Supporting Information

Self-assembly from Metal-Organic Vesicles to Globular Networks: Metallogel-Mediated Phenylation of Indole with Phenyl Boronic Acid

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I. General remarks

^{1}H NMR spectra were obtained with a Bruker AV-300 (300 MHz), a Bruker AV-400 (400 MHz), or a Bruker AV-600 (600 MHz) spectrometer, while ^{13}C NMR spectra were recorded with a Bruker AV-300 (75 MHz), or a Bruker AV-400 (100 MHz) spectrometer. The ^{1}H NMR chemical shifts were measured relative to tetramethylsilane, $CDCl_3$ or DMSO-d_6 as the internal reference, while the ^{13}C NMR chemical shifts were recorded with $CDCl_3$ or DMSO-d_6 as the internal standard. Mass spectra were obtained on a Waters Quattro Premier XE Mass Spectrometer or a Finnigan-LCQ^{DECA} instrument. GC-MS analyses were performed using an Agilent 6890-5973 set-up. The ESI-TOF mass spectra were recorded with a Waters Q-Tof premier instrument. High-resolution FAB mass spectra was obtained using a JEOL JMS-SX/SX 102A instrument. The optical rotations were determined with a Rudolph Autopol V polarimeter or a WZZ-2B polarimeter. Elemental analyses were performed with a CARLO ERBA1106 instrument or a Heraeus CHN-O-RAPID instrument. Melting points were determined with XRC-1 and are uncorrected. Dynamic light scattering (DLS) experiments were recorded on a Malvern Nano-ZS ZEN3600 instrument. Transmission electron microscopy (TEM) studies were carried out on a JEM100CXⅡ, operating at 100 kV (Fig. 3c), or a HITACHI H-600, operating at 75 kV (others). Tapping mode AFM imaging was performed under ambient conditions on a SEIKO SPA400 instrument by using BS-Tap 300Al levers (Olympus AC160TS, silicone cantilevers). FTIR spectra were measured with a NEXUS 670 FT-IR spectrometer.

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. Anhydrous solvents were dried by heating at reflux for at least

24 h over CaH_2 (dichloromethane and DMF) or sodium/benzophenone (tetrahydrofuran, toluene, and diethyl ether) and were freshly distilled prior to use. Unless otherwise indicated, all syntheses and manipulations were carried out under dry nitrogen atmosphere. *n*BuLi in Et_2O was prepared according to the literature.[1] Compounds **10a-b** were prepared by literature procedures.[2] Compounds **12a-c** were synthesized according to the procedures reported by Hampton et al.[3] Compounds **13-16** and ligand **7** were synthesized according to our previously reported method.[4] Ligands **1**,[5] **2**,[6] **3**,[7] **4**,[7] and **5**[7-8] were prepared using a modification of literature procedures.

II. Preparation of samples for TEM, AFM and DLS

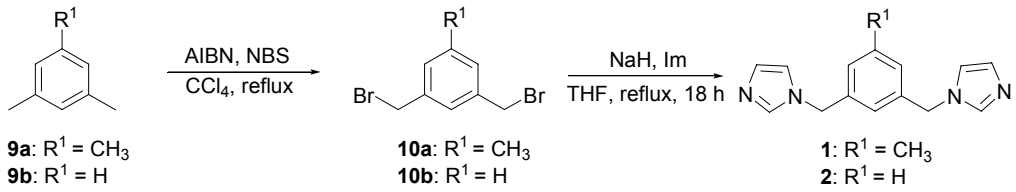
Preparation of samples for TEM: TEM specimens were prepared by gently placing a carbon-coated copper grid on a surface of the sample. The TEM grid was removed, dried for 30 min at room temperature, and then subjected to observation.

Preparation of samples for AFM: The samples of $\{[Pd\text{-}\mathbf{1}](OAc)_2\}_n$ (0.02 wt%, 0.1 mM) and $\{[Pd\text{-}\mathbf{2}](OAc)_2\}_n$ (0.02 wt%, 0.1 mM) in DMSO were cast on a freshly cleaved mica under ambient conditions, and then dried at 55 °C for 1 h before making AFM images.

Preparation of samples for DLS: DLS specimens of $\{[Pd\text{-}\mathbf{1}](OAc)_2\}_n$ and $\{[Pd\text{-}\mathbf{2}](OAc)_2\}_n$ were prepared in DMSO under ambient conditions.

III. Procedures for the preparation of ligands 1-7

i. Synthesis of ligands 1 and 2



9a: $R^1 = CH_3$ **10a**: $R^1 = CH_3$ **1**: $R^1 = CH_3$
9b: $R^1 = H$ **10b**: $R^1 = H$ **2**: $R^1 = H$

Scheme S1 Synthetic route for ligands **1** and **2**.

1,3-Bis(imidazol-1-ylmethyl)-5-methylbenzene (1)

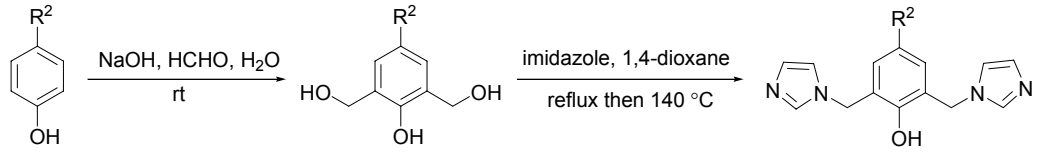
To a flame-dried three-neck round-bottom flask charged with imidazole (1.79 g, 26.2 mmol) and NaH (in 60% oil dispersion, 2.16 g, 52.4 mmol) was added dry THF (50 mL) with stirring at 0 °C under nitrogen. The reaction mixture was then allowed to warm to room temperature, and became a white suspension in 3 h. A solution of **10a** (2.43 g, 8.7 mmol) in 50 mL of THF was added dropwise under reflux, and the resulting mixture was stirred at the same temperature for 18 h. Subsequently, water (50 mL) was slowly added at 0 °C. The resulting mixture was stirred for 20 min and then concentrated under reduced pressure. Dichloromethane (30 mL) was added to the residue and the biphasic mixture was stirred until the solid was dissolved completely. The organic layer was separated, and the aqueous layer was extracted with CH_2Cl_2 (2 × 30 mL). The combined organic layers were washed with brine (35 mL), dried over Na_2SO_4, and concentrated in vacuo. The crude product was purified by silica gel flash column chromatography eluting with CH_2Cl_2/CH_3OH (15:1) to give **1** as a pale white solid (1.50 g, 67.9%).[5] M.p. 105-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.27 (s, 3H), 5.02 (s, 4H), 6.71 (s, 1H), 6.85 (dd, *J* = 1.2 Hz, 1.6 Hz, 2H), 6.86-6.87 (m, 2H), 7.05 (dd, *J* = 1.2 Hz, 1.2 Hz, 2H), 7.50 (s, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.2, 50.4, 119.3, 123.2, 127.8, 129.7, 137.1, 137.3, 139.8 ppm; MS (ESI) *m/z*: 253 $[M+H]^+$.

1,3-Bis(imidazol-1-ylmethyl)benzene (2)

This compound was prepared following the same procedure described above for **1** but using

10b as the starting material. Compound **2** was obtained as a pale yellow solid in 56.3% yield after purification by column chromatography on silica gel eluting with CH_2Cl_2/MeOH (15:1 to 13:1).[6] M.p. 53-55 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.07 (s, 4H), 6.85 (dd, J = 1.2 Hz, 1.2 Hz, 2H), 6.90 (s, 1H), 7.06-7.09 (m, 4H), 7.30 (t, J= 5.9 Hz, 1H), 7.50 (s, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 50.4, 119.3, 125.9, 127.1, 129.7, 129.8, 137.2, 137.4 ppm; MS (ESI) *m/z*: 239 $[M+H]^+$.

ii. Synthesis of ligands 3-5[7]



11a: R^2 = Cl
11b: R^2 = CH_3
11c: R^2 = *t*-Butyl

12a: R^2 = Cl
12b: R^2 = CH_3
12c: R^2 = *t*-Butyl

3: R^2 = Cl
4: R^2 = CH_3
5: R^2 = *t*-Butyl

Scheme S2 Synthetic route for ligands **3**-**5**.

Dihydroxymethyl phenol **12** (25 mmol) and imidazole (62.5 mmol) were added to 1,4-dioxane (10 mL), and stirred under reflux for 2 h. After the solvent was evaporated, the reaction was continued at 130-140 °C for 3 h. The agglomerating mixture was first dissolved in ethanol and then poured into water. The solid was collected and recrystallized from ethanol.

2,6-Bis(imidazol-1-yl)methyl-4-chlorophenol (3)

Yield: 81.3%; M.p. 176-177 °C; ^{1}H NMR (600 MHz, DMSO-d_6): δ 5.19 (s, 4H), 6.90 (s, 2H), 6.95 (s, 2H), 7.17 (s, 2H), 7.71 (s, 2H), 9.80 (br s, 1H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6): δ 45.2, 120.2, 124.0, 128.6, 128.9, 138.1, 151.7 ppm; MS (ESI) *m/z*: 287 $[M-H]^+$.

