Electronic Supplementary Material (ESI) for Chemical Science
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Supporting Information

Copper-Catalyzed Decarboxylative Alkenylation of Sp^3 C-H Bonds with Cinnamic Acids via A Radical Process

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Context

General Information

^{1}H and ^{13}C NMR spectra were recorded on a Bruker advance Ⅲ 400 spectrometer in $CDCl_3$ with TMS as internal standard. Mass spectra were determined on a Hewlett Packard 5988A spectrometer by direct inlet at 70 eV. High-resolution mass spectral analysis (HRMS) data were measured on a Bruker Apex II. Element analysis (EA) data were measured on a Vario EL. All products were identified by ^{1}H and ^{13}C NMR, MS, HRMS, and Element Analysis. The starting materials were purchased from Aldrich, Acros Organics, J&K Chemicals or TCI and used without further purification.

Typical procedure

A mixture of cinnamic acid (1 equiv., 0.5 mmol), Cu (0.02 equiv., 0.01 mmol), TBHP (1.2 equiv., 0.6 mmol) and alcohol or ether (3 ml) was heated under reflux at 110 ^{o}C for 12 h. After the reaction finished, the mixture was evaporated under vacuum and purified by column chromatography to afford the desired product.

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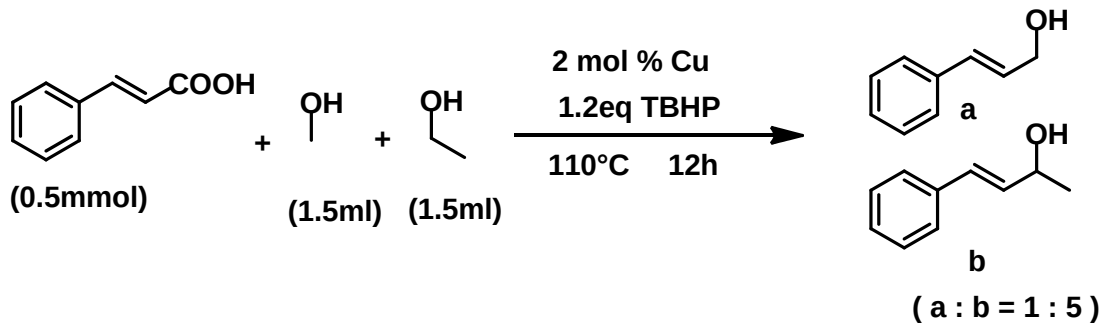
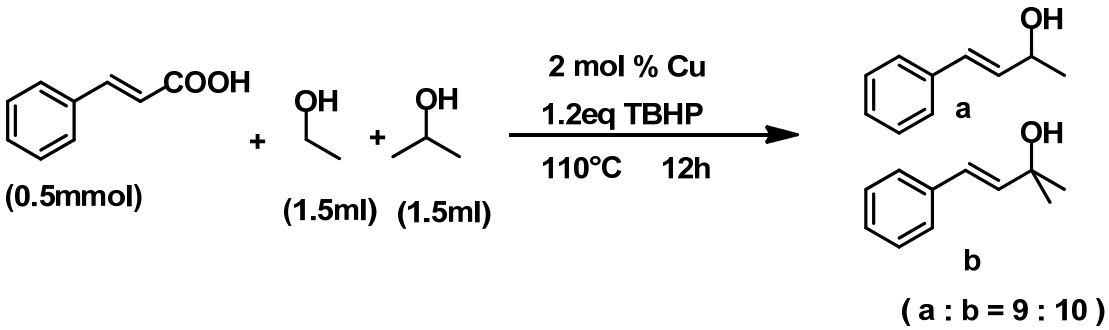
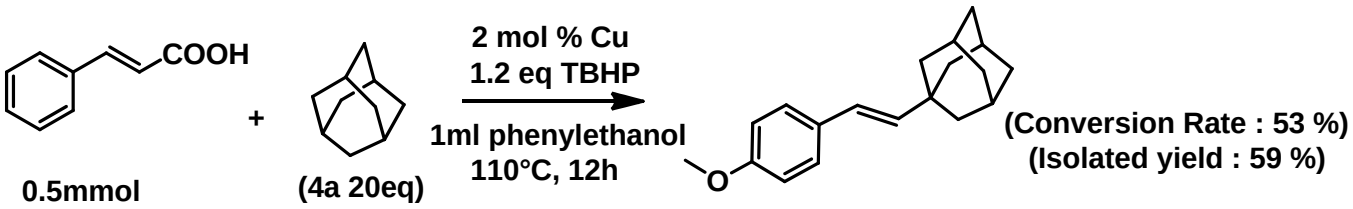
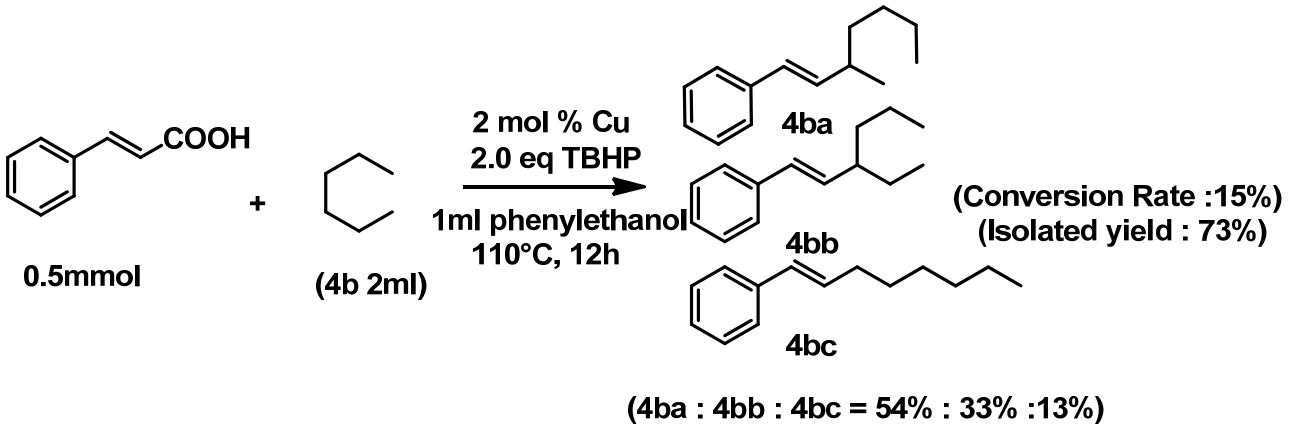
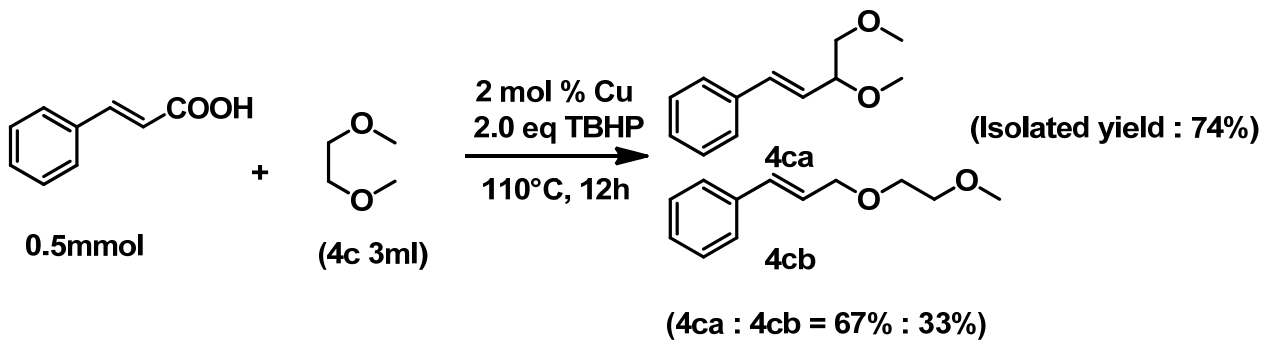
Regiospecificity studies











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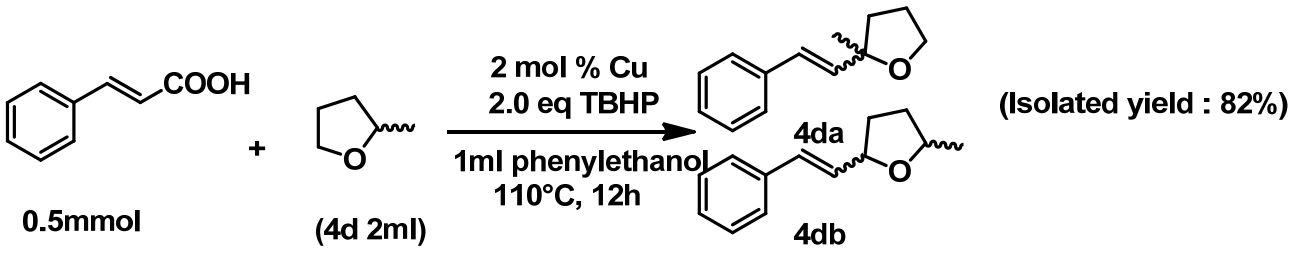
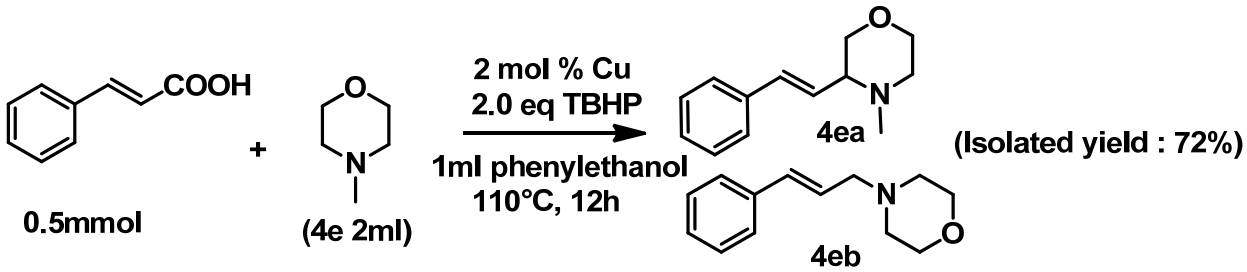
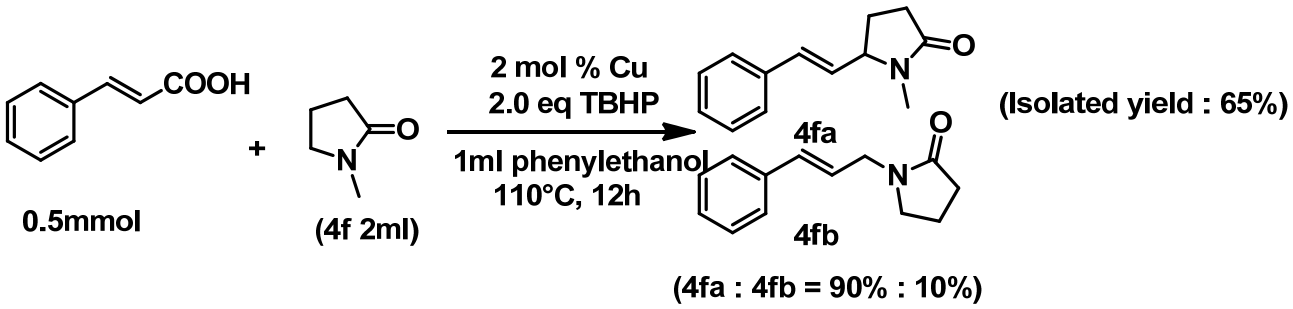
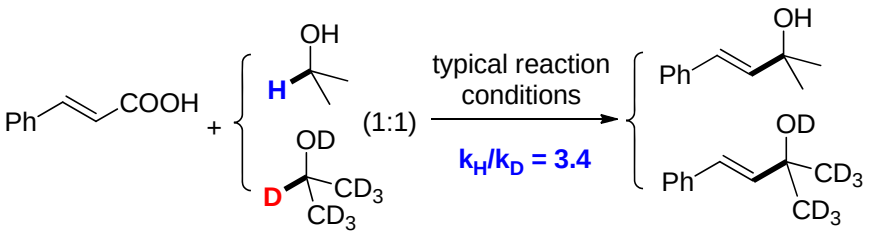






Competing Kinetic Isotope Effect (KIE) Experiment:



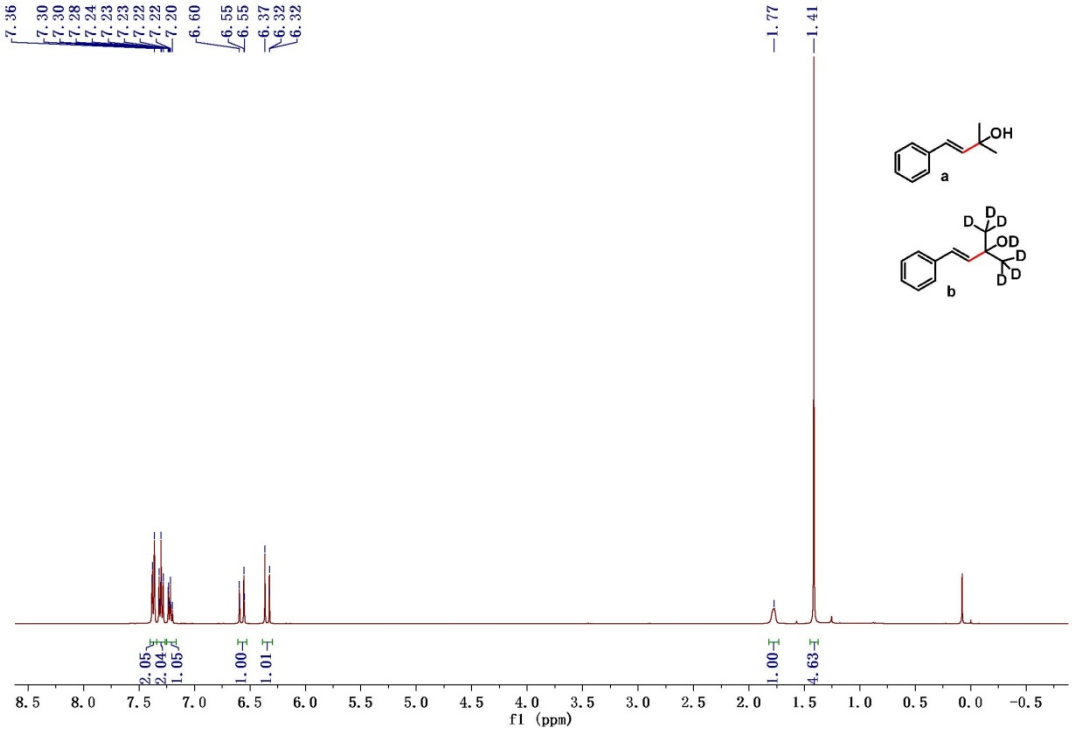


Figure ^{1}H NMR spectra of the mixture of compound **a** and **b**.

Note: The value of k_H/k_D was calculated from the ^{1}H NMR spectra above which should be the mixture of compound **a** and **b** (the KIE scheme). The sum of the integral of **a** and **b** at chemical shift 6.55-6.60 was integrated as 1.00 (both **a** and **b** keep the same double bond hydrogen). Compound **a** has 6 hydrogen atoms at chemical shift 1.41, while **b** has no H atoms. The amount of **a** could be defined as 0.77(4.63/6=0.77), on the other hand, the sum of **a** and **b** is 1.00, so the amount of **b** is 0.23 (1.00-0.77=0.23). As a result, k_H/k_D=0.77/0.23=3.4.

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Physical data and references for the following products

All known compounds are determined by ^{1}H NMR and ^{13}C NMR, MS analysis and compared with which were cited in the following references, and the new compounds were further confirmed by HRMS and/or element analysis.

References:

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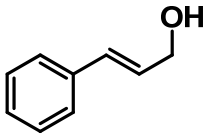
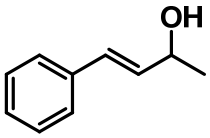
Physical data for the following products:

1a: (*E*)-3-phenylprop-2-en-1-ol



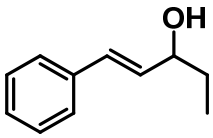
^{1}H NMR (400MHz, $CDCl_3$): δ 7.40－7.38 (m, 2H), 7.34－7.30 (m, 2H), 7.26－7.22 (m, 1H), 6.64－6.60 (d, *J* = 16.0 Hz, 1H), 6.40－6.33 (m, 1H), 4.32－4.31 (m, 2H), 1.58 (s, 1H)
^{13}C NMR (100 MHz, $CDCl_3$): δ 136.6, 131.1, 128.6, 128.5, 127.7, 126.4, 63.7.
MS (EI): *m*/*z* (%): 134 (M+, 47), 117 (15), 105 (45), 91 (55), 77 (34), 57 (100).

1b: (*E*)-4-phenylbut-3-en-2-ol



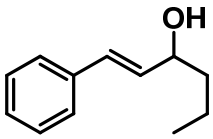
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30－7.28 (m, 2H), 7.24－7.21 (m, 2H), 7.17－7.13 (m, 1H), 6.49－6.45 (d, *J* = 16.0 Hz, 1H), 6.20－6.15 (dd, *J* = 16.0 Hz, J=4.0Hz, 1H), 4.49－4.46 (m, 1H), 1.84 (s, 1H), 1.29 －1.28 (d, *J* = 4.0 Hz, 3H).
^{13}C NMR (100MHz, $CDCl_3$): δ 136.7, 133.5, 129.3, 128.5, 127.6, 126.4, 68.8, 23.3.
MS (EI):*m*/*z* 148 (M+, 59), 131 (62), 105 (100), 91 (63), 77 (33), 43 (62).

1c: (*E*)-1-phenylpent-1-en-3-ol



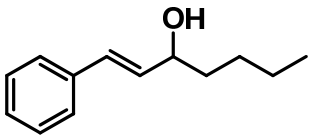
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38－7.36 (m, 2H), 7.32－7.28 (m, 2H), 7.24－7.21 (m, 1H), 6.57－6.53 (d, *J* = 16.0 Hz, 1H), 6.23－6.17 (dd, *J* = 16.0 Hz, *J* = 8.0 Hz, 1H), 4.25－4.20 (m, 1H), 1.92 (s, 1H), 1.69 －1.60 (m, 2H), 0.98－0.94 (t, *J* = 8.0Hz, 3H)
^{13}C NMR (100 MHz, $CDCl_3$): δ 136.7, 132.2, 130.3, 128.5, 127.5, 126.4, 74.31, 30.2, 9.7.
MS (EI): *m*/*z* (%): 162 (M+, 29), 133 (100), 105 (61), 91 (37), 77 (30), 55 (33).

1d: (*E*)-1-phenylhex-1-en-3-ol



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38－7.36 (m, 2H), 7.32－7.29 (m, 2H), 7.24－7.23 (m, 1H), 6.57－6.53 (d, *J* = 16.0 Hz, 1H), 6.24－6.18 (dd, *J* = 16.0 Hz, *J* = 8.0 Hz, 1H), 4.30－4.25 (m, 1H), 1.78 (s, 1H), 1.63 －1.53 (m, 2H), 1.44－1.38 (m, 2H), 0.97－0.93 (t, *J* =8.0Hz, 3H)
^{13}C NMR (100 MHz, $CDCl_3$): δ 136.7, 132.6, 130.1, 128.5, 127.6, 126.4, 72.8, 39.4, 18.6, 14.0.
MS (EI): *m*/*z* (%): 176 (M+, 26), 133 (100), 105 (47), 91 (32), 77 (18), 55 (27), 43 (15).

1e: (*E*)-1-phenylhept-1-en-3-ol



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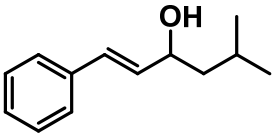
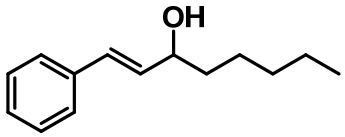
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41－7.39 (m, 2H), 7.34－7.31 (m, 2H), 7.26－7.25 (m, 1H), 6.60－6.56 (d, *J* = 16.0 Hz, 1H), 6.26－6.21 (dd, *J* = 16.0 Hz, *J* = 8.0 Hz, 1H), 4.31－4.26 (m, 1H), 1.69－0.91 (m, 10H)
^{13}C NMR (100 MHz, $CDCl_3$): δ 136.8, 132.6, 130.2, 128.5, 127.6, 126.4, 73.1, 37.1, 27.6, 22.6, 14.0
MS (EI): *m*/*z* (%): 190 (M+, 16), 133 (100), 105 (59), 91 (43), 77 (20), 57 (20).

1f: (*E*)-5-methyl-1-phenylhex-1-en-3-ol



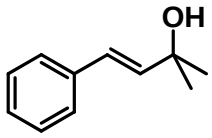
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39－7.37 (m, 2H), 7.33－7.29 (m, 2H), 7.25－7.21 (m, 1H), 6.59－6.55 (d, *J* = 16.0 Hz, 1H), 6.24－6.18 (dd, *J* = 16.0 Hz, *J* = 8.0 Hz, 1H), 4.36－4.34 (m, 1H), 1.79－0.88 (m, 10H).
^{13}C NMR (100 MHz, $CDCl_3$):δ 136.7, 132.8, 130.0, 128.5, 127.6, 126.4, 71.31, 46.4, 24.6, 23.0, 22.6, 22.5.
MS (EI): *m*/*z* (%): 190 (M+, 12), 165 (100), 105 (31), 91 (25), 77 (16), 57 (19), 43 (40).

1g: (*E*)-1-phenyloct-1-en-3-ol



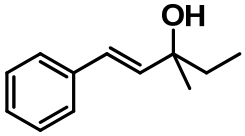
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39－7.37 (m, 2H), 7.31－7.29 (m, 2H), 7.25－7.23 (m, 1H), 6.58－6.54 (d, *J* = 16.0 Hz, 1H), 6.25－6.19 (dd, *J* = 16.0 Hz, *J* = 8.0 Hz, 1H), 4.31－4.26 (m, 1H), 1.71－0.87 (m, 12H)
^{13}C NMR (100 MHz, $CDCl_3$): δ 136.8, 132.6, 130.2, 128.5, 127.6, 126.4, 73.1, 37.3, 31.8, 25.10, 22.6, 14.0
MS (EI): *m*/*z* (%): 204 (M+, 5), 133 (100), 105 (47), 91 (39), 77 (17), 55 (32).

1h: (*E*)-2-methyl-4-phenylbut-3-en-2-ol



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38－7.20 (m, 5H), 6.60－6.56 (d, *J* = 16.0 Hz, 1H) 6.37－6.33 (d, *J* = 16.0 Hz, 1H), 1.73 (s, 1H), 1.42 (s, 6H)
^{13}C NMR (100 MHz, $CDCl_3$): δ 137.5, 136.9, 128.5, 127.4, 126.4, 126.3, 71.0, 29.8.
MS (EI): *m*/*z* (%): 162 (M+, 34), 147 (100), 129 (76), 91 (59), 77 (16), 43 (52).

1i: (*E*)-3-methyl-1-phenylpent-1-en-3-ol.



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38－7.36 (m, 2H), 7.29－7.27 (m, 2H), 7.23－7.21 (m, 1H), 6.60－6.55 (d, *J* = 16.0 Hz, 1H), 6.28－6.24 (d, *J* = 16.0 Hz, 1H), 1.74 (s, 1H), 1.68－1.62 (q, 2H), 1.36 (s, 3H), 0.94－0.90 (t, 3H)
^{13}C NMR (100 MHz, $CDCl_3$): δ 137.0, 136.5, 128.5, 127.2, 127.2, 126.3, 73.34, 35.3, 27.5, 8.3
MS (EI): *m*/*z* (%): 176 (M+, 6), 147 (100), 129 (39), 91 (16), 57 (8), 43 (19).

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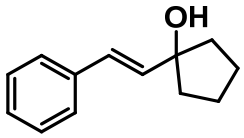
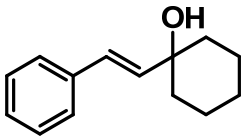
1j: (*E*)-1-styrylcyclopentanol



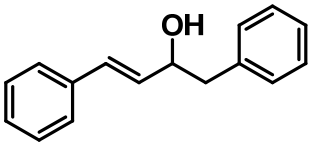
^{1}H NMR (400 MHz, $CDCl_3$):δ 7.39－7.37 (m, 2H), 7.32－7.28 (m, 2H), 7.23－7.19 (m, 1H), 6.67－6.63 (d, *J* = 16.0 Hz, 1H), 6.40－6.36 (d, *J* = 16.0 Hz, 1H) , 1.94－1.90 (m, 2H), 1.80－1.73 (m, 7H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 137.0, 136.0, 128.5, 127.2, 126.7, 126.3, 82.1, 40.7, 23.7.
Anal. Calcd. for $C_{13}H_6O$: C, 82.98; H, 8.51. Found: C, 83.12; H: 8.77

1k: (*E*)-1-styrylcyclohexanol



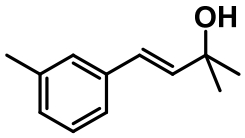
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39－7.37 (m, 2H), 7.32－7.28 (m, 2H), 7.24－7.21 (m, 1H), 6.65－6.61 (d, *J* = 10.0 Hz, 1H), 6.36－6.31 (d, *J* = 10.0 Hz, 1H), 1.68－0.86 (m, 11H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 137.5, 137.1, 128.5, 127.32, 127.0, 126.3, 71.7, 38.0, 25.5, 22.1.
MS (EI): *m*/*z* (%): 202 (M+, 68), 159 (100), 145 (73), 91 (55), 77 (24), 55 (23).

1l: (E)-1,4-diphenylbut-3-en-2-ol



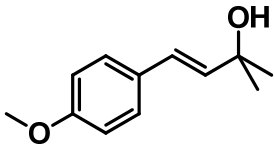
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37－7.23 (m, 10H), 6.60－6.56 (d, *J* = 16.0 Hz, 1H), 6.30－6.24 (dd, *J* = 16.0 Hz, *J* = 8.0 Hz, 1H),4.54－4.51 (m, 1H), 2.98－2.85 (m, 2H). 1.81 (s, 1H)
^{13}C NMR (100 MHz, $CDCl_3$): δ 137.6, 136.7, 131.5, 130.3, 129.6, 128.5, 128.5, 127.62, 126.6, 126.5, 73.4, 44.2
MS (EI): *m*/*z* (%): 224 (M+, 1), 133 (100), 115 (23), 91 (20), 77 (10), 55 (18).

2a: (*E*)-2-methyl-4-(m-tolyl)but-3-en-2-ol



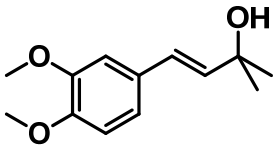
^{1}H NM R(400 MHz,$CDCl_3$): δ 7.20－7.17 (m, 3H), 7.03－7.02 (m, 1H), 6.55－6.51 (d, *J* = 16.0 Hz,1H), 6.34－6.30 (d, *J* = 16.0 Hz, 1H), 2.32 (s, 3H), 1.96 (s, 1H), 1.40 (s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 138.0, 137.3, 136.8, 128.4, 128.1, 127.0, 126.3, 123.5, 70.9, 29.8, 21.3.
Anal. Calcd. for $C_{12}H_{16}O$: C, 81.82; H,9.09. Found: C, 81.53; H: 9.32

2b: (*E*)-4-(4-methoxyphenyl)-2-methylbut-3-en-2-ol



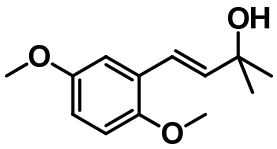
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32－7.30 (m, 2H), 6.86－6.84 (m, 2H),6.54－6.50 (d, *J* = 16.0 Hz, 1H), 6.24－6.20 (d, *J* = 16.0 Hz, 1H) ,3.80 (s, 3H), 1.62 (s, 1H), 1.41 (s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 159.0, 135.4, 129.6, 127.5, 125.8, 114.0, 71.0, 55.3, 29.9.
MS (EI): *m*/*z* (%): 192 (M+, 34), 177 (100), 121 (95), 91 (13), 43 (33).

2c: (*E*)-4-(3,4-dimethoxyphenyl)-2-methylbut-3-en-2-ol



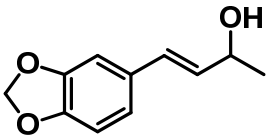
^{1}H NMR (400 MHz, $CDCl_3$): δ 6 .95－6.91 (m, 2H), 6.83－6.81 (d,J = 8.0 Hz, 1H), 6.54－6.50 (d, *J* = 16.0 Hz, 1H), 6.25－6.21 (d, *J* = 16.0 Hz, 1H), 3.91－3.88 (d, 6H), 1.57(s, 1H), 1.43 (s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 149.0, 148.6, 135.5, 129.9, 126.1, 119.5, 111.1, 108.6, 71.0, 55.9, 55.8, 29.9.
MS (EI): *m*/*z* (%): 222 (M+, 52), 207 (92), 189 (24), 151 (100), 91 (10), 43 (24).

2d: (*E*)-4-(2,5-dimethoxyphenyl)-2-methylbut-3-en-2-ol



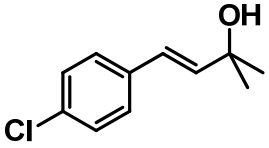
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.0 (d, 1H), 6.91－6.98 (d, *J* = 16.0 Hz, 1H), 6.81－6.77 (m, 2H), 6.38－6.33 (d, *J* = 16.0 Hz, 1H), 3.80－3.78 (d, *J* = 8.0 Hz, 6H), 1.43 (s, 6H), 1.25 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 153.7, 151.2, 138.3, 126.7, 120.9, 113.5, 112.2, 112.0, 71.3, 56.1, 55.8, 29.8.
MS (EI): *m*/*z* (%): 222 (M+, 77), 207 (42), 151 (100), 91 (32), 77 (11), 43 (49).

2e: (*E*)-4-(benzo[d][1,3]dioxol-5-yl)but-3-en-2-ol



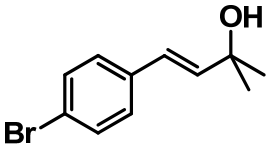
^{1}H NMR (400 MHz, $CDCl_3$): δ 6.91 (d, 2H), 6.81－6.74 (m, 2H), 6.48－6.45 (d, *J* = 12.0 Hz, 1H), 6.11－6.06 (dd, *J* = 16.0 Hz, *J* = 8.0 Hz, 1H), 5.94 (s, 2H), 4.46－4.43 (m, 1H),1.36－1.34 (d, *J*=8.0Hz, 3H)
^{13}C NMR (100 MHz, $CDCl_3$): δ 148.0, 147.2, 131.8, 131.1, 129.1, 121.1, 108.3, 105.7, 101.02, 68. 9, 23.4
Anal. Calcd. for $C_{11}H_{12}O_3$: C, 68.75; H, 6.25. Found: C, 68.46; H: 6.44

2f: (*E*)-4-(4-chlorophenyl)-2-methylbut-3-en-2-ol



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29－7.24 (m, 4H), 6.54－6.50 (d, *J* = 16.0 Hz, 1H), 6.33－6.29 (d, *J* = 16.0 Hz, 1H), 1.95 (s, 1H), 1.41 (s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 138.1, 135.4, 132.9, 128.6, 127.5, 125.1, 70.9, 29.8.
MS (EI): *m*/*z* (%): 196 (M+, 34), 183 (32), 181 (100), 128 (46), 91 (5), 43 (67).

2g: (*E*)-4-(4-bromophenyl)-2-methylbut-3-en-2-ol



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41－7.39 (m, 2H), 7.22－7.20 (m, 2H), 6.53－6.49 (d, *J* = 16.0 Hz, 1H), 6.34－6.30 (d, *J* = 16.0 Hz, 1H), 2.02 (s, 1H), 1.40 (s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 138.2, 135.8, 131.5, 127.9, 125.2, 121.0, 70.9, 29.8.
Anal. Calcd. for $C_{11}H_{13}BrO$: C, 54.77; H, 5.39. Found: C, 55.02; H: 5.36

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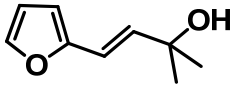
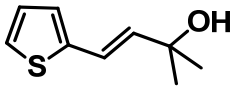
2h: (*E*)-4-(furan-2-yl)-2-methylbut-3-en-2-ol



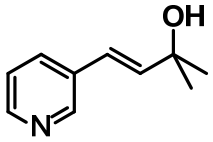
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 (d, 1H), 6.45－6.41 (d, *J* = 16.0 Hz, 1H), 6.37－6.36 (m, 1H), 6.33－6.29 (d, *J* = 16.0 Hz, 1H), 6.23－6.22 (d, *J* = 4.0 Hz, 1H), 1.68(s, 1H), 1.40(s, 6H)
^{13}C NMR (100 MHz, $CDCl_3$): δ 152.6, 141.7, 136.2, 115.2, 111.2, 107.7, 70.83, 29.9.
MS (EI): *m*/*z* (%): 152(M+, 45), 137 (42), 133 (81), 91 (46), 57 (85), 43 (100).

2i: (*E*)-2-methyl-4-(thiophen-2-yl)but-3-en-2-ol



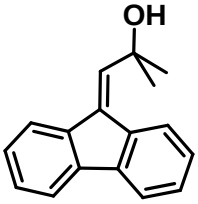
^{1}H NMR (400 MHz, $CDCl_3$): 7.16－7.14 (m, 1H), 6.97－6.95 (m, 2H), 6.76－6.72 (d, *J* = 16.0 Hz, 1H), 6.23－6.19 (d, *J* = 16.0 Hz, 1H), 1.70 (s, 1H), 1.42 (s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 142.1, 137.2, 127.3, 125.5, 123.9, 119.9, 70.9, 29.8
MS (EI): *m*/*z* (%): 168 (M+, 41), 153 (59), 125 (68), 97 (100), 57 (69), 43 (90).

2j: (*E*)-2-methyl-4-(pyridin-3-yl)but-3-en-2-ol



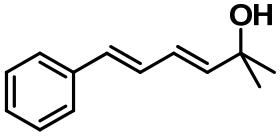
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (s, 1H), 8.42－8.41 (d, *J* = 4.0 Hz, 1H), 7.71－7.69 (m, 1H), 7.26－7.23 (m, 1H), 6.61－6.57 (d, 1H), 6.46－6.42 (d, 1H), 3.62 (s, 1H), 1.44 (s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$) :δ 147.7, 147.6, 140.5, 133.2, 132.9, 123.5, 122.4, 70.6, 29.7.
MS (EI): *m*/*z* (%): 163 (M+, 19), 148 (100), 130 (22), 106 (40), 105 (35), 43 (20).

2k: 1-(9H-fluoren-9-ylidene)-2-methylpropan-2-ol



^{1}H NMR (400 MHz, $CDCl_3$): δ 8.62－8.60 (d, *J* = 8.0 Hz, 1H), 7.65－7.61 (m, 2H), 7.56－7.54 (d, 1H), 7.31－7.22 (m, 4H), 6.73 (s, 1H), 2.01 (s, 1H), 1.60 (s, 6H)
^{13}C NMR (100 MHz, $CDCl_3$): 141.5, 139.8, 138.9, 136.3, 135.4, 135.2, 128.9, 128.2, 128.0, 126.8, 126.75, 119.8, 119.28, 119.27, 70.8, 30.5.
MS (EI): *m*/*z* (%):236 (M+, 39), 193 (38), 178 (40), 165 (100), 110 (47), 43 (26).

2l: (3*E*,5*E*)-2-methyl-6-phenylhexa-3,5-dien-2-ol



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39－7.37 (m, 2H), 7.32－7.28 (m, 2H), δ=7.23－7.21 (m, 1H), 6.79－6.72 (m, 1H), 6.57－6.53 (d, *J*=16.0 Hz, 1H) , 6.42－6.36 (m, 1H), 5.97－5.93 (d, *J*=16.0 Hz, 1H), 1.64(s, 1H), 1.38 (s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 141.7, 137.3, 132.3, 128.6, 128.5, 127.4, 127.0, 126.3, 70.9, 29.8.
MS (EI): *m*/*z* (%): 188 (M+, 38), 173 (19), 117 (72), 104 (29), 91 (100), 43 (34).

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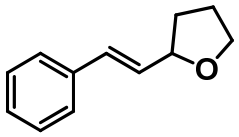
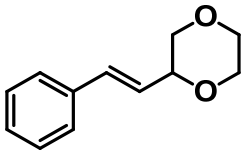
3a: (*E*)-2-styryl-tetrahydrofuran.



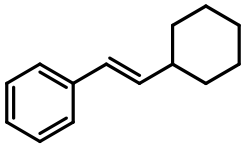
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39－7.37 (m, 2H), 7.32－7.28 (m, 2H), 7.24－7.20 (m, 1H), 6.60－6.56 (d, *J* = 16.0 Hz, 1H), 6.24－6.18 (dd, *J* = 16.0 Hz, *J* = 8.0 Hz, 1H), 4.50-4.45 (m, 1H),4.0－3.95 (m, 1H),3.87－3.81 (m, 1H), 2.15－2.09 (m, 1H), 1.98－1.92 (m, 2H), 1.76－1.69 (m, 1H)
^{13}C NMR (100 MHz, $CDCl_3$): δ 136.8, 130.5, 130.4, 128.5, 127.5, 126.4, 79.7, 68.2, 32.4, 25.9
MS (EI): *m*/*z* (%): 174 (M+, 69), 146 (42), 131 (100), 105 (15), 91 (23), 77 (34), 57 (29).

3b: (*E*)-2-styryl-1,4-dioxane



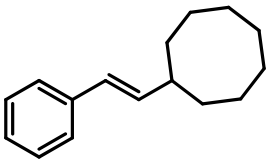
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38－7.36 (m, 2H), 7.32－7.28 (m, 2H), 7.25－7.23 (m, 1H), 6.70－6.66 (d, *J* = 16.0Hz, 1H), 6.10－6.05 (dd, *J* = 16.0 Hz, *J* = 8.0 Hz, 1H), 4.26－4.22 (m, 1H), 3.88－3.78 (m, 3H), 3.75－3.72 (m, 1H), 3.68－3.62 (m, 1H), 3.44－3.38 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 136.3, 132.6, 128.5, 127.9, 126.4, 125.1, 76.0, 70.9, 66.5, 66.2.
MS (EI): *m*/*z* (%): 190 (M+, 30), 131 (78), 99 (24), 86 (100), 77 (12), 57 (9), 43 (6).

3c: (*E*)-(2-cyclohexylvinyl)benzene



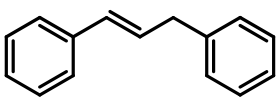
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35－7.33 (m, 2H), 7.29－7.24 (m, 2H), 7.19－7.17 (m, 1H), 6.36－6.32(d, *J* = 16.0 Hz, 1H), 6.20－6.14 (dd, *J* = 16.0 Hz, *J* = 8.0Hz, 1H), 2.14－1.14 (m, 11H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 138.1, 136.8, 128.4, 127.2, 126.7, 125.9, 41.2, 33.0, 26.2, 26.1
MS (EI): *m*/*z* (%):186 (M+, 27), 129 (30), 115 (22), 104 (100), 91 (41), 55 (22).

3d: (*E*)-styrylcyclooctane



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34－7.32 (m, 2H), 7.29－7.23 (m, 2H), 7.18－7.16 (m, 1H), 6.33－6.29 (d, *J* = 16.0 Hz, 1H), 6.23－6.18 (dd, *J* = 16.0 Hz, *J* = 8.0 Hz, 1H) , 2.38－0.85 (m, 15H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 138.1, 137.8, 128.4, 126.8, 126.6, 125.9, 41.3, 31.8, 27.4, 26.0, 25.1.
MS (EI): *m*/*z* (%): 214 (M+, 29), 129 (58), 104 (100), 91 (36), 55(9).

3e: (*E*)-prop-1-ene-1,3-diyldibenzene



^{1}H NMR (400 MHz, $CDCl_3$):δ 7.36－7.19 (m, 10H), 6.47－6.43 (d, 1H), 6.39－6.33 (m, 1H), 3.55－3.53 (d, *J* = 8.0 Hz, 2H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 140.2, 137.5, 131.1, 129.2, 128.7, 128.5, 127.1, 126.2, 126.1, 39.3.
MS (EI): *m*/*z* (%):194 (M+, 100), 193 (62), 179 (42), 178 (39), 116 (37), 115 (66).

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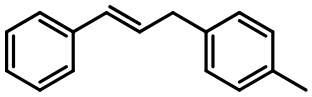
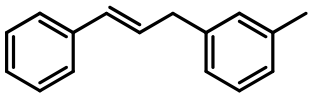
3f: 1-cinnamyl-4-methylbenzene



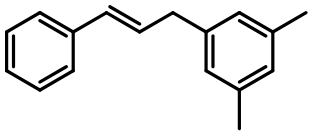
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35－7.12 (m, 9H), 6.46－6.42 (d, 1H), 6.37－6.30 (m, 1H), 3.51－3.49 (d, *J* = 8.0 Hz, 2H), 2.32 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 137.6, 137.1, 135.7, 130.8, 129.5, 129.2, 128.5, 127.0, 126.1, 38.9, 21.0.
MS (EI): *m*/*z* (%): 208 (M+, 100), 193 (96), 179 (12), 129 (16), 115 (83).

