Electronic Supplementary Information

Direct arylation of unactivated aromatic C–H bonds catalyzed by stable organic radical

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General methods

All aryl halides and KO*t*-Bu were purchased from Aladdin Reagent Company (Shanghai). Hbipo$^{-\bullet}$ radical (**Rad-A**) was synthesized following previously published procedure.[S1] All other reagents and solvents were commercially available and used without further purification. All reactions were performed in air-dried or oven-dried glassware. Analytical thin-layer chromatography (TLC) was performed on pre-coated, glass-backed silica gel plates. Flash column chromatography was performed using 200-300 mesh silica gel with the indicated solvent system according to standard techniques.

^{1}H and ^{13}C NMR spectra were obtained on Bruker Avance 300 MHz or 400 MHz NMR spectrometers using $CDCl_3$ as solvent and tetramethylsilane (TMS) as the internal standard. High-resolution mass spectra (HRMS) were recorded with an EI mode. Microanalytical data (C, H, N) were collected on Vario ELIII elemental analyzer. FT-IR spectra (KBr disk, 4000–400 cm^{-1}) were recorded on Bruker EQUINOX55 FT-IR spectrophotometer. The EPR spectrum was recorded on a JES-FA 200 ESR spectrometer at X-band.

The X-ray diffraction measurement was performed on a Gemini S Ultra CCD diffractometer (Oxford diffraction Ltd.) using graphite monochromated Cu-Kα radiation (λ = 1.54184 Å). The structure was solved by direct method (SHELXL 97) and completed by difference Fourier method (SHELXL 97). Refinement was performed against F^2 by weighted full-matrix least-squares (SHELXL 97),[S2] and empirical absorption correction (SCALE3 ABSPACK) was applied. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were placed in geometrically calculated positions. Weighted *R* factor (R_w) and all goodness of fit S are based on F^2, conventional *R* factor (*R*) is based on *F*.

General procedure for the direct arylation of arene with aryl halides in the presence of a substoichiometric amount of Hbipo$^{-\bullet}$ (Rad-A) radical:

An oven-dried three-necked flask was charged with **Rad-A** (75 mg, 0.3 mmol) and KO*t*-Bu (336 mg, 3 mmol) under a nitrogen atmosphere at room temperature. Then arene (10 mL, also as a solvent) and aryl halides (1.5 mmol) were added. The

resulting mixture was stirred at 120 °C under a nitrogen atmosphere for 24 h. After cooling to room temperature and some residue was filtered and washed by ethyl acetate, silica gel then was added to filtrate (including ethyl acetate) and evaporated to dryness under reduced pressure at 65 ºC. The product was purified through flash column chromatography on 200–300 mesh silica gel with petroleum ether (60–90)/ethyl acetate as eluent.

Recovery of Hbipo$^{-\bullet}$ radical after the coupling reaction:

A mixture of **Rad-A** (150 mg, 0.6 mmol), KO*t*-Bu (672 mg, 6 mmol), iodobenzene (612 mg, 3 mmol) and benzene (20 mL, 225 mmol) in a 50 mL oven-dried three-necked flask was stirred at 120 °C for 24 h under a nitrogen atmosphere. After cooling to room temperature and being filtered, the resulting residue was dissolved with H_2O (5 mL). After filtered, the filtrate was acidified with 37 % HCl to pH 6, leading to a yellow precipitate which then was recrystallized from DMF to give about 12 % (based on initial **Rad-A**) recoverable **Rad-A**, which was verified by the same methods as previously reported.[S1] The recoverable Hbipo$^{-\bullet}$ also proves there exists a key intermediate (anion radical complex **4**) in this HAS reaction system, because this anion radical complex can be dissolved in H_2O and acidified to form Hbipo$^{-\bullet}$.

Isolation 2-(imidazo[1,2-*a*]pyridin-2-yl)-2-oxo-*N*-(pyridin-2-yl)acetamide (Rad-B) from solid residue:

After the coupling reaction finished in the Hbipo$^{-\bullet}$ catalyzed HAS reaction system, the resulting residue was purified by column chromatography on silica gel (eluting with ethyl acetate). The removal of eluent under reduced pressure afforded a tiny amount of **Rad-B** as a yellow solid (based on initial **Rad-A**), which was identified by X-ray single crystal diffraction and EPR spectrum.

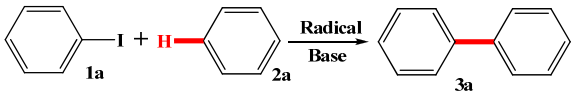
General procedure for preparation of Rad-B:

Indeed, **Rad-B** can also be synthesized by *m*-chloroperoxybenzonic acid promoted ring-opening reaction of zwitterionic Hbipo$^{-\bullet}$ radical under mild conditions. *m*-Chloroperoxybenzonic acid (4.8 g, 24 mmol) was added into an ice-bath cooled DMF (120 mL) solution of Hbipo$^{-\bullet}$ (5.5 g, 22 mmol), leading to a dark red solution. The reaction mixture was stirred for 2 h, giving rise to the yellow solid, which was collected by filtration and washed with water and methanol, recrystallization from ethanol afforded yellow solid of **Rad-B**. Yield: 2.66 g (10 mmol), 45.5 %. IR (KBr): 3364(s), 3156(w), 3108(w), 3044(w), 1708(s), 1669(vs), 1639(m), 1589(w), 1577(w), 1521(vs), 1472(w), 1440(s), 1306(w), 1154(w), 1125(w), 1055(w), 1044(w), 763(m) cm^{-1}. HRMS (EI, m/z, [M]$^+$): Calcd for $C_{14}H_{10}N_4O_2$: 266.0804, Found: 266.0806. Anal. Calc. (%) for $C_{14}H_{10}N_4O_2$: C, 63.15; H, 3.79; N, 21.04. Found: C, 63.90; H, 3.91; N, 21.21.

The proposed mechanism for this *m*-chloroperoxybenzonic acid promoted ring-opening reaction under mild conditions is shown in Scheme S3. According to ring-opening reaction of Hbipo$^{-\bullet}$ radical, when reaction (Table 2, entry 1) catalyzed by Hbipo$^{-\bullet}$ was carried out without using nitrogen atmosphere, only about 25% of

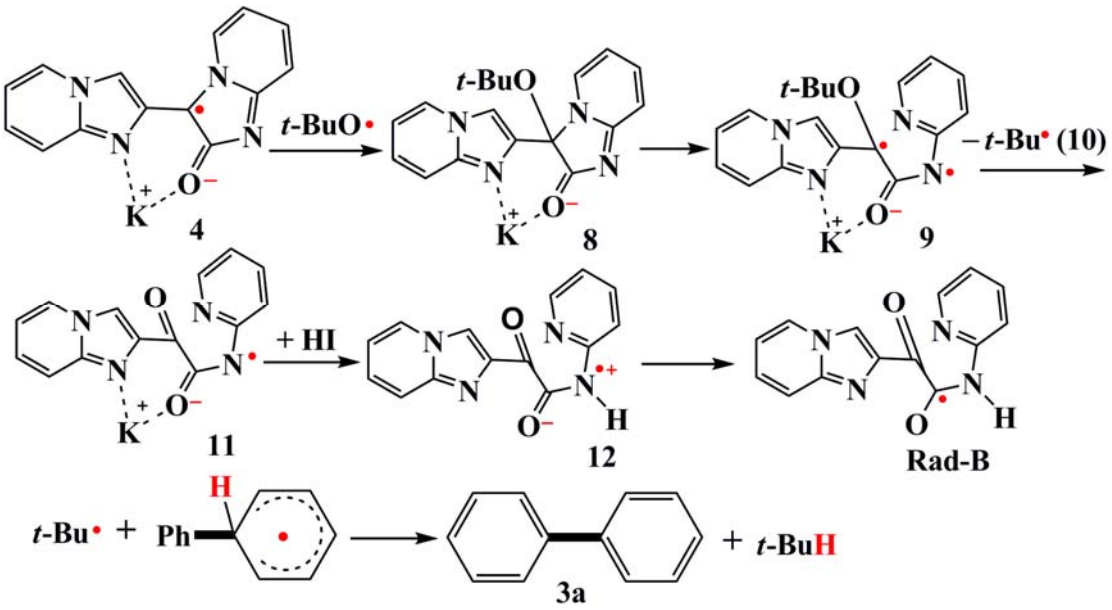
coupling product **3a** was isolated, probably attributed to $Hbipo^{-\bullet}$ mainly transferring to low efficiency **Rad-B** (the intercept effect of stable radical) under strong base, high temperature and air conditions.

Table S1 Arylation of benzene with iodobenzene [a]



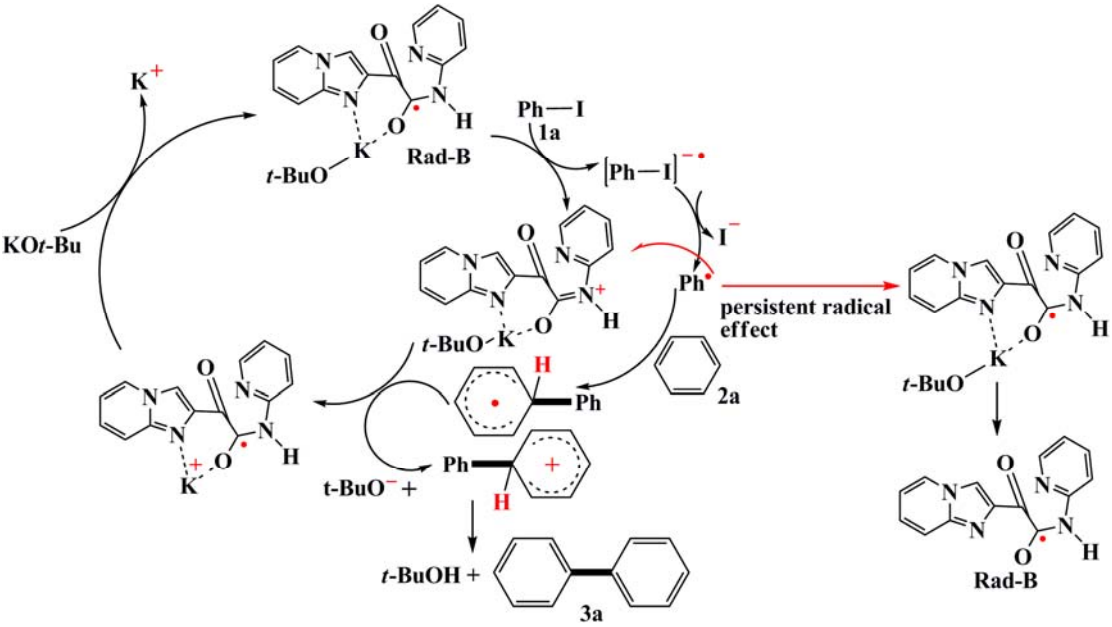
Entry	Base (equiv)	Radical (mol %)	Temp (°C)	Time (h)	Yield (%) [b]
1	KO*t*-Bu (2)	**A** (20)	120	6	40
2	KO*t*-Bu (2)	**A** (20)	120	12	59
3	KO*t*-Bu (2)	**A** (20)	120	24	76
4	KO*t*-Bu (2)	**A** (20)	120	36	74
5	KO*t*-Bu (2)	**A** (20)	80	24	54
6	KO*t*-Bu (2)	**A** (20)	100	24	65
7	KO*t*-Bu (2)	**A** (20)	160	24	70
8	KO*t*-Bu (2)	**A** (10)	120	24	63
9	KO*t*-Bu (2)	**A** (30)	120	24	75
10	KO*t*-Bu (2)	**A** (40)	120	24	76
11	KO*t*-Bu (2)	–	120	24	trace
12	KO*t*-Bu (1)	**A** (20)	120	24	61
13	KO*t*-Bu (3)	**A** (20)	120	24	72
14	KO*t*-Bu (4)	**A** (20)	120	24	74
15	NaO*t*-Bu (2)	**A** (20)	120	24	66
16	–	**A** (20)	120	24	trace
17	MeOK (2)	**A** (20)	120	24	trace
18	KOH (2)	**A** (20)	120	24	trace
19	K_2CO_3 (2)	**A** (20)	120	24	trace
20	Et_3N (2)	**A** (20)	120	24	trace
21	KO*t*-Bu (2)	**B** (20)	120	24	< 15
22	KO*t*-Bu (2)	**B** (100)	120	24	< 15
23	KO*t*-Bu (2)	**A** (20) /TEMPO(20)	120	24	0

[a] The reaction was carried out under a nitrogen atmosphere using iodobenzene (**1a**: 1.5 mmol) and benzene (**2a**: 10 mL, 112.5 mmol) in a three-necked flask. [b] Isolated yield based on **1a**.