2,6-Bis(imidazol-1-yl)methyl-4-methylphenol (4)

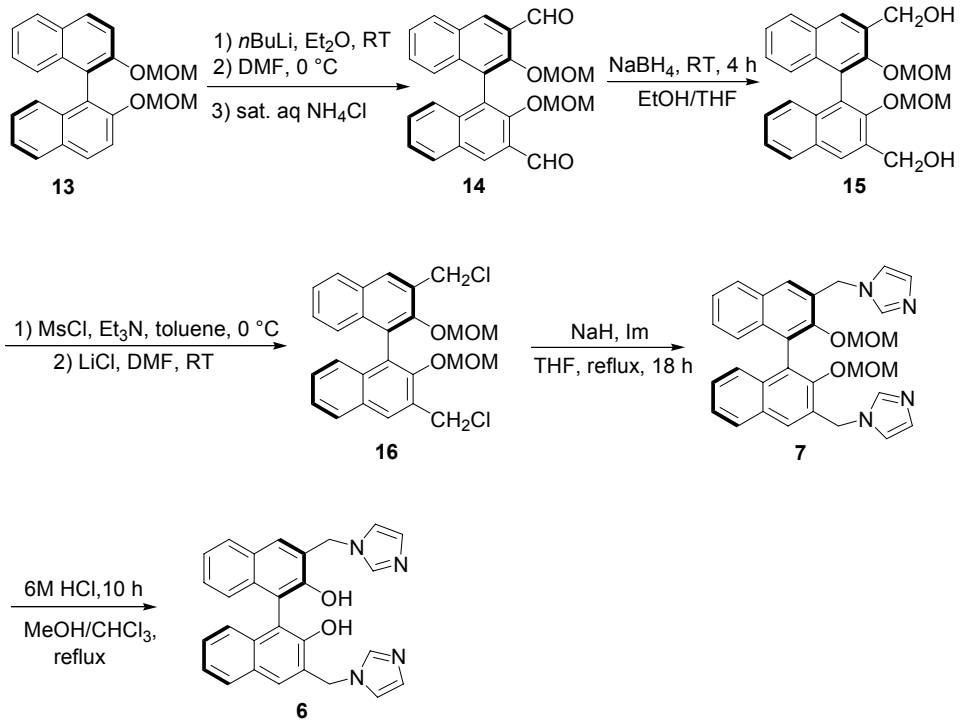
Yield: 67.1%; M.p. 174-175 °C; ^{1}H NMR (600 MHz, DMSO-d_6): δ 2.11 (s, 3H), 5.14 (s, 4H),

6.77 (s, 2H), 6.87 (s, 2H), 7.12 (s, 2H), 7.67 (s, 2H), 9.14 (s, 1H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6): δ 20.6, 45.5, 120.1, 126.2, 128.8, 129.4, 129.9, 137.9, 150.3 ppm; MS (ESI) *m/z*: 267 $[M-H]^+$.

2,6-Bis(imidazol-1-yl)methyl-4-*tert*-butylphenol (5)[7-8]

Yield: 42.7%; M.p. 158-160 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.15 (s, 9H), 5.17 (s, 4H), 6.87 (s, 2H), 7.02 (s, 2H), 7.14 (s, 2H), 7.69 (s, 2H), 9.23 (s, 1H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6): δ 31.6, 34.2, 45.9, 120.1, 125.6, 126.6, 128.7, 137.9, 142.9, 150.5 ppm; MS (ESI) *m/z*: 310 $[M]^+$.

iii. Synthesis of ligands 6 and 7



13 **14** **15** **16** **7** **6**

Scheme S3 Synthetic route for ligands **6** and **7**.

(*R*)-3,3′-Bis(imidazol-1-ylmethyl)-2,2′-dimethoxymethoxy-1,1′-binaphthyl (7)[4]

This compound was prepared following the same procedure described above for **1** but using **16** as the starting material. Compound **7** was obtained in 82.0% yield as a pale yellow

powder after purification by column chromatography on silica gel eluting with CH_2Cl_2/MeOH (25:1). M.p. 143-145 °C; $[\alpha]^{20}_D$ = −90.4 (c = 0.25, CH_3OH); ^{1}H NMR (300 MHz, $CDCl_3$): δ 3.10 (s, 6H), 4.36 (dd, *J* = 5.9 Hz, 6.0 Hz, 4H), 5.41 (dd, *J* = 16.0 Hz, 16.0 Hz, 4H), 7.10-7.18 (m, 6H), 7.26-7.32 (m, 2H), 7.40-7.45 (m, 2H), 7.50 (s, 2H), 7.71 (s, 2H), 7.79 (d, *J* = 8.1 Hz, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 46.9, 57.1, 99.6, 119.6, 125.0, 125.7, 125.8, 127.3, 128.2, 128.5, 129.8, 130.7, 133.8, 137.8, 152.1 ppm; MS (ESI) *m/z*: 557 $[M+Na]^+$.

(*R*)-3,3'-Bis(imidazol-1-ylmethyl)-1,1'-bi-2-naphthol (6)

Aqueous HCl (6 *M*, 4.0 mL) was added to a solution of **7** (1.28 g, 2.4 mmol) in chloroform (60 mL) and methanol (20 mL). The resulting solution was refluxed for 15 h until the conversion of **7** was complete. The solution was then cooled to room temperature and neutralized by addition of saturated aqueous $NaHCO_3$ solution. After the resulting mixture was stirred for a further 12 h, the organic layer was separated, and the aqueous phase was extracted with ethyl acetate/THF (1:3, 3 × 40 mL). The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure. The resulting residue was purified by flash column chromatography on silica gel eluting with CH_2Cl_2/MeOH (10:1 to 7:1) to give **6** (0.90 g, 84.1%) as a pale-yellow solid. M.p. 248-250 °C; $[\alpha]^{20}_D$ = + 101.4 (c = 0.50, DMSO); ^{1}H NMR (400 MHz, DMSO-d_6): δ 5.39 (s, 4H), 6.81 (d, *J* = 8.4 Hz, 2H), 6.94 (s, 2H), 7.16 (dd, *J* = 6.8 Hz, 8.0 Hz, 2H), 7.24-7.28 (m, 4H), 7.59 (s, 2H), 7.76-7.80 (m, 4H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6): δ 46.6, 114.8, 120.4, 123.5, 124.4, 126.7, 127.9, 128.4, 128.6, 128.8, 134.3, 138.1, 152.5 ppm; HRMS (FAB) calcd. for $C_{28}H_{23}N_4O_2$ $[M+H]^+$: 447.1821, found: 447.1824; Anal. Calcd. for $C_{28}H_{22}N_4O_2$: C, 75.32; H, 4.97; N, 12.55. Found: C, 74.98;

H, 5.07; N, 12.34.

IV. Gelation test of 3-6 with $Pd(OAc)_2$ in a 1:1 molar ratio in different solvents

Gelation tests: When a DMSO solution of ligands **3-6** reacted with a DMSO solution of $Pd(OAc)_2$ at the 1:1 molar ratio of ligand: metal salt, a clear yellow or red solution was formed initially. After the mixture was left to stand at room temperature for a few hours, an opaque but stable metallogel was formed, which was simply confirmed by the "stable to inversion of a test tube" method. Gelation properties in different solvents were summarized in Tables S1 and S2.

Table S1 Gelation test of **3-6** with $Pd(OAc)_2$ in different solvents

Entry	Solvent	{[Pd-**3**]OAc}$_n$[a]	{[Pd-**4**]OAc}$_n$[b]	{[Pd-**5**]OAc}$_n$[c]	{[Pd-**6**]OAc}$_n$[d]
1	methanol	P	P	P	P
2	ethanol	P	P	P	P
3	DMF	G	P	S	G
4	DMSO	G	G	G	G
5	DMA	G	S	S	G[e]
6	NMP	G	G	WG[e]	PG[e]
7	1,4-dioxane	I	I	I	I
8	acetonitrile	I	I	I	I
9	toluene	I	I	I	I

[a] Gelator: 1.15 wt%. [b] Gelator: 1.11 wt%. [c] Gelator: 1.20 wt%. [d] Gelator: 1.87 wt%. [e] Gels were formed by standing at room temperature for a few days. G: steady gel; PG: partial gel; WG: weak gel; P: precipitate; I: Ligand is insoluble; S: solution.

Table S2 Gelation properties of **3-6** with $Pd(OAc)_2$ in a mixture of DMSO/solvent (v/v 2:1) at room temperature

Entry	Solvent	{[Pd-**3**]OAc}$_n$ [a]	{[Pd-**4**]OAc}$_n$ [b]	{[Pd-**5**]OAc}$_n$ [c]	{[Pd-**6**]OAc}$_n$ [d]
1	acetone	P	P	P	P
2	tetrahydrofuran	G	G	G	G
3	diethyl ether	P	P	P	P
4	1,4-dioxane	G	G	G	PG
5	ethyl acetate	P	P	P	P
6	acetonitrile	P	P	P	P
7	water	S	S	S	S
8	methanol	S	S	S	S
9	ethanol	S	S	S	S
10	toluene	G	WG	WG	G
11	DCM	P	P	P	P
12	DCE	P	P	P	P
13	$CHCl_3$	P	P	P	P
14	m-xylene	G	WG	WG	G
15	benzene	G	WG	WG	G
16	HOAc	S	S	S	S
17	pyridine	S	S	S	S

[a] Gelator: 1.15 wt%. [b] Gelator: 1.11 wt%. [c] Gelator: 1.20 wt%. [d] Gelator: 1.87 wt%. G: steady gel; PG: partial gel; WG: weak gel; P: precipitate; S: solution.

V. Morphology analysis of the $\{[Pd\text{-}L](OAc)_2\}_n$ aggregates

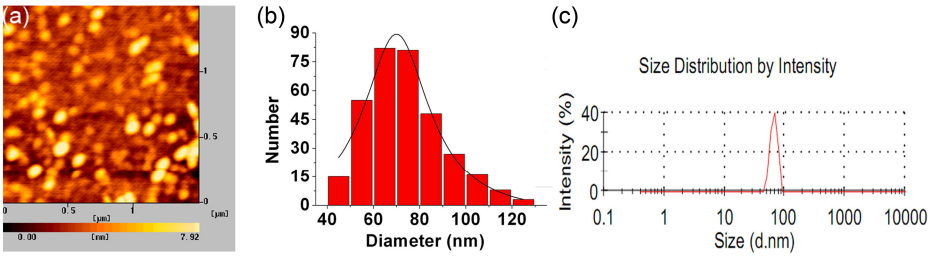


Fig. S1 (a) Tapping-mode AFM height image of aggregates of $\{[Pd\text{-}\mathbf{2}](OAc)_2\}_n$ in DMSO (0.02 wt%) on a freshly cleaved mica surface after the solvent was evaporated. (b) The corresponding histogram (Lorentzian fit) of $\{[Pd\text{-}\mathbf{2}](OAc)_2\}_n$. (c) The intensity-weighted distribution of the aggregates obtained from the DLS measurement of the sample of $\{[Pd\text{-}\mathbf{2}](OAc)_2\}_n$ (1.3 wt%) in DMSO at 25 °C.

