

Supporting Information

for

Highly selective and additive-free Pd(OAc)₂/CPP catalyzed

hydroaminocarbonylation of alkynes

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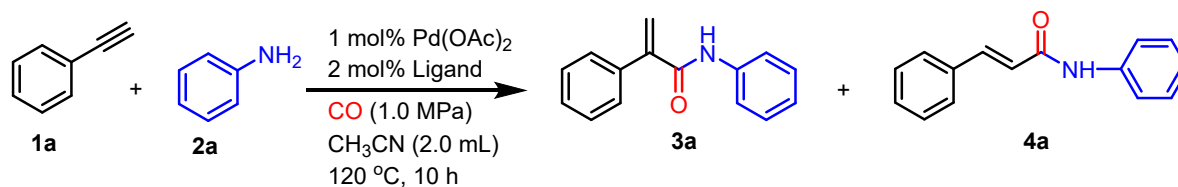
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S1. General Information: Materials and Methods

All commercial reagents were ordered from commercial suppliers, unless otherwise stated, commercial reagents were used without purification.

NMR spectra, including ^1H NMR (400 MHz), ^{13}C NMR (100 MHz) and ^{31}P NMR (162 MHz), were recorded on the Bruker AVANCE III HD-400 spectrometer. Chemical shifts δ (ppm) are given relative to solvent: references for CDCl_3 were 7.26 ppm (^1H NMR) and 77.16 ppm (^{13}C NMR), for CD_3CN were 1.94 ppm (^1H NMR) and 117.34 ppm (^{13}C NMR), for $\text{DMSO}-d_6$ were 2.50 ppm (^1H NMR) and 39.52 ppm (^{13}C NMR). Signals were assigned as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), m (multiplet) and br. s (broad singlet). All measurements were carried out at room temperature unless otherwise stated. GC analysis was performed with Agilent 7890B (KB-1, 30 m $\times$ 0.32 mm $\times$ 0.25 μm) and AT (C- 2000, 3 m $\times$ 3 mm). GC-Mass analysis was performed with SHIMADZU GCMS-QP2020 (SH-Rtx- 35MS, 30 m $\times$ 0.25 mm $\times$ 0.25 μm). High resolution mass spectra (HRMS) were measured on SHIMADZU LCMS-IT-TOF (ESI) mass spectrometer, and the corresponding molecular ion, such as $[\text{M}]^+$, $[\text{M}+\text{H}]^+$, were given in m/z units. Column chromatography was carried out using silica gel (200-300 mesh) eluting with petroleum ether/ethyl acetate.

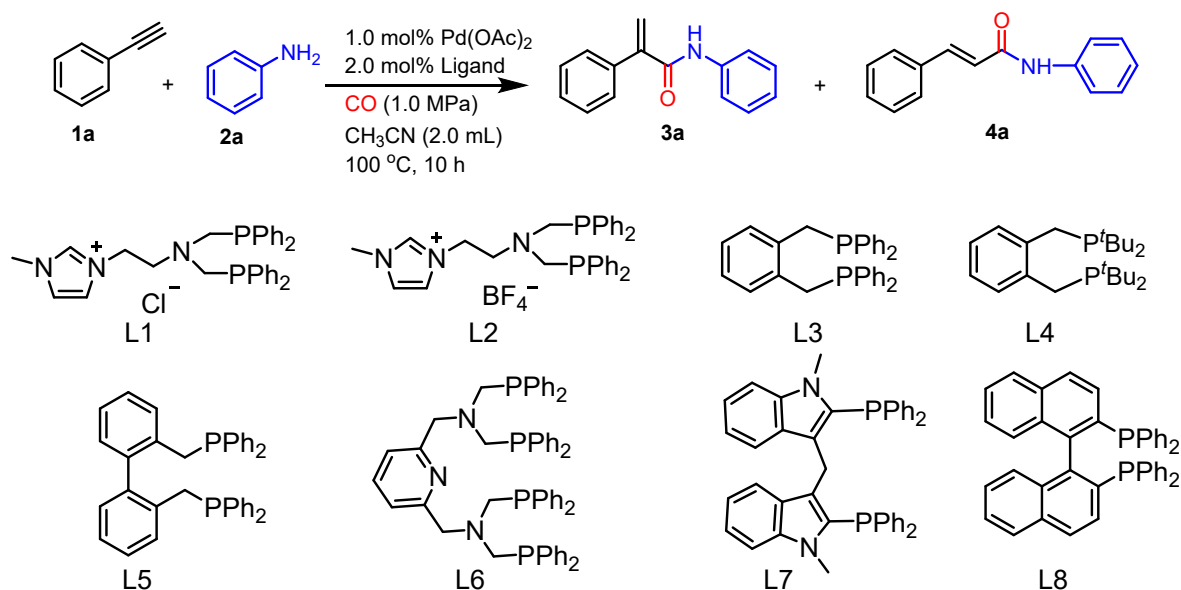
S2. General Procedure for the synthesis of products



Under nitrogen protection, a mixture of alkyne (1.0 mmol), amine (1.25 mmol), Pd(OAc)₂ (1.0 mol%), **CPP** (2.0 mol%), an oven-dried stirring bar and CH₃CN (2.0 mL) was added to a stainless-steel autoclave. The autoclave was flushed three times with CO and then pressurized to appointed pressure of CO. The reaction was heated under specified temperature for 10 hours. Then, the stainless-steel autoclave was cooled to room temperature and slowly depressurized. The reaction solution was analyzed by GC to determine the conversion and selectivity use n-dodecane as internal standard. Finally, the solvent was removed under vacuum and the obtained residue was purified by flash column chromatography on a silica gel (eluted with ethyl acetate/petroleum ether = 1/10 ~ 1/0) to furnish the desired α,β -unsaturated amides products.

S3. Optimization of reaction conditions

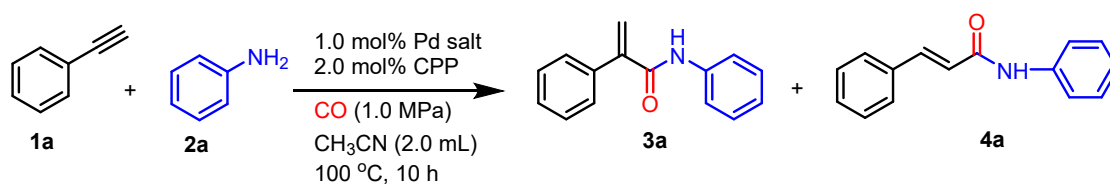
S3.1. The effect of ligand



Entry	Ligand	Conversion (%)	Yield 3a (%)	b:l
1	L1	78	78	>99:1
2	L2	49	48	99:1
3	L3	55	49	90:10
4	L4	52	33	78:22
5	L5	37	21	88:12
6	L6	60	55	93:7
7	L7	48	45	92:8
8	L8	70	68	98:2

Table S1. Reaction conditions: Phenylacetylene (1.0 mmol), aniline (1.25 mmol), Pd(OAc)₂ (1.0 mol%), Ligand (1.0 mol% or 2.0 mol%), CO (1.0 MPa), CH₃CN (2.0 mL), 100 °C, 10 h; the ratio of products and yields were determined by GC analysis with n-dodecane as the internal standard. **b:l** = **3a:4a**.

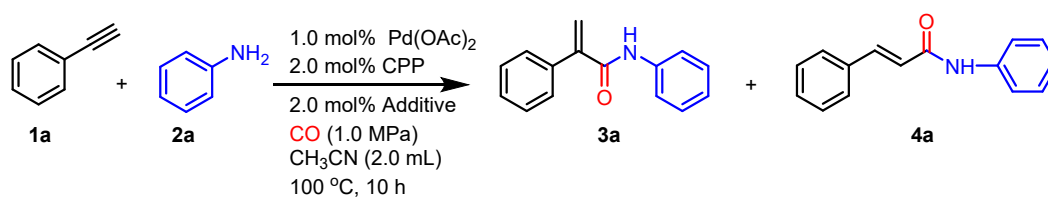
S3.2. The effect of Palladium precursor



Entry	Pd salt	Conversion (%)	Yield 3a (%)	b:l
1	Pd(OAc) ₂	78	78	>99:1
2	PdCl ₂ (CH ₃ CN) ₂	4	3	86:14
3	Pd(PPh ₃) ₄	22	17	79:21
4	PdCl ₂	7	6	86:14
5	Pd(TFA) ₂	3	2	71:29

Table S2. Reaction conditions: Phenylacetylene (1.0 mmol), aniline (1.25 mmol), Pd salt (1.0 mol%), CPP (2.0 mol%), CO (1.0 MPa), CH₃CN (2.0 mL), 100 °C, 10 h; the ratio of products and yields were determined by GC analysis with n-dodecane as the internal standard. b:l = **3a**:**4a**.

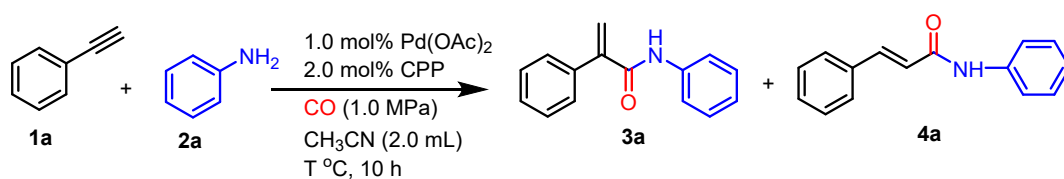
S3.3. The effect of additive



Entry	Additive	Conversion (%)	Yield 3 (%)	b:l
1	Al(OTf) ₃	Trace		
2	PTSA·H ₂ O	NR		
3	-	78	78	>99:1
4	Cs ₂ CO ₃	42	28	2:1
5	KO ^t Bu	96	81	84:16
6	NaO ^t Bu	87	84	93:7
7	KOH	42	40	97:3

Table S3. Reaction conditions: Phenylacetylene (1.0 mmol), aniline (1.25 mmol), Pd(OAc)₂ (1.0 mol%), CPP (2.0 mol%), additive (2.0 mol%), CO (1.0 MPa), CH₃CN (2.0 mL), 100 °C, 10 h; the ratio of products and yield were determined by GC analysis with n-dodecane as the internal standard. b:l = **3a**:**4a**.

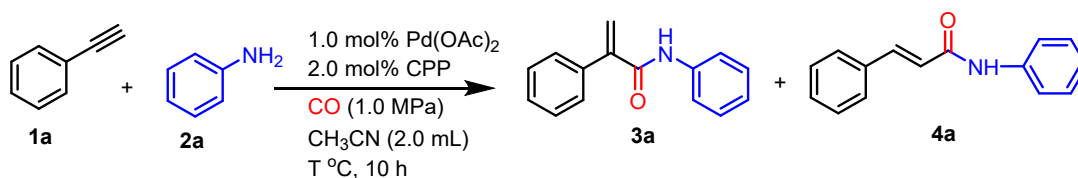
S3.4. The effect of CO pressure



Entry	CO (MPa)	Conversion (%)	Yield 3a (%)	b:l
1	0.5	44	43	>99:1
2	1	78	78	>99:1
3	2	55	54	>99:1

Table S4. Reaction conditions: Phenylacetylene (1.0 mmol), aniline (1.25 mmol), Pd(OAc)₂ (1.0 mol%), CPP (2.0 mol%), CO, CH₃CN (2.0 mL), 100 °C, 10 h; the ratio of products and yield were determined by GC analysis with n-dodecane as the internal standard. b:l = **3a**:**4a**.

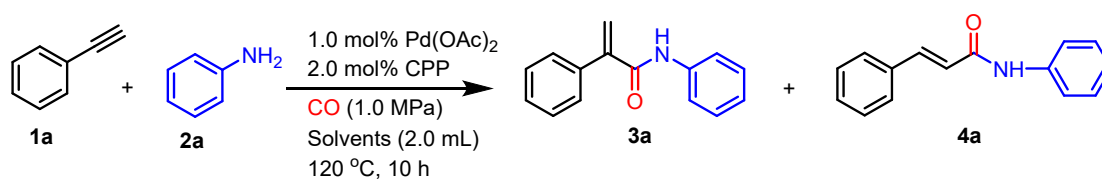
S3.5. The effect of reaction temperature



Entry	T (°C)	Conversion (%)	Yield 3a (%)	b:l
1	60	10	8	87:13
2	80	29	28	>99:1
3	100	78	77	>99:1
4	120	91	91	>99:1

Table S5. Reaction conditions: Phenylacetylene (1.0 mmol), aniline (1.25 mmol), Pd(OAc)₂ (1.0 mol%), CPP (2.0 mol%), CO (1.0 MPa), CH₃CN (2.0 mL), T °C, 10 h; the ratio of products and yield were determined by GC analysis with n-dodecane as the internal standard. b:l = **3a**:**4a**.

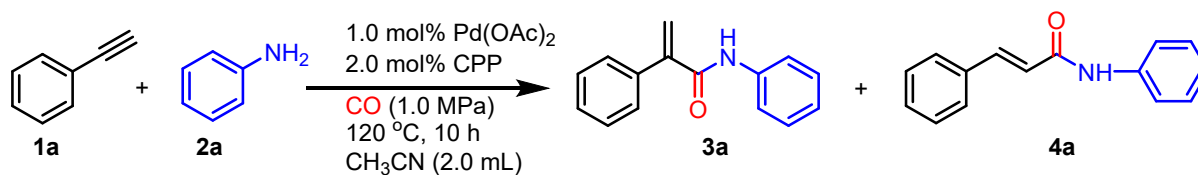
S3.6. The effect of solvents



Entry	Solvent	Conversion (%)	Yield 3a (%)	b:l
1	THF	45	44	>99:1
2	CH ₃ CN	91	91	>99:1
3	Toluene	82	82	99:1
4	NMP	4	4	87:13

Table S6. Reaction conditions: Phenylacetylene (1.0 mmol), aniline (1.25 mmol), Pd(OAc)₂ (1.0 mol%), CPP (2.0 mol%), CO (1.0 MPa), solvents (2.0 mL), 120 °C, 10 h; the ratio of products and yield were determined by GC analysis with n-dodecane as the internal standard. b:l = **3a:4a**.

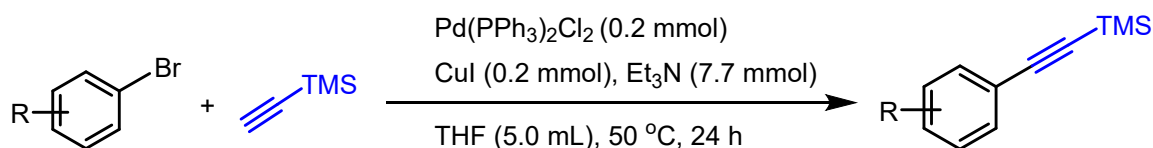
S3.7. Optimal reaction conditions



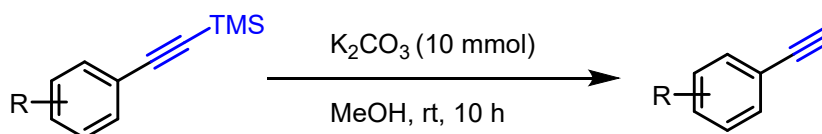
Conversion (%)	Yield 3a (%)	b:l
91	91	>99:1

Table S7. Reaction conditions: Phenylacetylene (1.0 mmol), aniline (1.25 mmol), Pd(OAc)₂ (1.0 mol%), CPP (2.0 mol%), CO (1.0 MPa), CH₃CN (2.0 mL), 120 °C, 10 h; the ratio of products and yield were determined by GC analysis with n-dodecane as the internal standard. b:l = **3a:4a**.

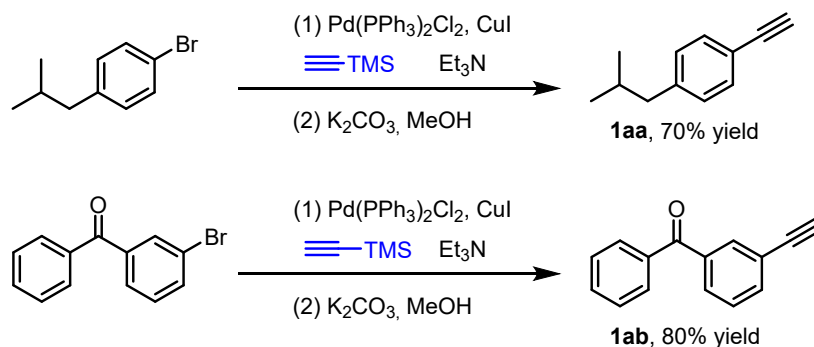
S4. General Procedure for the synthesis of substrates



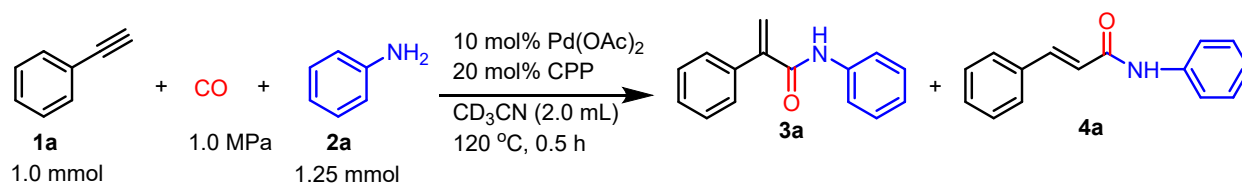
Reactions were set up in a nitrogen-filled glove box. To round-bottom flask with magnetic stirring bar were added $\text{Pd(PPh}_3)_2\text{Cl}_2$ (0.2 mmol), CuI (0.2 mmol), aryl bromides (5.0 mmol), THF (5.0 mL) and Et_3N (7.7 mmol). Then the flask was sealed with a rubber plug, removed from glovebox and stirred at 0 °C 15 min. Trimethylsilylacetylene (10 mmol) was slowly added to the reaction mixture and the color of the reactants gradually darkened. Then, the flask was transferred to oil bath and the mixture was reacted for 24 h at 50 °C. After the reaction was completed, the reaction mixture was cooled to room temperature and dissolved in ethyl acetate, which was then washed with water/ brine sequentially. The organic phase was dried with anhydrous Na_2SO_4 and concentrated *via* vacuum to get the crude products¹. Finally, the crude products were purified by a short fast column to get the chromatography 1-Aryl-2-trimethylphenylacetyl derivatives.



1-Aryl-2-trimethylphenylacetyl derivative (1.0 equiv.) was added to a mixture of potassium carbonate (2 equiv.) and anhydrous MeOH. Then, the reaction was stirred at room temperature for 10 hours under the protection of nitrogen and the reaction process was observed by TLC or GC-MS, When the reaction finished, the reaction mixture was quenched by saturated NH_4Cl . The MeOH were evaporated under reduced pressure and the residue was dissolved in ethyl acetate, which was washed with water/ brine sequentially and concentrated *via* vacuum to get crude products. Then, the crude products were purified by a short fast column chromatography to obtain the terminal alkyne substrates.

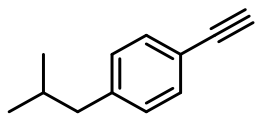


S5. Procedure for the NMR studies on the crude reaction mixture



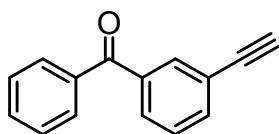
Given the low concentration of Palladium active species, the catalyst amount was increased by a factor of 10 in NMR experiments. The specific experimental steps are as follows: under nitrogen protection, Pd(OAc)₂ (10 mol%), **CPP** (20 mol%), Phenylacetylene (1.0 mmol), amine (1.25 mmol), an oven-dried stirring bar and CD₃CN (2.0 mL) was added to a stainless-steel autoclave. The reaction was heated at 120 °C under CO (1.0 MPa) for 0.5 hours. Then, the stainless-steel autoclave was cooled to room temperature and slowly depressurized. The reaction solution was analyzed by NMR immediately to analyze active species.

S6. NMR spectra of drug-derived substrates



Ethynyl-4-isobutyl benzene 1aa¹

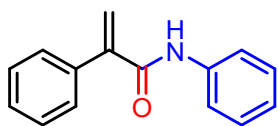
¹H NMR (400 MHz, CDCl₃) δ 7.42 (d, *J* = 8.2 Hz, 2H), 7.11 (d, *J* = 8.2 Hz, 2H), 3.04 (s, 1H), 2.48 (d, *J* = 7.2 Hz, 2H), 1.93 – 1.80 (m, 1H), 0.90 (d, *J* = 6.6 Hz, 6H). **¹³C NMR** (100 MHz, CDCl₃) δ 142.8, 131.9, 129.1, 119.3, 83.9, 77.4, 45.3, 30.2, 22.3.



(3-ethynylphenyl) (phenyl)methanone 1ab²

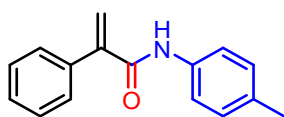
¹H NMR (400 MHz, CDCl₃) δ 7.90 (t, *J* = 1.7 Hz, 1H), 7.79 (ddd, *J* = 7.7, 3.7, 2.0 Hz, 3H), 7.69 (d, *J* = 7.7 Hz, 1H), 7.60 (s, 1H), 7.52 – 7.39 (m, 3H), 3.12 (s, 1H). **¹³C NMR** (100 MHz, CDCl₃) δ 195.77, 137.85, 137.12, 135.71, 133.55, 132.74, 130.09 (d, *J* = 9.5 Hz), 128.45 (d, *J* = 2.6 Hz), 122.47, 82.63, 78.34, 29.71.

S7. Structural characterization of products



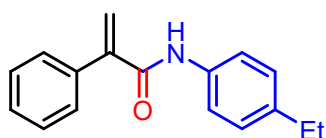
N,2-diphenylacrylamide (**3aa**)³

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.27 (s, 1H), 7.72 (d, *J* = 7.7 Hz, 2H), 7.51 – 7.47 (m, 2H), 7.41 – 7.30 (m, 5H), 7.10 – 7.06 (m, 1H), 5.94 (s, 1H), 5.72 (s, 1H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 167.8, 145.7, 139.5, 136.8, 129.6 – 128.2 (m), 127.4, 124.2, 120.4, 118.1.



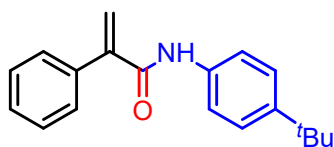
2-Phenyl-*N*-(*p*-tolyl) acrylamide (**3ab**)⁴

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.17 (s, 1H), 7.61 (d, *J* = 8.3 Hz, 2H), 7.54 – 7.46 (m, 2H), 7.44 – 7.33 (m, 3H), 7.14 (d, *J* = 8.3 Hz, 2H), 5.93 (s, 1H), 5.72 (s, 1H), 2.28 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 145.8, 136.9 (d, *J* = 16.7 Hz), 133.0, 129.5, 128.9, 128.7, 128.4 – 127.9 (m), 127.3, 120.4, 117.9, 21.0.



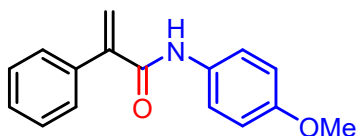
N-(4-ethylphenyl)-2-phenylacrylamide (**3ac**)

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.18 (s, 1H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.53 – 7.44 (m, 2H), 7.44 – 7.29 (m, 3H), 7.16 (d, *J* = 8.5 Hz, 2H), 5.92 (s, 1H), 5.71 (s, 1H), 2.57 (q, *J* = 7.6 Hz, 2H), 1.16 (t, *J* = 7.6 Hz, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 167.6, 139.6, 137.2, 136.8, 128.9, 128.7, 128.3, 127.3, 120.5, 117.9, 28.1, 16.2. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₇H₁₇NO: 252.1383; Found: 252.1387.



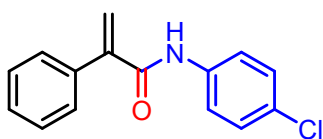
N-(4-(*tert*-butyl) phenyl)-2-phenylacrylamide (**3ad**)⁵

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.18 (s, 1H), 7.63 (d, *J* = 8.6 Hz, 2H), 7.53 – 7.46 (m, 2H), 7.43 – 7.26 (m, 5H), 5.92 (s, 1H), 5.71 (s, 1H), 1.27 (s, 10H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 167.6, 146.5, 145.8, 136.90 (d, *J* = 9.6 Hz), 128.9, 128.7, 127.3, 125.7, 120.2, 118.0, 34.5, 31.7.



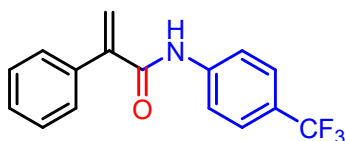
(4-methoxyphenyl)-2-phenylacrylamide (3ae)⁶

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.11 (s, 1H), 7.62 (d, *J* = 9.0 Hz, 2H), 7.51 – 7.45 (m, 2H), 7.42 – 7.29 (m, 3H), 6.90 (d, *J* = 9.0 Hz, 2H), 5.90 (s, 1H), 5.71 (s, 1H), 3.73 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 167.4, 156.0, 145.8, 136.9, 132.6, 128.9, 128.7, 127.3, 122.0, 117.9, 114.2, 55.7.



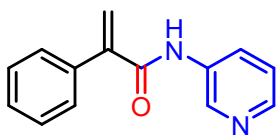
N-(4-chlorophenyl)-2-phenylacrylamide (3af)⁶

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.40 (s, 1H), 7.79 – 7.71 (m, 2H), 7.54 – 7.45 (m, 2H), 7.43 – 7.28 (m, 5H), 5.96 (s, 1H), 5.75 (s, 1H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 167.9, 145.5, 138.5, 136.6, 128.99 (d, *J* = 6.8 Hz), 128.8, 127.7, 127.3, 121.9, 118.5.



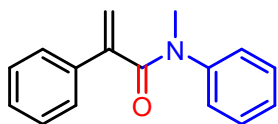
2-Phenyl-N-(4-(trifluoromethyl) phenyl) acrylamide (3ag)

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.64 (s, 1H), 7.95 (d, *J* = 8.5 Hz, 2H), 7.71 (d, *J* = 8.5 Hz, 2H), 7.58 – 7.47 (m, 2H), 7.45 – 7.25 (m, 3H), 6.00 (s, 1H), 5.80 (s, 1H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 167.1, 144.1, 139.4, 138.0, 131.6, 130.1, 129.7 (d, *J* = 31.2 Hz), 129.1, 125.3 (q, *J* = 3.9 Hz), 124.6 (d, *J* = 273.4 Hz), 124.3, 120.9, 120.6. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₆H₁₂NOF₃: 292.0944; Found: 292.0935.



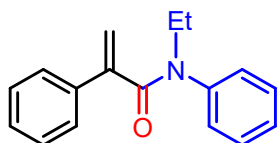
2-Phenyl-N-(pyridin-3-yl) acrylamide (3ah)

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.48 (s, 1H), 8.88 (d, *J* = 2.2 Hz, 1H), 8.31 (dd, *J* = 4.7, 1.4 Hz, 1H), 8.16 (ddd, *J* = 8.3, 2.2, 1.5 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.46 – 7.35 (m, 4H), 6.00 (s, 1H), 5.82 (s, 1H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 168.2, 160.6, 145.3, 145.0, 142.0, 136.6, 136.2, 129.0, 128.8, 127.40, 127.36, 124.0, 119.0. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₄H₁₂NO: 225.1022; Found: 225.1027.



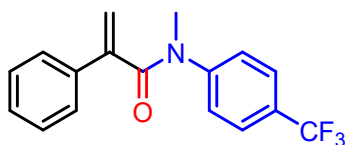
N-Methyl-N,2-diphenylacrylamide (3ai)⁴

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.93 – 6.69 (m, 10H), 5.61 (br, 1H), 5.22 (br, 1H), 3.29 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 169.8, 145.0, 144.1, 136.6, 135.2, 129.3, 129.0, 128.6, 128.0, 127.7, 127.2, 126.2, 37.5.



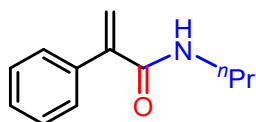
N-(2-phenylacryloyl) isonicotinamide (3aj)

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.32 – 6.96 (m, 10H), 5.56 (s, 1H), 5.22 (s, 1H), 3.94 – 3.71 (m, 2H), 1.07 (d, *J* = 5.8 Hz, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 169.3, 145.2, 142.4, 130.1, 129.3, 128.9, 128.7, 128.5, 128.4, 128.1, 128.0, 127.5, 127.3, 126.2, 117.0, 44.1, 13.3. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₇H₁₇NO: 252.1383; Found: 252.1385.



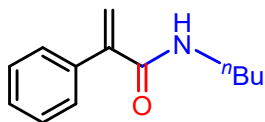
N-methyl-2-phenyl-N-(4-(trifluoromethyl) phenyl)acrylamide (3ak)

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.42 (d, *J* = 7.7 Hz, 2H), 7.43 – 7.22 (m, 5H), 5.74 (s, 1H), 5.36 (s, 1H), 3.35 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 169.2, 147.6, 144.8, 136.2, 129.3, 129.0, 128.8, 128.4, 128.2 (q, *J* = 35.80 Hz), 127.2, 126.35 (q, *J* = 3.8 Hz), 124.4 (q, *J* = 273.1 Hz), 37.5. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₇H₁₄F₃NO: 306.1100; Found: 306.1099.



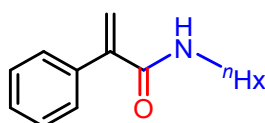
2-Phenyl-N-propylacrylamide (3al)³

¹H NMR (400 MHz, DMSO-*d*₆) δ 8.15 (s, 1H), 7.56 – 7.07 (m, 5H), 5.70 (s, 1H), 5.54 (s, 1H), 3.11 (dd, *J* = 13.0, 6.9 Hz, 2H), 1.47 (dd, *J* = 14.3, 7.3 Hz, 2H), 0.85 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 168.7, 146.0, 137.2, 128.8, 128.5, 127.4, 117.4, 41.1, 22.8, 11.9.



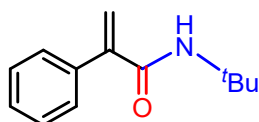
***N*-Butyl-2-phenylacrylamide (3am)**

¹H NMR (400 MHz, DMSO-*d*₆) δ 8.16 (t, *J* = 5.1 Hz, 1H), 7.78 – 7.19 (m, 5H), 5.72 (s, 1H), 5.55 (s, 1H), 3.16 (dd, *J* = 12.9, 7.0 Hz, 2H), 1.51 – 1.39 (m, 2H), 1.30 (dd, *J* = 15.0, 7.4 Hz, 2H), 0.89 (t, 3H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 168.7, 146.0, 137.2, 128.8, 128.5, 127.4, 117.4, 38.9, 31.6, 20.1, 14.2. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₇H₁₇NO: 204.1383; Found: 294.1381.



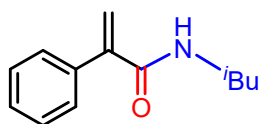
***N*-Exyl-2-phenylacrylamide (3an)**

¹H NMR (400 MHz, DMSO-*d*₆) δ 8.17 (s, 1H), 7.43 – 7.29 (m, 5H), 5.74 (s, 1H), 5.56 (s, 1H), 3.22 – 3.11 (m, 2H), 1.54 – 1.43 (m, 2H), 1.33 – 1.24 (m, 6H), 0.88 (t, *J* = 6.8 Hz, 3H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 168, 146.0, 137.2, 128.7, 128.5, 127.4, 117.3, 39.2, 31.4, 29.4, 26.6, 22.6, 14.4. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₅H₂₁NO: 232.1896; Found: 232.1899.



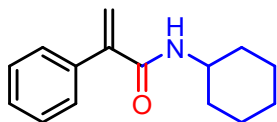
***N*-(*tert*-butyl)-2-phenylacrylamide (3ao)⁷**

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.67 (s, 1H), 7.54 – 7.18 (m, 5H), 5.69 (s, 1H), 5.44 (s, 1H), 1.33 (s, 9H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 168.9, 146.4, 137.3, 128.8, 128.4, 127.1, 116.2, 51.1, 28.9.



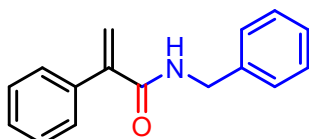
***N*-Isobutyl-2-phenylacrylamide (3ap)**

¹H NMR (400 MHz, DMSO-*d*₆) δ 8.17 (s, 1H), 7.63 – 6.94 (m, 5H), 5.73 (s, 1H), 5.56 (s, 1H), 3.00 (dd, *J* = 6.8, 6.2 Hz, 2H), 1.80 (dt, *J* = 13.5, 6.8 Hz, 1H), 0.87 (d, *J* = 6.7 Hz, 7H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 168.8, 146.0, 137.2, 128.8, 128.5, 127.4, 117.3, 46.8, 28.6, 20.7. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₇H₁₇NO: 204.1383; Found: 204.1381.



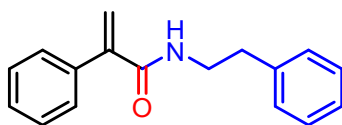
***N*-Cyclohexyl-2-phenylacrylamide (3aq)³**

¹H NMR (400 MHz, DMSO-*d*₆) δ 8.03 (d, *J* = 7.9 Hz, 1H), 7.65 – 7.06 (m, 5H), 5.72 (s, 1H), 5.49 (s, 1H), 3.83 – 3.50 (m, 1H), 1.69 (ddd, *J* = 52.5, 42.4, 10.7 Hz, 6H), 1.41 – 1.18 (m, 4H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 168.1, 145.9, 137.2, 128.8, 128.5, 127.2, 116.7, 48.4, 32.7, 25.7, 25.3.



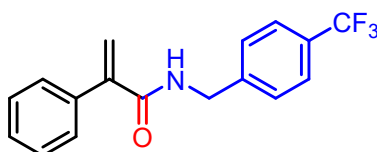
***N*-Benzyl-2-phenylacrylamide (3ar)³**

¹H NMR (400 MHz, DMSO-*d*₆) δ 8.76 (t, *J* = 5.8 Hz, 1H), 7.88 – 6.83 (m, 10H), 5.79 (s, 1H), 5.68 (s, 1H), 4.40 (d, *J* = 6.1 Hz, 2H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 168.7, 145.6, 140.1, 137.2, 128.78 (d, *J* = 1.3 Hz), 128.6, 127.6, 127.5, 127.2, 118.2, 42.8.



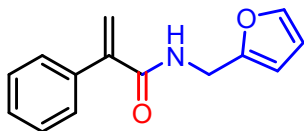
***N*-Phenethyl-2-phenylacrylamide (3as)³**

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.27 (s, 1H), 7.72 (d, *J* = 7.7 Hz, 2H), 7.51 – 7.47 (m, 2H), 7.41 – 7.30 (m, 5H), 7.10 – 7.06 (m, 1H), 5.94 (s, 1H), 5.72 (s, 1H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 168.6, 145.9, 139.9, 137.1, 129.2, 129.0, 128.74 (d, *J* = 3.8 Hz), 128.5, 127.5, 126.5, 117.6, 40.8, 35.4.



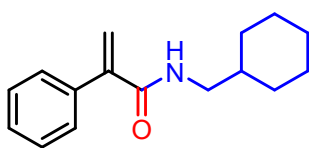
***2*-phenyl-*N*-(4-(trifluoromethyl) benzyl) acrylamide (3at)**

¹H NMR (400 MHz, DMSO-*d*₆) δ 8.86 (t, *J* = 6.0 Hz, 1H), 7.72 (d, *J* = 8.1 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.48 – 7.42 (m, 2H), 7.42 – 7.31 (m, 5H), 5.82 (s, 1H), 5.74 (s, 1H), 4.49 (d, *J* = 6.0 Hz, 2H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 168.8, 145.5, 145.0, 137.1, 128.8, 128.6, 128.3, 128.0 (q, *J* = 32.0 Hz), 127.6, 125.2 (q, *J* = 3.9 Hz), 124.8 (q, *J* = 273.10 Hz), 118.6, 42.6. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₇H₁₄F₃NO: 306.1100; Found: 306.1117.



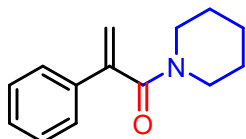
***N*-(furan-2-ylmethyl)-2-phenylacrylamide (3au)**

¹H NMR (400 MHz, DMSO-*d*₆) δ 8.69 (t, *J* = 5.9 Hz, 1H), 7.59 (dd, *J* = 1.9, 0.9 Hz, 1H), 7.53 – 7.17 (m, 5H), 6.41 (dd, *J* = 3.2, 1.9 Hz, 1H), 6.28 (dd, *J* = 3.2, 0.9 Hz, 1H), 5.78 (s, 1H), 5.65 (s, 1H), 4.41 (dd, *J* = 5.8, 0.9 Hz, 2H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 168.7, 152.8, 145.4, 142.5, 137.1, 128.8, 128.6, 127.5, 118.2, 111.0, 107.1, 36.3. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₄H₁₄NO₂: 228.1019; Found: 228.1018.



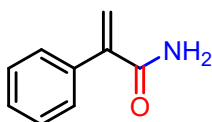
***N*-(cyclohexylmethyl)-2-phenylacrylamide (3av)**

¹H NMR (400 MHz, DMSO-*d*₆) δ 8.15 (s, 1H), 7.68 – 7.12 (m, 5H), 5.73 (s, 1H), 5.56 (s, 1H), 3.02 (t, *J* = 6.4 Hz, 2H), 1.77 – 1.40 (m, 6H), 1.28 – 1.07 (m, 3H), 1.07 – 0.78 (m, 2H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 168.8, 146.0, 137.3, 128.8, 128.5, 127.4, 117.4, 45.5, 37.9, 31.0, 26.6, 25.9. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₆H₂₂NO: 244.1696; Found: 244.1693.



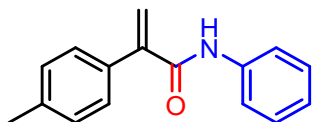
2-Phenyl-1-(piperidin-1-yl) prop-2-en-1-one (3aw)

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.62 – 7.25 (m, 5H), 5.78 (s, 1H), 5.23 (s, 1H), 3.58 – 3.52 (m, 2H), 3.28 – 3.21 (m, 2H), 1.54 (ddd, *J* = 15.5, 9.3, 2.9 Hz, 4H), 1.34 – 1.25 (m, 2H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 168.3, 145.0, 136.0, 129.3, 129.0, 128.4, 125.9, 113.4, 47.7, 42.0, 26.4, 25.7, 24.4. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₄H₁₇NO: 216.1383; Found: 216.1385.



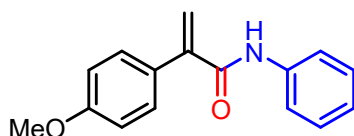
2-Phenylacrylamide (3ax)⁸

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.59 – 7.19 (m, 1H), 5.73 (s, 1H), 5.68 (s, 1H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 170.5, 145.6, 137.4, 132.0 – 125.3 (m), 118.3 (s).



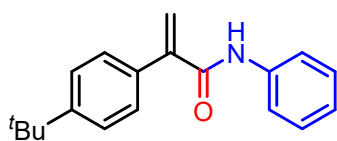
***N*-phenyl-2-(*p*-tolyl) acrylamide (3ba)⁶**

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.22 (s, 1H), 7.72 (d, *J* = 7.7 Hz, 2H), 7.44 – 7.26 (m, 4H), 7.19 (d, *J* = 7.9 Hz, 2H), 7.10 – 7.03 (m, 1H), 5.88 (s, 1H), 5.65 (s, 1H), 2.31 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 168.0, 145.6, 139.6, 138.2, 133.9, 129.5, 129.1, 127.2, 124.1, 120.4, 117.0, 21.2.



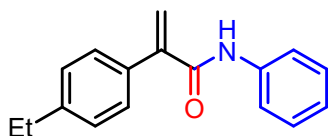
***2*-(4-methoxyphenyl)-*N*-phenylacrylamide (3ca)⁶**

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.20 (s, 1H), 7.71 (d, *J* = 7.7 Hz, 2H), 7.51 – 7.39 (m, 2H), 7.38 – 7.24 (m, 2H), 7.16 – 7.02 (m, 1H), 7.01 – 6.83 (m, 2H), 5.82 (s, 1H), 5.59 (s, 1H), 3.76 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 168.1, 159.8, 145.2, 139.6, 129.1, 128.6, 124.1, 120.4, 116.0, 114.3, 55.6.



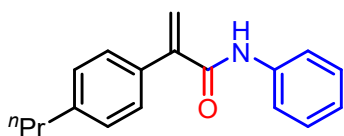
***2*-(4-(*tert*-butyl) phenyl)-*N*-phenylacrylamide (3da)**

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.22 (s, 1H), 7.73 (d, *J* = 7.8 Hz, 2H), 7.40 (dd, *J* = 9.4, 0.9 Hz, 4H), 7.32 (t, *J* = 7.9 Hz, 2H), 7.08 (t, *J* = 7.4 Hz, 1H), 5.88 (s, 1H), 5.68 (s, 1H), 1.28 (s, 10H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 167.9, 151.2, 145.6, 139.6, 134.0, 129.1, 127.1, 125.7, 124.1, 120.4, 117.4, 117.3, 34.8, 31.5. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₉H₂₁NO: 280.1696; Found: 280.1698.



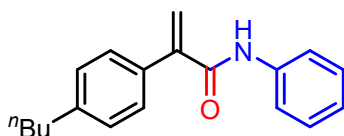
***2*-(4-ethylphenyl)-*N*-phenylacrylamide (3ea)⁶**

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.24 (s, 1H), 7.74 (d, *J* = 7.7 Hz, 2H), 7.47 – 7.39 (m, 2H), 7.34 (dd, *J* = 10.8, 5.1 Hz, 2H), 7.24 (d, *J* = 8.3 Hz, 2H), 7.12 – 7.04 (m, 1H), 5.90 (s, 1H), 5.68 (s, 1H), 2.62 (q, *J* = 7.6 Hz, 2H), 1.19 (t, *J* = 7.6 Hz, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 168.0, 145.7, 144.5, 139.6, 134.2, 129.1, 128.3, 127.3, 124.1, 120.4, 117.2, 28.4, 16.0.