3g: 1-cinnamyl-3-methylbenzene



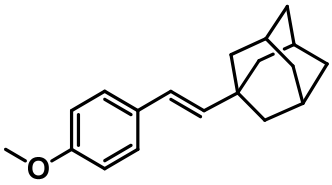
^{1}H NMR (400 MHz, $CDCl_3$):δ 7.36－7.02 (m, 9H), 6.47－6.43 (d, 1H), 6.38－6.32 (m, 1H), 3.52－3.50 (d, *J* = 8.0 Hz, 2H), 2.33 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 140.1, 138.1, 137.5, 130.9, 129.4, 129.4, 128.5, 128.4, 127.1, 126.90, 126.1, 125.7, 39.3, 21.4.
MS (EI): *m*/*z* (%):208 (M+, 100), 194(23), 193 (91), 115 (81), 105 (40), 91 (29).

3h: 1-cinnamyl-3,5-dimethylbenzene.



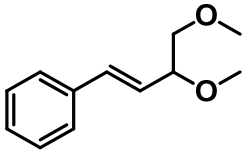
^{1}H NMR (400 MHz, $CDCl_3$):δ 7.36－6.85 (m, 8H), 6.47－6.43 (d, 1H),6.37－6.31 (m, 1H), 3.47－3.46 (d, *J* = 4.0 Hz, 2H), 2.29 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 140.0, 138.0, 137.5, 130.8, 129.5, 128.5, 127.8, 127.0, 126.4, 126.1, 39.3, 21.3.
MS (EI): *m*/*z* (%): 222 (M+, 96), 207 (100), 192 (28), 179 (14), 91 (28), 44 (11).

4a: (1s,3s)-1-((*E*)-4-methoxystyryl)adamantane



^{1}H NM R(400 MHz,$CDCl_3$): δ 7.30－7.28 (m, 2H), 6.84－6.82 (m, 2H), 6.20－6.16 (d, *J* = 16.0 Hz,1H), 5.99－5.95 (d, *J* = 16.0 Hz, 1H), 3.79 (s, 3H), 2.02 (s, 3H), 1.76－1. 67 (m, 12H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 158.5, 140.1, 131.0, 127.0, 123.7, 113.9, 55.3, 42.3, 36.9, 35.0, 28.5.
MS (EI): *m*/*z* (%):268 (M+, 100), 211(35), 134 (12), 121 (16), 91 (11), 77 (5).

4ca: (*E*)-1-(3,4-dimethoxybut-1-enyl)benzene



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42－7.39 (m, 2H), 7.34－7.30 (m, 2H), 7.27－7.23 (m, 1H), 6.66－6.62 (d, *J* = 16.0 Hz, 1H), 6.13－6.07 (dd, *J* = 16.0 Hz, *J* = 8.0 Hz, 1H), 3.98－3.94 (m, 1H), 3.55－3.46 (m, 2H), 3.41 (s, 3H), 3.38 (s, 3H)
^{13}C NMR (101 MHz, $CDCl_3$): δ 136.3, 133.6, 128.5, 127.9, 126.5, 126.5, 81.3, 75.6, 59.3, 56.6.
HRMS (ESI, m/z): Calculated for $C_{12}H_{16}O_2$ $(M+Na)^+$ 215.1048, found 215.1048.

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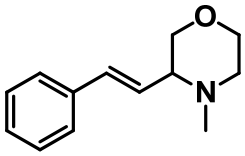
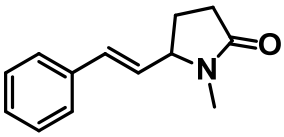
4ea: (*E*)-4-methyl-3-styrylmorpholine



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38－7.36 (m, 2H), 7.33－7.30 (m, 2H), 7.26－7.22 (m, 1H), 6.64－6.60 (d, *J* = 16.0 Hz, 1H), 6.03－5.96 (dd, *J* = 16.0 Hz, *J* = 12.0 Hz, 1H), 3.88－3.84 (m, 1H), 3.75-3.67 (m, 2H), 3.42－3.37 (m, 1H), 3.78－3.76 (m, 2H), 2.37－2.31 (m, 1H), 2.29 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 136.5, 134.0, 128.6, 127.8, 127.4, 126.3, 71.1, 67.1, 66.6, 54.8, 43.8.
HRMS (ESI, m/z): Calculated for $C_{13}H_{18}NO$ $(M+H)^+$ 204.1388, found 204.1377.

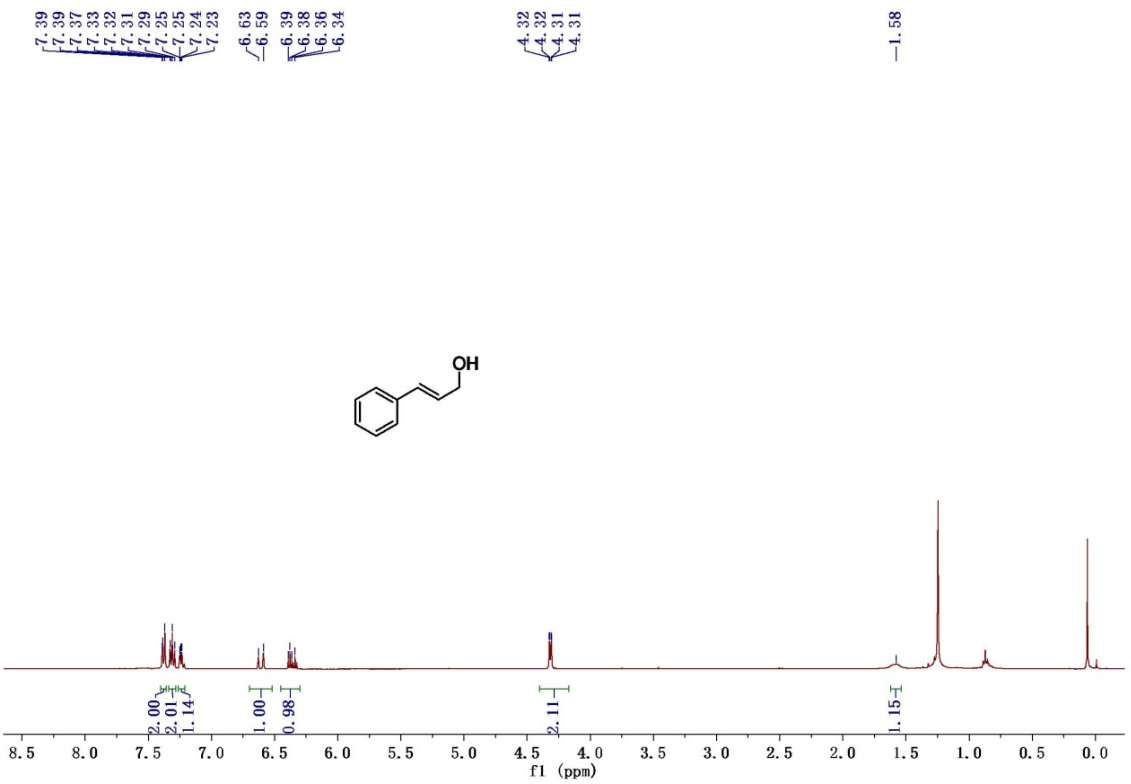
4fa: (*E*)-1-methyl-5-styrylpyrrolidin-2-one



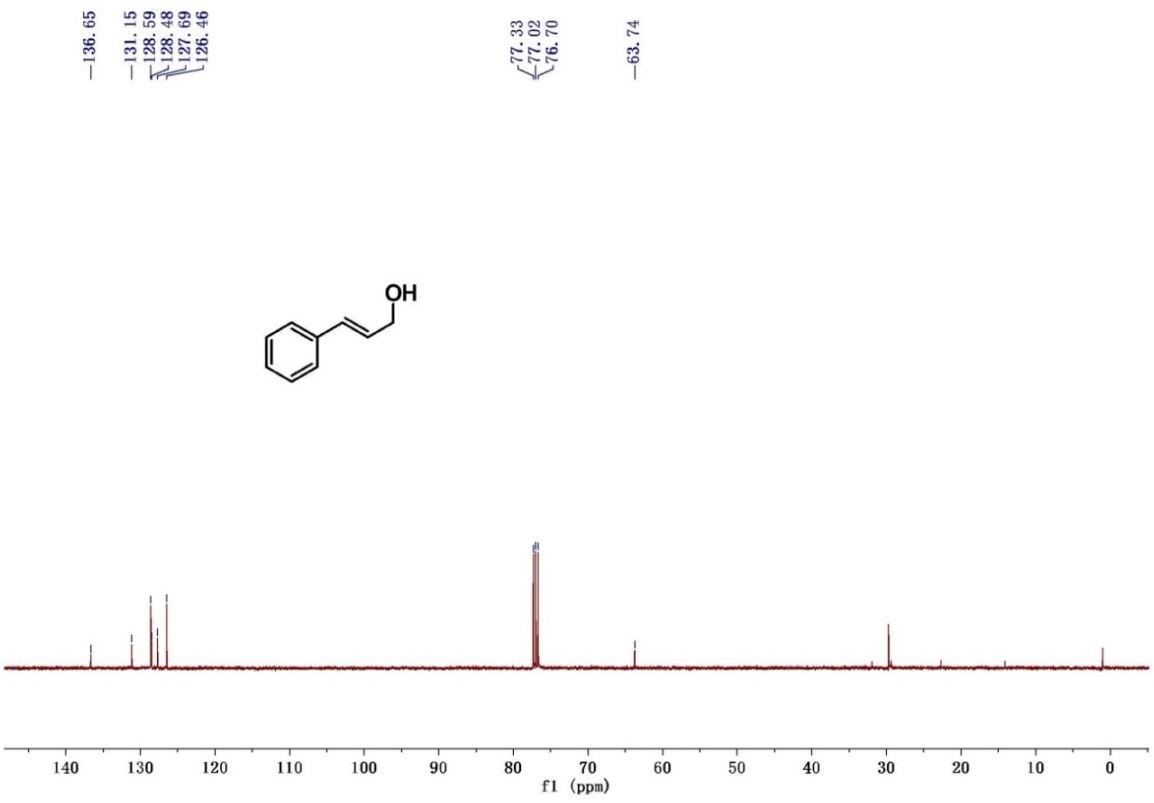
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41－7.40 (m, 2H), 7.36－7.34 (m, 2H), 7.32－7.27 (m, 1H), 6.59－6.55 (d, *J* = 16.0 Hz, 1H), 6.05－5.99 (dd, *J* = 16.0 Hz, *J* = 8.0 Hz, 1H), 4.13－4.09 (m, 1H), 2.79 (s, 3H), 2.51－2.27 (m, 3H), 1.87－1.82 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 175.0, 135.8, 132.9, 128.8, 128.7, 128.1, 126.5, 62.9, 30.0, 27.9, 25.7.
HRMS (ESI, m/z): Calculated for $C_{13}H_{16}NO$ $(M+H)^+$ 202.1232, found 202.1222.

Copies of the ^{1}H NMR and ^{13}C NMR

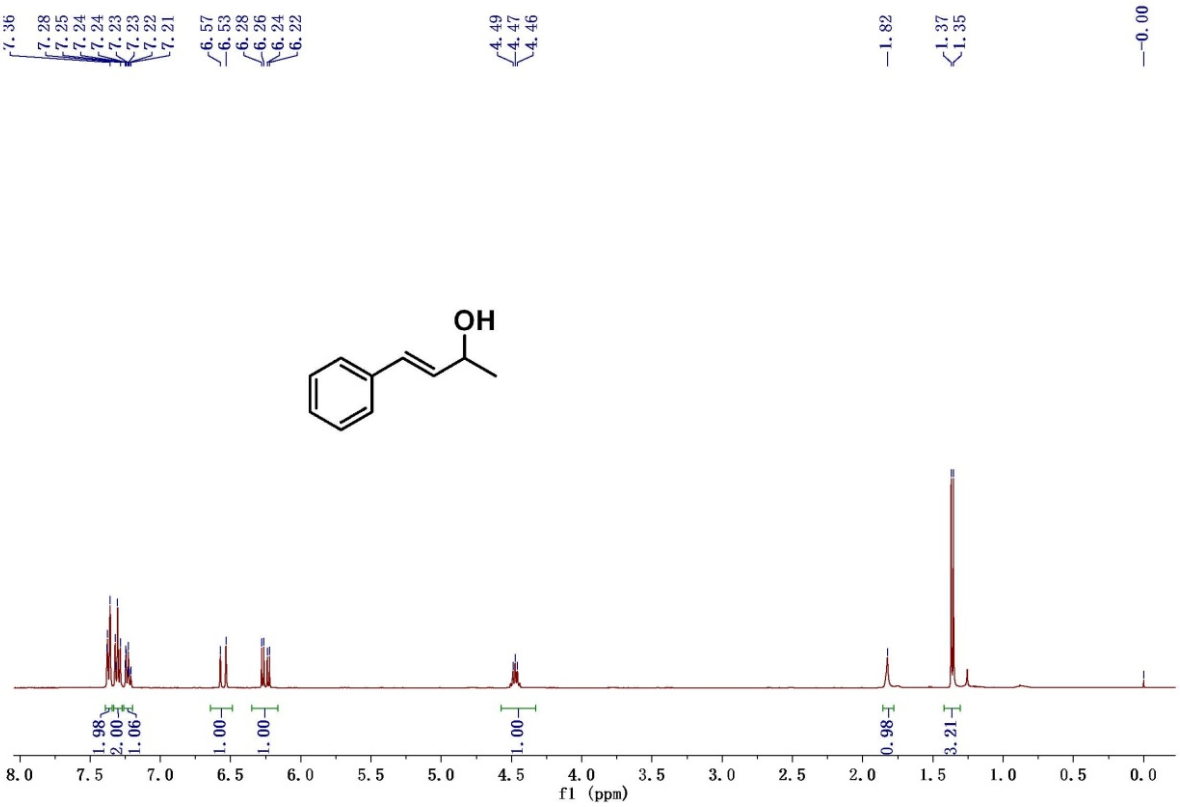
1a- ^{1}H NMR



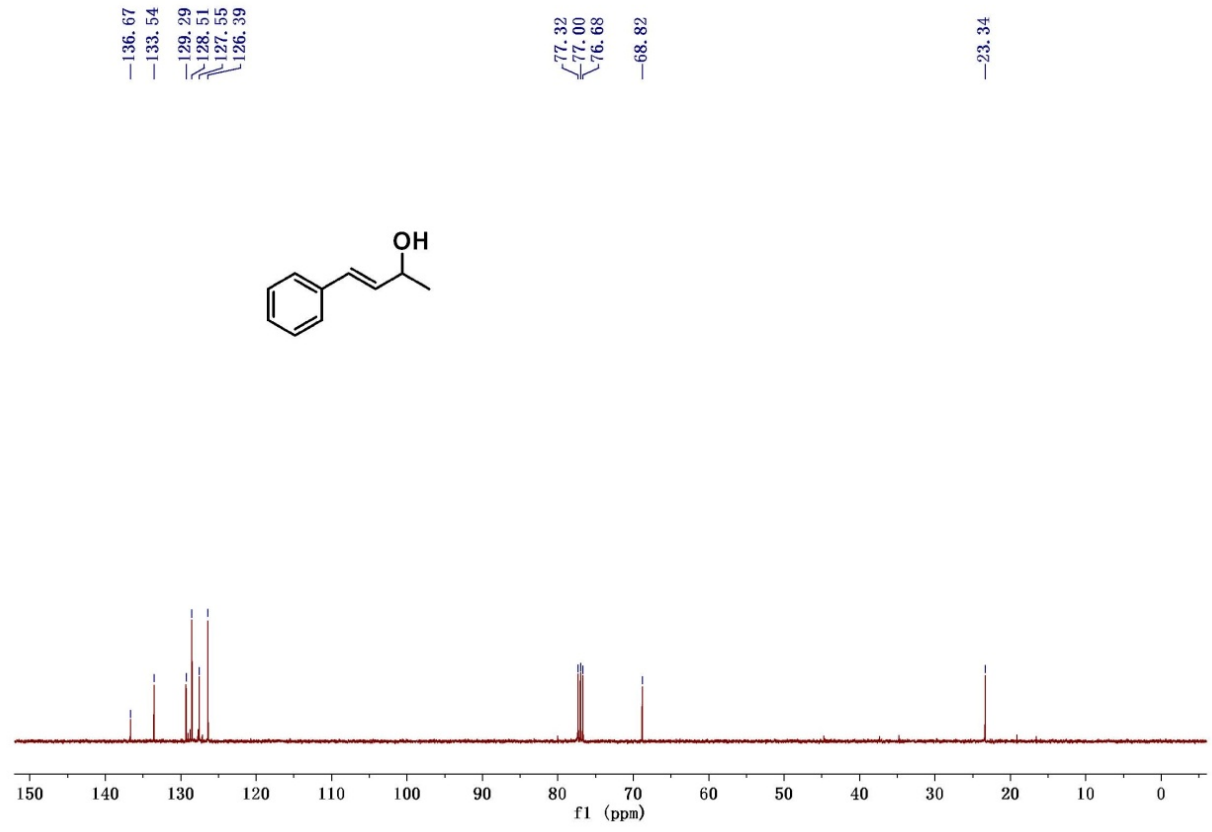
1a- ^{13}C NMR



1b- ^{1}H NMR



1b- ^{13}C NMR



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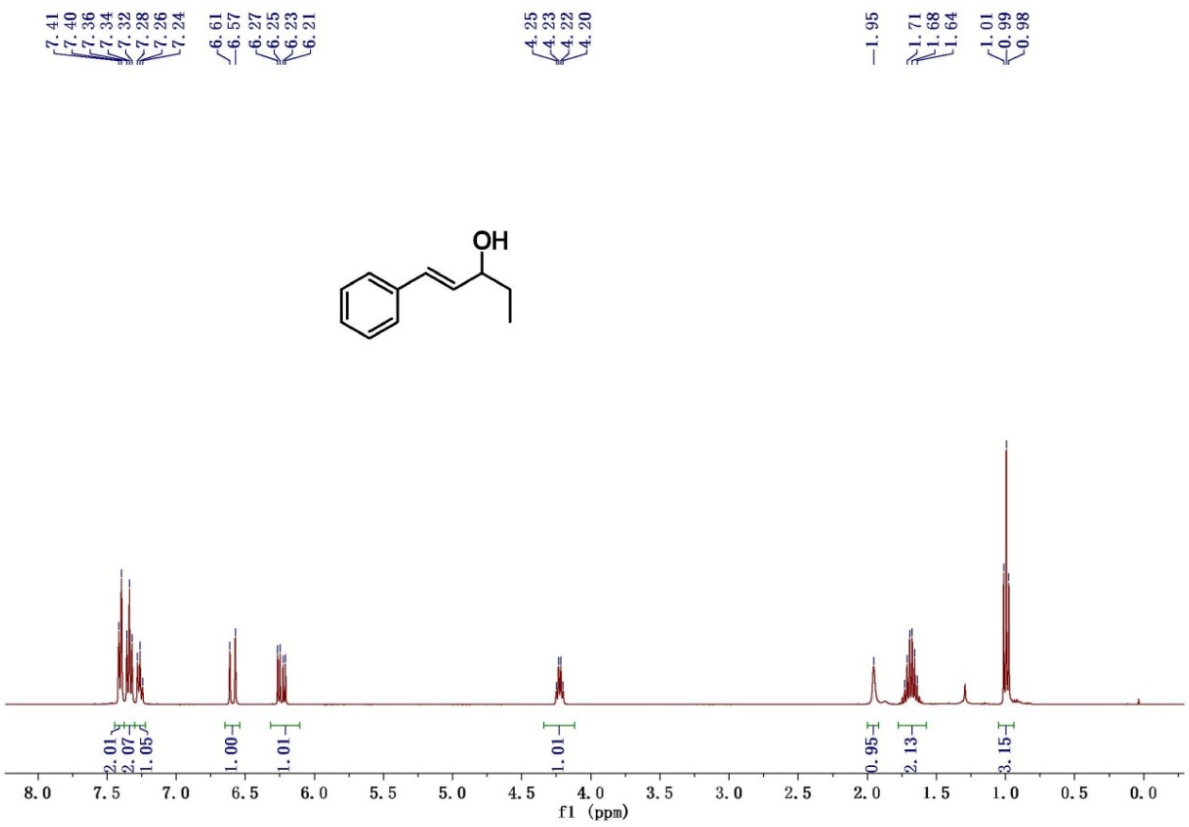
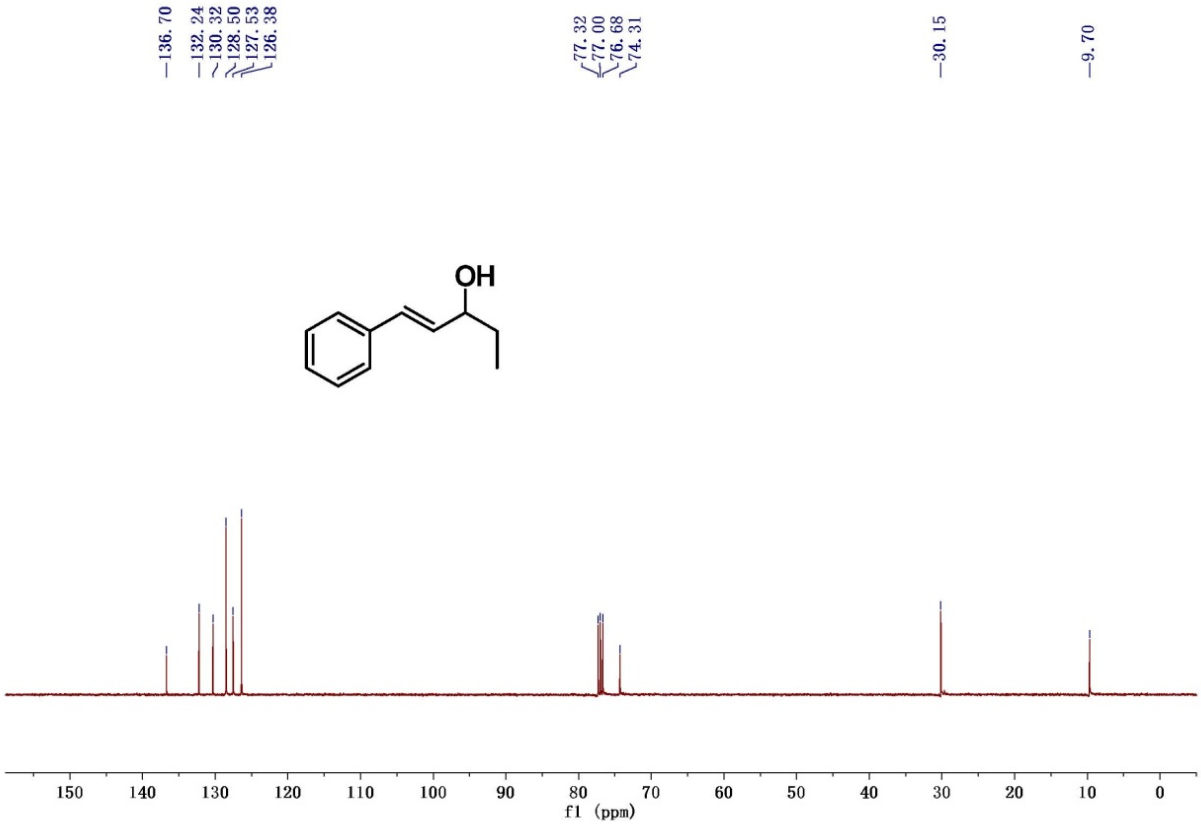
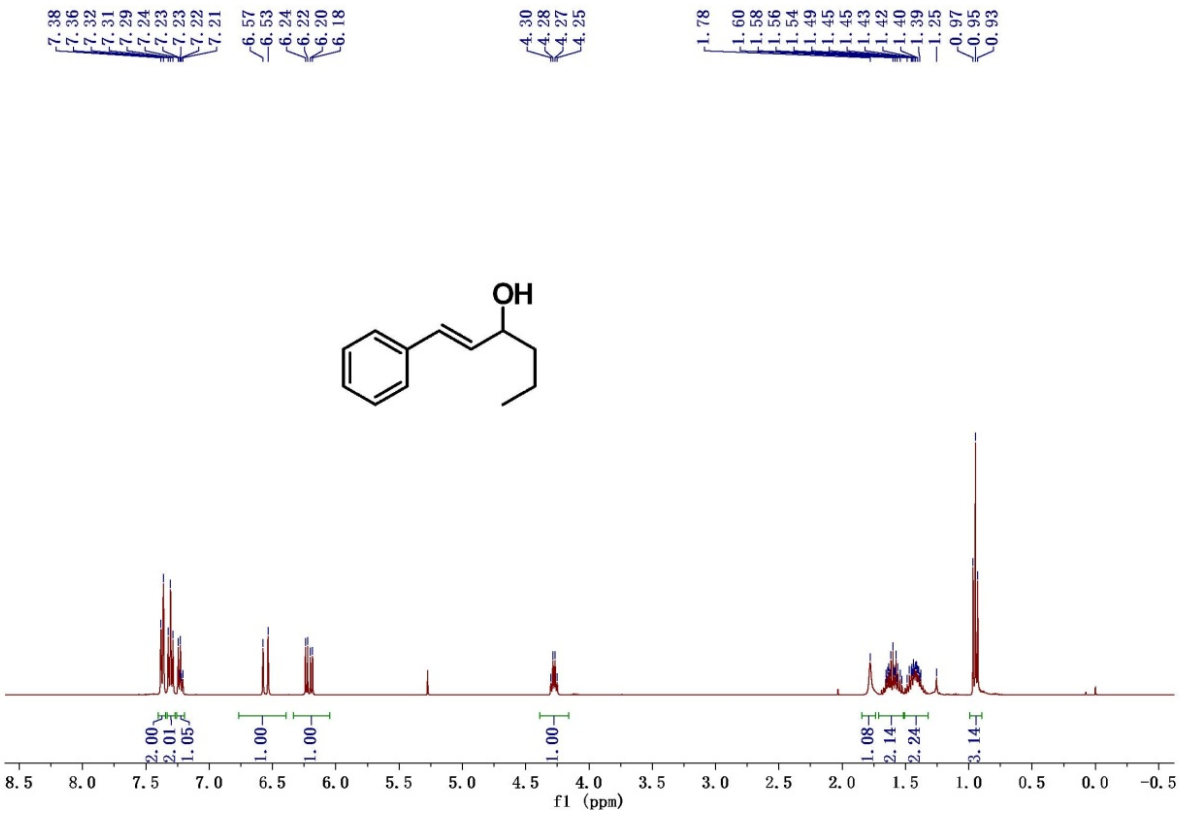
1c- ^{1}H NMR



