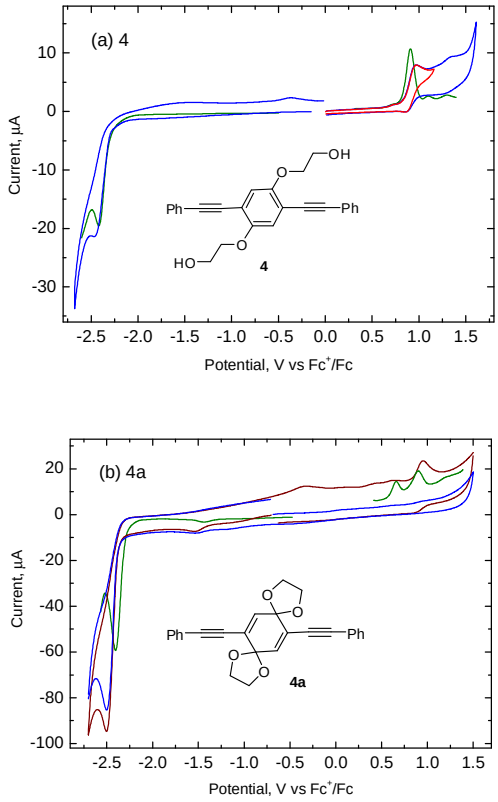


Figure S11. Cyclic and square wave voltammograms for the oxidation and reduction of a solution of **4** (a) and **4a** (b) in acetonitrile containing 0.15 M $TBAPF_6$ at 25°C on a Pt working electrode. (a) CV: v = 0.1 Vs^{-1} with different positive switching potentials (blue and red). SWV: scan increment = 2 mV, SW amplitude = 25 mV, frequency = 15 Hz (green). (b) CV: v = 1 Vs^{-1}, initial scan in the positive (blue) or in the negative (brown) direction. SWV (green): plotted signals have been fourfold enlarged, scan increment = 2 mV, SW amplitude = 25 mV, frequency = 15 Hz (reduction) or 60 Hz (oxidation). Data shown for SWV oxidation in (b) are obtained after a prior reduction scan, otherwise no peaks are observed.

Compounds **4** and **4a** show a reduction peak at -2.42 V, which probably derived from the reduction of the alkyne subunit[18]: We could not observe this peak in closely related structures **2** and **2a** because it is close to the detection limit using acetonitrile as solvent.

[18] A. Dalen, A. Nilsson and G. Hilmersson, *J. Org. Chem.* 2006, **71**, 1576-1580.

