Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting information for

Direct allylation of benzaldehydes via Copper-catalyzed domino Knoevenagel-decarboxylation-sp3-C-H-activation sequence

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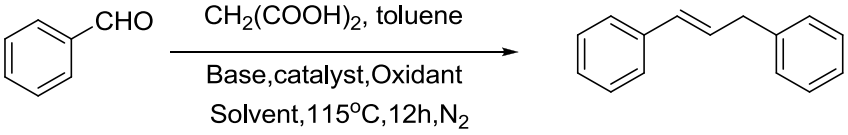
General Information: All reactions were carried out under an N_2 atmosphere condition. CuO was purchased from Aladdin-reagent with high purity (99.5%). All reagents were used as supplied without further purified and dried. Flash column chromatography was performed over silica gel 48-75 μm and reactions were monitored by thin layer chromatography (TLC) using UV light (254 nm). ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded on a BrukerAvance 400 MHz NMR spectrometer using d_6-DMSO as solvent and tetramethylsilane as internal standard (s = singlet, d = doublet, t = triplet, m = multiplet). MS analyses were performed on Agilent 5975 GC-MS instrument (EI). HRMS analyses were performed on Waters Micromass GCT instrument (EI).

General procedures for Copper-catalyzed allylation of benzaldehydes. Malonic (52 mg, 0.5 mmol) and CuO (4.8 mg, 0.06 mol) were added into a 10 mL Schlenk flask. Then toluene (2 mL), benzaldehyde (31 μl, 0.3 mmol), DTBP (120 μl, 1.2mmol), piperidine(20 μl, 0.2 mmol) were added at room temperature. The reaction vessel was purged with N_2 for three times. The mixture was stirred at 125 ℃ for 12 h. After cooling to room temperature, the mixture was diluted with CH_2Cl_2 and water. The organic phase was washed with brine, dried with $MgSO_4$, and concentrated under reduced pressure. The residue was purified by silica gel chromatography (petroleum ether/ethyl acetate = 100 : 1) to afford the corresponding product.

Experimental data:

Table S1 : Optimization of reaction conditions.[a]

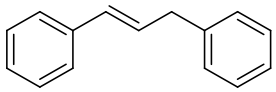


entry	catalyst	oxidant	base	solvent	yield[b](%)
1	CuO	DTBP	piperidine	toluene	68
2	$CuBr_2$	DTBP	piperidine	toluene	53
3	$CuCl_2$	DTBP	piperidine	toluene	22
4	$Cu(OAc)_2$	DTBP	piperidine	toluene	40
5	$CuSO_4$	DTBP	piperidine	toluene	38
6	CuI	DTBP	piperidine	toluene	50
7	Cu_2O	DTBP	piperidine	toluene	21
8	CuCl	DTBP	piperidine	toluene	34
9	CuBr	DTBP	piperidine	toluene	38
10	Cu	DTBP	piperidine	toluene	44
11	Fe_3O_4	DTBP	piperidine	toluene	30
12	Ferrocene	DTBP	piperidine	toluene	42
13	CuO	DCP	piperidine	toluene	48
14	CuO	H_2O_2	piperidine	toluene	NR
15	CuO	PhCOOOtBu	piperidine	toluene	33
16	CuO	TBHP	piperidine	toluene	24
17	CuO	DTBP	DBU	toluene	11
18	CuO	DTBP	Triethylamine	toluene	5
19	CuO	DTBP	-	toluene	trace
20[c]	CuO	DTBP	piperidine	toluene	43
21[d]	CuO	DTBP	piperidine	toluene	69
22	CuO	DTBP	piperidine 0.1mmol	toluene	8
23	CuO	DTBP	piperidine 0.3mmol	toluene	65

24	CuO	DTBP	piperidine 0.5mmol	toluene	36
25	CuO	DTBP	piperidine	DMF	trace
26	CuO	DTBP	piperidine	DMSO	trace
27	CuO	DTBP	piperidine	NMP	trace
28	CuO	DTBP	piperidine	chlorobenzene	trace
29	CuO	DTBP 2.0equiv	piperidine	toluene	33
30	CuO	DTBP 6.0equiv	piperidine	toluene	40
31[e]	CuO105 ^{o}C	DTBP	piperidine	toluene	NR
32[f]	CuO125 ^{o}C	DTBP	piperidine	toluene	77
33[g]	CuO135 ^{o}C	DTBP	piperidine	toluene	69
34[h]	CuO125^{o}C	DTBP	piperidine	toluene	49
35	CuO 10mmol%	DTBP	piperidine	toluene	55
36	CuO 30mmol%	DTBP	piperidine	toluene	42
37	-	DTBP	piperidine	toluene	11

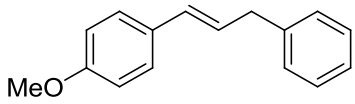
[a] Catalytic conditions: benzaldehyde (0.3 mmol), malonic (0.5mmol), toluene (0.5mmol), solvent (2 mL), base (0.2 mmol), catalyst (20mol%), oxidant (4 equiv), 115 ^{o}C (oil bath temperature, unless otherwise noted), 12h, N_2. [b] GC yields were given using dodecane as the internal standard. [c] 6h. [d] 24h. [e] 105 ^{o}C, N_2. [f] 125 ^{o}C, N_2. [g] 135 ^{o}C, N_2. [h] 125 ^{o}C, air.

Characterization of the corresponding products:



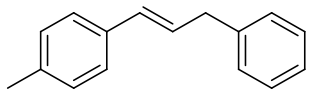
(E)-1-1, 3-diphenylpropene (3-1a).

^{1}H NMR (400 MHz, DMSO) δ 7.38 – 7.41 (m, *2*H), 7.24-7.33 (m, *6*H), 7.18 – 7.22 (m, 2H), 6.48 (d, J = 15.9 Hz, 1H), 6.46 – 6.38 (m, 1H), 3.52 (d, J = 5.8 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 140.52, 137.50, 130.99, 129.88, 129.02, 128.96, 128.92, 127.58, 126.53, 126.44, 39.06. GC/MS (m/z): $[M]^{+}$ calcd for C15H14, 194.1; found, 194.1. HRMS (EI+) calcd for C15H14 [M+]: 194.1095. Found: 194.1096.



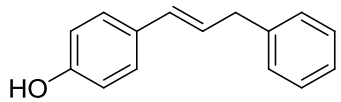
(E)-1-(4-Methoxyphenyl)-3-phenylpropene (3-1b).

^{1}H NMR (400 MHz, DMSO) δ 7.35 – 7.18 (m, 7H), 6.87 (d, J = 8.8 Hz, 2H), 6.42 (d, J = 15.8 Hz, 1H), 6.30 – 6.22 (m, 1H), 3.73 (s, 3H), 3.69 (d, J = 6.9 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 158.97, 140.80, 130.46, 130.17, 128.91, 128.89, 127.63, 127.43, 126.46, 114.43, 55.51, 39.05. GC/MS (m/z): $[M]^{+}$ calcd for C16H16O, 224.1; found, 224.1. HRMS (EI+) calcd for C16H16O [M+]: 224.1201. Found: 224.1202.



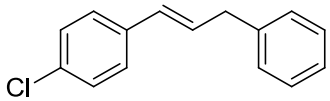
(E)-1-(4-Methyl)-3-phenylpropene (3-1c).

^{1}H NMR (400 MHz, DMSO) δ 7.33 – 7.18 (m, 7H), 7.11 (d, J = 7.9 Hz, 2H), 6.44 (d, J = 15.9 Hz, 1H), 6.39 – 6.32 (m, 1H), 3.50 (d, J = 6.4 Hz, 2H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 140.65, 136.79, 134.73, 130.84, 129.59, 128.93, 128.90, 128.77, 126.49, 126.36, 39.06, 21.19. GC/MS (m/z): $[M]^{+}$ calcd for C16H16, 208.1; found, 208.1. HRMS (EI+) calcd for C16H16 [M+]: 208.1252. Found: 208.1251.



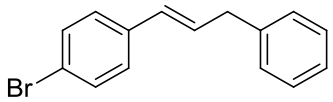
(E)-4-(3-phenylprop-1-enyl)phenol (3-1d).

^{1}H NMR (400 MHz, DMSO) δ 9.48 (s, 1H), 7.38 (s, 1H), 7.20 (d, J = 8.5 Hz, 3H), 6.75 (d, J = 8.5 Hz, 3H), 6.66 (dd, J = 17.7, 11.0 Hz, 1H), 5.78 – 5.55 (m, 2H), 5.07 (d, J = 11.2 Hz, 1H), 3.56 (dd, J = 15.9, 9.3 Hz, 1H), 3.11 (dd, J = 15.9, 8.1 Hz, 1H). ^{13}C NMR (100 MHz, DMSO) δ 164.36, 162.50, 141.74, 136.89, 135.27, 132.84, 132.02, 127.58, 120.43, 116.28, 113.90, 89.25, 42.20. GC/MS (m/z): $[M]^{+}$ calcd for C15H14O, 210.1; found, 210.1. HRMS (EI+) calcd for C15H14O [M+]: 210.1045. Found: 210.1046.



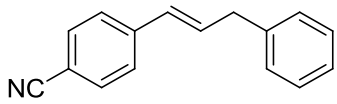
(E)-1-(4-Chlorophenyl)-3-phenylpropene (3-1e).

^{1}H NMR (400 MHz, DMSO) δ 7.43 (d, J = 8.6 Hz, 2H), 7.35-7.29 (m, *4*H), 7.26 – 7.19 (m, 3H), 6.48 – 6.46 (m, 2H), 3.52 (d, J = 4.5 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 140.31, 136.46, 131.91, 130.97, 129.71, 128.96, 128.93, 128.14, 126.57, 39.01. GC/MS (m/z): $[M]^+$ calcd for C15H13Cl, 228.1; found, 228.1. HRMS (EI+) calcd for C15H13Cl [M+]: 228.0706. Found: 228.0706.



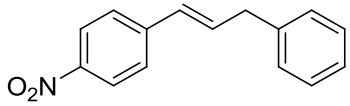
(E)-1-(4-Bromophenyl)-3-phenylpropene (3-1f).

^{1}H NMR (400 MHz, DMSO) δ 7.48 (d, J = 8.5 Hz, 2H), 7.38 – 7.19 (m, 7H), 6.49 – 6.42 (m, 2H), 3.51 (d, J = 5.3 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 140.27, 136.81, 131.88, 131.08, 129.78, 128.97, 128.93, 128.49, 126.58, 120.44, 39.03. GC/MS (m/z): $[M]^+$ calcd for C15H13Br, 272.0; found, 272.0. HRMS (EI+) calcd for C15H13Br [M+]: 272.0201. Found: 272.0200.



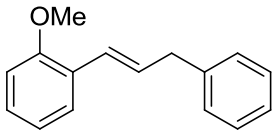
(E)-4-(3-phenylprop-1-enyl)benzonitrile (3-1g).

^{1}H NMR (400 MHz, DMSO) δ 7.75 (d, J = 8.3 Hz, 2H), 7.60 (d, J = 8.3 Hz, 2H), 7.34 – 7.19 (m, 5H), 6.72 – 6.64 (m, 1H), 6.56 (d, J = 15.9 Hz, 1H), 3.56 (d, J = 6.9 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 142.26, 139.92, 134.38, 132.98, 129.70, 129.02, 129.00, 128.98, 127.23, 126.68, 119.45, 109.73, 39.09. GC/MS (m/z): $[M]^+$ calcd for C16H13N, 219.1; found, 219.1. HRMS (EI+) calcd for C16H13N [M+]: 219.1048. Found: 219.1047.



(E)-4-(3-phenylprop-1-enyl)nitrobenzene (3-1h).

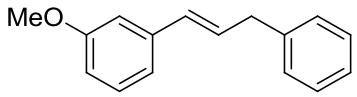
^{1}H NMR (400 MHz, DMSO) δ 8.13 (d, J = 8.8 Hz, 2H), 7.65 (d, J = 8.8 Hz, 2H), 7.37 – 7.15 (m, 6H), 6.73 (m, 1H), 6.60 (d, J = 15.9 Hz, 1H), 3.57 (d, J = 6.8 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 151.26, 149.11, 144.52, 140.28, 134.03, 133.78, 133.73, 132.11, 131.45, 129.06, 43.92. GC/MS (m/z): $[M]^+$ calcd for C15H13NO2, 239.1; found, 239.1. HRMS (EI+) calcd for C15H13NO2 [M+]: 239.0946. Found: 239.0949.



(E)-1-(2-Methoxyphenyl)-3-phenylpropene (3-1i).

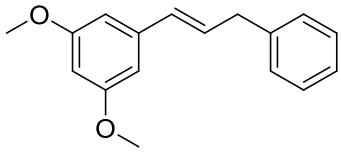
^{1}H NMR (400 MHz, DMSO) δ 7.44 (dd, J = 7.6, 1.6 Hz, 1H), 7.32-7.18(m, 6H), 6.97 (d, J = 7.6 Hz, 1H), 6.89 (t, J = 7.5 Hz, 1H), 6.72 (d, J = 15.9 Hz, 1H), 6.42 – 6.34 (m, 1H), 3.78 (s, 3H), 3.52 (d, J = 7.0 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 156.47, 140.73, 130.22, 128.93, 128.90, 128.79, 126.67, 126.47, 125.96, 125.57,

120.96, 111.70, 55.81, 39.37. GC/MS (m/z): $[M]^+$ calcd for C16H16O, 224.1; found, 224.1. HRMS (EI+) calcd for C16H16O [M+]: 224.1201. Found: 224.1202.



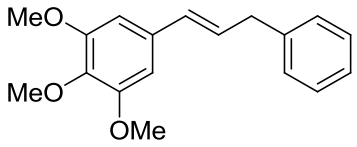
(E)-1-(3-Methoxyphenyl)-3-phenylpropene (3-1j).

^{1}H NMR (400 MHz, DMSO) δ 7.34 – 7.29 (m, 2H), 7.27 – 7.19 (m, 4H), 6.98 (d, J = 8.3 Hz, 2H), 6.78 (dd, J = 9.4, 2.1 Hz, 1H), 6.46 (d, J = 4.2 Hz, 1H), 6.45-6.40 (m, 1H), 3.74 (s, 3H), 3.52 (d, J = 4.6 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 159.99, 140.48, 138.99, 130.93, 130.22, 130.01, 128.97, 128.92, 126.53, 118.99, 118.99, 113.46, 111.51, 55.44, 39.04. GC/MS (m/z): $[M]^+$ calcd for C16H16O, 224.1; found, 224.1. HRMS (EI+) calcd for C16H16O [M+]: 224.1201. Found: 224.1202.



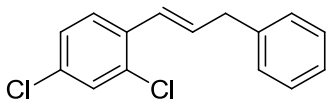
(E)-1-(3,5-Dimethoxyphenyl)-3-phenylpropene (3-1k).

^{1}H NMR (400 MHz, DMSO) δ 7.34-7.29 (m, 2H), 7.26 – 7.19 (m, 3H), 6.58 (d, J = 2.1 Hz, 2H), 6.50 – 6.43 (m, 1H), 6.40 (d, J = 15.9 Hz, 1H), 6.37 (t, J = 2.1 Hz, 1H), 3.73 (s, 6H), 3.51 (d, J = 6.2 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 161.07, 140.44, 139.59, 131.03, 130.46, 128.99, 128.91, 128.82, 126.54, 104.42, 99.92, 55.58, 39.03. GC/MS (m/z): $[M]^+$ calcd for C17H18O2, 254.1; found, 254.1. HRMS (EI+) calcd for C17H18O2 [M+]: 254.1307. Found: 254.1308.



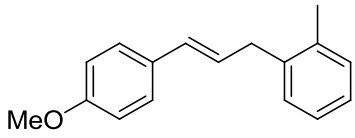
(E)-1-(3,4,5-Trimethoxyphenyl)-3-phenylpropene (3-1l).

^{1}H NMR (400 MHz, DMSO) δ 7.33-7.19 (m, 5H), 6.71 (s, 2H), 6.42 – 6.36 (m, 2H), 3.77 (s, 6H), 3.64 (s, 3H), 3.50 (d, J = 4.9 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 153.45, 140.58, 137.34, 133.28, 131.04, 129.30, 129.01, 128.91, 126.52, 103.80, 60.47, 56.25, 39.06. GC/MS (m/z): $[M]^+$ calcd for C18H20O2, 284.1; found, 284.1. HRMS (EI+) calcd for C18H20O2 [M+]: 284.1412. Found: 284.1413.



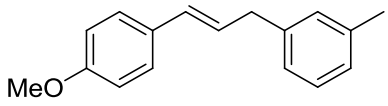
(E)-1-(2,4-Chlorophenyl)-3-phenylpropene (3-1m).

^{1}H NMR (400 MHz, DMSO) δ 7.67 (t, J = 7.0 Hz, 1H), 7.55 (d, J = 2.0 Hz, 1H), 7.37 – 7.29 (m, 3H), 7.28 – 7.19 (m, 3H), 6.77 – 6.67 (m, 1H), 6.59 – 6.47 (m, 1H), 3.57 (d, J = 6.9 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 139.85, 134.46, 134.25, 132.62, 129.28, 129.01, 128.96, 128.58, 128.01, 126.66, 125.48, 39.15. GC/MS (m/z): $[M]^+$ calcd for C15H12Cl2, 262.0; found, 262.0. HRMS (EI+) calcd for C15H12Cl2 [M+]: 262.0316. Found: 262.0320.



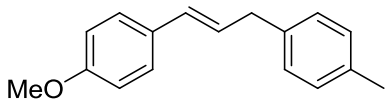
(E)-3-(2-Methylphenyl)-1-(4-methoxyphenyl)-propene (3-2b)

^{1}H NMR (400 MHz, DMSO) δ 7.31 (d, J = 6.8 Hz, 2H), 7.19-7.10 (m, 4H), 6.85 (d, J = 9.7 Hz, 2H), 6.33 (d, J = 15.9 Hz, 1H), 6.26-6.18 (m, 1H), 3.72 (s, 3H), 3.46 (d, J = 6.4 Hz, 2H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.70, 143.58, 141.08, 135.20, 135.07, 134.96, 134.16, 132.33, 131.38, 131.35, 131.21, 119.17, 60.25, 41.41, 24.21. GC/MS (m/z): $[M]^{+}$ calcd for C17H18O, 238.1; found, 238.1. HRMS (EI+) calcd for C17H18O [M+]: 238.1358. Found: 238.1359.



