# Supporting Information

# Acrylamides from 1,2-Dichloroethane via Palladium-Catalyzed Carbonylation

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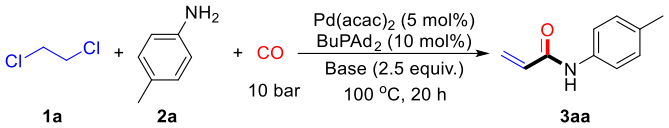
## 1. General Information

Unless otherwise noted, all reactions were carried out under a carbon monoxide or nitrogen atmosphere. All reagents were from commercial sources, all solvents are extra dry solvents and used as received without further purification. Column chromatography was performed on silica gel (200-300 meshes) using petroleum ether (b.p. 60-90 $^{o}$C) and ethyl acetate as the eluents. $^{1}$H and $^{13}$C NMR spectra were taken on Bruker AVANCE III 400 MHz or 700 MHz spectrometers and spectral data were reported in ppm relative to tetramethylsilane (TMS) as the internal standard and $CDCl_3$ or DMSO-$D_6$ as solvent. All coupling constants (J) are reported in Hz with the following abbreviations: s = singlet, d = doublet, dd = double doublet, t = triplet, dt = double triplet, q = quatriplet, m = multiplet, br = broad. Gas chromatography (GC) analyses were performed on an Agilent HP-7890A instrument with a FID detector and HP-5 capillary column (polydimethylsiloxane with 5% phenyl groups, 30 m, 0.32 mm i.d. 0.25 μm film thickness) using argon as carrier gas. Gas chromatography mass spectrometer (GC-MS) analyses were performed on a Shimadzu QP2020 NX instrument. Because of the high toxicity of carbon monoxide, all of the reactions should be performed in an autoclave. The laboratory should well-equipped with a CO detector and alarm system.

## 2. Optimization of the Reaction Conditions

(1) **Table S1**: Optimization of base

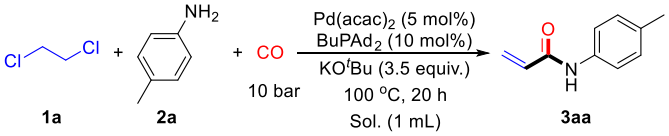



1a 2a 3aa

| Entry | Base | Yield |
|---|---|---|
| 1 | $Na_2CO_3$ | N.D. |
| 2 | $K_2CO_3$ | N.D. |
| 3 | $Cs_2CO_3$ | N.D. |
| 4 | $K_3PO_4$ | N.D. |
| 5 | CsF | N.D. |
| 6 | Li$O^tBu$ | 25% |
| 7 | DBU | 31% |
| 8 | DABCO | 18% |
| 9 | $Et_3N$ | 21% |
| 10 | DIPEA | 21% |
| 11 | K$O^tBu$ | 54% |
| 12 | K$O^tBu$ (3 equiv.) | 79% |
| 13 | K$O^tBu$ (3.5 equiv.) | 91% |
| 14 | K$O^tBu$ (4 equiv.) | 82% |

[a] Reaction conditions: **1a** (1 mL), **2a** (0.2 mmol), base (2.5 equiv.), yields were determined by GC-FID analysis using *n*-dodecane as internal standard.

(2) **Table S2**: Optimization of solvent

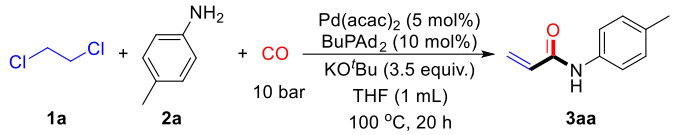



1a 2a 3aa

| Entry | Sol. | Yield |
|---|---|---|
| 1 | MeCN | 46% |
| 2 | 1,4-dioxane | 75% |
| 3 | THF | 91% |
| 4 | DMF | 73% |
| 5 | DMSO | 27% |
| 6 | NMP | 73% |
| 7 | DCM | 70% |
| 8 | Toluene | 68% |
| 9 | $PhCF_3$ | 73% |
| 10 | EA | 37% |
| 11 | Acetone | 39% |

[a] Reaction conditions:**1a** (2 mmol, 10 equiv.), **2a** (0.2 mmol), solvent (1 mL), yields were determined by GC-FID analysis using *n*-dodecane as internal standard.

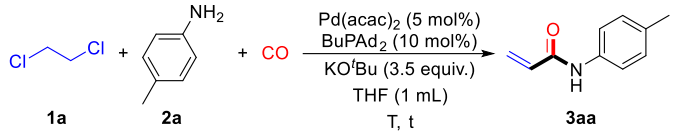
(3) **Table S3**: Optimization the amount of DCE




| Entry | DCE (equiv.) | Yield |
|---|---|---|
| 1 | 10 | 91% |
| 2 | 8 | 84% |
| 3 | 6 | 83% |
| 4 | 4 | 81% |

[a] Reaction conditions: **1a** (x equiv.), **2a** (0.2 mmol), yields were determined by GC-FID analysis using *n*-dodecane as internal standard.

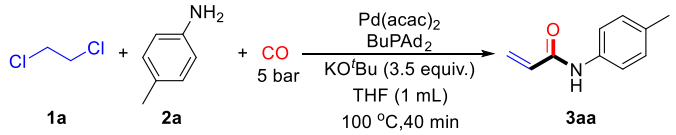
(4) **Table S4**: Optimization of temperature and time




| Entry | Temperature + Time | Yield |
|---|---|---|
| 1 | 5 bar + 100 °C + 12 h | 91% |
| 2 | 5 bar + 100 °C + 5 h | 88% |
| 3 | 5 bar + 100 °C + 3 h | 90% |
| 4 | 5 bar + 100 °C + 2 h | 99% |
| 5 | 5 bar + 100 °C + 1 h | 99% |
| 6 | 5 bar + 100 °C + 50 min | 99% |
| 7 | 5 bar + 100 °C + 40 min | 99% |
| 8 | 5 bar + 80 °C + 40 min | 83% |
| 9 | 1 bar + 100 °C + 40 min | 53% |
| 10 | 5 bar + 100 °C + 30 min | 85% |
| 11 | 5 bar + 100 °C + 15 min | 86% |

[a] Reaction conditions: **1a** (2 mmol, 10 equiv.), **2a** (0.2 mmol), yields were determined by GC-FID analysis using *n*-dodecane as internal standard.

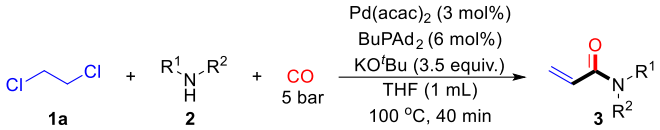
(5) **Table S5**: Optimization the amount of $Pd(acac)_2$ and $BuPAd_2$



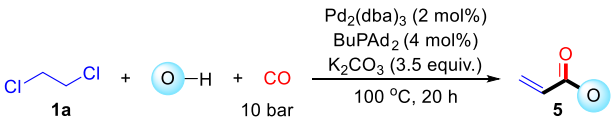

| Entry | $Pd(acac)_2$ (mol%) + $BuPAd_2$ (mol%) | Yield |
|---|---|---|
| 1 | $Pd(acac)_2$ (3 mol%) + $BuPAd_2$ (6 mol%) | 99% (96%[b]) |
| 2 | $Pd(acac)_2$ (2.5 mol%) + $BuPAd_2$ (5 mol%) | 94% |
| 3 | $Pd(acac)_2$ (2 mol%) + $BuPAd_2$ (4 mol%) | 88% |

[a] Reaction conditions: **1a** (2 mmol, 10 equiv.), **2a** (0.2 mmol), yields were determined by GC-FID analysis using *n*-dodecane as internal standard. [b] isolated yield.

## 3. General Procedure

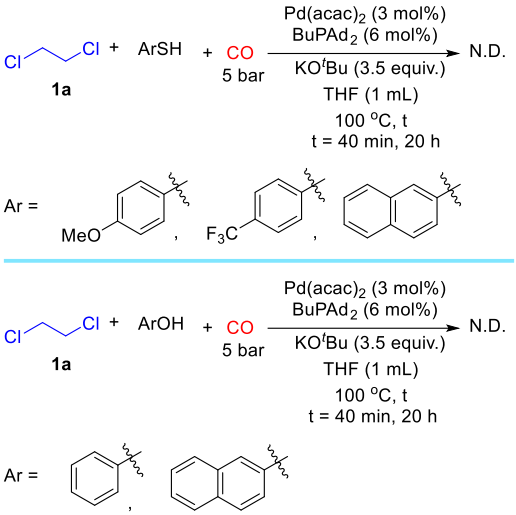



A 4 mL screw-cap vial was charged with $Pd(acac)_2$ (1.8 mg, 3 mol%), $BuPAd_2$ (4.3 mg, 6 mol%), KO$^t$Bu (3.5 equiv., 78.5 mg), and an oven-dried stir atm. The vial was closed with a Teflon septum and cap and connected to the atmosphere via a needle. After DCE (10 equiv., 160 uL), and THF (1 mL, 0.2 M), amines (1 equiv., 0.2 mmol) were added with a syringe under nitrogen atmosphere, the vial was moved to an alloy plate and put into a Parr 4560 series autoclave (300 mL) under an argon atmosphere. At room temperature, the autoclave was flushed with CO three times and charged with 5 atm of CO. The autoclave was placed on a heating plate equipped with a magnetic stirrer and an aluminum block. The reaction mixture was heated to 100 °C for 40 min. After the reaction was complete, the autoclave was cooled down with ice water to room temperature and the pressure was released carefully. After cooling to room temperature, the reaction mixture was directly purified by column chromatography on silica gel using petroleum ether and ethyl acetate to afford the corresponding product.




A 4 mL screw-cap vial was charged with $Pd_2(dba)_3$ (3.6 mg, 2 mol%), $BuPAd_2$ (2.9 mg, 4 mol%), $K_2CO_3$ (3.5 equiv., 96.8 mg), and an oven-dried stir atm. The vial was closed with a Teflon septum and cap and connected to the atmosphere via a needle. After DCE (1 mL), and alcohols (1 equiv., 0.2 mmol) were added with a syringe under nitrogen atmosphere, the vial was moved to an alloy plate and put into a Parr 4560 series autoclave (300 mL) under an argon atmosphere. At room temperature, the autoclave was flushed with CO three times and charged with 10 atm of CO. The autoclave was placed on a heating plate equipped with a magnetic stirrer and an aluminum block. The reaction mixture was heated to 100 °C for 20 h. After the reaction was complete, the autoclave was cooled down with ice water to room temperature and the pressure was released carefully. After cooling to room temperature, the reaction mixture was directly purified by column chromatography on silica gel using petroleum ether and ethyl acetate to afford the corresponding product.

## 4. Testing of Phenols and Thiophenols




A 4 mL screw-cap vial was charged with $Pd(acac)_2$ (1.8 mg, 3 mol%), $BuPAd_2$ (4.3 mg, 6 mol%), KO$^t$Bu (3.5 equiv., 78.5 mg), and an oven-dried stir atm. The vial was closed with a Teflon septum and cap and connected to the atmosphere via a needle. After DCE (10 equiv., 160 uL), and THF (1 mL, 0.2 M), phenols or thiophenols (1 equiv., 0.2 mmol) were added with a syringe under nitrogen atmosphere, the vial was moved to an alloy plate and put into a Parr 4560 series autoclave (300 mL) under an argon atmosphere. At room temperature, the autoclave was flushed with CO three times and charged with 5 atm of CO. The autoclave was placed on a heating plate equipped with a magnetic stirrer and an aluminum block. The reaction mixture was heated to 100 °C for 40 min or 20 h. After the reaction was complete, the autoclave was cooled down with ice water to room temperature and the pressure was released carefully. After cooling to room temperature, the reaction mixture was detected by GC-MS.

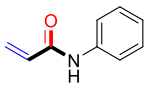
## 5. Characterization of Products

***N*-(*p*-tolyl)acrylamide (3aa)**[1]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.3) to give the titled product **3aa** as a white solid (31.0 mg, 96%).

**$^1$H NMRf (400 MHz, $CDCl_3$)** $\delta$ 7.98 (s, 1H), 7.47 (d, $J$ = 8.1 Hz, 2H), 7.10 (d, $J$ = 7.9 Hz, 2H), 6.40 (d, $J$ = 16.8 Hz, 1H), 6.28 (dd, $J$ = 16.9, 10.0 Hz, 1H), 5.71 – 5.68 (m, 1H), 2.30 (s, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 163.8, 135.2, 134.1, 131.3, 129.4, 127.3, 120.2, 20.8.

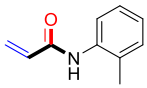


***N*-phenylacrylamide (3ab)**[1]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.3) to give the titled product **3ab** as a white solid (28.8 mg, 98%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 8.01 (s, 1H), 7.60 (d, $J$ = 7.9 Hz, 2H), 7.31 (t, $J$ = 7.8 Hz, 2H), 7.11 (t, $J$ = 7.3 Hz, 1H), 6.44 – 6.27 (m, 2H), 5.74 – 5.70 (m, 1H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 163.8, 137.8, 131.2, 128.9, 127.7, 124.5, 120.1.

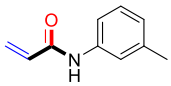


***N*-(*o*-tolyl)acrylamide (3ac)**[2]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.3) to give the titled product **3ac** as a white solid (28.7 mg, 88%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 7.77 (d, $J$ = 7.2 Hz, 1H), 7.45 (s, 1H), 7.20 – 7.07 (m, 3H), 6.41 – 6.26 (m, 2H), 5.72 (d, $J$ = 11.0 Hz, 1H), 2.23 (s, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 163.8, 135.4, 131.2, 130.5, 129.7, 127.5, 126.7, 125.5, 123.6, 17.8.

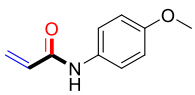


***N*-(*m*-tolyl)acrylamide (3ad)**[3]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.3) to give the titled product **3ad** as a yellow oil (31.8 mg, 94%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 8.05 (s, 1H), 7.46 (s, 1H), 7.37 (d, $J$ = 7.8 Hz, 1H), 7.18 (t, $J$ = 7.8 Hz, 1H), 6.92 (d, $J$ = 7.4 Hz, 1H), 6.43 – 6.27 (m, 2H), 5.71 (d, $J$ = 9.9 Hz, 1H), 2.30 (s, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 163.9, 138.8, 137.7, 131.3, 128.7, 127.5, 125.3, 120.8, 117.2, 21.4.

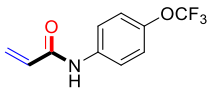


***N*-(4-methoxyphenyl)acrylamide (3ae)**[1]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.3) to give the titled product **3ae** as a white solid (34.0 mg, 96%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 8.22 (s, 1H), 7.48 (d, $J$ = 9.0 Hz, 2H), 6.81 (d, $J$ = 9.0 Hz, 2H), 6.37 (dd, $J$ = 16.9, 1.7 Hz, 1H), 6.28 (dd, $J$ = 16.9, 9.8 Hz, 1H), 5.67 (dd, $J$ = 9.8, 1.8 Hz, 1H), 3.76 (s, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 163.8, 156.4, 131.2, 130.9, 127.1, 122.0, 114.0, 55.4.



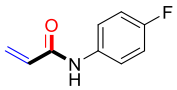

***N*-(4-(trifluoromethoxy)phenyl)acrylamide (3af)**[1]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.3) to give the titled product **3af** as a white solid (35.6 mg, 77%).

**$^1$H NMR (400 MHz, DMSO)** $\delta$ 10.34 (s, 1H), 7.78 (d, $J$ = 9.1 Hz, 2H), 7.32 (d, $J$ = 8.5 Hz, 2H), 6.43 (dd, $J$ = 17.0, 10.0 Hz, 1H), 6.29 (dd, $J$ = 17.0, 2.0 Hz, 1H), 5.78 (dd, $J$ = 10.0, 1.2 Hz, 1H).

**$^{13}$C NMR (101 MHz, DMSO)** $\delta$ 163.7, 144.2, 138.7, 132.1, 127.7, 122.1, 121.1, 120.6 (q, $J$ = 255.6 Hz).

**$^{19}$F NMR (376 MHz, DMSO)** $\delta$ -57.2.




***N*-(4-fluorophenyl)acrylamide (3ag)**[1]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.3) to give the titled product **3ag** as a white solid (31.0 mg, 94%).

**$^1$H NMR (400 MHz, DMSO)** $\delta$ 10.21 (s, 1H), 7.71 – 7.66 (m, 2H), 7.19 – 7.12 (m, 2H), 6.41 (dd, $J$ = 17.0, 10.1 Hz, 1H), 6.26 (dd, $J$ = 17.0, 2.1 Hz, 1H), 5.75 (dd, $J$ = 10.0, 2.1 Hz, 1H).

**$^{13}$C NMR (101 MHz, DMSO)** $\delta$ 163.5, 158.6 (d, $J$ = 240.1 Hz), 135.9 (d, $J$ = 2.5 Hz), 132.2, 127.4, 121.5 (d, $J$ = 7.8 Hz), 115.8 (d, $J$ = 22.2 Hz).

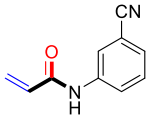
**$^{19}$F NMR (376 MHz, DMSO)** $\delta$ -119.0.


***N*-(4-chlorophenyl)acrylamide (3ah)**[2]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.2) to give the titled product **3ah** as a white solid (26.8 mg, 74%).

**$^1$H NMR (400 MHz, DMSO)** $\delta$ 10.27 (s, 1H), 7.70 (d, $J$ = 8.8 Hz, 2H), 7.37 (d, $J$ = 8.8 Hz, 2H), 6.42 (dd, $J$ = 17.0, 10.0 Hz, 1H), 6.27 (dd, $J$ = 17.0, 1.8 Hz, 1H), 5.77 (dd, $J$ = 10.0, 1.9 Hz, 1H).

**$^{13}$C NMR (101 MHz, DMSO)** $\delta$ 163.7, 138.4, 132.1, 129.2, 127.7, 127.5, 121.3.

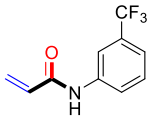



***N*-(3-cyanophenyl)acrylamide (3ai)**[5]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 3/1, $R_f$ = 0.3) to give the titled product **3ai** as a white solid (9.6 mg, 28%).

**$^1$H NMR (400 MHz, DMSO)** $\delta$ 10.48 (s, 1H), 8.167 – 8.165 (m, 1H), 7.87 – 7.83 (m, 1H), 7.56 – 7.51 (m, 2H), 6.42 (dd, *J* = 17.0, 10.0 Hz, 1H), 6.30 (dd, *J* = 17.0, 2.0 Hz, 1H), 5.81 (dd, *J* = 9.9, 2.0 Hz, 1H).

**$^{13}$C NMR (101 MHz, DMSO)** $\delta$ 164.1, 140.2, 131.8, 130.7, 128.4, 127.5, 124.4, 122.5, 119.1, 112.1.



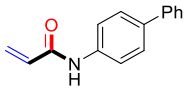

***N*-(3-(trifluoromethyl)phenyl)acrylamide (3aj)**[5]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.3) to give the titled product **3aj** as a white solid (29.2 mg, 68%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 8.25 (s, 1H), 7.89 (s, 1H), 7.78 (d, *J* = 7.9 Hz, 1H), 7.43 – 7.34 (m, 2H), 6.44 (dd, *J* = 16.9, 1.2 Hz, 1H), 6.31 (dd, *J* = 16.9, 10.1 Hz, 1H), 5.78 (dd, *J* = 10.1, 1.2 Hz, 1H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 164.2, 138.3, 131.4 (q, *J* = 32.5 Hz), 130.7, 129.6, 128.6, 123.8 (q, *J* = 272.4 Hz), 123.3, 121.1 (q, *J* = 3.7 Hz), 117.0 (d, *J* = 2.9 Hz).

**$^{19}$F NMR (376 MHz, $CDCl_3$)** $\delta$ -62.8.

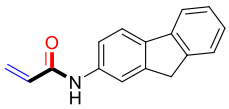



***N*-([1,1'-biphenyl]-4-yl)acrylamide (3ak)**[4]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.3) to give the titled product **3ak** as a white solid (41.0 mg, 92%).

**$^1$H NMR (400 MHz, DMSO)** $\delta$ 10.27 (s, 1H), 7.80 – 7.78 (m, 2H), 7.65 (d, *J* = 8.6 Hz, 4H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 6.48 (dd, *J* = 17.0, 10.1 Hz, 1H), 6.30 (dd, *J* = 17.0, 1.8 Hz, 1H), 5.78 (dd, *J* = 10.1, 2.0 Hz, 1H).

**$^{13}$C NMR (101 MHz, DMSO)** $\delta$ 163.6, 140.1, 139.0, 135.6, 132.3, 129.4, 127.53, 127.46, 126.7, 120.2.

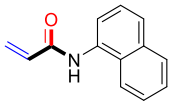



***N*-(9*H*-fluoren-2-yl)acrylamide (3al)**[6]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.2) to give the titled product **3al** as a white solid (43.2 mg, 92%).

**$^1$H NMR (400 MHz, DMSO)** $\delta$ 10.26 (s, 1H), 8.04 (s, 1H), 7.82 (t, *J* = 8.3 Hz, 2H), 7.64 (d, *J* = 8.2 Hz, 1H), 7.54 (d, *J* = 7.4 Hz, 1H), 7.35 (t, *J* = 7.3 Hz, 1H), 7.26 (t, *J* = 7.4 Hz, 1H), 6.50 (dd, *J* = 16.9, 10.1 Hz, 1H), 6.30 (dd, *J* = 16.9, 1.5 Hz, 1H), 5.77 (dd, *J* = 10.1, 1.9 Hz, 1H), 3.91 (s, 2H).

**$^{13}$C NMR (101 MHz, DMSO)** $\delta$ 163.6, 144.3, 143.3, 141.4, 138.6, 137.1, 132.4, 127.24, 127.21, 126.6, 125.5, 120.7, 112.0, 118.6, 116.6, 37.0.

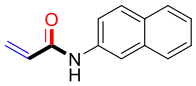


***N*-(naphthalen-1-yl)acrylamide (3am)**[4]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.2) to give the titled product **3am** as a white solid (24.8 mg, 63%).

**$^1$H NMR (400 MHz, DMSO)** $\delta$ 10.15 (s, 1H), 8.10 – 8.07 (m, 1H), 7.96 – 7.93 (m, 1H), 7.80 (dd, *J* = 14.3, 7.8 Hz, 2H), 7.60 – 7.50 (m, 3H), 6.73 (dd, *J* = 16.9, 10.2 Hz, 1H), 6.33 (dd, *J* = 17.0, 1.9 Hz, 1H), 5.82 (dd, *J* = 10.2, 1.5 Hz, 1H).

**$^{13}$C NMR (101 MHz, DMSO)** $\delta$ 164.4, 134.2, 133.7, 132.3, 128.7, 128.0, 127.4, 126.5, 126.4, 126.1, 125.8, 123.1, 122.0.

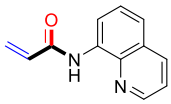


***N*-(naphthalen-2-yl)acrylamide (3an)**[4]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.2) to give the titled product **3an** as a white solid (26.4 mg, 67%).

**$^1$H NMR (400 MHz, DMSO)** $\delta$ 10.36 (s, 1H), 8.41 (s, 1H), 7.88 (d, *J* = 8.8 Hz, 1H), 7.83 (dd, *J* = 7.9, 4.4 Hz, 2H), 7.66 (dd, *J* = 8.8, 1.9 Hz, 1H), 7.49 – 7.45 (m, 1H), 7.40 (dd, *J* = 10.9, 4.1 Hz, 1H), 6.51 (dd, *J* = 17.0, 10.1 Hz, 1H), 6.32 (dd, *J* = 17.0, 1.9 Hz, 1H), 5.79 (dd, *J* = 10.1, 1.9 Hz, 1H).

**$^{13}$C NMR (101 MHz, DMSO)** $\delta$ 163.9, 137.1, 133.9, 132.3, 130.4, 128.9, 127.9, 127.8, 127.5, 126.9, 125.2, 120.5, 116.0.

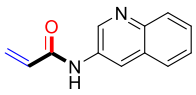


***N*-(quinolin-8-yl)acrylamide (3ao)**[7]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 3/1, $R_f$ = 0.2) to give the titled product **3ao** as a white solid (26.1 mg, 66%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 9.96 (s, 1H), 8.86 (d, *J* = 7.5 Hz, 1H), 8.80 – 8.79 (m, 1H), 8.15 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.45 – 7.43 (m, 1H), 6.53 – 6.46 (m, 2H), 5.82 (dd, *J* = 8.9, 2.4 Hz, 1H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 163.7, 148.2, 138.5, 136.4, 134.4, 131.8, 127.9, 127.5, 127.4, 121.8, 121.7, 116.9.

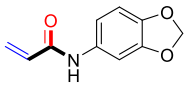


***N*-(quinolin-3-yl)acrylamide (3ap)**[8]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.3) to give the titled product **3ap** as a white solid (31.7 mg, 80%).

**$^1$H NMR (400 MHz, DMSO)** $\delta$ 10.65 (s, 1H), 8.96 (d, $J$ = 2.5 Hz, 1H), 8.80 (d, $J$ = 2.3 Hz, 1H), 7.97 – 7.92 (m, 2H), 7.67 – 7.63 (m, 1H), 7.59 – 7.55 (m, 1H), 6.52 (dd, $J$ = 17.0, 10.1 Hz, 1H), 6.35 (dd, $J$ = 17.0, 1.9 Hz, 1H), 5.85 (dd, $J$ = 10.1, 1.9 Hz, 1H).

