

Supplementary Information

Synthesis, Structure and Catalysis of NHC-Pd(II) Complex Based on Tetradentate Mixed Ligand

Qing-Xiang Liu*, Kang-Qing Cai, Zhi-Xiang Zhao

Tianjin Key Laboratory of Structure and Performance for Functional Molecules; Key Laboratory of Inorganic-Organic Hybrid Functional Material Chemistry, Ministry of Education; College of Chemistry, Tianjin Normal University, Tianjin 300387, China.

** Corresponding author, E-mail: tjnulqx@163.com*

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1. The figures for the crystal packings of complex 1

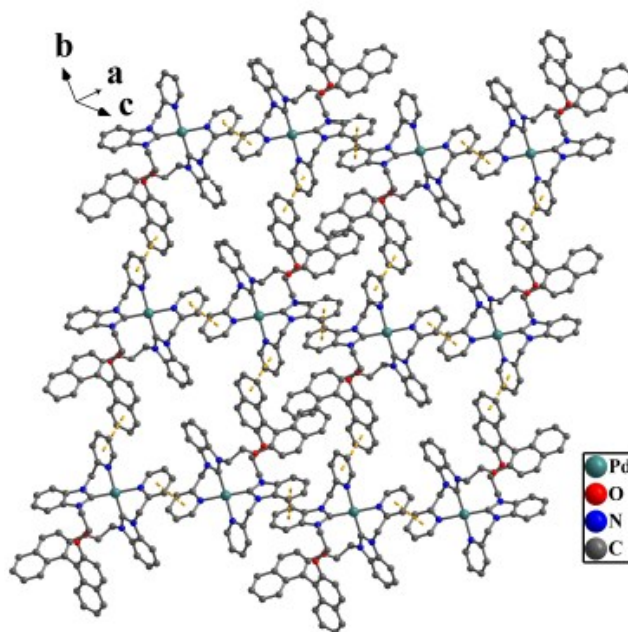


Figure S1. 2D supramolecular layer of complex **1** via $\pi \cdots \pi$ contacts. All hydrogen atoms were omitted for clarity.

2. Optimization of the reaction conditions for the Suzuki-Miyaura, Heck-Mizoroki and Sonogashira reactions (Table S1-Table S3)

Table S1 Suzuki-Miyaura reaction of 4-bromotoluene with phenylboronic acid catalyzed by complex **1**^[a]

Entry	Base	Solvent	Time (h) ^[b]	Ancillary catalysts	Yields (%) ^[c]
1	K ₂ CO ₃	H ₂ O	12	-	97%
2	K ₂ CO ₃	MeOH/H ₂ O (1:1)	6	-	98%
3	K ₂ CO ₃	MeOH	12	-	80%
4	K ₂ CO ₃	C ₂ H ₅ OH	12	-	25%
5	K ₂ CO ₃	1,4-dioxane	12	-	40%
6	K ₂ CO ₃	THF	12	-	7%
7	K ₂ CO ₃	C ₂ H ₅ OH/H ₂ O (1:1)	12	-	72%
8	^t BuOK	H ₂ O	12	-	72%
9	K ₃ PO ₄ ·3H ₂ O	H ₂ O	12	-	74%

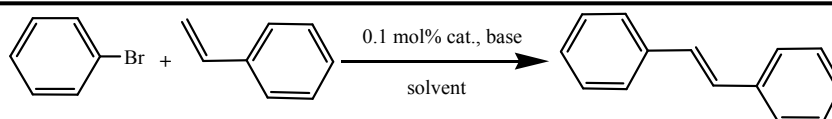
10	NaOAc	H ₂ O	12	-	52%
11	K ₂ CO ₃	H ₂ O	6	TBAB	99%
12	K ₂ CO ₃	H ₂ O	6	PEG-400	94%
13	K ₂ CO ₃	MeOH	6	PEG-400	93%
14	K ₂ CO ₃	MeOH	6	TBAB	97%

[a] Reaction conditions: 4-bromotoluene (0.5 mmol), phenylboronic acid (0.6 mmol), base (1.2 mmol), PEG-400 (10 mol%), TBAB (10 mol%), complex **1** 0.1 mol%, solvent (6.0 mL) at 40 °C and in air .

[b] Monitored by TLC.

[c] Determined by a GC method using n-tridecane as internal standard, and using 4-bromotoluene as a standard.

Table S2 Heck-Mizoroki reaction of bromobenzene with styrene catalyzed by NHC-Pd(II) complex **1**^[a]



Entry	Solvent	Base	T (°C)	Ancillary catalysts	Time (h) ^[b]	Yield (%) ^[c]
1	1,4-dioxane	NaOAc	120	-	24	92
2	1,4-dioxane	K ₂ CO ₃	120	-	24	65
3	1,4-dioxane	K ₃ PO ₄ ·3H ₂ O	120	-	24	78
4	1,4-dioxane	Et ₃ N	120	-	24	15
5	1,4-dioxane	^t BuOK	120	-	24	36
6	1,4-dioxane	KOH	120	-	24	25
7	1,4-dioxane	NaHCO ₃	120	-	24	83
8	1,4-dioxane	Cs ₂ CO ₃	120	-	24	39
9	H ₂ O	NaOAc	120	-	24	Trace
10	DMF	NaOAc	120	-	24	45
11	CH ₃ CN	NaOAc	120	-	24	14
12	THF	NaOAc	120	-	24	27
13	DME	NaOAc	120	-	24	52
14	DMSO	NaOAc	120	-	24	11
15	1,4-dioxane	NaOAc	100	-	30	61
16	1,4-dioxane	NaOAc	100	PEG-400	24	95
17	1,4-dioxane	NaOAc	100	TBAB	24	90

[a] Reaction conditions: bromobenzene (0.5 mmol), styrene (0.6 mmol), base (1.2 mmol), complex **1** (0.1 mol%), PEG-400 (10 mol%), TBAB (10 mol%), solvent (6 mL) in air.

[b] Monitored by TLC.

[c] Isolated yield using bromobenzene as a standard.

Table S3 Sonogashira reaction of 4-bromoanisole with phenylacetylene catalyzed by NHC-Pd(II) complex **1**^{[a], [b]}

COc1ccc(Br)cc1 + C#Cc1ccccc1
 $\xrightarrow[\text{solvent, 24 h}]{0.1 \text{ mol\% cat., base}}$
COc1ccc(C#Cc2ccccc2)cc1

Entry	Solvent	Base	Ancillary catalysts	Yield (%) ^[c]
1	1,4-dioxane/H ₂ O (1:1)	K ₃ PO ₄ ·3H ₂ O	-	79
2	1,4-dioxane/H ₂ O (1:1)	K ₃ PO ₄ ·3H ₂ O	TBAB	93
3	1,4-dioxane	Cs ₂ CO ₃	-	35
4	DMF	Cs ₂ CO ₃	-	21
5	DMSO	Cs ₂ CO ₃	-	10
6	CH ₃ CN	Cs ₂ CO ₃	-	25
7	H ₂ O	Cs ₂ CO ₃	-	29
8	THF	Cs ₂ CO ₃	-	trace
9	DMF/H ₂ O (1:1)	Cs ₂ CO ₃	-	53
10	1,4-dioxane/H ₂ O (1:1)	Cs ₂ CO ₃	-	69
11	1,4-dioxane/H ₂ O (1:1)	Cs ₂ CO ₃	PPh ₃	82
12	1,4-dioxane/H ₂ O (1:1)	Cs ₂ CO ₃	TBAB	91
13	1,4-dioxane/H ₂ O (1:1)	K ₂ CO ₃	TBAB	86
14	1,4-dioxane/H ₂ O (1:1)	KOH	TBAB	78

15	1,4-dioxane/H ₂ O (1:1)	NaOAc	TBAB	70
16	1,4-dioxane/H ₂ O (1:1)	Et ₃ N	TBAB	89
17	1,4-dioxane/H ₂ O (1:1)	NaHCO ₃	TBAB	82

[a] Reaction conditions: 4-bromoanisole (0.5 mmol), phenylacetylene (0.6 mmol), base (1.2 mmol), complex **1** (0.1 mol%), TBAB (10 mol%), PPh₃ (10 mol%), solvent (6 mL) at 100 °C in air.

[b] Reactions were monitored by TLC.

[c] Isolated yield using 4-bromoanisole as a standard.

3. The comparison of the reaction conditions between the present paper and literatures in three types of C-C coupling reactions

Table S4 The comparison of the reaction conditions between the present paper and literatures in three types of C-C coupling reactions

Reaction types		catalyst loading (mol%)	T (°C)	solvents	bases
Suzuki-Miyaura	a	0.1	40	H ₂ O	K ₂ CO ₃
	b	0.1-5	25-140	H ₂ O, THF, DMA, Dioxane, Toluene, THF/H ₂ O, Toluene/EtOH/H ₂ O	K ₂ CO ₃ , KOH, K ₃ PO ₄ , KO ^t Bu, Cs ₂ CO ₃ , CsF
Heck-Mizoroki	a	0.1	100	Dioxane	NaOAc
	b	0.1-3	80-150	DMSO, DMA, H ₂ O	DMF, NaOAc, Na ₂ CO ₃ , NaHCO ₃ , K ₃ PO ₄ , K ₂ CO ₃ , KHCO ₃ , Cs ₂ CO ₃ , Et ₃ N
Sonogashira	a	0.1	100	Dioxane/H ₂ O	K ₃ PO ₄
	b	1-4	80-120	DMSO, Dioxane, DMA/H ₂ O	DMF, DMF/H ₂ O, K ₃ PO ₄ , K ₂ CO ₃ , Cs ₂ CO ₃ , Et ₃ N

a: the data of the present paper; b: the data of literatures.

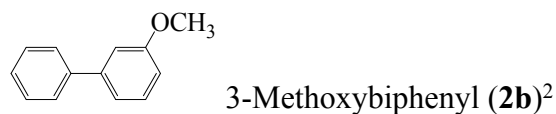
4. The data of ¹H NMR and ¹³C NMR spectra for all coupling products in the

Suzuki-Miyaura, Heck-Mizoroki and Sonogashira reactions

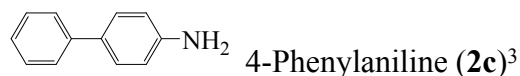


¹H NMR (400 MHz, CDCl₃): δ 3.84 (s, 3H, CH₃), 6.98 (d, J = 8.4 Hz, 2H, ArH), 7.29 (t, J = 7.4 Hz, 1H, ArH), 7.41 (t, J = 7.6 Hz, 2H, ArH), 7.55 (t, J = 8.4 Hz, 4H, ArH).

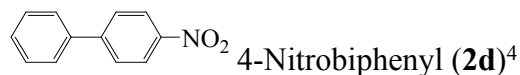
¹³C NMR (100 MHz, CDCl₃): δ 55.3 (CH₃), 114.2 (ArC), 126.7 (ArC), 128.1 (ArC), 128.7 (ArC), 133.7 (ArC), 140.8 (ArC), 159.1 (ArC).



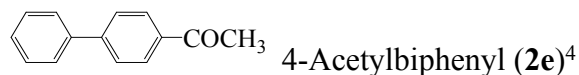
¹H NMR (400 MHz, CDCl₃): δ 3.83 (s, 3H, CH₃), 6.89 (d, J = 8.0 Hz, 1H, ArH), 7.12 (d, J = 1.6 Hz, 1H, ArH), 7.18 (d, J = 7.6 Hz, 1H, ArH), 7.35 (m, 2H, ArH), 7.41 (t, J = 7.6 Hz, 2H, ArH), 7.58 (d, J = 7.6 Hz, 2H, ArH). ¹³C NMR (100 MHz, CDCl₃): δ 55.2 (CH₃), 112.6 (ArC), 112.9 (ArC), 119.6 (ArC), 127.1 (ArC), 127.3 (ArC), 128.7 (ArC), 129.7 (ArC), 141.0 (ArC), 142.7 (ArC), 159.9 (ArC).



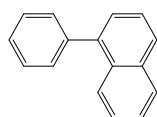
¹H NMR (400 MHz, CDCl₃): δ 3.67 (s, 2H, NH₂), 6.73 (d, J = 8.4 Hz, 2H, ArH), 7.25 (d, J = 7.2 Hz, 1H, ArH), 7.41 (m, 4H, ArH), 7.53 (d, J = 7.2 Hz, 2H, ArH). ¹³C NMR (100 MHz, CDCl₃): δ 115.3 (ArC), 126.2 (ArC), 126.3 (ArC), 127.9 (ArC), 128.6 (ArC), 131.5 (ArC), 141.1 (ArC), 145.8 (ArC).



¹H NMR (400 MHz, CDCl₃): δ 7.51 (m, 3H, ArH), 7.64 (t, J = 4.2 Hz, 2H, ArH), 7.75 (d, J = 8.8 Hz, 2H, ArH), 8.31 (d, J = 8.8 Hz, 2H, ArH). ¹³C NMR (100 MHz, CDCl₃): δ 124.1 (ArC), 127.3 (ArC), 127.8 (ArC), 128.9 (ArC), 129.1 (ArC), 138.7 (ArC), 147.1 (ArC), 147.6 (ArC).

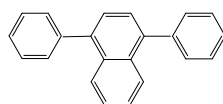


^1H NMR (400 MHz, CDCl_3): δ 2.64 (s, 3H, CH_3), 7.40 (t, $J = 7.2$ Hz, 1H, ArH), 7.47 (t, $J = 7.6$ Hz, 2H, ArH), 7.62 (d, $J = 7.2$ Hz, 2H, ArH), 7.70 (d, $J = 8.4$ Hz, 2H, ArH), 8.04 (d, $J = 8.4$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 26.6 (CH_3), 127.24 (ArC), 127.28 (ArC), 128.2 (ArC), 128.92 (ArC), 128.96 (ArC), 135.8 (ArC), 139.8 (ArC), 145.8 (ArC), 197.7 (CO).



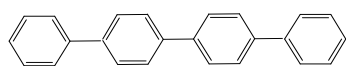
1-Phenylnaphthalene (**2f**)²

^1H NMR (400 MHz, CDCl_3): δ 7.51 (m, 3H, ArH), 7.62 (m, 6H, ArH), 7.92 (d, $J = 8.4$ Hz, 1H, ArH), 8.00 (q, $J = 4.0$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 125.4 (ArC), 125.8 (ArC), 126.0 (ArC), 126.9 (ArC), 127.23 (ArC), 127.29 (ArC), 127.6 (ArC), 128.3 (ArC), 128.8 (ArC), 130.1 (ArC), 131.6 (ArC), 133.8 (ArC), 140.3 (ArC), 140.8 (ArC).



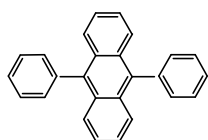
1,4-Diphenylnaphthalene (**2g**)⁵

^1H NMR (400 MHz, CDCl_3): δ 7.52 (m, 6H, ArH), 7.60 (m, 8H, ArH), 8.02 (q, $J = 3.3$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 125.8 (ArC), 126.3 (ArC), 126.4 (ArC), 127.2 (ArC), 128.2 (ArC), 130.1 (ArC), 131.9 (ArC), 139.8 (ArC), 140.8 (ArC).



4,4'-Diphenylbiphenyl (**2h**)⁶

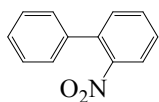
^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 7.52 (t, $J = 7.4$ Hz, 4H, ArH), 7.70 (d, $J = 4.4$ Hz, 4H, ArH), 7.74 (d, $J = 7.6$ Hz, 4H, ArH), 7.79 (s, 6H, ArH). ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 126.5 (ArC), 127.0 (ArC), 127.2 (ArC), 127.6 (ArC), 128.6 (ArC), 129.0 (ArC), 131.8 (ArC).



9,10-Diphenylanthracene (**2i**)⁷

¹H NMR (400 MHz, DMSO-*d*₆): δ 7.47 (q, *J* = 5.3 Hz, 8H, *ArH*), 7.67 (m, 10H, *ArH*).

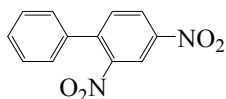
¹³C NMR (100 MHz, DMSO-*d*₆): δ 125.4 (ArC), 126.3 (ArC), 128.6 (ArC), 129.1 (ArC), 130.8 (ArC).



2-Nitrobiphenyl (**2j**)²

¹H NMR (400 MHz, CDCl₃): δ 7.33 (q, *J* = 3.2 Hz, 2H, *ArH*), 7.50 (m, 5H, *ArH*),

7.63 (m, 1H, *ArH*), 7.86 (q, *J* = 3.0 Hz, 1H, *ArH*). ¹³C NMR (100 MHz, CDCl₃): δ 124.0 (ArC), 127.9 (ArC), 128.1 (ArC), 128.2 (ArC), 128.7 (ArC), 131.9 (ArC), 132.2 (ArC), 136.3 (ArC), 137.3 (ArC), 149.3 (ArC).



2,4-Dinitrobiphenyl (**2k**)⁸

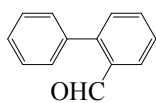
¹H NMR (400 MHz, CDCl₃): δ 7.38 (q, *J* = 3.2 Hz, 2H, *ArH*), 7.52 (t, *J* = 3.2 Hz, 3H,

ArH), 7.72 (d, *J* = 8.8 Hz, 1H, *ArH*), 8.51 (q, *J* = 3.6 Hz, 1H, *ArH*), 8.74 (d, *J* = 2.0

Hz, 1H, *ArH*). ¹³C NMR (100 MHz, CDCl₃): δ 119.7 (ArC), 126.4 (ArC), 127.6

(ArC), 129.1 (ArC), 129.5 (ArC), 133.2 (ArC), 135.2 (ArC), 142.2 (ArC), 146.8

(ArC), 149.1 (ArC).



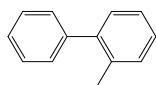
Biphenyl-2-carbaldehyde (**2l**)⁴

¹H NMR (400 MHz, CDCl₃): δ 7.33 (m, 7H, *ArH*), 7.56 (q, *J* = 2.9 Hz, 1H, *ArH*),

7.97 (q, *J* = 3.2 Hz, 1H, *ArH*), 10.52 (s, 1H, CHO). ¹³C NMR (100 MHz, CDCl₃): δ

126.5 (ArC), 127.3 (ArC), 128.0 (ArC), 129.4 (ArC), 129.6 (ArC), 129.7 (ArC), 130.6

(ArC), 133.2 (ArC), 135.1 (ArC), 135.3 (ArC), 189.8 (CHO).



2-Methylbiphenyl (**2m**)²

¹H NMR (400 MHz, CDCl₃): δ 2.26 (s, 3H, CH₃), 7.24 (m, 3H, *ArH*), 7.33 (m, 3H,

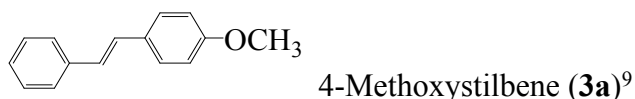
ArH), 7.43 (m, 3H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 20.5 (CH_3), 125.8 (ArC), 126.8 (ArC), 127.2 (ArC), 127.3 (ArC), 128.1 (ArC), 128.8 (ArC), 129.2 (ArC), 129.8 (ArC), 130.3 (ArC), 135.3 (ArC), 142.0 (ArC).



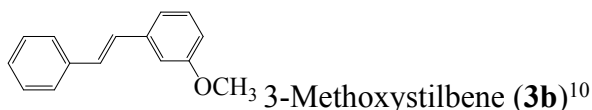
^1H NMR (400 MHz, CDCl_3): δ 7.44 (t, $J = 7.2$ Hz, 2H, ArH), 7.53 (t, $J = 7.4$ Hz, 4H, ArH), 7.70 (d, $J = 7.6$ Hz, 4H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 127.2 (ArC), 127.3 (ArC), 128.8 (ArC), 141.3 (ArC).



^1H NMR (400 MHz, CDCl_3): δ 2.38 (s, 3H, CH_2), 7.24 (d, $J = 8.0$ Hz, 2H, ArH), 7.30 (t, $J = 7.4$ Hz, 1H, ArH), 7.40 (t, $J = 7.6$ Hz, 2H, ArH), 7.47 (d, $J = 8.0$ Hz, 2H, ArH), 7.55 (d, $J = 8.4$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 21.1 (CH_3), 127.0 (ArC), 127.2 (ArC), 128.7 (ArC), 129.5 (ArC), 137.0 (ArC), 138.4 (ArC), 141.2 (ArC).

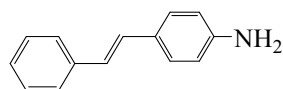


^1H NMR (400 MHz, CDCl_3): δ 3.88 (s, 3H, CH_3), 6.97 (d, $J = 8.8$ Hz, 2H, ArH), 7.06 (d, $J = 16.0$ Hz, 1H, =CH), 7.12 (d, $J = 16.0$ Hz, 1H, =CH), 7.30 (t, $J = 7.2$ Hz, 1H, ArH), 7.41 (t, $J = 7.6$ Hz, 2H, ArH), 7.56 (q, $J = 7.7$ Hz, 4H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 55.2 (CH_3), 114.1 (ArC), 126.2 (ArC), 126.5 (ArC), 127.1 (=CH or ArC), 127.7 (=CH or ArC), 128.1 (ArC), 128.6 (ArC), 130.1 (ArC), 137.6 (ArC), 159.2 (ArC).



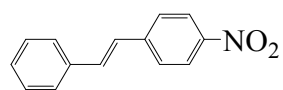
^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 3.80 (s, 3H, CH_3), 6.86 (d, $J = 7.6$ Hz, 1H, ArH), 7.19 (d, $J = 6.8$ Hz, 2H, =CH or ArH), 7.31 (m, 4H, =CH or ArH), 7.40 (t, $J = 7.6$ Hz,

2H, ArH), 7.61 (d, $J = 7.6$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, DMSO- d_6): δ 55.0 (CH₃), 111.4 (ArC), 113.4 (ArC), 119.0 (ArC), 119.1 (ArC), 126.4 (ArC), 127.6 (=CH or ArC), 128.3 (ArC), 128.6 (ArC), 129.6 (ArC), 136.9 (ArC), 138.4 (ArC), 159.5 (ArC).



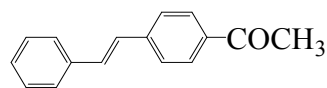
4-Anilinstilbene (**3c**)¹¹

^1H NMR (400 MHz, CDCl₃): δ 3.71 (s, 2H, NH₂), 6.67 (d, $J = 8.0$ Hz, 2H, ArH), 6.93 (d, $J = 16.0$ Hz, 1H, =CH), 7.00 (d, $J = 16.0$ Hz, 1H, =CH), 7.22 (t, $J = 7.0$ Hz, 1H, ArH), 7.34 (d, $J = 6.8$ Hz, 4H, ArH), 7.47 (d, $J = 7.6$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl₃): δ 115.1 (ArC), 125.0 (ArC), 126.0 (ArC), 126.8 (ArC), 127.7 (=CH or ArC), 127.9 (=CH or ArC), 128.5 (ArC), 128.6 (ArC), 137.9 (ArC), 146.1 (ArC).



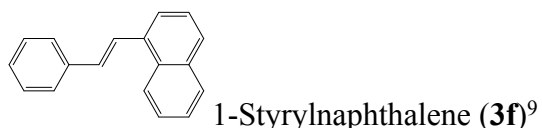
4-Nitrostilbene (**3d**)¹²

^1H NMR (400 MHz, CDCl₃): δ 7.19 (d, $J = 16.4$ Hz, 1H, =CH), 7.28 (d, $J = 16.4$ Hz, 1H, =CH), 7.36 (m, 1H, ArH), 7.43 (t, $J = 7.4$ Hz, 2H, ArH), 7.57 (d, $J = 7.2$ Hz, 2H, ArH), 7.67 (d, $J = 8.4$ Hz, 2H, ArH), 8.26 (d, $J = 8.8$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl₃): δ 124.1 (ArC), 126.3 (ArC), 126.8 (ArC), 127.0 (=CH or ArC), 128.8 (ArC), 128.9 (ArC), 133.3 (ArC), 136.2 (ArC), 143.8 (ArC), 146.8 (ArC).

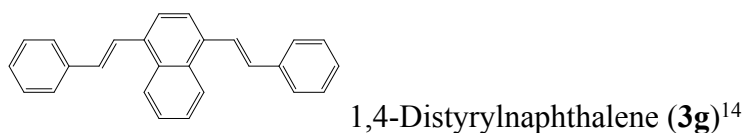


4-Acetylstilbene (**3e**)¹³

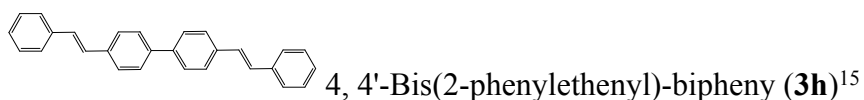
^1H NMR (400 MHz, CDCl₃): δ 2.63 (s, 3H, CH₃), 7.18 (d, $J = 16.4$ Hz, 1H, =CH), 7.24 (d, $J = 16.4$ Hz, 1H, =CH), 7.33 (q, $J = 8.5$ Hz, 1H, ArH), 7.41 (t, $J = 7.6$ Hz, 2H, ArH), 7.58 (d, $J = 7.2$ Hz, 2H, ArH), 7.62 (d, $J = 8.4$ Hz, 2H, ArH), 7.99 (d, $J = 8.4$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl₃): δ 26.5 (CH₃), 126.4 (ArC), 126.8 (ArC), 127.4 (=CH or ArC), 128.3 (ArC), 128.7 (ArC), 128.8 (ArC), 131.4 (ArC), 135.9 (ArC), 136.6 (ArC), 141.9 (ArC), 197.4 (CO).



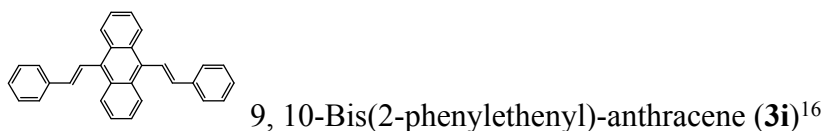
¹H NMR (400 MHz, CDCl₃): δ 7.14 (d, *J* = 16.0 Hz, 1H, =CH), 7.27 (t, *J* = 7.4 Hz, 1H, ArH), 7.37 (t, *J* = 7.6 Hz, 2H, ArH), 7.52 (m, 3H, =CH or ArH), 7.57 (d, *J* = 7.6 Hz, 2H, ArH), 7.70 (d, *J* = 7.2 Hz, 1H, ArH), 7.76 (d, *J* = 8.0 Hz, 1H, ArH), 7.84 (q, *J* = 7.2 Hz, 2H, ArH), 8.21 (d, *J* = 8.0 Hz, 1H, ArH). ¹³C NMR (100 MHz, CDCl₃): δ 123.5 (ArC), 123.7 (ArC), 125.6 (ArC), 125.7 (ArC), 125.8 (ArC), 126.0 (ArC), 126.6 (ArC), 127.7 (=CH or ArC), 128.0 (ArC), 128.5 (ArC), 128.7 (ArC), 131.3 (ArC), 131.7 (ArC), 133.6 (ArC), 134.9 (ArC), 137.5 (ArC).



¹H NMR (400 MHz, CDCl₃): δ 7.17 (d, *J* = 16.0 Hz, 2H, =CH), 7.29 (t, *J* = 7.4 Hz, 2H, ArH), 7.39 (t, *J* = 7.6 Hz, 4H, ArH), 7.54 (q, *J* = 1.8 Hz, 2H, ArH), 7.59 (d, *J* = 7.2 Hz, 4H, ArH), 7.75 (s, 2H, ArH), 7.86 (d, *J* = 16.0 Hz, 2H, =CH), 8.26 (q, *J* = 3.2 Hz, 2H, ArH). ¹³C NMR (100 MHz, CDCl₃): δ 123.5 (ArC), 124.3 (ArC), 125.7 (ArC), 126.0 (ArC), 126.6 (ArC), 127.7 (=CH or ArC), 128.7 (ArC), 131.5 (ArC), 134.8 (ArC), 137.6 (ArC).

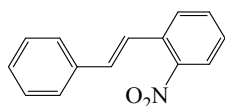


¹H NMR (400 MHz, CDCl₃): δ 7.16 (s, 2H, ArH), 7.39 (m, 6H, =CH or ArH), 7.43 (d, *J* = 8.0 Hz, 2H, ArH), 7.55 (t, *J* = 11.2 Hz, 2H, =CH or ArH), 7.62 (t, *J* = 6.0 Hz, 6H, ArH). ¹³C NMR (100 MHz, CDCl₃): δ 126.5 (ArC), 126.6 (ArC), 126.9 (ArC), 127.2 (=CH or ArC), 127.6 (=CH or ArC), 127.7 (ArC), 128.2 (ArC), 128.3 (ArC), 128.71 (ArC), 128.78 (ArC).



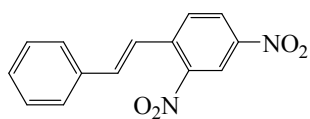
¹H NMR (400 MHz, DMSO-*d*₆): δ 7.40 (q, *J* = 2.2 Hz, 4H, ArH), 7.50 (t, *J* = 7.4 Hz, 4H, =CH or ArH), 7.58 (q, *J* = 3.4 Hz, 6H, ArH), 7.84 (d, *J* = 7.2 Hz, 4H, =CH or

ArH), 8.40 (q, $J = 3.3$ Hz, 4H, ArH). ^{13}C NMR (100 MHz, DMSO- d_6): δ 119.0 (ArC), 121.6 (ArC), 122.3 (ArC), 123.4 (ArC), 123.6 (ArC), 124.0 (ArC), 124.9 (ArC), 125.6 (ArC), 127.3 (=CH or ArC), 129.0 (ArC), 131.5 (ArC), 133.7 (ArC), 136.2 (ArC), 140.6 (ArC), 140.8 (ArC).



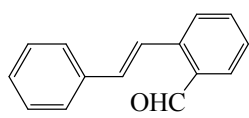
1-Nitro-2-(2-phenylethenyl)-stilbene (**3j**)¹⁷

^1H NMR (400 MHz, CDCl_3): δ 7.16 (d, $J = 16.4$ Hz, 1H, =CH), 7.25 (d, $J = 16.4$ Hz, 1H, =CH), 7.33 (t, $J = 7.2$ Hz, 1H, ArH), 7.40 (t, $J = 7.4$ Hz, 2H, ArH), 7.54 (d, $J = 7.2$ Hz, 2H, ArH), 7.64 (d, $J = 8.8$ Hz, 2H, ArH), 8.21 (d, $J = 8.8$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 124.3 (ArC), 127.2 (=CH or ArC), 129.0 (ArC), 130.4 (ArC), 130.7 (ArC), 132.2 (ArC), 133.7 (ArC), 136.2 (ArC), 136.3 (ArC), 143.7 (ArC).



