Supporting Information

Perfect symmetrical cyclic aromatic trimer motif in tripodal molecule

Shankar Deval Sathiyashivan, Chakka Kiran Kumar, Bhaskaran Shankar, Malaichamy Sathiyendiran and Dhanraj T. Masram

Department of Chemistry, University of Delhi 110 007, India
School of Chemistry, University of Hyderabad, Hyderabad 500 046, India

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General experimental methods

o-phenylenediamine, *p*-anisaldehyde, 3,4-dimethoxybenzaldehyde, 3,4,5-trimethoxybenzaldehyde, $NaHSO_3$, sodium hydride (NaH), 1,3,5-tris(bromomethyl)benzene, 1,3,5-tris(bromomethyl)-2,4,6-trimethylbenzene, 1,3,5-tris(bromomethyl)-2,4,6-triethylbenzene, tetrahydrofuran (THF) and dimethylformamide (DMF) were purchased from commercial sources and used as received. 2-(4-methoxyphenyl)benzimidazole (L^1), 2-(3,4-dimethoxyphenyl)benzimidazole (L^2) and 2-(3,4,5-trimethoxyphenyl)benzimidazole (L^3) were prepared according to previously reported methods.[3] All reactions were carried out in inert atmosphere. NMR spectra were recorded on Bruker Avance III 400 and 500 MHz instruments. The chemical shifts (δ) were reported in parts per million (ppm) relative to residual solvent signal. HR-MS were recorded on a Bruker maXis mass spectrometer. Elemental analysis was performed on a Flash EA series 1112 CHNS analyzer.

General procedure for the synthesis of tripodal molecules

To a solution of 2-substituted benzimidazole derivative (L^1-L^3, 1.0 equiv.) in dry THF at 0^0C, NaH (1.2 equiv.) was added and allowed stir at room temperature for 1 h. To this solution, solid tribromo compound was added and allowed to stir for 72 h at 40-45 °C. The progress of the reaction was monitored by TLC. After completion of reaction, the solvent was removed under reduced pressure and ice water was added to the resulting mixture. The precipitated solid was collected by filtration under vacuum, washed with hexane and air dried.

1,3,5-Tris(2-(4-methoxyphenyl)benzimidazol-1-ylmethyl)benzene (1): According to general procedure, 176 mg of product was prepared from L^1 (188.5 mg, 0.8405 mmol), NaH (24.0 mg, 1.0 mmol), 1,3,5-tris(bromomethyl) benzene (100 mg, 0.2802 mmol) and obtained as white solid. Yield: 80%. ^{1}H-NMR (500 MHz, d_6-DMSO, ppm): δ 7.69 (d, 3H, J_{HH} = 7.9 Hz, H^4), 7.28-7.23 (m, 9H, H^5 & $H^{a,d}$), 7.20-7.13 (m, 6H, $H^{b,c}$), 6.58 (m, 6H, $H^{6,7}$), 6.58 (s, 3H, arene), 5.31 (s, 6H, -CH_2-) and 3.77 (s, 9H, -OCH_3). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 160.91, 153.92, 143.10, 138.78, 135.71, 130.52, 123.63, 122.96, 122.78, 121.95, 120.00, 114.43, 114.23, 109.92 (aromatic), 55.40 (-OCH_3) and 47.99 (-CH_2-). HR-MS (*m/z*): Calc. for $C_{51}H_{43}N_6O_3$ $(M+H)^+$: 787.3397; found, 787.3401. Anal. Calc. for $C_{51}H_{42}N_6O_3$: C, 77.84; H, 5.38; N, 10.68 Found: C, 77.93; H, 5.32; N, 10.59.

1,3,5-Tris(2-(4-methoxyphenyl)benzimidazol-1-ylmethyl)-2,4,6-trimethylbenzene (2): According to general procedure, 136 mg of product was prepared from L^1 (168.6 mg, 0.7511 mmol), NaH (22.0 mg, 0.9013 mmol), 1,3,5-tris(bromomethyl)-2,4,6-trimethylbenzene (100 mg, 0.2506 mmol) and obtained as white solid. Yield: 66%. ^{1}H-NMR (500 MHz, d_6-DMSO, ppm): δ 7.71 (d, 6H, J_{HH} = 8.7 Hz, $H^{a,d}$), 7.57 (d, 3H, J_{HH} = 7.9 Hz, H^4), 7.11-7.06 (m, 9H, H^5 & $H^{b,c}$), 6.63 (t, 3H, J_{HH} = 7.7 Hz, H^6), 6.31 (d, 3H, J_{HH} = 8.2 Hz, H^7), 5.47 (s, 6H, -CH_2-), 3.83 (s, 9H, -OCH_3), and 1.84 (s, 9H, -CH_3). ^{13}C NMR (100 MHz, d_6-DMSO, ppm): δ 160.74, 154.48, 154.34, 143.16, 138.28, 137.47, 134.97, 131.65, 130.81, 128.50, 123.17, 122.52, 121.75, 119.44, 114.79, 114.47, 111.50 (aromatic), 55.76 (-OCH_3), 46.17 (-CH_2-) and 16.67 (-CH_3). HR-MS (*m/z*): Calc. for $C_{54}H_{49}N_6O_3$ $(M+H)^+$: 829.3866; found, 829.3867. Anal. Calc. for $C_{54}H_{48}N_6O_3$: C, 78.24; H, 5.84; N, 10.14. Found: C, 78.32; H, 5.78, N, 10.07.

1,3,5-Tris(2-(4-methoxyphenyl)benzimidazol-1-ylmethyl)-2,4,6-triethylbenzene (3): According to general procedure, 148 mg of product was prepared from L^1 (152.5 mg, 0.68 mmol), NaH (20.0 mg, 0.82 mmol), 1,3,5-tris(bromomethyl)-2,4,6-triethylbenzene (100 mg, 0.2267 mmol) and obtained as white solid. Yield: 75%. ^{1}H NMR (400 MHz, d_6-DMSO, ppm): δ 7.68 (d, 3H, J_{HH} = 8.7 Hz, $H^{a,d}$), 7.60 (d, 3H, J_{HH} = 8.0 Hz, H^4), 7.12 (d, 9H, J_{HH} = 8.8 Hz, H^5 & $H^{b,c}$), 6.40 (t, 3H, J_{HH} = 7.3 Hz, H^6), 6.24 (d, 3H, J_{HH} = 8.2 Hz, H^7), 5.45 (s, 6H, -CH_2-), 3.84 (s, 9H, -OCH_3), 2.43 (d, 6H, J_{HH} = 7.2 Hz, -CH_2-CH_3), and 0.45 (t, 9H, J_{HH} = 6.7 Hz, -CH_2-CH_3). ^{13}C NMR (100 MHz, d_6-DMSO/$CDCl_3$, ppm): δ 160.79, 154.16, 145.30, 143.21, 134.79, 131.47, 130.79, 122.73, 122.56, 121.59, 119.40, 114.32, 111.96 (aromatic), 55.56 (-OCH_3), 44.89 (-CH_2-), 23.29 and 14.59 (-CH_2-CH_3). HR-MS (*m/z*): Calc. for $C_{57}H_{55}N_6O_3$ $(M+H)^+$: 871.4336; found, 871.4336. Anal. Calc. for $C_{57}H_{54}N_6O_3$: C, 78.59; H, 6.25; N, 9.65. Found: C, 78.45; H, 6.31, N, 9.58.

1,3,5-Tris(2-(3,4-dimethoxyphenyl)benzimidazol-1-ylmethyl)benzene (4): According to the general procedure, 417 mg of product was prepared from L^2 (427.5 mg, 1.6812 mmol), NaH (49.0 mg, 2.01 mmol), 1,3,5-tris(bromomethyl)benzene (200 mg, 0.5604 mmol) and obtained as white solid. Yield: 85%. ^{1}H-NMR (500 MHz, d_6-DMSO, ppm): δ 7.68 (d, 3H, J_{HH} = 8.0 Hz, H^4), 7.23 (t, 3H, J_{HH} = 7.5 Hz, H^5), 7.18 (d, 3H, J_{HH} = 7.9 Hz, H^6), 7.14 (d, 3H, J_{HH} = 7.4 Hz, H^7), 7.05 (d, 3H, J_{HH} = 1.7 Hz, H^a), 6.85 (dd, 3H, J_{HH} = 8.3 and 1.9 Hz, H^c), 6.74 (d, 3H, J_{HH} = 8.4 Hz, H^d), 6.68 (s, 3H, arene), 5.37 (s, 6H, -CH_2-), 3.77 (s, 9H, -OCH_3), and 3.49 (s, 9H, -OCH_3). ^{13}C NMR (100 MHz, d_6-DMSO, ppm): δ 153.66, 150.29, 148.88, 143.06, 138.98, 136.16, 123.56, 122.81, 122.51, 121.90, 119.52, 112.54, 111.78, 110.99 (aromatic), 55.94 and 55.57 (-OCH_3), 47.76 (-CH_2-). HR-MS (*m/z*): Calc. for $C_{54}H_{49}N_6O_6$ $(M+H)^+$: 877.3714; found, 877.3713. Anal. Calc. for $C_{54}H_{48}N_6O_6$: C, 73.95; H, 5.52; N, 9.58 Found: C, 73.85; H, 5.46; N, 9.48.

1,3,5-Tris(2-(3,4-dimethoxyphenyl)benzimidazol-1-ylmethyl)-2,4,6-trimethylbenzene (5): According to general procedure, 623 mg of product was prepared from L^2 (573.6 mg, 2.2558 mmol), NaH (65.0 mg, 2.70 mmol), 1,3,5-tris(bromomethyl)-2,4,6-trimethylbenzene (300 mg, 0.7519 mmol) and obtained as white solid. Yield: 90%. ^{1}H-NMR (500 MHz, d_6-DMSO, ppm): δ 7.60 (d, 3H, J_{HH} = 7.6 Hz, H^4), 7.33-7.32 (m, 6H, $H^{a,d}$), 7.10-7.07 (m, 6H, H^5 & H^c), 6.60 (t, 3H, J_{HH} = 7.6 Hz, H^6), 6.30 (d, 3H, J_{HH} = 8.1 Hz, H^7), 5.51 (s, 6H, -CH_2-), 3.82 (s, 9H, -OCH_3), 3.80 (s, 9H, -OCH_3), and 1.87 (s, 9H, -CH_3). ^{13}C NMR (100 MHz, d_6-DMSO, ppm): δ 154.45, 150.43, 149.00, 143.11, 138.24, 134.99, 131.60, 123.27, 122.95, 122.54, 121.74, 119.43, 113.50, 111.82, 111.51 (aromatic), 56.13 and 56.00 (-OCH_3), 46.13 (-CH_2-) and 16.79 (-CH_3). HR-MS (*m/z*): Calc. for $C_{57}H_{55}N_6O_6$ $(M+H)^+$: 919.4183; found, 919.4184. Anal. Calc. for $C_{57}H_{54}N_6O_6$: C, 74.49; H, 5.92; N, 9.14. Found: C, 74.32; H, 5.85, N, 9.23.

1,3,5-Tris(2-(3,4-dimethoxyphenyl)benzimidazol-1-ylmethyl)-2,4,6-triethylbenzene (6): According to general procedure, 390 mg of product was prepared from L^2 (345.9 mg, 1.3604 mmol), NaH (39.0 mg, 1.63 mmol), 1,3,5-tris(bromomethyl)-2,4,6-triethylbenzene (200 mg, 0.4534 mmol) and obtained as white solid. Yield: 90%. ^{1}H NMR (400 MHz, d_6-DMSO, ppm): δ 7.59 (d, 3H, J_{HH} = 8.1 Hz, H^4), 7.40-7.34 (m, 6H, $H^{a,d}$), 7.16-7.08 (m, 6H, H^5 & H^c), 6.39 (br s, 3H, H^6), 6.22 (d, 3H, J_{HH} = 8.1 Hz, H^7), 5.48 (s, 6H, -CH_2-), 3.84 (s, 9H, -OCH_3), 3.81 (s, 9H, -OCH_3), 2.46 (s, 6H, -CH_2-CH_3), and 0.49 (s, 9H, -CH_2-CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 153.92, 150.56, 149.37, 145.28, 143.16, 134.54, 130.68, 123.12, 122.83, 122.36, 122.09, 119.89, 112.95, 111.58, 110.88 (aromatic), 56.22 and 56.01 (-OCH_3), 44.95 (-CH_2-), 29.70 and 14.12 (-CH_2-CH_3). HR-MS (*m/z*): Calc. for $C_{60}H_{61}N_6O_6$ $(M+H)^+$: 961.4653; found, 961.4653. Anal. Calc. for $C_{60}H_{60}N_6O_6$: C, 74.98; H, 6.29; N, 8.74. Found: C, 74.83; H, 6.21, N, 8.86.

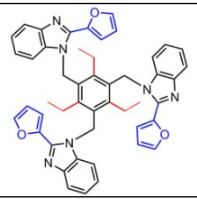
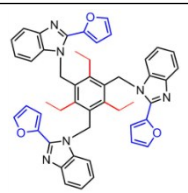
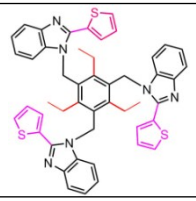
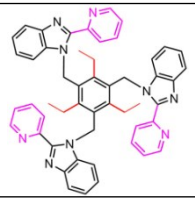
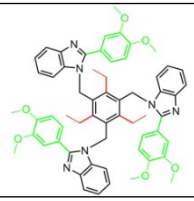
1,3,5-Tris(2-(3,4,5-trimethoxyphenyl)benzimidazol-1-ylmethyl)benzene (7): According to the general procedure 436 mg of product was prepared from L^3 (477.9 mg, 1.6812 mmol), NaH (48.0 mg, 2.02 mmol), 1,3,5-tris(bromomethyl) benzene (200 mg, 0.5604 mmol) and obtained as white solid. Yield: 80%. ^{1}H-NMR (500 MHz, d_6-DMSO, ppm): δ 7.64 (d, 3H, J_{HH} = 8.0 Hz, H^4), 7.22-7.18 (m, 3H, H^5), 7.10-7.07 (m, 6H, H^{6-7}), 6.80 (s, 6H, $H^{a,d}$), 6.62 (s, 3H, arene) and 5.43 (s, 6H, -CH_2-), 3.68 (s, 9H, -OCH_3), and 3.52 (s, 18H, -OCH_3). ^{13}C NMR (100 MHz, d_6-DMSO, ppm): δ 153.33, 153.30, 142.85, 139.04, 136.15, 125.50, 123.22, 122.99, 122.64, 119.61, 110.88, 106.70 (aromatic), 60.49 and 56.05 (-OCH_3) and 47.81 (-CH_3). HR-MS (*m/z*): Calc. for $C_{57}H_{55}N_6O_9$ $(M+H)^+$: 967.4031; found, 967.4032. Anal. Calc. for $C_{57}H_{54}N_6O_9$: C, 70.79; H, 5.63; N, 8.69. Found: C, 70.65; H, 5.71, N, 8.59.