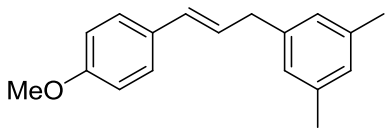
(E)-3-(3-Methylphenyl)-1-(4-methoxyphenyl)-propene (3-2c)

^{1}H NMR (400 MHz, DMSO) δ 7.33 (d, J= 8.7 Hz, 2H), 7.19 (t, J= 7.5 Hz, 1H), 7.05-7.00 (m, 3H), 6.89 – 6.50 (m, 2H), 6.41 (d, J= 15.8 Hz, 1H), 6.28-6.20 (m, 1H), 3.73 (s, 3H), 3.45 (d, J= 6.9 Hz, 2H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 158.97, 140.69, 137.92, 130.37, 130.19, 129.55, 128.77, 127.63, 127.49, 127.10, 125.99, 114.43, 55.51, 39.04, 21.45. GC/MS (m/z): $[M]^{+}$ calcd for C17H18O, 238.1; found, 238.1. HRMS (EI+) calcd for C17H18O [M+]: 238.1358. Found: 238.1360.



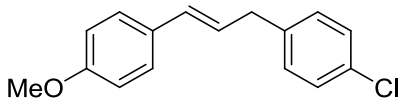
(E)-3-(4-Methylphenyl)-1-(4-methoxyphenyl)-propene (3-2d)

^{1}H NMR (400 MHz, DMSO) δ 7.33 (d, J = 8.7 Hz, 2H), 7.12 (s, 4H), 6.86 (d, J = 8.7 Hz, 2H), 6.39 (d, J = 15.8 Hz, 1H), 6.31 – 6.17 (m, 1H), 3.73 (s, 3H), 3.44 (d, J = 6.9 Hz, 2H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 158.94, 137.65, 135.37, 130.24, 130.21, 129.45, 128.80, 127.67, 127.59, 114.43, 55.51, 38.63, 21.07. GC/MS (m/z): $[M]^{+}$ calcd for C17H18O, 238.1; found, 238.1. HRMS (EI+) calcd for C17H18O [M+]: 238.1358. Found: 238.1359.



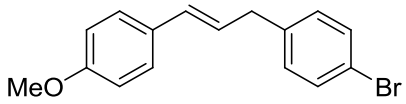
(E)-1-(4-Methoxyphenyl)-3-(3,5-dimethylphenyl)-propene (3-2e)

^{1}H NMR (400 MHz, DMSO) δ 7.32 (d, J = 11.6 Hz, 2H), 6.85 – 6.82 (m, 5H), 6.40 (d, J = 15.8 Hz, 1H), 6.26 – 6.18 (m, 1H), 3.73 (s, 3H), 3.40 (d, J = 6.9 Hz, 2H), 2.23 (s, 6H). ^{13}C NMR (100 MHz, DMSO) δ 163.70, 145.34, 142.51, 135.01, 134.96, 132.63, 132.37, 132.31, 131.43, 119.18, 60.27, 43.77, 26.10. GC/MS (m/z): $[M]^{+}$ calcd for C18H20O, 252.1; found, 252.1. HRMS (EI+) calcd for C18H20O [M+]: 252.1514. Found: 252.1513.



(E)-1-(4-Methoxyphenyl)-3-(4-chlorophenyl)-propene (3-2f)

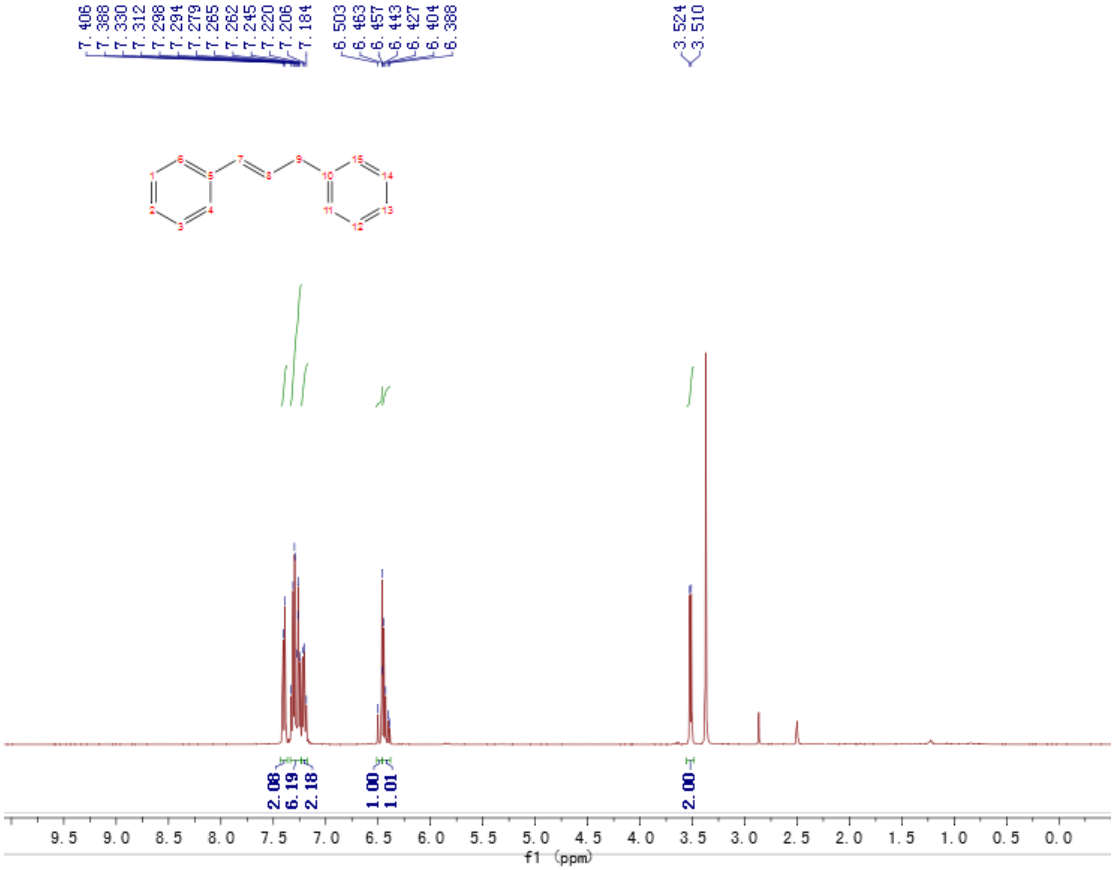
^{1}H NMR (400 MHz, DMSO) δ 7.37 – 7.32 (m, 4H), 7.27 (d, J = 8.5 Hz, 2H), 6.87 (d, J = 8.8 Hz, 2H), 6.41 (d, J = 15.8 Hz, 1H), 6.28 – 6.20 (m, 1H), 3.74 (s, 3H), 3.48 (d, J = 6.9 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 159.03, 139.86, 131.09, 130.83, 130.78, 130.06, 128.80, 127.68, 126.88, 114.44, 55.53, 38.21. GC/MS (m/z): $[M]^{+}$ calcd for C16H15ClO, 258.1; found, 258.1. HRMS (EI+) calcd for C16H15ClO [M+]: 258.0811. Found: 258.0813.

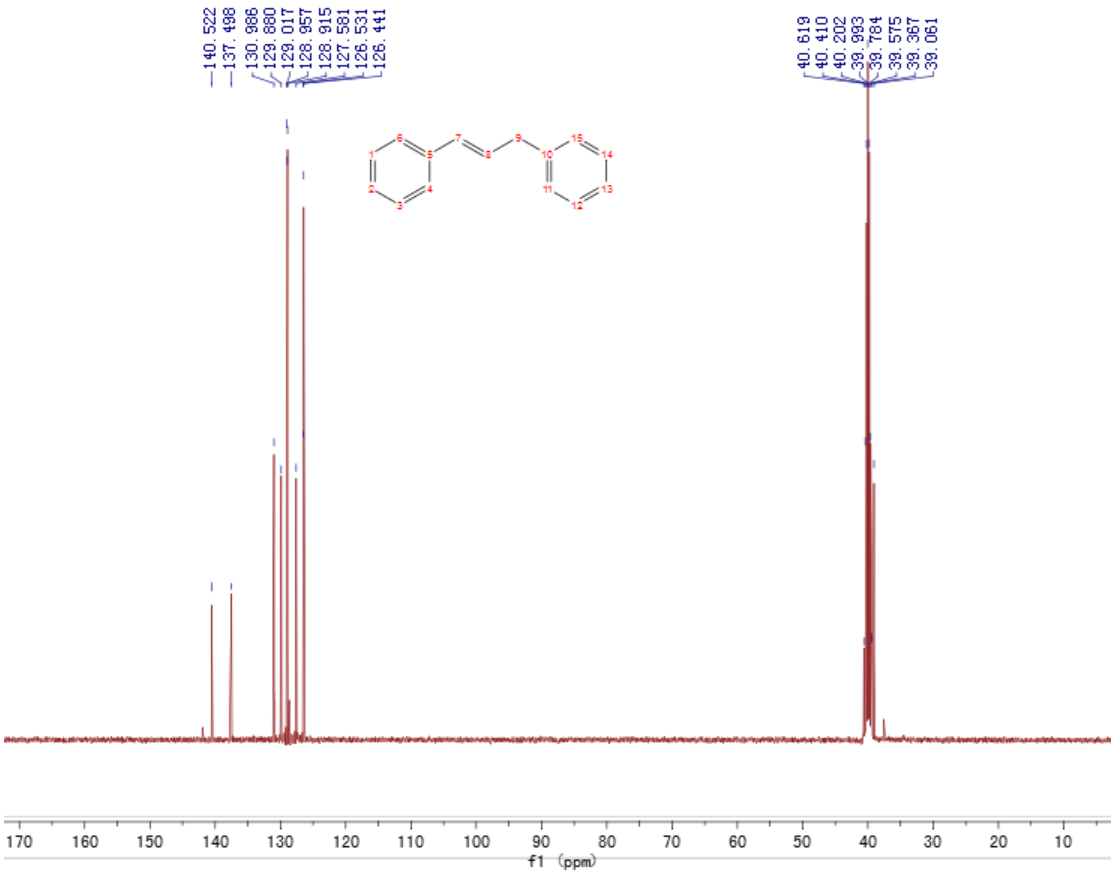


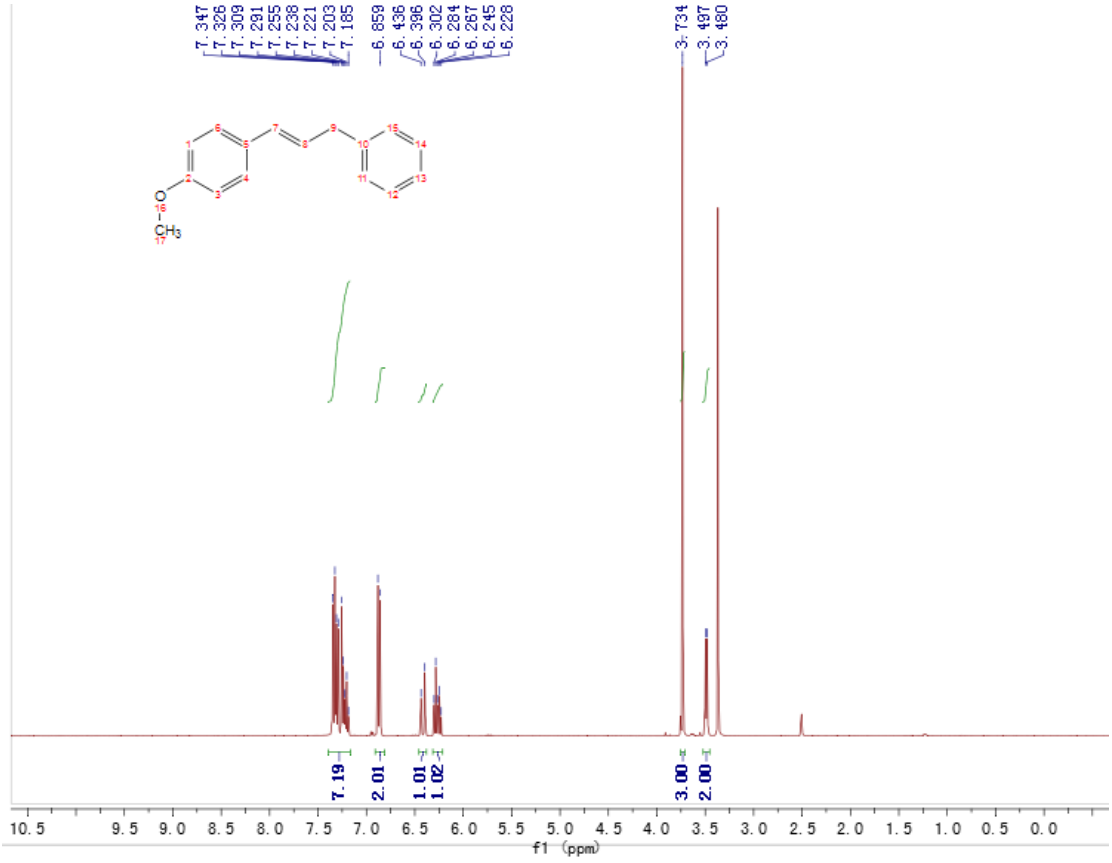
(E)-3-(4-Bromophenyl)-1-(4-methoxyphenyl)-propene (3-2g)

^{1}H NMR (400 MHz, DMSO) δ 7.49 (d, J = 8.4 Hz, 2H), 7.34 (d, J = 8.7 Hz, 2H), 7.22 (d, J = 8.4 Hz, 2H), 6.87 (d, J = 8.8 Hz, 2H), 6.41 (d, J = 15.8 Hz, 1H), 6.28 – 6.20 (m, 1H), 3.74 (s, 3H), 3.47 (d, J = 6.9 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 159.04, 140.30, 131.72, 131.20, 130.86, 130.05, 127.68, 126.80, 119.51, 114.44, 55.53, 38.27. GC/MS (m/z): $[M]^{+}$ calcd for C16H15BrO, 302.0; found, 302.0. HRMS (EI+) calcd for C16H15BrO [M+]: 302.0306. Found: 302.0306.

Copy of NMR Spectra for desired products:



