Supporting Information

Selective N-N or N-S bond cleavage of 1-trifluoromethyl benzotriazoles enables divergent synthesis of 1,2,4-benzotriazines and benzotriazoles

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1. General Information

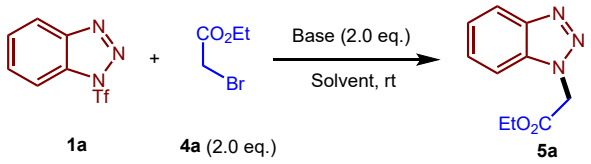
^{1}H and ^{13}C spectra were measured on a 600 MHz or 400 MHz NMR spectrometer using $CDCl_3$ as the solvent with tetramethylsilane (TMS) as the internal standard. Chemical shifts (δ) are given in parts per million relatives to TMS, and the coupling constants are given in hertz. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, brs = broad singlet. High-resolution mass spectrometry (HRMS) analysis was carried out using a TOF MS instrument with an APCI or ESI, EI source. Single-crystal X-ray diffraction studies were conducted at 293 K on the Bruker D8 VENTURE diffractometer equipped with a PHOTON-II detector (MoKα, λ = 0.71073 Å). An oil bath was used for heating when was needed. Column chromatography was performed using silica gel (200-300 mesh).

Commercially available materials purchased from Bidepharm and Energy Chemical were used as received. Unless otherwise specified, all reactions were carried out under nitrogen atmosphere in 10 mL Schlenk tubes. Benzotriazole were prepared according to previous literature procedures.

2. Optimization of reaction conditions for the synthesis of 5a

The results of the optimization of reaction conditions for the synthesis of **5a** are shown in Table S1. Different solvents were studied for the transformation mediated by LiOH (entries 1-5), and the reaction in DMF was found to be more effective than others (entry 3). Then different bases were also screened. The yield of **5a** was decreased when KOH, DBU or *t*-BuOK was utilized (entries 6-8). However, the use of Cs_2CO_3 afforded a better result (entry 9). Further investigation indicated that 1,4-dioxane was the most suitable solvent for the reaction mediated by Cs_2CO_3 (entry 14 vs entries 9-13). Therefore, the optimal reaction conditions for the synthesis of **5a** was established as following: using Cs_2CO_3 (2.0 eq) as the base and 1,4-dioxane as the solvent, and being stirred at room temperature.

Table S1 Optimization of reaction conditions for the synthesis of **5a** [a]



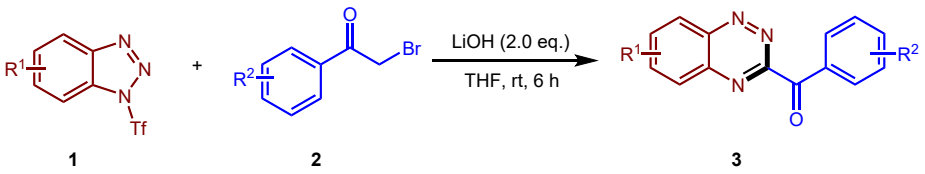
1a **4a** (2.0 eq.) **5a**

Entry	Base	Solvent	Yield of **5a** (%) [b]
1	LiOH	THF	40
2	LiOH	1,4-dioxane	46
3	LiOH	DMF	53
4	LiOH	MeCN	32
5	LiOH	PhCl	trace
6	KOH	DMF	27
7	DBU	DMF	nd [c]
8	*t*-BuOK	DMF	35
9	Cs_2CO_3	DMF	61
10	Cs_2CO_3	DCE	68
11	Cs_2CO_3	Acetone	27
12	Cs_2CO_3	THF	52
13	Cs_2CO_3	Toluene	76
14	**Cs_2CO_3**	**1,4-dioxane**	**80** [d]

[a] Reaction conditions: a mixture of 1-Tf-substituted benzotriazole **1a** (0.20 mmol), α-bromoacetophenone **4a** (0.40 mmol, 2 equiv), and base (0.40 mmol, 2 equiv) was stirred at rt under air atmosphere for about 6 h (monitored by TLC). [b] Yields of the products approximately determined by the crude ^{1}H NMR spectra. [c] nd = no desired product was detected. [d] Yields of isolated products.

3. General procedure for the synthesis of products 3 and 5

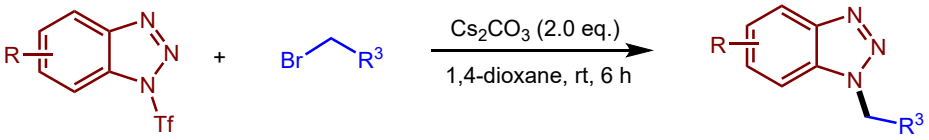
3.1 General procedure for the synthesis of products 3



1 2 3

Under nitrogen atmosphere, in a dry Schlenk tube, benzotriazole **1** (0.20 mmol) was added to tetrahydrofuran (2.0 mL) and stirred at room temperature. Then, bromide **2** (0.4 mmol) and LiOH (9.6 mg, 0.4 mmol) were added in sequence. The mixture was stirred for 6 h at room temperature. When the reaction was completed (monitored by TLC). The mixture was directly concentrated under reduced pressure. The resulting crude residue was purified via column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1 to 20:1) to afford the desired product **3** in good yields.

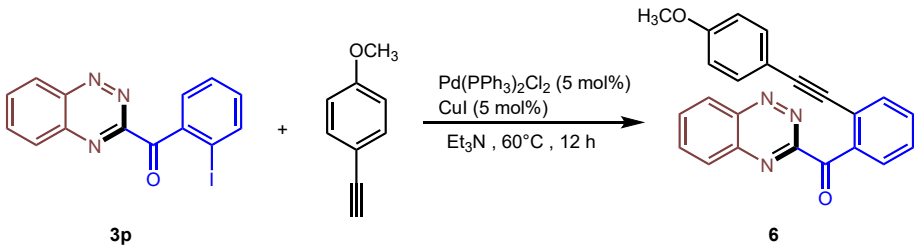
3.2 General procedure for the synthesis of products 5



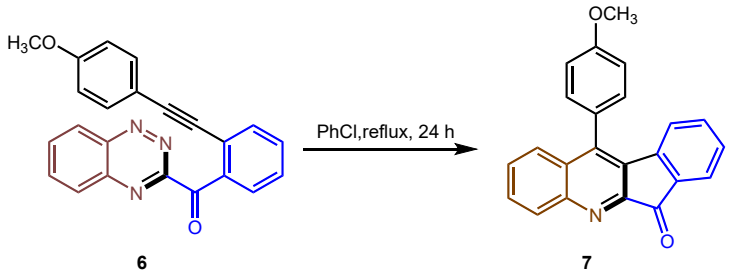
1 4 5

In a dry Schlenk tube, benzotriazole **1** (0.20 mmol) was added to 1,4-dioxane (2.0 mL) and stirred at room temperature. Then, bromide **4** (0.4 mmol) and Cs_2CO_3 (130.33mg, 0.4 mmol) were added in sequence. The mixture was stirred 6 h at room temperature. When the reaction was completed (monitored by TLC). The mixture was directly concentrated under reduced pressure. The resulting crude residue was purified via column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1 to 20:1) to afford the desired product **5** in good yields.

4. General procedure for the transformations of 3p



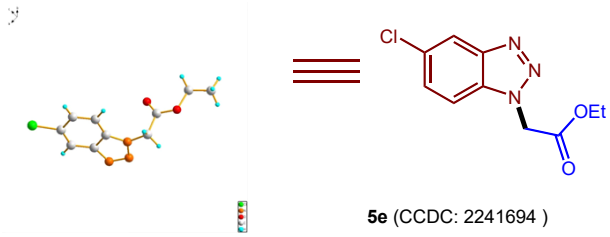
Under nitrogen atmosphere ,in a dry Schlenk tube with a magnetic stir bar, was added **3p** (72.2 mg, 0.20 mmol) and the reaction solvent Et_3N (2.0 mL) were added, followed by $Pd(PPh_3)_2Cl_2$ (7.0 mg,0.01 mmol) and CuI (1.9 mg, 0.01 mmol), 10 min later by *p*-methoxyphenylacetylene (29.07 mg, 0.22 mmol) and the reaction mixture was stirred at 60℃ for 12 h until the **3p** was complete consumed (monitored by TLC). The reaction was quenched with HCl (1.0 M, pH = 6-7), and extracted with EA (10 mL×3). The organic extracts were combined and dried over Na_2SO_4 and concentrated under reduced pressure. The resulting crude residue was purified via column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford the desired product **6** with 90% (65.7 mg) yield.



Under nitrogen atmosphere ,in a dry Schlenk tube with a magnetic stir bar, was added **6** (73.0 mg, 0.20 mmol) and the reaction solvent PhCl (2.0 mL) were added, the reaction mixture was stirred at 160℃ for 24 h until the **6** was complete consumed (monitored by TLC). The system was cooled to room temperature and the solvent was spin-dried over the column (petroleum ether/ethyl acetate = 8:1) to afford the desired product **7** with 75% (50.6 mg) yield.

5. Crystal structures of 5e

Product **5e** was crystallized as a yellow crystal via vaporization of a petroleum ether/ethyl acetate solution, and its absolute configuration was determined by x-ray structure analysis. The CCDC number was 2241694. The supplementary crystallographic data that could be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data request/cif.



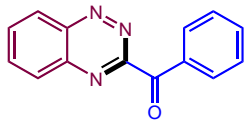
5e (CCDC: 2241694)

Crystal data and structure refinement for 5e.

CCDC Number	2241694
Identification code	**5e**
Empirical formula	$C_{10}H_{10}ClN_3O_2$
Formula weight	239.66
Temperature/K	298.00
Crystal system	monoclinic
Space group	C2/c
a/Å	21.347(2)
b/Å	11.8842(11)
c/Å	9.4684(9)
α/°	90
β/°	111.351(3)
γ/°	90
Volume/Å3	2237.2(4)
Z	8
ρcalcg/cm3	1.423
μ/mm-1	0.330
F(000)	992.0
Crystal size/mm3	0.19 × 0.178 × 0.154
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.648 to 50.742
Index ranges	-25 ≤ h ≤ 25, -14 ≤ k ≤ 14, -11 ≤ l ≤ 11
Reflections collected	9082
Independent reflections	2050 [Rint = 0.0395, Rsigma = 0.0306]
Data/restraints/parameters	2050/0/146
Goodness-of-fit on F2	1.029
Final R indexes [I>=2σ (I)]	R1 = 0.0545, wR2 = 0.1320
Final R indexes [all data]	R1 = 0.0744, wR2 = 0.1481
Largest diff. peak/hole / e Å-3	0.37/-0.27

6. Characterization of Products

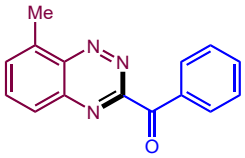
Benzo[*e*][1,2,4]triazin-3-yl(phenyl)methanone (3a)



Isolated in 78% yield (36.7 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.26 – 8.19 (m, 1H), 8.14 – 8.08 (m, 3H), 8.06 – 8.01 (m, 1H), 7.69 – 7.63 (m, 1H), 7.55 – 7.48 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.55, 158.10, 147.60, 140.33, 136.65, 135.16, 134.24, 132.73, 131.23, 129.80, 129.68, 128.69. HRMS (ESI) calcd. for $C_{14}H_{10}N_3O$ [M+H$^+$]: 236.0810, found: 236.0819.

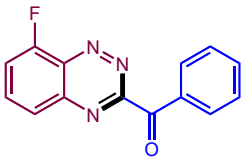
(8-Methylbenzo[*e*][1,2,4]triazin-3-yl)(phenyl)methanone (3b)



Isolated in 67% yield (33.4 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 – 8.13 (m, 2H), 8.08 (d, *J* = 8.5 Hz, 1H), 8.03 – 7.97 (m, 1H), 7.85 – 7.81 (m, 1H), 7.71 – 7.64 (m, 1H), 7.57 – 7.51 (m, 2H), 3.11 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.80, 158.00, 146.89, 140.97, 139.40, 136.79, 135.39, 134.13, 132.45, 131.32, 128.60, 127.40, 17.02. HRMS (ESI) calcd. for $C_{15}H_{12}N_3O$ [M+H$^+$]: 250.0975, found: 250.0976.

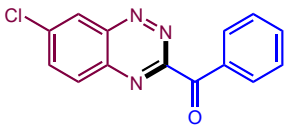
(8-Fluorobenzo[*e*][1,2,4]triazin-3-yl)(phenyl)methanone (3c)



Isolated in 65% yield (32.9 mg) as yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.15 – 8.05 (m, 4H), 7.74 – 7.66 (m, 2H), 7.60 – 7.50 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 190.08 (s), 158.56 (s), 157.74 (d, *J* = 270.2 Hz), 141.04 (s), 139.23 (d, *J* = 12.5 Hz), 136.68 (d, *J* = 8.4 Hz), 134.95 (s), 134.47 (s), 131.25 (s), 128.79 (s), 125.66 (d, *J* = 5.2 Hz), 116.45 (d, *J* = 17.7 Hz). HRMS (ESI) calcd. for $C_{14}H_9FN_3O$ [M+H$^+$]: 254.0724, found: 254.0724.

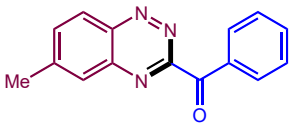
(7-Chlorobenzo[*e*][1,2,4]triazin-3-yl)(phenyl)methanone (3d)



Isolated in 67% yield (36.1 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 1.9 Hz, 1H), 8.22 (d, *J* = 9.0 Hz, 1H), 8.12 (d, *J* = 7.5 Hz, 2H), 8.05 (dd, *J* = 9.0, 2.1 Hz, 1H), 7.72 – 7.65 (m, 1H), 7.58 – 7.52 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.17, 158.19, 147.52, 139.12, 138.98, 137.97, 135.08, 134.41, 131.27, 128.79, 128.41 (1 peak is missing). HRMS (ESI) calcd. for $C_{14}H_9ClN_3O$ [M+H$^+$]: 270.0429, found: 270.0431.

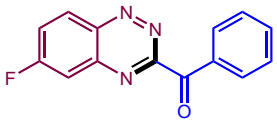
(6-Methylbenzo[*e*][1,2,4]triazin-3-yl)(phenyl)methanone (3e)



Isolated in 69% yield (34.4 mg) as yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.53 (d, *J* = 8.6 Hz, 1H), 8.12 (d, *J* = 7.6 Hz, 2H), 7.98 (s, 1H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.71 – 7.63 (m, 1H), 7.58 – 7.49 (m, 2H), 2.70 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 190.71, 158.29, 148.63, 146.62, 140.69, 135.31, 135.29, 134.13, 131.22, 129.26, 128.63, 127.86, 22.79. HRMS (ESI) calcd. for $C_{15}H_{12}N_3O$ [M+H$^+$]:250.0975, found:250.0976.

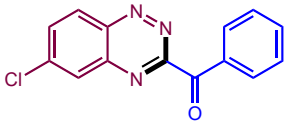
(6-Fluorobenzo[*e*][1,2,4]triazin-3-yl)(phenyl)methanone (3f)



Isolated in 78% yield (39.5 mg) as yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.74 – 8.68 (m, 1H), 8.12 – 8.07 (m, 2H), 7.84 – 7.79 (m, 2H), 7.70 – 7.65 (m, 1H), 7.55 – 7.51 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 190.27, 166.64 (d, *J* = 264.1 Hz), 158.39, 145.61, 142.28 (d, *J* = 14.8 Hz), 135.01, 134.41, 132.96 (d, *J* = 10.9 Hz), 131.22, 128.77, 124.19 (d, *J* = 27.3 Hz), 112.82 (d, *J* = 21.9 Hz). HRMS (ESI) calcd. for $C_{14}H_9FN_3O$ [M+H$^+$]: 254.0724, found: 254.0726.

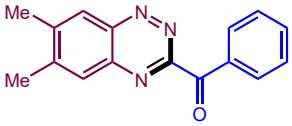
(6-Chlorobenzo[*e*][1,2,4]triazin-3-yl)(phenyl)methanone (3g)



Isolated in 58% yield (31.2 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 9.0 Hz, 1H), 8.23 (d, *J* = 2.0 Hz, 1H), 8.14 – 8.06 (m, 2H), 7.97 (dd, *J* = 9.0, 2.1 Hz, 1H), 7.73 – 7.65 (m, 1H), 7.59 – 7.48 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 190.20, 158.56, 146.26, 143.37, 140.86, 134.99, 134.45, 134.19, 131.24, 131.19, 128.80, 128.40. HRMS (ESI) calcd. for $C_{14}H_9ClN_3O$ [M+H$^+$]: 270.0429, found: 270.0431.

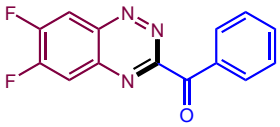
(6,7-Dimethylbenzo[*e*][1,2,4]triazin-3-yl)(phenyl)methanone (3h)



Isolated in 63% yield (33.2 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 8.12 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.95 (s, 1H), 7.69 – 7.62 (m, 1H), 7.53-7.50 (m, 2H), 2.61 (s, 3H), 2.59 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.80, 157.80, 148.92, 146.91, 144.35, 139.63, 135.37, 133.94, 131.19, 128.51, 128.07, 128.01, 21.23, 20.80. HRMS (ESI) calcd. for $C_{16}H_{14}N_3O$ [M+H$^+$]: 264.1131, found: 264.1131.

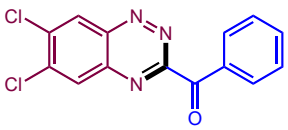
(6,7-Difluorobenzo[*e*][1,2,4]triazin-3-yl)(phenyl)methanone (3i)



Isolated in 55% yield (29.8 mg) as yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.42 (t, *J* = 8.4 Hz, 1H), 8.09 (d, *J* = 7.5 Hz, 2H), 8.02 – 7.93 (m, 1H), 7.69 (t, *J* = 7.4 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.91, 158.33 (d, *J* = 2.4 Hz), 157.12 (dd, *J* = 269.4, 16.9 Hz), 153.99 (dd, *J* = 265.7, 17.0 Hz), 145.54 (d, *J* = 10.4 Hz), 139.15 (d, *J* = 12.6 Hz), 134.91, 134.45, 131.19, 128.77, 115.47 (d, *J* = 2.3 Hz), 115.34 (dd, *J* = 9.8, 7.8 Hz). HRMS (ESI) calcd. for $C_{14}H_8F_2N_3O$ [M+H$^+$]: 272.0630, found: 272.0639.

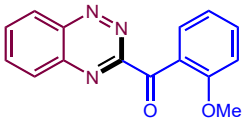
(6,7-Dichlorobenzo[*e*][1,2,4]triazin-3-yl)(phenyl)methanone (3j)



Isolated in 57% yield (34.5 mg) as yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.81 (s, 1H), 8.37 (s, 1H), 8.09 (d, *J* = 7.7 Hz, 2H), 7.71 – 7.67 (m, 1H), 7.54 (t, *J* = 7.7 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.86, 158.44, 146.09, 142.57, 139.10, 138.18, 134.90, 134.53, 131.22, 130.34, 130.19, 128.83. HRMS (ESI) calcd. for $C_{14}H_8Cl_2N_3O$ [M+H$^+$]: 304.0039, found: 304.0042.

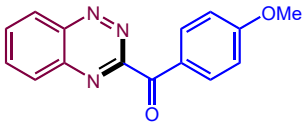
Benzo[*e*][1,2,4]triazin-3-yl(2-methoxyphenyl)methanone (3k)



Isolated in 60% yield (31.8 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (dd, *J* = 8.4, 0.7 Hz, 1H), 8.23 (d, *J* = 8.1 Hz, 1H), 8.11 – 8.04 (m, 1H), 8.02 – 7.94 (m, 2H), 7.63 – 7.56 (m, 1H), 7.19 – 7.13 (m, 1H), 6.95 (d, *J* = 8.4 Hz, 1H), 3.41 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 192.09, 159.84, 159.46, 147.31, 140.74, 136.15, 135.29, 132.06, 131.53, 129.82, 129.76, 126.51, 121.37, 112.01, 55.81. HRMS (ESI) calcd. for $C_{15}H_{12}N_3O_2$ [M+H$^+$]: 266.0924, found: 266.0925.

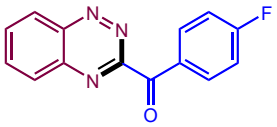
Benzo[*e*][1,2,4]triazin-3-yl(4-methoxyphenyl)methanone (3l)



Isolated in 56% yield (29.7 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 8.3 Hz, 1H), 8.24 (d, *J* = 8.4 Hz, 1H), 8.18 – 8.08 (m, 3H), 8.07 – 7.99 (m, 1H), 7.01 (d, *J* = 8.9 Hz, 2H), 3.92 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.98, 164.64, 158.70, 147.62, 140.47, 136.54, 133.84, 132.51, 129.86, 129.72, 128.22, 114.12, 55.76. HRMS (ESI) calcd. for $C_{15}H_{12}N_3O_2$ [M+H$^+$]: 266.0924, found: 266.0926.

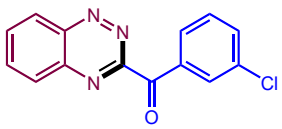
Benzo[*e*][1,2,4]triazin-3-yl(4-fluorophenyl)methanone (3m)



Isolated in 64% yield (32.4 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (dd, *J* = 8.4, 0.5 Hz, 1H), 8.29 – 8.19 (m, 3H), 8.17 – 8.12 (m, 1H), 8.10 – 8.04 (m, 1H), 7.26 – 7.19 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.86, 166.52 (d, *J* = 257.3 Hz), 157.87, 144.04 (d, *J* = 731.1 Hz), 136.78, 134.20, 133.50 (d, *J* = 121.9 Hz), 131.65 (d, *J* = 3.0 Hz), 129.87, 129.74, 116.14, 115.92. HRMS (ESI) calcd. for $C_{14}H_9FN_3O$ [M+H$^+$]: 254.0724, found: 254.0726.

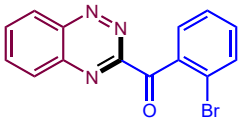
Benzo[*e*][1,2,4]triazin-3-yl(3-chlorophenyl)methanone (3n)



Isolated in 57% yield (30.7 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 – 8.60 (m, 1H), 8.27 (d, *J* = 8.5 Hz, 1H), 8.18 – 8.11 (m, 2H), 8.11 – 7.98 (m, 2H), 7.70 – 7.61 (m, 1H), 7.49 (t, *J* = 7.9 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.06, 157.33, 147.58, 140.25, 136.70, 134.86, 133.98, 132.90, 130.94, 129.89, 129.76, 129.66, 129.32. HRMS (ESI) calcd. for $C_{14}H_9ClN_3O$ [M+H$^+$]: 270.0429, found: 270.0431.

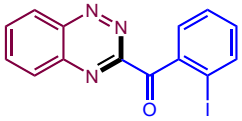
Benzo[*e*][1,2,4]triazin-3-yl(2-bromophenyl)methanone (3o)



Isolated in 59% yield (36.9 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 8.3 Hz, 1H), 8.27 (d, *J* = 8.4 Hz, 1H), 8.16 – 8.10 (m, 1H), 8.09 – 8.03 (m, 1H), 7.82 – 7.74 (m, 1H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.47 (td, *J* = 7.6, 1.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.86, 156.67, 147.36, 140.74, 139.12, 136.62, 133.34, 133.13, 133.05, 131.37, 130.02, 129.82, 127.76, 121.26. HRMS (ESI) calcd. for $C_{14}H_9BrN_3O$ [M+H$^+$]: 313.9924, found: 313.9926.

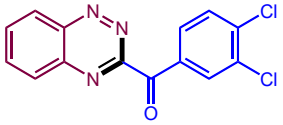
Benzo[*e*][1,2,4]triazin-3-yl(2-iodophenyl)methanone (3p)



Isolated in 60% yield (43.3 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 8.3 Hz, 1H), 8.26 (d, *J* = 8.4 Hz, 1H), 8.13 (t, *J* = 7.5 Hz, 1H) 8.07 (t, *J* = 7.6 Hz, 1H), 7.94 (d, *J* = 7.9 Hz, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.28 (t, *J* = 7.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.77, 155.94, 147.25, 142.63, 140.70, 139.85, 136.65, 133.22, 132.75, 131.09, 130.02, 129.80, 128.29, 93.47. HRMS (ESI) calcd. for $C_{14}H_9IN_3O$ [M+H$^+$]: 361.9785, found: 361.9786.

benzo[*e*][1,2,4]triazin-3-yl(3,4-dichlorophenyl)methanone (3q)

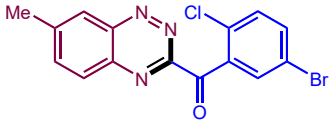


Isolated in 77% yield (46.7 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (dd, *J* = 8.4, 0.7 Hz, 1H), 8.30 (d, *J* = 2.0 Hz, 1H), 8.27 (d, *J* = 8.4 Hz, 1H), 8.18 – 8.13 (m, 1H), 8.11 – 8.02 (m, 2H), 7.63 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$)

δ 188.14, 157.10, 147.75, 140.41, 139.02, 136.97, 134.86, 133.45, 133.23, 133.08, 130.86, 130.33, 129.92, 129.83. HRMS (ESI) calcd. for $C_{14}H_8Cl_2N_3O$ [M+H$^+$]: 304.0039, found: 304.0041.

