Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Electronic Supporting Information

Salen-Porphyrin-based conjugated microporous polymer supported Pd nanoparticles: highly efficient heterogeneous catalysts for aqueous C–C coupling reactions

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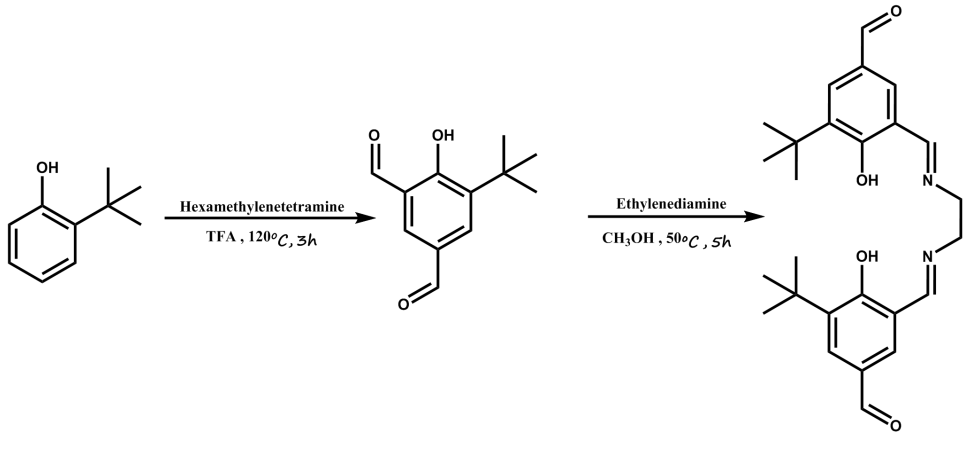
Synthetic procedures

Compound 2 (1-hydroxy-2-t-butyl-isophthalaldehyde). 2-tert-butyl phenol (6 g, 0.04 mmol) and hexamethylenetetramine (6.72 g, 0.048 mmol) were dissolved in TFA (36 mL) and the solution was heated at 120 ^{o}C for 3 h. After cooling to room temperature 10 % aq. H_2SO_4 (36 mL) was added and again the temperature maintained at 100 ^{o}C for 3 h. After completion the solution was basified with Na_2CO_3 to pH=8 and extracted with 90 mL of $CHCl_3$. The combined organic layers were dried on Na_2SO_4, filtered and concentrated to dryness under reduced pressure. The crude product was purified on silica gel column using petroleum ether-ethyl acetate (5:1, v/v) as eluent to afford compound **2** (4.2 g, 51 % yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.40 (s, 1H), 9.99 (s, 1H), 9.93 (s, 1H), 8.07 (d, J = 2.0 Hz, 1H), 7.98 (d, J = 2.0 Hz, 1H), 1.46 (s, 9H) ppm.

Monomer 3. Compound **2** (1.03 g, 5 mmol) was poured in a round-bottomed flask which containing 25 mL methanol. And then ethylenediamine (150 mg, 2.5 mmol) was added and the reaction mixture was refluxed for 5 h. After cooling to room temperature, the yellow precipitate was collected by filtration, washed with cool methanol, and dried under vacuum to give a yellow solid in 90 % yield (1.4 g). ^{1}H NMR (400 MHz, d_6-DMSO): δ 14.74 (d, J = 6.5 Hz, 1H), 9.68 (s, 1H), 8.68 (d, J = 7.1 Hz, 1H), 7.80 (d, J = 2.0 Hz, 1H), 7.69 (d, J = 2.0 Hz, 1H), 4.01 (s, 2H), 1.35 (s, 9H) ppm.



1 2 3

Scheme S1. Schematic representation for the synthesis of monomer **3**.

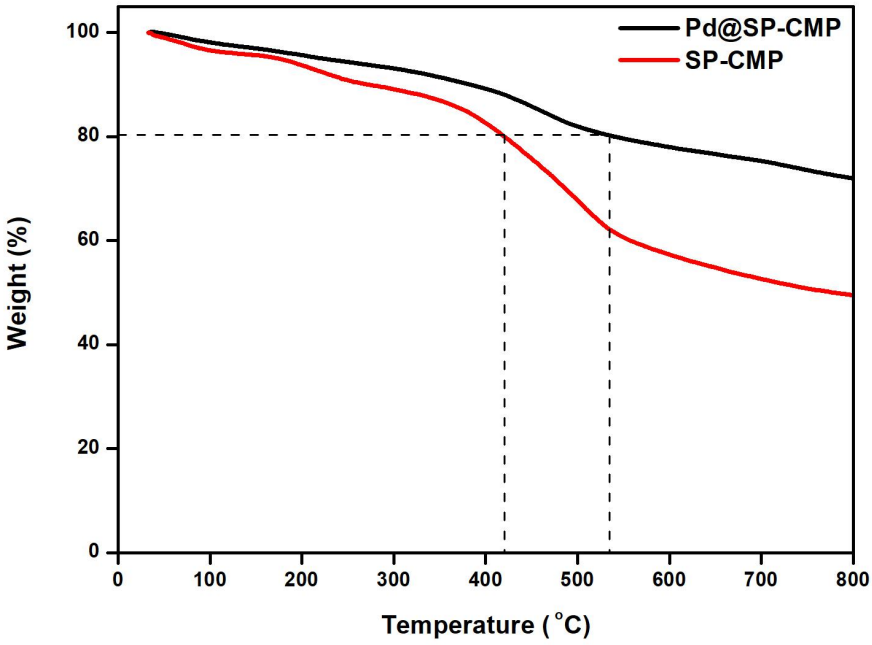


Fig. S1. TGA date of **SP-CMP** and **Pd@SP-CMP**.

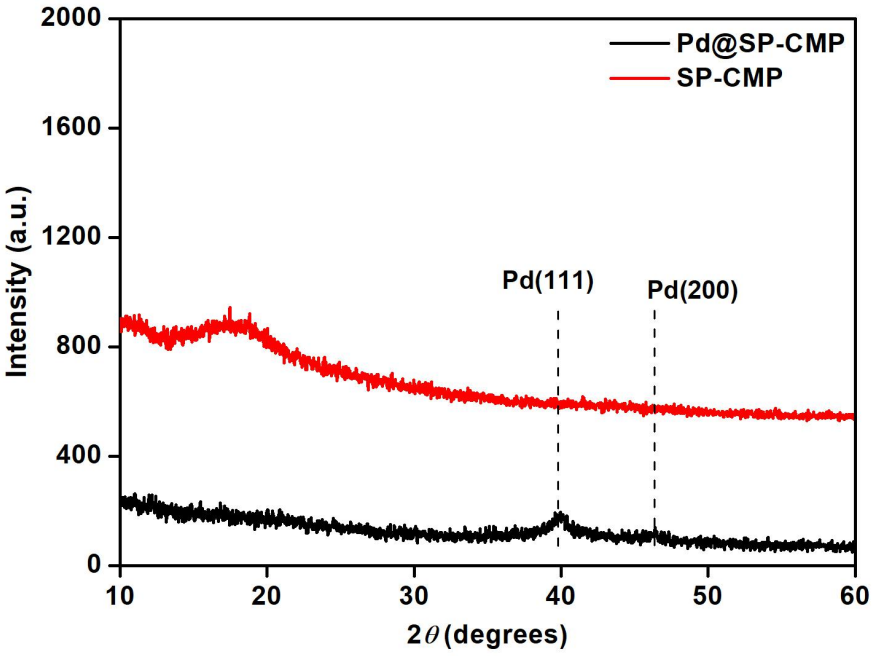


Fig. S2. PXRD date of **SP-CMP** and **Pd@SP-CMP**.

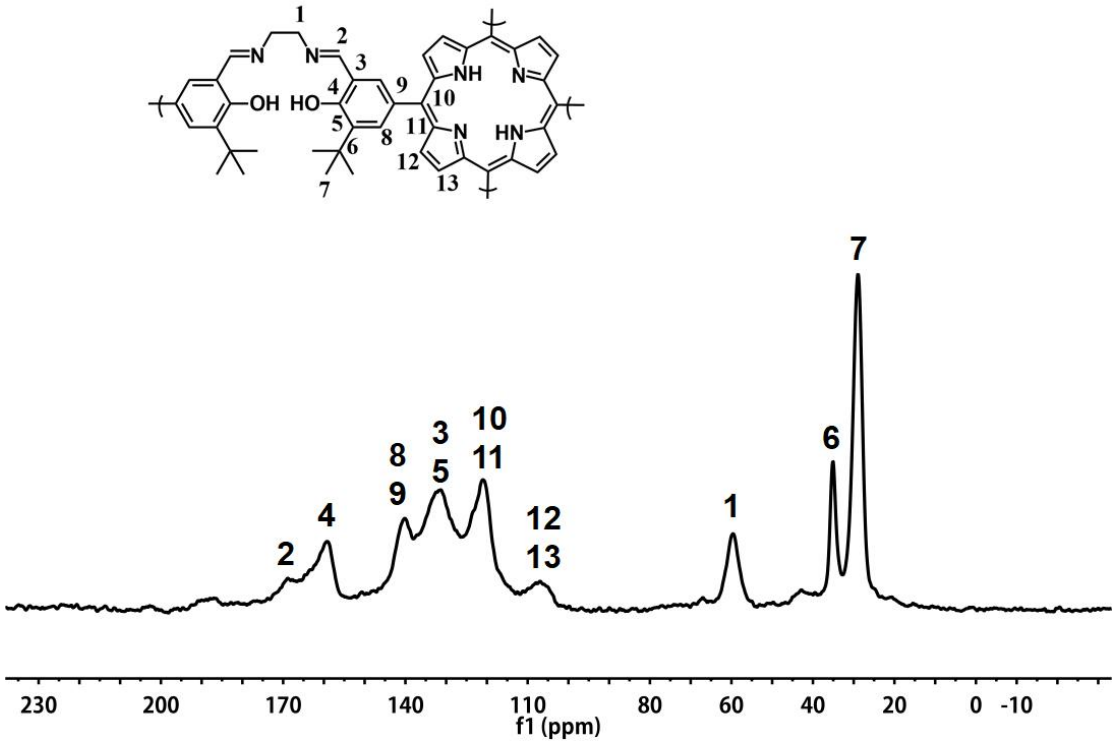


Fig. S3. Solid-state ^{13}C NMR spectrum of **SP-CMP**.

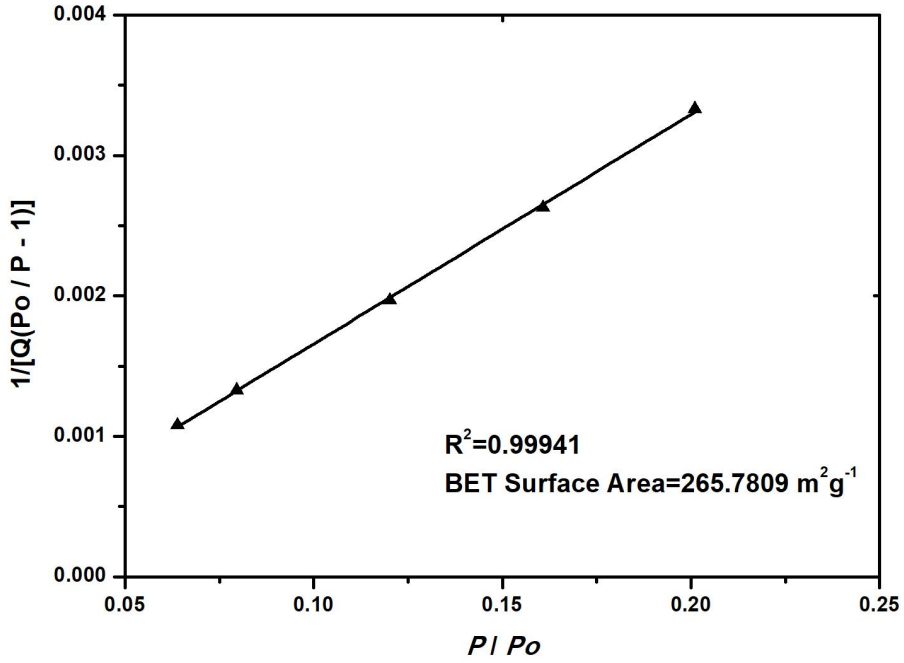


Fig. S4. BET surface area plot for **Pd@SP-CMP** calculated from the N_2 absorption isotherm.