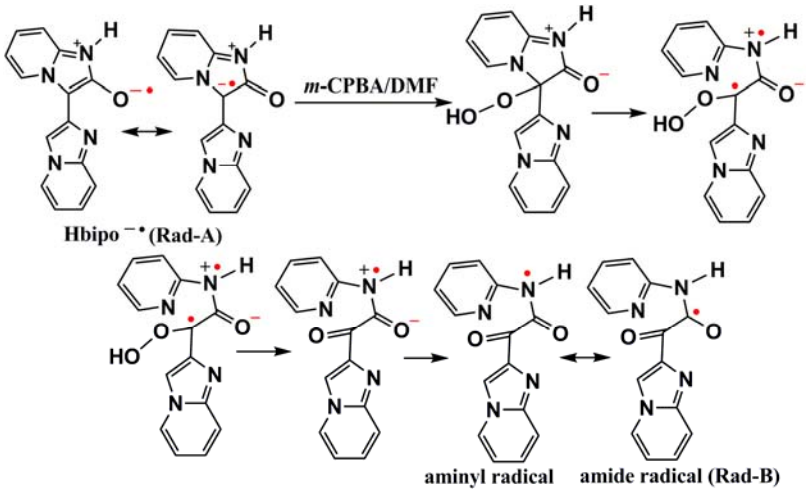


Scheme S1 A plausible mechanism for *in situ* forming **Rad-B**.

As suggested by Shirakawa,[S3] the *t*-BuO• can be formed from *t*-BuOH. The partial *t*-BuO• is considered to react with anion radical complex **4**, giving rise to the formation of another complex **8**. According to the steric hinderance of *t*-BuO, **8** occurs the ring-opening reaction, affording biradical intermediate **9** which eliminates *t*-Bu• **10**, leading to the formation of another radical complex **11**. Then, **11** further converts to **Rad-B**. The active *t*-Bu• **10** can react with cyclohexadienyl radical **7**, further affording coupling product **3a**. However, it should be specially noted that because only a tiny amount of **Rad-B** was obtained in reaction system, and the radical reaction mechanism in Scheme S1 is nonchain, the resulting coupling product **3a** by *t*-Bu• must be tiny.

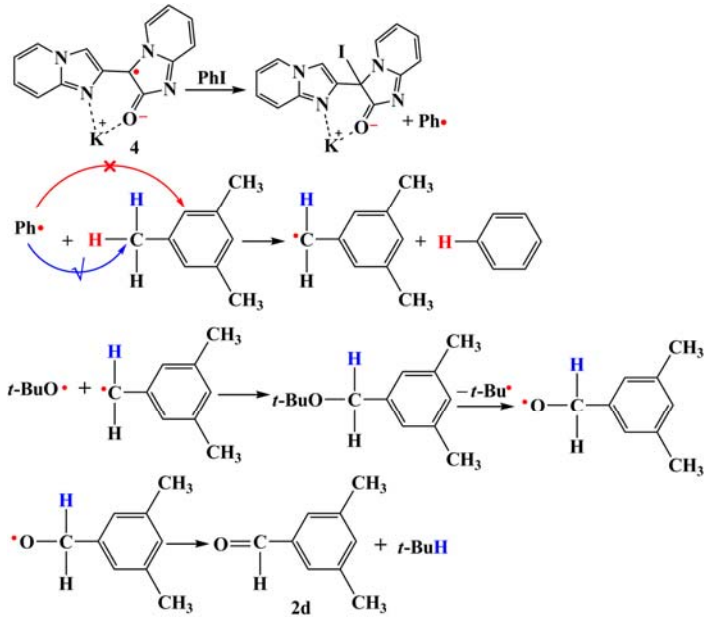


Scheme S2 A proposed SET mechanism catalyzed by neutral **Rad-B**.

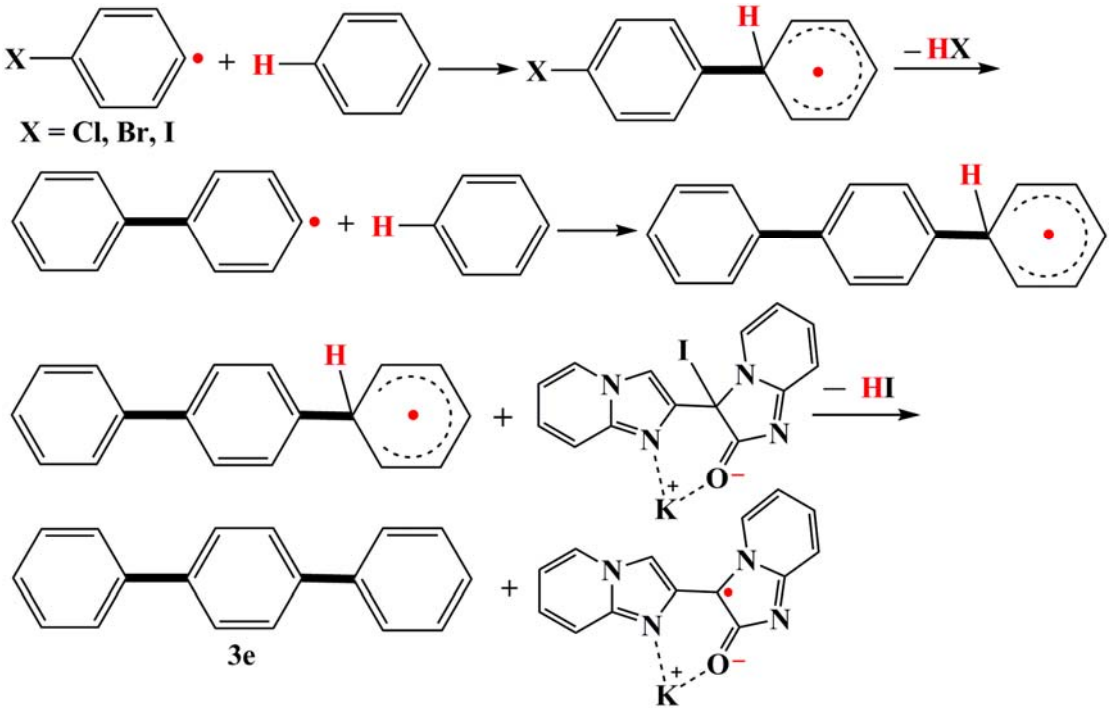


Scheme S3 Proposed mechanism for *m*-CPBA promoted ring-opening reaction of Hbipo$^{-\bullet}$.

The dihedral angle between imidazo[1, 2-*a*]pyridine ring and pyridine ring is 7.57°, showing they are almost coplanar. In **Rad-B**, 2-oxo-acetamide moiety displays interesting valent bond character from crystal structure analysis. The C–C bond length between two carbonyl carbon atom is 1.545(5) Å, typical of C–C σ signal bond; the C–O distance of two carbonyl is 1.216(5) and 1.226(5) Å, respectively, typical length of C=O bond. However, the C–N distance of amide moiety is 1.342(5) Å, typical distance of conjugated C=N bond. These valent bond characters indicate signal electron does not center on nitrogen atom of amide moiety as aminyl radical but delocalize in three atoms (C, N and O) of amide moiety as a stable amide radical (Scheme S3), which can be demonstrated by its isotropic EPR signal (g = 2.000, see Fig. S1).



Scheme S4 The possible mechanism for forming 3,5-dimethylbenzaldehyde from mesitylene catalyzed by Hbipo$^{-\bullet}$ radical.



Scheme S5 A HAS mechanism for formation of *p*-terphenyl **3e**.

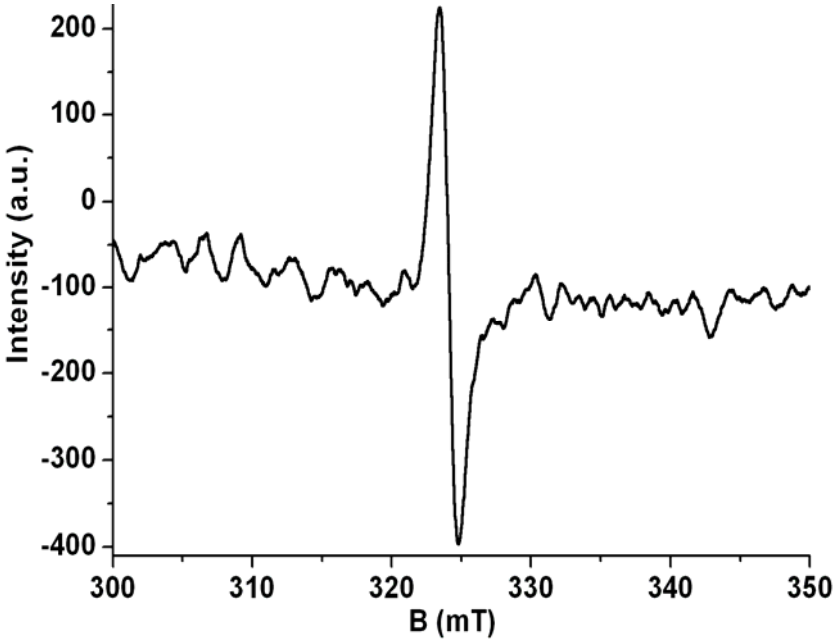


Fig. S1 Solid-state EPR spectrum of **Rad-B** at room temperature.

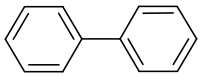
References

S1 G. P. Yong, C. F. Li, Y. Z. Li and S. W. Luo, *Chem. Commun.*, 2010, **46**, 3194.

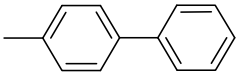
S2 G. M. Sheldrick, *SHELX-97, Programs for Crystal Structure Solution and Refinement*, University of Göttingen, Germany, 1997.

S3 E. Shirakawa, K. Itoh, T. Higashino and T. Hayashi, *J. Am. Chem. Soc.*, 2010, **132**, 15537.

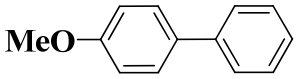
The spectroscopic data of all the products are presented below. All the known compounds gave satisfactory spectroscopic values and accorded to spectroscopic data reported in the literatures.



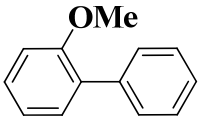
Biphenyl (3a) [1]: A white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.62 (d, J = 8.2 Hz, 4H), 7.51–7.41 (t, J = 7.6 Hz, 4H), 7.36 (t, J = 7.2 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 127.1, 127.2, 128.7, 141.2. MS (EI): Calcd for $C_{12}H_{10}$ (M^+): 154.08. Found: 154 (M^+).



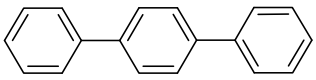
4-Methylbiphenyl (3b) [1]: A white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.58 (d, J = 7.2 Hz, 2H), 7.50 (d, J = 8.0 Hz, 2H), 7.43 (t, J = 7.4 Hz, 2H), 7.33 (t, J = 7.3 Hz, 1H), 7.25 (d, J = 8.0 Hz, 2H), 2.40 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 21.1, 126.9, 128.7, 129.4, 137.0, 138.3, 141.1. MS (EI): Calcd for $C_{13}H_{12}$ (M^+): 168.09. Found: 168 (M^+).