1,3,5-Tris(2-(3,4,5-trimethoxyphenyl)benzimidazol-1-ylmethyl)-2,4,6-trimethylbenzene (8): According to the general procedure 321 mg of product was prepared from L^3 (427.5 mg, 1.5039 mmol), NaH (43.3 mg, 1.80 mmol), 1,3,5-tris(bromomethyl)-2,4,6-trimethylbenzene (200 mg, 0.5013 mmol) and obtained as white solid. Yield: 81%. ^{1}H-NMR (500 MHz, d_6-DMSO, ppm): δ 7.60 (d, 3H, J_{HH} = 8.0 Hz, H^4), 7.11 (t, 3H, J_{HH} = 7.6 Hz, H^5), 6.98 (s, 6H, $H^{a,d}$), 6.65 (t, 3H, J_{HH} = 7.4 Hz, H^6), 6.42 (d, 3H, J_{HH} = 8.2 Hz, H^7), 5.51 (s, 6H, -CH_2-), 3.79 (s, 18H, -OCH_3), 3.71 (s, 9H, -OCH_3), and 1.85 (s, 9H, -CH_3). ^{13}C NMR (100 MHz, d_6-DMSO, ppm): δ 154.31, 153.19, 142.94, 138.97, 138.12, 135.08, 131.53, 126.48, 122.73, 121.88, 119.56, 111.48, 107.65 (aromatic), 60.51 and 56.51 (-OCH_3), 45.90 (-CH_2-), 16.90 (-CH_3). HR-MS (*m/z*): Calc. for $C_{60}H_{61}N_6O_9$ $(M+H)^+$: 1009.4500; found, 1009.4510. Anal. Calc. for $C_{60}H_{60}N_6O_9$: C, 71.41; H, 5.99; N, 8.33. Found: C, 71.28; H, 5.92, N, 8.41.

1,3,5-Tris(2-(3,4,5-trimethoxyphenyl)benzimidazol-1-ylmethyl)-2,4,6-triethylbenzene (9): According to the general procedure 368 mg of product was prepared from L^3 (386.7 mg, 1.3604 mmol), NaH (39.0 mg, 1.63 mmol), 1,3,5-tris(bromomethyl)-2,4,6-triethylbenzene (200 mg, 0.4534 mmol) and obtained as white solid. Yield: 78%. ^{1}H NMR (500 MHz, d_6-DMSO, ppm): δ 7.62 (d, 3H, J_{HH} = 8.0 Hz, H^4), 7.12 (t, 3H, J_{HH} = 7.6 Hz, H^5), 7.09 (s, 6H, $H^{a,d}$), 6.46 (br s, 3H, H^6), 6.34 (br d, 3H, J_{HH} = 6.4 Hz, H^7), 5.49 (s, 6H, -CH_2-), 3.81 (s, 18H, -OCH_3), 3.73 (s, 9H, -OCH_3), 2.49 (s, 6H, -CH_2-CH_3), and 0.48 (s, 9H, -CH_2-CH_3). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 148.92, 148.75, 138.22, 135.11, 134.12, 133.08, 130.72, 124.26, 123.45, 120.53, 120.09, 118.62, 118.55, 118.31, 115.48, 104.93, 101.84 (aromatic), 56.19 and 51.37 (-OCH_3), 43.27 (-CH_2-), 26.81 and 16.67 (-CH_2-CH_3). HR-MS (*m/z*): Calc. for $C_{63}H_{67}N_6O_9$ $(M+H)^+$: 1051.4970; found, 1051.4968. Anal. Calc. for $C_{63}H_{66}N_6O_9$: C, 71.98; H, 6.33; N, 7.99. Found: C, 71.85; H, 6.29, N, 7.88.

X-ray Crystallography. Intensity data of suitably sized crystals of **3** and **6** were carried out on a Bruker D8 QUEST diffractometer [λ(Mo Kα) = 0.71073 Å] for unit cell determination and three-dimensional intensity data collection. The structures were solved by direct methods using SHELXS-97[2] which revealed the atomic positions and refined using the SHELXL-2014/7 program (within the WinGX program package).[3] Non-H atoms were refined anisotropically.

Table S1. Geometrical parameters (*d*, Å= distance between the COM of benzene of benzimidazolyl residues; τ, ° = dihedral angle between the benzimidazolyl units) in the X-ray structures **I** (phenyl substituted porphyrin-Zn complex)[2], **II**-**IV** (II = 1,3,5-tris(2-furyl)benzimidazol-1-ylmethyl)-2,4,6-triethylbenzene, **IIa** = optimized structure of **II, III =** 1,3,5-tris(2-thiophenyl)benzimidazol-1-ylmethyl)-2,4,6-triethylbenzene, **IV** = 1,3,5-tris(2-pyridyl)benzimidazol-1-ylmethyl)-2,4,6-triethylbenzene)[4], and **6** (1,3,5-Tris(2-(3,4-dimethoxyphenyl)benzimidazol-1-ylmethyl)-2,4,6-trimethylbenzene).

	I	**II**	**IIa**	**III**	**IV**	**6**
d_{ab}	4.973(4)	5.13	5.74	5.09	5.30	4.88
d_{bc}	4.623(4)	5.19	5.77	5.40	5.07	4.88
d_{ac}	5.004(4)	5.06	5.76	5.43	4.97	4.88
τ_{ab}	67.7(3)	64	60	65	56	60
τ_{bc}	32.7(3)	54	59	59	62	60
τ_{ca}	59.2(3)	61	60	55	62	60
	[phenyl substituted porphyrin-Zn complex]$_3$					

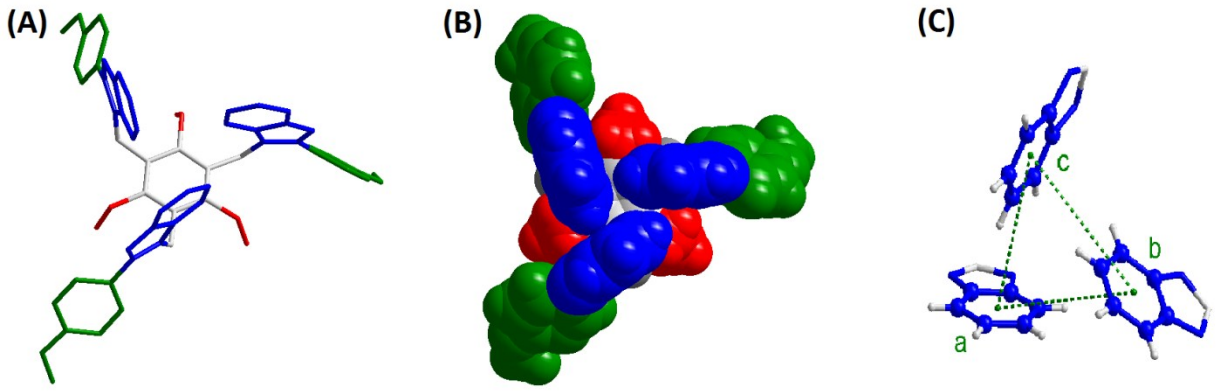
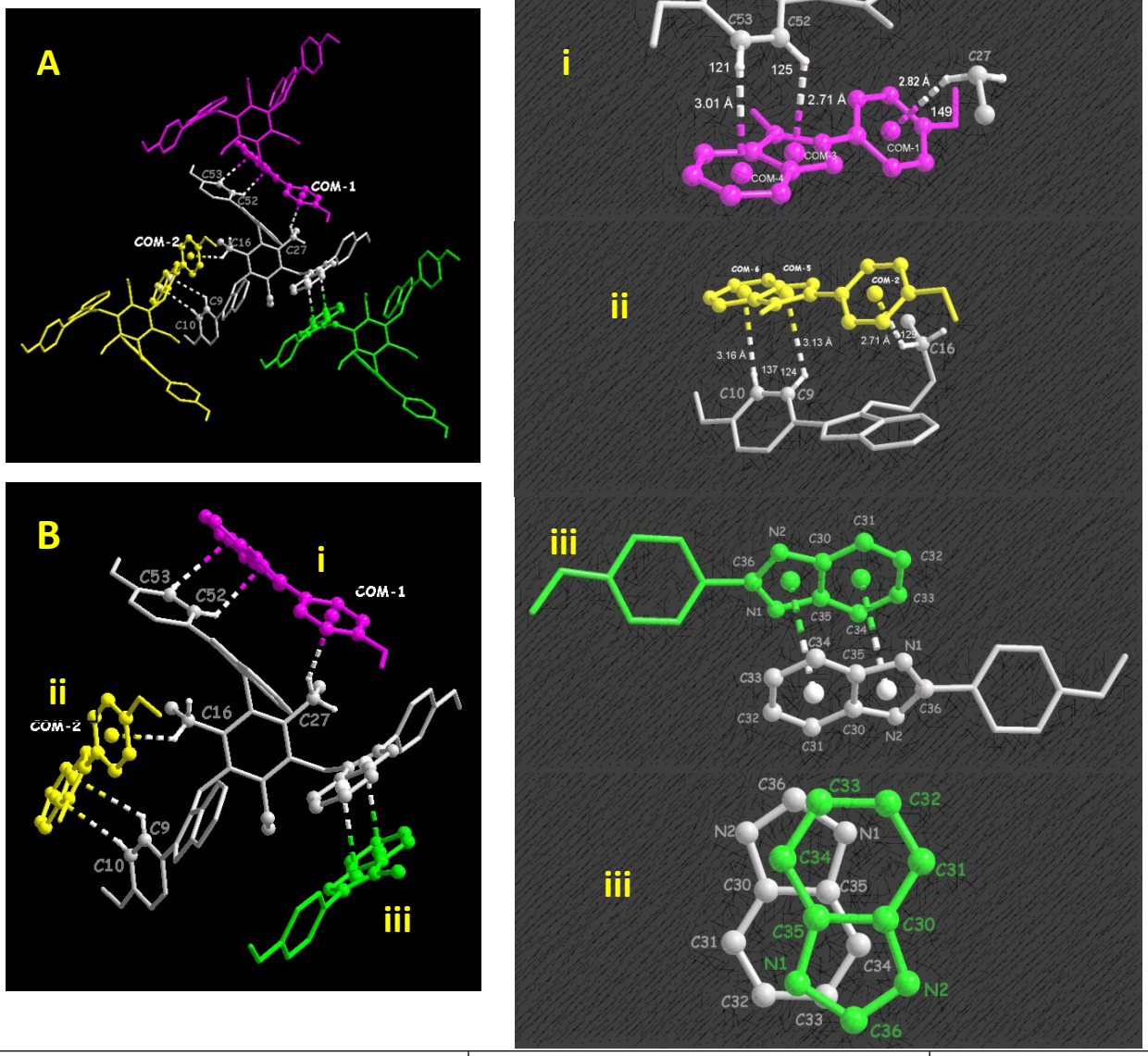


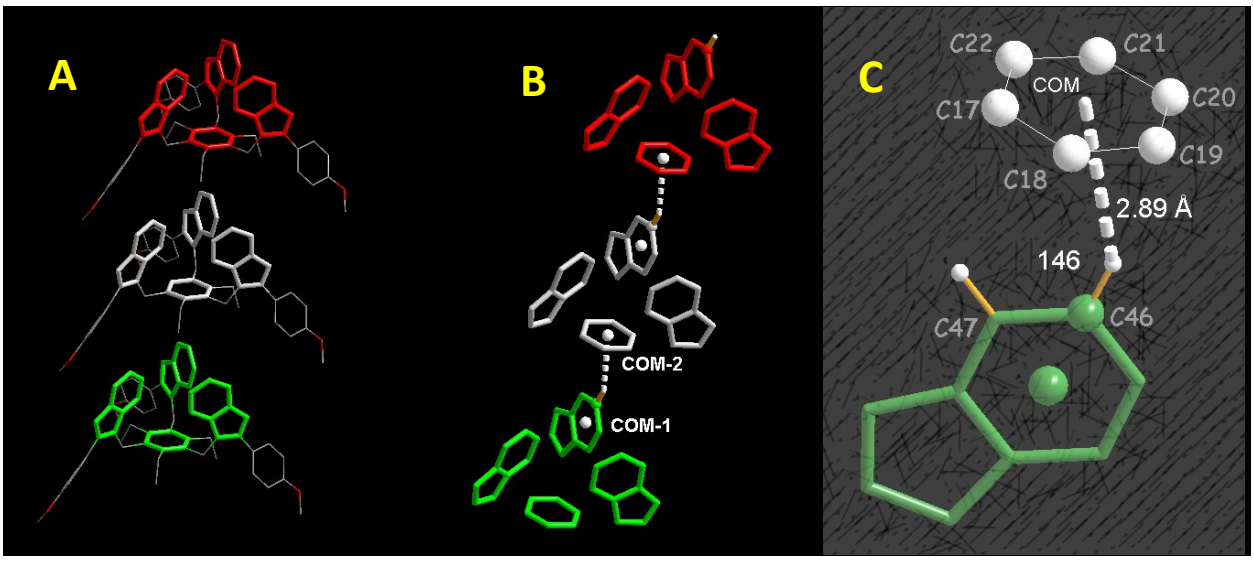
Fig. S1 Molecular structures of **3** (A: stick model, H-atoms are removed; B: space-filling model; C: Three benzimidazolyl units of **3**). a, b and c are the COM of benzene ring. (Color code: methoxyphenyl = green, ethyl = red, benzene = grey, benzimidazolyl = blue, and H atoms in C = grey).



