

Supporting Information

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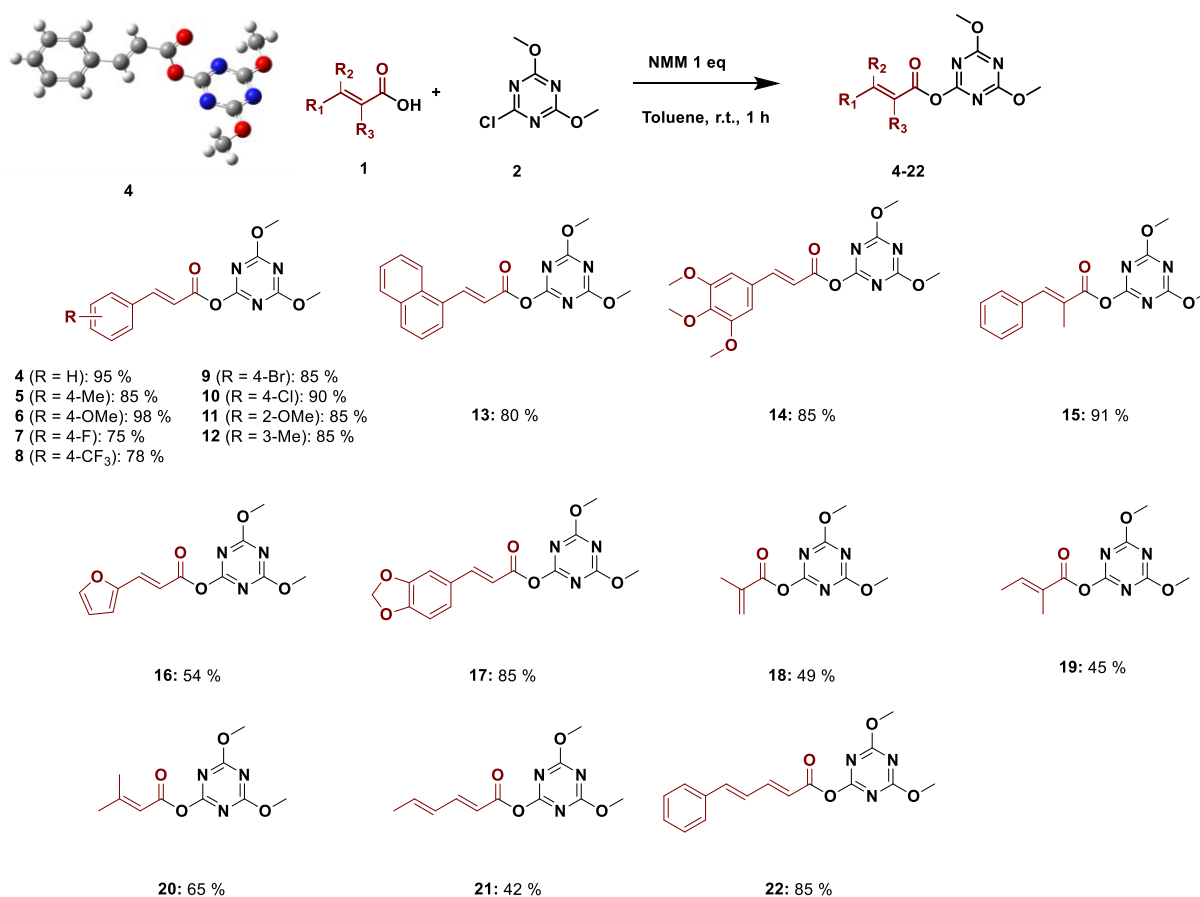
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1. General Information

All reactions were performed using 27.5x72.5 mm screw-capped vial under air, unless otherwise stated. Glassware was dried in an oven before use. All reactions were stirred with magnetic followers. All stated temperatures refer to external bath/heating aluminum block temperatures. Reagents were purchased from commercial sources and were used as received unless mentioned otherwise. Reactions were monitored by thin layer chromatography using silica gel. The thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (boiling point was between 60-90 °C). Gradient flash chromatography was conducted eluting with a continuous gradient from petroleum to the indicated solvent, and they were listed as volume/volume ratios. ¹H NMR and ¹³C NMR were recorded on a Bruker-400 MHz Spectrometer (¹H: 400 MHz, ¹³C: 101 MHz), using CDCl₃ as the solvent at room temperature. The chemical shifts (δ) were expressed in ppm and the coupling constants (J) were expressed in Hz. High-resolution mass spectra (HRMS) were recorded on a Bruker MAXIS spectrometer.

2. Synthesis and Analysis of α , β - Unsaturated triazine esters

2.1 Synthesis of α , β - Unsaturated triazine esters



Scheme S1 Synthesis of α, β - Unsaturated triazine esters **4-22**

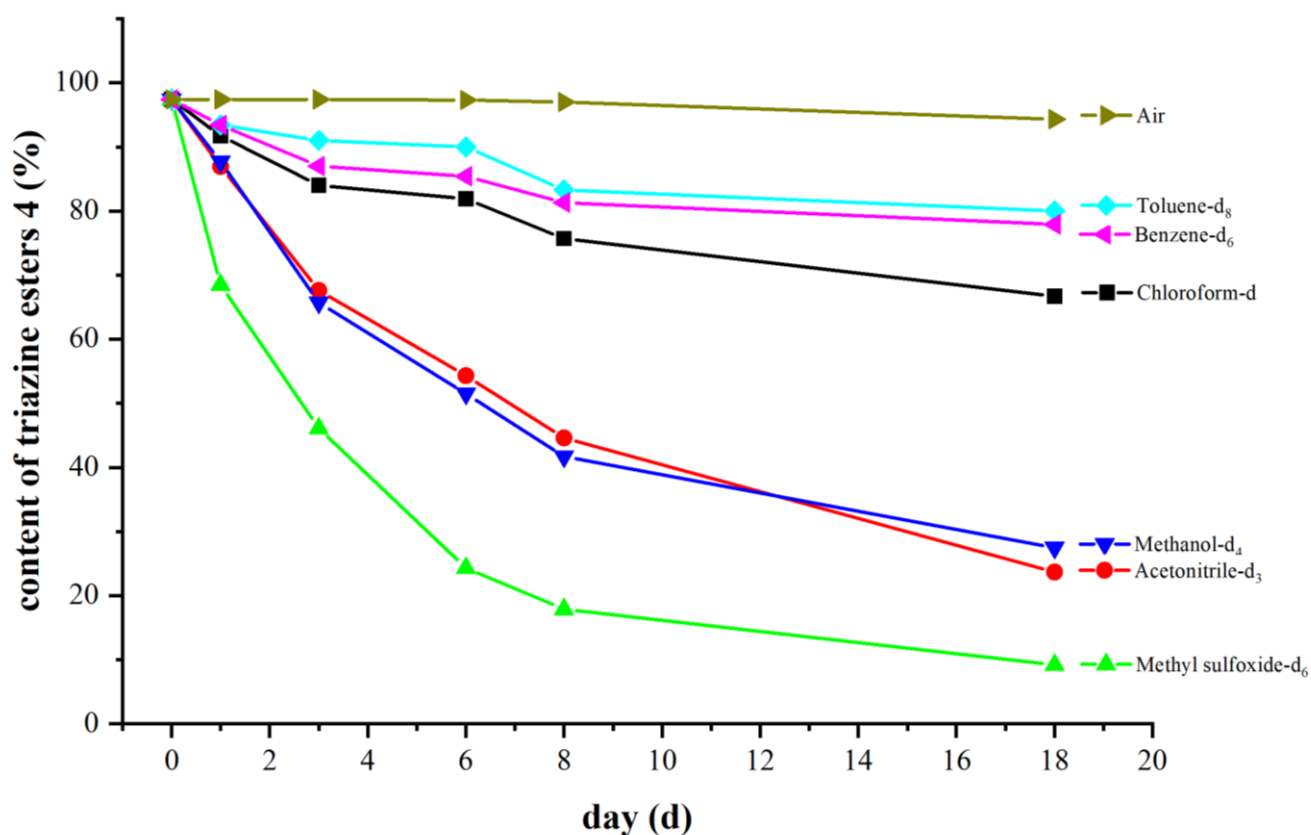
General Procedure 1(**GP1**): Under an air atmosphere, a round-bottom flask of 150 mL equipped with a magnetic stir bar was charged successively with α, β - unsaturated carboxylic acid (**1a-1s** 1.0 mmol), NMM(1.2 mmol), and 10 mL of Toulene. The reaction mixture was stirred at room temperature to completely dissolved. Then add CDMT (**2**, 1.2 mmol) which is dissolved in 10 mL toluene into the reaction mixture dropwise. After the reaction was completed, the resulting mixture was diluted with 20.0 mL of ethyl acetate, and filtrated. The residue was washed with 1N citric acid solution, H₂O, and 1N sodium bicarbonate, respectively. The organic layer was dried over anhydrous MgSO₄ and concentrated under reduced pressure. Purification of the crude product by flash chromatography on silica gel using the mixed solvent system of petroleum ether (PE) and ethyl acetate (EA) afforded the desired products (**4-22**).

2.2 Stability testing of α , β - Unsaturated triazine esters

Table S1 Stability of triazine esters **4** in solvents

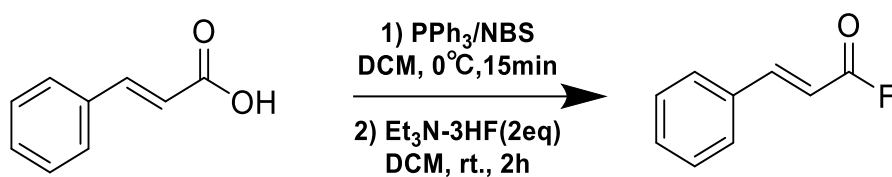
	0 day	1 day	3 day	6 day	8 day	18 day
air	97%	97%	97%	97%	97%	94%
Chloroform-d	97%	92%	84%	82%	76%	67%
Acetonitrile-d ₃	97%	87%	68%	54%	45%	24%
Methyl sulfoxide-d ₆	97%	69%	46%	24%	18%	9%
Methanol-d ₄	97%	88%	66%	52%	42%	28%
Toluene-d ₈	97%	93%	91%	90%	83%	80%
Benzene-d ₆	97%	93%	87%	85%	81%	78%

Figure S1 The content of α , β - Unsaturated triazine esters **4** in different solvents



Procedure: α , β - Unsaturated triazine esters **4** was dissolved in different deuterated solvents and allowed to stand at room temperature for 0-18 days, respectively, using NMR spectroscopy to monitor the remaining content of **4** of the solution during this period.

2.3 Activity Comparison of triazine ester 4 and cinnamic fluoride

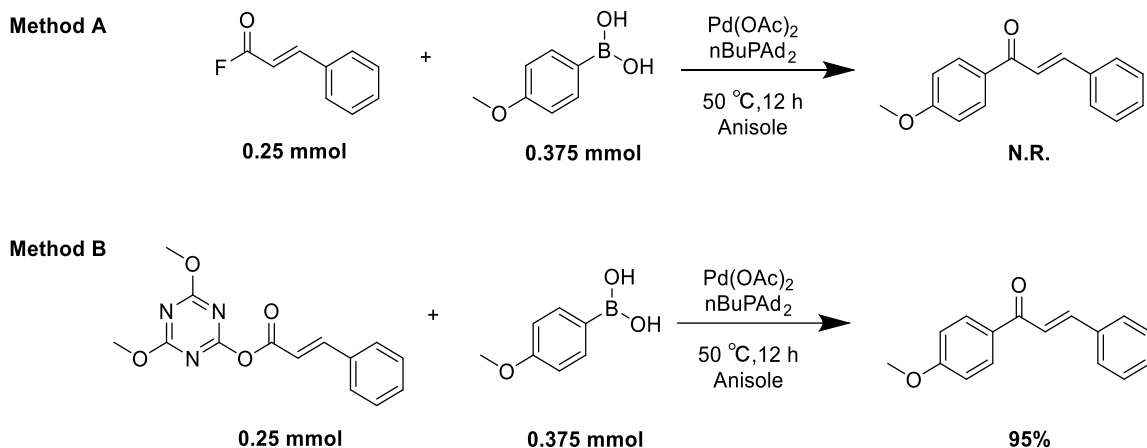


Scheme S2 Preparation of Cinnamic Fluoride, PhC=CCOF

PhC=CCOF was prepared with the literature method using a Phosphine/Fluoride Deoxyfluorination Reagent System (G. K. Prakash, et al., *Org. Lett.* 2019, **21**, 1659-1663).

Procedure: On the bench-top, cinnamic acid **1** (1 equiv, 0.5 mmol) and triphenylphosphine, PPh₃ (2 equiv, 1 mmol, 262.3 mg) and anhydrous DCM (5 mL) were charged into an oven-dried screw-cap vial equipped with a magnetic stir bar. The vial was capped, and this mixture was then cooled to 0 °C using an ice-bath. Subsequently, N-bromosuccinimide, NBS (2.1 equiv, 1.05 mmol, 187 mg) was added as a solid in one portion, the vial was re-capped, and the mixture was kept in the ice-bath for two minutes. After this time, the ice-bath was removed, and this solution was further stirred for 15 min. After this time, the vial was opened and 3HF-Et₃N (2 equiv, 1 mmol, 163 μ L) was added via micropipette. This mixture was stirred further for 2 h at room temperature. After this time, the vial was opened, and the reaction mixture was diluted with hexanes (20 mL), and the mixture was stirred for 10 min. During this time, large amounts of succinimide and triphenylphosphine oxide precipitate, which are then removed by passing the mixture through a short pad of silica (2 cm thick x 3 cm diameter). Purification of the crude product by flash chromatography on silica gel using the mixed solvent system of petroleum ether (PE) and ethyl acetate (EA) afforded the desired products. (38.9 mg, 37%)

¹H NMR (400 MHz, CDCl₃) δ 7.83 (d, J = 16.0 Hz, 1H), 7.64 - 7.50 (m, 2H), 7.53 - 7.38 (m, 3H), 6.36 (dd, J = 16.0, 7.4 Hz, 1H). ¹⁹F NMR (376 MHz, CDCl₃) δ 25.7 (d, J = 6.6 Hz, 1F).



Scheme S3 Comparison of Suzuki coupling reaction activities with different substrates

An oven-dried 30-mL screw-capped vial equipped with a magnetic stirring bar was charged with the indicated Pd(OAc)_2 (2.0 mol%) and the nBuPAD₂ (4.0 mol%). Then, cinnamic fluoride substrates (0.25 mmol, 1.0 equiv), (4-methoxyphenyl)boronic acid (3a, 57 mg, 0.375 mmol, 1.5 equiv) and Anisole (2.0 mL) were added in. The reaction mixture was stirred at 50 °C for the indicated reaction time. After the reaction, no enone product was monitored by Method **A**, while the isolated yield of (E)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one was 95% by Method **B**.

2.4 Single crystal X-ray analysis of triazine ester 4

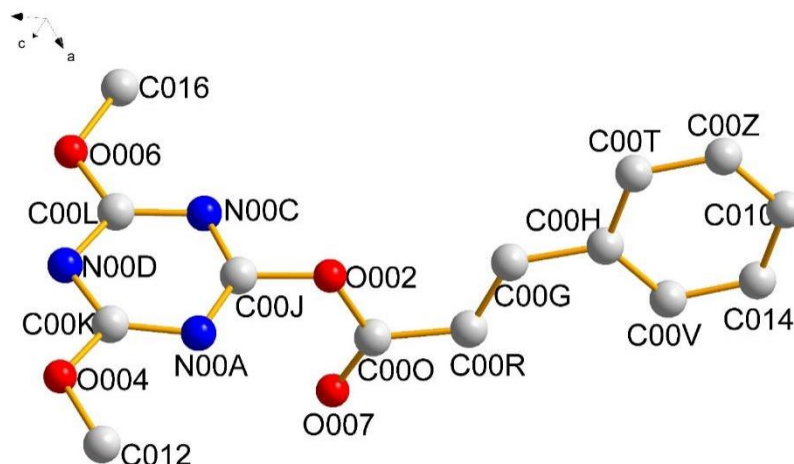


Figure S2. Molecular structure of triazine ester 4

Summary of X-ray crystallographic data for triazine ester 4

CDCC number	2236141
Empirical formula	C ₁₁ H ₁₀ NO
Formula weight	172.20
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	8.3286(3)
b/Å	11.3682(5)
c/Å	15.5301(5)
α/°	93.171(3)
β/°	96.973(3)
γ/°	104.307(4)
Volume/Å ³	1408.69(10)
Z	6
ρ _{calc} /cm ³	1.218
μ/mm ⁻¹	0.627
F(000)	546.0
Crystal size/mm ³	0.5 × 0.4 × 0.3
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	8.058 to 143.156
Index ranges	-8 ≤ h ≤ 10, -13 ≤ k ≤ 13, -18 ≤ l ≤ 19
Reflections collected	25876
Independent reflections	5429 [R _{int} = 0.0338, R _{sigma} = 0.0211]
Data/restraints/parameters	5429/0/378
Goodness-of-fit on F ²	1.028
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0469, wR ₂ = 0.1210
Final R indexes [all data]	R ₁ = 0.0542, wR ₂ = 0.1287
Largest diff. peak/hole / e Å ⁻³	0.18/-0.31

Selected geometric informations (bond angle)

C00K—O004—C012	118.83(14)	C00H—C00V—H00V	119.700
C00N—O005—C015	118.18(14)	C014—C00V—C00H	120.54(17)
C00L—O006—C016	118.58(14)	C014—C00V—H00V	119.700
C00F—N008—C00N	112.35(13)	C00U—C00W—H00W	119.600
C00J—N00A—C00K	112.12(13)	C00X—C00W—C00U	120.73(17)
C00I—N00B—C00N	113.72(13)	C00X—C00W—H00W	119.600
C00J—N00C—C00L	111.97(14)	C00W—C00X—H00X	120.300
C00K—N00D—C00L	113.79(13)	C00W—C00X—C011	119.35(16)
C00F—N00E—C00I	111.88(13)	C011—C00X—H00X	120.300
N008—C00F—O001	114.67(14)	C00M—C00Y—H00Y	119.700
N008—C00F—N00E	128.97(13)	C011—C00Y—C00M	120.64(17)
N00E—C00F—O001	116.23(14)	C011—C00Y—H00Y	119.700
C00H—C00G—H00G	116.000	C00T—C00Z—H00Z	119.900
C00R—C00G—H00G	116.000	C010—C00Z—C00T	120.21(18)
O003—C00I—N00E	119.54(14)	C00X—C011—C00Y	120.50(18)
N00B—C00I—O003	113.68(13)	C00X—C011—H011	119.700

Selected geometric informations (dihedral angle)

C00J—O002—C00O—O007	-2.5(3)	C00W—C00X—C011—C00Y	0.8(3)
C00J—O002—C00O—C00R	177.63(14)	C00Y—C00M—C00U—C00W	0.3(3)
C00J—N00A—C00K—O004	-179.16(13)	C00Y—C00M—C1—C00S	178.61(18)
C00J—N00A—C00K—N00D	-0.5(2)	C00Z—C010—C014—C00V	-1.2(4)
C00J—N00C—C00L—O006	178.64(13)	C012—O004—C00K—N00A	-2.4(2)
C00J—N00C—C00L—N00D	-0.9(2)	C012—O004—C00K—N00D	178.76(14)
C00K—N00A—C00J—O002	175.61(12)	C013—O003—C00I—N00B	179.69(14)
C00K—N00A—C00J—N00C	0.4(2)	C013—O003—C00I—N00E	0.2(2)
C00K—N00D—C00L—O006	-178.78(13)	C015—O005—C00N—N008	0.6(2)
C00K—N00D—C00L—N00C	0.7(2)	C015—O005—C00N—N00B	-178.50(16)
C00L—N00C—C00J—O002	-175.06(12)	C016—O006—C00L—N00C	-2.0(2)
C00L—N00C—C00J—N00A	0.3(2)	C016—O006—C00L—N00D	177.58(15)
C00L—N00D—C00K—O004	178.75(12)	C1—C00M—C00U—C00W	-178.32(17)
C00L—N00D—C00K—N00A	0.0(2)	C1—C00M—C00Y—C011	179.07(18)

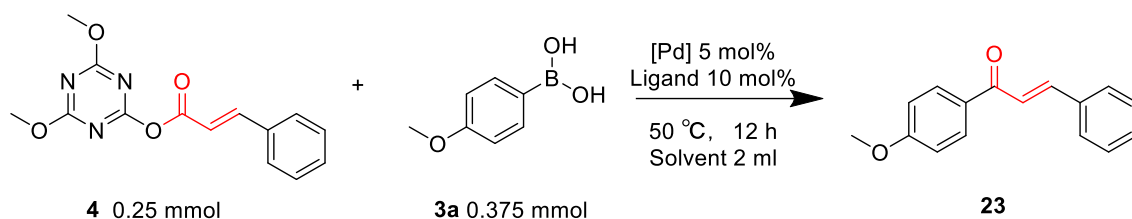
Selected geometric informations (bond length)

O001—C00F	1.3791(17)	C00Q—C00S	1.462(2)
O001—C00Q	1.3707(18)	C00R—H00R	0.9300
O002—C00J	1.3784(17)	C00S—H00S	0.9300
O002—C00O	1.3674(18)	C00S—C1	1.315(2)
O003—C00I	1.3288(19)	C00T—H00T	0.9300
O003—C013	1.436(2)	C00T—C00Z	1.380(2)
O004—C00K	1.3202(19)	C00U—H00U	0.9300
O004—C012	1.438(2)	C00U—C00W	1.381(2)
O005—C00N	1.319(2)	C00V—H00V	0.9300
O005—C015	1.437(2)	C00V—C014	1.380(2)
O006—C00L	1.3224(19)	C00W—H00W	0.9300
O006—C016	1.443(2)	C00W—C00X	1.371(3)
O007—C00O	1.1867(19)	C00X—H00X	0.9300
N008—C00F	1.309(2)	C00X—C011	1.373(3)
N008—C00N	1.3361(19)	C00Y—H00Y	0.9300

3. Optimization Study

General procedure for the optimization reactions. An oven-dried 30-mL screw-capped vial equipped with a magnetic stirring bar was charged with the indicated palladium catalyst (2.0 mol%) and the indicated ligand. Then, α,β -Unsaturated triazine esters (**4**, 0.25 mmol, 1.0 equiv), (4-methoxyphenyl)boronic acid (**3a**, 57 mg, 0.375 mmol, 1.5 equiv) and the indicated solvents (2.0 mL) were added in. The reaction mixture was stirred at 50 °C for the indicated reaction time and subsequently analyzed by GC analysis.

Table S2. Optimization of the palladium-catalyzed cross-coupling of a α, β -Unsaturated triazine ester and a (4-methoxyphenyl) boronic acid.^[a]



Entry	Catalyst	Ligand	Solvent	Yield[%]
1	Pd(OAc) ₂	/	THF	11
2	Pd(PPh ₃) ₄	/	THF	nd
3	PdCl ₂	/	THF	5
4	PdCl ₂ (PPh) ₂	/	THF	4
5	[(Cinnamyl)PdCl] ₂	/	THF	3
6	PdCl ₂ (dppf) ₂	/	THF	3
7	Pd(OAc) ₂	PPh ₃	THF	15
8	Pd(OAc) ₂	<i>t</i> -Bu ₃ PBF ₄ ·H ⁺	THF	12
9	Pd(OAc) ₂	dppb	THF	2
10	Pd(OAc) ₂	dppf	THF	3
11	Pd(OAc) ₂	dppp	THF	5
12	Pd(OAc) ₂	nBuPAd ₂	THF	33
13	Pd(OAc) ₂	nBuPAd ₂	Cyclopentyl Methyl Ether	56
14	Pd(OAc) ₂	nBuPAd ₂	Anisole	68
15	Pd(OAc) ₂	nBuPAd ₂	Toluene	41
16	Pd(OAc) ₂	nBuPAd ₂	acetonitrile	27
17	Pd(OAc) ₂	nBuPAd ₂	dioxane	62
18 ^[b]	Pd(OAc) ₂	nBuPAd ₂	Anisole	51
19 ^[c]	Pd(OAc) ₂	nBuPAd ₂	Anisole	95
20 ^[c]	Pd(OAc) ₂	PPh ₃	Anisole	43
21 ^[c]	Pd(OAc) ₂	<i>t</i> -Bu ₃ PBF ₄ ·H ⁺	Anisole	21
22 ^[c]	Pd(OAc) ₂	dppb	Anisole	26
23 ^[c]	Pd(OAc) ₂	dppf	Anisole	23
24 ^[c]	Pd(OAc) ₂	dppp	Anisole	16
25 ^[d]	Pd(OAc) ₂	nBuPAd ₂	Anisole	72
26 ^[e]	Pd(OAc) ₂	nBuPAd ₂	Anisole	68

[a] Unless otherwise noted, all reactions were performed on a 0.25 mmol scale in 2 mL of solvent, and yields were determined by calibrated GC analysis with biphenyl as an internal standard. [b] Ligand (20% mol) was used. [c] Ligand (5% mol) was used. [d] Run at 70 °C and Ligand (5% mol) was used. [e] Run at 90 °C and Ligand (5% mol) was used. dppb = 1,4-bis(diphenylphosphino)butane; dppf = 1,1'-bis(diphenylphosphino)ferrocene; dppp = 1,3-bis(diphenylphosphino)propane; dppe = 1,2-bis(diphenylphosphino)ethane.

4. General Procedure for the Coupling of α, β - Unsaturated Triazine Esters and Boronic Acid (GP2)

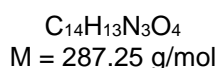
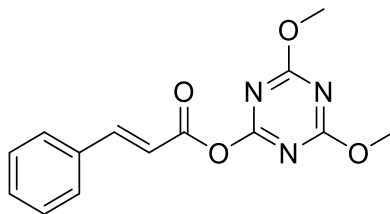
General procedure for the optimization reactions. An oven-dried 30-mL screw-capped vial equipped with a magnetic stirring bar was charged with the corresponding α - β unsaturated triazine esters (0.25 mmol, 1.0 equiv), boronic acid (0.375 mmol, 1.5 equiv), Pd(OAc)₂ (5.0 mol%) and nBuPAD₂ (5.0 mol%). Then, anisole (2.0 mL) was added in. The reaction mixture was stirred at 50 °C. The conversion was monitored by TLC analysis, and unless otherwise noted, the triazine esters were fully converted within 12 h. A color change from brown to yellow was observed.

The reaction mixture was diluted with 20.0 mL of ethyl acetate, filtrated, and concentrated under reduced pressure. Purification of the crude product by flash chromatography on silica gel using the mixed solvent system of petroleum ether (PE) and ethyl acetate (EA) afforded the desired products.

5. Characterization and procedure of the products

5.1 Characterization Data for α - β Unsaturated triazine esters

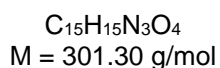
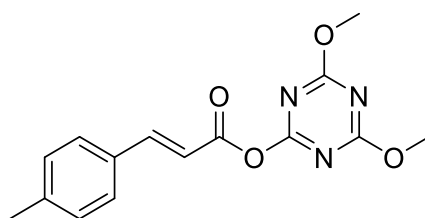
4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**):



Prepared according to GP1 from the cinnamic acid (**1a**, 148.2 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **4** (272.9 mg, 0.95 mmol, 95 %) as a white solid.

¹H NMR (400 MHz, CDCl₃): δ /ppm = 7.91 (d, J = 16.0 Hz, 1H), 7.60 – 7.53 (m, 2H), 7.47 – 7.37 (m, 5H), 6.57 (d, J = 16.0 Hz, 1H), 4.08 (s, 6H). **¹³C NMR** (101 MHz, CDCl₃): δ /ppm = 174.23 , 170.70 , 162.38 , 149.11 , 133.75 , 131.40 , 129.17 , 128.68 , 115.88 , 56.01 . **IR(KBr)**: ν (C=O): 1742 cm⁻¹. **HRMS(ESI) m/z**: [M+Na]⁺ calcd for C₁₄H₁₃N₃NaO₄: 310.0795; Found: 310.0798.

4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(p-tolyl)acrylate (**5**):

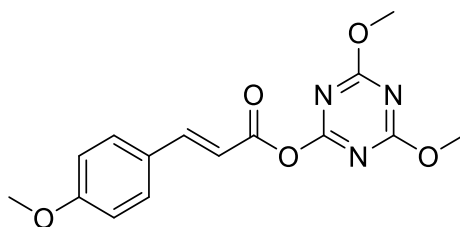


Prepared according to GP1 from the (E)-3-(p-tolyl)acrylic acid (**1b**, 148.2 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **5** (256.1 mg, 0.85 mmol, 85 %) as a white solid.

¹H NMR (400 MHz, CDCl₃): δ /ppm = 7.88 (d, J = 15.9 Hz, 1H), 7.47 (d, J = 8.0 Hz, 2H), 7.22 (d, J = 7.9 Hz, 2H), 6.51 (d, J = 15.9 Hz, 1H), 4.07 (s, 6H), 2.39 (s, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ /ppm = 174.21 , 170.75 , 162.57 , 149.21 , 142.13 , 131.05 , 129.92 , 128.74 ,

114.69 , 56.00 , 21.71 . **IR(KBr)**: $\nu(\text{C}=\text{O})$: 1756 cm^{-1} . **HRMS(ESI) m/z**: $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{15}\text{H}_{15}\text{N}_3\text{NaO}_4$: 324.0948; Found: 324.0955.

4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(4-methoxyphenyl)acrylate (6):

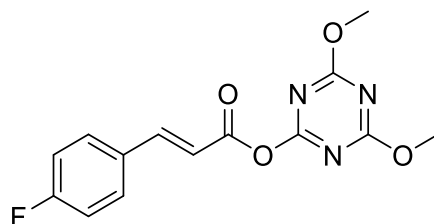


$\text{C}_{15}\text{H}_{15}\text{N}_3\text{O}_5$
M = 315.33 g/mol

Prepared according to GP1 from the (E)-3-(4-methoxyphenyl)acrylic acid (**1c**, 178.2 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **6** (309 mg, 0.98 mmol, 98 %) as a white solid.

^1H NMR (400 MHz, CDCl_3): δ/ppm = 7.84 (d, J = 15.9 Hz, 01H), 7.51 (d, J = 8.7 Hz, 2H), 6.92 (d, J = 8.7 Hz, 2H), 6.41 (d, J = 15.8 Hz, 1H), 4.05 (s, 6H), 3.84 (s, 3H). **^{13}C NMR** (101 MHz, CDCl_3): δ/ppm = 174.19, 170.80, 162.69, 162.32, 148.93, 130.58, 126.49, 114.61, 113.09, 55.99, 55.56. **IR(KBr)**: $\nu(\text{C}=\text{O})$: 1744 cm^{-1} . **HRMS(ESI) m/z**: $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{15}\text{H}_{15}\text{N}_3\text{NaO}_5$: 340.0903; Found: 340.0904.

4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(4-fluorophenyl)acrylate (7):



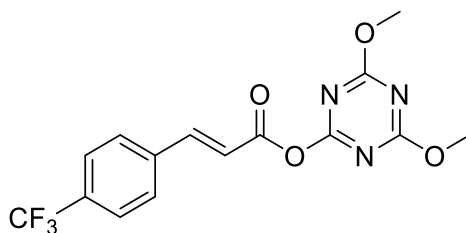
$\text{C}_{14}\text{H}_{12}\text{FN}_3\text{O}_4$
M = 320.30 g/mol

Prepared according to GP1 from the (E)-3-(4-fluorophenyl)acrylic acid (**1d**, 166.2 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **7** (240.2 mg, 0.75 mmol, 75 %) as a white solid.

^1H NMR (400 MHz, CDCl_3): δ/ppm = 7.86 (d, J = 16.0 Hz, 1H), 7.57 (dd, J = 8.6, 5.4 Hz, 2H), 7.11 (t, J = 8.6 Hz, 2H), 6.49 (d, J = 16.0 Hz, 1H), 4.07 (s, 1H). **^{13}C NMR** (101 MHz, CDCl_3): δ/ppm = 174.22 , 170.64 , 162.28 , 147.73 , 130.71 , 130.01 , 116.44 , 115.59 , 56.04. **IR(KBr)**: $\nu(\text{C}=\text{O})$: 1745 cm^{-1} . **HRMS(ESI) m/z**: $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{14}\text{H}_{12}\text{FN}_3\text{NaO}_4$: 328.0695;

Found: 328.0704.

4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(4-(trifluoromethyl)phenyl)acrylate (8):

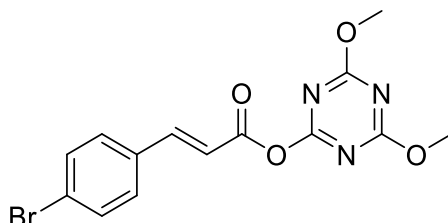


$C_{15}H_{12}F_3N_3O_4$
M = 355.27 g/mol

Prepared according to GP1 from the (E)-3-(4-(trifluoromethyl)phenyl)acrylic acid (**1e**, 216.2 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **7** (277.1 mg, 0.78 mmol, 78 %) as a white solid.

¹H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.91 (d, J = 16.0 Hz, 1H), 7.68 (s, 4H), 6.64 (d, J = 16.0 Hz, 1H), 4.07 (s, 6H). **¹³C NMR** (101 MHz, $CDCl_3$): δ /ppm = 174.25, 170.52, 161.87, 146.94, 137.02, 128.76, 126.16, 118.52, 56.05. **IR(KBr)**: ν (C=O): 1754 cm^{-1} . **HRMS(ESI) m/z**: $[M+H]^+$ calcd for $C_{15}H_{13}FN_3O_4$: 356.0648; Found: 356.0641.

4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(4-bromophenyl)acrylate (9):

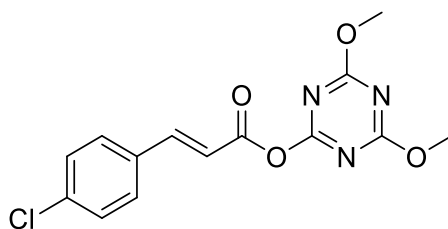


$C_{14}H_{12}BrN_3O_4$
M = 366.17 g/mol

Prepared according to GP from the (E)-3-(4-bromophenyl)acrylic acid (**1f**, 227.1 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **9** (311.2 mg, 0.85 mmol, 85 %) as a white solid.

¹H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.82 (d, J = 15.9 Hz, 1H), 7.54 (m, 2H), 7.46 - 7.37 (m, 2H), 6.54 (d, J = 16.0 Hz, 1H), 4.06 (s, 6H). **¹³C NMR** (101 MHz, $CDCl_3$): δ /ppm = 174.23, 170.60, 162.17, 147.62, 132.48, 130.00, 125.87, 116.55, 56.05. **IR(KBr)**: ν (C=O): 1767 cm^{-1} . **HRMS(ESI) m/z**: $[M+Na]^+$ calcd for $C_{14}H_{12}BrN_3NaO_4$: 387.9906; Found: 387.9903.

4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(4-chlorophenyl)acrylate (10):

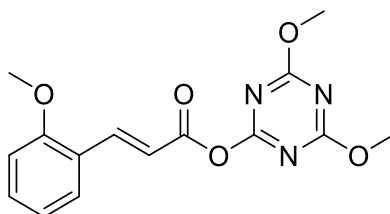


$C_{14}H_{12}ClN_3O_4$
M = 321.72 g/mol

Prepared according to GP1 from the (E)-3-(4-chlorophenyl)acrylic acid (**1g**, 182 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **10**(289.5 mg, 0.95 mmol, 90 %) as a white solid.

1H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.85 (d, J = 16.0 Hz, 1H), 7.50 (d, J = 8.5 Hz, 2H), 7.40 (d, J = 8.4 Hz, 2H), 6.53 (d, J = 16.0 Hz, 1H), 4.07 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ /ppm = 174.21, 170.59, 162.20, 147.58, 137.44, 132.20, 129.83, 129.51, 116.40, 56.06. **IR(KBr)**: $\nu(C=O)$: 1750 cm^{-1} . **HRMS(ESI) m/z**: $[M+Na]^+$ calcd for $C_{14}H_{12}ClN_3NaO_4$: 344.0410; Found: 344.0409.

4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(2-methoxyphenyl)acrylate (**11**):

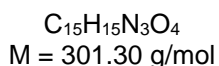
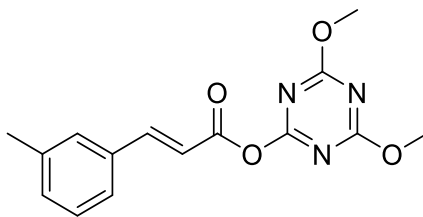


$C_{15}H_{15}N_3O_5$
M = 317.30 g/mol

Prepared according to GP1 from the (E)-3-(2-methoxyphenyl)acrylic acid (**1h**, 178.2 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **11** (269.7 mg, 0.85 mmol, 85 %) as a white solid.

1H NMR (400 MHz, $CDCl_3$): δ /ppm = 8.19 (d, J = 16.1 Hz, 1H), 7.53 (dd, J = 7.7, 1.4 Hz, 1H), 7.43 - 7.37 (m, 1H), 7.02 - 6.90 (m, 2H), 6.68 (d, J = 16.1 Hz, 1H), 4.06 (s, 6H), 3.89 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ /ppm = 174.22, 170.88, 162.97, 158.96, 144.80, 132.71, 129.83, 122.76, 120.90, 116.32, 111.37, 55.95, 55.60. **IR(KBr)**: $\nu(C=O)$: 1753 cm^{-1} . **HRMS(ESI) m/z**: $[M+Na]^+$ calcd for $C_{15}H_{15}N_3NaO_5$: 340.0906; Found: 340.0904.

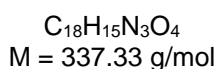
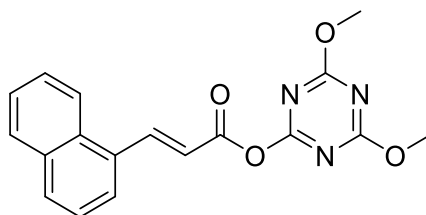
4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(m-tolyl)acrylate (**12**):



Prepared according to GP1 from the (E)-3-(4-chlorophenyl)acrylic acid (**1i**, 162.2 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **12** (256.1 mg, 0.85 mmol, 85 %) as a white solid.

¹H NMR (400 MHz, acetonitrile-*d*₃): δ/ppm = 7.88 (d, *J* = 16.0 Hz, 1H), 7.61 – 7.43 (m, 2H), 7.38 – 7.29 (m, 2H), 6.67 (d, *J* = 16.0 Hz, 1H), 4.01(s, 3H), 2.37(s, 3H). **¹³C NMR** (101 MHz, acetonitrile-*d*₃): δ/ppm = 174.23, 170.72, 162.45, 149.36, 138.90, 133.71, 132.27, 129.32, 129.05, 125.91, 115.62, 56.00, 21.42. **IR(KBr)**: ν(C=O): 1744 cm⁻¹. **HRMS(ESI) m/z**: [M+Na]⁺ calcd for C₁₅H₁₅N₃NaO₄: 324.0960; Found: 324.0955.

4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(naphthalen-1-yl)acrylate (**13**):

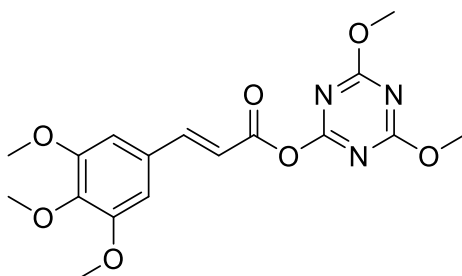


Prepared according to GP1 from the (E)-3-(naphthalen-1-yl)acrylic acid (**1j**, 198.2 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **13**(269.8 mg, 0.80 mmol, 80 %) as a white solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.76 (d, *J* = 15.9 Hz, 1H), 8.20 (d, *J* = 8.4 Hz, 1H), 7.98 – 7.81 (m, 3H), 7.64 – 7.49 (m, 3H), 6.68 (d, *J* = 15.9 Hz, 1H), 4.09(s, 6H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 174.27, 170.76, 162.30, 145.99, 133.77, 131.70, 131.48, 130.98, 128.95, 127.36, 126.55, 125.78, 125.56, 123.25, 118.29, 56.03. **IR(KBr)**: ν(C=O): 1687 cm⁻¹.

HRMS(ESI) m/z: $[M+Na]^+$ calcd for $C_{18}H_{15}N_3NaO_4$: 360.0956; Found: 360.0955.

4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(3,4,5-trimethoxyphenyl)acrylate (14):

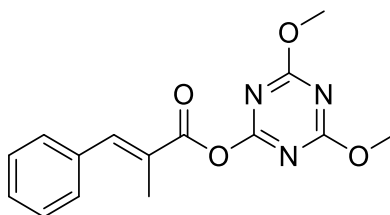


$C_{17}H_{19}N_3O_7$
M = 377.35 g/mol

Prepared according to GP1 from the (E)-3-(3,4,5-trimethoxyphenyl)acrylic acid (**1k**, 238.2 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **14** (320.7 mg, 0.85 mmol, 85 %) as a yellow solid.

1H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.81 (d, J = 15.9 Hz, 1H), 6.79 (s, 2H), 6.46 (d, J = 15.8 Hz, 1H), 4.06 (s, 6H), 3.89 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ /ppm = 174.23, 170.70, 162.33, 153.60, 149.08, 141.06, 129.20, 115.01, 105.83, 61.11, 56.28, 55.99. **IR(KBr)**: $\nu(C=O)$: 1769 cm^{-1} . **HRMS(ESI) m/z:** $[M+Na]^+$ calcd for $C_{17}H_{19}N_3NaO_7$: 400.1120; Found: 400.1115.

4,6-dimethoxy-1,3,5-triazin-2-yl (E)-2-methyl-3-phenylacrylate (15):



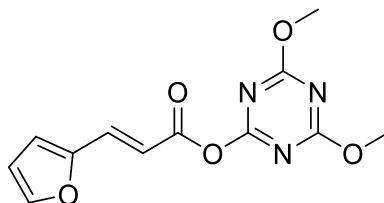
$C_{15}H_{15}N_3O_4$
M = 301.30 g/mol

Prepared according to GP1 from the (E)-2-methyl-3-phenylacrylic acid (**1l**, 162.2 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **15** (274.2 mg, 0.91 mmol, 91 %) as a white solid.

1H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.93 (s, 1H), 7.52 - 7.31 (m, 5H), 4.08 (s, 6H), 2.23 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ /ppm = 174.23, 171.21, 164.62, 143.28, 135.17, 130.09,

129.32, 128.66, 126.55, 56.03, 14.23. **IR(KBr)**: $\nu(\text{C}=\text{O})$: 1734 cm^{-1} . **HRMS(ESI) m/z**: $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{15}\text{H}_{15}\text{N}_3\text{NaO}_4$: 324.0952; Found: 324.0955.

4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(furan-2-yl)acrylate (16):

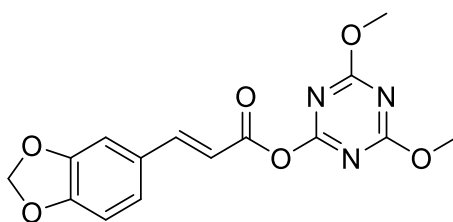


$\text{C}_{12}\text{H}_{11}\text{N}_3\text{O}_5$
M = 277.23 g/mol

Prepared according to GP1 from the (E)-3-(furan-2-yl)acrylic acid (**1m**, 138.1 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **16** (149.7 mg, 0.54 mmol, 54 %) as a brown solid.

¹H NMR (400 MHz, CDCl_3): δ/ppm = 7.62 (d, J = 15.6 Hz, 1H), 7.55 (d, J = 0.8 Hz, 1H), 7.26 (s, 1H), 6.74 (d, J = 3.4 Hz, 1H), 6.42 (d, J = 15.6 Hz, 1H), 4.06 (s, 6H). **¹³C NMR** (101 MHz, CDCl_3): δ/ppm = 174.19, 170.70, 162.45, 150.44, 146.07, 134.71, 117.28, 113.20, 112.88, 56.00. **IR(KBr)**: $\nu(\text{C}=\text{O})$: 1739 cm^{-1} . **HRMS(ESI) m/z**: $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{12}\text{H}_{11}\text{N}_3\text{NaO}_5$: 300.0587; Found: 300.0591.

4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(benzo[d][1,3]dioxol-5-yl)acrylate (17):



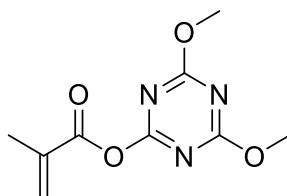
$\text{C}_{17}\text{H}_{17}\text{N}_3\text{O}_6$
M = 331.28 g/mol

Prepared according to GP1 from the (E)-3-(benzo[d][1,3]dioxol-5-yl)acrylic acid (**1n**, 192.2 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **17** (281.6 mg, 0.85 mmol, 85 %) as a white solid.

¹H NMR (400 MHz, CDCl_3): δ/ppm = 7.80 (d, J = 15.9 Hz, 1H), 7.05 (m, 2H), 6.83 (m, 1H), 6.37 (d, J = 16.0 Hz, 1H), 6.03(s, 2H), 4.06(s, 6H). **¹³C NMR** (101 MHz, CDCl_3): δ/ppm =

174.20, 170.74, 162.55, 150.65, 148.87, 148.62, 128.19, 113.57, 108.80, 106.76, 101.91, 55.99. **IR(KBr)**: $\nu(\text{C}=\text{O})$: 1755 cm^{-1} . **HRMS(ESI) m/z**: $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{17}\text{H}_{17}\text{N}_3\text{NaO}_6$: 354.0696; Found: 354.0697.

4,6-dimethoxy-1,3,5-triazin-2-yl methacrylate (**18**):

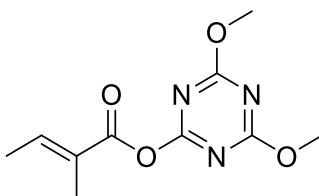


$\text{C}_9\text{H}_{11}\text{N}_3\text{O}_4$
M = 225.20 g/mol

Prepared according to GP1 from the methacrylic acid (**1o**, 86.1 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **18** (110.3 mg, 0.49 mmol, 49 %) as a white solid.

^1H NMR (400 MHz, CDCl_3): δ/ppm = 6.38 (s, 1H), 5.86 (s, 1H), 4.05 (s, 6H), 2.03 (s, 3H). **^{13}C NMR** (101 MHz, CDCl_3): δ/ppm = 174.20, 170.93, 163.16, 134.80, 129.85, 56.02, 18.17. **IR(KBr)**: $\nu(\text{C}=\text{O})$: 1748 cm^{-1} . **HRMS(ESI) m/z**: $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_9\text{H}_{11}\text{N}_3\text{NaO}_4$: 248.0644; Found: 248.0642.

4,6-dimethoxy-1,3,5-triazin-2-yl (E)-2-methylbut-2-enoate (**19**):



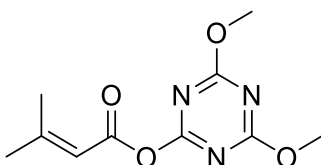
$\text{C}_{10}\text{H}_{13}\text{N}_3\text{O}_4$
M = 239.23 g/mol

Prepared according to GP1 from the (E)-2-methylbut-2-enoic acid (**1p**, 100.1 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **19** (107.6 mg, 0.45 mmol, 45 %) as a white solid.

^1H NMR (400 MHz, CDCl_3): δ/ppm = 7.14 (qd, J = 7.0, 1.2 Hz, 1H), 4.03 (s, 6H), 1.91 (s, 3H), 1.87 (dd, J = 6.9, 0.7 Hz, 3H). **^{13}C NMR** (101 MHz, CDCl_3): δ/ppm = 174.16, 171.20, 163.68, 142.80, 127.39, 55.90, 14.99, 12.05. **IR(KBr)**: $\nu(\text{C}=\text{O})$: 1740 cm^{-1} . **HRMS(ESI) m/z**: $[\text{M}+\text{Na}]^+$

calcd for C₁₀H₁₃N₃NaO₄: 262.0799; Found: 262.0798.

4,6-dimethoxy-1,3,5-triazin-2-yl 3-methylbut-2-enoate (**20**):

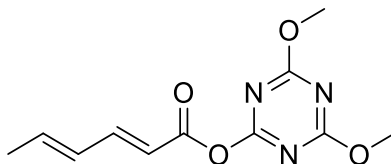


C₁₀H₁₃N₃O₄
M = 239.23 g/mol

Prepared according to GP1 from the 3-methylbut-2-enoic acid (**1q**, 100.1 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **20** (150.7 mg, 0.63 mmol, 60 %) as a white solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 5.85 (p, J = 1.4 Hz, 1H), 4.04 (s, 6H), 2.23 (d, J = 1.3 Hz, 3H), 1.99 (d, J = 1.4 Hz, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 174.15, 170.71, 164.16, 161.28, 114.21, 55.84, 27.91, 20.99. **IR(KBr)**: ν(C=O): 1760 cm⁻¹. **HRMS(ESI) m/z**: [M+Na]⁺ calcd for C₁₀H₁₃N₃NaO₄: 262.0795; Found: 262.0798.

4,6-dimethoxy-1,3,5-triazin-2-yl (2E,4E)-hexa-2,4-dienoate (**21**):

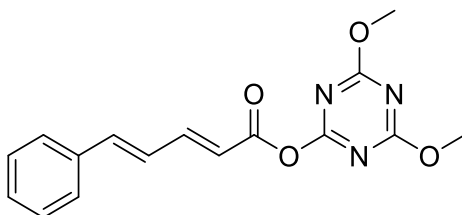


C₁₁H₁₃N₃O₄
M = 251.24 g/mol

Prepared according to GP1 from the (2E,4E)-hexa-2,4-dienoic acid (**1r**, 112.1 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **21** (105.5 mg, 0.42 mmol, 42 %) as a white solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 7.47 (ddd, J = 15.3, 6.6, 3.2 Hz, 1H), 6.30 - 6.25 (m, 2H), 5.89 (d, J = 15.0 Hz, 1H), 4.05 (s, 6H), 1.90 (d, J = 4.9 Hz, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 174.17, 170.75, 162.59, 149.53, 142.81, 129.71, 116.61, 55.95, 19.02. **IR(KBr)**: ν(C=O): 1745 cm⁻¹. **HRMS(ESI) m/z**: [M+Na]⁺ calcd for C₁₁H₁₃N₃NaO₄: 274.0795; Found: 274.0798.

4,6-dimethoxy-1,3,5-triazin-2-yl (2E,4E)-5-phenylpenta-2,4-dienoate (22):



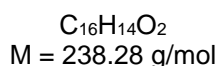
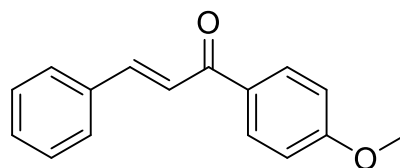
$C_{16}H_{15}N_3O_4$
M = 313.31g/mol

Prepared according to GP1 from the (2E,4E)-5-phenylpenta-2,4-dienoic acid (**1s**, 174.2 mg, 1.0 mmol, 1.0 equiv) and CDMT (210.7 mg, 1.2 mmol, 1.2 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(2:1) as eluent afforded the title compound **22** (260.1 mg, 0.83 mmol, 81 %) as a white solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 7.65 (dd, J = 15.2, 10.2 Hz, 1H), 7.50 - 7.45 (m, 2H), 7.40 - 7.32 (m, 3H), 7.03 - 6.93 (m, 2H), 6.10 (d, J = 15.2 Hz, 1H), 4.05 (s, 6H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 174.19, 170.74, 162.38, 149.11, 143.22, 135.61, 129.80, 129.01, 127.65, 125.75, 118.58, 55.99. **IR(KBr)**: ν(C=O): 1748 cm⁻¹. **HRMS(ESI) m/z**: [M+Na]⁺ calcd for C₁₆H₁₅N₃NaO₄: 336.0951; Found: 336.0955.

5.2 Characterization Data for Ketene

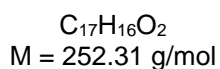
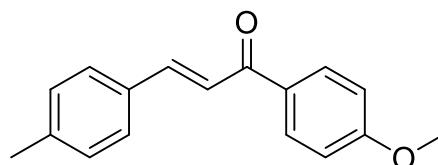
(E)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one (**23**)^[1]:



Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and phenylboronic acid (**2a**, 45.7 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **23** (59.6 mg, 0.237 mmol, 95 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.42 - 8.35 (m, 2H), 8.15 (d, J = 15.7 Hz, 1H), 7.99 (dd, J = 6.6, 2.9 Hz, 2H), 7.90 (d, J = 15.7 Hz, 1H), 7.76 (dd, J = 5.1, 1.9 Hz, 3H), 7.36 - 7.29 (m, 2H), 4.24(m, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 188.82, 163.22, 143.97, 130.93, 130.45, 129.03, 128.47, 121.91, 113.94, 55.62.

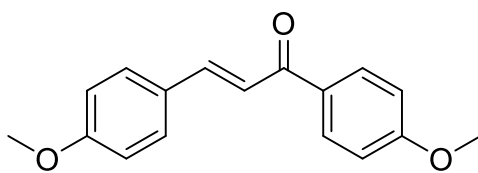
(E)-1-(4-methoxyphenyl)-3-(p-tolyl)prop-2-en-1-one (**24**)^[7]:



Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(p-tolyl)acrylate (**5**, 75.3 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (**2a**, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **24** (51.7 mg, 0.205 mmol, 82 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.08 - 8.00 (m, 2H), 7.79 (d, J = 15.6 Hz, 1H), 7.53 (m, 3H), 7.22 (d, J = 8.0 Hz, 2H), 7.01 - 6.95 (m, 2H), 3.89 (s, 3H), 2.39 (s, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 188.88, 163.44, 144.14, 140.93, 132.41, 131.30, 130.87, 129.77, 128.49, 120.91, 113.90, 55.58, 21.63.

(E)-1,3-bis(4-methoxyphenyl)prop-2-en-1-one (25)^[3]:

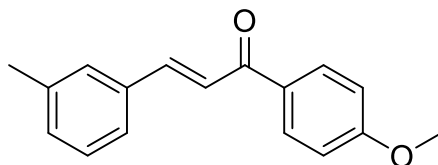


$C_{17}H_{16}O_3$
M = 268.31 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(4-methoxyphenyl)acrylate (**6**, 79.3 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (**2a**, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **25** (63.7 mg, 0.203 mmol, 95 %) as a yellow solid.

¹H NMR (400 MHz, $CDCl_3$): δ /ppm= 8.03 (d, J = 8.9 Hz, 2H), 7.77 (d, J = 15.6 Hz, 1H), 7.59 (d, J = 8.7 Hz, 2H), 7.43 (d, J = 15.6 Hz, 1H), 6.97 (d, J = 8.8 Hz, 2H), 6.93 (d, J = 8.7 Hz, 2H), 3.87 (s, 3H), 3.84 (s, 3H). **¹³C NMR** (151 MHz, $CDCl_3$): δ /ppm= 187.72, 162.25, 160.49, 142.77, 130.34, 129.67, 129.07, 126.80, 118.55, 113.36, 112.76, 54.44, 54.37.

(E)-3-(2-methoxyphenyl)-1-(2-methylphenyl)prop-2-en-1-one (26)^[5]:

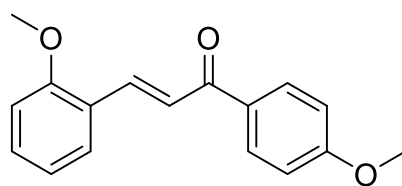


$C_{17}H_{16}O_2$
M = 252.31 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(2-methylphenyl)acrylate (**12**, 75.3 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (**2a**, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **26** (51.7 mg, 0.205 mmol, 77 %) as a yellow solid.

¹H NMR (400 MHz, $CDCl_3$): δ /ppm = 8.09 - 8.02 (m, 2H), 7.78 (d, J = 15.6 Hz, 1H), 7.54 (d, J = 15.7 Hz, 1H), 7.45 (d, J = 6.8 Hz, 2H), 7.31 (dd, J = 8.8, 7.1 Hz, 1H), 7.22 (d, J = 7.6 Hz, 1H), 7.03 - 6.95 (m, 2H), 3.89 (s, 3H), 2.40 (s, 3H). **¹³C NMR** (101 MHz, $CDCl_3$): δ /ppm = 188.83, 163.49, 144.27, 138.67, 135.10, 131.31, 130.91, 128.99, 125.73, 121.72, 113.92, 55.58, 21.46.

(E)-3-(2-methoxyphenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (27)^[8]:

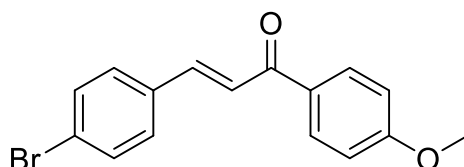


C₁₇H₁₆O₃
M = 268.31 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(2-methoxyphenyl)acrylate (**11**, 79.3mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (2a, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **27** (58.4 mg, 0.218 mmol, 87 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.10 (d, J = 15.8 Hz, 1H), 8.05 – 8.01 (m, 2H), 7.65 – 7.60 (m, 2H), 7.36 (ddd, J = 8.8, 7.4, 1.7 Hz, 1H), 7.01 – 6.90 (m, 4H), 3.90 (s, 3H), 3.87 (s, 3H). ¹³C NMR (101 MHz, CDCl₃): δ/ppm = 189.44, 163.32, 158.82, 139.64, 132.33, 131.63, 130.91, 129.26, 124.18, 122.76, 120.80, 113.85, 111.29, 55.62, 55.57.

(E)-3-(4-bromophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (28)^[8]:

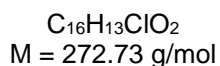
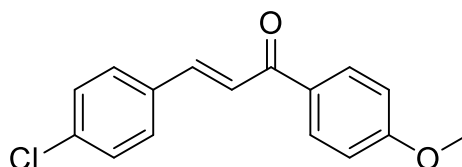


C₁₆H₁₃BrO₂
M = 317.18 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(4-bromophenyl)acrylate (**9**, 91.5 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (2a, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **28** (43.6 mg, 0.137 mmol, 55 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.03 (d, J = 8.9 Hz, 2H), 7.72 (d, J = 15.6 Hz, 1H), 7.57 – 7.46 (m, 5H), 6.98 (d, J = 8.9 Hz, 2H), 3.89 (s, 3H). ¹³C NMR (101 MHz, CDCl₃): δ/ppm = 188.49, 163.65, 142.61, 134.10, 132.26, 130.94, 129.82, 124.63, 122.46, 114.00, 55.61.

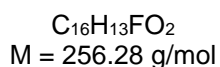
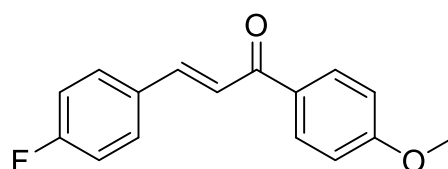
(E)-3-(4-chlorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (29)^[6]:



Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(4-chlorophenyl)acrylate (**10**, 80.4 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (2a, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **29** (54.5 mg, 0.203 mmol, 81 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.07 - 8.00 (m, 2H), 7.74 (d, J = 15.6 Hz, 1H), 7.59 - 7.54 (m, 2H), 7.51 (d, J = 15.6 Hz, 1H), 7.40 - 7.36 (m, 2H), 7.01 - 6.96 (m, 2H), 3.89 (s, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 188.47, 163.63, 142.54, 136.26, 133.66, 130.93, 129.60, 129.29, 122.35, 113.98, 55.61 .

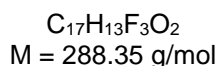
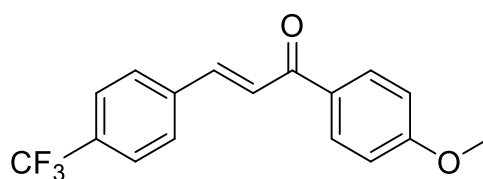
(E)-3-(4-fluorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (30)^[9]:



Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(4-fluorophenyl)acrylate (**7**, 76.3 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (2a, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **30** (57.6 mg, 0.225 mmol, 90 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.06 - 8.01 (m, 2H), 7.77 (d, J = 15.8 Hz, 1H), 7.66 - 7.61 (m, 2H), 7.48 (d, J = 15.9 Hz, 2H), 7.14 - 7.07 (m, 2H), 7.01 - 6.96 (m, 2H), 3.89(s, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 188.58, 163.56, 142.77, 130.91, 130.34 (d, J = 8.5 Hz), 121.58 (d, J = 1.8 Hz), 116.18 (d, J = 21.8 Hz), 113.96, 55.62.

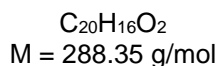
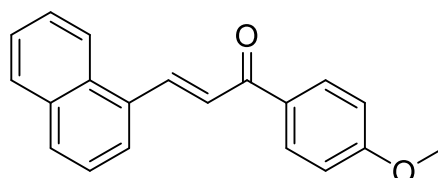
(E)-1-(4-methoxyphenyl)-3-(4-(trifluoromethyl)phenyl)prop-2-en-1-one (31)^[9]:



Prepared according to GP from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(4-trifluoromethylphenyl)acrylate (**8**, 88.8mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (2a, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **31** (47.6 mg, 0.165 mmol, 66%) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.08 - 8.03 (m, 2H), 7.80 (d, J = 15.8 Hz, 1H), 7.74 (d, J = 8.2 Hz, 2H), 7.67 (d, J = 8.3 Hz, 2H), 7.61 (d, J = 15.7 Hz, 1H), 7.02 - 6.98 (m, 2H), 3.90 (s, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 188.28, 163.79, 141.99, 138.56, 132.33, 131.02, 130.77, 128.51, 125.96 (d, J = 15.0 Hz), 124.15, 114.06, 55.63.

(E)-1-(4-methoxyphenyl)-3-(naphthalen-1-yl)prop-2-en-1-one (32)^[6]:

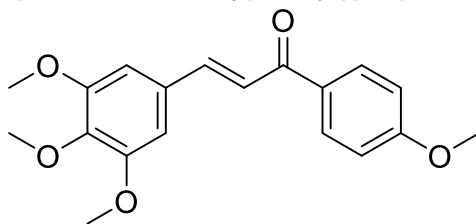


Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(naphthalen-1-yl)acrylate (**13**, 84.3 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (2a, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **32** (64.9 mg, 0.225 mmol, 90 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.11 - 8.07 (m, 2H), 8.04 - 7.94 (m, 2H), 7.90 - 7.79 (m, 4H), 7.67 (d, J = 15.6 Hz, 1H), 7.55 - 7.50 (m, 2H), 7.02 - 6.98 (m, 2H), 3.90 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ/ppm = 188.65, 163.60, 141.06, 133.82, 132.76, 132.34, 131.86, 131.13, 131.03, 130.69, 128.82, 127.01, 126.37, 125.54, 125.08, 124.67, 123.69, 114.00, 55.62.

(E)-1-(4-methoxyphenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one (33)^[5]:

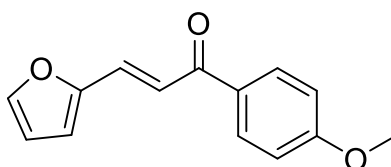


C₁₉H₂₀O₅
M = 328.36 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(3,4,5-trimethoxyphenyl)acrylate (**14**, 94.3 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (2a, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **33** (55.8 mg, 0.170 mmol, 68 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.03 (d, J = 8.8 Hz, 2H), 7.71 (d, J = 15.6 Hz, 1H), 7.42 (d, J = 15.6 Hz, 1H), 6.98 (d, J = 8.9 Hz, 2H), 6.85(s, 2H), 3.91(s, 6H), 3.89(s, 3H), 3.88(s, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 188.77, 163.48, 153.53, 144.24, 140.27, 131.18, 130.90, 130.66, 121.28, 113.92, 105.59, 61.10, 56.29, 55.59.

(E)-3-(furan-2-yl)-1-(4-methoxyphenyl)prop-2-en-1-one (34)^[10]:

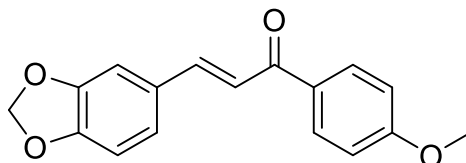


C₁₄H₁₂O₃
M = 228.25 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(furan-2-yl)acrylate (**16**, 69.3 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (2a, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **34** (47.9 mg, 0.210 mmol, 82 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.09 - 7.95 (m, 2H), 7.62 - 7.37 (m, 3H), 7.05 - 6.87 (m, 2H), 6.69 (d, J = 3.4 Hz, 1H), 6.50 (dd, J = 3.4, 1.8 Hz, 1H), 3.88 (s, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 188.20, 163.50, 151.90, 144.80, 131.14, 130.85, 130.10, 119.24, 115.96, 113.91, 112.71, 55.59.

(E)-3-(benzo[d][1,3]dioxol-5-yl)-1-(4-methoxyphenyl)prop-2-en-1-one (35)^[6]:

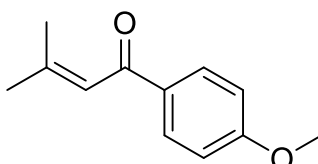


C₁₇H₁₄O₄
M = 282.30 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(benzo[d][1,3]dioxol-5-yl)acrylate (**17**, 82.8 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (**2a**, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **35** (53.6 mg, 0.190 mmol, 76 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.02 (d, J = 8.8 Hz, 2H), 7.72 (d, J = 15.5 Hz, 1H), 7.38 (d, J = 15.5 Hz, 1H), 7.18 - 7.08 (m, 2H), 6.97 (d, J = 8.8 Hz, 2H), 6.84 (d, J = 8.0 Hz, 1H), 6.02 (s, 2H), 3.88 (s, 3H). ¹³C NMR (101 MHz, CDCl₃): δ/ppm = 188.70, 163.43, 149.82, 148.47, 143.92, 131.34, 130.81, 129.64, 125.13, 119.97, 113.90, 108.75, 106.71, 101.69, 55.58.

(E)-1-(4-methoxyphenyl)-3-methylbut-2-en-1-one(36):

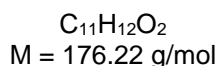
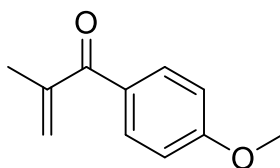


C₁₂H₁₄O₂
M = 190.24 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl 3-methylbut-2-enoate(**20**, 59.8 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (**2a**, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **36** (23.3 mg, 0.123 mmol, 49 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 7.95 - 7.91 (m, 2H), 6.94 - 6.91 (m, 2H), 6.72 - 6.70 (m, 1H), 3.86(s, 3H), 2.18 (d, J = 1.2 Hz, 3H), 2.00 (d, J = 1.2 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃): δ/ppm = 190.46, 163.01, 155.44, 132.20, 130.56, 121.27, 113.67, 55.53, 28.02, 21.17.

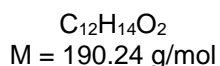
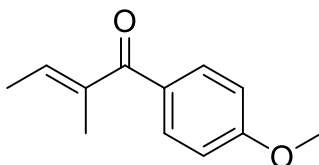
1-(4-methoxyphenyl)-2-methylprop-2-en-1-one (37):



Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl methacrylate (1p, 56.3 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (**18**, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **37** (24.2 mg, 0.137 mmol, 55 %) as a yellow solid.

1H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.81 - 7.76 (m, 2H), 6.95 - 6.89 (m, 2H), 5.80 - 5.79 (m, 1H), 5.53 (s, 1H), 3.86 (s, 3H), 2.06 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ /ppm = 1197.29, 163.08, 143.96, 131.99, 130.08, 124.99, 113.51, 55.53, 19.20.

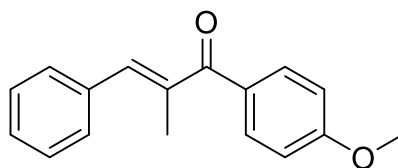
(E)-1-(4-methoxyphenyl)-2-methylbut-2-en-1-one (38):



Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-2-methylbut-2-enoate(**19**, 59.8 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (2a, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **38** (23.8 mg, 0.125 mmol, 50 %) as a yellow solid.

1H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.66 (d, J = 8.8 Hz, 2H), 6.90 (d, J = 8.8 Hz, 2H), 6.32 (qd, J = 6.9, 1.5 Hz, 1H), 3.85(s, 3H), 1.95(s, 3H), 1.86 (d, J = 6.9 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ /ppm = 198.03, 162.49, 139.28, 137.53, 131.77, 131.07, 113.35, 55.50, 14.70, 12.74.

(E)-1-(4-methoxyphenyl)-2-methyl-3-phenylprop-2-en-1-one (39):



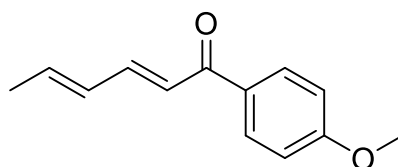
$C_{17}H_{16}O_2$
M = 252.31 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-2-methyl-3-phenylacrylate (**15**, 75.3 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (**2a**, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **39** (57.3 mg, 0.227 mmol, 91 %) as a yellow solid.

1H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.83 - 7.77 (m, 2H), 7.43 - 7.38 (m, 4H), 7.36 - 7.28 (m, 1H), 7.10 (d, J = 1.3 Hz, 1H), 6.98 - 6.92 (m, 2H), 3.86 (s, 3H), 2.25 (d, J = 1.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ /ppm = 198.42, 162.88, 140.19, 137.06, 136.04, 132.10, 130.74, 129.70, 128.56, 128.44, 113.59, 55.55, 15.02 .

(2E,4E)-1-(4-methoxyphenyl)hexa-2,4-dien-1-one (40):

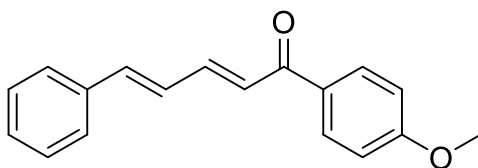


$C_{13}H_{16}O_2$
M = 202.25 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (2E,4E)-hexa-2,4-dienoate(**21**, 62.8 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (**2a**, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **40** (32.8 mg, 0.163 mmol, 65 %) as a yellow solid.

1H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.97 - 7.90 (m, 2H), 7.38 (dd, J = 15.0, 10.5 Hz, 1H), 6.96 - 6.90 (m, 2H), 6.87 (d, J = 15.0 Hz, 1H), 6.37 - 6.17 (m, 2H), 3.85 (s, 3H), 1.87 (d, J = 6.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ /ppm = 189.20, 163.29, 144.50, 140.65, 131.24, 130.71, 123.15, 113.81, 55.55, 18.98.

(2E,4E)-1-(4-methoxyphenyl)-5-phenylpenta-2,4-dien-1-one (41):

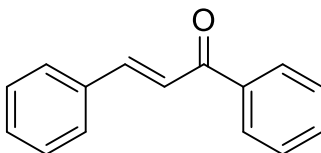


$C_{18}H_{16}O_2$
M = 264.32 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (2E,4E)-5-phenylpenta-2,4-dienoate (**22**, 78.3 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (2a, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **41** (59.5 mg, 0.225 mmol, 90 %) as a yellow solid.

¹H NMR (400 MHz, $CDCl_3$): δ /ppm = 8.05 - 7.97 (m, 2H), 7.60 (ddd, J = 14.9, 8.4, 1.8 Hz, 1H), 7.50 (d, J = 7.1 Hz, 2H), 7.40 - 7.29 (m, 3H), 7.12 (d, J = 14.9 Hz, 1H), 7.04 - 6.95 (m, 4H), 3.88 (s, 3H). **¹³C NMR** (101 MHz, $CDCl_3$): δ /ppm = 188.78, 163.42, 144.11, 141.51, 136.29, 131.20, 130.79, 129.21, 128.94, 127.34, 127.15, 125.33, 113.90, 55.59.

(E)-chalcone(42)^[1]:

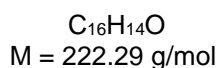
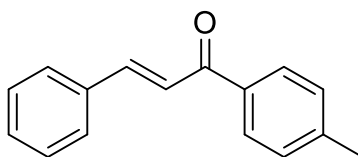


$C_{15}H_{12}O$
M = 208.26 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and phenylboronic acid (2b, 45.7 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **42** (42.2 mg, 0.203 mmol, 81 %) as a yellow solid.

¹H NMR (400 MHz, $CDCl_3$): δ /ppm = 8.06 - 8.00 (m, 2H), 7.82 (d, J = 11.9 Hz, 1H), 7.65 (dd, J = 5.1, 2.2 Hz, 2H), 7.59 (t, J = 5.6 Hz, 1H), 7.57 - 7.48 (m, 3H), 7.45 - 7.38 (m, 3H). **¹³C NMR** (101 MHz, $CDCl_3$): δ /ppm = 190.68, 144.97, 138.29, 134.97, 132.91, 130.67, 129.07, 128.74, 128.61, 128.56.

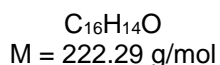
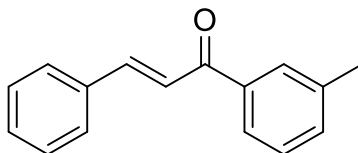
(E)-3-phenyl-1-(p-tolyl)prop-2-en-1-one (43)^[1]:



Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and p-tolylboronic acid (**2c**, 51.0 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **43** (45,5 mg, 0.205 mmol, 82 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.04 – 8.00 (m, 2H), 7.80 (d, J = 16 Hz, 1H), 7.62 – 7.47 (m, 6H), 7.23 (d, J = 8.0 Hz, 2H), 2.40(s, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 190.79, 145.07, 141.21, 138.44, 132.78, 132.23, 129.81, 128.69, 128.58, 121.17, 21.65.

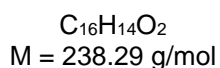
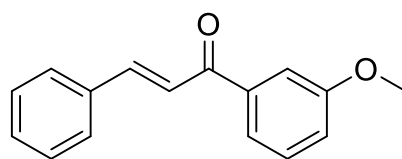
(E)-3-phenyl-1-(m-tolyl)prop-2-en-1-one (44):



Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (3-methyl)boronic acid (**2d**, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **44** (52.8mg, 0.237 mmol, 95 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 7.85 – 7.78 (m, 3H), 7.66 (dd, J = 6.5, 2.8 Hz, 2H), 7.54 (d, J = 15.9 Hz, 1H), 7.45 – 7.38 (m, 5H), 2.45(s, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 190.87, 144.79, 138.58, 138.32, 135.01, 133.71, 130.62, 129.14, 129.06, 128.59, 128.56, 125.82, 122.32, 21.53.

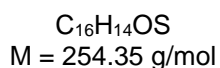
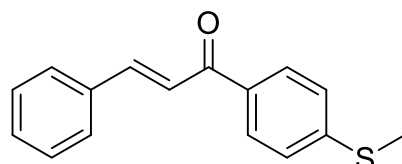
(E)-1-(3-methoxyphenyl)-3-phenylprop-2-en-1-one (45)^[2]:



Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (3-methoxyphenyl)boronic acid (**2e**, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **45** (53.6 mg, 0.225 mmol, 90 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 7.82 (d, J = 15.7 Hz, 1H), 7.67 - 7.59 (m, 3H), 7.56 - 7.49 (m, 2H), 7.43 (m, 4H), 7.16 - 7.12 (m, 1H), 3.89 (s, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 190.39, 160.01, 144.98, 139.69, 134.98, 130.67, 129.68, 129.07, 128.57, 122.21, 121.16, 119.43, 112.94, 55.59.

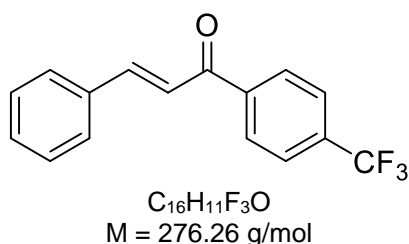
(E)-1-(4-(methylthio)phenyl)-3-phenylprop-2-en-1-one (46):



Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (4-methylthiophenyl)boronic acid (**2f**, 51 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **3ak** (52.1 mg, 0.205 mmol, 82 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 7.96 (d, J = 8.5 Hz, 2H), 7.82 (d, J = 15.7 Hz, 1H), 7.65 (dd, J = 6.6, 2.8 Hz, 2H), 7.53 (d, J = 15.7 Hz, 1H), 7.42 (dd, J = 5.0, 1.7 Hz, 3H), 7.31 (d, J = 8.5 Hz, 2H), 2.54 (s, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 189.30, 145.80, 144.63, 135.01, 134.45, 130.62, 129.07, 128.55, 125.12, 121.76, 14.90.

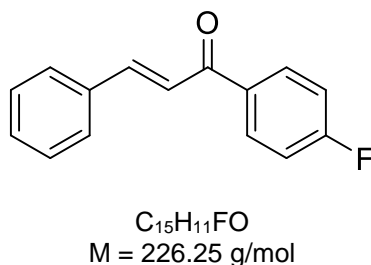
(E)-3-phenyl-1-(4-(trifluoromethyl)phenyl)prop-2-en-1-one (47)^[1]



Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (4-trifluoromethyl)boronic acid (2g, 71.2 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **3ab** (37.9 mg, 0.203 mmol, 55 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.10 (d, J = 8.2 Hz, 2H), 7.84 (d, J = 15.8 Hz, 1H), 7.77 (d, J = 8.3 Hz, 2H), 7.66 (m, 2H), 7.49 (d, J = 15.7 Hz, 1H), 7.47 - 7.41 (m, 3H). ¹³C NMR (101 MHz, CDCl₃): δ/ppm = 189.78, 146.24, 141.12, 134.57, 131.09, 129.16, 128.87, 128.71, 125.77(d, J = 3.65 Hz), 121.64.

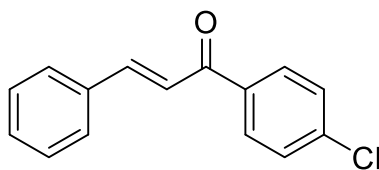
(E)-1-(4-fluorophenyl)-3-phenylprop-2-en-1-one (48)^[1]:



Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (4-fluorophenyl)boronic acid (2h, 52.5mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **48** (44.1 mg, 0.195 mmol, 78 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 8.10 - 8.02 (m, 2H), 7.82 (d, J = 15.7 Hz, 1H), 7.65 (dd, J = 6.7, 3.0 Hz, 2H), 7.51 (d, J = 15.7 Hz, 1H), 7.45 - 7.40 (m, 3H), 7.23 - 7.13 (m, 2H). ¹³C NMR (101 MHz, CDCl₃): δ/ppm = 188.94, 165.70 (d, J = 253.3 Hz), 145.18, 134.83, 134.60, 131.20 (d, J = 35.3 Hz), 130.77, 129.09, 128.58, 121.63, 115.85.

(E)-1-(4-chlorophenyl)-3-phenylprop-2-en-1-one (49)^[1]:

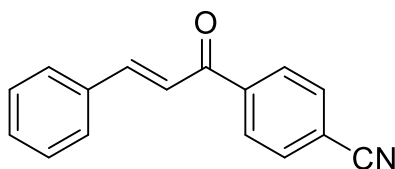


$C_{15}H_{11}ClO$
M = 242.70 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (4-chlorophenyl)boronic acid (**2i**, 58.6 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **49** (54.6 mg, 0.225 mmol, 90%) as a yellow solid.

¹H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.97 (d, J = 8.5 Hz, 2H), 7.82 (d, J = 15.7 Hz, 1H), 7.64 (m, 2H), 7.52 - 7.46 (m, 3H), 7.44 - 7.40 (m, 3H). **¹³C NMR** (101 MHz, $CDCl_3$): δ /ppm = 189.29, 145.47, 139.32, 136.57, 134.76, 130.86, 130.02, 129.11, 129.05, 128.62, 121.55 .

4-cinnamoylbenzotrile (50):

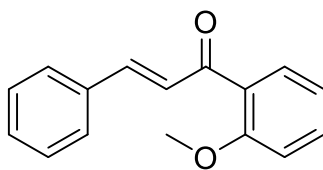


$C_{19}H_{14}NO$
M = 258.32 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (4-methoxyphenyl)boronic acid (**2j**, 55.1 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **50** (52.3 mg, 0.203 mmol, 81%) as a yellow solid.

¹H NMR (400 MHz, $CDCl_3$): δ /ppm = 8.09 (d, J = 8.3 Hz, 2H), 7.83 (m, 3H), 7.66 (m, 2H), 7.46 (m, 4H). **¹³C NMR** (101 MHz, $CDCl_3$): δ /ppm = 189.30, 146.73, 141.55, 134.42, 132.61, 131.28, 129.20, 128.97, 128.77, 121.23, 118.15, 116.04.

(E)-1-(2-methoxyphenyl)-3-phenylprop-2-en-1-one (51):

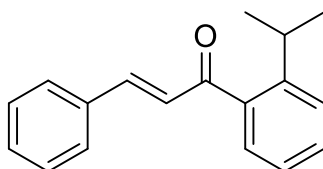


$C_{16}H_{14}O_2$
M = 238.29 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (2-methoxyphenyl)boronic acid (**2k**, 57 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **51** (39.3 mg, 0.165 mmol, 66%) as a yellow solid.

1H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.68 - 7.56 (m, 4H), 7.48 (ddd, J = 8.4, 7.5, 1.8 Hz, 1H), 7.41 - 7.35 (m, 4H), 7.08 - 6.94 (m, 2H), 3.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ /ppm = 193.14, 158.21, 143.36, 135.23, 132.99, 130.45, 130.36, 129.37, 128.98, 128.51, 127.18, 120.84, 111.73, 55.85.

(E)-1-(2-isopropylphenyl)-3-phenylprop-2-en-1-one (52):

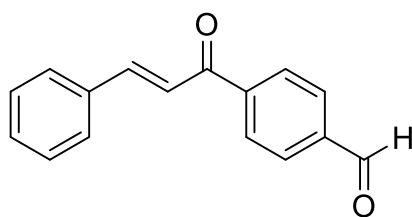


$C_{18}H_{18}O$
M = 250.34 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (2-isopropylphenyl)boronic acid (**2l**, 61.5 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **52** (44.4 mg, 0.177 mmol, 71%) as a yellow solid.

1H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.65 - 7.58 (m, 2H), 7.51 - 7.46 (m, 2H), 7.44 - 7.33 (m, 5H), 7.31 - 7.26 (m, 1H), 7.13 (d, J = 16 Hz, 1H), 3.15 (hept, J = 6.8 Hz, 1H), 1.21 (d, J = 5.2 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ /ppm = 197.74, 146.89, 146.19, 139.14, 134.61, 130.84, 130.36, 129.08, 128.59, 127.80, 127.28, 126.19, 125.58, 30.00, 23.43.

4-Cinnamoylbenzaldehyde (**53**):

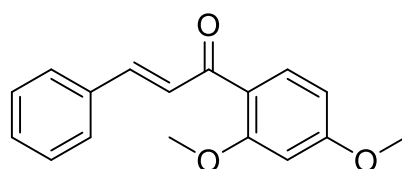


$C_{16}H_{12}O_2$
M = 236.27 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (4-formyl)boronic acid (2m, 61.5 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **53** (46 mg, 0.195 mmol, 78%) as a yellow solid.

1H NMR (400 MHz, $CDCl_3$): δ /ppm = 10.12(s, 1H), 8.14 (d, J = 8.1 Hz, 2H), 8.01 (d, J = 8.1 Hz, 2H), 7.83 (d, J = 15.9 Hz, 1H), 7.66 (dd, J = 6.5, 2.8 Hz, 2H), 7.51 (d, J = 15.9 Hz, 1H), 7.46 – 7.41 (m, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ /ppm = 191.80, 190.11, 146.26, 142.86, 138.82, 134.56, 131.12, 129.96, 129.17, 129.08, 128.74, 121.77.

(E)-1-(2,4-dimethoxyphenyl)-3-phenylprop-2-en-1-one (**54**)^[4]:



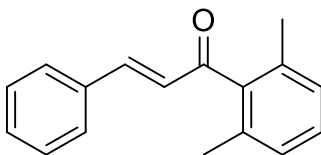
$C_{17}H_{16}O_3$
M = 268.31 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (4,6-methoxyphenyl)boronic acid (2n, 68.2 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **54** (60.4 mg, 0.225 mmol, 90%) as a yellow solid.

1H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.77 (d, J = 8.6 Hz, 1H), 7.69 (d, J = 15.8 Hz, 1H), 7.63 – 7.57 (m, 2H), 7.52 (d, J = 15.8 Hz, 1H), 7.43 – 7.35 (m, 3H), 6.57 (dd, J = 8.6, 2.1 Hz, 1H), 6.50 (d, J = 2.1 Hz, 1H), 3.91 (s, 3H), 3.87 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ /ppm = 190.61, 164.29, 160.51, 142.11, 135.54, 133.02, 130.07, 128.93, 128.41, 127.24,

122.26 , 105.24 , 98.70 , 55.85 , 55.67 .

(E)-1-(2,6-dimethylphenyl)-3-phenylprop-2-en-1-one (55):

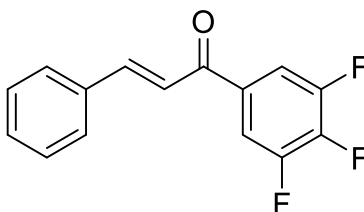


C₁₇H₁₆O
M = 236.31 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (2,6-methylphenyl)boronic acid (**2o**, 56.2 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **3aq** (18.9 mg, 0.080 mmol, 32%) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 7.54 - 7.48 (m, 2H), 7.42 - 7.35 (m, 3H), 7.24 - 7.15 (m, 2H), 7.08 (d, J = 7.6 Hz, 2H), 6.95 (d, J = 16.3 Hz, 1H), 2.23 (s, 6H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 201.37 , 147.12 , 139.91 , 134.43 , 134.18 , 131.01 , 129.09 , 128.75 , 128.62 , 128.25 , 127.72 , 19.46

(E)-3-phenyl-1-(3,4,5-trifluorophenyl)prop-2-en-1-one (56):

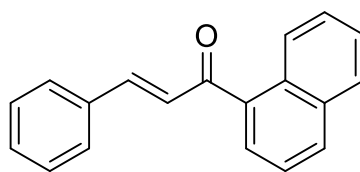


C₁₅H₉F₃O
M = 262.23 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (3,4,5-trifluorophenyl)boronic acid (**2p**, 65.9 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **56** (17 mg, 0.065 mmol, 26 %) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 7.86 (d, J = 15.6 Hz, 1H), 7.71 - 7.62 (m, 4H), 7.48 - 7.37 (m, 4H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 186.68, 146.70, 134.37, 131.28, 129.19, 128.77, 120.16, 113.19, 112.97.