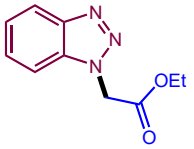
(5-Bromo-2-chlorophenyl)(7-methylbenzo[*e*][1,2,4]triazin-3-yl)methanone (3r)



Isolated in 56% yield (40.4 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (s, 1H), 8.16 (d, *J* = 8.7 Hz, 1H), 7.96 (dd, *J* = 8.7, 1.4 Hz, 1H), 7.89 (d, *J* = 2.3 Hz, 1H), 7.65 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.32 (d, *J* = 8.5 Hz, 1H), 2.73 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.93, 156.16, 147.47, 145.00, 139.50, 139.45, 138.83, 135.70, 133.66, 131.89, 131.64, 129.48, 128.07, 120.98, 22.47. HRMS (ESI) calcd. for $C_{15}H_{10}BrClN_3O$ [M+H$^+$]: 361.9690, found: 361.9695.

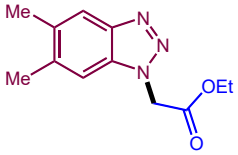
Ethyl 2-(1H-benzo[*d*][1,2,3]triazol-1-yl)acetate (5a)



Isolated in 80% yield (32.8 mg) as yellow liquid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.04 (m, 1H), 7.52 – 7.43 (m, 2H), 7.40 – 7.34 (m, 1H), 5.40 (s, 2H), 4.22 (q, *J* = 7.1 Hz, 2H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.45, 146.06, 133.45, 127.97, 124.18, 120.21, 109.33, 62.39, 49.14, 14.12. HRMS (ESI) calcd. for $C_{10}H_{12}N_3O_2$ [M+H$^+$]: 206.0924, found: 206.0921.

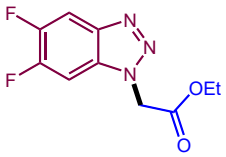
Ethyl 2-(5,6-dimethyl-1H-benzo[*d*][1,2,3]triazol-1-yl)acetate (5b)



Isolated in 66% yield (30.8 mg) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.21 (s, 1H), 5.35 (s, 2H), 4.25 (q, *J* = 7.1 Hz, 2H), 2.41 (s, 3H), 2.40 (s, 3H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.68, 145.35, 138.49, 134.08, 132.56, 119.36, 108.76, 62.37, 49.16, 21.11, 20.53, 14.21. HRMS (ESI) calcd. for $C_{12}H_{16}N_3O_2$ [M+H$^+$]: 234.1237, found: 234.1234.

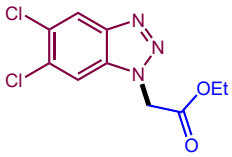
Ethyl 2-(5,6-difluoro-1H-benzo[*d*][1,2,3]triazol-1-yl)acetate (5c)



Isolated in 63% yield (30.4 mg) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, J = 9.0, 7.1 Hz, 1H), 7.30 (dd, J = 8.6, 6.6 Hz, 1H), 5.39 (s, 2H), 4.28 (q, J = 7.1 Hz, 2H), 1.30 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.05, 150.67 (dd, J = 524.7, 16.7 Hz), 150.64 (dd, J = 22.3, 16.5 Hz), 141.29 (d, J = 9.7 Hz), 129.47 (d, J = 11.4 Hz), 106.81 (dd, J = 20.2, 1.7 Hz), 97.16 (d, J = 23.7 Hz), 62.72, 49.47, 14.17. HRMS (ESI) calcd. for $C_{10}H_{10}F_2N_3O_2$ [M+H$^+$]: 242.0736, found: 242.0735.

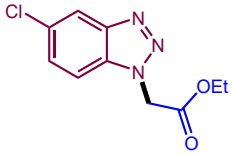
Ethyl 2-(5,6-dichloro-1H-benzo[*d*][1,2,3]triazol-1-yl)acetate (5d)



Isolated in 82% yield (44.8 mg) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.64 (s, 1H), 5.37 (s, 2H), 4.27 (q, J = 7.1 Hz, 2H), 1.28 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.89, 144.96, 133.18, 132.44, 129.11, 121.07, 110.85, 62.68, 49.29, 14.08. HRMS (ESI) calcd. for $C_{10}H_{10}Cl_2N_3O_2$ [M+H$^+$]: 274.0145, found: 274.0144.

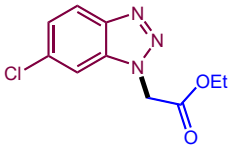
Ethyl 2-(5-chloro-1H-benzo[*d*][1,2,3]triazol-1-yl)acetate (5e)



Isolated in 31% yield (14.8 mg) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 1.1 Hz, 1H), 7.47 (dd, J = 8.8, 1.6 Hz, 1H), 7.41 (d, J = 8.8 Hz, 1H), 5.40 (s, 2H), 4.25 (q, J = 7.1 Hz, 2H), 1.26 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.17, 146.78, 132.21, 130.20, 128.97, 119.66, 110.46, 62.61, 49.38, 14.17. HRMS (ESI) calcd. for $C_{10}H_{11}ClN_3O_2$ [M+H$^+$]: 240.0534, found: 240.0534.

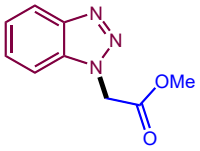
Ethyl 2-(6-chloro-1H-benzo[*d*][1,2,3]triazol-1-yl)acetate (5e')



Isolated in 38% yield (18.2 mg) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.8 Hz, 1H), 7.47 (d, *J* = 1.3 Hz, 1H), 7.31 (dd, *J* = 8.8, 1.7 Hz, 1H), 5.35 (s, 2H), 4.22 (q, *J* = 7.1 Hz, 2H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.16, 144.61, 134.41, 134.03, 125.39, 121.08, 109.36, 62.52, 49.12, 14.08. HRMS (ESI) calcd. for $C_{10}H_{11}ClN_3O_2$ [M+H$^+$]: 240.0534, found: 240.0534.

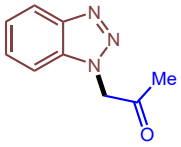
Methyl 2-(1H-benzo[*d*][1,2,3]triazol-1-yl)acetate (5f)



Isolated in 74% yield (28.3 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.4 Hz, 1H), 7.50 – 7.42 (m, 2H), 7.38 – 7.33 (m, 1H), 5.40 (s, 2H), 3.74 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.92, 146.01, 133.39, 127.99, 124.18, 120.15, 109.27, 52.99, 48.89. HRMS (ESI) calcd. for $C_9H_{10}N_3O_2$ [M+H$^+$]: 192.0768, found: 192.0764.

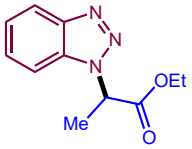
1-(1H-Benzo[*d*][1,2,3]triazol-1-yl)propan-2-one (5g)



Isolated in 20% yield (7.0 mg) as yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.3 Hz, 1H), 7.55 – 7.48 (m, 1H), 7.43 – 7.36 (m, 2H), 5.45 (s, 2H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.04, 146.09, 133.53, 128.16, 124.34, 120.34, 109.19, 56.92, 27.23. HRMS (ESI) calcd. for $C_{19}H_{10}N_3O$ [M+H$^+$]: 176.0818, found: 176.0813.

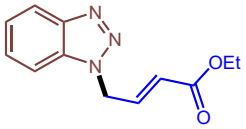
Ethyl 2-(1H-benzo[*d*][1,2,3]triazol-1-yl)propanoate (5h)



Isolated in 79% yield (34.6 mg) as yellow liquid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.4 Hz, 1H), 7.58 – 7.46 (m, 2H), 7.42 – 7.36 (m, 1H), 5.71 (q, *J* = 7.4 Hz, 1H), 4.21 (q, *J* = 7.1 Hz, 2H), 2.03 (d, *J* = 7.4 Hz, 3H), 1.20 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.31, 146.44, 132.61, 127.67, 124.17, 120.37, 110.08, 62.38, 57.42, 16.83, 14.12. HRMS (ESI) calcd. for $C_{11}H_{14}N_3O_2$ [M+H$^+$]: 220.1081, found: 220.1076.

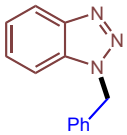
Ethyl-4-(1H-benzo[*d*][1,2,3]triazol-1-yl)but-2-enoate (5i)



Isolated in 35% yield (16.2 mg) as yellow liquid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 – 8.06 (m, 1H), 7.56 – 7.46 (m, 2H), 7.45 – 7.40 (m, 1H), 7.12 (dt, *J* = 15.7, 5.2 Hz, 1H), 5.75 (dt, *J* = 15.7, 1.8 Hz, 1H), 5.46 (dd, *J* = 5.2, 1.8 Hz, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.33, 146.24, 139.83, 132.95, 127.99, 124.40, 124.35, 120.42, 109.30, 61.00, 48.67, 14.23. HRMS (ESI) calcd. for $C_{12}H_{14}N_3O_2$ [M+H$^+$]: 232.1081, found: 232.1080.

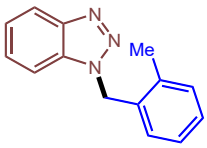
1-Benzyl-1H-benzo[*d*][1,2,3]triazole (5j)



Isolated in 84% yield (35.1 mg) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 8.06 (m, 1H), 7.44 – 7.27 (m, 8H), 5.86 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.46, 134.87, 132.93, 129.15, 128.62, 127.72, 127.55, 124.08, 120.22, 109.86, 52.42. HRMS (ESI) calcd. for $C_{13}H_{12}N_3$ [M+H$^+$]: 210.1026, found: 210.1022.

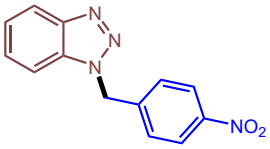
1-(2-Methylbenzyl)-1H-benzo[*d*][1,2,3]triazole (5k)



Isolated in 82% yield (36.6 mg) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 7.9 Hz, 1H), 7.39 – 7.29 (m, 2H), 7.28 – 7.12 (m, 4H), 7.04 (d, *J* = 7.6 Hz, 1H), 5.83 (s, 2H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.32, 136.61, 133.06, 132.65, 131.01, 128.74, 128.57, 127.40, 126.48, 123.94, 120.10, 109.93, 50.84, 19.33. HRMS (ESI) calcd. for $C_{14}H_{14}N_3$ [M+H$^+$]: 224.1182, found: 224.1180.

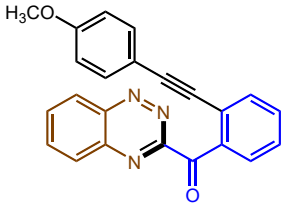
1-(4-Nitrobenzyl)-1H-benzo[*d*][1,2,3]triazole (5l)



Isolated in 92% yield (46.8 mg) as yellow solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.6 Hz, 2H), 8.09 (d, *J* = 8.2 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.43 – 7.35 (m, 4H), 5.97 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.97, 146.34, 141.95, 132.77, 128.33, 128.07, 124.41, 124.31, 120.40, 109.19, 51.17. HRMS (ESI) calcd. for $C_{13}H_{11}N_3O_2$ [M+H$^+$]: 255.0877, found: 255.0878.

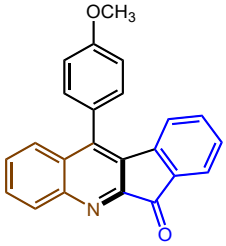
Benzo[*e*][1,2,4]triazin-3-yl(2-((4-methoxyphenyl)ethynyl)phenyl)methanone (6)



Isolated in 90% yield (65.7 mg) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.4 Hz, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 8.05 – 7.94 (m, 2H), 7.92 – 7.84 (m, 1H), 7.63 – 7.49 (m, 3H), 6.67 (d, *J* = 8.7 Hz, 2H), 6.51 (d, *J* = 8.7 Hz, 2H), 3.70 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.17, 159.71, 158.74, 147.46, 140.69, 138.71, 136.18, 133.14, 132.64, 132.61, 132.37, 130.41, 129.73, 129.68, 128.45, 124.30, 113.84, 113.69, 97.07, 86.67, 55.35. HRMS (ESI) calcd. for $C_{23}H_{16}N_3O_2$ [M+H$^+$]: 366.1237, found: 366.1239.

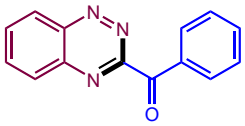
11-(4-Methoxyphenyl)-6H-indeno[2,1-*b*]quinolin-6-one (7)



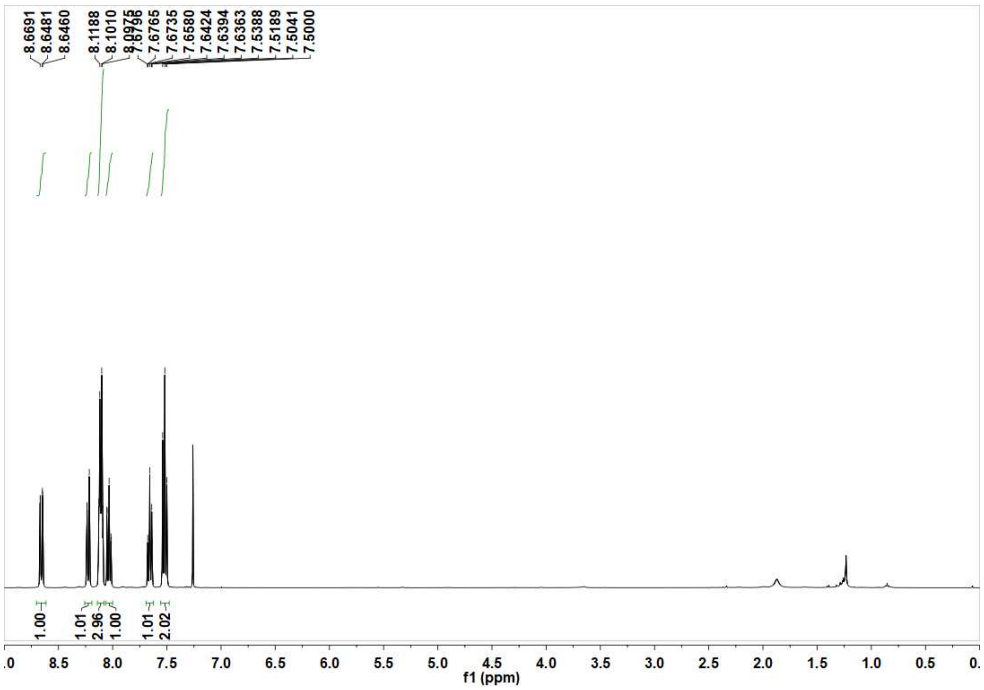
Isolated in 75% yield (50.6 mg) as white solid.

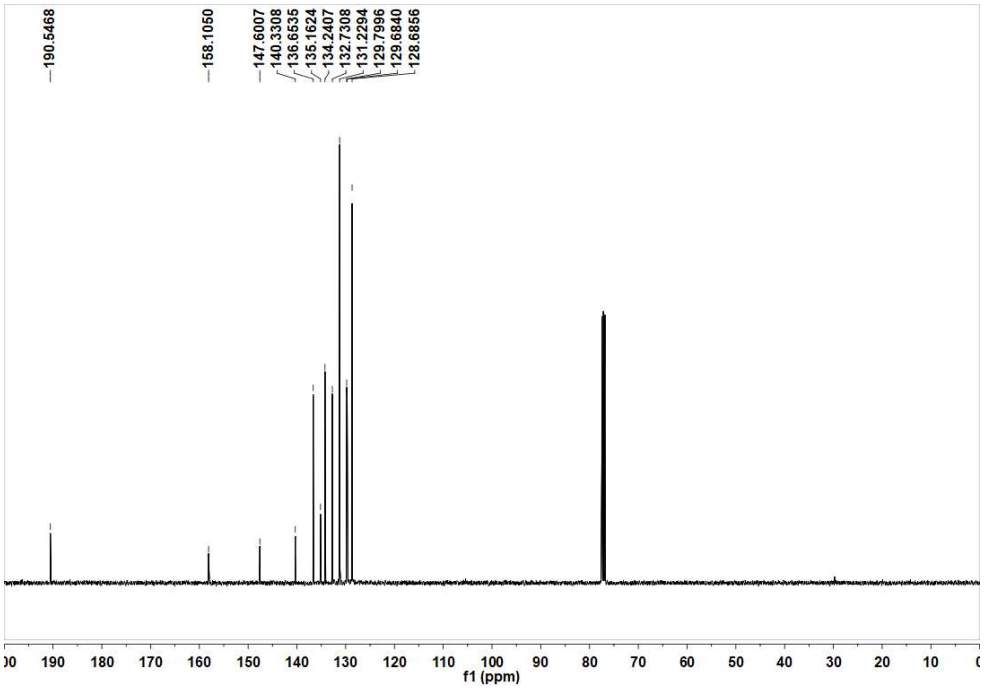
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.1 Hz, 1H), 7.81 (s, 1H), 7.68 (t, *J* = 7.1 Hz, 1H), 7.57 (d, *J* = 7.9 Hz, 1H), 7.54 – 7.48 (m, 1H), 7.39 – 7.28 (m, 4H), 7.17 (d, *J* = 8.0 Hz, 2H), 6.71 – 6.60 (m, 1H), 3.97 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.75, 160.26, 154.16, 148.60, 143.44, 141.86, 135.92, 134.71, 131.94, 131.34, 130.35, 130.19, 130.00, 129.52, 129.23, 127.02, 126.75, 124.91, 124.09, 114.95, 55.59. HRMS (ESI) calcd. for $C_{23}H_{16}NO_2$ [M+H$^+$]: 338.1176, found: 338.1177.

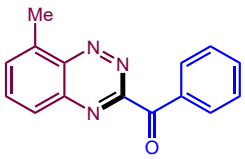
7. Spectra of new compounds



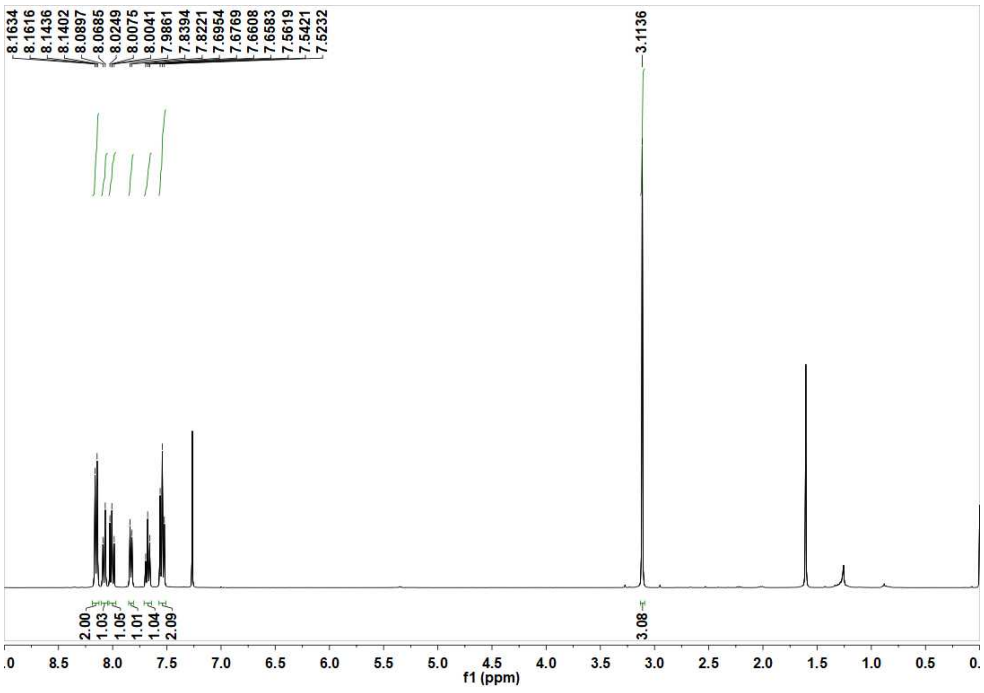
3a






Me
N
N
N
O

3b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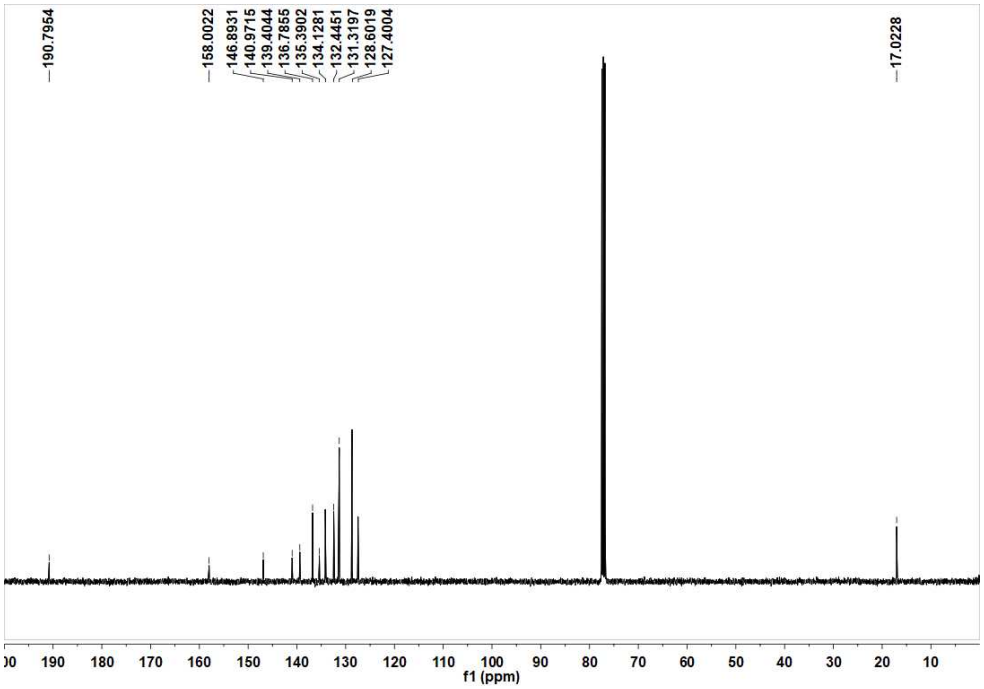
8.1436
8.1402
8.0897
8.0685
8.0249
8.0075
8.0041
7.9861
7.8394
7.8221
7.6954
7.6769
7.6608
7.6583
7.5619
7.5421
7.5232
3.1136
2.00
1.03
1.05
1.01
1.04
2.09
3.08
f1 (ppm)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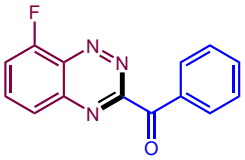
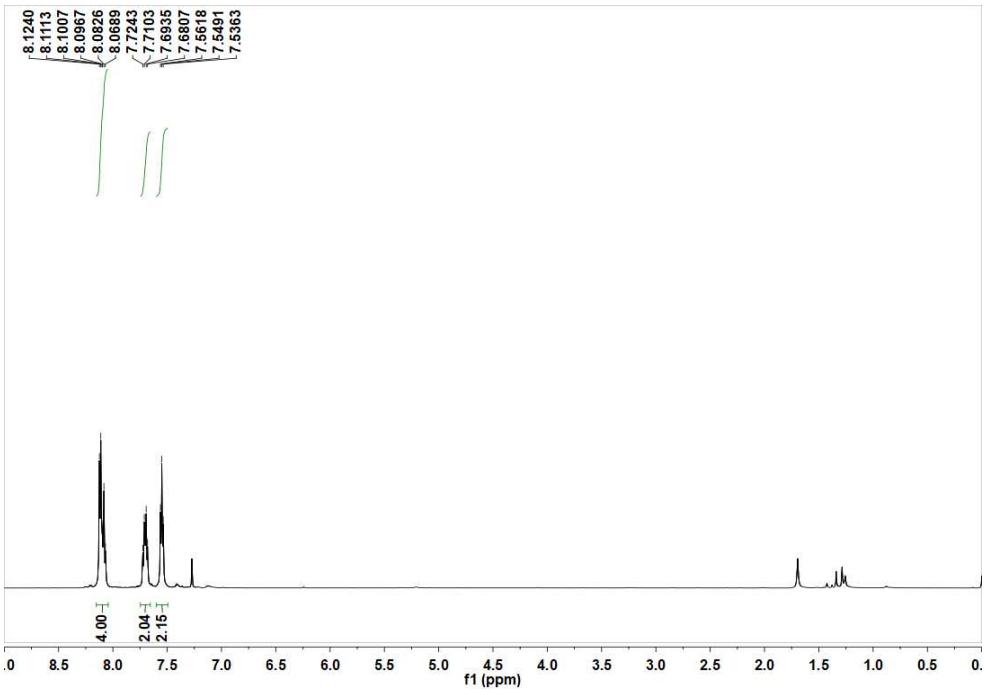
158.0022
146.8931
140.9715
139.4044
136.7855
135.3902
134.1281
132.4451
131.3197
128.6019
127.4004
17.0228
f1 (ppm)