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7.291
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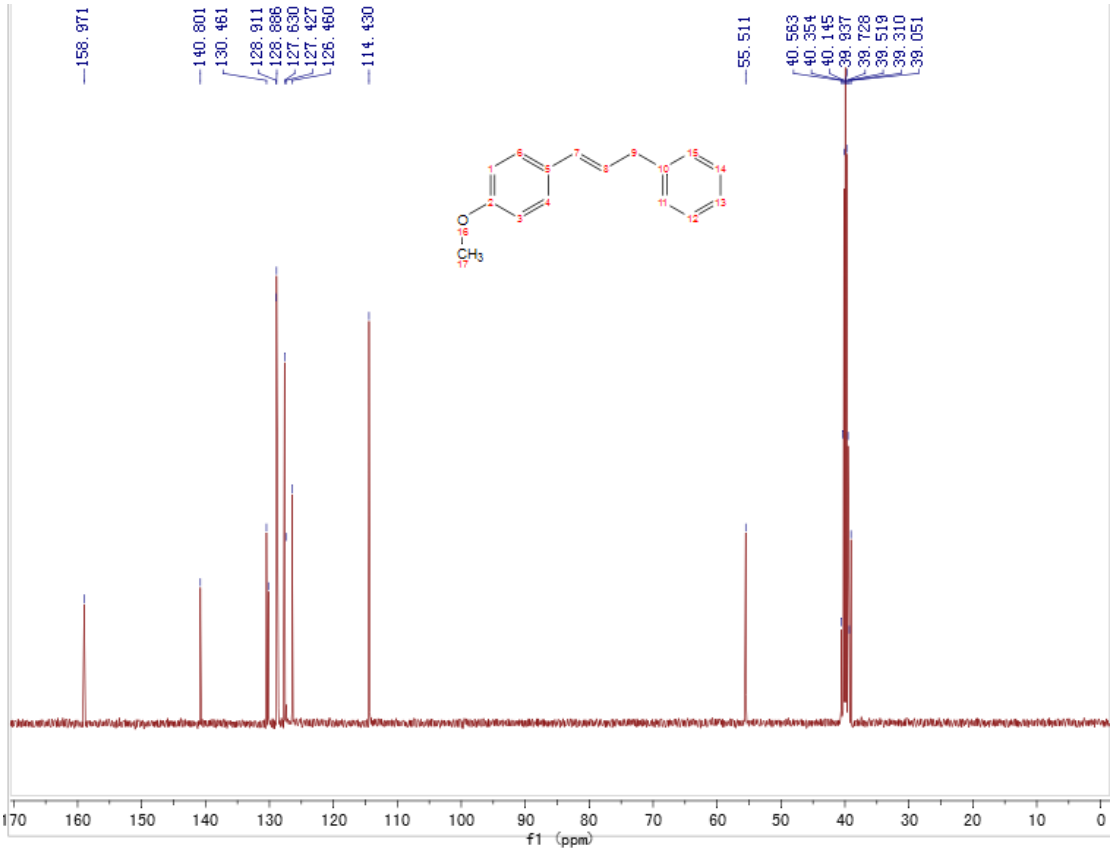
7.238
7.221
7.203
7.185
6.859
6.436
6.396
6.302
6.284
6.267
6.245
6.228
3.734
3.497
3.480
O
CH3
7.19
2.01
1.01
1.02
3.00
2.00
f1 (ppm)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140.801
130.461
128.911
128.886
127.630
127.427
126.460
114.430
55.511
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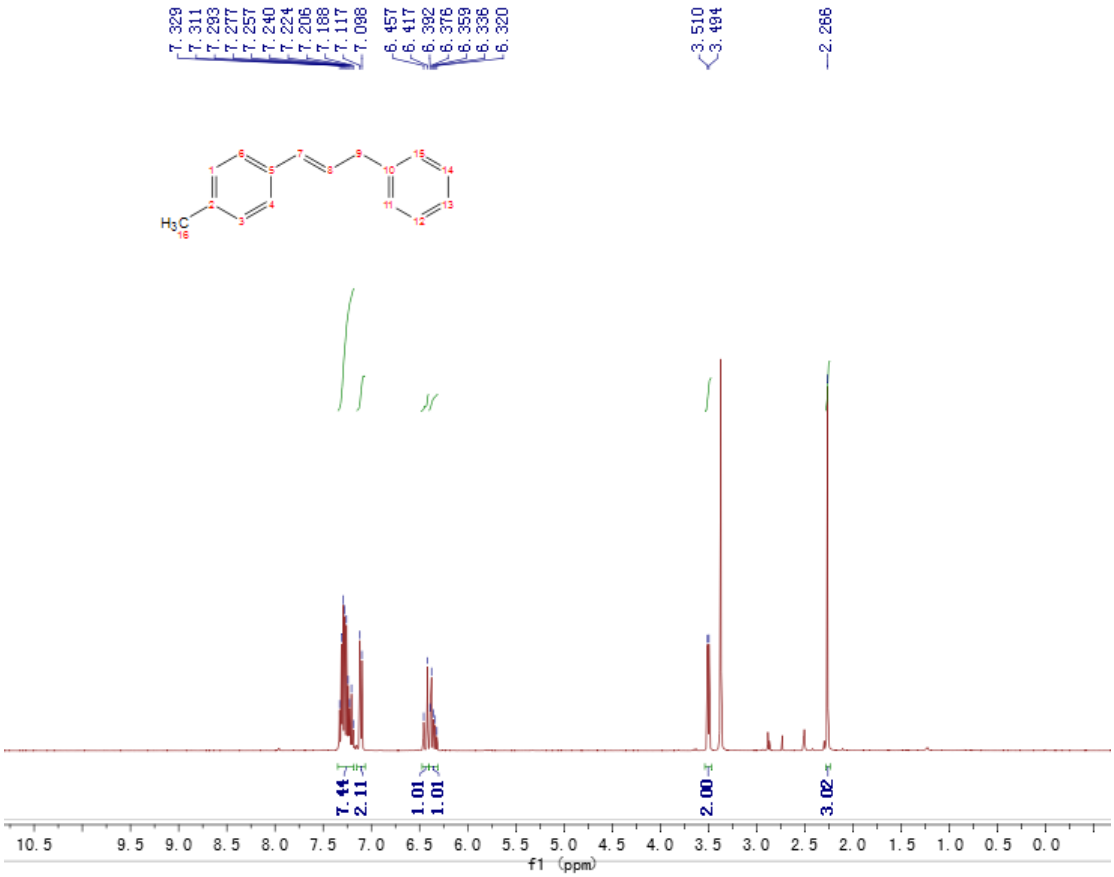
40.354
40.145
39.937
39.728
39.519
39.310
39.051
O
CH3
f1 (ppm)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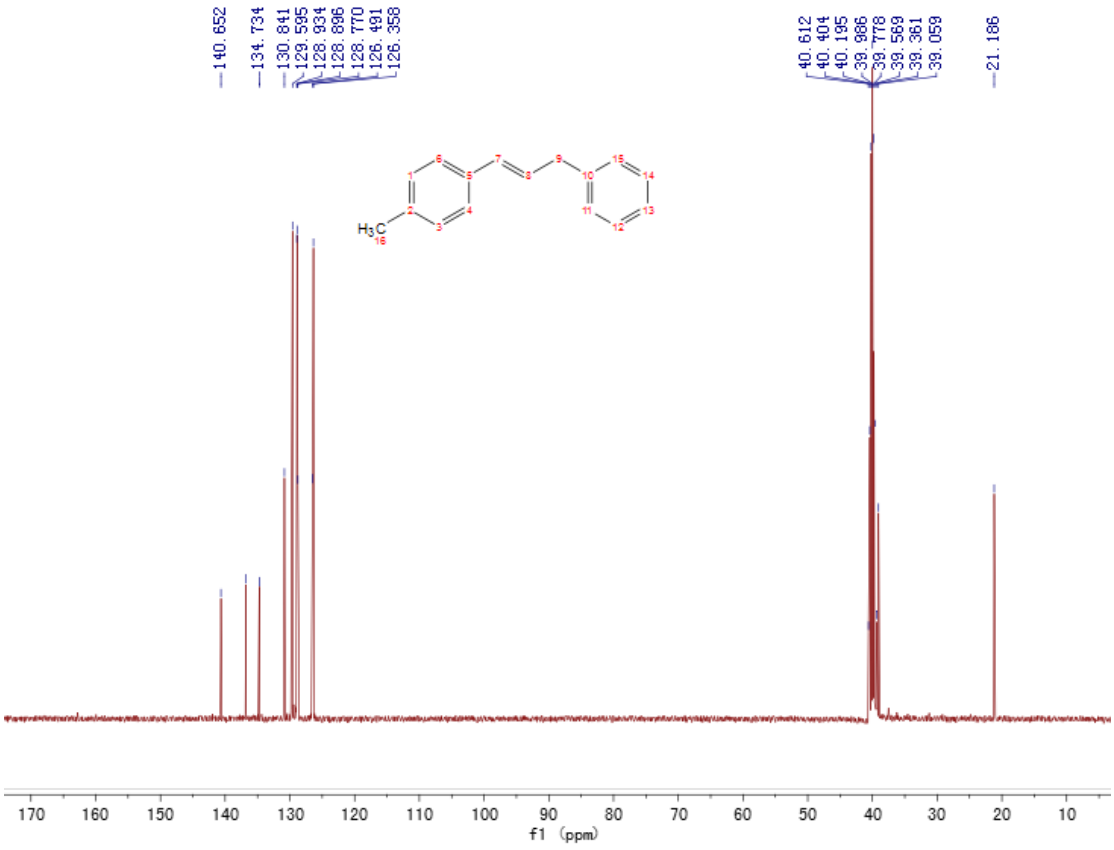
7.293
7.277
7.257
7.240
7.224
7.206
7.188
7.117
7.088
6.457
6.417
6.392
6.376
6.359
6.336
6.320
3.510
3.494
2.266
7.44
2.11
1.01
1.01
2.00
3.02
f1 (ppm)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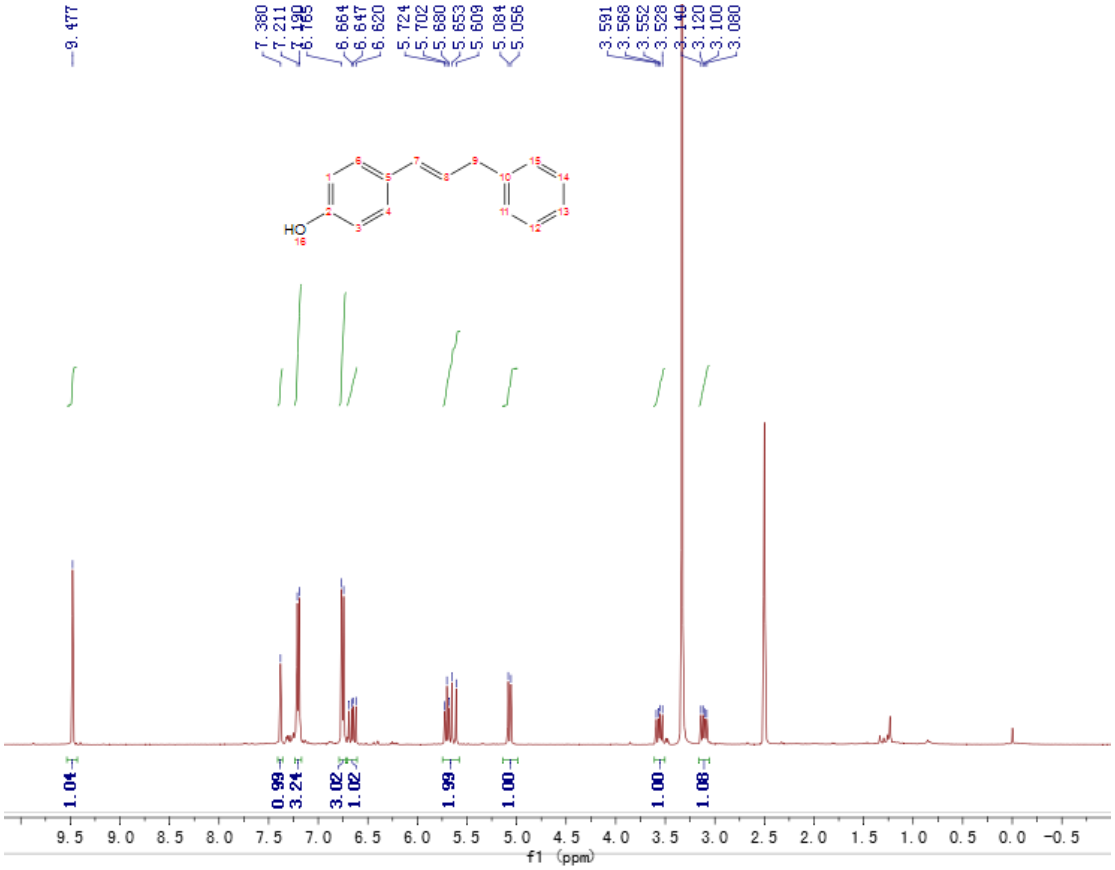
134.734
130.841
129.595
128.934
128.886
128.770
126.491
126.358
40.612
40.404
40.195
39.986
39.778
39.569
39.361
39.059
21.186
f1 (ppm)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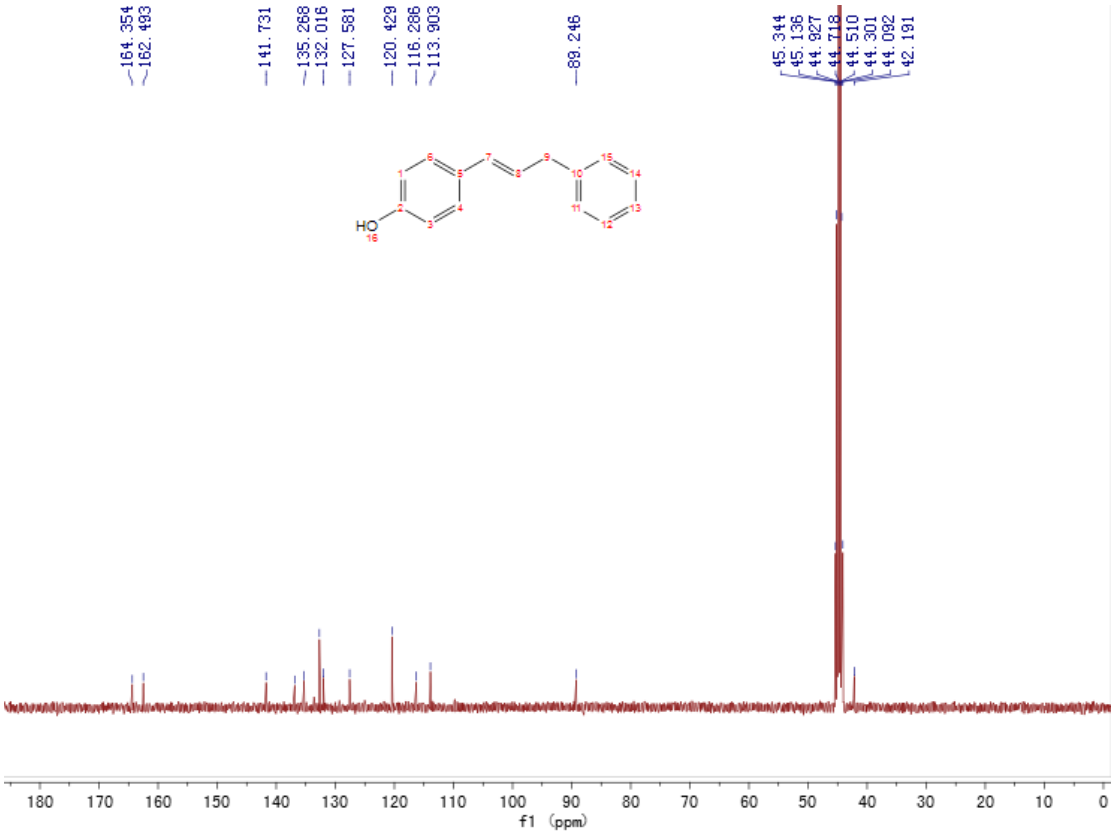
7.380
7.211
6.664
6.647
6.620
5.724
5.702
5.680
5.653
5.609
5.084
5.056
3.591
3.568
3.552
3.528
3.140
3.120
3.100
3.080
HO
1.04
0.99
3.24
3.02
1.02
1.99
1.00
1.00
1.08
f1 (ppm)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162.493
141.731
135.268
132.016
127.581
120.429
116.286
113.903
89.246
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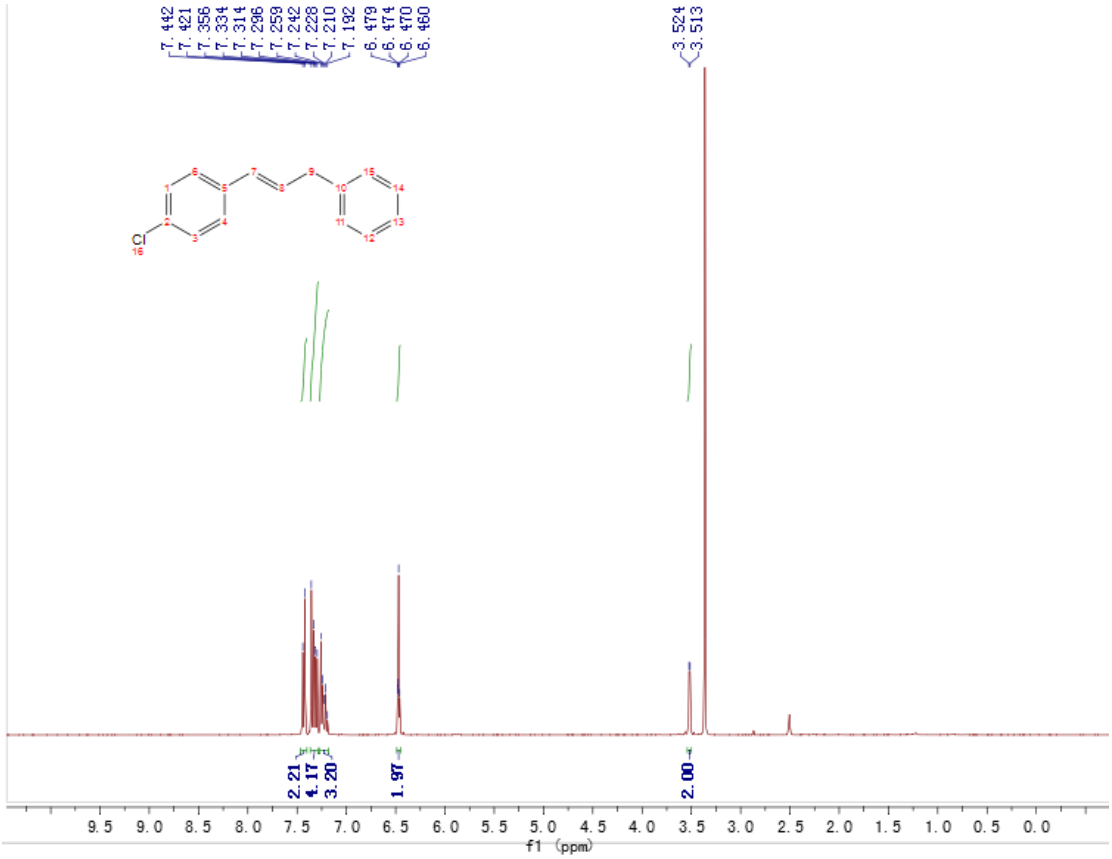
45.136
44.927
