Supporting Information

Pd/Cu-Catalyzed Amide-Enabled Selectivity-Reversed Borocarbonylation of Unactivated Alkenes

Fu-Peng Wu and Xiao-Feng Wu*

Leibniz-Institut für Katalyse e.V. an der Universität Rostock, Albert-Einstein-Straße 29a, 18059 Rostock, Germany; Dalian National Laboratory for Clean Energy, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 116023, Dalian, Liaoning, China

* E-mail: xiao-feng.wu@catalysis.de

Table of Contents

1. General Information

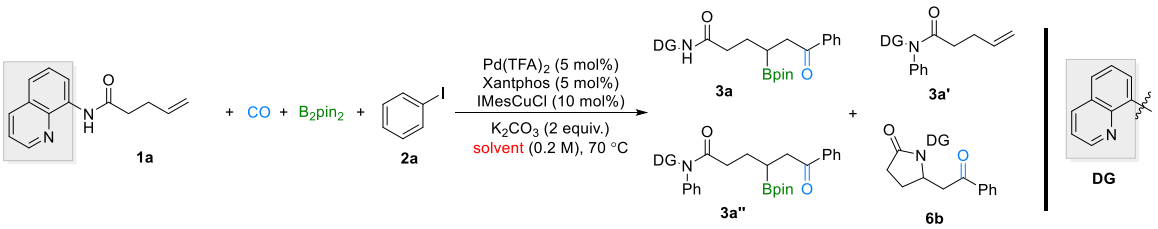
Reagents, solvents, and analytical methods:

Unless otherwise noted, all reactions were carried out under a carbon monoxide or nitrogen atmosphere. Alkenes were synthesized according to existing method. The reagents were ordered from Sigma-Aldrich, TCI, ABCR, and Acros, and used without purification. All solvents were dried by standard techniques and distilled prior to use. Column chromatography was performed on silica gel (200-300 meshes) using *N*-pentane (bp. 36.1 °C), dichloromethane and ethyl acetate as eluent. All NMR spectra were recorded at ambient temperature using Bruker Avance III HD 300 NMR (^{1}H, 300 MHz; ^{13}C{^{1}H}, 75 MHz; ^{11}B, 96 MHz), Bruker ARX 400 NMR spectrometers (^{1}H, 400 MHz; ^{13}C{^{1}H}, 101 MHz, ^{11}B 128 MHz). ^{1}H NMR chemical shifts are reported relative to TMS and were referenced via residual proton resonances of the corresponding deuterated solvent ($CDCl_3$: 7.26 ppm) whereas ^{13}C{^{1}H} NMR spectra are reported relative to TMS via the carbon signals of the deuterated solvent ($CDCl_3$: 77.0 ppm,). Data for ^{1}H are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet, br = broad), coupling constant (Hz), and integration. All ^{13}C NMR spectra were broad-band ^{1}H decoupled. However, signals for the carbon attach to boron, C(alkyl)-B, are usually too broad to observe in the ^{13}C{^{1}H} NMR spectra. Coupling constants are reported to 0.5 or 1 Hz accuracy. Gas chromatography (**GC**) analyses were performed on an Agilent HP-7890A instrument with an FID detector and HP-5 capillary column (polydimethylsiloxane with 5% phenyl groups, 30 m, 0.32 mm i.d. 0.25 μm film thickness) using argon as carrier gas. High resolution mass spectra (**HRMS**) were recorded on an Agilent 6210 system.

Because of the high toxicity of carbon monoxide, all the reactions should be performed in an autoclave. The laboratory should be well-equipped with a CO detector and alarm system.

2. Optimization of Reaction Conditions

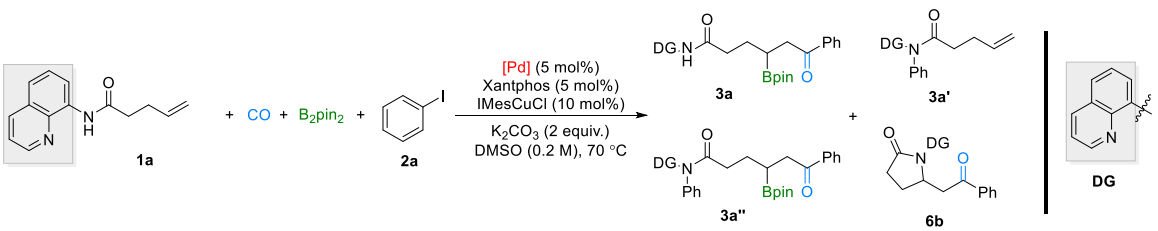
Table S1. Optimization of solvent.



Entry	solvent	**3a** (%)	**3a'** (%)	**3a''** (%)	**6b** (%)
1	Toluene	17	30	6	0
2	CH_3CN	11	9	0	0
3	THF	13	26	3	0
4	1,4-dioxane	17	30	9	0
5	DMSO	29	8	0	8
6	DCM	29	18	9	0
7	DCE	29	19	10	0
8	$CHCl_3$	24	14	18	0
9	PhCl	20	28	9	0
10	DCE/CH_3CN (4:1)	29	20	7	0
11	^{t}AmylOH	-	-	-	-
12	HFIP	-	-	-	-

Reaction conditions: *N*-(quinolin-8-yl)pent-4-enamide (0.1 mmol), iodobenzene (2.0 equiv.), B_2pin_2 (1.5 equiv.), $Pd(TFA)_2$ (5 mol%), Xantphos (5 mol%), IMesCuCl (10 mol%), K_2CO_3 (2 equiv.), CO (10 bar), solvent (0.2 M), 70 °C, 18 h. Yields were determined by ^{1}H NMR analysis of the crude reaction mixture using 1,3,5-trimethoxybenzene as internal standard. N.R. = No reaction.

Table S2. Optimization of palladium source.

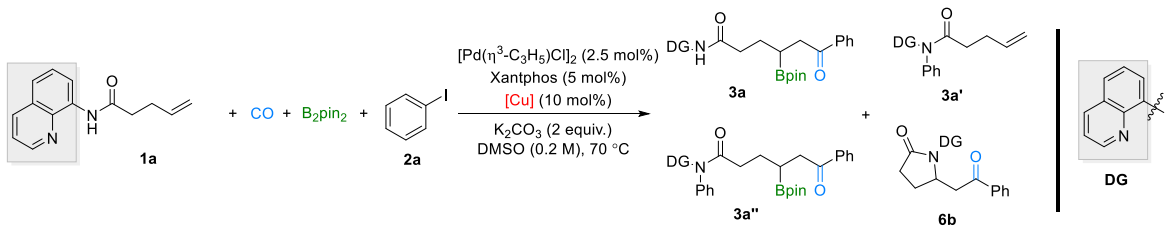


Entry	[Pd]	**3a** (%)	**3a'** (%)	**3a''** (%)	**6b** (%)
1	$Pd(TFA)_2$	29	8	0	8
2	$Pd(OAc)_2$	34	8	0	0

3	$PdCl_2$	26	8	0	8
4	Pd_2dba_3 (2.5)	25	8	0	10
5	[Pd(η-C_3H_5)Cl]$_2$ (2.5)	41	14	0	4
6	[Pd(cinnamyl)Cl]$_2$ (2.5)	36	14	0	7
7	$Pd(PPh_3)_4$	24	8	0	10

Reaction conditions: *N*-(quinolin-8-yl)pent-4-enamide (0.1 mmol), iodobenzene (2.0 equiv.), B_2pin_2 (1.5 equiv.), [Pd] (5 mol%), Xantphos (5 mol%), IMesCuCl (10 mol%), K_2CO_3 (2 equiv.), CO (10 bar), DMSO (0.2 M), 70 °C, 18 h. Yields were determined by ^{1}H NMR analysis of the crude reaction mixture using 1,3,5-trimethoxybenzene as internal standard.