(E)-1-(naphthalen-1-yl)-3-phenylprop-2-en-1-one (57):

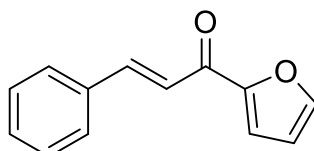


$C_{19}H_{14}O$
M = 258.32 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and 1-naphthylboronic Acid (2q, 64.5 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **57** (54.9 mg, 0.213 mmol, 85 %) as a yellow solid.

¹H NMR (400 MHz, $CDCl_3$): δ /ppm = 8.34 - 8.31 (m, 1H), 8.01 (m, 1H), 7.94 - 7.90 (m, 1H), 7.78 (m, 1H), 7.64 - 7.52 (m, 6H), 7.42 (m, 3H), 7.31 (d, J = 16.0 Hz, 1H). **¹³C NMR** (101 MHz, $CDCl_3$): δ /ppm = 195.93, 146.13, 137.14, 134.67, 133.93, 131.72, 130.84, 130.58, 129.10, 128.61, 128.55, 127.56, 127.24, 127.21, 126.59, 125.74, 124.62.

(E)-1-(furan-2-yl)-3-phenylprop-2-en-1-one (58):

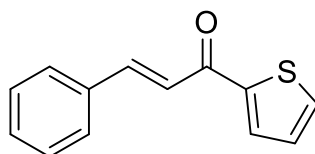


$C_{13}H_{10}O_2$
M = 198.22 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and 2-furylboronic acid (2r, 41.9 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **58** (47 mg, 0.237 mmol, 95%) as a yellow solid.

¹H NMR (400 MHz, $CDCl_3$): δ /ppm = 7.88 (d, J = 16.0 Hz, 1H), 7.67 - 7.63 (m, 3H), 7.48 - 7.39 (m, 4H), 7.34 (d, J = 3.5 Hz, 1H), 6.59 (dd, J = 3.5, 1.5 Hz, 1H). **¹³C NMR** (101 MHz, $CDCl_3$): δ /ppm = 178.11, 153.77, 146.66, 144.09, 134.79, 130.73, 129.05, 128.64, 121.21, 117.66, 112.67.

(E)-3-phenyl-1-(thiophen-2-yl)prop-2-en-1-one (59)^[1]:

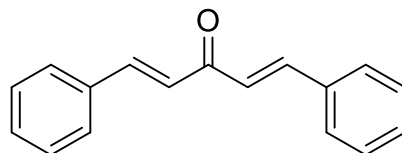


C₁₃H₁₀OS
M = 214.28 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and 2-thiopheneboronic acid (**2s**, 47.9 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **59** (49.8 mg, 0.233 mmol, 93%) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 7.91 - 7.80 (m, 2H), 7.71 - 7.63 (m, 3H), 7.47 - 7.40 (m, 4H), 7.21 - 7.16 (m, 1H). ¹³C NMR (101 MHz, CDCl₃): δ/ppm = 182.14, 145.62, 144.18, 134.78, 134.05, 131.94, 130.72, 129.07, 128.60, 128.38, 121.68.

(1E,4E)-1,5-diphenylpenta-1,4-dien-3-one (60):

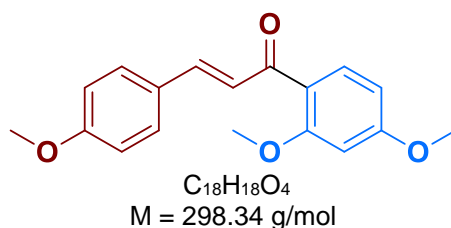


C₁₇H₁₄O
M = 234.30 g/mol

Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl cinnamate (**4**, 71.8 mg, 0.25 mmol, 1.0 equiv) and (E)-styrylboronic acid (**2t**, 55.5 mg, 0.375 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **60** (48.0 mg, 0.205 mmol, 82%) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 7.75 (d, J = 16.0 Hz, 2H), 7.62 (dd, J = 6.8, 2.9 Hz, 4H), 7.49 - 7.31 (m, 6H), 7.10 (d, J = 15.9 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃): δ/ppm = 189.04, 143.44, 134.87, 130.63, 129.08, 128.52, 125.50.

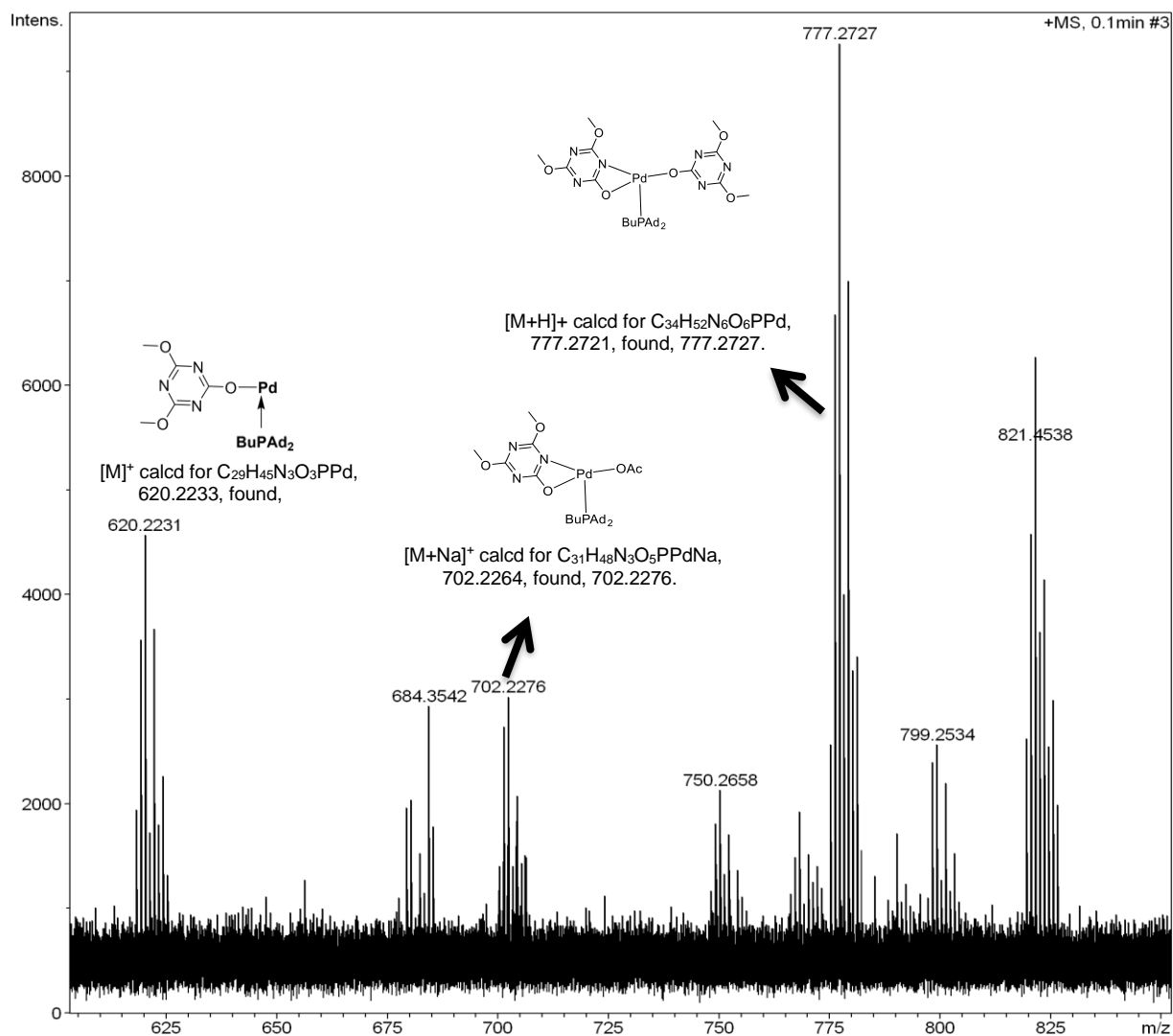
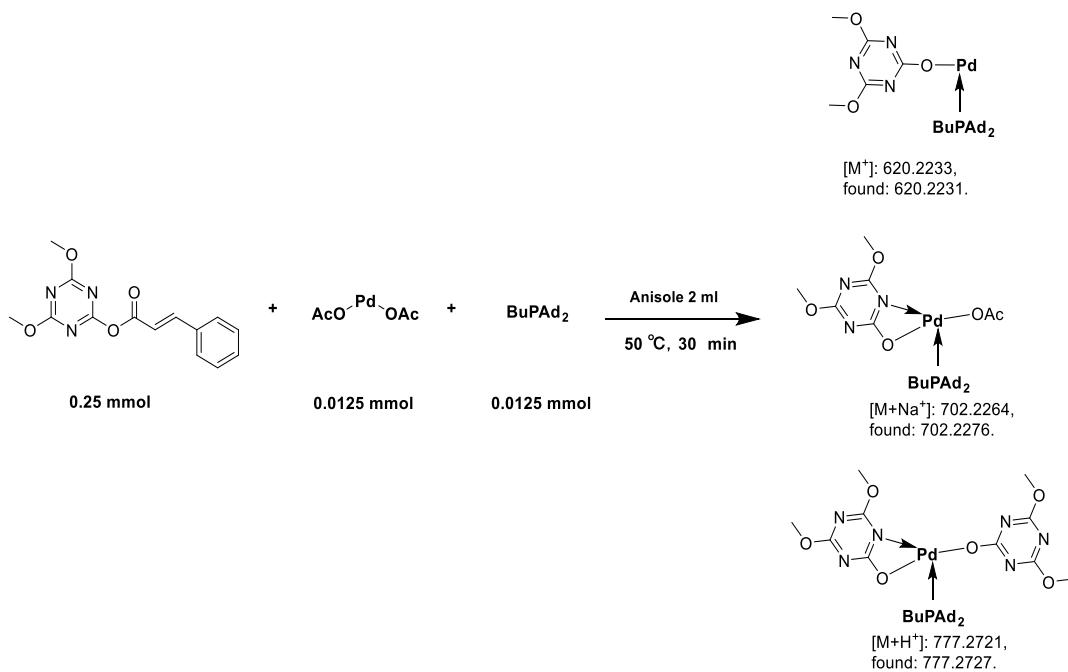
metochalcone (61)^[5]:



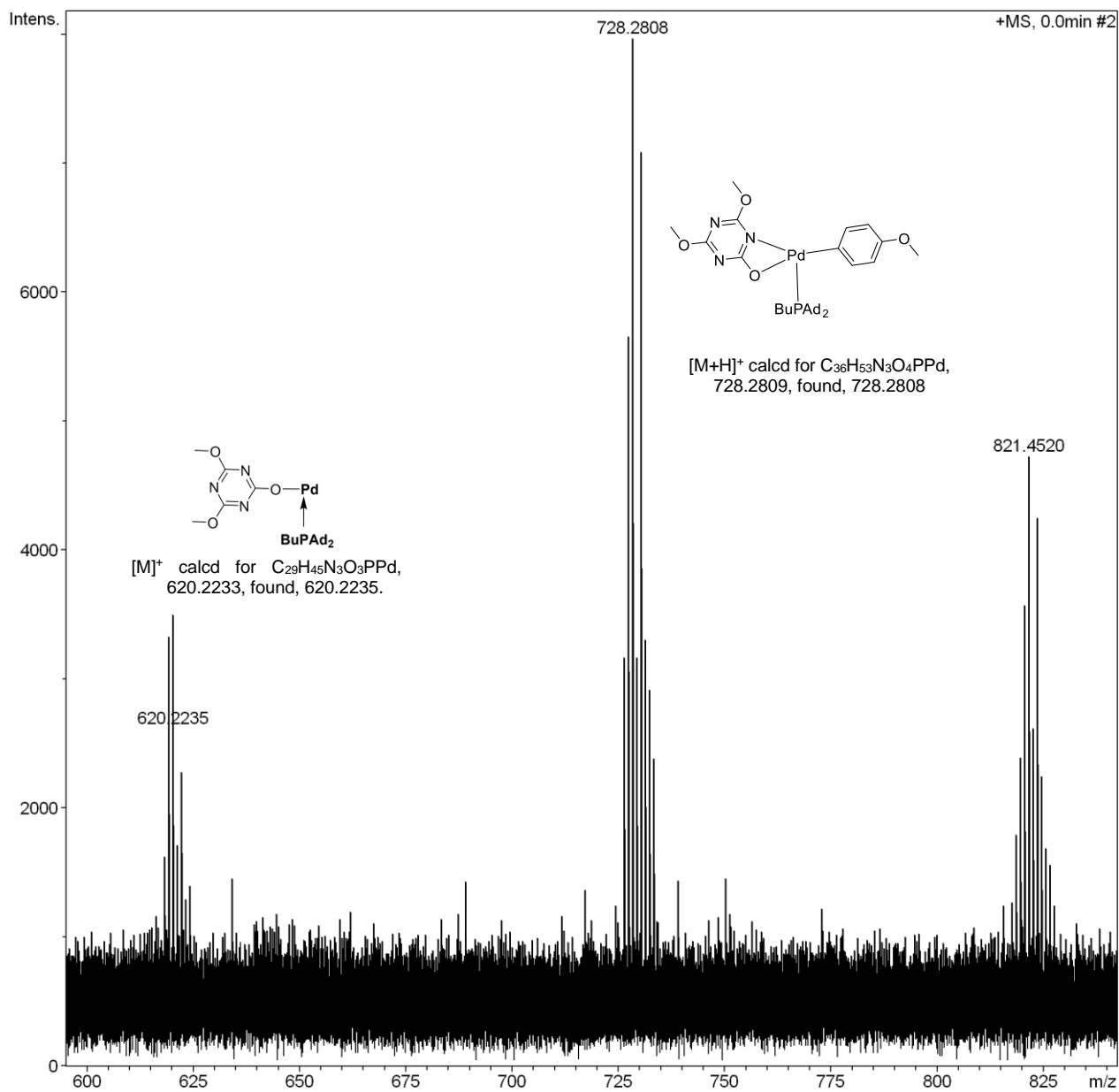
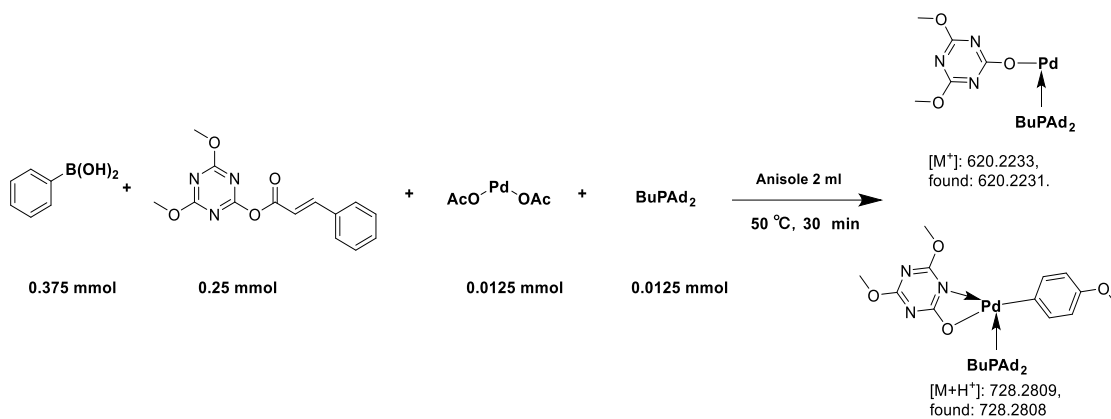
Prepared according to GP2 from the 4,6-dimethoxy-1,3,5-triazin-2-yl (E)-3-(4-methoxyphenyl)acrylate (**6**, 1.59 g, 5 mmol, 1.0 equiv) and (4,6-methoxyphenyl)boronic acid (2n, 1.37 g, 7.5 mmol, 1.5 equiv). Purification by flash column chromatography on silica gel using petroleum ether(PE):ethyl acetate(EA)(20:1) as eluent afforded the title compound **61** (1.35 g, 4.5 mmol, 90%) as a yellow solid.

¹H NMR (400 MHz, CDCl₃): δ/ppm = 7.74 (d, J = 8.5 Hz, 1H), 7.65 (d, J = 15.8 Hz, 1H), 7.54 (d, J = 8.5 Hz, 2H), 7.39 (d, J = 15.8 Hz, 1H), 6.91 (d, J = 8.4 Hz, 2H), 6.55 (dd, J = 8.5, 1.9 Hz, 1H), 6.49 (d, J = 1.6 Hz, 1H), 3.89 (s, 3H), 3.86 (s, 3H), 3.83 (s, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ/ppm = 190.76, 164.05, 161.31, 160.33, 142.17, 132.83, 130.09, 128.22, 125.07, 122.52, 114.37, 105.16, 98.73, 55.83, 55.63, 55.47.

6. Detecting Pd Intermediates via HR ESI-Mass



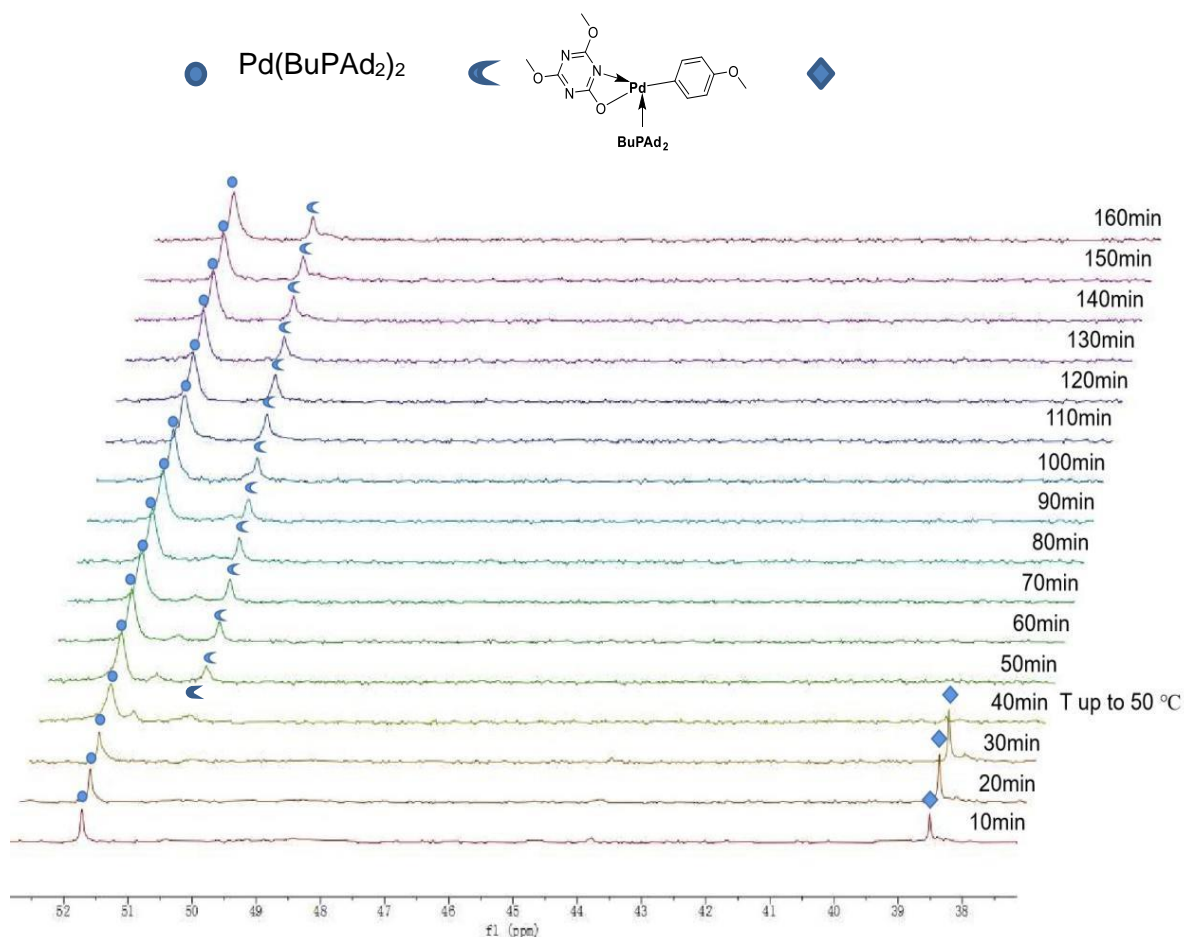
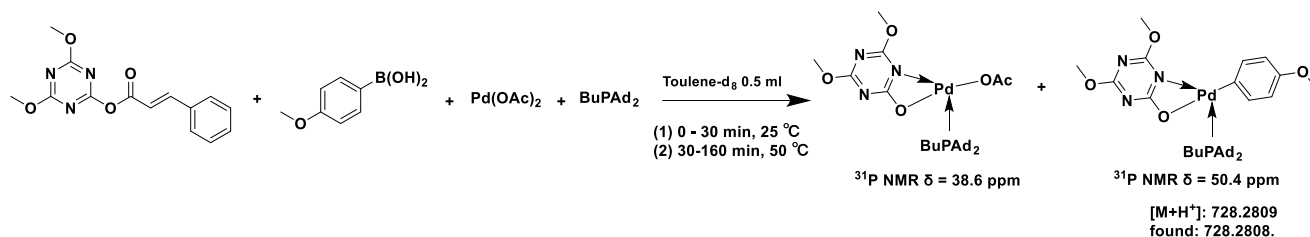
Scheme S4



Scheme S5

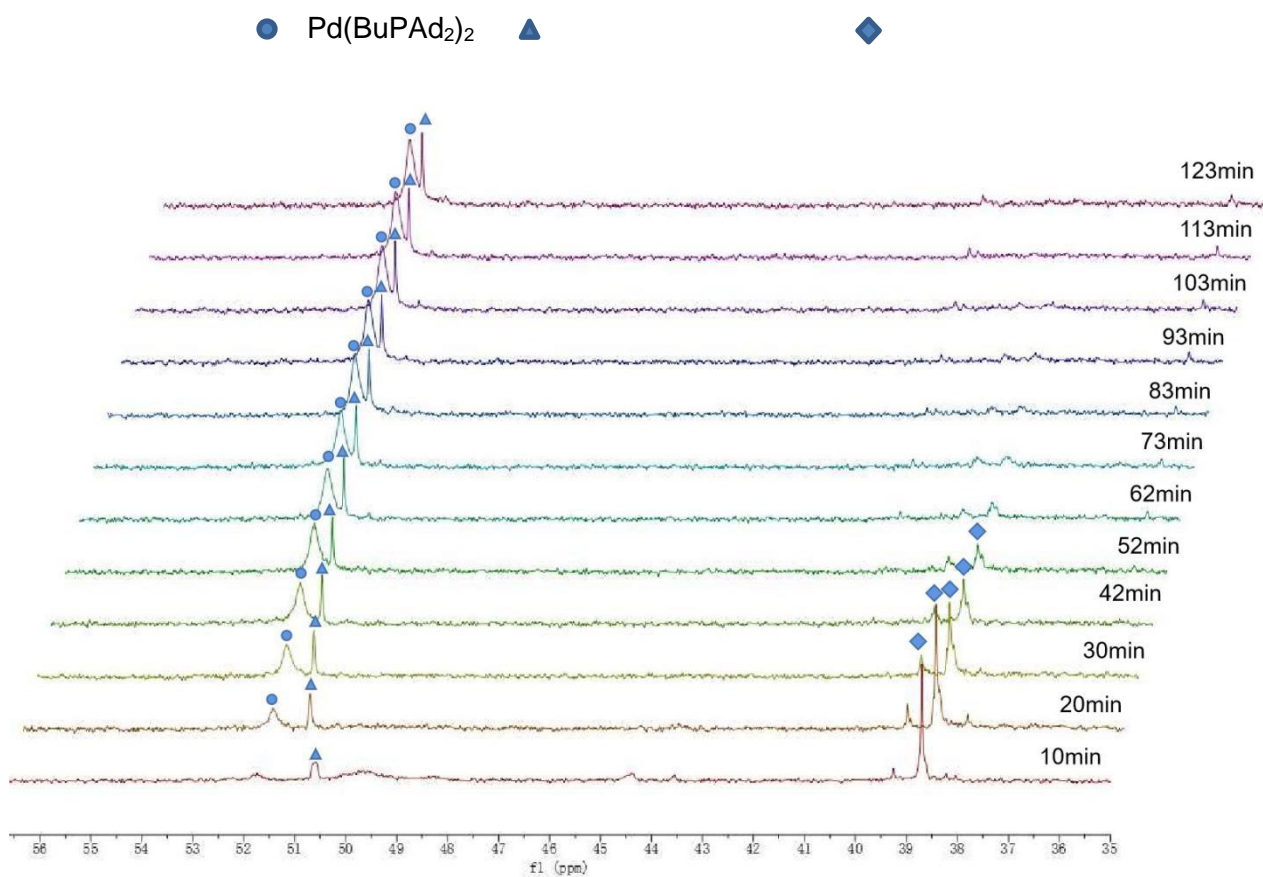
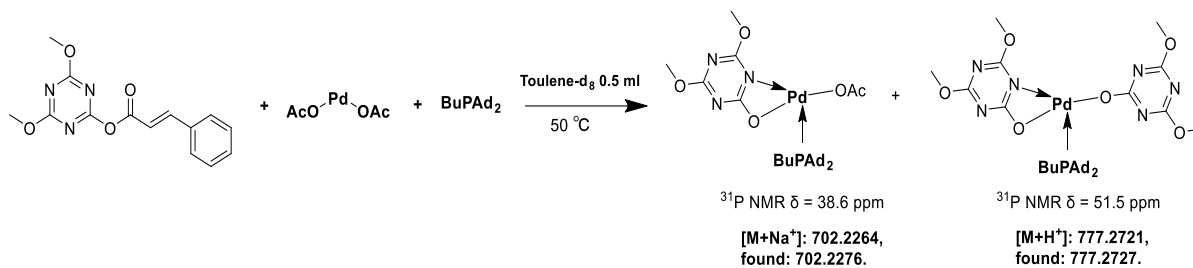
7. Monitoring the reaction by ^{31}P NMR

Procedure: The reaction mixture contained 0.1 mmol of **4**, 0.15 mmol of **3a**, 0.05 mmol of $\text{Pd}(\text{OAc})_2$, and 0.05 mmol of BuPAD_2 , all dissolved in 0.5 mL of deuterated toluene- d_8 . The experiment was carried out in an NMR tube at 25°C for 30 minutes, after which the temperature was raised to 50°C and the reaction continued for 160 minutes.



Scheme **S6** ^{31}P Spectrum of reaction of coupling of triazine ester with boron acid in presence of stoichiometric amount $\text{Pd}(\text{OAc})_2$ and BuPAD_2

Procedure: The reaction mixture consisted of 0.1 mmol of **4**, 0.05 mmol of Pd(OAc)₂, and 0.05 mmol of BuPAD₂ dissolved in 0.5 mL of deuterated toluene-d₈. The experiment was carried out in a NMR tube.



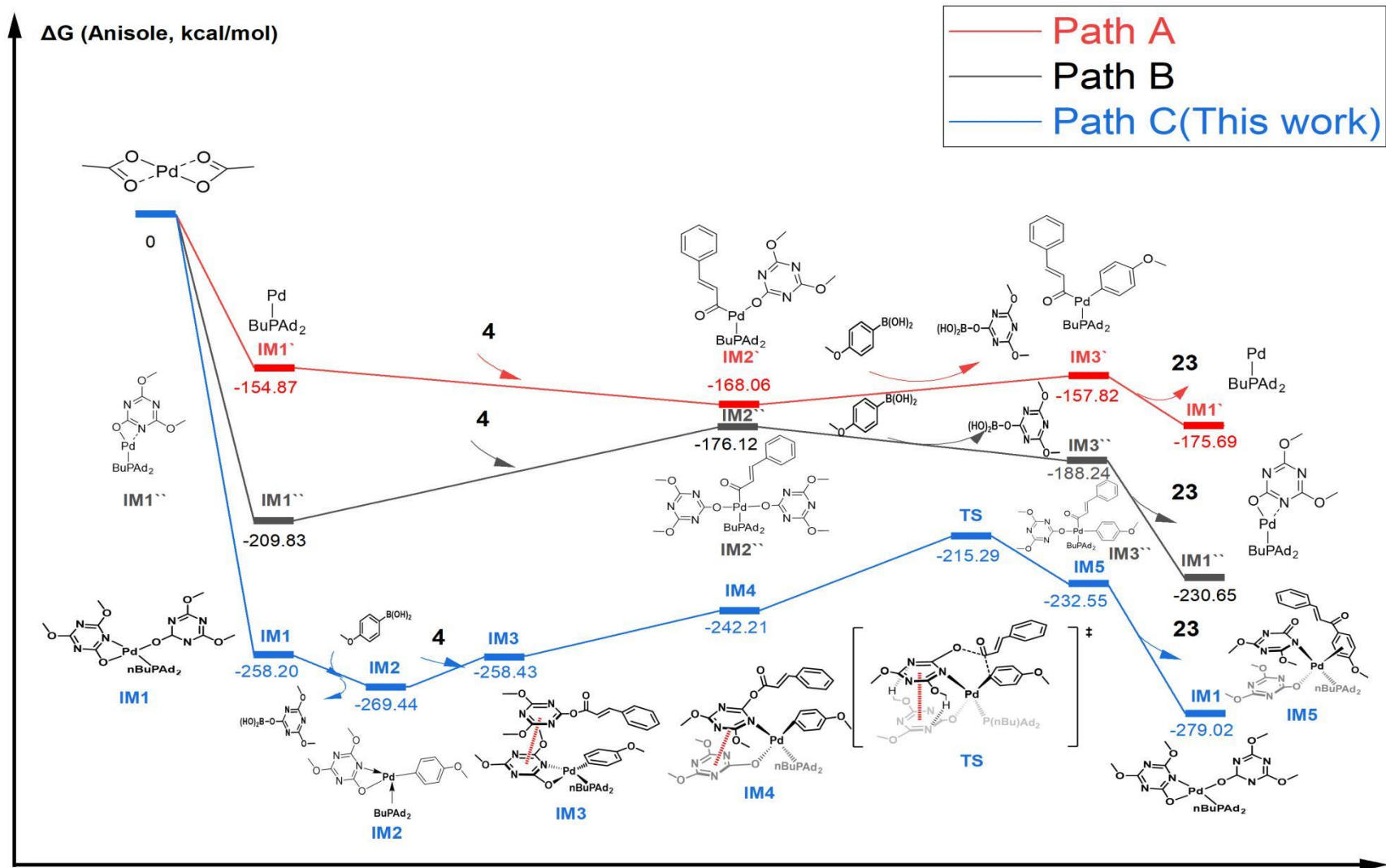
Scheme S7 ³¹P Spectrum of reaction between triazine ester, Pd(OAc)₂ and BuPAD₂

8. Density Functional Theory (DFT) Calculations

DFT Method:

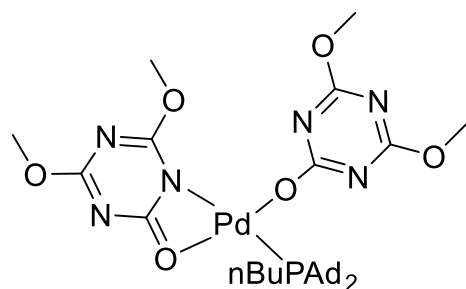
All calculations were performed with the Gaussian 16 program. (Full citation of Gaussian 16: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016. Gaussian 16, Revision A.03).

For the DFT calculation (Figure 4 in the manuscript): Geometry optimizations and frequency analysis were conducted with the Gaussian 16 software package, B3LYP functional [with gd3(BJ) dispersion correction], and LANL2DZ basis set for Pd and 6-31g(d) basis set for all other atoms. Single-point energy calculations were conducted with the M06 functional and Def2-TVZP basis set for all other atoms, along with the SMD Anisole as solvent for correction. Concentration was corrected from 1 atm to 1 mol/L by addition 1.89 kcal/mol to the Gibbs energy of each species. Reaction paths were traced by the intrinsic reaction coordinate method for all transition states. All energetics reported throughout the text are in kcal/mol.



Scheme S8. The comparison of energy profiles of reaction pathways A, B and C

Coordinates and Energies of Stationary Points



IM1

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -2575.052415 a.u.

Thermal correction to Gibbs Free Energy at 298.15 K: 0.7603638 a.u.

Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

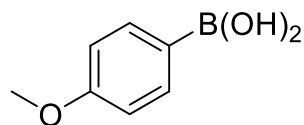
-2574.292051 a.u.

P	0.29996000	1.23702900	0.46535300
C	1.49001300	1.40133100	1.87165500
C	-1.40771000	1.60085400	1.20249700
C	0.86858100	2.51560400	-0.79881600
C	2.50792100	-0.68065300	5.01945000
C	2.56750500	0.41257700	3.95001900
C	1.40964000	0.31456200	2.95103300
C	-1.33701400	2.67367800	2.32107500
C	-2.73887400	2.88763200	2.93511100
C	-3.72548000	3.35025000	1.84940200
C	-3.80929500	2.27677500	0.75170400
C	-2.41539600	2.08108600	0.12754100

C	-4.30086400	0.94858400	1.35090000
C	-3.32359000	0.49632000	2.44861500
C	-1.92698900	0.28234200	1.83821000
C	-3.24057000	1.56843400	3.54868300
C	0.09556300	2.32600500	-2.13054800
C	0.60661600	3.32309700	-3.18607800
C	0.42314900	4.76254000	-2.67214200
C	1.22813100	4.95199200	-1.37361600
C	0.70706900	3.97128000	-0.30221200
C	2.71758800	4.68043700	-1.64721600
C	2.88799900	3.23946200	-2.16049700
C	2.37343000	2.25881400	-1.08976600
C	2.09456600	3.05679000	-3.46409700
H	3.34224200	-0.59745200	5.72467900
H	1.57625400	-0.62037000	5.59468800
H	2.55057400	-1.67691300	4.56335800
H	3.51724100	0.34441300	3.40630200
H	2.55357400	1.40212100	4.42844800
H	1.41851400	-0.67184700	2.47150200
H	0.46667200	0.38520600	3.50263600
H	2.47747700	1.34817600	1.41843800
H	1.37619700	2.39882600	2.31050600
H	-0.65302600	2.35738900	3.11556700
H	-0.95998700	3.62373200	1.92677700
H	-2.65845800	3.65407200	3.71682000

H	-4.71477900	3.52262400	2.29351000	H	2.22784200	2.03703800	-3.84783200
H	-3.39451200	4.30526300	1.41845800	H	2.46968600	3.74526200	-4.23292500
H	-4.49687500	2.60196300	-0.03830700	Pd	0.47045900	-0.81413000	-0.55603100
H	-2.08544700	3.03926800	-0.28738200	O	1.01083300	-2.82512500	-1.42419300
H	-2.46461200	1.36468900	-0.69255800	C	2.16793000	-2.76542600	-0.92244900
H	-5.30856400	1.07315200	1.76944300	C	3.64550700	-1.38726200	0.22103500
H	-4.36558900	0.18823700	0.56347200	C	4.28106600	-3.41742800	-0.51686500
H	-3.66104800	-0.45481500	2.87868600	N	2.40319500	-1.58285200	-0.20464100
H	-1.24315400	-0.05371600	2.62278400	N	3.11151600	-3.71612500	-1.05367500
H	-1.95953800	-0.51791700	1.10076700	N	4.63131700	-2.26974200	0.10639200
H	-4.22602200	1.72178300	4.00805600	O	5.21277200	-4.36726500	-0.62834200
H	-2.56033400	1.23903000	4.34612200	O	3.90086600	-0.20469200	0.79479400
H	0.22349300	1.29957000	-2.48712500	C	6.50603800	-4.10538400	-0.07619200
H	-0.97583200	2.46555600	-1.98388600	H	7.08768700	-5.00525600	-0.27949000
H	0.02584200	3.18185900	-4.10542900	H	6.96778500	-3.23699600	-0.55430000
H	-0.64070200	4.96415100	-2.48849300	H	6.44395600	-3.92716300	1.00100100
H	0.76137400	5.48150700	-3.42985800	C	5.25197400	0.03942800	1.21264900
H	1.09967300	5.97659200	-1.00212700	H	5.93321700	-0.01557100	0.36070900
H	-0.34496300	4.19139800	-0.09697100	H	5.23870700	1.04655000	1.63084100
H	1.25898300	4.11802500	0.63521000	H	5.56100700	-0.68683500	1.96761500
H	3.09868800	5.39345600	-2.38985900	O	-1.32777400	-0.40269400	-1.42728700
H	3.30316200	4.82677900	-0.72907500	C	-2.29447900	-1.25150600	-1.24684100
H	3.95108900	3.03280700	-2.33833900	C	-4.39740600	-1.89900700	-1.70369800
H	2.97065100	2.39295800	-0.18280800	C	-3.17155700	-3.07115100	-0.24414600
H	2.51514200	1.22307600	-1.41918800	N	-3.43623400	-1.01238000	-1.92992100

N	-2.12105300	-2.26964000	-0.37158500
N	-4.34444900	-2.95682500	-0.87989700
C	-6.60722300	-2.59854900	-2.17371900
H	-6.92323100	-2.60650600	-1.12640500
H	-7.41585000	-2.23989000	-2.81249200
H	-6.31590000	-3.61296200	-2.46033500
C	-4.10442200	-4.97903800	0.79320900
H	-4.35171500	-5.47183100	-0.15115400
H	-3.76031900	-5.71079400	1.52546300
H	-4.99266900	-4.45744000	1.16165400
O	-3.00969300	-4.07475600	0.62710700
O	-5.53333400	-1.67816600	-2.37959000



2a

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -522.6768638 a.u.

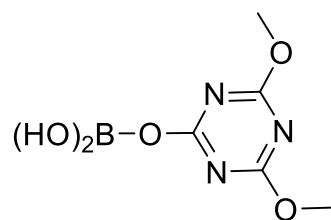
Thermal correction to Gibbs Free Energy at 298.15 K: 0.1188864 a.u.

Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

-522.5579774 a.u.

C	0.46531000	1.29004000	-0.00000100
C	-0.91451200	1.42558700	-0.00002000

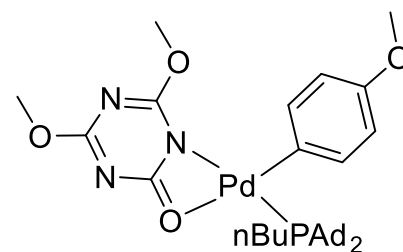
C	-1.72858000	0.28301100	-0.00006600
C	-1.14387500	-0.98924400	-0.00012100
C	0.24650600	-1.10080100	-0.00007200
C	1.08346100	0.02395000	-0.00003000
H	1.08690400	2.18073500	0.00006600
H	-1.39243000	2.40018400	-0.00001400
H	-1.75466600	-1.88447800	-0.00008000
H	0.69353900	-2.09086800	-0.00018700
O	-3.07235800	0.51530700	-0.00010900
C	-3.94135000	-0.60481200	0.00018900
H	-3.79821800	-1.22526400	0.89458600
H	-4.95434000	-0.19875500	-0.00004200
H	-3.79808600	-1.22590000	-0.89371900
B	2.62962700	-0.12074700	-0.00001200
O	3.16693100	-1.38916100	0.00001500
H	4.13370200	-1.41514800	0.00029100
O	3.39132700	1.02658500	0.00007800
H	4.34649700	0.87500100	0.00001200



Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -760.6463226 a.u.
 Thermal correction to Gibbs Free Energy at 298.15 K: 0.1166346 a.u.
 Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):
 -760.529688 a.u.

O	2.03339800	-1.07461000	-0.22058800
C	0.78071800	-0.63025300	-0.13321500
C	-0.68224400	1.05932600	-0.09876200
C	-1.39964800	-1.06120600	-0.00425700
N	0.59774500	0.69610200	-0.16887300
N	-0.16602900	-1.56449700	-0.05577900
N	-1.73364800	0.23627800	-0.01612700
O	-0.89184700	2.37660100	-0.12199700
O	-2.36941600	-1.97304300	0.06959400
C	-3.71928000	-1.49769300	0.13142200
H	-4.33318700	-2.39712600	0.18640300
H	-3.87243200	-0.87405900	1.01628600

H	-3.96897500	-0.91693500	-0.76061300
C	-2.25070300	2.82692200	-0.05839800
H	-2.72670500	2.49815600	0.86923600
H	-2.18967900	3.91509700	-0.09238700
H	-2.82641400	2.44829300	-0.90714900
B	3.12313400	-0.24996500	0.07303700
O	3.19529300	0.27703700	1.32953600
H	3.93052800	0.88630400	1.47343300
O	4.06342000	-0.15432500	-0.91072300
H	4.86488100	0.31905200	-0.65227000



IM2

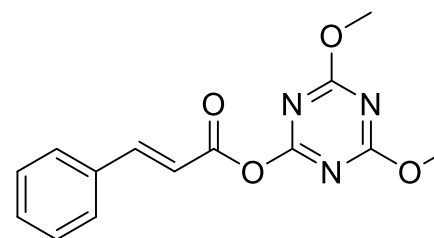
Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -2337.100008 a.u.
 Thermal correction to Gibbs Free Energy at 298.15 K: 0.7617471 a.u.
 Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):
 -2336.3382609 a.u.

P	-0.40884400	0.83026200	0.41025200	C	-0.54863700	4.54229900	-1.70614400
C	0.70815400	1.40513200	1.77637200	C	-0.80251100	3.53256500	-0.56715100
C	-2.15509800	0.84424700	1.15166200	C	0.96405700	4.71444500	-1.92514500
C	-0.19286600	2.15887400	-0.92686400	C	1.57933100	3.35636900	-2.30543100
C	2.26334800	-0.15097400	5.00724400	C	1.33025400	2.35291400	-1.16383800
C	2.08431500	0.80082600	3.82254600	C	0.94033600	2.84676900	-3.60692500
C	0.87045500	0.44001000	2.95859600	H	3.13806400	0.11841200	5.60958400
C	-2.36517900	2.02449600	2.13516200	H	1.38595600	-0.13373700	5.66532600
C	-3.78172100	1.96326700	2.74596800	H	2.39880300	-1.18313500	4.66246900
C	-4.83728600	2.03168300	1.62842600	H	2.98137900	0.78319600	3.19148900
C	-4.64755100	0.83986600	0.67451000	H	1.97977200	1.83293000	4.18678400
C	-3.24112700	0.90843100	0.05024600	H	0.99150000	-0.58162400	2.57582700
C	-4.80587700	-0.48094800	1.44622700	H	-0.02806500	0.43721700	3.58628000
C	-3.75421900	-0.53683900	2.56690200	H	1.68543100	1.50811600	1.30481000
C	-2.34819600	-0.47760300	1.94250000	H	0.39862100	2.39917400	2.11968700
C	-3.94854400	0.64856600	3.52665500	H	-1.62937000	1.97717000	2.94496800
C	-0.80158700	1.65073100	-2.25738900	H	-2.22714900	2.98524100	1.63062400
C	-0.57067000	2.67161900	-3.38643700	H	-3.90426000	2.81723700	3.42455500
C	-1.20071100	4.02203800	-2.99998800	H	-5.84512700	2.01339300	2.06373900

H	-4.74205300	2.97637400	1.07528400	H	1.14790500	5.45060400	-2.71878600
H	-5.38905400	0.88915600	-0.13308000	H	1.43578900	5.10013900	-1.01110100
H	-3.15508100	1.84035900	-0.51701700	H	2.66293400	3.46462200	-2.44079400
H	-3.10846500	0.07947300	-0.64912800	H	1.81257100	2.73356400	-0.26002900
H	-5.81685400	-0.55255600	1.86917900	H	1.79777400	1.38894100	-1.39178700
H	-4.67258300	-1.33212800	0.76615300	H	1.39064100	1.88918100	-3.89910900
H	-3.84941800	-1.48157900	3.11635600	H	1.12700100	3.55669100	-4.42361200
H	-1.59390400	-0.56494700	2.72961700	Pd	0.57875600	-1.10809100	-0.33230400
H	-2.21318300	-1.32708400	1.27495300	O	1.89868900	-2.80236200	-0.82844800
H	-4.94497700	0.60800000	3.98642800	C	2.97982000	-2.21333500	-0.52174900
H	-3.21433700	0.59858000	4.34229600	C	3.93557000	-0.25743500	0.23396200
H	-0.32814900	0.69705600	-2.51750300	C	5.21021400	-2.03348500	-0.26592200
H	-1.87258700	1.46195800	-2.14897200	N	2.82169800	-0.90272300	-0.07304700
H	-1.03930100	2.29314400	-4.30348100	N	4.19244800	-2.79942400	-0.61855100
H	-2.28357200	3.90596200	-2.85547600	N	5.16828900	-0.75434100	0.16536300
H	-1.06014900	4.74946200	-3.81019000	O	6.41165700	-2.61598900	-0.35744100
H	-0.99584000	5.50493700	-1.42731500	O	3.77599800	1.01334900	0.64850300
H	-1.88093700	3.44652400	-0.40653600	C	7.55567200	-1.84171300	0.00865500
H	-0.36444300	3.90747400	0.36649900	H	8.40778900	-2.50621100	-0.14116700

H	7.64922700	-0.95429900	-0.62392400
H	7.49887200	-1.52555800	1.05425000
C	4.96002100	1.74825000	0.98037000
H	5.62202900	1.82759900	0.11469900
H	4.60420400	2.73387500	1.28366100
H	5.50028800	1.26687400	1.79917000
C	-1.12795100	-2.03823700	-0.78214900
C	-1.40793900	-3.19097900	-0.02779900
C	-1.97036800	-1.72902300	-1.84816600
C	-2.51833200	-3.97962200	-0.30855100
H	-0.75385900	-3.47740100	0.79078200
C	-3.09084700	-2.51970100	-2.14689300
H	-1.77759700	-0.86369500	-2.47065300
C	-3.37494300	-3.64233100	-1.36631200
H	-2.73973600	-4.86762700	0.27562400
H	-3.72144900	-2.24548700	-2.98508400
C	-5.32907500	-4.17398200	-2.61833800
H	-6.10254800	-4.94396900	-2.59537800
H	-5.79579100	-3.18708100	-2.49163600

H	-4.81690300	-4.20321000	-3.58966900
O	-4.44619900	-4.47259700	-1.55420200



4

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -768.2995456 a.u.

Thermal correction to Gibbs Free Energy at 298.15 K: 0.2105935 a.u.

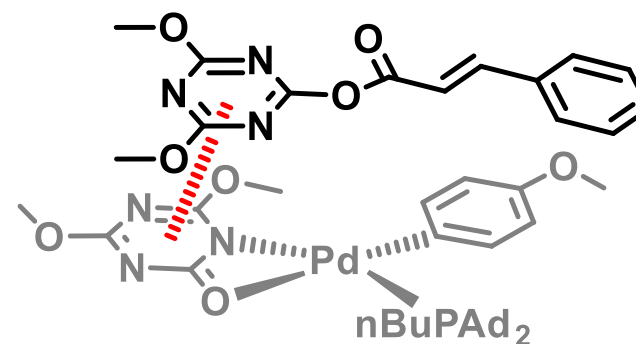
Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

-768.0889521 a.u.

C	-6.87163100	0.32969200	-0.66252000
C	-5.96997700	1.12631600	-1.36828900
C	-4.60595500	1.03246500	-1.10397400
C	-4.11617200	0.14362100	-0.13124300
C	-5.03893600	-0.65346800	0.57183400
C	-6.40009100	-0.56019100	0.30803100
H	-7.93639800	0.39927000	-0.86538600
H	-6.32823400	1.81974600	-2.12349600

H	-3.90270100	1.65308500	-1.65319300
H	-4.68803400	-1.34924200	1.32723500
H	-7.09896700	-1.18254900	0.85937000
C	-2.67505900	0.09091000	0.10155800
H	-2.07658800	0.75498800	-0.51713800
C	-2.02561100	-0.68281600	0.99213000
H	-2.53746900	-1.37499600	1.65189400
C	-0.57149800	-0.69019900	1.16570500
O	0.03731200	-1.39366100	1.93307300
O	0.05355600	0.26685800	0.36541500
C	1.40013500	0.17625500	0.17317300
C	3.18813500	-0.94689400	-0.52010700
C	3.38532300	1.17274700	0.18679500
N	1.86713800	-0.96358400	-0.32359300
N	2.07812700	1.28342900	0.44846400
N	4.00628600	0.08698800	-0.28717000
O	3.69509700	-2.07849200	-1.00274200
O	4.09775700	2.26780700	0.44133500
C	5.50897700	2.20936700	0.19551000

H	5.88455800	3.19453400	0.47266800
H	5.97715500	1.43343600	0.80681900
H	5.71114000	2.00358100	-0.85898400
C	5.10887700	-2.12296100	-1.23604800
H	5.66038200	-1.95835200	-0.30669500
H	5.29945900	-3.12445400	-1.62215800
H	5.40595900	-1.36604000	-1.96681500



IM3

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -3343.3470472 a.u.

Thermal correction to Gibbs Free Energy at 298.15 K: 0.998867 a.u.

Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

-3342.3481802 a.u.

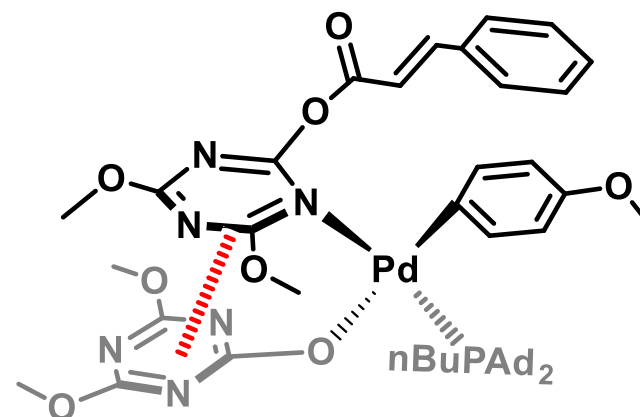
P	-1.73694100	0.47309800	-1.11662100
C	-0.48109900	0.04846300	-2.41591000

C	-1.86424700	2.35791600	-1.12024700	C	-4.77230200	-1.86042500	-3.91168200
C	-3.30606100	-0.35485800	-1.80178800	C	-4.21115900	-2.57041400	-2.66730600
C	3.33897300	0.46572300	-3.10386000	C	-2.95604200	-1.82067800	-2.18154000
C	1.91545600	-0.08503900	-3.21857300	C	-5.27625700	-2.58995000	-1.55922300
C	0.94629600	0.56828000	-2.22564200	H	3.99746500	0.02671800	-3.86265700
C	-1.72692600	2.96640000	-2.53983600	H	3.35103600	1.55486800	-3.23624200
C	-1.75303600	4.50785200	-2.45674200	H	3.75462900	0.23957100	-2.11860000
C	-3.08007600	4.97056900	-1.82948000	H	1.92864600	-1.16657800	-3.03573800
C	-3.20609600	4.38665200	-0.41140000	H	1.53789900	0.05876300	-4.24201100
C	-3.19081200	2.84750400	-0.49141200	H	1.28032800	0.34925900	-1.20944500
C	-2.03405500	4.87390300	0.45862900	H	0.99295600	1.65462400	-2.34464600
C	-0.71148800	4.41702000	-0.17896800	H	-0.43673600	-1.04100100	-2.40502400
C	-0.69127800	2.88184400	-0.25284500	H	-0.87619100	0.35423400	-3.39298300
C	-0.57816300	5.00080500	-1.59440400	H	-0.78533300	2.65160500	-2.99993000
C	-4.38508100	-0.41313200	-0.69399200	H	-2.53514300	2.62555300	-3.19335100
C	-5.64477100	-1.14292500	-1.19402800	H	-1.66424100	4.91090800	-3.47417300
C	-6.20595500	-0.42048200	-2.43156000	H	-3.11428000	6.06758500	-1.79185200
C	-5.14402600	-0.41357400	-3.54593100	H	-3.92642200	4.64246600	-2.44933000
C	-3.89233100	0.34121800	-3.05086700	H	-4.15754300	4.70164100	0.03639900

H	-4.04503200	2.51822600	-1.09281500	H	-3.92427900	-3.59811800	-2.92463600
H	-3.30813400	2.42420600	0.50916700	H	-2.21045600	-1.84131400	-2.98128600
H	-2.06046700	5.96885100	0.54454100	H	-2.51680500	-2.33254400	-1.31822800
H	-2.12257200	4.46227000	1.47240900	H	-4.89107400	-3.11372400	-0.67447100
H	0.13715600	4.73834500	0.43597400	H	-6.16609700	-3.13643700	-1.89920700
H	0.26922500	2.55793900	-0.65029400	Pd	-1.23170800	-0.69700400	0.80287100
H	-0.77447900	2.47546800	0.75275800	O	-0.94561700	-2.27245300	2.35113200
H	-0.57638300	6.09876400	-1.55752400	C	-0.49044800	-3.13926700	1.54365300
H	0.37721300	4.68781500	-2.03486200	C	0.20307400	-3.54162100	-0.61721300
H	-3.96915800	-0.94423300	0.16940600	C	0.32844700	-5.14717900	0.94882900
H	-4.64943400	0.59296100	-0.35767800	N	-0.32615500	-2.68299300	0.23844500
H	-6.39390600	-1.14113600	-0.39215600	N	-0.19029200	-4.40314700	1.90820200
H	-6.48620500	0.60961800	-2.17246100	N	0.56912200	-4.79169500	-0.33298100
H	-7.11648900	-0.92382100	-2.78267400	O	0.64481200	-6.39643000	1.31267500
H	-5.53819400	0.10367900	-4.43004300	O	0.37115300	-3.08256500	-1.86714300
H	-4.17300500	1.37223000	-2.81832500	C	1.17155500	-7.27046800	0.31362900
H	-3.14344700	0.38176400	-3.85150000	H	1.30854100	-8.22813100	0.81786800
H	-5.65637700	-2.39307900	-4.28657500	H	0.47714000	-7.37657100	-0.52462200
H	-4.02590000	-1.86562300	-4.71770500	H	2.13017700	-6.90547600	-0.06731900

C	0.97118900	-3.96541000	-2.82144300	C	2.15250200	-1.62072000	2.57462800
H	0.39571600	-4.88950600	-2.91321500	C	3.11953300	-1.86821000	0.56472400
H	0.96588800	-3.41018300	-3.75992200	C	2.46594600	0.15178500	1.25002500
H	1.99711400	-4.20487100	-2.53153800	O	1.75243800	-2.18953000	3.69126800
C	-1.93455000	0.67883700	2.06879700	O	3.69543100	-2.59000800	-0.39504800
C	-0.98193800	1.40120300	2.80783800	O	2.30092100	1.48328000	1.05538800
C	-3.27806800	0.81149500	2.41569100	C	3.12317000	2.19323600	0.16522500
C	-1.37250900	2.25172700	3.83809400	C	4.55418400	1.88525600	0.23605400
H	0.07507000	1.30063000	2.58790700	C	5.40064200	2.48217000	-0.62535500
C	-3.68343300	1.66684900	3.45139200	H	4.88700200	1.16933100	0.97631400
H	-4.04382700	0.25572900	1.88847800	H	4.96159300	3.17718600	-1.33822300
C	-2.72834700	2.39897900	4.16025200	C	6.84356500	2.29511200	-0.71706000
H	-0.63848200	2.81467700	4.40693000	C	7.56184100	3.05753600	-1.65537000
H	-4.73871100	1.74442100	3.68778600	C	7.55144900	1.38113500	0.08688700
C	-4.36846100	3.44765000	5.53120000	C	8.94164700	2.92004500	-1.78478000
H	-4.37748400	4.17483700	6.34549400	H	7.02444400	3.76292000	-2.28365300
H	-4.95715200	3.83842100	4.68956700	C	8.92816600	1.24321500	-0.04302500
H	-4.82361000	2.50971600	5.87783100	H	7.01935700	0.77185600	0.81046500
O	-3.01042600	3.26976000	5.17850000	C	9.62913500	2.01254900	-0.97801500

H	9.47908300	3.51879000	-2.51420000
H	9.45975400	0.53284500	0.58339000
H	10.70499600	1.90109900	-1.07669400
O	2.61058600	3.05435600	-0.50802600
N	2.71325800	-2.45776600	1.68164700
N	3.01918000	-0.55786500	0.27546900
N	2.00827100	-0.29627600	2.41433500
C	0.99329000	-1.38762500	4.62013000
H	0.08376800	-1.03295800	4.13636300
H	0.75329000	-2.06900300	5.43514400
H	1.59444800	-0.54707800	4.97476200
C	3.92708000	-3.98345800	-0.12283300
H	4.47776500	-4.10658300	0.81244400
H	2.97888000	-4.52022100	-0.06330200
H	4.51833000	-4.33656200	-0.96890200



IM4

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -3343.349788 a.u.

Thermal correction to Gibbs Free Energy at 298.15 K: 1.0274481 a.u.

Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

-3342.32234 a.u.

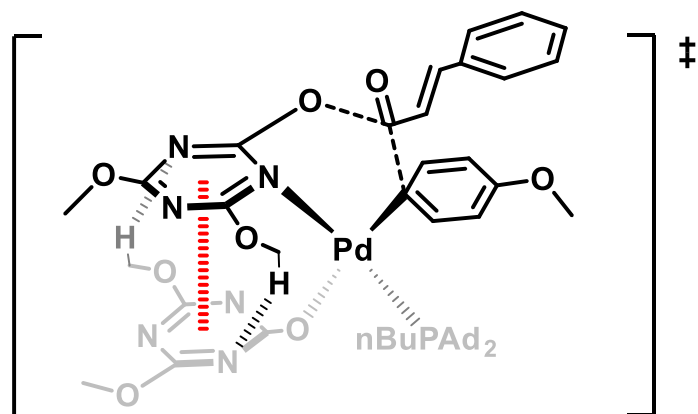
P	1.48222000	-0.66975500	-1.40618700
C	0.83203700	-1.84959900	-2.67934000
C	3.27987300	-1.19013100	-1.10548000
C	1.36592500	1.01438500	-2.27371500
C	-0.28407000	-5.57905100	-2.92088900
C	-0.26980400	-4.06897300	-3.16803500
C	0.72395000	-3.32378600	-2.26884900
C	3.98431200	-1.64318500	-2.41070500

C	5.42606400	-2.10354600	-2.10559900	H	0.69820000	-6.02310400	-3.12491700
C	6.21928200	-0.94838600	-1.46973600	H	-1.26733800	-3.64489900	-2.99866800
C	5.53733400	-0.52294700	-0.15815400	H	-0.02178500	-3.87699600	-4.22169200
C	4.10288600	-0.04988200	-0.45824400	H	0.38674100	-3.38909000	-1.22810800
C	5.49183100	-1.71009600	0.81870100	H	1.70402200	-3.81382900	-2.32071300
C	4.70663000	-2.86351500	0.17184500	H	-0.18175300	-1.49428100	-2.86224200
C	3.27051700	-2.39544600	-0.12689300	H	1.40478400	-1.74090800	-3.60786700
C	5.39310400	-3.29575300	-1.13440000	H	3.43543600	-2.47309200	-2.86806300
C	1.44431400	2.12939400	-1.20370700	H	4.01041400	-0.83264000	-3.14372200
C	1.25965000	3.51359800	-1.84616600	H	5.90121000	-2.40494200	-3.04814400
C	2.34882800	3.73533000	-2.90988100	H	7.25265900	-1.26554000	-1.27588200
C	2.23544400	2.65310700	-3.99898200	H	6.26769800	-0.09695600	-2.16259000
C	2.43726300	1.26137500	-3.36050500	H	6.09050100	0.30900200	0.29585700
C	0.84726800	2.73249800	-4.65548300	H	4.14809800	0.81737300	-1.12373700
C	-0.22972700	2.50018100	-3.58338000	H	3.62458500	0.27187000	0.46832800
C	-0.02877200	1.11118000	-2.94877600	H	6.51136600	-2.03585500	1.06577100
C	-0.13077700	3.58214000	-2.49719900	H	5.00701500	-1.40600300	1.75541000
H	-0.53792900	-5.80882600	-1.87964400	H	4.65765500	-3.71260600	0.86557500
H	-1.01798600	-6.08242600	-3.56009600	H	2.69784000	-3.22477700	-0.55106200

H	2.78018800	-2.10829500	0.80230800	C	-2.65770200	-0.64056800	-1.11818500
H	6.41477600	-3.64422000	-0.93170100	C	-3.64153500	1.36357800	-0.68348000
H	4.84876200	-4.13588600	-1.58704000	C	-4.89145700	-0.35076000	-1.36837000
H	0.65841100	1.95963800	-0.45998900	N	-2.51953500	0.66558200	-0.72102800
H	2.40545100	2.09511400	-0.68149200	N	-3.86193000	-1.17577000	-1.47384200
H	3.34336300	3.69888900	-2.44365100	N	-4.87041400	0.93516100	-0.98343200
H	2.24076600	4.73152800	-3.35942800	O	-6.08128000	-0.89831100	-1.67015000
H	3.01546300	2.80462700	-4.75648500	O	-3.49370600	2.64508500	-0.28598500
H	3.44427900	1.21463200	-2.93728000	C	-7.24464200	-0.10861400	-1.40894700
H	2.37378900	0.48685300	-4.13547000	H	-8.08727800	-0.73801900	-1.70072600
H	0.71113000	3.71466800	-5.12799900	H	-7.30570600	0.14432100	-0.34674800
H	0.76078700	1.97719200	-5.44862200	H	-7.23719500	0.81339500	-1.99627000
H	-1.22586200	2.52613300	-4.04336000	C	-4.69032200	3.40565700	-0.08813700
H	-0.12129400	0.35596200	-3.73563000	H	-4.35412000	4.37658900	0.28019600
H	-0.81077900	0.92903300	-2.20866800	H	-5.23962500	3.52215300	-1.02604300
H	-0.90817400	3.41883300	-1.74234000	H	-5.33725100	2.92175100	0.64774900
H	-0.29777900	4.57766600	-2.93122300	C	0.98588200	6.57058400	0.60450200
Pd	-0.05142800	-0.79347200	0.31460500	C	-0.27953000	6.22513500	0.12614200
O	-1.62803100	-1.39407300	-1.11357500	C	-0.88811100	5.04806000	0.55456200

C	-0.25284100	4.20628000	1.48450200	N	-1.76125400	-1.32163400	1.75525000
C	1.02603500	4.56182300	1.95245900	N	-3.47950500	-2.90232300	1.30942400
C	1.63870400	5.73128700	1.51351100	O	-5.62968300	-2.09182600	1.25208200
H	1.46787100	7.48226900	0.26342900	O	-1.25106300	-3.44918000	1.22053500
H	-0.78524000	6.86521100	-0.59092800	C	-1.64605600	-4.68423200	0.60000300
H	-1.85936200	4.75822500	0.16631300	H	-0.71823100	-5.24055500	0.47171400
H	1.54519200	3.90693900	2.64519200	H	-2.34153900	-5.23280100	1.23855800
H	2.63006200	5.98881100	1.87518300	H	-2.11115200	-4.47364900	-0.36528800
C	-0.93838300	2.98838000	1.90741500	C	-5.97833000	-3.28108700	0.51634000
H	-1.75478400	2.65966500	1.27106100	H	-5.72588100	-4.17444400	1.09182200
C	-0.63203800	2.25379500	2.99507400	H	-7.05505900	-3.20806700	0.36657100
H	0.16240400	2.51477600	3.68379000	H	-5.45447400	-3.28036000	-0.44097000
C	-1.29337100	0.99385100	3.30836100	C	1.25952100	-0.44577300	1.78433000
O	-1.01722200	0.22425500	4.19062300	C	1.44018700	-1.47345600	2.71643900
O	-2.40411500	0.77809900	2.46160600	C	1.91022900	0.77104400	2.02380500
C	-2.74116900	-0.46336400	2.08796200	C	2.24895500	-1.30867300	3.84564400
C	-4.34759500	-1.90327100	1.51790200	H	0.93400800	-2.42400900	2.57660300
C	-2.20659100	-2.55327500	1.43455600	C	2.72002200	0.95266500	3.14456300
N	-4.04209700	-0.69108700	1.99689300	H	1.78796500	1.60069500	1.34056200

C	2.89676100	-0.08748100	4.06297800
H	2.35126200	-2.12883200	4.54701100
H	3.22851300	1.89614500	3.32411800
O	3.71019800	0.18488900	5.12940800
C	3.88973900	-0.83479400	6.09425400
H	4.35645800	-1.72807800	5.65651300
H	4.55319300	-0.41826200	6.85469300
H	2.93769700	-1.12212000	6.56016800
H	1.34399400	4.27539300	-1.06591000



TS

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -3343.279562 a.u.

Thermal correction to Gibbs Free Energy at 298.15 K: 1.0001212 a.u.

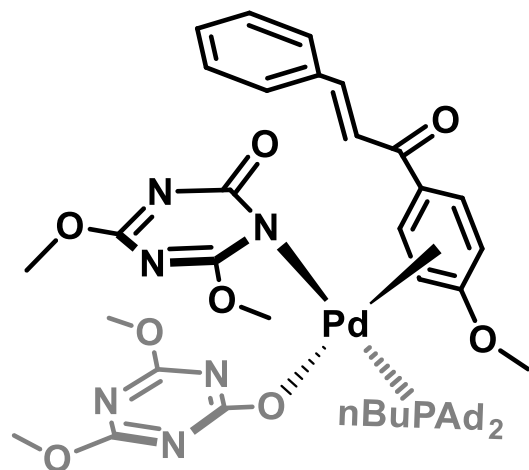
Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):
-3342.279441 a.u.

P	1.74619400	0.21806000	-1.15683400
C	1.17717200	-0.18056400	-2.88019600
C	3.41669900	-0.70784000	-1.02971000
C	1.99766500	2.09390200	-1.24179500
C	-0.18969200	-3.10475800	-5.04878400
C	-0.03664400	-1.69279100	-4.47994300
C	0.80823900	-1.63726700	-3.19920200
C	4.11289300	-0.84397900	-2.41252000
C	5.39547900	-1.69232800	-2.29320900
C	6.37673900	-1.02115300	-1.31910000
C	5.70713400	-0.90221500	0.05908700
C	4.43052400	-0.04431900	-0.06883300
C	5.35656900	-2.30776400	0.57812000
C	4.37387800	-2.97808500	-0.39719600
C	3.09234200	-2.13006100	-0.50028400
C	5.03145100	-3.09749100	-1.78241200
C	2.35878800	2.67109800	0.14905400
C	2.53066300	4.20242200	0.06970400
C	3.62590100	4.55644900	-0.95066800
C	3.21845900	4.02919000	-2.33811600
C	3.08373600	2.49646600	-2.26904500
C	1.87478800	4.64289000	-2.76908400
C	0.79670500	4.27803700	-1.73415500

C	0.65119900	2.74324900	-1.66512900	H	4.34487400	-3.58700900	-2.48604900
C	1.20441900	4.84126000	-0.36496600	H	1.55480400	2.43047300	0.85385600
H	-0.67645700	-3.77318800	-4.33126900	H	3.28088200	2.22439800	0.53060700
H	-0.79895600	-3.10128500	-5.95957900	H	4.58785700	4.11689400	-0.65137000
H	0.78597800	-3.54031700	-5.30000700	H	3.76590300	5.64475800	-0.98569600
H	-1.02148300	-1.26751300	-4.25376400	H	3.99475200	4.27970500	-3.07262500
H	0.42319000	-1.04914700	-5.24436800	H	4.05203600	2.06955600	-1.99228700
H	0.23791200	-2.06322600	-2.37083800	H	2.82969300	2.10668100	-3.26114700
H	1.70920900	-2.25009500	-3.32800700	H	1.96704600	5.73415000	-2.84854500
H	0.27271000	0.41050600	-3.00816100	H	1.59494400	4.26852800	-3.76321700
H	1.92640000	0.18779000	-3.58782300	H	-0.16998900	4.70235600	-2.03127700
H	3.45029000	-1.32356600	-3.13387300	H	0.34168100	2.37905600	-2.64891800
H	4.36496000	0.14270300	-2.81281700	H	-0.13758000	2.46075900	-0.96022400
H	5.85272000	-1.76758800	-3.28811500	H	0.43057500	4.63551900	0.37325000
H	7.30006900	-1.61063600	-1.24335400	H	1.31212700	5.93243500	-0.42552400
H	6.65746200	-0.02656900	-1.69162200	Pd	-0.06693900	-0.50845300	0.21903500
H	6.38835000	-0.40708400	0.76307000	O	-1.23390900	-0.25992400	-1.59633700
H	4.71284400	0.94561900	-0.43958600	C	-2.49032200	-0.04332300	-1.44345200
H	3.98566100	0.09130400	0.91557600	C	-4.21336700	0.82908200	-0.25249700
H	6.27138300	-2.90977200	0.66395400	C	-4.62886600	-0.55103400	-1.96105400
H	4.91836000	-2.24591400	1.57971000	N	-2.90318000	0.80775100	-0.46567600
H	4.10366700	-3.97508200	-0.02567700	N	-3.34758400	-0.71424400	-2.26015400
H	2.37099800	-2.62371900	-1.16004200	N	-5.14340600	0.17357400	-0.95916900
H	2.61773600	-2.05968400	0.47965300	O	-5.48386300	-1.22858800	-2.74878900
H	5.93259800	-3.72215200	-1.72207700	O	-4.59654500	1.58846000	0.77668700

C	-6.88030500	-1.02604600	-2.51004900	O	-2.19586200	-0.34404000	2.83709600
H	-7.38833600	-1.67831400	-3.22250500	C	-2.63878100	-1.12256200	1.97459200
H	-7.14843700	-1.28971100	-1.48433000	C	-4.31642300	-2.37516300	1.07438300
H	-7.15748000	0.01763500	-2.68593400	C	-2.26903400	-2.59071800	0.20410300
C	-5.92873100	1.39337700	1.27175500	N	-3.96074100	-1.47949800	1.96848700
H	-6.01452600	2.07304300	2.12030400	N	-1.78202600	-1.62311600	0.98730300
H	-6.67101800	1.63526500	0.50651600	N	-3.51733700	-3.03270100	0.20701800
H	-6.04907100	0.35785100	1.59892100	O	-5.62606400	-2.66185100	1.03869800
C	-1.87959700	6.22000200	1.24538200	O	-1.38239800	-3.14065000	-0.63199800
C	-2.36304700	5.20399700	0.42017800	C	-1.92088900	-3.91766000	-1.71631000
C	-2.08723200	3.87030000	0.71588100	H	-1.04732700	-4.30245900	-2.24141200
C	-1.31583300	3.53209100	1.84252900	H	-2.53523700	-4.73668400	-1.33795400
C	-0.84435100	4.56551000	2.67382700	H	-2.51216700	-3.26628800	-2.36471700
C	-1.12212800	5.89495500	2.37621300	C	-6.06310900	-3.59898100	0.04880500
H	-2.09235800	7.26014800	1.01496300	H	-5.63507100	-4.58894000	0.23150200
H	-2.95752500	5.44891600	-0.45547400	H	-7.14912700	-3.63306500	0.15164500
H	-2.45638200	3.06901000	0.08541500	H	-5.77987600	-3.27068100	-0.95401000
H	-0.25582000	4.32905800	3.55506900	C	0.87786600	-0.79849300	2.09486000
H	-0.74824500	6.68242900	3.02453300	C	0.80218800	-2.18536900	2.44210700
C	-1.04389900	2.11508300	2.07879300	C	2.10622100	-0.14753500	2.43455600
H	-1.51414400	1.43552800	1.37367900	C	1.81376600	-2.84700500	3.10897400
C	-0.33088200	1.60858500	3.09574600	H	-0.10912800	-2.71979700	2.20524300
H	0.10680200	2.23175800	3.87246800	C	3.10842100	-0.77579600	3.14104700
C	-0.16912800	0.18200900	3.41251800	H	2.21161200	0.90469300	2.19687700
O	-0.07505100	-0.32107000	4.48250300	C	2.97094000	-2.13454500	3.48295400

H	1.70383900	-3.89621300	3.35565100
H	4.01602600	-0.26004600	3.43756300
O	4.00704100	-2.66886600	4.15392800
C	3.95181200	-4.04492700	4.52727700
H	3.88368500	-4.68864000	3.64308800
H	4.88512100	-4.24305200	5.05446400
H	3.10315000	-4.23764300	5.19260700
H	2.81287900	4.57328000	1.06351900



IM5

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -3343.3339871 a.u.

Thermal correction to Gibbs Free Energy at 298.15 K: 1.0270443 a.u.

Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

-3342.306943 a.u.

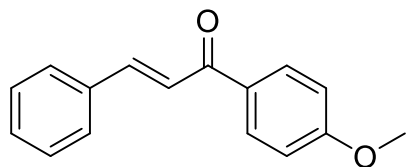
P	-2.05229000	-0.35565800	0.67370900
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C	-1.74516800	0.02142600	2.47882400
C	-2.99702200	-1.98691100	0.52203700
C	-3.04804800	1.18364800	0.16266600
C	-0.63035800	-1.48262100	5.88955000
C	-0.96572400	-0.43519700	4.82554600
C	-1.44492000	-1.07257700	3.51423000
C	-4.17278100	-2.11787500	1.51955900
C	-4.81061100	-3.51860500	1.40622200
C	-5.36158800	-3.71546600	-0.01651900
C	-4.20796200	-3.59693800	-1.02682800
C	-3.55755200	-2.20360300	-0.90475000
C	-3.15789300	-4.68375300	-0.74355700
C	-2.61007500	-4.49264300	0.68005700
C	-1.95105000	-3.10731700	0.78853100
C	-3.75529900	-4.59905400	1.70267600
C	-3.40554000	1.21604600	-1.34244000
C	-4.05988400	2.55973100	-1.72539900
C	-5.35701700	2.73884400	-0.91960100
C	-5.02279600	2.72132700	0.58165500

C	-4.37093700	1.36957700	0.94693500	H	-4.59405500	-3.70995200	-2.04776900
C	-4.05699500	3.87482900	0.90402500	H	-4.31036600	-1.44485800	-1.13725400
C	-2.76648800	3.71257400	0.08247000	H	-2.75606400	-2.12500900	-1.64392300
C	-2.09949600	2.37943000	0.45782500	H	-3.60701700	-5.67996000	-0.85210500
C	-3.09466400	3.71671500	-1.41783400	H	-2.33916900	-4.60969700	-1.47159400
H	0.16177300	-2.15453200	5.53801500	H	-1.85149800	-5.25673400	0.89317700
H	-0.28446200	-1.01401700	6.81762900	H	-1.50016600	-2.98976400	1.77464900
H	-1.50562800	-2.09858700	6.13183800	H	-1.13381800	-3.02461600	0.06287300
H	-0.08009200	0.17599500	4.61266000	H	-4.21587900	-5.59471500	1.65470000
H	-1.73545300	0.25098000	5.20783800	H	-3.36190200	-4.47350200	2.72007800
H	-0.66415800	-1.73185700	3.13858800	H	-2.51398900	1.07556400	-1.94930400
H	-2.33034400	-1.68471100	3.71973900	H	-4.09555800	0.40523200	-1.59018200
H	-0.87075000	0.67807000	2.44099200	H	-6.06590800	1.93437500	-1.15921800
H	-2.59304900	0.61604400	2.83288300	H	-5.84155700	3.68670400	-1.18758000
H	-3.83348500	-1.95113500	2.54404100	H	-5.94387700	2.83055400	1.16824000
H	-4.93267100	-1.35925200	1.30697000	H	-5.06645500	0.56036800	0.69861300
H	-5.62861200	-3.58979000	2.13417500	H	-4.20465100	1.33101100	2.02796600
H	-5.84073400	-4.69944300	-0.10419600	H	-4.53412200	4.83641300	0.67364100
H	-6.13114800	-2.96148200	-0.23122600	H	-3.81947700	3.88212800	1.97633800

H	-2.07255200	4.52476600	0.31404600	C	3.66816600	3.40189000	2.96377400
H	-1.82532700	2.40808100	1.51536900	H	3.31366500	4.42681700	3.08042200
H	-1.16504100	2.25358800	-0.09879200	H	4.25182300	3.09315200	3.83524000
H	-2.17032200	3.61518400	-2.00138000	H	4.28443000	3.31023000	2.06628300
H	-3.54978600	4.67354700	-1.70531800	C	-0.00767700	6.38900700	1.24799500
Pd	0.06099000	-0.60347400	-0.37650600	C	0.46619900	5.12717200	1.61485800
O	0.68453800	-1.31808900	1.46685000	C	0.77082000	4.18629300	0.63440800
C	1.69859800	-0.64011200	1.93674300	C	0.61643400	4.49509100	-0.72923600
C	2.64183600	1.30920600	2.55821000	C	0.14236500	5.76916000	-1.08765400
C	3.90928400	-0.51999300	2.34560400	C	-0.16821300	6.70607700	-0.10603300
N	1.52110900	0.66524700	2.24831800	H	-0.25523500	7.12351300	2.00953000
N	2.87014000	-1.29830900	2.05034300	H	0.59459100	4.86358900	2.66066900
N	3.87290800	0.79326700	2.60335000	H	1.13389100	3.20478700	0.91887300
O	5.09134000	-1.14439400	2.34056000	H	0.00083300	6.01629700	-2.13589700
O	2.48014400	2.61068600	2.83690400	H	-0.54160700	7.68516000	-0.39331900
C	6.26003600	-0.31218700	2.29469400	C	0.92454500	3.43898200	-1.68907500
H	7.09927500	-1.00737100	2.25295700	H	1.10720400	2.46927500	-1.23752100
H	6.23392500	0.30723800	1.39516300	C	1.10031900	3.54539000	-3.02213300
H	6.32607500	0.31958300	3.18383900	H	1.09251800	4.50133900	-3.54070000

C	1.51188800	2.39839000	-3.85706700	C	1.04219200	1.01219500	-3.51234100
O	2.19086700	2.56428500	-4.86731300	C	1.70964000	-0.08805900	-4.06550600
O	2.57116900	1.23990800	-0.65616900	C	-0.14843900	0.77409700	-2.81936500
C	2.98964600	0.08961200	-0.80470000	C	1.23250900	-1.39332100	-3.93723500
C	4.63588700	-1.49936100	-0.78651600	H	2.61649900	0.10339900	-4.62988300
C	2.52297700	-2.20676200	-0.90265400	C	-0.66075000	-0.52996400	-2.67463000
N	4.32629000	-0.22395200	-0.78513300	H	-0.72733900	1.61266500	-2.45838300
N	2.05815100	-0.96073500	-0.95207500	C	0.02984300	-1.62311700	-3.26604900
N	3.79418400	-2.55837200	-0.85498800	H	1.78942200	-2.21061300	-4.37826600
O	5.94884300	-1.76570700	-0.69662200	H	-1.69443800	-0.68602800	-2.39938500
O	1.57373600	-3.16127200	-0.92330200	O	-0.58556900	-2.81723600	-3.15416400
C	1.94995500	-4.43624800	-0.38269500	C	0.08645700	-3.97285400	-3.64779700
H	1.02794300	-5.01994900	-0.36923900	H	1.05594100	-4.08731200	-3.15572900
H	2.70608000	-4.92008900	-1.00597600	H	-0.55862600	-4.81609200	-3.39880500
H	2.33695900	-4.30527400	0.63018500	H	0.21575800	-3.91683000	-4.73509500
C	6.32691100	-3.12239800	-0.45239400	H	-4.28845700	2.53762800	-2.79849000
H	6.01138300	-3.77740100	-1.26909300				
H	7.41597300	-3.10521100	-0.38066300				
H	5.88831400	-3.47692900	0.48451600				



23

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -768.2995456 a.u.

Thermal correction to Gibbs Free Energy at 298.15 K: 0.2105935 a.u.

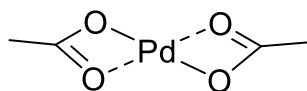
Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

-768.0889521 a.u.

C	-5.61806100	-1.16397200	-0.09079500
C	-4.57385500	-1.97762400	-0.53021300
C	-3.26915000	-1.49028500	-0.53875700
C	-2.97949000	-0.18313300	-0.11090300
C	-4.04421400	0.62455900	0.32973000
C	-5.34650700	0.13871400	0.33899500
H	-6.63723900	-1.53941700	-0.08219500
H	-4.77476400	-2.99092200	-0.86597700
H	-2.45598000	-2.12537100	-0.88144600
H	-3.84986800	1.63759300	0.66714300
H	-6.15573600	0.77681000	0.68250100
C	-1.58796800	0.27024000	-0.13701700

H	-0.87449700	-0.47219100	-0.48795000
C	-1.12416800	1.49058700	0.19590400
H	-1.80012800	2.29183600	0.48323000
C	0.27845500	1.94196800	0.03791100
O	0.49626000	3.13552800	-0.16419200
C	1.40596000	0.96601400	0.09733800
C	2.59138500	1.29026400	-0.57388600
C	1.36612000	-0.22364900	0.84606100
C	3.69701600	0.44703500	-0.54286700
H	2.62944700	2.22343600	-1.12603800
C	2.46608700	-1.06641600	0.90043300
H	0.47776200	-0.47358800	1.41564200
C	3.63611700	-0.74247500	0.19775800
H	4.59366100	0.72063300	-1.08598800
H	2.45083600	-1.97918600	1.48687400
O	4.65418200	-1.63752500	0.30277200
C	5.87106000	-1.35033500	-0.37034300
H	6.53817500	-2.18477600	-0.14934000
H	5.72210400	-1.28010400	-1.45535300

H	6.31997400	-0.41772500	-0.00584500
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Pd(OAc)₂

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -584.8714249 a.u.

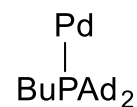
Thermal correction to Gibbs Free Energy at 298.15 K: 0.0649773 a.u.

Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

-584.8064476 a.u.

C	3.93911500	0.00013200	0.03697100
H	4.32697100	0.89689500	-0.45151800
H	4.26698200	0.00623600	1.08306500
H	4.32726300	-0.90174400	-0.44167400
C	2.44477600	-0.00007600	-0.00475200
O	1.77270000	-1.08852500	-0.00996800
O	1.77270500	1.08840500	-0.00997700
C	-3.93909800	0.00017500	0.03696800
H	-4.32725700	-0.89656300	-0.45131700
H	-4.26690600	-0.00567800	1.08309300
H	-4.32701800	0.90207100	-0.44181500
C	-2.44477300	0.00011800	-0.00476800

O	-1.77259500	1.08851000	-0.00997300
O	-1.77276500	-1.08837500	-0.00997000
Pd	-0.00001100	-0.00007500	-0.00972300



IM1`

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -1991.038705 a.u.

Thermal correction to Gibbs Free Energy at 298.15 K: 0.6447261 a.u.

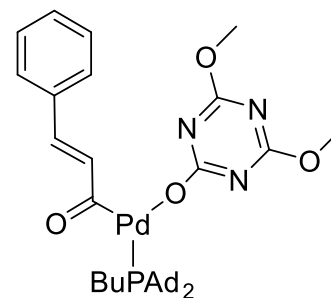
Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

-1990.393979 a.u.

P	0.00593500	0.56827100	0.17382300
C	-0.31200600	1.73761900	-1.24817000
C	-1.31616500	-0.78676900	-0.04154800
C	1.73584100	-0.10810300	-0.24733000
C	-2.97143300	4.47038900	-2.13025600
C	-1.65791800	3.68606600	-2.18114700
C	-1.62187700	2.53032500	-1.17462500
C	-1.68052200	-1.09182100	-1.51398900
C	-2.80082700	-2.15074200	-1.58176800
C	-2.33151700	-3.44597400	-0.89602800

C	-2.00469600	-3.15419300	0.57964700	H	-1.50192300	3.29187500	-3.19536400
C	-0.88231500	-2.10064600	0.64979000	H	-1.74425100	2.92176300	-0.15583300
C	-3.26142500	-2.62833100	1.29171100	H	-2.47999400	1.87411400	-1.36118500
C	-3.72044300	-1.33071500	0.60647200	H	0.51198200	2.45513900	-1.20818400
C	-2.59302200	-0.28538300	0.68900900	H	-0.23291700	1.21323900	-2.20877500
C	-4.05488900	-1.61633900	-0.86841600	H	-2.02187200	-0.18157100	-2.01833000
C	2.27504700	-0.91117500	0.96472600	H	-0.80460600	-1.45131400	-2.06302500
C	3.71824100	-1.38316000	0.71053700	H	-3.03209100	-2.35309700	-2.63568400
C	3.75876900	-2.25770800	-0.55636200	H	-3.11339200	-4.21405400	-0.96536600
C	3.27165900	-1.43693500	-1.76450400	H	-1.44362400	-3.84262900	-1.40740300
C	1.81719900	-0.98152500	-1.51899100	H	-1.65694300	-4.07281300	1.06969400
C	4.18017200	-0.20928300	-1.94860100	H	0.00822600	-2.51206800	0.16596300
C	4.12889600	0.65742300	-0.67755300	H	-0.62003700	-1.89335600	1.69501100
C	2.67657900	1.11251300	-0.43974300	H	-4.05976400	-3.38199400	1.25620500
C	4.62923400	-0.15966500	0.52416100	H	-3.04227100	-2.43693200	2.35047800
H	-2.97554800	5.29516600	-2.85164000	H	-4.60759900	-0.93493500	1.11729700
H	-3.82651700	3.82217000	-2.35825800	H	-2.93615200	0.65911600	0.25722200
H	-3.13606900	4.89584400	-1.13295500	H	-2.34078000	-0.07369100	1.73524400
H	-0.81505100	4.36237600	-1.98201400	H	-4.86947000	-2.34990200	-0.93709100

H	-4.40478300	-0.69854900	-1.36042700
H	2.22870900	-0.27297300	1.85619100
H	1.64333400	-1.77871500	1.16782700
H	4.05622100	-1.96979700	1.57442400
H	3.12312800	-3.14380900	-0.42261500
H	4.78070400	-2.61830600	-0.73481900
H	3.29977600	-2.05793800	-2.66932900
H	1.18328700	-1.86799100	-1.41921700
H	1.45288800	-0.42107600	-2.38948200
H	5.21144000	-0.53049600	-2.14731500
H	3.85119700	0.37643800	-2.81782800
H	4.75852400	1.54661800	-0.81090100
H	2.36068900	1.70549700	-1.30405500
H	2.61325400	1.76151300	0.44354000
H	4.61789000	0.45836500	1.43161000
H	5.66795000	-0.47701900	0.35963300
Pd	-0.03669700	1.55296800	2.17624500



IM2`

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -2413.303013 a.u.

Thermal correction to Gibbs Free Energy at 298.15 K: 0.7691079 a.u.

Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

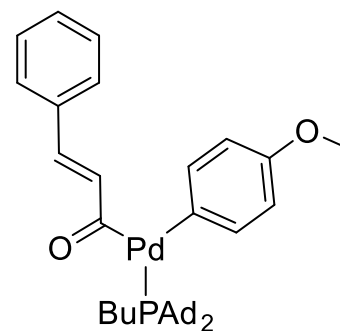
-2412.533905 a.u.

P	0.59221500	-1.39701900	0.10350200
C	-0.54577900	-2.83872400	0.34646600
C	1.26523700	-0.97971700	1.82184300
C	1.93441200	-2.04281900	-1.05539400
C	-4.18435600	-3.27871500	1.71639900
C	-2.91910900	-3.56460300	0.90414800
C	-1.80135000	-2.55475000	1.18549400
C	1.44048400	-2.22266600	2.72698400
C	1.91875000	-1.79261800	4.12995800

C	3.26523700	-1.05583300	4.01936400	H	-3.15097600	-3.53710100	-0.16895000
C	3.08963100	0.19291100	3.13818500	H	-2.55962900	-4.58139000	1.11555900
C	2.61735500	-0.23493200	1.73558500	H	-2.17652000	-1.54897100	0.96645100
C	2.05213900	1.13504000	3.77023200	H	-1.56148900	-2.56578800	2.25545300
C	0.70821600	0.39637400	3.88643300	H	-0.86719800	-3.10083900	-0.66283700
C	0.23693500	-0.01768800	2.48106200	H	0.01265500	-3.69197100	0.74774400
C	0.87452700	-0.85676200	4.76435500	H	0.49491100	-2.76527900	2.82483000
C	2.76673500	-0.84258900	-1.57947300	H	2.16497500	-2.91659100	2.28689000
C	3.81761500	-1.32330500	-2.59633200	H	2.03715800	-2.69028100	4.75029400
C	4.74327000	-2.35804800	-1.93004600	H	3.62029800	-0.77049900	5.01861100
C	3.91365700	-3.56688600	-1.45885700	H	4.02441600	-1.72030500	3.58448700
C	2.87057300	-3.09761000	-0.42287900	H	4.05085100	0.71423800	3.03801800
C	3.20041300	-4.20111400	-2.66525800	H	3.38089500	-0.88404100	1.29723200
C	2.27341700	-3.15825200	-3.31423700	H	2.52245900	0.64376000	1.09609900
C	1.23145200	-2.69298200	-2.27933300	H	2.39213100	1.46472100	4.76118800
C	3.10554300	-1.96066300	-3.80023000	H	1.93465600	2.03119800	3.14749800
H	-4.97304000	-4.00754300	1.49778300	H	-0.04459100	1.06139600	4.32793300
H	-3.98119400	-3.32082300	2.79353600	H	-0.74565800	-0.49455000	2.54662900
H	-4.57932300	-2.28153900	1.49110400	H	0.11749900	0.87123000	1.85108000

H	1.19213500	-0.57112600	5.77596600	C	-0.31527000	3.13762200	-1.14010700
H	-0.08776800	-1.37721100	4.86347200	C	0.66548700	5.14310200	-0.84890800
H	2.09180700	-0.11668500	-2.04922600	C	1.76067700	3.30600600	-0.18026500
H	3.26325000	-0.31944300	-0.75991200	N	-0.39068400	4.47786200	-1.28724400
H	4.40721400	-0.45897900	-2.92698500	N	0.77514000	2.50733900	-0.56180400
H	5.26415600	-1.90286900	-1.07638100	N	1.78143100	4.63397000	-0.28849200
H	5.51404100	-2.68724500	-2.63942600	C	1.70289200	7.24940900	-0.53862200
H	4.57235800	-4.30614100	-0.98519600	H	2.61666100	6.97816000	-1.07507800
H	3.39304300	-2.68584900	0.44563600	H	1.43057600	8.28427200	-0.75098600
H	2.28558600	-3.95669700	-0.06955200	H	1.86965200	7.11195400	0.53369600
H	3.94017500	-4.55757600	-3.39433300	C	3.90038000	3.51260000	0.82376100
H	2.61813600	-5.07490700	-2.34261900	H	3.55542000	4.21266300	1.58885500
H	1.74290600	-3.61032000	-4.16150400	H	4.62797600	2.81602200	1.24292700
H	0.64856400	-3.56372400	-1.96202500	H	4.33994600	4.07656500	-0.00274200
H	0.52595200	-1.98698800	-2.72767300	O	2.82385900	2.68912800	0.36315100
H	2.45510300	-1.22156400	-4.28560900	O	0.59174300	6.47220600	-0.99013900
H	3.83978900	-2.28913200	-4.54804300	C	-1.93924400	-0.57633000	-1.48790000
Pd	-0.39854300	0.47796900	-0.83044400	C	-3.19684500	0.09481300	-1.08815000
O	-1.25156700	2.36189100	-1.51979100	C	-4.33747400	-0.62207900	-1.01765200

C	-5.63560000	-0.16317600	-0.53156400
C	-6.68220300	-1.09568500	-0.41690400
C	-5.88532500	1.17312600	-0.16448000
C	-7.93596100	-0.71243600	0.05398800
H	-6.50013800	-2.12938100	-0.69941100
C	-7.13734700	1.55537400	0.30290600
H	-5.09667700	1.91346400	-0.25386400
C	-8.16730900	0.61512200	0.41599000
H	-8.73087400	-1.44803200	0.13691600
H	-7.31469900	2.59084600	0.57887300
H	-9.14378400	0.91884000	0.78223200
O	-1.88424600	-1.59647800	-2.14242800
H	-3.12562700	1.13376600	-0.79116700
H	-4.28910600	-1.66426200	-1.32851700



IM3'

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -2175.313972 a.u.

Thermal correction to Gibbs Free Energy at 298.15 K: 0.7680869 a.u.

Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

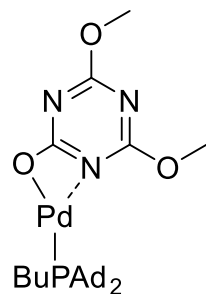
-2174.545885 a.u.

P	-1.41802400	0.32841700	0.01221600
C	-1.22921600	2.17412200	-0.12086500
C	-2.21118300	0.00089100	1.69720200
C	-2.59329100	-0.09658000	-1.40988900
C	1.05892700	4.94346900	1.42554000
C	0.11444100	4.25288200	0.44021500
C	-0.27743400	2.83793100	0.88196600
C	-3.26659200	1.04434100	2.12628600
C	-3.79367200	0.71969100	3.53882300
C	-4.42964300	-0.68230900	3.54051500

C	-3.37005200	-1.72935400	3.15084200	H	-0.79460800	4.85645200	0.30704800
C	-2.83895900	-1.41423700	1.73895300	H	0.62718700	2.22677200	0.98579100
C	-2.21320300	-1.69337500	4.16287900	H	-0.73863400	2.88752700	1.87550900
C	-1.57593400	-0.29435200	4.14817800	H	-0.80882100	2.32490900	-1.11981900
C	-1.05020000	0.00981800	2.73330100	H	-2.20872700	2.66822800	-0.11009400
C	-2.62751400	0.75864000	4.54227700	H	-2.82706200	2.04848200	2.12468300
C	-2.46412400	-1.61785700	-1.68872700	H	-4.09966800	1.06004600	1.41674300
C	-3.32242800	-2.01768800	-2.90208600	H	-4.54677200	1.46783300	3.81739100
C	-4.79468700	-1.65512600	-2.63507500	H	-4.83581000	-0.91031600	4.53479700
C	-4.92094300	-0.13677700	-2.40992700	H	-5.27016000	-0.71505700	2.83392100
C	-4.07671900	0.27105300	-1.18365700	H	-3.82354000	-2.72846900	3.14095100
C	-4.42021600	0.60806600	-3.65890500	H	-3.66456100	-1.49232600	1.02646400
C	-2.94641400	0.24504600	-3.90764200	H	-2.08796600	-2.15894700	1.44381500
C	-2.11032200	0.65738100	-2.68040600	H	-2.58298000	-1.93182200	5.16892600
C	-2.81537400	-1.26830800	-4.14527600	H	-1.46219700	-2.45179300	3.90520900
H	1.33120000	5.94600600	1.07824900	H	-0.73486000	-0.26077100	4.85195500
H	0.59556300	5.04378200	2.41497300	H	-0.53591400	0.97423800	2.73076000
H	1.98593800	4.37243600	1.54129500	H	-0.30088700	-0.74491900	2.45080300
H	0.59706500	4.19542500	-0.54383200	H	-2.99603400	0.55996500	5.55734200

H	-2.17430700	1.75922000	4.55381000	C	2.65096200	1.50445700	-0.77689400
H	-1.41201500	-1.85993700	-1.87563600	C	3.36736600	2.77174600	-0.66733900
H	-2.77614700	-2.19626300	-0.81414200	C	3.23707200	3.80829600	-1.60981900
H	-3.23013800	-3.09979400	-3.05819800	C	4.19291800	2.98310900	0.45100300
H	-5.16266000	-2.19839300	-1.75369300	C	3.91179600	5.01208300	-1.43674600
H	-5.41999600	-1.95965400	-3.48487700	H	2.58880100	3.67261000	-2.47012400
H	-5.97000600	0.12321900	-2.21782500	C	4.87691100	4.18505200	0.61918300
H	-4.47340400	-0.23579900	-0.29920500	H	4.29717200	2.18810000	1.18479400
H	-4.17440800	1.35039400	-1.00654300	C	4.73526100	5.20502600	-0.32285100
H	-5.03079100	0.33511900	-4.52989400	H	3.79373100	5.80591900	-2.16872100
H	-4.52429600	1.69281900	-3.51869400	H	5.51423000	4.32796900	1.48693100
H	-2.57198800	0.79147900	-4.78262400	H	5.25908900	6.14715100	-0.19010000
H	-2.21627600	1.73834900	-2.53885700	O	0.99667400	-0.89179400	-2.83164400
H	-1.05441200	0.44429300	-2.86795200	H	2.02804100	1.50242500	-2.82454300
H	-1.76698700	-1.52853500	-4.33615400	H	2.63797900	0.88520200	0.11806000
H	-3.39533500	-1.56168400	-5.03071100	C	2.40069700	-1.93970100	0.07671000
Pd	0.65554600	-0.87541700	-0.04322400	C	2.72962700	-2.95938100	-0.82563400
C	1.30118700	-0.28785200	-1.82498600	C	3.25636500	-1.76370200	1.18311100
C	2.01764900	1.00742400	-1.85490900	C	3.83261000	-3.79884700	-0.63087300

H	2.11862400	-3.10417700	-1.71384700
C	4.35932200	-2.58718600	1.39585700
H	3.05952500	-0.97329800	1.90648300
C	4.65139500	-3.61266500	0.48780100
H	4.04432700	-4.57941100	-1.35368500
H	5.01182200	-2.45450400	2.25442100
O	5.75812800	-4.36821600	0.77757900
C	6.09627500	-5.40722000	-0.11991200
H	6.31362400	-5.02071300	-1.12519700
H	6.99359800	-5.87871300	0.28635400
H	5.29570800	-6.15613300	-0.19428300



IM1^{..}

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -1991.038705 a.u.

Thermal correction to Gibbs Free Energy at 298.15 K: 0.6447261 a.u.

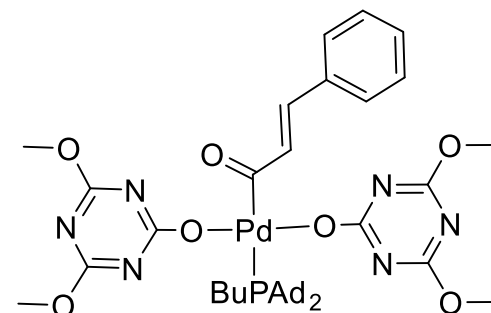
Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

-1990.393979 a.u.	P	1.12701500	-0.05670600	0.38221200
	C	0.87628400	0.11042100	2.21724700
	C	1.05805500	1.70168000	-0.30945100
	C	2.84987800	-0.81877000	0.22769300
	C	-2.17784500	0.91204100	4.52442400
	C	-0.79421500	0.39422700	4.12263500
	C	-0.50330900	0.63218100	2.63741500
	C	1.67100500	2.76035800	0.63702800
	C	1.50687200	4.17053200	0.03441900
	C	2.21995200	4.23517200	-1.32779500
	C	1.59247400	3.20508400	-2.28412100
	C	1.75683300	1.79309000	-1.68726600
	C	0.10035000	3.52312700	-2.47596800
	C	-0.60787000	3.44684300	-1.11366300
	C	-0.44479500	2.03034900	-0.53491000
	C	0.00980100	4.47613500	-0.15059100
	C	3.04706700	-1.31187300	-1.23021300
	C	4.39675700	-2.03699400	-1.38005400

C	5.53801900	-1.07911000	-0.99007600	H	2.13262400	5.24426200	-1.75149000
C	5.36251800	-0.63421600	0.47369100	H	3.29199700	4.03025600	-1.20182300
C	4.01885100	0.10977000	0.62337700	H	2.10735500	3.23778000	-3.25263200
C	5.37901600	-1.86963900	1.39062200	H	2.82541800	1.57753500	-1.59321000
C	4.23122400	-2.81546400	0.99353700	H	1.32997800	1.04545300	-2.36781000
C	2.89193300	-2.06980800	1.14789000	H	-0.01798900	4.52330600	-2.91382100
C	4.41694800	-3.27021900	-0.46290900	H	-0.35170100	2.80725200	-3.17476700
H	-2.38843900	0.72275600	5.58272200	H	-1.67865000	3.65127600	-1.23864900
H	-2.25711300	1.99336700	4.35556200	H	-1.01208100	1.94178300	0.39280400
H	-2.96042900	0.42618900	3.93017300	H	-0.87613600	1.29324900	-1.22137300
H	-0.72839200	-0.68195400	4.33447400	H	-0.12071900	5.49197700	-0.54671800
H	-0.02127100	0.87755900	4.73692200	H	-0.50344100	4.43960700	0.82005700
H	-1.27793100	0.14803800	2.03583600	H	2.22444500	-1.99065600	-1.49682400
H	-0.58390300	1.70545300	2.42985600	H	3.00377500	-0.47669700	-1.93255900
H	0.98520400	-0.90631500	2.60590300	H	4.51596600	-2.34823000	-2.42519900
H	1.67925400	0.71111000	2.66227400	H	5.53775700	-0.20294200	-1.65275100
H	1.17715700	2.72873700	1.61396900	H	6.50779800	-1.57788900	-1.11676300
H	2.73307600	2.55467700	0.80832200	H	6.17644800	0.04652600	0.75370500
H	1.95283000	4.90161200	0.72087900	H	4.03314400	1.00236600	-0.00970200

H	3.89501700	0.45158500	1.65903400
H	6.34262100	-2.38877200	1.30516900
H	5.26983400	-1.56275300	2.43964200
H	4.22409200	-3.68856900	1.65794700
H	2.78166400	-1.77437700	2.19620900
H	2.05250700	-2.73636000	0.90686900
H	3.61541300	-3.96417300	-0.74800500
H	5.36685800	-3.81015600	-0.57108000
Pd	-0.45160700	-1.43652400	-0.58547500
O	-2.01325600	-2.68954300	-1.46738900
C	-3.00431700	-2.01067600	-1.05261800
C	-3.67576600	-0.16318800	0.14802600
C	-5.18651200	-1.50136400	-0.82903300
N	-2.67089400	-0.90562600	-0.28517900
N	-4.28689000	-2.32919600	-1.33412800
N	-4.96731800	-0.39760500	-0.08298400
O	-6.45826400	-1.81719400	-1.10655700
O	-3.33004000	0.90796400	0.88320000
C	-7.48128900	-0.96340800	-0.59112000

H	-8.41859200	-1.40389400	-0.93440000
H	-7.45389100	-0.93113900	0.50194100
H	-7.37578100	0.05495200	-0.97629000
C	-4.39041400	1.73376600	1.37534400
H	-5.06540100	1.16187200	2.01713100
H	-3.89424800	2.51862400	1.94778300
H	-4.96426700	2.16327300	0.55001500



IM2''

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -2997.246136 a.u.

Thermal correction to Gibbs Free Energy at 298.15 K: 0.8783972 a.u.

Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

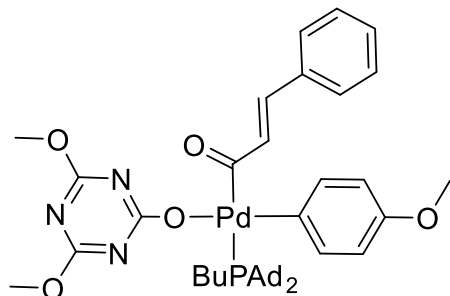
-2996.367739 a.u.

P	-1.48576500	-0.99719100	0.55221900
C	-2.49355300	-0.04855700	1.78918700
C	-0.54731900	-2.32091700	1.51933600

C	-2.78698400	-1.71828000	-0.61764900	C	-4.77839400	-1.06284400	-2.05343400
C	-1.94760100	2.55668100	4.62808300	C	-3.72432200	-0.55957100	-1.05087300
C	-2.70169500	1.62519800	3.67805700	C	-4.08460700	-1.62690800	-3.30315100
C	-1.75707500	0.68181900	2.92062000	H	-2.63797600	3.18529300	5.20180200
C	-1.35701100	-2.91146800	2.70035900	H	-1.33652100	1.99041200	5.34261500
C	-0.48750000	-3.92250500	3.48017800	H	-1.28815600	3.21603000	4.05402900
C	-0.04612200	-5.06352700	2.54597000	H	-3.25439600	2.23565300	2.95360200
C	0.77287100	-4.48084600	1.38090300	H	-3.44893200	1.03510100	4.22829800
C	-0.10340500	-3.48431300	0.59882800	H	-0.93189400	1.26070400	2.49851400
C	2.01989600	-3.76747900	1.93005200	H	-1.32508600	-0.03263400	3.63034700
C	1.58095700	-2.63479400	2.87309500	H	-3.01333100	0.70359700	1.19070100
C	0.72312600	-1.62808700	2.08716300	H	-3.26609900	-0.71443600	2.19478500
C	0.75791500	-3.21143200	4.03822400	H	-1.68227200	-2.11768400	3.38056300
C	-2.10551600	-2.26742400	-1.89693600	H	-2.25966100	-3.41115100	2.33468100
C	-3.16646000	-2.78668700	-2.88449000	H	-1.08356900	-4.32932200	4.30730500
C	-4.00080900	-3.89468600	-2.21734200	H	0.55277000	-5.79454000	3.10549500
C	-4.70787700	-3.32688500	-0.97330100	H	-0.92532900	-5.59599000	2.15826800
C	-3.64679900	-2.82816700	0.03100800	H	1.07732400	-5.28358700	0.69846800
C	-5.62437500	-2.16279600	-1.38895700	H	-0.98183400	-4.01735500	0.22163300

H	0.43630700	-3.10598300	-0.27002800	H	-4.25035500	-0.14775500	-0.18301100
H	2.65766400	-4.48307300	2.46641200	H	-3.13832100	0.25267000	-1.48792100
H	2.61459400	-3.35949600	1.10325500	H	-3.49653900	-0.84012600	-3.79241900
H	2.46365500	-2.11224300	3.26334800	H	-4.83351300	-1.97477100	-4.02776800
H	0.44286000	-0.79605500	2.73971000	Pd	0.09465900	0.42150700	-0.64913400
H	1.31309900	-1.20113100	1.27170900	O	-0.33703300	2.08876900	0.46971100
H	1.36471900	-3.91933300	4.61856400	C	-1.42351700	2.74195700	0.22520600
H	0.45852100	-2.40585900	4.72243500	C	-2.91653400	4.31742100	0.82262900
H	-1.51490300	-1.47669300	-2.36646200	C	-3.30124300	3.06561700	-0.99033200
H	-1.40443600	-3.06877800	-1.65725500	N	-1.76186900	3.72486600	1.09288200
H	-2.65196500	-3.19068700	-3.76497300	N	-2.16757600	2.38902900	-0.85420200
H	-3.35259100	-4.73426100	-1.93148400	N	-3.75125800	4.04135600	-0.19362600
H	-4.74429000	-4.28731000	-2.92385700	O	-4.05252400	2.68988700	-2.03611000
H	-5.30214700	-4.11417300	-0.49146200	O	-3.26776100	5.27895900	1.68697100
H	-3.02175400	-3.67384300	0.33346400	C	-5.29940700	3.36508000	-2.22427100
H	-4.14140500	-2.44978400	0.93484800	H	-5.73819400	2.90849700	-3.11243500
H	-6.39513300	-2.52295900	-2.08349500	H	-5.95411700	3.22584500	-1.35930500
H	-6.14492400	-1.75995200	-0.50910300	H	-5.14470200	4.43601000	-2.38121500
H	-5.41639700	-0.21461200	-2.33199900	C	-4.50994300	5.94800500	1.45674800

H	-5.34712500	5.24484100	1.49084300	O	4.38481800	-3.94443000	-1.98958100
H	-4.59336700	6.67818100	2.26304800	C	1.30599600	1.75375800	-1.70935800
H	-4.51182300	6.45034800	0.48525600	C	2.32507800	2.37244700	-0.87388200
O	0.78698400	-1.23551300	-1.67972100	C	3.40739900	2.93862000	-1.44996700
C	2.02347400	-1.48384400	-1.41305700	C	4.57952000	3.44811200	-0.74981800
C	3.84042700	-2.80616000	-1.54370000	C	5.55216300	4.15534300	-1.47867200
C	3.97102800	-0.88086300	-0.41006200	C	4.78552100	3.24357100	0.62858400
N	2.56801900	-2.63230100	-1.87419200	C	6.68991800	4.65779500	-0.85190200
N	2.70193000	-0.58136900	-0.65152000	H	5.40508200	4.31152000	-2.54420700
N	4.61562300	-1.97696200	-0.81861500	C	5.92201600	3.74516700	1.25217800
C	5.74948600	-4.20110800	-1.64858100	H	4.06764200	2.66700300	1.20021000
H	5.88044700	-4.24842200	-0.56369000	C	6.87731900	4.45526600	0.51611600
H	5.97874700	-5.16629700	-2.10235200	H	7.42931100	5.20441100	-1.42973000
H	6.40737500	-3.42499400	-2.04960800	H	6.06788900	3.58139400	2.31607700
C	6.02150100	-0.20019500	0.56281100	H	7.76441600	4.84367300	1.00800700
H	6.56731000	-0.32399800	-0.37603400	O	1.05355800	1.84893400	-2.87238600
H	6.36752400	0.69029200	1.08818700	H	2.20287800	2.25673600	0.19252200
H	6.16308400	-1.09406500	1.17681400	H	3.43005300	3.00614500	-2.53621400
O	4.63103300	0.03290900	0.31591400				



IM3''

Total SCF energy (M06/def2-TZVP/SMD(Anisole)): -2759.296453 a.u.

Thermal correction to Gibbs Free Energy at 298.15 K: 0.8811017 a.u.

Gibbs free energy at 298.15 K (M06/def2-TZVP/SMD(Anisole)):

-2758.415351 a.u.

P	-0.50406100	-1.44182600	0.27691300
C	0.35446300	-2.97330000	-0.31610600
C	-2.24954200	-1.96901000	0.77242500
C	0.52387600	-0.89872200	1.79156900
C	0.42492400	-5.08575400	-3.59383800
C	0.89748700	-4.48885500	-2.26678700
C	-0.15703900	-3.57470800	-1.63253500
C	-2.28426600	-3.33192800	1.50781700
C	-3.74192300	-3.71808900	1.83856000

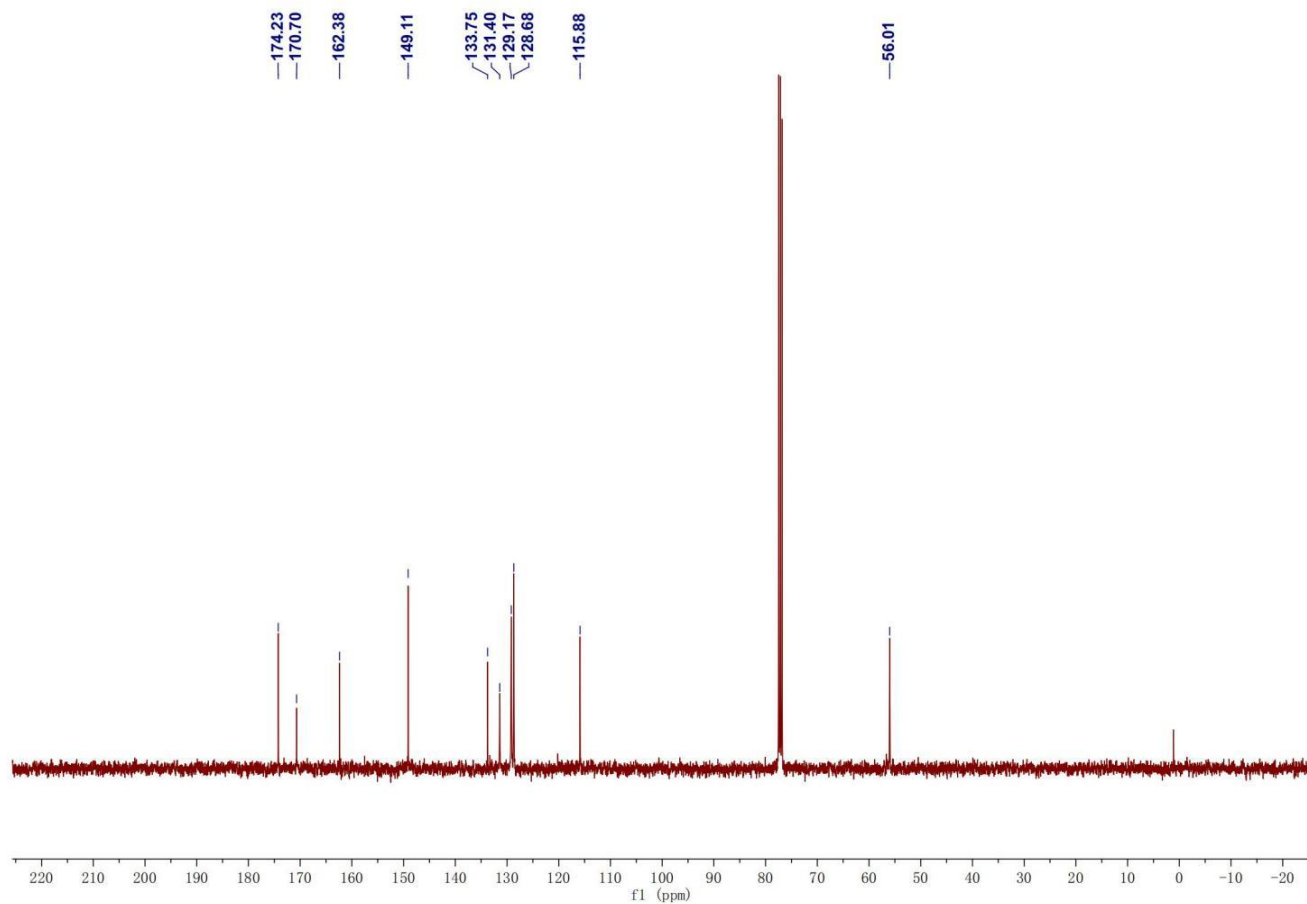
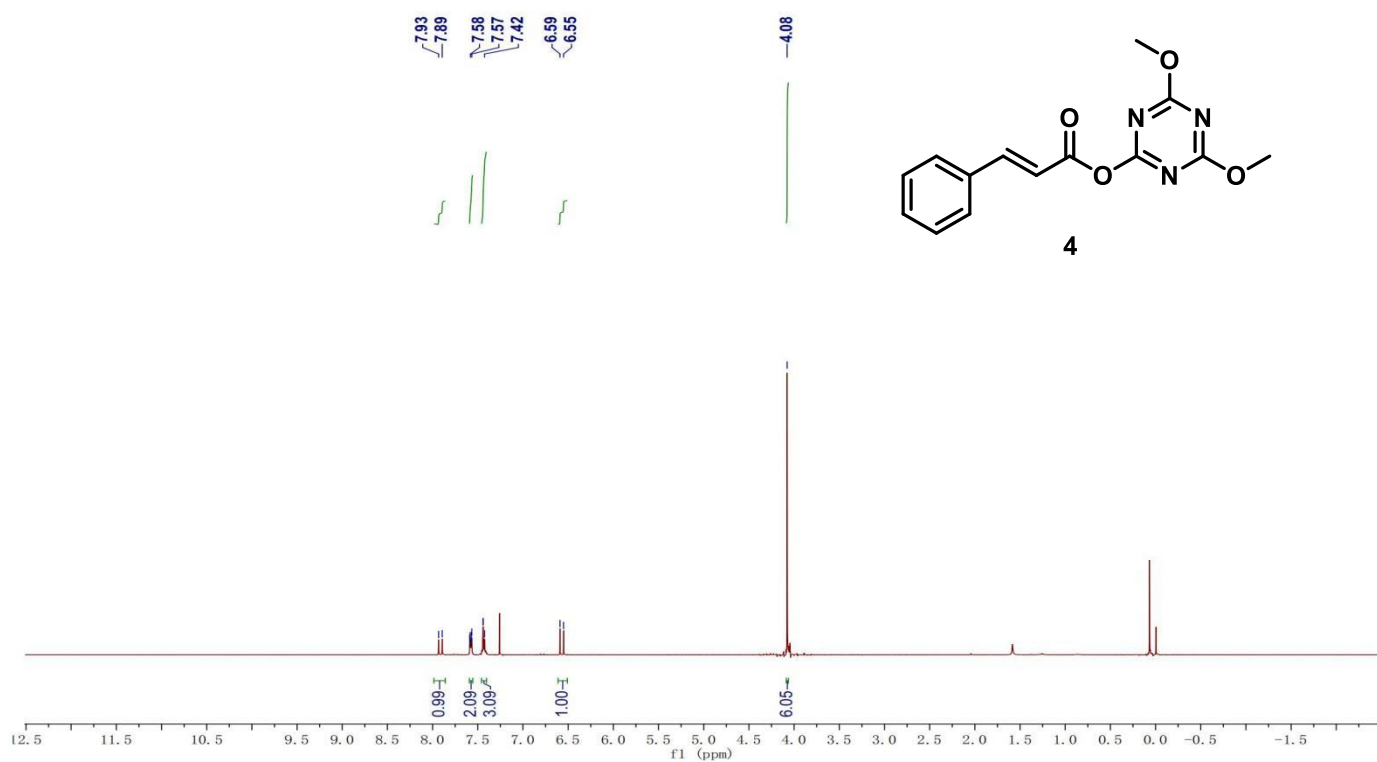
C	-4.37845900	-2.63323800	2.72602500
C	-4.37635200	-1.28993300	1.97538100
C	-2.92566900	-0.88776600	1.65123100
C	-5.17634600	-1.41931700	0.66839400
C	-4.53377300	-2.50704800	-0.20886400
C	-3.07962800	-2.11441200	-0.53131500
C	-4.54892500	-3.85253800	0.53610700
C	0.28328200	0.61170100	2.02665700
C	1.16636900	1.13676300	3.17178500
C	0.84771300	0.35533300	4.45892800
C	1.13850400	-1.14109100	4.23768700
C	0.24592400	-1.67885500	3.09677800
C	2.62121300	-1.32735800	3.87387800
C	2.92100800	-0.54941900	2.58291600
C	2.02388200	-1.08103400	1.45038300
C	2.64625000	0.94674600	2.79887700
H	1.19071400	-5.73366300	-4.03496300
H	-0.48588200	-5.68468100	-3.46382400
H	0.20141800	-4.29315900	-4.31834900

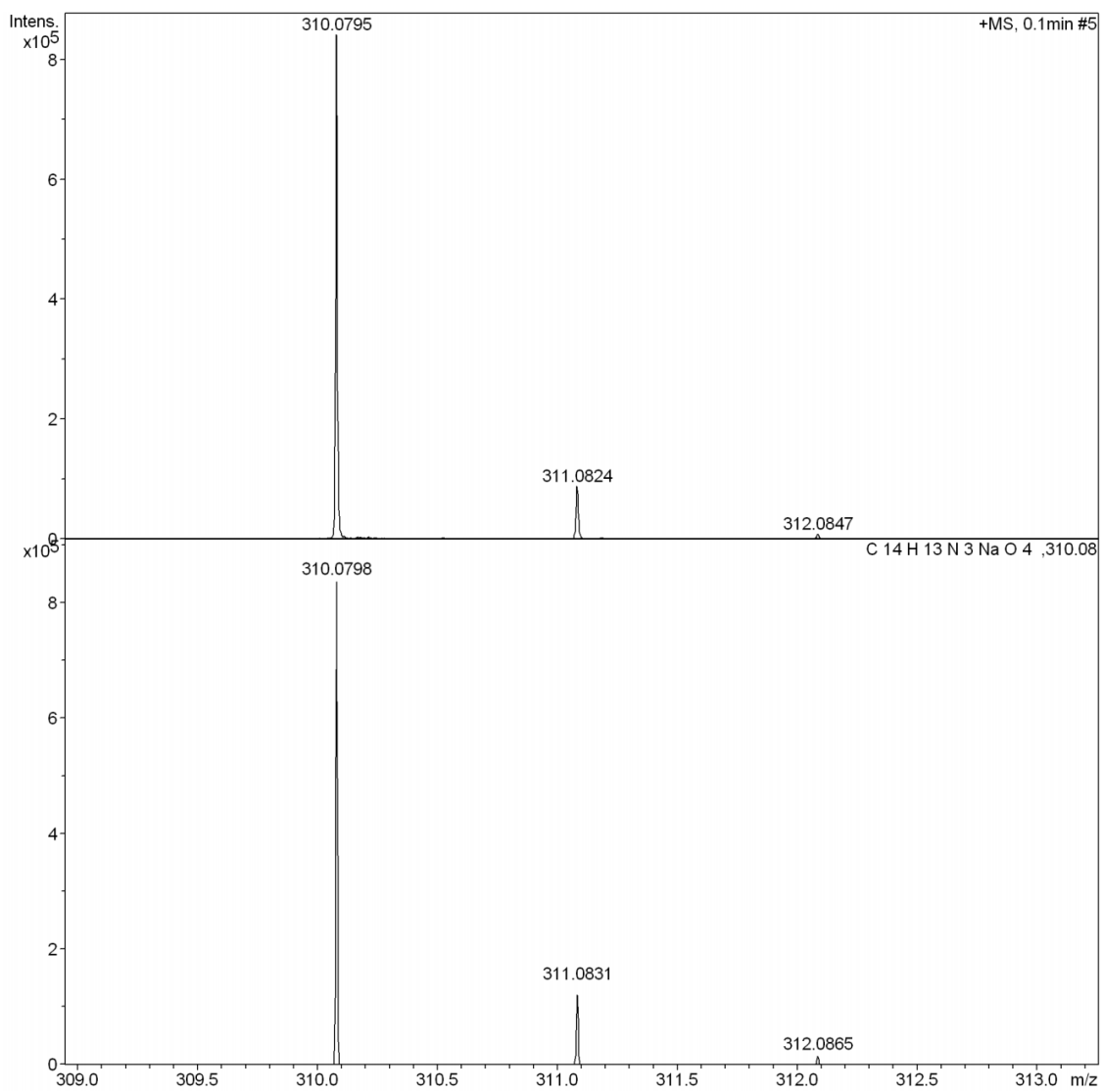
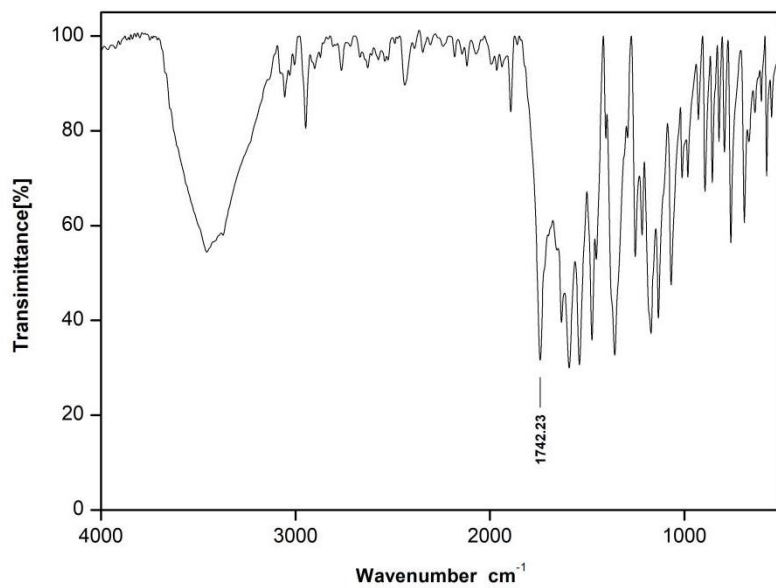
H	1.81239400	-3.90506800	-2.41884000	H	-5.58150200	-4.15087200	0.76187800
H	1.14912200	-5.29728200	-1.56463300	H	-4.11571800	-4.63935600	-0.09610900
H	-0.38860000	-2.76466200	-2.33341700	H	0.51887900	1.15511200	1.10428100
H	-1.08278000	-4.14020900	-1.46858000	H	-0.77039800	0.80084800	2.25362300
H	1.38770500	-2.67049200	-0.48877200	H	0.95628400	2.20399100	3.31546200
H	0.36323300	-3.72221800	0.48549200	H	-0.20609500	0.49771600	4.73505200
H	-1.84032300	-4.10950400	0.87576900	H	1.45334500	0.73391100	5.29303200
H	-1.70093100	-3.29584900	2.43143200	H	0.90706500	-1.70148600	5.15261900
H	-3.73611400	-4.67713700	2.37236900	H	-0.80044900	-1.58461000	3.39751100
H	-5.40560500	-2.91951700	2.98859900	H	0.44604200	-2.74696000	2.94508500
H	-3.81945600	-2.53959700	3.66737400	H	3.25823600	-0.96834500	4.69330700
H	-4.82163400	-0.51036400	2.60632900	H	2.84440400	-2.39367200	3.73359100
H	-2.37758400	-0.75430300	2.58859700	H	3.96674300	-0.69827600	2.28482800
H	-2.91575500	0.07255000	1.13176200	H	2.25692200	-2.13642200	1.28508200
H	-6.22085500	-1.67868300	0.88851400	H	2.25052600	-0.53961600	0.53370200
H	-5.17994700	-0.45964800	0.13611900	H	2.87766100	1.50537600	1.88478900
H	-5.08701900	-2.59793800	-1.15238000	H	3.29161700	1.34026700	3.59636100
H	-2.63602700	-2.87147500	-1.18245200	Pd	-0.28643500	0.21946500	-1.45126300
H	-3.06762400	-1.17084000	-1.07532500	O	1.42620100	-0.82336700	-2.27101100

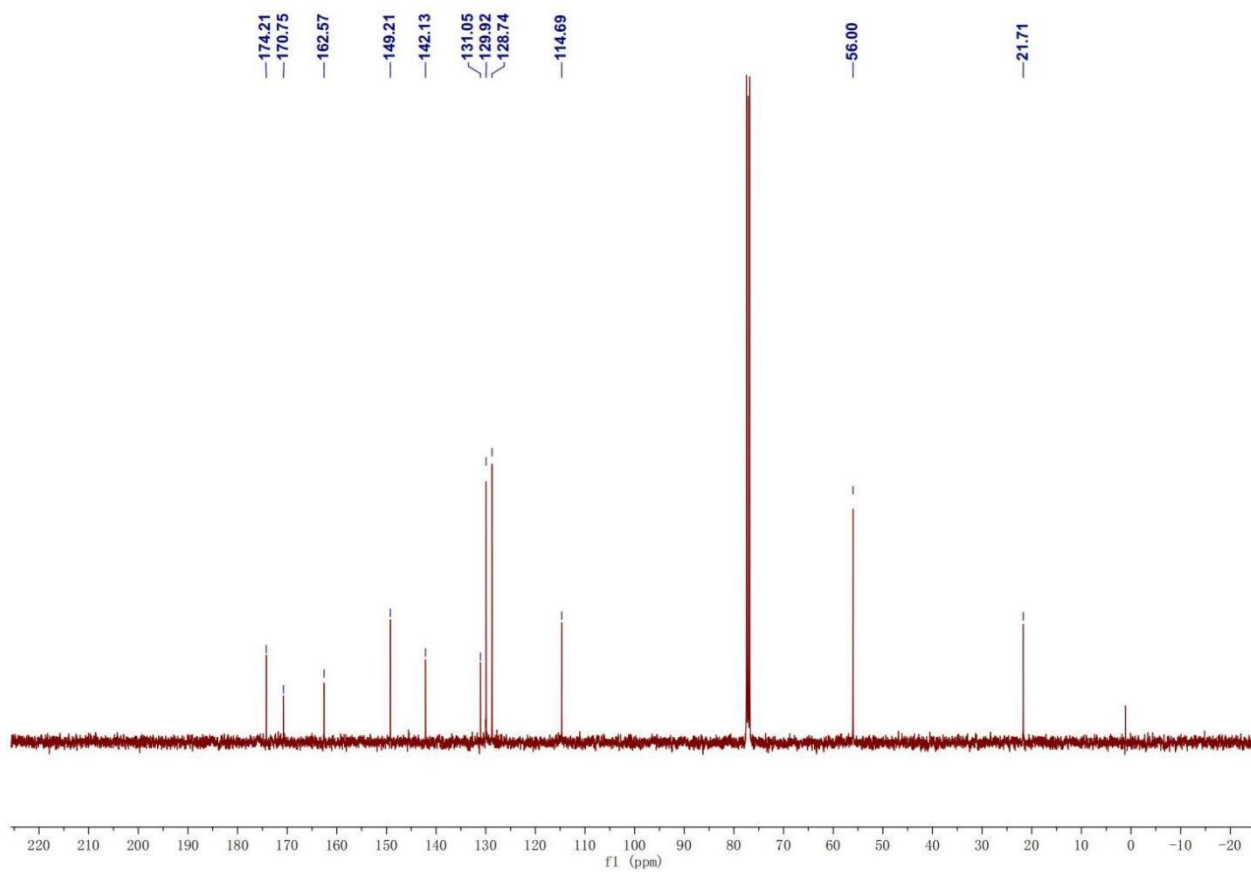
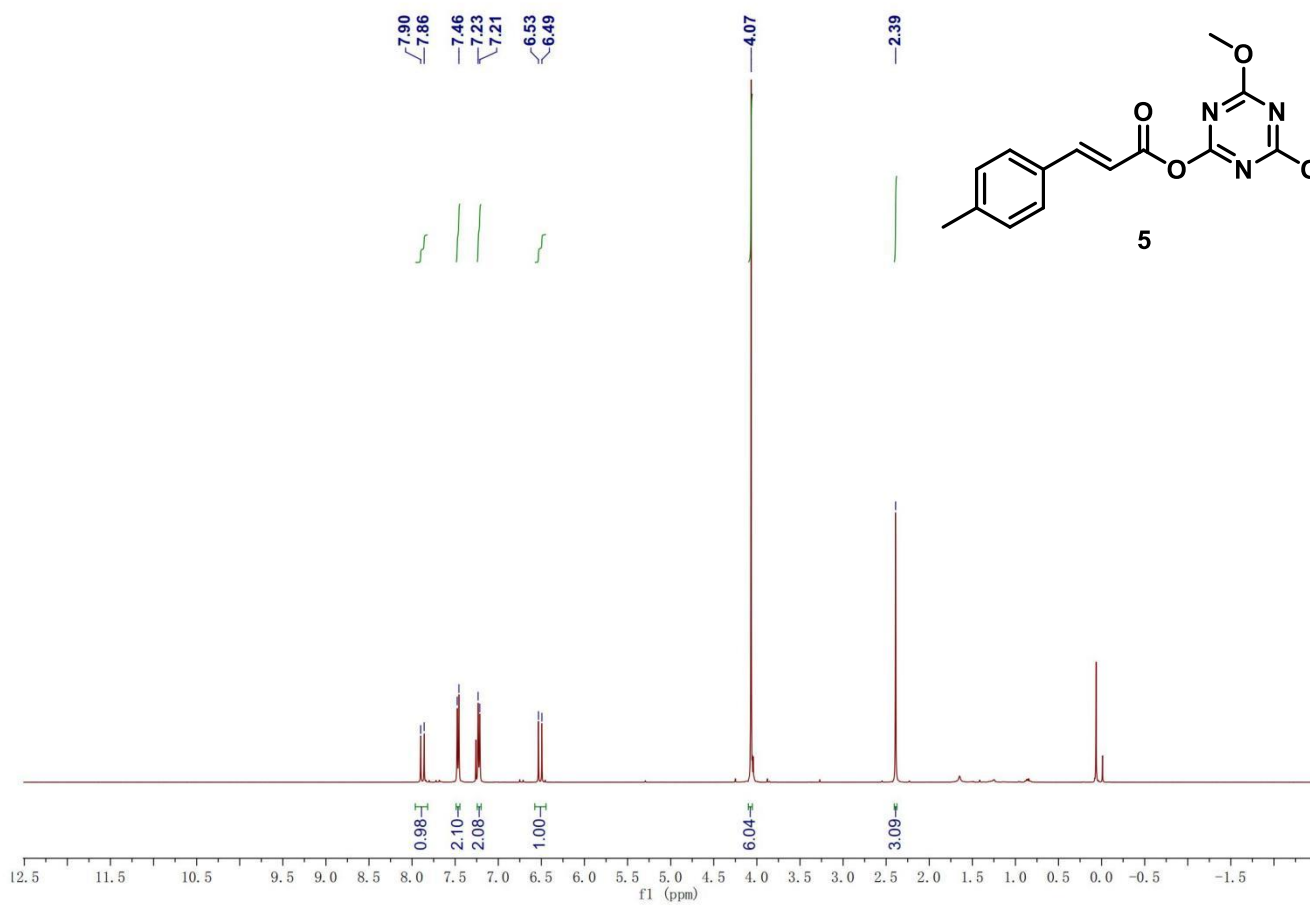
C	2.61308400	-0.69935000	-1.82767100	C	0.78909300	4.15686000	-0.50837700
C	4.56450200	-1.65050800	-1.16469000	C	0.08725700	5.19993500	0.13470400
C	4.25141100	0.53364600	-0.83228000	C	2.02133900	3.73516800	0.04000000
N	3.39086600	-1.81675600	-1.74974200	C	0.59289600	5.79727100	1.28387500
N	3.05798500	0.52989300	-1.40411500	H	-0.86981400	5.51813300	-0.26998600
N	5.06449400	-0.51042700	-0.65247700	C	2.52114700	4.33979100	1.18658500
O	4.64365300	1.73625900	-0.36703700	H	2.57977900	2.92797300	-0.41839100
O	5.30735900	-2.76212300	-1.06451500	C	1.81290200	5.36971200	1.81672900
C	5.90144500	1.79971700	0.31125300	H	0.03498800	6.59301500	1.76916800
H	6.02979600	2.85096500	0.57377500	H	3.46717600	3.99809200	1.59621900
H	5.88884400	1.17981900	1.21234700	H	2.20740400	5.83326100	2.71636500
H	6.71432500	1.46510700	-0.33805200	O	-0.59250400	1.41198600	-4.19704000
C	6.57789900	-2.64872100	-0.42002800	H	1.69513400	2.00202500	-2.07693500
H	6.46478900	-2.31921000	0.61711700	H	-0.81033200	3.85098500	-1.92393100
H	7.00549300	-3.65187300	-0.45526100	C	-1.97858200	1.22859900	-1.00328000
H	7.22444200	-1.94006200	-0.94525700	C	-3.08396600	1.08063300	-1.84606000
C	-0.08407700	1.60141700	-3.14612200	C	-2.06563200	2.18301700	0.02148500
C	0.72088200	2.43212500	-2.32579700	C	-4.25757300	1.82567400	-1.66336800
C	0.18611500	3.51535500	-1.65278800	H	-3.04780900	0.38085400	-2.67679700

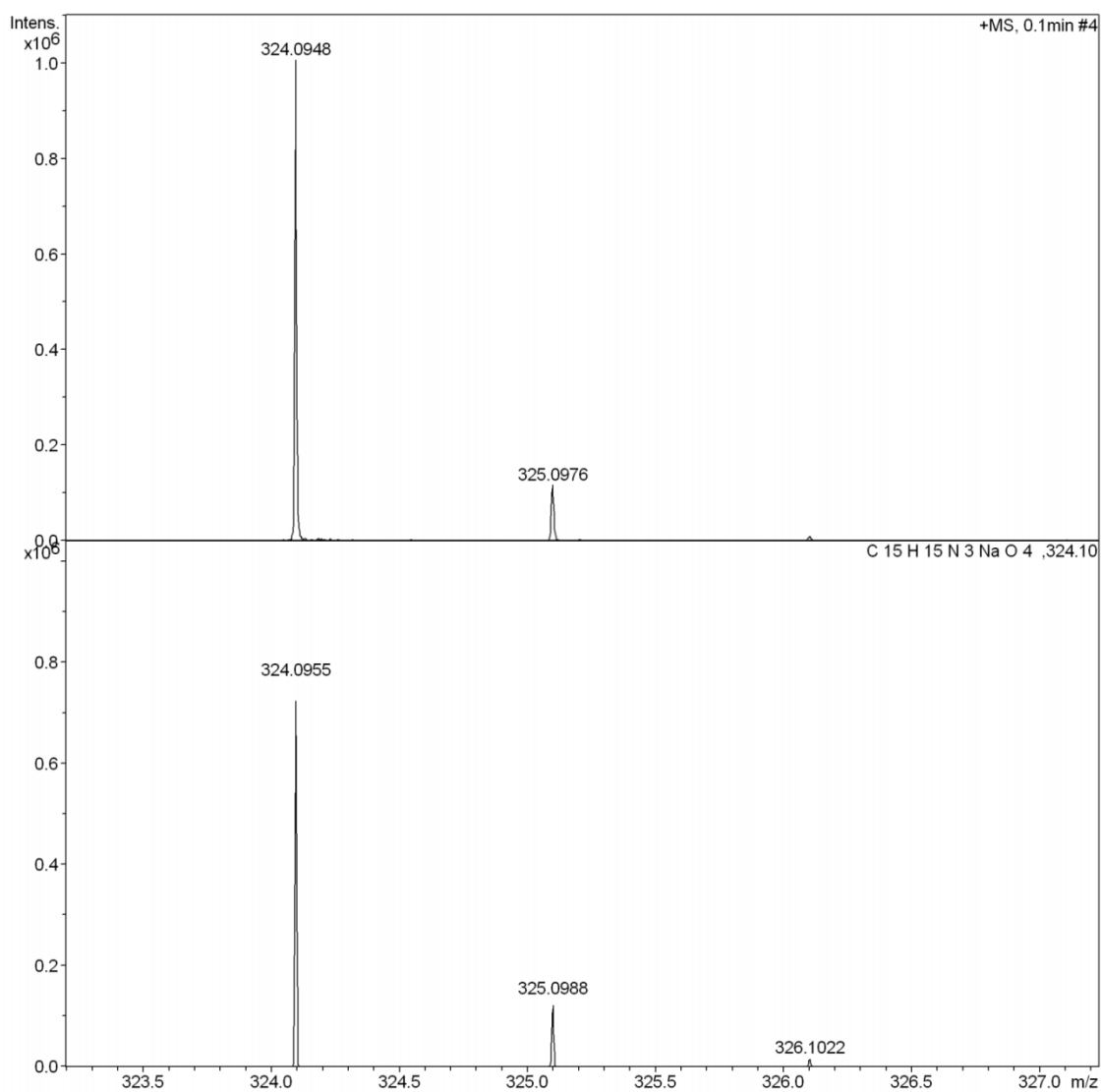
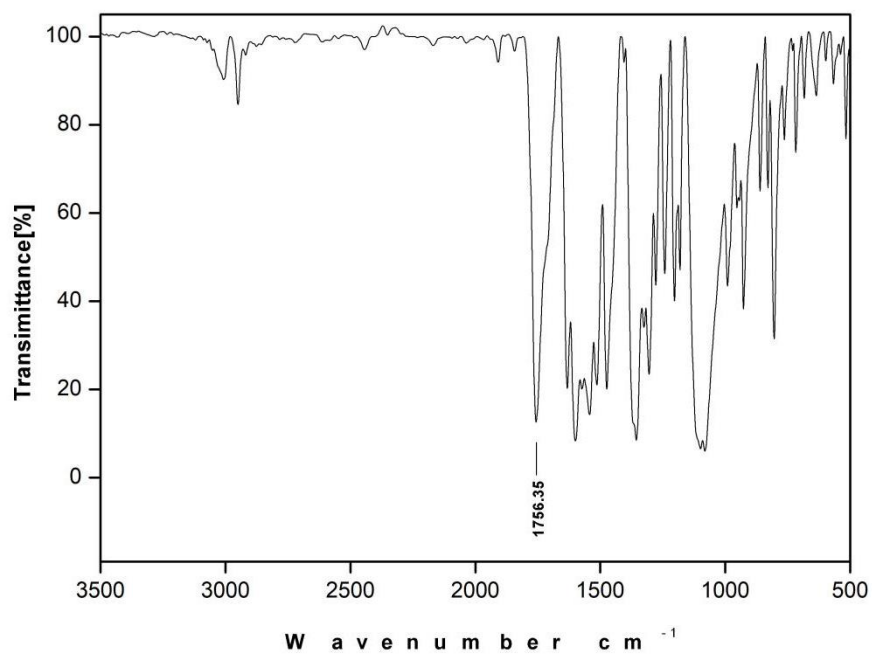
C	-3.22306100	2.93185900	0.21825800
H	-1.22195300	2.36492600	0.67485700
C	-4.33374500	2.74932500	-0.61642600
H	-5.08884500	1.67768400	-2.34326200
H	-3.28737100	3.66530200	1.01661200
O	-5.42721300	3.52063900	-0.33526500
C	-6.57790500	3.34795000	-1.14201500
H	-6.95711000	2.31839000	-1.08745900
H	-7.33048900	4.03196600	-0.74559900
H	-6.37737200	3.59879800	-2.19239800

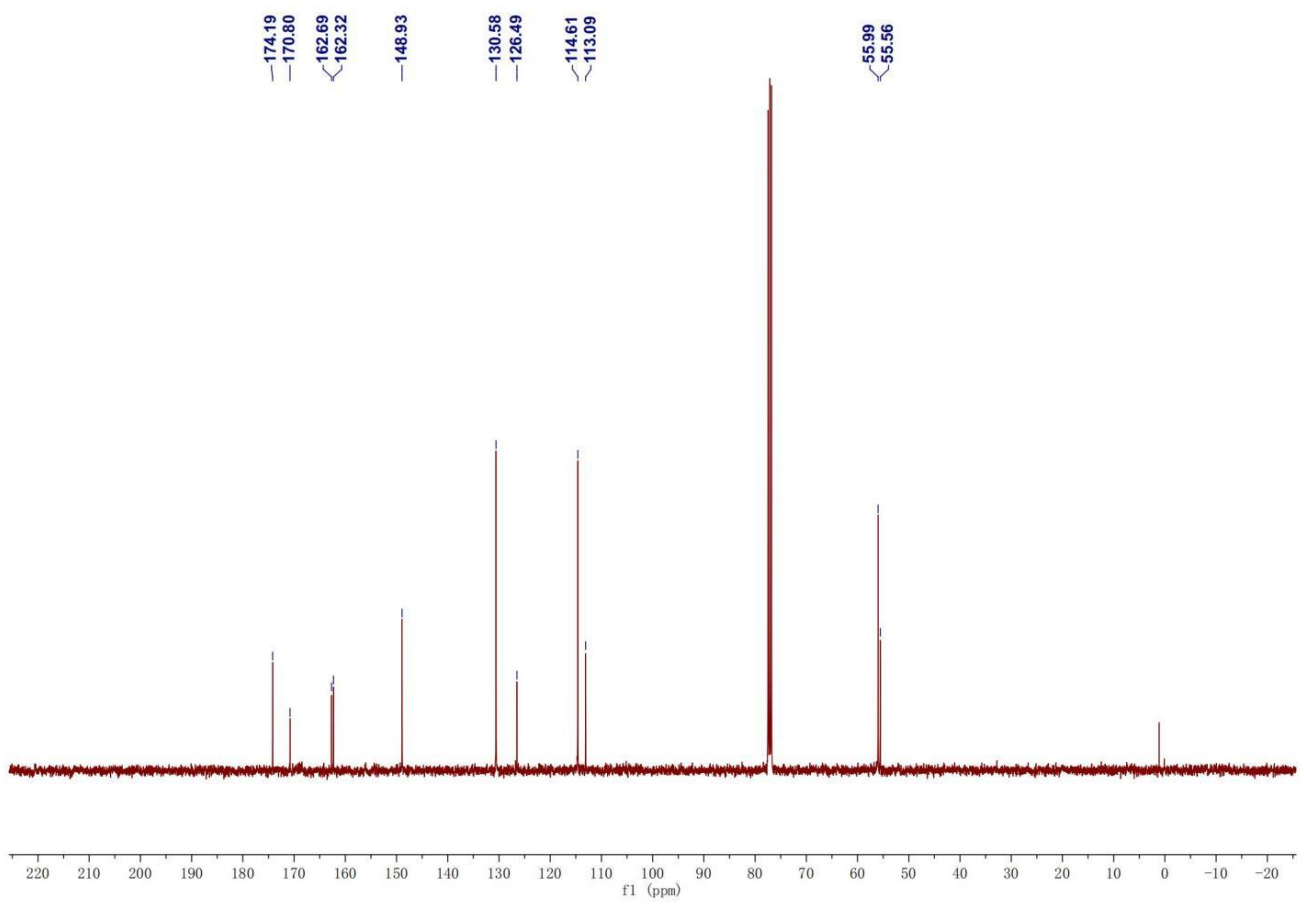
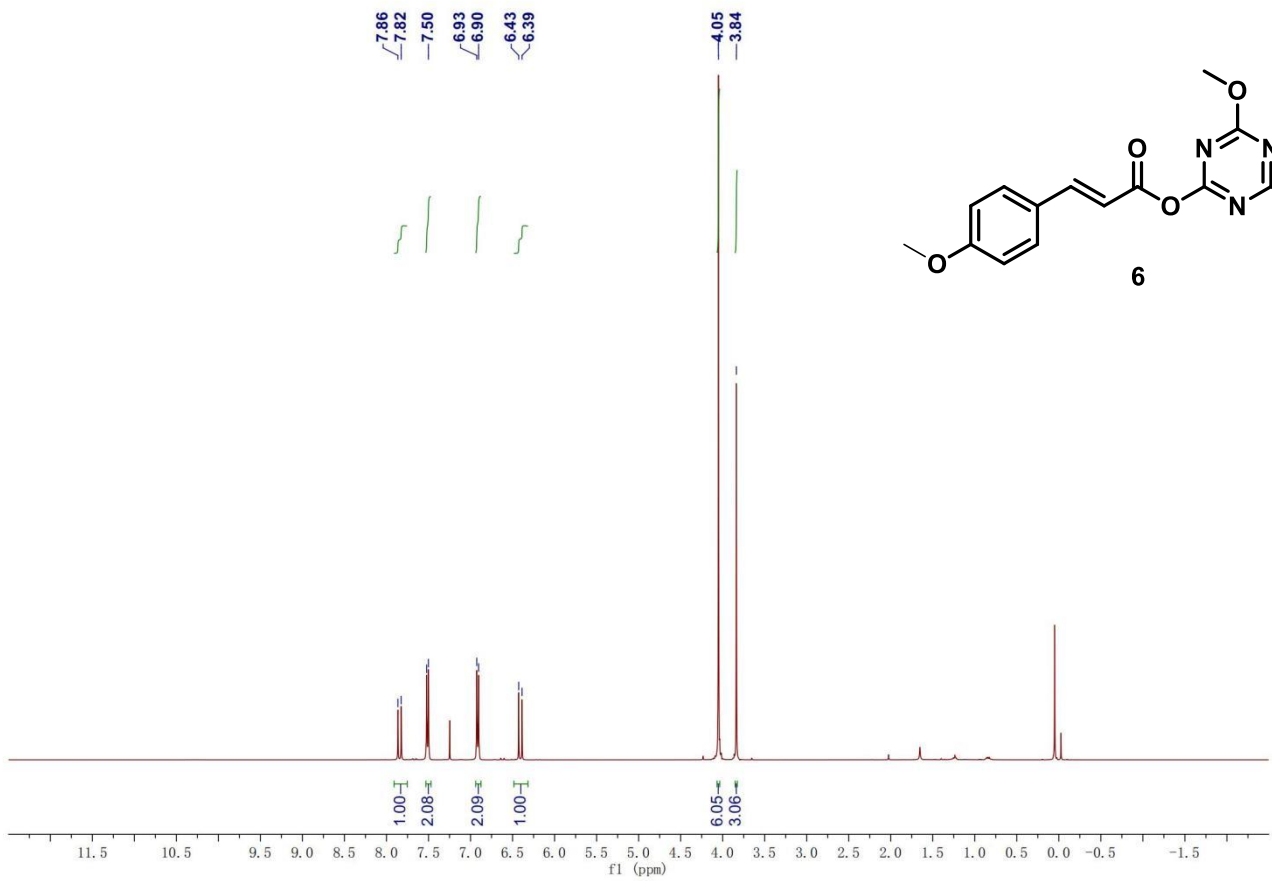
9. NMR Spectra of products: ^1H NMR, ^{13}C NMR, IR and HRMS

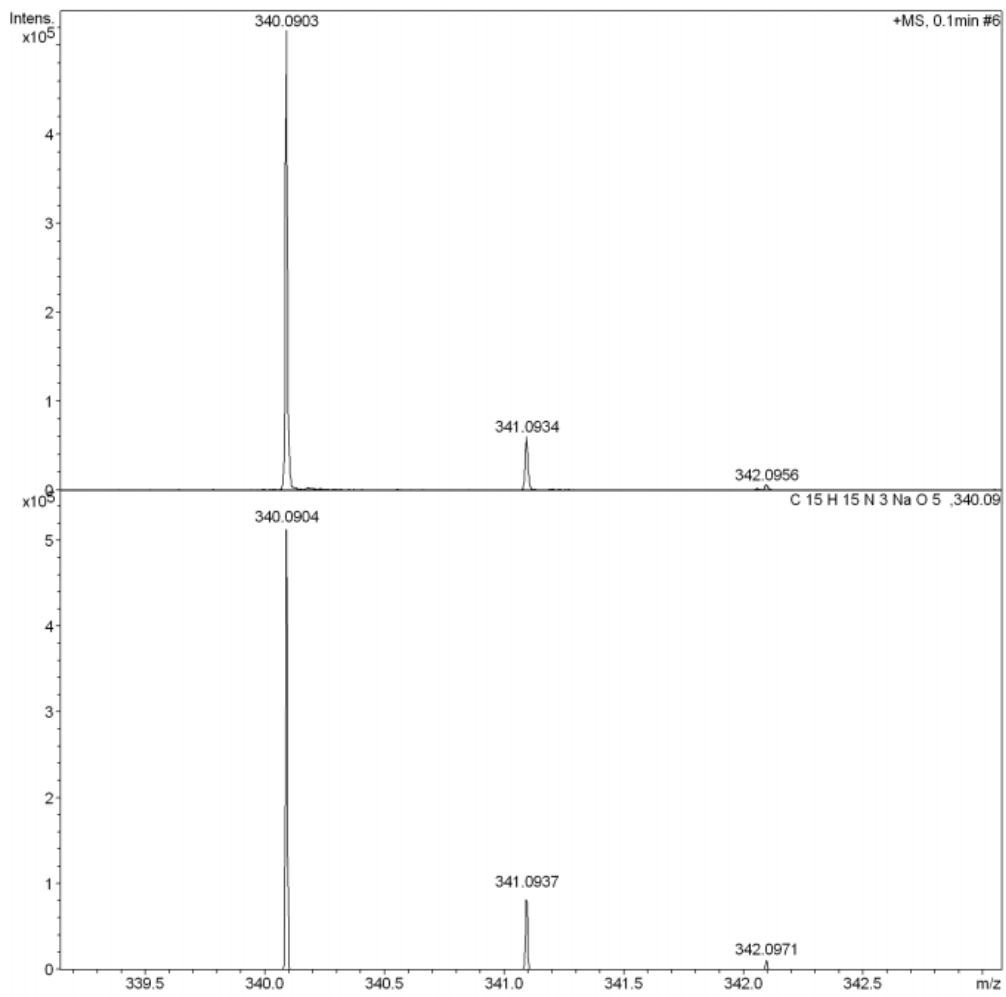
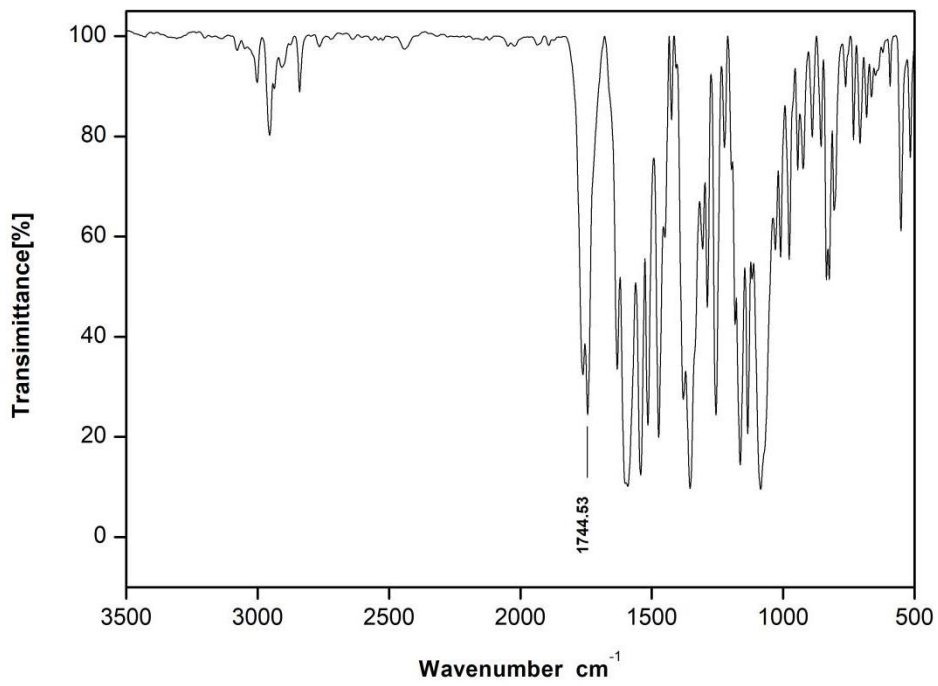


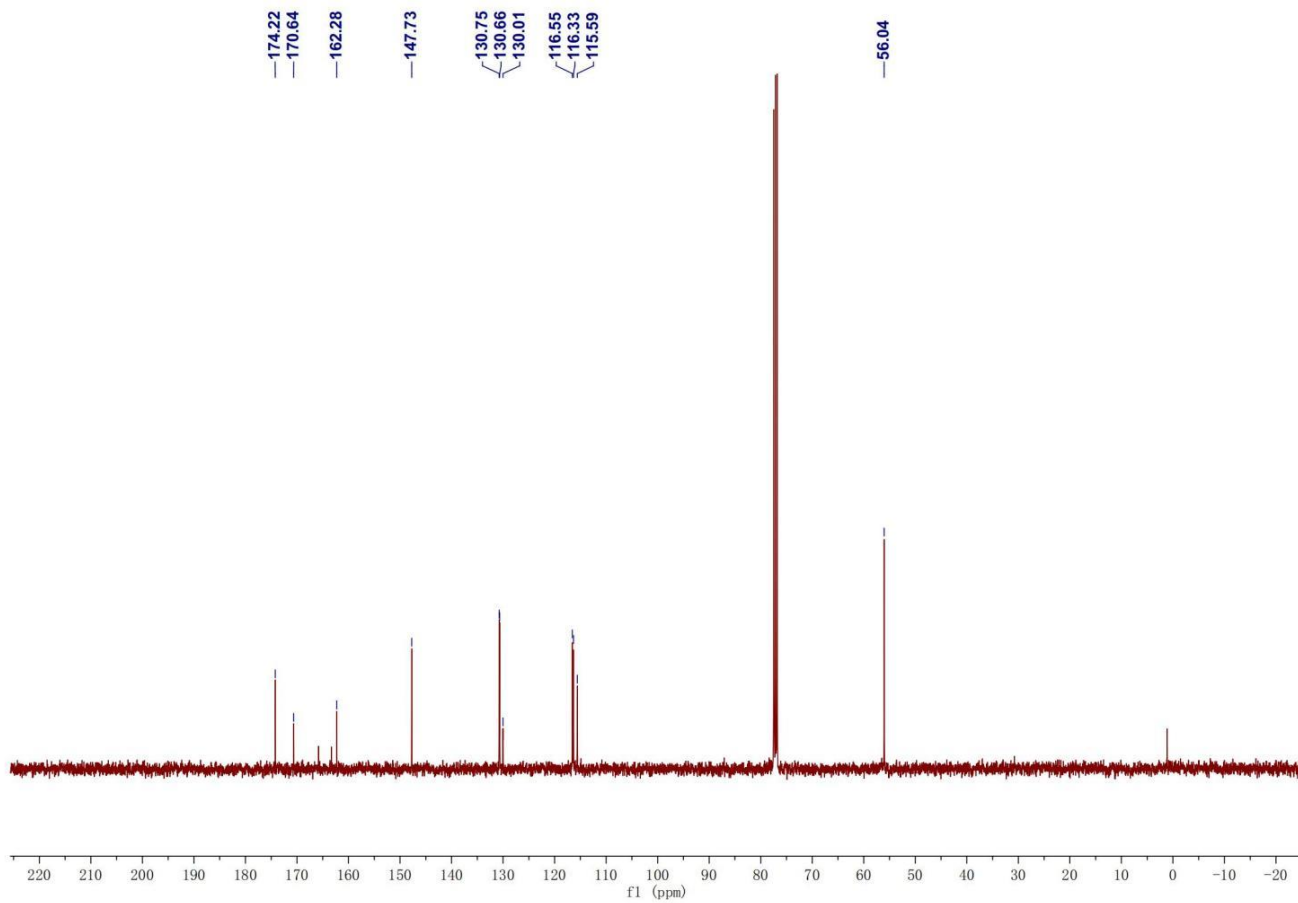
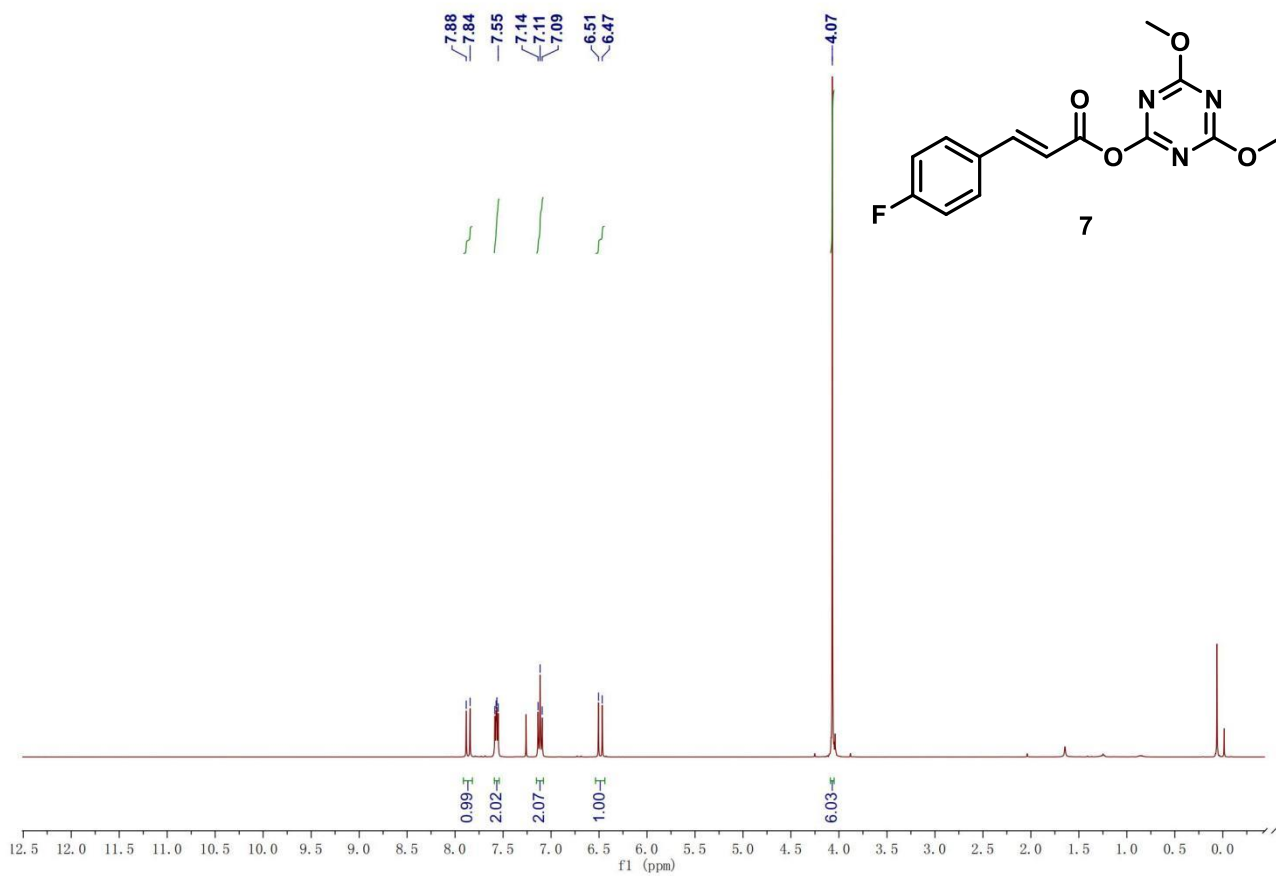


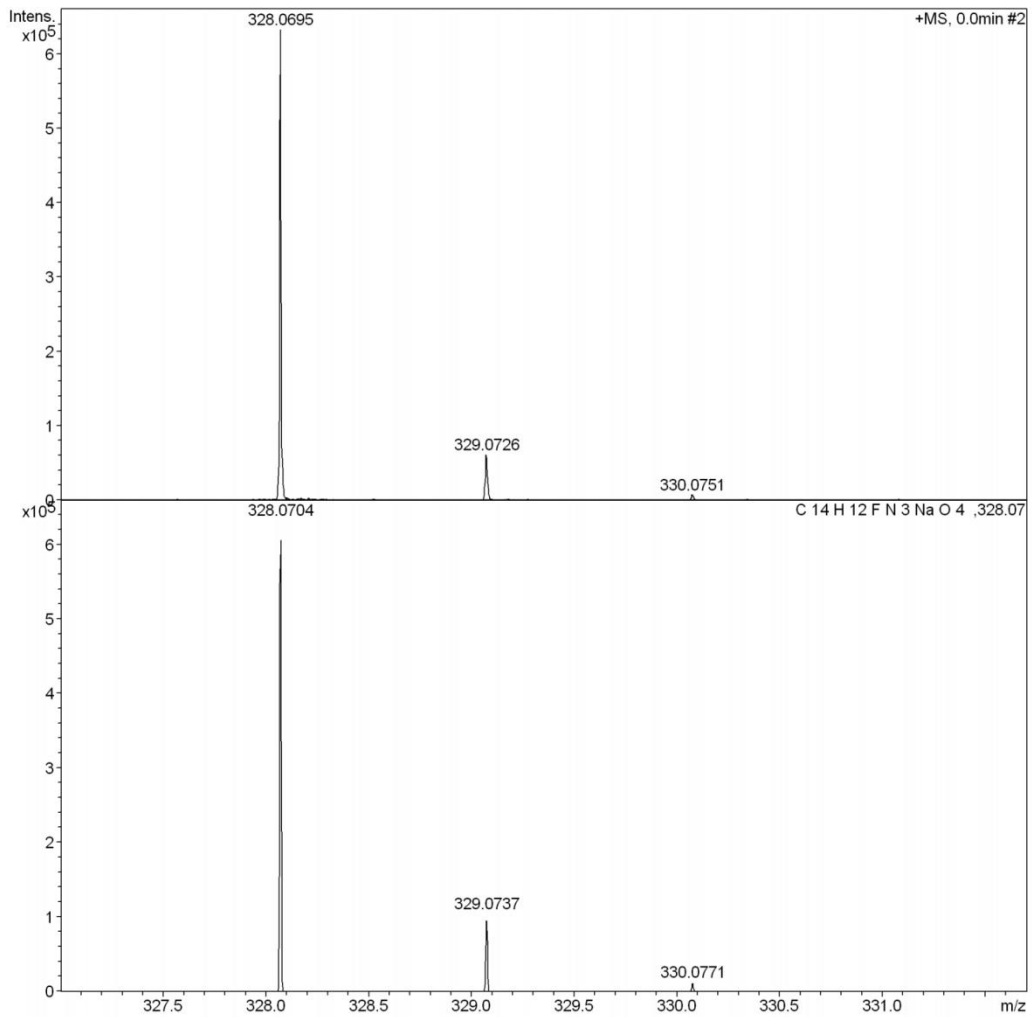
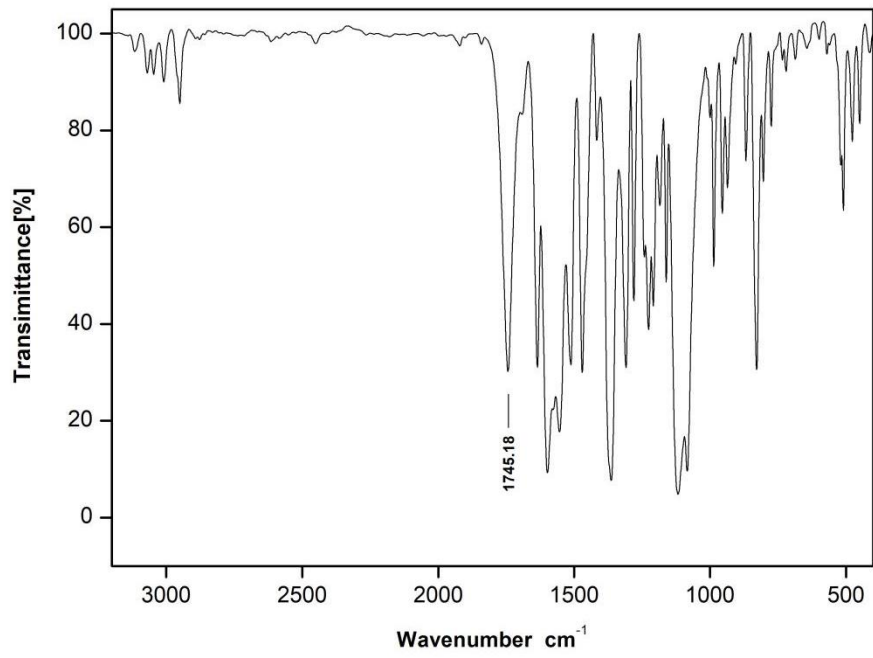


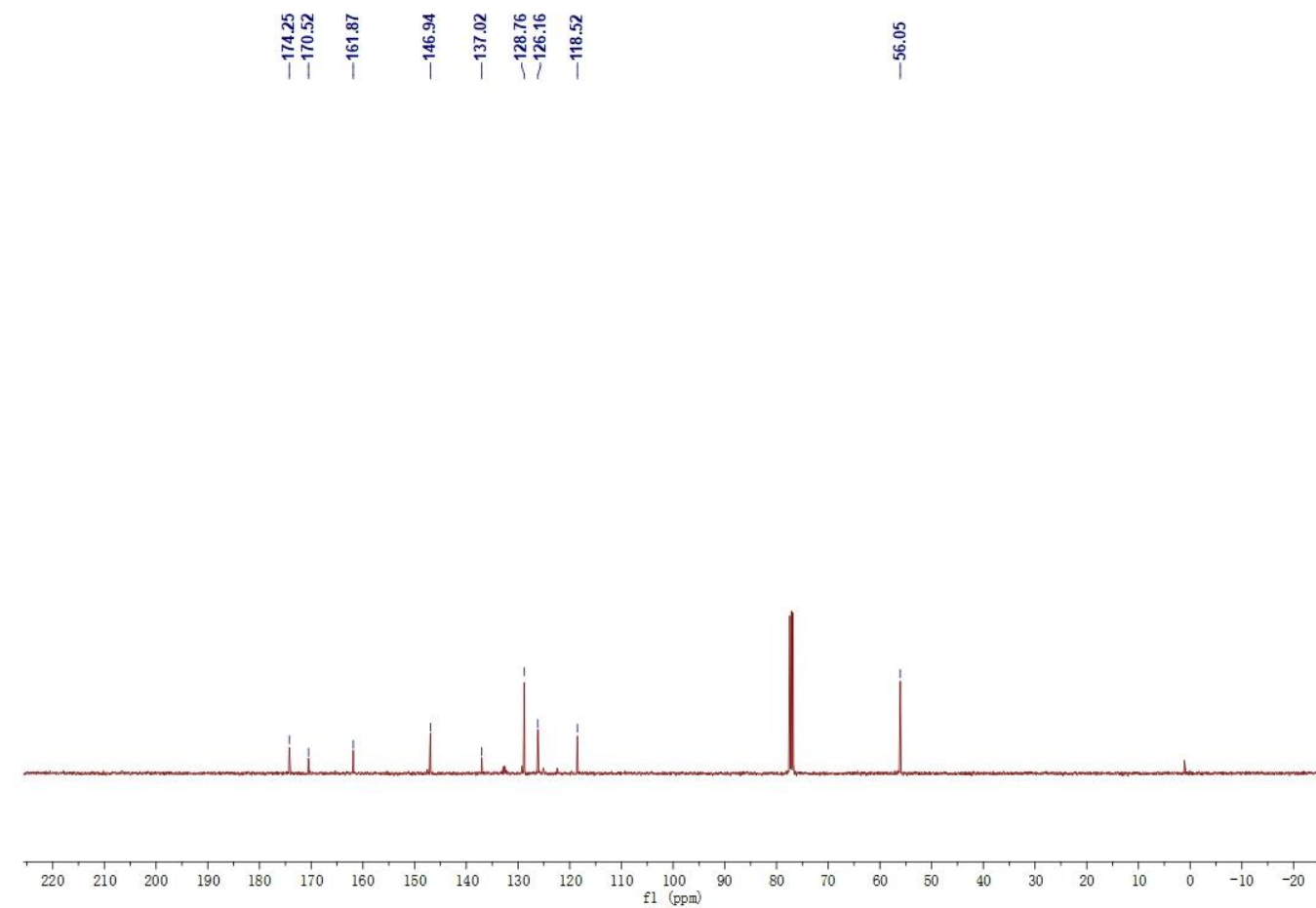
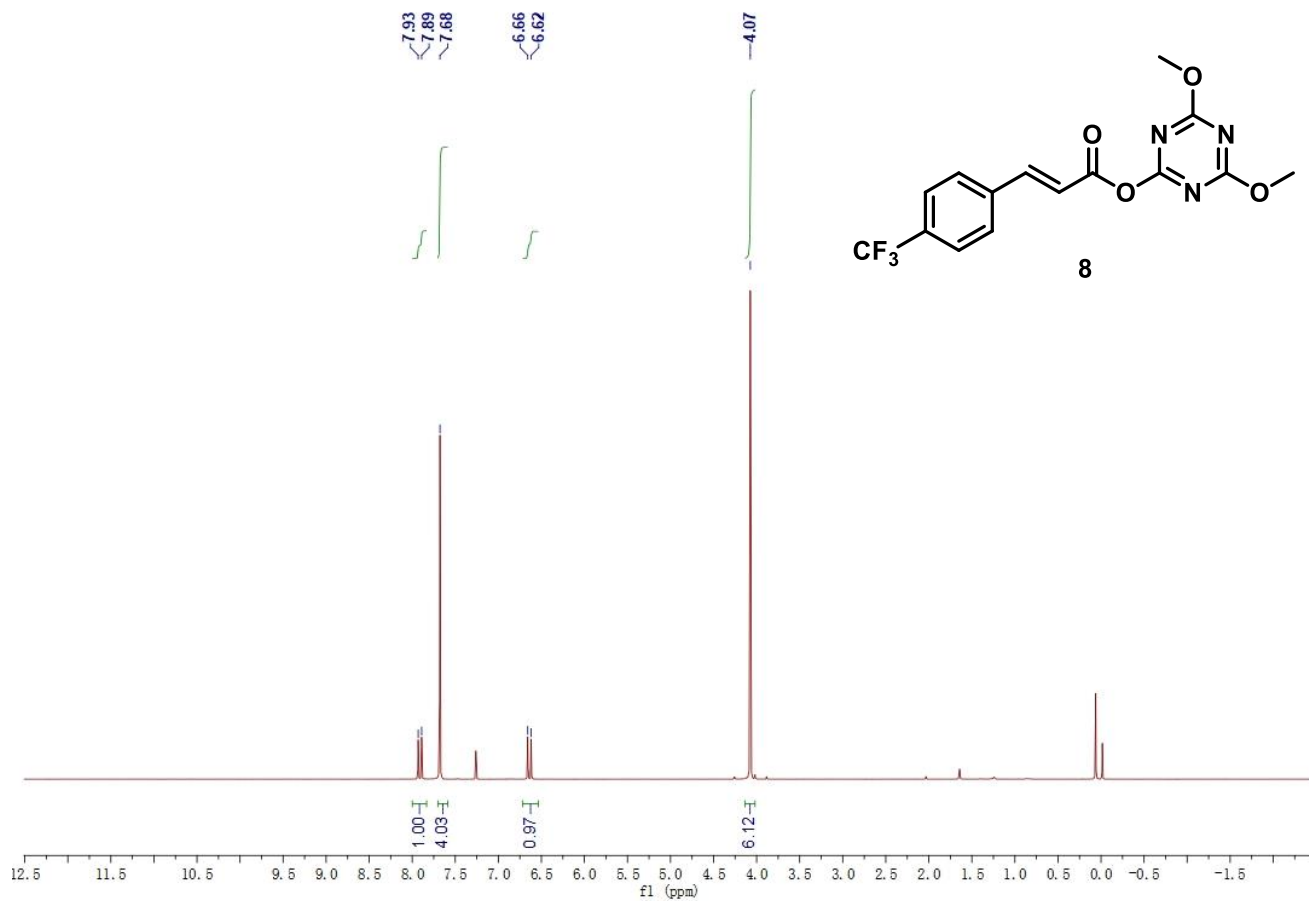


