Supporting Information

Dimeric Packing of Molecular Clips Induced by Interactions Between π-Systems

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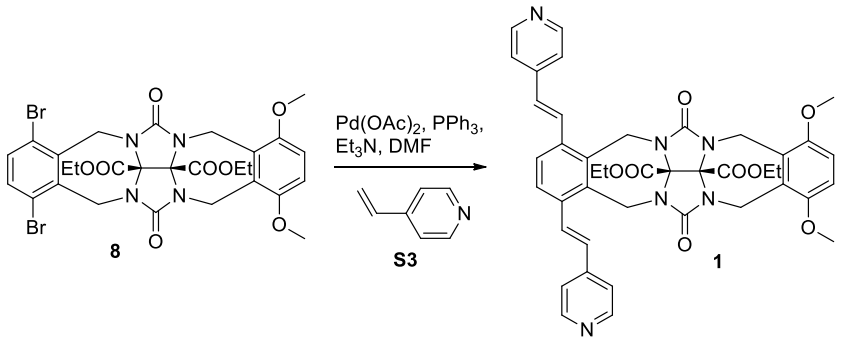
Table of contents **Page**

General Experimental. The reagents and solvents employed were commercially available and used as received without further purification. Dichloromethane was distilled from CaH_2 immediately before use. NEt_3 was distilled from KOH immediately before use. Compound **8** and **9** were prepared according to the reported methods.[1,2] IR spectra were recorded on a Perkin-Elmer PE-983 infrared spectrometer as KBr pellets with absorption in 4000-400 cm^{-1}. NMR spectra were recorded on a Varian Mercury 400 or 600 MHz spectrometer and resonances (δ) are given in parts per million relative to tetramethylsilane (TMS) as internal standard. High resolution mass spectra were obtained on a Bruker Apex-Ultra 7.0T FTMS equipped with an electrospray ionization source (ESI). Melting points were determined using an XT-4 apparatus and were not corrected.

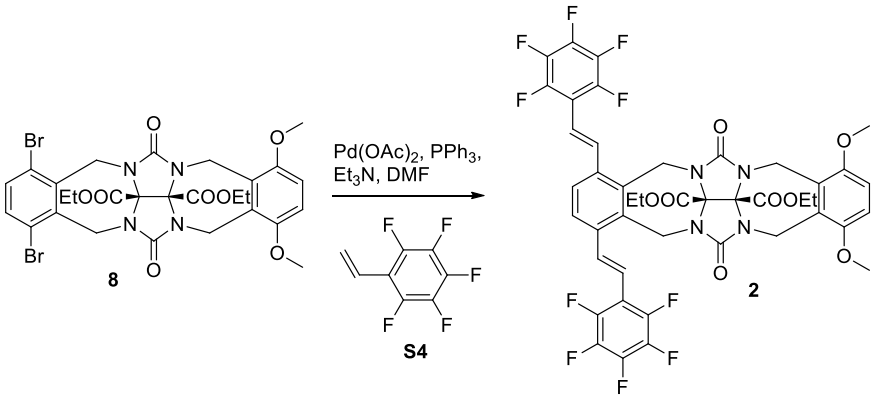
Synthesis and characterization of compounds 1 – 7



Scheme S1. Synthesis of Compounds **1** by Heck coupling.

Experimental procedure for compound 1. To a solution of $Pd(OAc)_2$ (2.3 mg, 0.01 mmol), PPh_3 (6.0 mg, 0.02 mmol) and **8**[1] (142 mg, 0.2 mmol) in freshly distilled Et_3N (5 mL) and DMF (5 mL) under Ar atmosphere at room temperature was added 4-vinylpyridine (63 mg, 0.6 mmol). The mixture was warmed to 110 ˚C for 12 h (monitored by TLC), and then the solvent was removed under reduced pressure. The solid residue was purified by flash chromatography (SiO_2, CH_2Cl_2/CH_3OH, 50:1) to give crude **1** (113 mg, 0.15 mmol, 75%) as a yellow solid. To further purify the crude product, about 2 mL ethyl acetate was added and the solution was vibrated by

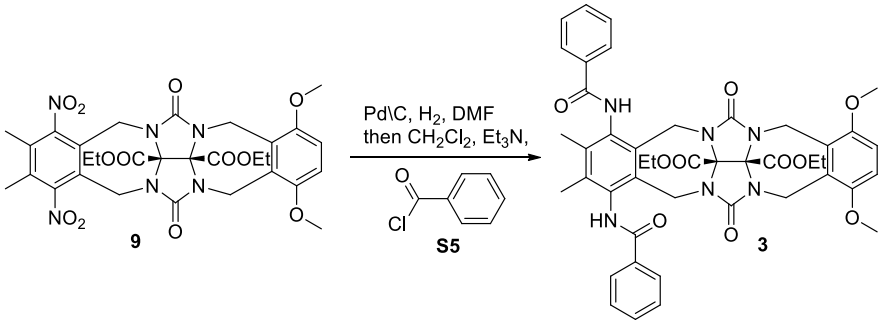
ultrasonic oscillator. Finally, the solvent and the desired solid compound **1** were separated by centrifugation (98 mg, 0.13 mmol, 65%). M.p. > 300 °C. TLC ($CHCl_3$/MeOH 50:1) R_f 0.14. IR (KBr, cm^{-1}): 3420m, 2964w, 1758s, 1717s, 1596s, 1467s, 1433s, 1360w, 1307m, 1258s, 1019m, 943w. ^1H NMR (600 MHz, $CDCl_3$): δ = 8.40 (d, J = 4.8 Hz, 4H), 7.89 (d, J = 16.2 Hz, 2H), 7.33 (d, J = 5.4 Hz, 4H), 6.80 (d, J = 16.2 Hz, 2H), 6.42 (brs, 2H), 6.32 (s, 2H), 5.65 (d, J = 16.2 Hz, 2H), 5.21 (d, J = 16.2 Hz, 2H), 4.31 (q, J = 7.2 Hz, 2H), 4.28-4.24 (m, 4H), 4.18 (d, J = 16.8 Hz, 2H), 3.50 (s, 6H), 1.35 (t, J = 7.2 Hz, 3H), 1.34 (t, J = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ = 166.1, 165.8, 156.4, 150.6, 149.8, 144.8, 135.6, 134.5, 129.9, 129.4, 126.6, 125.7, 120.9, 111.1, 80.7, 79.3, 63.4, 63.2, 55.9, 40.0, 37.1, 14.0, 14.0. HRMS (ESI): *m/z* [M + H]+ calcd for $C_{42}H_{41}N_6O_8$: 757.2980; found: 757.2967.



Scheme S2. Synthesis of Compounds **2** by Heck coupling.

Experimental procedure for compound 2. To a solution of $Pd(OAc)_2$ (2.3 mg, 0.01 mmol), PPh_3 (6.0 mg, 0.02 mmol) and **8** (142 mg, 0.2 mmol) in freshly distilled Et_3N (5 mL) and DMF (5 mL) under Ar atmosphere at room temperature was added 1,2,3,4,5-pentafluoro-6-vinylbenzene (116.4 mg, 0.6 mmol). The mixture was warmed to 110 ˚C for 12 h (monitored by TLC), and then the solvent was removed under reduced pressure. The solid residue was purified by flash chromatography (SiO_2, CH_2Cl_2/CH_3OH, 50:1) to give **2** (134 mg, 0.143 mmol, 72%) as a yellow solid. To further purify the crude product, about 2 mL ethyl acetate was added and the solution was vibrated by ultrasonic oscillator. Finally, the solvent and the desired solid compound **2** was separated by centrifugation (114 mg, 0.122 mmol, 61%). M.p. >

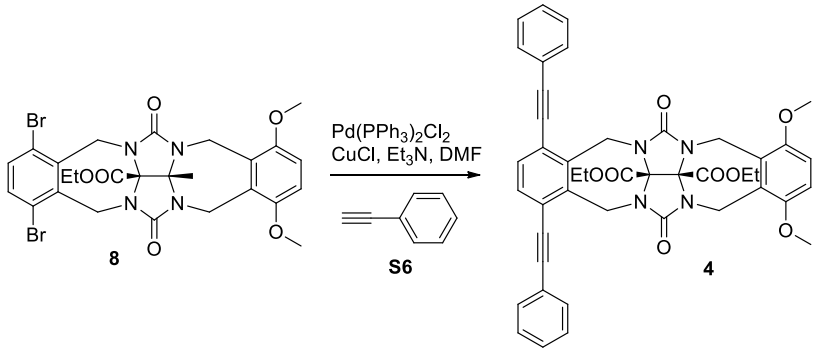
300 °C. TLC ($CHCl_3$/MeOH 50:1) R_f 0.17. IR (KBr, cm^{-1}): 3442w, 2986w, 2360w, 1724s, 1463s, 1259s, 1081m, 917w. ^1H NMR (600 MHz, $CDCl_3$): δ = 8.27 (d, J = 16.8 Hz, 2H), 7.45 (s, 2H), 6.77 (d, J = 16.2 Hz, 2H), 6.66 (s, 2H), 5.17 (d, J = 16.8 Hz, 2H), 4.98 (d, J = 15.0 Hz, 2H), 4.45 (d, J = 15.0 Hz, 2H), 4.28-4.23 (m, 4H), 4.04 (q, J = 7.2 Hz, 2H), 3.69 (s, 6H), 1.31 (t, J = 7.2 Hz, 3H), 1.20 (t, J = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ = 166.1, 165.8, 156.6, 150.9, 137.6, 135.7, 127.0, 125.8, 116.5, 111.9, 80.6, 79.6, 63.4, 63.0, 56.5, 40.5, 37.5, 14.0, 13.9. HRMS (APCI): *m/z* $[M + H]^+$ calcd for $C_{44}H_{33}F_{10}N_4O_8$: 935.2138; found: 935.2133.



Scheme S3. Synthesis of **3** via Pd/H_2 reduction and amide bond formation.