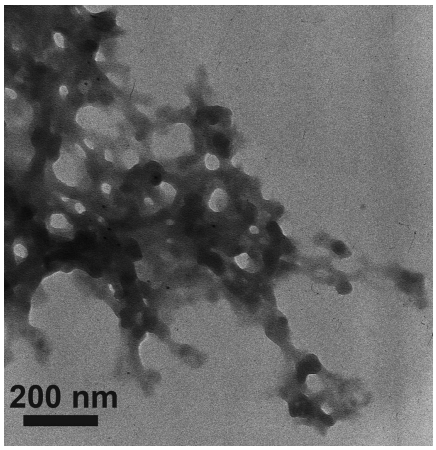


Fig. S2 TEM images (unstained) obtained from the metallogel of $\{[Pd\text{-}\mathbf{3}](OAc)_2\}_n$ in DMSO (1.2 wt%).

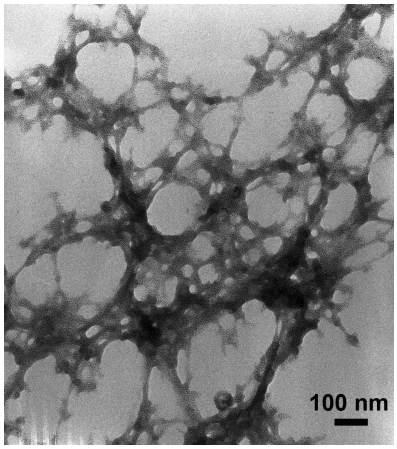


Fig. S3 TEM images (unstained) obtained from the metallogel of {[Pd-**4**](OAc)$_2$}$_n$ in DMSO (0.7 wt%).

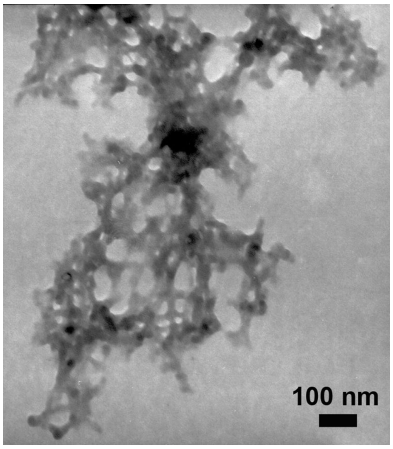


Fig. S4 TEM images (unstained) obtained from the metallogel of {[Pd-**6**](OAc)$_2$}$_n$ in DMSO (2.1 wt%).

VI. Catalytic procedure for 2-phenylation of indole[9]

A flame-dried reaction vessel was charged with indole (58.5 mg, 0.5 mmol, 1.0 equiv), phenyl boronic acid (91.5 mg, 0.75 mmol, 1.5 equiv), the freshly prepared gel of $\{[Pd\text{-}\mathbf{3}](OAc)_2\}_n$ (0.025 mmol of Pd(II), 0.4 mL of DMF) and AcOH (5.0 mL). The resulting solution was degassed twice and refilled with O_2 (1.0 atm.). After the reaction mixture was stirred at room temperature for 10 h, AcOH was removed in *vacuo*. The residue was extracted with CH_2Cl_2 (50 mL) and washed with aqueous $NaHCO_3$ (2 × 30 mL). The organic layer was dried over $MgSO_4$, and concentrated under reduced pressure. Purification of the residue by flash chromatography eluting with petroleum ether/ethyl acetate (6: 1) afforded the desired product. M.p. 138-139 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.85 (s, 1H), 7.12 (t, J= 7.6 Hz, 1H), 7.19 (t, J= 8.0 Hz, 1H), 7.32 (t, J= 7.2 Hz, 1H), 7.41-7.48 (m, 3H), 7.64-7.69 (m, 3H), 8.36 (s, 1H) ppm; GC-MS: *m/z* 193 $[M]^+$.

VII. X-Ray crystallography of the complex $\{[Pd\text{-}3]Cl_2\}_2$ (8)

A DMSO solution (2 mL) of **3** (28.9 mg, 0.1 mmol) was added slowly with constant stirring to a DMSO solution (2 mL) of $PdCl_2(CH_3CN)_2$ (25.9 mg, 0.1 mmol) to give a yellow solution. The reaction mixture was stirred for 30 min and was then filtered to remove a trace amount of undissolved substance. Yellow block crystals $\{[Pd\text{-}\mathbf{3}]Cl_2\}_2$ (**8**) suitable for X-ray analysis were obtained by slow diffusion of acetone into the corresponding DMSO solution at ambient temperature after several days (yield 71%). Anal. Calcd. for $C_{28}H_{26}N_8O_2Pd_2Cl_6 \cdot 2DMSO$: C, 35.31; H, 3.52; N, 10.30. Found: C, 35.17; H, 3.65; N, 10.07.

X-Ray single-crystal diffraction data for **8** was collected on a Bruker SMART 1000 CCD areadetector diffractometer at 100 K with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) with ω scan mode. The structure was solved by direct methods using the SHELXS program and refined by full-matrix least-squares methods with SHELXL.[10] All non-hydrogen atoms were located in successive difference Fourier syntheses and refined with anisotropic thermal parameters on F^2. Hydrogen atoms were included in calculated positions and refined with constrained thermal parameters riding on their parent atoms. The crystal parameters, data collection and refinement results for the complex **8** are summarized in Table S3.

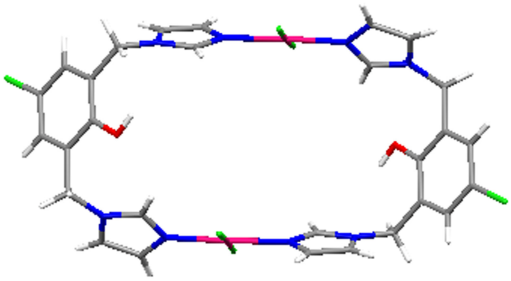


Fig. S5 The crystal structure of the metallomacrocycle {[Pd-**3**]Cl_2}$_2$ (**8**). Atom color code: C (dark gray), N (blue), O (red), Pd (pink), Cl (green), H (white). The hydrogen-bond interactions (Å) are shown as black dashed lines. The solvent DMSO molecules are omitted for clarity.

Table S3 The crystal parameters, data collection and refinement results for **8**

	8
chemical formula	$C_{35}H_{47}Cl_6N_8O_{5.5}Pd_2S_{3.5}$
formula weight (M)	1205.52
temperature (K)	100(2)
wavelength (Å)	0.71073
crystal system	triclinic

space group	*P*-1
crystal size (mm^3)	0.43×0.40×0.25
a (Å)	10.4624(5)
b (Å)	10.9371(3)
c (Å)	11.9010(4)
α (deg)	94.927(2)
β (deg)	112.740(4)
γ (deg)	99.666(3)
volume ($Å^3$)	1220.98(8)
Z	1
calculated density (g cm^{-3})	1.640
μ (mm^{-1})	1.263
reflections collected	11094
independent reflections	5565 [R_{int} = 0.0163]
F(000)	607
GOF	1.178
final R indices [I>2sigma(I)]	R_1 = 0.0349, wR_2 = 0.1257
R indices (all data)	R_1 = 0.0399, wR_2 = 0.1289

VIII. Copy of ESI-MS spectrum of the complex $\{[Pd\text{-}3](OAc)_2\}_2$

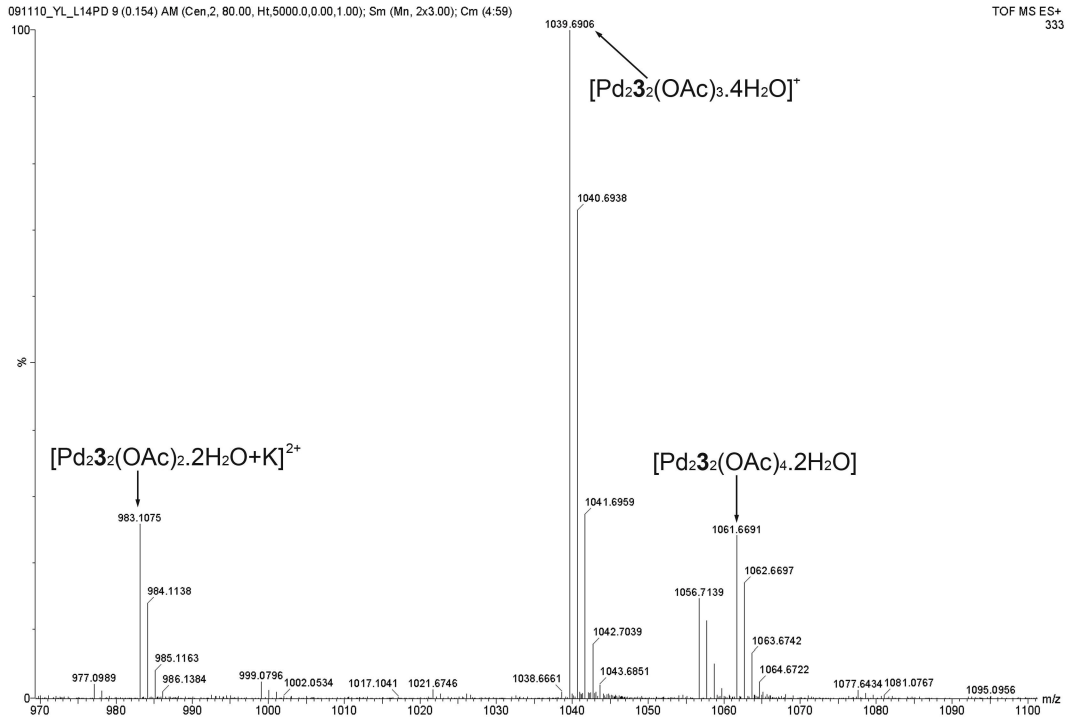


Fig. S6 The ESI-TOF mass spectrum of $\{[Pd\text{-}\mathbf{3}](OAc)_2\}_2$.