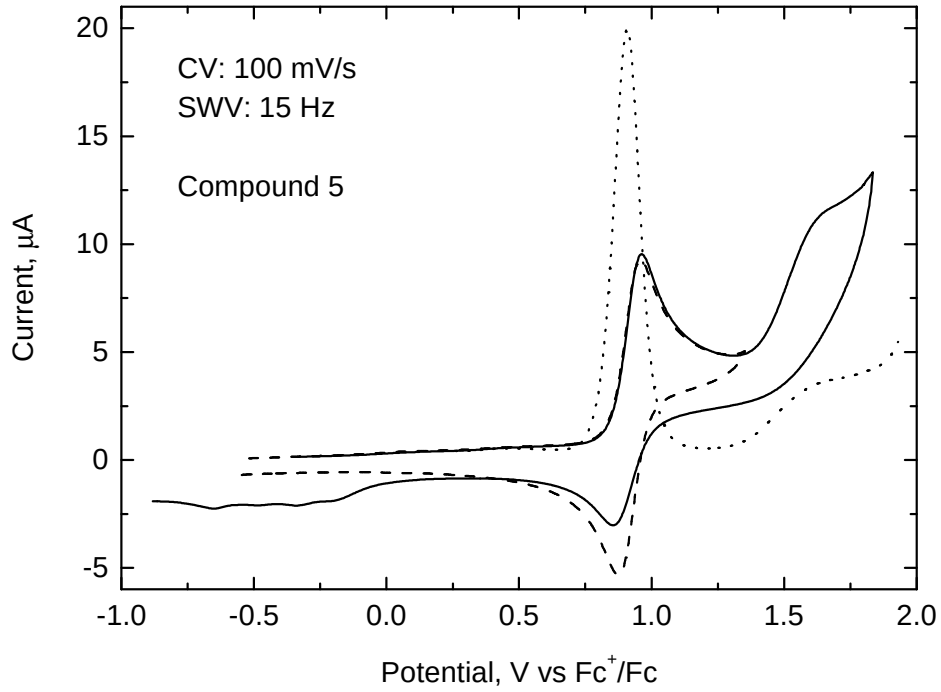


Figure S12. Cyclic and square wave voltammograms for the oxidation of a solution of **5** in acetonitrile containing 0.15 M $TBAPF_6$ at 25°C on a Pt working electrode. CV: v = 0.1 Vs^{-1} with different positive switching potentials (— and ---). SWV: scan increment = 2 mV, SW amplitude = 25 mV, frequency = 15 Hz (···).

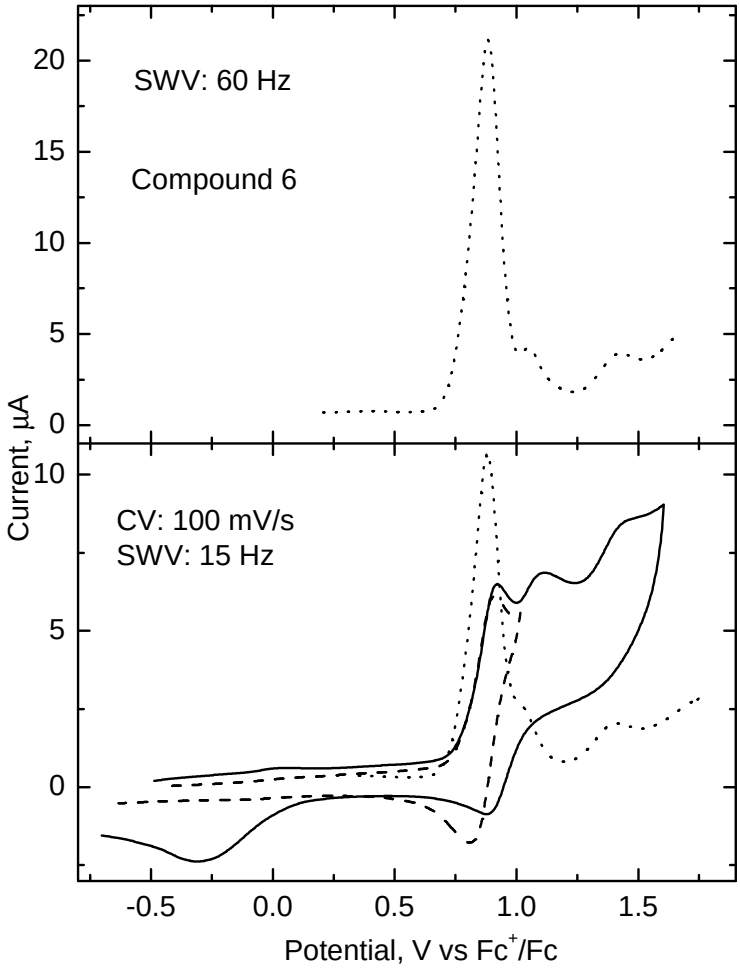


Figure S13. Cyclic and square wave voltammograms for the oxidation of a solution of **6** in acetonitrile containing 0.15 M $TBAPF_6$ at 25°C on a Pt working electrode. CV: v = 0.1 Vs^{-1} with different positive switching potentials (— and ---). SWV: scan increment = 2 mV, SW amplitude = 25 mV, frequency = 15 Hz or 60 Hz, as indicated in the figure (···) and top panel.