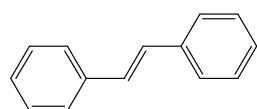
2, 4-Dinitro-1-(2-phenylethenyl)-stilbene (**3k**)¹⁸

^1H NMR (400 MHz, CDCl_3): δ 7.40 (m, 2H, =CH or ArH), 7.54 (m, 6H, =CH or ArH), 8.04 (t, $J = 4.2$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 121.2 (ArC), 121.8 (ArC), 126.1 (ArC), 128.2 (=CH or ArC), 128.4 (ArC), 128.6 (ArC), 128.7 (ArC), 130.1 (ArC), 131.6 (ArC), 139.7 (ArC), 140.2 (ArC), 159.0 (ArC).



2-(2-Phenylethenyl)-stilbene (**3l**)¹⁹

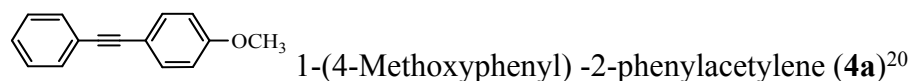
^1H NMR (400 MHz, CDCl_3): δ 7.06 (d, $J = 16.4$ Hz, 1H, =CH), 7.06 (d, $J = 16.4$ Hz, 1H, =CH), 7.16, (d, $J = 8.0$ Hz, 2H, ArH), 7.23 (t, $J = 6.8$ Hz, 1H, ArH), 7.34 (t, $J = 7.6$ Hz, 2H, ArH), 7.39 (d, $J = 8.0$ Hz, 2H, ArH), 7.48 (d, $J = 7.6$ Hz, 2H, ArH), 11.02 (s, 1H, CHO). ^{13}C NMR (100 MHz, CDCl_3): δ 126.7 (=CH or ArC), 129.1 (ArC), 129.4 (ArC), 132.5 (ArC), 133.5 (ArC), 135.1 (ArC), 135.3 (ArC), 141.7 (ArC), 186.2 (CHO).



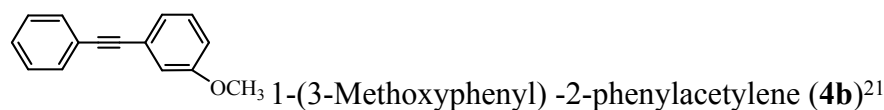
Stilbene (**3n**)⁹

^1H NMR (400 MHz, CDCl_3): δ 7.19 (s, 2H, ArH), 7.33 (t, $J = 7.4$ Hz, 2H, ArH), 7.43

(t, $J = 7.6$ Hz, 4H, =CH or ArH), 7.58 (d, $J = 7.6$ Hz, 4H, =CH or ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 126.5 (ArC), 127.6 (=CH or ArC), 128.6 (ArC), 137.3 (ArC).



^1H NMR (400 MHz, CDCl_3): δ 3.86 (s, 3H, CH_3), 6.93 (d, $J = 8.8$ Hz, 2H, ArH), 7.39 (m, 3H, ArH), 7.57 (m, 4H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 55.2 (CH_3), 88.0 ($\equiv\text{C}$), 89.3 ($\equiv\text{C}$), 113.9 (ArC), 115.3 (ArC), 123.5 (ArC), 127.9 (ArC), 128.3 (ArC), 131.4 (ArC), 133.0 (ArC), 159.6 (ArC).



^1H NMR (400 MHz, CDCl_3): δ 3.85 (s, 3H), 6.94 (m, 1H, ArH), 7.10 (q, $J = 1.3$ Hz, 1H, ArH), 7.17 (t, $J = 3.8$ Hz, 1H, ArH), 7.30 (t, $J = 8.0$ Hz, 1H, ArH), 7.39 (m, 3H, ArH), 7.57 (m, 2H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 55.0 (CH_3), 88.4 ($\equiv\text{C}$), 88.9 ($\equiv\text{C}$), 111.4 (ArC), 113.4 (ArC), 119.0 (ArC), 126.4 (ArC), 127.6 (ArC), 128.3 (ArC), 128.8 (ArC), 129.6 (ArC), 136.9 (ArC), 138.4 (ArC), 159.5 (ArC).



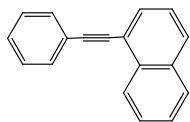
^1H NMR (400 MHz, CDCl_3): δ 3.78 (s, 2H, NH_2), 7.37 (m, 5H, ArH), 7.54 (q, $J = 3.2$ Hz, 4H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 73.9 ($\equiv\text{C}$), 81.5 ($\equiv\text{C}$), 121.8 (ArC), 128.3 (ArC), 128.4 (ArC), 129.2 (ArC), 132.5 (ArC).



^1H NMR (400 MHz, CDCl_3): δ 7.43 (m, 3H, ArH), 7.60 (q, $J = 3.2$ Hz, 2H, ArH), 7.70 (d, $J = 8.8$ Hz, 2H, ArH), 8.26 (d, $J = 8.8$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 87.5 ($\equiv\text{C}$), 94.7 ($\equiv\text{C}$), 122.0 (ArC), 123.6 (ArC), 128.5 (ArC), 129.2 (ArC), 130.2 (ArC), 131.8 (ArC), 132.2 (ArC), 146.9 (ArC).

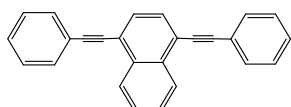


^1H NMR (400 MHz, CDCl_3): δ 2.61 (s, 3H, CH_3), 7.37 (t, $J = 3.2$ Hz, 3H, ArH), 7.56 (m, 2H, ArH), 7.62 (d, $J = 8.4$ Hz, 2H, ArH), 7.95 (d, $J = 8.4$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl_3): δ 26.6 (CH_3), 88.6 ($\equiv\text{C}$), 92.7 ($\equiv\text{C}$), 122.7 (ArC), 128.2 (ArC), 128.4 (ArC), 128.8 (ArC), 131.72 (ArC), 131.76 (ArC), 136.2 (ArC), 197.2 (CO).



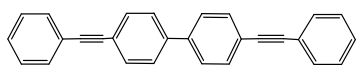
1-(2-Phenylethynyl)naphthalene (**4f**)²³

¹H NMR (400 MHz, CDCl₃): δ 7.43 (s, 4H, ArH), 7.69 (d, $J = 5.6$ Hz, 4H, ArH), 7.77 (s, 2H, ArH), 8.51 (t, $J = 2.6$ Hz, 2H, ArH). ¹³C NMR (100 MHz, CDCl₃): δ 89.5 (\equiv C), 96.8 (\equiv C), 122.1 (ArC), 126.2 (ArC), 127.8 (ArC), 128.5 (ArC), 128.9 (ArC), 131.6 (ArC), 134.5 (ArC), 137.7 (ArC).



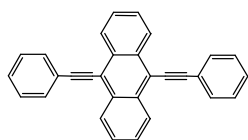
1, 4-Bis(2-phenylethynyl)-naphthalene (**4g**)²⁵

¹H NMR (400 MHz, DMSO-*d*₆): δ 7.23 (s, 1H, ArH), 7.44 (m, 2H, ArH), 7.51 (m, 5H, ArH), 7.75 (q, $J = 3.2$ Hz, 3H, ArH), 7.81 (d, $J = 3.3$ Hz, 2H, ArH), 7.88 (d, $J = 10.8$ Hz, 2H, ArH), 8.48 (q, $J = 3.2$ Hz, 1H, ArH). ¹³C NMR (100 MHz, DMSO-*d*₆): δ 87.0 (\equiv C), 96.2 (\equiv C), 120.6 (ArC), 122.0 (ArC), 124.3 (ArC), 126.2 (ArC), 127.1 (ArC), 128.1 (ArC), 128.8 (ArC), 128.9 (ArC), 129.2 (ArC), 129.9 (ArC), 131.5 (ArC), 132.2 (ArC).



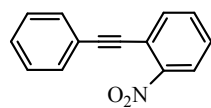
4, 4'-Bis(2-phenylethynyl)-1,1'-biphenyl (**4h**)²⁶

¹H NMR (400 MHz, CDCl₃): δ 7.35 (d, $J = 2.0$ Hz, 2H, ArH), 7.37 (q, $J = 2.1$ Hz, 2H, ArH), 7.45 (s, 1H, ArH), 7.47 (d, $J = 8.4$ Hz, 2H, ArH), 7.54 (t, $J = 1.8$ Hz, 2H, ArH), 7.56 (d, $J = 3.2$ Hz, 5H, ArH), 7.58 (d, $J = 2.0$ Hz, 3H, ArH), 7.61 (s, 1H, ArH). ¹³C NMR (100 MHz, CDCl₃): δ 89.1 (\equiv C), 90.3 (\equiv C), 93.5 (\equiv C), 103.6 (\equiv C), 121.9 (ArC), 123.2 (ArC), 126.8 (ArC), 128.3 (ArC), 128.5 (ArC), 131.6 (ArC), 131.9 (ArC), 132.1 (ArC).



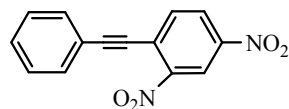
9, 10-Bis(2-phenylethynyl)-anthracene (**4i**)²⁵

¹H NMR (400 MHz, DMSO-*d*₆): δ 7.60 (m, 7H, ArH), 7.64 (m, 2H, ArH), 7.84 (q, $J = 3.3$ Hz, 3H, ArH), 7.93 (q, $J = 3.0$ Hz, 3H, ArH), 7.84 (q, $J = 3.2$ Hz, 3H, ArH). ¹³C NMR (100 MHz, DMSO-*d*₆): δ 85.7 (\equiv C), 87.1 (\equiv C), 117.5 (ArC), 122.1 (ArC), 126.8 (ArC), 127.8 (ArC), 128.6 (ArC), 128.8 (ArC), 128.9 (ArC), 129.4 (ArC), 131.2 (ArC), 131.4 (ArC), 131.5 (ArC), 131.6 (ArC).



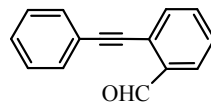
(2-Nitrophenyl)phenylacetylene (**4j**)²⁷

¹H NMR (400 MHz, CDCl₃): δ 7.40 (m, ArH), 7.57 (q, $J = 3.0$ Hz, 4H, ArH). ¹³C NMR (100 MHz, CDCl₃): δ 73.9 (\equiv C), 81.5 (\equiv C), 121.8 (ArC), 128.4 (ArC), 129.2 (ArC), 132.5 (ArC).



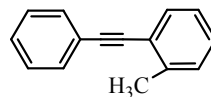
2,4-Dinitro-1-(2-phenylethynyl)-acetylene (**4k**)²⁸

¹H NMR (400 MHz, CDCl₃): δ 7.39 (d, $J = 7.2$ Hz, 5H, ArH), 7.57 (d, $J = 6.8$ Hz, 3H, ArH). ¹³C NMR (100 MHz, CDCl₃): δ 73.9 (\equiv C), 81.5 (\equiv C), 121.8 (ArC), 128.4 (ArC), 129.2 (ArC), 132.5 (ArC).



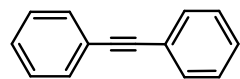
2-(Phenylethynyl) benzaldehyde (**4l**)²⁹

¹H NMR (400 MHz, CDCl₃): δ 7.36 (m, 3H, ArH), 7.51 (q, $J = 6.8$ Hz, 5H, ArH), 8.04 (d, $J = 7.6$ Hz, 1H, ArH), 11.08 (s, 1H, CHO). ¹³C NMR (100 MHz, CDCl₃): δ 89.8 (\equiv C), 92.2 (\equiv C), 126.7 (ArC), 128.4 (ArC), 131.5 (ArC), 132.4 (ArC), 132.5 (ArC), 133.5 (ArC), 134.7 (ArC), 136.7 (ArC), 157.0 (ArC), 193.3 (CHO).



2-Methylphenylacetylene (**4m**)³⁰

¹H NMR (400 MHz, CDCl₃): δ 1.56 (s, 3H, ArH), 7.39 (m, 6H, ArH), 7.56 (t, $J = 4.0$ Hz, 3H, ArH). ¹³C NMR (100 MHz, CDCl₃): δ 26.6 (CH₃), 88.6 (\equiv C), 92.7 (\equiv C), 122.7 (ArC), 128.2 (ArC), 128.4 (ArC), 128.8 (ArC), 131.72 (ArC), 131.76 (ArC), 136.2 (ArC).



Diphenylacetylene (**4n**)³⁰

¹H NMR (400 MHz, CDCl₃): δ 7.27 (d, $J = 3.6$ Hz, 2H, ArH), 7.37 (d, $J = 8.0$ Hz, 4H, ArH), 7.54 (d, $J = 7.8$ Hz, 4H, ArH). ¹³C NMR (100 MHz, CDCl₃): δ 83.8 (\equiv C), 125.6

(ArC), 127.2 (ArC), 128.1 (ArC), 128.3 (ArC), 128.9 (ArC), 131.9 (ArC), 137.7 (ArC).

5. The figures of ^1H NMR and ^{13}C NMR spectra for all intermediates, precursor [(S)-LH₂] \cdot (PF₆)₂, complex 1, and all coupling products in Suzuki-Miyaura, Heck-Mizoroki and Sonogashira reactions

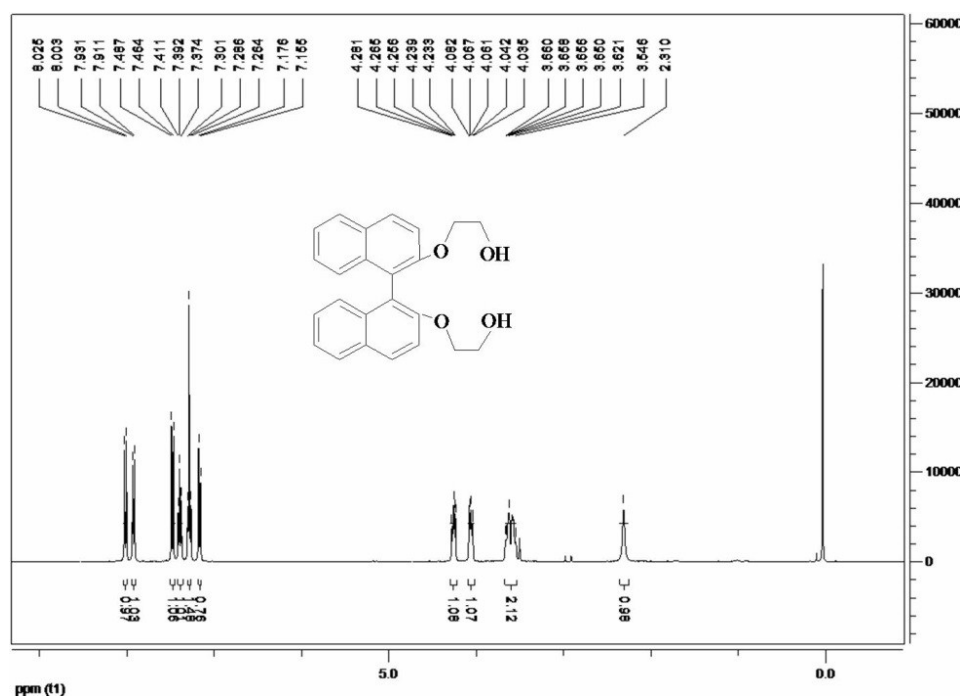


Fig. S2 The ^1H NMR (400 MHz, CDCl_3) spectrum of (S)-2,2'-di(2'-hydroxyethoxy)-1,1'-binaphthyl.

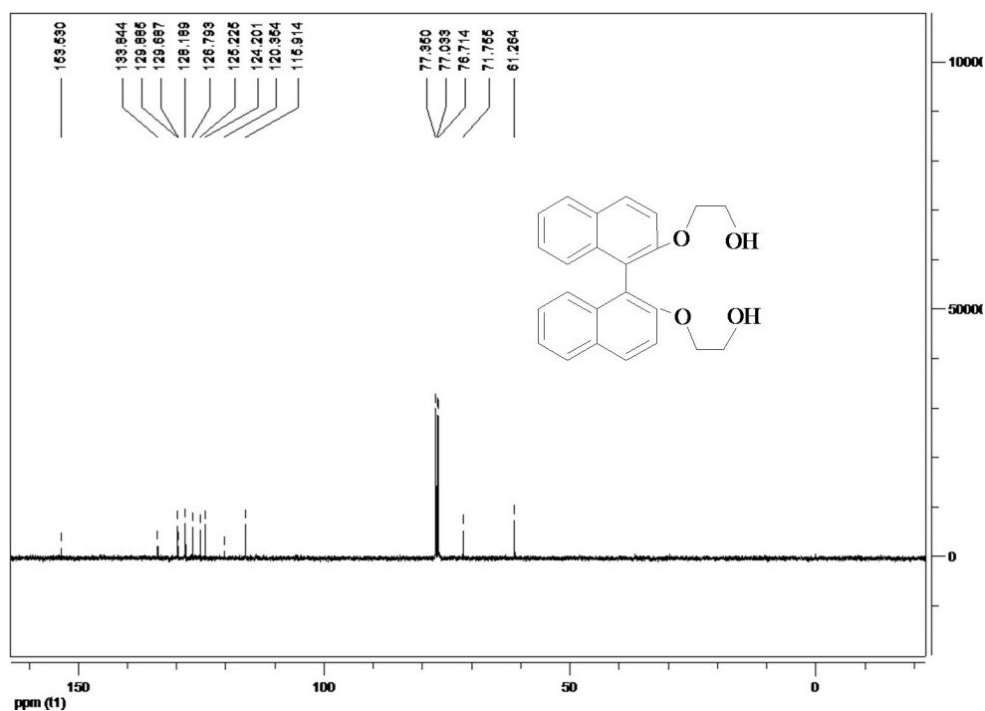


Fig. S3 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of (S)-2,2'-di(2'-hydroxyethoxy)-1,1'-binaphthyl.

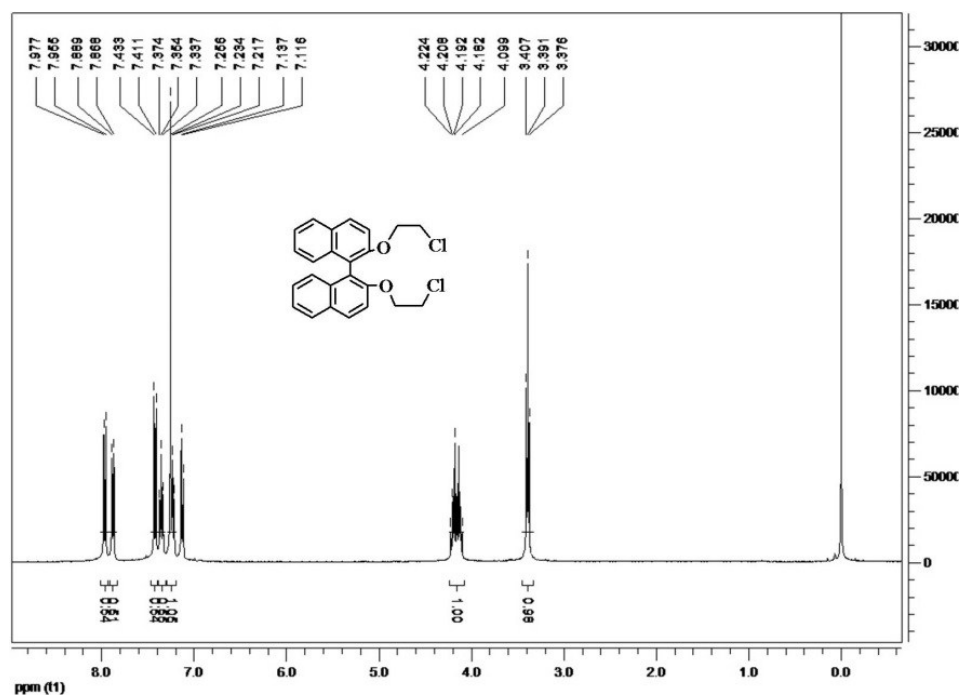


Fig. S4 The ^1H NMR (400 MHz, CDCl_3) spectrum of (S)-2,2'-di(2'-chloroethoxy)-1,1'-binaphthyl

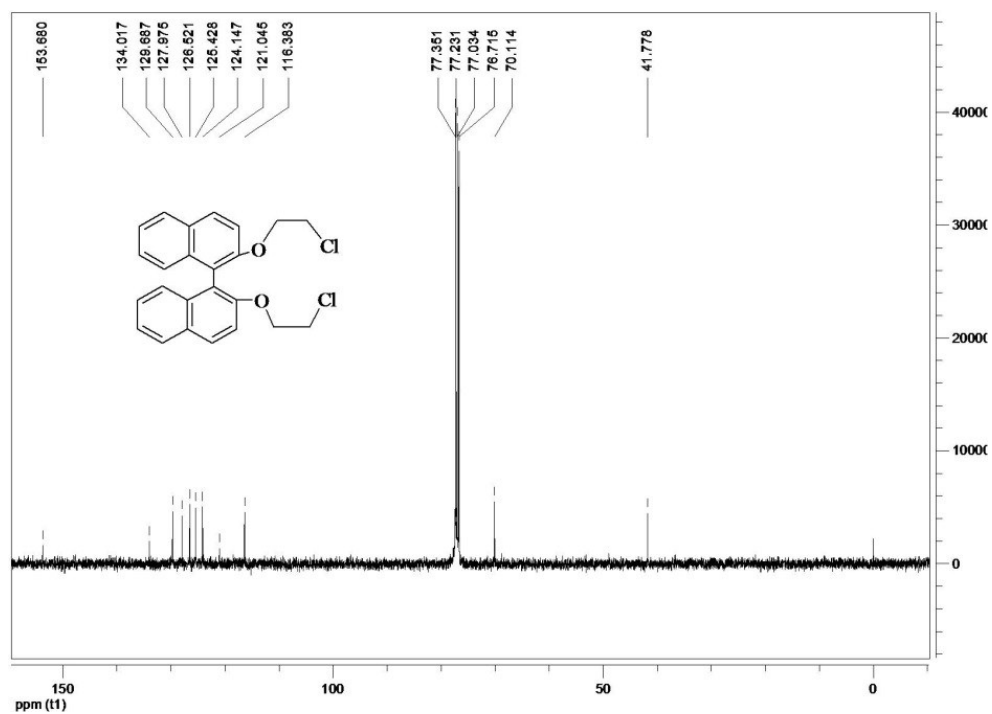


Fig. S5 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of (S)-2,2'-di(2'-chloroethoxy)-1,1'-binaphthyl.

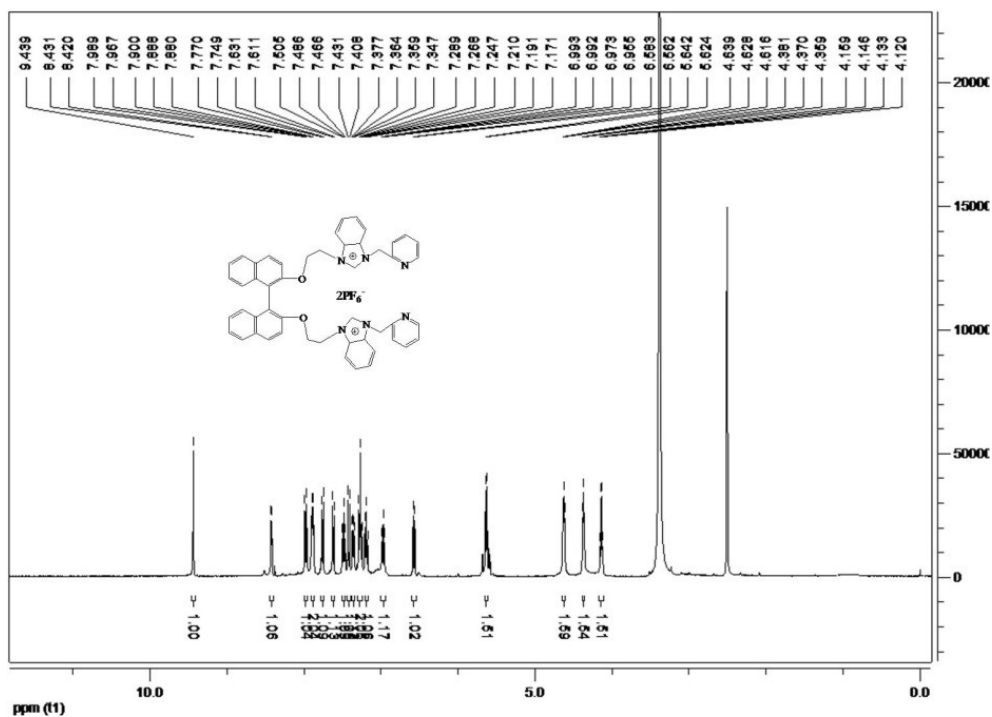


Fig. S6 The ^1H NMR (400 MHz, DMSO-d_6) spectrum of [(S)-LH₂] \cdot (PF₆)₂.

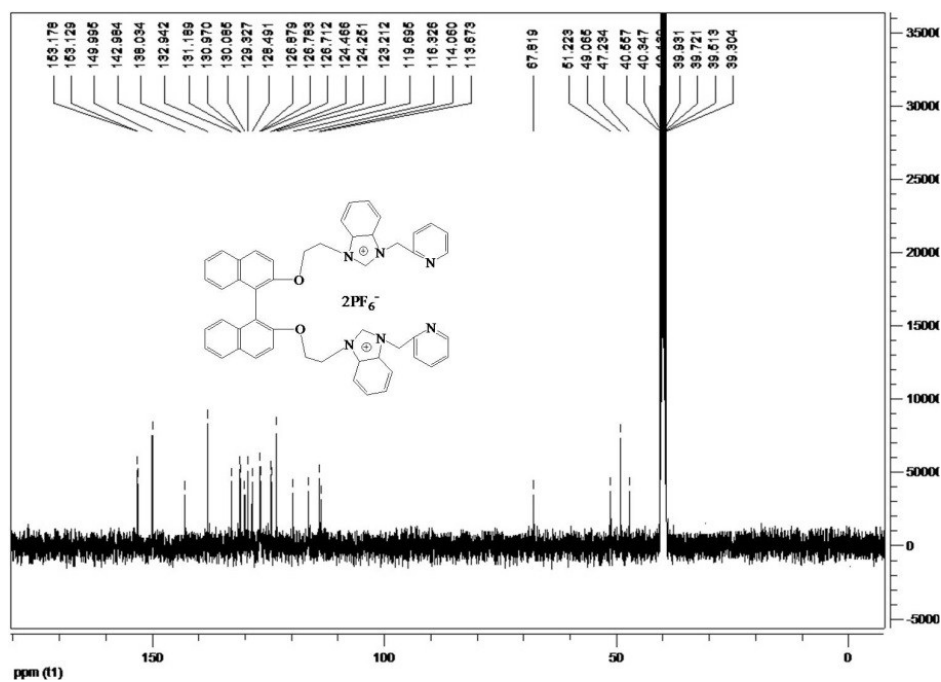


Fig. S7 The ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of $[(S)\text{-LH}_2] \cdot (\text{PF}_6)_2$.

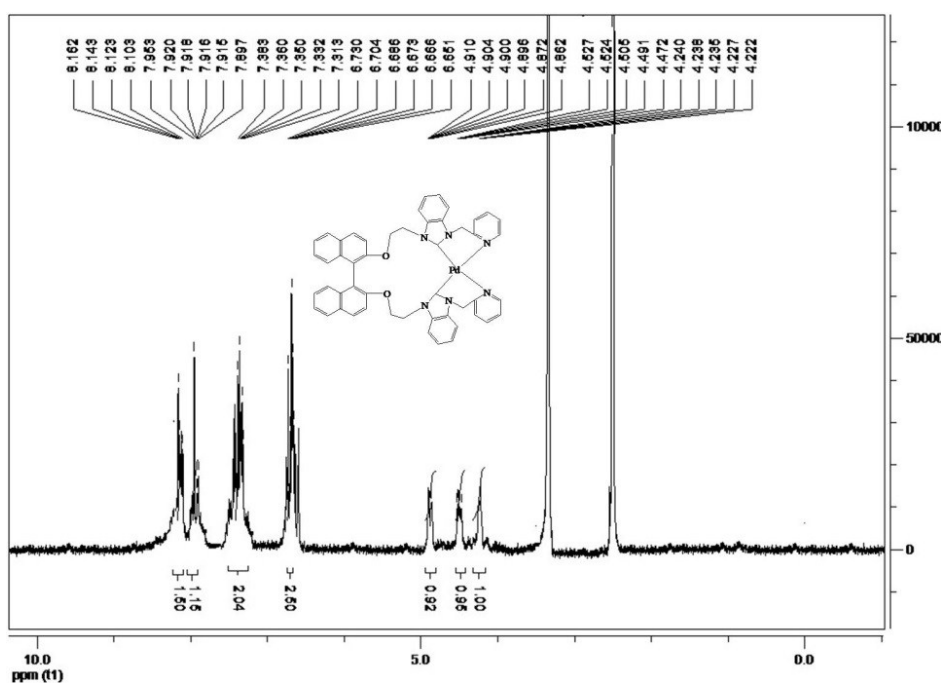


Fig. S8 The ^1H NMR (400 MHz, DMSO-d_6) spectrum of **1**.

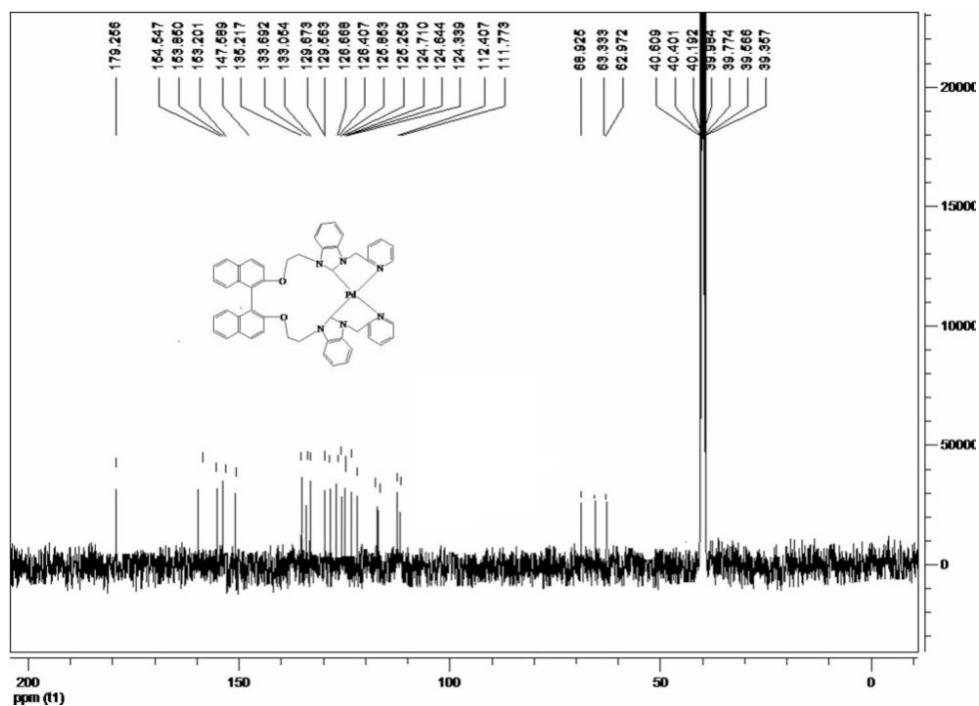


Fig. S9 The ¹³C NMR (100 MHz, DMSO-d₆) spectrum of 1.