IX. FTIR spectra of 3 and the metallogel of $\{[Pd\text{-}3](OAc)_2\}_n$

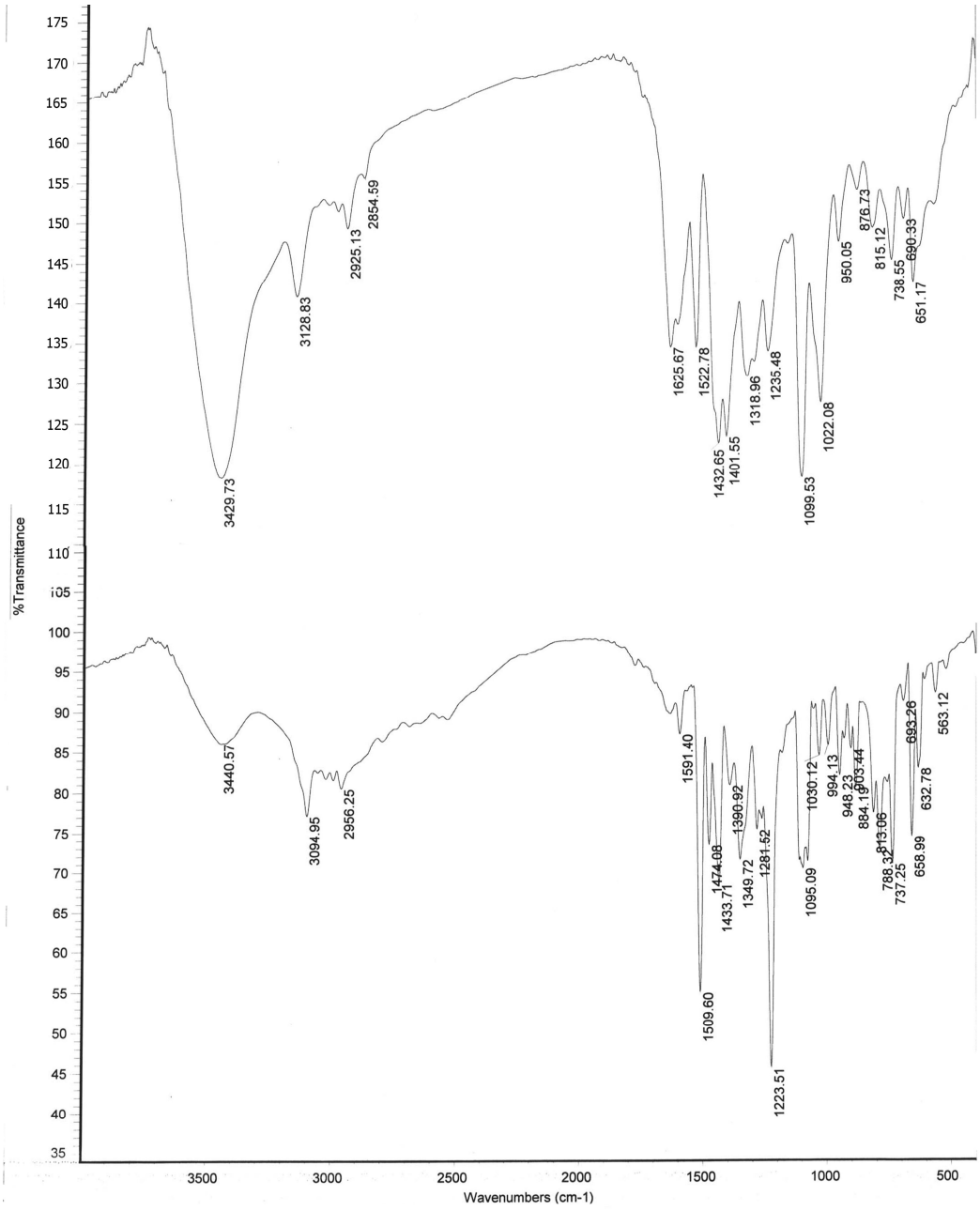


Fig. S7 The FTIR spectra of **3** and the dry metallogel of $\{[Pd\text{-}\mathbf{3}](OAc)_2\}_n$: top: metallogel; bottom: **3**.

X. References

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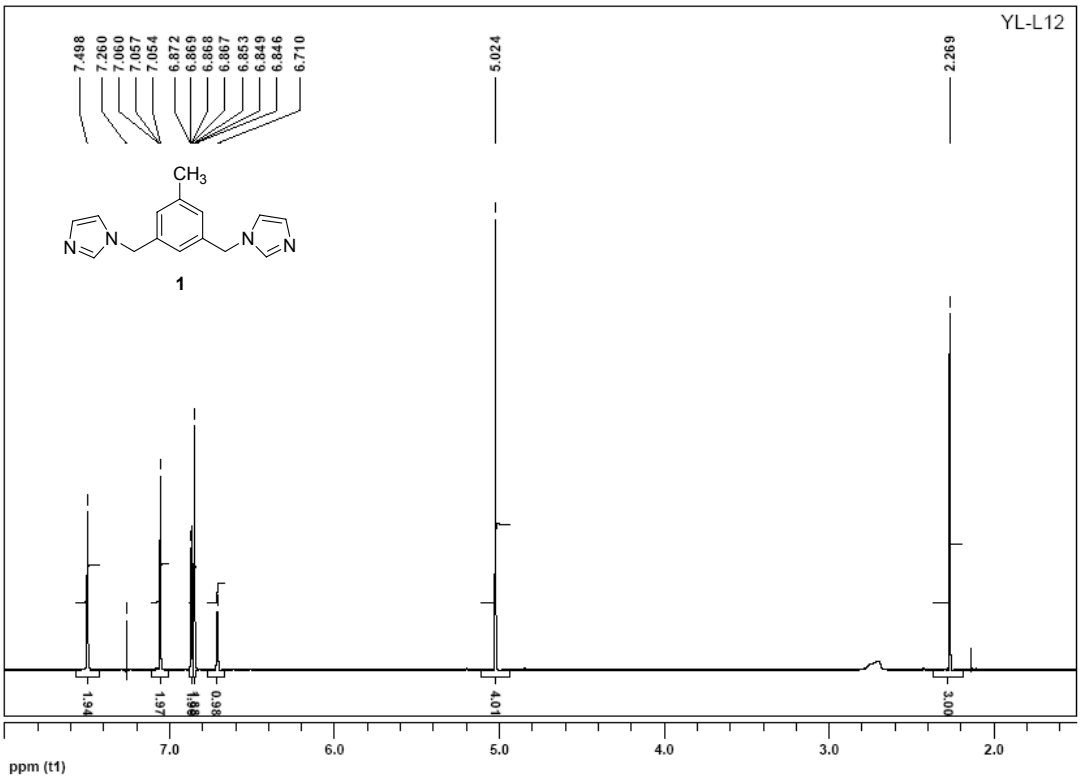
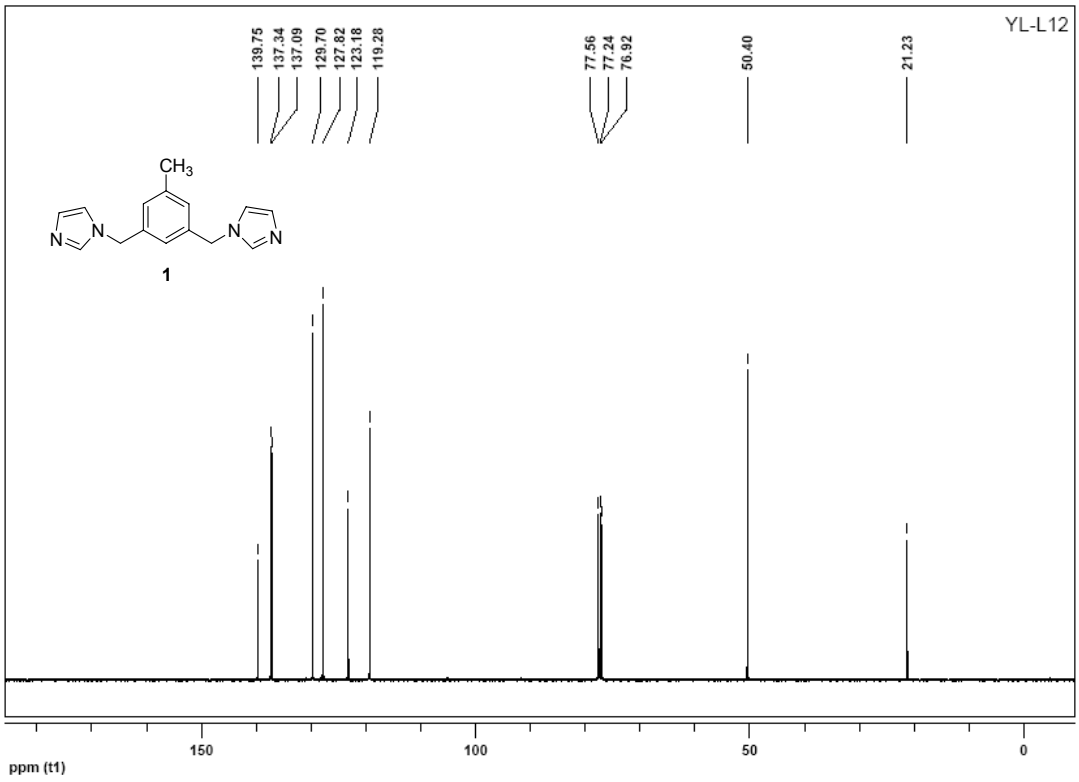
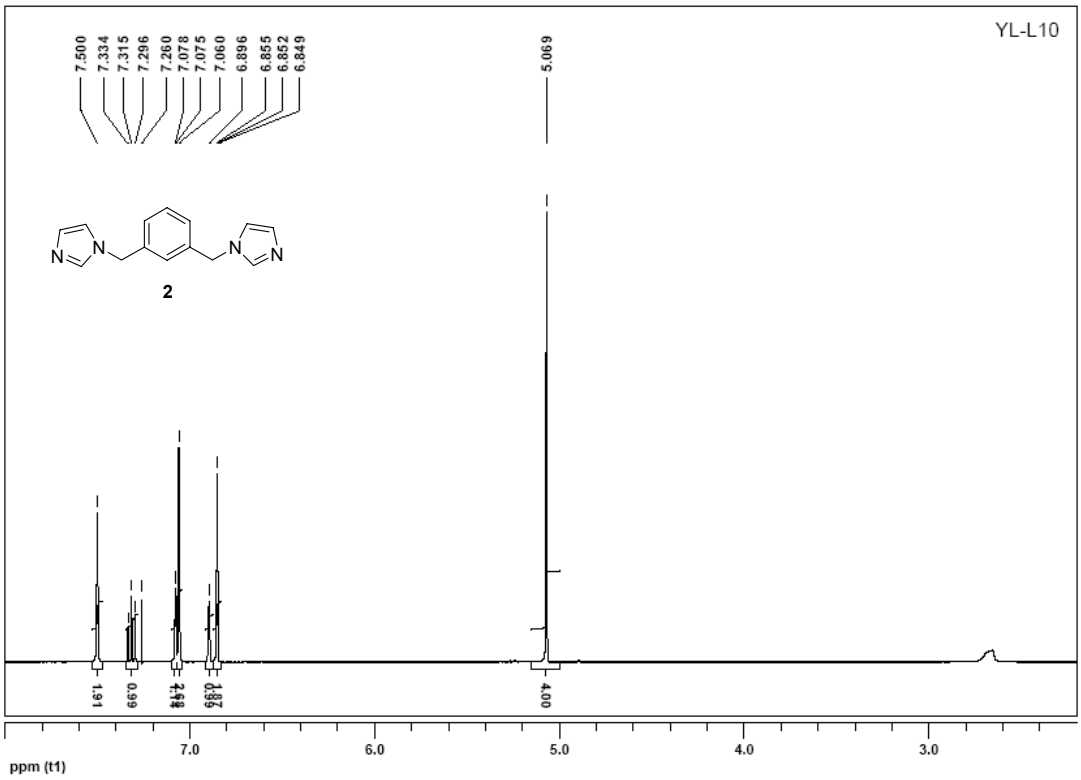
XI. Copies of ^{1}H and ^{13}C NMR spectra of ligands 1-7 and 2-phenyl indole