Experimental procedure for compound 3. A mixture of **9**[2] (66.8 mg, 0.10 mmol) and 10% Pd/C (20 mg,) in anh. DMF (5 mL) was stirred under H_2 (10-20 psi) at RT for 5 h. The reaction mixture was filtered under Ar, and concentrated under high vacuum at RT. The residue was dissolved in a mixture of anh. degassed CH_2Cl_2 (10 mL) and Et_3N (0.05 mL, 0.30 mmol). This solution was added to a solution of benzoyl chloride (14 μL, 0.11 mmol) in anh. degassed CH_2Cl_2 (10 mL) at -78 °C. After 15 min., the cooling bath was removed and stirring was continued at RT for 12 h. The reaction mixture was diluted with $CHCl_3$ (200 mL), washed with sat. aq. $NaHCO_3$ dried over anh. $MgSO_4$ and concentrated. Flash chromatography (SiO_2, $CHCl_3$/MeOH, 50:1) gave slightly impure **3** (70 mg, 0.085 mmol, 85%). To get highest purity material, the white solid was washed with EtOAc (1.0 mL), centrifuged, the supernatant decanted, and the residual solid dried under high vacuum yielding **3** (60 mg, 0.073 mmol, 73%). M.p. > 300 °C. TLC ($CHCl_3$/MeOH 50:1) R_f 0.34. IR (KBr, cm^{-1}): 3395m, 3322m, 2999w, 2964w, 2941w, 1759s, 1699s, 1682s, 1600w, 1580w, 1509m, 1470s, 1433s, 1356m, 1254s,

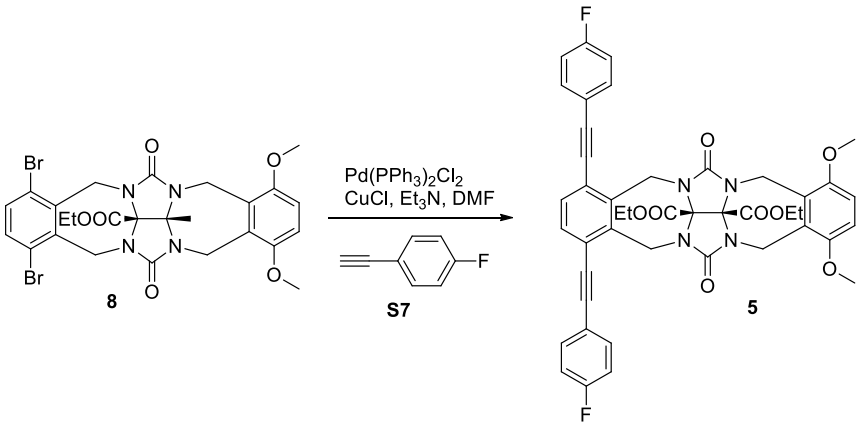
1154m, 1131m, 1079m, 1031w, 1012w, 942w. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.98 (s, 2H), 8.13 (d, J = 6.6 Hz, 4H), 7.58 (m, 2H), 7.53 (t, J = 7.2 Hz, 4H), 6.68 (s, 2H), 5.03 (d, J = 16.2 Hz, 2H), 4.88 (d, J = 15.0 Hz, 2H), 4.52 (d, J = 15.6 Hz, 2H), 4.31 (d, J = 16.2 Hz, 2H), 4.25 (q, J = 7.2 Hz, 2H), 3.99 (q, J = 6.6 Hz, 2H), 3.77 (s, 6H), 2.18 (s, 6H), 1.28 (t, J = 7.2 Hz, 3H), 1.17 (t, J = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ = 165.8, 165.7, 165.5, 157.7, 151.1, 136.6, 133.7, 133.2, 131.9, 131.0, 128.7, 127.5, 125.4, 111.9, 95.3, 80.0, 63.7, 63.1, 56.6, 40.7, 37.7, 16.1, 13.8, 13.7. HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{44}H_{45}N_6O_{10}$: 817.3192, found: 817.3197.



Scheme S4. Synthesis of **4** by Sonogashira coupling.

Experimental procedure for compound 4. To a solution of $Pd(PPh_3)_2Cl_2$ (36 mg, 0.05 mmol), CuI (19 mg, 0.10 mmol) and **8** (354 mg, 0.50 mmol) in freshly distilled Et_3N (2 mL) and DMF (10 mL) under Ar atmosphere at room temperature was added ethynylbenzene (204 mg, 2.0 mmol). The mixture was warmed to 110 ˚C for 12 h (monitored by TLC) and then the solvent was removed under reduced pressure. The solid residue was purified by flash chromatography (SiO_2, CH_2Cl_2/CH_3OH, 50:1) to give **4** (251 mg, 0.335 mmol, 67%) as a white solid. In order to purify the crude product, about 2 mL ethyl acetate was added and the solution was vibrated by ultrasonic oscillator. Finally, the solvent and the desired solid compound **4** were separated by centrifugation (210 mg, 0.28 mmol, 56%). M.p. = 290-291 °C, TLC ($CHCl_3$/MeOH, 50:1) R_f 0.15. IR (KBr, cm^{-1}): 3438w, 2924w, 1725s, 1460s, 1427m, 1258s, 1081m, 757w. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.64 – 7.62 (m, 4H), 7.42 (s, 2H), 7.37 – 7.36 (m, 6H), 6.69 (s, 2H), 5.58 (d, *J* = 15.6 Hz, 2H), 5.06 (d, *J* = 15.6 Hz, 2H), 4.50 (d, J = 15.6 Hz, 2H), 4.42 (d, J = 15.6 Hz, 2H), 4.18 (q, J = 7.2 Hz, 2H), 4.04 (q, J = 6.6 Hz, 2H), 3.77 (s, 6H), 1.29 (t, J = 7.2 Hz, 3H), 1.20 (t, J

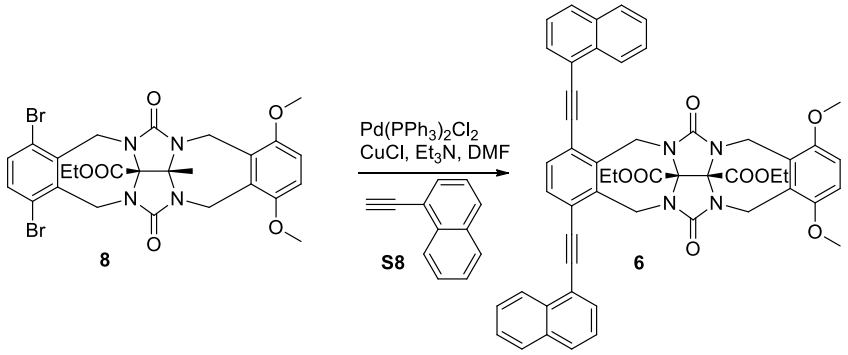
= 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.2 , 166.1 , 156.4, 151.1 , 138.2 , 131.9 , 131.7 , 128.5 , 128.24 , 125.9 , 123.7 , 122.9 , 112.2 , 95.7 , 87.1 , 80.1 , 63.4 , 63.0 , 56.8, 56.7. HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{44}H_{39}N_4O_8$: 751.2748; found: 751.2762.



Scheme S5. Synthesis of compound **5** by Sonogashira coupling.

Experimental procedure for compound 5. To a solution of $Pd(PPh_3)_2Cl_2$ (36 mg, 0.05 mmol), CuI (19 mg, 0.10 mmol) and **8** (354 mg, 0.50 mmol) in freshly distilled Et_3N (2 mL) and DMF (10 mL) under Ar atmosphere at room temperature was added 1-ethynyl-4-fluorobenzene (240 mg, 2.0 mmol). The mixture was warmed to 110 ˚C for 12 h (monitored by TLC) and then the solvent was removed under reduced pressure. The solid residue was purified by flash chromatography (SiO_2, CH_2Cl_2/CH_3OH, 50:1) to give **4** (298 mg, 0.38 mmol, 76%) as a white solid. In order to purify the crude product, about 2 mL ethyl acetate was added and the solution was vibrated by ultrasonic oscillator. Finally, the solvent and the desired solid compound **4** were separated by centrifugation (255 mg, 0.325 mmol, 65%). M.p. = 296-297 °C TLC ($CHCl_3$/MeOH, 50:1) R_f 0.12. IR (KBr, cm^{-1}): 3441w, 2986w, 1727s, 1510s, 1460s, 1427m, 1258s, 839m. ^{1}H NMR (600 MHz, DMSO) δ 7.71-7.69 (m, 4H), 7.44 (s, 2H), 7.33 (t, *J* = 9.0 Hz, 4H), 6.83 (s, 2H), 5.44 (d, *J* = 16.2 Hz, 2H), 5.16 (d, *J* = 16.2 Hz, 2H), 4.55 (d, *J* = 16.2 Hz, 2H), 4.28 (q, *J* = 7.2 Hz, 2H), 4.21 – 4.15 (m, 4H), 3.69 (s, 6H), 1.28 (t, *J* = 7.2 Hz, 3H), 1.22 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 166.1, 164.0, 161.6, 156.4, 151.2, 138.5,

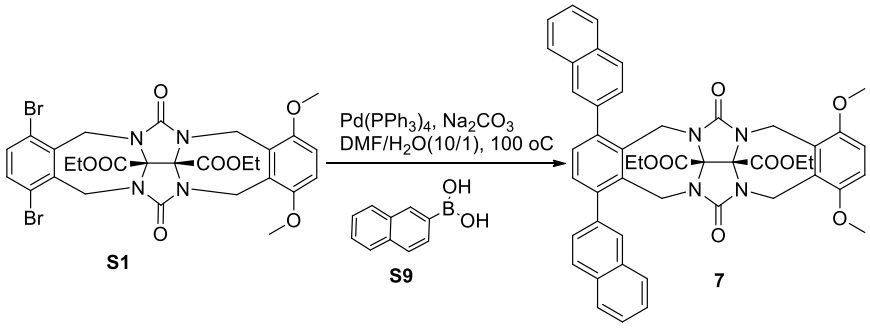
133.8, 133.7, 131.5, 126.1, 123.7, 119.1, 115.8, 115.6, 112.2, 94.7, 86.9, 63.4, 63.0, 56.8, 42.9, 37.6, 14.0, 13.9. HRMS (APCI): *m/z* $[M+H]^+$ calcd for $C_{44}H_{37}F_2N_4O_8$: 787.2572; found: 787.2574.



Scheme S6. Synthesis of compound **6** by Sonogashira coupling.