I			II			III	
	d, Å	∠C-H···COM,°		*d*, Å	∠C-H···COM,°	Cg··· Cw	*d*, Å
[a]C27-H···COM1	2.82	149	[a]C16-H···COM2	2.71	129	C33···C36	3.4808
C52-H···COM3	2.71	125	C9-H···COM5	3.13	124	C34···C30	3.5796
C53-H···COM4	3.01	121	C10-H···COM2	3.16	137	C34···C35	3.6413
						C35···C35	3.5299

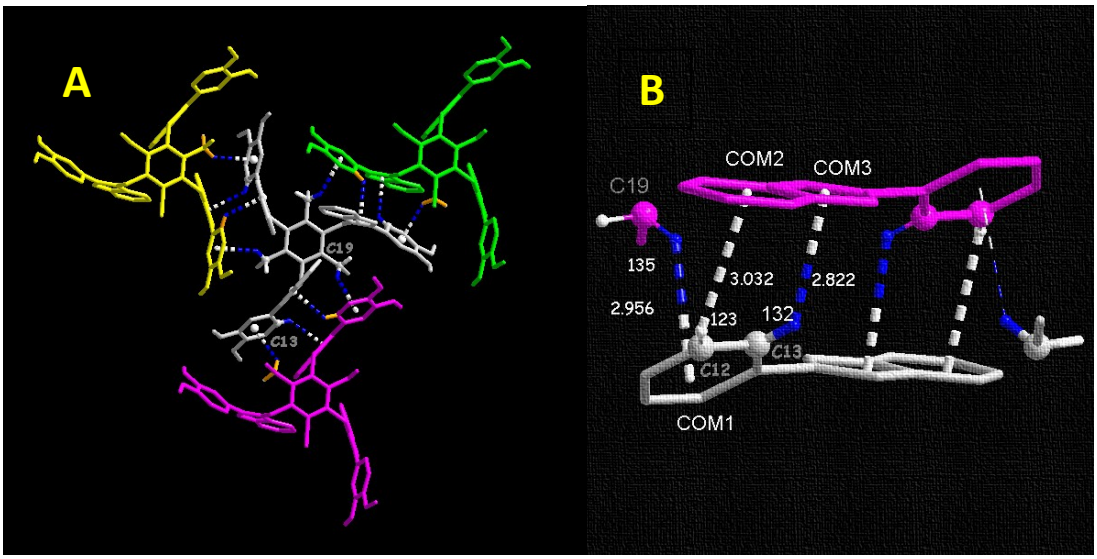
a = alkyl carbon, *d* = distance, COM = center of mass of six membered ring (or) five membered ring, Cg = green color carbon, Cw = white color carbon.

Fig. S2 Partial packing diagram showing four molecules of **3** (A). One full molecule with partial three molecules of **3** (B). **I**, **II**, and **III** are the portion of two neighboring methoxyphenylbenzimidazolyl units. Hydrogen atom is included only for carbon involving the C-H···π interactions.



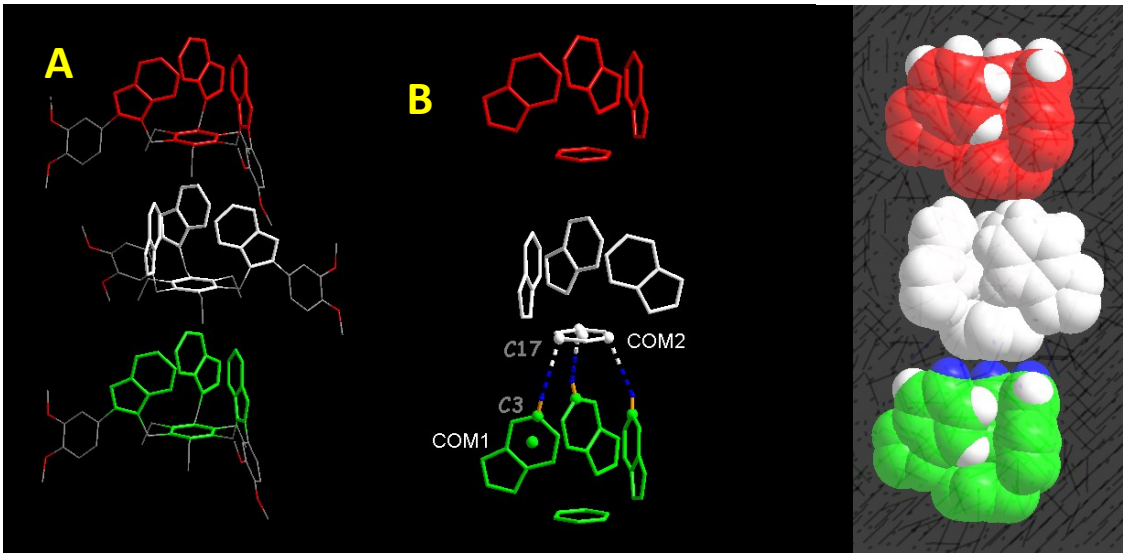
	d, Å	∠C-H···COM,°
[a]COM1···COM2	2.82	149
C46-H···COM	2.89	146
C46-H···C17	3.58	124
C46-H···C18	3.21	133
C46-H···C19	2.86	156
C46-H···C20	2.82	169
C46-H···C21	3.16	142
C46-H···C22	3.54	128

Fig. S3 Partial packing diagram showing three adjacent molecules of **3** (A). Spacer benzene and CBT core (B). Two aromatic units indicate the intermolecular *edge-to-face* C-H···π interactions. Hydrogen atom is included only for carbon involving the C-H···π interactions.



	d, Å	∠C-H···COM,°
[a]C19-H···COM1	2.956	135
C12-H···COM2	3.032	123
C13-H···COM4	2.822	132

Fig. S4 Partial packing diagram showing four molecules of **6** (A). Two neighboring phenylbenzimidazolyl units and CH_2 unit in ethyl group involve in noncovalent interactions (B). Hydrogen atom is included only for carbon involving the C-H···π interactions.



	d, Å	
[a]COM1···COM2	5.7918	τ = 86°
C3-H···COM2	3.078	∠C-H···COM = 156°

Fig. S5 Partial packing diagram showing three adjacent molecules of **6** (A). Spacer benzene and CBT core (B). CBT trimer unit, three benzene units, contacts with benzene spacer by intermolecular *edge-to-face* C-H···π interactions. Hydrogen atom is included only for carbon involving the C-H···π interactions.

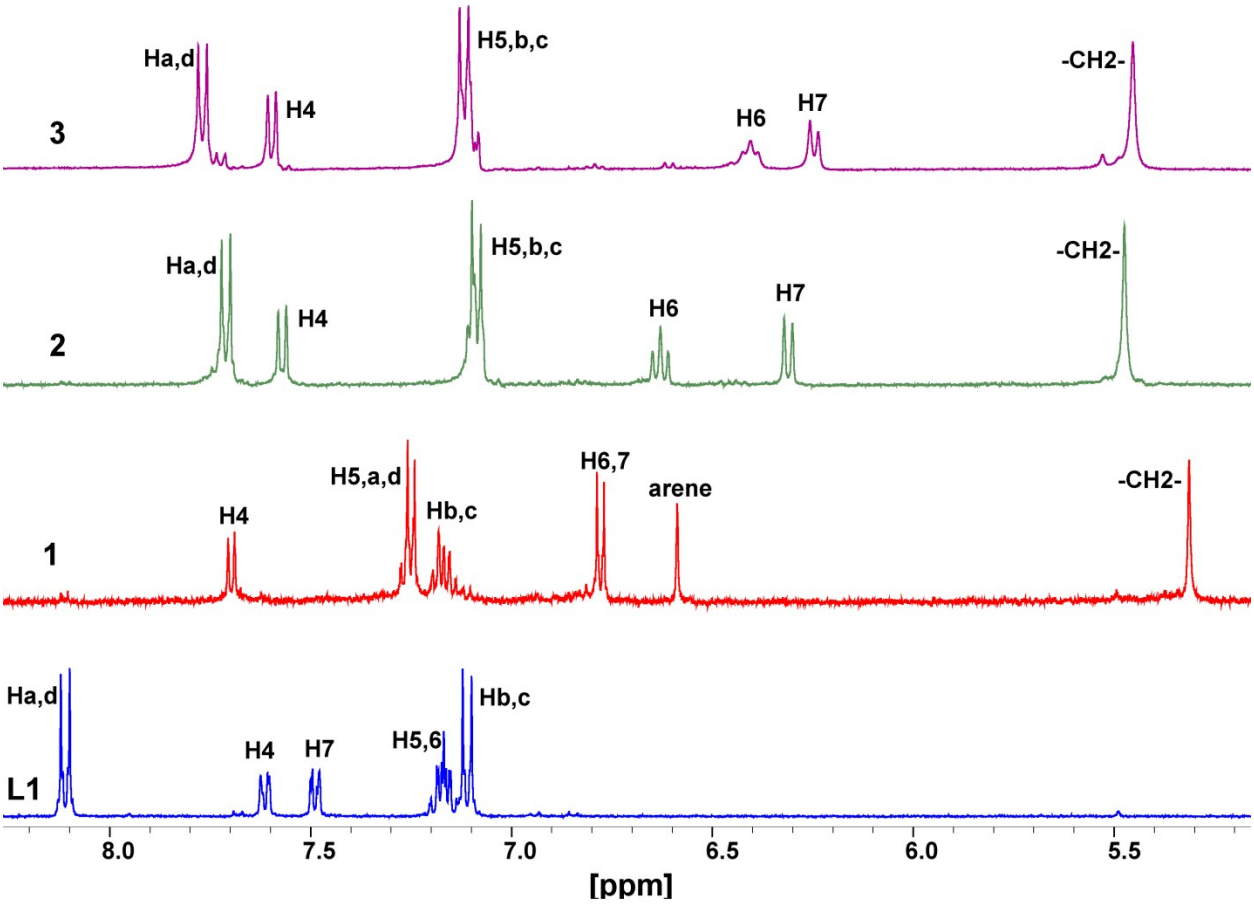


Fig. S6 Partial ^{1}H NMR spectra of L^{1}, **1**, **2** and **3** in d_6-DMSO.

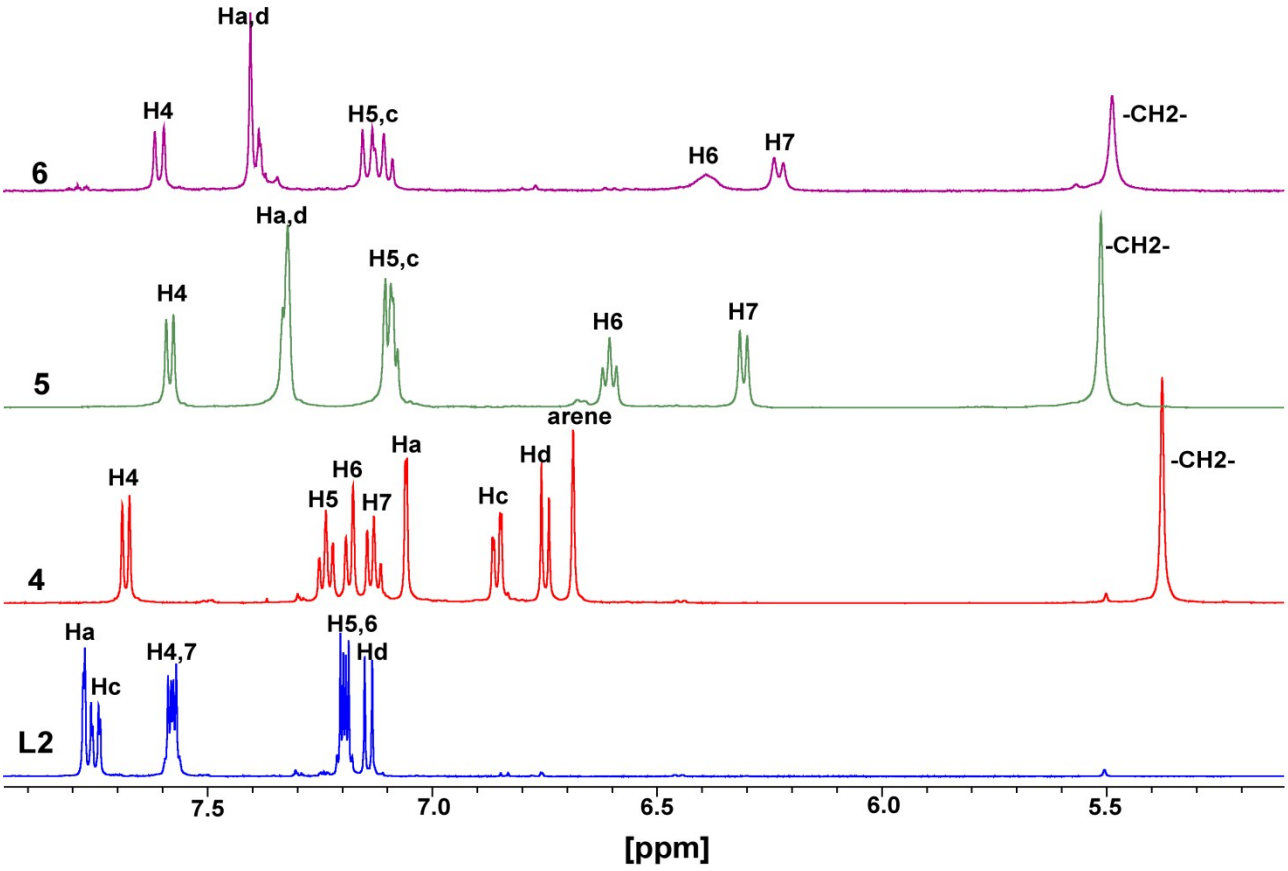


Fig. S7 Partial ^{1}H NMR spectra of L^{2}, **4, 5** and **6** in d_6-DMSO.