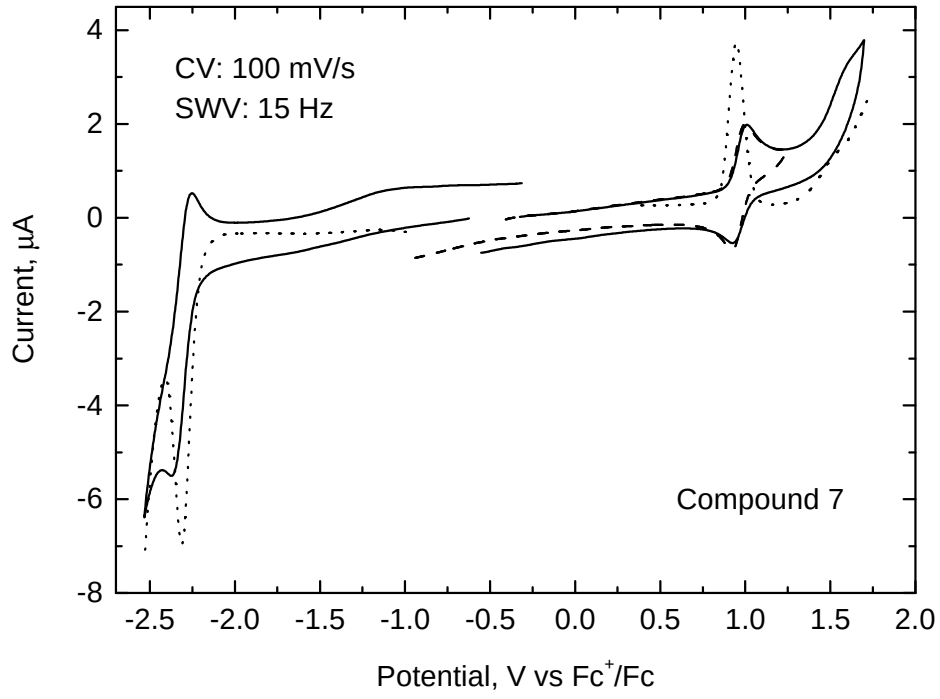


Figure S14. Cyclic and square wave voltammograms for the oxidation and the reduction of a solution of **7** in acetonitrile containing 0.15 M $TBAPF_6$ at 25°C on a Pt working electrode. CV: v = 0.1 Vs^{-1} with different positive switching potentials (— and ---). SWV: scan increment = 2 mV, SW amplitude = 25 mV, frequency = 15 Hz (···).