**$^{13}$C NMR (101 MHz, DMSO)** $\delta$ 164.4, 145.0, 144.8, 133.2, 131.8, 129.0, 128.4, 128.3, 128.2, 127.6, 122.8.

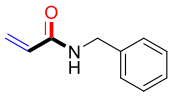


***N*-(benzo[d][1,3]dioxol-5-yl)acrylamide (3aq)**[4]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.4) to give the titled product **3aq** as a white solid (34.8 mg, 91%).

**$^1$H NMR (400 MHz, DMSO)** $\delta$ 10.06 (s, 1H), 7.40 (d, $J$ = 1.8 Hz, 1H), 7.03 (dd, $J$ = 8.4, 1.9 Hz, 1H), 6.86 (d, $J$ = 8.4 Hz, 1H), 6.39 (dd, $J$ = 17.0, 10.0 Hz, 1H), 6.23 (dd, $J$ = 17.0, 2.0 Hz, 1H), 5.98 (s, 2H), 5.72 (dd, $J$ = 10.0, 2.0 Hz, 1H).

**$^{13}$C NMR (101 MHz, DMSO)** $\delta$ 163.3, 147.5, 143.6, 133.9, 132.3, 127.0, 112.6, 108.6, 101.9, 101.5.

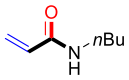


***N*-benzylacrylamide (3ar)**[1]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.5) to give the titled product **3ar** as a white solid (20.6 mg, 64%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 7.34 – 7.24 (m, 5H), 6.31 – 6.25 (m, 2H), 6.13 (dd, $J$ = 17.0, 10.2 Hz, 1H), 5.63 (dd, $J$ = 10.2, 1.5 Hz, 1H), 4.48 (d, $J$ = 5.8 Hz, 2H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 165.5, 138.1, 130.7, 128.7, 127.9, 127.6, 126.8, 43.7.

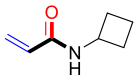


***N*-butylacrylamide (3as)**[9]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.5) to give the titled product **3as** as a yellow oil (22.1 mg, 87%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 6.27 (dd, $J$ = 17.0, 1.5 Hz, 1H), 6.12 (dd, $J$ = 17.0, 10.2 Hz, 1H), 5.95 (s, 1H), 5.62 (dd, $J$ = 10.2, 1.5 Hz, 1H), 3.36 – 3.31 (m, 2H), 1.56 – 1.49 (m, 2H), 1.41 – 1.32 (m, 2H), 0.93 (t, $J$ = 7.3 Hz, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 165.5, 131.0, 126.0, 39.3, 31.6, 20.0, 13.7.

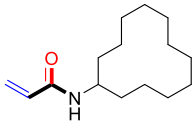


***N*-cyclobutylacrylamide (3at)**[10]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.4) to give the titled product **3at** as a yellow oil (19.0 mg, 76%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 6.42 (s, 1H), 6.23 (dd, $J$ = 17.0, 1.2 Hz, 1H), 6.09 (dd, $J$ = 17.0, 10.2 Hz, 1H), 5.58 (dd, $J$ = 10.2, 1.2 Hz, 1H), 4.48 – 4.38 (m, 1H), 2.35 – 2.28 (m, 2H), 1.94 – 1.84 (m, 2H), 1.72 – 1.65 (m, 2H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 164.6, 130.9, 126.4, 44.7, 31.1, 15.2.

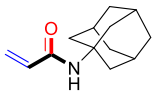


***N*-cyclododecylacrylamide (3au)**[10]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.4) to give the titled product **3au** as a white solid (38.9 mg, 82%).

**$^1$H NMR (400 MHz, DMSO)** $\delta$ 7.84 (d, $J$ = 8.4 Hz, 1H), 6.20 (dd, $J$ = 17.1, 10.1 Hz, 1H), 6.04 (dd, $J$ = 17.1, 2.4 Hz, 1H), 5.54 (dd, $J$ = 10.0, 2.4 Hz, 1H), 3.99 – 3.95 (m, 1H), 1.59 – 1.55 (m, 2H), 1.41 – 1.24 (m, 20H).

**$^{13}$C NMR (101 MHz, DMSO)** $\delta$ 164.3, 132.5, 125.1, 44.7, 30.5, 23.9, 23.7, 23.5, 23.2, 22.0.

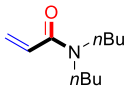


***N*-((3s,5s,7s)-adamantan-1-yl)acrylamide (3av)**[10]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.4) to give the titled product **3av** as a white solid (40.6 mg, 99%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 6.20 (dd, $J$ = 16.9, 0.6 Hz, 1H), 6.01 (dd, $J$ = 16.9, 10.2 Hz, 1H), 5.54 (dd, $J$ = 10.1, 1.0 Hz, 1H), 5.32 (s, 1H), 2.07 – 2.03 (m, 9H), 1.71 – 1.68 (m, 6H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 164.5, 132.2, 125.5, 52.1, 41.6, 36.3, 29.4.

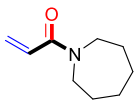


***N*,*N*-dibutylacrylamide (3aw)**[11]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.5) to give the titled product **3aw** as a yellow oil (30.4 mg, 83%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 6.51 (dd, $J$ = 16.7, 10.3 Hz, 1H), 6.33 – 6.28 (m, 1H), 5.64 – 5.60 (m, 1H), 3.36 – 3.24 (m, 4H), 1.57 – 1.47 (m, 4H), 1.34 – 1.25 (m, 4H), 0.93 – 0.88 (m, 6H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 165.9, 127.9, 127.5, 47.9, 46.4, 31.8, 29.9, 20.3, 20.0, 13.9, 13.8.

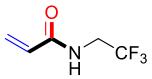


**1-(azepan-1-yl)prop-2-en-1-one (3ax)**[12]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.5) to give the titled product **3ax** as a yellow oil (23.6 mg, 77%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 6.58 – 6.51 (m, 1H), 6.31 – 6.27 (m, 1H), 5.64 – 5.61 (m, 1H), 3.57 – 3.54 (m, 2H), 3.49 – 3.46 (m, 2H), 1.75 – 1.67 (m, 4H), 1.57 – 1.50 (m, 4H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 166.2, 127.9, 127.4, 47.8, 46.3, 29.2, 27.4, 26.9, 26.5.



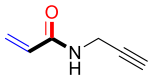
***N*-(2,2,2-trifluoroethyl)acrylamide (3ay)**[13]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.4) to give the titled product **3ay** as a white solid (20.8 mg, 68%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 6.36 (dd, $J$ = 17.0, 1.2 Hz, 1H), 6.24 – 6.13 (m, 2H), 5.75 (dd, $J$ = 10.3, 1.2 Hz, 1H), 4.03 – 3.94 (m, 2H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 165.7, 129.6, 128.4, 124.1 (q, $J$ = 278.3 Hz), 40.7 (q, $J$ = 34.8 Hz).

**$^{19}$F NMR (376 MHz, $CDCl_3$)** $\delta$ -72.4.

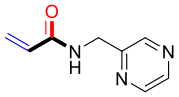


***N*-(prop-2-yn-1-yl)acrylamide (3az)**[14]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 5/1, $R_f$ = 0.5) to give the titled product **3az** as a yellow oil (8.9 mg, 41%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 6.31 (dd, $J$ = 17.0, 0.9 Hz, 1H), 6.15 – 6.04 (m, 2H), 5.68 (dd, $J$ = 10.3, 1.0 Hz, 1H), 4.13 (dd, $J$ = 5.3, 2.5 Hz, 2H), 2.24 (t, $J$ = 2.5 Hz, 1H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 165.2, 130.1, 127.3, 79.3, 71.8, 29.3.



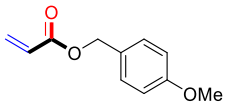
***N*-(pyrazin-2-ylmethyl)acrylamide (4aa)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 3/1, $R_f$ = 0.2) to give the titled product **4aa** as a yellow oil (22.8 mg, 70%).

**$^1$H NMR (400 MHz, DMSO)** $\delta$ 8.79 (s, 1H), 8.58 – 8.53 (m, 3H), 6.31 (dd, $J$ = 17.1, 10.2 Hz, 1H), 6.13 (dd, $J$ = 17.1, 2.1 Hz, 1H), 5.64 (dd, $J$ = 10.2, 2.1 Hz, 1H), 4.50 (d, $J$ = 5.9 Hz, 2H).

**$^{13}$C NMR (101 MHz, DMSO)** $\delta$ 165.4, 154.5, 144.4, 143.9, 143.7, 131.8, 126.3, 42.7.

HRMS (ES-TOF): m/z calcd. for $C_8H_9N_3NaO^+$ [M+$Na^+$] 186.0638, found 186.0643.



**4-methoxybenzyl acrylate (5aa)**[15]

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether/ethyl acetate = 10/1, $R_f$ = 0.5) to give the titled product **5aa** as a colorless oil (20.4 mg, 53%).

**$^1$H NMR (400 MHz, $CDCl_3$)** $\delta$ 7.33 – 7.31 (m, 2H), 6.92 – 6.88 (m, 2H), 6.43 (dd, $J$ = 17.3, 1.4 Hz, 1H), 6.14 (dd, $J$ = 17.3, 10.4 Hz, 1H), 5.83 (dd, $J$ = 10.4, 1.4 Hz, 1H), 5.14 (s, 2H), 3.81 (s, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** $\delta$ 166.1, 159.6, 130.9, 130.1, 128.4, 127.9, 113.9, 66.1, 55.3.

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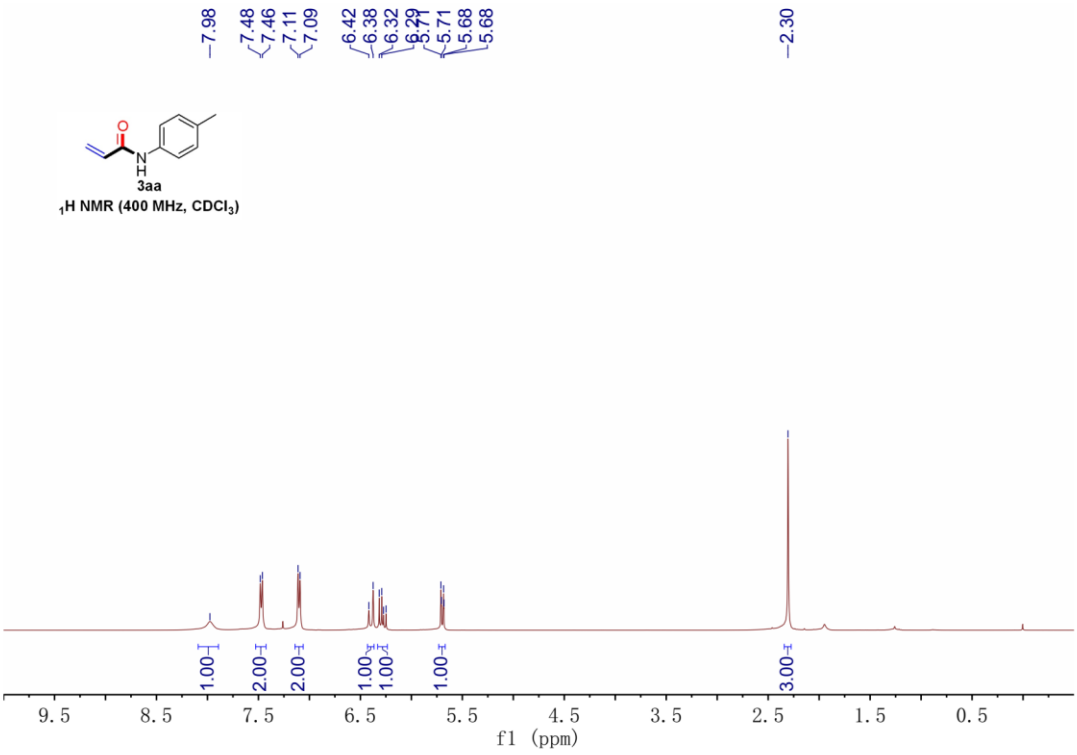
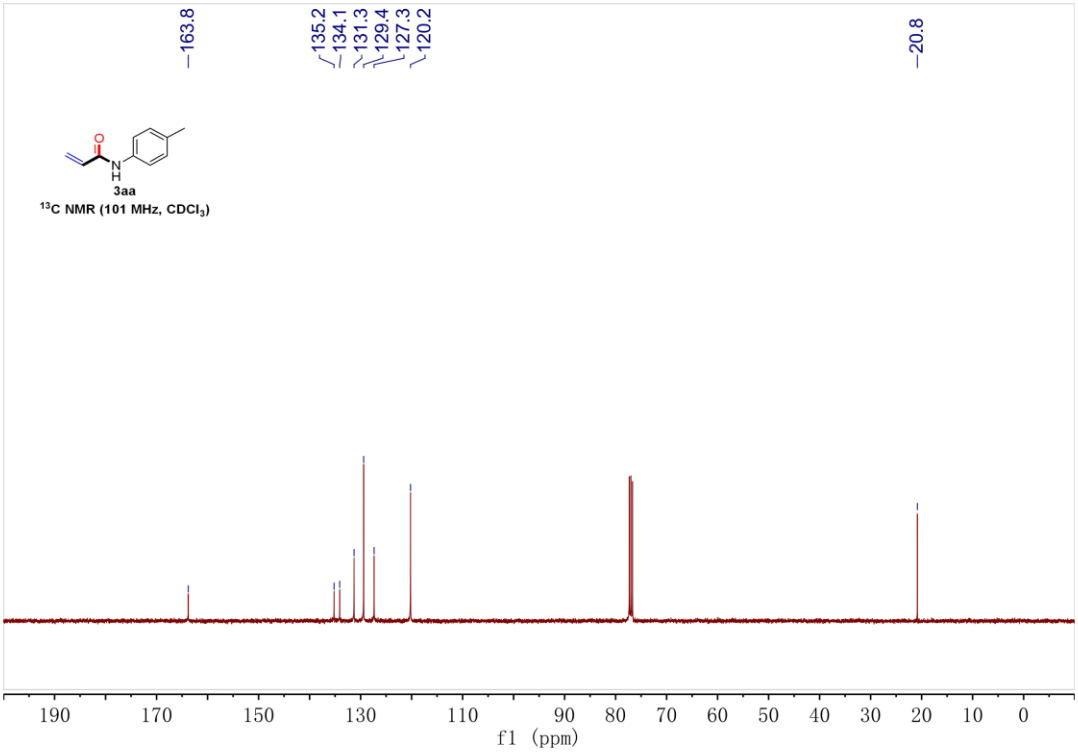
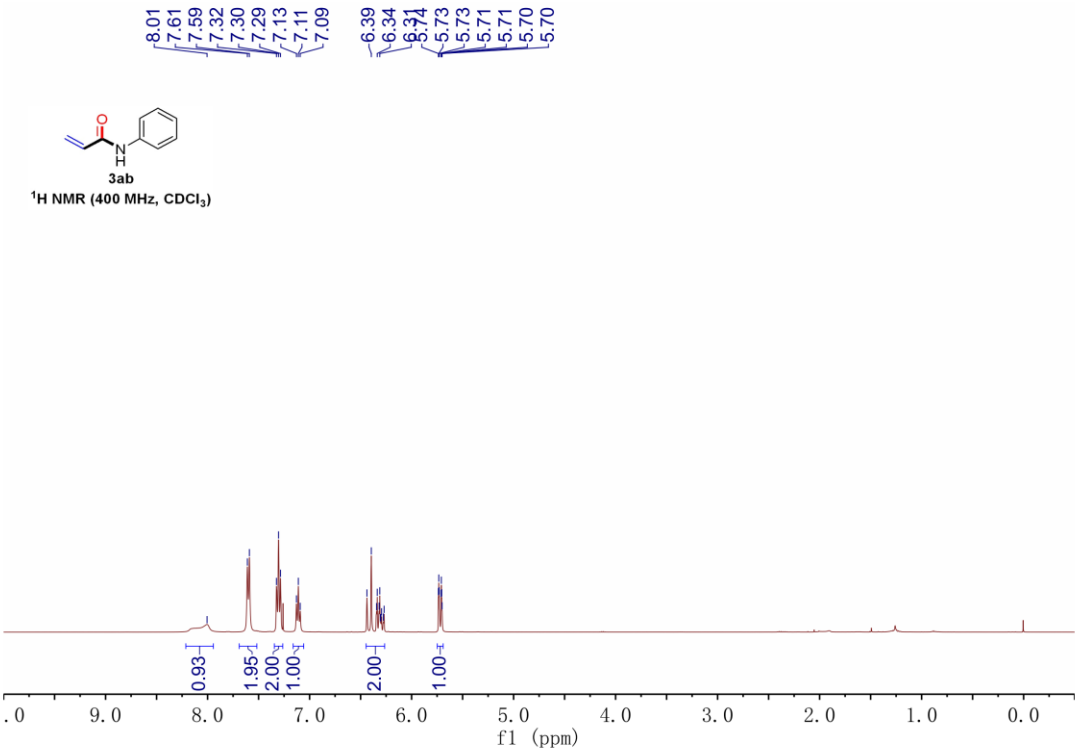
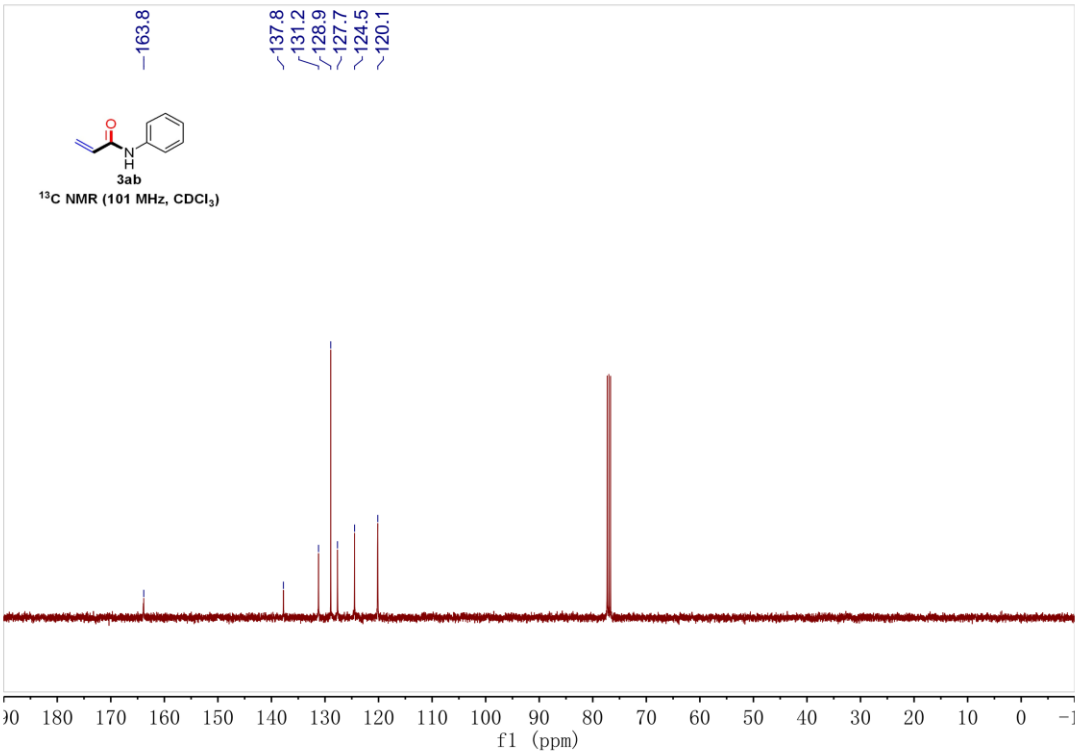
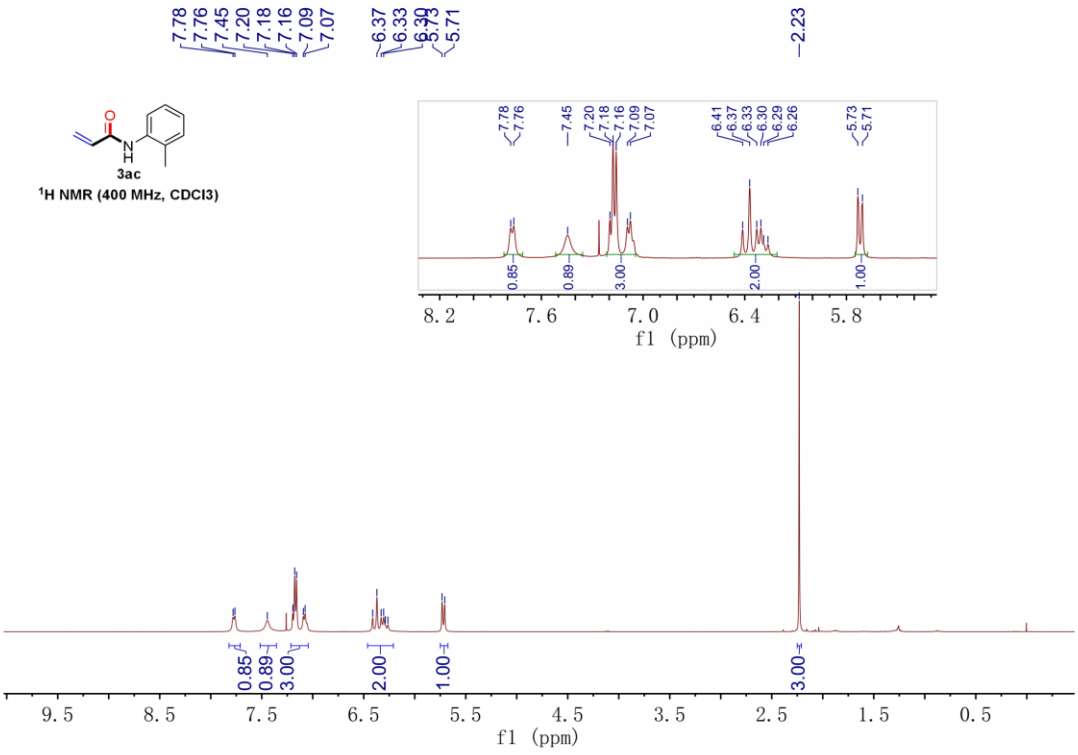
## 7. Copy of $^{1}H$, $^{13}C$ and $^{19}F$ NMR Spectra of Products