Experimental procedure for compound 6. To a solution of $Pd(PPh_3)_2Cl_2$ (36 mg, 0.05 mmol), CuI (19 mg, 0.10 mmol) and **8** (354 mg, 0.50 mmol) in freshly distilled Et_3N (2 mL) and DMF (10 mL) under Ar atmosphere at room temperature was added 1-ethynylnaphthalene (304 mg, 2.0 mmol). The mixture was warmed to 110 ˚C for 12 h (monitored by TLC) and then the solvent was removed under reduced pressure. The solid residue was purified by flash chromatography (SiO_2, CH_2Cl_2/CH_3OH, 50:1) to give **4** (314 mg, 0.37 mmol, 74%) as a white solid. In order to purify the crude product, about 2 mL ethyl acetate was added and the solution was vibrated by ultrasonic oscillator. Finally, the solvent and the desired solid compound **4** were separated by centrifugation (280 mg, 0.33 mmol, 66%). M.p. > 300 °C, TLC ($CHCl_3$/MeOH, 50:1) R_f 0.13. IR (KBr, cm^{-1}): 3431w, 2920w, 1758s, 1722s, 1462s, 1425m, 1258s, 1080m, 801m, 774w. ^1H NMR (600 MHz, DMSO) δ 8.54 (d, *J* = 8.4 Hz, 2H), 8.07 (t, *J* = 9.0 Hz, 4H), 7.94 (d, *J* = 7.8 Hz, 2H), 7.72 (t, *J* = 7.8 Hz, 2H), 7.68 – 7.65 (m, 3H), 7.62 (t, *J* = 7.2 Hz, 2H), 6.81 (s, 2H), 5.61 (d, *J* = 16.2 Hz, 2H), 5.21 (d, *J* = 16.2 Hz, 2H), 4.70 (d, *J* = 16.2 Hz, 2H), 4.30 (q, *J* = 6.6 Hz, 2H), 4.22 (q, *J* = 6.6, 7.3 Hz, 2H), 4.18 (d, *J* = 16.2 Hz, 2H), 3.68 (s, 6H), 1.29 (t, *J* = 7.2 Hz, 3H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR could not be obtained even with 12 h acquisition time because of

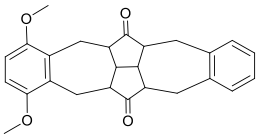
the low solubility of compound **6**. HRMS (APCI): *m/z* $[M+H]^+$ calcd for $C_{52}H_{43}N_4O_8$: 851.3082; found: 851.3075.



Scheme S7. Synthesis of compound **7** by Suzuki coupling.

Experimental procedure for compound 7. To a solution of $Pd(PPh_3)_4$ (35 mg, 0.03 mmol), Na_2CO_3 (106 mg, 1 mmol) and **S1** (142 mg, 0.20 mmol) in DMF (10 mL) and H_2O (1 mL) under Ar atmosphere at room temperature was added naphthalen-2-ylboronic acid (103 mg, 0.60 mmol). The mixture was warmed to 100 ˚C for 2 h (monitored by TLC) and then the solvent was removed under reduced pressure. The solid residue was purified by flash chromatography (SiO_2, Petroleum ether b.p. 60-90 ˚C/EtOAc, 40:1) to give **7** (144 mg, 0.18 mmol, 90%) as a white solid. M.p. = 197-198 °C. TLC (Petroleum ether b.p. 60-90 ˚C/EtOAc 40:1) R_f 0.14. IR (KBr, cm^{-1}): 3446m, 2987w, 1722s, 1463s, 1430m, 1238s, 1082m, 821w, 481w. ^1H NMR (600 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.91 – 7.89 (m, 6H), 7.69 (s, 2H), 7.53 – 7.52 (m, 4H), 7.44 (s, 2H), 6.80 (s, 2H), 5.39 (d, *J* = 15.6 Hz, 2H), 4.79 (d, *J* = 14.4 Hz, 2H), 4.48 (d, *J* = 12.0 Hz, 2H), 4.18 – 4.12 (m, 4H), 3.89 (q, *J* = 7.2 Hz, 3H), 3.82 (s, 6H), 1.28 (t, *J* = 6.6 Hz, 2H), 1.04 (t, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.4, 166.0, 157.1, 151.3, 142.2, 137.6, 133.1, 132.5, 132.4, 130.5, 128.2, 128.1, 128.0, 127.6, 127.2, 126.6, 126.2, 126.1, 112.7, 81.6, 79.3, 63.3, 63.1, 57.1, 43.6, 37.3, 13.9, 13.8. HRMS (APCI): *m/z* $[M + H]^+$ calcd for $C_{48}H_{43}N_4O_8$: 803.3077; found: 803.3075.

CSD search [CSD version 5.35 updates (May 2014)]



Total	monomer	dimer	
		in-in	out-out
36	13	22	0

Details :

CSD refcodes	packing	motif	CSD refcodes	packing	motif
AKAGUO	dimer	in-in	UFONUZ	dimer	in-in
AKAHAV	dimer	in-in	CIDSIS	monomer	
HAHDOJ	monomer		CIDSOY	dimer	in-in
HEBYAP	monomer		CIDSUE	dimer	in-in
JISDEU	monomer		CIDTAL	dimer	in-in
JISDEU10	monomer		CIDTEP	dimer	in-in
LANWAY[a]			CIDTIT	dimer	in-in
MUTFAI	dimer	in-in	HIRSIL	dimer	in-in
QIQDAV	dimer	in-in	KEKREY	dimer	in-in
ROBWEK	dimer	in-in	KEKSEZ	dimer	in-in
ROBWEK01[a,b]	dimer	in-in	KEKSID	dimer	in-in
SURDUE	monomer		KEKSOJ	dimer	in-in
VOKGUX	monomer		XEVCAD	monomer	
CURSIS	monomer		HEBYAP	monomer	
CURSOY	dimer	in-in	AKAGUO	dimer	in-in
CURSUE	dimer	in-in	AKAHAV	dimer	in-in
DIYYEQ	monomer		MUTFAI	dimer	in-in
OFOXEN	monomer		ROBWEK01	monomer	

[a]No structure available in CSD searched result, [b]the packing structure was according to the reference (*Recl. Trav. Chim. Pays-Bas,* **1993**, *112*, 404-406).

References.

1) Wang, Z.; Wang, Y.; Yin, G.; Wu, A. X. *J. Chem. Crystallogr.* **2008**, 38, 591-594.

2) Liu, Q.; Wang, J.; Zhao, G. *J. Chem. Crystallogr.* **2012**, *42*, 727-732.

Details of the refinements of 1 – 7

For **1**: In the refinement, the two chloroform solvent molecule (C43-Cl1-Cl2-Cl3 and C44-Cl4-Cl5-Cl6) were found to be disordered over two sites. The commands DFIX and EADP were used in the refinement to restrain some distances (e.g. C43-Cl1=1.73(1) Å) and thermal factors. The final most satisfactory occupancies for the C43, C44-involved chloroform were 0.57: 0.43 and 0.86:0.14 for the major and minor components, respectively.

For **4**: In the refinement, one of the ethoxy groups (C29-C30) was found to be disordered. The commands DFIX, and EADP were used in the refinement to restrain some distances (eg. C29-C30=1.51(1) Å and C29-O4=1.45(1) Å) and thermal factors. The final most satisfactory occupancies for the C29-, C29'-involved ethoxy were 0.51:0.49 for the major and minor components.

For **5**: In the refinement, one of the ethoxy groups (C34-C35) was found to be disordered. The commands DFIX, and EADP were used in the refinement to restrain some distances (eg. C34-C35=1.51(1) Å and thermal factors. The final most satisfactory occupancies for the C34-, C34'-involved ethoxy were 0.50:0.50 for the major and minor components. One of three dichloromethane (C46) was disordered. The commands DFIX, and EADP were used in the refinement to restrain some distances (eg. C46-Cl5=1.73(1) Å and Cl5-Cl6=2.90(1) Å) and thermal factors. The final most satisfactory occupancies for the C46-, C46'-involved ethoxy were

0.46:0.54 for the major and minor components.

For **6**: In the refinement, one of the ethoxy groups (C13-C14) was found to be disordered. The command DFIX was used in the refinement to restrain some distances (eg. C13-C14=1.51(1) Å and C13-O6=1.51(1) Å) and thermal factors. The final most satisfactory occupancies for the C13-, C13'-involved ethoxy were 0.68:0.32 for the major and minor components.

For **7**: In the refinement, one of the ethoxy groups (C37-C38) was found to be disordered. The command DFIX was used in the refinement to restrain some distances (eg. C37-C38=1.48 Å and C37-O6=1.38 Å) and thermal factors. The final most satisfactory occupancies for the C13-, C13'-involved ethoxy were 0.67:0.33 for the major and minor components. One chloroform solvent moleculer (C49-Cl1-Cl2-Cl3) wase found to be disordered over two sites. The command DFIX was used in the refinement to restrain some distances (eg. C43-Cl1=1.73 Å) and thermal factors. The final most satisfactory occupancies for the C49, C49'-involved chloroform were 0.87: 0.13 for the major and minor components. The naphthalene ring (C17-C26) was found to be disordered. The command DFIX was used in the refinement to restrain some distances (eg. C19- C24=2.42 Å and C19-C23=1.39 Å) and thermal factors. The final most satisfactory occupancies for the C19-, C19'-involved ethoxy were 0.80:0.20 for the major and minor components.

Table S1. Crystallographic Data and Structure Refinement Details for **1–7.**

empirical formula	**1**	**2**	**3**	**4**	**5**	**6**	**7**
CCDC deposition number	992389	992390	992391	992392	992393	992394	996879
formula	$C_{44}H_{42}N_6O_8Cl_6$	$C_{45}H_{33}N_4O_8F_{10}Cl_3$	$C_{46}H_{46}Cl_6N_6O_{10}$	$C_{45}H_{39}N_4O_8Cl_3$	$C_{47}H_{41}F_2N_3O_{8.5}Cl_3$	$C_{53.5}H_{43.5}N_4O_8Cl_{4.5}$	$C_{49}H_{43}N_4O_8Cl_3$
formula weight	995.54	1054.10	1055.59	870.15	928.18	1029.95	922.22
crystal system	Triclinic	Triclinic	Triclinic	Monoclinic	Triclinic	Triclinic	Triclinic
space group	P-1	P-1	P-1	P2(1)/n	P-1	P-1	P-1
a (Å)	10.7259(9)	10.8333(15)	11.0037(13)	11.1774(14)	12.9379(12)	13.1674(15)	10.9368(13)
b (Å)	14.2208(12)	14.2199(19)	13.2032(14)	13.9112(18)	13.0294(12)	13.8587(16)	14.8456(18)
c (Å)	14.8907(12)	15.066(2)	17.428(3)	26.663(3)	15.7092(14)	13.8587(16)	15.7583(19)
α (deg)	92.5080(10)	93.122(2)	89.128(2)	90.00	114.0830(10)	64.005(2)	71.070(2)
β (deg)	93.7200(10)	108.057(2)	76.376(2)	97.601(2)	111.3440(10)	85.984(2)	89.029(2)
γ (deg)	98.8250(10)	99.045(2)	72.207(11)	90.00	76.410(2)	67.813(2)	69.365(2)
Z	2	2	2	4	2	2	2
V($Å^3$)	2236.3(3)	2166.0(5)	2338.6(5)	4109.4(9)	2182.1(3)	2363.3(5)	2251.2(5)
Dcalcd(g cm^{-3})	1.478	1.616	1.499	1.406	1.413	1.447	1.361
μ (Mo Kα) (mm^{-1})	0.445	0.316	0.433	0.284	0.278	0.341	0.263
F(000)	1028	1072	1092	1808	962	1066	960
temp (K)	100(2)	100(2)	100(2)	220(2)	100(2)	100(2)	296(2)
θ min−max (deg)	2.22, 20.81	1.43, 25.50	1.96, 25.01	1.54, 16.19	1.74, 22.69	1.46, 23.09	1.37, 23.89
tot., unique data	13370，4582	15848, 7961	14575, 8145	9219, 2050	12070, 5719	13815, 6542	14305, 6825
R(int)	0.0315	0.0331	0.1022	0.0373	0.0251	0.0626	0.0335
obsd data [I > 2σ(I)]	3740	5667	6350	1700	4676	5135	3976
Nref, Npar	4582, 643	7961, 636	8145, 619	2050, 553	5719, 631	6542, 691	6825, 723
R1,wR2 (all data)	0.0782, 0.1951	0.0876, 0.1893	0.1276, 0.2575	0.0489, 0.1040	0.0671, 0.1746	0.0965, 0.2403	0.1059, 0.1818
S	1.080	1.157	1.135	1.077	1.051	1.042	1.033
min and max resd dens (e $Å^{-3}$)	-0.727, 0.882	-0.595, 0.824	-1.183, 1.700	-0.204, 0.308	-0.530, 0.642	-0. 948, 0.962	-0.333, 0.362