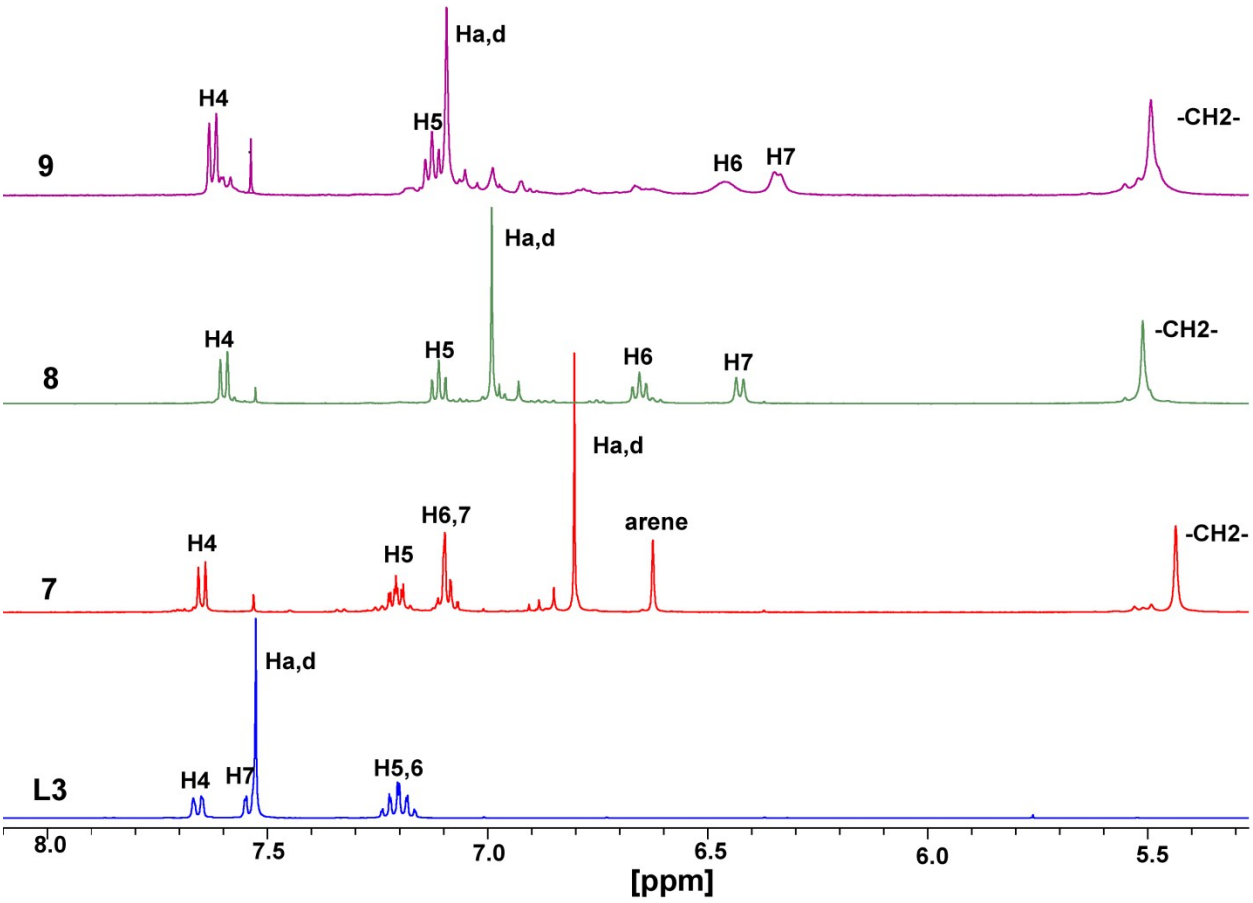


Fig. S8 Partial ^{1}H NMR spectra of L^{3}, **7, 8** and **9** in d_6-DMSO.

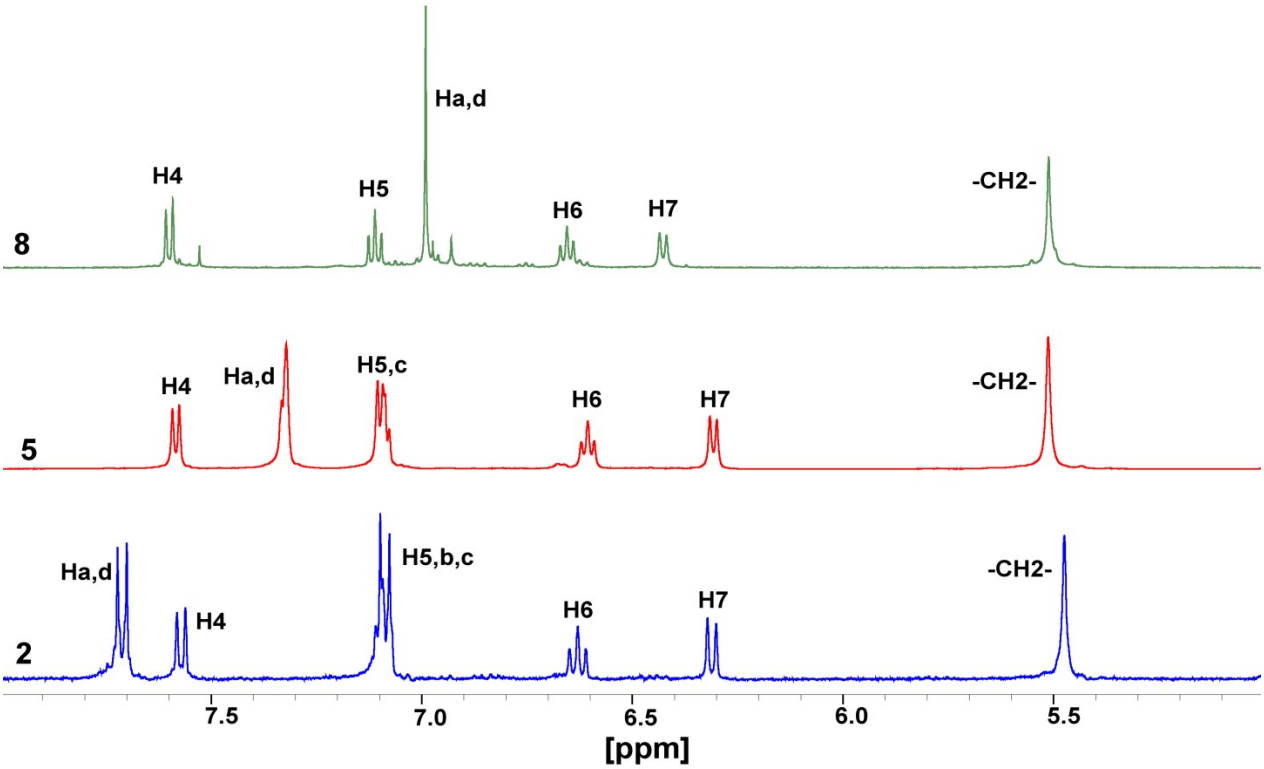


Fig. S9 Partial ^{1}H NMR spectra of **2, 5** and **8** in d_6-DMSO.

The methoxyphenyl protons in these molecules also display significant upfield shifts in the ^{1}H NMR spectra. The H^a and H^d of monomethoxyphenyl unit of molecule **2** remain almost same region relative to the free ligand (δ 6.69). Molecule **5** shows a merged peak (δ 7.33) for the H^a and H^d, which were appeared as two separate peaks (δ 7.77 and 7.14) in the free ligand. Compare to the molecule **2**, these two protons are slightly downfield shifted in **5**. This indicates that the dimethoxyphenyl units directed away to the center of molecule in **5** in compare to monomethoxyphenyl unit arrangement in **2**. In addition, it may be possible that the dimethoxyphenyl unit rotates in solution and H^a and H^d experience the similar chemical environment in the NMR time scale. Molecule **8** shows a sharp singlet for the H^a and H^d of trimethoxyphenyl unit, which was upfield shifted relative to free ligand. The peak position of these two protons in molecules **2** and **8** are in the similar region. The H^b and H^c of molecule **2** appeared at 7.6 ppm which was also significantly upfield shifted in compare to free ligand. Similar pattern was observed for H^c of molecule **5**.

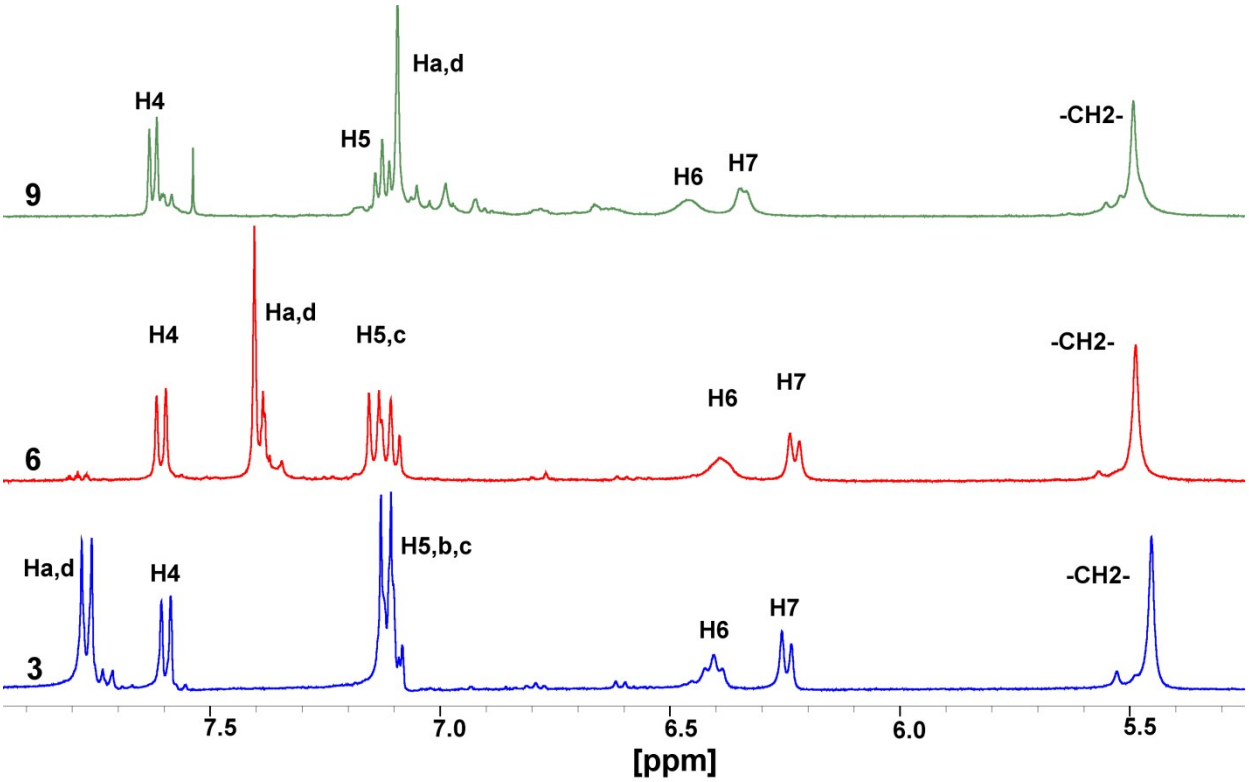


Fig. S10 Partial ^{1}H NMR spectra of **3, 6** and **9** in d_6-DMSO.

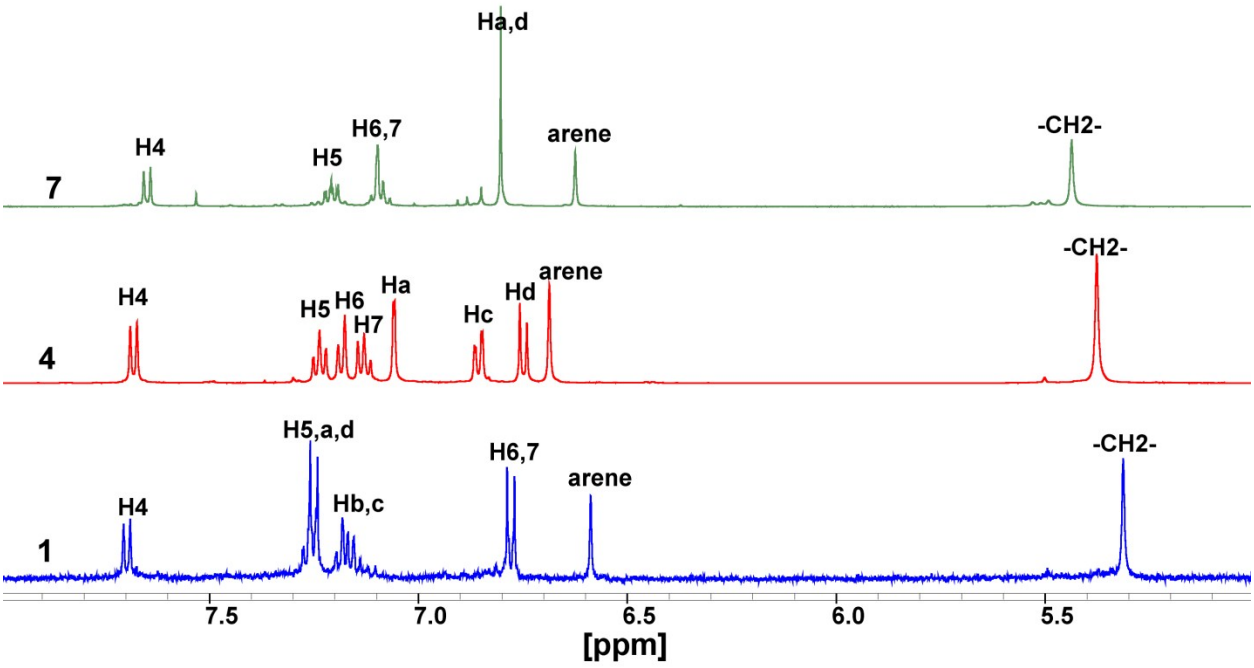


Fig. S11 Partial ^{1}H NMR spectra of **1, 4** and **7** in d_6-DMSO.