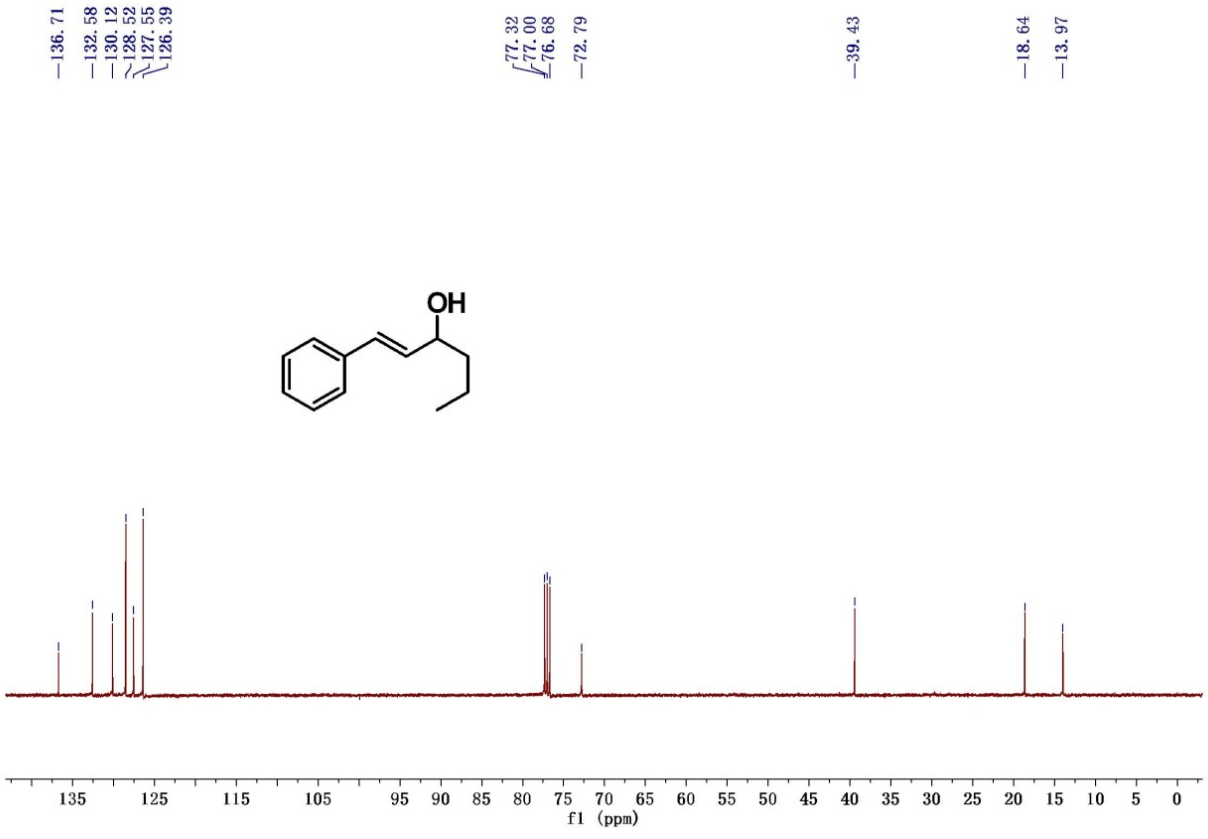
1c- ^{13}C NMR



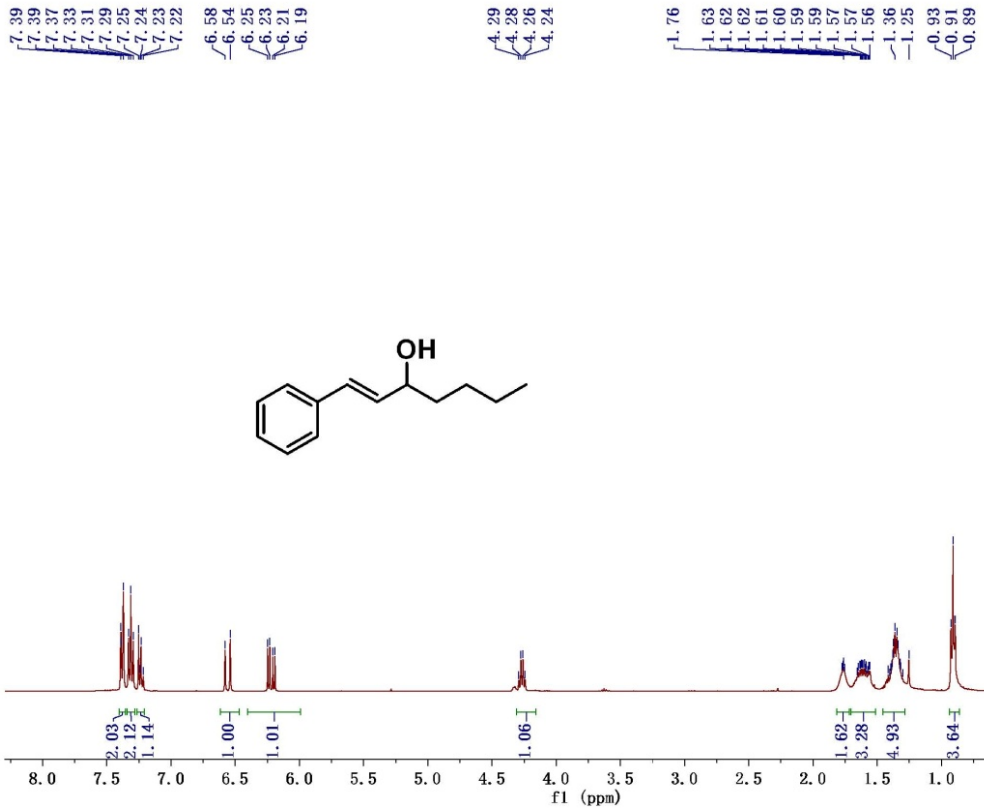
1d- ^{1}H NMR



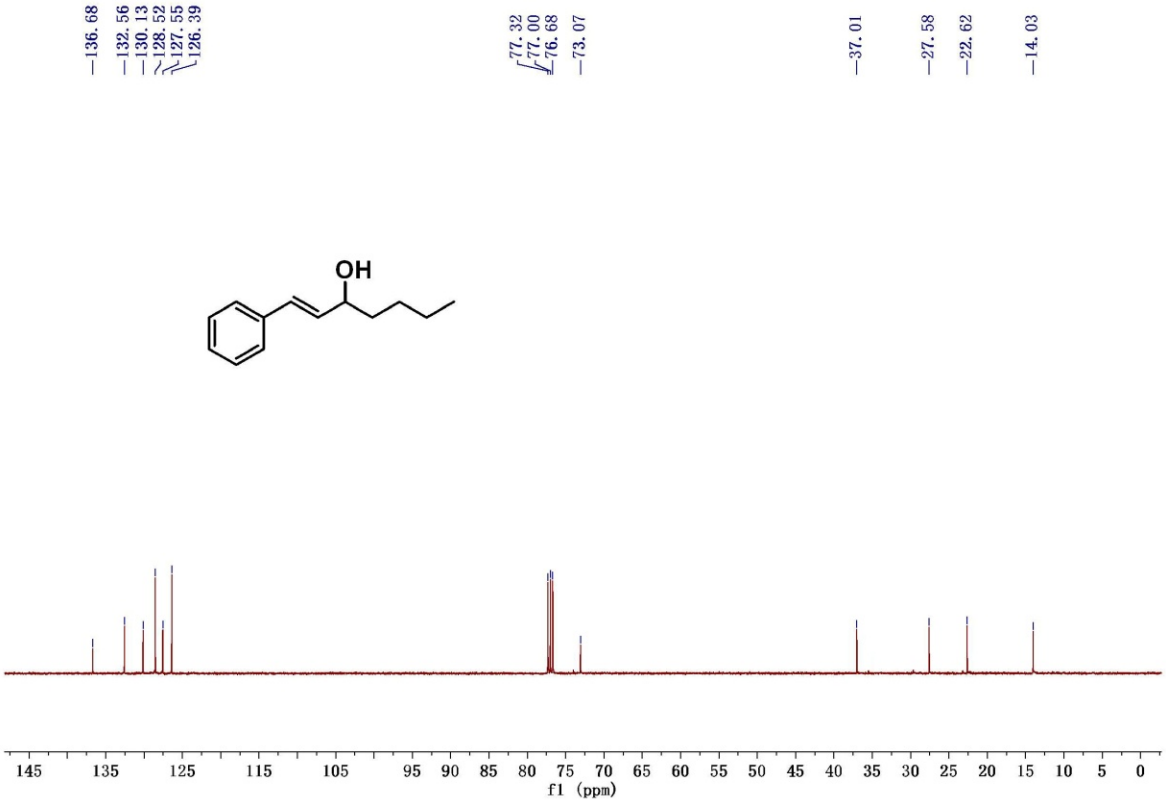
1d- ^{13}C NMR



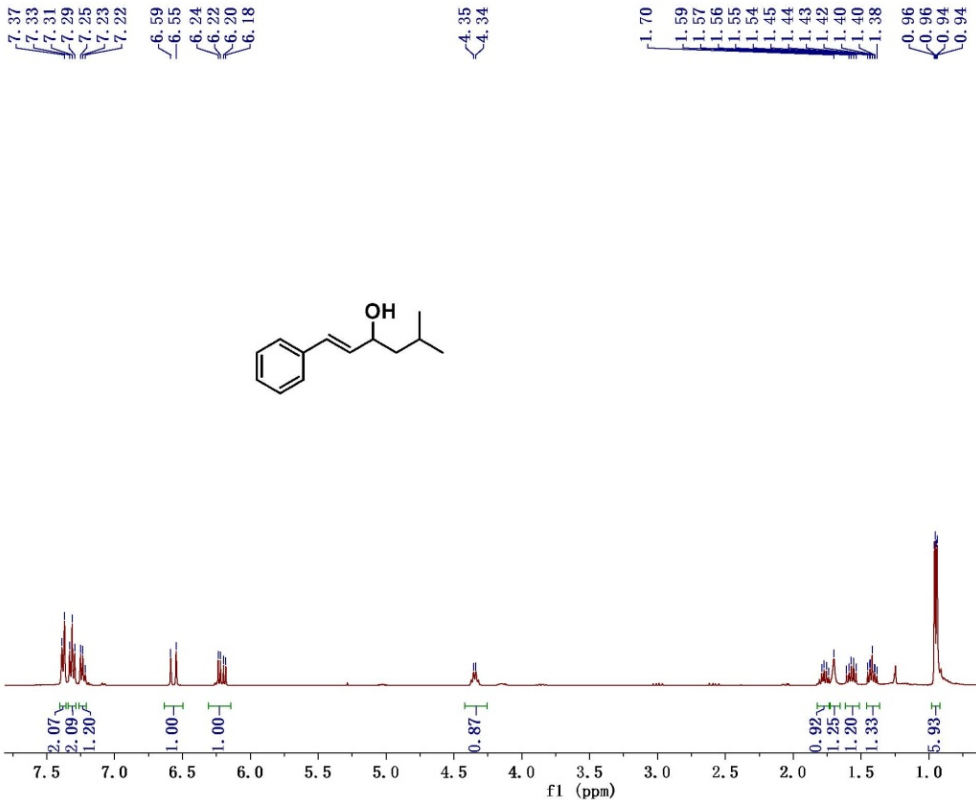
1e- ^{1}H NMR



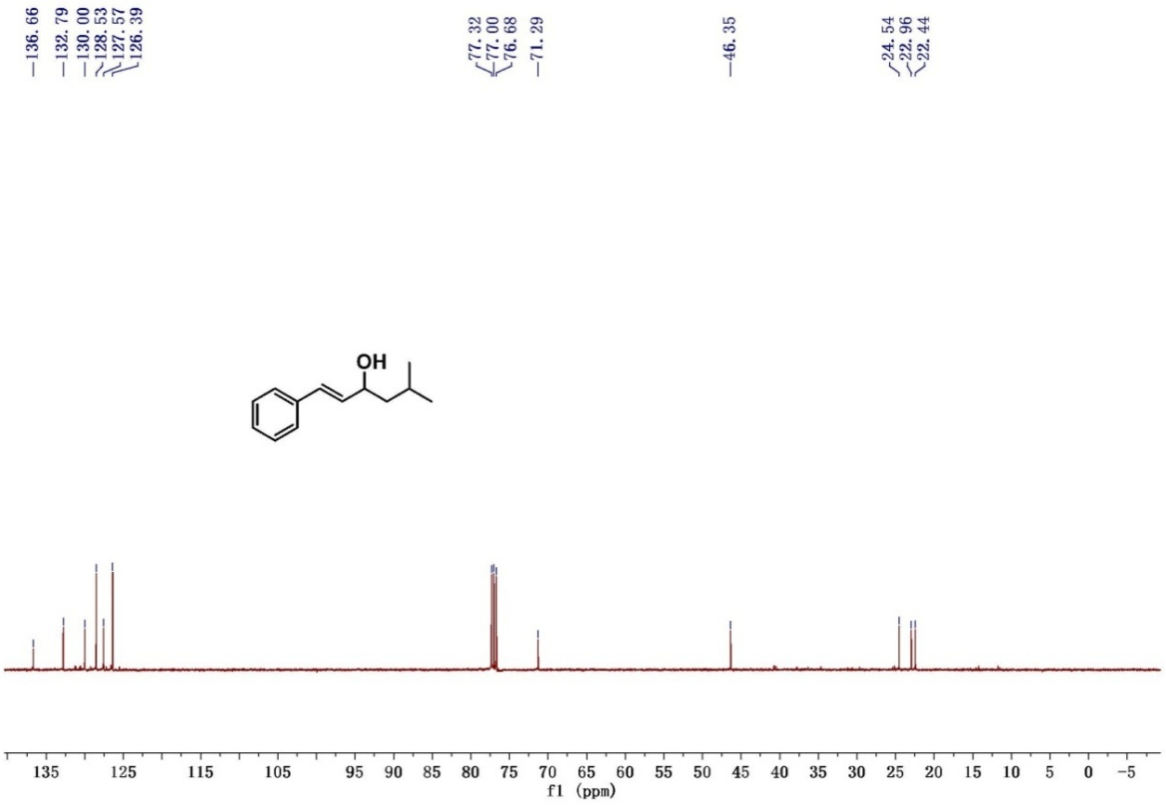
1e- ^{13}C NMR



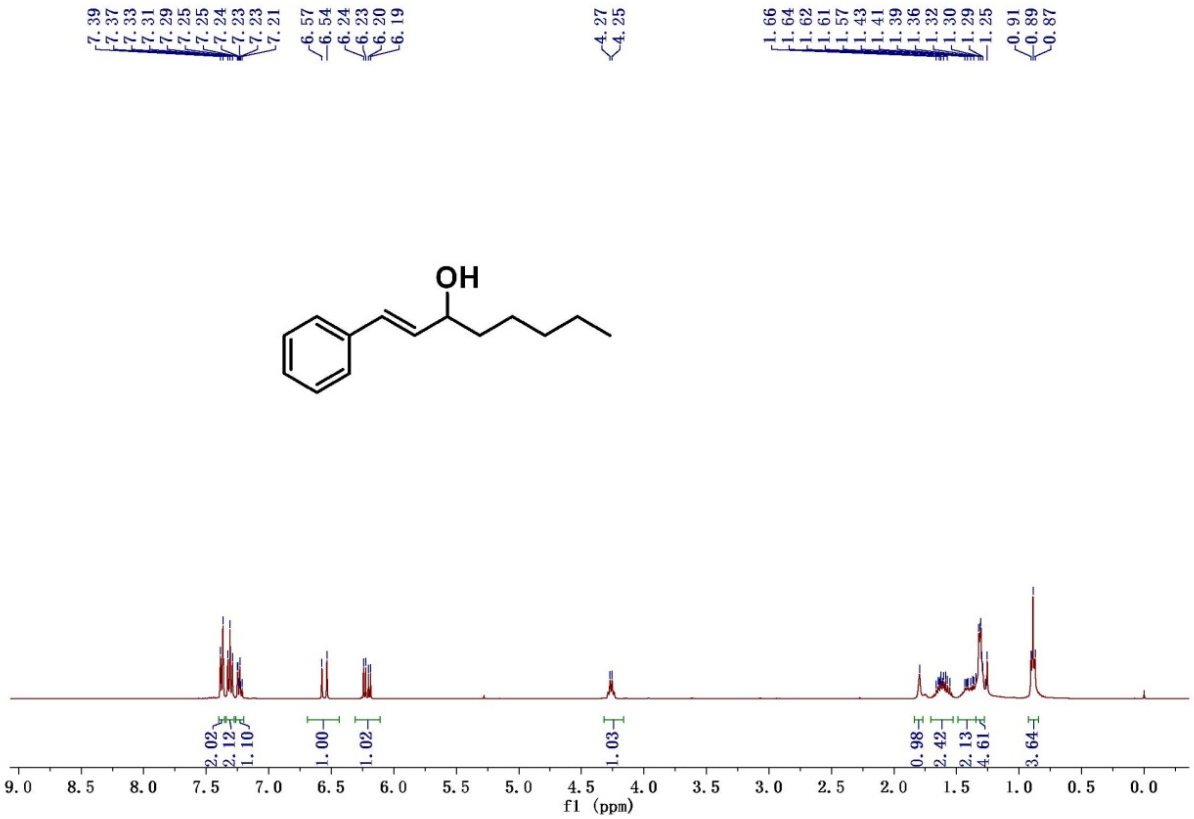
1f- ^{1}H NMR



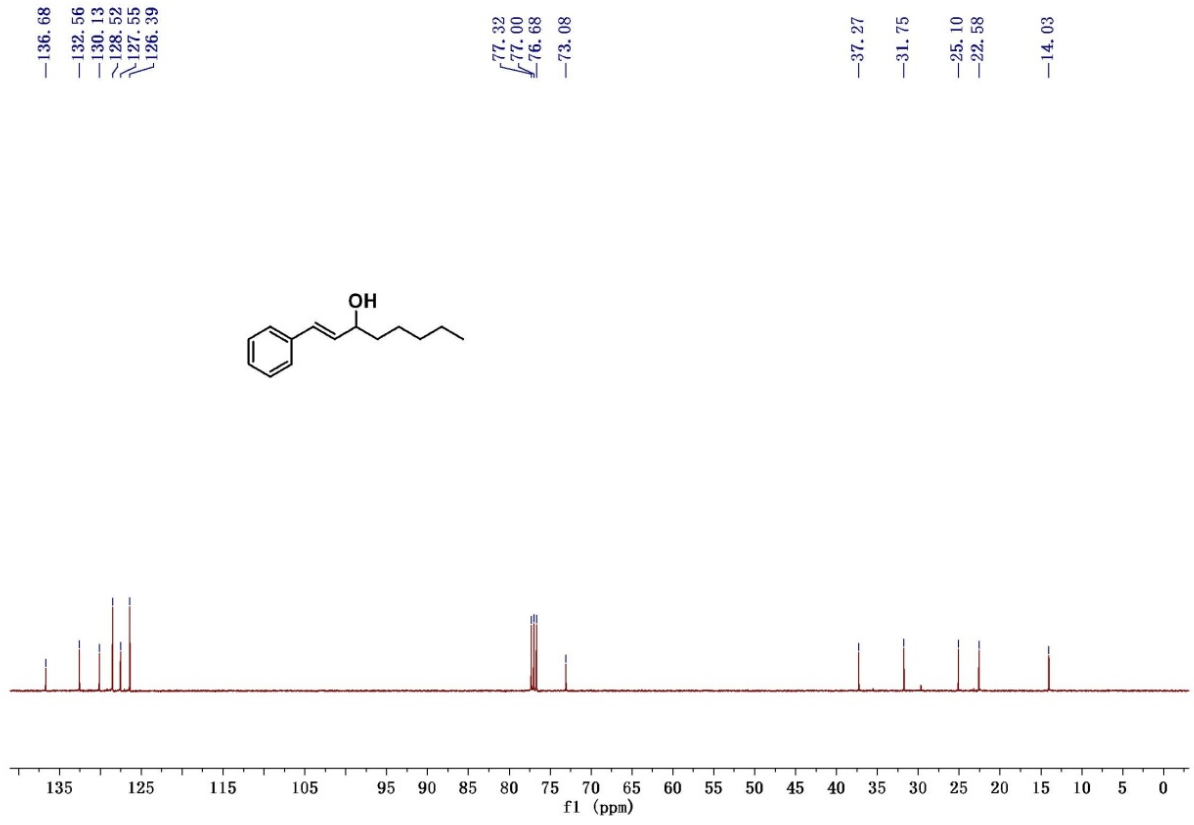
1f- ^{13}C NMR



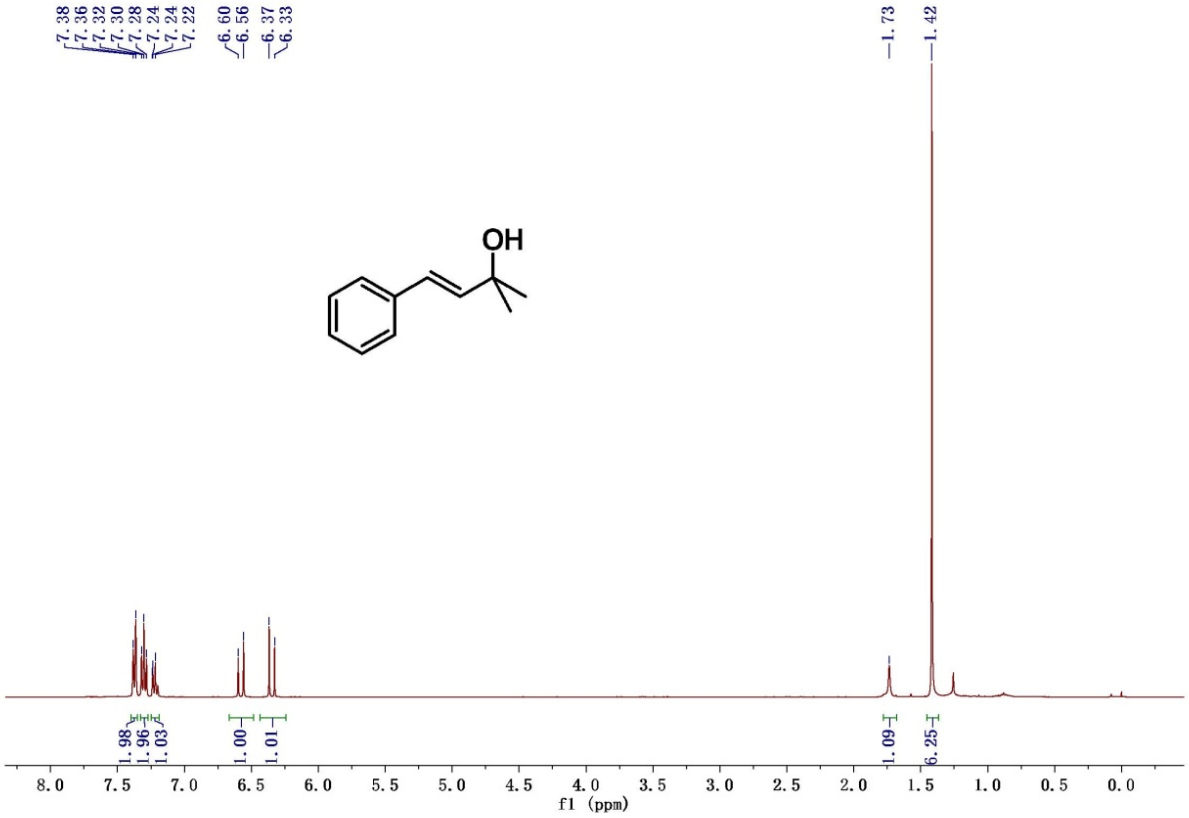
1g- ^{1}H NMR



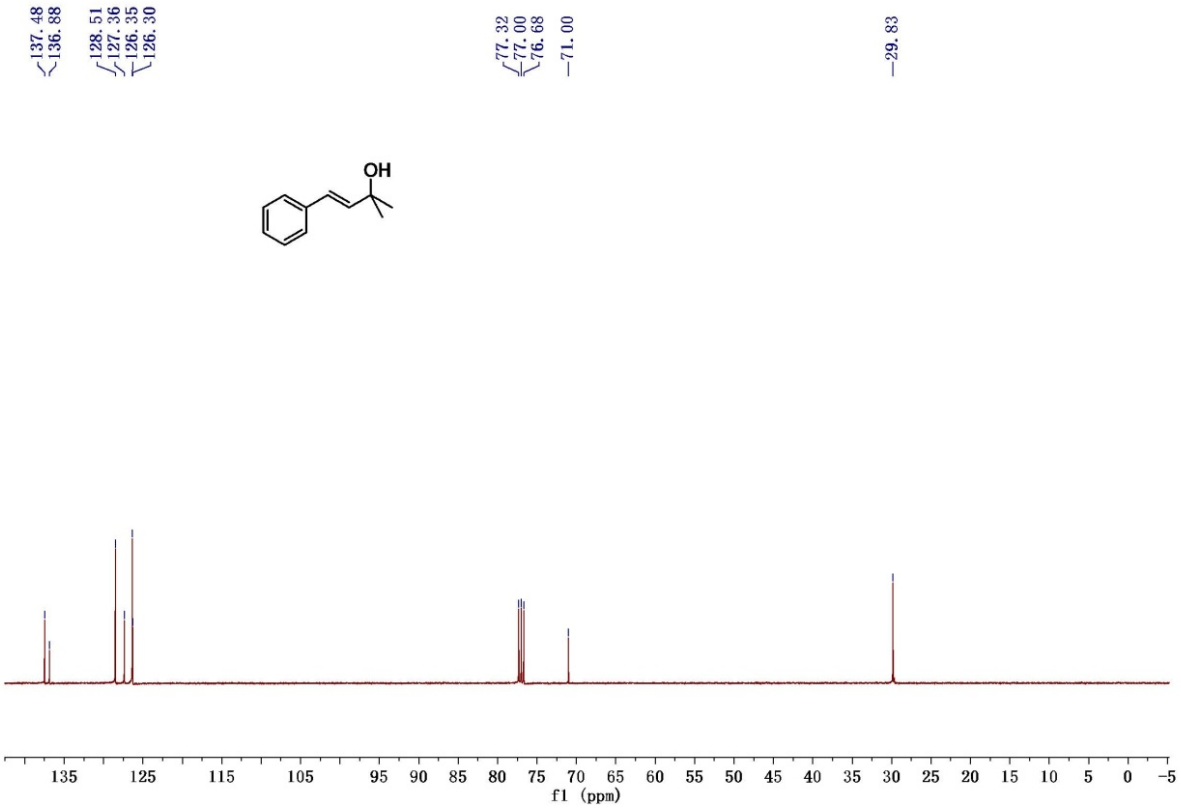
1g- ^{13}C NMR



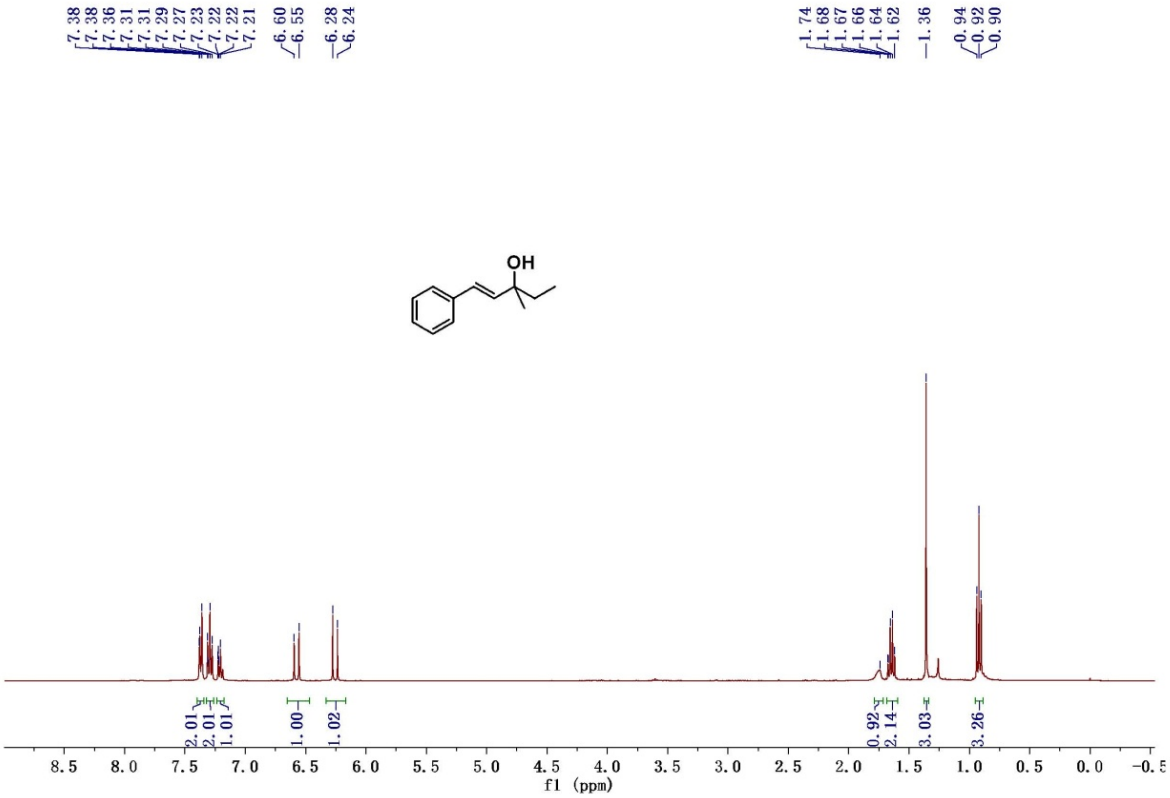
1h- ^{1}H NMR



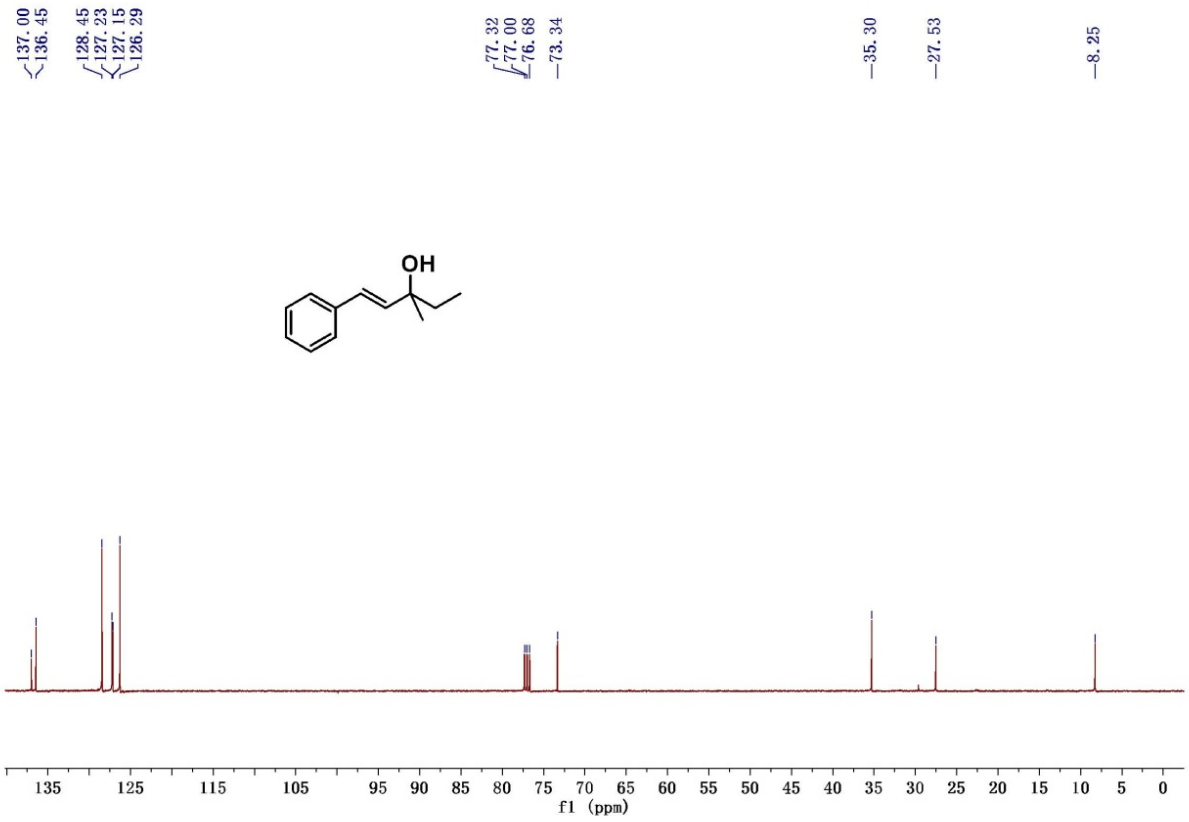
1h- ^{13}C NMR



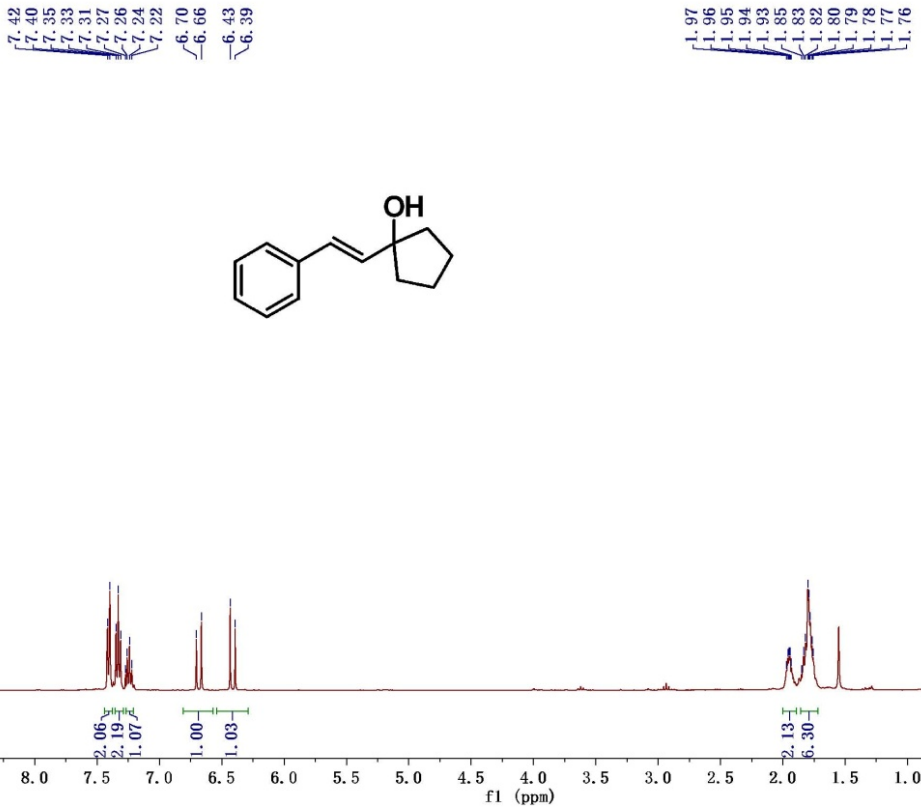
1i- ^{1}H NMR



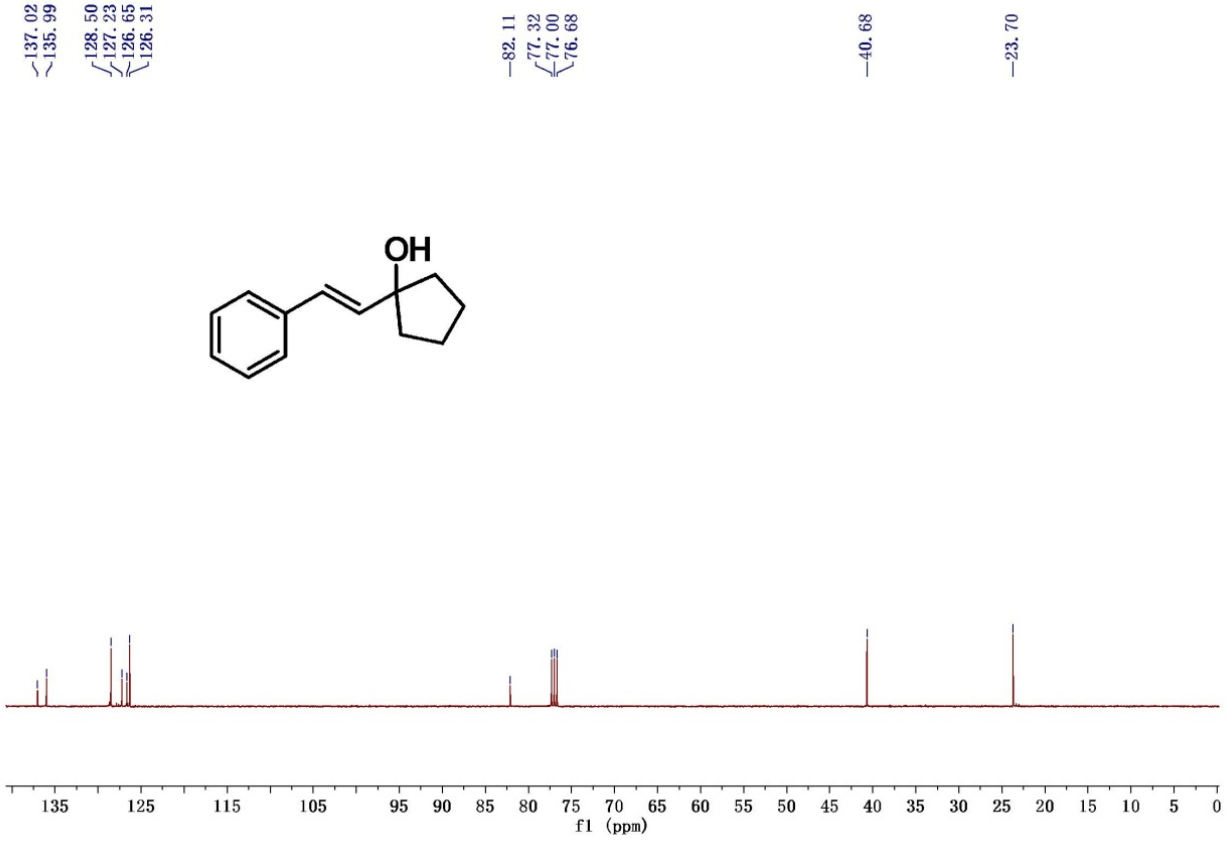
1i- ^{13}C NMR



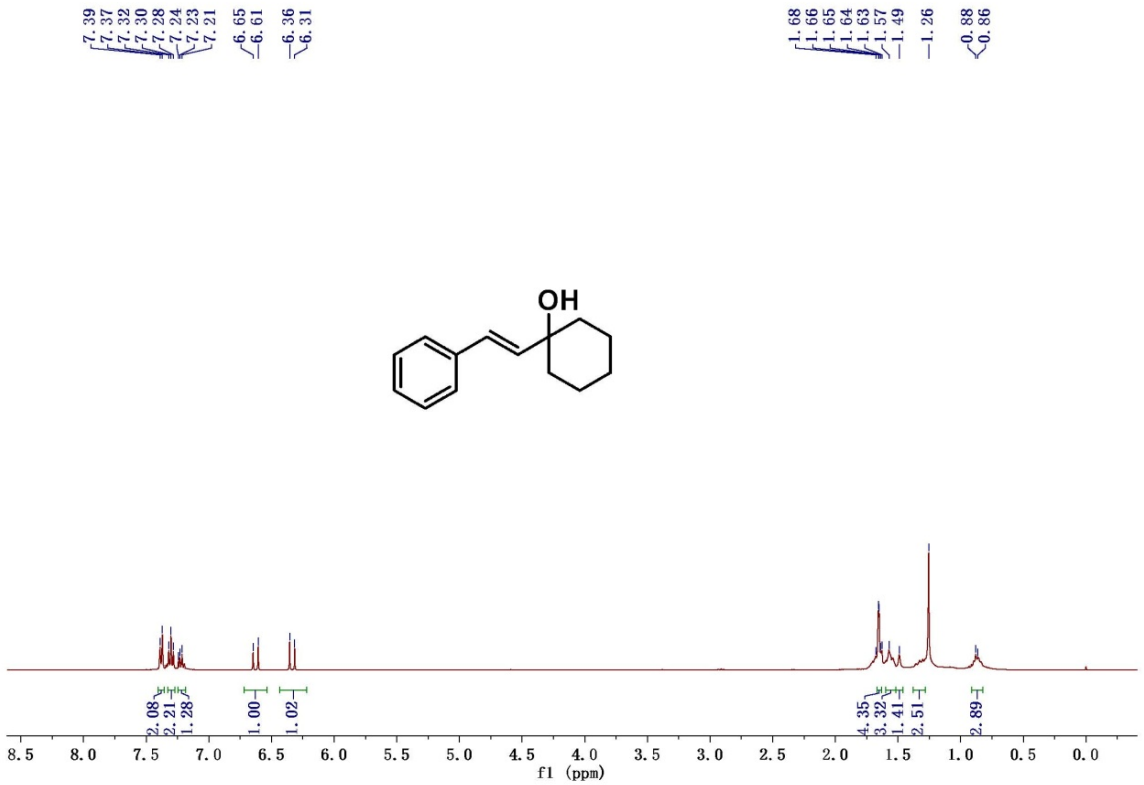