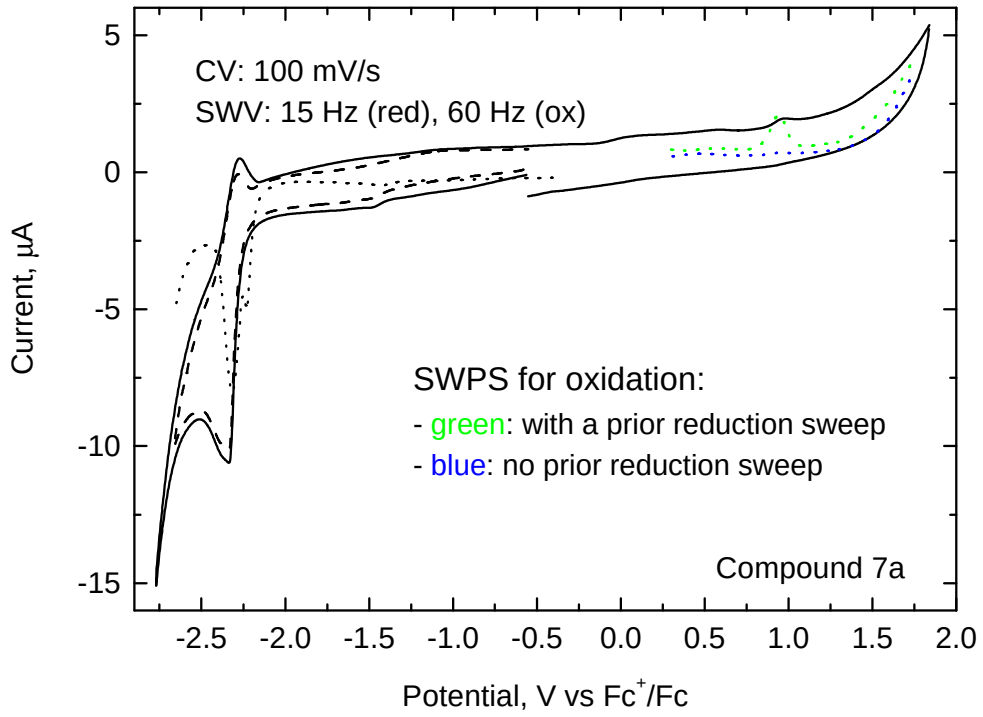


Figure S15. Cyclic and square wave voltammograms for the reduction and the oxidation of a solution of **7a** in acetonitrile containing 0.15 M $TBAPF_6$ at 25°C on a Pt working electrode. CV: v = 0.1 Vs^{-1} with different switching potentials (— and ---). SWV: scan increment = 2 mV, SW amplitude = 25 mV, frequency = 15 Hz (for reduction), 60 Hz (for oxidation) (···).

Compound **7** shows a reduction peak at -2.31 V, assigned to the reduction of the aromatic nitrile groups.[19] We could detect again a reduction peak corresponding to the nitrile reduction at -2.31 V of bisnitrile **7a**.

[19] A. M. Romanin, A. Gennaro and E. Vianello, *J. Electroanal. Chem.* 1978, **88**, 175-185.

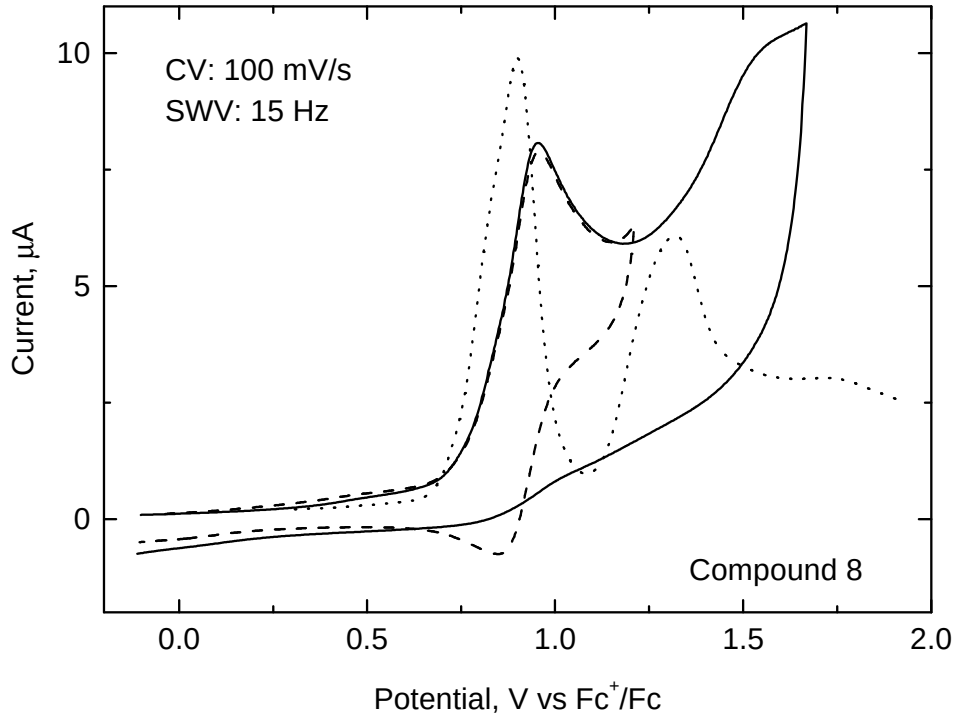


Figure S16. Cyclic and square wave voltammograms for the oxidation of a solution of **8** in acetonitrile containing 0.15 M $TBAPF_6$ at 25°C on a Pt working electrode. CV: v = 0.1 Vs^{-1} with different positive switching potentials (— and ---). SWV: scan increment = 2 mV, SW amplitude = 25 mV, frequency = 15 Hz (···).