Molecules with benzene center scaffold (**1, 4** and **7**) show different pattern in compare to remaining molecules. Though these molecules **1, 4** and **7** display a well-separated and a single set of peaks for all protons, assigning to a particular conformation based on the chemical resonances was fruitless. However, molecule **1** may exist as *syn*-conformer predominantly in the solution due to upfield shift observed for the H^6 and H^7protons which are very close the values found for the same proton in methyl/ethyl substituted molecules.

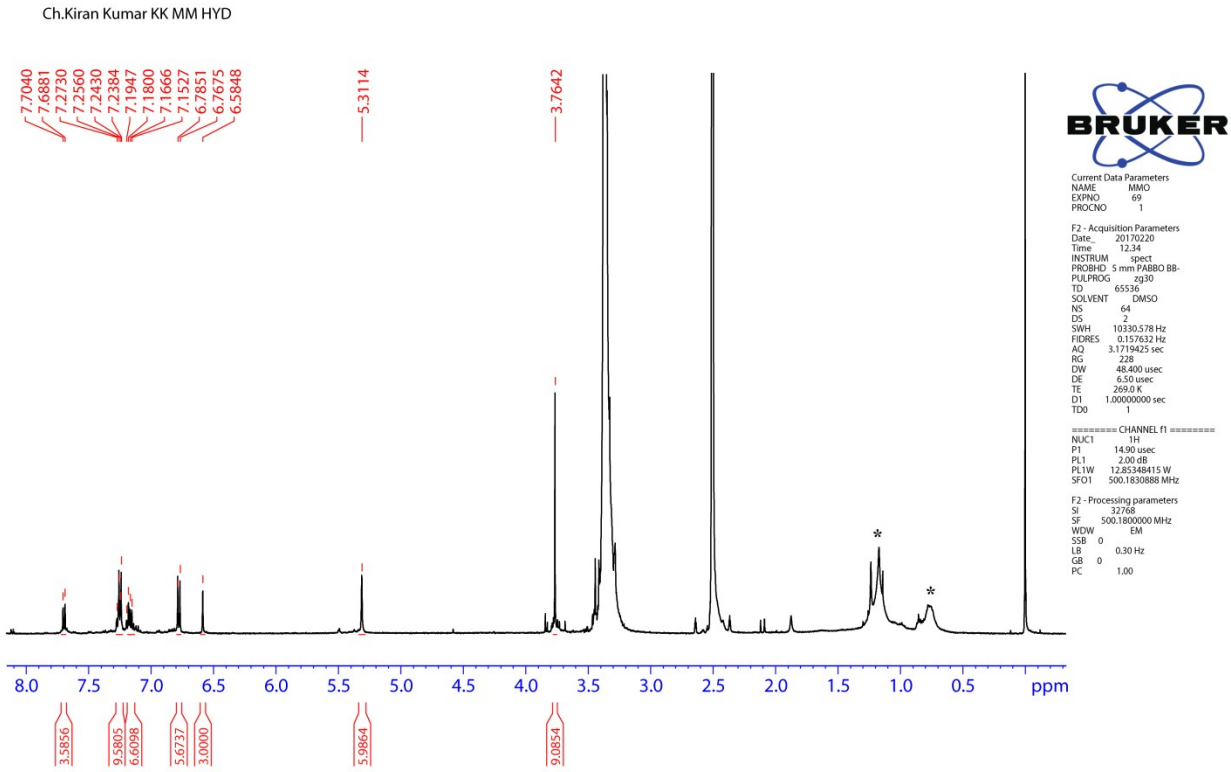


Fig. S12 ^{1}H NMR spectrum of **1** in d_6-DMSO (* = residual solvent peaks).

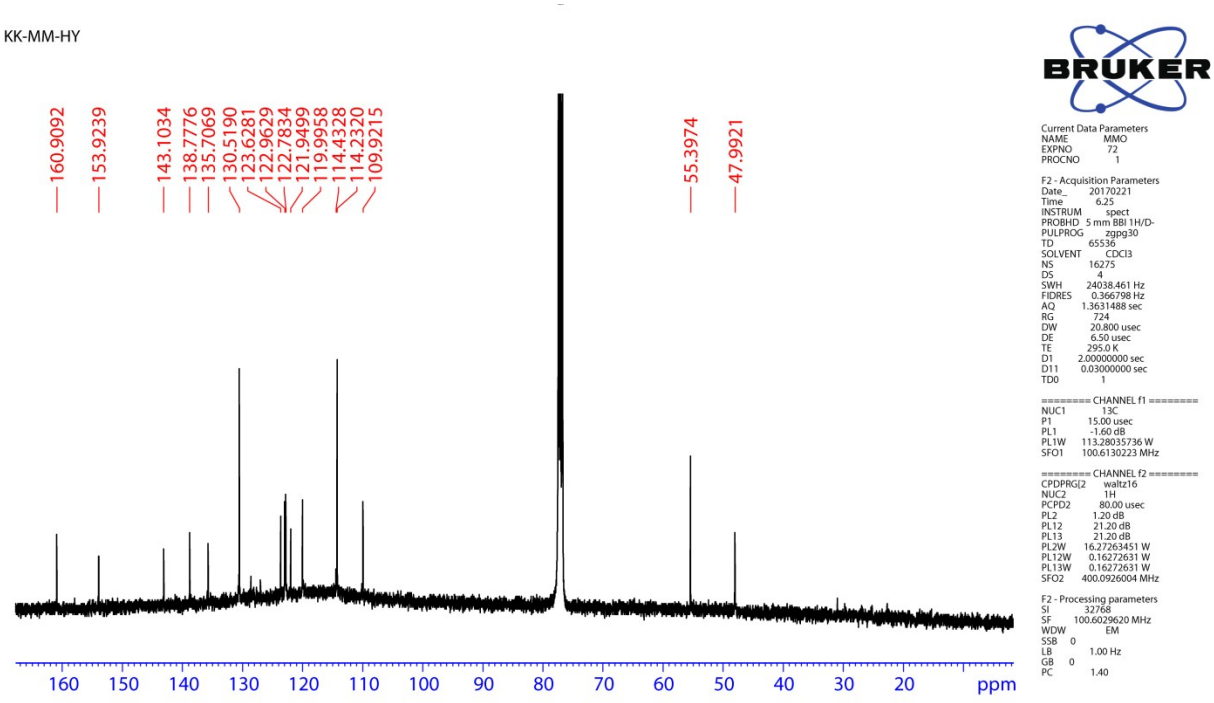


Fig. S13 ^{13}C NMR spectrum of **1** in $CDCl_3$.

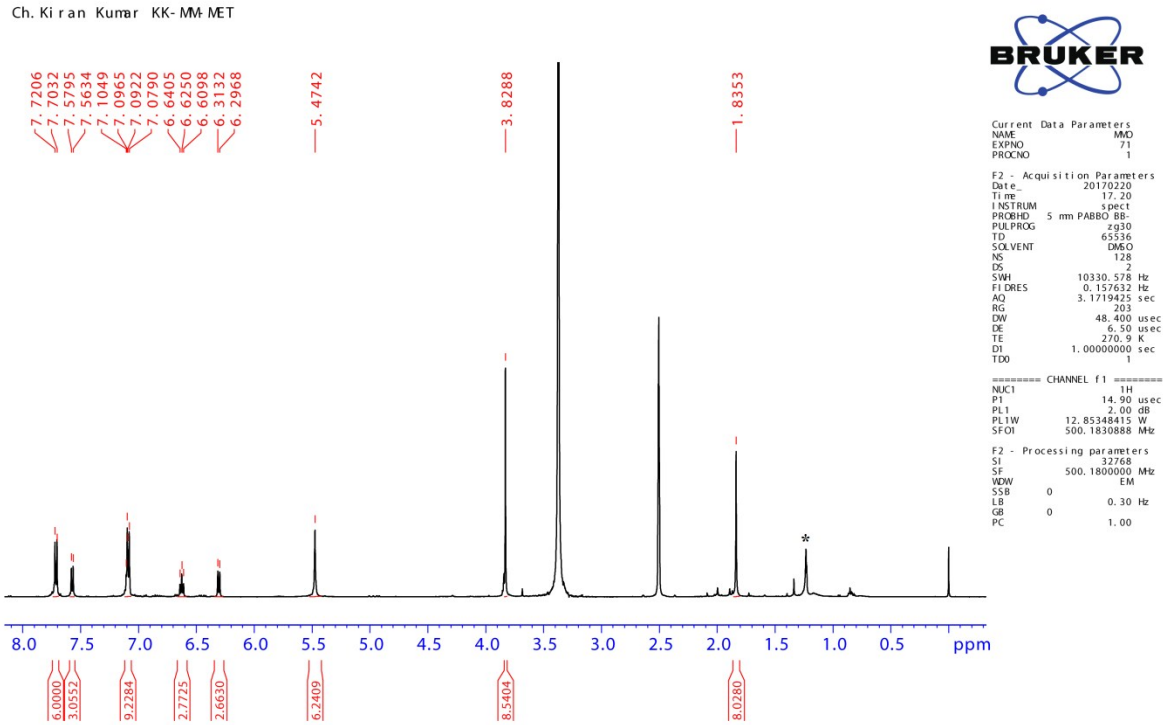


Fig. S14 ^{1}H NMR spectrum of **2** in d_6-DMSO (***** = residual solvent peak).

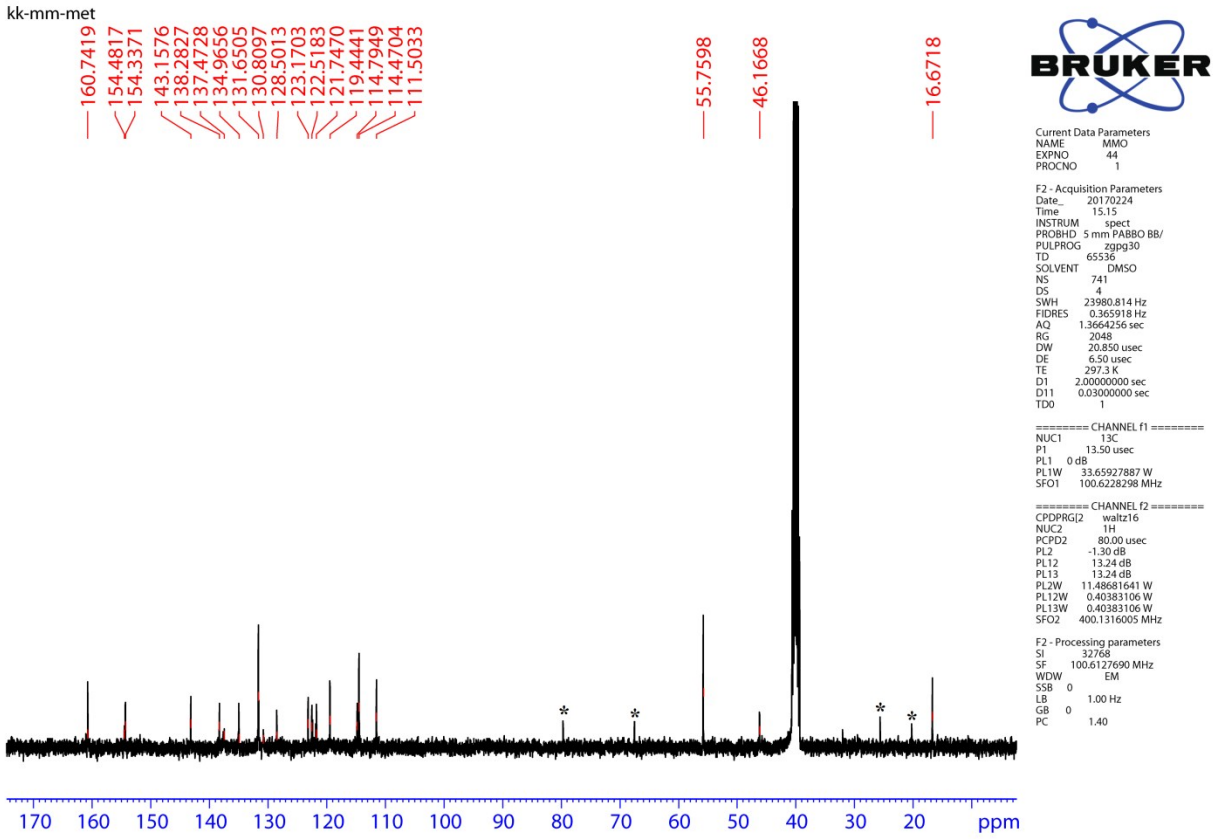


Fig. S15 ^{13}C NMR spectrum of **2** in d_6-DMSO (* = residual solvent peaks).