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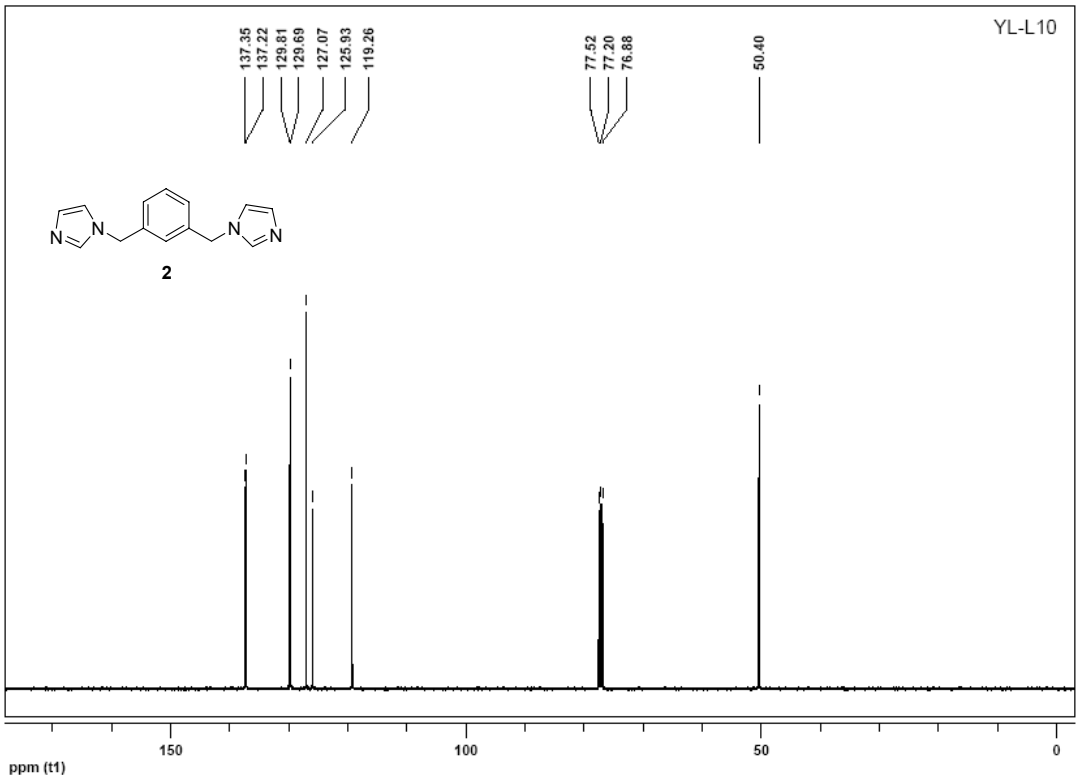
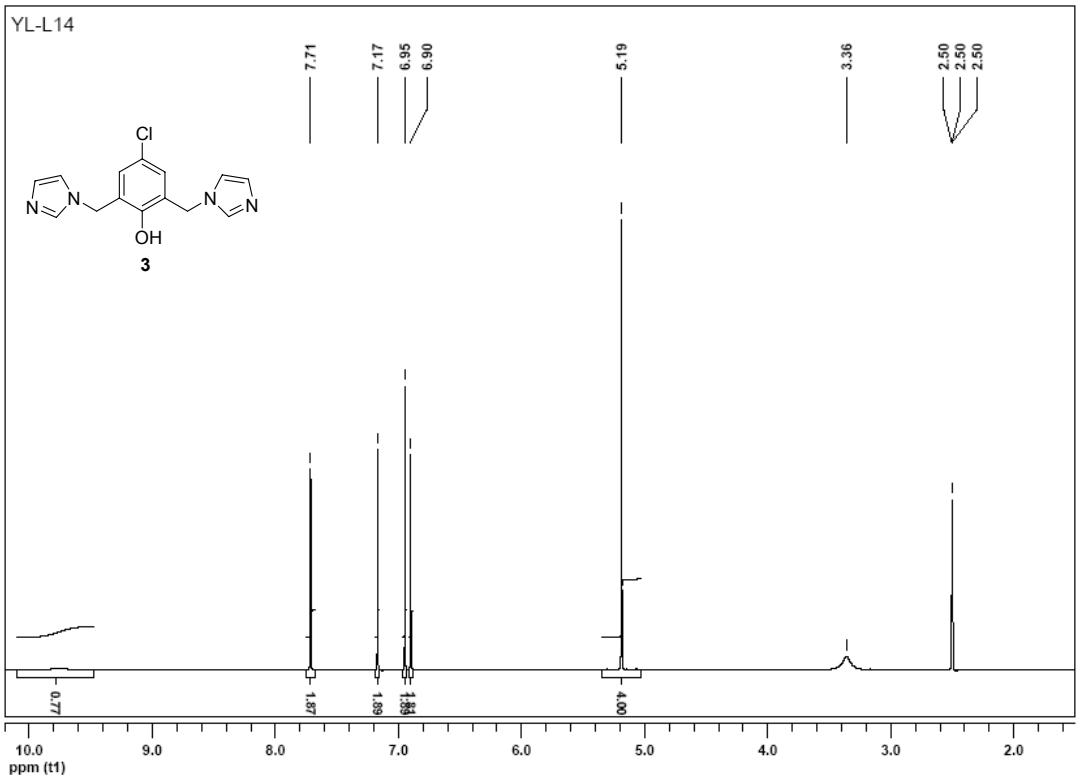
7.334
7.315
7.296
7.260
7.078
7.075
7.060
6.896
6.855
6.852
6.849
5.069
2
1.91
0.99
4.00
7.0
6.0
5.0
4.0
3.0
ppm (t1)