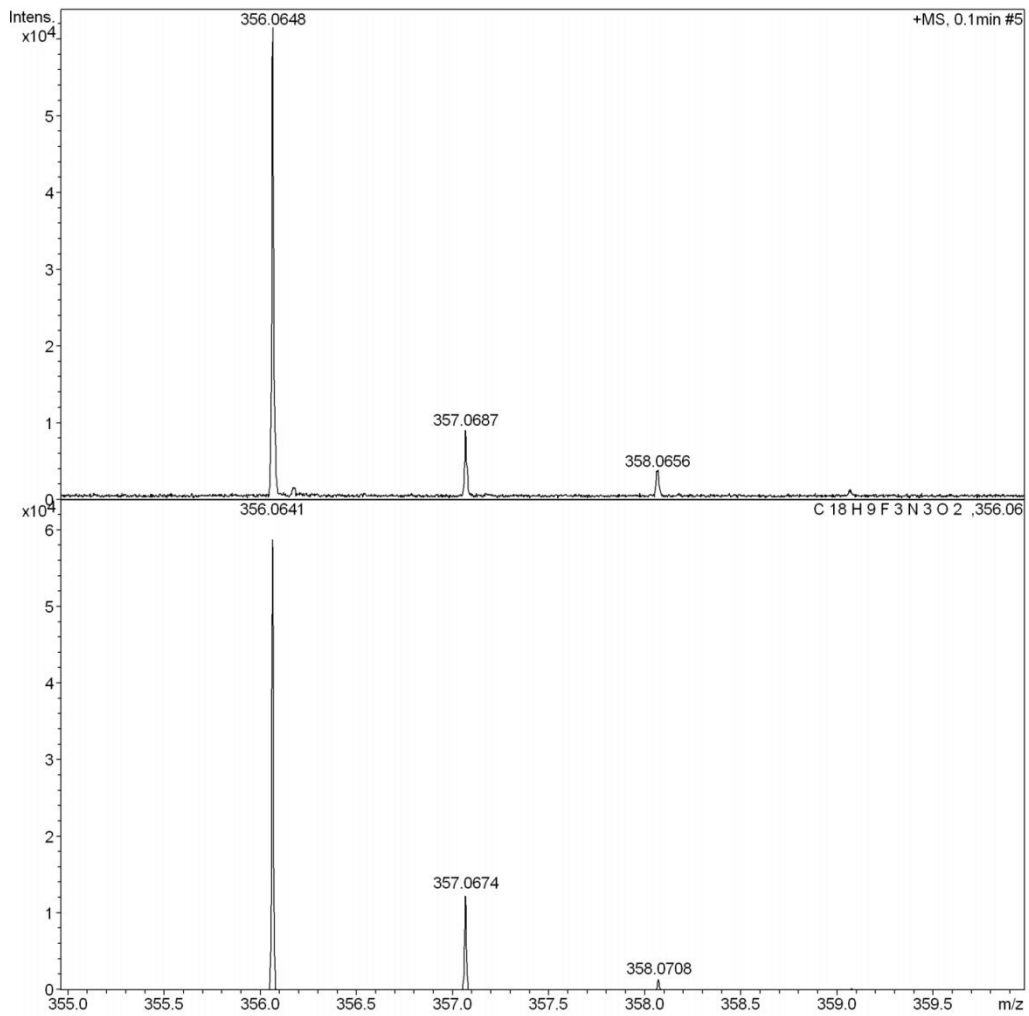
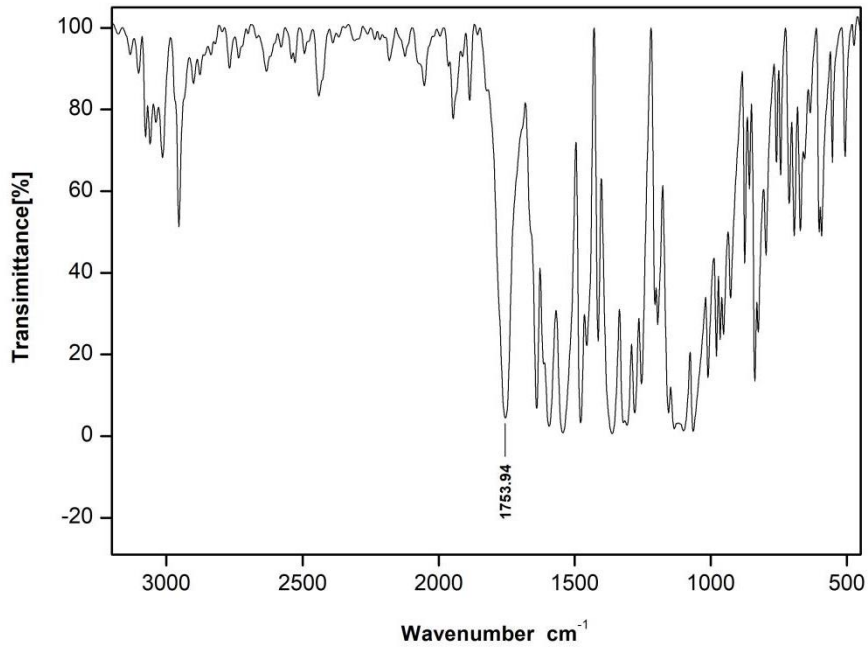


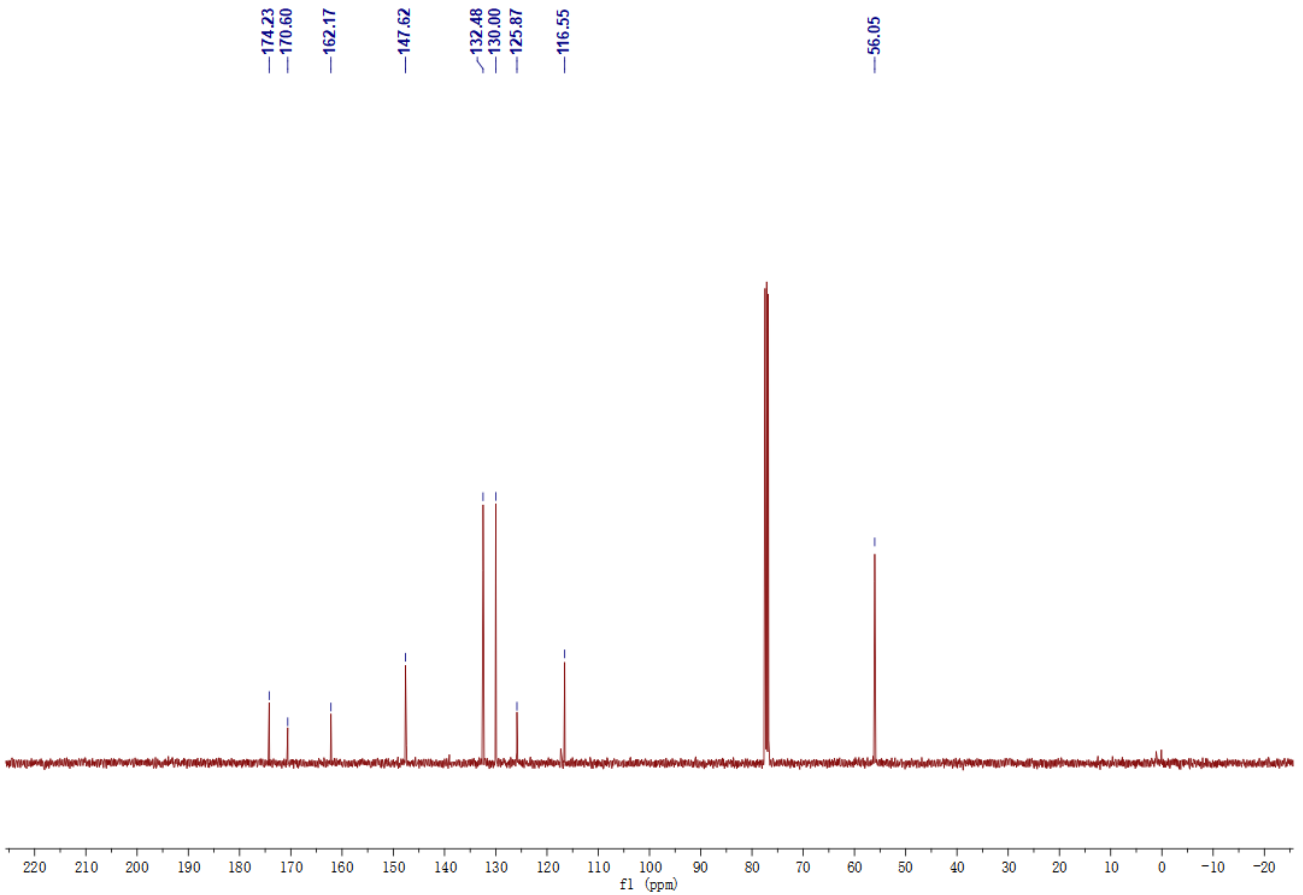
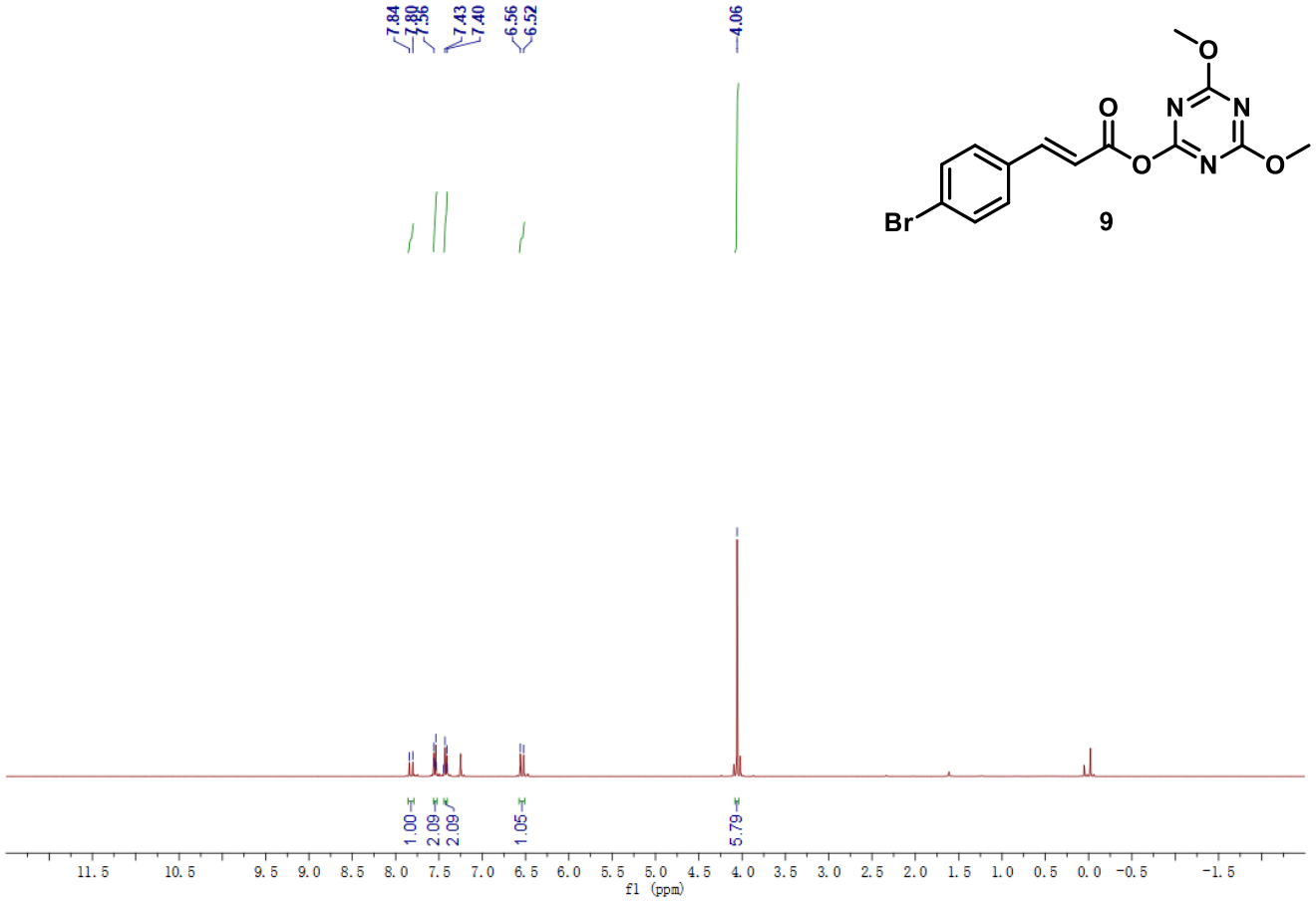
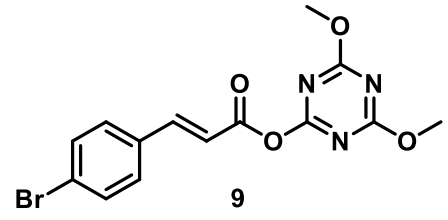


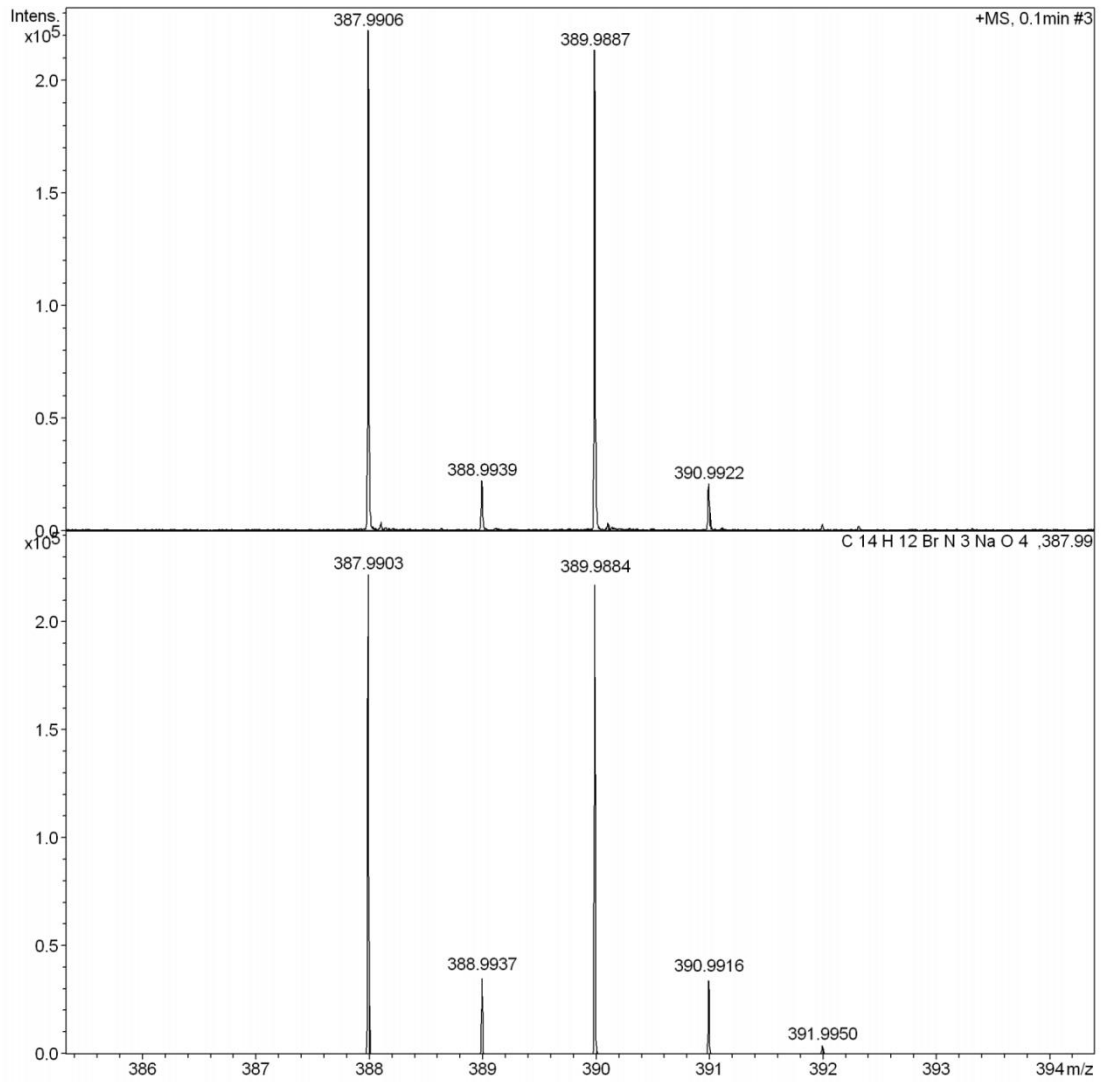
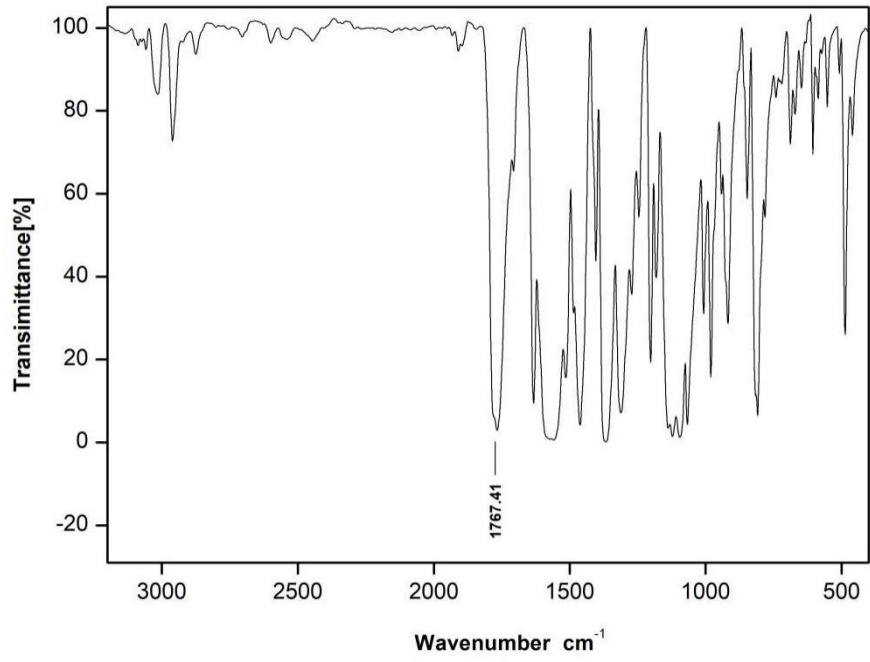


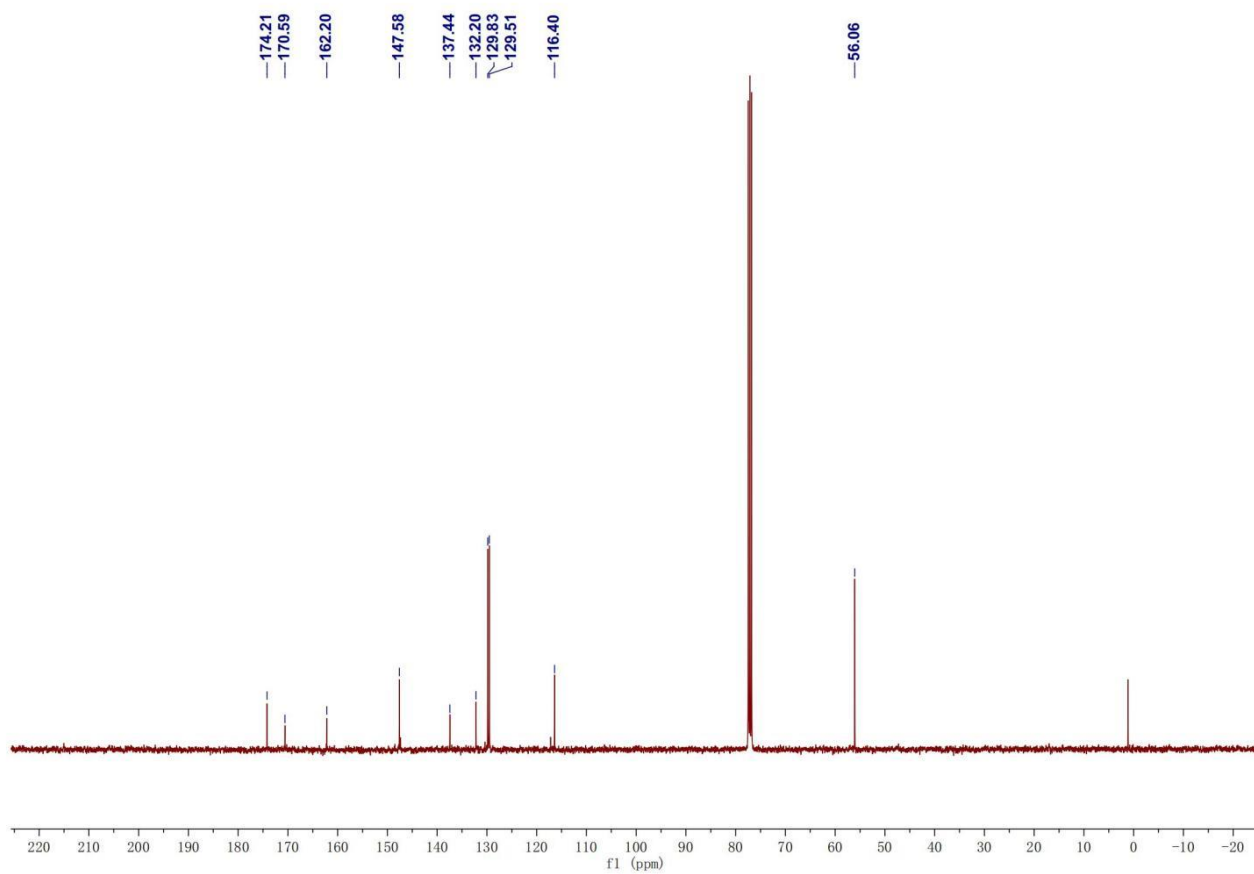
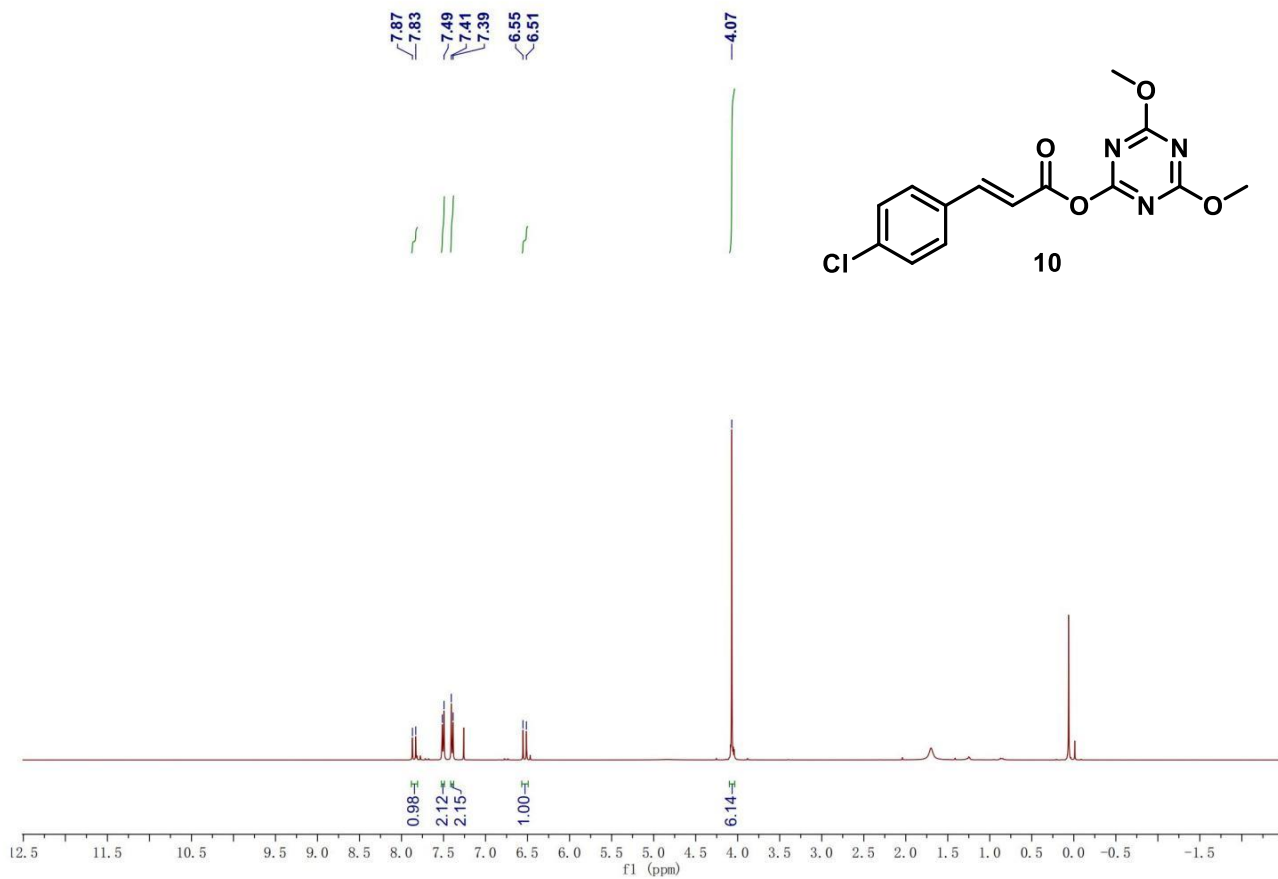


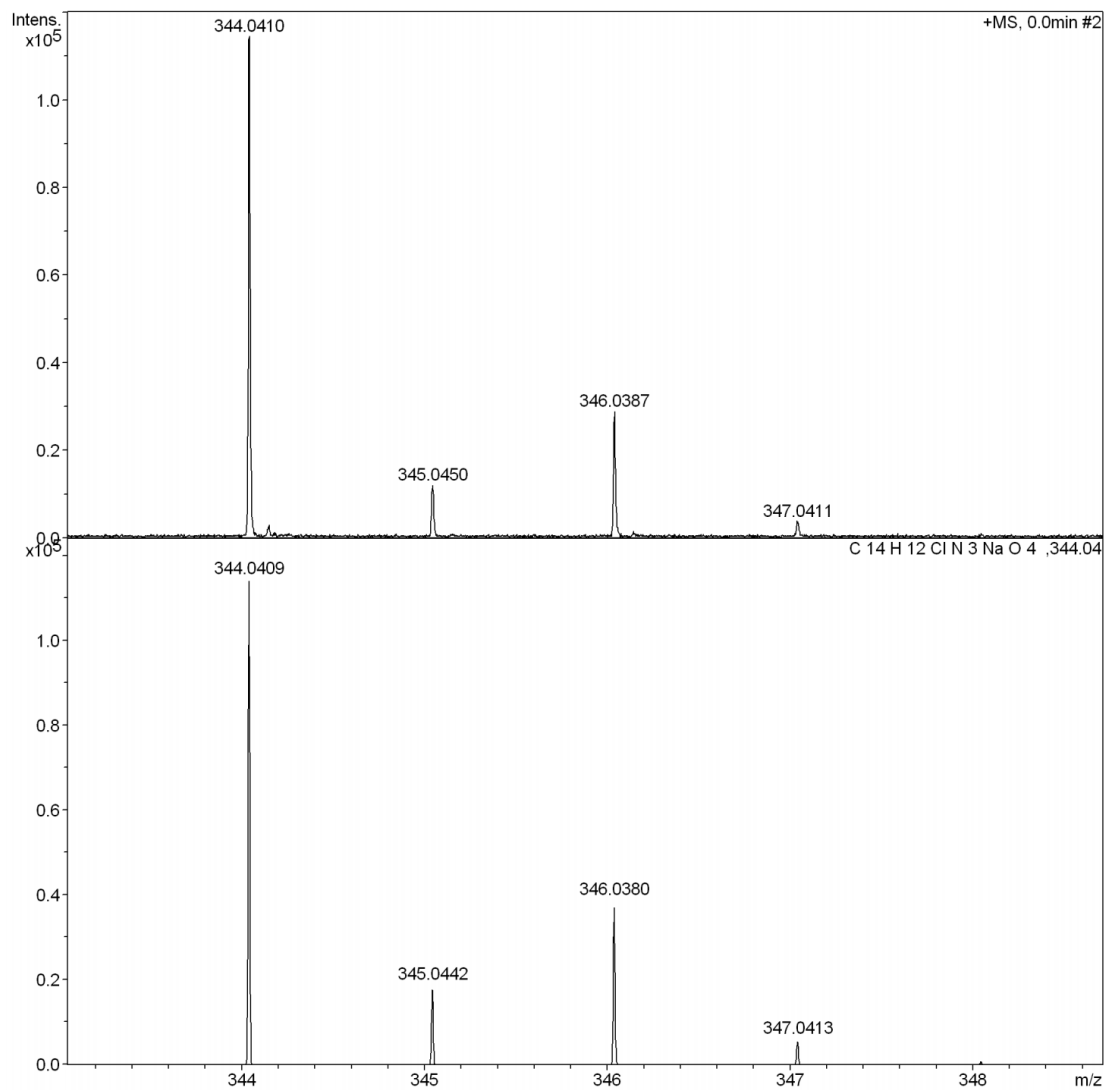
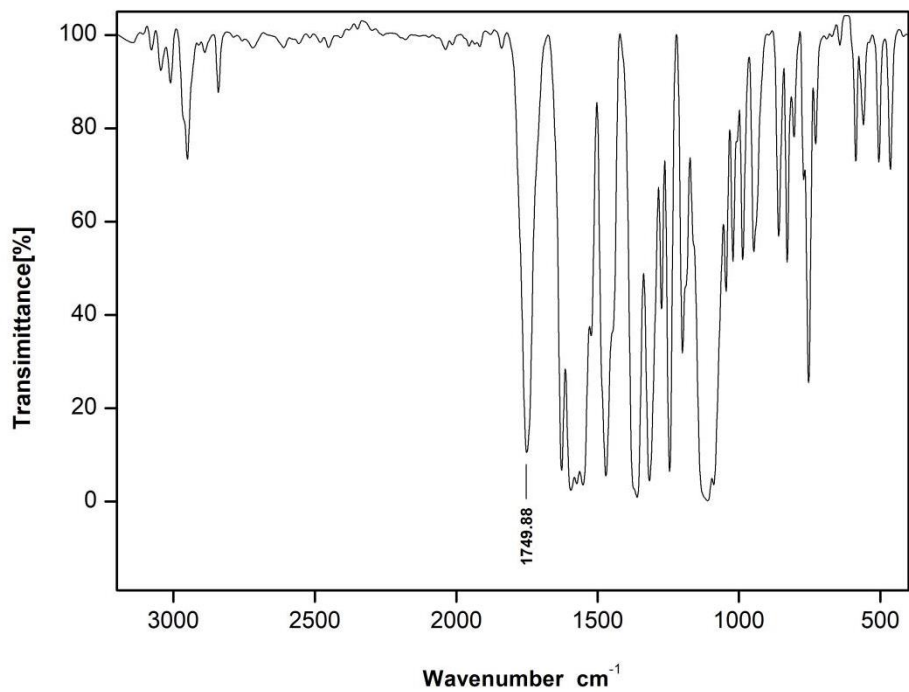


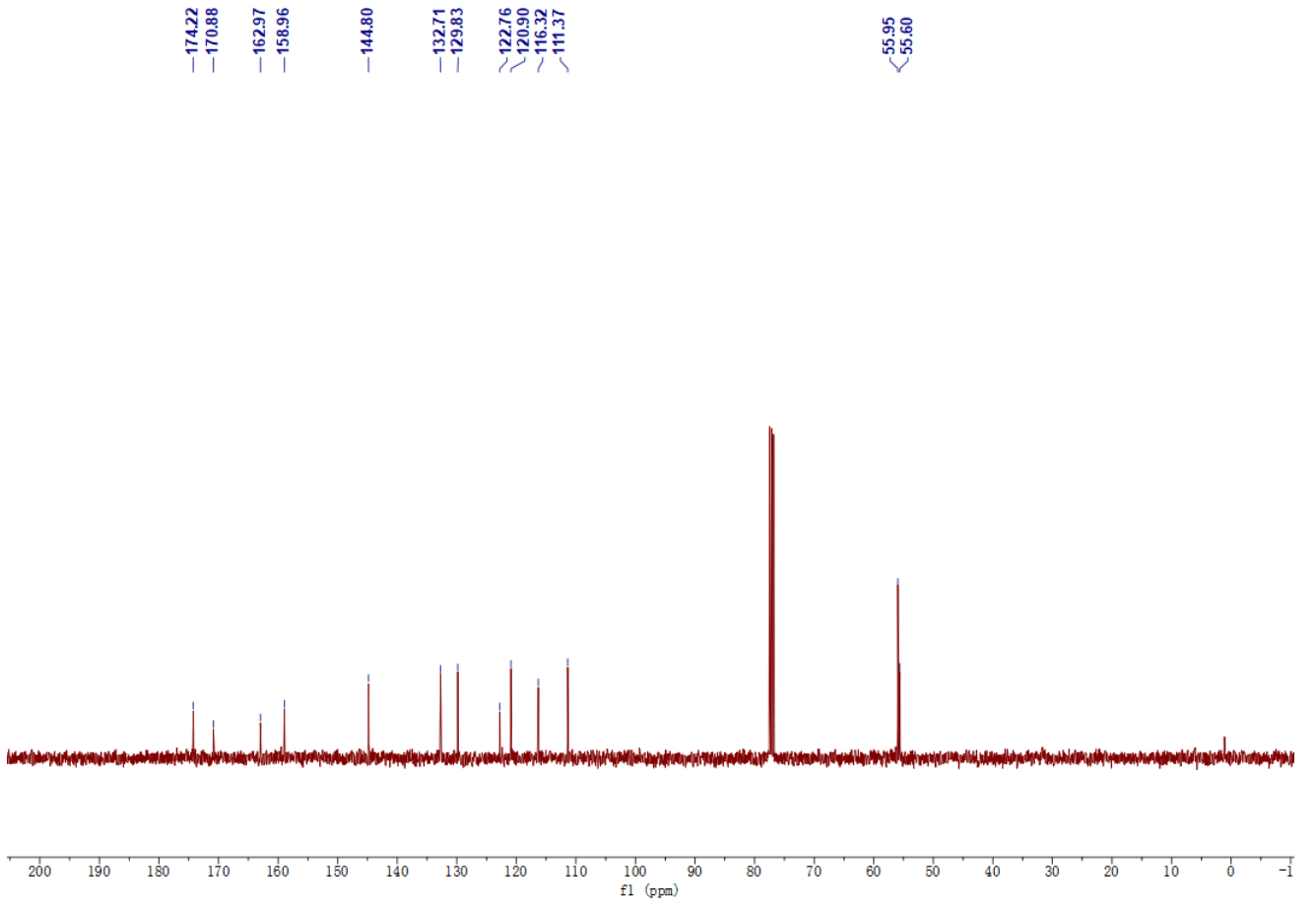
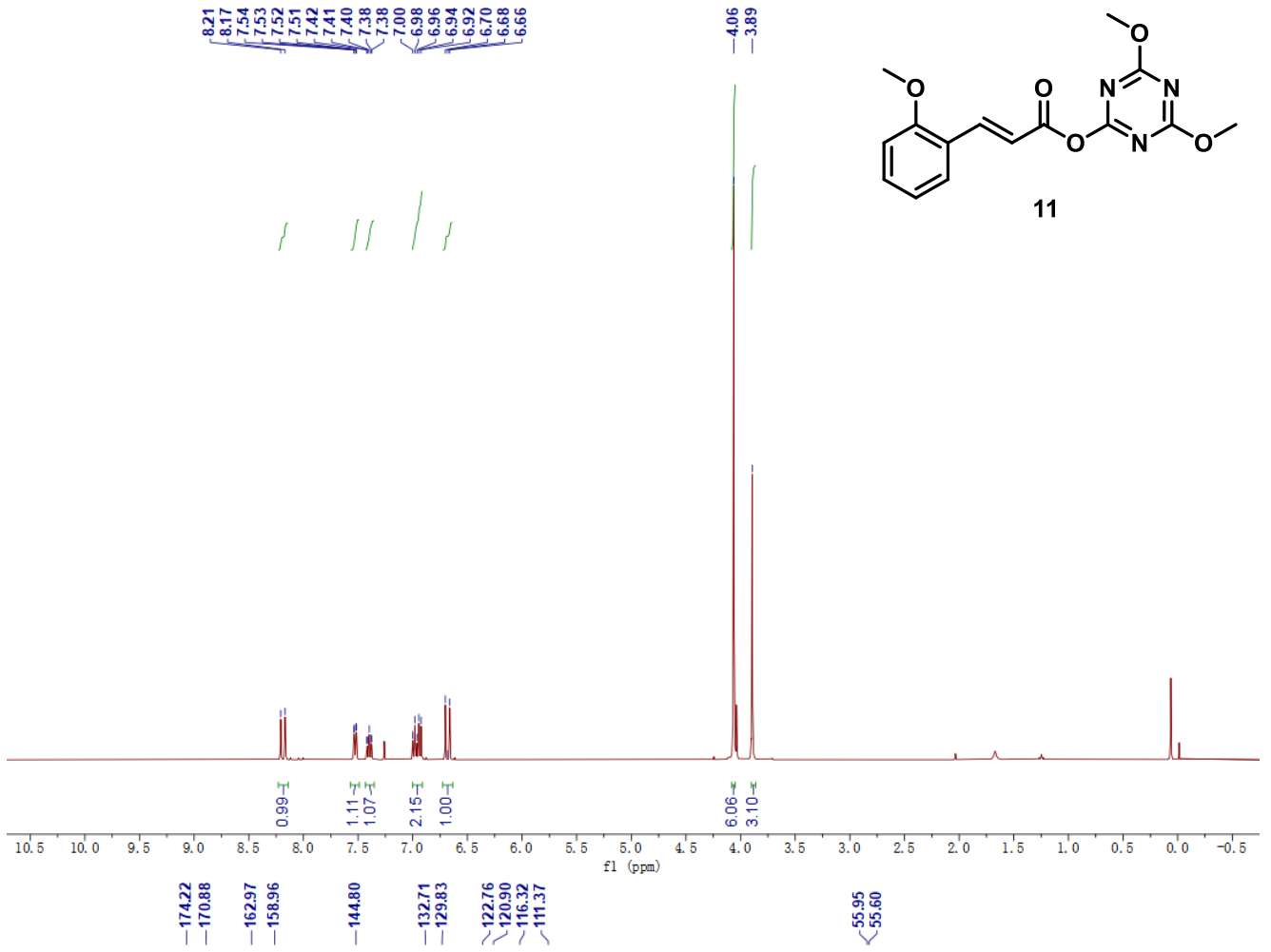


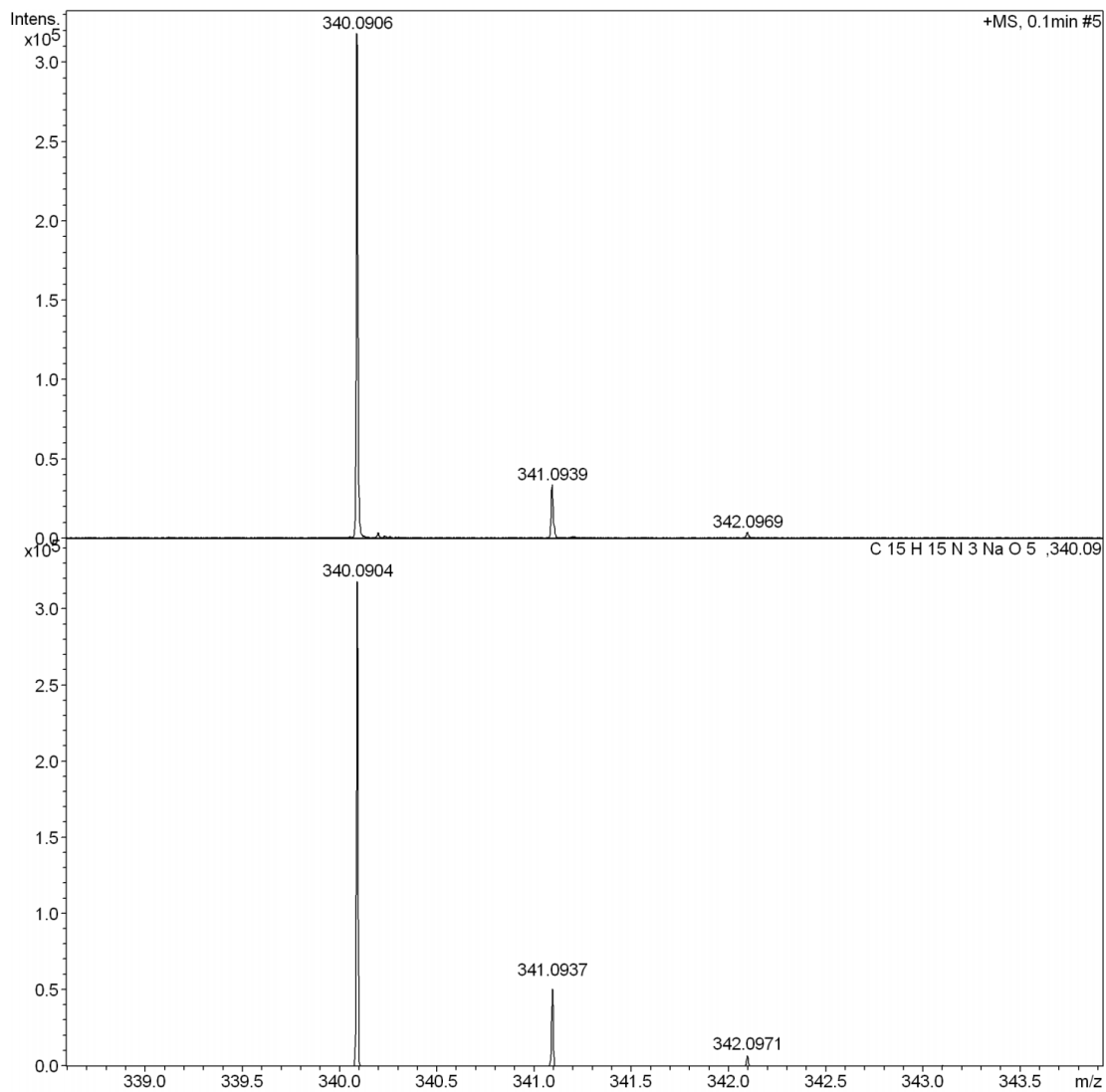
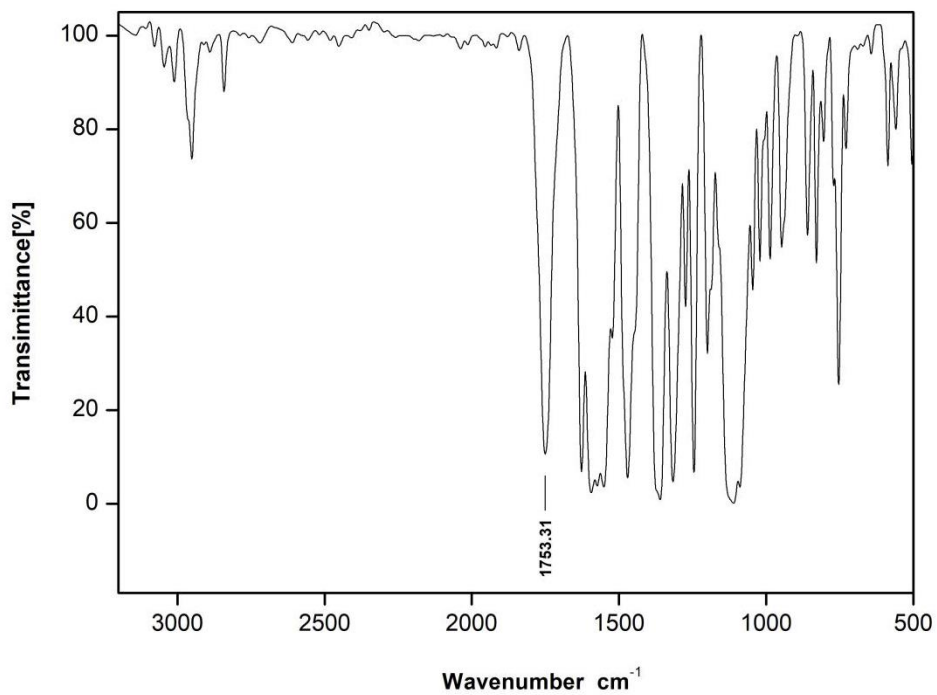


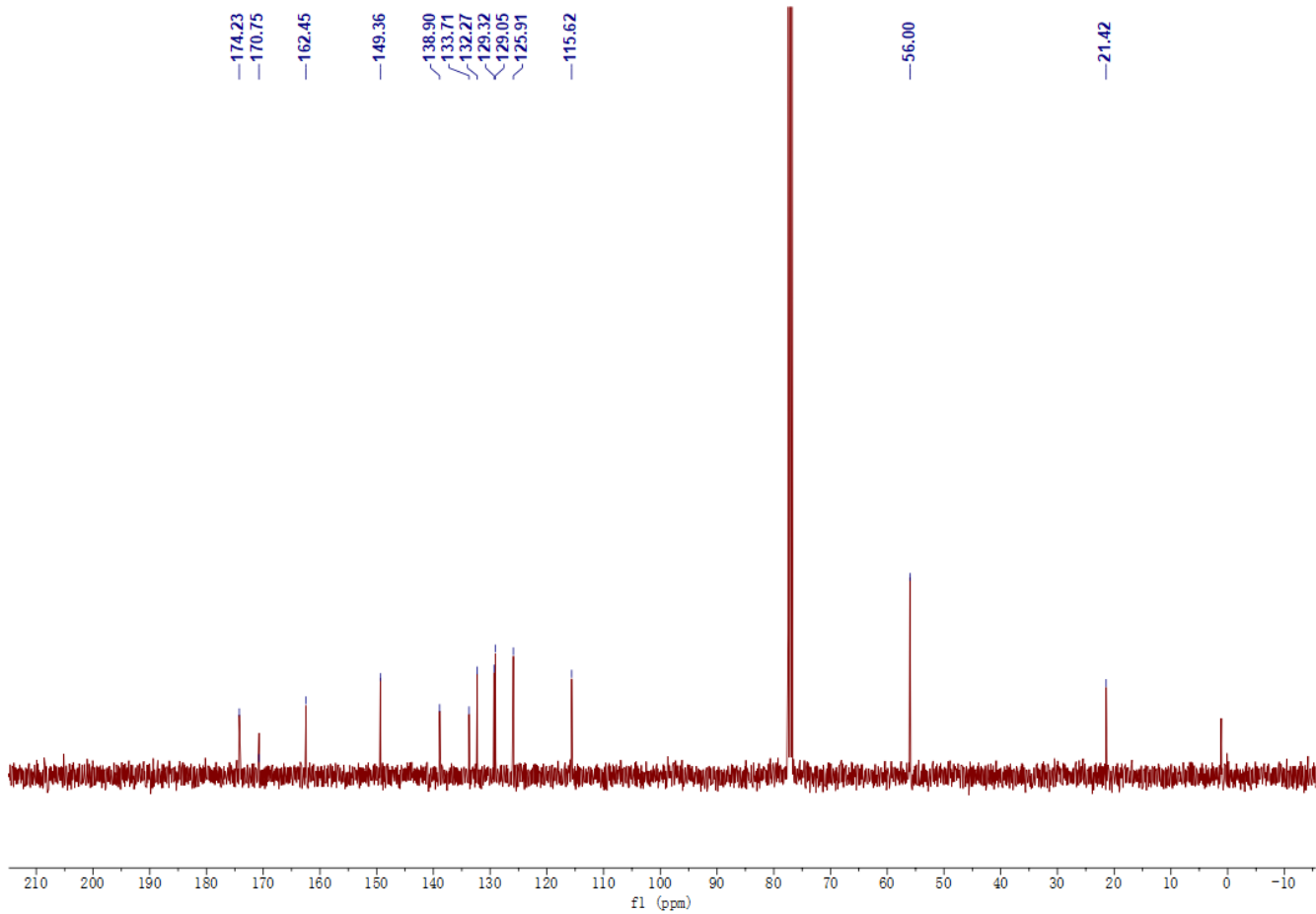
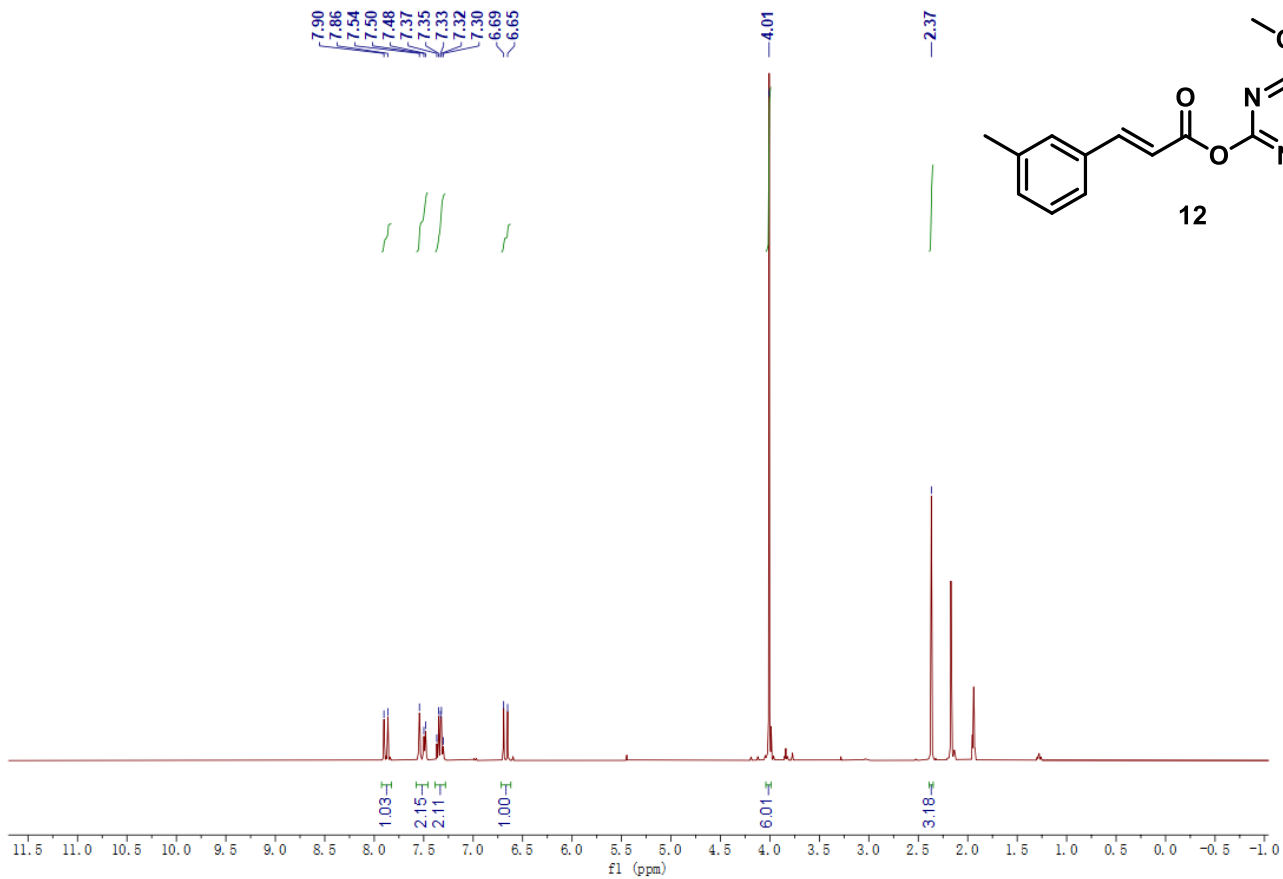


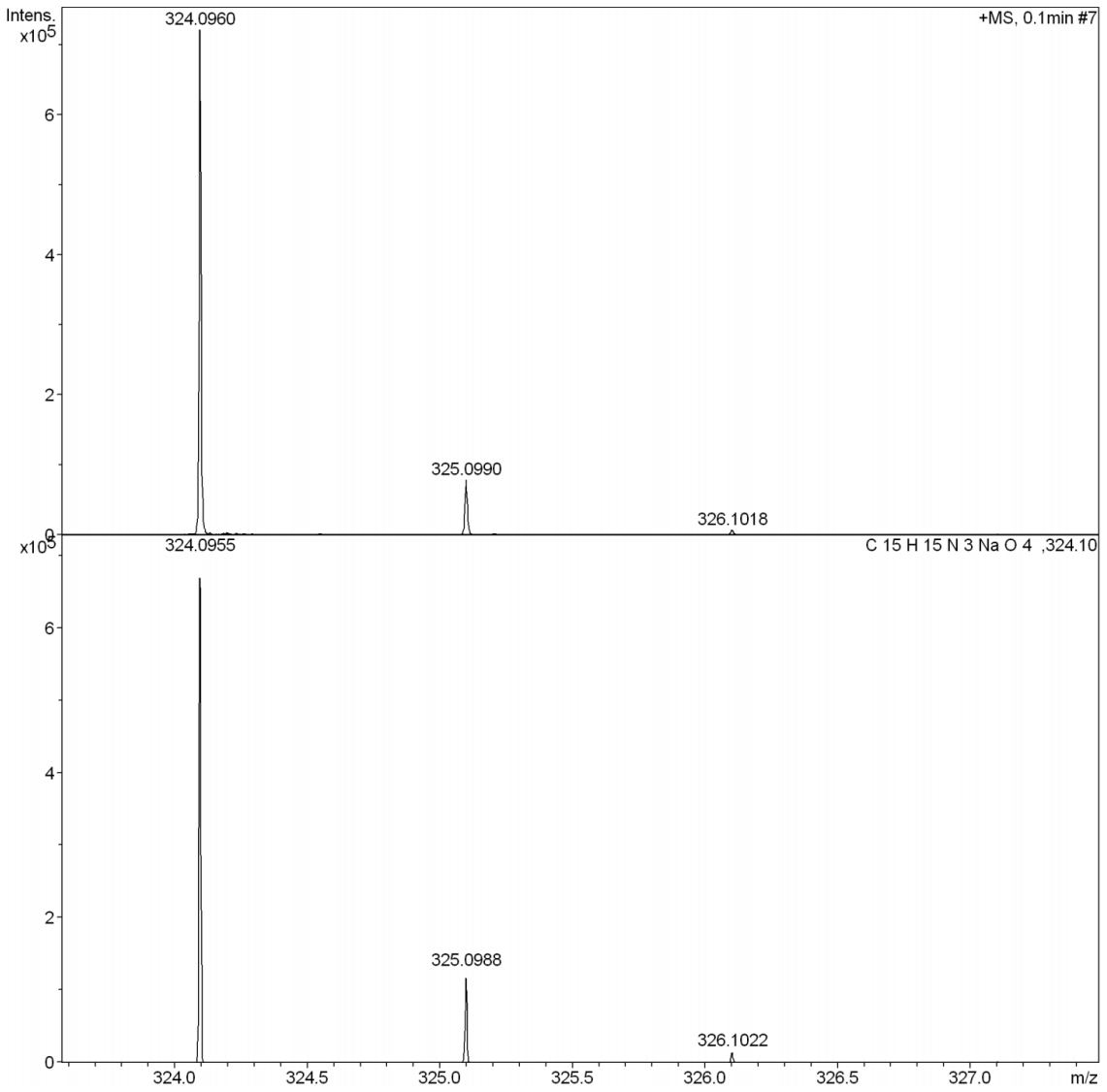
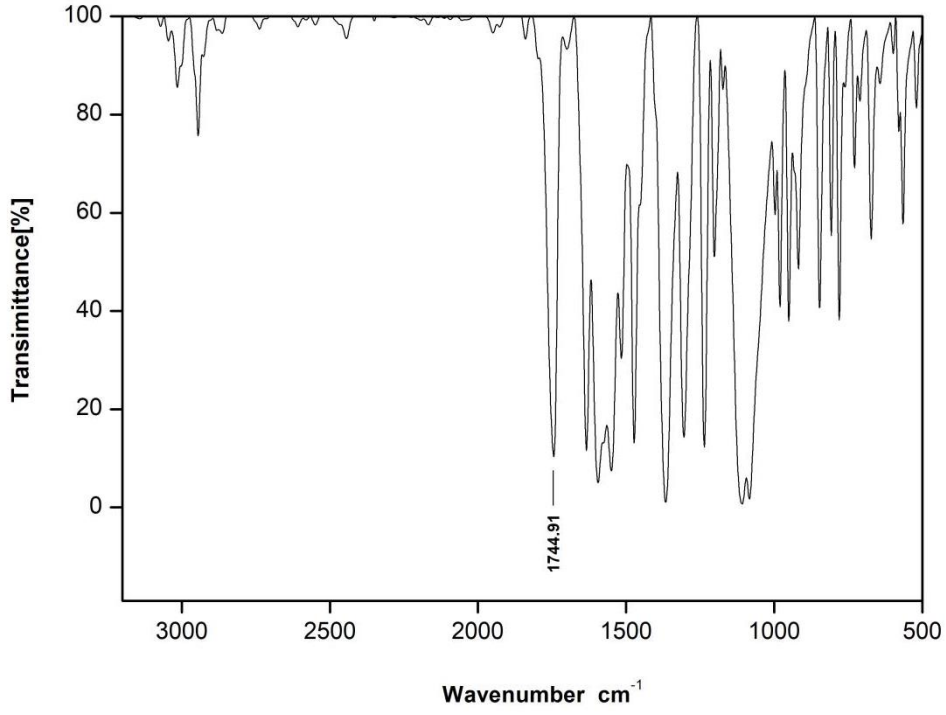


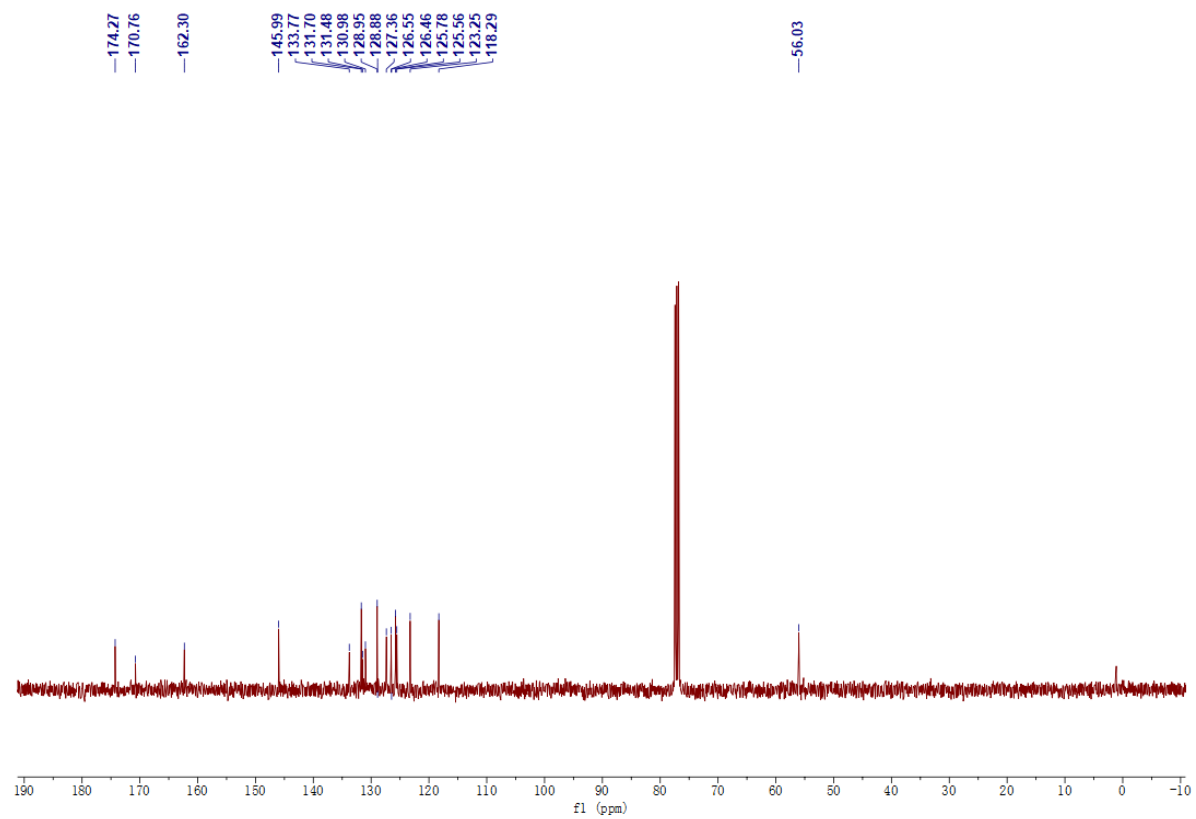
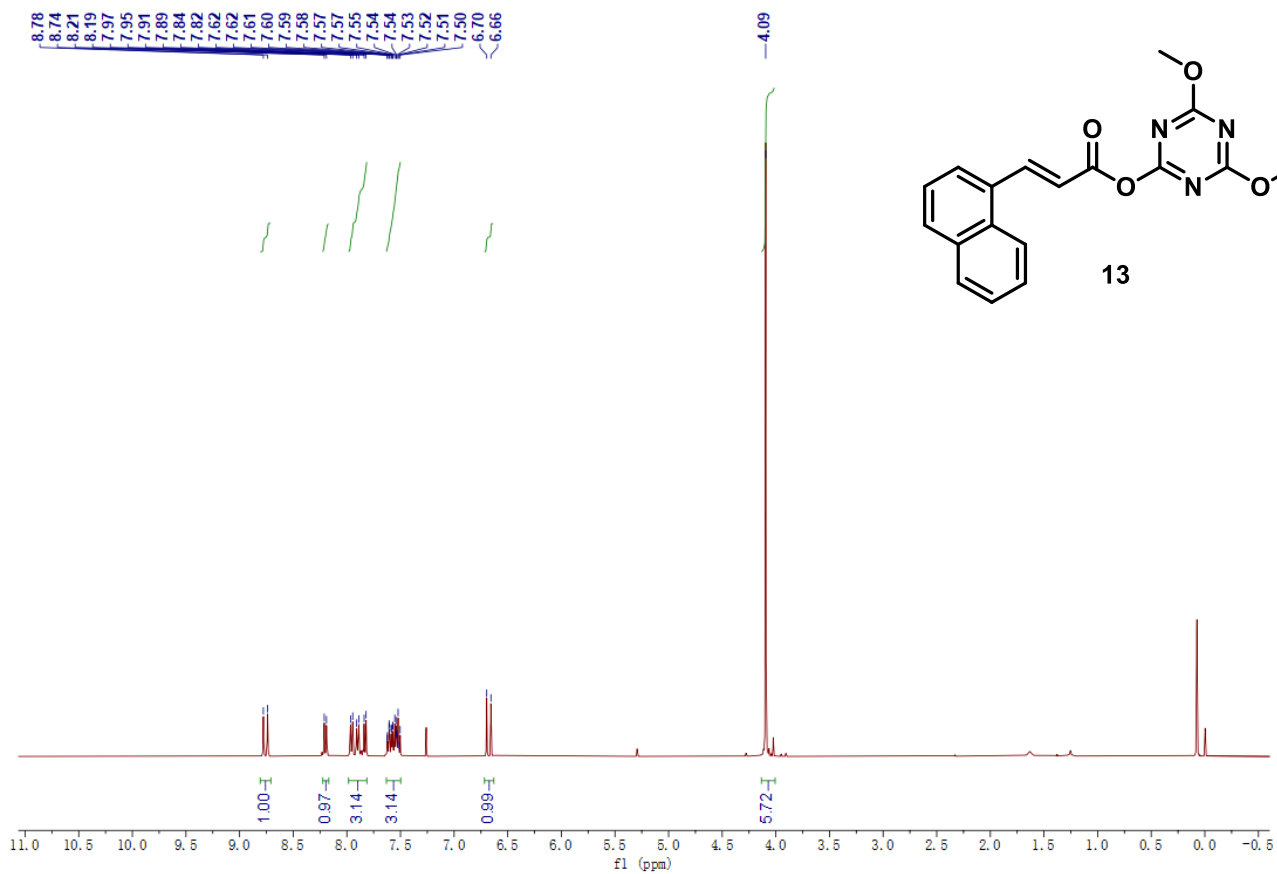


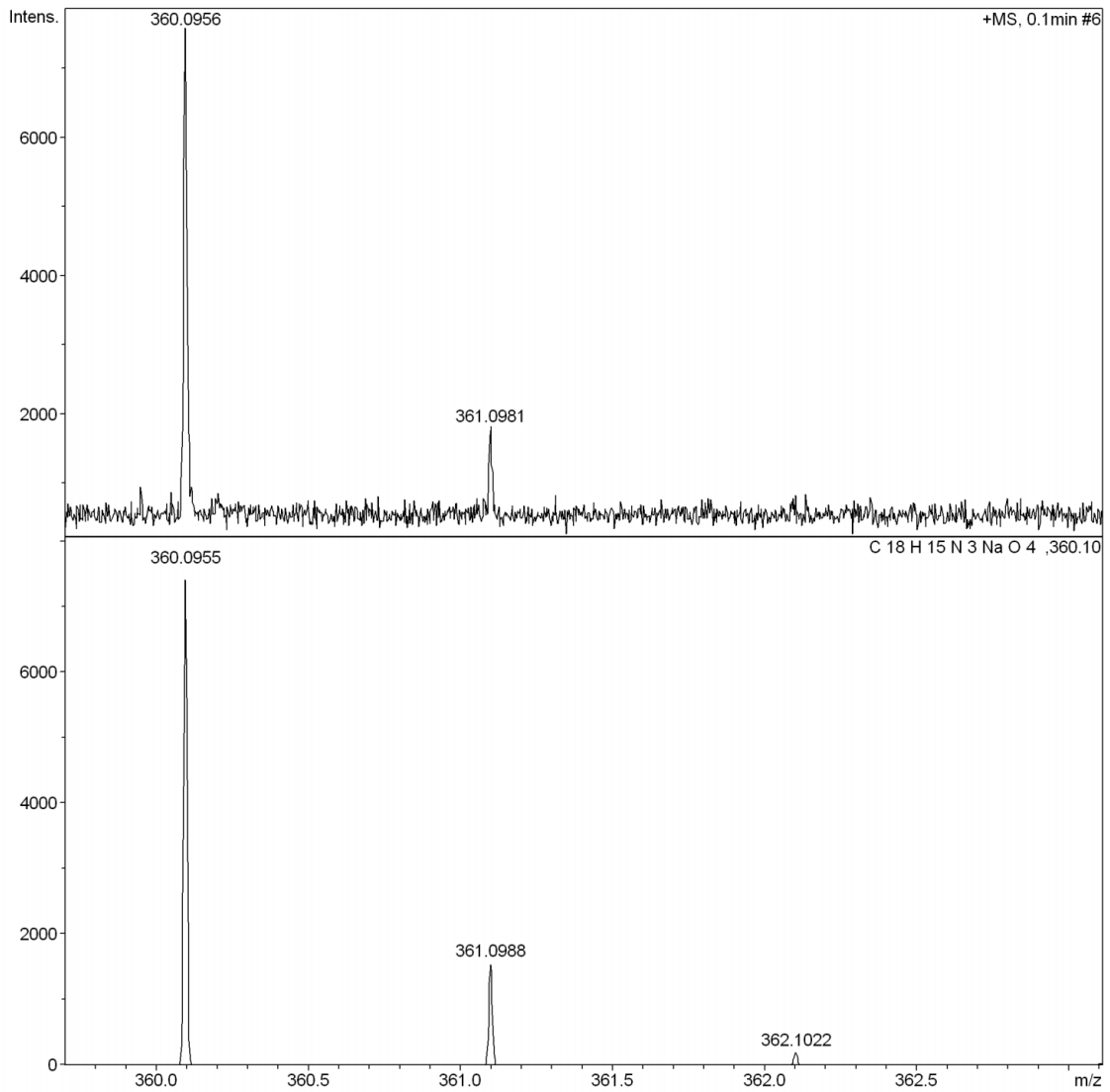
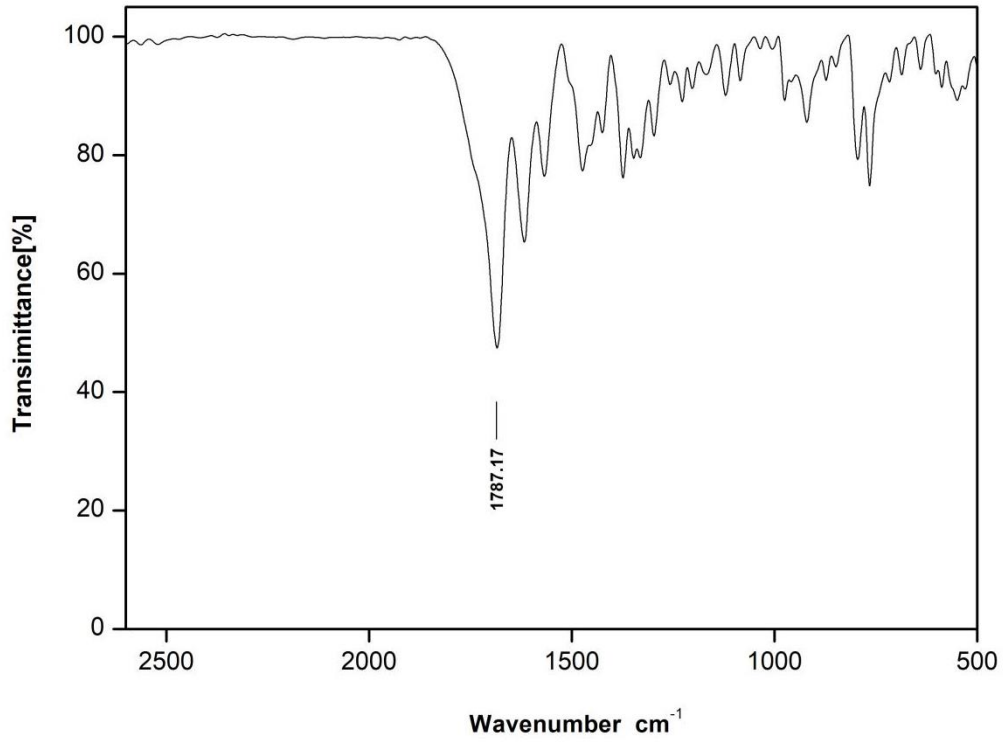










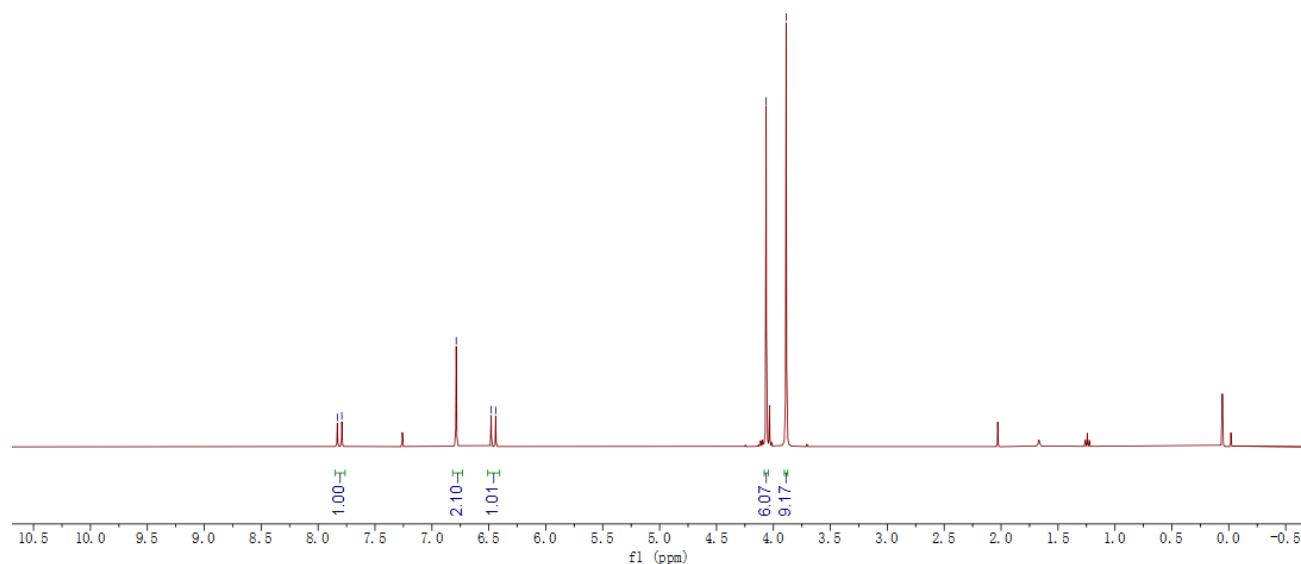
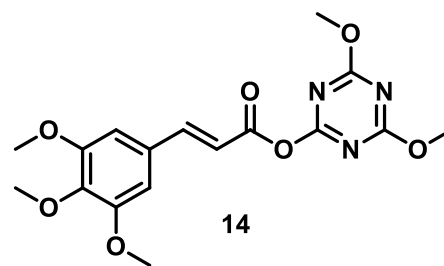


LDZ-3, 4, 5-tri-MeO-esters
single_pulse

7.83
7.79

6.79
6.48
6.44

4.06
3.89



LDZ-3, 4, 5-tri-MeO-esters
single_pulse decoupled gated NOE

174.23
170.70

162.33

153.60

149.08

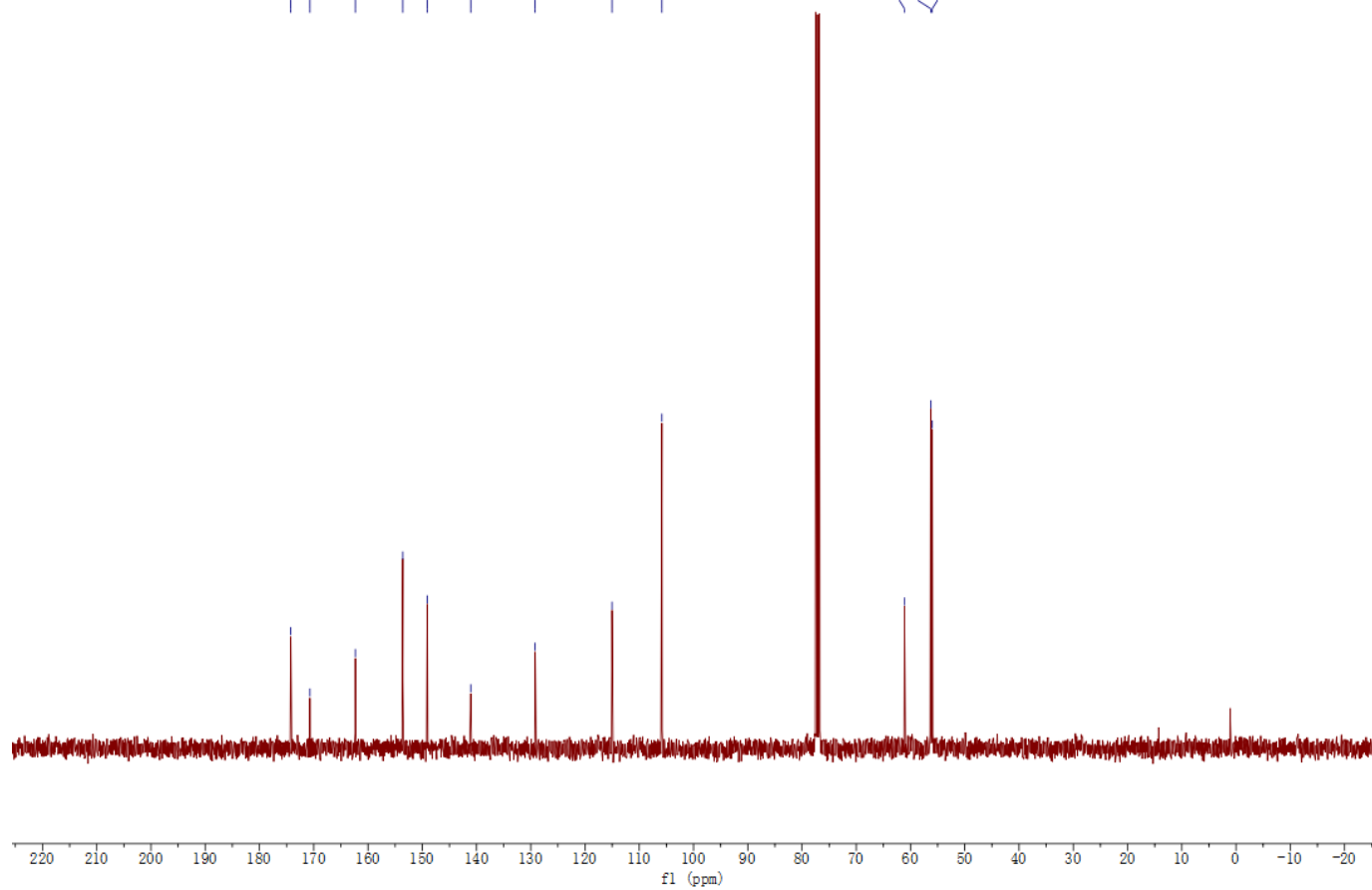
141.06

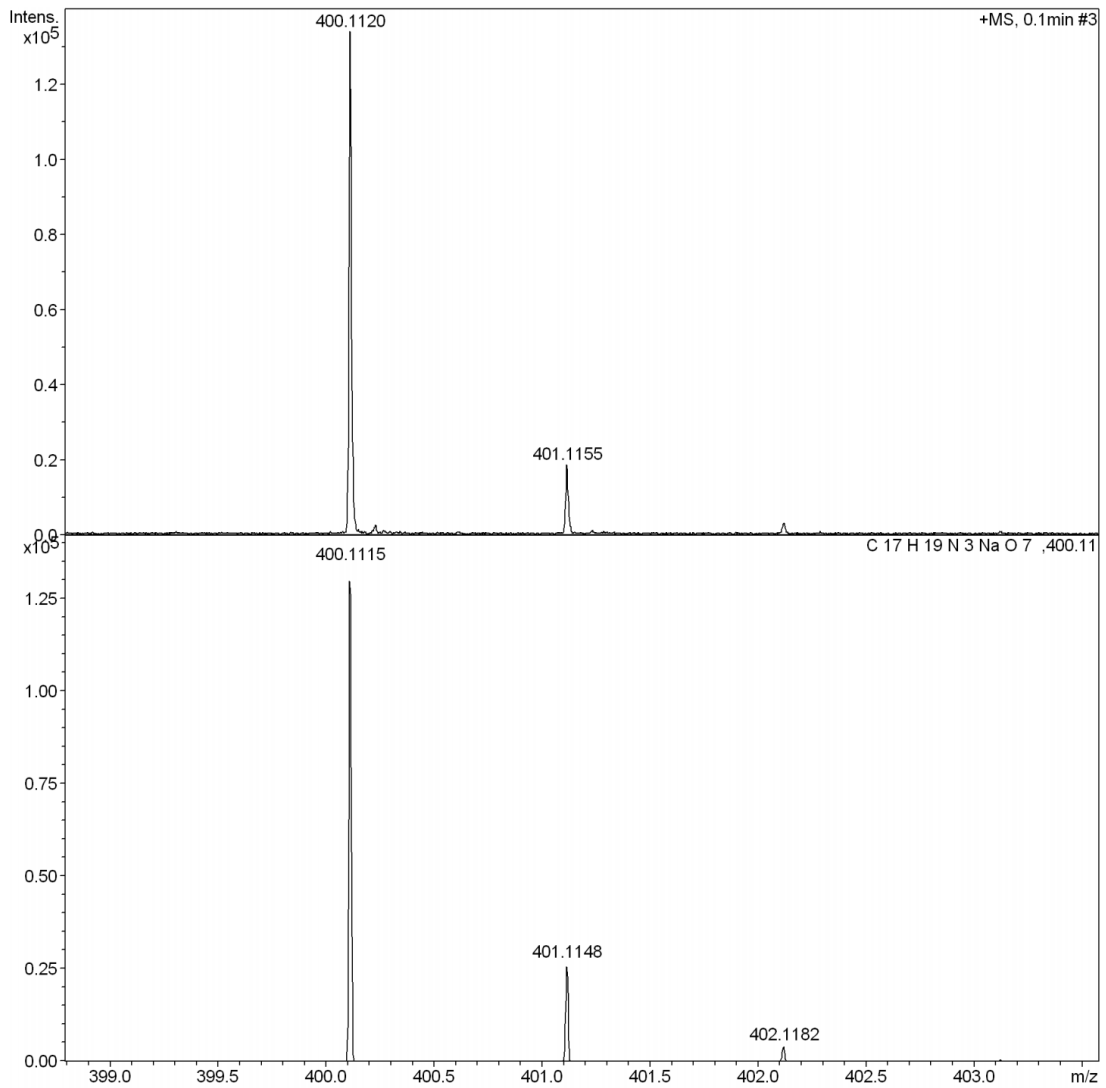
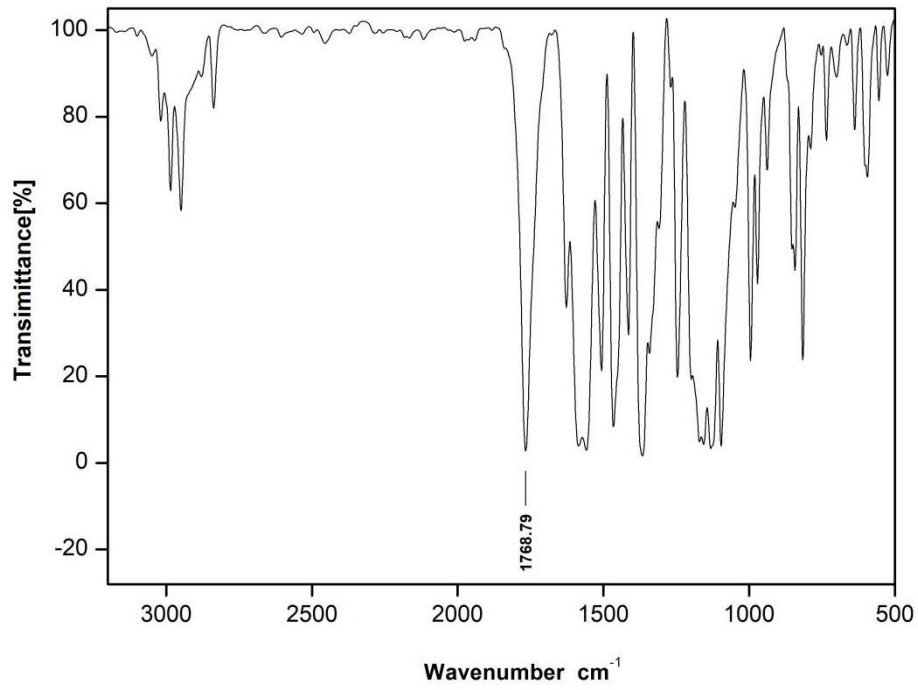
129.20