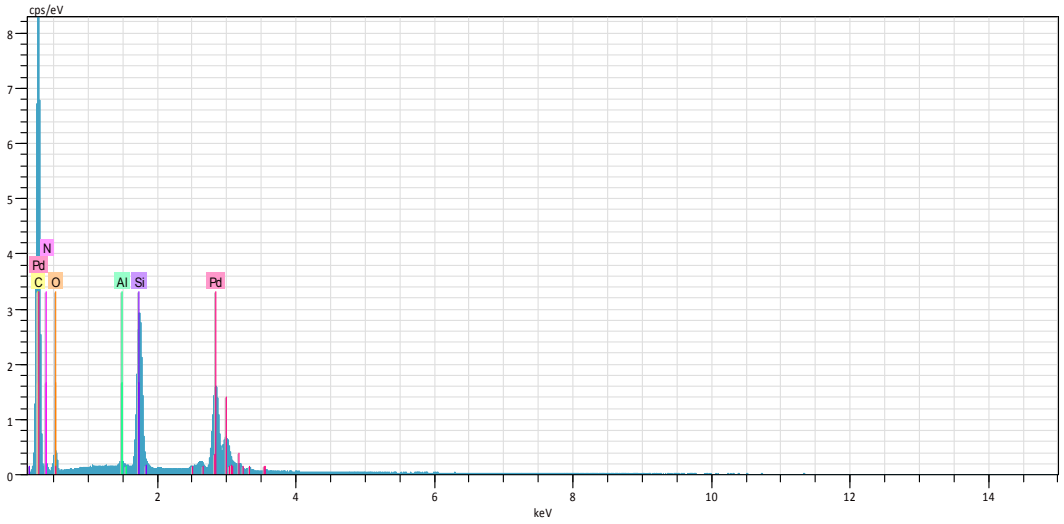


Fig. S5. SEM-EDX spectrum of **Pd@SP-CMP**. The aluminum element comes from the aluminum stage, and the silicon element comes from the silicon wafer.

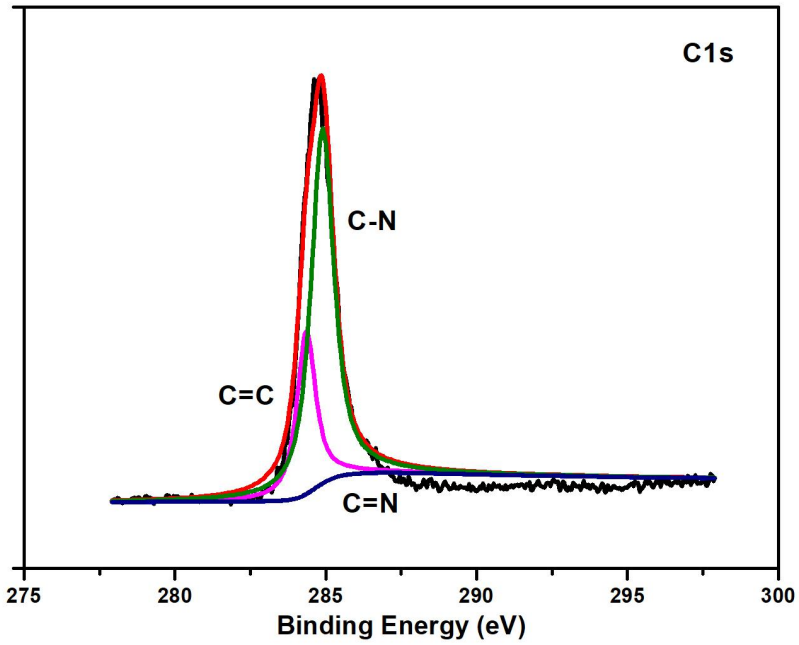


Fig. S6. The XPS spectra of **Pd@SP-CMP** showing typical peaks at 284.2 eV (C=C), 285 eV (C-N) and 286.5 eV (C=N) for C 1S.

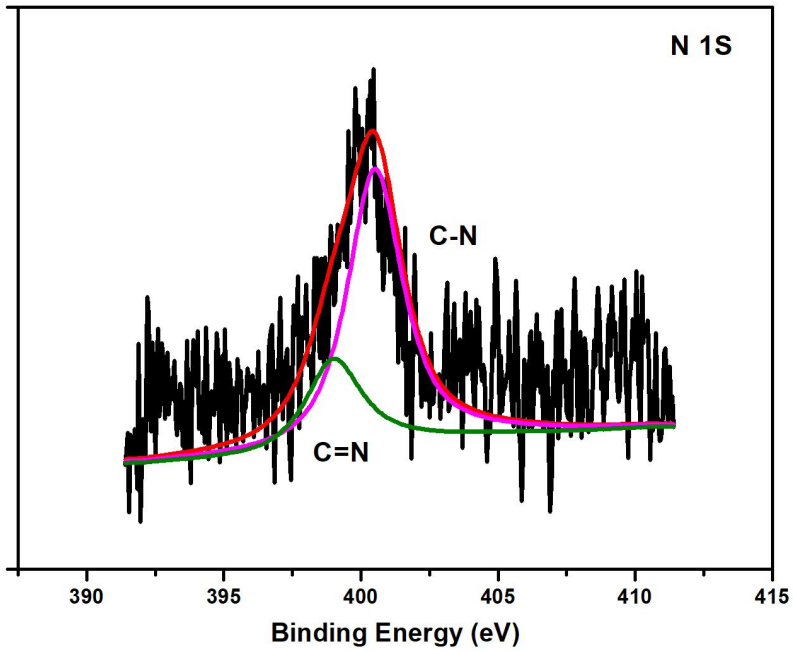


Fig. S7. The XPS spectra of **Pd@SP-CMP** showing typical peaks at 399 eV (C=N) and 401 (C-N) for N 1S**.**

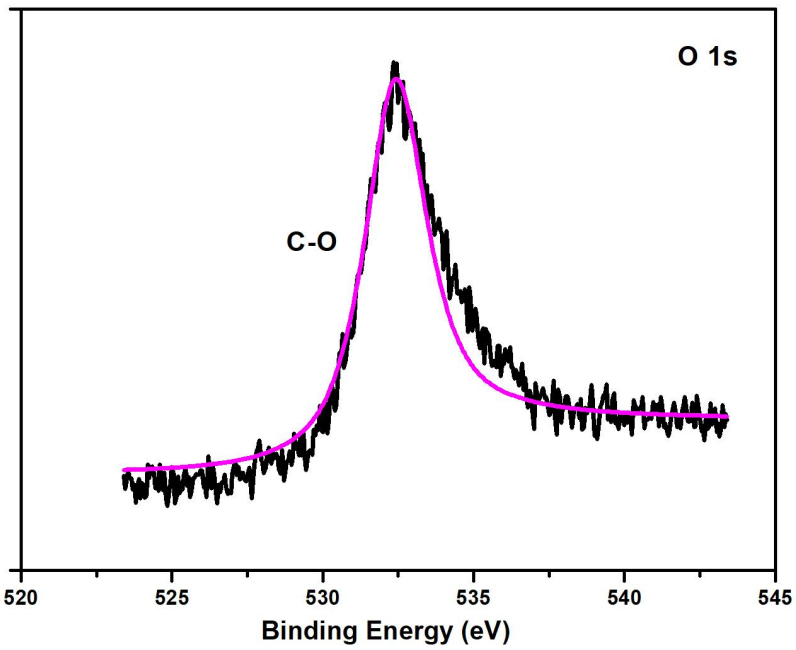


Fig. S8. The XPS spectra of **Pd@SP-CMP** showing typical peaks at 532.3 eV (C-O) for O 1S.

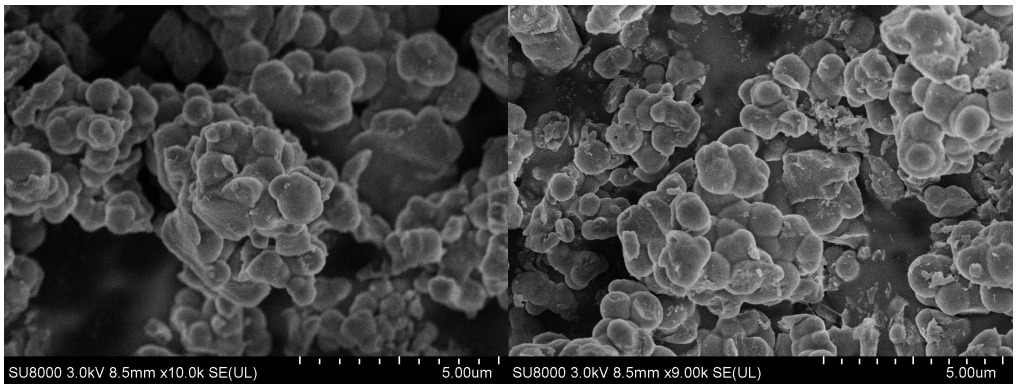


Fig. S9. SEM image of **Pd@SP-CMP** (left) and SEM image of **Pd@SP-CMP** after ten successive runs (right).

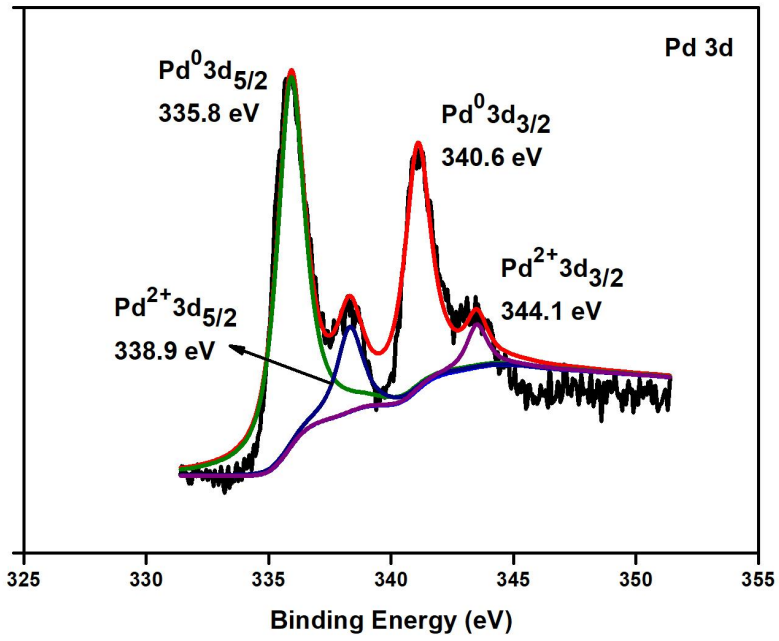


Fig. S10. XPS spectra of the **Pd@SP-CMP** after ten successive runs.

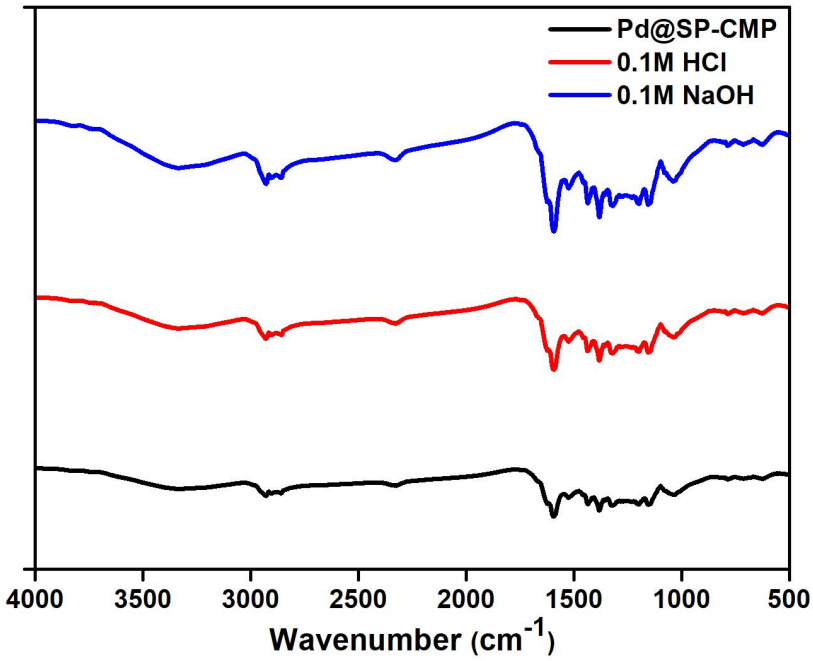
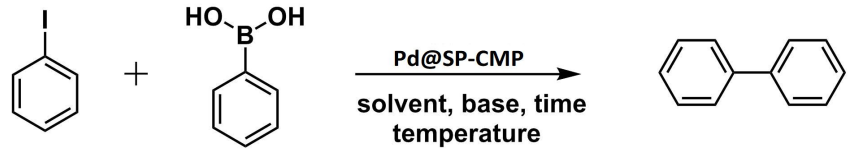


Fig. S11. The FT-IR spectra of **Pd@SP-CMP** and **Pd@SP-CMP** after treatment in aqueous solutions for 3 days (pH = 1 and 13).