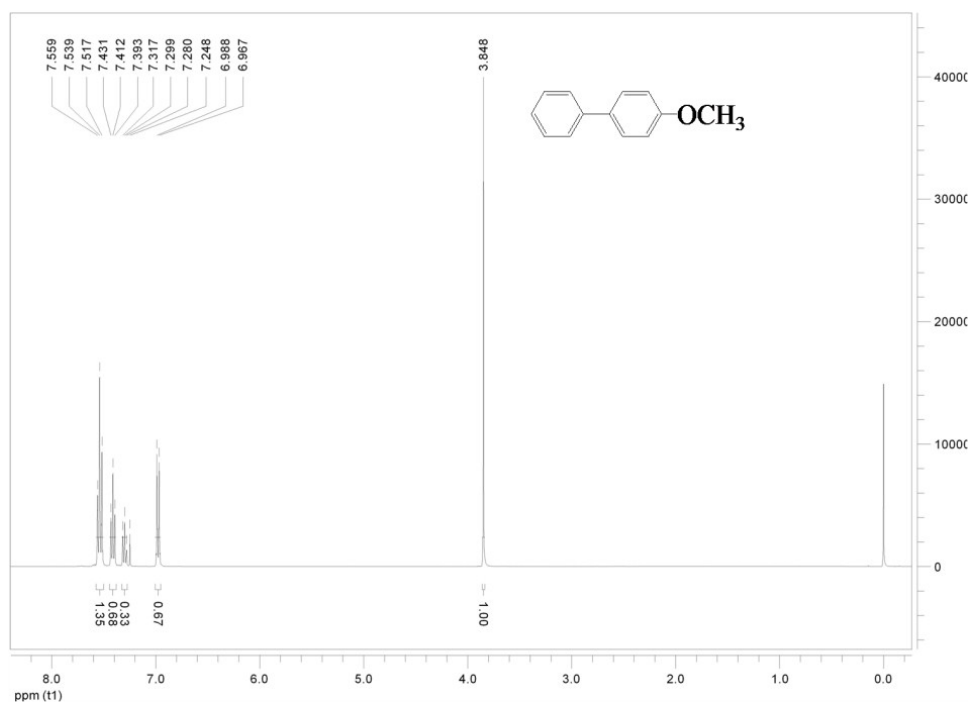


Fig. S10 The ¹H NMR (400 MHz, CDCl₃) spectrum of 4-methoxybiphenyl (2a).

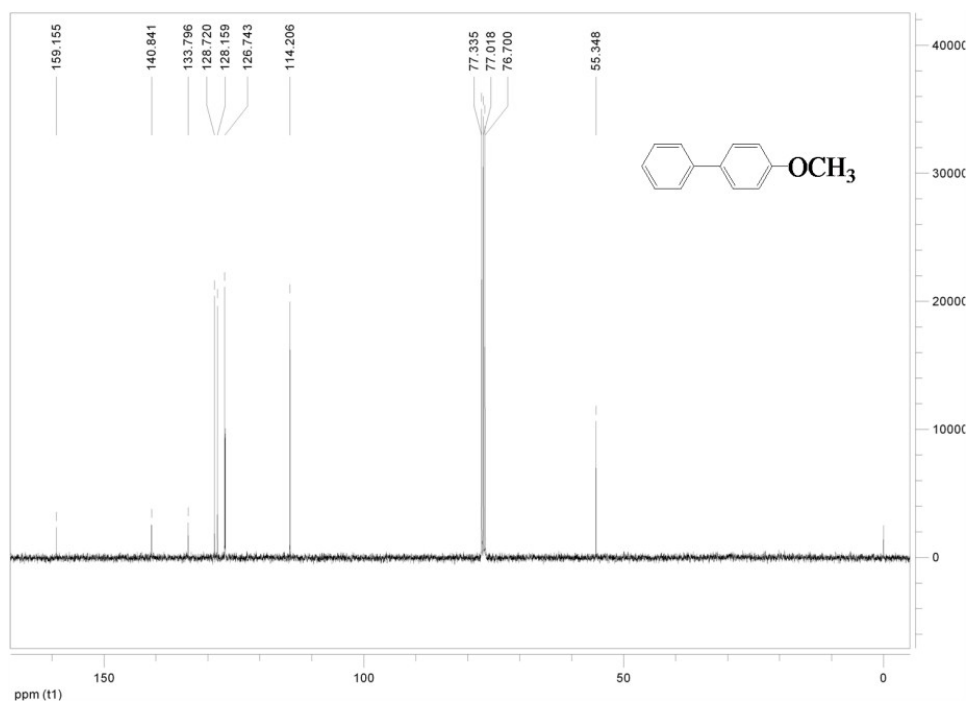


Fig. S11 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4-methoxybiphenyl (**2a**).

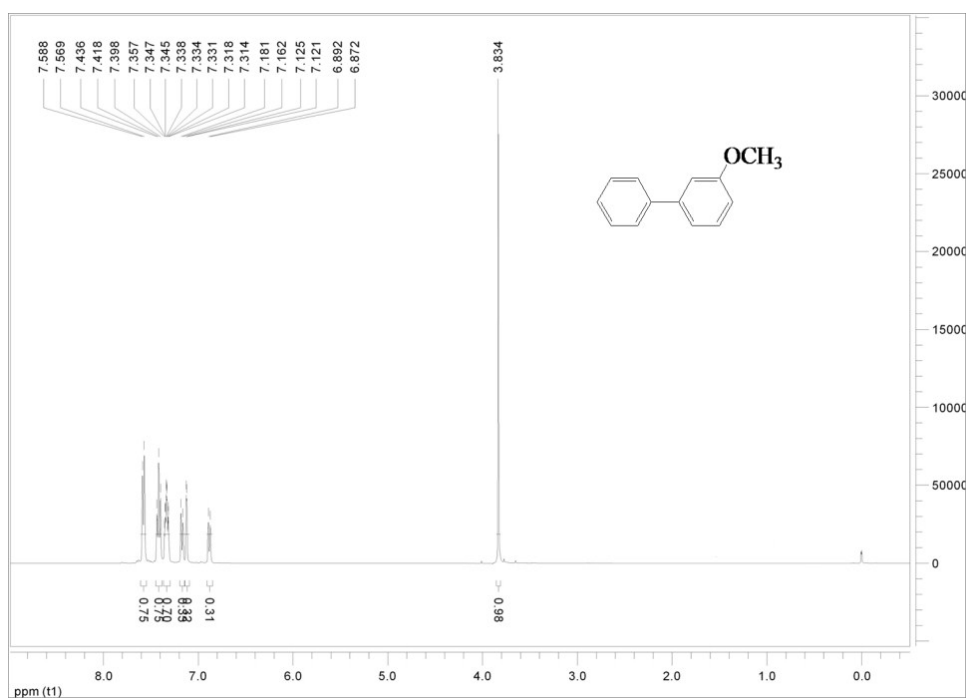


Fig. S12 The ^1H NMR (400 MHz, CDCl_3) spectrum of 3-methoxybiphenyl (**2b**).

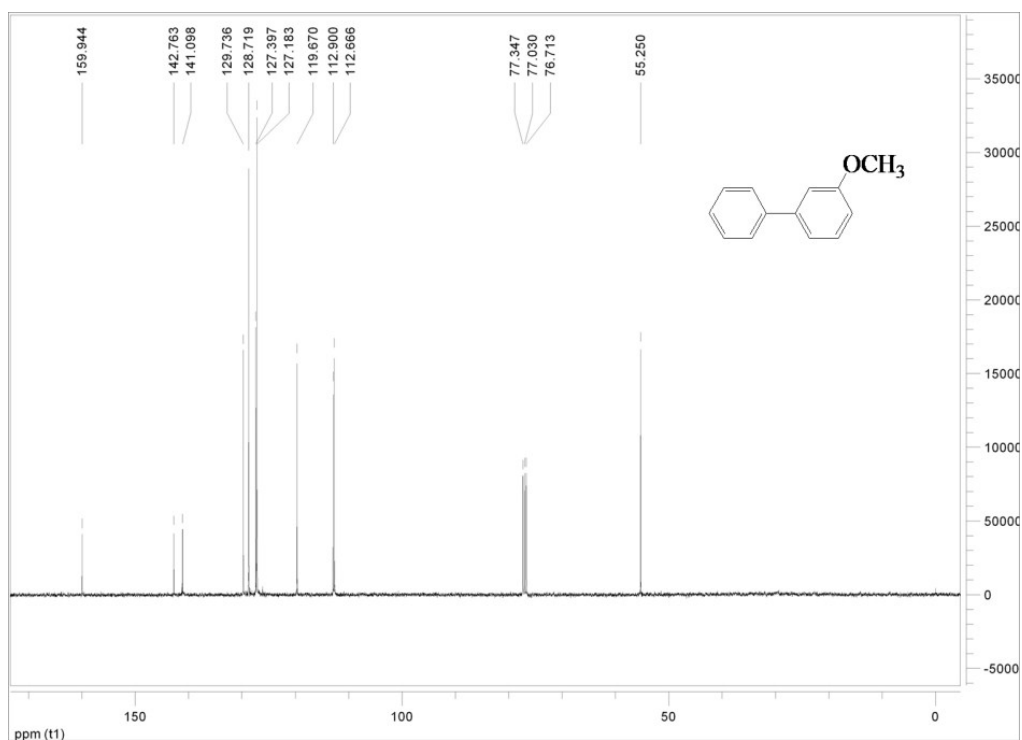


Fig. S13 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 3-methoxybiphenyl (**2b**).

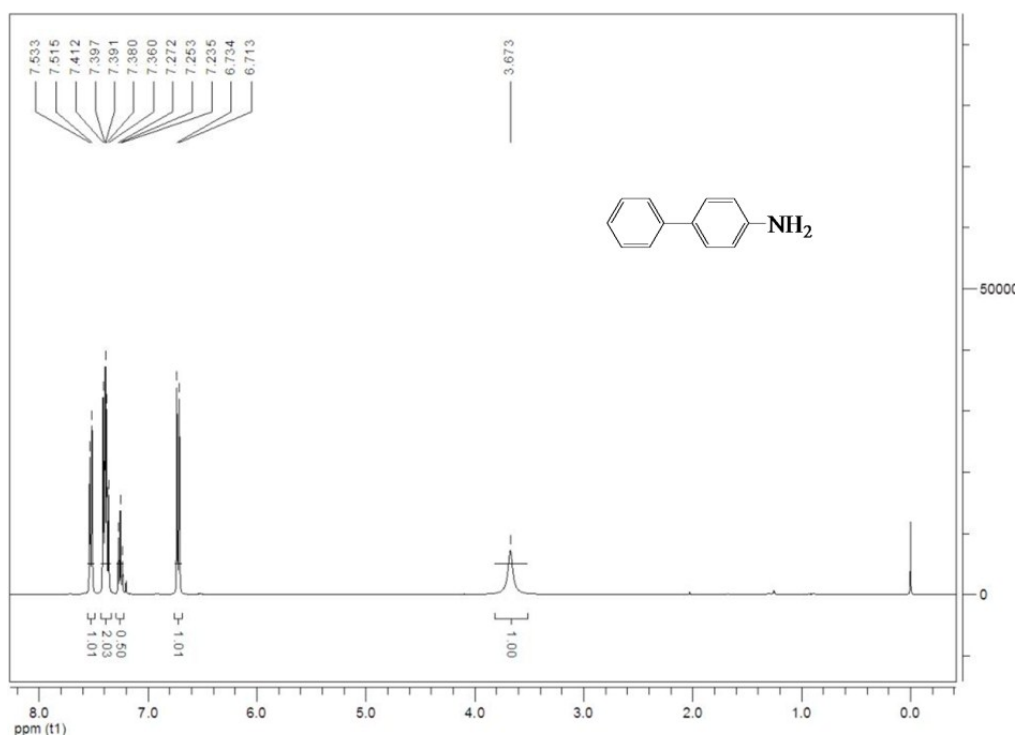


Fig. S14 The ^1H NMR (400 MHz, CDCl_3) spectrum of 4-phenylaniline (**2c**).

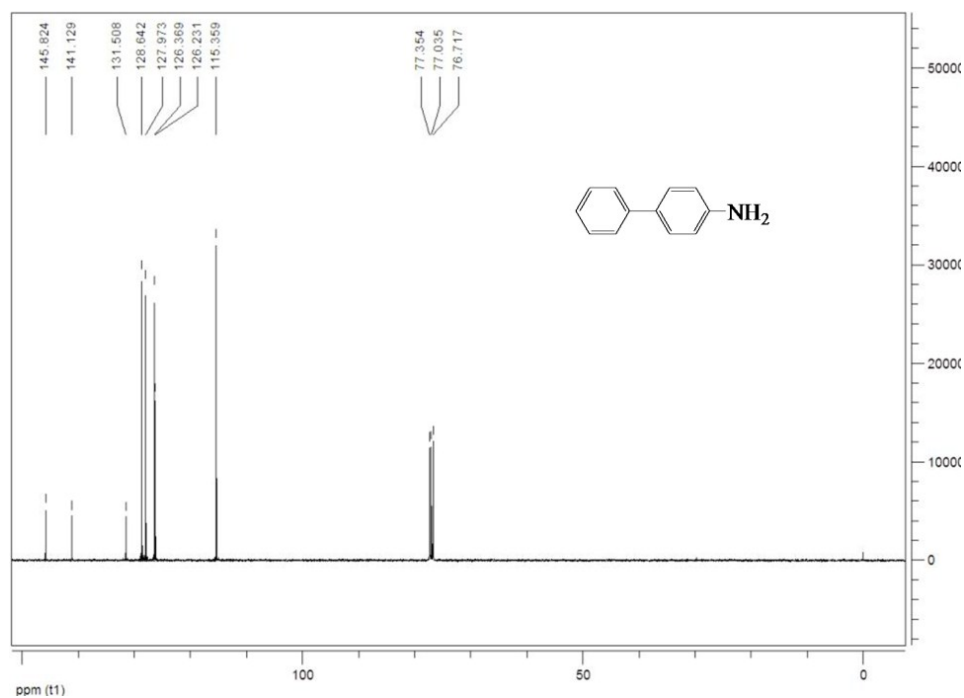


Fig. S15 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4-phenylaniline (**2c**).

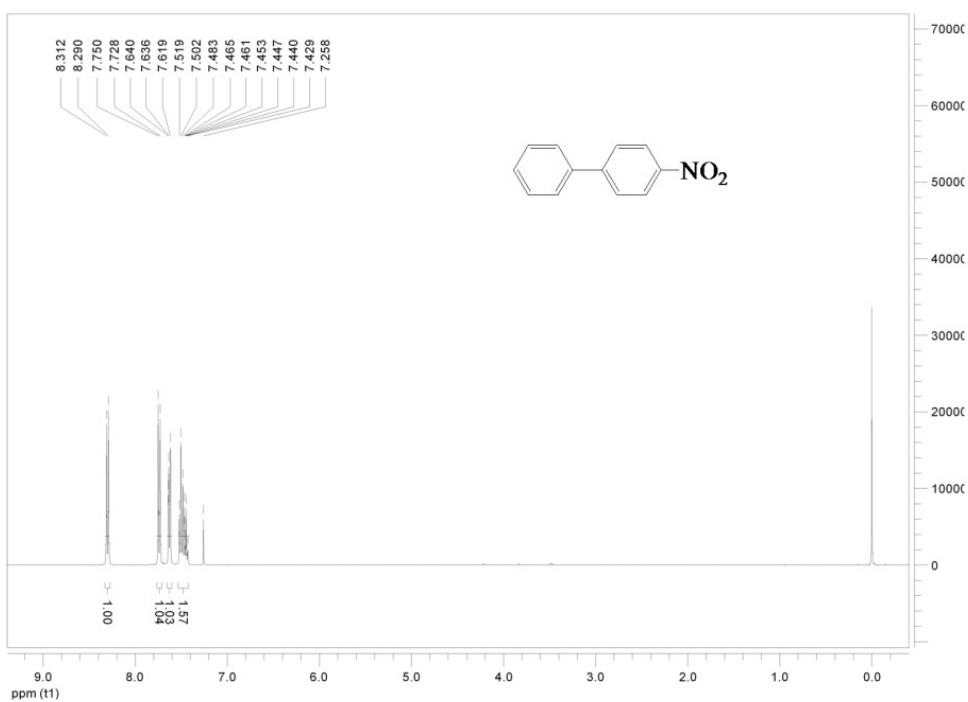


Fig. S16 The ^1H NMR (400 MHz, CDCl_3) spectrum of 4-nitrobiphenyl (**2d**).

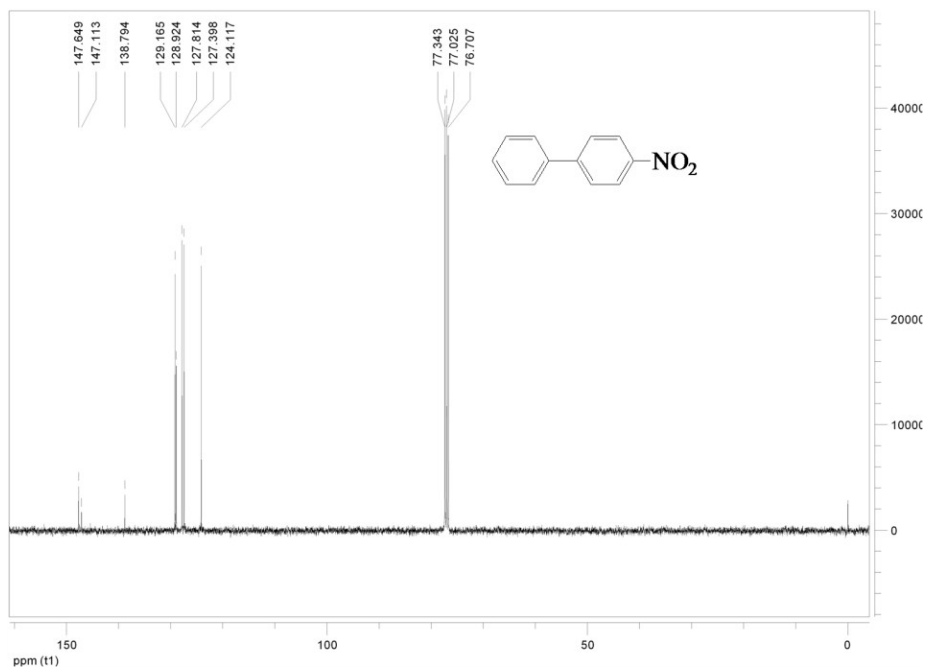


Fig. S17 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4-nitrobiphenyl (**2d**).

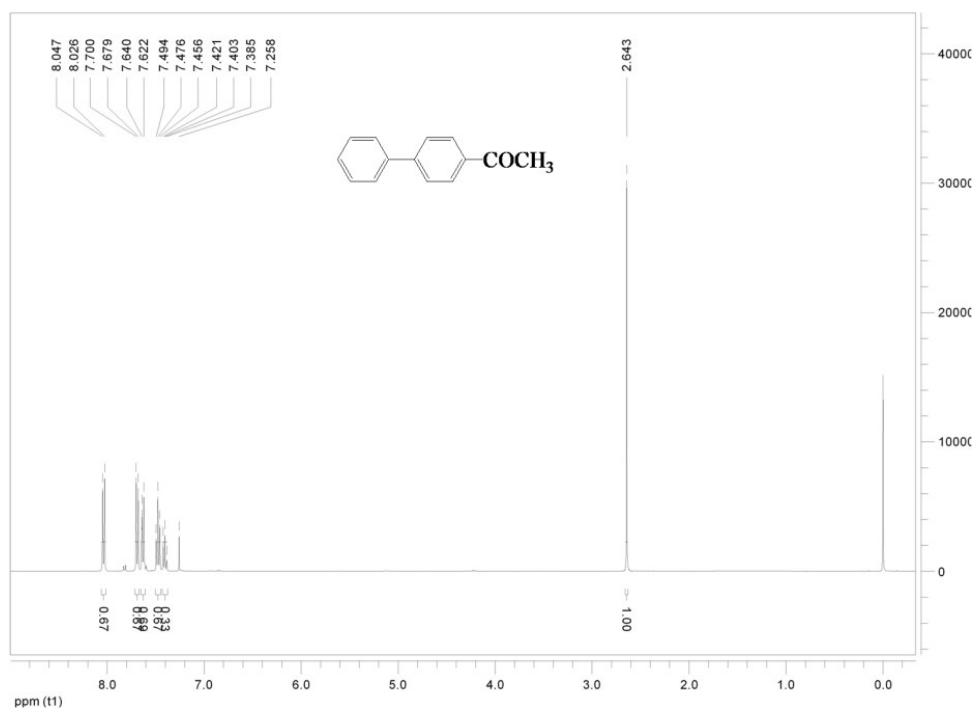


Fig. S18 The ^1H NMR (400 MHz, CDCl_3) spectrum of 4-acetylbiphenyl (**2e**).

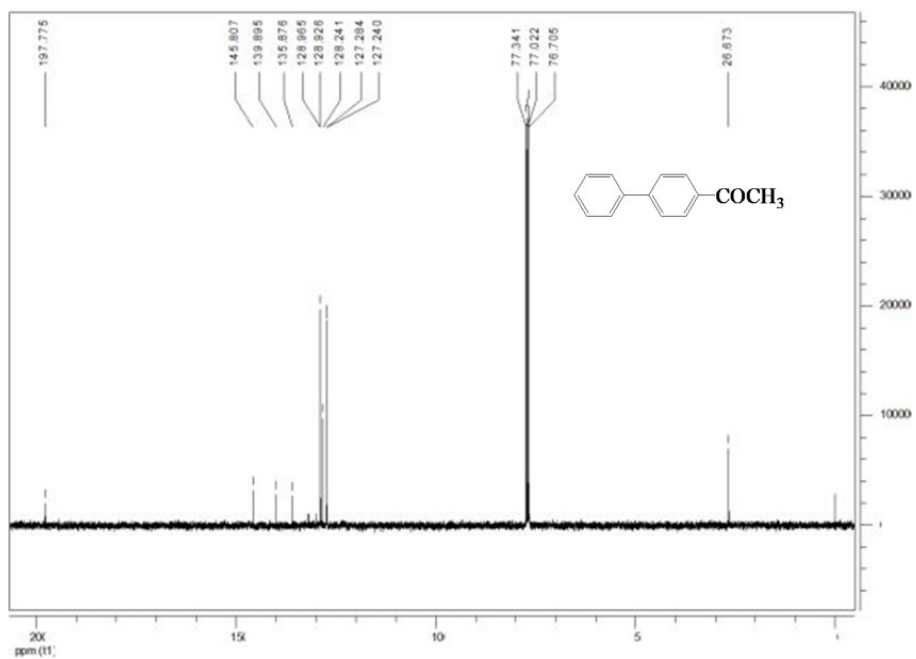


Fig. S19 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4-acetylbiphenyl (**2e**).

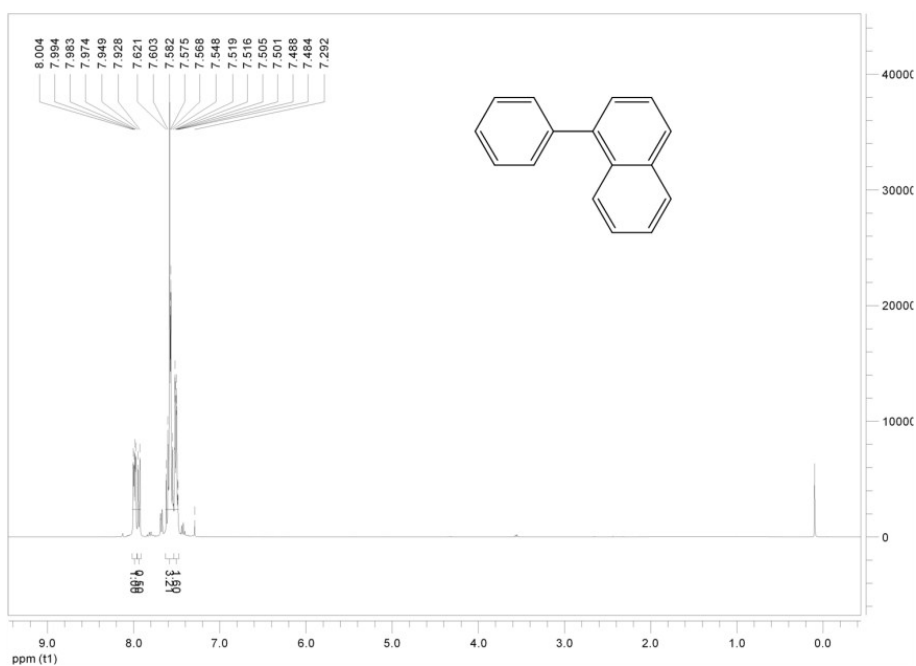


Fig. S20 The ^1H NMR (400 MHz, CDCl_3) spectrum of 1-phenylnaphthalene (**2f**).

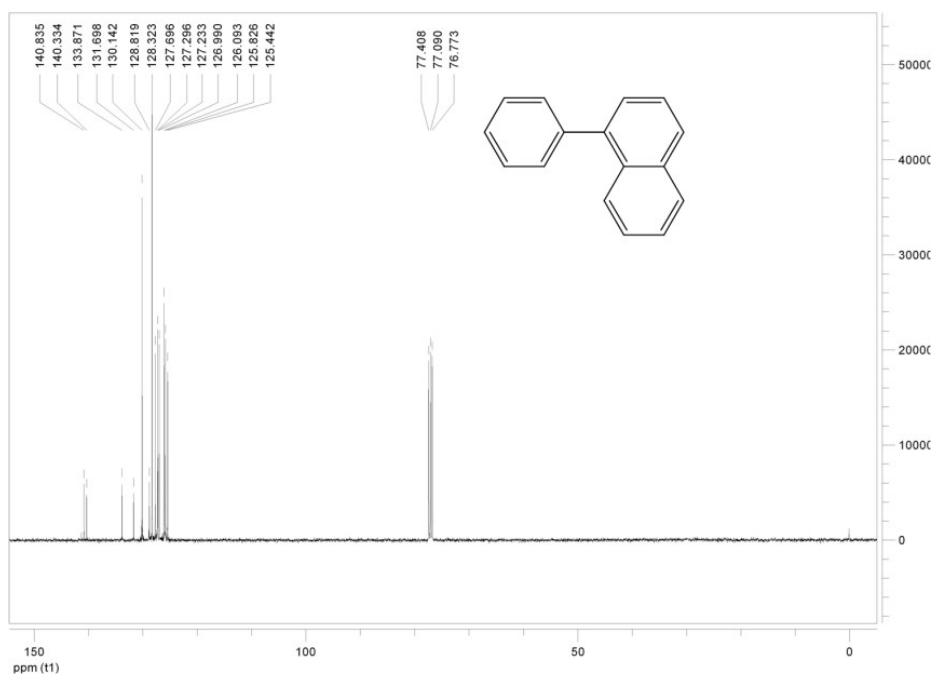


Fig. S21 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 1-phenylnaphthalene (**2f**).

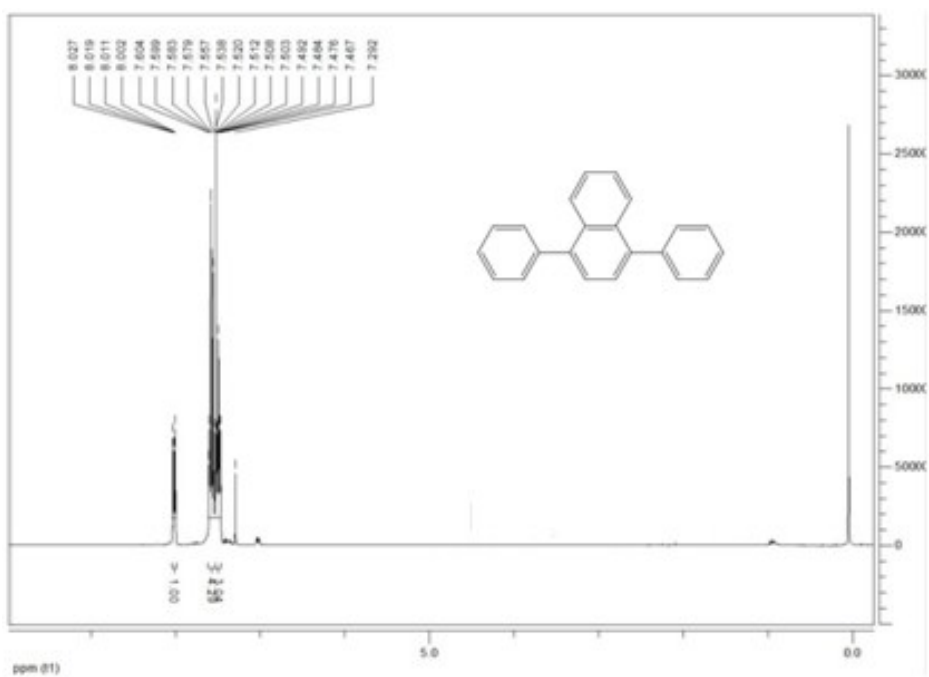


Fig. S22 The ^1H NMR (400 MHz, CDCl_3) spectrum of 1,4-diphenylnaphthalene (**2g**).