F
N
N
N
O

3c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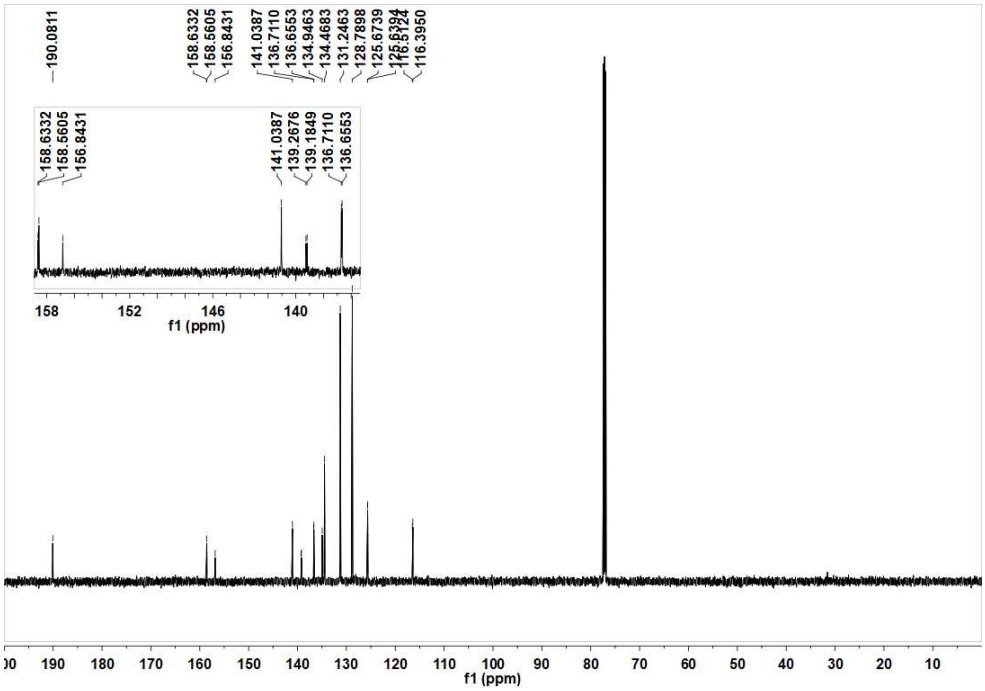
8.1113
8.1007
8.0967
8.0826
8.0689
7.7243
7.7103
7.6935
7.6807
7.5618
7.5491
7.5363
4.00
2.04
2.15
f1 (ppm)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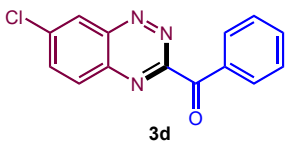
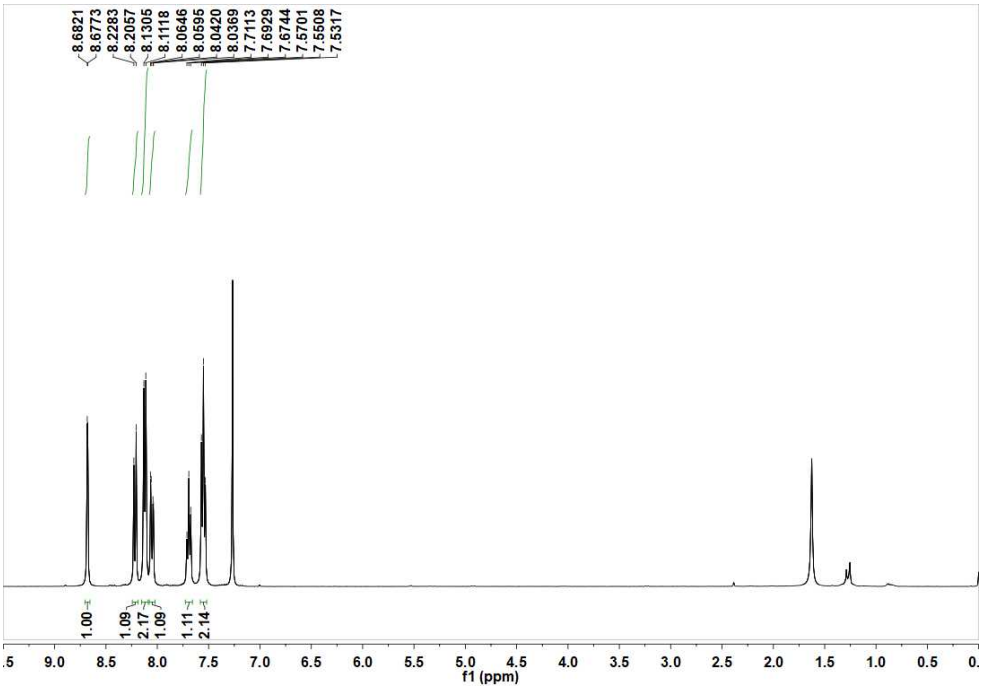
158.6332
158.5605
156.8431
141.0387
136.7110
136.6553
134.9463
134.4683
131.2463
128.7898
125.6739
116.3950
158.6332
158.5605
156.8431
141.0387
139.2676
139.1849
136.7110
136.6553
158
152
146
140
f1 (ppm)
f1 (ppm)


Cl
N
N
N
O

3d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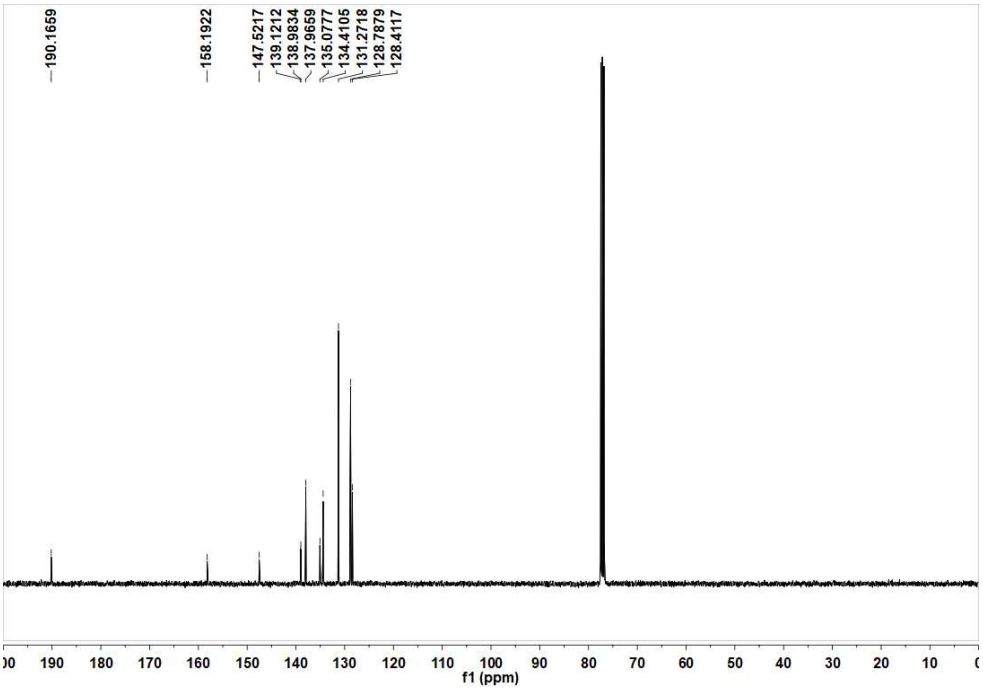
8.6773
8.2283
8.2057
8.1305
8.1118
8.0646
8.0595
8.0420
8.0369
7.7113
7.6929
7.6744
7.5701
7.5508
7.5317
1.00
1.09
2.17
1.09
1.11
2.14
f1 (ppm)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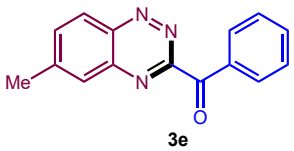
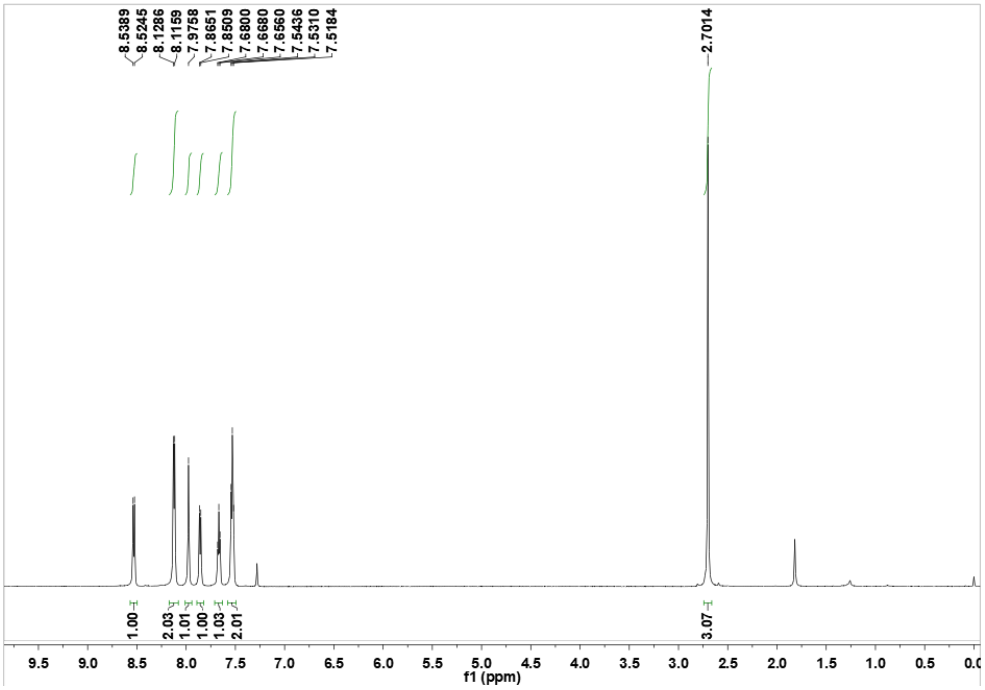
158.1922
147.5217
139.1212
138.9834
137.9659
135.0777
134.4105
131.2718
128.7879
128.4117
f1 (ppm)


Me
N
N
N
O

3e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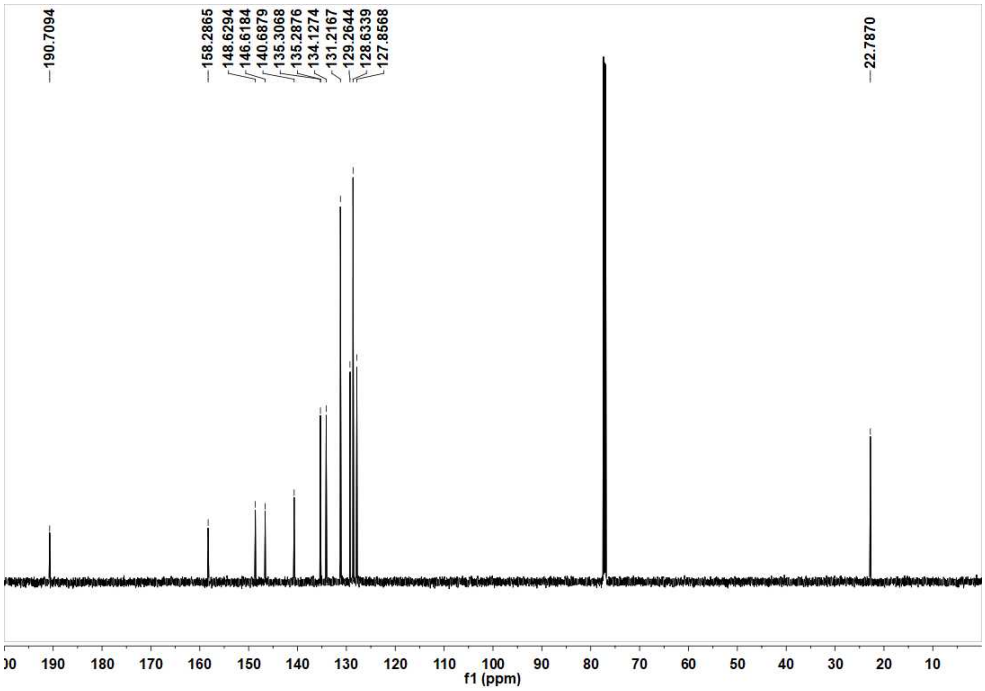
8.1286
8.1159
7.9758
7.8651
7.8509
7.6800
7.6680
7.6560
7.5436
7.5310
7.5184
2.7014
1.00
2.03
1.01
1.00
1.03
2.01
3.07
f1 (ppm)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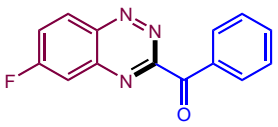
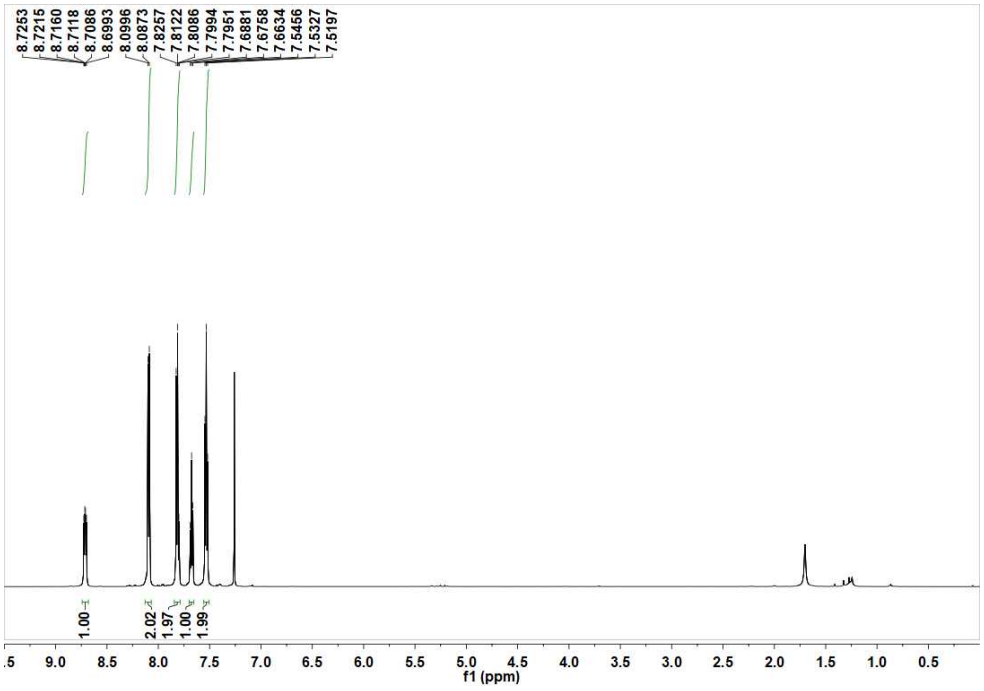
158.2865
148.6294
146.6184
140.6879
135.3068
135.2876
134.1274
131.2167
129.2644
128.6339
127.8568
22.7870
f1 (ppm)


N
N
N
F
O

3f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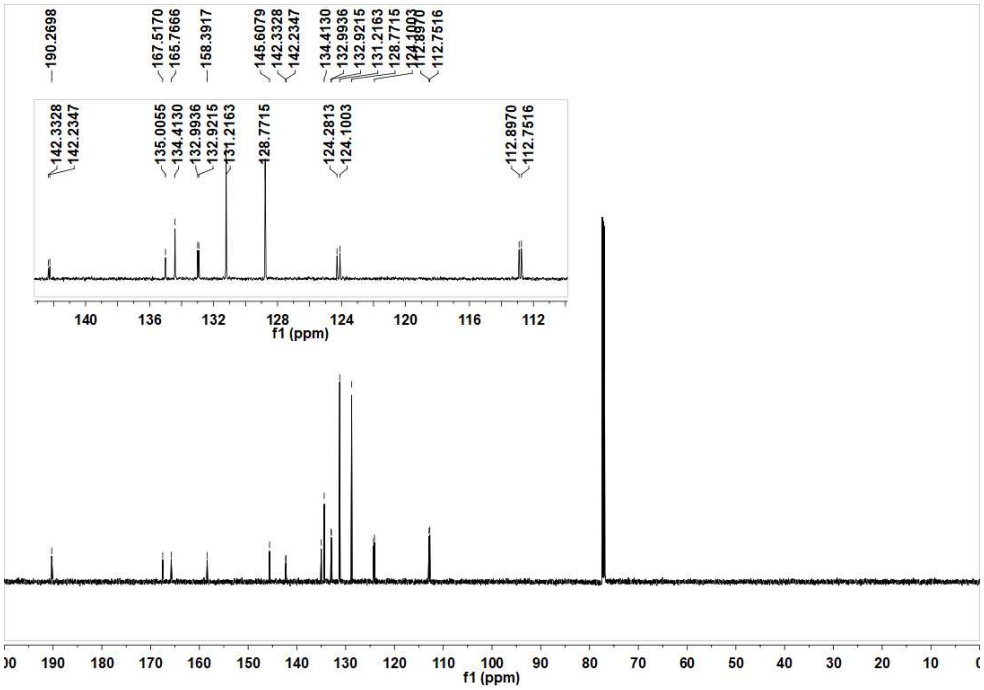
8.7215
8.7160
8.7118
8.7086
8.6993
8.0996
8.0873
7.8257
7.8122
7.8086
7.7994
7.7951
7.6881
7.6758
7.6634
7.5456
7.5327
7.5197
1.00
2.02
1.97
1.00
1.99
f1 (ppm)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165.7666
158.3917
145.6079
142.3328
142.2347
134.4130
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131.2163
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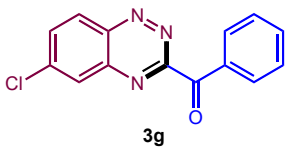
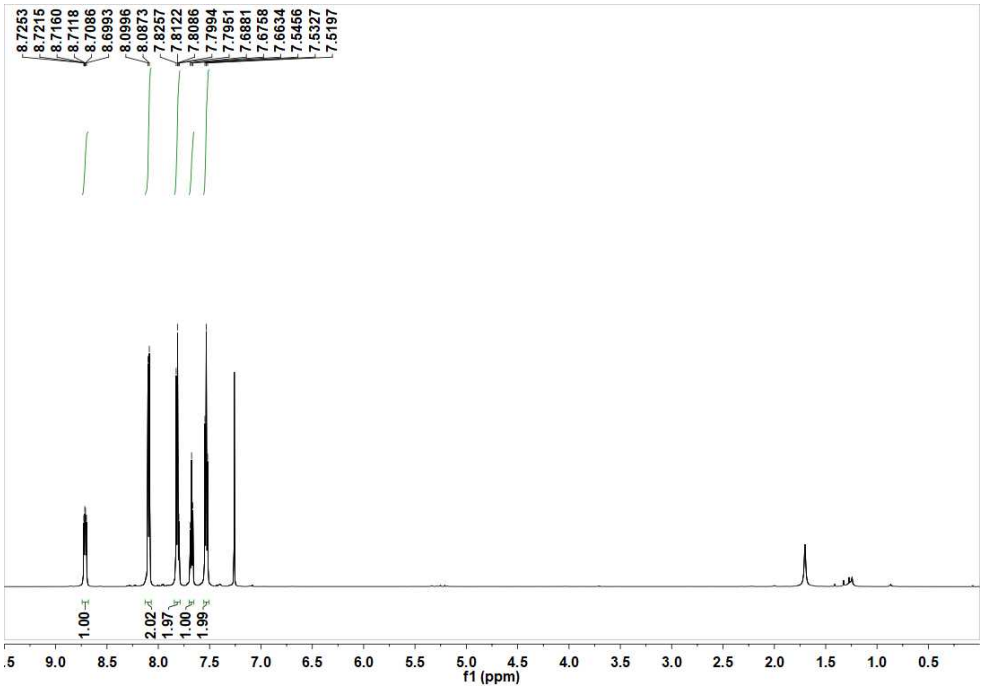
124.2813
124.1003
112.8970
112.7516
135.0055
f1 (ppm)


N
N
N
Cl
O

3g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8.7215
8.7160
8.7118
8.7086
8.6993
8.0996
8.0873
7.8257
7.8122
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7.7994
7.7951
7.6881
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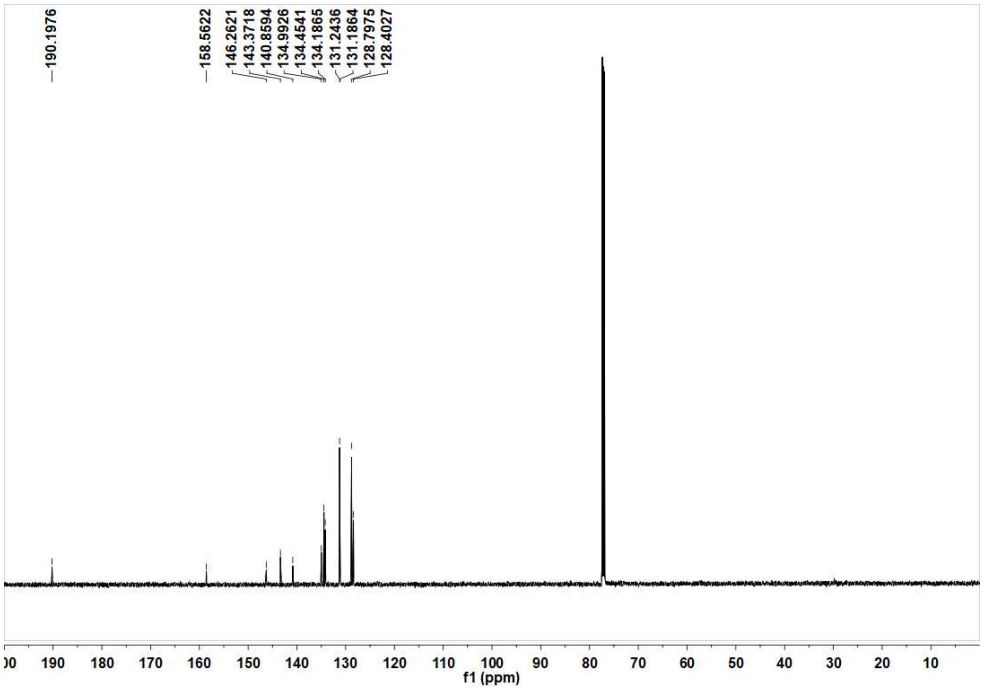
2.02
1.97
1.00
1.99
f1 (ppm)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134.9926
134.4541
134.1865
131.2436
131.1864
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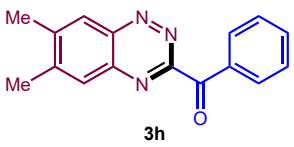
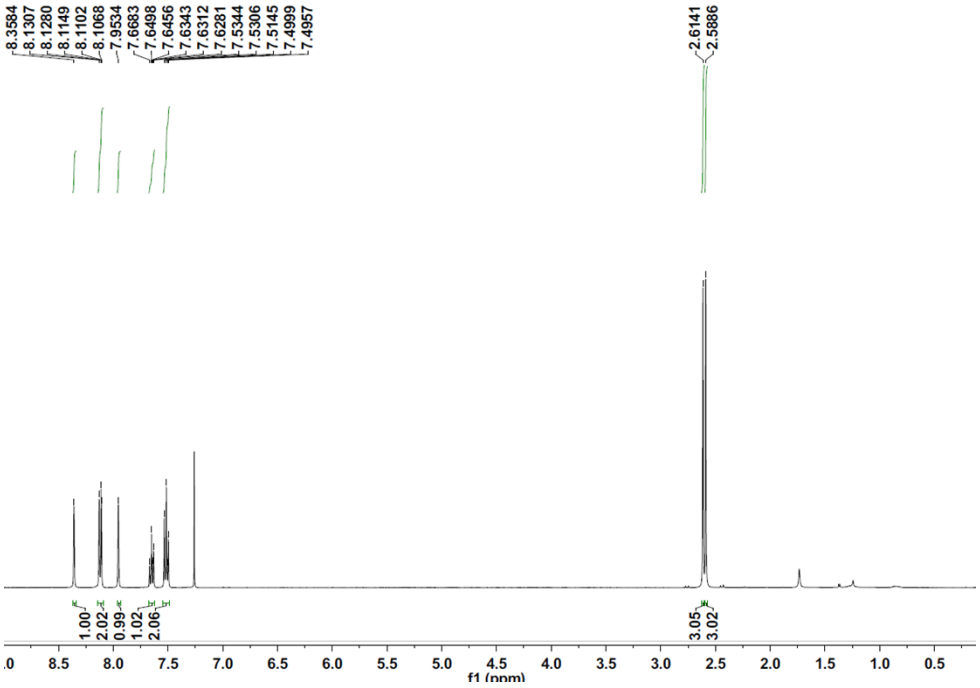
f1 (ppm)