Table S2. C-H---π interactions in the packing of **1** and **2**

C-H---π Interactions				
	C-H→R(j)	H---R (Å)	∠C-H---R (°)	C---R (Å)
1[a]	C(33)-H(33B)→R(C35-40)□	2.88	161	3.833(5)
2[b]	C(36)-H(36A)→R(C37-42)□	2.75	148	3.632(3)

[a]Symmetry codes: (□) 2-X, 1-Y, 1-Z; [b]Symmetry codes: (i) 1-X, -Y, 1-Z.

^{1}H and ^{13}C NMR Recorded for Compounds 1 – 7.

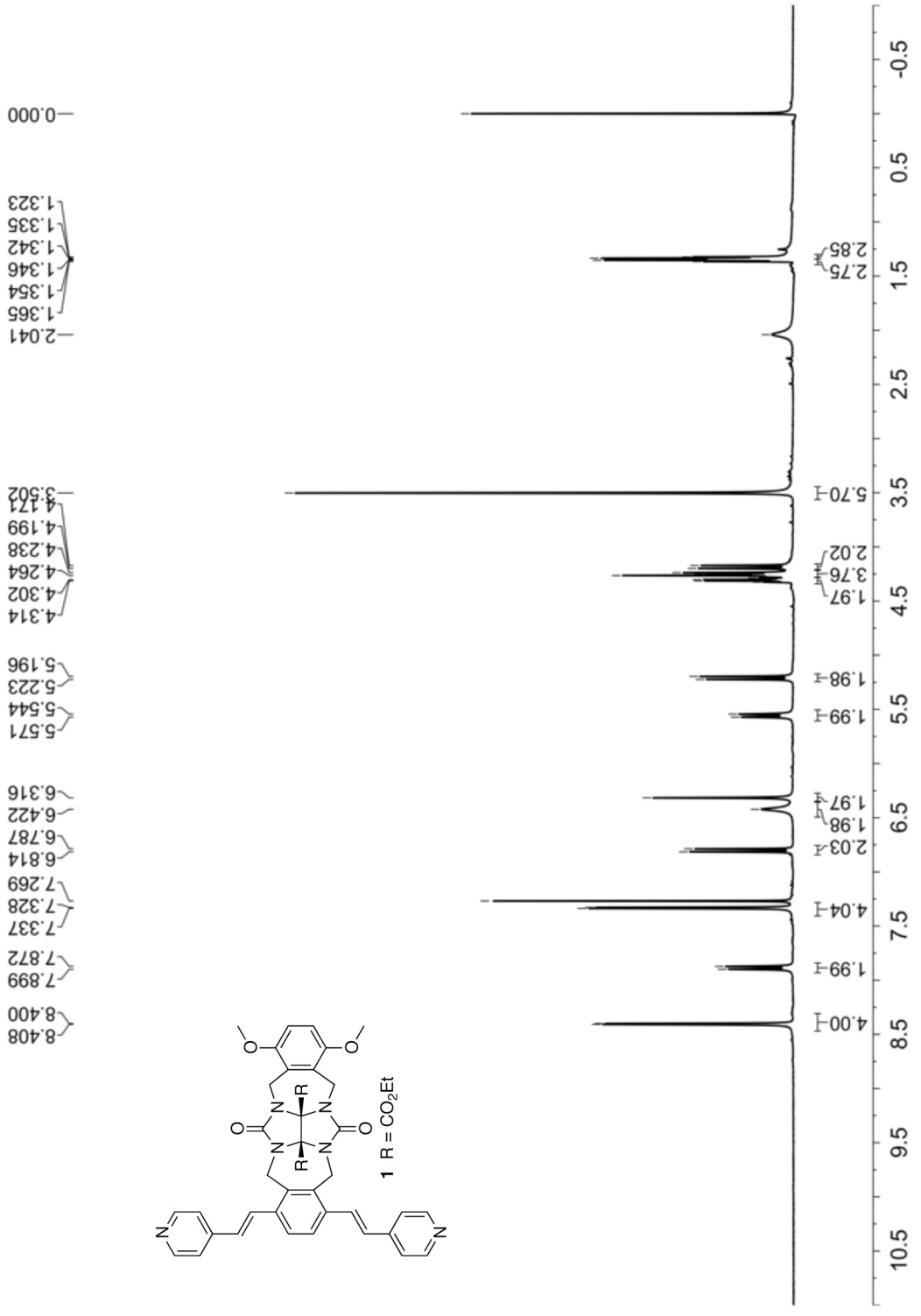


Figure S1. ^{1}H NMR spectrum recorded (600 MHz, $CDCl_3$, RT) for compound **1**.

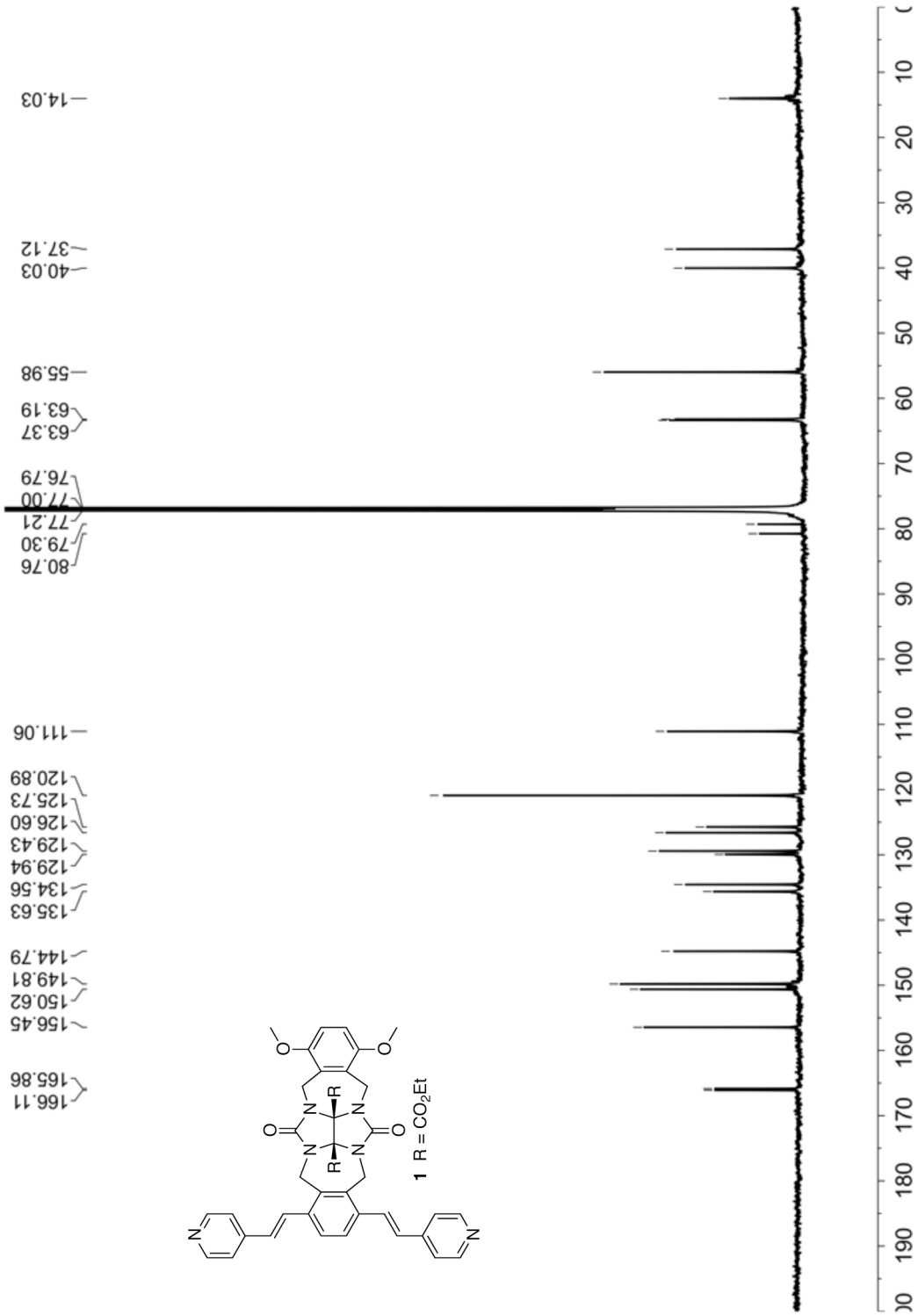


Figure S2. ^{13}C NMR spectrum recorded (150 MHz, $CDCl_3$, RT) for compound **1**.