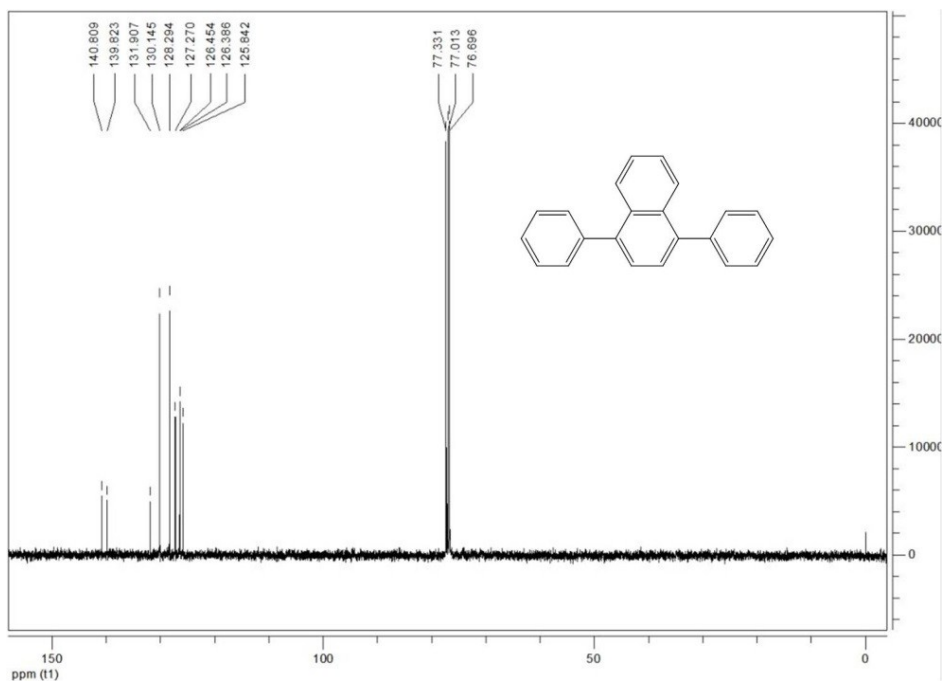


Fig. S23 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 1,4-diphenylnaphthalene (**2g**).

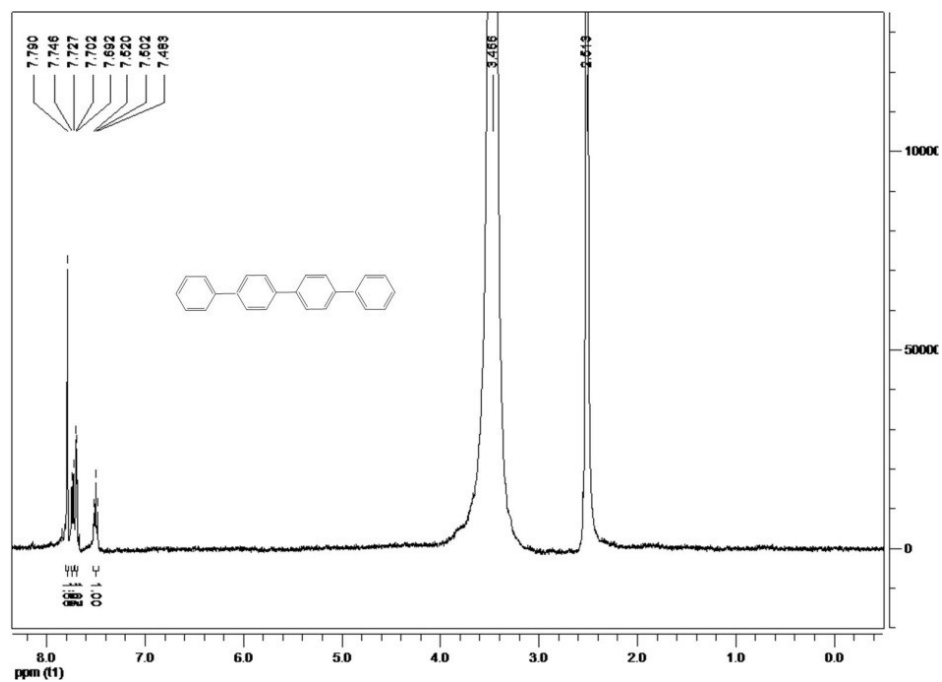


Fig. S24 The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) of 4, 4'-diphenylbiphenyl (**2h**).

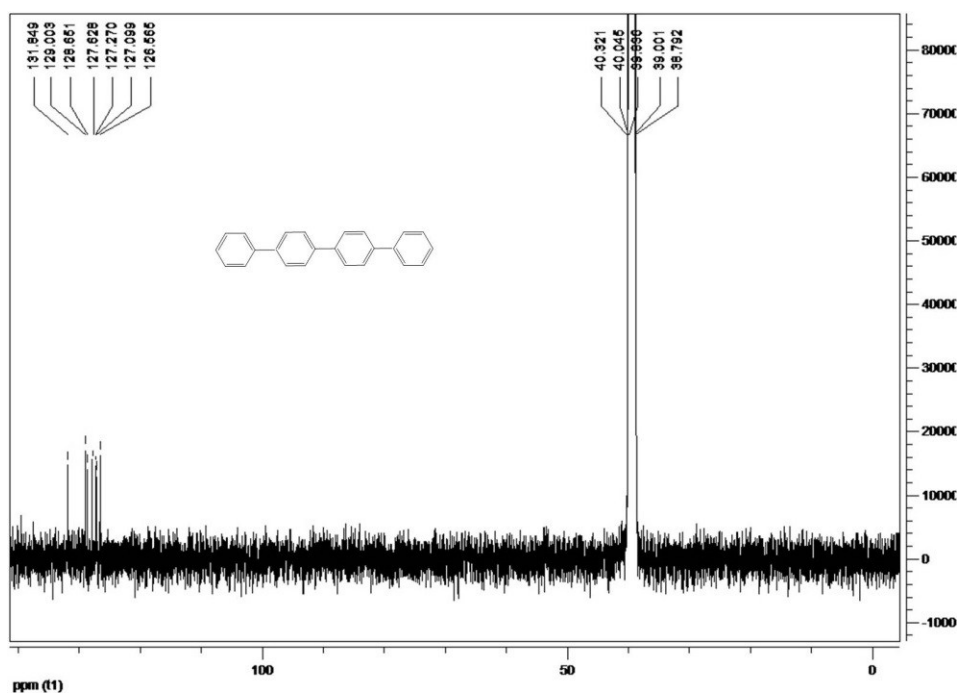


Fig. S25 The ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of 4, 4'-diphenylbiphenyl (2h).

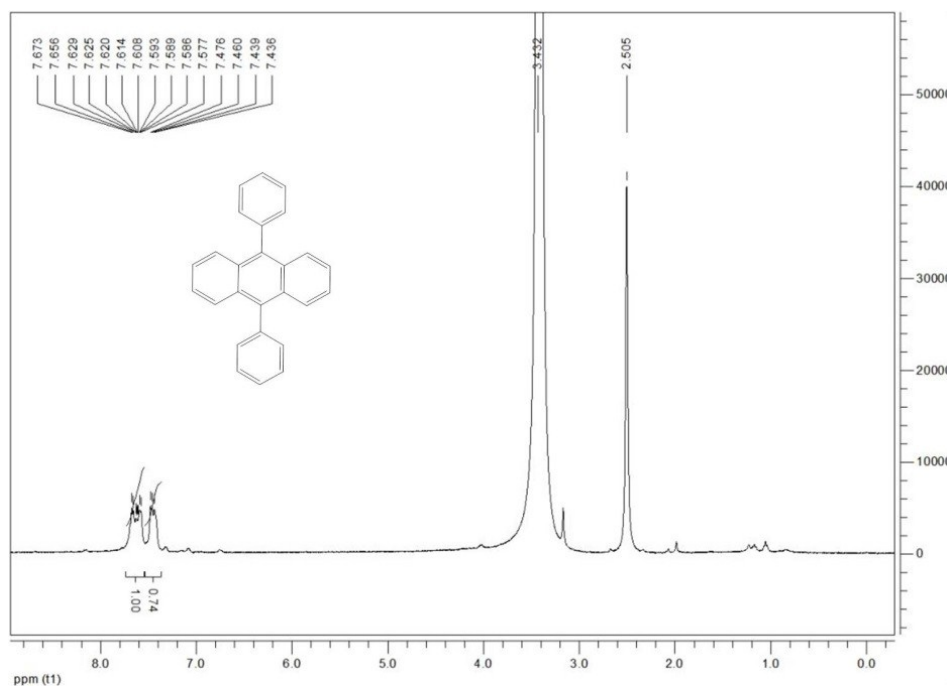


Fig. S26 The ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of 9,10-diphenylanthracene (2i).

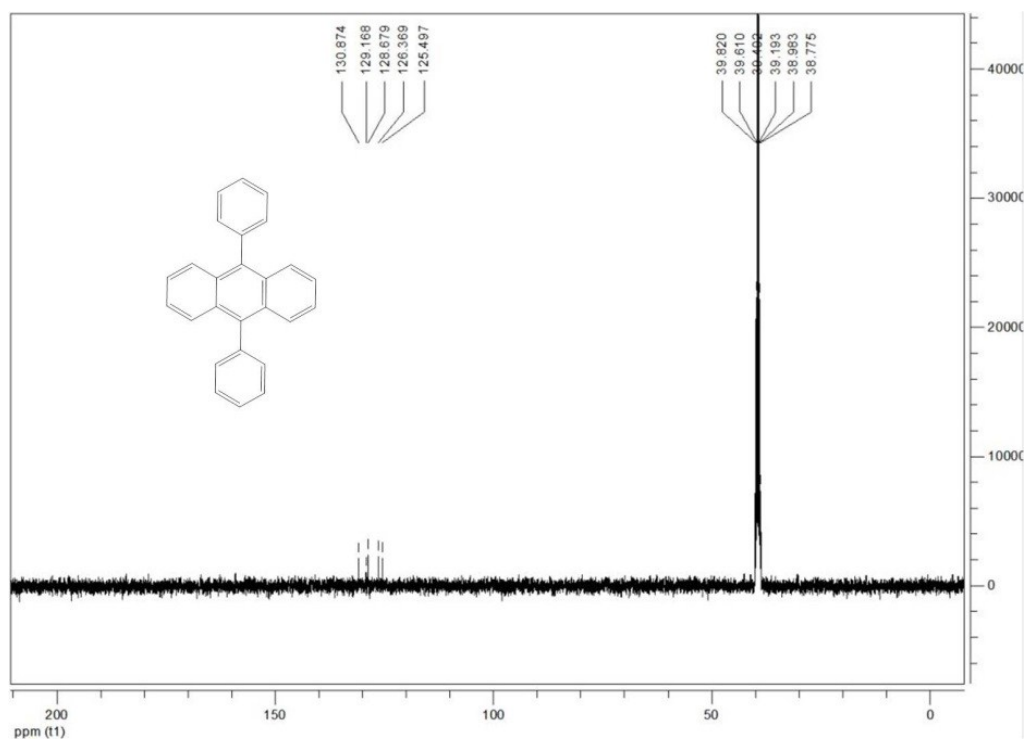


Fig. S27 The ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of 9,10-diphenylanthracene (**2i**).

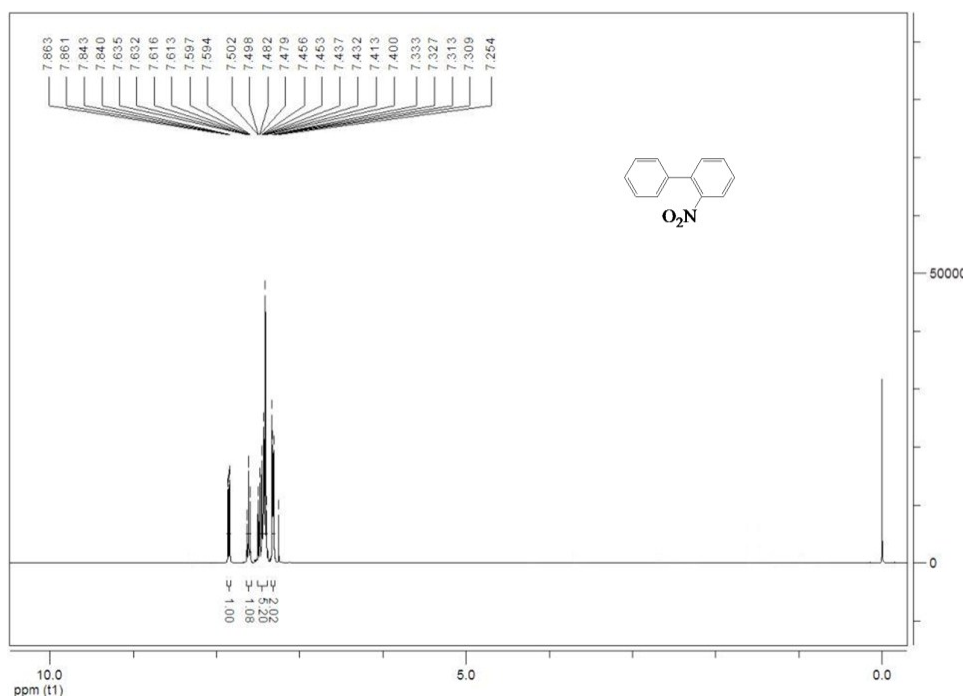


Fig. S28 The ^1H NMR (400 MHz, CDCl_3) spectrum of 2-nitrophenyl (**2j**).

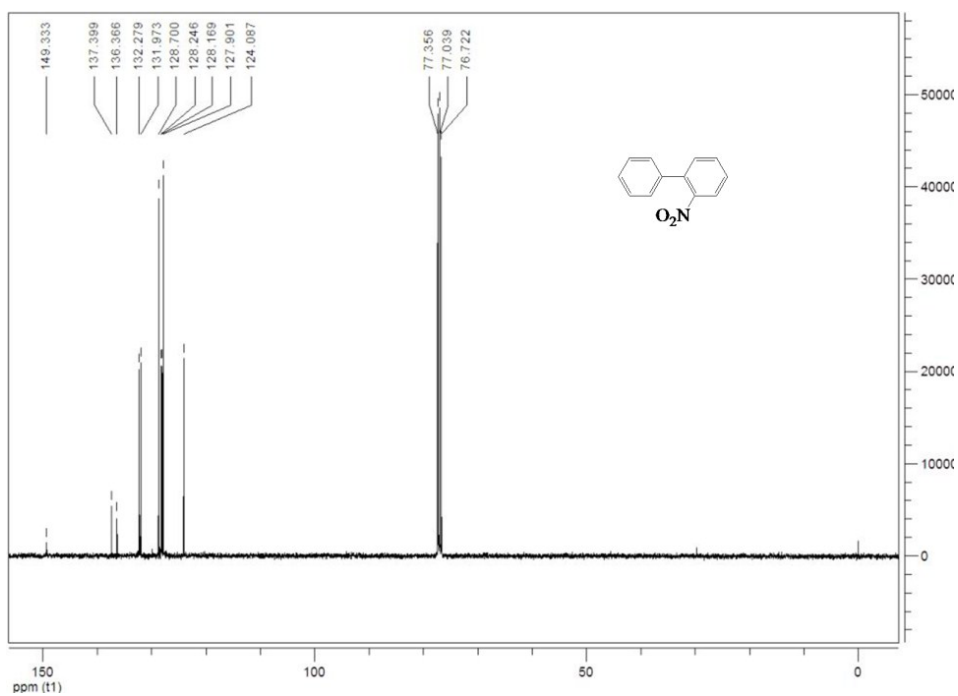


Fig. S29 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 2-nitrophenyl (**2j**).

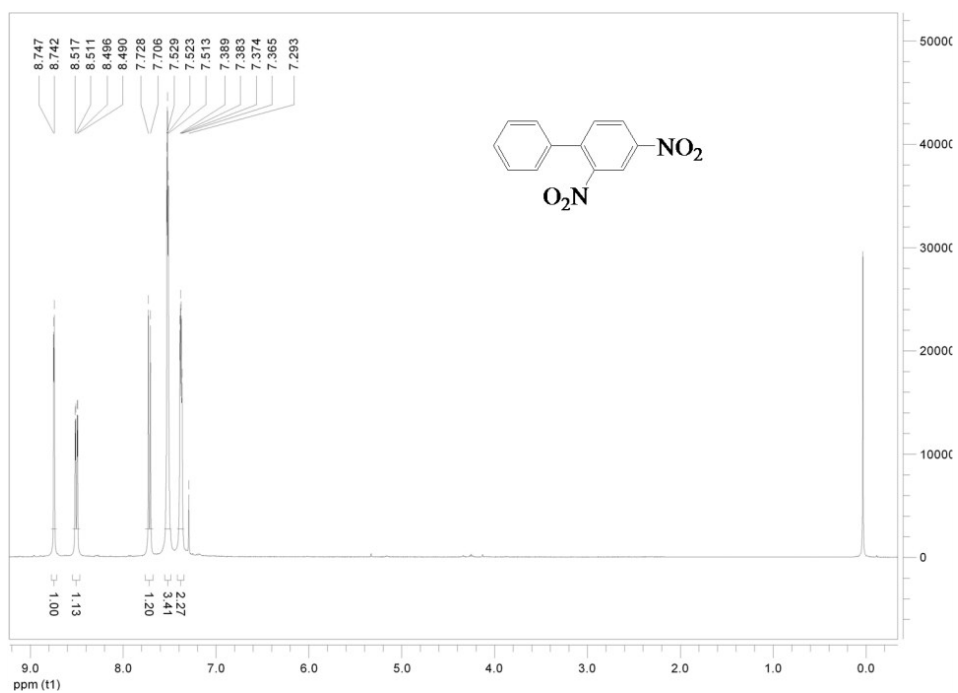


Fig. S30 The ^1H NMR (400 MHz, CDCl_3) spectrum of 2,4-dinitrophenyl (**2k**).

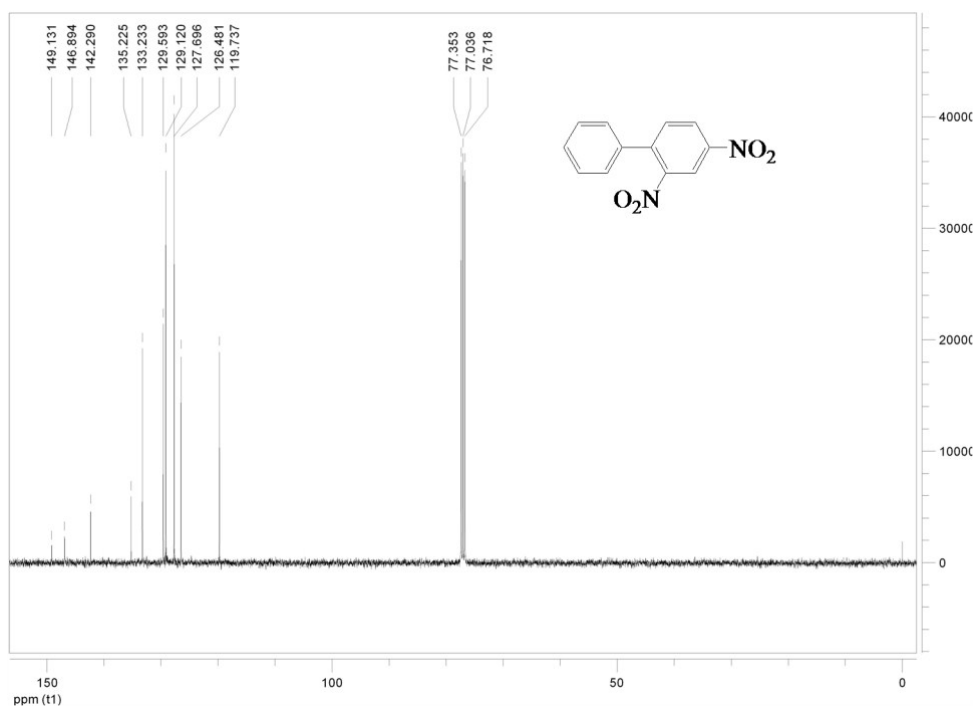


Fig. S31 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 2,4-dinitrobiphenyl (**2k**).

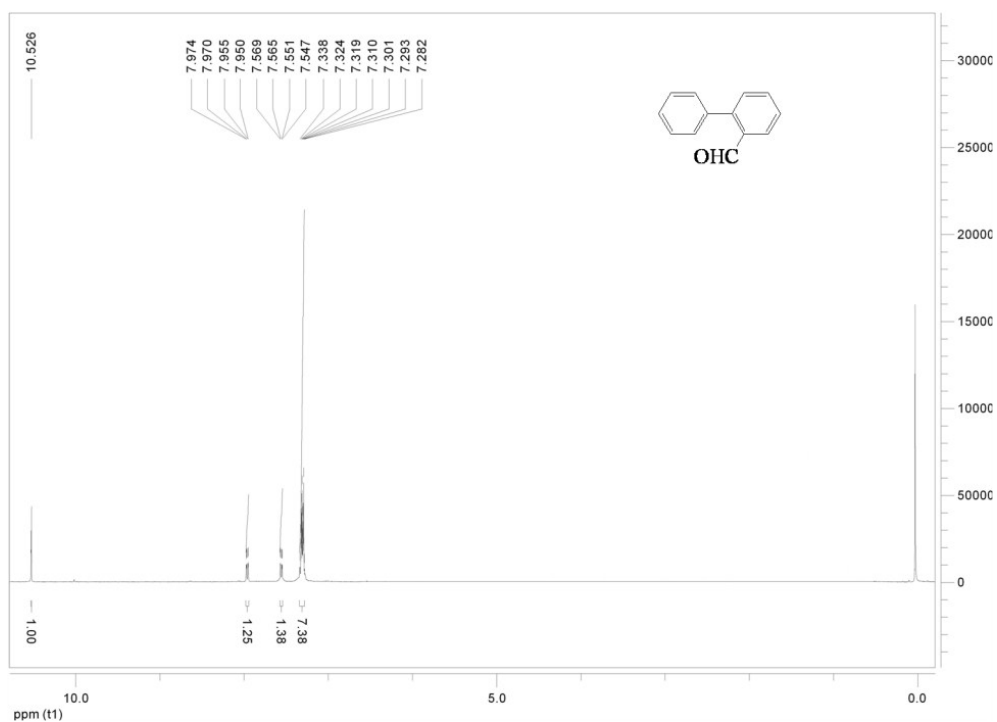


Fig. S32 The ^1H NMR (400 MHz, CDCl_3) spectrum of biphenyl-2-carbaldehyde (**2l**).

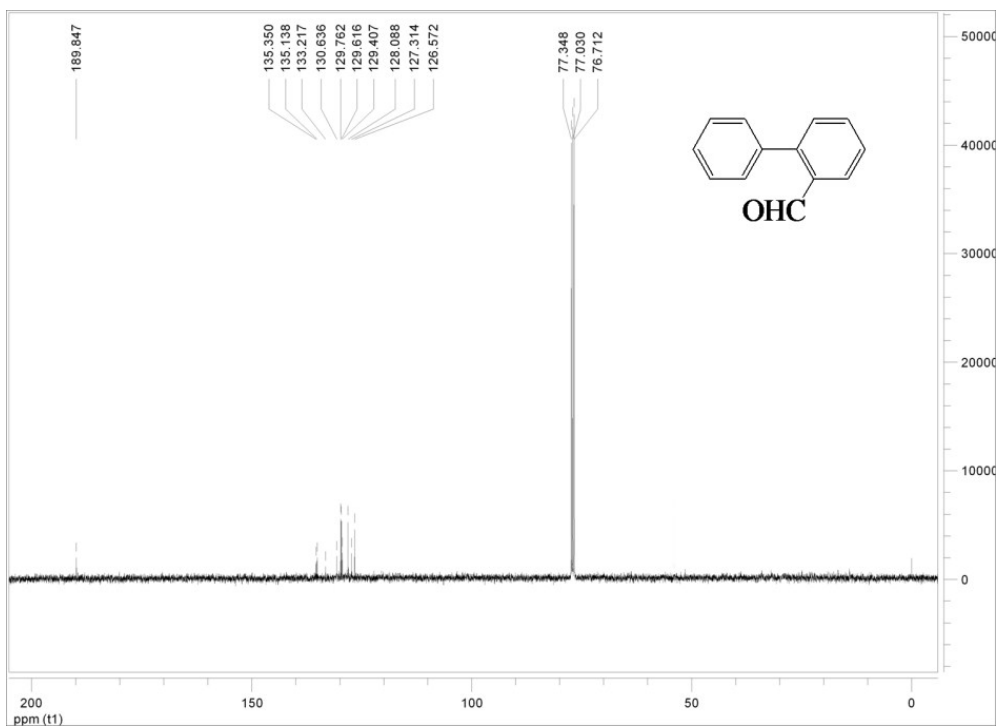


Fig. S33 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of biphenyl-2-carbaldehyde (**21**).

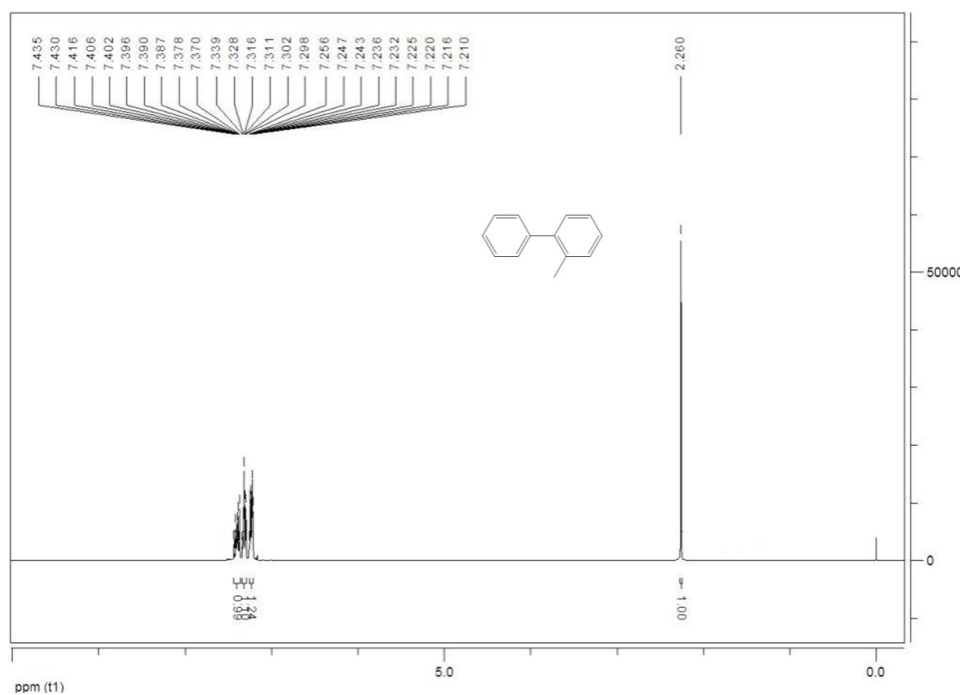


Fig. S34 The ^1H NMR (400 MHz, CDCl_3) spectrum of 2-methylbiphenyl (**2m**).

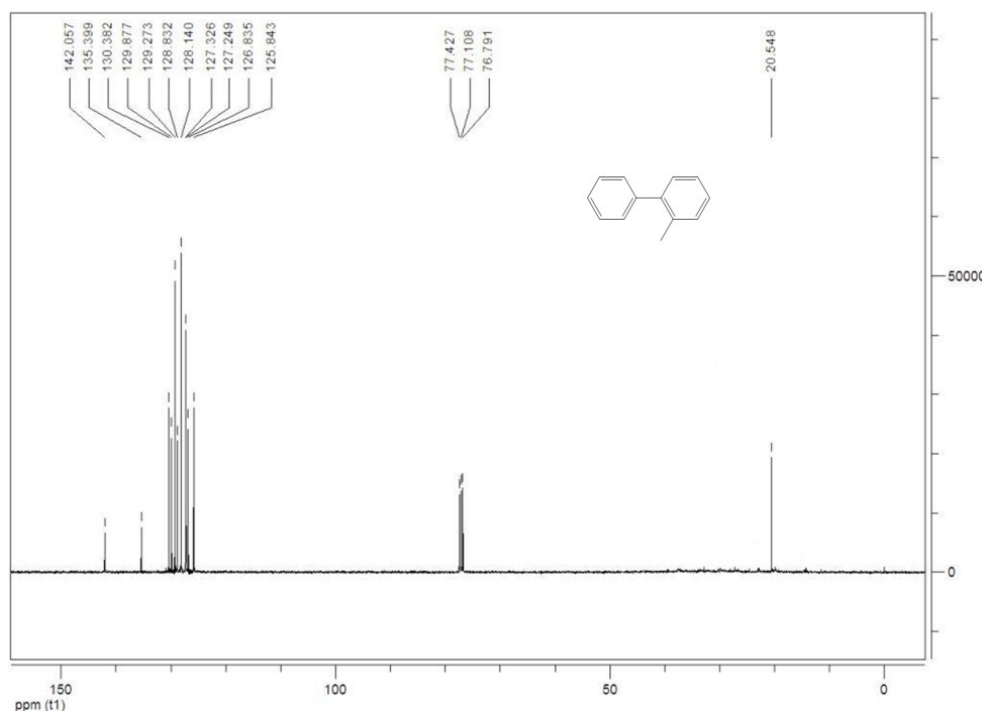


Fig. S35 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 2-methylbiphenyl (**2m**).

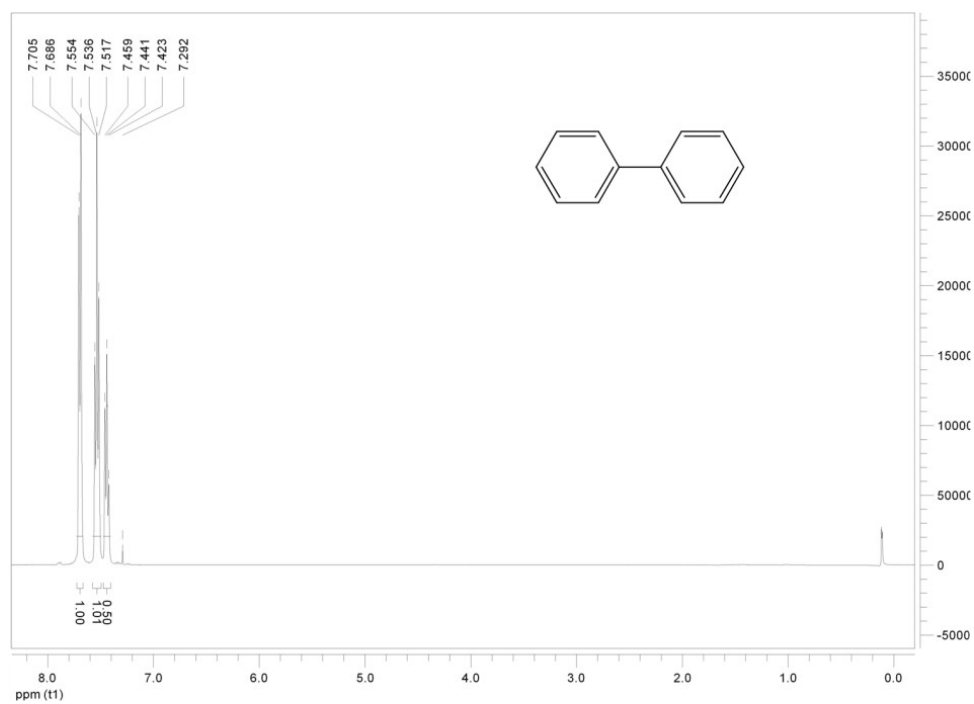


Fig. S36 The ^1H NMR (400 MHz, CDCl_3) spectrum of biphenyl (**2n**).