The electrochemical behaviour of isonitrile **8** seems to be more complex than the other compounds. The first oxidation wave is composed and quasirreversible, suggesting that two different processes are occurring at similar voltages. A simple explanation is the possible coordination of **8** with the electrode surface.

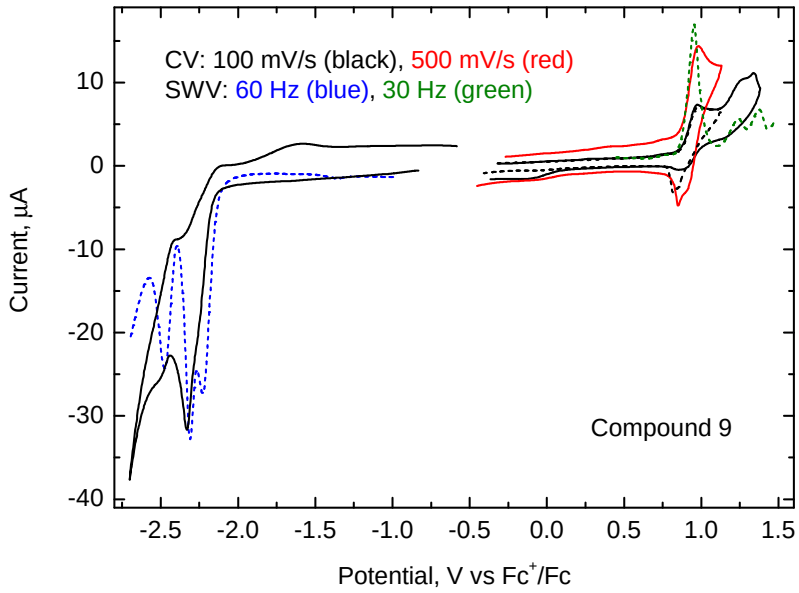


Figure S17. Cyclic and square wave voltammograms for the oxidation and the reduction of a solution of **9** in acetonitrile containing 0.15 M $TBAPF_6$ at 25°C on a Pt working electrode. CV: v = 0.1 Vs^{-1} with different positive switching potentials (— and --- black), and 0.5 Vs^{-1} (red). SWV: scan increment = 2 mV, SW amplitude = 25 mV, frequency = 30 Hz and 60 Hz, as indicated (---).

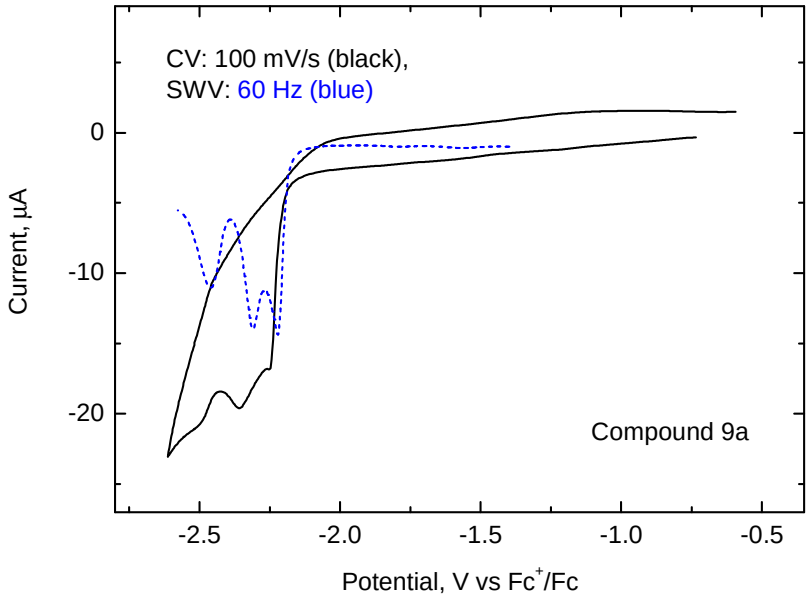


Figure S18. Cyclic and square wave voltammograms for the reduction of a solution of **9a** in acetonitrile containing 0.15 M $TBAPF_6$ at 25°C on a Pt working electrode. CV: v = 0.1 Vs^{-1} (—). SWV: scan increment = 2 mV, SW amplitude = 25 mV, frequency = 60 Hz (··· blue).

