Supporting Information for

Repurposing Cycloaddition of β-carbonyl Phosphonate and Azide to Synthesize Triazolyl phosphonates via Ionic-Liquid-Based Data-Driven Screening

Content

General Information and Materials:

Solvents were dried using traditional methods and freshly distilled before use. Reactions were monitored by thin-layer chromatography (TLC) on silica gel GF254 precoated plates and RP-HPLC. Compounds were detected under UV light and/or visualized by phosphomolybdic acid in ethanol solution. Solvents were evaporated under reduced pressure and below 50 °C. Mass spectra were obtained on Bruker APEX. High-resolution MS was performed with Bruker BIFLEX III and Bruker Daltonics. Inc. APEX II. 1H NMR spectra were recorded on 400 or 600 MHz using TMS as the internal standard. Chemical shifts were reported in parts per million and coupling constants were quoted in Hz. β-carbonyl phosphonates and azides were prepared based on the methods in the literatures in our previous work [1-3]. GC-MS analyses were performed with Thermo Fisher TRACE_1300_1310 for identifications of the compound library of 312 1,2,3-triazolyl phosphonates. 1,8-Diazabicyclo[5.4.0]undec-7-ene (Aldrich, 99%); 1,1,3,3-Tetramethylguanidine (Macklin, 99%); 7-Methyl-1,5,7-triazabicyclo[4.4.0] dec-5-ene (Aldrich, 99%); 1,5,7-triazabicyclo [4.4.0] decyl-5-ene (Macklin, 99%); 4-Dimethylaminopyridine (Macklin, 99%); 2-Aminopyridine; [Choline][OH] (Macklin, 45% aqueous solution); 1-Methylimidazole (Macklin, 99%); Ethanolamine (Alfa, 99%); Diethanolamine (Aldrich, 99%); Triethanolamine ((Macklin, 99%)); N,N-Dimethylethanolamine (Aldrich, 99%); Acetate (Aladdin, 99.5%); Propionic Acid (Alfa, 99%); Butyric acid (Alfa,99+%);Valeric acid (Sigma-Aldrich, 99%); Benzoic acid (Aladdin, 99.5%); *p*-Methoxybenzoic acid (Aladdin, 99%); Glycolic acid (Aladdin, 98%); Lactic acid (Alfa, 98%); Crotonic acid (Macklin, 98%); Trifluoroacetic Acid (Macklin, 99.5%); Phosphoric acid (Aladdin, 99%).

Abbreviations:

[DBU] = 1,8-Diazabicyclo[5.4.0]undec-7-ene;

[TMG] = N,N’-Tetramethylguanidine;

[MTBD] = 7-Methyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene

[TBD] = 1,5,7-triazabicyclo [4.4.0] decyl-5-ene

[DMAP] = 4-Dimethylaminopyridine

[2-AnPy] = 2-Aminopyridine

[MEIM] = N,N-Dimethylethanolamine

[MEOA] = 2-Methylaminoethanol

[DEOA] = Diethanolamine

[TEOA] = Triethanolamine

[DMEOA] = N,N-Dimethylethanolamine;

[Ac] = Acetate

[Pro] = Propionic Acid

[But] = Butyric acid

[Pen] = Valeric acid

[Ben] = Benzoic acid

[p-Ani] = *p*-Methoxybenzoic acid

[Gly] = Glycolic acid

[Lac] = Lactic acid

[Cro] = Crotonic acid

[TFA] = Trifluoroacetic Acid

[Pho] = Phosphoric acid

Preparative methods of the ionic liquid pool

1.5 mL centrifuge tubes were used to form a square of 144 tubes of 12 base×12 acid cross combinations. Then corresponding base (0.02 mmol) was added to each centrifuge tube in the ice bath, and 100 μL of methanol solution was added. The acid corresponding to the same amount of substance (0.02 mmol) was also added. When the heat release was over, covered the lid and removed the tubes from the ice bath. Place each of the tubes in a shaker for 48 hours at room temperature. The solvents were evaporated under reduced press after reactions. Considering the possible volatilities of acids and bases that are used for the building of the IL pool, we dried the samples under reduced pressures at 50^{o}C for 12 hours. The dried ILs were checked by ^{1}H NMR to confirm the 1:1 stoichiometry of cations to anions, and the water contents were measured by Karl fisher experiments to less than 0.5%.

Screening reactivity of β-carbonyl phosphonates with the ionic liquid pool

Adding 200 μL of stock solution (1.04 mmol/L at a concentration of 4-(Trifluoromethyl)phenyl azide (**1a**) soluble in phosphonate (**2a**) to each of the 144 centrifuge tubes that contained ionic liquids prepared by the above method. After the lid was tightly closed, each of the tubes was shocked on an oscillator for 20 seconds, then incubated in a table concentrator shaker at 30^{o}C for 24 hours. 300 μL ethyl acetate and 300 μL water were added to the reaction mixture to accelerate the separations of products from ionic liquids. Each of the phases of ethyl acetate was transferred into the glass vials containing 1-methylimidazole as the internal standards, and then run Gas Chromatograph with autosamplers. The qualitative analysis of products was conducted using a Gas Chromatograph (SHIMADZU GC-2014ATF+APL) and by comparing it with authentic samples. The yields of compounds were quantitatively analyzed by Gas Chromatograph (SHIMADZU GC-2014ATF+APL, equipped with a hydrogen flame-ionization detector, full electric pneumatic control, 280°C) based on internal standard curves and areas of integrated peak areas according to the Gas Chromatograph traces.

For the yields of the triazolyl phosphonates (compound **3a**)

The yield of product **3a** = Moles of product **3a** / Moles of phosphonate **2a** ×100%

For the yields of triazoles (compound **4a**)

The yield of product **4a** = Moles of product **4a** / Moles of phosphonate **2a** ×100%

For the calculations of reaction selectivity

Selectivity = (Yield of product **3a**)/(Yield of product **3a** + Yield of product **4a**) ×100%

NMR experimental procedures of mechanistic investigations

The NMR spectra were recorded on BrukerAnanc 400. The spectra were detected at 303K. To eliminate the effect of solvent, Wilmad coaxial insert NMR tubes were used for ^{1}H NMR and ^{31}PNMR. For ^{1}H NMR, the mixtures of phosphonates and ionic liquids with different molar ratios were prepared. DMSO-d6 as an internal standard was added to the inner tube, and the sample was added to the outer tube. The mixture (0.3 mL) was added to the outer tube, and the inner tube was inserted. The temperature was controlled at 303K. For ^{31}P NMR, the mixtures of phosphonates and ionic liquids with different molar ratios (1:2, 1:1, and 2:1) were prepared. DMSO-d6 as an internal standard was added to the inner tube, and the sample was added to the outer tube. The mixture (0.3 mL) was added to the outer tube, and the inner tube was inserted. The temperature was controlled at 303K.

Preparative methods of 1,2,3-triazolyl phosphonates

To an oven-dried round bottom flask, azide (0.20 mmol), phosphonates (0.22 mmol), and choline acetate (0.20 mmol) were added. The reaction mixture was stirred at 30^{o}C for 24 hours. After the completion of the reaction, the products and ionic liquids could separate automatically. Water was added to solute ionic liquids, and the products could be obtained by filtrating. Alternatively, ethyl acetate could be added to the reaction mixture to accelerate the separations of products from ionic liquids, and the products were obtained after evaporations to get off the solvents and dried in a vacuum drying oven. The structures of triazolyl phosphonates were identified by ^{1}H NMR, ^{13}C NMR, ^{31}P NMR, and HRMS. To study the reusability, the ionic liquid was dried under a vacuum at 50°C for 24 hours

High-throughput workflow for syntheses of 312 1,2,3-triazolyl phosphonates

1.5 mL Centrifuge tubes (×312) that each containing 0.05 mmol choline acetate, were used to form a square of 12 phosphonate×25 azide cross combinations. The corresponding 12 phosphonates (0.05 mmol) were added to each centrifuge tube, and then 26 azides were added to each centrifuge tube. After the lid was tightly closed, each of the tubes was shocked on an oscillator for 20 seconds, then incubated in a table concentrator shaker at 30^{o}C for 24 hours. 300 μl ethyl acetate and 300 μl saturated brine were added to the tubes to accelerate the separations of products from the ionic liquids. Each of the phases of ethyl acetate was transferred into the glass vials. After identifying the molecular weights of the products by Thermo Fisher TRACE_1300_1310, the solvents were removed under reduced press and the products were used in situ for the followed antifungal biological activity assays.

Bioactivity evaluations of 300 1,2,3-triazolyl phosphonates

To evaluate the antifungal activity of 1,2,3-triazolyl phosphonates, disc diffusion experiments were first performed. The spores of *Rhizoctonia solani* ((Thanatephorus cucumeris NBRC 6298), purchased from Guangdong culture collection center) were cultured into Petri dishes containing potato dextrose agar (PDA). The concentrated phosphonates (5mg/mL) were applied to sterilized paper discs (5mm in diameter) using a capillary pipette. The degree of growth inhibition was indicated by comparations of the non-growth zone. Based on the results of the disc diffusion experiments, compounds TA-101, TA-133, and TA-125 were further investigated as the antifungal agents using the followed Fungicide Disk Assays.

Fungicide Disk Assays: Compounds in EtOH were added to 10 mL of PDA, in a concentration of 5 mg/mL、1mg/mL、0.5 mg/mL、0.05 mg/mL and 0.005mg/mL. PDA plates containing only the solvents were used as controls. Seven-day-old cultures of test Thanatephorus cucumeris NBRC 6298, grown on PDA plates were used as an inoculum put onto the control and test plates. After 5 days of incubation at 25 °C, the mycelial growth diameter was measured, and the percentage of inhibition to the control was calculated according to the following formula described by Shin et al. [4] as follows:

inhibition (%) = (growth diameter in untreated control - growth diameter in treatment) × 100]/ [growth diameter in untreated control]

Table S1: Chemical structures of ionic liquids

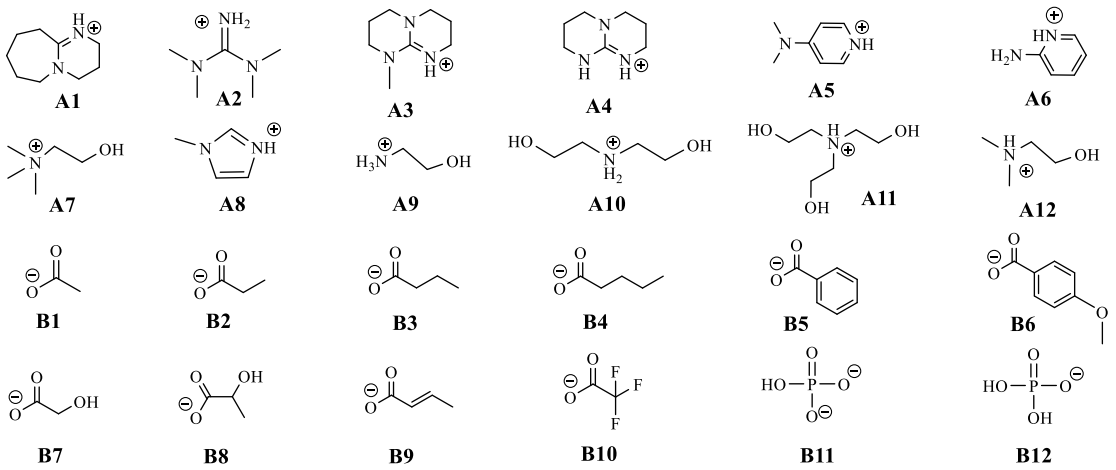


Table S2: Screening results using ionic liquid pool

Entry [a]	Name of ILs		Yield 3a (%)	Yield 4a (%)	Selectivity 3a (%)
1	A1-B1	[DBU][Ac]	70	3	96
2	A1-B2	[DBU][Pro]	50	1	98
3	A1-B3	[DBU][But]	30	5	86
4	A1-B4	[DBU][Val]	47	1	98
5	A1-B5	[DBU][Ben]	41	3	93
6	A1-B6	[DBU][Ani]	--[b]	5	--[c]
7	A1-B7	[DBU][Gly]	42	3	93
8	A1-B8	[DBU][Lac]	21	7	75
9	A1-B9	[DBU][Cro]	55	2	96
10	A1-B10	[DBU][TFA]	--[b]	6	--[c]
11	A1-B11	[DBU][H_2PO_4]	40	5	89
12	A1-B12	[DBU]$_2$[HPO_4]	--[b]	5	--[c]
13	A2-B1	[TMG][Ac]	78	5	94
14	A2-B2	[TMG][Pro]	44	5	90
15	A2-B3	[TMG][But]	20	21	49
16	A2-B4	[TMG][Val]	53	2	96
17	A2-B5	[TMG][Ben]	40	3	93
18	A2-B6	[TMG][Ani]	--[b]	4	--[c]
19	A2-B7	[TMG][Gly]	--[b]	10	--[c]
20	A2-B8	[TMG][Lac]	6	5	55
21	A2-B9	[TMG][Cro]	90	5	95
22	A2-B10	[TMG][TFA]	5	8	38

23	A2-B11	[TMG][H_2PO_4]	13	4	76
24	A2-B12	$[TMG]_2[HPO_4]$	20	5	80
25	A3-B1	[MTBD][Ac]	22	2	92
26	A3-B2	[MTBD][Pro]	27	9	75
27	A3-B3	[MTBD][But]	27	10	73
28	A3-B4	[MTBD][Val]	23	9	72
29	A3-B5	[MTBD][Ben]	55	11	83
30	A3-B6	[MTBD][Ani]	53	13	80
31	A3-B7	[MTBD][Gly]	80	11	88
32	A3-B8	[MTBD][Lac]	30	3	91
33	A3-B9	[MTBD][Cro]	33	2	94
34	A3-B10	[MTBD][TFA]	0	5	0
35	A3-B11	[MTBD][H_2PO_4]	0	6	0
36	A3-B12	$[MTBD]_2[HPO_4]$	77	1	99
37	A4-B1	[TBD][Ac]	90	7	93
38	A4-B2	[TBD][Pro]	22	6	79
39	A4-B3	[TBD][But]	14	9	61
40	A4-B4	[TBD][Val]	6	9	40
41	A4-B5	[TBD][Ben]	--[b]	10	--[c]
42	A4-B6	[TBD][Ani]	--[b]	9	--[c]
43	A4-B7	[TBD][Gly]	--[b]	9	--[c]
44	A4-B8	[TBD][Lac]	--[b]	3	--[c]
45	A4-B9	[TBD][Cro]	19	3	86
46	A4-B10	[TBD][TFA]	--[b]	4	--[c]

47	A4-B11	[TBD][H_2PO_4]	--[b]	4	--[c]
48	A4-B12	[TBD]$_2$[HPO_4]	61	8	88
49	A5-B1	[DMAP][Ac]	6	5	55
50	A5-B2	[DMAP][Pro]	5	8	38
51	A5-B3	[DMAP][But]	4	6	40
52	A5-B4	[DMAP][Val]	11	--[b]	100
53	A5-B5	[DMAP][Ben]	--[b]	--[b]	--[c]
54	A5-B6	[DMAP][Ani]	--[b]	--[b]	--[c]
55	A5-B7	[DMAP][Gly]	--[b]	5	--[c]
56	A5-B8	[DMAP][Lac]	--[b]	5	--[c]
57	A5-B9	[DMAP][Cro]	21	6	78
58	A5-B10	[DMAP][TFA]	--	5	--[c]
59	A5-B11	[DMAP][H_2PO_4]	3	4	43
60	A5-B12	[DMAP]$_2$[HPO_4]	27	5	84
61	A6-B1	[2-AnPy][Ac]	--[b]	7	--[c]
62	A6-B2	[2-AnPy][Pro]	--[b]	6	--[c]
63	A6-B3	[2-AnPy][But]	--[b]	5	--[c]
64	A6-B4	[2-AnPy][Val]	--[b]	9	--[c]
65	A6-B5	[2-AnPy][Ben]	--[b]	8	--[c]
66	A6-B6	[2-AnPy][Ani]	--[b]	5	--[c]
67	A6-B7	[2-AnPy][Gly]	--[b]	10	--[c]
68	A6-B8	[2-AnPy][Lac]	--[b]	10	--[c]
69	A6-B9	[2-AnPy][Cro]	--[b]	9	--[c]
70	A6-B10	[2-AnPy][TFA]	--[b]	9	--[c]

71	A6-B11	[2-AnPy][H_2PO_4]	--[b]	11	--[c]
72	A6-B12	[2-AnPy]$_2$[HPO_4]	--[b]	10	--[c]
73	A7-B1	[CH][Ac]	95	3	97
74	A7-B2	[CH][Pro]	91	6	95
75	A7-B3	[CH][But]	94	3	97
76	A7-B4	[CH][Val]	91	2	98
77	A7-B5	[CH][Ben]	45	4	92
78	A7-B6	[CH][Ani]	44	5	90
79	A7-B7	[CH][Gly]	--[b]	5	--[c]
80	A7-B8	[CH][Lac]	5	3	63
81	A7-B9	[CH][Cro]	86	--[b]	100
82	A7-B10	[CH][TFA]	--[b]	4	--[c]
83	A7-B11	[CH][H_2PO_4]	10	3	77
84	A7-B12	[CH]$_2$[HPO_4]	64	27	70
85	A8-B1	[MEIM][Ac]	--[b]	13	--[c]
86	A8-B2	[MEIM][Pro]	--[b]	11	--[c]
87	A8-B3	[MEIM][But]	--[b]	10	--[c]
88	A8-B4	[MEIM][Val]	--[b]	11	--[c]
89	A8-B5	[MEIM][Ben]	--[b]	8	--[c]
90	A8-B6	[MEIM][Ani]	--[b]	11	--[c]
91	A8-B7	[MEIM][Gly]	--[b]	8	--[c]
92	A8-B8	[MEIM][Lac]	--[b]	11	--[c]
93	A8-B9	[MEIM][Cro]	--[b]	13	--[c]
94	A8-B10	[MEIM][TFA]	--[b]	13	--[c]

95	A8-B11	[MEIM][H_2PO_4]	--[b]	6	--[c]
96	A8-B12	[MEIM]$_2$[HPO_4]	--[b]	7	--[c]
97	A9-B1	[EOA][Ac]	10	7	59
98	A9-B2	[EOA][Pro]	7	10	41
99	A9-B3	[EOA][But]	8	3	73
100	A9-B4	[EOA][Val]	4	8	33
101	A9-B5	[EOA][Ben]	--[b]	9	--[c]
102	A9-B6	[EOA][Ani]	5	12	29
103	A9-B7	[EOA][Gly]	--[b]	17	--[c]
104	A9-B8	[EOA][Lac]	--[b]	21	--[c]
105	A9-B9	[EOA][Cro]	--[b]	13	--[c]
106	A9-B10	[EOA][Tfa]	--[b]	12	--[c]
107	A9-B11	[EOA][H_2PO_4]	--[b]	13	--[c]
108	A9-B12	[EOA]$_2$[HPO_4]	--[b]	12	--[c]
109	A10-B1	[DEOA][Ac]	--[b]	6	--[c]
110	A10-B2	[DEOA][Pro]	--[b]	5	--[c]
111	A10-B3	[DEOA][But]	--[b]	4	--[c]
112	A10-B4	[DEOA][Val]	--	5	--[c]
113	A10-B5	[DEOA][Ben]	1	6	14
114	A10-B6	[DEOA][Ani]	--[b]	4	--[c]
115	A10-B7	[DEOA][Gly]	--[b]	7	--[c]
116	A10-B8	[DEOA][Lac]	--[b]	6	--[c]
117	A10-B9	[DEOA][Cro]	--[b]	3	--[c]
118	A10-B10	[DEOA][TFA]	--[b]	3	--[c]

119	A10-B11	[DEOA][H_2PO_4]	--[b]	7	--[c]
120	A10-B12	[DEOA]$_2$[HPO_4]	1	6	14
121	A11-B1	[TEOA][Ac]	--[b]	7	--[c]
122	A11-B2	[TEOA][Pro]	--[b]	6	--[c]
123	A11-B3	[TEOA][But]	--[b]	9	--[c]
124	A11-B4	[TEOA][Val]	--[b]	7	--[c]
125	A11-B5	[TEOA][Ben]	--[b]	10	--[c]
126	A11-B6	[TEOA][Ani]	--[b]	11	--[c]
127	A11-B7	[TEOA][Gly]	--[b]	8	--[c]
128	A11-B8	[TEOA][Lac]	--[b]	9	--[c]
129	A11-B9	[TEOA][Cro]	--[b]	9	--[c]
130	A11-B10	[TEOA][TFA]	--[b]	9	--[c]
131	A11-B11	[TEOA][H_2PO_4]	--[b]	12	--[c]
132	A11-B12	[TEOA]$_2$[HPO_4]	--[b]	17	--[c]
133	A12-B1	[DMEOA][Ac]	--[b]	8	--[c]
134	A12-B2	[DMEOA][Pro]	--[b]	8	--[c]
135	A12-B3	[DMEOA][But]	--[b]	8	--[c]
136	A12-B4	[DMEOA][Val]	--[b]	9	--[c]
137	A12-B5	[DMEOA][Ben]	--[b]	17	--[c]
138	A12-B6	[DMEOA][Ani]	--[b]	9	--[c]
139	A12-B7	[DMEOA][Gly]	--[b]	10	--[c]
140	A12-B8	[DMEOA][Lac]	--[b]	7	--[c]
141	A12-B9	[DMEOA][Cro]	--[b]	6	--[c]
142	A12-B10	[DMEOA][TFA]	--[b]	7	--[c]

143	A12-B11	[DMEOA][H_2PO_4]	--[b]	1	--[c]
144	A12-B12	[DMEOA]$_2$[HPO_4]	--[b]	2	--[c]

[a] The experiments were conducted based on the procedures described in the section "Screening reactivity of β-carbonyl phosphonates with the ionic liquid pool" in the supporting information. [b] Yields were less than 5%. [c] No calculations about reaction selectivity.

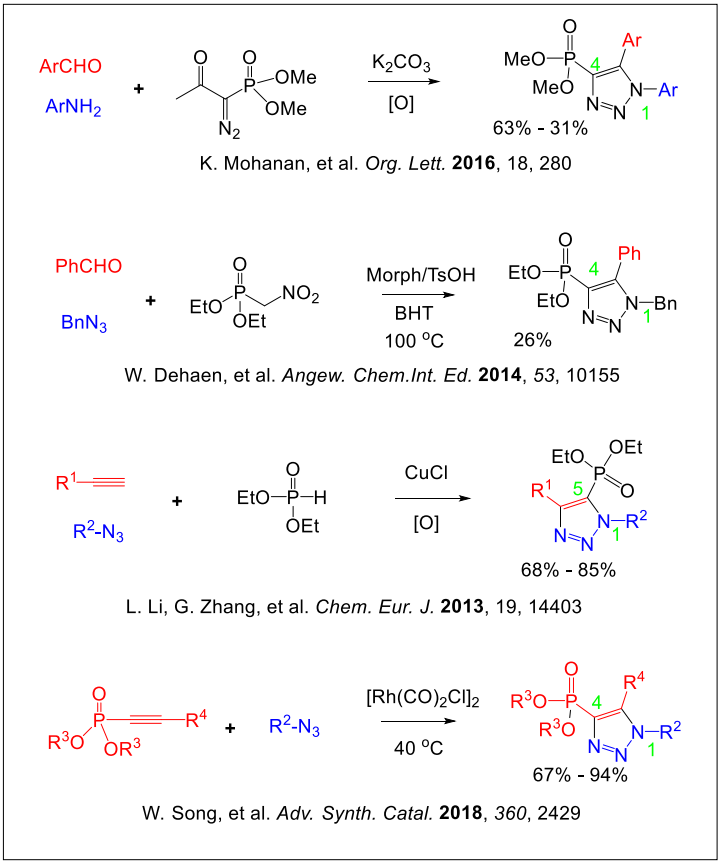


Figure S1 Synthesis of triazolyl phosphonates by different methods in literature.

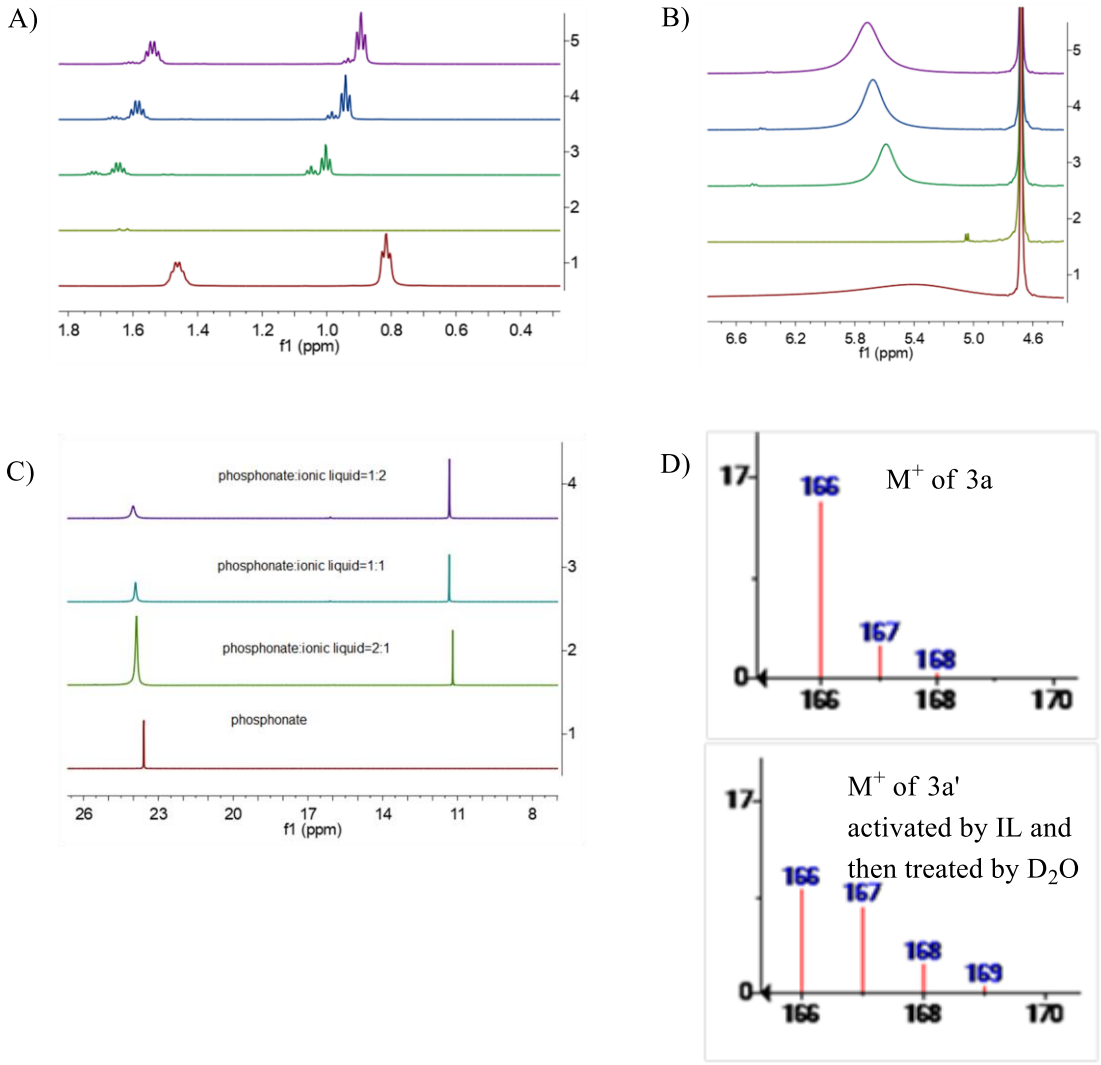


Figure S2:A) The magnified figure for ^{1}H NMR spectra showing the changing of the proton on hydroxyl group of ionic liquid after mixing with carbonyl phosphonates; B) The magnified figure for ^{1}H NMR spectra showing the changing of the proton on hydroxyl group of ionic liquid after mixing with carbonyl phosphonates; C) ^{31}P NMR analyses of the effects of A7-B3 on the proton shifts of β-carbonyl phosphonates; D) Mass spectra analyses of the effects of A7-B3 on deuterium reaction with β-carbonyl phosphonates;

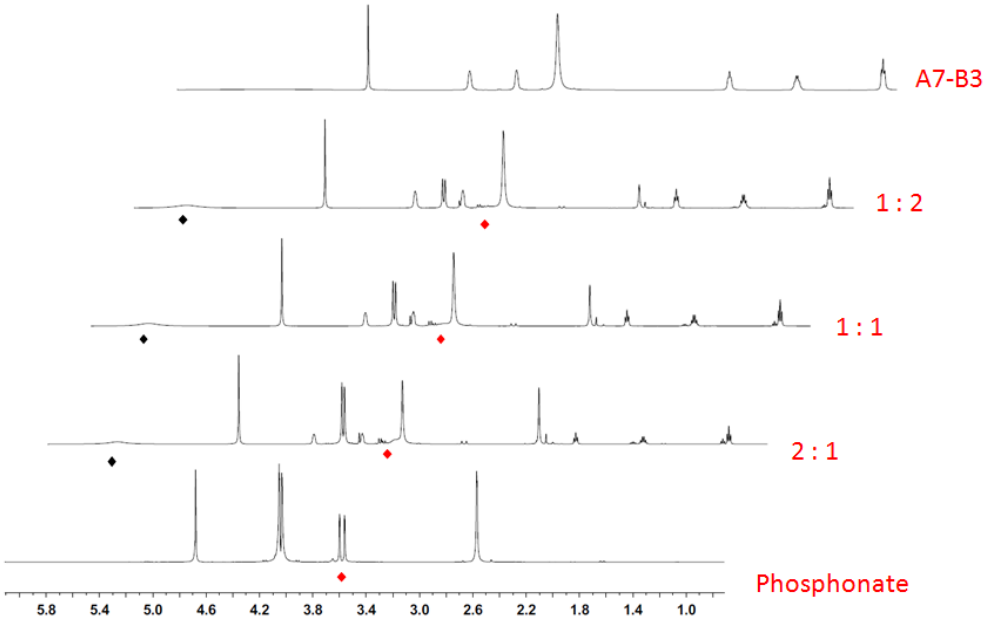


Figure S3: ^{1}H nuclear magnetic resonance (NMR) spectra of ionic liquid A7-B3, β-carbonyl phosphonate **1b,** and the mixtures with A7-B3 and **1b** with various molar ratios (molar ratio of A7-B3 to **1b** = 1:2, 1:1 and 2:1). The resonance band of -CH_2- of β-carbonyl phosphonate is labeled by the red asterisk. The resonance band of the newly formed H-bond is labeled by a black asterisk.

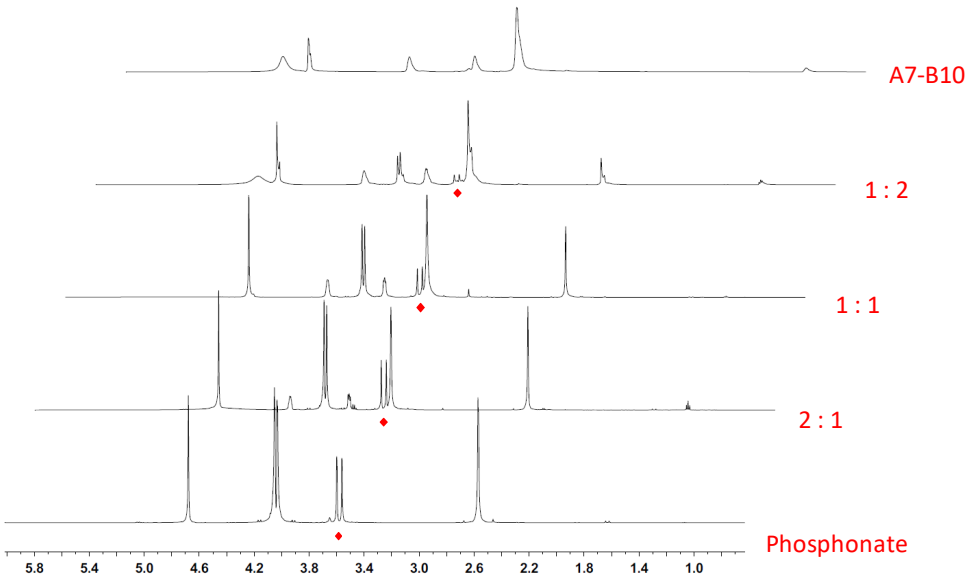


Figure S4: ^{1}H nuclear magnetic resonance (NMR) spectra of ionic liquid A7-B10, β-carbonyl phosphonate **1b,** and the mixtures with A7-B10 and **1b** with various molar ratios (molar ratio of A7-B10 to **1b** = 1:2, 1:1 and 2:1). The resonance band of -CH_2- of β-carbonyl phosphonate is labeled

by the red asterisk.

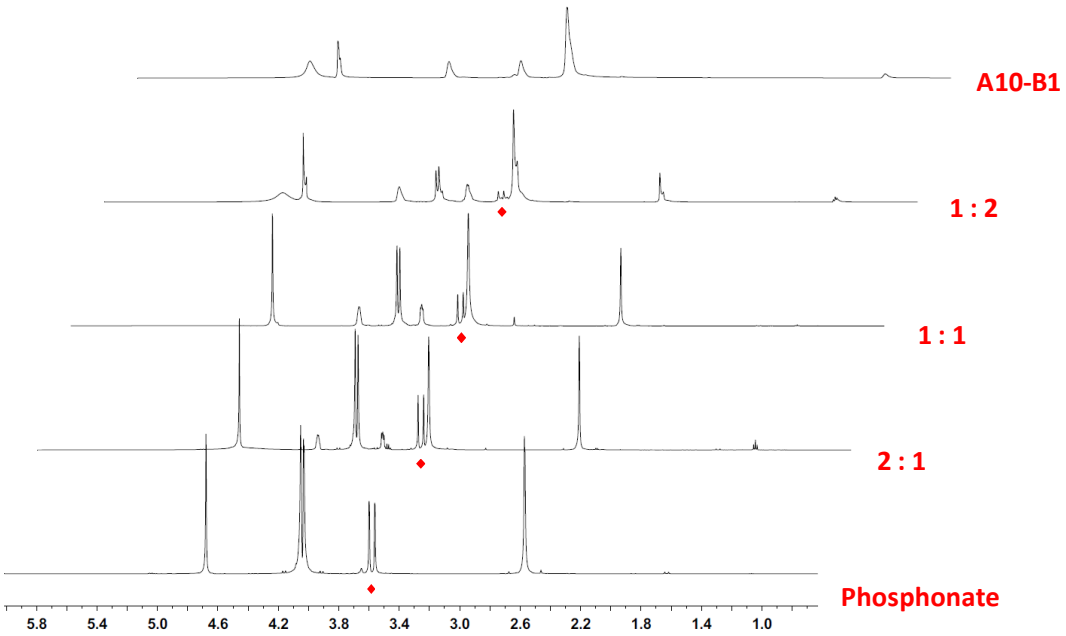


Figure S5: ^{1}H nuclear magnetic resonance (NMR) spectra of ionic liquid A10-B1, β-carbonyl phosphonate **1b,** and the mixtures with A10-B1 and **1b** with various molar ratios (molar ratio of A10-B1 to **1b** = 1:2, 1:1 and 2:1). The resonance band of -CH_2- of β-carbonyl phosphonate is labeled by the red asterisk.

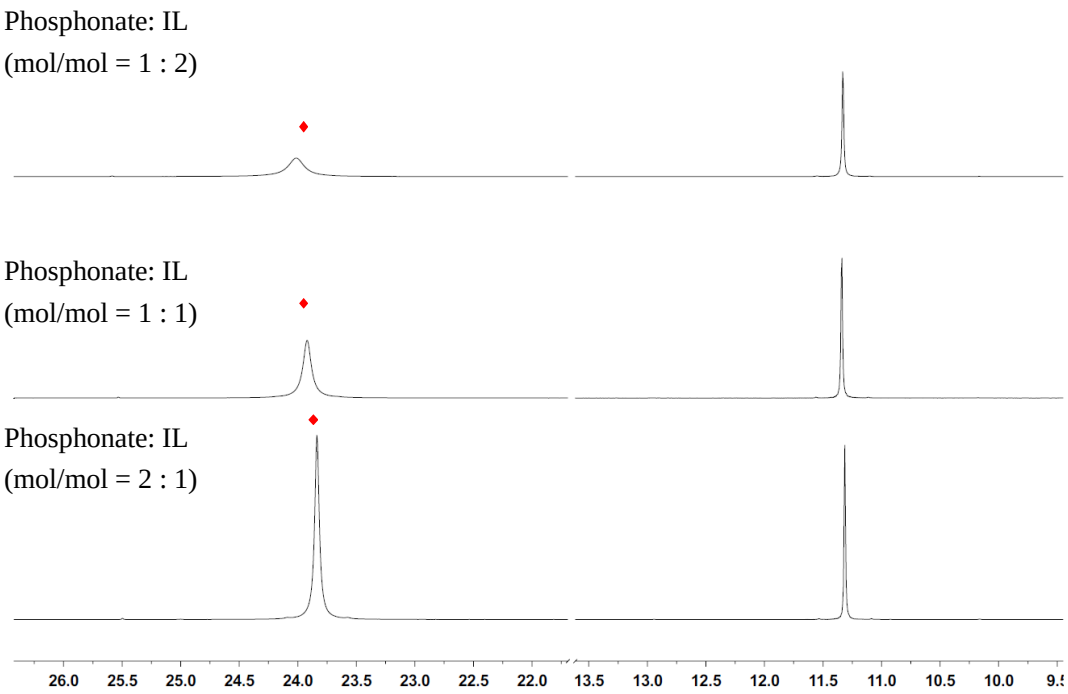


Figure S6: ^{31}P nuclear magnetic resonance (NMR) spectra of the mixtures of A7-B3 and **1b** (with various molar ratios (molar ratio of **1b** to A7-B3 = 1:2, 1:1, and 2:1). The resonance band of P of β-carbonyl phosphonate is labeled by the red asterisk.

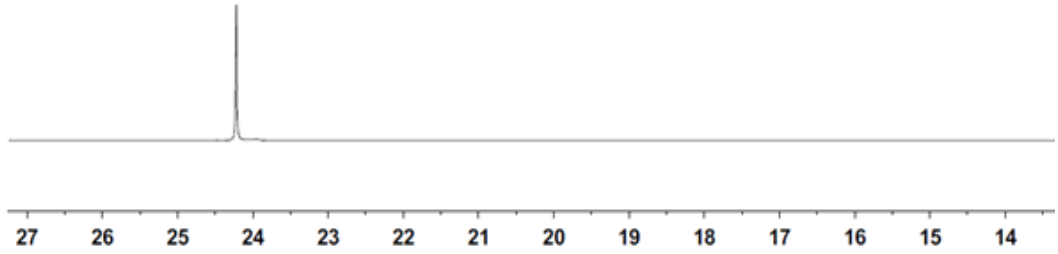


Figure S7: ^{31}P nuclear magnetic resonance (NMR) spectra of the mixtures with A7-B3 and **1b** (molar ratio of **1b** to A7-B3 = 1:2) after H_2O was added.

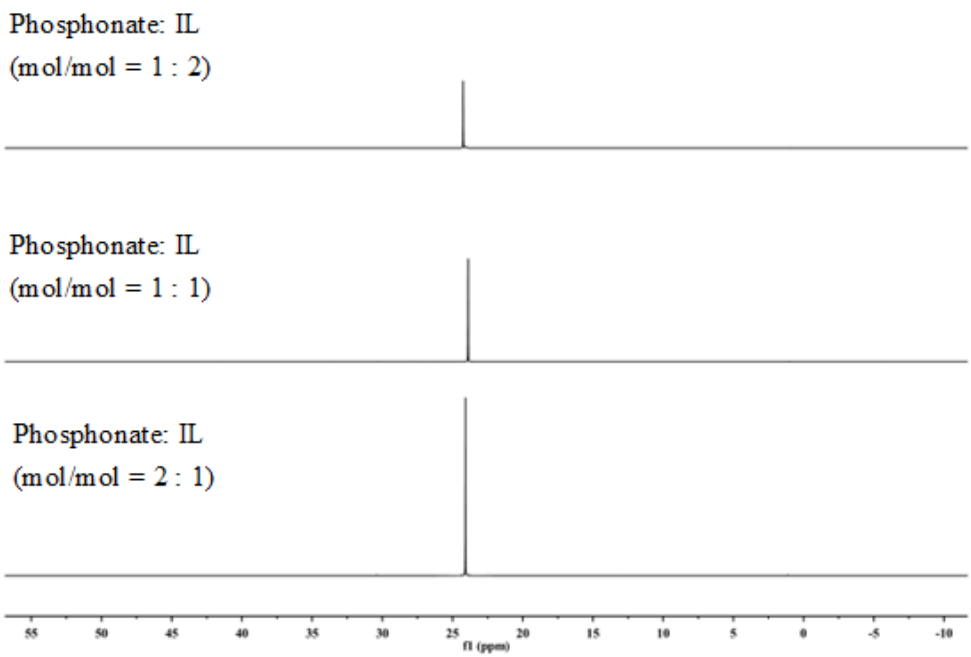


Figure S8: ^{31}P nuclear magnetic resonance (NMR) spectra of the mixtures of A7-B10 and **1b** (with various molar ratios (molar ratio of **1b** to A7-B10 = 1:2, 1:1, and 2:1).

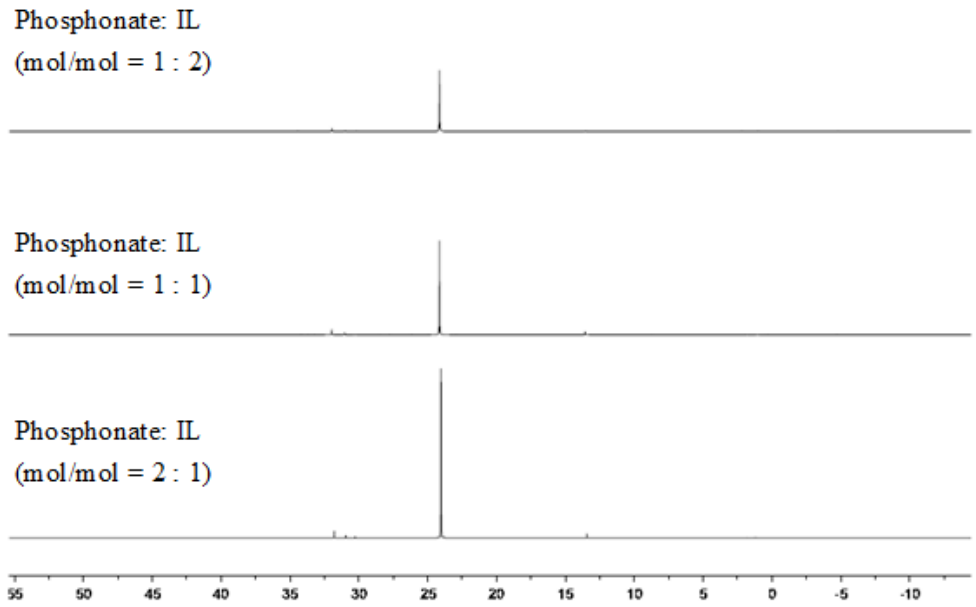
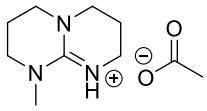


Figure S9: ^{31}P nuclear magnetic resonance (NMR) spectra of the mixtures of A10-B1 and **1b** (with various molar ratios (molar ratio of **1b** to A10-B1 = 1:2, 1:1, and 2:1).

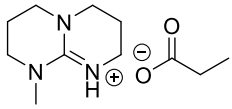
Characterization of synthesized ionic liquids

A3-B1: [MTBD][Ac]



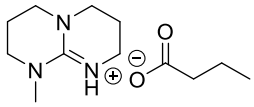
^{1}H NMR (400 MHz, D_2O) δ 3.27 - 3.20 (m, 8H), 2.84 (s, 3H), 1.94 - 1.86 (m, 4H), 1.84 (s, 3H). ^{13}C NMR (101 MHz, D_2O) δ 180.5, 151.1, 47.7, 47.1, 46.7, 38.4, 36.3, 22.9, 20.3.

A3-B2: [MTBD][Pro]



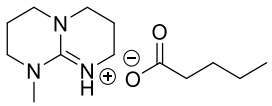
^{1}H NMR (400 MHz, D_2O) δ 3.27 - 3.20 (m, 8H), 2.84 (s, 3H), 2.11 - 2.05 (m, 2H), 1.94 - 1.83 (m, 4H), 0.96 (t, J = 8.0Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 184.5, 151.0, 47.7, 47.1, 46.7, 38.4, 36.3, 30.7, 20.3, 10.2.

A3-B3: [MTBD][But]



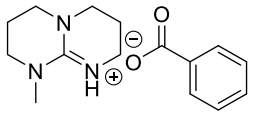
^{1}H NMR (400 MHz, D_2O) δ 3.27 - 3.20 (m, 8H), 2.84 (s, 3H), 2.06 (t, J = 8.0 Hz, 2H), 1.94 - 1.83 (m, 4H), 1.51 - 1.42 (m, 2H), 0.80 (t, J = 8.0 Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 183.6, 151.0, 47.7, 47.1, 46.7, 39.7, 38.4, 36.3, 20.3, 19.4, 13.3.

A3-B4: [MTBD][Val]



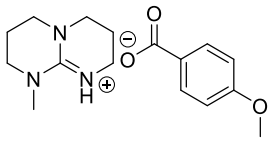
^{1}H NMR (400 MHz, D_2O) δ 3.27 - 3.20 (m, 8H), 2.84 (s, 3H), 2.08 (t, J = 8.0 Hz, 2H), 1.94 - 1.84 (m, 4H), 1.47 - 1.40 (m, 2H), 1.25 - 1.16 (m, 2H), 0.80 (t, J = 8.0 Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 183.9, 151.0, 47.7, 47.1, 46.7, 38.4, 37.4, 36.3, 28.1, 22.0, 20.3, 13.2.

A3-B5: [MTBD][Ben]



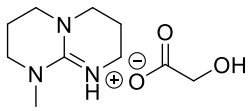
^{1}H NMR (400 MHz, D_2O) δ 7.78 (d, *J* = 8.0 Hz, 2H), 7.47 - 7.36 (m, 3H), 3.18 - 3.11 (m, 8H), 2.77 (s, 3H), 1.87 - 1.77 (m, 4H). ^{13}C NMR (101 MHz, D_2O) δ 174.9, 150.6, 136.3, 131.1, 128.8, 128.2, 47.5, 46.9, 46.5, 38.3, 36.2, 20.1.

A3-B6: [MTBD][Ani]



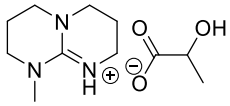
^{1}H NMR (400 MHz, D_2O) δ 7.79 - 7.75 (m, 2H), 6.93 - 6.89 (m, 2H), 3.76 (s, 3H), 3.16 - 3.08 (m, 8H), 2.75 (s, 3H), 1.85 - 1.75 (m, 4H). ^{13}C NMR (101 MHz, D_2O) δ 174.3, 161.1, 150.5, 131.0, 129.1, 113.2, 55.3, 47.5, 46.9, 46.5, 38.3, 36.1, 20.1.

A3-B7: [MTBD][Gly]



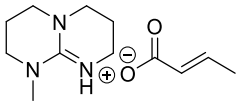
^{1}H NMR (400 MHz, D_2O) δ 3.82 (s, 2H), 3.26 - 3.19 (m, 8H), 2.84 (s, 3H), 1.94 - 1.81 (m, 4H). ^{13}C NMR (101 MHz, D_2O) δ 179.5, 151.1, 61.2, 47.7, 47.1, 46.7, 38.5, 36.3, 20.3.

A3-B8: [MTBD][Lac]



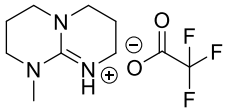
^{1}H NMR (400 MHz, D_2O) δ 4.04 (q, *J* = 8.0 Hz, 1H), 3.26 - 3.19 (m, 8H), 2.84 (s, 3H), 1.94 - 1.83 (m, 4H), 1.24 (d, *J* = 8.0 Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 181.6, 151.1, 68.1, 47.7, 47.1, 46.7, 38.4, 36.3, 20.3, 20.0.

A3-B9: [MTBD][Cro]



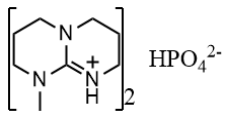
^{1}H NMR (400 MHz, D_2O) δ 6.62 - 6.53 (m, 1H), 5.74 (dd, *J* = 16.0, 4.0 Hz, 1H), 3.26 - 3.19 (m, 8H), 2.84 (s, 3H), 1.94 - 1.83 (m, 4H), 1.72 (dd, *J* = 8.0, 4.0 Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 175.3, 151.0, 141.4, 127.1, 47.7, 47.1, 46.7, 38.4, 36.3, 20.3, 17.0.

A3-B10: [MTBD][TFA]



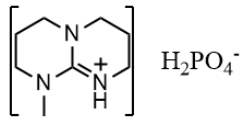
^{1}H NMR (400 MHz, D_2O) δ 3.27 - 3.20 (m, 8H), 2.85 (d, *J* = 4.0 Hz, 3H), 1.95 - 1.83 (m, 4H). ^{13}C NMR (101 MHz, D_2O) δ 162.7 (q, $J_{C\text{-}F}$ = 40.4 Hz), 151.0, 116.4 (q, $J_{C\text{-}F}$ = 292.9 Hz), 47.7, 47.1, 46.7, 38.4, 36.3, 20.4, 20.2.

A3-B11: [MTBD][HPO_4^{2-}]



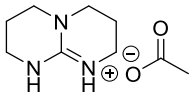
^{1}H NMR (400 MHz, D_2O) δ 3.26 - 3.19 (m, 8H), 2.84 (s, 3H), 1.93 - 1.82 (m, 4H). ^{13}C NMR (101 MHz, D_2O) δ 151.1, 47.7, 47.1, 46.6, 38.4, 36.3, 20.3.

A3-B12: [MTBD][$H_2PO_4^-$]



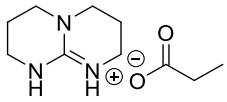
^{1}H NMR (400 MHz, D_2O) δ 3.25 - 3.17 (m, 16H), 2.82 (s, 6H), 1.92 - 1.81 (m, 8H). ^{13}C NMR (101 MHz, D_2O) δ 151.1, 47.7, 47.1, 46.7, 38.4, 36.3, 20.3.

A4-B1: [TBD][Ac]



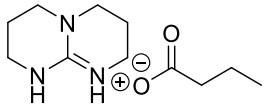
^{1}H NMR (400 MHz, D_2O) δ 3.24 (t, *J* = 4.0 Hz, 4H), 3.16 (t, *J* = 4.0 Hz, 4H), 1.91 - 1.85 (m, 4H), 1.82 (s, 3H). ^{13}C NMR (151 MHz, D_2O) δ 181.4, 151.0, 46.5, 37.8, 23.3, 20.2.

A4-B2: [TBD][Pro]



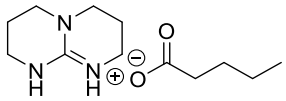
^{1}H NMR (400 MHz, D_2O) δ 3.26 (t, *J* = 6.0 Hz, 4H), 3.18 (t, *J* = 6.0 Hz, 4H), 2.11 (q, *J* = 7.2 Hz, 2H), 2.00 - 1.79 (m, 4H), 0.98 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (151 MHz, D_2O) δ 183.1, 150.9, 46.5, 37.8, 29.5, 20.2, 9.6.

A4-B3: [TBD][But]



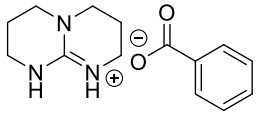
^{1}H NMR (400 MHz, D_2O) δ 3.28 (t, *J* = 6.0 Hz, 4H), 3.20 (t, *J* = 6.0 Hz, 4H), 2.09 (t, *J* = 7.4 Hz, 2H), 1.97 - 1.86 (m, 4H), 1.55 - 1.45 (m, 2H), 0.84 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, D_2O) δ 181.9, 150.9, 46.5, 38.0, 37.8, 20.2, 18.8, 13.0.

A4-B4: [TBD][Val]



^{1}H NMR (400 MHz, D_2O) δ 3.29 (t, *J* = 6.0 Hz, 4H), 3.22 (t, *J* = 6.0 Hz, 4H), 2.14 (t, *J* = 7.2 Hz, 2H), 1.99 - 1.88 (m, 4H), 1.53 - 1.44 (m, 2H), 1.32 - 1.22 (m, 2H), 0.85 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, D_2O) δ 181.9, 150.9, 46.5, 37.8, 35.6, 27.3, 21.8, 20.2, 13.0.

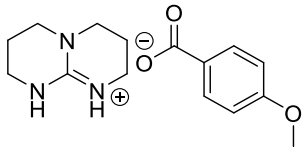
A4-B5: [TBD][Ben]



^{1}H NMR (400 MHz, D_2O) δ 7.83 (d, *J* = 4.0 Hz, 2H), 7.43 - 7.33 (m, 3H), 3.08 - 2.83

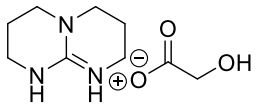
(m, 8H), 1.76 - 1.63 (m, 4H). ^{13}C NMR (101 MHz, D_2O) δ 174.6, 150.4, 136.1, 131.2, 128.9, 128.2, 46.2, 37.6, 20.0.

A4-B6: [TBD][Ani]



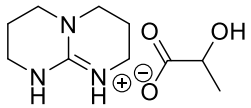
^{1}H NMR (400 MHz, D_2O) δ 7.80 (d, *J* = 8.8 Hz, 2H), 6.85 (d, *J* = 8.8 Hz, 2H), 3.70 (s, 3H), 3.00 (dd, *J* = 11.8, 5.8 Hz, 8H), 1.75 - 1.65 (m, 4H). ^{13}C NMR (101 MHz, D_2O) δ 174.2, 161.2, 150.4, 131.0, 128.9, 113.2, 55.3, 46.2, 37.7, 37.6, 20.0.

A4-B7: [TBD][Gly]



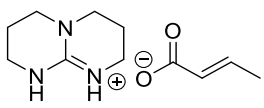
^{1}H NMR (400 MHz, D_2O) δ 3.90 (s, 2H), 3.30 (t, *J* = 4.0 Hz, 4H), 3.22 (t, *J* = 4.0 Hz, 4H), 2.00 - 1.86 (m, 4H). ^{13}C NMR (101 MHz, D_2O) δ 178.1, 150.9, 60.3, 46.4, 37.8, 20.2.

A4-B8: [TBD][Lac]



^{1}H NMR (400 MHz, D_2O) δ 4.04 (q, *J* = 8.0 Hz, 1H), 3.23 (t, *J* = 8.0 Hz, 4H), 3.16 (t, *J* = 8.0 Hz, 4H), 1.91 - 1.85 (m, 4H), 1.24 (d, *J* = 4.0 Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 181.9, 150.9, 68.2, 46.4, 37.8, 20.2, 20.0.

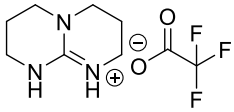
A4-B9: [TBD][Cro]



^{1}H NMR (400 MHz, D_2O) δ 6.64 - 6.55 (m, 1H), 5.78 - 5.73 (m, 1H), 3.23 (t, 8.0 Hz, 4H), 3.16 (t, 8.0 Hz, 4H), 1.91 - 1.84 (m, 4H), 1.76 - 1.70 (d, *J* = 8.0 Hz, 3H). ^{13}C NMR

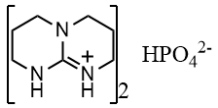
(101 MHz, D_2O) δ 175.4, 150.9 (s), 141.8, 126.8, 46.4, 37.8, 20.2, 17.0.

A4-B10: [TBD][TFA]



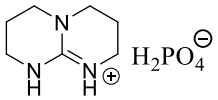
^{1}H NMR (400 MHz, D_2O) δ 3.24 (t, J = 8.0 Hz, 4H), 3.17 (t, J = 8.0 Hz, 4H), 1.92 - 1.86 (m, 4H). ^{13}C NMR (101 MHz, D_2O) δ 162.2 (q, $J_{C\text{-}F}$ = 40.4 Hz), 150.8, 116.2 (q, $J_{C\text{-}F}$ = 292.2 Hz), 46.4, 37.7, 20.1.

A4-B11: [TBD][H_2PO_4]



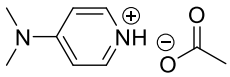
^{1}H NMR (400 MHz, D_2O) δ 3.22 (t, J = 8.0 Hz, 4H), 3.15 (t, J = 4.0 Hz, 4H), 1.90 - 1.84 (m, 4H). ^{13}C NMR (101 MHz, D_2O) δ 150.9, 46.4, 37.8, 20.2.

A4-B12: [TBD][$H_2PO_4^-$]



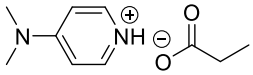
^{1}H NMR (400 MHz, D_2O) δ 3.23 (t, J = 8.0 Hz, 8H), 3.16 (t, J = 8.0 Hz, 8H), 1.91 - 1.85 (m, 8H). ^{13}C NMR (101 MHz, D_2O) δ 151.0, 46.4, 37.8, 20.2.

A5-B1: [DMAP][Ac]



^{1}H NMR (400 MHz, D_2O) δ 7.88 (d, J = 8.0 Hz, 2H), 6.74 (d, J = 8.0 Hz, 2H), 3.07 (s, 6H), 1.79 (s, 3H). ^{13}C NMR (101 MHz, D_2O) δ 181.3, 157.4, 138.4, 106.7, 39.2, 23.2.

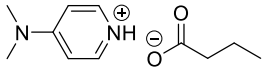
A5-B2: [DMAP][Pro]



^{1}H NMR (400 MHz, D_2O) δ 7.84 (d, J = 8.0 Hz, 2H), 6.66 (d, J = 8.0 Hz, 2H), 3.00 (s,

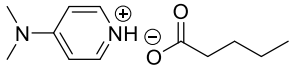
6H), 2.01 (q, *J* = 8.0 Hz, 2H), 0.89 (t, *J* = 8.0 Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 184.6, 157.1, 138.8, 106, 39.1, 30.7, 10.1.

A5-B3: [DMAP][But]



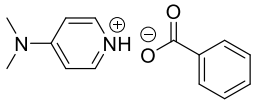
^{1}H NMR (400 MHz, D_2O) δ 7.85 (d, *J* = 8.0 Hz, 2H), 6.70 (d, *J* = 8.0 Hz, 2H), 3.03 (s, 6H), 1.98 (t, *J* = 8.0 Hz, 2H), 1.43 - 1.34 (m, 2H), 0.72 (t, *J* = 8.0 Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 183.8, 157.3, 138.2, 106.7, 39.6, 39.2, 19.3, 13.2.

A5-B4: [DMAP][Val]



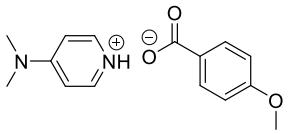
^{1}H NMR (400 MHz, D_2O) δ 7.84 (d, *J* = 7.0 Hz, 2H), 6.63 (d, *J* = 7.0 Hz, 2H), 2.97 (s, 6H), 1.97 (t, *J* = 7.6 Hz, 2H), 1.36 - 1.27 (m, 2H), 1.13 - 1.03 (m, 2H), 0.67 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 174.8, 161.1, 157.0, 138.8, 130.9, 128.8, 113.2, 106.6, 55.3, 39.1.

A5-B5: [DMAP][Ben]



^{1}H NMR (400 MHz,) δ 7.56 (d, *J* = 8.0 Hz, 2H), 7.50 - 7.48 (m, 2H), 7.18 - 7.14 (m, 1H), 7.10 - 7.06 (m, 2H), 6.37 (d, *J* = 8.0 Hz, 2H), 2.76 (s, 6H). ^{13}C NMR (101 MHz, D_2O) δ 175.0, 157.2, 137.9, 135.8, 131.2, 128.8, 128.2, 106.6, 39.1.

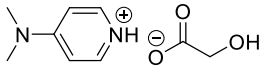
A5-B6: [DMAP][Ani]



^{1}H NMR (400 MHz, D_2O) δ 7.64 (s, 2H), 7.58 (d, *J* = 8.8 Hz, 2H), 6.60 (d, *J* = 8.8 Hz, 2H), 6.33 (d, *J* = 5.6 Hz, 2H), 3.56 (s, 3H), 2.77 (s, 6H). ^{13}C NMR (101 MHz, D_2O) δ

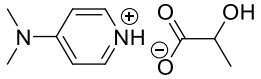
174.8, 161.1, 157.0, 138.8, 130.9, 128.8, 113.2, 106.6, 55.3, 391.

A5-B7: [DMAP][Gly]



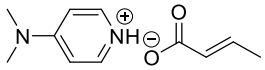
^{1}H NMR (400 MHz, D_2O) δ 7.91 (d, *J* = 8.0 Hz, 2H), 6.78 (d, *J* = 8.0 Hz, 2H), 3.84 (s, 2H), 3.11 (s, 6H). ^{13}C NMR (101 MHz, D_2O) δ 179.8, 157.5, 138.1, 106.7, 61.2, 39.3.

A5-B8: [DMAP][Lac]



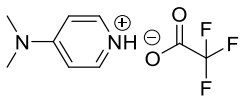
^{1}H NMR (400 MHz, D_2O) δ 7.90 (d, *J* = 6.8 Hz, 2H), 6.76 (d, *J* = 7.0 Hz, 2H), 4.04 (dd, *J* = 6.8, 0.6 Hz, 1H), 3.09 (d, *J* = 0.8 Hz, 6H), 1.23 (dd, *J* = 6.9, 0.7 Hz, 3H). ^{13}C NMR (151 MHz, D_2O) δ 181.8, 157.5, 138.1, 106.7, 68.2, 39.3, 20.0.

A5-B9: [DMAP][Cro]



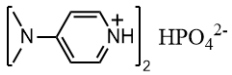
^{1}H NMR (400 MHz, D_2O) δ 7.80 (d, *J* = 7.6 Hz, 2H), 6.59 (d, *J* = 7.6 Hz, 2H), 6.43 (dd, *J* = 15.6, 6.8 Hz, 1H), 5.61 (dd, *J* = 15.6, 1.6 Hz, 1H), 2.95 (s, 6H), 1.58 (dd, *J* = 6.8, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 175.1, 157.4, 142.2, 138.1, 126.4, 106.7, 39.3, 17.0.

A5-B10: [DMAP][TFA]



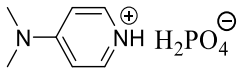
^{1}H NMR (400 MHz, D_2O) δ 7.82 (d, *J* = 8.0 Hz, 2H), 6.62 (d, *J* = 8.0 Hz, 2H), 2.97 (d, *J* = 4.0 Hz, 6H). ^{13}C NMR (151 MHz, D_2O) δ 162.7 (q, J_{C-F} = 40.4 Hz), 157.0, 139.1, 116.4 (q, J_{C-F} = 292.9 Hz), 106.6, 39.1.

A5-B11: [DMAP][HPO_4^{2-}]



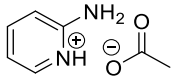
^{1}H NMR (400 MHz, D_2O) δ 7.85 (s, 2H), 6.70 (s, 2H), 3.03 (s, 6H). ^{13}C NMR (151 MHz, D_2O) δ 157.4, 138.1, 106.7, 39.2.

A5-B12: [DMAP][HPO_4^-]



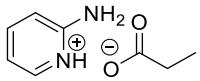
^{1}H NMR (400 MHz, D_2O) δ 7.84 (d, *J* = 8.0 Hz, 4H), 6.66 (d, *J* = 8.0 Hz, 4H), 3.00 (s, 12H). ^{13}C NMR (151 MHz, D_2O) δ 157.3, 138.3, 106.6, 39.2.

A6-B1: [2-AnPy][Ac]



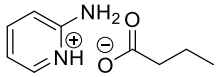
^{1}H NMR (400 MHz, D_2O) δ 7.69 - 7.65 (m, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 6.75 (dt, *J* = 12.0, 4.0 Hz, 1H), 6.71 - 6.67 (m, 1H), 1.78 (s, 3H). ^{13}C NMR (151 MHz, D_2O) δ 181.1, 154.2, 143.6, 136.1, 112.9, 23.1.

A6-B2: [2-AnPy][Pro]



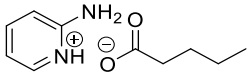
^{1}H NMR (400 MHz, D_2O) δ 7.67 - 7.60 (m, 2H), 6.74 (d, *J* = 12.0 Hz, 1H), 6.68 (t, *J* = 8.0 Hz, 1H), 2.02 (q, *J* = 8.0 Hz, 2H), 0.88 (t, *J* = 8.0 Hz, 3H). ^{13}C NMR (151 MHz, D_2O) δ 184.7, 154.6, 143.3, 137.0, 113.1, 112.8, 30.5, 10.0.

A6-B3: [2-AnPy][But]



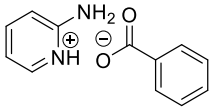
^{1}H NMR (400 MHz, D_2O) δ 7.65 - 7.61 (m, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 6.65 (t, *J* = 8.0 Hz, 1H), 1.96 (t, *J* = 8.0 Hz, 2H), 1.39 - 1.30 (m, 2H), 0.67 (t, *J* = 8.0 Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 183.7, 154.2, 143.7, 136.0, 113.0, 39.3, 19.2, 13.1.

A6-B4: [2-AnPy][Val]



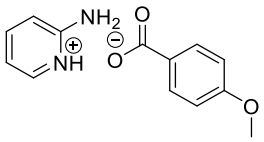
^{1}H NMR (400 MHz, D_2O) δ 7.65 - 7.48 (m, 2H), 6.72 - 6.58 (m, 2H), 1.96 (t, *J* = 7.5 Hz, 2H), 1.32 - 1.22 (m, 2H), 1.09 - 0.98 (m, 2H), 0.61 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 183.5, 153.9, 144.1, 135.3, 113.3, 112.8, 36.8, 27.8, 21.9, 13.1.

A6-B5: [2-AnPy][Ben]



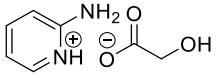
^{1}H NMR (400 MHz, DMSO) δ 8.01 (d, *J* = 4.0 Hz, 2H), 7.93 (d, *J* = 4.4 Hz, 1H), 7.62 (dt, *J* = 8.6, 1.2 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.46 - 7.37 (m, 1H), 6.52 (dd, *J* = 10.3, 3.9 Hz, 2H). ^{13}C NMR (101 MHz, DMSO) δ 168.5, 159.9, 147.3, 137.8, 133.0, 132.0, 129.7, 128.9, 112.2, 108.8.

A6-B6: [2-AnPy][Ani]



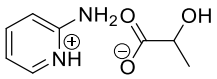
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.8 Hz, 2H), 7.90 (d, *J* = 4.8 Hz, 1H), 7.51 - 7.41 (m, 1H), 6.91 (d, *J* = 7.4 Hz, 2H), 6.64 - 6.57 (m, 1H), 6.55 (d, *J* = 8.5 Hz, 1H), 3.84 (dd, *J* = 4.0, 2.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.1, 162.8, 157.8 142.7, 139.9, 131.7, 125.5, 113.4, 112.6, 110.8, 77.4, 77.1, 76.8, 55.4.

A6-B7: [2-AnPy][Gly]



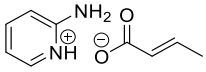
^{1}H NMR (400 MHz, D_2O) δ 7.54 - 7.43 (m, 2H), 6.63 - 6.49 (m, 2H), 3.70 (s, 2H). ^{13}C NMR (101 MHz, D_2O) δ 179.7, 153.8, 144.2, 135.0, 113.4, 112.8, 61.1.

A6-B8: [2-AnPy][Lac]



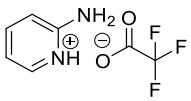
^{1}H NMR (400 MHz, D_2O) δ 7.68 - 7.53 (m, 2H), 6.76 - 6.63 (m, 2H), 3.98 (q, *J* = 6.8 Hz, 1H), 1.15 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 181.8, 153.7, 144.3, 134.8, 113.5, 112.8, 68.1, 19.9.

A6-B9: [2-AnPy][Cro]



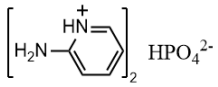
^{1}H NMR (400 MHz, D_2O) δ 7.77 - 7.56 (m, 2H), 6.85 - 6.68 (m, 2H), 6.53 (dq, *J* = 13.6, 6.8 Hz, 1H), 5.68 (d, *J* = 15.6 Hz, 1H), 1.65 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, D_2O) δ 174.9, 153.8, 143.9, 141.7, 135.1, 126.6, 113.2, 112.6, 16.9.

A6-B10: [2-AnPy][TFA]



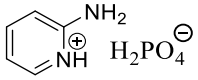
^{1}H NMR (400 MHz, D_2O) δ 7.82 - 7.78 (m, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 6.89 (d, *J* = 12.0 Hz, 1H), 6.79 (t, *J* = 8.0 Hz, 1H). ^{13}C NMR (101 MHz, D_2O) δ 162.9 (q, J_{C-F} = 40.4 Hz), 153.7, 144.5, 134.8, 116.4 (q, J_{C-F} = 292.9 Hz), 113.6, 112.8.

A6-B11: [2-AnPy][HPO_4]



^{1}H NMR (400 MHz, D_2O) δ 7.70 (t, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 6.79 (d, *J* = 8.0 Hz, 1H), 6.70 (t, *J* = 8.0 Hz, 1H). ^{13}C NMR (101 MHz, D_2O) δ 153.6, 144.3, 134.8, 113.5, 112.7.

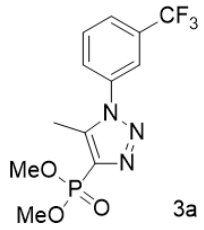
A6-B12: [2-AnPy][$H_2PO_4^-$]



^{1}H NMR (400 MHz, D_2O) δ 7.61 (dd, *J* = 14.2, 6.3 Hz, 4H), 6.67 (dd, *J* = 21.4, 15.0 Hz, 4H). ^{13}C NMR (101 MHz, D_2O) δ 154.4, 143.3, 136.6, 112.9, 112.8.

Characterization of synthesized 1,2,3-triazolyl phosphonates compounds

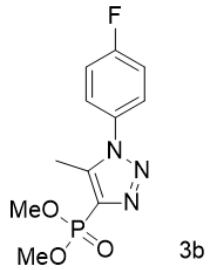
Dimethyl(5-methyl-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3a)



3a

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 1H), 7.80 - 7.76 (m, 2H), 7.71 (d, *J* = 8.0 Hz, 1H), 3.92 (d, *J* = 12.0 Hz, 6H), 2.61 (d, *J* = 4.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.5 (d, J_{C-F} = 23.2 Hz), 135.9, 134.9, 134.1 (d, J_{C-P} = 160.6 Hz), 132.5 (t, J_{C-F} = 23.2 Hz), 128.5, 126.8, 123.1 (q, J_{C-F} = 181.8 Hz), 122.3, 53.5 (d, *J* = 4.04 Hz), 9.6. ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.57. HRMS for $C_{12}H_{13}F_3N_3NaO_3P^+$: calcd. $[M+Na]^+$: 358.0539, found: 358.0538.

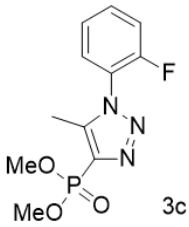
Dimethyl (1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3b)



3b

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (q, *J* = 4.0 Hz, 2H), 7.28 (t, *J* = 8.0 Hz, 2H), 3.91 (d, *J* = 8.0 Hz, 6H), 2.55 (d, *J* = 4.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.3 (d, J_{C-F} = 169.7 Hz), 141.6 (d, J_{C-F} = 169.7 Hz), 133.7 (d, J_{C-P} = 159.6 Hz), 131.5, 127.3 (d, *J* = 7.1 Hz), 116.8 (d, *J* = 15.2 Hz), 53.4 (d, *J* = 4.0 Hz), 9.6. ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.95. HRMS for $C_{11}H_{13}FN_3NaO_3P^+$: calcd. $[M+Na]^+$: 308.0571, found: 308.0570

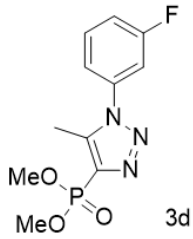
Dimethyl (1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3c)



3c

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (dd, *J* = 12.0, 8.0 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 1H), 7.41 - 7.33 (m, 2H), 3.91 (d, *J* = 12.0 Hz, 6H), 2.49 (t, *J* =4.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.1 (d, J_{C-F} = 254.5 Hz), 143.2 (d, J_{C-F} = 35.4 Hz), 133.4 (d, J_{C-P} = 182.8 Hz), 132.5 (d, *J* = 7.1 Hz), 128.6, 125.3 (d, *J* = 4.0 Hz), 123.2 (d, *J* = 13.1 Hz), 117.0 (d, *J* = 20.2 Hz), 53.4, 8.8. ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.93. HRMS for $C_{11}H_{14}FN_3O_3P^+$: calcd. $[M+H]^+$: 286.0751, found: 286.0751.

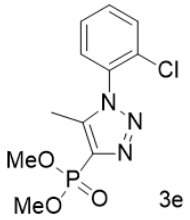
Dimethyl (1-(3-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3d)



3d

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (td, *J* = 16.0, 8.0 Hz, 1H), 7.24 - 7.16 (m, 3H), 3.83 (d, *J* = 12.0 Hz, 6H), 2.51 (d, *J* = 12.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7 (d, J_{C-F} = 250.5 Hz), 141.5 (d, J_{C-F} = 34.3 Hz), 136.5 (d, *J* = 10.1 Hz), 133.8 (d, J_{C-P} = 240.4 Hz), 131.1 (d, *J* = 9.1 Hz), 120.9 (d, *J* = 3.0 Hz), 117.2 (d, *J* = 23.2 Hz), 113.1 (d, *J* = 25.3 Hz), 53.5 (d, *J* = 6.1 Hz), 9.7. ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.84. HRMS for $C_{11}H_{14}FN_3O_3P^+$: calcd. $[M+H]^+$: 286.0751, found: 286.0752.

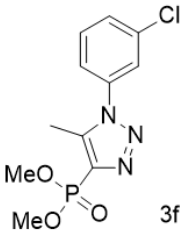
Dimethyl (1-(2-chlorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3e)



3e

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.0 Hz, 1H), 7.60 - 7.49 (m, 2H), 7.45 (d, *J* = 8.0 Hz, 1H), 3.92 (dd, *J* = 12.0, 1.2 Hz, 6H), 2.43 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.3 (d, J_{C-F} = 23.2 Hz), 133.6, 133.0, 132.2, 131.7, 130.7, 129.1, 128.1, 53.4, 8.9. ^{31}P NMR (243 MHz, $CDCl_3$) δ 10.04. HRMS for $C_{11}H_{13}ClN_3NaO_3P^+$: calcd. $[M+Na]^+$: 324.0275, found: 324.0279.

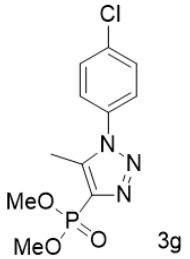
Dimethyl (1-(3-chlorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3f)



3f

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56 - 7.52 (m, 3H), 7.38 (d, *J* = 8.0 Hz, 1H), 3.91 (d, *J* = 4.0 Hz, 6H), 2.59 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.5 (d, *J* = 23.2 Hz), 136.4, 135.5, 133.9 (d, J_{C-P} = 160.6 Hz), 130.8, 130.3, 125.6, 123.4, 53.5 (d, *J* = 4.0 Hz), 9.7. ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.01. HRMS for $C_{11}H_{13}ClN_3NaO_3P^+$: calcd. $[M+Na]^+$: 324.0275, found: 324.0279.

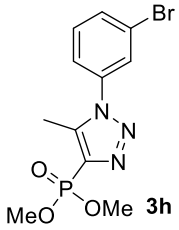
Dimethyl (1-(4-chlorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3g)



3g

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 6.0 Hz, 2H), 7.35 (d, *J* = 6.0 Hz, 2H), 3.83 (d, *J* = 12.0 Hz, 6H), 2.49 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.5 (d, *J* = 23.2 Hz), 136.3, 133.9, 133.9 (d, J_{C-P} = 159.6 Hz), 130.0, 126.5, 53.5 (d, *J* = 3.0 Hz), 9.6. ^{31}P NMR (243 MHz, $CDCl_3$) δ 10.07. HRMS for $C_{11}H_{13}ClN_3NaO_3P^+$: calcd. $[M+Na]^+$: 324.0275, found: 324.0277.

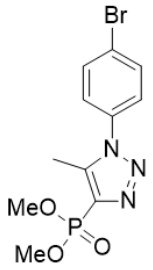
Dimethyl (1-(3-bromophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3h)



3h

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 - 7.67 (m, 2H), 7.50 - 7.42 (m, 2H), 3.90 (d, *J* = 12.0 Hz, 6H), 2.59 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.5 (d, *J* = 23.2 Hz), 136.5, 133.9 (d, J_{C-P} = 159.6 Hz), 133.2, 131.0, 128.4, 123.8, 123.1, 53.5 (d, *J* = 6.1 Hz), 9.6. ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.74. HRMS for $C_{11}H_{13}BrN_3NaO_3P^+$: calcd. $[M+Na]^+$: 367.9770, found: 367.9779.

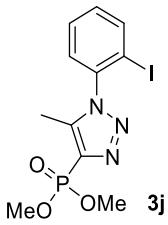
Dimethyl(1-(4-bromophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3i)



3i

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 16.0 Hz, 2H), 3.91 (d, *J* = 12.0 Hz, 6H), 2.57 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.5 (d, *J* = 23.2 Hz), 134.4, 133.9 (d, J_{C-P} = 159.6 Hz), 133.0, 126.7, 124.3, 53.5 (d, J = 3.0 Hz), 9.7. ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.81.HRMS for $C_{11}H_{13}BrN_3NaO_3P^+$: calcd. $[M+Na]^+$: 367.9770, found: 367.9773.

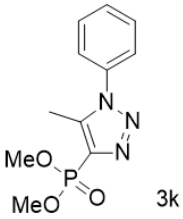
Dimethyl (1-(2-iodophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3j)



3j

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 8.0, 1.2Hz, 1H), 7.58 (td, *J* = 8.0, 1.2 Hz, 1H), 7.39 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.33 (td, *J* = 8.0, 1.6 Hz, 1H), 3.91 (d, *J* = 12.0 Hz, 6H), 2.42 (d, *J* = 1.6 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.8 (d, *J* = 23.2 Hz), 140.2, 138.2, 133.9 (d, J_{C-P} = 159.6 Hz), 132.3, 129.6, 128.5, 96.5, 53.5 (d, *J* = 4.0 Hz), 9.3. ^{31}P NMR (243 MHz, $CDCl_3$) δ 10.09.HRMS for $C_{11}H_{13}IN_3NaO_3P^+$: calcd. $[M+Na]^+$: 415.9631, found: 415.9640.

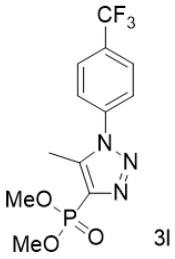
Dimethyl(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)phosphonate (3k)



3k

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (dd, *J* = 4.8 Hz, 5H), 3.91 (d, *J* = 8.0 Hz, 6H), 2.57 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.4 (d, *J* = 23.2 Hz), 135.4, 134.6 (d, J_{C-P} = 159.6 Hz), 130.1, 129.7, 125.3, 53.4 (d, *J* = 4.0 Hz), 9.6. ^{31}P NMR (243 MHz, $CDCl_3$) δ 10.21. HRMS for $C_{11}H_{14}N_3NaO_3P^+$: calcd. $[M+Na]^+$: 290.0665, found: 290.0658.

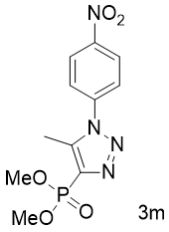
Dimethyl(5-methyl-1-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3l)



3l

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.0 Hz, 1H), 7.79 - 7.74 (m, 2H), 7.69 (d, *J* = 8.0 Hz, 1H), 3.91 (d, *J* = 12.0 Hz, 6H), 2.61 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.6 (d, J_{C-F} = 23.2 Hz), 136.0, 135.0, 133.4, 132.6 (q, J_{C-F} = 22.2 Hz), 127.2 (q, J_{C-F} = 252.5 Hz), 122.4, 53.5 (d, *J* = 4.0 Hz), 9.7. ^{31}P NMR (162 MHz, $CDCl_3$) δ 9.56. HRMS for $C_{12}H_{13}F_3N_3NaO_3P^+$: calcd. $[M+Na]^+$: 358.0539, found: 358.0532.

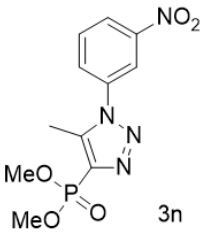
Dimethyl (5-methyl-1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3m)



3m

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 12.0 Hz, 2H), 7.76 (d, *J* = 8.0 Hz, 2H), 3.92 (d, *J* = 8.0 Hz, 6H), 2.67 (d, *J* = 2.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.3, 140.3, 135.5, 133.9, 125.8, 125.2, 53.6, 9.9. ^{31}P NMR (243 MHz, $CDCl_3$) δ 6.84. HRMS for $C_{11}H_{13}N_4NaO_5P^+$: calcd. $[M+Na]^+$: 335.0516, found: 335.0513.

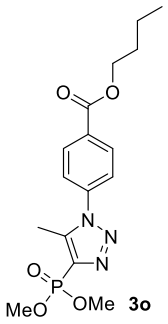
Dimethyl (5-methyl-1-(3-nitrophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3n)



3n

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 - 8.41 (m, 2H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.85 (t, *J* = 8.0 Hz, 1H), 3.92 (d, *J* = 12.0 Hz, 6H), 2.66 (d, *J* = 4.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.8, 136.4, 131.0, 130.9, 124.7, 120.3, 53.6, 9.7. ^{31}P NMR (243 MHz, $CDCl_3$) δ 6.84. HRMS for $C_{11}H_{13}N_4\ NaO_5P^+$: calcd. $[M+Na]^+$: 335.0516, found: 335.0521.

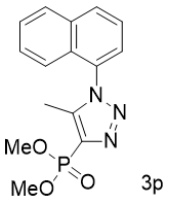
Butyl 4-(4-(dimethoxyphosphoryl)-5-methyl-1H-1,2,3-triazol-1-yl)benzoate (3o)



3o

1H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 12.0 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 4.39 (t, *J* = 8.0 Hz, 2H), 3.91 (d, *J* = 12.0 Hz, 6H), 2.61 (d, *J* = 4.0 Hz, 3H), 1.79 (t, *J* = 8.0 Hz, 2H), 1.53 - 1.50 (m, 2H), 1.00 (t, *J* = 8.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.3, 141.5 (d, *J* = 23.2 Hz), 138.8, 134.1 (d, J_{C-P} = 159.6 Hz), 132.0, 131.0, 125.0, 65.5, 53.5, 30.7, 19.3, 13.7, 9.8. ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.72. HRMS for $C_{16}H_{23}N_3O_5P^+$: calcd. $[M+H]^+$: 368.1370, found: 368.1363.

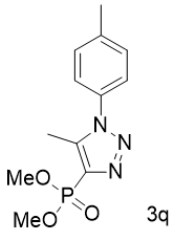
Dimethyl (5-methyl-1-(naphthalen-1-yl)-1H-1,2,3-triazol-4-yl)phosphonate (3p)



3p

^1H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 12.0 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.65 - 7.59 (m, 2H), 7.53 (q, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 1H), 3.97 (d, *J* = 8.0 Hz, 6H), 2.37 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.6, 141.4, 140.0, 135.3, 134.2, 132.6, 130.8, 129.4, 125.9, 122.3, 53.4, 53.4, 21.3, 9.6. ^{31}P NMR (243 MHz, $CDCl_3$) δ 10.30. HRMS for $C_{15}H_{16}N_3NaO_3P^+$: calcd.$[M+Na]^+$: 340.0821, found: 340.0824.

Dimethyl (5-methyl-1-(p-tolyl)-1H-1,2,3-triazol-4-yl)phosphonate (3q)

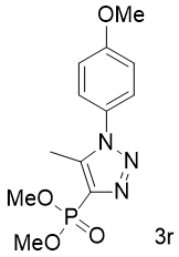


3q

^1H NMR (400 MHz, $CDCl_3$) δ 7.35 (dd, *J* = 20.0, 8.0 Hz, 4H), 3.90 (d, *J* = 12.0 Hz, 6H), 2.55 - 2.46 (m, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.5 (d, *J* = 23.2 Hz), 140.4,

133.3 (d, J = 161.6 Hz), 132.9, 130.2, 125.1, 53.4 (d, *J* = 3.0 Hz), 21.2, 9.6. ^{31}P NMR (243 MHz, $CDCl_3$) δ 10.35. HRMS for $C_{12}H_{16}N_3NaO_3P^+$: calcd. $[M+Na]^+$: 304.0821, found: 304.0816.

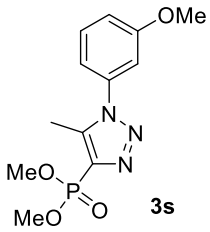
Dimethyl (1-(4-methoxyphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3r)



3r

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 12.0 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 3.92 (s, 3H), 3.89 (d, *J* = 1.6 Hz, 6H), 2.52 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.7, 141.3 (d, *J* = 23.2 Hz), 132.0, 130.2 (d, J_{C-P} = 159.6 Hz), 126.7, 114.8, 55.7, 53.4 (d, *J* = 4.0), 9.56. ^{31}P NMR (243 MHz, $CDCl_3$) δ 10.37 .HRMS for $C_{12}H_{16}N_3NaO_4P^+$: calcd. $[M+Na]^+$: 320.0770, found: 320.0765.

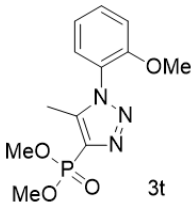
Dimethyl (1-(3-methoxyphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3s)



3s

^{1}H NMR (400 MHz, $CDCl_3$) δ7.47 (t, J = 8.0 Hz, 1H), 7.09 (dd, J = 8.5, 2.4 Hz, 1H), 7.00 (dd, J = 7.3, 5.2 Hz, 2H), 3.92 (s, 3H), 3.89 (s, 3H), 3.87 (s, 3H), 2.57 (d, J = 4.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.5, 141.5 (d, *J* = 23.2 Hz), 136.4, 133.2 (d, J_{C-P} = 159.6 Hz), 130.4, 117.3, 115.9, 111.2, 55.7, 53.5 (d, *J* = 4.1 Hz), 9.7. ^{31}P NMR (243 MHz, $CDCl_3$) δ 10.20. HRMS for $C_{12}H_{16}N_3NaO_4P^+$: calcd.$[M+Na]^+$: 320.0771, found: 320.0763.

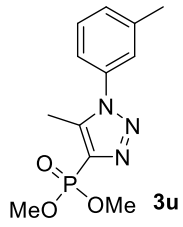
Dimethyl (1-(2-methoxyphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3t)



3t

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 - 7.53 (m, 1H), 7.35 (dd, *J* = 8.0, 4.0 Hz, 1H), 7.11 (q, *J* = 4.0 Hz, 2H), 3.91 (d, *J* =8.0 Hz, 6H), 3.81 (s, 3H), 2.40 (d, *J* = 1.6 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.9, 143.6 (d, *J* = 23.2 Hz), 132.4 (d, J_{C-P} = 161.6 Hz), 132.1, 128.5, 124.0, 121.1, 112.2, 55.8, 53.4, 8.9. ^{31}P NMR (243 MHz, $CDCl_3$) δ 10.76. HRMS for $C_{12}H_{16}N_3NaO_4P^+$: calcd.$[M+Na]^+$: 320.0771, found: 320.0765.

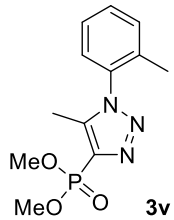
Dimethyl (5-methyl-1-(m-tolyl)-1H-1,2,3-triazol-4-yl)phosphonate (3u)



3u

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (t, *J* = 8.0 Hz, 1H), 7.37 - 7.36 (d, *J* = 4.0Hz,1H), 7.28 (s, 1H), 7.23 – 7.24 (m, 1H), 3.90 (d, *J* = 8.0 Hz, 6H), 2.55(d, *J* = 1.2 Hz, 3H), 2.46 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.5 (d, *J* = 23.2 Hz), 140.1, 135.3, 133.4 (d, J_{C-P} = 160.9 Hz), 130.9, 129.4, 126.0, 122.3, 53.4, 21.3, 9.6. ^{31}P NMR (162 MHz, $CDCl_3$) δ 10.32. HRMS for $C_{12}H_{16}N_3NaO_3P^+$: calcd. $[M+Na]^+$: 304.0821, found: 304.0811.

Dimethyl (5-methyl-1-(o-tolyl)-1H-1,2,3-triazol-4-yl)phosphonate (3v)

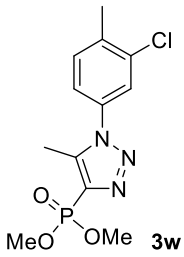


3v

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (t, *J* = 8.0 Hz, 1H), 7.40 (q, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 1H), 3.92 (d, *J* = 12.0 Hz, 6H), 2.38 (d, *J* = 1.6 Hz, 3H), 2.04 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 142.3 (d, J = 23.2 Hz), 135.5, 134.2, 132.8 (d, J_{C-P} = 160.6 Hz), 131.5, 130.8, 127.1, 53.4, 53.4, 17.2, 9.0. ^{31}P NMR (162 MHz, $CDCl_3$) δ 10.32. HRMS for $C_{12}H_{16}N_3NaO_3P^+$: calcd. $[M+Na]^+$: 304.0821, found: 304.0821.

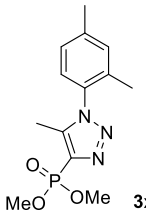
Dimethyl(1-(3-chloro-4-methylphenyl)-5-methyl-1H-1,2,3-triazol-4-yl) phosphonate (3w)



3w

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 2.0 Hz, 1H), 7.45 (d, J = 8.0 Hz, 1H), 7.28 (d, J = 8.0, Hz, 1H), 3.90 (d, J = 12.0 Hz, 6H), 2.57 (d, J = 1.6 Hz, 3H), 2.48 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.5 (d, J = 23.2 Hz), 138.6, 135.3, 134.4 (d, J_{C-P} = 159.6 Hz), 134.0, 131.7, 125.9, 123.3, 53.4 (d, J = 4.0 Hz), 20.0, 9.6. ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.93. HRMS for $C_{12}H_{15}ClN_3NaO_3P^+$: calcd. $[M+Na]^+$: 338.0432, found: 338.0435.

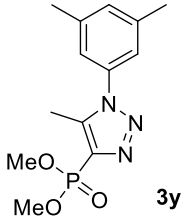
Dimethyl (1-(2,4-dimethylphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3x)



3x

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (s, 1H), 7.05 (s, 2H), 3.90 (d, J = 8.0 Hz, 6H), 2.55 (d, J = 4.0 Hz, 3H), 2.41 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.5 (d, J = 23.2 Hz), 139.7, 135.2, 133.2 (d, J_{C-P} = 159.6 Hz), 131.7, 123.0, 53.4 (d, J = 4.0 Hz), 21.2, 18.4, 9.6. ^{31}P NMR (243 MHz, $CDCl_3$) δ 10.40. HRMS for $C_{13}H_{19}N_3O_3P^+$: calcd. $[M+H]^+$: 296.1158, found: 296.1167.