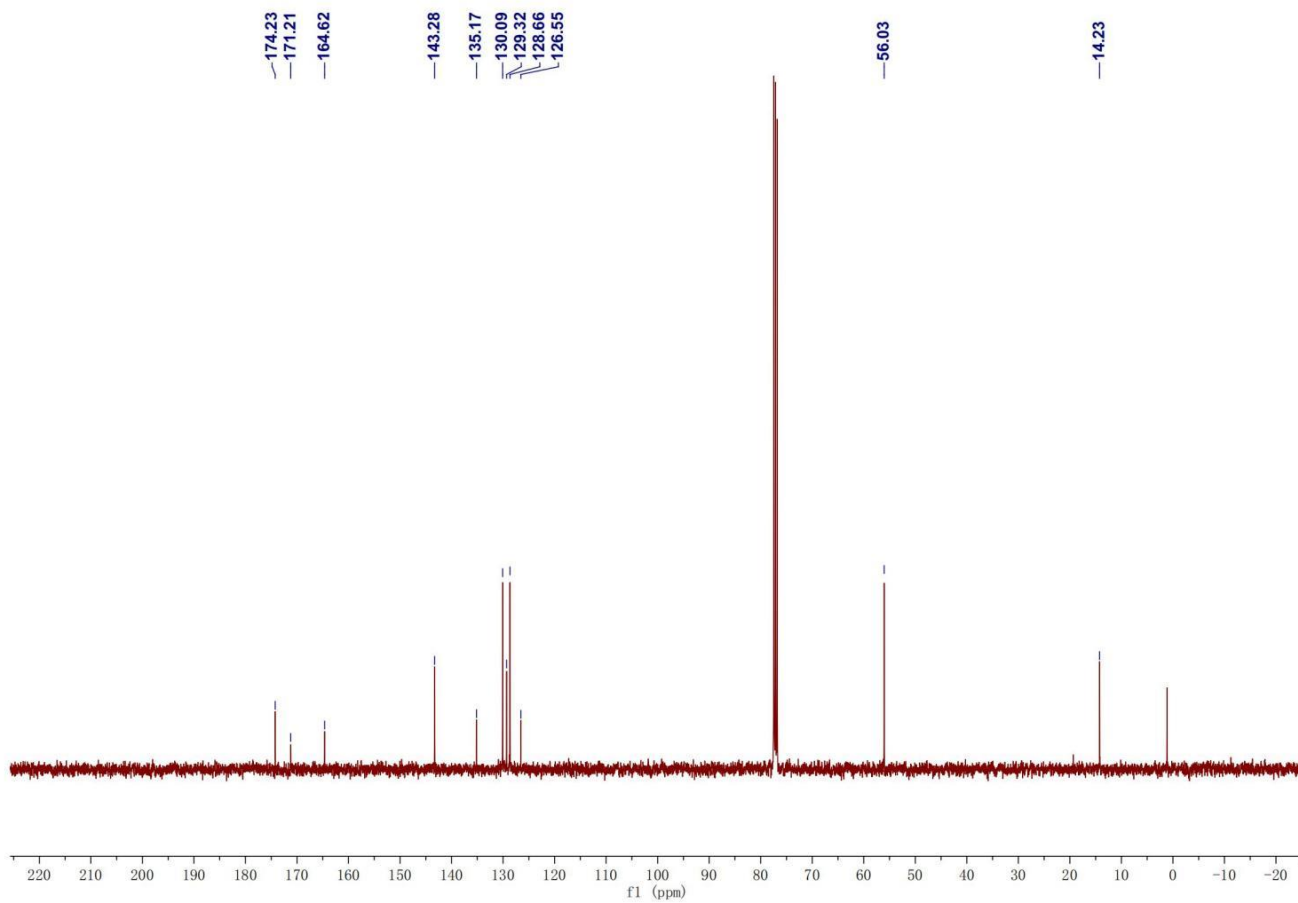
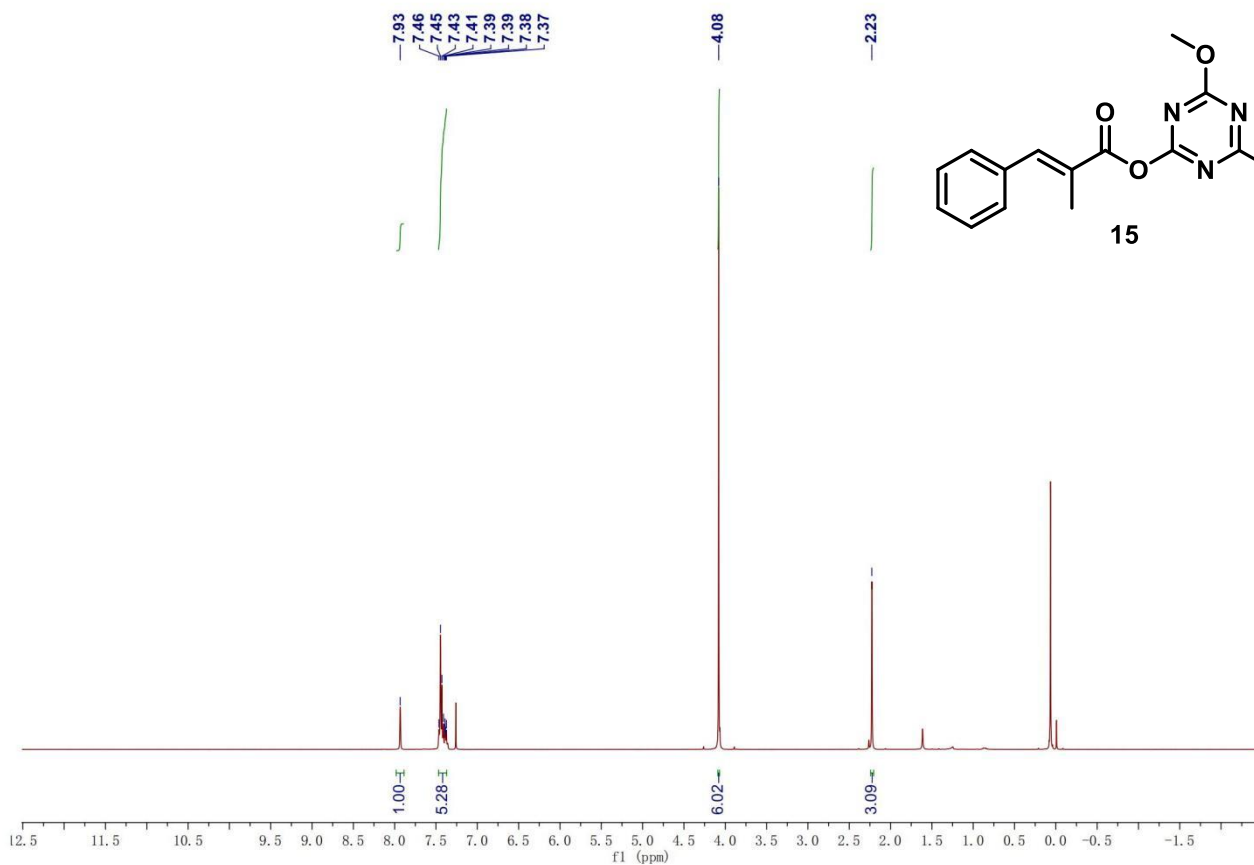
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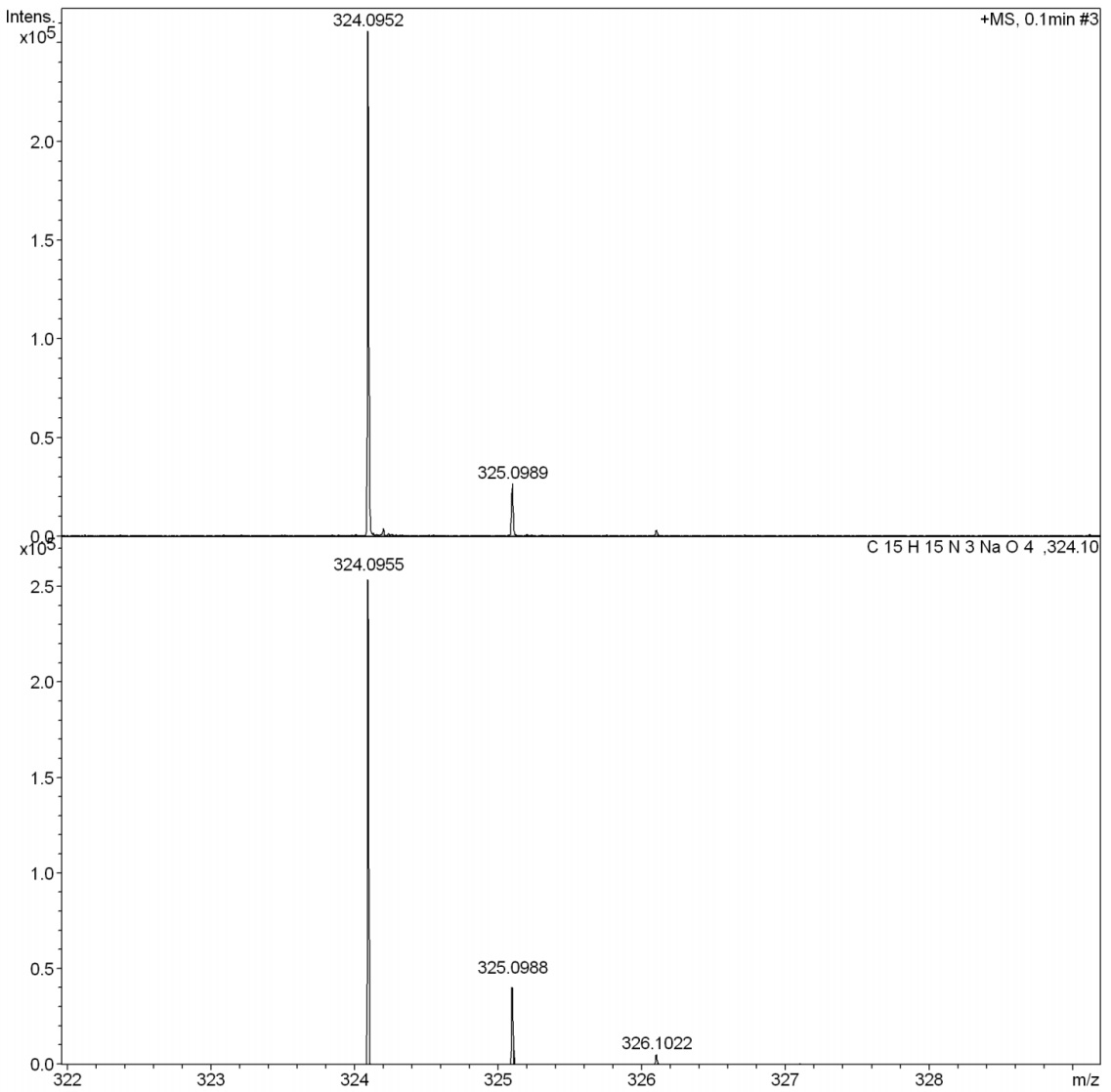
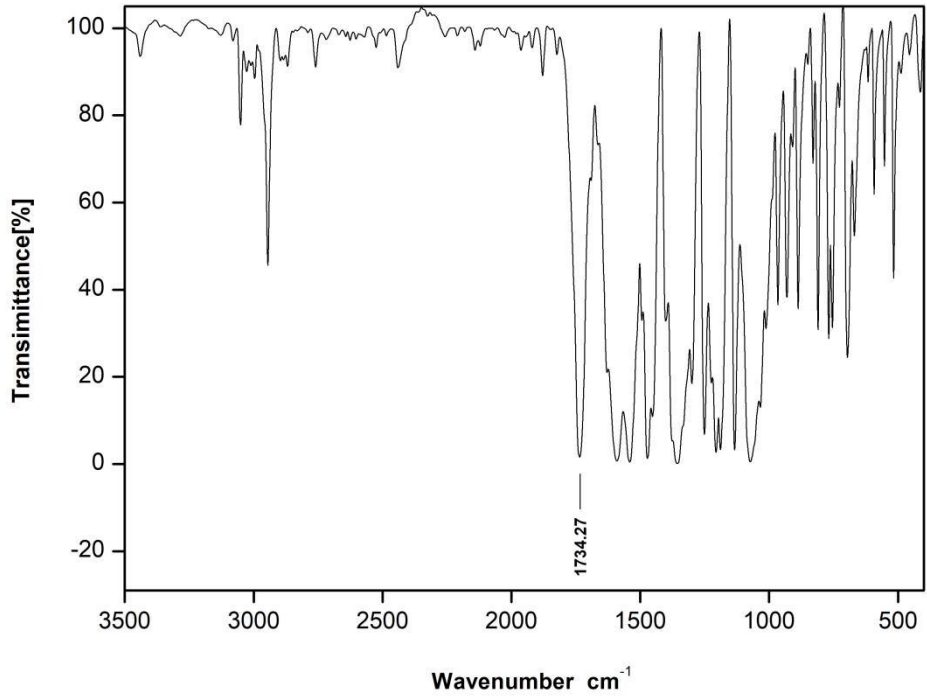
105.83

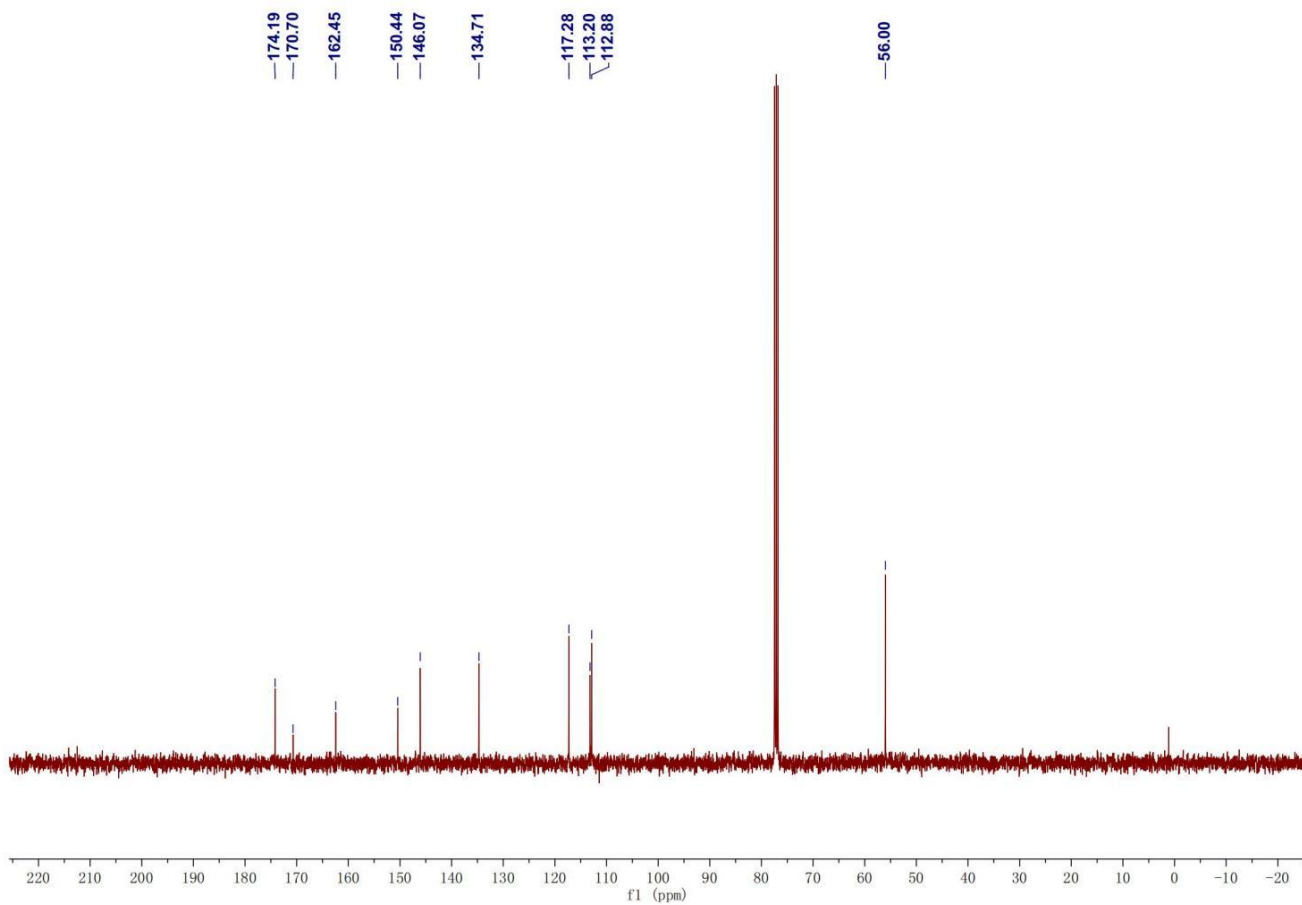
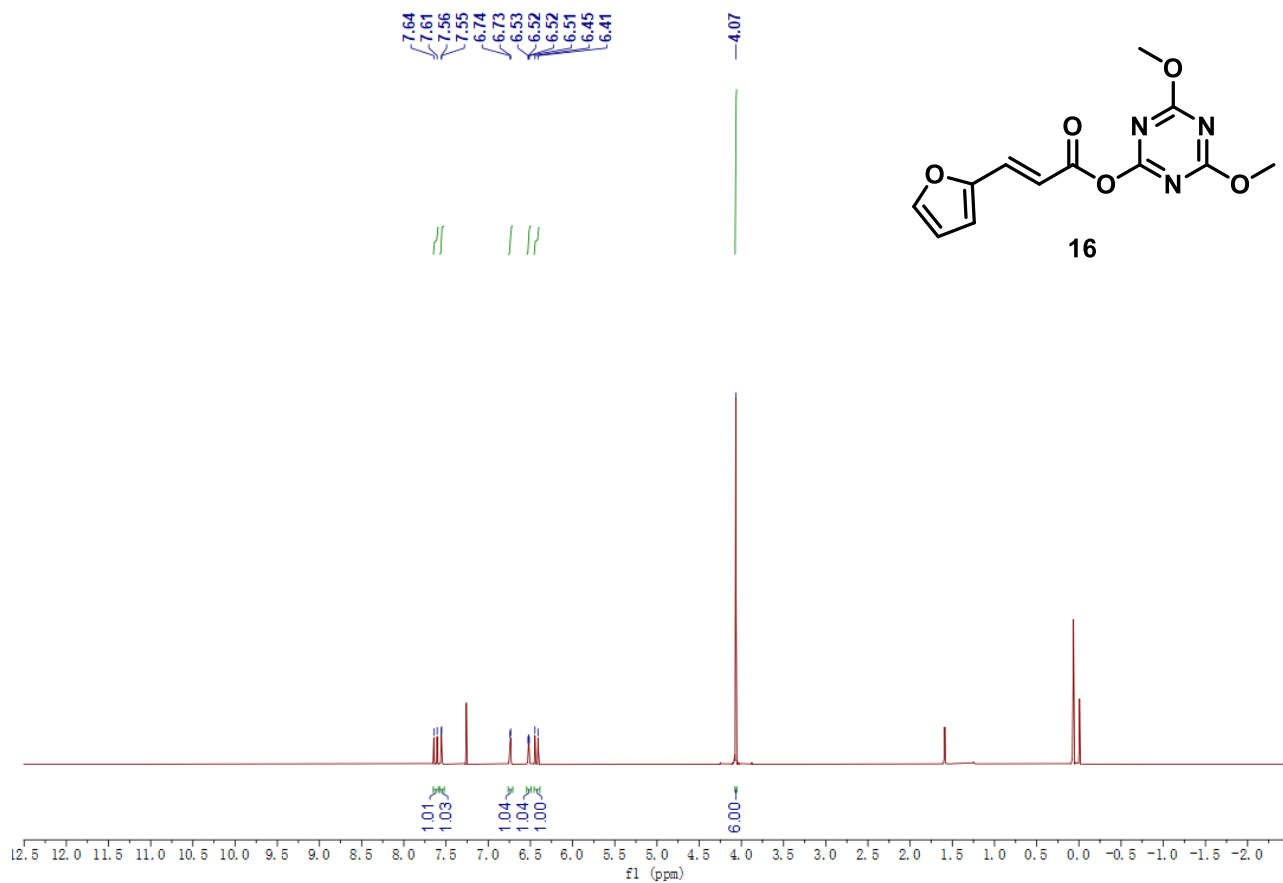
61.11
56.28
55.99

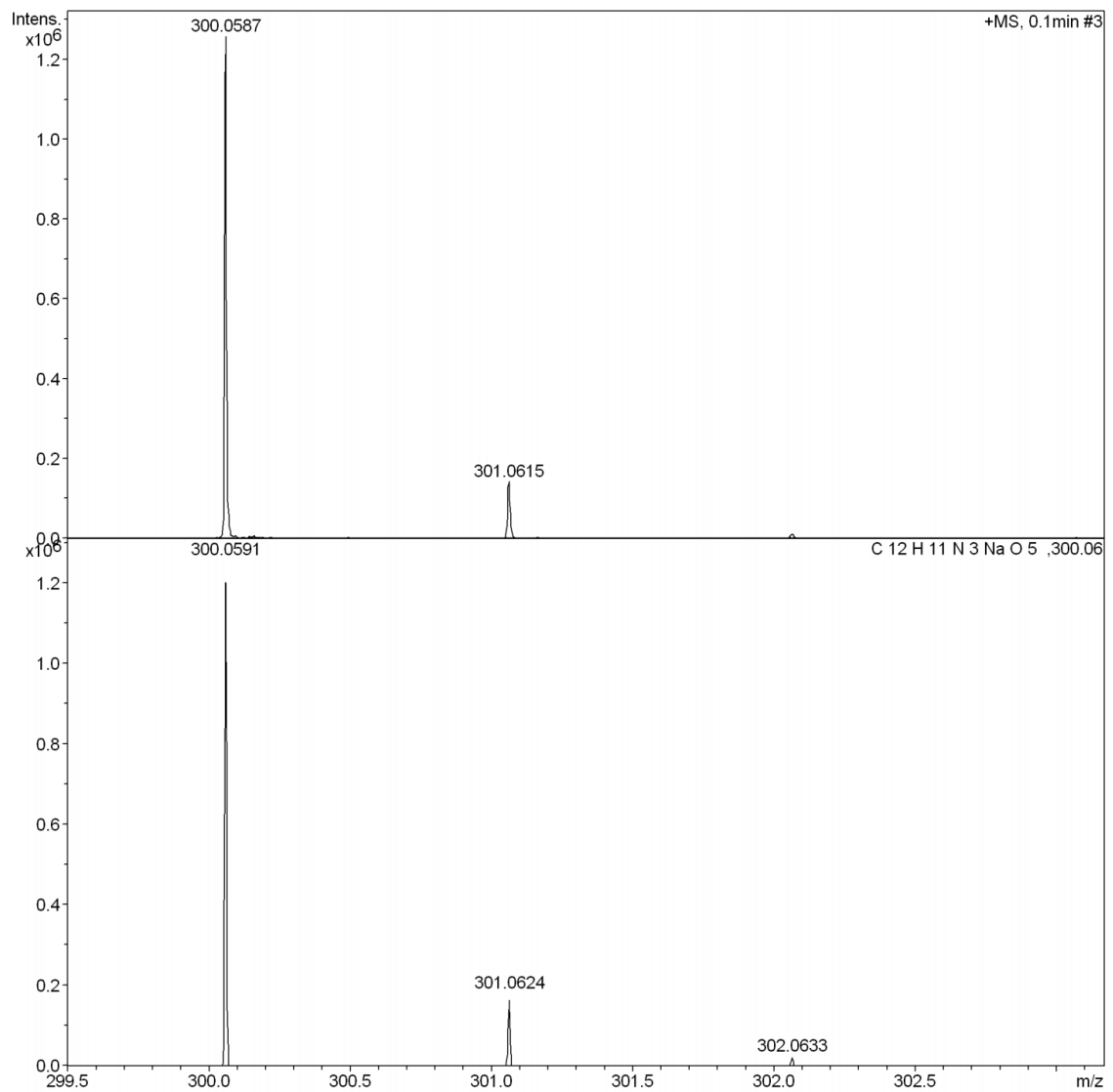
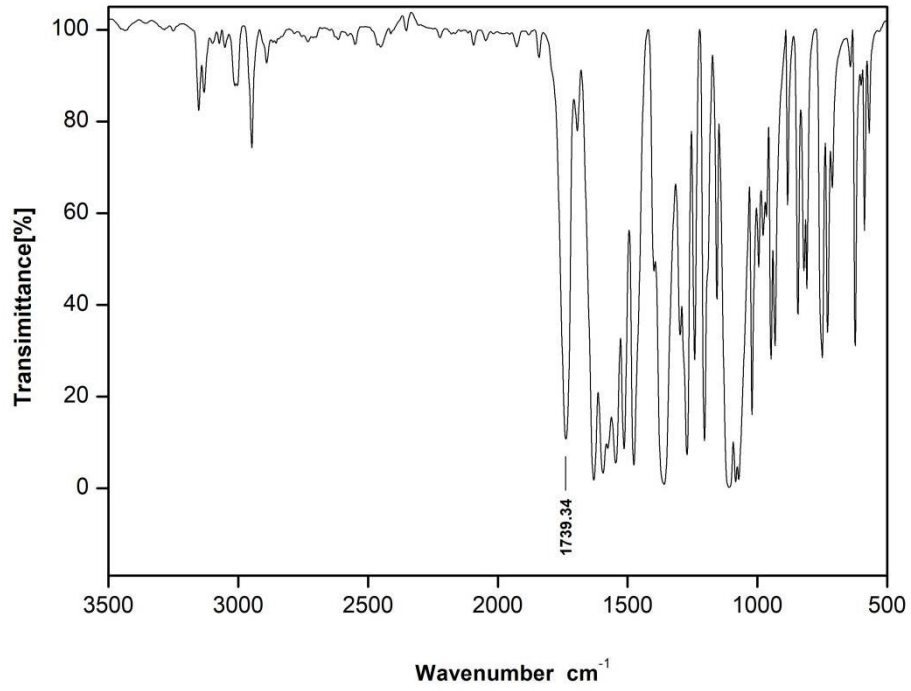


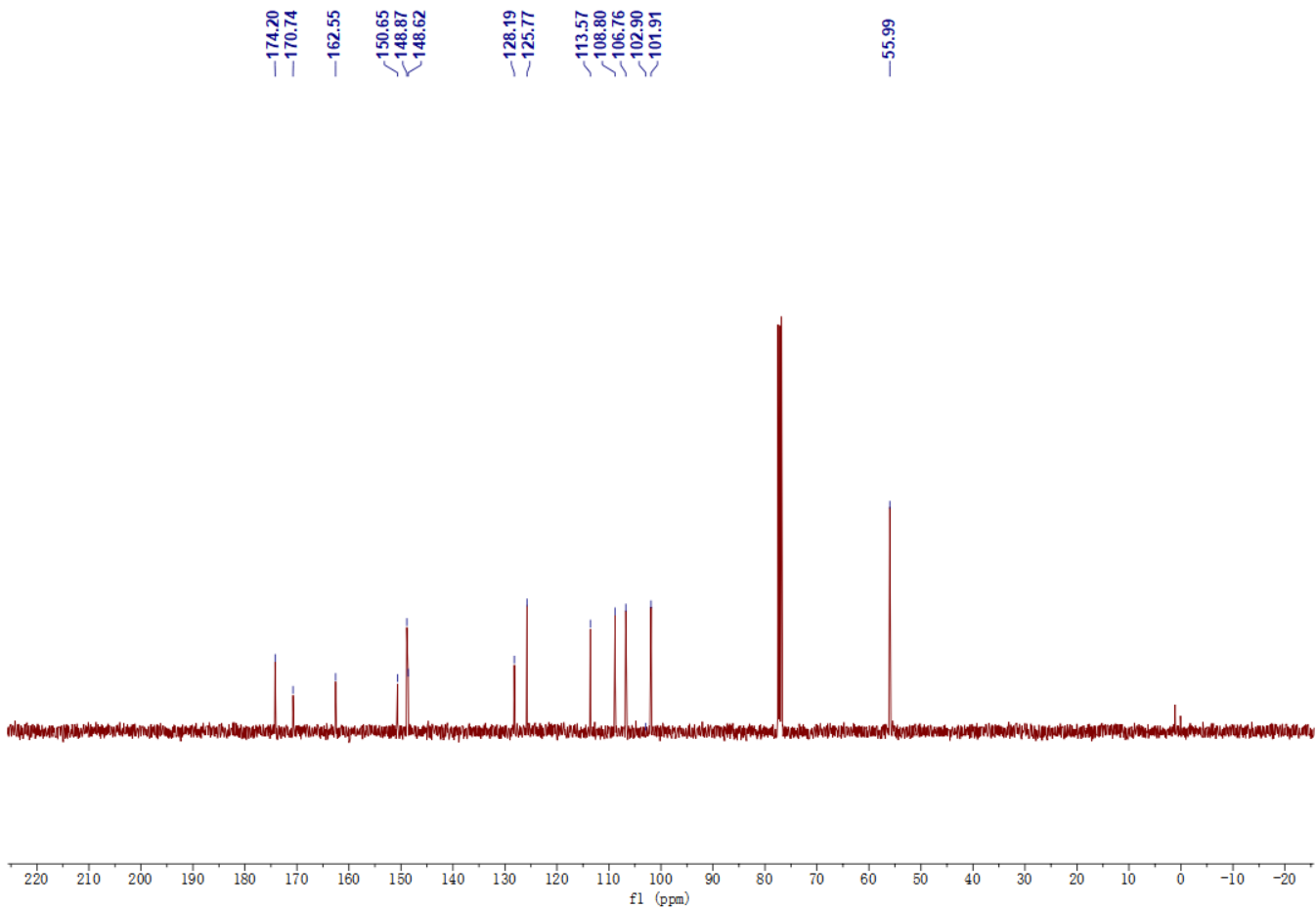
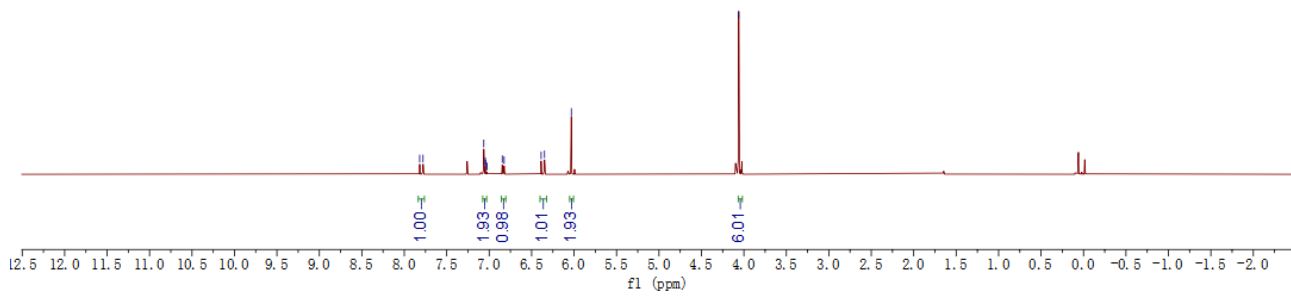
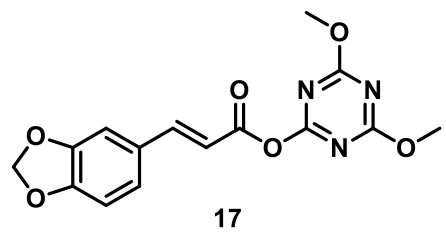


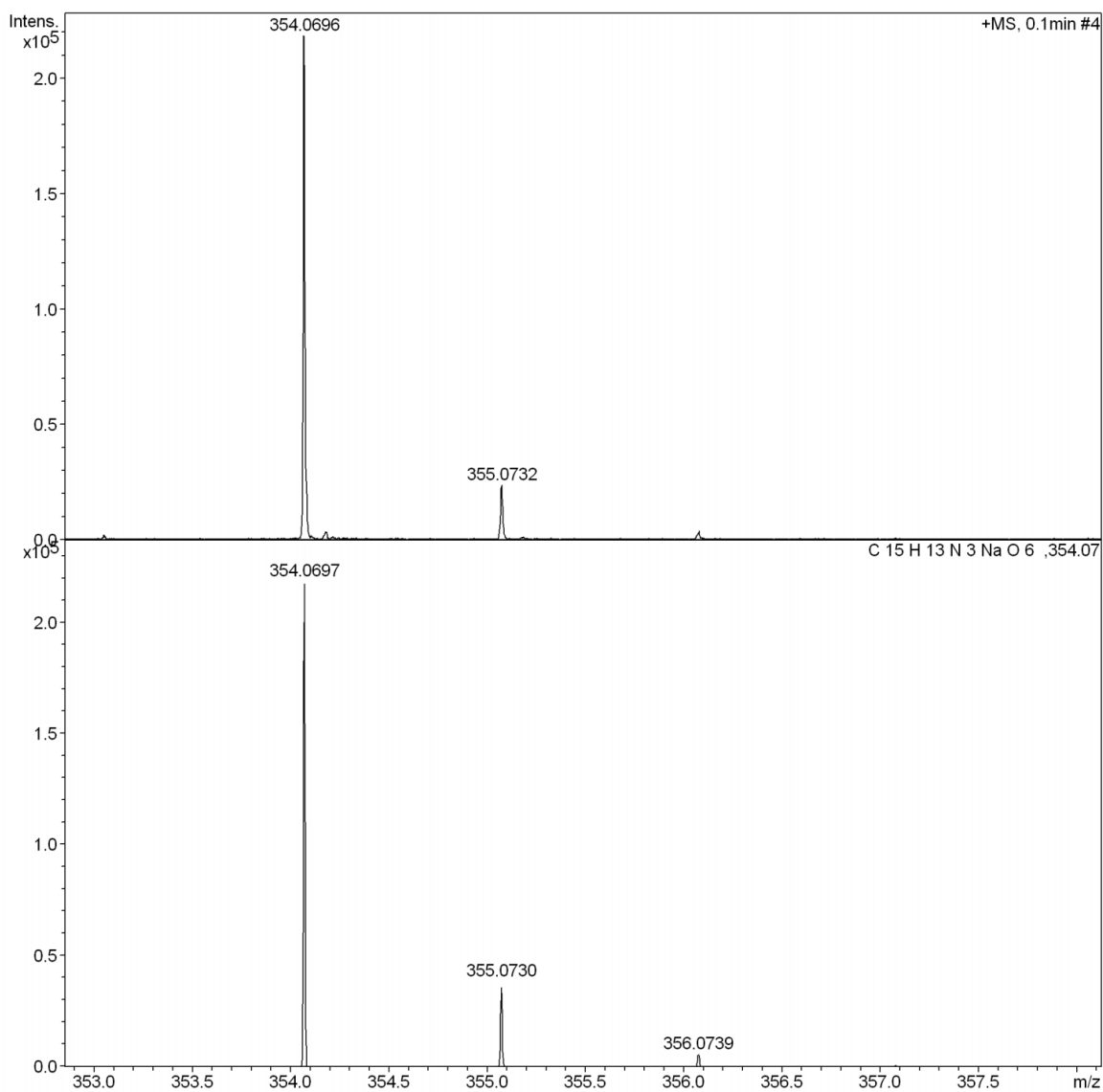
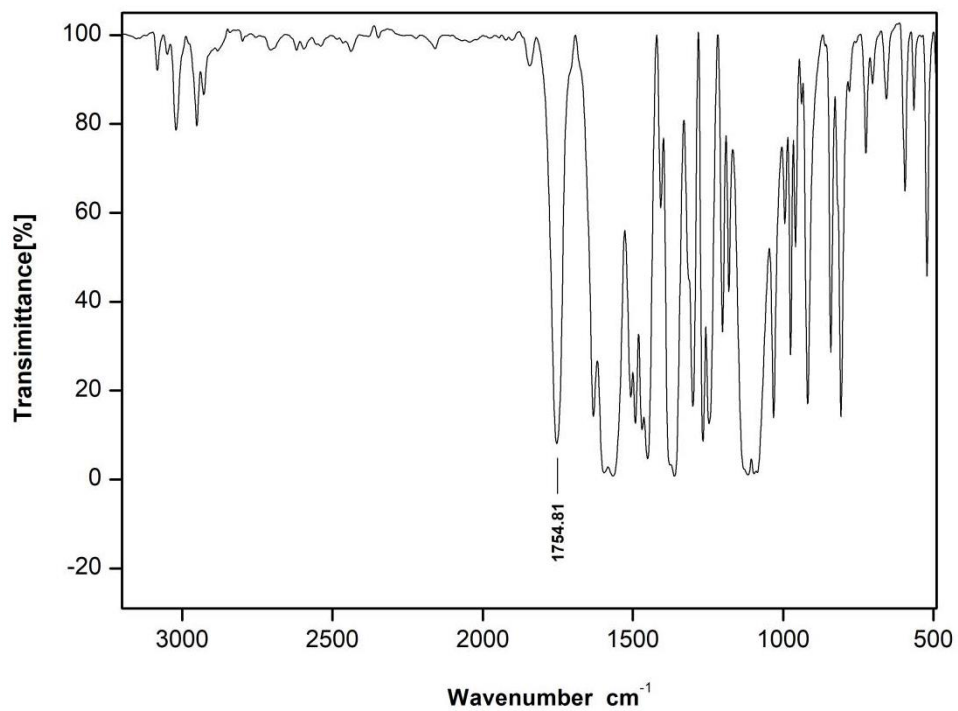


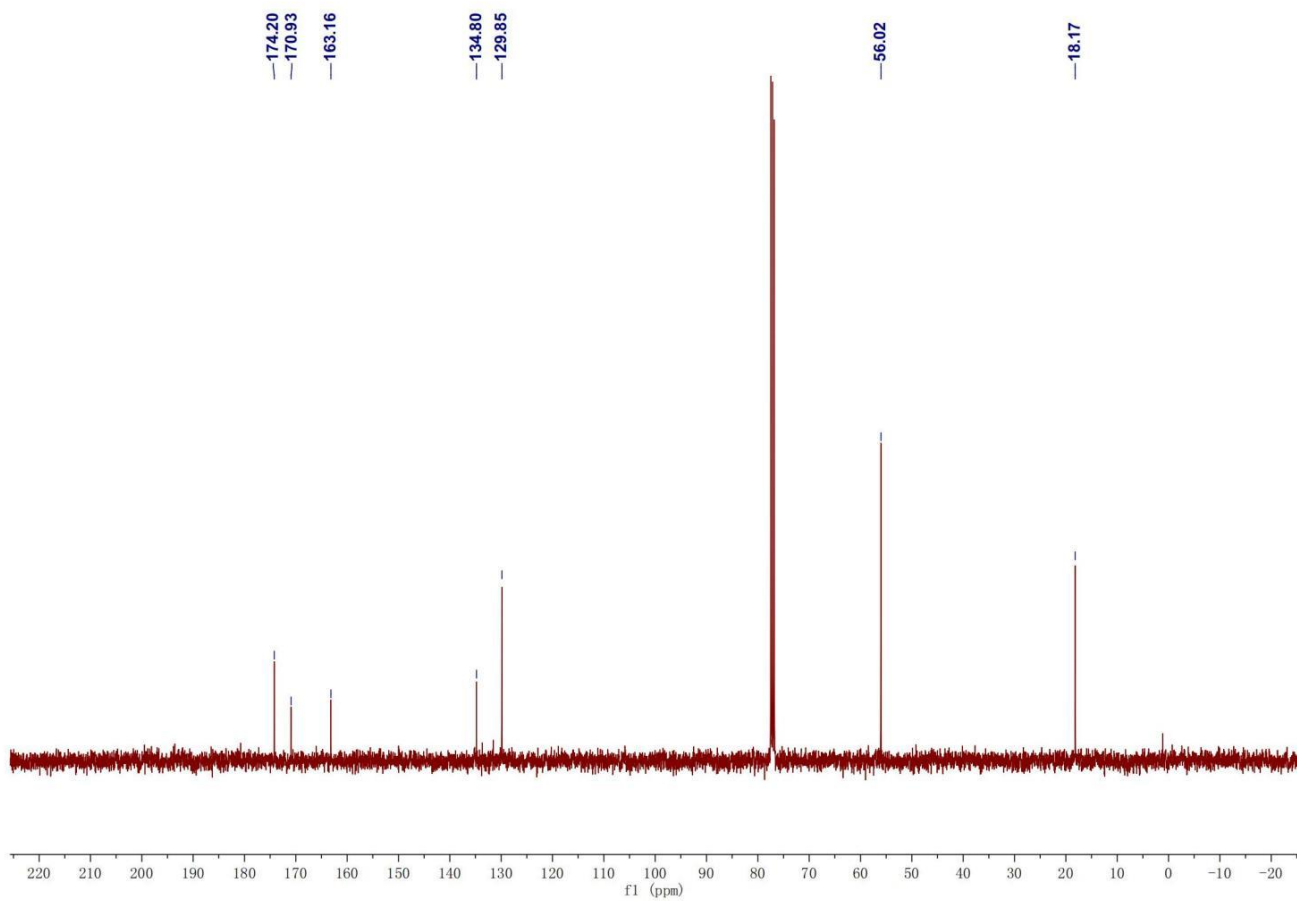
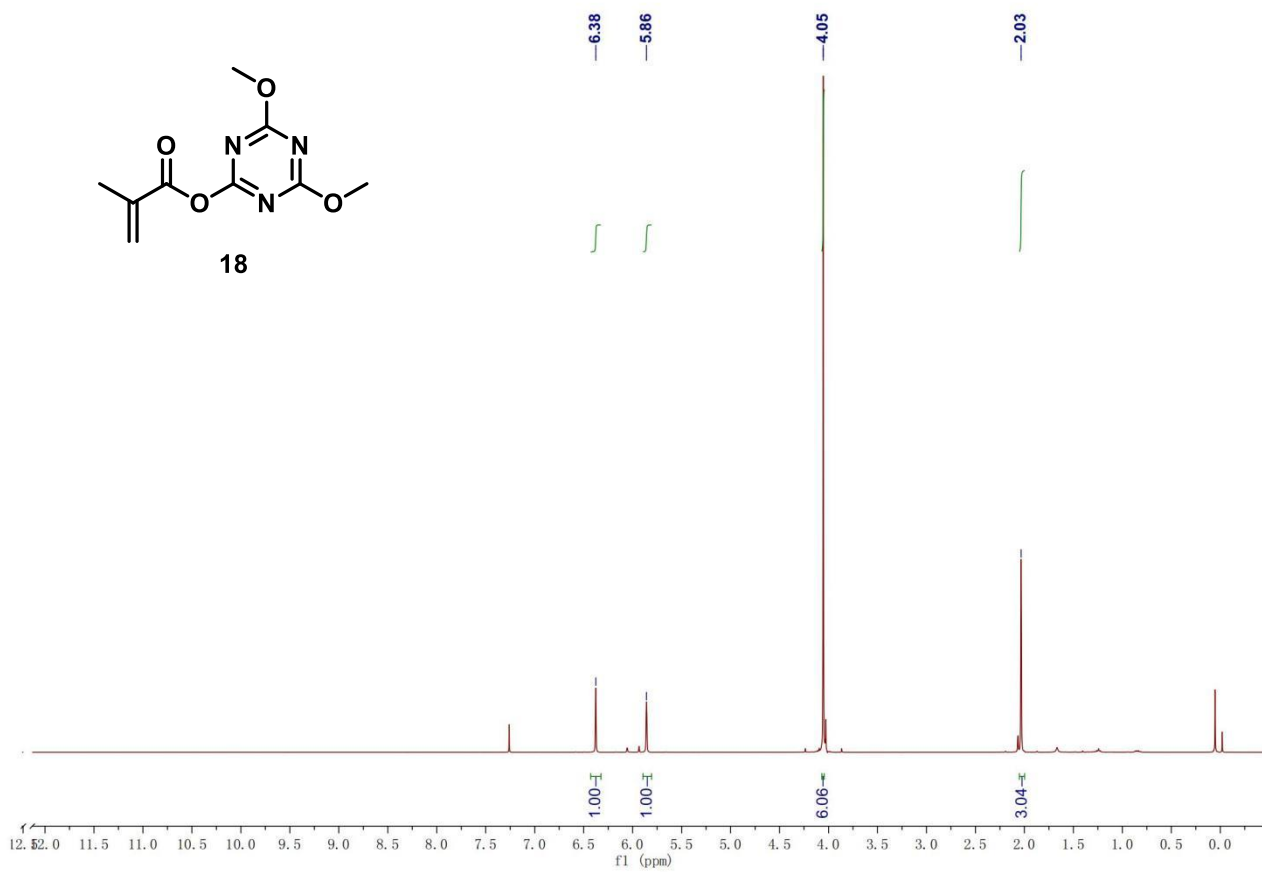
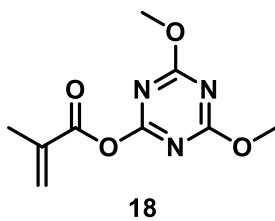


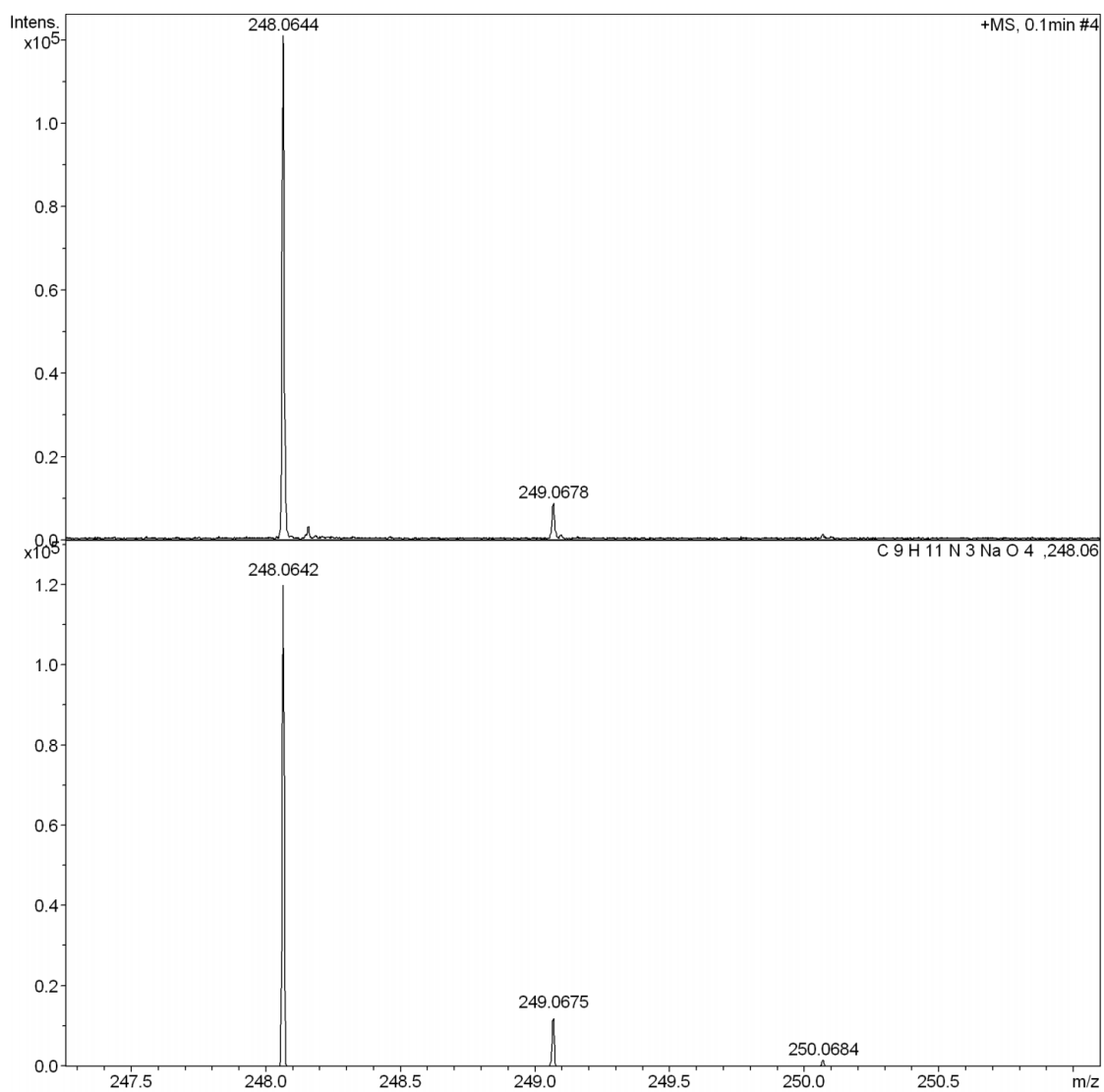
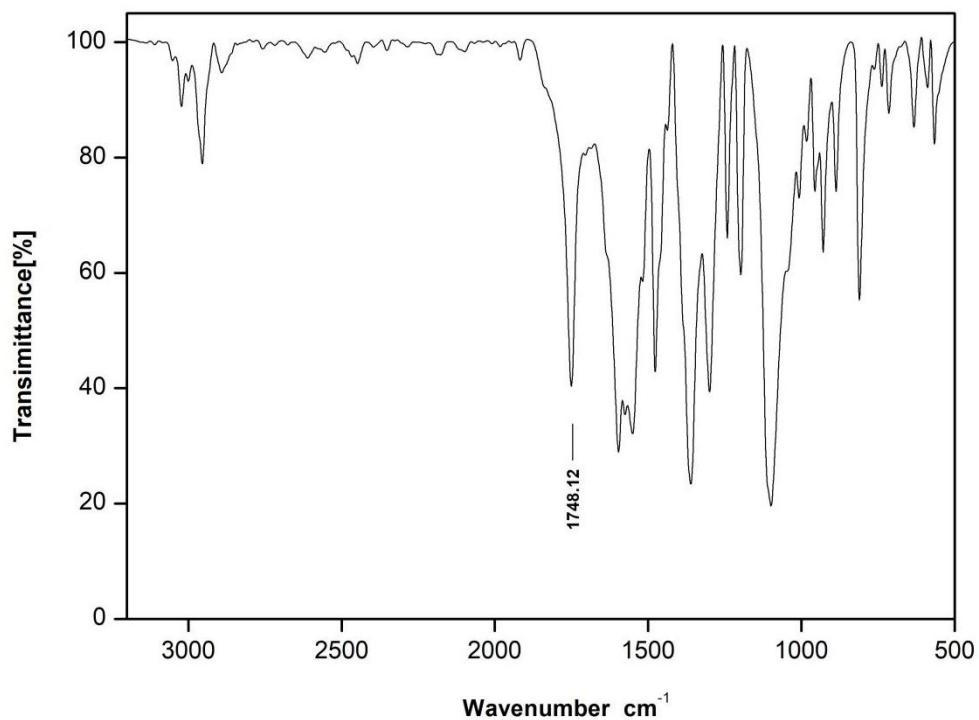


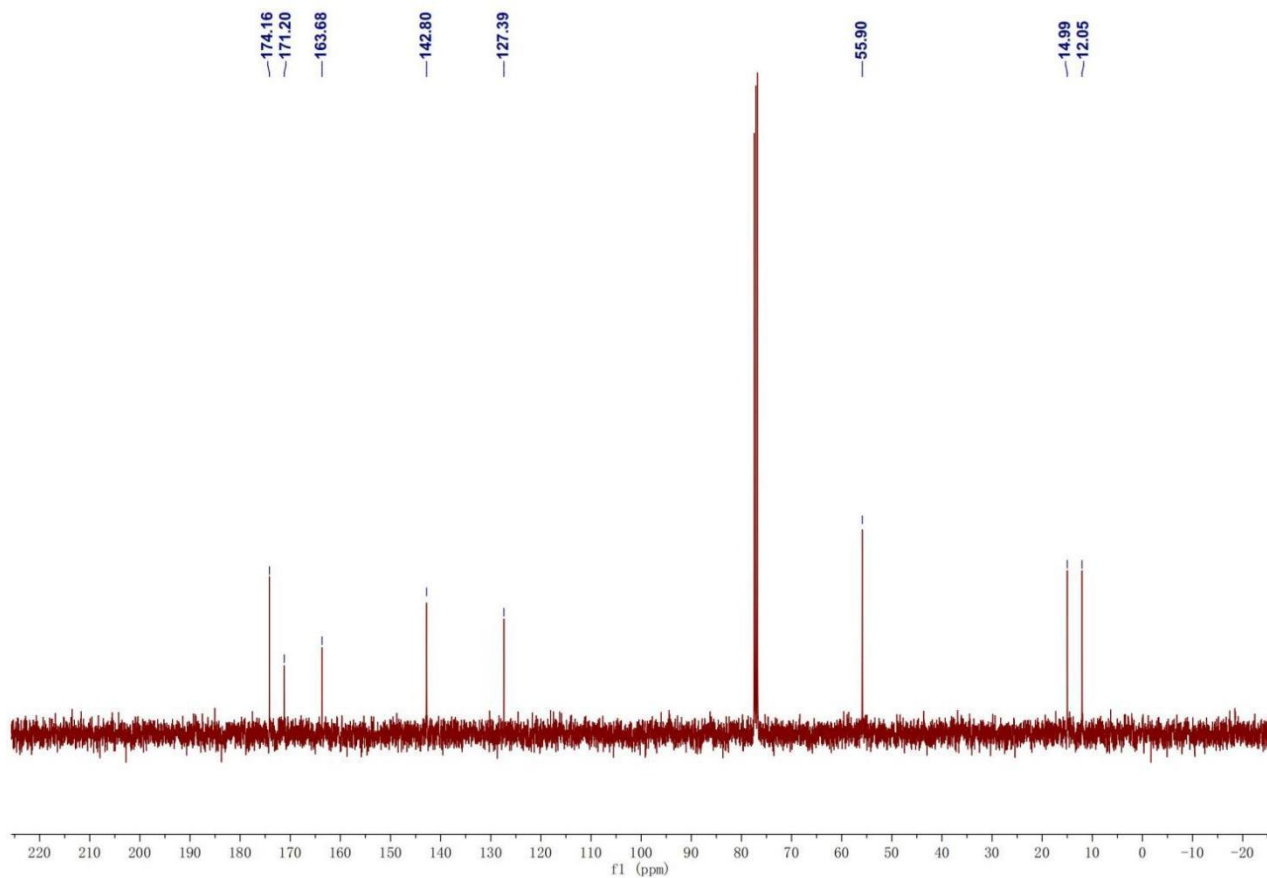
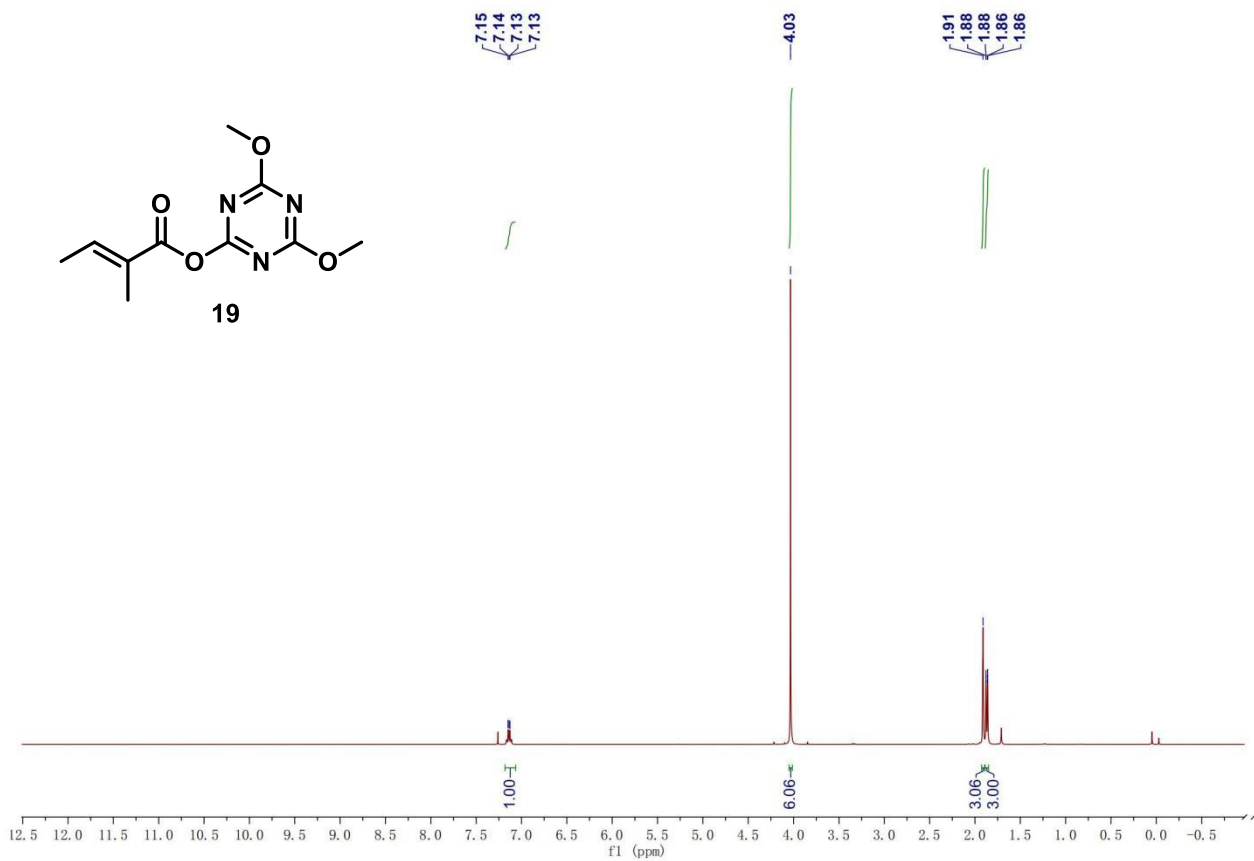
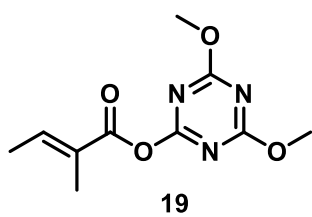


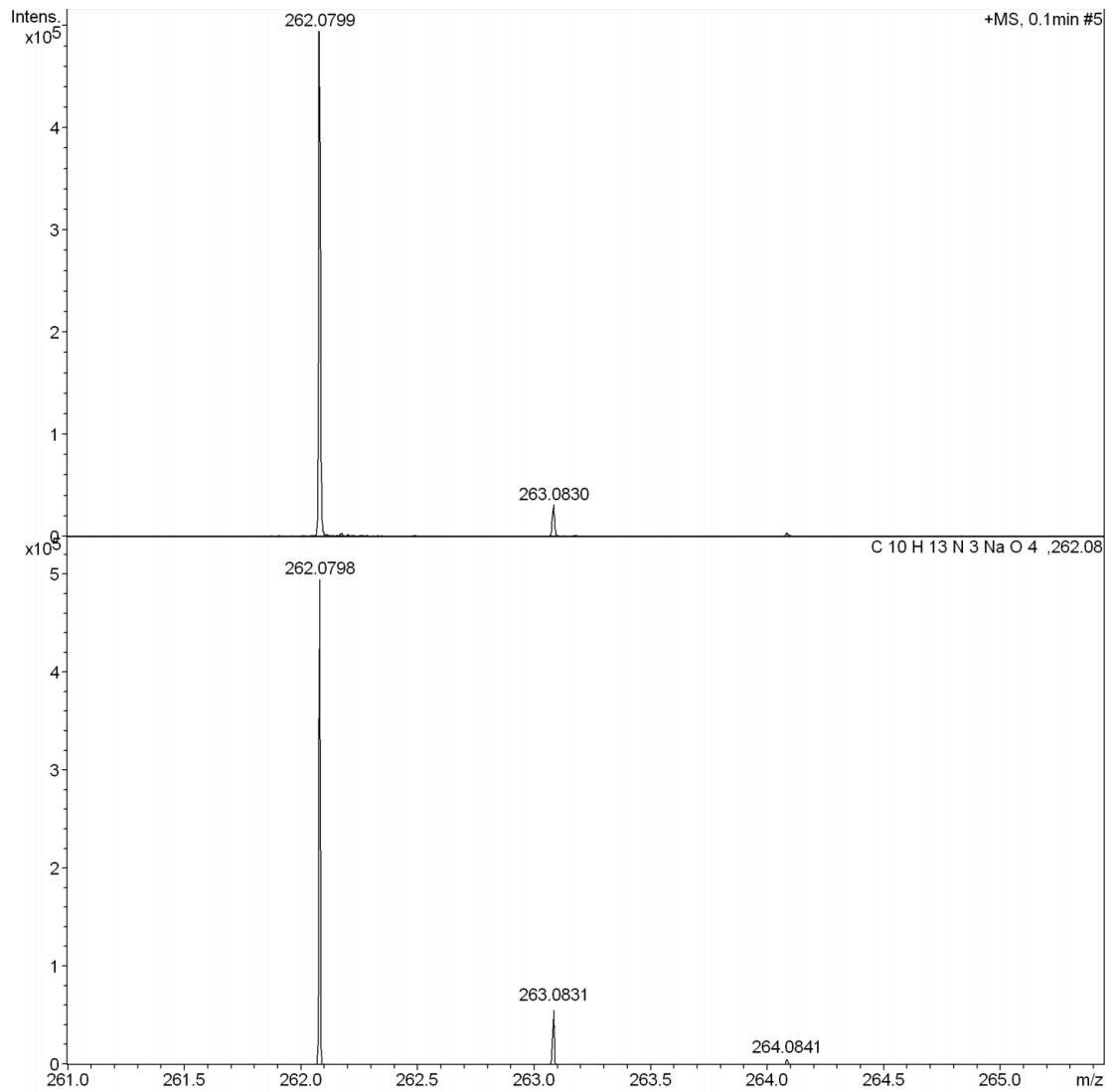
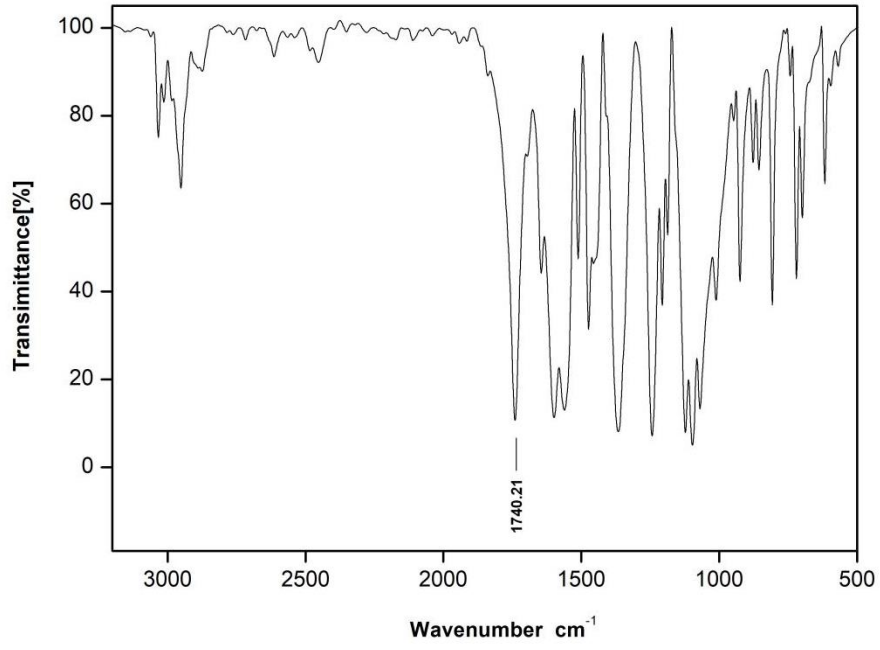


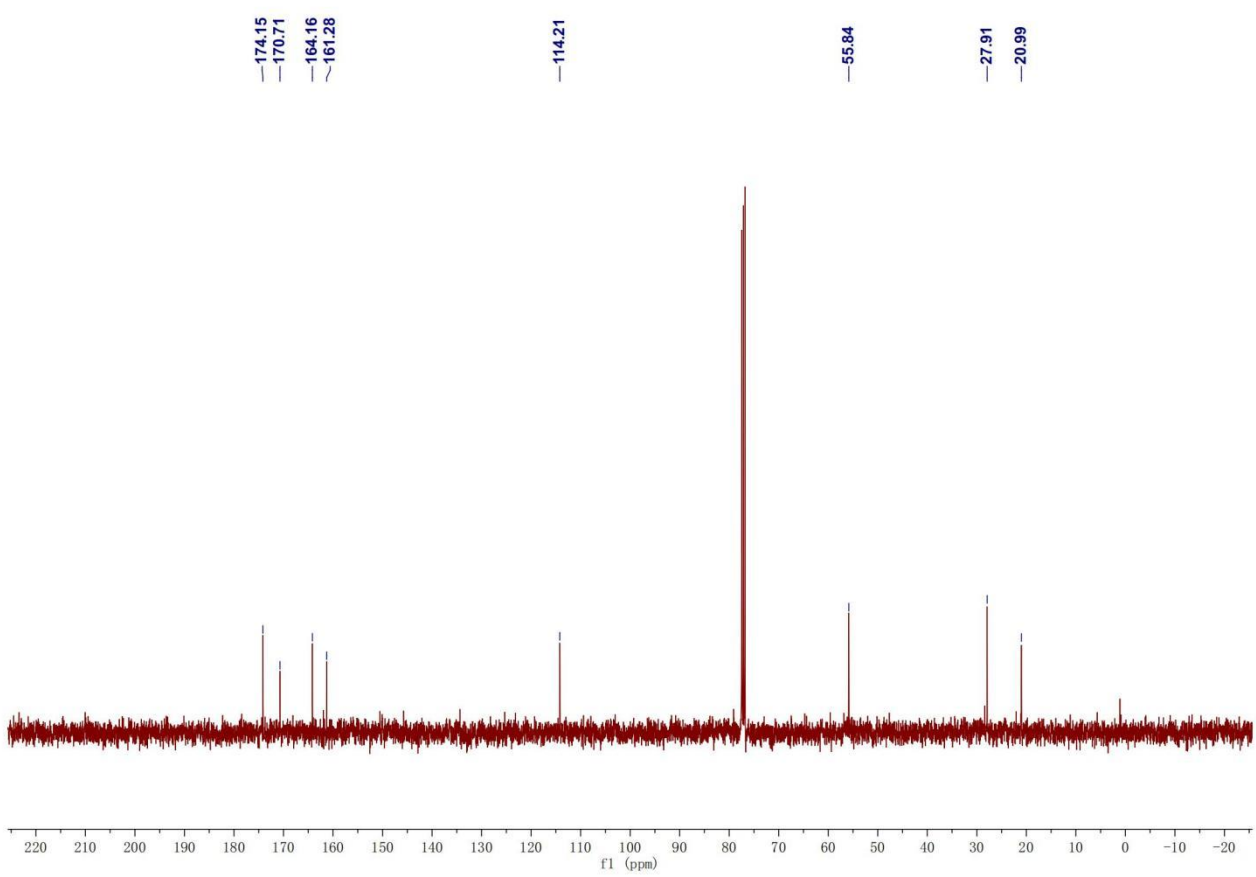
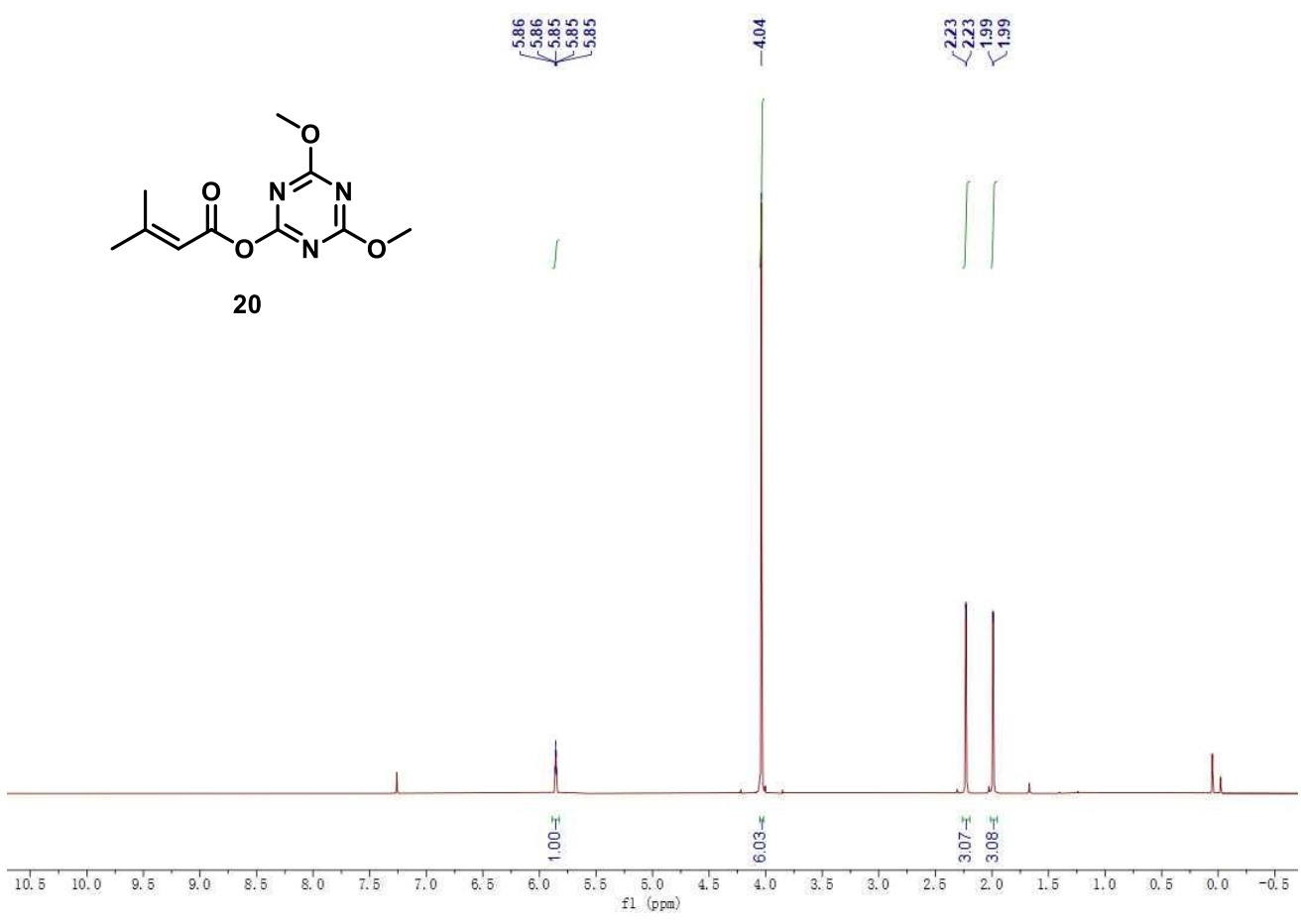
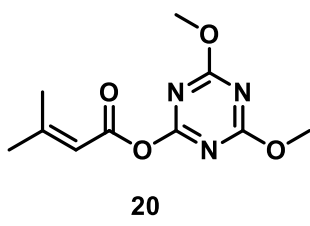


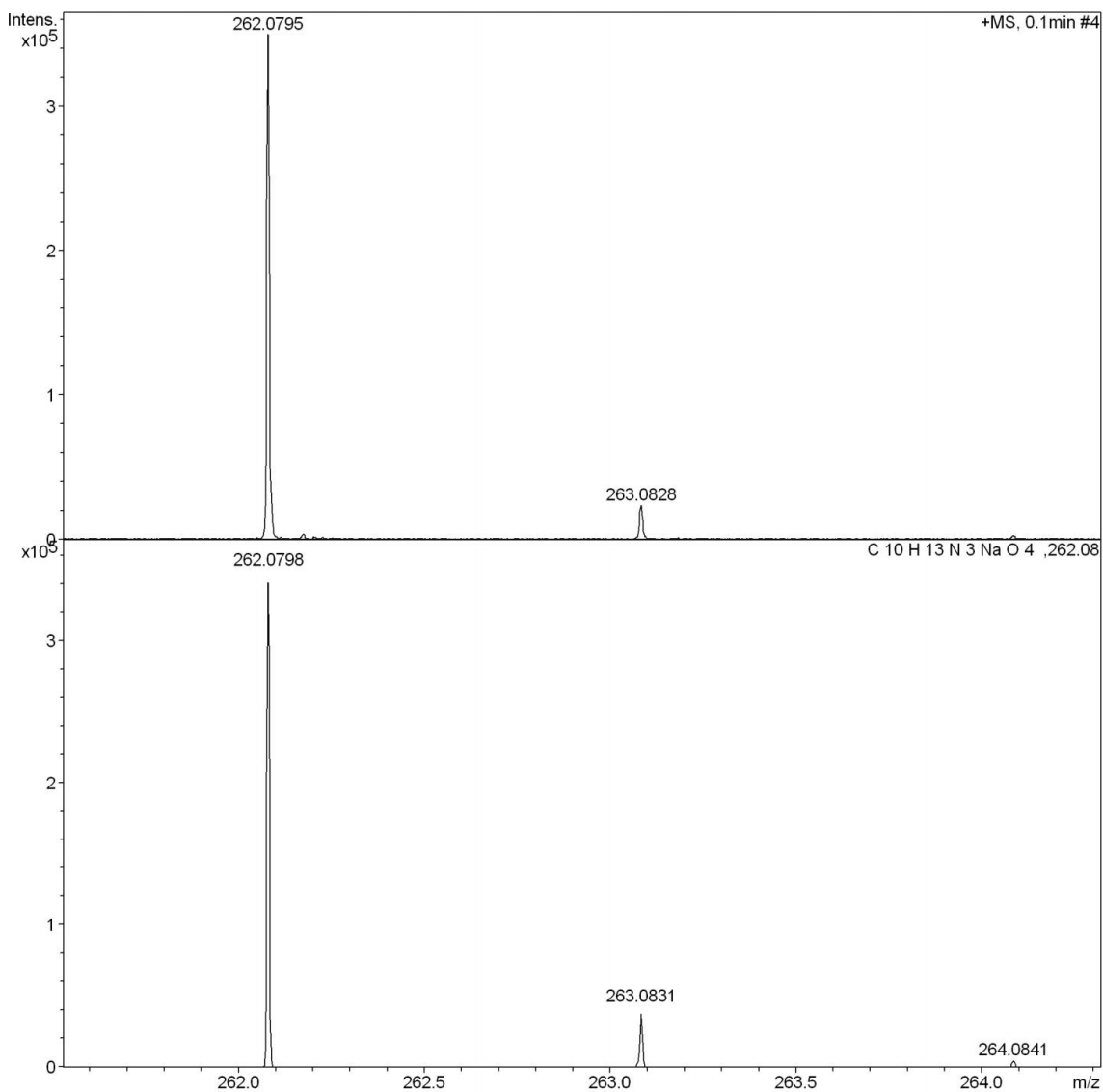
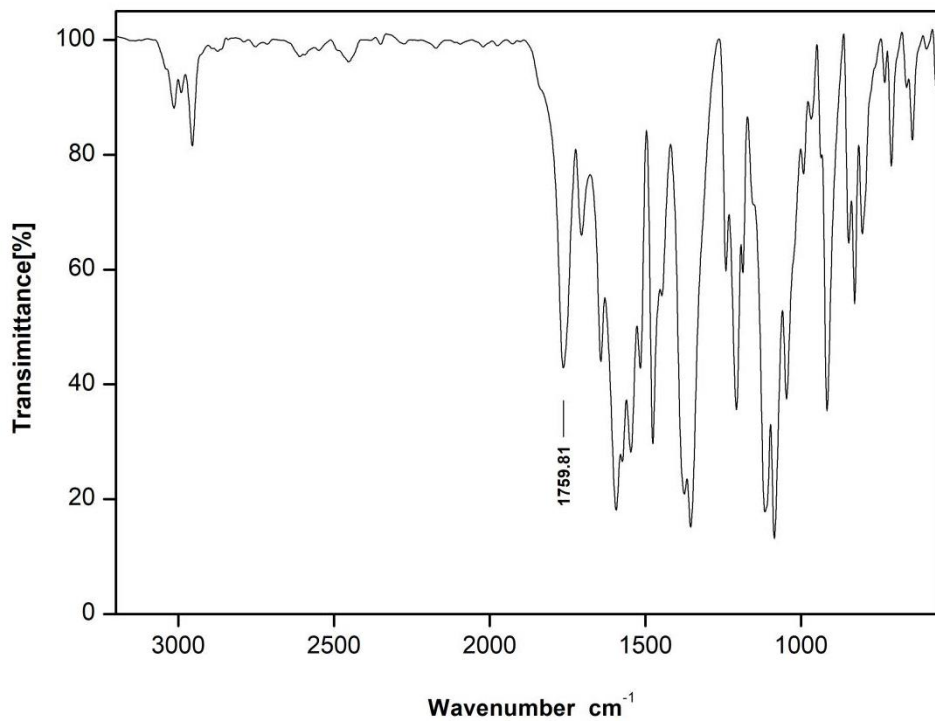


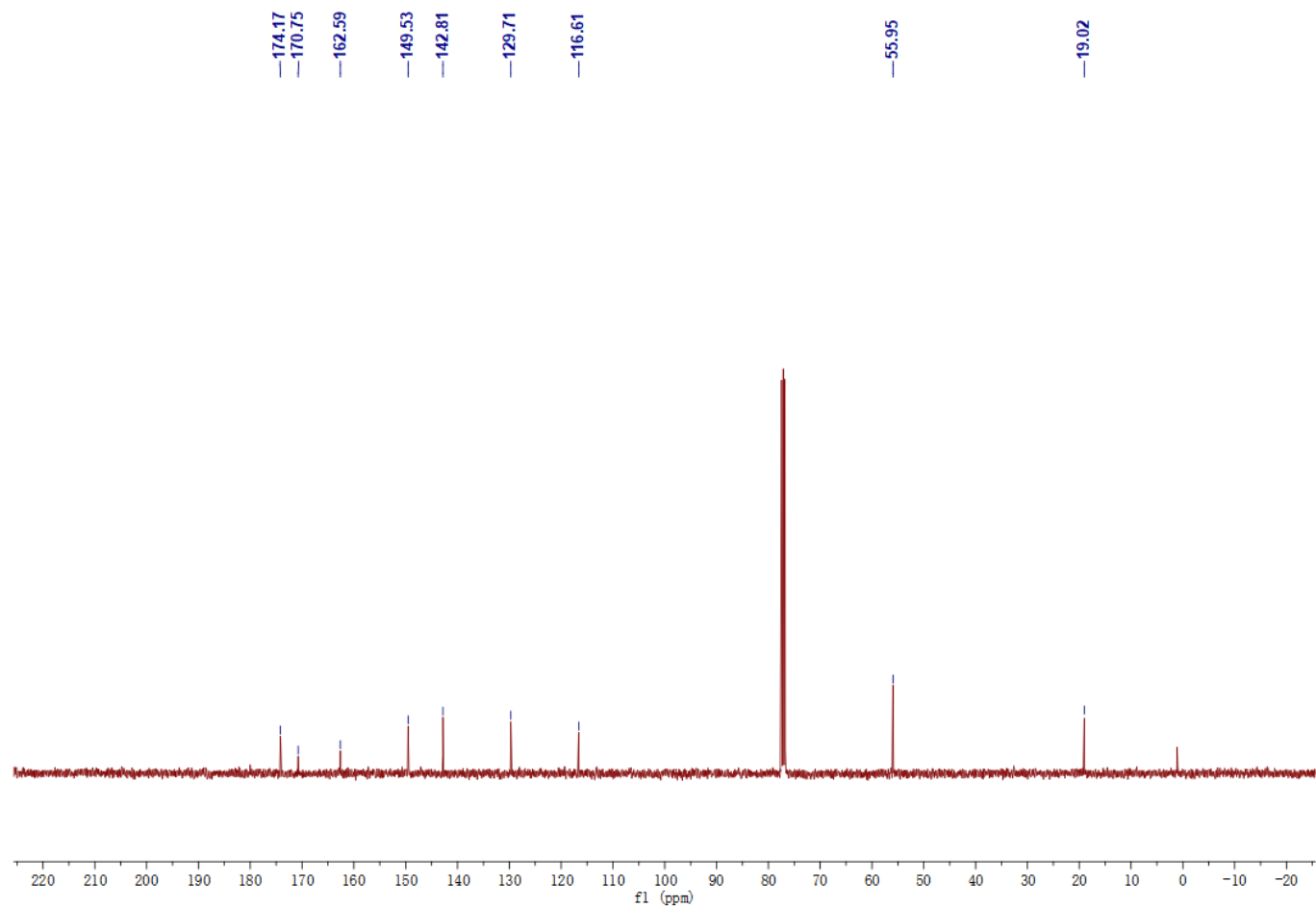
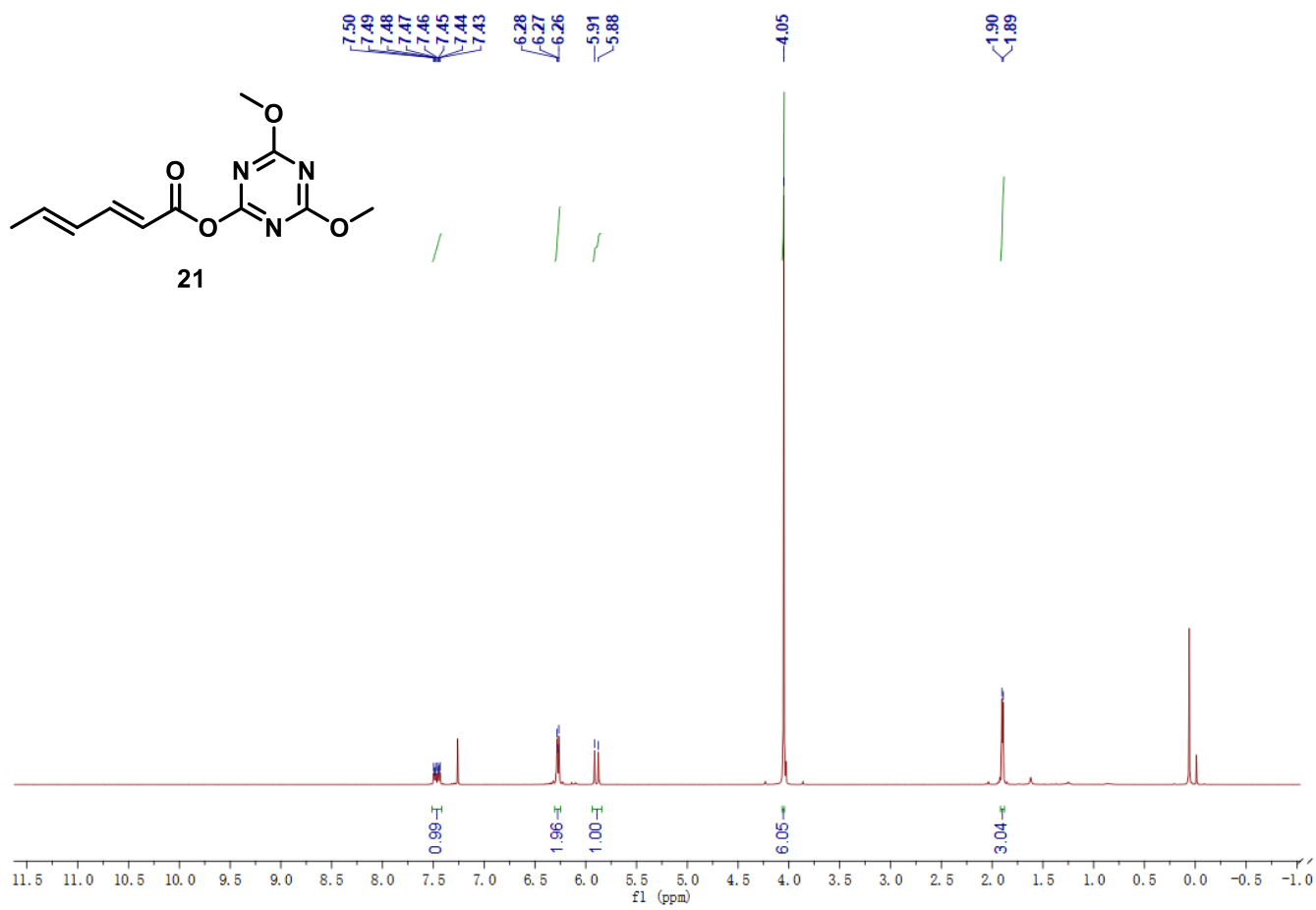
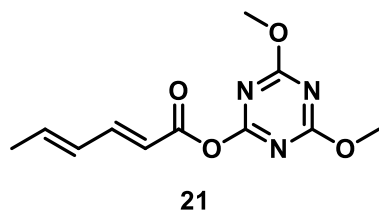


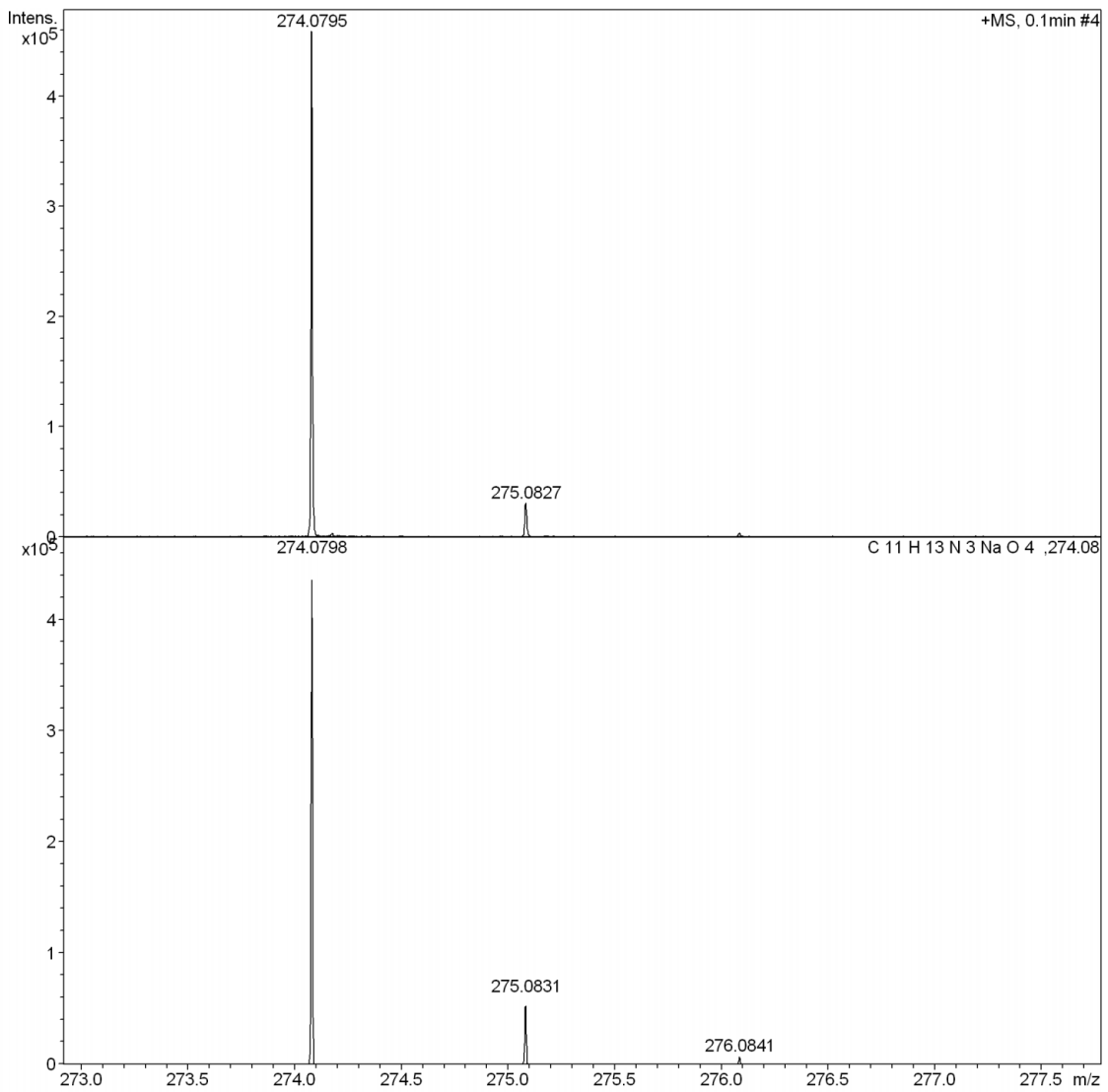
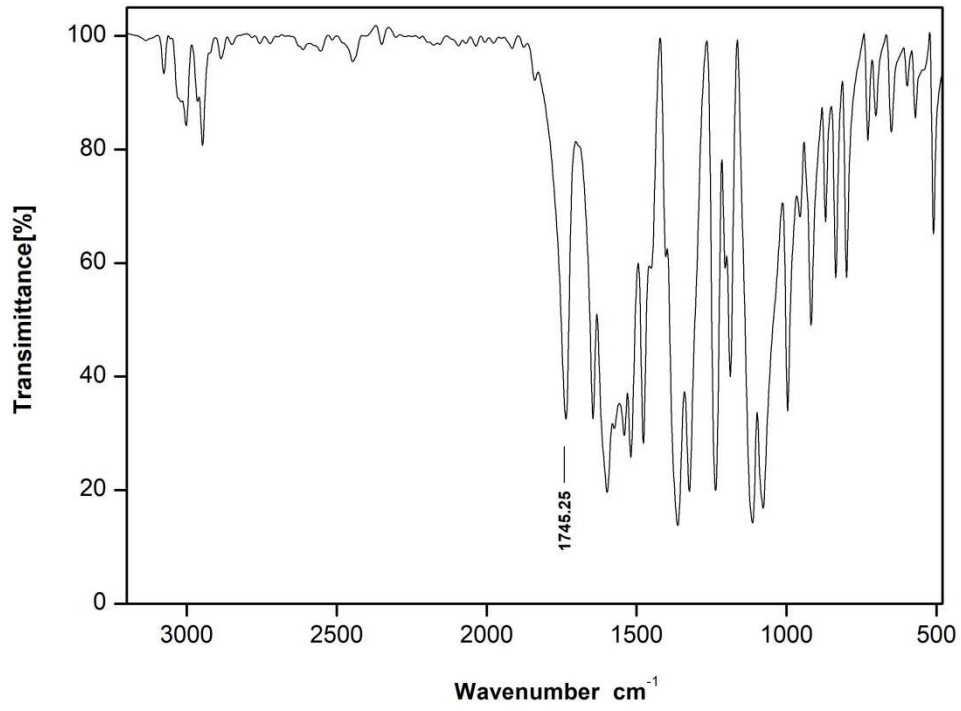