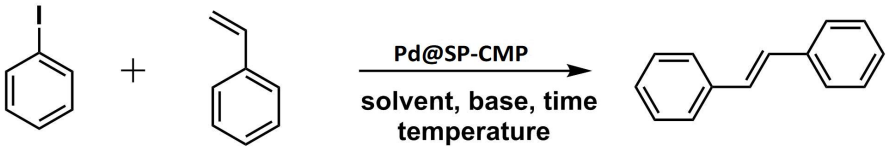
Table S1 The Suzuki–Miyaura coupling reactions of phenylboronic acid and iodobenzene under various reaction conditions.[a]



Entry	Solvent	Base	T / °C	Time / h	Yield / % [b]
1	DMF	K_2CO_3	90	8	99
2	DMF/H_2O	K_2CO_3	90	8	99
3	H_2O	K_2CO_3	90	8	99
4	H_2O	K_2CO_3	80	8	99
5	H_2O	K_2CO_3	50	8	95
6	H_2O	K_2CO_3	RT	8	51
7	H_2O	K_2CO_3	80	7	99
8	H_2O	K_2CO_3	80	5	99
9	H_2O	K_2CO_3	80	4	95
10	H_2O	Na_2CO_3	80	5	99
11	H_2O	Et_3N	80	5	99

[a] Iodobenzene (0.5 mmol), phenylboronic acid (0.75 mmol), base (0.75 mmol), solvent (5 mL), **Pd@SP-CMP** (0.3 mol%), N_2.
[b] Isolated yields based on iodobenzene.

Table S2 The Mizoroki-Heck coupling reactions of styrene and iodobenzene under various reaction conditions.[a]



Entry	Solvent	Base	T / °C	Time / h	Yield / % [b]
1	H_2O	K_2CO_3	90	12	55
2	1,4-dioxane	K_2CO_3	90	12	94
3	1,4-dioxane / H_2O	K_2CO_3	90	12	95
4	1,4-dioxane / H_2O	K_2CO_3	80	12	95
5	1,4-dioxane / H_2O	K_2CO_3	50	12	94
6	1,4-dioxane / H_2O	K_2CO_3	RT	12	51
7	1,4-dioxane / H_2O	Na_2CO_3	80	12	81
8	1,4-dioxane / H_2O	Et_3N	80	12	77

[a] Iodobenzene (0.5 mmol), styrene (0.6 mmol), base (0.75 mmol), solvent (5 mL), **Pd@SP-CMP** (0.6 mol%), N_2.
[b] Isolated yields based on iodobenzene.

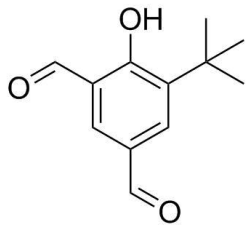
Table S3. Pd supported material catalysts for Suzuki–Miyaura cross coupling reactions reported to date.

Entry	Catalyst	Base	Solvent	Temp. (◦C)	Time (h)	Yield (%)	Reference
1	0.02 g **Pd-MPTAT-1**	NaOH	DMF:H_2O =1:5	85	10	85	*Green Chem.*, 2011, **13**, 1317–1331.
2	0.5 mol % **Pd/COF-LZU1**	K_2CO_3	*p*-xylene	150	3	97	*J. Am. Chem. Soc.*, 2011, **133**, 19816–19822.
3	0.01 mol % **Pd-CIN-1**	K_2CO_3	DMF	80	1.5	96	*Dalton Trans.*, 2012, **41**, 1304–1311
4	1 mg **MsMOP-1**	K_2CO_3	EtOH:H_2O =1:1	80	1	99	*J. Mater. Chem. A*, 2013, **1**, 14108–14114
5	20 mg **Pd(0)/MCoS-1**	K_2CO_3	H_2O	80	6	97	*Appl. Catal. A: Gen.*, 2014, **469** 320–327.
6	0.5 mol % of Pd **CelMcPd^0-1**	K_2CO_3	EtOH	65	0.25	91	*Ind. Eng. Chem. Res.*, 2014, **53**, 8339–8345.
7	0.6 mol % of Pd **CMC-Pd^{II}**	K_2CO_3	EtOH	78	0.25	90	*Ind. Eng. Chem. Res.*, 2015, **54**, 790–797.
8	0.8 mol% **Pd@NHC-MOP**	K_2CO_3	EtOH:H_2O =1:1	80	0.5	99	*ChemistrySelect*, 2016, **1**, 1371–1376.
9	0.1 mol % Pd **Pd(OAc)$_2$@COF-300**	K_2CO_3	MeOH:H_2O=4:1	70	0.33	100	*ChemCatChem.*, 2016, **8**, 743–750.
10	5 mg **Pd@CzMOP**	K_2CO_3	DMF	80	6	96	*Polym. Chem.*, 2017, **8**, 1488–1494.
11	0.1 mol % Pd **PdNPs@COF**	K_2CO_3	DMF:H_2O =1:1	50	3	99	*J. Am. Chem. Soc.*, 2017, **139**, 17082–17088.
12	0.5 mol % **Pd@PPPP-2**	K_2CO_3	*p*-xylene	150	3	94	*Polym. Chem.*, 2018, **9**, 1430–1438.
13	0.3 mol % **Pd@SP-CMP**	K_2CO_3	H_2O	80	5	99	**This work**

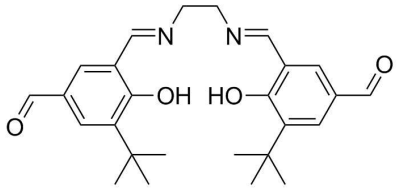
Table S4. Pd supported material catalysts for Heck–Mizoroki cross coupling reactions reported to date.

Entry	Catalyst	Base	Solvent	Temp. (◦C)	Time (h)	Yield (%)	Reference
1	0.3 mol % **PdNs-PAMAM--g-MWCNTs**	K_2CO_3	NMP	100	2.5	95	*Appl. Catal. A: Gen.*, 2011, **406** 124–132.
2	0.5 mol % **Pd catalyst**	K_2CO_3	DMF	120	1	93	*J. Organomet. Chem.*, 2011, **696**, 594-599.
3	1.2 mol % **PNP–SSS**	K_2CO_3	H_2O	100	1.5	95	*Green Chem.*, 2011, **13**, 2408-2415.
4	0.5 mol % **Pd/PRGO**	K_2CO_3	EtOH:H_2O =1:1	180	0.16	100	*ACS Catal.*, 2012, **2**, 145–154.
5	1 mg **MsMOP-1**	Et_3N	DMAc	130	12	76	*J. Mater. Chem. A*, 2013, **1**, 14108–14114.
6	0.1 mol % **Fe_3O_4@PUNP-Pd**	K_2CO_3	DMF:H_2O =1:1	120	8	95	*Green Chem.*, 2013, **15**, 3429–3437.
7	15 mg **Pd(0)@TpPa-1**	K_2CO_3	CH_3OH	105	6	92	*J. Mater. Chem. A*, 2014, **2**, 7944–7952.
8	0.006 mol % **Pd@MCOP**	K_2CO_3	DMSO:H_2O =1:1	90	10	98	*Green Chem.*, 2014, **16**, 4223–4233.
9	10 mg **C-(KTB-Pd)**	$K_3PO_4{\cdot}3H_2O$	DMF	120	2	99	*Dalton Trans.*, 2015, 44, 13906–13913.
10	1 mol % **Pd@NHC-MOP**	Et_3N	DMF	130	24	82	*ChemistrySelect*, 2016, **1**, 1371–1376.
11	5 mol % **Pd/CM**	Bu_3N	DMA	100	80	61	*RSC Adv.*, 2017, **7**, 1833–1840.
12	0.009 mol % **Fe_3O_4@SiO_2 -Dendrimer-Pd**	Et_3N	Solvent-free	120	2	92	*New J. Chem.*, 2018, **42**, 4748—4756.
13	0.6 mol % **Pd@SP-CMP**	K_2CO_3	1,4-dioxane: H_2O=1:1	80	12	99	**This work**

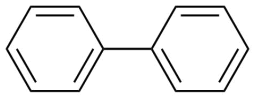
^{1}H NMR and ^{13}C NMR spectra



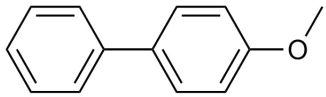
5-(tert-butyl)-4-hydroxyisophthalaldehyde: ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.40 (s, 1H), 9.99 (s, 1H), 9.93 (s, 1H), 8.07 (d, *J* = 2.0 Hz, 1H), 7.98 (d, *J* = 2.0 Hz, 1H), 1.46 (s, 9H) ppm.



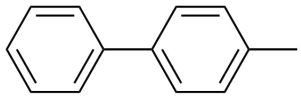
5,5'-((1E,1'E)-(ethane-1,2-diylbis(azanylylidene))bis(methanylylidene))bis(3-(tert-butyl)-4-hydroxybenzaldehyde): ^{1}H NMR (400 MHz, DMSO): δ 14.74 (d, *J* = 6.5 Hz, 1H), 9.68 (s, 1H), 8.68 (d, *J* = 7.1 Hz, 1H), 7.80 (d, *J* = 2.0 Hz, 1H), 7.69 (d, *J* = 2.0 Hz, 1H), 4.01 (s, 2H), 1.35 (s, 9H) ppm.



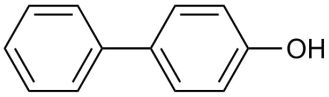
1,1'-biphenyl: ^{1}H NMR (400 MHz, $CDCl_3$) : δ 7.63 (d, *J* = 7.9 Hz, 4H), 7.47 (t, *J* = 7.5 Hz, 4H), 7.38 (t, *J* = 7.3 Hz, 2H) ppm.



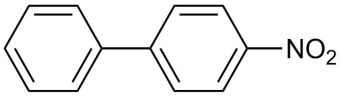
4-methoxy-1,1'-biphenyl: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54 (dd, *J* = 12.8, 5.0 Hz, 4H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.30 (t, *J* = 7.3 Hz, 1H), 6.98 (d, *J* = 8.7 Hz, 2H), 3.85 (s, 3H) ppm.



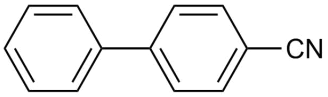
4-methyl-1,1'-biphenyl: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (d, *J* = 7.3 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.26 – 7.20 (m, 2H), 2.39 (s, 3H) ppm.



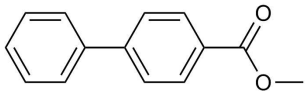
[1,1'-biphenyl]-4-ol: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54 (d, J = 7.5 Hz, 2H), 7.48 (d, *J* = 8.6 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.3 Hz, 1H), 6.91 (d, *J* = 8.6 Hz, 2H), 4.73 (s, 1H) ppm.



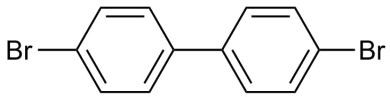
4-nitro-1,1'-biphenyl: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.30 (d, *J* = 8.8 Hz, 2H), 7.73 (d, *J* = 8.8 Hz, 2H), 7.65 – 7.60 (m, 2H), 7.52 – 7.44 (m, 3H) ppm.



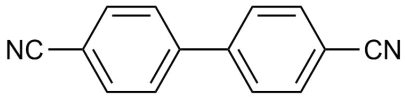
[1,1'-biphenyl]-4-carbonitrile: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 – 7.66 (m, 4H), 7.61 – 7.56 (m, 2H), 7.51 – 7.45 (m, 2H), 7.42 (ddd, *J* = 7.3, 3.6, 1.3 Hz, 1H) ppm.



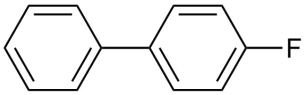
Methyl [1,1'-biphenyl]-4-carboxylate: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (d, *J* = 7.3 Hz, 2H), 7.64 (dd, *J* = 14.3, 7.6 Hz, 4H), 7.53 – 7.36 (m, 3H), 3.94 (s, 3H) ppm.



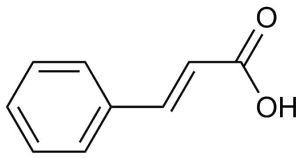
4,4'-dibromo-1,1'-biphenyl: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.5 Hz, 4H), 7.41 (d, *J* = 8.4 Hz, 4H) ppm.



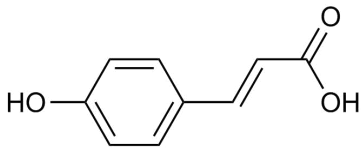
[1,1'-biphenyl]-4,4'-dicarbonitrile: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (d, *J* = 7.9 Hz, 4H), 7.37 (d, *J* = 8.1 Hz, 4H) ppm.



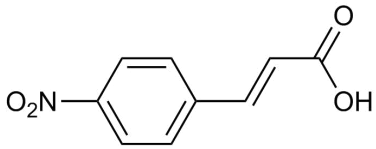
4-fluoro-1,1'-biphenyl: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54 (dd, *J* = 8.0, 3.8 Hz, 4H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.3 Hz, 1H), 7.12 (t, *J* = 8.6 Hz, 2H) ppm.