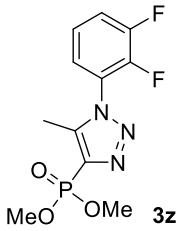
Dimethyl (1-(3,5-dimethylphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3y)



3y

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (s, 1H), 7.05 (s, 2H), 3.90 (d, *J* = 8.0 Hz, 6H), 2.52 (s, 3H), 2.39 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.4 (d, *J* = 6.1 Hz), 139.6 (d, *J* = 3.0 Hz), 135.6, 131.4 (d, *J* = 9.1 Hz), 123.2, 111.1 (d, *J* = 122.1 Hz), 52.2 (d, *J* = 4.0 Hz), 21.2, 11.02. ^{31}P NMR (243 MHz, $CDCl_3$) δ 10.30. HRMS for $C_{13}H_{19}N_3O_3P^+$: calcd. $[M+H]^+$: 296.1158, found: 296.1148.

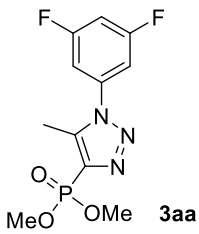
Dimethyl (1-(2,3-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3z)



3z

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 - 7.29 (m, 2H), 7.18 (t, *J* = 6.0 Hz, 1H), 3.83 (d, *J* = 12.0 Hz, 6H), 2.51 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ151.3 (d, J_{C-F} = 169.7 Hz), 150.5 (d, J_{C-F} = 169.7 Hz), 141.5 (d, J_{C-F} = 24.2 Hz), 134.0 (d, J_{C-F} = 155.5 Hz), 131.7, 121.7, 118.4 (d, *J* = 13.1 Hz), 115.4 (d, *J* = 14.1 Hz), 53.5, 9.5. ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.55. HRMS for $C_{11}H_{12}F_2N_3NaO_3P^+$: calcd.$[M+Na]^+$: 326.0477, found: 326.0477.

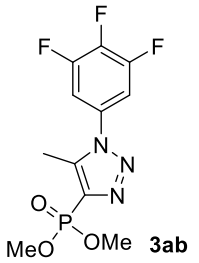
Dimethyl (1-(3,5-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3aa)



3aa

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.03 (d, *J* = 6.0 Hz, 2H), 6.98 (t, *J* = 12.0 Hz, 1H), 3.83 (d, *J* = 12.0 Hz, 6H), 2.55 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.1 (dd, *J* = 159.6, 9.1 Hz), 141.4 (d, *J* = 23.2 Hz), 137.2, 135.4 (d, J_{C-P} = 161.6 Hz), 109.0 (q, *J* = 5.1 Hz), 105.8 (t, *J* = 17.2 Hz),53.5 (d, *J* = 4.0 Hz), 9.7. ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.34. HRMS for $C_{11}H_{12}F_2N_3NaO_3P^+$: calcd. $[M+Na]^+$: 326.0477, found: 326.0476.

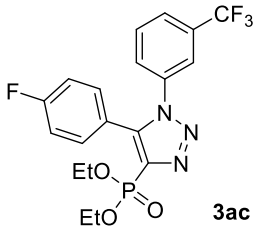
Dimethyl (5-methyl-1-(3,4,5-trifluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ab)



3ab

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 - 7.14 (m, 2H), 3.83 (d, *J* = 12.0 Hz, 6H), 2.53 (d, *J* = 1.6 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.5 (dq, J_{C-F} = 255.5, 5.1 Hz), 141.5 (d, *J* = 35.6 Hz), 141.0 (dt, *J* = 258.6, 15.6 Hz), 134.4 (d, J_{C-P} = 239.4 Hz), 130.6 (td, *J* = 10.1, 5.0 Hz), 110.5 (d, *J* = 25.6 Hz), 53.5 (d, *J* = 6.1 Hz), 9.64. ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.17. HRMS for $C_{11}H_{12}F_3N_3O_3P^+$: calcd.$[M+H]^+$: 322.0563, found: 322.0570.

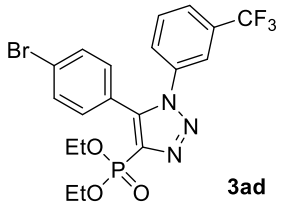
Diethyl(5-(4-fluorophenyl)-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ac)



3ac

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 1H), 7.64 (s, 1H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.36 (q, *J* = 4.0 Hz, 2H), 7.11 (t, *J* = 8.0 Hz, 2H), 4.24 - 4.19 (m, 4H), 1.30 (t, *J* = 8.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.8 (d, *J* = 168.7 Hz), 141.9 (d, *J* = 22.2 Hz), 136.6 (d, J_{C-P} = 160.6 Hz), 136.2, 132.3 (d, *J* = 6.1 Hz), 132.2 (q, *J* = 9.1 Hz), 130.2, 128.2, 127.7 (q, J_{C-F} = 252.5 Hz), 126.3, 122.2, 121.0 (d, *J* = 4.04 Hz), 116.1 (d, *J* = 15.2 Hz), 63.2 (d, *J* = 4.04 Hz), 16.2 (d, *J* = 4.04 Hz). ^{31}P NMR (243 MHz, $CDCl_3$) δ 6.20. HRMS for $C_{19}H_{18}F_4N_3NaO_3P^+$: calcd. $[M+Na]^+$: 466.0914, found: 466.0920.

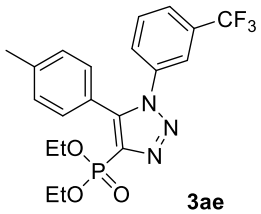
Diethyl(5-(4-bromophenyl)-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ad)



3ad

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 - 7.68 (m, 2H), 7.57 - 7.53 (m, 3H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 2H), 4.26 - 4.16 (m, 4H), 1.30 (t, *J* = 8.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.8 (d, *J* = 20.2 Hz), 136.8 (d, J_{C-P} = 141.4 Hz), 135.9, 132.2 (q, J_{C-F} = 9.1 Hz), 132.1, 131.6, 130.9 (d, *J* = 141.4 Hz), 130.2, 127.7 (q, J_{C-F} = 252.5 Hz), 123.0, 124.6 (d, *J* = 111.1 Hz), 122.4, 122.1, 63.3 (d, *J* = 4.04 Hz), 16.2 (d, *J* = 4.04 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 6.03. HRMS for $C_{19}H_{18}BrF_3N_3NaO_3P^+$: calcd. $[M+Na]^+$: 526.0113, found: 526.0113.

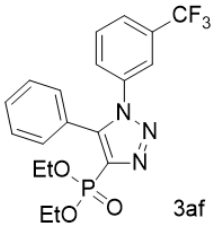
Diethyl(5-(p-tolyl)-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl) phosphonate (3ae)



3ae

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 - 7.66 (m, 2H), 7.52 (t, J = 8.0 Hz, 1H), 7.41 (d, J = 12.0 Hz, 1H), 7.25 – 7.17 (m, 4H),4.19 (q, J = 8.0 Hz, 4H), 2.38 (s, 3H), 1.28 (t, J = 8.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.0 (d, J = 22.2 Hz), 140.7, 137.5 (d, J = 15.6 Hz), 135.3 (d, J_{C-P} = 160.6 Hz), 132.1 (q, J_{C-F} = 22.2 Hz), 130.8 (d, J = 9.1 Hz), 130.0 (d, J = 3.0 Hz), 129.5, 128.2, 124.1 (d, J = 2.0 Hz), 124.1 (q, J_{C-F} = 181.8 Hz), 122.2 (d, J = 2.0 Hz), 63.1 (d, J = 3.0 Hz), 29.7, 21.4, 16.2 (d, J = 5.1 Hz). ^{31}P NMR (243 MHz, $CDCl_3$) δ 6.63. HRMS for $C_{20}H_{21}F_3N_3NaO_3P^+$: calcd. $[M+Na]^+$:462.1164, found: 462.1161.

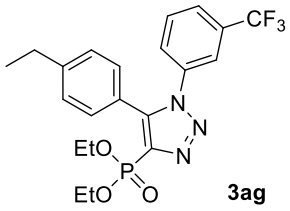
Diethyl(5-phenyl-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl) phosphonate (3af)



3af

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 4.0 Hz, 1H), 7.62 (s, 1H), 7.53 (t, J = 8.0 Hz, 1H), 7.46 - 7.39 (m, 4H), 7.35 (d, J = 8.0 Hz, 2H), 4.19 (q, J = 8.0 Hz, 4H), 1.26 (t, J = 8.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.8 (d, J = 22.0 Hz), 136.5 (d, J_{C-P} = 160.6 Hz), 136.3, 132.2, 132.0 (q, J_{C-F} = 23.2 Hz), 130.4, 130.1, 128.8, 128.1, 126.1 (d, J = 2.0 Hz), 125.1, 122.8 (q, J_{C-F} = 116.2 Hz), 122.1 (d, J = 3.0 Hz), 63.1 (d, J = 4.0 Hz), 16.1 (d, J = 5.0 Hz). ^{31}P NMR (243 MHz, $CDCl_3$) δ 6.46. HRMS for $C_{19}H_{20}F_3N_3O_3P^+$: calcd. $[M+H]^+$: 426.1188, found: 426.1186.

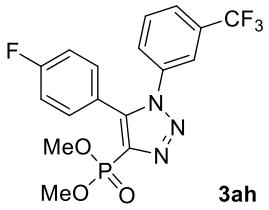
Diethyl(5-(4-ethylphenyl)-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ag)



3ag

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.0 Hz, 1H), 7.52 (s, 1H), 7.45 (t, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.17 - 7.14 (m, 4H), 4.17 - 4.07 (m, 4H), 2.60 (q, *J* = 8.0 Hz, 2H), 1.21 - 1.14 (m, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.9, 141.0, 135.6 (d, J_{C-P} = 160.6 Hz), 135.4, 133.9 (q, J_{C-F} = 22.2 Hz), 131.0 (d, *J* = 19.2 Hz), 130.9, 128.0, 127.2 (d, *J* = 17.0 Hz), 124.4 (q, J_{C-P} = 181.8 Hz), 123.1 (d, *J* = 2.0 Hz), 121.7, 62.1 (d, *J* = 4.0 Hz), 30.0, 21.7, 15.1 (d, *J* = 4.0 Hz), 14.2. ^{31}P NMR (162 MHz, $CDCl_3$) δ 6.66. HRMS for $C_{21}H_{24}F_3N_3O_3P^+$: calcd. $[M+H]^+$: 454.1501, found: 454.1491.

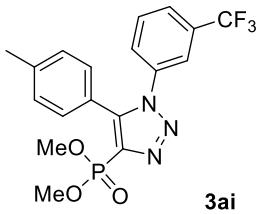
Dimethyl(5-(4-fluorophenyl)-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ah)



3ah

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.0 Hz, 1H), 7.64 (s, 1H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.36 (dd, *J* = 24.0, 8.0 Hz, 2H), 7.14 - 7.09 (m, 2H), 3.84 (d, *J* = 12.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.8 (d, *J* = 168.7 Hz), 142.3 (d, *J* = 23.2 Hz)， 136.1, 135.6 (d, J_{C-P} = 159.6 Hz), 134.8, 132.4, 132.2 (d, *J* = 5.1 Hz), 130.2, 128.2, 126.4 (q, *J* = 3.0 Hz), 123.0 (q, J_{C-F} = 181.8 Hz), 122.3, 120.8 (d, *J* = 2.0 Hz), 53.6 (d, *J* = 4.0 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 8.82. HRMS for $C_{17}H_{14}F_4N_3NaO_3P^+$: calcd. $[M+Na]^+$: 438.0631, found: 438.0637.

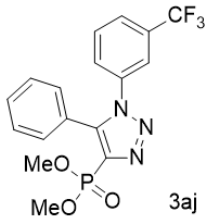
Dimethyl(5-(p-tolyl)-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ai)



3ai

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 - 7.65 (m, 2H), 7.53 (t, *J* = 8.0 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.28 - 7.19 (m, 4H), 3.82 (d, *J* = 8.0 Hz, 6H), 2.38 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.4 (d, *J* = 23.2 Hz), 140.8, 136.4, 135.3 (d, J_{C-P} = 160.6 Hz), 132.2 (q, J_{C-F} = 22.2 Hz), 130.0, 129.9, 129.6, 128.2, 126.2 (d, *J* = 2.0 Hz), 123.1 (q, J_{C-F} = 181.8 Hz), 122.2 (d, *J* = 2.0 Hz), 121.7, 53.6 (d, *J* = 4.0 Hz), 21.4. ^{31}P NMR (162 MHz, $CDCl_3$) δ 9.29. HRMS for $C_{18}H_{17}F_3N_3NaO_3P^+$: calcd. $[M+Na]^+$: 434.0851, found: 434.0851.

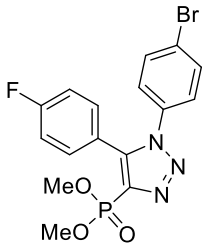
Dimethyl(5-phenyl-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3aj)



3aj

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 1H), 7.62 (s, 1H), 7.53 (t, *J* = 8.0 Hz, 1H), 7.47 - 7.45 (m, 4H), 7.39 (m, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 3.82 (d, *J* = 12.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.4 (d, *J* = 23.2 Hz), 140.8, 136.4, 135.3 (d, J_{C-P} = 160.6 Hz), 132.2 (q, J_{C-F} = 22.2 Hz), 130.0, 129.9, 129.6, 128.2, 126.2 (q, *J* = 2.0 Hz), 123.1 (q, J_{C-F} = 181.8 Hz), 122.2 (d, *J* = 2.0 Hz), 121.7, 53.6 (d, *J* = 4.0 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 9.09. HRMS for $C_{17}H_{15}F_3N_3NaO_3P^+$: calcd. $[M+Na]^+$: 420.0695, found: 420.0695.

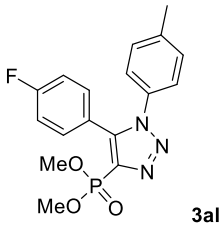
Dimethyl(1-(4-bromophenyl)-5-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ak)



3ak

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.0 Hz, 2H), 7.35 (q, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.11 (t, *J* = 8.0 Hz, 2H), 3.83 (d, *J* = 12.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.7 (d, J_{C-F} = 168.7 Hz), 142.0 (d, *J* = 22.2 Hz)， 135.4 (d, J_{C-P} = 161.6 Hz), 134.6, 132.8, 132.2, 132.2, 126.6, 123.9, 116.1 (d, *J* = 15.2 Hz), 53.6 (d, *J* = 4.0 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 9.11. HRMS for $C_{16}H_{14}BrFN_3NaO_3P^+$: calcd. $[M+Na]^+$: 447.9832, found: 447.9840.

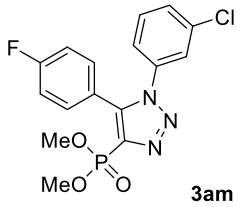
Dimethyl (5-(4-fluorophenyl)-1-(p-tolyl)-1H-1,2,3-triazol-4-yl)phosphonate (3al)



3al

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (q, *J* = 4.0 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 7.07 (t, *J* = 8.0 Hz, 2H), 3.83 (d, *J* = 12.0 Hz, 6H), 2.39 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.6 (d, J_{C-F} = 167.7 Hz), 142.1 (d, *J* = 20.2 Hz), 140.0, 132.7 (d, J_{C-P} = 87.8 Hz), 132.2, 132.1, 130.1, 125.1, 121.4, 115.9 (d, *J* = 14.2 Hz), 53.6, 21.2. ^{31}P NMR (162 MHz, $CDCl_3$) δ 9.64. HRMS for $C_{17}H_{17}FN_3NaO_3P^+$: calcd. $[M+Na]^+$: 384.0883, found: 384.0883.

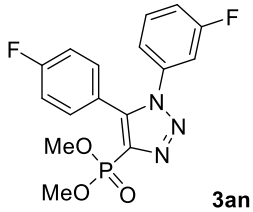
Dimethyl(1-(3-chlorophenyl)-5-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3am)



3am

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36 (d, *J* = 12.0 Hz, 2H), 7.30 - 7.25 (m, 3H), 7.03 (dd, *J* = 18.0, 6.0 Hz, 3H), 3.76 (d, *J* = 12.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.8 (d, J_{C-F} = 168.7 Hz), 136.3 (d, *J* = 22.2 Hz), 136.4 (d, *J* = 37.4 Hz), 135.0 (d, J_{C-P} = 78.8 Hz), 135.0, 132.2, (d, *J* = 6.06 Hz), 130.6, 130.4, 125.6, 123.3, 120.9 (d, J_{C-F} = 2.0 Hz), 116.1 (d, *J* = 15.6 Hz), 53.6 (d, *J* = 4.0 Hz). ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.06. HRMS for $C_{16}H_{14}ClFN_3NaO_3P^+$: calcd. $[M+Na]^+$: 404.0337, found: 404.0331.

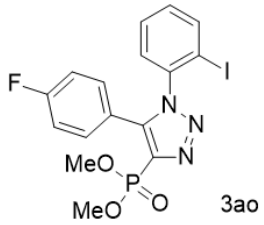
Dimethyl(1-(3-fluorophenyl)-5-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3an)



3an

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 - 7.32 (m, 5H), 7.11 (t, *J* = 8.0 Hz, 3H), 3.84 (d, *J* = 12.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.7 (d, J_{C-F} = 168.7 Hz), 142.2 (d, *J* = 22.2 Hz), 136.5, 135.3 (d, J_{C-P} = 160.6 Hz), 135.3, 132.2, 130.5, 130.2 (d, *J* = 50.5 Hz), 125.6, 123.3, 120.9 (d, *J* = 2.0 Hz), 116.1 (d, *J* = 15.2 Hz), 53.6 (d, *J* = 4.0 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 9.27. HRMS for $C_{16}H_{14}F_2N_3NaO_3P^+$: calcd. $[M+Na]^+$: 388.0633, found: 388.0633.

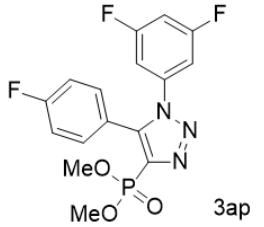
Dimethyl(5-(4-fluorophenyl)-1-(2-iodophenyl)-1H-1,2,3-triazol-4-yl)phosphonate(3ao)



3ao

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.39 (t, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.22 (t, *J* = 8.0 Hz, 1H), 7.02 (t, *J* = 8.0 Hz, 2H), 3.86 (d, *J* = 12.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.6 (d, J_{C-F} = 168.7 Hz), 143.4 (d, *J* = 22.2 Hz), 140.2, 138.4, 135.3 (d, J_{C-P} = 160.6 Hz), 132.2 (d, *J* = 21.2 Hz), 129.1 (d, J = 21.2 Hz), 121.8, 120.7 (d, *J* = 2.0 Hz), 115.7 (d, *J* = 15.6 Hz), 100.4, 96.7, 53.6 (d, *J* = 4.0 Hz). ^{31}P NMR (243 MHz, $CDCl_3$) δ 9.06. HRMS for $C_{16}H_{14}FIN_3NaO_3P^+$: calcd. $[M+Na]^+$: 495.9693, found: 495.9693.

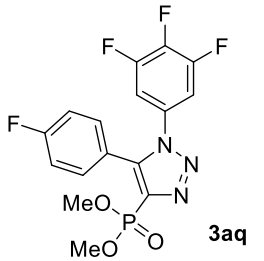
Dimethyl(1-(3,5-difluorophenyl)-5-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ap)



3ap

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (t, *J* = 4.0 Hz, 2H), 7.15 (t, *J* = 4.0 Hz, 2H), 6.93 (t, *J* = 8.0 Hz, 1H), 6.87 (d, *J* =4.0 Hz, 2H), 3.83 (d, *J* = 8.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.9 (d, J_{C-F} = 161.6 Hz), 162.9 (d, *J* = 151.5 Hz), 142.2 (d, *J* = 22.2 Hz), 136.6, 136.2 (d, J_{C-P} = 233.3 Hz), 132.1 (d, *J* = 6.1 Hz), 120.6 (d, *J* = 3.0 Hz), 116.4 (d, *J* = 15.6 Hz), 109.0 (d, *J* = 15.2 Hz), 105.5 (d, *J* = 33.3 Hz), 53.6 (d, *J* = 4.0 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 8.64. HRMS for $C_{16}H_{13}F_3N_3NaO_3P^+$: calcd. $[M+Na]^+$: 406.0538, found: 406.0528.

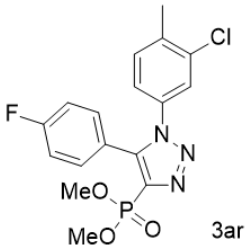
Dimethyl(5-(4-fluorophenyl)-1-(3,4,5-trifluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3aq)



3aq

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (q, *J* = 4.0 Hz, 2H), 7.16 (t, *J* = 8.0 Hz, 2H), 7.00 (t, *J* = 8.0 Hz, 2H), 3.83 (d, *J* = 12.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.0 (d, J_{C-F} = 169.7 Hz), 152.1, 150.3, 142.4, 142.4, 135.9 (d, J_{C-P} = 163.6 Hz), 132.1 (d, *J* = 6.1 Hz), 120.4 (d, *J* = 2.0 Hz), 116.5 (d, *J* = 15.2 Hz), 110.4 (d, *J* = 17.2 Hz), 53.6 (d, *J* = 4.0 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 8.45. HRMS for $C_{16}H_{12}F_4N_3NaO_3P^+$: calcd. $[M+Na]^+$: 424.0446, found: 424.0439.

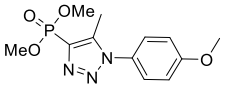
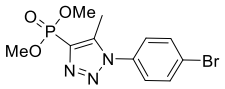
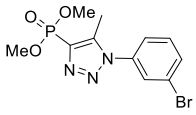
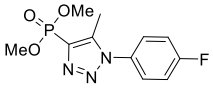
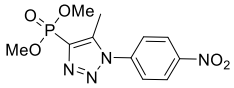
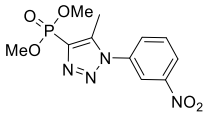
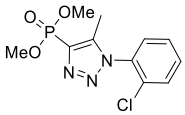
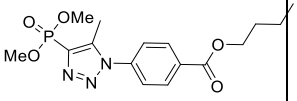
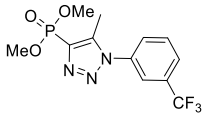
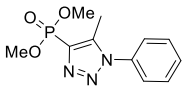
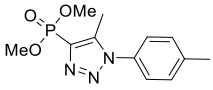
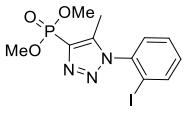
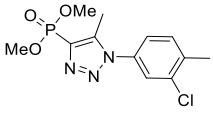
Dimethyl(1-(3-chloro-4-methylphenyl)-5-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ar)

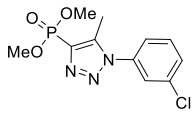
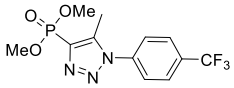
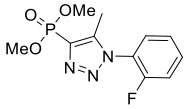
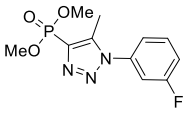
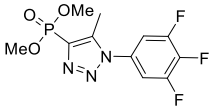
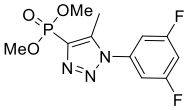
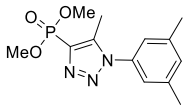
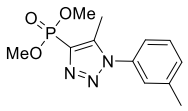
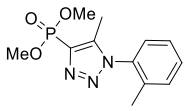
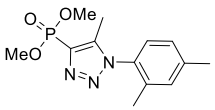
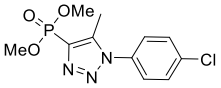
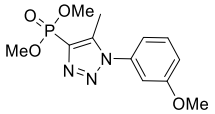
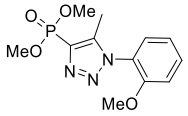


3ar

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 - 7.35 (m, 3H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.10 (t, *J* = 8.0 Hz, 2H), 6.98 (d, *J* = 12.0 Hz, 1H), 3.83 (d, *J* = 8.0 Hz, 6H), 2.41 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.7 (d, J_{C-F} = 168.7 Hz), 142.3, 138.2, 135.2 (d, J_{C-P} = 159.6 Hz), 135.2, 134.2, 132.2 (d, *J* = 6.1 Hz), 131.5, 125.8, 123.2, 121.0 (d, *J* = 2.0 Hz), 116.1 (d, *J* = 15.6 Hz), 53.6 (d, *J* = 4.0 Hz), 19.9. ^{31}P NMR (162 MHz, $CDCl_3$) δ 9.21. HRMS for $C_{17}H_{16}ClFN_3NaO_3P^+$: calcd. $[M+Na]^+$: 418.0494, found: 418.0493.

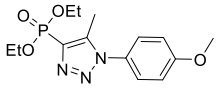
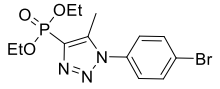
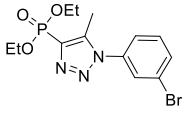
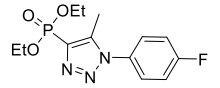
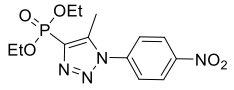
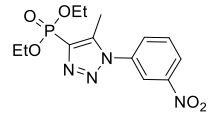
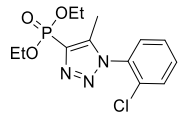
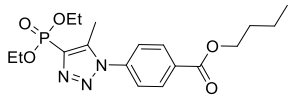
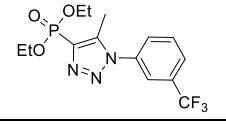
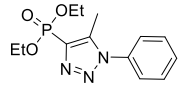
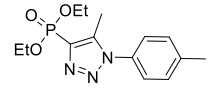
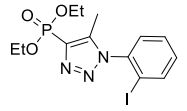
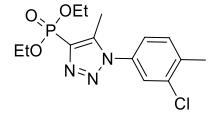
Table S3 GC/MS data of compound A1-B1 to A1-B26.[a]

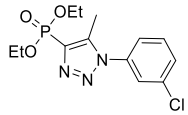
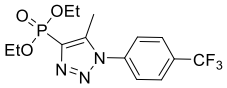
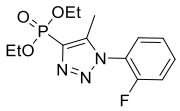
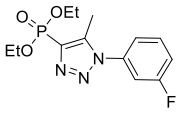
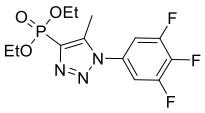
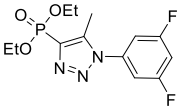
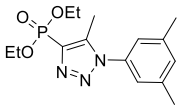
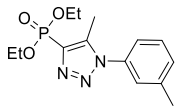
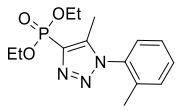
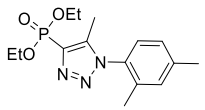
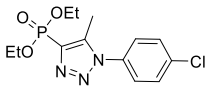
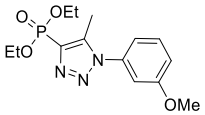
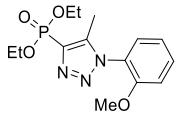
Code	Chemical structure	RT (min)	MW	Results of MS
A1-B1		9.4	297.2	297.2(M), 296.2(M-1), 269.3(M-28), 254.2, 222.1, 160.2, 159.2, 134.2, 109.1, 77.1
A1-B2		9.5	346.1	346.1(M), 345.2(M-1), 318.2(M-28), 210.0, 209.1, 208.1, 157.0, 155.0, 109.1, 93.0, 76.1, 75.0
A1-B3		9.4	346.1	346.1(M), 345.2(M-1), 318.2(M-28), 224.1, 210.1, 209.1, 208.1, 157.0, 155.0, 154.0
A1-B4		8.1	285.2	285.2(M), 284.7(M-1), 283.9, 257.2(M-28), 162.1, 148.1, 147.2, 147.1, 122.1, 106.1, 105.1
A1-B5		10.4	312.2	312.2(M), 311.2(M-1), 310.6, 284.3(M-28), 273.1, 175.1, 162.1, 135.1, 110.1, 109.1, 93.1
A1-B6		10.0	312.2	312.2(M), 311.1(M-1), 284.2(M-28), 175.1, 174.1, 173.1, 162.1, 135.1, 130.1, 129.1
A1-B7		8.7	301.7	301.6(M), 300.1(M-1), 299.8, 273.3(M-28), 178.1, 164.1, 163.1, 162.1, 110.1, 93.1
A1-B8		12.6	367.3	367.3(M), 366.1(M-1), 365.5, 339.4(M-28), 238.1, 230.2, 188.1, 174.1, 93.1, 86.5
A1-B9		7.8	335.22	335.3(M), 334.3(M-1), 333.3, 307.3(M-28), 212.2, 199.1, 198.1, 197.1, 196.1, 145.1
A1-B10		8.3	267.2	267.2(M), 266.1(M-1), 264.8, 239.5(M-28), 207.1, 185.1, 144.2, 131.1, 130.1
A1-B11		8.7	281.3	281.2(M), 280.2(M-1), 280.1, 253.2(M-28), 158.2, 145.2, 144.2, 143.2, 142.1, 118.1
A1-B12		9.6	393.1	393.1(M), 365.0(M-28), 220.2, 205.2, 177.2, 145.2, 105.0, 91.2, 80.9, 57.1
A1-B13		8.7	315.7	315.6(M), 314.2(M-1), 313.9, 287.2(M-28), 180.1, 179.1, 178.1, 177.1, 125.1, 123.1

A1-B14		8.9	301.7	301.6(M), 300.3(M-1), 300.1, 273.3(M-28), 166.1, 165.1, 164.1, 135.1, 111.1, 106.1
A1-B15		8.0	335.2	335.2(M), 334.2(M-1), 307.2(M-28), 333.5, 212.1, 199.1, 198.1, 197.1, 93.0
A1-B16		8.0	285.2	285.2(M), 284.6(M-1), 284.1, 257.1(M-28), 162.1, 148.1, 147.1, 135.1, 122.1, 95.1
A1-B17		8.0	285.2	285.2(M), 284.2(M-1), 283.4, 254.9(M-28), 162.1, 148.1, 147.1, 135.1, 110.1, 109.1, 95.1
A1-B18		7.7	321.2	321.2(M), 293.1(M-28), 198.1, 184.1, 162.1, 157.1, 135.1, 131.1
A1-B19		7.7	303.2	303.2(M), 302.1(M-1), 275.1(M-28), 180.1, 167.1, 166.1, 135.1, 113.1
A1-B20		9.0	295.3	295.2(M), 294.2(M-1), 267.1(M-28), 266.2, 172.2, 158.2, 157.2, 105.1
A1-B21		8.6	281.3	281.2(M), 280.1(M-1), 253.2(M-28), 255.3, 158.1, 145.2, 144.2, 143.2, 91.1, 65.1
A1-B22		8.6	281.3	281.1(M), 280.1(M-1), 253.3(M-28), 220.1, 158.2, 157.2, 156.1, 132.1, 77.1
A1-B23		8.6	295.3	295.2(M), 294.1(M-1), 267.3(M-28), 281.9, 220.1, 158.2, 157.2, 156.1, 132.1, 77.1
A1-B24		9.0	301.7	301.6(M), 300.2(M-1), 273.2(M-28), 299.9, 272.1, 178.1, 166.1, 165.1, 164.1, 111.1
A1-B25		9.2	297.3	297.2(M), 296.2(M-1), 269.2(M-28), 295.8, 268.1, 254.1, 161.1, 160.1, 158.1, 77.1
A1-B26		8.6	297.3	297.0(M), 296.2(M-1), 269.2(M-28), 252.1, 158.2, 144.1, 143.1, 93.1, 91.1, 65.1

[a] The purity of the triazolyl phosphonate compounds were > 96%.

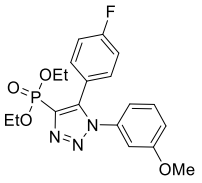
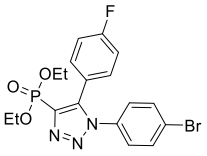
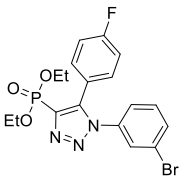
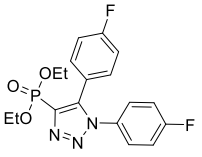
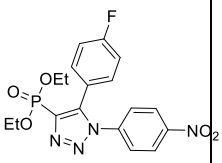
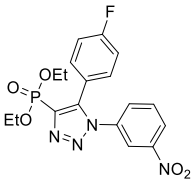
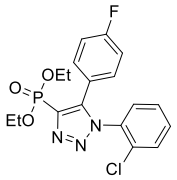
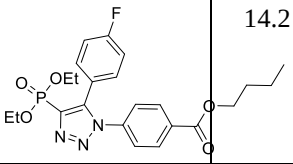
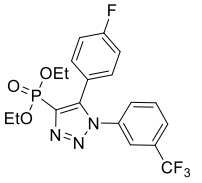
Table S4 GC/MS data of compound A2-B1 to A2-B26.[a]

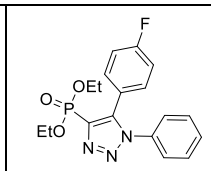
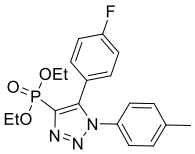
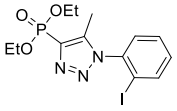
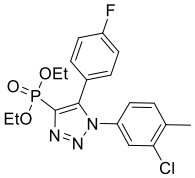
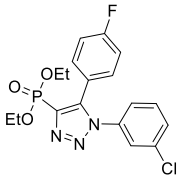
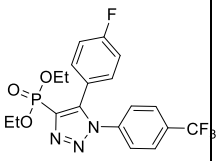
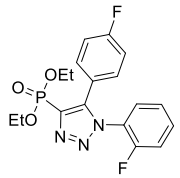
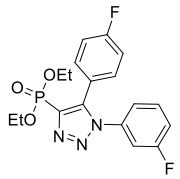
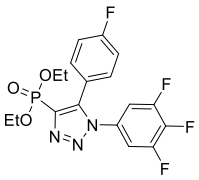
Code	Chemical structure	RT (min)	MW	Results of MS
A2-B1		9.9	325.3	325.1(M), 324.2(M-1), 297.2(M-28), 161.2, 160.1, 159.2, 159.1, 134.1, 92.1
A2-B2		10.0	374.2	374.1(M), 373.1(M-1), 346.1(M-28), 272.0, 210.1, 209.1, 208.1, 157.0, 136.1
A2-B3		9.8	374.2	374.1(M), 373.2(M-1), 346.2(M-28), 211.1, 210.1, 209.1, 208.1, 196.0, 157.0
A2-B4		8.4	313.3	313.2(M), 312.5(M-1), 285.1(M-28), 312.0, 149.1, 148.1, 147.1, 136.1, 122.1, 95.1
A2-B5		10.9	340.3	340.1(M), 339.1(M-1), 312.3(M-28), 256.1, 239.1, 176.1, 175.1, 136.1, 129.1
A2-B6		10.6	340.3	340.1(M), 339.1(M-1), 312.3(M-28), 266.1, 176.1, 175.1, 163.1, 136.1, 76.1
A2-B7		9.0	329.7	329.1(M), 328.1(M-1), 301.6(M-28), 166.1, 165.1, 164.1, 152.1, 121.1, 111.1, 75.1
A2-B8		13.7	395.4	395.4(M), 394.1(M-1), 367.3(M-28), 381.3, 231.2, 230.2, 174.1, 136.1, 121.1
A2-B9		8.1	363.3	363.0(M), 362.2(M-1), 335(M-28), 260.1, 199.1, 198.1, 186.1, 145.1, 136.1
A2-B10		8.6	295.3	295.2(M), 294.5(M-1), 267.2(M-28), 293.9, 131.1, 130.1, 118.1, 77.1
A2-B11		9.1	308.3	308.2(M), 307.4(M-1), 280.1(M-28), 208.2, 145.2, 144.1, 143.2, 118.1, 91.1, 65.1
A2-B12		10.1	421.2	421.1(M), 420.4(M-1), 393.2(M-28), 419.3, 473.1, 399.0, 256.0, 200.1, 172.1, 109.1, 107.1, 76.1
A2-B13		9.9	343.8	343.7(M), 342.5(M-1), 315.0(M-28), 181.1, 180.1, 179.1, 178.1, 166.1, 125.1, 89.1

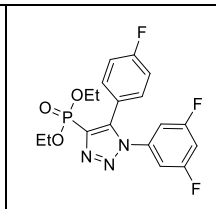
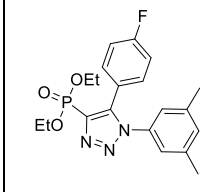
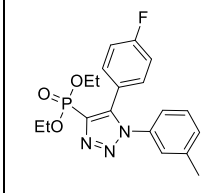
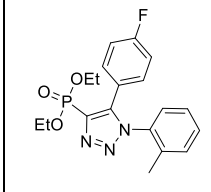
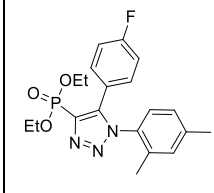
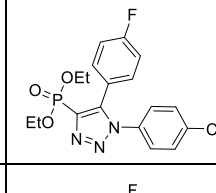
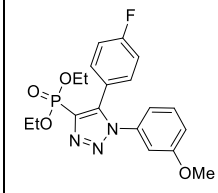
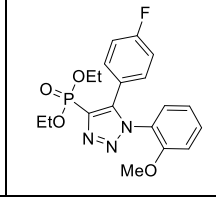
A2-B14		9.2	329.7	329.1(M), 328.4(M-1), 301.3(M-28), 326.0, 301.1, 281.1, 207.1, 165.1, 164.1
A2-B15		8.2	363.3	363.0(M), 362.7(M-1), 335.6(M-28), 361.9, 279.1, 199.1, 198.1, 186.1, 145.1, 121.1
A2-B16		8.4	313.3	313.2(M), 312.5(M-1), 285.2(M-28), 299.1, 149.1, 148.1, 147.1, 136.1121.1, 95.1
A2-B17		8.3	313.3	313.2(M), 312.6(M-1), 285.3(M-28), 312.1, 229.1, 149.1, 148.1, 136.1, 121.1, 95.1
A2-B18		8.0	349.3	349.2(M), 348.1(M-1), 321.1(M-28), 347.4, 265.1, 85.1, 184.1, 172.1, 131.1
A2-B19		8.0	331.3	331.2(M), 330.6(M-1), 303.2(M-28), 329.7, 247.1, 167.1, 154.1, 121.1, 113.1
A2-B20		9.4	323.3	323.3(M), 322.2(M-1), 295.3(M-28), 159.2, 158.2, 105.1, 77.1,
A2-B21		9.0	309.3	309.3(M), 308.4(M-1), 281.3(M-28), 307.5, 145.1, 144.1, 143.1, 91.1, 66.1, 65.1,
A2-B22		8.5	309.3	309.3(M), 308.7(M-1), 281.4(M-28), 308.2, 145.2, 144.2, 1423.2, 142.2, 91.1
A2-B23		15.9	323.3	323.5(M), 322.7(M-1), 295.3(M-28), 295.3, 158.2, 156.2, 144.1, 132.3, 121.2, 103.1
A2-B24		9.4	329.7	329.1(M), 328.1(M-1), 301.3(M-28), 165.1, 164.1, 163.1, 136.1, 111.1, 92.1, 75.7
A2-B25		9.6	325.3	325.1(M), 324.2(M-1), 297.2(M-28), 161.1, 160.1, 134.1, 107.1, 92.1, 77.1
A2-B26		9.6	325.3	325.3(M), 324.8(M-1), 297.3(M-28), 282.1, 160.1, 146.1, 134.1, 120.1, 92.1, 77.1

[a] The purity of the triazolyl phosphonate compounds were > 96%.

Table S5 GC/MS data of compound A3-B1 to A3-B26.[a]

Code	Chemical structure	RT (min)	MW	Results of MS
A3-B1		12.5	405.4	405.3(M), 404.3(M-1), 377.2(M-28), 303.1, 200.1, 172.1, 160.2, 134.1, 123.1,
A3-B2		12.7	454.2	454.1(M), 453.4(M-1), 426.1(M-28), 353.0, 208.1, 200.1, 172.1, 107.1, 108.1, 76.1, 65.0
A3-B3		12.3	454.2	454.1(M), 453.2(M-1), 426.1(M-28), 353.0, 208.1, 200.1, 172.1, 123.1, 107.1, 76.1
A3-B4		10.0	393.3	393.3(M), 392.1(M-1), 365.2(M-28), 291.1, 229.1, 200.1, 172.1, 123.1, 107.1, 95.1
A3-B5		10.0	420.3	420.2(M), 419.2(M-1), 392.3(M-28), 317.1, 230.2, 200.1, 172.1, 107.0, 65.0
A3-B6		11.1	420.3	420.2(M), 419.3(M-1), 381.1, 307.1, 245.1, 200.1, 123.1, 107.1, 75.1, 65.1
A3-B7		13.7	409.8	409.7(M), 408.4(M-1), 407.3, 392.2, 318.1, 209.1, 200.1, 172.1, 123.1, 107.1, 76.1
A3-B8		14.2	475.5	475.1(M), 474.1(M-1), 447.1(M-28), 392.2, 364.2, 336.1, 318.1, 256.1, 208.1, 200.1, 192.1, 123.1
A3-B9		9.4	443.3	443.3(M), 442.1(M-1), 415.2(M-28), 430.4, 415.2, 387.1, 389.1, 279.1, 200.1, 172.1, 123.1, 107.1

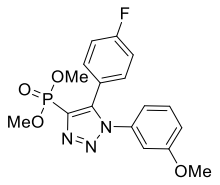
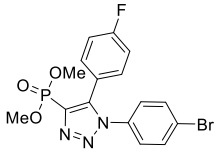
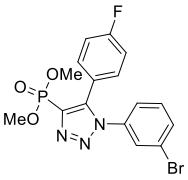
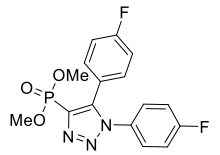
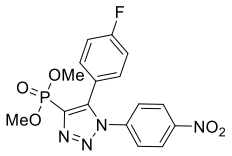
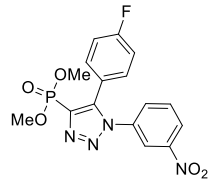
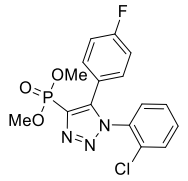
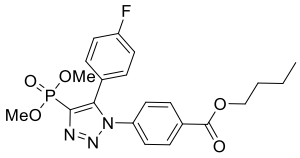
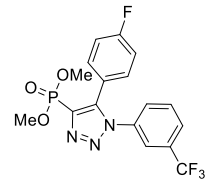
A3-B10		10.3	375.3	375.2(M), 374.1(M-1), 347.1(M-28), 291.1, 273.0, 200.1, 123.1, 107.1, 77.1, 65.0
A3-B11		11.1	389.4	389.2(M), 388.9(M-1), 347.4(M-28), 361.2, 305.1, 287.1, 200.1, 172.1, 123.1, 107.1
A3-B12		13.1	501.2	501.1(M), 500.1(M-1), 473.1(M-28), 399.0, 256.0, 200.1, 172.1, 107.1, 76.1, 65.0
A3-B13		12.4	423.8	423.1(M), 422.0(M-1), 395.2(M-28), 321.1, 200.1, 172.1, 123.1, 107.0
A3-B14		11.3	409.8	409.2(M), 408.1(M-1), 381.2(M-28), 381.2, 339.1, 321.1, 207.1, 200.1, 172.1, 107.1
A3-B15		9.5	443.3	443.3(M), 442.1(M-1), 415.2(M-28), 341.1, 200.1, 172.1, 123.1, 107.1
A3-B16		10.0	393.3	393.1(M), 392.1(M-1), 365.2(M-28), 291.1, 200.1, 172.1, 107.1, 95.1
A3-B17		9.9	393.3	393.3(M), 392.1(M-1), 365.2(M-28), 385.2, 309.1, 291.1, 200.1, 172.1, 123.1, 107.1
A3-B18		9.2	429.3	429.2(M), 428.0(M-1), 401.5(M-28), 327.1, 265.1, 200.1, 172.1, 107.1, 81.0, 65.0

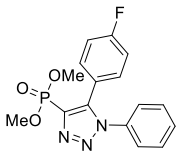
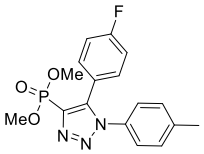
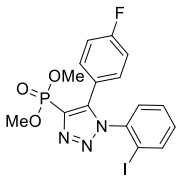
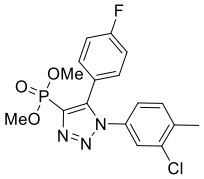
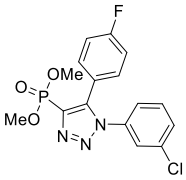
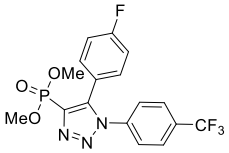
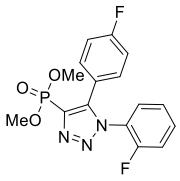
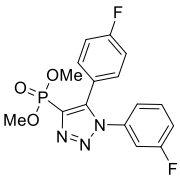
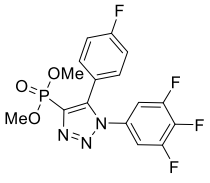
A3-B19		9.3	411.3	411.1(M), 410.1(M-1), 383.2(M-28), 309.1, 247.1, 200.1, 172.1, 107.1
A3-B20		11.3	403.4	403.4(M), 402.4(M-1), 375.2(M-28), 301.1, 239.2, 200.1, 172.0, 132.1, 107.1
A3-B21		10.8	389.4	389.1(M), 388.1(M-1), 361.2(M-28), 305.1, 287.1, 255.2, 200.1, 172.0, 107.1, 65.1
A3-B22		10.3	389.4	389.3(M), 388.2(M-1), 361.2(M-28), 304.1, 222.1, 172.0, 144.1, 123.1, 91.1
A3-B23		10.9	403.4	403.0(M), 402.2(M-1), 375.2(M-28), 318.1, 238.2.200.1, 172.0, 158.2, 123.1
A3-B24		11.6	409.8	409.7(M), 408.2(M-1), 381.1(M-28), 307.1, 245.1, 200.1, 172.0, 107.0, 75.1
A3-B25		11.9	405.4	405.3(M), 404.2(M-1), 377.2(M-28), 321.1, 303.1, 200.1, 172.1, 107.1, 77.1
A3-B26		11.3	405.4	404.3(M-1), 377.2(M-28), 303.1, 225.1, 200.1, 172.1, 160.1, 123.1, 109.1

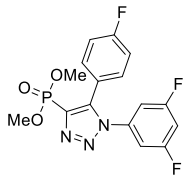
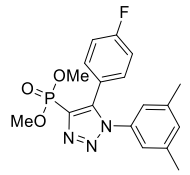
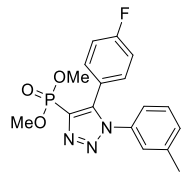
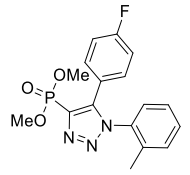
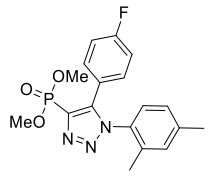
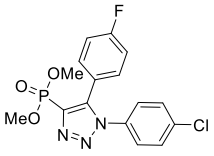
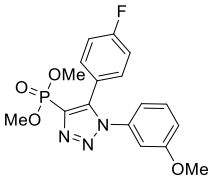
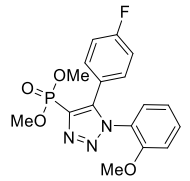
[a] The purity of the triazolyl phosphonate compounds were > 96%.

Table S6 GC/MS data of compound A4-B1 to A4-B26.[a]

Code	Chemical structure	RT (min)	MW	Results of MS

A4-B1		11.8	377.3	377.3(M), 376.1(M-1), 349.2(M-28), 254.2, 171.1, 123.1, 93.1, 63.1
A4-B2		12.0	426.2	426.1(M), 425.5(M-1), 398.1(M-28), 397.0, 186.1, 171.1, 107.1, 93.0, 75.1
A4-B3		11.6	426.2	426.1(M), 425.6(M-1), 398.1(M-28), 186.1, 171.0, 123.1, 107.1, 93.1
A4-B4		9.6	365.3	364.1(M-1), 337.1(M-28), 242.2, 186.1, 171.1, 93.1, 75.1
A4-B5		13.3	392.3	392.1(M), 391.2(M-1), 364.7(M-28), 208.1, 186.1, 171.1, 123.1, 93.1
A4-B6		12.9	392.3	392.2(M), 391.3(M-1), 364.1(M-28), 209.1, 186.1, 123.1, 93.1, 76.1
A4-B7		10.6	381.7	381.7(M), 380.5(M-1), 353.1(M-28), 186.1, 171.1, 107.1, 93.0, 75.1
A4-B8		17.6	447.4	447.4(M), 446.1(M-1), 419.2(M-28), 186.1, 171.0, 123.1, 107.1, 93.0
A4-B9		9.1	415.3	415.1(M), 414.1(M-1), 387.1(M-28), 292.1, 186.1, 171.0, 107.1, 93.0

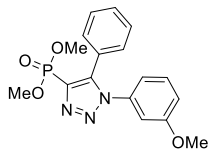
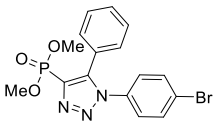
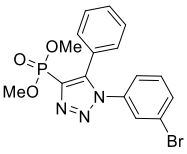
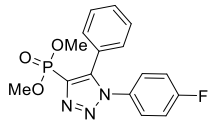
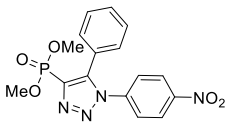
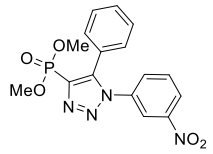
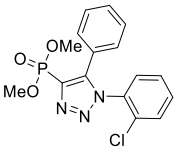
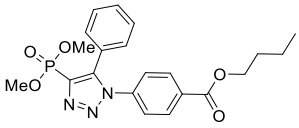
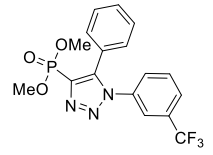
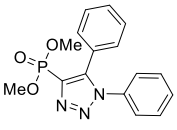
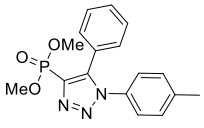
A4-B10		9.9	347.3	347.0(M), 346.9(M-1), 319.1(M-28), 224.2, 186.1, 171.0, 123.1, 107.1
A4-B11		10.5	361.3	361.3(M), 360.2(M-1), 333.2 (M-28), 238.2, 186.1, 171.0, 107.1, 93.1
A4-B12		12.4	473.2	473.0(M), 472.1(M-1), 445.0(M-28), 243.0, 222.1, 186.1, 123.1, 107.1, 93.1,
A4-B13		11.7	395.8	395.7(M), 394.1(M-1), 367.1(M-28), 272.1, 186.1, 171.1, 123.1, 107.1, 93.1, 63.1
A4-B14		10.8	381.7	381.7(M), 380.2(M-1), 353.1(M-28), 379.6, 353.1, 258.1, 186.1, 171.0, 107.1, 93.0
A4-B15		9.2	415.3	415.2(M), 414.5(M-1), 387.1(M-28), 292.1, 186.1, 171.0, 107.1, 93.0
A4-B16		9.6	365.3	365.2(M), 364.1(M-1), 337.1(M-28), 242.2, 186.1, 171.1, 107.1, 93.1
A4-B17		9.5	365.3	365.1(M), 364.0(M-1), 337.1(M-28), 338.1, 242.1, 186.1, 171.0, 123.1, 93.0, 75.0
A4-B18		8.9	401.3	401.2(M), 400.1(M-1), 373.2(M-28), 278.1, 186.1, 107.1, 93.1, 79.0

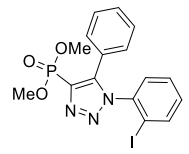
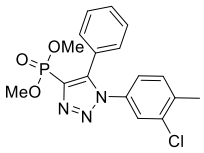
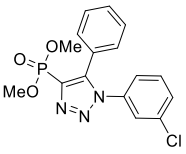
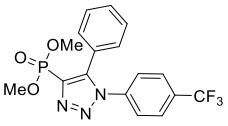
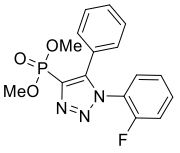
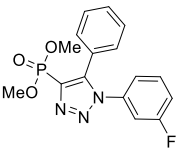
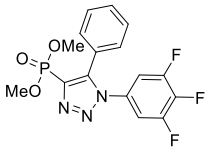
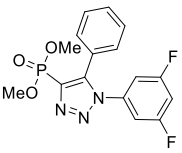
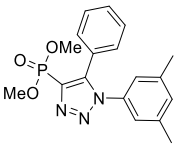
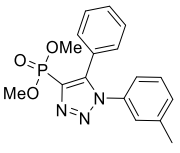
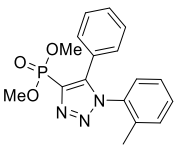
A4-B19		8.9	383.3	383.2(M), 382.2(M-1), 355.1(M-28), 186.1, 171.1, 107.1, 93.1, 79.0
A4-B20		10.7	375.3	375.3(M), 374.1(M-1), 347.5(M-28), 252.2, 186.1, 171.1, 107.1, 77.1
A4-B21		10.3	361.3	361.3(M), 360.2(M-1), 333.2(M-28), 238.2, 186.1, 171.0, 107.1, 93.1
A4-B22		9.8	361.3	361.2(M), 360.1(M-1), 333.2(M-28), 286.1, 222.1, 171.1, 123.1, 93.1
A4-B23		9.8	375.3	375.1(M), 333.2(M-28), 286.1, 222.1, 171.1, 123.1, 93.1, 65.1, 51.3
A4-B24		10.5	381.7	381.1(M), 380.1(M-1), 353.1(M-28), 304.1, 303.1, 227.1, 226.1, 183.1, 181.1, 152.4
A4-B25		11.3	377.3	377.3(M), 376.1(M-1), 349.2(M-28), 254.2, 186.1, 171.1, 123.1, 92.1
A4-B26		10.8	377.3	377.3(M), 376.6(M-1), 349.2(M-28) 287.1, 186.1, 123.1, 107.1, 77.1

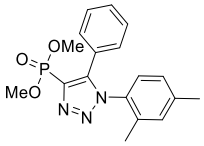
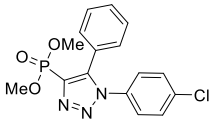
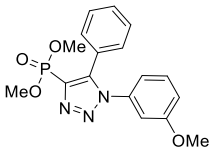
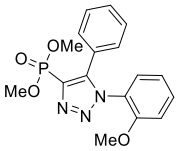
[a] The purity of the triazolyl phosphonate compounds were > 96%.

Table S7 GC/MS data of compound A5-B1 to A5-B26.[a]

Code	Chemical structure	RT (min)	MW	Results of MS

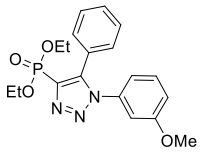
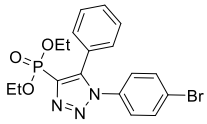
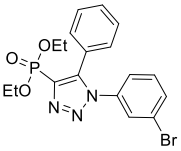
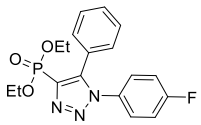
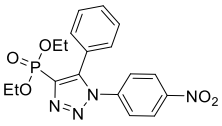
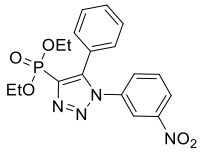
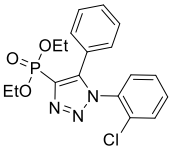
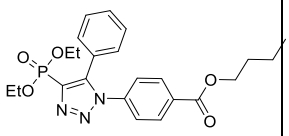
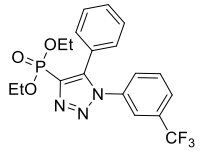
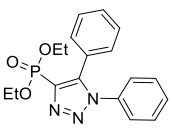
A5-B1		12.5	359.3	359.3(M), 358.2(M-1), 331.2(M-28), 236.2, 168.1, 105.1, 98.1, 77.1
A5-B2		12.6	408.2	408.1(M), 407.3(M-1), 380.3(M-28), 380.3, 204.2, 168.1, 105.1, 98.1, 63.1
A5-B3		12.2	408.2	408.1(M), 407.2(M-1), 380.3(M-28), 379.1, 204.2, 168.1, 105.1, 98.1, 63.1
A5-B4		9.9	347.3	347.3(M), 346.2(M-1), 319.1(M-28), 224.2, 168.1, 105.1, 98.1, 63.1
A5-B5		14.1	374.3	374.1(M), 373.1(M-1), 346.1(M-28), 204.1, 168.1, 105.1, 76.1, 63.1
A5-B6		13.6	374.3	374.2(M), 373.6(M-1), 346.1(M-28), 191.2, 168.1, 105.1, 76.1, 63.1
A5-B7		11.1	363.7	363.7(M), 362.3(M-1), 335.1(M-28), 204.1, 168.1, 105.1, 98.1, 63.0
A5-B8		19.3	429.4	429.2(M), 428.2(M-1), 401.2(M-28), 168.1, 130.1, 105.1, 93.1, 89.1,
A5-B9		9.4	397.3	397.2(M), 396.5(M-1), 369.1(M-28), 168.1, 153.1, 109.0, 89.1, 63.0
A5-B10		8.3	329.3	329.5(M), 328.4(M-1), 301.2(M-28), 206.2, 168.1, 153.1, 105.1, 89.1, 77.1
A5-B11		11.0	343.3	343.4(M), 342.0(M-1), 315.2(M-28), 220.2, 168.1, 153.1, 131.1, 105.1, 89.1

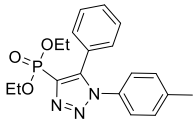
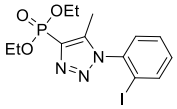
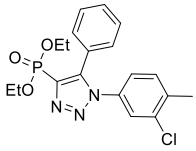
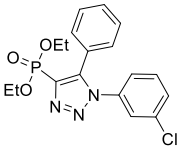
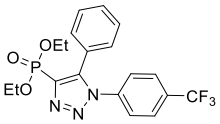
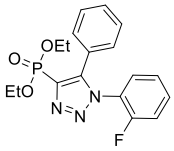
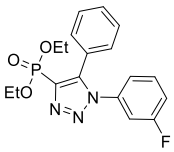
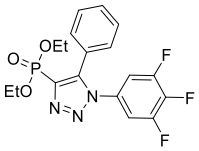
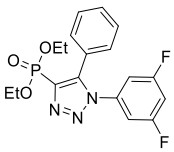
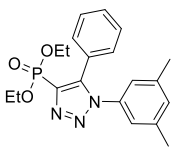
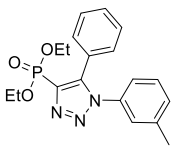
A5-B12		13.2	455.2	455.1(M), 454.2(M-1), 427.1(M-28), 222.1, 204.1, 168.1, 153.1, 105.1, 90.1, 76.1
A5-B13		12.4	377.8	377.4(M), 376.1(M-1), 349.1(M-28), 254.1, 168.1, 105.1, 89.1, 63.0
A5-B14		11.2	363.7	363.7(M), 362.3(M-1), 335.1(M-28), 240.1, 168.1, 105.1, 89.1, 63.0
A5-B15		9.4	397.3	397.2(M), 396.0(M-1), 369.1(M-28), 274.2, 168.1, 105.1, 89.1, 63.1
A5-B16		10.0	347.3	347.2(M), 346.2(M-1), 319.1(M-28), 224.1, 168.1, 105.1, 89.1, 63.1
A5-B17		9.8	347.3	347.0(M), 346.9(M-1), 319.1(M-28), 224.1, 168.1, 105.1, 89.1, 63.0
A5-B18		9.1	383.3	383.2(M), 355.1(M-28), 260.1, 168.1, 109.0, 89.1, 63.1
A5-B19		9.2	365.3	365.2(M), 364.0(M-1), 337.1(M-28), 242.1, 168.1, 93.1, 90.1, 63.1
A5-B20		11.3	357.4	357.3(M), 356.2(M-1), 329.2(M-28), 234.2, 168.1, 105.1, 79.1
A5-B21		10.8	343.3	343.3(M), 342.2(M-1), 315.2(M-28), 220.2, 168.1, 105.1, 91.1, 65.1
A5-B22		9.2	343.3	343.3(M), 342.2(M-1), 315.9(M-28), 260.2, 205.2, 204.1, 105.1, 91.1, 65.1,

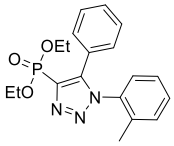
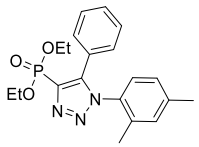
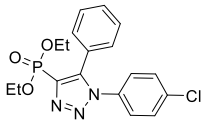
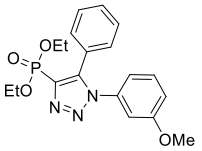
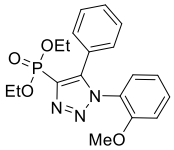
A5-B23		10.9	357.4	357.3(M), 356.4(M-1), 329.2(M-28), 282.1, 218.2, 153.1, 105.1, 93.1
A5-B24		11.3	363.7	363.7(M), 362.1(M-1), 335.1(M-28), 240.1, 168.1, 105.1, 89.1, 63.0
A5-B25		11.9	359.3	359.3(M), 358.0(M-1), 331.2(M-28), 236.2, 168.1, 105.1, 98.1, 77.1
A5-B26		11.3	359.3	359.3(M), 358.2(M-1), 331.2(M-28), 269.1, 220.1, 153.1, 105.1, 77.1

[a] The purity of the triazolyl phosphonate compounds were > 96%.

Table S8 GC/MS data of compound A6-B1 to A6-B26.[a]

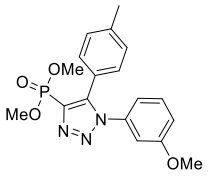
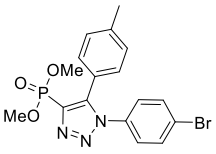
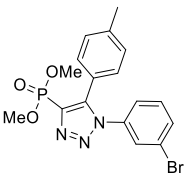
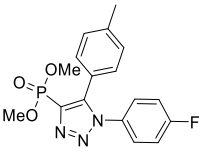
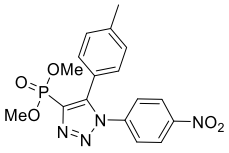
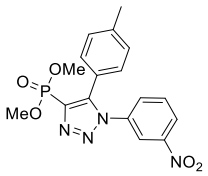
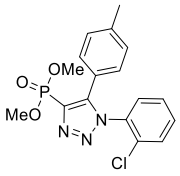
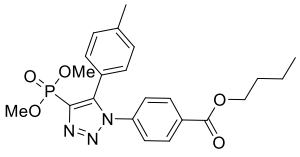
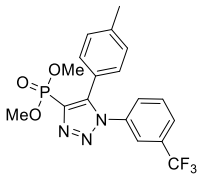
Code	Chemical structure	RT (min)	MW	Results of MS
A6-B1		13.4	387.4	387.1(M), 386.2(M-1), 285.1, 359.2(M-28), 182.1, 154.1, 105.1, 89.1
A6-B2		13.5	436.3	436.1(M), 435.2(M-1), 408.1(M-28), 208.0, 182.1, 154.1, 105.1, 91.1, 89.1
A6-B3		13.1	436.3	436.1(M), 435.4(M-1), 408.1(M-28), 208.0, 182.1, 154.1, 105.1, 89.1, 76.1
A6-B4		10.4	375.3	375.3(M), 374.2(M-1), 360.2, 347.2(M-28), 273.1, 211.1, 182.1, 105.1, 89.1
A6-B5		15.2	402.4	402.3(M), 401.1(M-1), 388.4, 374.2(M-28), 300.1, 182.1, 154.1, 105.1, 89.1
A6-B6		14.6	402.4	402.2(M), 401.0(M-1), 400.9, 374.2(M-28), 300.1, 182.2, 154.1, 105.1, 89.1
A6-B7		11.7	391.8	391.7(M), 390.0(M-1), 378.5, 363.1(M-28), 289.1, 182.1, 154.0, 105.1, 89.1
A6-B8		21.4	457.5	457.3(M), 456.3(M-1), 429.2(M-28), 230.2, 182.1, 154.1, 89.1, 65.0
A6-B9		9.5	425.4	425.2(M), 424.1(M-1), 397.2(M-28), 323.1, 261.1, 182.1, 154.1, 89.1
A6-B10		10.8	357.4	357.2(M), 356.2(M-1), 329.2(M-28), 255.1, 182.1, 154.1, 89.1, 77.1

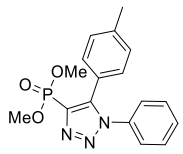
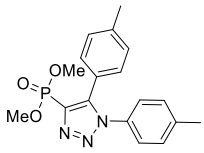
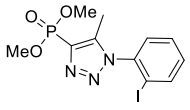
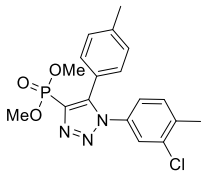
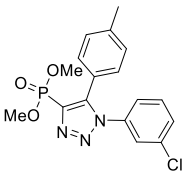
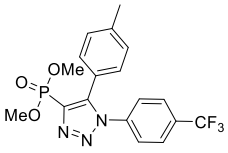
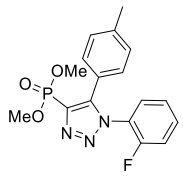
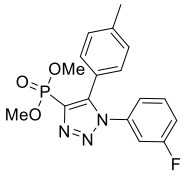
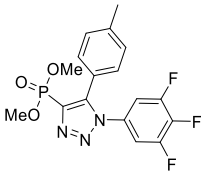
A6-B11		11.7	371.4	371.2(M), 370.1(M-1), 343.2(M-28), 269.1, 182.1, 154.1, 89.1, 65.1
A6-B12		13.5	483.3	483.2(M), 482.9(M-1), 455.1(M-28), 381.0, 319.0, 256.0, 230.0, 182.1, 154.1
A6-B13		13.2	405.8	405.8(M), 404.5(M-1), 380.3(M-28), 377.1, 303.1, 182.1, 154.1, 105.1, 89.1
A6-B14		11.9	391.8	391.7(M), 390.4(M-1), 390.2, 363.1(M-28), 289.1, 182.1, 154.0, 105.1, 89.1
A6-B15		9.9	425.4	425.2(M), 424.1(M-1), 397.2(M-28), 323.1, 261.1, 182.1, 164.1, 89.1
A6-B16		10.5	375.3	375.2(M), 374.1(M-1), 347.2(M-28), 273.1, 182.1, 154.1, 105.1, 89.1,
A6-B17		10.3	375.3	375.2(M), 374.1(M-1), 347.4(M-28), 273.1, 182.1, 154.0, 105.1, 89.1
A6-B18		9.5	411.3	411.2(M), 410.1(M-1), 383.1(M-28), 309.0, 182.1, 154.1, 105.1, 89.1
A6-B19		9.6	393.3	393.2(M), 392.2(M-1), 365.1(M-28), 291.1, 182.0, 154.1, 105.1, 89.1
A6-B20		11.9	385.4	385.2(M), 384.1(M-1), 357.2(M-28), 221.1, 182.1, 154.0, 105.1, 89.1
A6-B21		11.3	371.4	371.2(M), 370.1(M-1), 343.2(M-28), 269.0, 182.1, 154.1, 105.1, 89.1

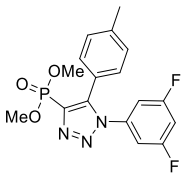
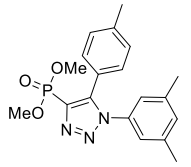
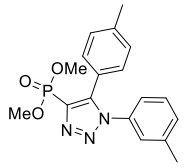
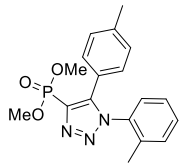
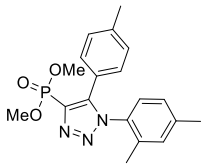
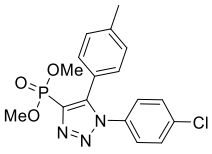
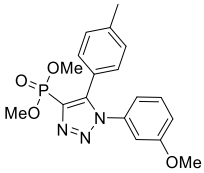
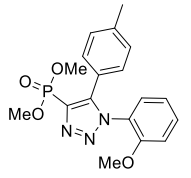
A6-B22		10.7	371.4	371.2(M), 370.2(M-1), 343.2(M-28), 204.1, 182.1, 154.0, 91.1, 89.1
A6-B23		11.4	385.4	385.3(M), 384.1(M-1), 357.2(M-28), 282.1, 218.2, 182.1, 157.0, 105.1
A6-B24		21.2	391.8	391.5(M), 390.1(M-1), 363.1(M-28), 289.1, 182.1, 154.1, 105.1, 89.1
A6-B25		12.7	387.4	387.3(M), 386.1(M-1), 359.2 (M-28), 258.1, 182.1, 154.1, 89.1, 77.1
A6-B26		11.9	387.4	387.3(M), 386.0(M-1), 359.2(M-28), 207.1, 182.1, 154.1, 105.0, 77.1, 65.0

[a] The purity of the triazolyl phosphonate compounds were > 96%.

Table S9 GC/MS data of compound A7-B1 to A7-B26.[a]

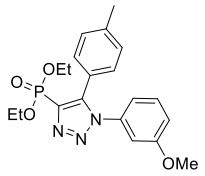
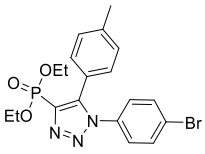
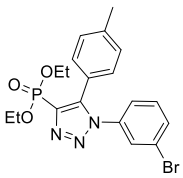
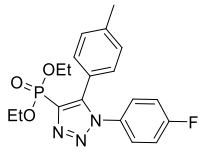
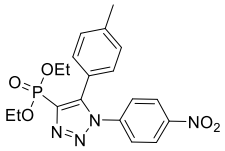
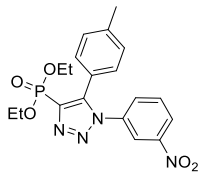
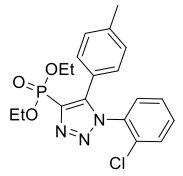
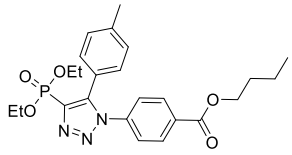
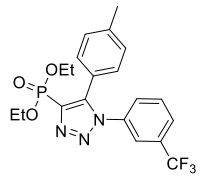
Code	Chemical structure	RT (min)	MW	Results of MS
A7-B1		13.5	373.4	373.3(M), 372.2(M-1), 345.2(M-28), 182.1, 119.1, 103.1, 77.1, 63.0
A7-B2		13.6	422.2	422.1(M), 421.0(M-1), 394.1(M-28), 393.1, 182.1, 119.1, 103.1, 93.1, 77.1
A7-B3		13.2	422.2	422.1(M), 421.4(M-1), 394.1(M-28), 182.1, 119.1, 103.1, 93.0, 77.1
A7-B4		10.5	361.3	361.3(M), 360.4(M-1), 333.1(M-28), 238.2, 182.1, 119.1, 93.0, 77.1
A7-B5		15.3	388.3	388.3(M), 387.1(M-1), 360.1(M-28), 182.1, 167.1, 119.1, 93.0, 76.1
A7-B6		14.6	388.3	388.3(M), 387.0(M-1), 360.1(M-28), 267.1, 182.1, 119.1, 93.0, 76.1
A7-B7		11.9	377.8	377.7(M), 376.4(M-1), 349.1(M-28), 182.1, 167.1, 119.1, 103.1, 93.0
A7-B8		21.5	443.4	443.3(M), 442.2(M-1), 415.2(M-28), 182.1, 167.0, 119.1, 103.1, 77.1
A7-B9		9.9	411.3	411.3(M), 410.5(M-1), 383.2(M-28), 182.1, 167.1, 103.1, 93.0, 77.1

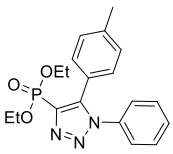
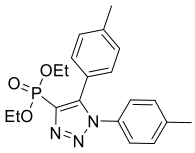
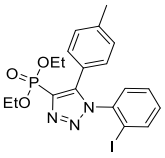
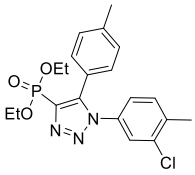
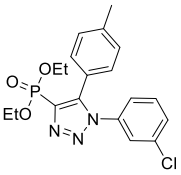
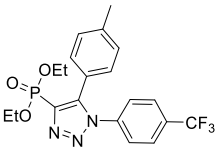
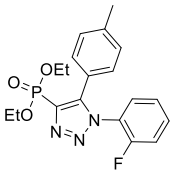
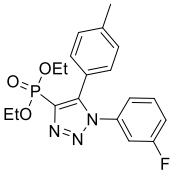
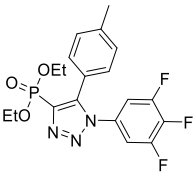
A7-B10		10.9	343.3	343.3(M), 342.0(M-1), 315.2 (M-28), 182.1, 167.1, 103.1, 92.9, 77.1
A7-B11		11.8	357.4	357.3(M), 356.7(M-1), 329.2(M-28), 234.2, 182.1, 119.1, 103.1, 65.1
A7-B12		8.9	469.2	469.1(M), 468.9(M-1), 441.8(M-28), 439.1, 340.3, 284.2207.1, 177.2, 161.2, 149.1, 91.3
A7-B13		13.3	391.8	391.6(M), 390.0(M-1), 363.1(M-28), 268.1, 182.1, 119.1, 103.1, 77.1
A7-B14		12.0	377.8	377.1(M), 376.1(M-1), 349.1(M-28), 182.1, 167.0, 119.1, 77.1, 63.0,
A7-B15		9.9	411.3	411.3(M), 410.1(M-1), 383.2(M-28), 182.1, 167.1, 103.1, 93.0, 77.1
A7-B16		10.6	361.3	361.3(M), 360.1(M-1), 333.1(M-28), 182.1, 167.1, 119.1, 93.0, 91.1
A7-B17		10.4	361.3	361.0(M), 360.0(M-1), 333.1(M-28), 238.2, 182.1, 119.1, 103.1, 77.1
A7-B18		9.5	397.3	397.1(M), 396.1(M-1), 369.1(M-28), 182.1, 167.1, 119.1, 103.1, 77.1

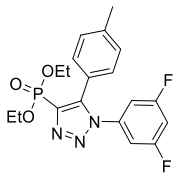
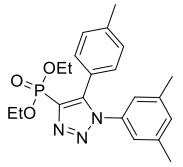
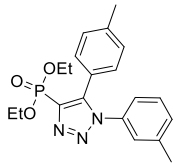
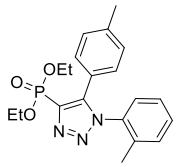
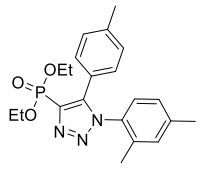
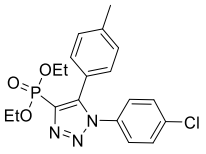
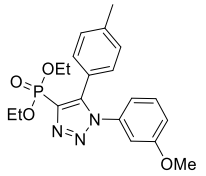
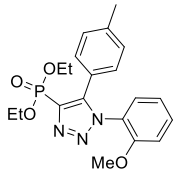
A7-B19		9.6	379.3	379.1(M), 378.1(M-1), 351.1(M-28), 182.1, 167.1, 119.1, 103.1, 77.1
A7-B20		12.1	371.4	371.3(M), 370.6(M-1), 343.2(M-28), 248.2, 182.1, 167.1, 119.1, 93.0
A7-B21		9.1	357.4	357.3(M), 356.0(M-1), 329.2(M-28), 263.2, 235.2, 234.2, 193.2, 130.1, 103.1, 77.1
A7-B22		10.9	357.4	357.3(M), 356.9(M-1), 329.2(M-28), 218.2, 204.1, 167.1, 119.1, 91.1
A7-B23		8.8	371.4	371.3(M), 370.3(M-1), 343.0(M-28), 235.2, 220.2, 205.2, 193.2, 130.1, 103.1, 77.1
A7-B24		12.4	377.8	377.7(M), 376.6(M-1), 349.1(M-28), 182.1, 119.1, 103.1, 93.0, 77.1
A7-B25		12.9	373.4	373.3(M), 372.1(M-1), 345.2(M-28), 250.2, 182.0, 119.1, 93.0, 77.1
A7-B26		12.1	373.3	373.3(M), 372.2(M-1), 345.2(M-28), 283.1, 220.1, 167.1, 119.1, 93.1, 77

[a] The purity of the triazolyl phosphonate compounds were > 96%.

Table S10 GC/MS data of compound A8-B1 to A8-B26.[a]

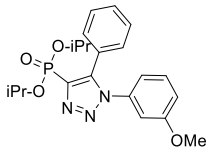
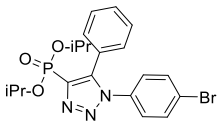
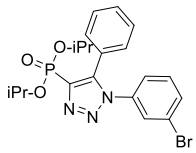
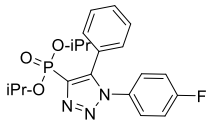
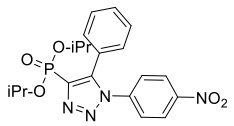
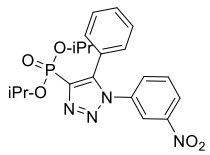
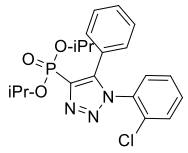
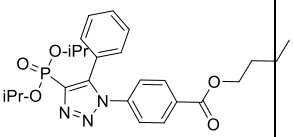
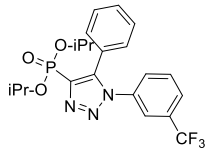
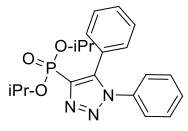
Code	Chemical structure	RT (min)	MW	Results of MS
A8-B1		14.5	401.4	401.1(M), 400.5(M-1), 373.2(M-28), 317.1, 237.2, 196.1, 160.1, 119.1
A8-B2		14.6	450.3	450.1(M), 449.4(M-1), 422.1(M-28), 421.1, 196.1, 119.1, 105.1, 77.1, 76.1
A8-B3		14.0	450.3	450.1(M), 449.3(M-1), 422.1(M-28), 421.1, 349.0, 196.1, 168.1, 103.1, 91.1
A8-B4		11.0	389.4	389.3(M), 388.1(M-1), 361.2(M-28), 305.2, 287.1, 168.1, 119.1, 103.1
A8-B5		16.4	416.4	416.3(M), 415.1(M-1), 388.2(M-28), 314.1, 196.1, 168.1, 103.1, 91.1
A8-B6		15.8	416.4	416.2(M), 415.0(M-1), 388.2(M-28), 314.1, 196.1, 168.0, 119.1, 76.1
A8-B7		12.6	405.8	405.1(M), 404.1(M-1), 377.1(M-28), 303.1, 196.1, 168.1, 103.1, 77.1
A8-B8		23.7	471.5	471.4(M), 470.1(M-1), 443.2(M-28), 196.1, 168.1, 119.1, 103.1, 65.0
A8-B9		10.2	439.4	439.3(M), 438.3(M-1), 411.2(M-28), 412.2, 411.2, 337.1, 196.1, 168.0, 103.1, 77.1

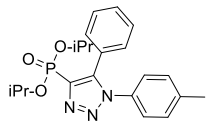
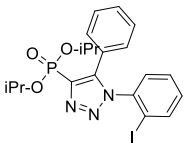
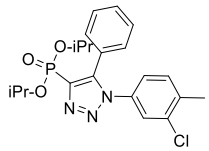
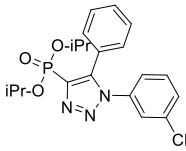
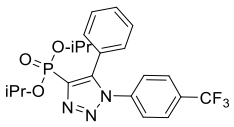
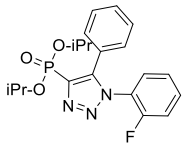
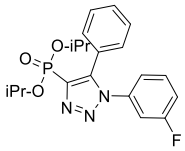
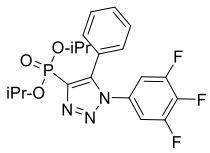
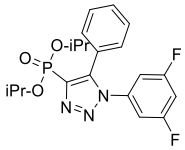
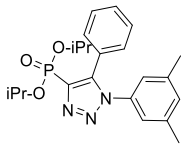
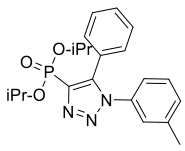
A8-B10		11.5	371.4	371.3(M), 370.1(M-1), 343.2(M-28), 287.1, 196.1, 168.1, 103.1, 77.1
A8-B11		12.5	385.4	385.4(M), 384.0(M-1), 357.2(M-28), 283.1, 196.1, 168.1, 119.1, 91.1,
A8-B12		15.2	497.3	497.2(M), 496.0(M-1), 469.1(M-28), 395.0, 196.1, 158.1, 119.1, 103.1, 77.1, 65.0
A8-B13		14.2	419.9	419.8(M), 418.0(M-1), 391.2(M-28), 317.1, 196.1, 168.1, 103.1, 77.1
A8-B14		12.7	405.8	405.8(M), 404.4(M-1), 377.1(M-28), 303.0, 196.1, 168.1, 103.1, 77.1
A8-B15		10.3	439.4	439.3(M), 438.1(M-1), 411.4(M-28), 337.1, 196.1, 168.1, 103.1, 77.1
A8-B16		11.1	389.4	389.2(M), 388.9(M-1), 361.2(M-28), 287.1, 196.1, 168.1, 103.1, 77.1
A8-B17		10.8	389.4	389.3(M), 388.9(M-1), 361.2(M-28), 287.1, 196.1, 168.1, 103.1, 77.1
A8-B18		9.9	425.4	425.2(M), 424.1(M-1), 397.2(M-28), 323.1, 196.1, 168.1, 103.1, 77.1

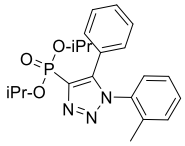
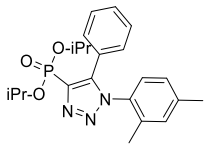
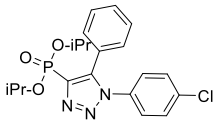
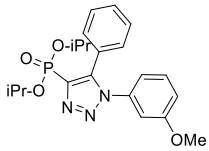
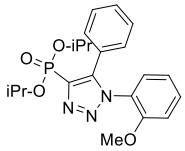
A8-B19		10.0	407.3	407.2(M), 406.1(M-1), 380.2(M-28), 379.2, 305.1, 108.1, 103.1, 65.0
A8-B20		12.7	399.4	399.4(M), 398.1(M-1), 371.2(M-28), 297.1, 196.1, 168.1, 103.1, 77.1
A8-B21		12.1	385.4	385.4(M), 384.0(M-1), 357.2(M-28), 196.1, 168.1, 103.1, 91.2,
A8-B22		11.4	385.4	385.4(M), 384.8(M-1), 357.2(M-28), 220.2, 196.1, 168.1, 91.1, 65.0
A8-B23		12.2	399.4	399.4(M), 398.8(M-1), 371.2(M-28), 234.2, 168.1, 119.1, 77.1, 65.0
A8-B24		13.0	405.8	405.5(M), 404.0(M-1), 377.2(M-28), 303.1, 279.1, 196.1, 168.1, 103.1, 77.1
A8-B25		13.6	401.4	401.4(M), 400.0(M-1), 373.2(M-28), 299.1, 196.1, 168.1, 103.1, 77.1
A8-B26		12.7	401.4	401.4(M), 400.0(M-1), 373.2(M-28), 196.1, 168.1, 119.1, 77.1, 65.0

[a] The purity of the triazolyl phosphonate compounds were > 96%.

Table S11 GC/MS data of compound A9-B1 to A9-B26.[a]

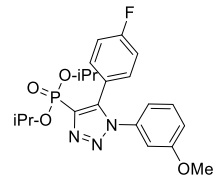
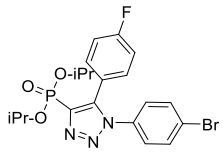
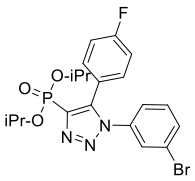
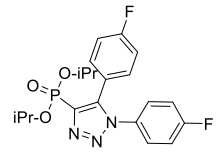
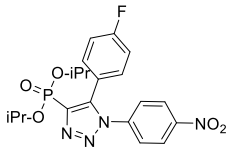
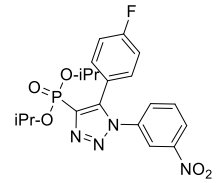
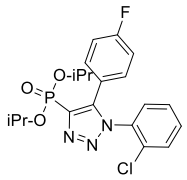
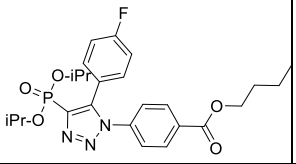
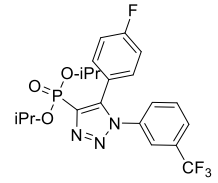
Code	Chemical structure	RT (min)	MW	Results of MS
A9-B1		8.4	415.4	415.2(M), 414.3(M-1), 387.5(M-28), 304.1, 303.1, 208.1, 105.1, 89.2, 77.1
A9-B2		13.4	464.3	464.3(M), 463.3(M-1), 436.1(M-28), 353.0, 333.0, 105.1, 89.1, 76.1,
A9-B3		12.9	464.3	464.1(M), 463.7(M-1), 436.1(M-28), 353.0, 335.0, 191.1, 165.1, 105.1, 89.1, 77.1, 76.1
A9-B4		10.3	403.4	403.3(M), 402.3(M-1), 375.0(M-28), 291.1, 273.1, 105.1, 89.0
A9-B5		9.9	430.4	430.3(M), 429.1(M-1), 402.4(M-28), 319.1, 318.1, 300.1, 191.1, 105.1, 89.1
A9-B6		9.8	430.4	430.2(M), 429.1(M-1), 402.5(M-28), 319.1, 318.1, 300.1, 199.1, 105.1, 89.1
A9-B7		11.	419.9	419.8(M), 418.1(M-1), 391.1 (M-28), 309.1, 307.1, 289.1, 105.1, 89.1
A9-B8		21.3	485.5	485.1(M), 484.2(M-1), 457.2(M-28), 373.1, 374.2, 299.1, 207.0, 137.1
A9-B9		9.7	453.4	453.4(M), 452.1(M-1), 425.7(M-28), 342.1, 341.1, 323.1, 105.1, 89.1
A9-B10		10.7	385.4	385.4(M), 384.1(M-1), 357.2(M-28), 274.1, 273.1,255.1,105.1,89.1, 77.1

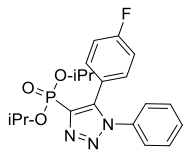
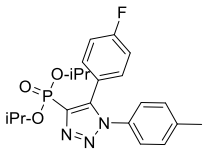
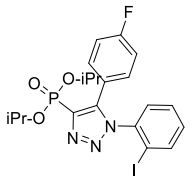
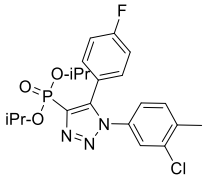
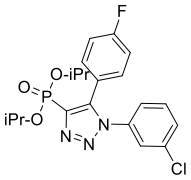
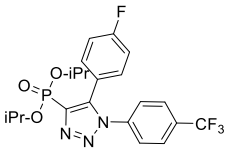
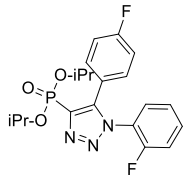
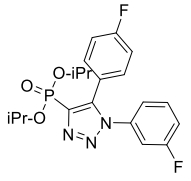
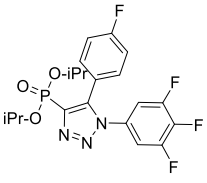
A9-B11		11.6	399.4	399.2(M), 398.2(M-1), 371.3(M-28), 287.1, 269.1, 206.1, 105.1, 89.1, 65.1
A9-B12		13.8	511.3	511.3(M), 510.3(M-1), 483.5 (M-28), 400.0, 399.0, 381.0, 207.1, 190.1, 179.1, 105.1, 89.1
A9-B13		13.0	433.9	433.8(M), 432.2(M-1), 405.8(M-28), 323.1, 321.1, 303.1, 105.1, 89.1
A9-B14		11.8	419.9	419.3(M), 418.1(M-1), 391.2(M-28), 309.1, 307.1, 289.1, 105.1, 89.1
A9-B15		9.8	453.4	453.3(M), 452.1(M-1), 425.2(M-28), 342.1, 341.1, 343.1, 105.1, 89.1
A9-B16		10.4	403.4	403.1(M), 402.2(M-1), 375.5(M-28), 292.1, 291.1, 237.1, 105.1, 89.1
A9-B17		10.2	403.4	403.2(M), 402.2(M-1), 375.2(M-28), 291.1, 273.1, 105.1, 89.1
A9-B18		9.4	439.4	439.0(M), 438.2(M-1), 411.4(M-28), 327.1, 309.1, 105.1, 89.1
A9-B19		9.6	421.4	421.3(M), 420.2(M-1), 393.3(M-28), 309.1, 291.1, 105.1, 89.1
A9-B20		11.8	413.5	413.4(M), 412.2(M-1), 385.2(M-28), 302.2, 301.1, 283.1, 105.1, 89.0, 79.1
A9-B21		11.3	399.4	399.2(M), 398.1(M-1), 371.2(M-28), 288.1, 287.1, 269.1, 105.1, 89.1, 65.1

A9-B22		10.7	399.4	399.4(M), 398.2(M-1), 371.7(M-28), 287.1, 207.2, 206.2, 105.1, 91.1, 65.1
A9-B23		11.4	413.5	413.4(M), 412.2(M-1), 385.3(M-28), 301.2, 218.2, 200.2, 204.1, 105.1, 77.1
A9-B24		12.1	419.9	419.3(M), 418.1(M-1), 391.3(M-28), 309.1, 307.1, 289.1, 105.1, 89.1
A9-B25		12.5	415.4	415.1(M), 414.2(M-1), 387.5(M-28), 304.1, 303.1, 285.1, 105.1, 89.1, 77.1
A9-B26		11.8	415.4	415.4(M), 414.1(M-1), 387.9(M-28), 303.1, 285.1, 282.2, 203.1, 105.1, 77.1

[a] The purity of the triazolyl phosphonate compounds were > 96%.