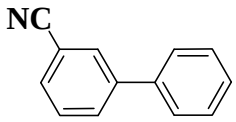
4-Methoxybiphenyl (3c) [1]: A white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.55 (t, J = 7.2 Hz, 4H), 7.43 (t, J = 7.6 Hz, 2H), 7.33 (d, J = 7.3 Hz, 1H), 6.99 (d, J = 8.7 Hz, 2H), 3.86 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 55.3, 114.1, 126.6, 126.7, 128.1, 128.7, 133.8, 140.8, 159.0. MS (EI): Calcd for $C_{13}H_{12}O$ (M^+): 184.09. Found: 184 (M^+).



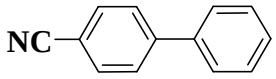
2-Methoxybiphenyl (3d) [1]: A colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.52 (dt, *J* = 8.2, 1.7 Hz, 2H), 7.42–7.36 (m, 2H), 7.34–7.26 (m, 3H), 7.04–6.93 (m, 2H), 3.78 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 55.4, 111.1, 120.7, 126.8, 127.9, 128.5, 129.4, 130.8, 138.4, 156.4. MS (EI): Calcd for $C_{13}H_{12}O$ (M^+): 184.09. Found: 184 (M^+).



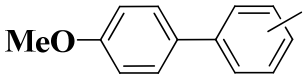
***p*-Terphenyl (3e) [1]:** A white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.84–7.58 (m, 8H), 7.48 (t, J = 7.7 Hz, 4H), 7.38 (t, J = 7.3 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 127.0, 127.3, 127.5, 128.8, 140.1, 140.7. MS (EI): Calcd for $C_{18}H_{14}$ (M^+): 230.11. Found: 230 (M^+).



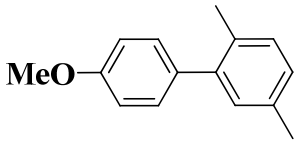
3-Cyanobiphenyl (3f) [2]: A colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.88–7.74 (m, 2H), 7.64–7.38 (m, 7H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 112.9, 118.8, 127.0, 128.3, 129.0, 129.5, 130.8, 131.4, 138.7, 142.3. MS (EI): Calcd for $C_{13}H_9N$ (M^+): 179.07. Found: 179 (M^+).



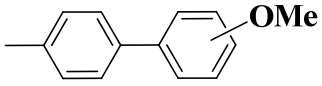
4-Cyanobiphenyl (3g) [1]: A pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.77–7.66 (m, 4H), 7.62–7.39 (m, 5H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 111.0, 118.9, 127.2, 127.7, 128.6, 129.1, 139.2, 145.7. MS (EI): Calcd for $C_{13}H_9N$ (M^+): 179.07. Found: 179 (M^+).



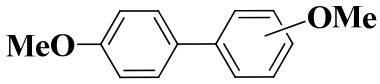
Mixture of 4'-Methoxy-2-methylbiphenyl, 4'-Methoxy-3-methylbiphenyl and 4'-Methoxy-4-methylbiphenyl (3h) [1]: A white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.56–7.07 (6H), 6.96 (2H), 3.85 (3H), 2.41–2.28 (3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 20.5, 20.7, 21.0, 55.2, 55.3, 55.4, 113.5, 114.1, 114.2, 123.9, 125.7, 126.5, 127.0, 127.9, 128.1, 128.6, 129.4, 129.9, 130.2, 130.3, 135.4, 158.5, 158.9, 159.1. MS (EI): Calcd for $C_{14}H_{14}O$ (M^+): 198.10. Found: 198 (M^+).



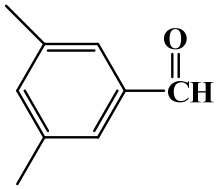
2,5-Dimethyl-4'-methoxybiphenyl (3i) [1]: A light yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.24 (d, J = 8.7 Hz, 2H), 7.14 (d, J = 8.2 Hz, 1H), 7.04 (d, J = 5.3 Hz, 2H), 6.93 (d, J = 8.7 Hz, 2H), 3.83 (s, 3H), 2.33 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 20.0, 20.9, 55.2, 113.4, 127.6, 129.0, 130.2, 130.6, 132.2, 134.5, 135.1, 141.3, 158.4. MS (EI): Calcd for $C_{15}H_{16}O$ (M^+): 212.12. Found: 212 (M^+).



Mixture of 2-Methoxy-4'-methylbiphenyl, 3-Methoxy-4'-methylbiphenyl and 4-Methoxy-4'-methylbiphenyl (3j)[1]: A colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.56–7.38 (2H), 7.41–7.04 (4H), 7.12–6.77 (2H), 3.88–3.77 (3H), 2.39 (3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 21.0, 21.1, 21.2, 55.2, 55.3, 55.5, 111.2, 112.4, 112.7, 114.1, 114.8, 114.9, 119.5, 120.6, 120.8, 126.5, 127.0, 127.9, 128.3, 128.7, 129.4, 129.4, 129.7, 130.7, 136.5, 156.5, 158.9, 159.9. MS (EI): Calcd for $C_{14}H_{14}O$ (M^+): 198.10. Found: 198 (M^+).



Mixture of 2,4'-Dimethoxybiphenyl, 3,4'-Dimethoxybiphenyl and 4,4'-Dimethoxybiphenyl (3k) [1]: A white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.47 (2H), 7.2–6.81 (6H), 3.82–3.78 (6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 55.2, 55.3, 55.5, 111.2, 112.0, 112.5, 113.5, 114.1, 119.2, 120.8, 127.7, 128.1, 128.2, 130.6, 130.7, 130.9, 142.4, 156.4, 158.6, 158.7, 159.2, 159.9. MS (EI): Calcd for $C_{14}H_{14}O_2$ (M^+): 214.10. Found: 214 (M^+).

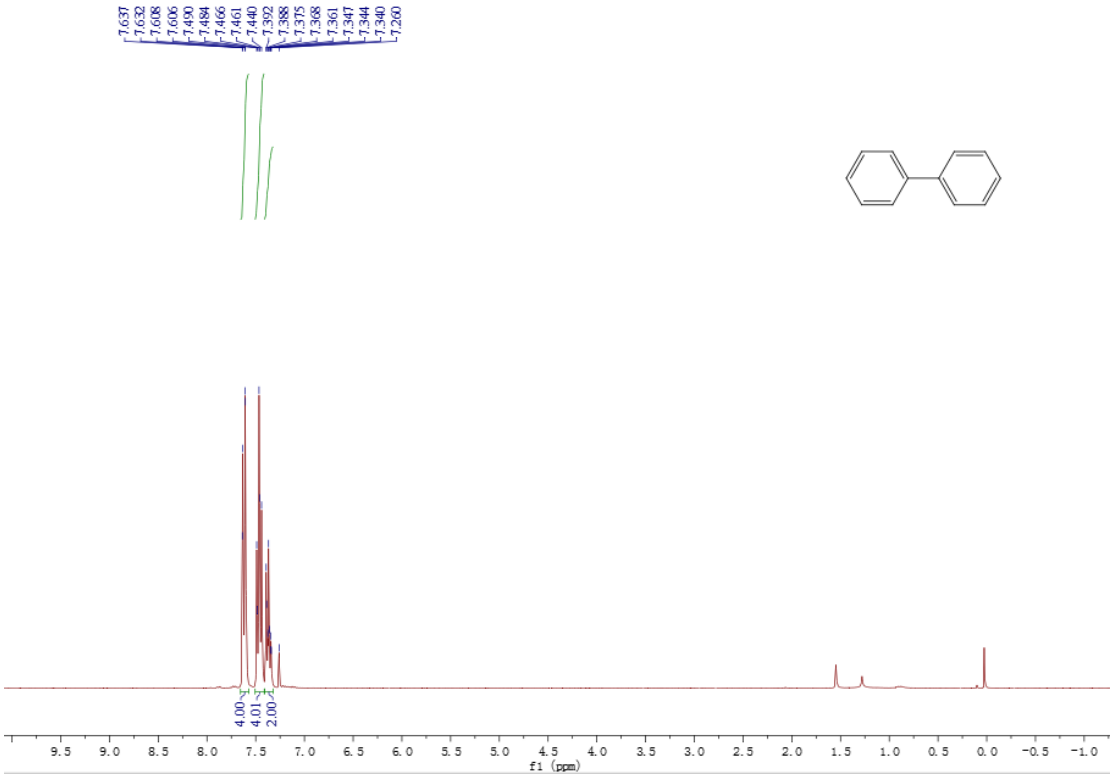


3,5-Dimethylbenzaldehyde (2d): A colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ = 9.85 (s, 1H), 7.40 (s, 2H), 7.17 (s, 1H), 2.30 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 192.8, 138.8, 136.6, 136.2, 127.6, 21.1. Calcd for $C_9H_{10}O$ (M^+): 134.07. Found: 134 (M^+).

References:

[1] (*a*) C. L. Sun, H. Li, D. G. Yu, M. Yu, X. Zhou, X. Y. Lu, K. Huang, S. F. Zheng, B. J. Li and Z. J. Shi, *Nature Chem.*, 2010, **2**, 1044; (*b*) F. Vallée, J. J. Mousseau and A. B. Charette, *J. Am. Chem. Soc.*, 2010, **132**, 1514; (*c*) E. Shirakawa, K. I. Itoh, T. Higashino and T. Hayashi, *J. Am. Chem. Soc.*, 2010, **132**, 15537; (*d*) W. Liu, H. Cao, H. Zhang, H. Zhang, K. H. Chung, C. He, H. Wang, F. Y. Kwong and A. W. Lei, *J. Am. Chem. Soc.*, 2010, **132**, 16737.