1j- ^{1}H NMR



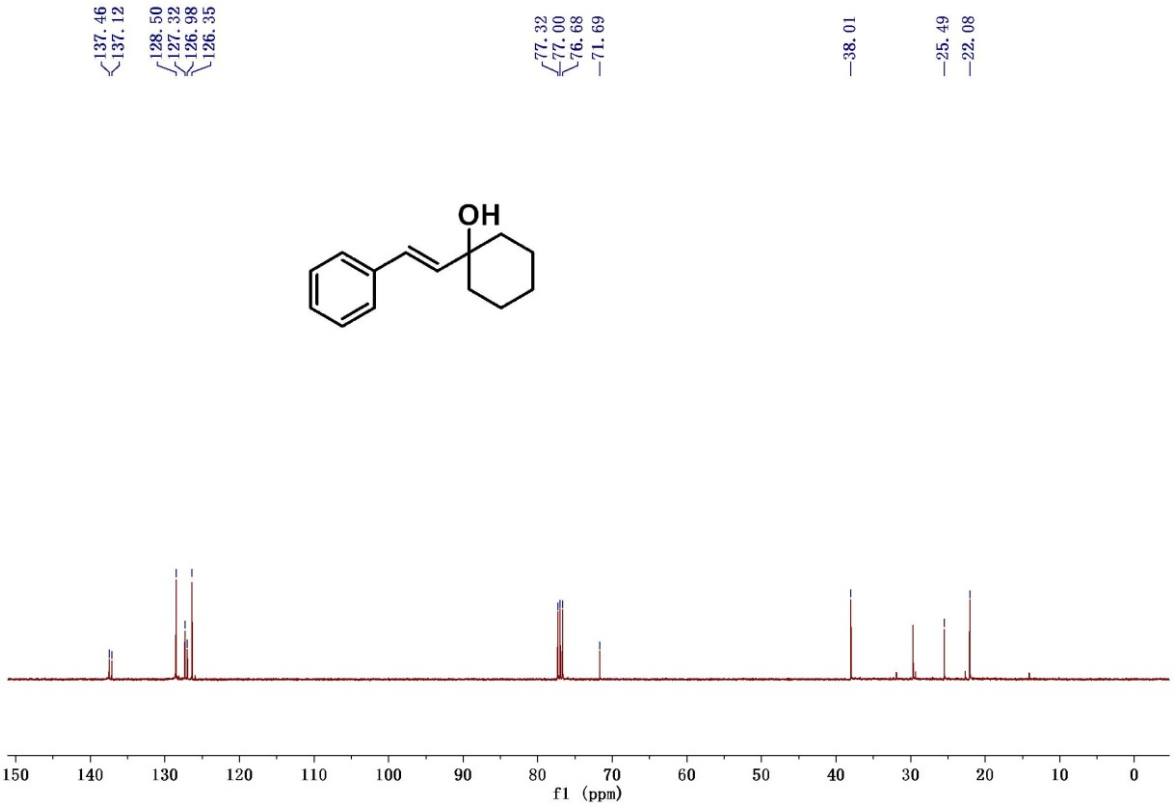
1j- ^{13}C NMR



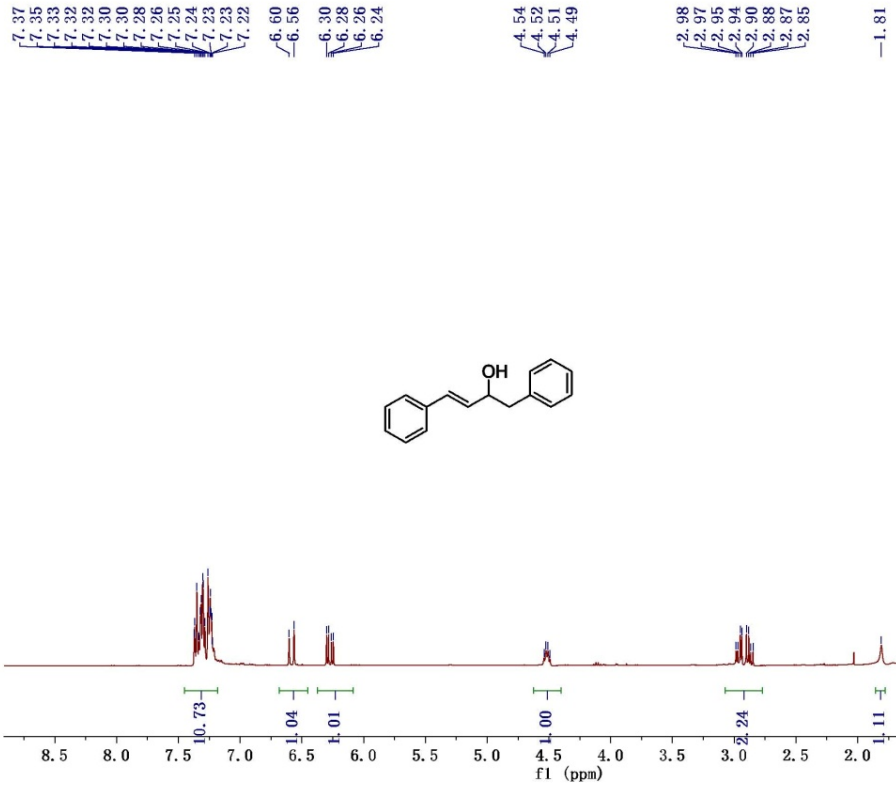
1k- ^{1}H NMR



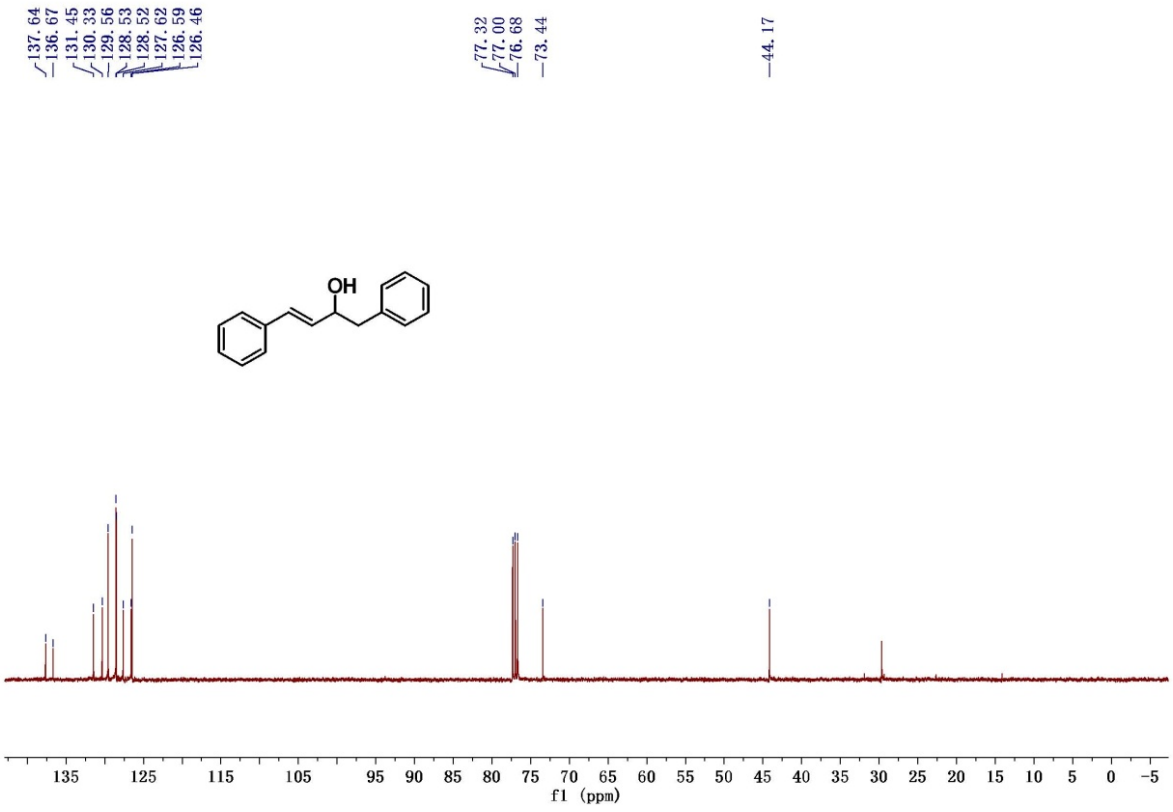
1k- ^{13}C NMR



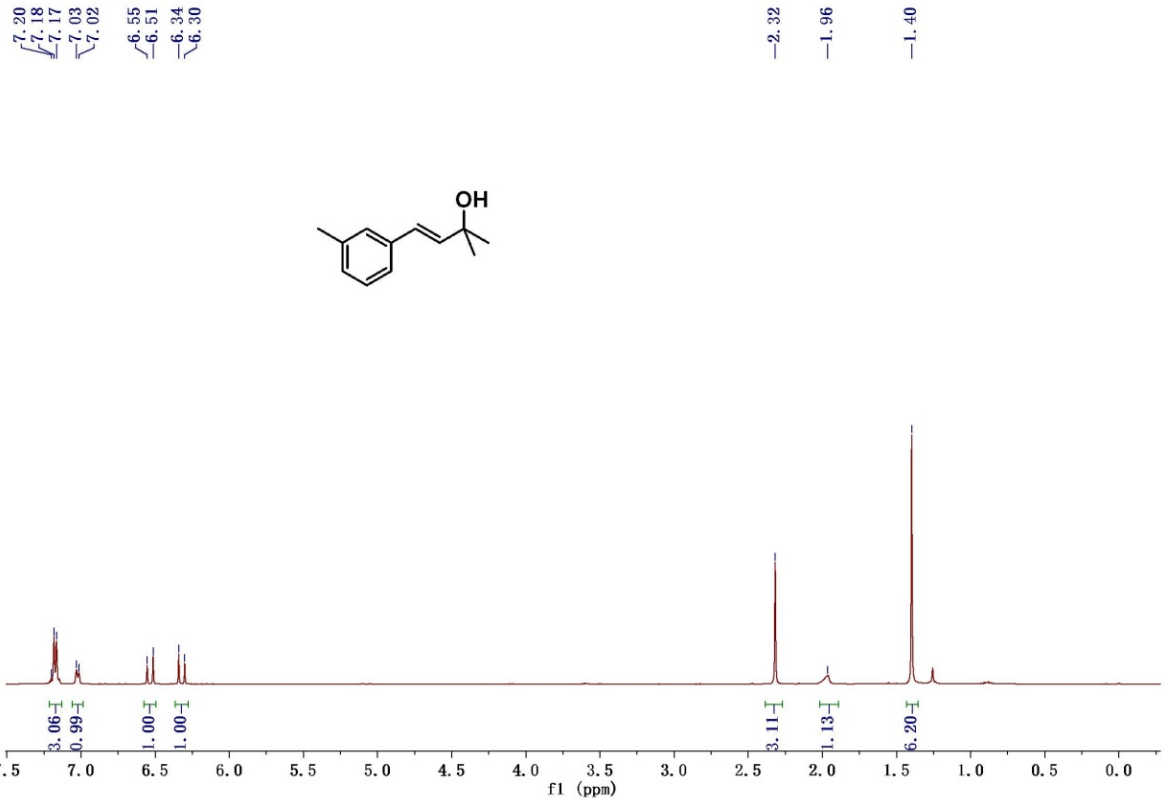
1l- ^{1}H NMR



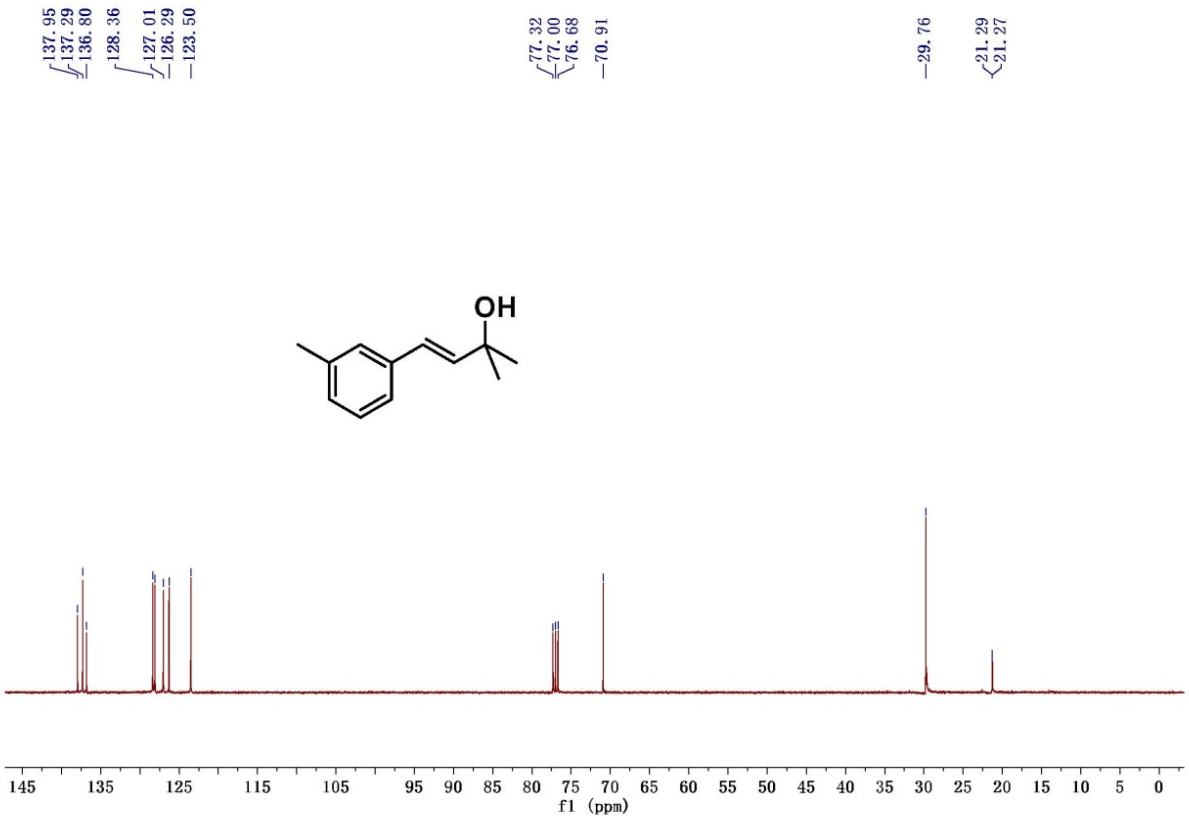
1l- ^{13}C NMR



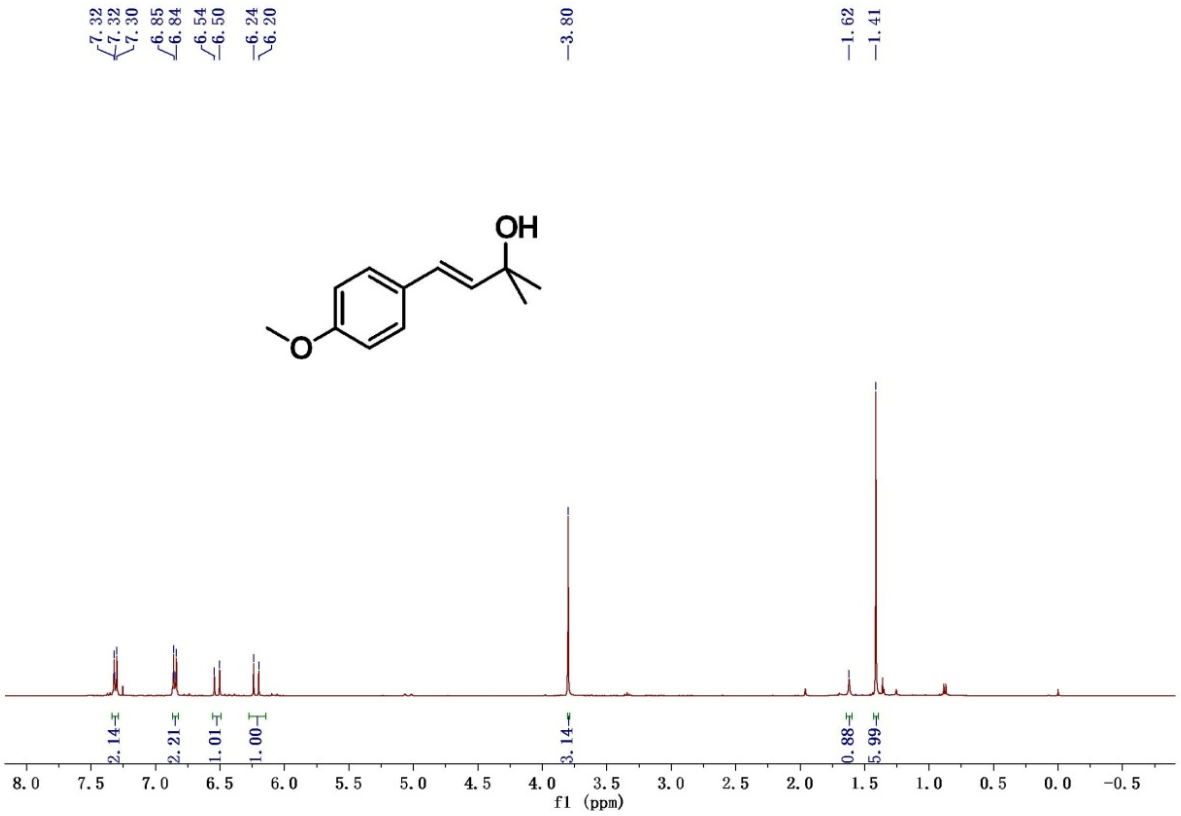
2a- ^{1}H NMR



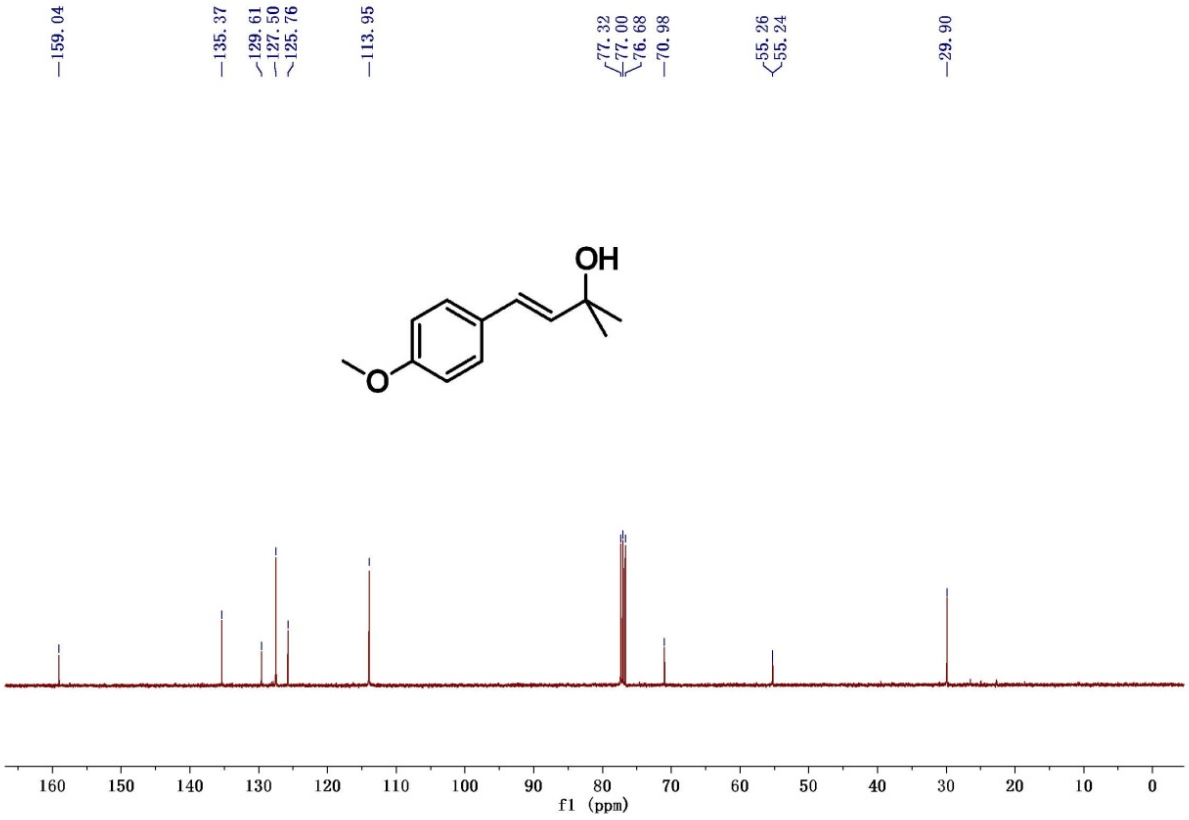
2a- ^{13}C NMR



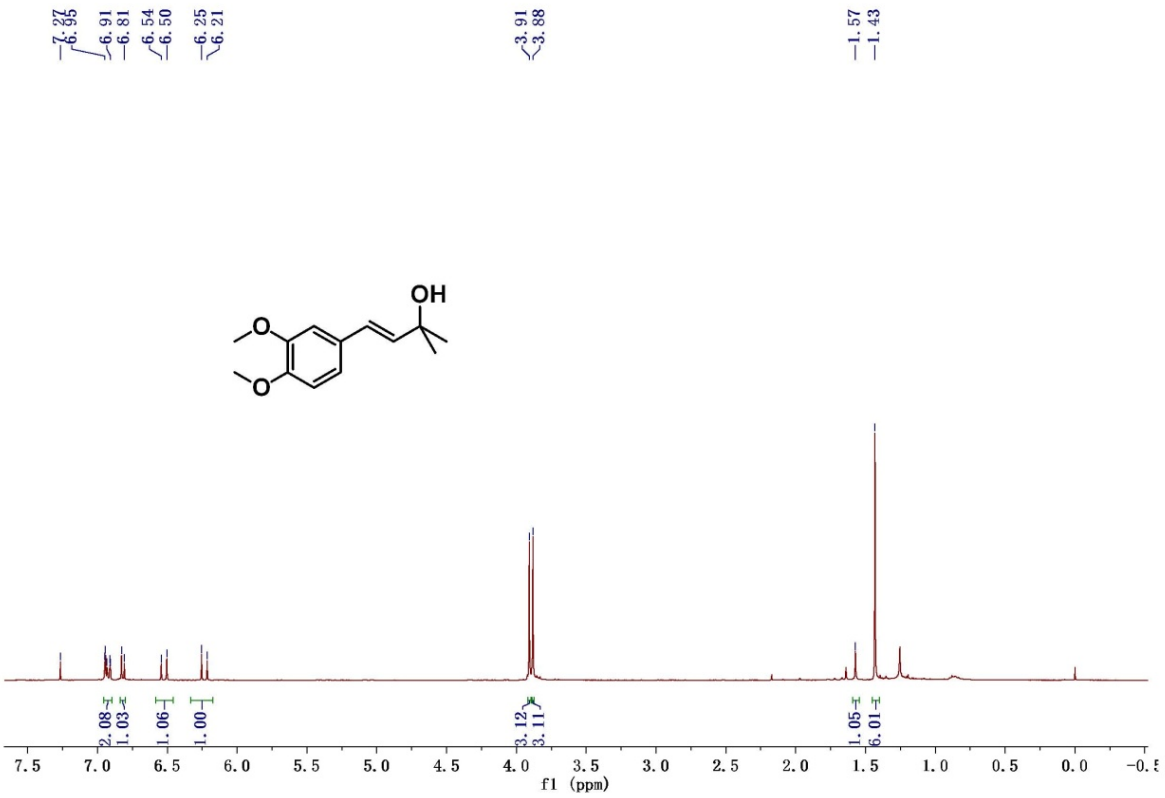
2b- ^{1}H NMR



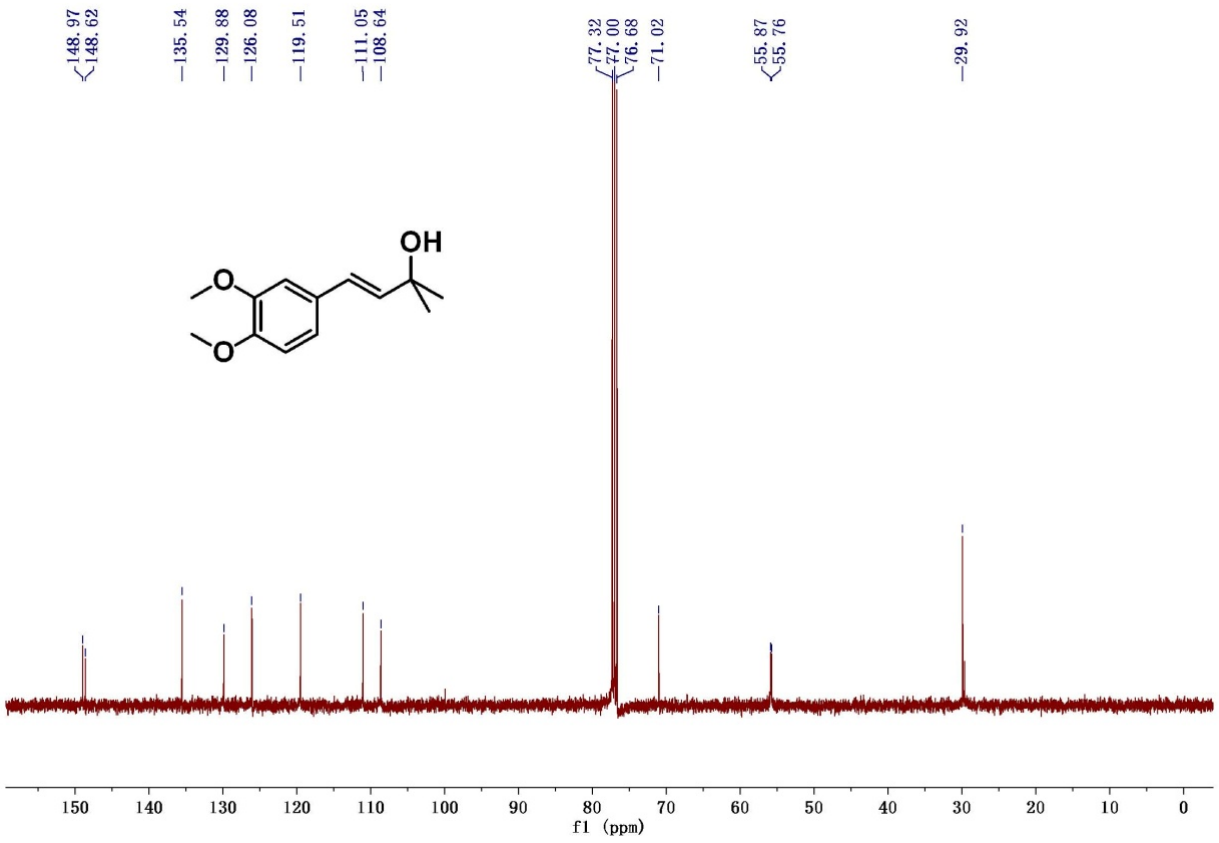
2b- ^{13}C NMR



2c- ^{1}H NMR



2c- ^{13}C NMR



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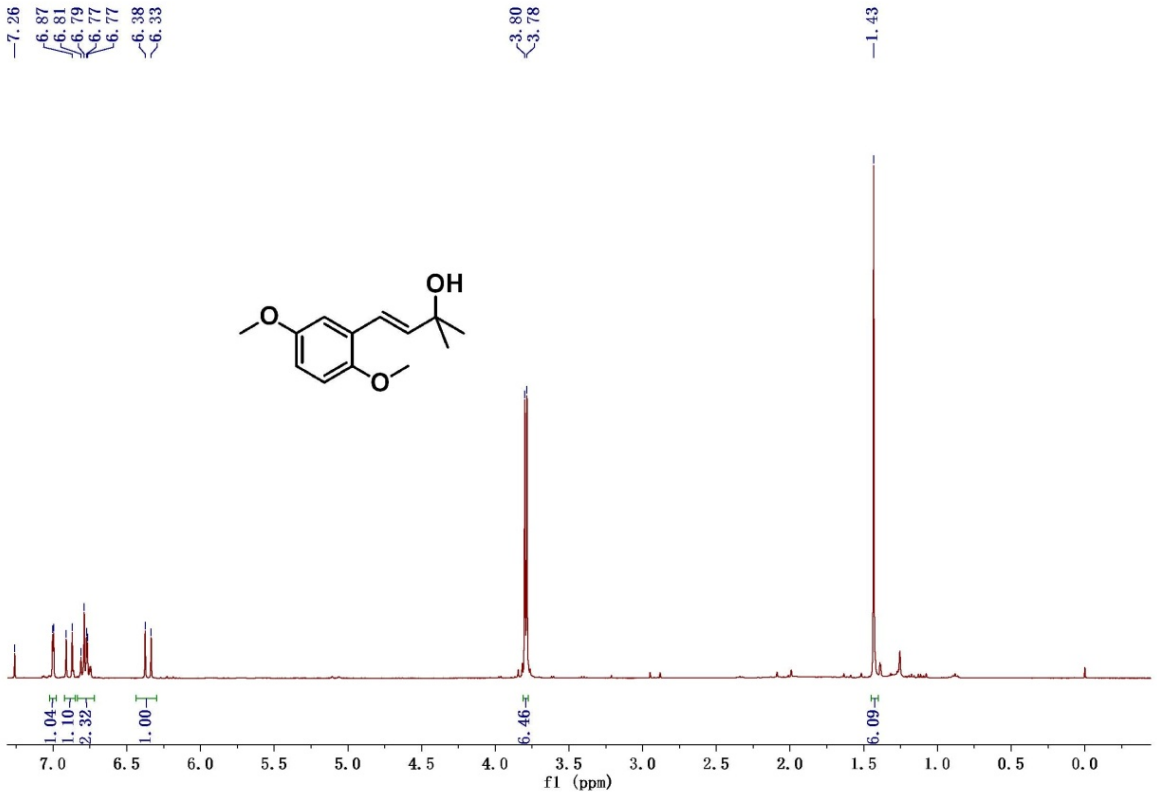
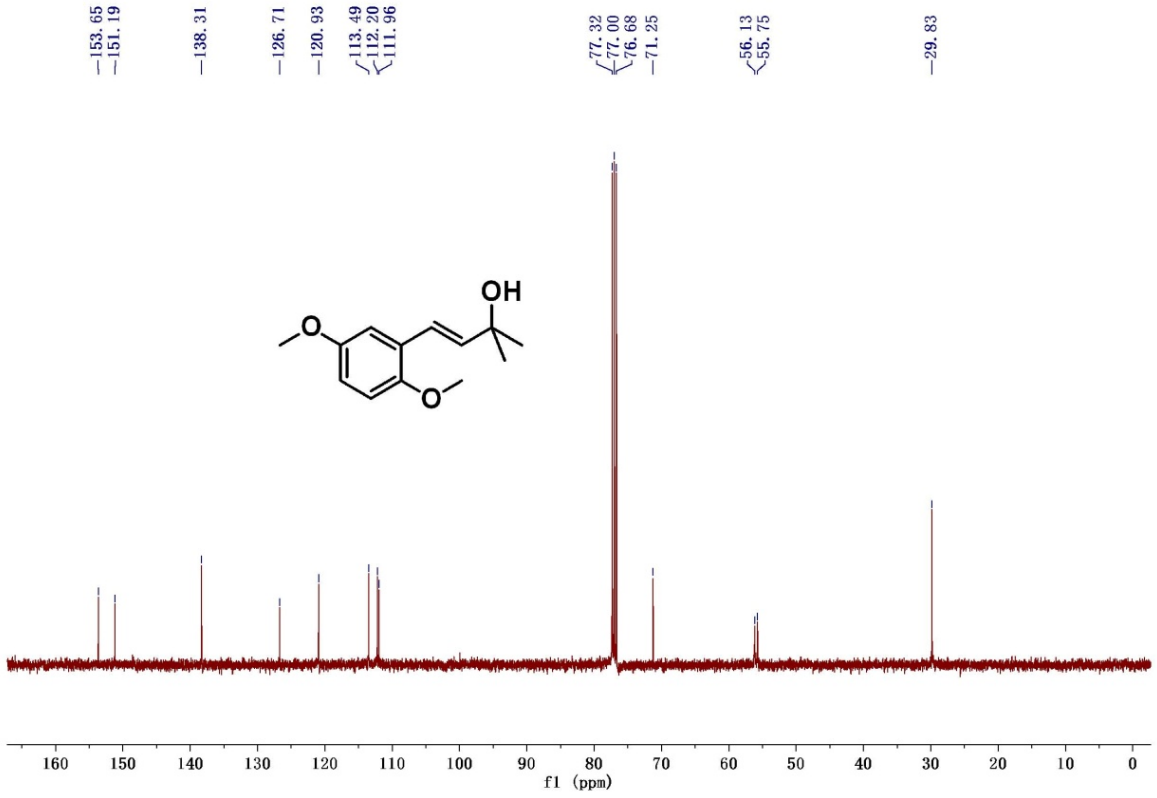
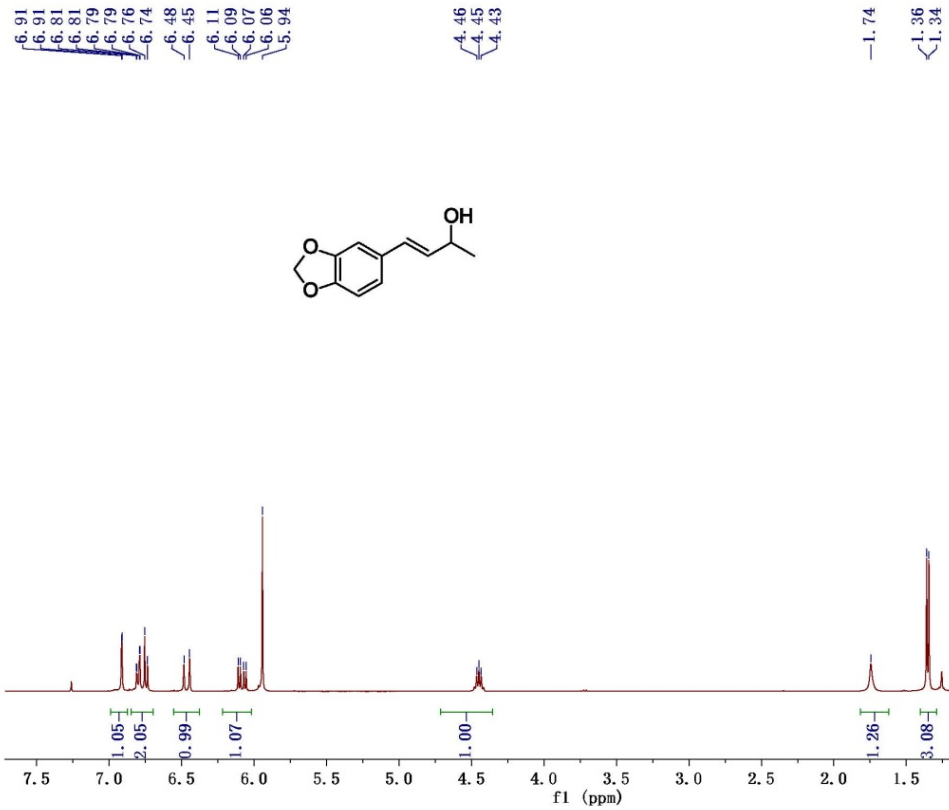
2d- ^{1}H NMR