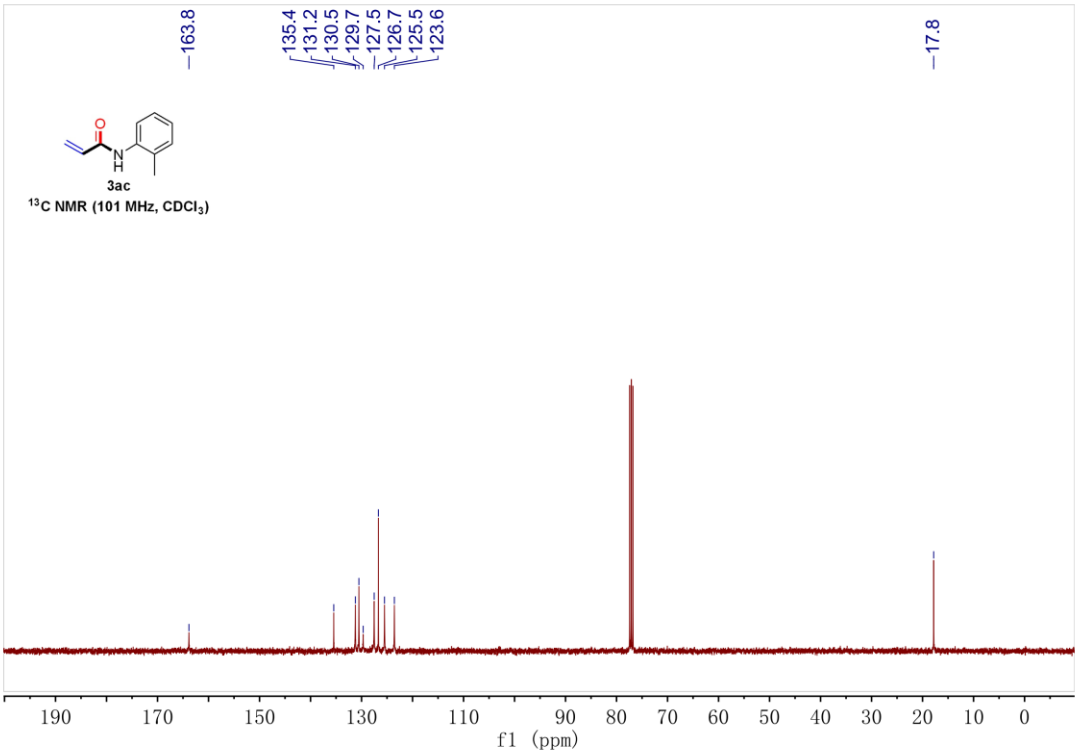


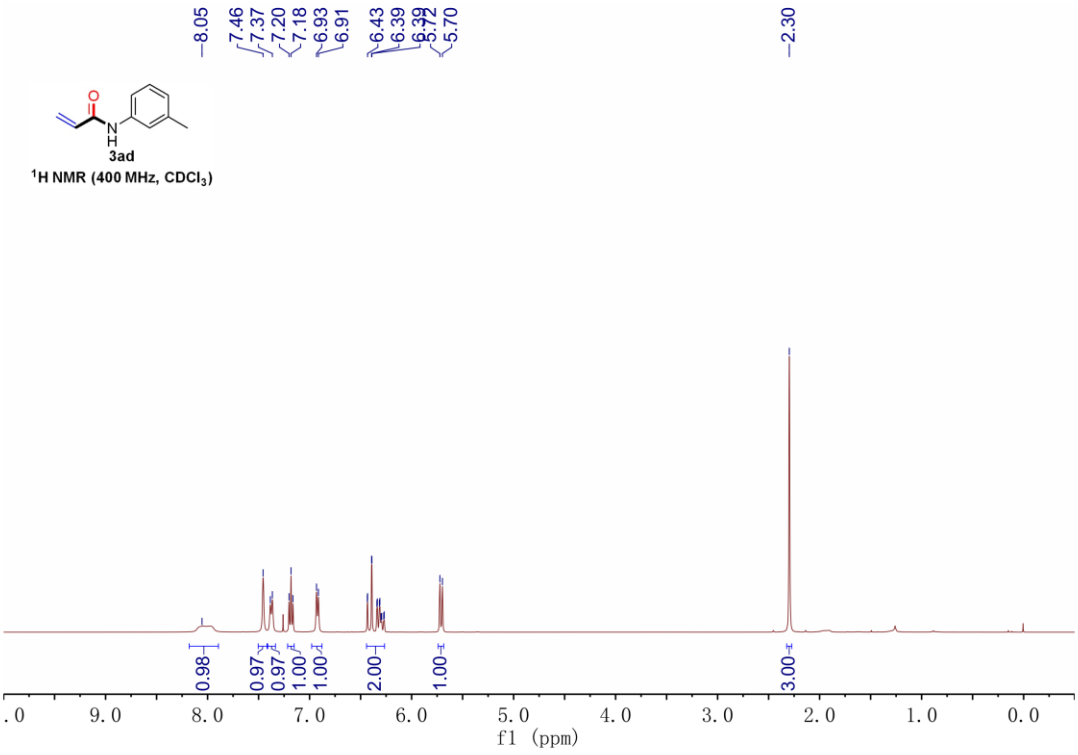



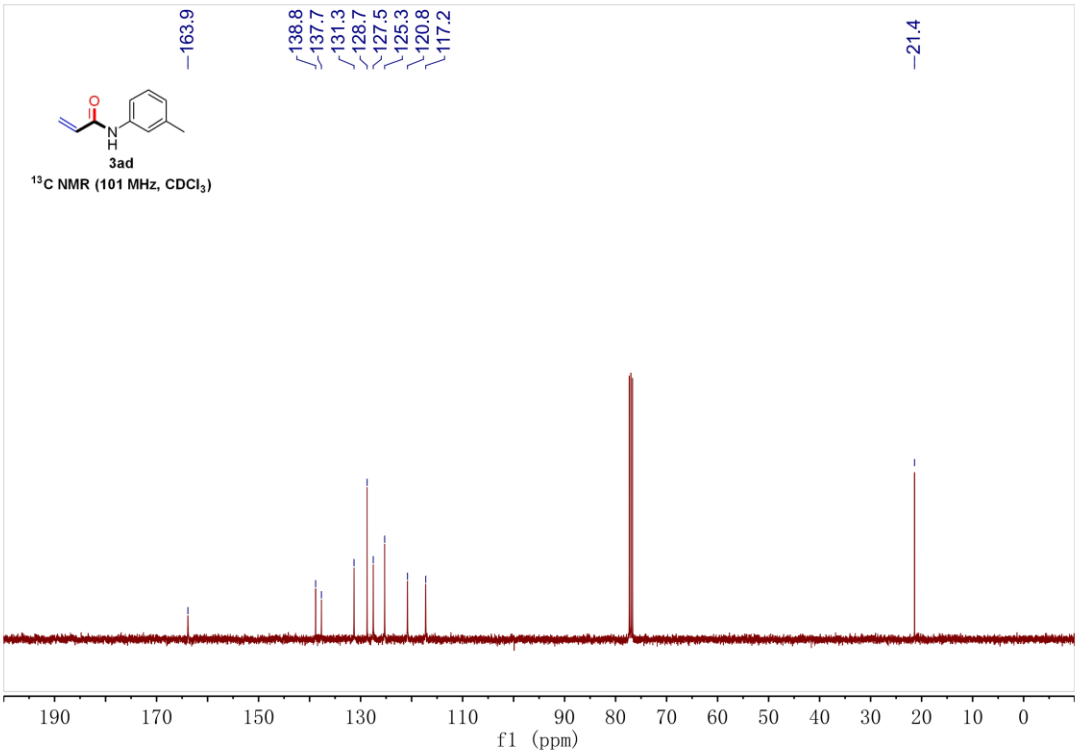

8.01
7.61
7.59
7.32
7.30
7.29
7.13
7.11
7.09
6.39
6.34
6.31
5.74
5.73
5.73
5.71
5.71
5.70
5.70
3ab
¹H NMR (400 MHz, CDCl₃)
0.93
1.95
2.00
1.00
2.00
1.00
f1 (ppm)

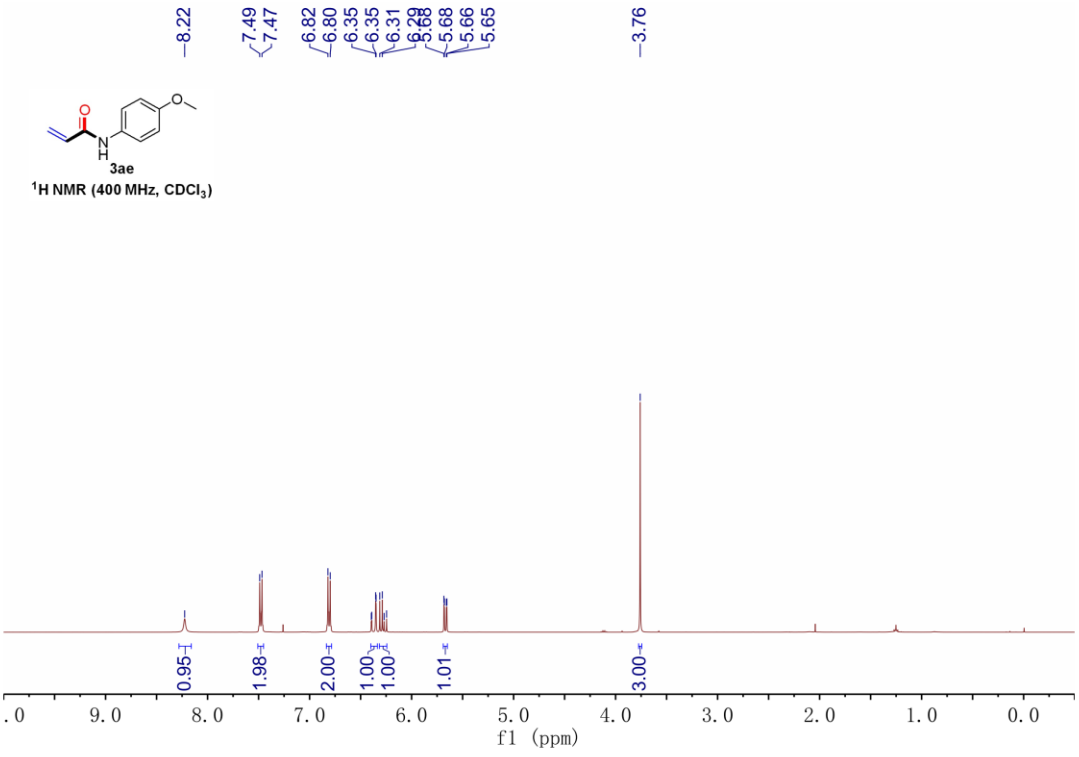

163.8
137.8
131.2
128.9
127.7
124.5
120.1
3ab
¹³C NMR (101 MHz, CDCl₃)
f1 (ppm)

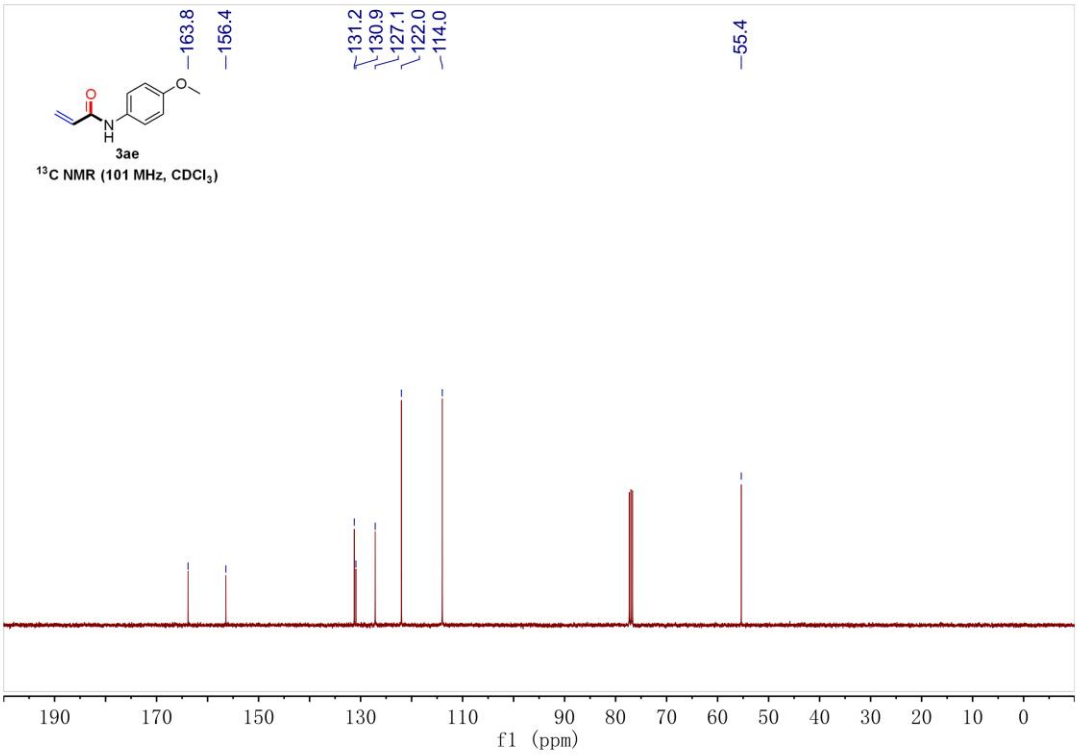

7.78
7.76
7.45
7.20
7.18
7.16
7.09
7.07
6.37
6.33
5.73
5.71
2.23
3ac
1H NMR (400 MHz, CDCl3)
0.85
0.89
3.00
2.00
1.00
3.00
f1 (ppm)

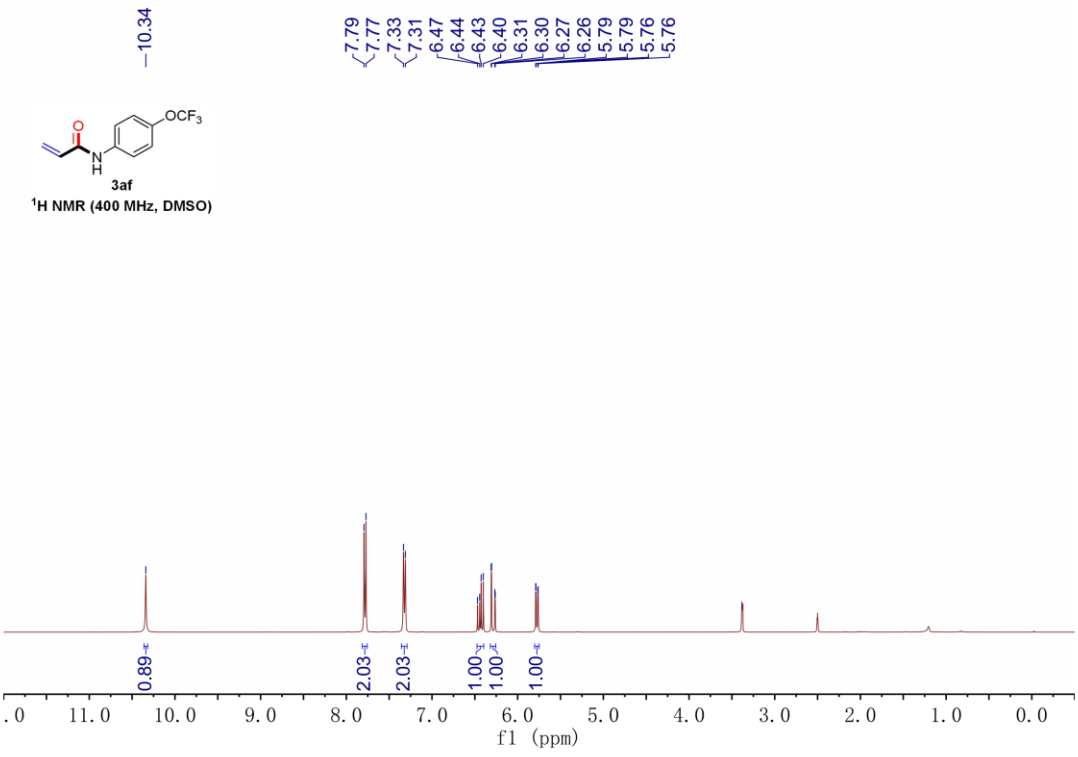

163.8
135.4
131.2
130.5
129.7
127.5
126.7
125.5
123.6
17.8
3ac
13C NMR (101 MHz, CDCl3)
f1 (ppm)

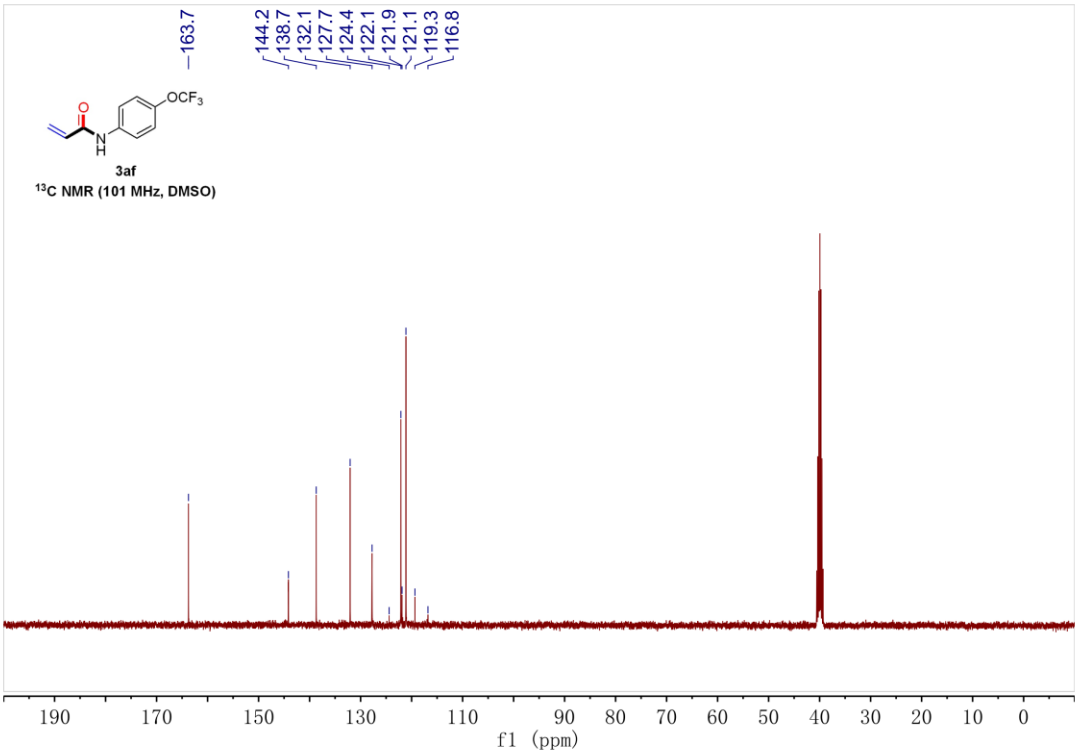

8.05
7.46
7.37
7.20
7.18
6.93
6.91
6.43
6.39
5.72
5.70
2.30
3ad
$^{1}$H NMR (400 MHz, $CDCl_3$)
0.98
0.97
0.97
1.00
1.00
2.00
1.00
3.00
f1 (ppm)

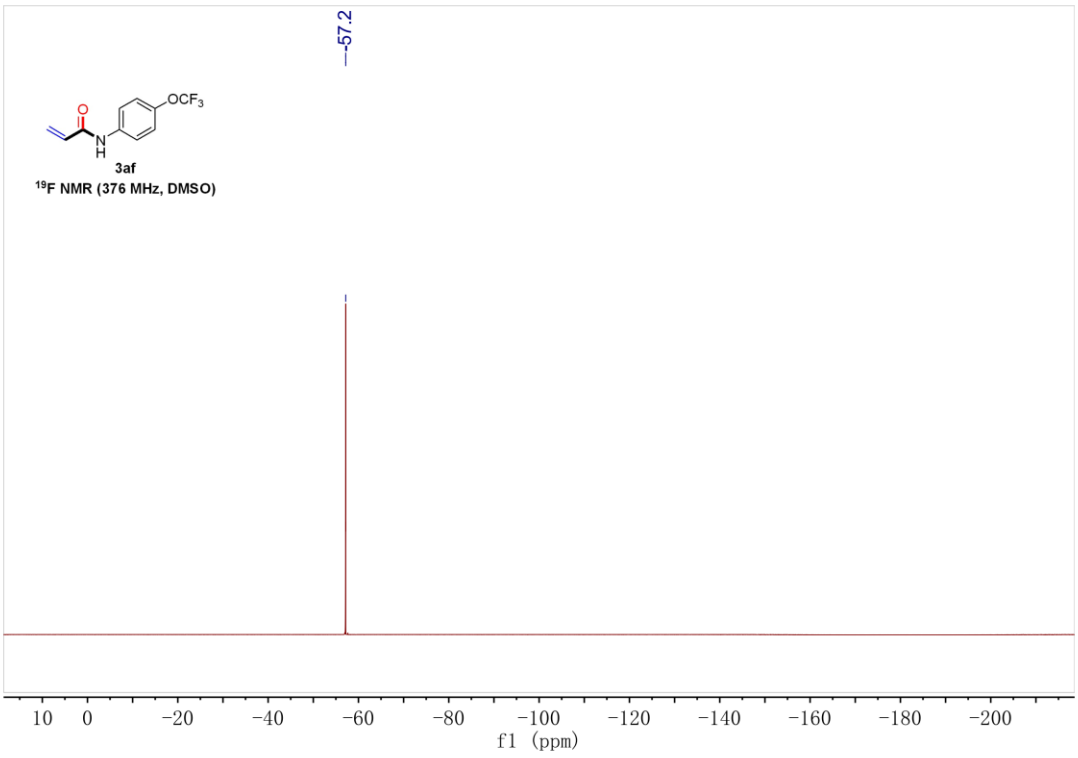

163.9
138.8
137.7
131.3
128.7
127.5
125.3
120.8
117.2
21.4
3ad
$^{13}$C NMR (101 MHz, $CDCl_3$)
f1 (ppm)


8.22
7.49
7.47
6.82
6.80
6.35
6.35
6.31
6.29
5.68
5.66
5.65
3.76
3ae
$^1$H NMR (400 MHz, CDCl$_3$)
0.95
1.98
2.00
1.00
1.00
1.01
3.00
f1 (ppm)


163.8
156.4
131.2
130.9
127.1
122.0
114.0
55.4
3ae
$^{13}$C NMR (101 MHz, CDCl$_3$)
f1 (ppm)

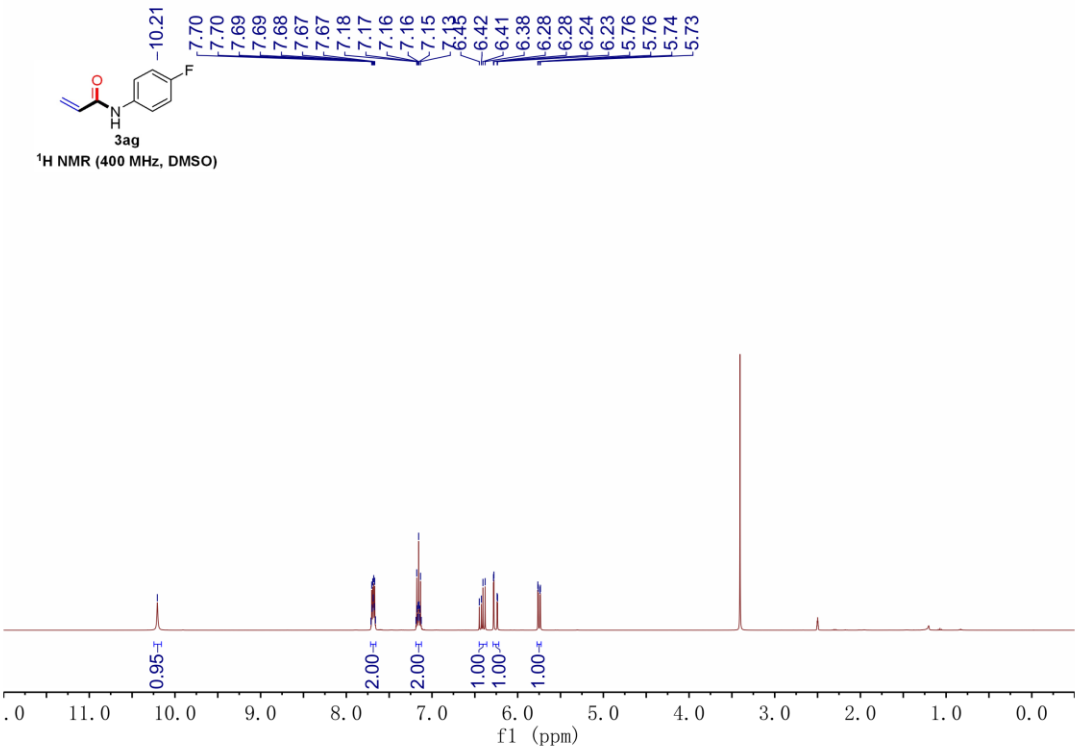

10.34
7.79
7.77
7.33
7.31
6.47
6.44
6.43
6.40
6.31
6.30
6.27
6.26
5.79
5.79
5.76
5.76
OCF3
O
N
H
3af
1H NMR (400 MHz, DMSO)
0.89
2.03
2.03
1.00
1.00
1.00
f1 (ppm)

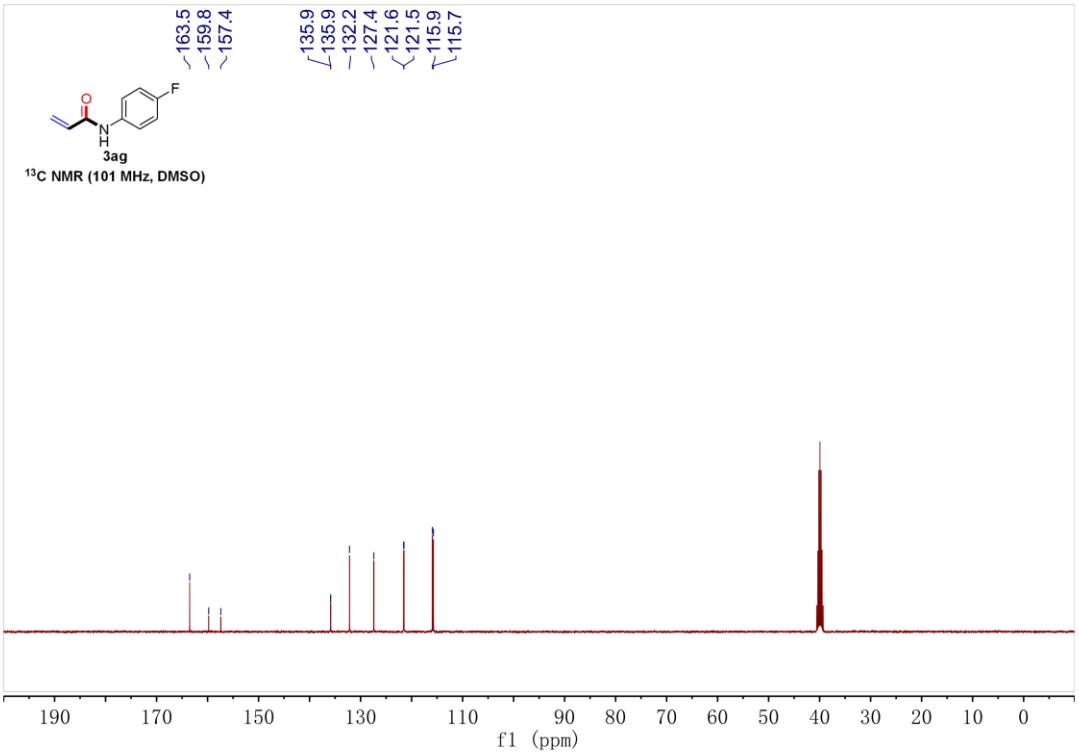

163.7
144.2
138.7
132.1
127.7
124.4
122.1
121.9
121.1
119.3
116.8
OCF3
O
N
H
3af
13C NMR (101 MHz, DMSO)
f1 (ppm)