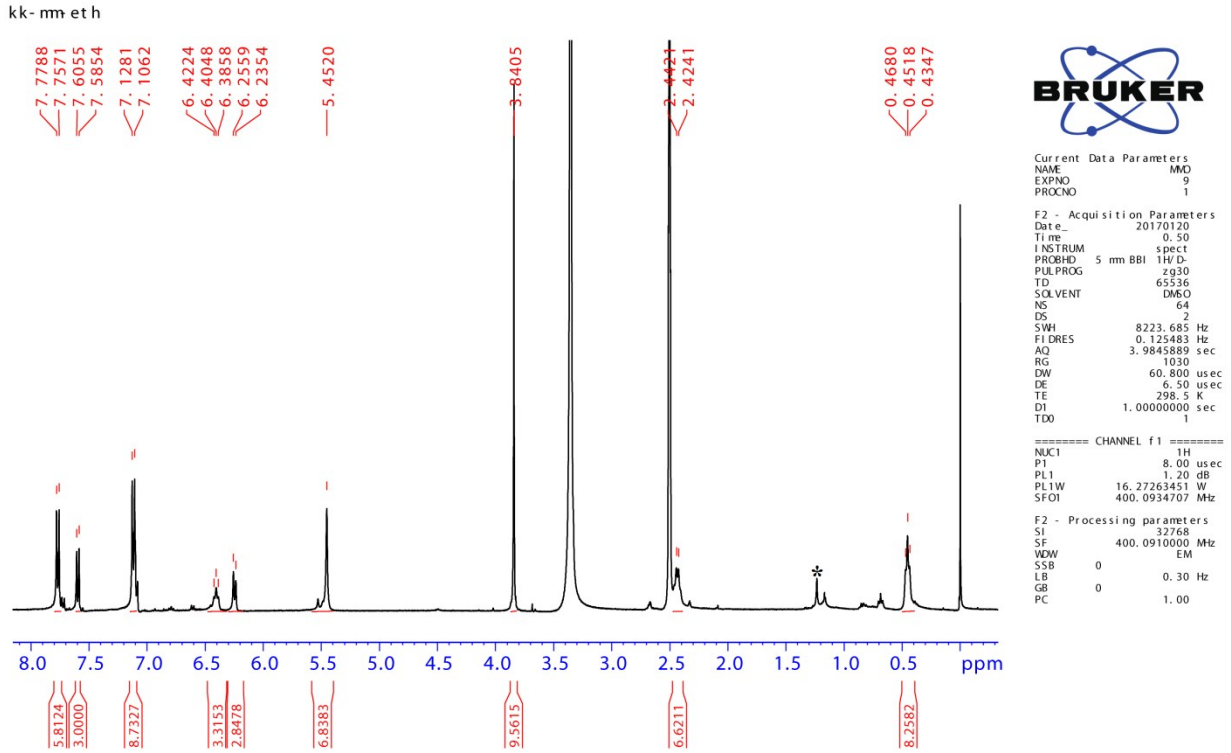


Fig. S16 ^{1}H NMR spectrum of **3** in d_6-DMSO (* = residual solvent peak).

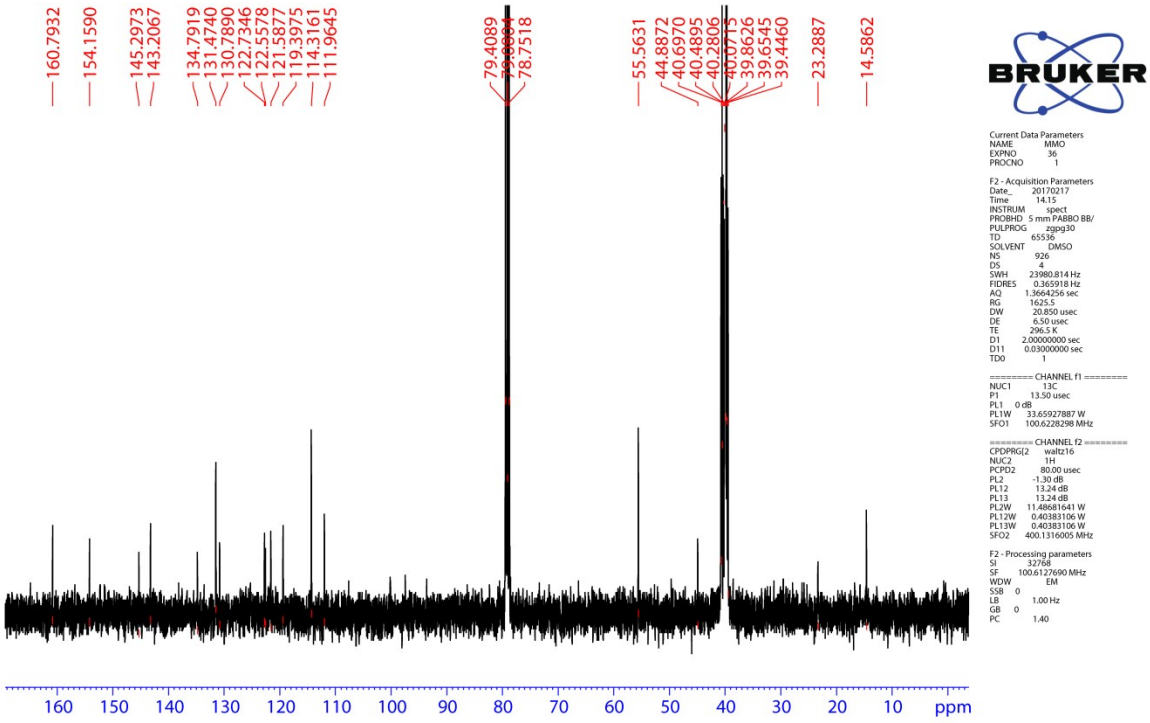


Fig. S17 ^{13}C NMR spectrum of **3** in $CDCl_3$/d_6-DMSO.

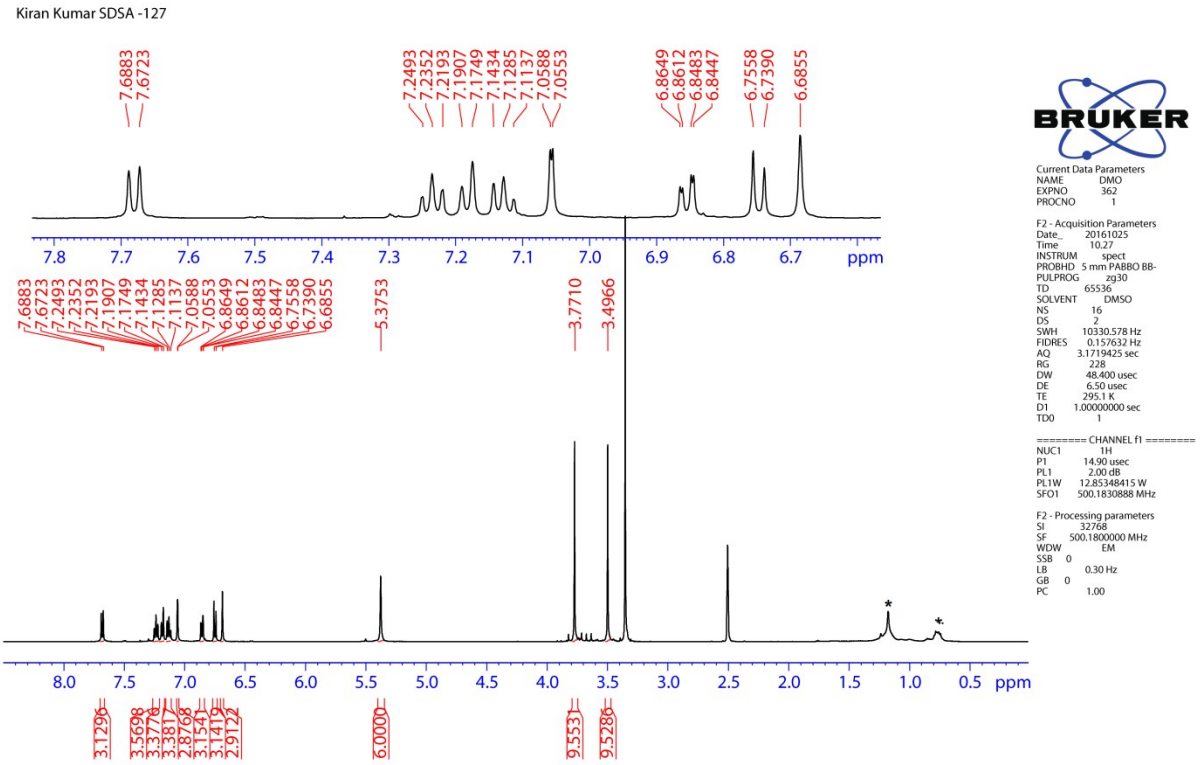


Fig. S18 ^{1}H NMR spectrum of **4** in d_6-DMSO (* = residual solvent peaks).

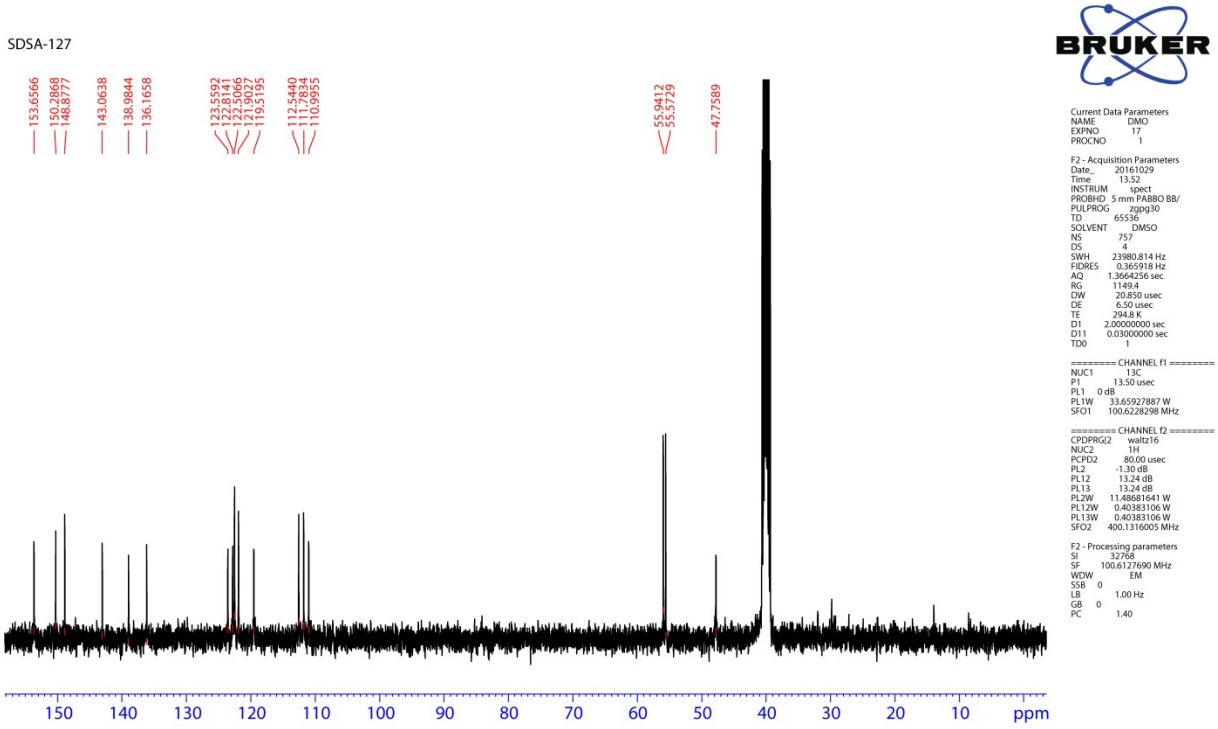


Fig. S19 ^{13}C NMR spectrum of **4** in d_6-DMSO.

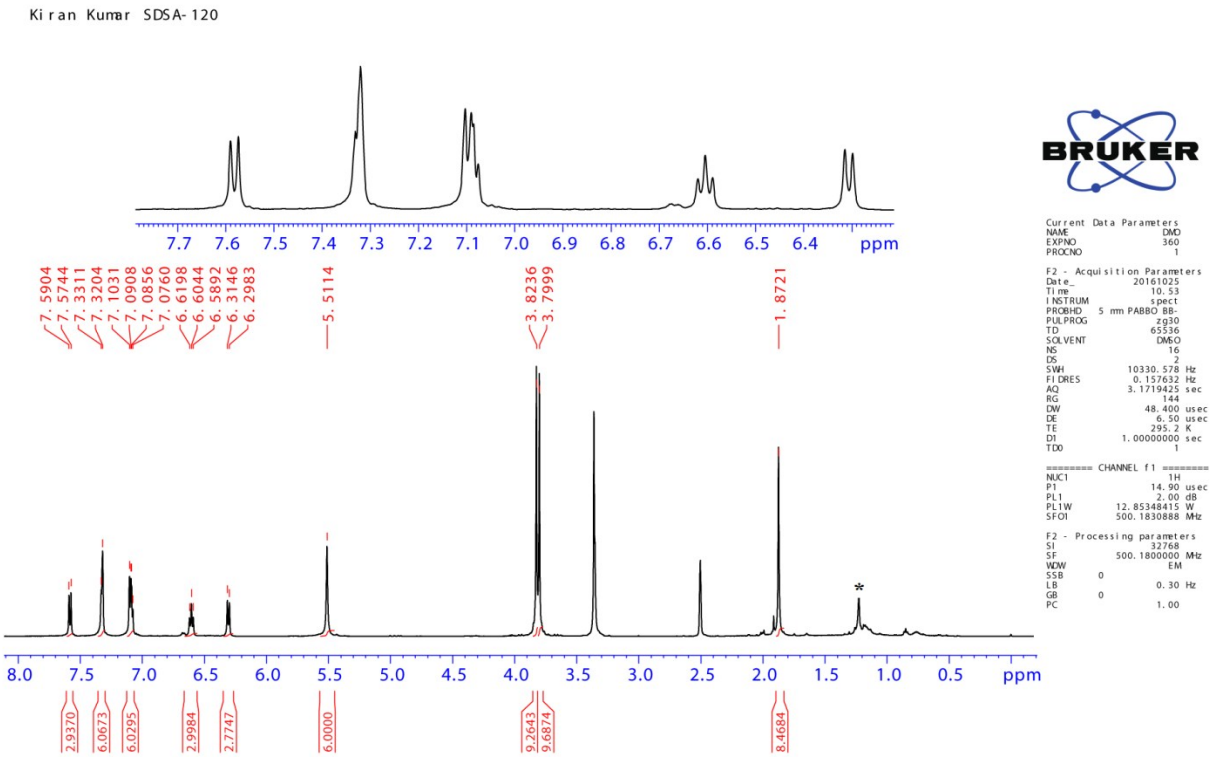


Fig. S20 ^{1}H NMR spectrum of **5** in d_6-DMSO (* = residual solvent peak).