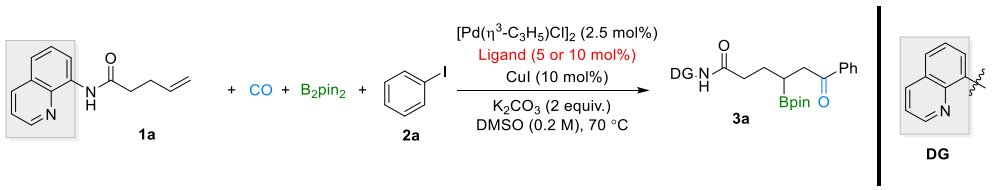
Table S3. Optimization of copper source.



Entry	[Cu]	**3a** (%)	**3a'** (%)	**3a''** (%)	**6b** (%)
1	IMesCuCl	41	14	0	4
2	IPrCuCl	-	-	-	-
3	CuCl	33	6	0	14
4	CuBr	41	12	0	6
5	CuI	50	12	0	11
6	$Cu(OTf)_2$	20	10	0	21
7	$CuCl_2$	16	6	0	5
8	$Cu(CH_3CN_4)BF_4$	42	12	0	13
9	CuBr●SMe_2	-	-	-	-

Reaction conditions: *N*-(quinolin-8-yl)pent-4-enamide (0.1 mmol), iodobenzene (2.0 equiv.), B_2pin_2 (1.5 equiv.), [Pd(η^3-C_3H_5)Cl]$_2$ (2.5 mol%), Xantphos (5 mol%), [Cu] (10 mol%), K_2CO_3 (2 equiv.), CO (10 bar), DMSO (0.2 M), 70 °C, 18 h. Yields were determined by ^{1}H NMR analysis of the crude reaction mixture using 1,3,5-trimethoxybenzene as internal standard. N.R. = No reaction.

Table S4. Optimization of ligand.



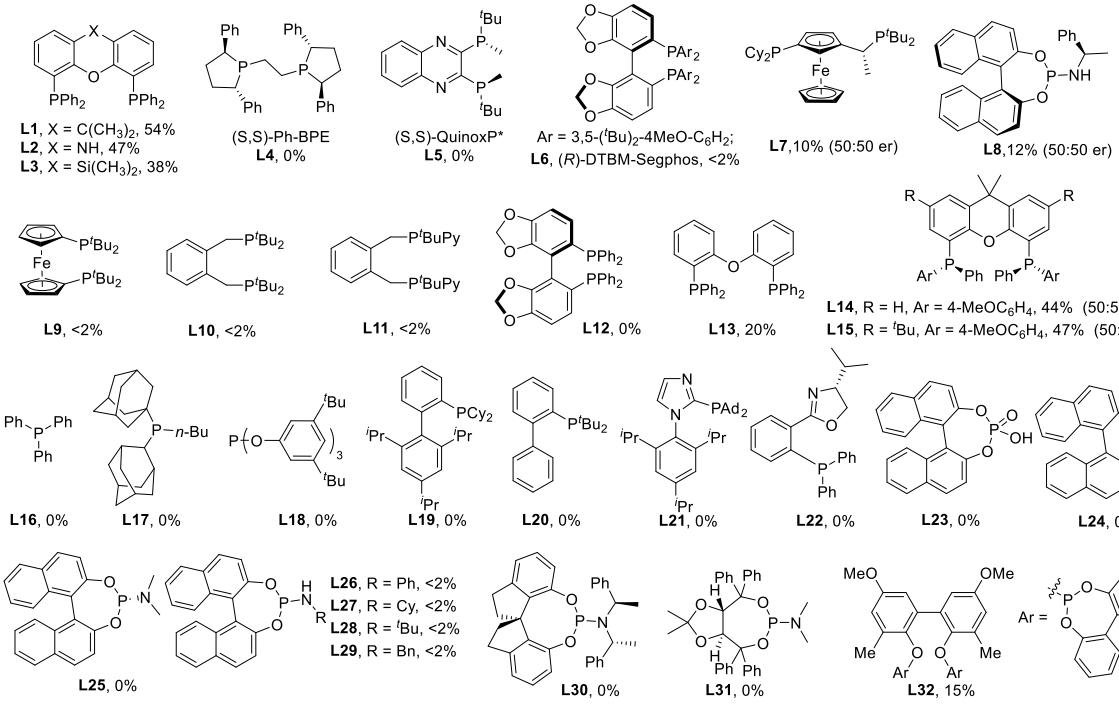
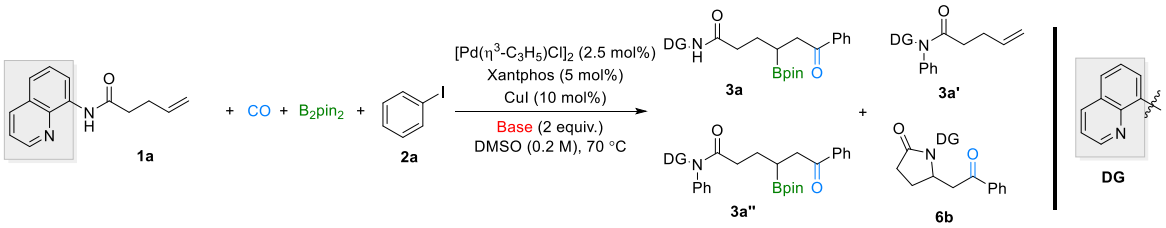


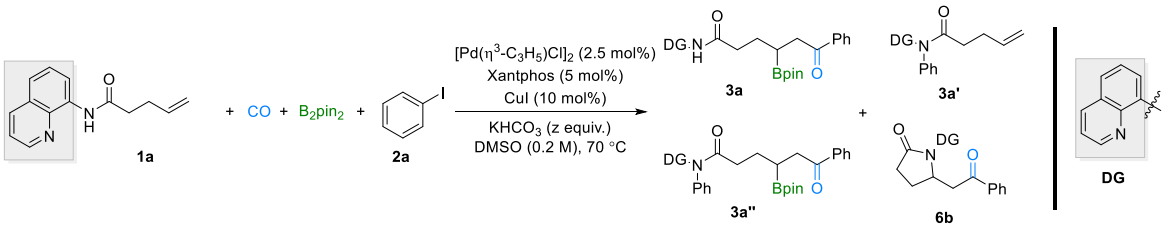
Table S5. Optimization of base.



Entry	Base	**3a** (%)	**3a'** (%)	**3a''** (%)	**6b** (%)
1	K_2CO_3	50	12	0	11
2	$KHCO_3$	58	14	0	13
3	Na_2CO_3	-	-	-	-
4	$NaHCO_3$	-	-	-	-
5	K_3PO_4	-	-	-	-
6	K_2HPO_4	26	12	0	0
7	KH_2PO_4	-	-	-	-
8	Et_3N	-	-	-	-
9	NaO^tBu	11	22	2	0
10	LiOMe	-	-	-	-
11	NaOEt	11	16	0	0
12	LiO^tBu	-	-	-	-
13	KF	-	-	-	-
14	KOAc	-	-	-	-

Reaction conditions: *N*-(quinolin-8-yl)pent-4-enamide (0.1 mmol), iodobenzene (2.0 equiv.), B_2pin_2 (1.5 equiv.), $[Pd(\eta^3\text{-}C_3H_5)Cl]_2$ (2.5 mol%), Xantphos (5 mol%), CuI (10 mol%), Base (2 equiv.), CO (10 bar), DMSO (0.2 M), 70 °C, 18 h. Yields were determined by ^1H NMR analysis of the crude reaction mixture using 1,3,5-trimethoxybenzene as internal standard.