44.718
44.510
44.301
44.092
42.191
HO
f1 (ppm)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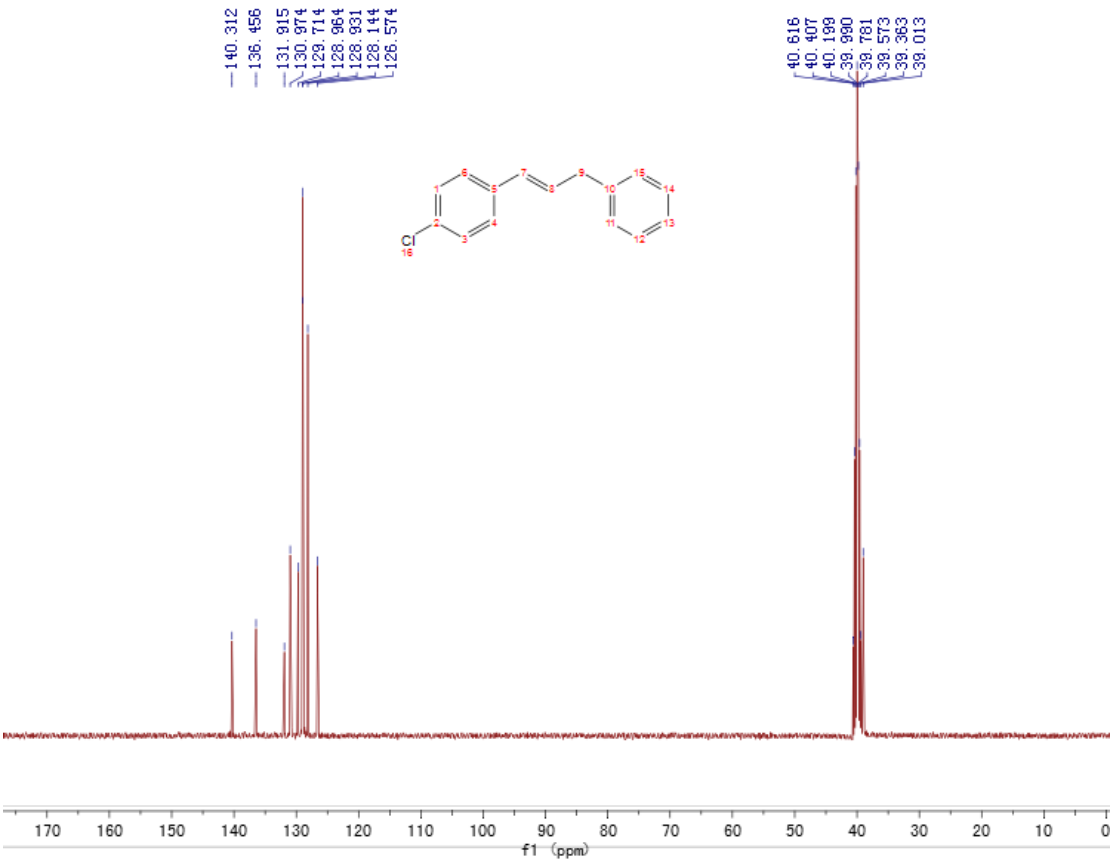
7.356
7.334
7.314
7.296
7.259
7.242
7.228
7.210
7.192
6.479
6.474
6.470
6.460
3.524
3.513
Cl
16
2.21
4.17
3.20
1.97
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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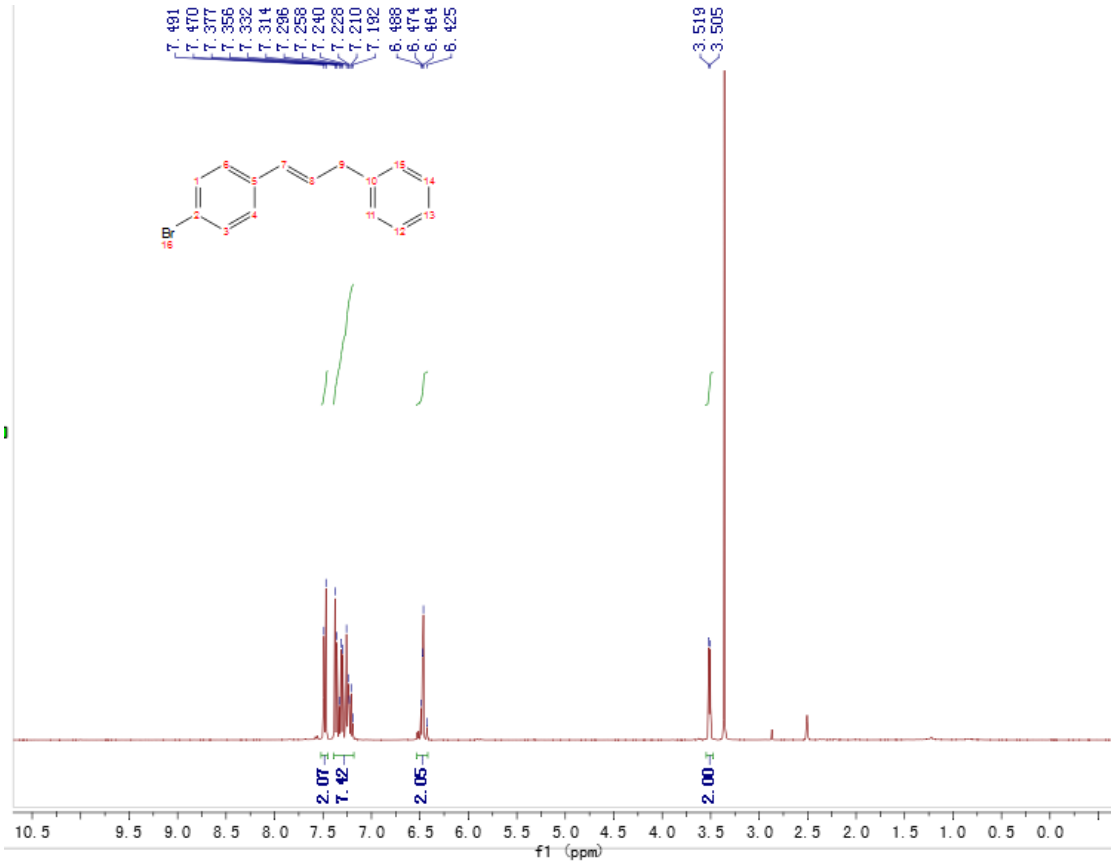
130.974
129.714
128.964
128.931
128.144
126.574
40.616
40.407
40.199
39.990
39.781
39.573
39.363
39.013
Cl
16
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.258
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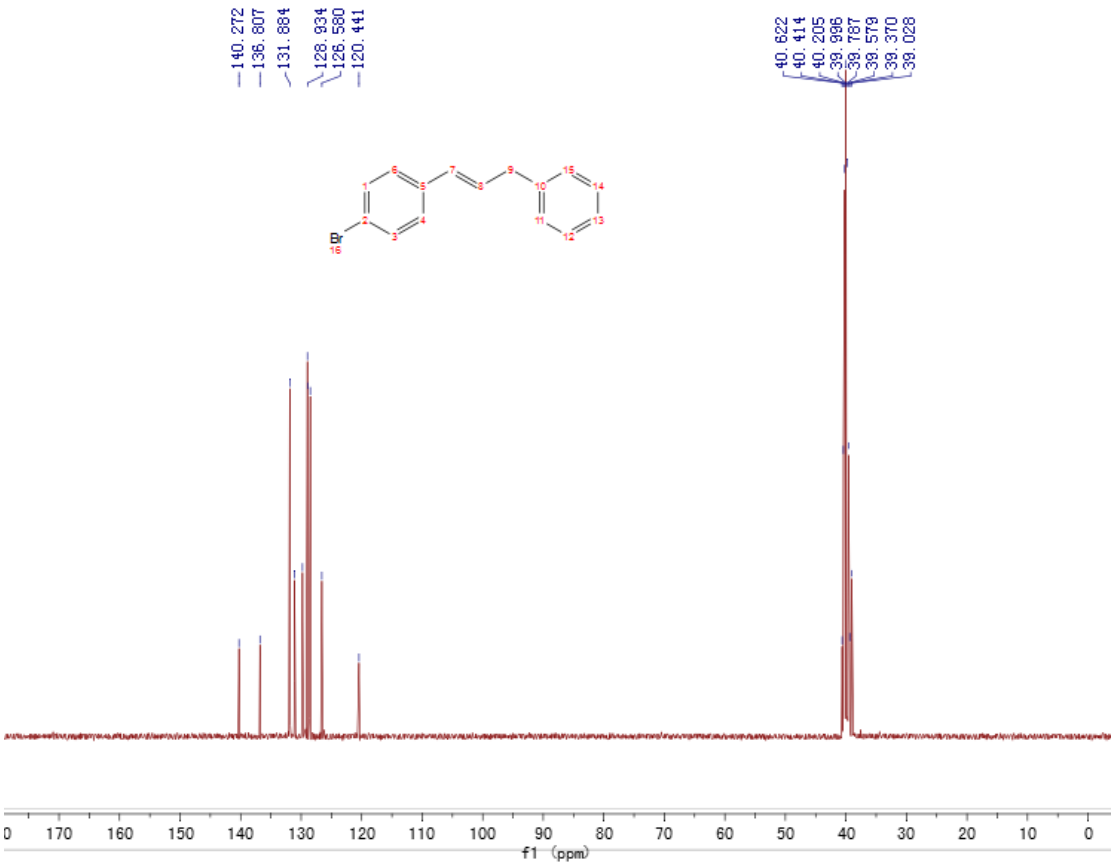
7.228
7.210
7.192
6.488
6.474
6.464
6.425
3.519
3.505
Br
16
2.07
7.42
2.05
2.00
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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40.414
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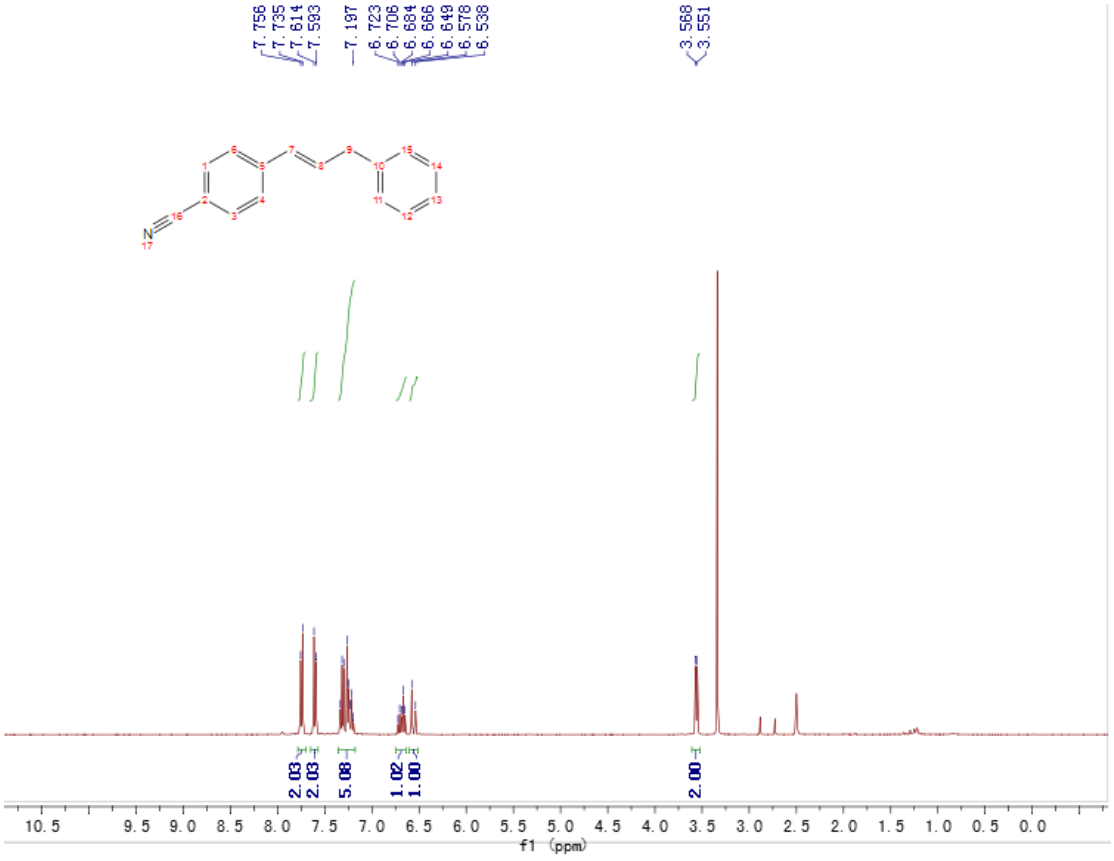
39.579
39.370
39.028
Br
16
0 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.735
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6.706
6.684
6.666
6.649
6.578
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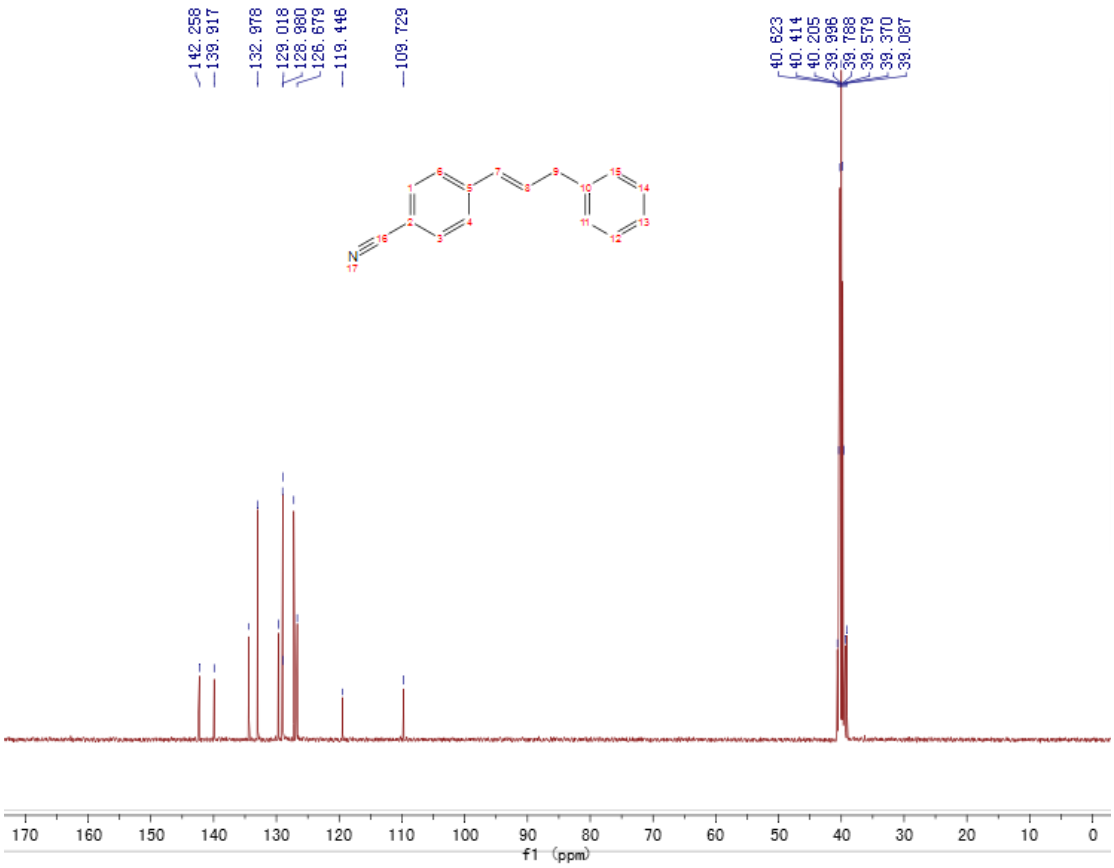
3.551
2.03
2.03
5.08
1.02
1.00
2.00
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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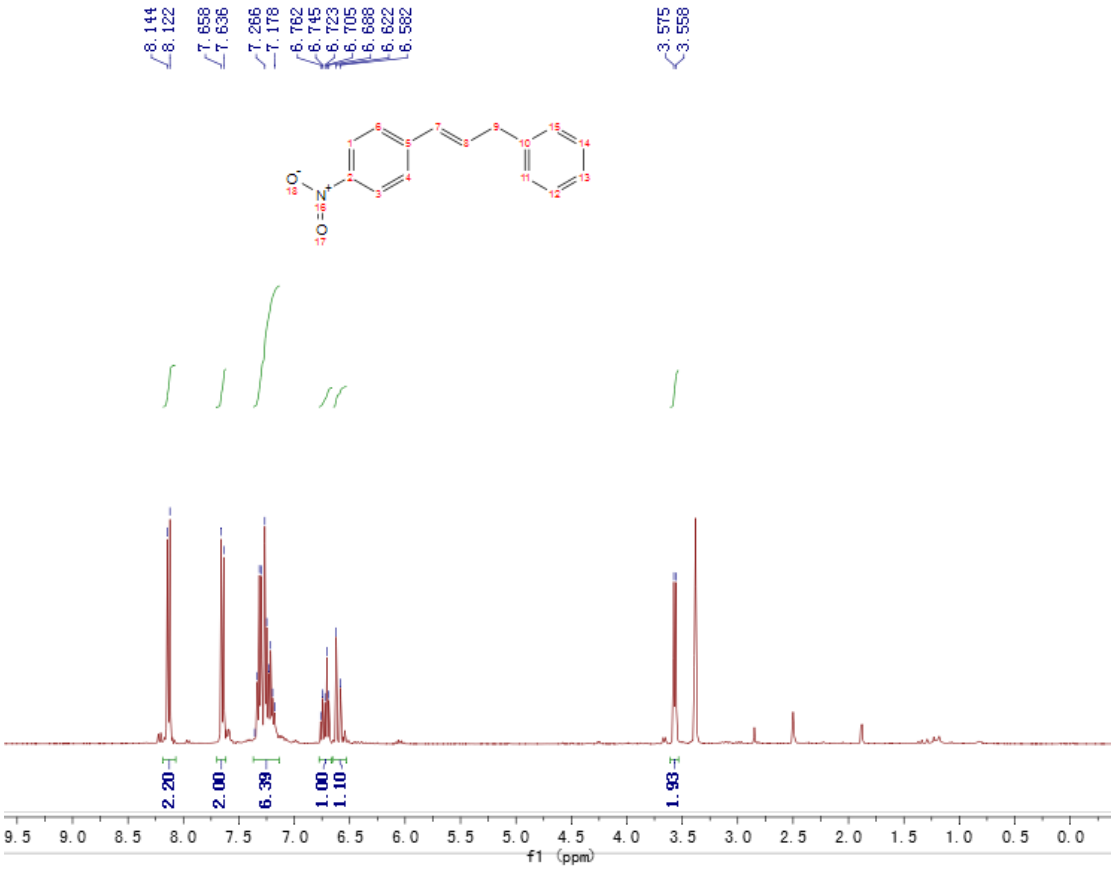
139.917
132.978
129.018
128.980
126.679
119.446
109.729
40.623
40.414
40.205
39.996
39.788
39.579
39.370
39.087
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.636