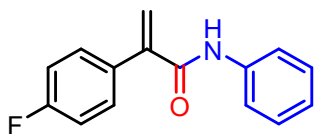
***N*-phenyl-2-(4-propylphenyl) acrylamide (3fa)⁶**

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.23 (s, 1H), 7.90 – 7.62 (m, 2H), 7.44 – 7.29 (m, 4H), 7.24 – 7.16 (m, 2H), 7.11 – 7.06 (m, 1H), 5.89 (s, 1H), 5.66 (s, 1H), 2.58 (t, *J* = 7.7 Hz, 2H), 1.55 (ddt, *J* = 8.9, 7.6, 3.5 Hz, 2H), 1.30 (q, *J* = 7.4 Hz, 2H), 0.89 (t, *J* = 7.3 Hz, 3H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 168.0, 145.7, 142.9, 139.7, 134.2, 129.1, 128.94, 128.90, 127.2, 124.1, 120.4, 117.1, 37.4, 24.5, 14.1.



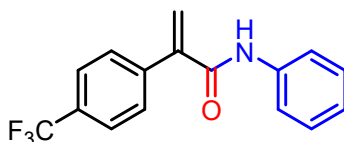
***2*-(4-butylphenyl)-*N*-phenylacrylamide (3ga)**

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.23 (s, 1H), 7.90 – 7.62 (m, 2H), 7.44 – 7.29 (m, 4H), 7.24 – 7.16 (m, 2H), 7.11 – 7.06 (m, 1H), 5.89 (s, 1H), 5.66 (s, 1H), 2.58 (t, *J* = 7.7 Hz, 2H), 1.55 (ddt, *J* = 8.9, 7.6, 3.5 Hz, 2H), 1.30 (q, *J* = 7.4 Hz, 2H), 0.89 (t, *J* = 7.3 Hz, 3H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 168.0, 145.7, 143.6, 139.6, 134.1, 129.1, 128.9, 127.2, 124.1, 120.4, 117.1, 35.0, 33.5, 22.2, 14.2. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₉H₂₁NO: 280.1696; Found: 280.1697.



***2*-(4-fluorophenyl)-*N*-phenylacrylamide (3ha)⁶**

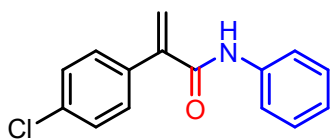
¹H NMR (400 MHz, DMSO-*d*₆) δ 10.27 (s, 1H), 7.79 – 7.69 (m, 2H), 7.57 – 7.52 (m, 2H), 7.37 – 7.29 (m, 2H), 7.26 – 7.19 (m, 2H), 7.12 – 7.04 (m, 1H), 5.94 (s, 1H), 5.77 (s, 1H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 167.6, 162.53 (d, *J* = 245.4 Hz), 144.6, 139.5, 133.30 (d, *J* = 3.3 Hz), 129.56 (d, *J* = 8.3 Hz), 129.1, 124.2, 120.5, 118.5, 115.76 (d, *J* = 21.6 Hz).



***N*-Phenyl-2-(4-(trifluoromethyl) phenyl) acrylamide (3ia)**

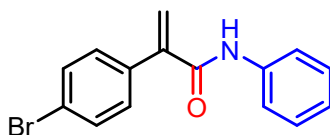
¹H NMR (400 MHz, DMSO-*d*₆) δ 10.34 (s, 1H), 7.77 – 7.69 (m, 6H), 7.34 (dd, *J* = 8.5, 7.4 Hz, 2H), 7.15 – 7.06 (m, 1H), 6.11 (s, 1H), 5.94 (s, 1H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 167.1, 144.4, 141.0,

139.4, 128.5 (q, $J = 31.7$ Hz), 125.8 (q, $J = 3.9$ Hz), 125.0 (q, $J = 173.2$ Hz), 124.3, 121.0, 120.5, 119.6, 112.6. HRMS (ESI-TOF) m/z : $[M+H]^+$ Calcd. for $C_{16}H_{12}F_3NO$: 292.0944; Found: 292.0941.



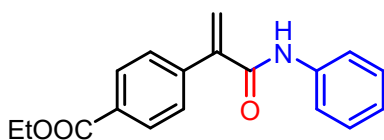
2-(4-chlorophenyl)-N-phenylacrylamide (3ja)⁶

1H NMR (400 MHz, DMSO- d_6) δ 10.29 (s, 1H), 7.81 – 7.64 (m, 2H), 7.55 – 7.50 (m, 2H), 7.47 – 7.42 (m, 2H), 7.34 (dd, $J = 8.5, 7.3$ Hz, 2H), 7.13 – 7.02 (m, 1H), 5.99 (s, 1H), 5.81 (s, 1H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 167.3, 144.5, 139.4, 136.0, 132.5, 131.9, 130.0, 129.5, 129.3, 129.1, 124.2, 122.0, 120.5, 119.2.



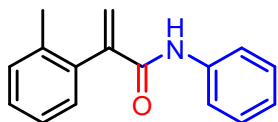
2-(4-bromophenyl)-N-phenylacrylamide (3ka)

1H NMR (400 MHz, DMSO- d_6) δ 10.29 (s, 1H), 7.78 – 7.68 (m, 2H), 7.62 – 7.55 (m, 2H), 7.50 – 7.41 (m, 2H), 7.33 (dd, $J = 8.5, 7.3$ Hz, 2H), 7.15 – 6.99 (m, 1H), 5.99 (s, 1H), 5.81 (s, 1H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 167.3, 144.5, 139.4, 136.0, 132.5, 131.7, 130.1, 129.6, 129.3, 129.1, 124.2, 122.0, 120.5, 119.2. HRMS (ESI-TOF) m/z : $[M+H]^+$ Calcd. for $C_{15}H_{12}BrNO$: 392.0175; Found: 392.0166.



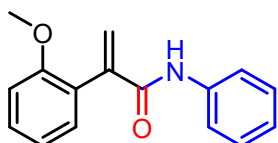
Ethyl 4-(3-oxo-3-(phenylamino) prop-1-en-2-yl) benzoate (3la)

1H NMR (400 MHz, DMSO- d_6) δ 10.34 (s, 1H), 8.06 – 7.91 (m, 2H), 7.87 – 7.53 (m, 4H), 7.48 – 7.27 (m, 2H), 7.23 – 7.01 (m, 1H), 6.11 (s, 1H), 5.90 (s, 1H), 4.33 (q, $J = 7.1$ Hz, 2H), 1.33 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 167.2, 165.9, 144.8, 141.3, 139.4, 129.9, 129.8, 129.1, 127.7, 124.2, 120.4, 61.3, 14.6. HRMS (ESI-TOF) m/z : $[M+H]^+$ Calcd. for $C_{18}H_{17}NO_3$: 296.1281; Found: 296.1281.



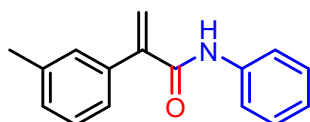
***N*-Phenyl-2-(*o*-tolyl)acrylamide (3ma)⁶**

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.07 (s, 1H), 7.71 (d, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.9 Hz, 3H), 7.23 (tt, *J* = 15.2, 5.1 Hz, 4H), 7.08 (t, *J* = 7.4 Hz, 1H), 6.10 (s, 1H), 5.67 (s, 1H), 2.23 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 167.0, 146.6, 139.6, 138.4, 136.0, 130.28 (d, *J* = 13.5 Hz), 129.0, 128.5, 126.3, 124.1, 122.8, 120.6, 20.1.



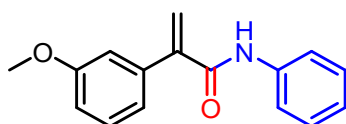
***2*-(2-methoxyphenyl)-*N*-phenylacrylamide (3na)**

¹H NMR (400 MHz, DMSO-*d*₆) δ 9.93 (s, 1H), 7.70 (d, *J* = 7.6 Hz, 2H), 7.41 – 7.23 (m, 4H), 7.14 – 6.89 (m, 3H), 5.84 (s, 1H), 5.71 (s, 1H), 3.67 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 167.5, 157.1, 144.7, 140.0, 130.8, 130.3, 129.0, 127.8, 123.7, 121.1, 121.0, 120.4, 112.0, 56.2. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₆H₁₅NO₂:254.1176; Found: 254.1179.



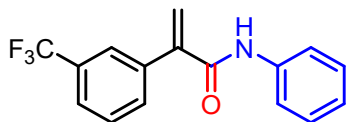
***N*-phenyl-2-(*m*-tolyl)acrylamide (3oa)**

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.24 (s, 1H), 7.86 – 7.67 (m, 2H), 7.36 – 7.25 (m, 5H), 7.20 – 7.13 (m, 1H), 7.12 – 7.05 (m, 1H), 5.91 (s, 1H), 5.71 (s, 1H), 2.32 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 167.9, 145.9, 139.6, 138.0, 136.8, 129.4, 129.1, 128.8, 127.8, 124.5, 124.1, 120.4, 117.9, 21.5. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₆H₁₅NO:238.1226; Found: 238.1228.



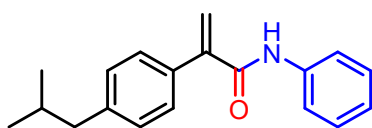
***2*-(3-methoxyphenyl)-*N*-phenylacrylamide (3pa)⁶**

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.36 (s, 1H), 7.88 – 7.77 (m, 2H), 7.77 – 7.70 (m, 4H), 7.65 (t, *J* = 7.7 Hz, 1H), 7.35 (dd, *J* = 8.5, 7.4 Hz, 2H), 7.14 – 7.04 (m, 1H), 6.14 (s, 1H), 5.95 (s, 1H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 167.7, 159.8, 145.6, 139.5, 138.2, 130.0, 129.1, 124.1, 120.4, 119.8, 118.5, 114.2, 113.0, 55.6.



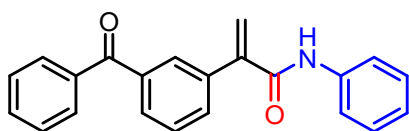
***N*-phenyl-2-(3-(trifluoromethyl) phenyl) acrylamide (3qa)**

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.36 (s, 1H), 7.88 – 7.77 (m, 2H), 7.77 – 7.70 (m, 4H), 7.65 (t, *J* = 7.7 Hz, 1H), 7.35 (dd, *J* = 8.5, 7.4 Hz, 2H), 7.14 – 7.04 (m, 1H), 6.14 (s, 1H), 5.95 (s, 1H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 167.1, 144.0, 139.4, 138.0, 131.6, 130.0, 129.7 (q, *J* = 31.7 Hz), 129.1, 125.3 (q, *J* = 3.9 Hz), 124.3, 124.0 (q, *J* = 273.4 Hz), 121.0, 120.6. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₆H₁₂F₃NO:292.0944; Found: 292.0935.



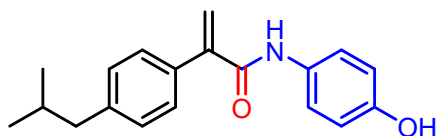
2-(4-isobutylphenyl)-*N*-phenylacrylamide (3ra)

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.24 (s, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.44 – 7.38 (m, 2H), 7.33 (t, *J* = 7.9 Hz, 2H), 7.17 (d, *J* = 8.1 Hz, 2H), 7.11 – 7.03 (m, 1H), 5.90 (s, 1H), 5.66 (s, 1H), 2.45 (d, *J* = 7.2 Hz, 2H), 1.83 (dp, *J* = 13.4, 6.6 Hz, 1H), 0.87 (d, *J* = 6.6 Hz, 6H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 168.0, 145.7, 141.9, 139.6, 134.2, 129.5, 129.1, 127.0, 124.1, 120.4, 117.0, 44.74, 30.1, 22.6. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₉H₂₁NO:280.1696; Found: 280.1698.



2-(3-benzoylphenyl)-*N*-phenylacrylamide (3sa)

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.33 (s, 1H), 7.89 – 7.82 (m, 2H), 7.81 – 7.49 (m, 9H), 7.42 – 7.30 (m, 2H), 7.20 – 7.03 (m, 1H), 6.06 (s, 1H), 5.90 (s, 1H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 196.0, 167.3, 144.8, 139.4, 137.7, 137.27 (d, *J* = 4.2 Hz), 133.3, 131.6, 130.2, 130.0, 129.3, 129.09 (d, *J* = 7.0 Hz), 128.5, 124.2, 120.5, 120.1. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₂₂H₁₇NO₂:328.1332; Found: 328.1329.



***N*-(4-hydroxyphenyl)-2-(4-isobutylphenyl) acrylamide (3ta)**

¹H NMR (400 MHz, DMSO-*d*₆) δ 9.99 (s, 1H), 9.24 (s, 1H), 7.50 (d, *J* = 8.9 Hz, 2H), 7.40 (d, *J* = 8.2 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 6.73 (d, *J* = 8.9 Hz, 1H), 5.85 (s, 1H), 5.61 (s, 1H), 2.45 (d, *J* = 7.1 Hz, 2H), 1.82 (dq, *J* = 13.5, 6.8 Hz, 1H), 0.86 (d, *J* = 6.6 Hz, 6H). **¹³C NMR** (100 MHz, DMSO-*d*₆) δ 167.4, 154.1, 145.8, 141.8, 134.3, 131.2, 129.5, 127.0, 122.1, 116.6, 115.4, 44.7, 30.1, 22.6. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd. for C₁₉H₂₁NO₂:296.1645; Found: 296.1648.

References

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- 5 B. El Ali and J. Tijani, *Applied Organom Chemis*, 2003, **17**, 921–931.
- 6 X. Zhou, Z. Wang, B. Yu, S. Kuang, W. Sun and Y. Yang, *Green Chem.*, 2022, **24**, 4463–4469.
- 7 B. El Ali and J. Tijani, *Applied Organometallic Chemistry*, 2003, **17**, 921–931.
- 8 D. Wang, W. Guo, Q. Zhou, L. Liu, Y. Lu and Y. Liu, *ChemCatChem*, 2018, **10**, 4264–4268.

S8. The NMR spectra relevant to elucidating CPP coordination behavior

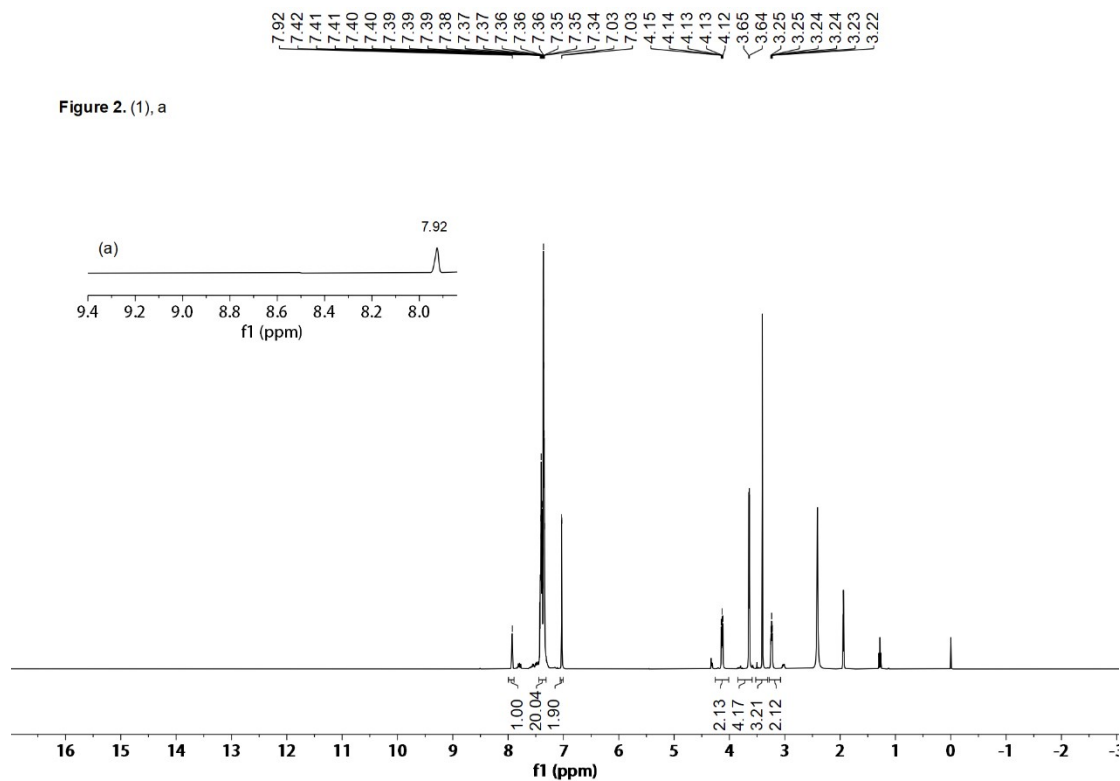


Figure 2. (1), a

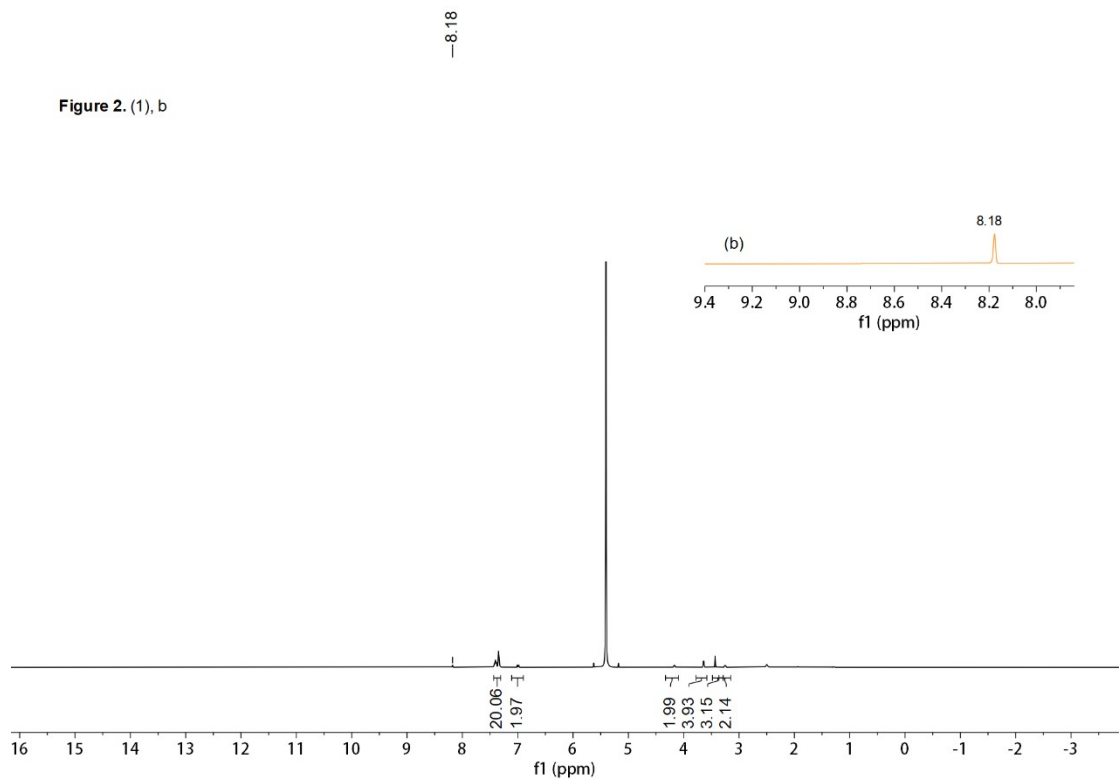


Figure 2. (1), b

Figure 2. (1), c

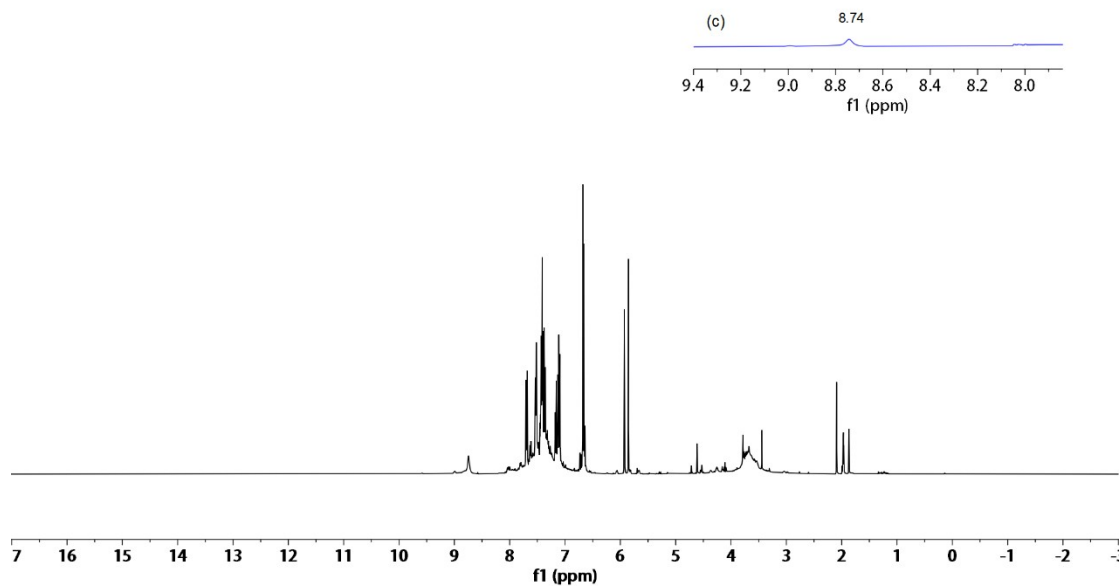


Figure 2. (1), c

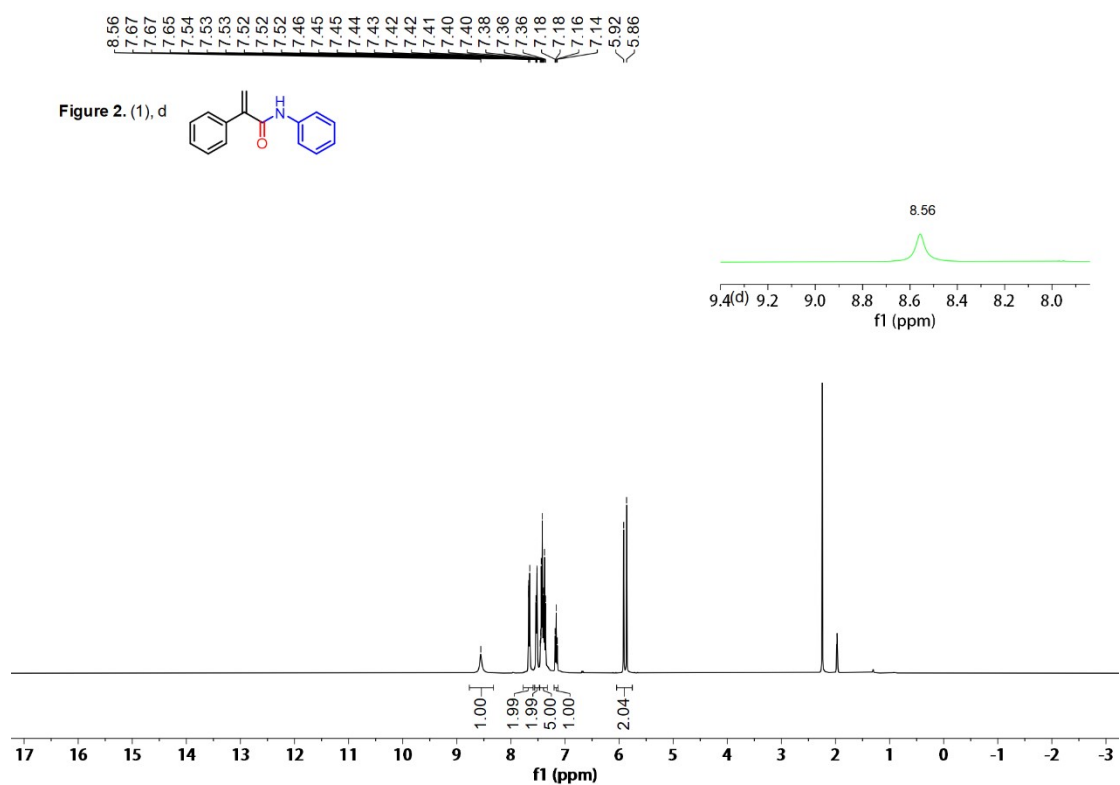


Figure 2. (1), d

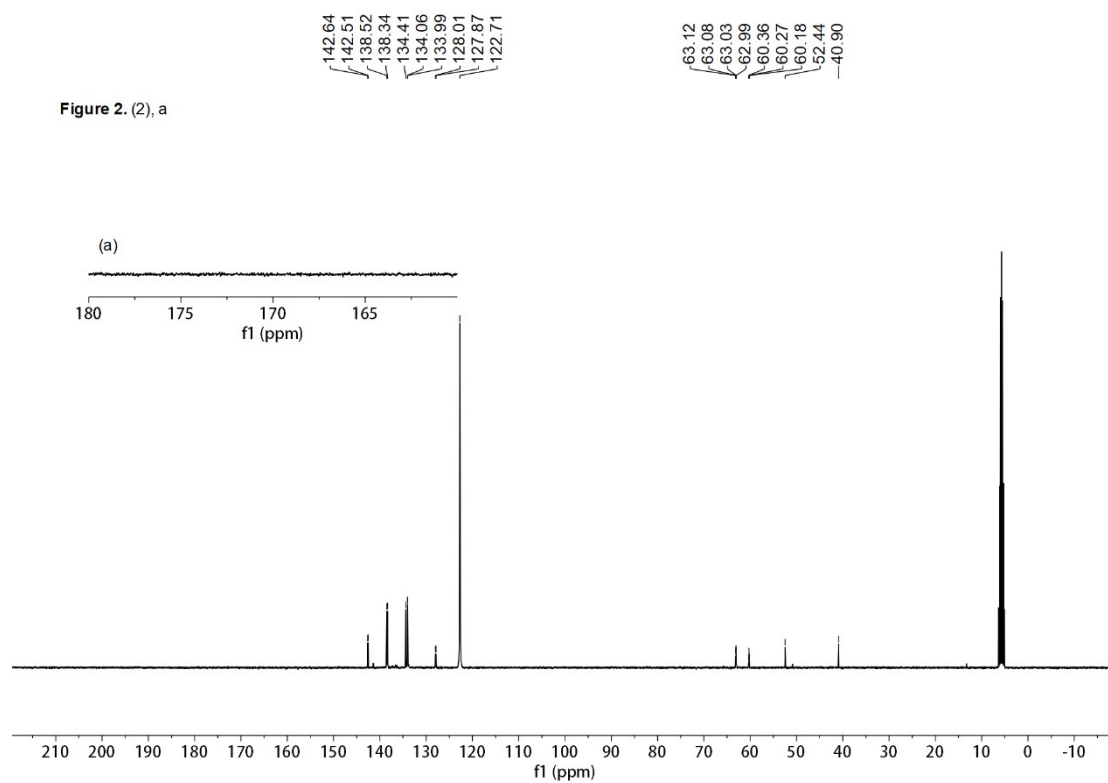


Figure 2. (2), a

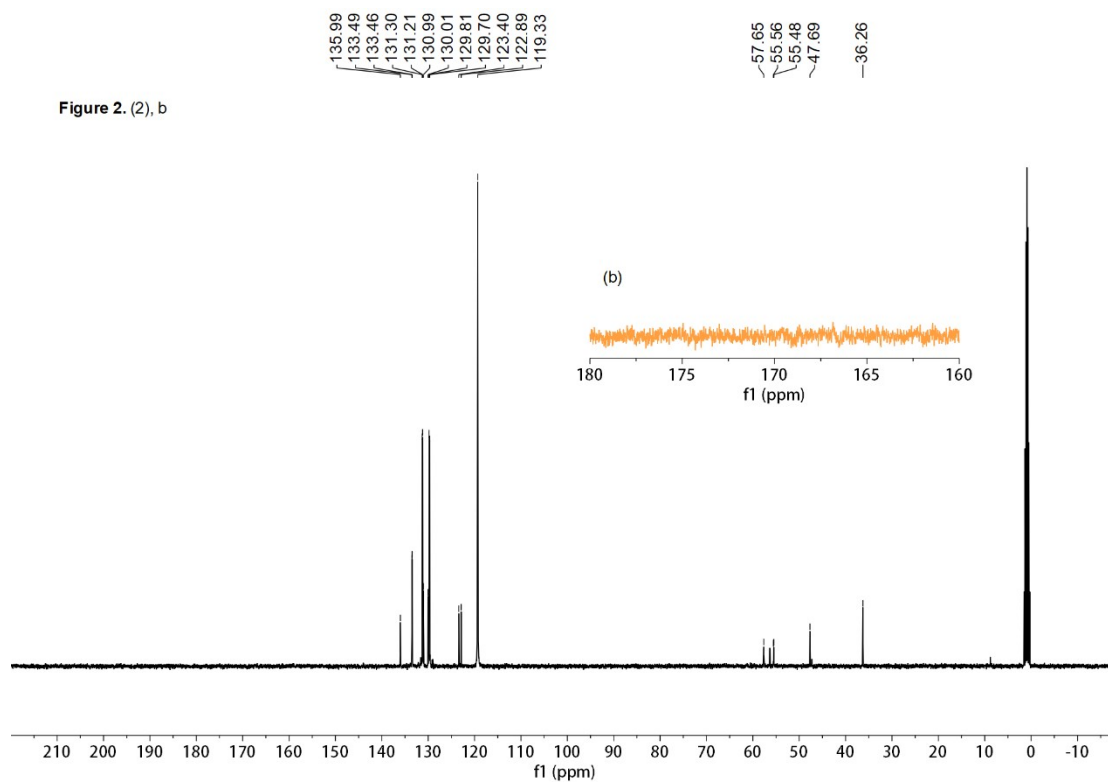


Figure 2. (2), b

Figure 2. (2), c

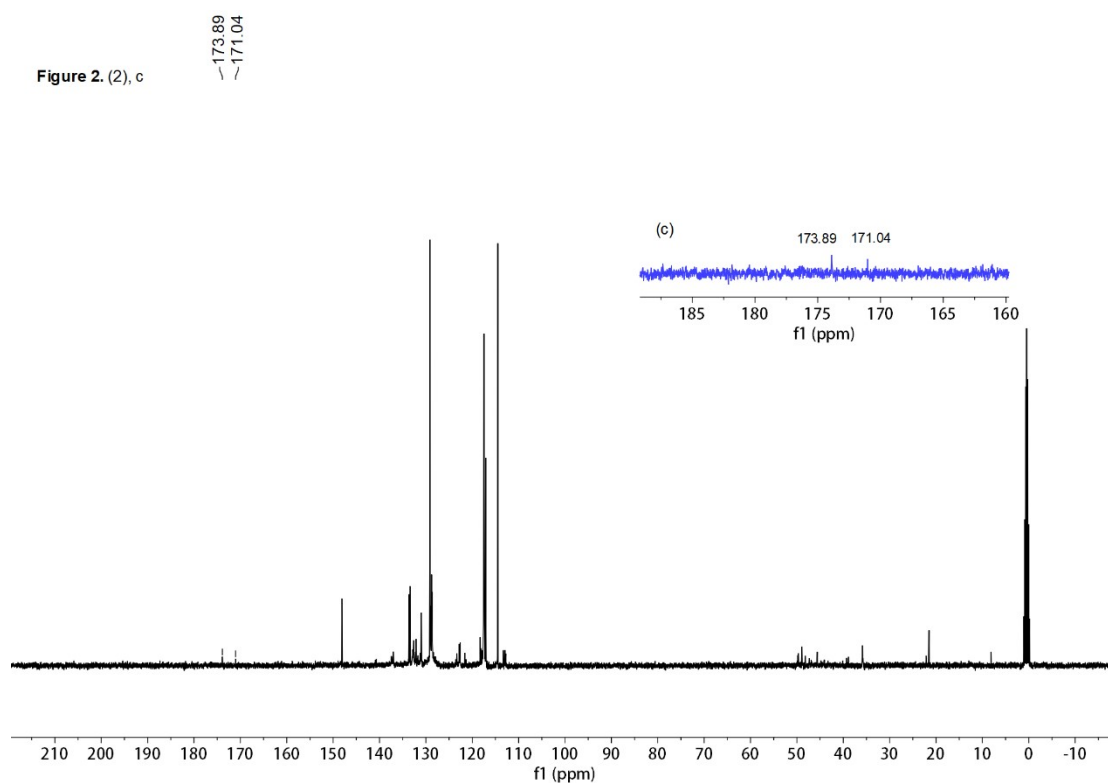


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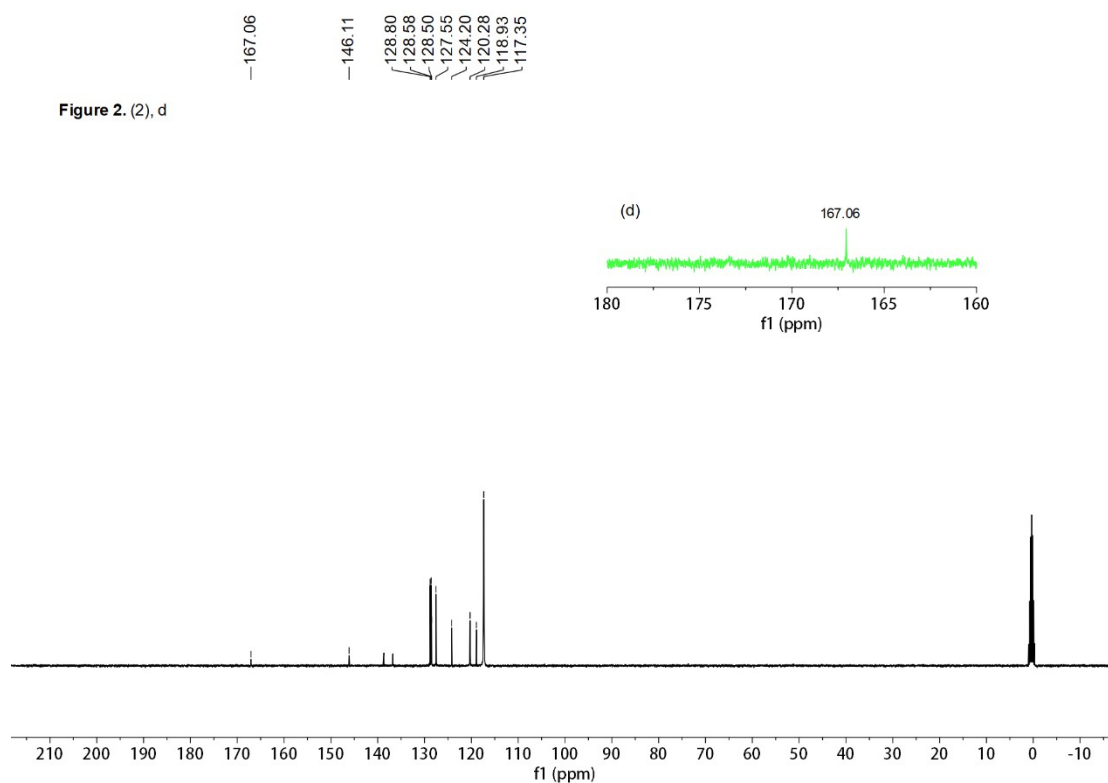