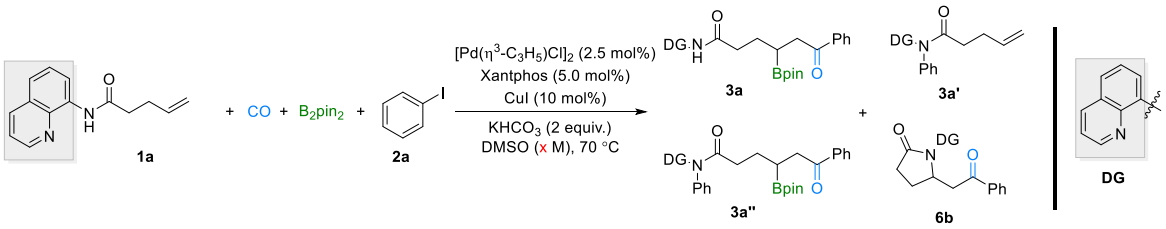
Table S6. Optimization of amount of B_2pin_2, iodobenzene and base.



Entry	B_2pin_2	**2a**	$KHCO_3$	**3a** (%)	**3a'** (%)	**3a''** (%)	**6b** (%)
1	1.5	2.0	1.5	41	12	0	10
2	1.5	2.0	2.0	58	14	0	13
3	1.5	2.0	2.5	49	18	0	5
4	1.5	2.0	3.0	50	20	0	8
5	1.5	1.5	2.0	45	16	0	6
6	1.5	1.7	2.0	49	16	0	6
7	1.5	2.0	2.0	58	14	0	13
8	1.5	2.5	2.0	51	14	0	10
9	1.5	3.0	2.0	34	16	9	10
10	1.3	2.0	2.0	43	14	0	14
11	1.5	2.0	2.0	58	14	0	13
12	1.7	2.0	2.0	49	14	0	5
13	2.0	2.0	2.0	47	16	0	2

Reaction conditions: *N*-(quinolin-8-yl)pent-4-enamide (0.1 mmol), iodobenzene (x equiv.), B_2pin_2 (y equiv.), $[Pd(\eta^3\text{-}C_3H_5)Cl]_2$ (2.5 mol%), Xantphos (5 mol%), CuI (10 mol%), $KHCO_3$ (z equiv.), CO (10 bar), DMSO (0.4 M), 70 °C, 18 h. Yields were determined by ^1H NMR analysis of the crude reaction mixture using 1,3,5-trimethoxybenzene as internal standard.

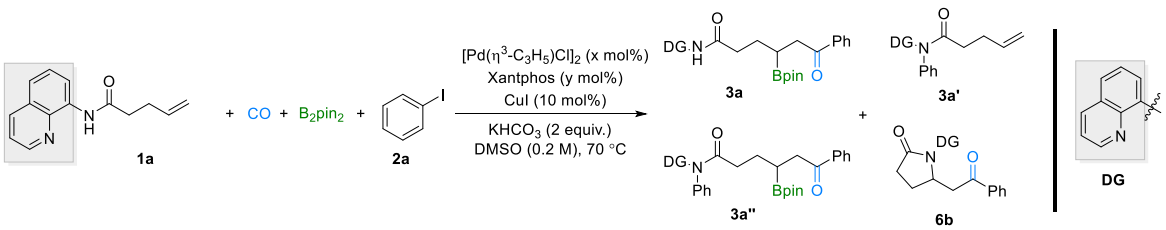
Table S7. Optimization of concentration.



Entry	DMSO (x M)	**3a** (%)	**3a'** (%)	**3a''** (%)	**6b** (%)
1	0.4 M	43	14	0	2
2	0.2 M	58	14	0	13
3	0.1 M	40	12	0	24

Reaction conditions: *N*-(quinolin-8-yl)pent-4-enamide (0.1 mmol), iodobenzene (2.0 equiv.), B_2pin_2 (1.5 equiv.), $[Pd(\eta^3\text{-}C_3H_5)Cl]_2$ (2.5 mol%), Xantphos (5.0 mol%), CuI (10 mol%), $KHCO_3$ (2 equiv.), CO (10 bar), DMSO (0.2 M), 70 °C, 18 h. Yields were determined by ^{1}H NMR analysis of the crude reaction mixture using 1,3,5-trimethoxybenzene as internal standard.

Table S8. Optimization of catalyst and ligand ratio.

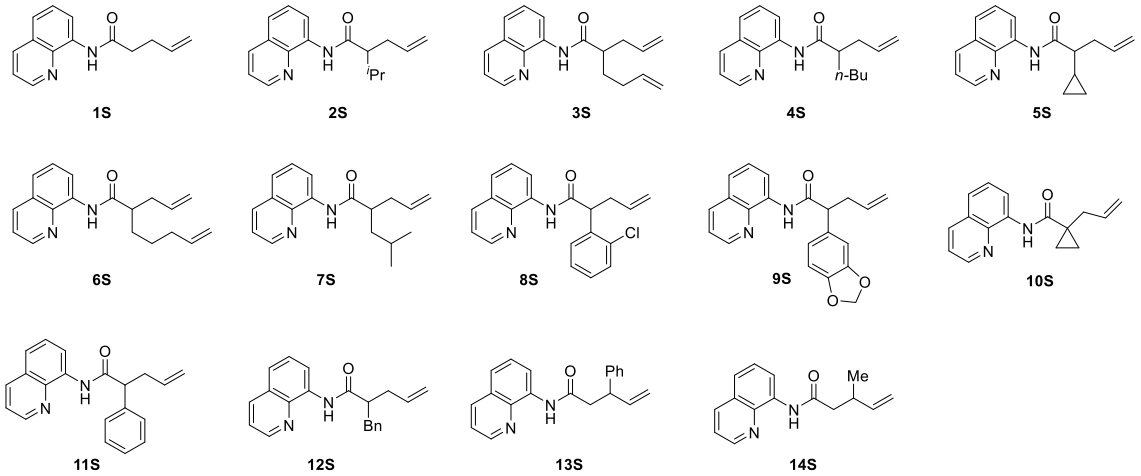


Entry	x : y	**3a** (%)	**3a'** (%)	**3a''** (%)	**6b** (%)
1	1:2	14	2	8	0
2	2:4	49	18	0	4
3	2.5:5	58	14	0	13
4	3:6	36	10	0	14
5	4:8	44	20	0	17
6	2.5:6	45	10	0	12

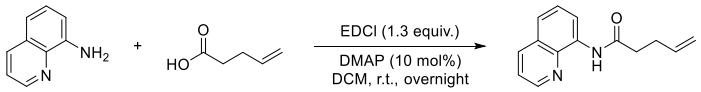
Reaction conditions: *N*-(quinolin-8-yl)pent-4-enamide (0.1 mmol), iodobenzene (2.0 equiv.), B_2pin_2 (1.5 equiv.), $[Pd(\eta^3\text{-}C_3H_5)Cl]_2$ (x mol%), Xantphos (y mol%), CuI (10 mol%), $KHCO_3$ (2 equiv.), CO (10 bar), DMSO (0.2 M), 70 °C, 18 h. Yields were determined by ^{1}H NMR analysis of the crude reaction mixture using 1,3,5-trimethoxybenzene as internal standard.