7.286
7.178
6.762
6.745
6.723
6.705
6.688
6.622
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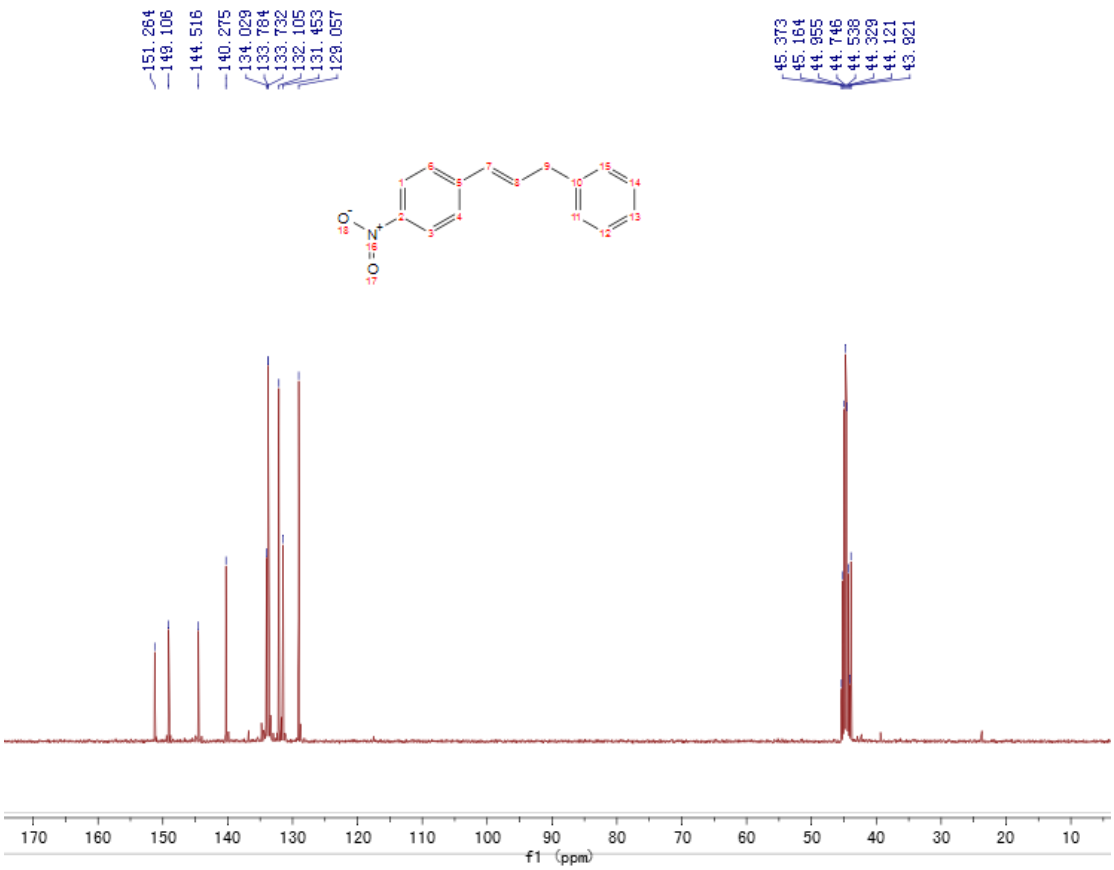
3.575
3.558
2.20
2.00
6.39
1.00
1.10
1.93
f1 (ppm)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133.732
132.105
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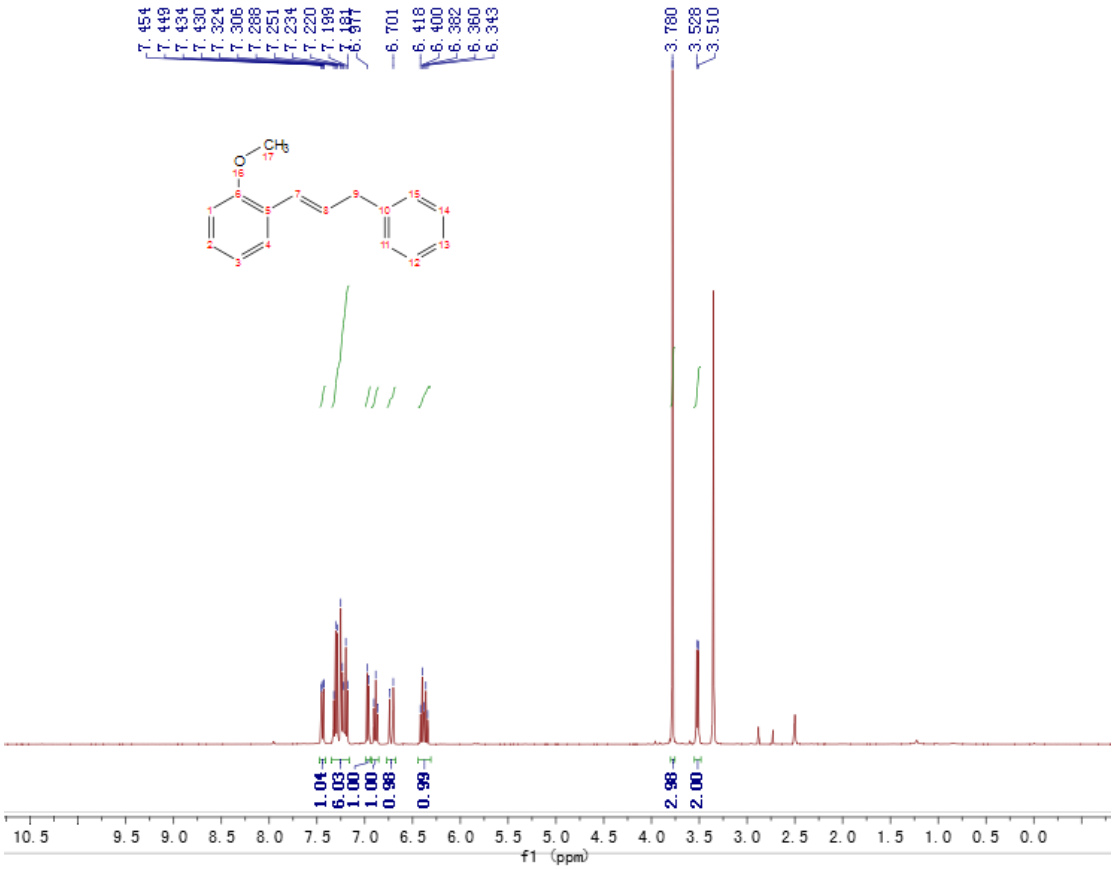
44.746
44.538
44.329
44.121
43.921
f1 (ppm)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6.400
6.382
6.360
6.343
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1.04
6.03
1.00
1.00
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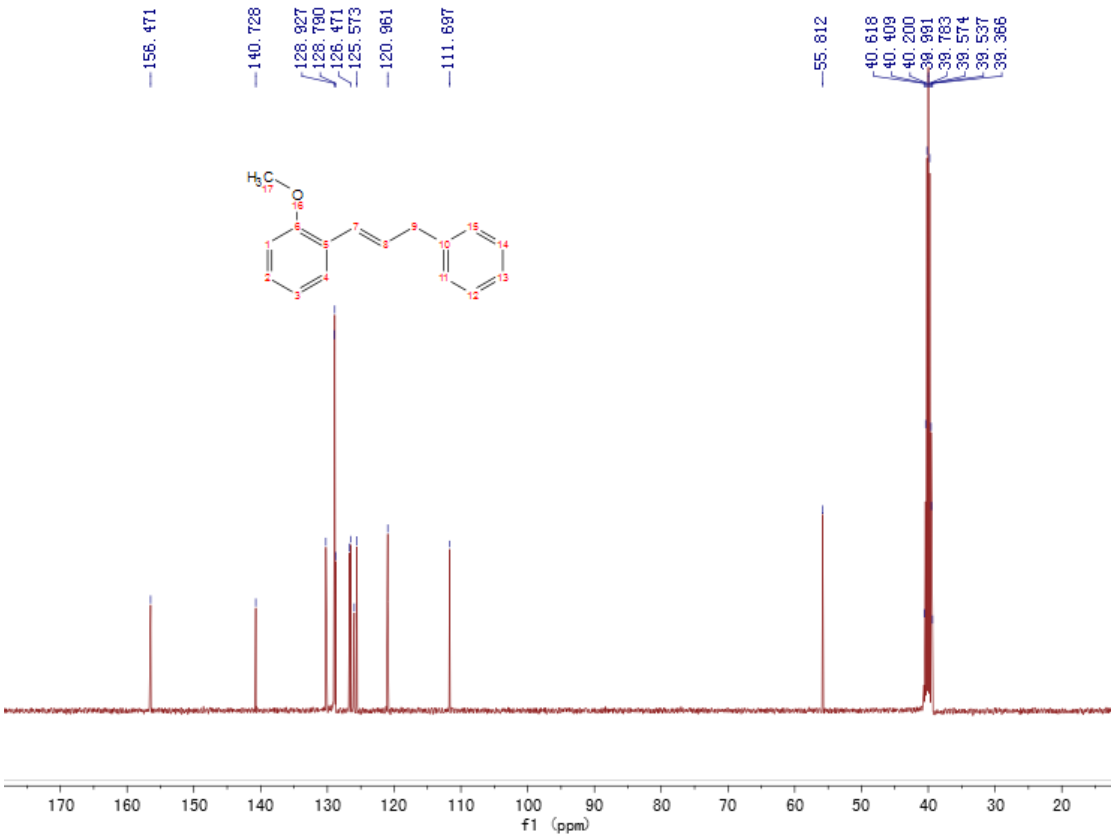
2.00
f1 (ppm)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38.574
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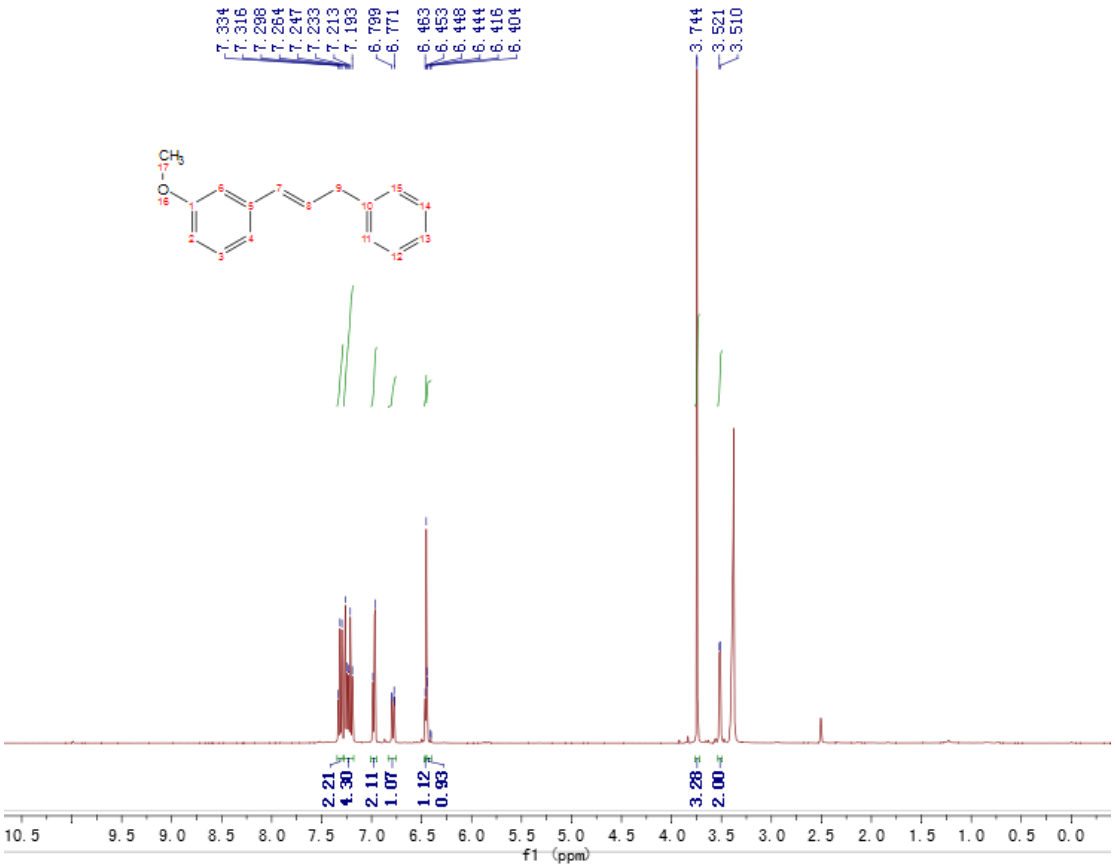
38.366
f1 (ppm)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6.444
6.416
6.404
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1.07
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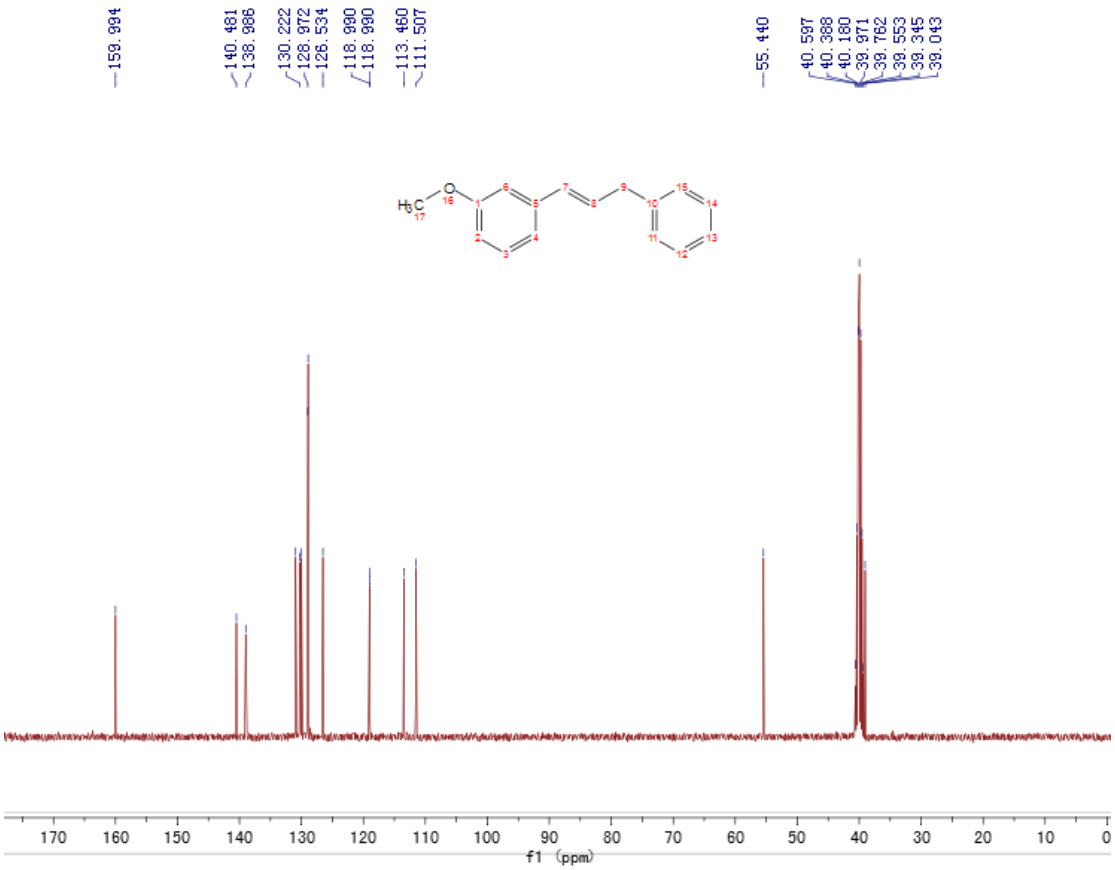
f1 (ppm)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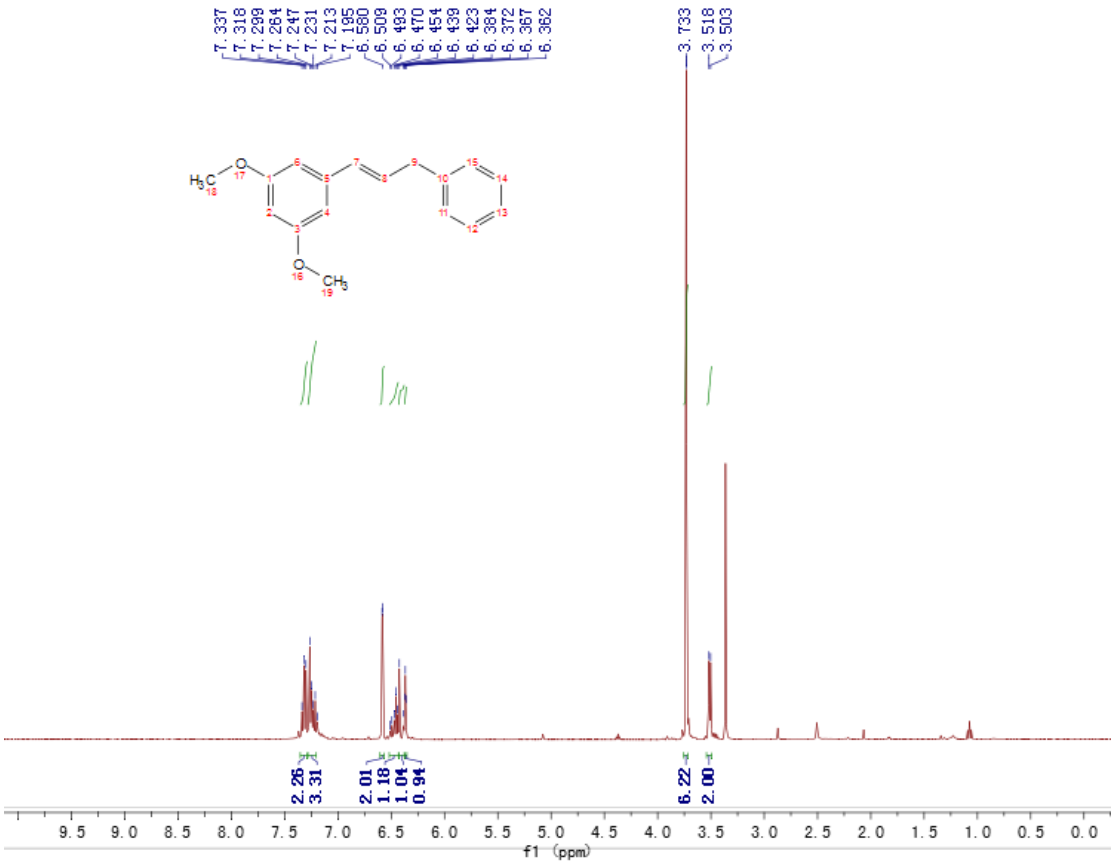
f1 (ppm)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6.367
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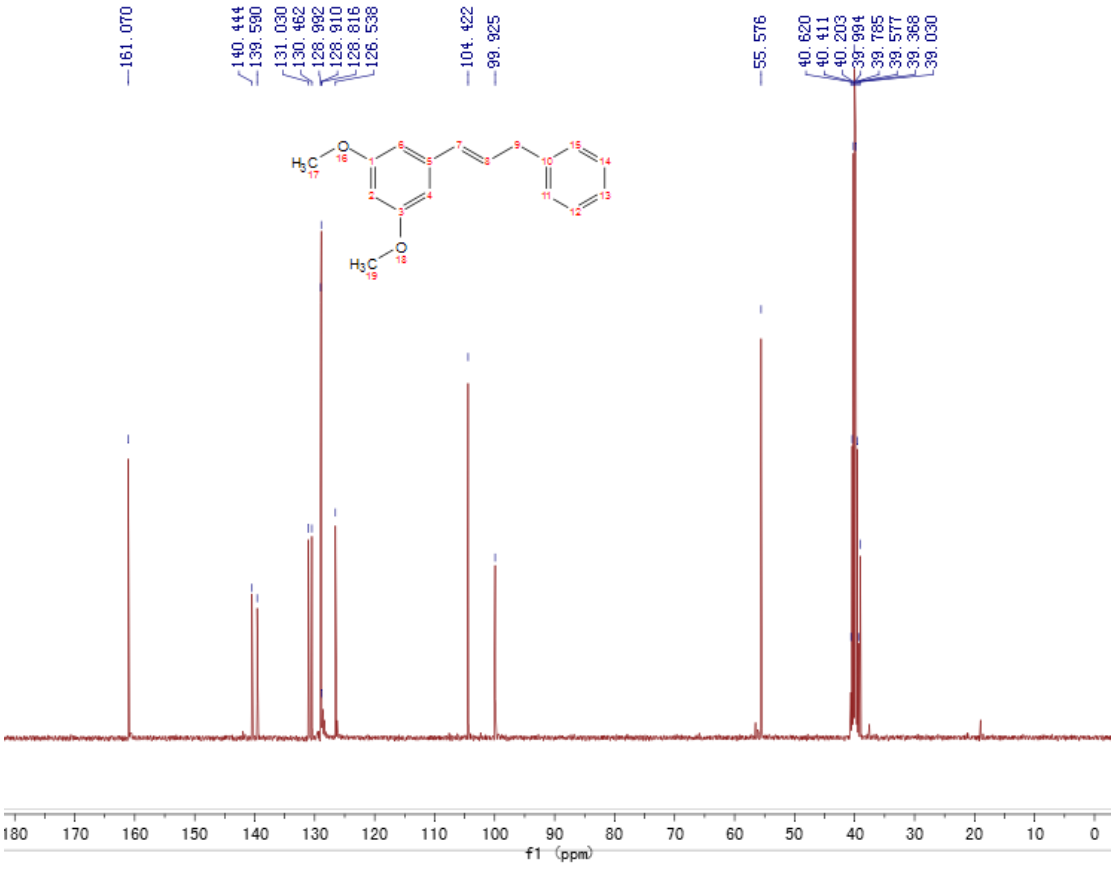
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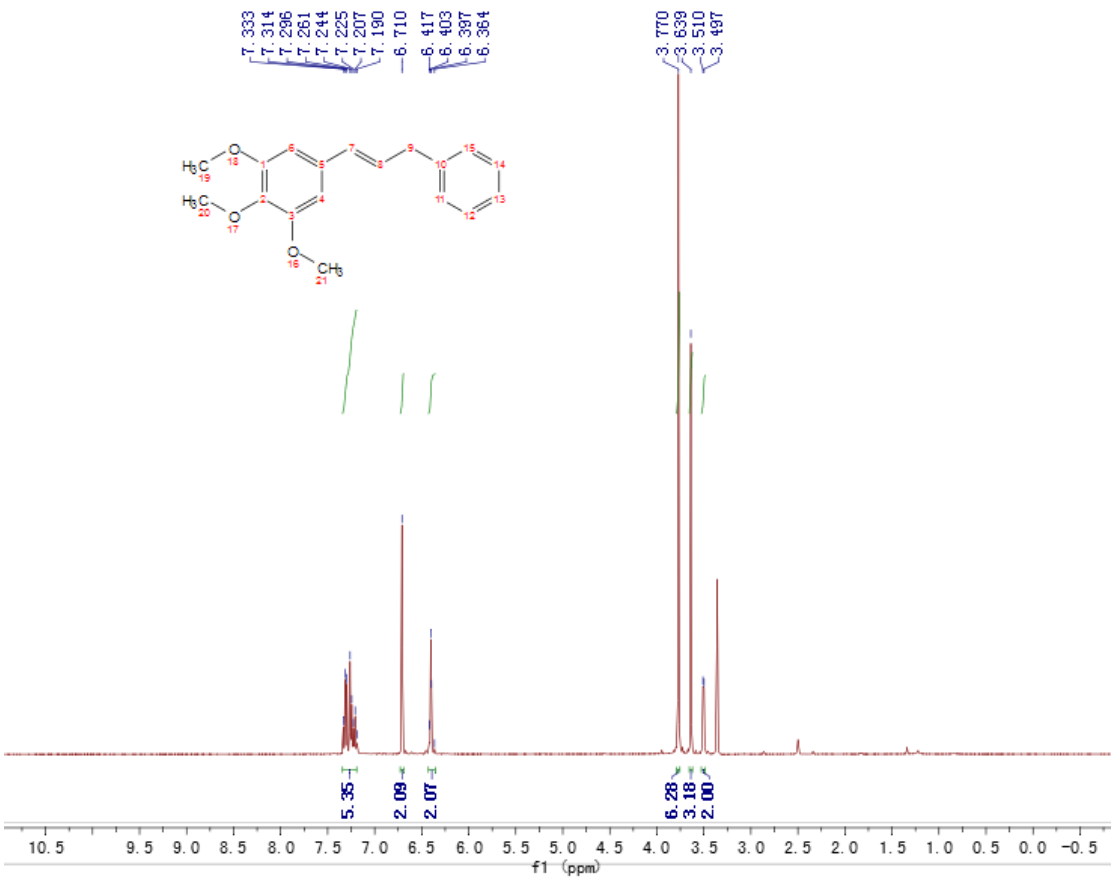
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5.35
2.09
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6.28