[2] (*a*) L. Wang, Y. H. Zhang, L. F. Liu and Y. G. Wang, *J. Org. Chem.*, 2006, 71, 1284; (*b*) W. M. Dai, Y. N. Li, Y. Zhang, C. Y. Yue and J. L. Wu, *Chem. Eur. J.*, 2008, **14**, 5538; (*c*) W. J. Zhou, K. H. Wang and J. X. Wang, *J. Org. Chem.*, 2009, **74**, 5599.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7.606
7.490
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7.466
7.461
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7.392
7.388
7.375
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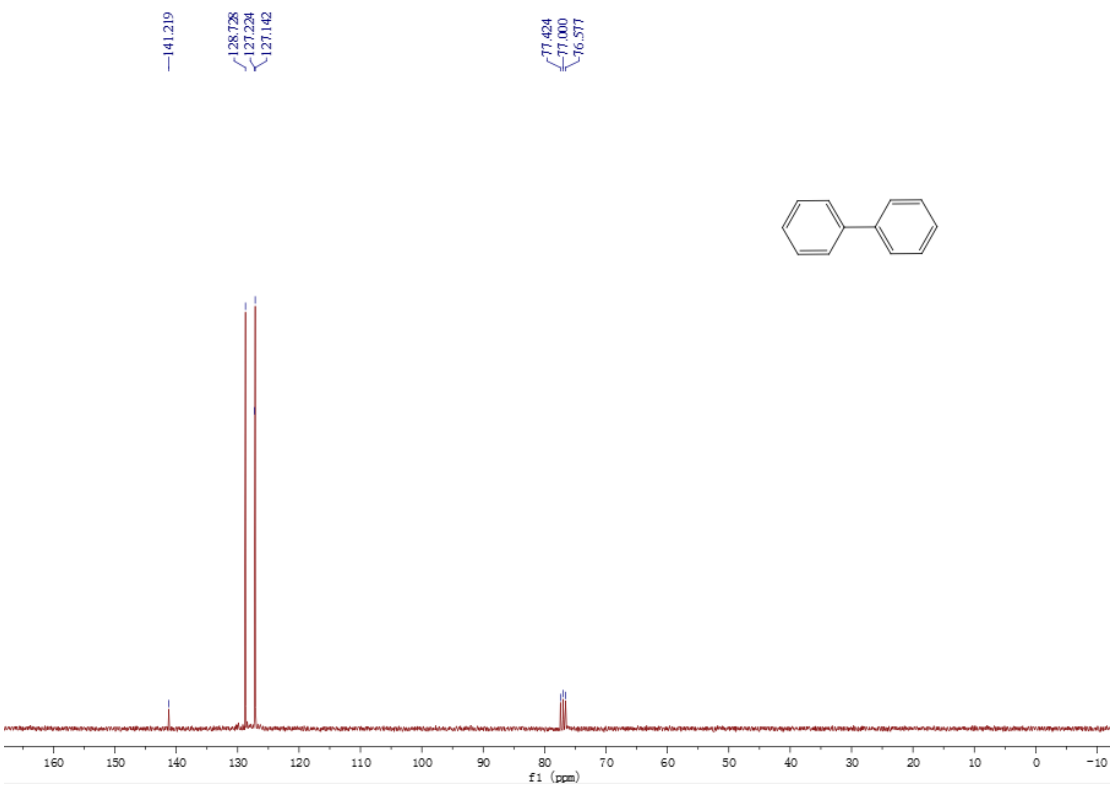
7.361
7.347
7.344
7.340
7.260
4.00
4.01
2.00
f1 (ppm)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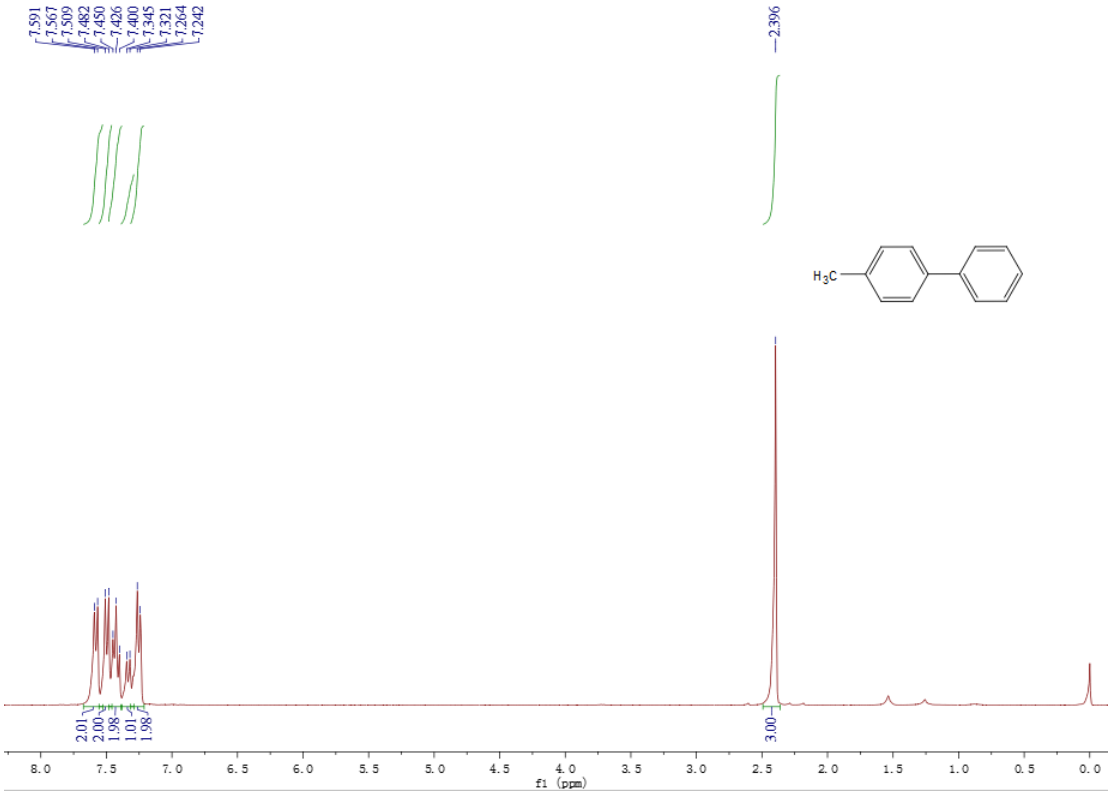
f1 (ppm)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7.567
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7.426
7.400
7.345
7.321
7.264
7.242
2.396
H3C
2.01
2.00
1.98
1.01
1.98
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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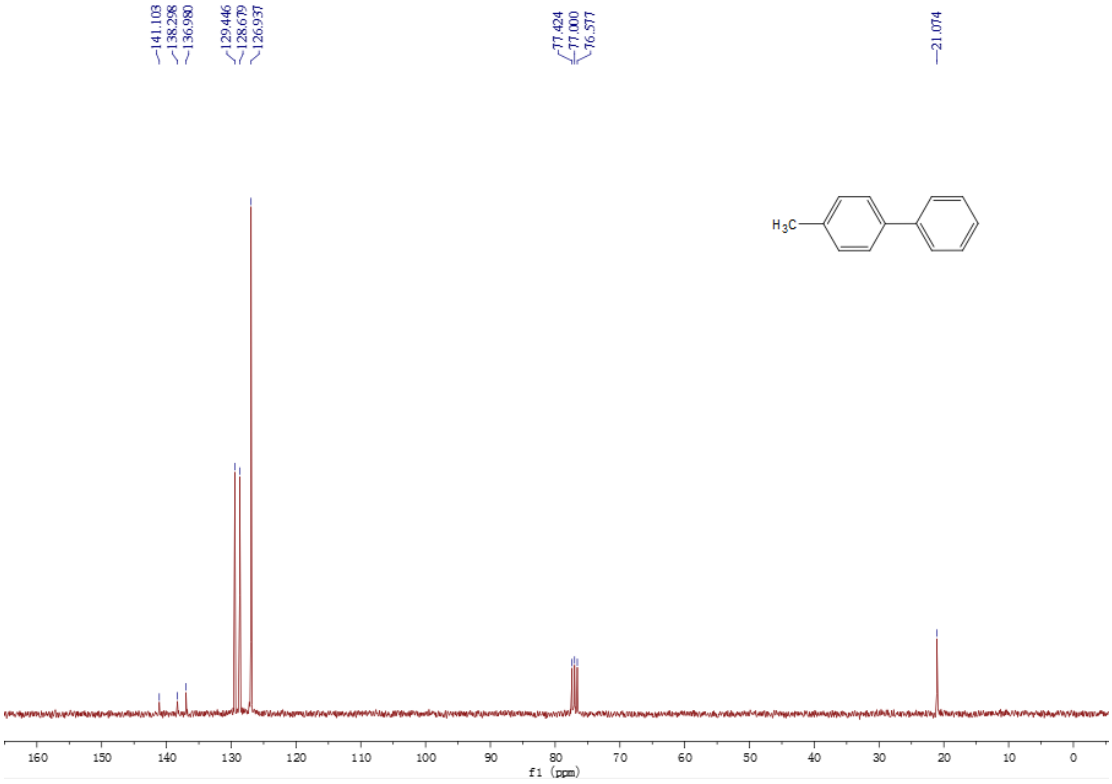
0.0
f1 (ppm)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136.980
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126.937
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77.000
76.577
21.074
H3C
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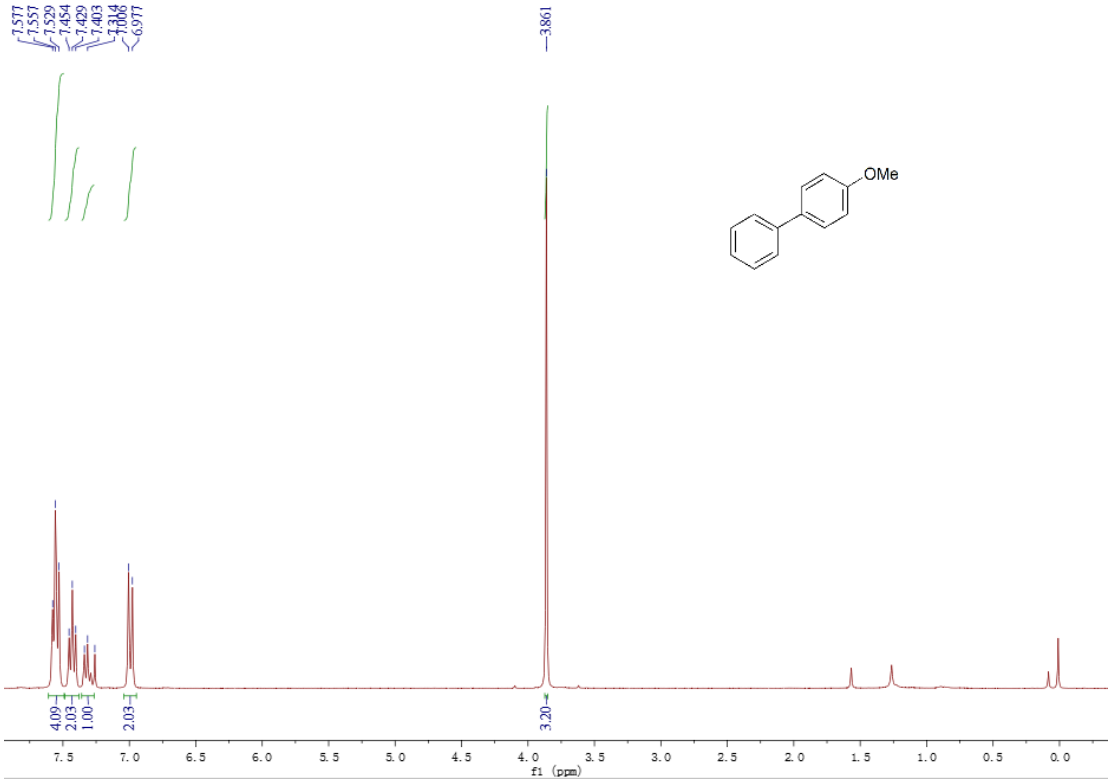