Me
Me
N
N
N
O

3h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8.1149
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7.6498
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7.6281
7.5344
7.5306
7.5145
7.4999
7.4957
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2.5886
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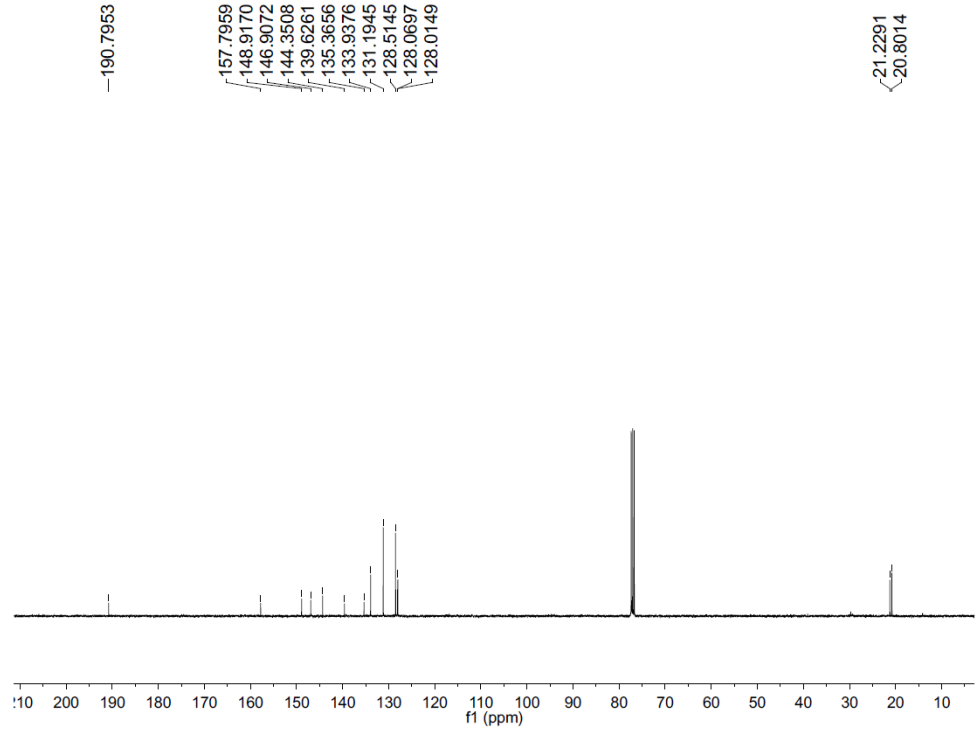
2.02
0.99
1.02
2.06
3.05
3.02
f1 (ppm)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128.0149
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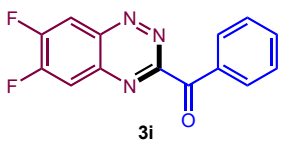
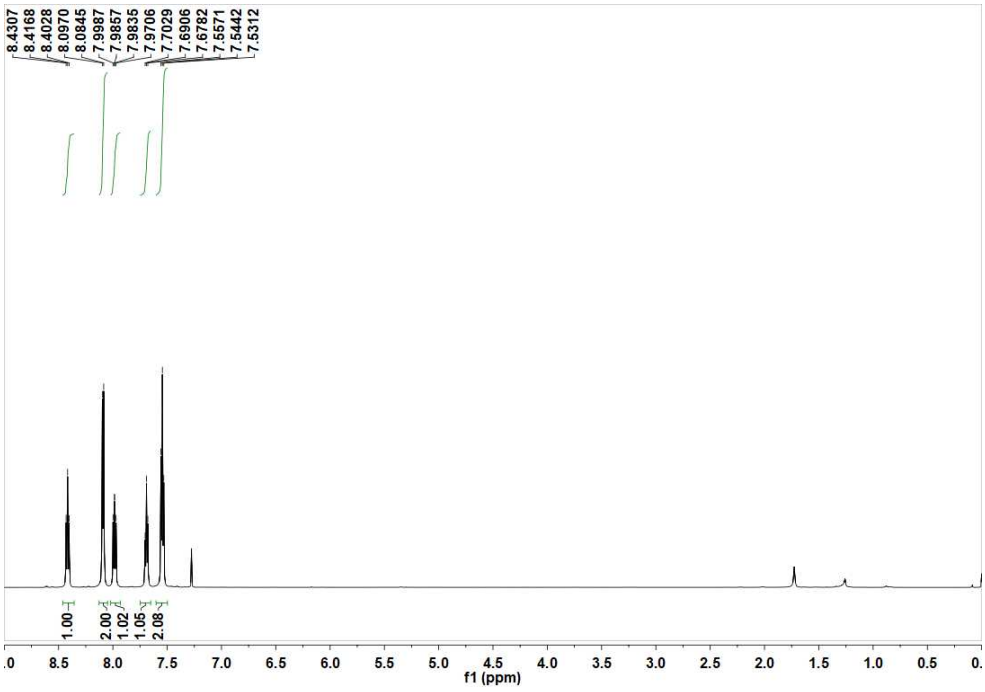
20.8014
f1 (ppm)


F
F
N
N
N
O

3i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7.9857
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7.9706
7.7029
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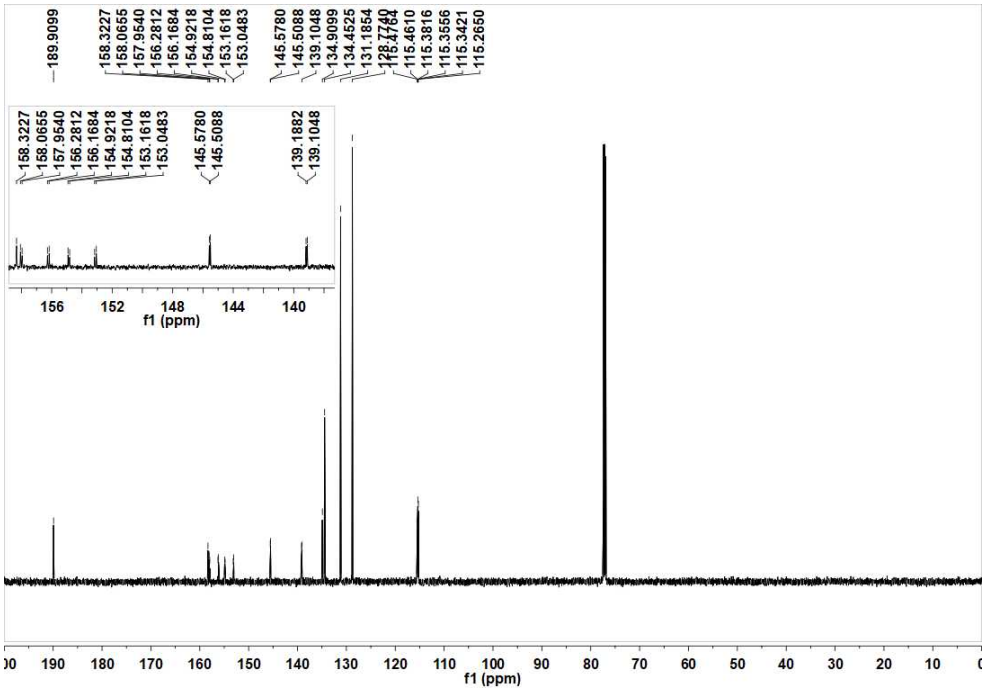
7.6782
7.5571
7.5442
7.5312
1.00
2.00
1.02
1.05
2.08
f1 (ppm)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156.2812
156.1684
154.9218
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153.1618
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145.5780
145.5088
139.1048
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115.3816
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115.3421
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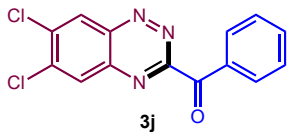
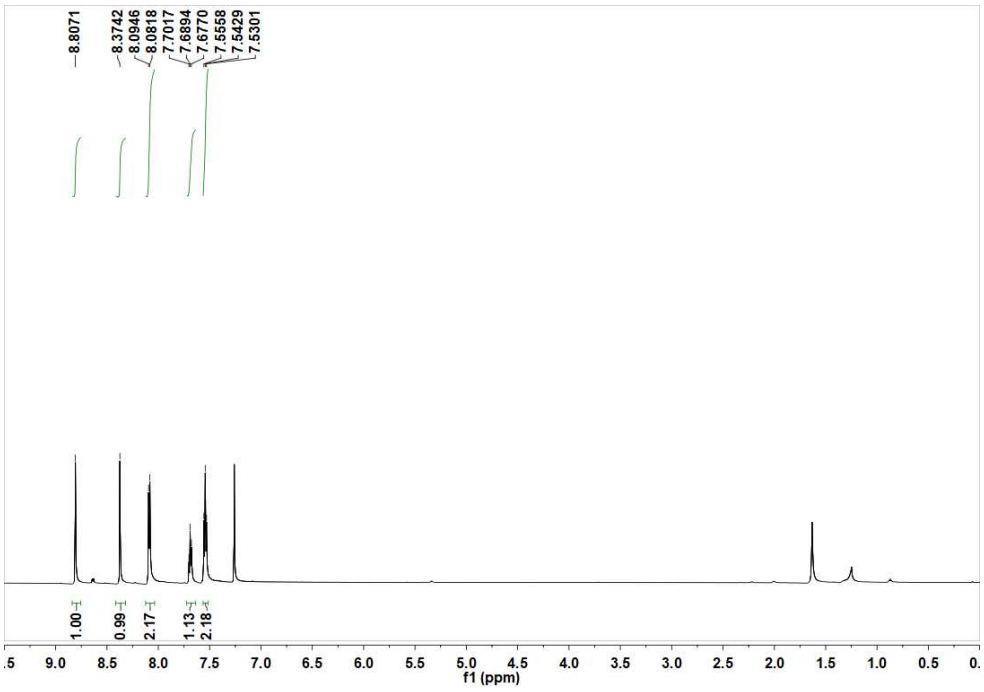
139.1882
f1 (ppm)


Cl
Cl
N
N
N
O

3j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7.6770
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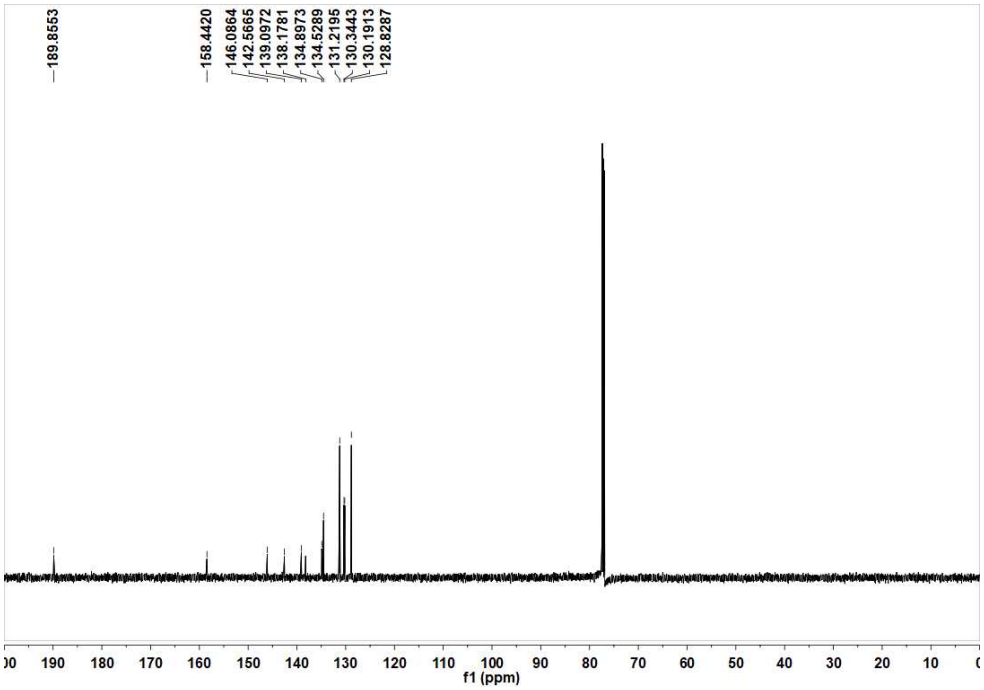
7.5429
7.5301
1.00
0.99
2.17
1.13
2.18
f1 (ppm)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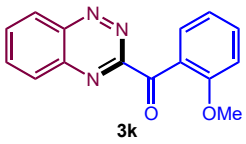
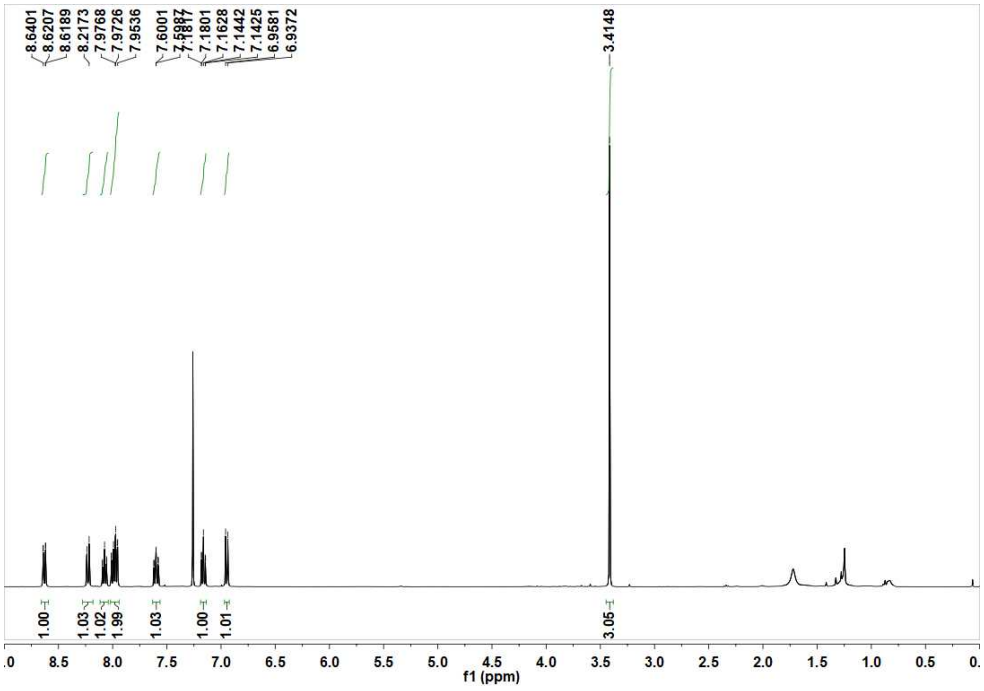
128.8287
f1 (ppm)


N
N
N
O
OMe

3k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7.9536
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7.1801
7.1628
7.1442
7.1425
6.9581
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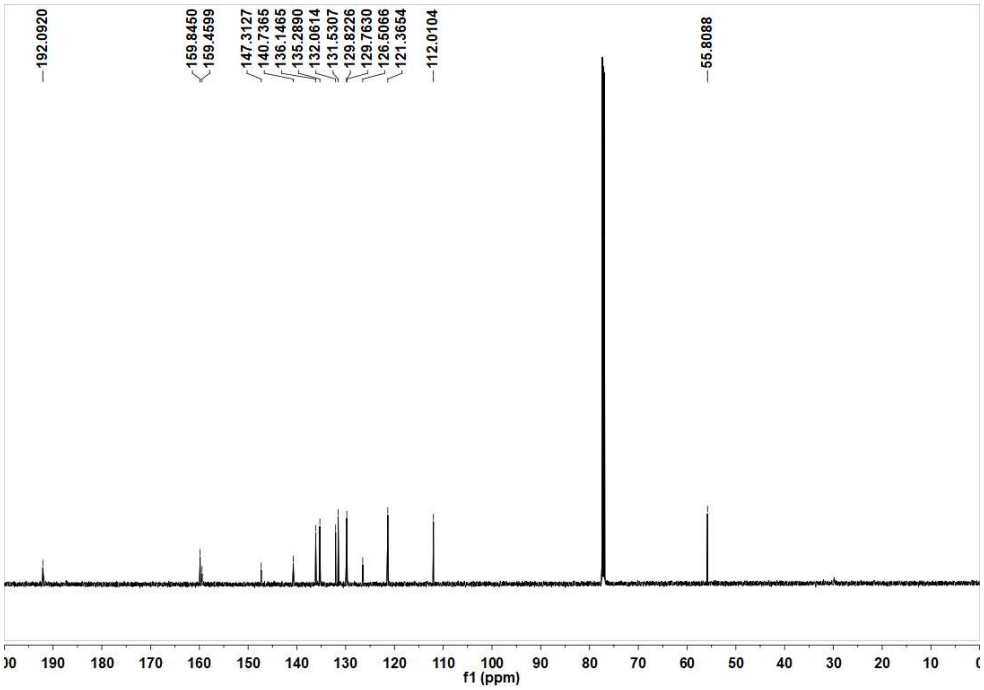
1.03
1.02
1.99
1.03
1.00
1.01
3.05
f1 (ppm)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140.7365
136.1465
135.2890
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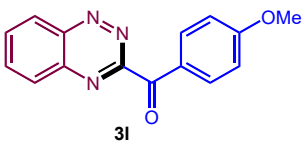
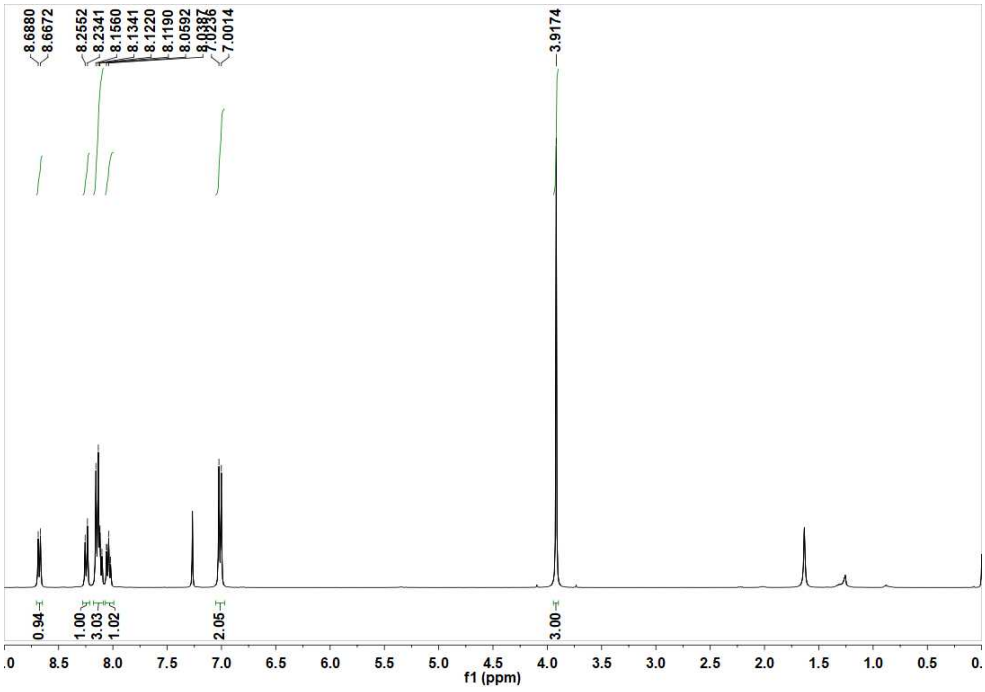
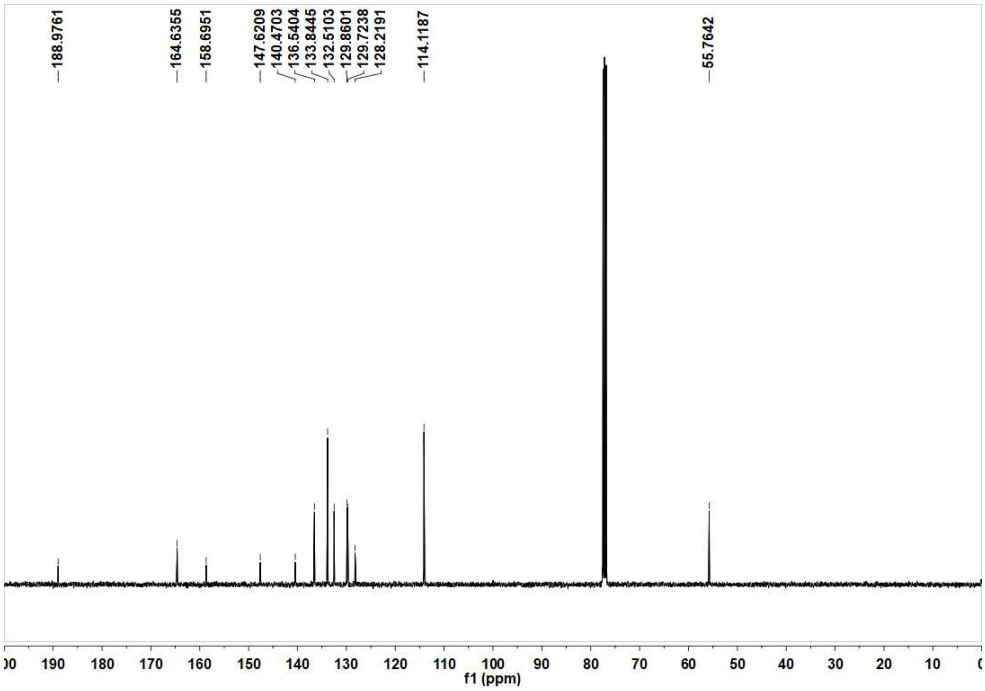
121.3654
112.0104
55.8088
f1 (ppm)


N
N
N
OMe
O

3l


8.6880
8.6672
8.2552
8.2341
8.1560
8.1341
8.1220
8.1190
8.0592
7.0236
7.0014
3.9174
0.94
1.00
3.03
1.02
2.05
3.00
f1 (ppm)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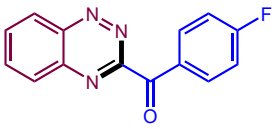
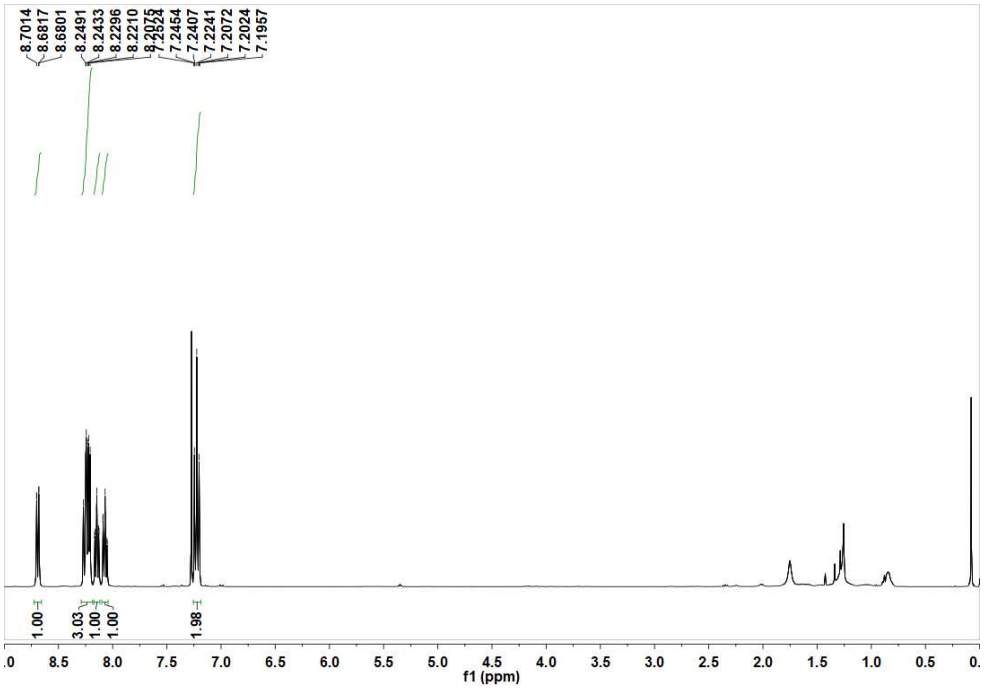
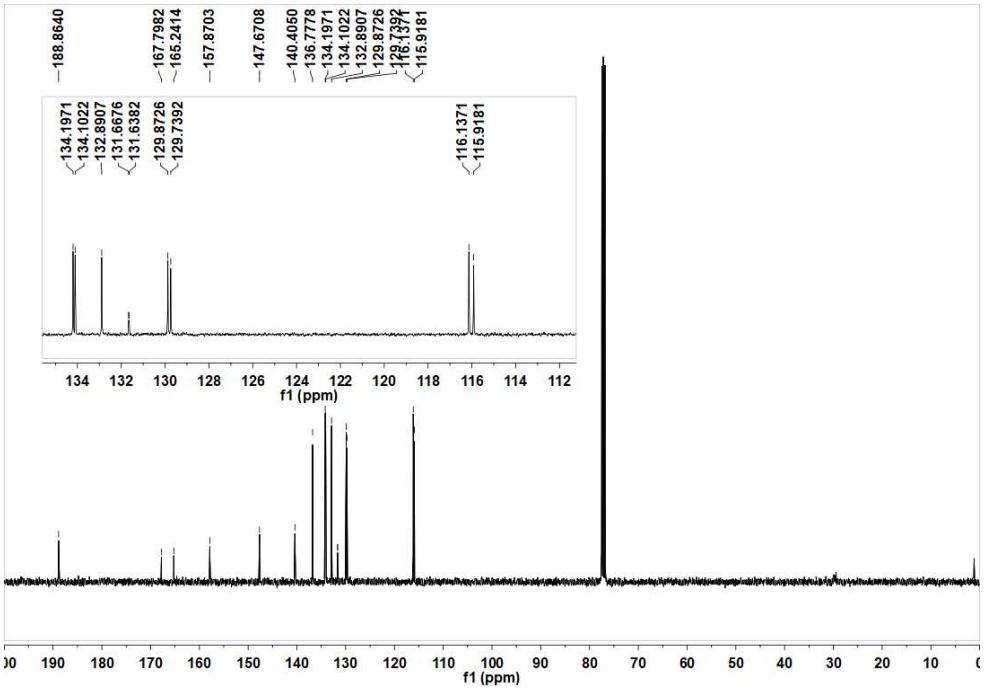
164.6355
158.6951
147.6209
140.4703
136.5404
133.8445
132.5103
129.8601
129.7238
128.2191
114.1187
55.7642
f1 (ppm)