Figure 2. (2), d

Figure 2. (3), a

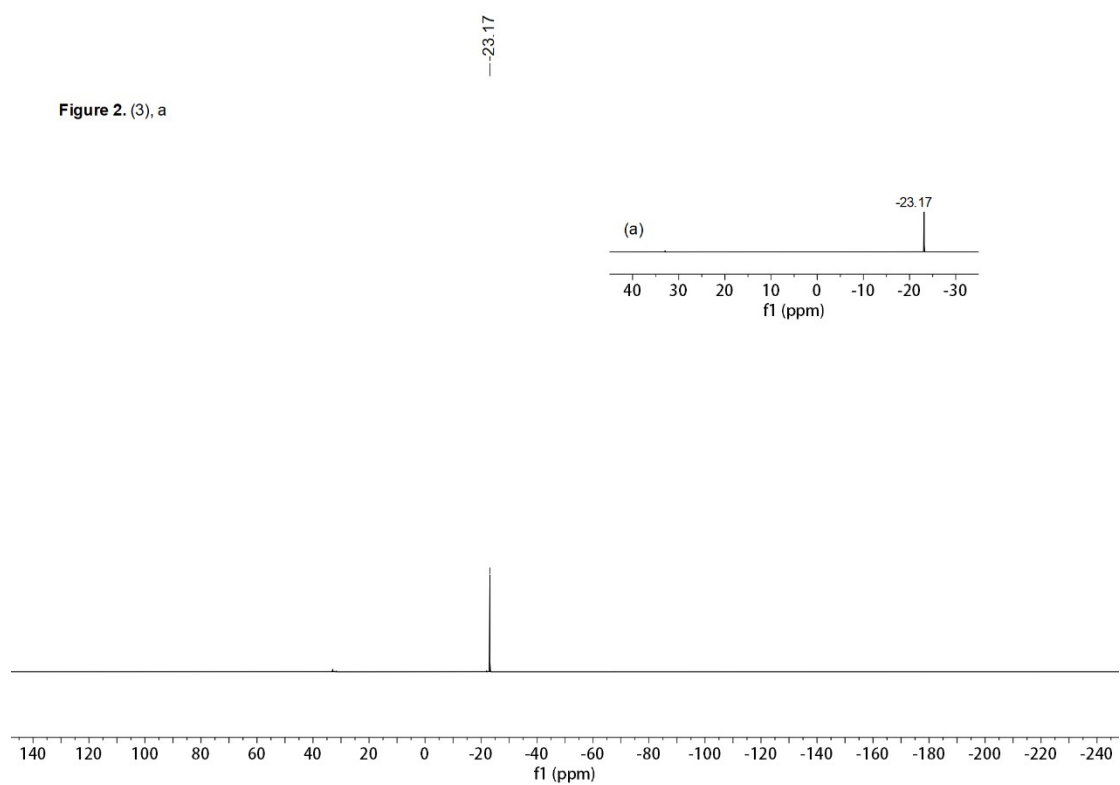


Figure 2. (3), a

Figure 2. (3), b

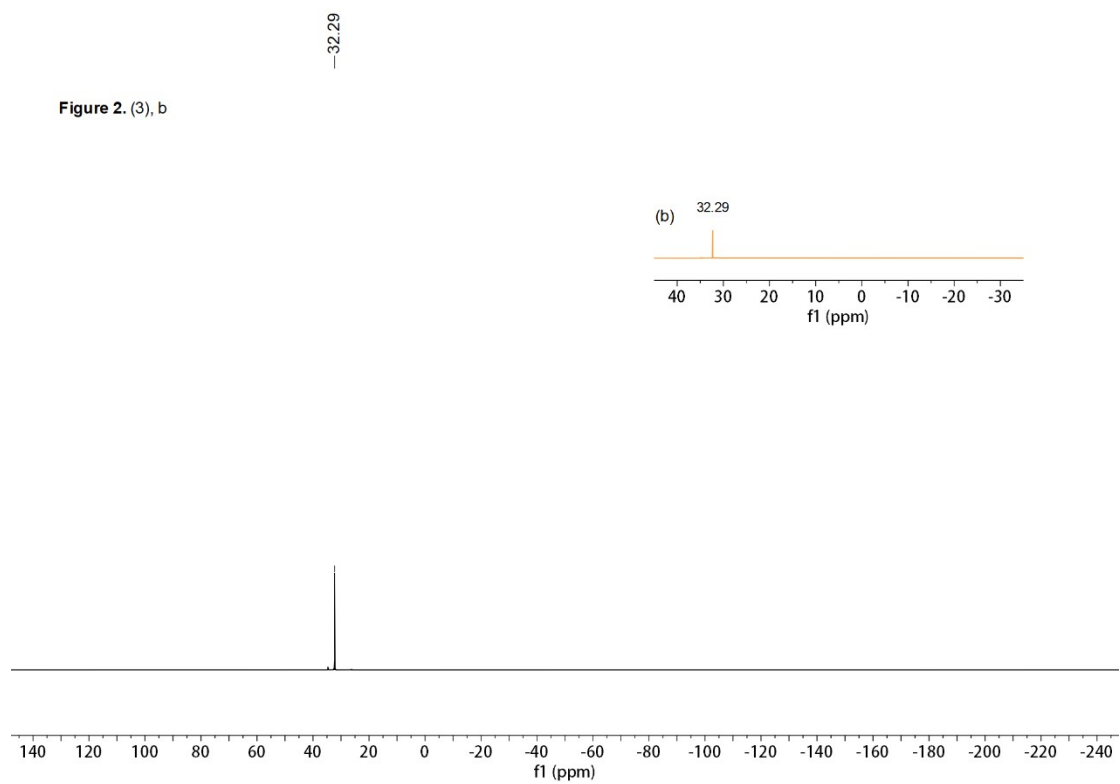


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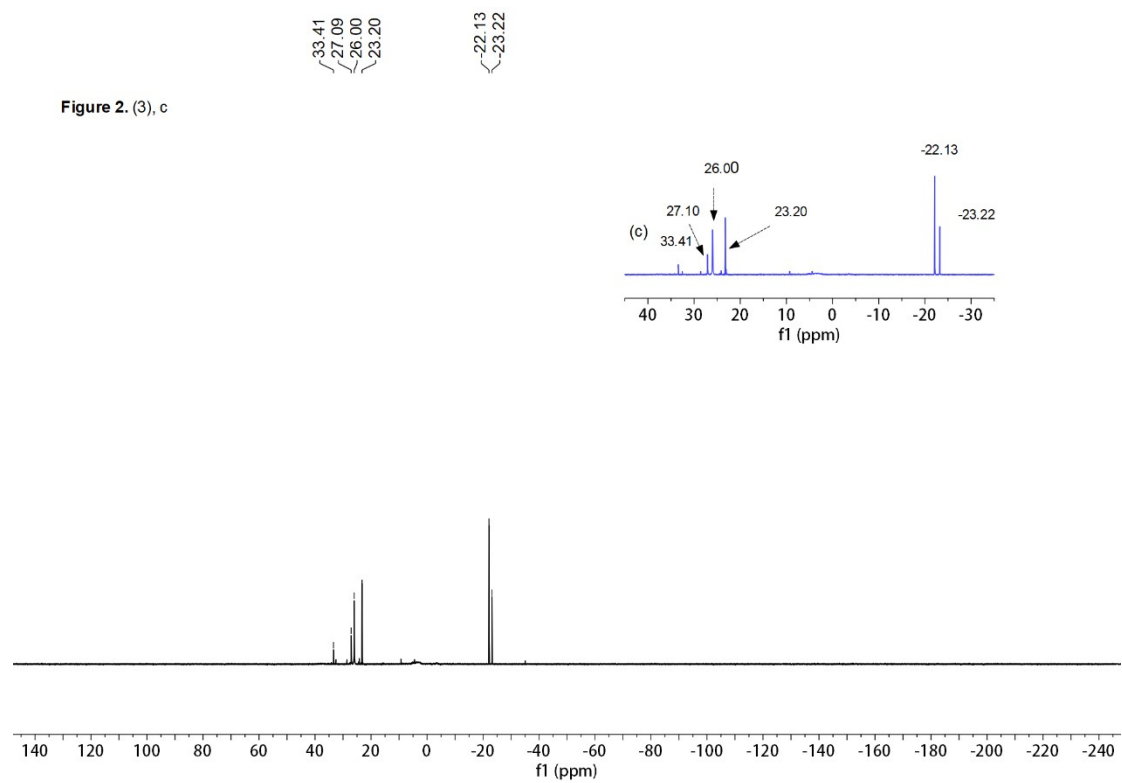
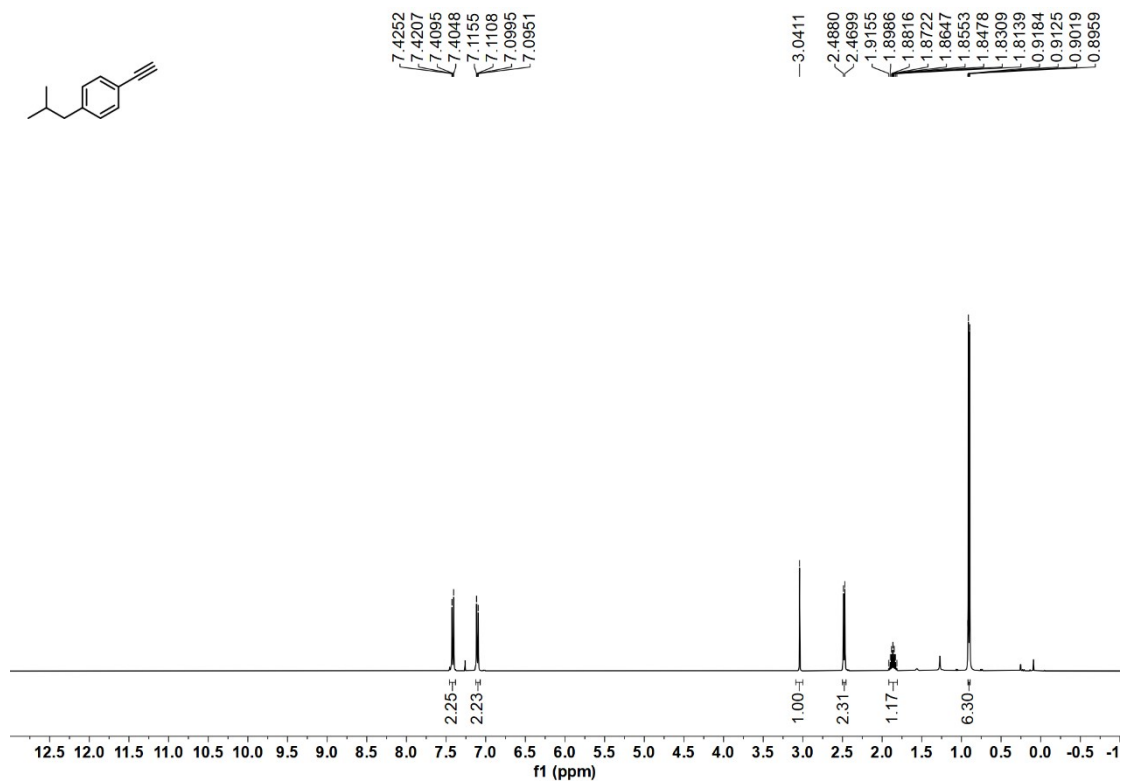
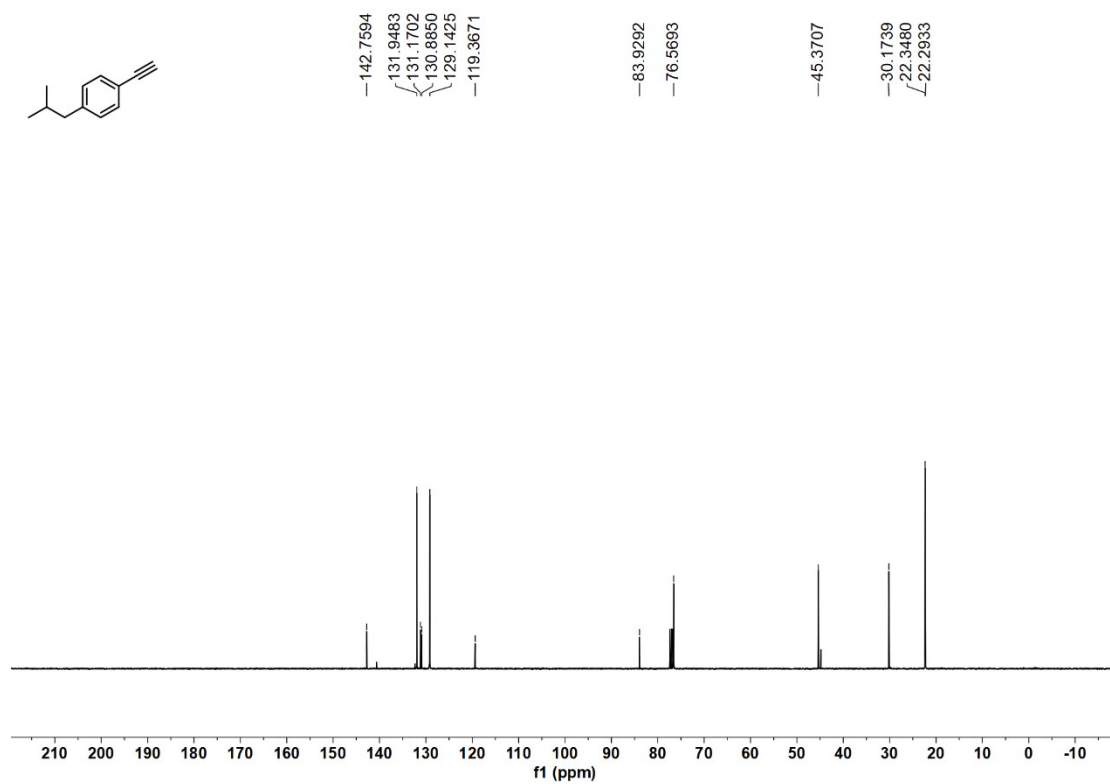


Figure 2. (3), c

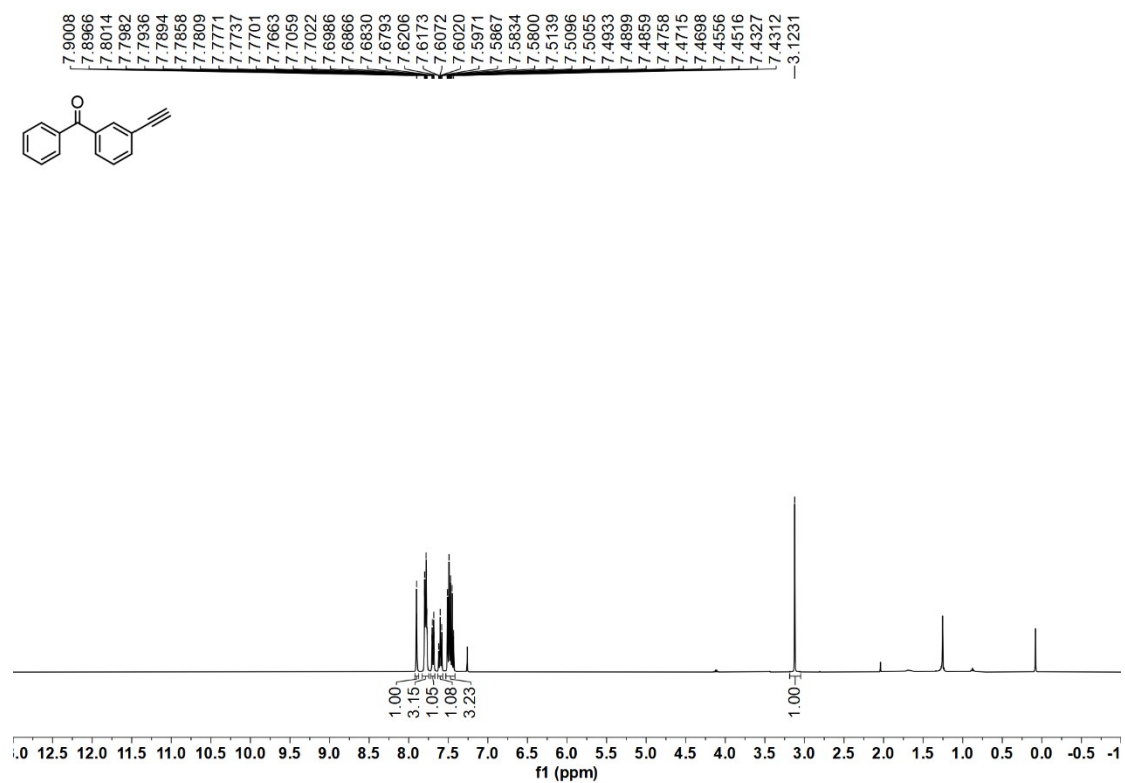
S9. NMR spectra of substrates and products



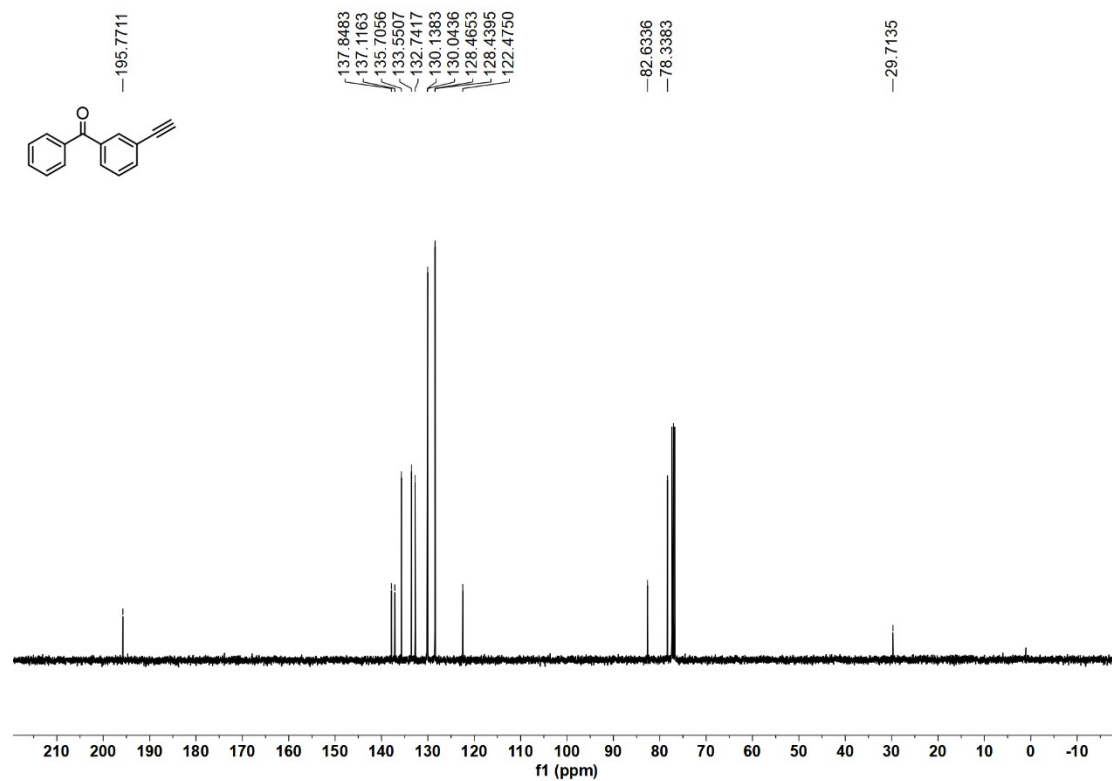
¹H NMR (400 MHz, CDCl₃) spectrum of 1aa



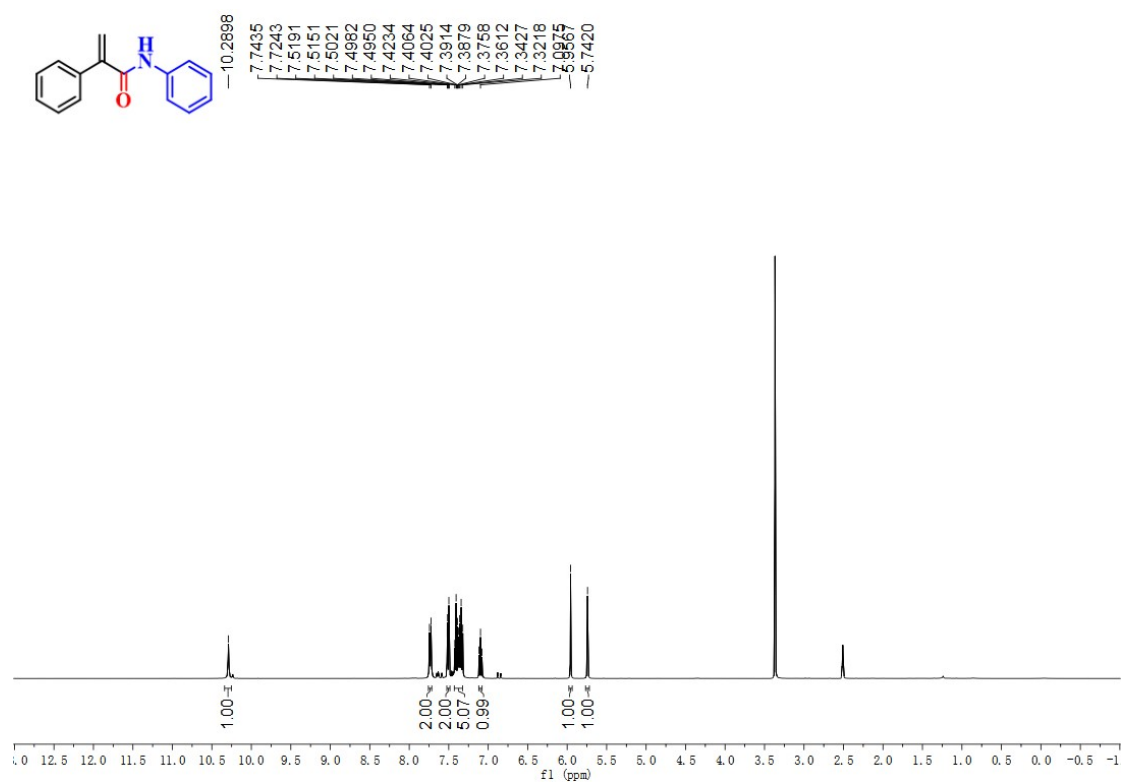
¹³C NMR (100 MHz, CDCl₃) spectrum of 1aa



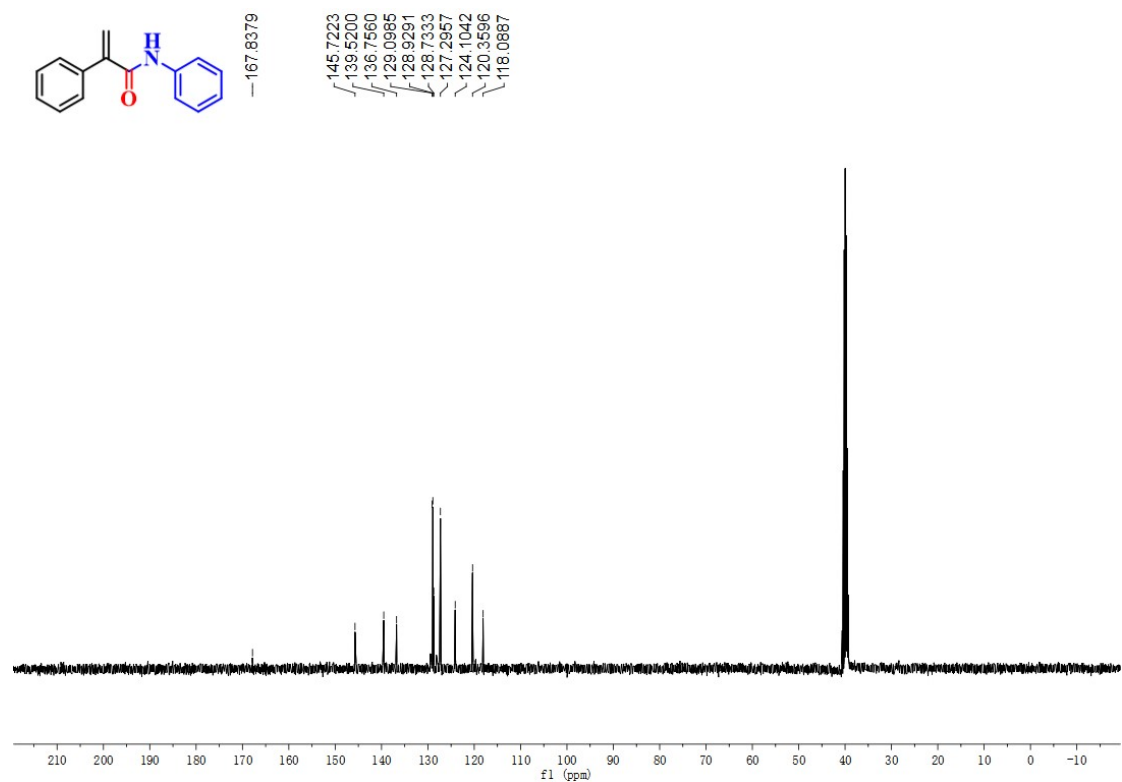
¹H NMR (400 MHz, CDCl₃) spectrum of 1a



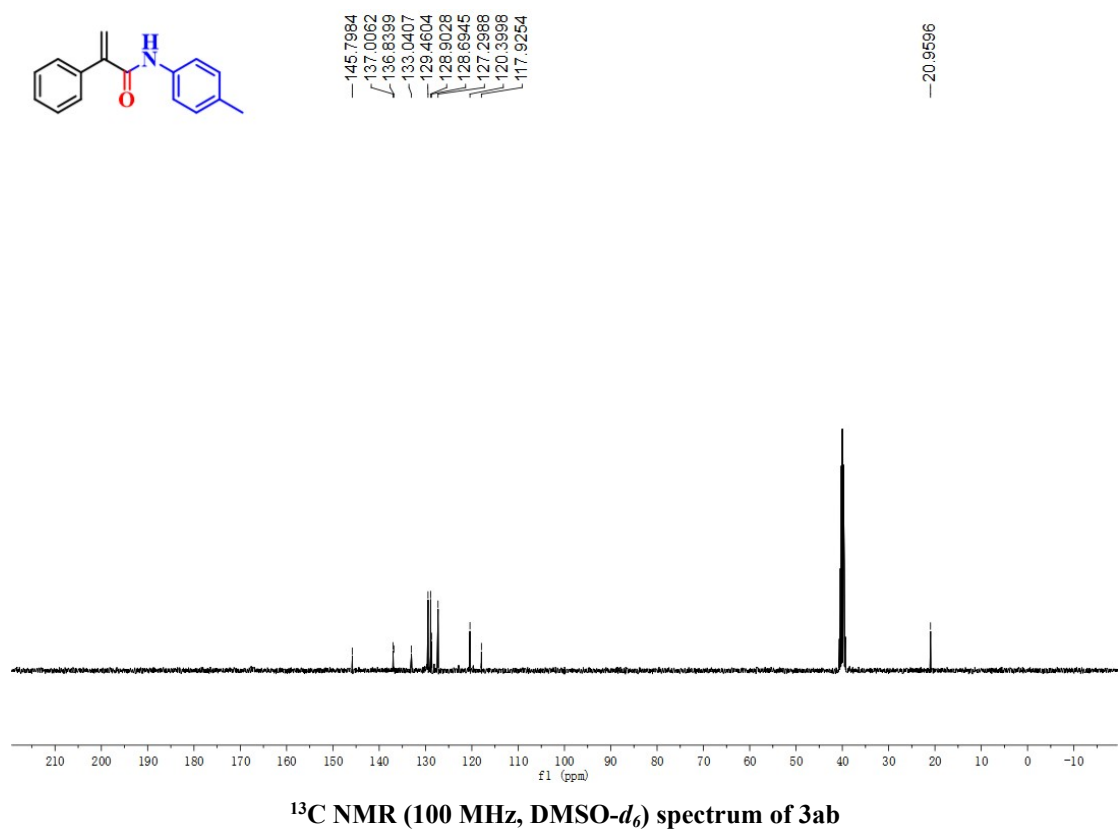
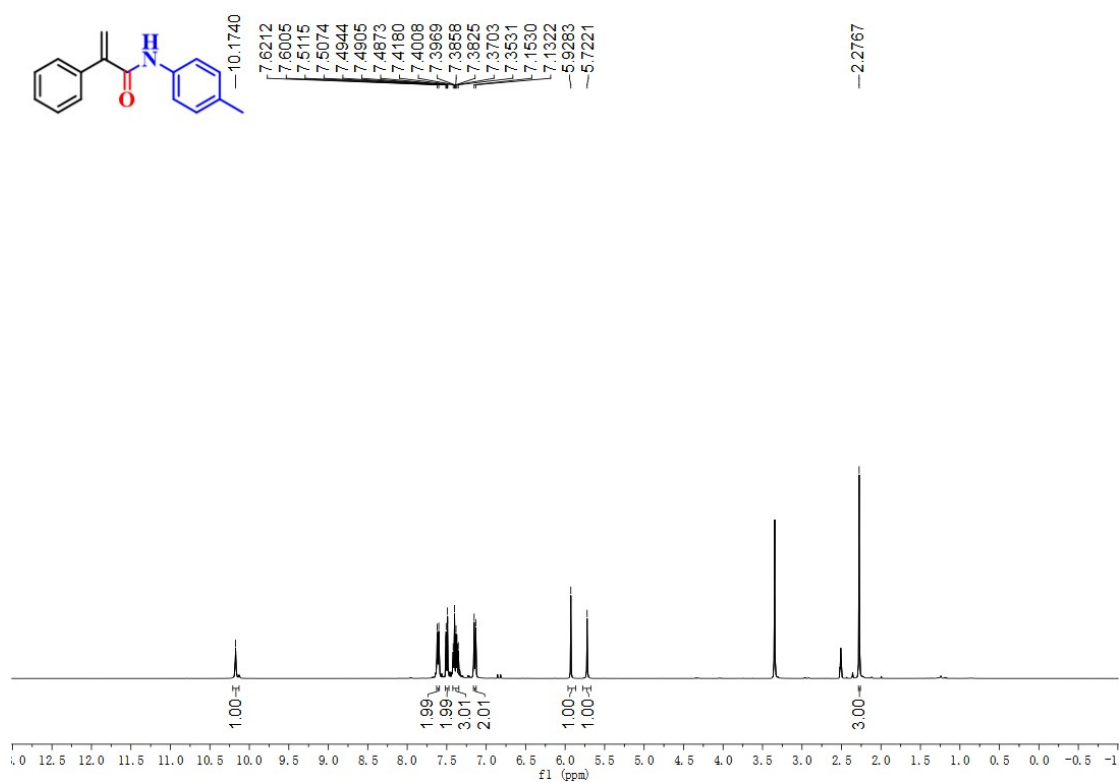
¹³C NMR (100 MHz, CDCl₃) spectrum of 1a

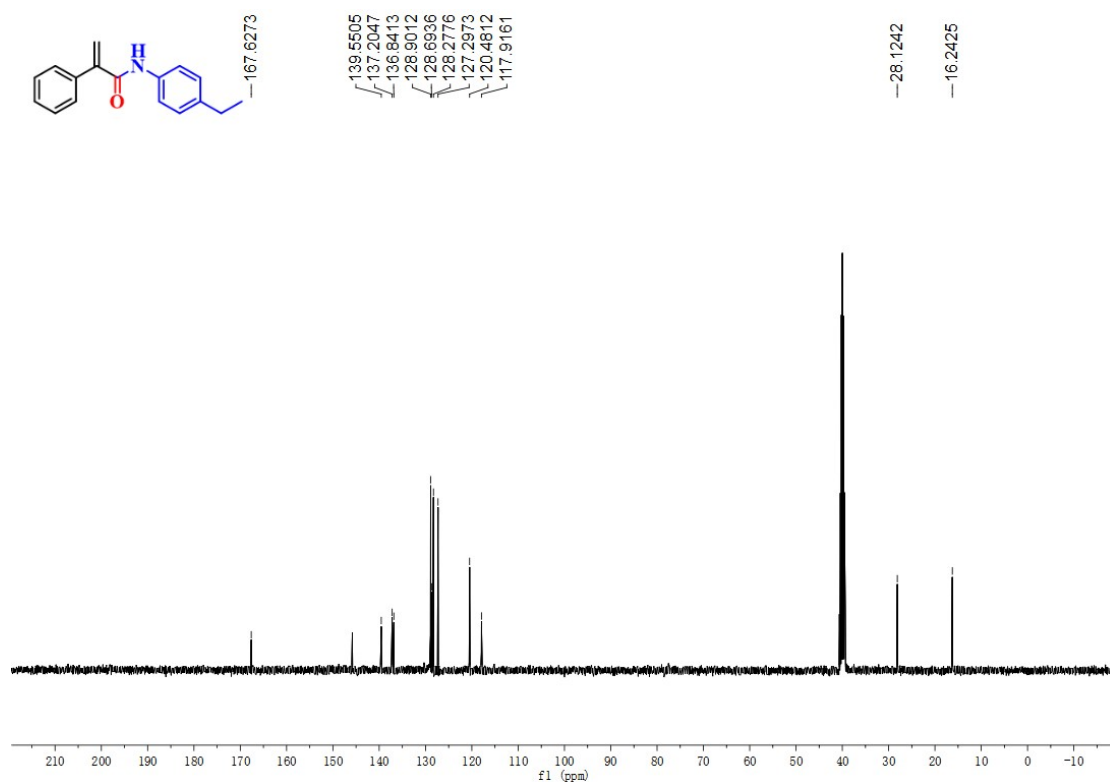
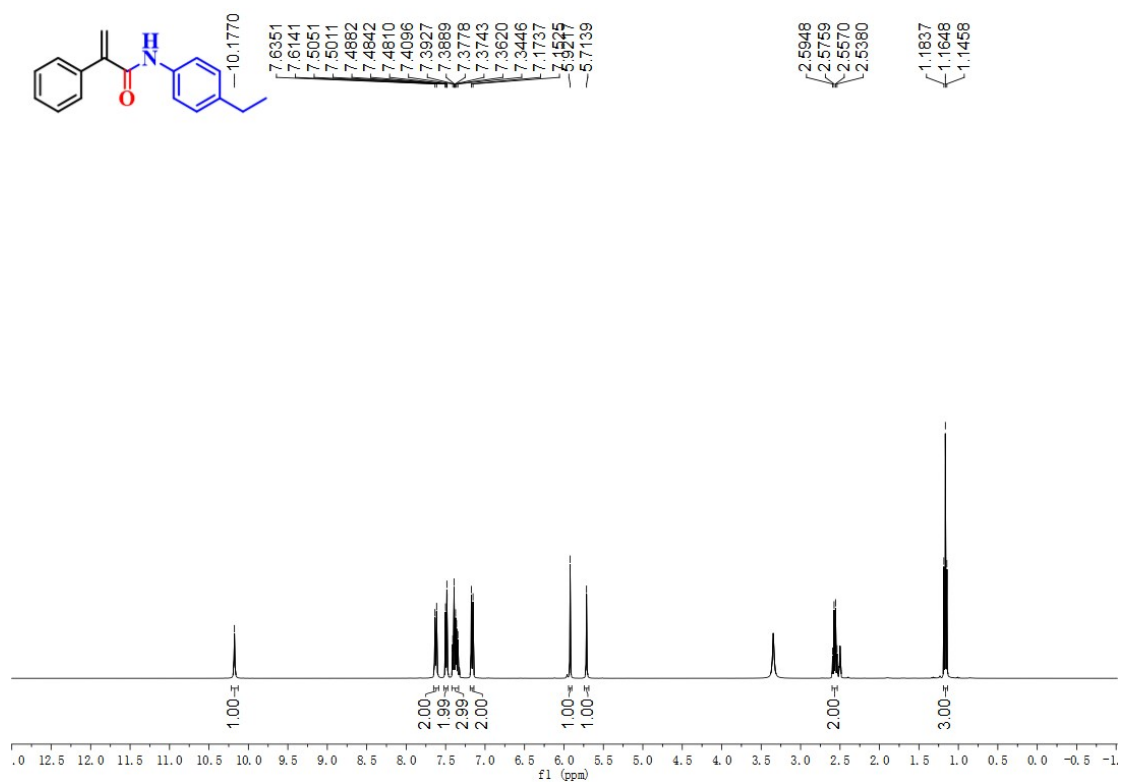


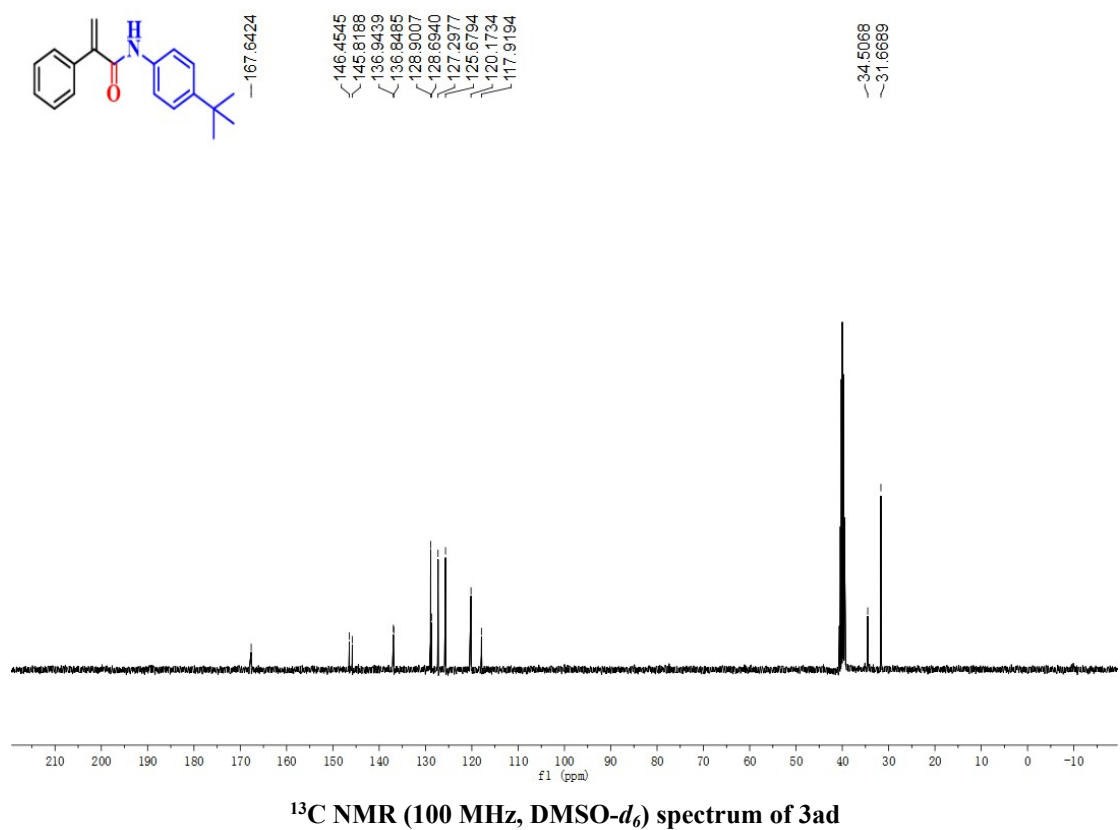
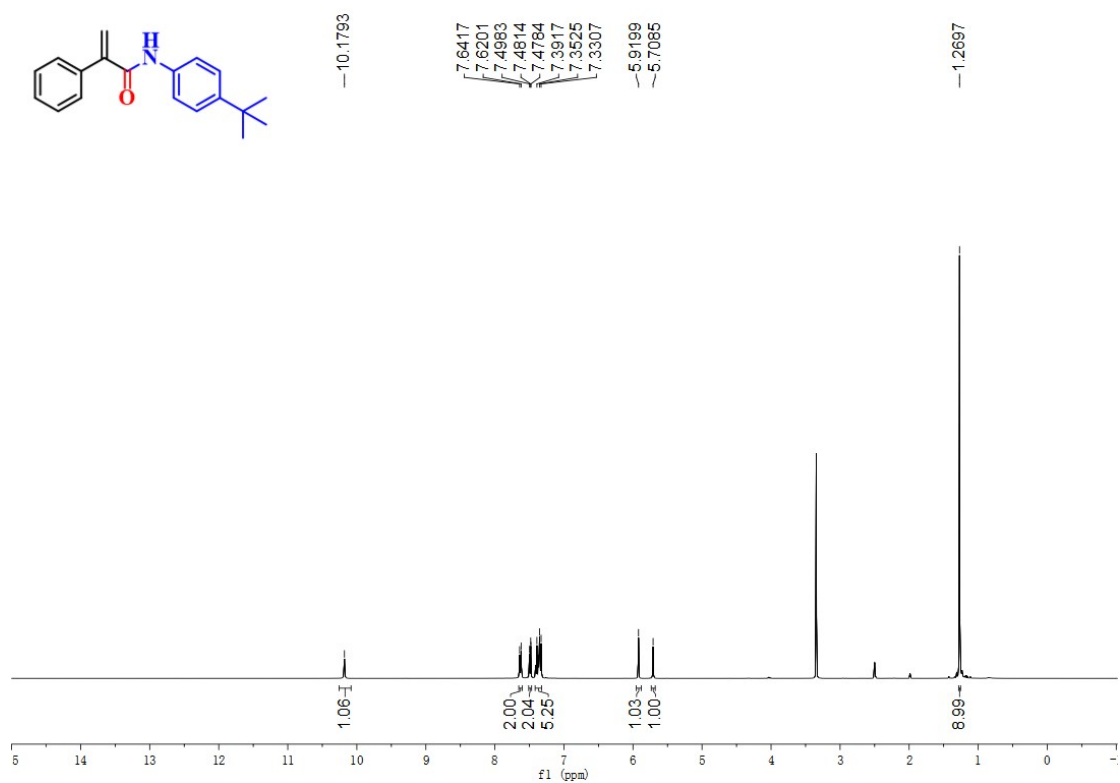
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 3aa

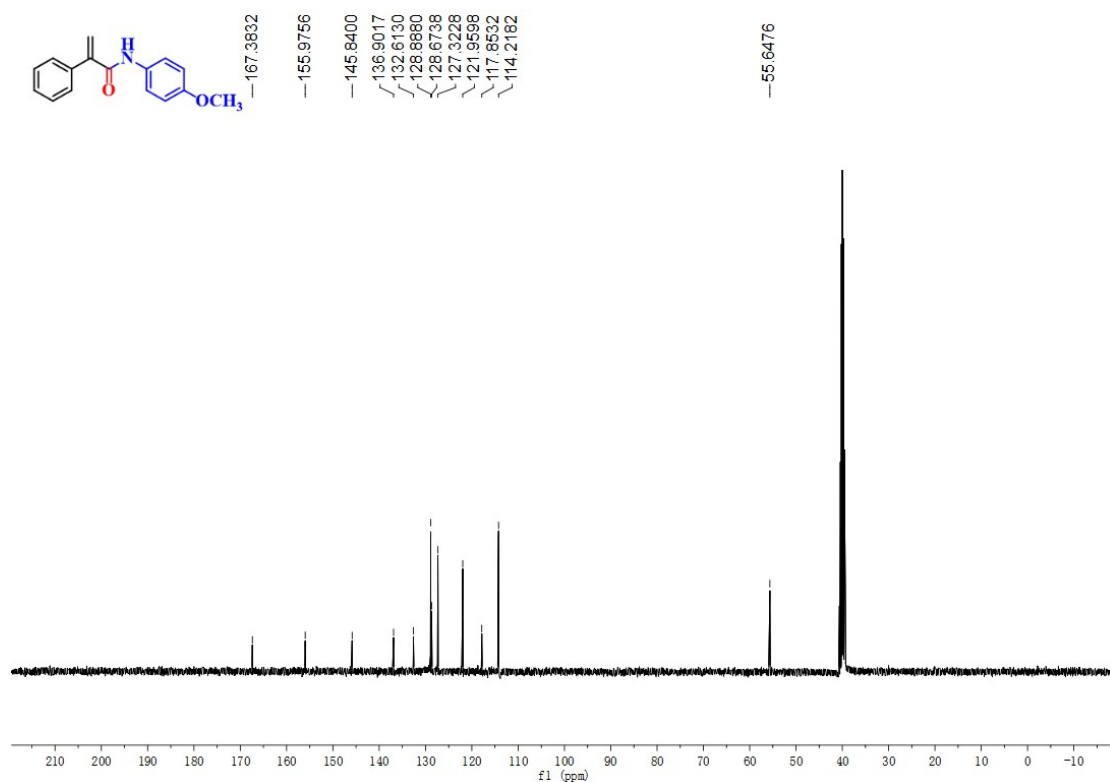
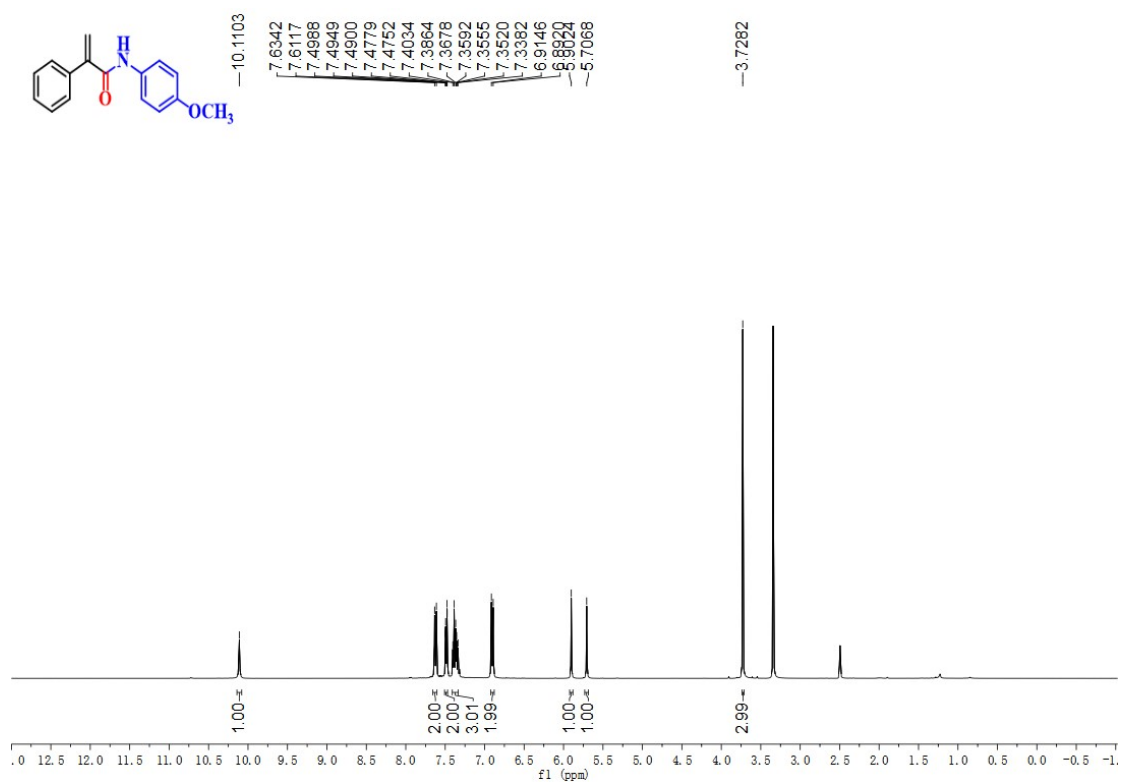