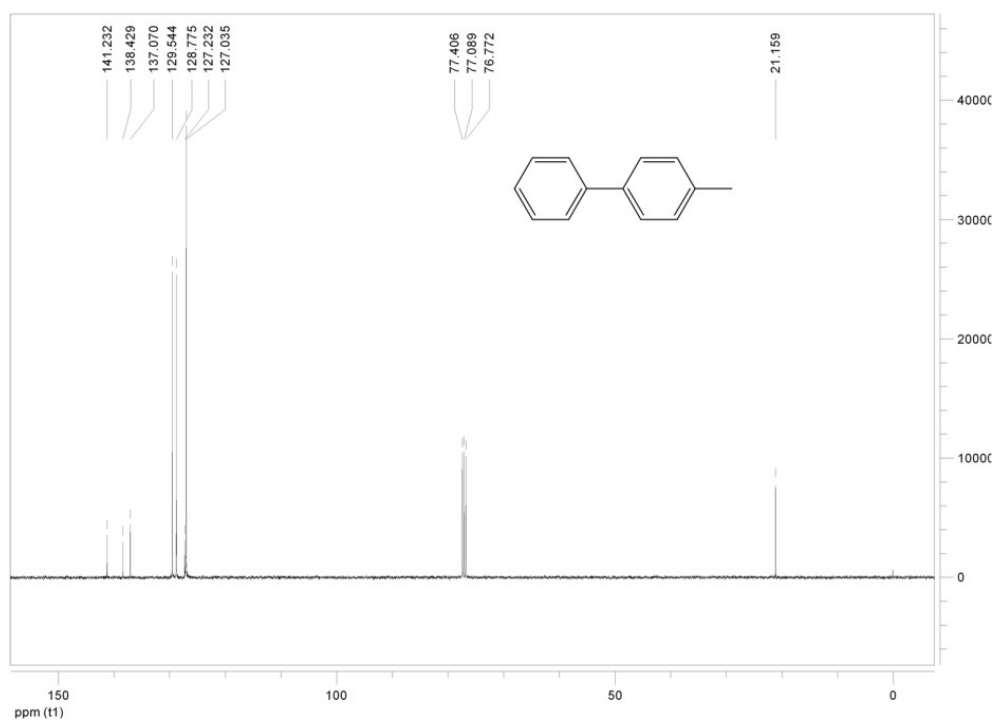


Fig. S39 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4-methylbiphenyl (**2o**).

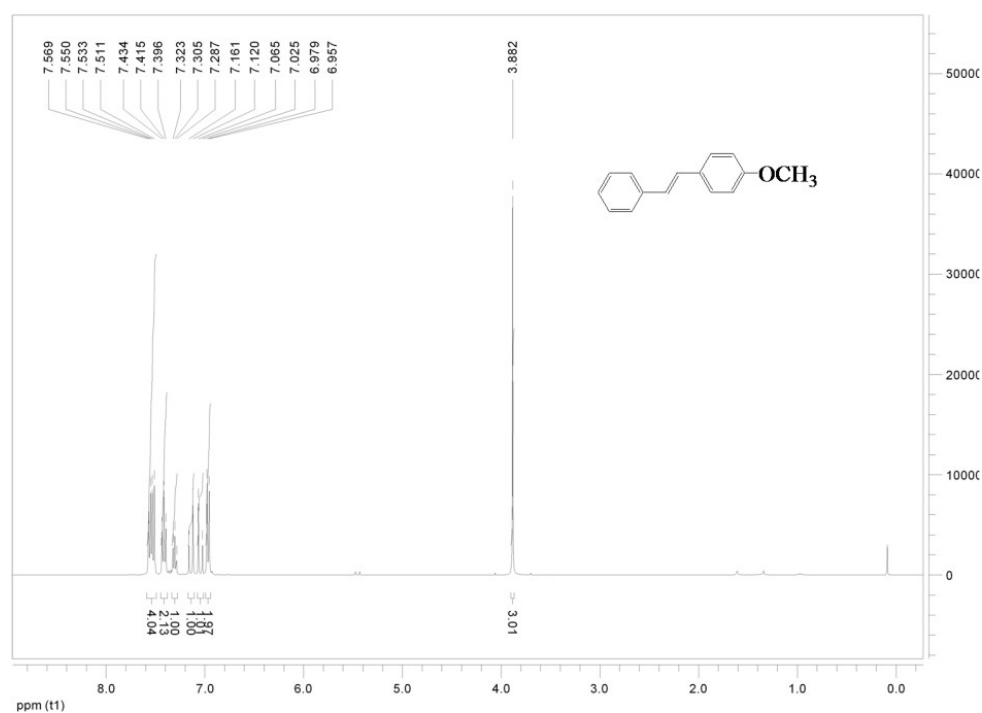


Fig. S40 The ^1H NMR (400 MHz, CDCl_3) spectrum of 4-methoxystilbene (**3a**).

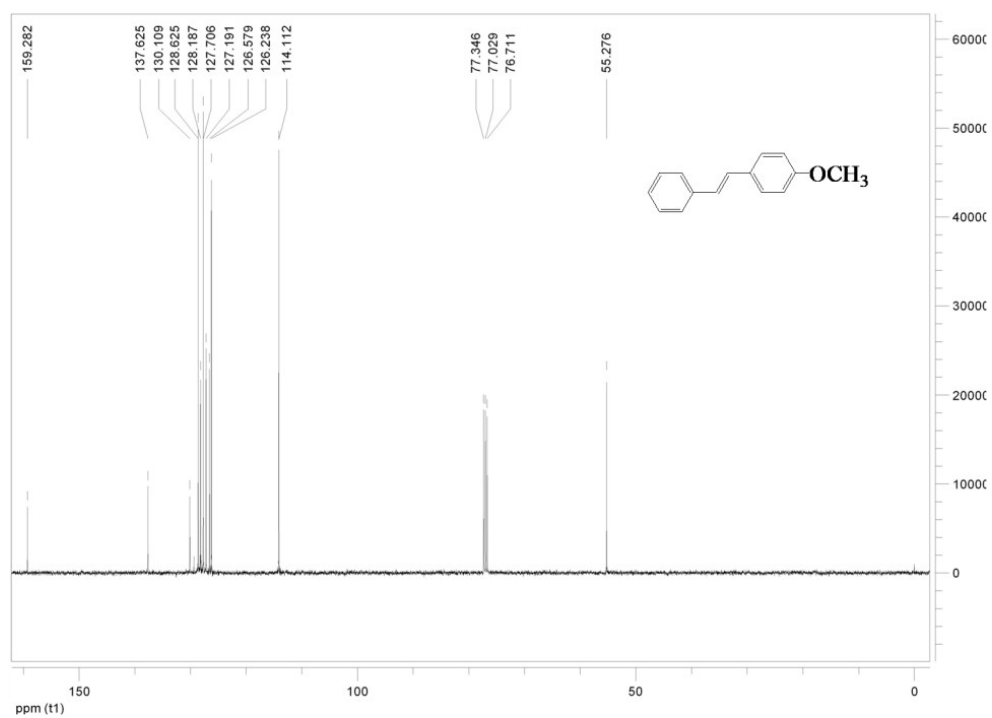


Fig. S41 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4-methoxystilbene (**3a**).

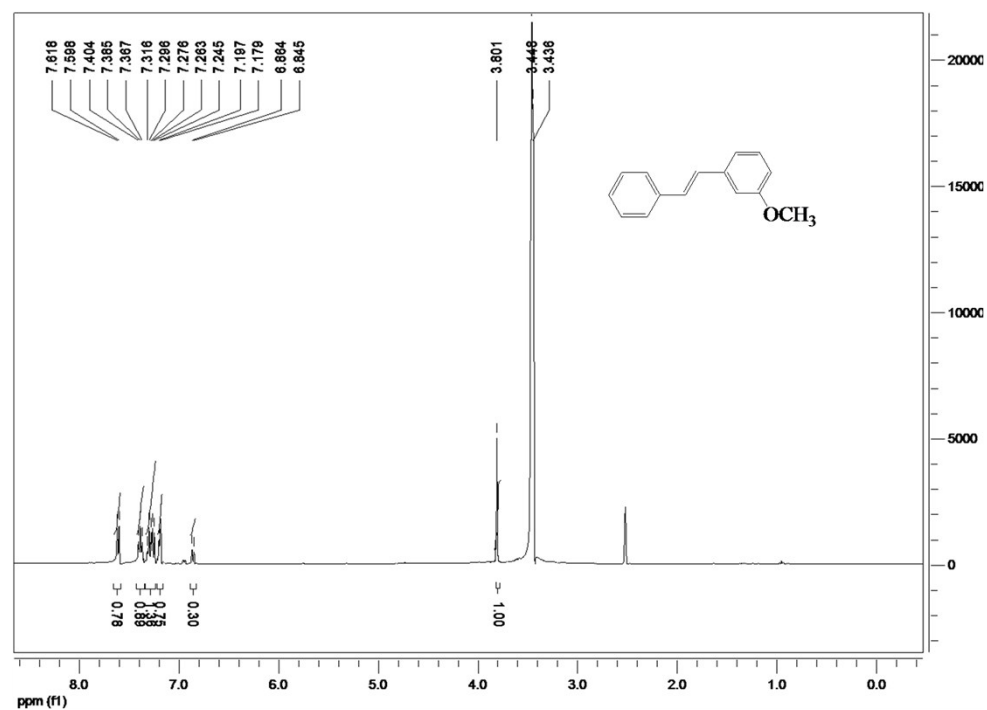


Fig. S42 The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of 3-methoxystilbene (**3b**).

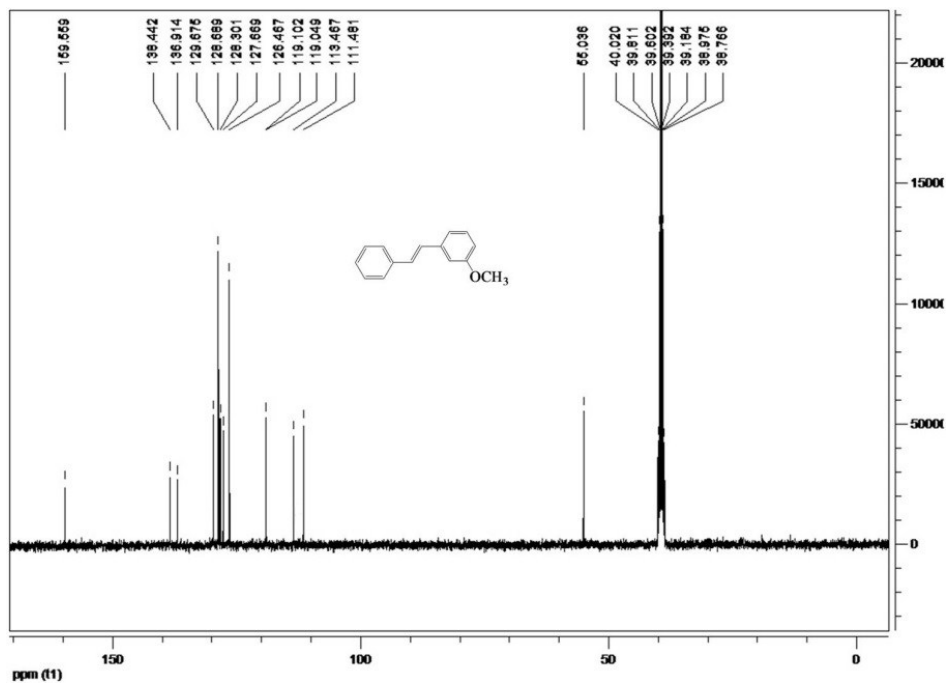


Fig. S43 The ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of 3-methoxystilbene (**3b**).

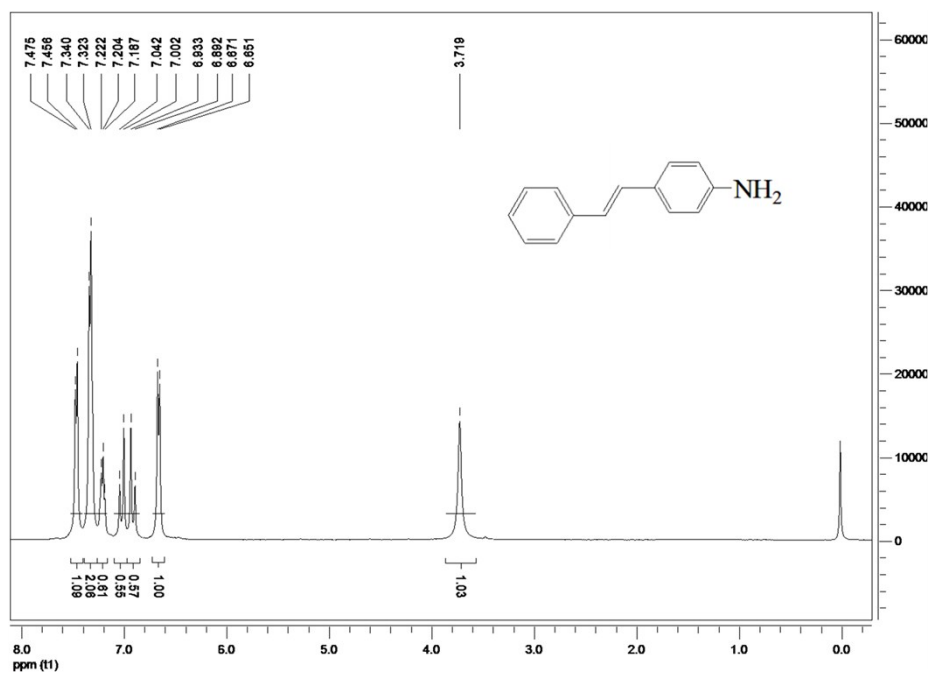


Fig. S44 The ^1H NMR (400 MHz, CDCl_3) spectrum of 4-anilinstilbene (**3c**).

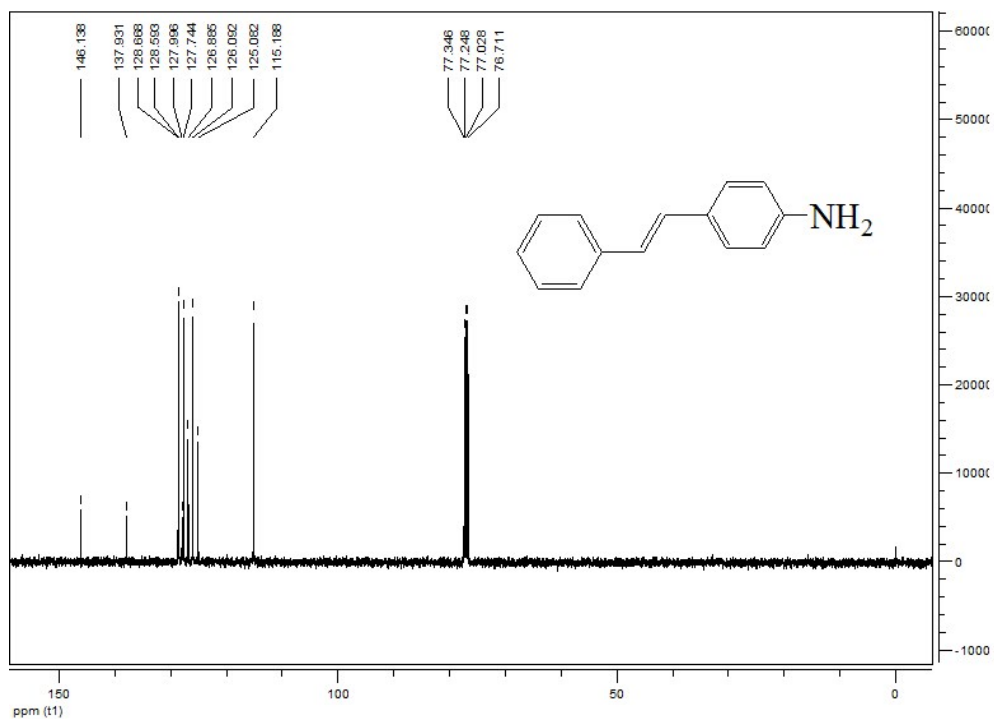


Fig. S45 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4-anilinstilbene (**3c**).

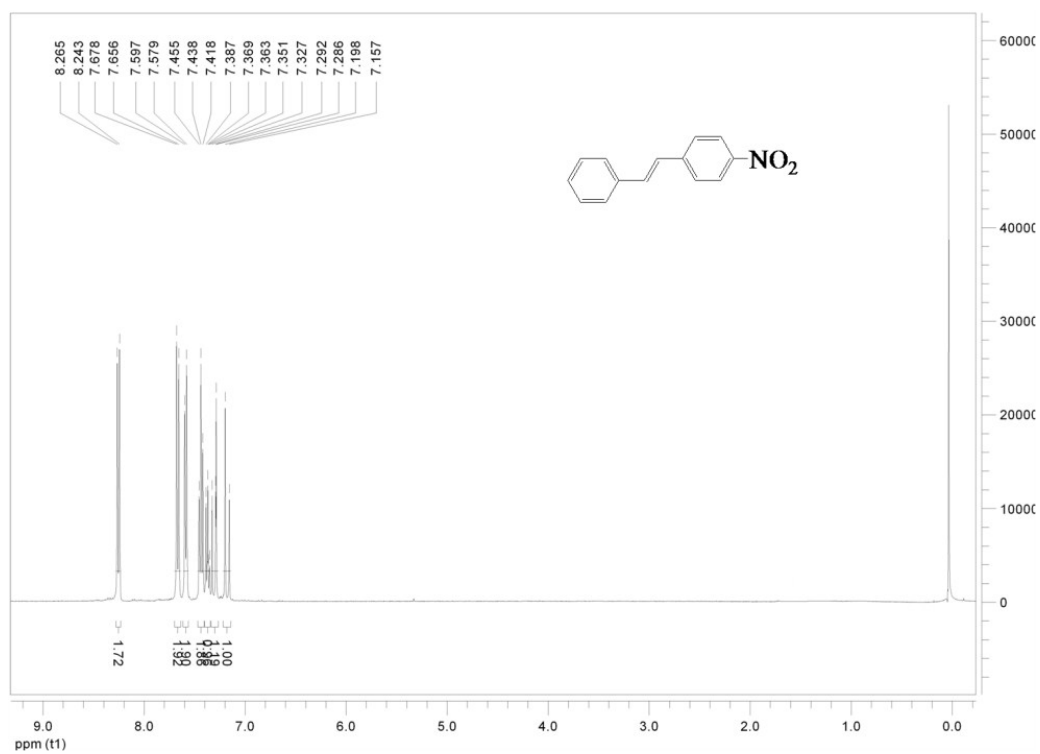


Fig. S46 The ^1H NMR (400 MHz, CDCl_3) spectrum of 4-nitrostilbene (**3d**).

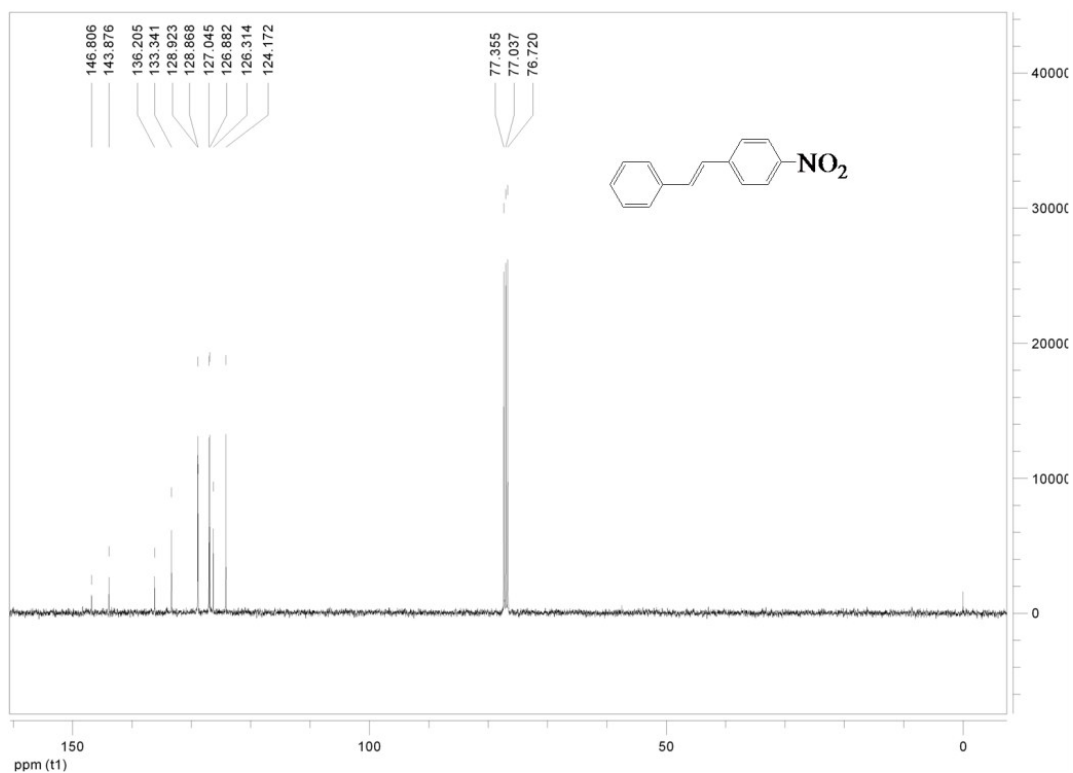


Fig. S47 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4-nitrostilbene (**3d**).

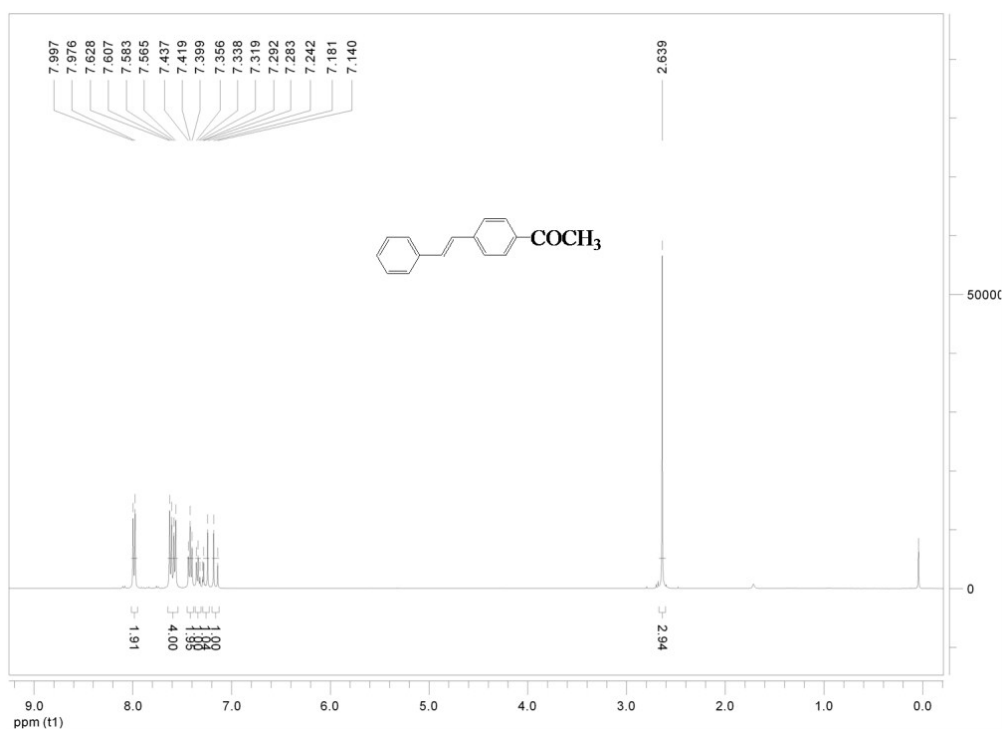


Fig. S48 The ^1H NMR (400 MHz, CDCl_3) spectrum of 4-acetylstilbene (**3e**).

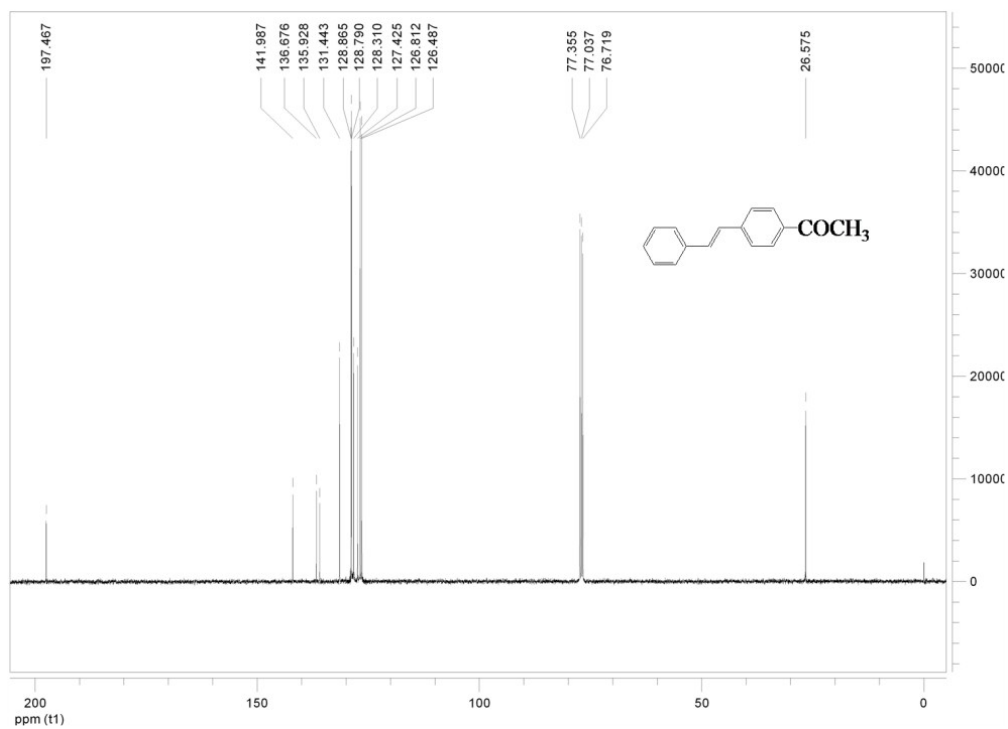


Fig. S49 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4-acetylstilbene (**3e**).

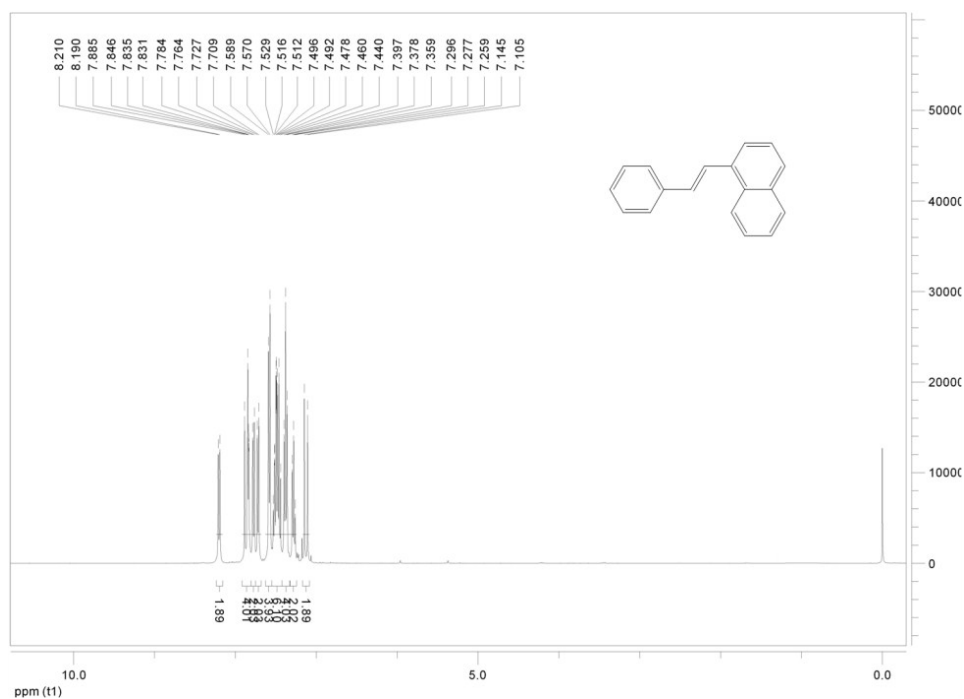


Fig. S50 The ^1H NMR (400 MHz, CDCl_3) spectrum of 1-styrylnaphthalene (**3f**).

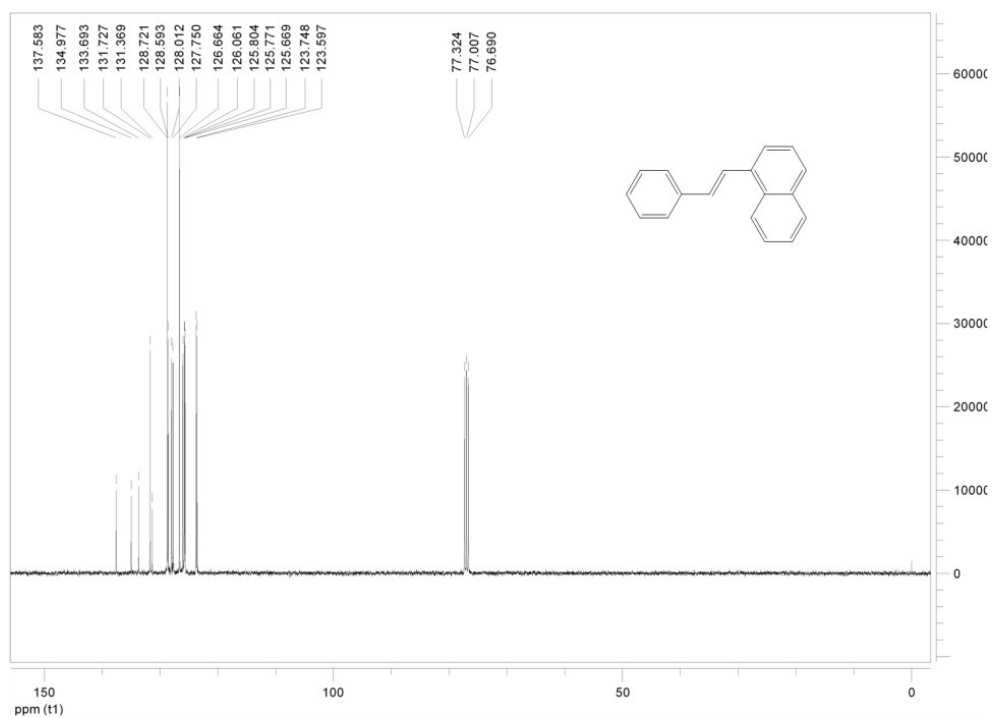


Fig. S51 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 1-styrylnaphthalene (**3f**).