Table S12 GC/MS data of compound A10-B1 to A10-B26.[a]

Code	Chemical structure	RT (min)	MW	Results of MS
A10-B1		12.4	433.4	432.9(M), 432.1(M-1), 405.3(M-28), 332.1, 321.1, 241.1, 240.1, 226.1, 123.1, 107.1
A10-B2		12.6	482.3	482.0(M), 481.3(M-1), 454.1(M-28), 372.0, 369.0, 123.1, 107.0, 76.1, 64.6, 57.4
A10-B3		12.2	482.3	482.1(M), 481.2(M-1), 480.6, 454.1(M-28), 372.0, 369.0, 209.3, 123.1, 107.1, 75.1, 65.5
A10-B4		10.0	421.4	421.1(M), 420.6(M-1), 393.4(M-28), 309.1, 291.1, 123.1, 107.1, 95.2, 75.2, 57.2
A10-B5		14.2	448.4	448.3(M), 447.9(M-1), 446.2, 420.3(M-28), 336.1, 318.01, 209.1, 123.1, 107.1, 76.5, 65.4
A10-B6		13.6	448.4	448.3(M), 447.9(M-1), 447.0, 432.6, 420.3(M-28), 337.1, 318.1, 209.1, 107.1, 76.1, 62.3
A10-B7		11.1	437.8	437.7(M), 436.6(M-1), 409.5(M-28), 327.1, 307.0, 243.6, 229.7, 123.1, 107.1
A10-B8		11.0	503.5	475.5(M-28), 392.2, 391.2, 335.1, 317.1, 208.1, 207.1, 123.1, 107.1, 65.1
A10-B9		9.4	471.4	471.3(M), 470.2(M-1), 443.8(M-28), 401.5, 370.2, 341.1, 279.6, 172.4, 145.3, 123.1

A10-B10		10.3	403.4	402.8(M-1), 375.7(M-28), 333.7, 302.5, 273.1, 211.3, 183.3, 123.1, 107.1
A10-B11		11.0	417.4	417.4(M), 416.2(M-1), 389.4(M-28), 347.7, 305.1, 224.8, 123.1, 107.1, 91.3, 65.6
A10-B12		13.0	529.3	529.2(M), 528.9(M-1), 501.5(M-28), 417.0, 399.0, 230.1, 208.1, 197.1, 183.1, 123.1, 107.1
A10-B13		12.3	451.9	451.5(M), 450.1(M-1), 423.2(M-28), 381.8, 339.1, 258.0, 224.5, 172.4, 123.1, 107.0
A10-B14		11.2	437.8	437.5(M), 436.1(M-1), 409.3(M-28), 327.1, 245.5, 183.5, 132.6, 123.1, 75.5
A10-B15		9.5	471.4	471.3(M), 470.0(M-1), 443.3(M-28), 370.3, 341.1, 279.3, 172.5, 123.1, 95.5
A10-B16		10.0	421.4	421.3(M), 420.1(M-1), 393.3(M-28), 351.4, 309.1, 230.0, 123.1, 107.1, 95.3, 75.4
A10-B17		9.8	421.4	421.3(M), 420.1(M-1), 393.4(M-28), 229.5, 123.1, 107.0, 95.4, 75.3
A10-B18		9.2	457.4	457.0(M), 456.1(M-1), 429.4(M-28), 387.7, 345.1, 365.3, 237.4, 158.6, 123.1, 81.6

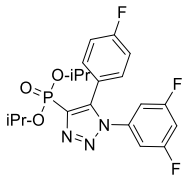
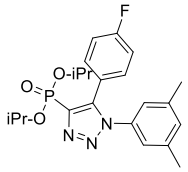
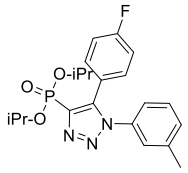
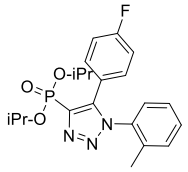
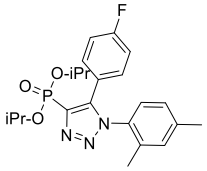
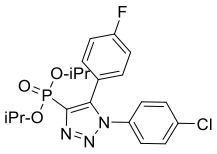
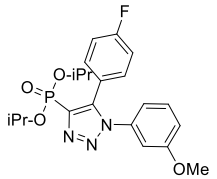
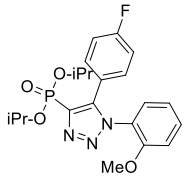
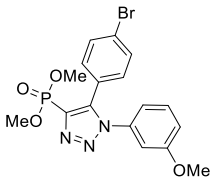
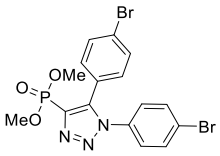
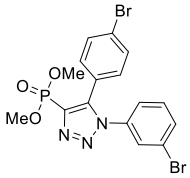
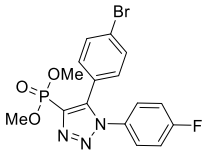
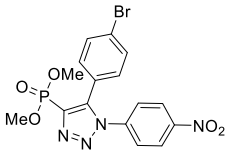
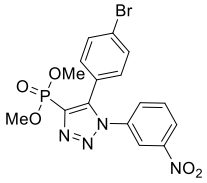
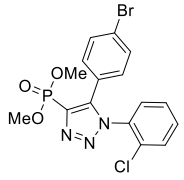
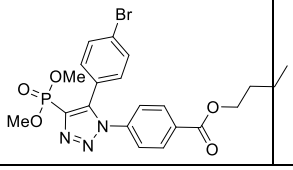
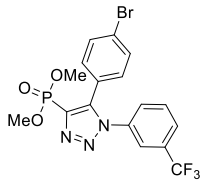
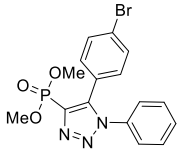
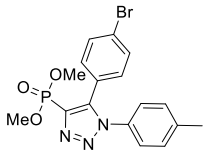
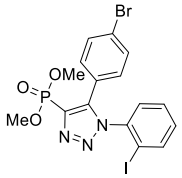
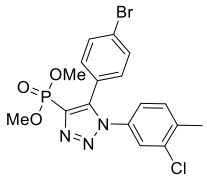
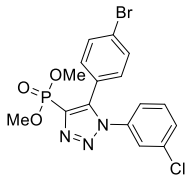
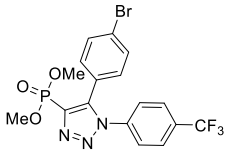
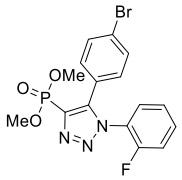
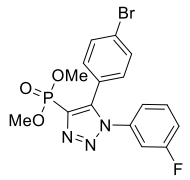
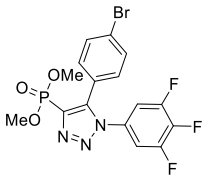
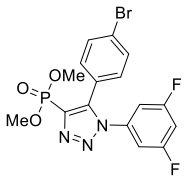
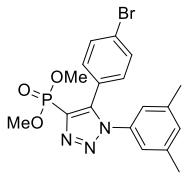
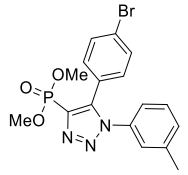
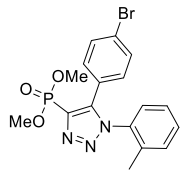
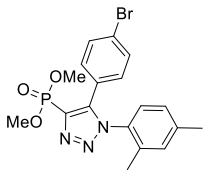
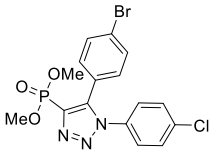
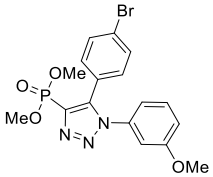
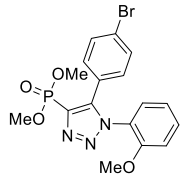
A10-B19		9.2	439.4	439.0(M), 438.2(M-1), 411.5(M-28), 369.6, 327.1, 247.3219.5, 123.1, 107.1, 95.4
A10-B20		11.2	431.4	431.4(M), 430.1(M-1), 403.3(M-28), 320.1, 319.1, 238.2, 207.1, 123.1, 107.1, 77.1
A10-B21		11.7	417.4	417.2(M), 416.6(M-1), 403.2(M-28), 306.1, 305.1, 225.0, 224.1, 123.1, 107.1, 91.1
A10-B22		10.2	417.4	417.3(M), 416.5(M-1), 389.3(M-28), 320.1, 319.1, 237.1, 222.1, 123.0, 77.1, 65.7
A10-B23		10.8	431.4	431.4(M), 430.2(M-1), 403.5(M-28), 320.1, 319.1, 237.1, 236.1, 222.1, 123.1, 77.1
A10-B24		11.5	437.8	437.3(M), 436.7(M-1), 409.3(M-28), 327.1, 326.1, 307.0, 123.1, 107.0, 75.3, 65.3
A10-B25		11.8	433.4	433.3(M), 432.3(M-1), 405.2(M-28), 321.1, 303.1, 107.1, 77.1, 64.6, 62.7, 57.4
A10-B26		11.2	433.4	433.4(M), 432.3(M-1), 405.5(M-28), 322.1, 303.1, 123.1, 107.1, 92.1, 77.1, 64.5

Table S13 GC/MS data of compound A11-B1 to A11-B26.

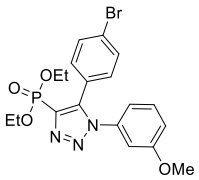
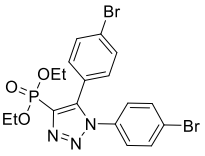
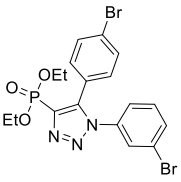
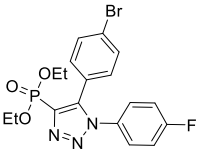
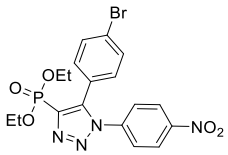
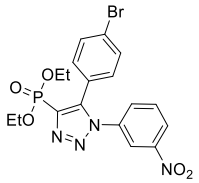
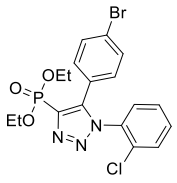
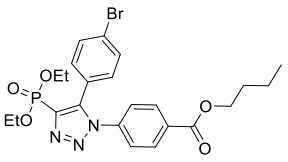
Code	Chemical structure	RT (min)	MW	Results of MS
A11-B1		15.8	438.2	439.1(M), 437.1(M), 411.1(M-28), 409.1(M-28), 248.0, 246.0, 233.0, 231.0, 167.0, 165.0
A11-B2		16.3	487.1	489.0(M), 487.5(M), 461.0(M-28), 458.0(M-28), 246.0, 231.0, 233.0, 183.0, 167.0, 155.0
A11-B3		15.6	487.1	486.8(M), 488.0(M), 458.0(M-28), 461.0(M-28), 248.0, 231.0, 230.0, 185.0, 183.0, 167.0
A11-B4		11.8	426.2	425.2(M), 427.1(M), 397.0(M-28), 399.0(M-28), 248.0, 246.0, 233.0, 231.0, 169.0, 167.0
A11-B5		18.9	453.2	452.3(M), 454.2(M), 424.1(M-28), 426.1(M-28), 246.0, 248.0, 231.0, 233.0, 190.1, 191.1
A11-B6		18.0	453.2	452.2(M), 454.2(M), 424.1(M-28), 426.1(M-28), 246.0, 248.0, 190.1, 191.2, 79.0, 75.1
A11-B7		13.7	442.6	441.0(M), 443.0(M), 413.0(M-28), 415.0(M-28), 246.0, 248.0, 231.0, 233.0, 167.0, 169.0, 183.0, 185.0
A11-B8		14.6	508.3	507.0(M), 509.9(M), 481.0(M-28), 479.3(M-28), 373.1, 317.1, 315.1, 270.0, 272.1, 194.0

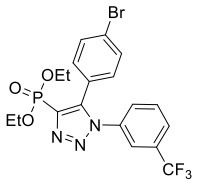
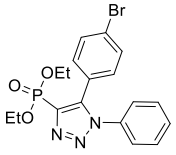
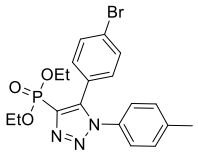
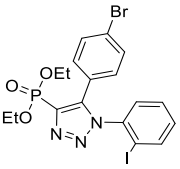
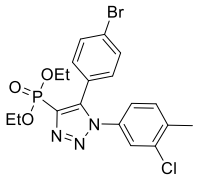
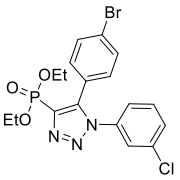
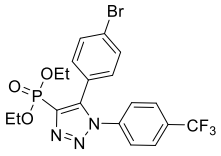
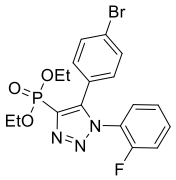
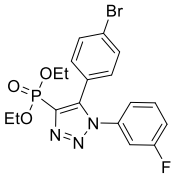
A11-B9		10.8	476.2	475.4(M), 477.1(M), 447.1(M-28), 449.1(M-28), 272.1, 248.0, 246.0, 233.0, 231.0, 93.0
A11-B10		12.4	408.2	409.0(M), 407.0(M), 381.0(M-28), 379.0(M-28), 248.0, 246.0, 232.9, 230.9, 185.0, 183.0
A11-B11		13.5	422.2	423.1(M), 421.1(M), 395.1(M-28), 393.1(M-28), 248.0, 246.0, 233.0, 231.0, 185.0, 183.0
A11-B12		11.2	534.1	535.0(M), 533.8(M), 507.0(M-28), 505.2(M-28), 426.9, 425.1, 398.9, 396.9, 191, 1, 190.1
A11-B13		15.7	456.7	457.2(M), 455.1(M), 429.0(M-28), 427.0(M-28), 248.0, 246.0, 169.0, 167.0, 79.0, 78.5
A11-B14		13.9	442.6	443.2(M), 441.1(M), 415.0(M-28), 413.0(M-28), 248.0, 246.0, 185.0, 183.0, 111.0, 109.0
A11-B15		11.0	476.2	477.7(M), 475.1(M), 449.1(M-28), 447.0(M-28), 248.0, 246.0, 233.0, 231.0, 185.1, 183.0
A11-B16		11.8	426.2	427.1(M), 425.1(M), 399.1(M-28), 397.1(M-28), 248.0, 246.0, 231.0, 233.0, 167.0, 93.0
A11-B17		11.6	426.2	427.2(M), 425.4(M), 399.1(M-28), 246.0, 239.0, 233.1, 207.1, 183.0, 167.0, 135.1,

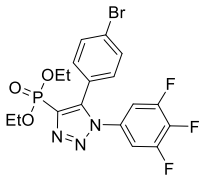
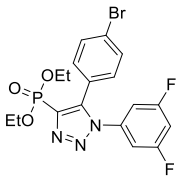
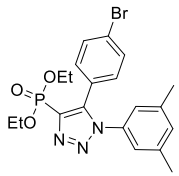
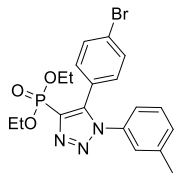
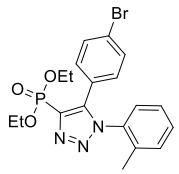
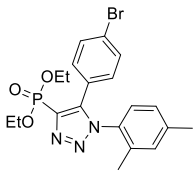
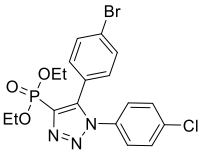
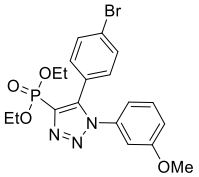
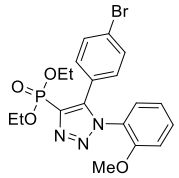
A11-B18		10.4	462.2	461.9(M), 463.0(M), 435.1(M-28), 433.1(M-28), 246.0, 248.0, 235.1, 185.0, 169.1, 183.0
A11-B19		11.6	444.2	455.5(M), 443.9(M), 417.1(M-28), 415.1(M-28), 248.0, 246.0, 207.1, 183.2, 109.4
A11-B20		138	436.3	437.1(M), 435.1(M), 409.1(M-28), 407.1(M-28), 314.1, 312.1, 246.0, 248.0, 103.1, 105.1
A11-B21		13.0	422.2	423.1(M), 421.1(M), 395.1(M-28), 393.1(M-28), 293.1, 295.1, 300.1, 298.1, 248.0, 246.0, 233.0, 231.0
A11-B22		12.3	422.2	423.1(M), 421.1(M), 395.1(M-28), 393.1(M-28), 285.1, 283.1, 93.0, 91.0, 65.1, 63.1
A11-B23		13.2	436.3	437.4(M), 435.1(M), 409.1(M-28), 407.1(M-28), 299.1, 297.1, 219.2, 217.1, 185.0, 183.0, 79.1, 77.1
A11-B24		14.4	442.6	443.2(M), 441.2(M), 415.0(M-28), 413.0(M-28), 248.0, 246.0, 233.0, 231.0, 185.0, 183.0
A11-B25		14.9	438.2	439.2(M), 437.2(M), 411.1(M-28), 409.1(M-28), 248.0, 246.0, 233.0, 231.0, 185.1, 183.0
A11-B26		13.9	438.2	439.1(M), 437.1(M), 411.1(M-28), 409.1(M-28), 300.0, 298.0, 246.0, 248.0, 185.0, 183.0

[a] The purity of the triazolyl phosphonate compounds were > 96%.

Table S14 GC/MS data of compound A12-B1 to A12-B26.[a]

Code	Chemical structure	RT (min)	MW	Results of MS
A12-B1		17.2	466.3	467.3(M), 465.2(M), 439.1(M-28), 437.1(M-28), 383.0, 381.0, 365.0, 363.0, 185.0, 183.0
A12-B2		17.6	515.1	487.0(M-28), 489.0(M-28), 431.0, 412.9, 351.0, 262.0, 260.0, 234.0, 232.0, 210.0, 208.0, 185.0
A12-B3		16.8	515.1	488.0(M-28), 486.0(M-28), 461.0, 457.0, 262.0, 260.0, 234.0, 232.0, 185.0, 183.0
A12-B4		13.4	454.2	455.1(M), 453.3(M), 427.1(M-28), 425.1(M-28), 353.0, 351.0, 234.0, 232.0, 169.0, 167.0
A12-B5		20.7	481.2	482.4(M), 480.1(M), 454.1(M-28), 452.1(M-28), 426.0, 424.0, 318.0, 316.0, 262.0, 260.0
A12-B6		19.5	481.2	482.1(M), 480.2(M), 454.1(M-28), 452.1(M-28), 380.0, 378.0, 262.0, 260.0.234.0, 232.0
A12-B7		14.6	470.7	471.0(M), 469.0(M), 443.0(M-28), 441.0(M-28), 387.0, 385.0, 369.0, 367.0, 262.0, 260.0
A12-B8		16.6	536.36	535.1(M), 537.1(M), 507.3(M-28), 509.5(M-28), 488.8, 487.0, 348.7, 351.0, 260.0, 262.0, 169.0, 167.0, 88.1, 81.0

A12-B9		11.3	504.2	477.1(M-28), 475.4(M-28), 403.3, 401.3, 340.0, 339.0, 262.0, 260.0, 234.0, 232.0, 198.1, 169.0
A12-B10		12.0	436.3	437.2(M), 435.1(M), 407.1(M-28), 409.1(M-28), 335.0, 333.0, 373.0, 371.1, 262.0, 260.0
A12-B11		14.4	450.3	451.3(M), 449.2(M), 423.1(M-28), 421.1(M-28), 367.0, 365.0, 3459.0, 347.0, 234.0, 232.0
A12-B12		11.1	562.1	563.6(M), 535.2(M-28), 533.3(M-28), 459.1, 207.1, 190.1, 163.0, 127.0, 128.0, 76.1, 73.1
A12-B13		16.9	484.7	485.0(M), 483.4(M), 457.1(M-28), 455.1(M-28), 401.0, 399.0, 383.0, 381.0, 234.0, 232.0
A12-B14		14.9	470.7	471.1(M), 469.1(M), 443.0(M-28), 441.0(M-28), 387.0, 385.0, 369.0, 367.0, 262.0, 260.0
A12-B15		11.5	504.2	477.1(M-28), 475.2(M-28), 403.0, 401.1, 341.0, 339.0, 262.0, 260.0, 234.0, 232.0
A12-B16		12.5	454.2	455.2(M), 453.1(M), 427.1(M-28), 425.1(M-28), 353.0, 351.0, 234.0, 232.0, 169.0, 167.0
A12-B17		12.2	454.2	455.2(M), 453.1(M), 427.1(M-28), 425.1(M-28), 371.0, 369.0, 353.0, 351.0, 262.0, 260.0

A12-B18		10.9	490.2	491.1(M), 489.1(M), 463.1(M-28), 461.1(M-28), 389.1, 387.0, 262.0, 260.0, 234.0, 232.0
A12-B19		11.1	472.2	473.1(M), 471.1(M), 445.1(M-28), 443.1(M-28), 389.0, 387.0, 371.0, 369.0, 234.0, 232.0
A12-B20		14.7	464.3	465.2(M), 463.2(M), 437.1(M-28), 435.1(M-28), 381.1, 379.0, 363.0, 361.0262.0, 260
A12-B21		13.9	450.3	451.3(M), 449.2(M), 423.1(M-28), 421.1(M-28), 349.0, 347.0, 262.0, 260.0, 234.0, 232.0
A12-B22		13.0	450.2	451.1(M), 449.1(M), 423.1(M-28), 421.1(M-28), 262.0, 260.0, 234.0, 232.0, 204.1, 144.1
A12-B23		14.1	464.3	465.2(M), 463.1(M), 437.1(M-28), 435.1(M-28), 300.1, 298.1, 262.0, 260.0, 234.0, 232.0
A12-B24		15.5	470.7	471.2(M), 469.2(M), 443.0(M-28), 441.0(M-28), 369.0, 367.0, 262.0, 260.0, 232.0, 234.0
A12-B25		16.0	466.3	467.4(M), 465.2(M), 439.1(M-28), 437.1(M-28), 365.0, 363.0, 262.0, 260.0, 234.0, 232.0
A12-B26		14.9	466.3	467.3(M), 464.0(M), 439.1(M-28), 437.1(M-28), 262.0, 260.0, 234.0, 232.0, 185.0, 183.0, 121.0, 120.0

[a] The purity of the triazolyl phosphonate compounds were > 96%.

Table S15: Inhibition rate of compound TA-101 against the growth of *Rhizoctonia solani*

Concentration（mg/mL）	0	0.005	0.05	0.5	1	5
Growth diameter (mm)	14.3	8.2	3.7	0.5	0	0
Inhibitory (%)		42.7%	74.1%	96.5%	100%	100%
Growth diameter (mm)	14.0	8.0	3.0	1.0	0	0
Inhibitory (%)		42.9%	78.6%	93.0%	100%	100%
Growth diameter (mm)	12.0	7.2	2.0	0.5	0	0
Inhibitory (%)		40%	83.3%	95.8%	100%	100%

Table S16: Inhibition rate of compound TA-125 against the growth of *Rhizoctonia solani*

Concentration（mg/mL）	0	0.005	0.05	0.5	1	5
Growth diameter (mm)	14.0	8.5	4.0	0.5	0	0
Inhibitory (%)		39.3%	71.4%	96.4%	100%	100%
Growth diameter (mm)	15.0	8.5	4.2	2.0	0	0
Inhibitory (%)		43.3%	72.0%	86.7%	100%	100%
Growth diameter (mm)	15.0	10	6.3	2.5	0	0
Inhibitory (%)		33.3%	58%	83.3%	100%	100%

Table S17: Inhibition rate of compound TA-133 against the growth of *Rhizoctonia solani*

Concentration（mg/mL）	0	0.005	0.05	0.5	1	5
Growth diameter (mm)	14.0	8.0	5.0	0.5	0	0
Inhibitory (%)		42.9%	64.2%	96.4%	100%	100%
Growth diameter (mm)	13.0	7.0	3.5	0.5	0	0
Inhibitory (%)		46.2%	73.1%	96.2%	100%	100%
Growth diameter (mm)	15.0	14.0	6.0	2.5	1.2	0
Inhibitory (%)		6.7%	60.0%	83.3%	92.0%	100%

Table S18 The benefits of the integrated workflow for bioactive molecule discovery triggered by ILDDS.

Retry	Items	Solution
1	High atom efficincy and waste minimization	*H_2O as solely by-product; The optimized catalyst choline acetate (A7-B1) is recoverable and reused.*
2	Safe solvents and reagents	*No reaction solvents; The optimized ionic liquid A7-B1 is biocompatible and nontoxic.*
3	Elimination of unnecessary steps	*No chromatographic separations; In-situ biological assays for target products.*
4	Energy utilization minimization	*Reaction and isolation are conducted in parallel in tubes under open; No specialized and high energy-consumption instruments.*
5	Low cost	*Raw materials are Inexpensive and widely used bulk chemicals. acetic acid (*$55per 1L*); choline chloride (*$20 per100g*);* aniline($35 per100g*).*

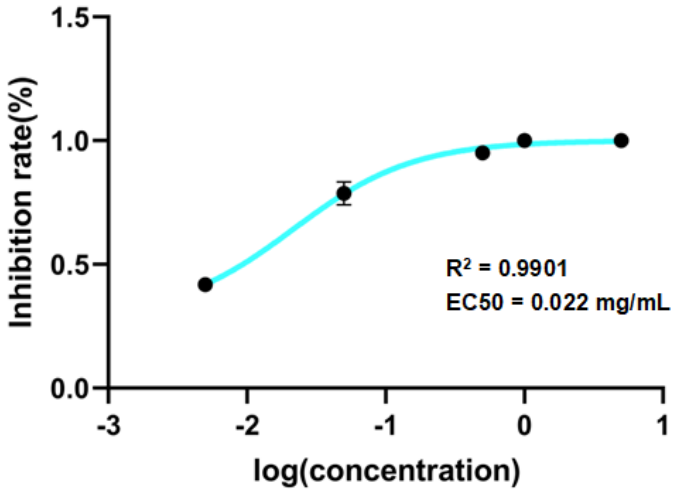


Figure S10 Inhibition rate curve of compound TA-101

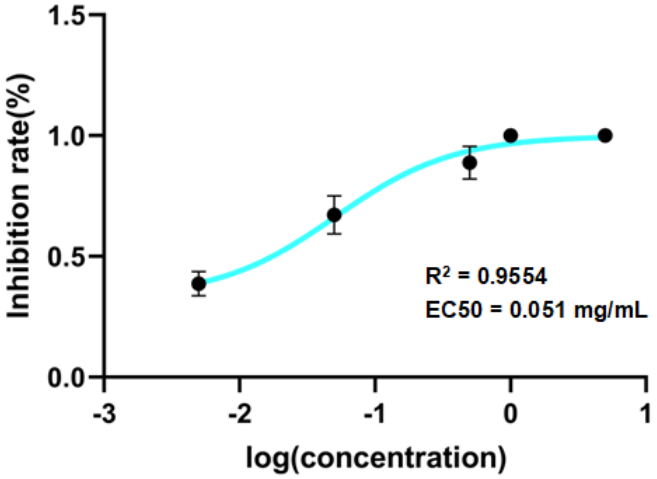


Figure S11 Inhibition rate curve of compound TA-125

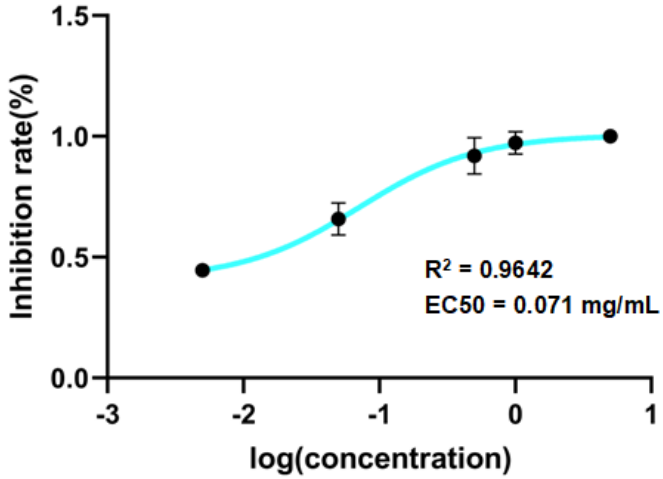


Figure S12 Inhibition rate curve of compound TA-133

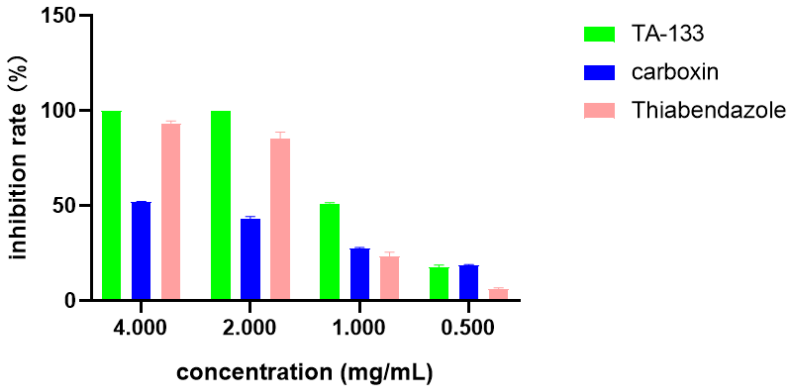


Figure S13 Comparison of inhibitive bioactivity of TA-133 with Carboxin and Thiabendazole at different concentrations.

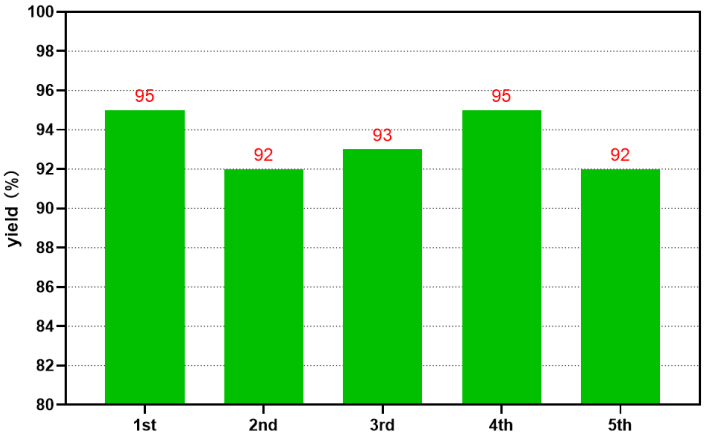
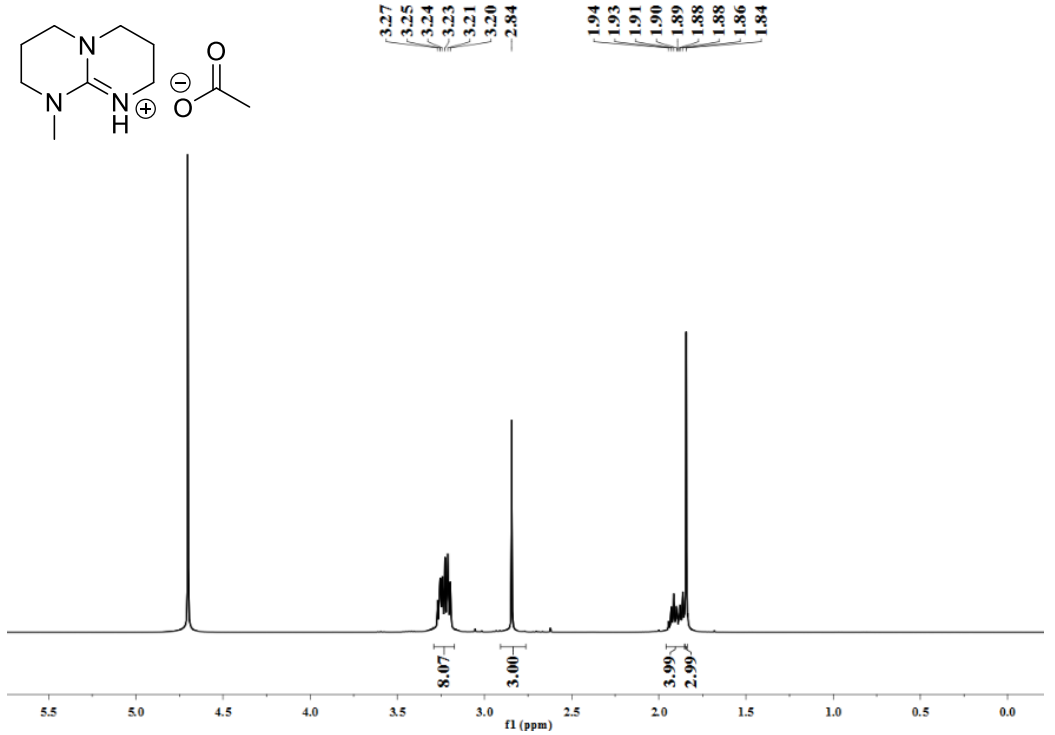
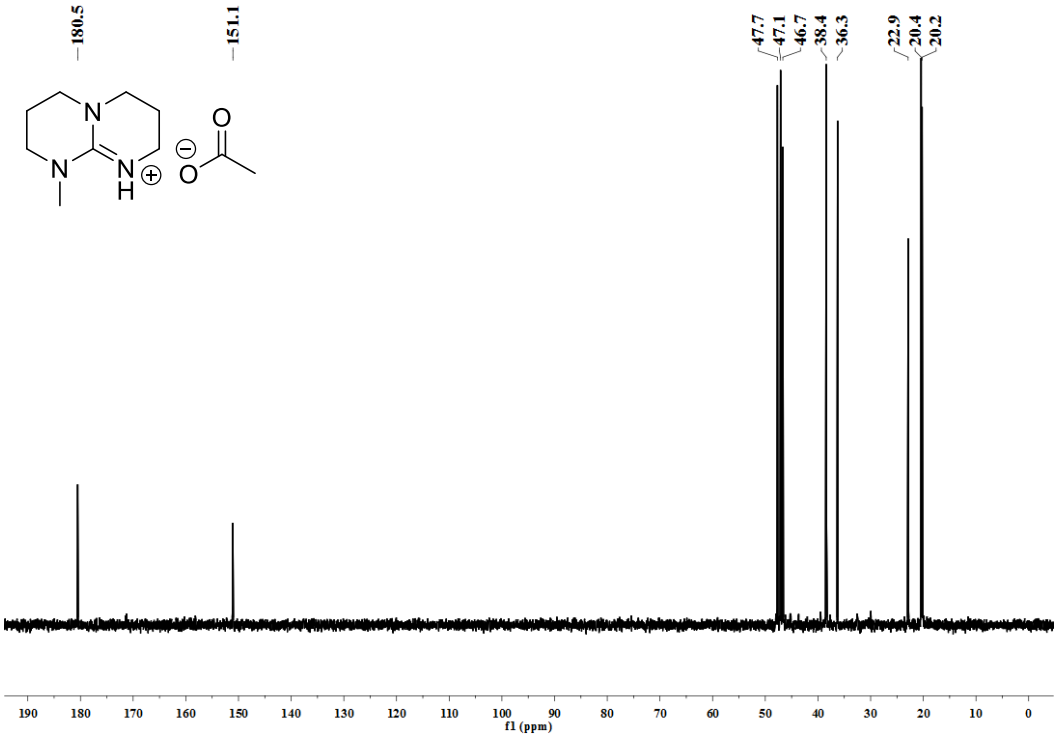


Figure S14 Recycling and reuse of ionic liquid A7-B1 in the synthesis of triazolyl phosphonate.

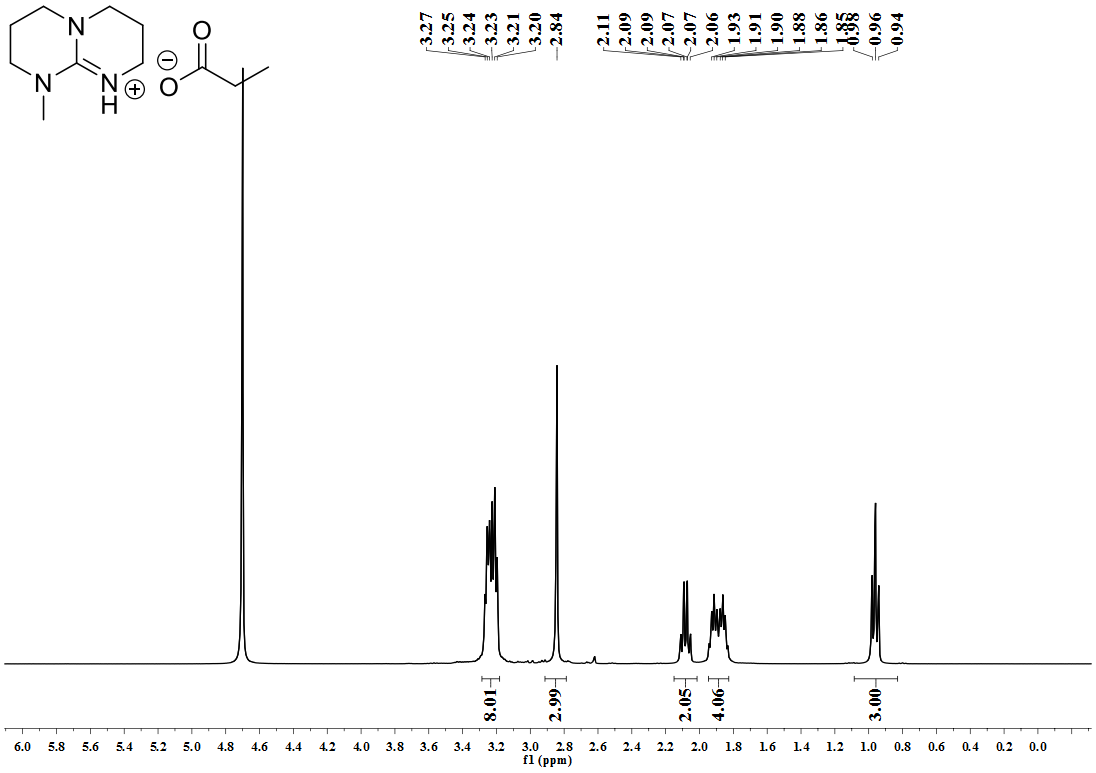
^{1}H NMR and ^{13}C NMR spectra of ionic liquids

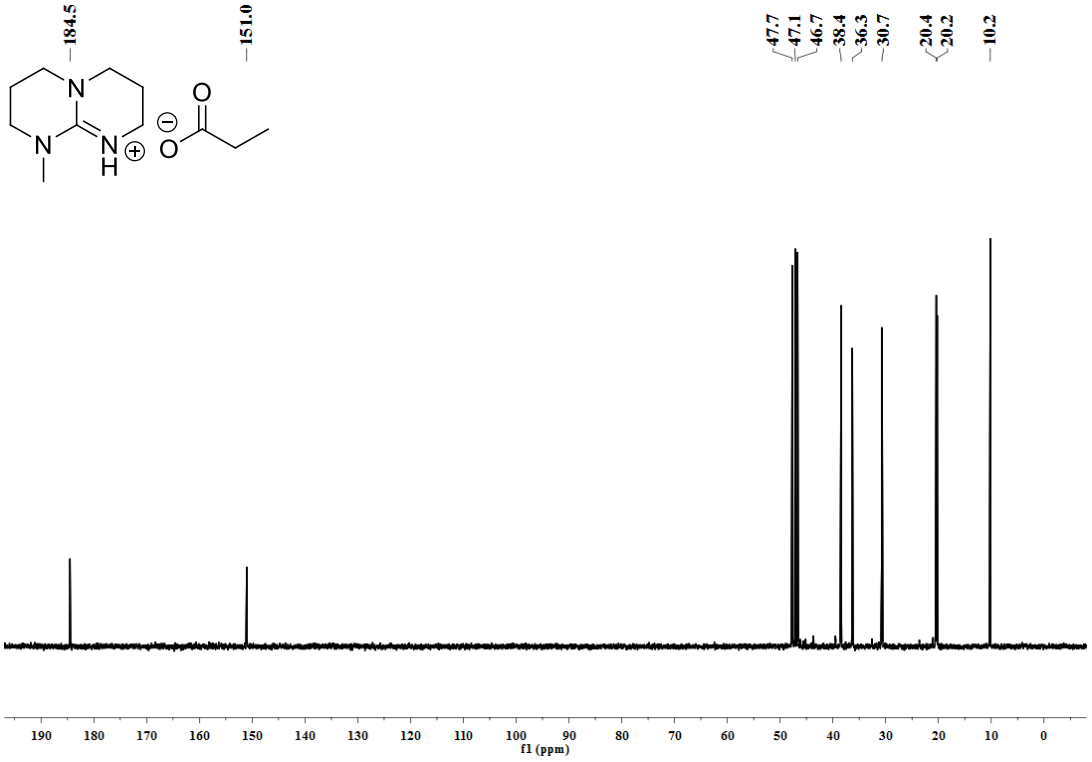
A3-B1: [MTBD][Ac]



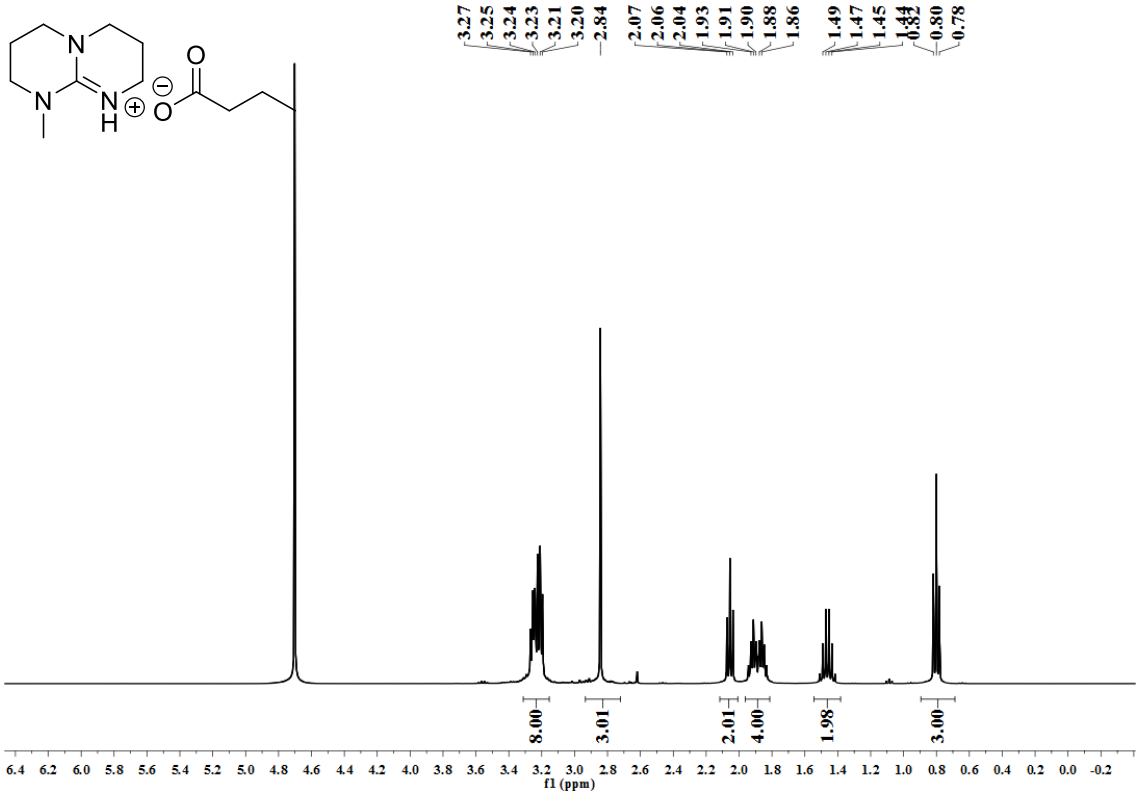


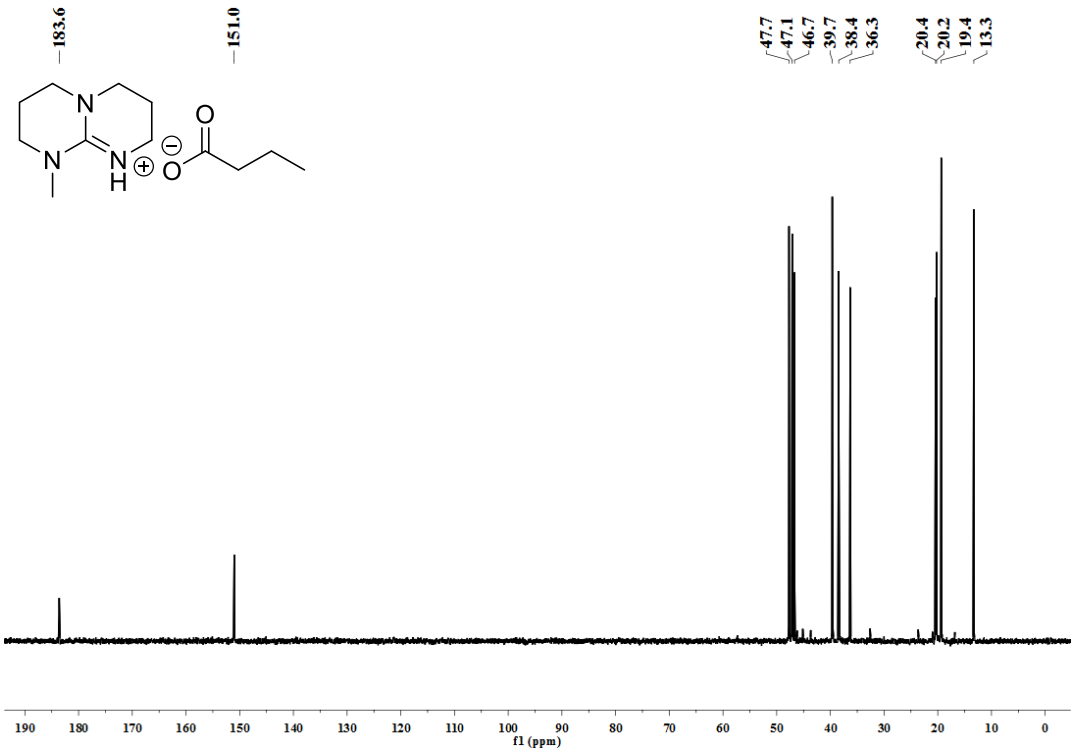
A3-B2: [MTBD][Pro]



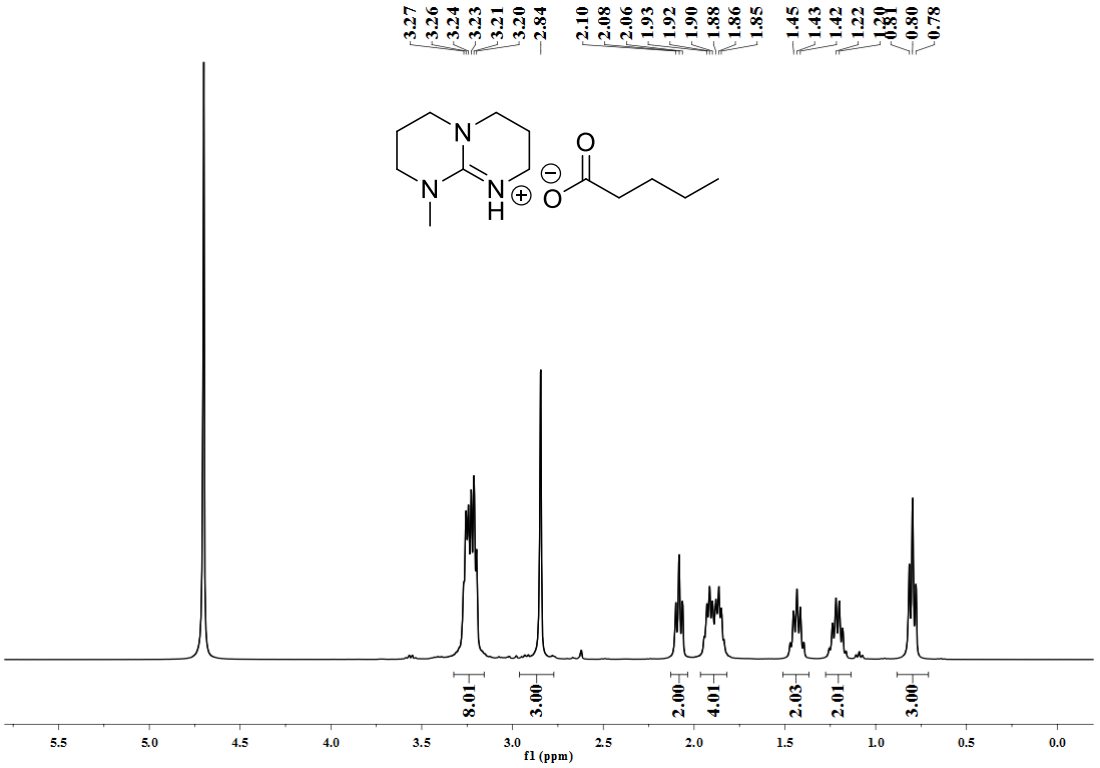


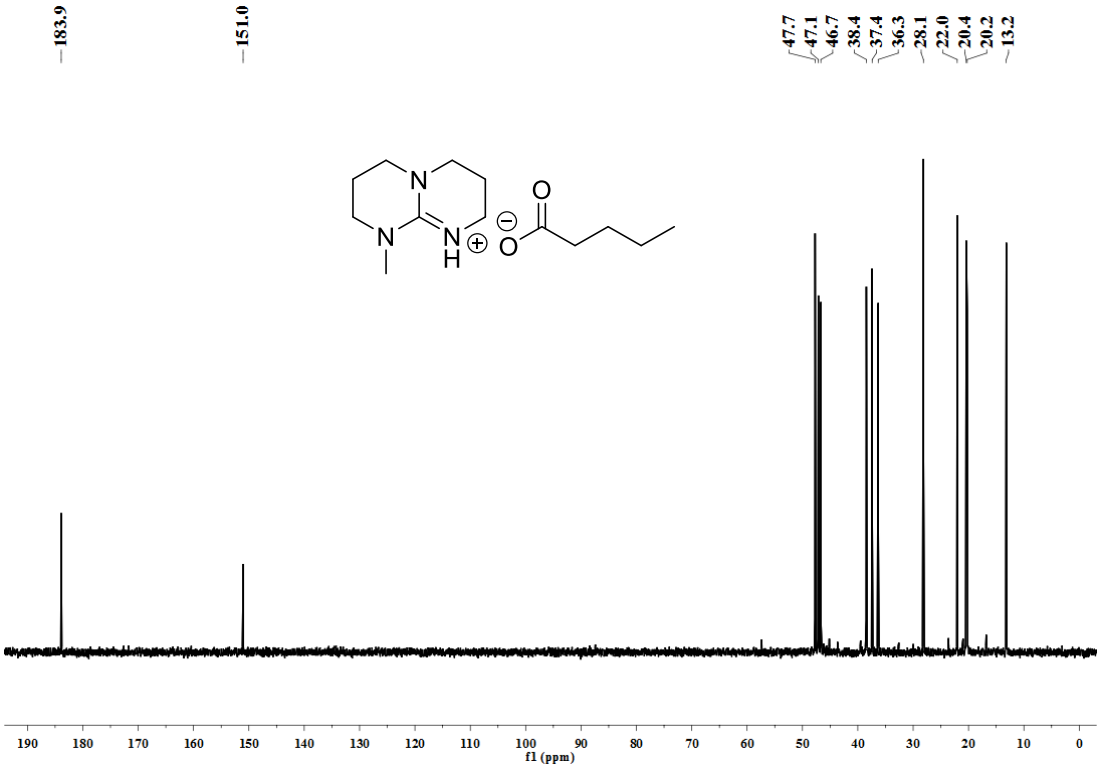
A3-B3: [MTBD][But]



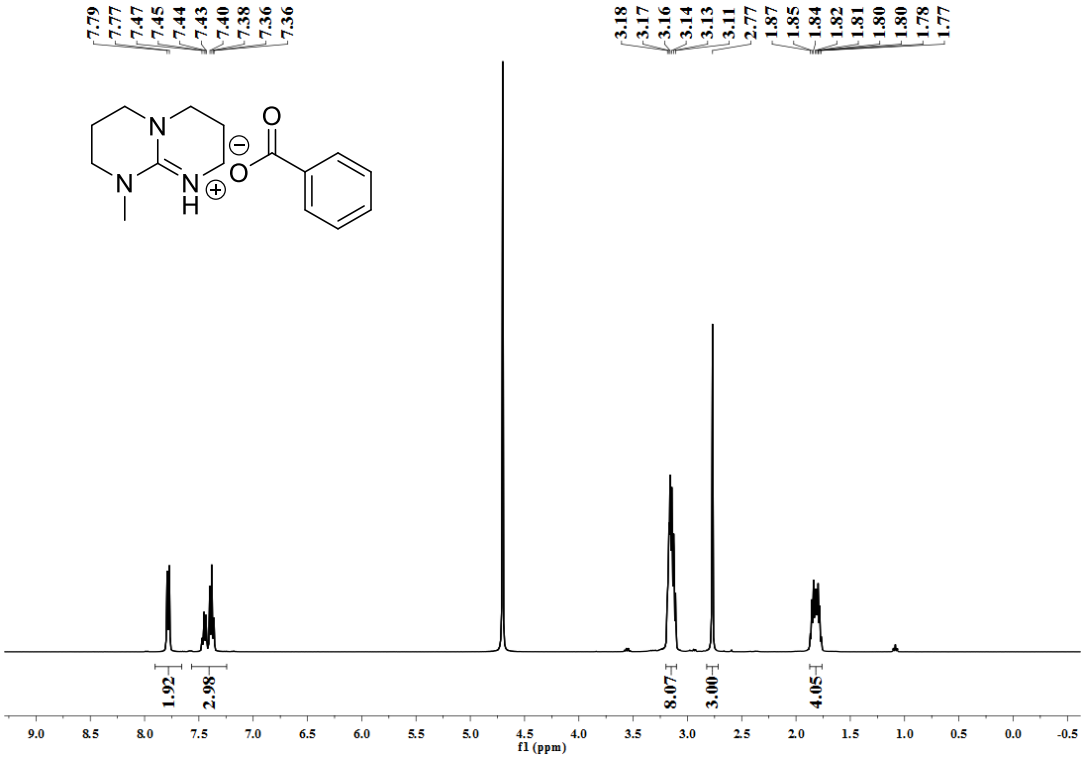


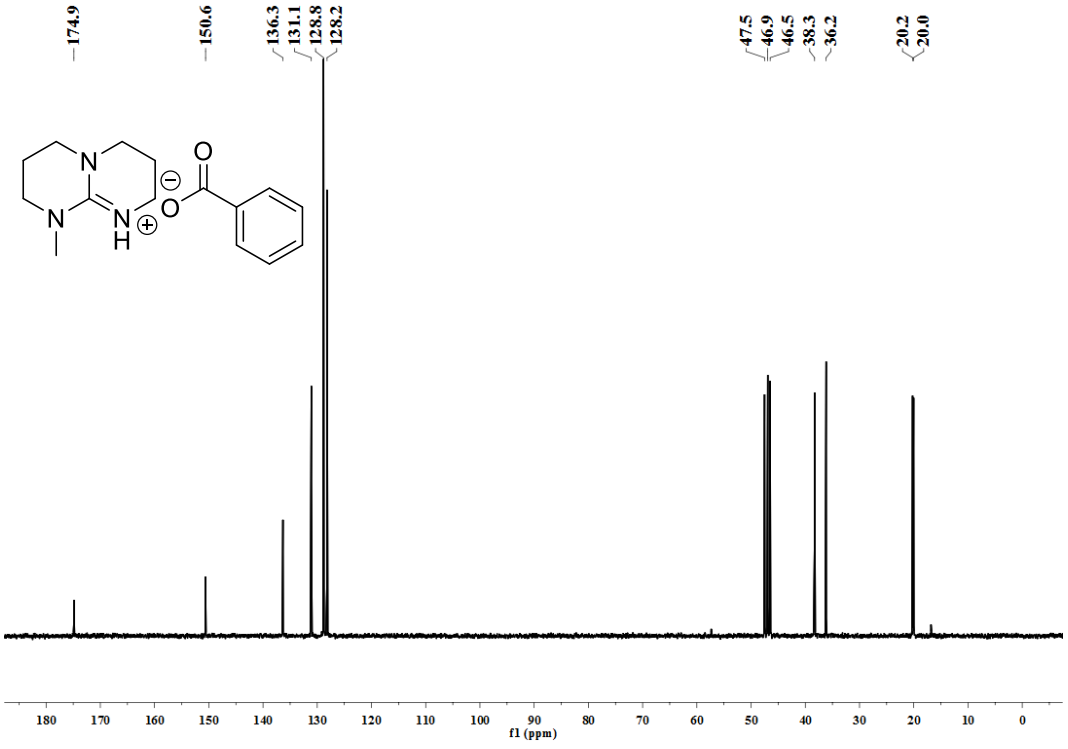
A3-B4: [MTBD][Val]



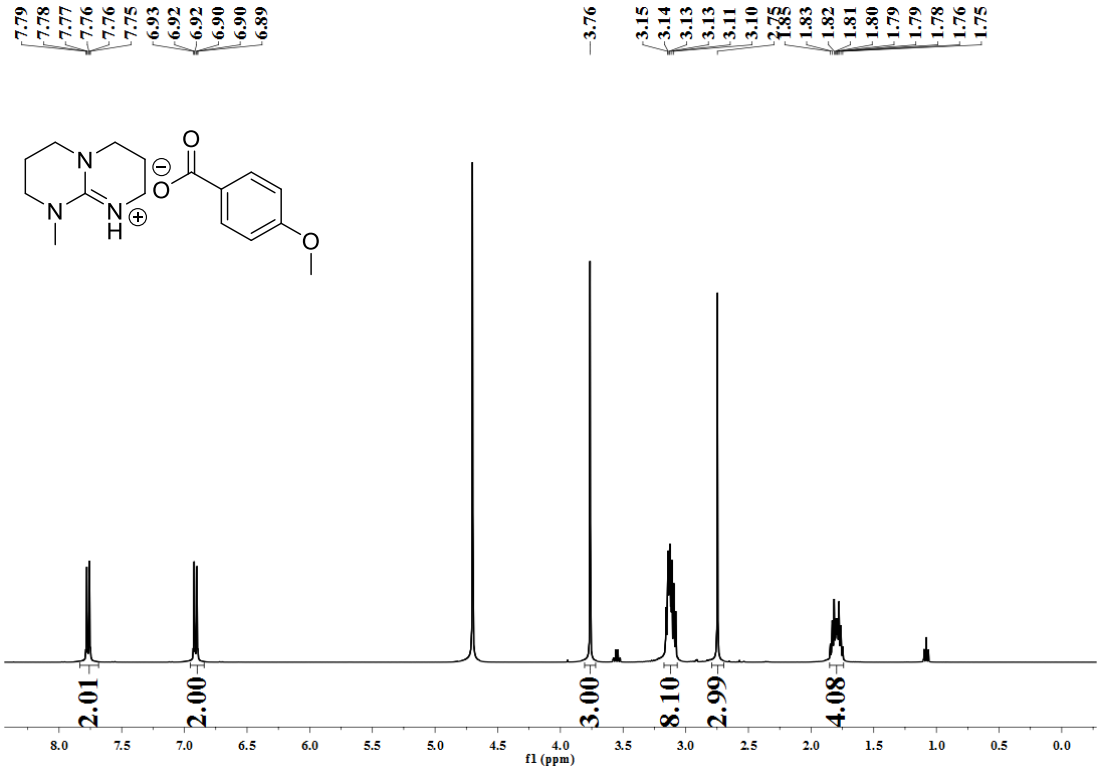


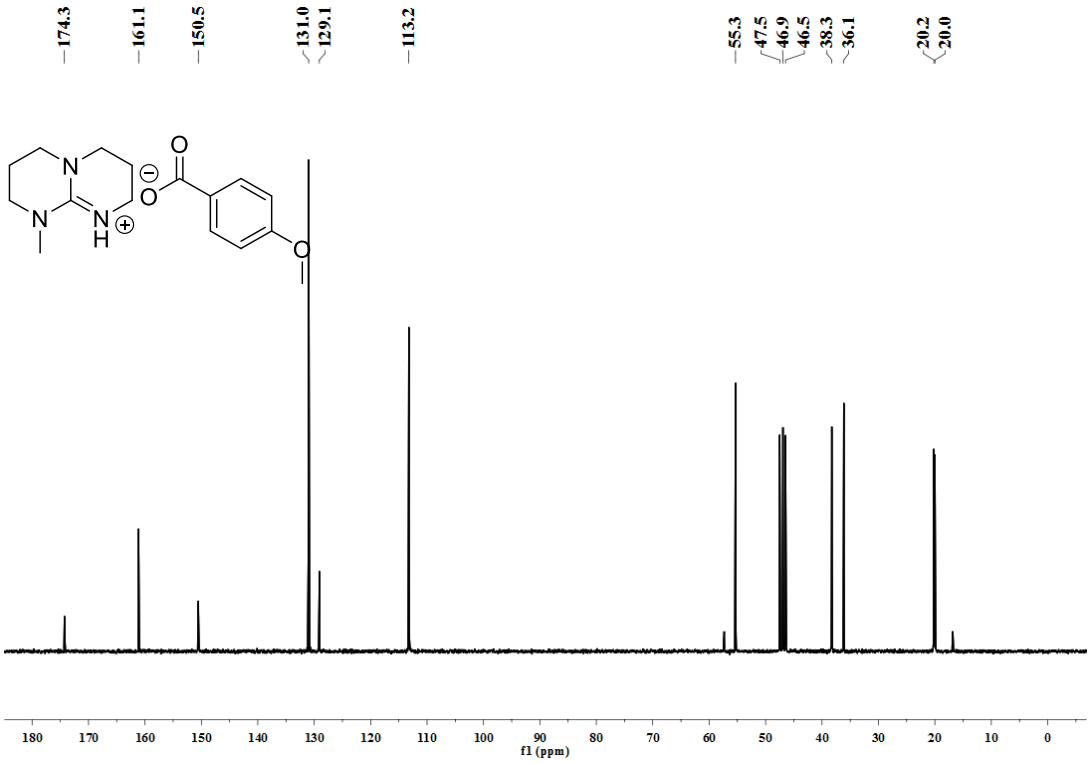
A3-B5: [MTBD][Ben]



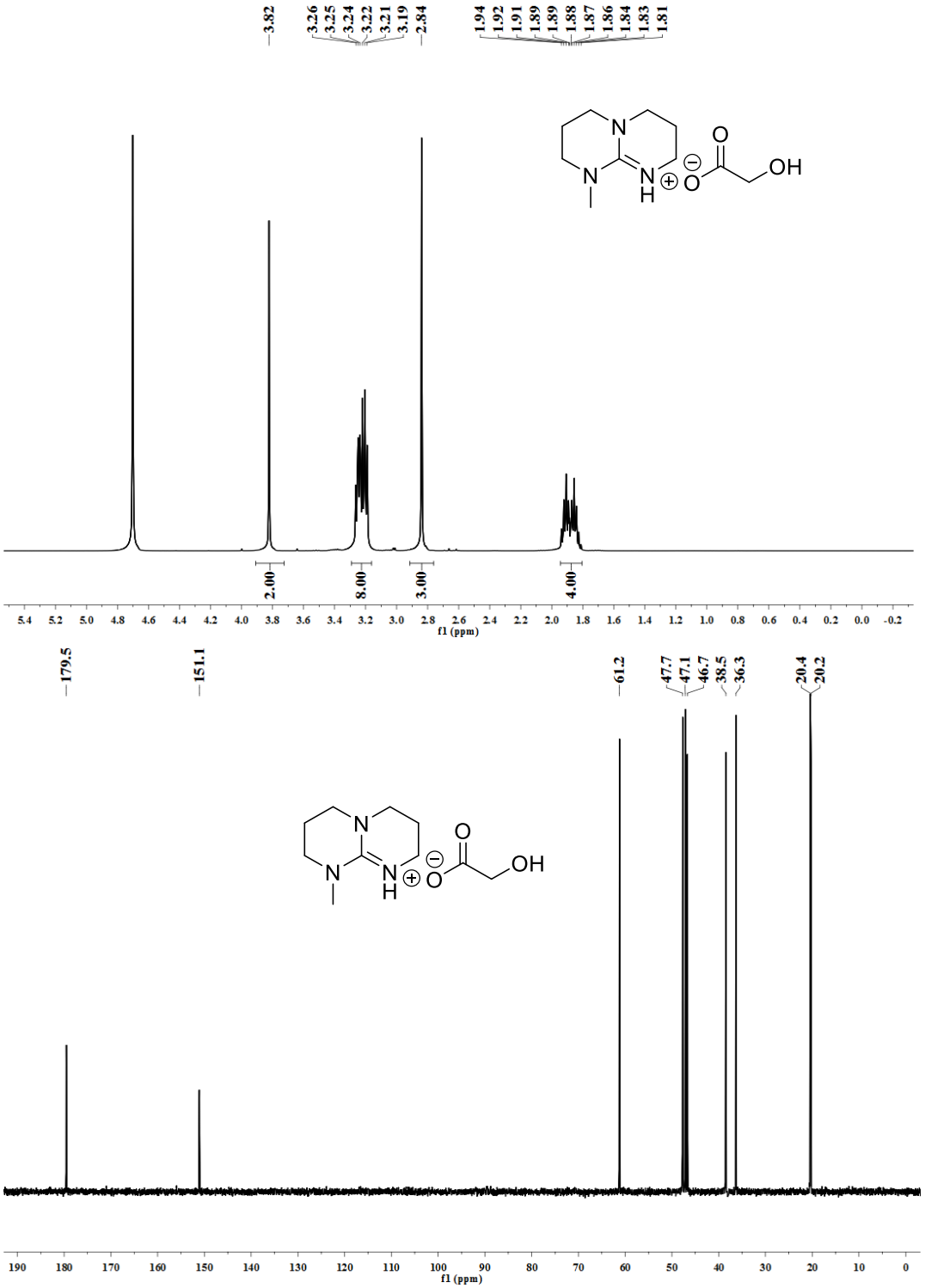


A3-B6: [MTBD][Ani]

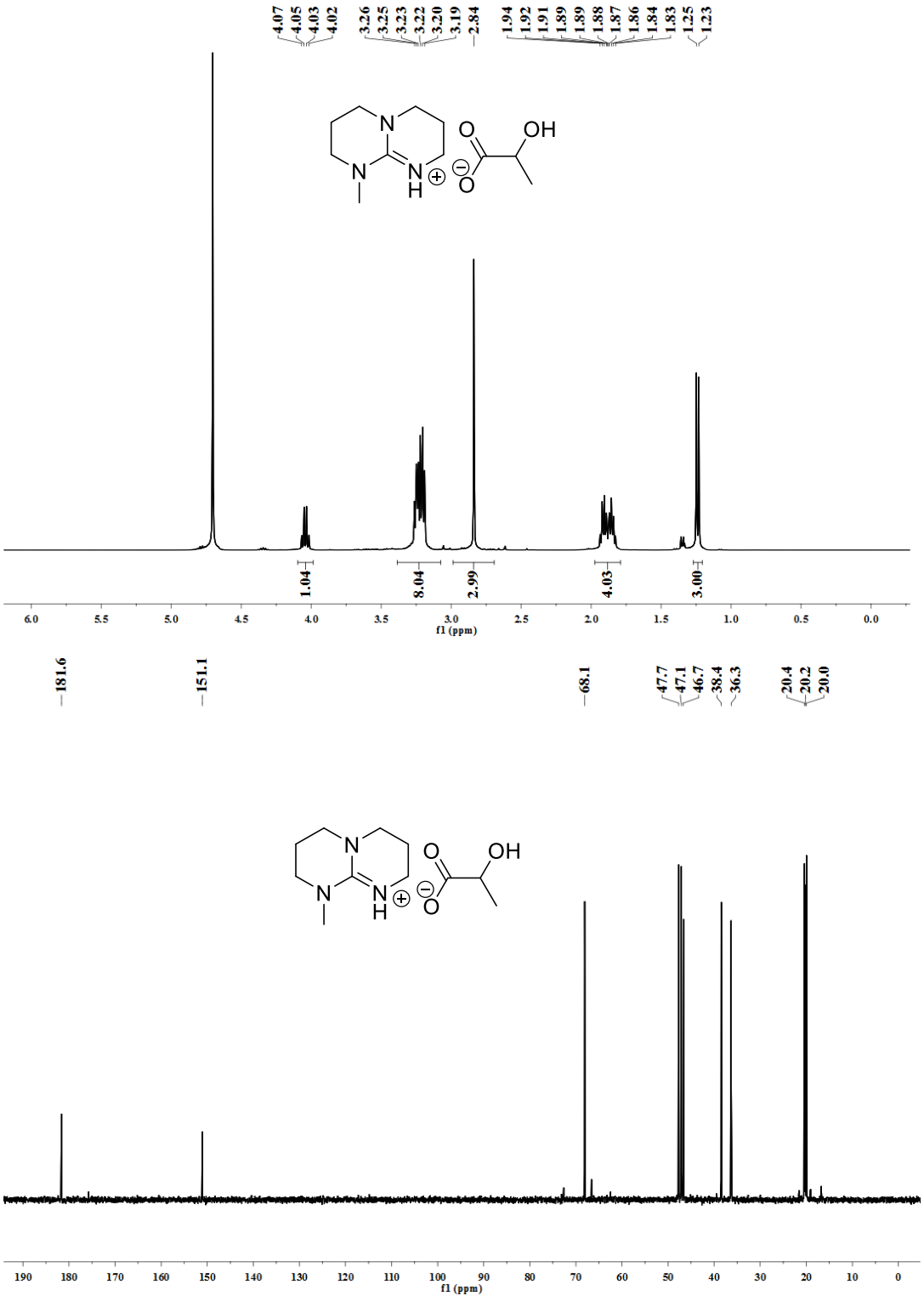




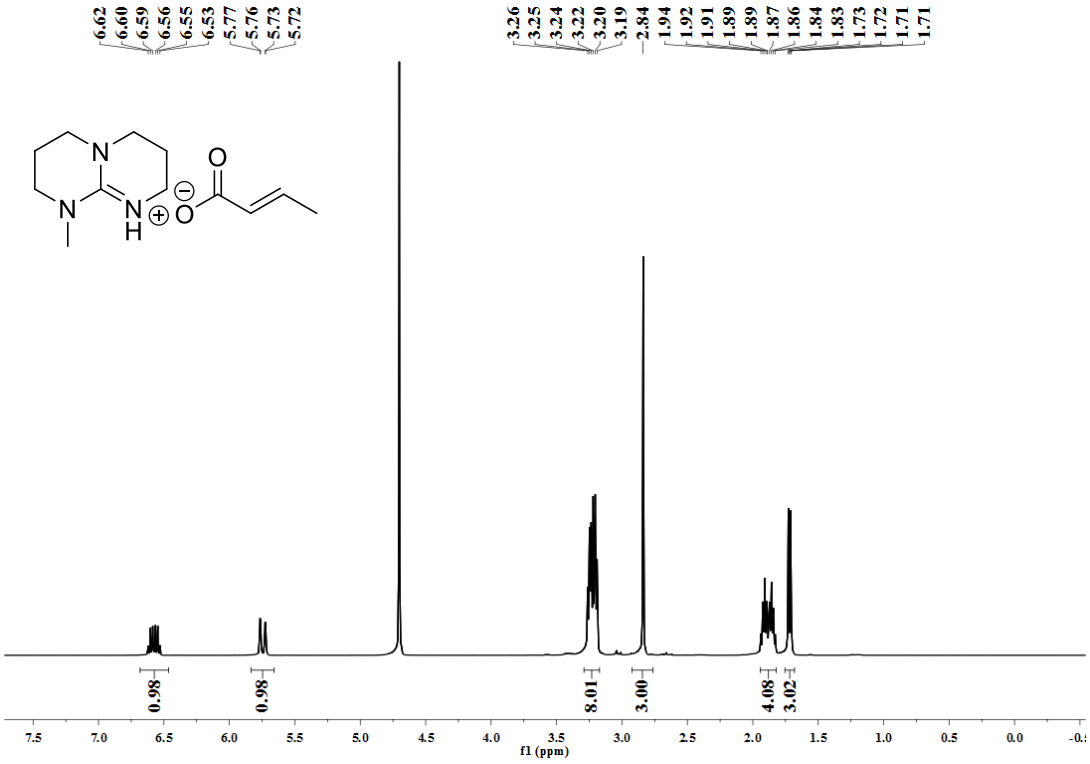
A3-B7: [MTBD][Gly]

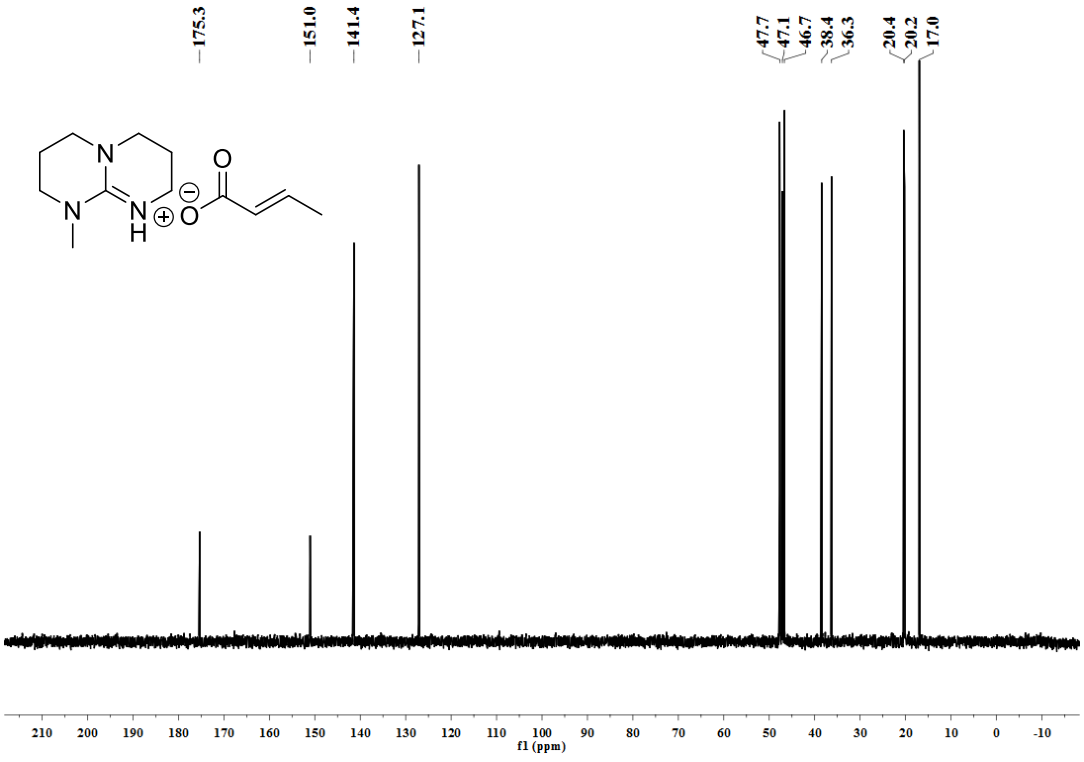


A3-B8: [MTBD][Lac]

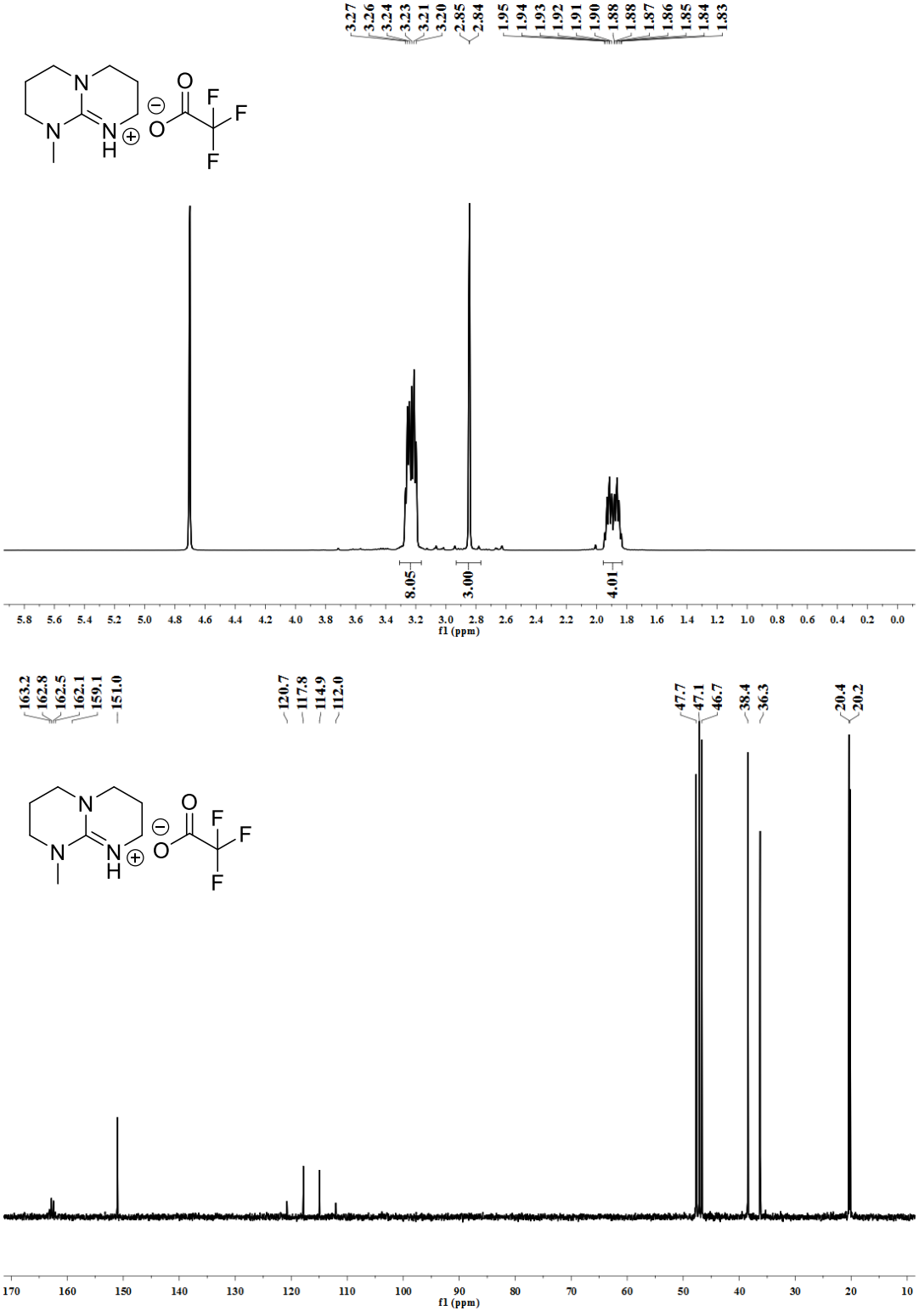


A3-B9: [MTBD][Cro]

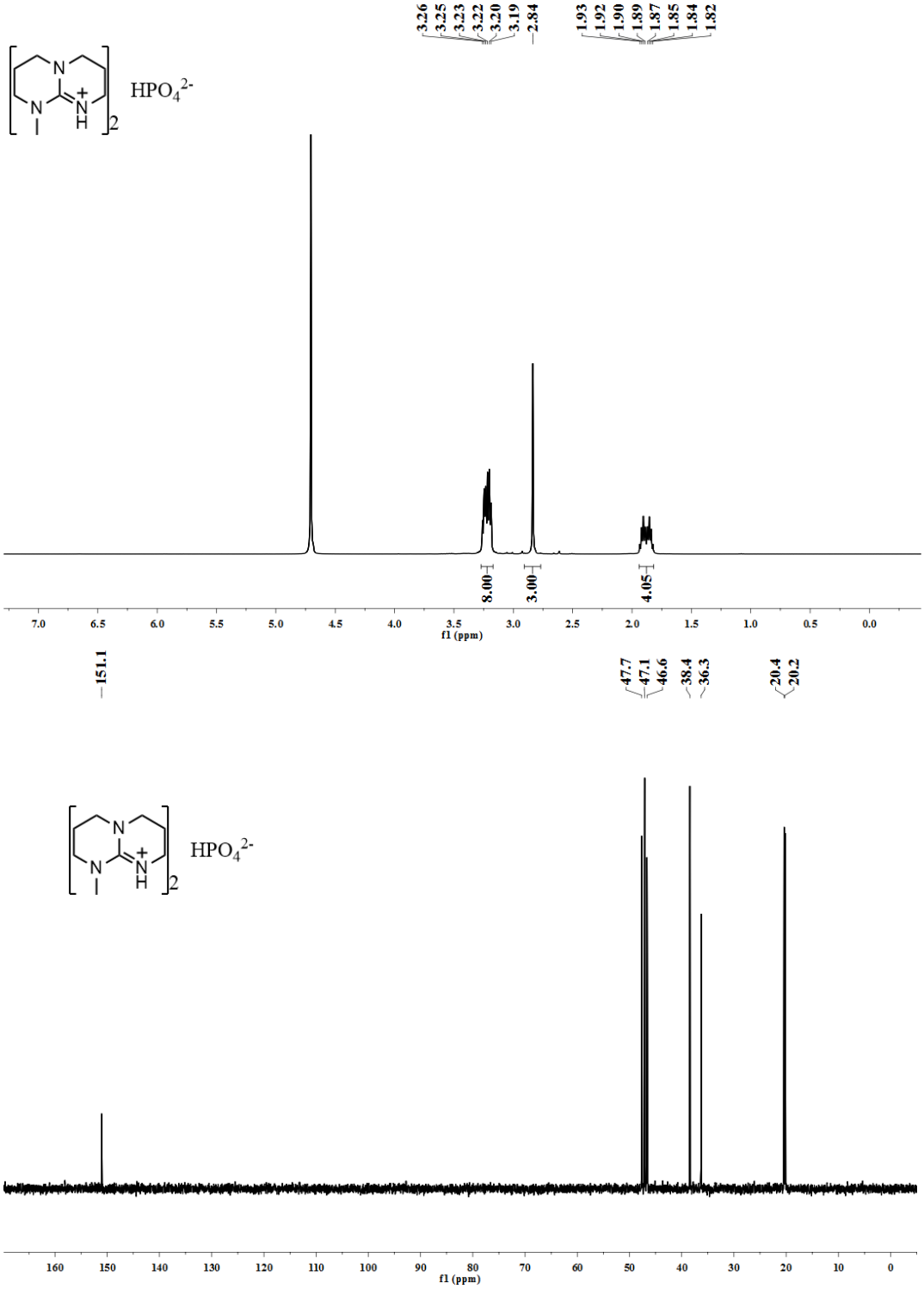




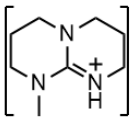
A3-B10: [MTBD][TFA]



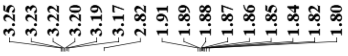
A3-B11: [MTBD][H_2PO_4]

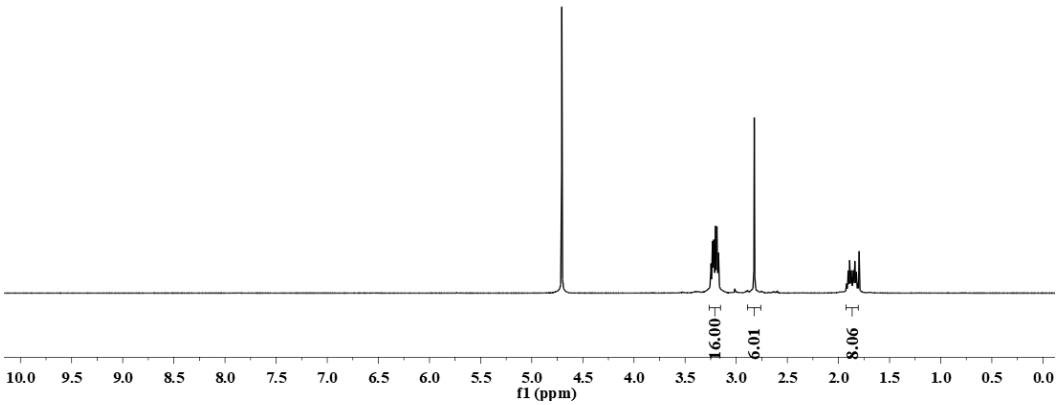


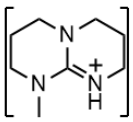
A3-B12: [MTBD][H_2PO_4]



$H_2PO_4^-$

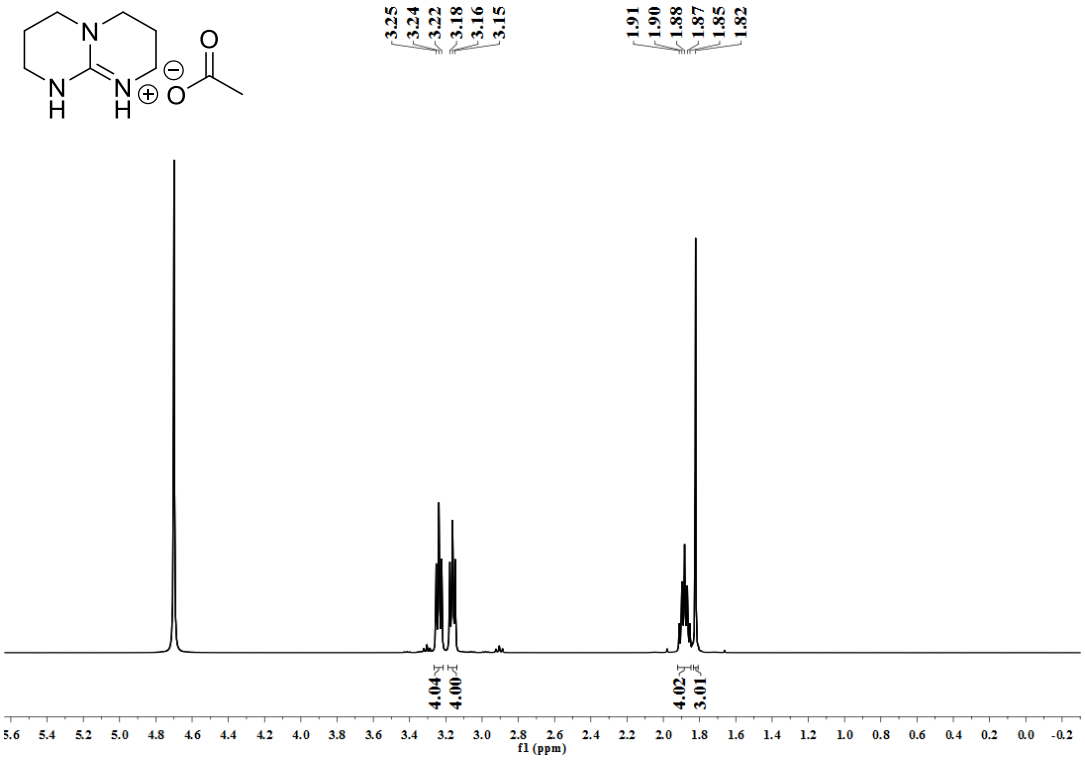


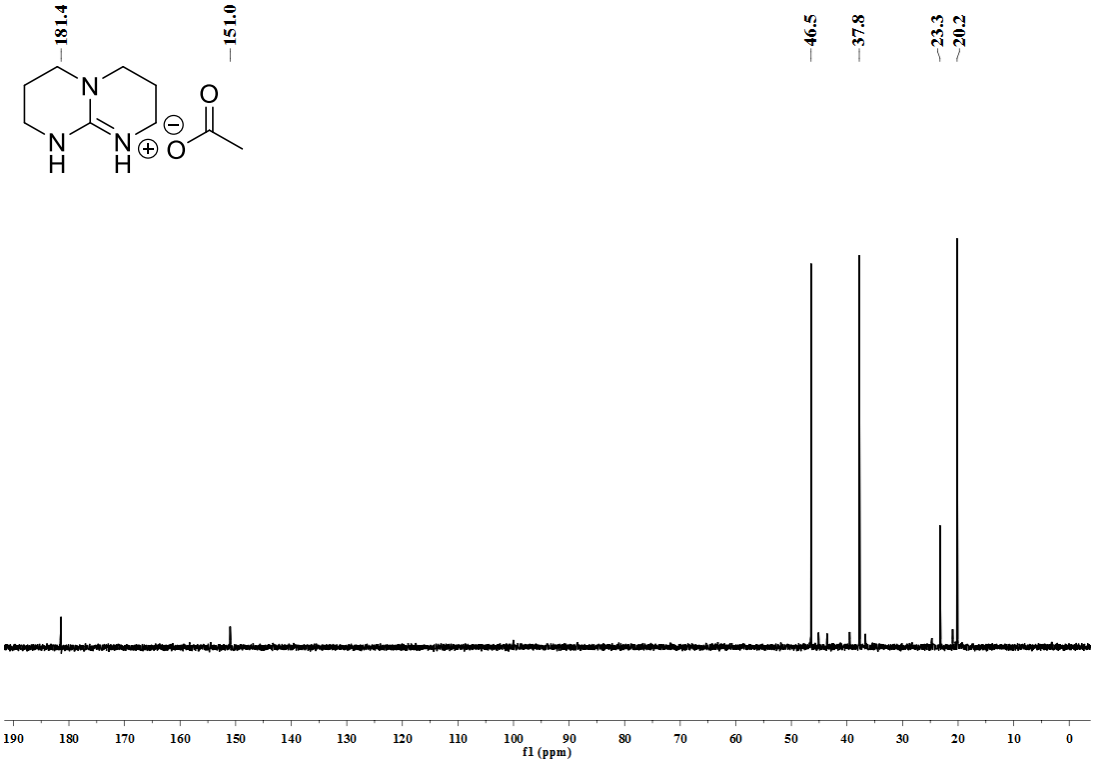




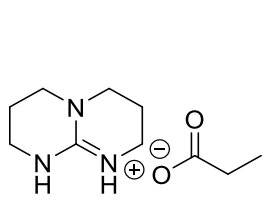
$H_2PO_4^-$

A4-B1: [TBD][Ac]

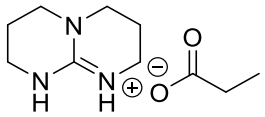

3.25
3.24
3.22
3.18
3.16
3.15
1.91
1.90
1.88
1.87
1.85
1.82
4.04
4.00
4.02
3.01
f1 (ppm)


181.4
151.0
46.5
37.8
23.3
20.2
f1 (ppm)

A4-B2: [TBD][Pro]

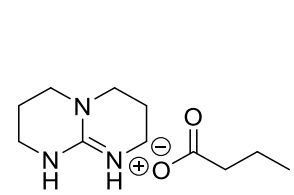


3.27
3.26
3.24
3.19
3.18
3.17
2.12
2.10
1.91
1.90
1.88
1.00
0.98
0.96
8.00
2.05
4.03
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

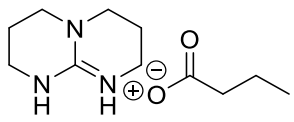


183.1
150.9
46.5
37.8
29.5
20.2
9.6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

A4-B3: [TBD][But]

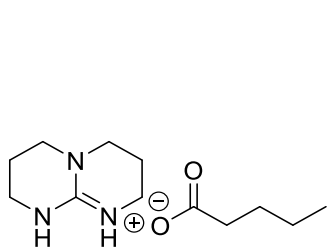


3.29
3.28
3.26
3.22
3.20
3.19
2.09
1.93
1.92
1.90
1.51
0.84
0.83
8.00
2.00
4.00
2.06
3.00
f1 (ppm)



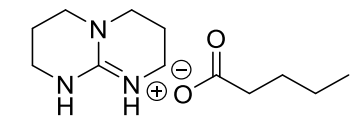
181.9
150.9
46.5
38.0
37.8
20.2
18.8
13.0
f1 (ppm)

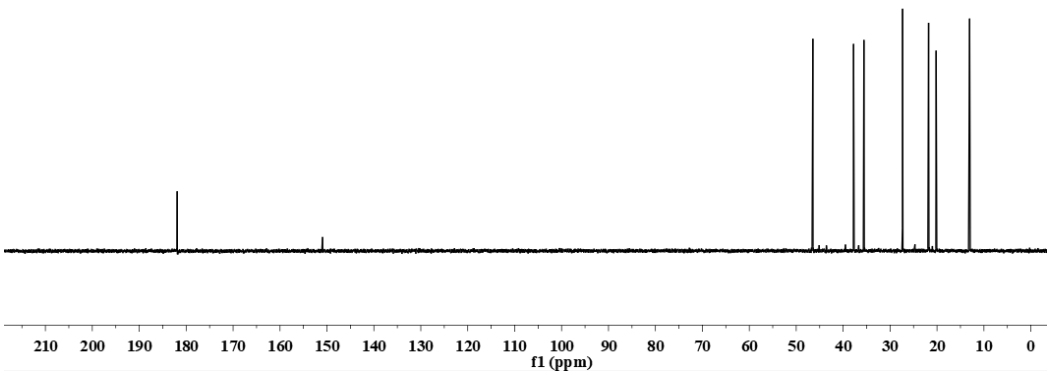
A4-B4: [TBD][Val]