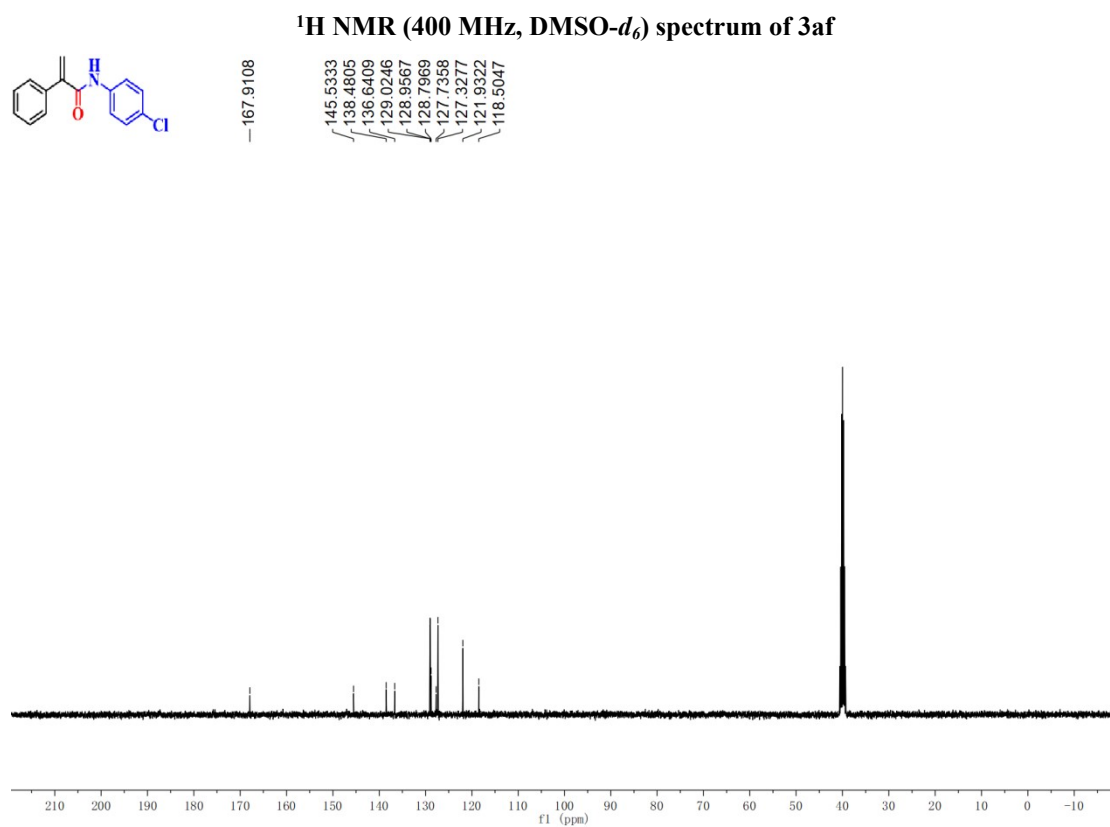
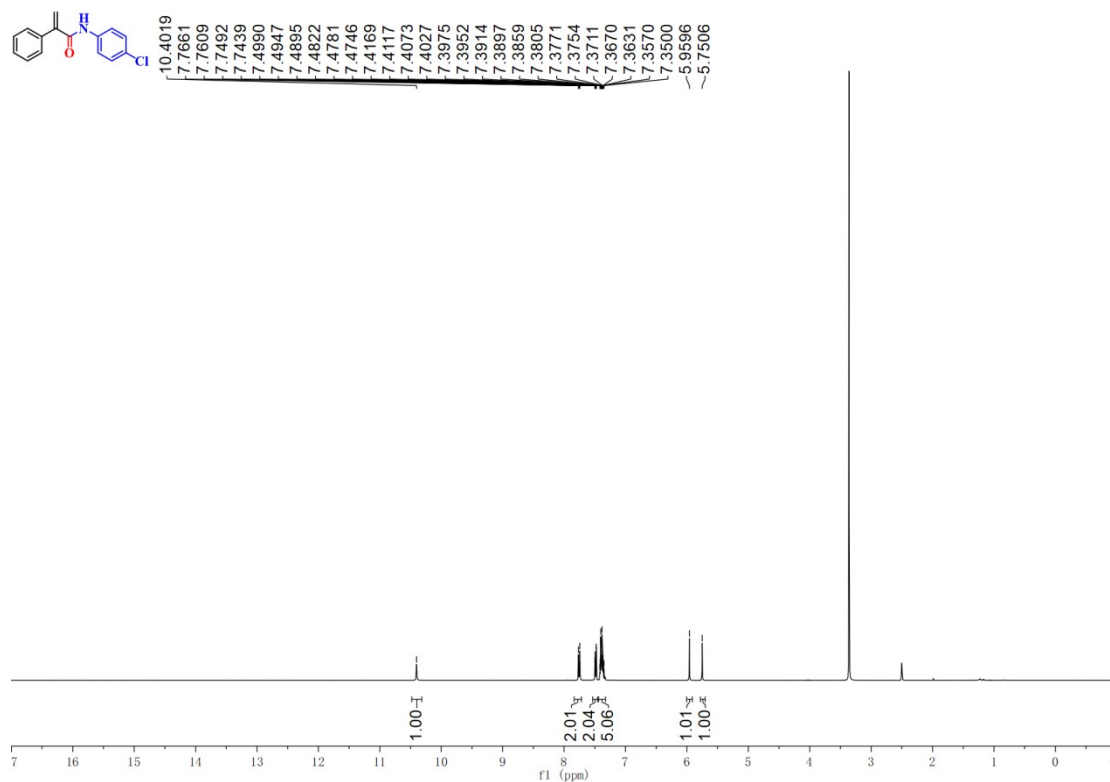
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 3aa

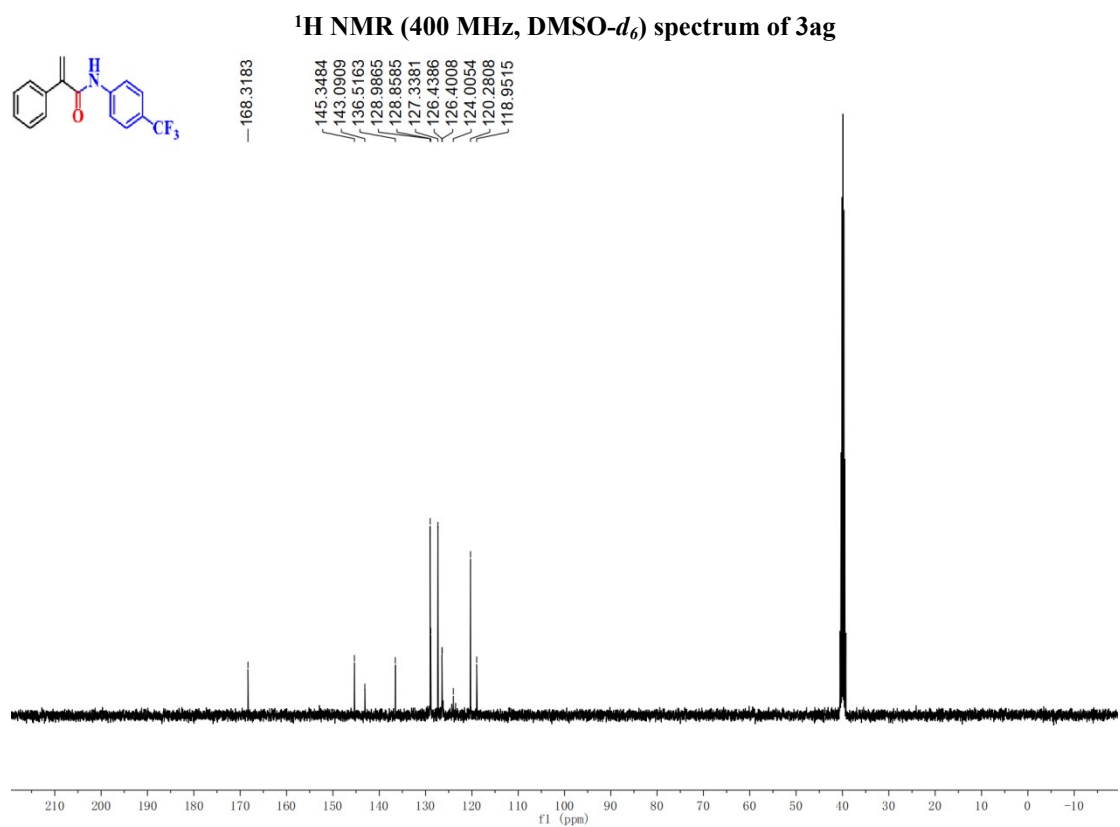
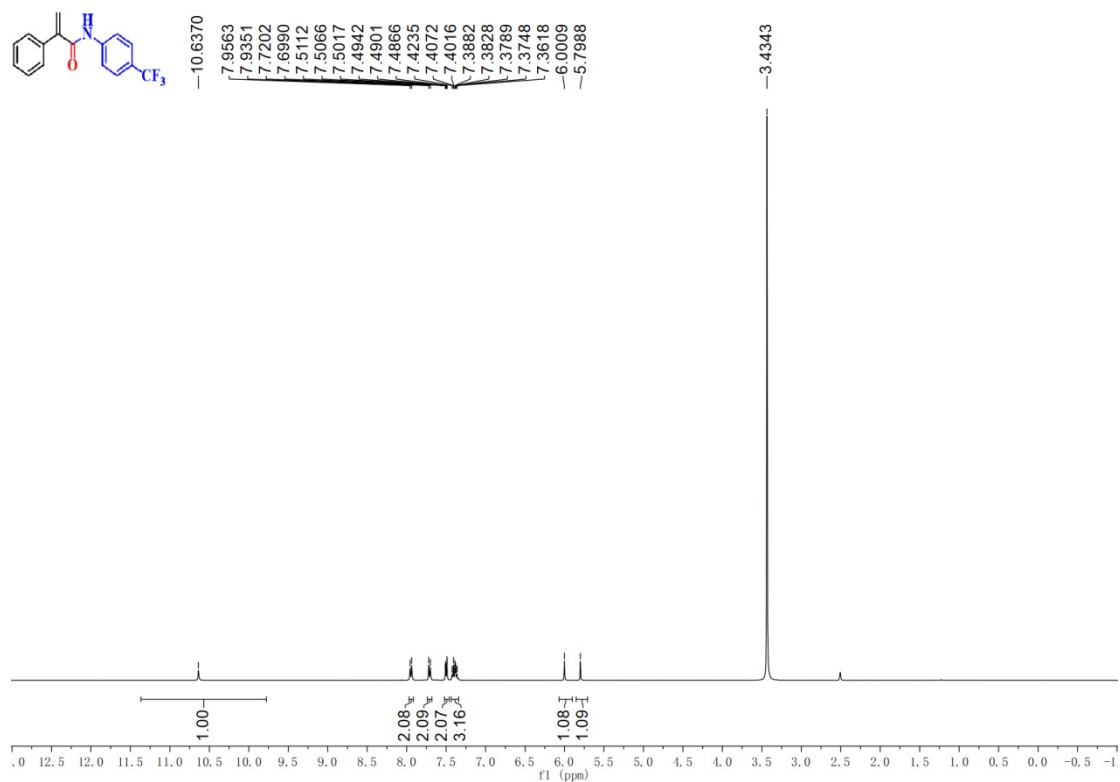


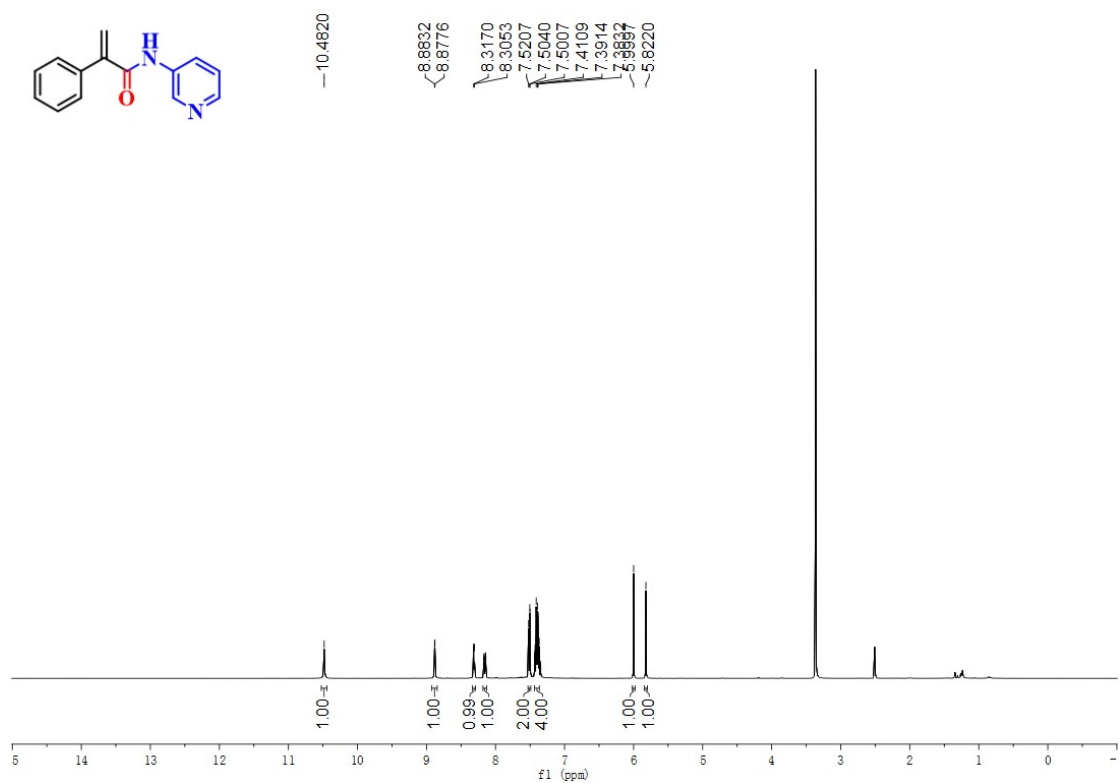




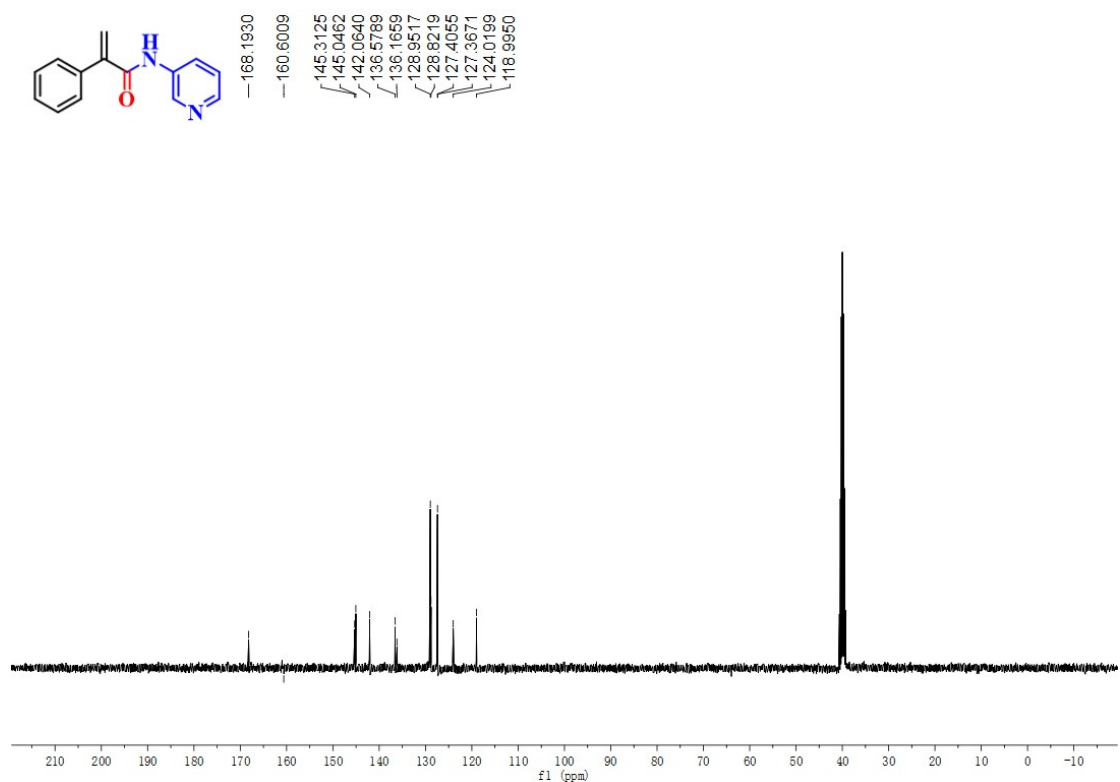




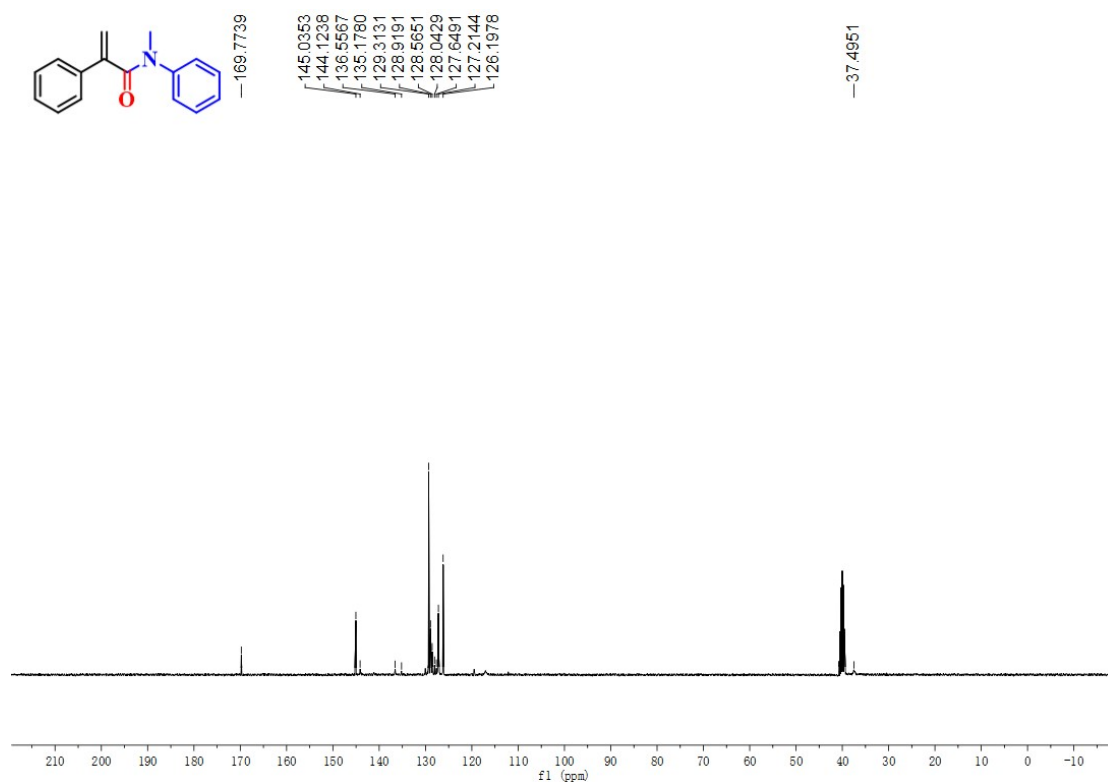
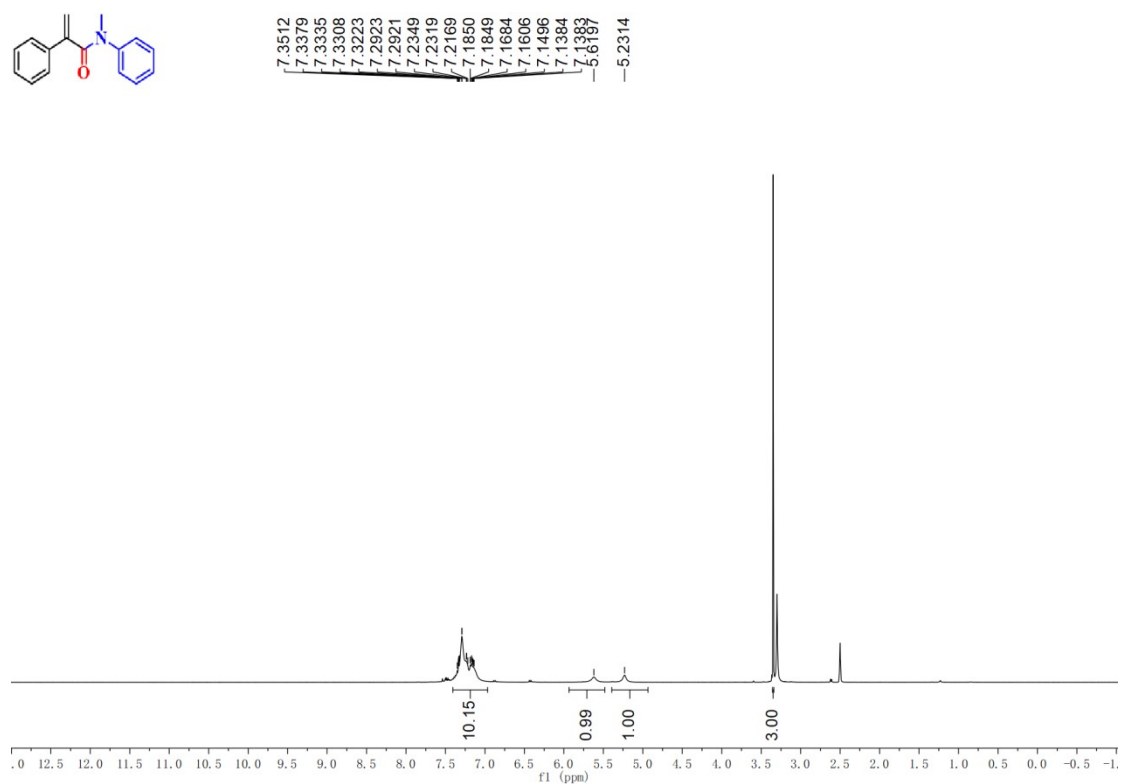


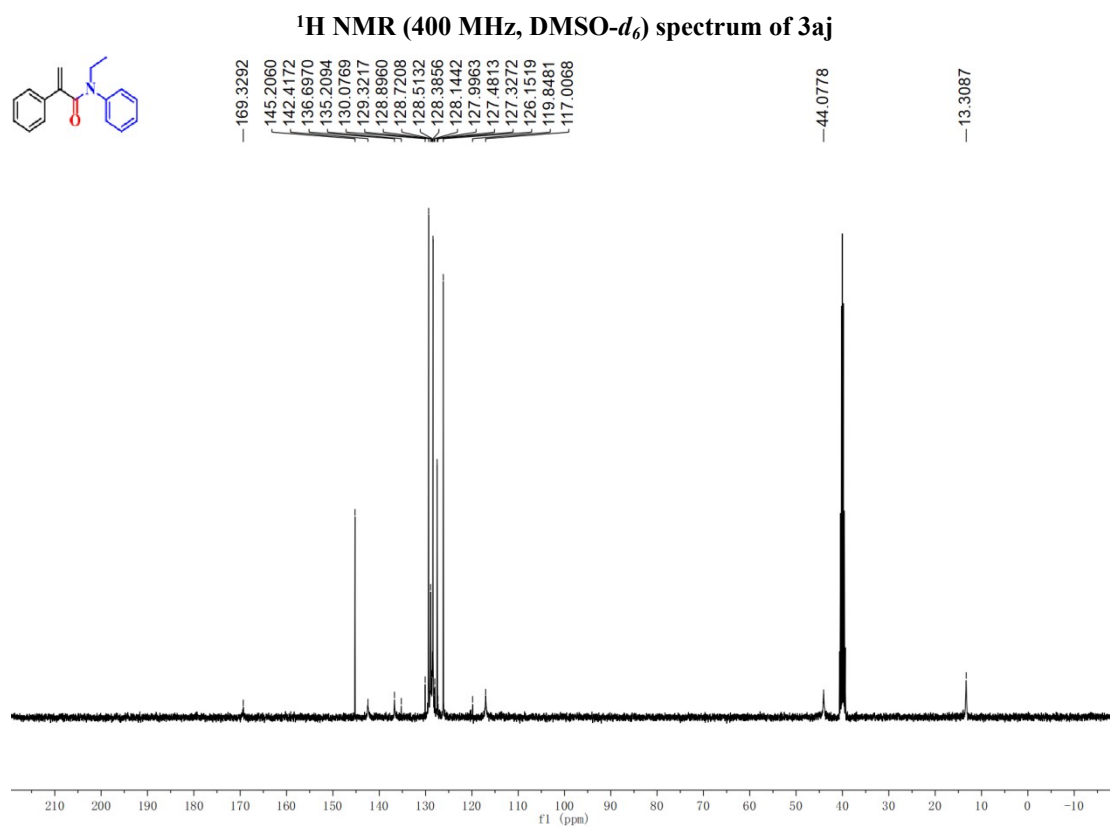
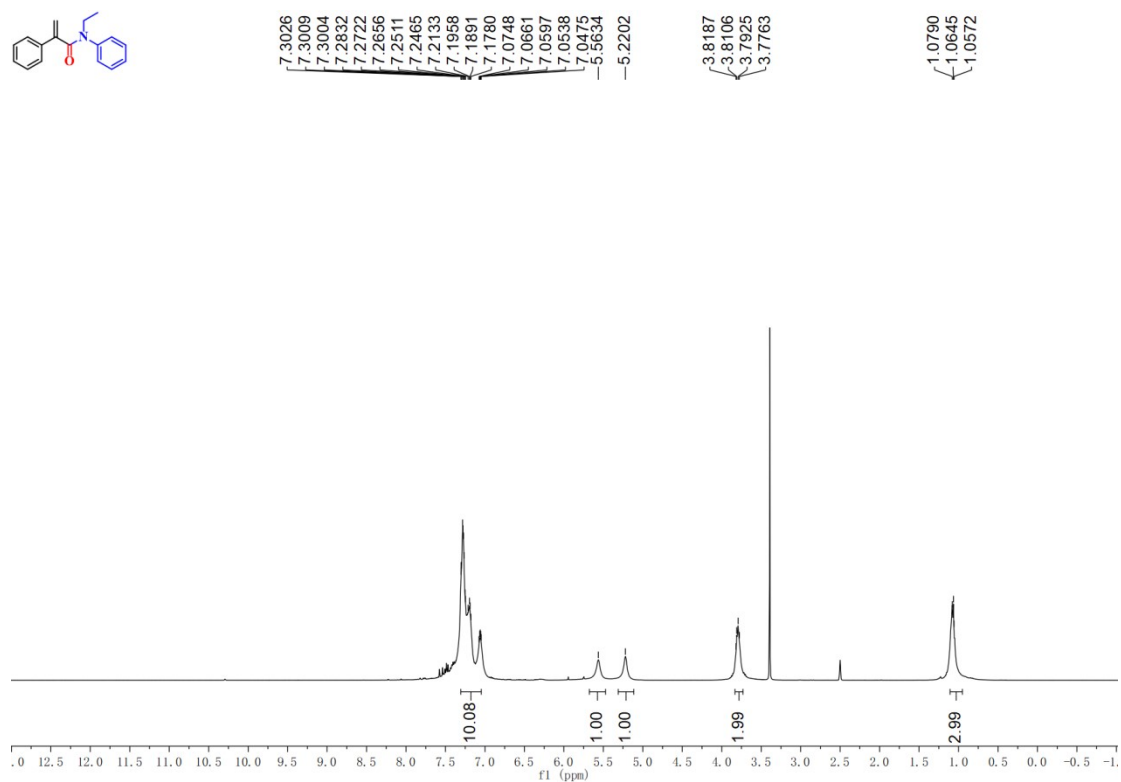


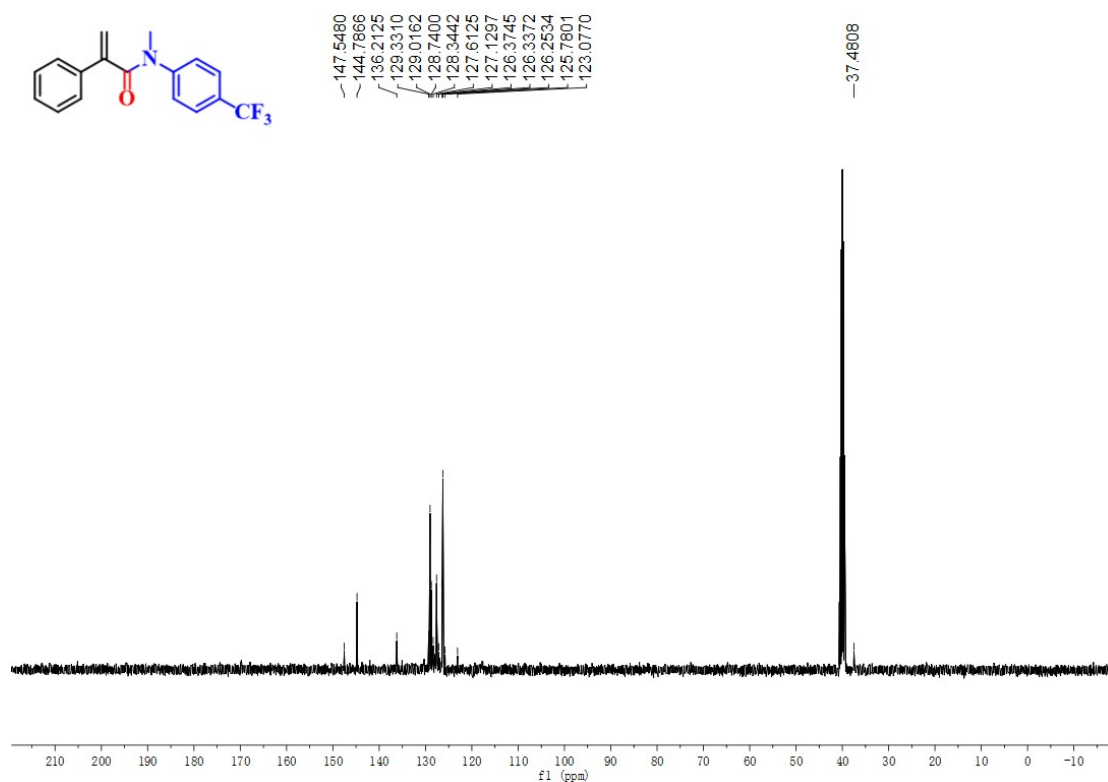
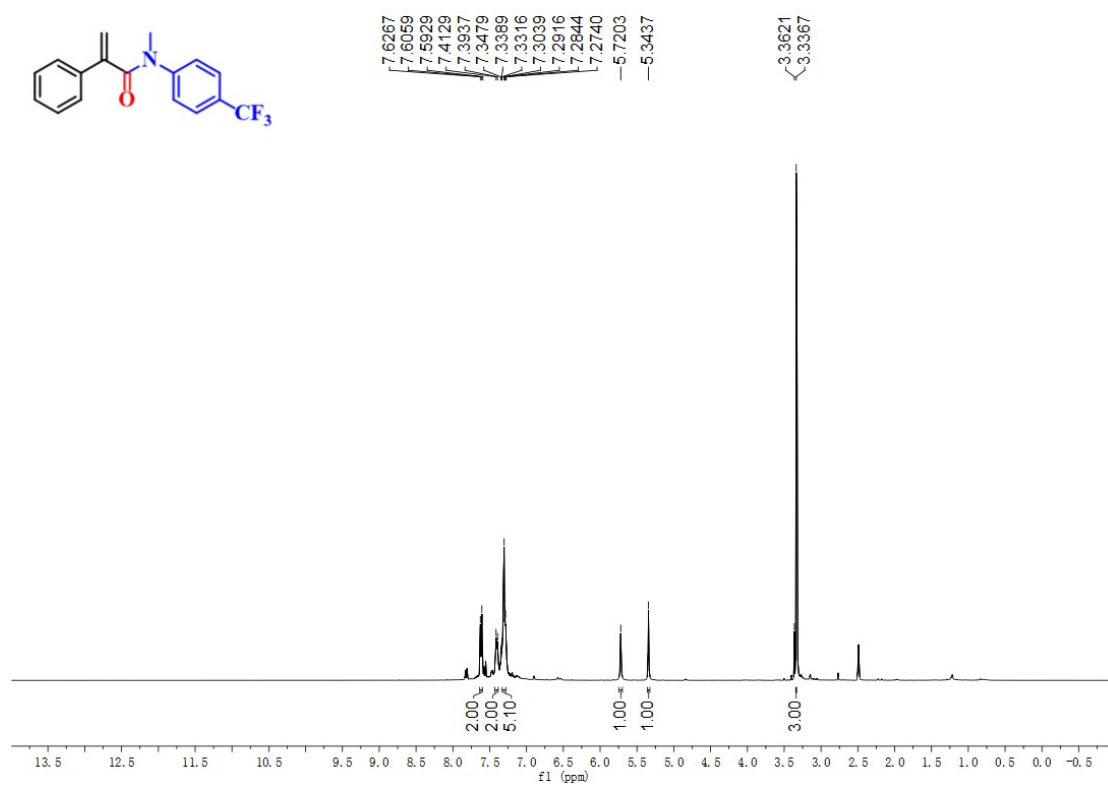
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 3ah

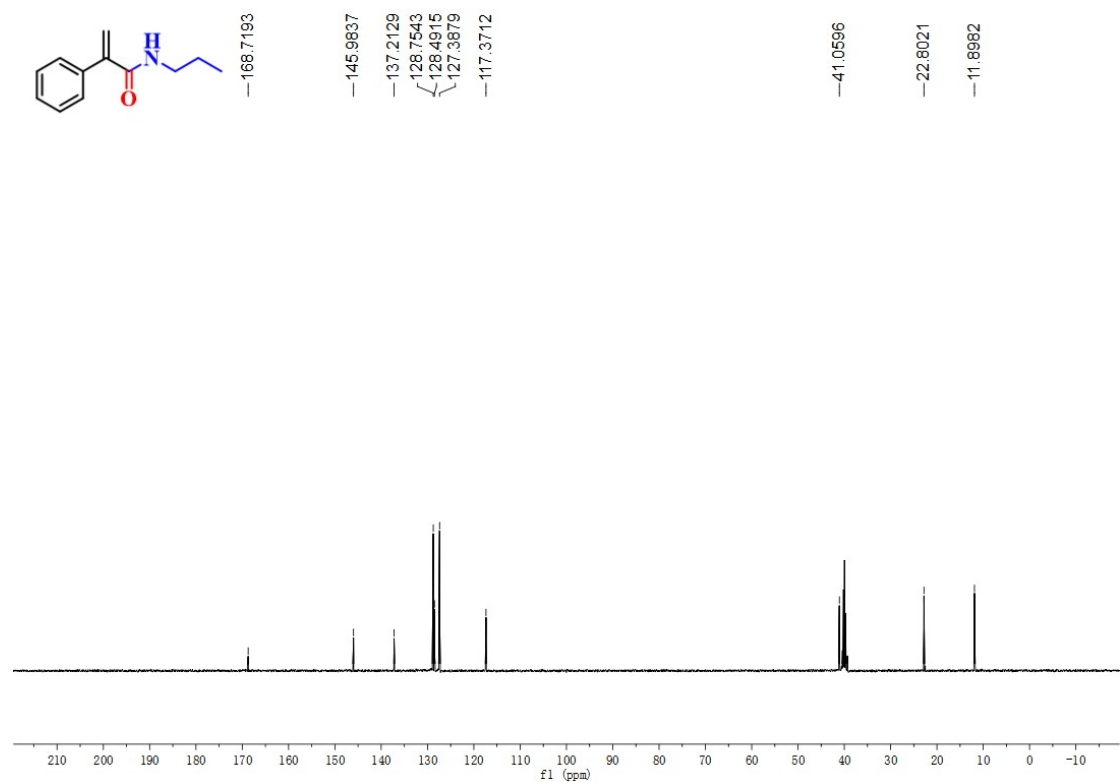
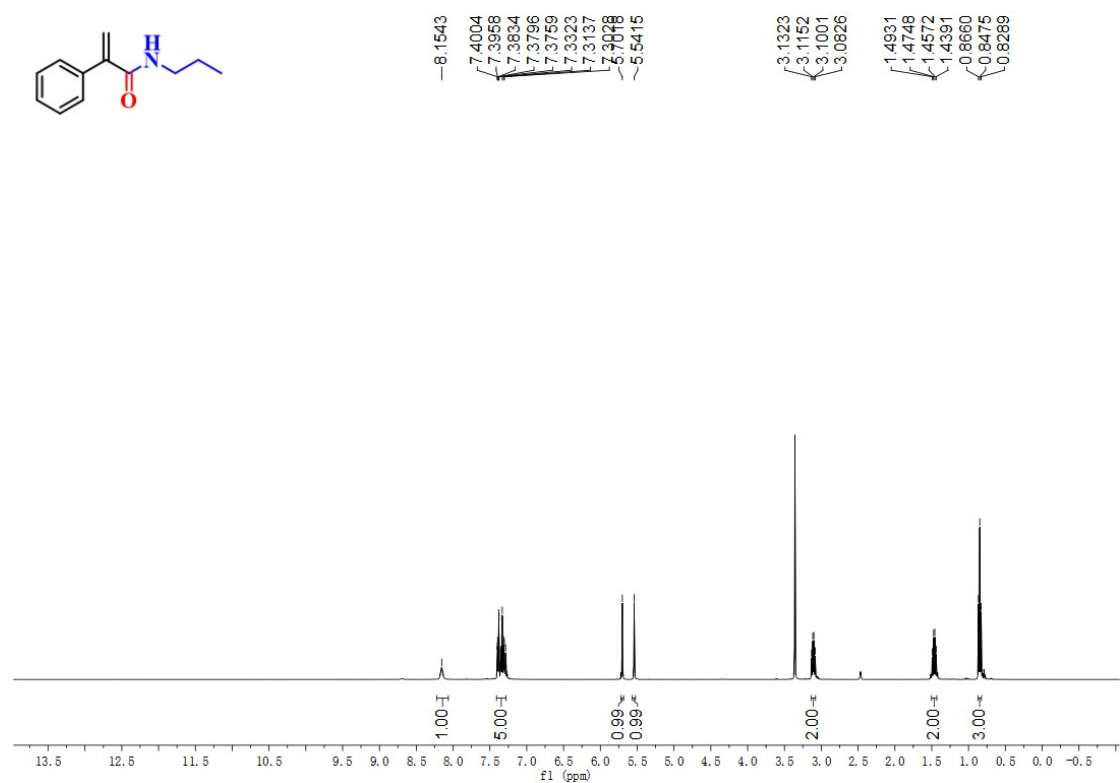


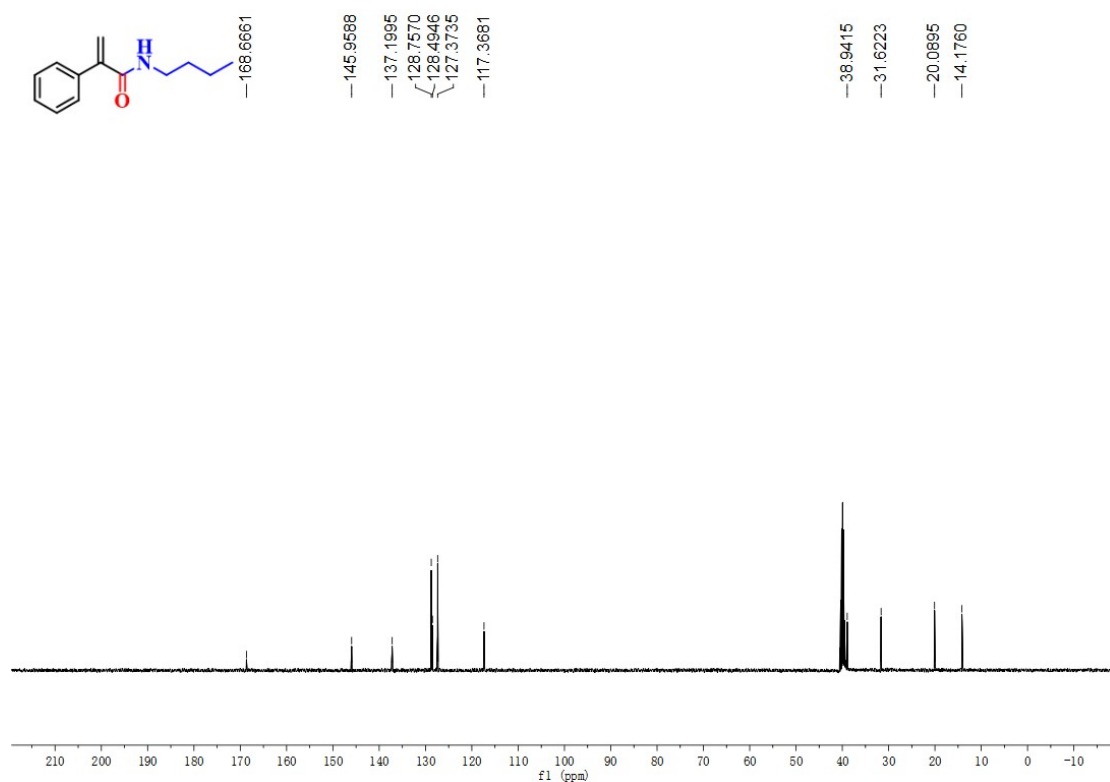
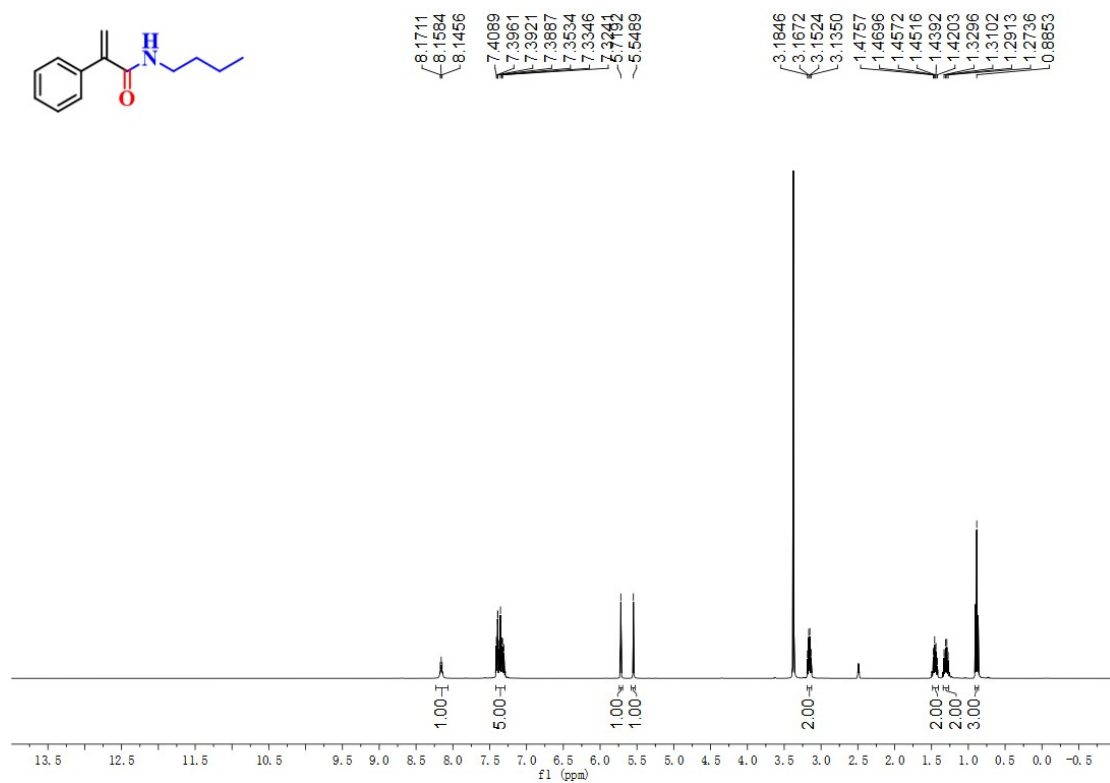
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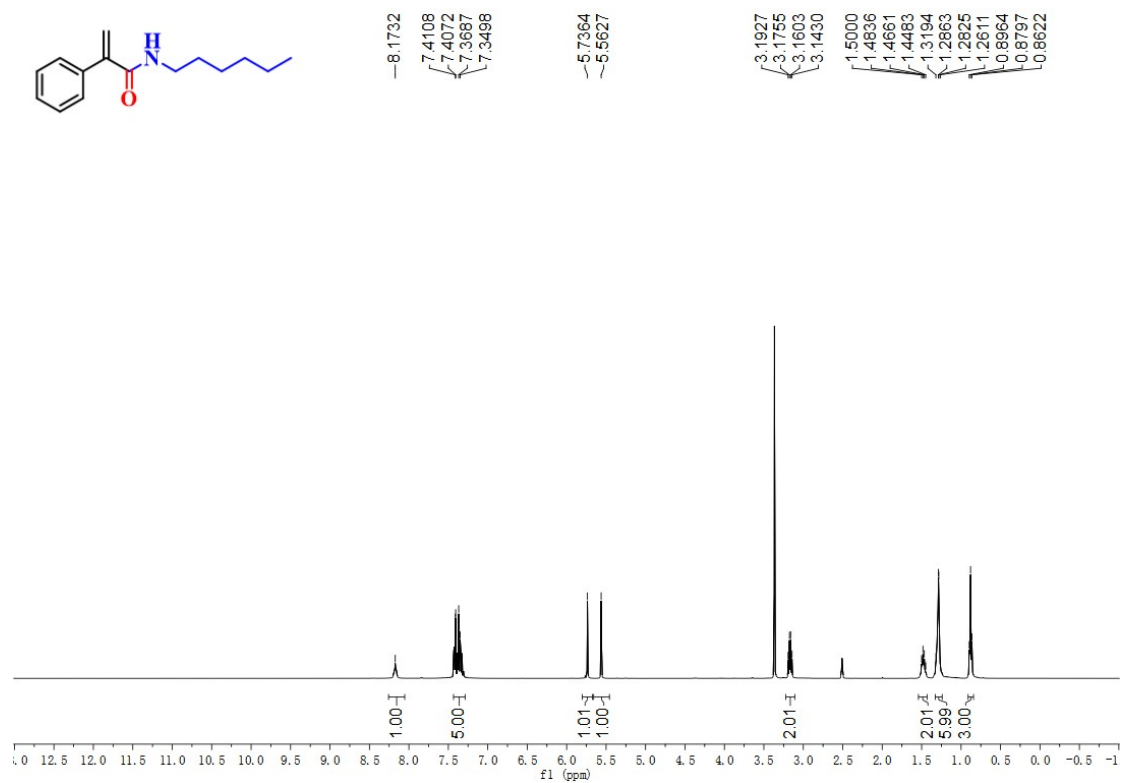