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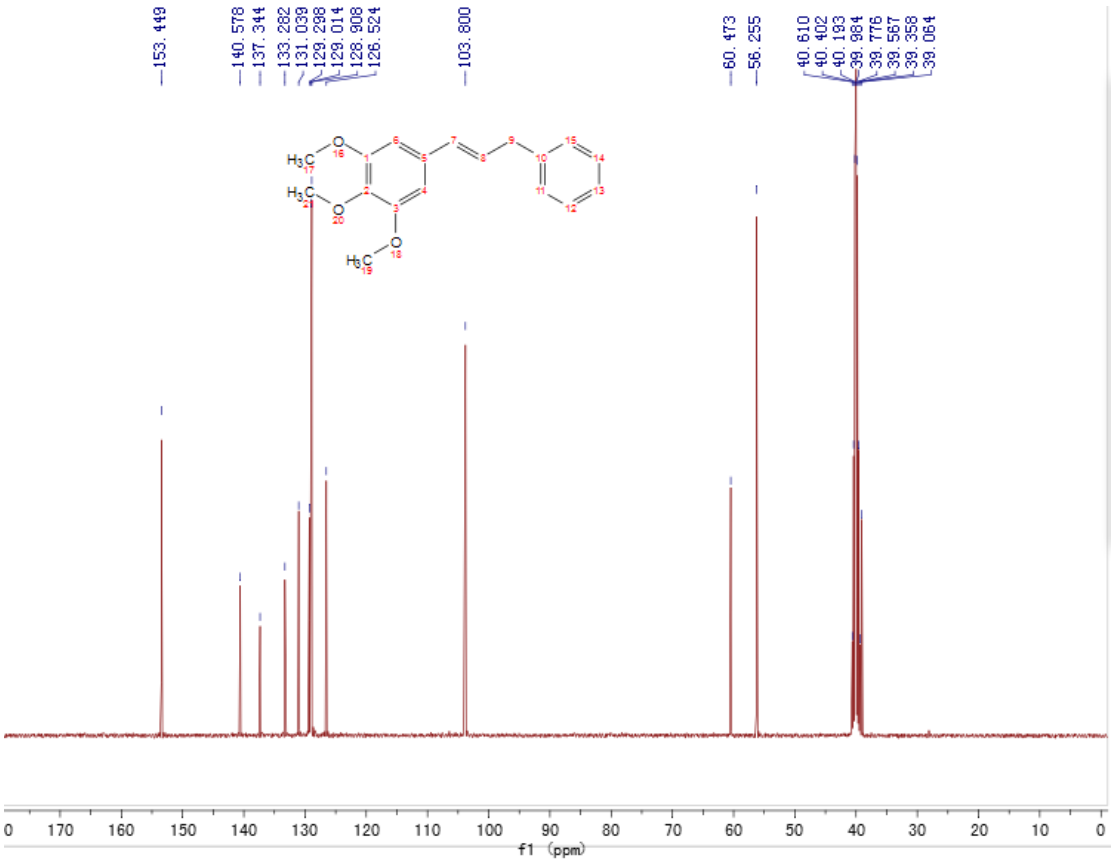
2.00
f1 (ppm)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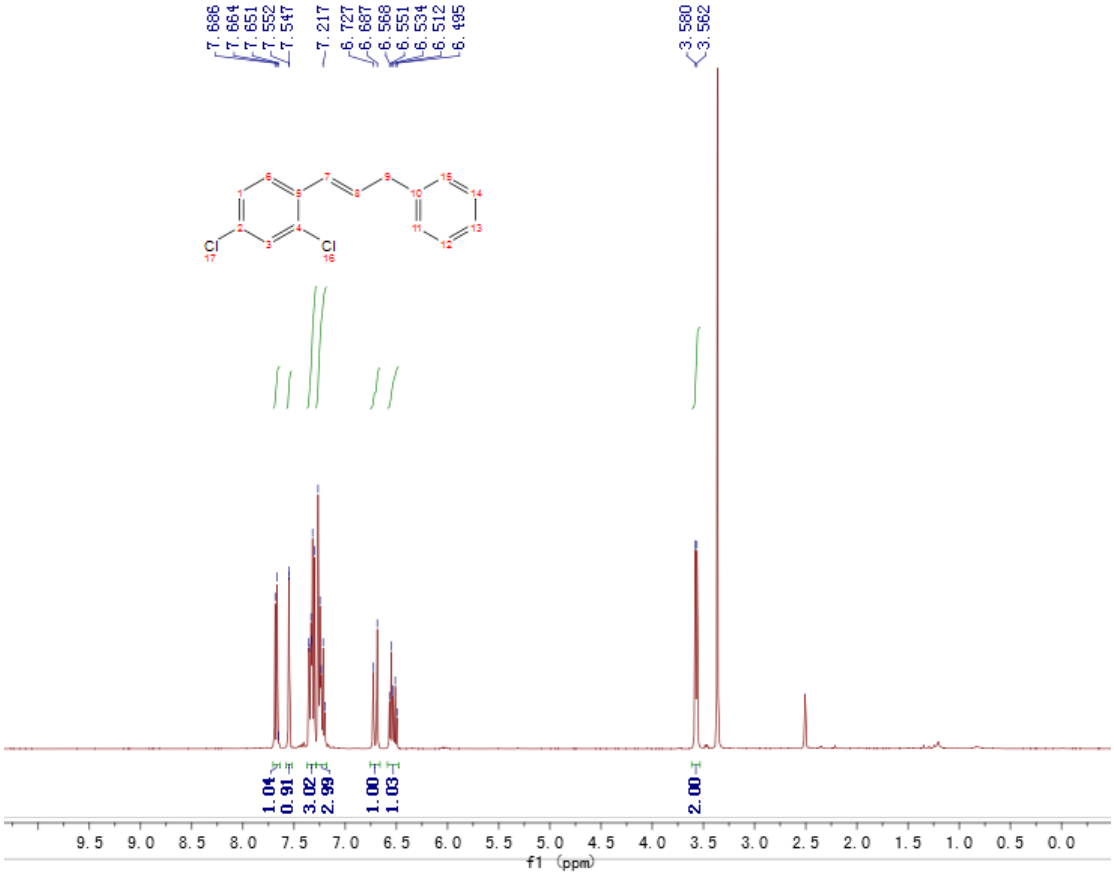
39.064
f1 (ppm)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7.547
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6.687
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6.551
6.534
6.512
6.495
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Cl
Cl
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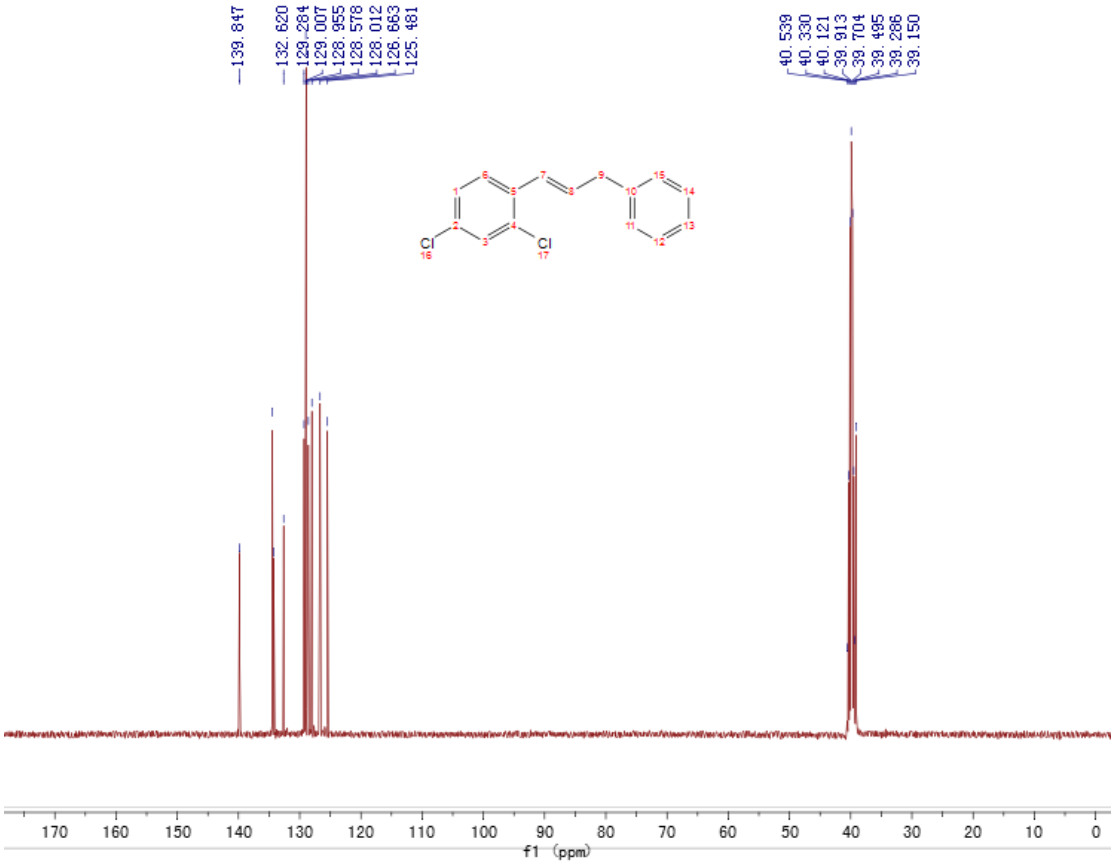
0.91
3.02
2.99
1.00
1.03
2.00
f1 (ppm)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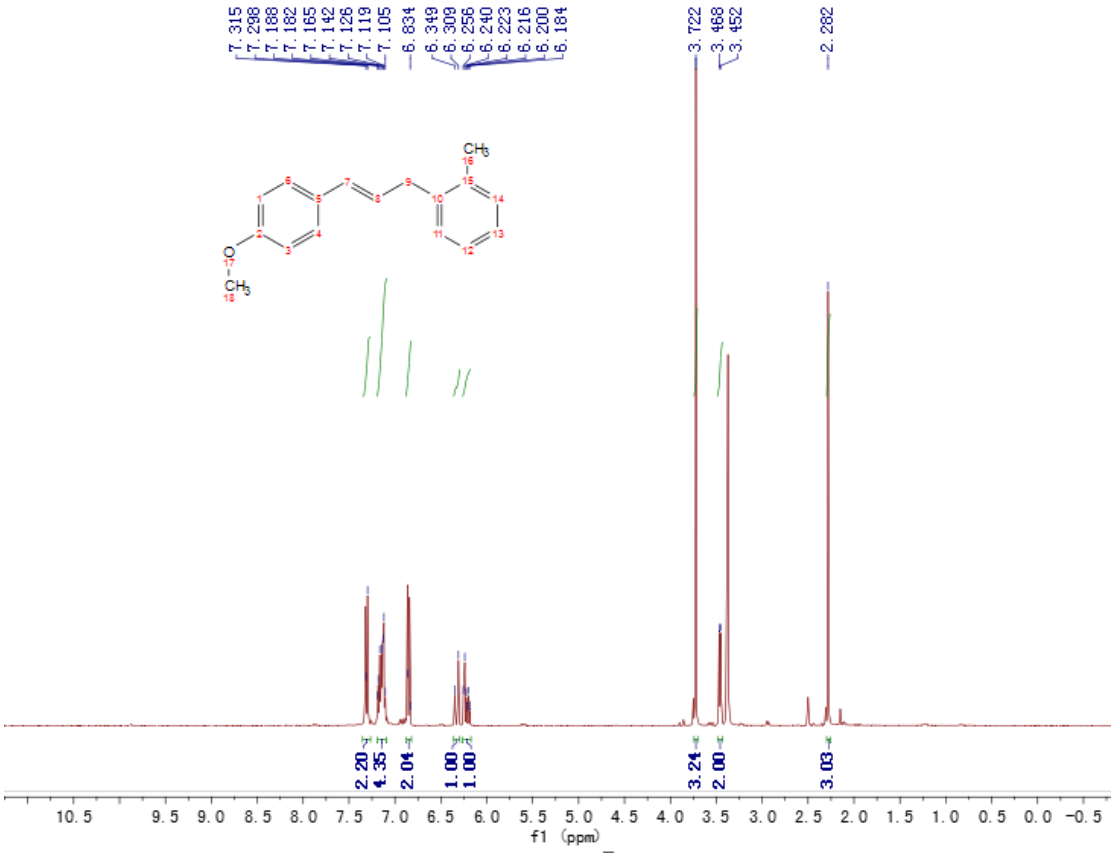
Cl
Cl
f1 (ppm)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6.256
6.240
6.223
6.216
6.200
6.184
3.722
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1.00
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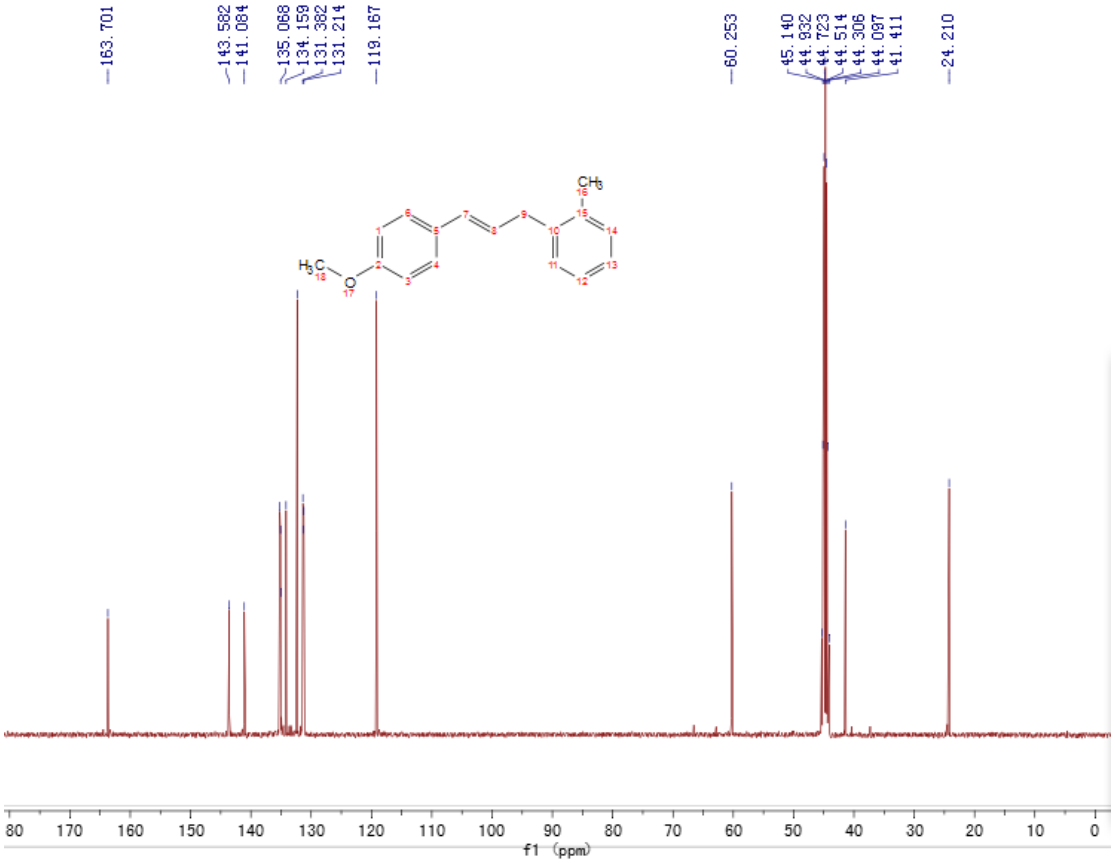
3.24
2.00
3.03
f1 (ppm)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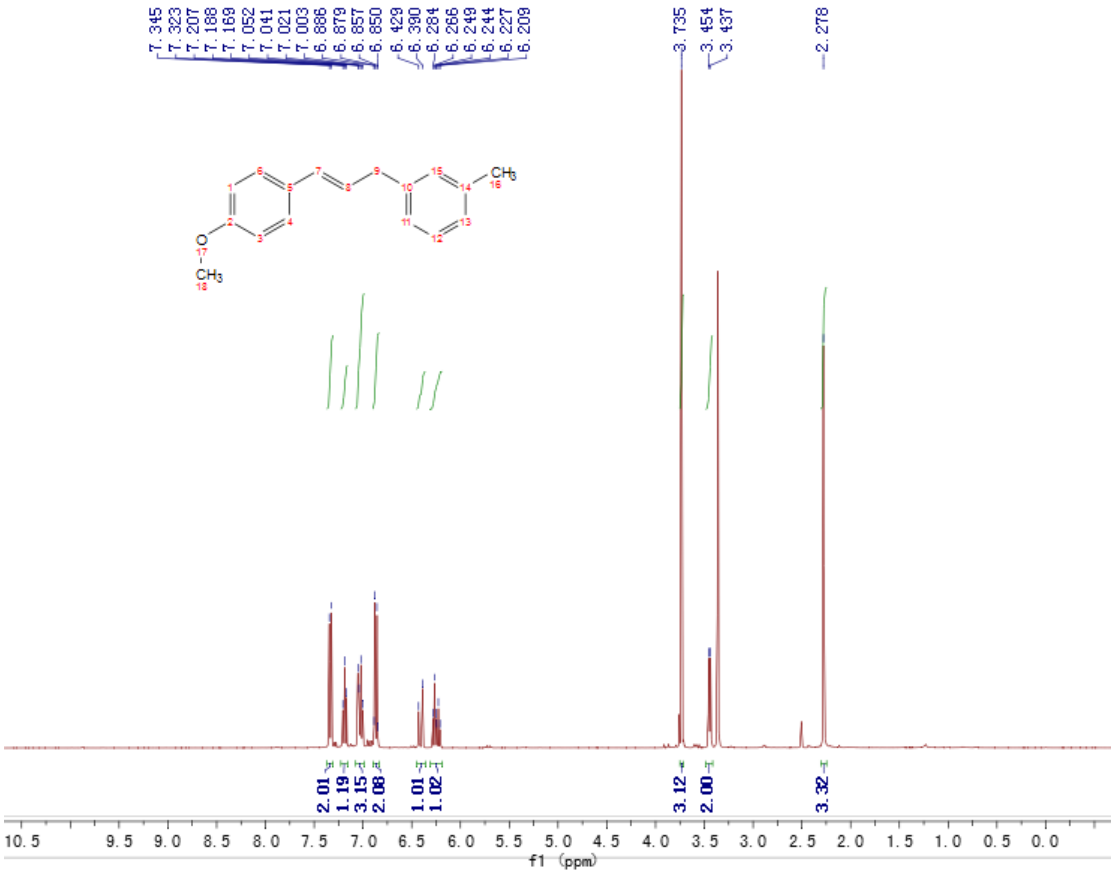
143.582
141.084
135.068
134.159
131.382
131.214
119.167
60.253
45.140
44.932
44.723
44.514
44.306
44.097
41.411
24.210
f1 (ppm)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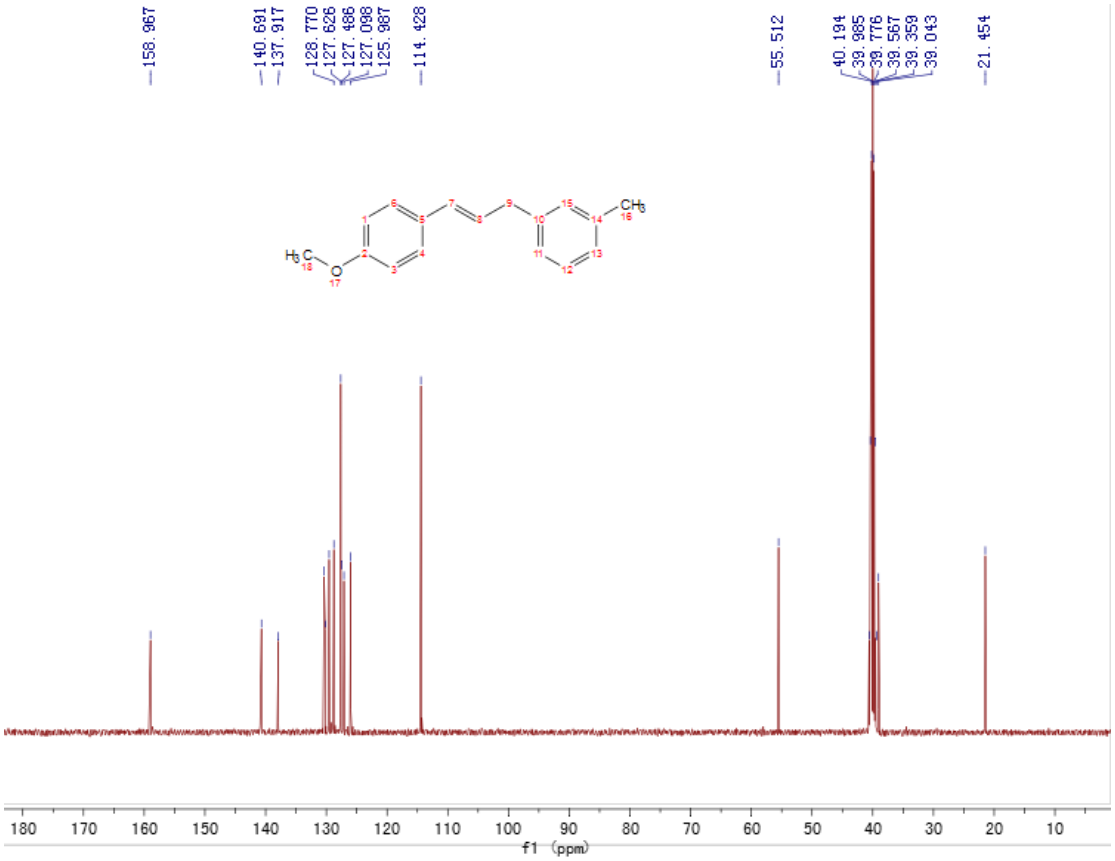
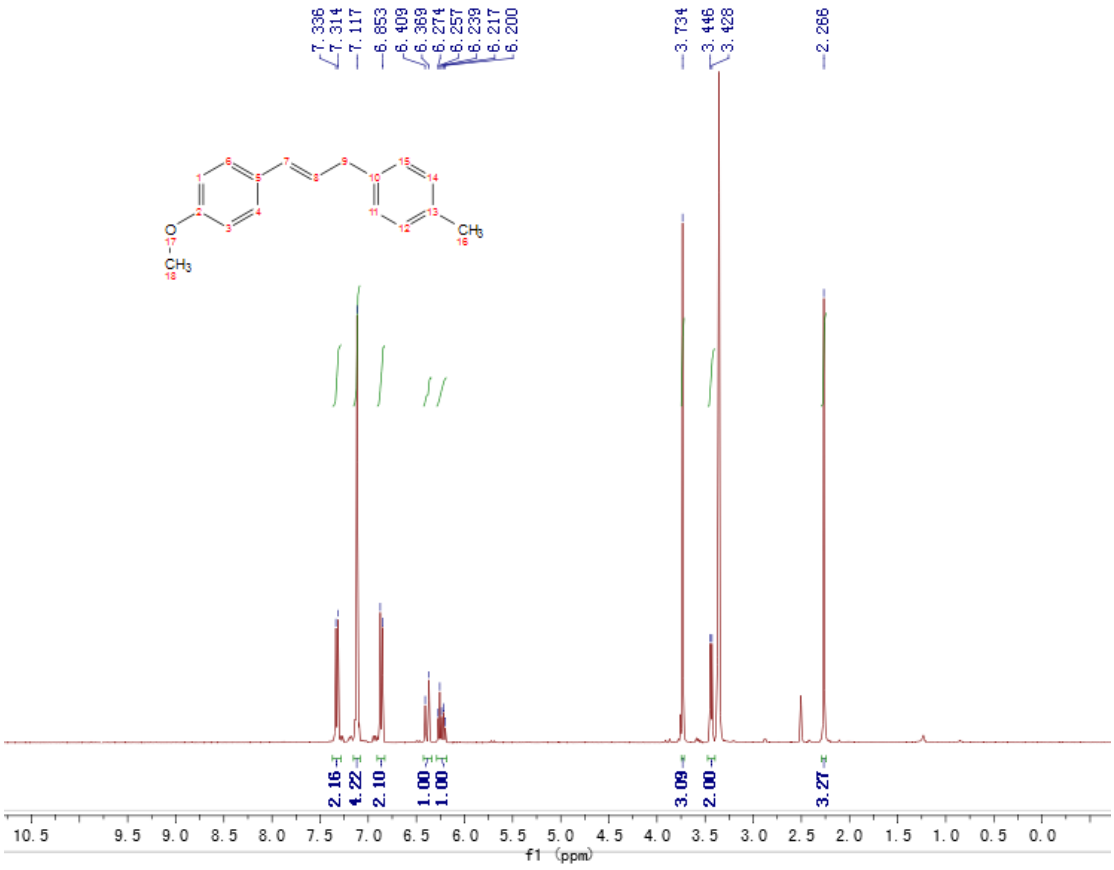
7.323
7.207
7.188
7.169
7.052
7.041
7.021
7.003
6.886
6.879
6.857
6.850
6.429
6.390
6.284
6.266
6.249
6.244
6.227
6.209
3.735
3.454
3.437
2.278
2.01
1.19
3.15
2.08
1.01
1.02
3.12
2.00
3.32
f1 (ppm)