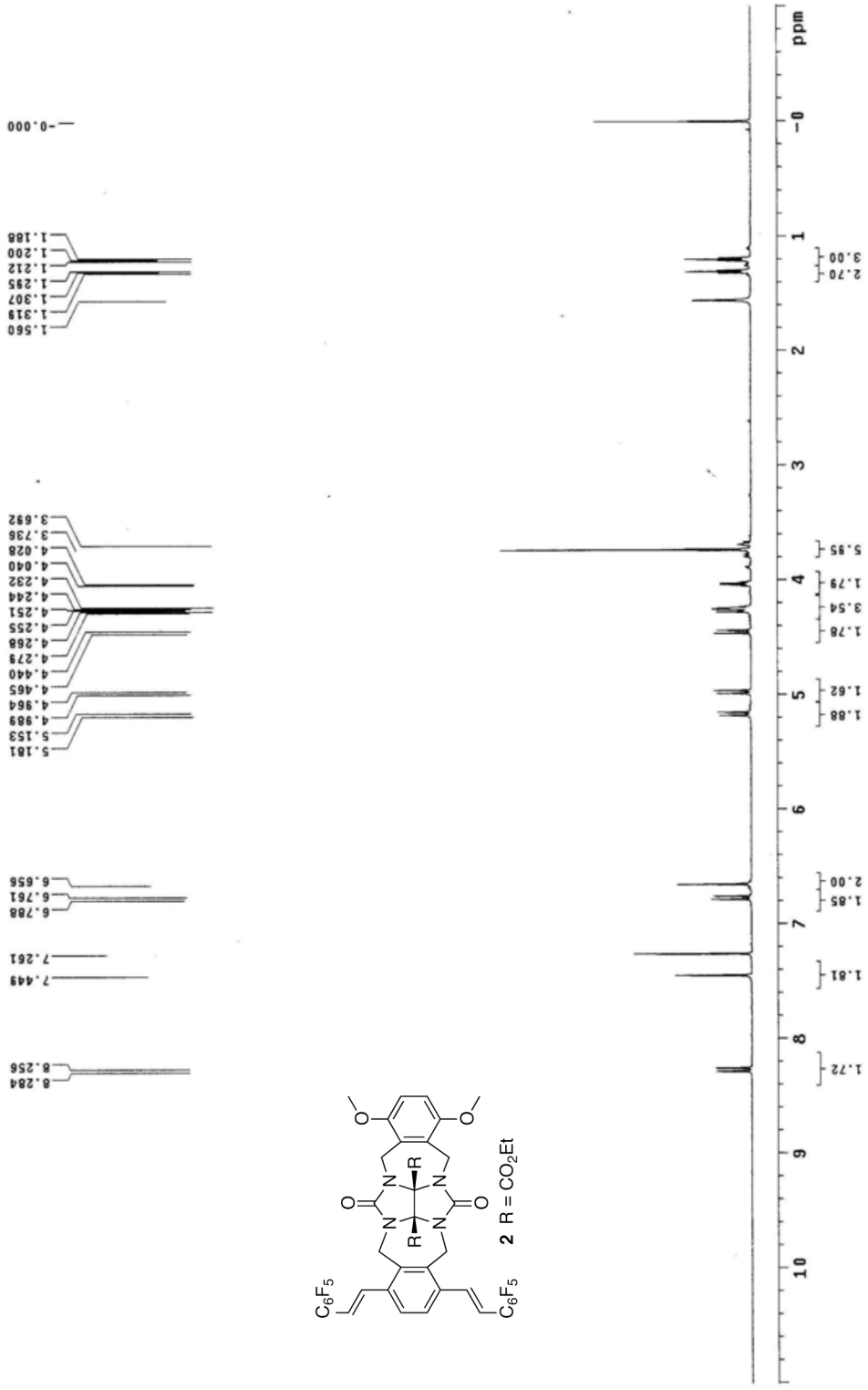


Figure S3. ^{1}H NMR spectrum recorded (600 MHz, $CDCl_3$, RT) for compound **2**.

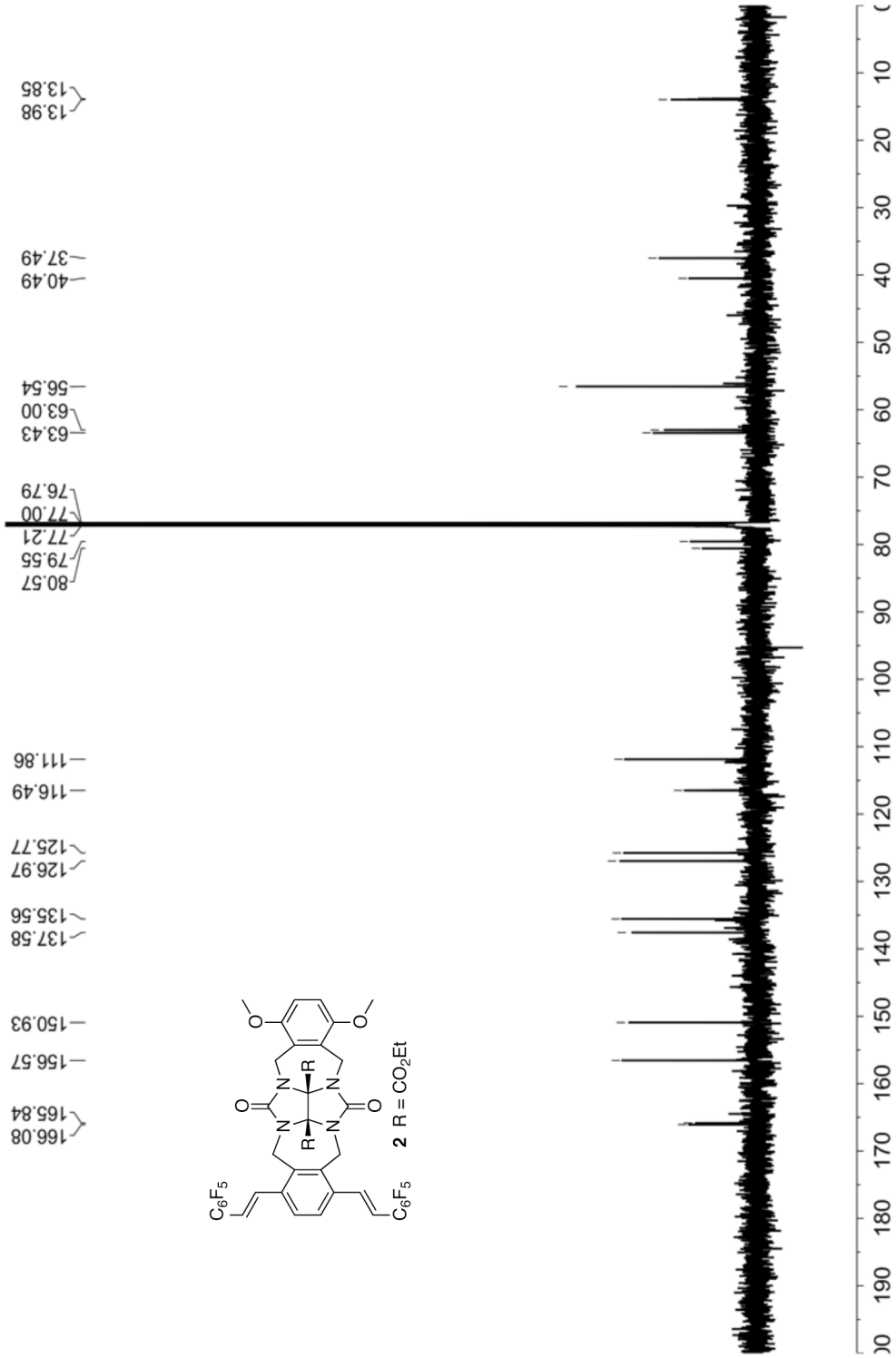


Figure S4. ^{13}C NMR spectrum recorded (150 MHz, $CDCl_3$, RT) for compound **2**.

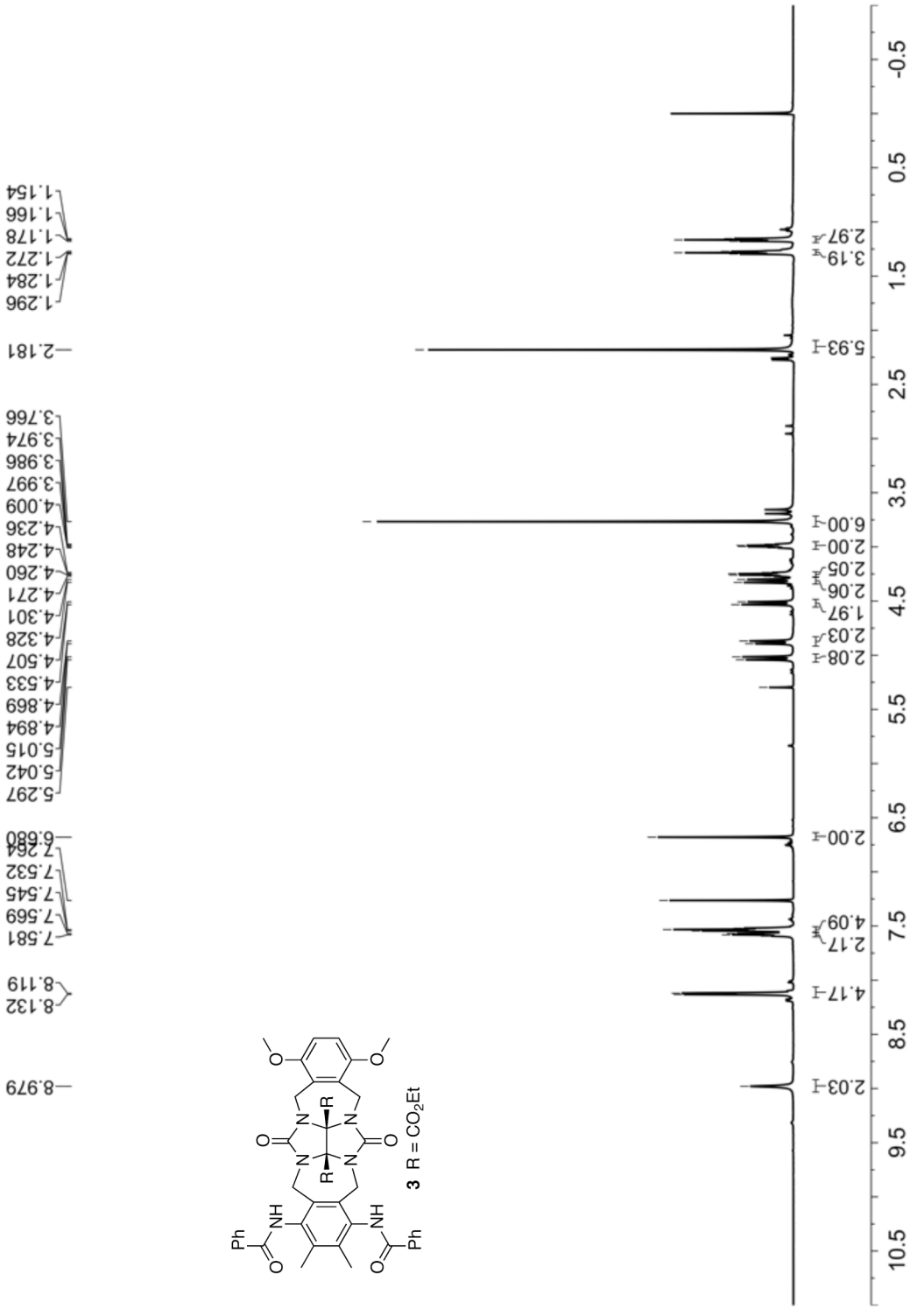


Figure S5. ^{1}H NMR spectrum recorded (600 MHz, $CDCl_3$, RT) for compound **3**.