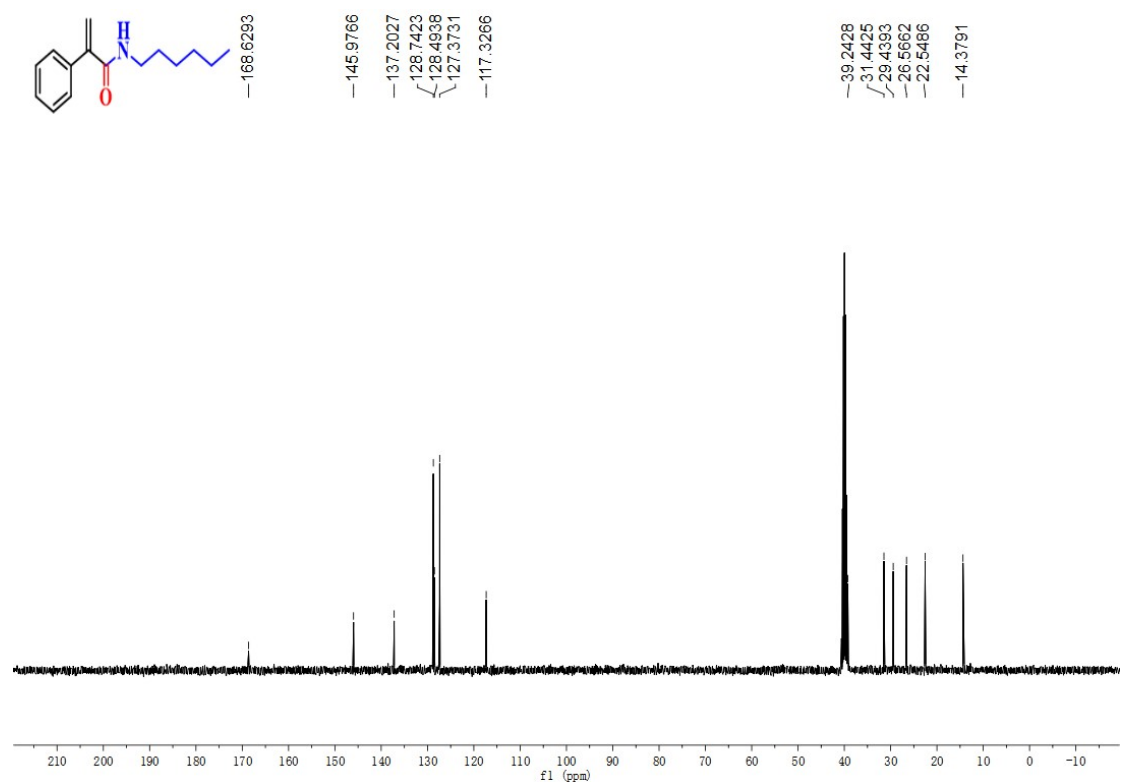




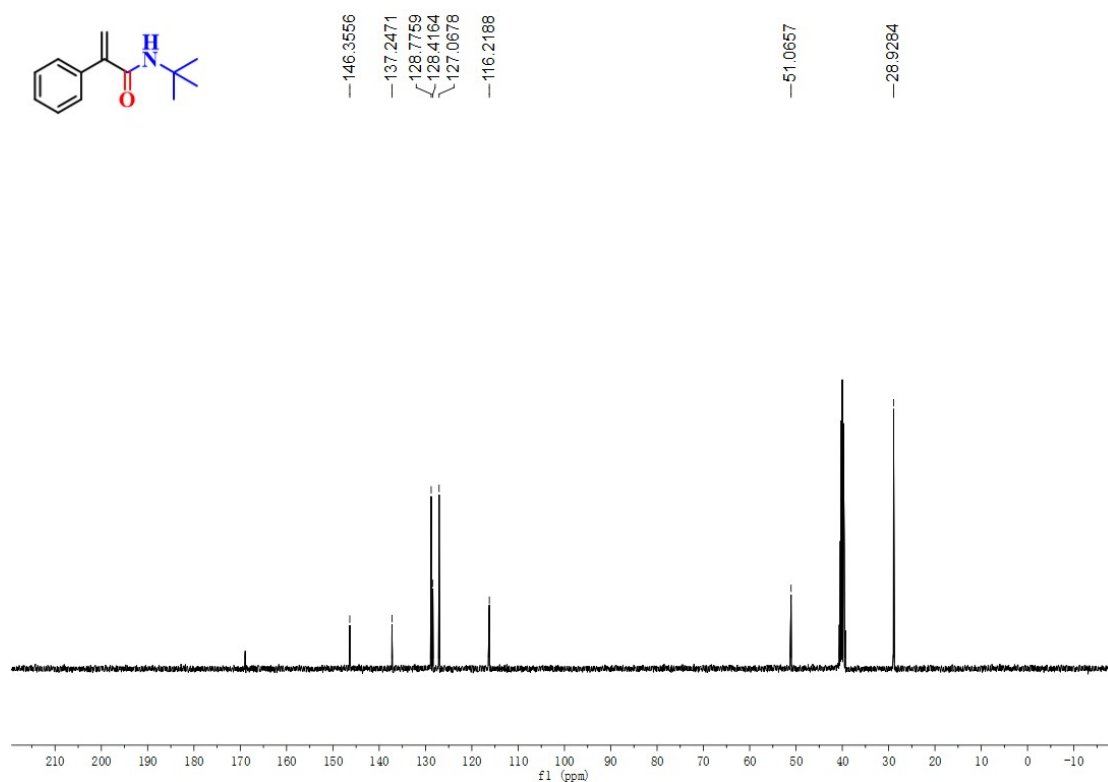
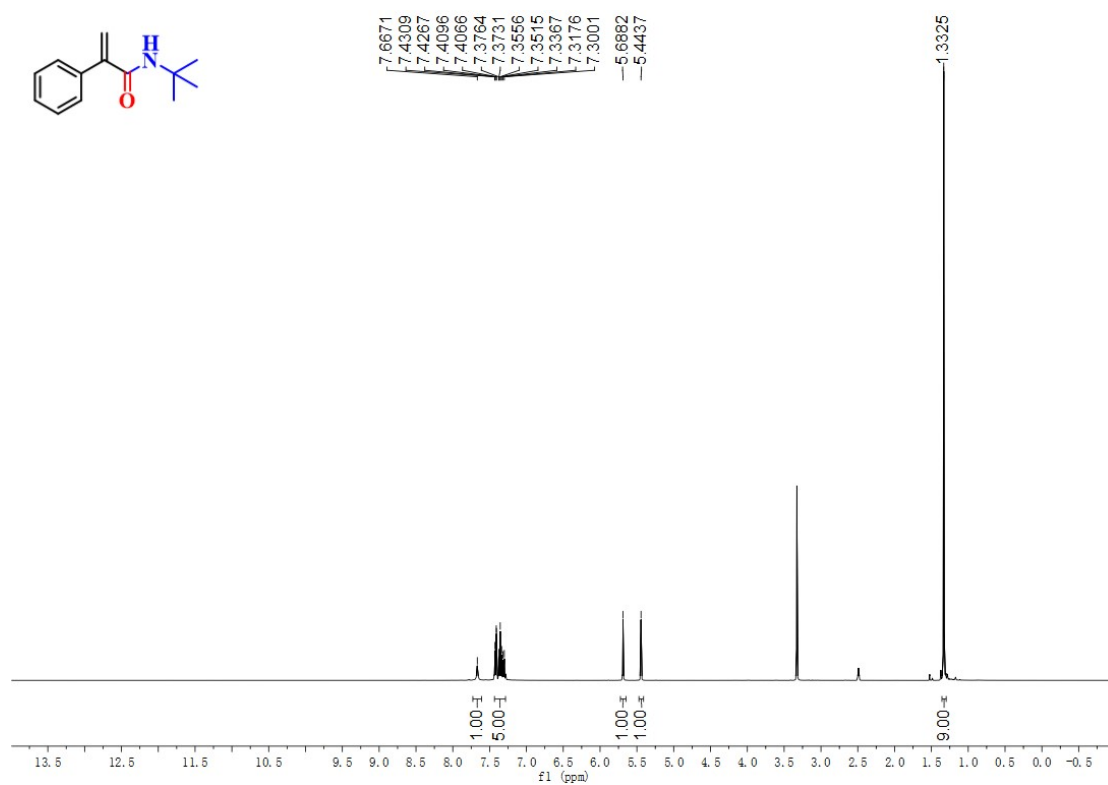


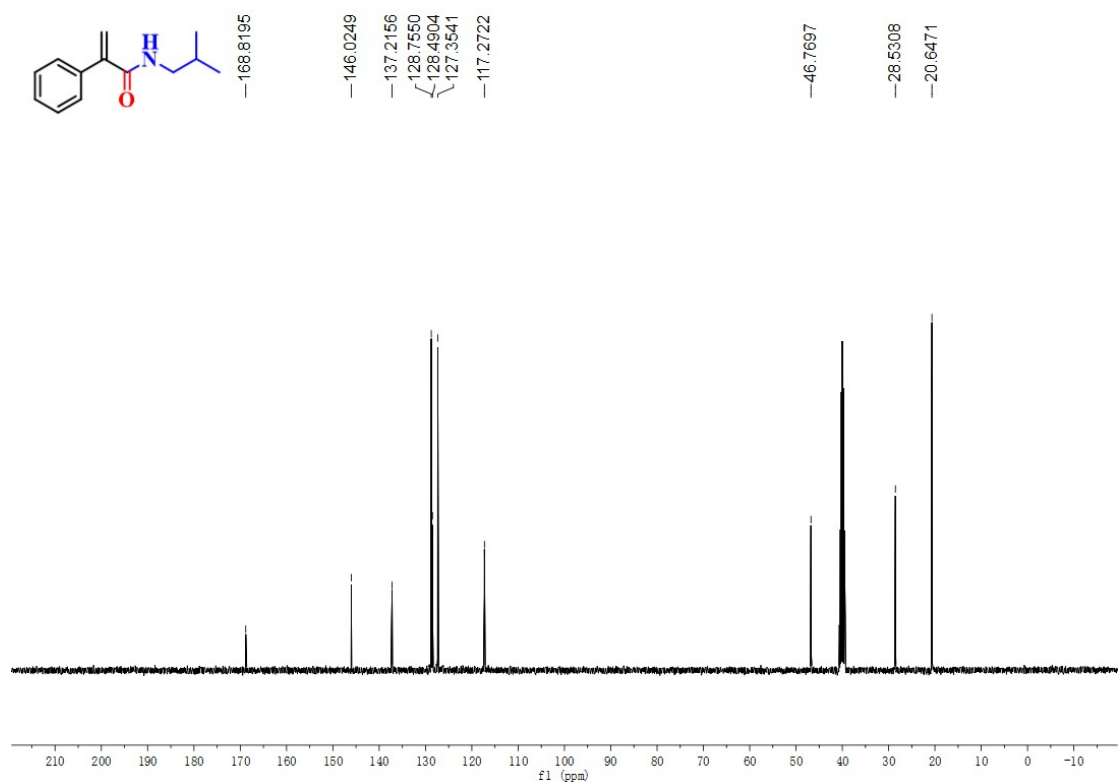
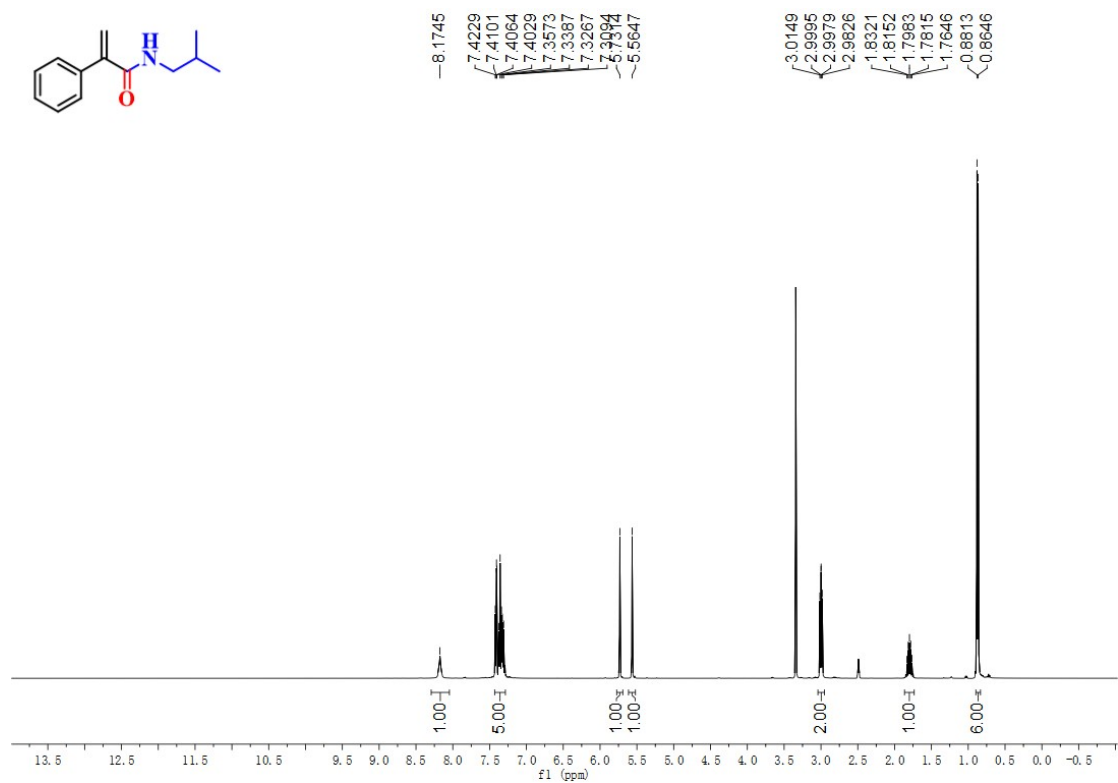


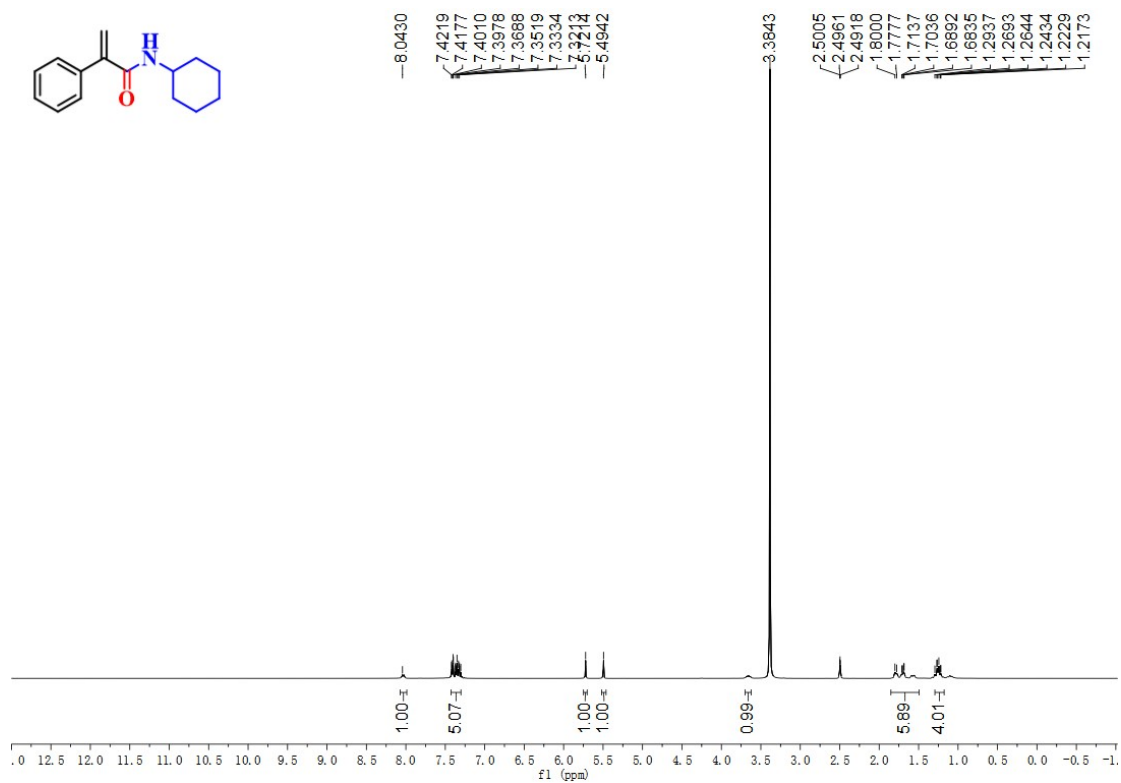
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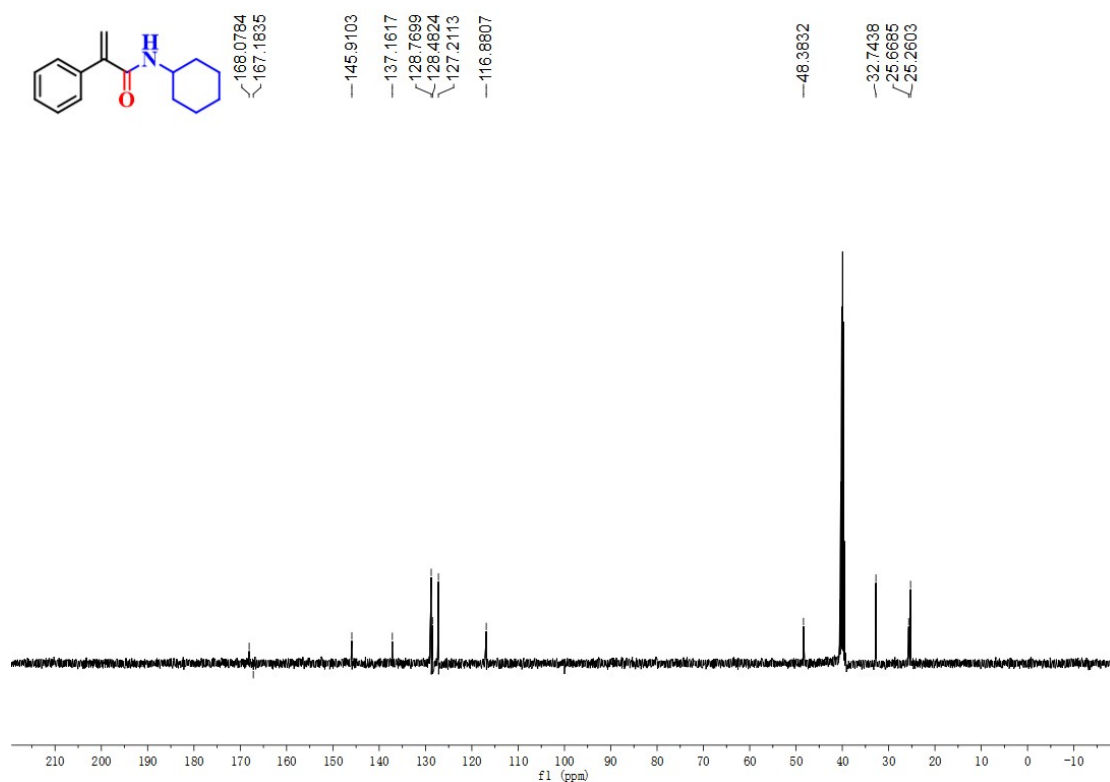
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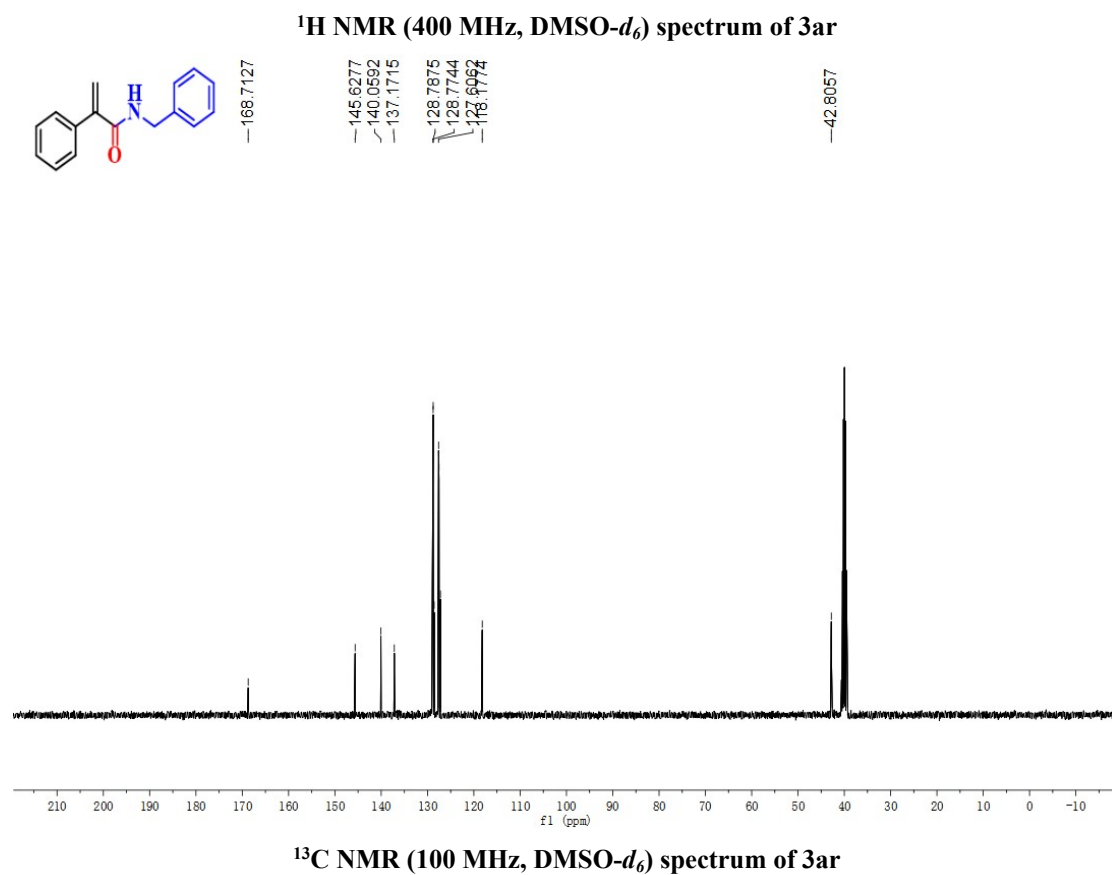
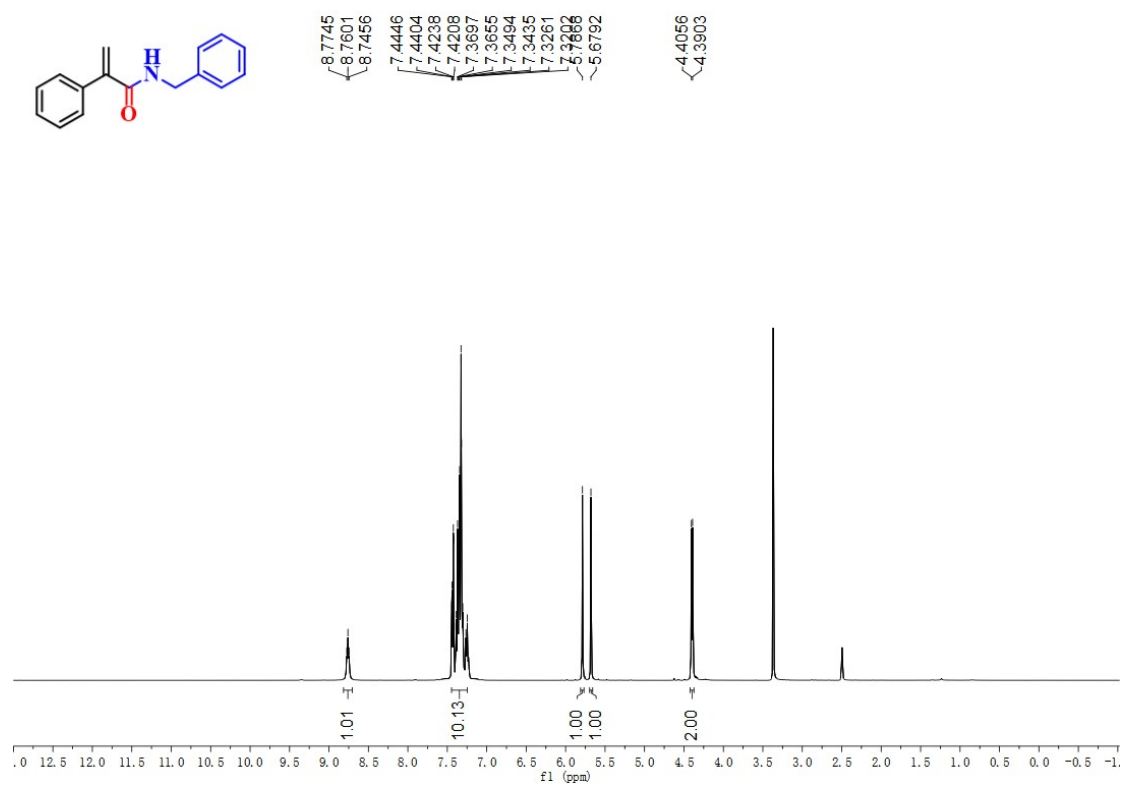


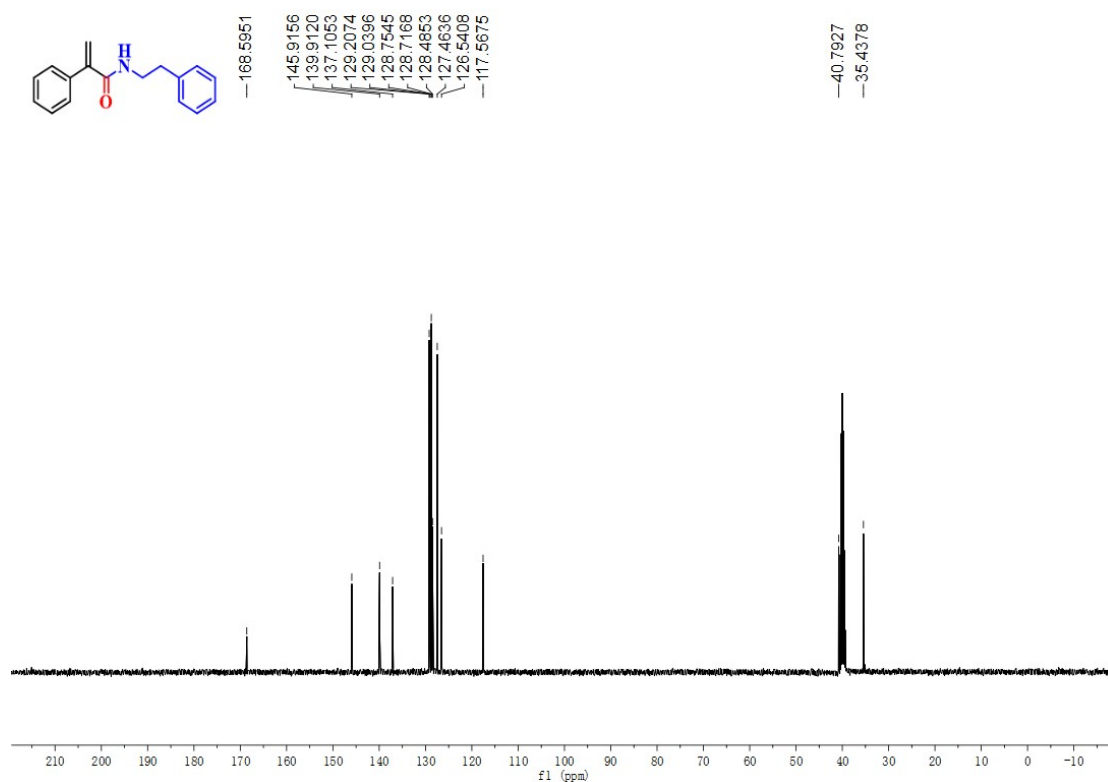
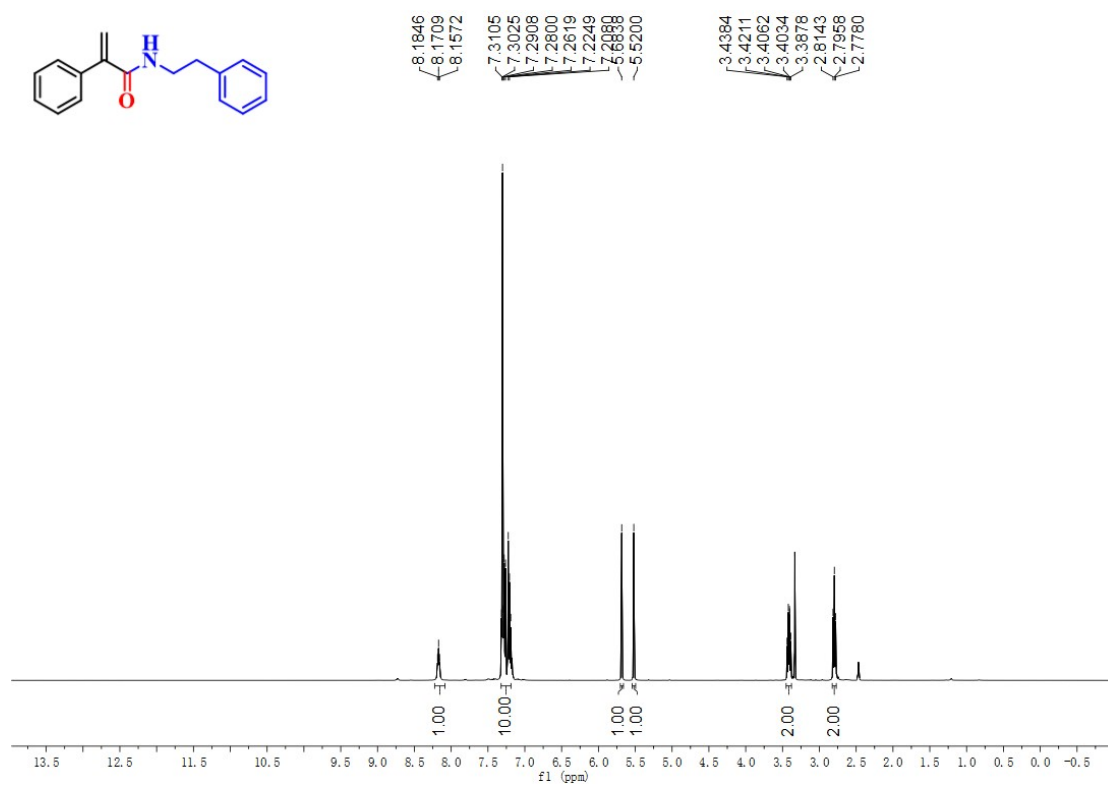


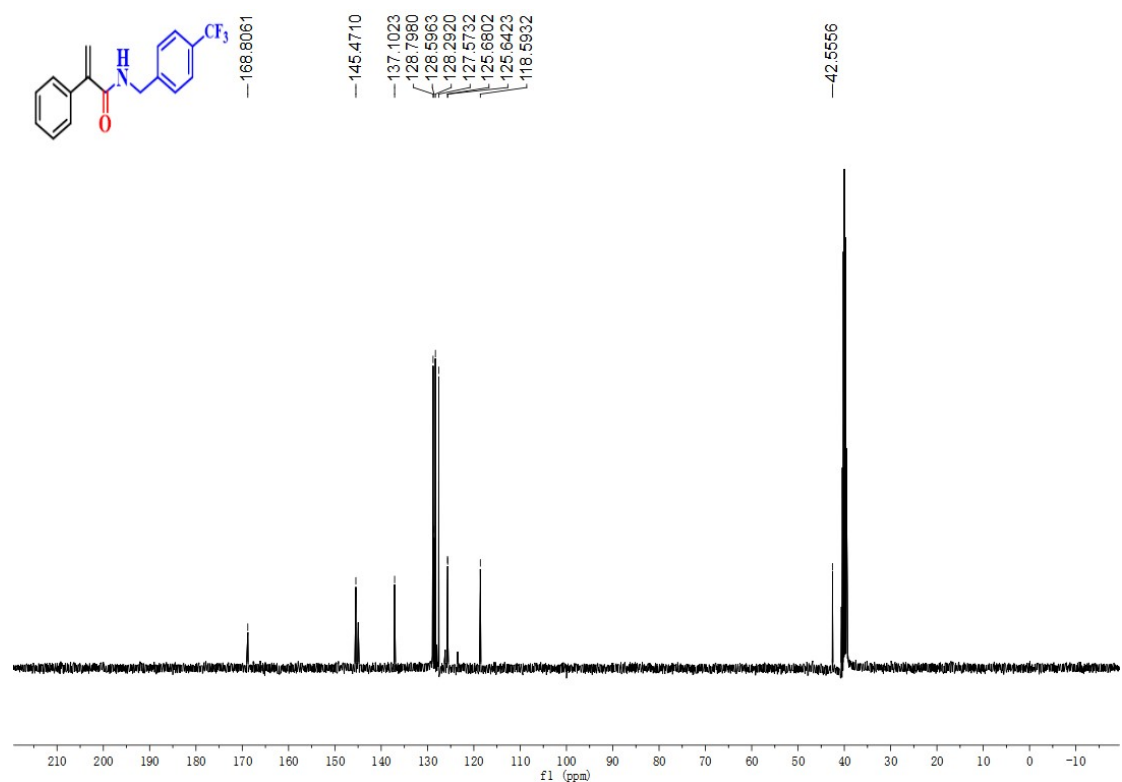
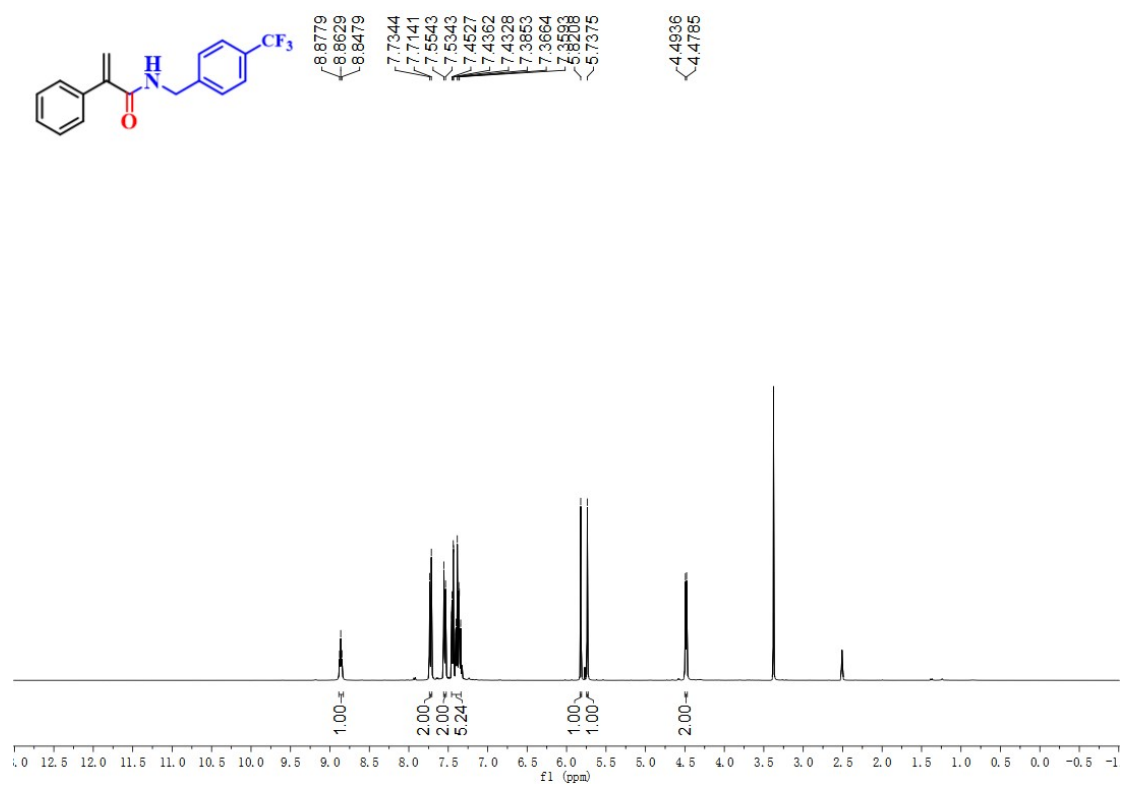
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 3aq