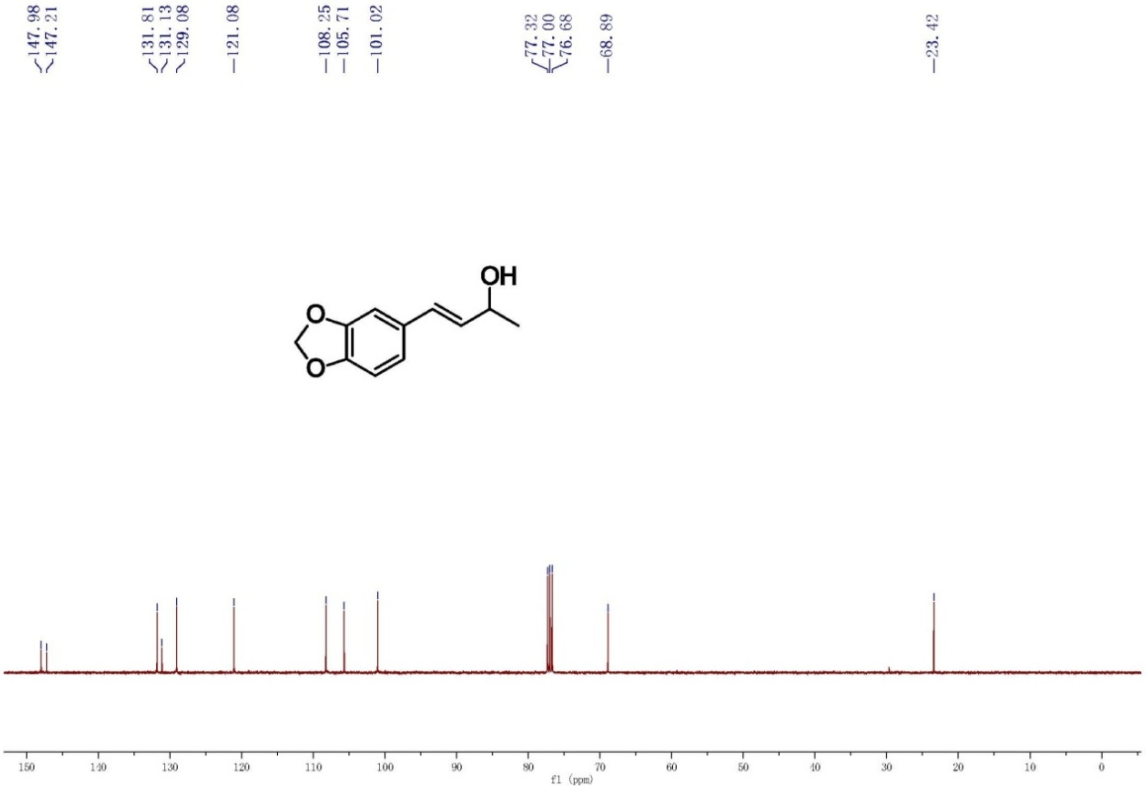
2d- ^{13}C NMR



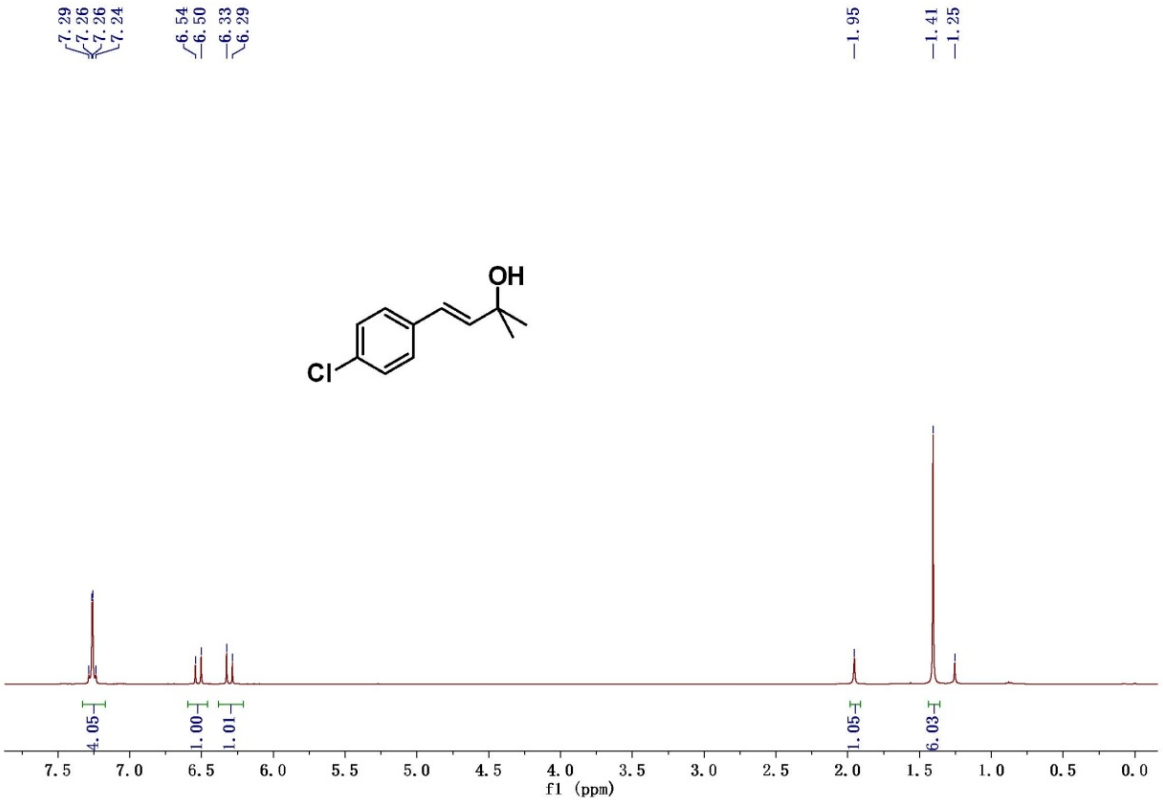
2e- ^{1}H NMR



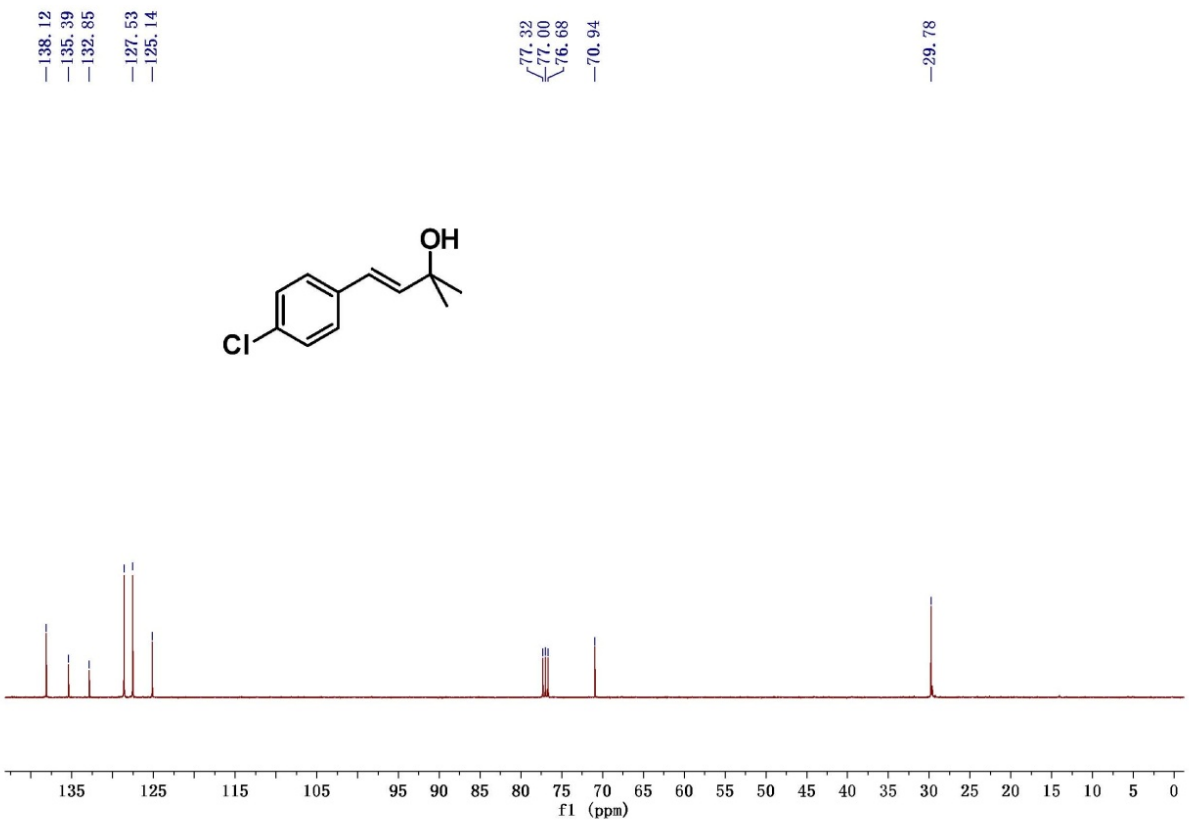
2e- ^{13}C NMR



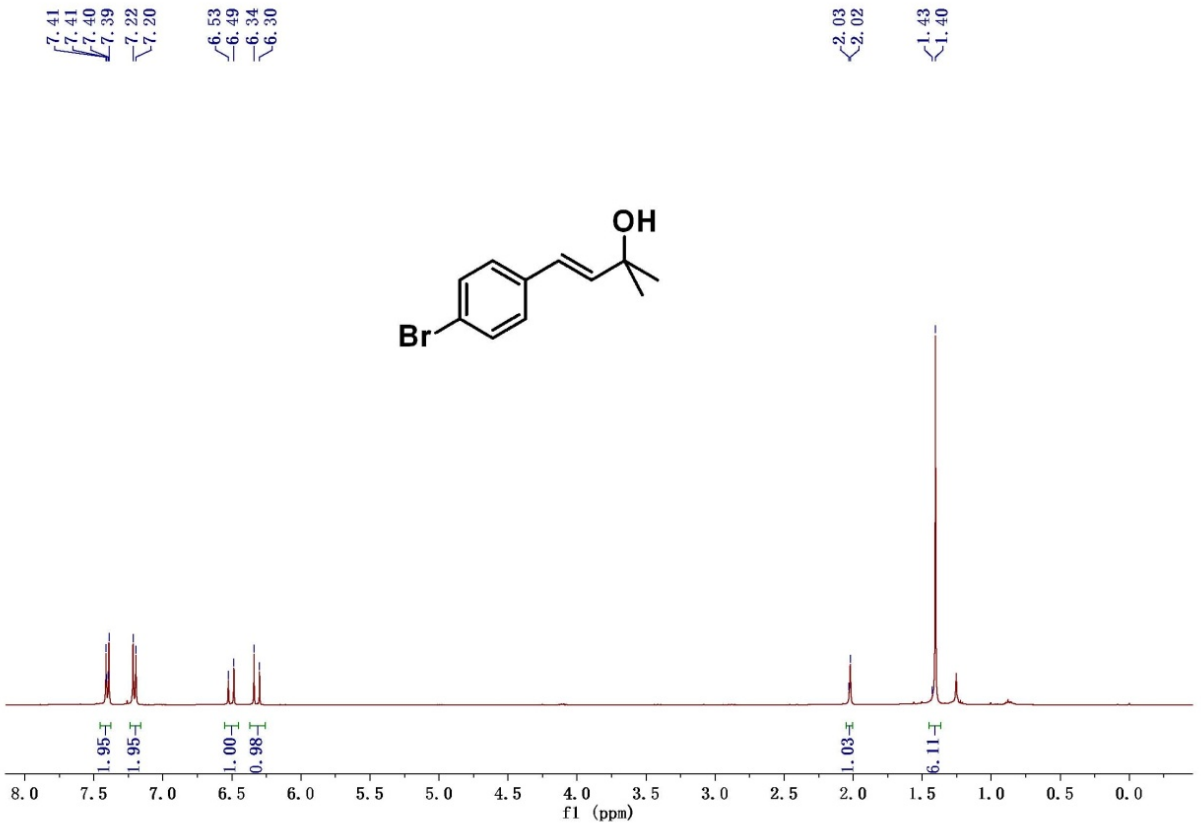
2f- ^{1}H NMR



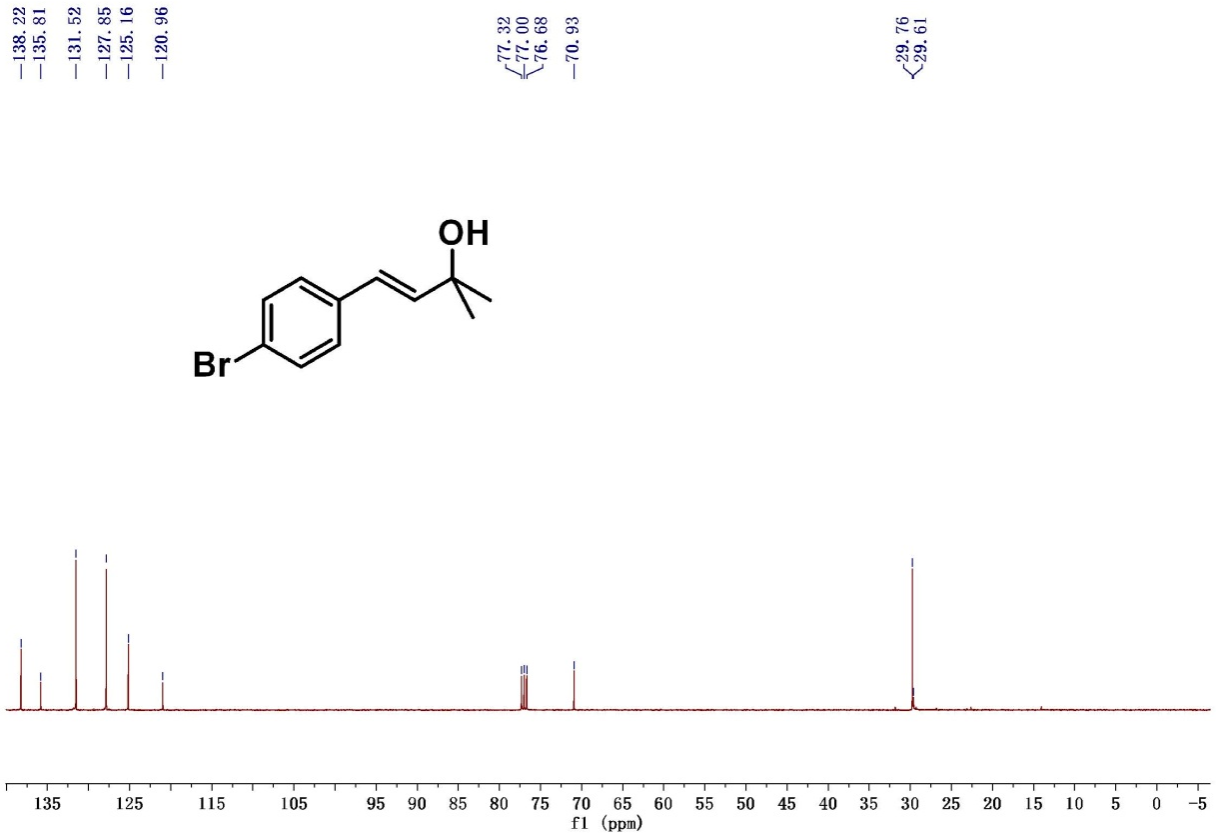
2f- ^{13}C NMR



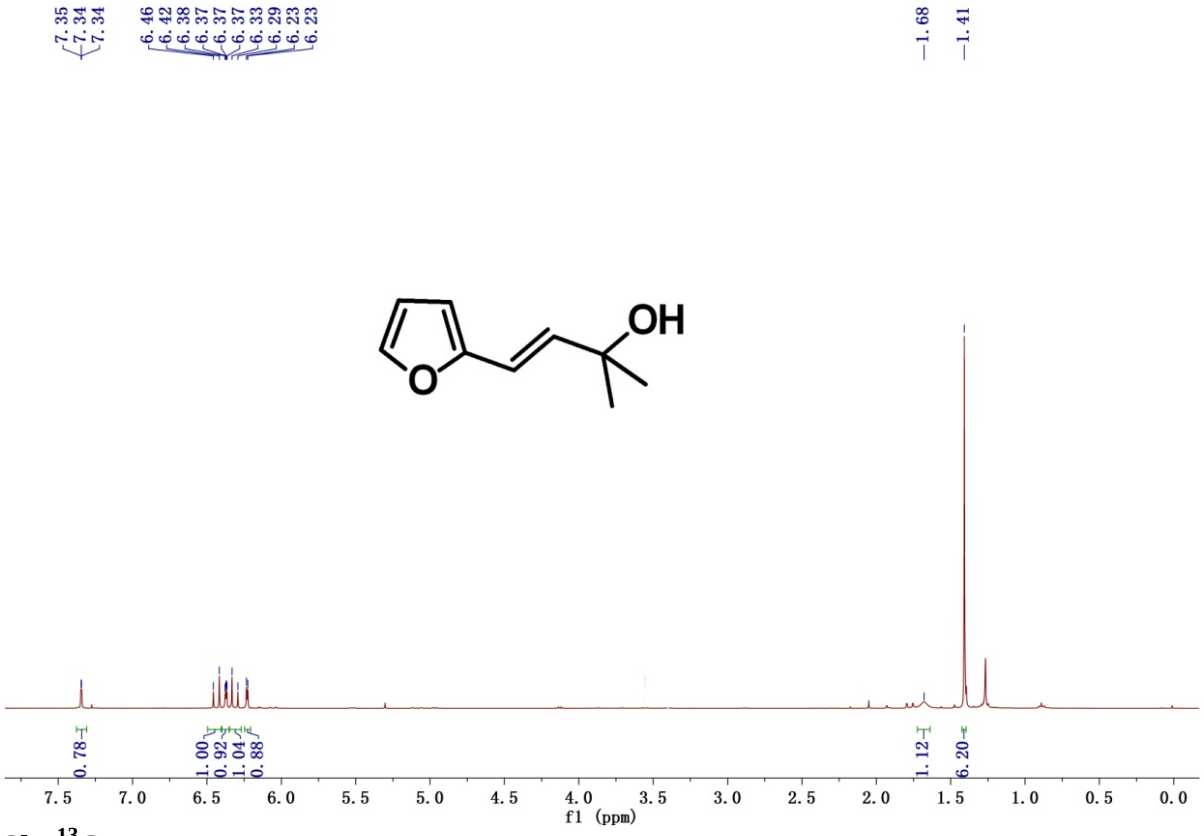
2g- ^{1}H NMR



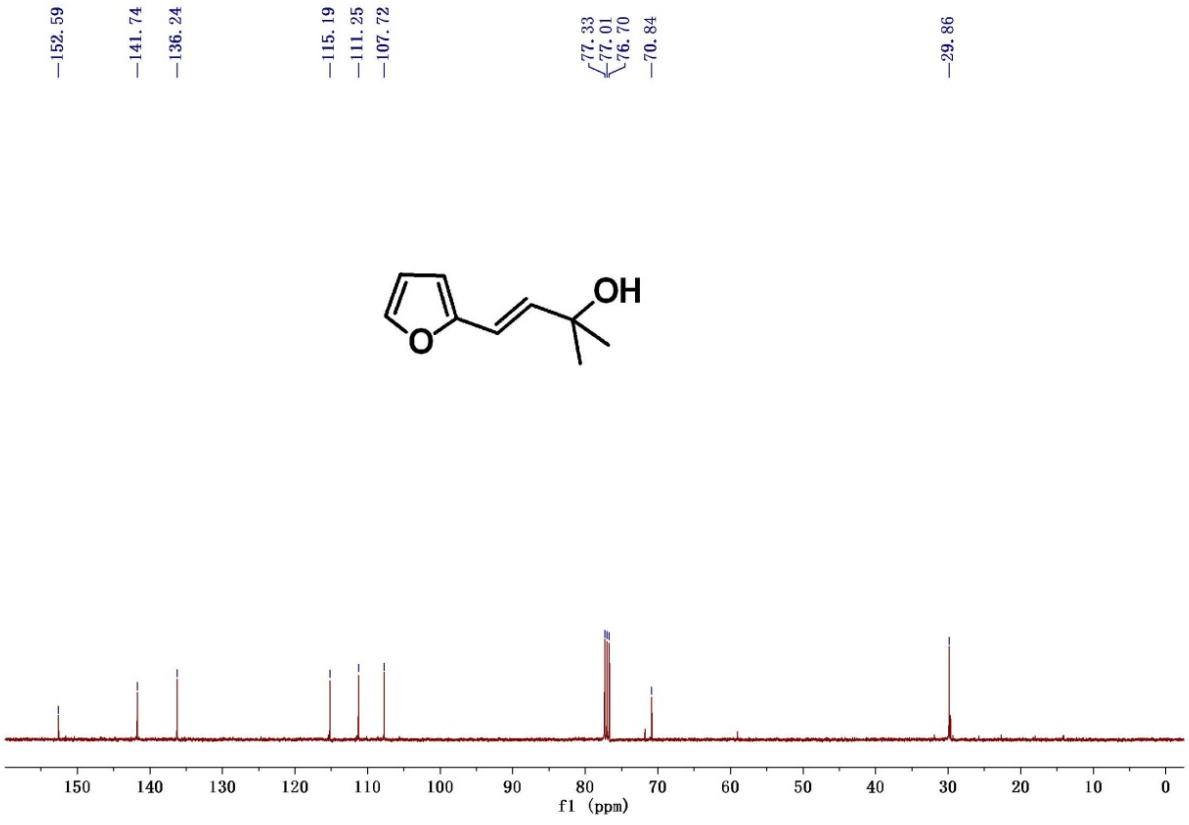
2g- ^{13}C NMR



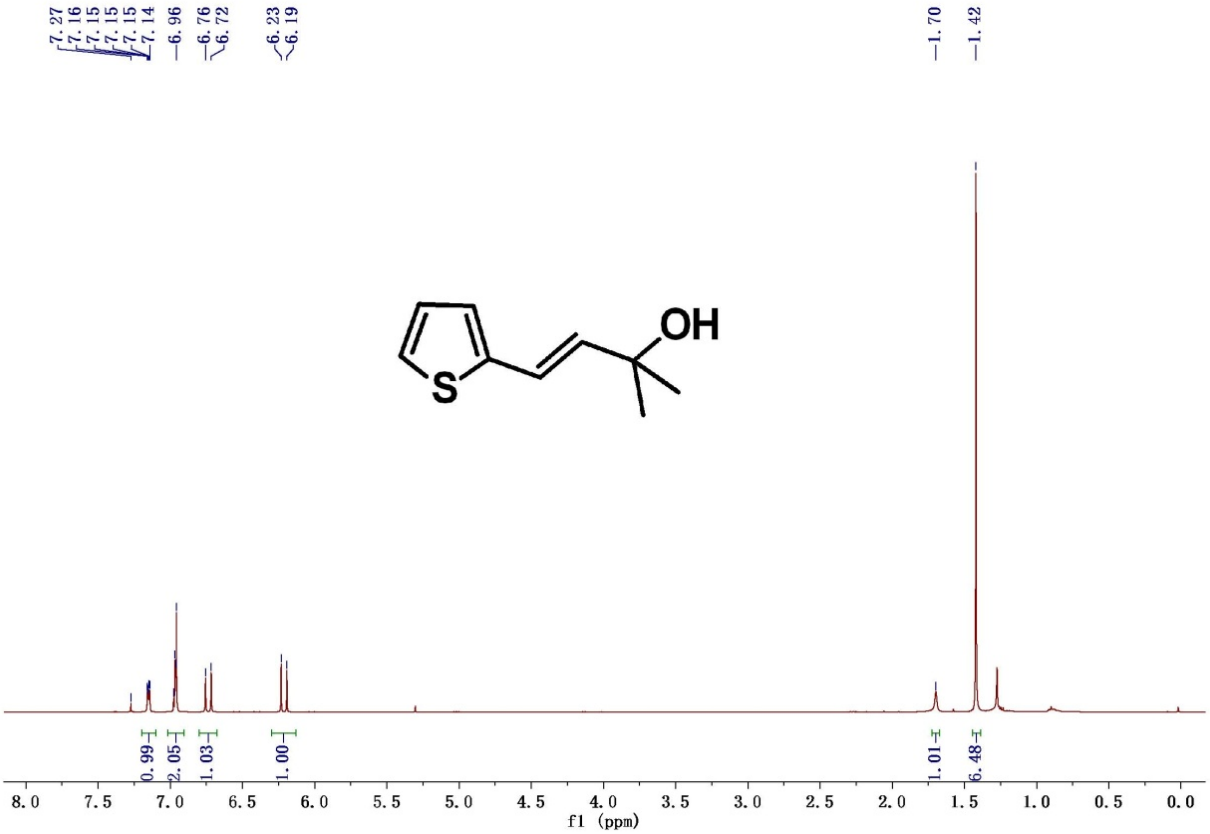
2h- ^{1}H NMR



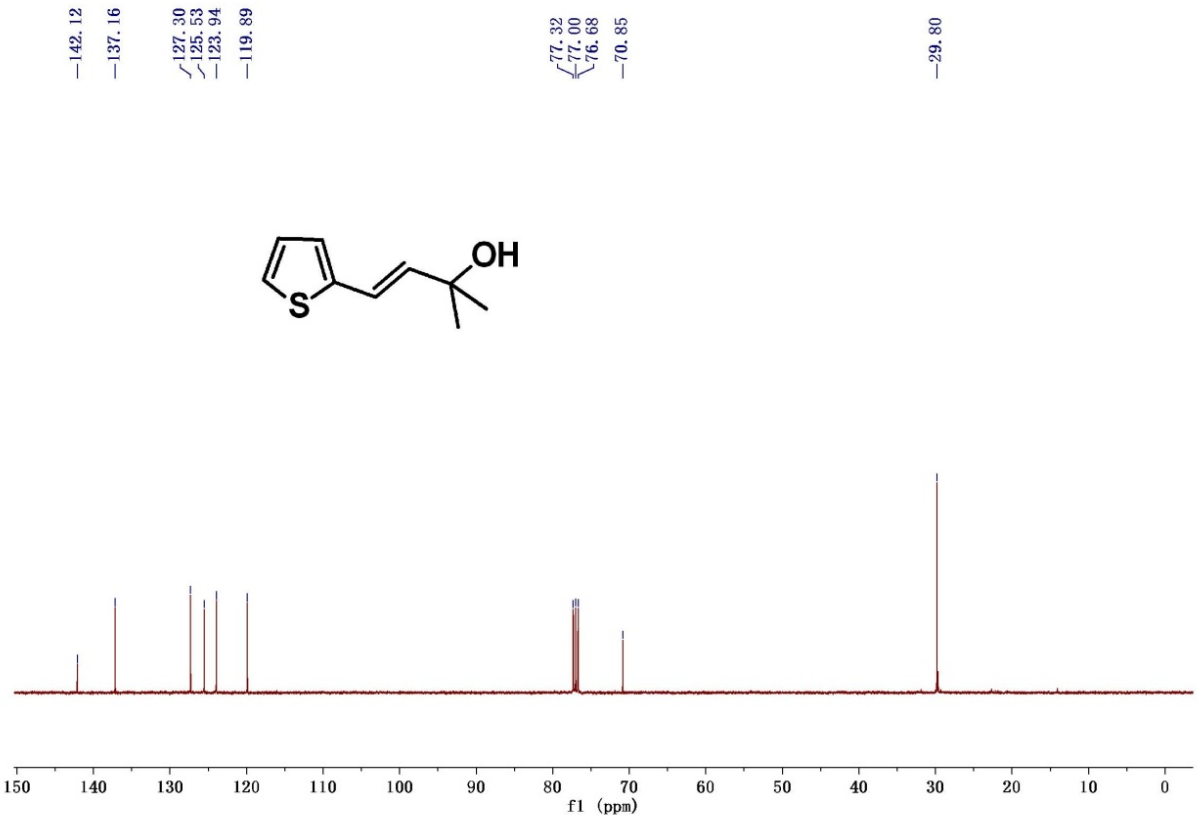
2h- ^{13}C NMR



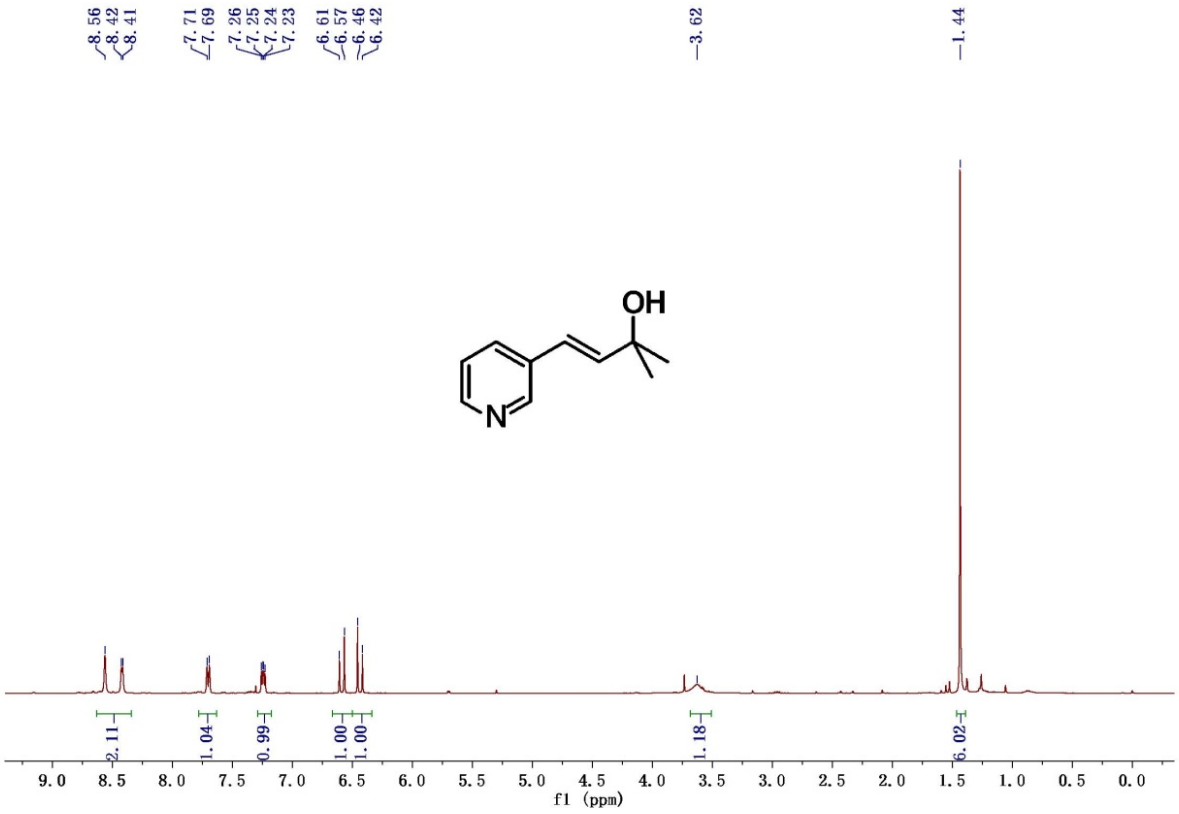
2i- ^{1}H NMR



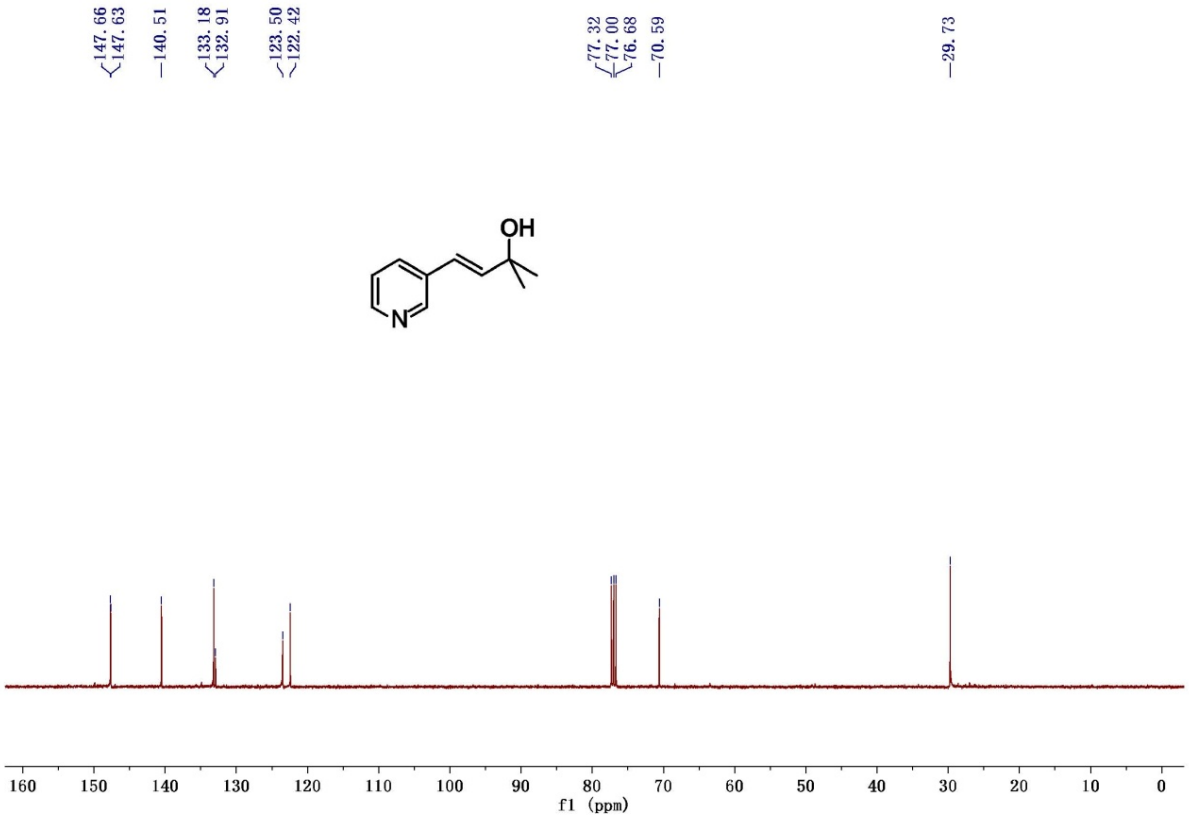
2i- ^{13}C NMR



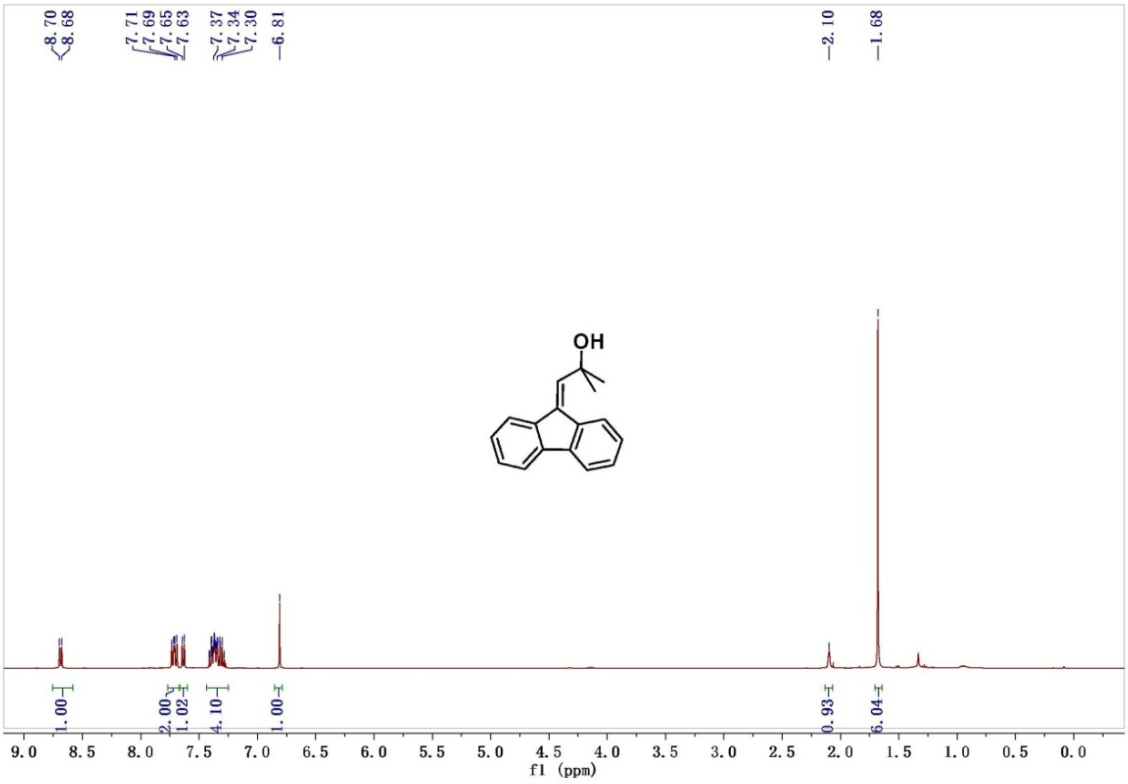
2j- ^{1}H NMR



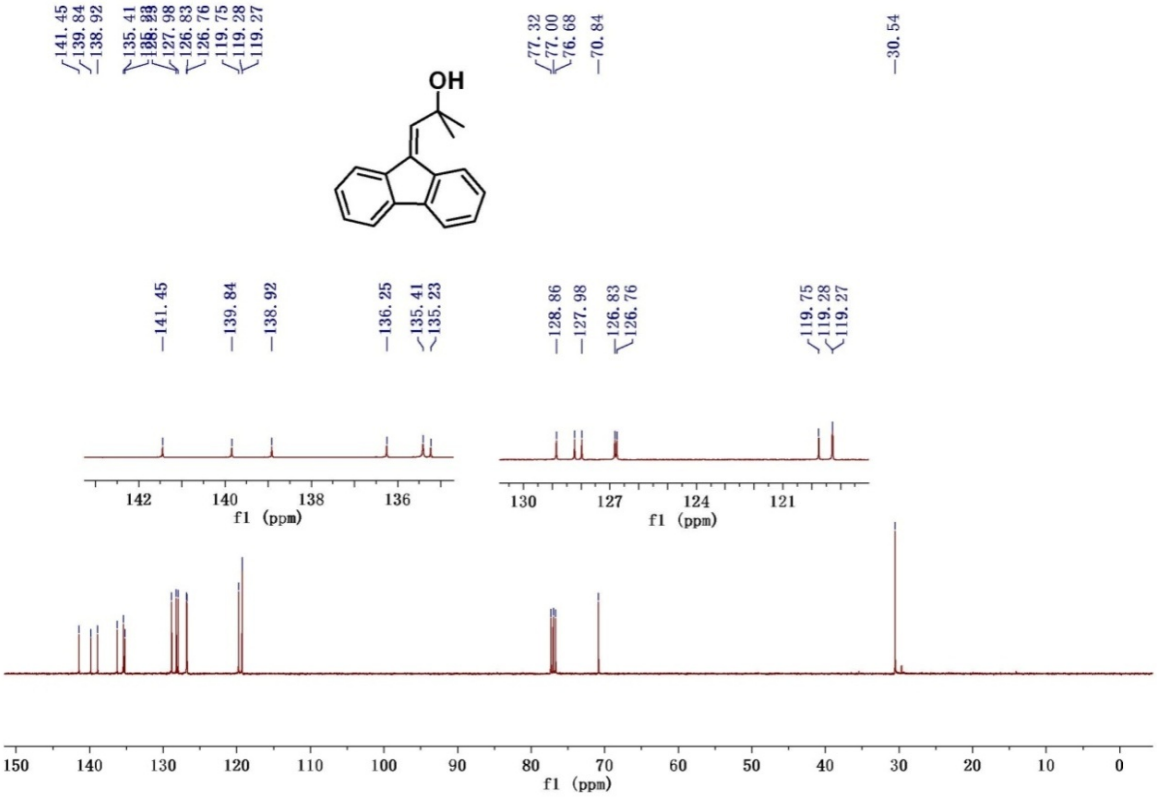
2j- ^{13}C NMR



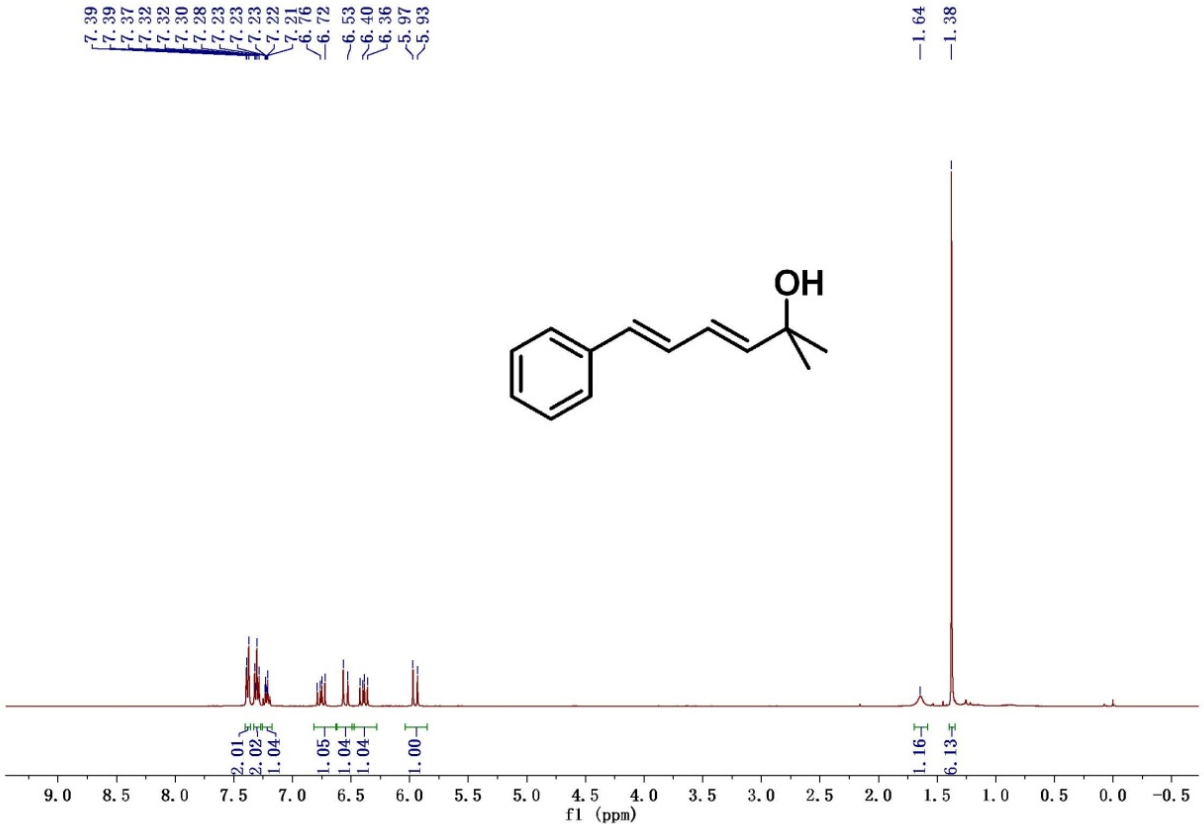
2k- ^{1}H NMR



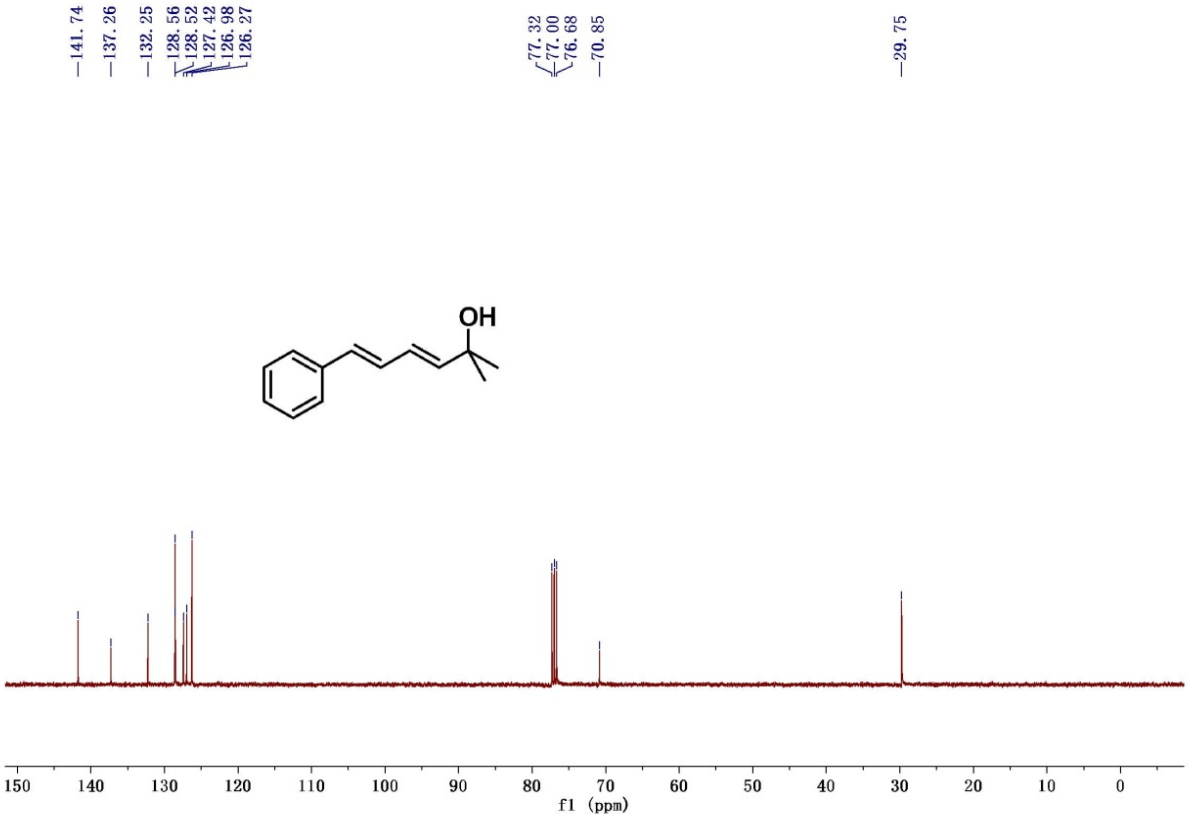
2k- ^{13}C NMR



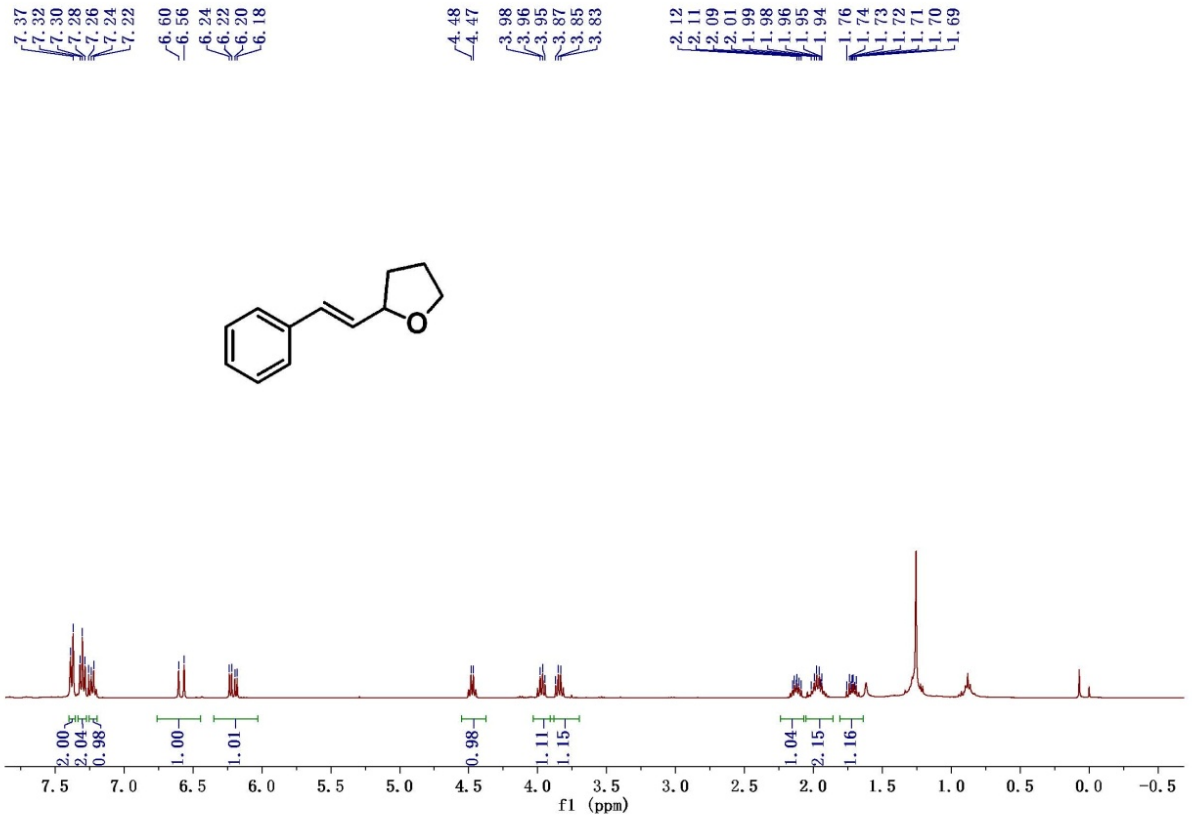
2l- ^{1}H NMR



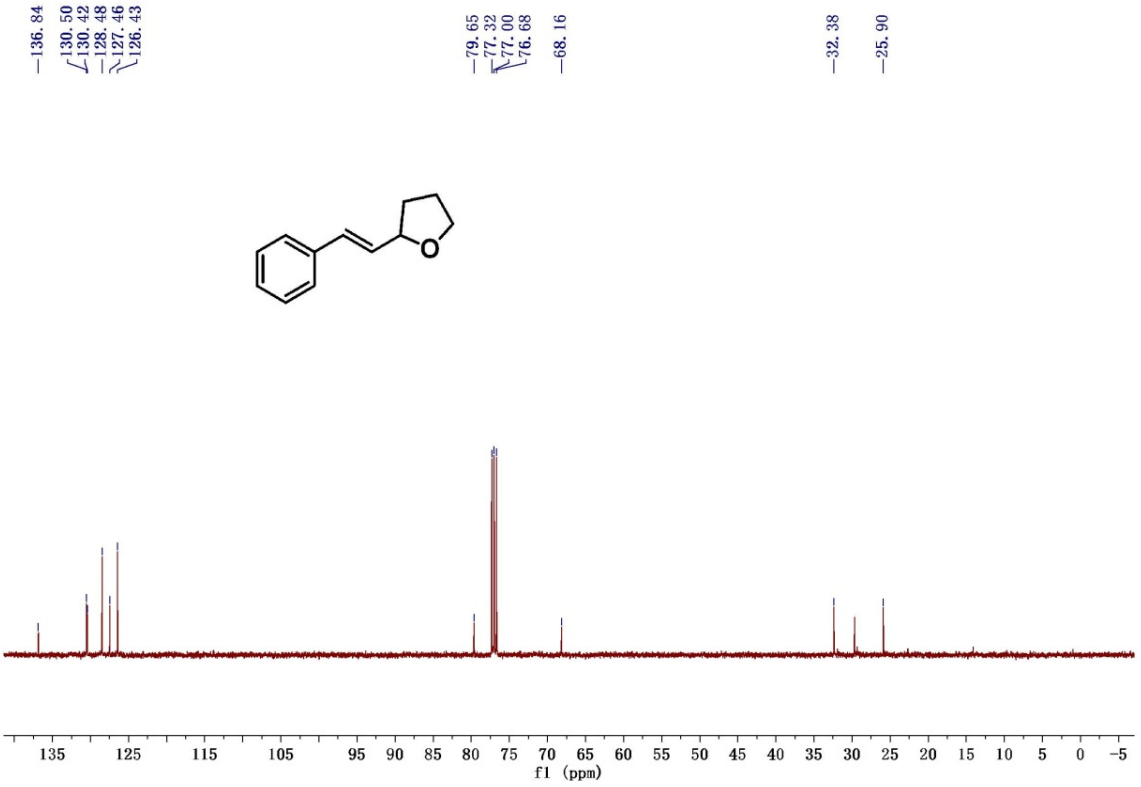
2l- ^{13}C NMR



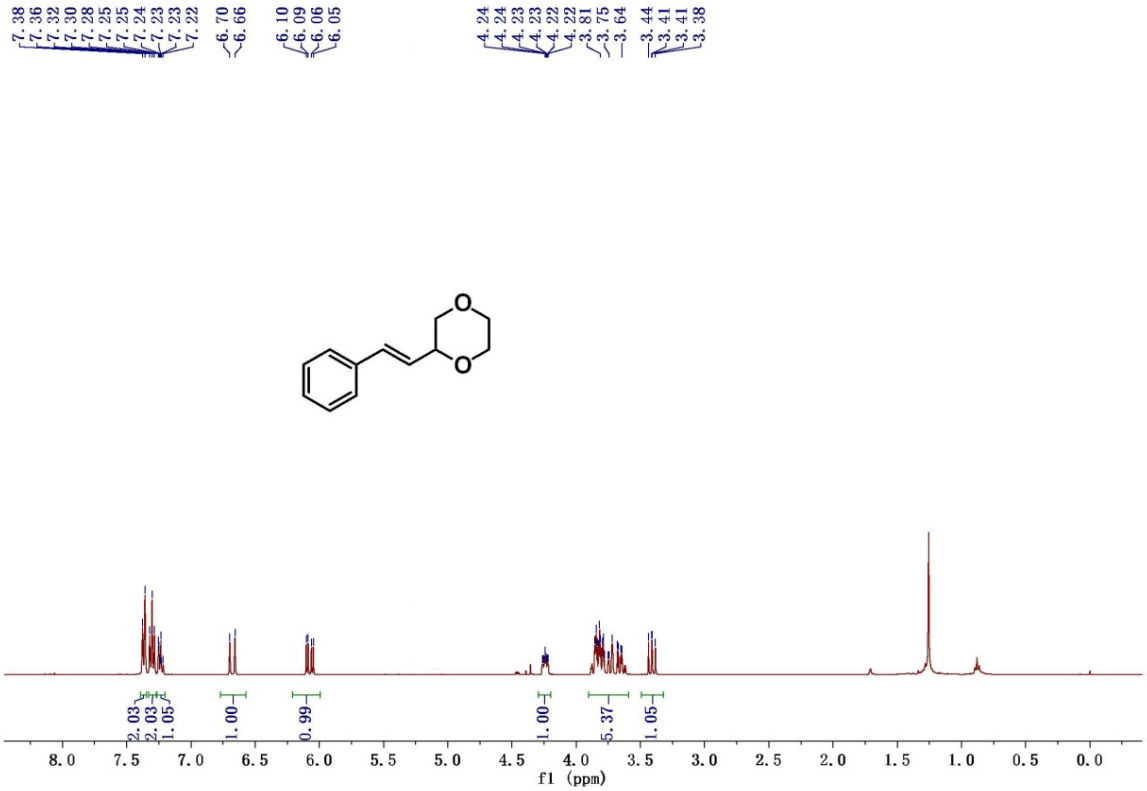
3a- ^{1}H NMR



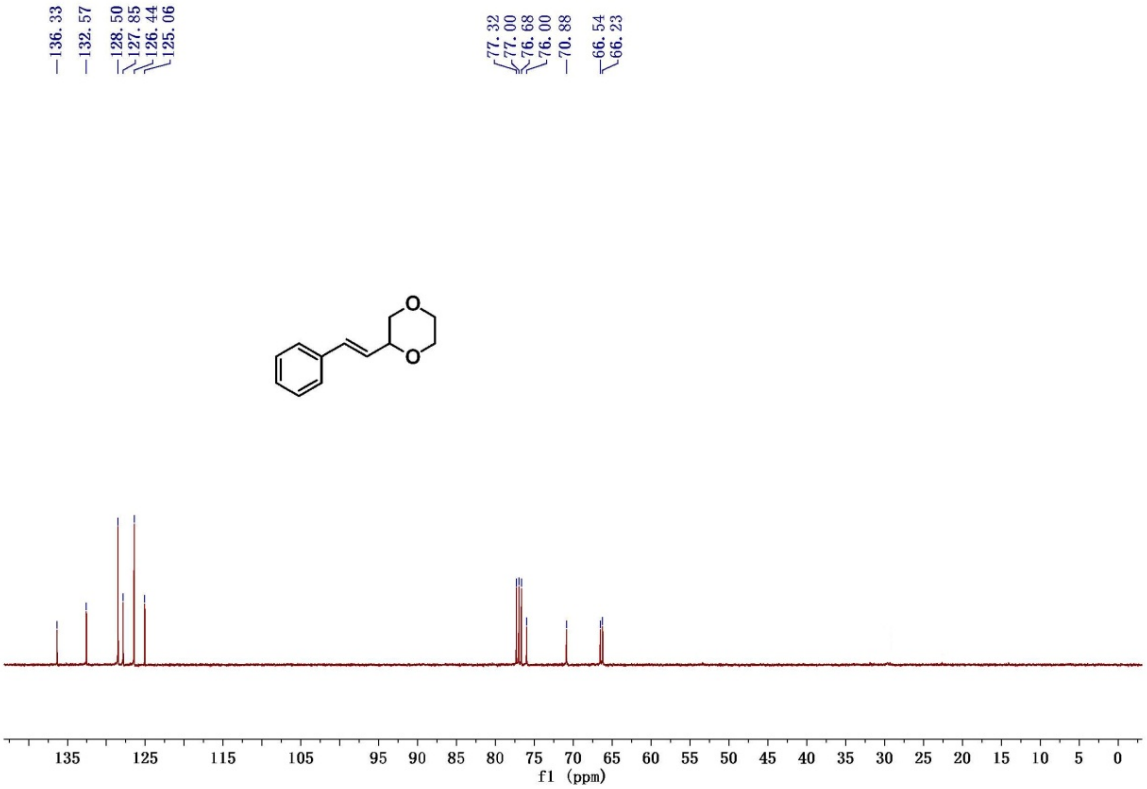
3a- ^{13}C NMR



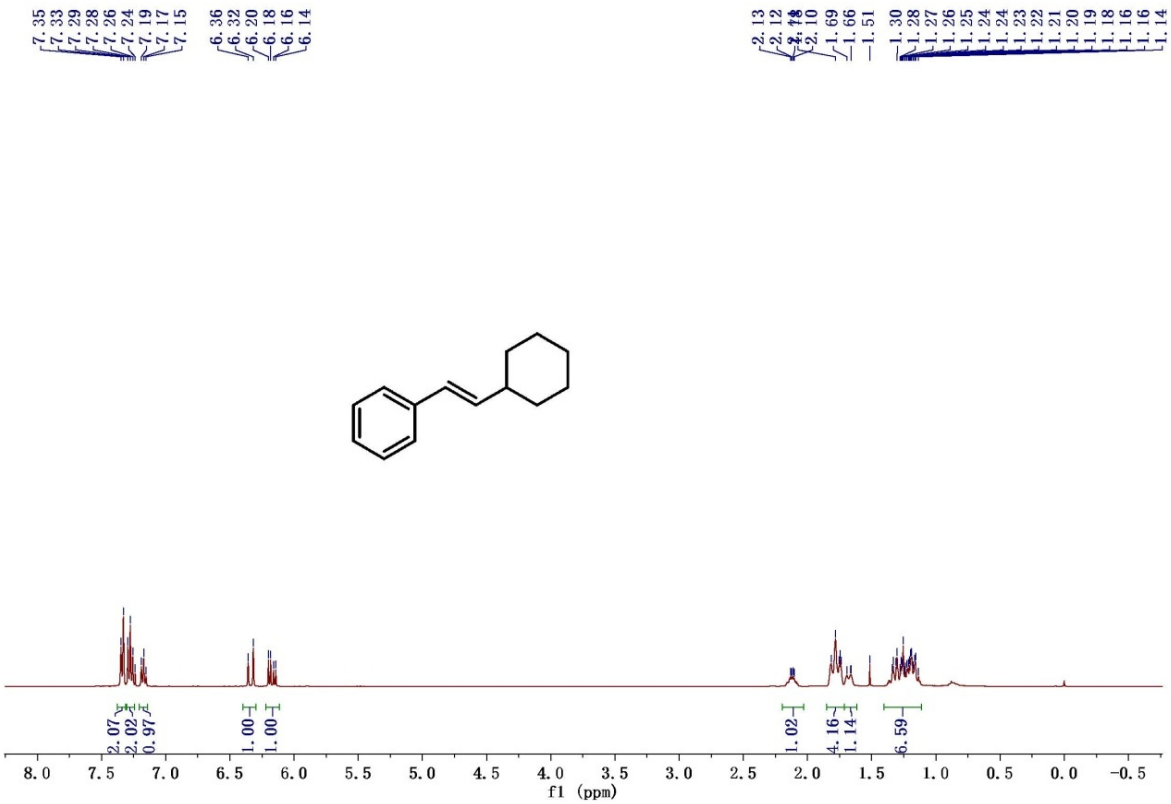
3b- ^{1}H NMR



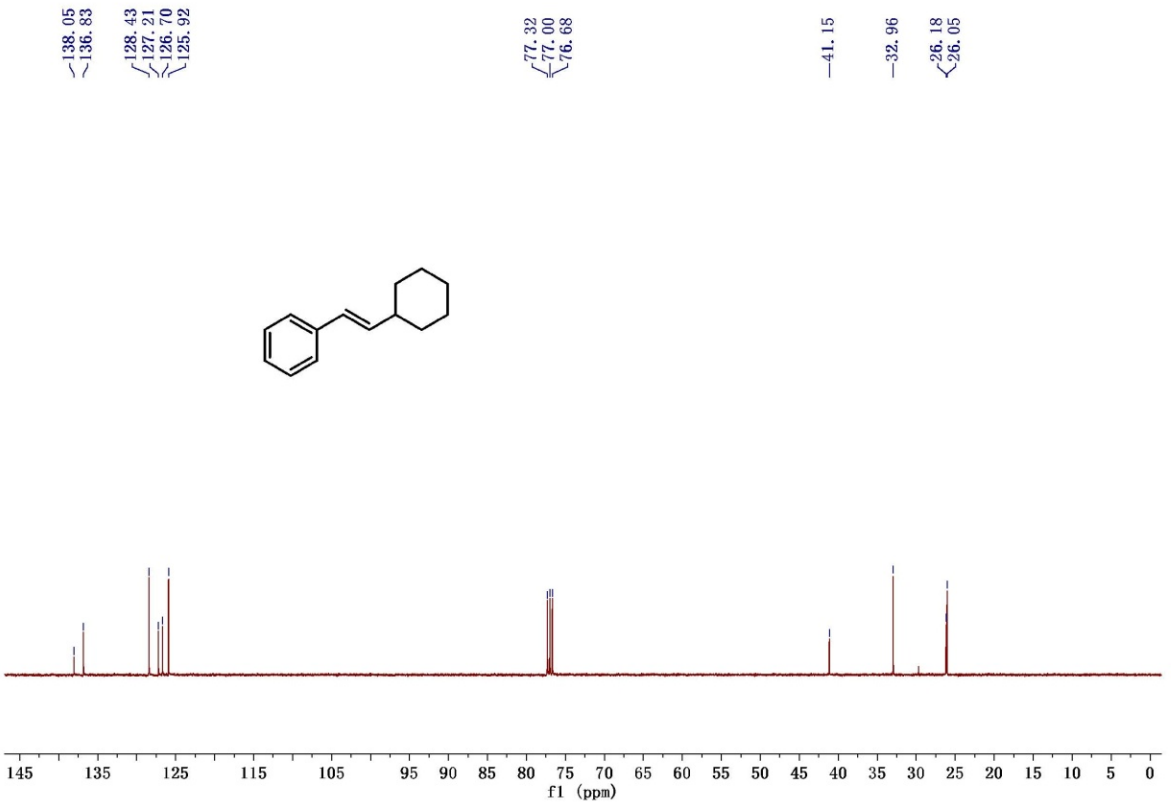
3b- ^{13}C NMR



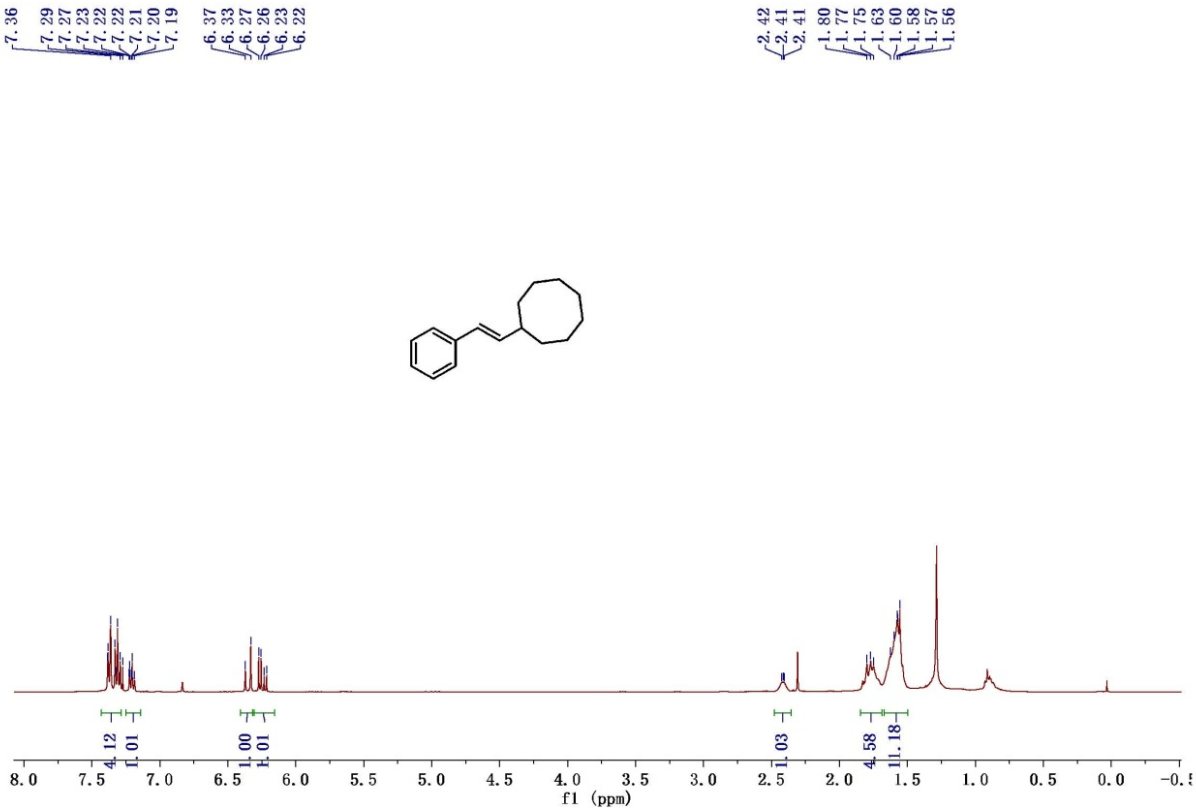
3c- ^{1}H NMR



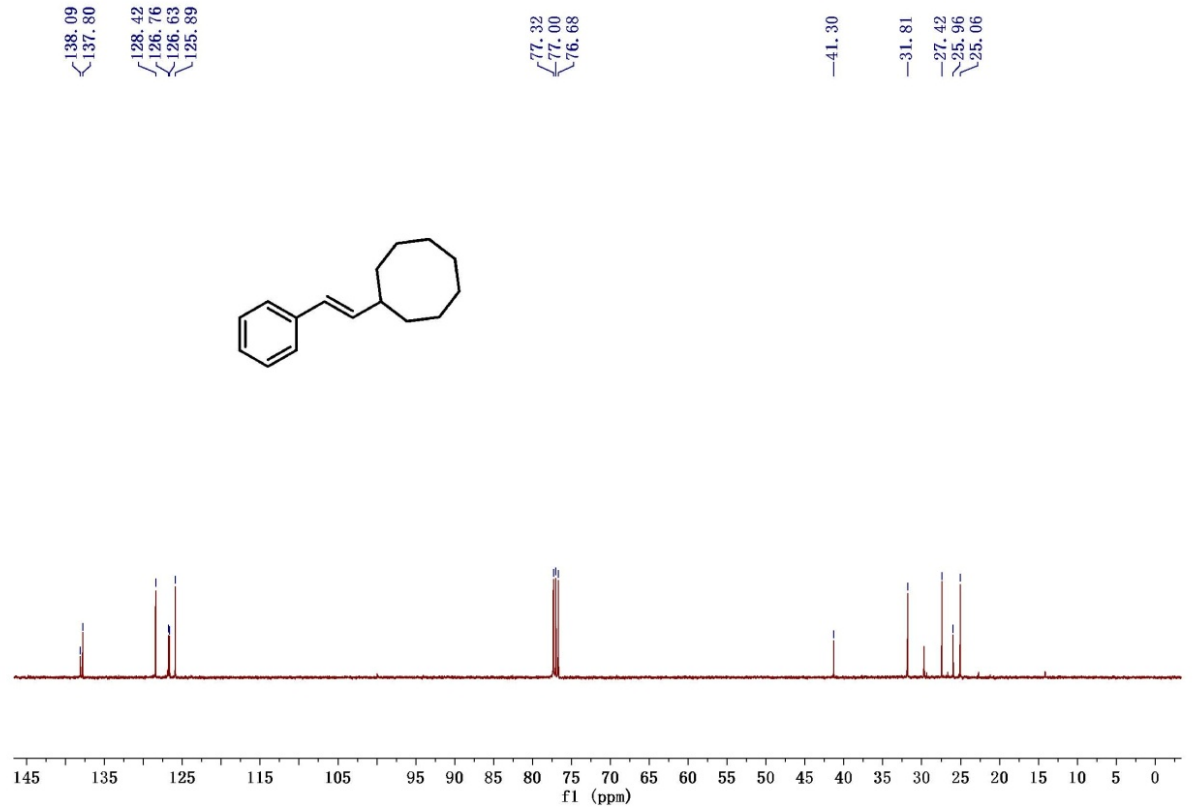