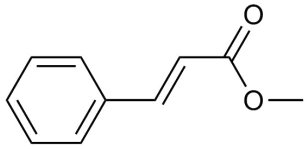
Cinnamic acid: ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.71 (s, 1H), 7.80 (d, *J* = 16.0 Hz, 1H), 7.55 (dd, *J* = 6.6, 2.9 Hz, 2H), 7.41 (dd, *J* = 6.2, 3.7 Hz, 3H), 6.46 (d, *J* = 16.0 Hz, 1H) ppm.



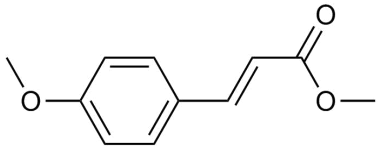
(E)-3-(4-hydroxyphenyl)acrylic acid: ^{1}H NMR (400 MHz, DMSO): δ 12.71 (s, 1H), 8.24 (d, *J* = 8.4 Hz, 2H), 7.99 (d, *J* = 8.5 Hz, 2H), 7.70 (d, *J* = 16.1 Hz, 1H), 6.75 (d, *J* = 16.1 Hz, 1H) ppm.



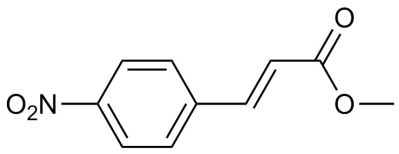
(E)-3-(4-nitrophenyl)acrylic acid: ^{1}H NMR (400 MHz, DMSO): δ 12.73 (s, 1H), 8.24 (d, *J* = 8.8 Hz, 2H), 7.99 (d, *J* = 8.8 Hz, 2H), 7.70 (d, *J* = 16.1 Hz, 1H), 6.76 (d, *J* = 16.1 Hz, 1H) ppm.



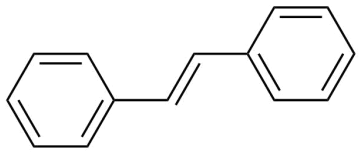
Methyl cinnamate: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52 – 7.43 (m, 4H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.23 (t, *J* = 7.4 Hz, 1H), 7.02 (dd, *J* = 38.1, 16.3 Hz, 2H), 6.93 – 6.88 (m, 2H), 3.83 (s, 3H) ppm.



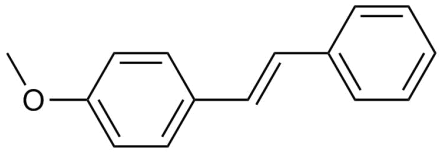
Methyl (E)-3-(4-methoxyphenyl)acrylate: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65 (d, J = 16.0 Hz, 1H), 7.47 (d, *J* = 7.2 Hz, 2H), 6.90 (d, *J* = 7.2 Hz, 2H), 6.31 (d, *J* = 15.9 Hz, 1H), 3.83 (s, 3H), 3.79 (s, 3H) ppm.



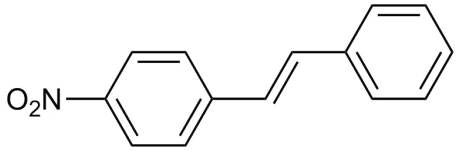
Methyl (E)-3-(4-nitrophenyl)acrylate: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, *J* = 15.9 Hz, 1H), 7.51 (d, *J* = 8.5 Hz, 2H), 6.92 (d, J = 8.5 Hz, 2H), 6.32 (d, *J* = 15.9 Hz, 1H), 3.85 (s, 3H) ppm.



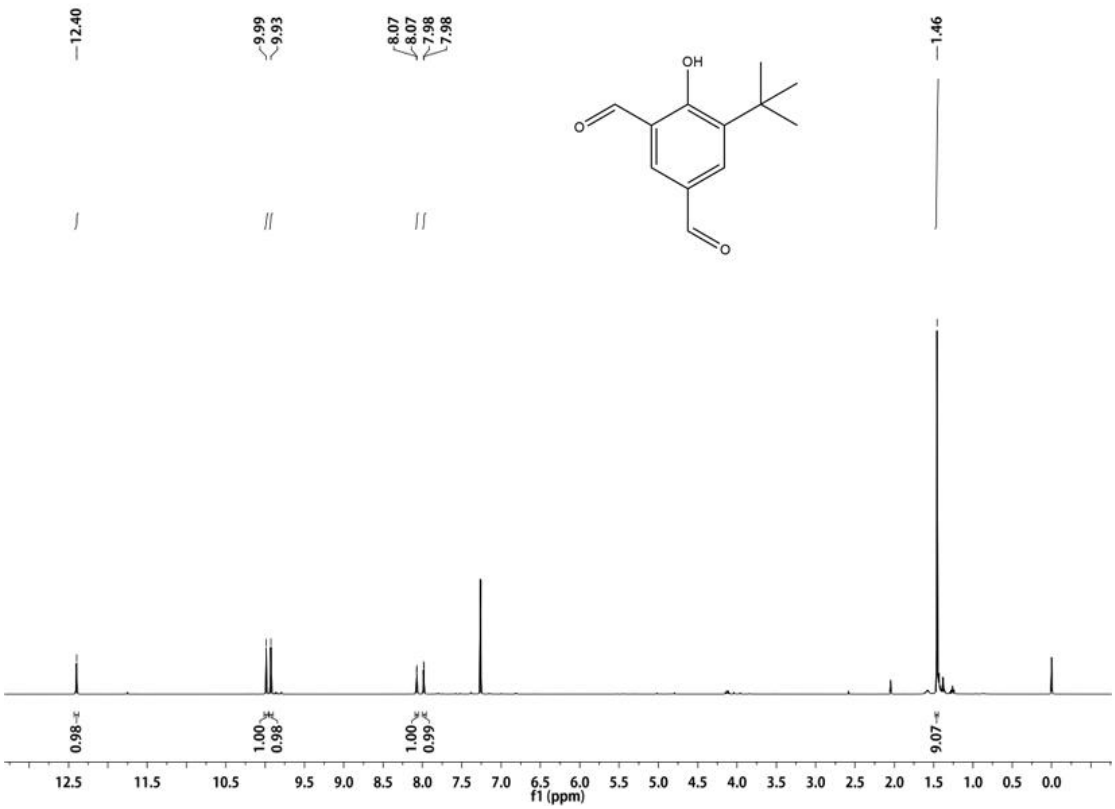
(E)-1,2-diphenylethene: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52 (d, *J* = 7.3 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.28 (d, *J* = 3.7 Hz, 1H), 7.12 (d, *J* = 5.5 Hz, 1H) ppm.



(E)-1-methoxy-4-styrylbenzene: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52 – 7.43 (m, 4H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.23 (t, *J* = 7.4 Hz, 1H), 7.02 (dd, *J* = 38.1, 16.3 Hz, 2H), 6.93 – 6.88 (m, 2H), 3.83 (s, 3H) ppm.