3. General Procedure for Preparing Alkene.

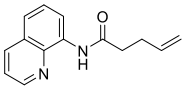
Substrate Synthesis (Yields are unoptimized)



3.1 Synthesis of substrate 1S.



Enoic acid (1.3 mmol, commercial sources) was charged into a 100 mL RB flask containing 10 mL DCM at room temperature. Aminopyridine (10 mmol), EDCI (2.5 g, 13 mmol) and DMAP (122 mg, 1 mmol) were added sequentially, and the reaction was stirred at room temperature for 16 h. The brown solution was diluted with DCM (100 mL), washed with HCl (100 mL, 0.1 mol/L), sat. $NaHCO_3$ (100 mL, ×2) and brine (100 mL, ×1), and purified by column chromatography (20% EtOAc in *n*-pentane) to afford desired amide substrates.

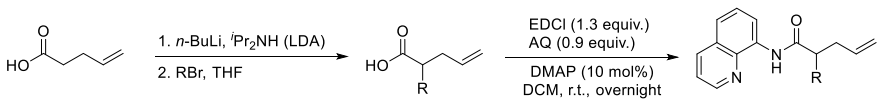


***N*-(Quinolin-8-yl)pent-4-enamide (1S)**

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.82 (s, 1H), 8.90 – 8.71 (m, 2H), 8.16 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.59 – 7.41 (m, 3H), 6.04 – 5.85 (m, 1H), 5.22 – 5.00 (m, 2H), 2.71 – 2.47 (m, 4H).

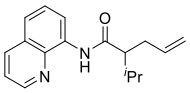
^{13}C NMR (75 MHz, $CDCl_3$) δ 170.9, 148.1, 138.3, 136.9, 136.4, 134.5, 127.9, 127.4, 121.6, 121.4, 116.5, 115.7, 37.3, 29.5.

3.2 Synthesis of substrate 2S-7S.



n-BuLi (4.1 mL, 2.7 M in toluene 11 mmol) was added dropwise to a cold (0 °C) solution of ^{i}Pr$_2$NH (1.54 mL, 5.05 mmol) in THF (10 mL), and the mixture was stirred for 30 min. Then, a solution of pent-4-enoic acid (5 mmol) in THF (10 mL) was added dropwise over 20 min and stirring was continued for another 30 min at the same temperature. Alkyl bromide (6.5 mmol) was added, and the stirring was continued for another 6 h. The solvent was removed under reduced pressure. The resulting residue was diluted with water (50 mL) and extracted with ethyl acetate (50 mL). pH of the separated aqueous layer was adjusted to 2 by HCl (6 M) and then extracted with

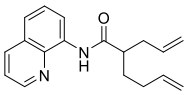
ethyl acetate. The combined organic layers were washed with brine, dried with Na_2SO_4, and filtered. The solvent was evaporated, and the crude acid was taken forward to the next step without further purification. The crude acid (~2-5 mmol) was charged into a 100 mL RB flask containing 10 mL DCM. 8-Aminoquinoline (0.9 equiv), EDCl (1.3 equiv) and DMAP (0.1 equiv) were added sequentially, and the reaction was stirred at room temperature for 16 h. The brown solution was diluted with DCM (100 mL), washed with HCl (100 mL, 0.1 mol/L), sat. $NaHCO_3$ (100 mL, ×2) and brine (100 mL, ×1), and purified by column chromatography (20% EtOAc in *n*-pentane) to afford desired amide substrates.



2-Isopropyl-*N*-(quinolin-8-yl)pent-4-enamide (2S)

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.80 (s, 1H), 8.93 – 8.70 (m, 2H), 8.14 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.59 – 7.38 (m, 3H), 5.87 (ddt, *J* = 17.0, 10.0, 7.0 Hz, 1H), 5.19 – 5.06 (m, 1H), 4.98 (ddt, *J* = 10.0, 2.0, 1.0 Hz, 1H), 2.64 – 2.37 (m, 2H), 2.30 (ddd, *J* = 10.0, 7.5, 4.2 Hz, 1H), 2.06 (dp, *J* = 8.0, 6.5 Hz, 1H), 1.06 (dd, *J* = 8.5, 6.5 Hz, 6H).

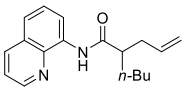
^{13}C NMR (75 MHz, $CDCl_3$) δ 173.4, 148.1, 138.4, 136.3, 136.0, 134.4, 127.9, 127.4, 121.5, 121.3, 116.6, 116.4, 56.1, 34.5, 30.8, 20.7, 20.4.



2-Allyl-*N*-(quinolin-8-yl)hex-5-enamide (3S)

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.85 (s, 1H), 8.89 – 8.73 (m, 2H), 8.10 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.57 – 7.37 (m, 3H), 5.95 – 5.68 (m, 2H), 5.20 – 4.92 (m, 4H), 2.66 – 2.30 (m, 3H), 2.26 – 2.07 (m, 2H), 2.01 – 1.84 (m, 1H), 1.69 (dddd, *J* = 13.5, 9.0, 7.0, 4.5 Hz, 1H).

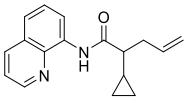
^{13}C NMR (75 MHz, $CDCl_3$) δ 173.6, 148.0, 138.3, 137.7, 136.1, 135.4, 134.2, 127.8, 127.2, 121.4, 121.3, 116.9, 116.3, 115.3, 47.9, 37.1, 31.4.



2-Allyl-*N*-(quinolin-8-yl)hexanamide (4S)

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.84 (s, 1H), 8.90 – 8.73 (m, 2H), 8.14 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.58 – 7.40 (m, 3H), 5.87 (dddd, *J* = 17.0, 10.0, 7.0, 6.5 Hz, 1H), 5.21 – 4.94 (m, 2H), 2.55 (dtdd, *J* = 11.0, 8.0, 6.0, 4.5 Hz, 2H), 2.37 (tdt, *J* = 8.0, 5.5, 1.5 Hz, 1H), 1.87 – 1.72 (m, 1H), 1.68 – 1.55 (m, 1H), 1.46 – 1.29 (m, 4H), 0.93 – 0.82 (m, 3H).

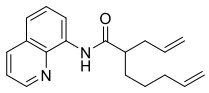
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.0, 148.1, 138.3, 136.2, 135.7, 134.4, 127.8, 127.3, 121.5, 121.3, 116.8, 116.4, 48.9, 37.2, 32.2, 29.6, 22.7, 13.9.



2-Cyclopropyl-*N*-(quinolin-8-yl)pent-4-enamide (5S)

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.06 (s, 1H), 8.84 – 8.64 (m, 2H), 8.06 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.52 – 7.26 (m, 3H), 5.86 (ddt, *J* = 17.0, 10.0, 7.0 Hz, 1H), 5.13 – 4.85 (m, 2H), 2.69 – 2.40 (m, 2H), 1.74 (ddd, *J* = 10.0, 7.5, 6.0 Hz, 1H), 1.15 – 1.00 (m, 1H), 0.68 – 0.52 (m, 2H), 0.45 – 0.34 (m, 1H), 0.23 (ddd, *J* = 9.5, 5.0, 1.5 Hz, 1H).

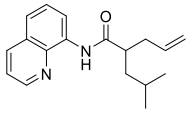
^{13}C NMR (75 MHz, $CDCl_3$) δ 173.2, 148.1, 138.5, 136.2, 135.8, 134.6, 127.9, 127.4, 121.5, 121.3, 116.7, 116.4, 53.5, 36.8, 13.5, 4.9, 4.3.