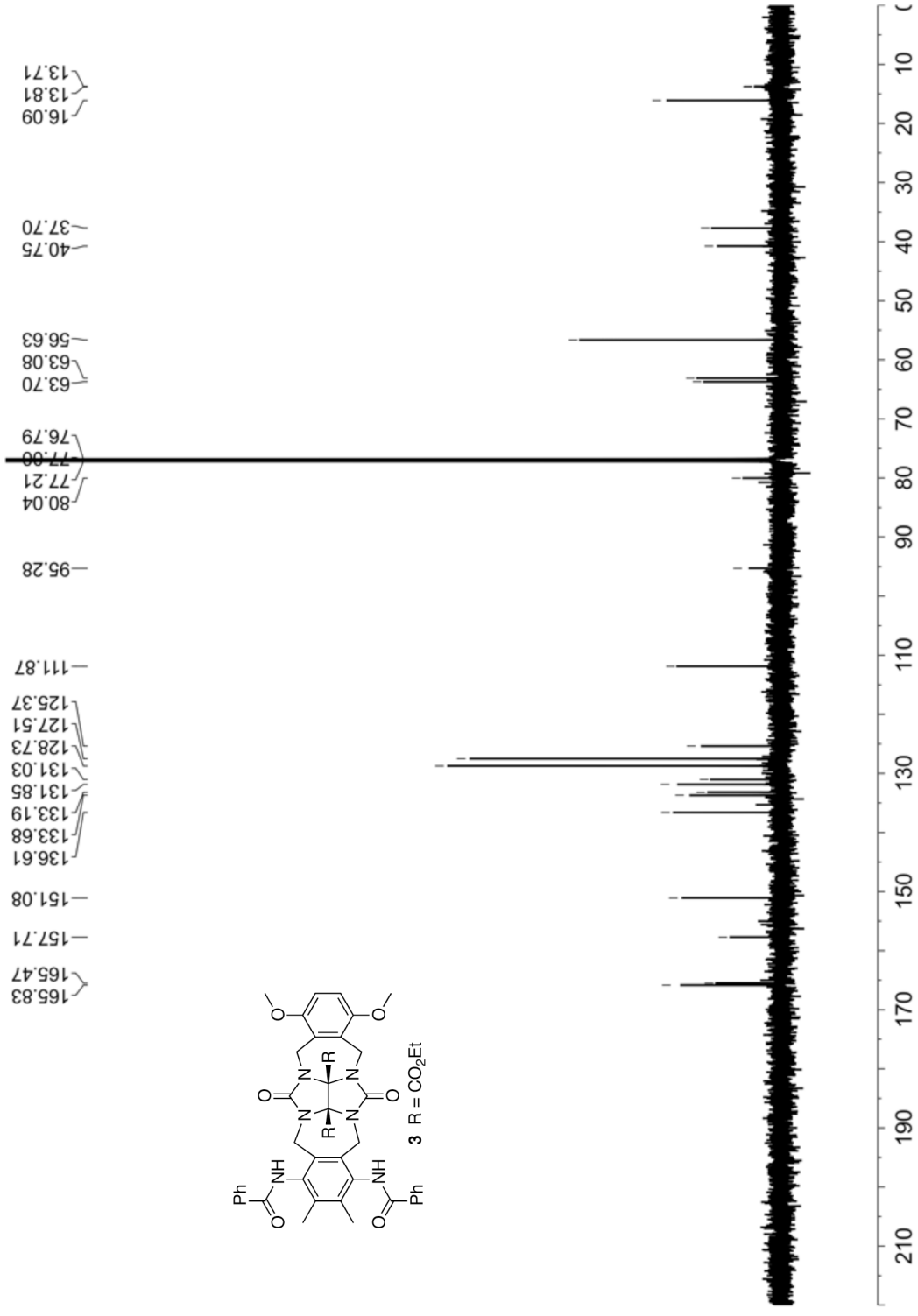


Figure S6. ^{13}C NMR spectrum recorded (150 MHz, $CDCl_3$, RT) for compound **3**.

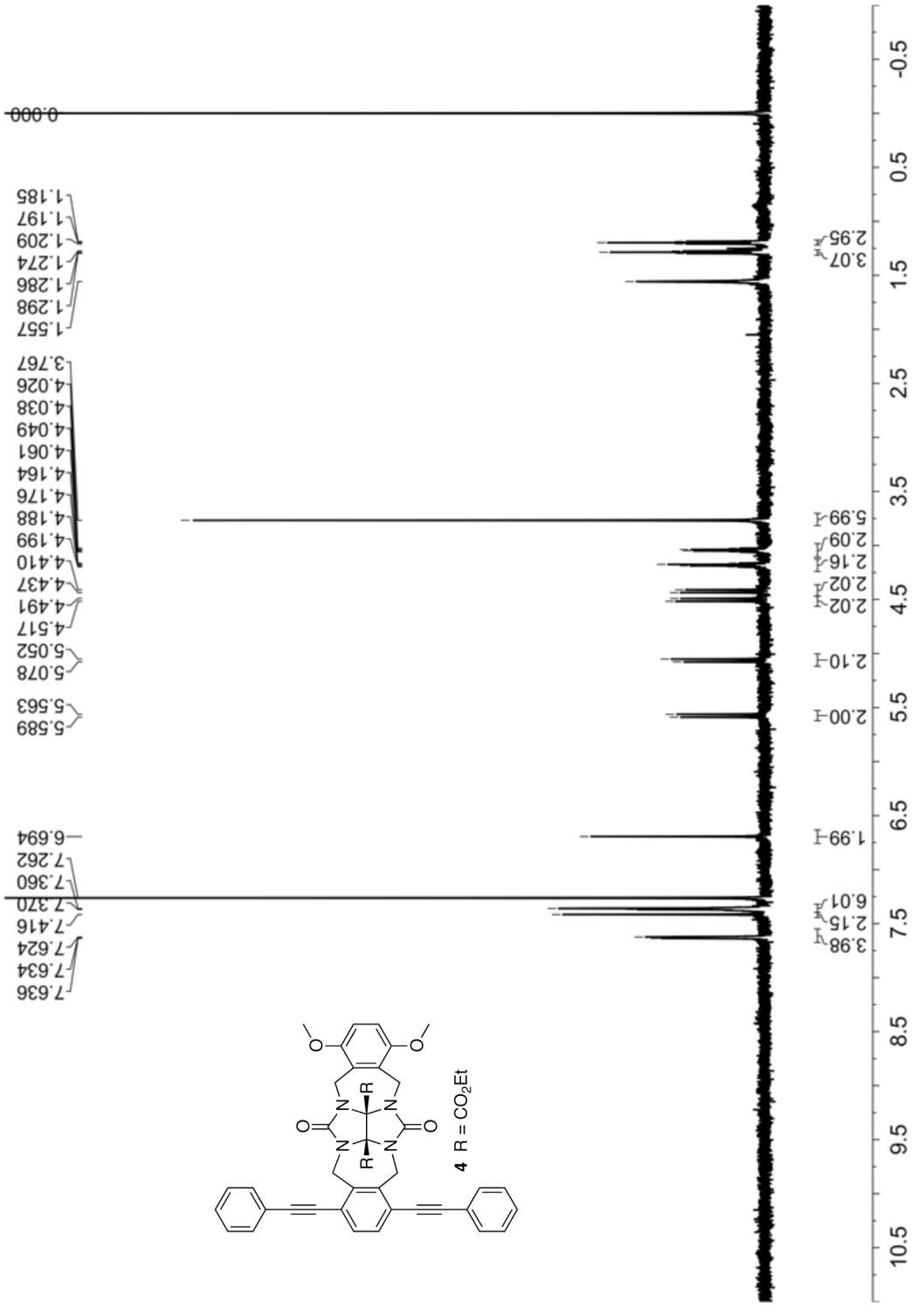


Figure S7. ^{1}H NMR spectrum recorded (600 MHz, $CDCl_3$, RT) for compound **4**.

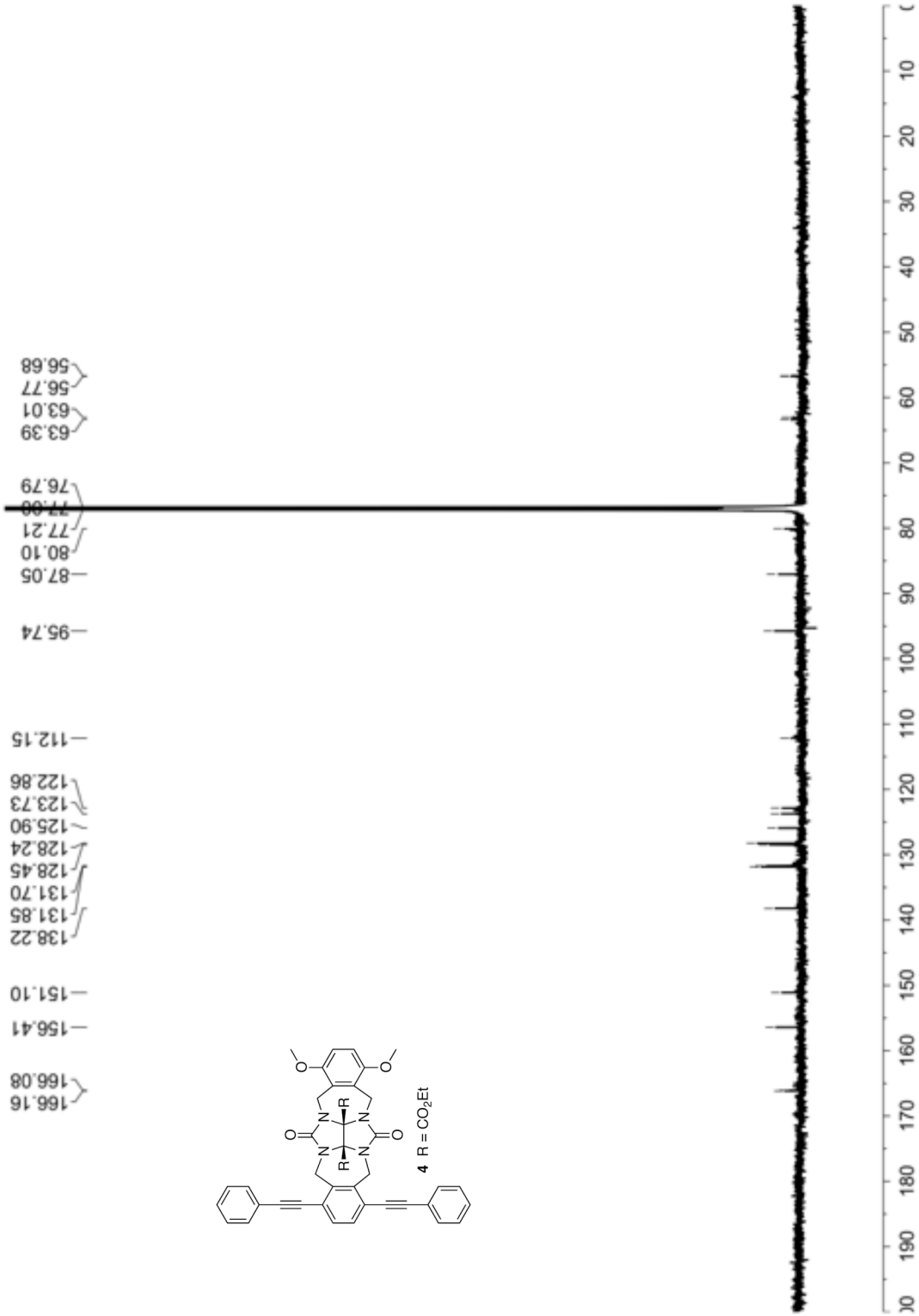


Figure S8. ^{13}C NMR spectrum recorded (150 MHz, $CDCl_3$, RT) for compound **4**.