158.967
140.691
137.917
128.770
127.626
127.486
127.098
125.987
114.428
55.512
40.194
39.985
39.776
39.567
39.359
39.043
21.454
f1 (ppm)


7.336
7.314
7.117
6.853
6.409
6.369
6.274
6.257
6.239
6.217
6.200
3.734
3.446
3.428
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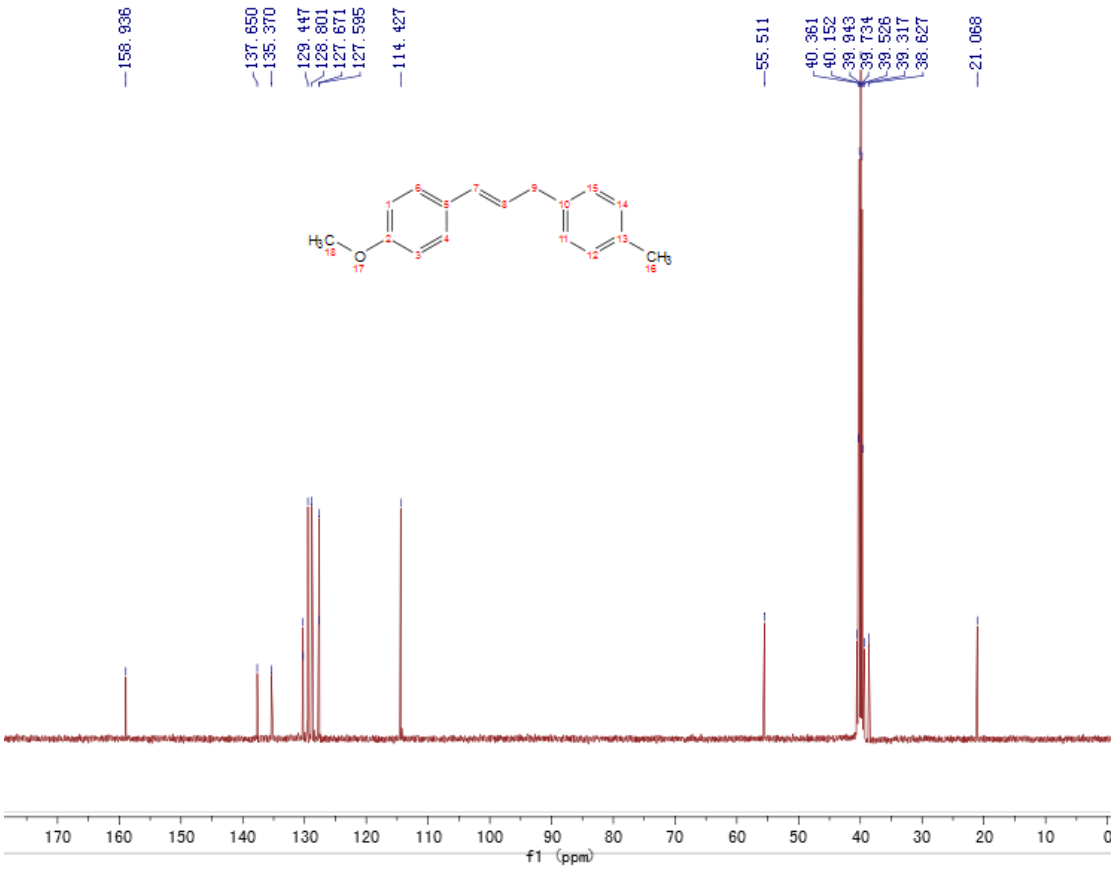
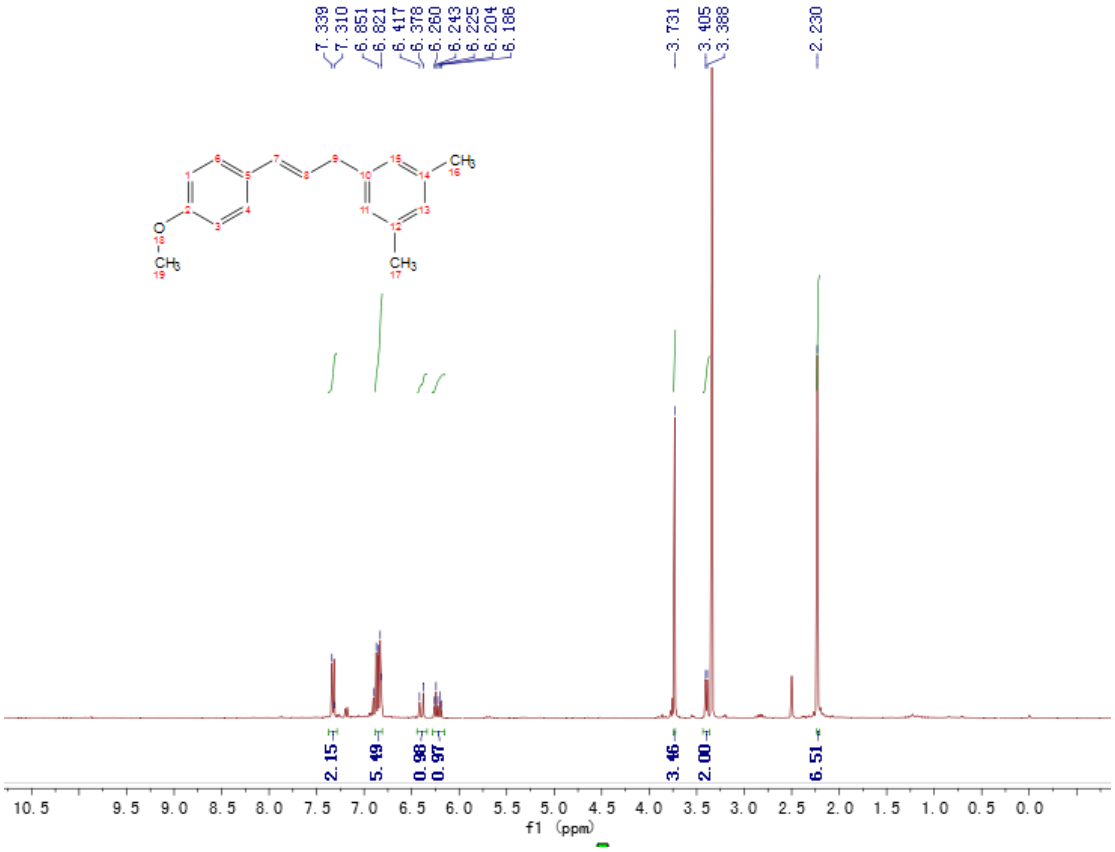
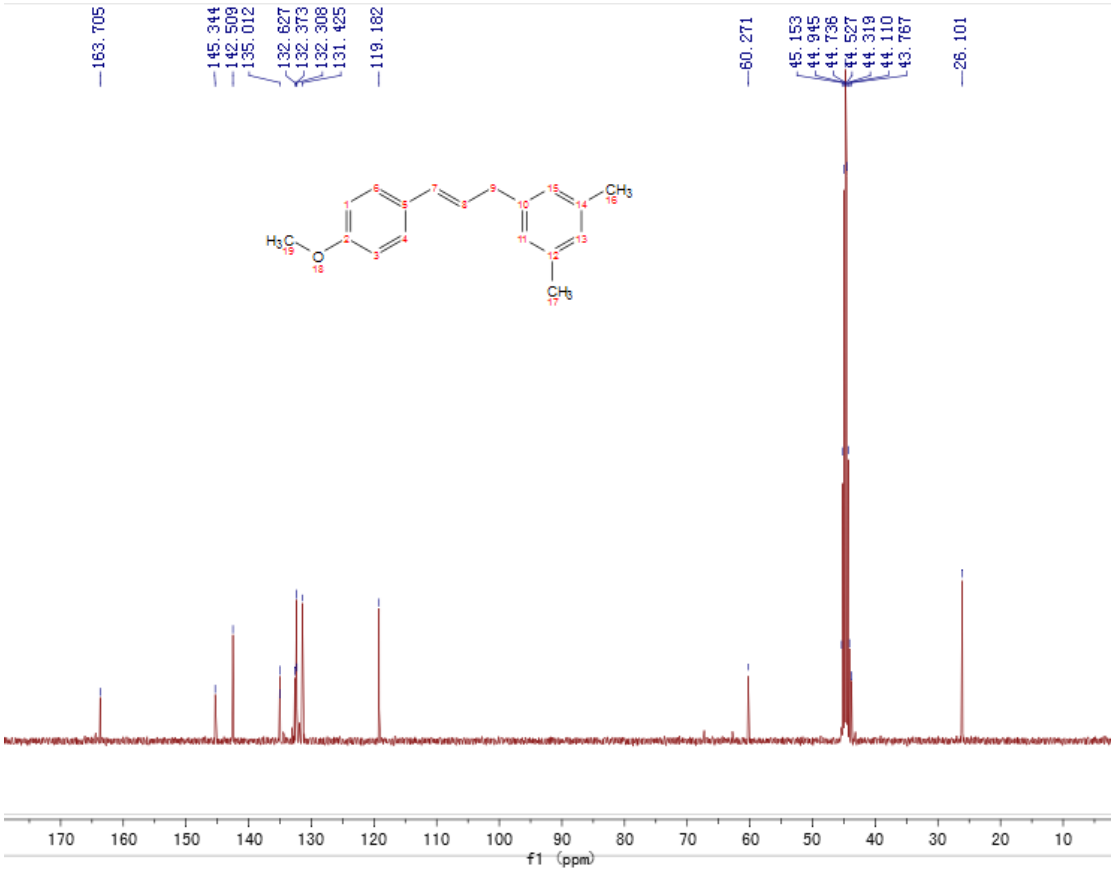
2.16
4.22
2.10
1.00
1.00
3.09
2.00
3.27
f1 (ppm)