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.454
7.429
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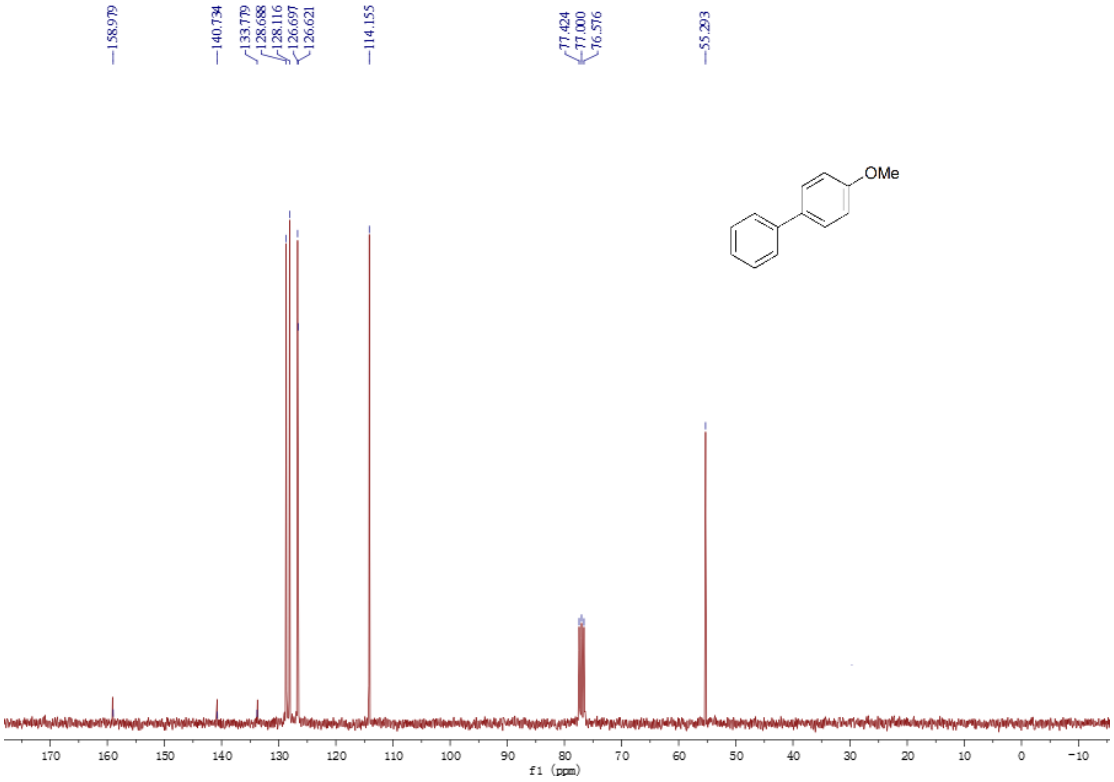
OMe
4.09
2.03
1.00
2.03
3.20
f1 (ppm)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77.424
77.000
76.576
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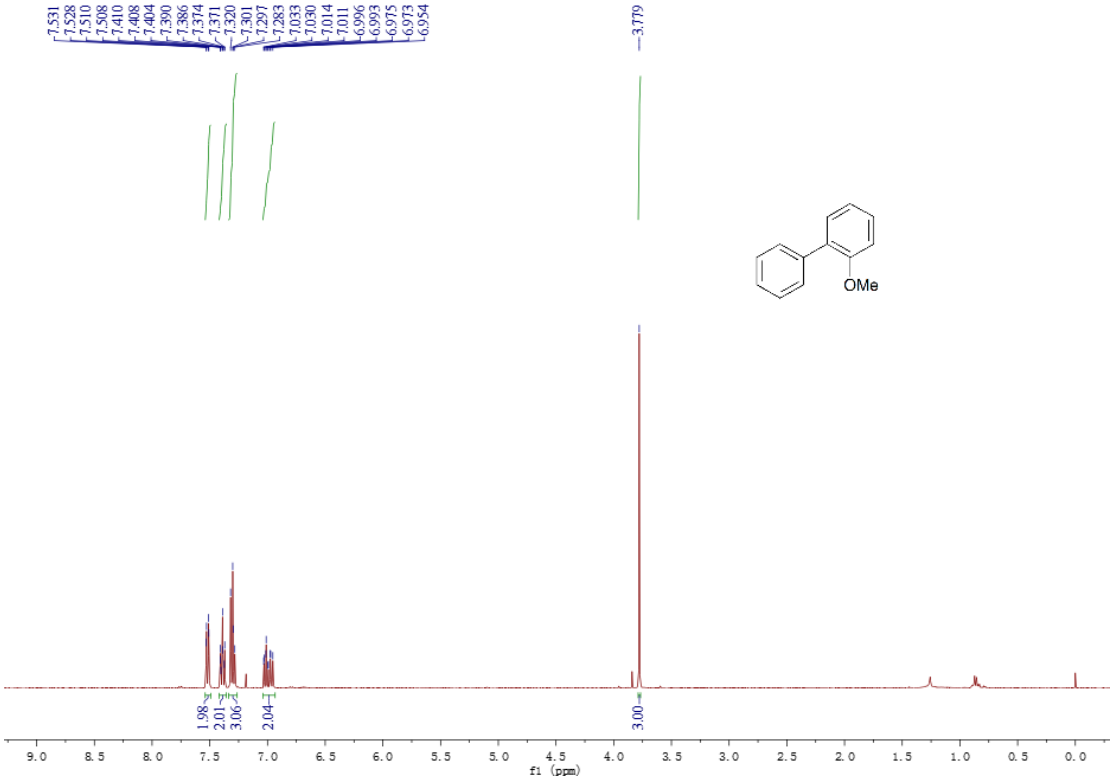
OMe
f1 (ppm)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7.410
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7.390
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7.297
7.283
7.033
7.030
7.014
7.011
6.996
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OMe
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3.06
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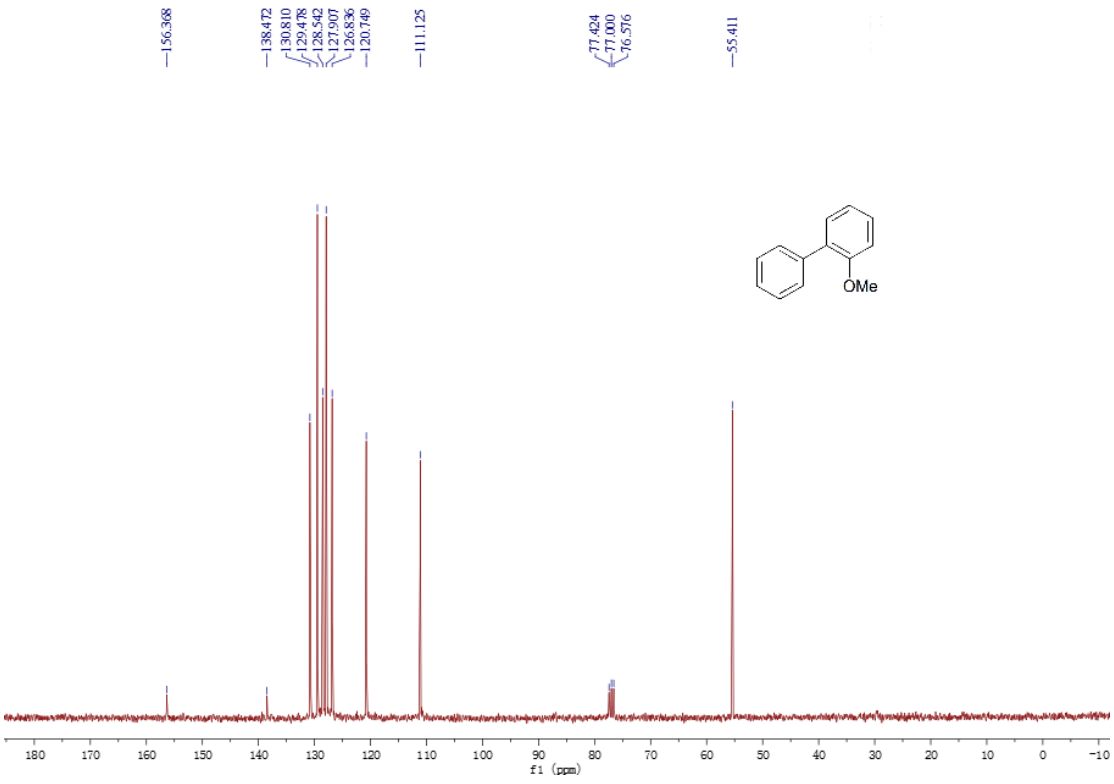
3.00
f1 (ppm)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77.000
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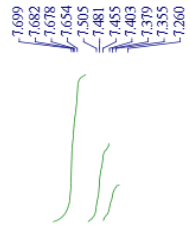
OMe
f1 (ppm)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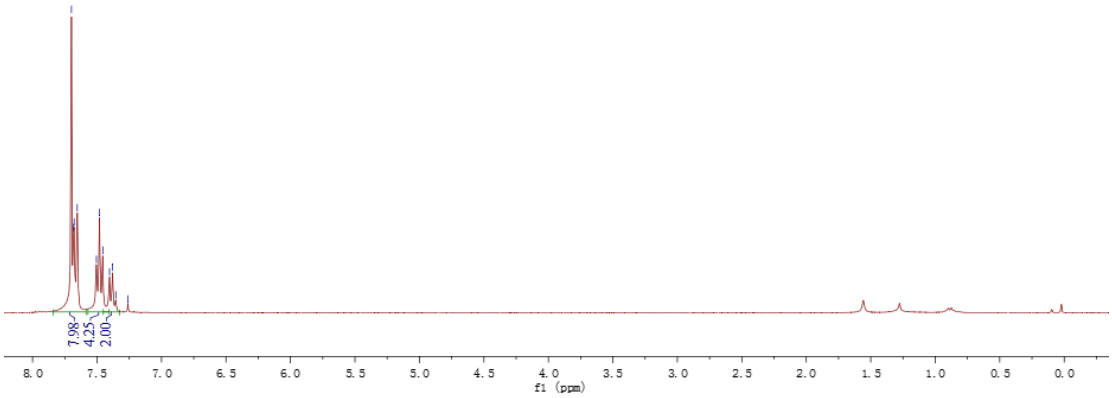
7.403
7.379
7.355
7.260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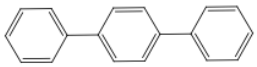
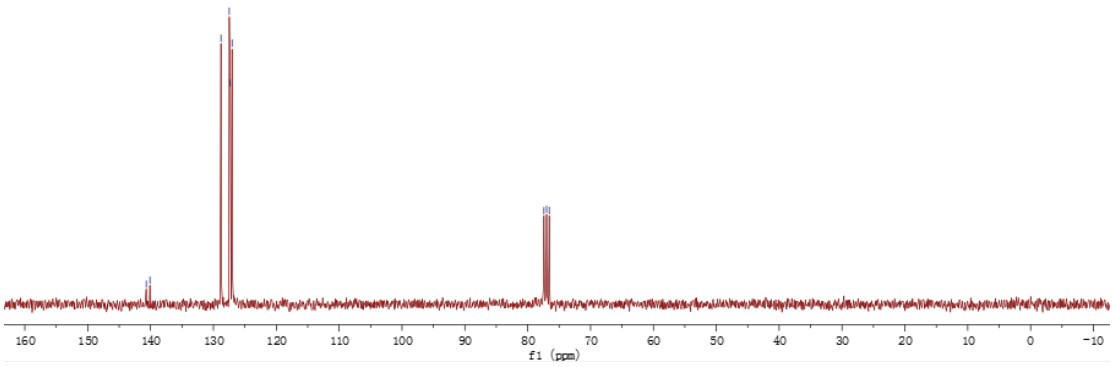
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