2-Allyl-*N*-(quinolin-8-yl)hept-6-enamide (6S)

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.85 (s, 1H), 8.88 – 8.74 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.57 – 7.41 (m, 3H), 5.95 – 5.69 (m, 2H), 5.19 – 4.88 (m, 4H), 2.56 (dddd, *J* = 9.5, 8.0, 6.5, 4.0 Hz, 2H), 2.43 – 2.29 (m, 1H), 2.16 – 2.04 (m, 2H), 1.90 – 1.74 (m, 1H), 1.70 – 1.57 (m, 1H), 1.57 – 1.42 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 173.9, 148.1, 138.4, 136.3, 135.6, 134.4, 127.9, 127.4, 121.5, 121.4, 116.9, 116.5, 114.7, 48.8, 37.2, 33.7, 32.0, 26.7.

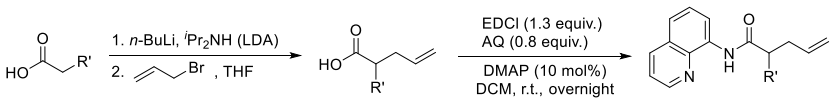


2-Isobutyl-*N*-(quinolin-8-yl)pent-4-enamide (7S)

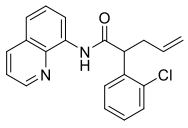
^{1}H NMR (300 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.87 – 8.71 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.61 – 7.37 (m, 3H), 5.87 (dddd, *J* = 16.5, 10.0, 7.5, 6.5 Hz, 1H), 5.19 – 4.97 (m, 2H), 2.70 – 2.47 (m, 2H), 2.33 (dddt, *J* = 14.0, 7.0, 6.0, 1.0 Hz, 1H), 1.87 – 1.62 (m, 2H), 1.40 (ddd, *J* = 13.0, 8.5, 5.0 Hz, 1H), 0.98 (d, *J* = 6.5 Hz, 3H), 0.93 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 174.1, 148.2, 138.4, 136.3, 135.7, 134.4, 127.9, 127.4, 121.5, 121.3, 116.9, 116.4, 46.9, 41.7, 37.7, 26.0, 23.3, 22.2.

3.3 Synthesis of substrate 8S-12S.



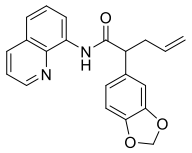
n-BuLi (4.1 mL, 2.7 M in toluene 11 mmol) was added dropwise to a cold (0 °C) solution of $^{i}Pr_2NH$ (1.54 mL, 5.05 mmol) in THF (10 mL), and the mixture was stirred for 30 min. Then, a solution of carboxylic caid (5 mmol) in THF (10 mL) was added dropwise over 20 min and stirring was continued for another 30 min at the same temperature. Ally bromide (6.5 mmol) was added, and the stirring was continued for another 6 h. The solvent was removed under reduced pressure. The resulting residue was diluted with water (50 mL) and extracted with ethyl acetate (50 mL). pH of the separated aqueous layer was adjusted to 2 by HCl (6 M) and then extracted with ethyl acetate. The combined organic layers were washed with brine, dried with Na_2SO_4, and filtered. The solvent was evaporated, and the crude acid was taken forward to the next step without further purification. The crude acid (~2-5 mmol) was charged into a 100 mL RB flask containing 10 mL DCM. 8-Aminoquinoline (0.9 equiv), EDCI (1.3 equiv) and DMAP (0.1 equiv) were added sequentially, and the reaction was stirred at room temperature for 16 h. The brown solution was diluted with DCM (100 mL), washed with HCl (100 mL, 0.1 mol/L), sat. $NaHCO_3$ (100 mL, ×2) and brine (100 mL, ×1), and purified by column chromatography (20% EtOAc in *n*-pentane) to afford desired amide substrates.



2-(2-Chlorophenyl)-*N*-(quinolin-8-yl)pent-4-enamide (8S)

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.11 (s, 1H), 8.82 (dd, *J* = 7.5, 1.5 Hz, 1H), 8.71 (dd, *J* = 4.5, 1.5 Hz, 1H), 7.99 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.68 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.50 – 7.35 (m, 3H), 7.29 (ddd, *J* = 7.5, 4.5, 3.0 Hz, 2H), 7.19 (td, *J* = 7.5, 1.5 Hz, 1H), 5.92 (ddt, *J* = 17.0, 10.0, 7.0 Hz, 1H), 5.35 – 4.93 (m, 2H), 4.53 (dd, *J* = 8.0, 7.0 Hz, 1H), 3.15 (dddt, *J* = 14.5, 8.0, 6.5, 1.5 Hz, 1H), 2.74 (dtt, *J* = 14.0, 7.0, 1.5 Hz, 1H).

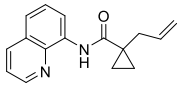
^{13}C NMR (75 MHz, $CDCl_3$) δ 170.1, 147.9, 138.0, 136.6, 135.8, 135.0, 134.2, 133.7, 129.4, 128.6, 128.3, 127.5, 127.2, 126.9, 121.4, 121.3, 117.1, 116.1, 49.4, 36.3.



2-(Benzo[d][1,3]dioxol-5-yl)-*N*-(quinolin-8-yl)pent-4-enamide (9S)

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.90 (s, 1H), 8.78 – 8.73 (m, 2H), 8.12 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.56 – 7.45 (m, 2H), 7.42 (dd, *J* = 8.5, 4.0 Hz, 1H), 7.04 – 6.87 (m, 2H), 6.80 (dd, *J* = 8.0, 0.5 Hz, 1H), 5.95 – 5.91 (m, 2H), 5.81 (ddt, *J* = 17.0, 10.0, 7.0 Hz, 1H), 5.20 – 4.96 (m, 2H), 3.73 (t, *J* = 7.5 Hz, 1H), 3.06 – 2.96 (m, 1H), 2.70 – 2.56 (m, 1H).

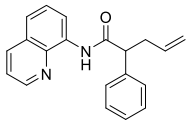
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.4, 148.1, 148.0, 146.9, 138.4, 136.2, 135.6, 134.4, 133.1, 127.8, 127.3, 121.5, 121.5, 121.4, 117.0, 116.3, 108.4, 108.2, 101.0, 54.2, 37.5.



1-Allyl-*N*-(quinolin-8-yl)cyclopropane-1-carboxamide (10S)

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.36 (s, 1H), 8.81 (dd, *J* = 4.0, 1.5 Hz, 1H), 8.76 (dd, *J* = 7.0, 2.0 Hz, 1H), 8.14 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.55 – 7.48 (m, 2H), 7.44 (dd, *J* = 8.5, 4.0 Hz, 1H), 5.99 (ddt, *J* = 17.0, 10.0, 6.5 Hz, 1H), 5.46 (dq, *J* = 17.0, 1.5 Hz, 1H), 5.19 (dt, *J* = 10.5, 1.5 Hz, 1H), 2.64 (dt, *J* = 6.5, 1.5 Hz, 2H), 1.44 – 1.39 (m, 2H), 0.86 – 0.80 (m, 2H).

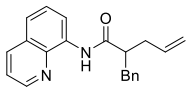
^{13}C NMR (75 MHz, $CDCl_3$) δ 172.7, 148.0, 138.7, 136.2, 134.9, 134.7, 127.9, 127.4, 121.5, 121.1, 117.9, 116.2, 38.2, 24.8, 15.3.