In the CV of the oxidation of compound **9** we can also observe a small peak in the reverse sweep at +0.82 V, which can be related with adsorption processes of the molecule on the electrode. The absence of this peak in the other compounds may be related with favoured stapled adsorptions of these molecules owing to the presence of two nitrile groups in *meta* position.
We can also observe (much better resolved in SWV) cathodic peaks corresponding to the reduction of nitrile (-2.22, -2.30 V) and alkyne (-2.47 V) functionalities. Taking into account that compound **9** is symmetric, the presence of the two reduction peaks of nitrile groups can be again related with adsorption processes. A possible electronic coupling is dismissed because similar peaks are observed in oxidized compound **9a**.
As expected based on the CV and SWV of compound **9**, three cathodic peaks corresponding to the reduction of nitrile (-2.22, -2.28 V) and alkyne (-2.47 V) functionalities could be observed.

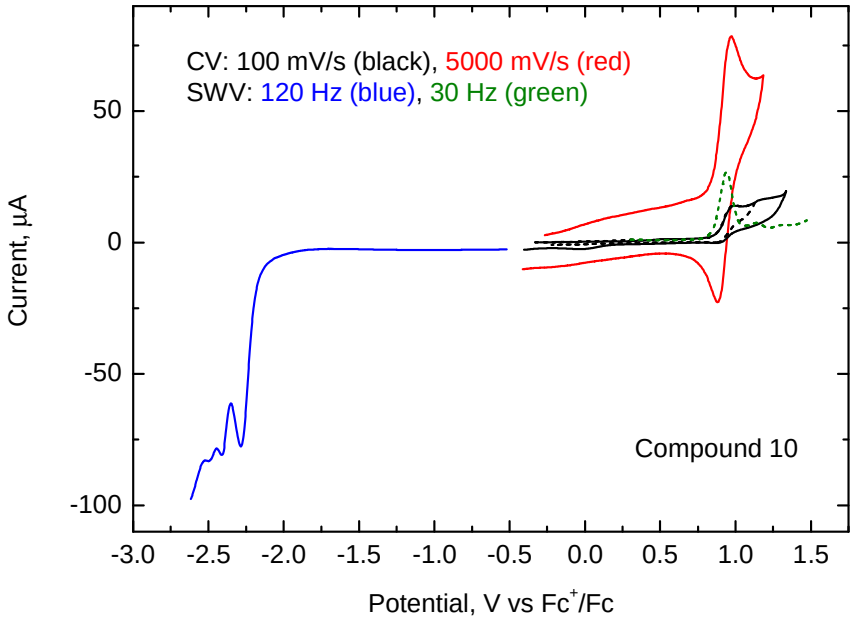


Figure S19. Cyclic and square wave voltammograms for the oxidation and the reduction of a solution of **10** in acetonitrile containing 0.15 M $TBAPF_6$ at 25°C on a Pt working electrode. CV: v = 0.1 Vs^{-1} with different positive switching potentials (— and --- black), and 5 Vs^{-1} (red). SWV: scan increment = 2 mV, SW amplitude = 25 mV, frequency = 30 Hz (green) and 120 Hz (blue), as indicated.