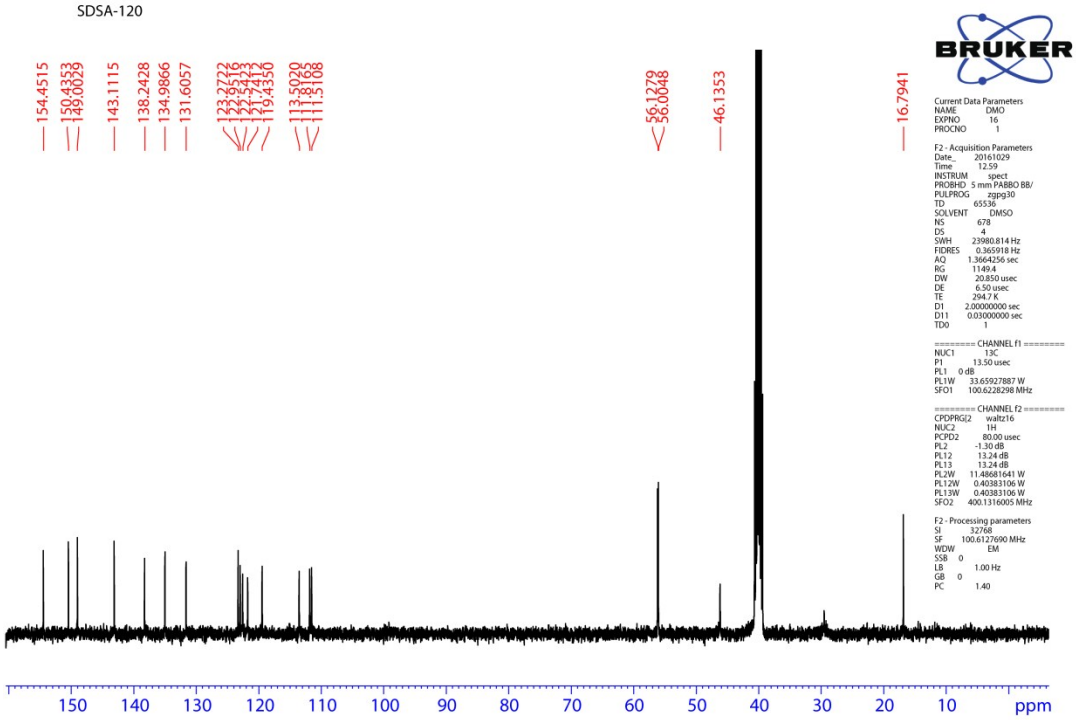


Fig. S21 ^{13}C NMR spectrum of **5** in d_6-DMSO.

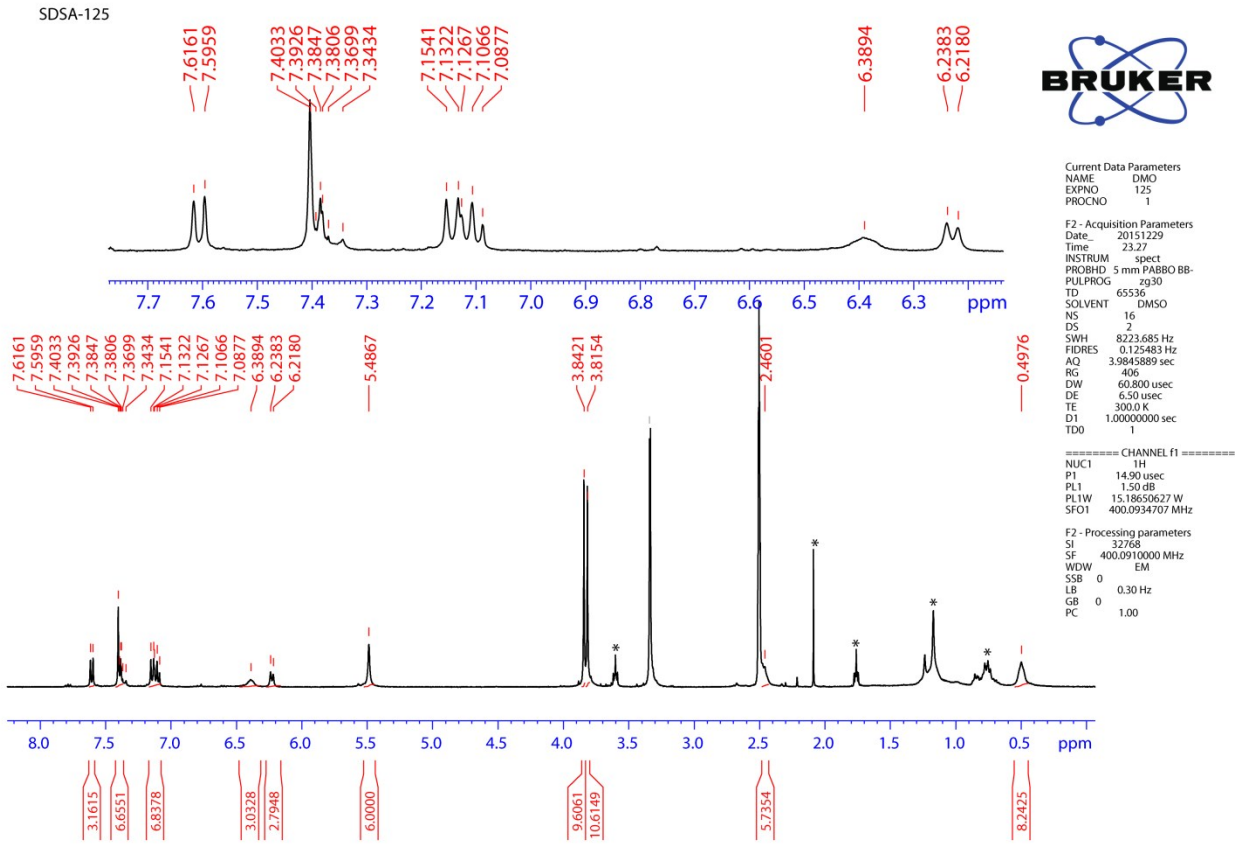


Fig. S22 ^{1}H NMR spectrum of **6** in d_6-DMSO (* = residual solvent peaks).

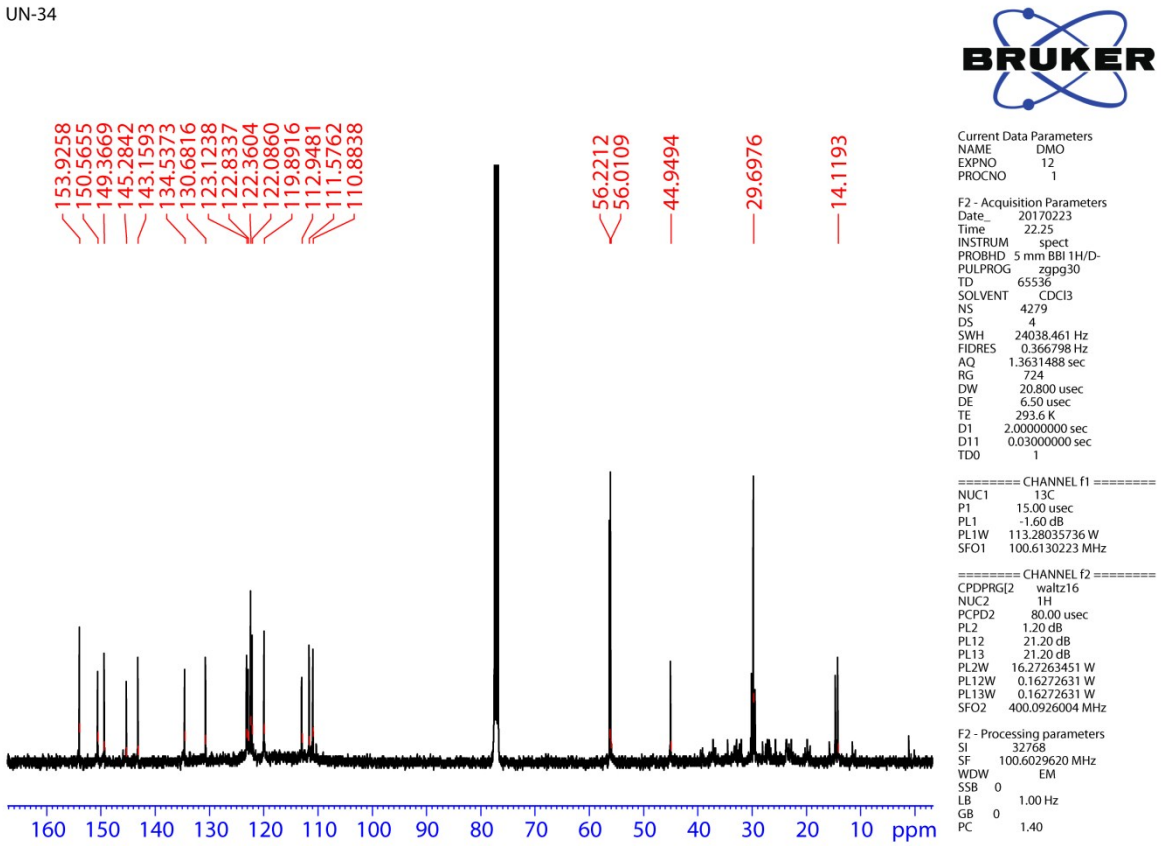


Fig. S23 ^{13}C NMR spectrum of **6** in $CDCl_3$.

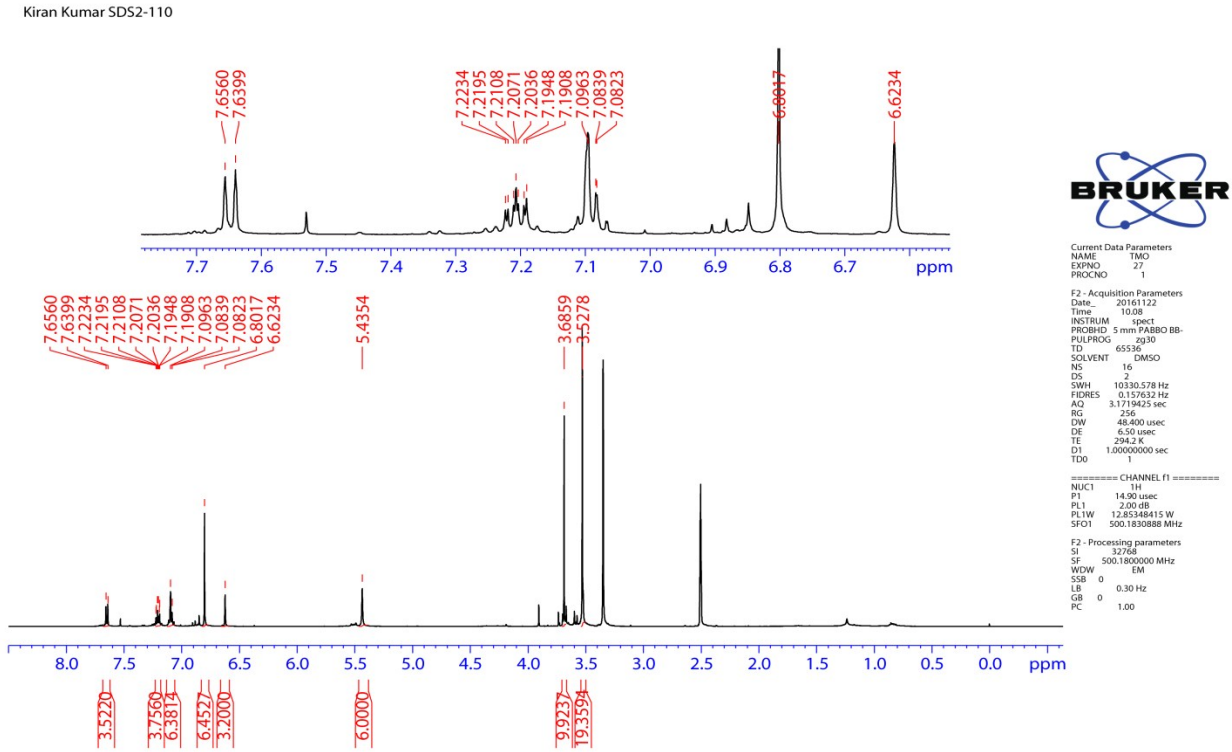


Fig. S24 ^{1}H NMR spectrum of **7** in d_6-DMSO.