140.690
140.106

128.800
127.484
127.325
127.035


77.422
77.000
76.577

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140
130
120
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100
90
80
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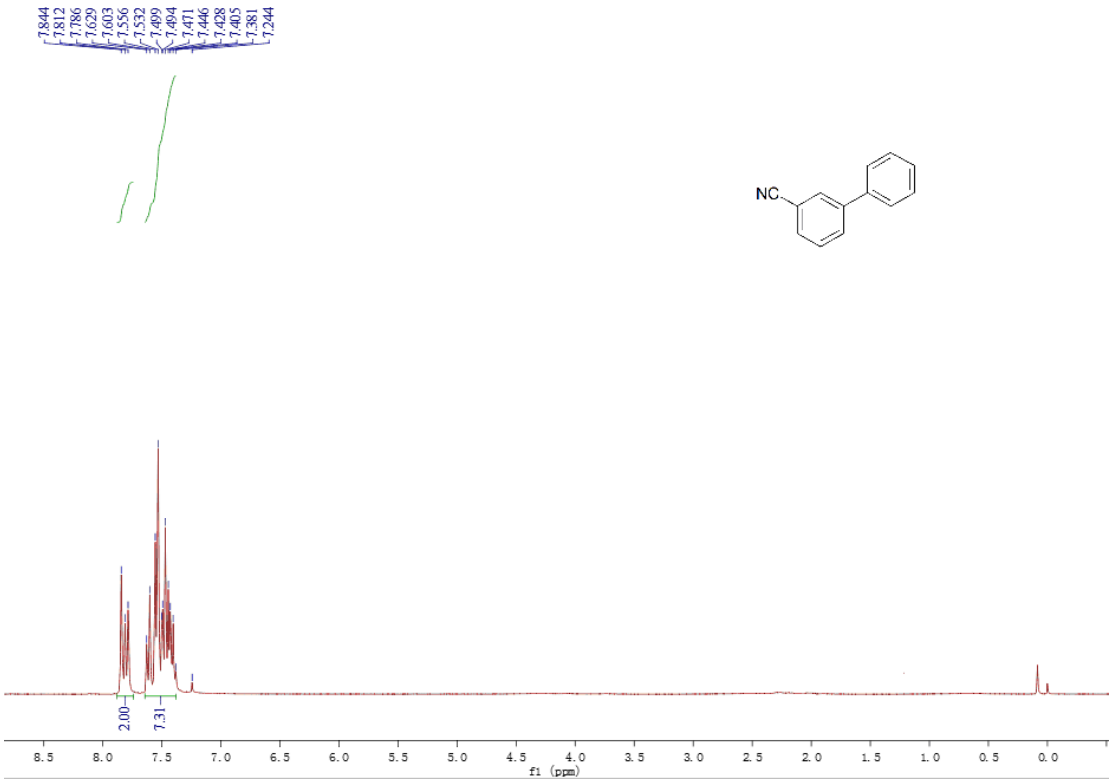
60
50
40
30
20
10
0
-10
f1 (ppm)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7.405
7.381
7.244
NC
2.00
7.31
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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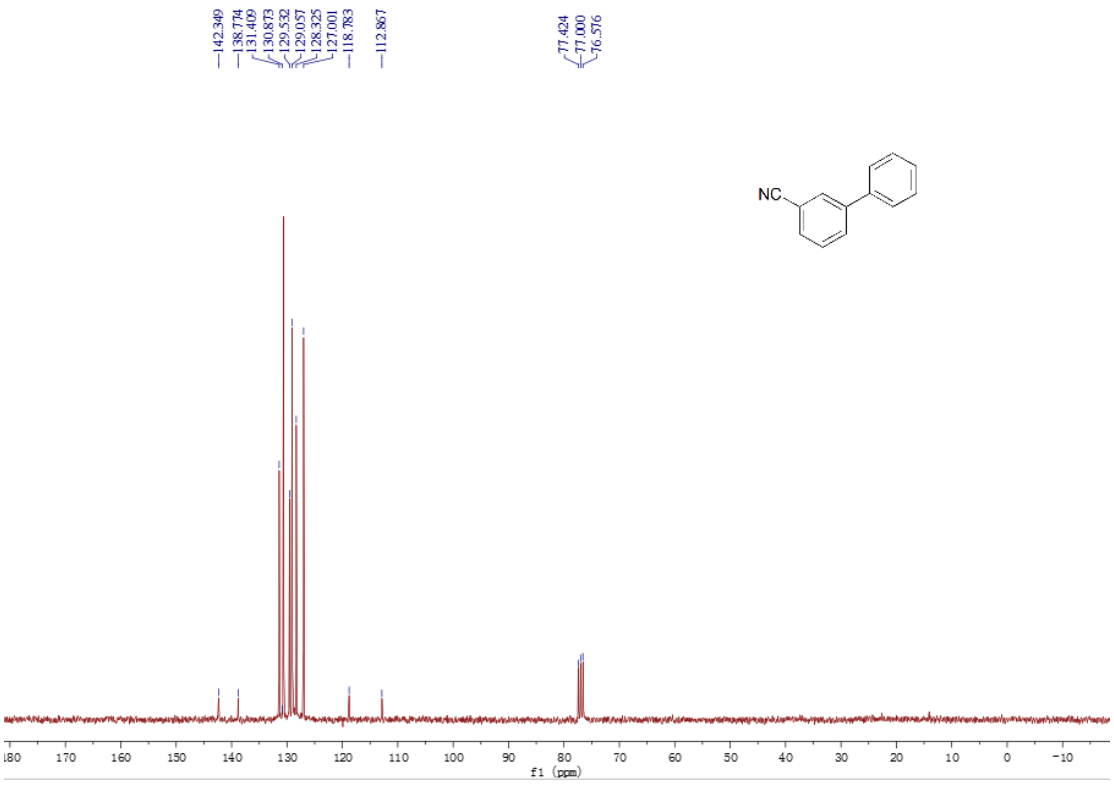
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.057
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112.867
77.424
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76.576
NC
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.747
7.744
7.742
7.739
7.727
7.722
7.719
7.701
7.698
7.693
7.682
7.678
7.676
7.673
7.606
7.602
7.597
7.589
7.585
7.582
7.576
7.509
7.506
7.501
7.493
7.488
7.484
7.473
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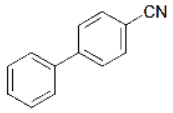
7.420
7.412
7.409
7.405
7.260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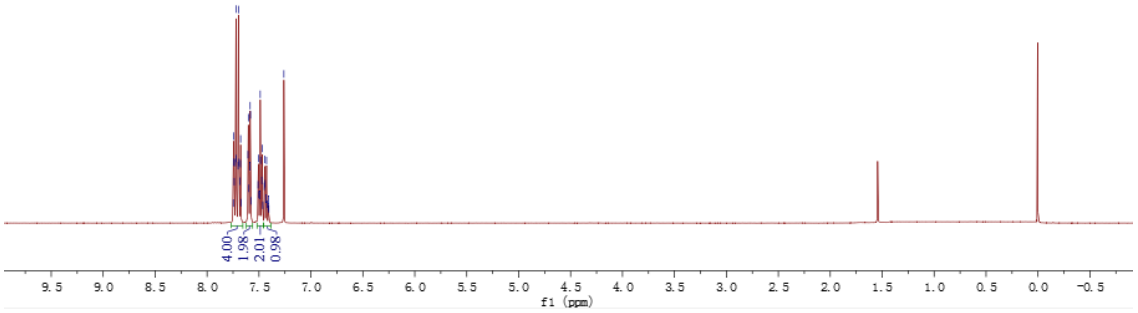
4.00
1.98
2.01
0.98
f1 (ppm)


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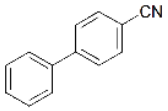
77.000
76.682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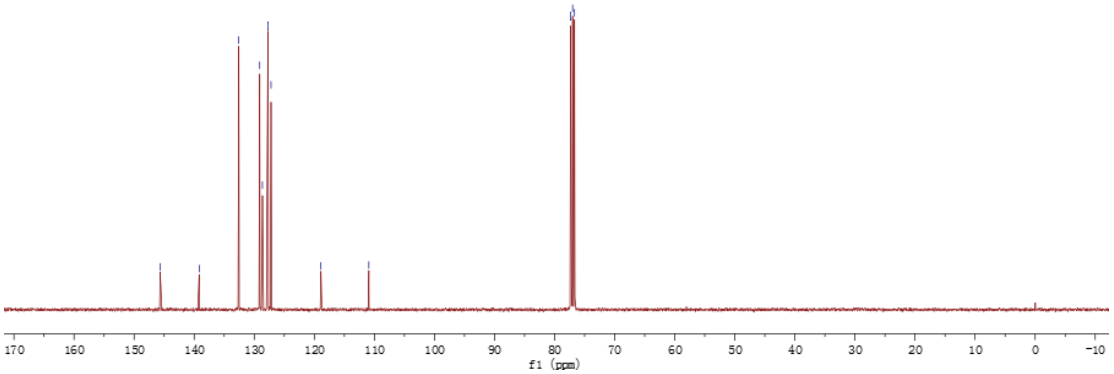
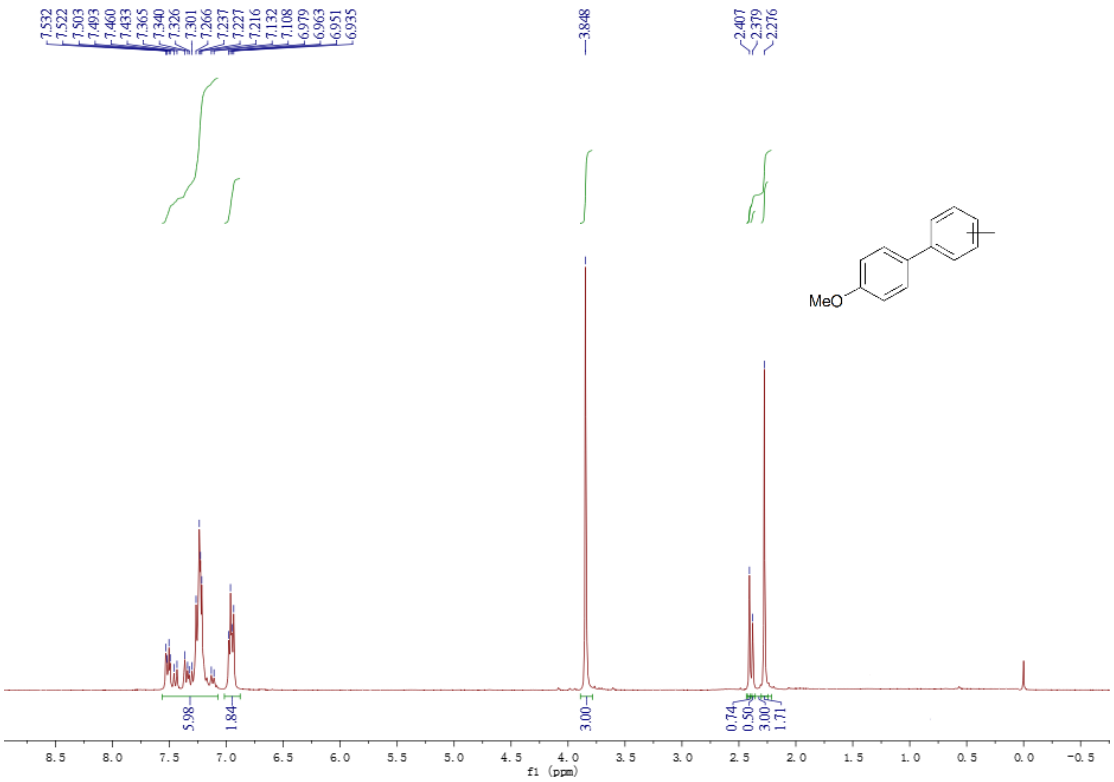