3c- ^{13}C NMR



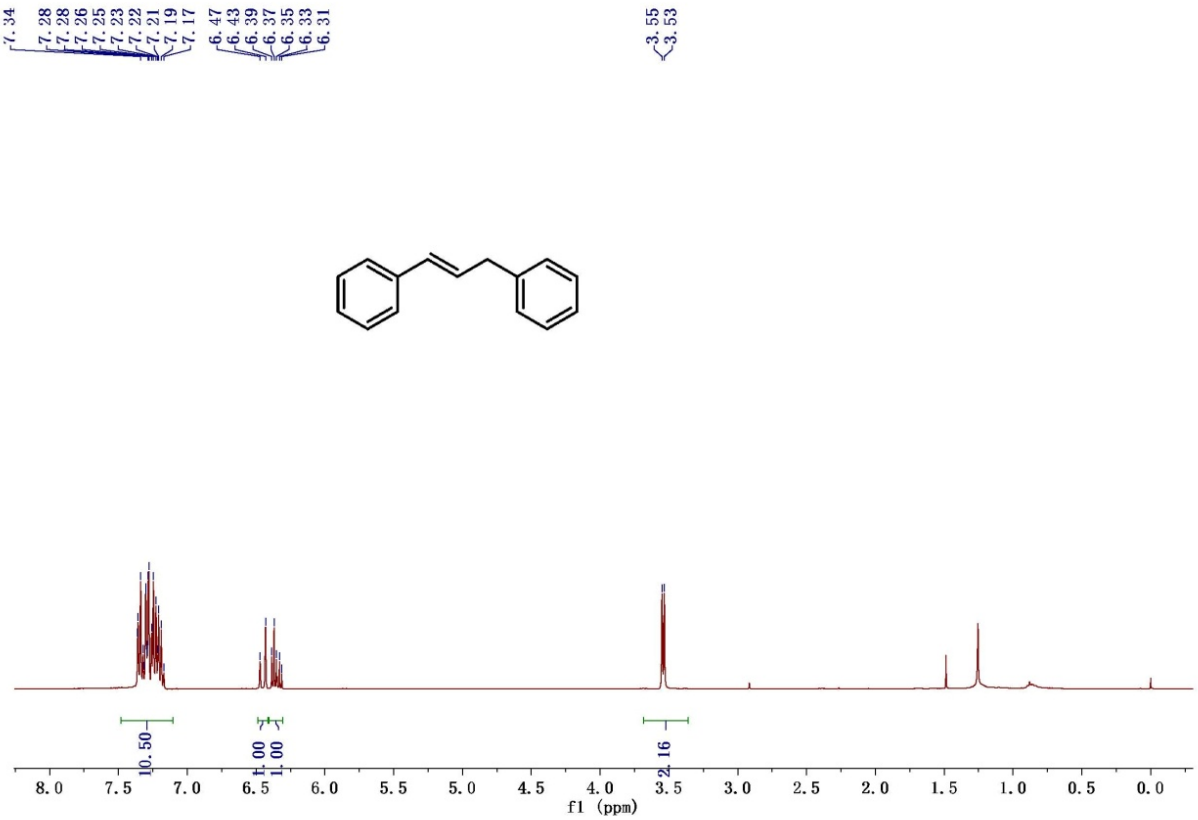
3d- ^{1}H NMR



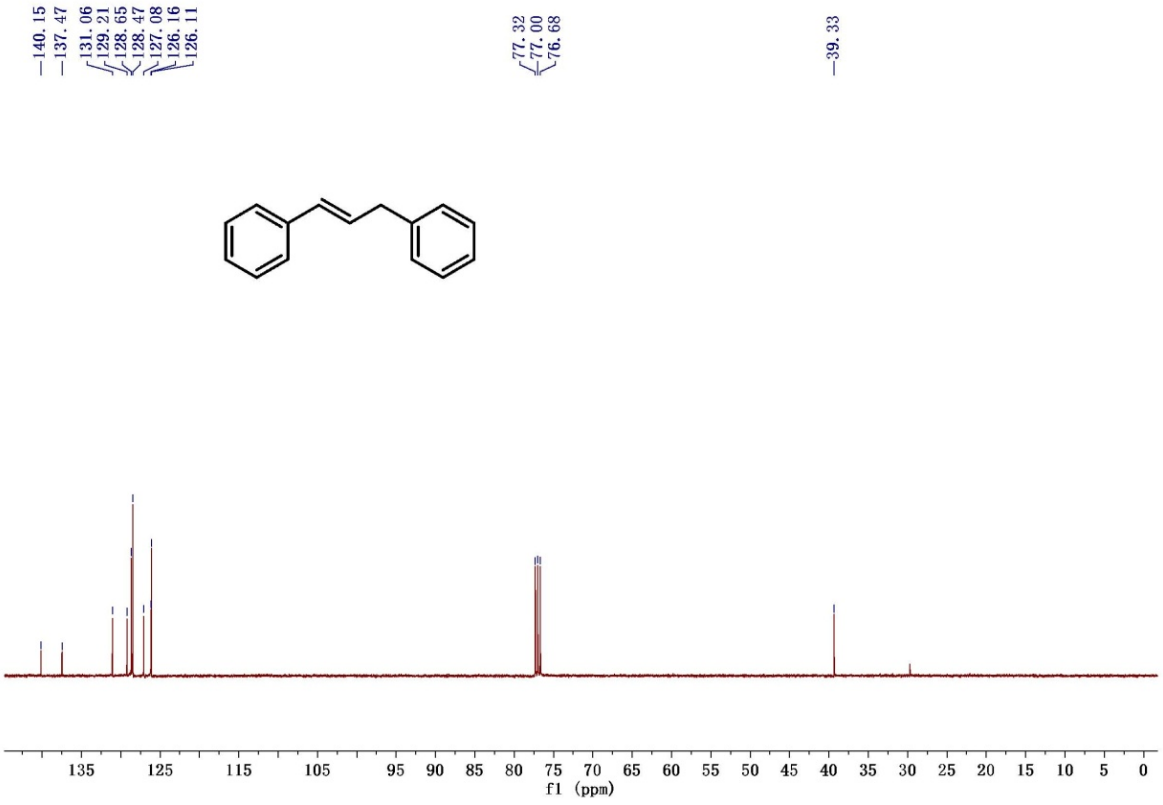
3d- ^{13}C NMR



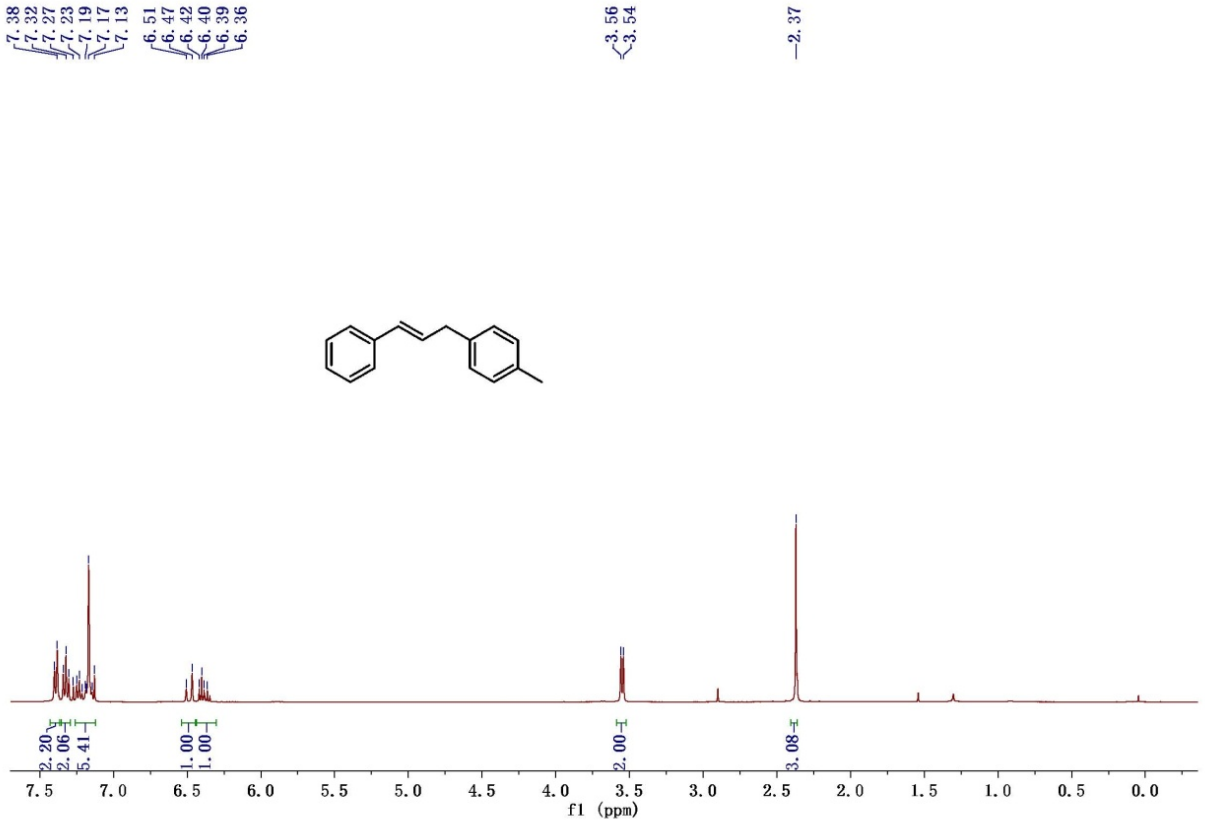
3e- ^{1}H NMR



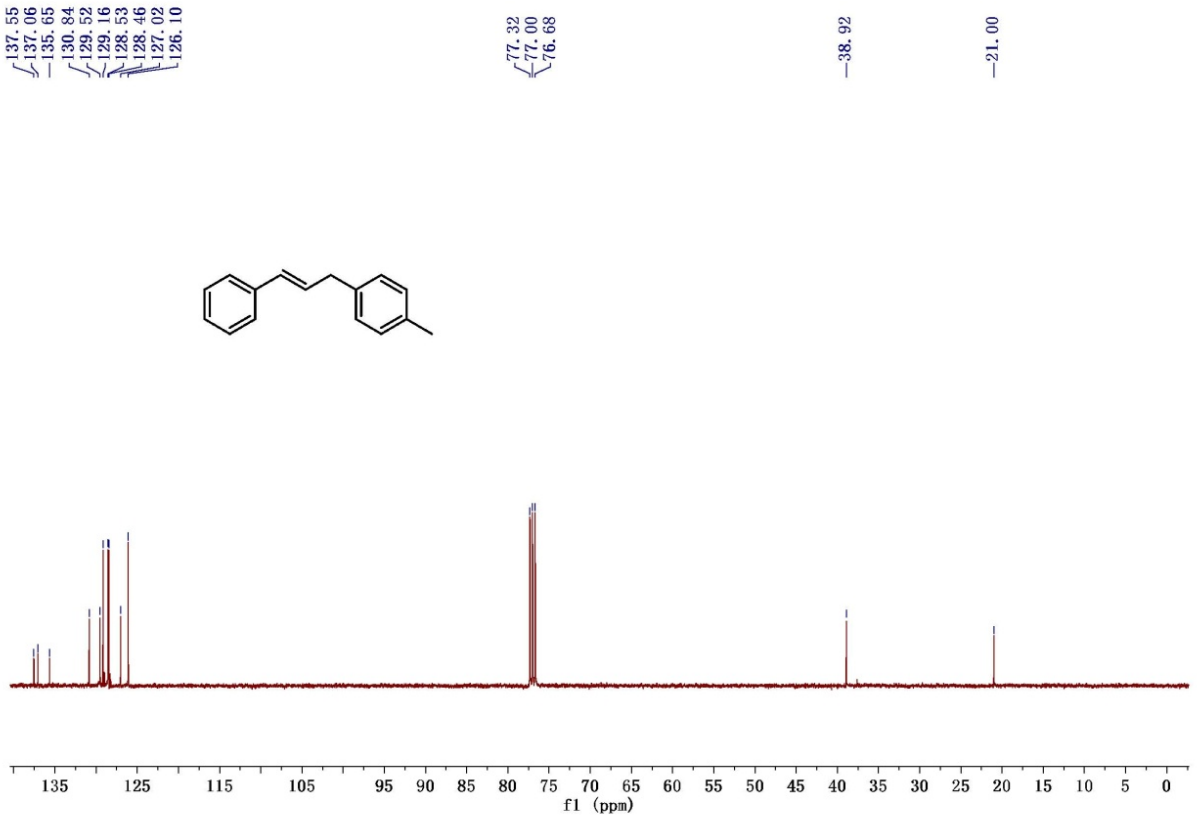
3e- ^{13}C NMR



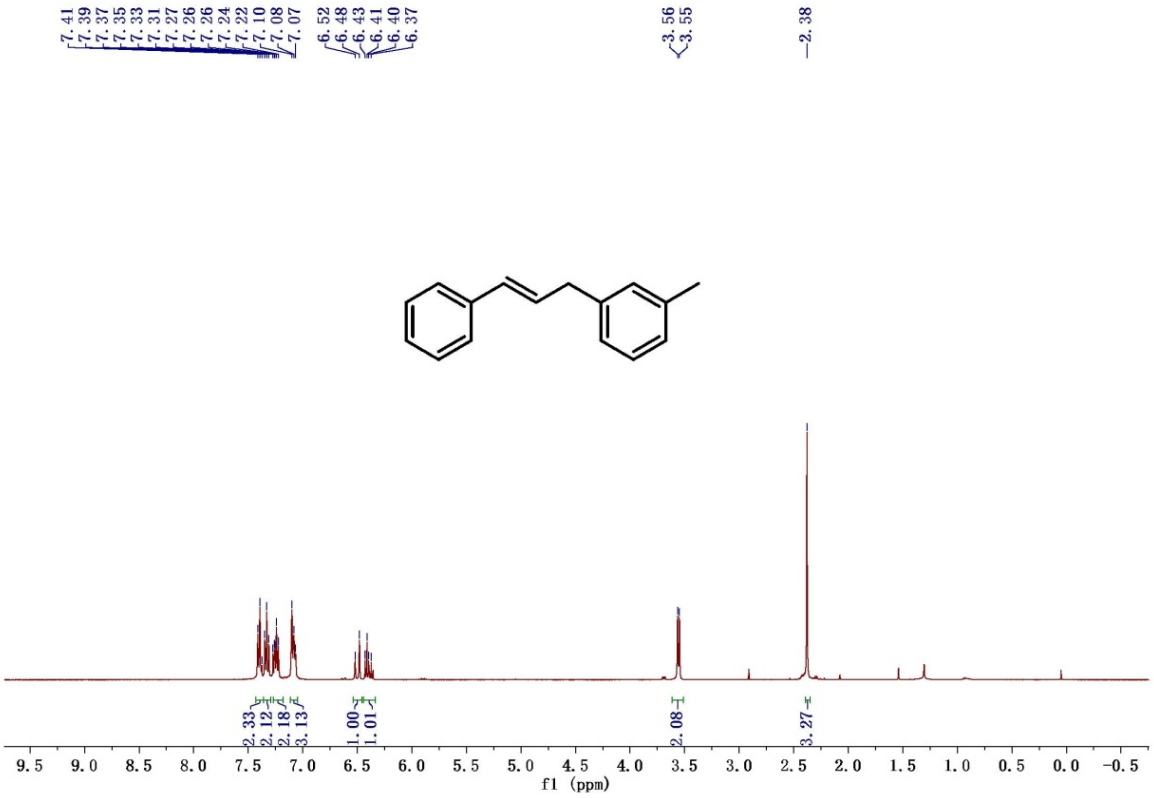
3f- ^{1}H NMR



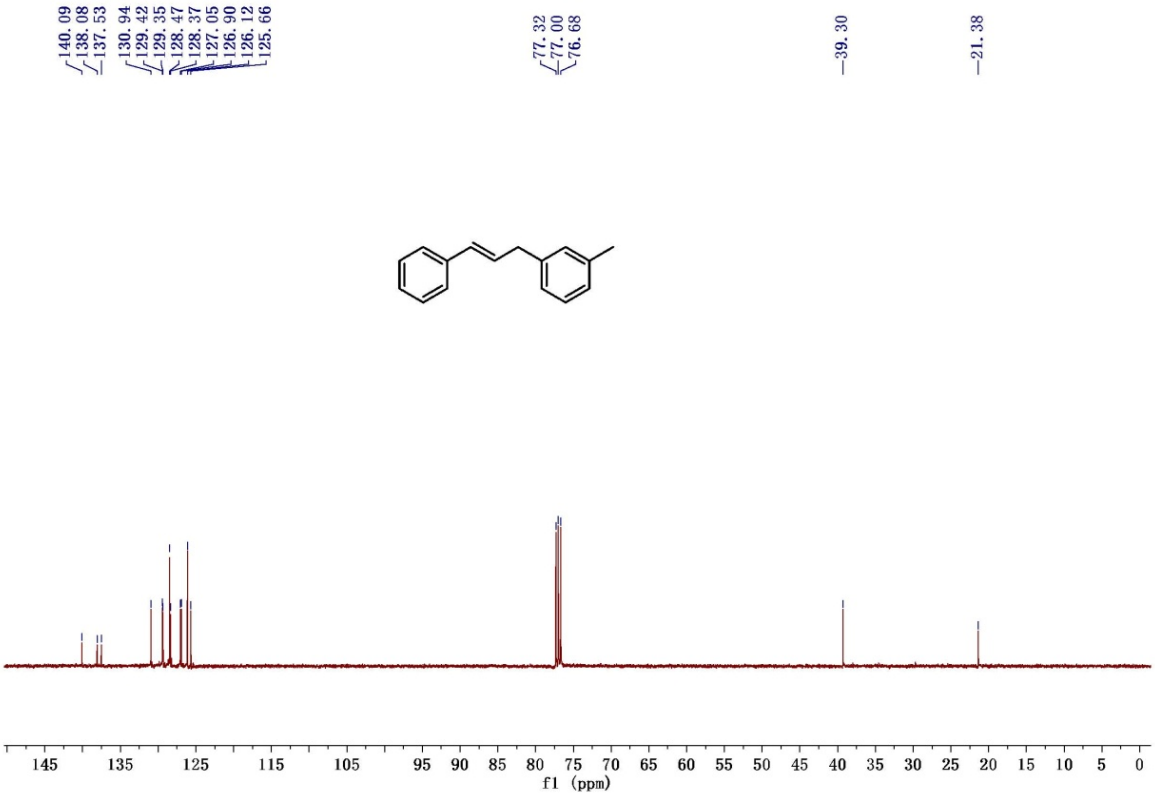
3f- ^{13}C NMR



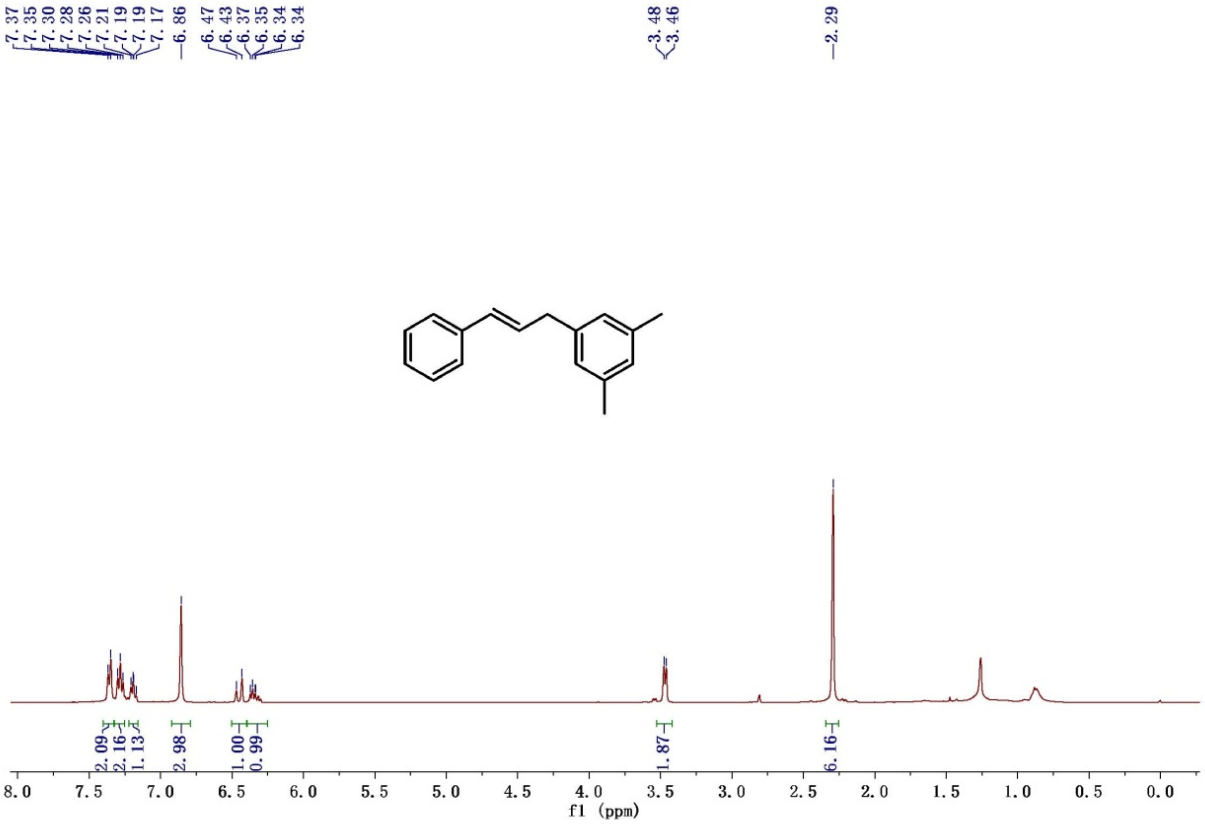
3g- ^{1}H NMR



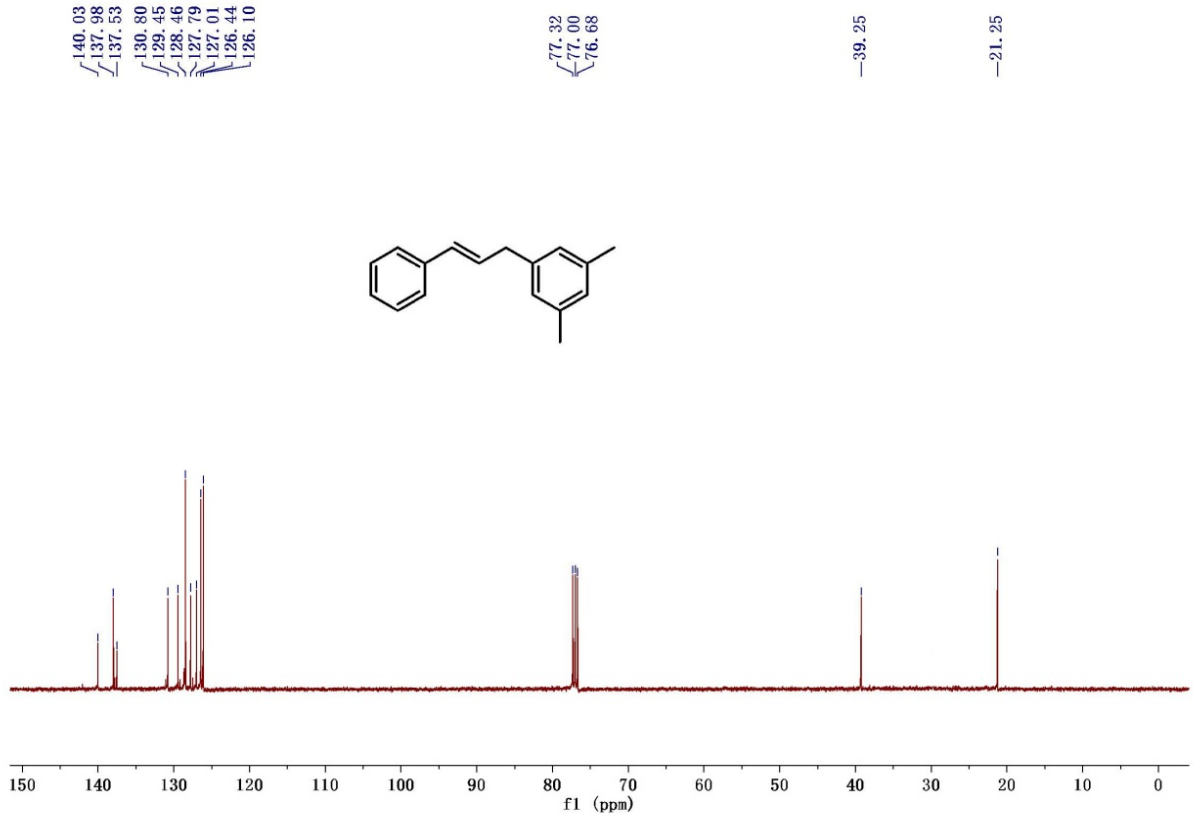
3g- ^{13}C NMR



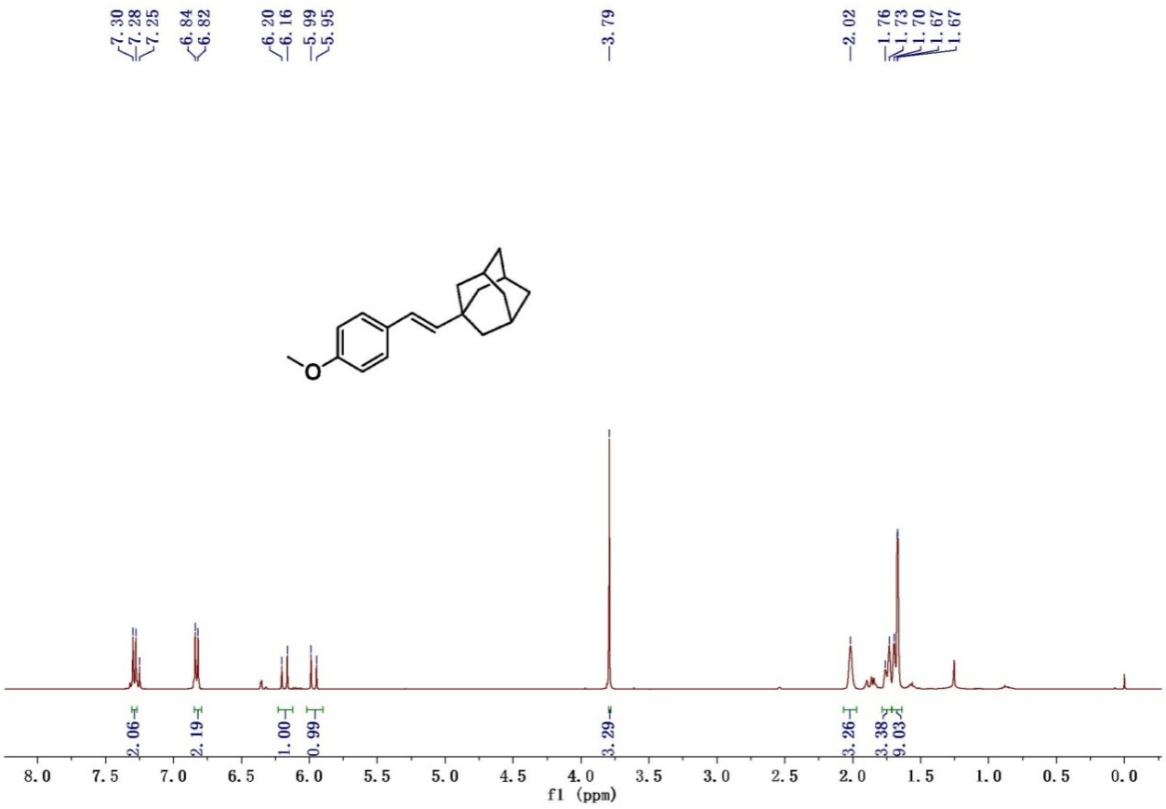
3h- ^{1}H NMR



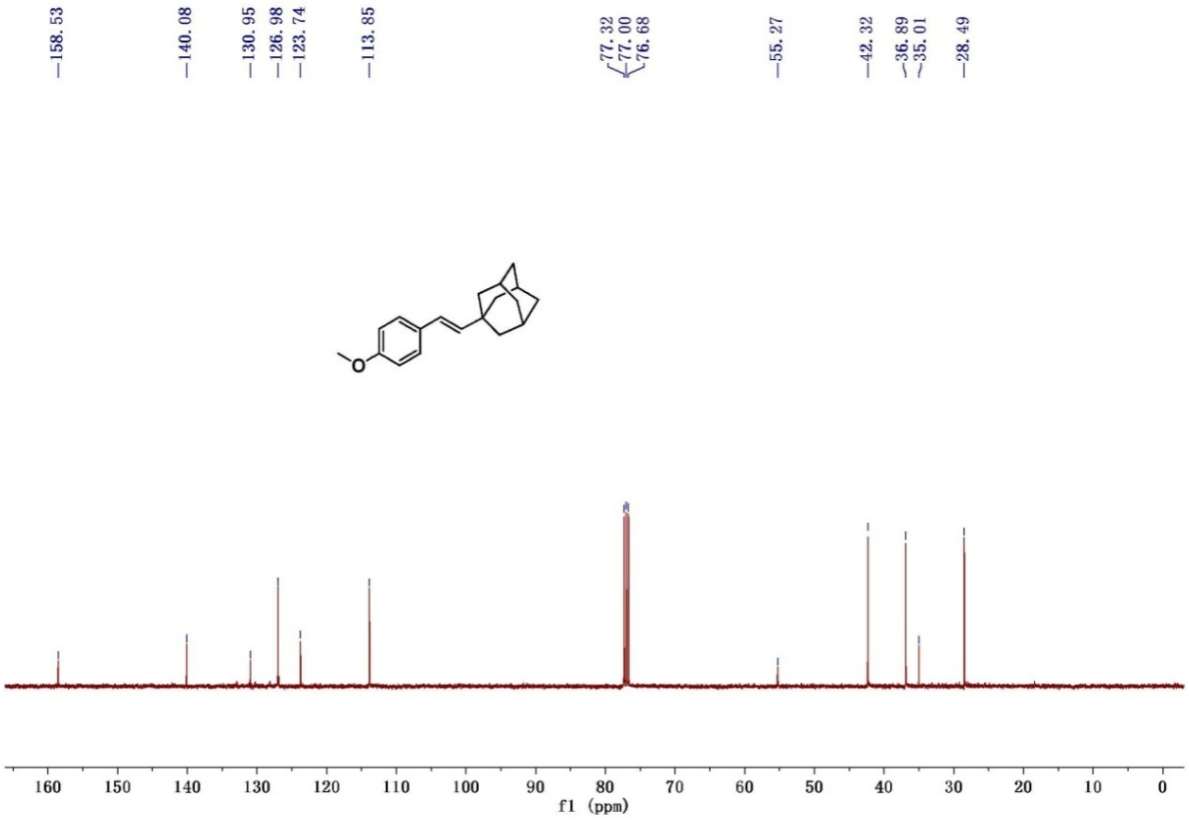
3h- ^{13}C NMR

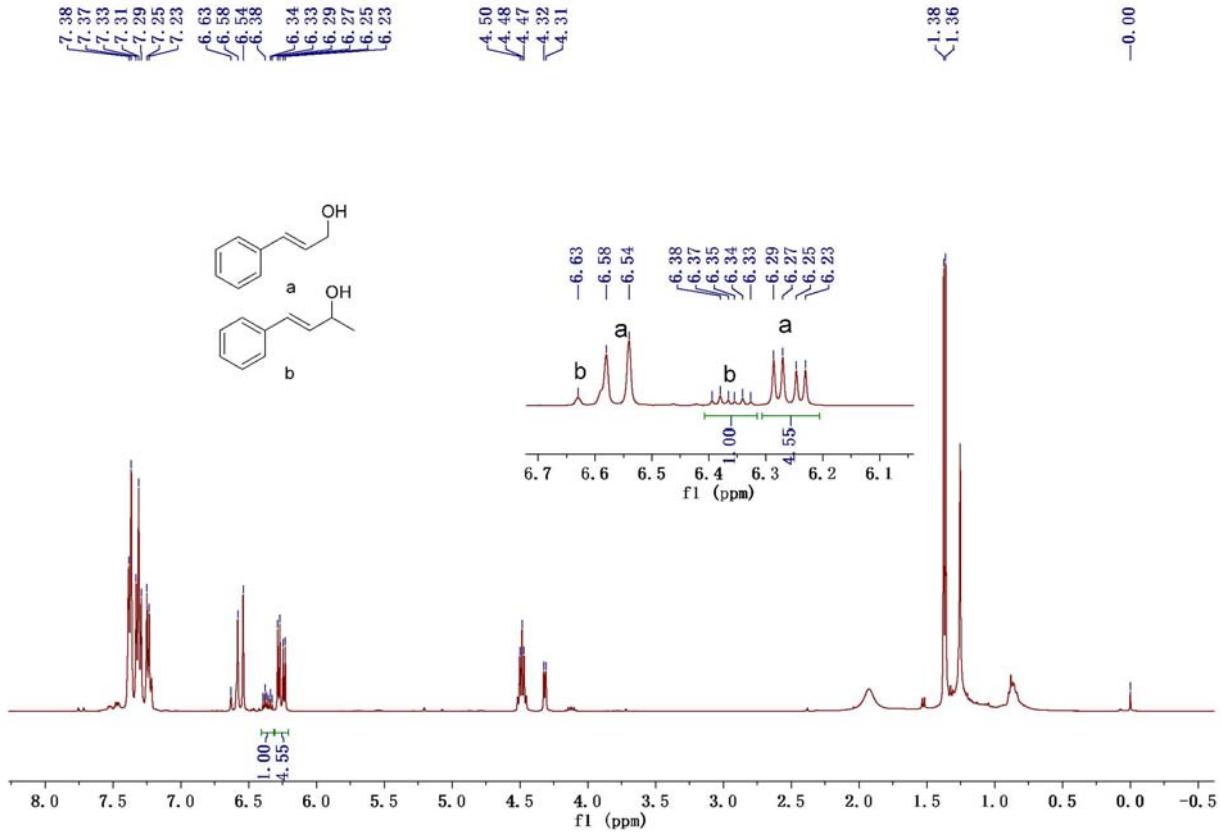


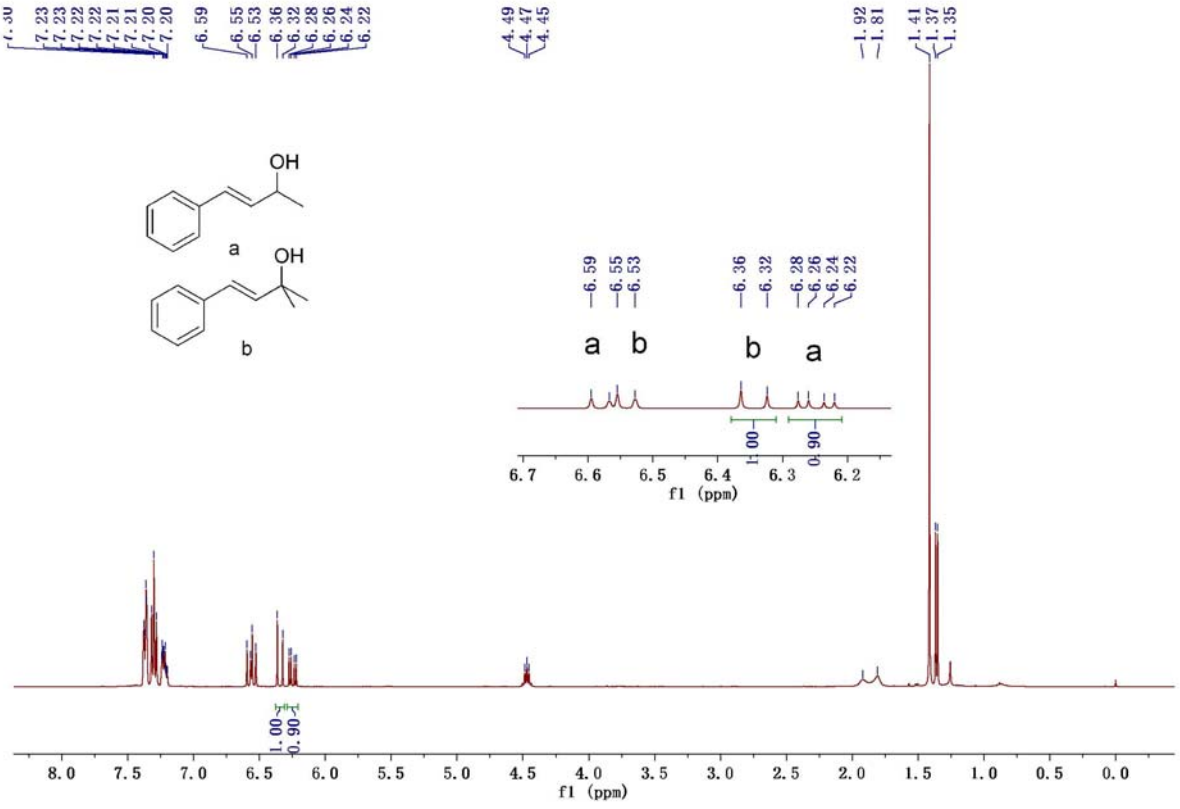
4a- ^{1}H NMR



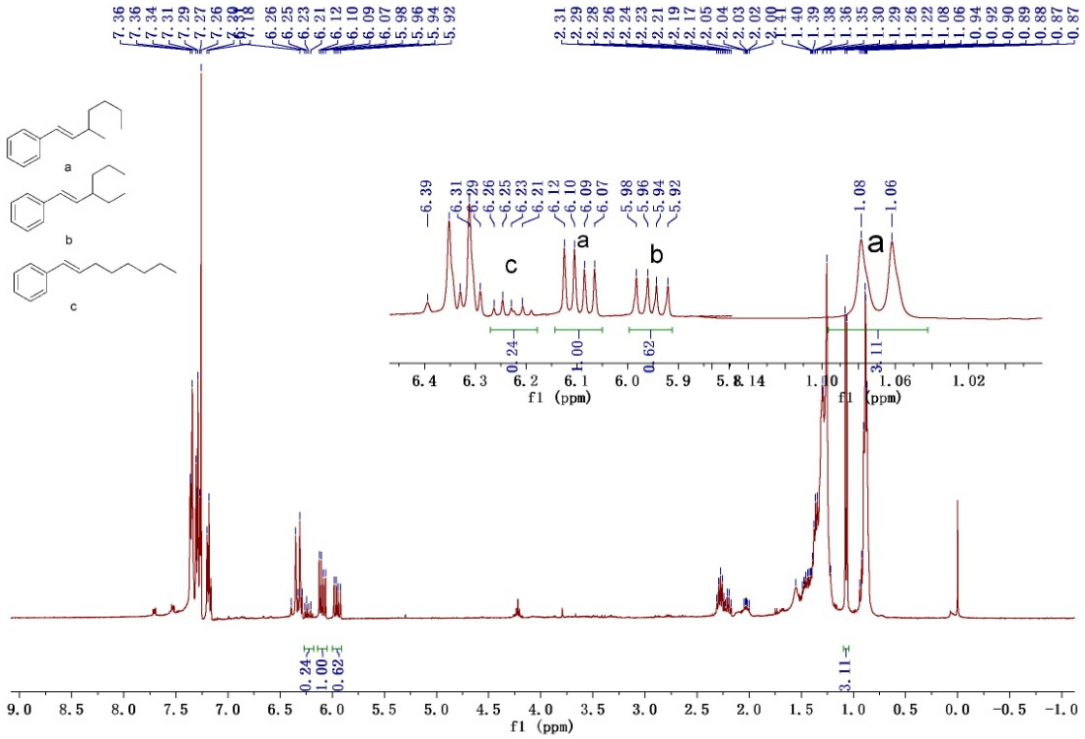
4a- ^{13}C NMR



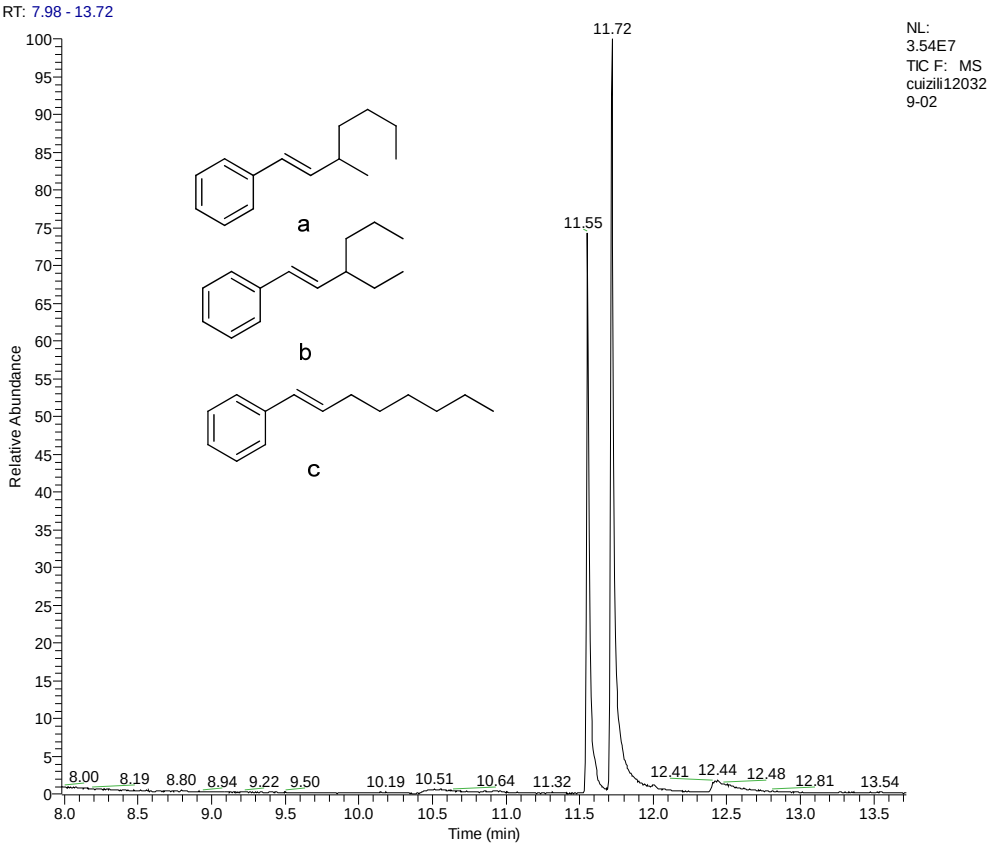

7.38
7.37
7.33
7.31
7.29
7.25
7.23
6.63
6.58
6.54
6.38
6.34
6.33
6.29
6.27
6.25
6.23
4.50
4.48
4.47
4.32
4.31
1.38
1.36
0.00
OH
a
OH
b
6.63
6.58
6.54
6.38
6.37
6.35
6.34
6.33
6.29
6.27
6.25
6.23
a
b
a
b
1.00
4.55
6.7 6.6 6.5 6.4 6.3 6.2 6.1
f1 (ppm)
1.00
4.55
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


7.30
7.23
7.23
7.22
7.22
7.21
7.21
7.20
7.20
6.59
6.55
6.53
6.36
6.32
6.28
6.26
6.24
6.22
4.49
4.47
4.45
1.92
1.81
1.41
1.37
1.35
OH
a
OH
b
6.59
6.55
6.53
6.36
6.32
6.28
6.26
6.24
6.22
a
b
b
a
1.00
0.90