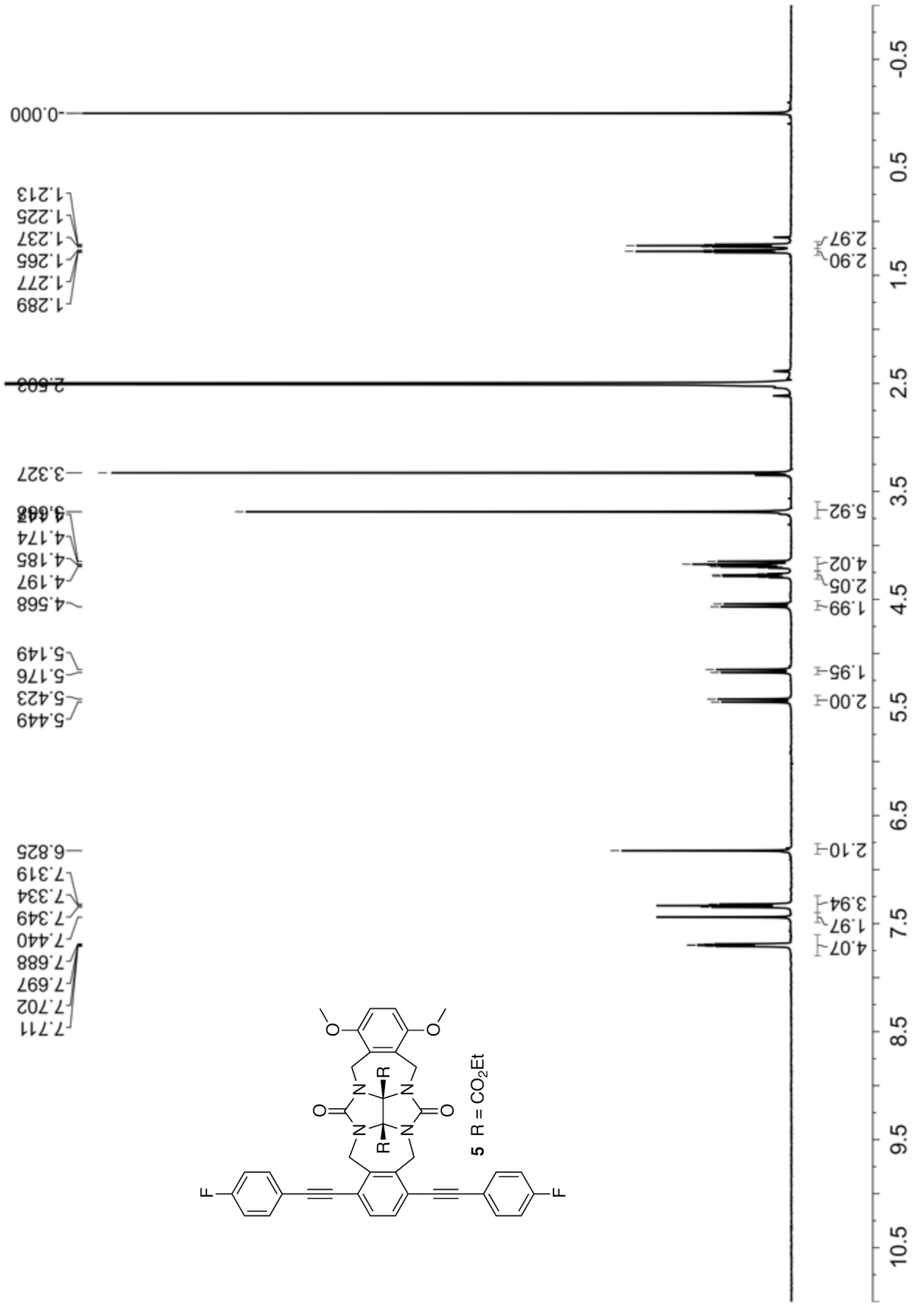


Figure S9. ^{1}H NMR spectrum recorded (600 MHz, DMSO, RT) for compound **5**.

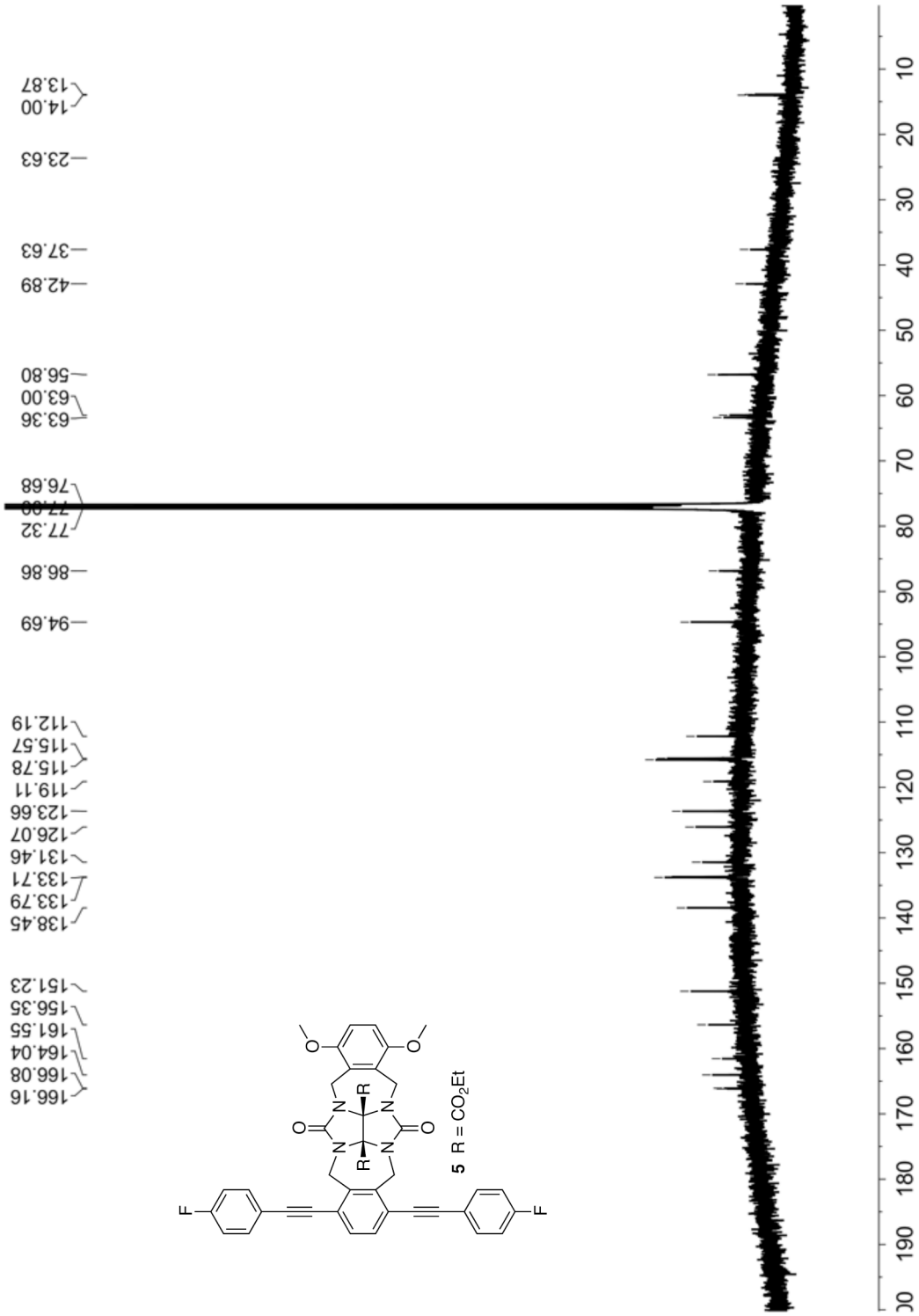


Figure S10. ^{13}C NMR spectrum recorded (150 MHz, $CDCl_3$, RT) for compound **5**.