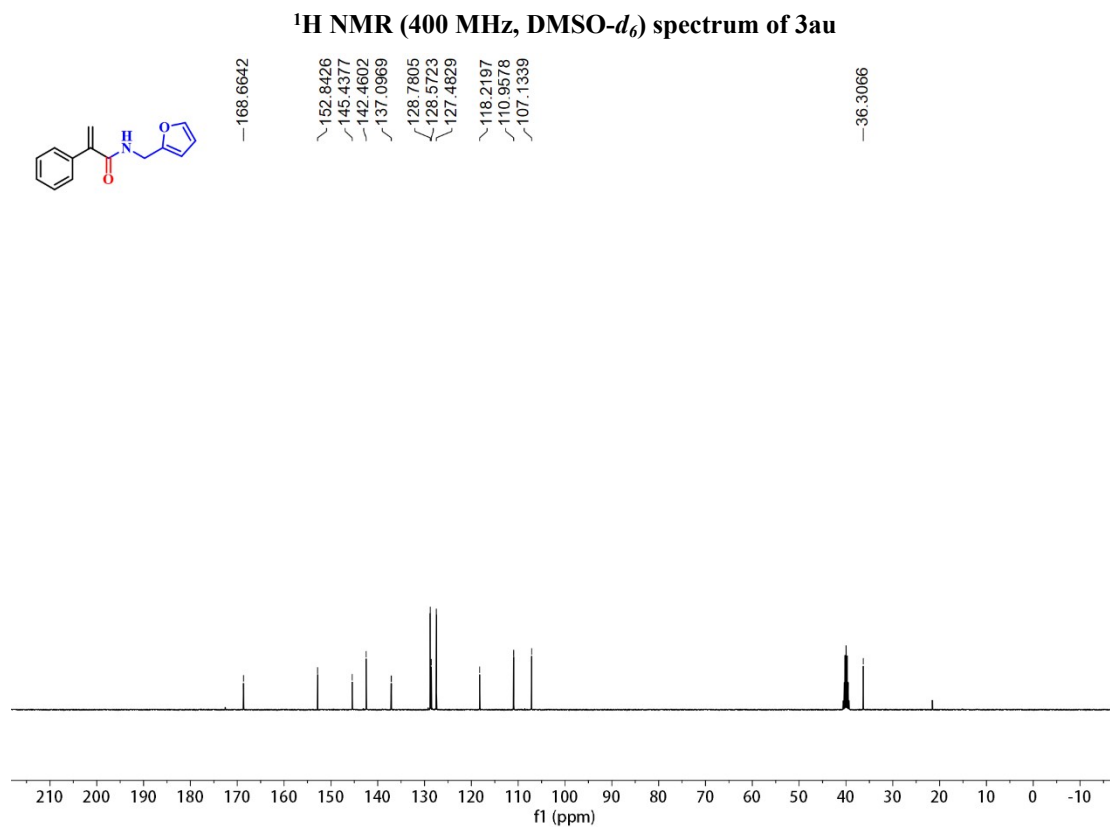
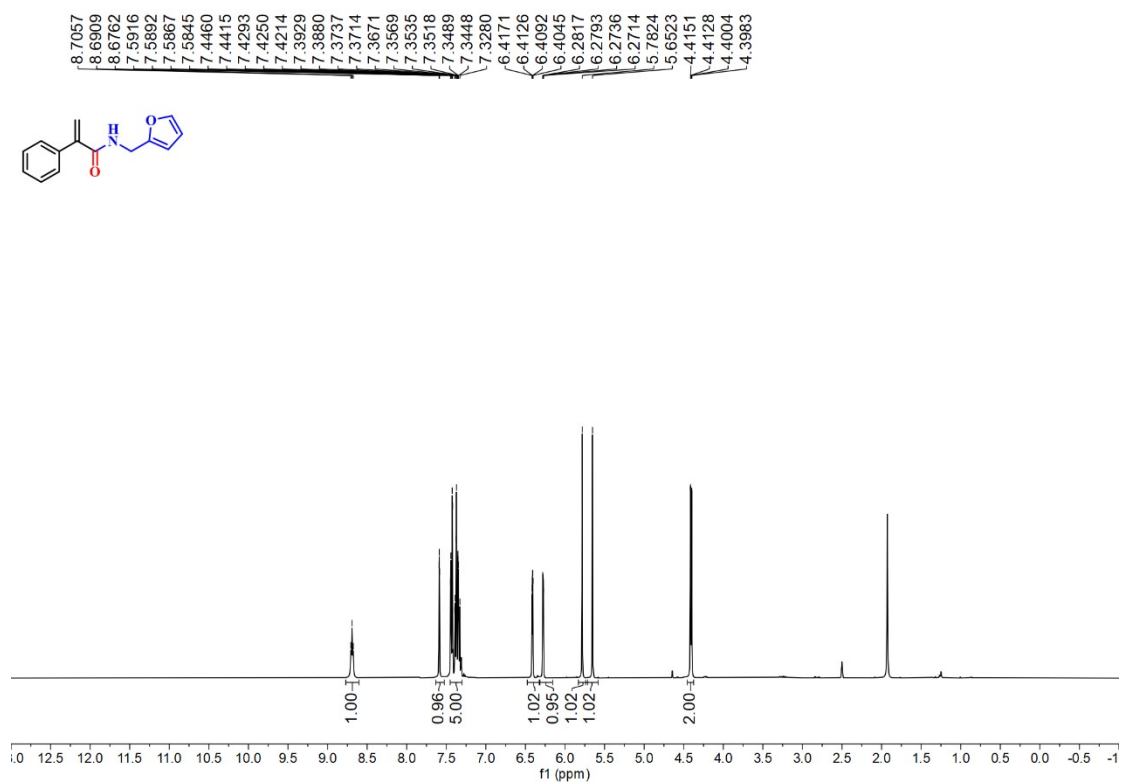


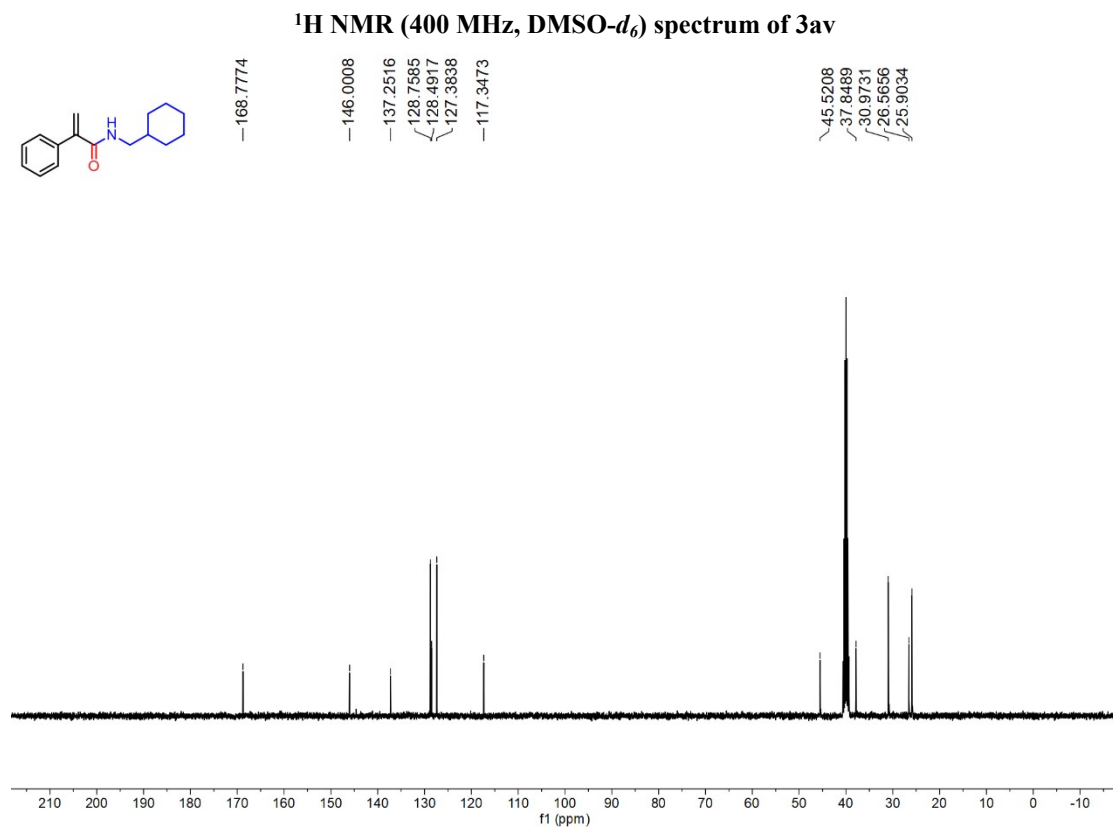
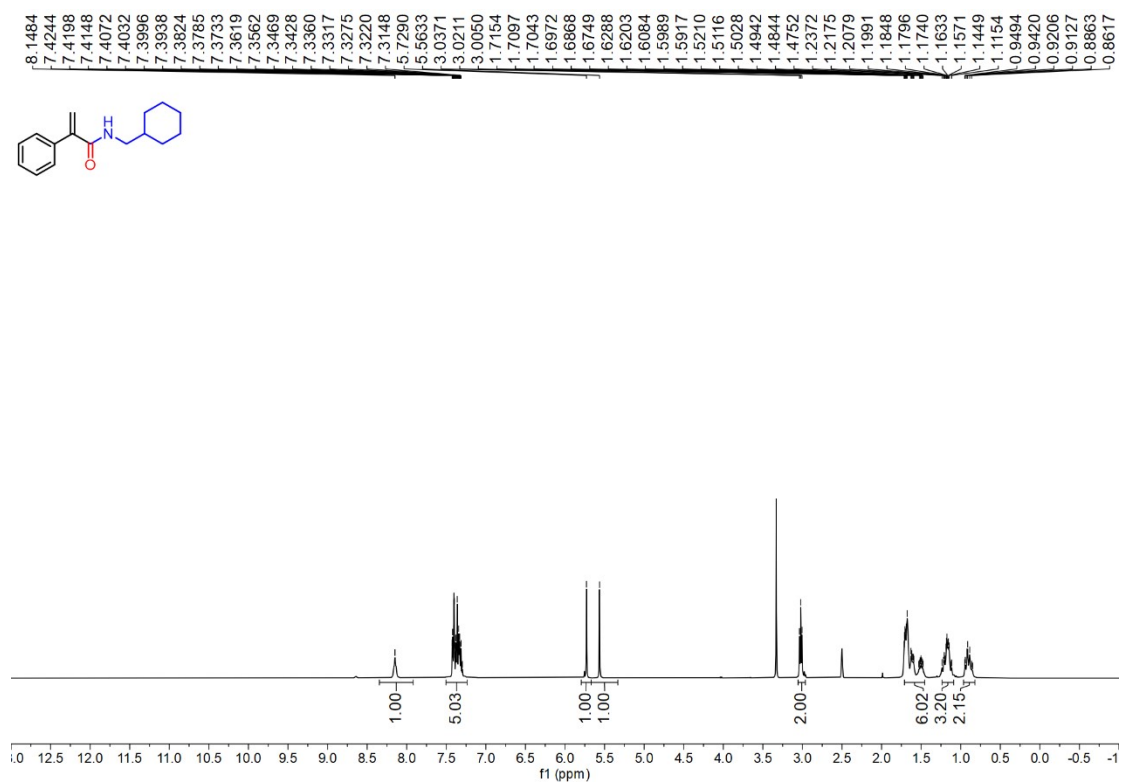
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 3aq

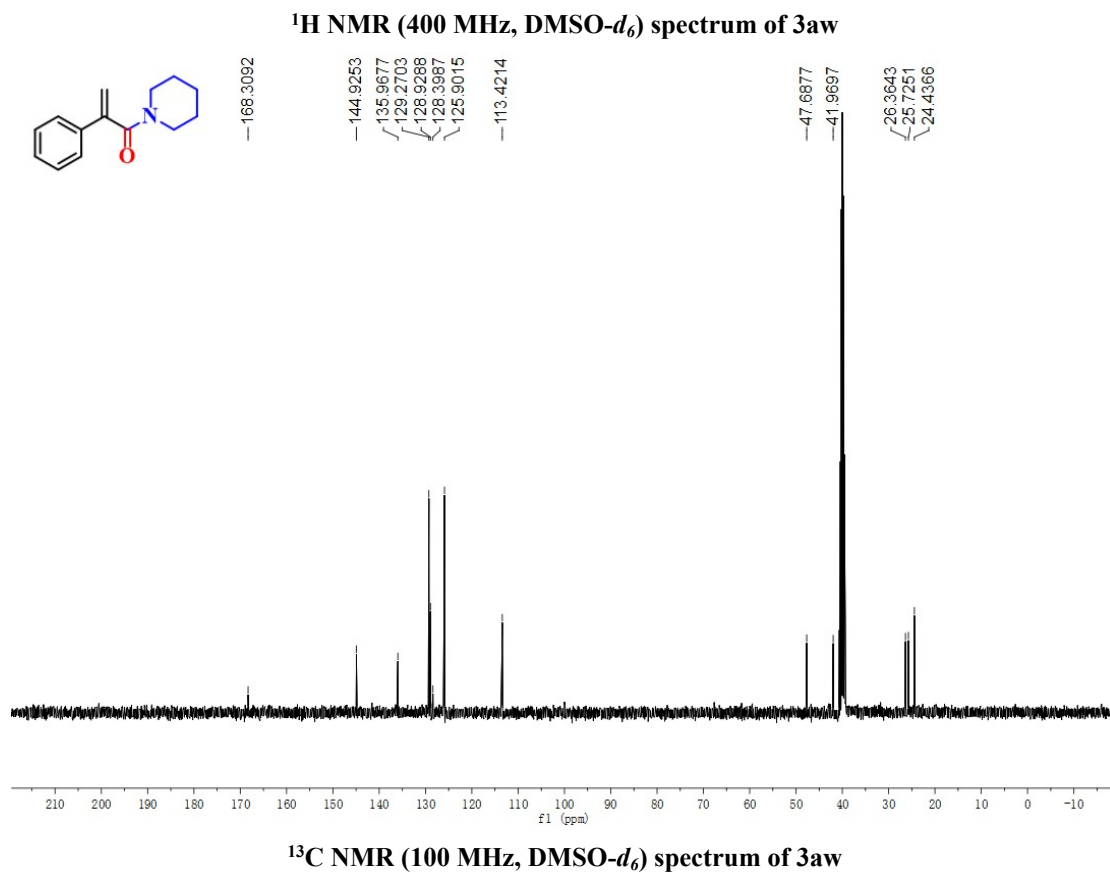
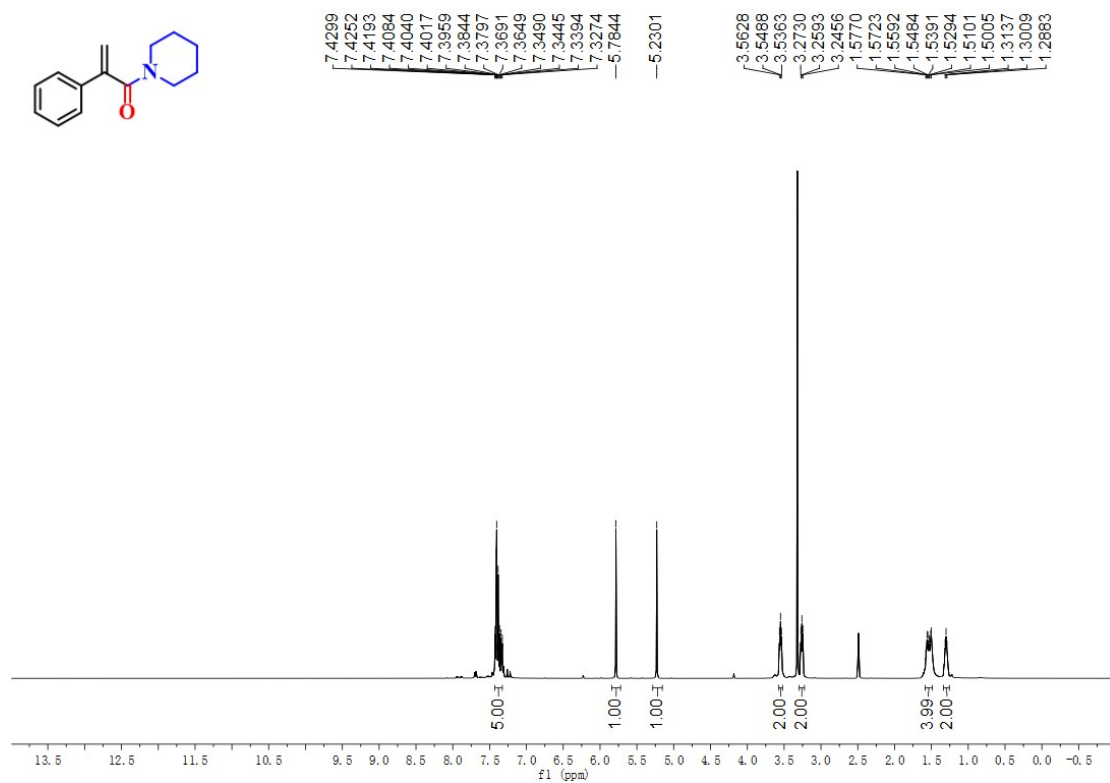


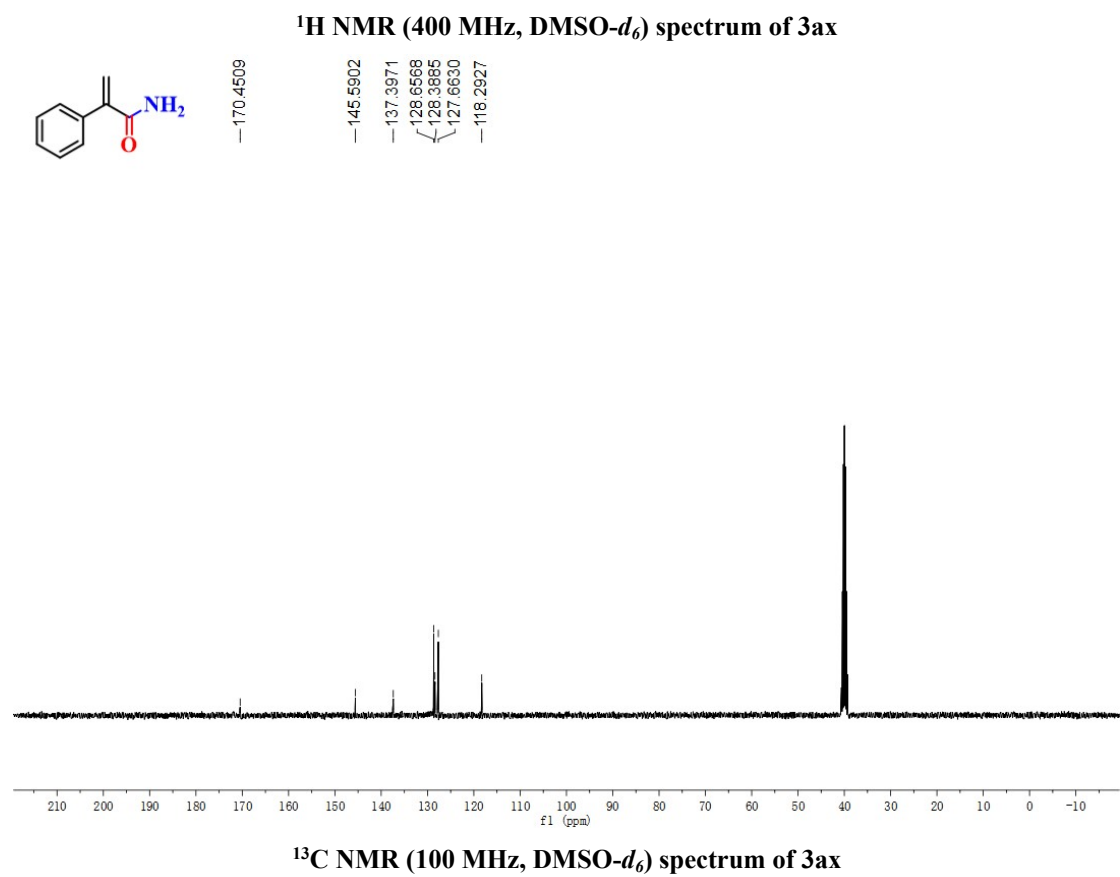
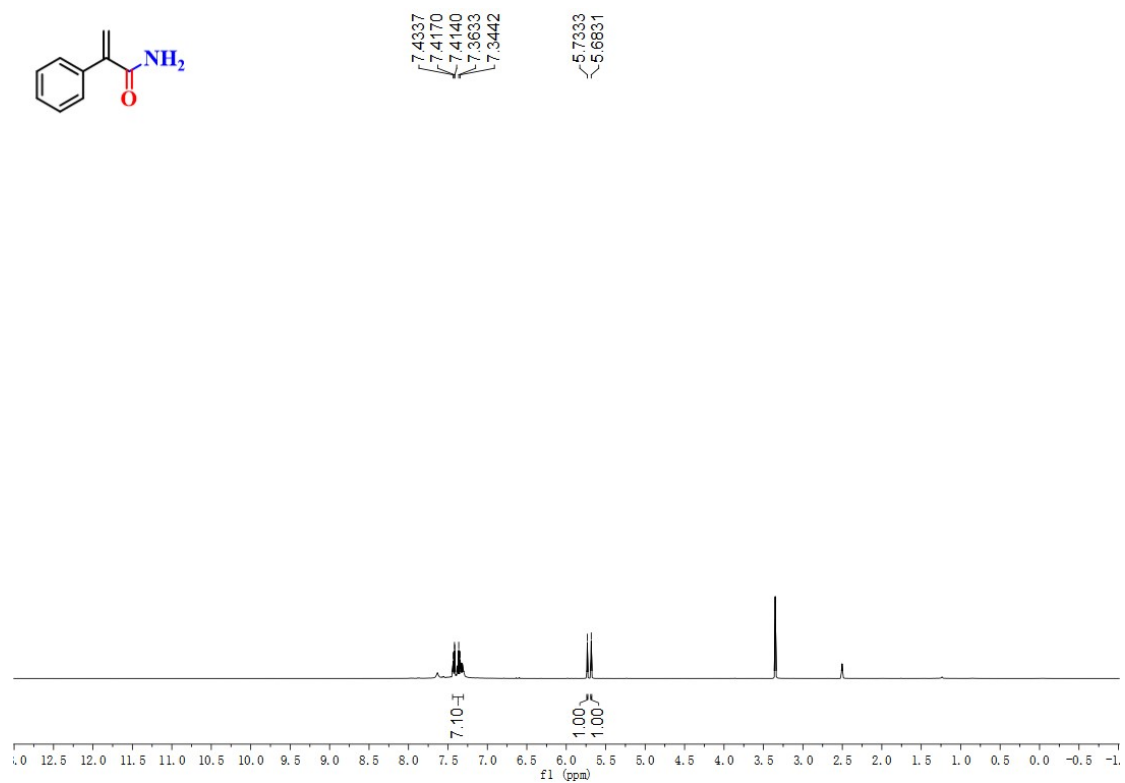


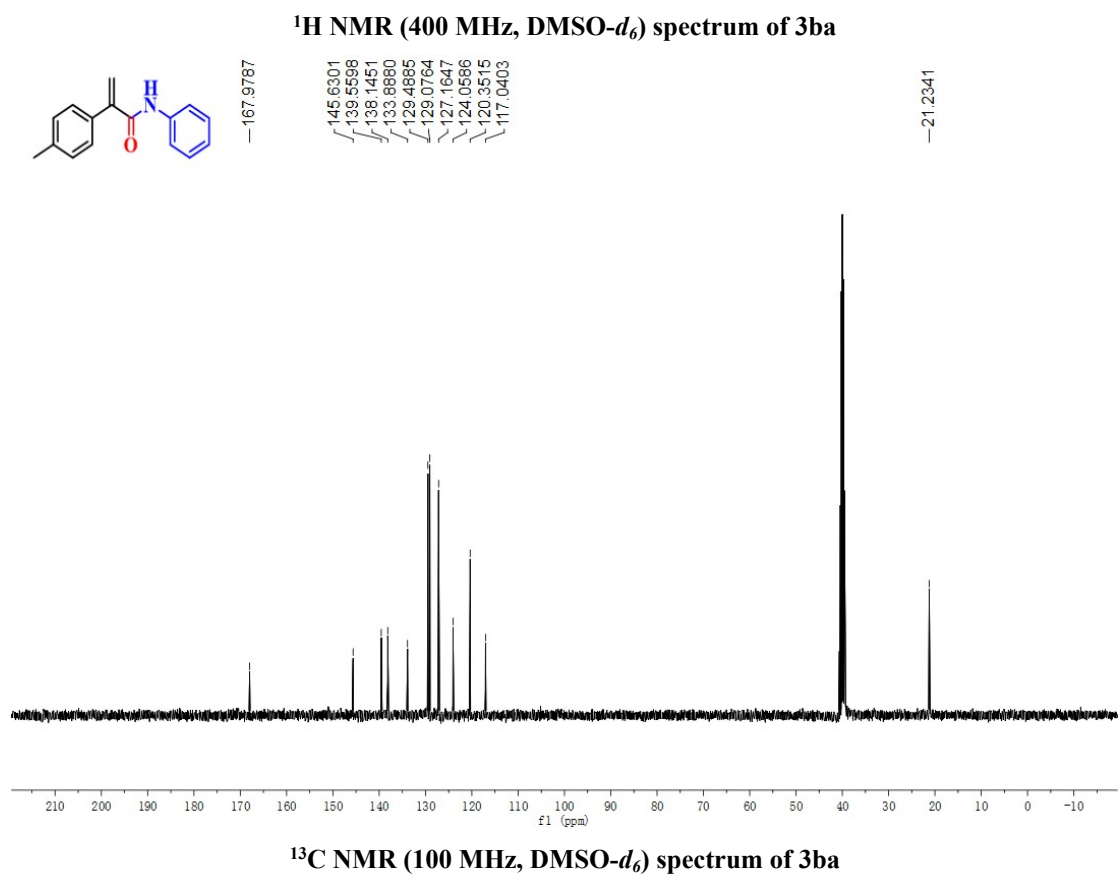
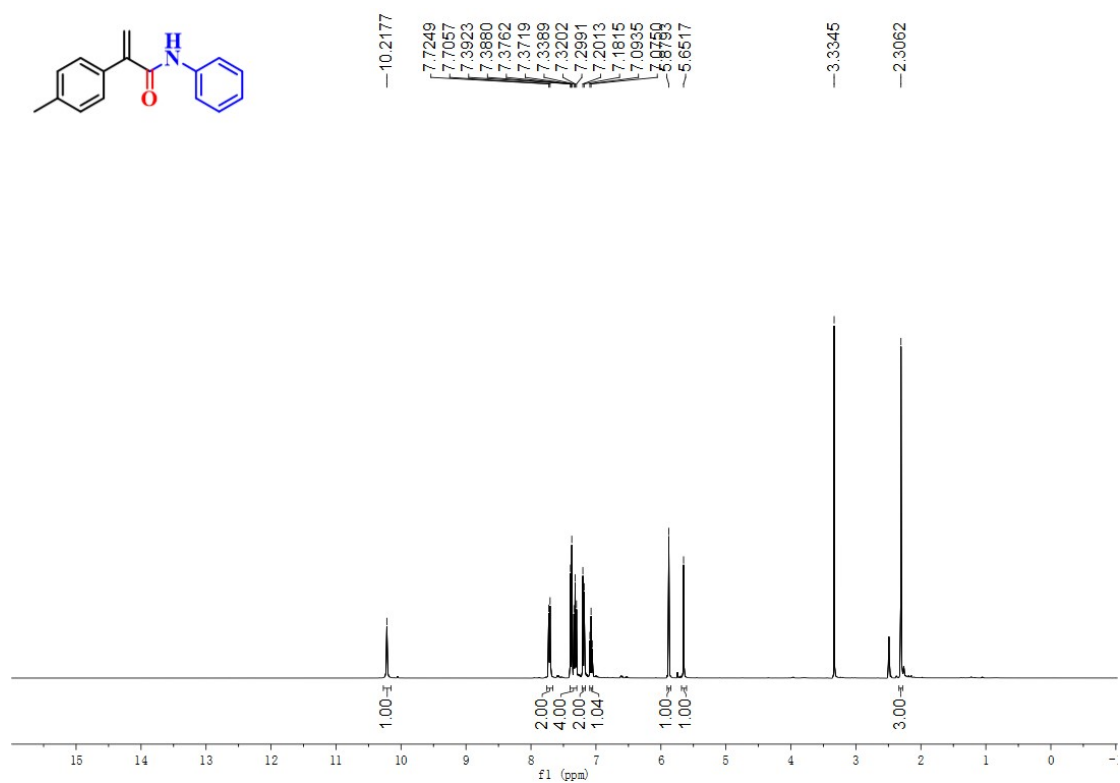


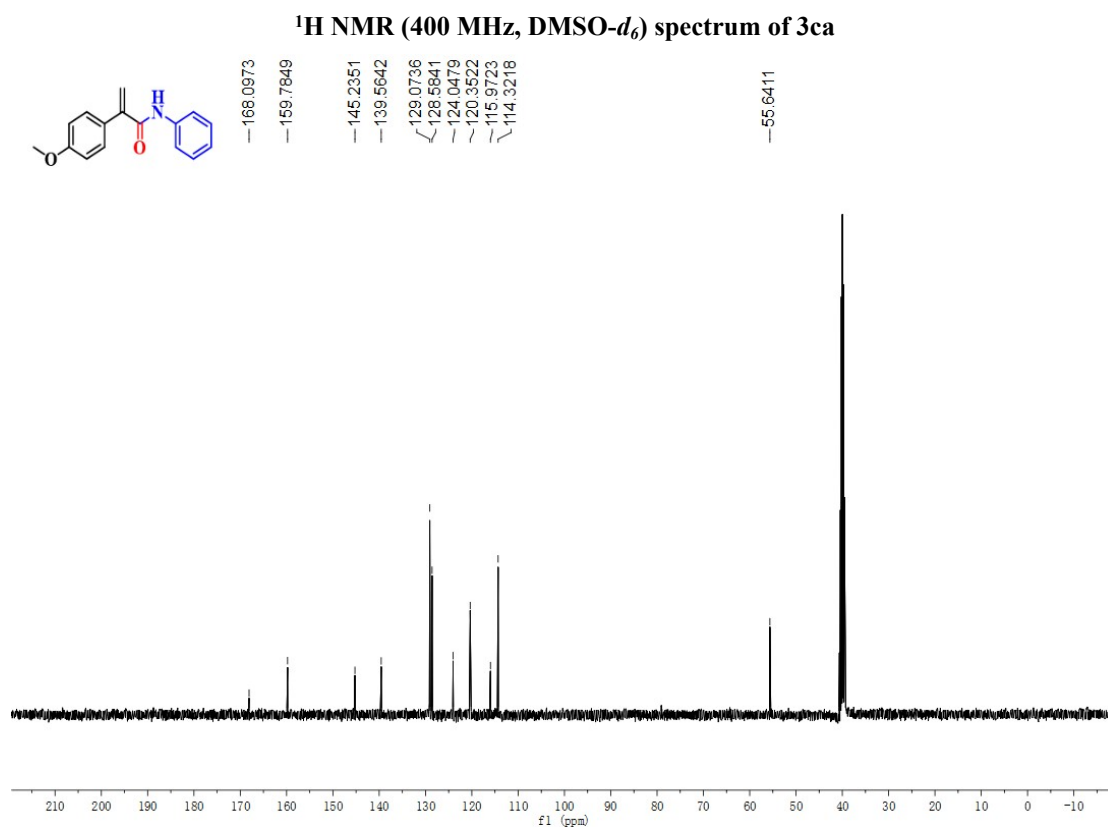
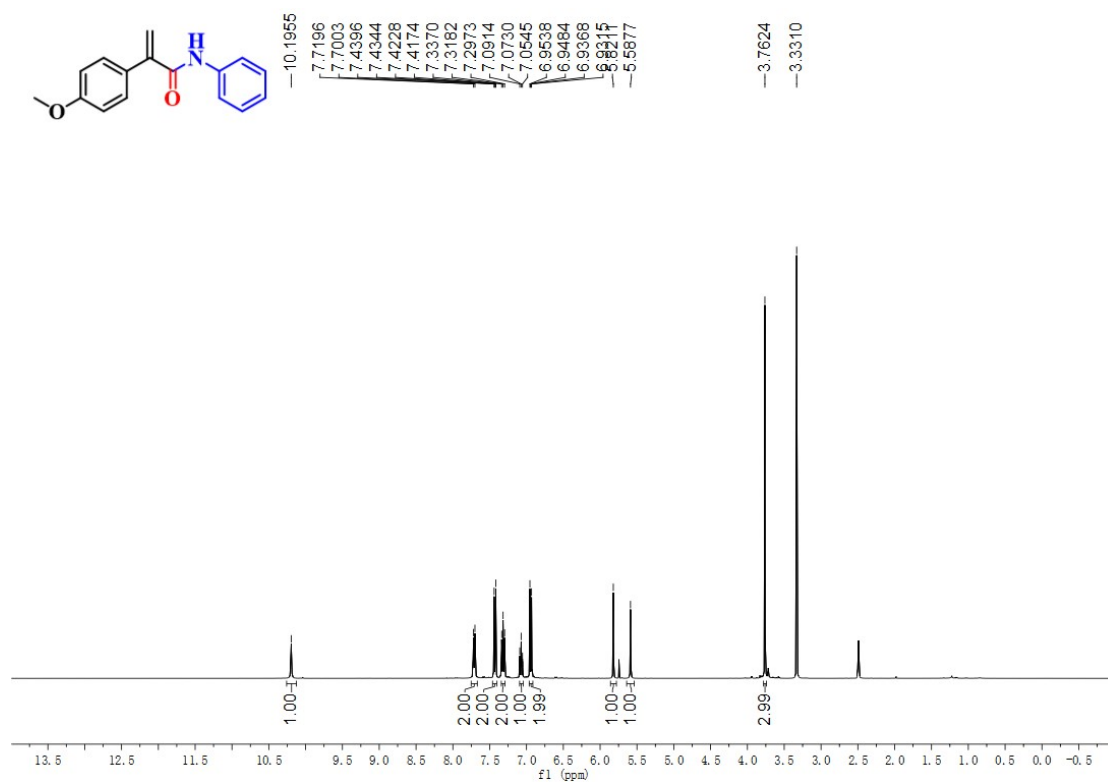


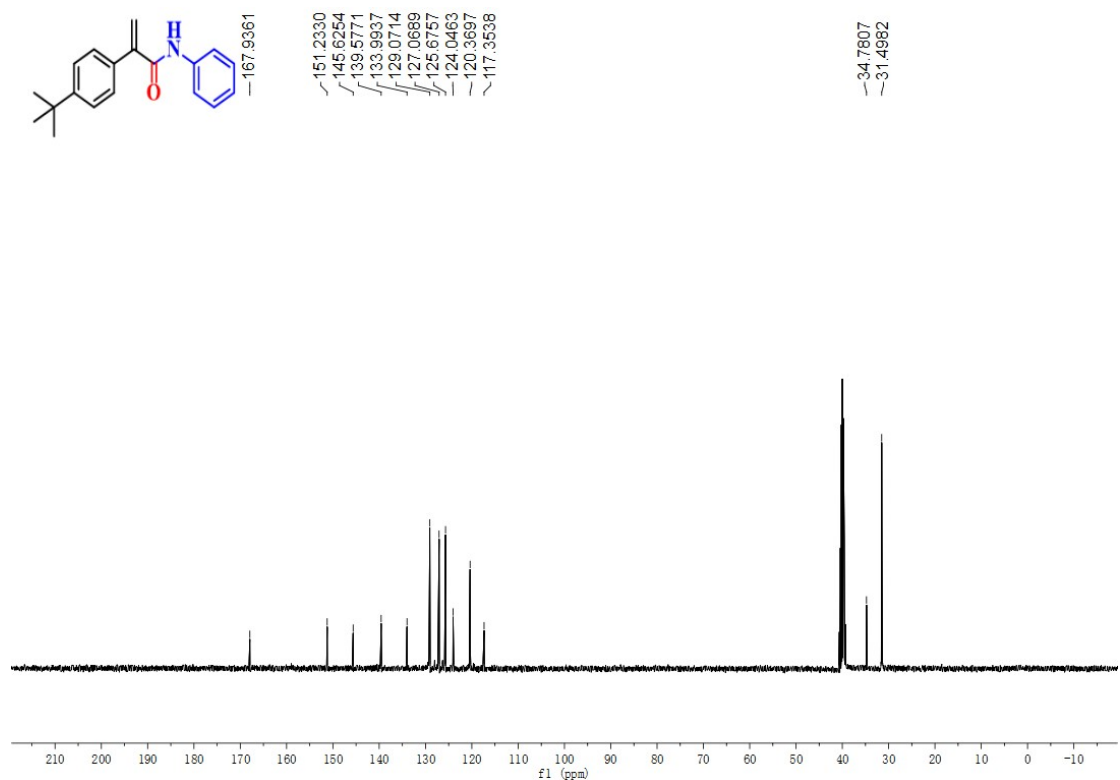
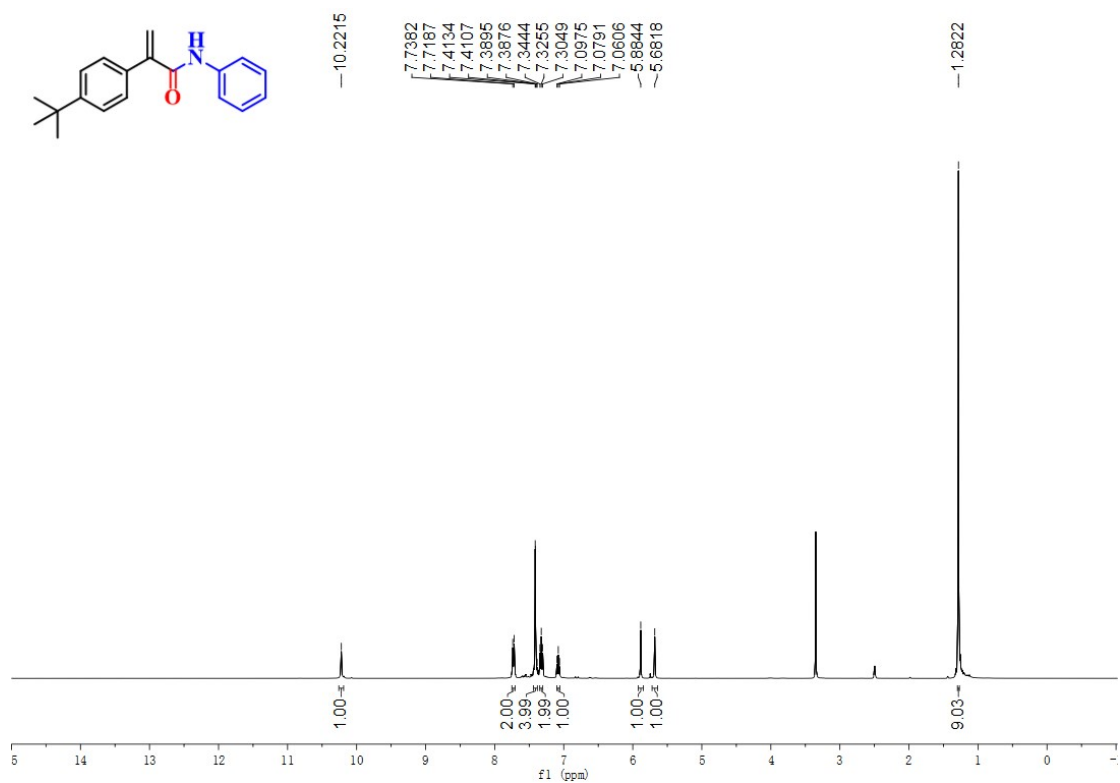


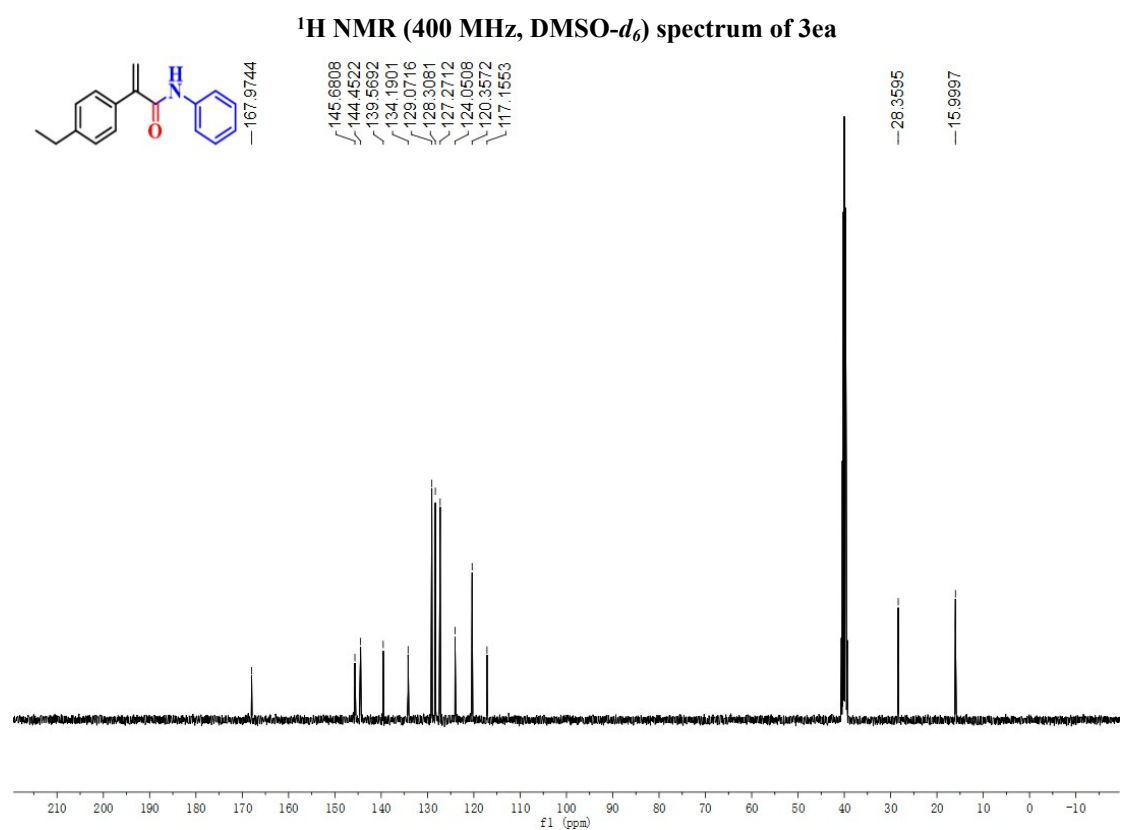
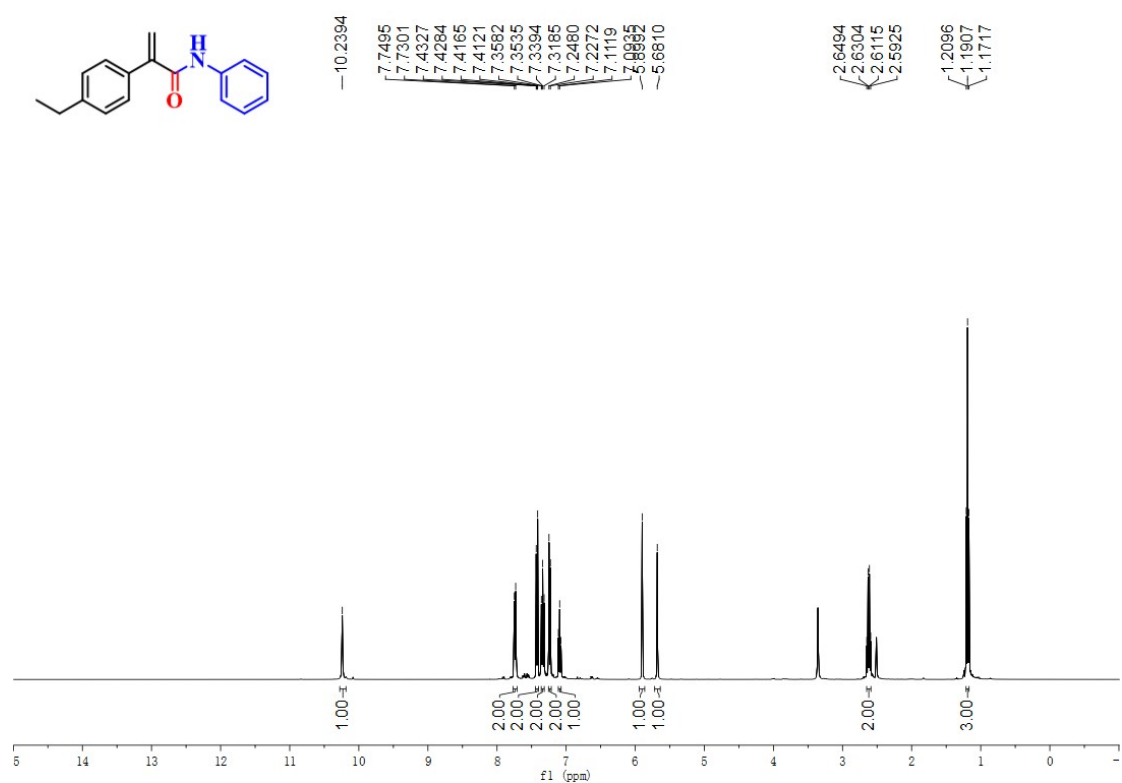