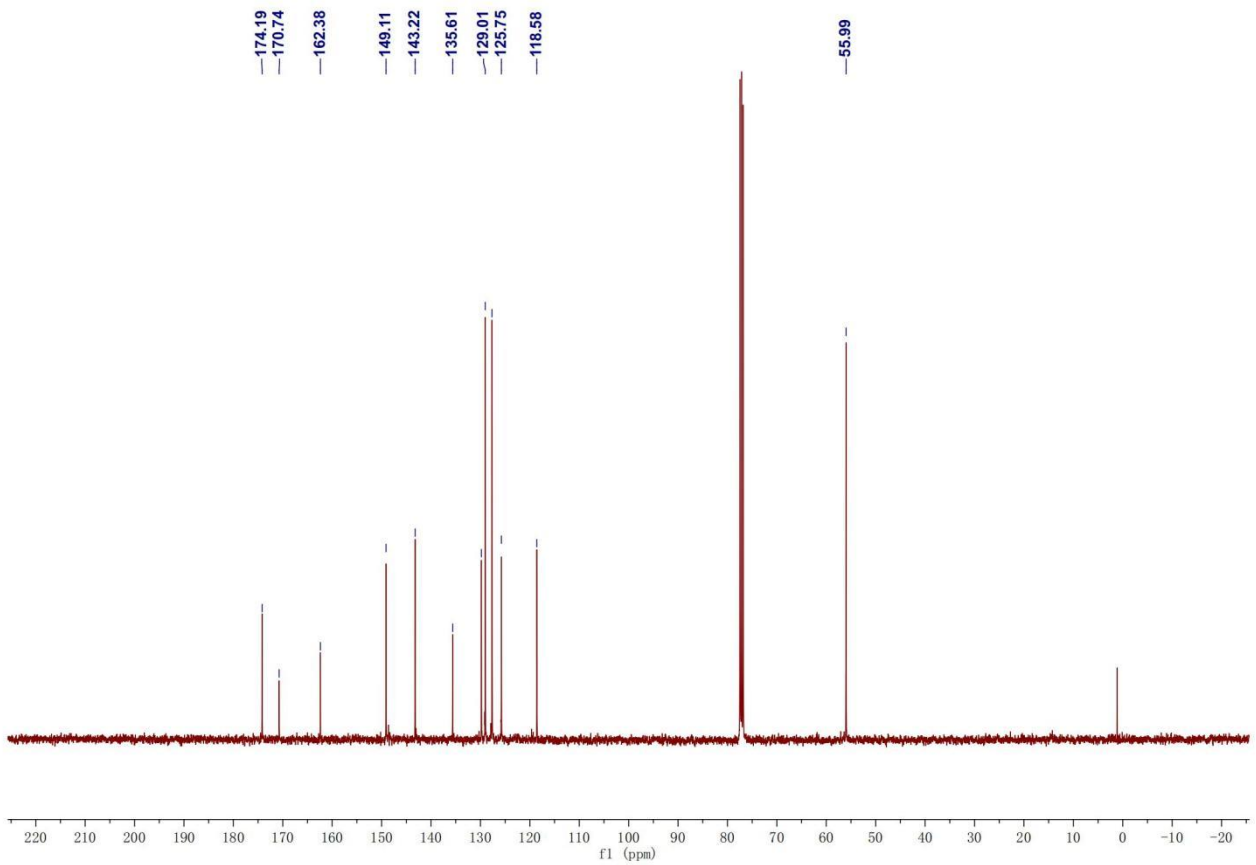
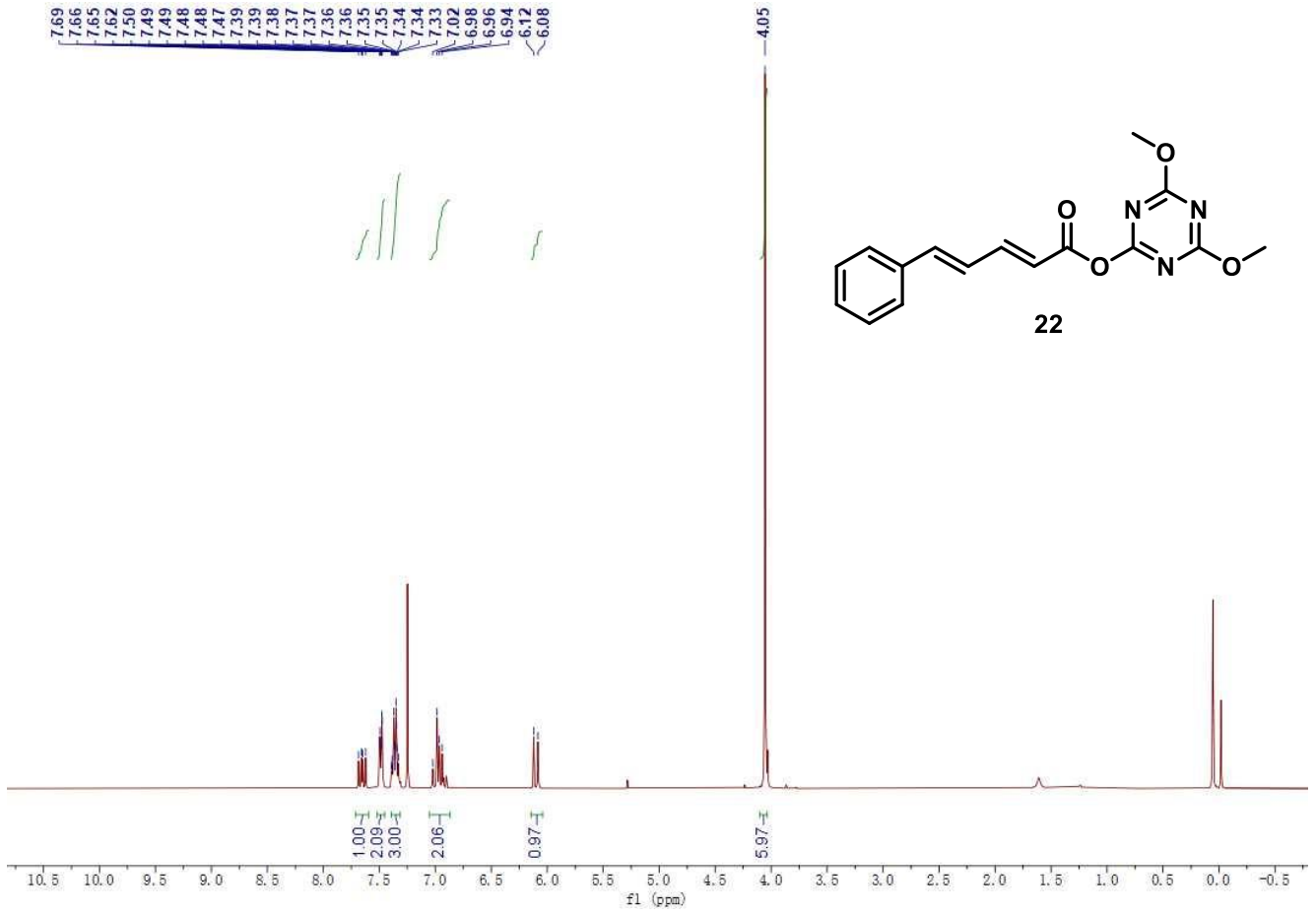


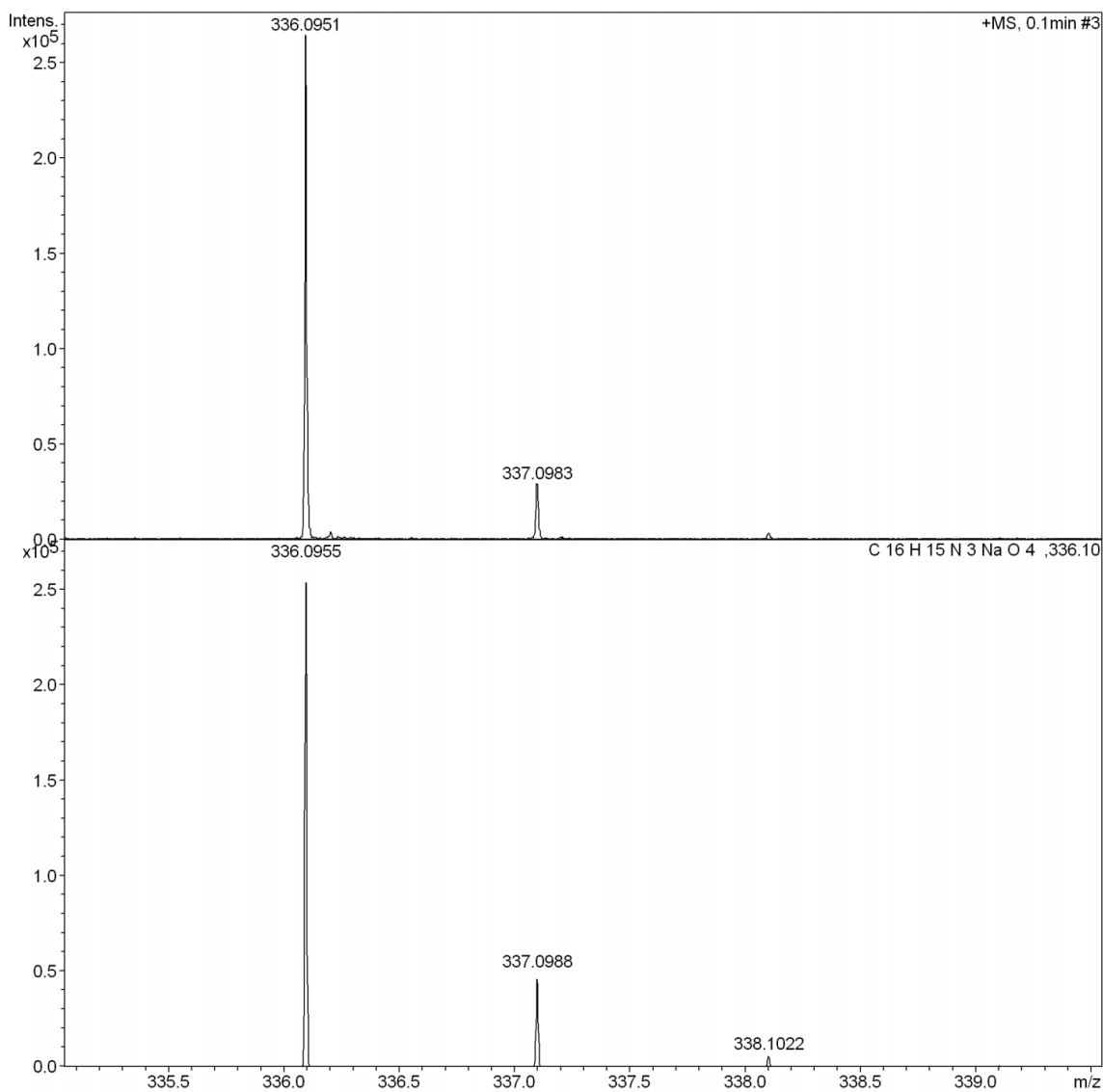
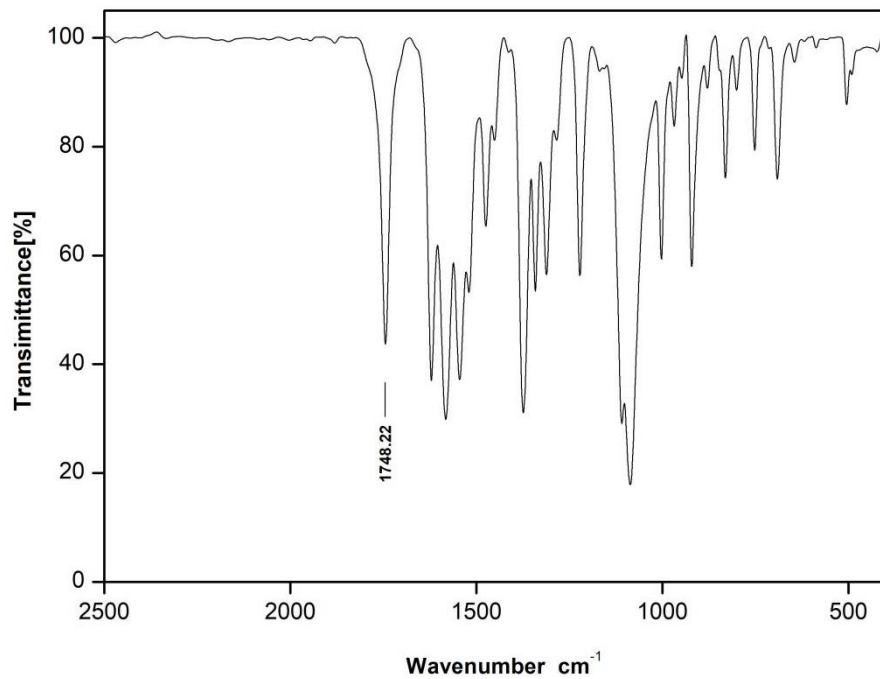


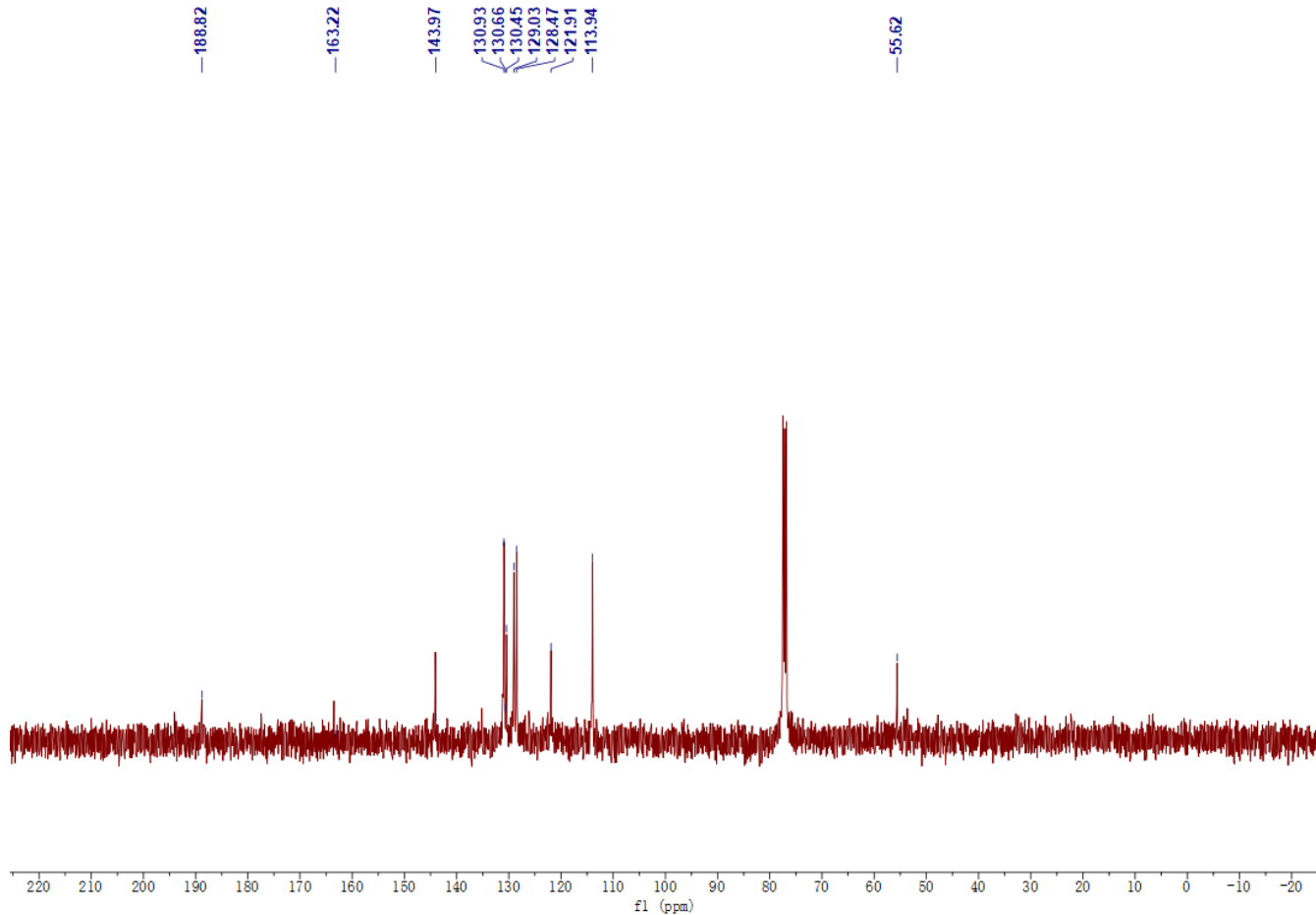
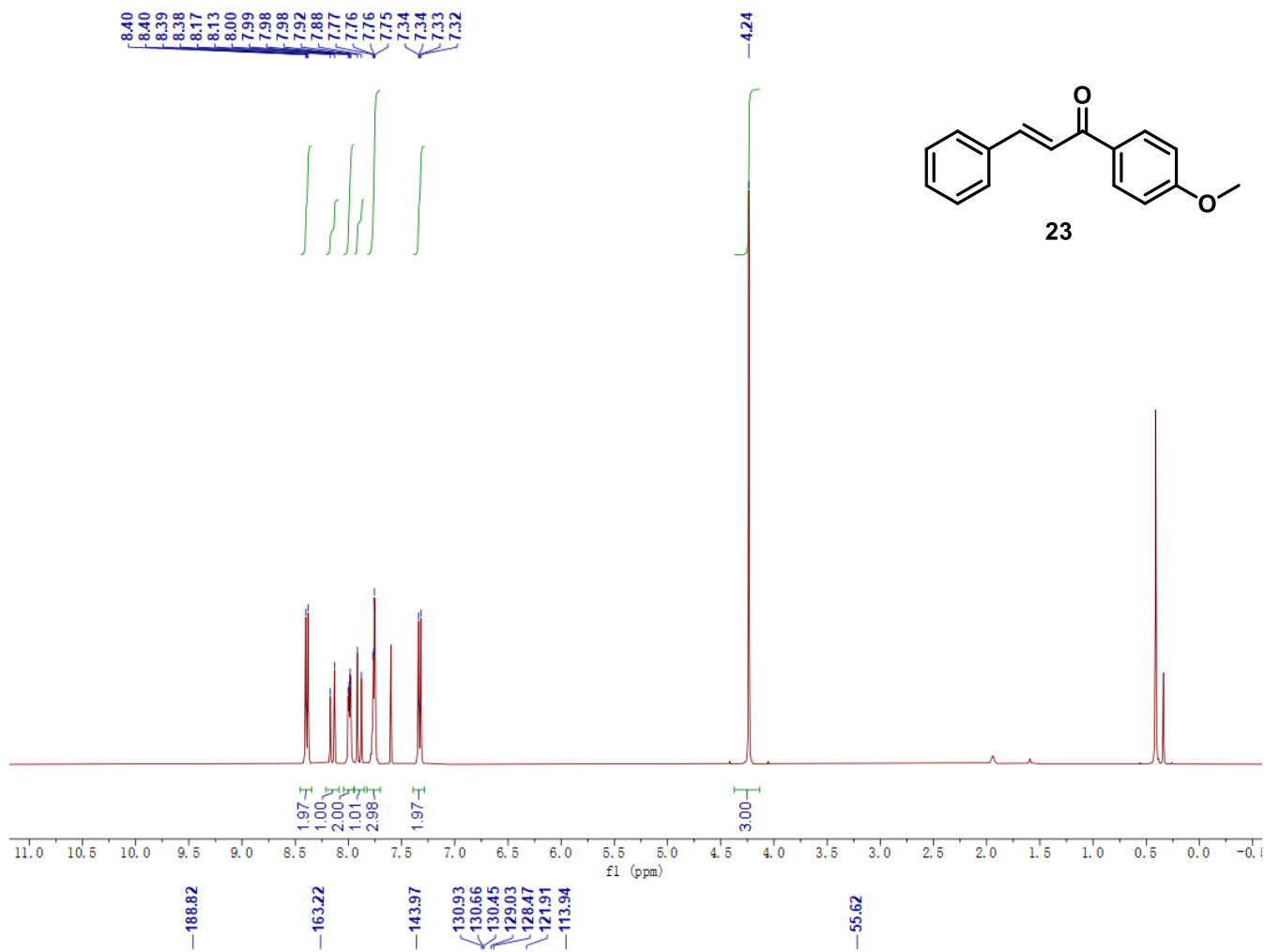


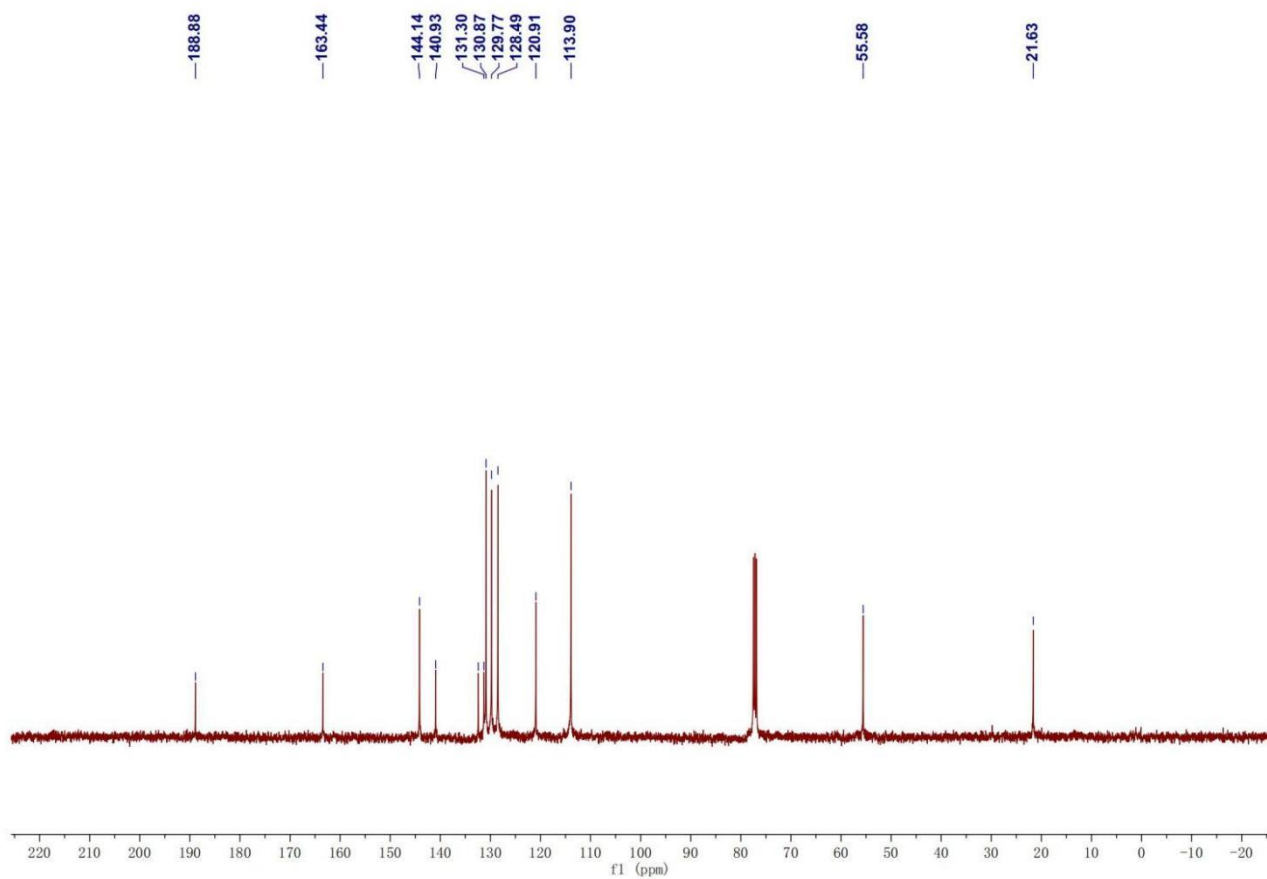
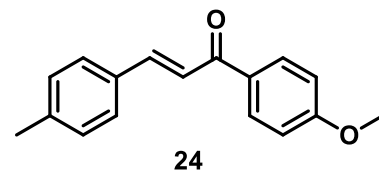
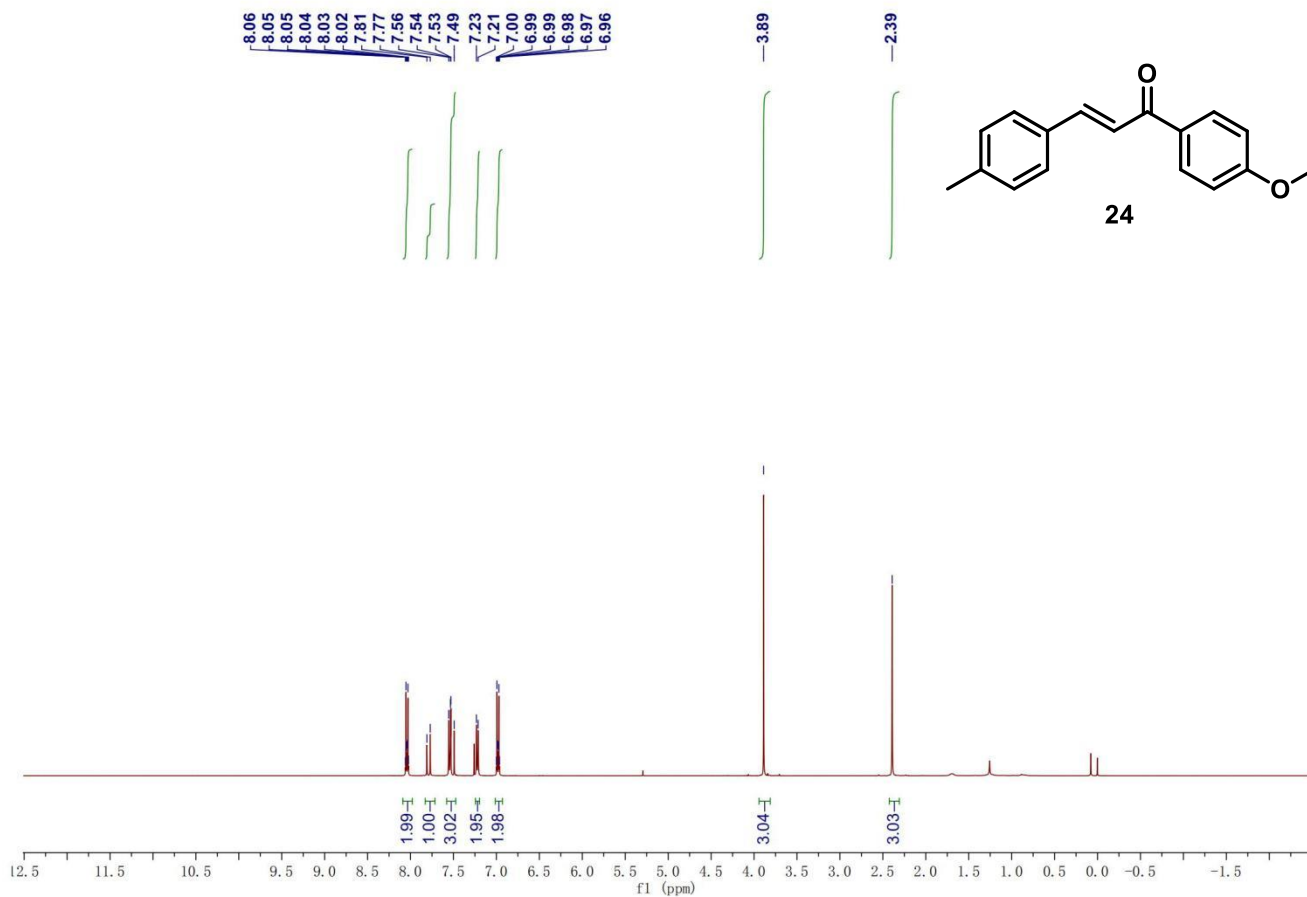


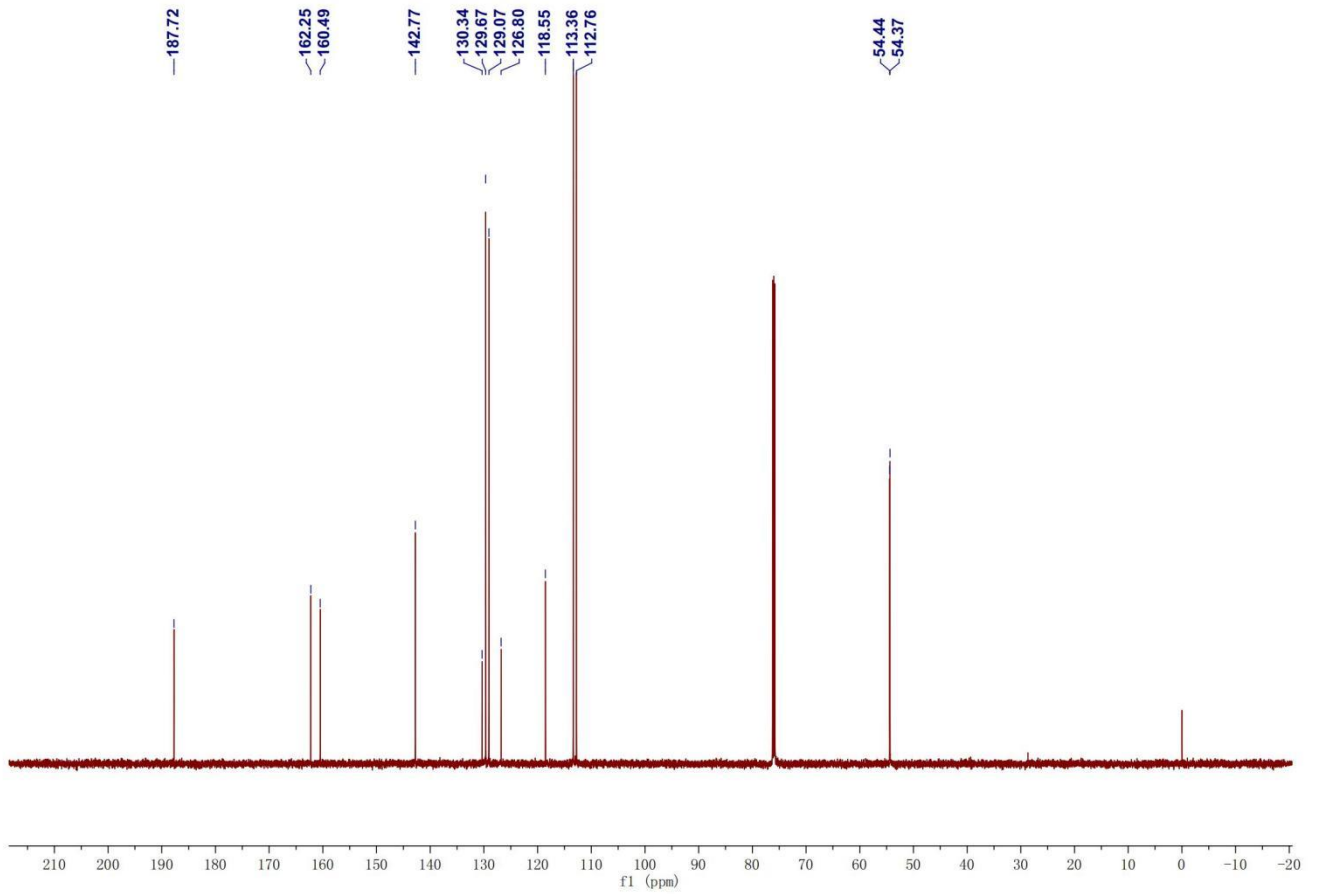
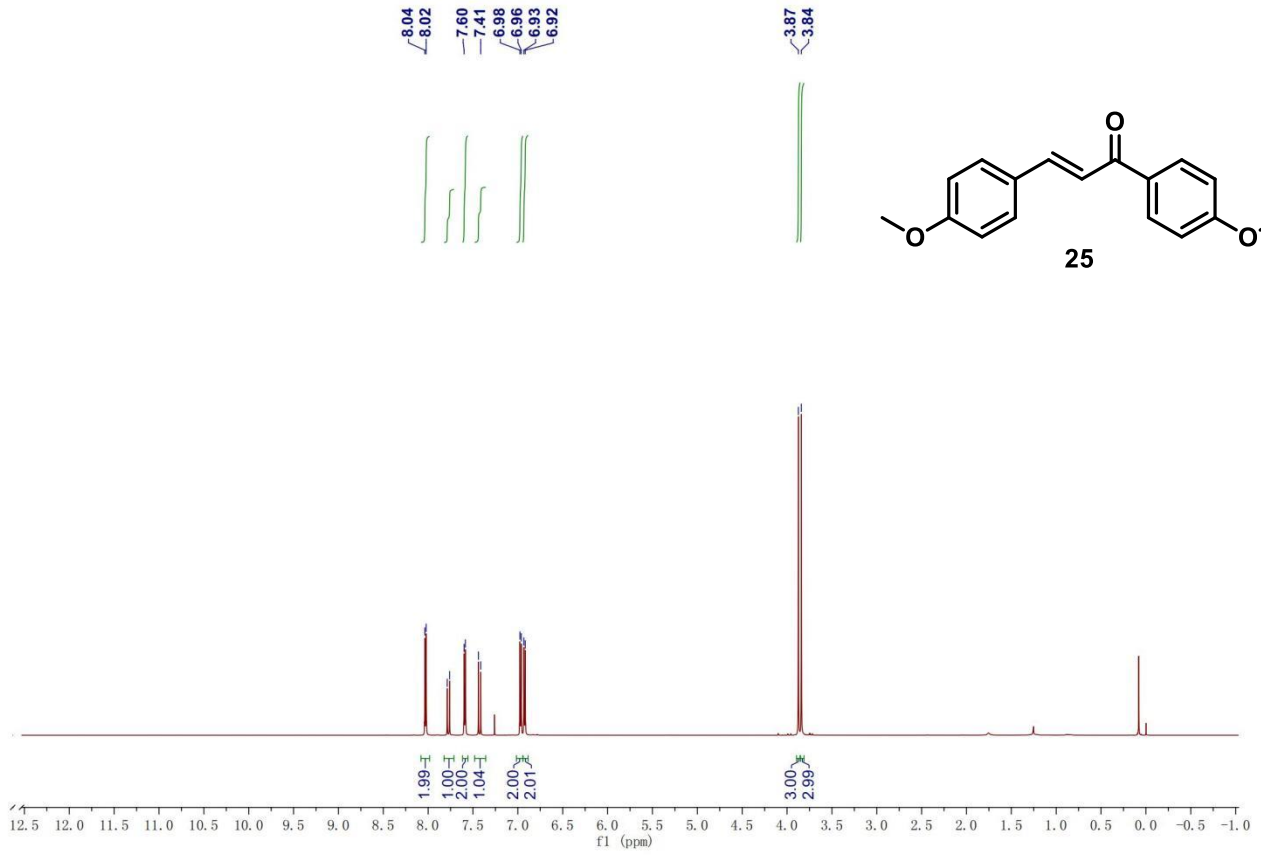


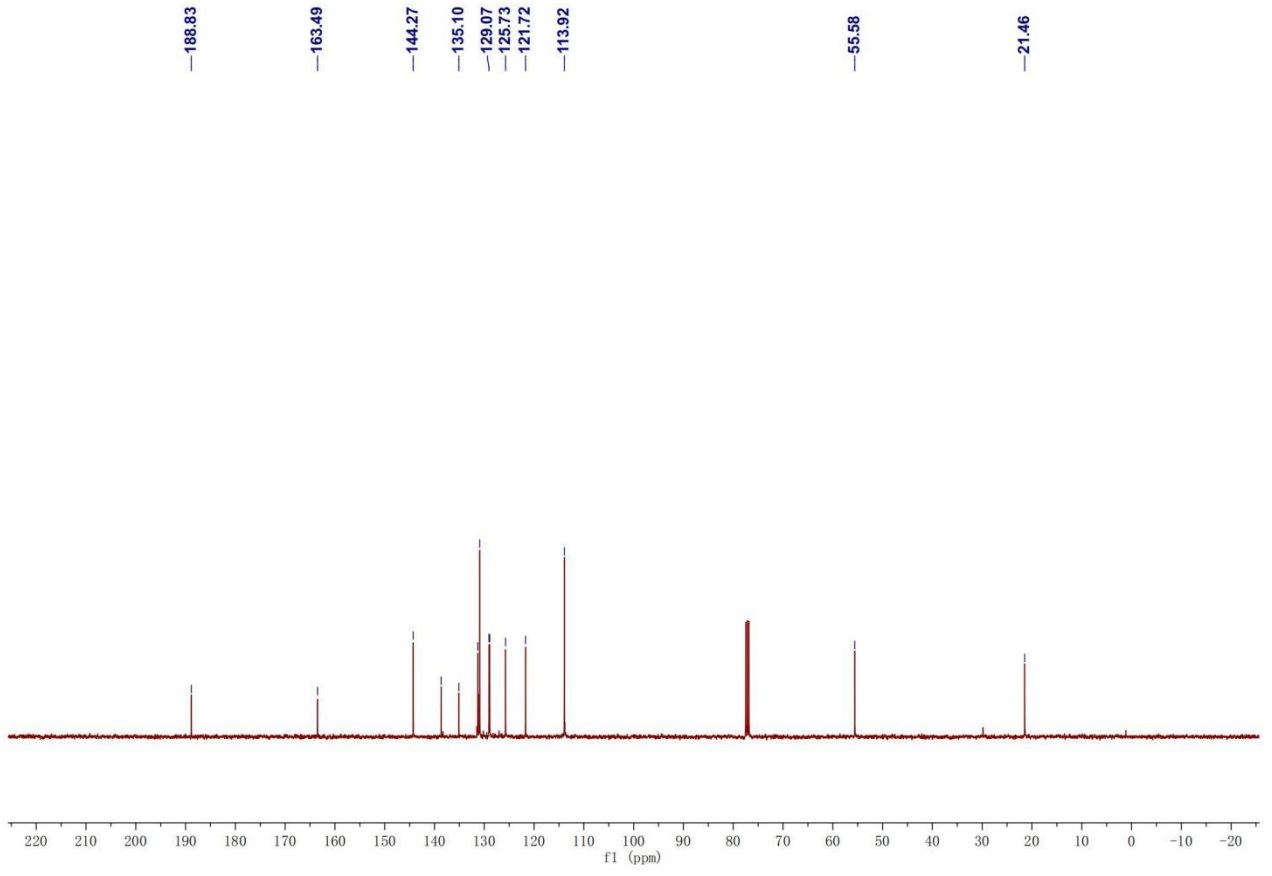
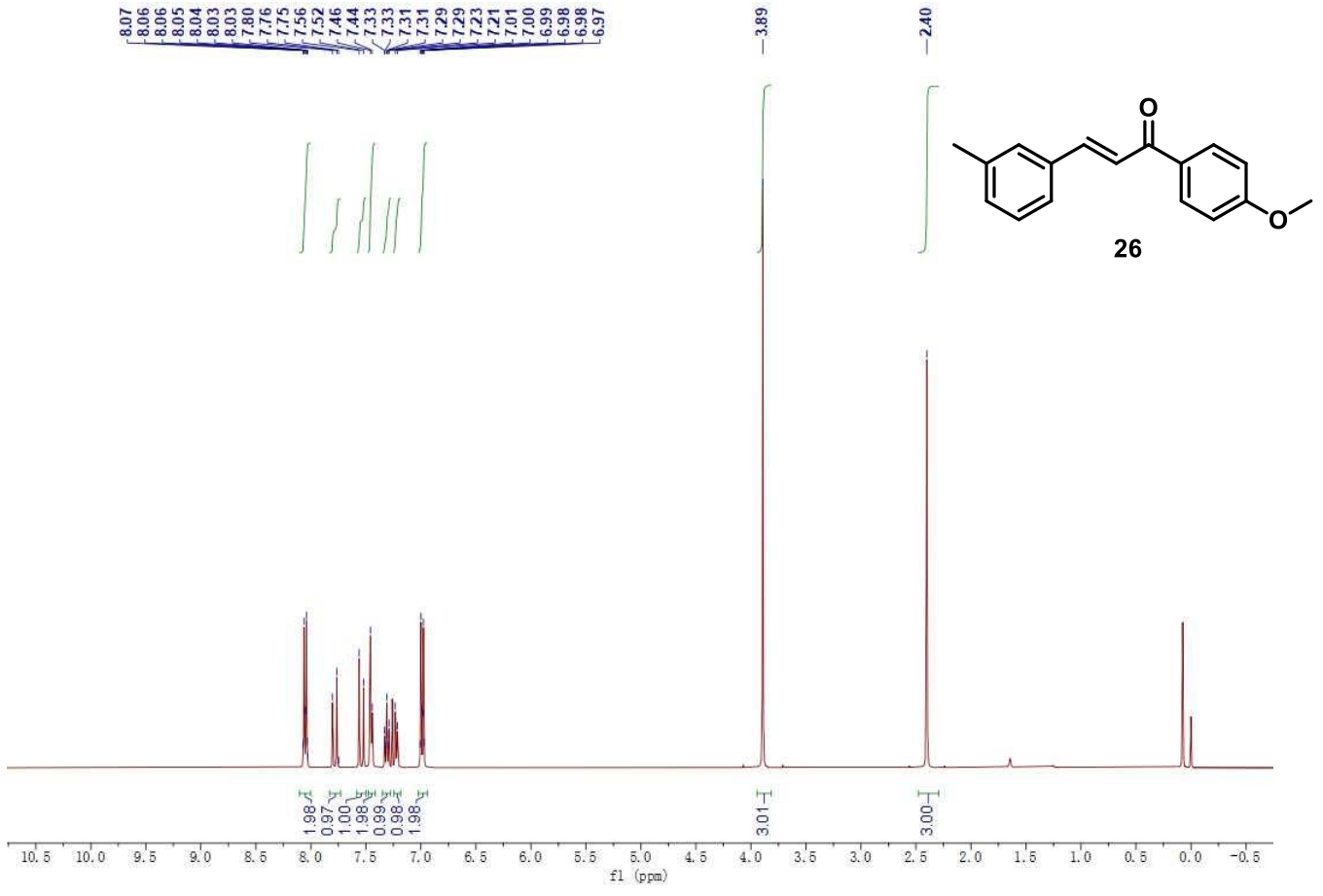






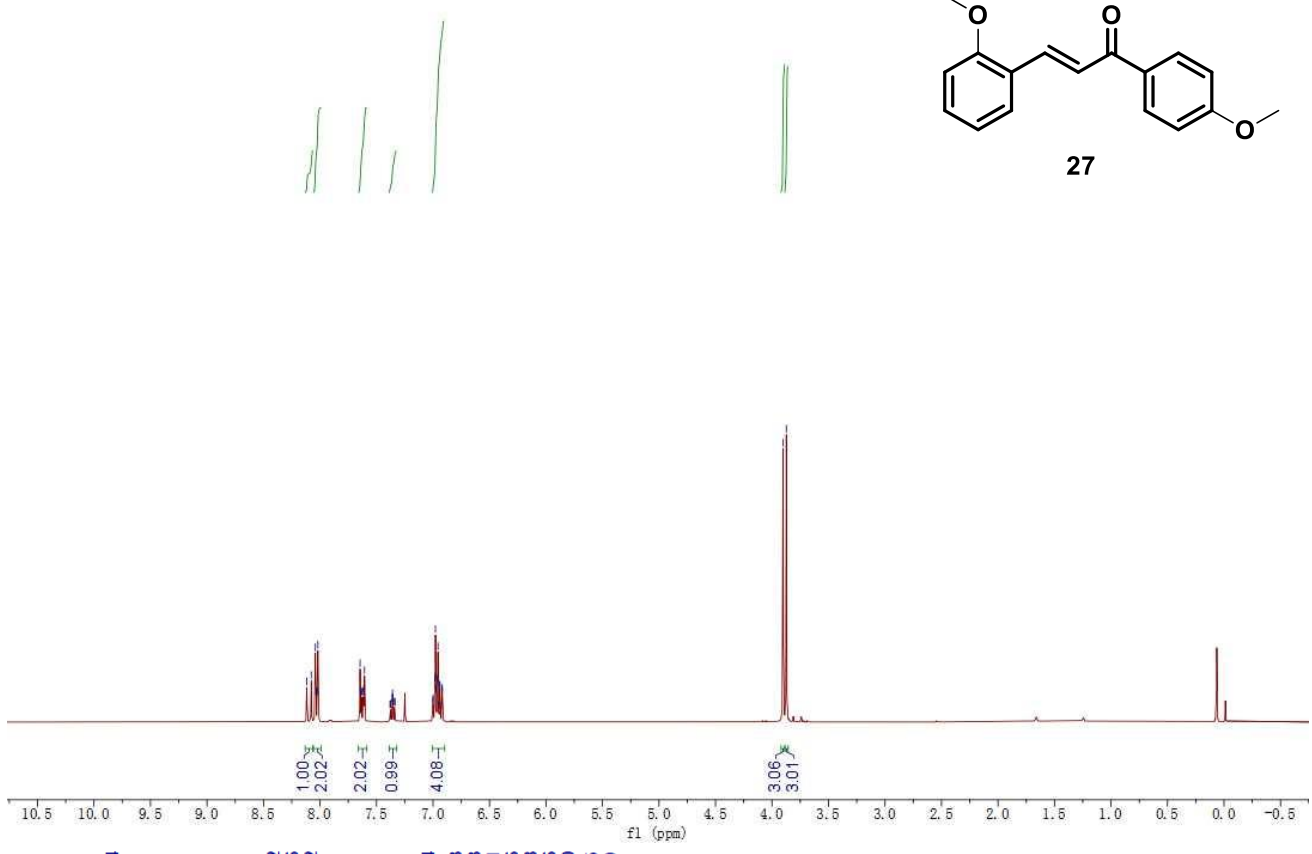
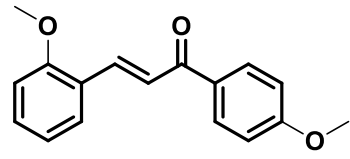






8.12
8.08
8.04
8.02
8.02
7.85
7.64
7.63
7.62
7.61
7.61
7.38
7.38
7.36
7.36
7.34
7.34
7.00
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6.95
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6.92

3.90
3.87

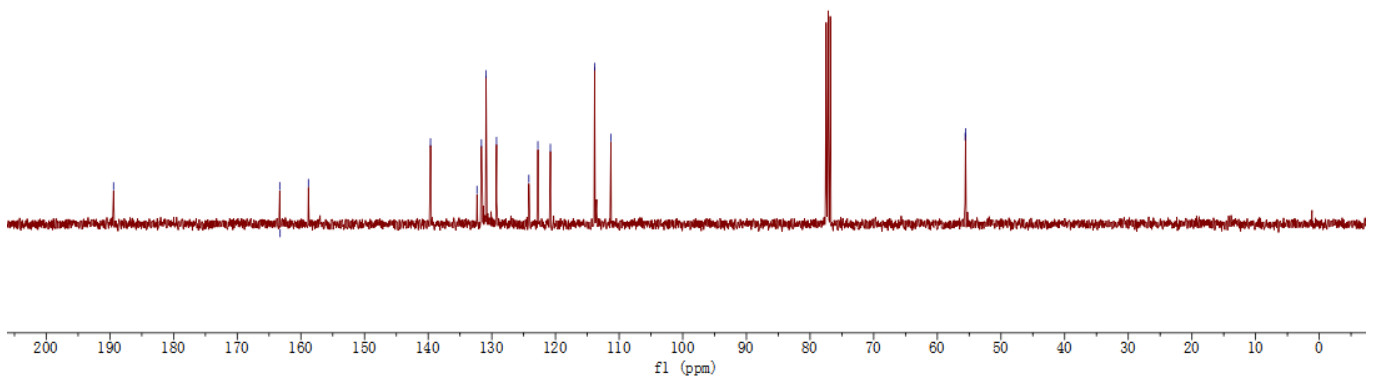


189.44

163.32
163.26
158.82

139.64
132.33
131.63
130.91
129.26
124.18
122.76
120.80
113.85
111.29

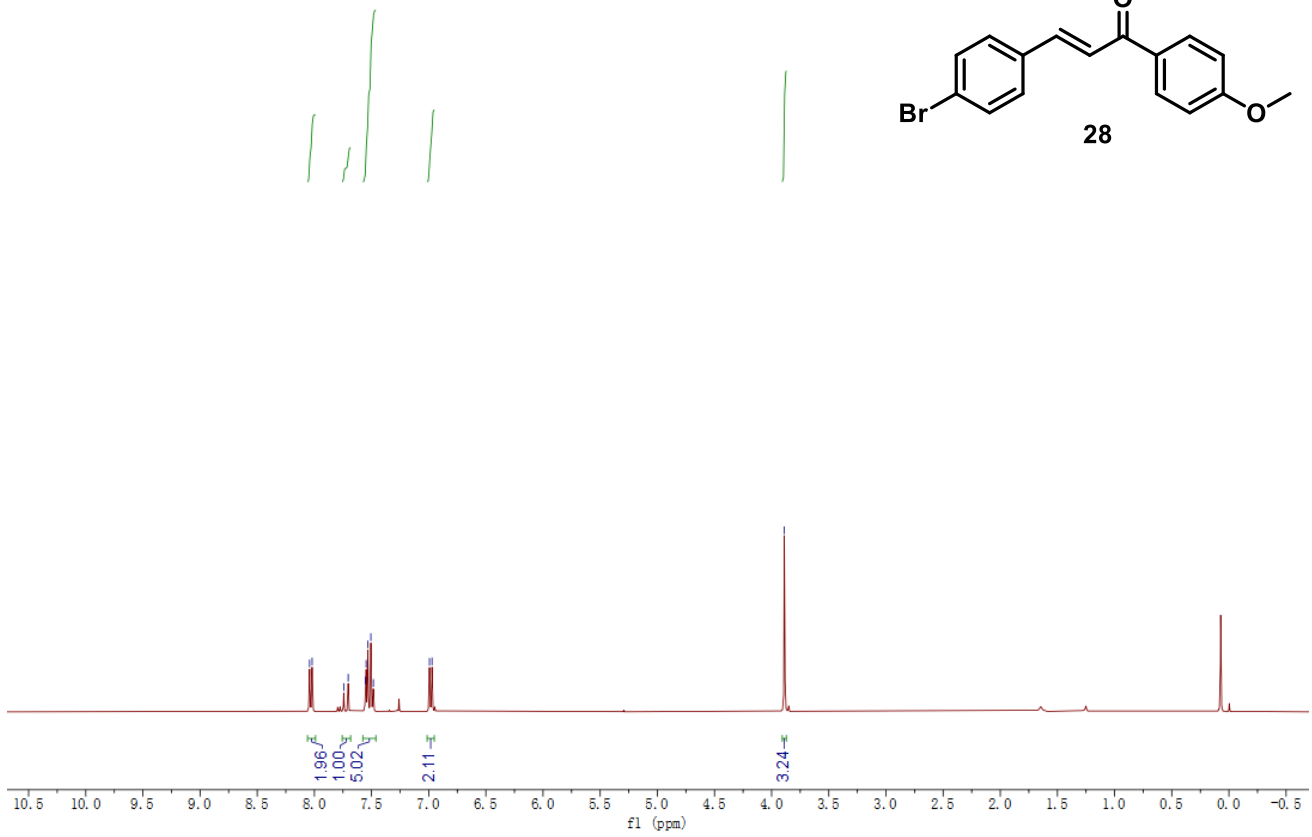
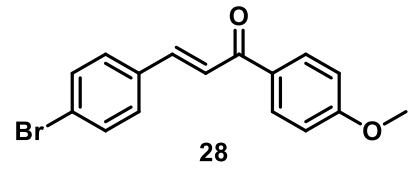
55.62
55.57



ldz062902
single_pulse

8.04
8.02
7.74
7.70
7.55
7.53
7.51
7.48
6.99
6.97

3.89



ldz062902
single pulse decoupled NOE

188.19

163.65

142.61

134.10

132.26

130.94

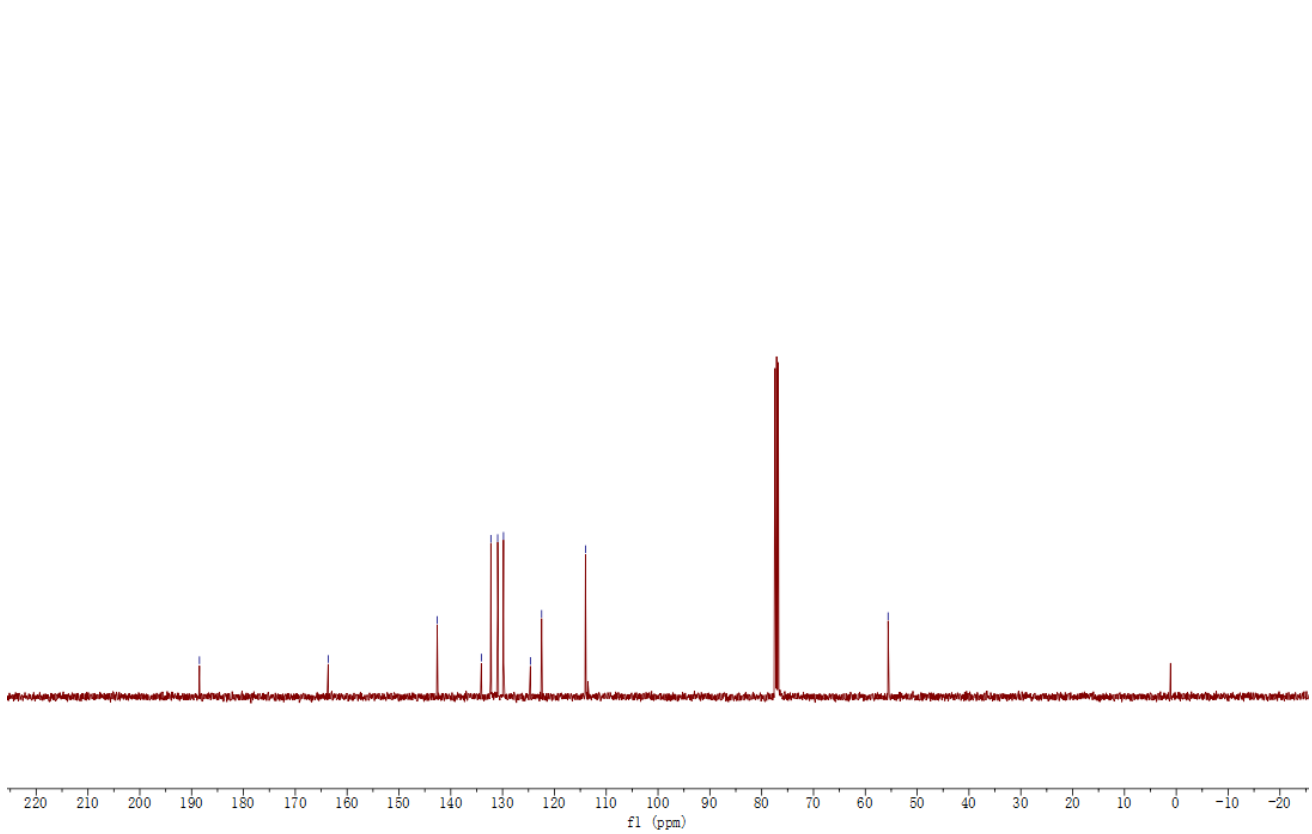
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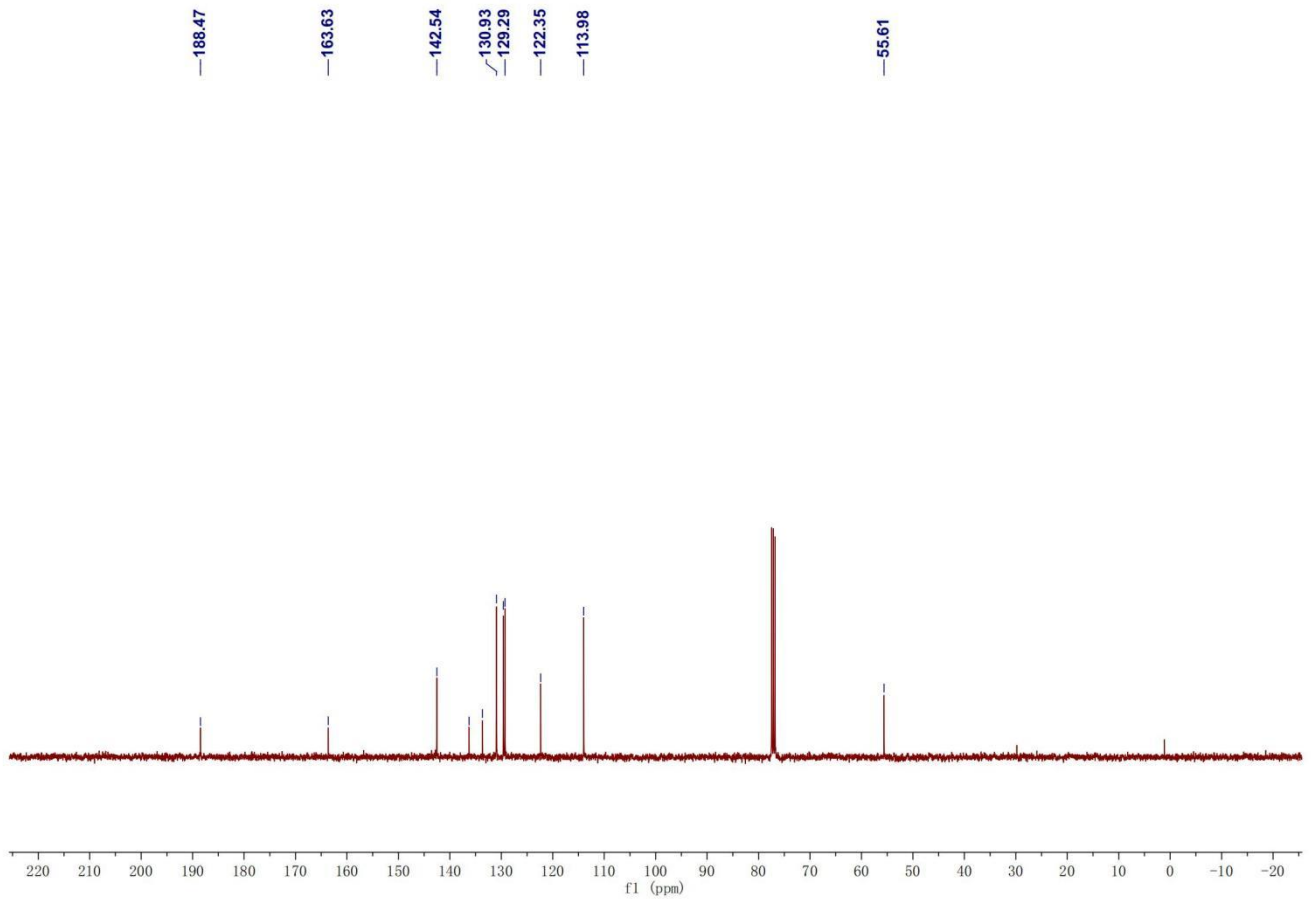
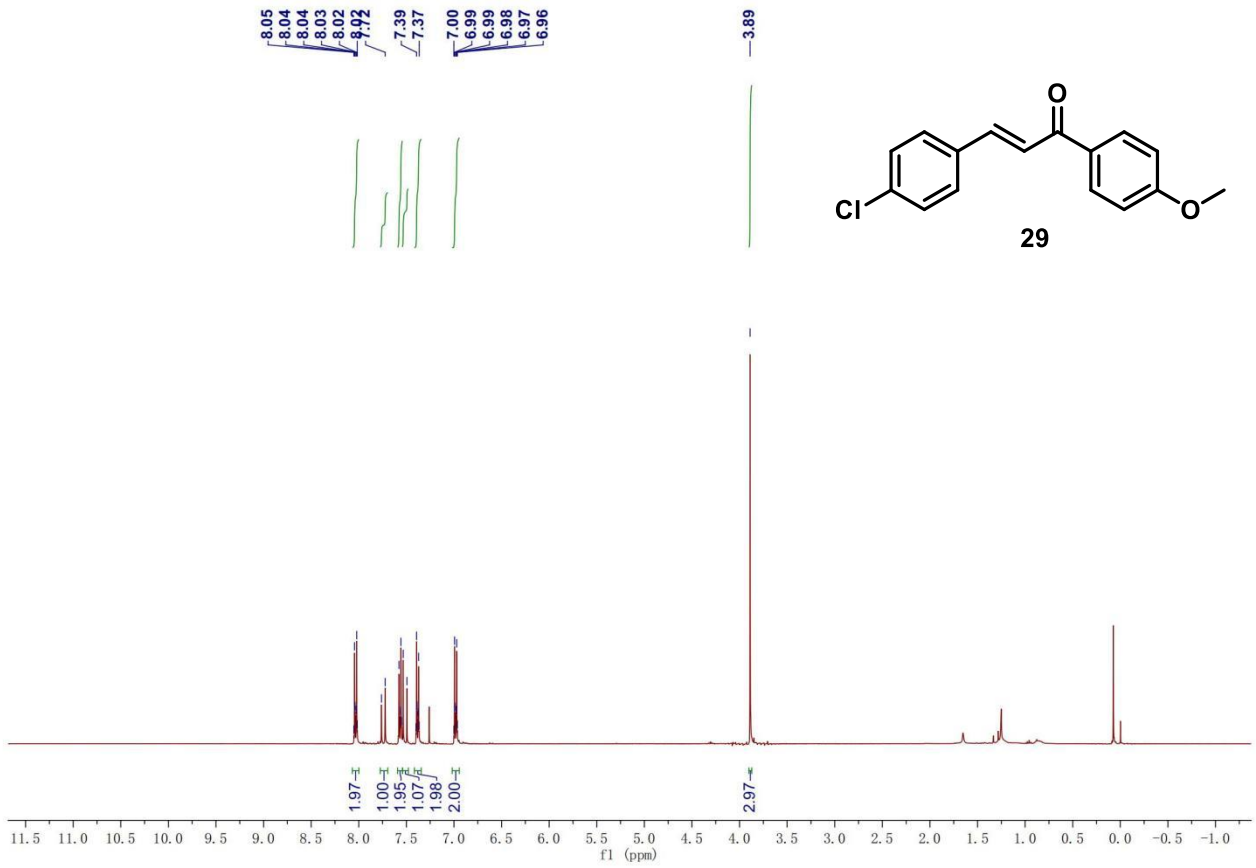
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122.46

114.00

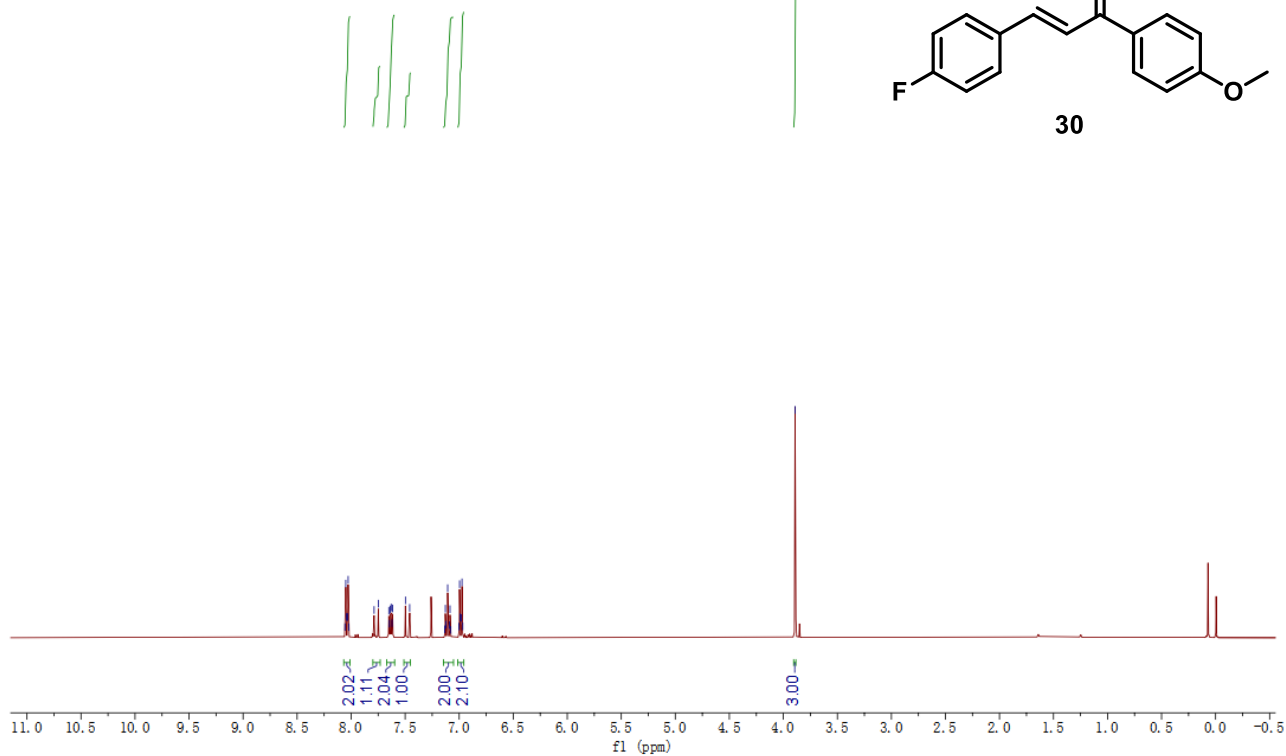
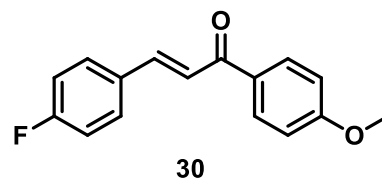
55.61





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8.03
8.02
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7.62
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7.46
7.14
7.13
7.12
7.11
7.09
7.08
7.08
7.00
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6.98
6.97
6.97

3.89



188.58

163.56

142.77

130.91

130.38

130.30

121.59

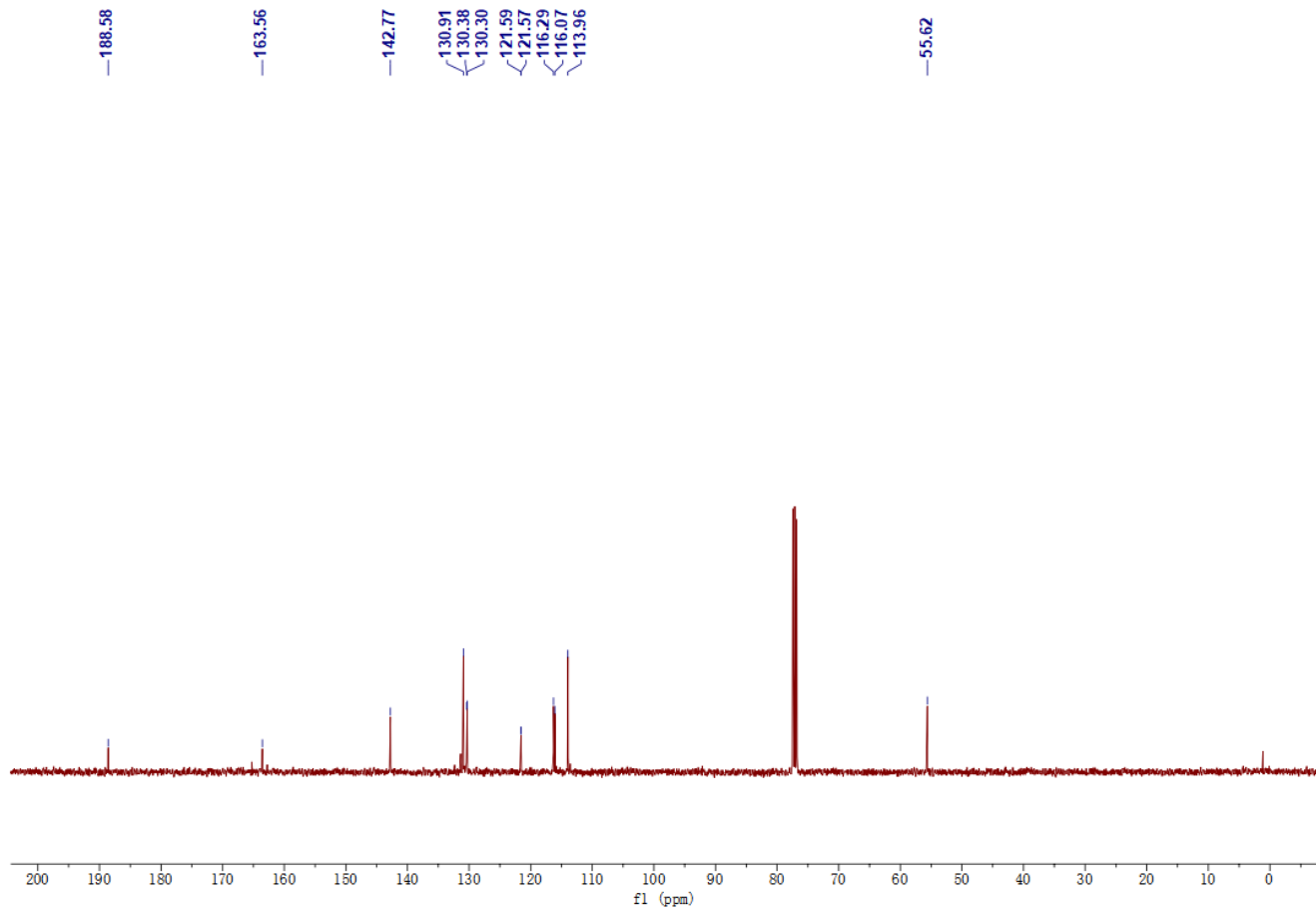
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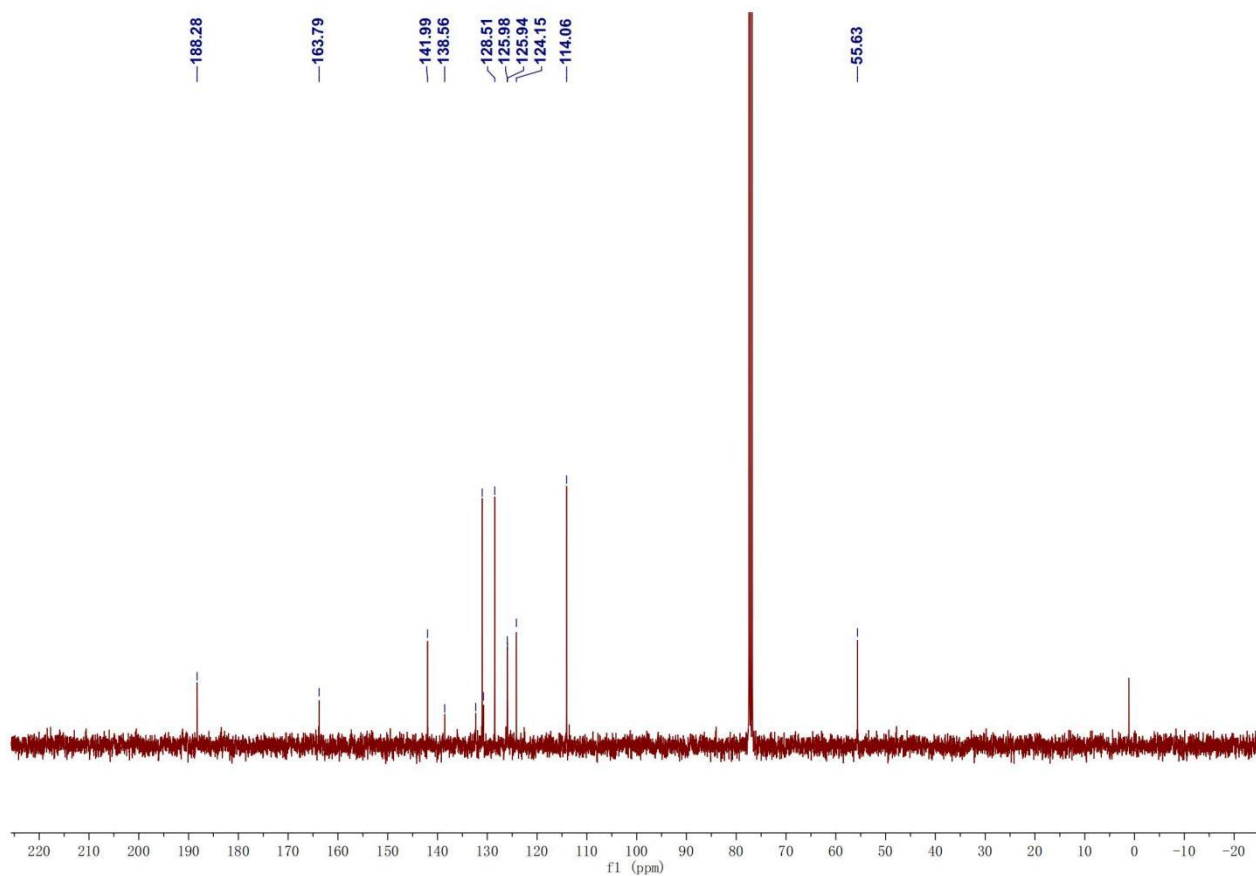
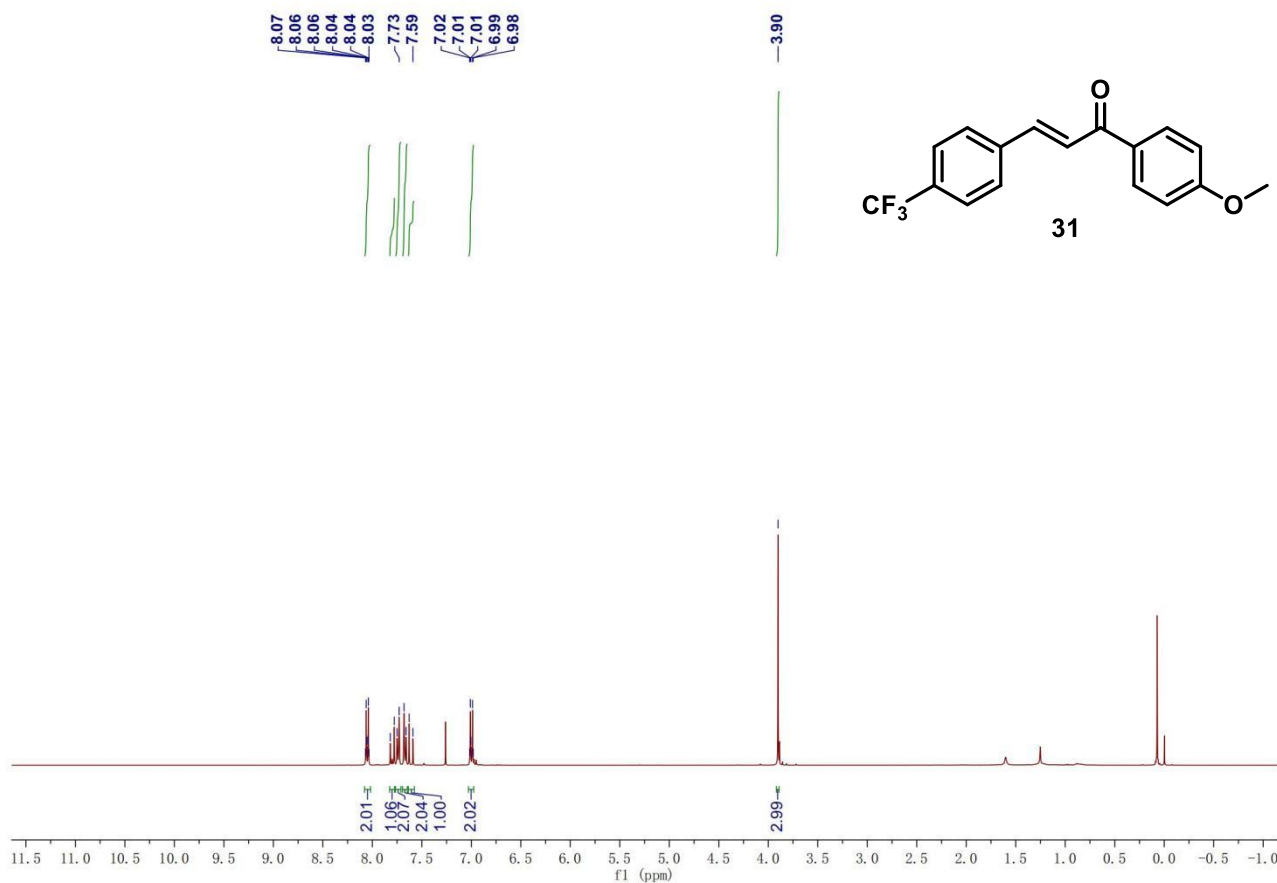
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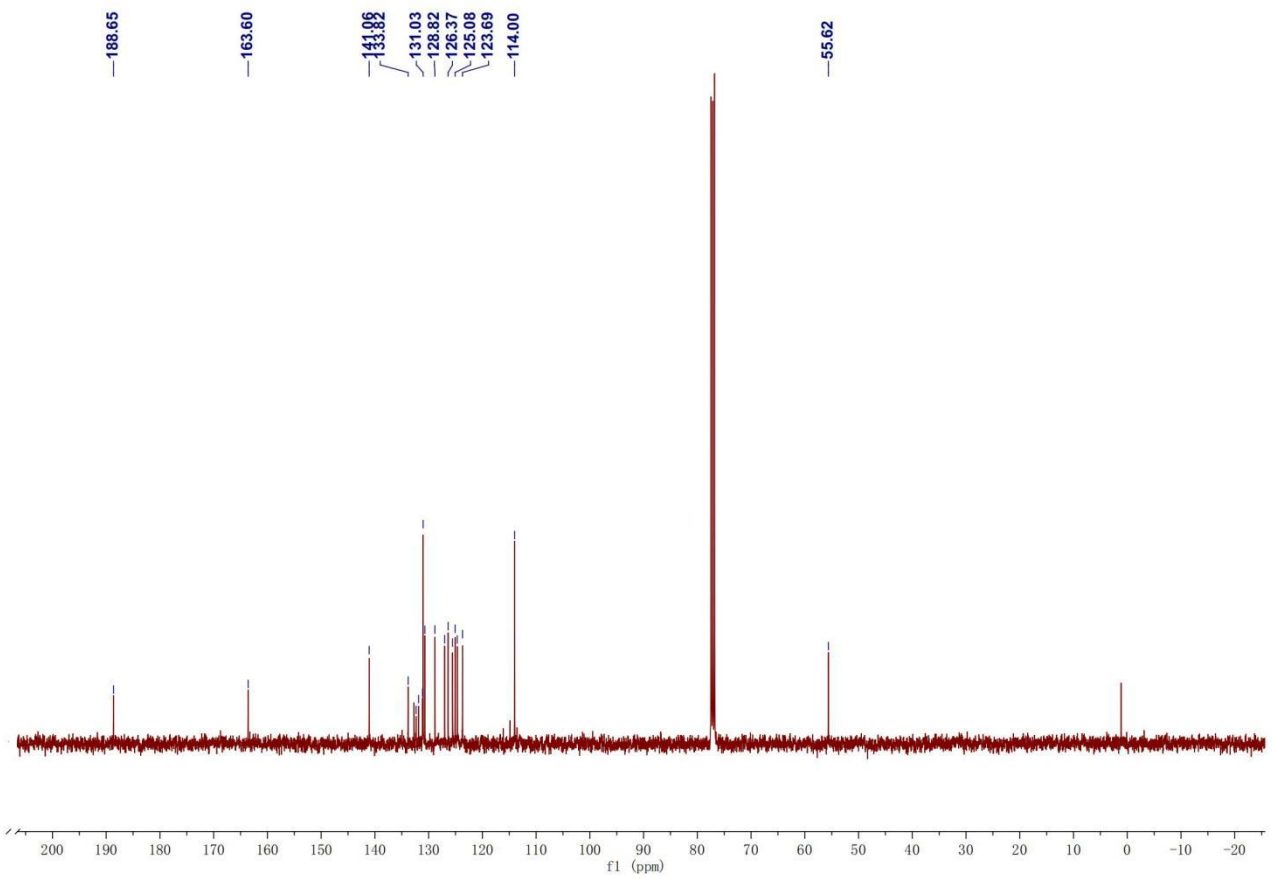
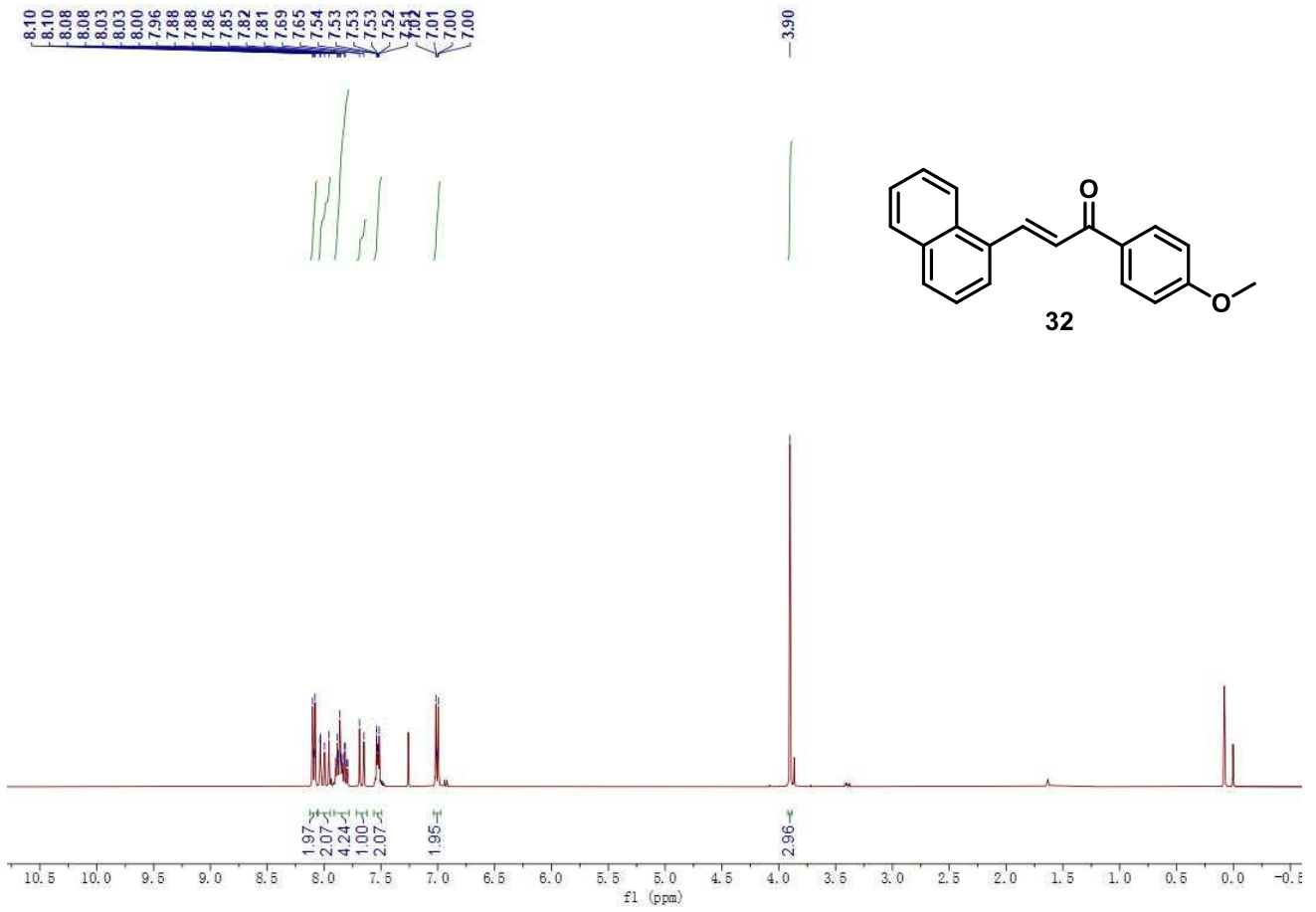
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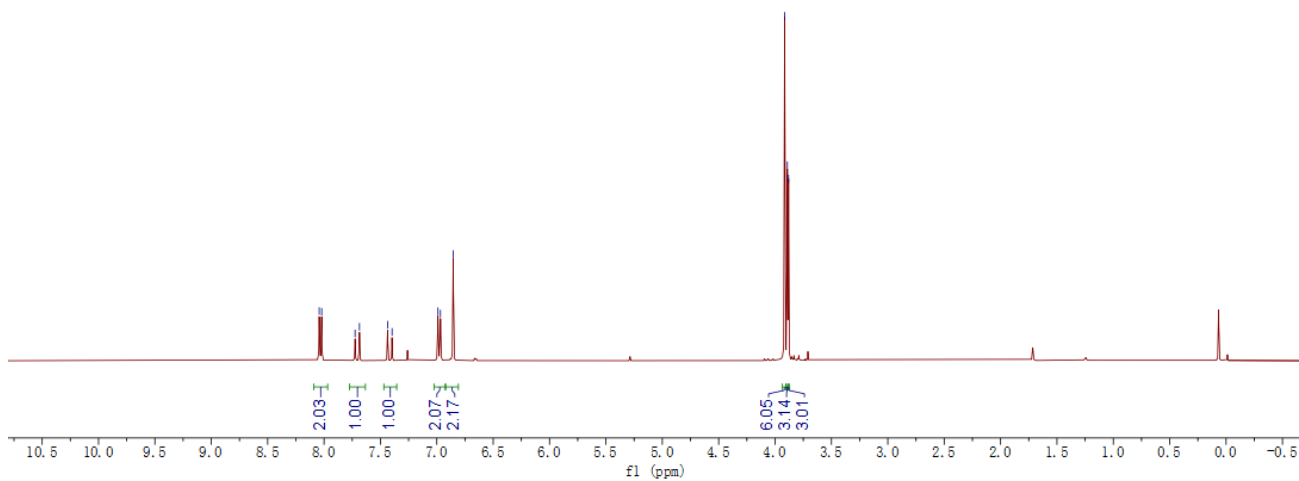
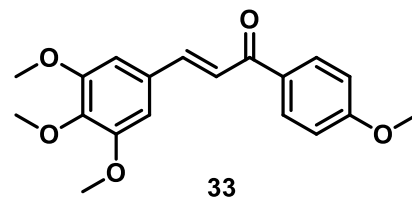
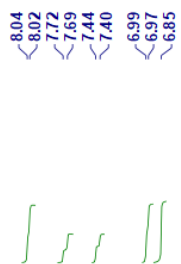
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55.62