2-Phenyl-*N*-(quinolin-8-yl)pent-4-enamide (11S)

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.93 (s, 1H), 8.79 (dd, *J* = 7.5, 2.0 Hz, 1H), 8.72 (dd, *J* = 4.0, 1.5 Hz, 1H), 8.08 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.57 – 7.43 (m, 4H), 7.43 – 7.24 (m, 4H), 5.85 (ddt, *J* = 17.0, 10.0, 7.0 Hz, 1H), 5.24 – 4.97 (m, 2H), 3.83 (t, *J* = 7.5 Hz, 1H), 3.21 – 3.00 (m, 1H), 2.80 – 2.61 (m, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.3, 148.0, 139.2, 138.3, 136.1, 135.6, 134.4, 128.8, 128.0, 127.7, 127.3, 127.2, 121.4, 121.4, 116.9, 116.2, 54.6, 37.5.



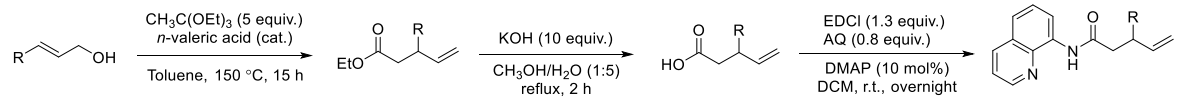
2-Benzyl-N-(quinolin-8-yl)pent-4-enamide (12S)

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.88 (dd, *J* = 7.5, 1.5 Hz, 1H), 8.72 (dd, *J* = 4.0, 1.5 Hz, 1H), 8.02 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.55 – 7.47 (m, 1H), 7.42 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.37 – 7.23 (m, 5H), 7.19 – 7.11 (m,

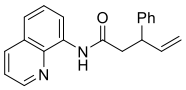
1H), 5.95 (ddt, *J* = 17.0, 10.0, 7.0 Hz, 1H), 5.27 – 5.06 (m, 2H), 3.28 – 3.15 (m, 1H), 3.02 – 2.87 (m, 2H), 2.73 – 2.61 (m, 1H), 2.53 – 2.41 (m, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.7, 147.7, 139.2, 138.0, 135.8, 135.1, 134.0, 128.7, 128.2, 127.5, 127.0, 126.1, 121.2, 121.2, 117.2, 116.2, 50.5, 38.3, 36.6.

3.4 Synthesis of substrate 13S and 14S.



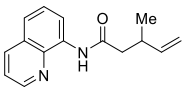
To the mixture of allyl alcohol (10 mmol) and triethyl orthoacetate (9.2 mL, 50 mmol) in toluene (30 mL) was added n-valeric acid (cat.). The mixture was heated at 150 °C for 15 h. The mixture was cooled and concentrated under reduced pressure. The crude product was dissolved in methanol (5 mL), and a solution of potassium hydroxide (100 mmol) in water (25 mL) was added. The mixture was refluxed for 2 h. After cooling, the solution was washed with ethyl ether and acidified with concentrated HCl to pH 2. The acidic solution was extracted with ethyl acetate (3 × 20 mL), and combined organic phases were dried over Na_2SO_4, filtered, and concentrated under a vacuum. The crude acid was taken forward to the next step without further purification. The crude acid (~4mmol) was charged into a 100 mL RB flask containing 10 mL DCM. 8-Aminoquinoline (0.65 g, 4.5 mmol), EDCI (1.24 g, 6.5 mmol) and DMAP (61 mg, 0.5 mmol) were added sequentially, and the reaction was stirred at room temperature for 16 h. The brown solution was diluted with DCM (100 mL), washed with HCl (100 mL, 0.1 mol/L), sat. $NaHCO_3$ (100 mL, ×2) and brine (100 mL, ×1), and purified by column chromatography (20% EtOAc in *n*-pentane) to afford the desired product.



3-Phenyl-*N*-(quinolin-8-yl)pent-4-enamide (13S)

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.82 (s, 1H), 8.83 (dd, *J* = 7.5, 1.5 Hz, 1H), 8.77 (dd, *J* = 4.0, 1.5 Hz, 1H), 8.07 (dt, *J* = 8.5, 1.5 Hz, 1H), 7.54 – 7.42 (m, 2H), 7.40 – 7.30 (m, 5H), 7.29 – 7.20 (m, 1H), 6.15 (ddd, *J* = 17.0, 10.5, 7.0 Hz, 1H), 5.27 – 5.11 (m, 2H), 4.24 – 4.11 (m, 1H), 3.11 – 2.89 (m, 2H).

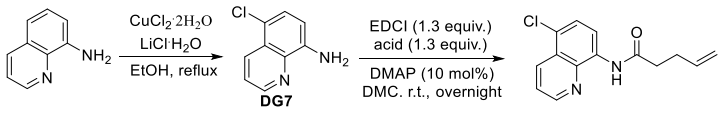
^{13}C NMR (75 MHz, $CDCl_3$) δ 169.3, 147.8, 142.5, 140.2, 138.0, 136.0, 134.1, 128.4, 127.6, 127.4, 127.0, 126.4, 121.3, 121.2, 116.2, 114.9, 45.6, 43.7.



3-Methyl-*N*-(quinolin-8-yl)pent-4-enamide (14S)

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.80 (s, 1H), 8.85 – 8.75 (m, 2H), 8.14 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.60 – 7.41 (m, 3H), 5.90 (ddd, *J* = 17.0, 10.5, 7.0 Hz, 1H), 5.18 – 4.93 (m, 2H), 2.89 (dq, *J* = 13.5, 7.0 Hz, 1H), 2.70 – 2.40 (m, 2H), 1.17 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.4, 148.1, 142.6, 138.3, 136.3, 134.4, 127.9, 127.4, 121.5, 121.4, 116.4, 113.6, 45.2, 34.8, 19.7.



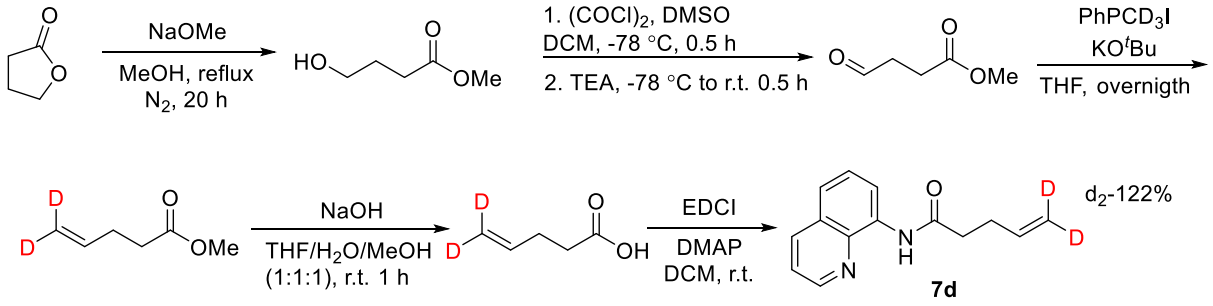
A round-bottomed flask (25 mL) was charged with substrate (720 mg, 5 mmol), $CuCl_2 \cdot 2H_2O$ (2.5 g, 6 mmol), $LiCl \cdot H_2O$ (0.3 g, 2 mmol) and EtOH (10 mL). The resulting reaction mixture was stirred at reflux. After the completion of the reaction monitored by TLC, EtOH was removed under reduced pressure. Then ammonium hydroxide (10 mL, 25% w/w) and water (10 mL) were added, and the aqueous phase was extracted with EA (30 mL). The combined organic phase was washed with brine (30 mL) and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure. The crude mixture was purified by chromatography on silica gel to obtain the desired 5-chloroquinolin-8-amine (220 mg, 25% yield, yellow solid).