N
N
N
F
O

3m


8.7014
8.6817
8.6801
8.2491
8.2433
8.2296
8.2210
7.2524
7.2454
7.2407
7.2241
7.2072
7.2024
7.1957
1.00
3.03
1.00
1.00
1.98
f1 (ppm)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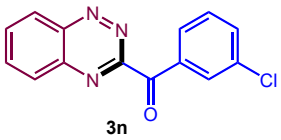
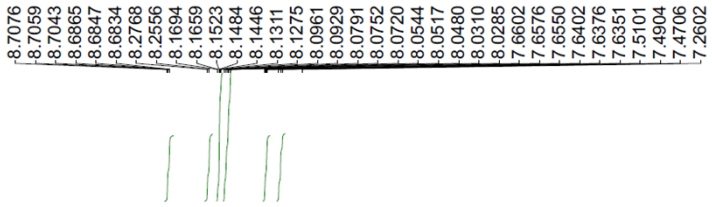
167.7982
165.2414
157.8703
147.6708
140.4050
136.7778
134.1971
134.1022
132.8907
129.8726
129.7392
116.1371
115.9181
134.1971
134.1022
132.8907
131.6676
131.6382
129.8726
129.7392
116.1371
115.9181
f1 (ppm)
f1 (ppm)


N
N
N
O
Cl

3n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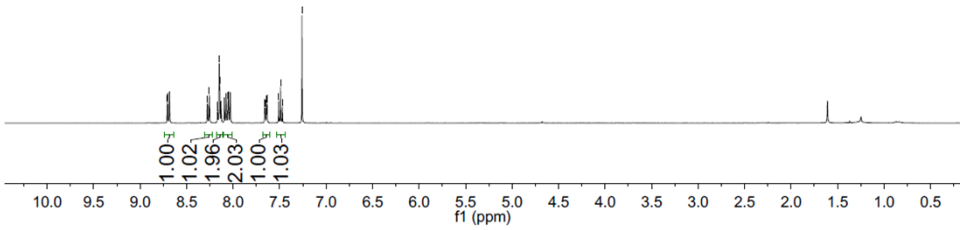
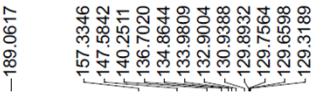
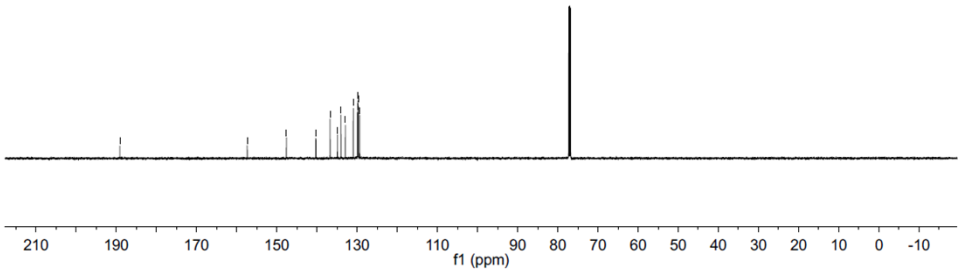
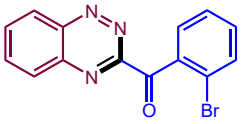
8.7059
8.7043
8.6865
8.6847
8.6834
8.2768
8.2556
8.1694
8.1659
8.1523
8.1484
8.1446
8.1311
8.1275
8.0961
8.0929
8.0791
8.0752
8.0720
8.0544
8.0517
8.0480
8.0310
8.0285
7.6602
7.6576
7.6550
7.6402
7.6376
7.6351
7.5101
7.4904
7.4706
7.2602

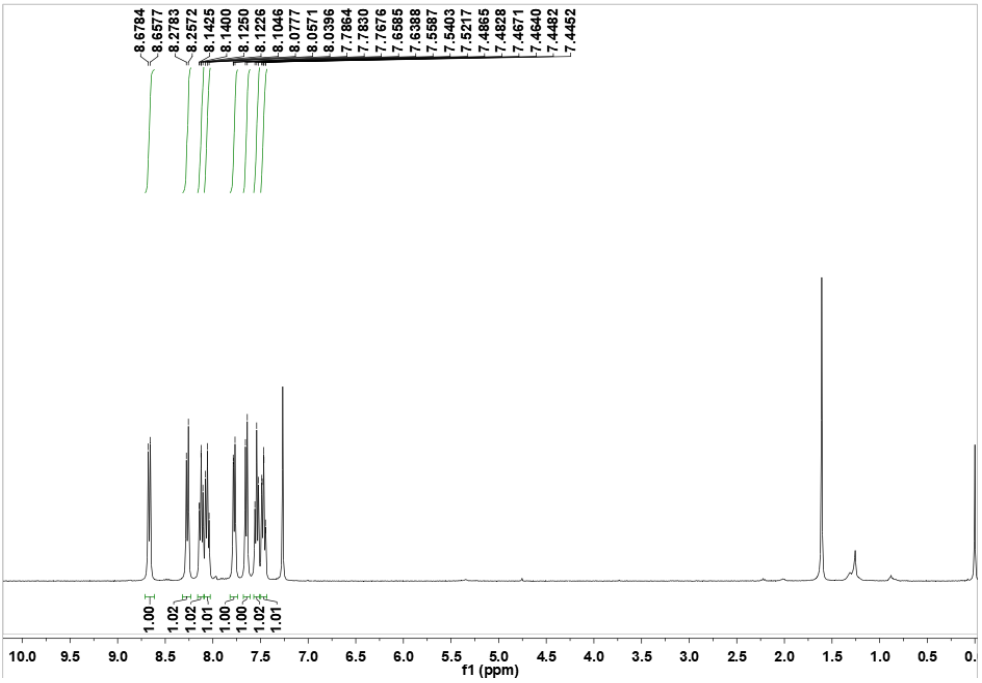

1.00
1.02
1.96
2.03
1.00
1.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


189.0617
157.3346
147.5842
140.2511
136.7020
134.8644
133.9809
132.9004
130.9388
129.8932
129.7564
129.6598
129.3189


210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


N
N
N
O
Br

3o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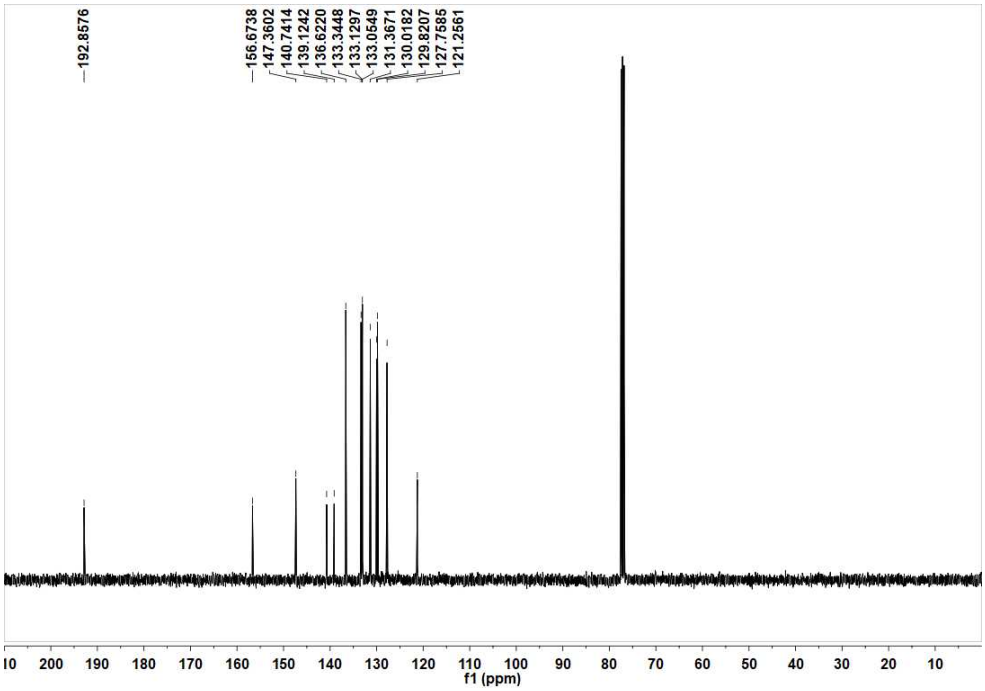
8.6577
8.2783
8.2572
8.1425
8.1400
8.1250
8.1226
8.1046
8.0777
8.0571
8.0396
7.7864
7.7830
7.7676
7.6585
7.6388
7.5687
7.5403
7.5217
7.4885
7.4828
7.4671
7.4640
7.4482
7.4452
1.00
1.02
1.02
1.01
1.00
1.00
1.02
1.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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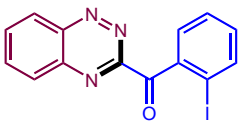
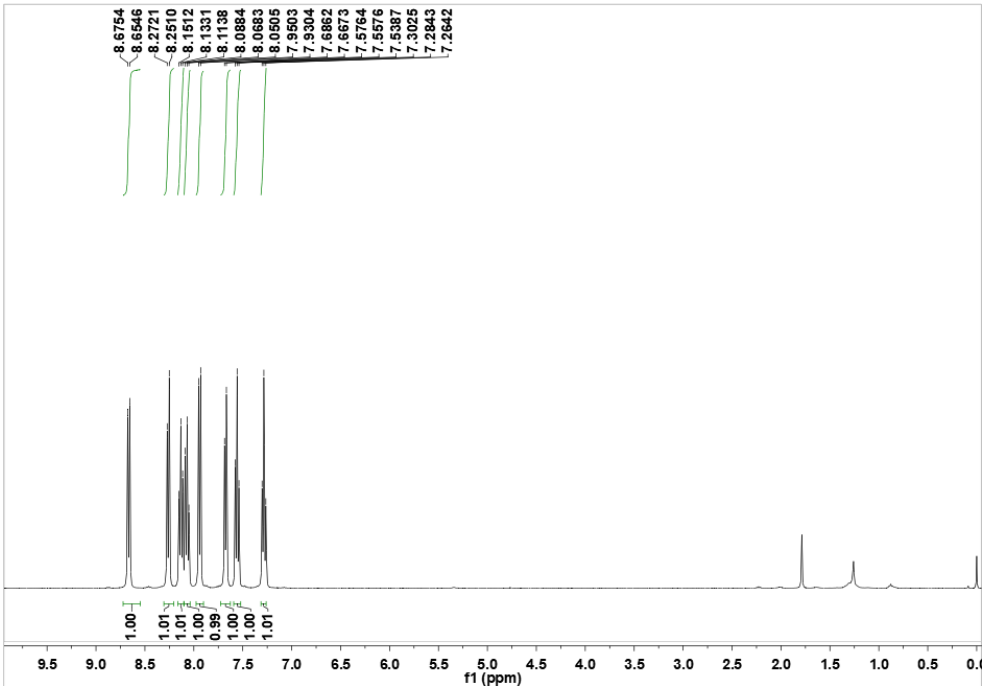
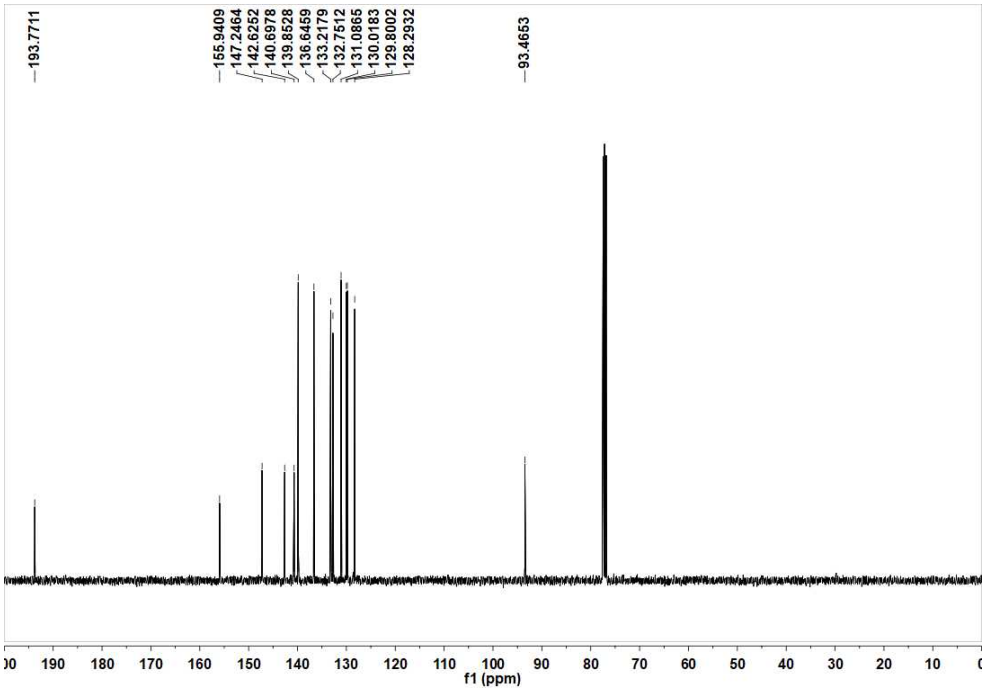
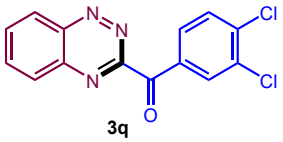
156.6738
147.3602
140.7414
139.1242
136.6220
133.3448
133.1297
133.0549
131.3671
130.0182
129.8207
127.7585
121.2561
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)



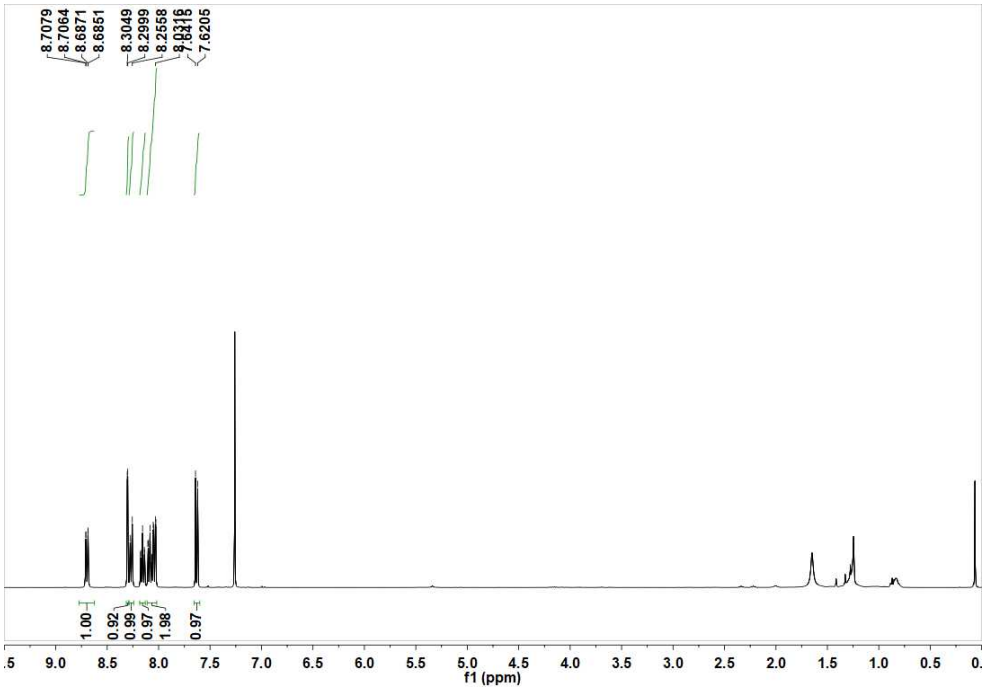
3p

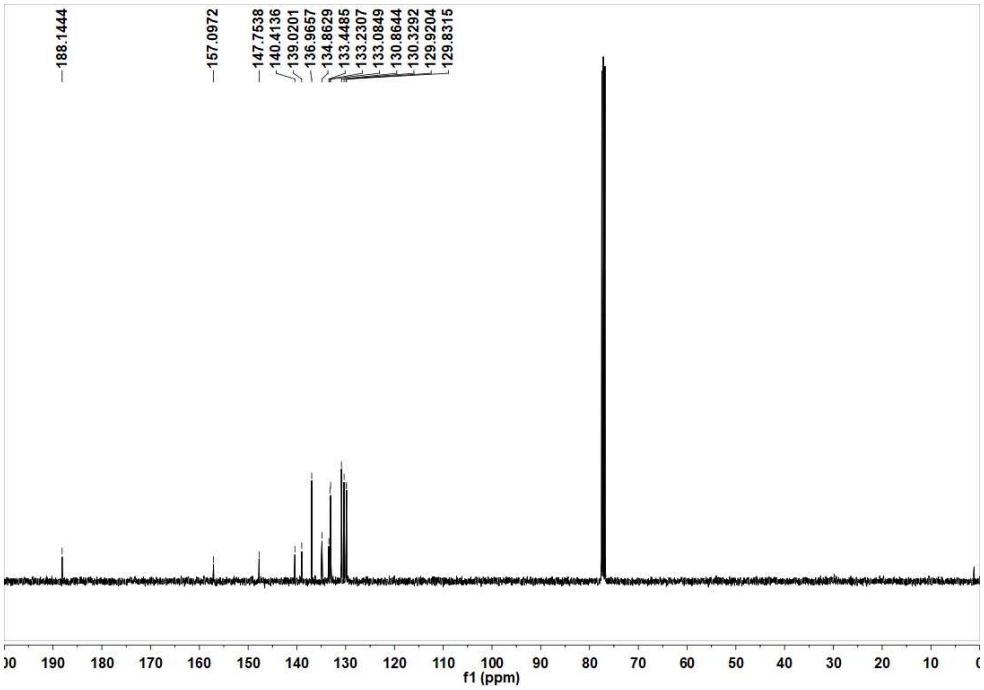

8.6754
8.6546
8.2721
8.2510
8.1512
8.1331
8.1138
8.0884
8.0683
8.0505
7.9503
7.9304
7.6862
7.6673
7.5764
7.5576
7.5387
7.3025
7.2843
7.2642
1.00
1.01
1.01
1.00
0.99
1.00
1.00
1.01
f1 (ppm)

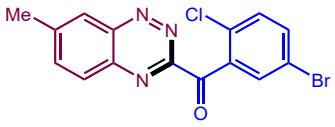

193.7711
155.9409
147.2464
142.6252
140.6978
139.8528
136.6459
133.2179
132.7512
131.0865
130.0183
129.8002
128.2932
93.4653
f1 (ppm)


N
N
N
Cl
Cl
O

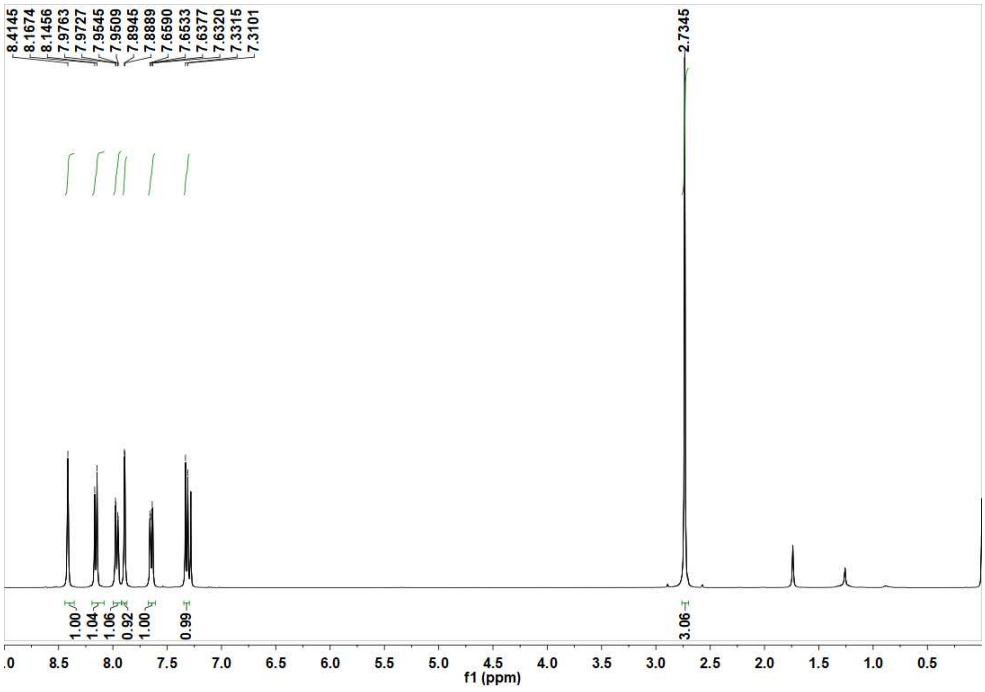
3q

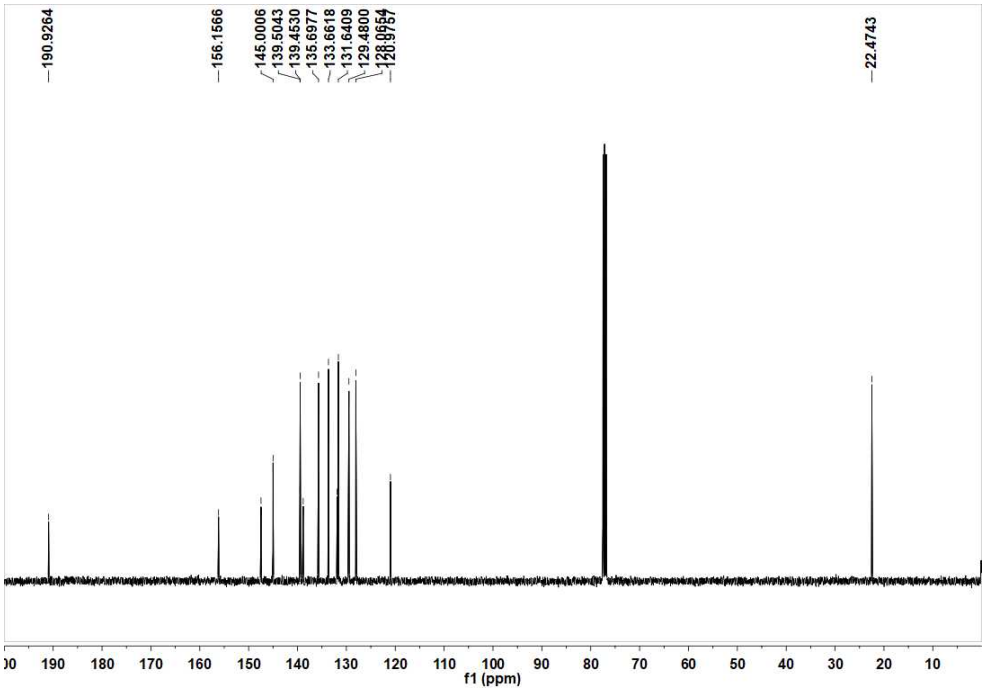

8.7079
8.7064
8.6871
8.6851
8.3049
8.2999
8.2558
8.0316
8.0315
7.6415
7.6205
1.00
0.92
0.99
0.97
1.98
0.97
f1 (ppm)


188.1444
157.0972
147.7538
140.4136
139.0201
136.9657
134.8629
133.4485
133.2307
133.0849
130.8644
130.3292
129.9204
129.8315
f1 (ppm)


Me
N
N
N
Cl
Br
O

3r


8.4145
8.1674
8.1456
7.9763
7.9727
7.9545
7.9509
7.8945
7.8889
7.6590
7.6533
7.6377
7.6320
7.3315
7.3101
2.7345
1.00
1.04
1.06
0.92
1.00
0.99
3.06
f1 (ppm)