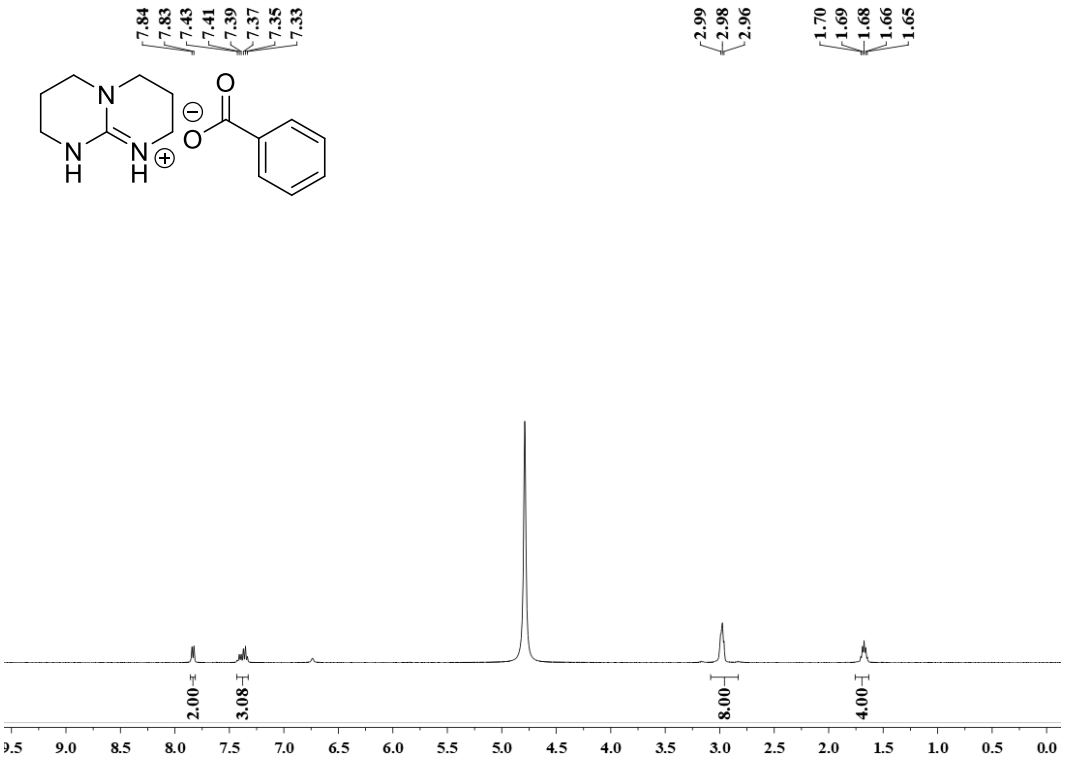
3.31
3.29
3.28
3.23
3.22
3.20
2.15
2.14
2.12
1.96
1.95
1.93
1.92
1.90
1.52
1.50
1.49
1.47
1.45
1.31
1.29
1.27
1.25
1.24
1.22
0.87
0.85
0.83
8.00
2.09
3.94
2.12
2.11
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5 -3.0
f1 (ppm)

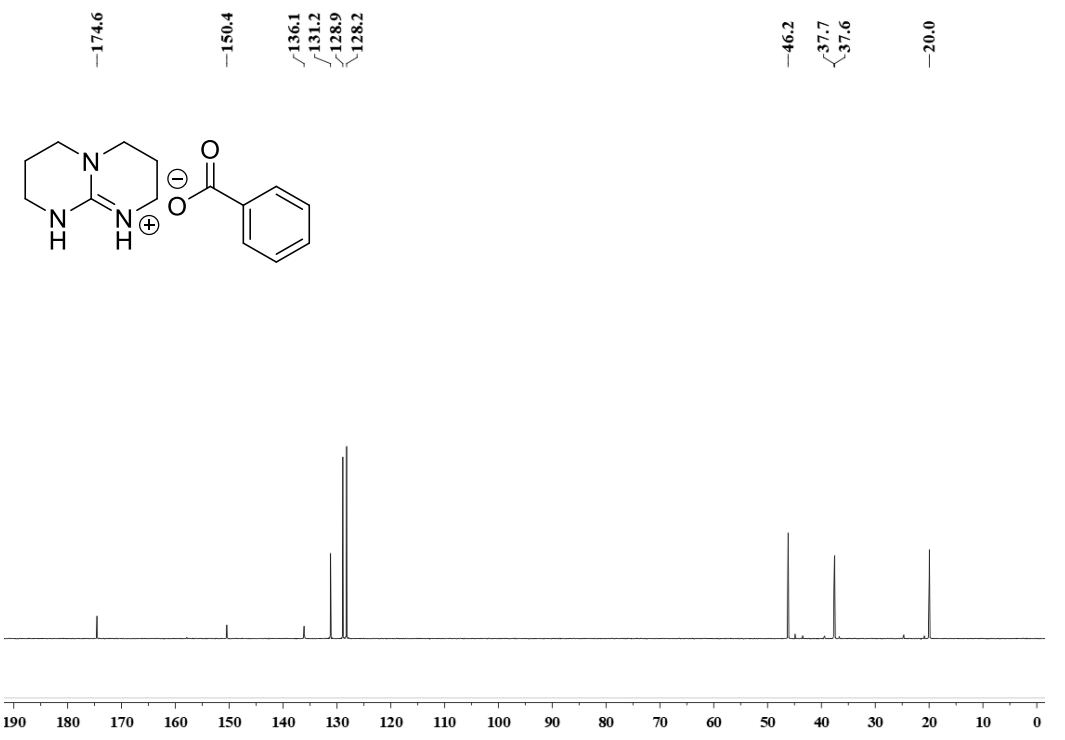
181.9
150.9
46.5
37.8
35.6
27.3
21.8
20.2
13.0



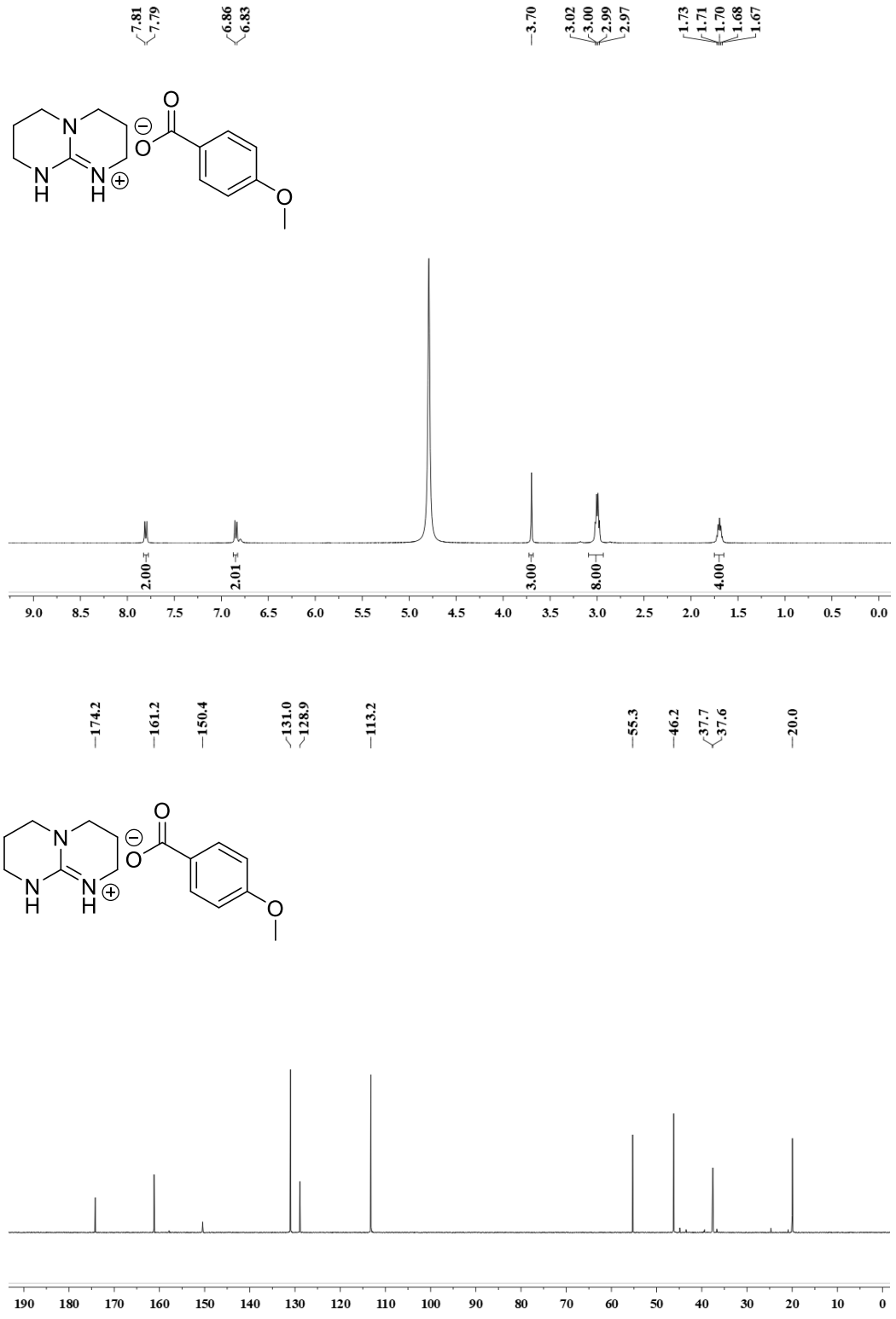

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

A4-B5: [TBD][Ben]

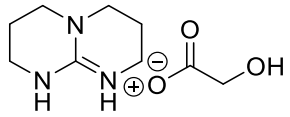

7.84
7.83
7.43
7.41
7.39
7.37
7.35
7.33
2.99
2.98
2.96
1.70
1.69
1.68
1.66
1.65
2.00
3.08
8.00
4.00


174.6
150.4
136.1
131.2
128.9
128.2
46.2
37.7
37.6
20.0

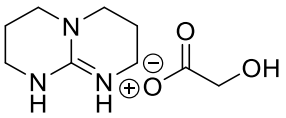
A4-B6: [TBD][Ani]


7.81
7.79
6.86
6.83
3.70
3.02
3.00
2.99
2.97
1.73
1.71
1.70
1.68
1.67
2.00
2.01
3.00
8.00
4.00
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 0.0
174.2
161.2
150.4
131.0
128.9
113.2
55.3
46.2
37.7
37.6
20.0
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

A4-B7: [TBD][Gly]

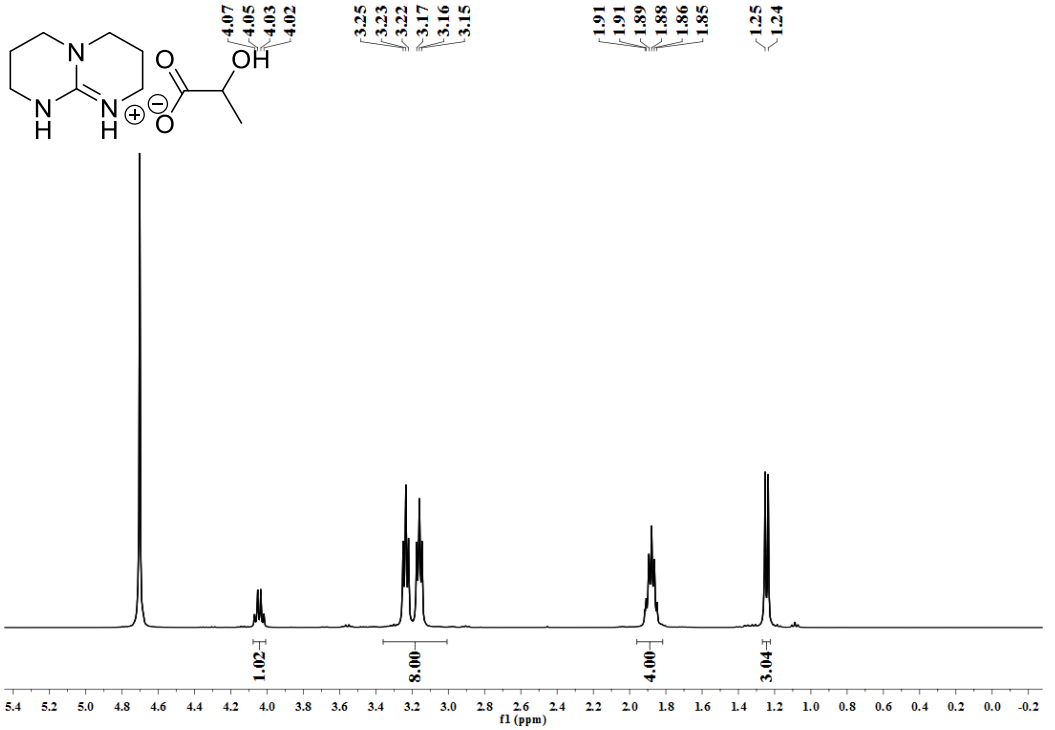

N
O
N
H
N
H
O
OH

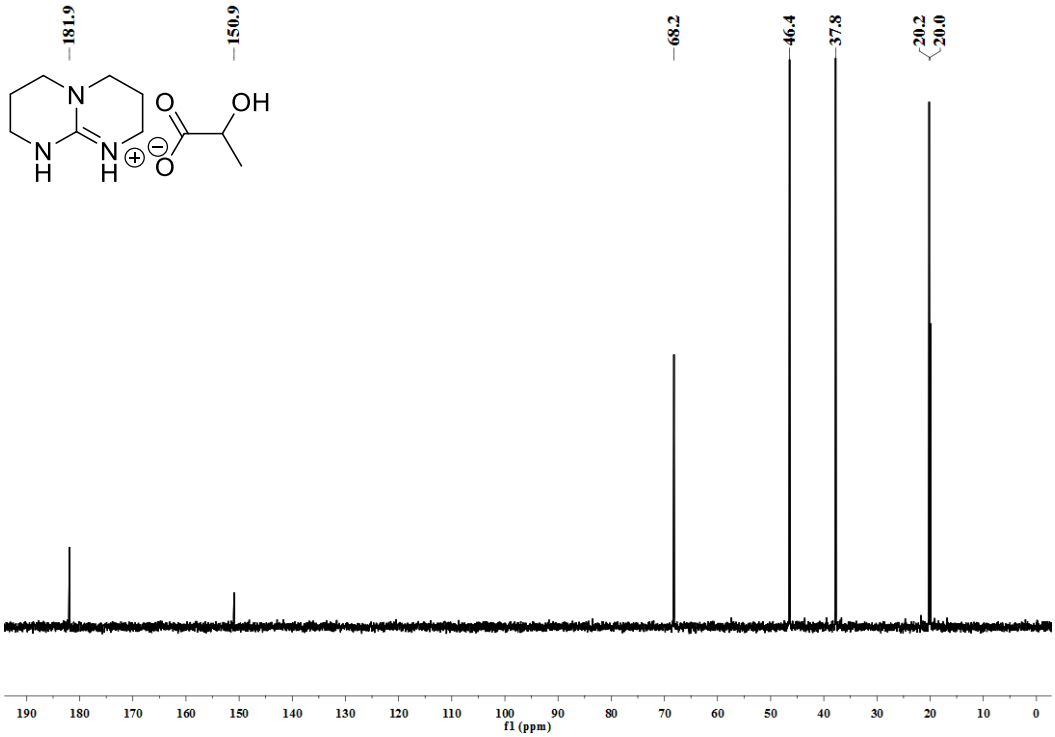
3.90
3.31
3.30
3.28
3.23
3.22
3.21
1.96
1.95
1.94
1.92
1.91
2.00
8.00
4.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


N
O
N
H
N
H
O
OH

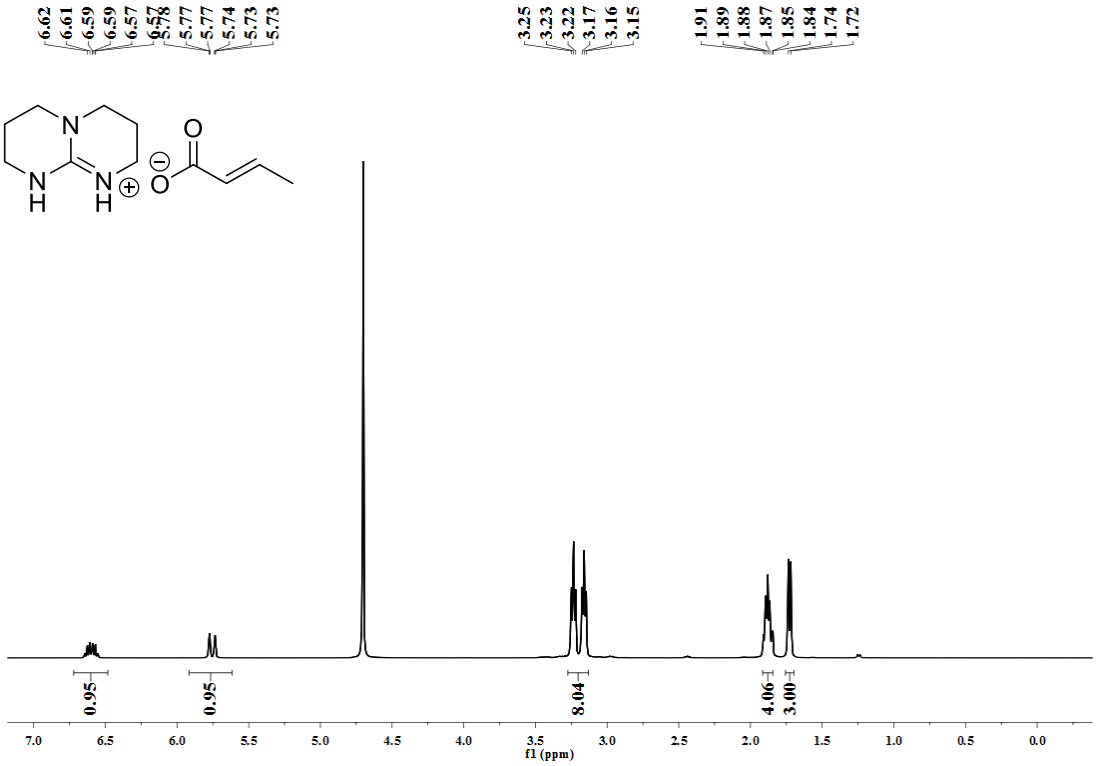
178.1
150.9
60.3
46.4
37.8
20.2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

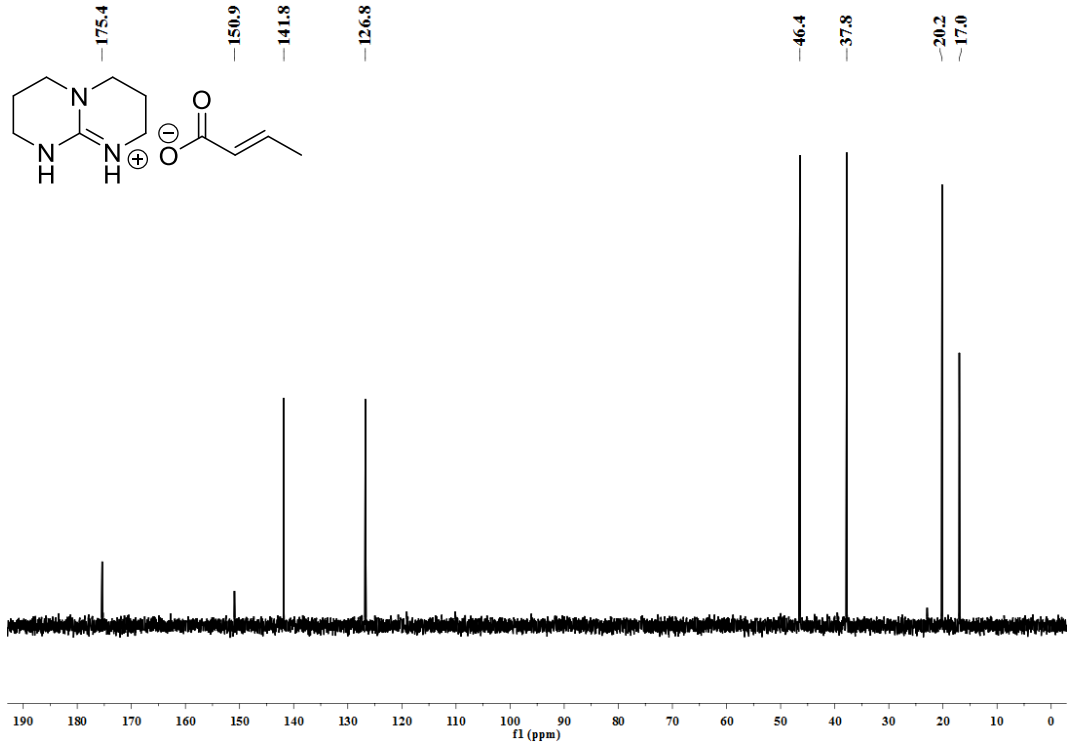
A4-B8: [TBD][Lac]


4.07
4.05
4.03
4.02
3.25
3.23
3.22
3.17
3.16
3.15
1.91
1.91
1.89
1.88
1.86
1.85
1.25
1.24
OH
1.02
8.00
4.00
3.04
f1 (ppm)

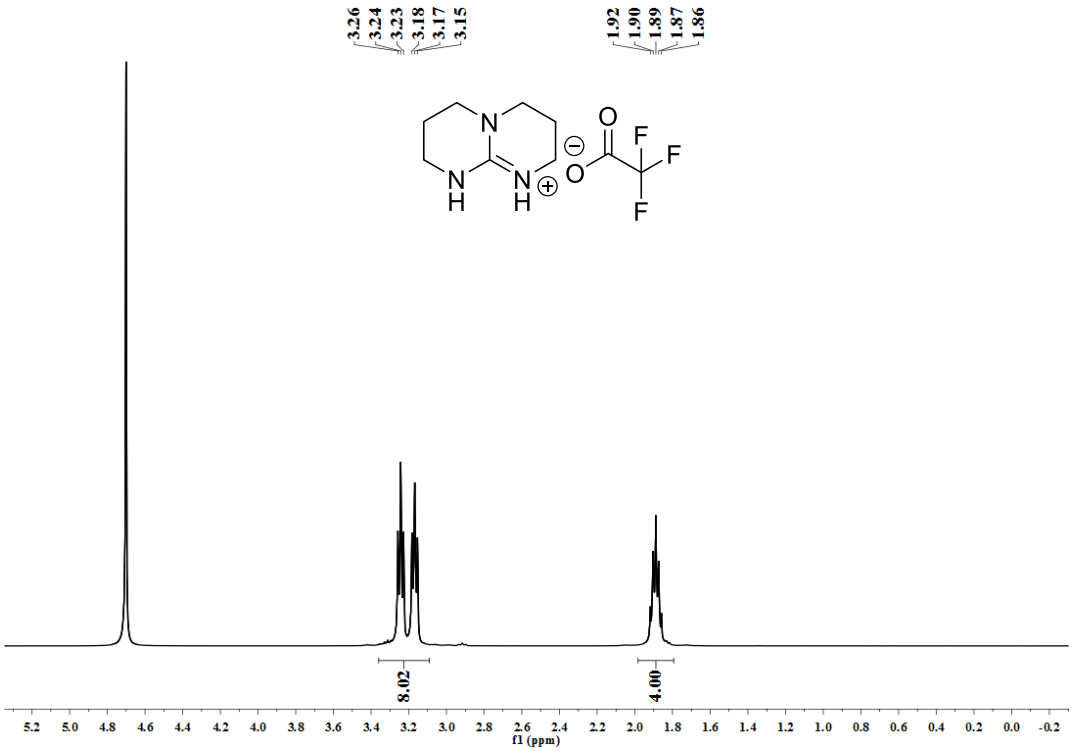

181.9
150.9
68.2
46.4
37.8
20.2
20.0
OH
f1 (ppm)

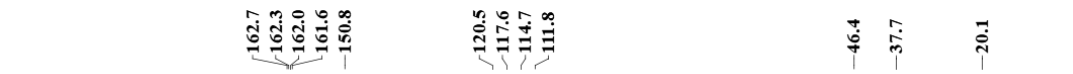
A4-B9: [TBD][Cro]

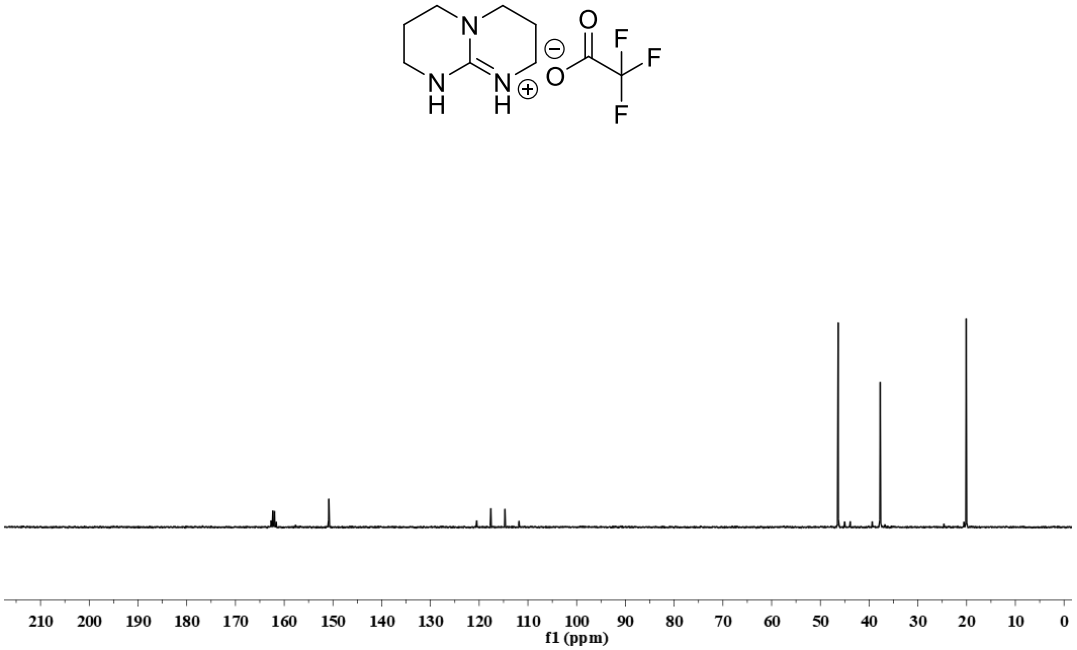

6.62
6.61
6.59
6.59
6.57
6.57
5.78
5.77
5.77
5.74
5.73
5.73
3.25
3.23
3.22
3.17
3.16
3.15
1.91
1.89
1.88
1.87
1.85
1.84
1.74
1.72
0.95
0.95
8.04
4.06
3.00
f1 (ppm)


175.4
150.9
141.8
126.8
46.4
37.8
20.2
17.0
f1 (ppm)

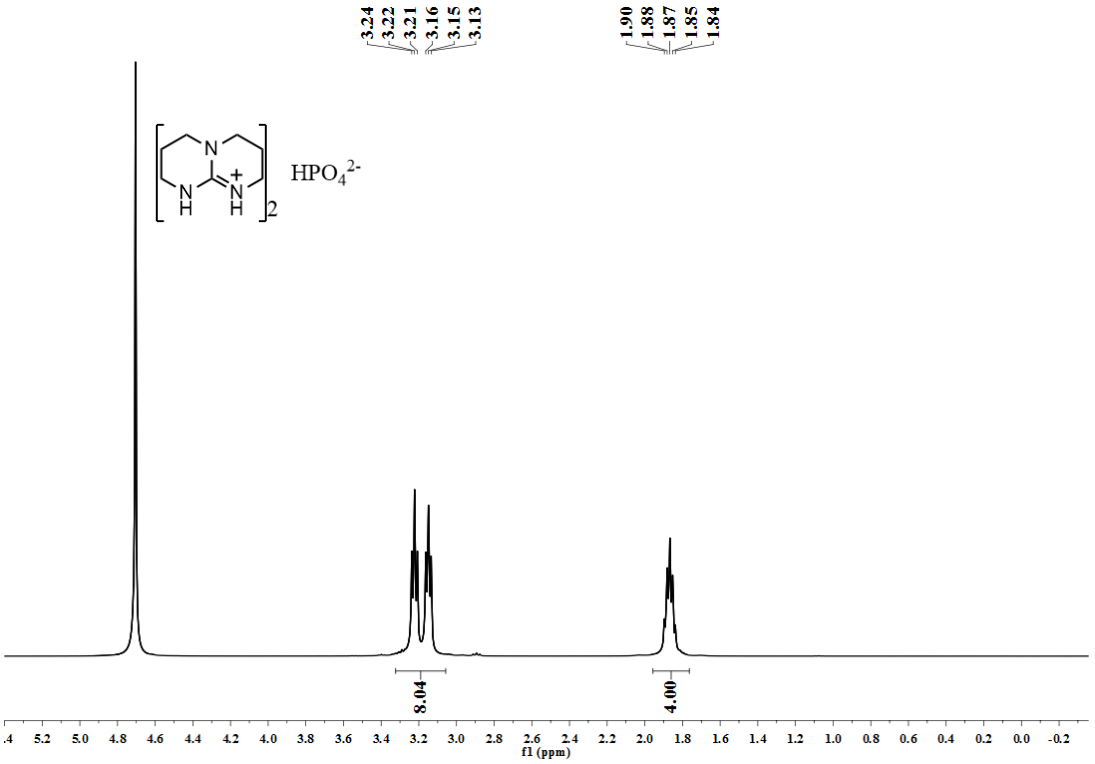
A4-B10: [TBD][TFA]

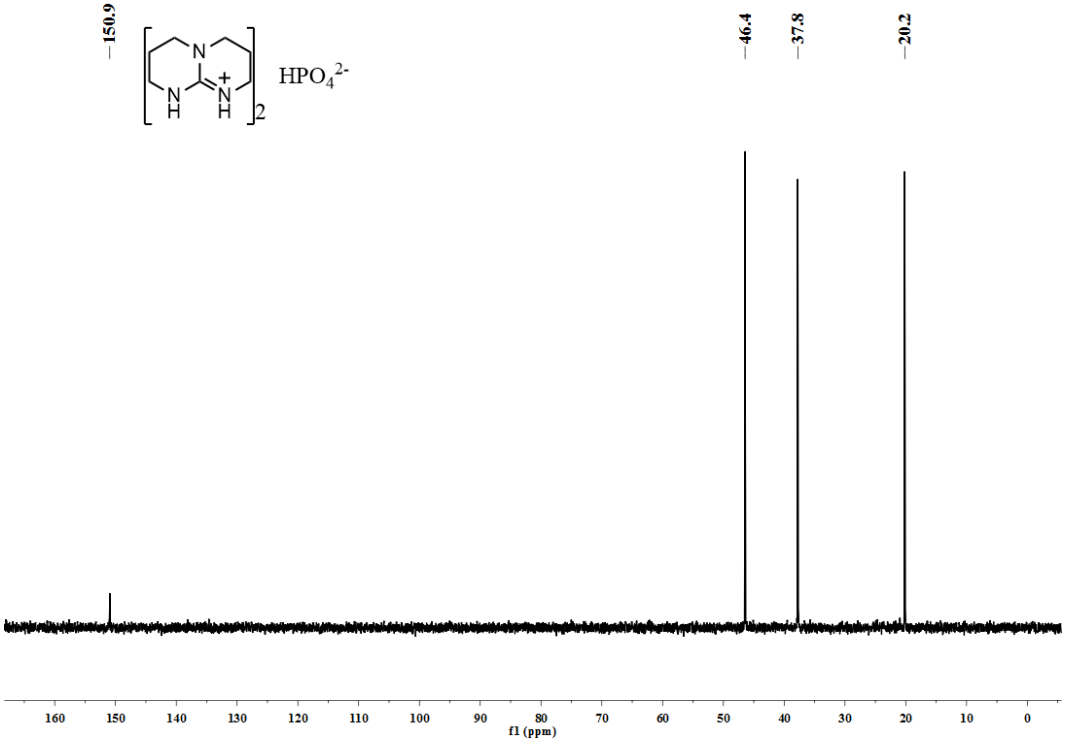




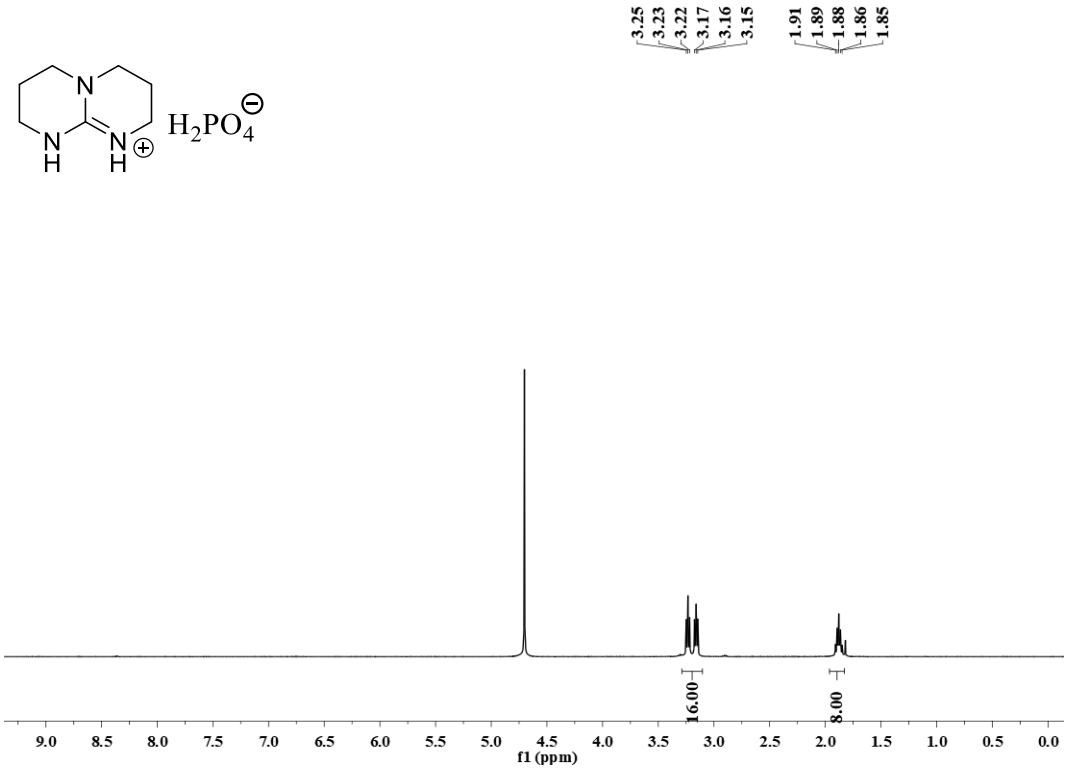


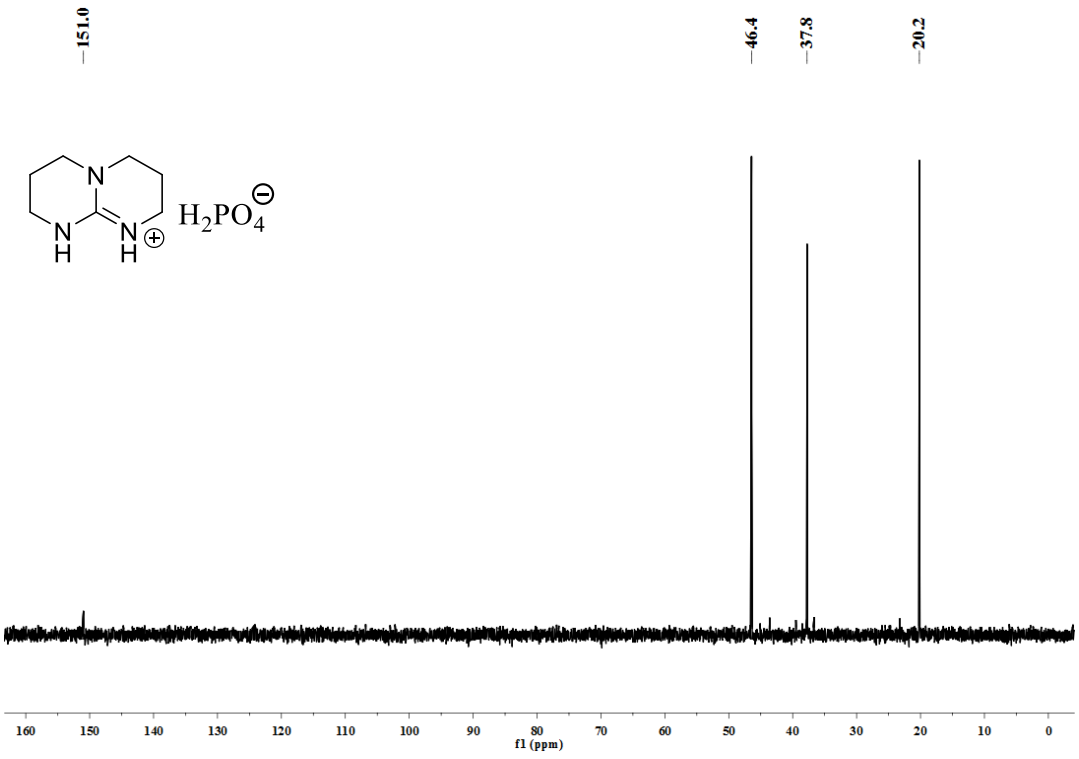
A4-B11: [TBD][H_2PO_4]



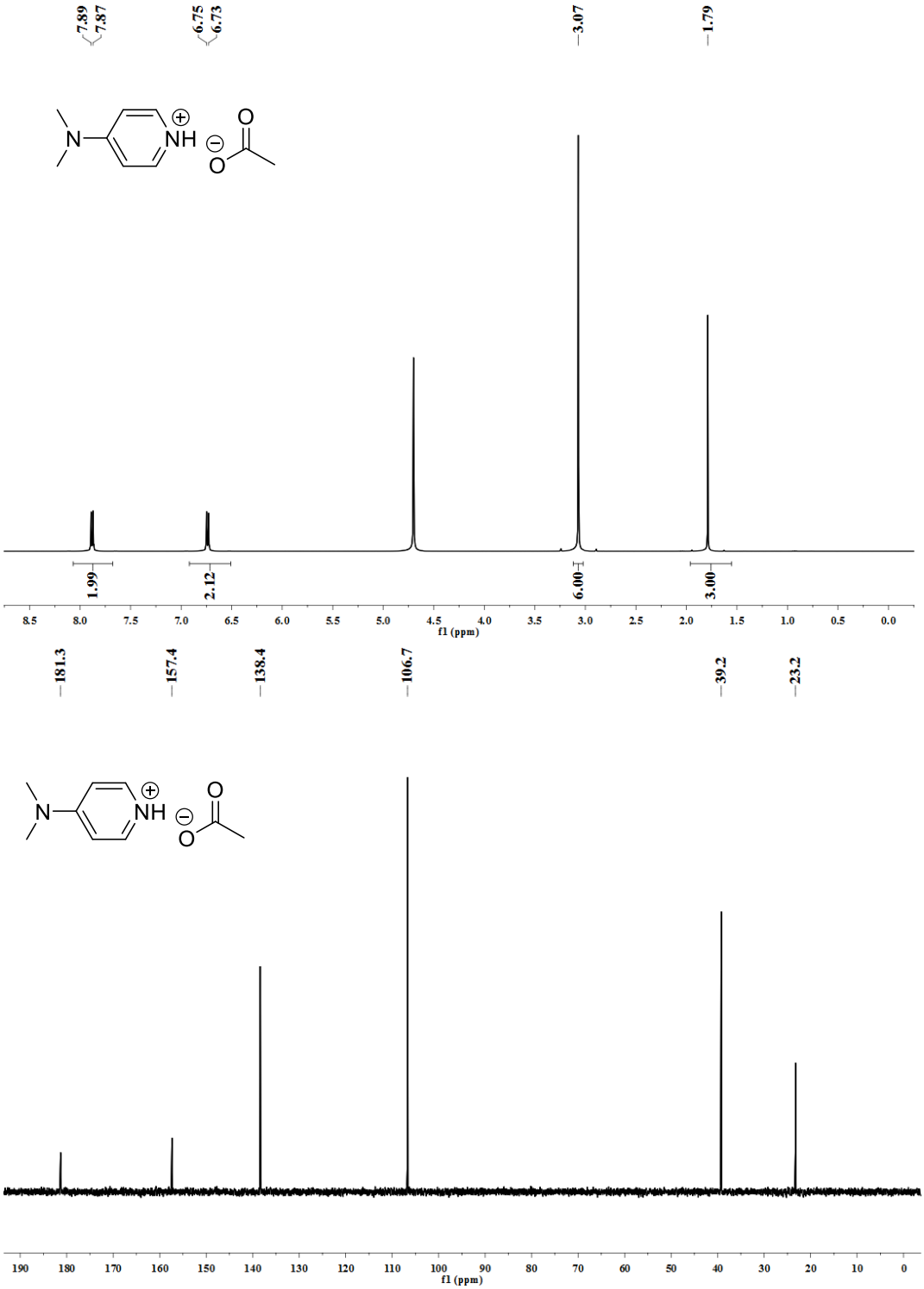


A4-B12: [TBD][H_2PO_4]

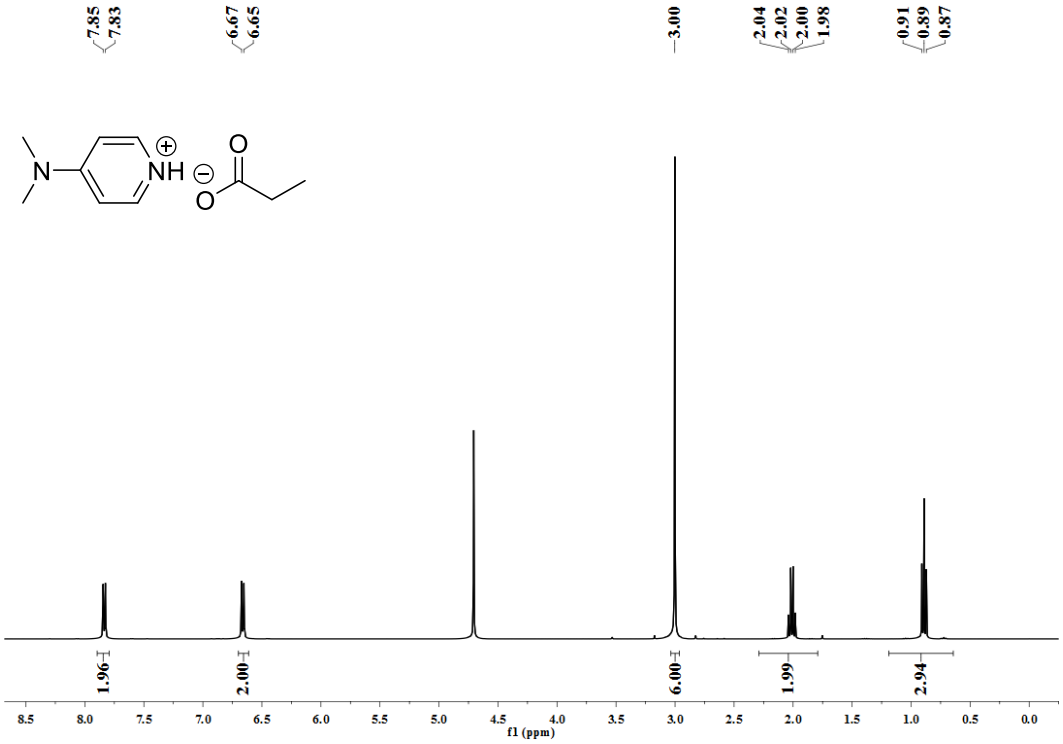


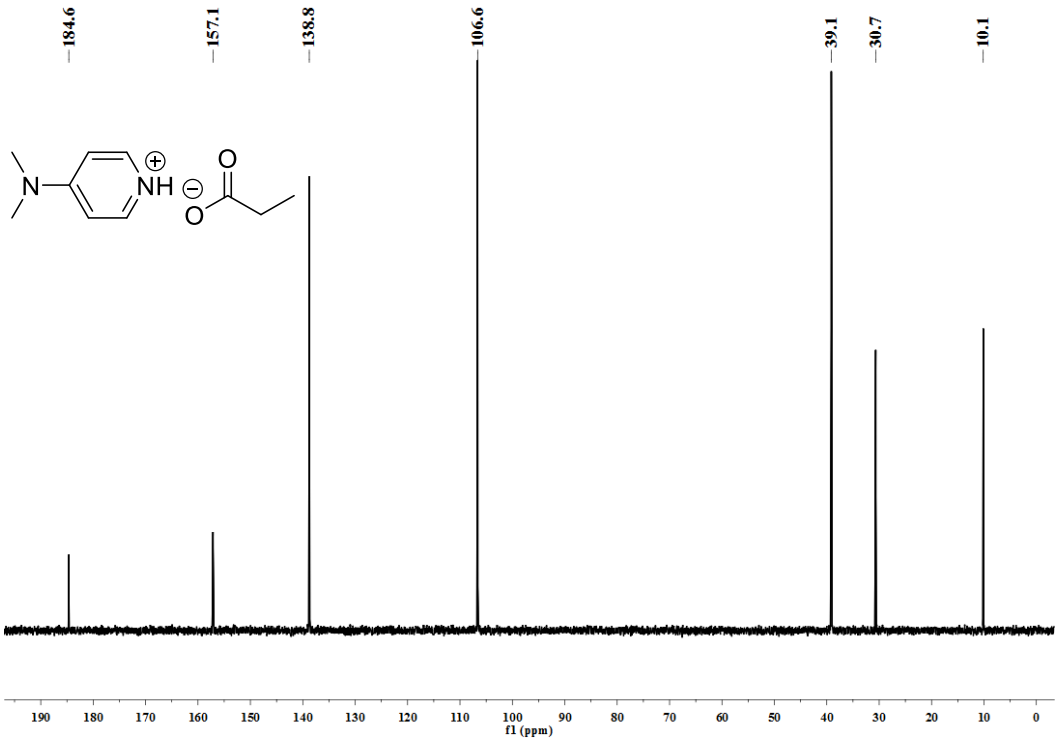


A5-B1: [DMAP][Ac]


7.89
7.87
6.75
6.73
3.07
1.79
1.99
2.12
6.00
3.00
f1 (ppm)
181.3
157.4
138.4
106.7
39.2
23.2
f1 (ppm)

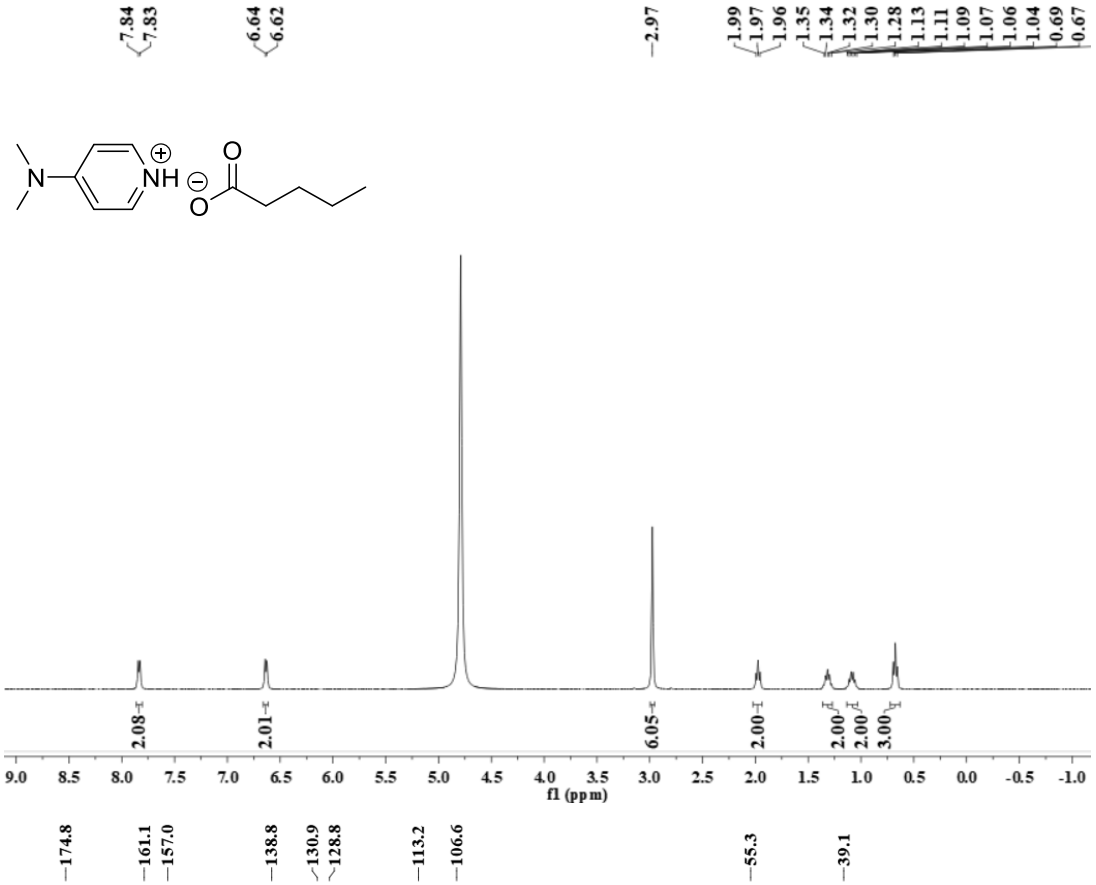
A5-B2: [DMAP][Pro]

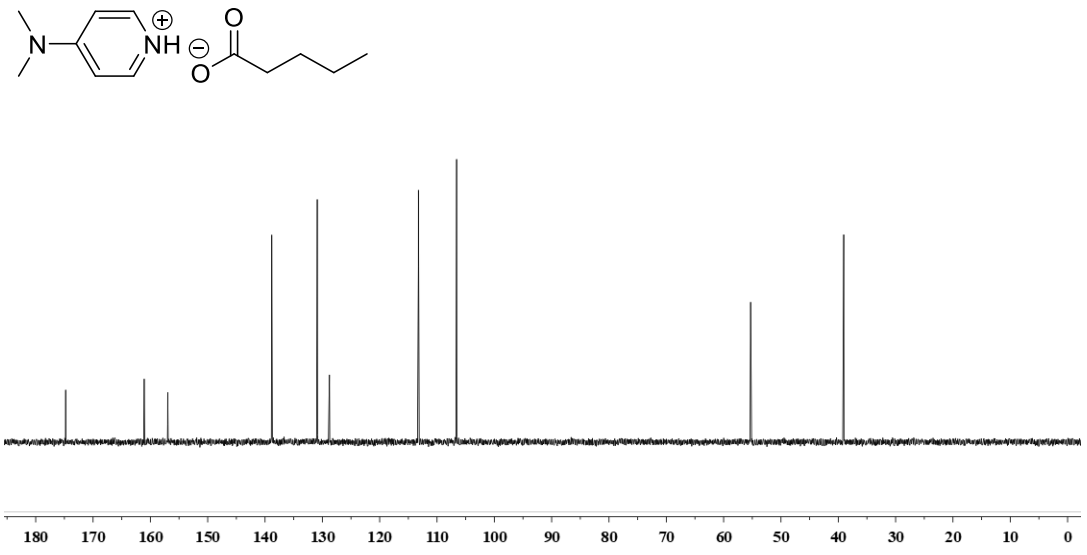




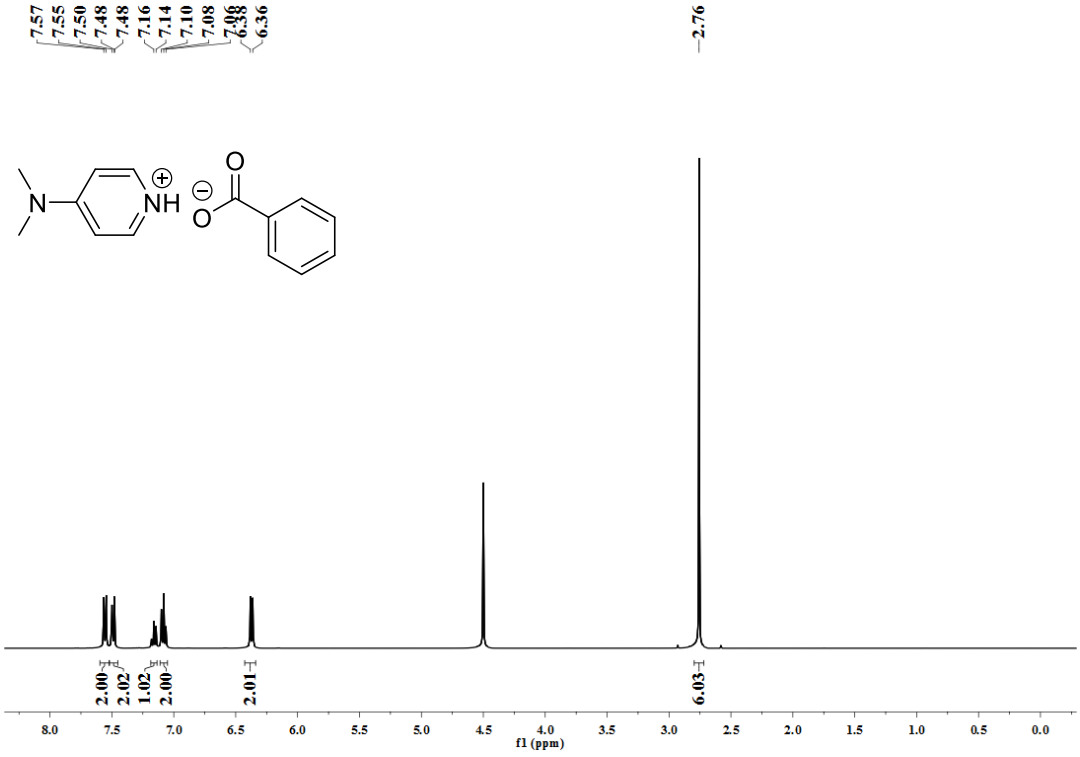
A5-B3: [DMAP][But]

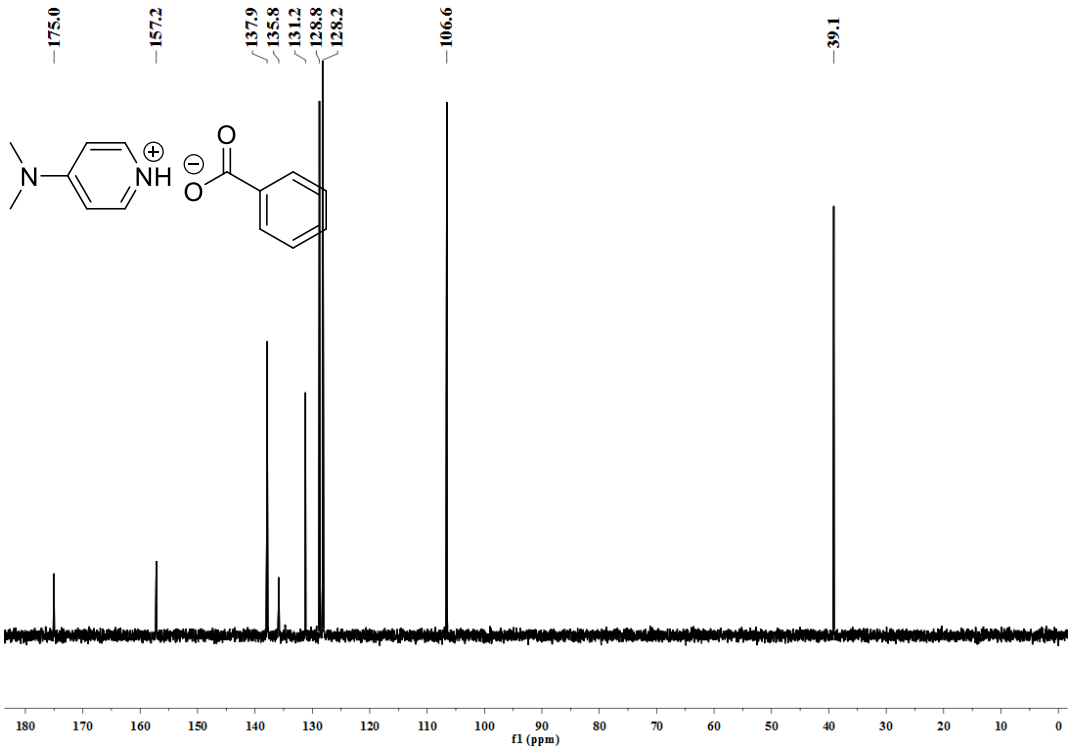
A5-B4: [DMAP][Val]



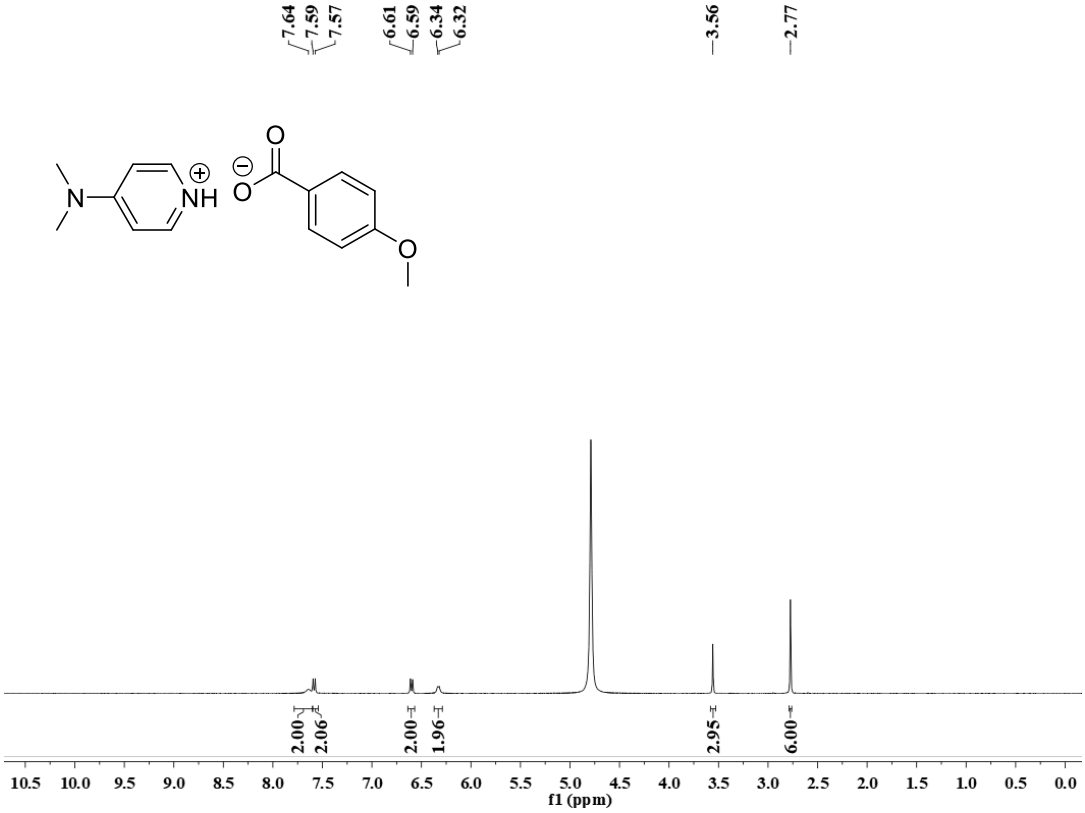


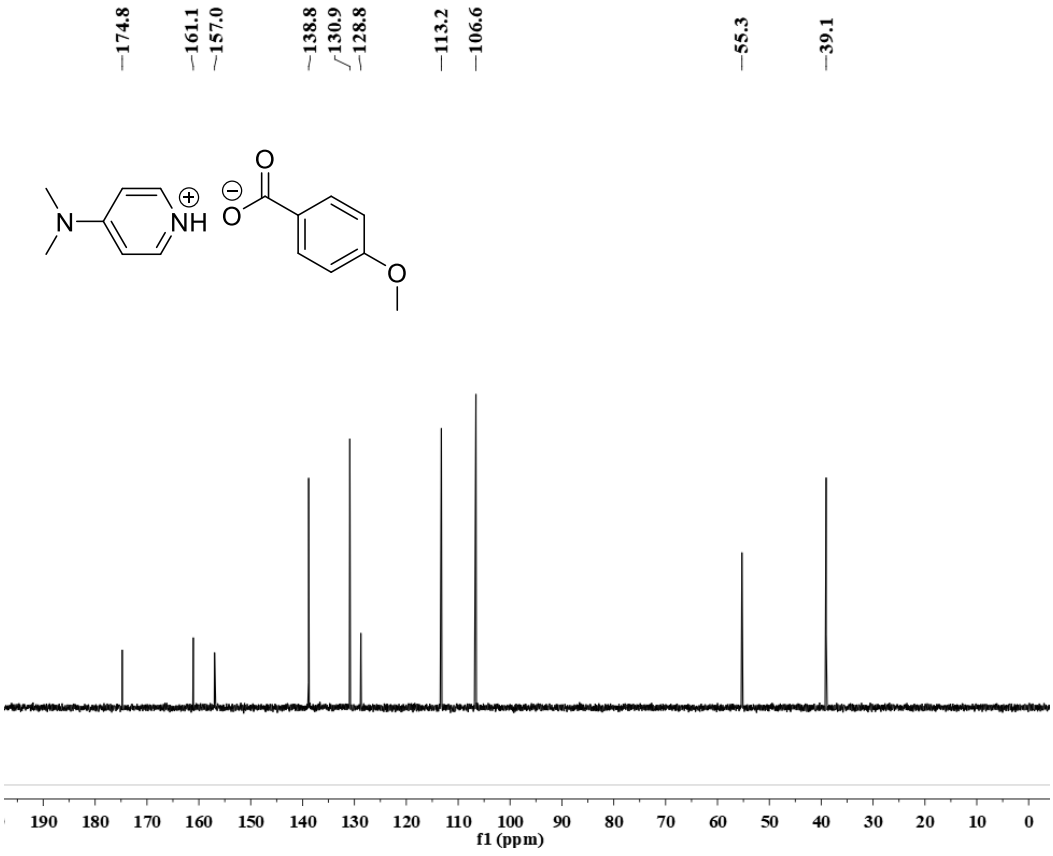
A5-B5: [DMAP][Ben]



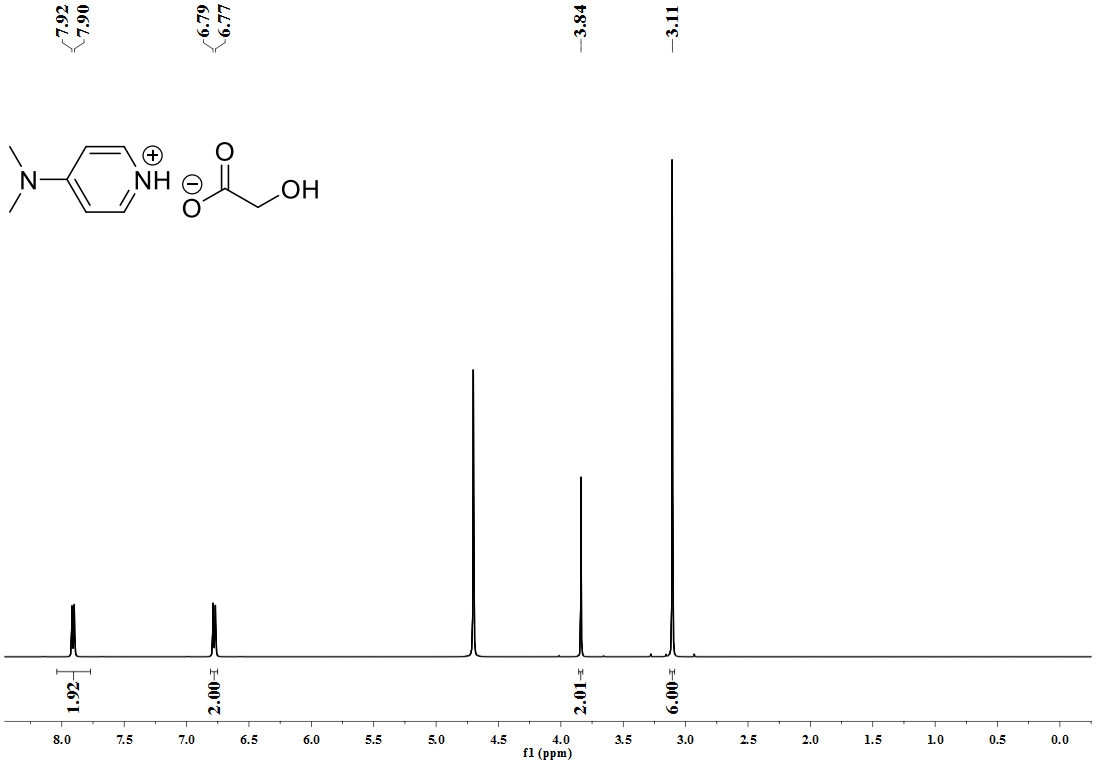


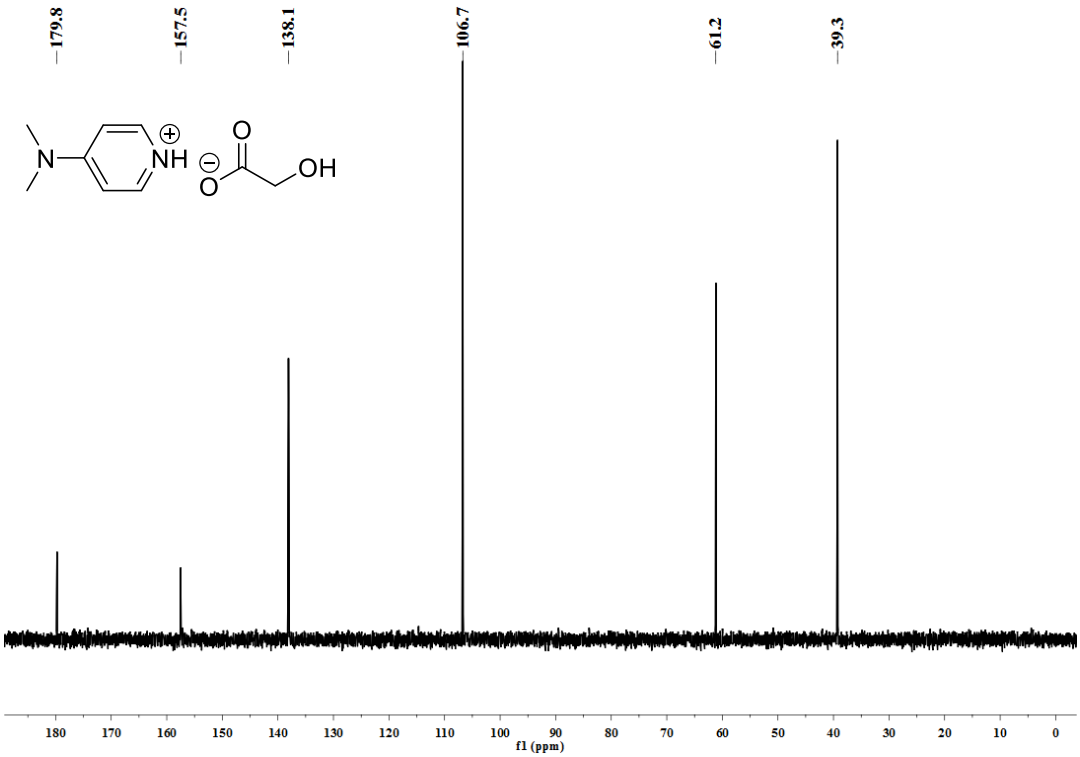
A5-B6: [DMAP][Ani]



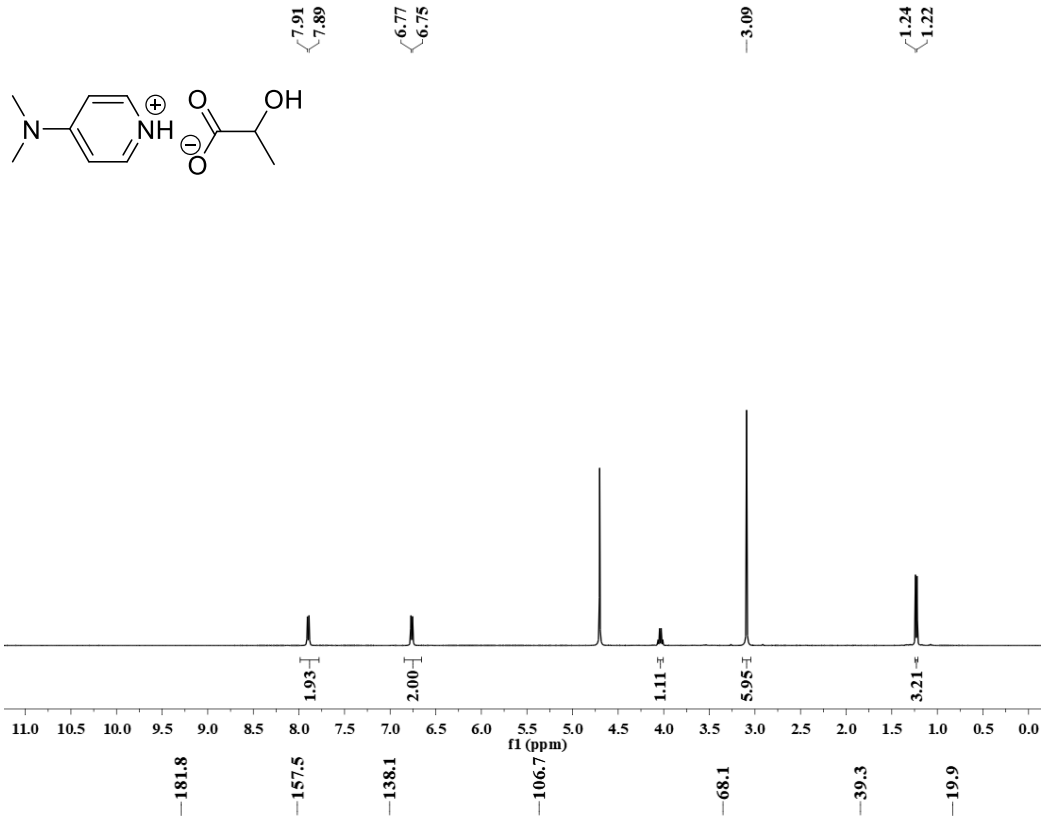


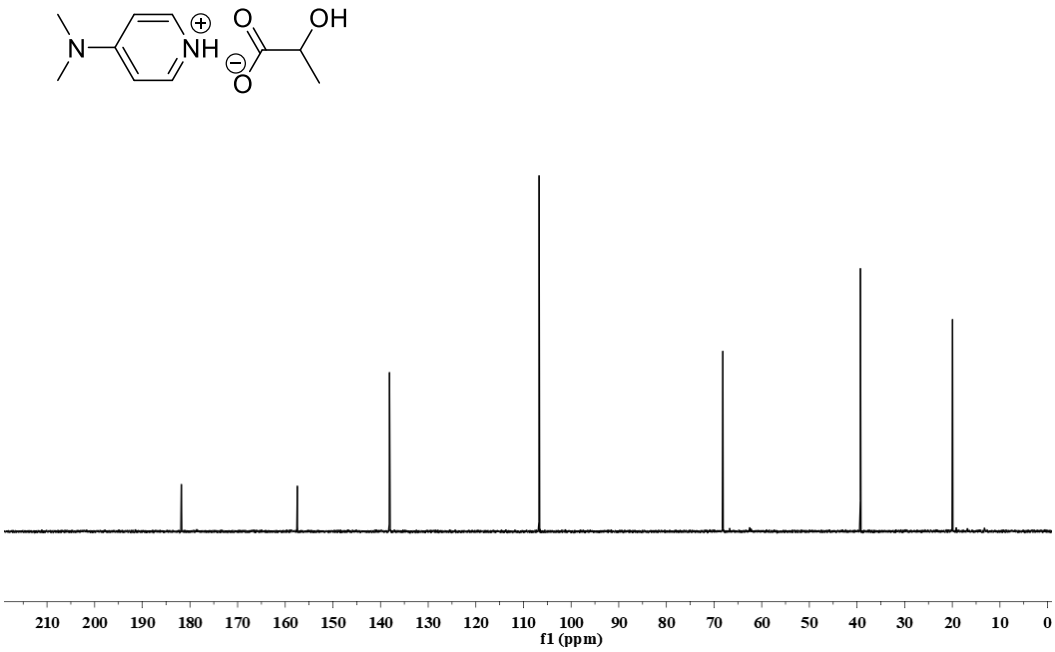
A5-B7: [DMAP][Gly]



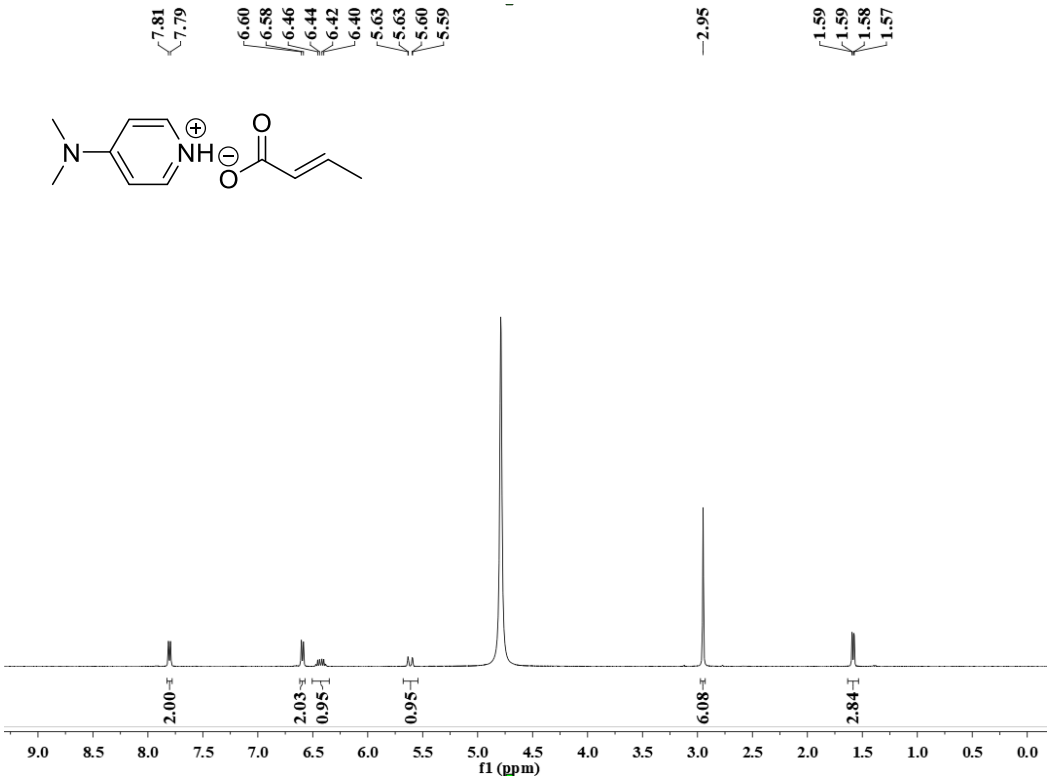


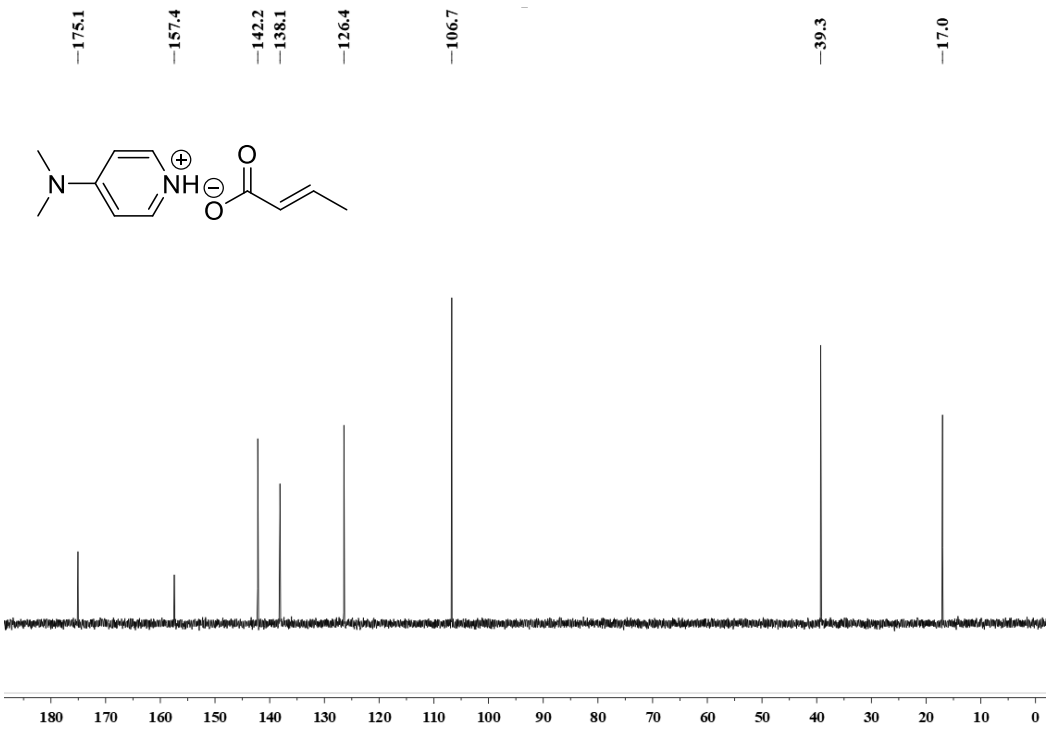
A5-B8: [DMAP][Lac]



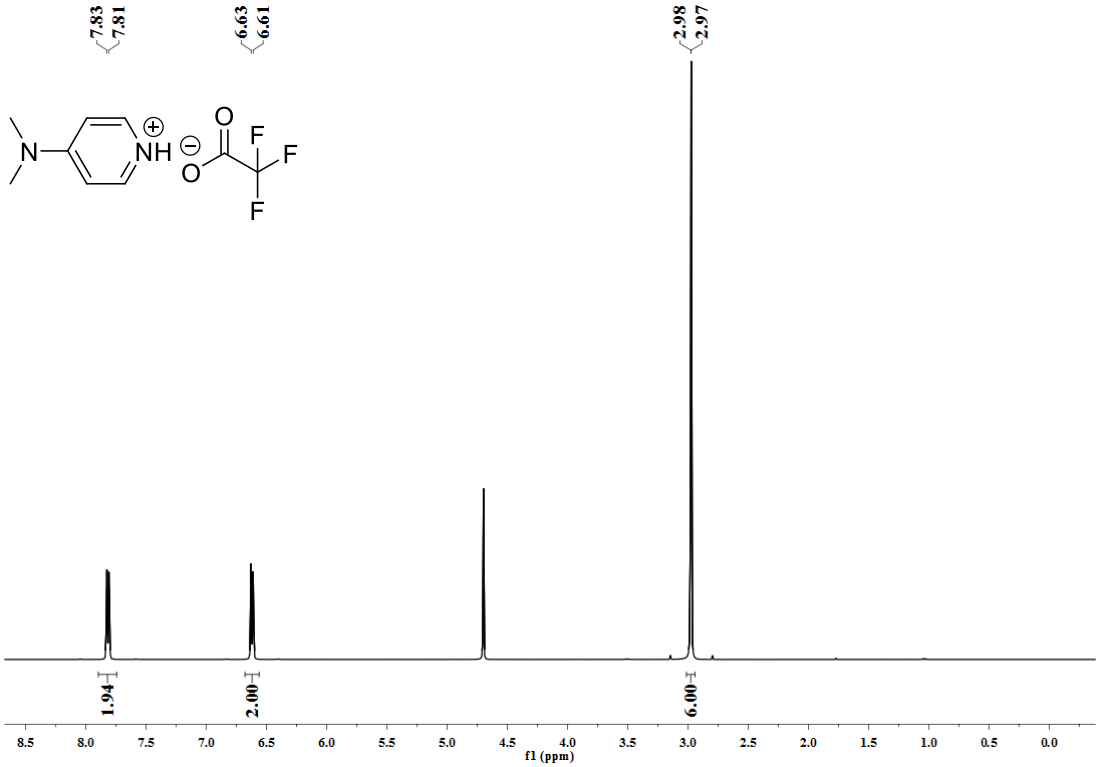


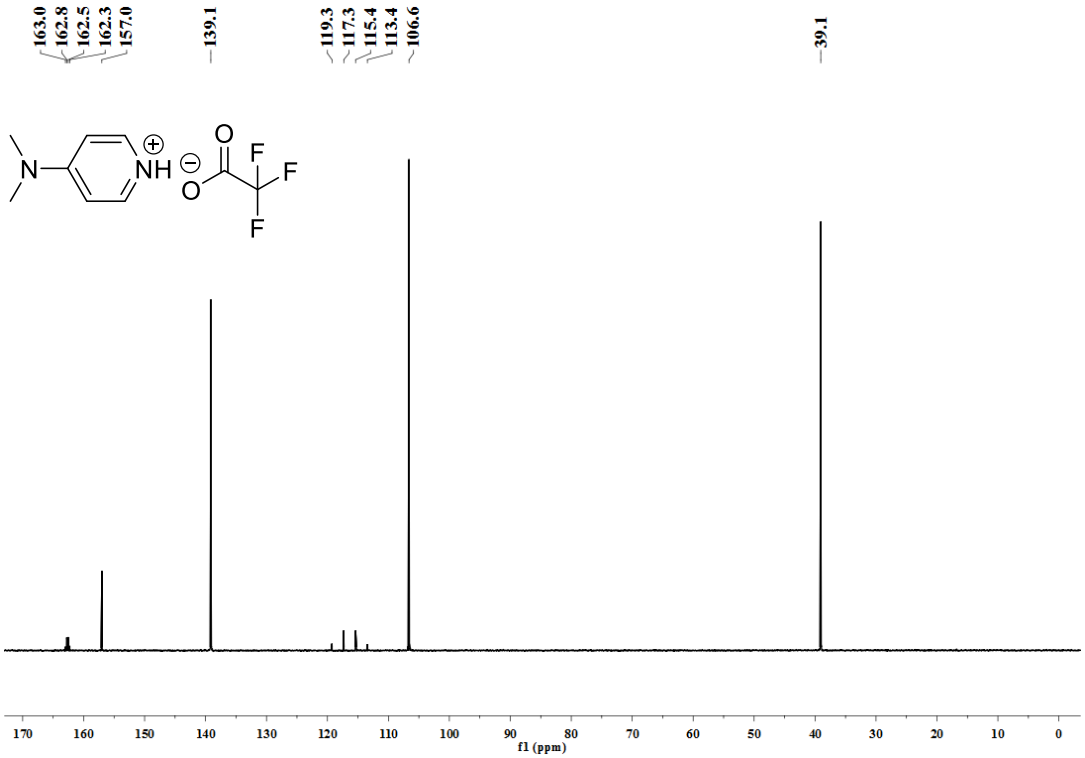
A5-B9: [DMAP][Cro]



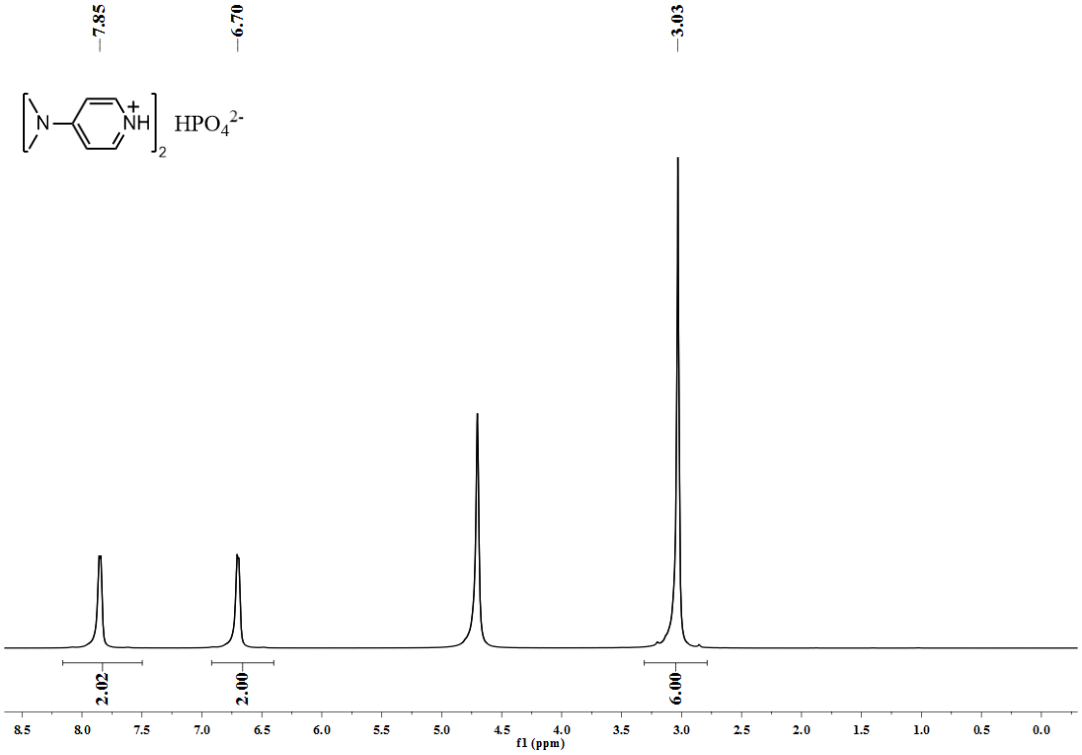


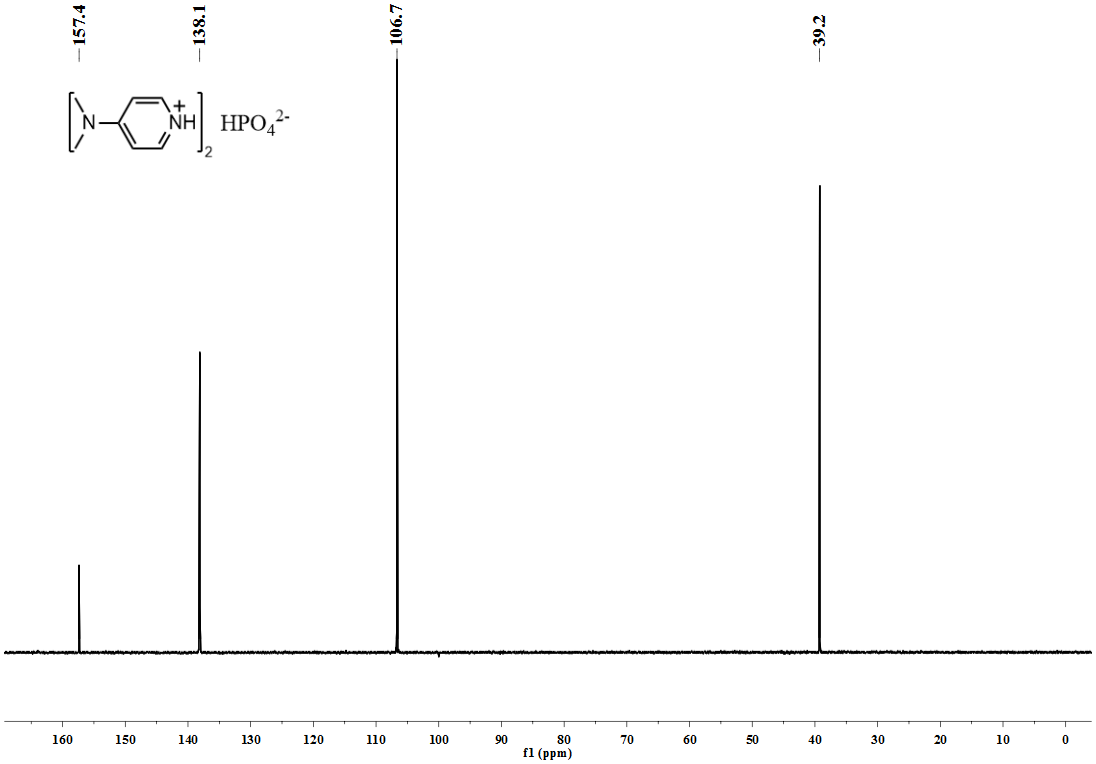
A5-B10: [DMAP][Tfa]



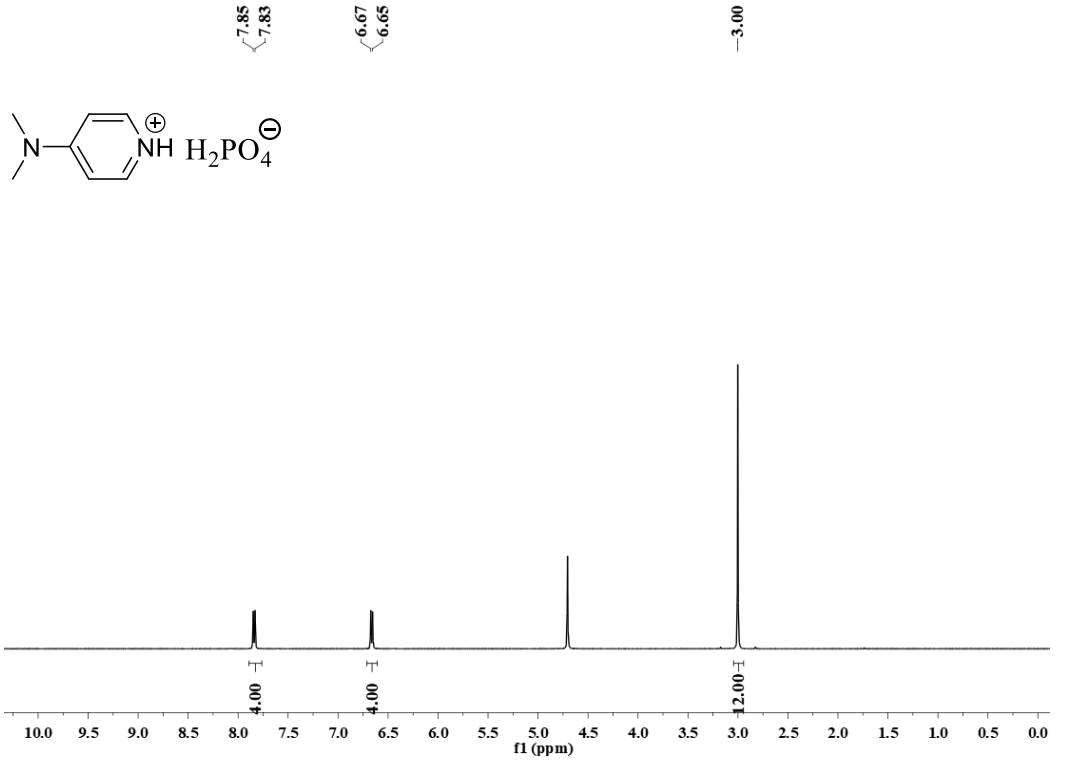


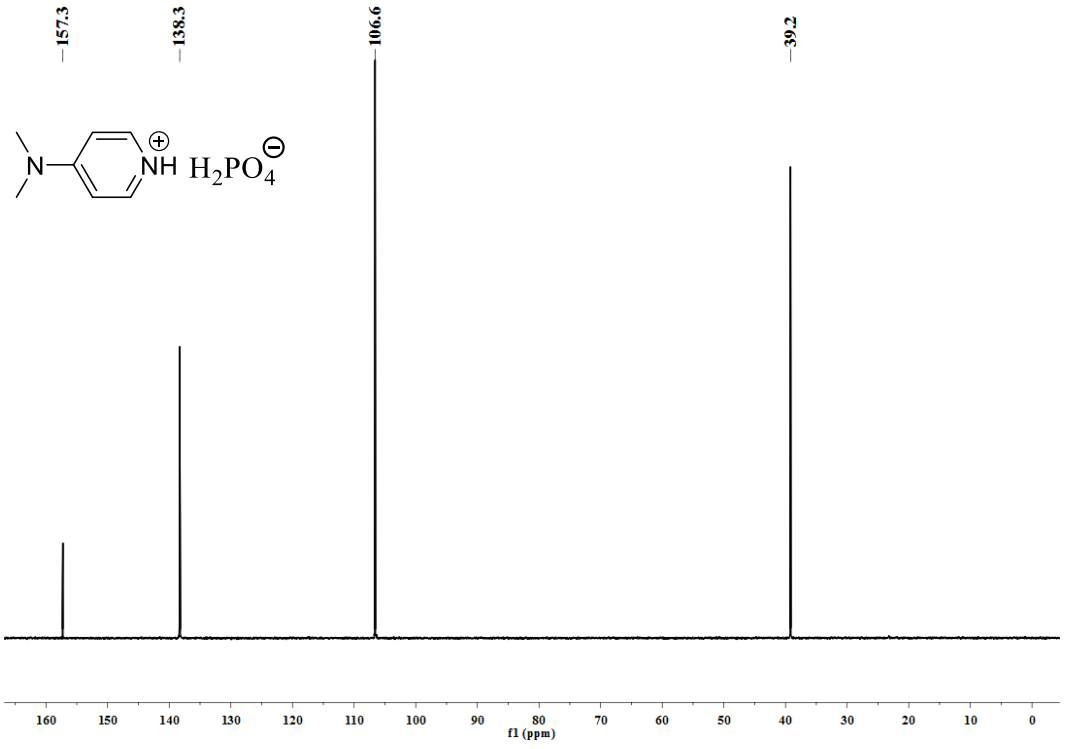
A5-B11: [DMAP][H_2PO_4]