YL-L10
137.35
137.22
129.81
129.69
127.07
125.93
119.26
77.52
77.20
76.88
50.40
2
150
100
50
0
ppm (t1)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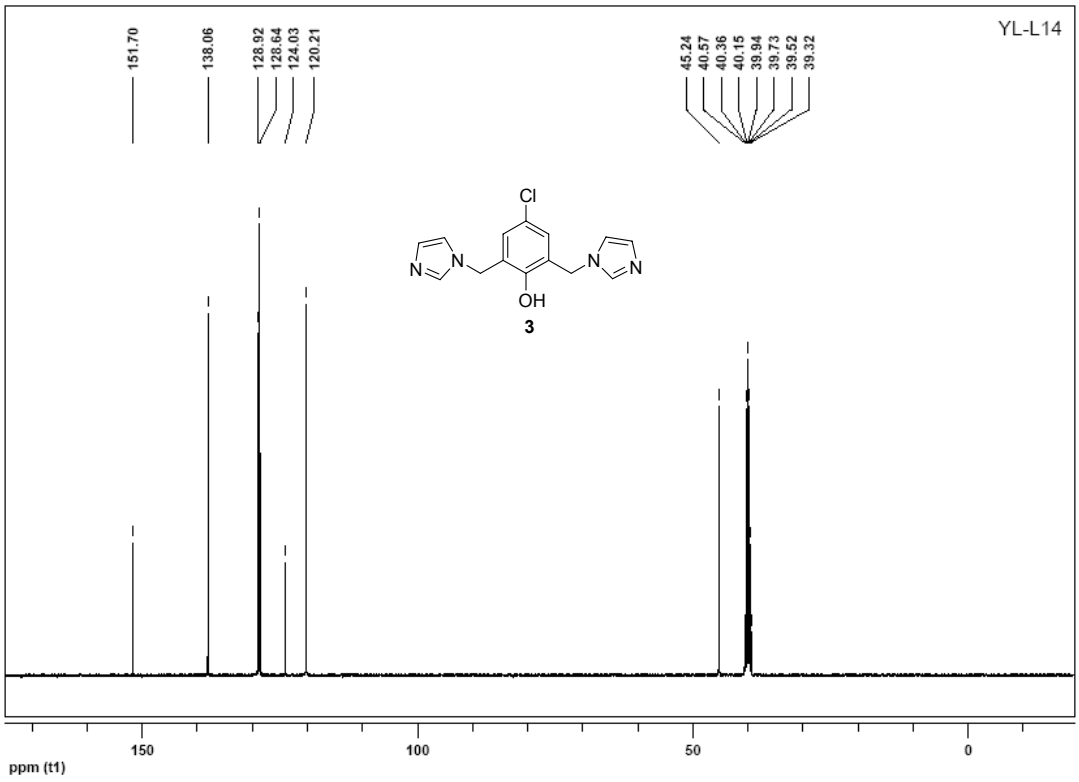
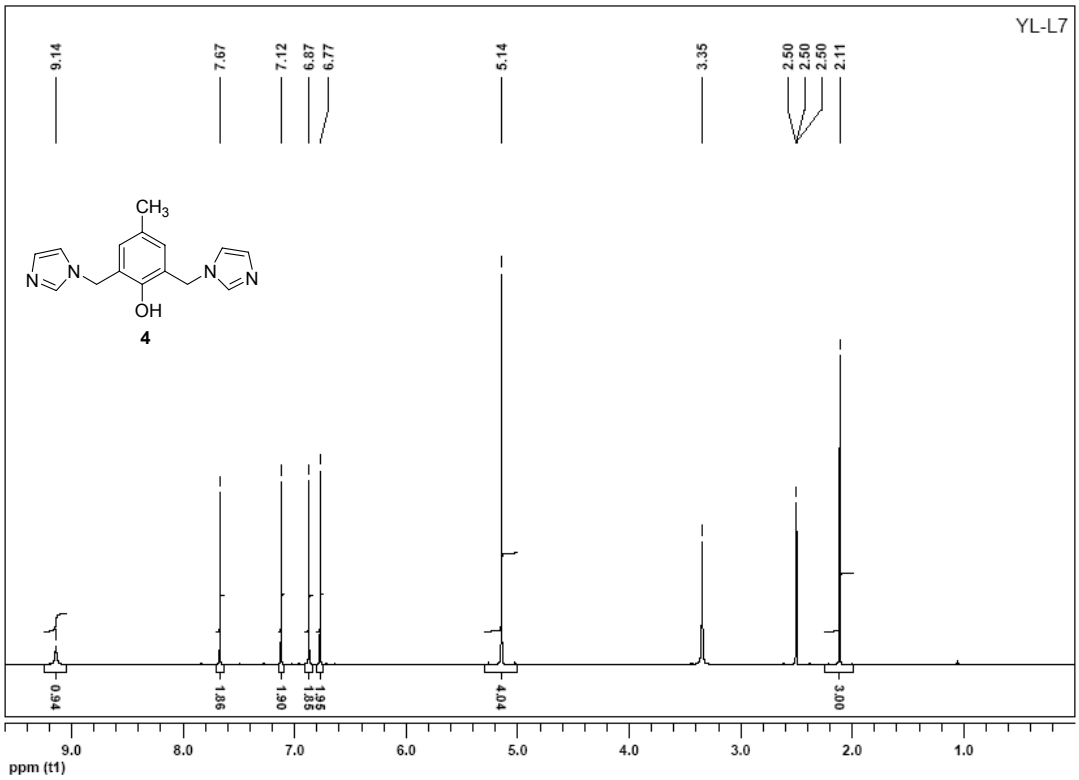
7.71
7.17
6.95
6.90
5.19
3.36
2.50
2.50
2.50
Cl
N
N
N
N
OH
3
0.77
1.87
1.69
4.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm (t1)


YL-L14
151.70
138.06
128.92
128.64
124.03
120.21
45.24
40.57
40.36
40.15
39.94
39.73
39.52
39.32
Cl
N
N
N
N
OH
3
150
100
50
0
ppm (t1)