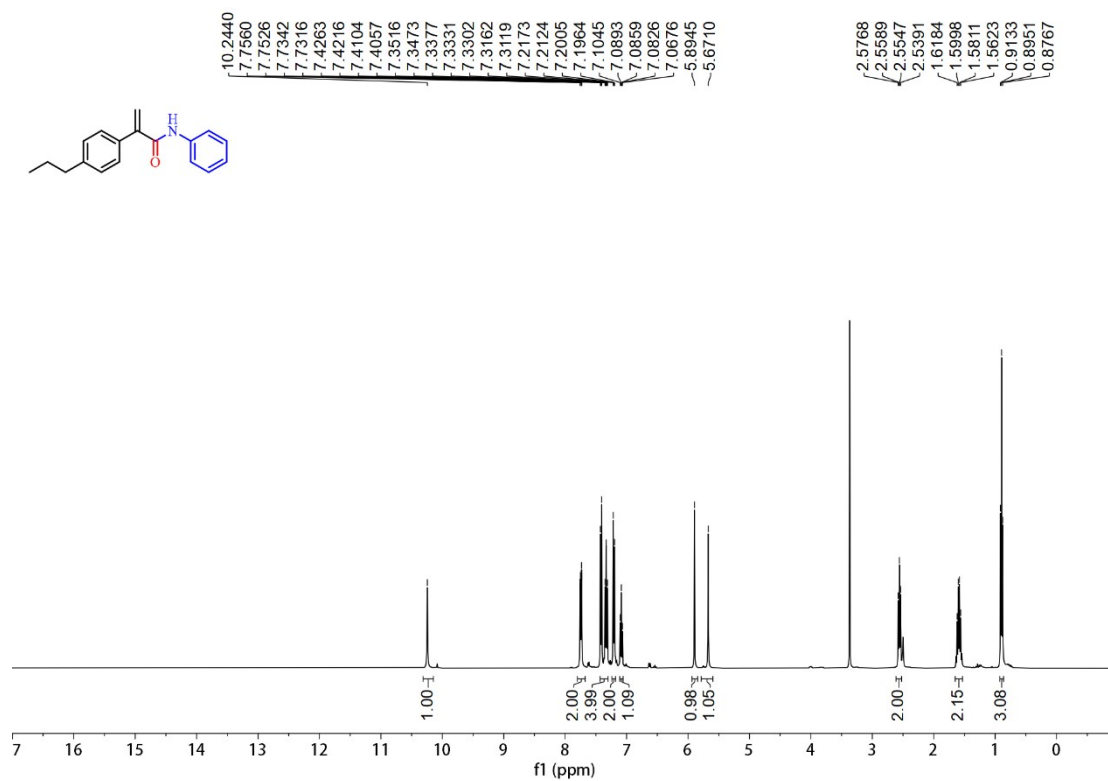




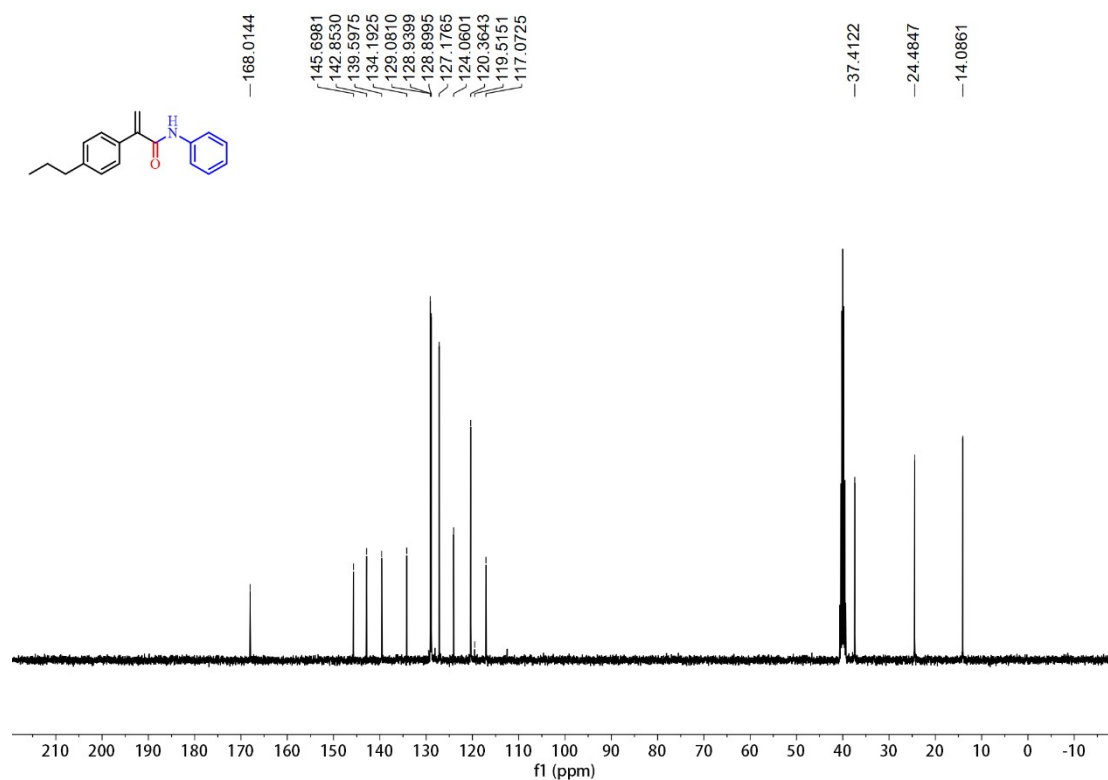




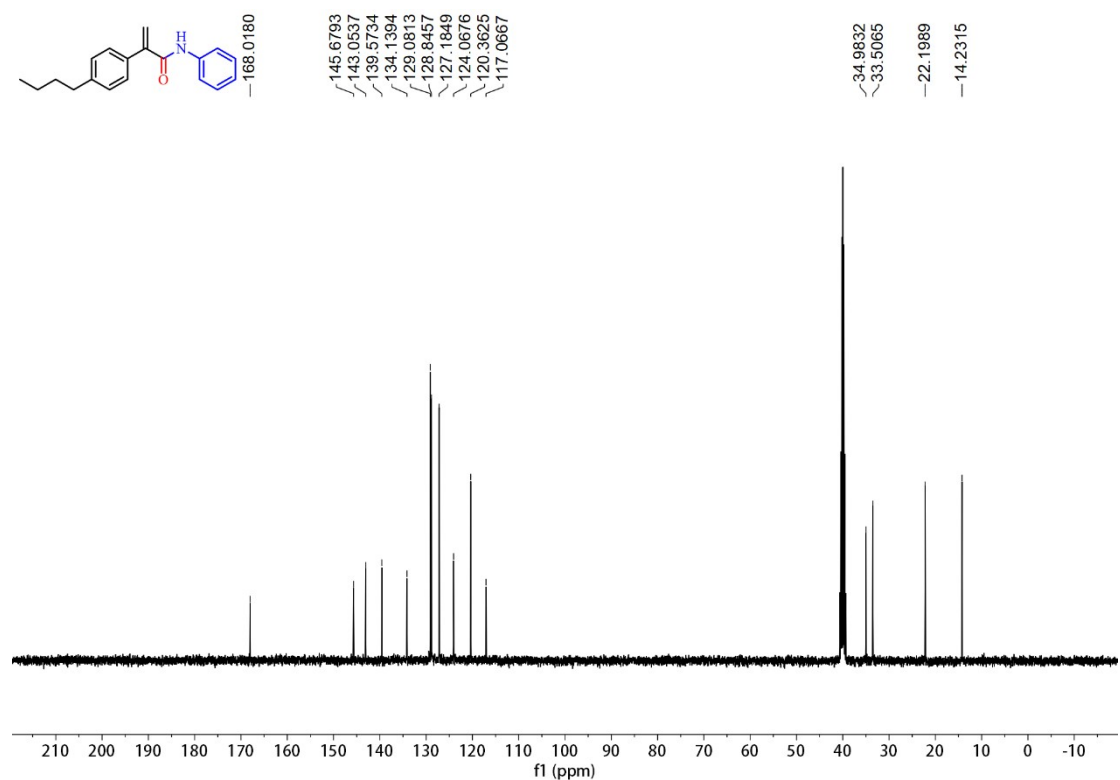
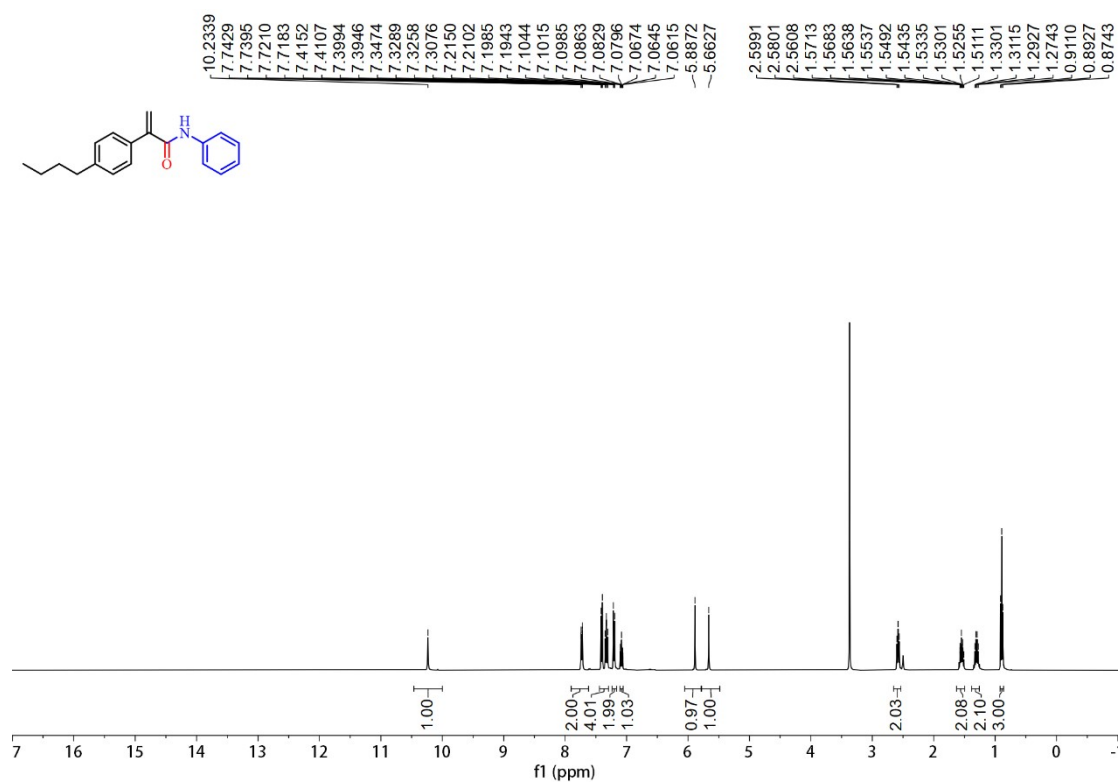


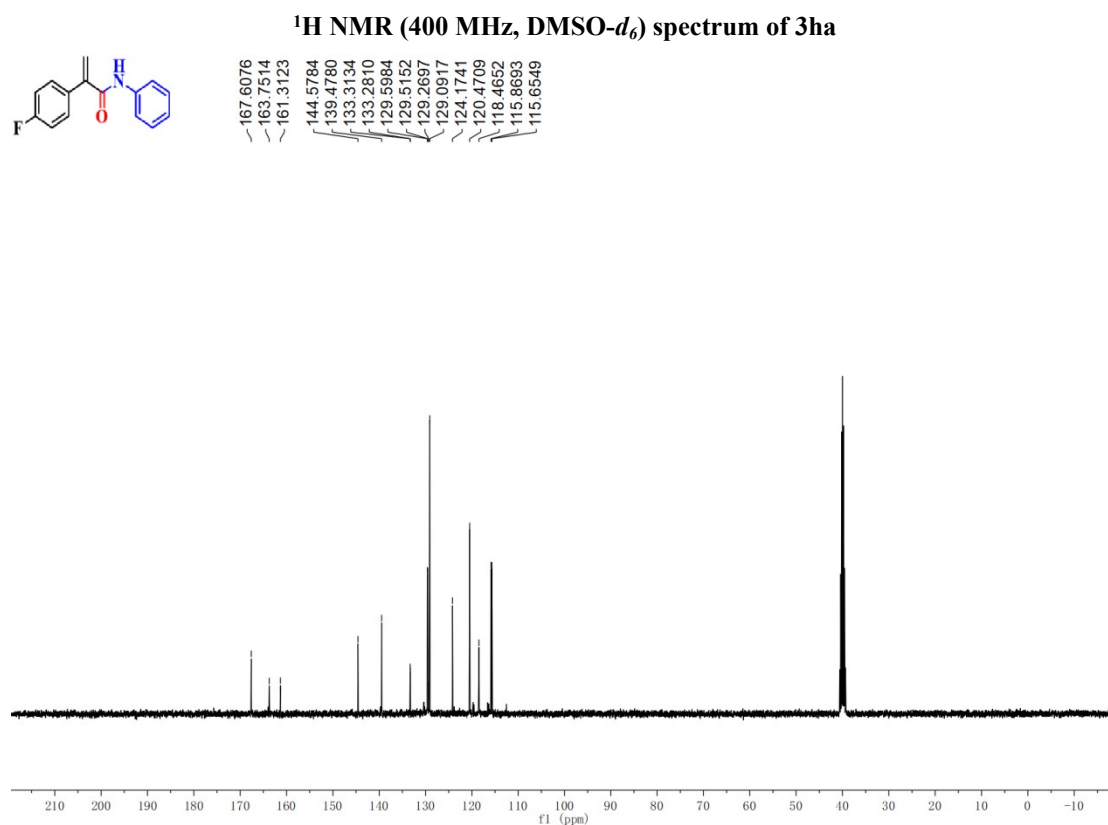
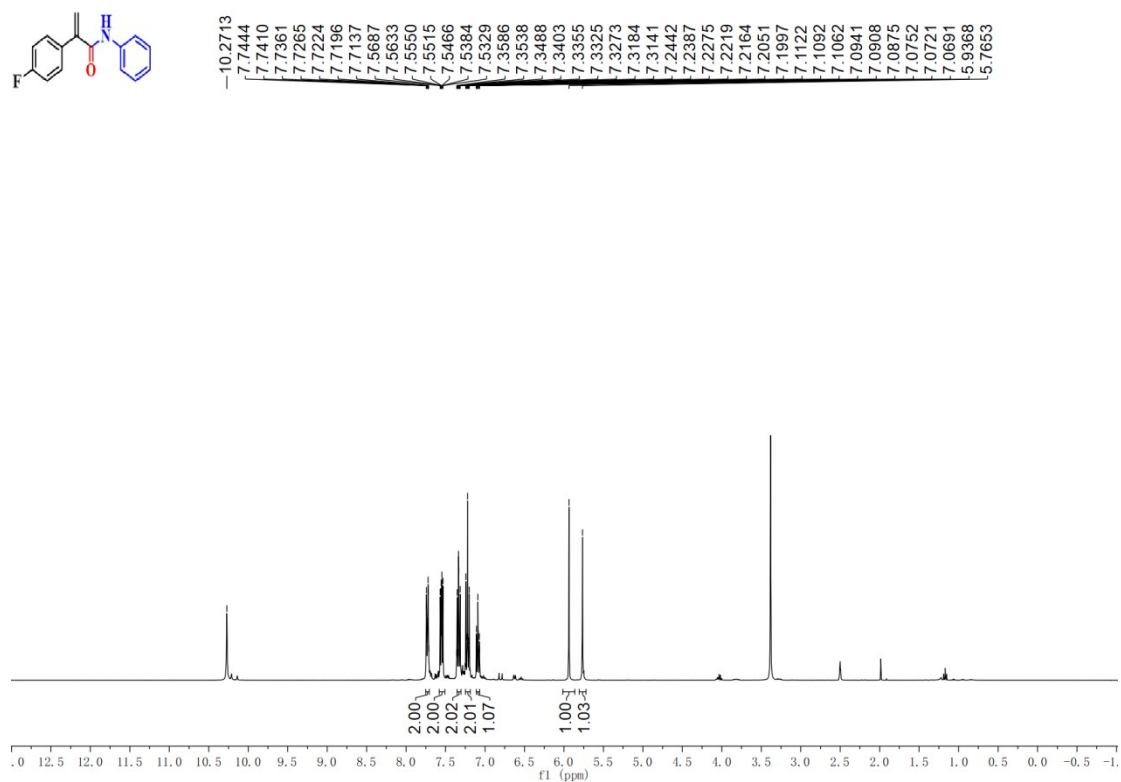


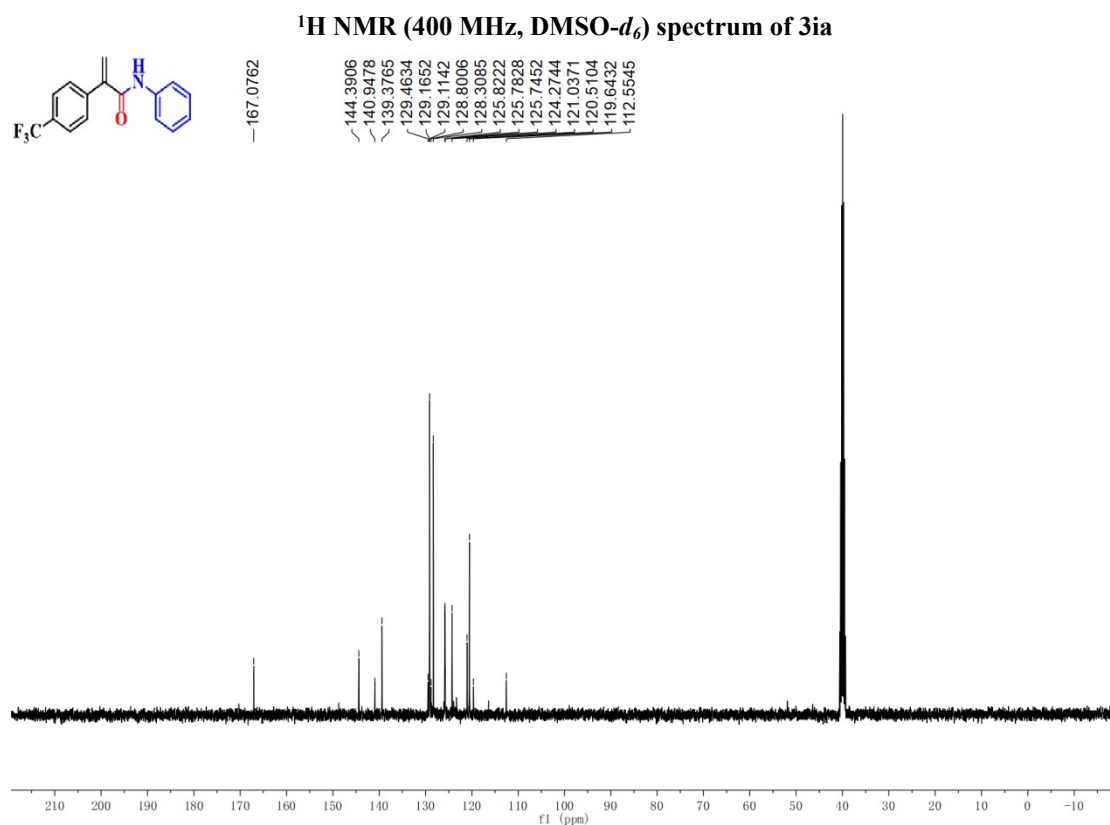
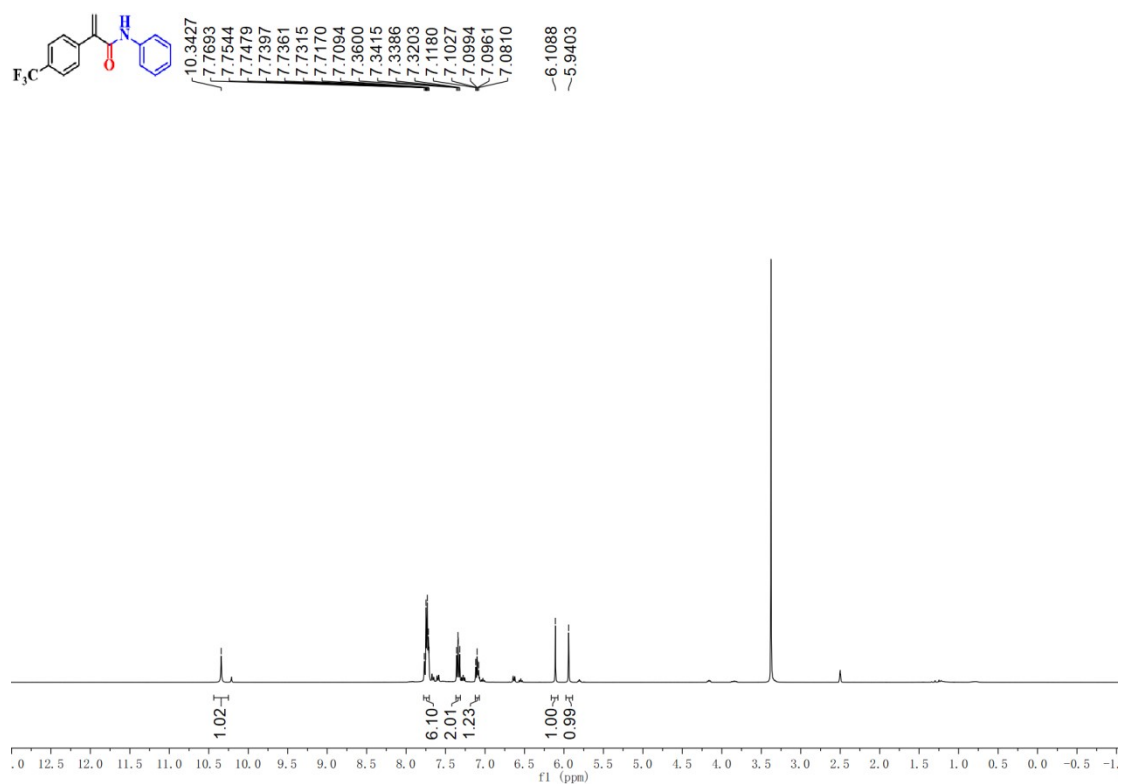
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 3fa

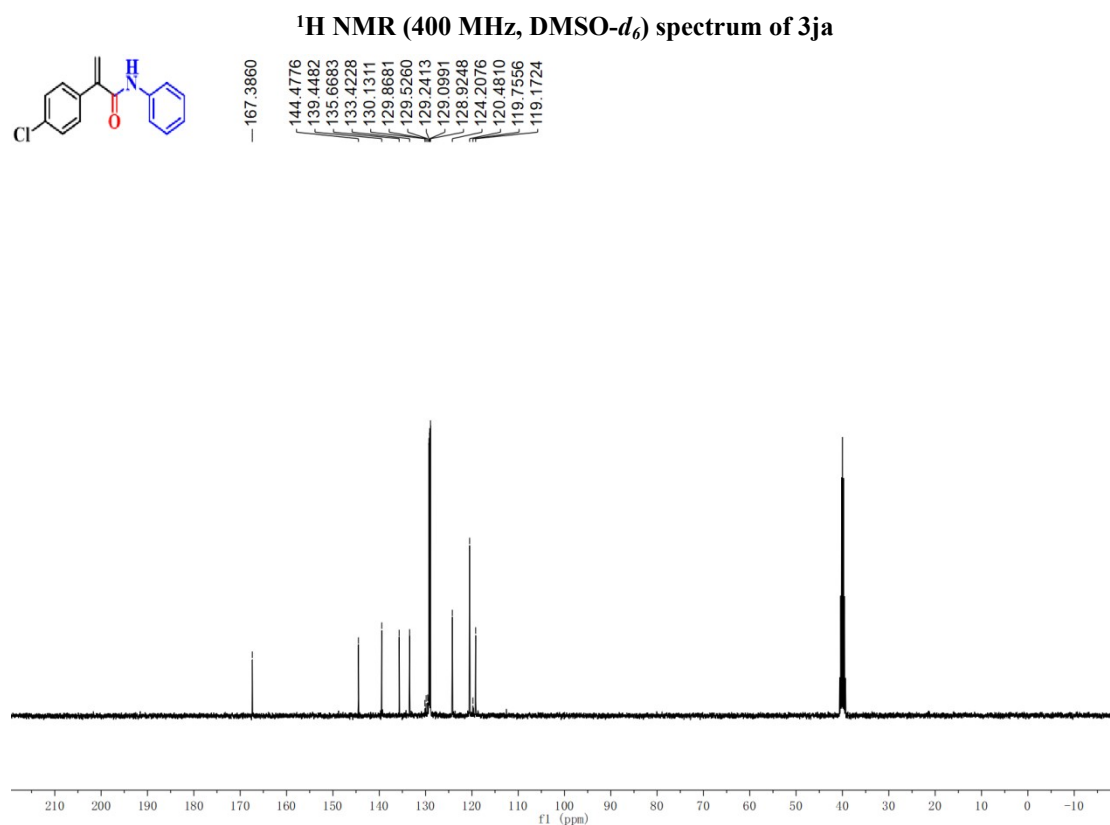
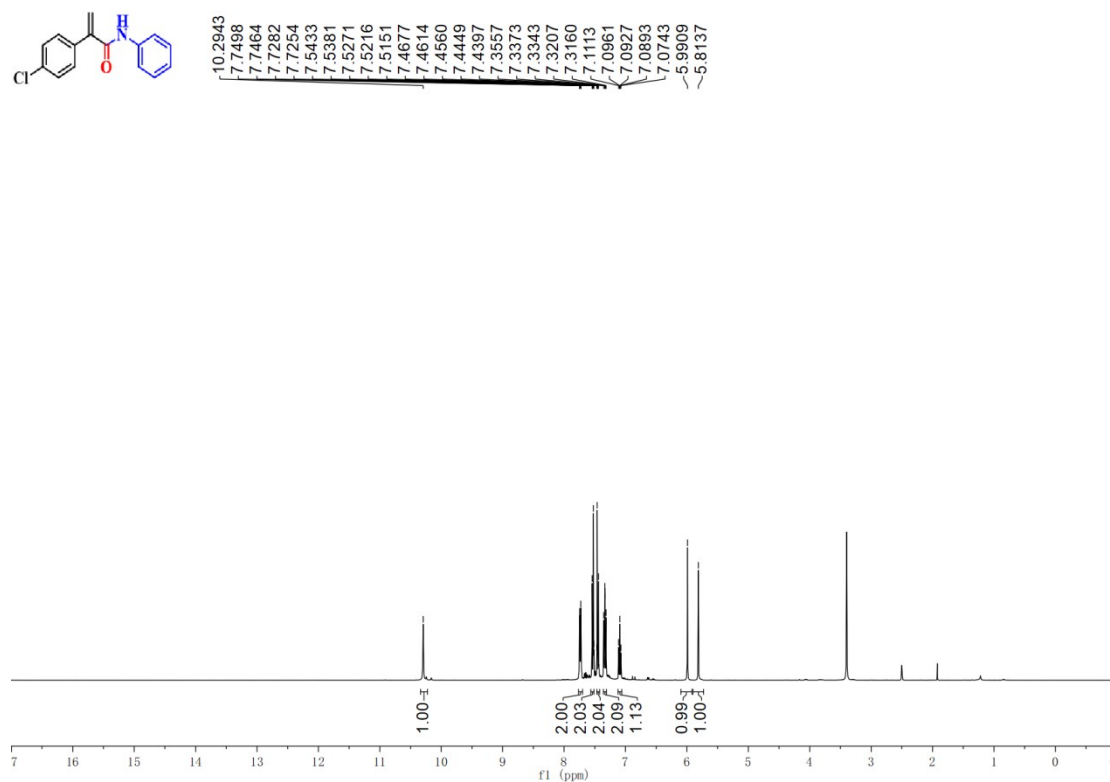


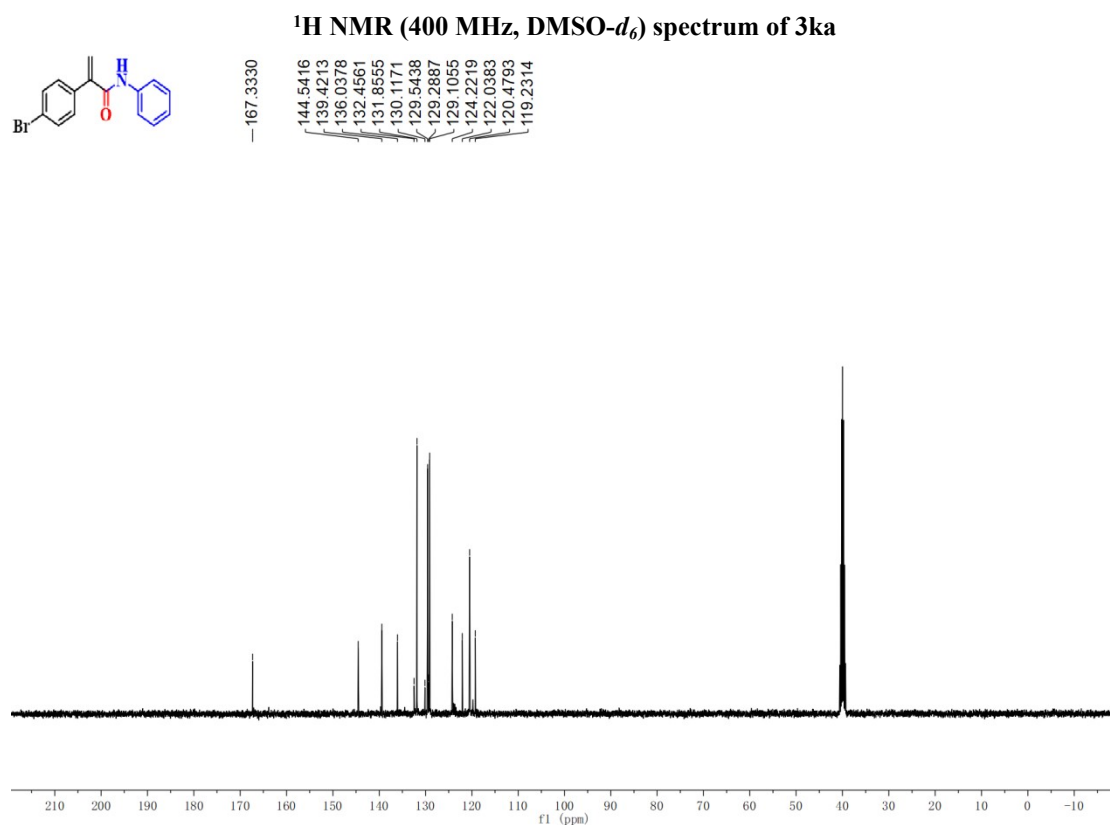
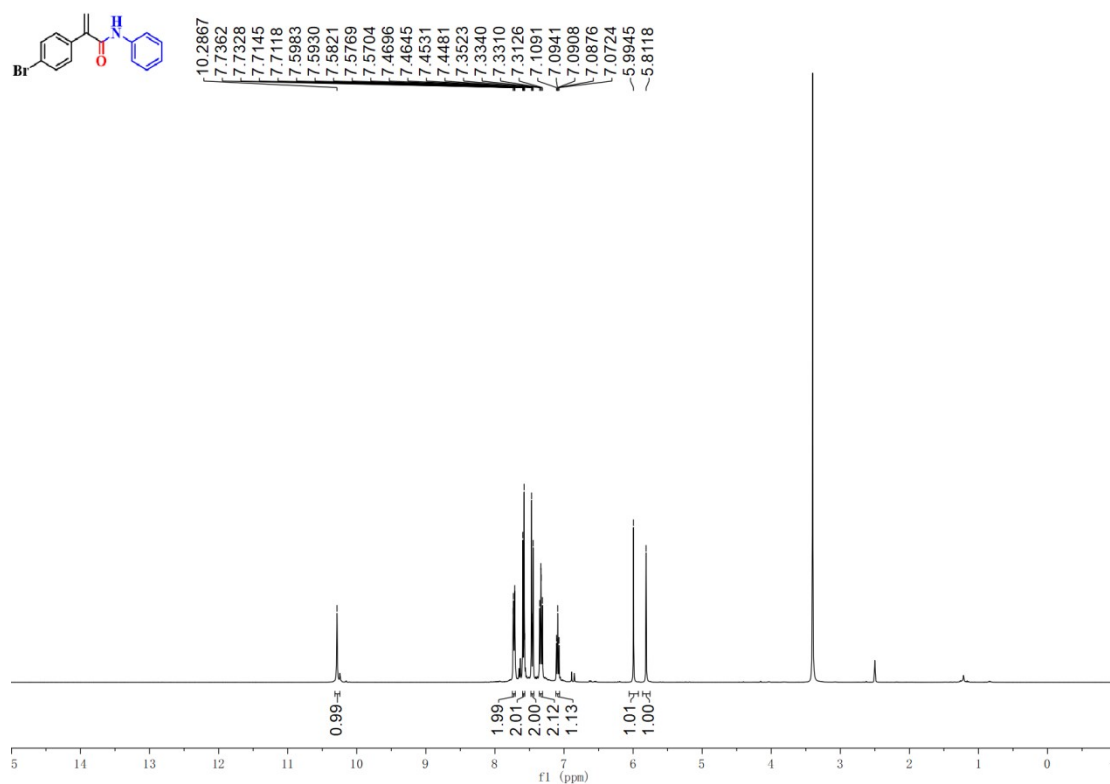
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 3fa

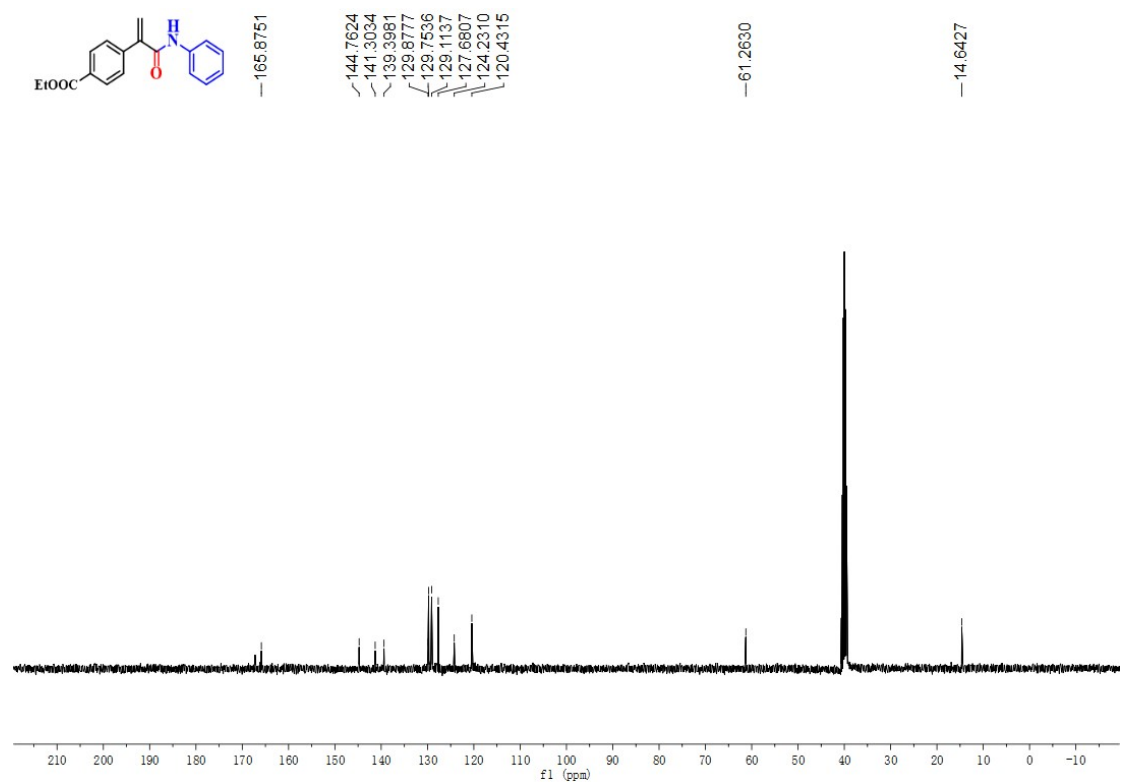
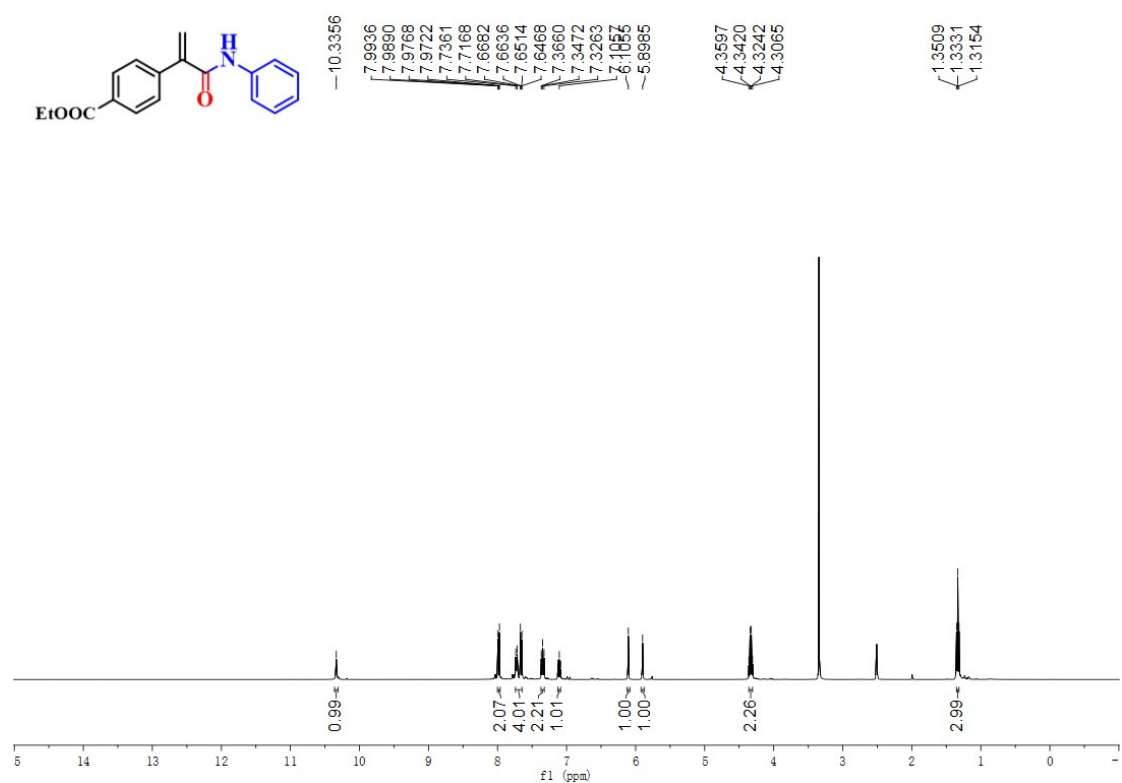