(E)-1-nitro-4-styrylbenzene: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (d, *J* = 8.8 Hz, 2H), 7.64 (d, *J* = 8.8 Hz, 2H), 7.56 (d, *J* = 7.3 Hz, 2H), 7.46 – 7.28 (m, 4H), 7.15 (d, *J* = 16.3 Hz, 1H) ppm.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8.07
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7.98
1.46
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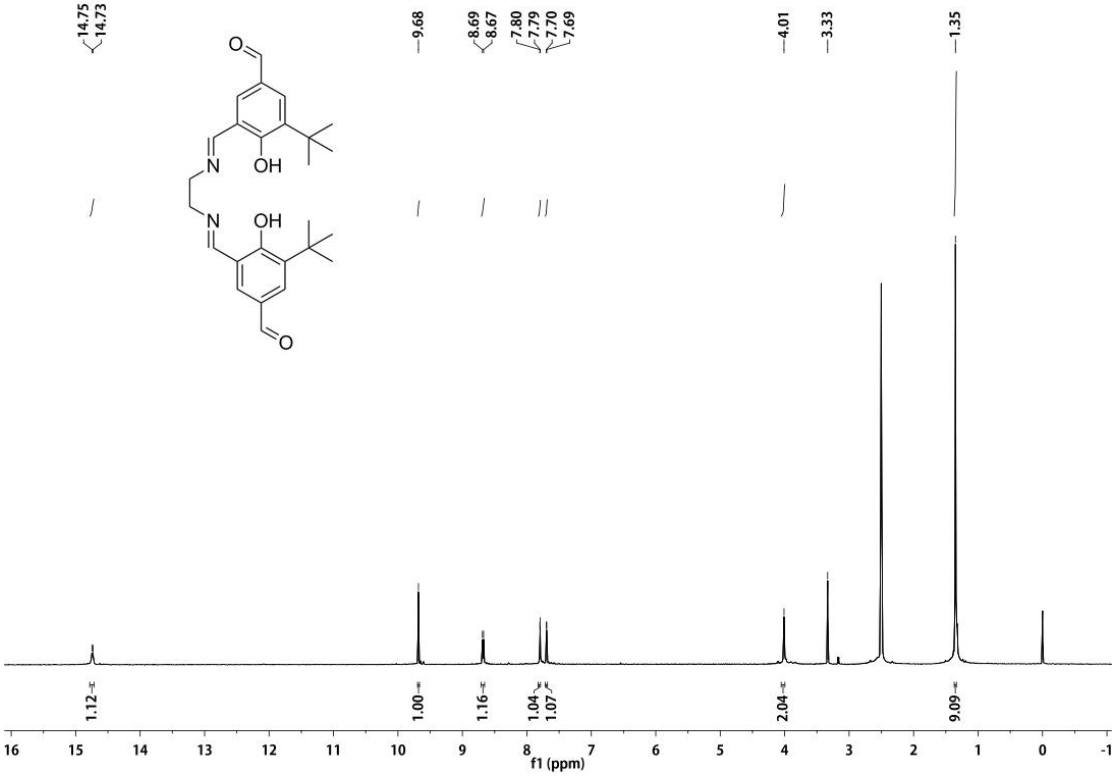
O
0.98
1.00
0.98
1.00
0.99
9.07
f1 (ppm)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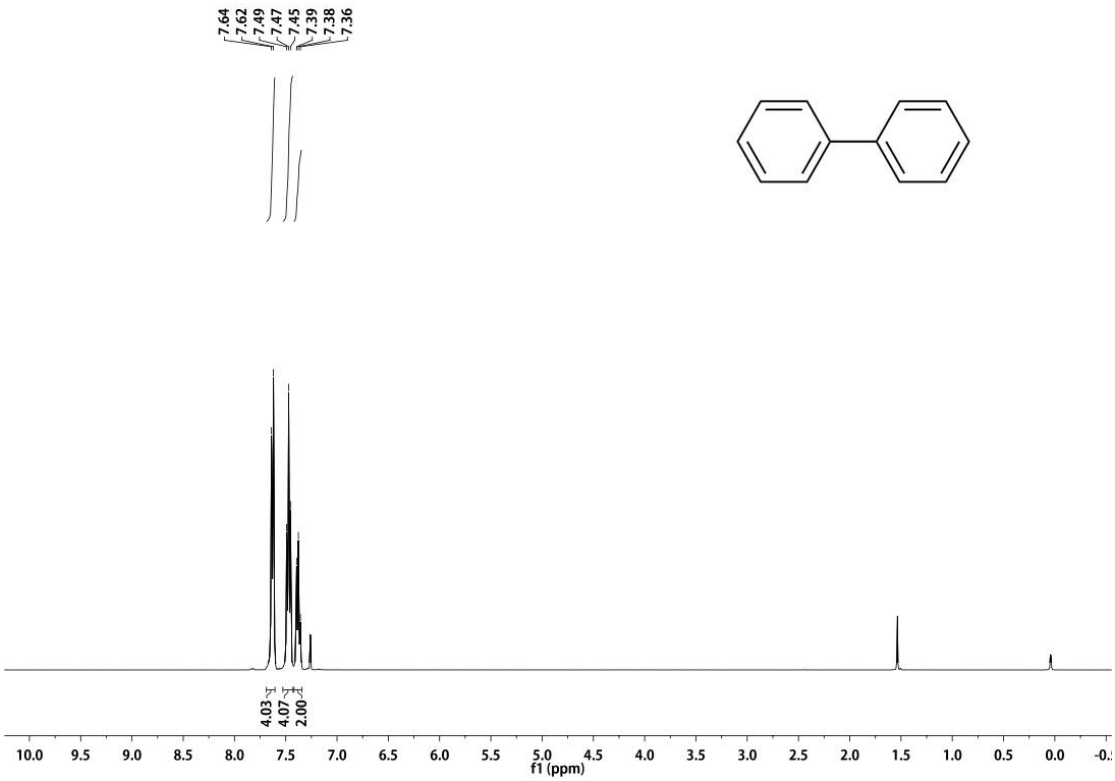
8.69
8.67
7.80
7.79
7.70
7.69
4.01
3.33
1.35
O
N
OH
N
OH
O
1.12
1.00
1.16
1.04
1.07
2.04
9.09
f1 (ppm)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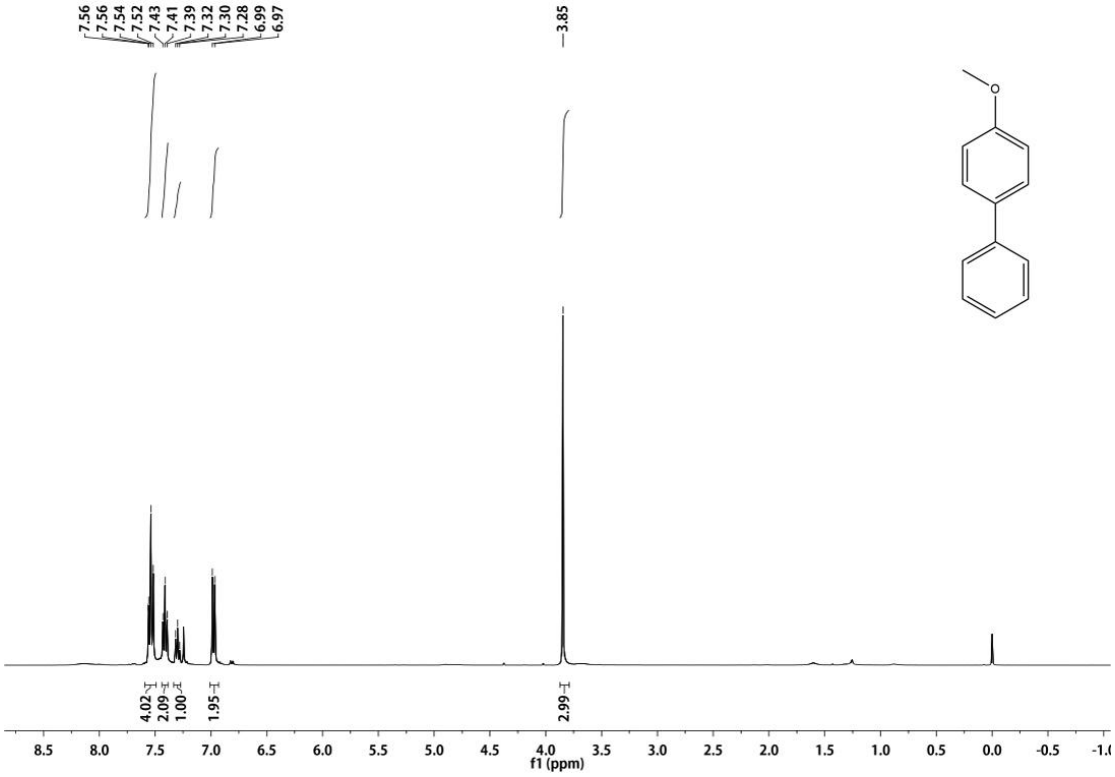
7.39
7.38
7.36
4.03
4.07
2.00
f1 (ppm)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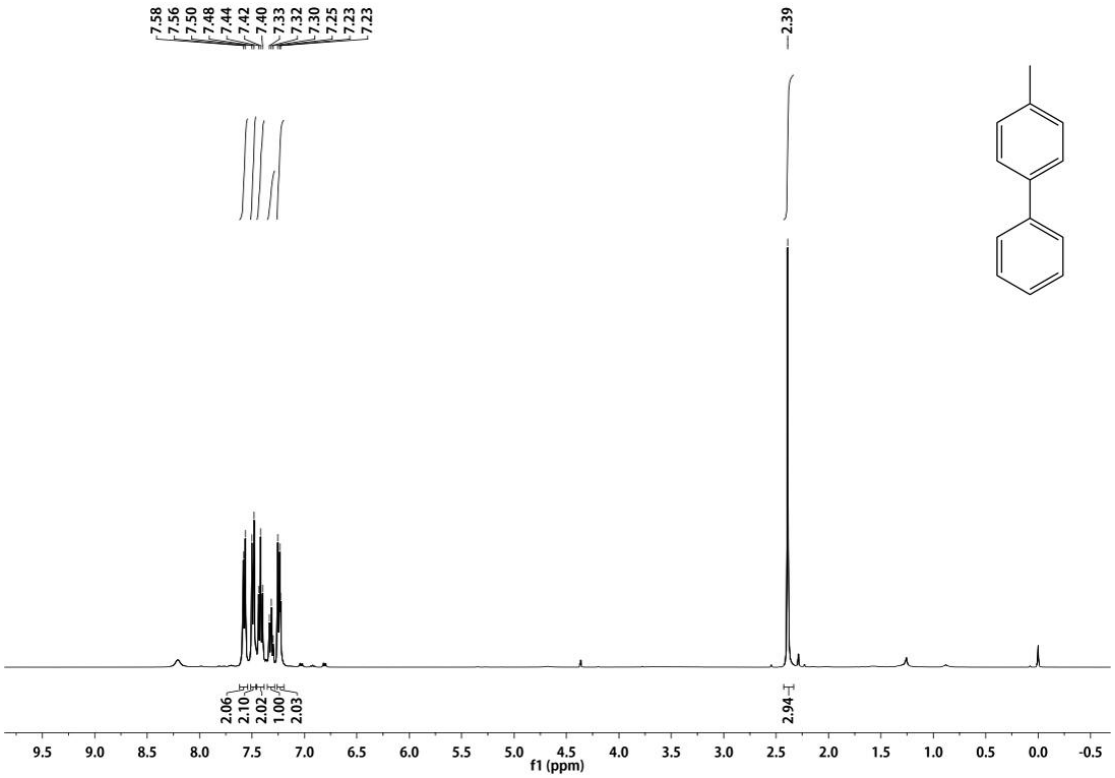
2.09
1.00
1.95
2.99
f1 (ppm)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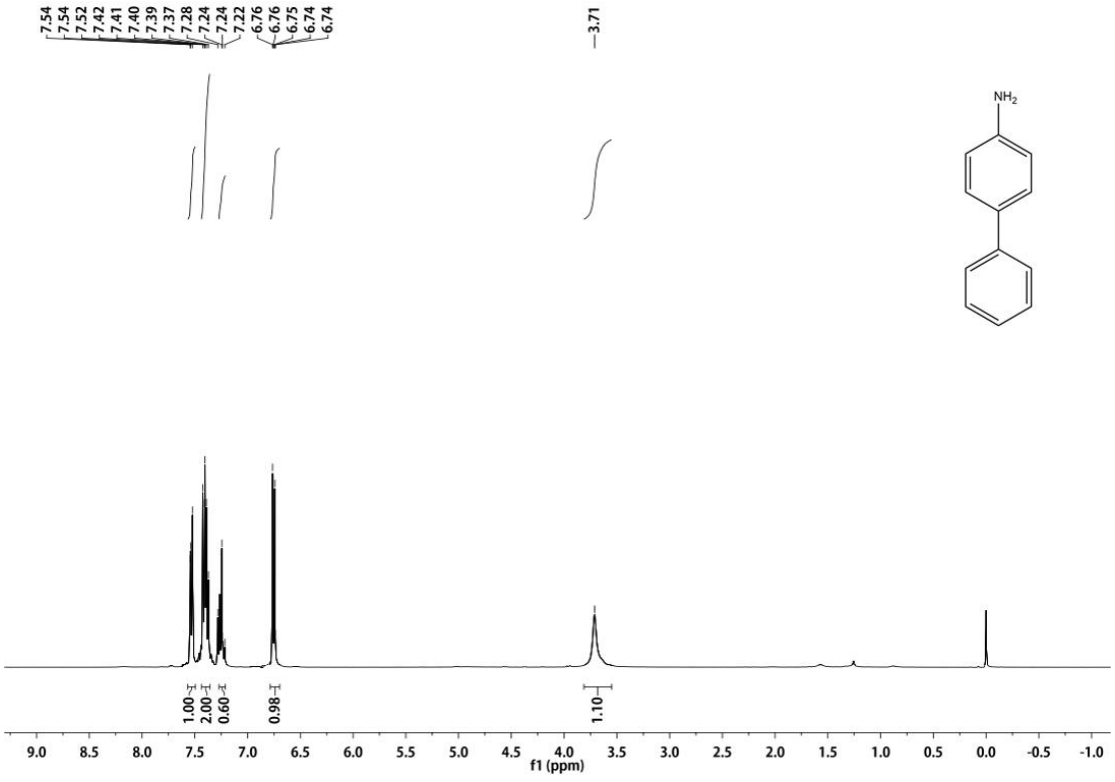