YL-L7
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7.67
7.12
6.87
6.77
5.14
3.35
2.50
2.50
2.50
2.11
CH3
N
N
N
N
OH
4
0.94
1.86
1.90
1.85
1.95
4.04
3.00
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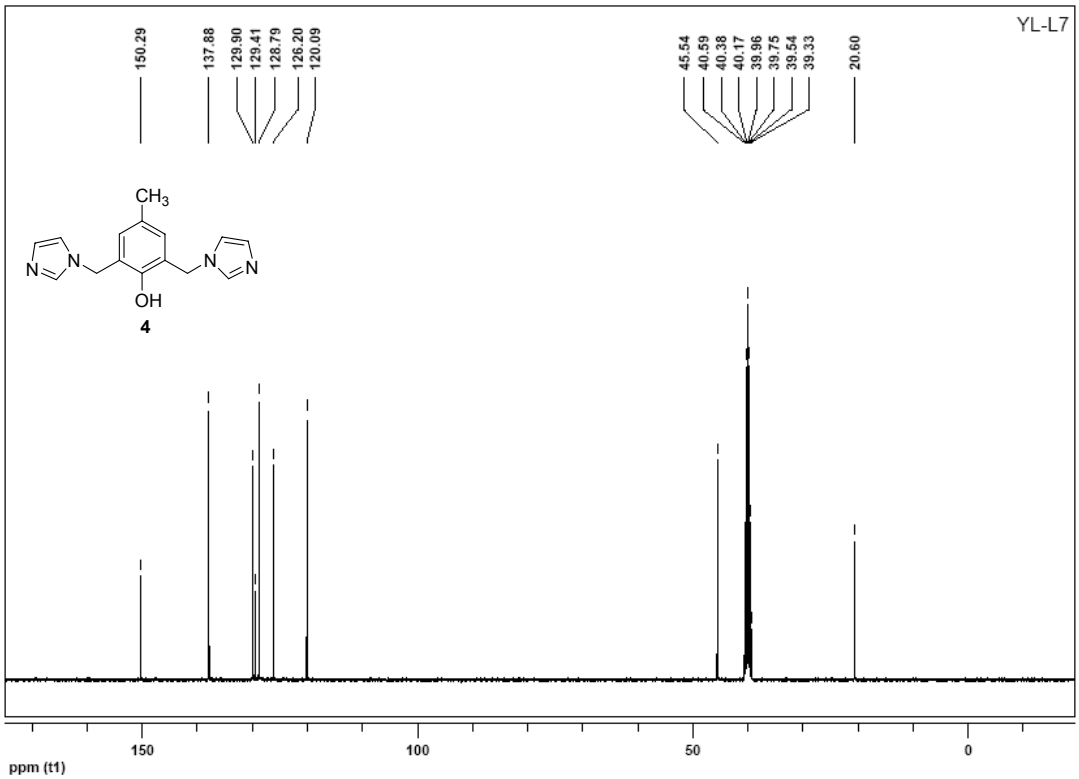
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)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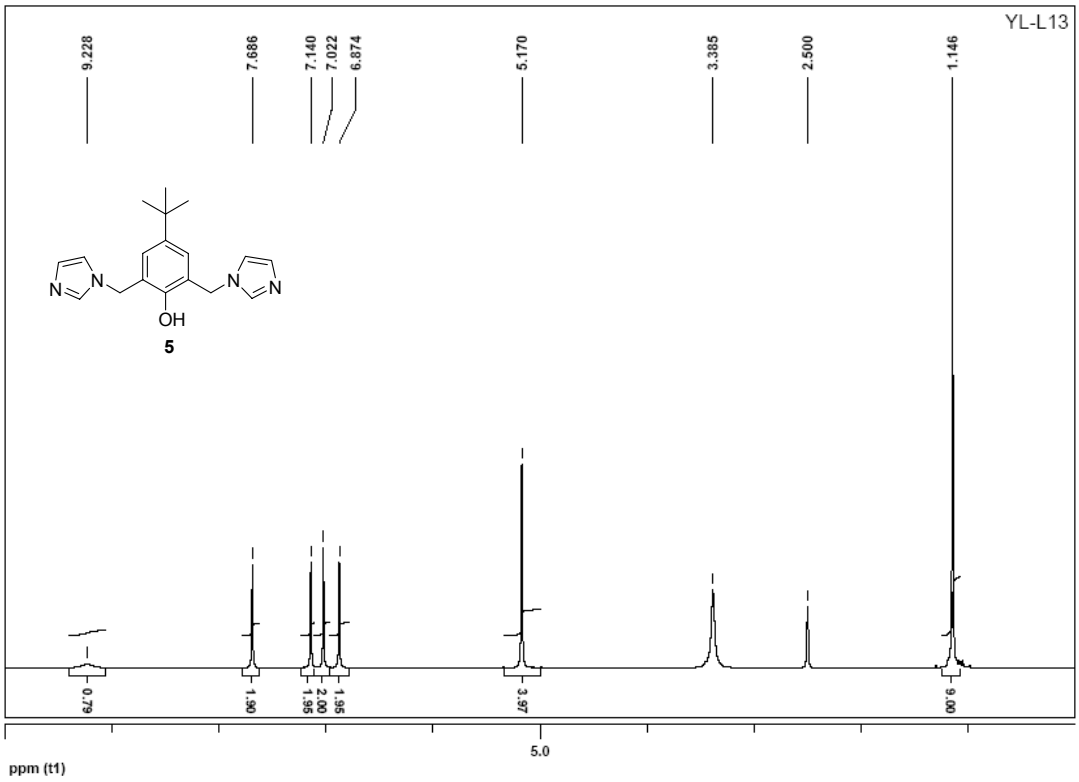
137.88
129.90
129.41
128.79
126.20
120.09
45.54
40.59
40.38
40.17
39.96
39.75
39.54
39.33
20.60
CH3
N
N
N
N
OH
4
150
100
50
0
ppm (t1)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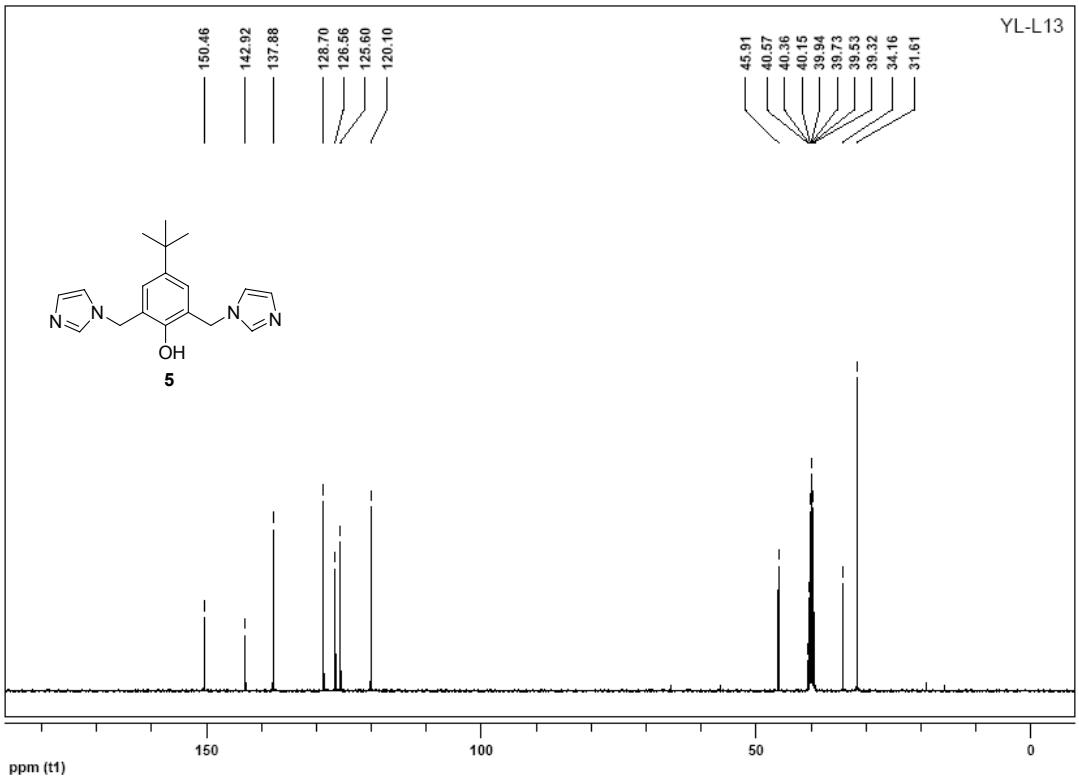
7.140
7.022
6.874
5.170
3.385
2.500
1.146
OH
5
0.79
1.00
1.96
2.00
1.96
3.97
9.00
5.0
ppm (t1)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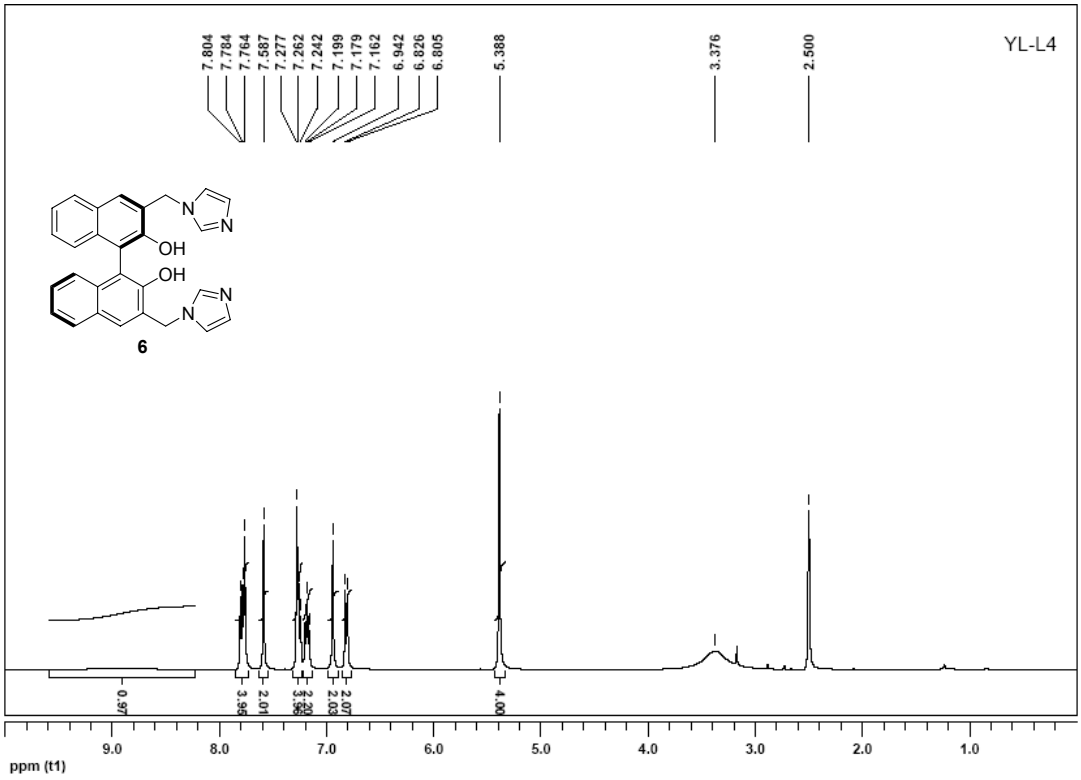
150.46
142.92
137.88
128.70
126.56
125.60
120.10
45.91
40.57
40.36
40.15
39.94
39.73
39.53
39.32
34.16
31.61
OH
5
150
100
50
0
ppm (t1)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7.587
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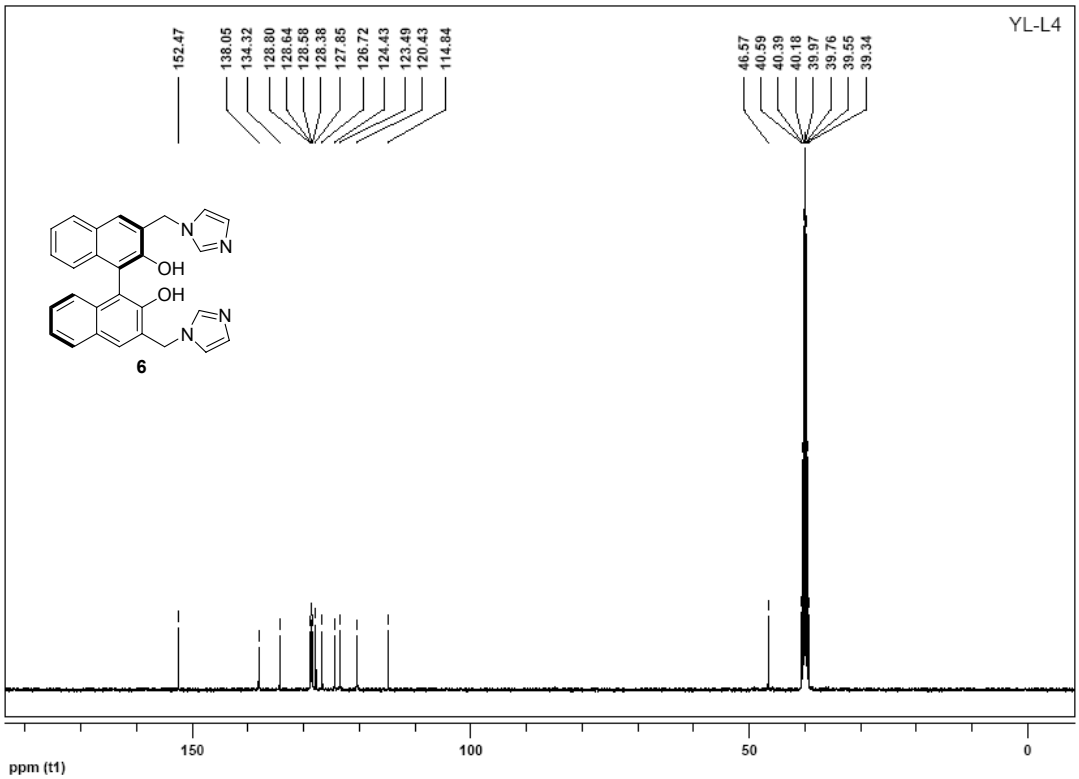
7.262
7.242
7.199
7.179
7.162
6.942
6.826
6.805
5.388
3.376
2.500
OH
OH
N
N
N
N
6
0.97
3.95
2.01
2.20
3.56
2.03
2.07
4.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)