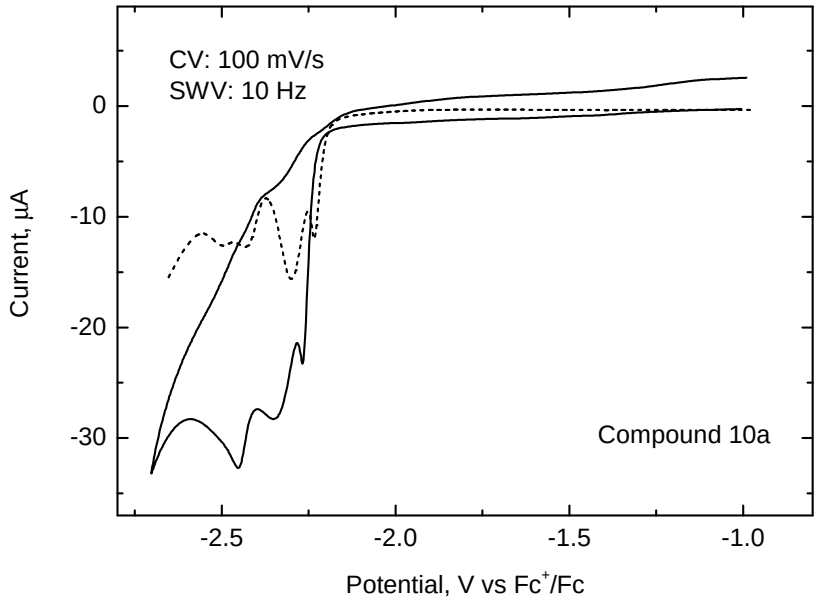


Figure S20. Cyclic and square wave voltammograms for the reduction of a solution of **10a** in acetonitrile containing 0.15 M $TBAPF_6$ at 25°C on a Pt working electrode. CV: v = 0.1 Vs^{-1} (—). SWV: scan increment = 2 mV, SW amplitude = 25 mV, frequency = 10 Hz (···).

Compound **10,** having a nitrile and two non-equivalent alkyne groups, presents the corresponding three irreversible cathodic peaks at -2.28, -2.41 and -2.50 V.
Beside the expected reduction peaks at -2.30, -2.41 and -2.49 V and consistently with CV and SWV of compounds **7a** and **9a**, a peak corresponding to adsorption processes is observed in compound **10a** at -2.24 V.

Table S3. Oxidation and reduction processes for compounds **5-10**.

Compound	Oxidations [V][a]	Reductions [V]
5	0.91 rev. 1.56 irrev.	-
5a	-	-
6	0.88 rev. 1.05 irrev. 1.43 irrev.	-
6a	-	-
7	0.95 rev. 1.52 irrev.	-2.31 rev
7a[b]	-	-2.31 rev
8	0.90 quasirev. 1.31 irrev.	-
8a	-	-
9	0.95 rev. 1.24 irrev. 1.37 irrev.	-2.22 irrev. -2.30 irrev. -2.47 irrev.
9a	-	-2.22 irrev. -2.28 irrev. -2.47 irrev.
10	0.94 rev. 1.14 irrev. 1.34 irrev.	-2.28 irrev. -2.41 irrev. -2.50 irrev.
10a[c]	-	-2.30 irrev. -2.41 irrev. -2.49 irrev.

[a] In acetonitrile containing 0.15 M $TBAPF_6$ at 25 °C on a Pt working electrode. E values measured versus $E_{1/2}$ of the internal reference ferrocenium/ferrocene (Fc^+/Fc). Data taken from SWV measurements. [b] A minor peak at -2.27 V could also be observed. [c] A minor peak at -2.24 V could also be observed

HOMO-LUMO electrochemical gaps for compounds 1-10

The CV of compounds **1-3**, **5-6** and **8**, did not present reduction peaks because the solvent was reduced at a lower voltage. Consequently, for these structures we could only assign an electrochemical HOMO-LUMO gap higher than 3.30 eV.

In the oxidized compounds **1a-3a**, **5a-6a** and **8a**, the absence of oxidation and reduction peaks must be related with an electrochemical gap higher than 4.2 V. The first reduction peak was observed in structures **4**, **7, 9** and **10**. The corresponding electrochemical gaps are 3.33, 3.26, 3.17 and 3.22 eV, respectively, whilst the gaps for the related bisketals **4a**, **7a**, **9a** and **10a** were estimated to be higher than 4.0 eV.