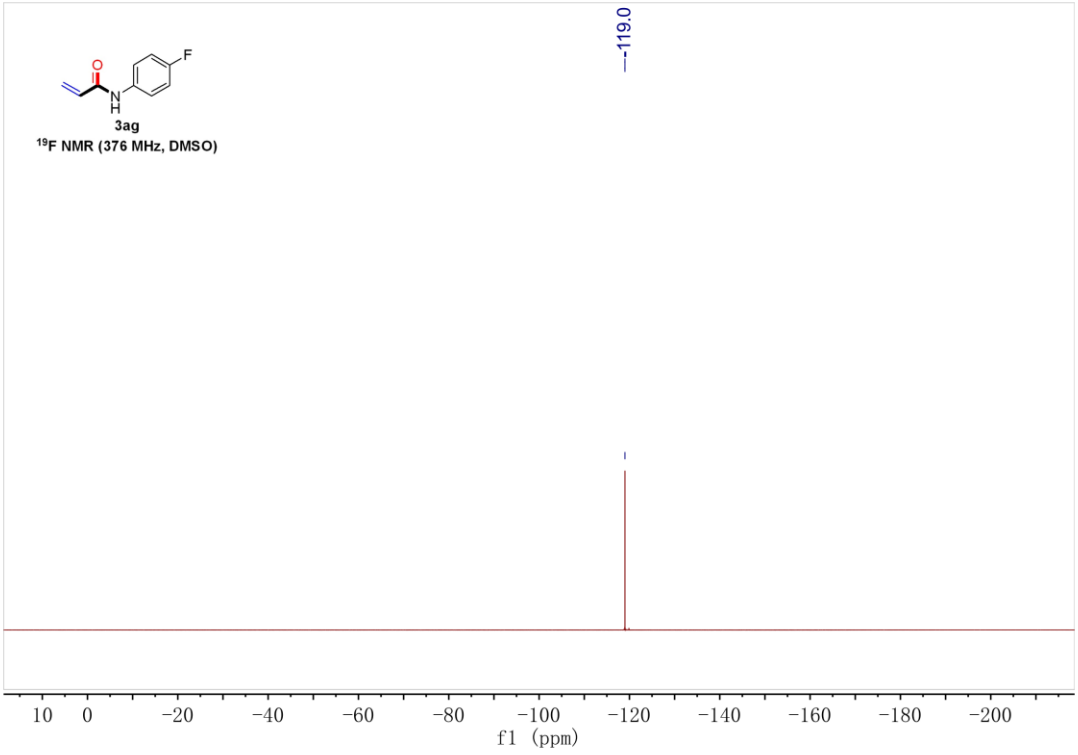


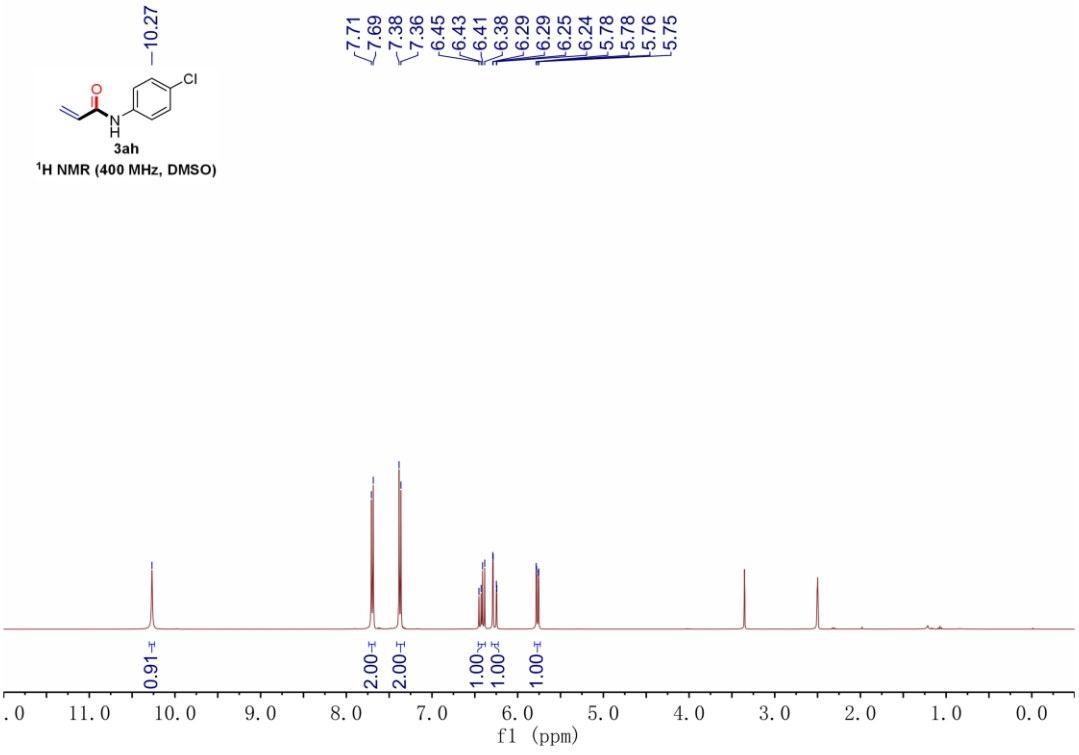

3af

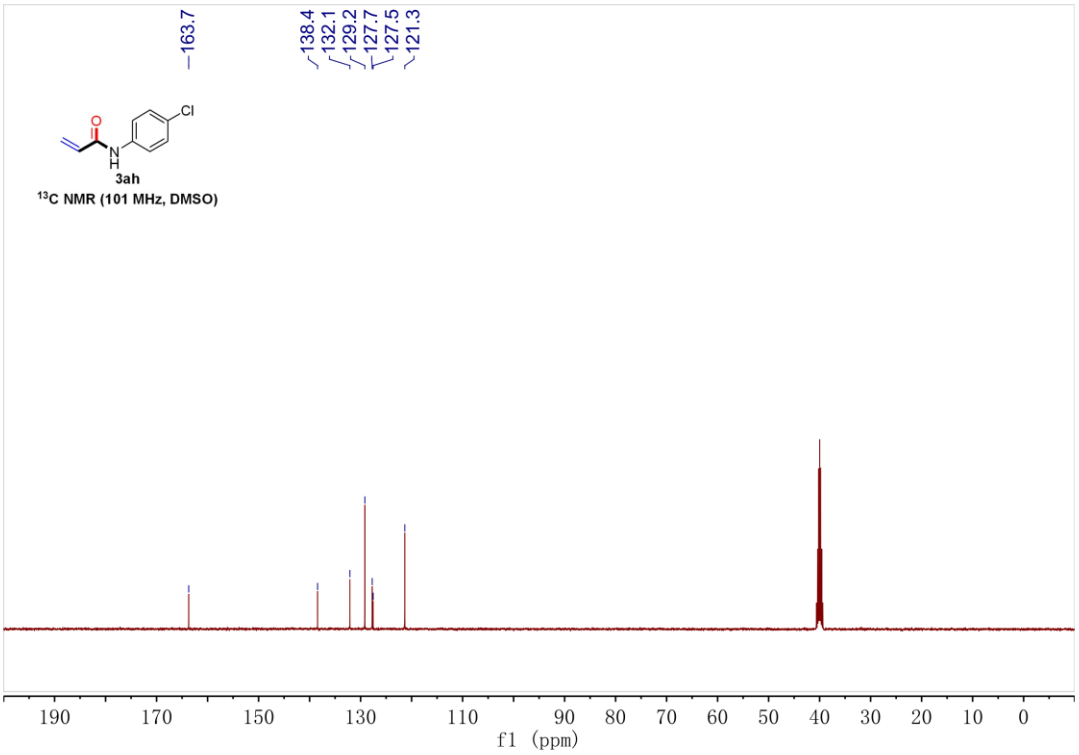
$^{19}$F NMR (376 MHz, DMSO)

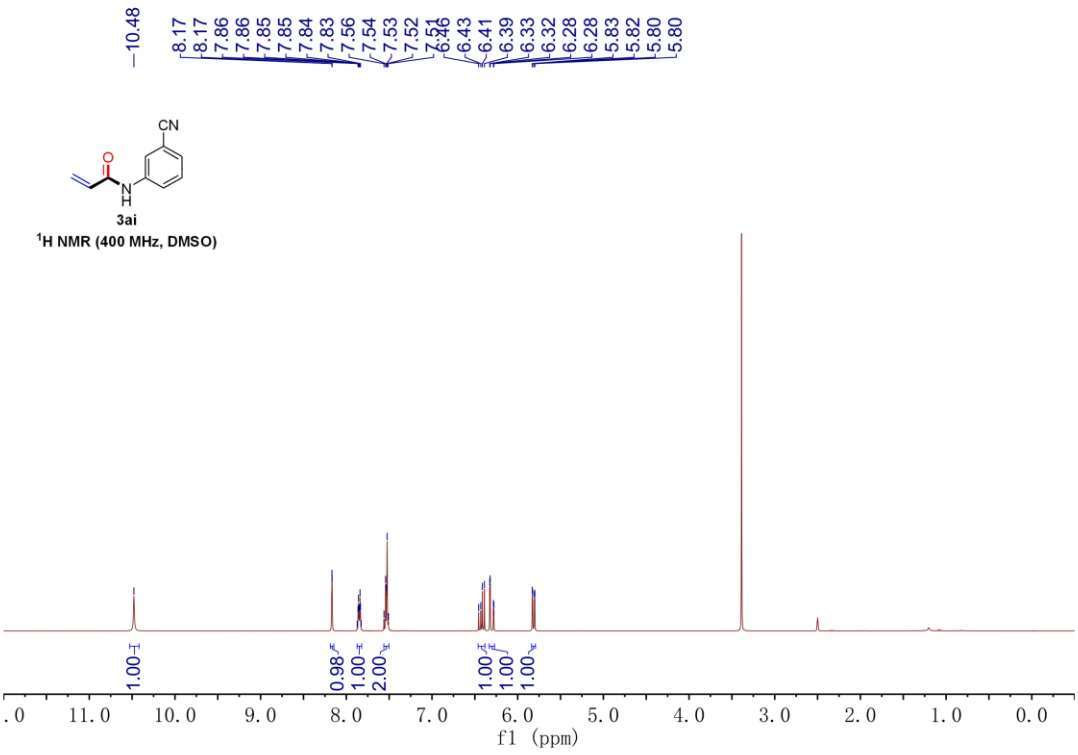

10.21
7.70
7.70
7.69
7.69
7.68
7.67
7.67
7.18
7.17
7.16
7.16
7.15
6.45
6.42
6.41
6.38
6.28
6.28
6.24
6.23
5.76
5.76
5.74
5.73
F
O
N
H
3ag
1H NMR (400 MHz, DMSO)
0.95
2.00
2.00
1.00
1.00
1.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

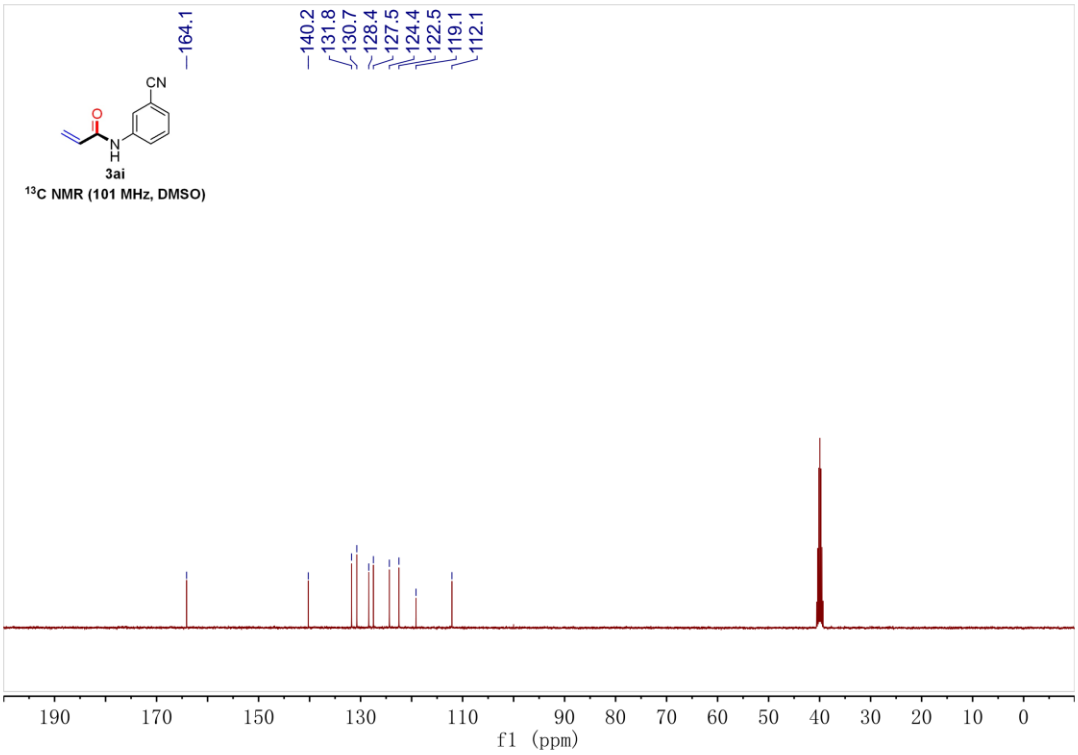

163.5
159.8
157.4
135.9
135.9
132.2
127.4
121.6
121.5
115.9
115.7
F
O
N
H
3ag
13C NMR (101 MHz, DMSO)
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

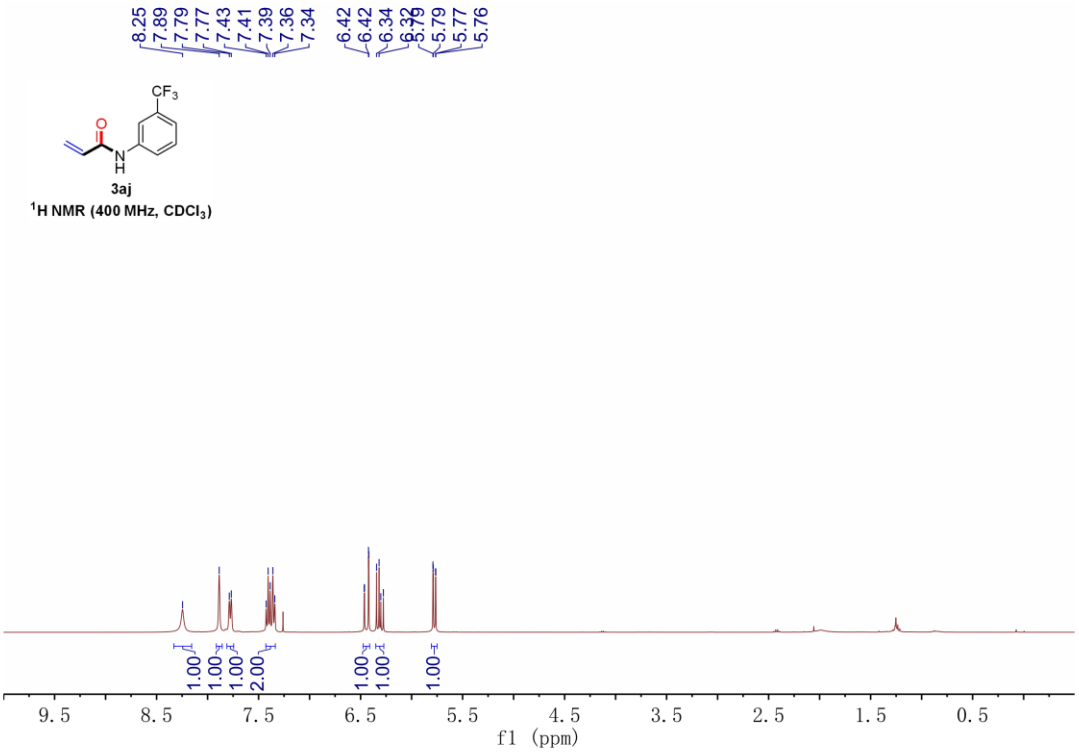

-119.0
F
O
N
H
3ag
19F NMR (376 MHz, DMSO)
10
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

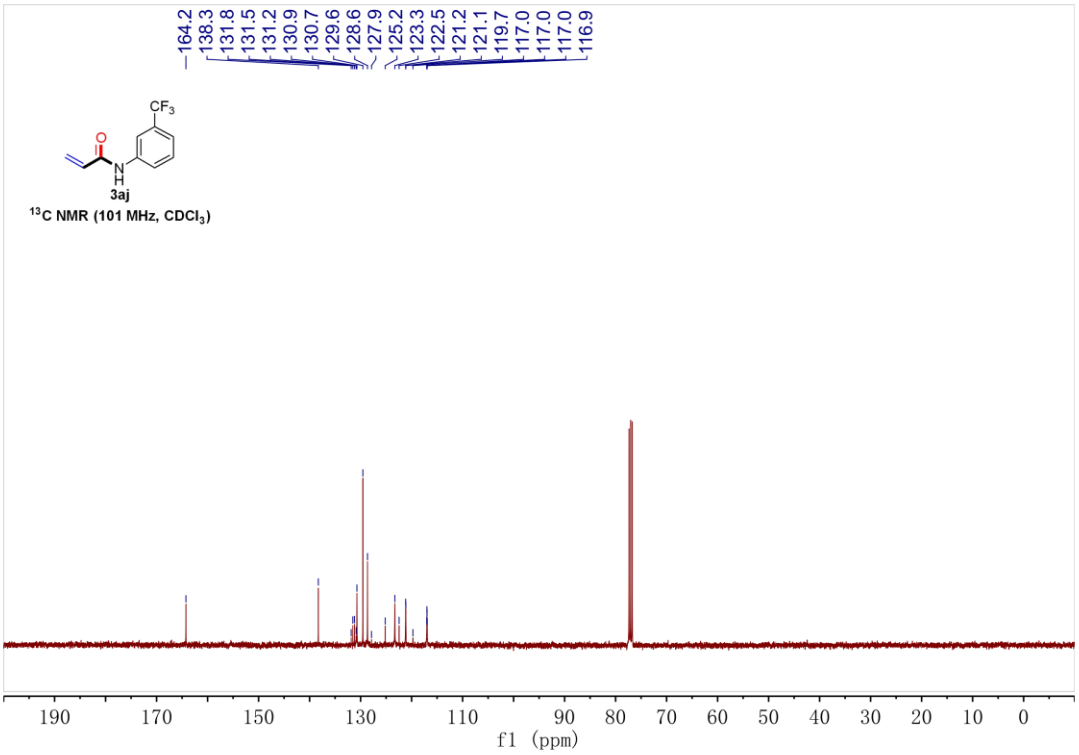

10.27
7.71
7.69
7.38
7.36
6.45
6.43
6.41
6.38
6.29
6.29
6.25
6.24
5.78
5.78
5.76
5.75
Cl
O
N
H
3ah
1H NMR (400 MHz, DMSO)
0.91
2.00
2.00
1.00
1.00
1.00
f1 (ppm)

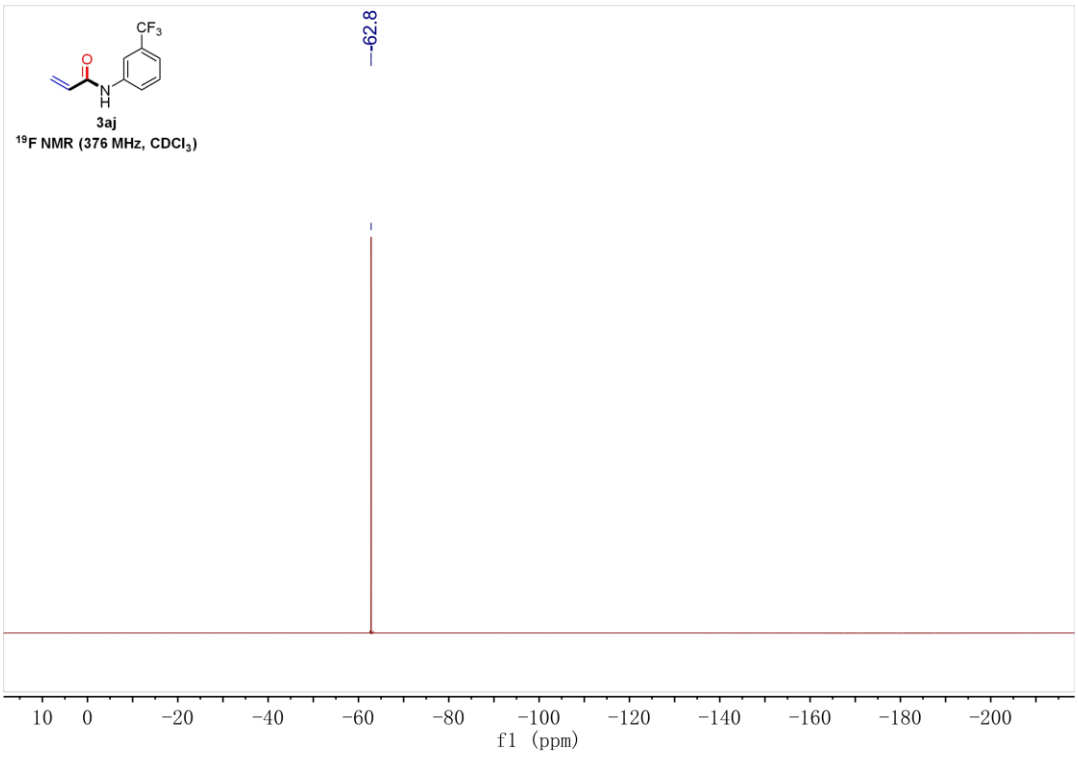

163.7
138.4
132.1
129.2
127.7
127.5
121.3
Cl
O
N
H
3ah
13C NMR (101 MHz, DMSO)
f1 (ppm)

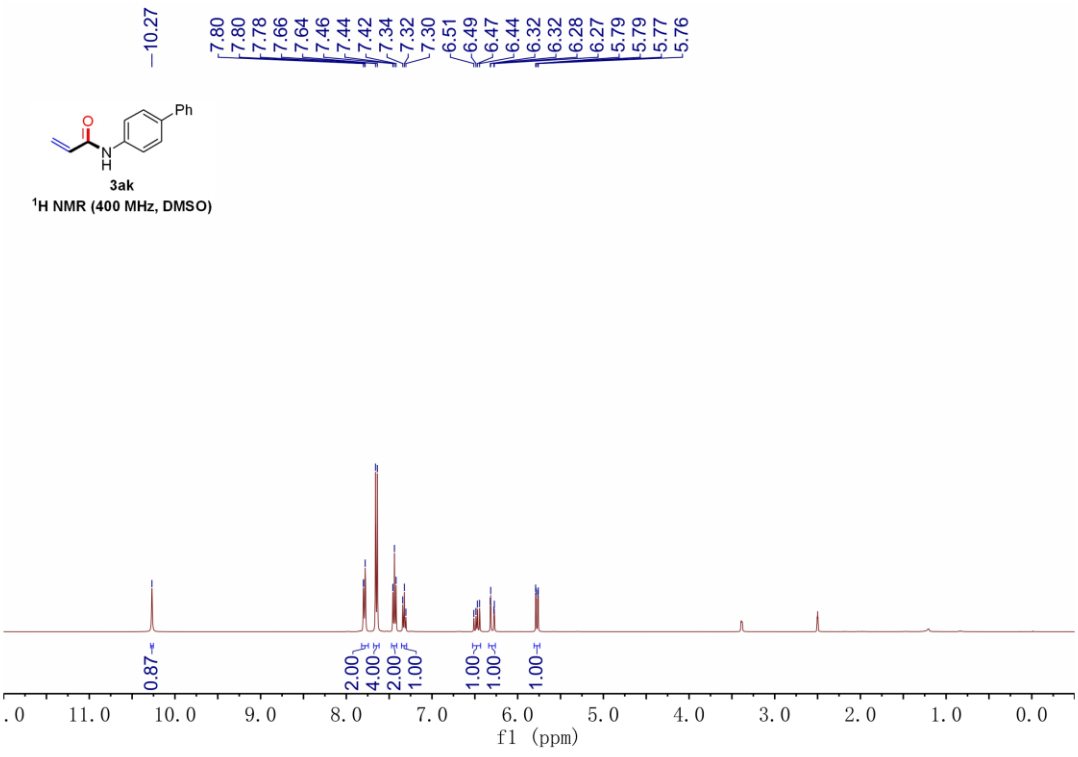

10.48
8.17
8.17
7.86
7.86
7.85
7.85
7.84
7.83
7.56
7.54
7.53
7.52
7.51
6.43
6.41
6.39
6.33
6.32
6.28
5.83
5.82
5.80
5.80
CN
O
N
H
3ai
1H NMR (400 MHz, DMSO)
1.00
0.98
1.00
2.00
1.00
1.00
1.00
f1 (ppm)


164.1
140.2
131.8
130.7
128.4
127.5
124.4
122.5
119.1
112.1
CN
O
N
H
3ai
13C NMR (101 MHz, DMSO)
f1 (ppm)


8.25
7.89
7.79
7.77
7.43
7.41
7.39
7.36
7.34
6.42
6.42
6.34
5.79
5.77
5.76
CF3
O
N
H
3aj
1H NMR (400 MHz, CDCl3)
1.00
1.00
1.00
2.00
1.00
1.00
1.00
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