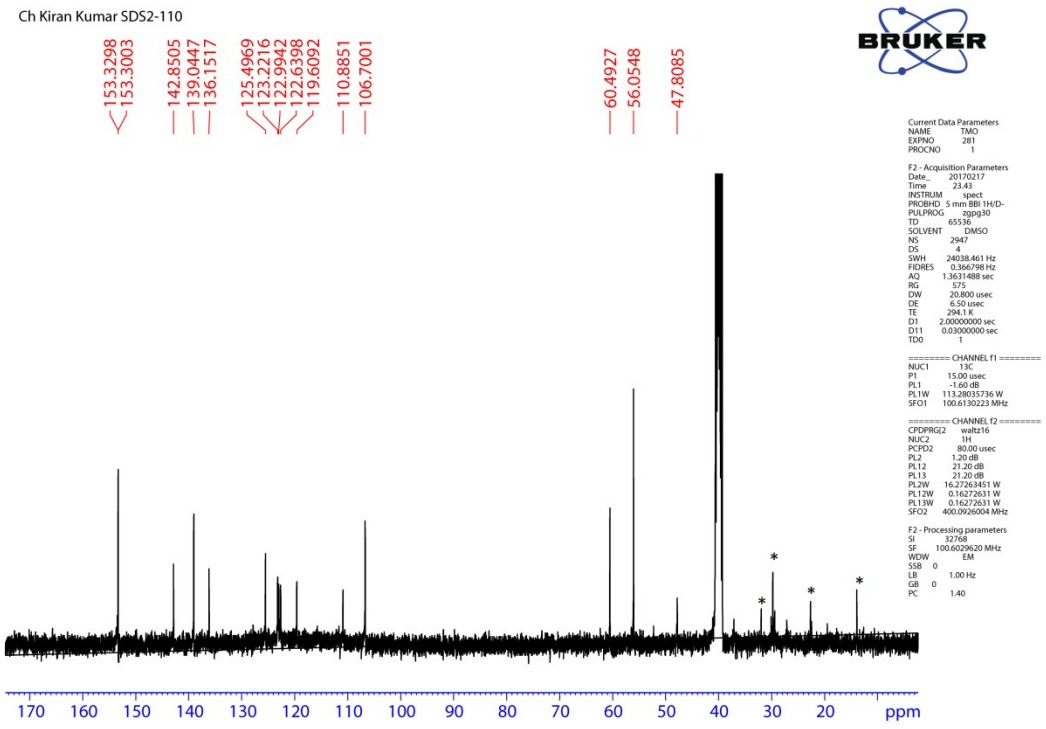


Fig. S25 ^{13}C NMR spectrum of **7** in d_6-DMSO (* = residual solvent peaks).

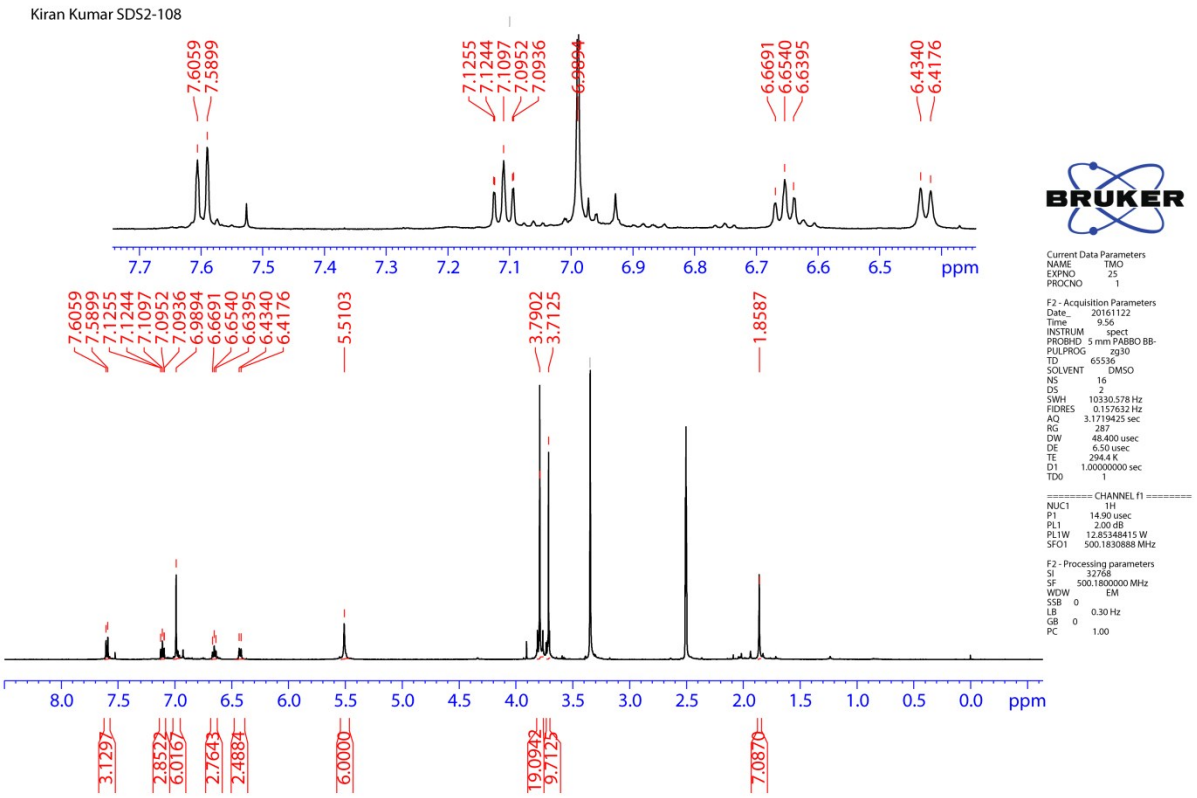


Fig. S26 ^{1}H NMR spectrum of **8** in d_6-DMSO.

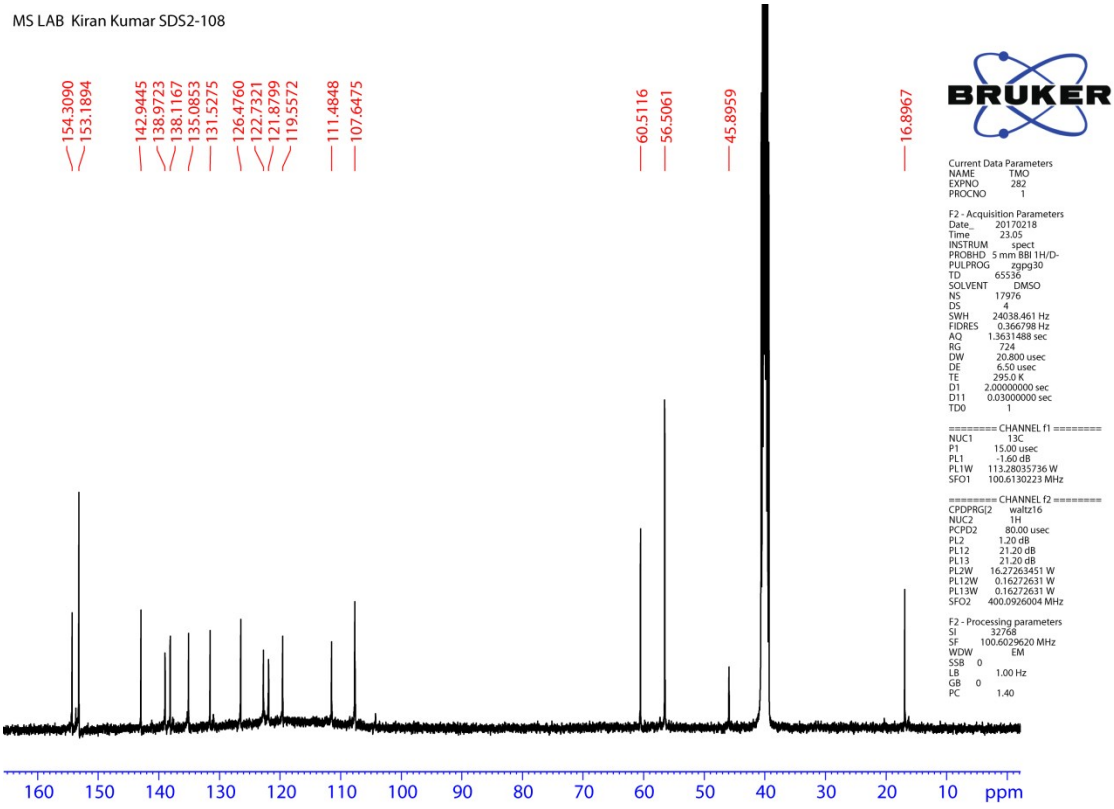


Fig. S27 ^{13}C NMR spectrum of **8** in d_6-DMSO.

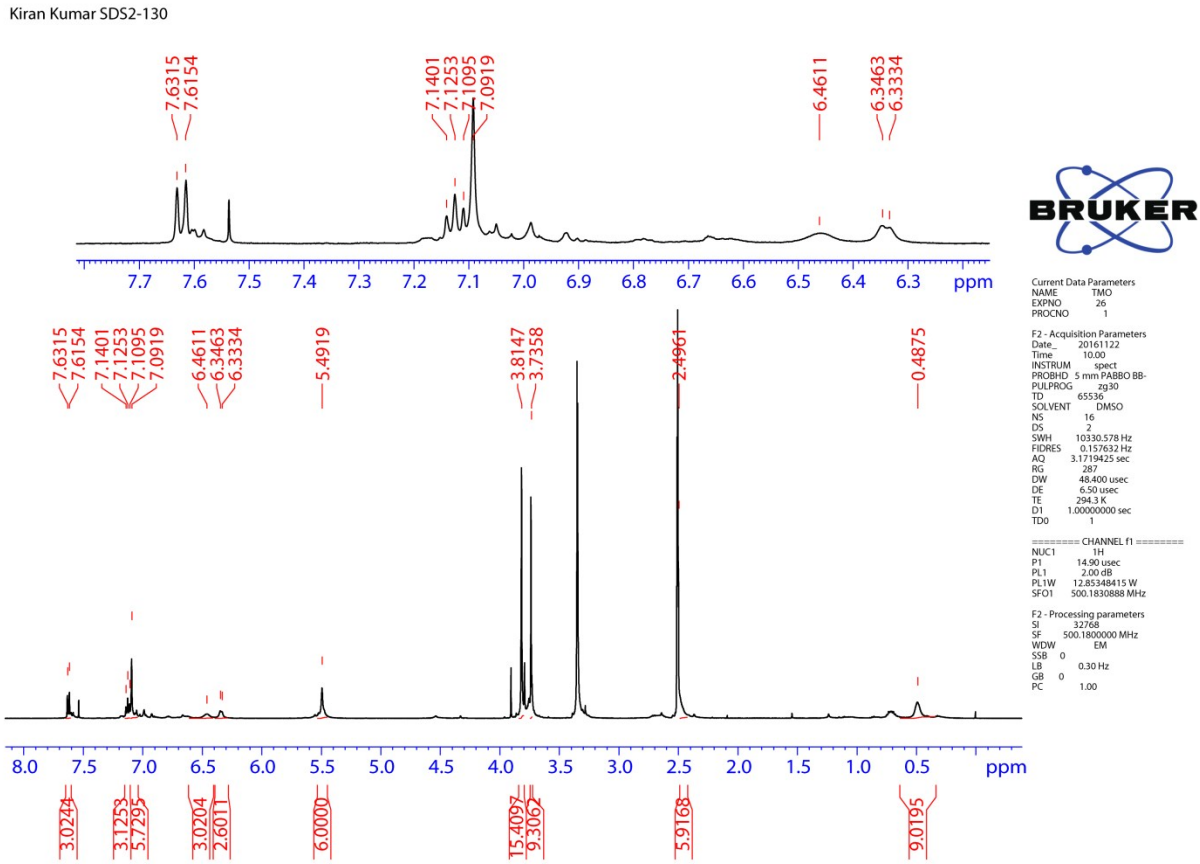
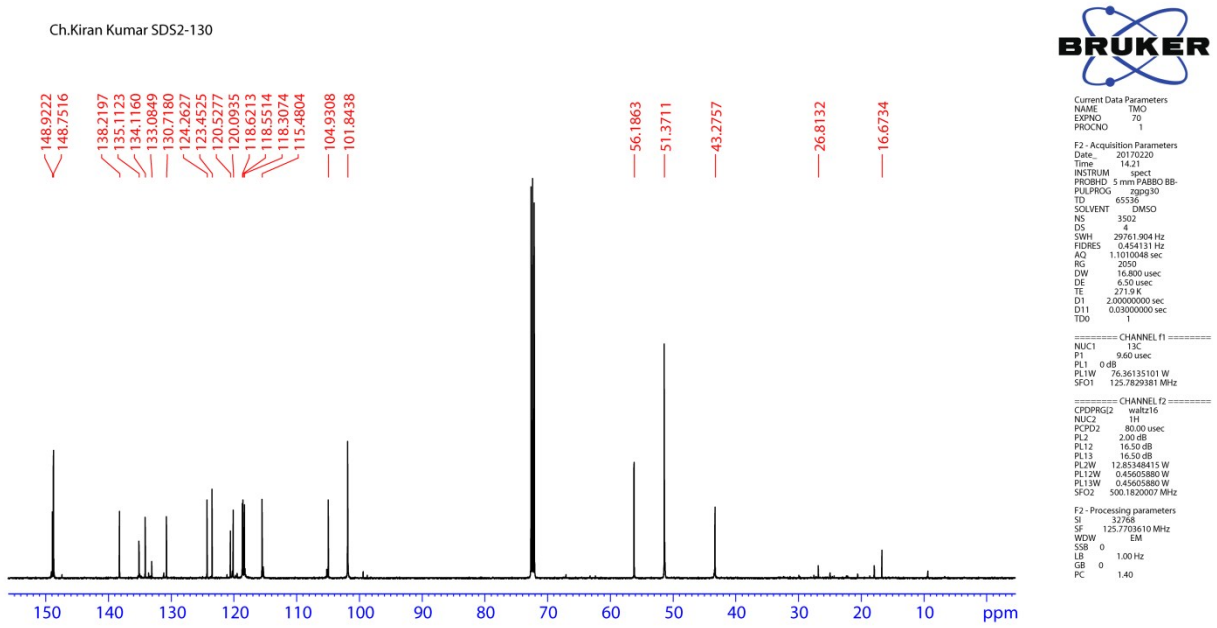


Fig. S28 ^{1}H NMR spectrum of **9** in d_6-DMSO.



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ig. S29 ^{13}C NMR spectrum of **9** in $CDCl_3$.

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