190.9264
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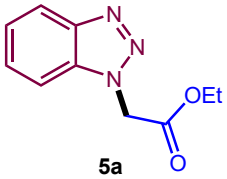
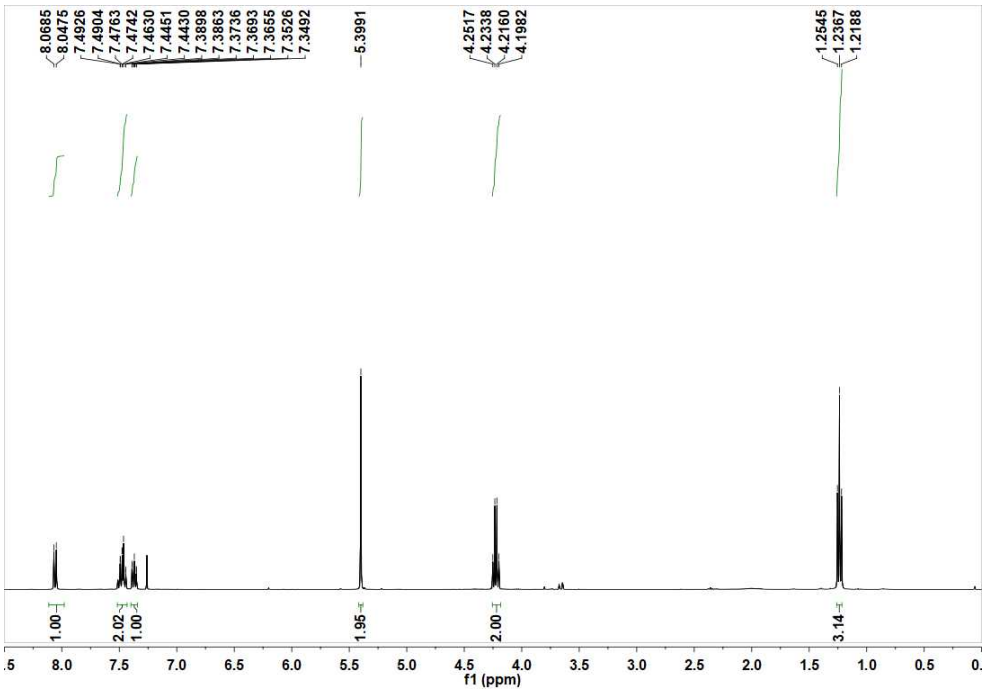
145.0006
139.5043
139.4530
135.6977
133.6618
131.6409
129.4800
22.4743
f1 (ppm)


N
N
N
OEt
O

5a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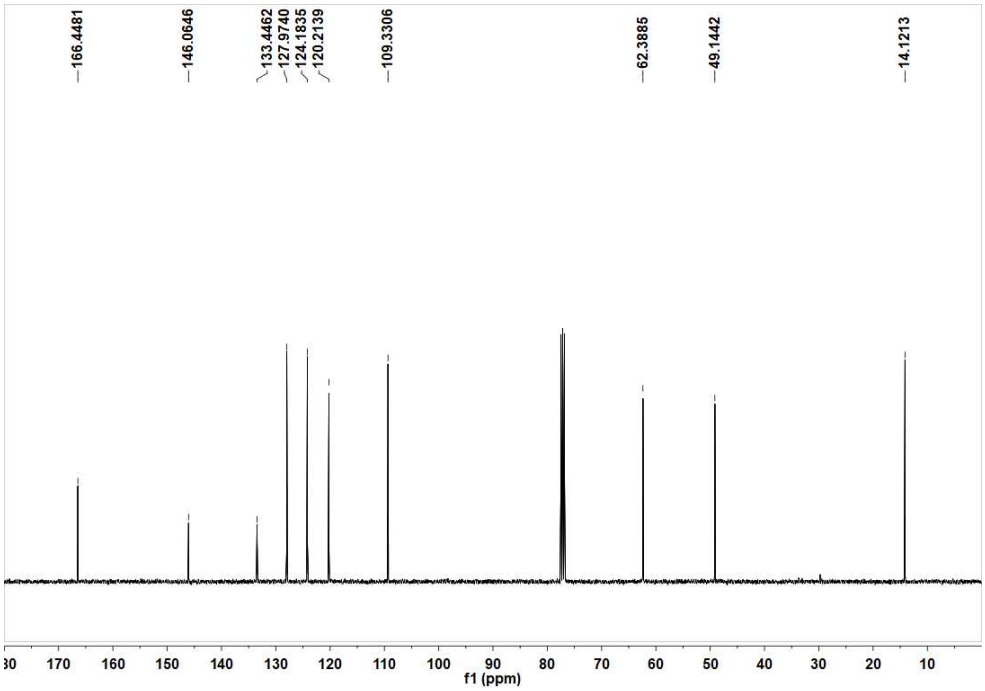
8.0475
7.4926
7.4904
7.4763
7.4742
7.4630
7.4451
7.4430
7.3898
7.3863
7.3736
7.3693
7.3655
7.3526
7.3492
5.3991
4.2517
4.2338
4.2160
4.1982
1.2545
1.2367
1.2188
1.00
2.02
1.00
1.95
2.00
3.14
f1 (ppm)


166.4481
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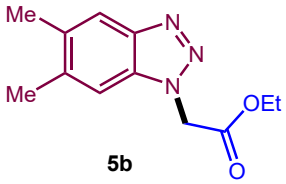
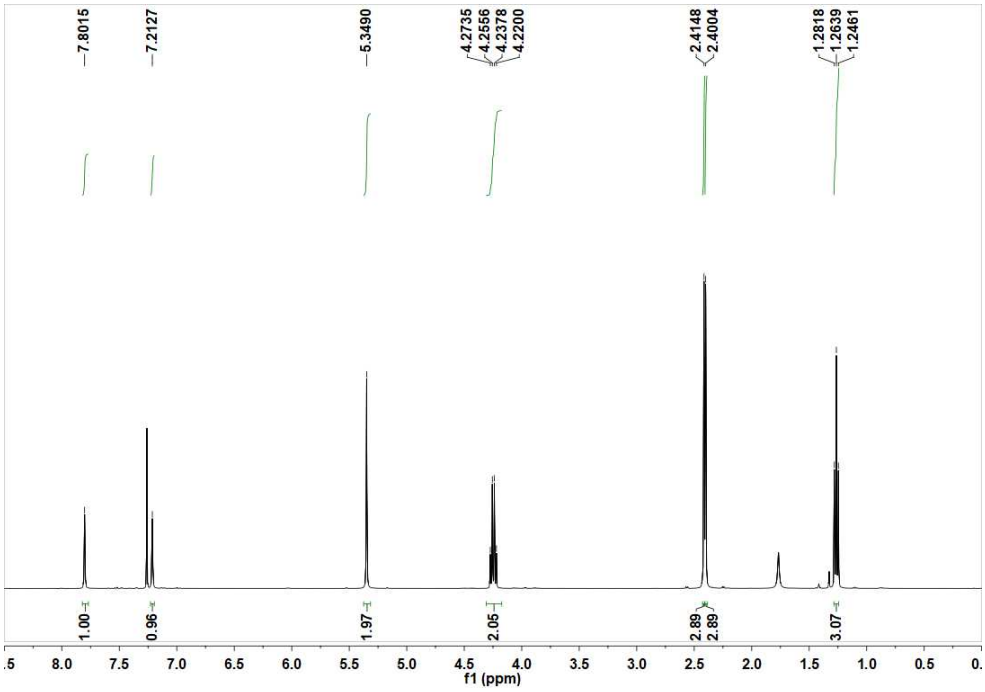
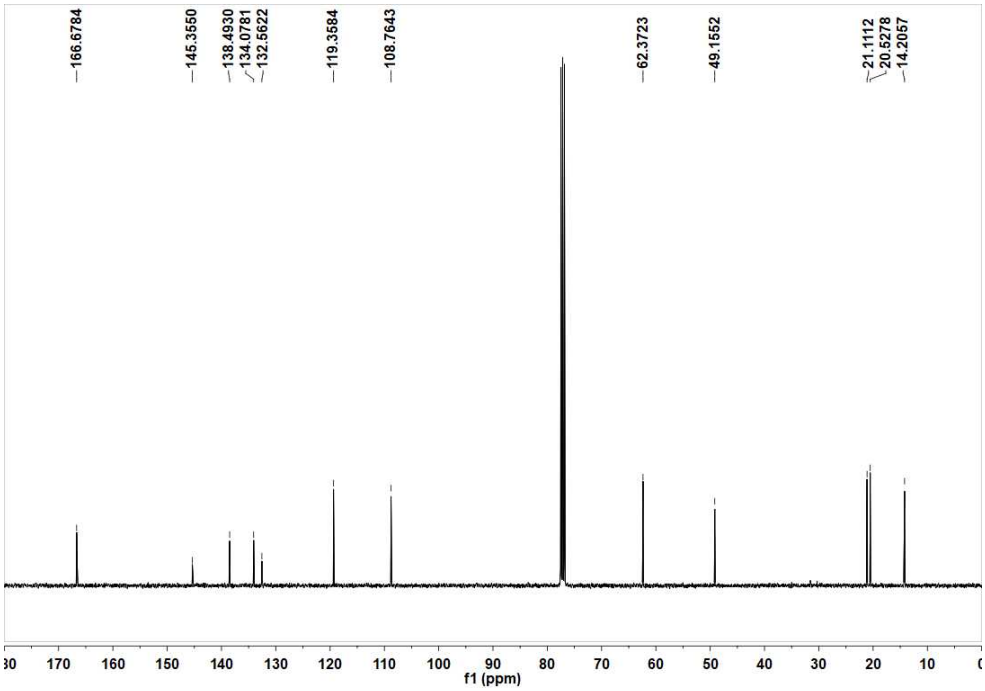
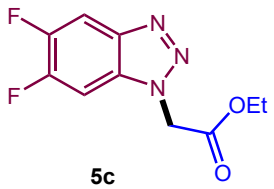
133.4462
127.9740
124.1835
120.2139
109.3306
62.3885
49.1442
14.1213
f1 (ppm)


Me
Me
N
N
N
OEt
O

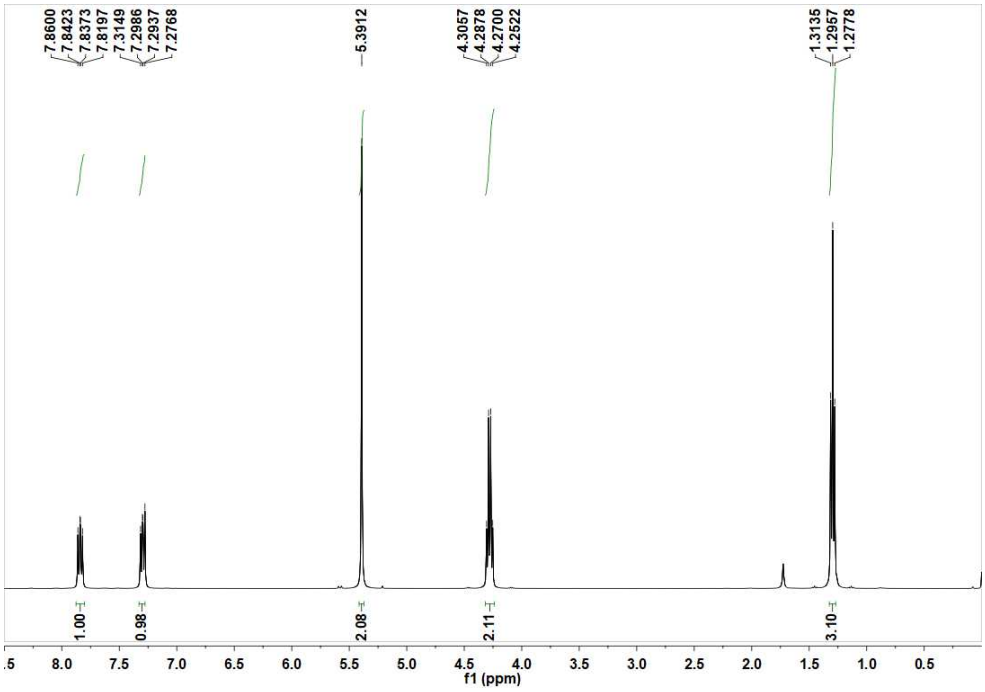
5b

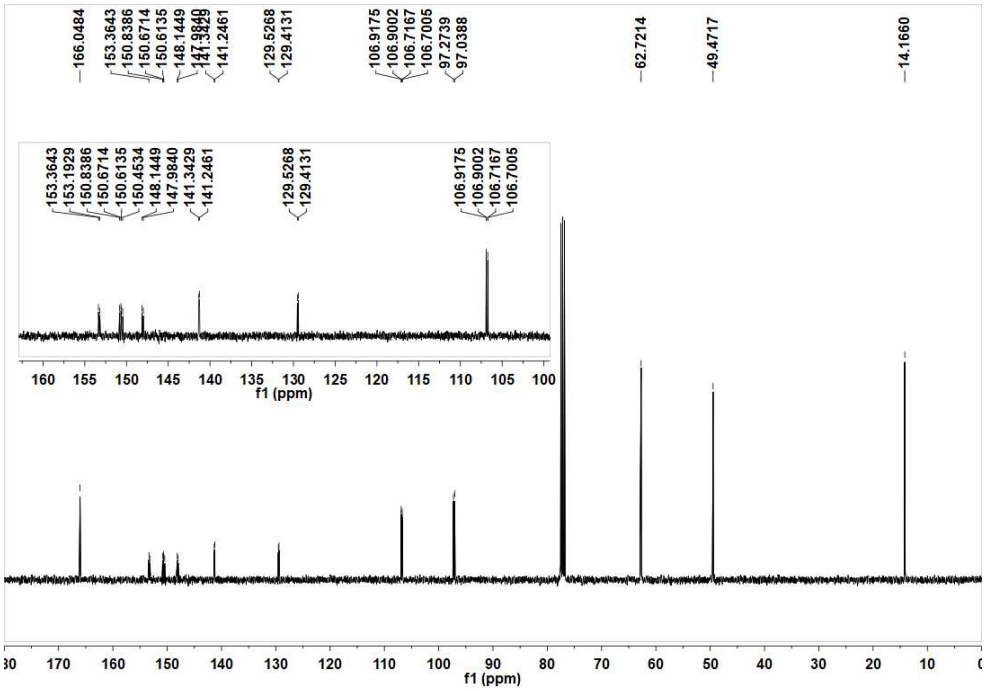

7.8015
7.2127
5.3490
4.2735
4.2556
4.2378
4.2200
2.4148
2.4004
1.2818
1.2639
1.2461
1.00
0.96
1.97
2.05
2.89
2.89
3.07
f1 (ppm)

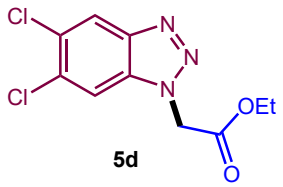

166.6784
145.3550
138.4930
134.0781
132.5622
119.3584
108.7643
62.3723
49.1552
21.1112
20.5278
14.2057
f1 (ppm)


F
F
N
N
N
OEt
O

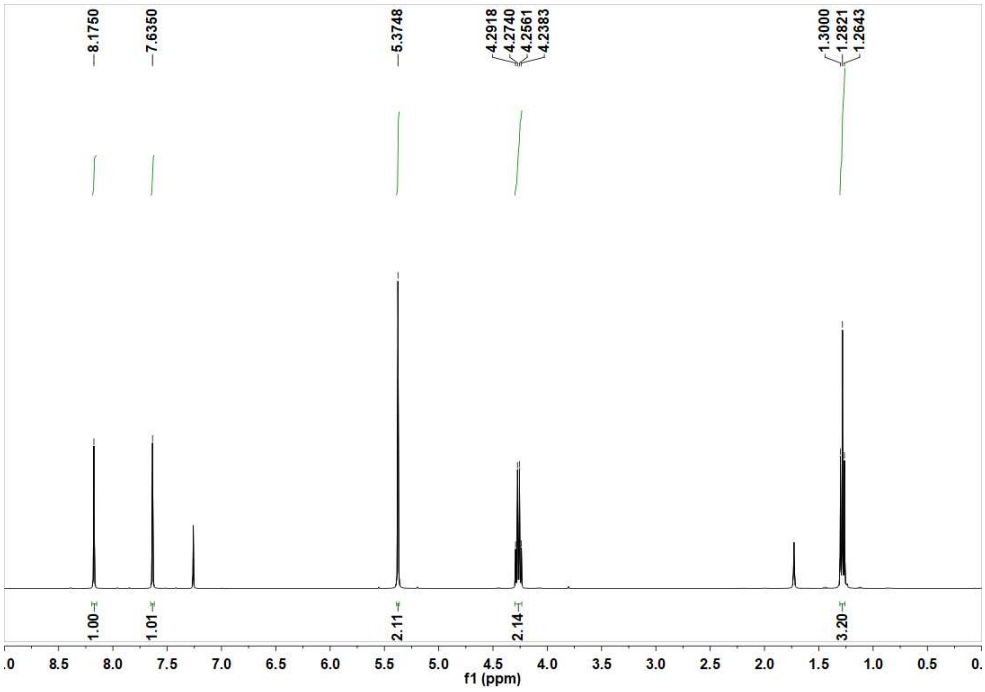
5c

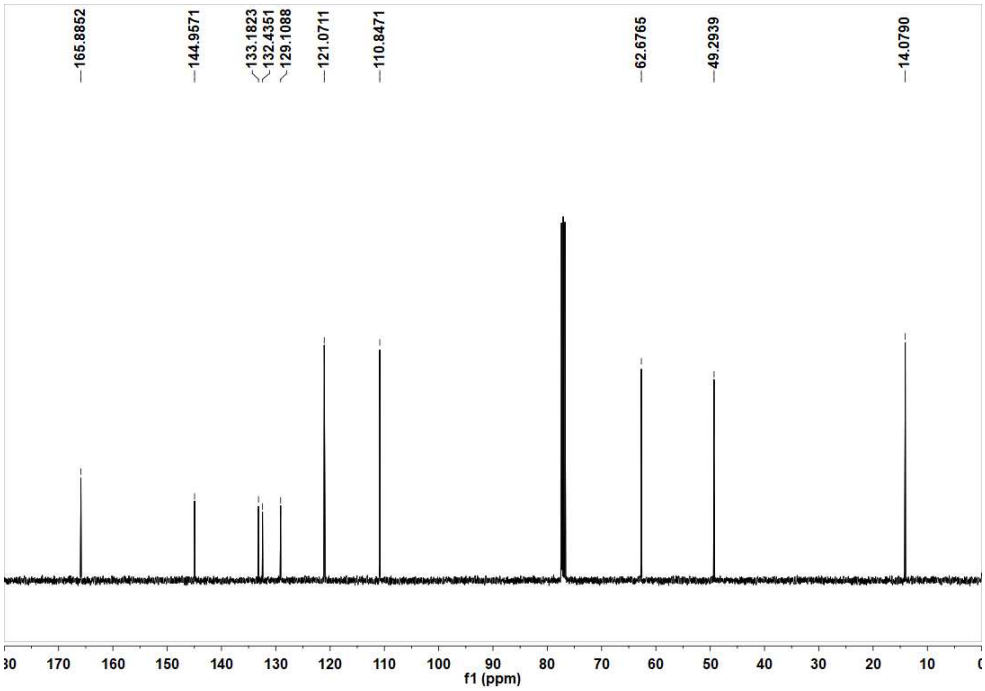

7.8600
7.8423
7.8373
7.8197
7.3149
7.2986
7.2937
7.2768
5.3912
4.3057
4.2878
4.2700
4.2522
1.3135
1.2967
1.2778
1.00
0.98
2.08
2.11
3.10
f1 (ppm)

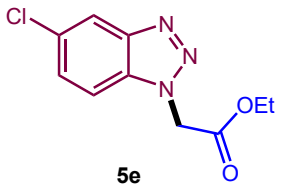

166.0484
153.3643
150.8386
150.6714
150.6135
148.1449
147.9840
141.3429
141.2461
129.5268
129.4131
106.9175
106.9002
106.7167
106.7005
97.2739
97.0388
62.7214
49.4717
14.1660
153.3643
153.1929
150.8386
150.6714
150.6135
150.4534
148.1449
147.9840
141.3429
141.2461
129.5268
129.4131
106.9175
106.9002
106.7167
106.7005
f1 (ppm)


Cl
Cl
N
N
N
OEt
O

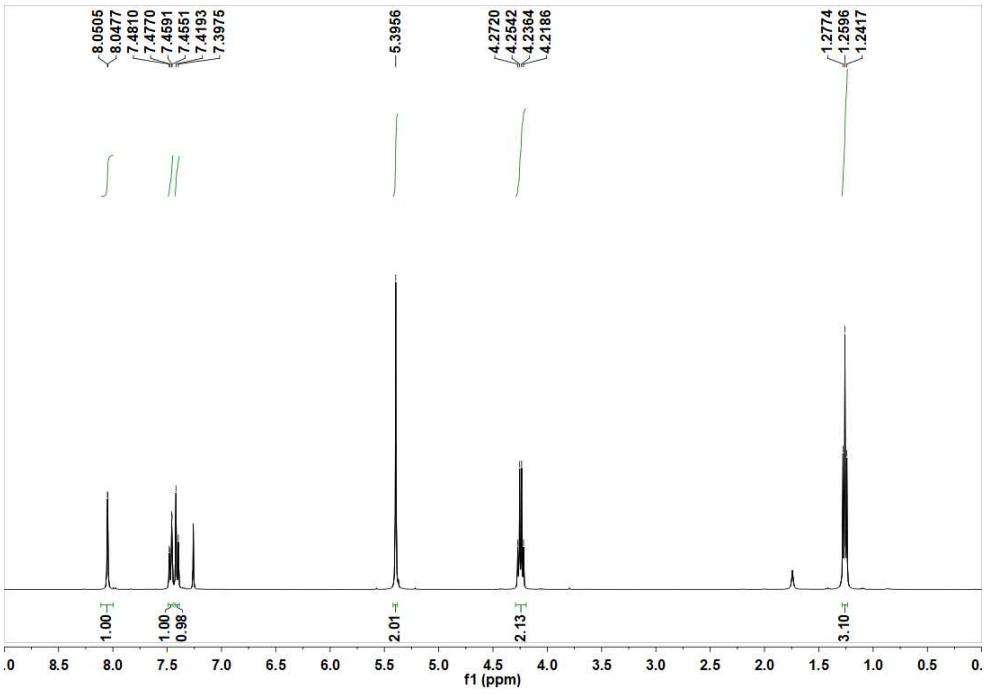
5d

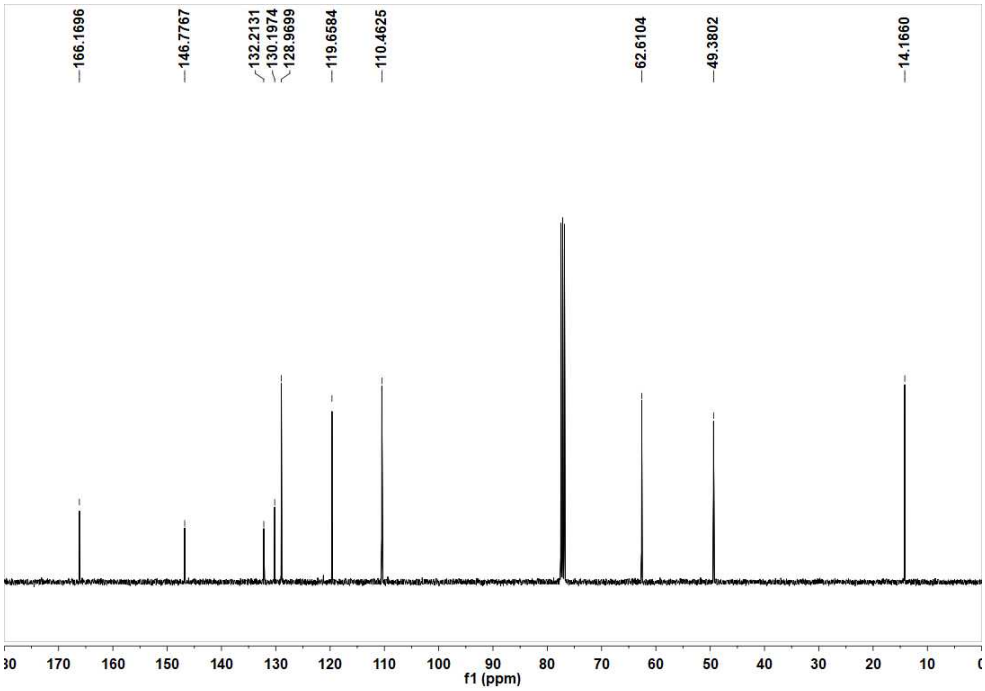

8.1750
7.6350
5.3748
4.2918
4.2740
4.2561
4.2383
1.3000
1.2821
1.2643
1.00
1.01
2.11
2.14
3.20
f1 (ppm)

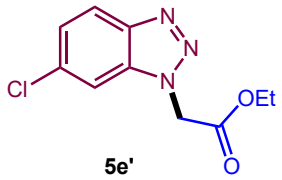

165.8852
144.9571
133.1823
132.4351
129.1088
121.0711
110.8471
62.6765
49.2939
14.0790
f1 (ppm)


Cl
N
N
N
OEt
O

5e


8.0505
8.0477
7.4810
7.4770
7.4591
7.4551
7.4193
7.3975
5.3956
4.2720
4.2542
4.2364
4.2186
1.2774
1.2596
1.2417
1.00
1.00
0.98
2.01
2.13
3.10
f1 (ppm)