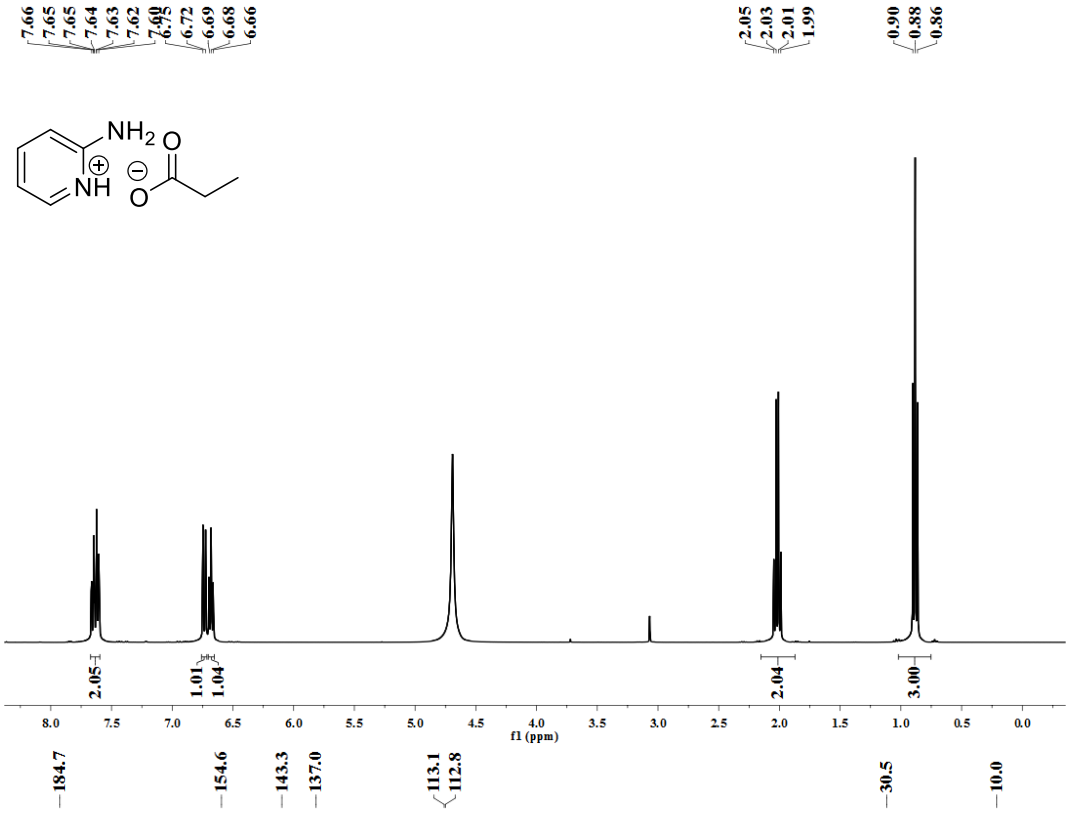
A5-B12: [DMAP][HPO_4]

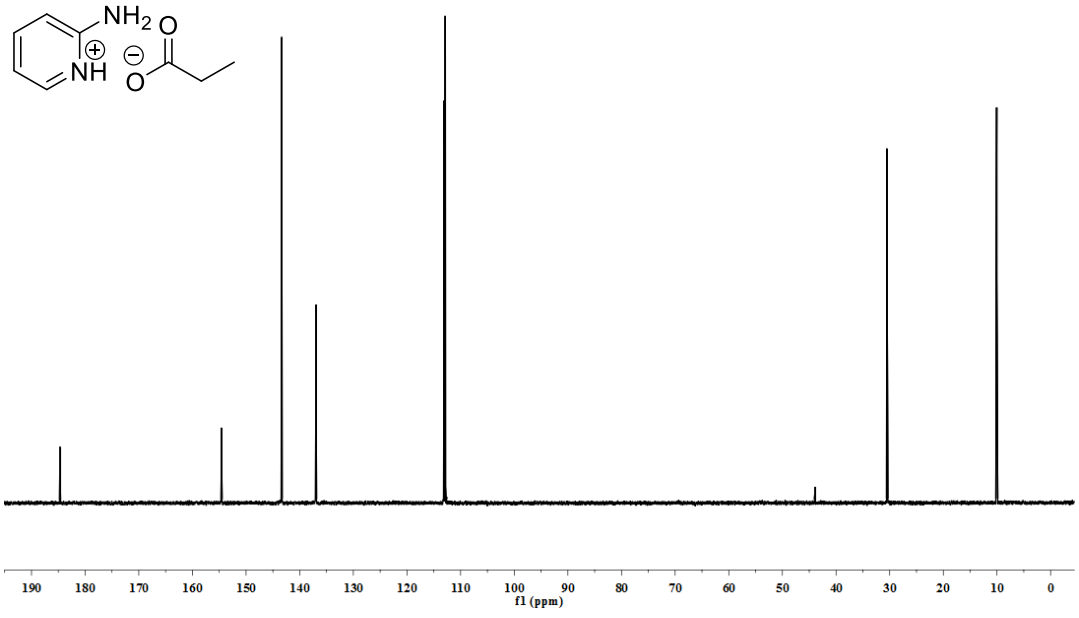




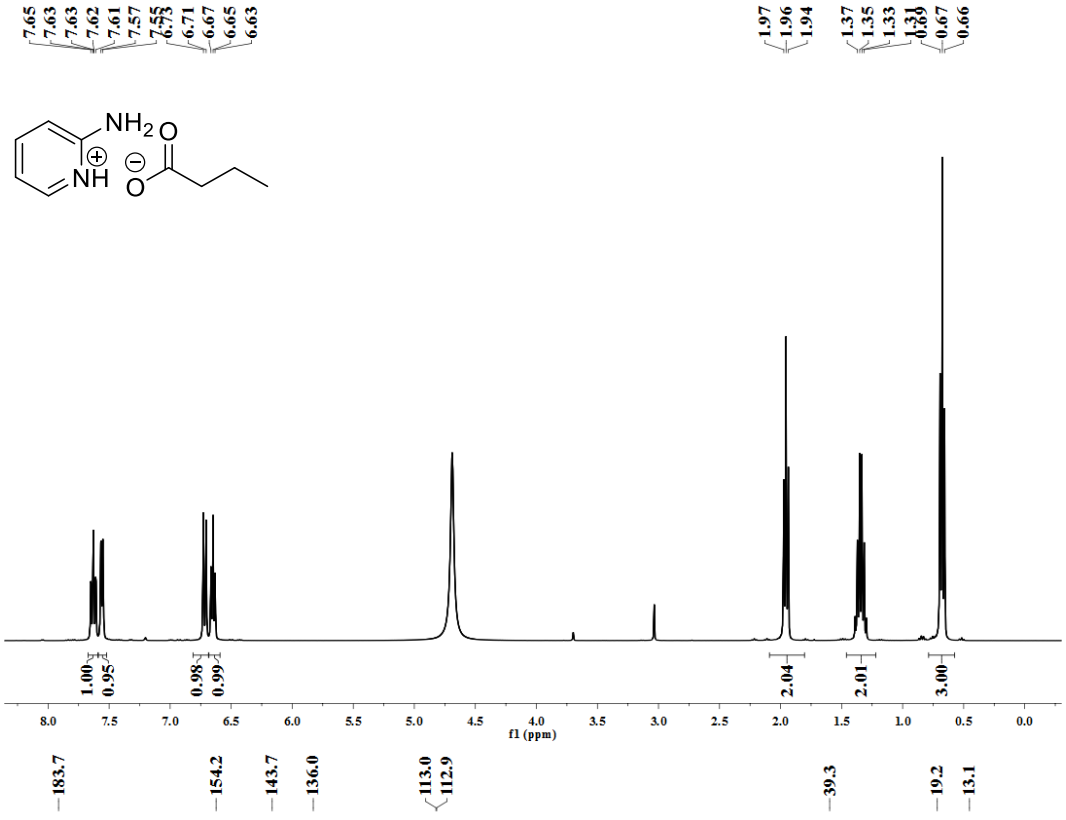
A6-B1: [2-AnPy][Ac]

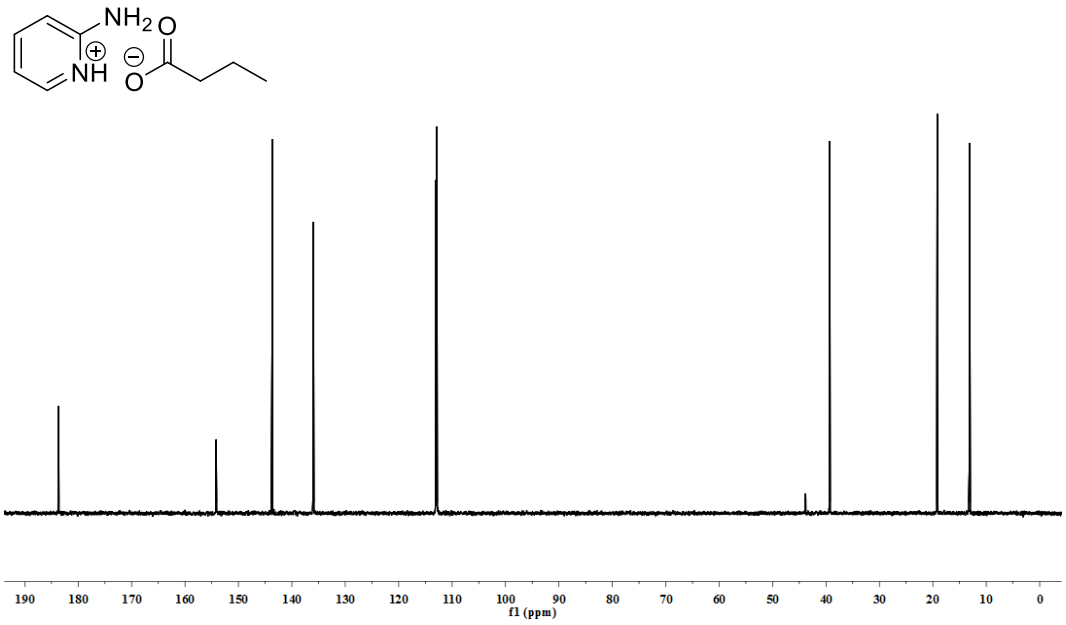
A6-B2: [2-AnPy][Pro]



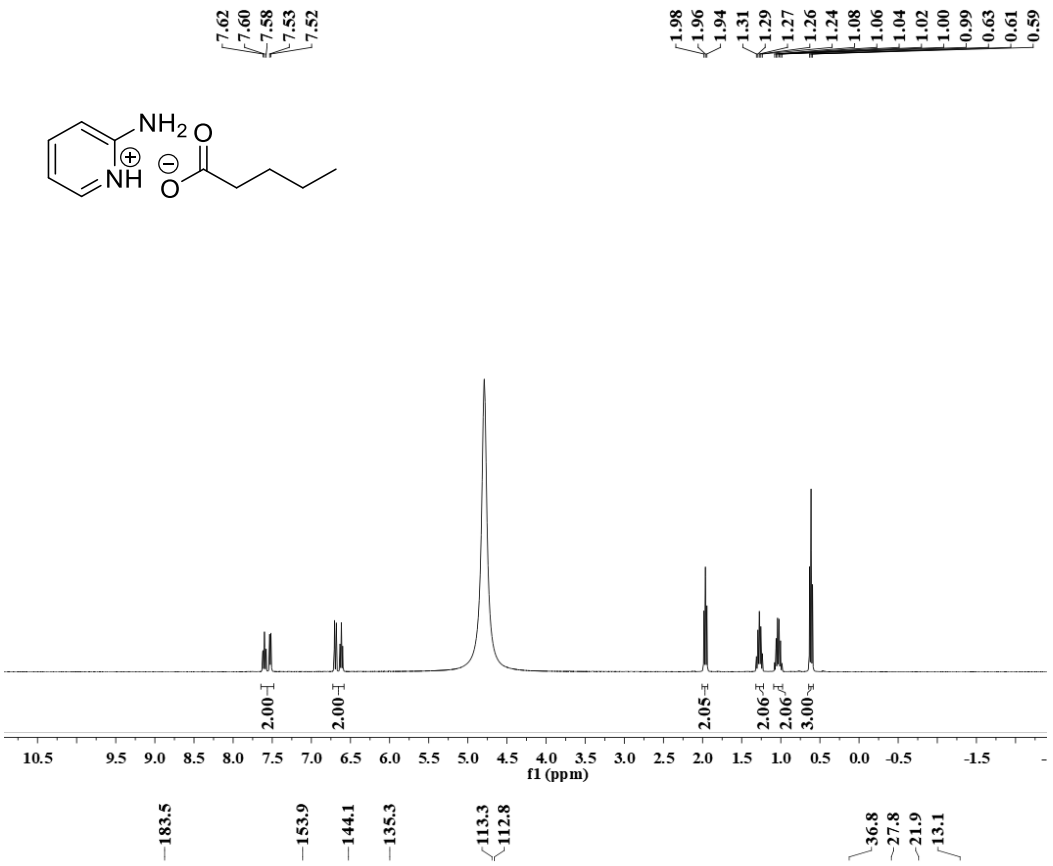


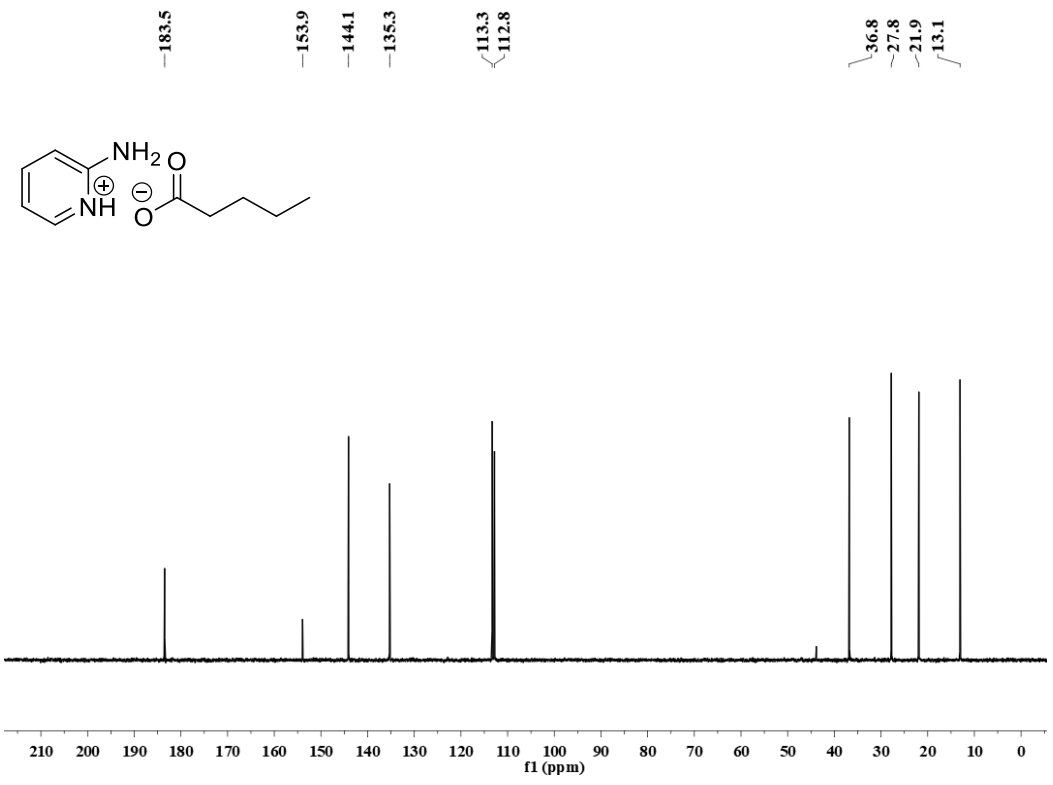
A6-B3: [2-AnPy][But]



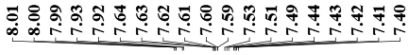


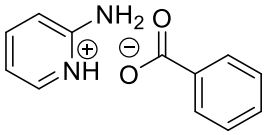
A6-B4: [2-AnPy][Val]

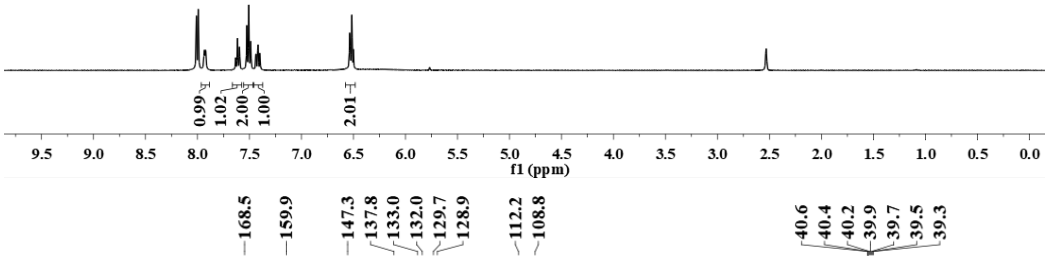


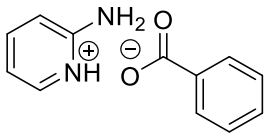


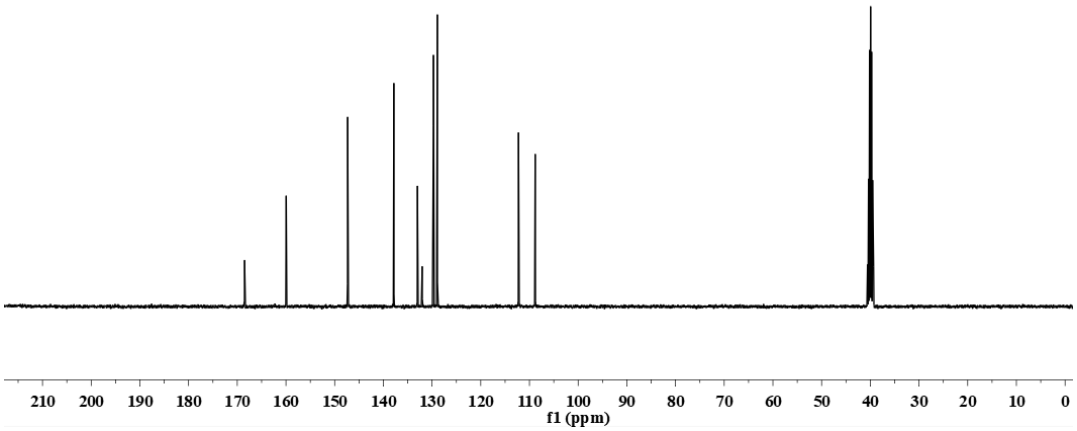
A6-B5: [2-AnPy][Ben]



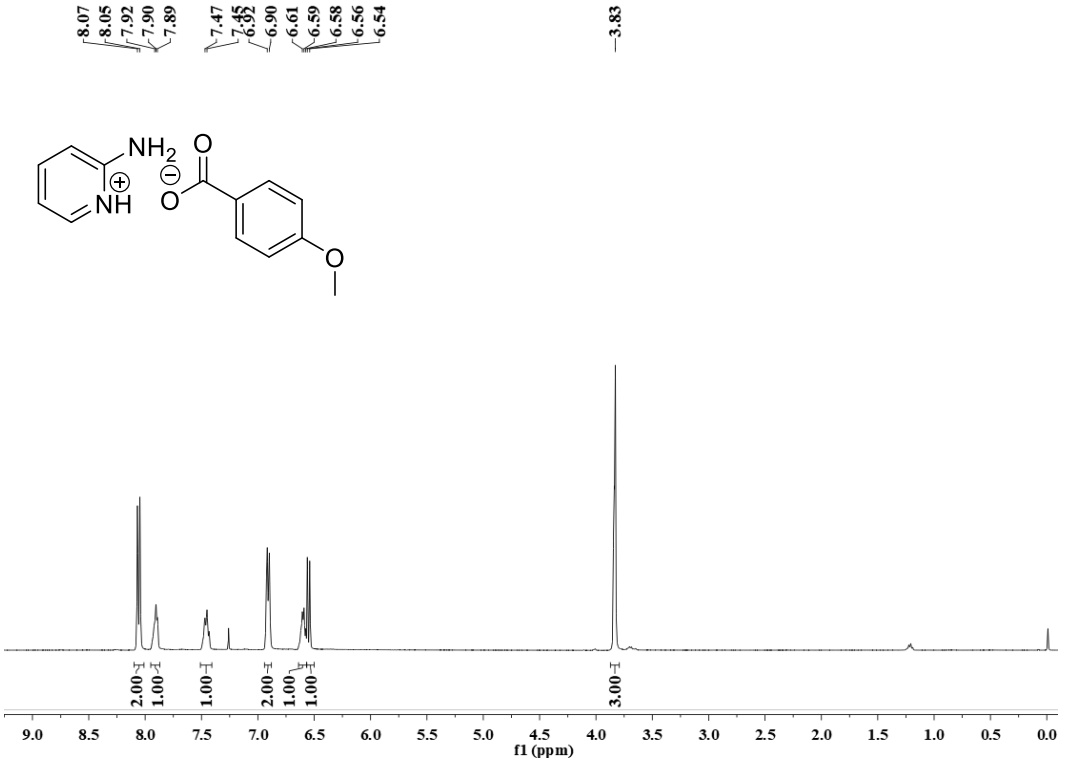


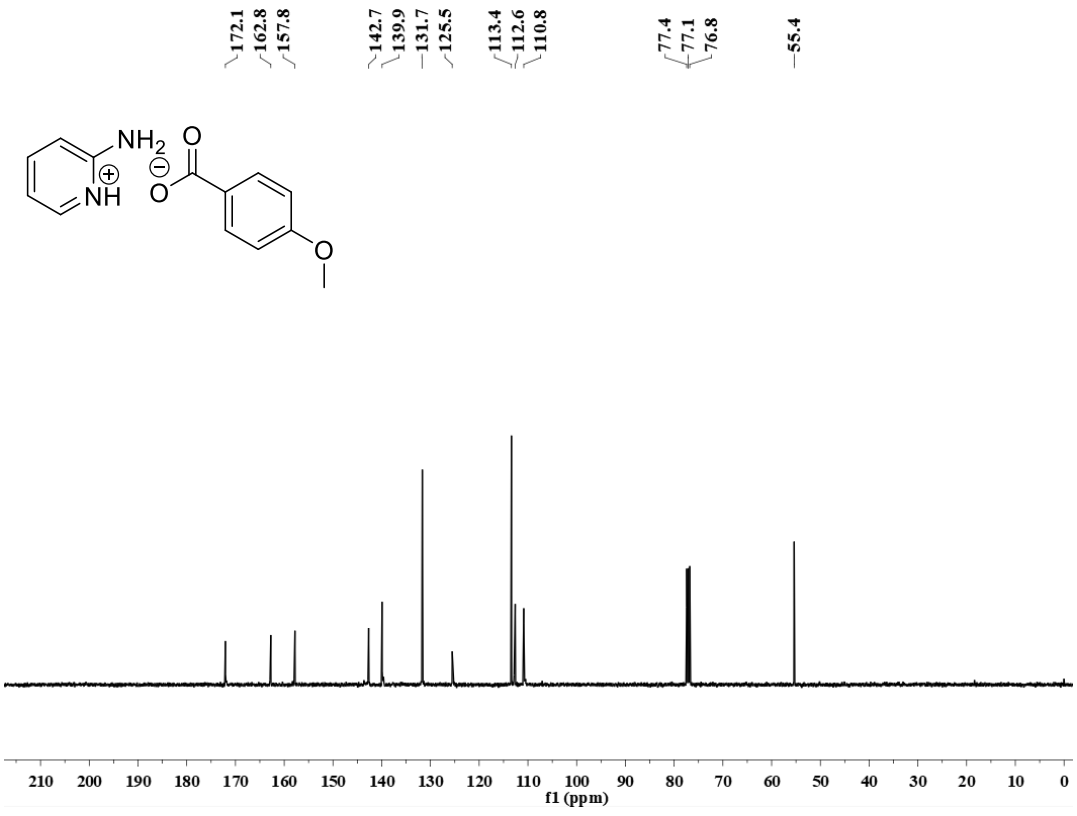




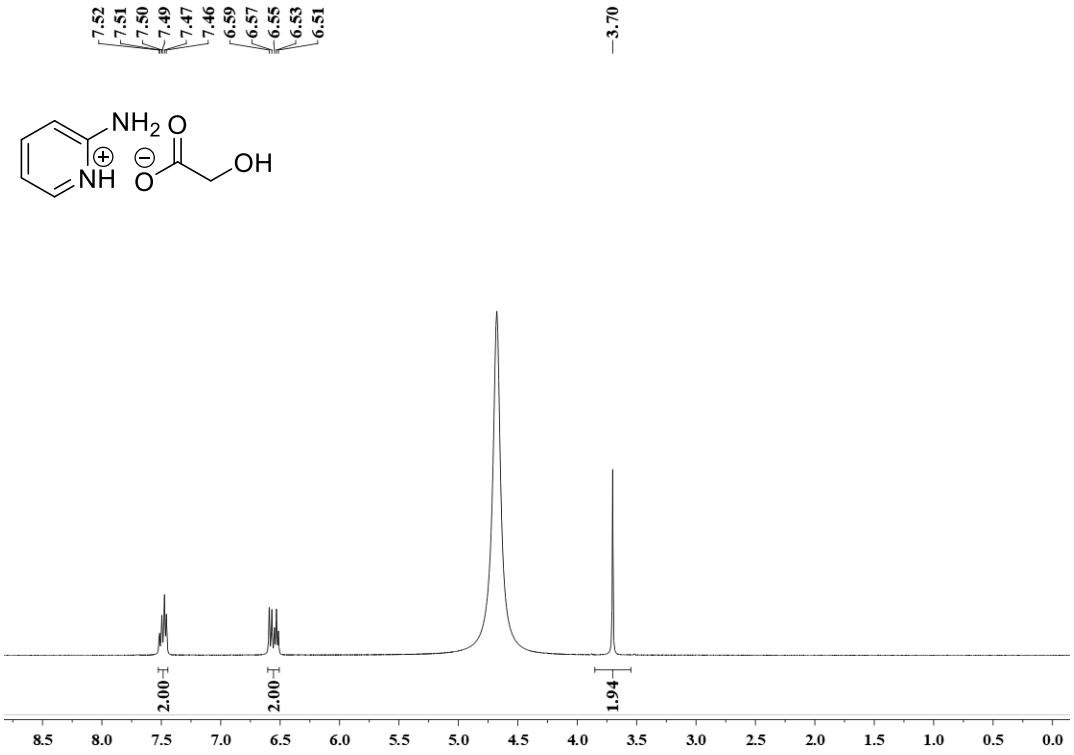


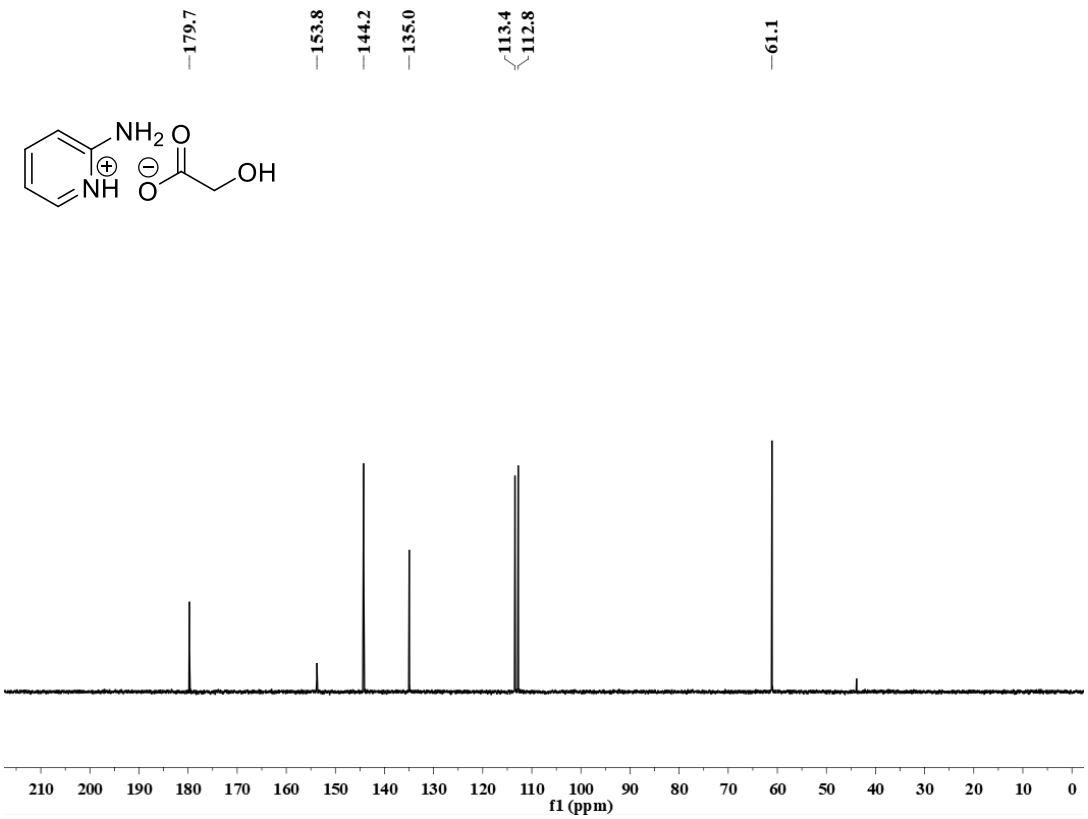
A6-B6: [2-AnPy][Ani]



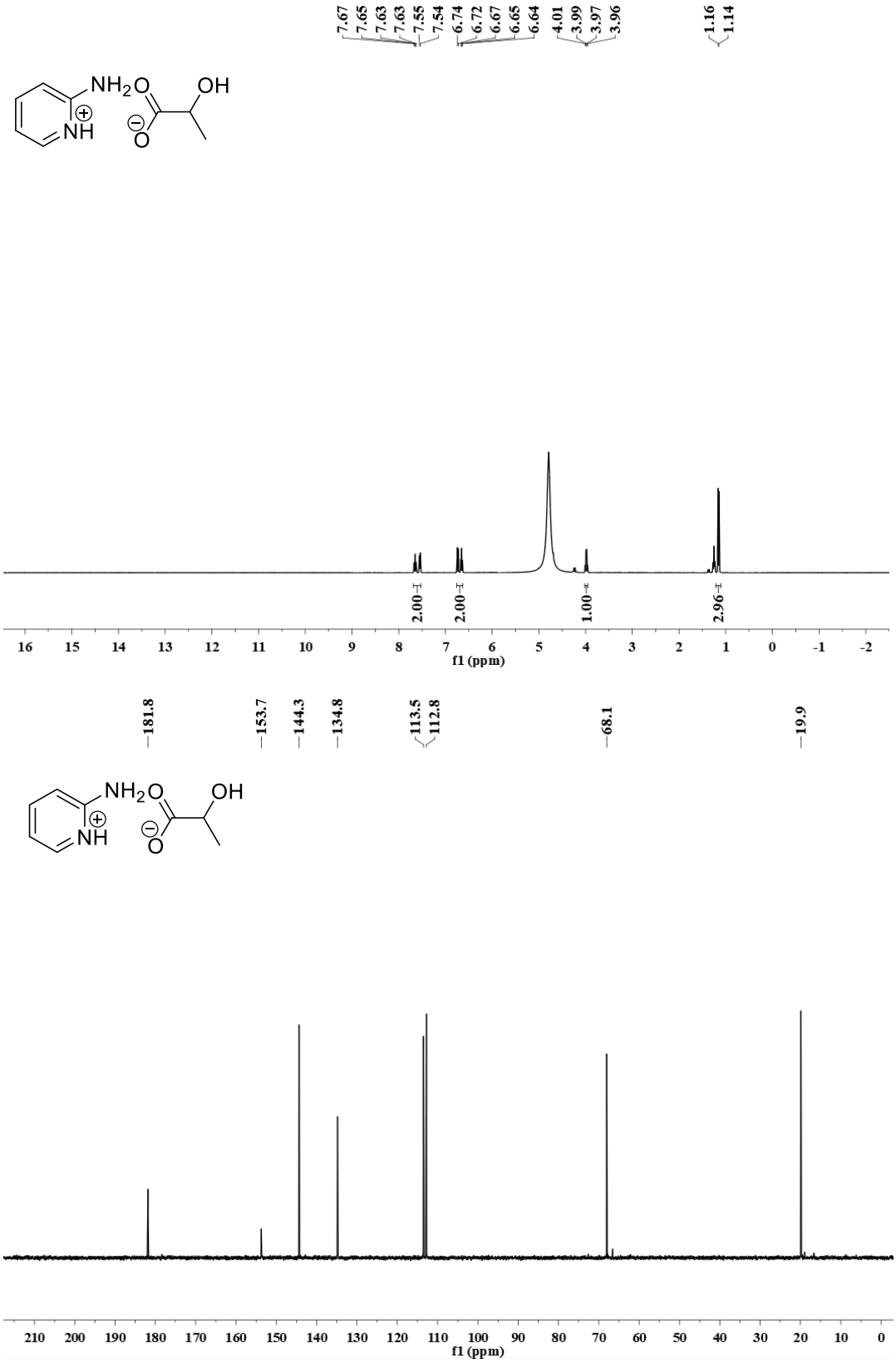


A6-B7: [2-AnPy][Gly]

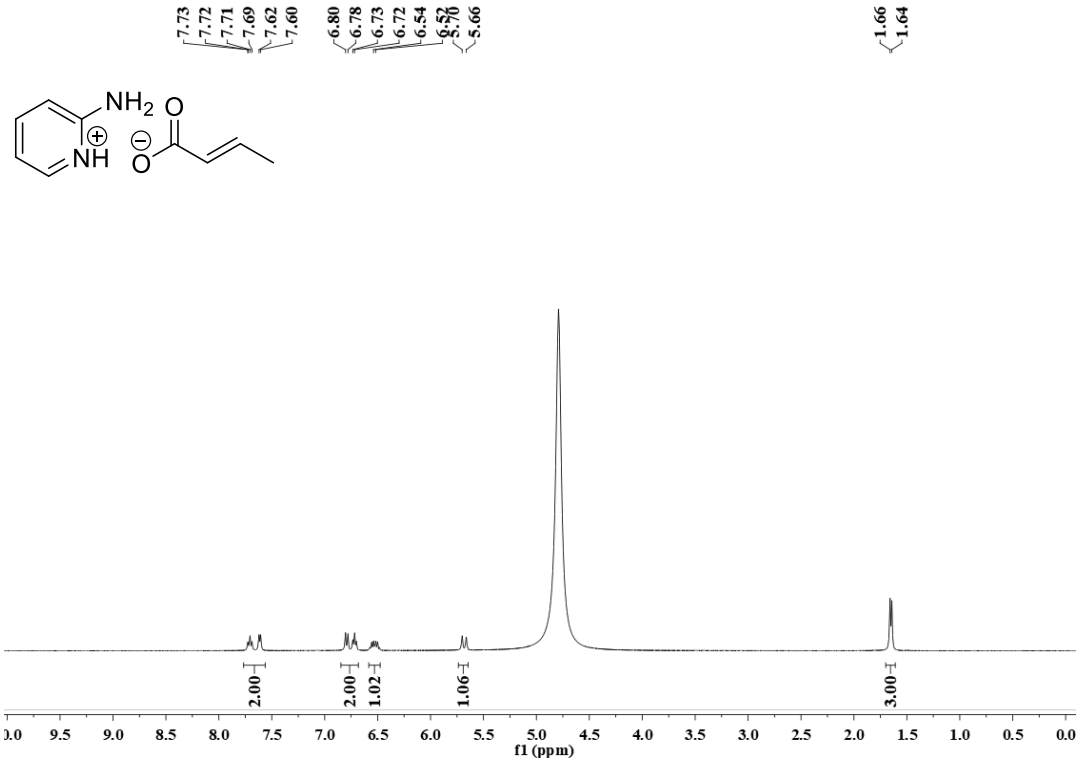


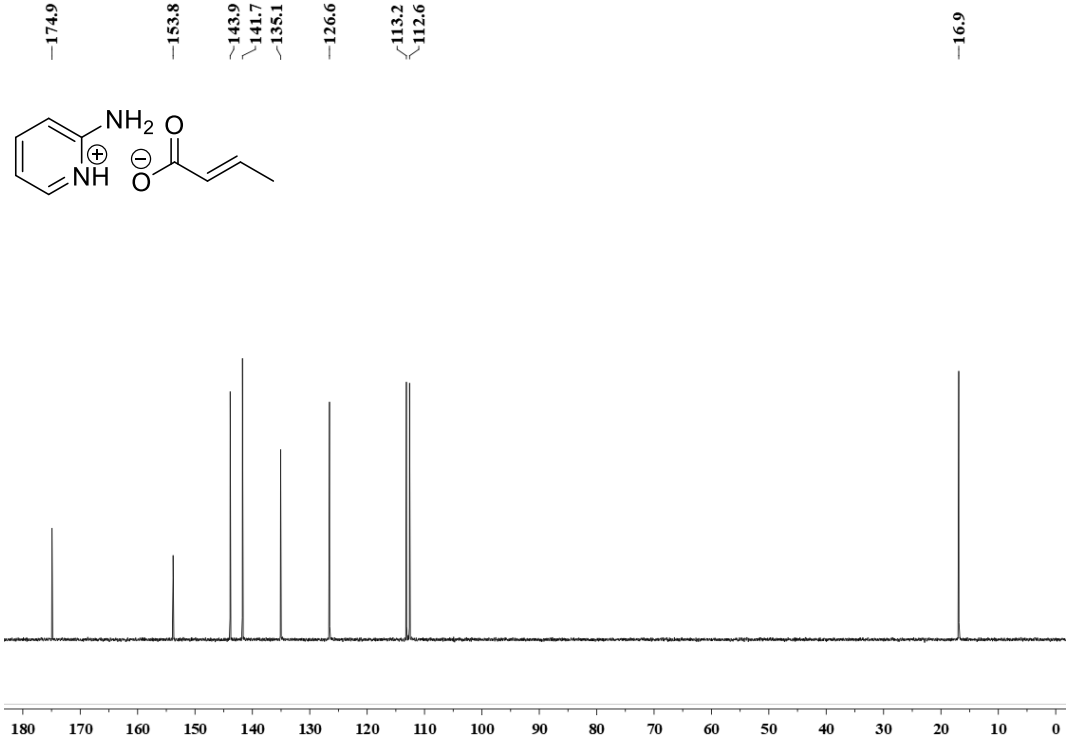


A6-B8: [2-AnPy][Lac]

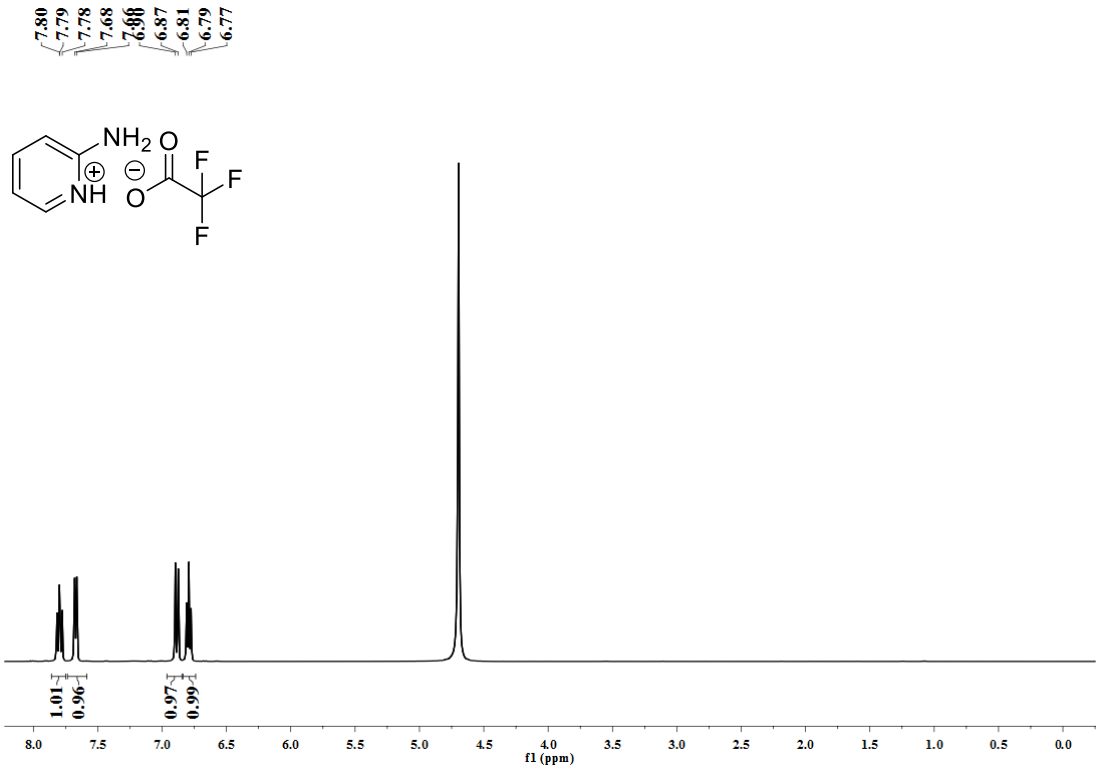


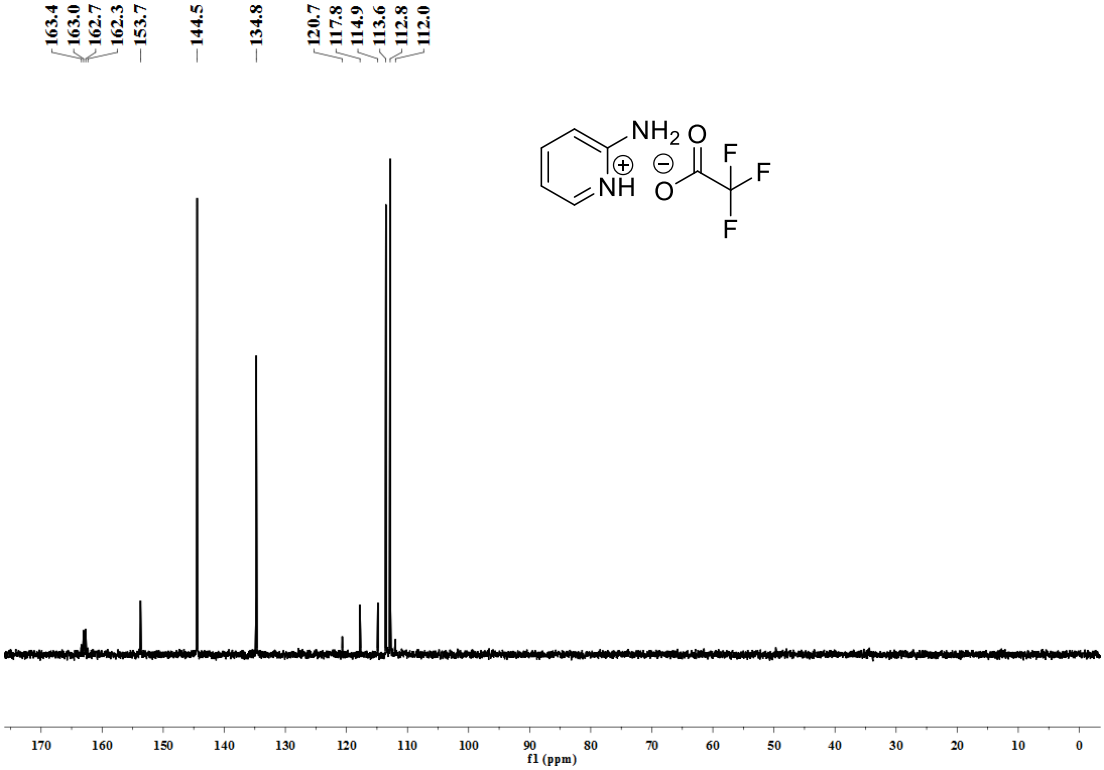
A6-B9: [2-AnPy][Cro]



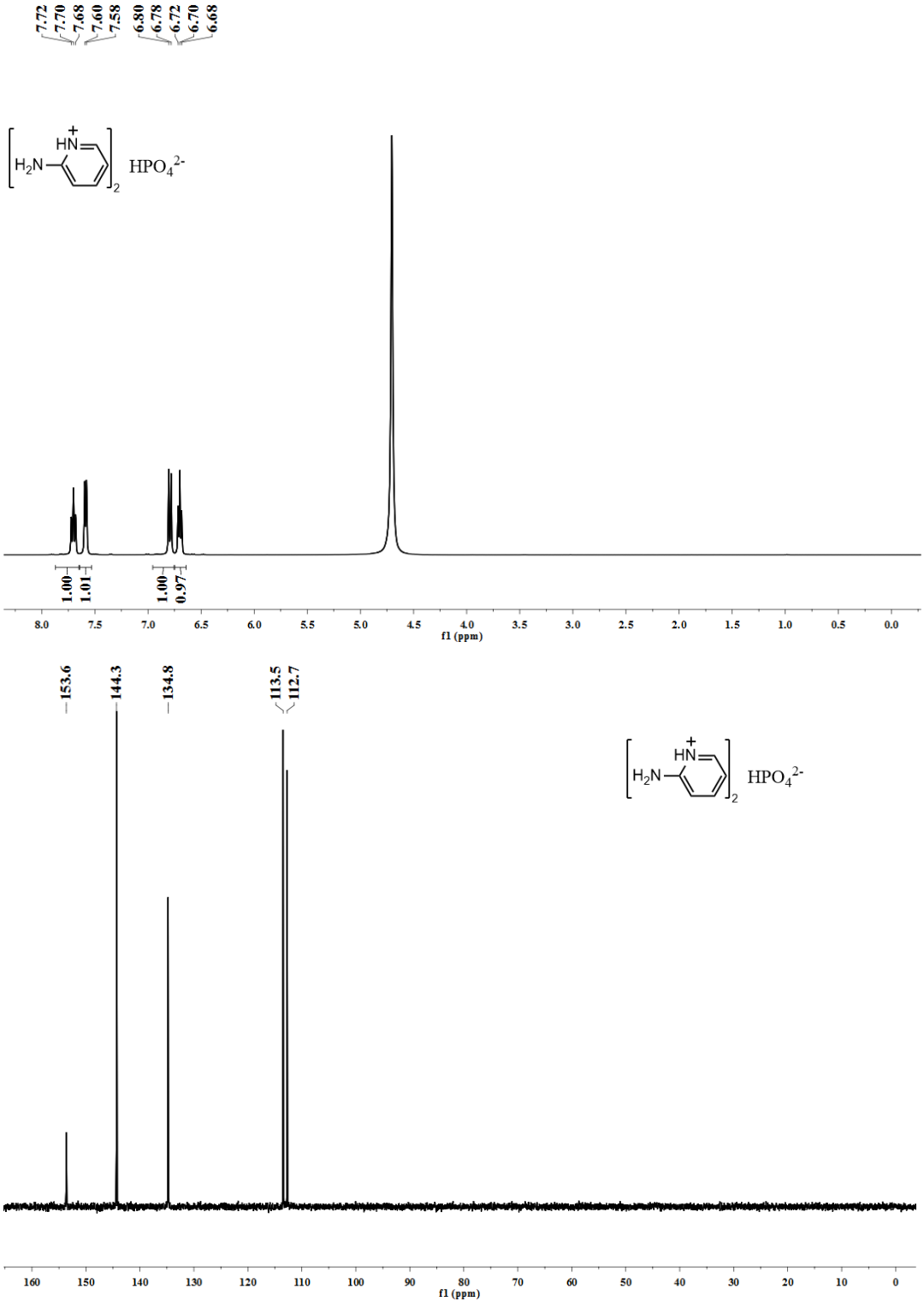


A6-B10: [2-AnPy][Tfa]

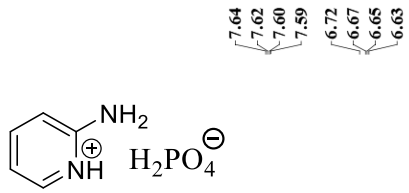


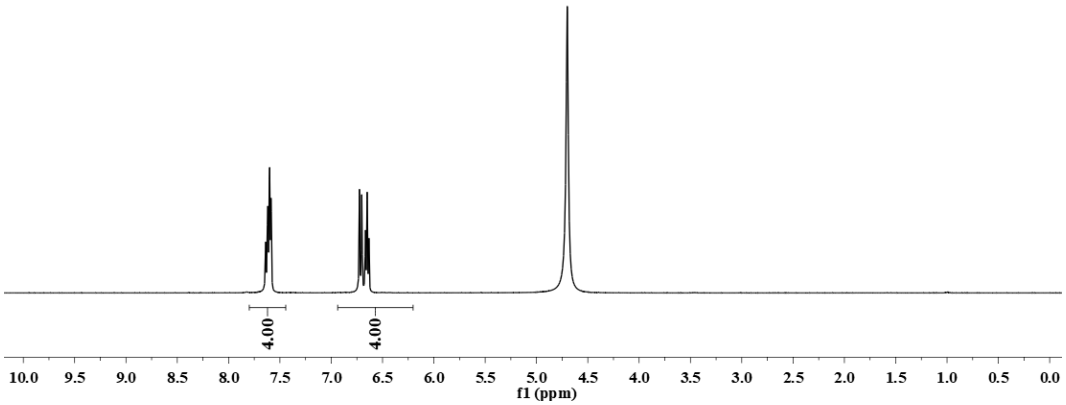


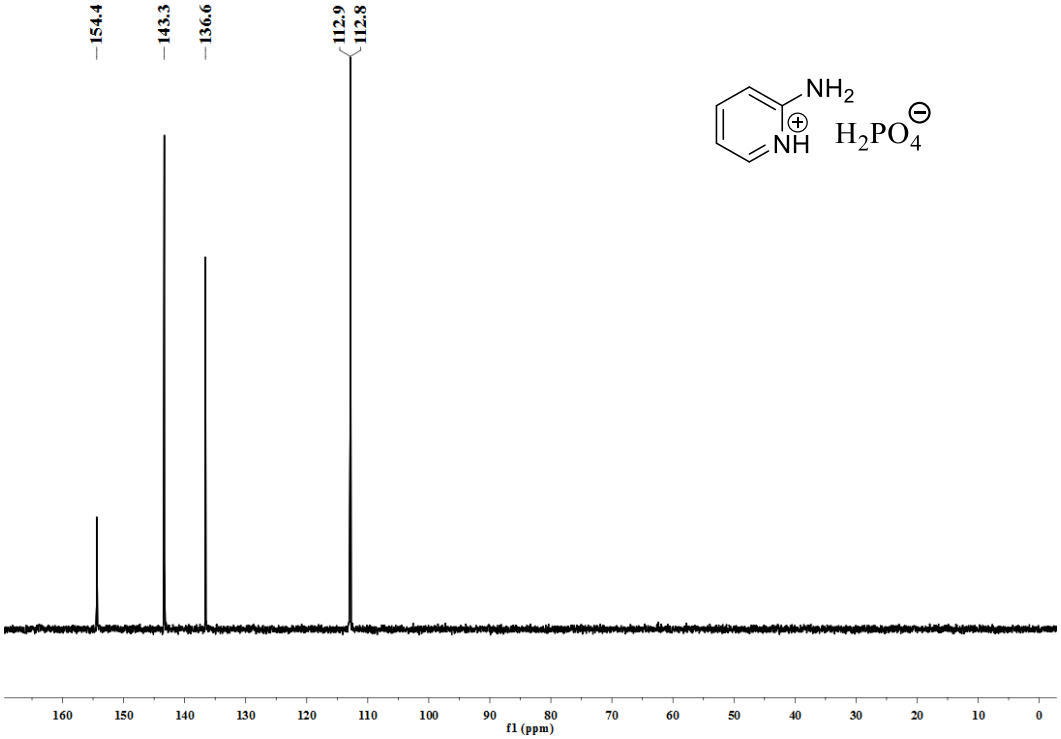
A6-B11: [2-AnPy][HPO_4]



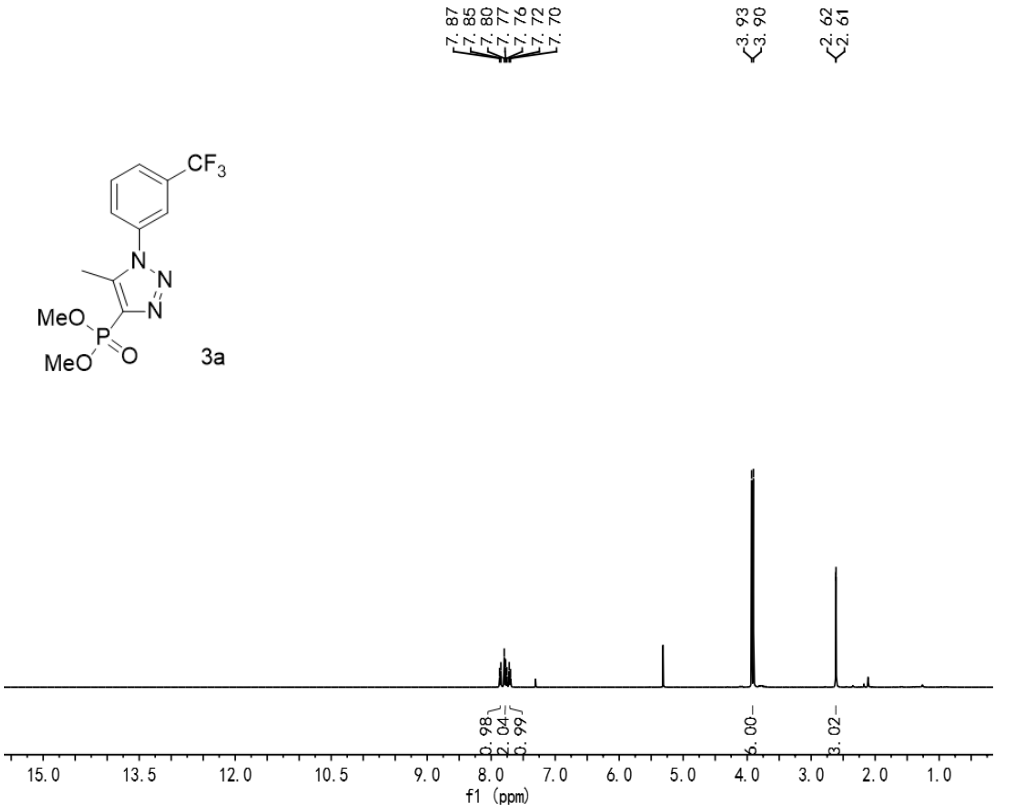
A6-B12: [2-AnPy][H_2PO_4]

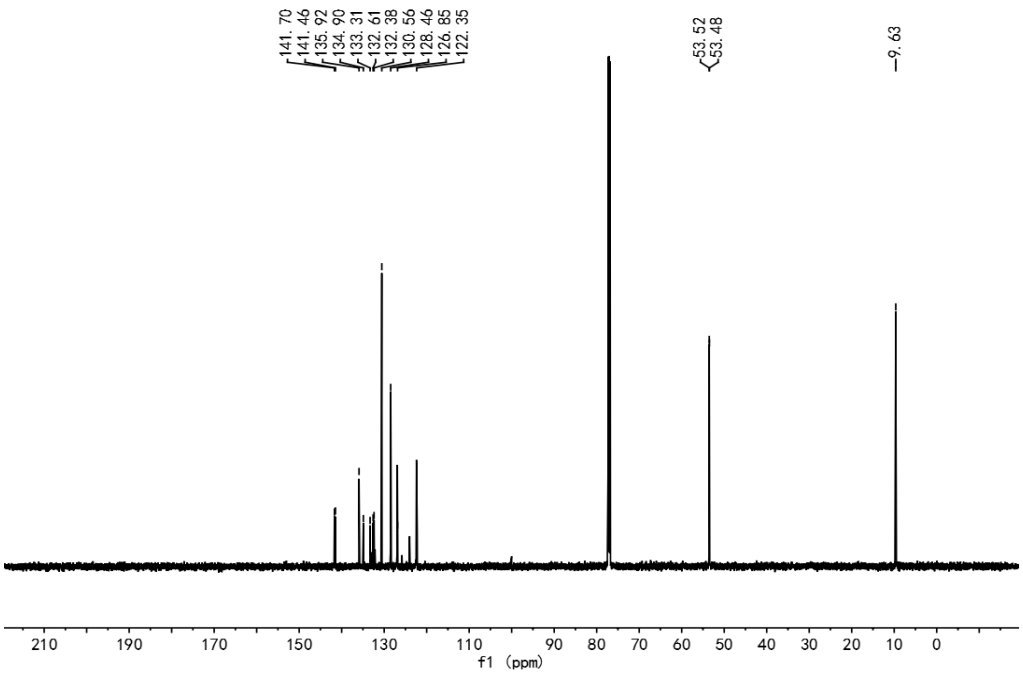


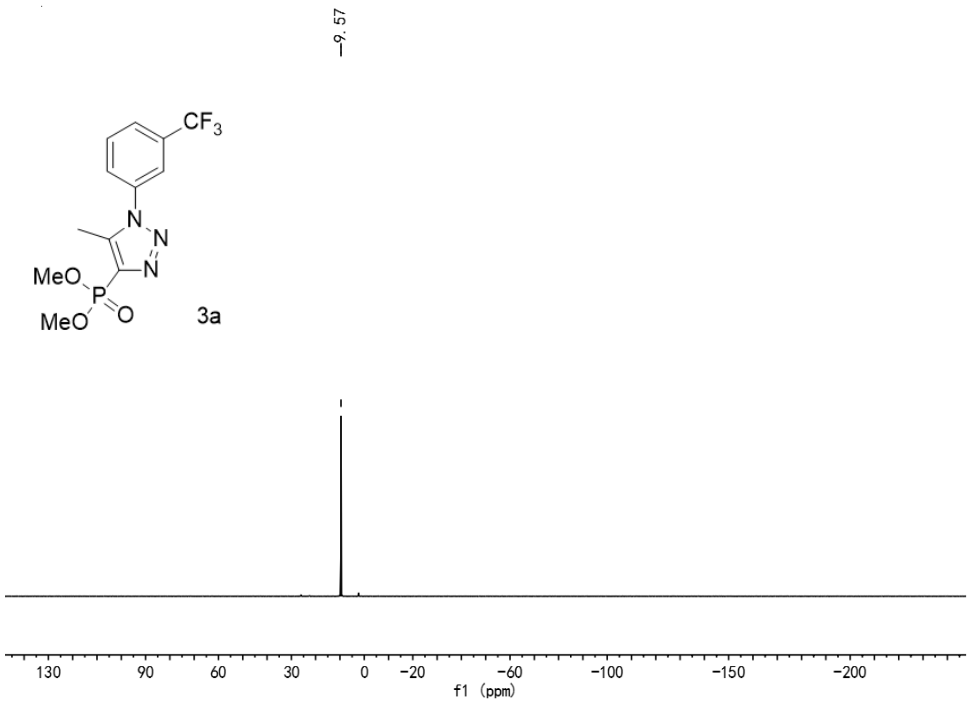




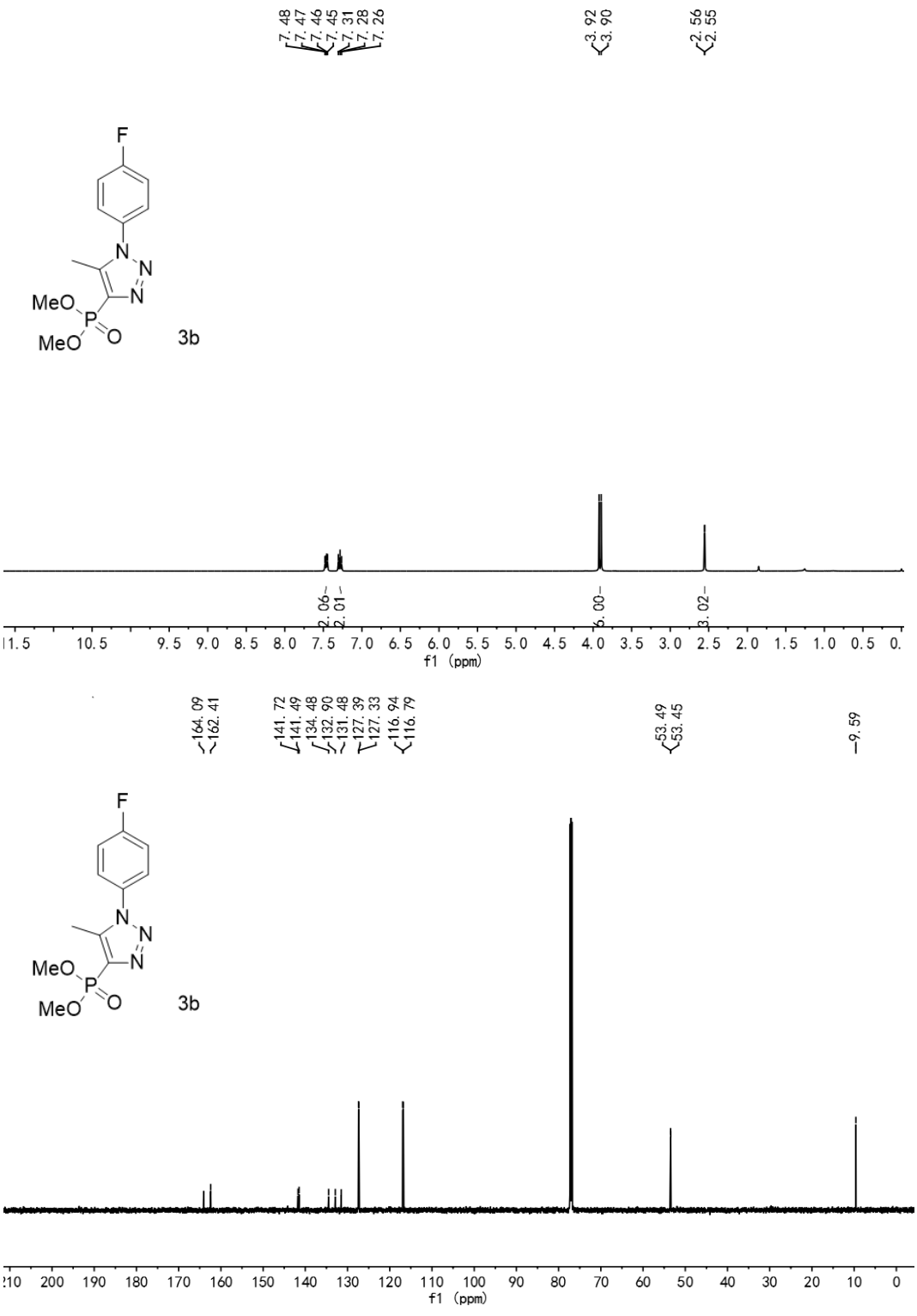
Dimethyl(5-methyl-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3a)

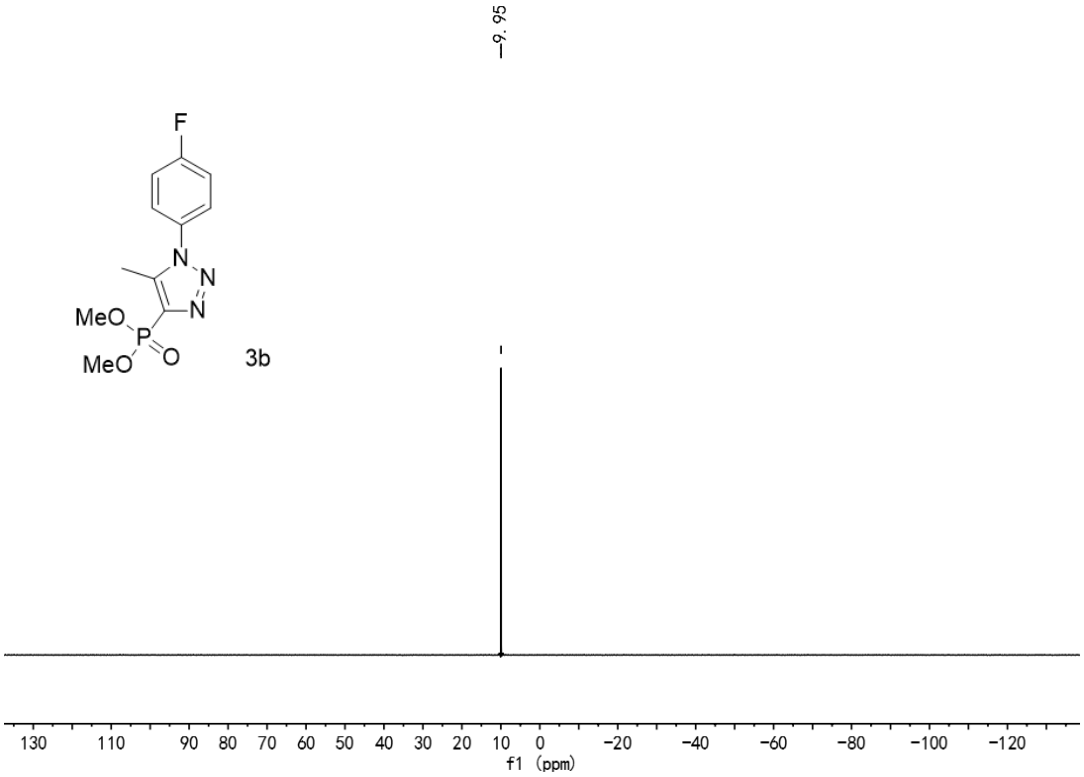




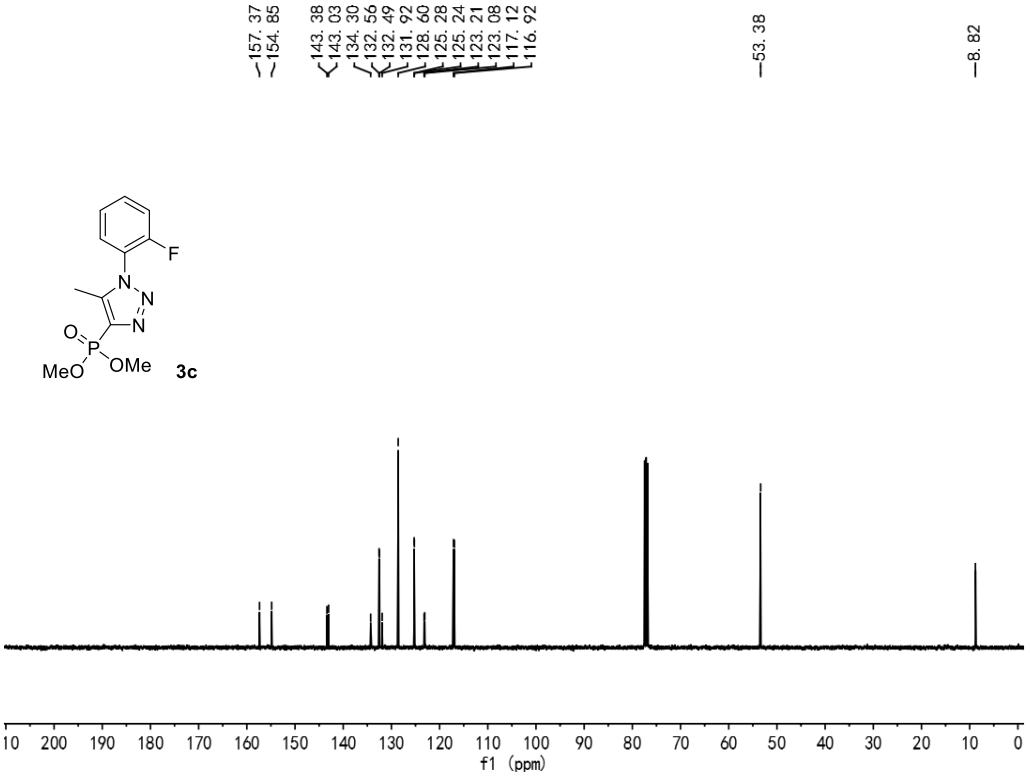

−9.57
CF3
N
N
N
MeO
P
O
MeO
3a
130
90
60
30
0
−20
−60
−100
−150
−200
f1 (ppm)

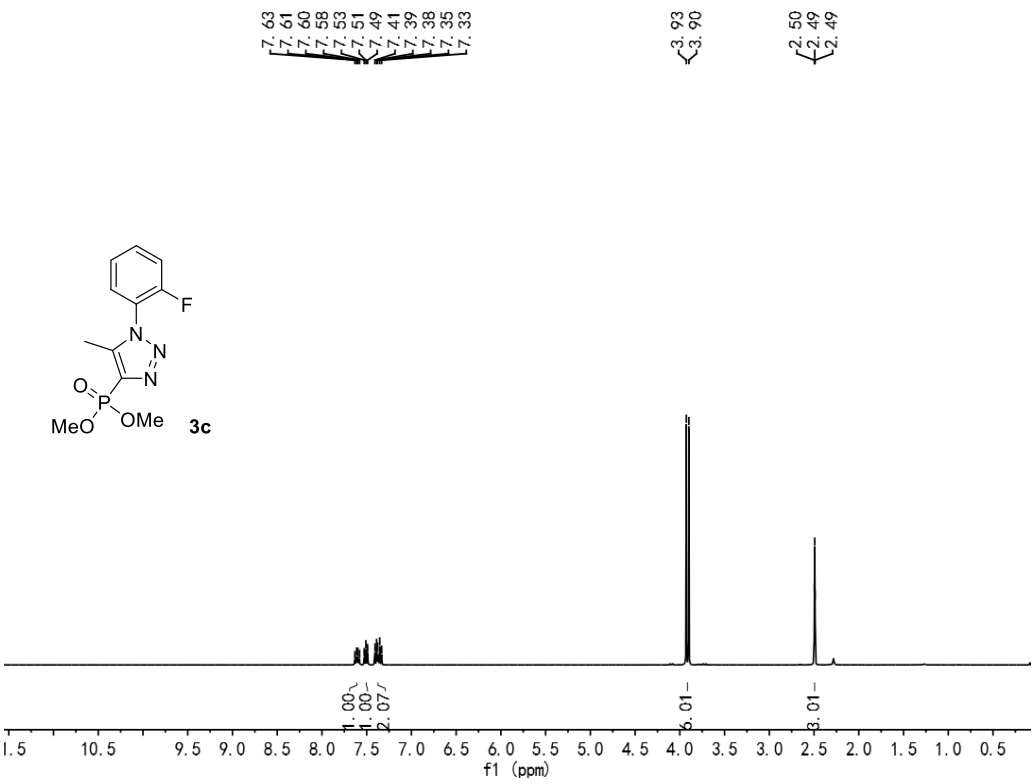
Dimethyl(1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate(3b)

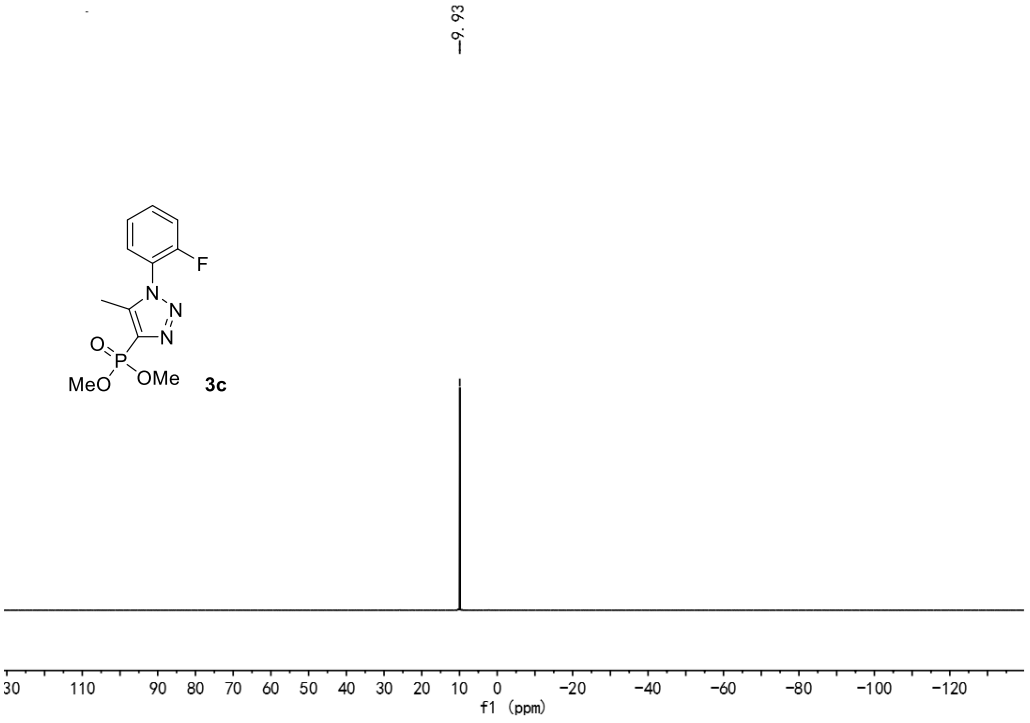




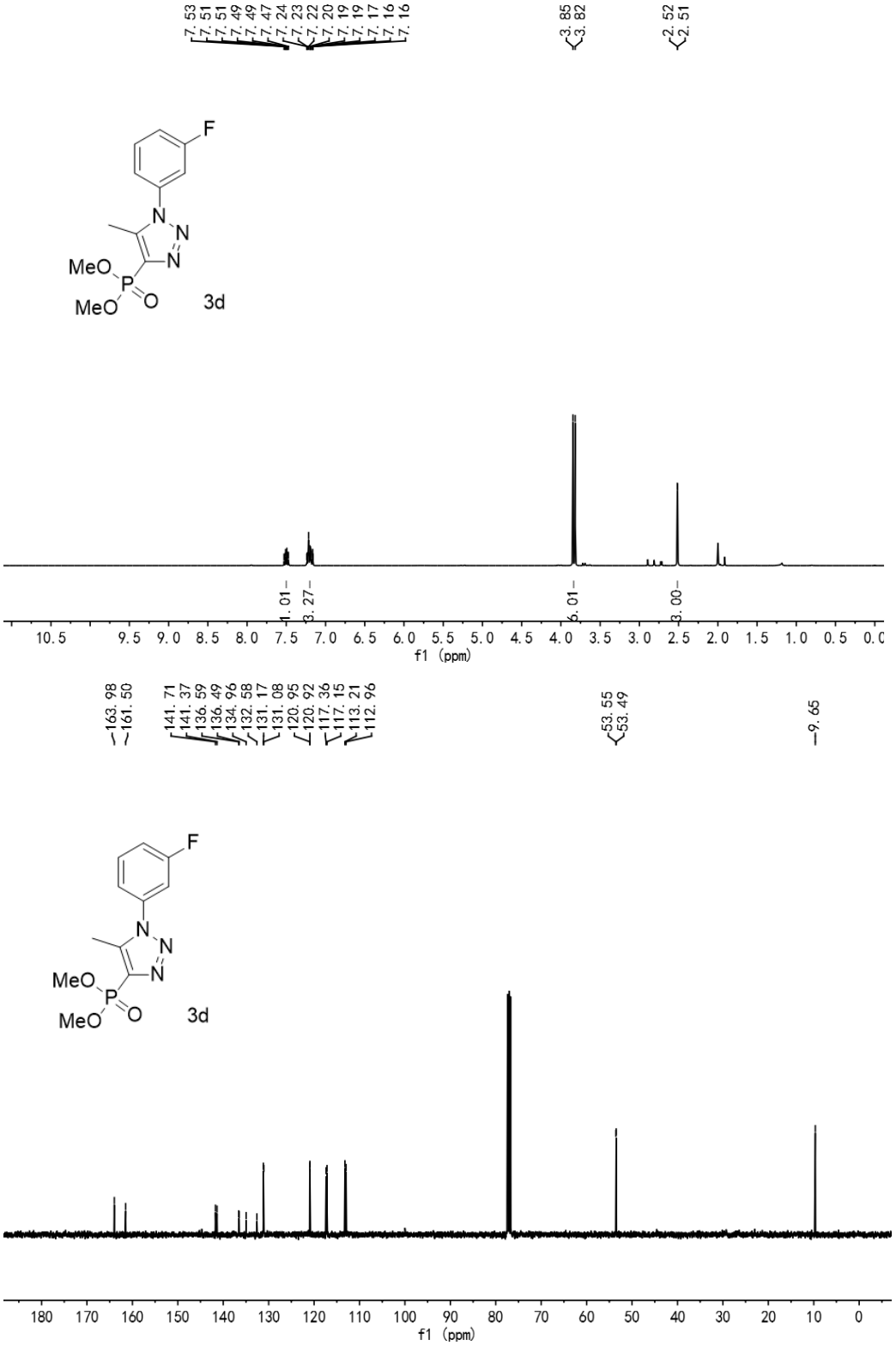
Dimethyl (1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3c)

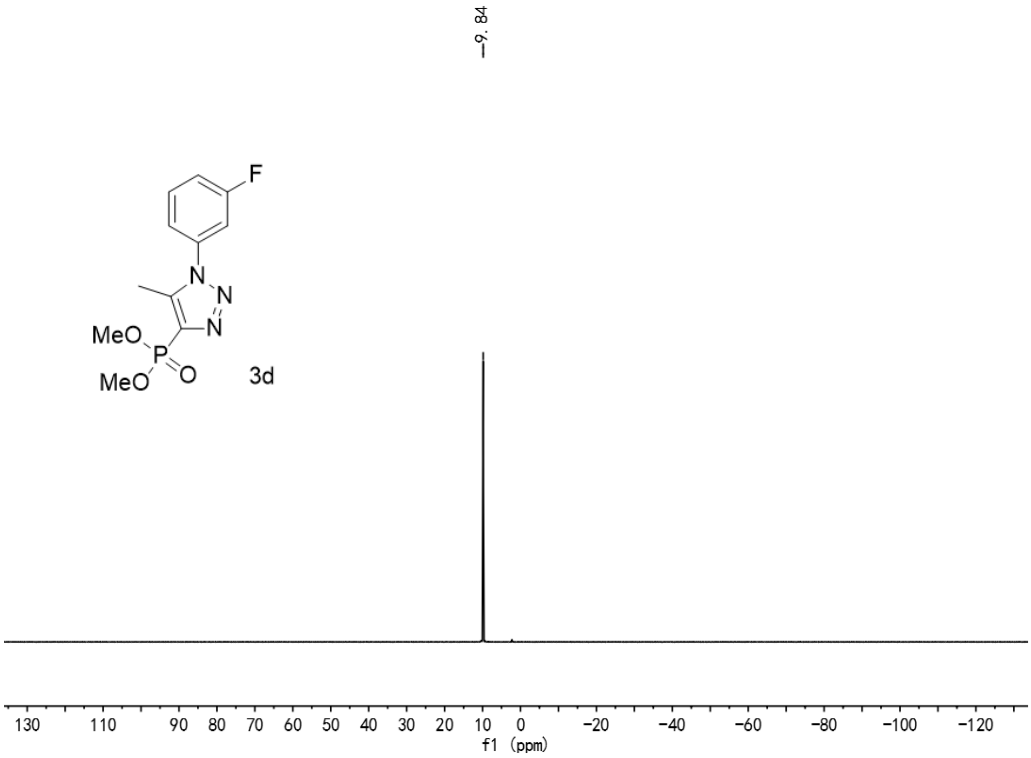



7.63
7.61
7.60
7.58
7.53
7.51
7.49
7.41
7.39
7.38
7.35
7.33
3.93
3.90
2.50
2.49
2.49
F
N
N
N
O
P
MeO
OMe
3c
1.00
1.00
2.07
6.01
3.01
f1 (ppm)

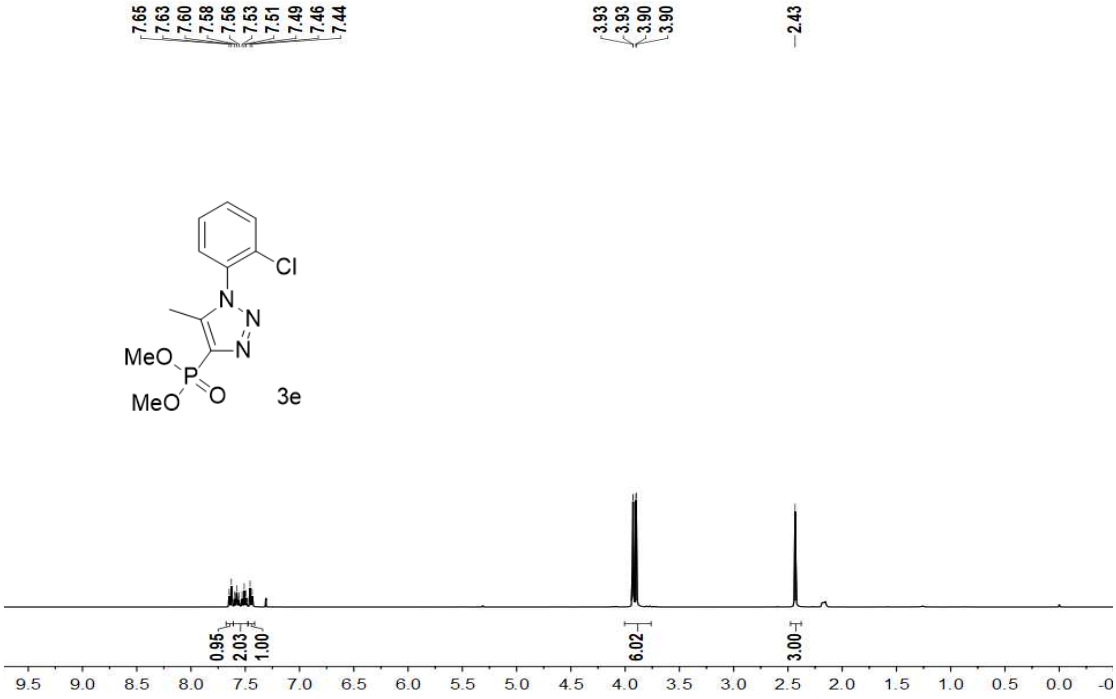

-9.93
F
N
N
N
O
P
MeO
OMe
3c
f1 (ppm)

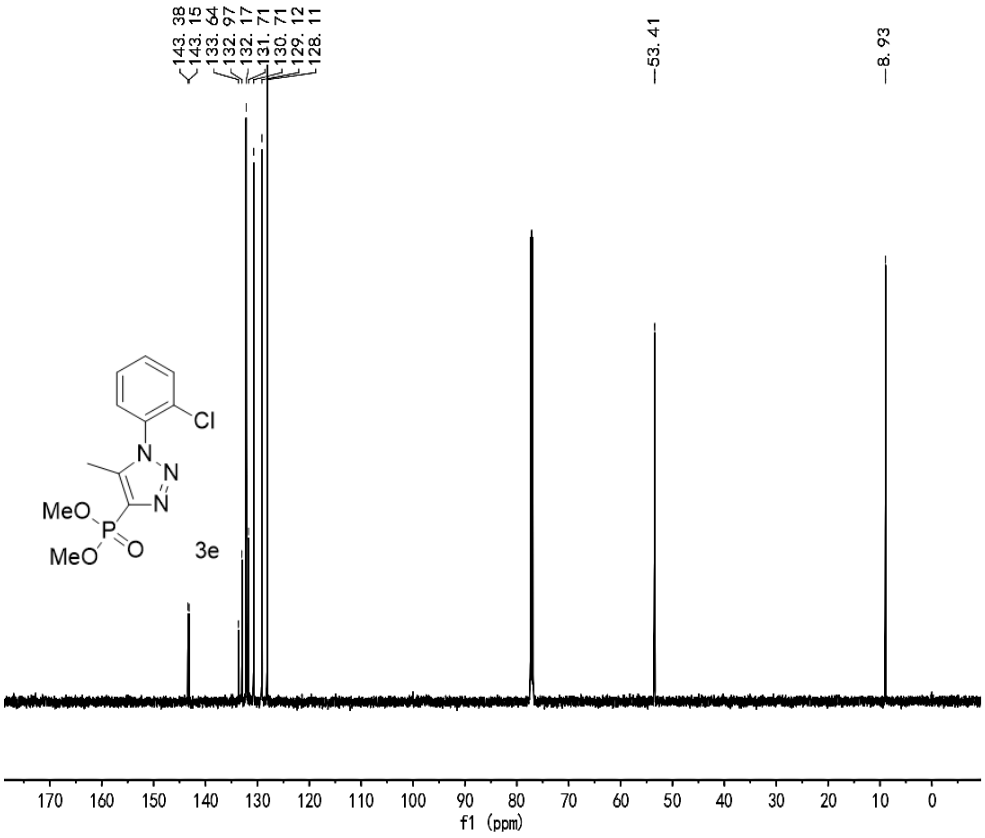
Dimethyl (1-(3-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3d)

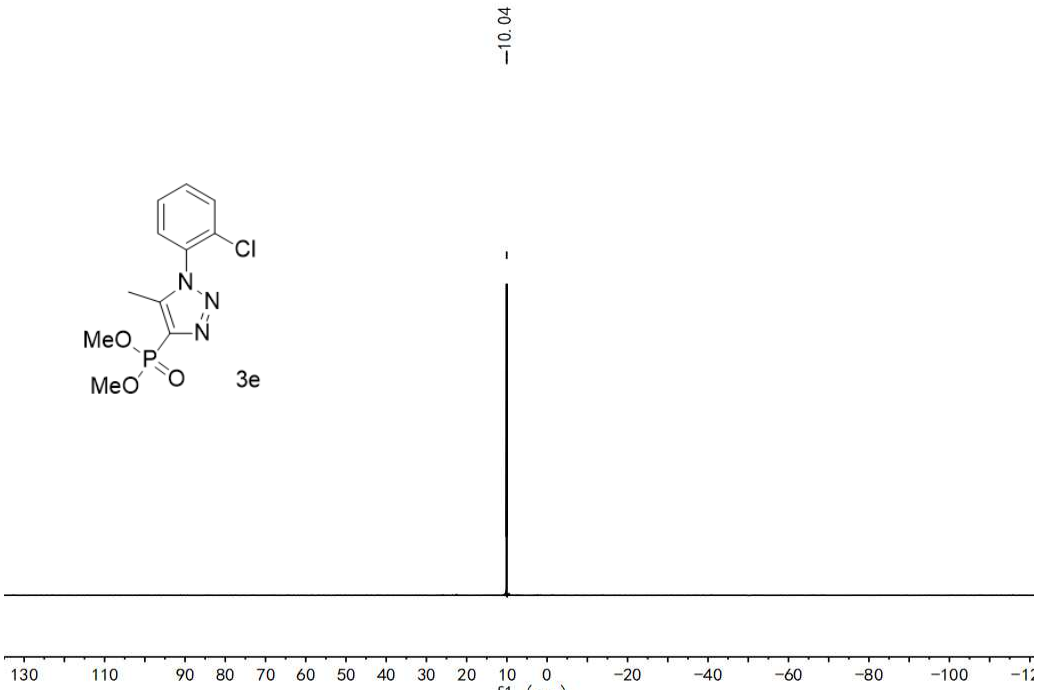




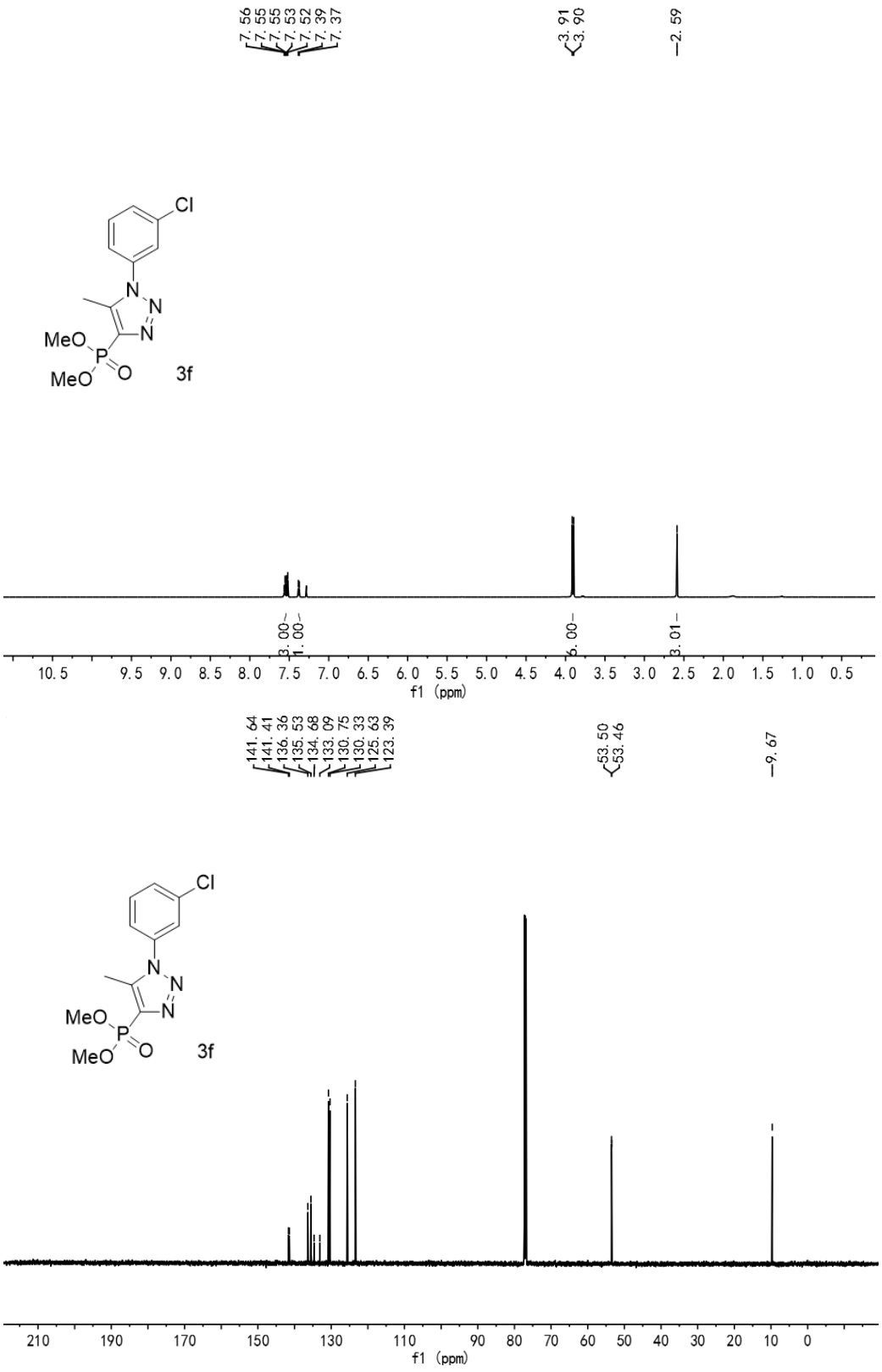
Dimethyl (1-(2-chlorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3e)