f1 (ppm)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7.340
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7.301
7.266
7.237
7.227
7.216
7.132
7.108
6.979
6.963
6.951
6.935
3.848
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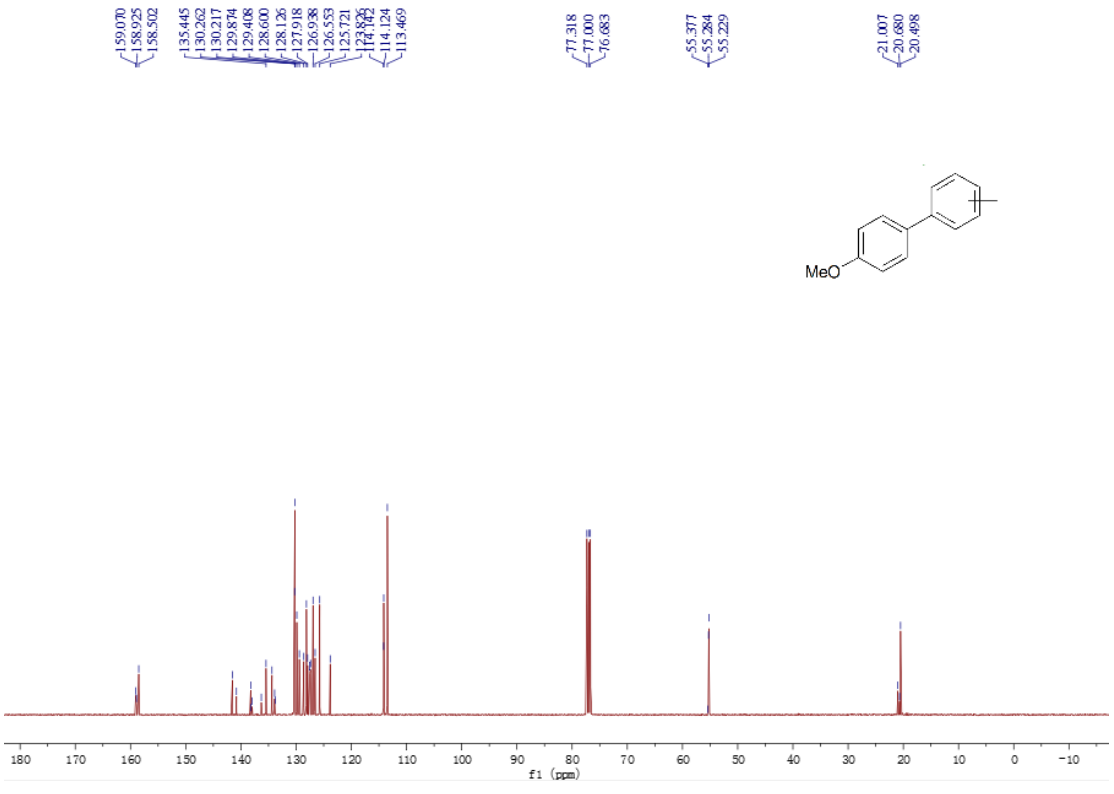
0.50
3.00
1.71
f1 (ppm)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126.938
126.553
125.721
123.826
114.142
114.124
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77.318
77.000
76.683
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55.284
55.229
21.007
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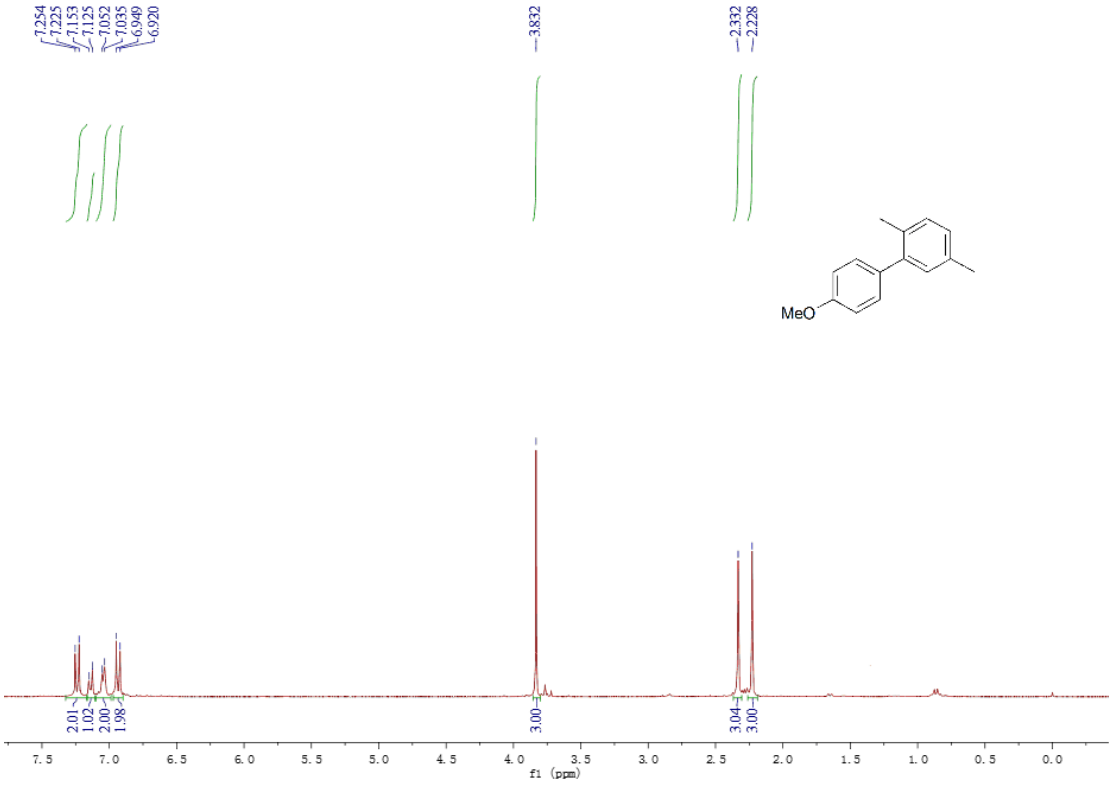
20.498
MeO
f1 (ppm)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7.035
6.949
6.920
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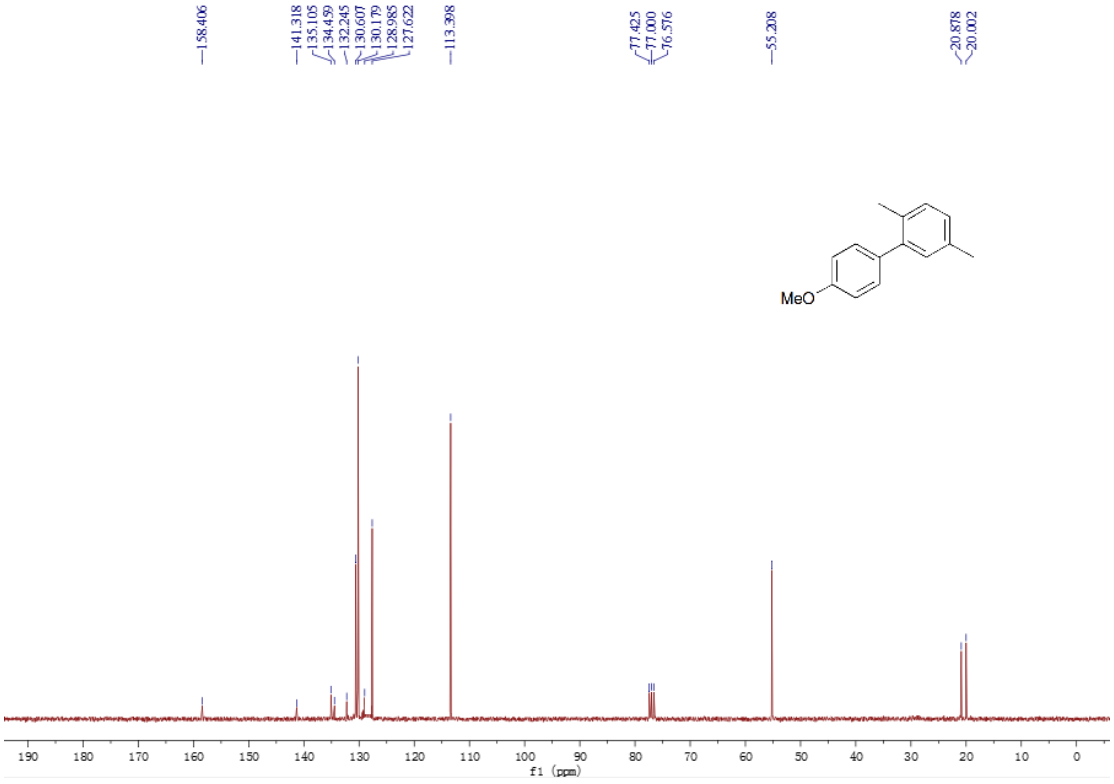
3.00
3.04
3.00
f1 (ppm)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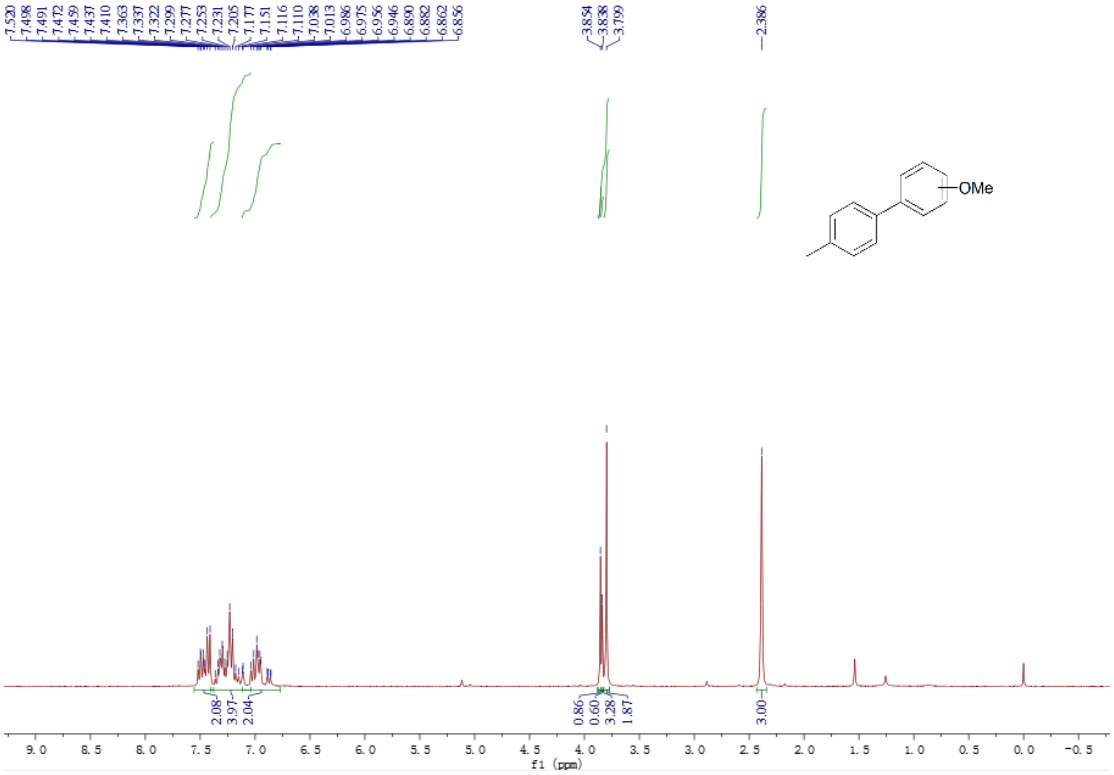
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7.322
7.299
7.277
7.253
7.231
7.205
7.177
7.151
7.116
7.110
7.038
7.013
6.986
6.975
6.956
6.946
6.890
6.882
6.862
6.856
3.854
3.838
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2.04
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0.60