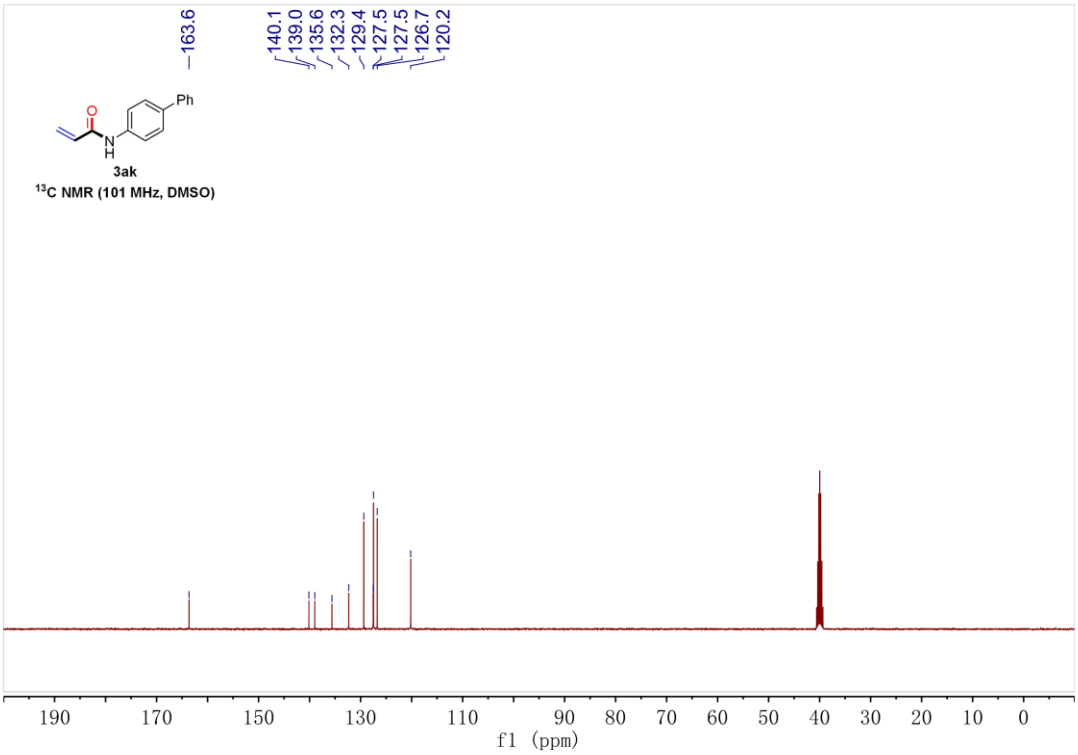

164.2
138.3
131.8
131.5
131.2
130.9
130.7
129.6
128.6
127.9
125.2
123.3
122.5
121.2
121.1
119.7
117.0
117.0
117.0
116.9
CF3
O
N
H
3aj
13C NMR (101 MHz, CDCl3)
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


CF3
O
N
H
3aj
19F NMR (376 MHz, CDCl3)
-62.8
10
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)



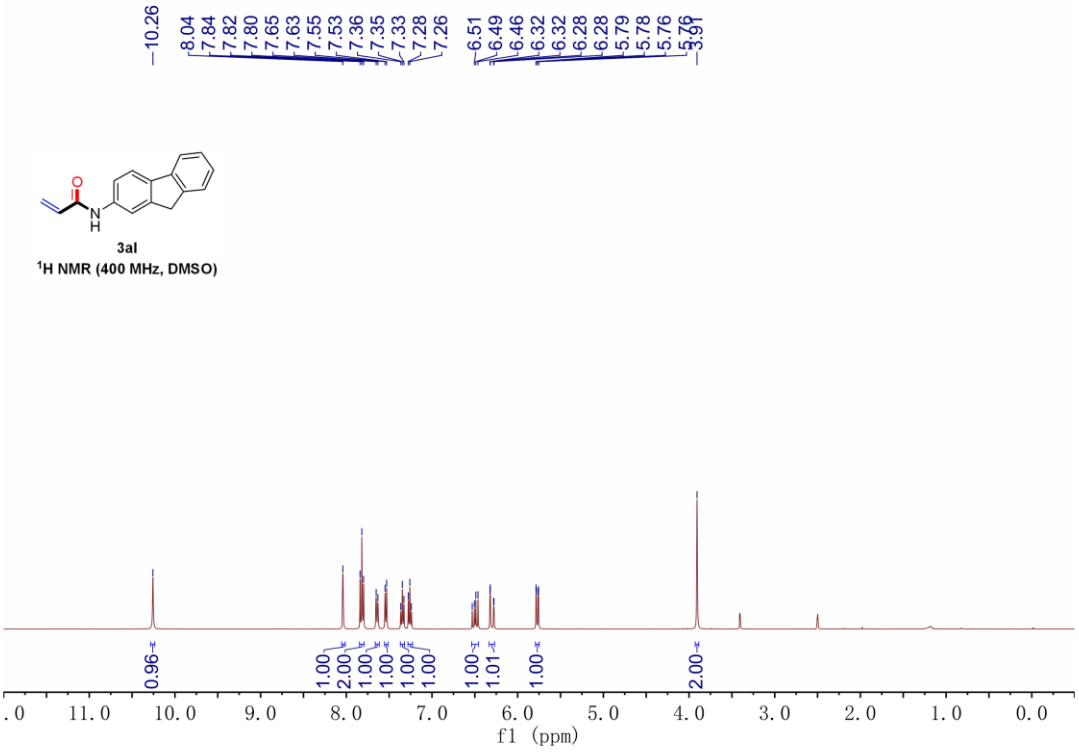

3ak

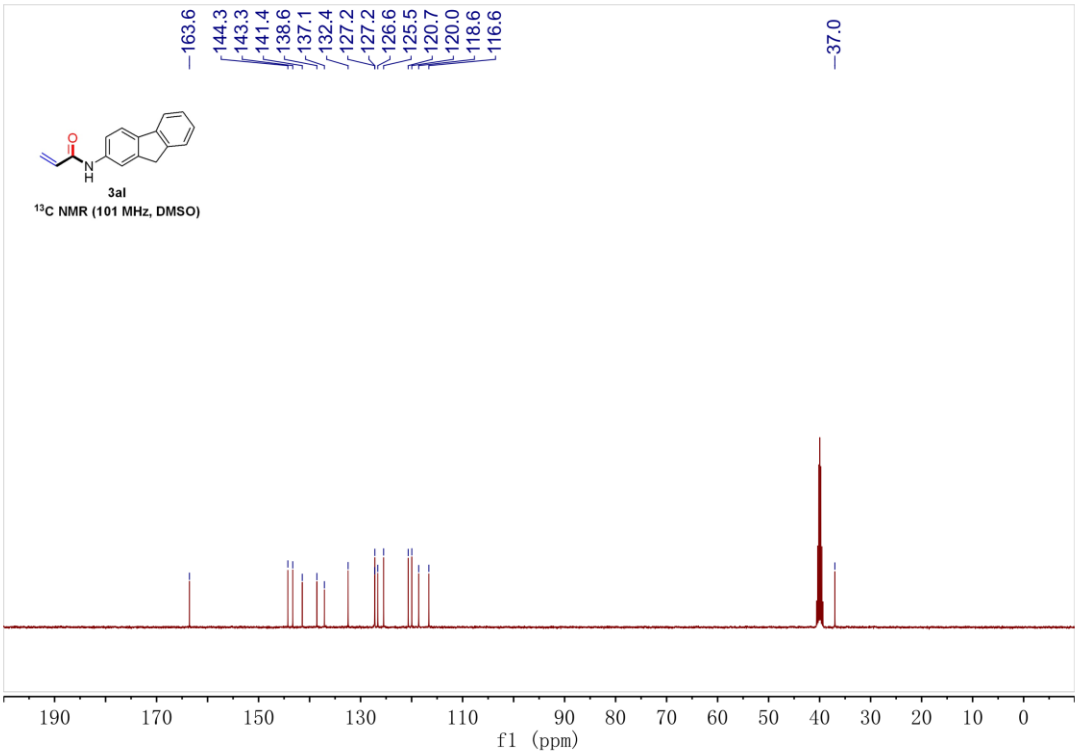
$^{1}$H NMR (400 MHz, DMSO)

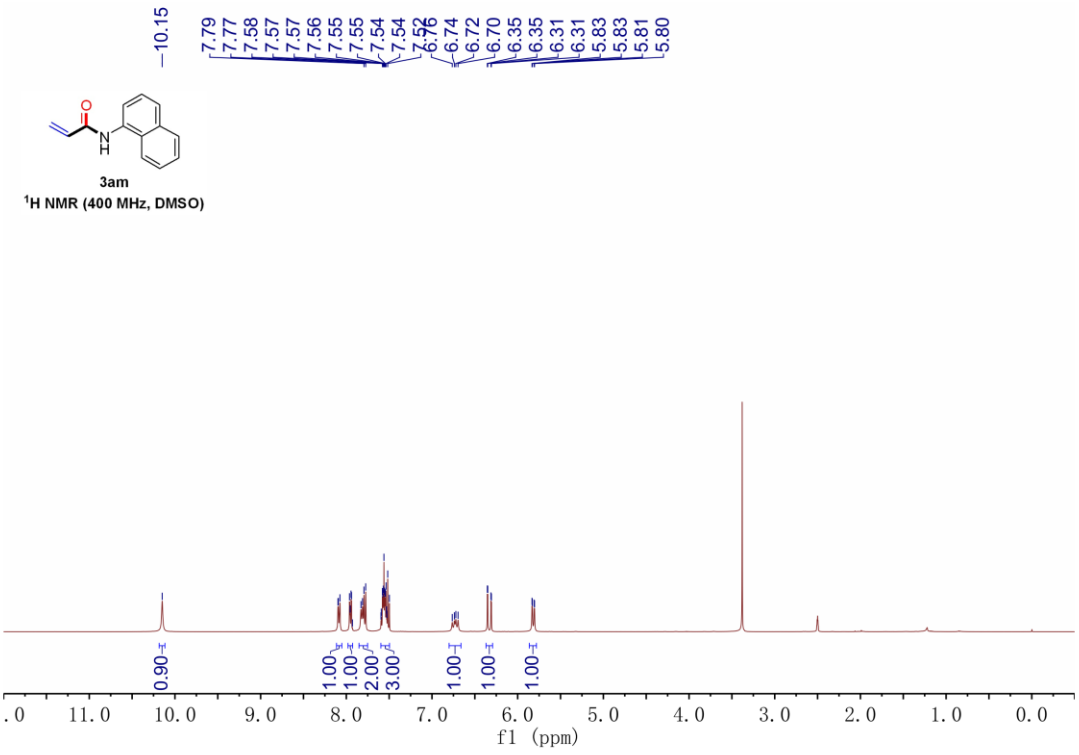


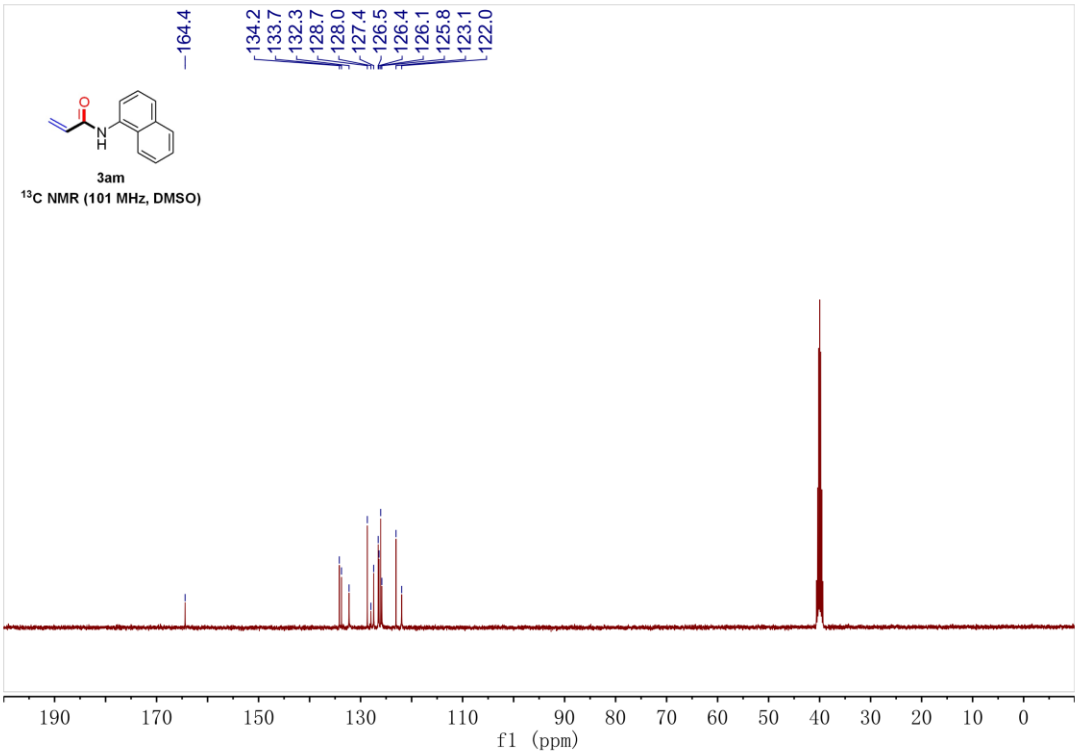

3ak

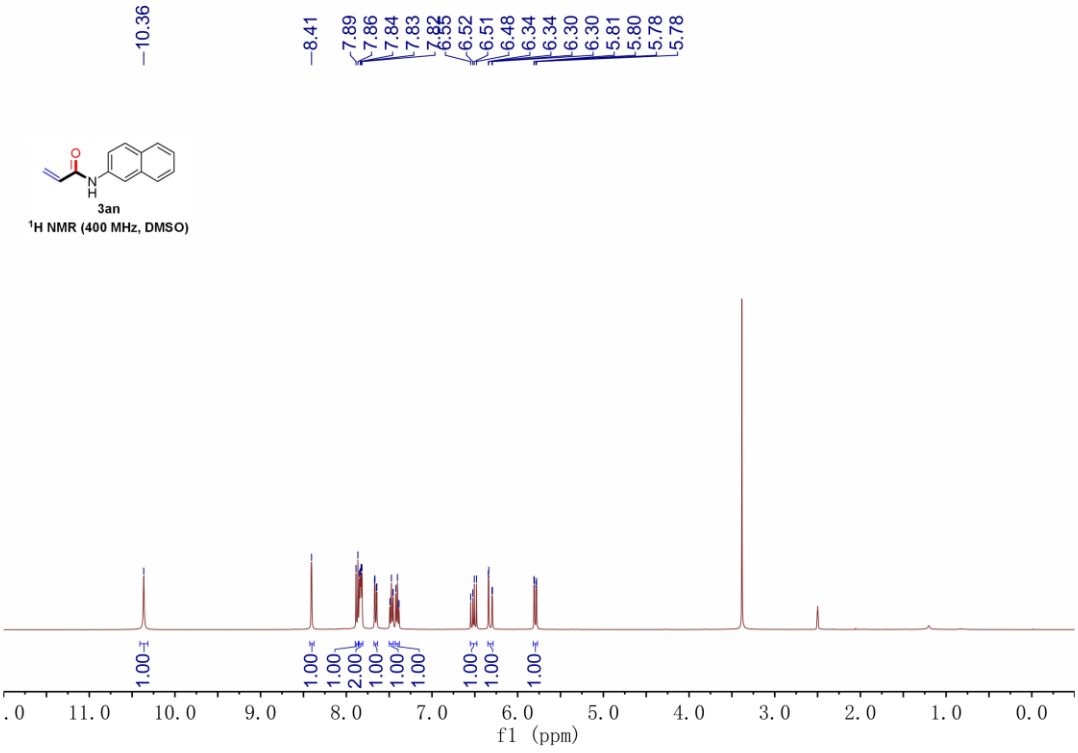
$^{13}$C NMR (101 MHz, DMSO)

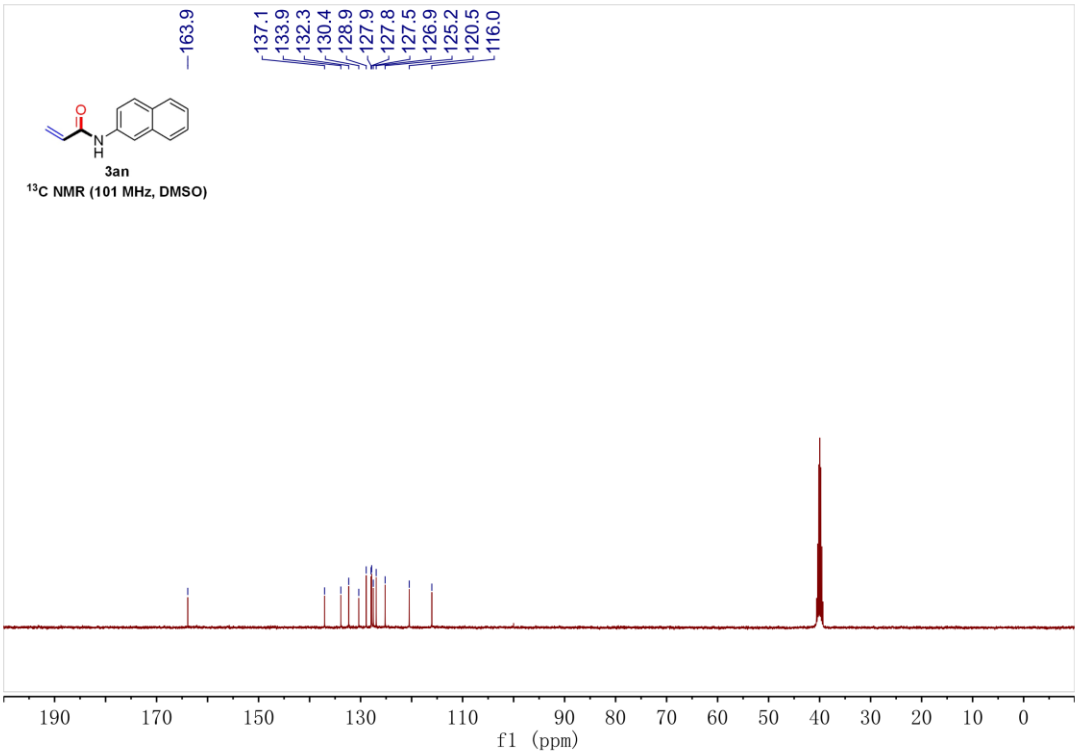

10.26
8.04
7.84
7.82
7.80
7.65
7.63
7.55
7.53
7.36
7.35
7.33
7.28
7.26
6.51
6.49
6.46
6.32
6.28
6.28
5.79
5.78
5.76
3.91
3al
1H NMR (400 MHz, DMSO)
0.96
1.00
2.00
1.00
1.00
1.00
1.00
1.01
1.00
2.00
f1 (ppm)

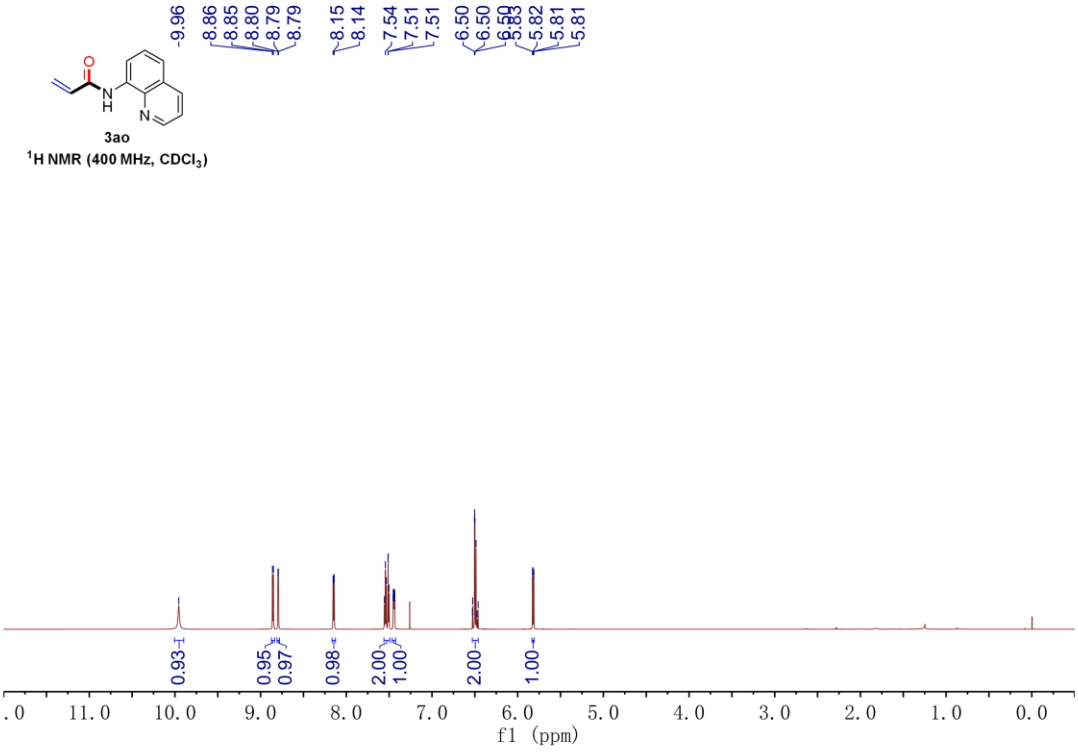

163.6
144.3
143.3
141.4
138.6
137.1
132.4
127.2
127.2
126.6
125.5
120.7
120.0
118.6
116.6
37.0
3al
13C NMR (101 MHz, DMSO)
f1 (ppm)


10.15
7.79
7.77
7.58
7.57
7.57
7.56
7.55
7.55
7.54
7.54
7.52
6.76
6.74
6.72
6.70
6.35
6.35
6.31
6.31
5.83
5.83
5.81
5.80
3am
1H NMR (400 MHz, DMSO)
0.90
1.00
1.00
2.00
3.00
1.00
1.00
1.00
f1 (ppm)


164.4
134.2
133.7
132.3
128.7
128.0
127.4
126.5
126.4
126.1
125.8
123.1
122.0
3am
13C NMR (101 MHz, DMSO)
f1 (ppm)

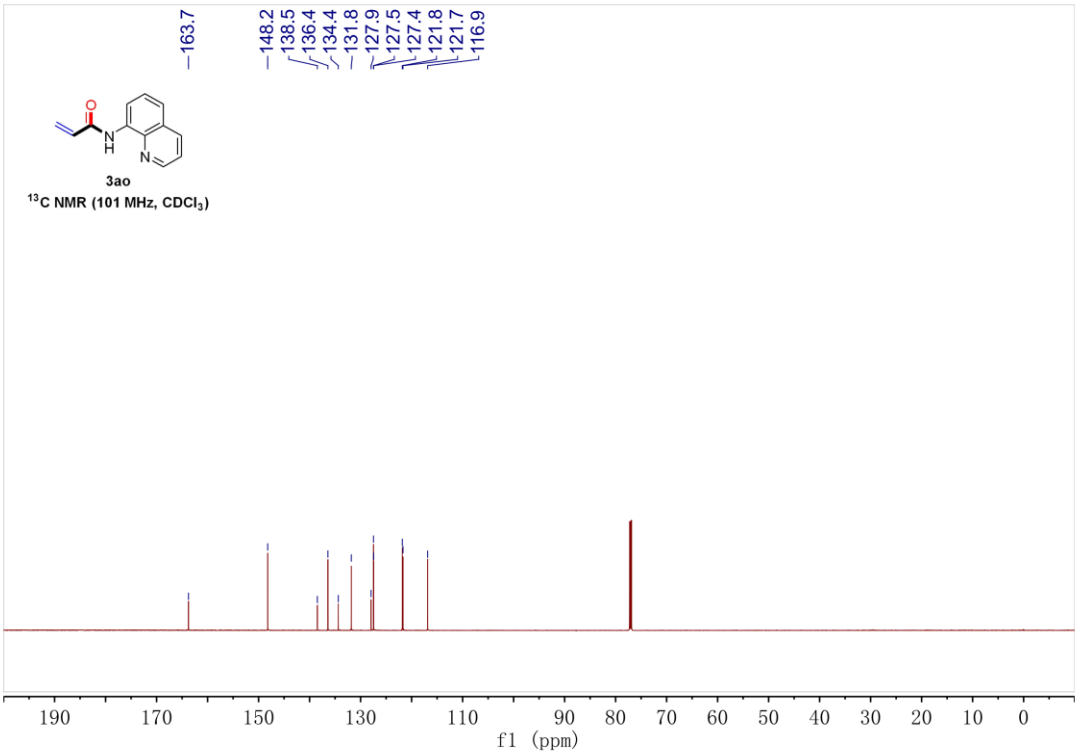

10.36
8.41
7.89
7.86
7.84
7.83
6.55
6.52
6.51
6.48
6.34
6.34
6.30
6.30
5.81
5.80
5.78
5.78
3an
1H NMR (400 MHz, DMSO)
1.00
1.00
1.00
2.00
1.00
1.00
1.00
1.00
1.00
f1 (ppm)


163.9
137.1
133.9
132.3
130.4
128.9
127.9
127.8
127.5
126.9
125.2
120.5
116.0
3an
13C NMR (101 MHz, DMSO)
f1 (ppm)