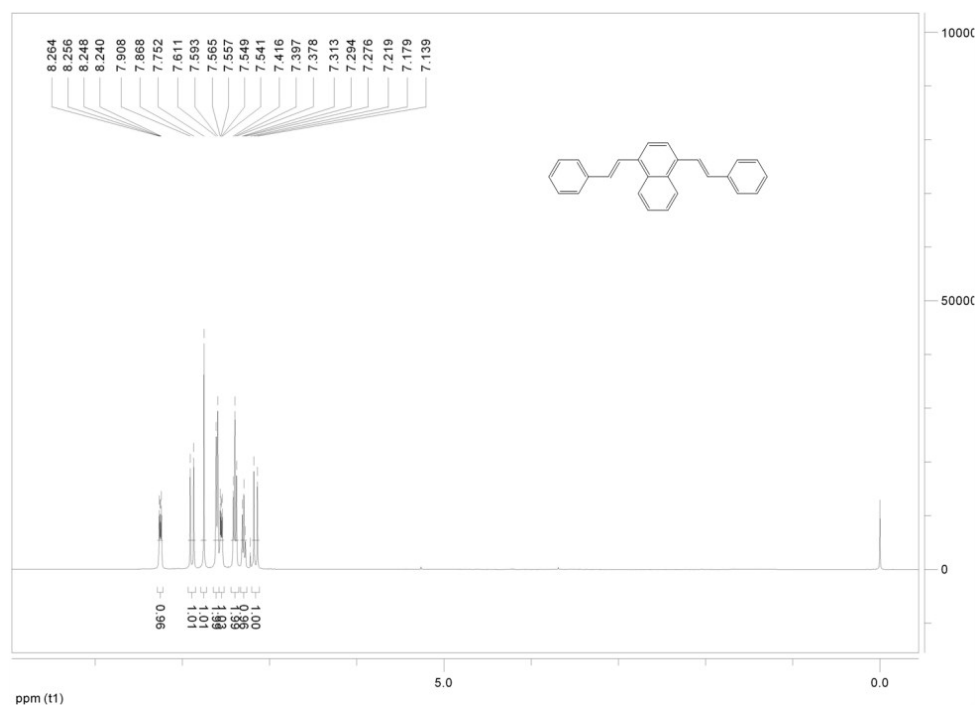


Fig. S52 The ^1H NMR (400 MHz, CDCl_3) spectrum of 1,4-distyrylnaphthalene (**3g**).

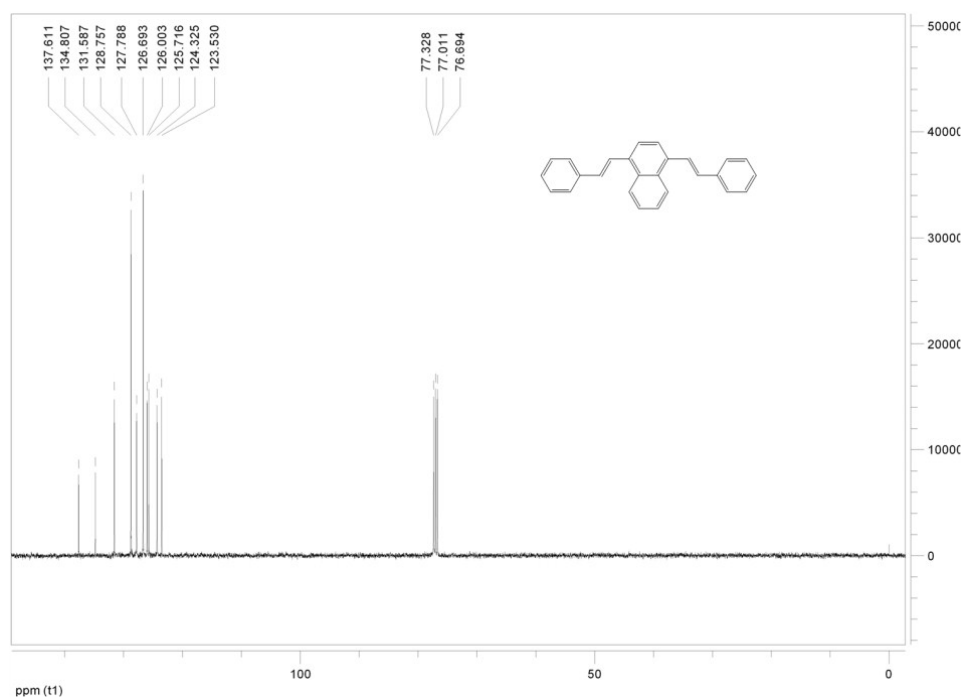


Fig. S53 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 1,4-distyrylnaphthalene (**3g**).

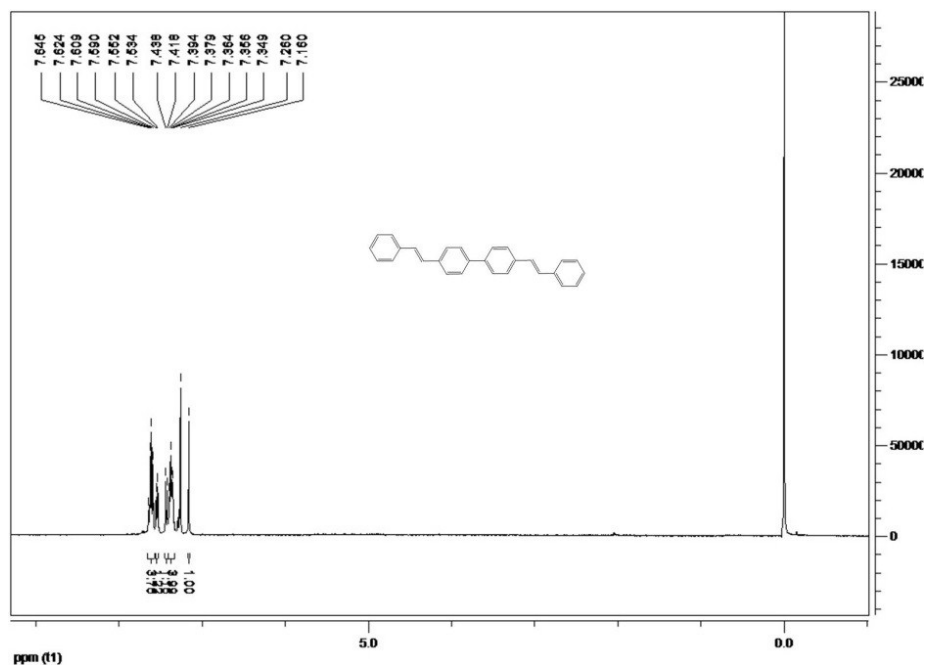


Fig. S54 The ^1H NMR (400 MHz, CDCl_3) spectrum of 4, 4'-bis(2-phenylethenyl)-bipheny (**3h**).

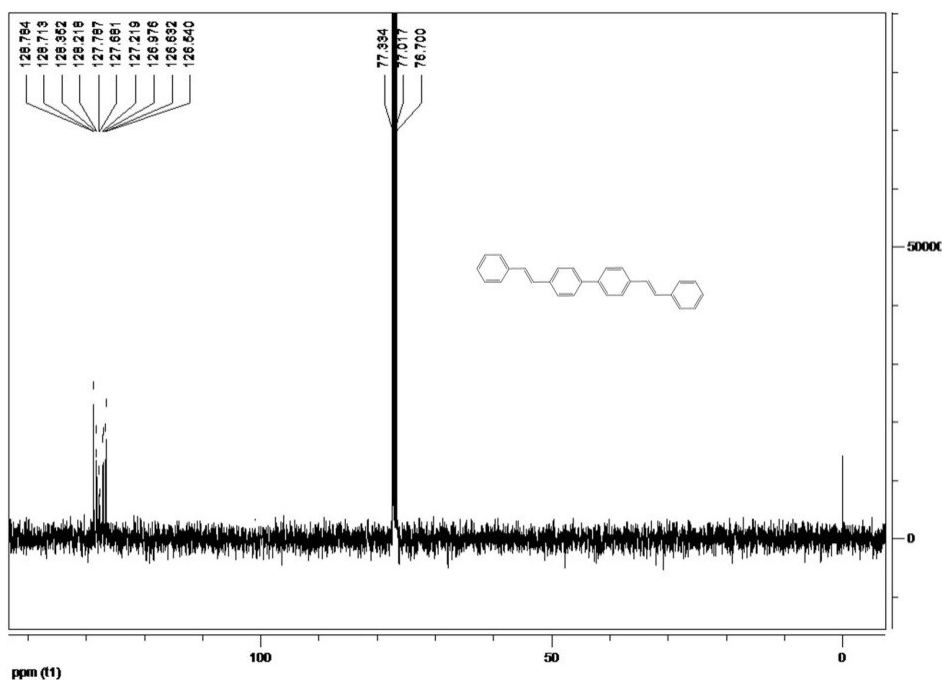


Fig. S55 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4, 4'-bis(2-phenylethenyl)-bipheny (**3h**).

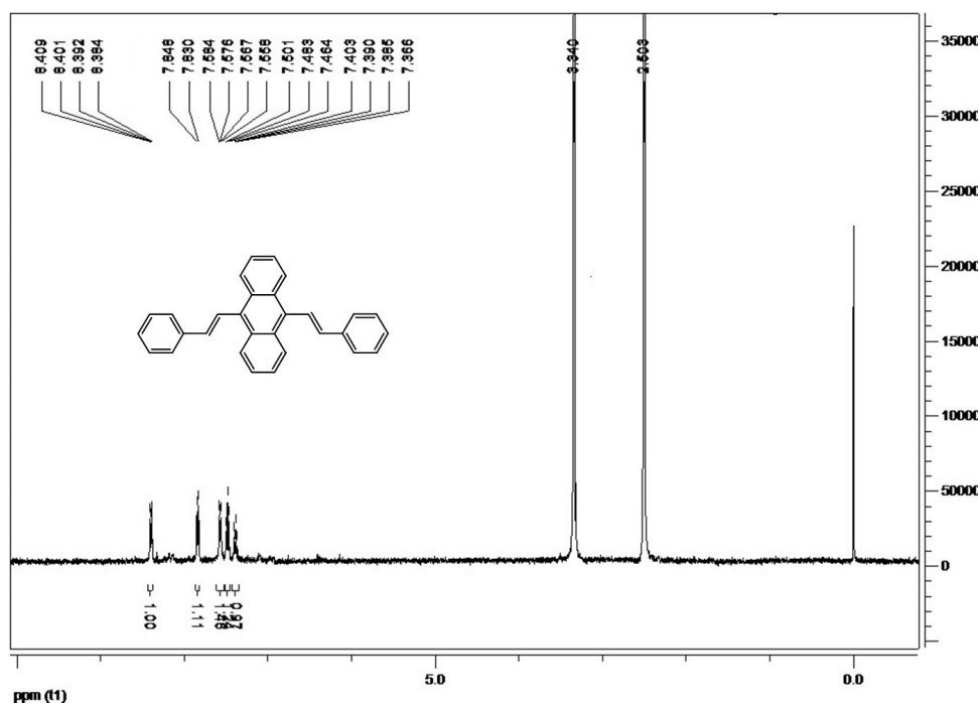


Fig. S56 The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of 9, 10-bis(2-phenylethenyl)-anthracene (**3i**).

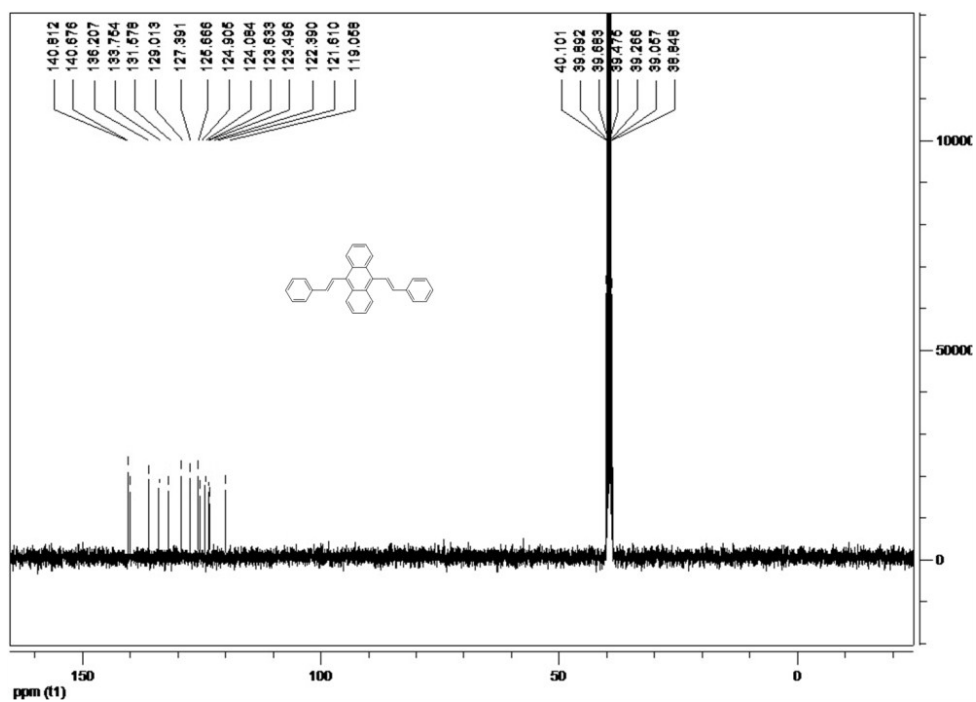


Fig. S57 The ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of 9, 10-bis(2-phenylethenyl)-anthracene (**3i**).

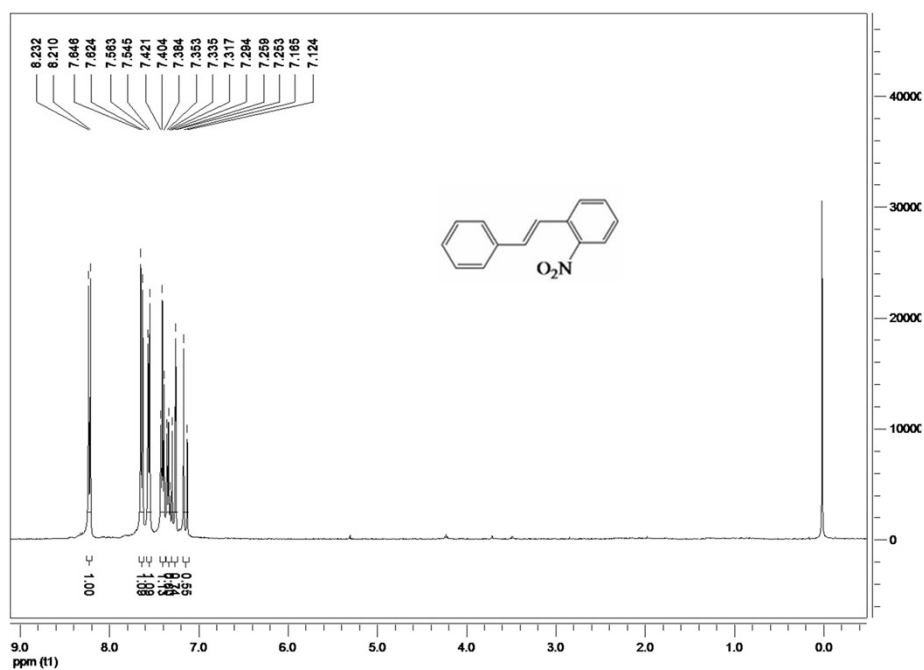


Fig. S58 The ^1H NMR (400 MHz, CDCl_3) spectrum of 1-nitro-2-(2-phenylethenyl)-stilbene (**3j**).

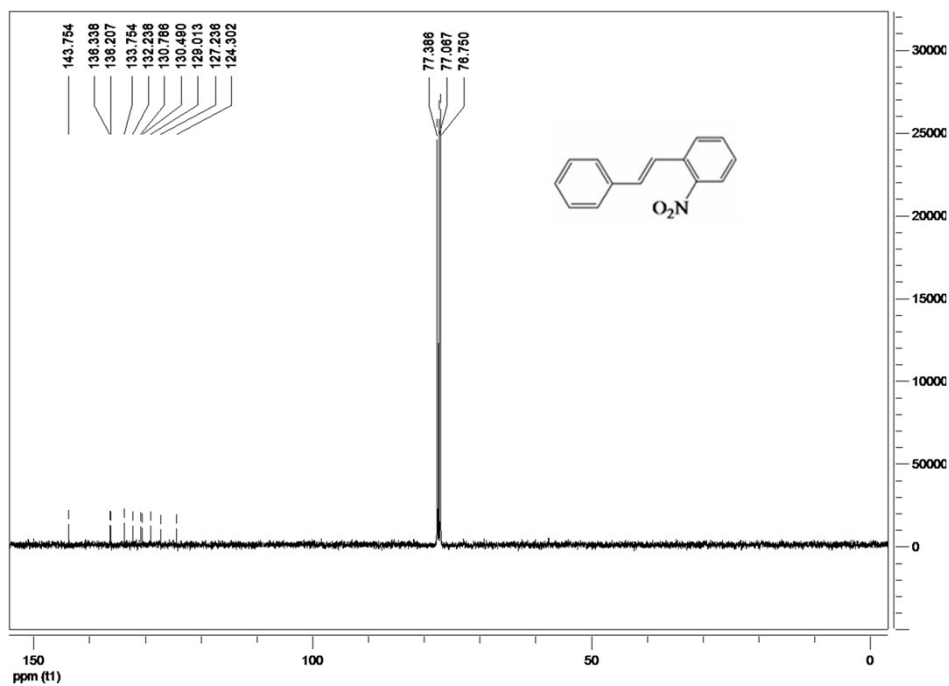


Fig. S59 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 1-nitro-2-(2-phenylethenyl)-stilbene (**3j**).

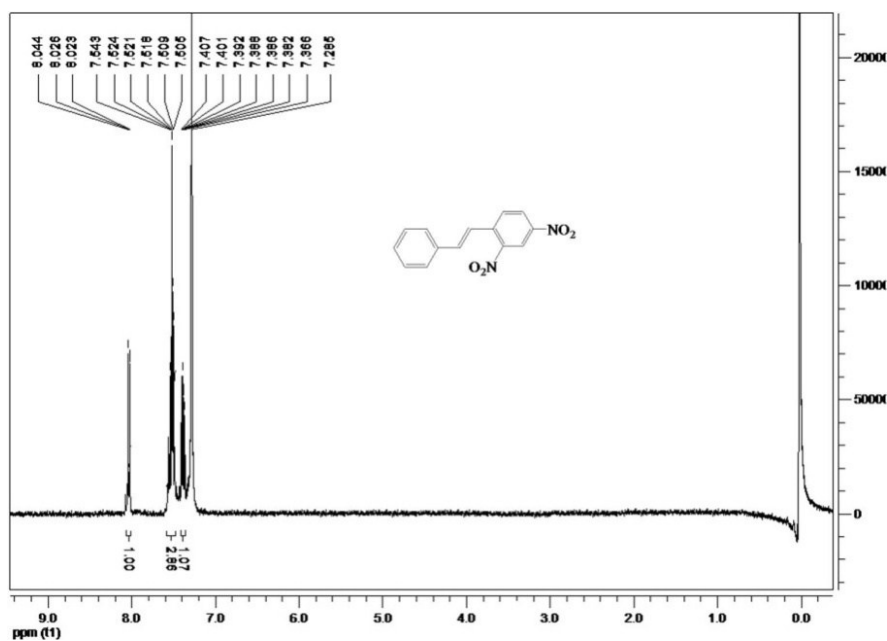


Fig. S60 The ^1H NMR (400 MHz, CDCl_3) spectrum of 2,4-dinitro-1-(2-phenylethenyl)-stilbene (**3k**).

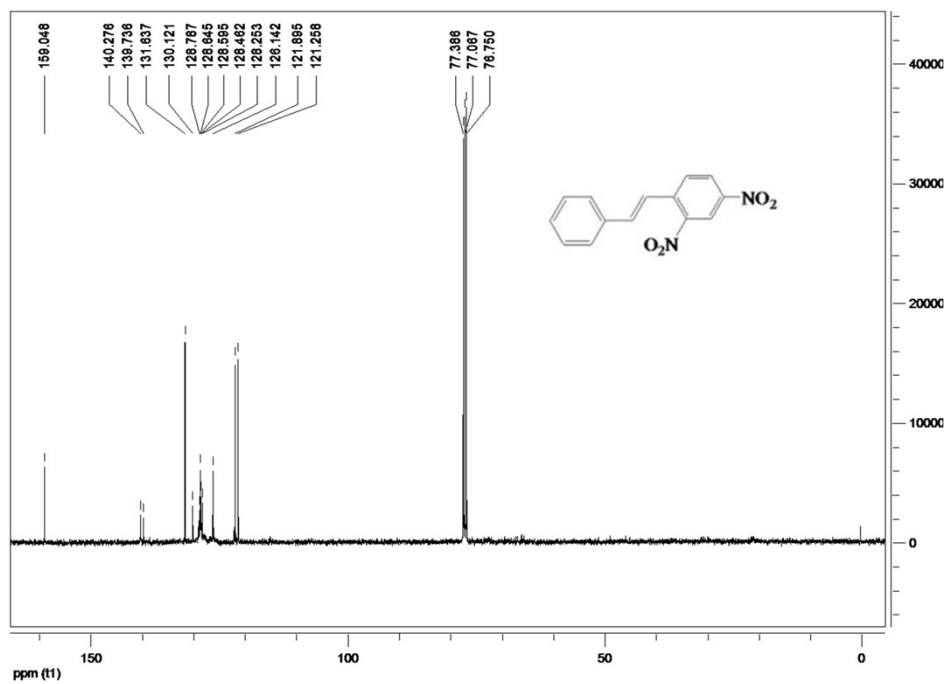


Fig. S61 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 2, 4-dinitro-1-(2-phenylethenyl)-stilbene (**3k**).

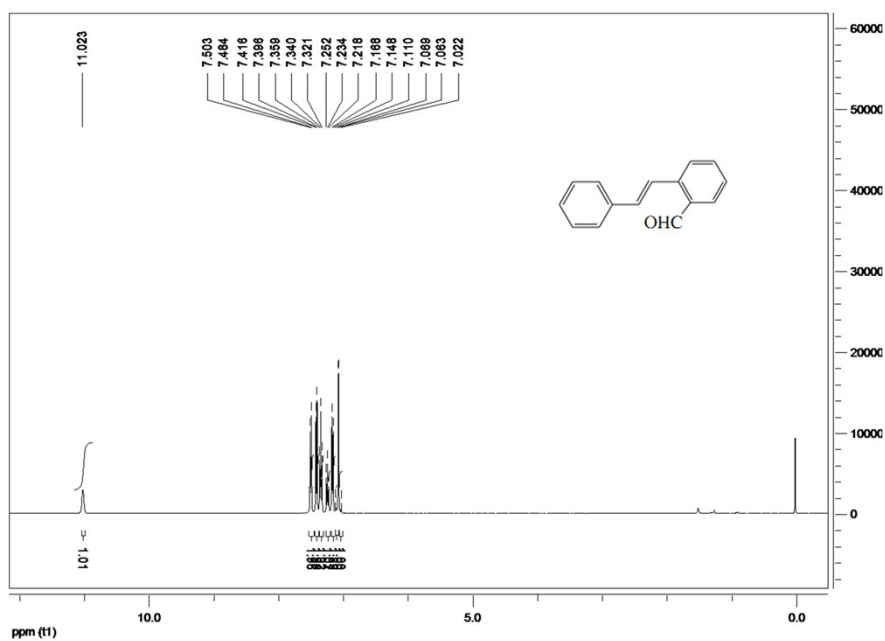


Fig. S62 The ^1H NMR (400 MHz, CDCl_3) spectrum of 2-(2-phenylethenyl)-stilbene (**3l**).

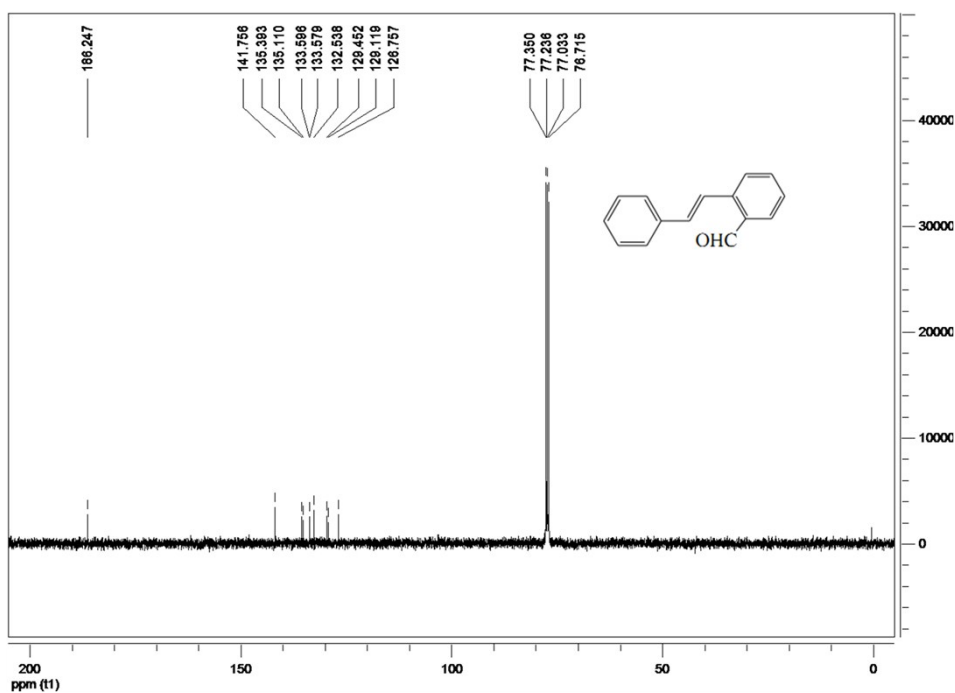


Fig. S63 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 2-(2-phenylethenyl)-stilbene (**3l**).

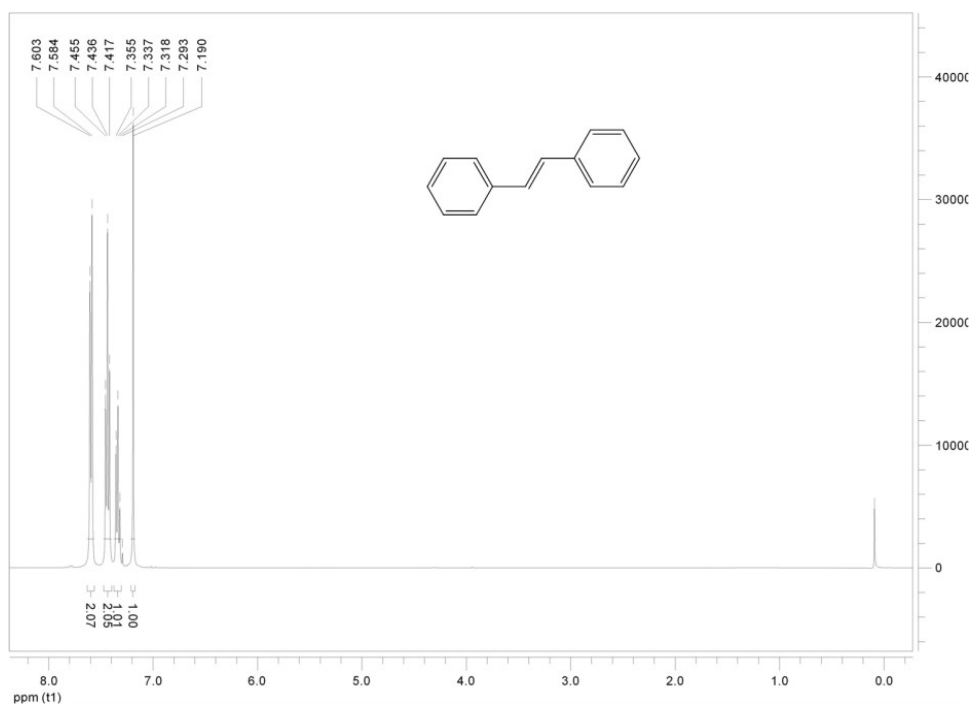


Fig. S64 The ^1H NMR (400 MHz, CDCl_3) spectrum of stilbene (**3n**).

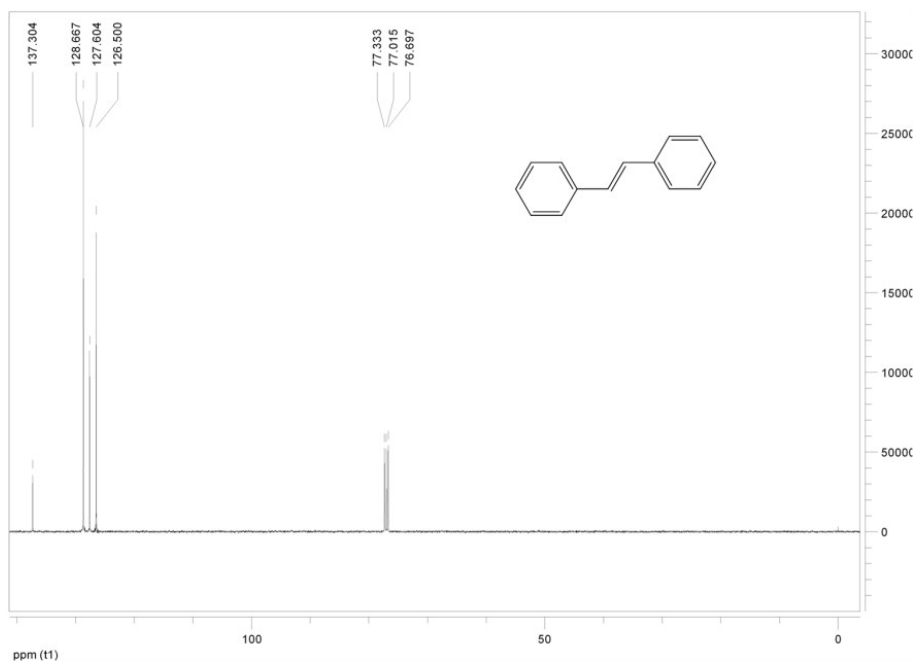


Fig. S65 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of stilbene (**3n**).