7.23
7.23
2.39
2.06
2.10
2.02
1.00
2.03
2.94
f1 (ppm)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6.76
6.75
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6.74
3.71
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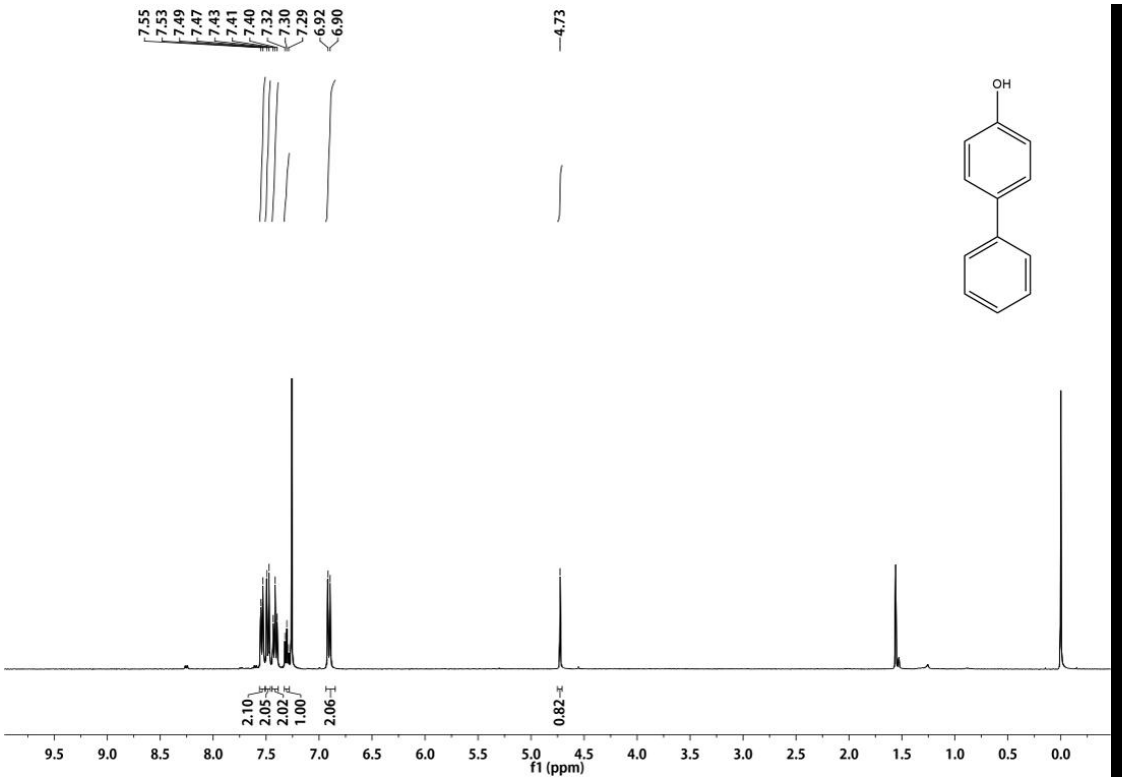
0.60
0.98
1.10
f1 (ppm)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4.73
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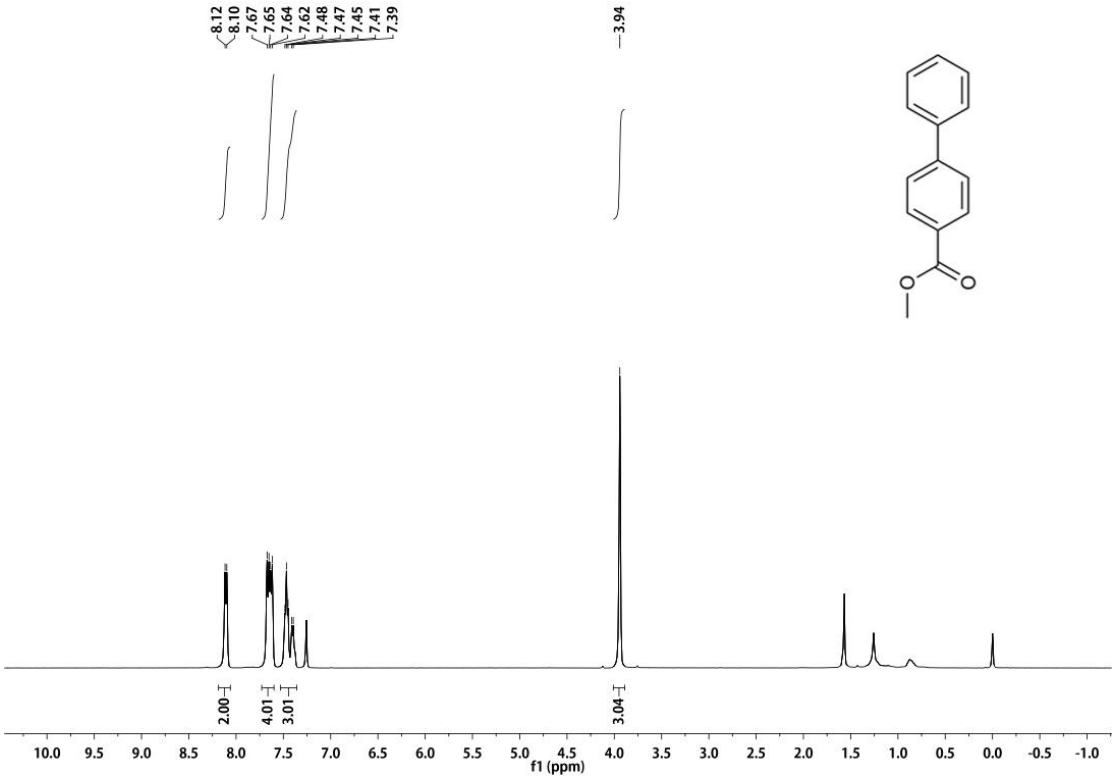
2.02
1.00
2.06
0.82
f1 (ppm)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7.47
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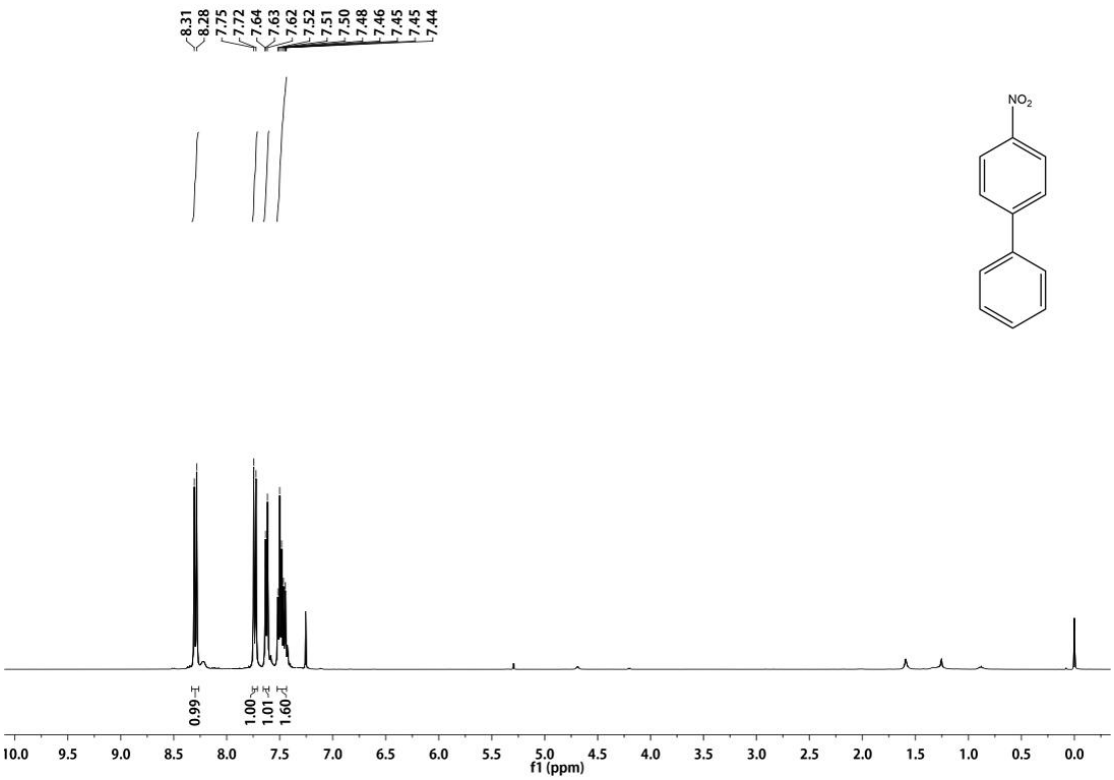
7.41
7.39
3.94
2.00
4.01
3.01
3.04
f1 (ppm)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8.28
7.75
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7.63
7.62
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7.45
7.45
7.44
NO2
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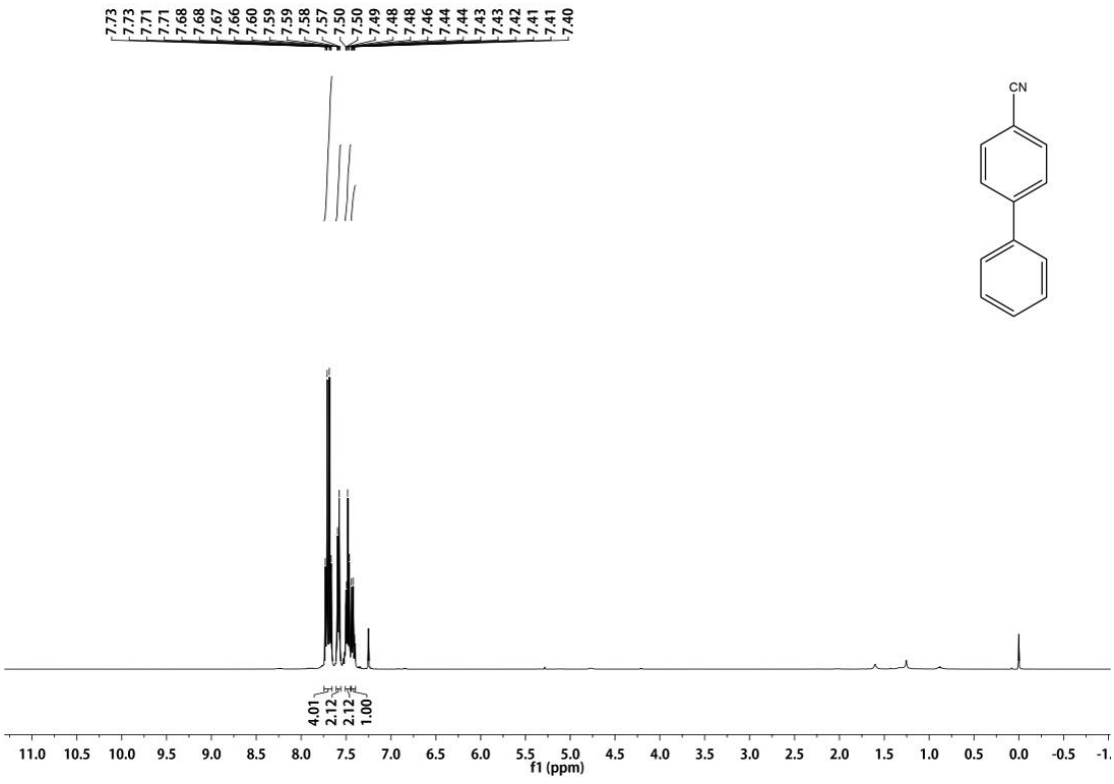