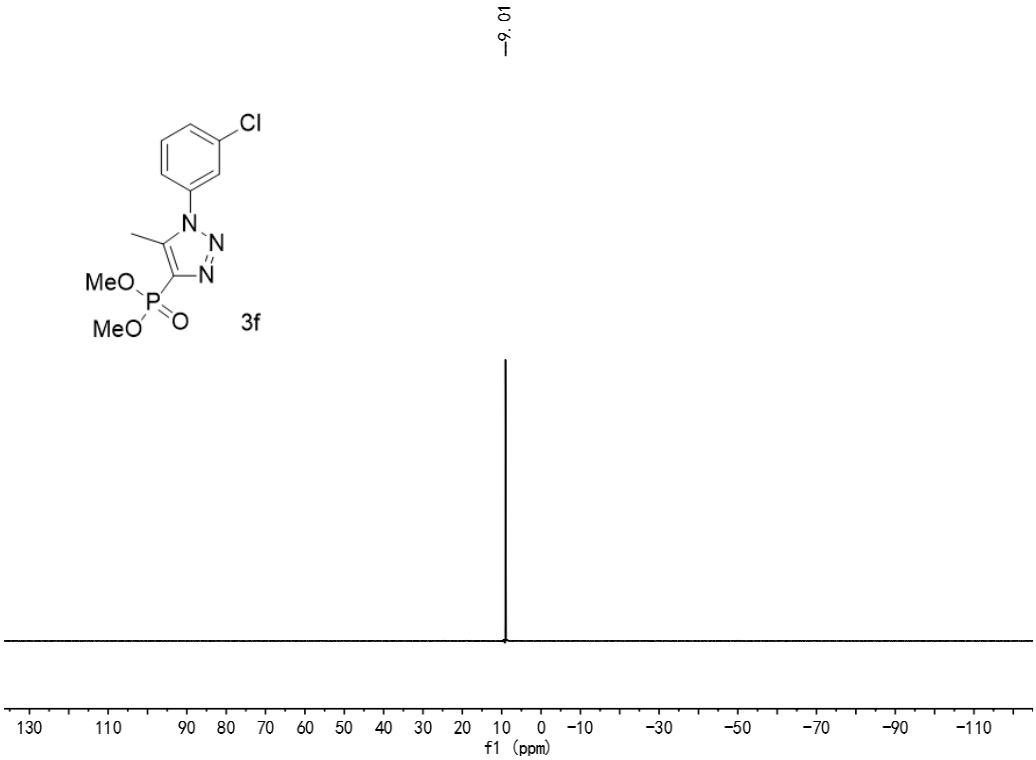



143.38
143.15
133.64
132.97
132.17
131.71
130.71
129.12
128.11
53.41
8.93
Cl
N
N
N
MeO
P
O
MeO
3e
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

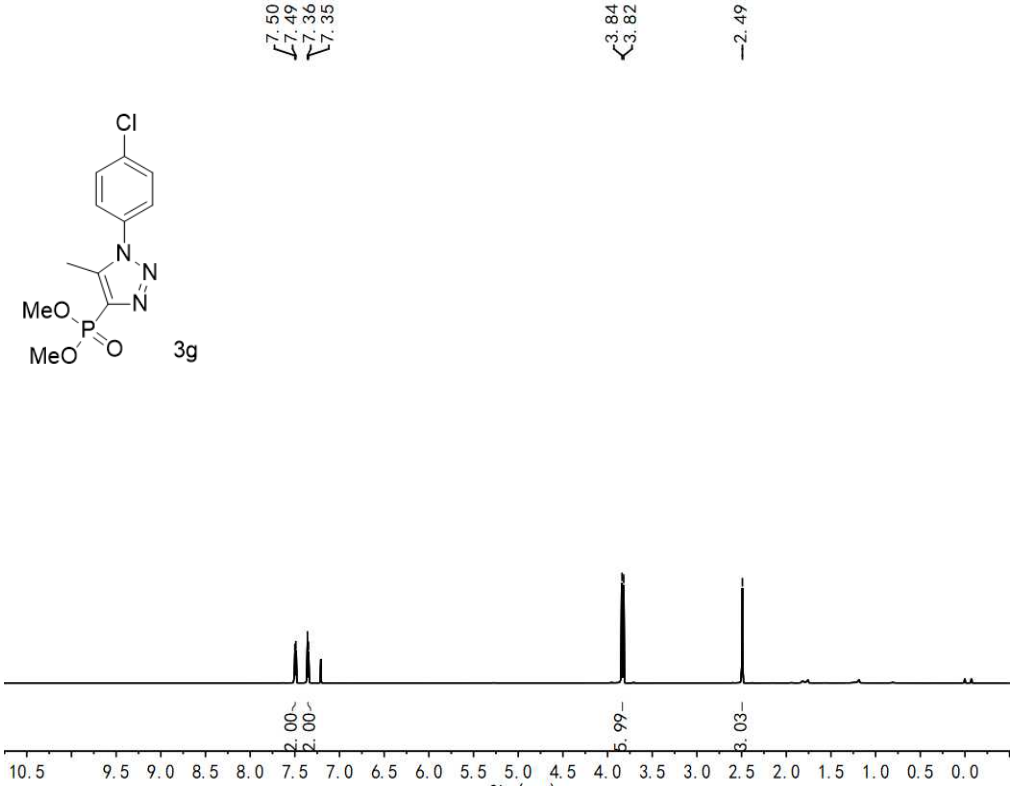

10.04
Cl
N
N
N
MeO
P
O
MeO
3e
130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100

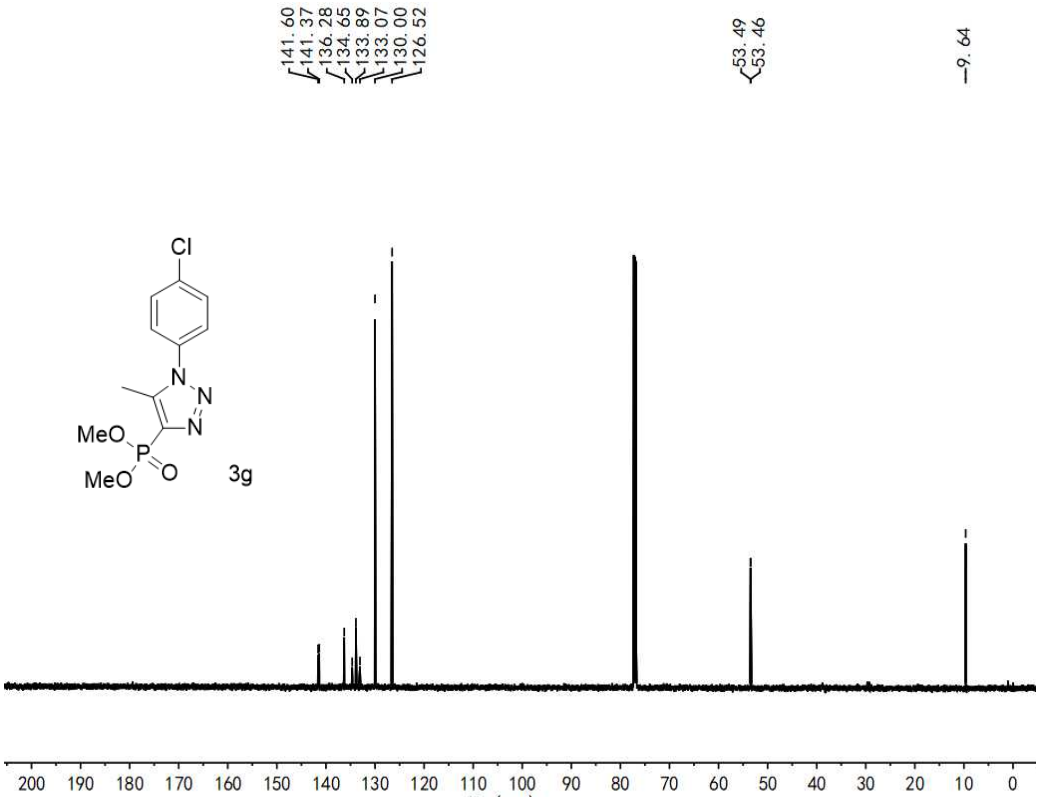
Dimethyl (1-(3-chlorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3f)

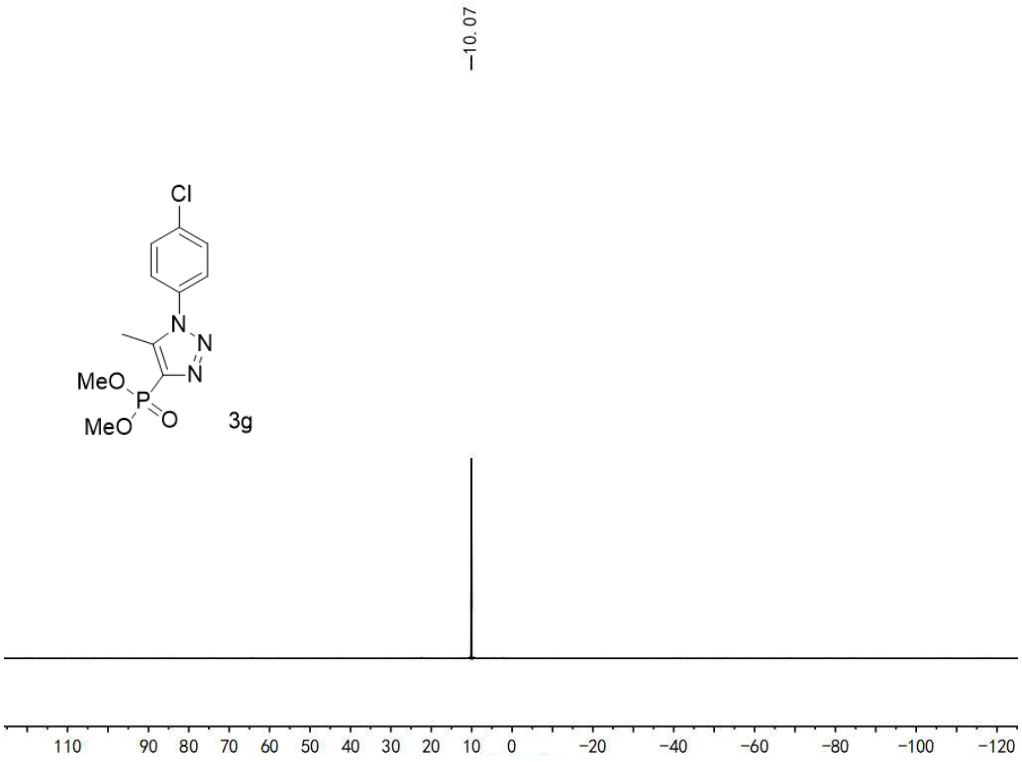




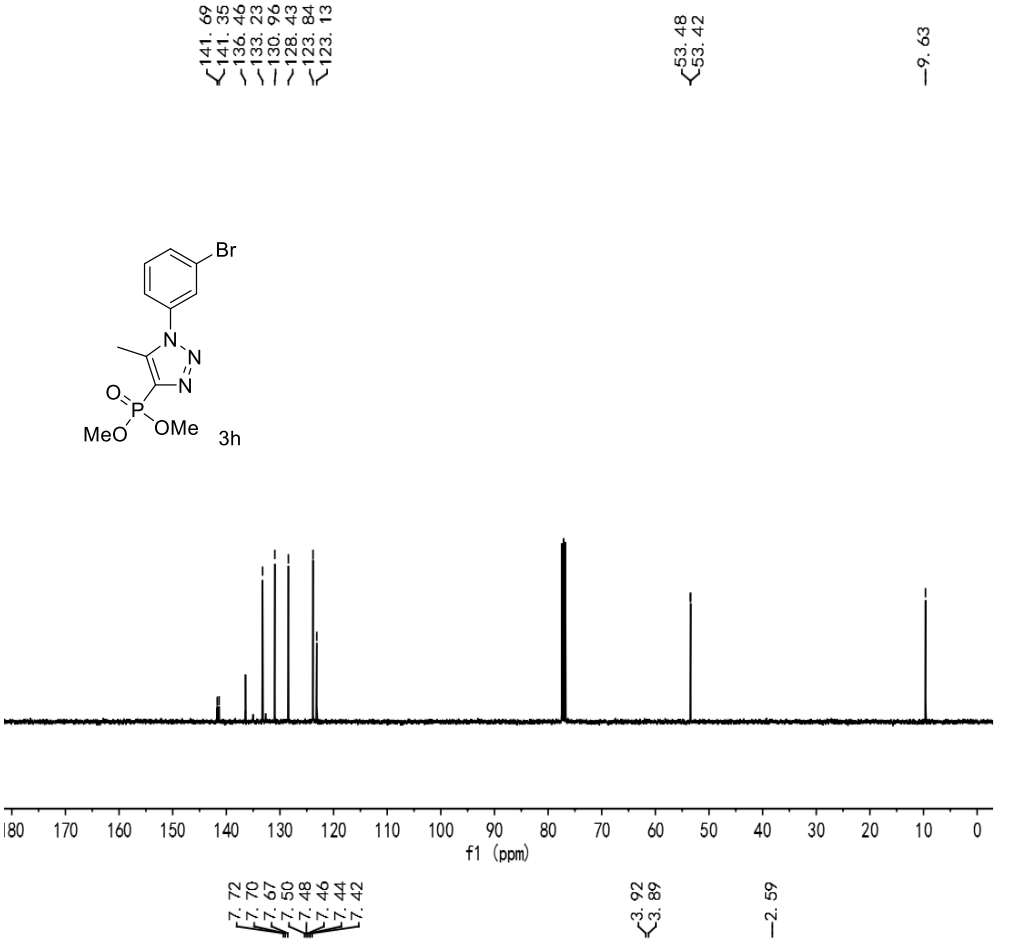
Dimethyl (1-(4-chlorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3g)

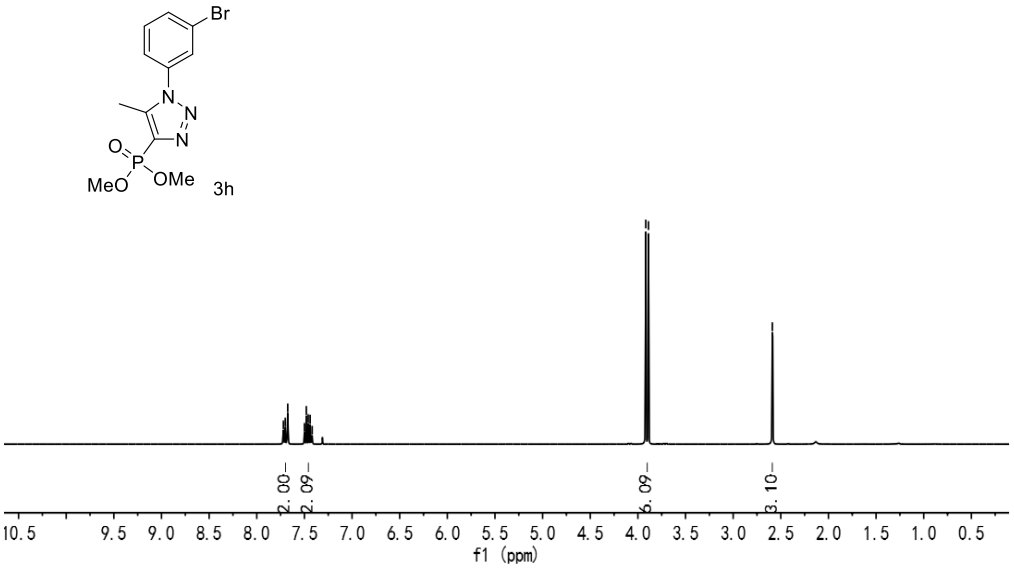


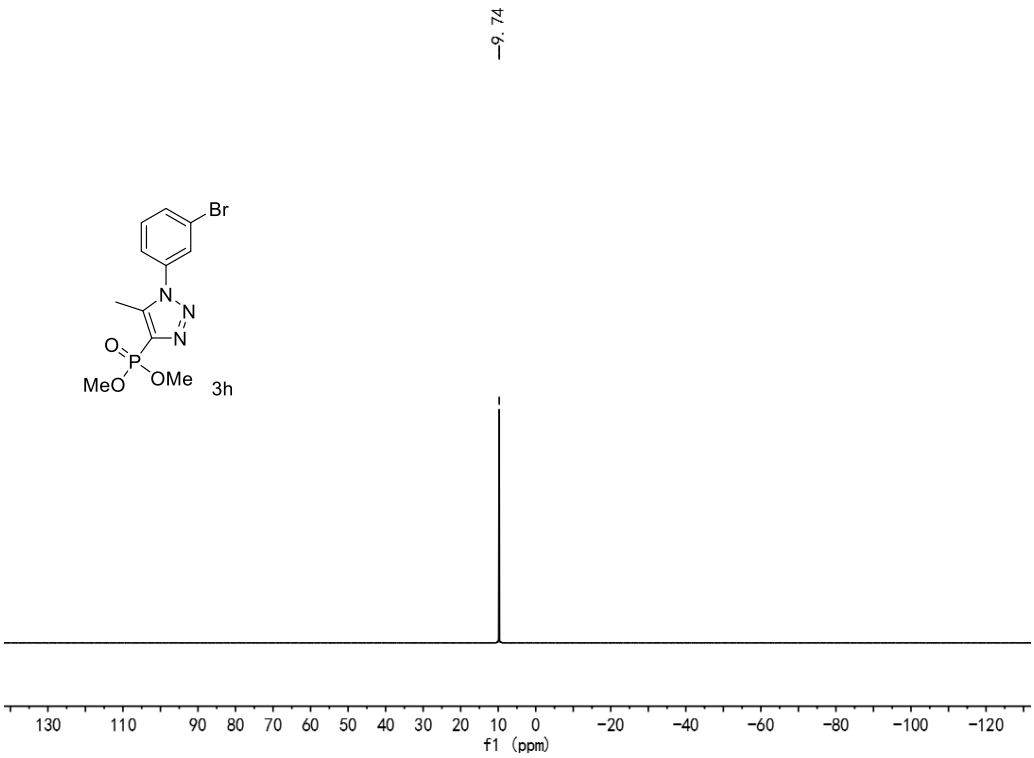

141.60
141.37
136.28
134.65
133.89
133.07
130.00
126.52
53.49
53.46
9.64
Cl
N
N
N
MeO
P
O
MeO
3g
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


10.07
Cl
N
N
N
MeO
P
O
MeO
3g
110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120

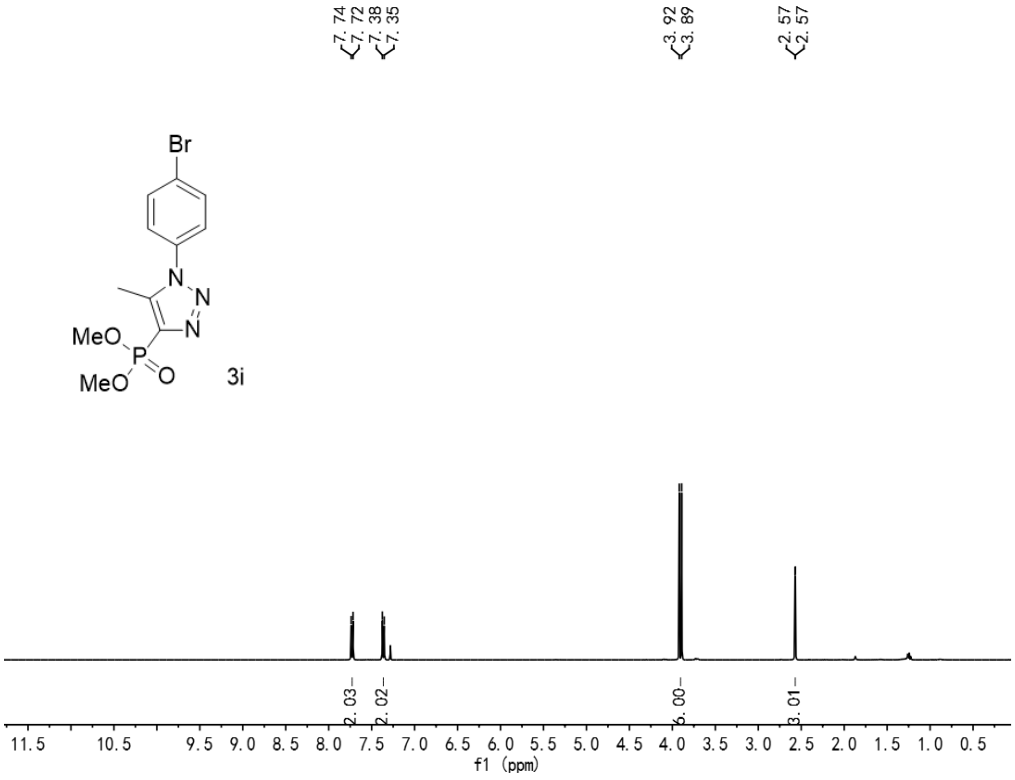
Dimethyl (1-(3-bromophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3h)

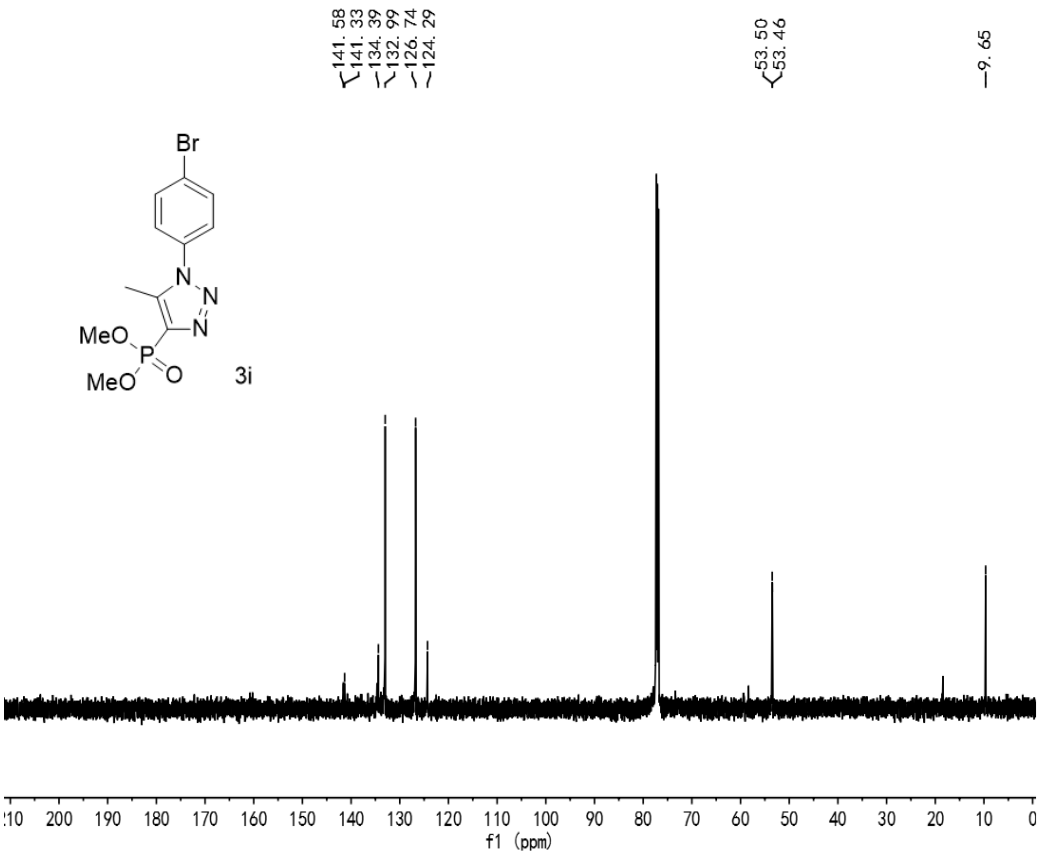


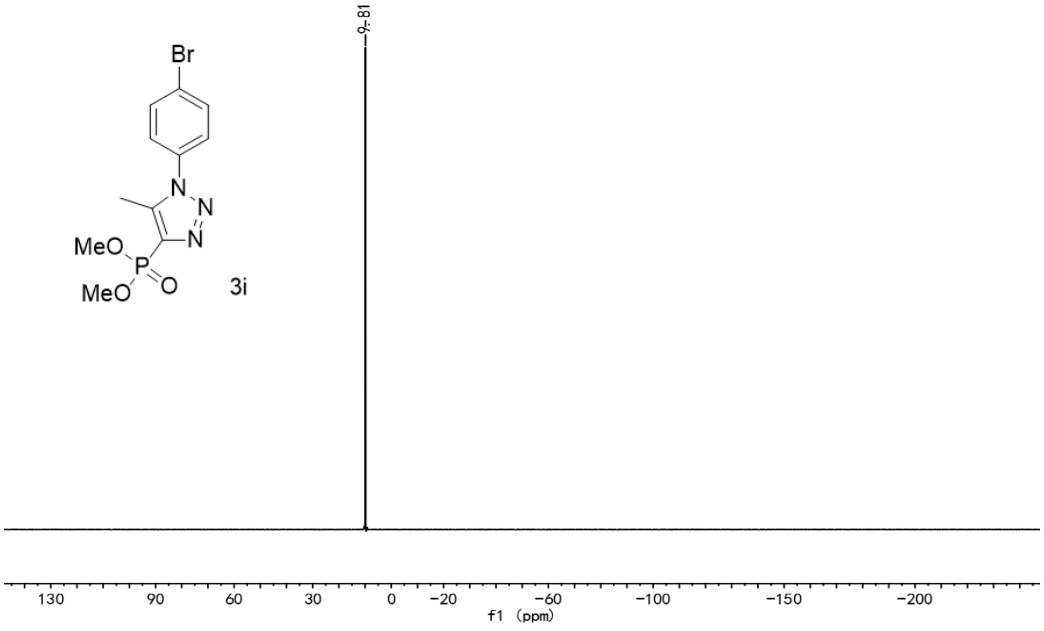




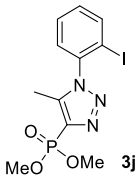
Dimethyl(1-(4-bromophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3i)



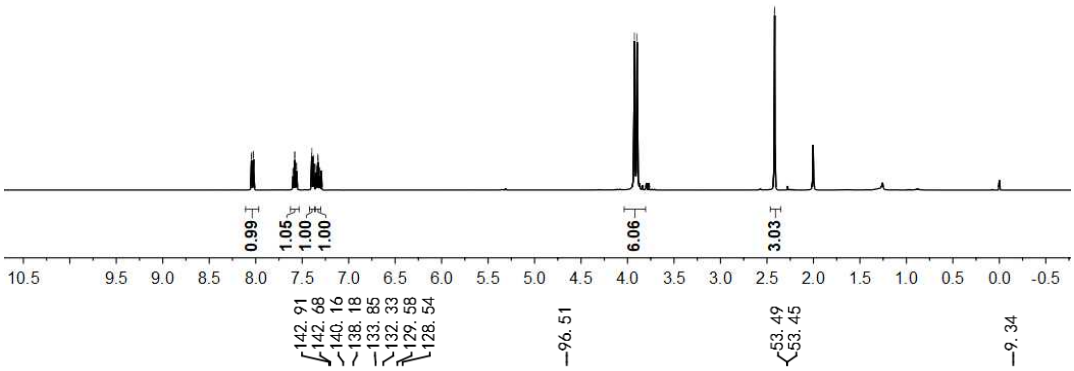

141.58
141.33
134.39
132.99
126.74
124.29
53.50
53.46
9.65
Br
N
N
N
MeO
P
O
MeO
3i
f1 (ppm)

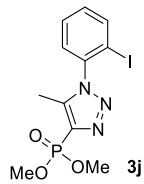

9.81
Br
N
N
N
MeO
P
O
MeO
3i
f1 (ppm)

Dimethyl(1-(2-iodophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3j)

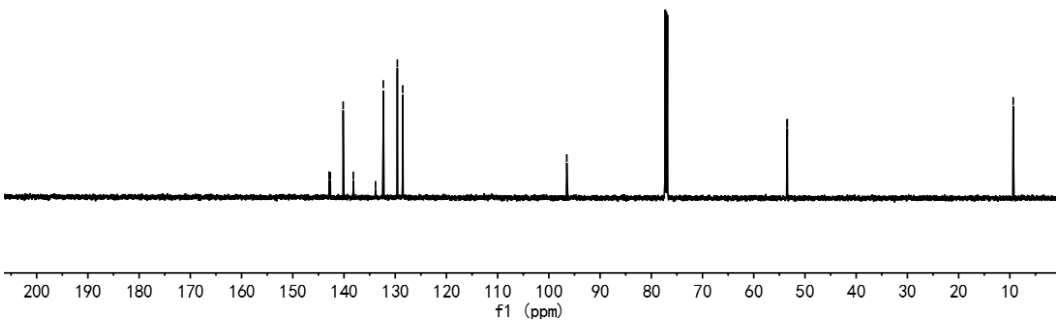


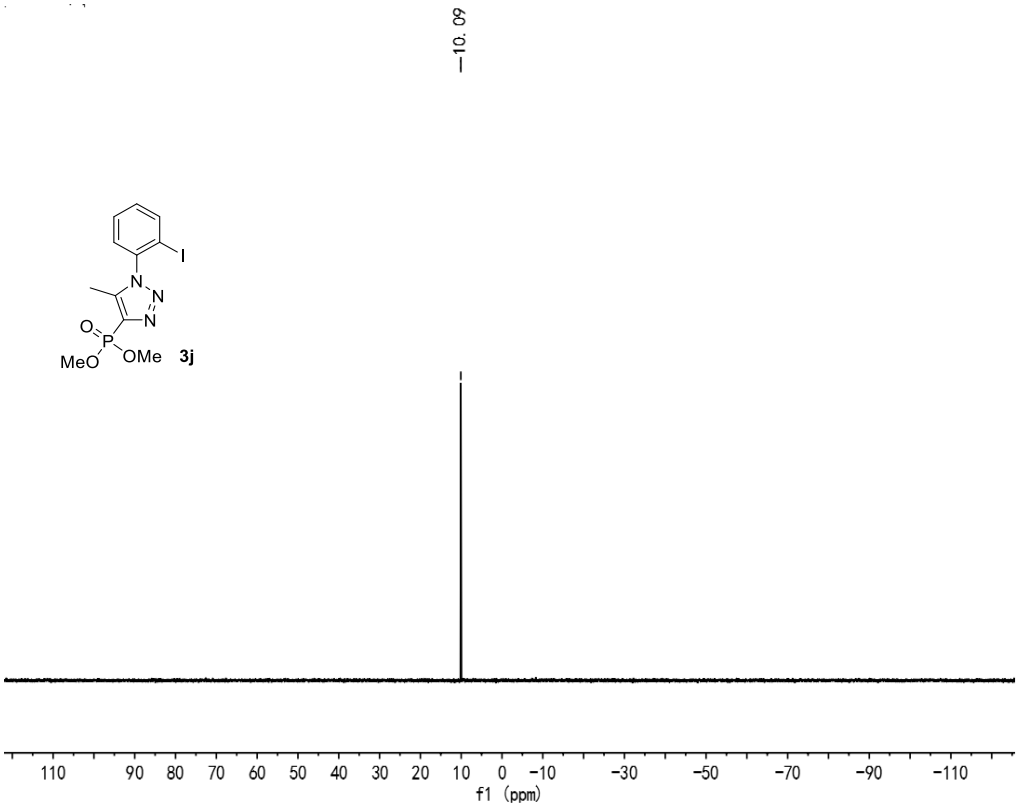
3j



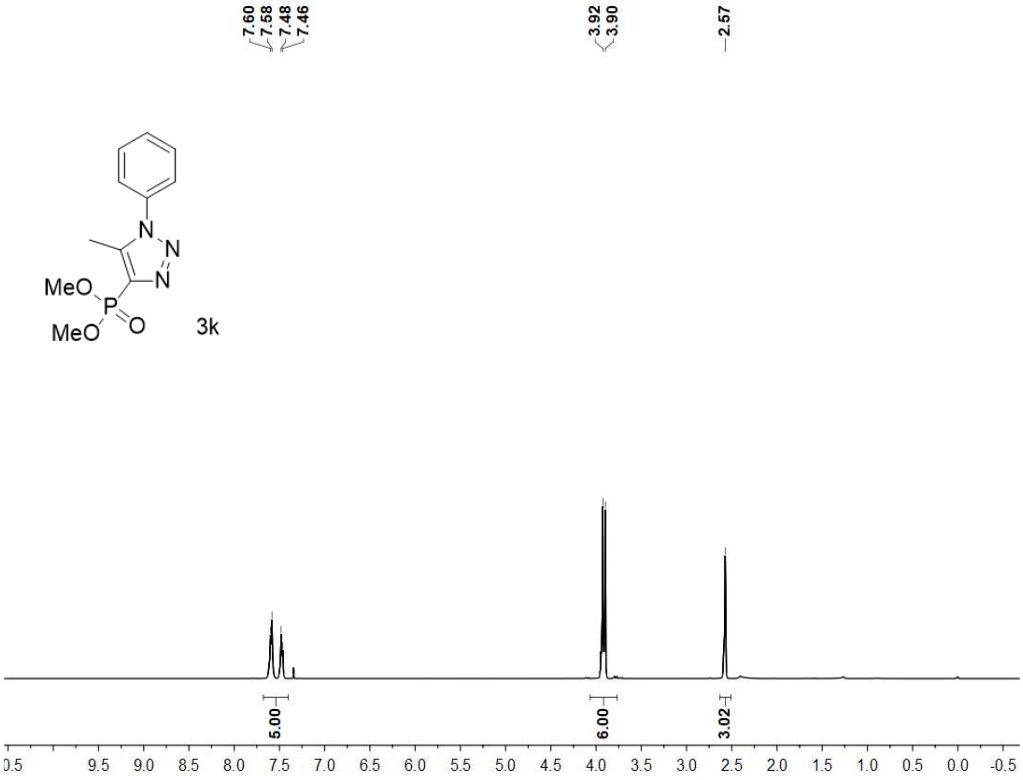


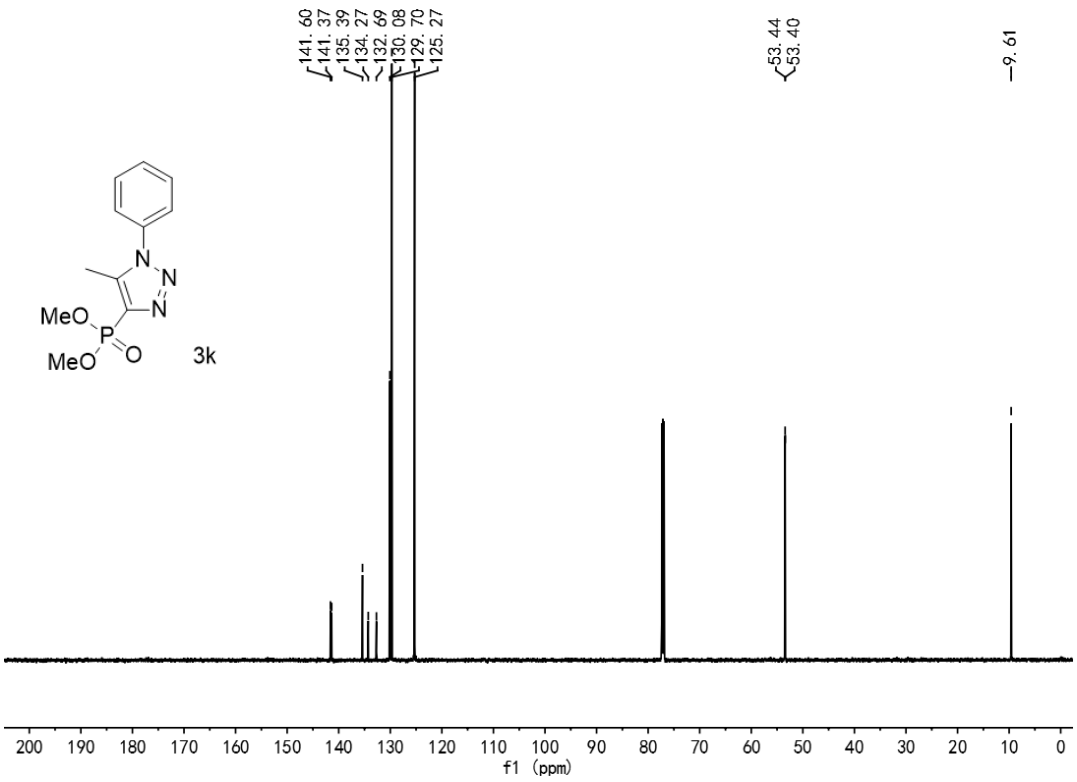
3j

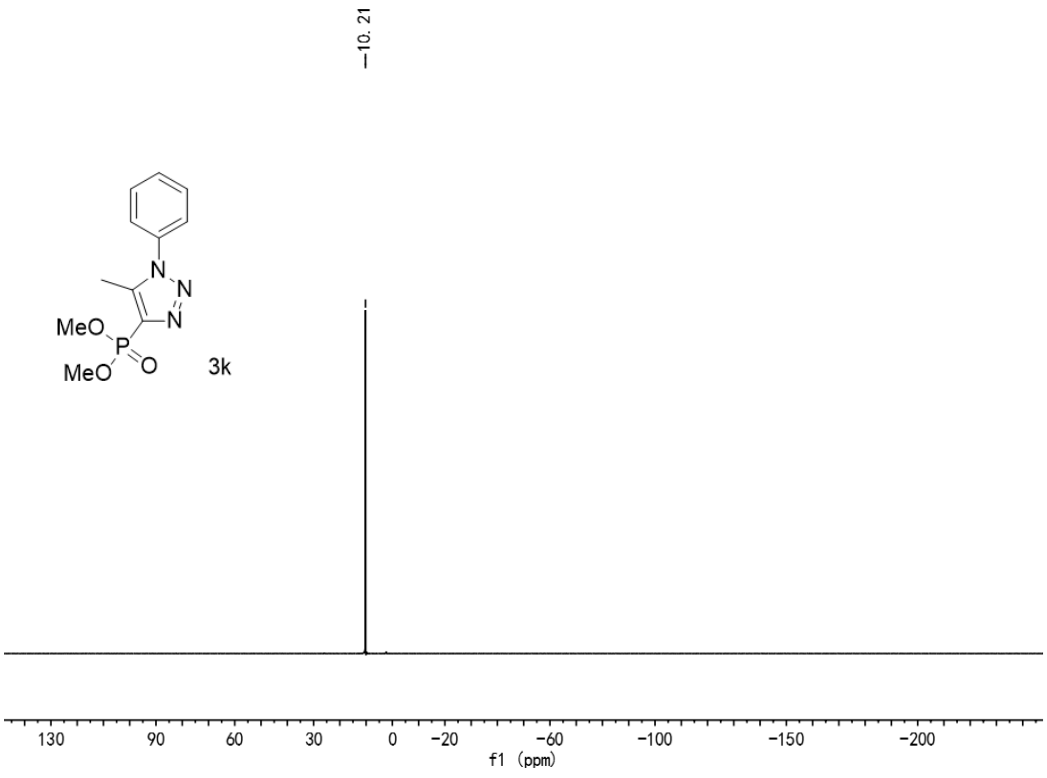




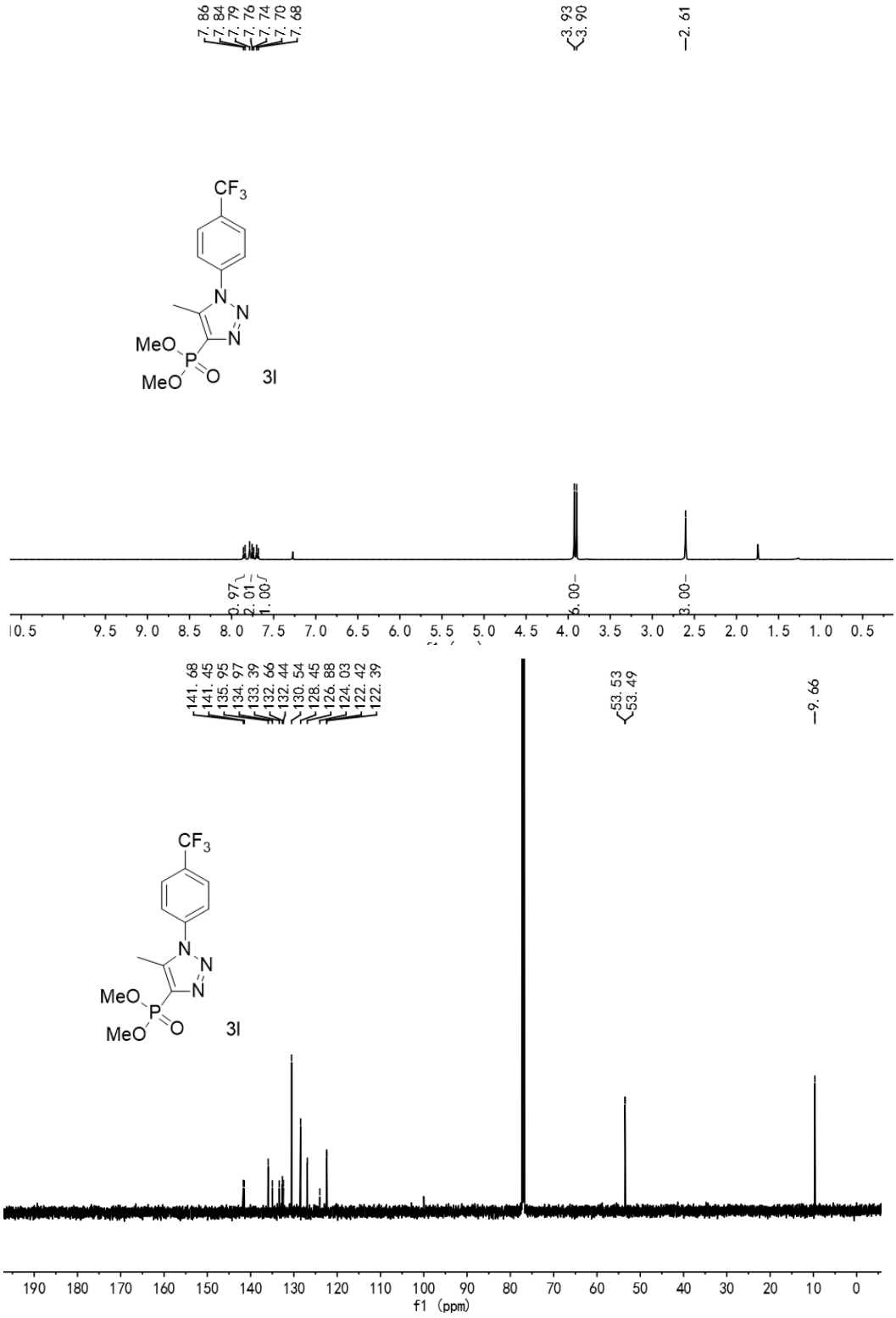
Dimethyl(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)phosphonate (3k)

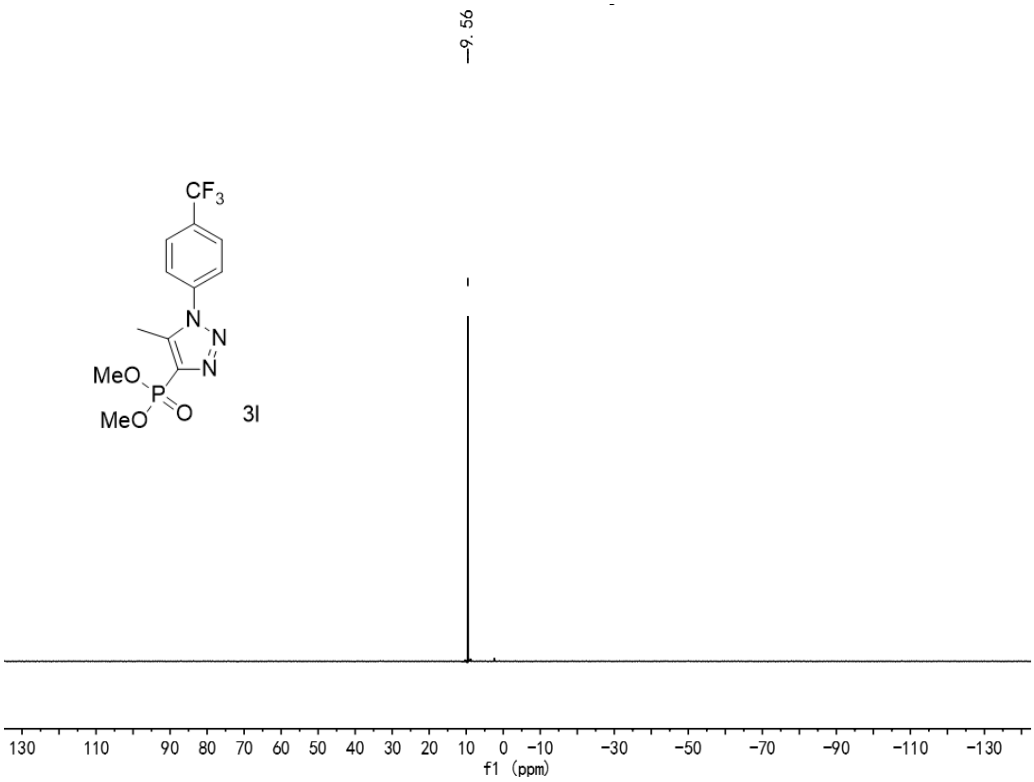



141.60
141.37
135.39
134.27
132.69
130.08
129.70
125.27
53.44
53.40
9.61
MeO
MeO
P
O
N
N
N
3k
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

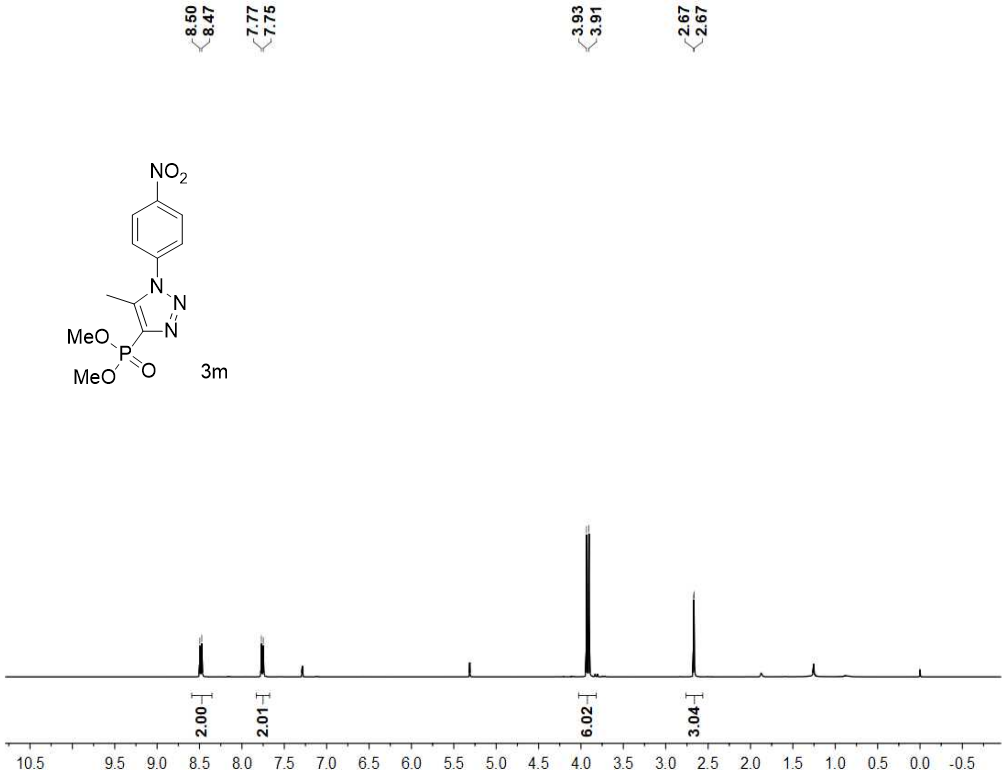

10.21
MeO
MeO
P
O
N
N
N
3k
130 90 60 30 0 -20 -60 -100 -150 -200
f1 (ppm)

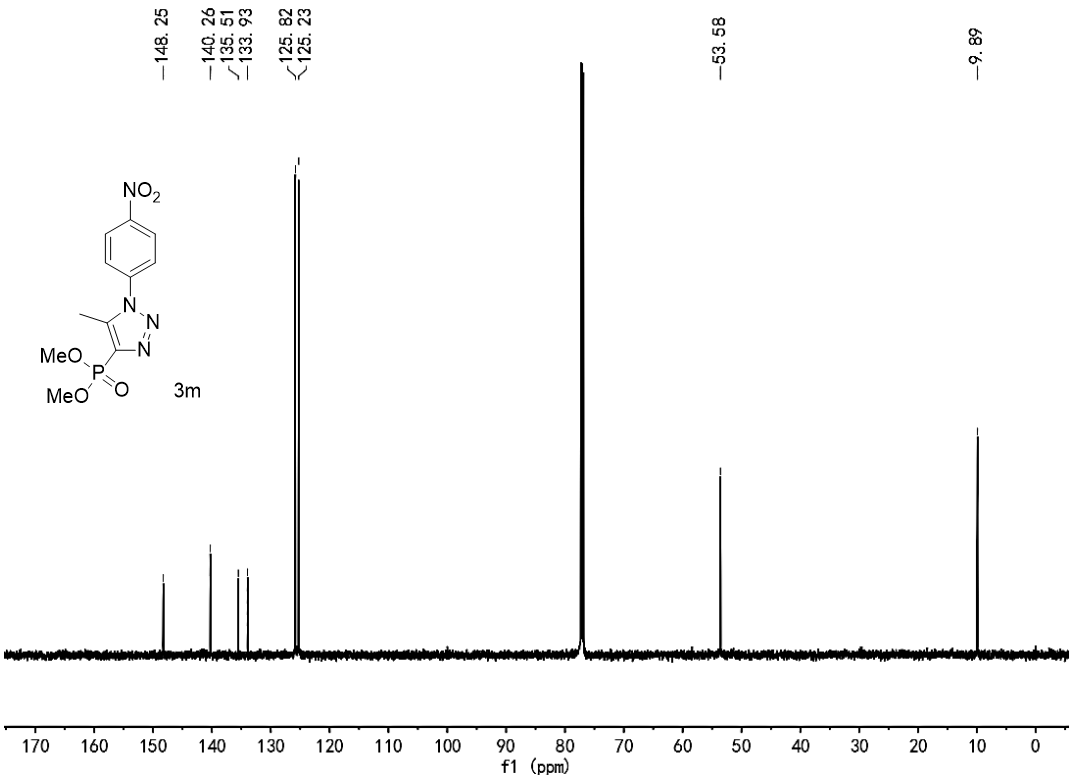
Dimethyl(5-methyl-1-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3l)

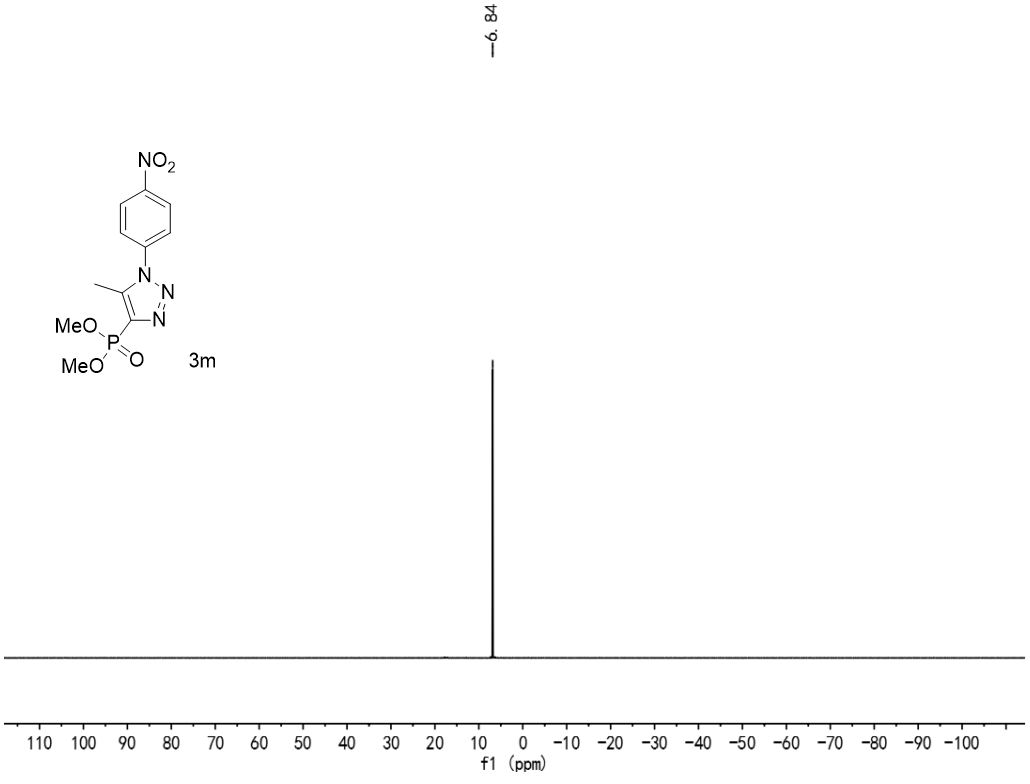




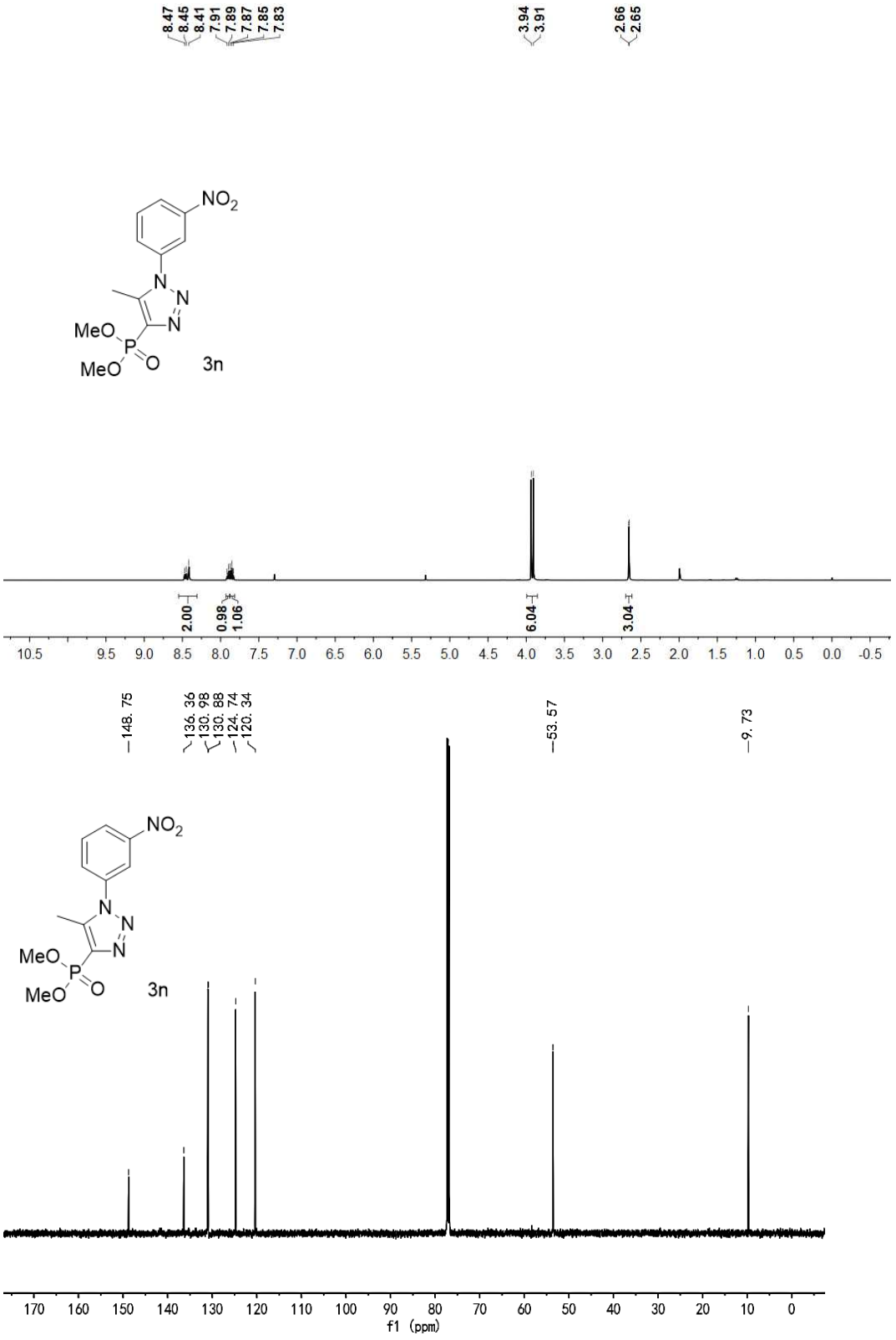
Dimethyl (5-methyl-1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3m)

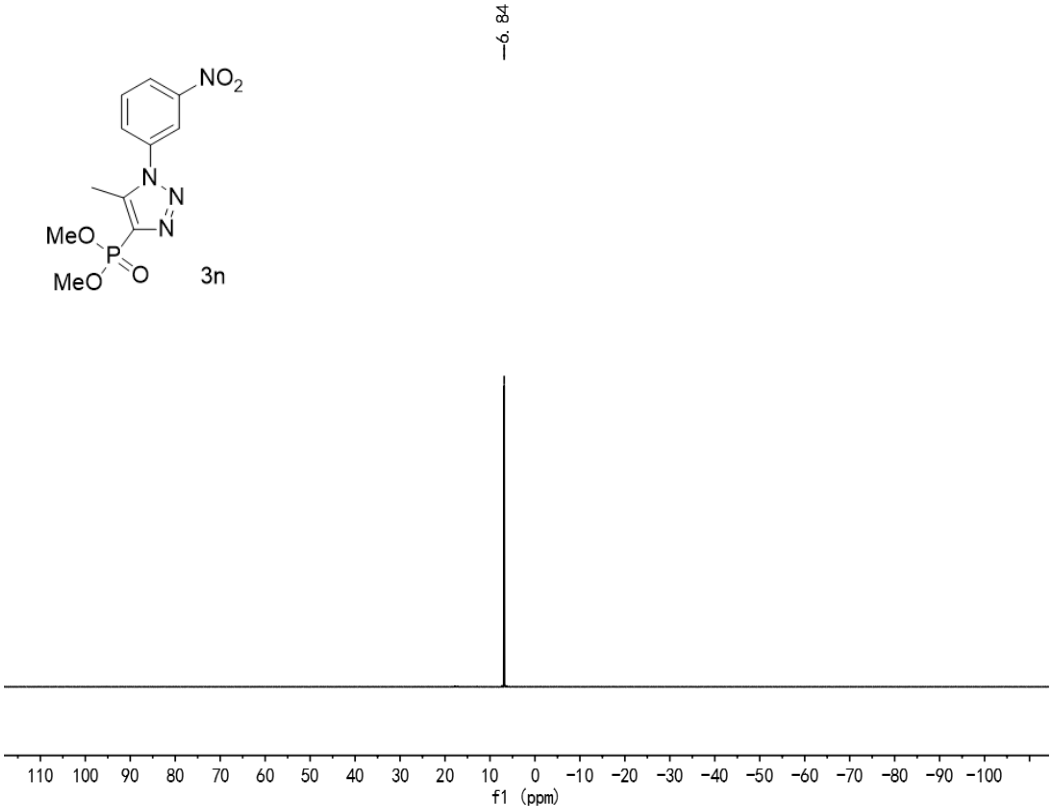



148.25
140.26
135.51
133.93
125.82
125.23
53.58
9.89
NO2
N
N
N
MeO
P
O
MeO
3m
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

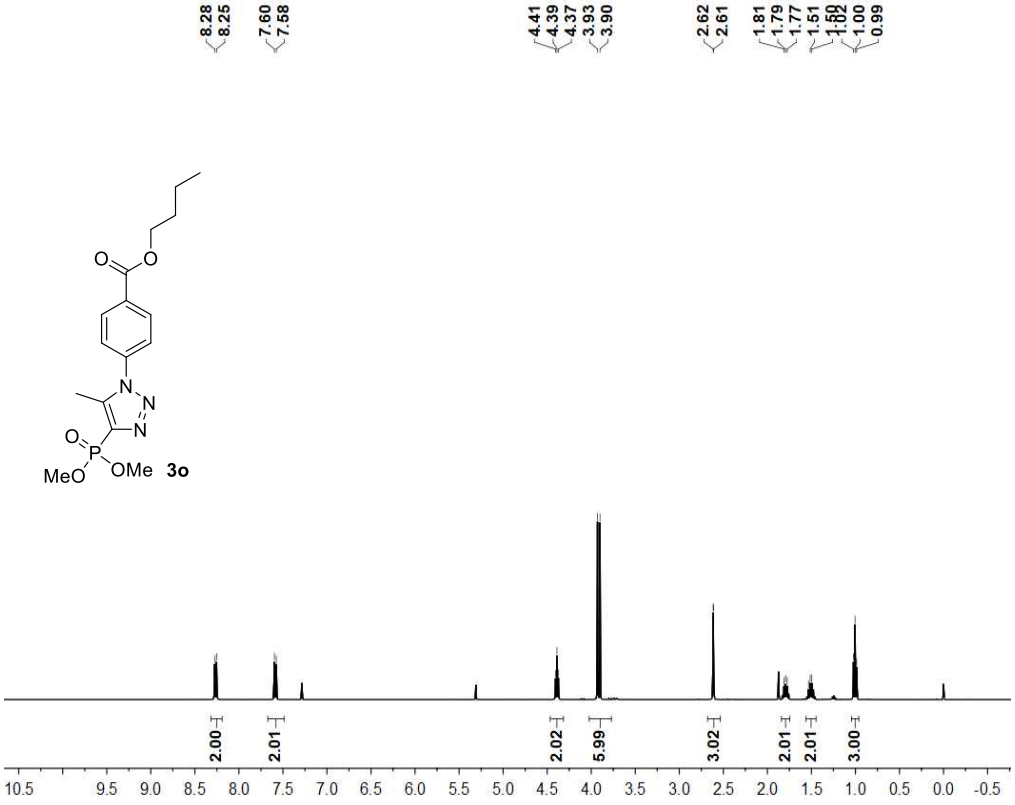

6.84
NO2
N
N
N
MeO
P
O
MeO
3m
110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100
f1 (ppm)

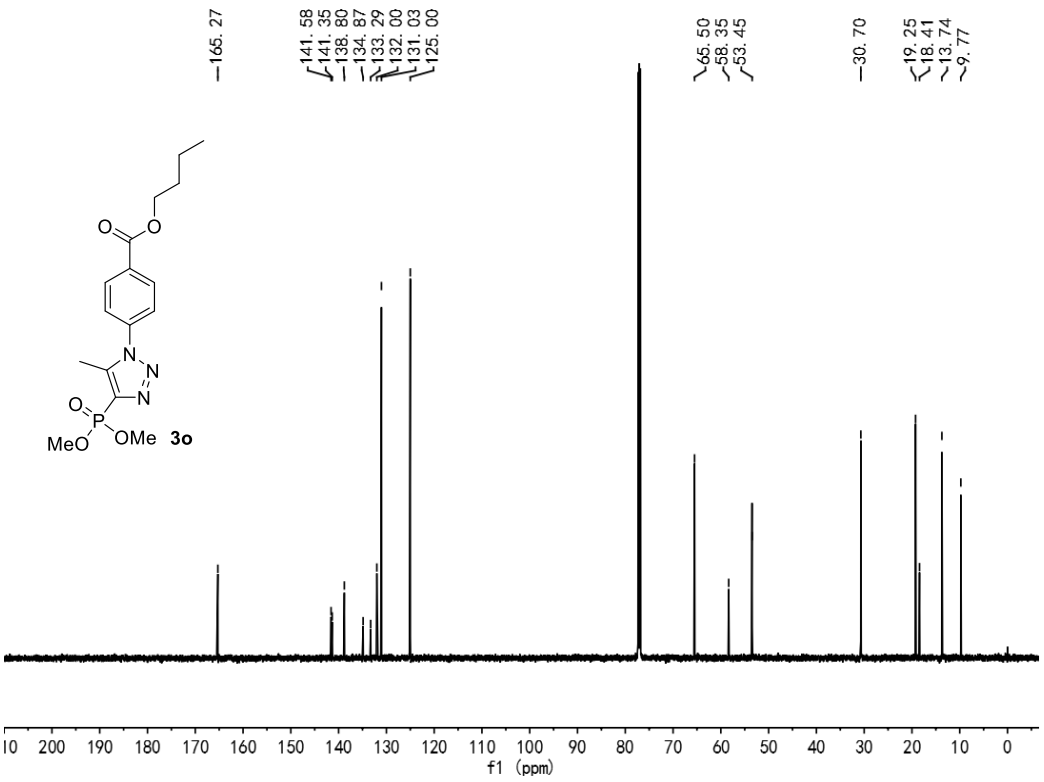
Dimethyl(5-methyl-1-(3-nitrophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3n)

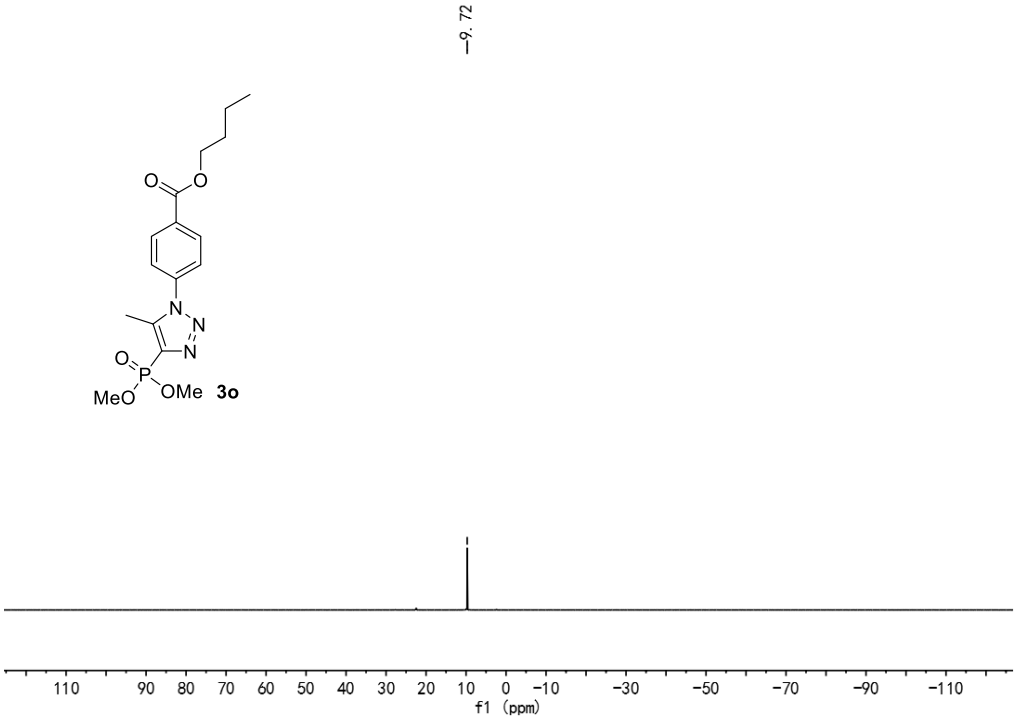




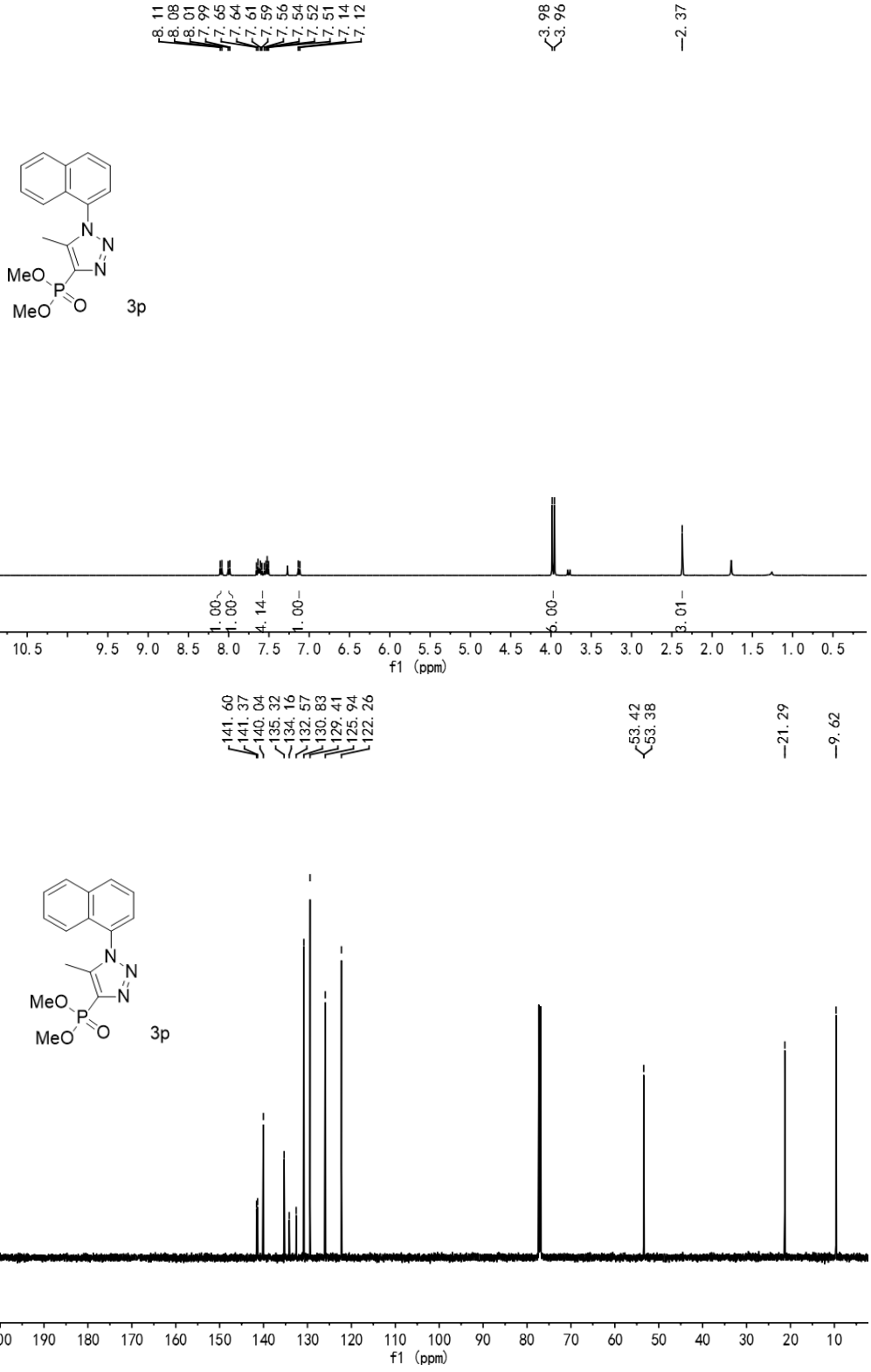
Butyl 4-(4-(dimethoxyphosphoryl)-5-methyl-1H-1,2,3-triazol-1-yl)benzoate (3o)

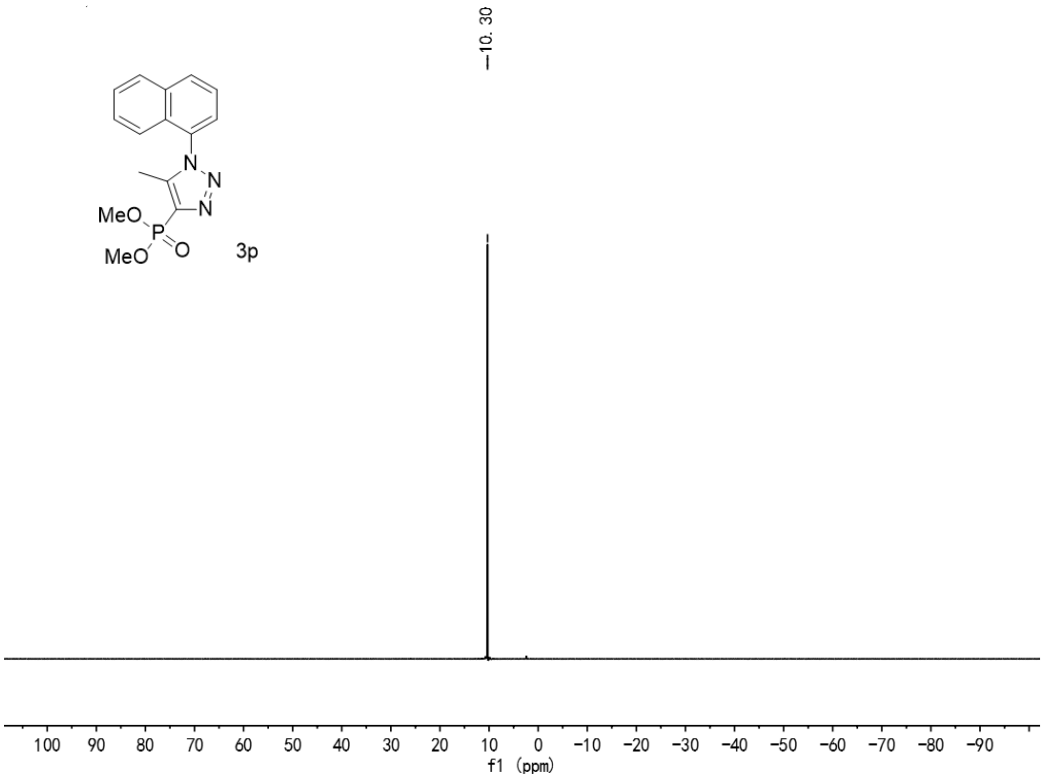



165.27
141.58
141.35
138.80
134.87
133.29
132.00
131.03
125.00
65.50
58.35
53.45
30.70
19.25
18.41
13.74
9.77
MeO
OMe
3o
f1 (ppm)

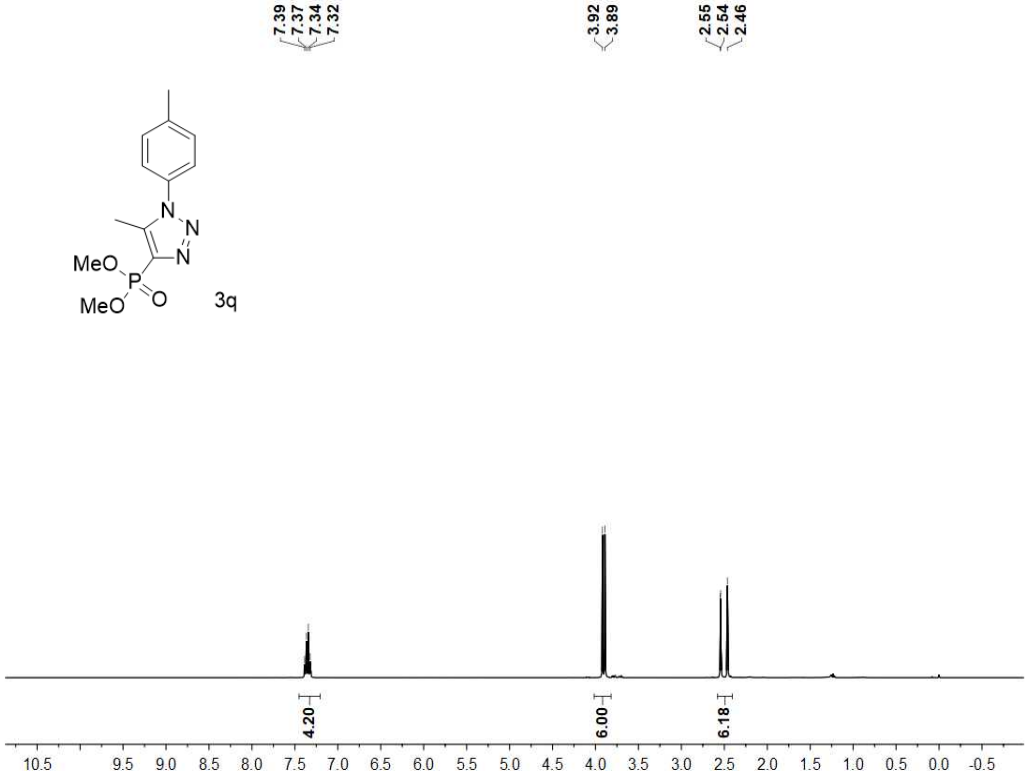

9.72
MeO
OMe
3o
f1 (ppm)

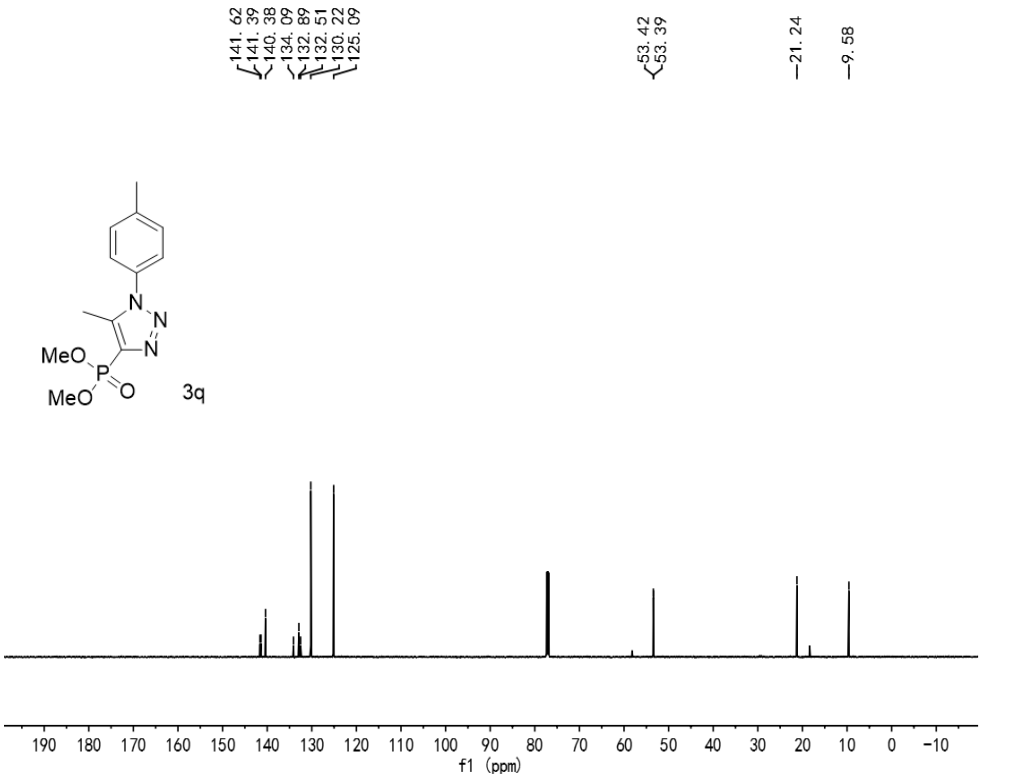
Dimethyl(5-methyl-1-(naphthalen-1-yl)-1H-1,2,3-triazol-4-yl)phosphonate (3p)

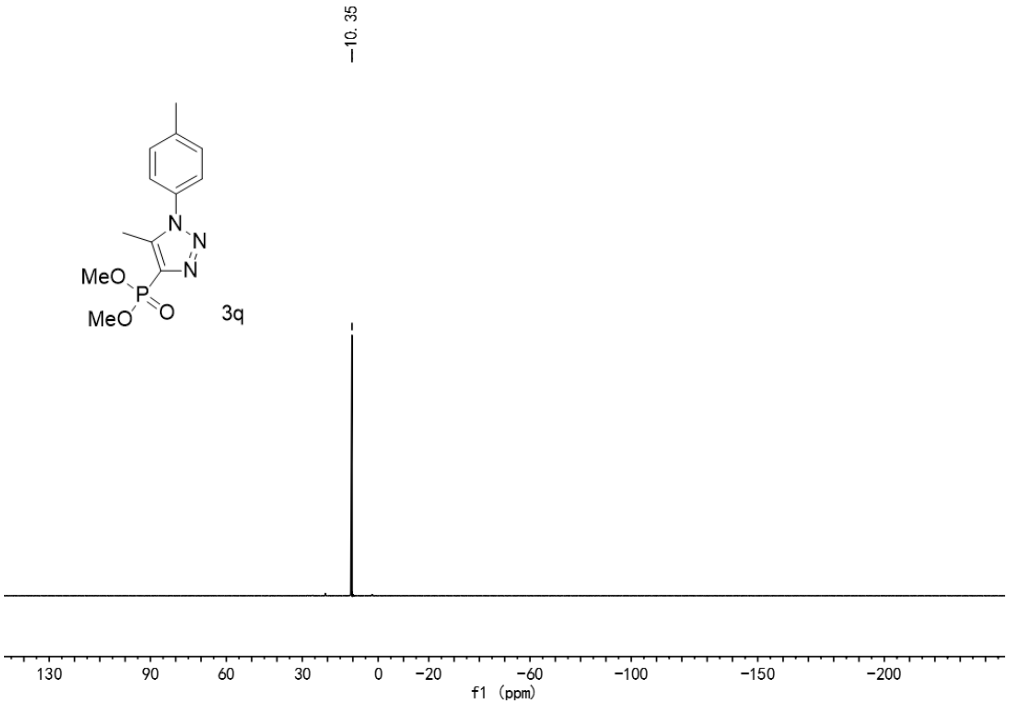




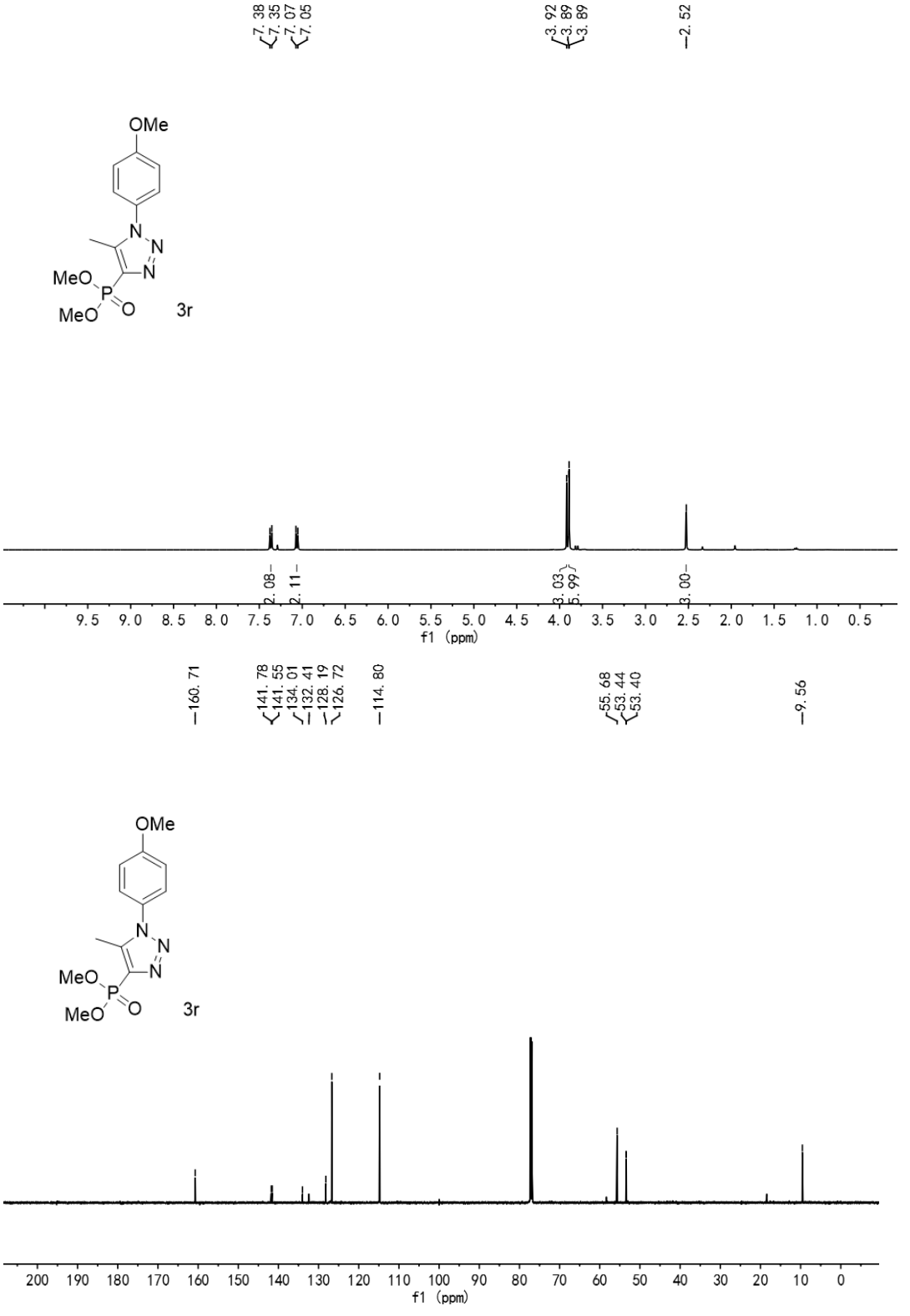
Dimethyl (5-methyl-1-(p-tolyl)-1H-1,2,3-triazol-4-yl)phosphonate (3q)

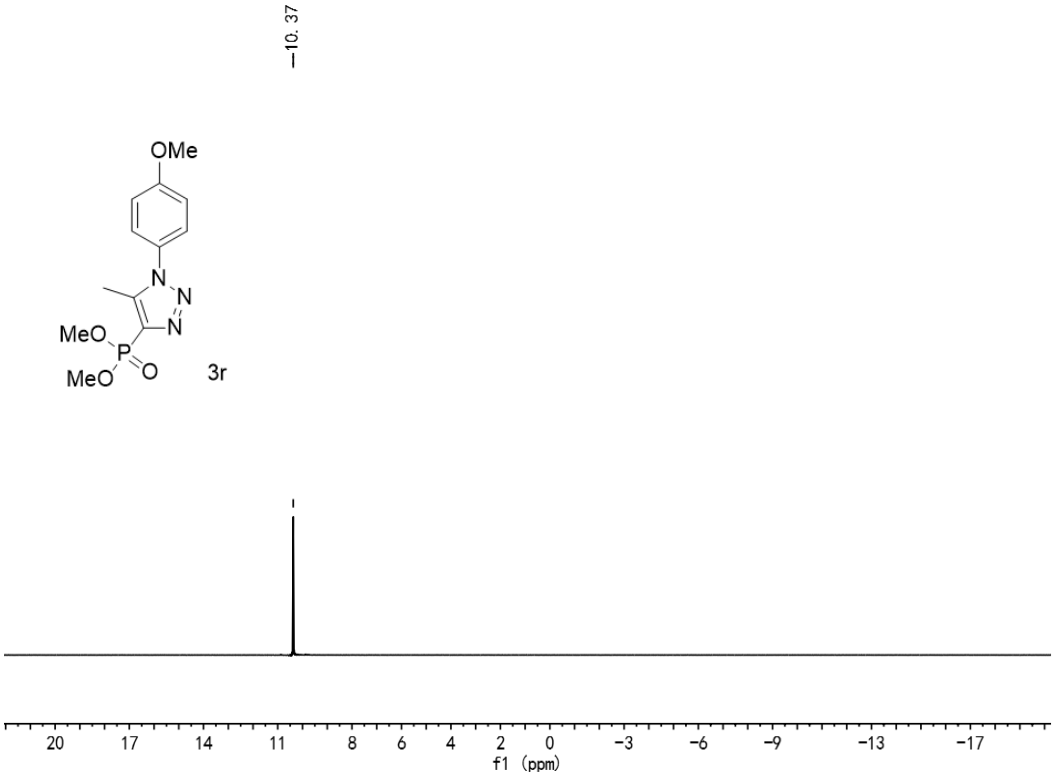



141.62
141.39
140.38
134.09
132.89
132.51
130.22
125.09
53.42
53.39
21.24
9.58
MeO
MeO
P
O
N
N
N
3q
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