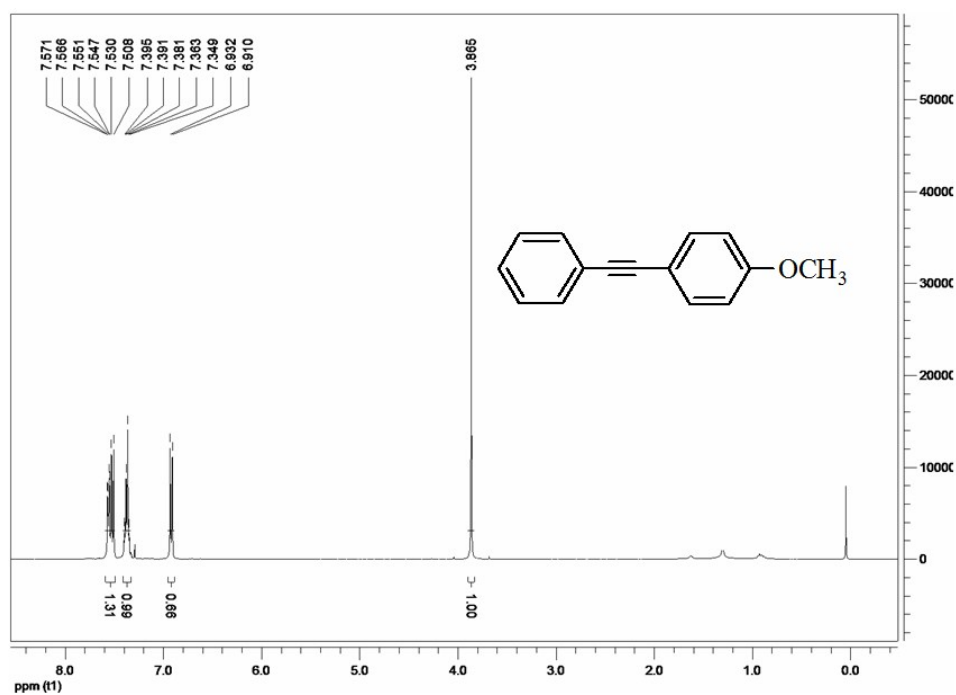


Fig. S66 The ^1H NMR (400 MHz, CDCl_3) spectrum of 1-(4-Methoxyphenyl)-2-phenylacetylene (**4a**).

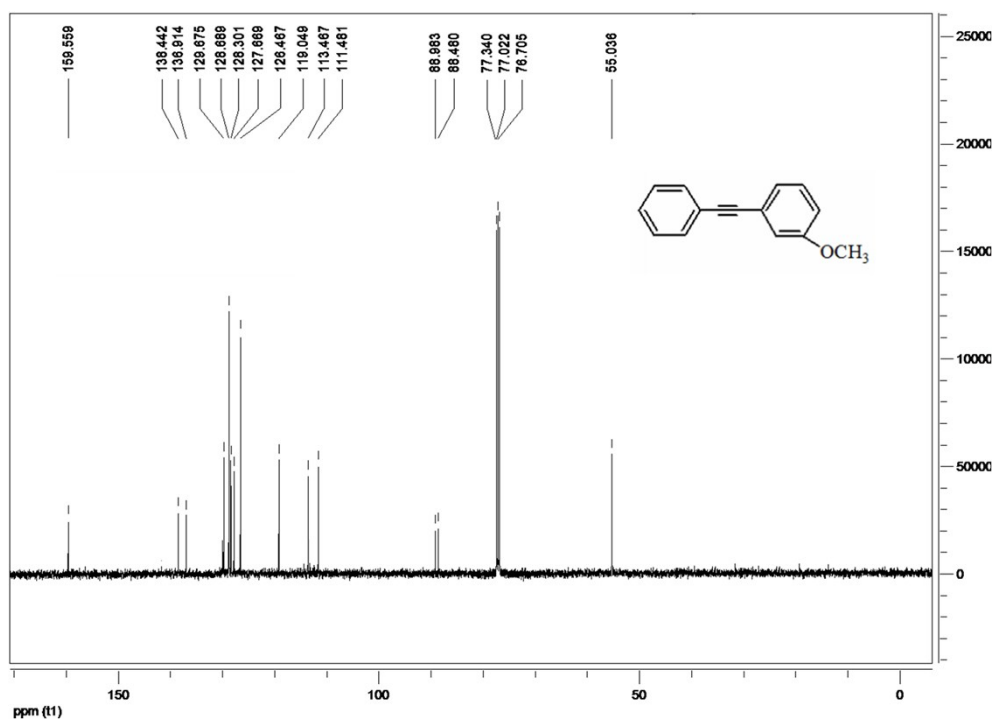


Fig. S69 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 1-(3-Methoxyphenyl)-2-phenylacetylene (**4b**).

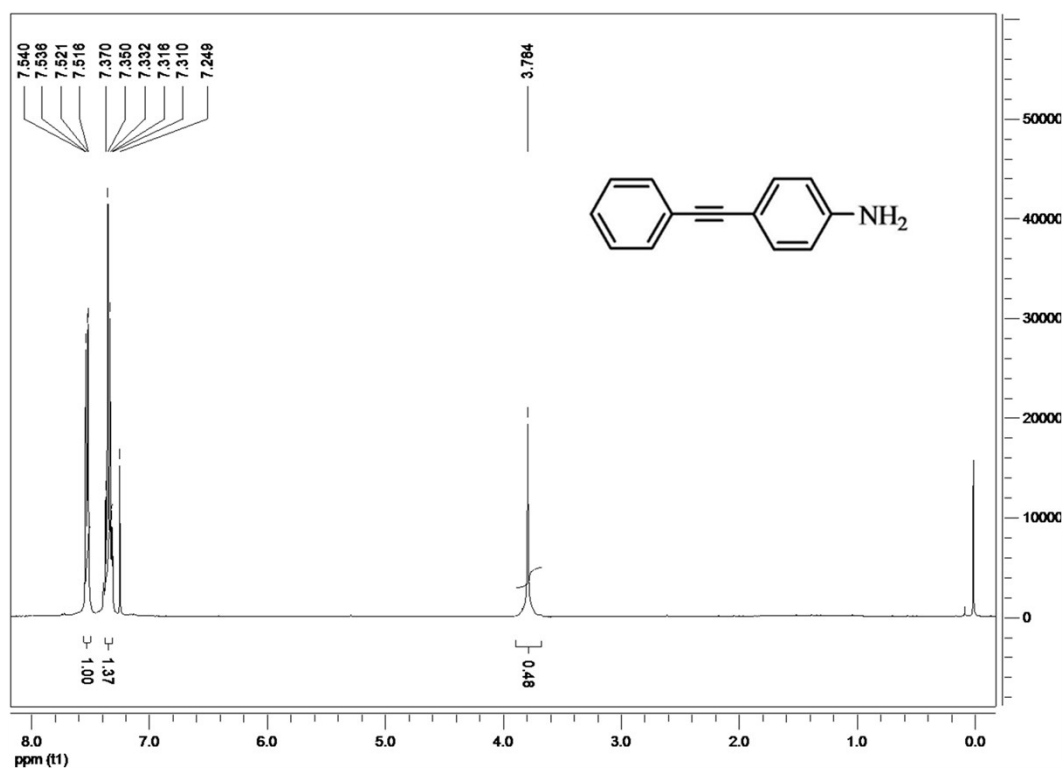


Fig. S70 The ^1H NMR (400 MHz, CDCl_3) spectrum of 4-(2-phenylethynyl)-aniline (**4c**).

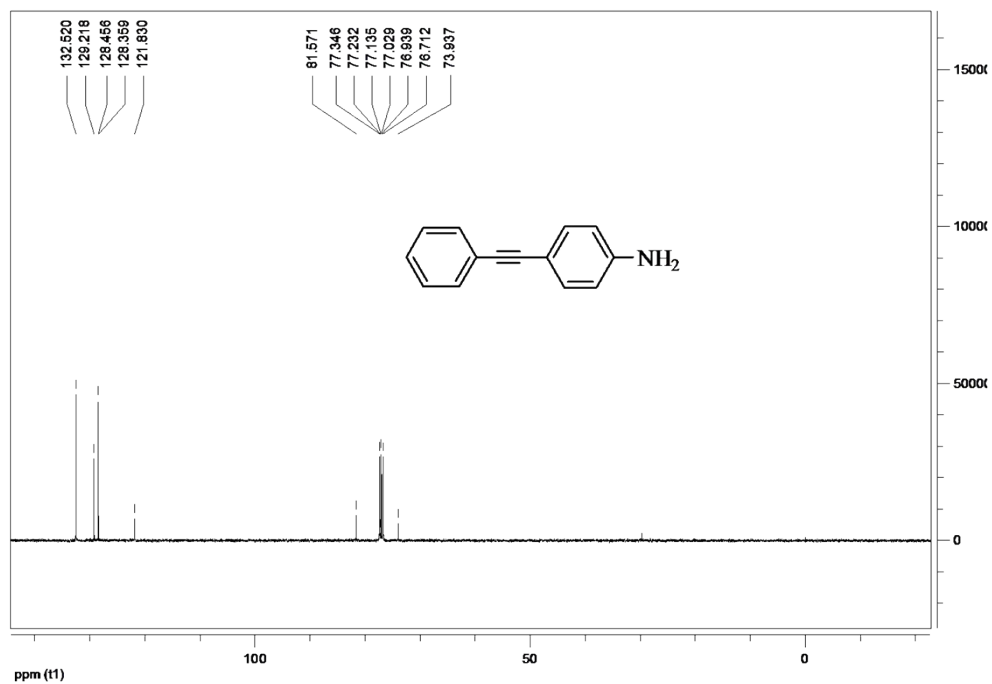


Fig. S71 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4-(2-phenylethynyl)-aniline (**4c**).

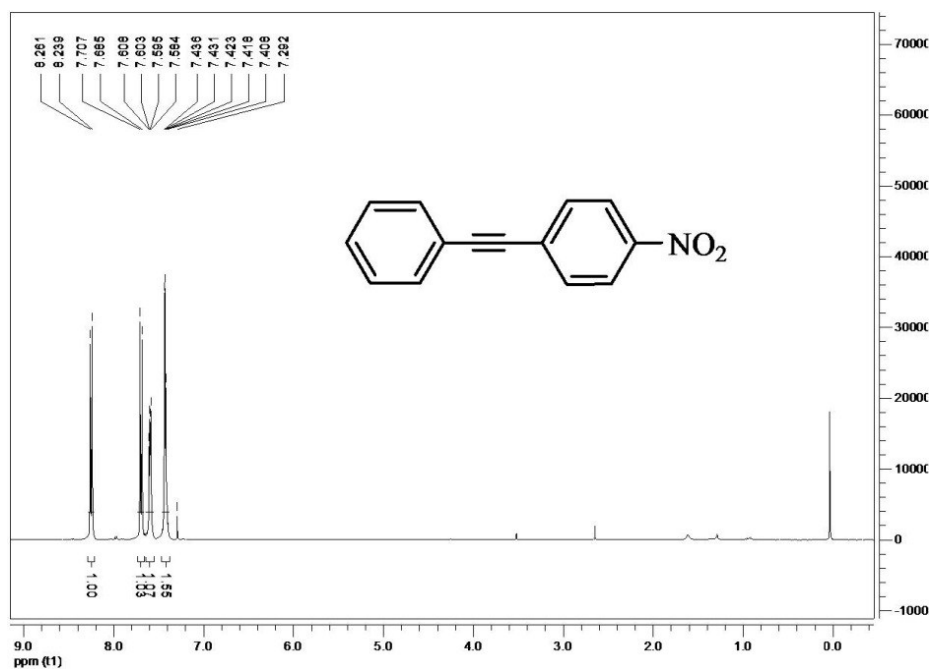


Fig. S72 The ^1H NMR (400 MHz, CDCl_3) spectrum of 1-(4-nitrophenyl)-2-phenylacetylene (**4d**).

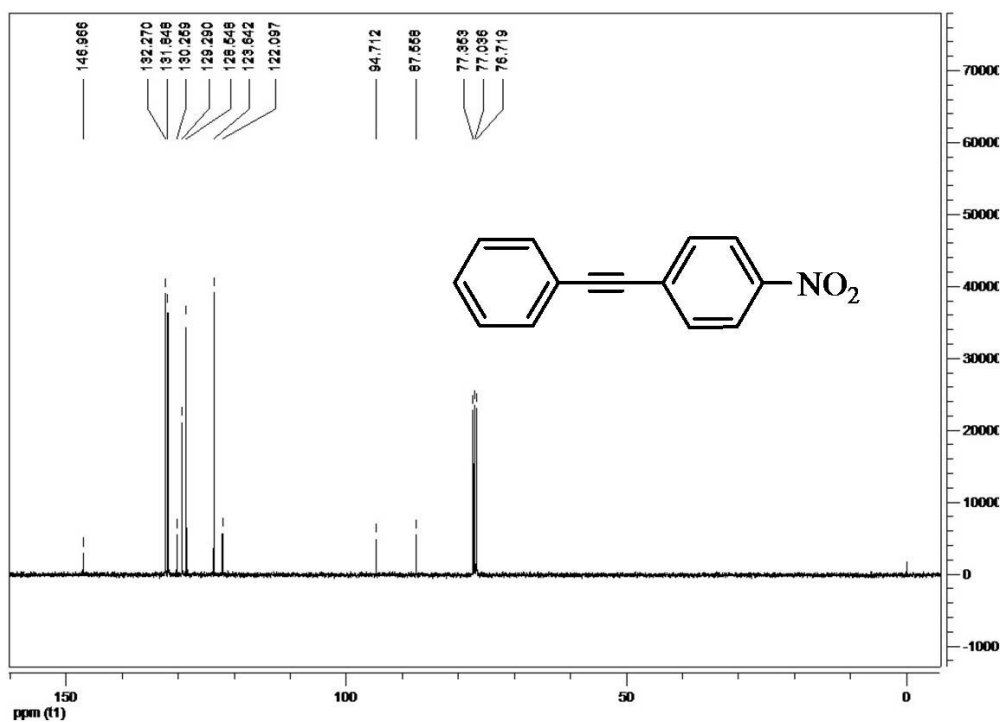


Fig. S73 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 1-(4-nitrophenyl)-2-phenylacetylene (**4d**).

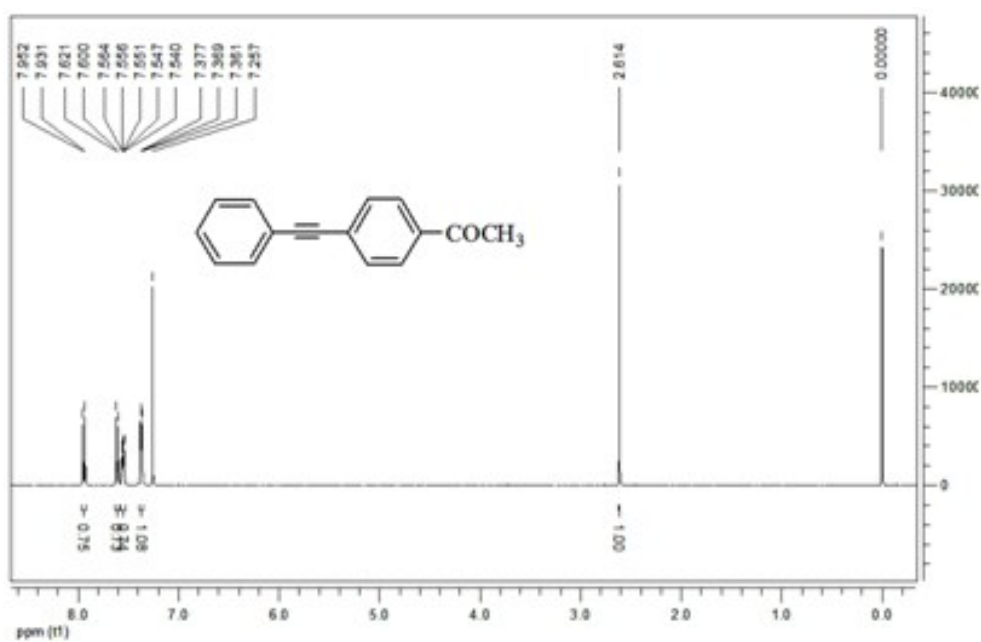


Fig. S74 The ^1H NMR (400 MHz, CDCl_3) spectrum of 1-(4-acetylphenyl)-2-phenylacetylene (**4e**).

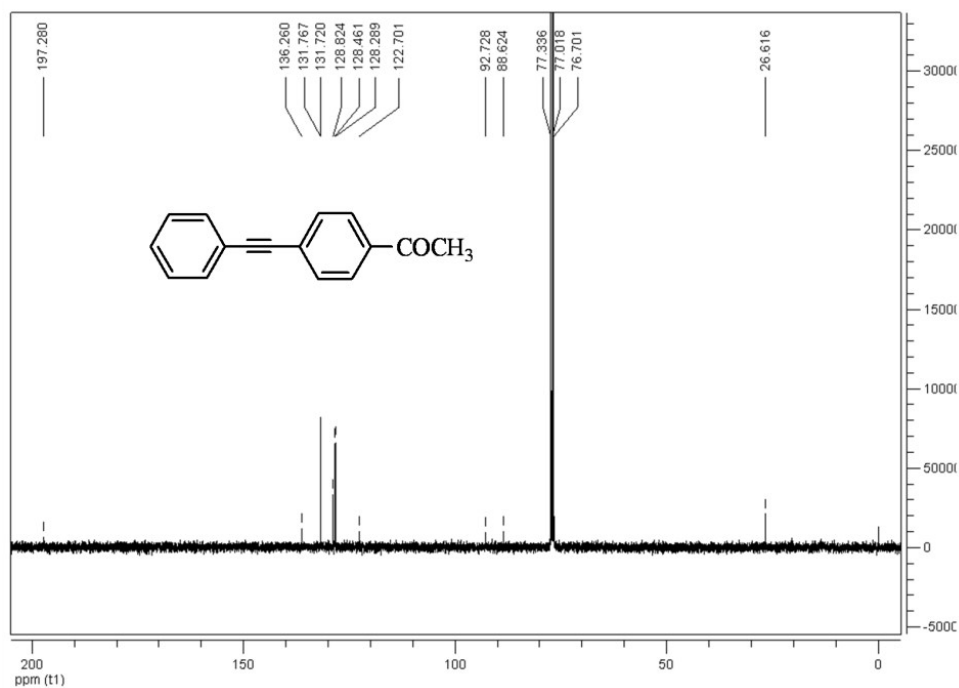


Fig. S75 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 1-(4-acetylphenyl)-2-phenylacetylene (**4e**).

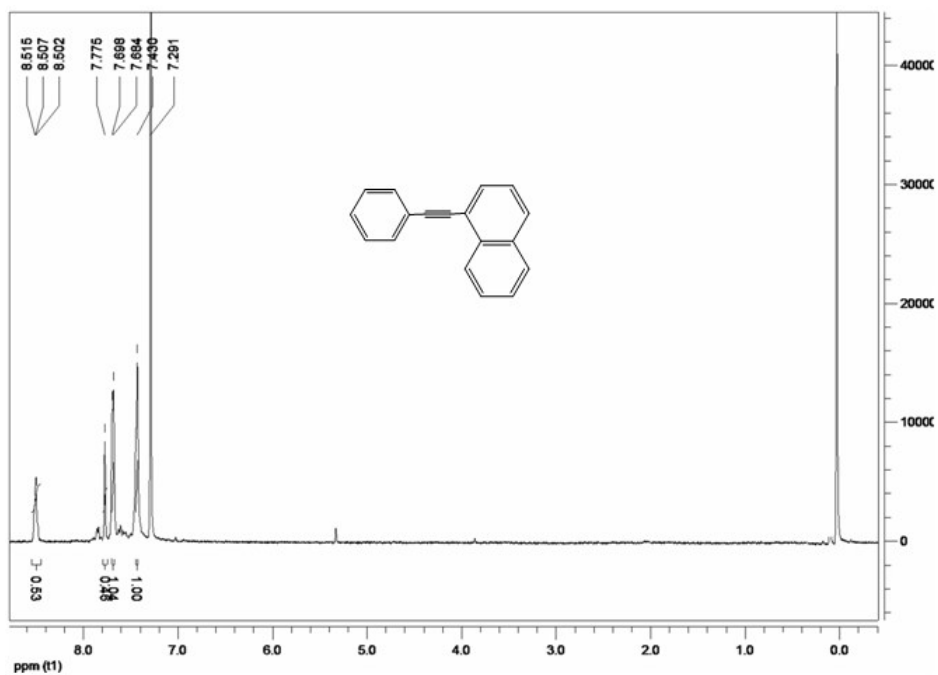


Fig. S76 The ^1H NMR (400 MHz, CDCl_3) spectrum of 1-(2-phenylethynyl)naphthalene (**4f**).

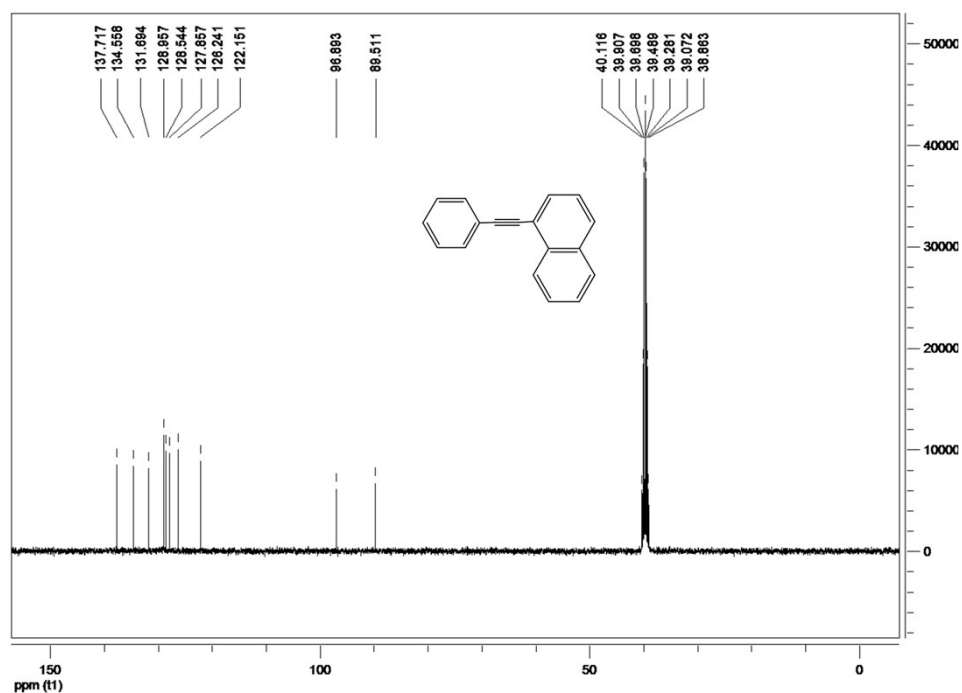


Fig. S77 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 1-(2-phenylethynyl)naphthalene (**4f**).

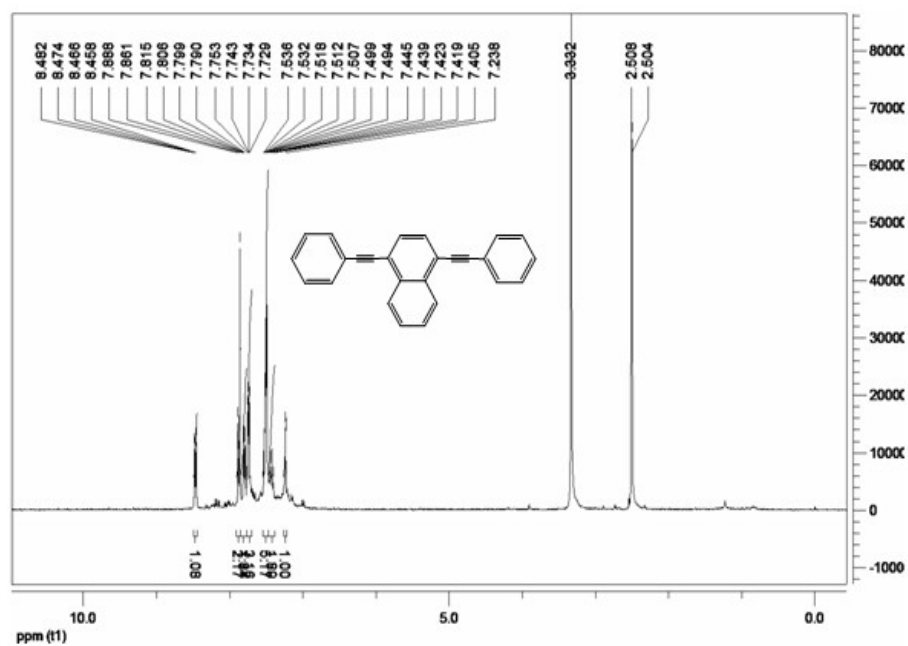


Fig. S78 The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of 1,4-bis(2-phenylethynyl)naphthalene (**4g**).

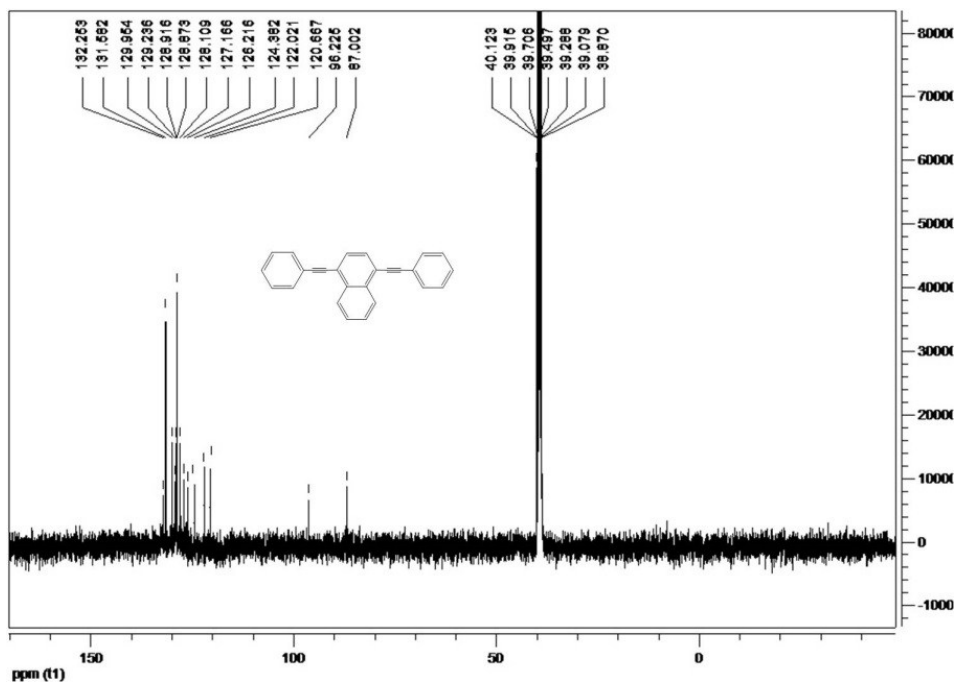


Fig. S79 The ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of 1,4-bis(2-phenylethynyl)-naphthalene (**4g**).

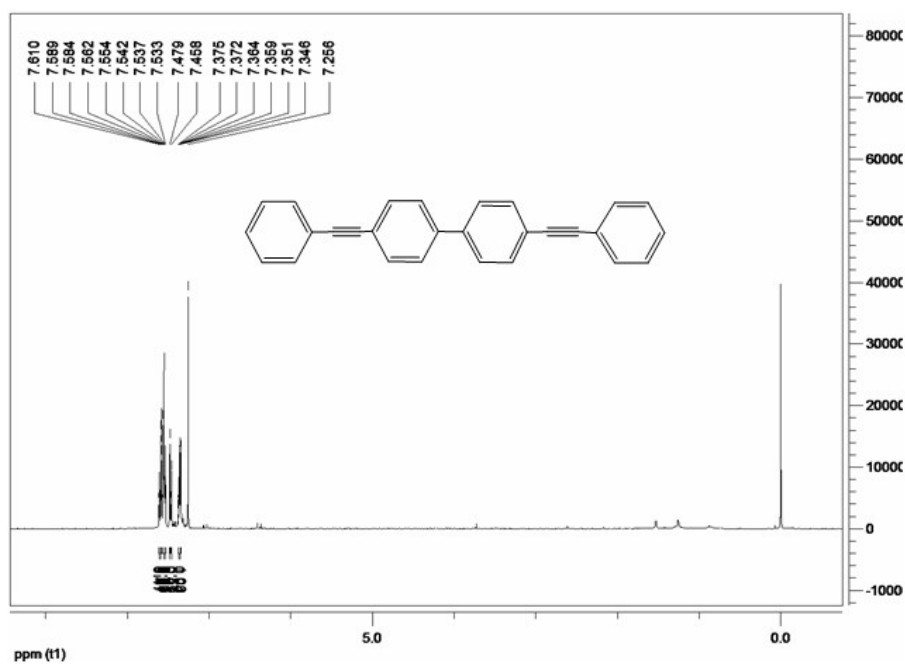


Fig. S80 The ^1H NMR (400 MHz, CDCl_3) spectrum of 4,4'-bis(2-phenylethynyl)-1,1'-biphenyl (**4h**).

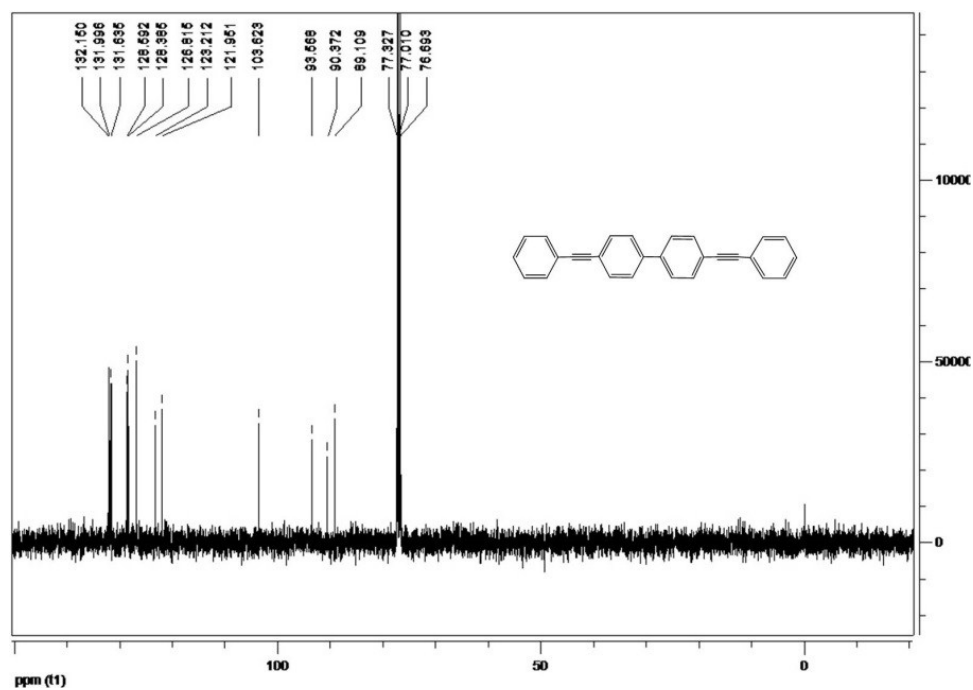


Fig. S81 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4,4'-bis(2-phenylethynyl)-1,1'-biphenyl (**4h**).