6.7 6.6 6.5 6.4 6.3 6.2
f1 (ppm)
1.00
0.90
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)

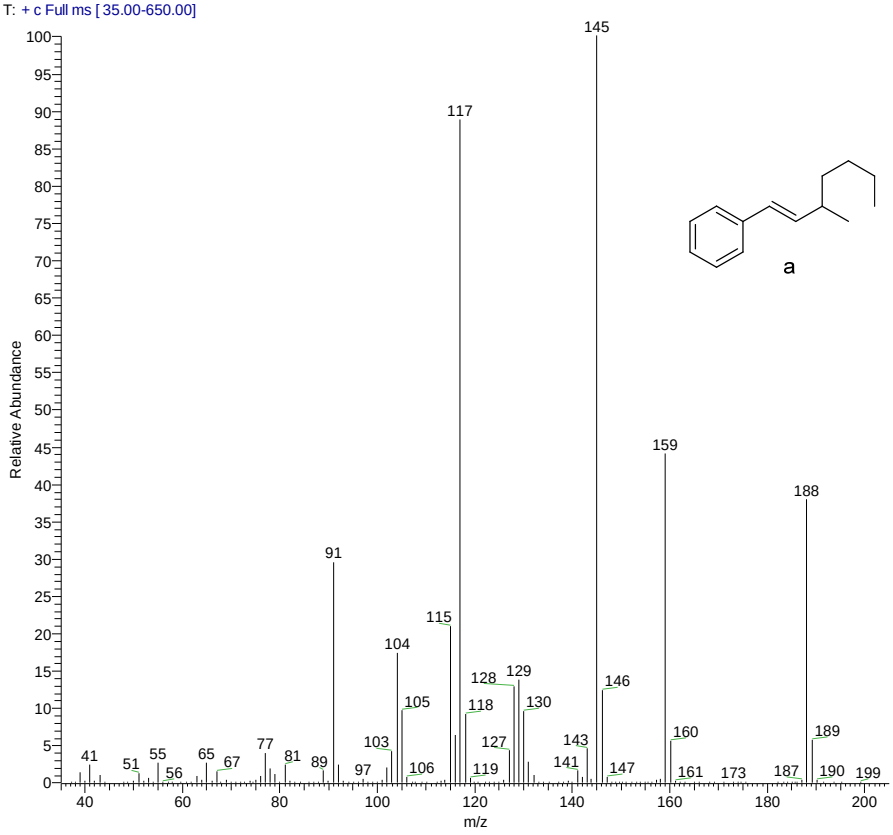
4b- ^{1}H NMR



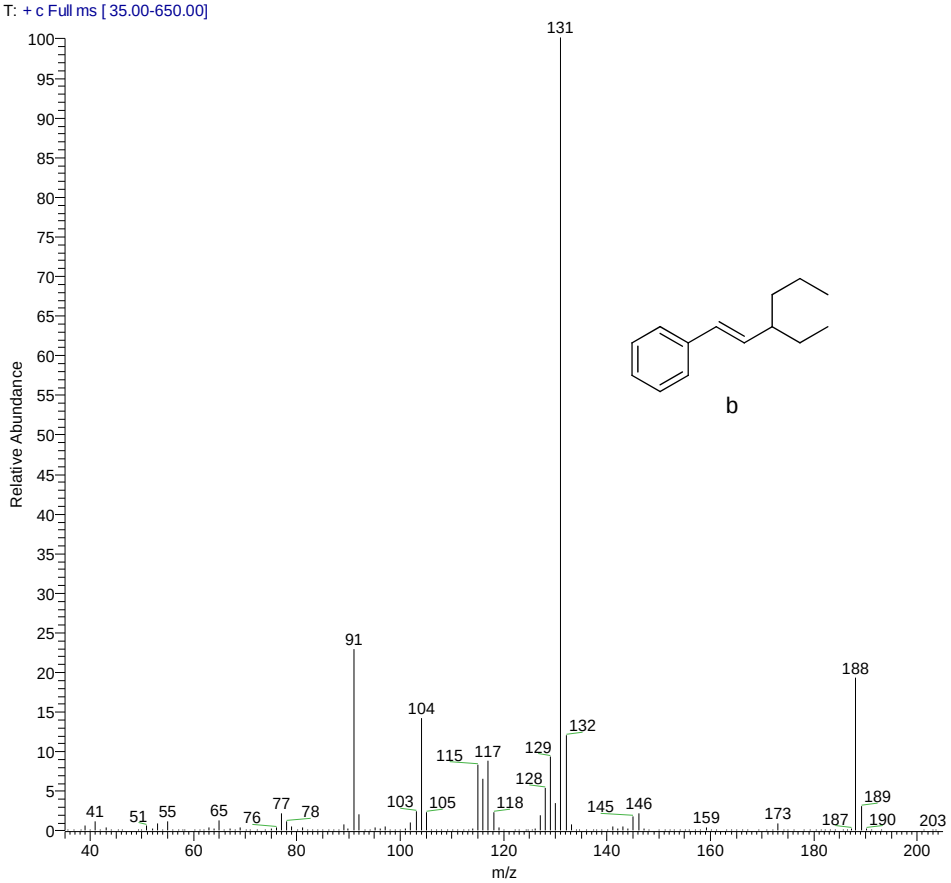
4b- GC – MS

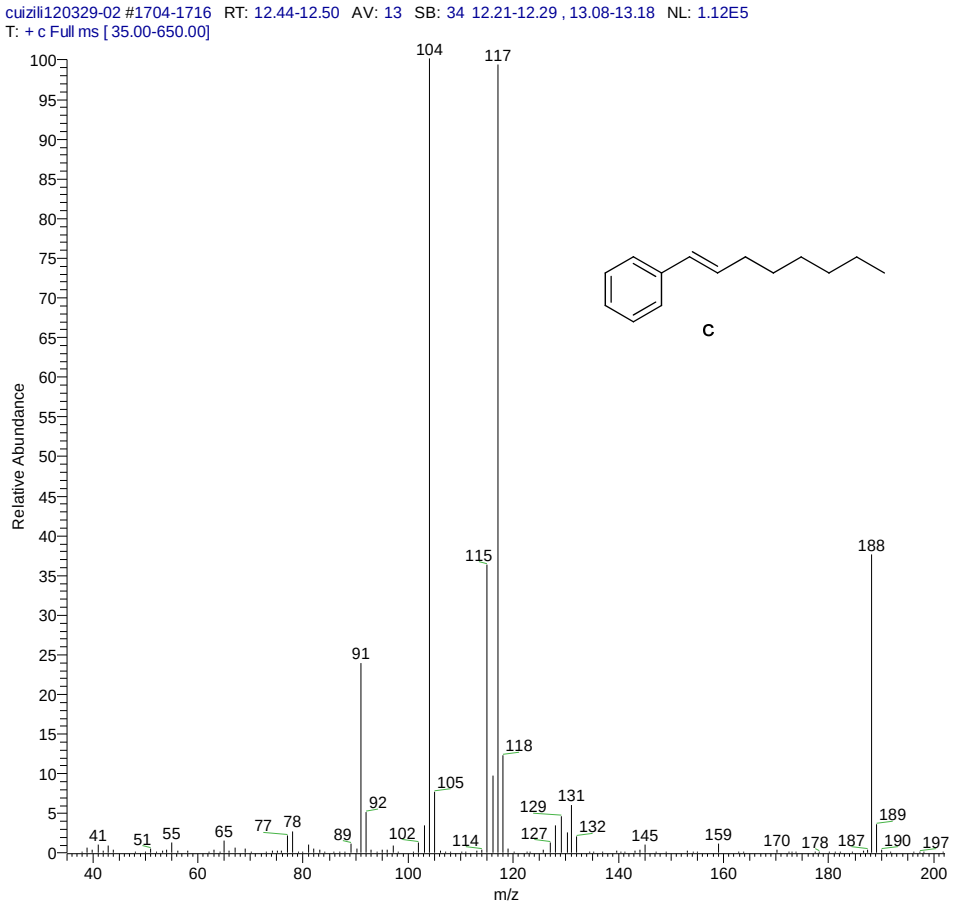


cuizili120329-02 #1544-1546 RT: 11.55-11.56 AV: 3 SB: 15 11.46-11.49 , 12.01-12.05 NL: 4.60E6
T: + c Full ms [35.00-650.00]

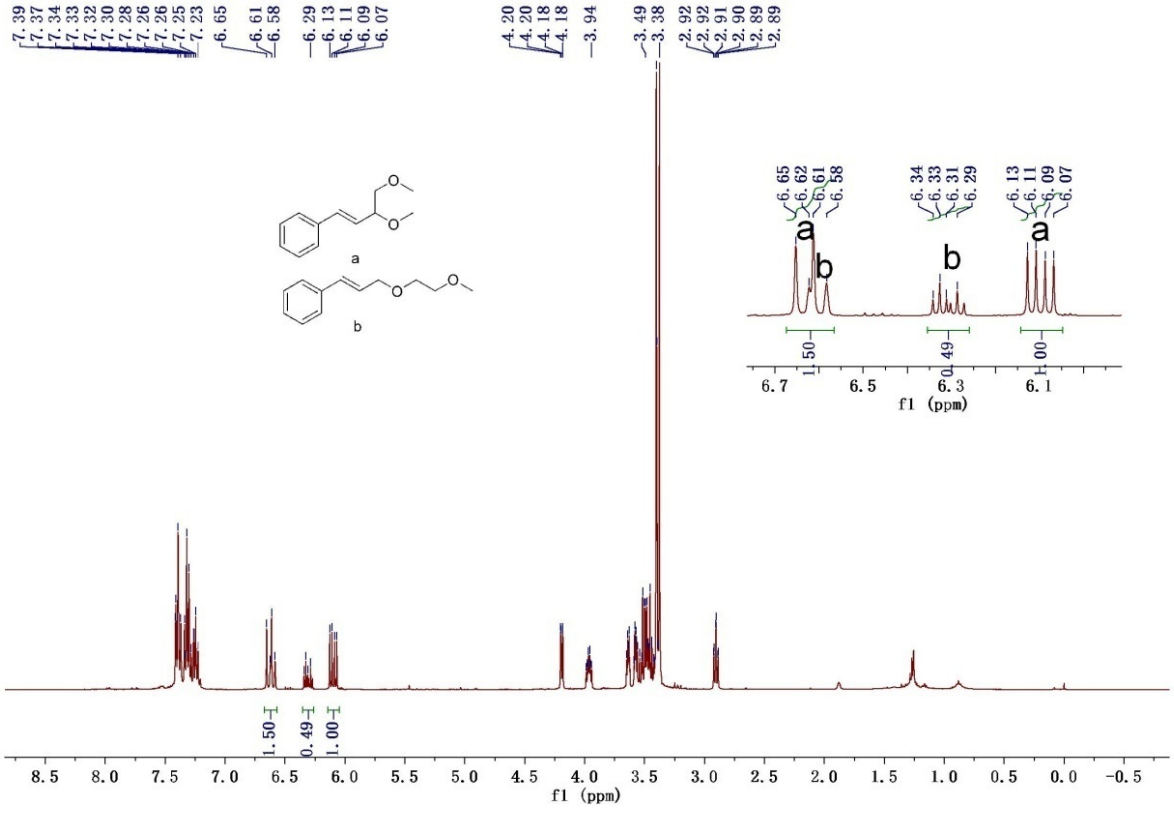


cuizili120329-02 #1574-1576 RT: 11.72-11.73 AV: 3 SB: 15 11.46-11.49 , 12.01-12.05 NL: 1.25E7
T: + c Full ms [35.00-650.00]

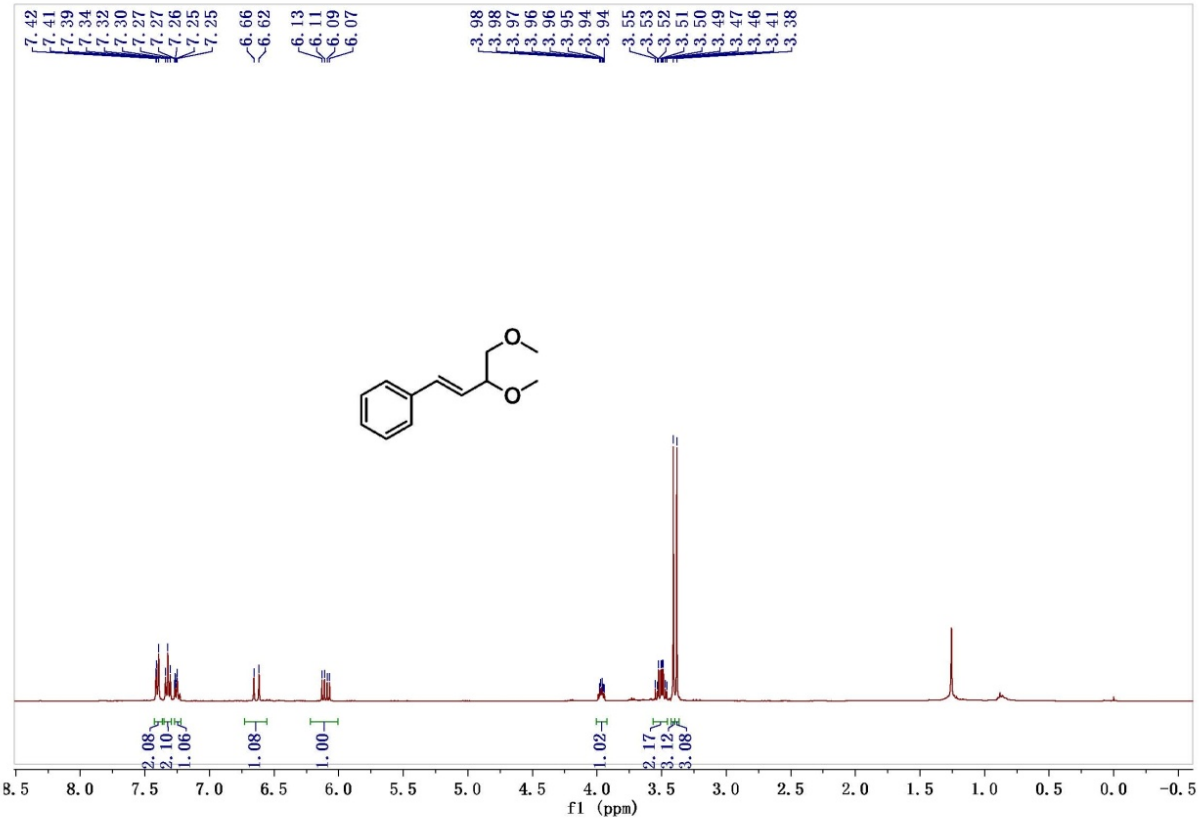



cuizili120329-02 #1704-1716 RT: 12.44-12.50 AV: 13 SB: 34 12.21-12.29 , 13.08-13.18 NL: 1.12E5
T: + c Full ms [35.00-650.00]
Relative Abundance
m/z
104
117
115
188
91
118
105
92
129
131
189
41
51
55
65
77
78
89
102
114
127
132
145
159
170
178
187
190
197
c

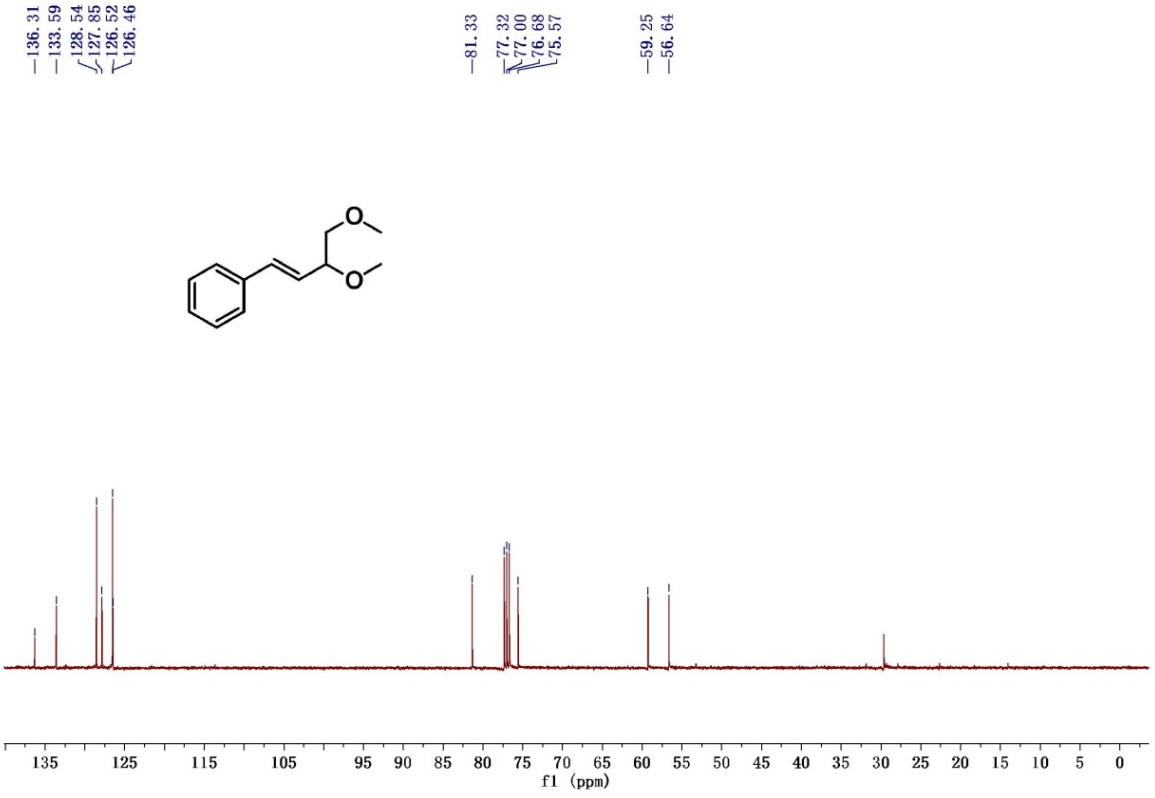
4c- ^{1}H NMR


a
b
f1 (ppm)

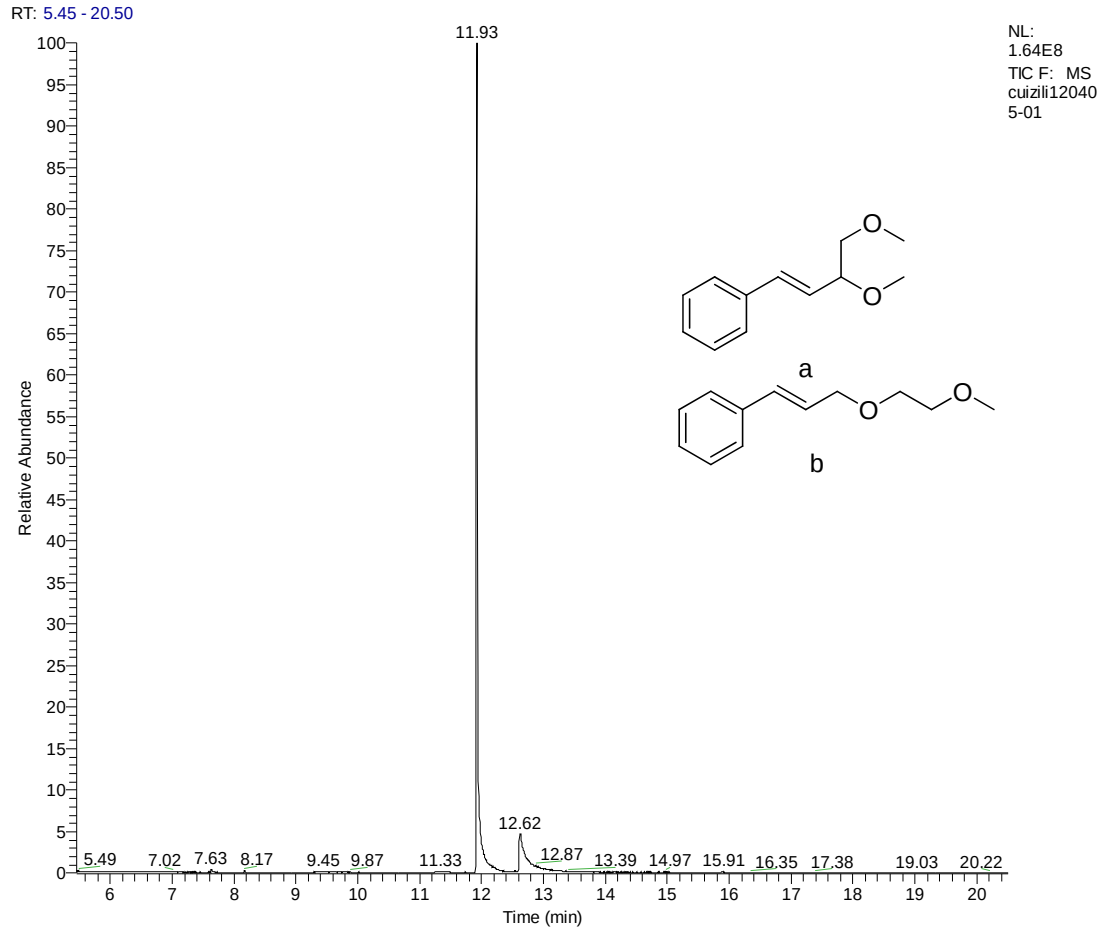
4ca- ^{1}H NMR

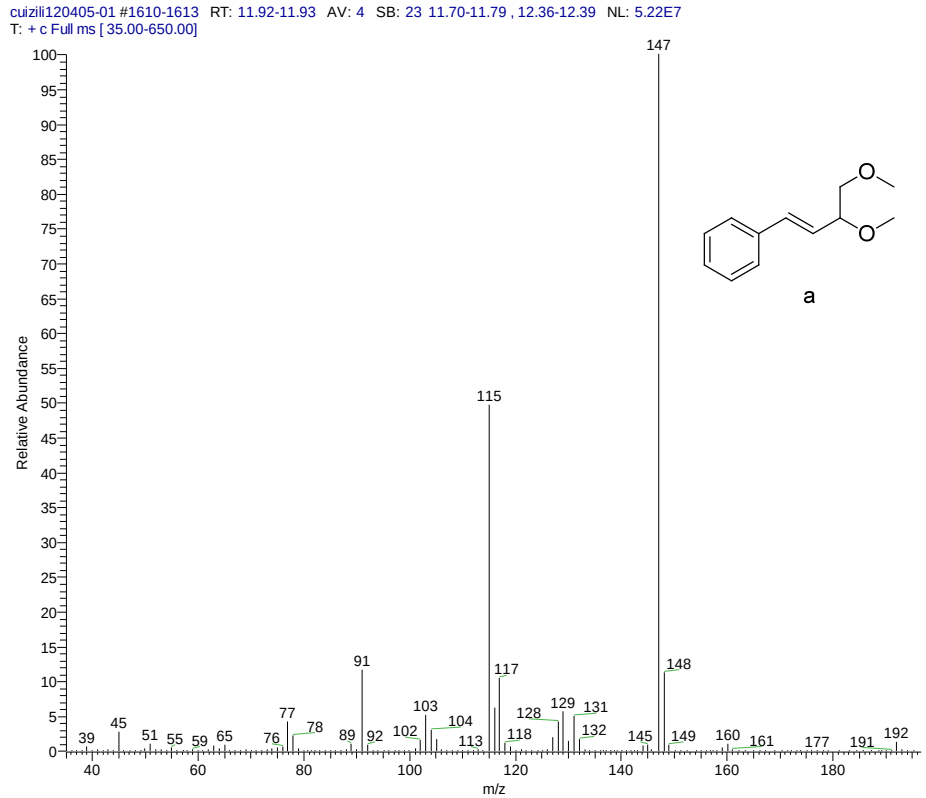


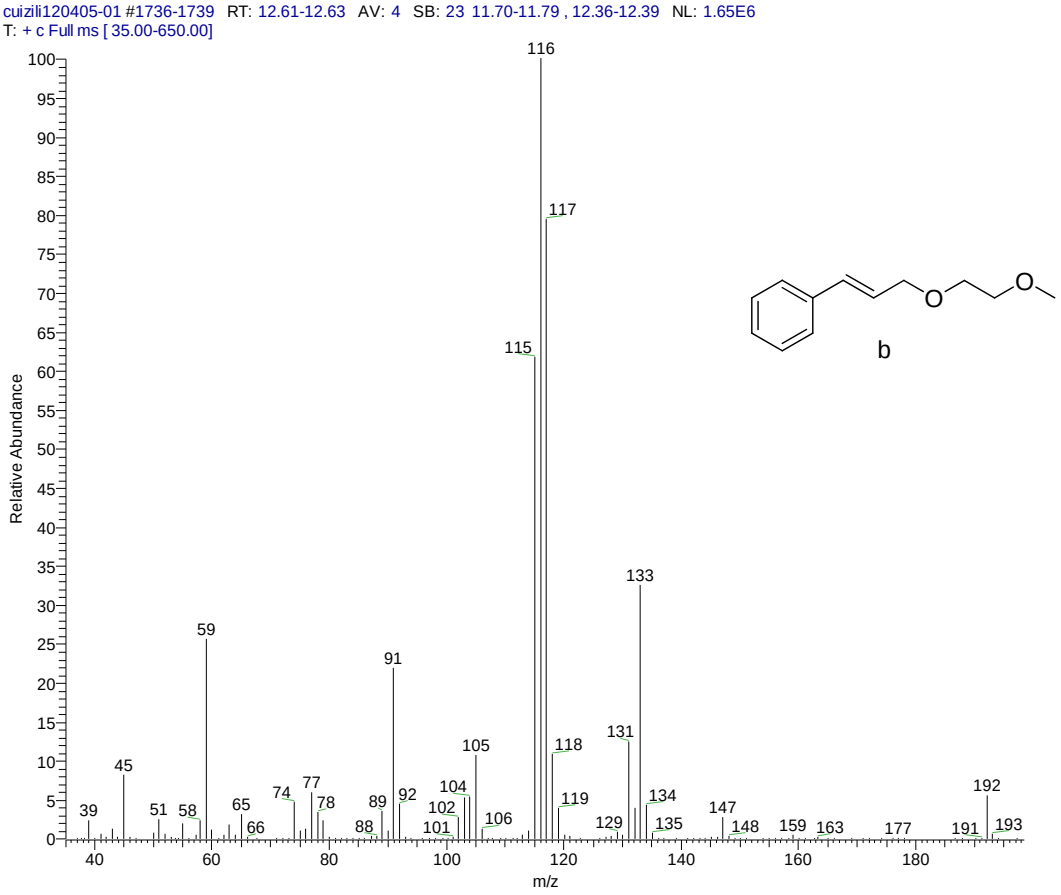
4ca- ^{13}C NMR



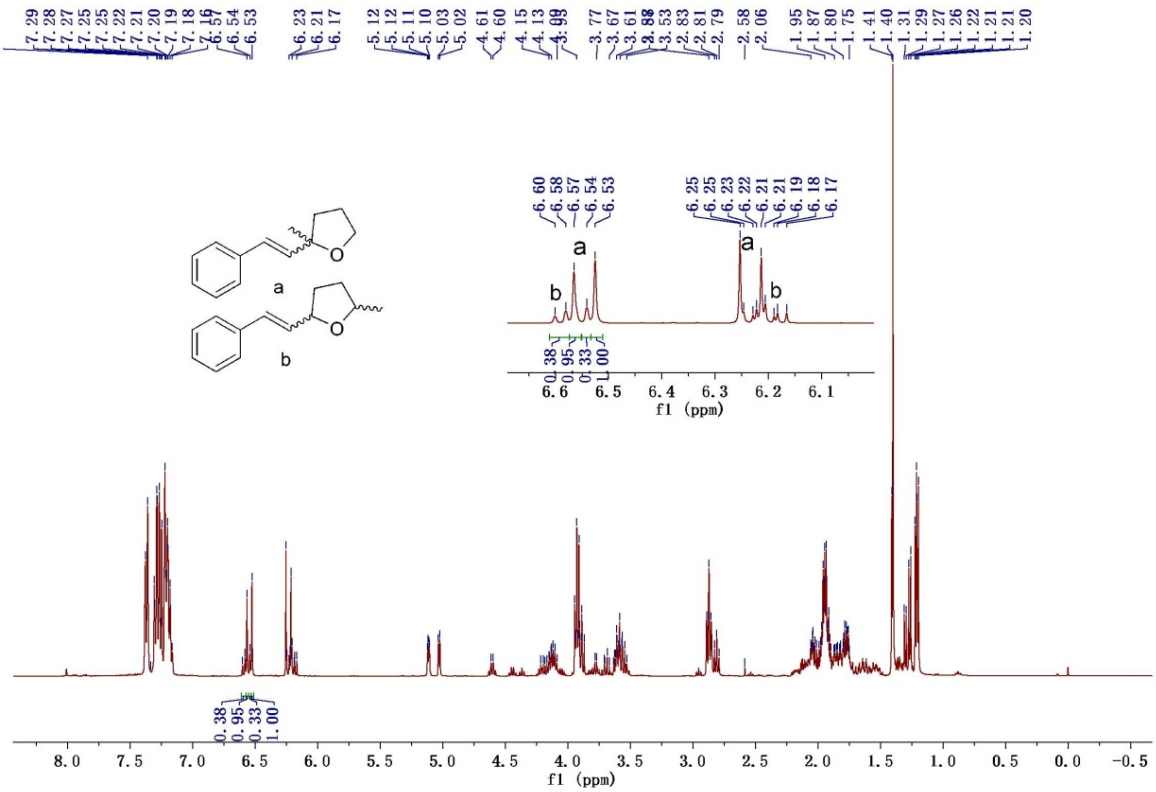
4c- GC - MS


RT: 5.45 - 20.50
NL:
1.64E8
TIC F: MS
cuizili12040
5-01
Relative Abundance
Time (min)
11.93
12.62
5.49
7.02
7.63
8.17
9.45
9.87
11.33
12.87
13.39
14.97
15.91
16.35
17.38
19.03
20.22
a
b