The pent-4-enoic acid (111uL, 1.1 mmol) was charged into a 50 mL RB flask containing 10 mL DCM. 5-Chloroquinolin-8-amine (142 mg, 0.8 mmol), EDCI (256 mg, 1.1 mmol) and DMAP (15.2 mg, 0.11 mmol) were added sequentially, and the reaction was stirred at room temperature for 16 h. The yellow solution was diluted with DCM (50 mL), washed with HCl (20 mL, 0.1 mol/L), sat. $NaHCO_3$ (50 mL, ×2) and brine (50 mL, ×1), and purified by column chromatography (20% EtOAc in *n*-pentane) to afford the desired product **16S** (130 mg, 63% yield, white sold).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.82 (dd, *J* = 4.0, 1.5 Hz, 1H), 8.71 (d, *J* = 8.5 Hz, 1H), 8.54 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.65 – 7.45 (m, 2H), 5.92 (ddt, *J* = 17.0, 10.5, 6.5 Hz, 1H), 5.15 (dq, *J* = 17.0, 1.5 Hz, 1H), 5.05 (dq, *J* = 10.5, 1.5 Hz, 1H), 2.66 (ddd, *J* = 8.0, 6.5, 1.5 Hz, 2H), 2.56 (qq, *J* = 6.5, 1.5 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 148.5, 138.8, 136.7, 133.7, 133.4, 127.2, 125.8, 124.1, 122.2, 116.3, 115.8, 37.2, 29.3.

3.5 Procedure for synthesis of *d2-N*-(quinolin-8-yl)pent-4-enamide (*d*$_2$-7d)[3]



Lactone cleavage.[4]

To the 0.5 M NaOMe solution in MeOH (4.0 mL, 2.0 mmol) diluted with MeOH (16.0 mL, 1.0 M) was added γ-butyrolactone (1.72 g, 20.0 mmol). The reaction mixture was heated at reflux for 20 h. The reaction mixture was monitored by TLC using DCM/pentane as the mobile phase. After disappearance of starting material, the reaction mixture was diluted with Et_2O (50 mL), filtered off through a pad of celite and silica. After washing with Et_2O, the filtrate was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (DCM/pentane) to give methyl 4-hydroxybutanoate as pale yellow oil (1.45 g, 52%).

Alcohol oxidation.[4]

To a solution of oxalyl chloride (1.1 mL, 13.5 mmol) in DCM (30 mL, 0.3 M) was added DMSO (1.95 mL, 26.9 mmol) dropwisely at -78 oC under argon atmosphere. After stirring for 30 min at -78 oC, the solution of 4-hydroxybutanoate (1.45 g, 12.3 mmol) in DCM (12 mL) was added to the reaction mixture, and resulting mixture

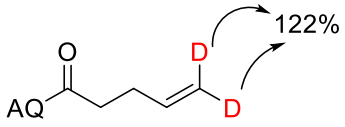
was stirred at -78 °C for 30 min. Triethylamine (8.5 mL, 61.0 mmol) was added, and the mixture could warm to room temperature gradually and stirred for 30 min. The reaction mixture was monitored by TLC using EA/penatene = 1:1 as the mobile phase. After disappearance of starting material, the reaction mixture was quenched with distilled water (50 mL) and extracted with DCM (3×50 mL). The combined organic layer was washed with aqueous NH_4Cl (2×100 mL) and brine and dried over $MgSO_4$ and concentrated under reduced pressure to give methyl 4-oxobutanoate as pale-yellow oil (1.43, quant.). The residue was used in the next step without further purification.

Wittig reaction[5]

In an oven dried flask, methyl d_2-triphenylphosphonium iodide (0.91 g, 1.2 equiv.) was taken and to this abs. THF (1.6 mL/mmol) was added. The suspension was cooled to 0 °C, *t*-BuOK (0.4 g, 1.2 equiv.) was added and the resulting yellow suspension was stirred at 0 °C for 45 min. To this suspension, a solution of methyl 4-oxobutanoate (3 mmol) in THF (0.7 mL/mmol) was added dropwise and the resulting mixture was warmed gradually to rt. and stirred at rt for 16 h. Reaction mixture was concentrated under reduced pressure and filtered over Celite®. The filtrate was concentrated under reduced pressure to afford yellow oil. The residue was used in the next step without further purification.

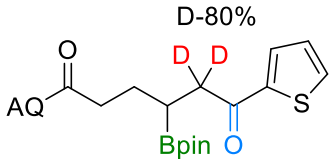
Ester hydrolysis and amide bond formation (***d2***-7d)

To a solution of methyl pent-4-enoate-5,5-d_2 (~115 mg, ~1.0 mmol) in THF/H_2O/MeOH = 1:1:1 (2.0 mL, 1.0 M) was added lithium hydroxide monohydrate (83.5 mg, 2.0 mmol). The reaction mixture was stirred at room temperature for 1 h. The reaction mixture was monitored by TLC using EA/pentane = 1:3 as the mobile phase. After disappearance of starting material, the reaction mixture was diluted with distilled water (25 mL) and extracted with EA (3×25 mL). The aqueous layer was acidified with 2 M HCl at 0 °C and extracted with EA (3×25 mL). The combined organic layer was dried over $MgSO_4$ and concentrated under reduced pressure to give pent-4-enoic-5,5-d_2 acid as pale-yellow oil (~1 mmol). The residue was used in the next step without further purification. The crude acid (~1 mmol) was charged into a 100 mL RB flask containing 10 mL DCM. 8-Aminoquinoline (187 mg, 1.3 mmol), EDCl (24.8 g, 1.3 mmol) and DMAP (15 mg, 0.1 mmol) were added sequentially, and the reaction was stirred at room temperature for 16 h. The brown solution was diluted with DCM (100 mL), washed with HCl (30 mL, 0.1 mol/L), sat. $NaHCO_3$ (30 mL×2) and brine (30 mL×1), and purified by column chromatography (20% EtOAc in *n*-pentane) to afford the desired product.



7d

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.82 (s, 1H), 8.85 – 8.75 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.57 – 7.41 (m, 3H), 6.00 – 5.87 (m, 1H), 5.19 – 5.11 (m, 0.39H), 5.09 – 5.00 (m, 0.39H), 2.67 (ddd, *J* = 8.0, 6.5, 1.5 Hz, 1.84H), 2.62 – 2.53 (m, 1.88H).



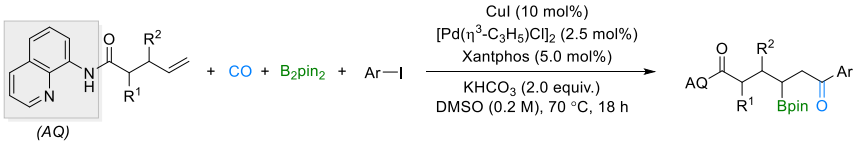
***d*$_2$-6-Oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(thiophen-2-yl)hexanamide (7e)**

Pentane/EA = 3:1 (Rf = 0.35), yellow oil (25.0 mg, 54% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.89 – 8.67 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.72 (dd, *J* = 3.8, 1.1 Hz, 1H), 7.58 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.56 – 7.46 (m, 2H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.09 (dd, *J* = 5.0, 3.8 Hz, 1H), 3.18 – 3.13 (m, 1.2H), 2.74 – 2.59 (m, 1.82H), 2.10 – 1.85 (m, 2H), 1.52 (td, *J* = 8.2, 7.3, 5.1 Hz, 1H), 1.28 (d, *J* = 3.8 Hz, 12H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.9, 171.7, 148.0, 144.0, 138.4, 136.3, 134.6, 133.1, 131.8, 127.9, 127.9, 127.4, 121.5, 121.3, 116.4, 83.3, 41.4, 37.6, 26.6, 24.8, 24.8.