166.1696
146.7767
132.2131
130.1974
128.9699
119.6584
110.4625
62.6104
49.3802
14.1660
f1 (ppm)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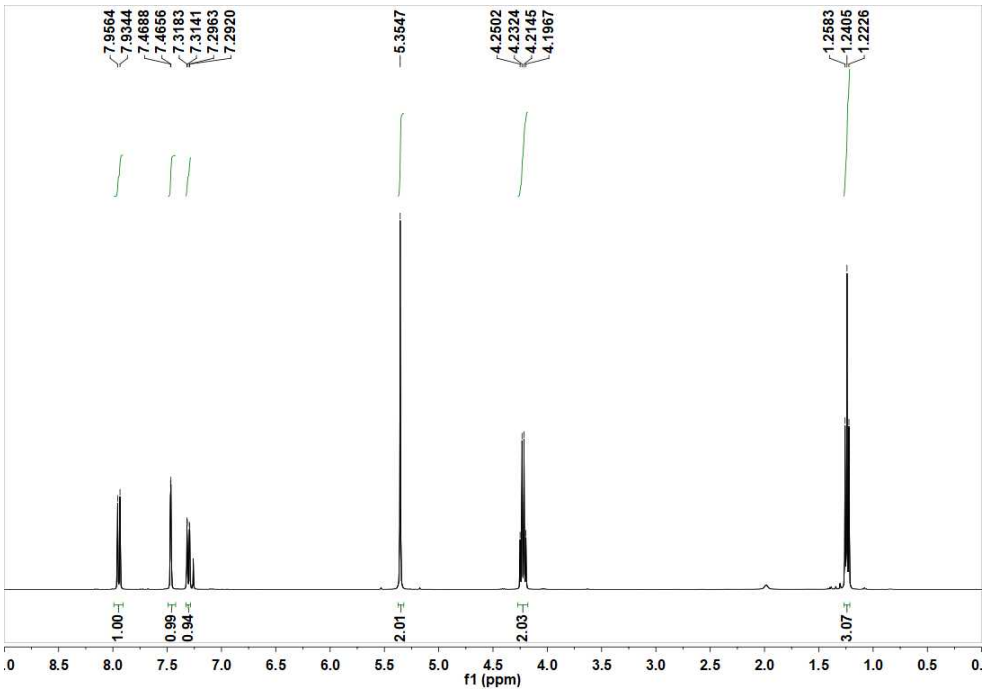
N
N
Cl
OEt
O

5e'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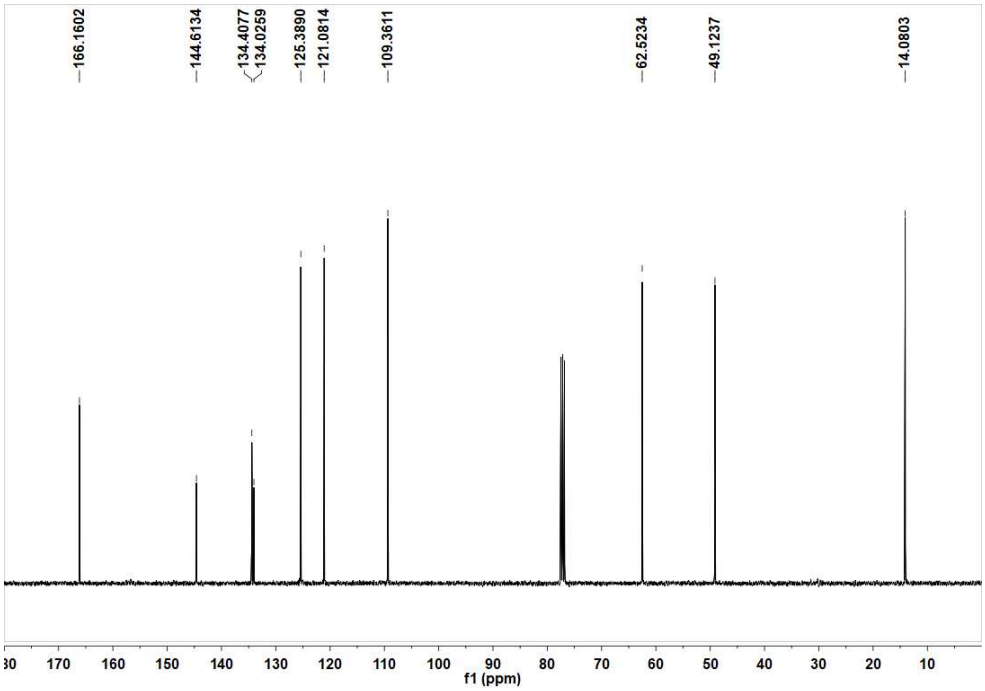
7.9344
7.4688
7.4656
7.3183
7.3141
7.2963
7.2920
5.3547
4.2502
4.2324
4.2145
4.1967
1.2583
1.2405
1.2226
1.00
0.99
0.94
2.01
2.03
3.07
f1 (ppm)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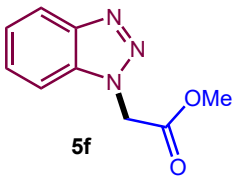
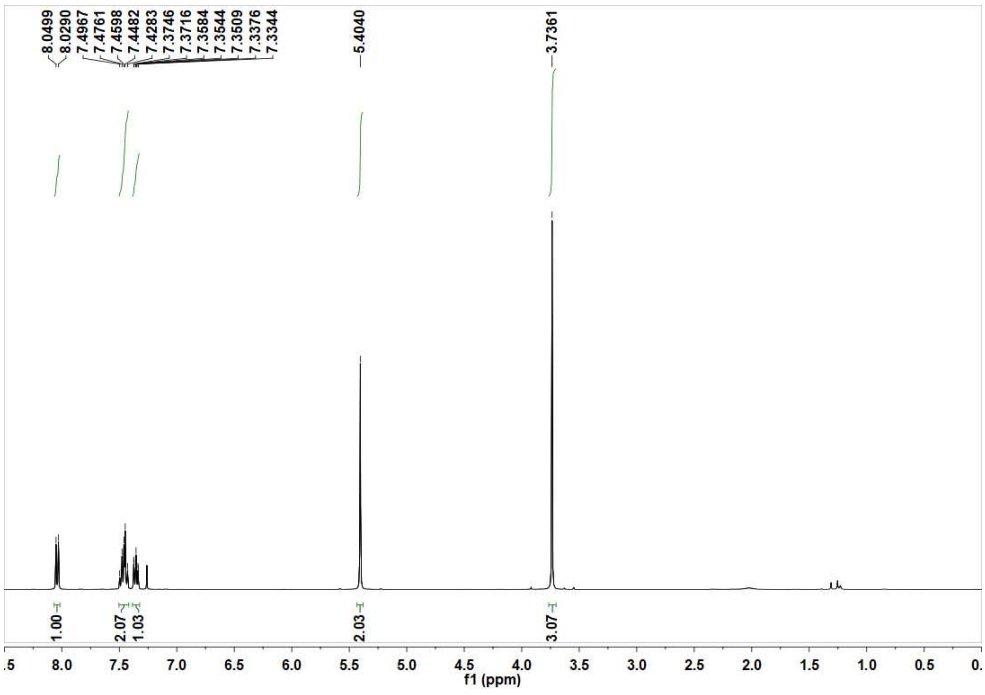
144.6134
134.4077
134.0259
125.3890
121.0814
109.3611
62.5234
49.1237
14.0803
f1 (ppm)


N
N
N
OMe
O

5f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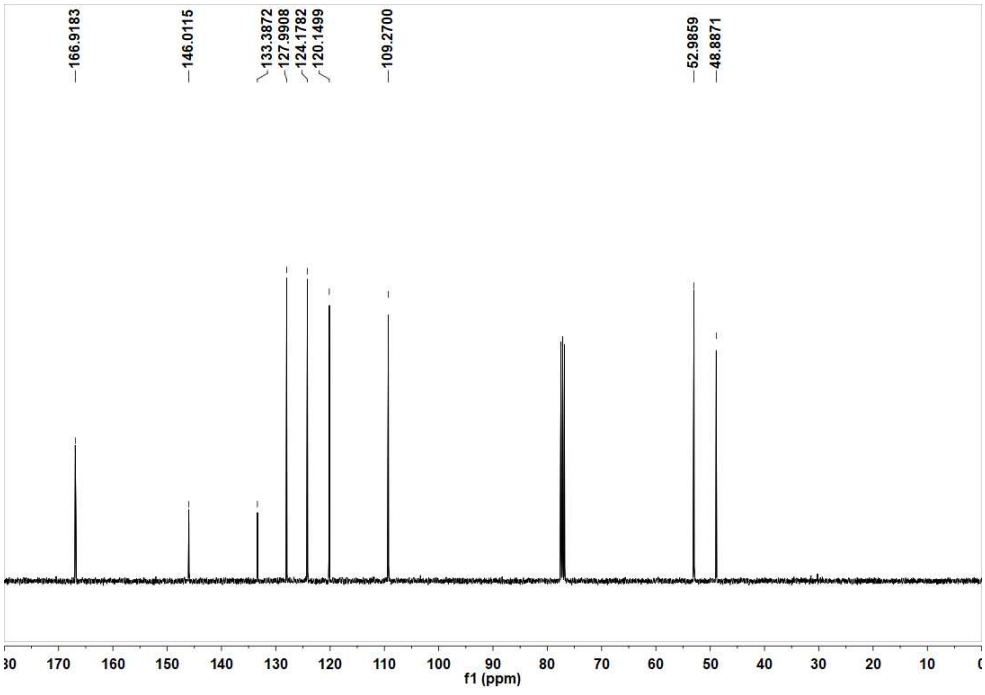
8.0290
7.4967
7.4761
7.4698
7.4482
7.4283
7.3746
7.3716
7.3584
7.3544
7.3509
7.3376
7.3344
5.4040
3.7361
1.00
2.07
1.03
2.03
3.07
f1 (ppm)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146.0115
133.3872
127.9908
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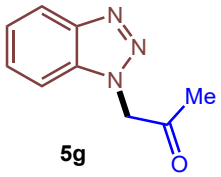
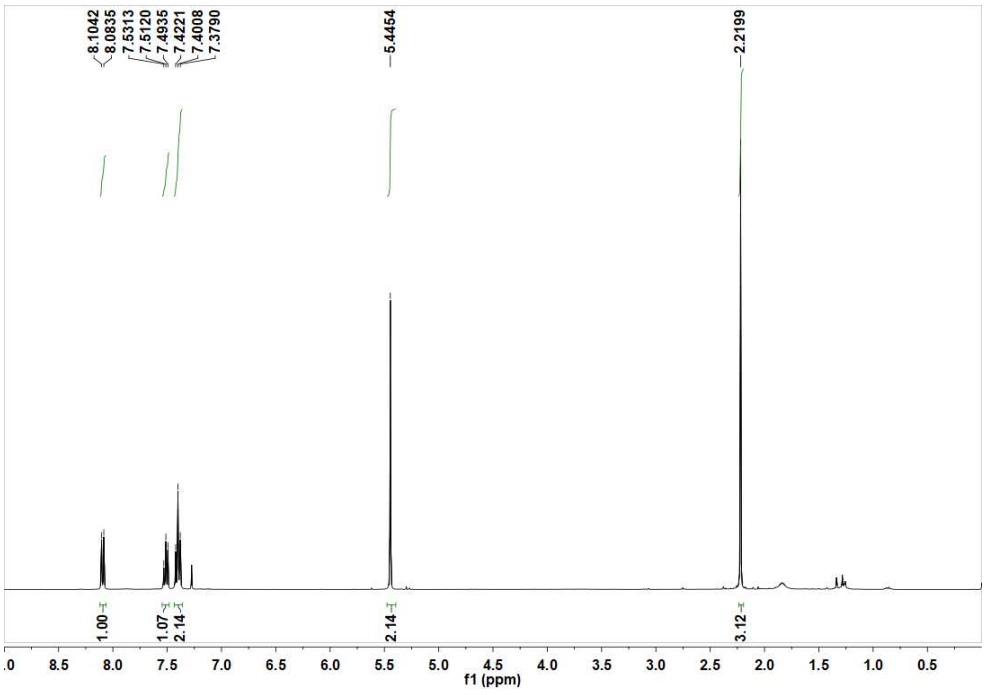
120.1499
109.2700
52.9859
48.8871
f1 (ppm)


N
N
N
Me
O

5g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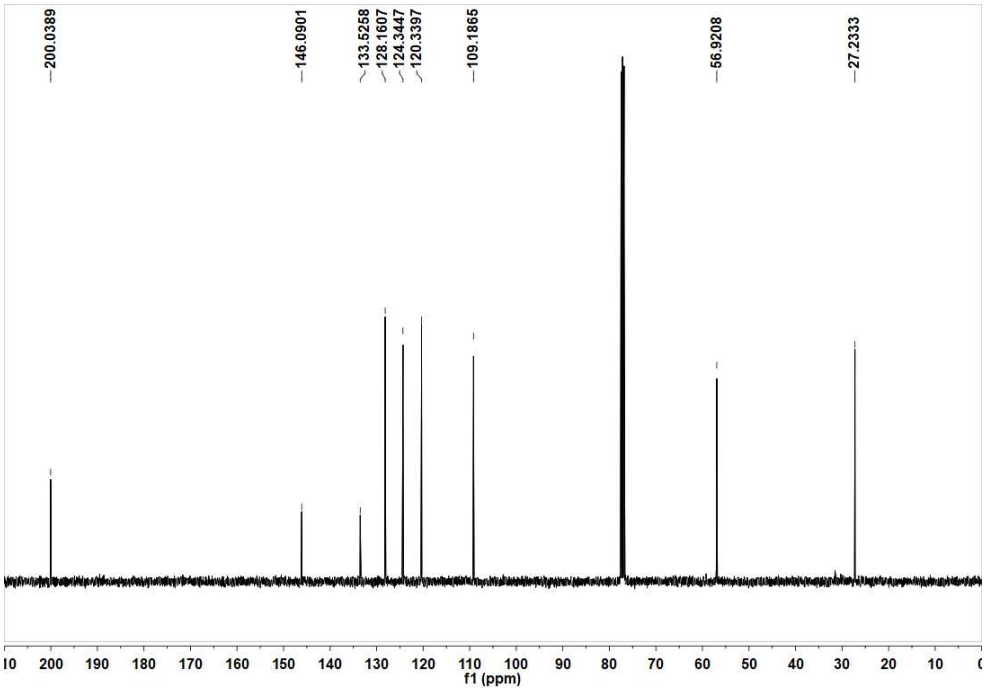
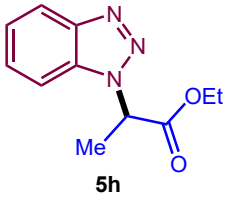
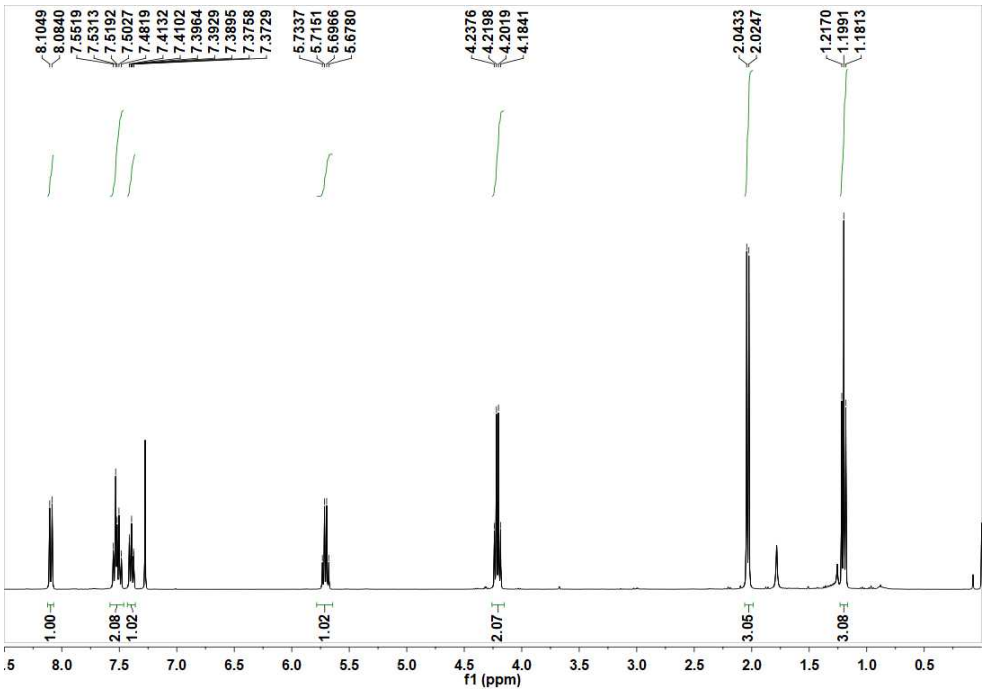
8.0835
7.5313
7.5120
7.4935
7.4221
7.4008
7.3790
5.4454
2.2199
1.00
1.07
2.14
2.14
3.12
f1 (ppm)


200.0389
146.0901
133.5258
128.1607
124.3447
120.3397
109.1865
56.9208
27.2333
f1 (ppm)


N
N
N
OEt
Me
O

5h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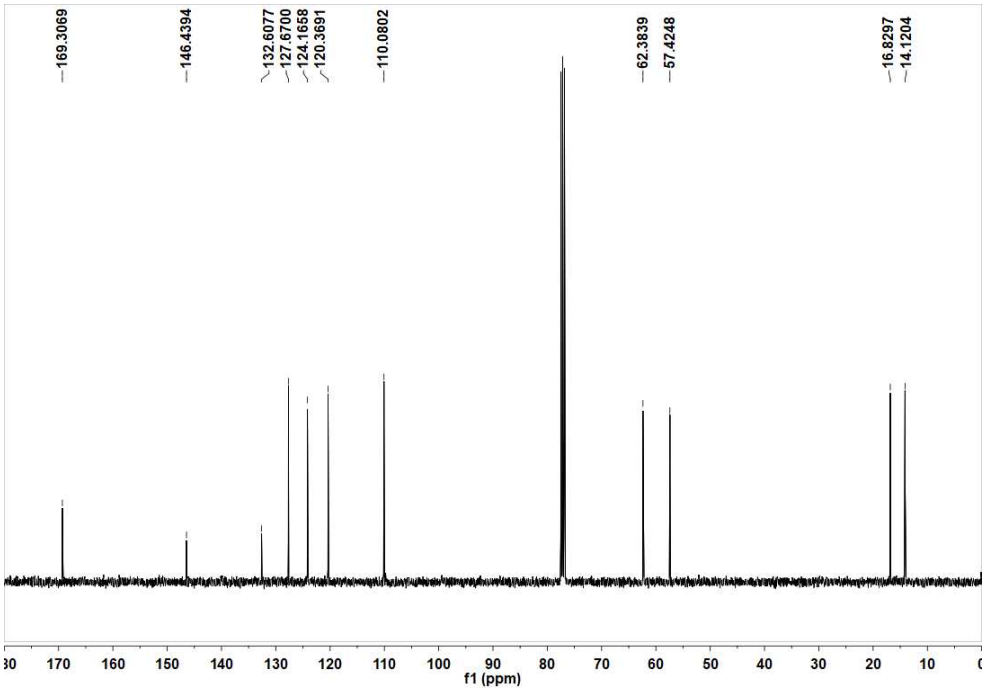
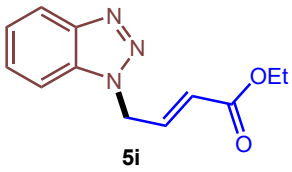
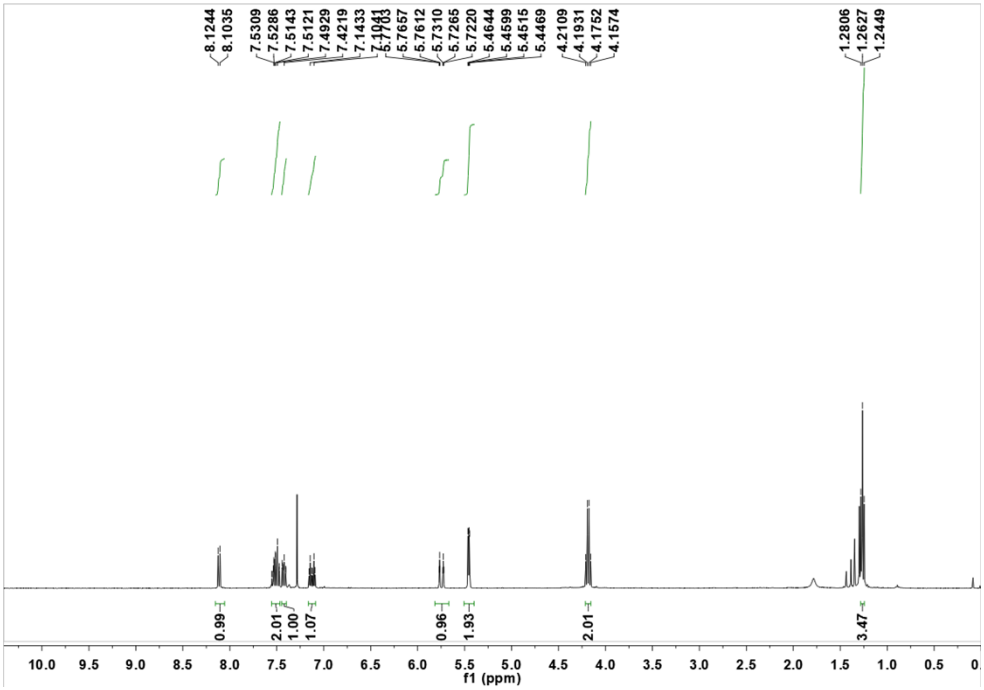
8.0840
7.5519
7.5313
7.5192
7.5027
7.4819
7.4132
7.4102
7.3964
7.3929
7.3895
7.3758
7.3729
5.7337
5.7151
5.6966
5.6780
4.2376
4.2198
4.2019
4.1841
2.0433
2.0247
1.2170
1.1991
1.1813
1.00
2.08
1.02
1.02
2.07
3.05
3.08
f1 (ppm)


169.3069
146.4394
132.6077
127.6700
124.1658
120.3691
110.0802
62.3839
57.4248
16.8297
14.1204
f1 (ppm)