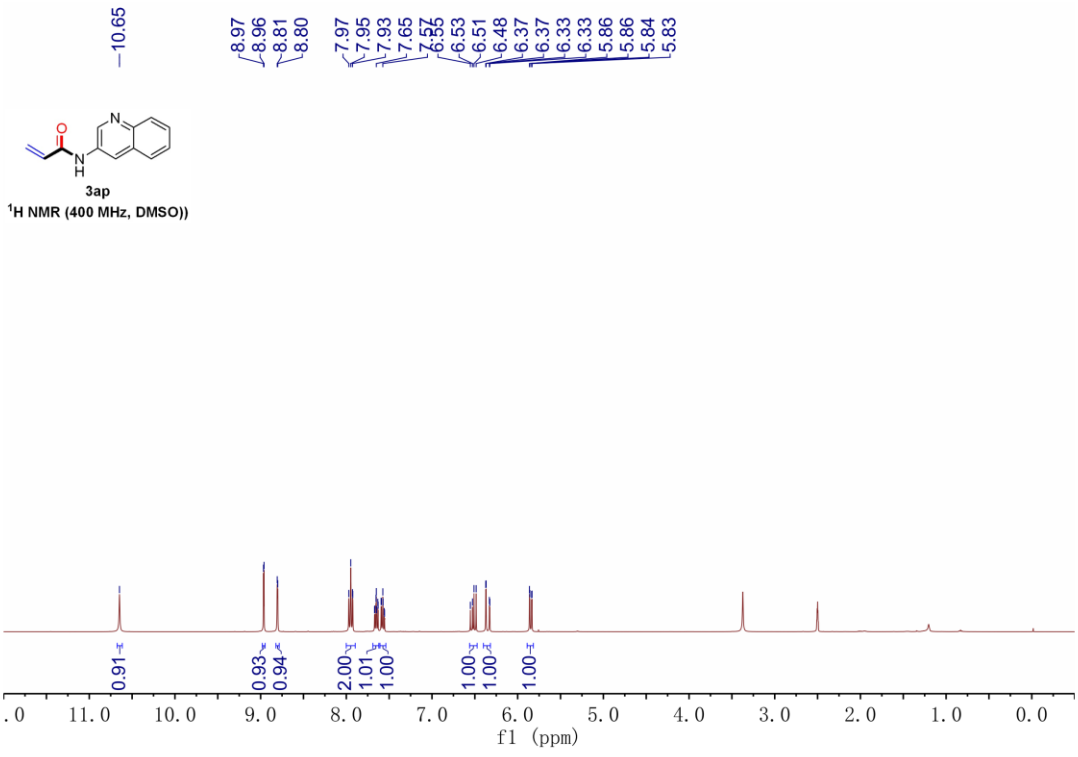

3ao

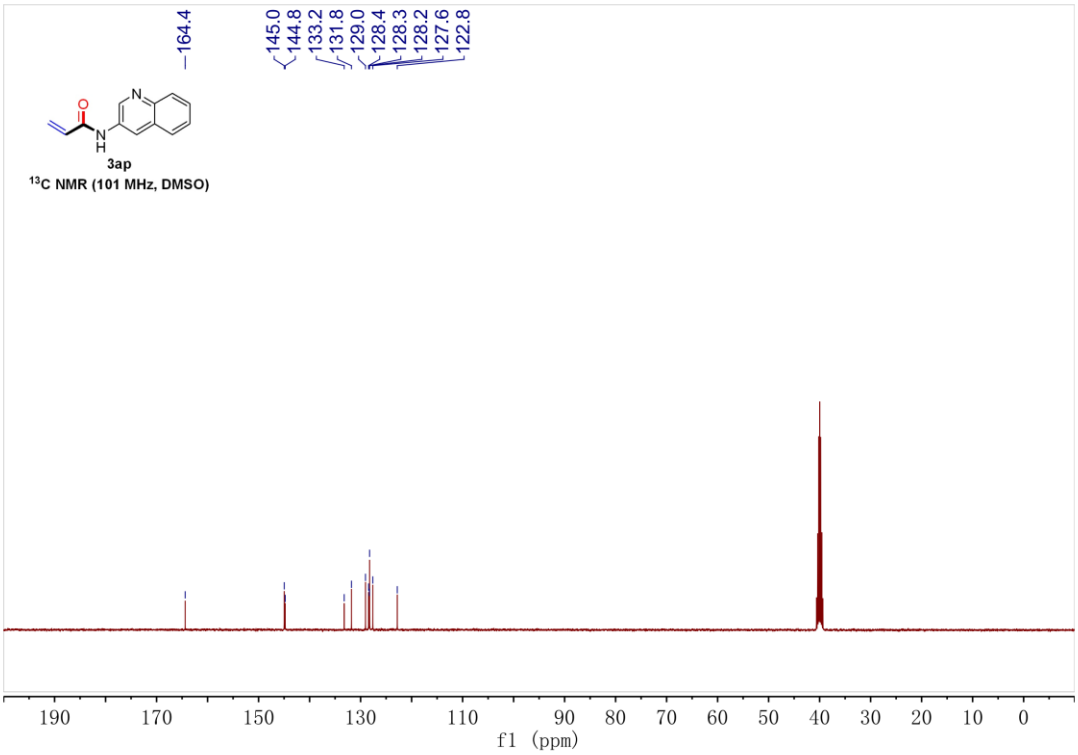
$^{1}$H NMR (400 MHz, $CDCl_3$)

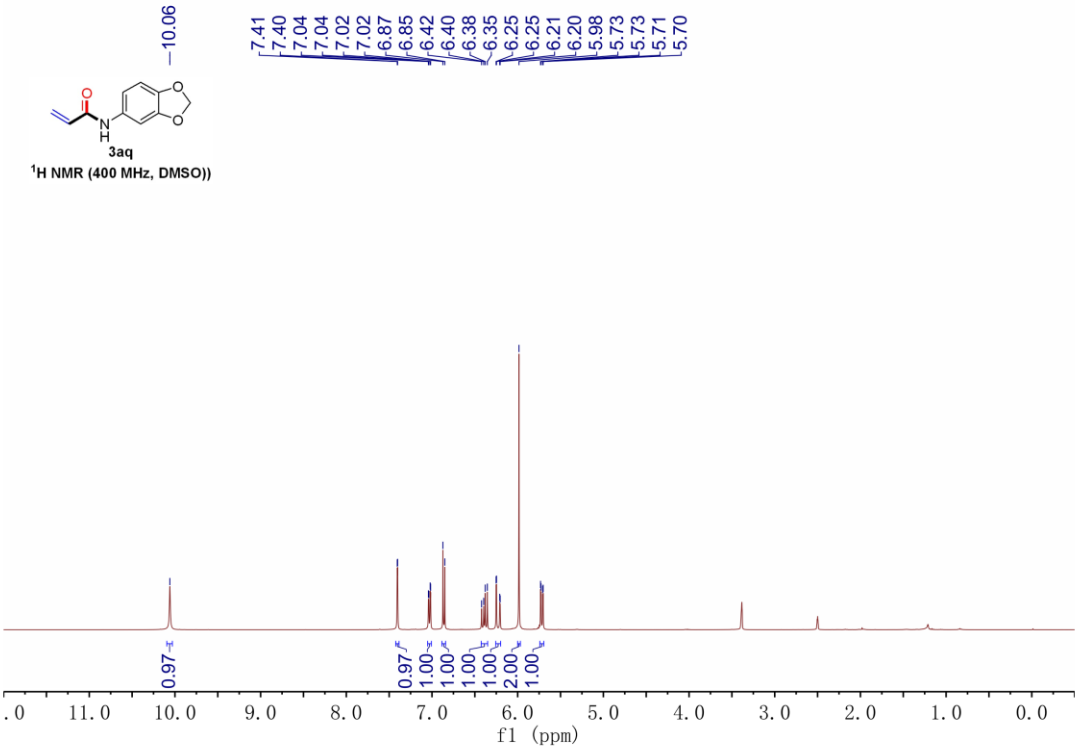


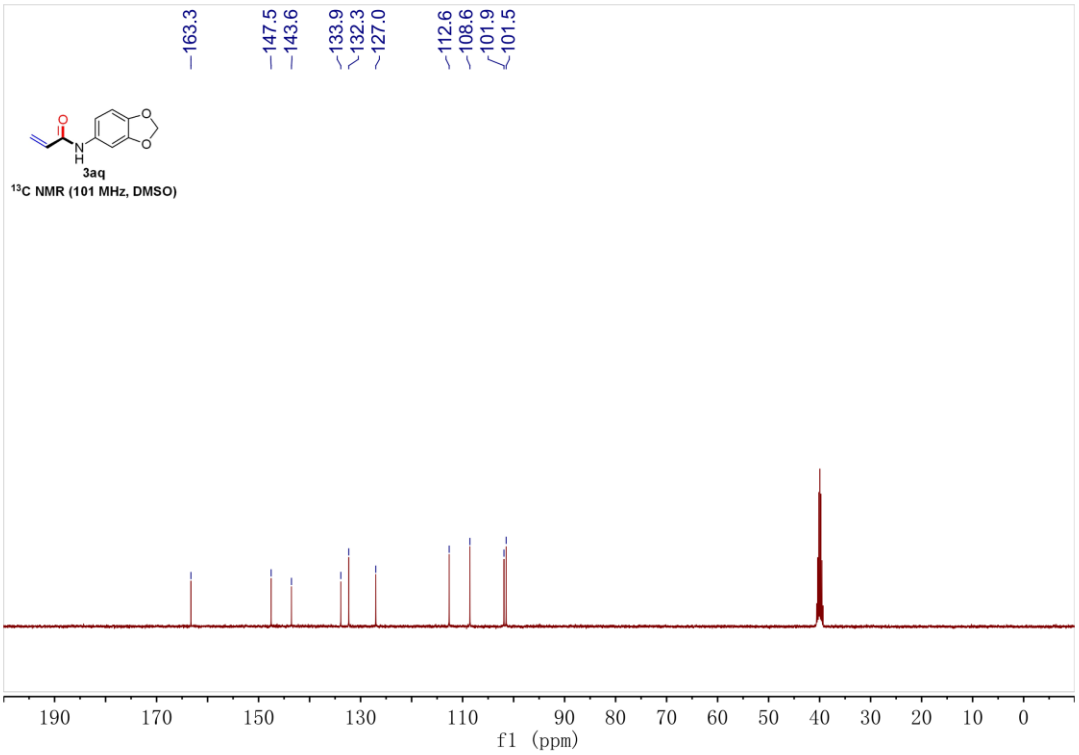

3ao

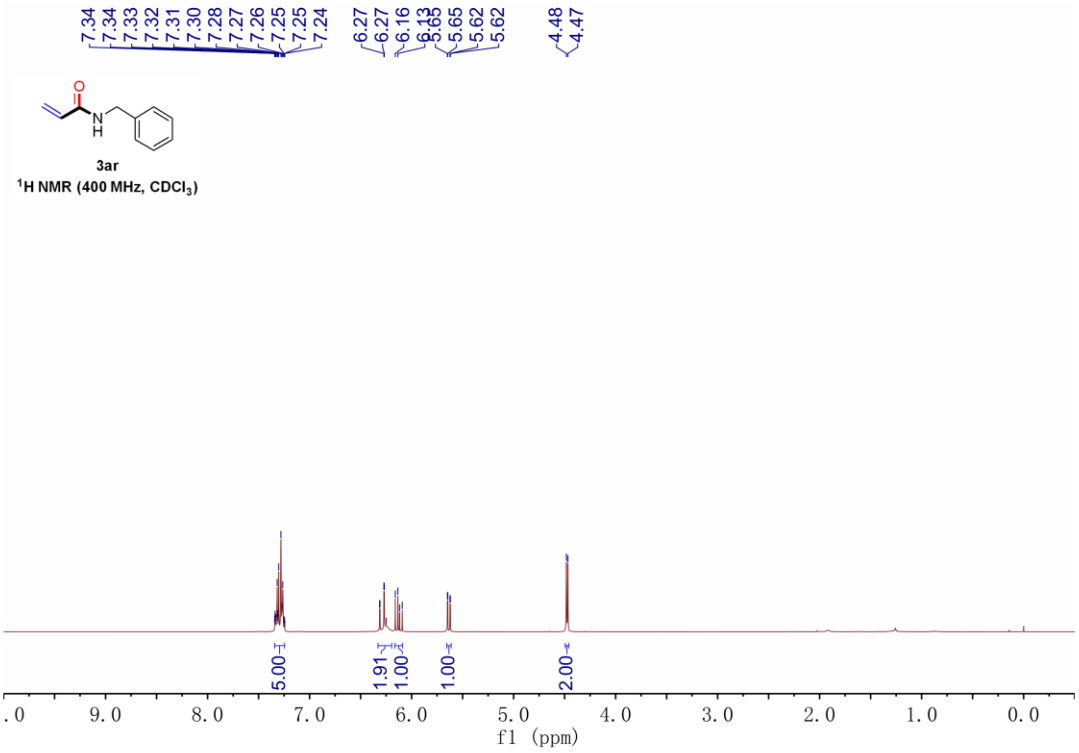
$^{13}$C NMR (101 MHz, $CDCl_3$)

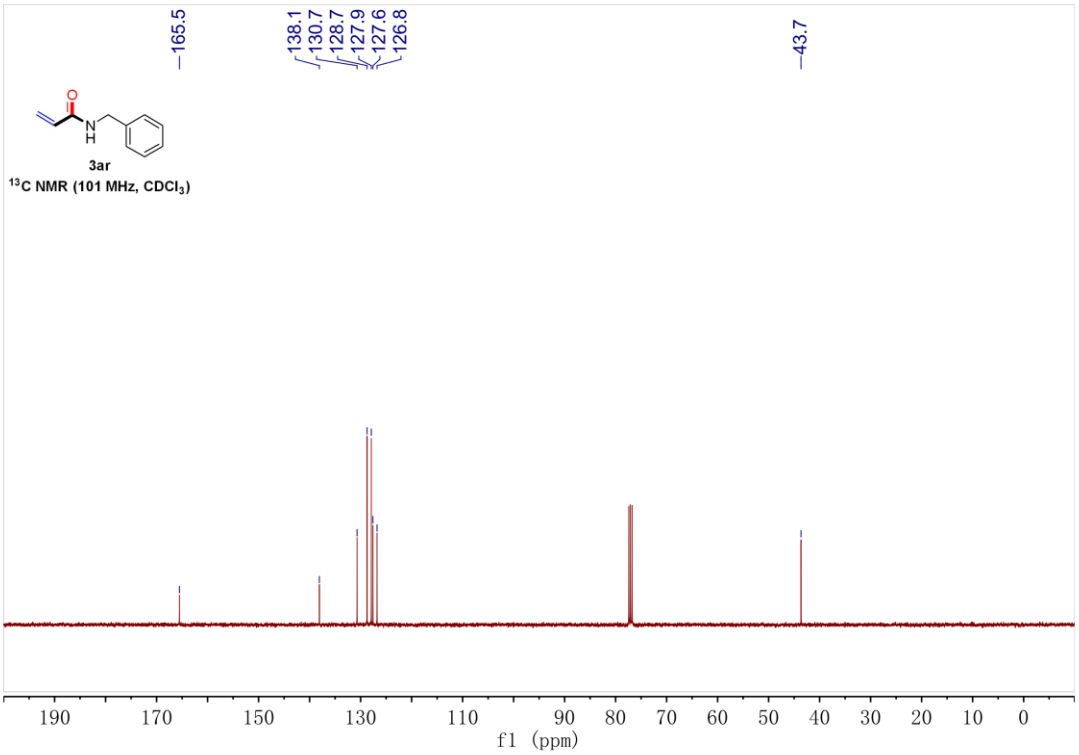

10.65
8.97
8.96
8.81
8.80
7.97
7.95
7.93
7.65
7.57
7.55
6.53
6.51
6.48
6.37
6.37
6.33
6.33
5.86
5.86
5.84
5.83
3ap
1H NMR (400 MHz, DMSO))
0.91
0.93
0.94
2.00
1.01
1.00
1.00
1.00
1.00
f1 (ppm)

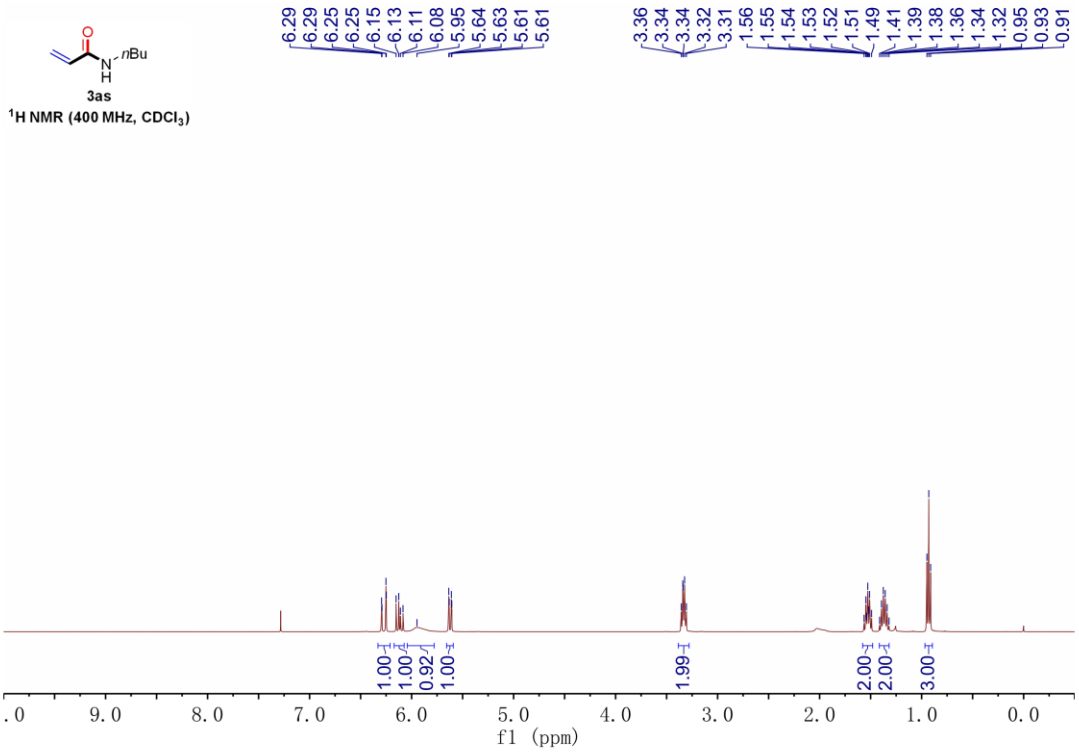

164.4
145.0
144.8
133.2
131.8
129.0
128.4
128.3
128.2
127.6
122.8
3ap
13C NMR (101 MHz, DMSO)
f1 (ppm)

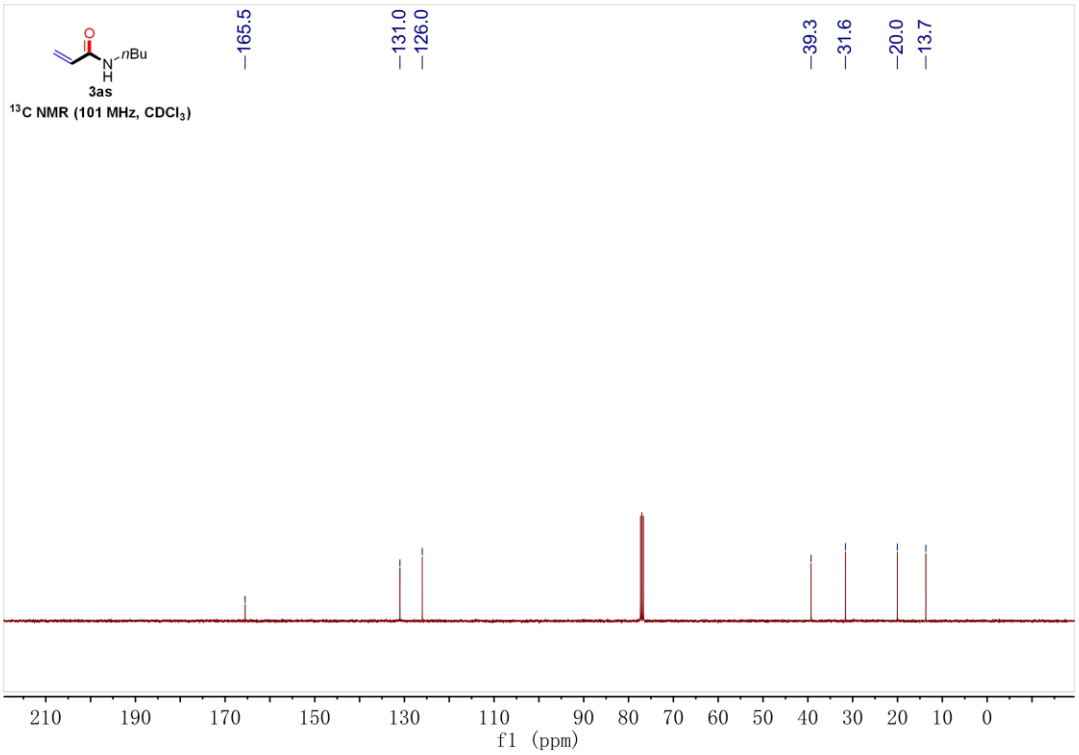

10.06
7.41
7.40
7.04
7.04
7.02
7.02
6.87
6.85
6.42
6.40
6.38
6.35
6.25
6.25
6.21
6.20
5.98
5.73
5.73
5.71
5.70
3aq
1H NMR (400 MHz, DMSO))
0.97
0.97
1.00
1.00
1.00
1.00
2.00
1.00
f1 (ppm)

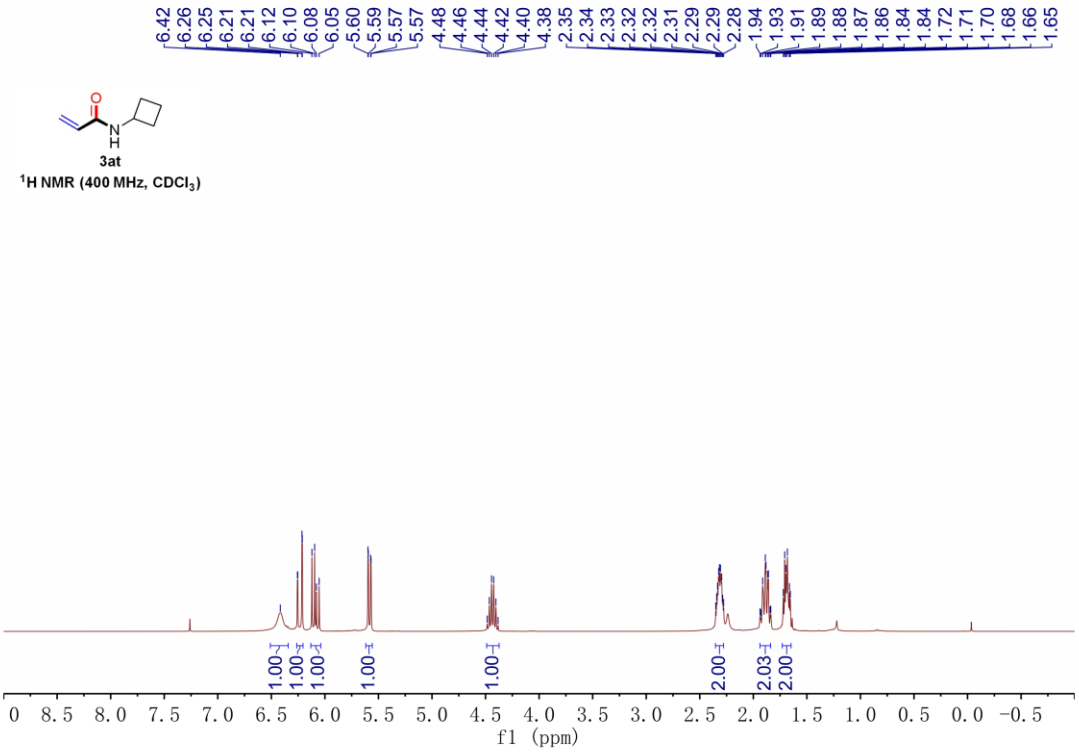

163.3
147.5
143.6
133.9
132.3
127.0
112.6
108.6
101.9
101.5
3aq
13C NMR (101 MHz, DMSO)
f1 (ppm)

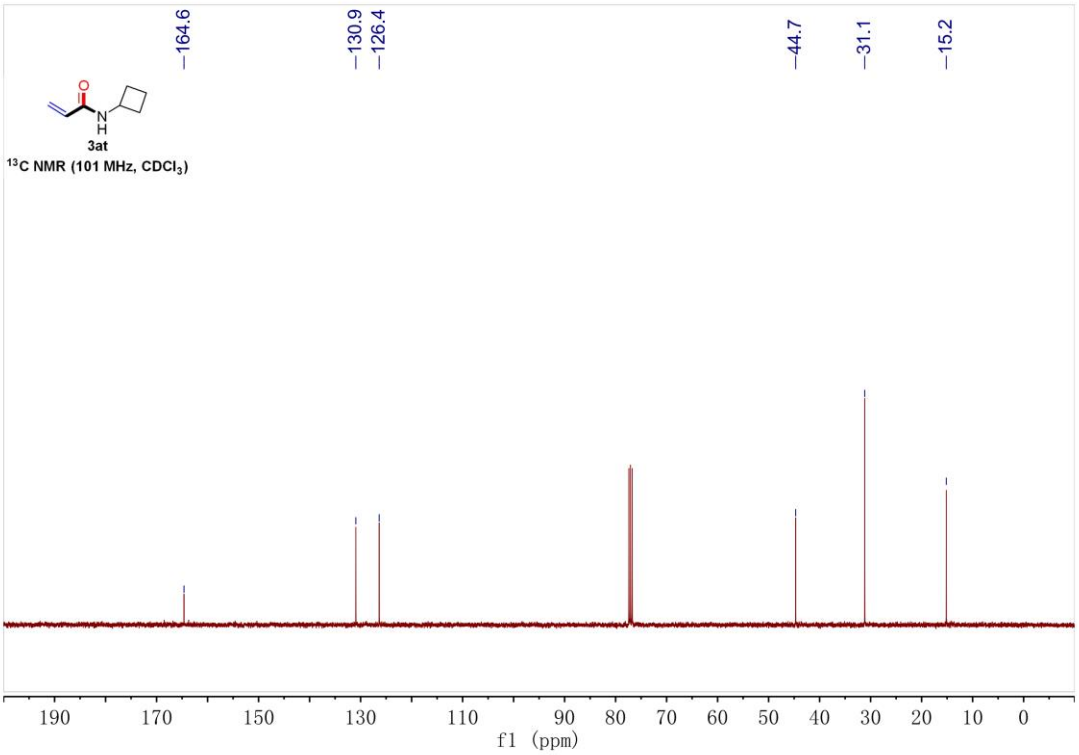

7.34
7.34
7.33
7.32
7.31
7.30
7.28
7.27
7.26
7.25
7.25
7.24
6.27
6.27
6.16
6.13
5.65
5.62
5.62
4.48
4.47
3ar
1H NMR (400 MHz, CDCl3)
5.00
1.91
1.00
1.00
2.00
.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