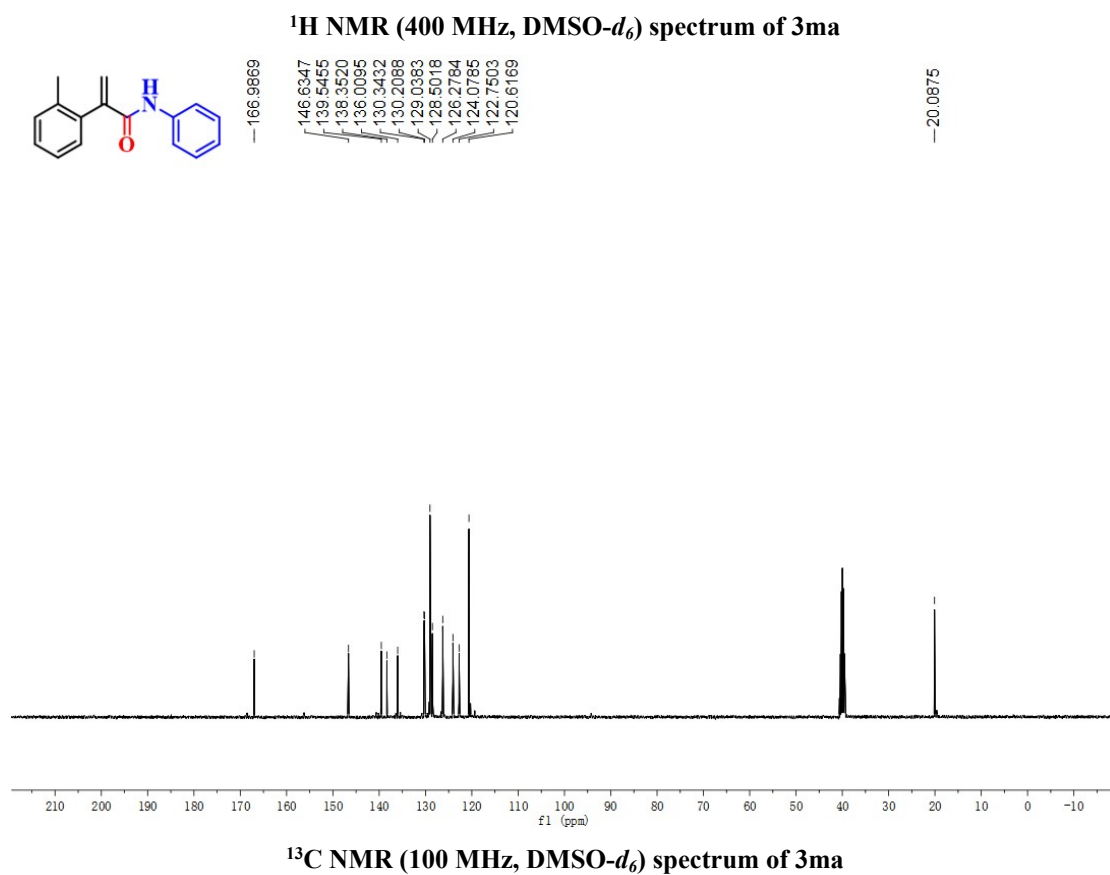
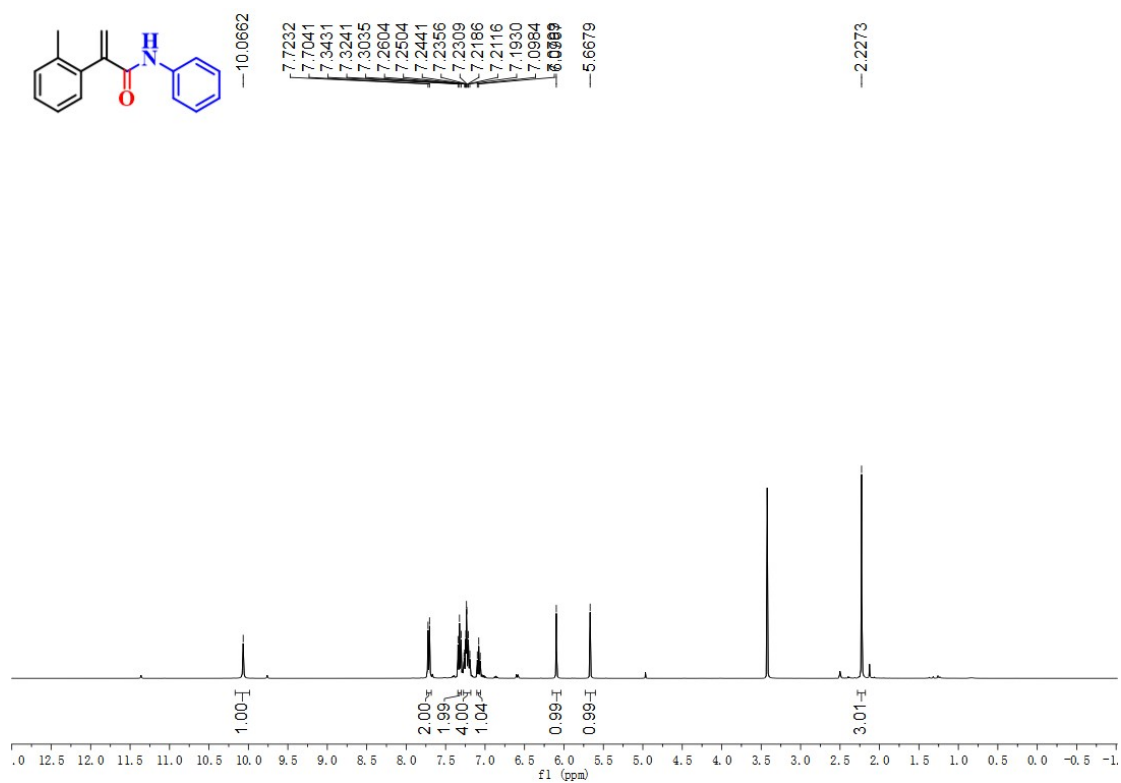


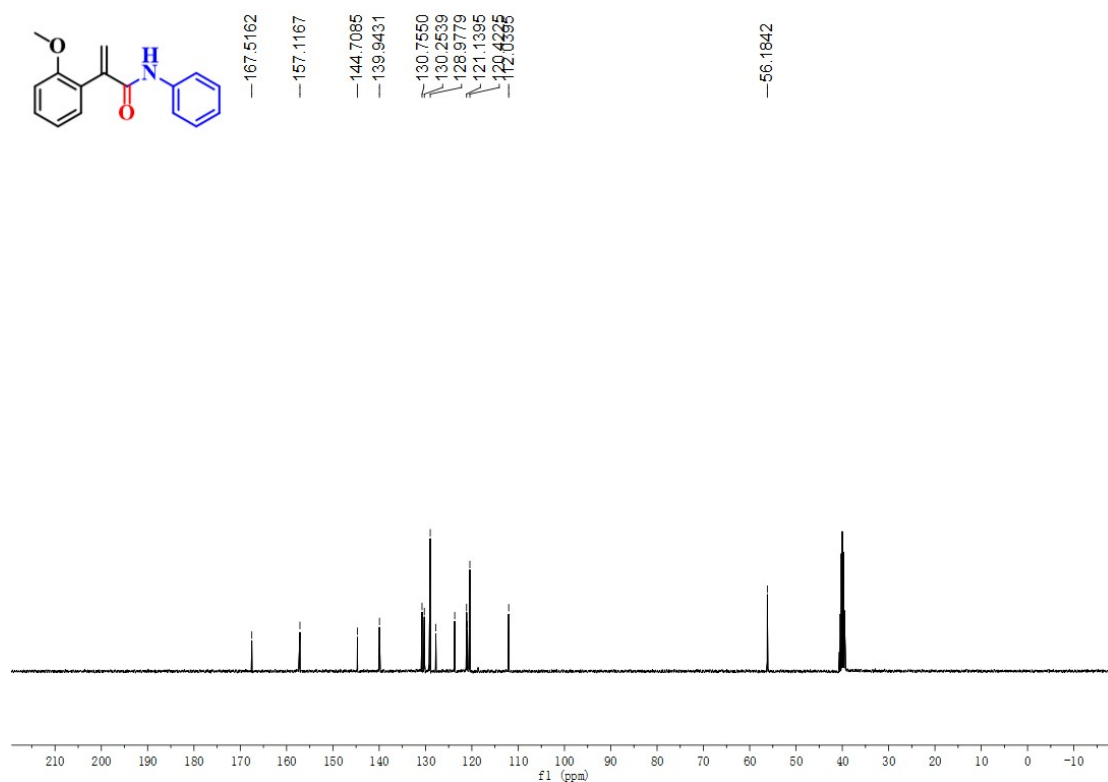
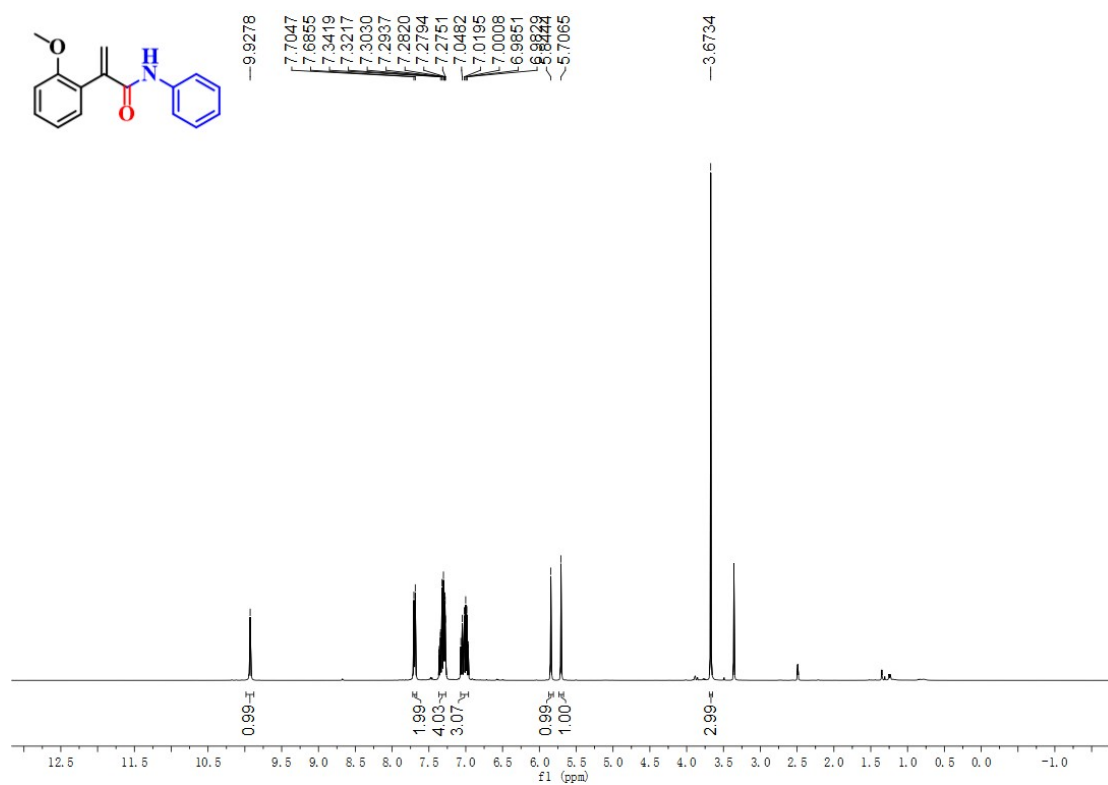


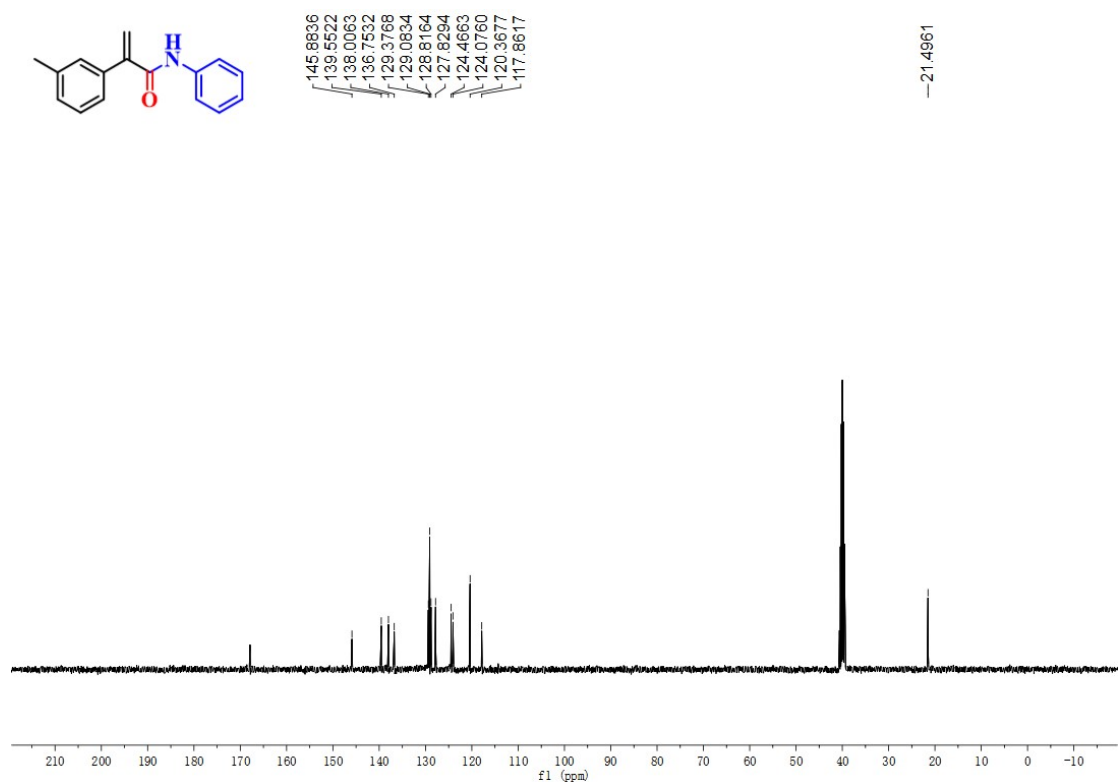
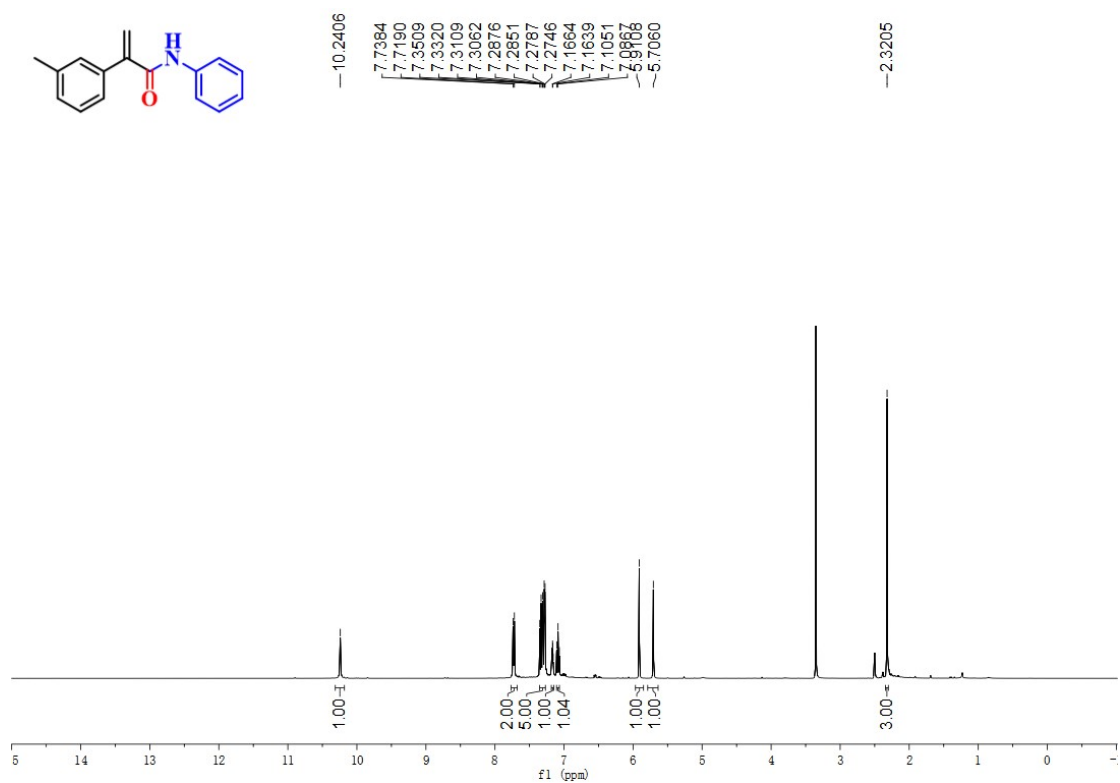


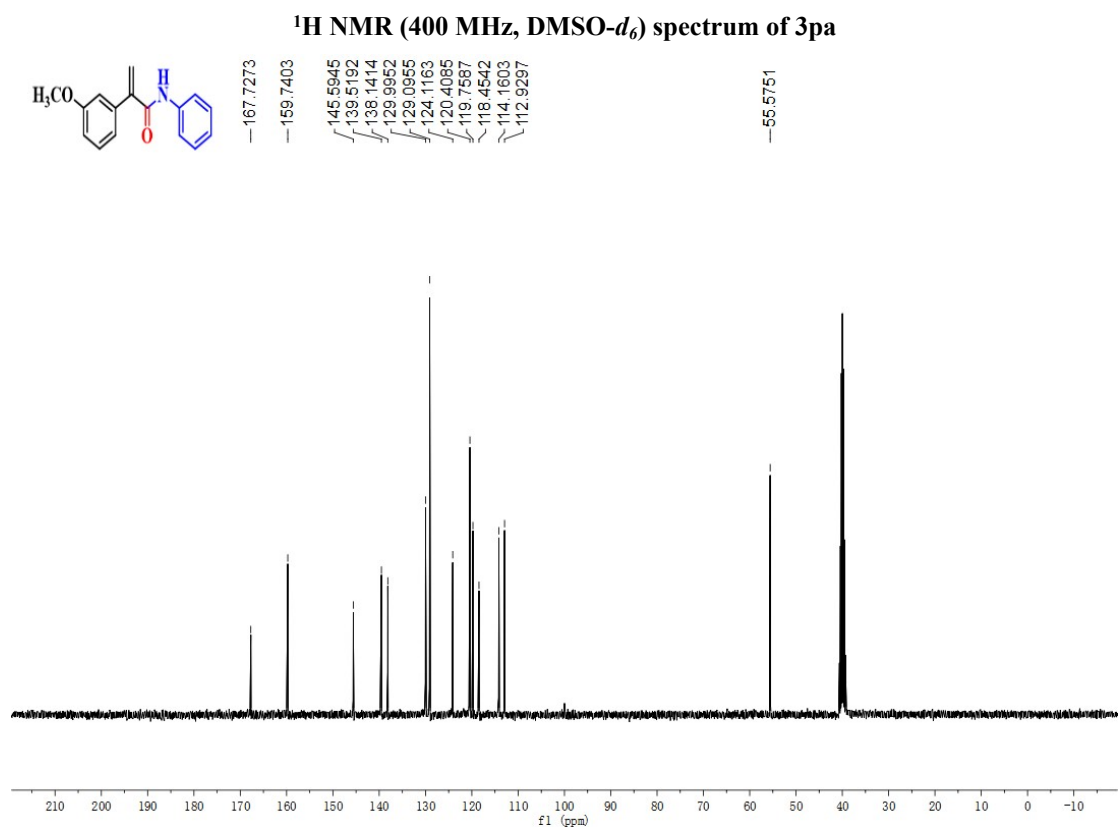
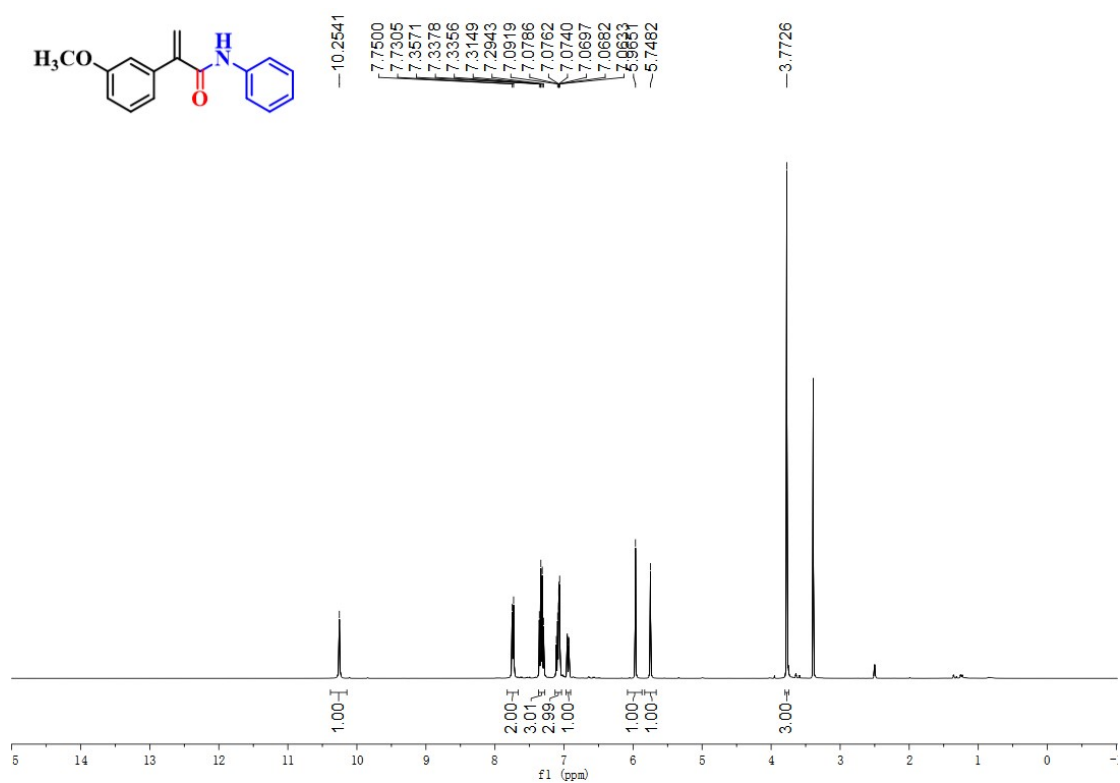


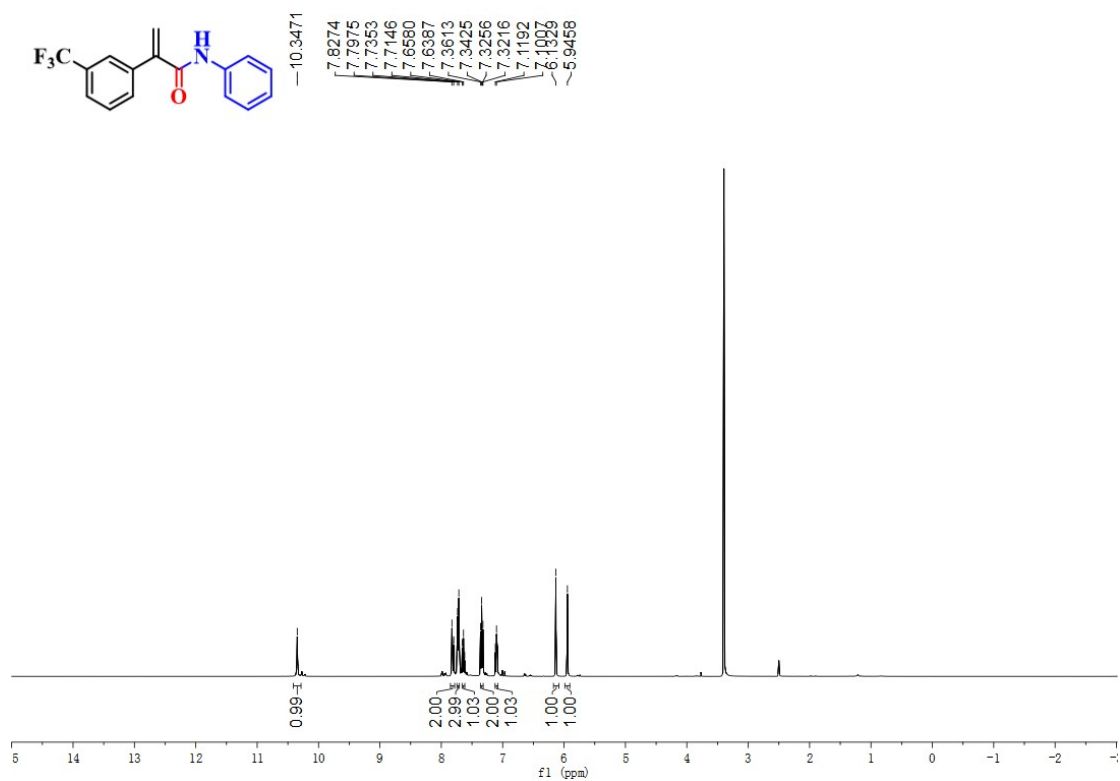




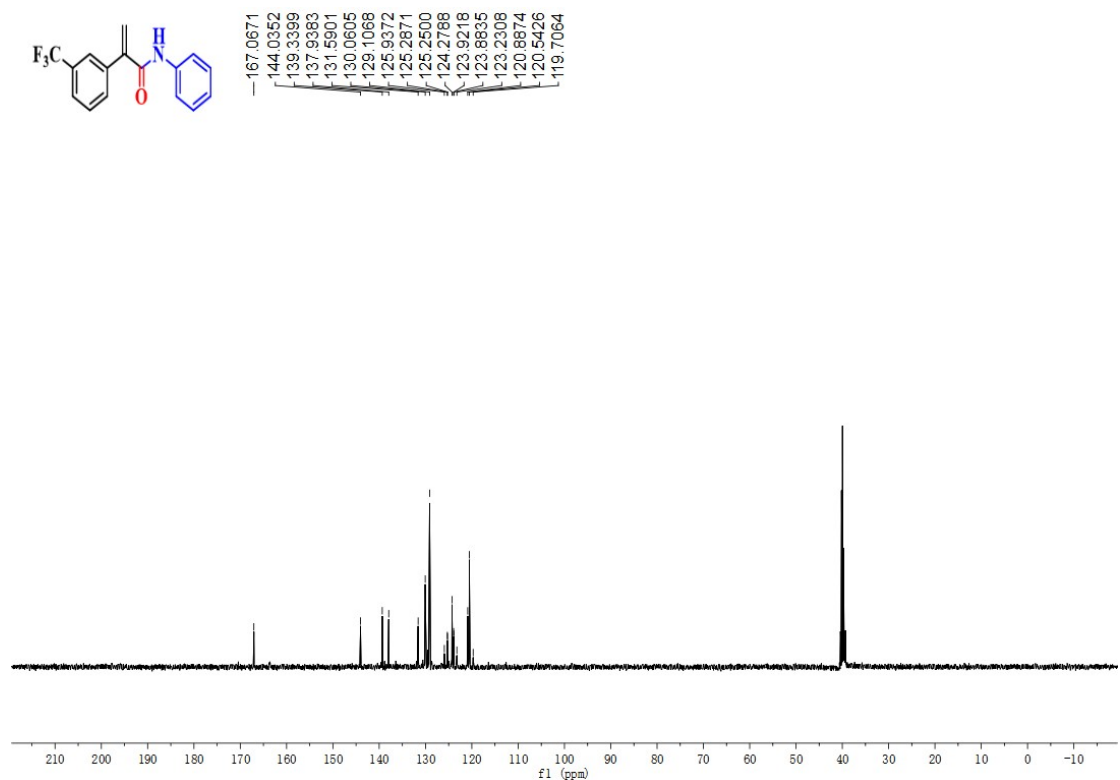




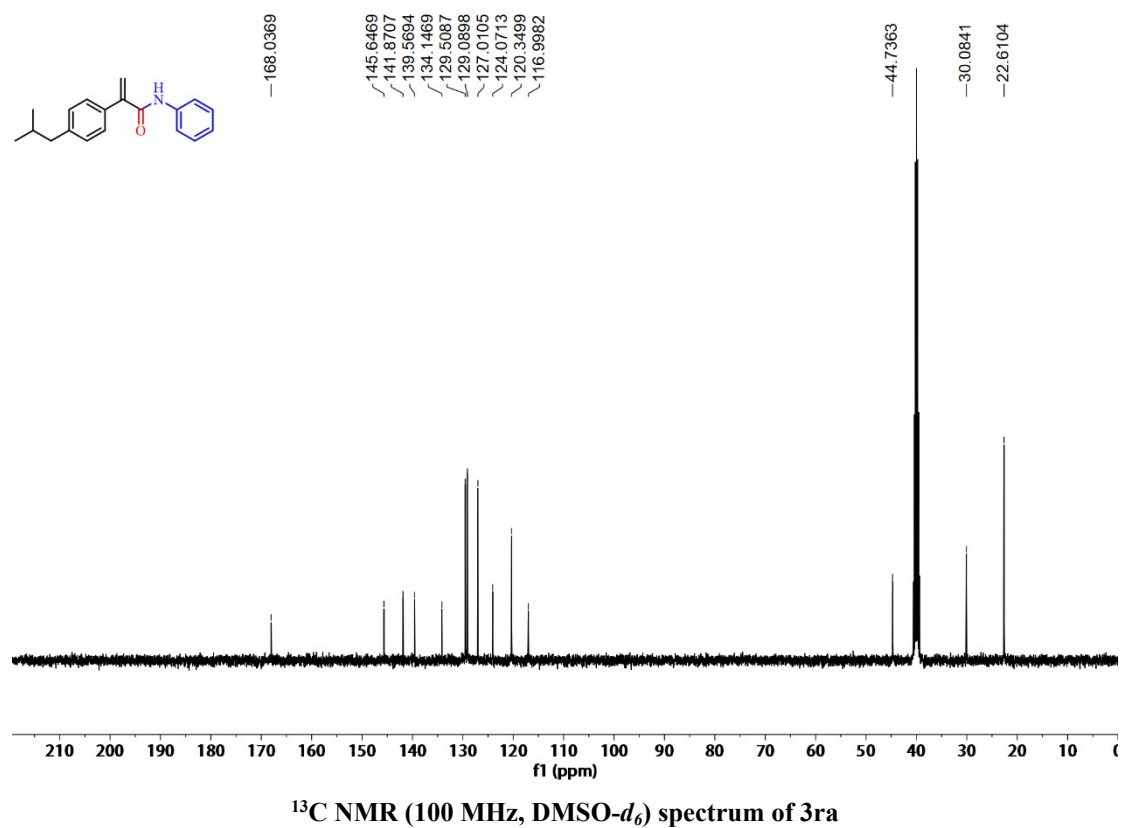
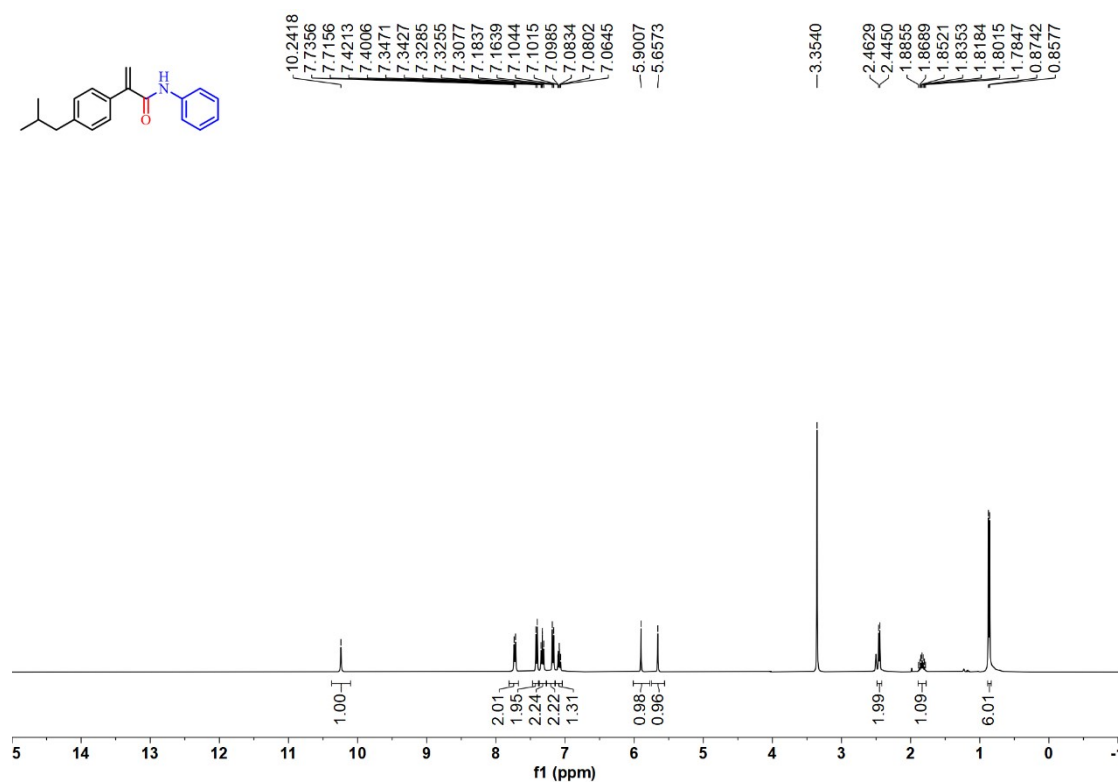


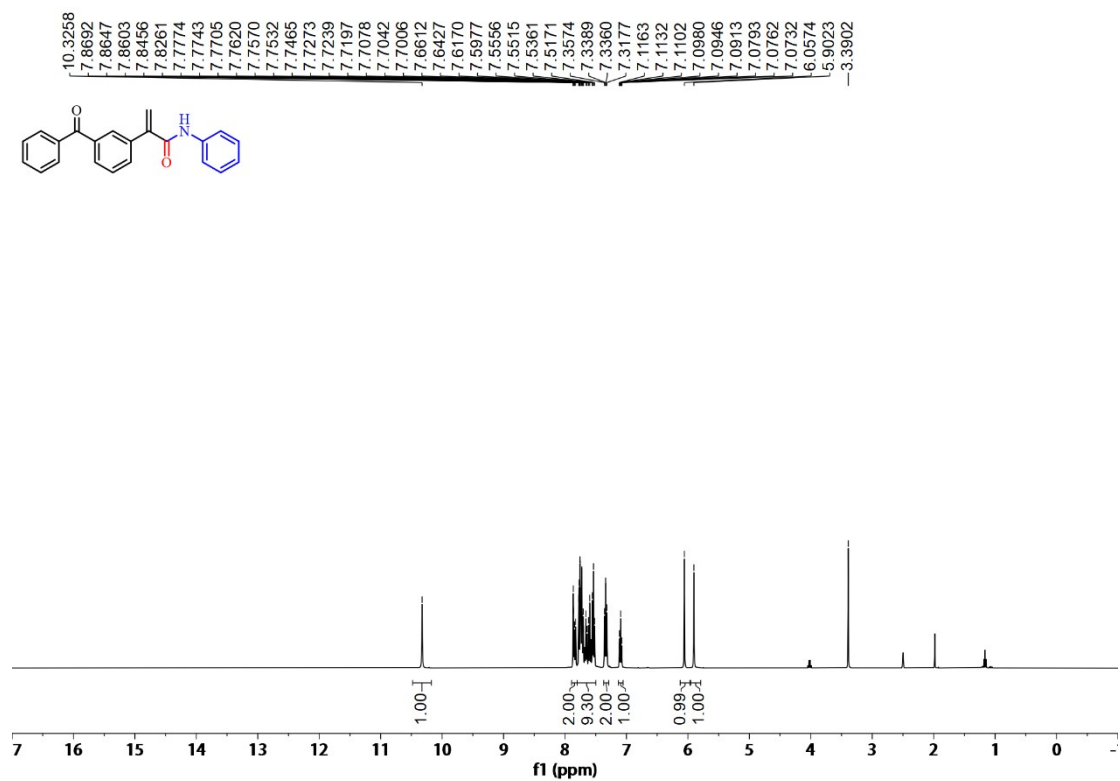


¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 3a

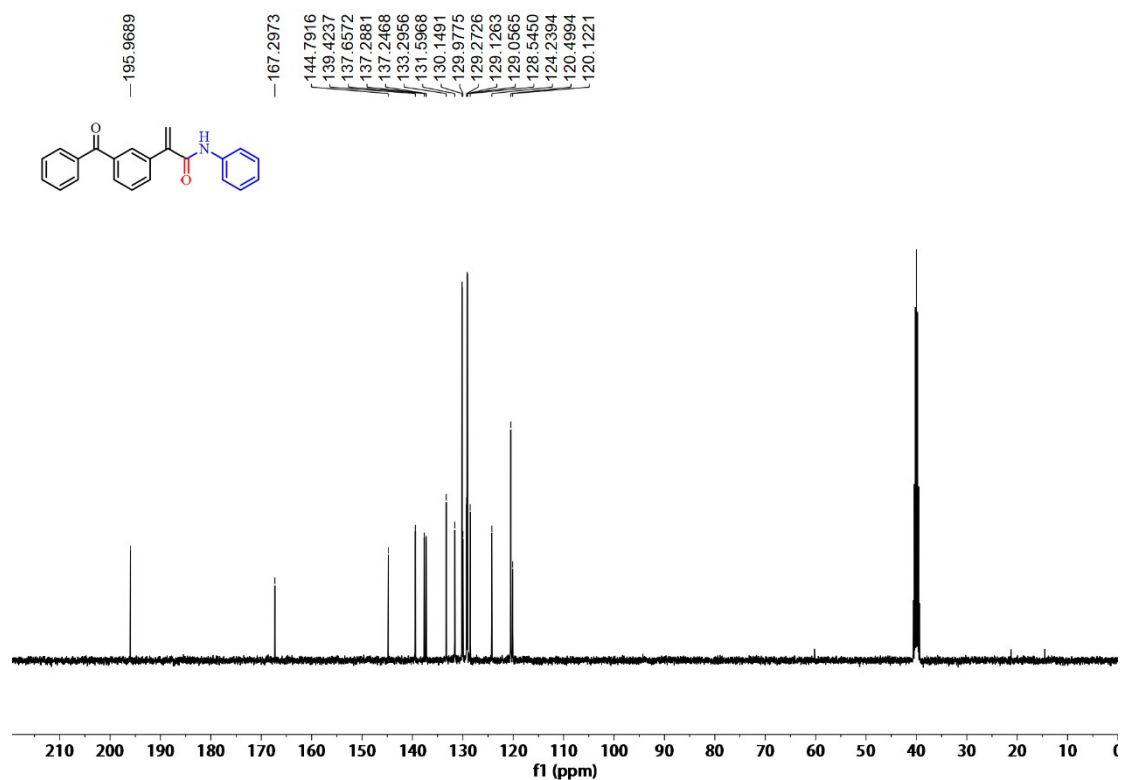


¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 3a

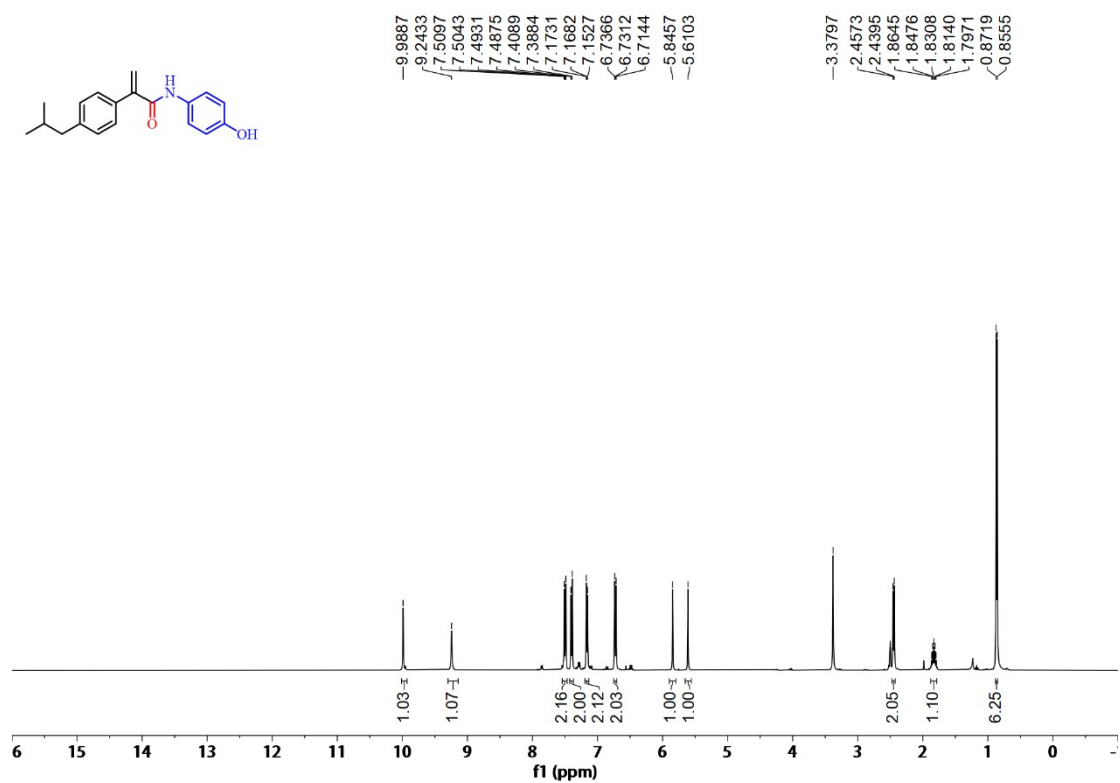




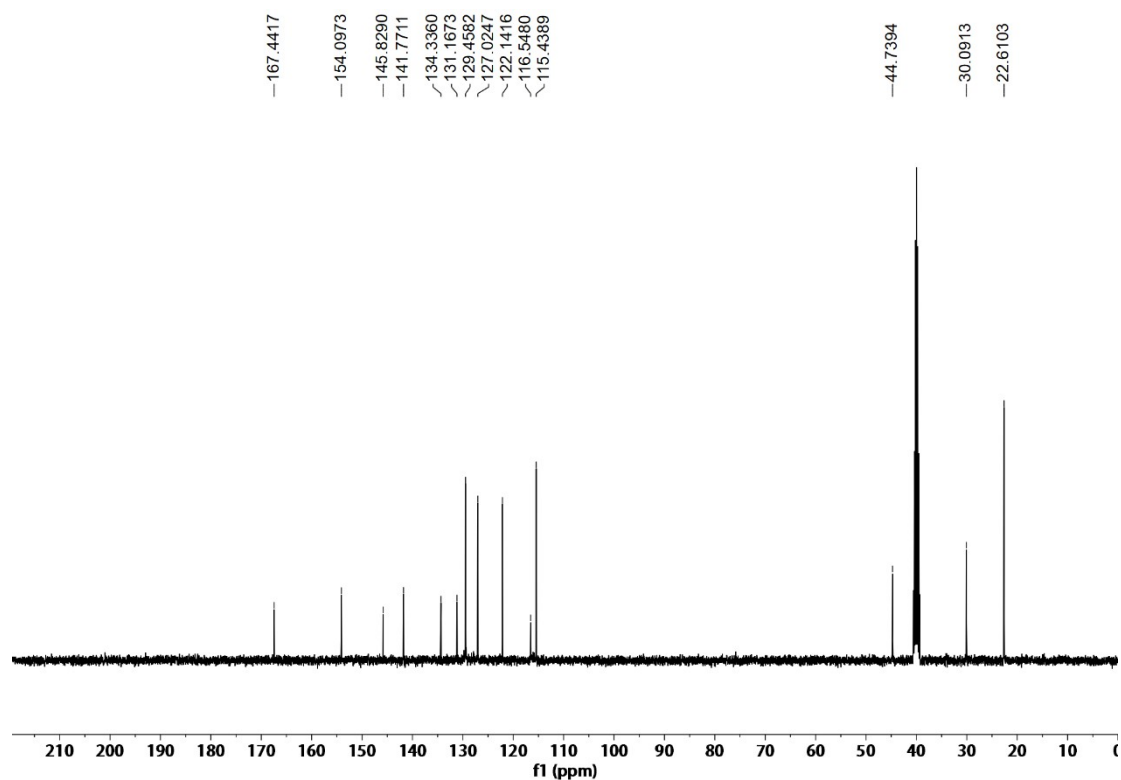
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 3sa



¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 3sa



¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 3ta



¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 3ta