N
N
N
OEt
O

5i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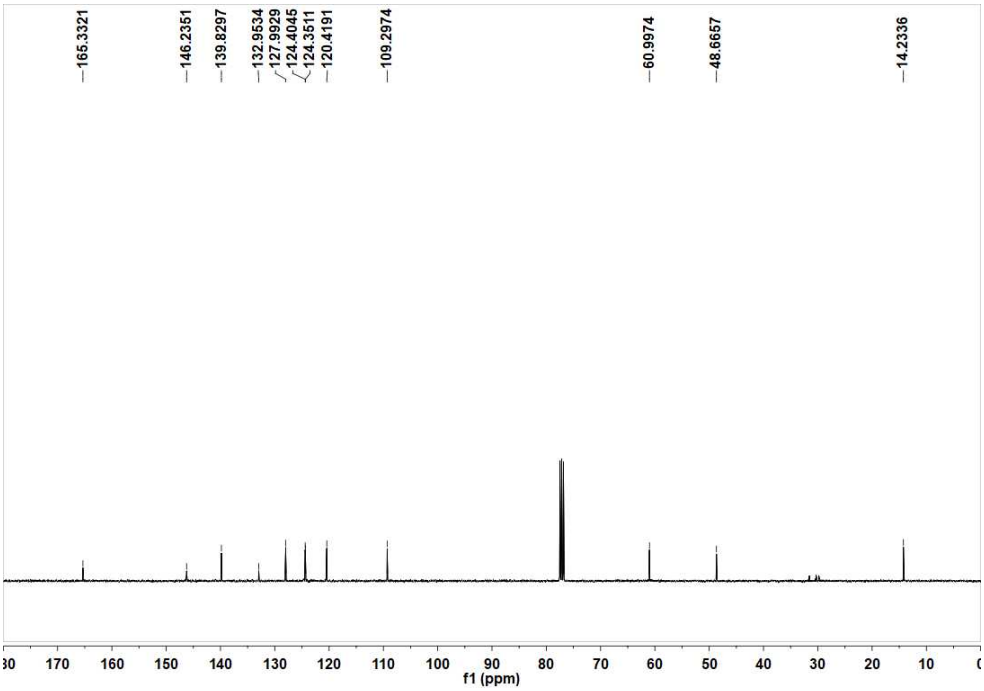
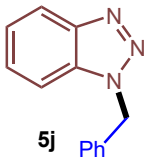
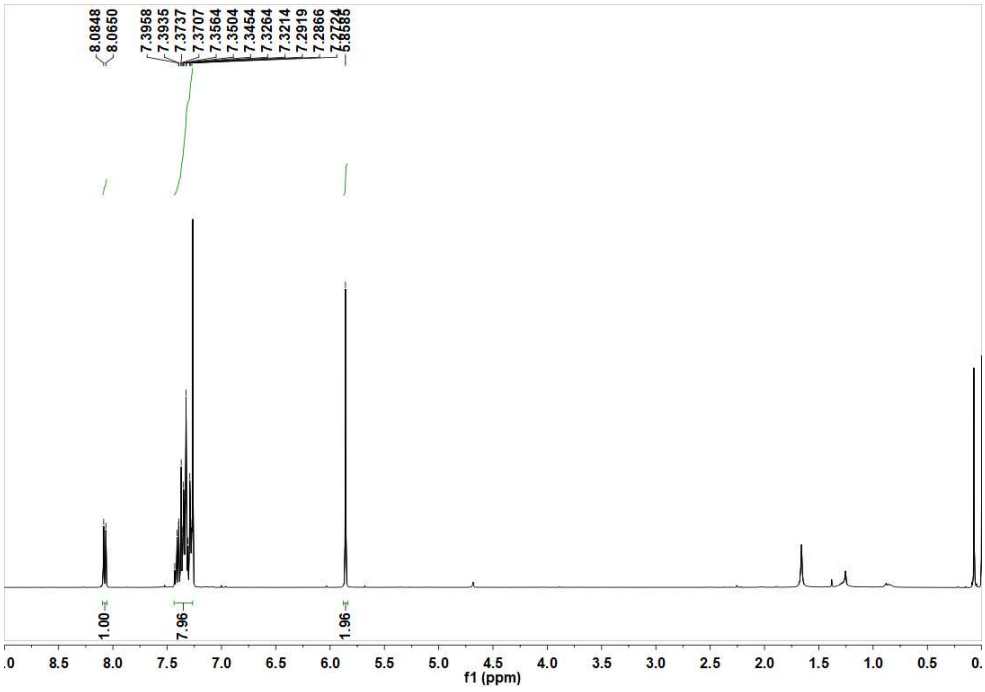
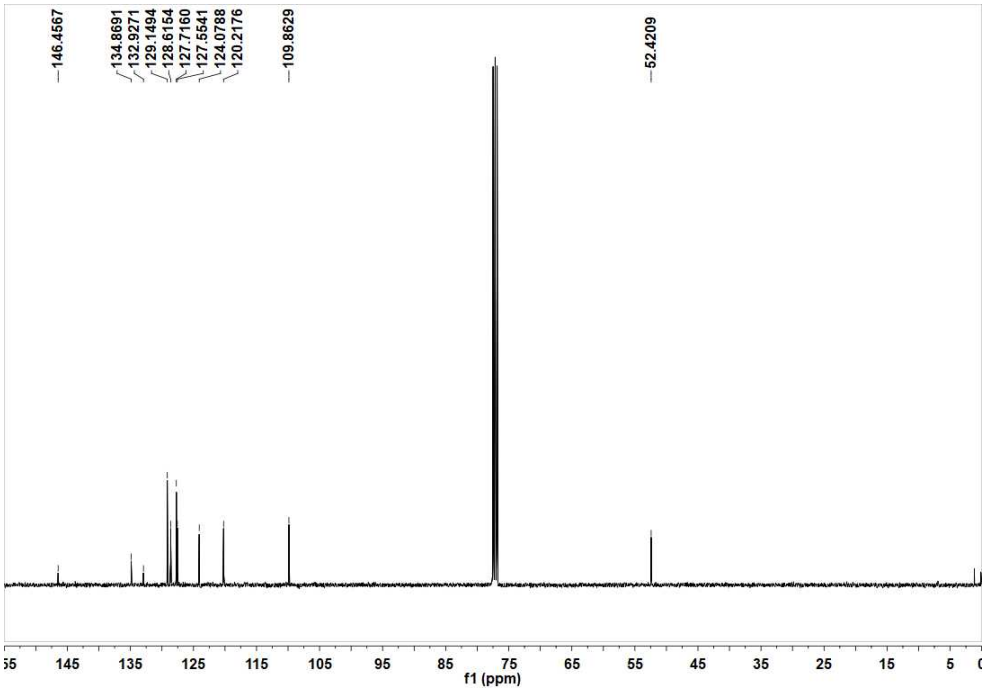
8.1035
7.5309
7.5286
7.5143
7.5121
7.4929
7.4219
7.1433
7.1041
7.1003
5.7657
5.7612
5.7310
5.7265
5.7220
5.4644
5.4599
5.4515
5.4469
4.2109
4.1931
4.1752
4.1574
1.2806
1.2627
1.2449
0.99
2.01
1.00
1.07
0.96
1.93
2.01
3.47
f1 (ppm)


165.3321
146.2351
139.8297
132.9534
127.9929
124.4045
124.3511
120.4191
109.2974
60.9974
48.6657
14.2336
f1 (ppm)


N
N
N
Ph

5j


8.0848
8.0650
7.3958
7.3935
7.3737
7.3707
7.3564
7.3504
7.3454
7.3264
7.3214
7.2919
7.2866
1.00
7.96
1.96
f1 (ppm)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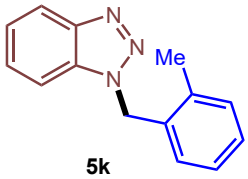
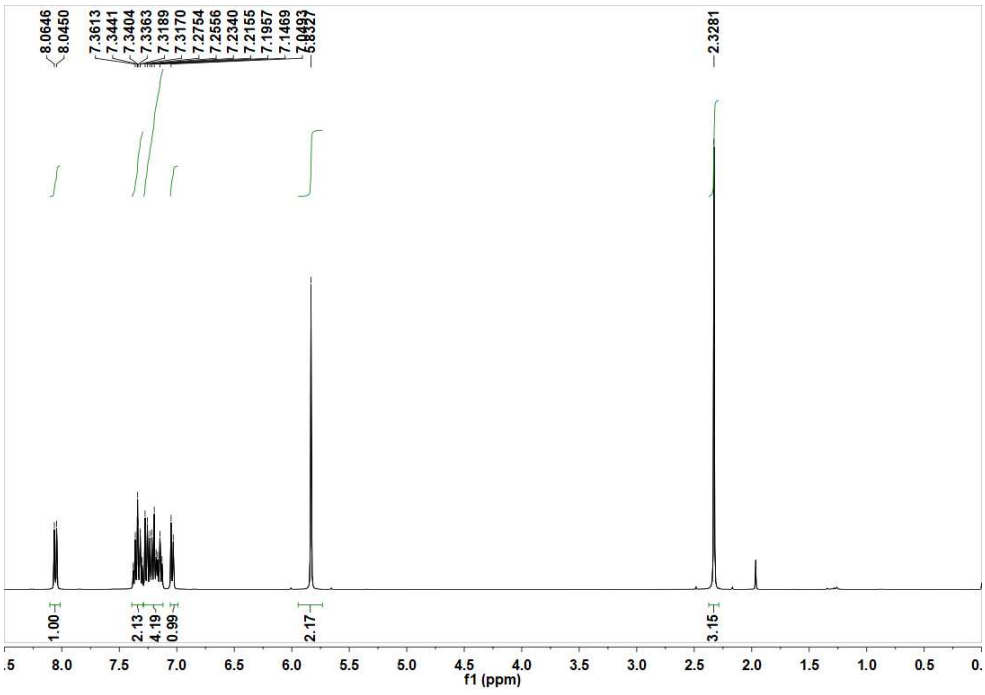
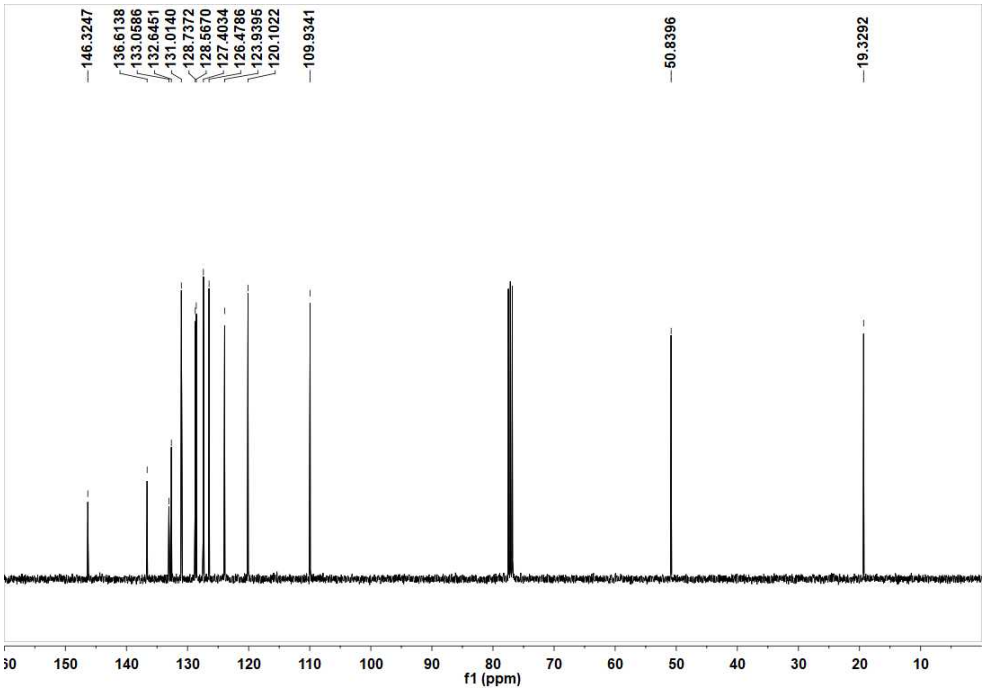
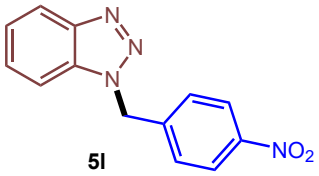
134.8691
132.9271
129.1494
128.6154
127.7160
127.5541
124.0788
120.2176
109.8629
52.4209
f1 (ppm)


N
N
N
Me

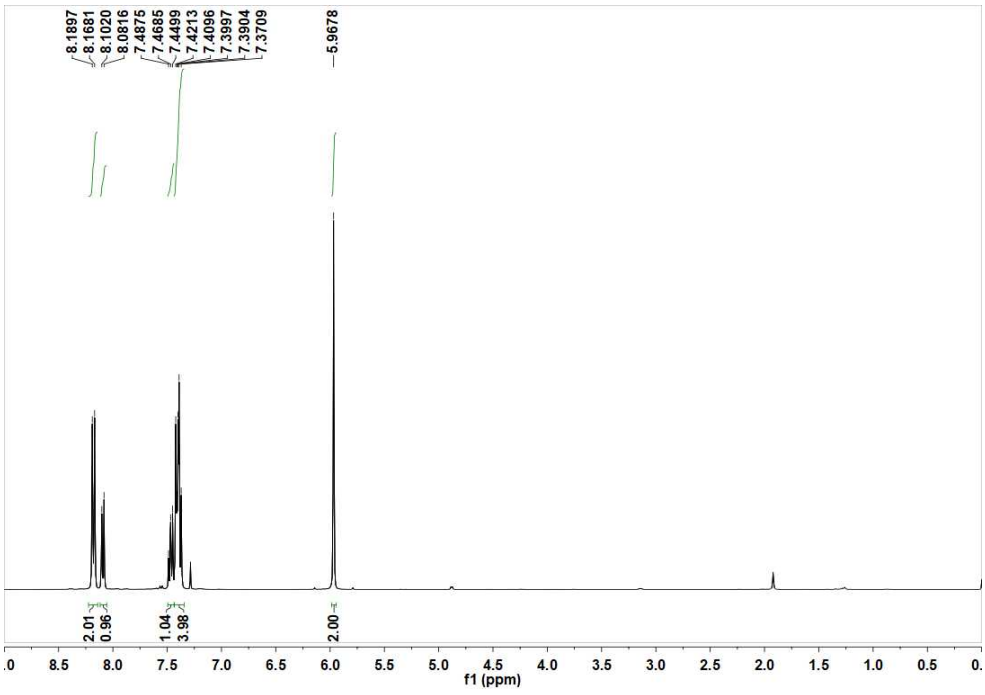
5k


8.0646
8.0450
7.3613
7.3441
7.3404
7.3363
7.3189
7.3170
7.2754
7.2656
7.2340
7.2155
7.1957
7.1469
5.8327
2.3281
1.00
2.13
4.19
0.99
2.17
3.15
f1 (ppm)


146.3247
136.6138
133.0586
132.6451
131.0140
128.7372
128.5670
127.4034
126.4786
123.9395
120.1022
109.9341
50.8396
19.3292
f1 (ppm)


N
N
N
NO2

5l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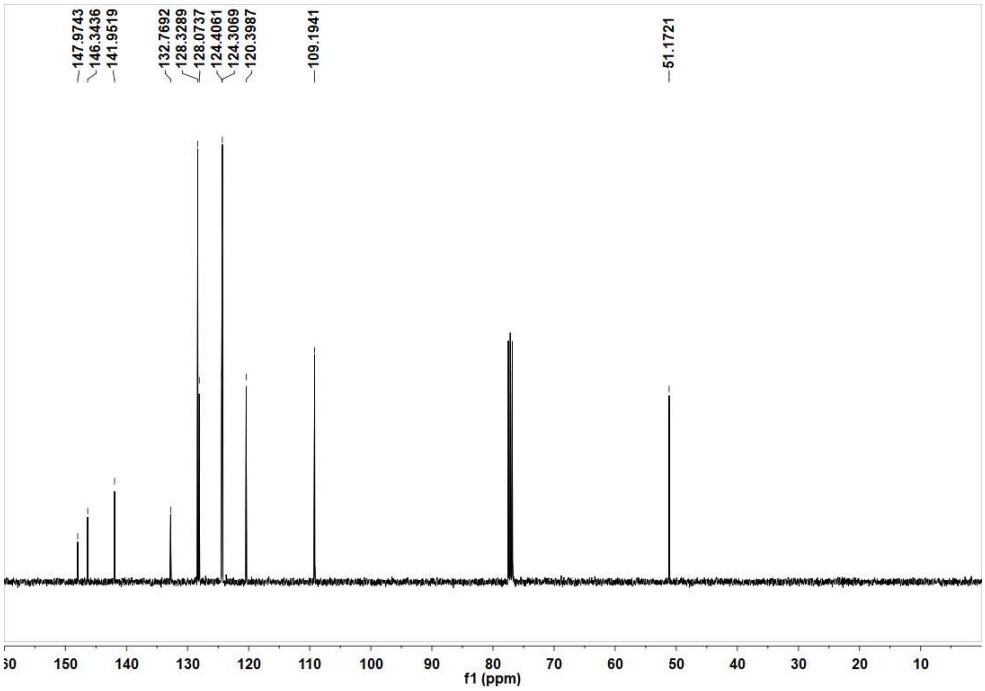
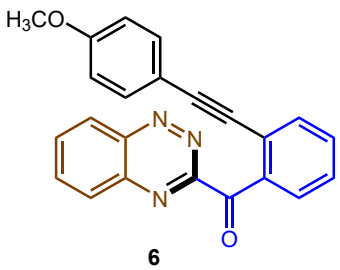
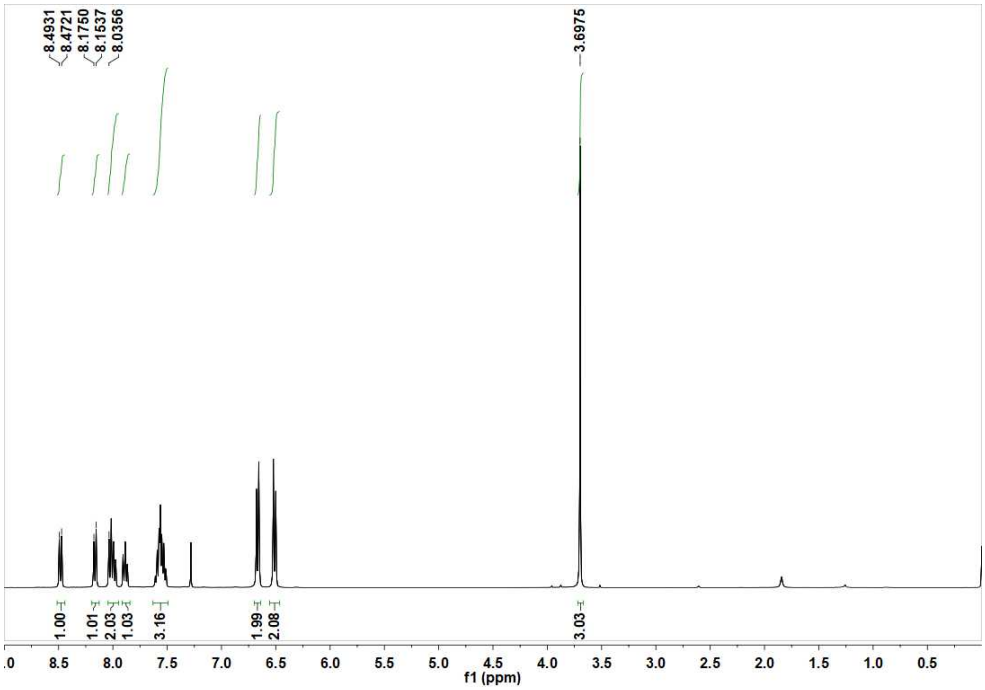
8.1681
8.1020
8.0816
7.4875
7.4685
7.4499
7.4213
7.4096
7.3997
7.3904
7.3709
5.9678
2.01
0.96
1.04
3.98
2.00
f1 (ppm)


147.9743
146.3436
141.9519
132.7692
128.3289
128.0737
124.4061
124.3069
120.3987
109.1941
51.1721
f1 (ppm)


H3CO
N
N
N
O

6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8.4721
8.1750
8.1537
8.0356
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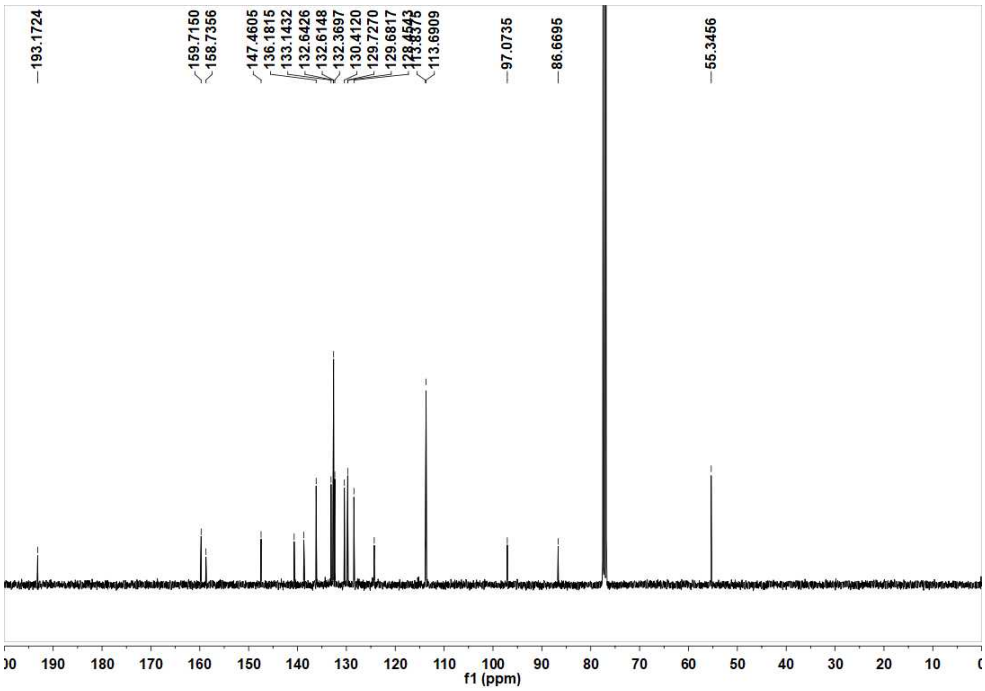
1.01
2.03
1.03
3.16
1.99
2.08
3.03
f1 (ppm)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159.7150
158.7356
147.4605
136.1815
133.1432
132.6426
132.6148
132.3697
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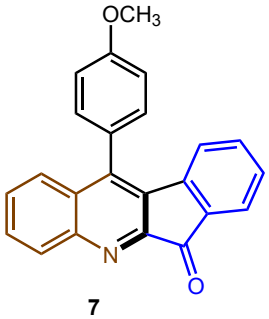
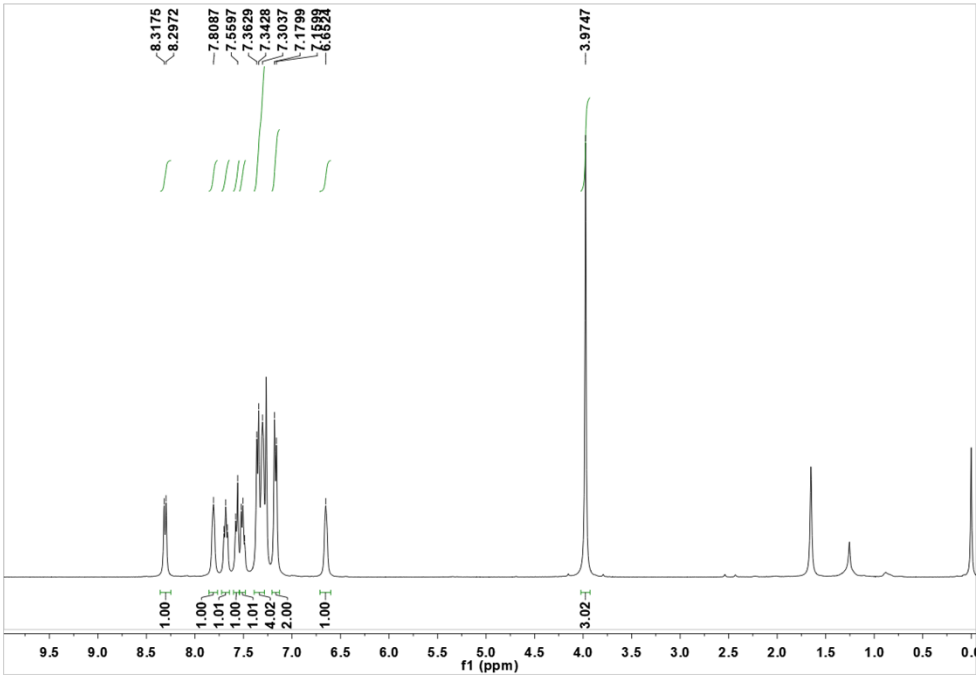
129.7270
129.6817
113.6909
97.0735
86.6695
55.3456
f1 (ppm)


OCH3
N
O

7


8.3175
8.2972
7.8087
7.6597
7.3629
7.3428
7.3037
7.1799
6.6824
3.9747
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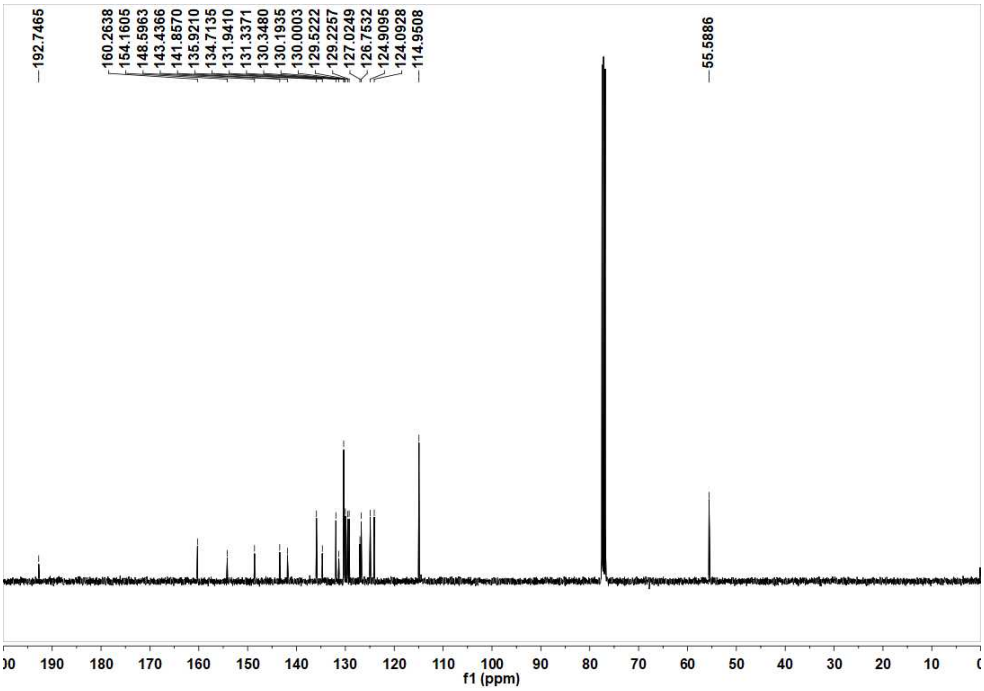
4.02
2.00
1.00
3.02
f1 (ppm)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148.5963
143.4366
141.8570
135.9210
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131.9410
131.3371
130.3480
130.1935
130.0003
129.5222
129.2257
127.0249
126.7532
124.9095
124.0928
114.9508
55.5886
f1 (ppm)