YL-L4
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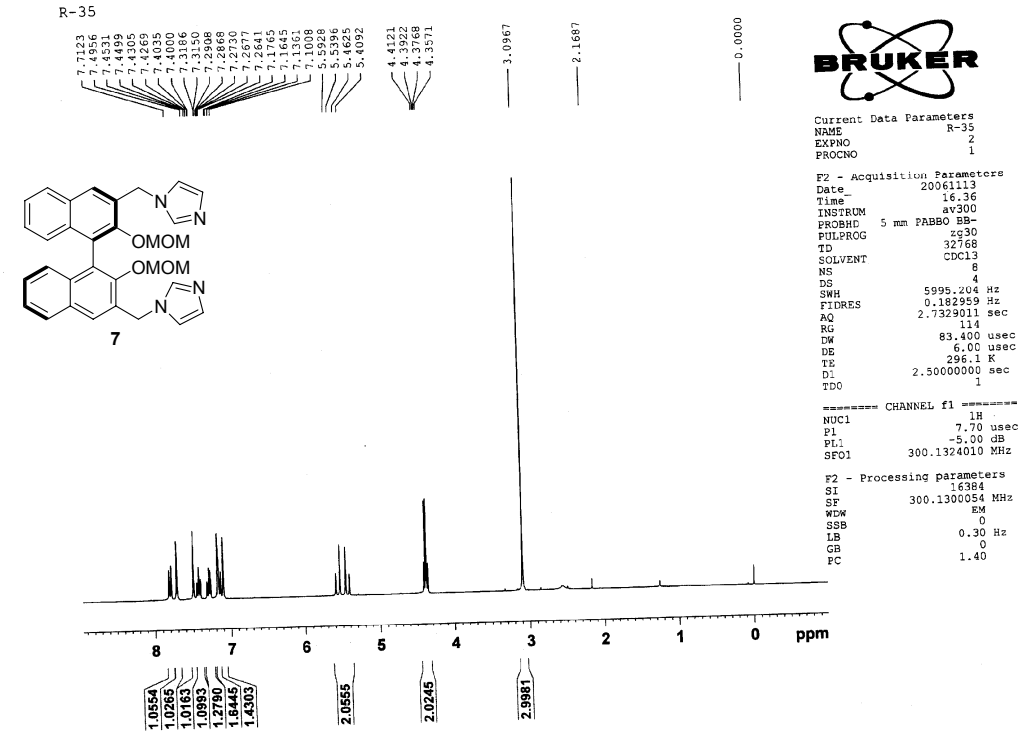
138.05
134.32
128.80
128.64
128.58
128.38
127.85
126.72
124.43
123.49
120.43
114.84
46.57
40.59
40.39
40.18
39.97
39.76
39.55
39.34
OH
OH
N
N
N
N
6
150
100
50
0
ppm (t1)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7.4499
7.4305
7.4269
7.4035
7.4000
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7.3150
7.2908
7.2668
7.2730
7.2677
7.2641
7.1765
7.1645
7.1361
7.1008
5.5928
5.5396
5.4695
5.4092
4.4121
4.3922
4.3768
4.3571
3.0967
2.1687
0.0000
OMOM
OMOM
7
1.0554
1.0266
1.0163
1.0993
1.2790
1.6445
1.4303
2.0555
2.0245
2.9981
8
7
6
5
4
3
2
1
0
ppm
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PROCNO 1
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SOLVENT CDCl3
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FIDRES 0.182959 Hz
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RG 114
DW 83.400 usec
DE 6.00 usec
TE 296.1 K
D1 2.50000000 sec
TD0 1
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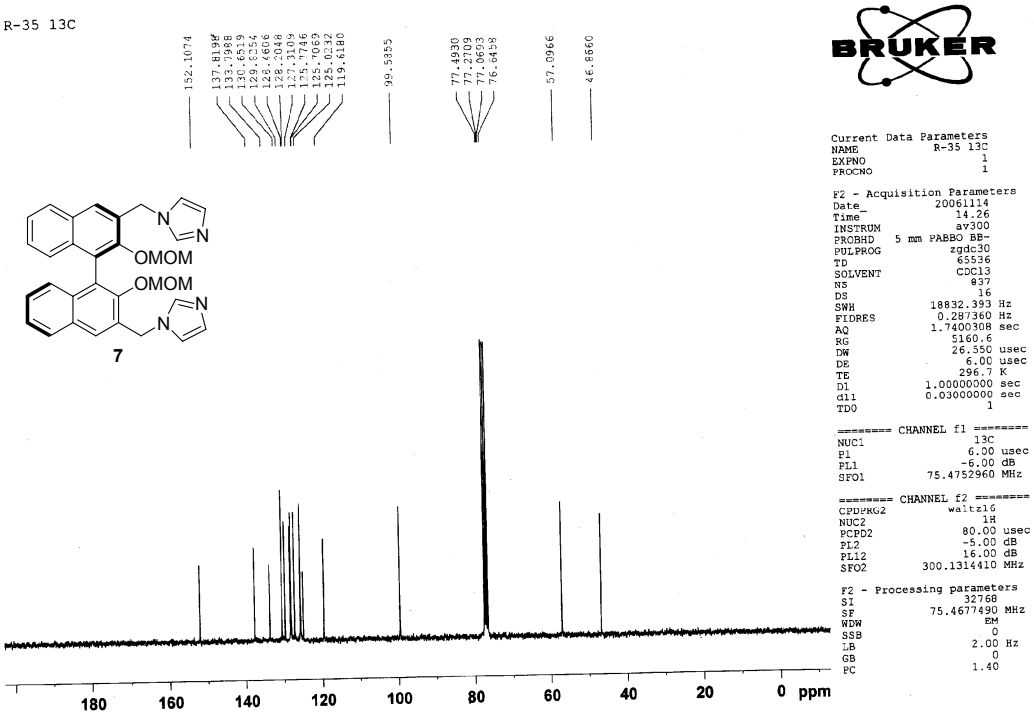
NUC1 1H
P1 7.70 usec
PL1 -5.00 dB
SFO1 300.1324010 MHz
F2 - Processing parameters
SI 16384
SF 300.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40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129.8254
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127.3109
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125.7069
125.0232
119.6180
99.5355
77.4930
77.2709
77.0693
76.6458
57.0966
46.8660
OMOM
OMOM
7
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
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PROCNO 1
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PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 937
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SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5160.6
DW 26.550 usec
DE 6.00 usec
TE 296.7 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -6.00 dB
SFO1 75.4752960 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 16.00 dB
SFO2 300.1314410 MHz
F2 - Processing parameters
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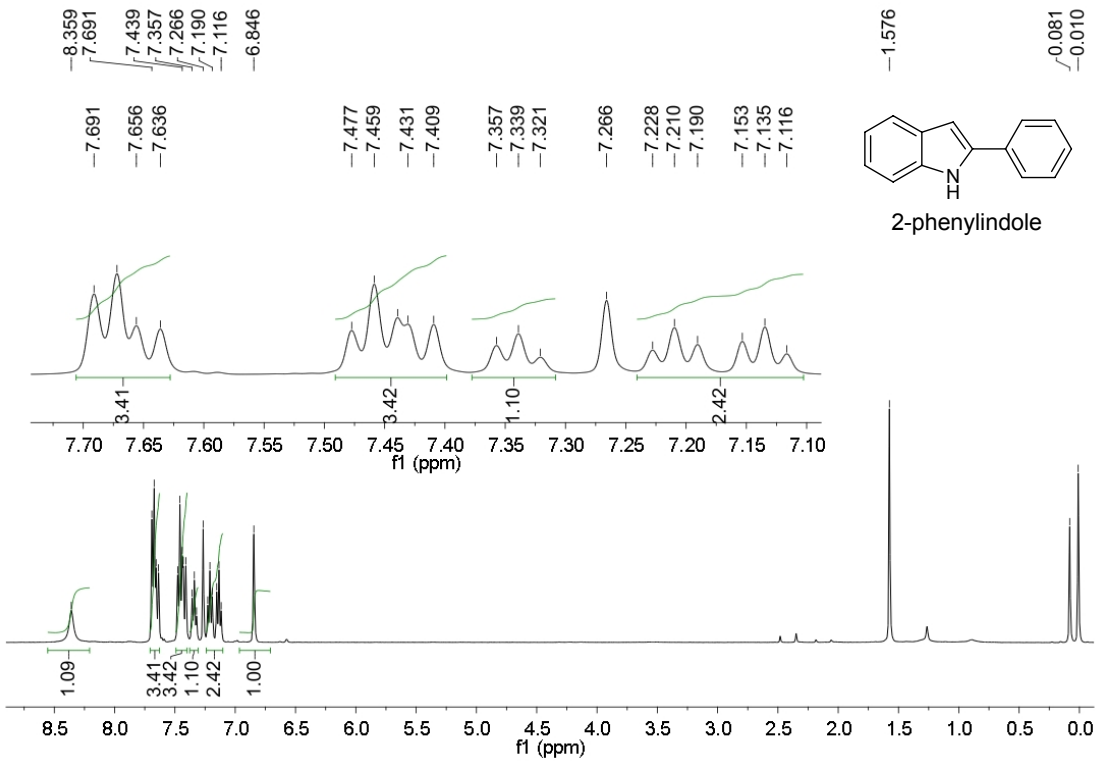
8.359
7.691
7.439
7.357
7.266
7.190
7.116
6.846
1.576
0.081
0.010
7.691
7.656
7.636
7.477
7.459
7.431
7.409
7.357
7.339
7.321
7.266
7.228
7.210
7.190
7.153
7.135
7.116
2-phenylindole
3.41
3.42
1.10
2.42
f1 (ppm)
1.09
3.41
3.42
1.10
2.42
1.00
f1 (ppm)