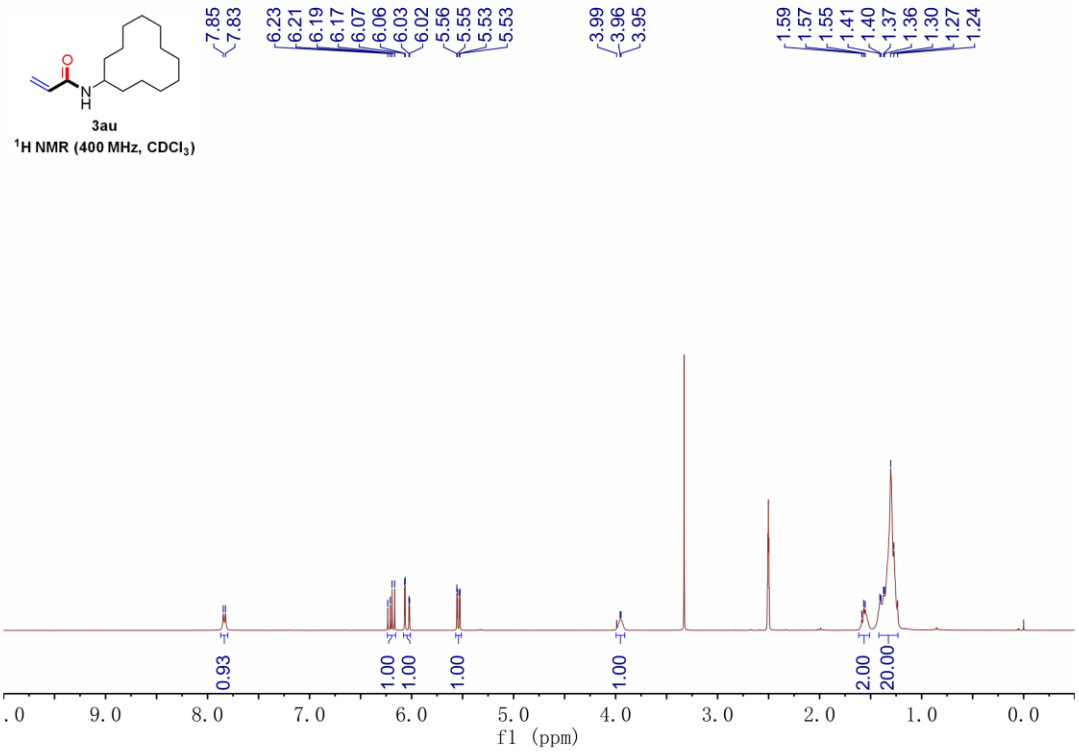

165.5
138.1
130.7
128.7
127.9
127.6
126.8
43.7
3ar
13C NMR (101 MHz, CDCl3)
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

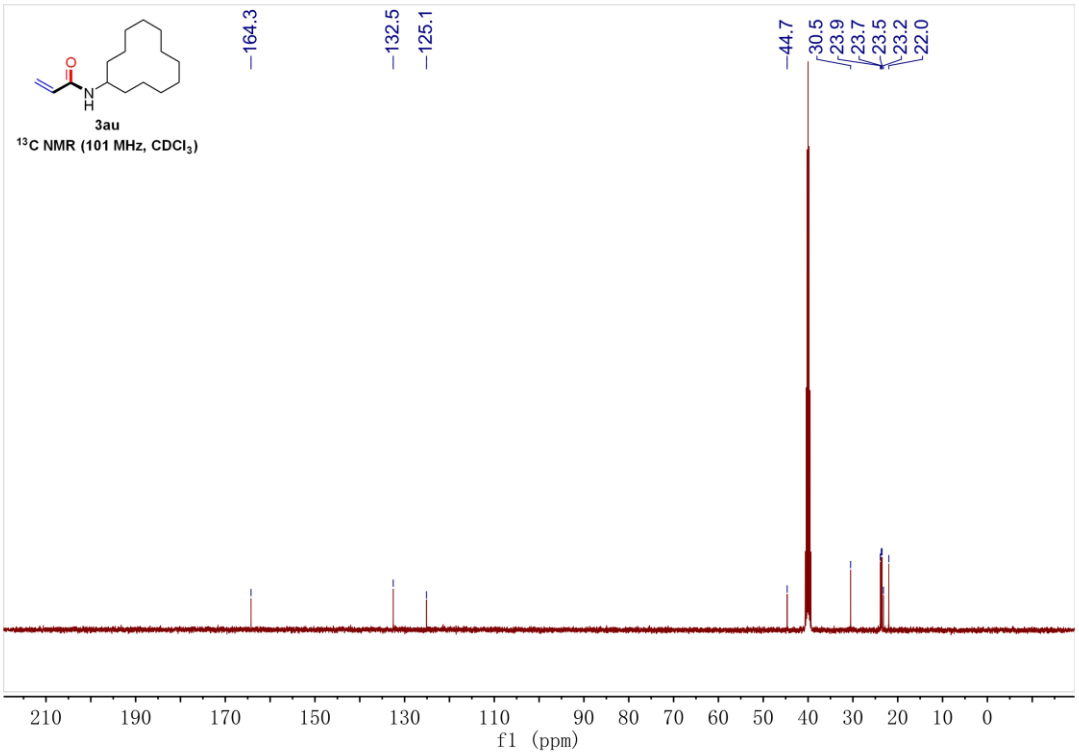

3as
1H NMR (400 MHz, CDCl3)
6.29
6.29
6.25
6.25
6.15
6.13
6.11
6.08
5.95
5.64
5.63
5.61
5.61
3.36
3.34
3.34
3.32
3.31
1.56
1.55
1.54
1.53
1.52
1.51
1.49
1.41
1.39
1.38
1.36
1.34
1.32
0.95
0.93
0.91
1.00
1.00
0.92
1.00
1.99
2.00
2.00
3.00
f1 (ppm)

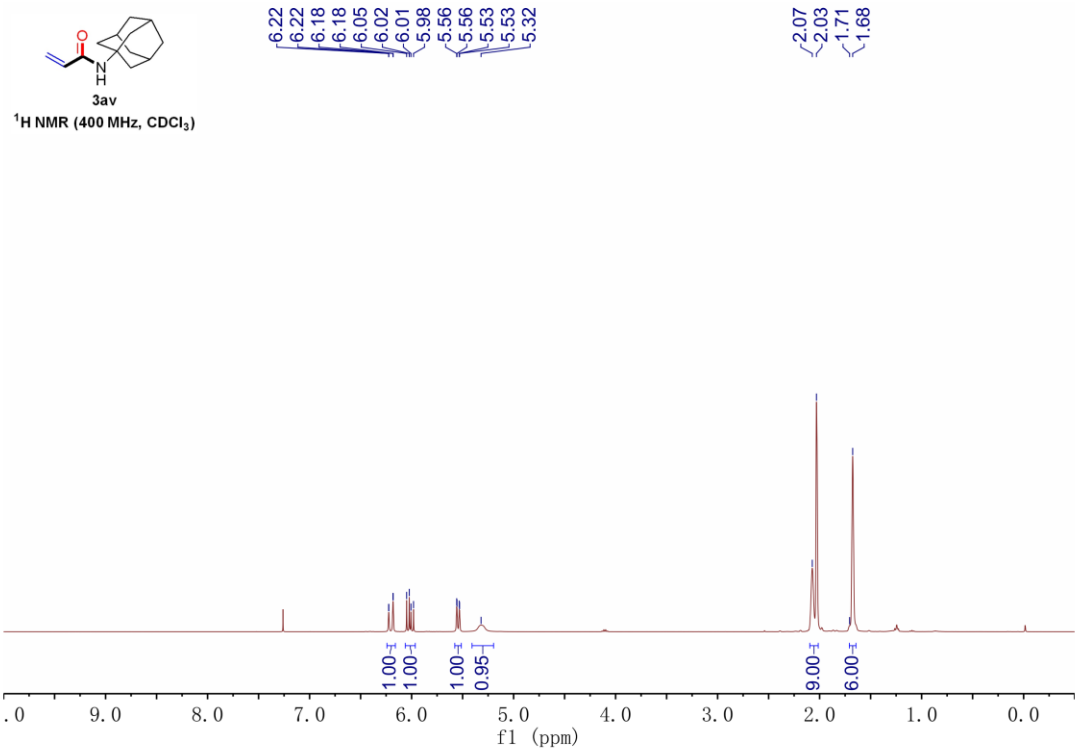

3as
13C NMR (101 MHz, CDCl3)
165.5
131.0
126.0
39.3
31.6
20.0
13.7
f1 (ppm)

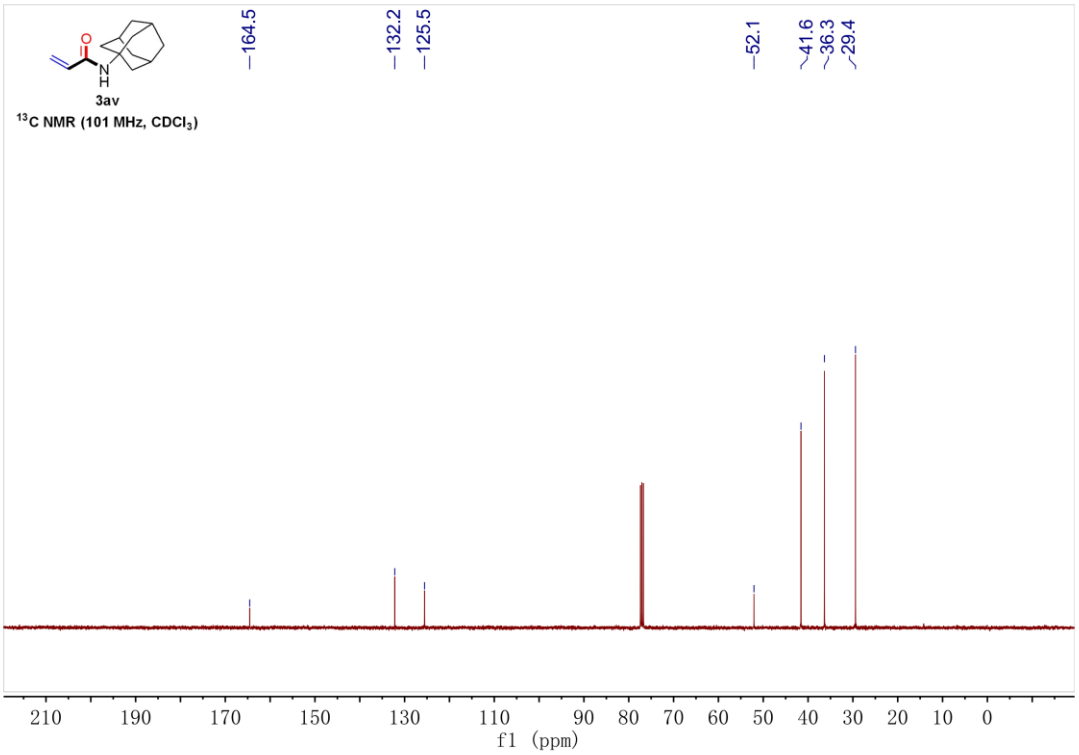

6.42 6.26 6.25 6.21 6.21 6.12 6.10 6.08 6.05 5.60 5.59 5.57 5.57 4.48 4.46 4.44 4.42 4.40 4.38 2.35 2.34 2.33 2.32 2.32 2.31 2.29 2.29 2.28 1.94 1.93 1.91 1.89 1.88 1.87 1.86 1.84 1.84 1.72 1.71 1.70 1.68 1.66 1.65
3at
$^1$H NMR (400 MHz, $CDCl_3$)
1.00 1.00 1.00 1.00 1.00 2.00 2.03 2.00
0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

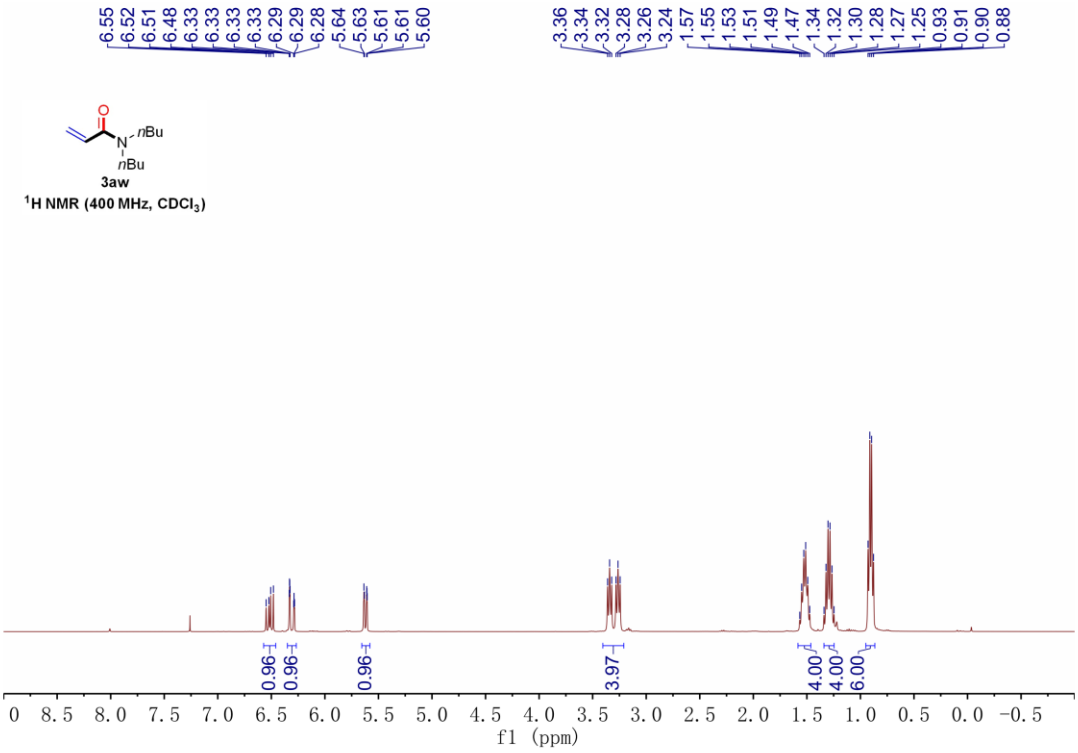

164.6
130.9
126.4
44.7
31.1
15.2
3at
$^{13}$C NMR (101 MHz, $CDCl_3$)
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

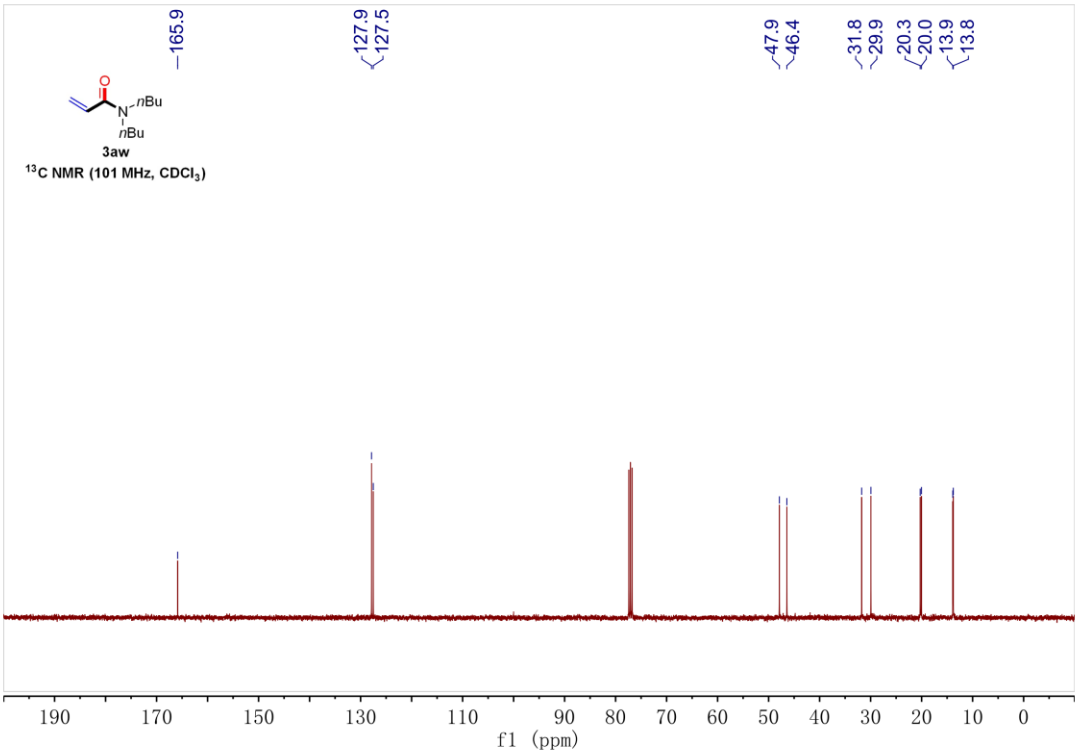

7.85
7.83
6.23
6.21
6.19
6.17
6.07
6.06
6.03
6.02
5.56
5.55
5.53
5.53
3.99
3.96
3.95
1.59
1.57
1.55
1.41
1.40
1.37
1.36
1.30
1.27
1.24
3au
1H NMR (400 MHz, CDCl3)
0.93
1.00
1.00
1.00
1.00
2.00
20.00
f1 (ppm)

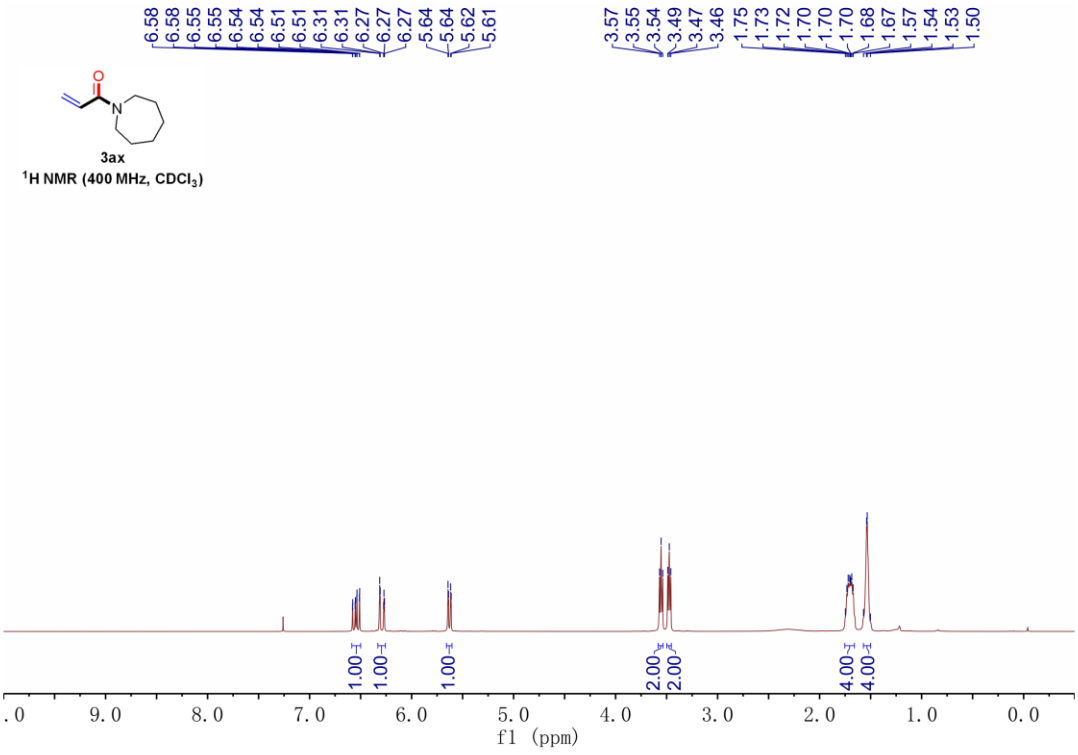

164.3
132.5
125.1
44.7
30.5
23.9
23.7
23.5
23.2
22.0
3au
13C NMR (101 MHz, CDCl3)
f1 (ppm)

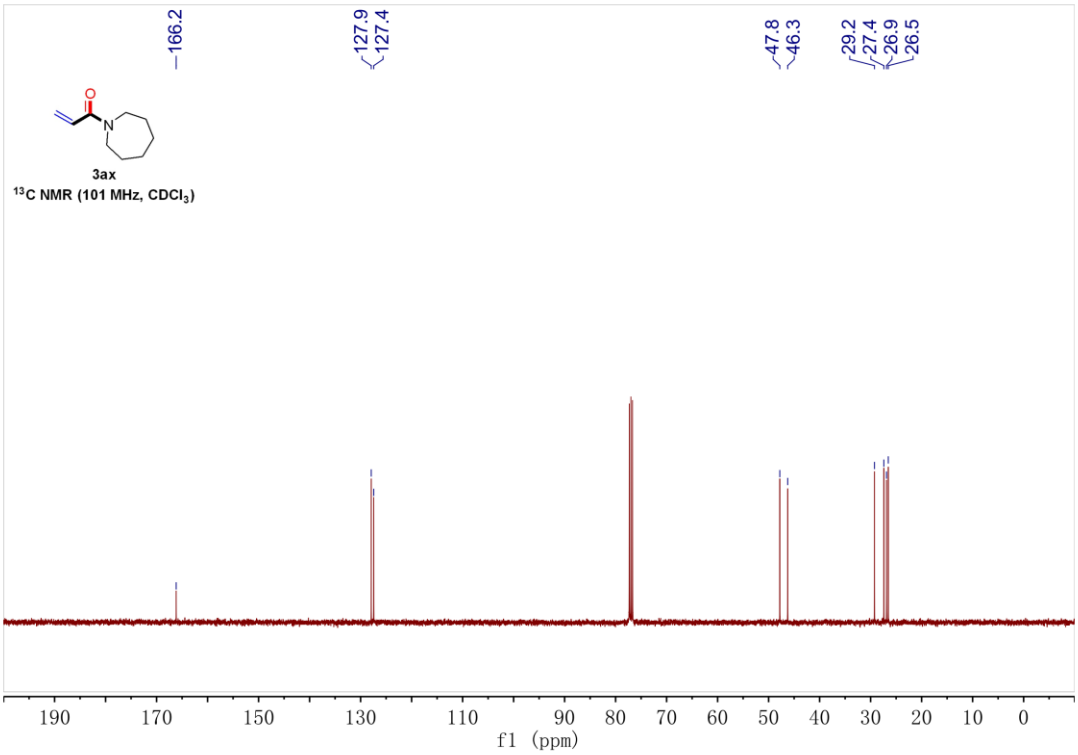

3av
$^1$H NMR (400 MHz, CDCl$_3$)
6.22
6.22
6.18
6.18
6.05
6.02
6.01
5.98
5.56
5.56
5.53
5.53
5.32
2.07
2.03
1.71
1.68
1.00
1.00
1.00
0.95
9.00
6.00
f1 (ppm)