1.00
1.01
1.60
f1 (ppm)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7.50
7.49
7.48
7.48
7.46
7.44
7.44
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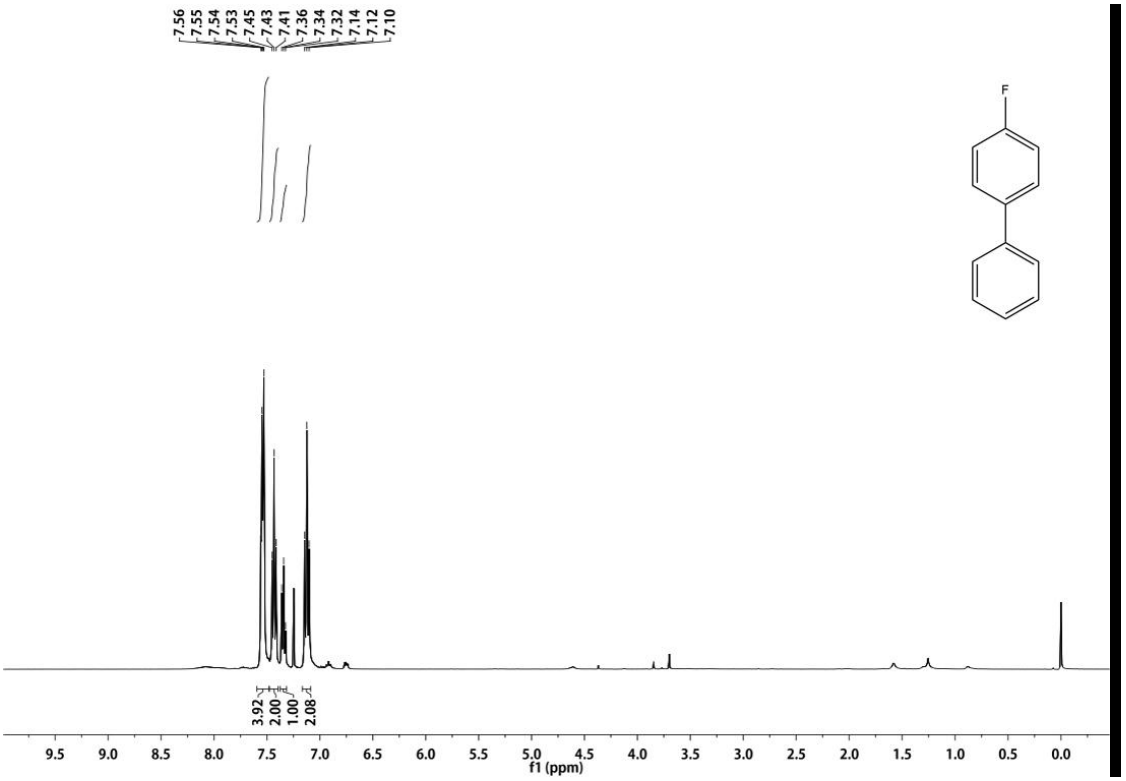
7.41
7.41
7.40
CN
4.01
2.12
2.12
1.00
f1 (ppm)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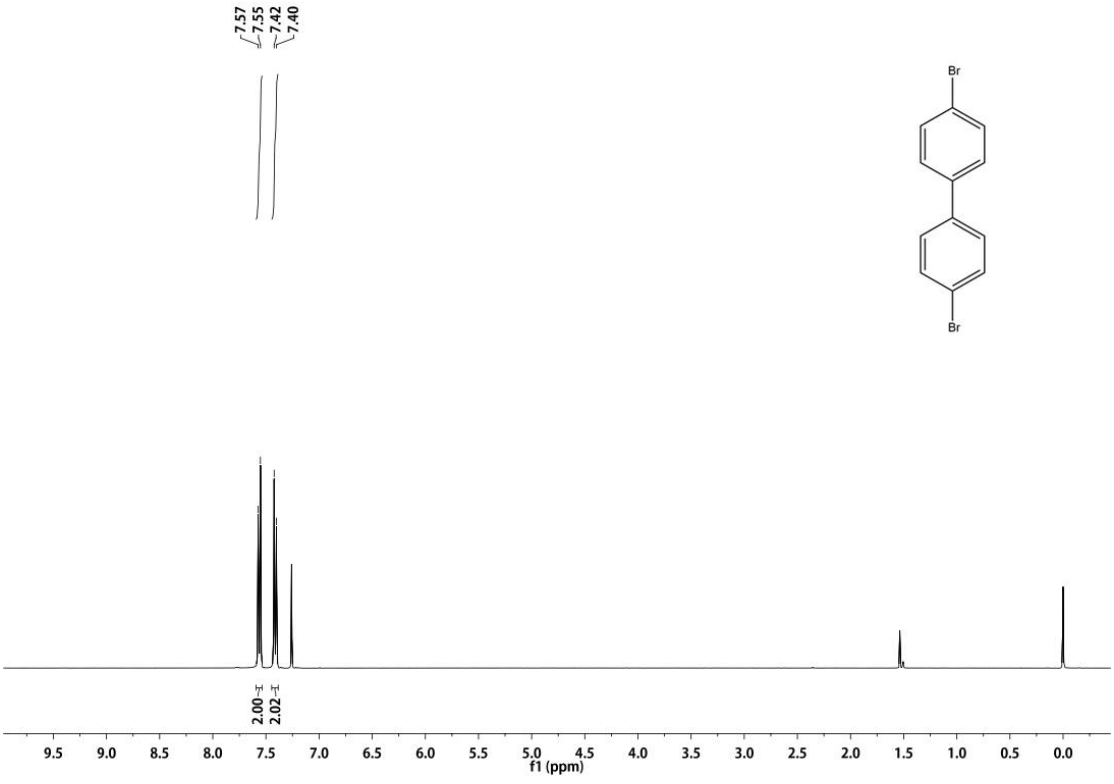
7.36
7.34
7.32
7.14
7.12
7.10
F
3.92
2.00
1.00
2.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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7.55
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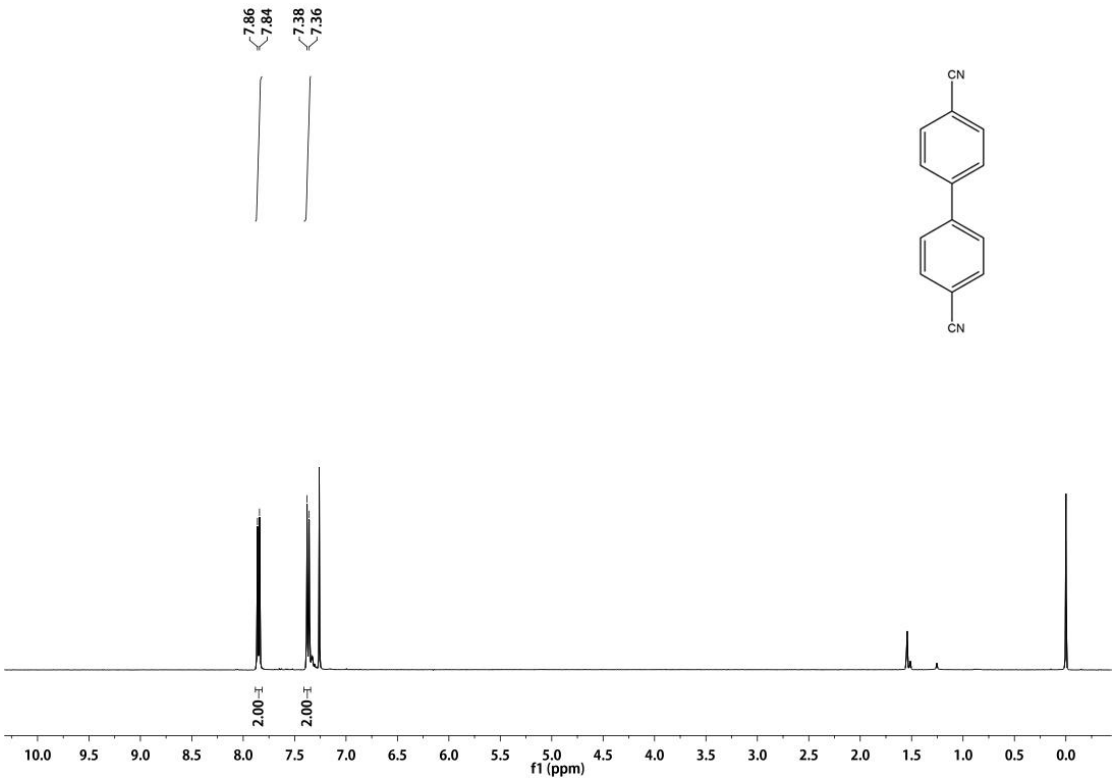
7.40
Br
Br
2.00
2.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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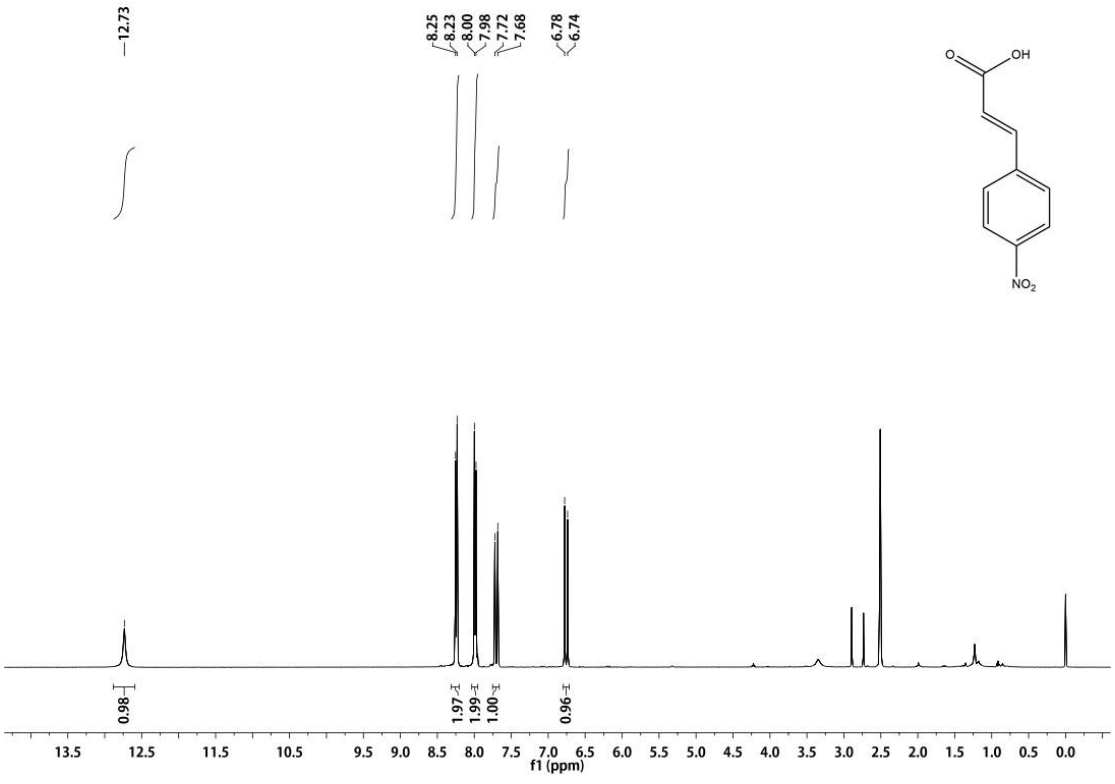
7.36
CN
CN
2.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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OH
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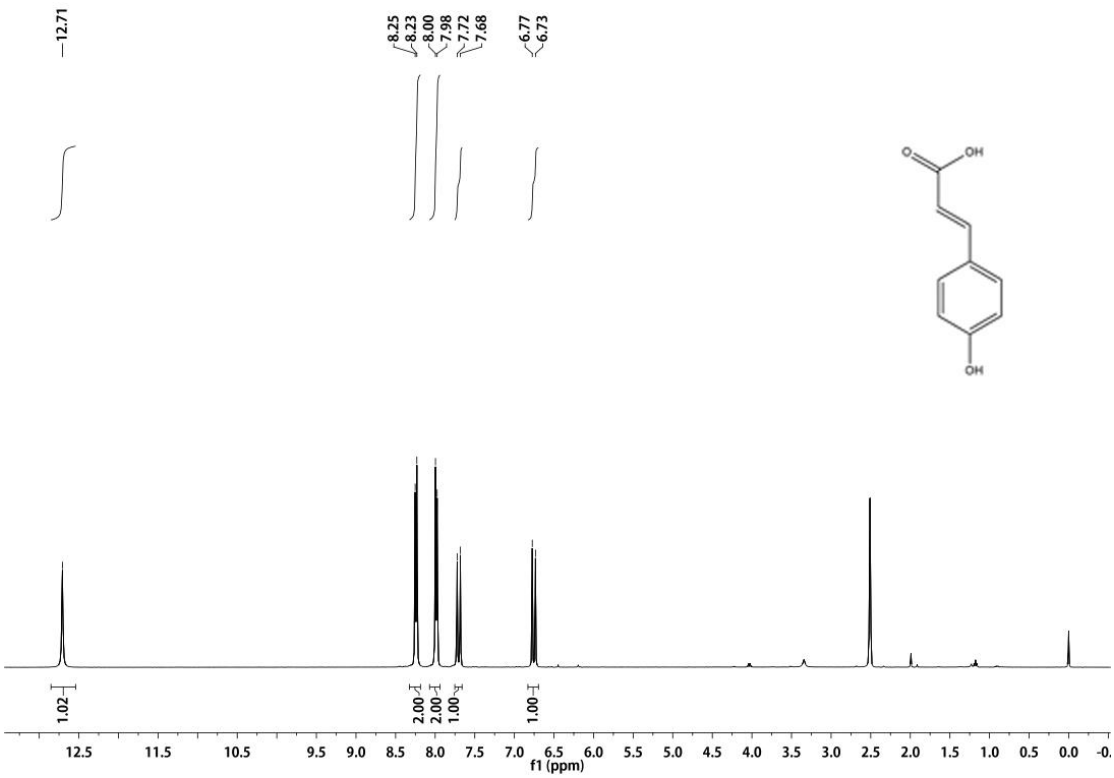
1.97