158.936
137.650
135.370
129.447
128.801
127.671
127.595
114.427
55.511
40.361
40.152
39.943
39.734
39.526
39.317
38.627
21.068
f1 (ppm)


7.339
7.310
6.851
6.821
6.417
6.378
6.260
6.243
6.225
6.204
6.186
3.731
3.405
3.388
2.230
2.15
5.49
0.98
0.97
3.46
2.00
6.51
f1 (ppm)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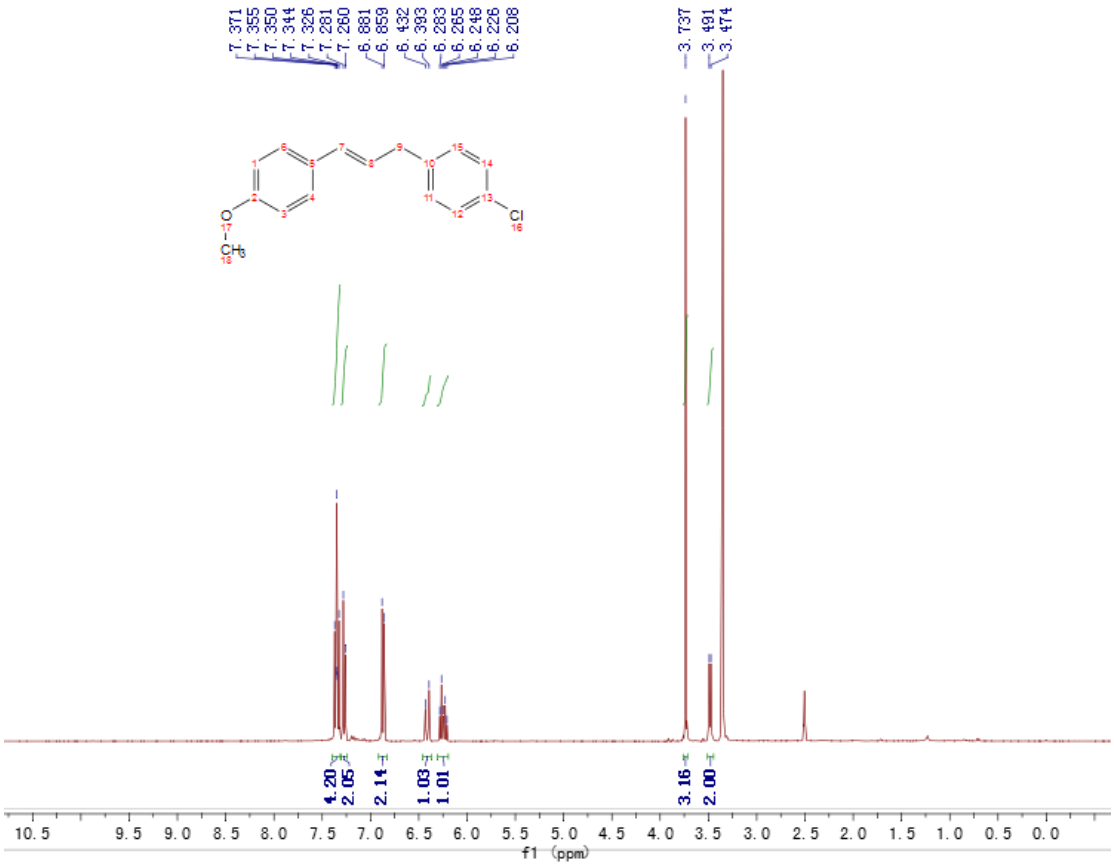
145.344
142.509
135.012
132.627
132.373
132.308
131.425
119.182
60.271
45.153
44.945
44.736
44.527
44.319
44.110
43.767
26.101
f1 (ppm)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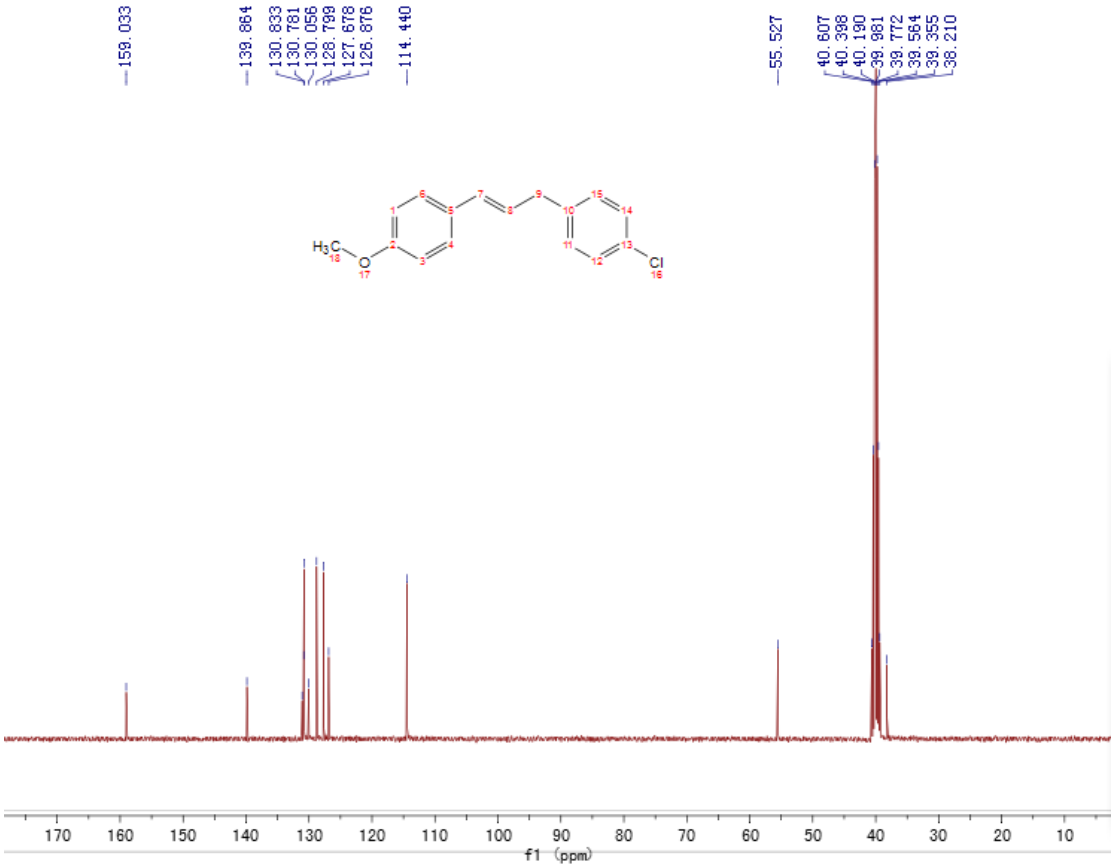
7.355
7.350
7.344
7.326
7.281
7.260
6.881
6.859
6.432
6.393
6.283
6.265
6.248
6.226
6.208
3.737
3.491
3.474
O
CH3
Cl
4.20
2.05
2.14
1.03
1.01
3.16
2.00
f1 (ppm)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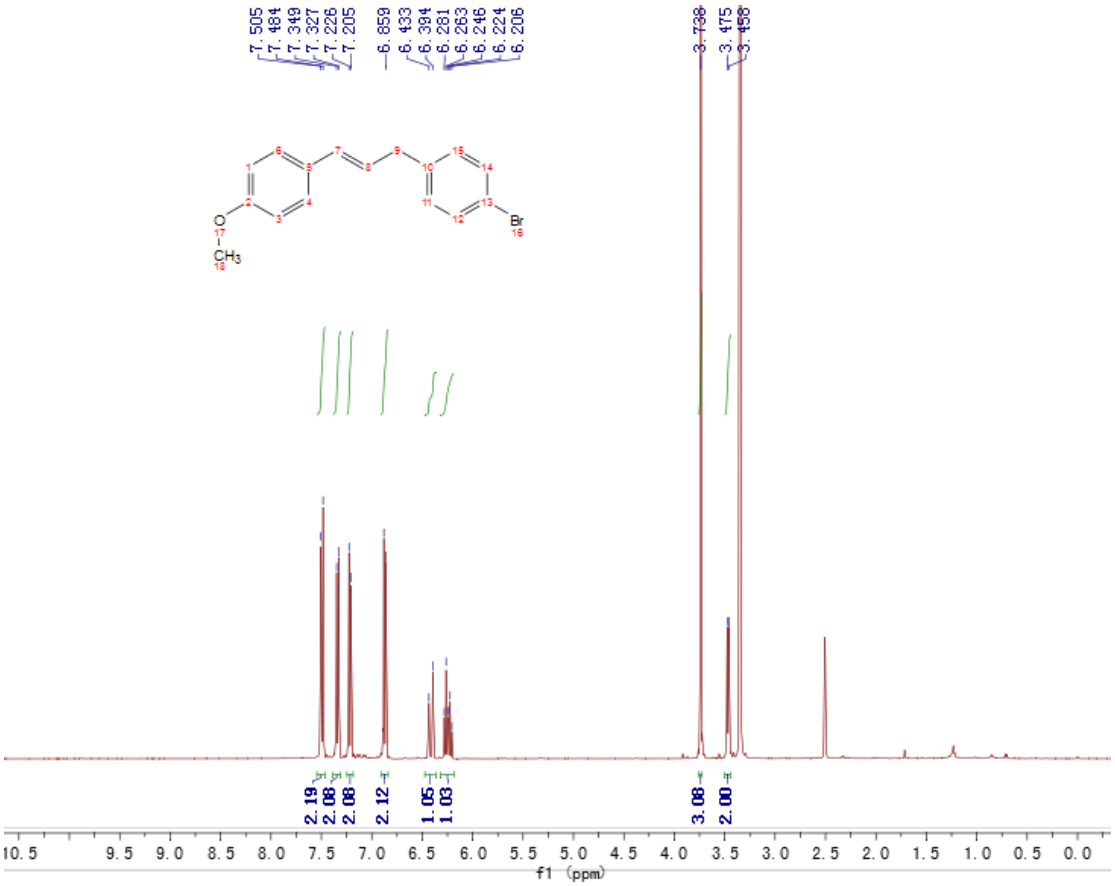
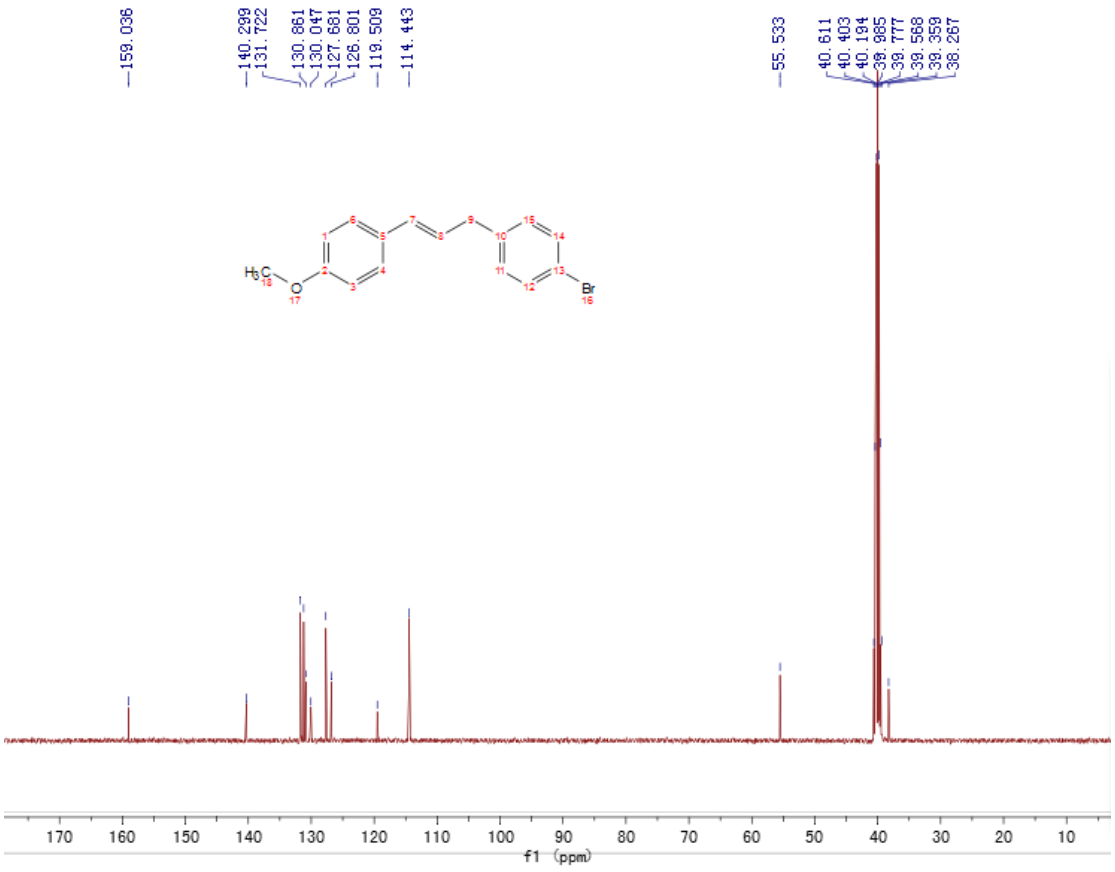
139.864
130.833
130.781
130.056
128.799
127.678
126.876
114.440
55.527
40.607
40.398
40.190
39.981
39.772
39.564
39.355
38.210
H3C
O
Cl
f1 (ppm)


7.505
7.484
7.349
7.327
7.226
7.205
6.859
6.433
6.394
6.281
6.263
6.246
6.224
6.206
3.738
3.475
3.458
2.19
2.06
2.08
2.12
1.05
1.03
3.08
2.00
f1 (ppm)


159.036
140.299
131.722
130.861
130.047
127.681
126.801
119.509
114.443
55.533
40.611
40.403
40.194
39.985
39.777
39.568
39.359
39.267
f1 (ppm)