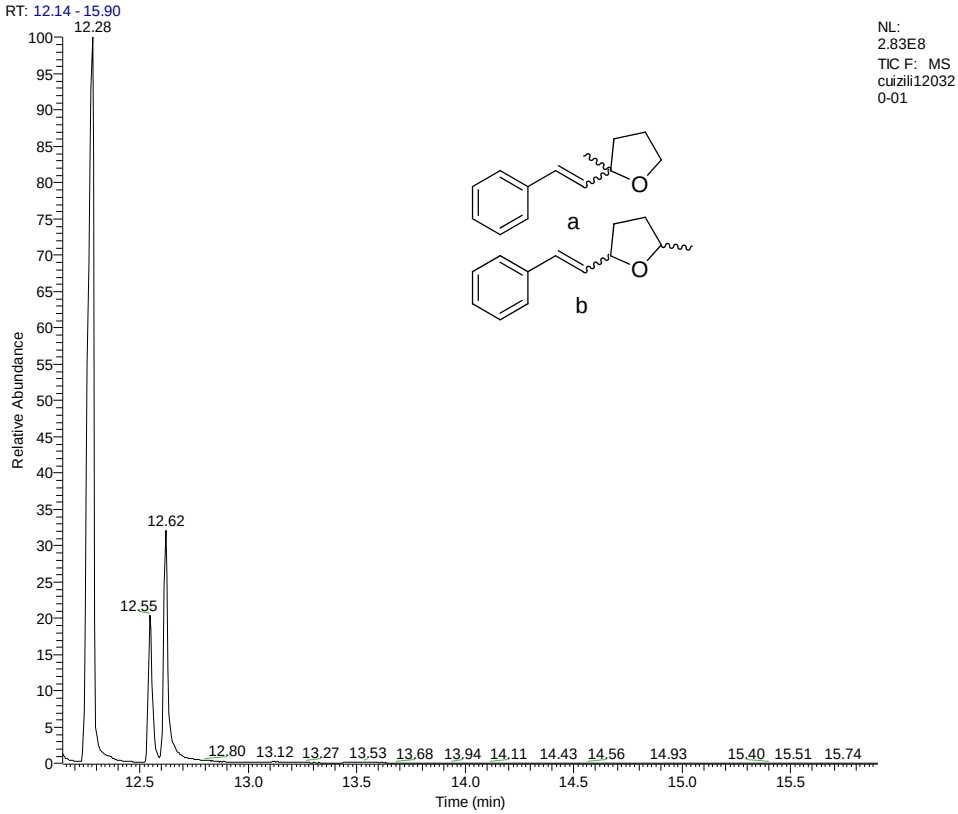

cuizili120405-01 #1610-1613 RT: 11.92-11.93 AV: 4 SB: 23 11.70-11.79 , 12.36-12.39 NL: 5.22E7
T: + c Full ms [35.00-650.00]
Relative Abundance
m/z
147
115
91
117
148
103
129
131
128
104
77
78
132
102
92
89
76
65
55
59
51
45
39
118
113
145
149
160
161
177
191
192
a

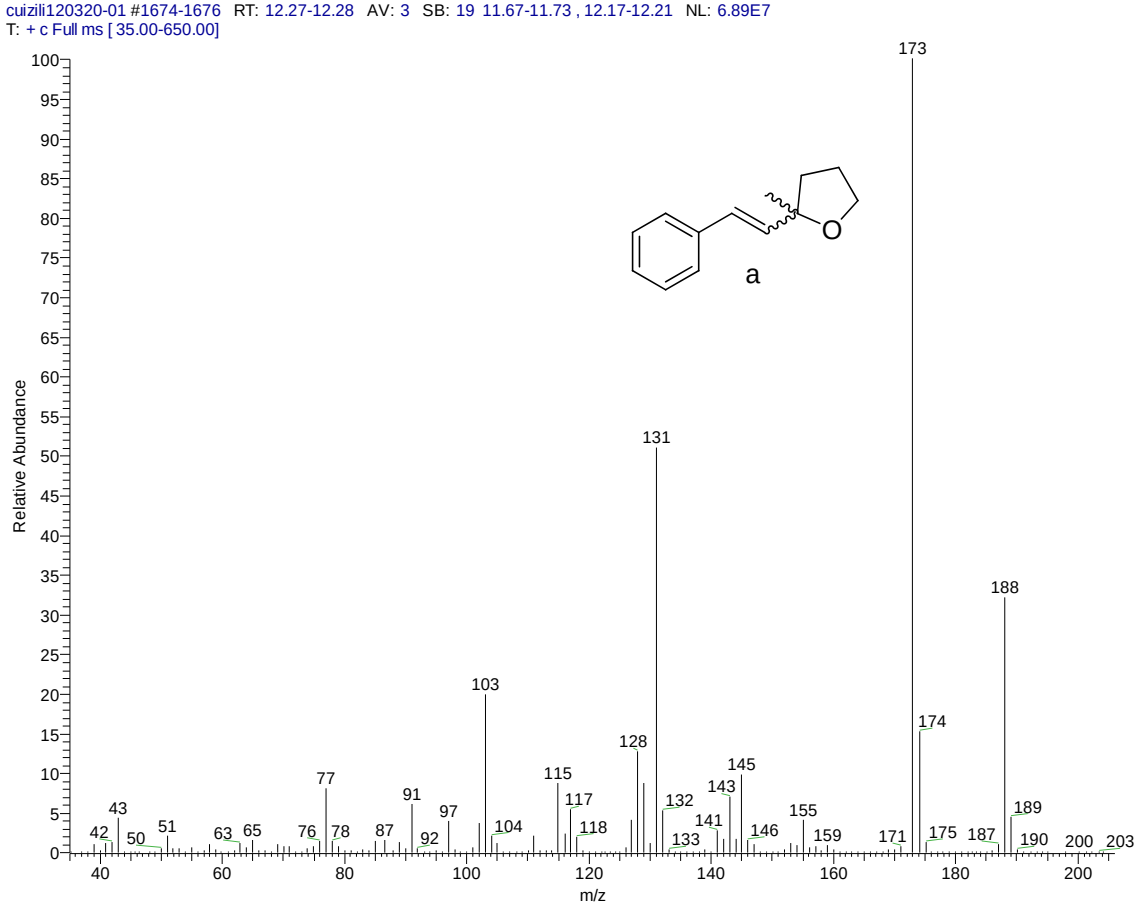

cuizili120405-01 #1736-1739 RT: 12.61-12.63 AV: 4 SB: 23 11.70-11.79 , 12.36-12.39 NL: 1.65E6
T: + c Full ms [35.00-650.00]
Relative Abundance
m/z
b

4d- ^{1}H NMR

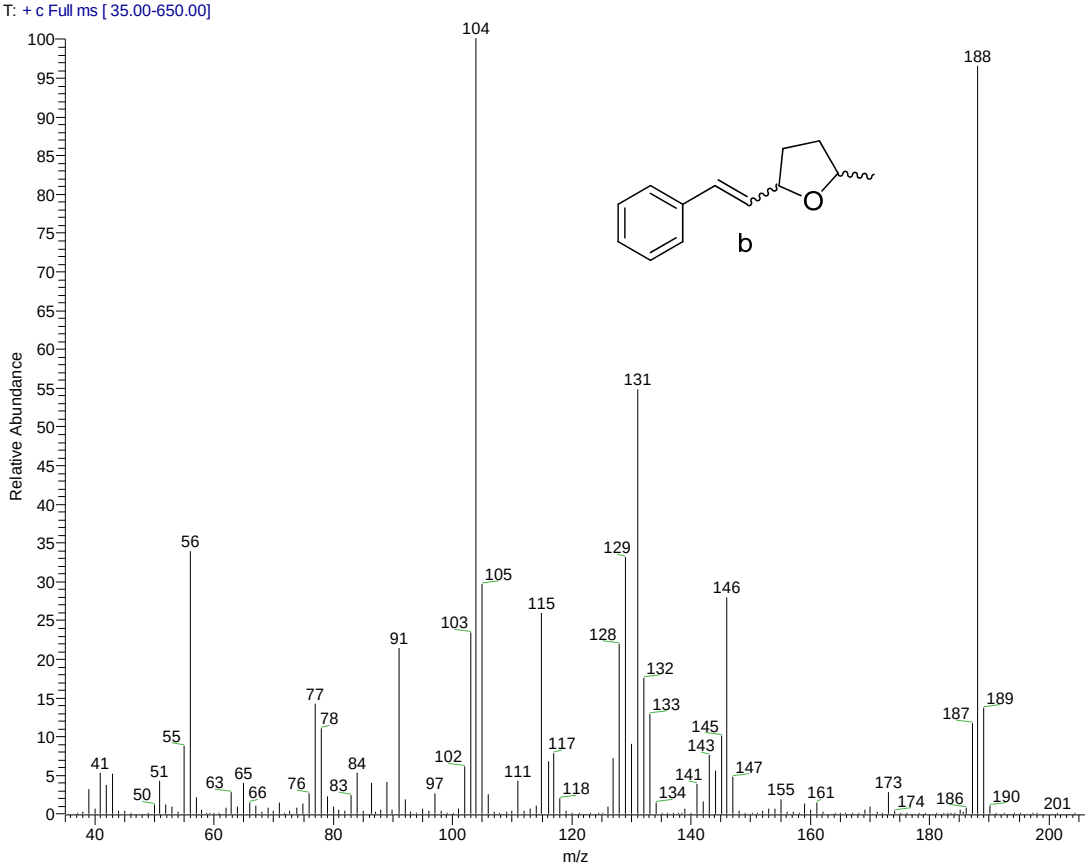

a
b
f1 (ppm)

4d- GC - MS

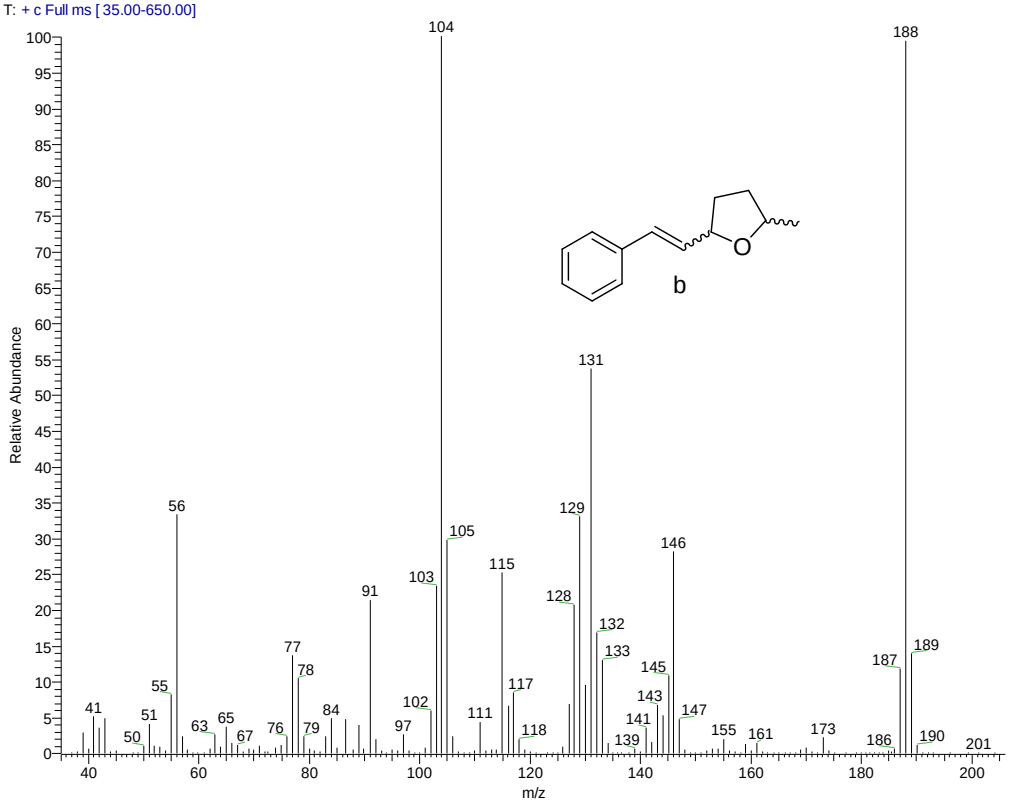

RT: 12.14 - 15.90
NL:
2.83E8
TIC F: MS
cuizili12032
0-01
12.28
12.62
12.55
12.80
13.12
13.27
13.53
13.68
13.94
14.11
14.43
14.56
14.93
15.40
15.51
15.74
Relative Abundance
Time (min)
a
b


cuizili120320-01 #1674-1676 RT: 12.27-12.28 AV: 3 SB: 19 11.67-11.73 , 12.17-12.21 NL: 6.89E7
T: + c Full ms [35.00-650.00]
Relative Abundance
m/z
a

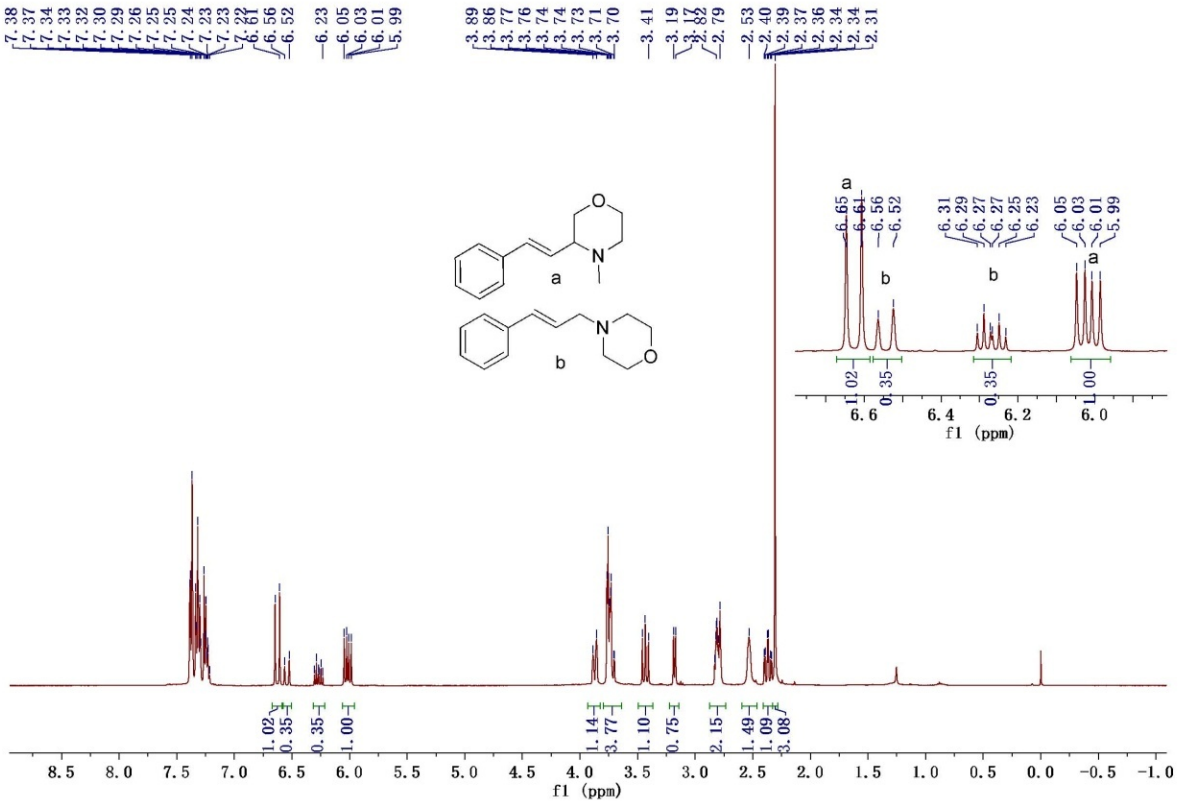
cuizili120320-01 #1724-1725 RT: 12.55-12.55 AV: 2 SB: 19 11.67-11.73 , 12.17-12.21 NL: 7.43E6
T: + c Full ms [35.00-650.00]



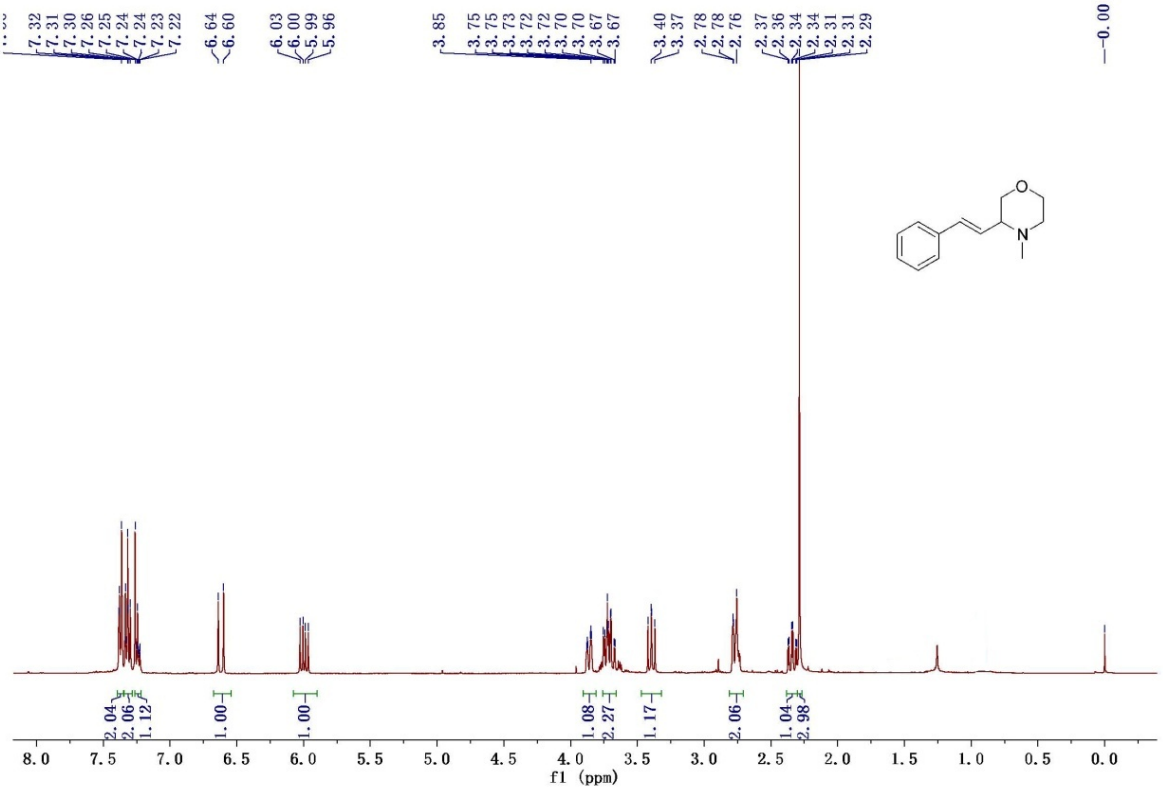
cuizili120320-01 #1736-1737 RT: 12.61-12.62 AV: 2 SB: 19 11.67-11.73 , 12.17-12.21 NL: 1.09E7
T: + c Full ms [35.00-650.00]



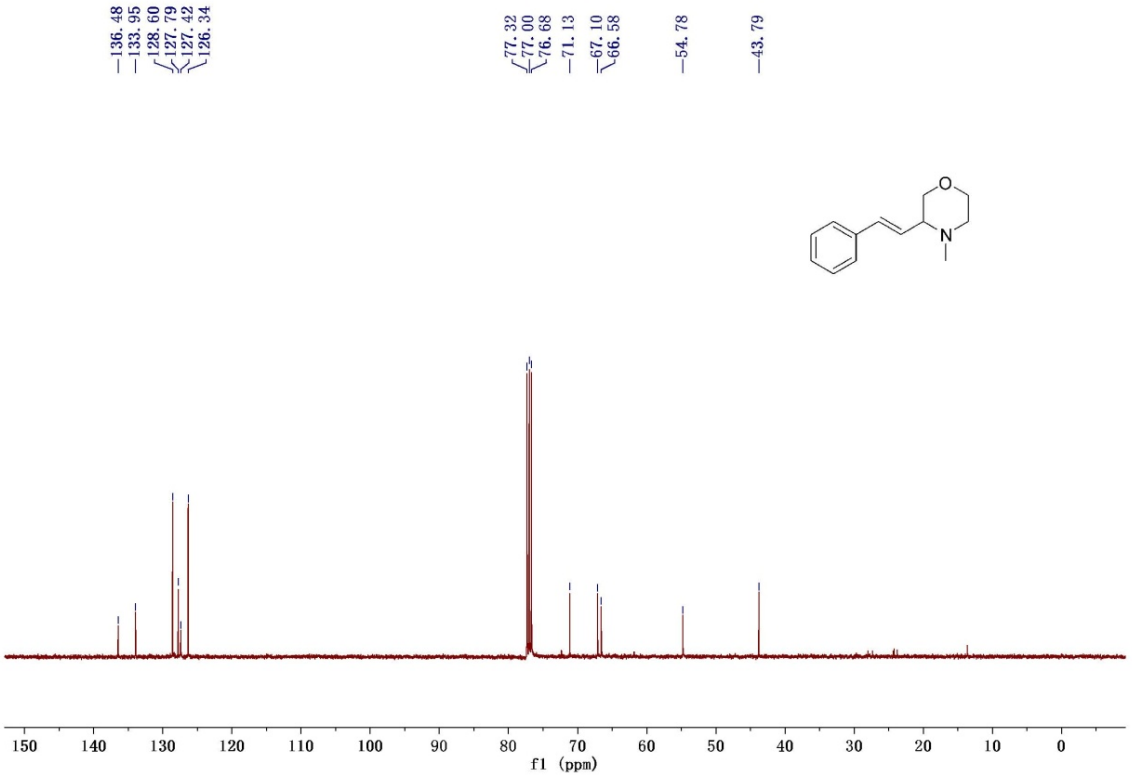
4e- ^{1}H NMR



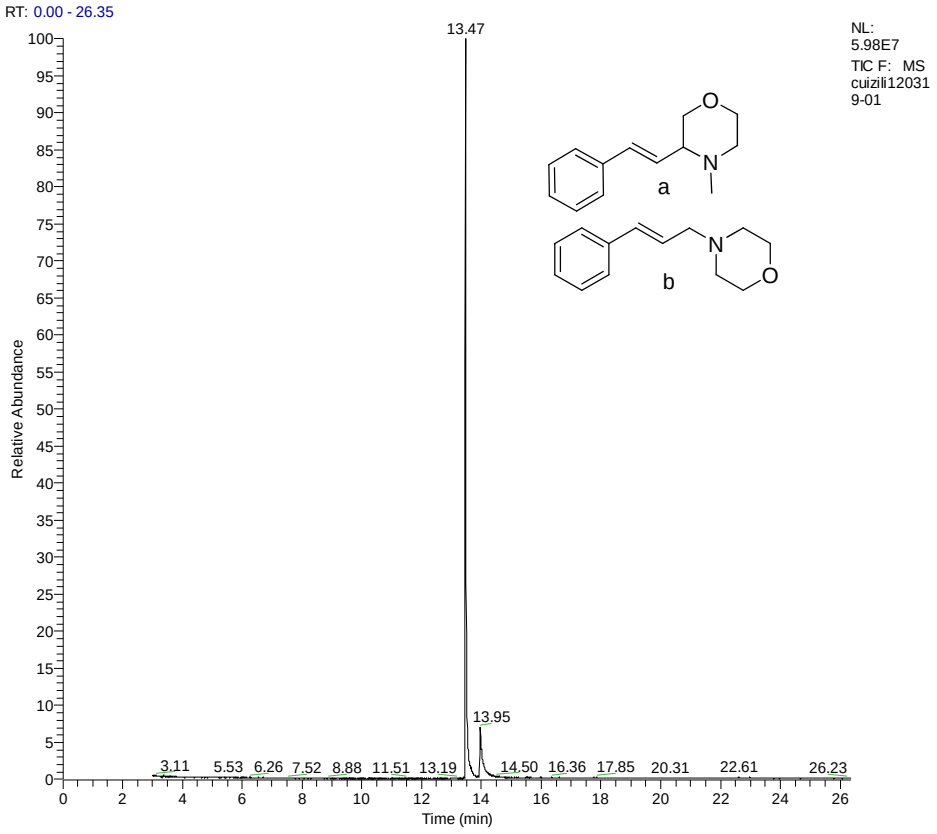
4ea- ^{1}H NMR



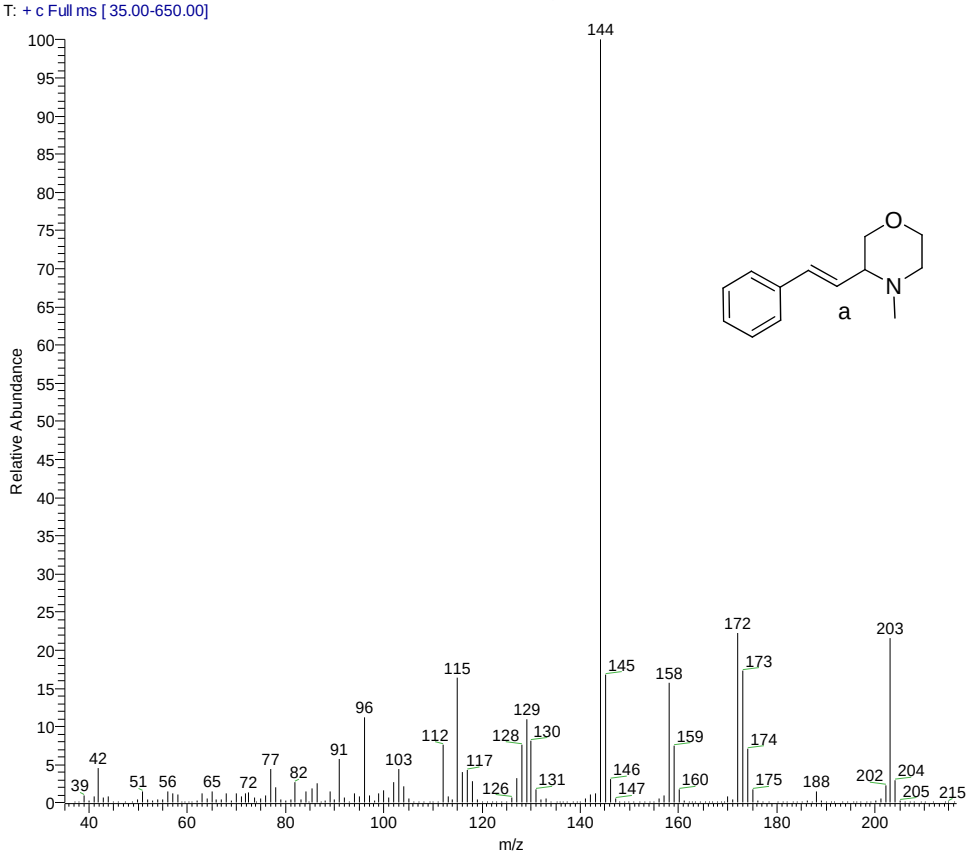
4ea- ^{13}C NMR



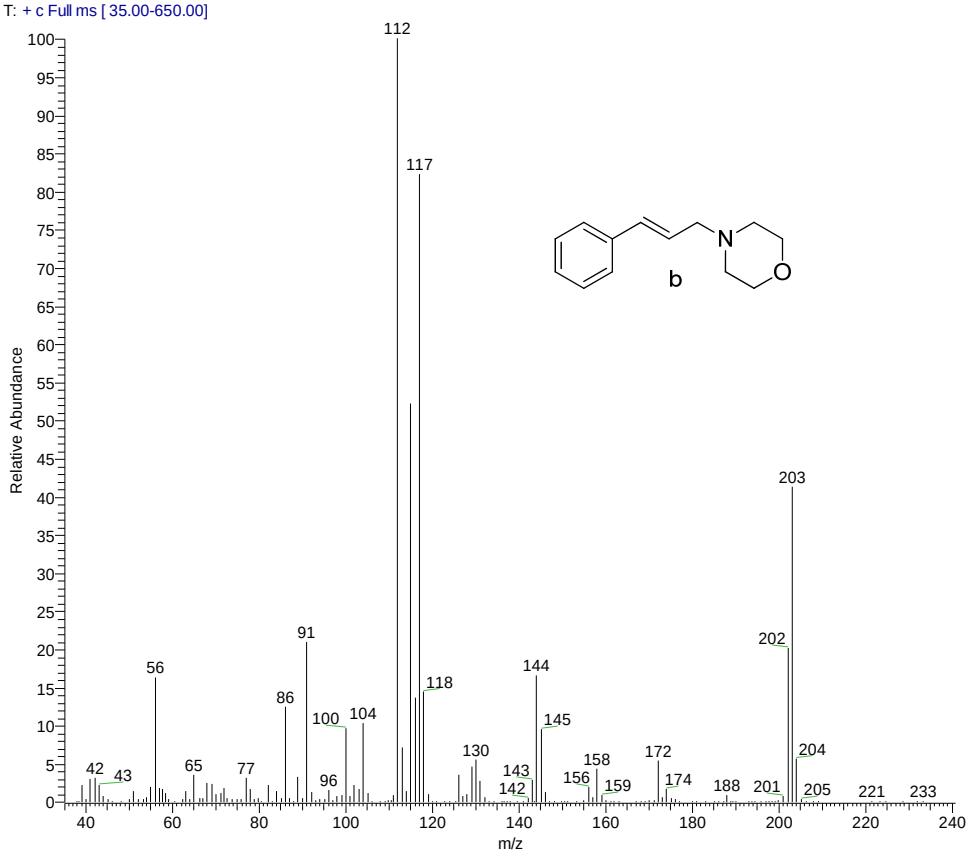
4e- GC – MS



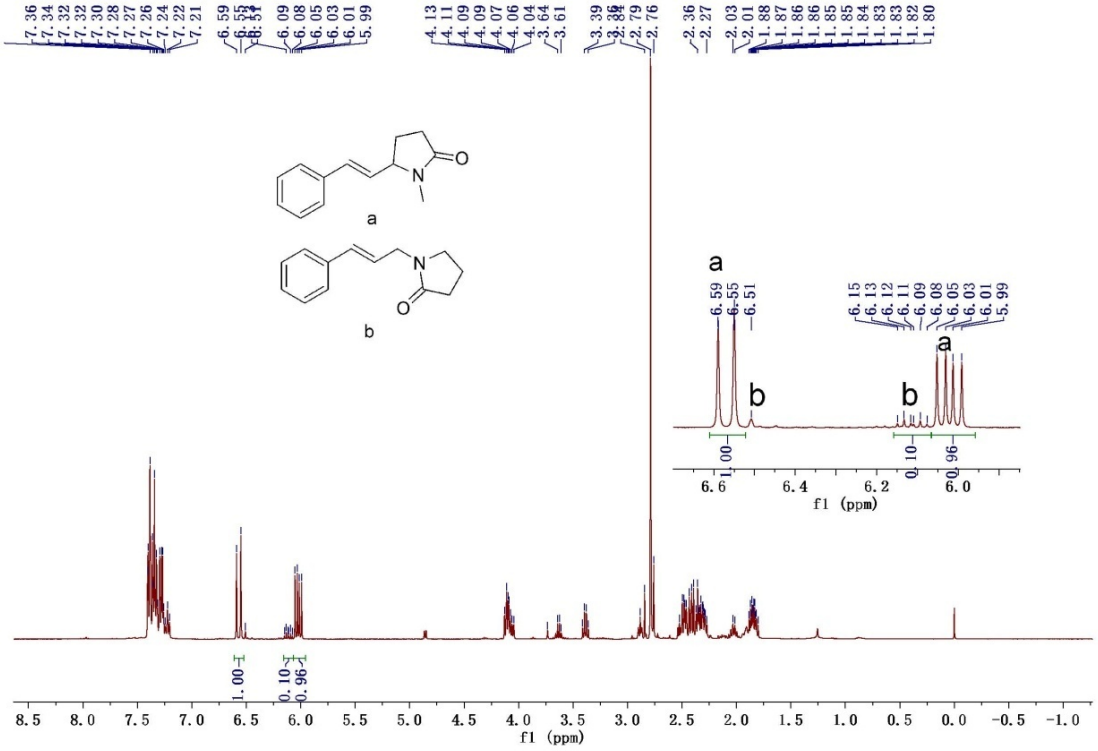
cuizili120319-01 #1890-1893 RT: 13.47-13.48 AV: 4 SB: 32 13.31-13.38 , 13.71-13.80 NL: 1.21E7
T: + c Full ms [35.00-650.00]



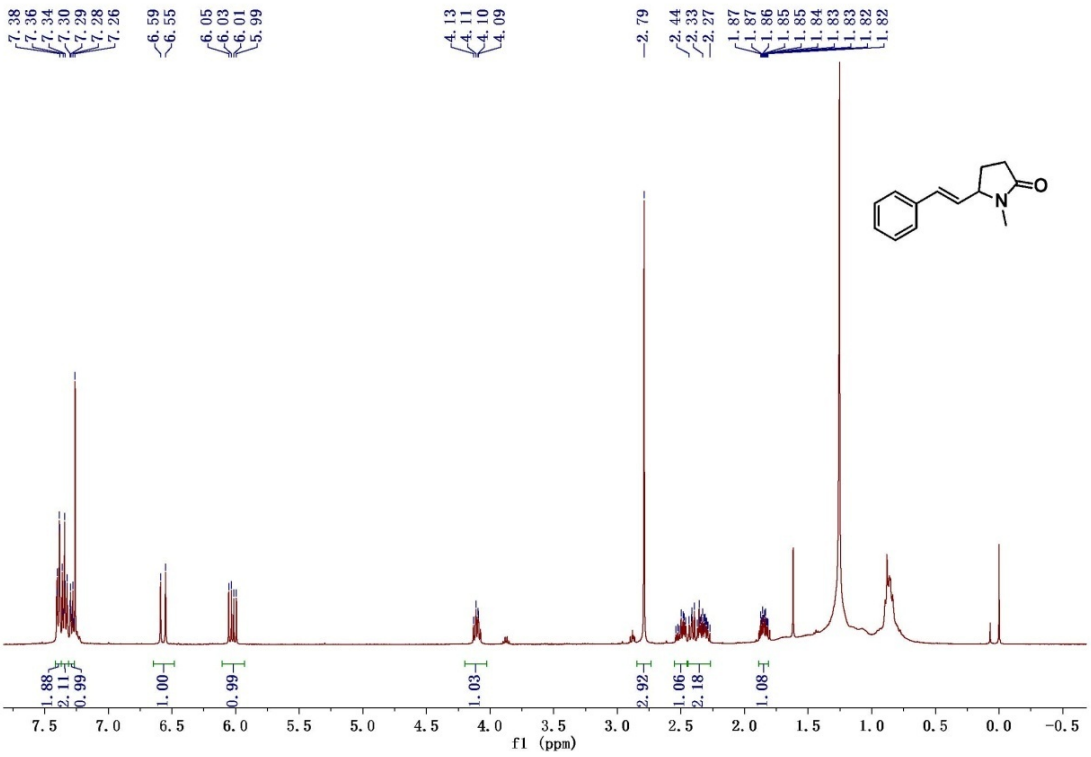
cuizili120319-01 #1977-1982 RT: 13.95-13.98 AV: 6 SB: 32 13.31-13.38 , 13.71-13.80 NL: 6.69E5
T: + c Full ms [35.00-650.00]



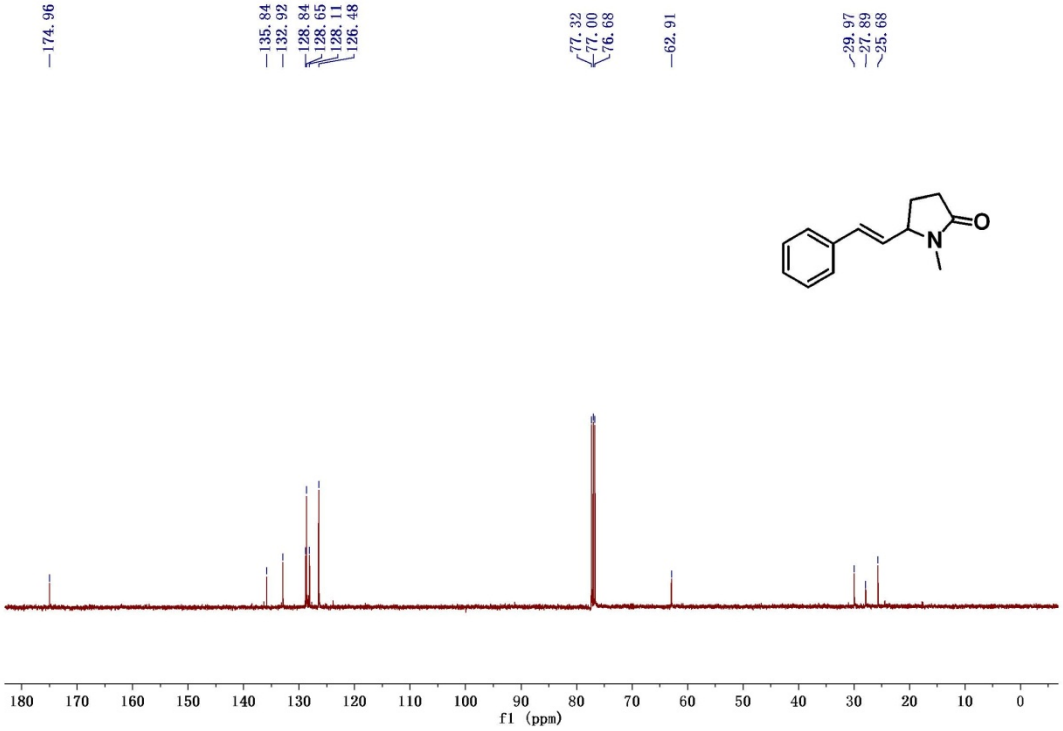
4f- ^{1}H NMR



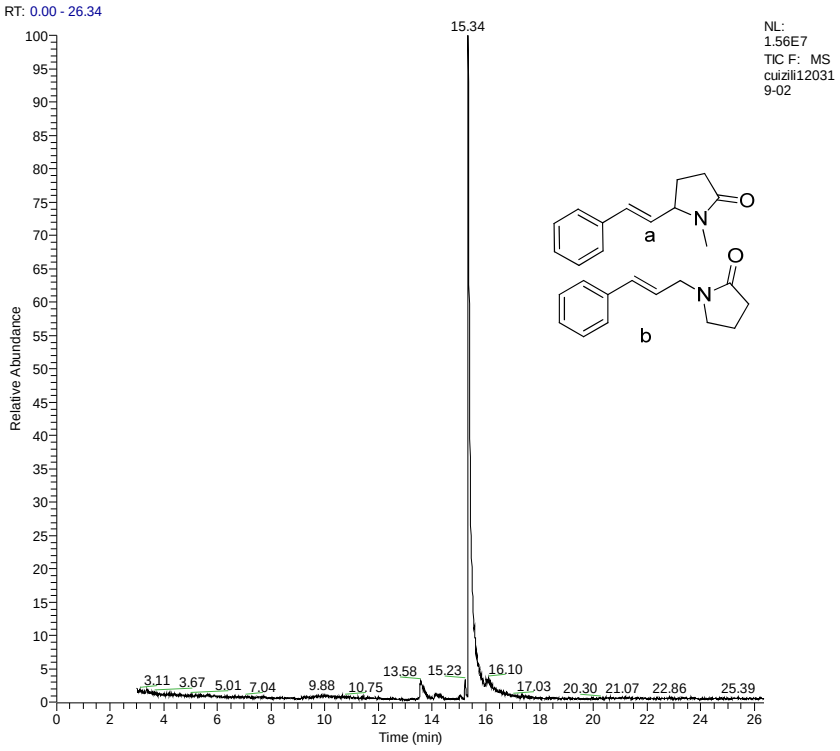
4fa- ^{1}H NMR



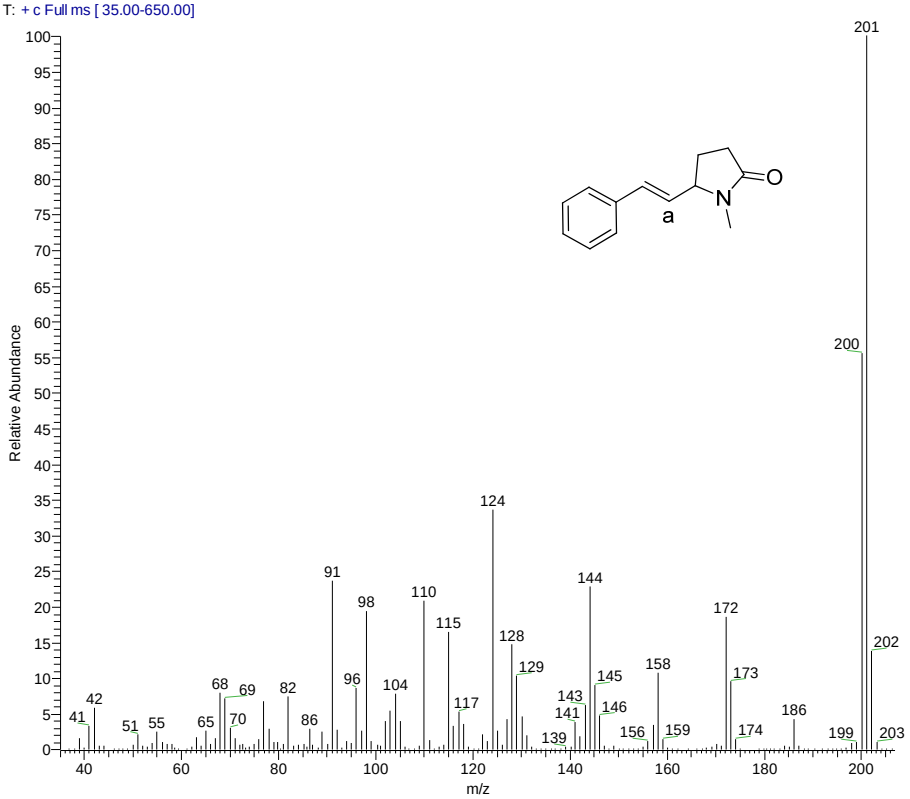
4fa- ^{13}C NMR



4f- GC – MS



cuizili120319-02 #2232-2254 RT: 15.36-15.48 AV: 23 SB: 107 14.52-14.84 , 16.69-16.95 NL: 1.01E6
T: + c Full ms [35.00-650.00]



cuizili120319-02 #2351-2362 RT: 16.02-16.08 AV: 12 SB: 80 14.59-14.73 , 17.50-17.79 NL: 5.68E4
T: + c Full ms [35.00-650.00]