188.77

163.48

153.53

144.24

140.27

131.18

130.90

130.66

121.28

113.92

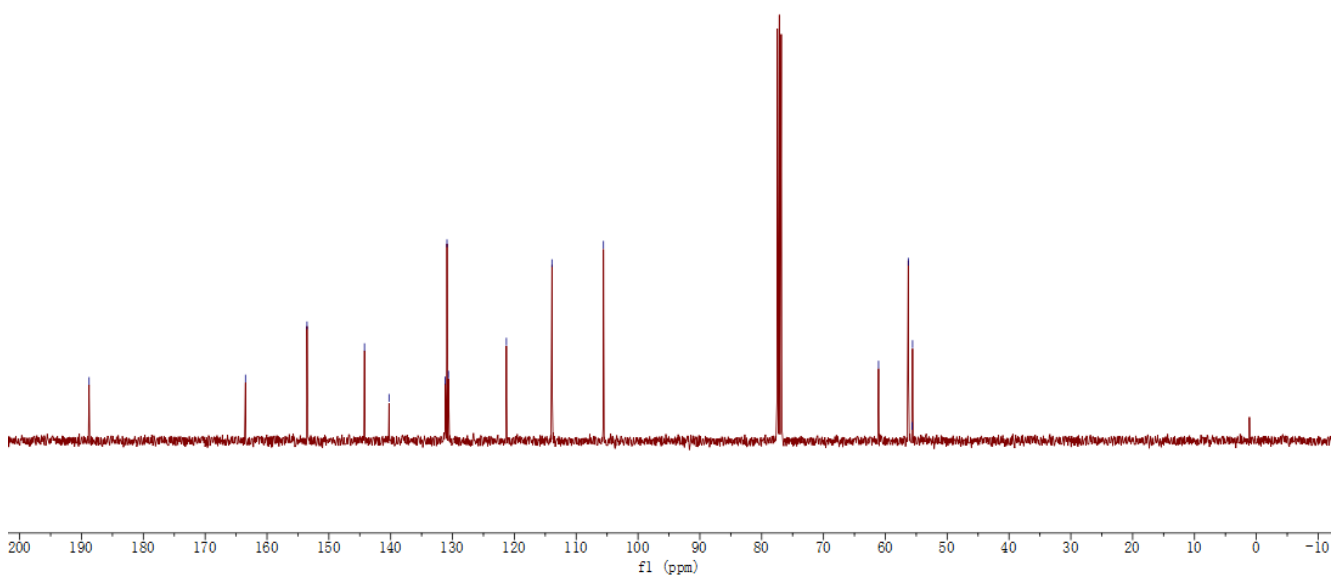
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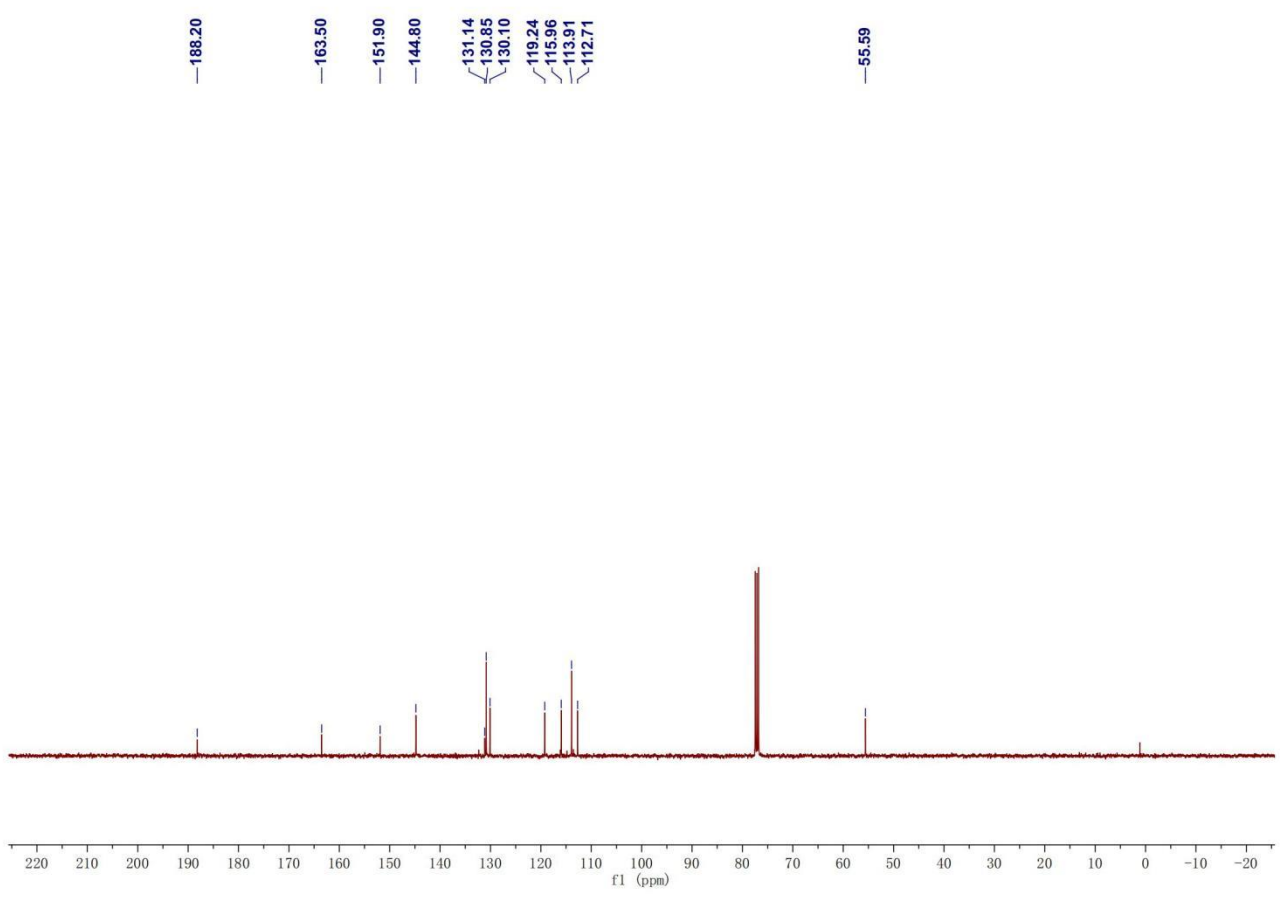
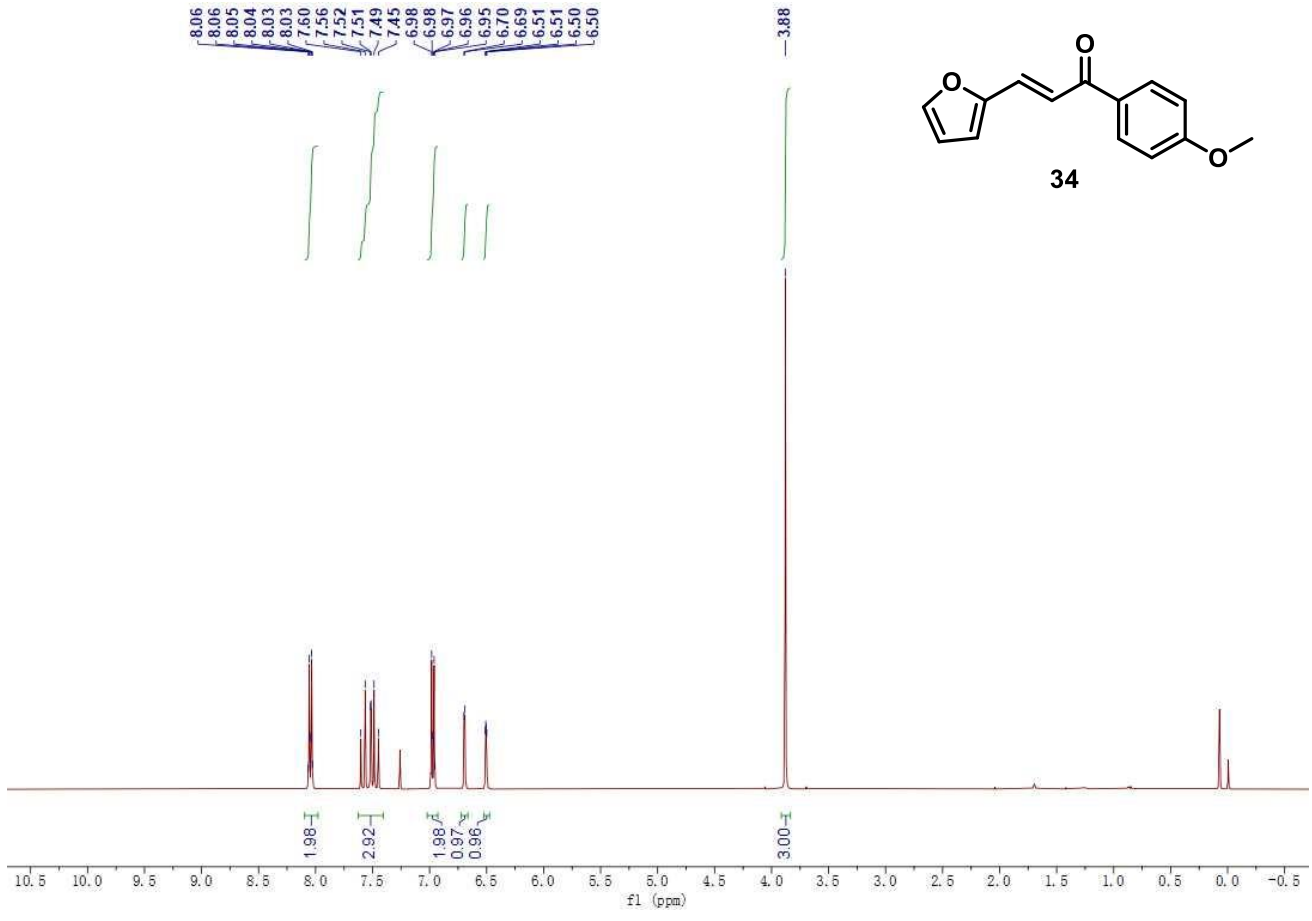
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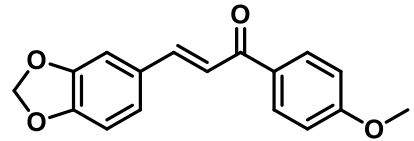
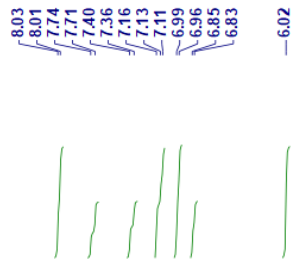
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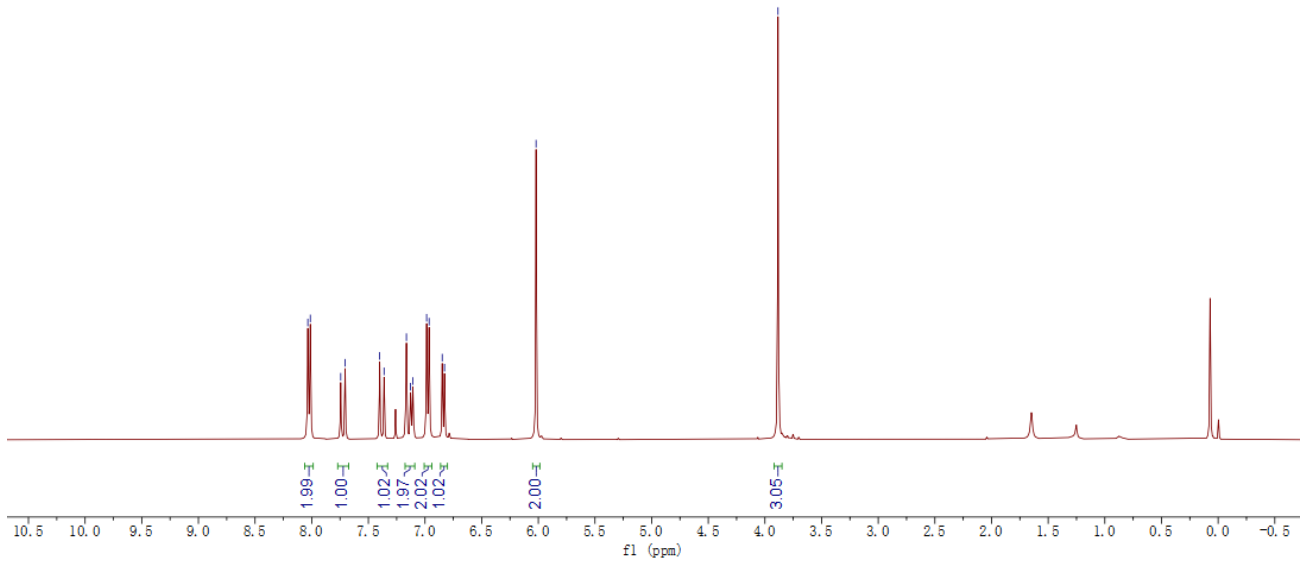




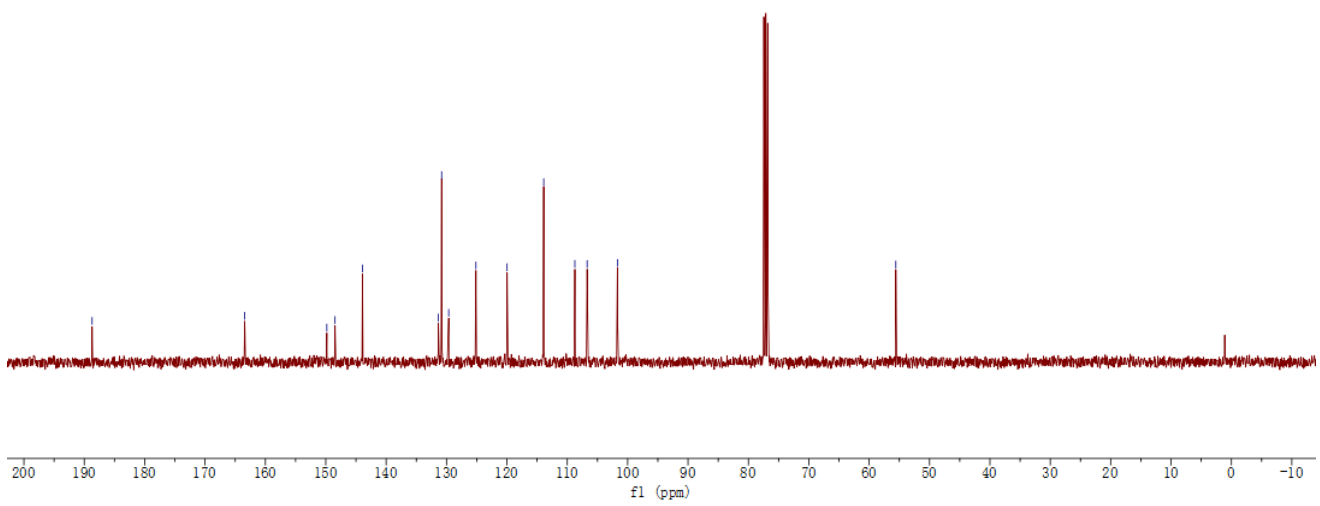
ldz062901
single_pulse

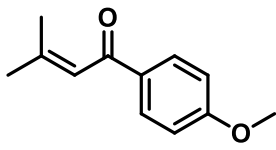


35



ldz062901
single_pulse decoupled gated



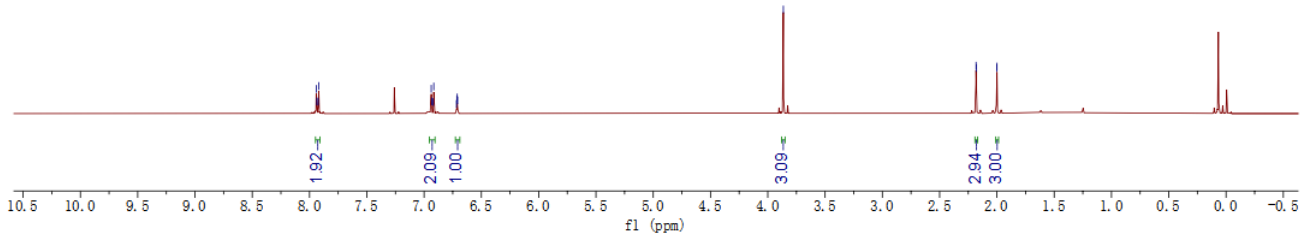


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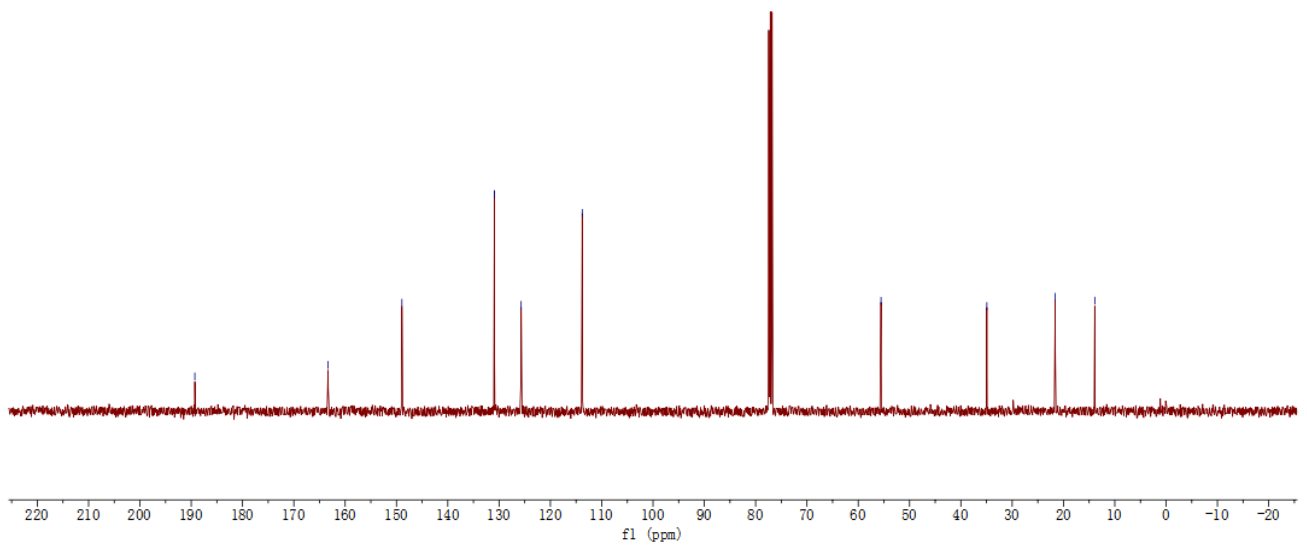
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6.71

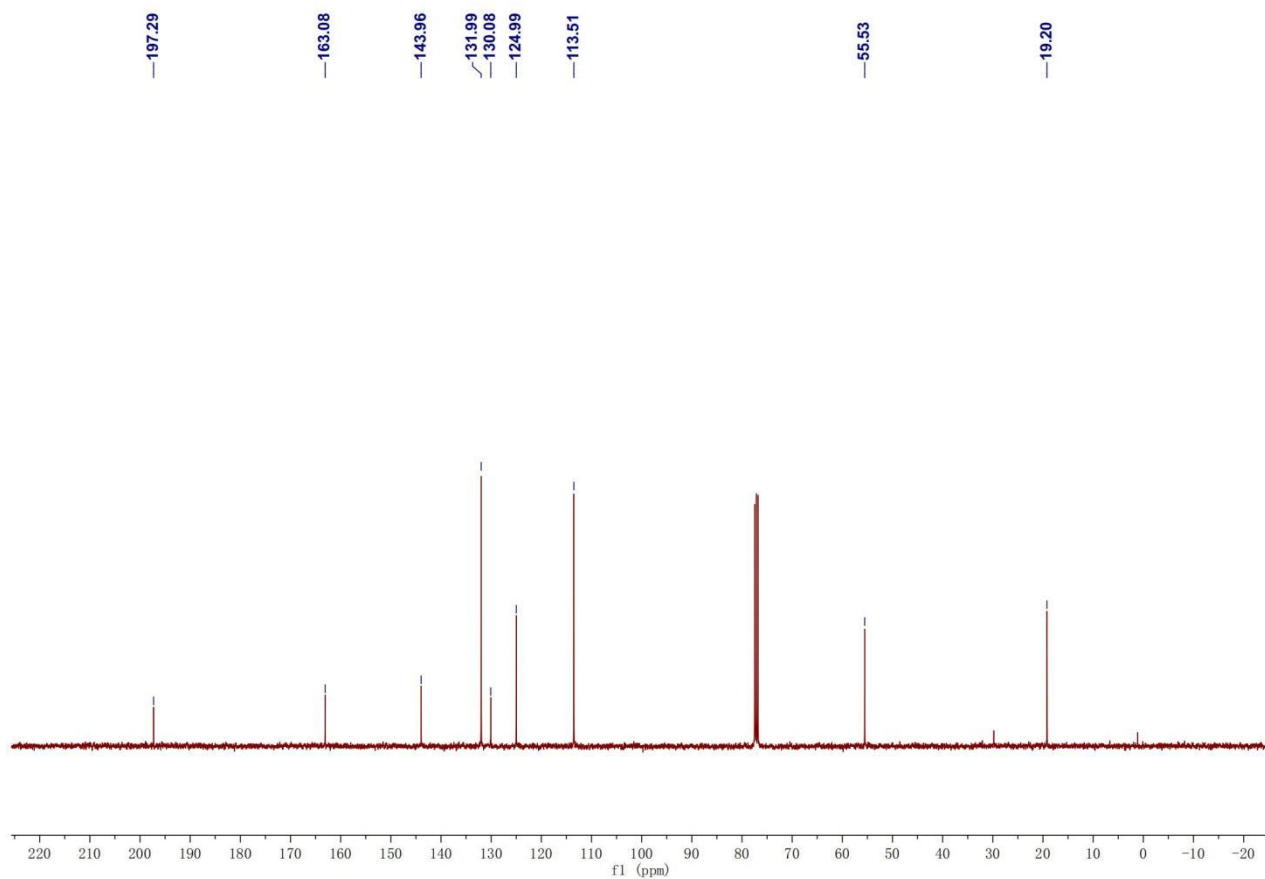
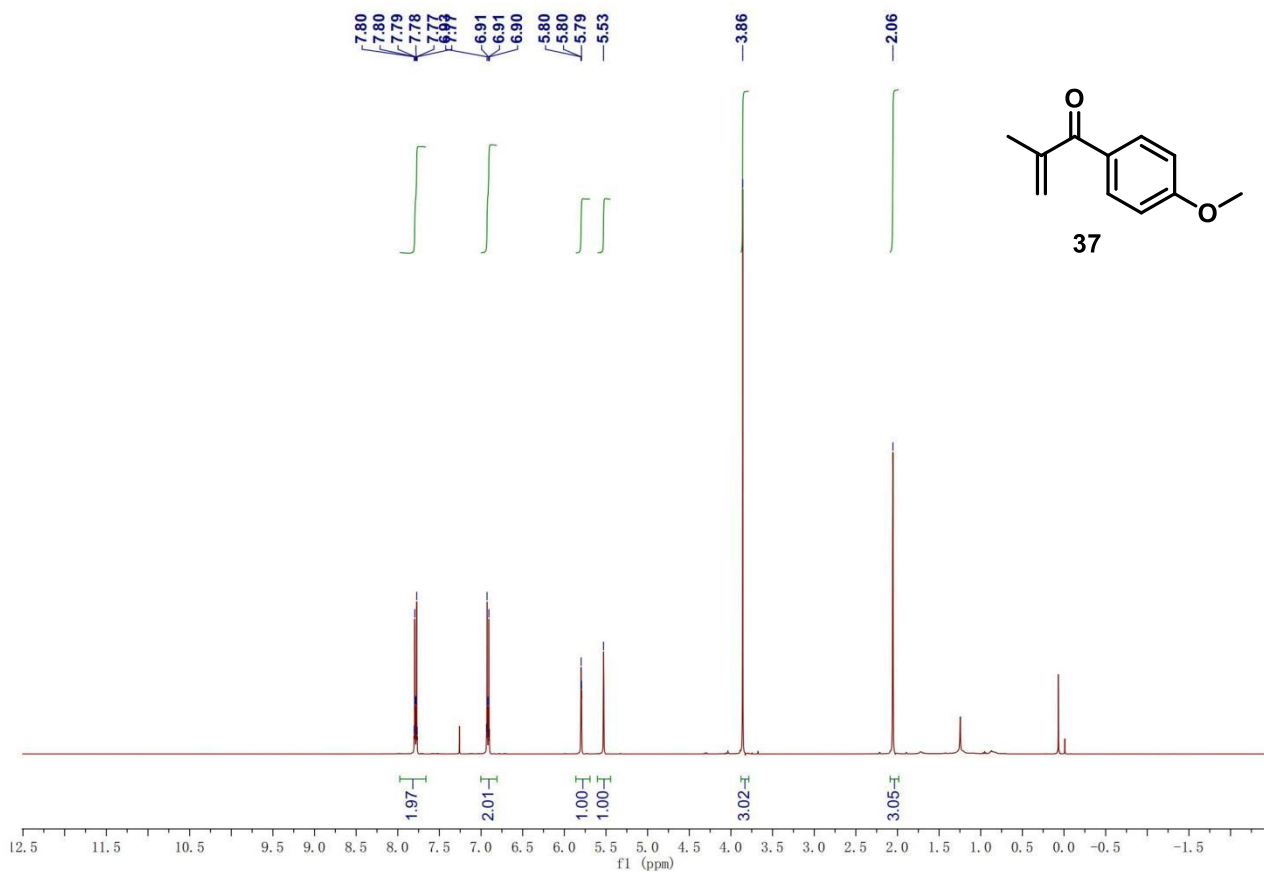
3.86

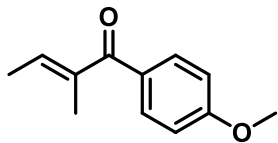
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2.18
2.00
2.00



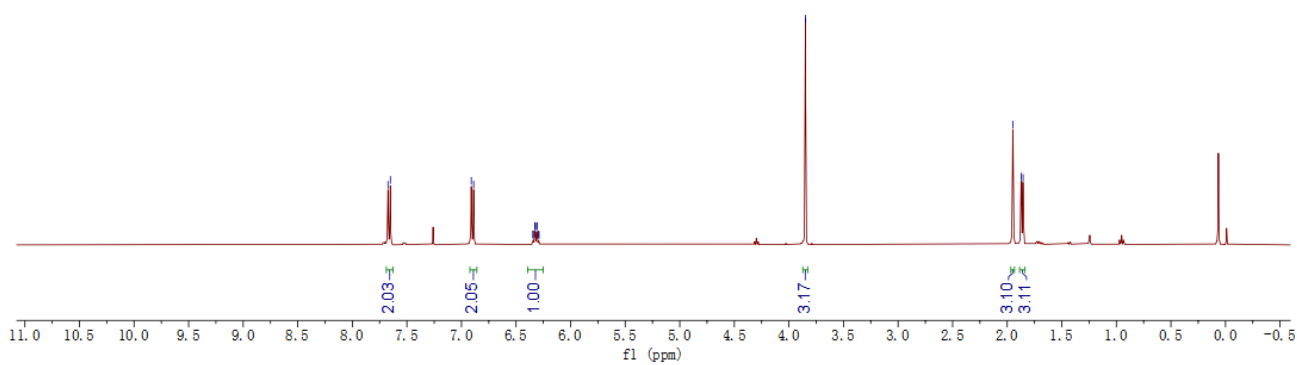
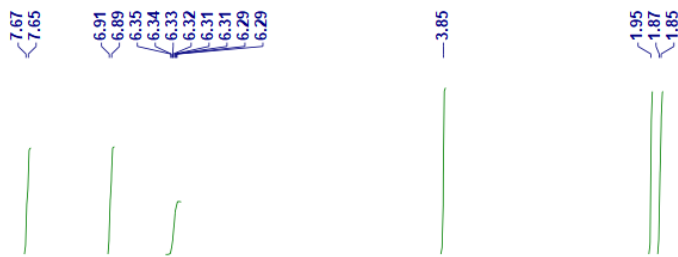
189.30
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148.94
130.91
125.70
113.79
55.56
34.94
21.60
13.90







38



198.03

162.49

139.28

137.53

131.77

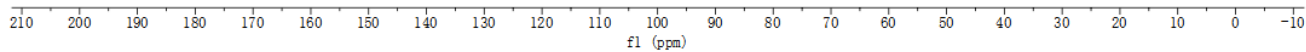
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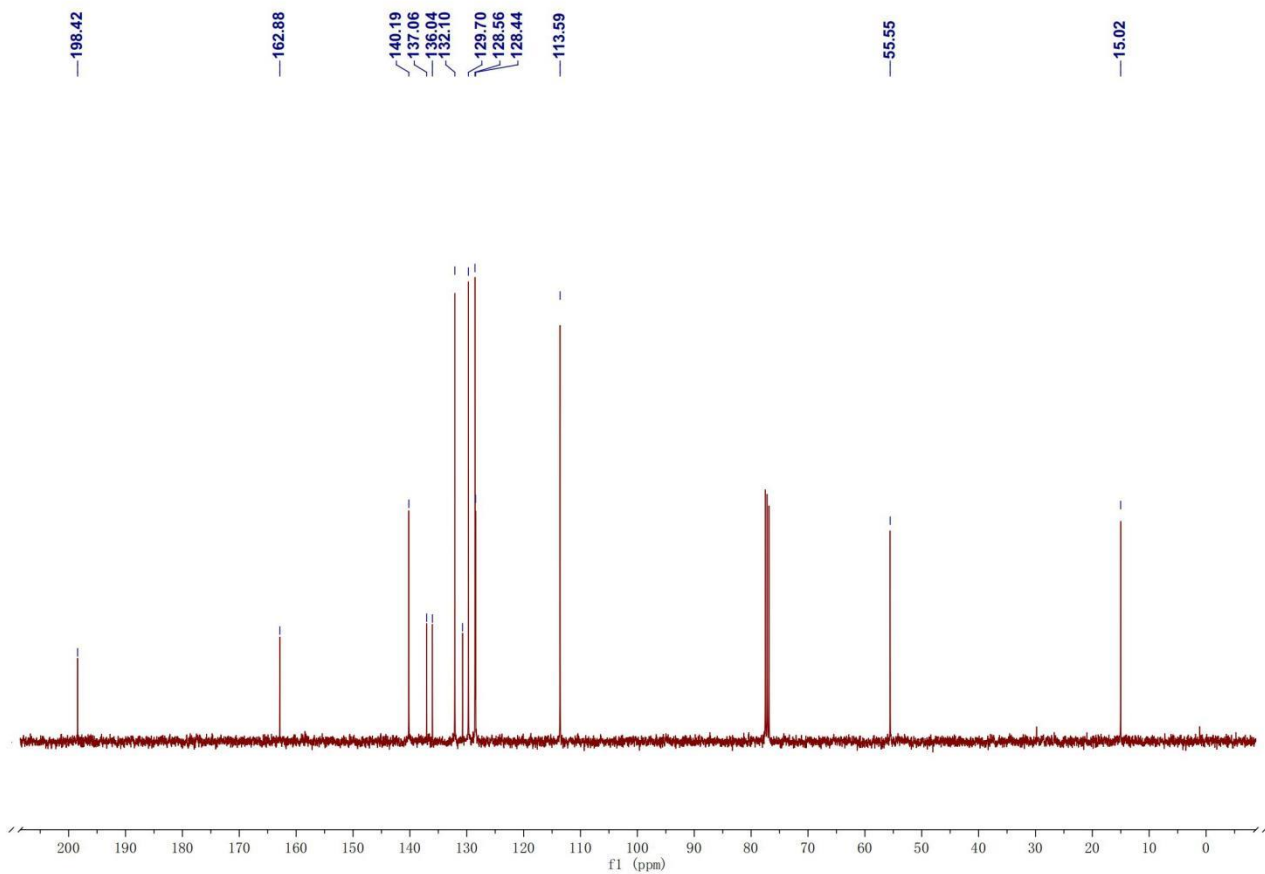
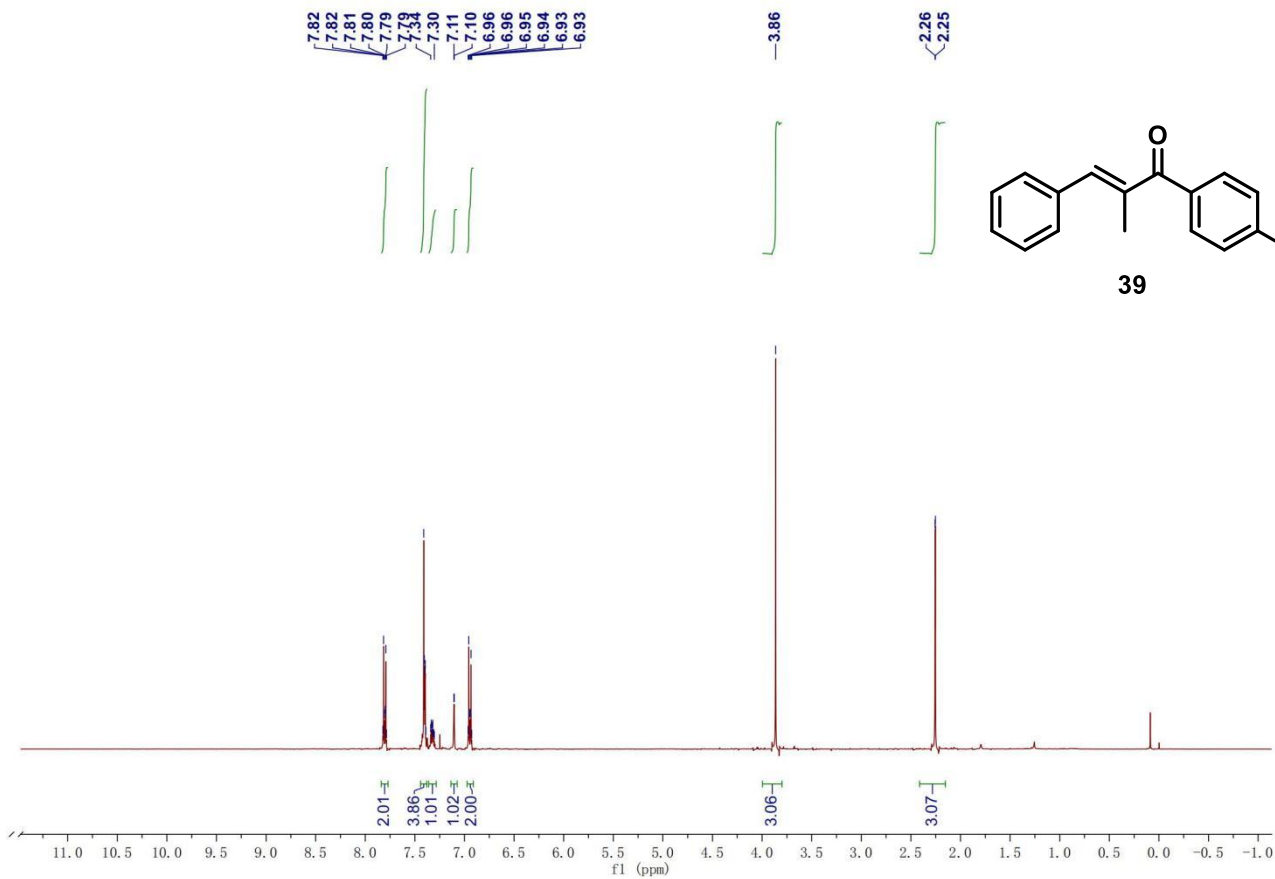
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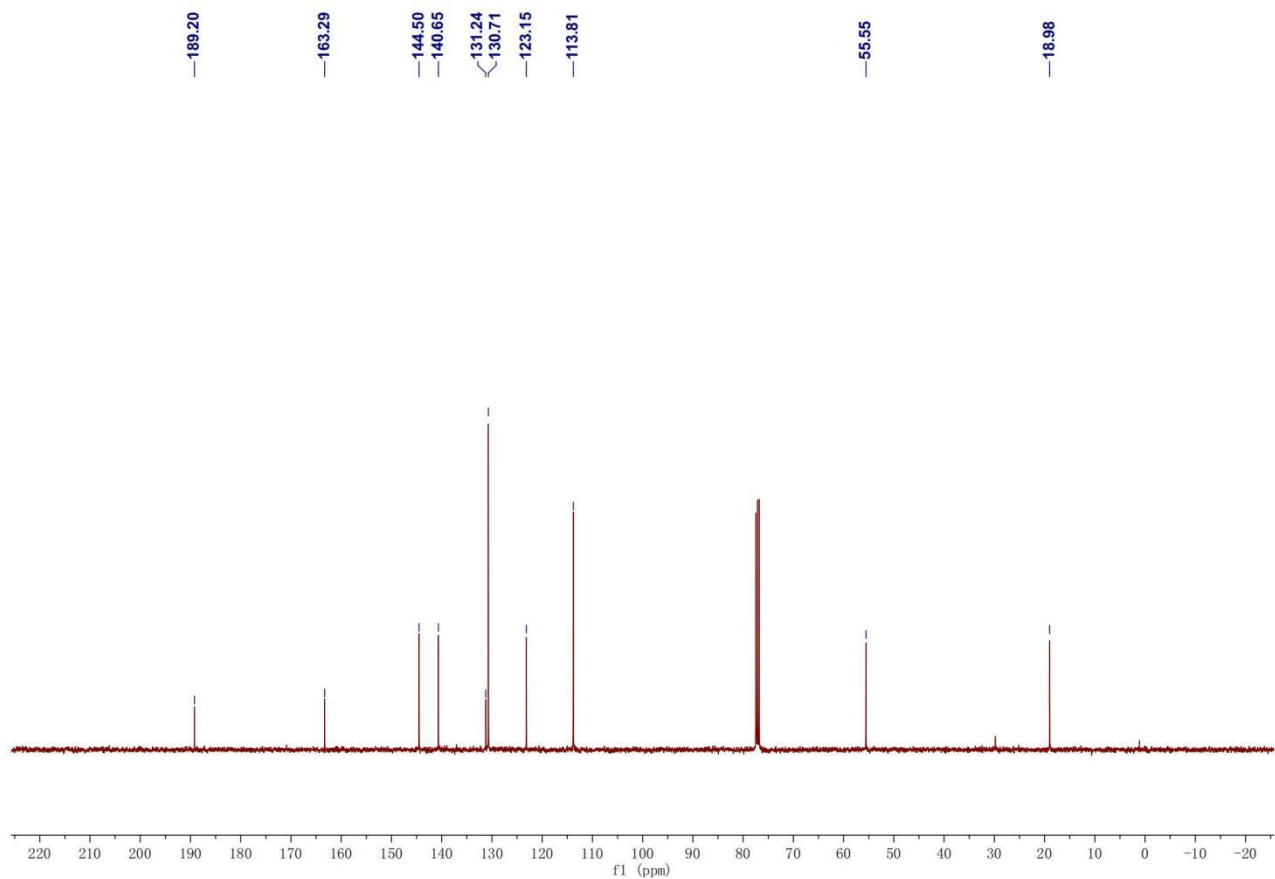
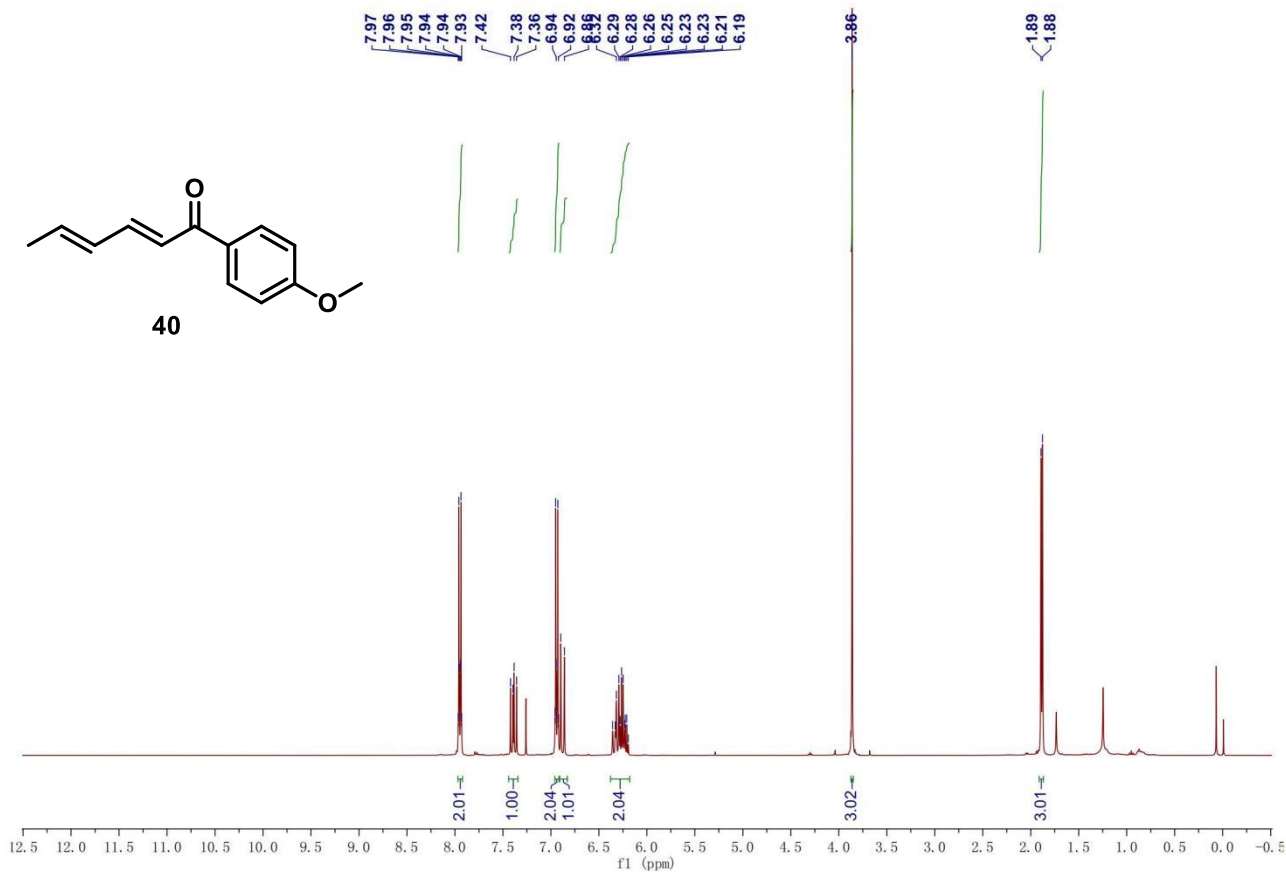
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12.74

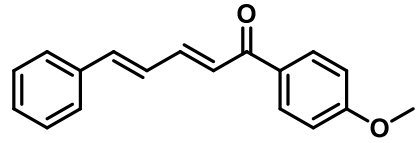




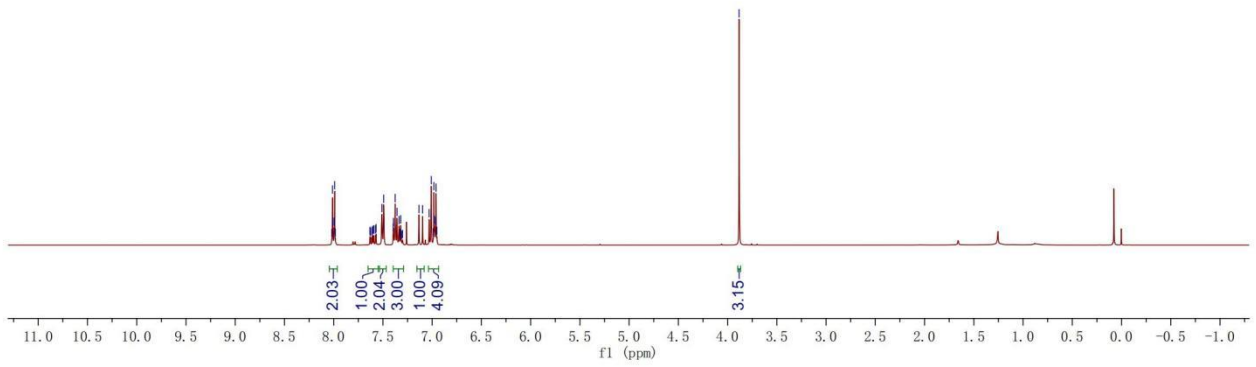


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8.01
8.01
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7.57
7.51
7.40
7.38
7.34
7.32
7.30
7.10
7.01
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6.96
6.95

3.88



41



188.78

163.42

144.11

141.51

136.29

130.79

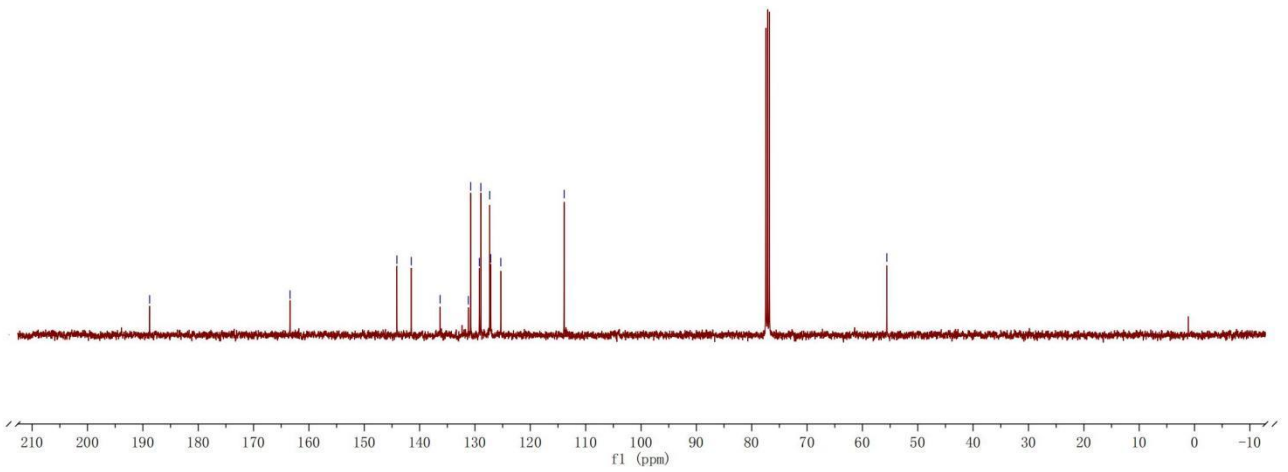
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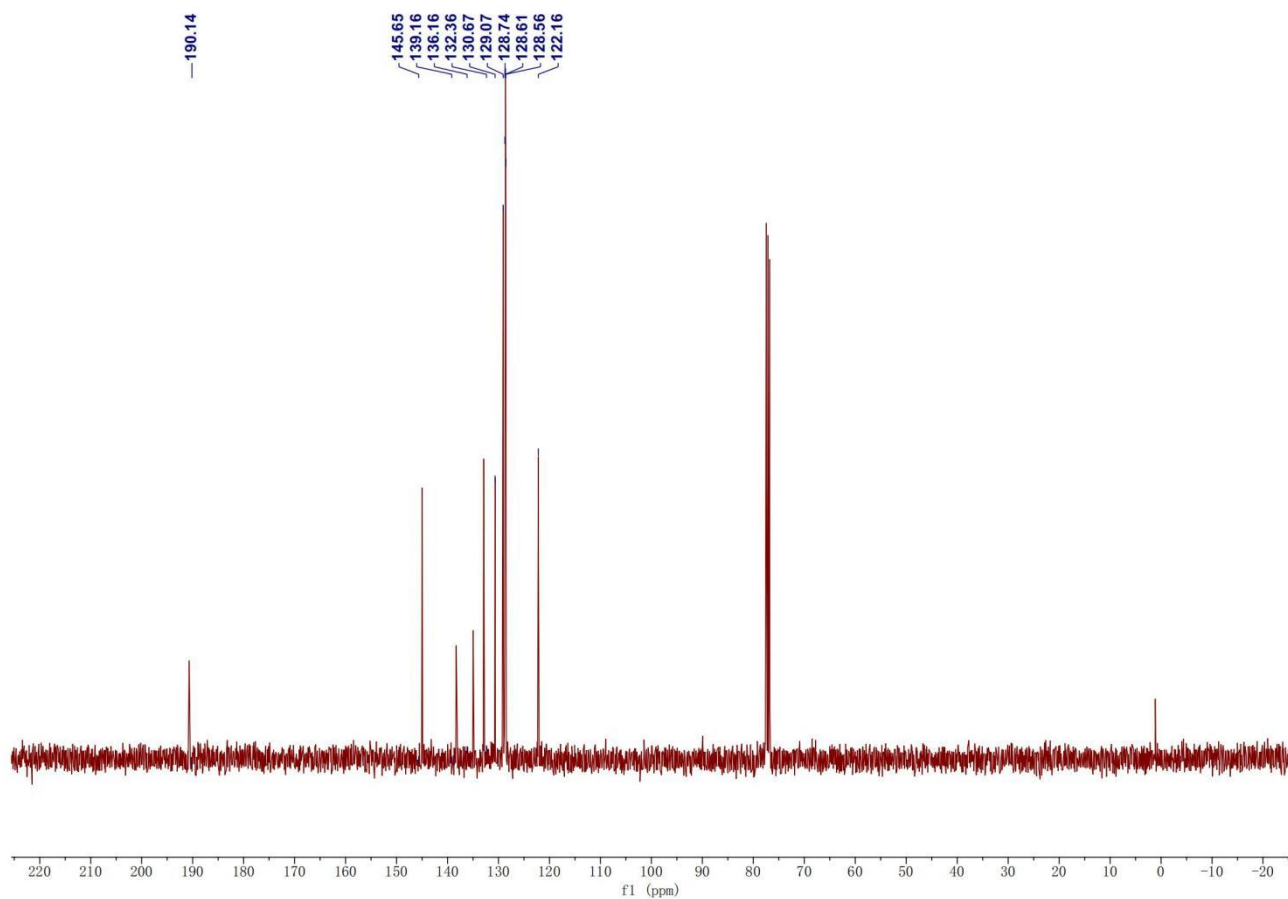
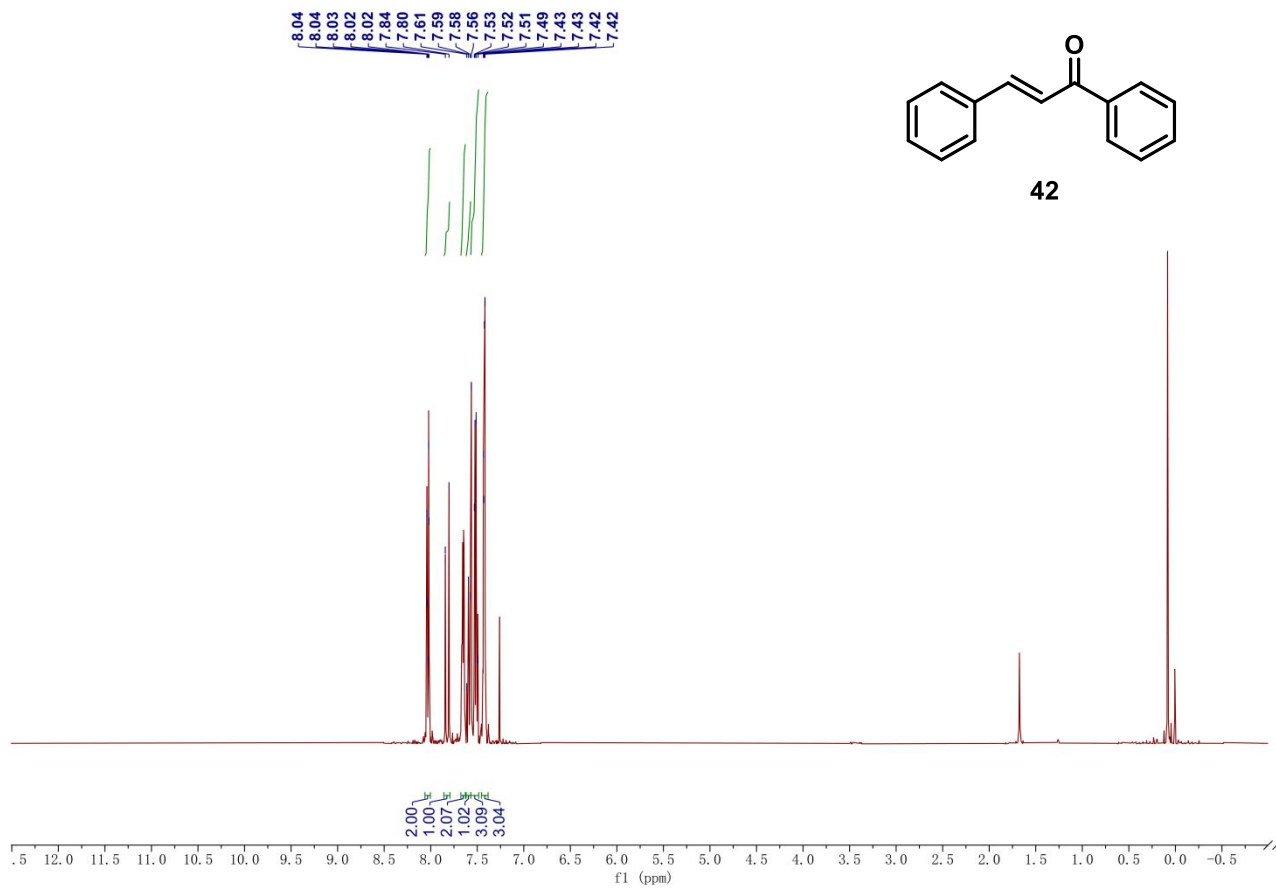
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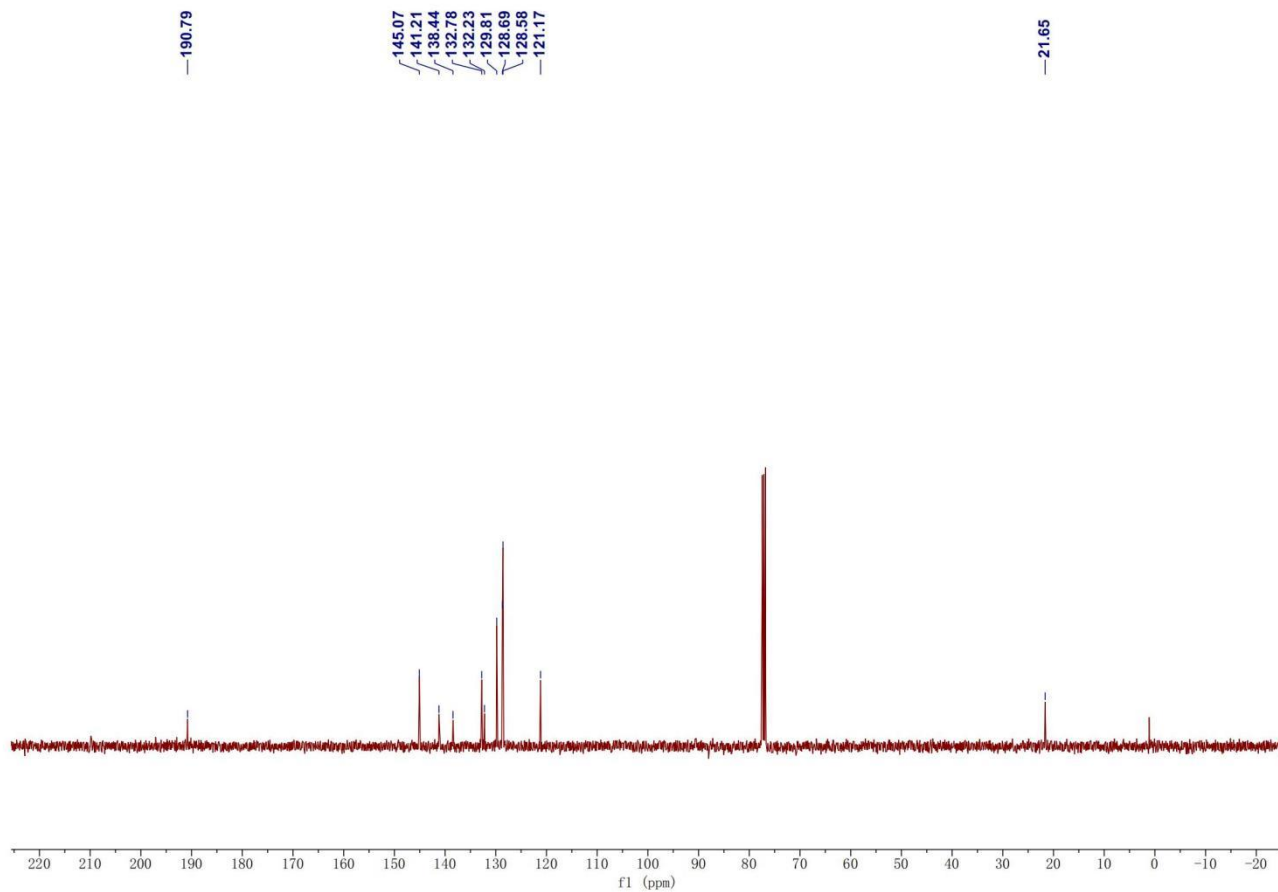
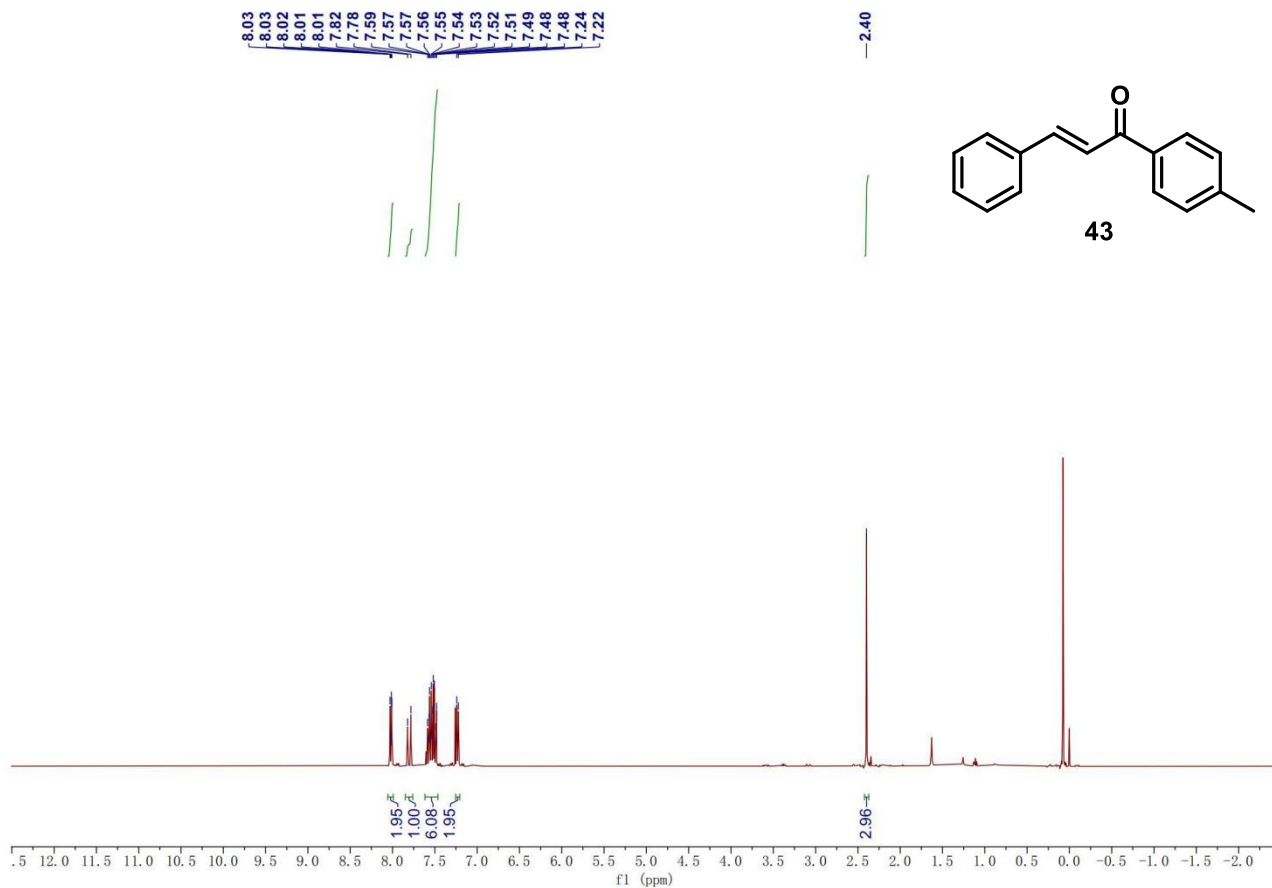
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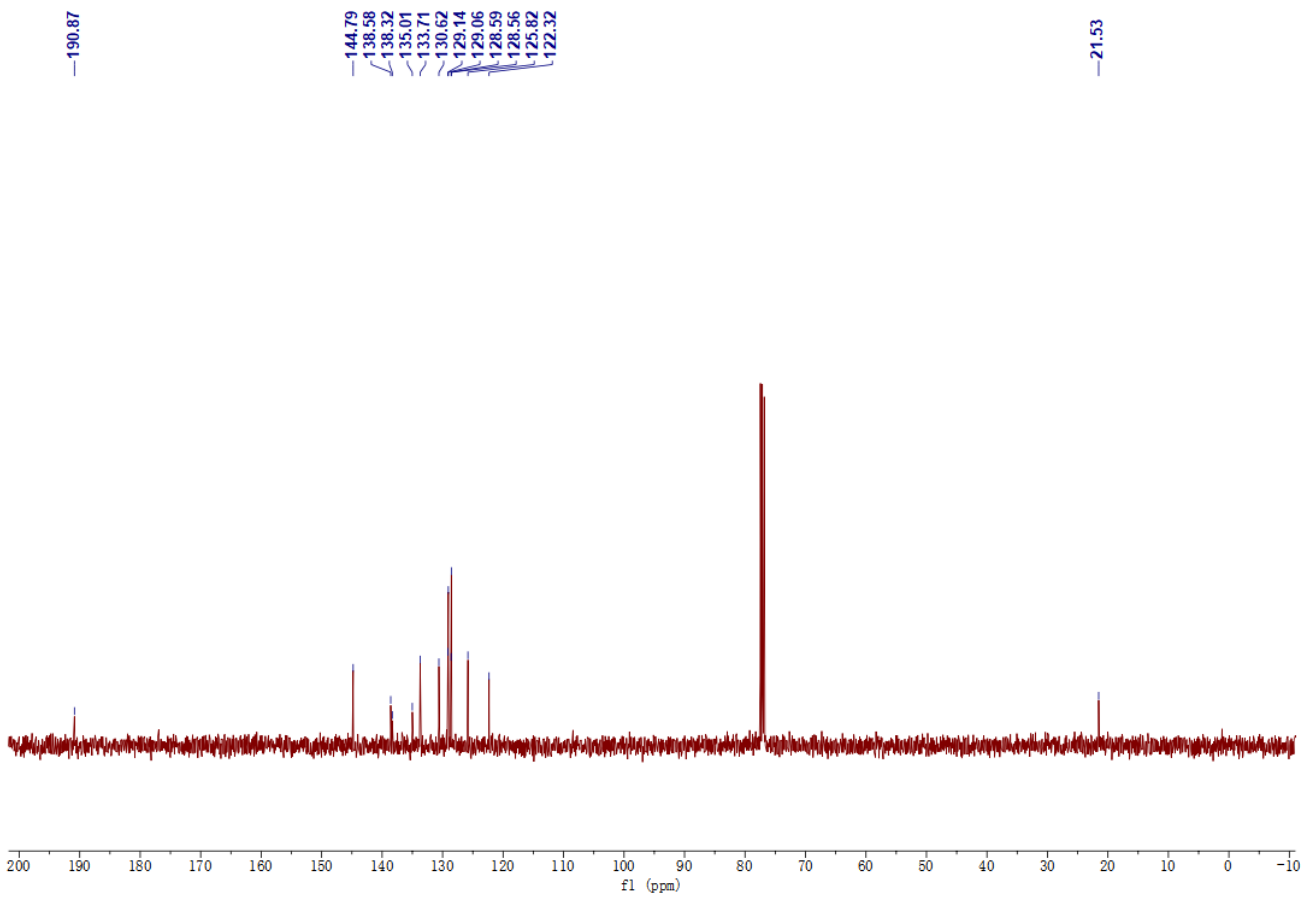
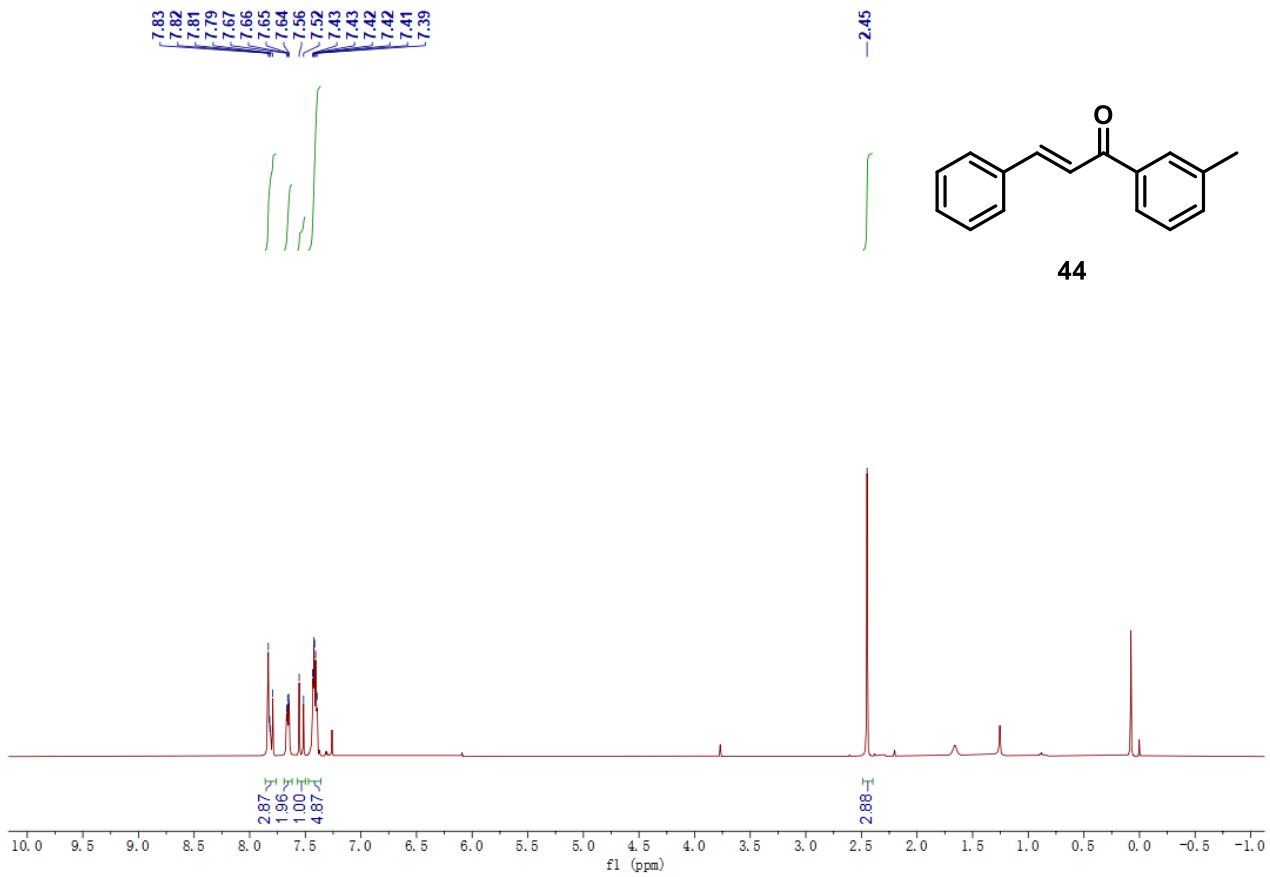
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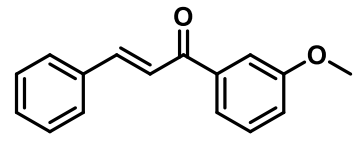
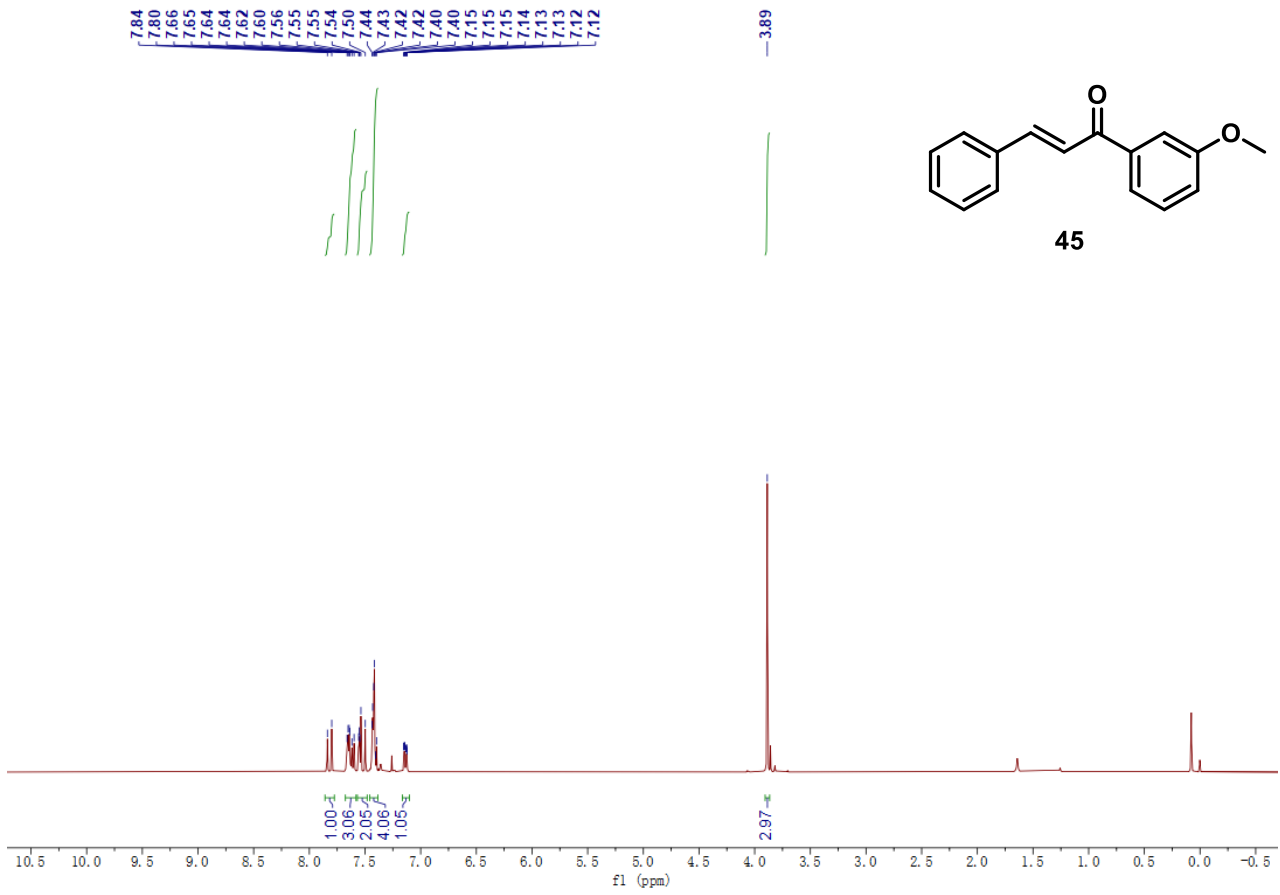
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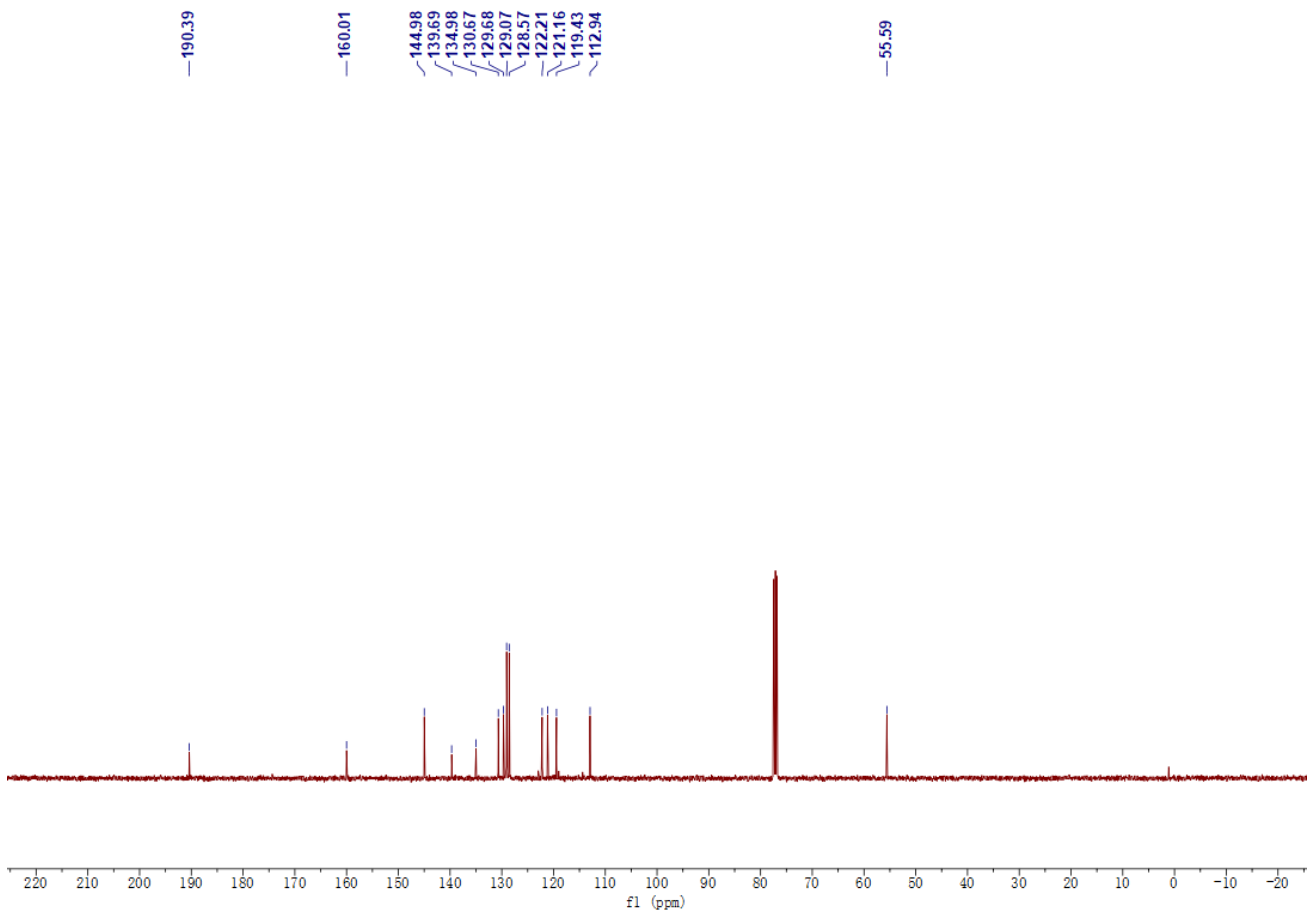


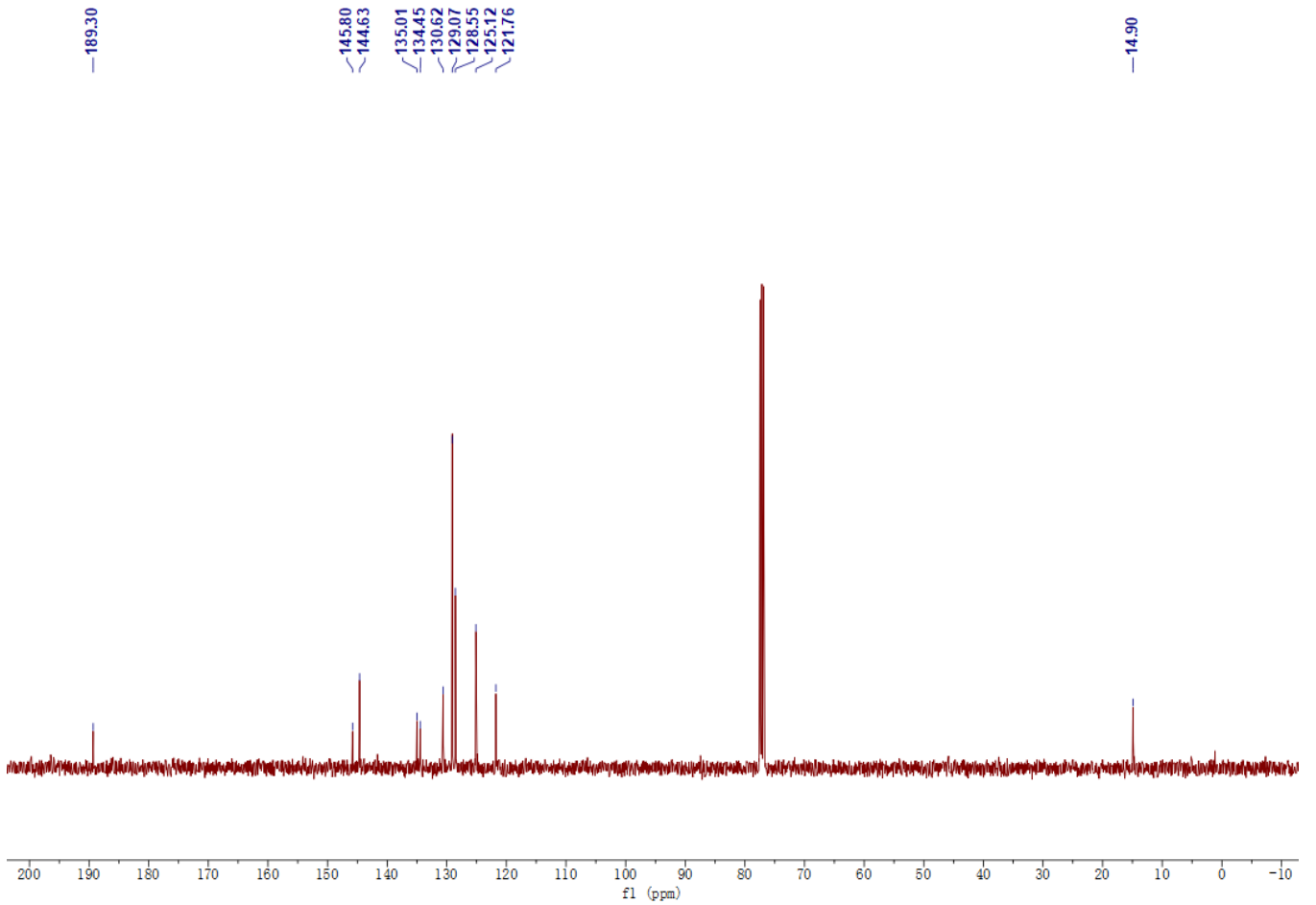
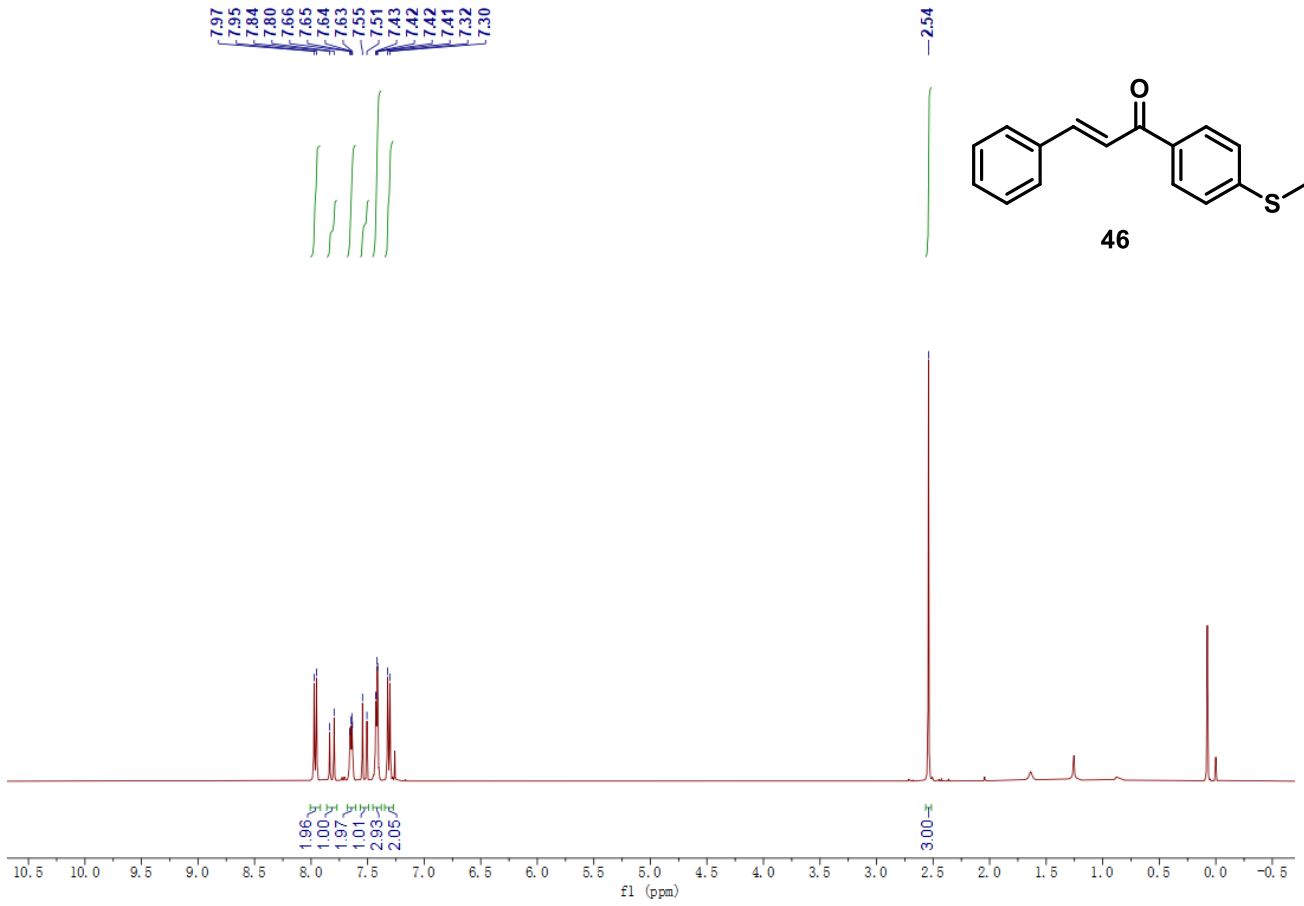




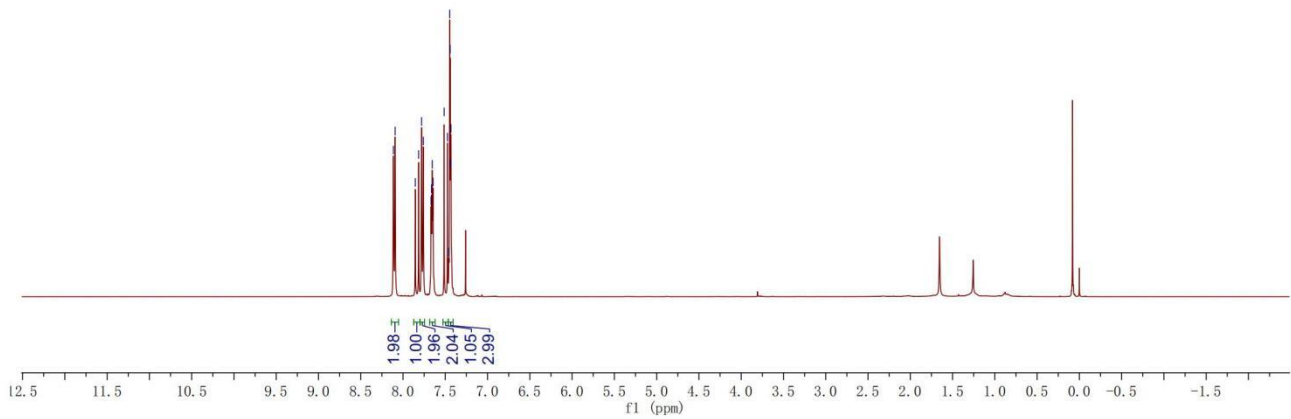
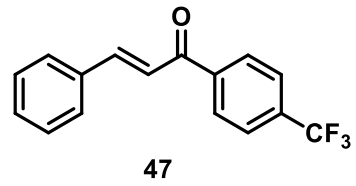