1.99
1.00
0.96
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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OH
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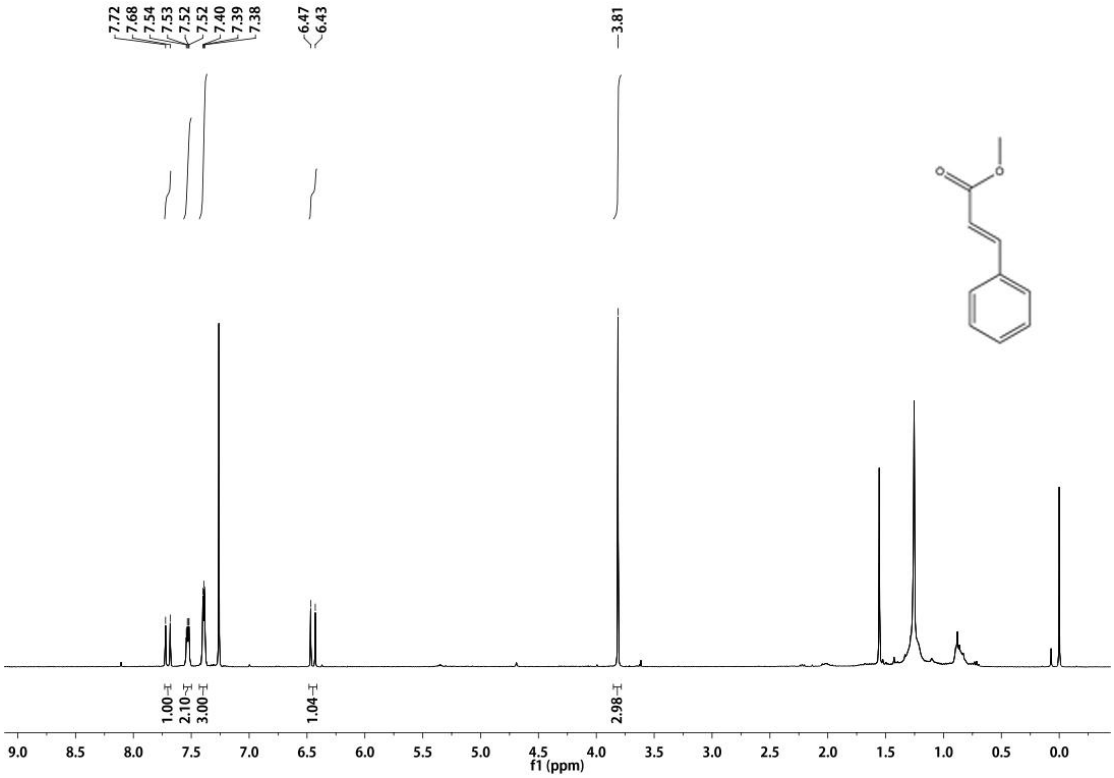
1.00
f1 (ppm)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3.00
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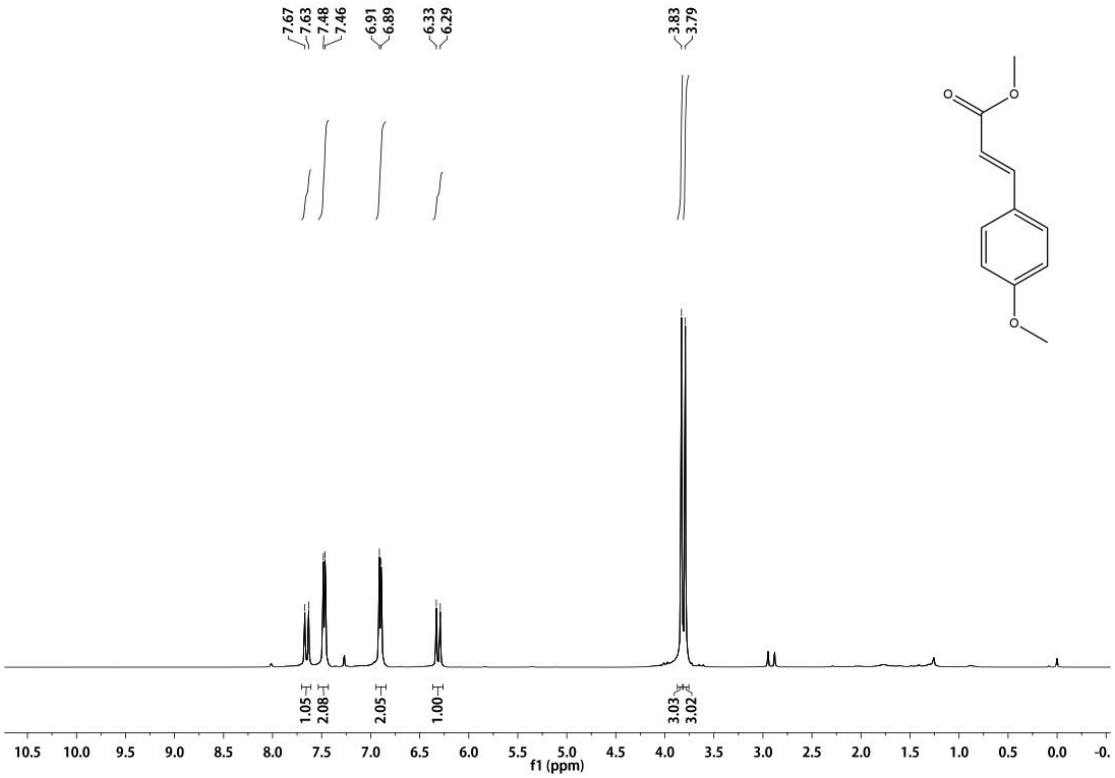
2.98
f1 (ppm)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2.05
1.00
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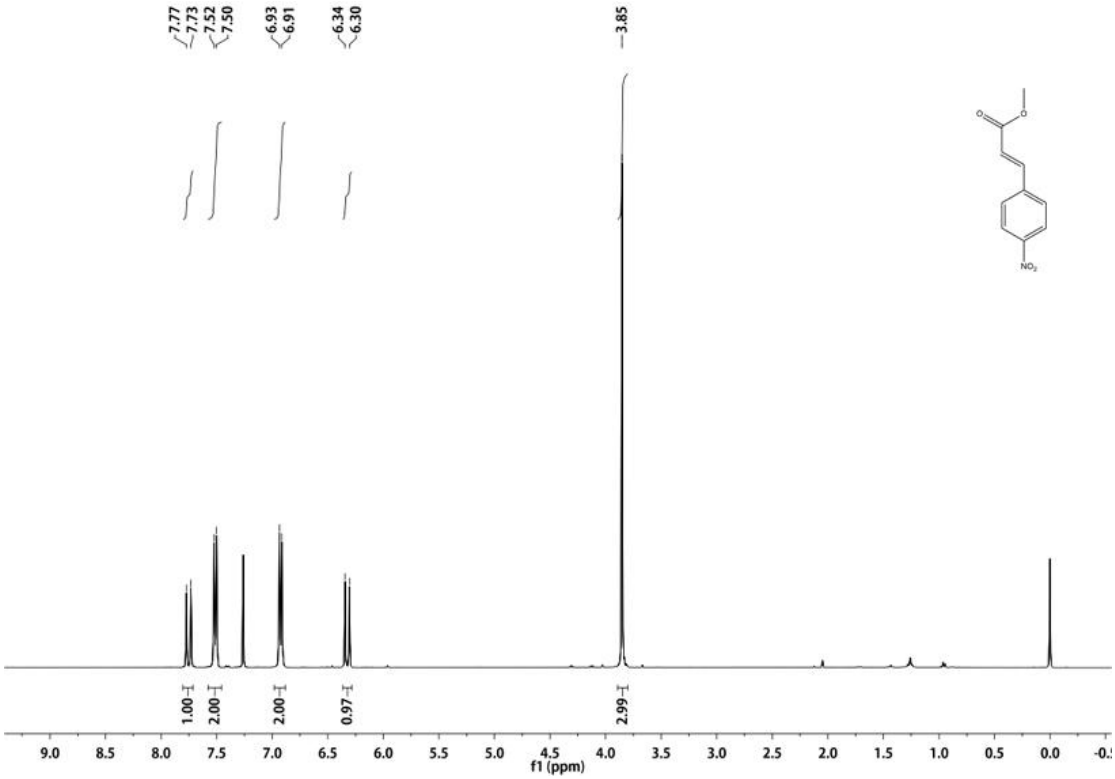
3.02
f1 (ppm)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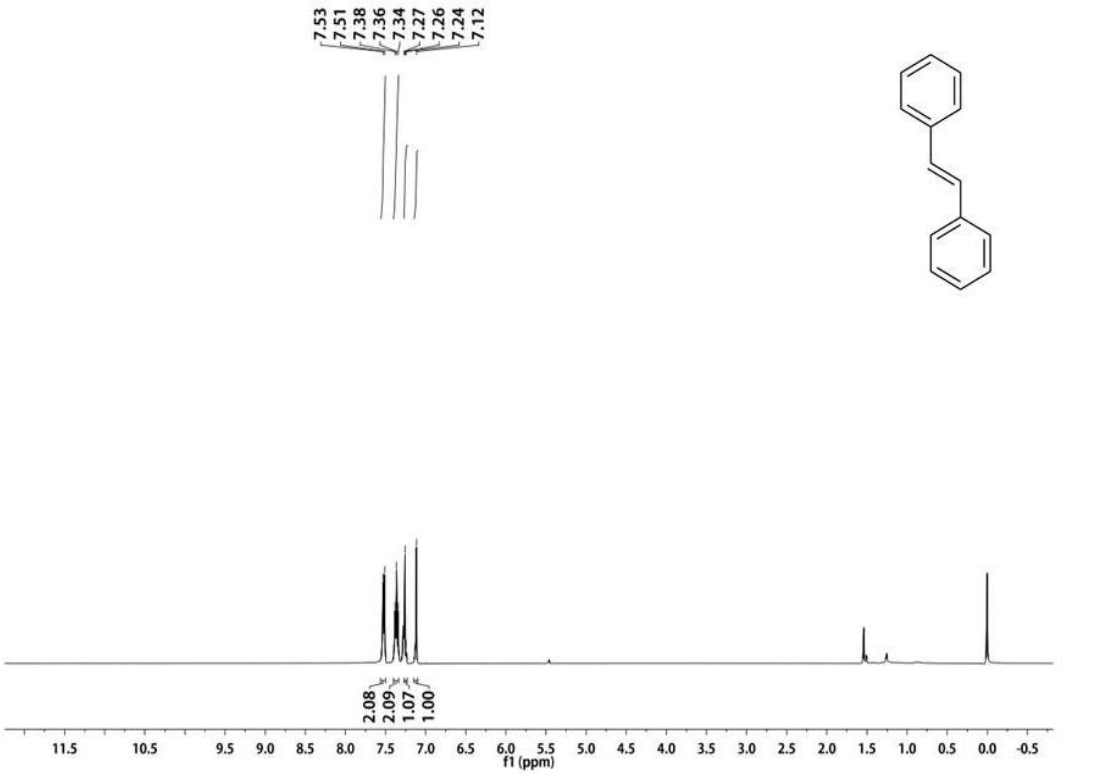
f1 (ppm)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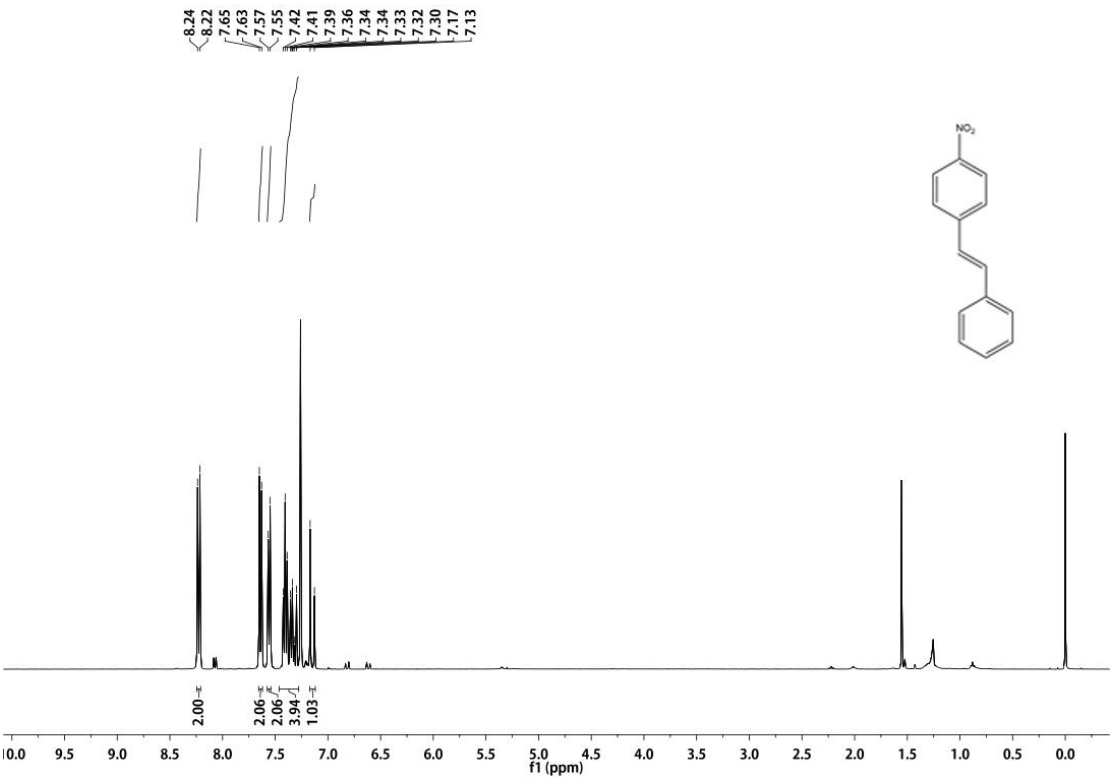
f1 (ppm)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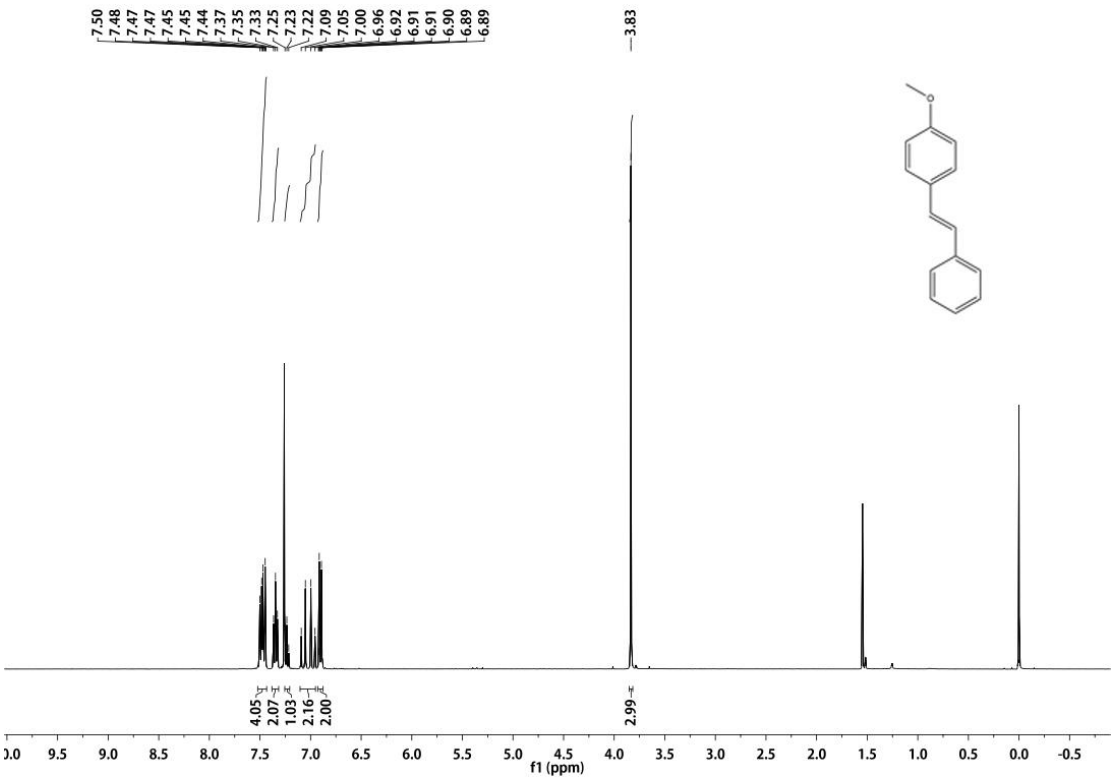
f1 (ppm)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6.91
6.90
6.89
6.89
3.83
4.05
2.07
1.03
2.16
2.00
2.99
f1 (ppm)