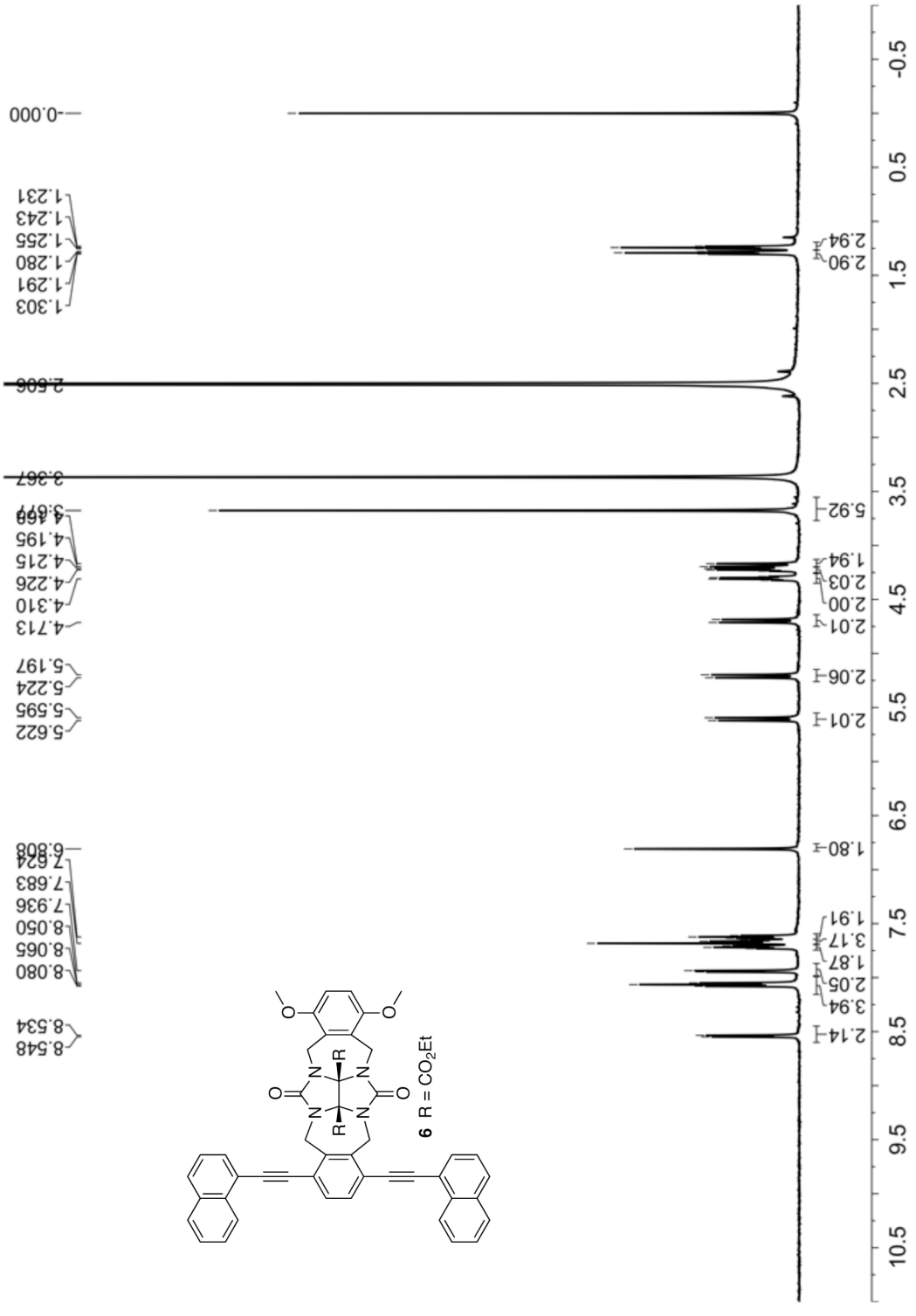


Figure S11. ^{1}H NMR spectrum recorded (600 MHz, DMSO, RT) for compound **6**.

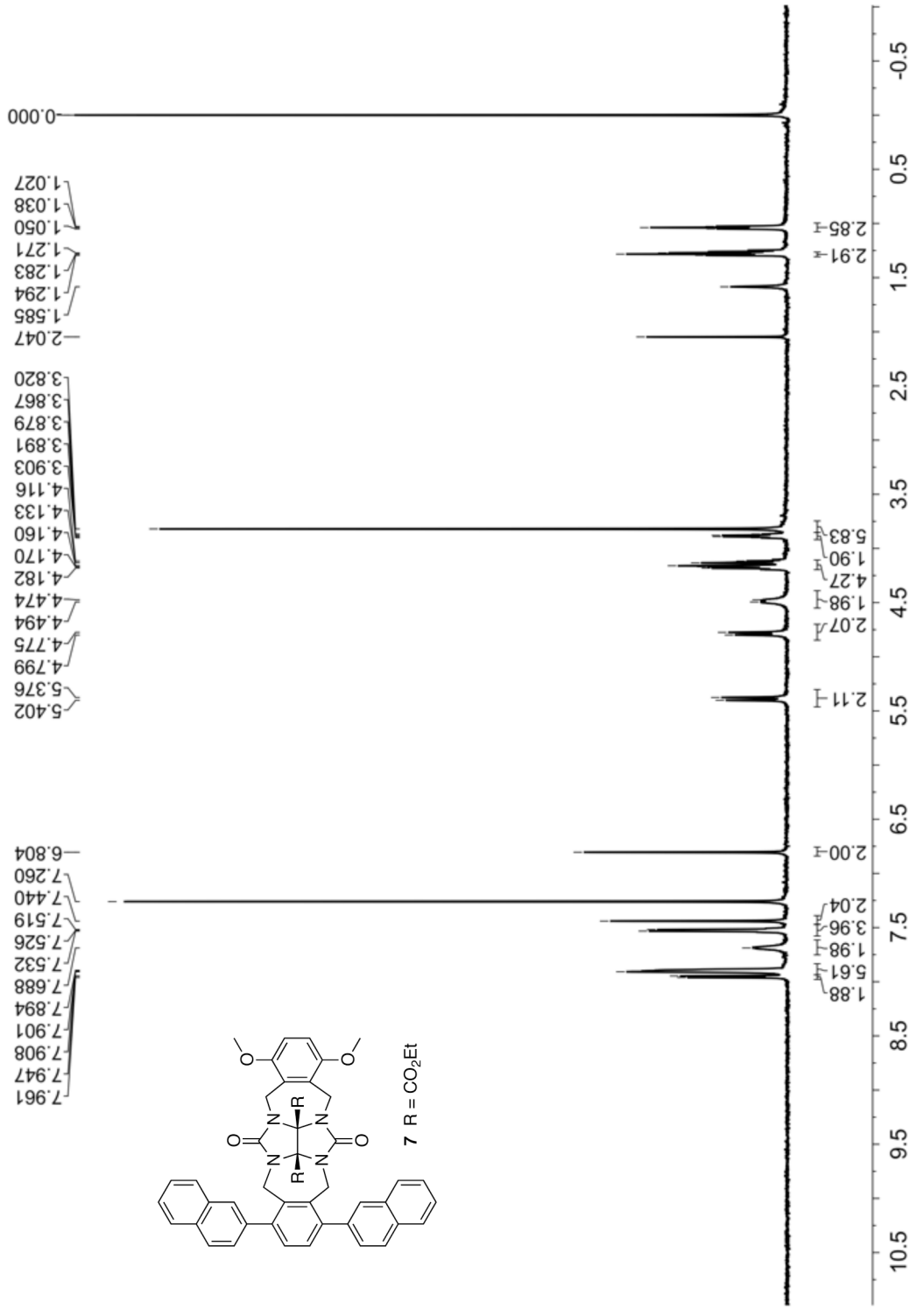


Figure S12. ^{1}H NMR spectrum recorded (600 MHz, $CDCl_3$, RT) for compound **7**.

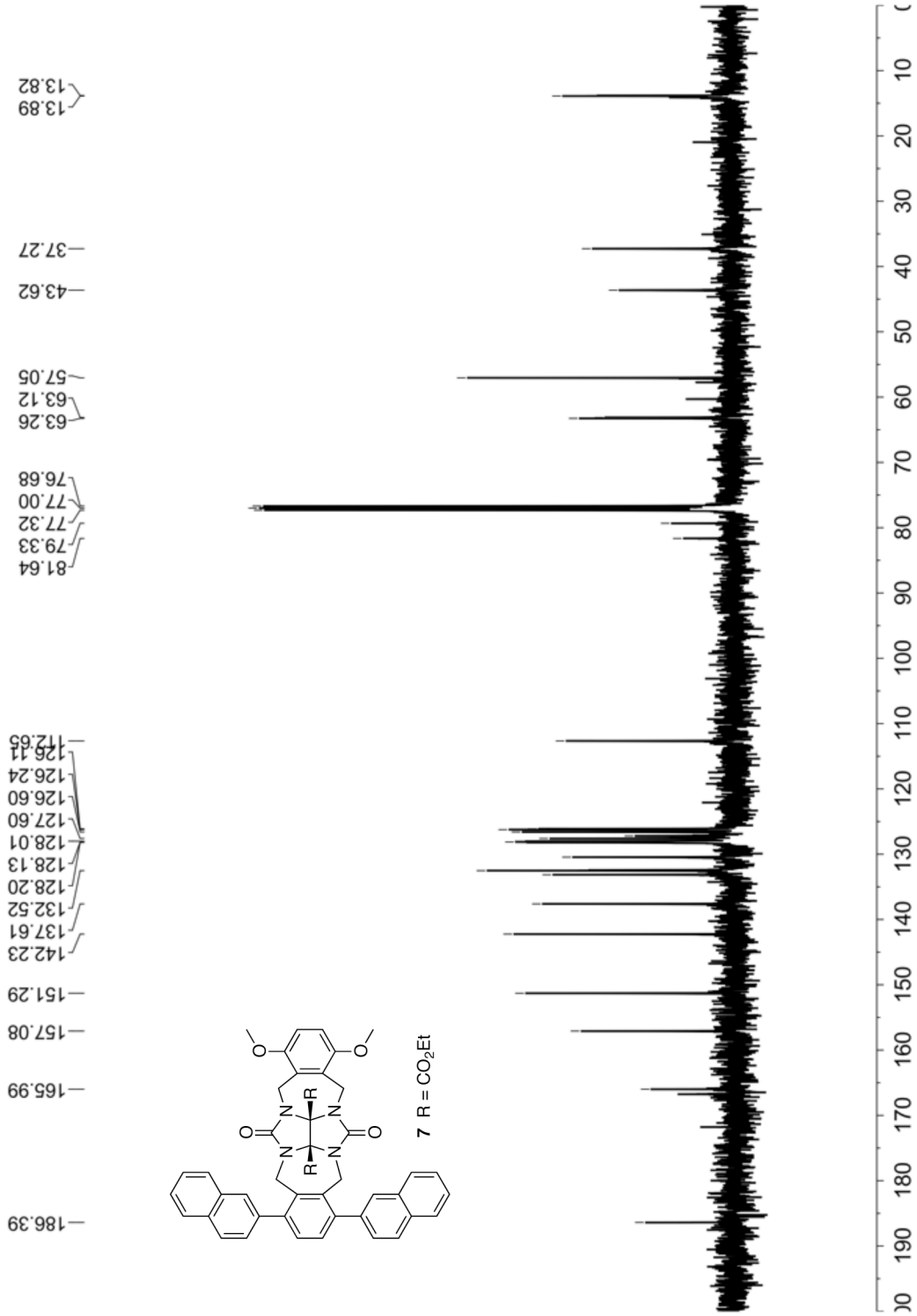


Figure S13. ^{13}C NMR spectrum recorded (100 MHz, $CDCl_3$, RT) for compound **7**.