45

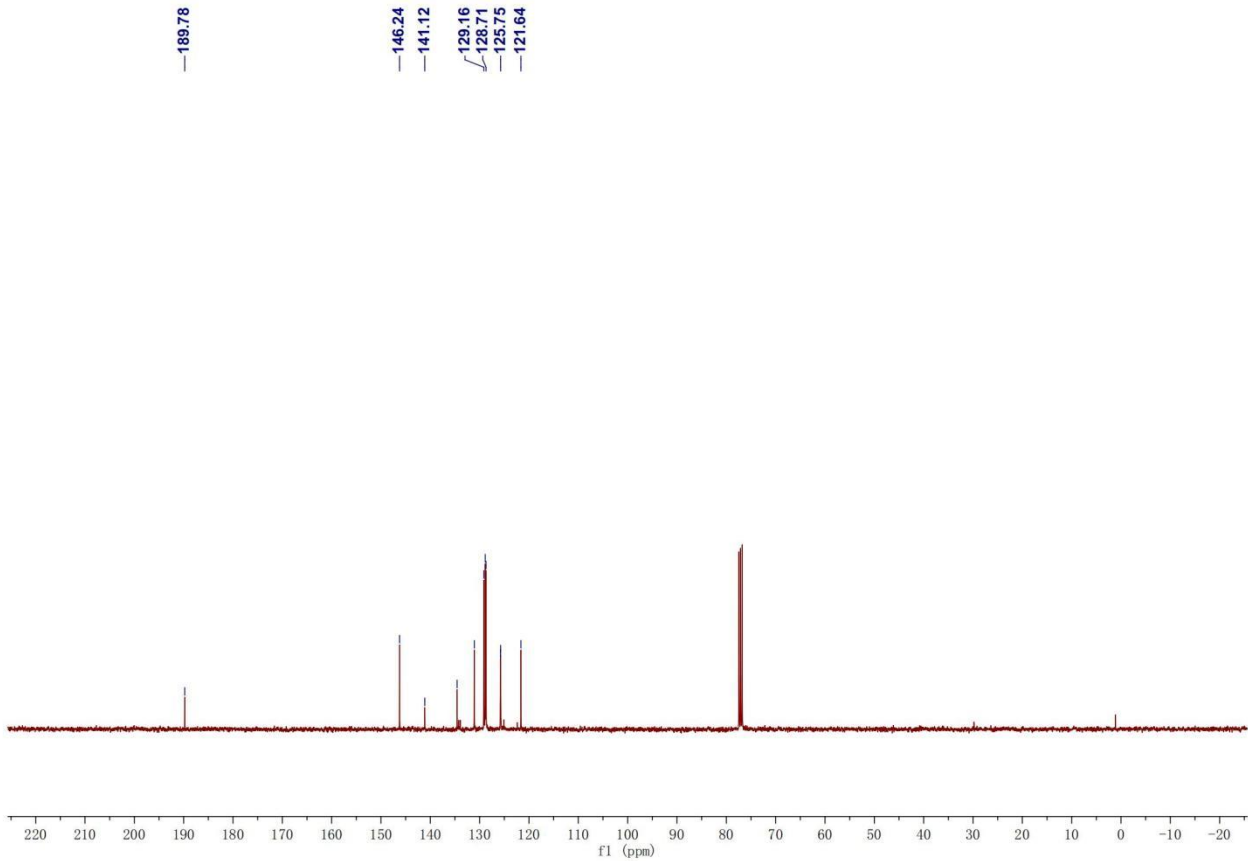




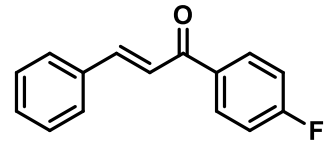
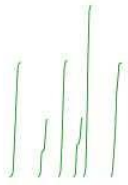
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7.44
7.43



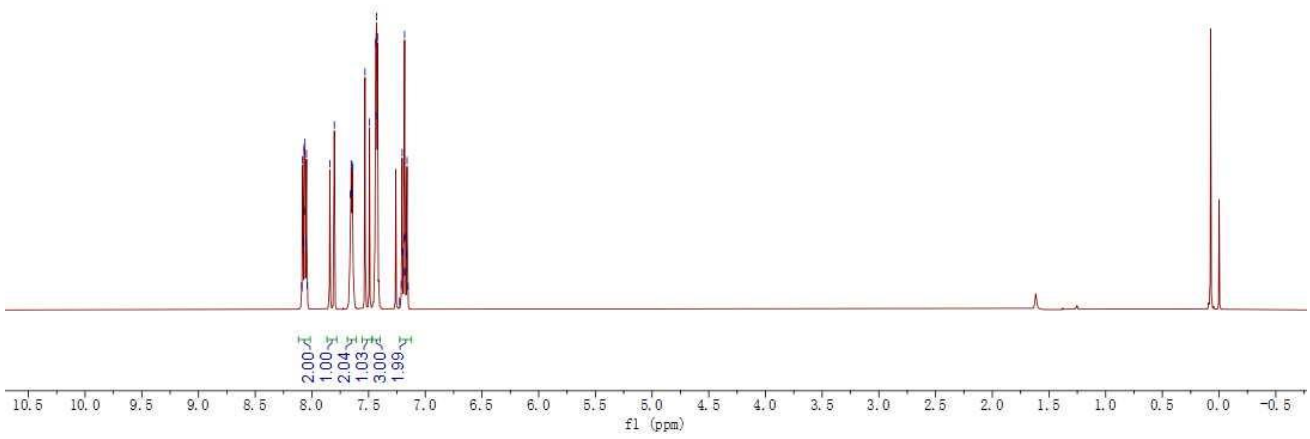
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129.16
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125.75
121.64



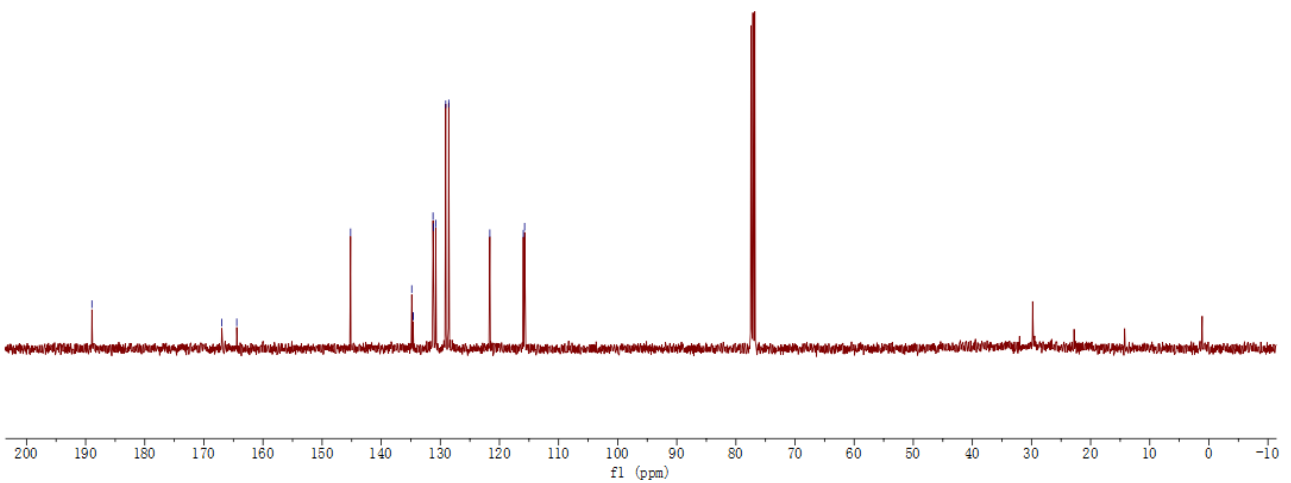
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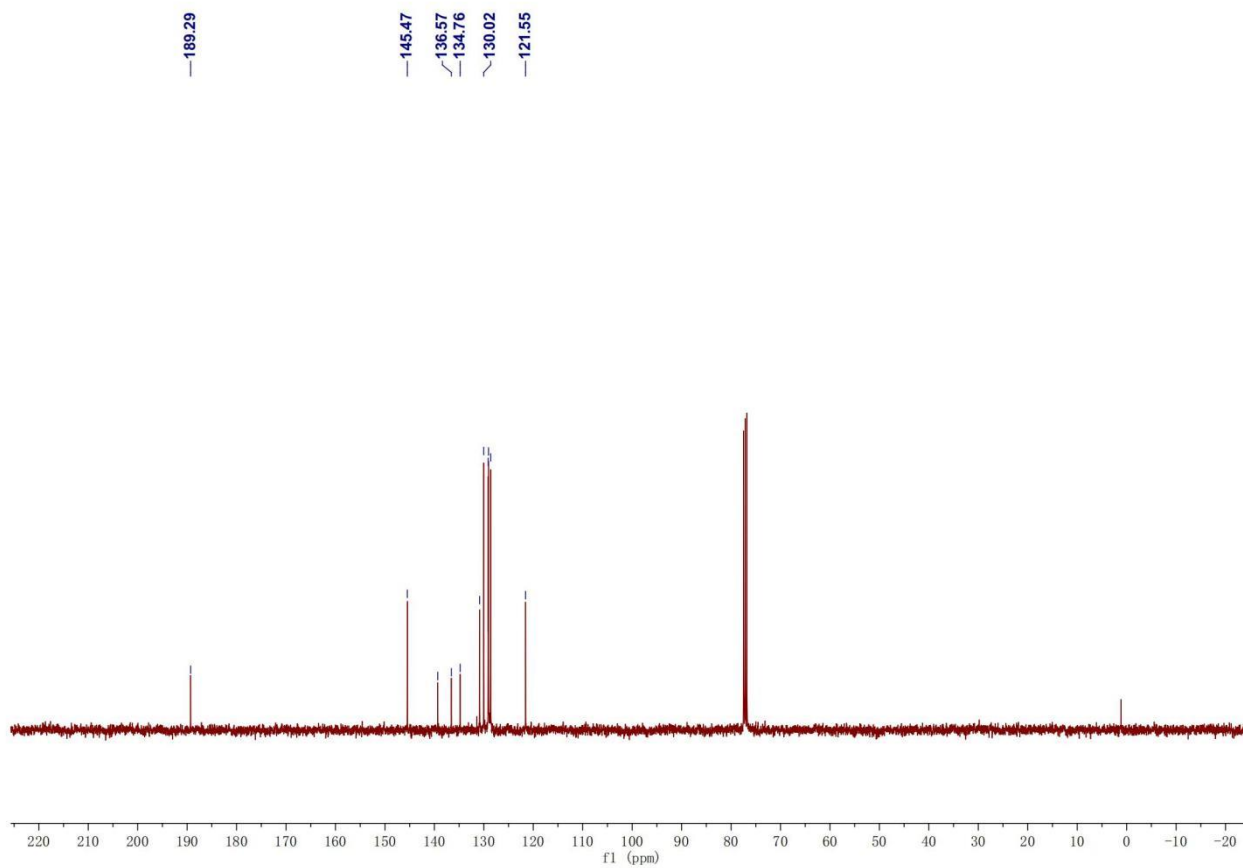
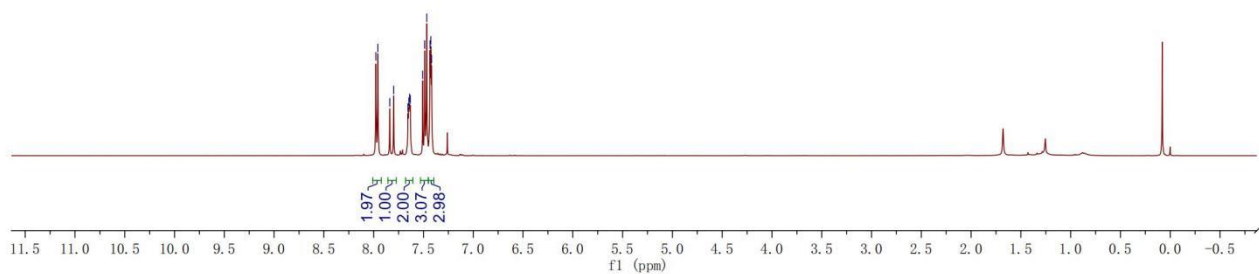
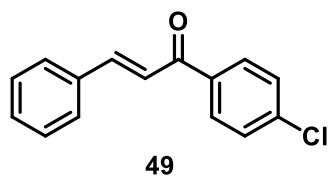
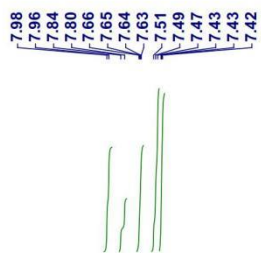


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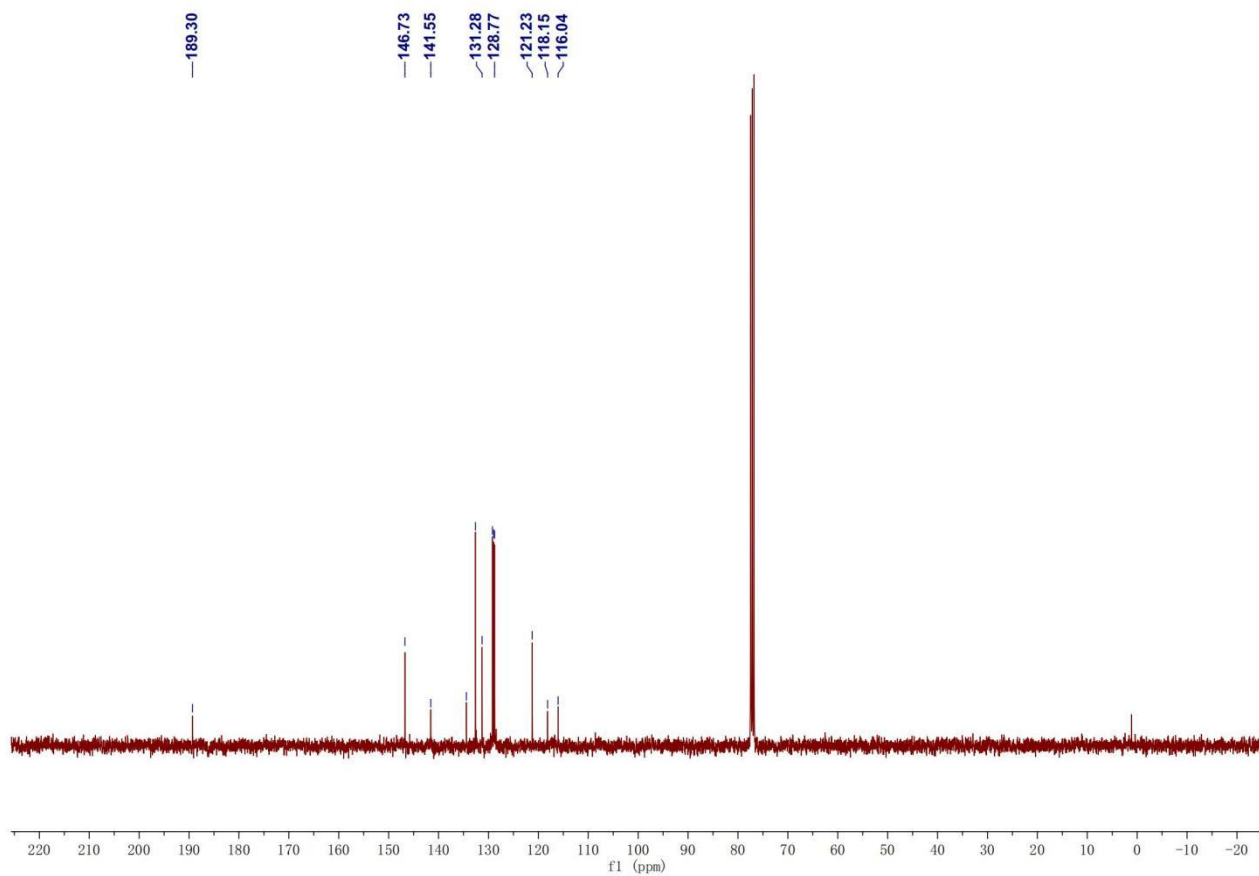
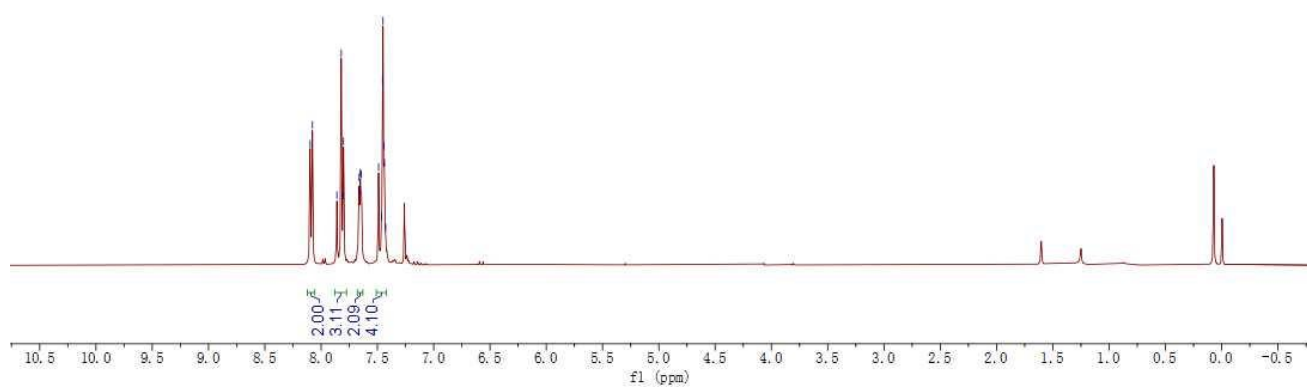
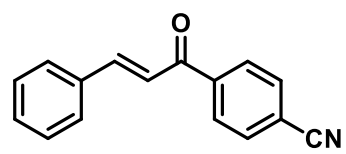
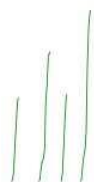


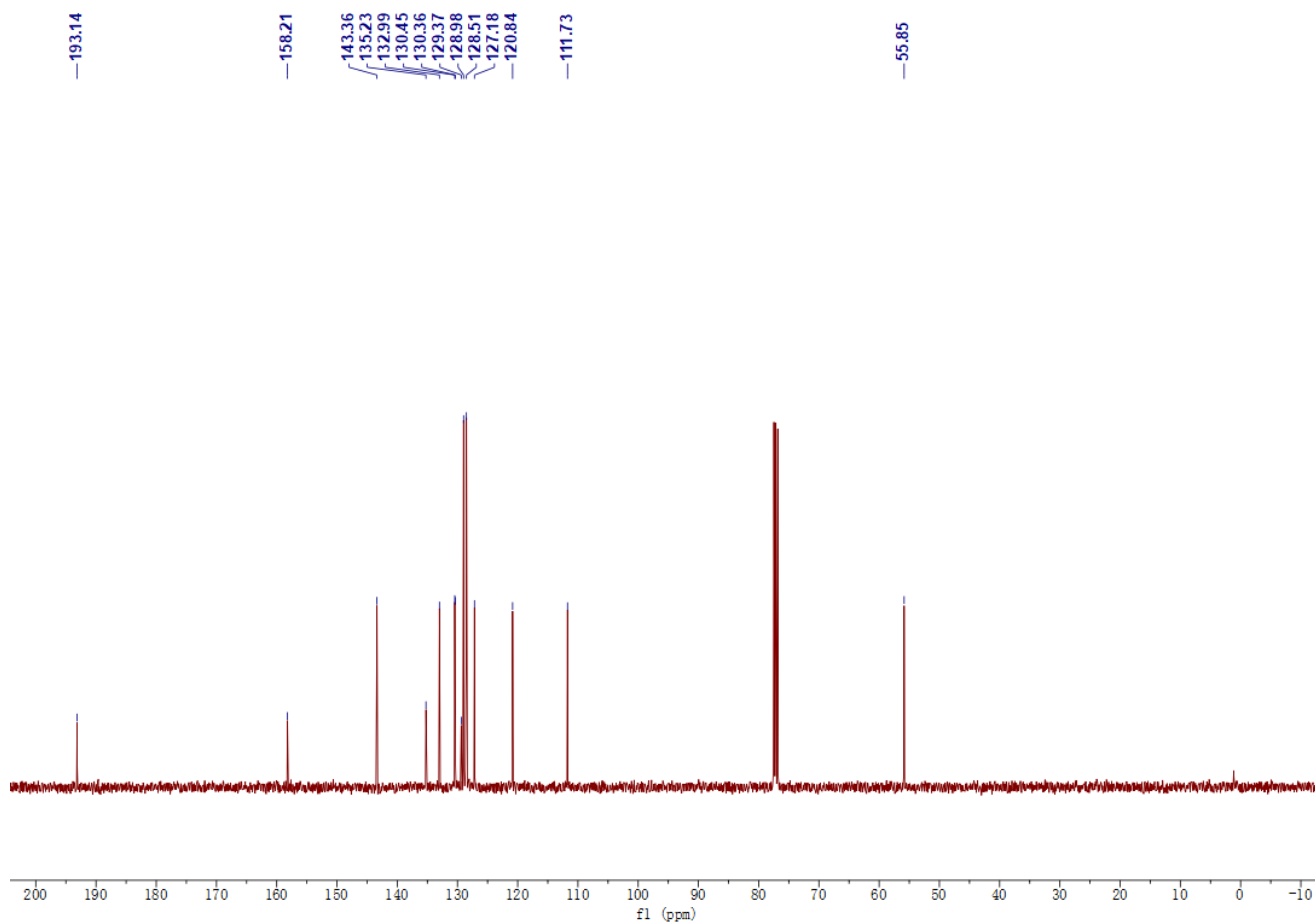
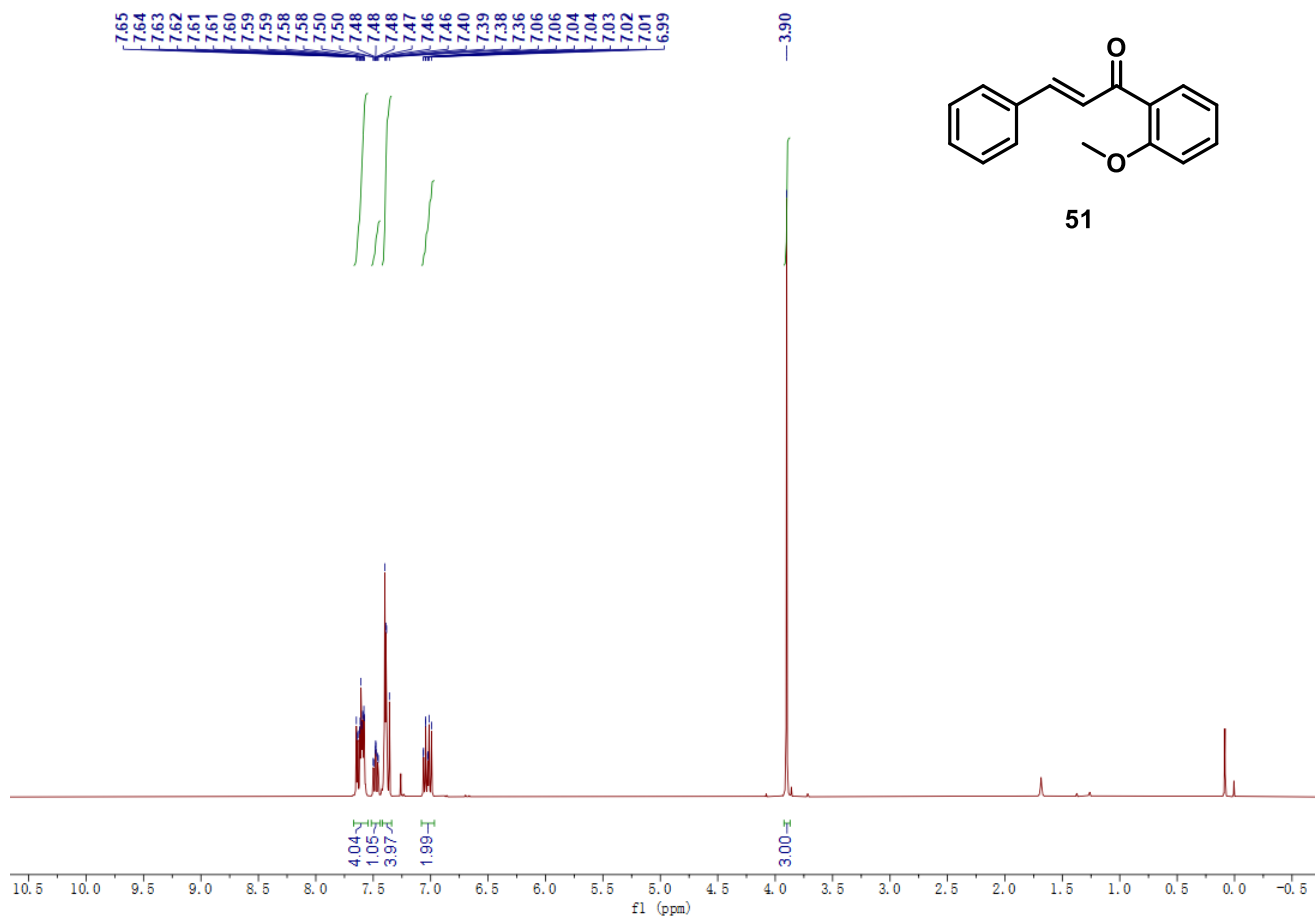
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121.63
115.96
115.74

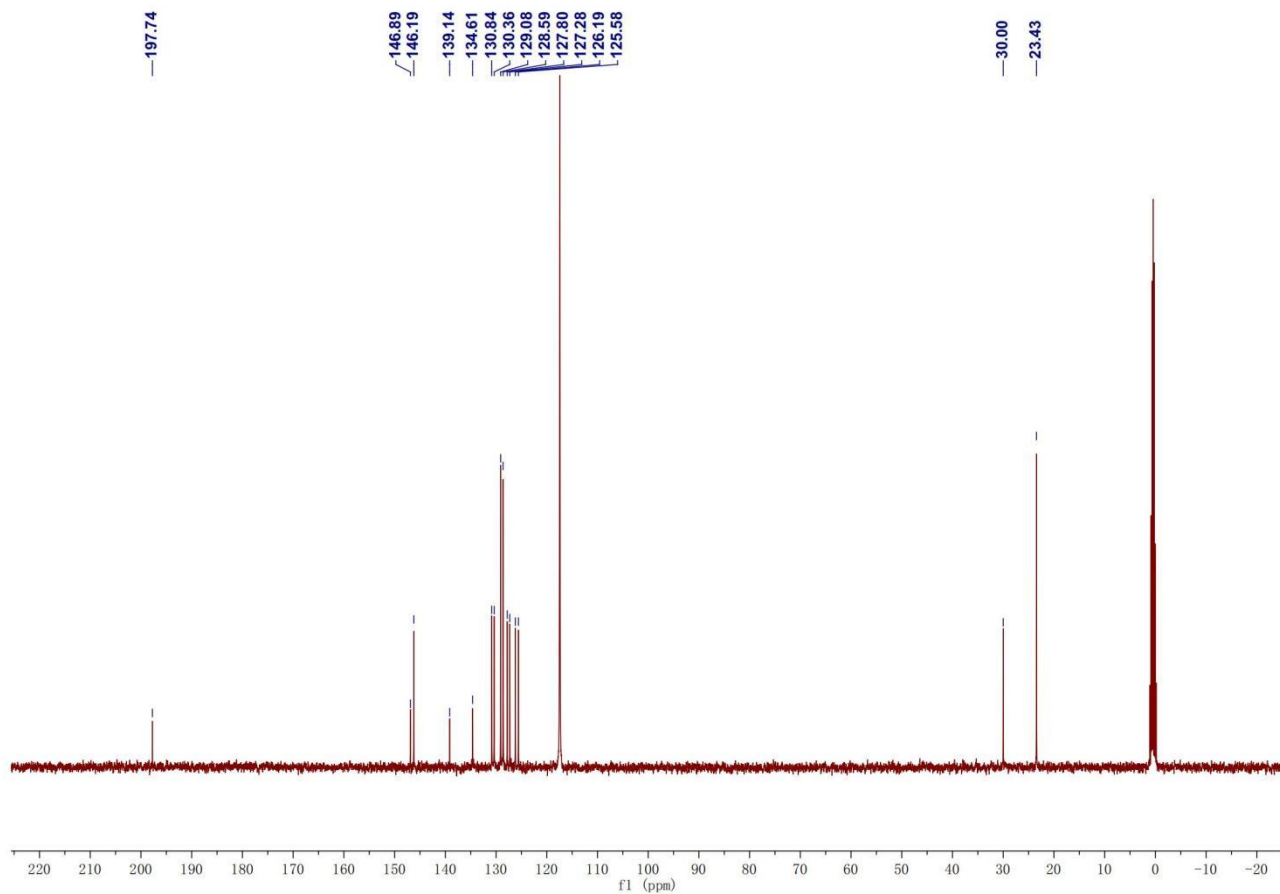
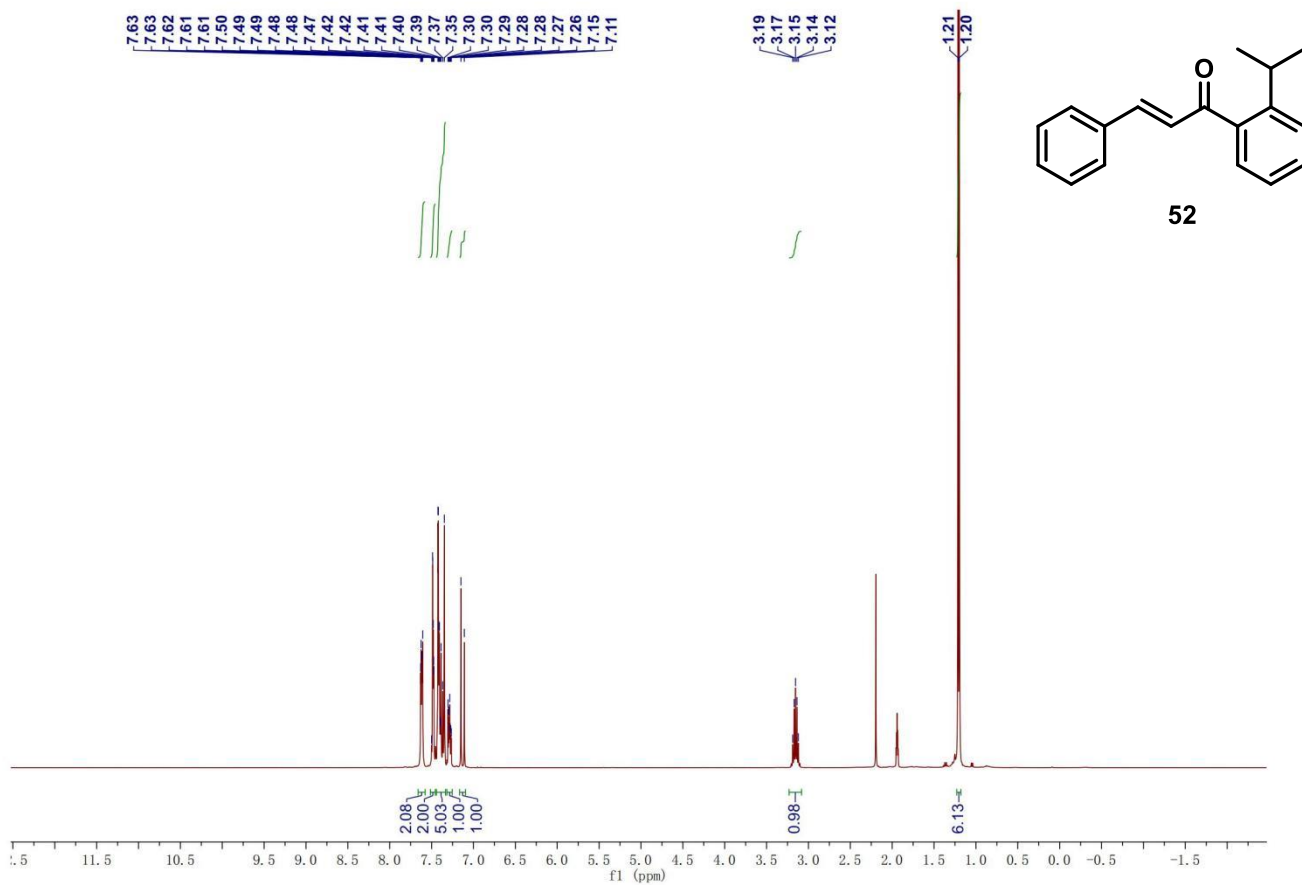


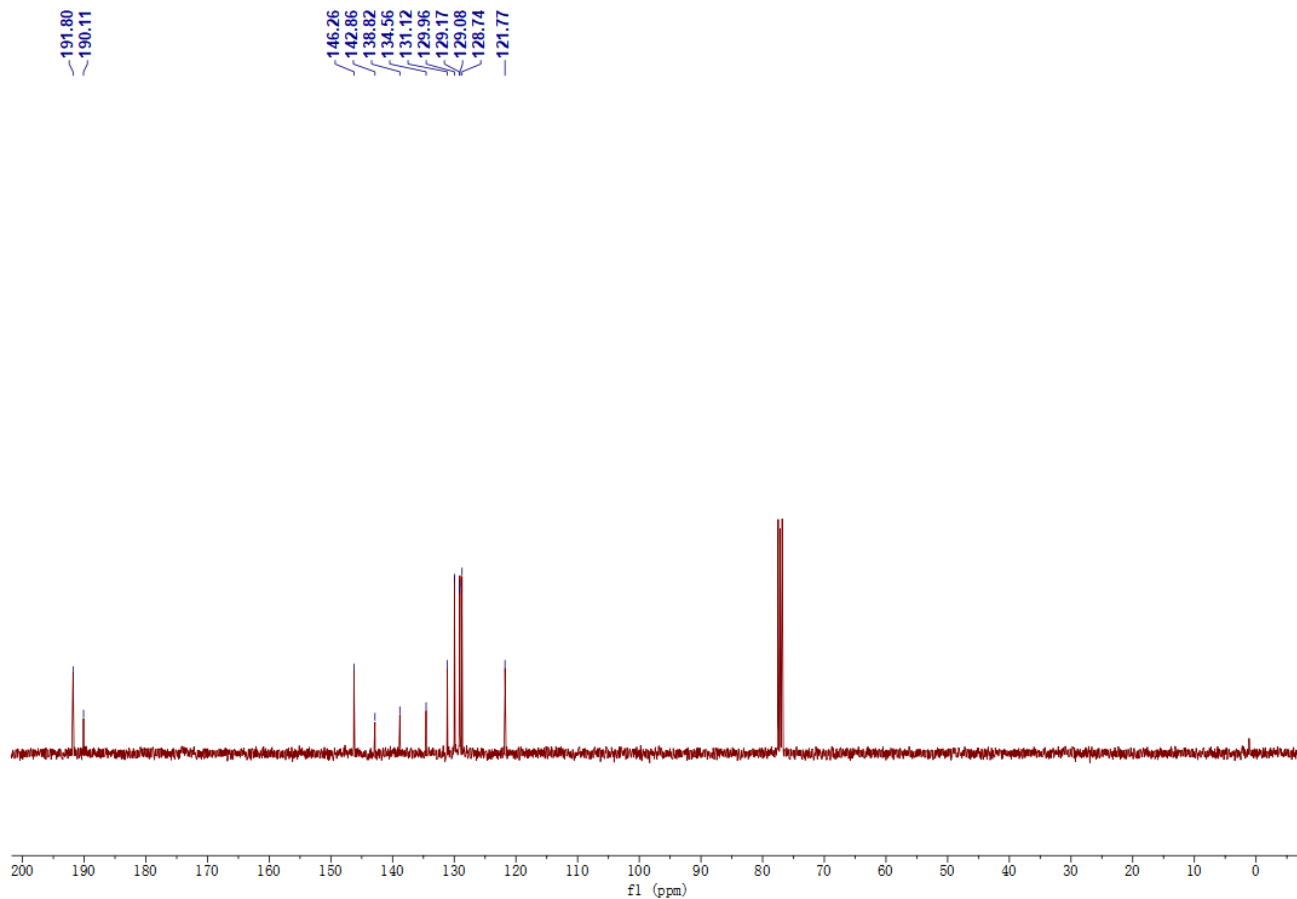
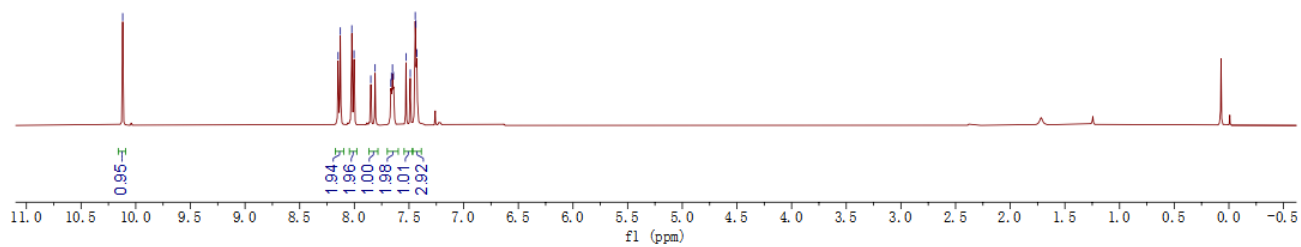
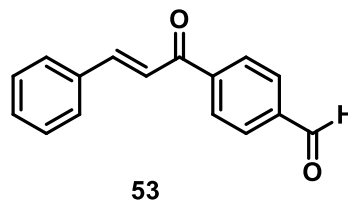
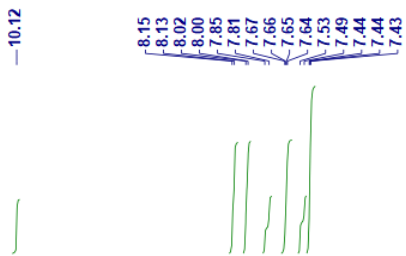


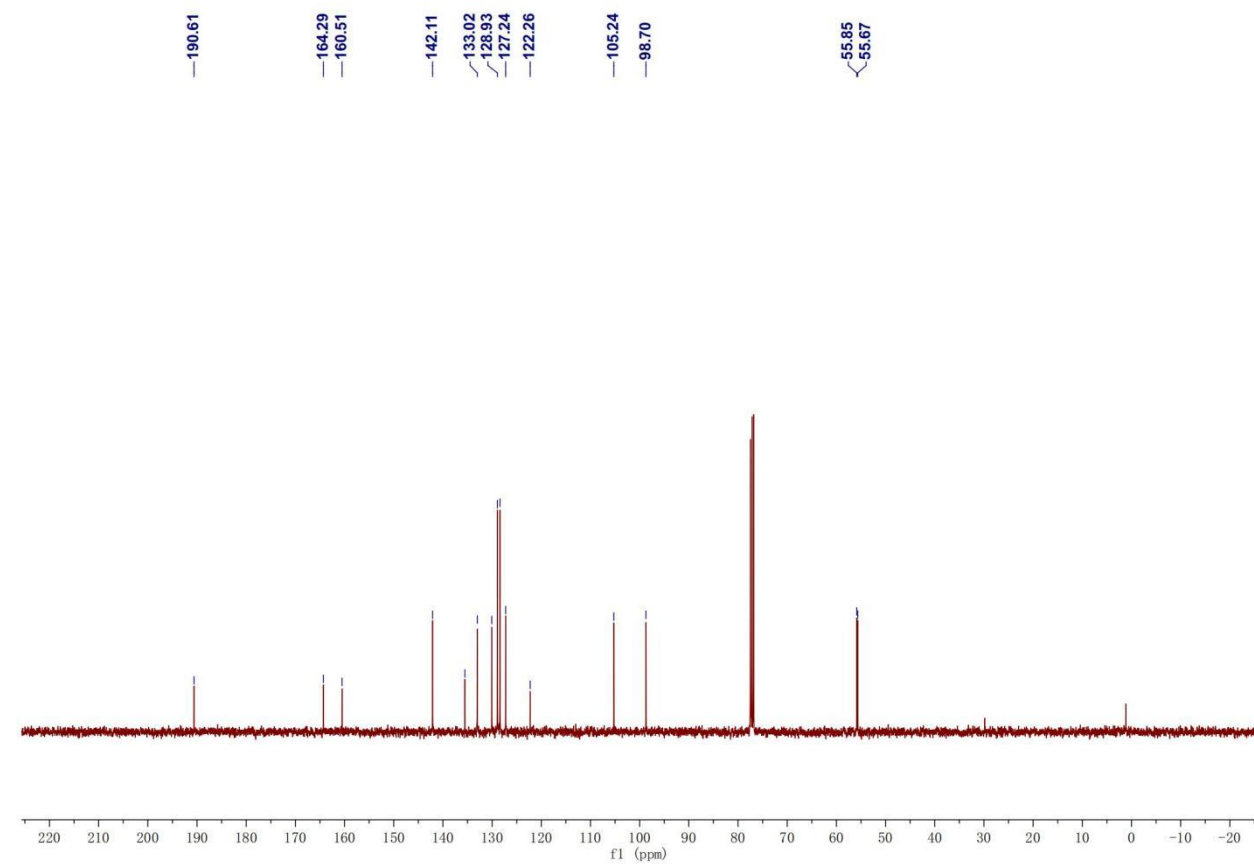
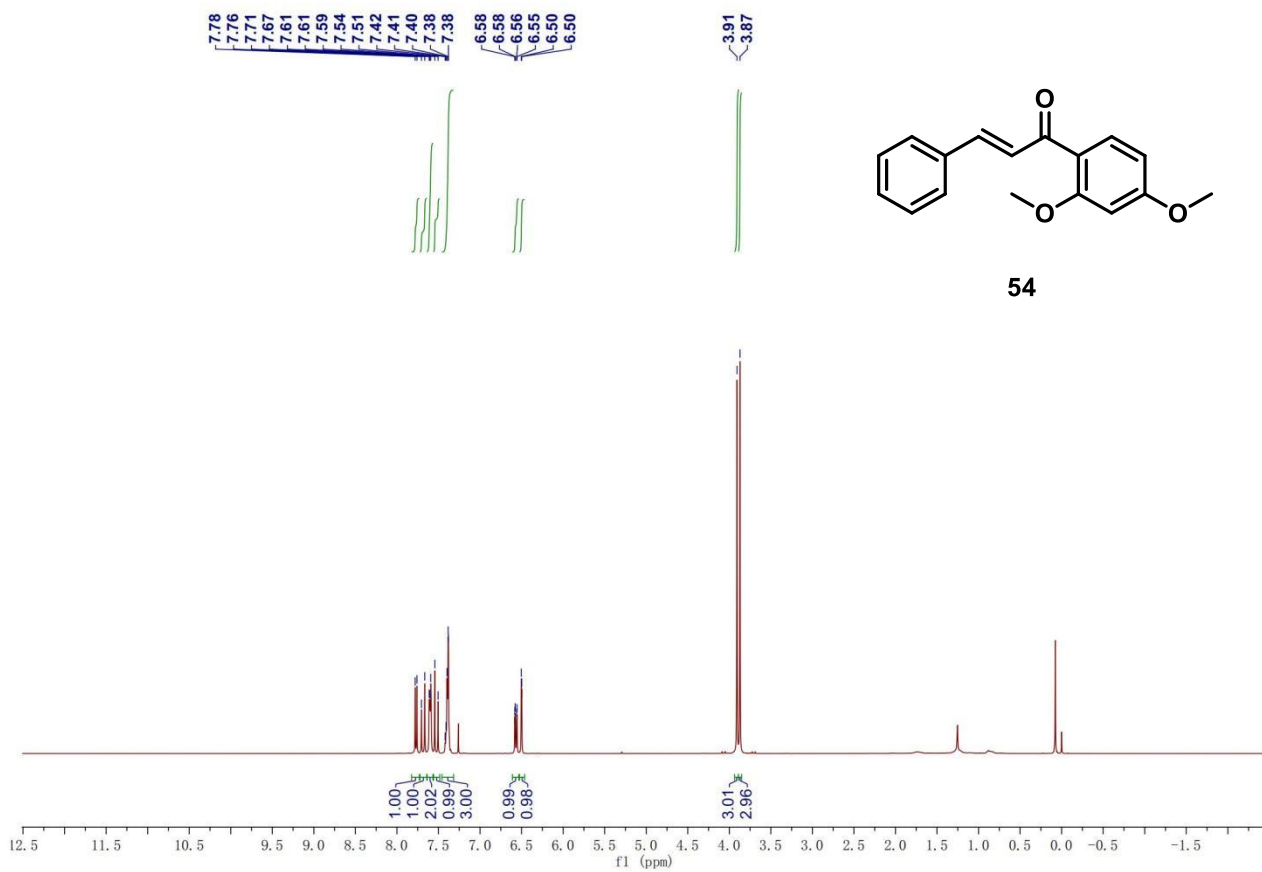
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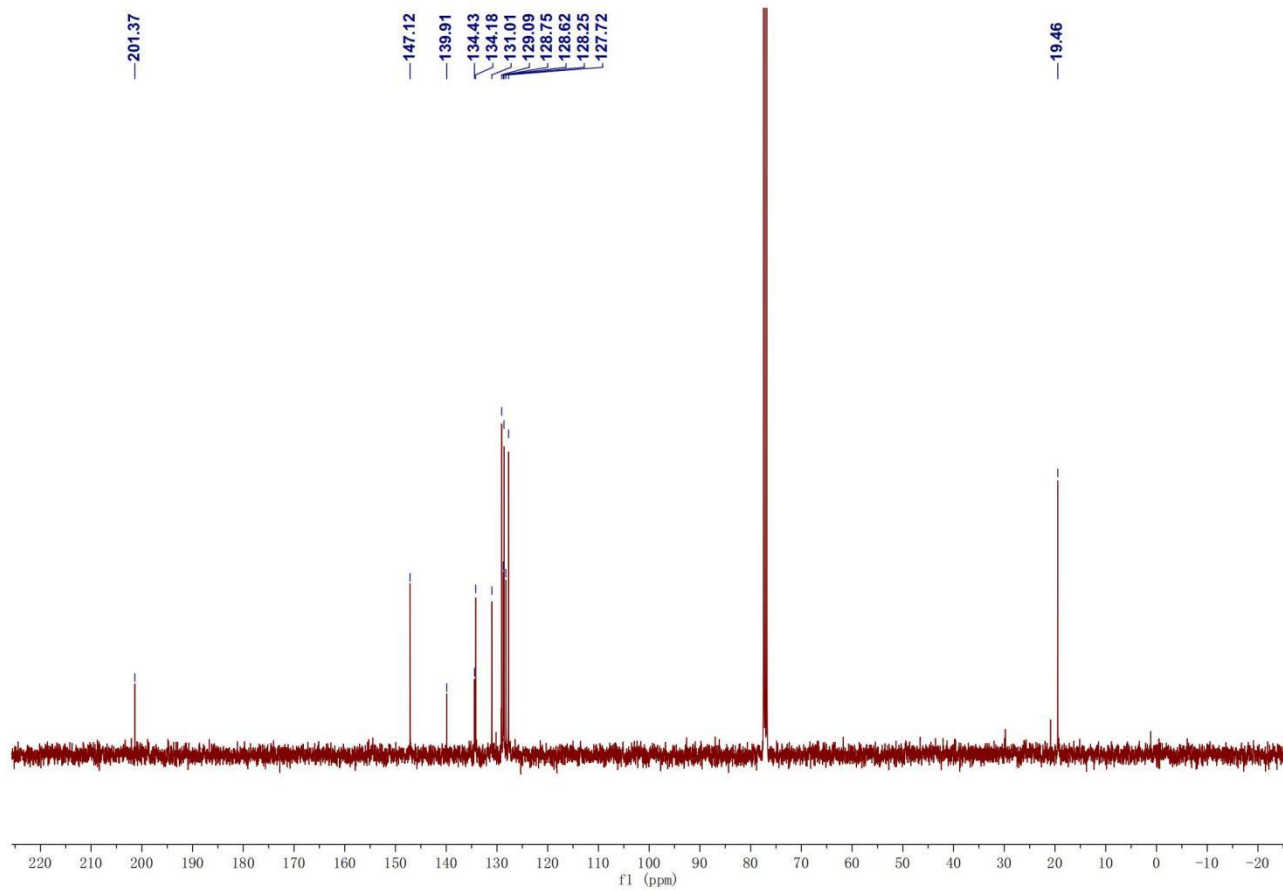
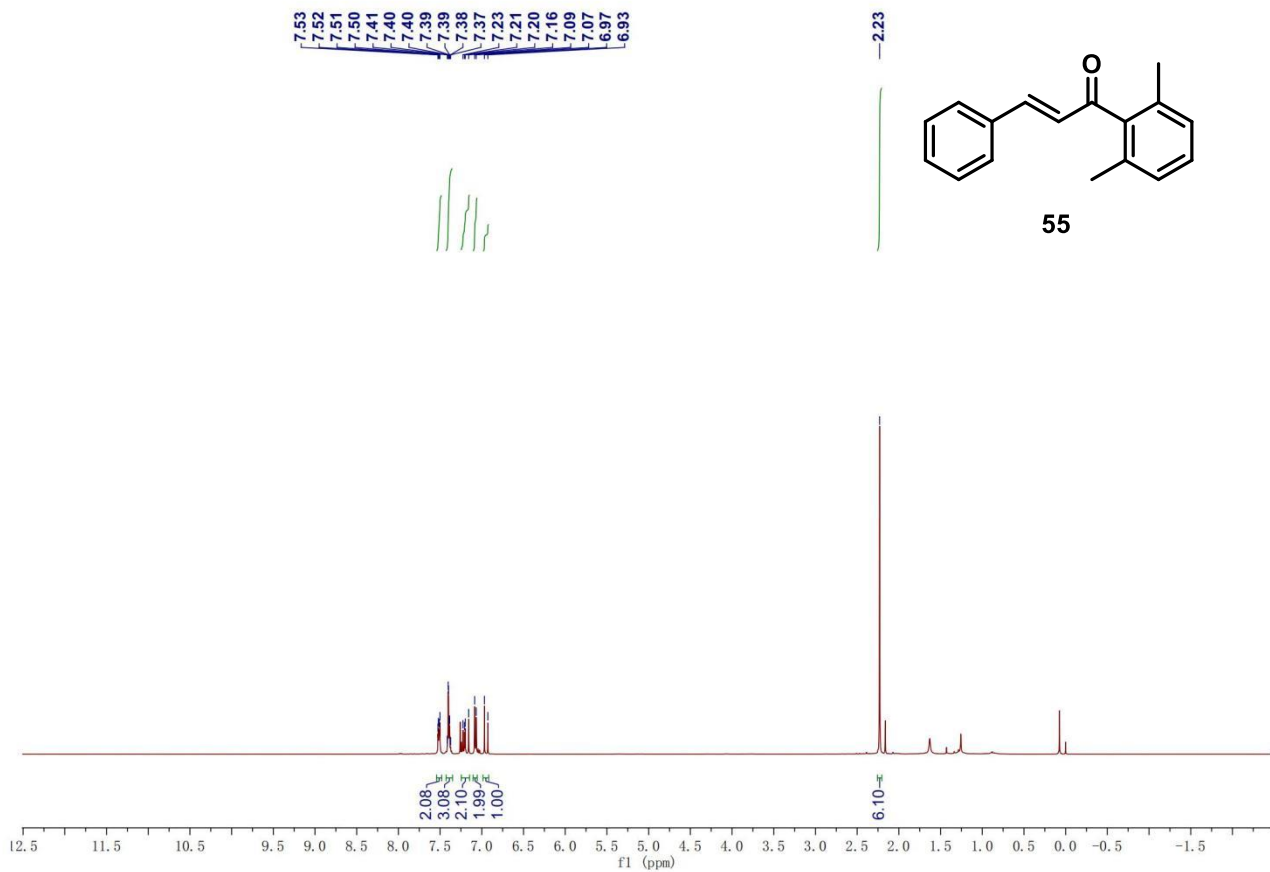


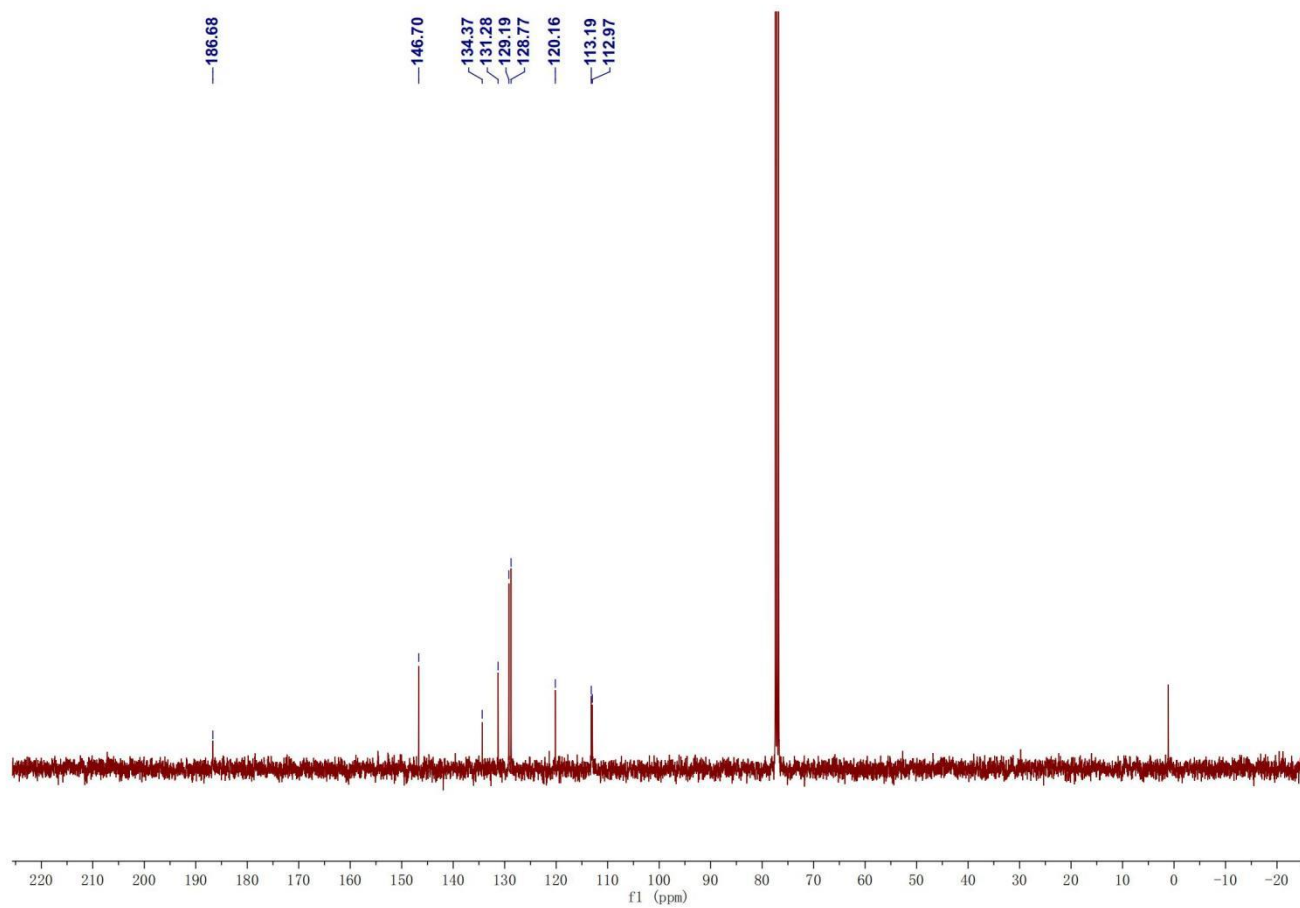
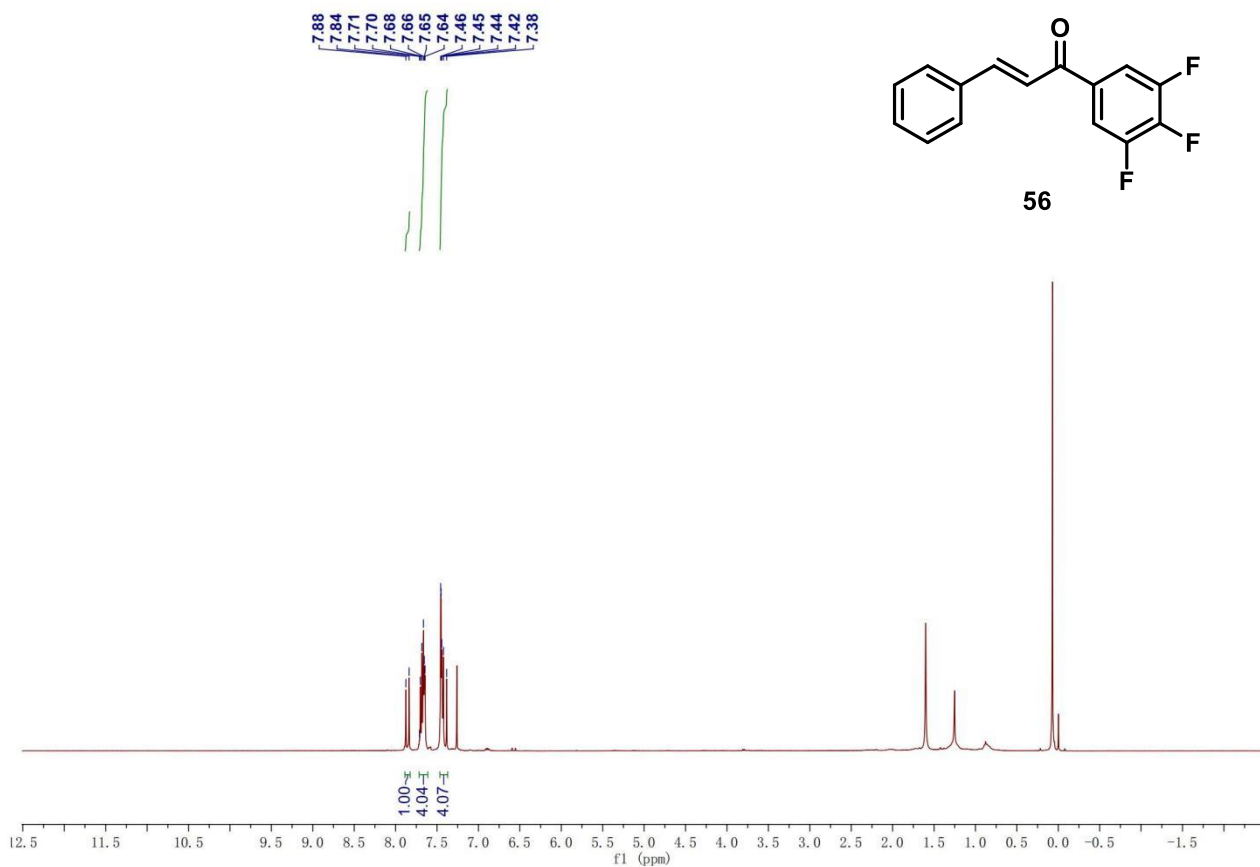




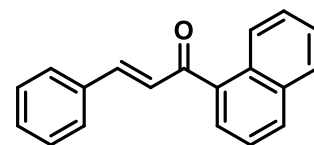




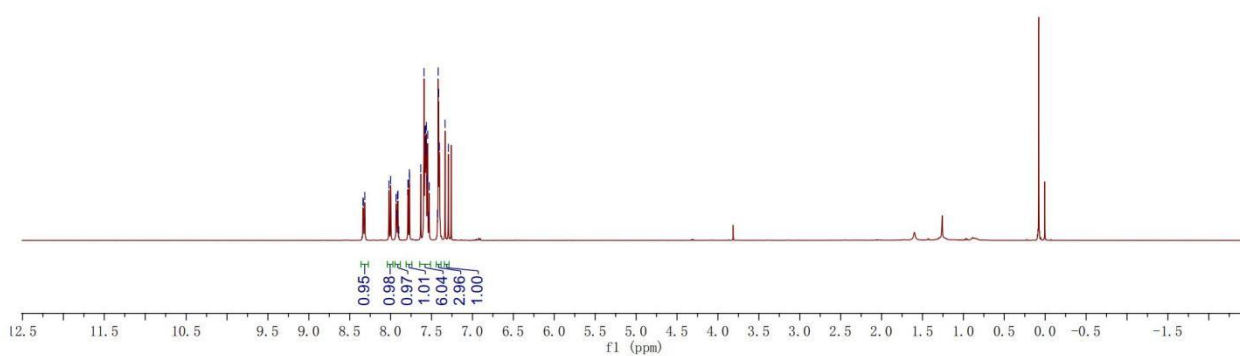




8.34
8.33
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7.33
7.29

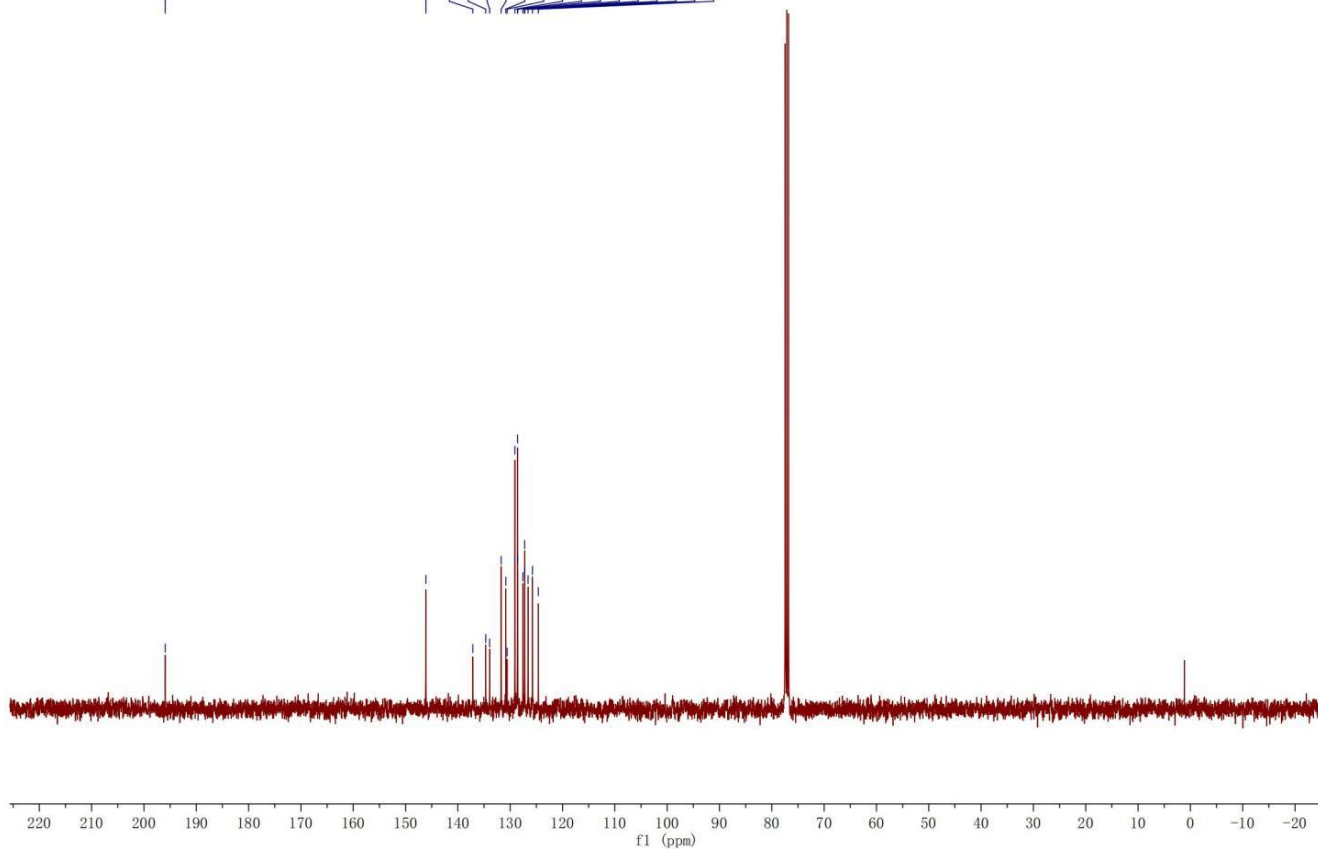


57

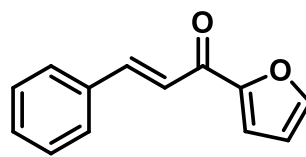
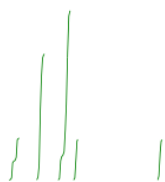


195.93

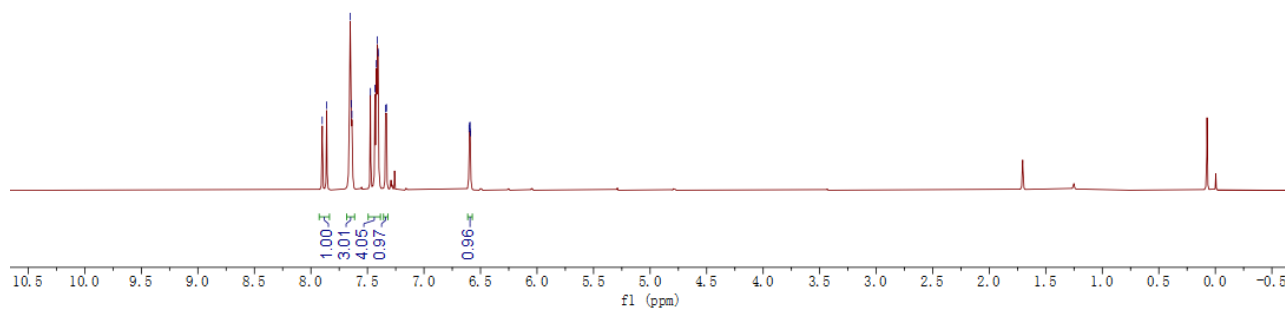
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137.14
134.67
133.93
131.72
130.84
130.58
129.10
128.61
128.55
127.56
127.24
127.21
126.59
125.74
124.62



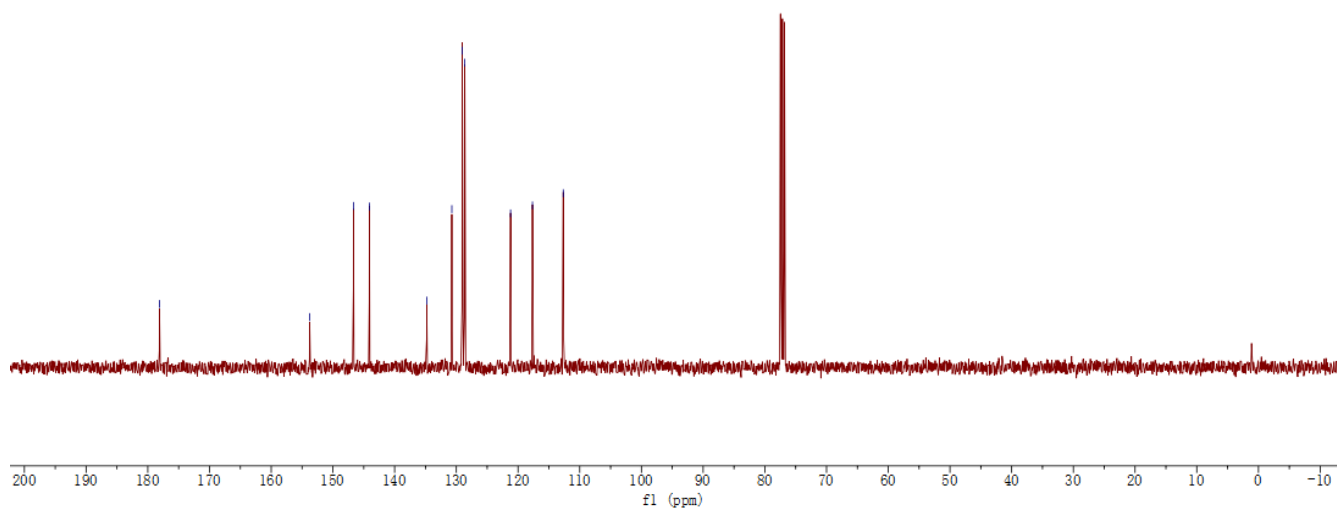
7.90
7.86
7.65
7.64
7.64
7.47
7.43
7.42
7.41
7.41
7.34
7.33
6.60
6.60
6.59



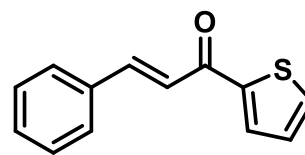
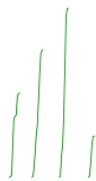
58



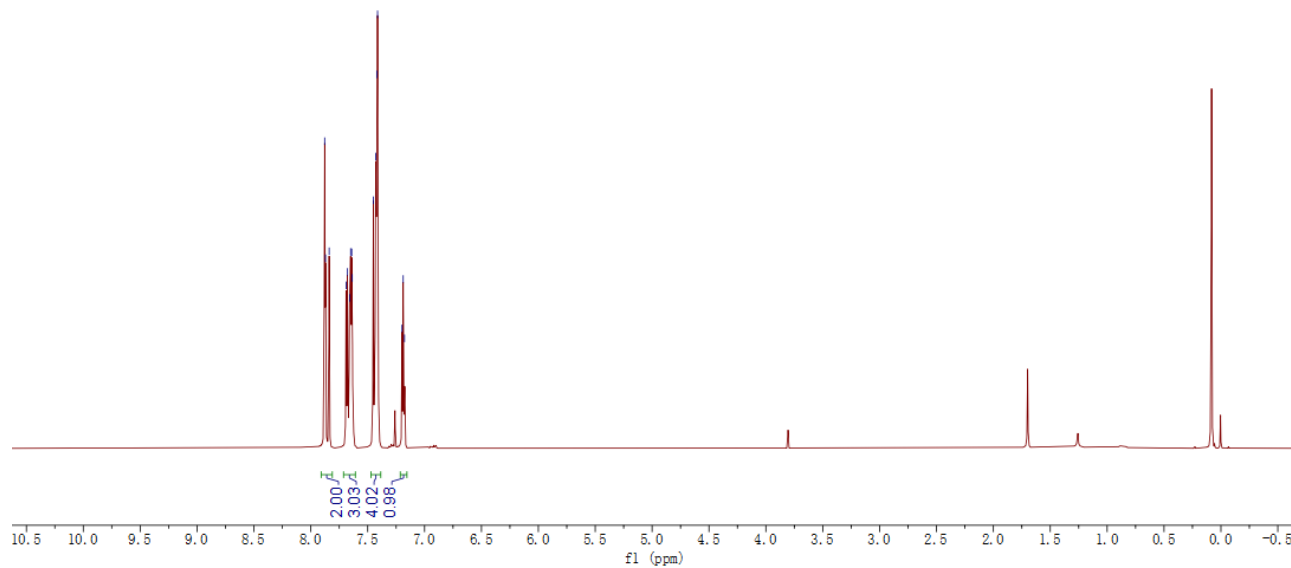
178.11
153.77
146.66
144.09
134.79
130.73
129.05
128.64
121.21
117.66
112.67



7.88
7.87
7.84
7.69
7.68
7.66
7.65
7.64
7.45
7.43
7.42
7.41
7.20
7.19
7.18

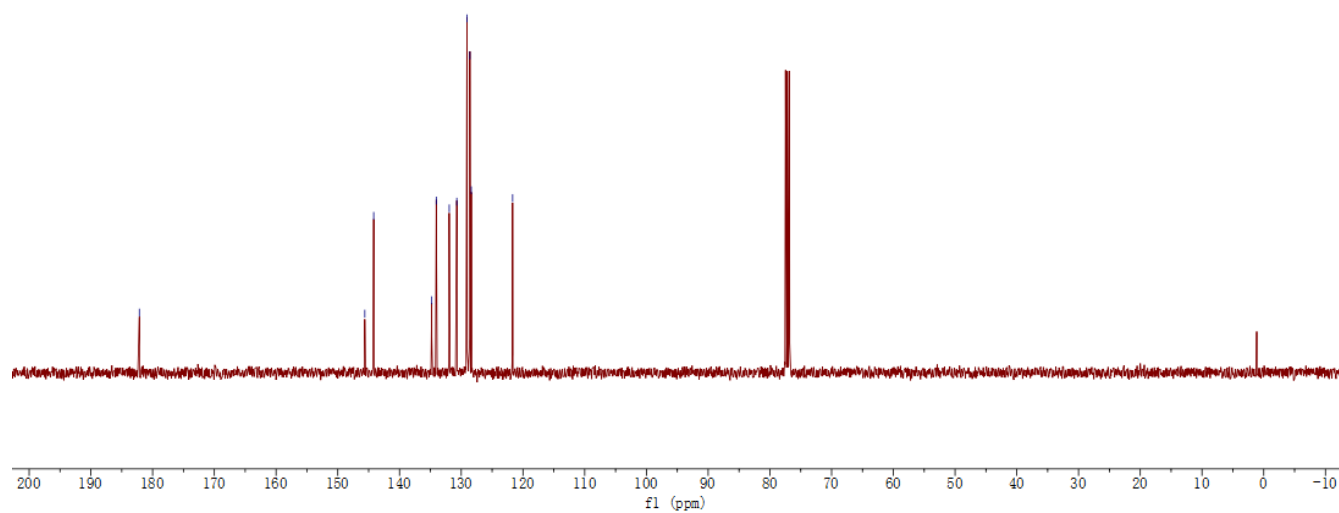


59

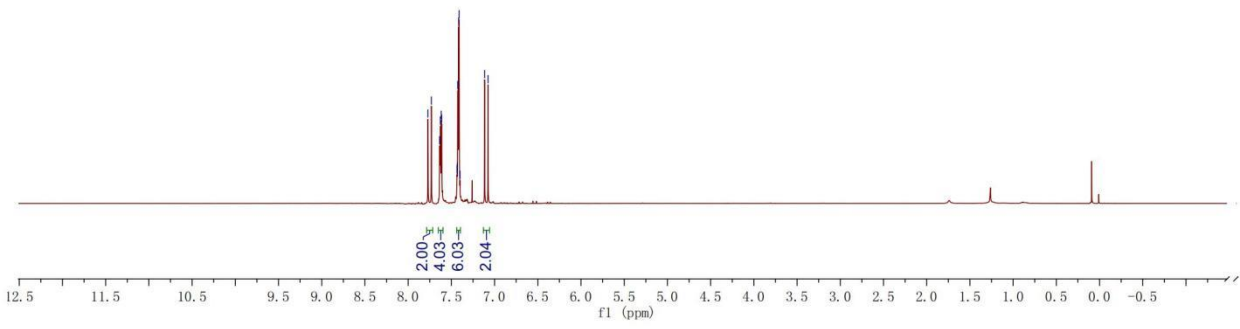
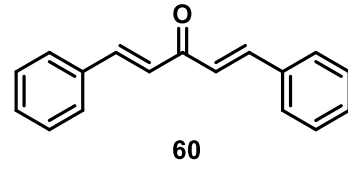


182.14

145.62
144.18
134.78
134.05
131.94
130.72
129.07
128.60
128.38
121.68

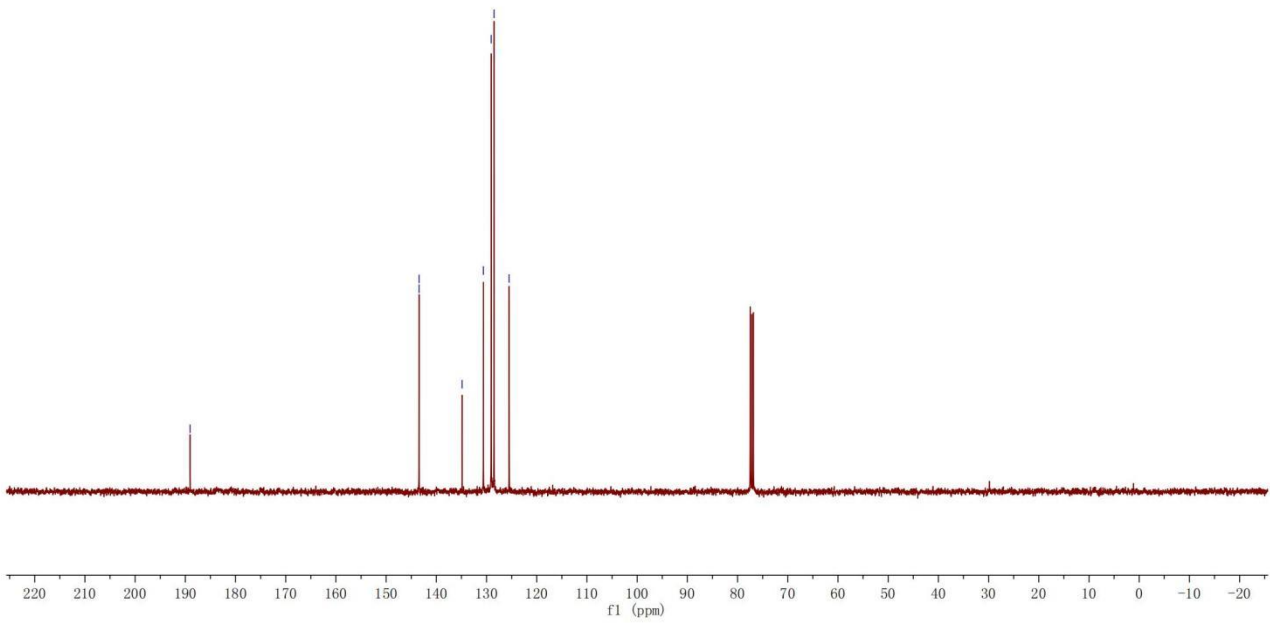


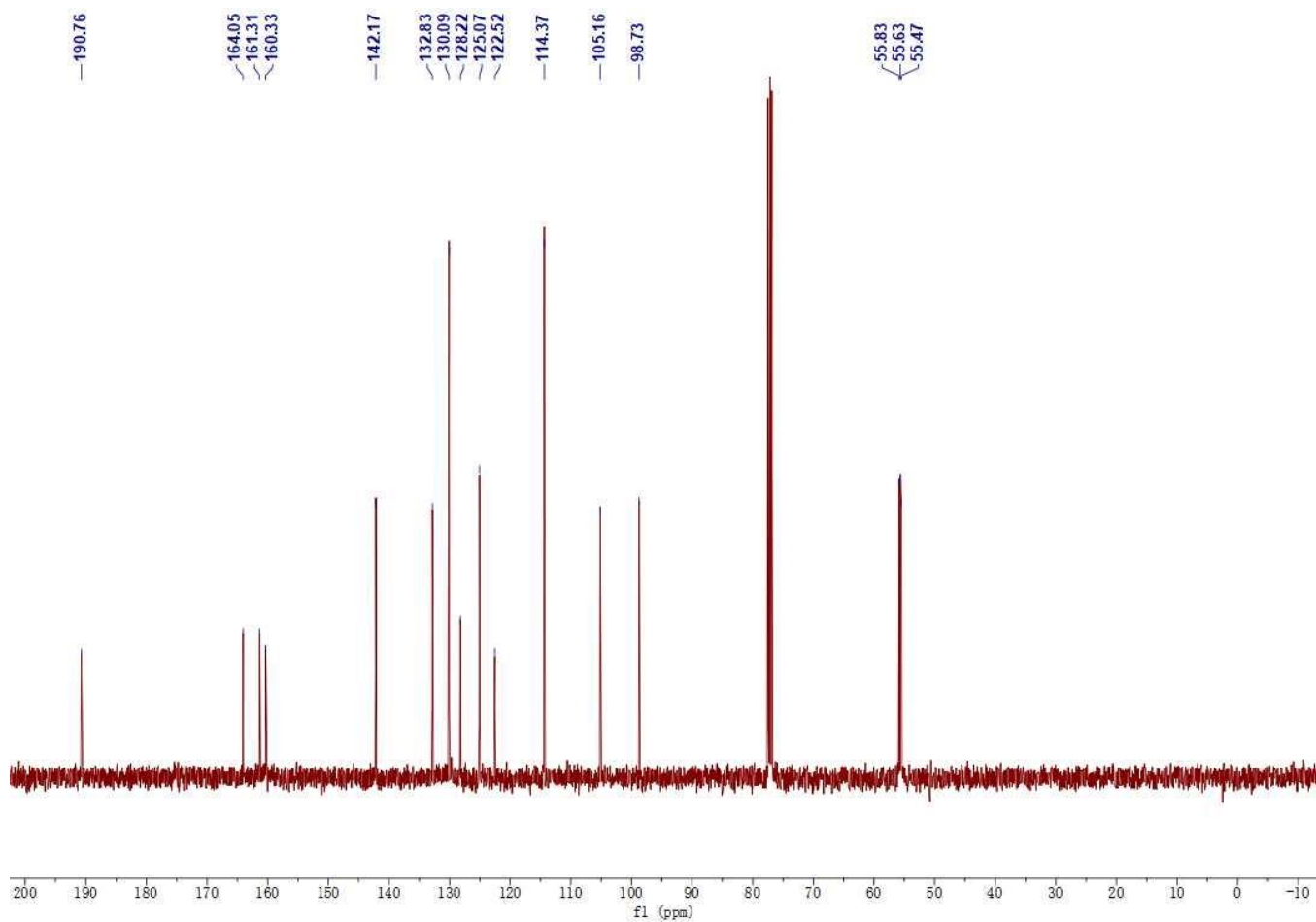
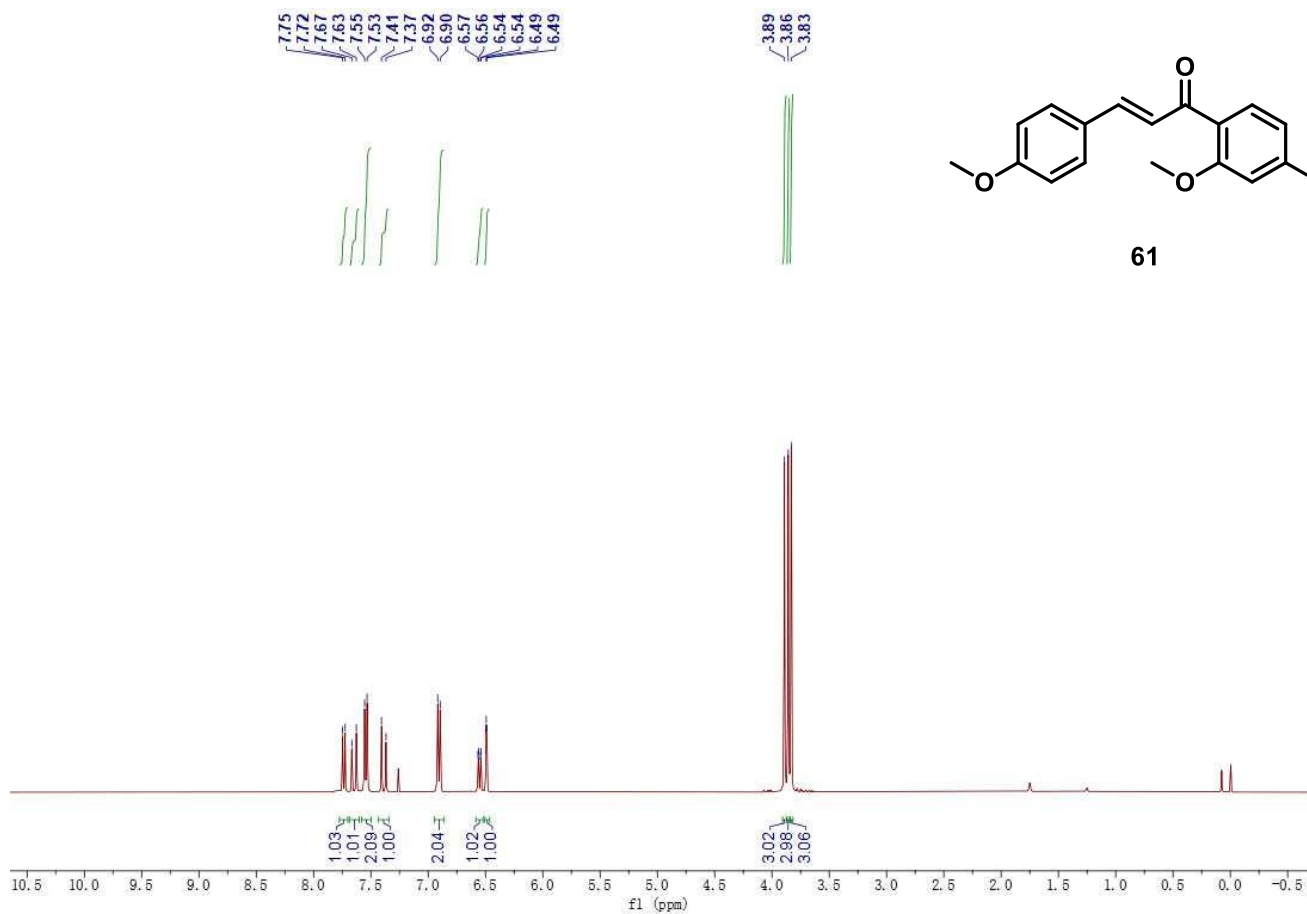
7.77
7.73
7.64
7.63
7.62
7.61
7.43
7.43
7.42
7.41
7.40
7.12
7.08



189.04

143.44
143.44
134.87
130.63
129.08
128.52
125.50





10. References

- [1] Wu, X. F.; Neumann, H.; Spannenberg, A.; Schulz, T.; Jiao, H.; Beller, M. J. *Am. Chem. Soc.* 2010, 132, 14596-14602.
- [2] Ishikawa, T.; Mizuta, T.; Hagiwara, K.; Aikawa, T.; Kudo, T.; Saito, S. *J. Org. Chem.* 2003, 68, 3702-3705.
- [3] Schmink, J. R.; Holcomb, J. L.; Leadbeater, N. E. *Org. Lett.* 2009, 11, 365-368.
- [4] Bianco, A.; Cavarischia, C.; Guiso, M. *Eur. J. Org. Chem.* 2004, 13, 2894-2898.
- [5] Hermange, P.; Gøgsig, T. M.; Lindhardt, T. M.; Taaning, R. H.; Skrydstrup, T. *Org. Lett.* 2011, 13, 9, 2444 - 2447
- [6] Chiaradia, L. D.; Mascarello, A.; Purificação, M.; Vernal, J.; Cordeiro, M. N. S.; Zenteno, M. E.; Villarino, A.; Nunes, R. J.; Yunes, R. A.; Terenzi, H. *Bioorg. Med. Chem. Lett.* 2008, 18, 6227-6230.
- [7] Montes-Avila, J.; Díaz-Camacho, S. P.; Sicairos-Félix, J.; Delgado-Vargas, F.; Rivero, I. A. *Bioorg. Med. Chem.* 2009, 17, 6780-6785.
- [8] Wu, J.; Wang, C.; Cai, Y.; Peng, J.; Liang, D.; Zhao, Y.; Yang, S.; Li, X.; Wu, X.; Liang, G. *Med Chem Res.* 2012, 21, 444 - 452.
- [9] Mathew, B.; Mathew, G. E.; Ucar, G.; Baysal, I.; Suresh, J.; Vilapurathu, K. J.; Prakasan, A.; Suresh, J. K.; Thomas, A. *Bioorganic Chemistry*, 2015, 62, 22 - 29
- [10] Ahmad, P.; Kwon, Y.; Rahman, A. F. M. M. P. *Bioorg. Med. Chem.*, 2016, 24, 1898 - 1908.