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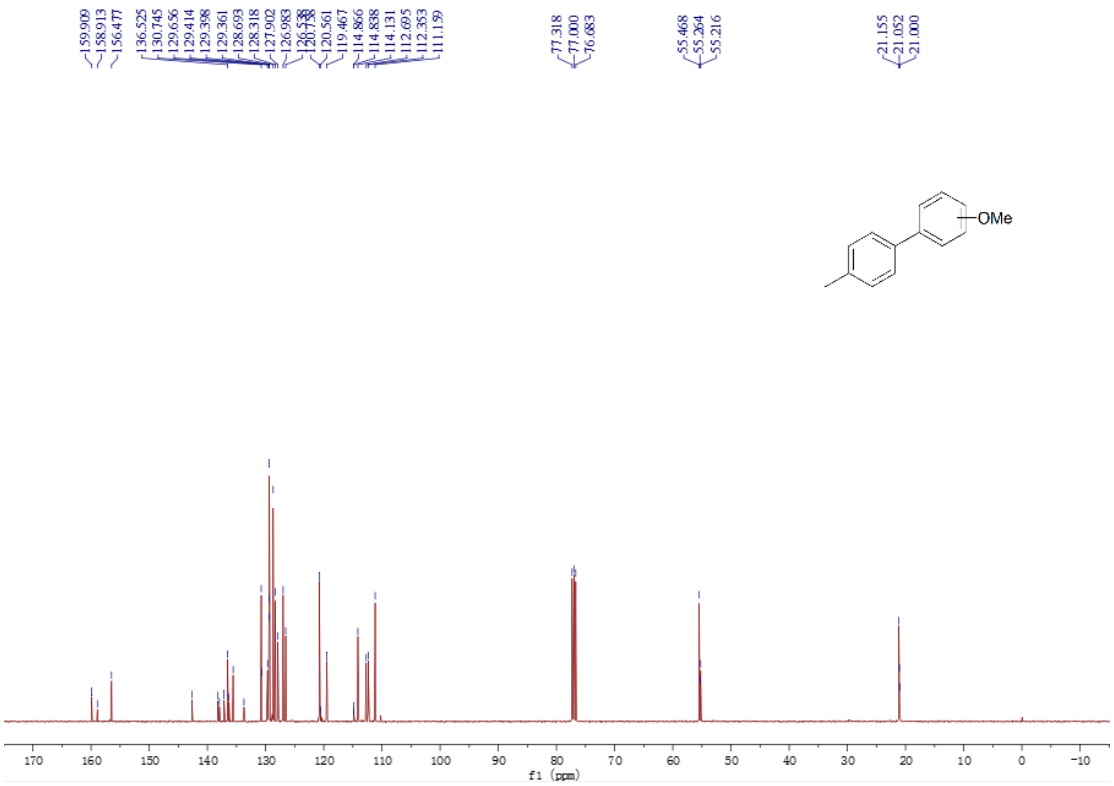
3.00
f1 (ppm)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120.561
119.467
114.866
114.838
114.131
112.695
112.353
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76.683
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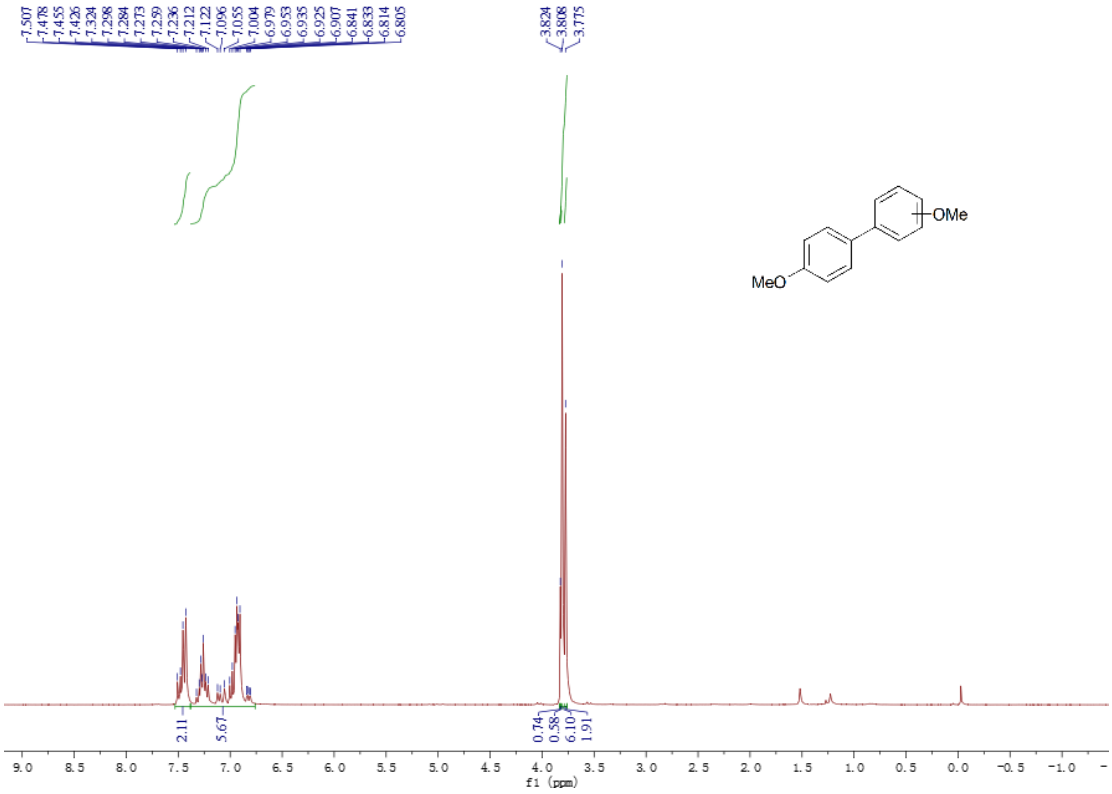
55.264
55.216
21.155
21.052
21.000
OMe
f1 (ppm)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7.212
7.122
7.096
7.055
7.004
6.979
6.953
6.935
6.925
6.907
6.841
6.833
6.814
6.805
3.824
3.808
3.775
OMe
MeO
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0.58
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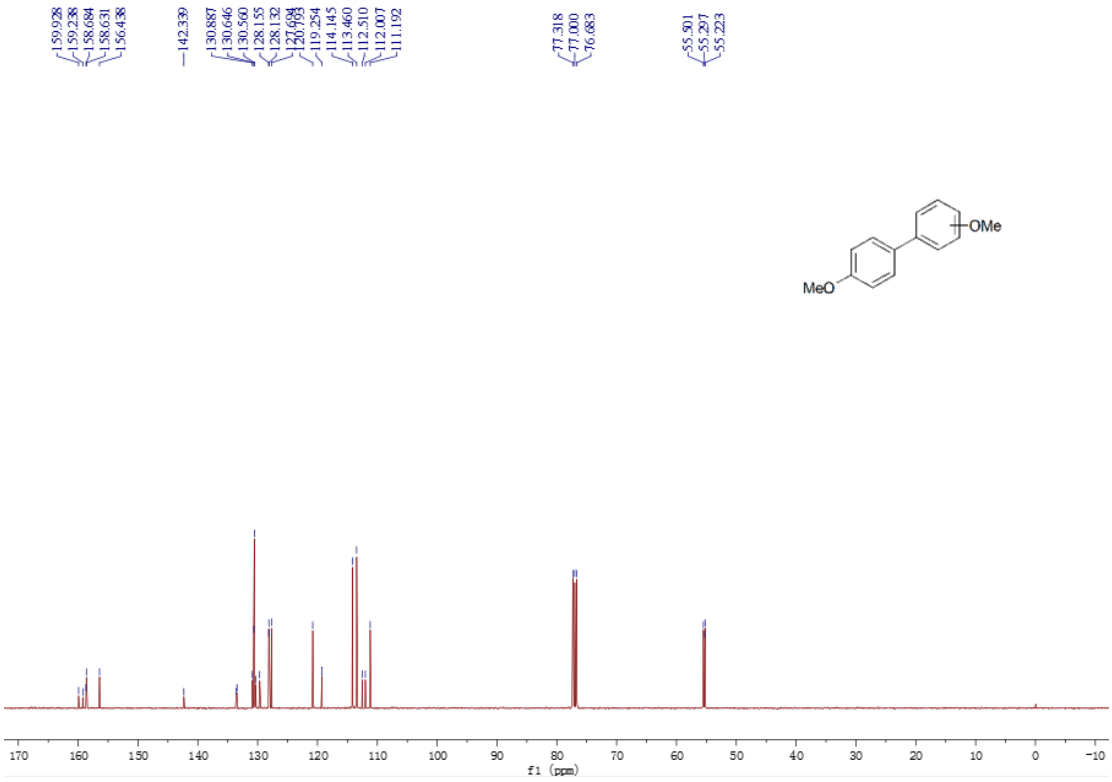
1.91
f1 (ppm)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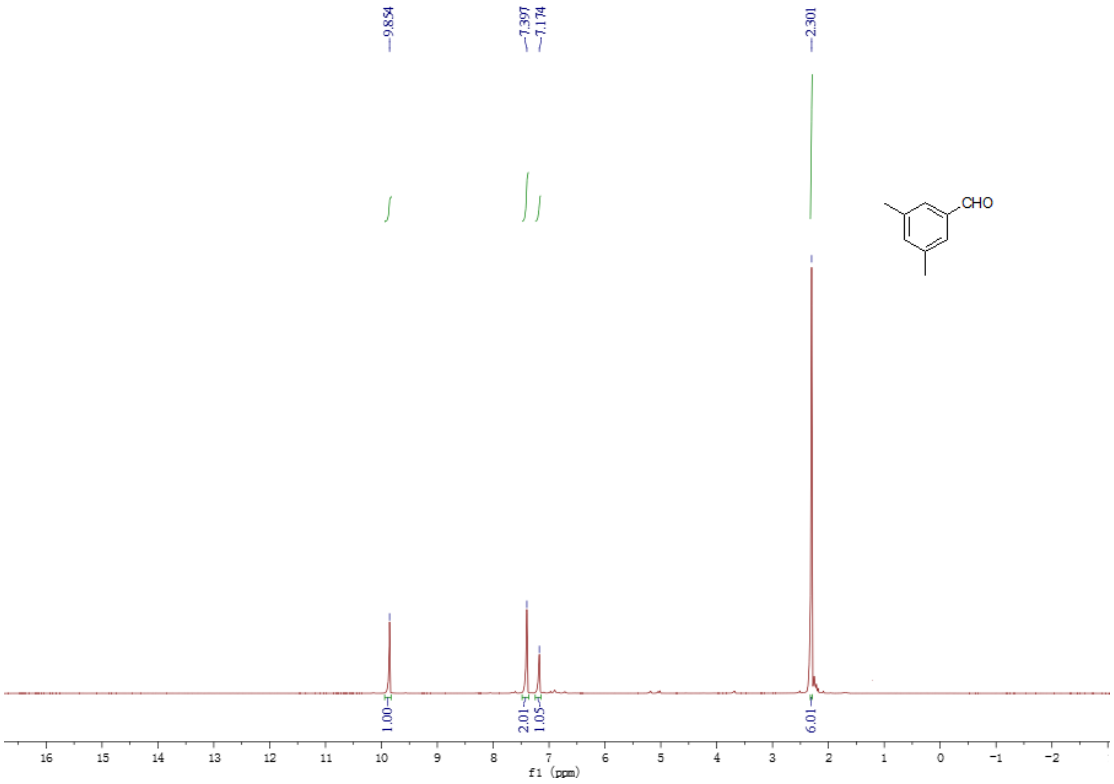
128.132
127.694
120.793
119.254
114.145
113.460
112.510
112.007
111.192
77.318
77.000
76.683
55.301
55.297
55.223
OMe
MeO
f1 (ppm)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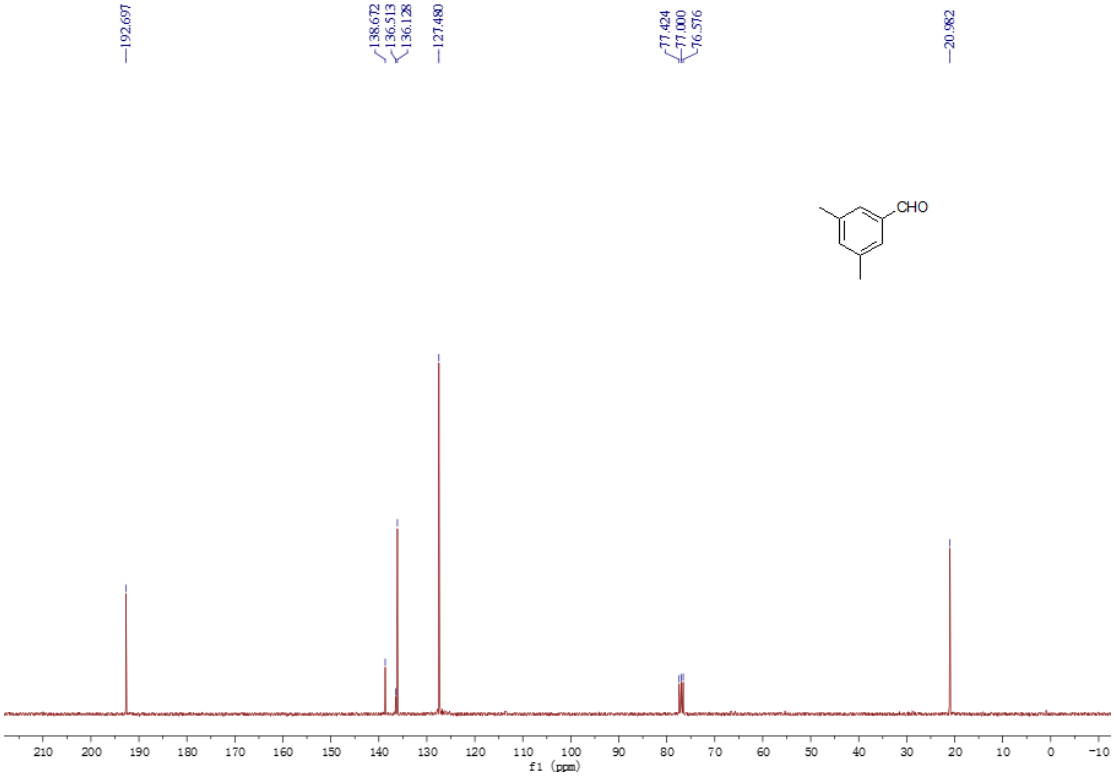
1.05
6.01
f1 (ppm)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77.424
77.000
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CHO
f1 (ppm)