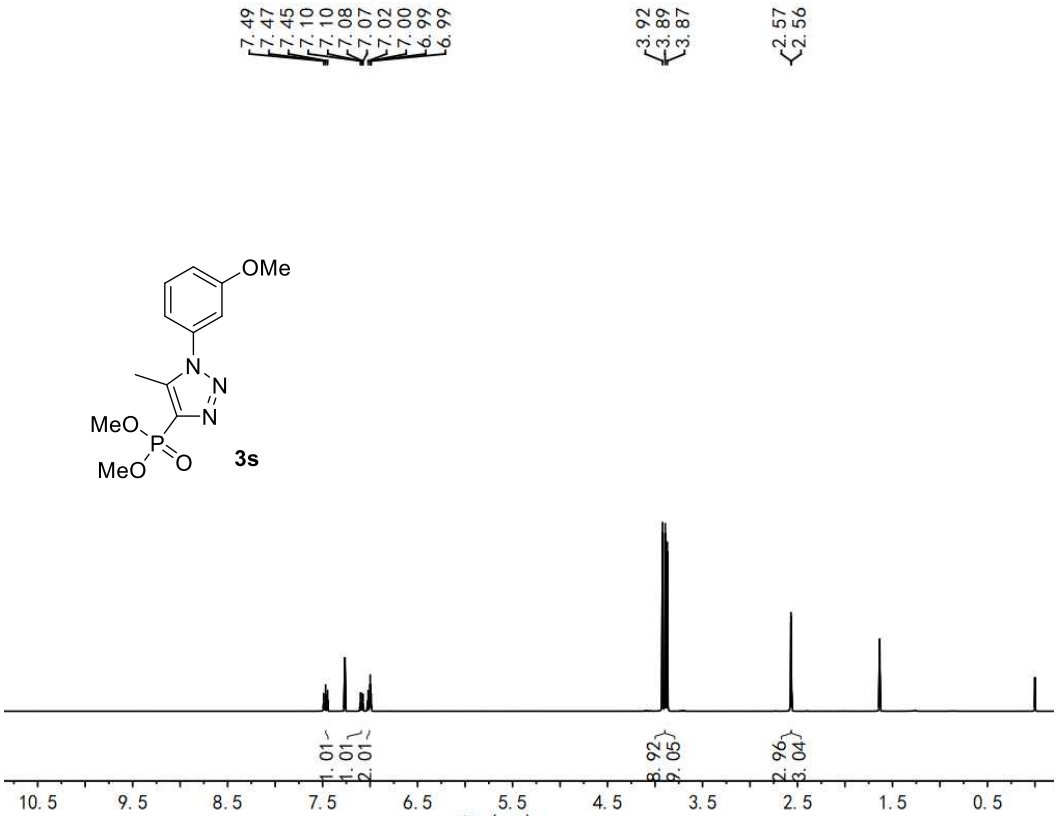

10.35
MeO
MeO
P
O
N
N
N
3q
130 90 60 30 0 -20 -60 -100 -150 -200
f1 (ppm)

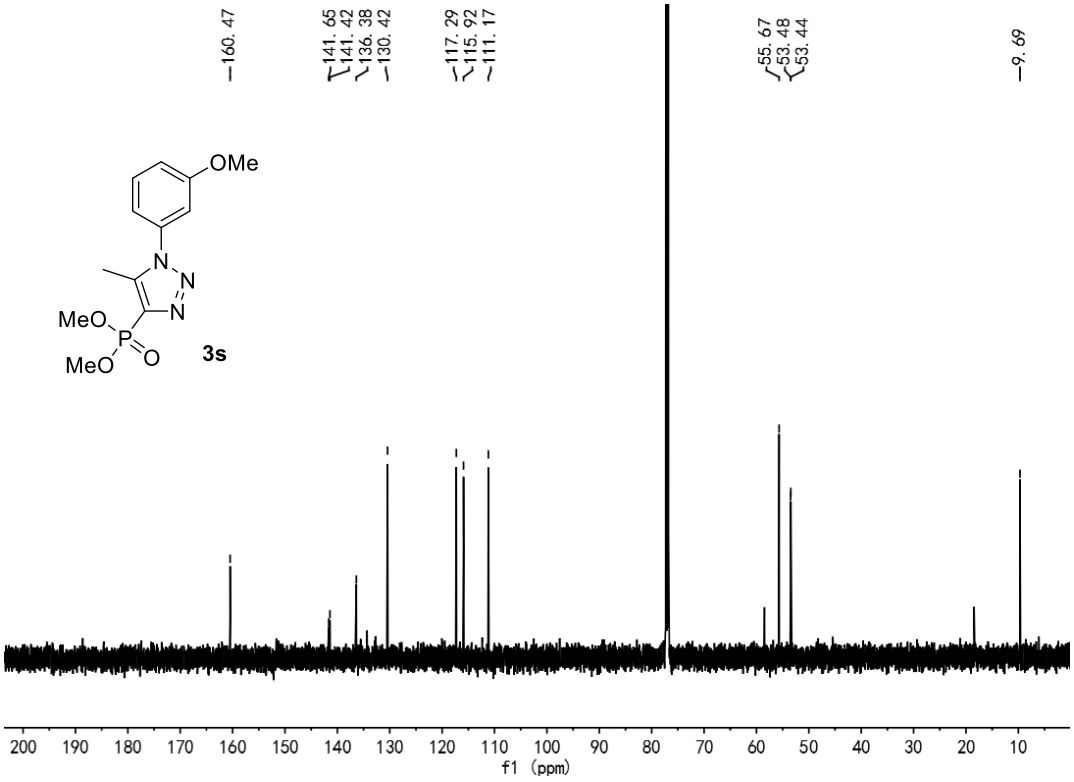
Dimethyl(1-(4-methoxyphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3r)

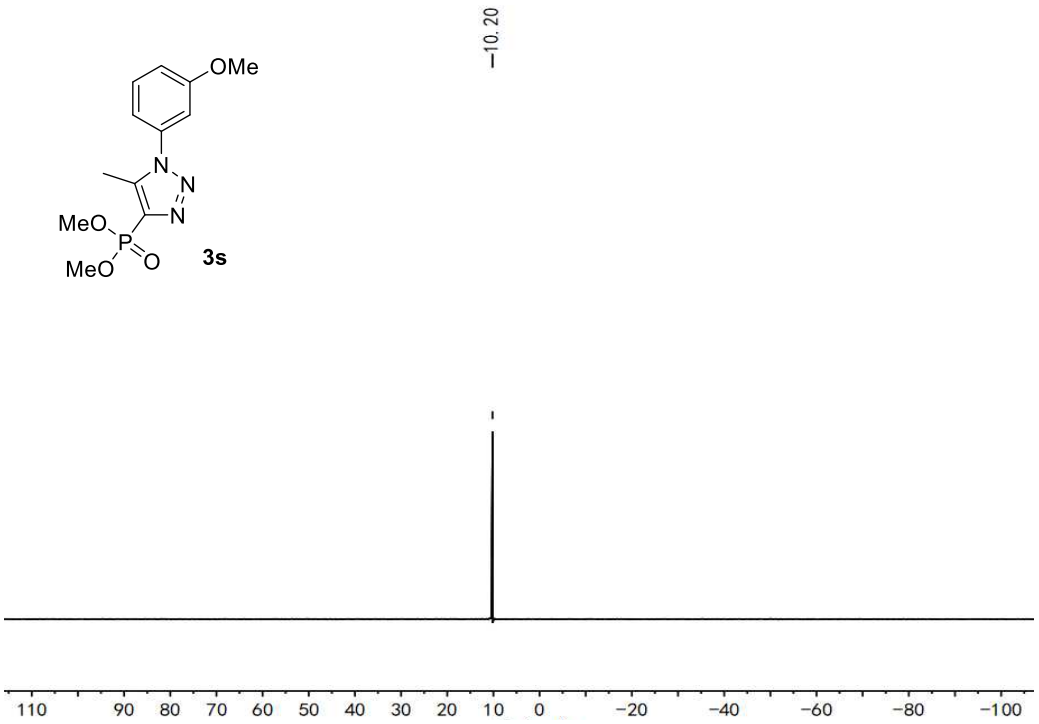




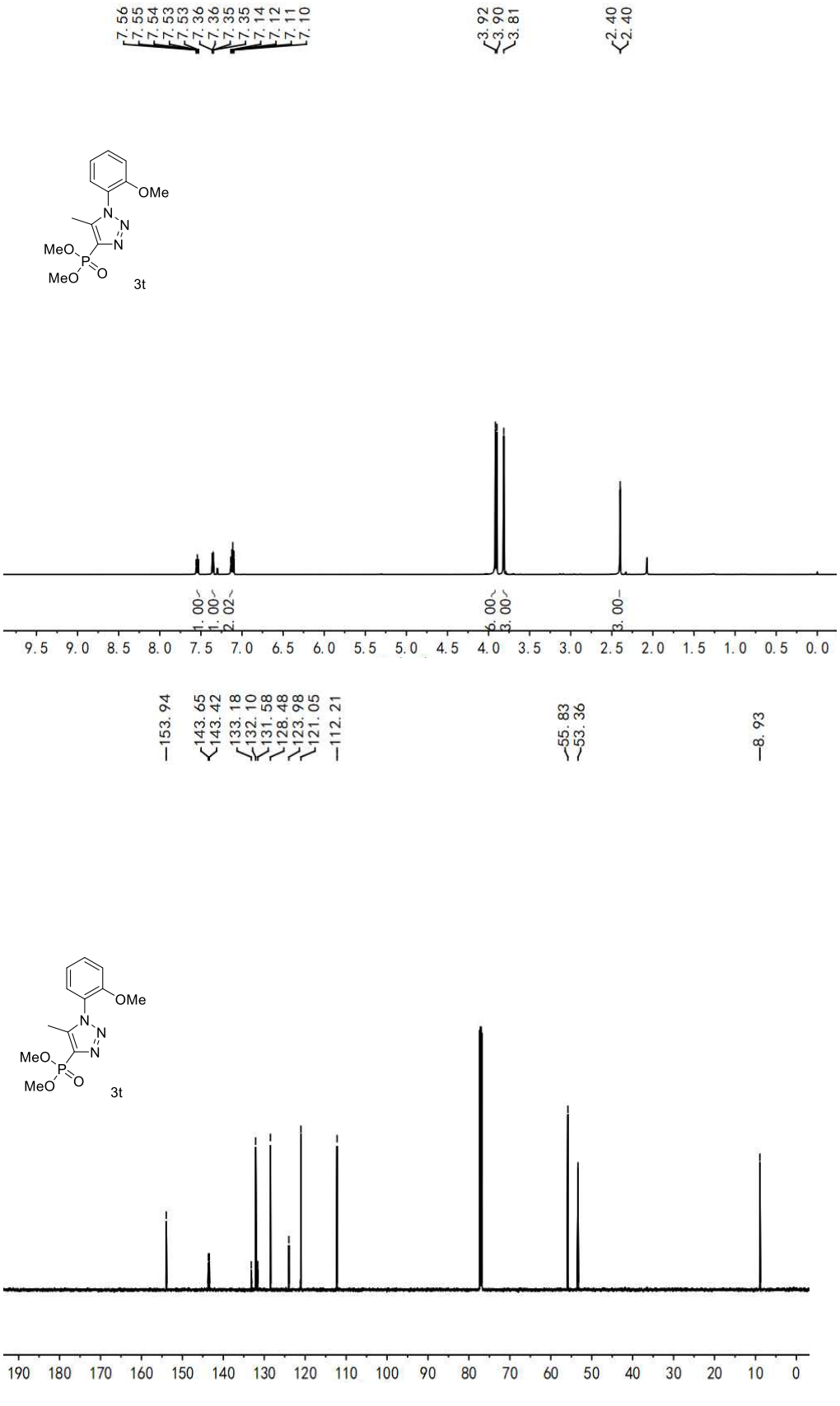
Dimethyl(1-(3-methoxyphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3s)

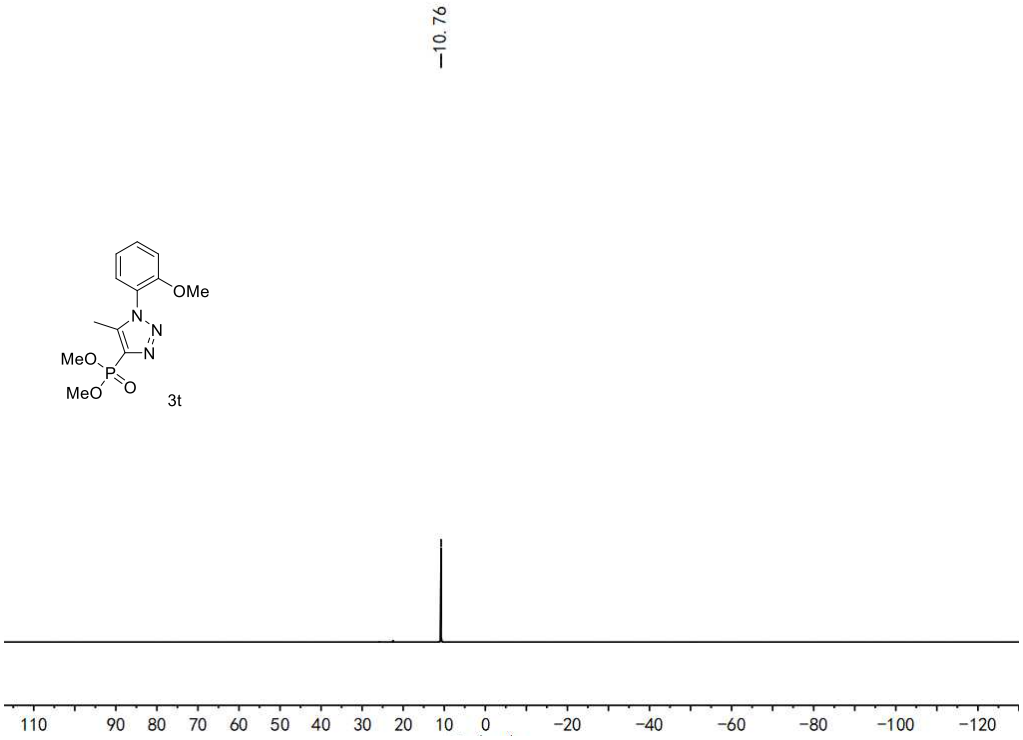



160.47
141.65
141.42
136.38
130.42
117.29
115.92
111.17
55.67
53.48
53.44
9.69
OMe
MeO
MeO
P
O
N
N
N
3s
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

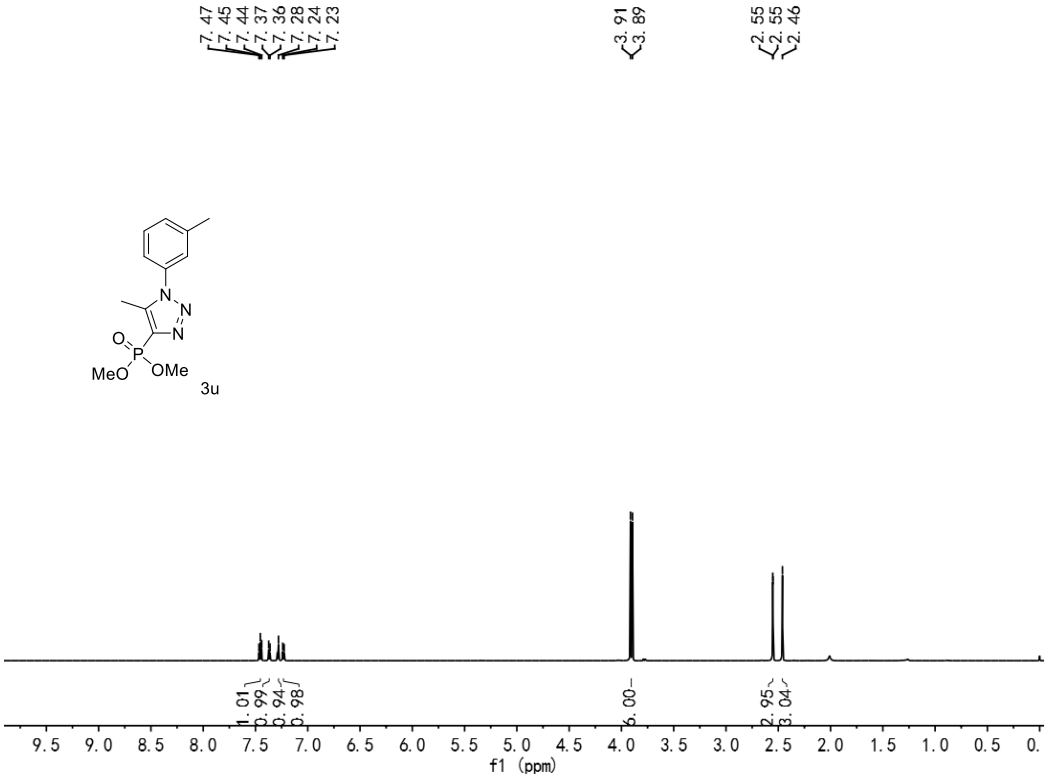

10.20
OMe
MeO
MeO
P
O
N
N
N
3s
110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100

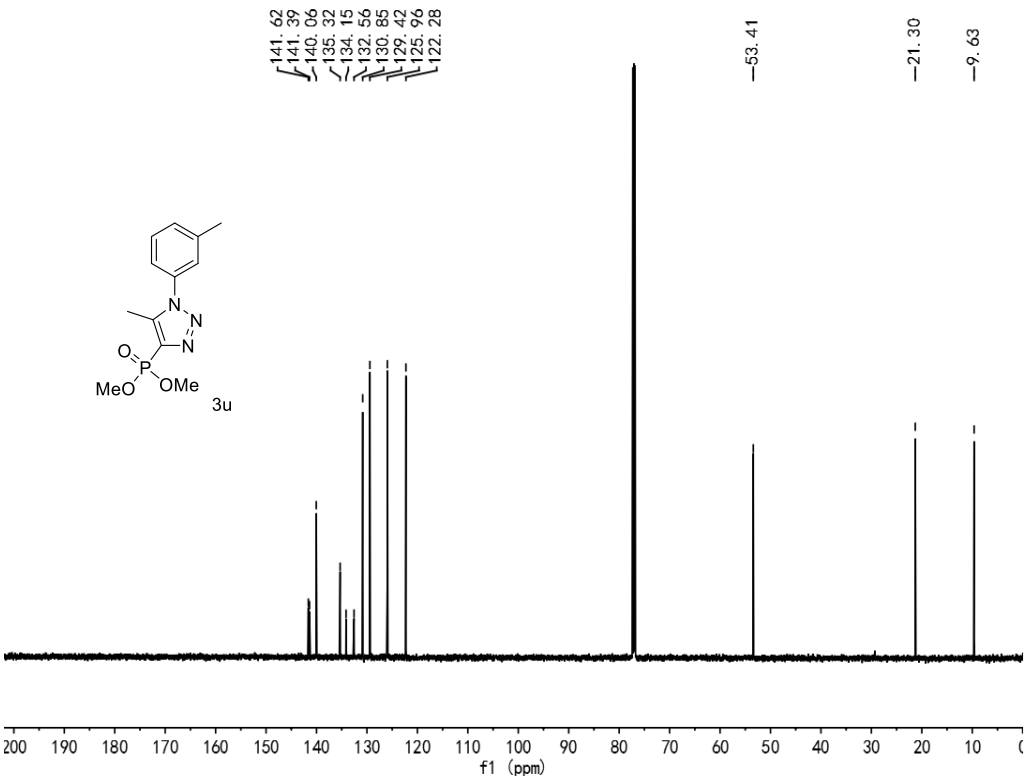
Dimethyl(1-(2-methoxyphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3t)

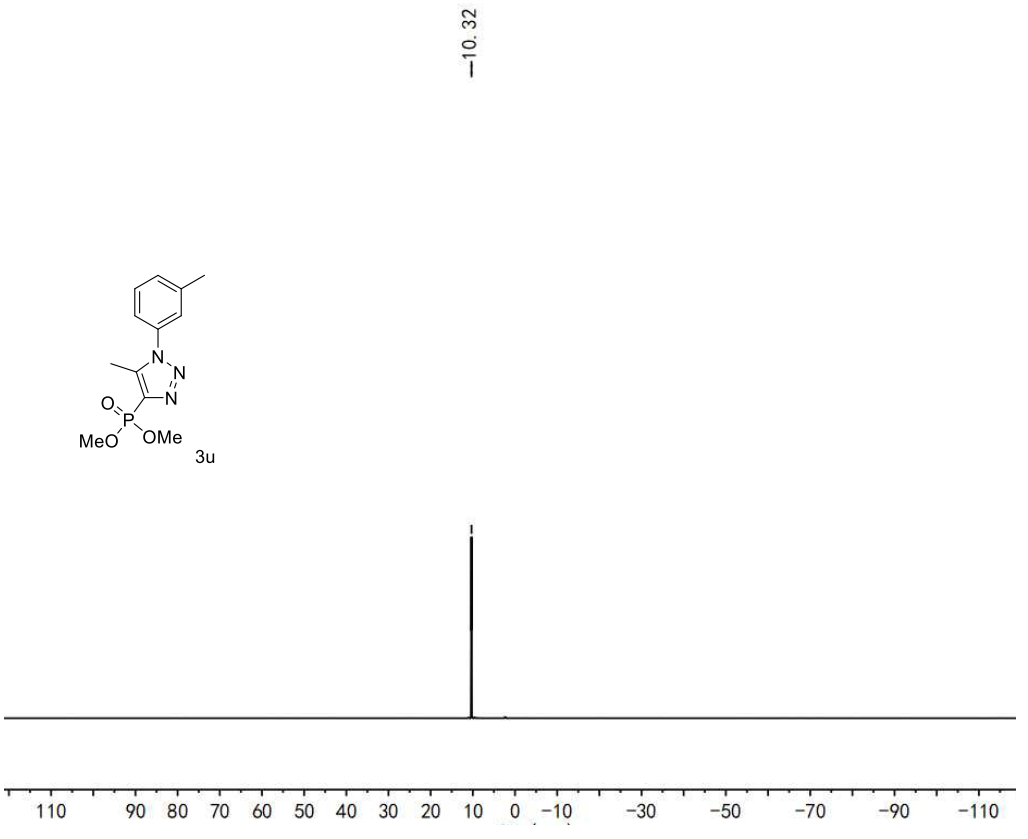




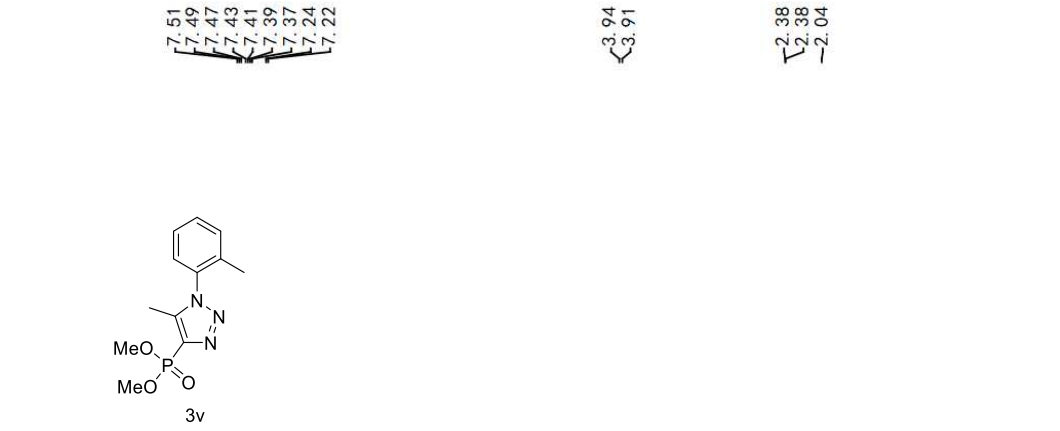
Dimethyl(5-methyl-1-(m-tolyl)-1H-1,2,3-triazol-4-yl)phosphonate (3u)

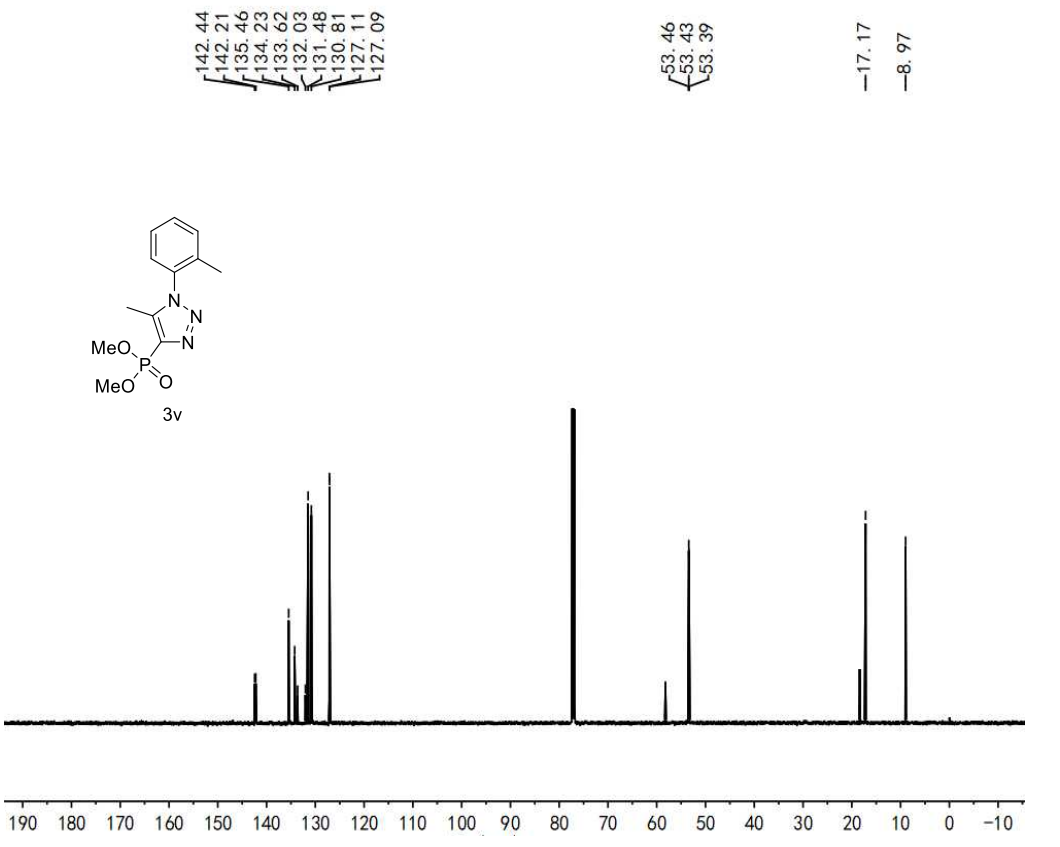


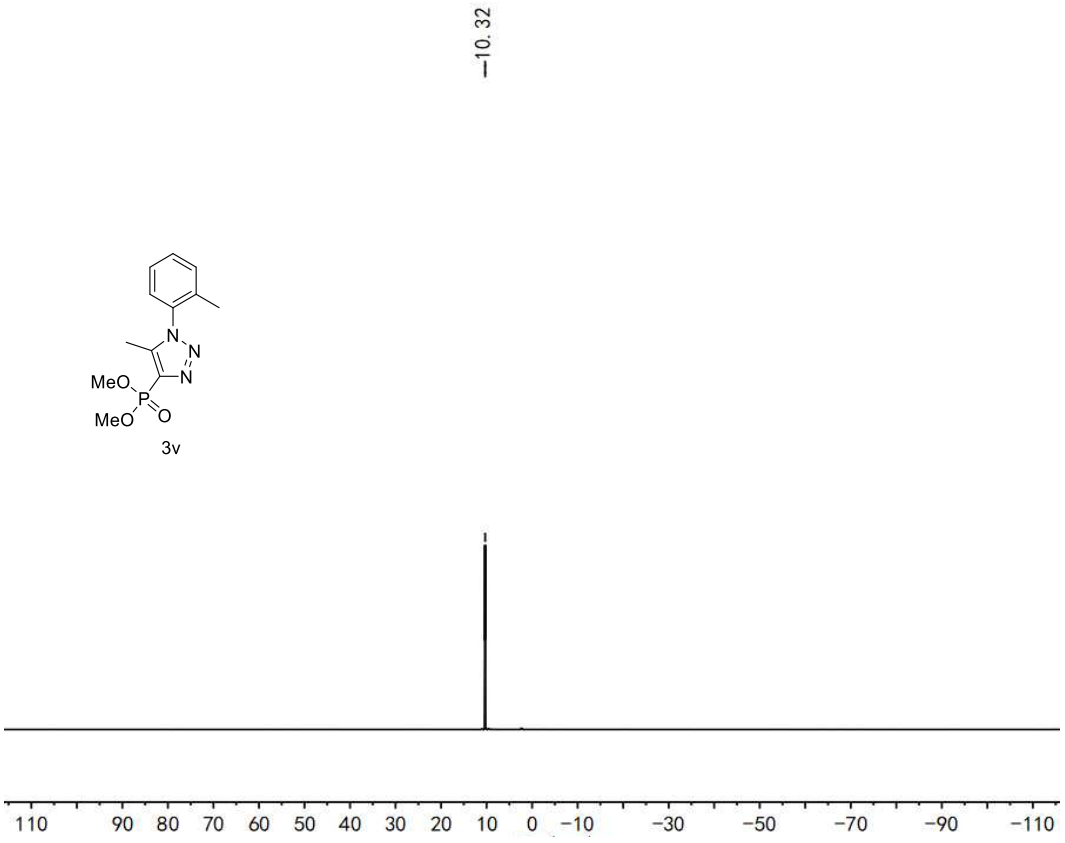

141.62
141.39
140.06
135.32
134.15
132.56
130.85
129.42
125.96
122.28
53.41
21.30
9.63
MeO
OMe
3u
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


10.32
MeO
OMe
3u
110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110

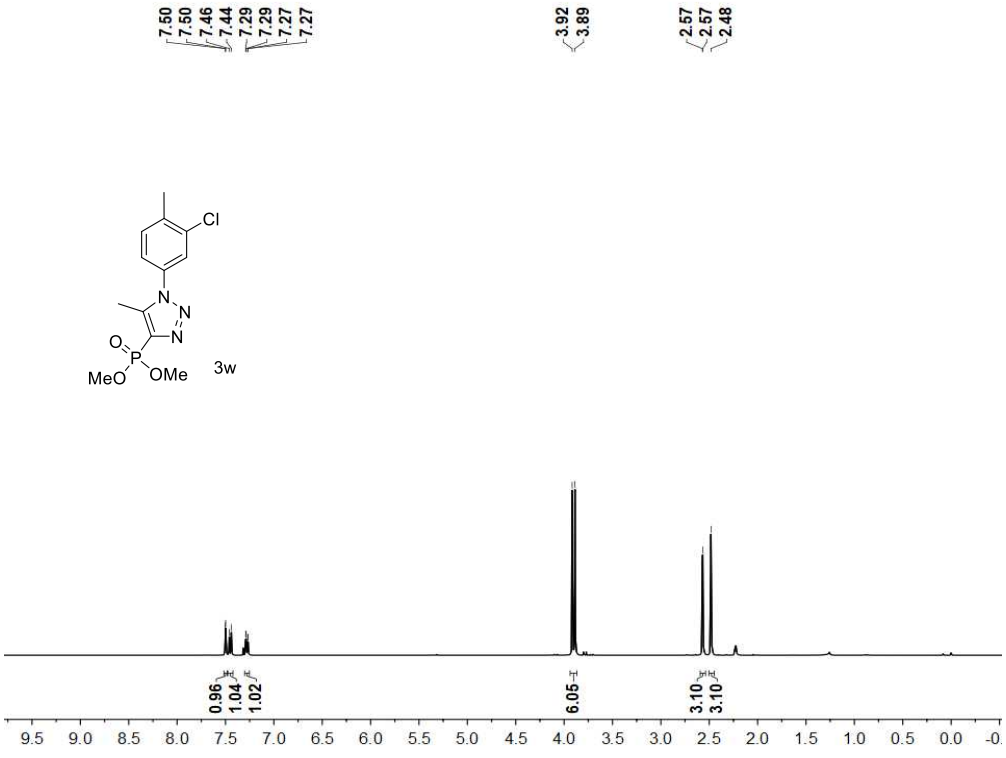
Dimethyl(1-(2-methoxyphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3v)

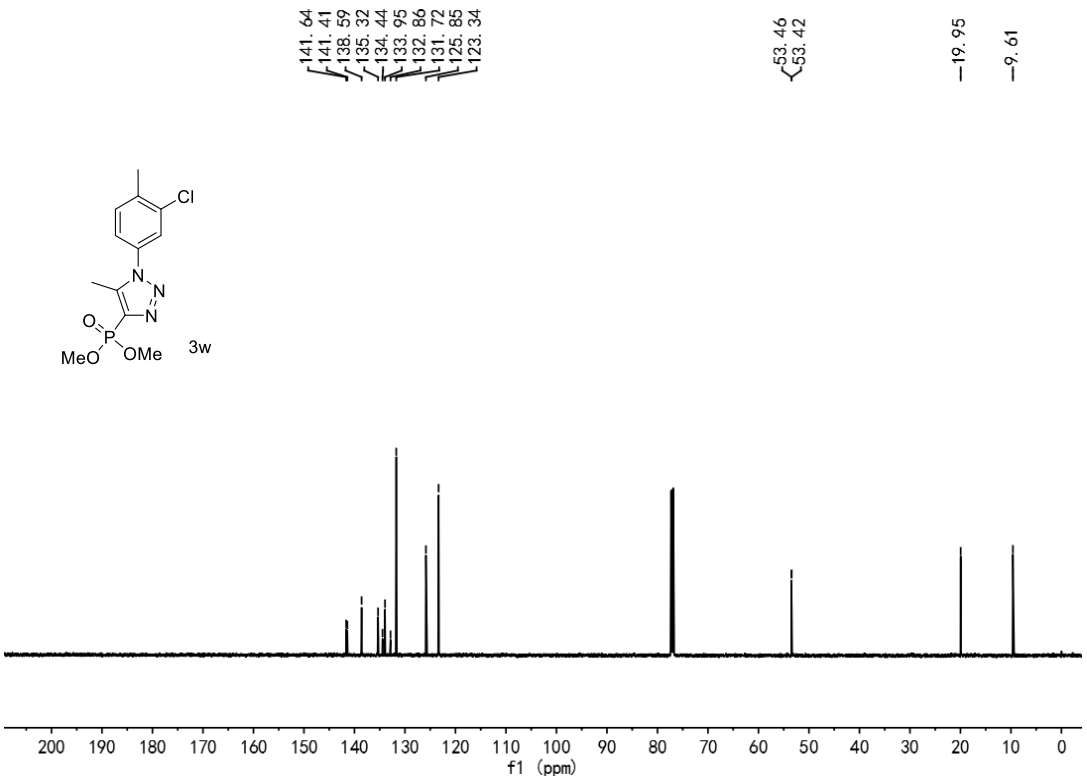


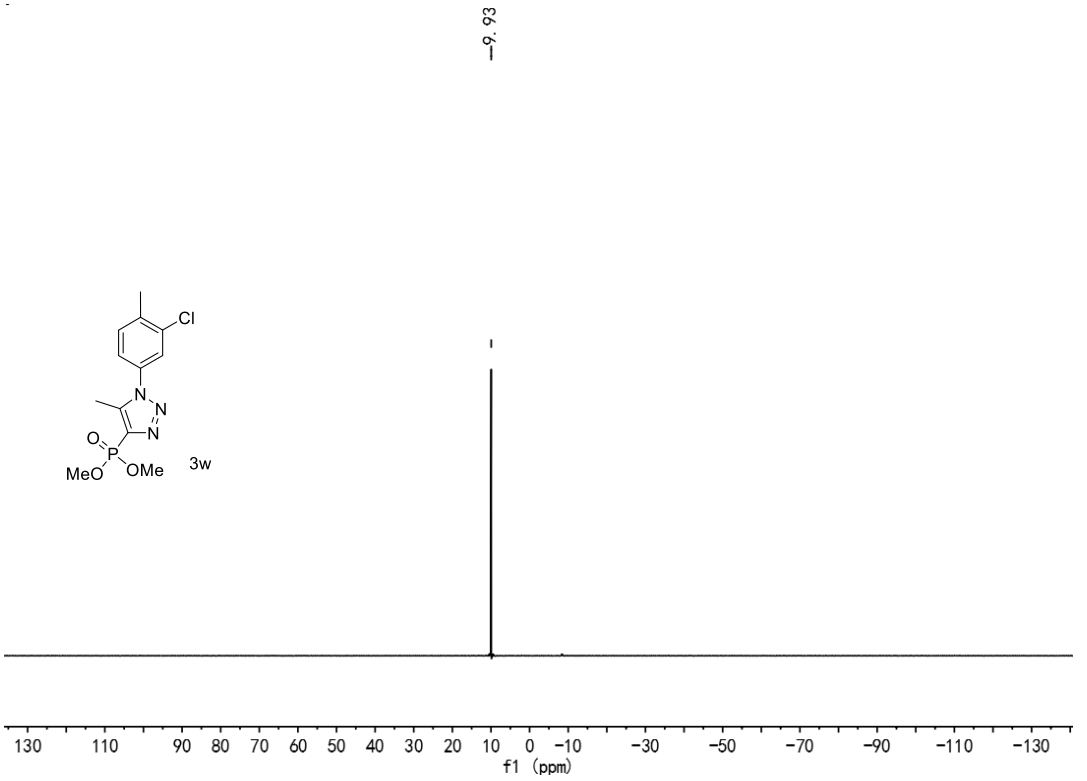




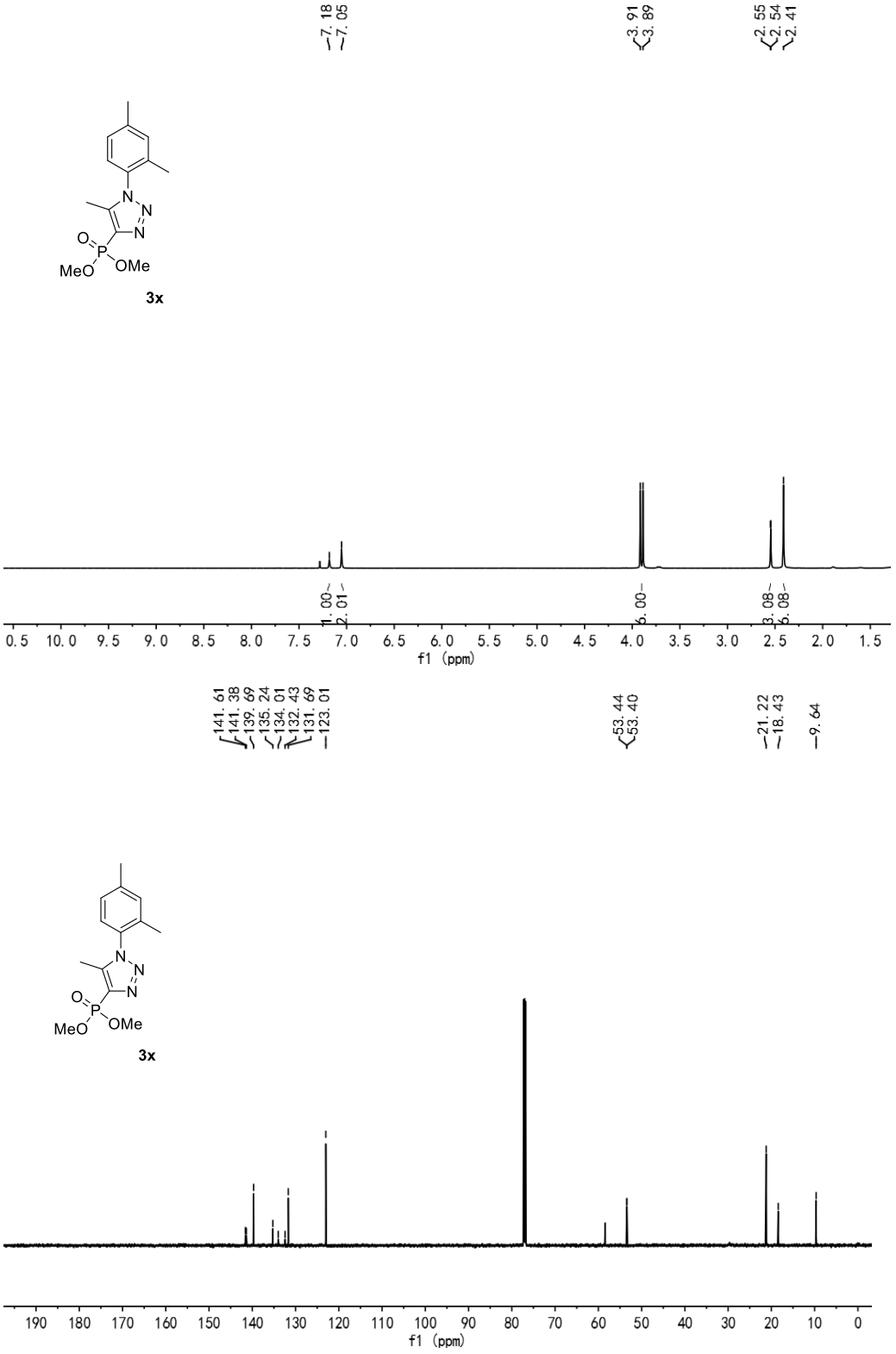
Dimethyl(1-(3-chloro-4-methylphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3w)

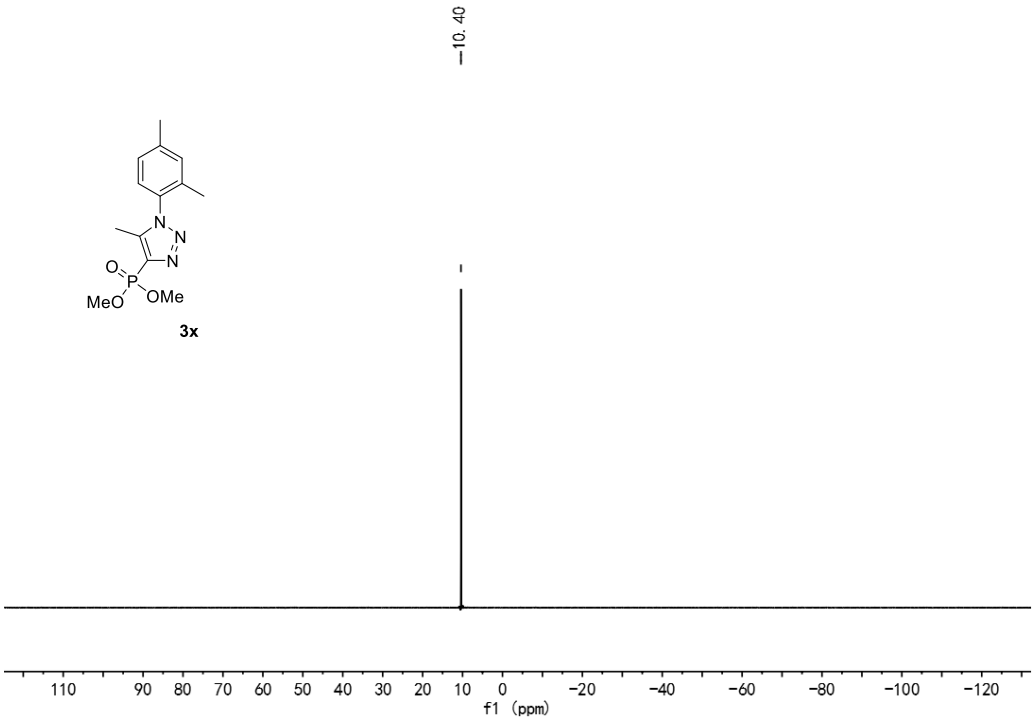



141.64
141.41
138.59
135.32
134.44
133.95
132.86
131.72
125.85
123.34
53.46
53.42
19.95
9.61
Cl
N
N
N
O
P
MeO
OMe
3w
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

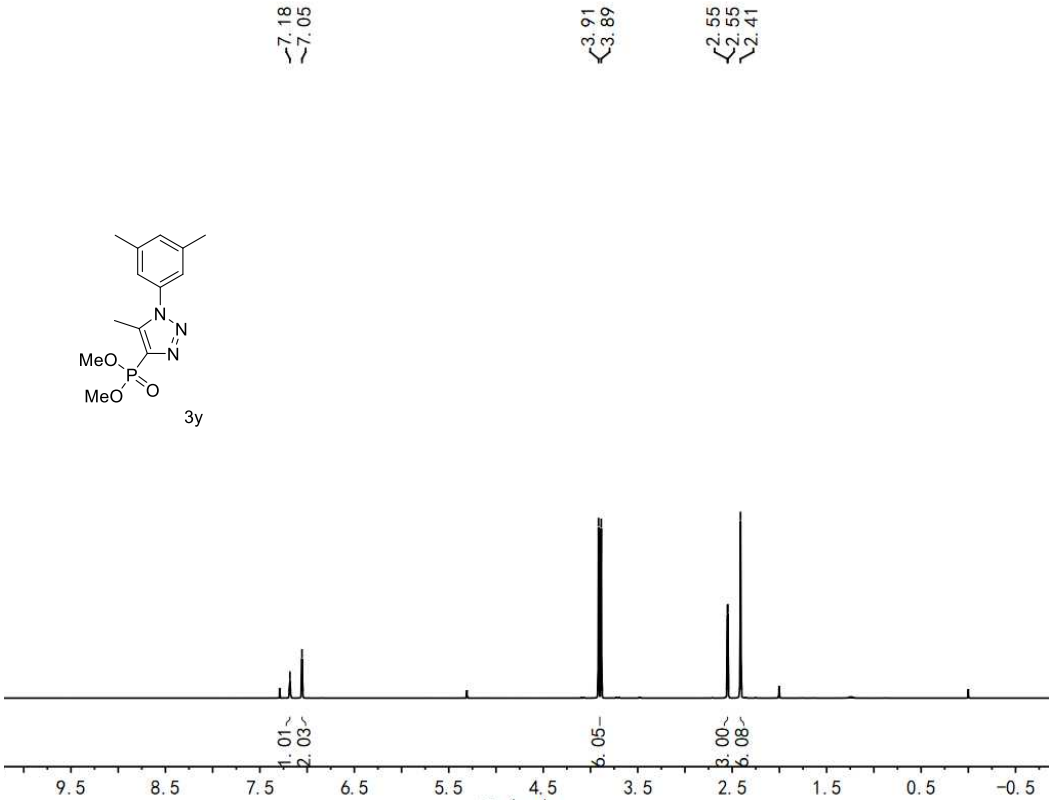

9.93
Cl
N
N
N
O
P
MeO
OMe
3w
130 110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130
f1 (ppm)

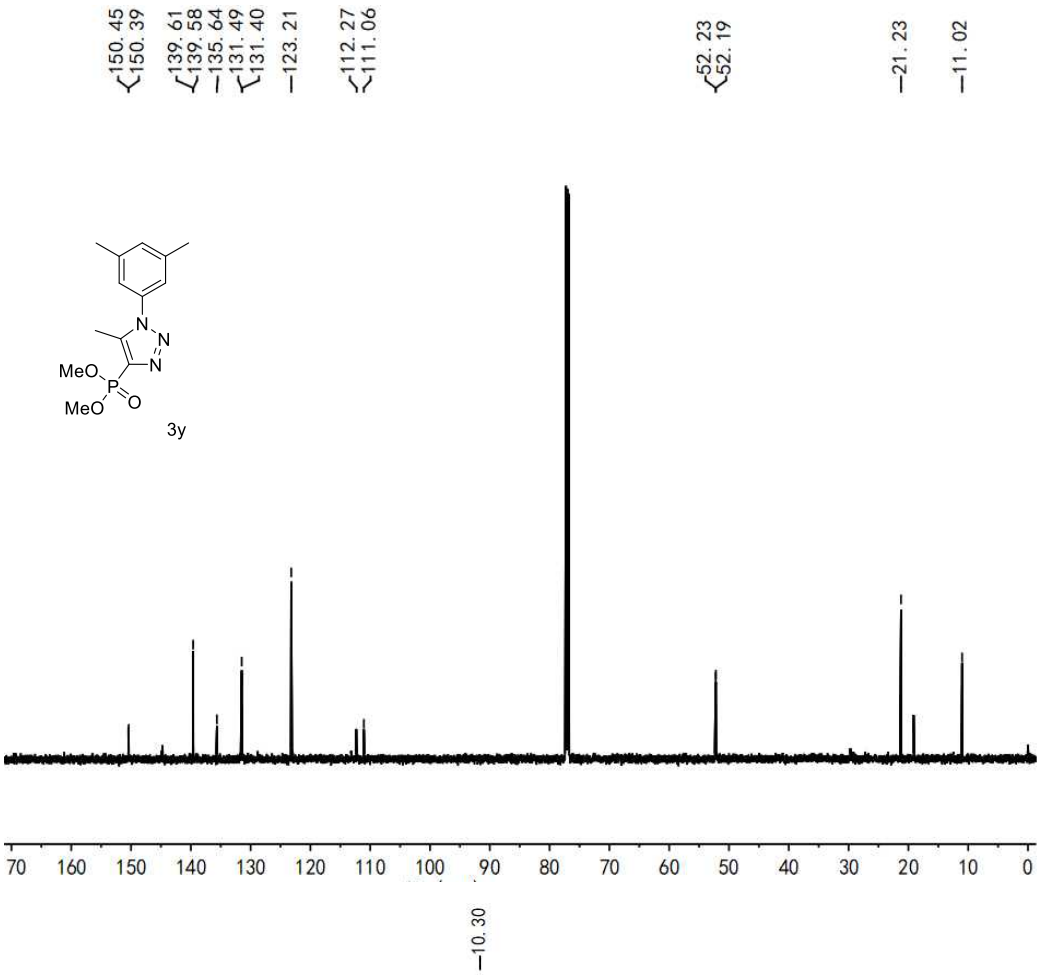
Dimethyl(1-(2,4-dimethylphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3x)

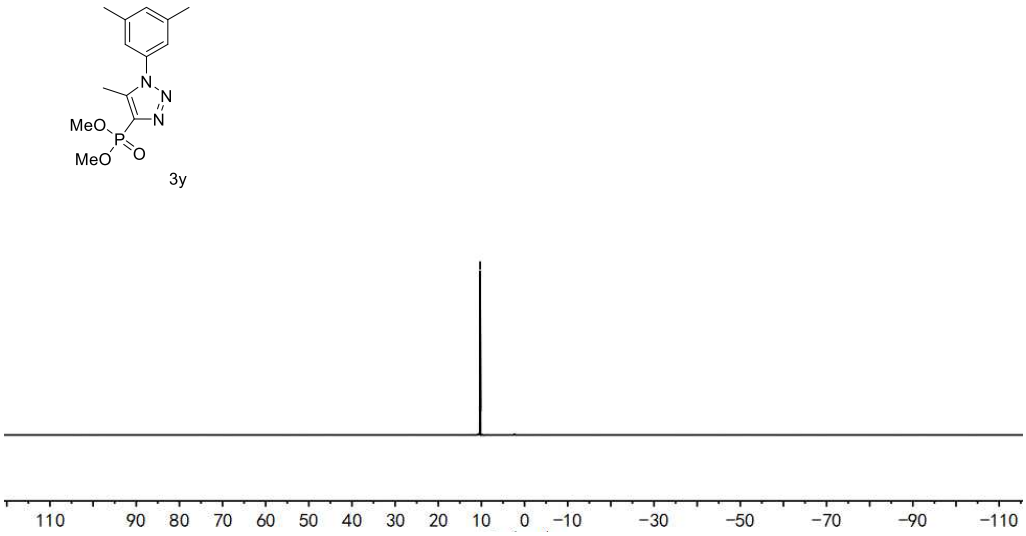




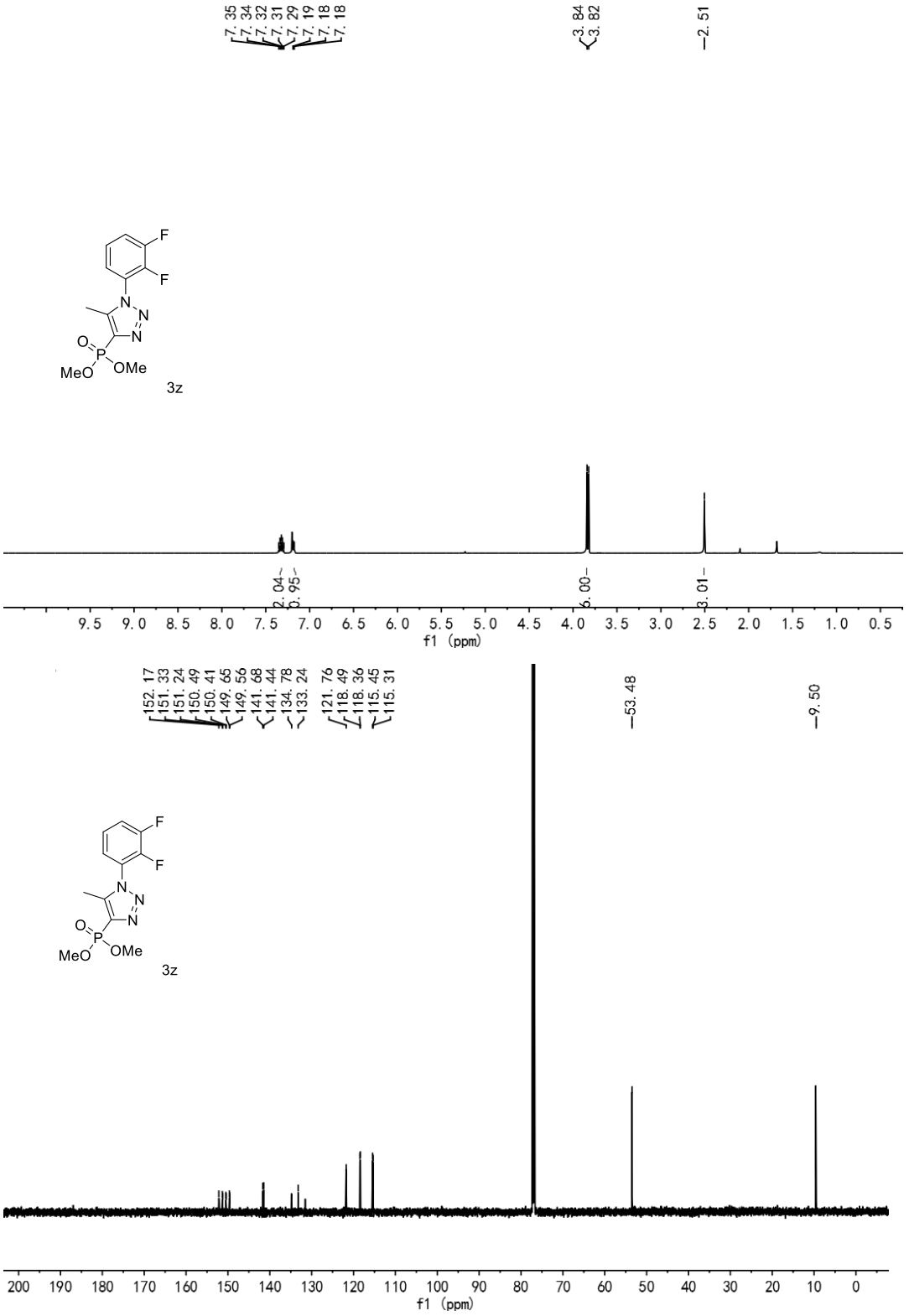
Dimethyl(1-(3,5-dimethylphenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3y)

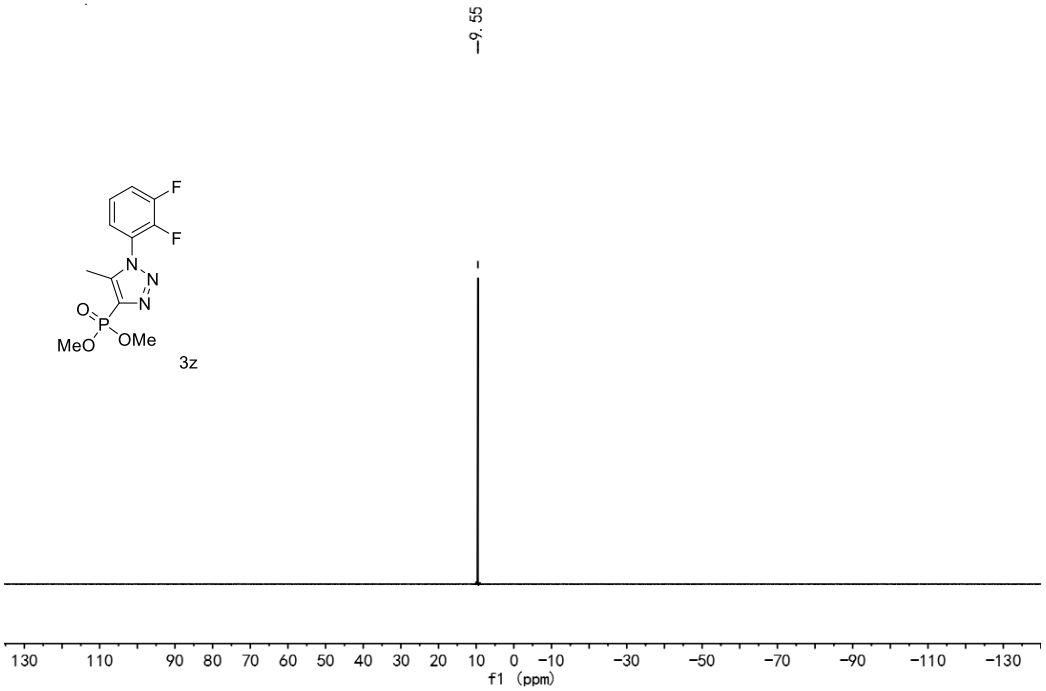



150.45
150.39
139.61
139.58
135.64
131.49
131.40
123.21
112.27
111.06
52.23
52.19
21.23
11.02
MeO
MeO
P
O
N
N
N
3y
70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
10.30

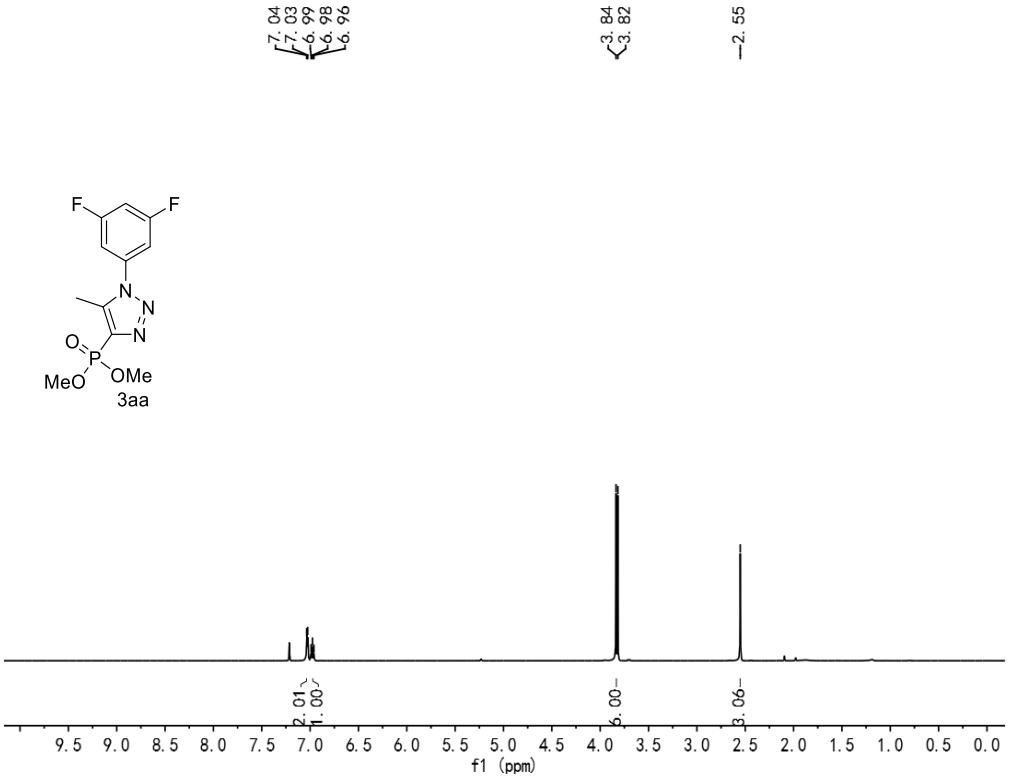

MeO
MeO
P
O
N
N
N
3y
110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110

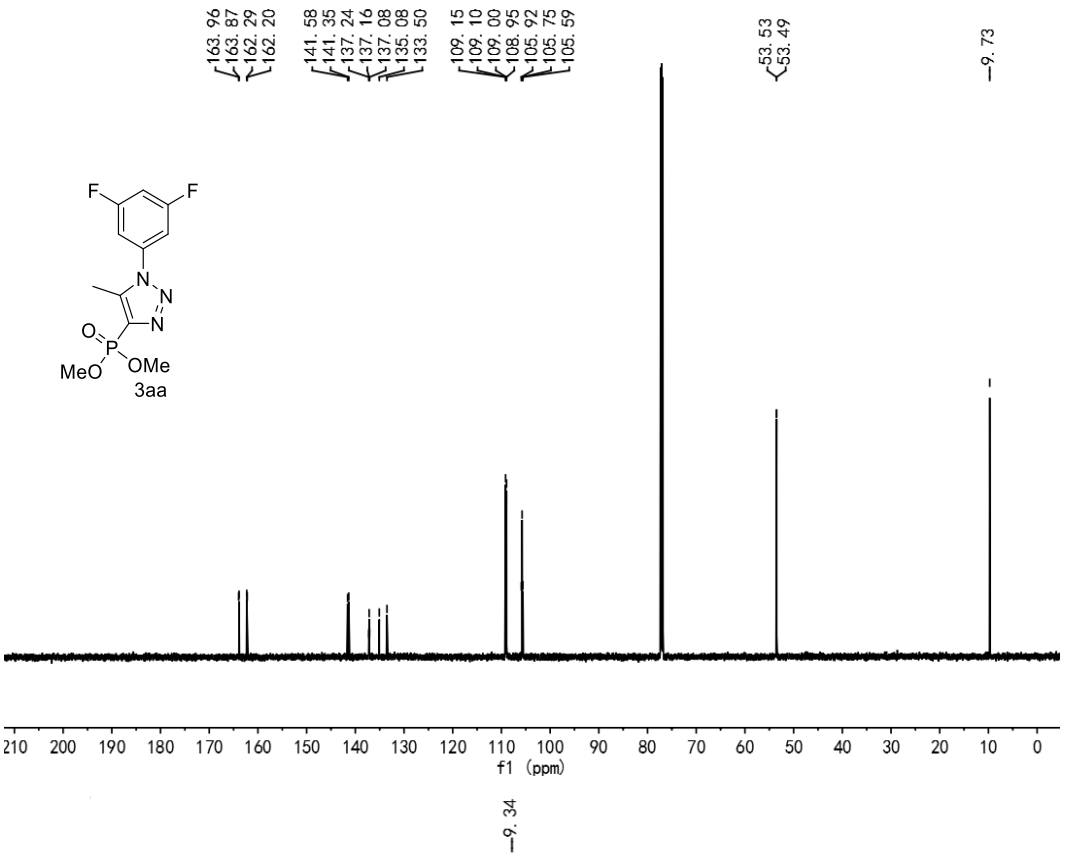
Dimethyl(1-(2,3-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3z)

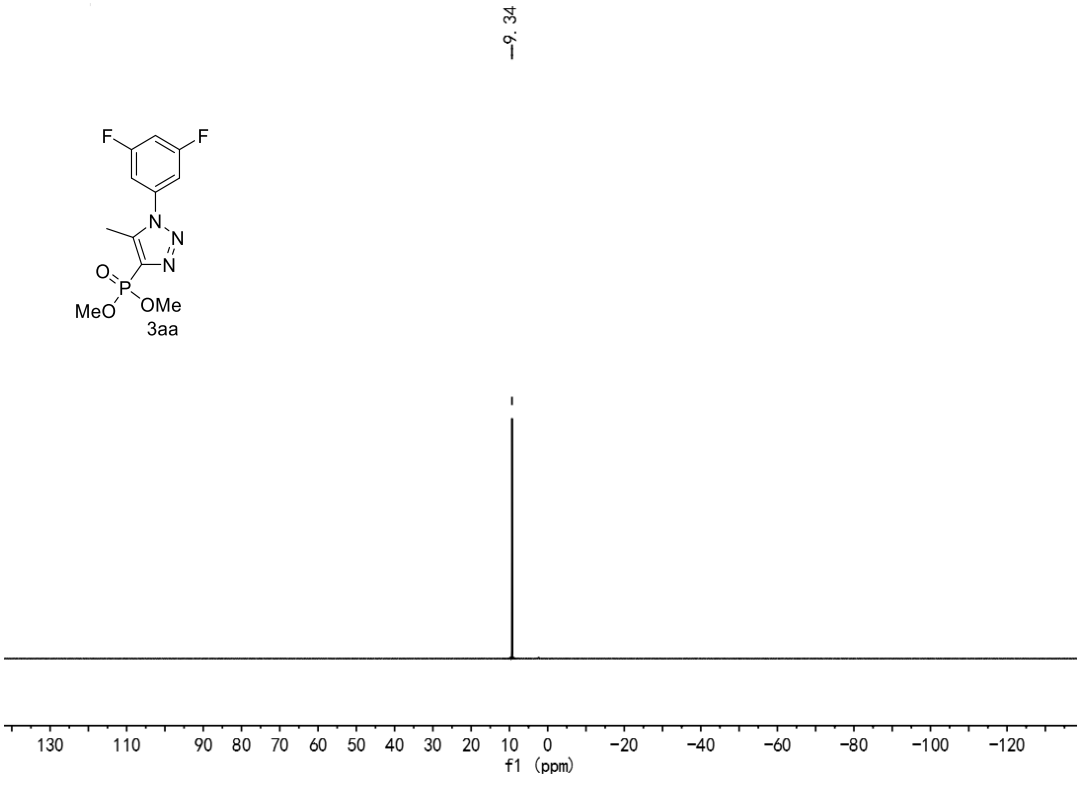




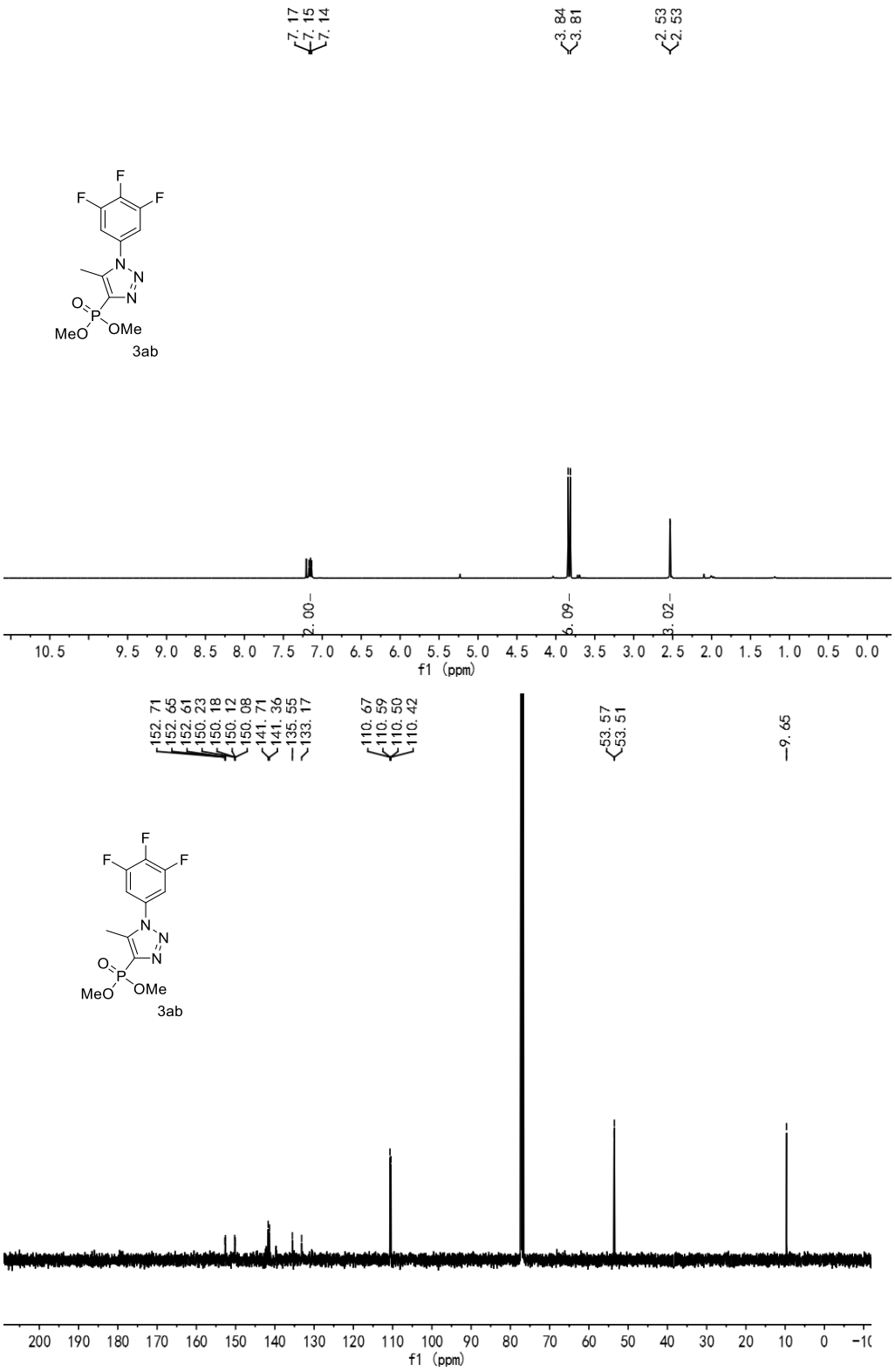
Dimethyl(1-(3,5-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl)phosphonate (3aa)

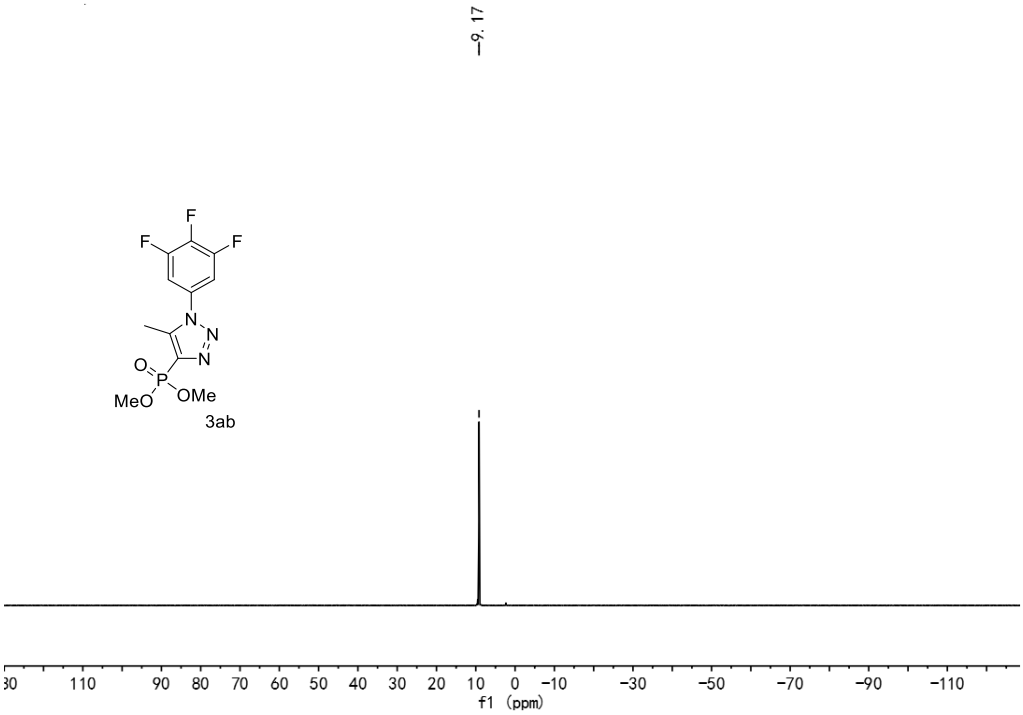



163.96
163.87
162.29
162.20
141.58
141.35
137.24
137.16
137.08
135.08
133.50
109.15
109.10
109.00
108.95
105.92
105.75
105.59
53.53
53.49
9.73
F
F
N
N
N
O
P
MeO
OMe
3aa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

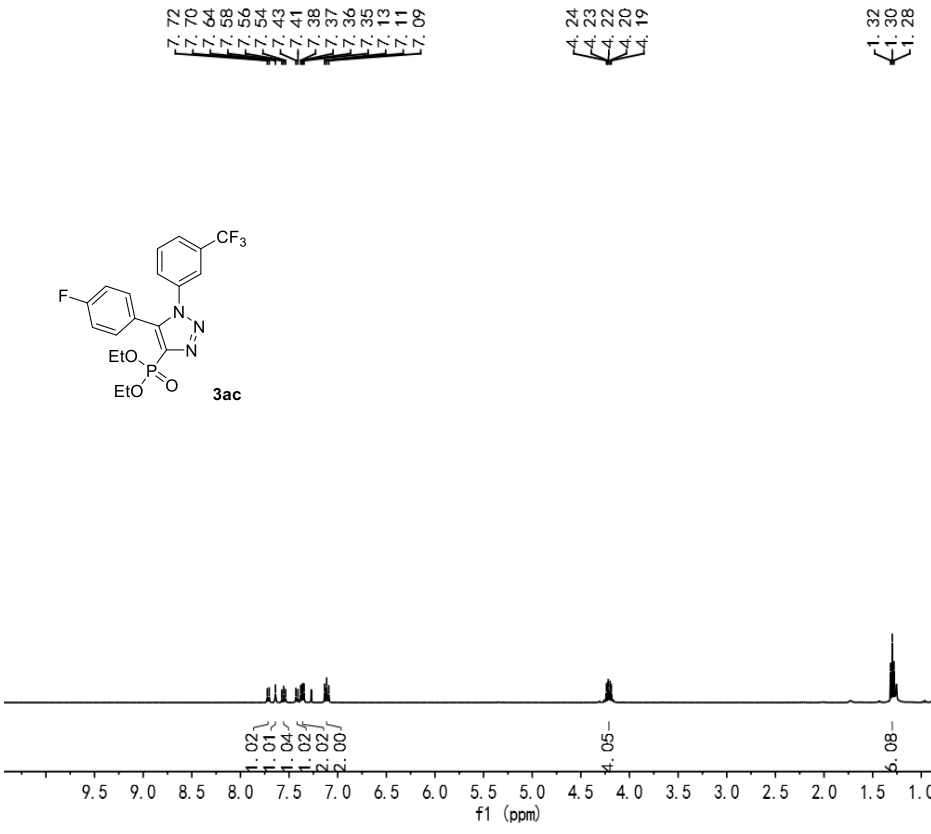

9.34
F
F
N
N
N
O
P
MeO
OMe
3aa
130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120
f1 (ppm)

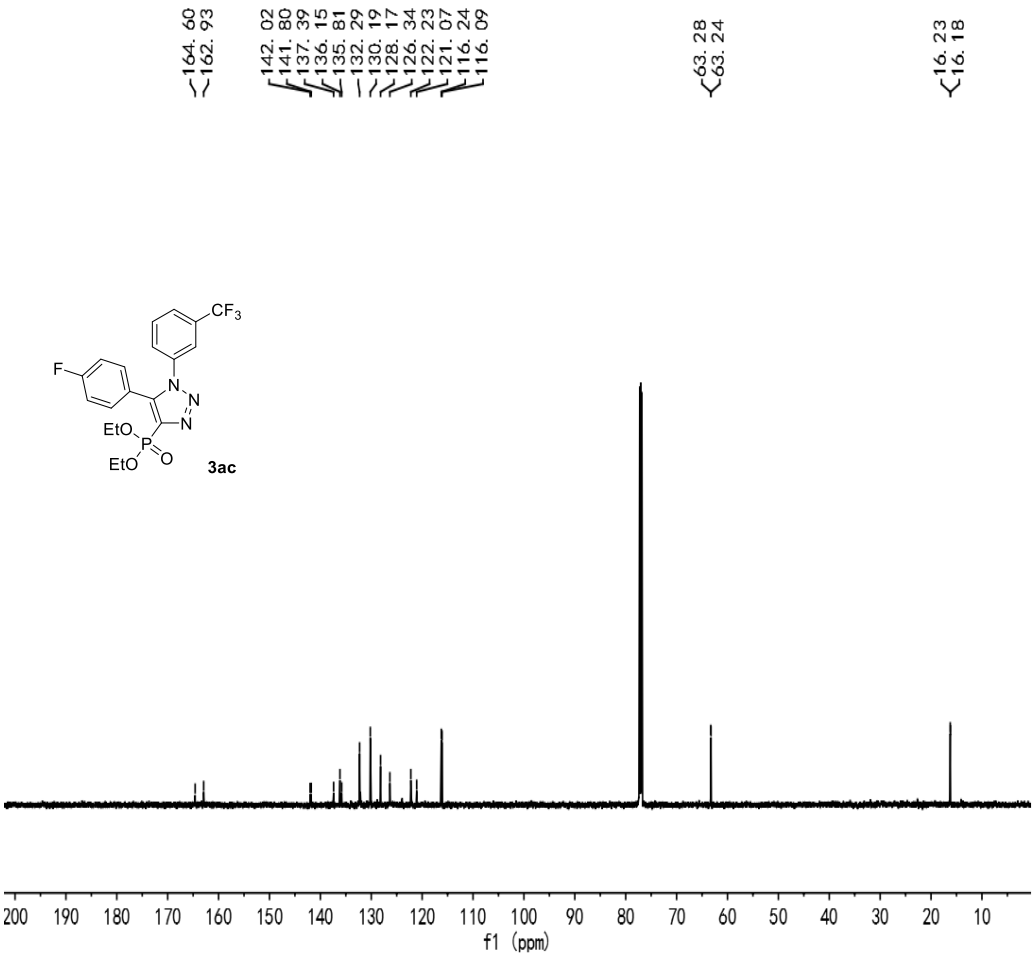
Dimethyl(5-methyl-1-(3,4,5-trifluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ab)

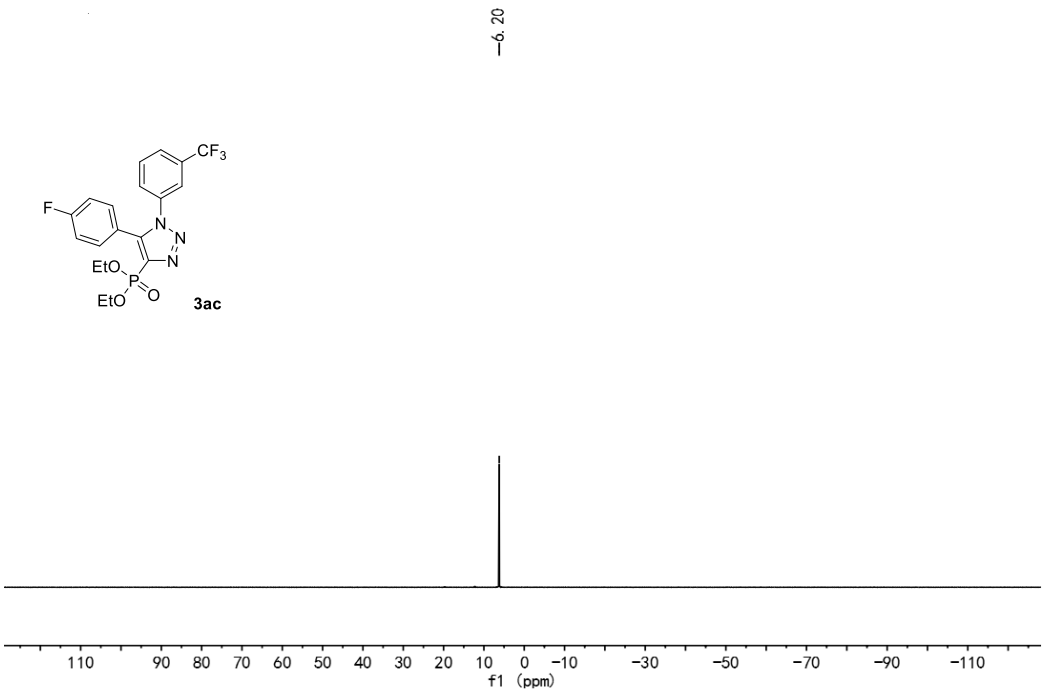




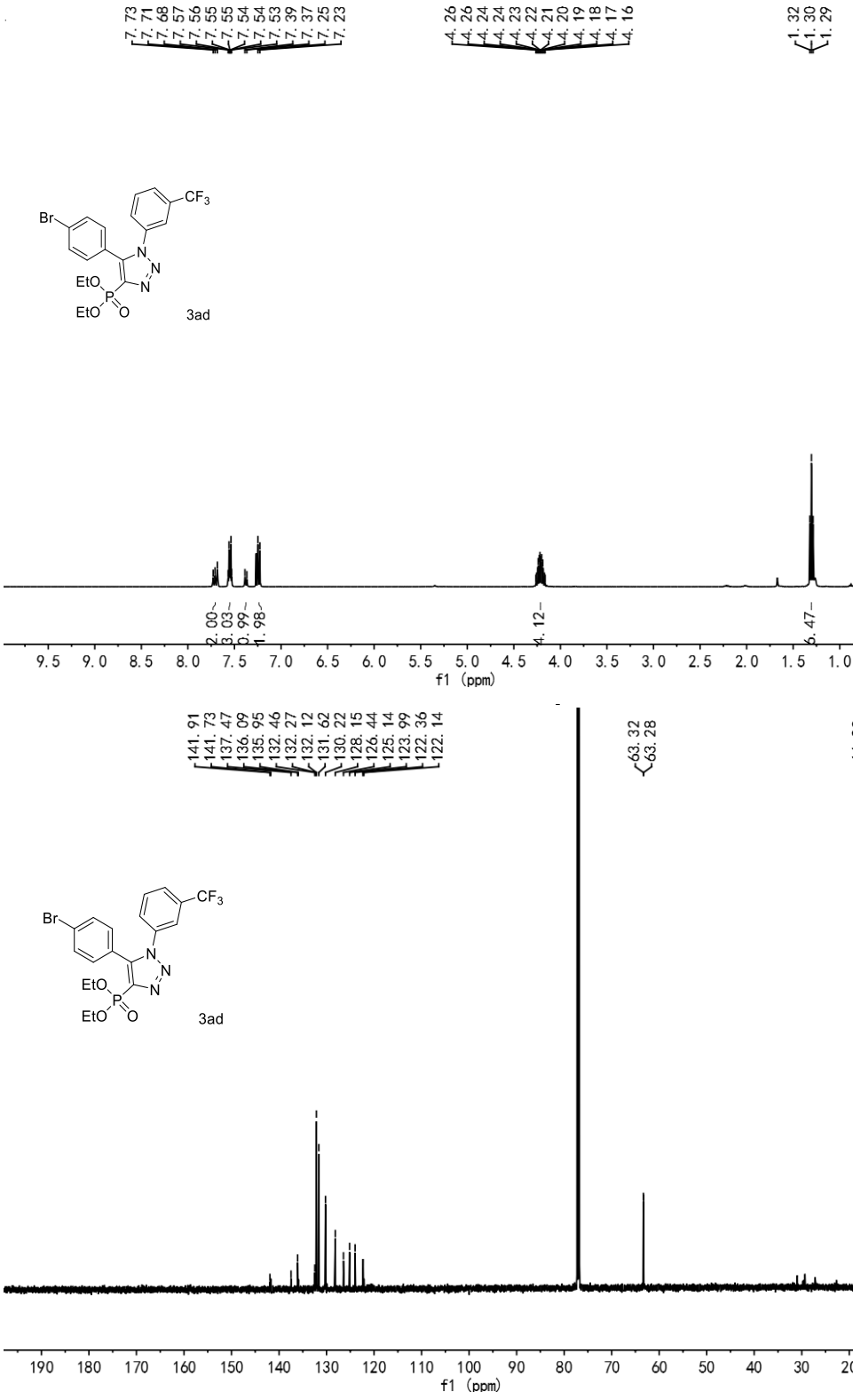
Diethyl(5-(4-fluorophenyl)-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ac)

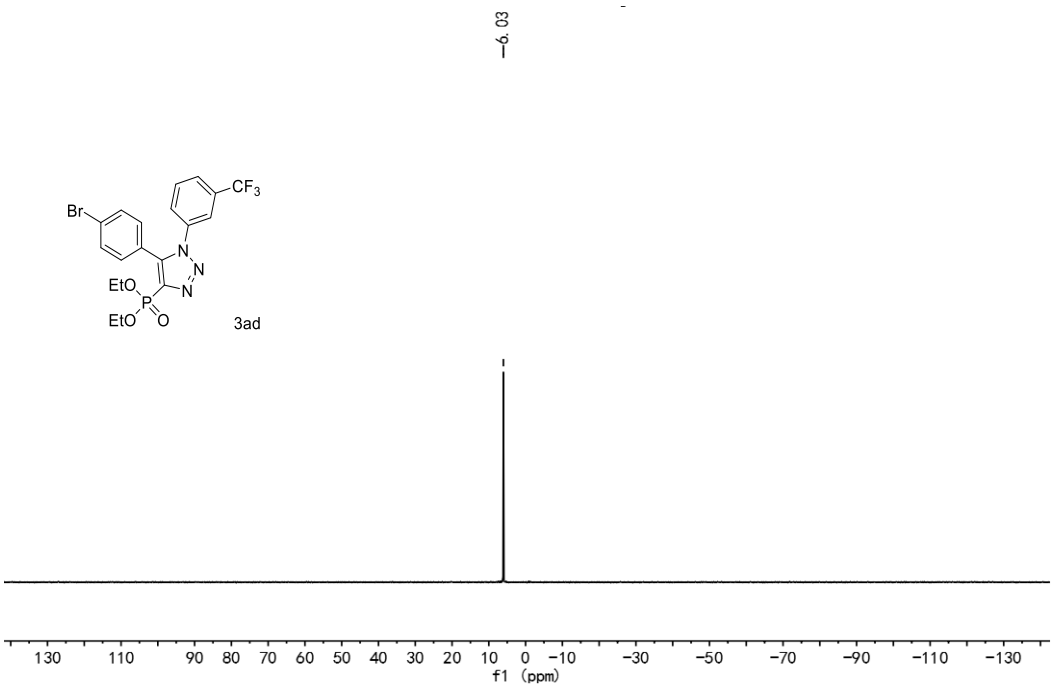



164.60
162.93
142.02
141.80
137.39
136.15
135.81
132.29
130.19
128.17
126.34
122.23
121.07
116.24
116.09
63.28
63.24
16.23
16.18
CF3
F
N
N
N
EtO
P
O
EtO
3ac
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

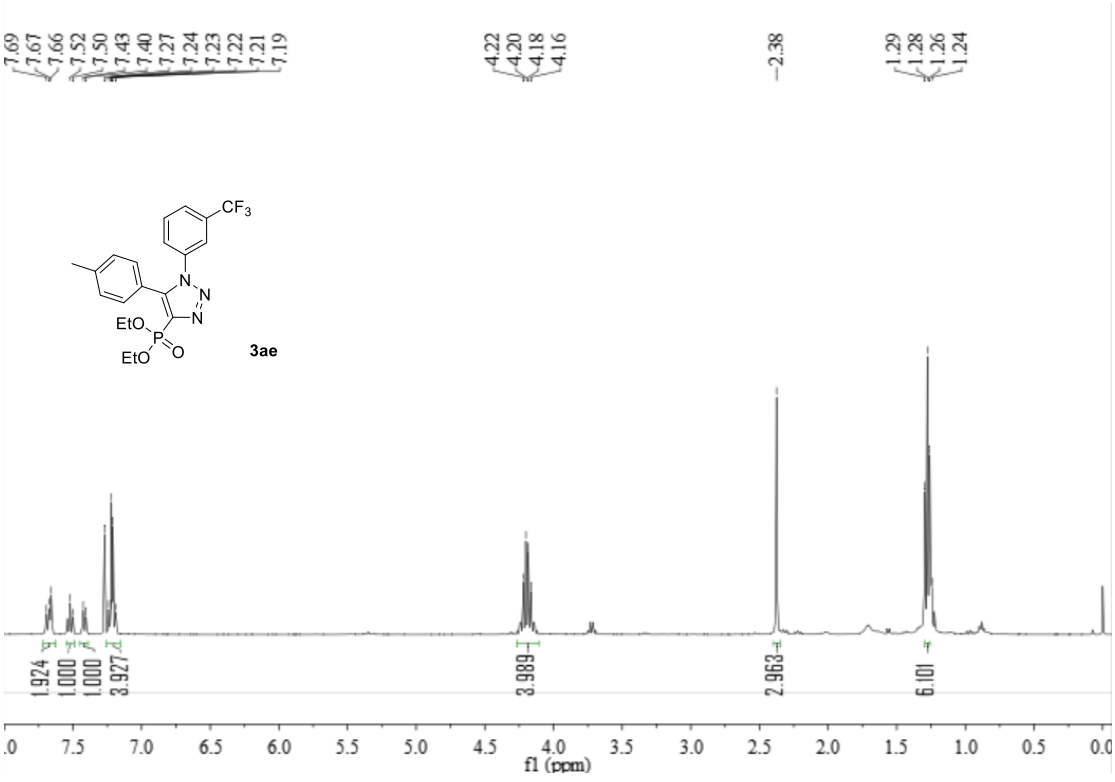

-6.20
CF3
F
N
N
N
EtO
P
O
EtO
3ac
110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110
f1 (ppm)

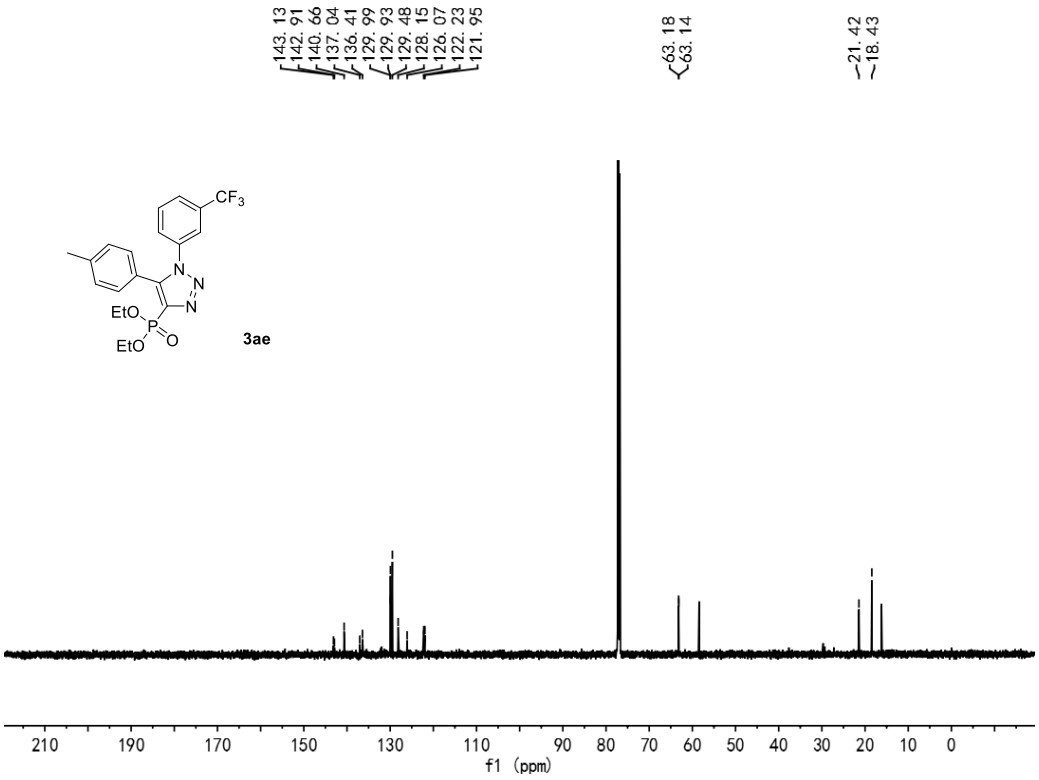
Diethyl(5-(4-bromophenyl)-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ad)