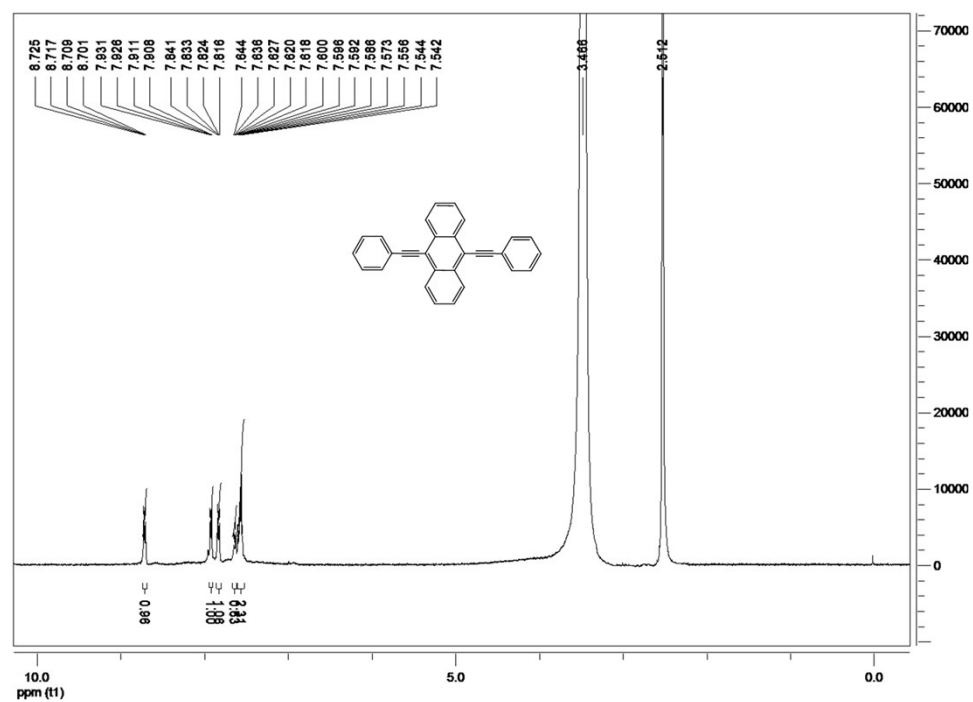


Fig. S82 The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of 9,10-bis(2-phenylethynyl)anthracene (**4i**).

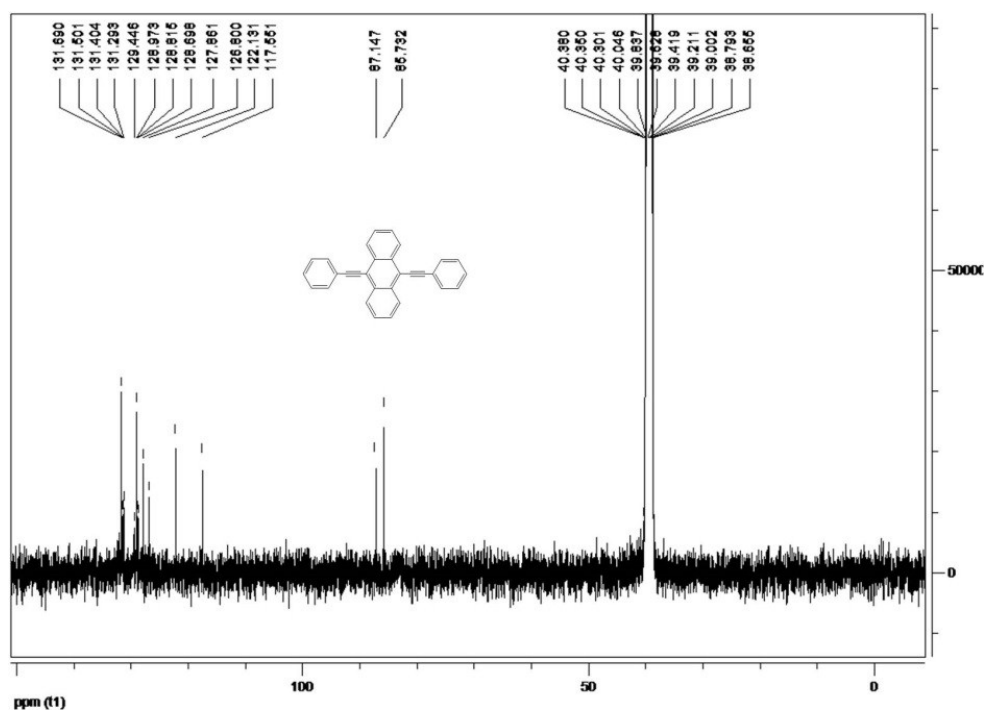


Fig. S83 The ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of 9,10-bis(2-phenylethynyl)anthracene (**4i**).

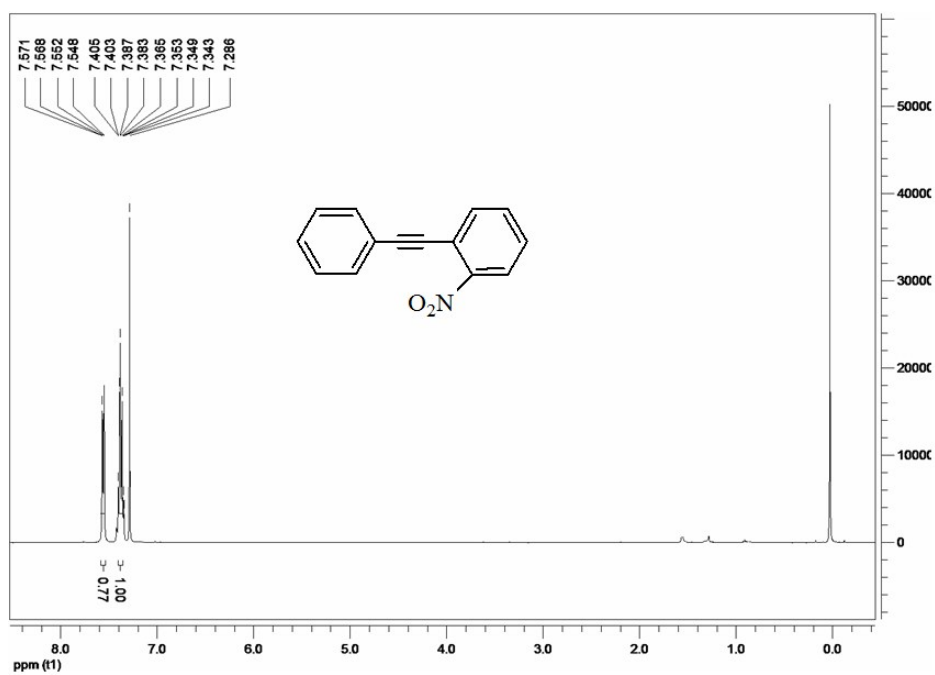


Fig. S84 The ^1H NMR (400 MHz, CDCl_3) spectrum of (2-nitrophenyl)phenylacetylene (**4j**).

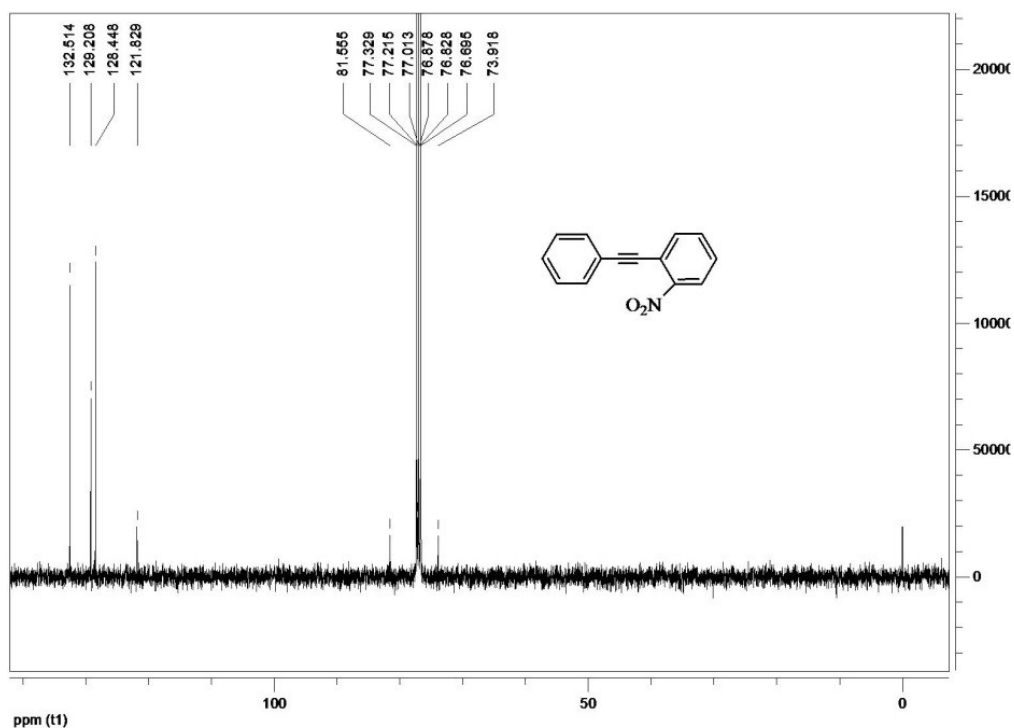


Fig. S85 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of (2-nitrophenyl)phenylacetylene (**4j**).

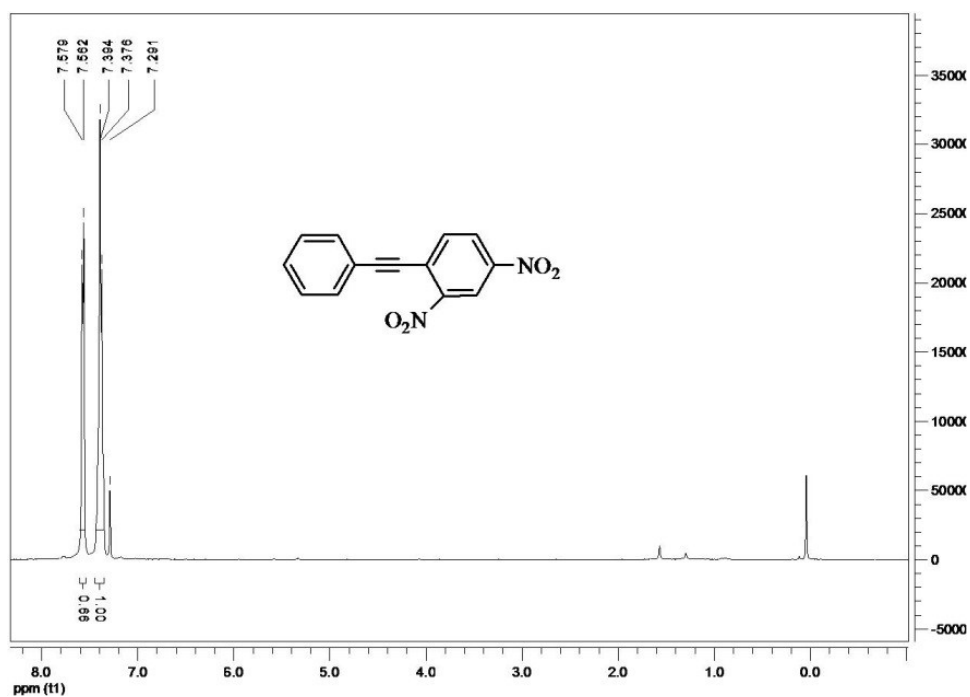


Fig. S86 The ^1H NMR (400 MHz, CDCl_3) spectrum of 2,4-dinitro-1-(2-phenylethynyl)acetylene (**4k**).

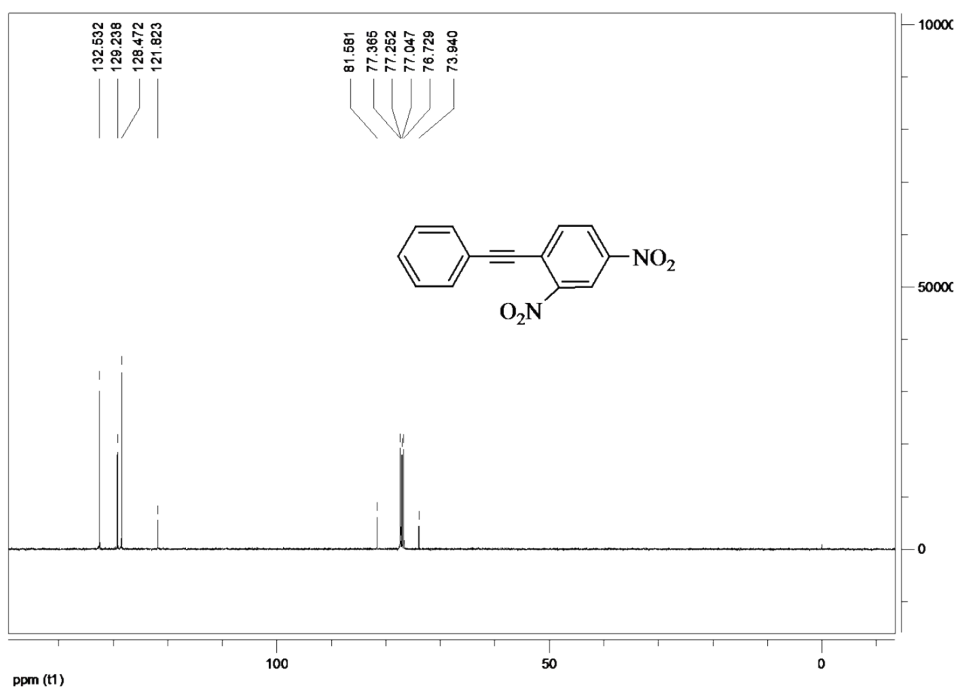


Fig. S87 The ¹³C NMR (100 MHz, CDCl₃) spectrum of 2,4-dinitro-1-(2-phenylethynyl)acetylene (**4k**).

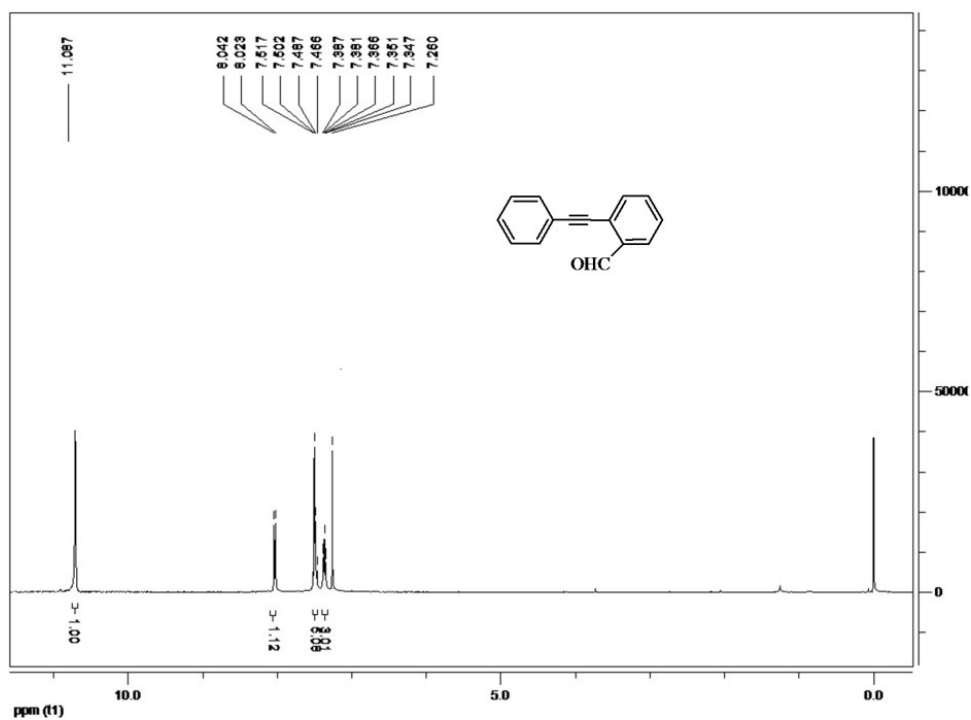


Fig. S88 The ¹H NMR (400 MHz, CDCl₃) spectrum of 2-(phenylethynyl)benzaldehyde (**4l**).

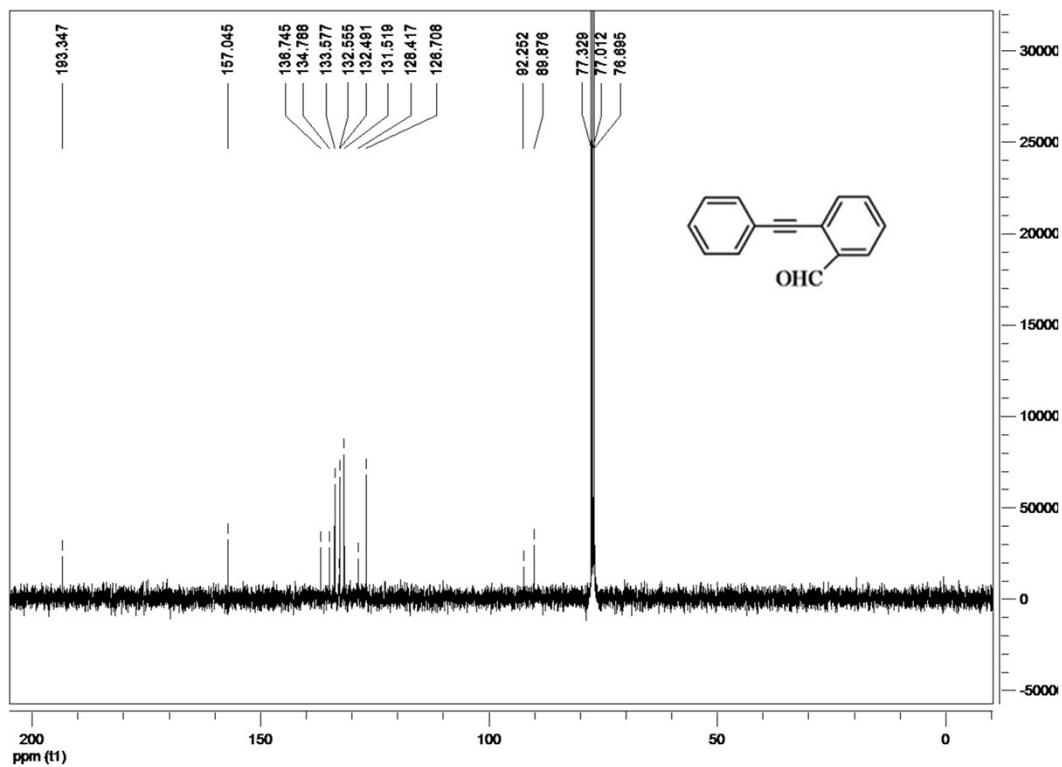


Fig. S89 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 2-(phenylethynyl)benzaldehyde (**4I**).

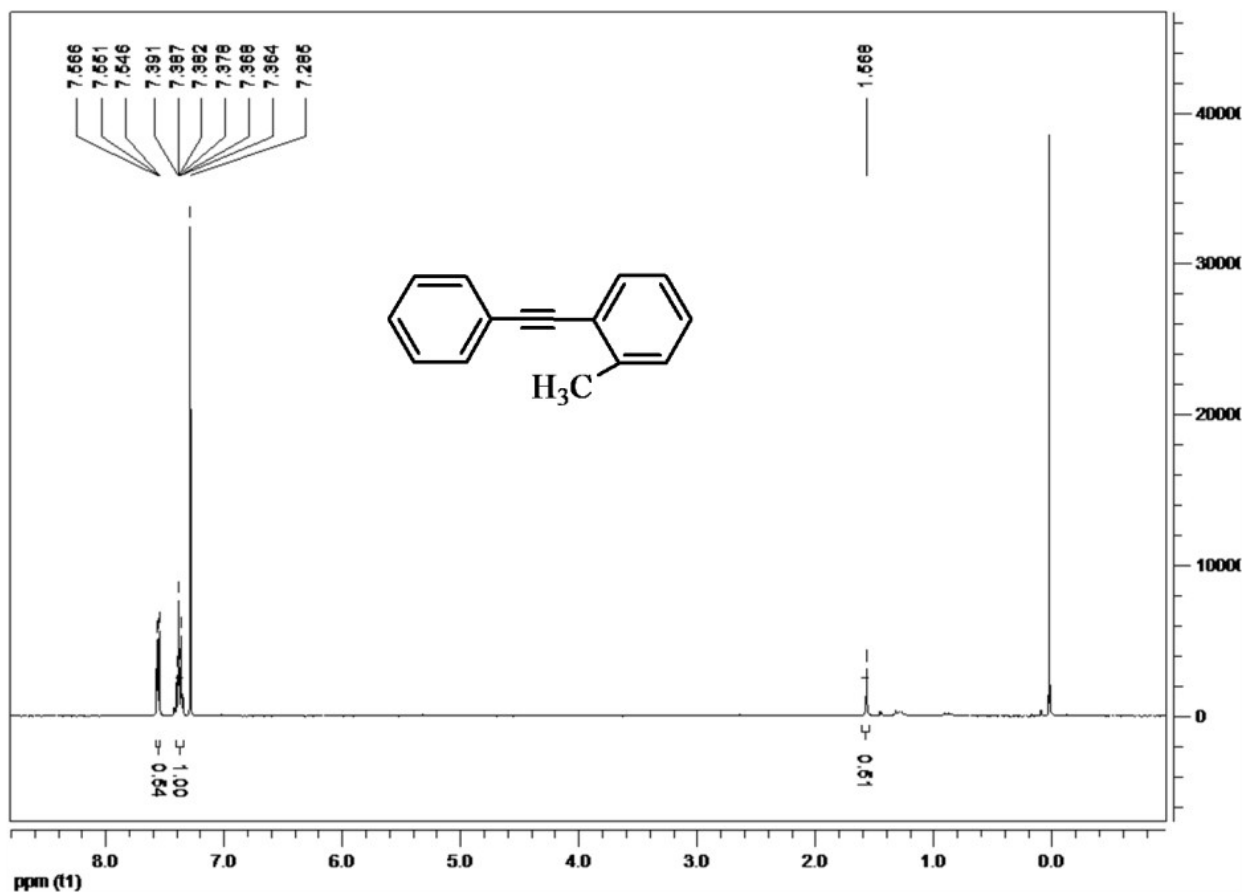


Fig. S90 The ^1H NMR (400 MHz, CDCl_3) spectrum of 2-methylphenylacetylene (**4m**).

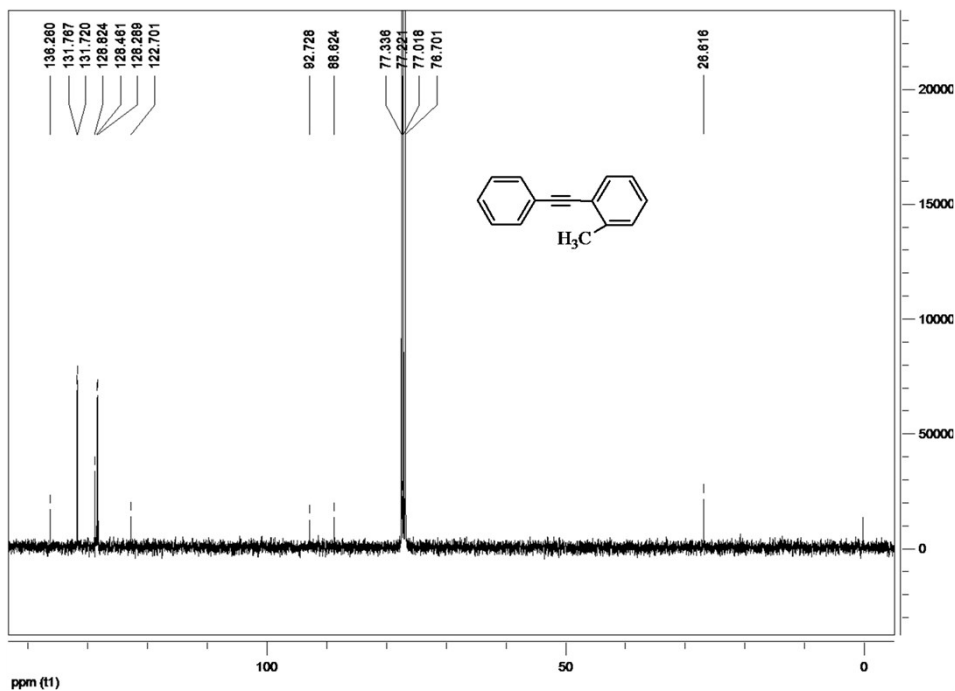


Fig. S91 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 2-methylphenylacetylene (**4m**).

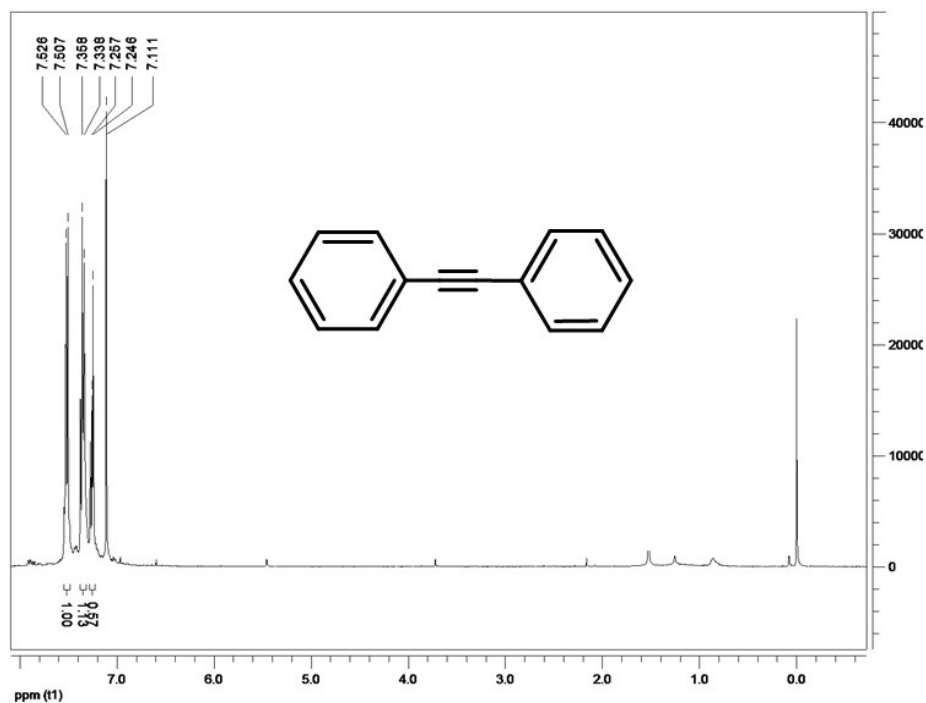


Fig. S92 The ^1H NMR (400 MHz, CDCl_3) spectrum of diphenylacetylene (**4n**).

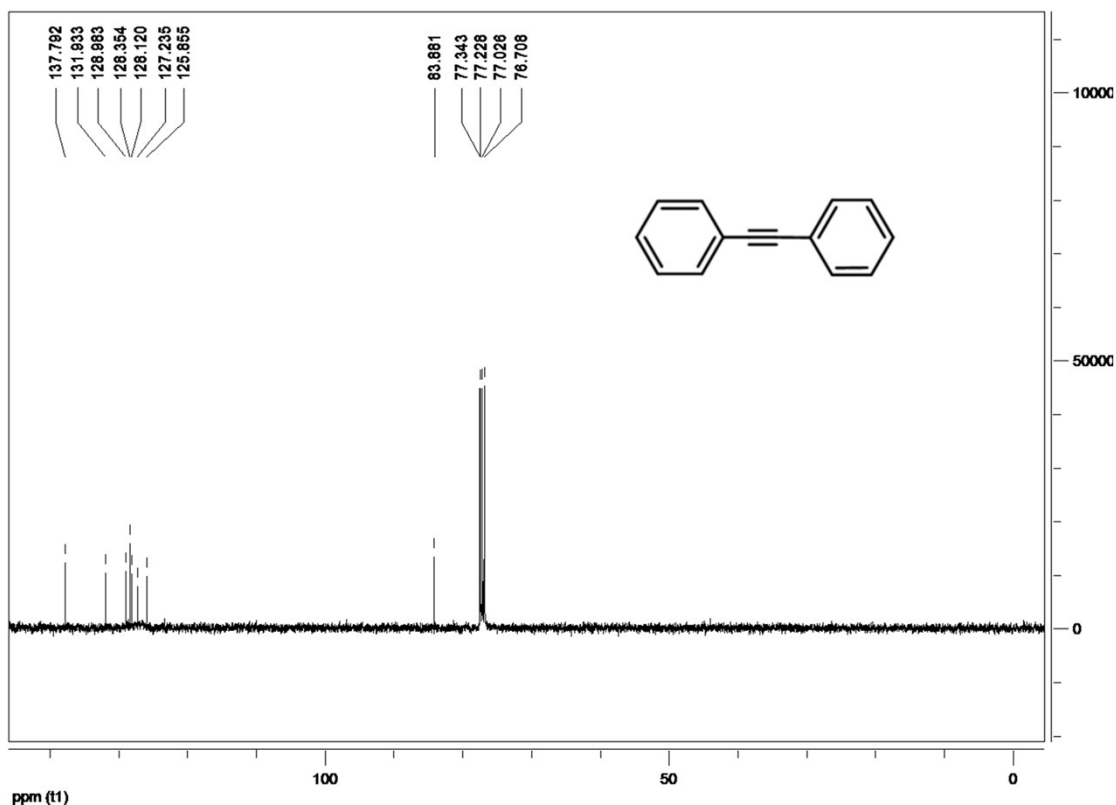


Fig. S93 The ^{13}C NMR (100 MHz, CDCl_3) spectrum of diphenylacetylene (**4n**).

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