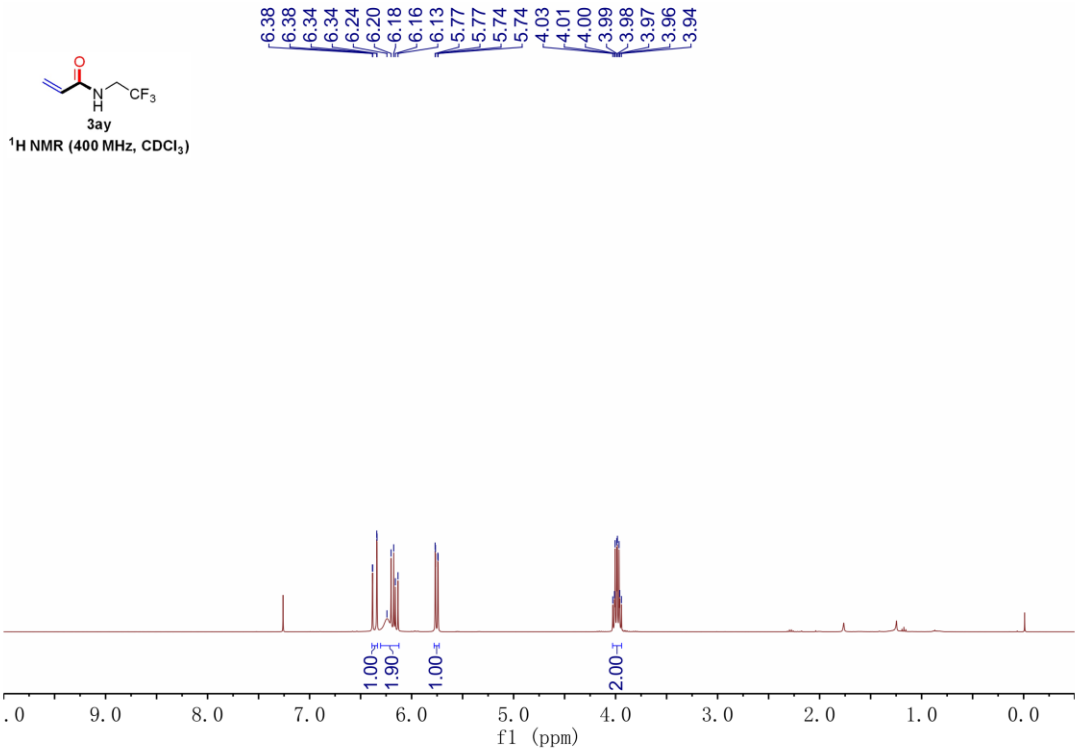

3av
$^{13}$C NMR (101 MHz, CDCl$_3$)
164.5
132.2
125.5
52.1
41.6
36.3
29.4
f1 (ppm)

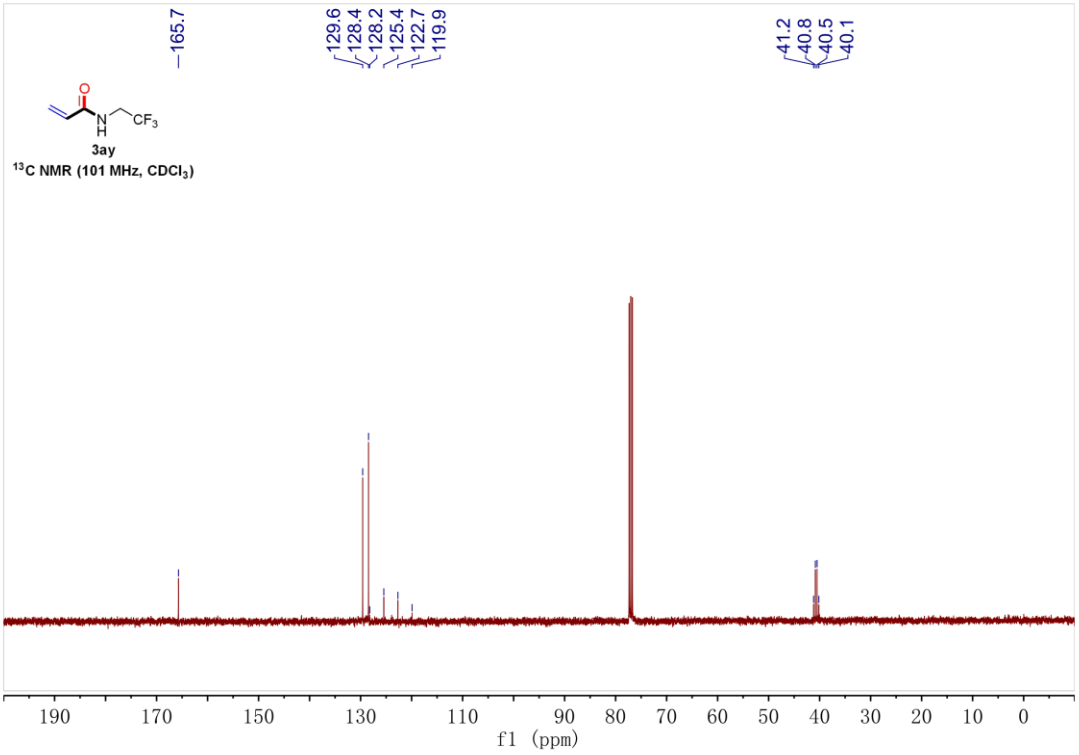

6.55
6.52
6.51
6.48
6.33
6.33
6.33
6.33
6.29
6.29
6.28
5.64
5.63
5.61
5.61
5.60
3.36
3.34
3.32
3.28
3.26
3.24
1.57
1.55
1.53
1.51
1.49
1.47
1.34
1.32
1.30
1.28
1.27
1.25
0.93
0.91
0.90
0.88
nBu
nBu
3aw
1H NMR (400 MHz, CDCl3)
0.96
0.96
0.96
3.97
4.00
4.00
6.00
f1 (ppm)

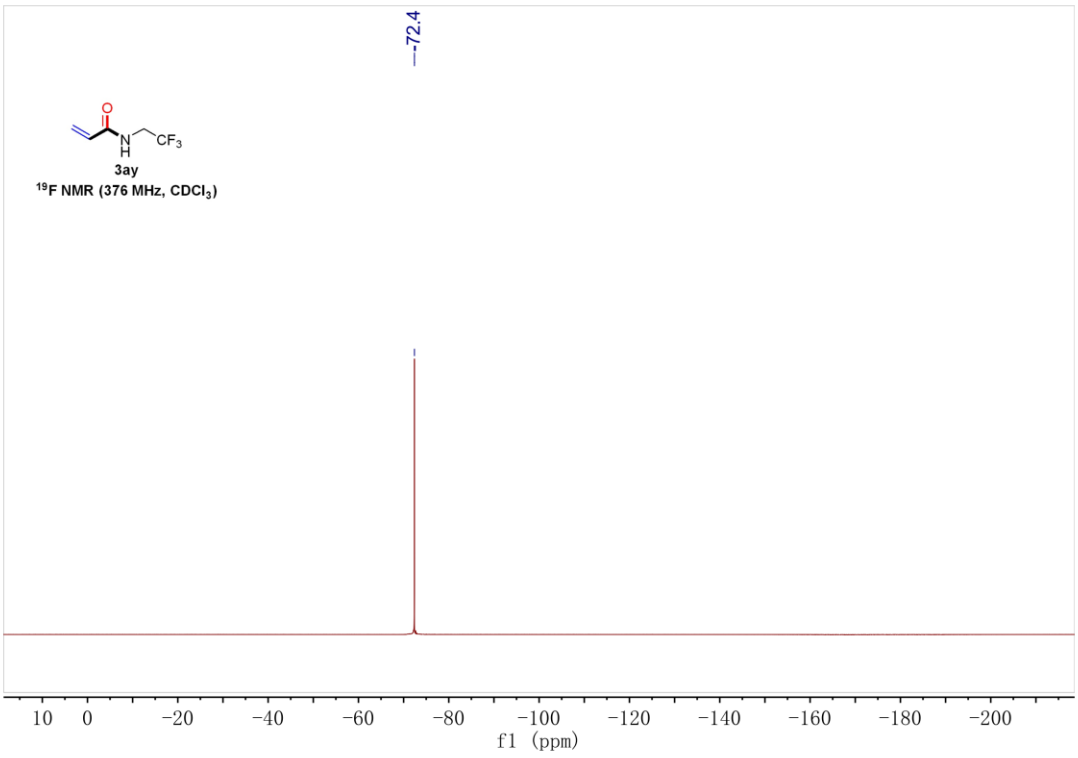

165.9
127.9
127.5
47.9
46.4
31.8
29.9
20.3
20.0
13.9
13.8
nBu
nBu
3aw
13C NMR (101 MHz, CDCl3)
f1 (ppm)

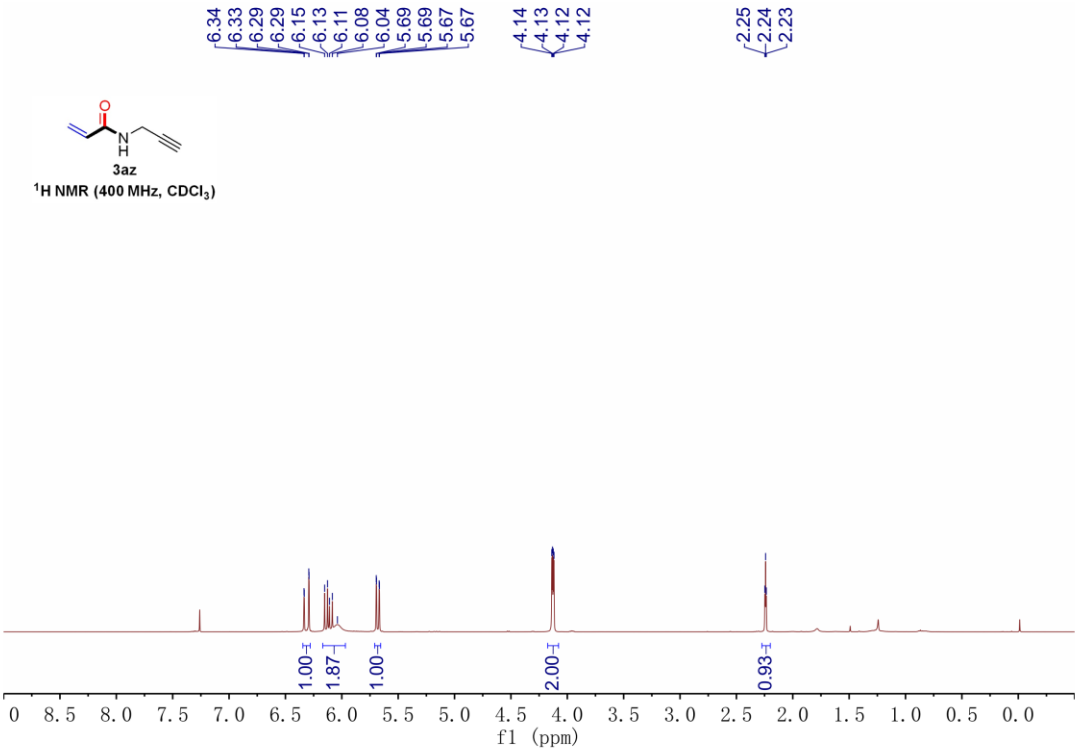

6.58
6.58
6.55
6.55
6.54
6.54
6.51
6.51
6.31
6.27
6.27
6.27
5.64
5.64
5.62
5.61
3.57
3.55
3.54
3.49
3.47
3.46
1.75
1.73
1.72
1.70
1.70
1.70
1.68
1.67
1.57
1.54
1.53
1.50
O
N
3ax
1H NMR (400 MHz, CDCl3)
1.00
1.00
1.00
2.00
2.00
4.00
4.00
.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

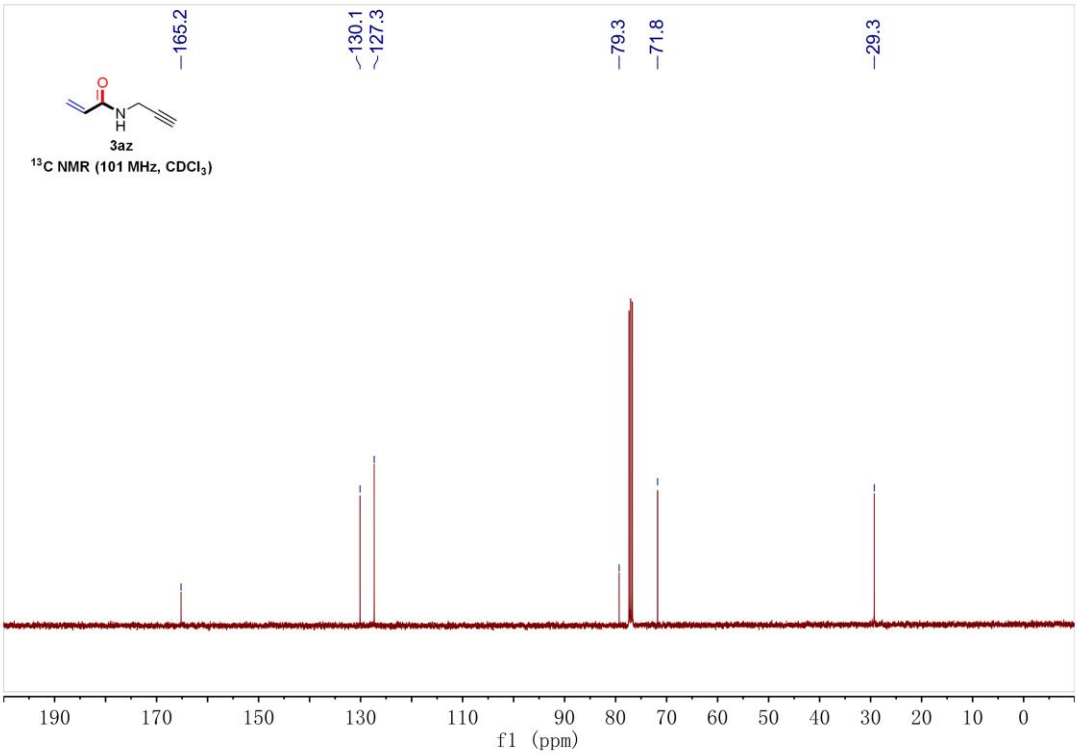

166.2
127.9
127.4
47.8
46.3
29.2
27.4
26.9
26.5
O
N
3ax
13C NMR (101 MHz, CDCl3)
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

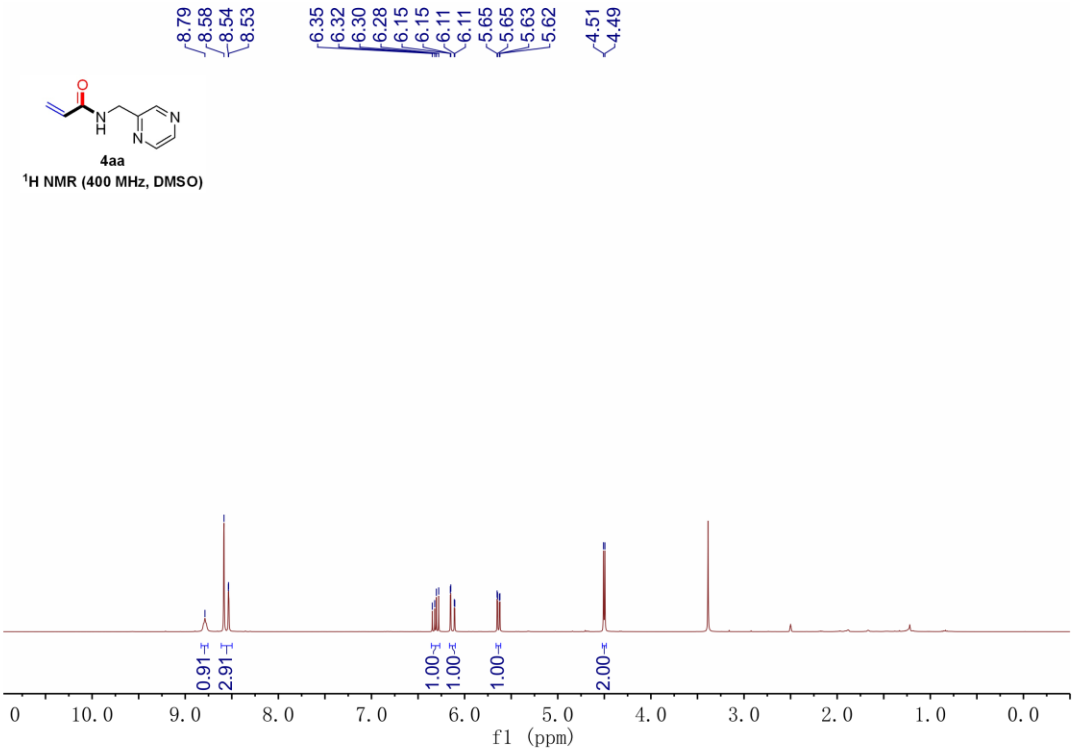

6.38
6.38
6.34
6.34
6.24
6.20
6.18
6.16
6.13
5.77
5.77
5.74
5.74
4.03
4.01
4.00
3.99
3.98
3.97
3.96
3.94
O
N
H
CF3
3ay
1H NMR (400 MHz, CDCl3)
1.00
1.90
1.00
2.00
.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

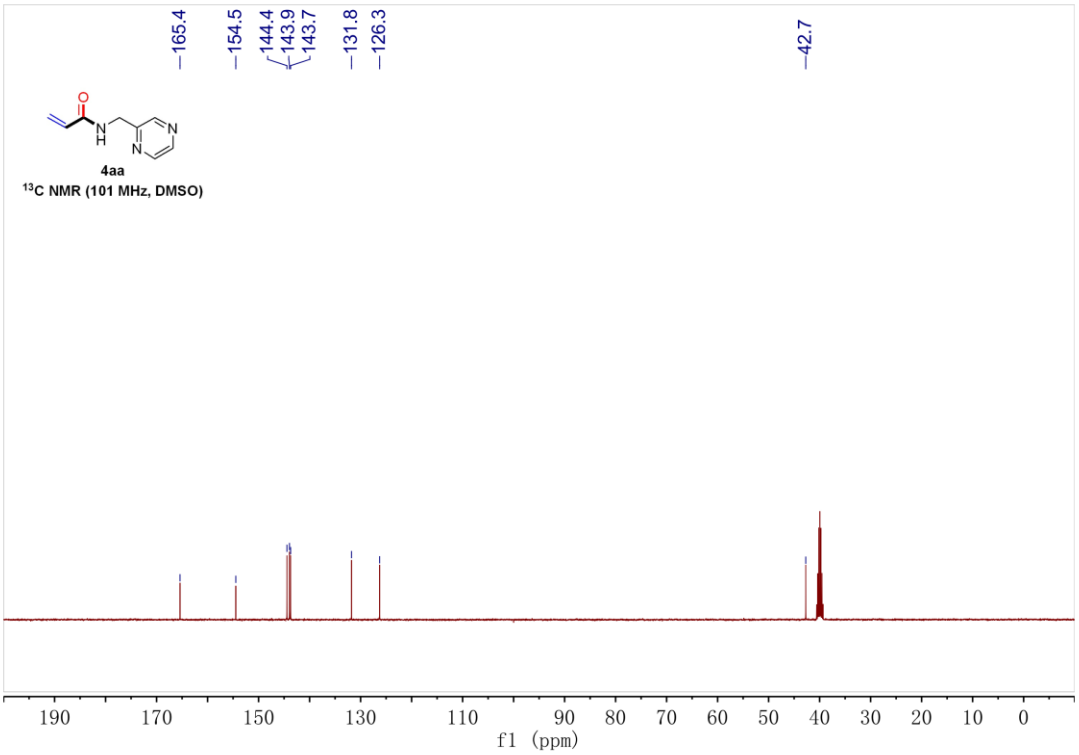

165.7
129.6
128.4
128.2
125.4
122.7
119.9
41.2
40.8
40.5
40.1
O
N
H
CF3
3ay
13C NMR (101 MHz, CDCl3)
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

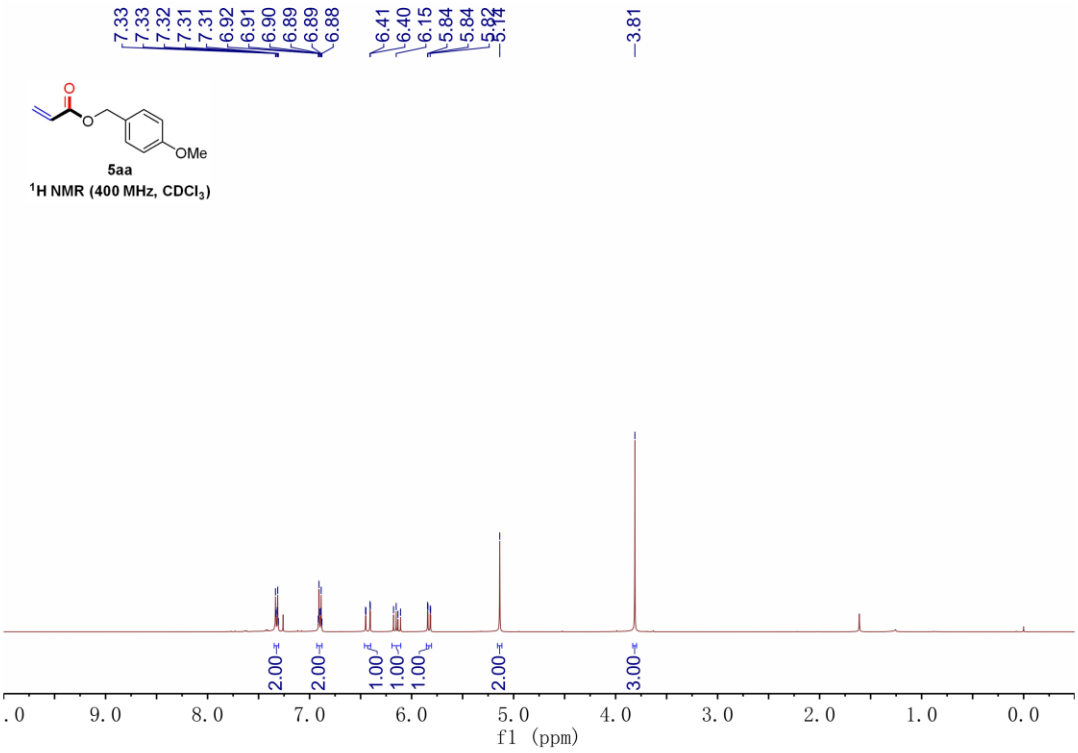

-72.4
O
N
H
CF3
3ay
19F NMR (376 MHz, CDCl3)
10
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

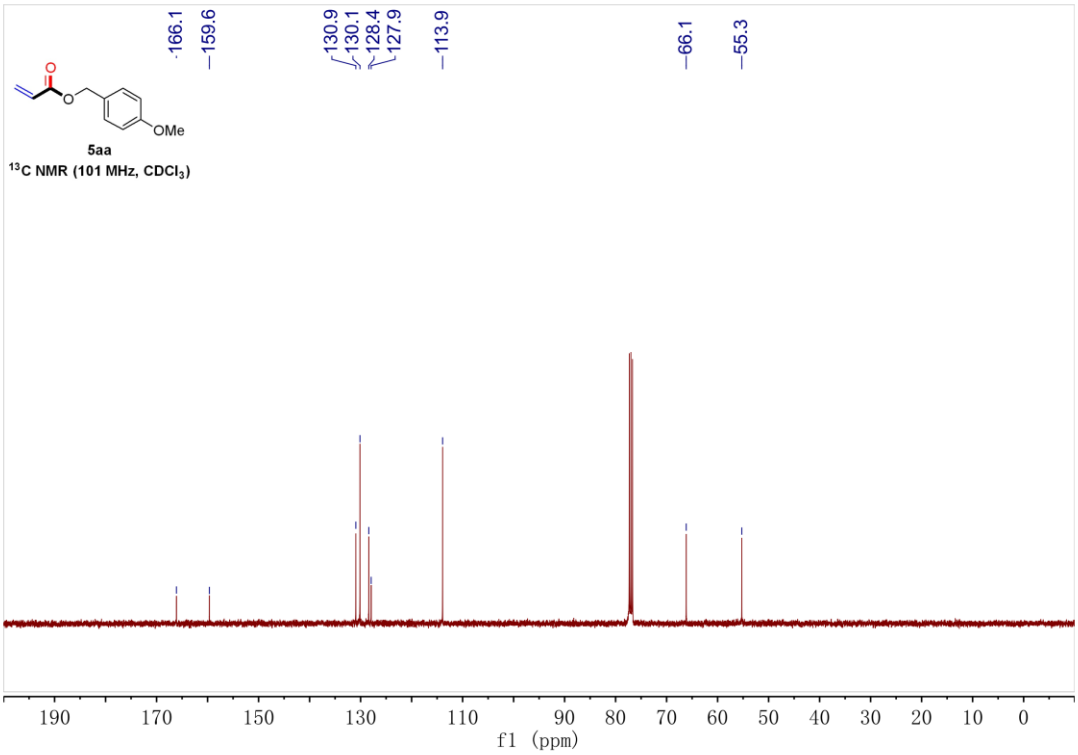

6.34
6.33
6.29
6.29
6.15
6.13
6.11
6.08
6.04
5.69
5.69
5.67
5.67
4.14
4.13
4.12
4.12
2.25
2.24
2.23
3az
1H NMR (400 MHz, CDCl3)
1.00
1.87
1.00
2.00
0.93
f1 (ppm)


165.2
130.1
127.3
79.3
71.8
29.3
3az
13C NMR (101 MHz, CDCl3)
f1 (ppm)


8.79
8.58
8.54
8.53
6.35
6.32
6.30
6.28
6.15
6.15
6.11
6.11
5.65
5.65
5.63
5.62
4.51
4.49
4aa
1H NMR (400 MHz, DMSO)
0.91
2.91
1.00
1.00
1.00
2.00
f1 (ppm)


165.4
154.5
144.4
143.9
143.7
131.8
126.3
42.7
4aa
13C NMR (101 MHz, DMSO)
f1 (ppm)


7.33
7.33
7.32
7.31
7.31
6.92
6.91
6.90
6.89
6.89
6.88
6.41
6.40
6.15
5.84
5.84
3.81
OMe
5aa
1H NMR (400 MHz, CDCl3)
2.00
2.00
1.00
1.00
1.00
2.00
3.00
f1 (ppm)


166.1
159.6
130.9
130.1
128.4
127.9
113.9
66.1
55.3
OMe
5aa
13C NMR (101 MHz, CDCl3)
f1 (ppm)