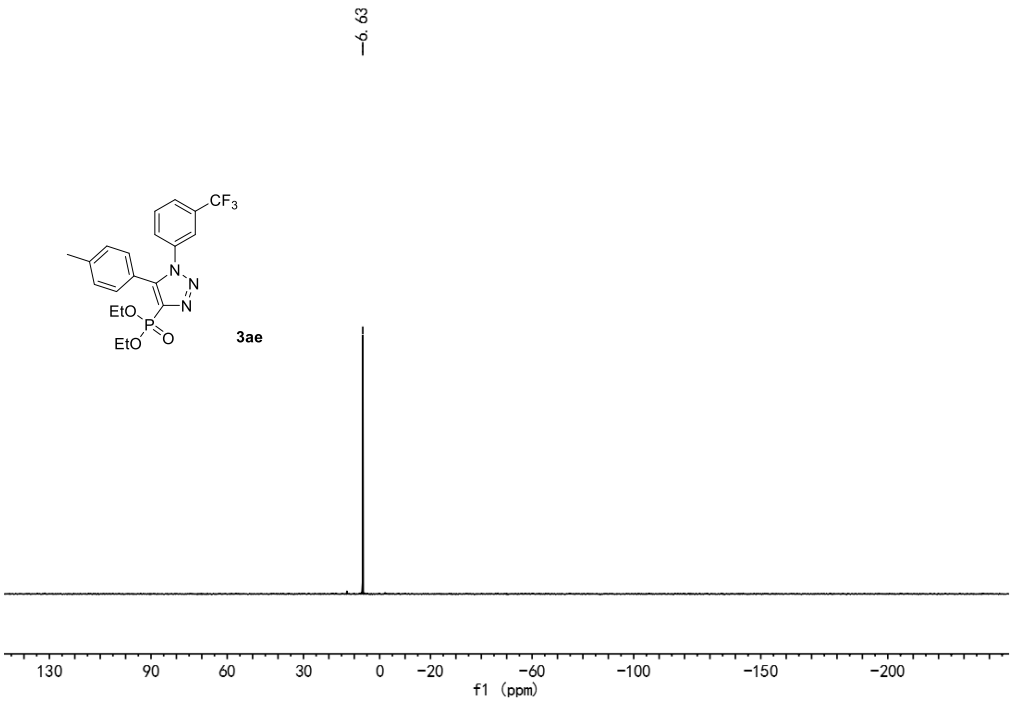




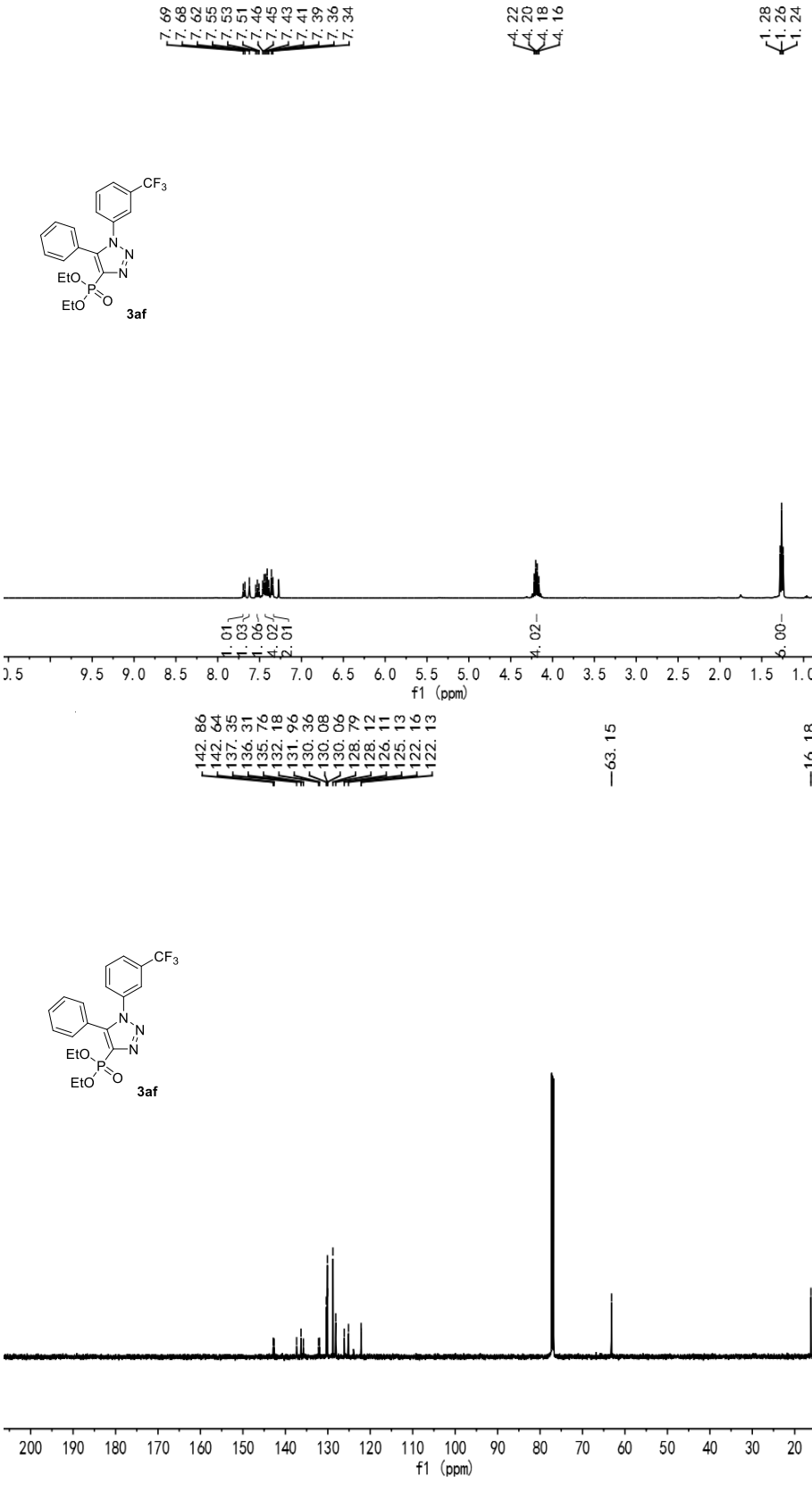
Diethyl(5-(p-tolyl)-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ae)

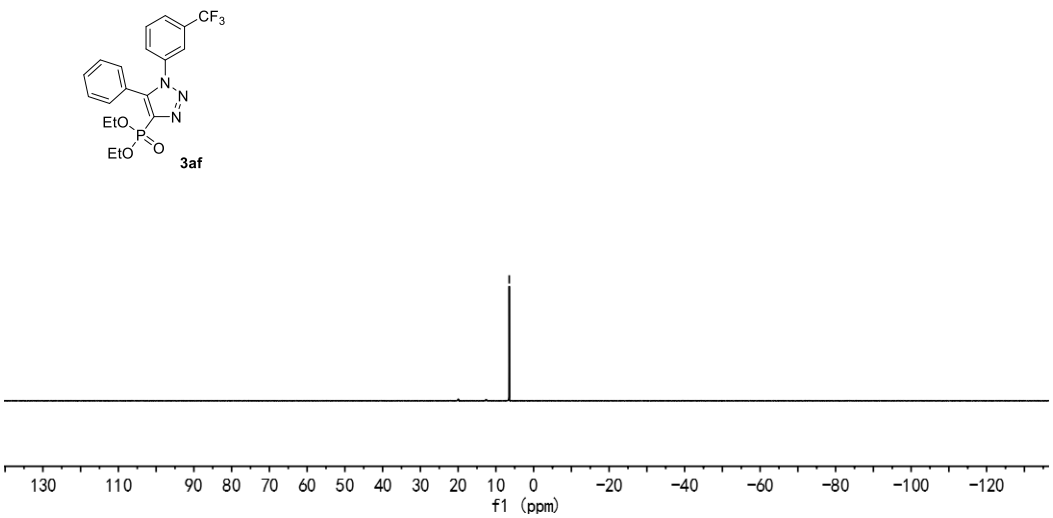



143.13
142.91
140.66
137.04
136.41
129.99
129.93
129.48
128.15
126.07
122.23
121.95
63.18
63.14
21.42
18.43
CF3
EtO
EtO
P
O
N
N
N
3ae
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

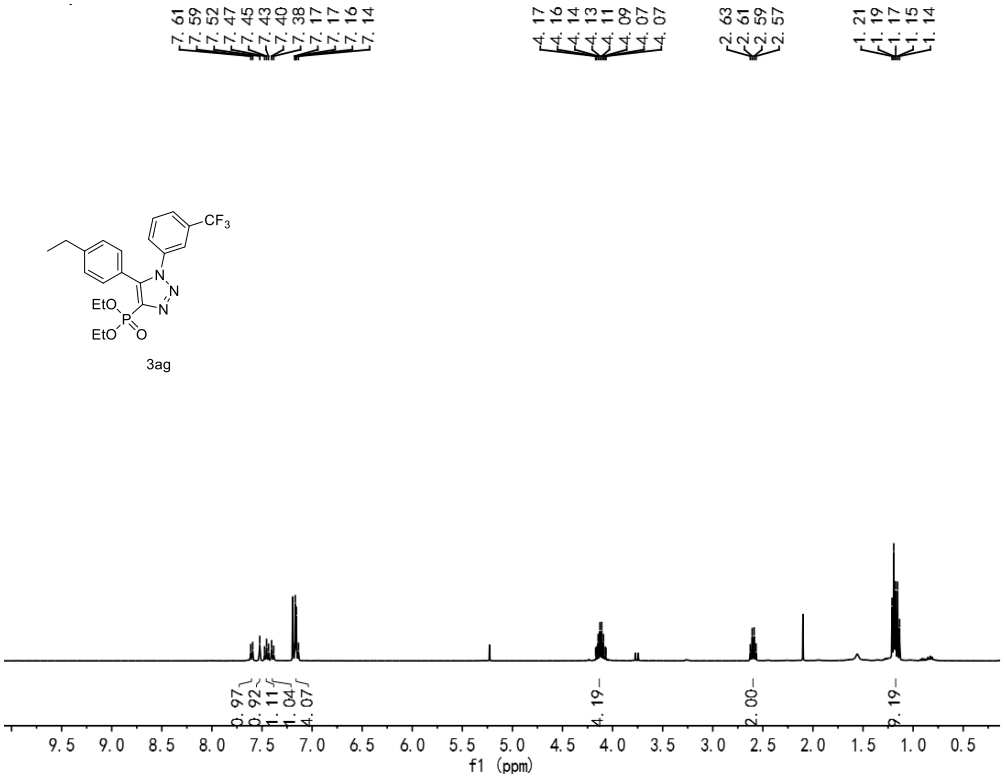

6.63
CF3
EtO
EtO
P
O
N
N
N
3ae
130
90
60
30
0
-20
-60
-100
-150
-200
f1 (ppm)

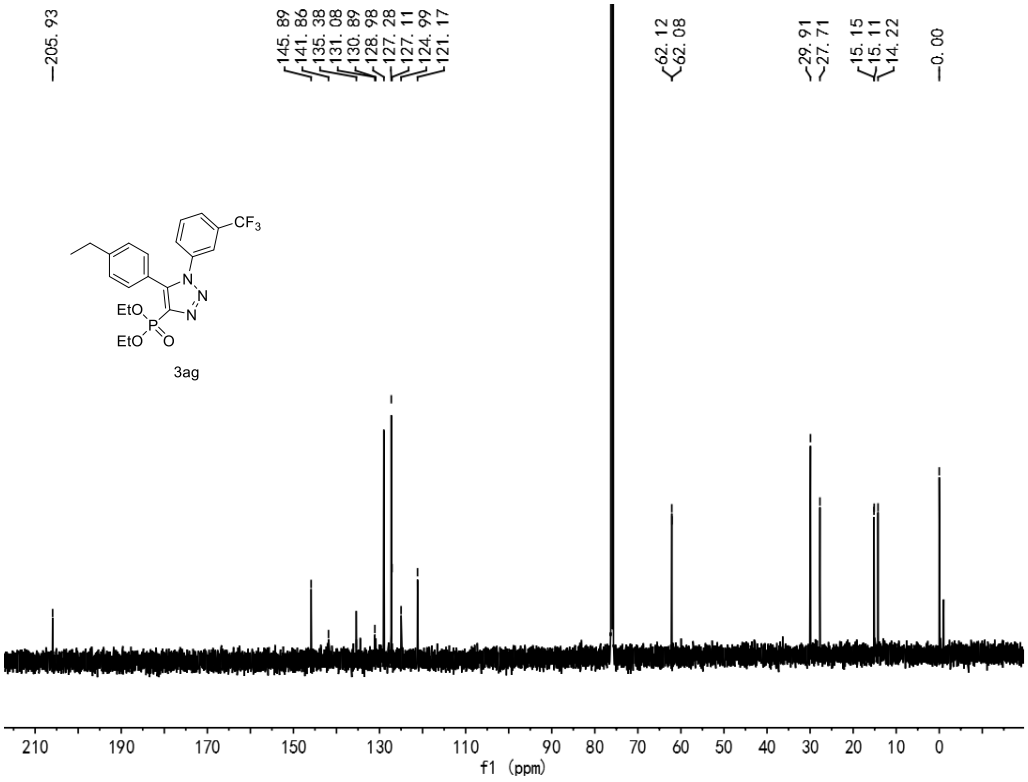
Diethyl(5-phenyl-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3af)

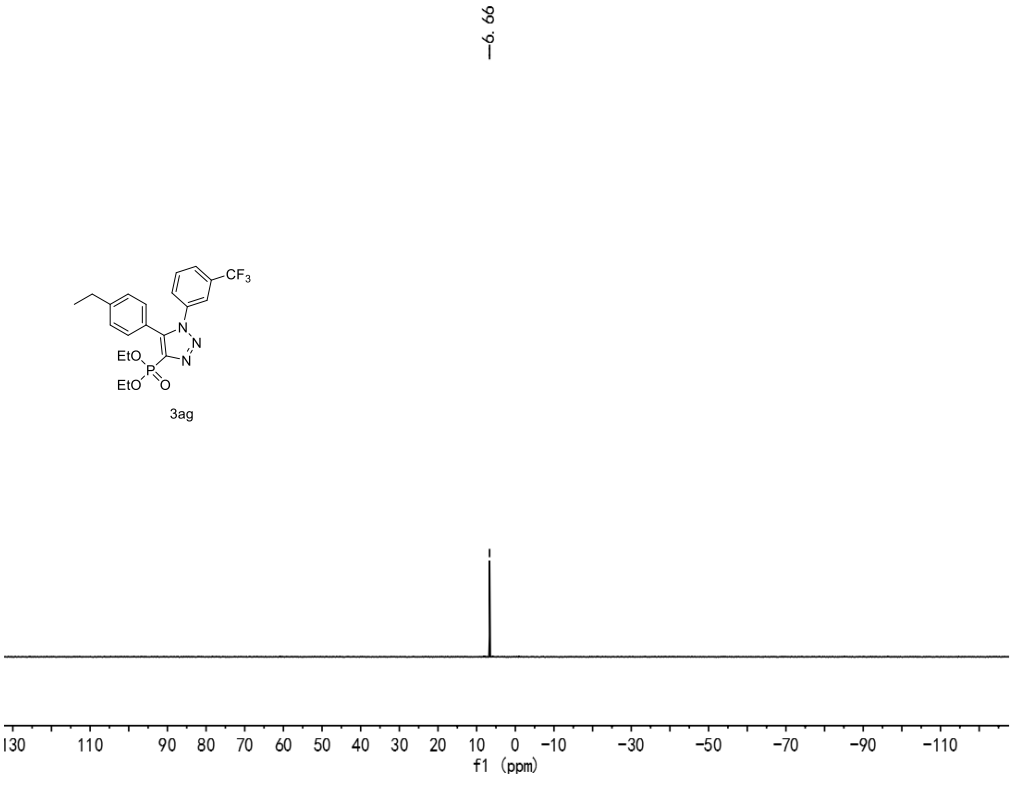




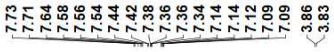
Diethyl(5-(4-ethylphenyl)-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate **(3ag)**

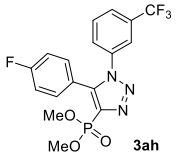


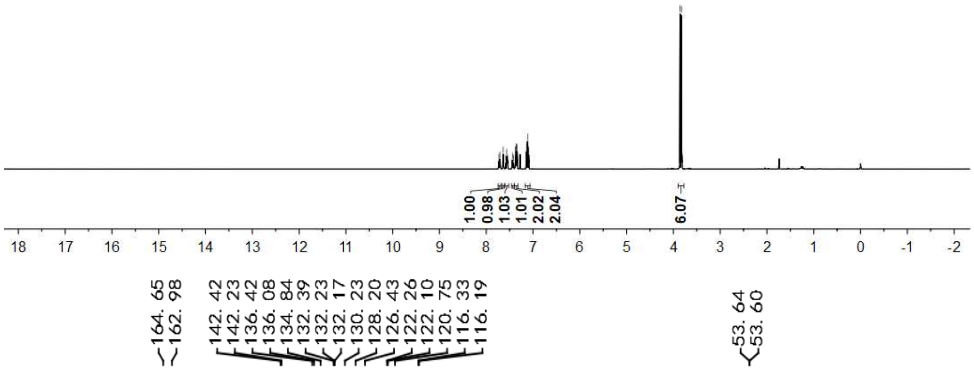

205.93
145.89
141.86
135.38
131.08
130.89
128.98
127.28
127.11
124.99
121.17
62.12
62.08
29.91
27.71
15.15
15.11
14.22
0.00
CF3
EtO
EtO
P
O
N
N
N
3ag
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

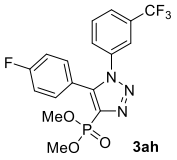

6.66
CF3
EtO
EtO
P
O
N
N
N
3ag
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
-50
-70
-90
-110
f1 (ppm)

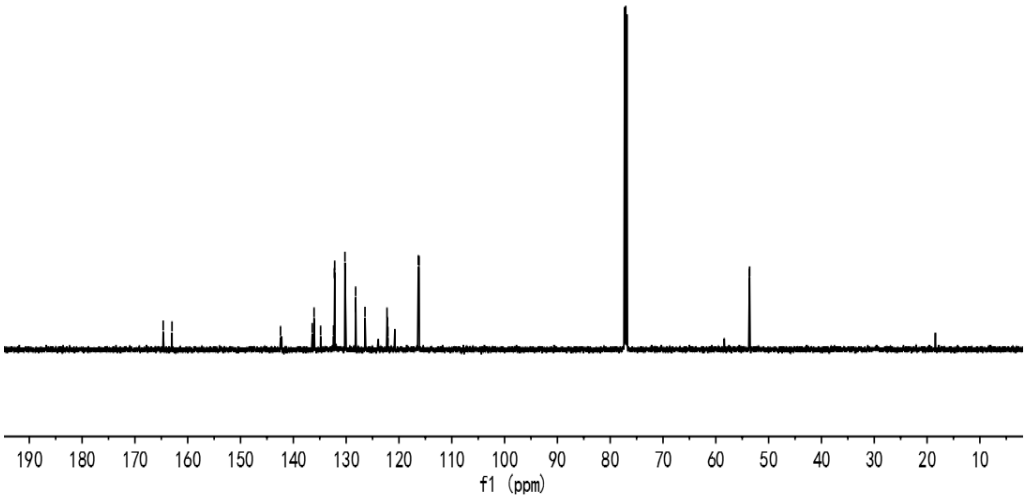
Dimethyl(5-(4-fluorophenyl)-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ah)

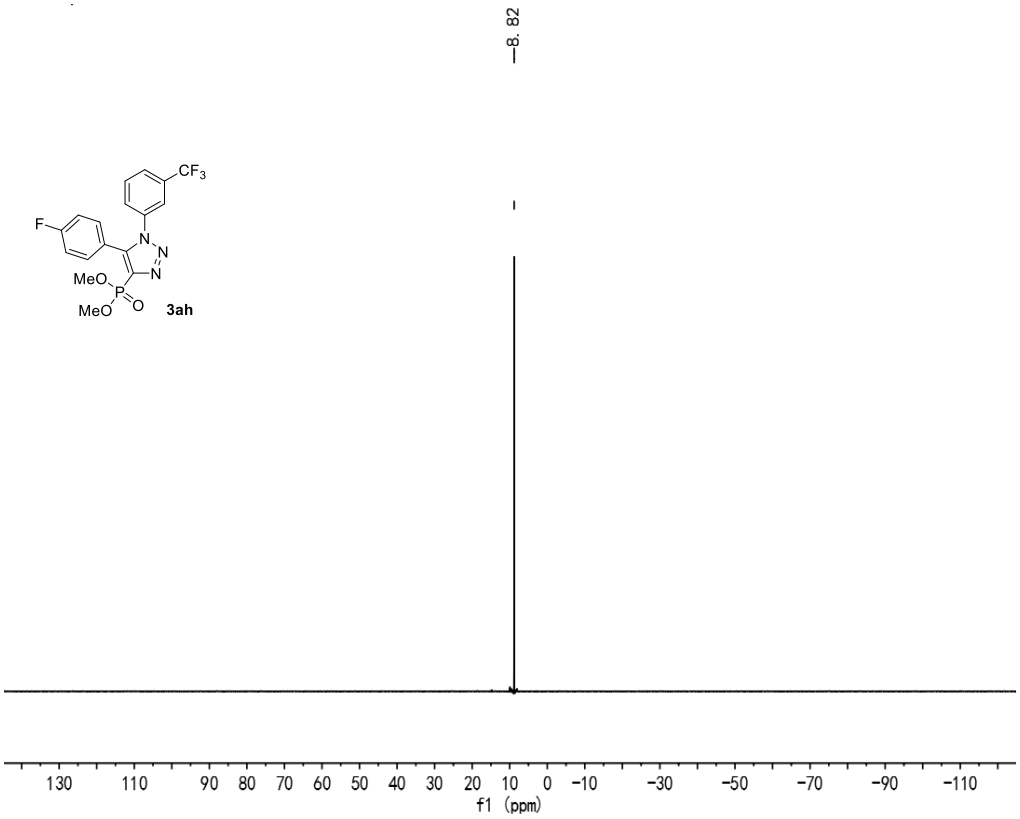




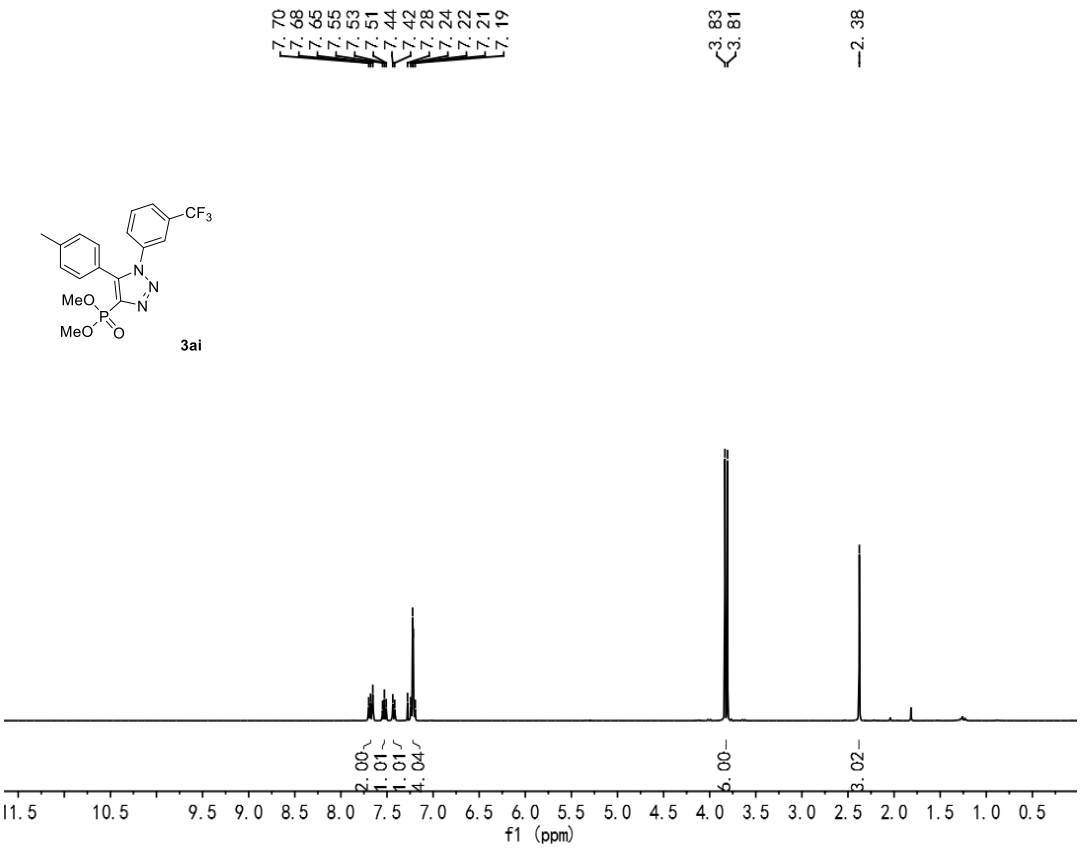


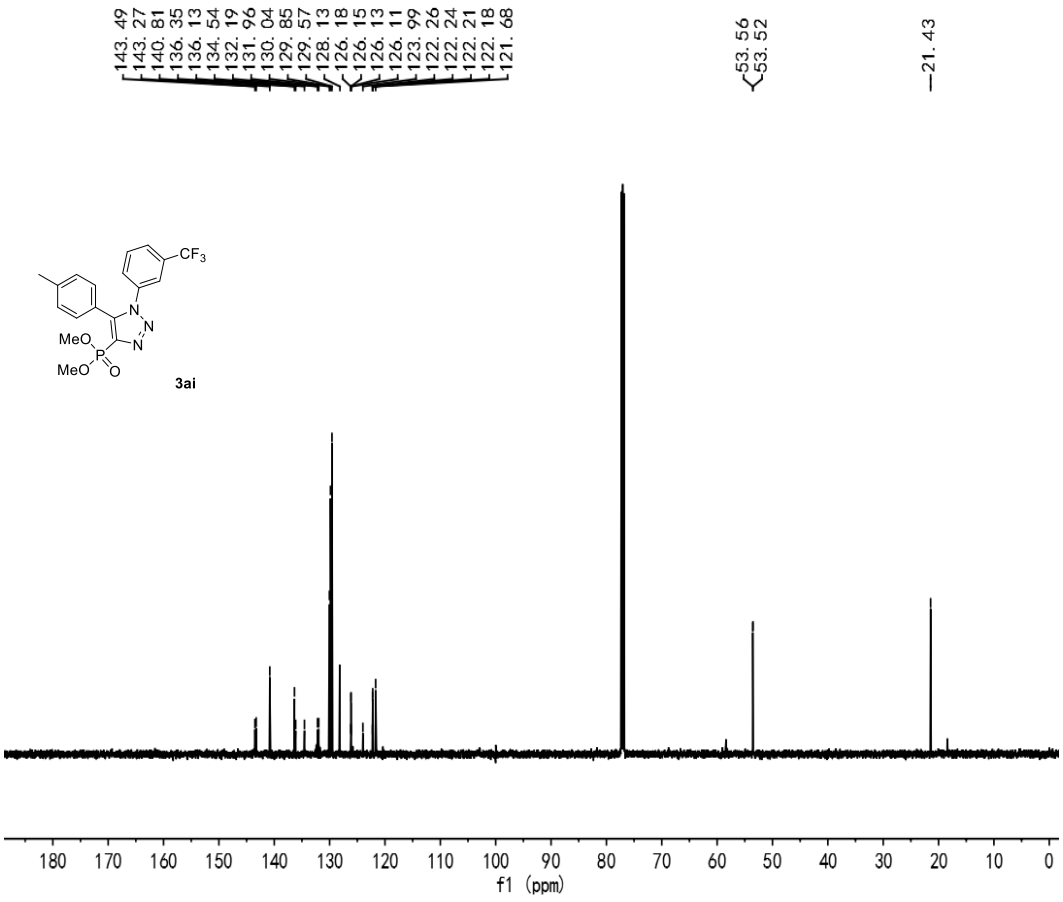


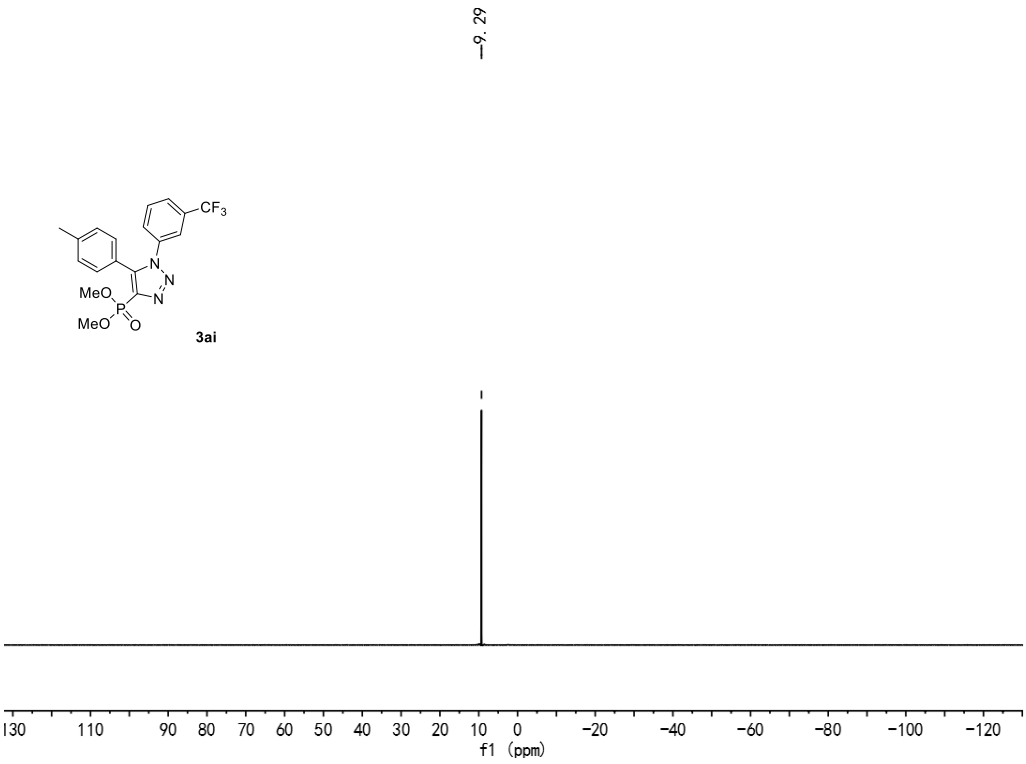




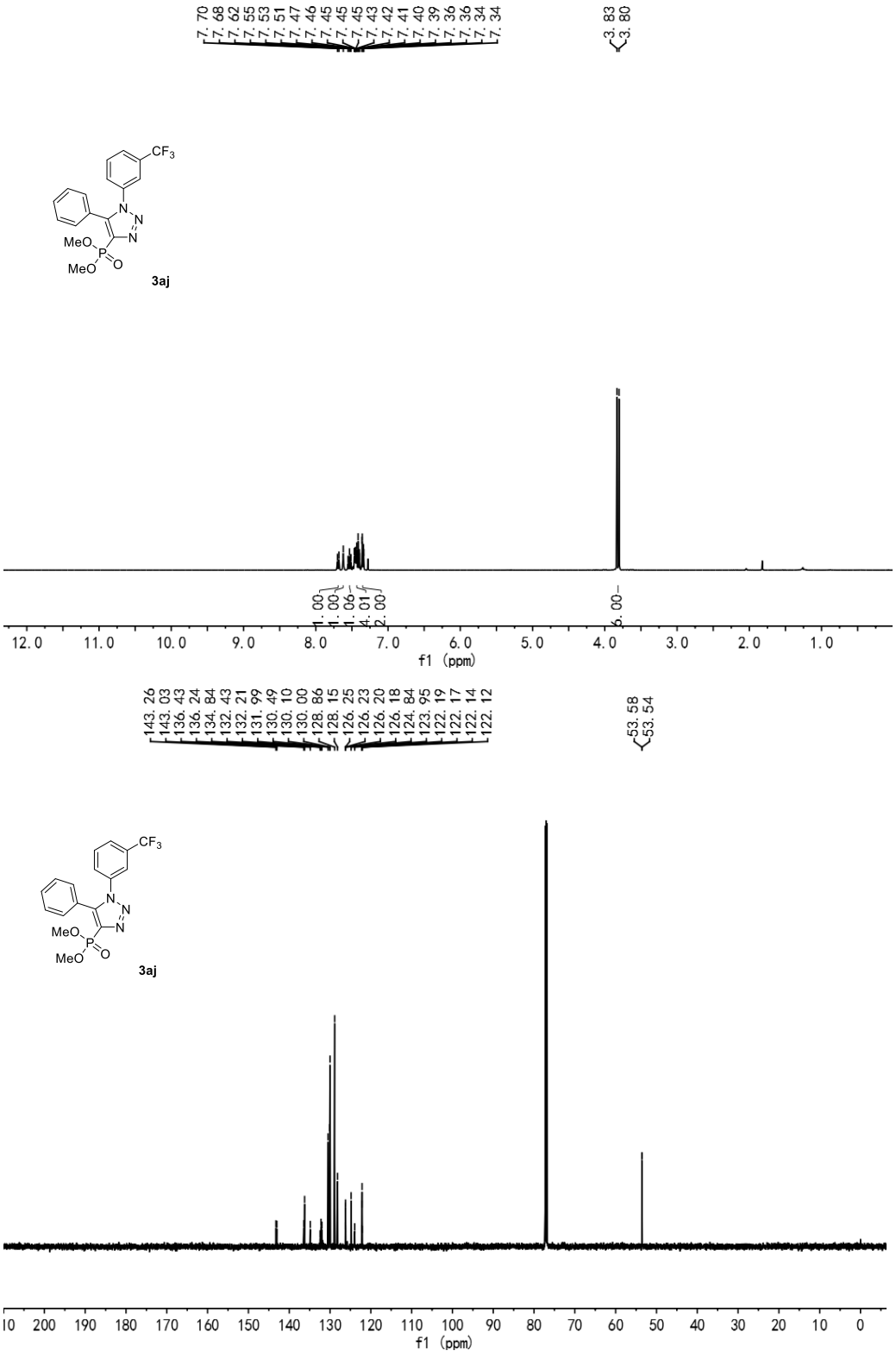
Dimethyl(5-(p-tolyl)-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate **(3ai)**

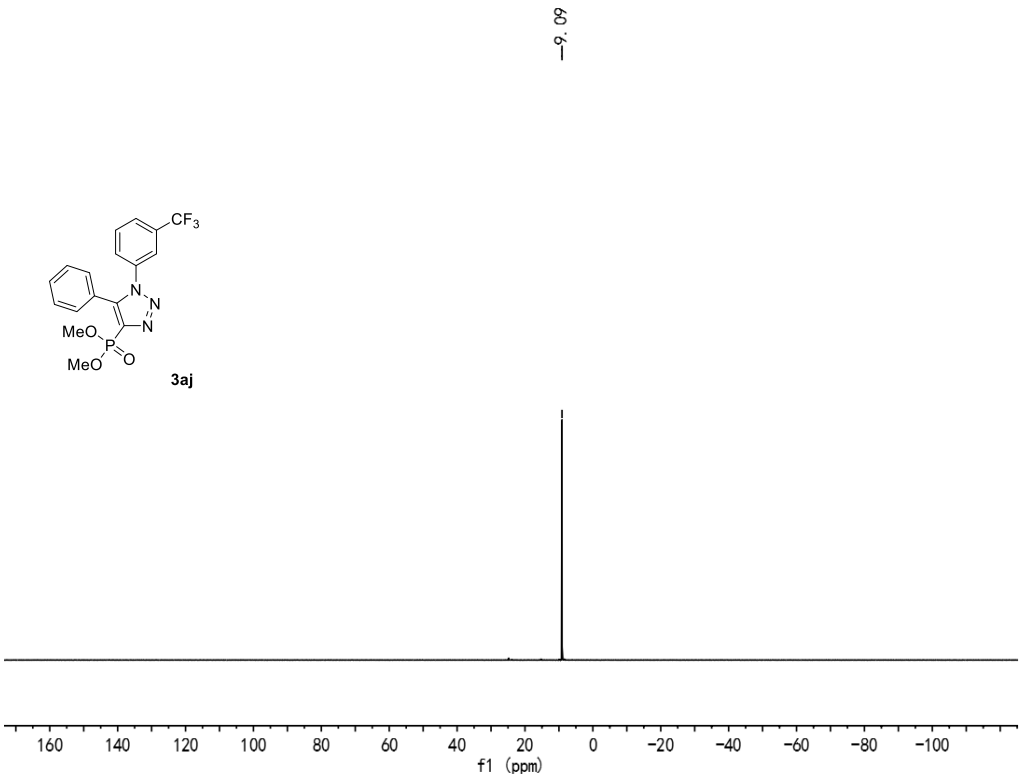



143.49
143.27
140.81
136.35
136.13
134.54
132.19
131.96
130.04
129.85
129.57
128.13
126.18
126.15
126.13
126.11
123.99
122.26
122.24
122.21
122.18
121.68
53.56
53.52
21.43
CF3
MeO
MeO
P
O
N
N
N
3ai
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

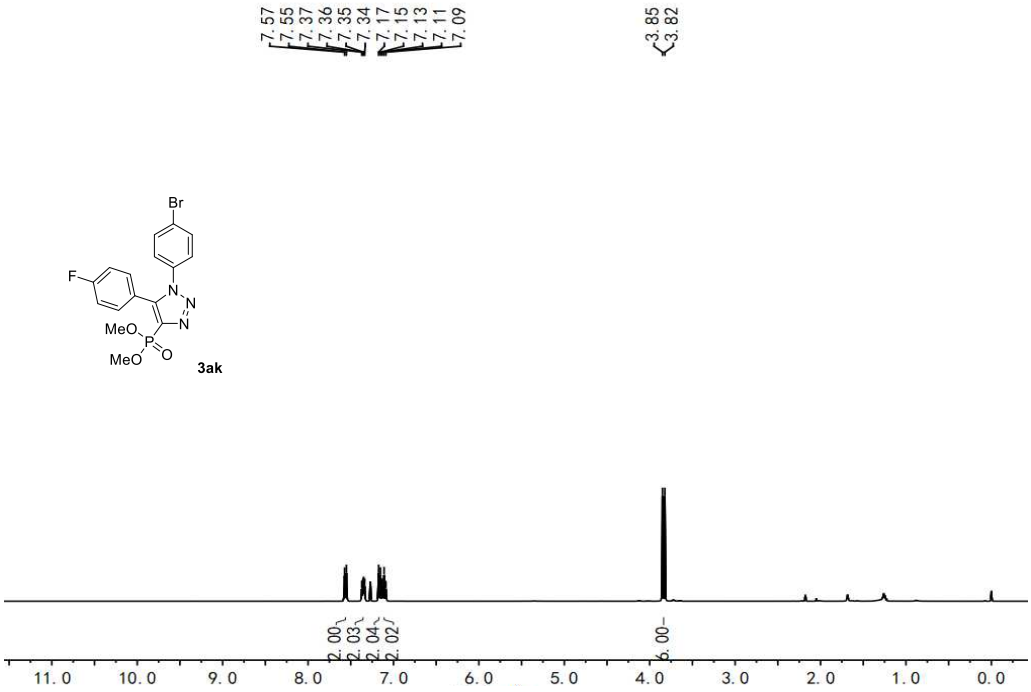

9.29
CF3
MeO
MeO
P
O
N
N
N
3ai
130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120
f1 (ppm)

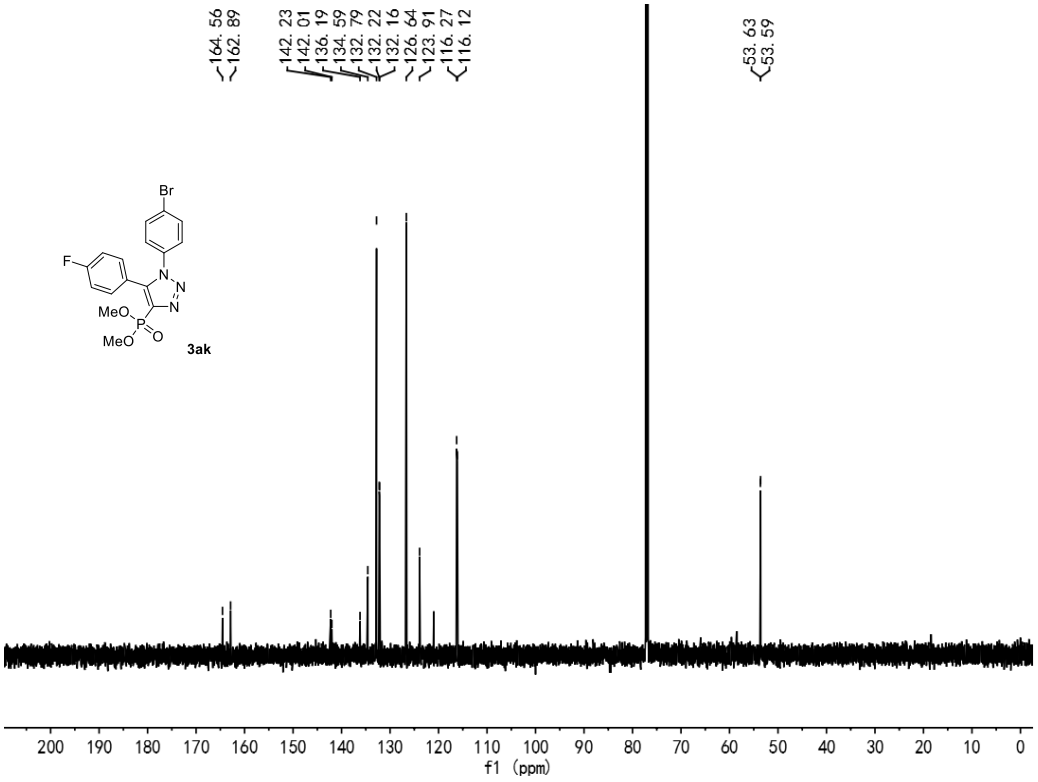
Dimethyl(5-phenyl-1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3aj)

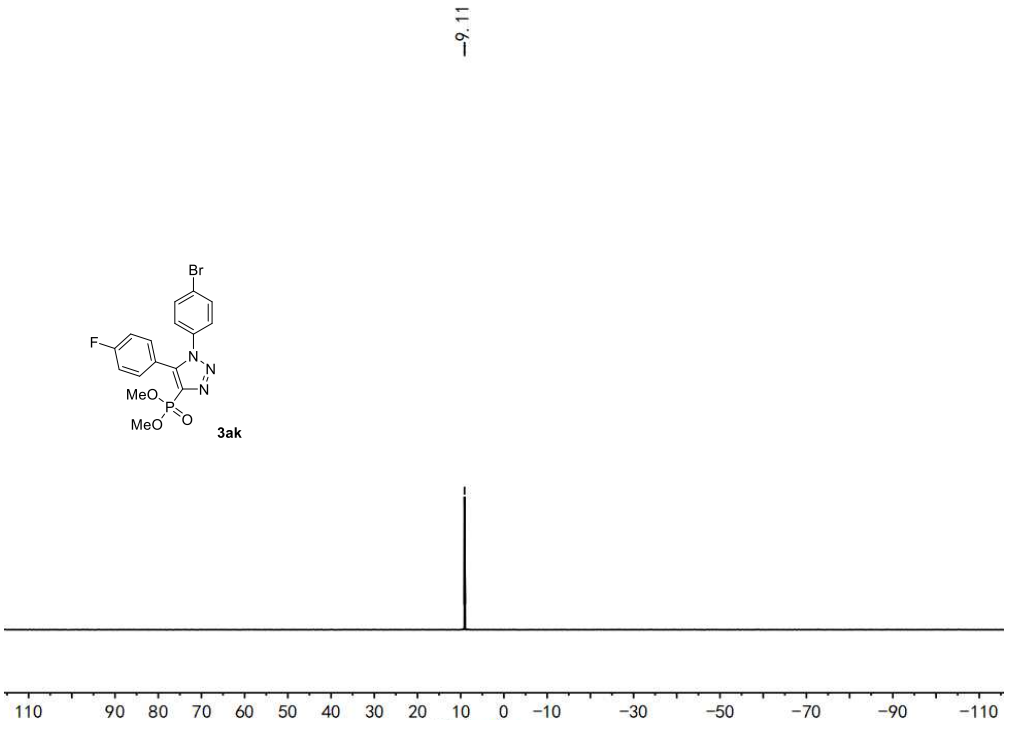




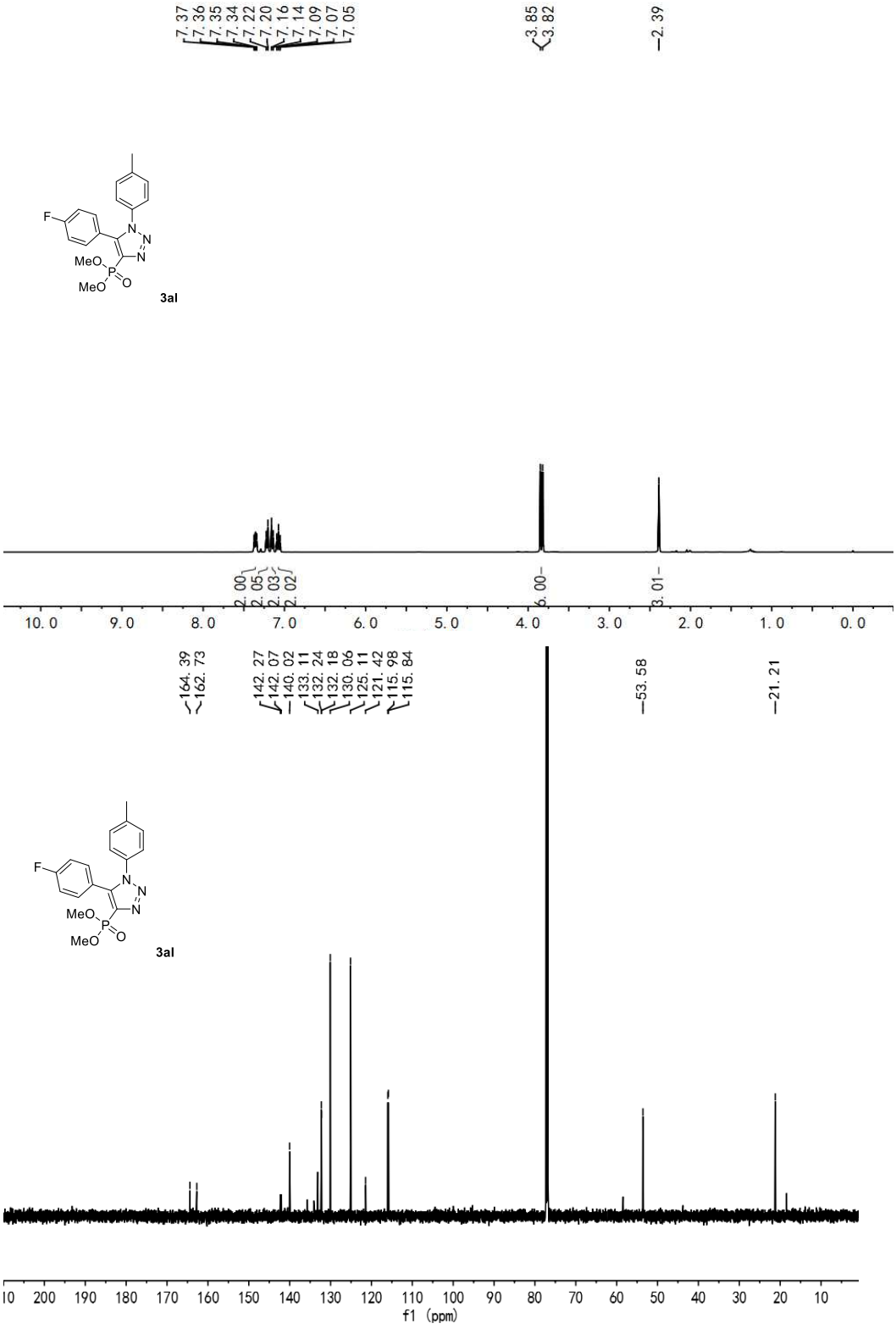
Dimethyl(1-(4-bromophenyl)-5-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ak)

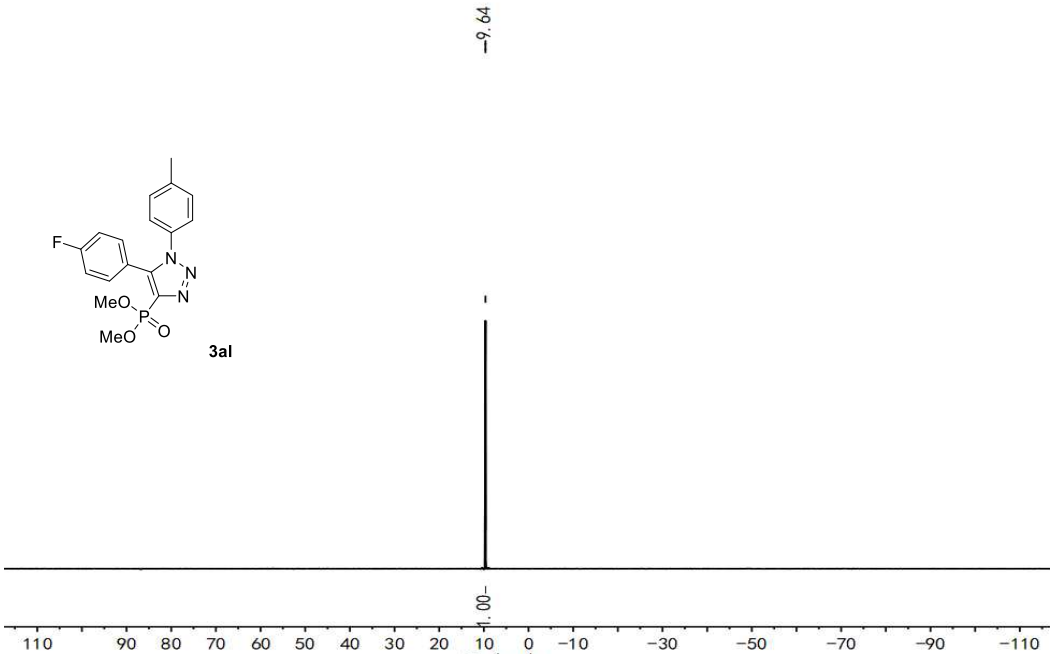



164.56
162.89
142.23
142.01
136.19
134.59
132.79
132.22
132.16
126.64
123.91
116.27
116.12
53.63
53.59
Br
F
N
N
N
MeO
MeO
P
O
3ak
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

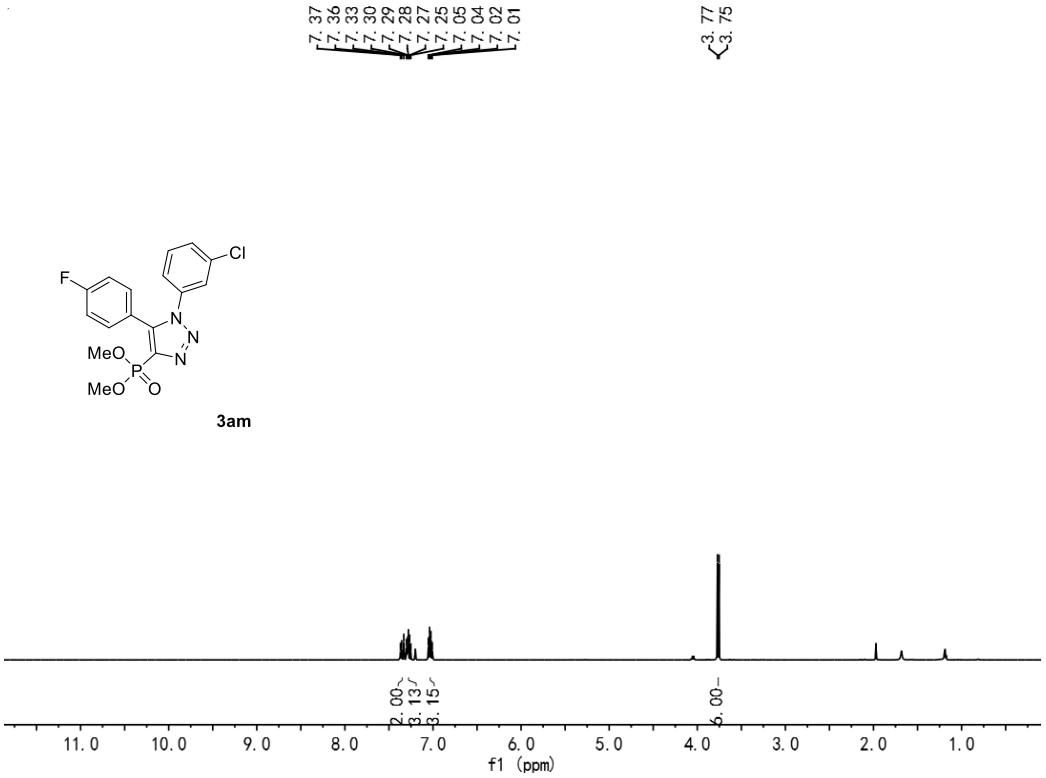

9.11
Br
F
N
N
N
MeO
MeO
P
O
3ak
110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110

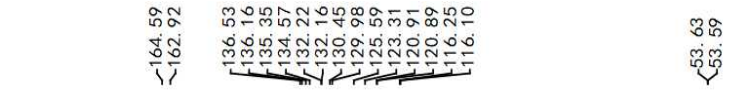
Dimethyl(5-(4-fluorophenyl)-1-(p-tolyl)-1H-1,2,3-triazol-4-yl)phosphonate (3al)

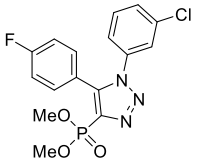




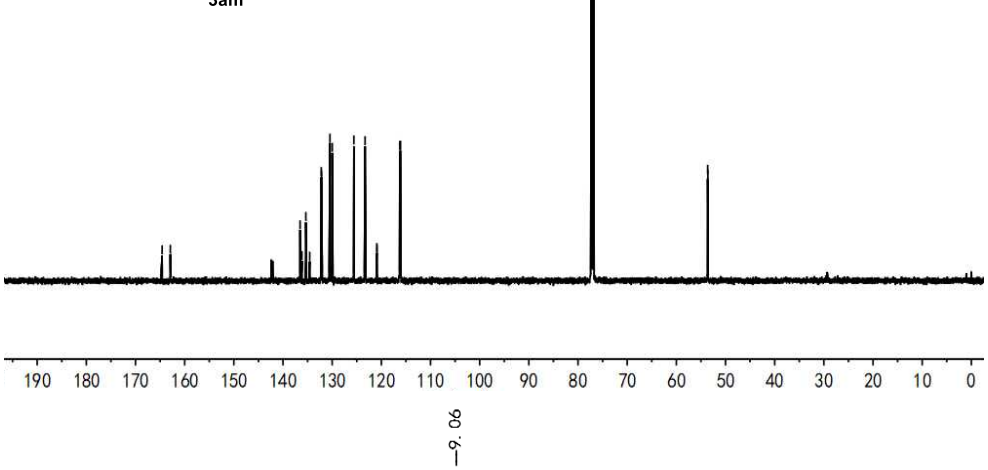
Dimethyl(1-(3-chlorophenyl)-5-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3am)

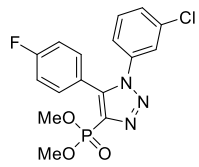



164.59
162.92
136.53
136.16
135.35
134.57
132.22
132.16
130.45
129.98
125.59
123.31
120.91
120.89
116.25
116.10
53.63
53.59

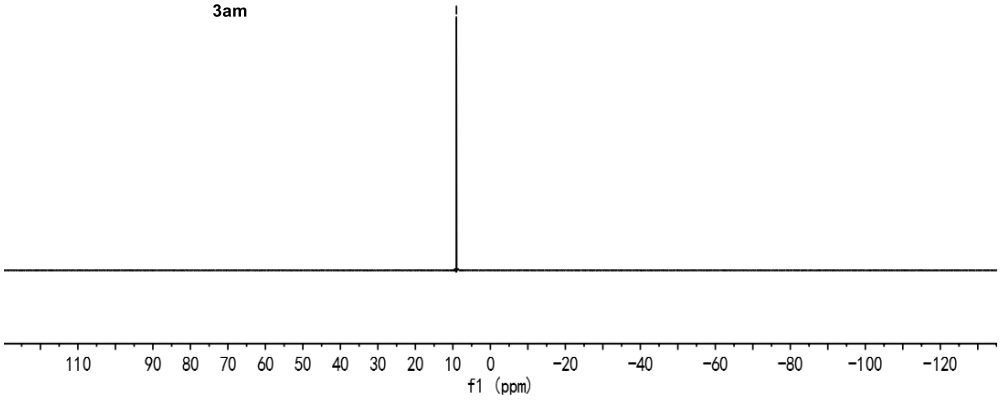

F
Cl
N
N
N
MeO
MeO
P
O

3am

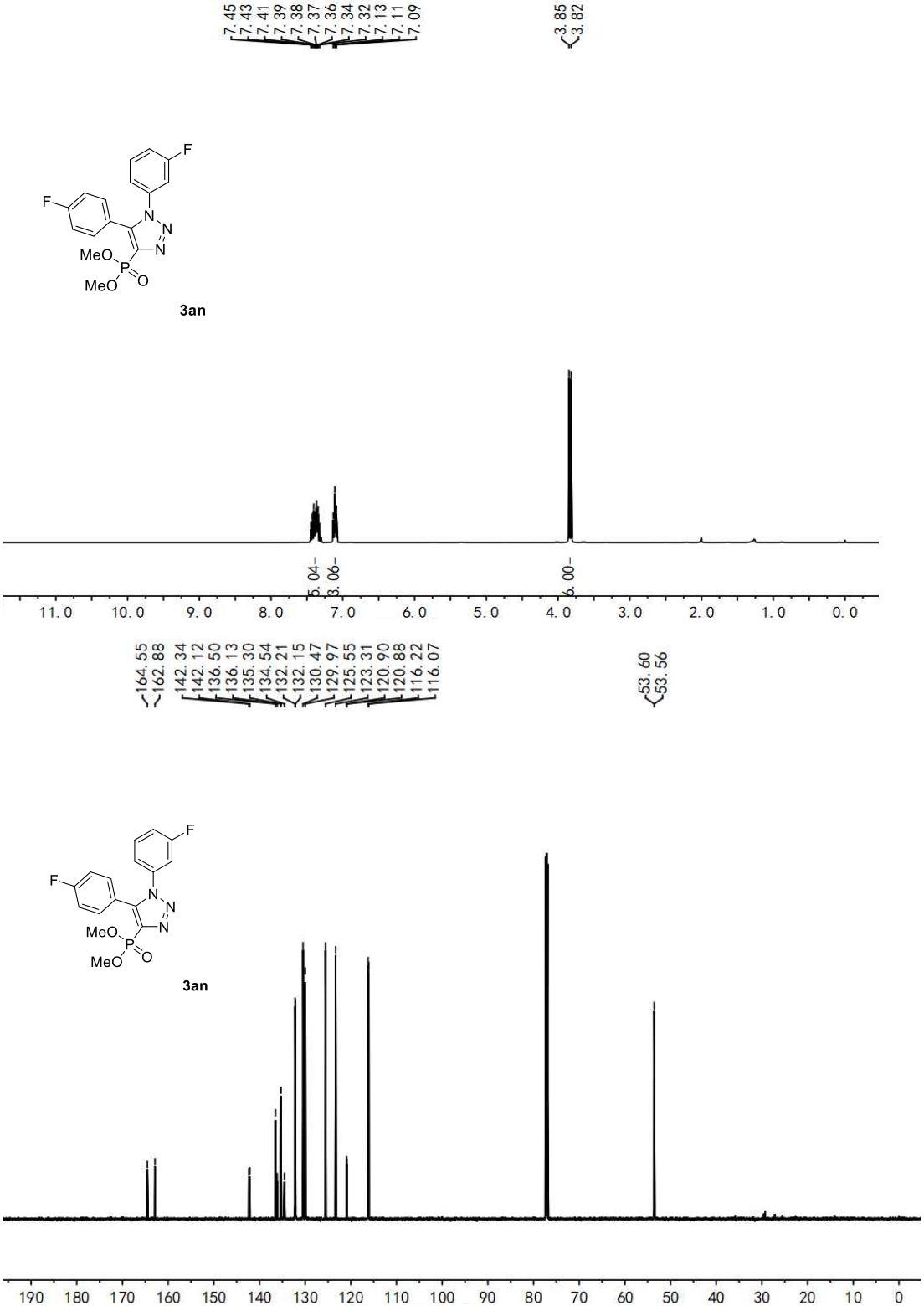

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
-9.06

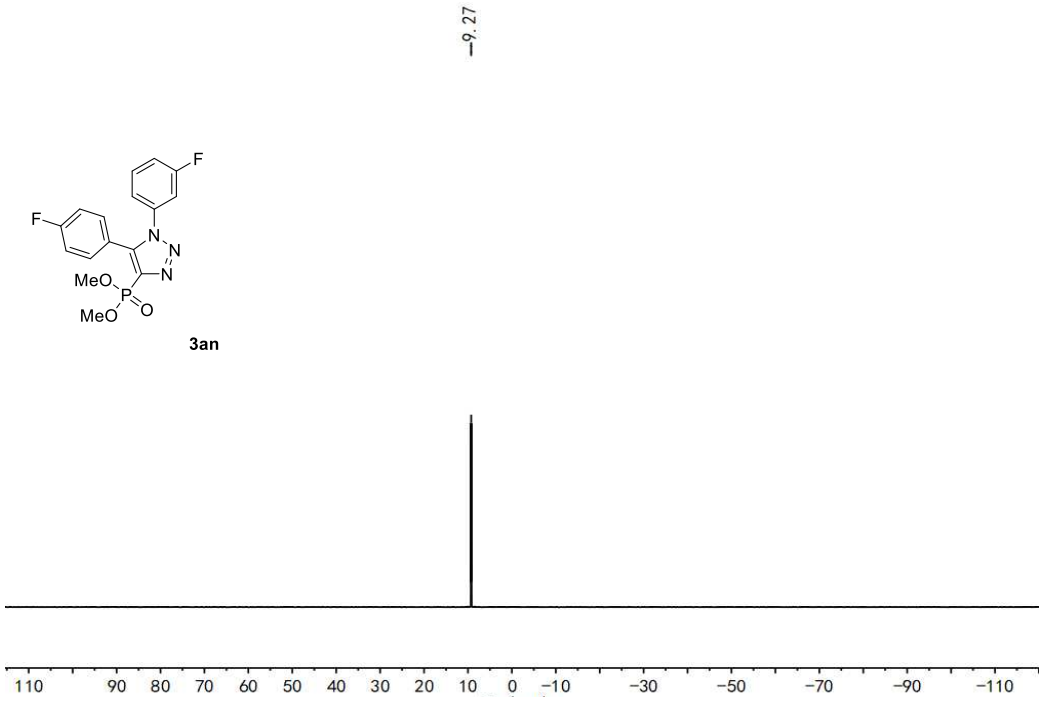

F
Cl
N
N
N
MeO
MeO
P
O

3am

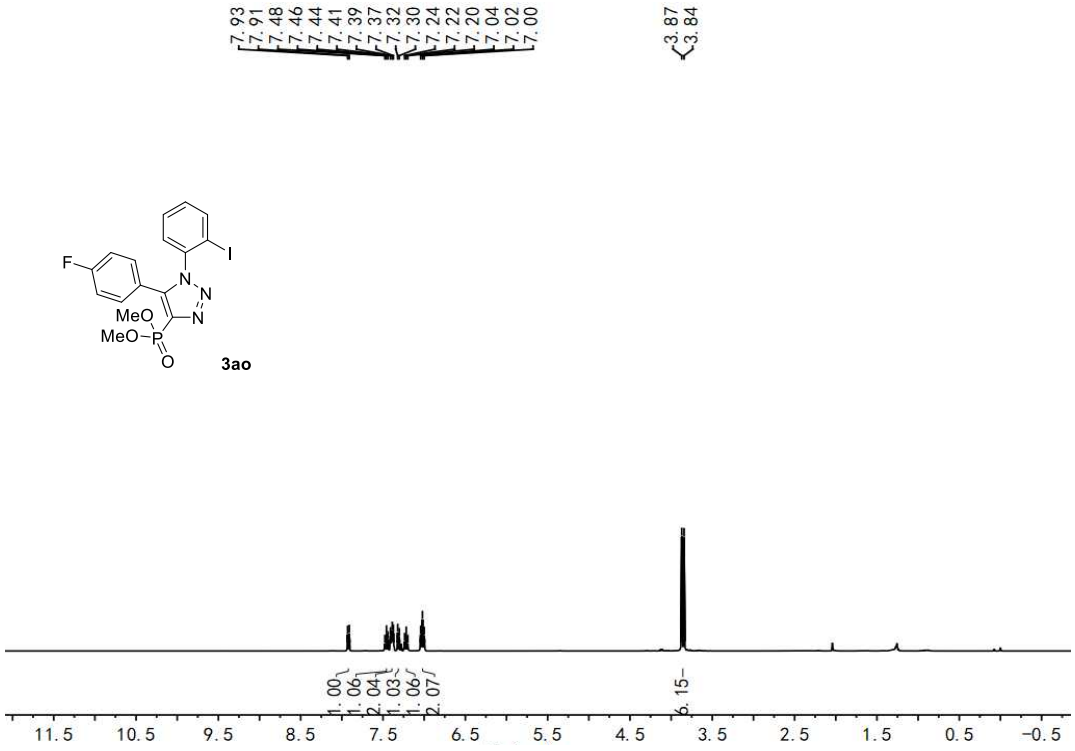

110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120
f1 (ppm)

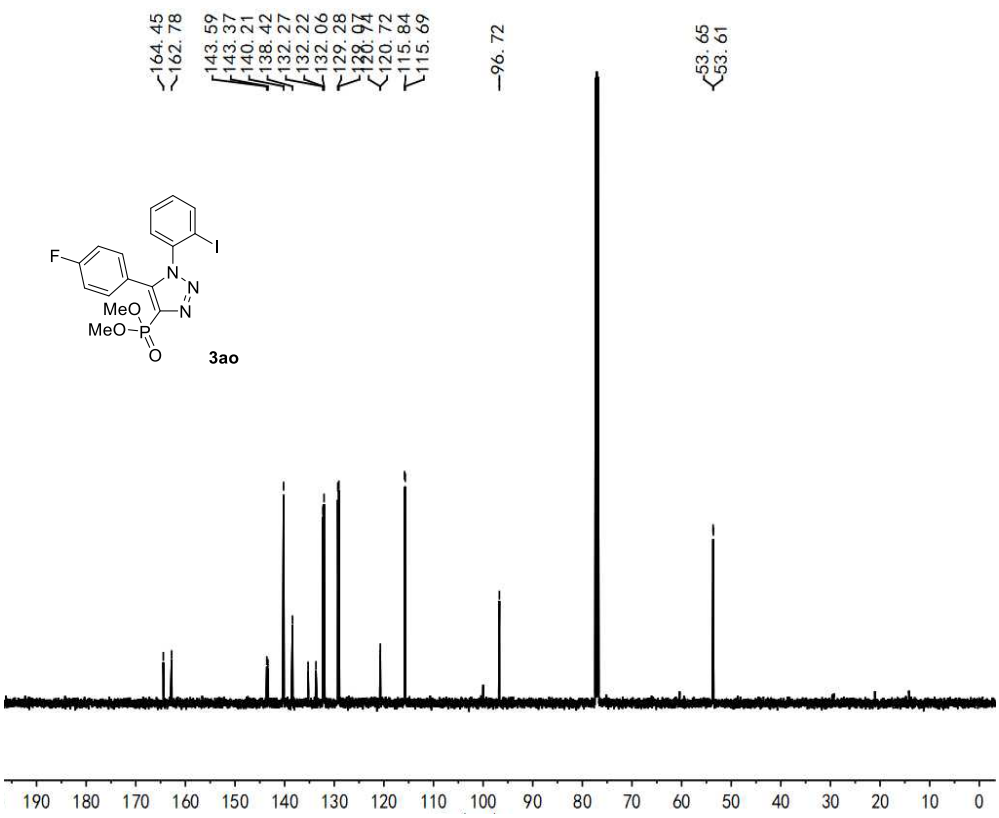
Dimethyl(1-(3-fluorophenyl)-5-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3an)

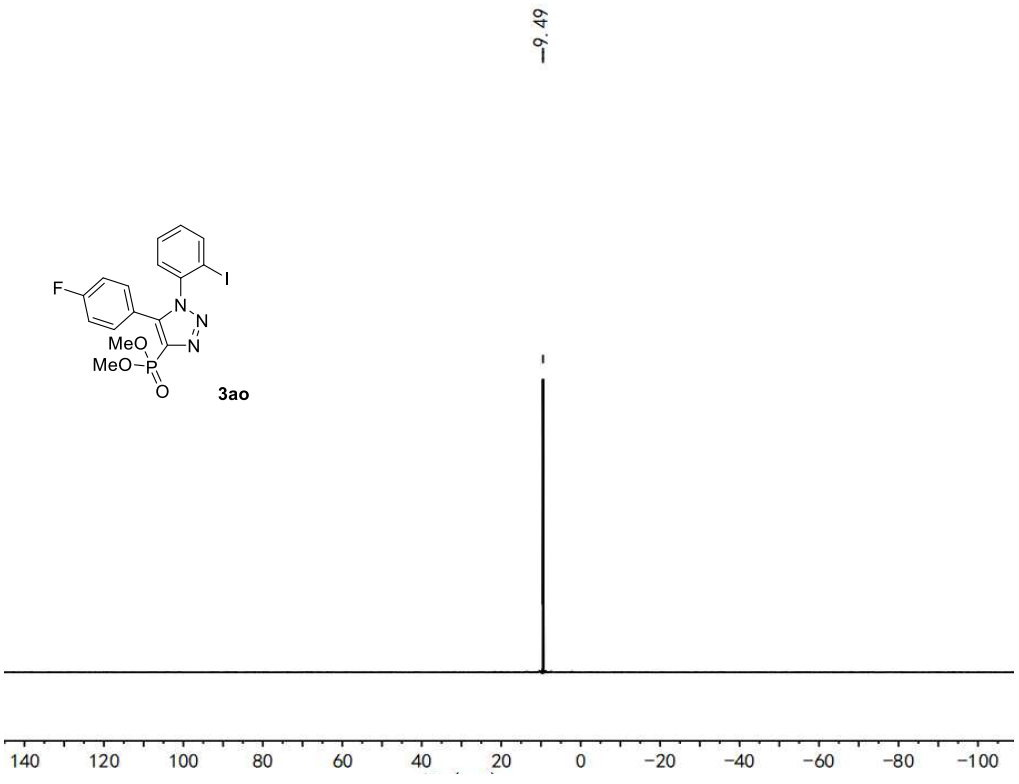




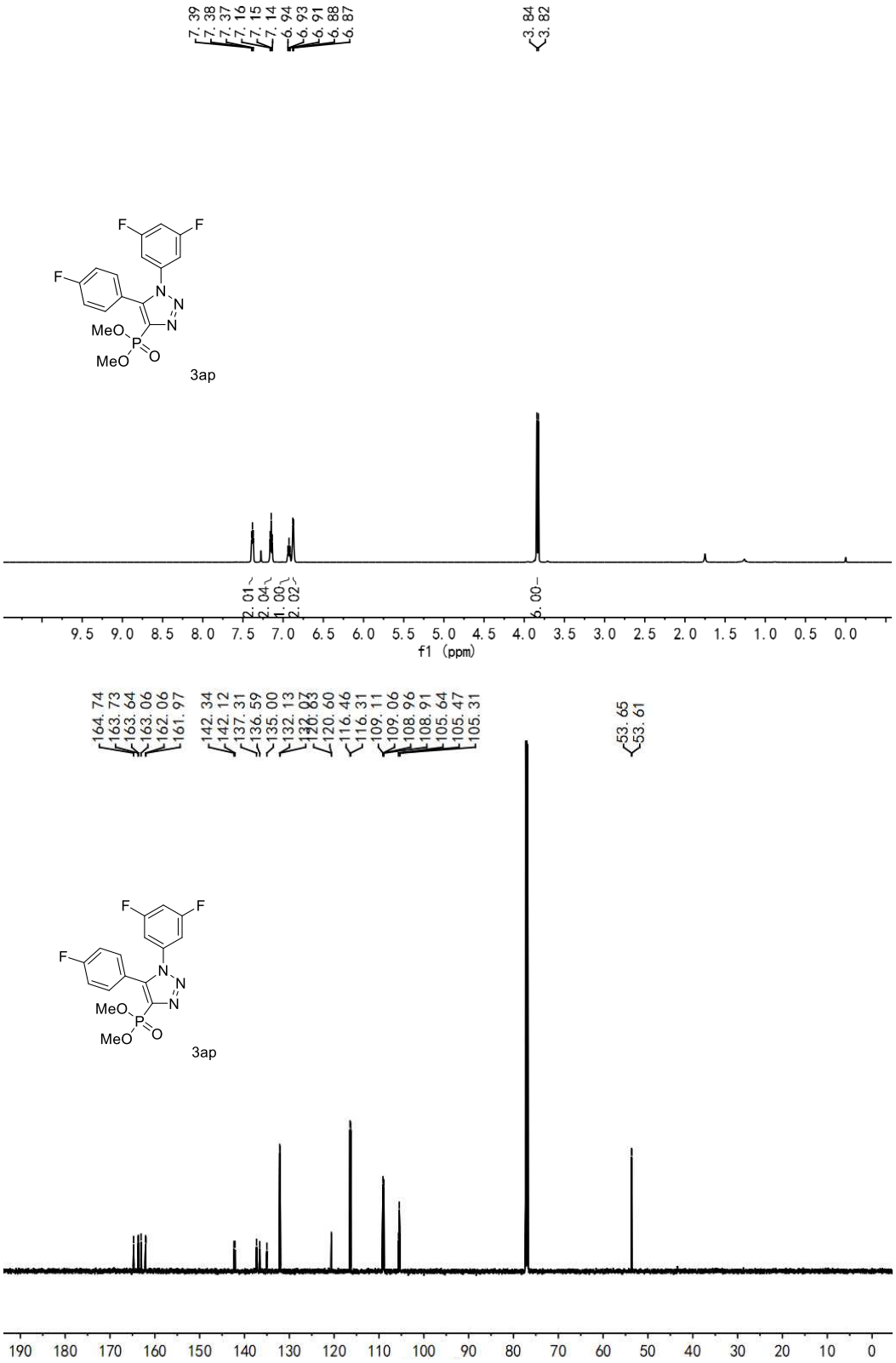
Dimethyl(5-(4-fluorophenyl)-1-(2-iodophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ao)

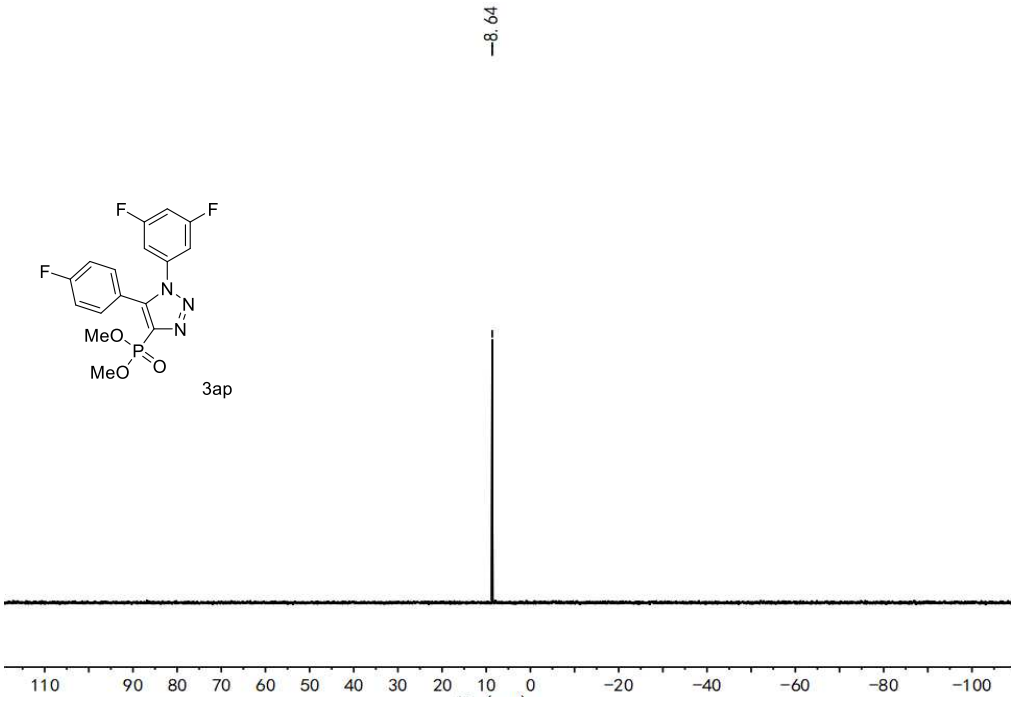



164.45
162.78
143.59
143.37
140.21
138.42
132.27
132.22
132.06
129.28
120.72
115.84
115.69
96.72
53.65
53.61
F
I
N
N
N
MeO
MeO
P
O
3ao
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

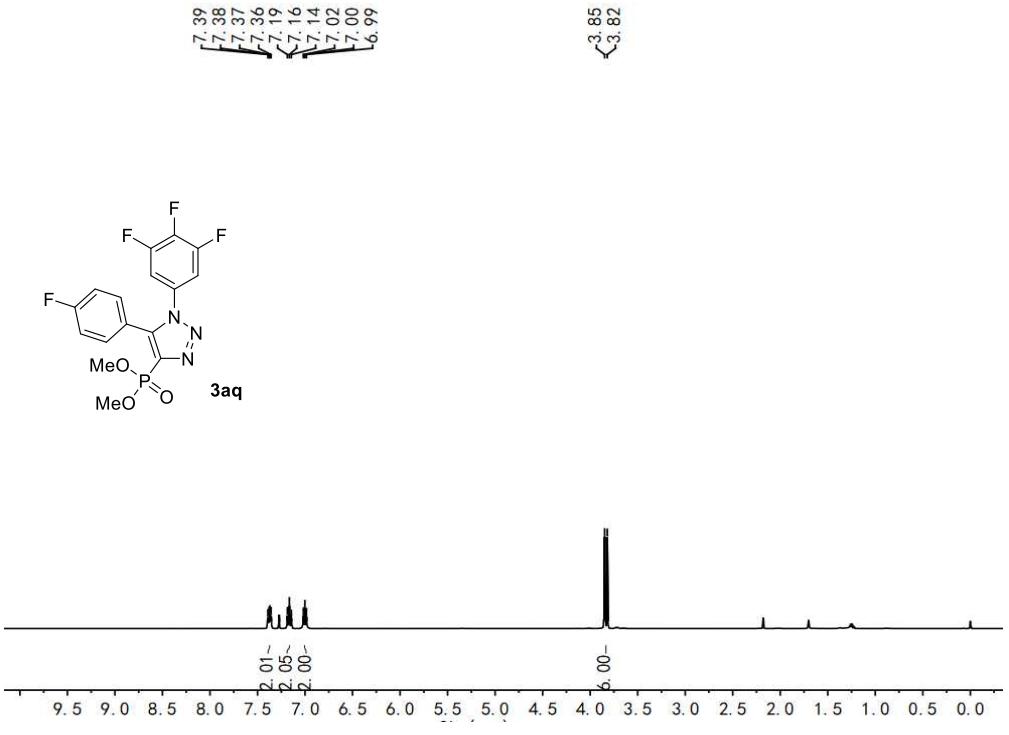

9.49
F
I
N
N
N
MeO
MeO
P
O
3ao
140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100

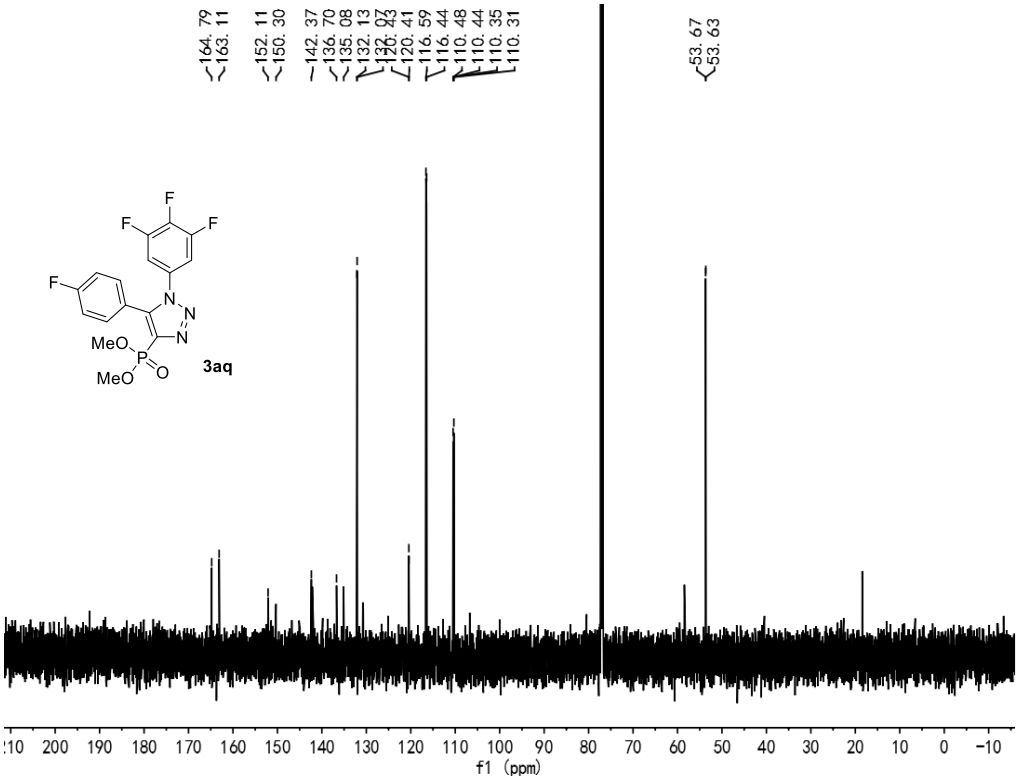
Dimethyl(1-(3,5-difluorophenyl)-5-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ap)

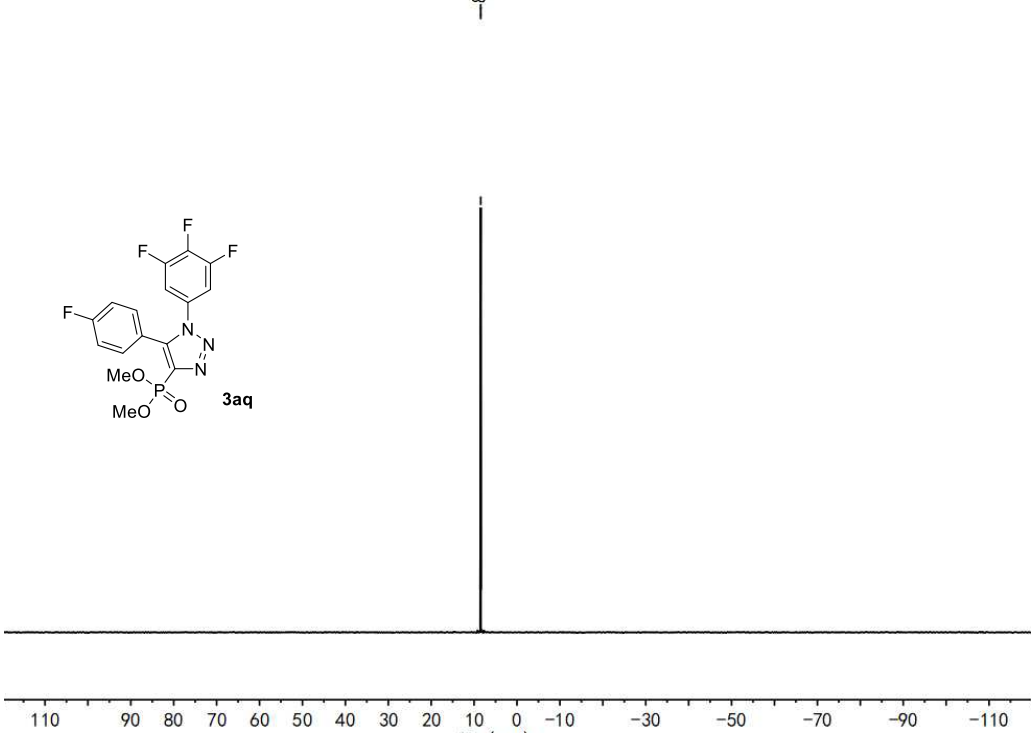




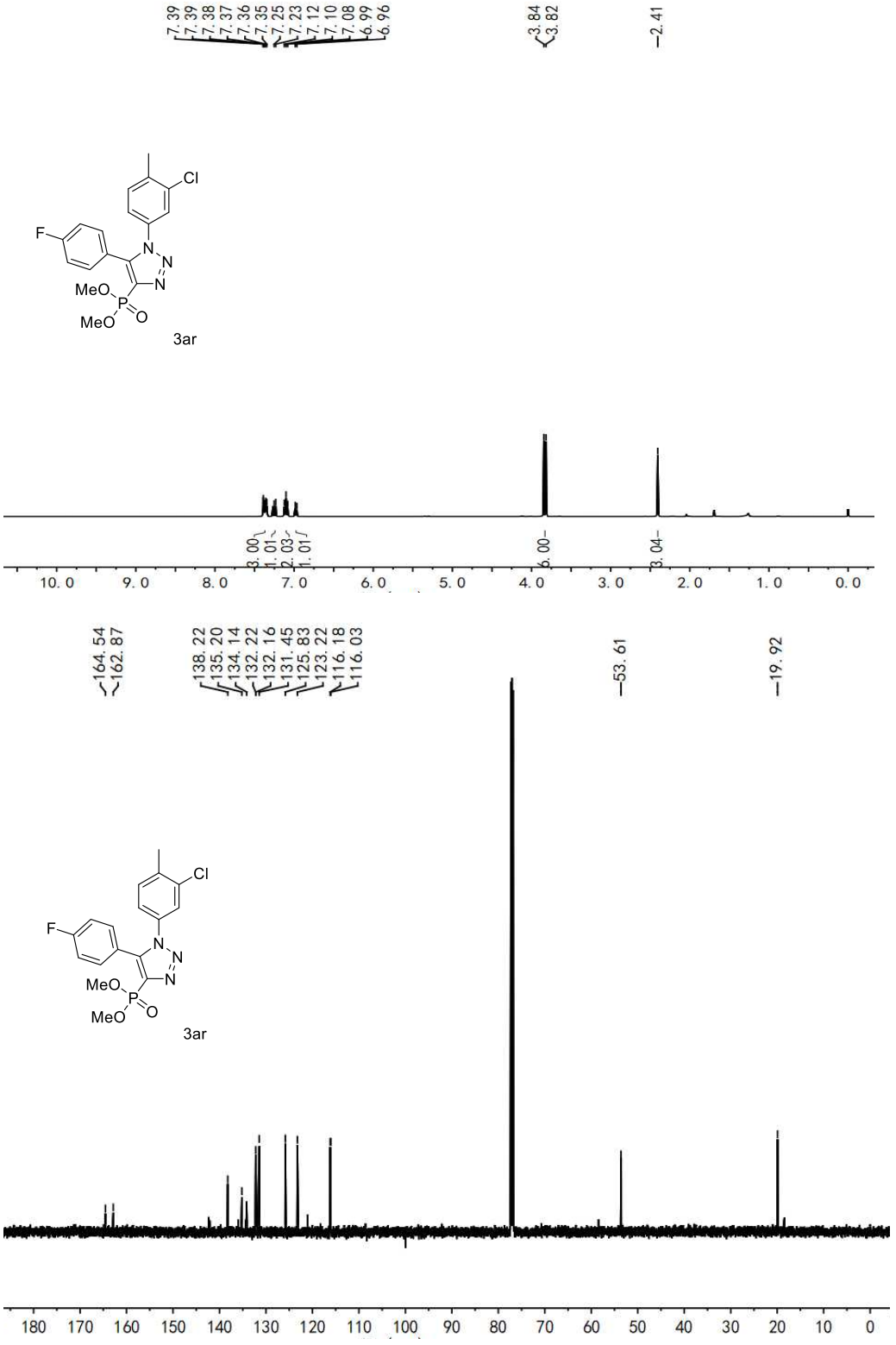
Dimethyl(5-(4-fluorophenyl)-1-(3,4,5-trifluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3aq)

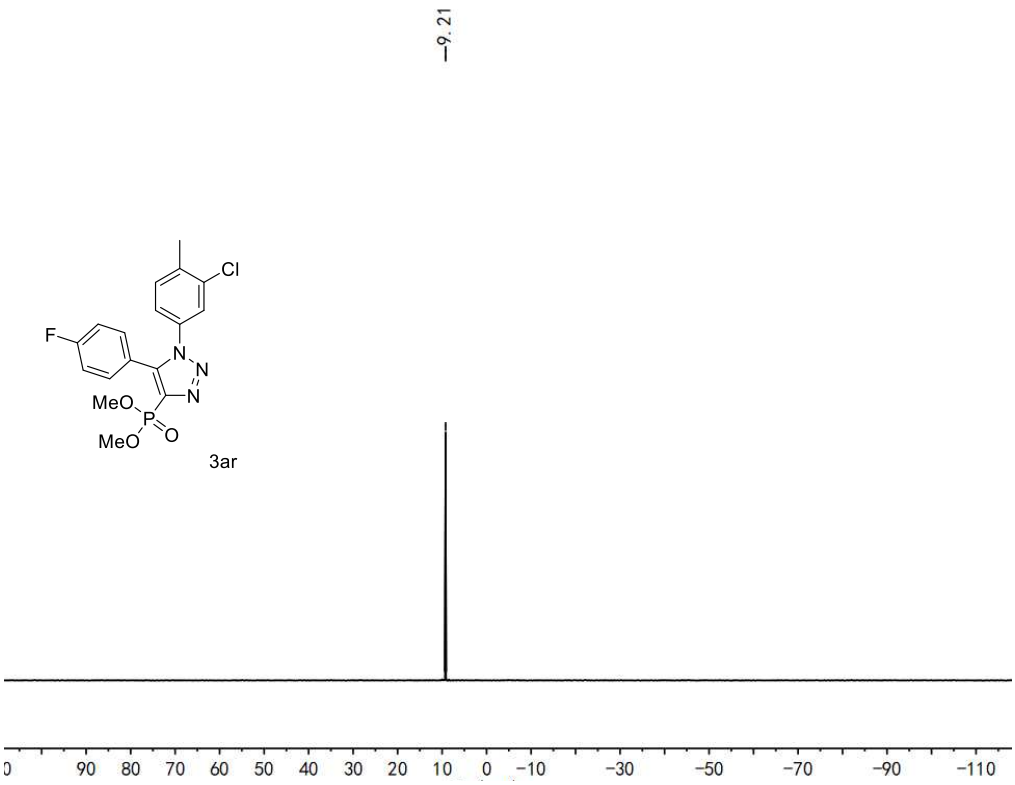



164.79
163.11
152.11
150.30
142.37
136.70
135.08
132.13
120.41
116.59
116.44
110.48
110.44
110.35
110.31
53.67
53.63
MeO
MeO
3aq
f1 (ppm)


8.45
MeO
MeO
3aq

Dimethyl(1-(3-chloro-4-methylphenyl)-5-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)phosphonate (3ar)





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