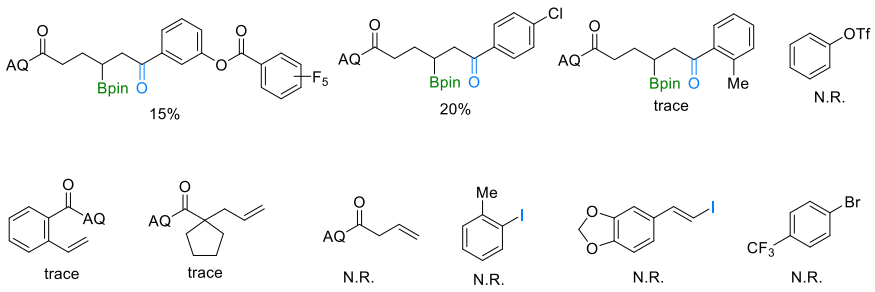
4. General Procedure for *anti*-Borocarbonylation of alkenes.



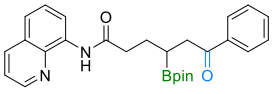
A 4 mL screw-cap vial was charged with $[Pd(\eta\text{-}C_3H_5)Cl]_2$ (0.9 mg, 2.5 mol%), CuI (1.9 mg, 10 mol%), Xantphos (2.9 mg, 5 mol%), B_2pin_2 (38.1 mg, 1.5 equiv.), *N*-(quinolin-8-yl)pent-4-enamide (0.1 mmol), $KHCO_3$ (20.0 mg, 2.0 equiv.) and an oven-dried stir bar. The vial was closed with a Teflon septum and cap and connected to the atmosphere via a needle. After DMSO (0.2 M) and iodobenzene (2.0 equiv.) were added with a syringe under argon atmosphere, the vial was moved to an alloy plate and put into a Parr 4560 series autoclave (300 mL) under an argon atmosphere. At room temperature, the autoclave was flushed with CO three times and charged with 10 bar of CO. The autoclave was placed on a heating plate equipped with a magnetic stirrer and an aluminum block. The reaction mixture was heated to 70 ºC for 12 h. The reaction was then quenched upon addition of water (10 mL) and the mixture was extracted with EA (10 mL). The combined organic phase was dried using Na_2SO_4 and then concentrated in vacuo. The crude product was purified by column chromatography on silica gel to afford the corresponding product.

5. Spectroscopic Data of Products

5.1 Failed substrates



5.2 Date of Products



6-Oxo-6-phenyl-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanamide (3a)

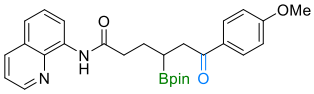
Pentane/EA = 3:1 (Rf = 0.35), yellow oil (23.3 mg, 51% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.83 – 8.74 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.99 – 7.91 (m, 2H), 7.57 – 7.46 (m, 3H), 7.46 – 7.40 (m, 3H), 3.24 (d, *J* = 7.0 Hz, 2H), 2.69 (t, *J* = 8.0 Hz, 2H), 2.09 – 1.90 (m, 2H), 1.51 (dq, *J* = 9.0, 6.5 Hz, 1H), 1.29 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 200.0, 171.8, 148.0, 138.4, 136.9, 136.3, 134.6, 132.8, 128.4, 128.0, 127.9, 127.4, 121.5, 121.3, 116.4, 83.2, 41.1, 37.7, 26.6, 24.8, 24.7.

^{11}B NMR (96 MHz, $CDCl_3$) δ 33.4.

HRMS (ESI): calcd for $[M+H]^+$ $C_{27}H_{31}BN_2O_4$ 459.2455, found: 459.2458.



6-(4-Methoxyphenyl)-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanamide (3b)

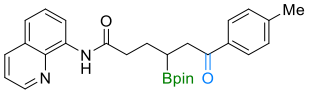
Pentane/EA = 3:1 (Rf = 0.20), colorless oil (32.4 mg, 66% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.86 – 8.72 (m, 2H), 8.14 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.97 – 7.90 (m, 2H), 7.56 – 7.41 (m, 3H), 6.93 – 6.86 (m, 2H), 3.85 (s, 3H), 3.18 (dd, *J* = 7.0, 1.5 Hz, 2H), 2.68 (dd, *J* = 8.5, 7.0 Hz, 2H), 2.12 – 1.86 (m, 2H), 1.54 – 1.43 (m, 1H), 1.29 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 198.5, 171.9, 163.3, 148.0, 138.4, 136.3, 134.6, 130.3, 130.0, 127.9, 127.4, 121.5, 121.2, 116.4, 113.5, 83.1, 55.4, 40.7, 37.8, 26.7, 24.8, 24.8.

^{11}B NMR (96 MHz, $CDCl_3$) δ 33.7.

HRMS (ESI): calcd for $[M+H]^+$ $C_{28}H_{33}BN_2O_5$ 489.2561, found: 489.2572.



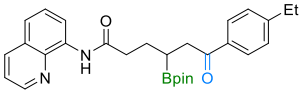
6-Oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(p-tolyl)hexanamide (3c)

Pentane/EA = 3:1 (Rf = 0.35), yellow oil (25.0 mg, 53% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.82 – 8.75 (m, 2H), 8.14 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.89 – 7.82 (m, 2H), 7.56 – 7.46 (m, 2H), 7.44 (dd, *J* = 8.5, 4.0 Hz, 1H), 7.24 – 7.18 (m, 2H), 3.29 – 3.12 (m, 2H), 2.68 (t, *J* = 8.0 Hz, 2H), 2.39 (s, 3H), 2.11 – 1.88 (m, 2H), 1.50 (dq, *J* = 8.5, 7.0 Hz, 1H), 1.29 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 199.6, 171.8, 148.0, 143.5, 138.4, 136.2, 134.6, 134.4, 129.1, 128.1, 127.9, 127.4, 121.5, 121.2, 116.4, 83.1, 41.0, 37.7, 26.7, 24.8, 24.7, 21.6.

HRMS (ESI): calcd for $[M+H]^+$ $C_{28}H_{33}BN_2O_4$ 473.2611, found: 473.2612.



6-(4-Ethylphenyl)-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanamide (3d)

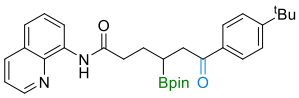
Pentane/EA = 3:1 (Rf = 0.35), yellow oil (34.0 mg, 70% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.95 – 9.81 (m, 1H), 8.86 – 8.70 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.92 – 7.84 (m, 2H), 7.57 – 7.46 (m, 2H), 7.44 (dd, *J* = 8.5, 4.0 Hz, 1H), 7.27 – 7.22 (m, 2H), 3.21 (d, *J* = 7.0 Hz, 2H), 2.69 (m, 4H), 2.11 – 1.87 (m, 2H), 1.56 – 1.44 (m, 1H), 1.29 (s, 6H), 1.27 (s, 6H), 1.23 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 199.6, 171.9, 149.7, 148.0, 138.4, 136.3, 134.7, 128.2, 127.9, 127.4, 121.5, 121.3, 116.4, 83.1, 41.0, 37.7, 28.9, 26.7, 24.8, 24.8, 15.2.

^{11}B NMR (96 MHz, $CDCl_3$) δ 33.6.

HRMS (ESI): calcd for $[M+H]^+$ $C_{29}H_{35}BN_2O_4$ 487.2768, found: 487.2772.



6-(4-(*tert*-Butyl)phenyl)-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanamide (3e)

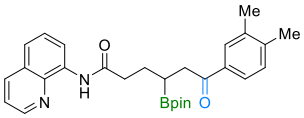
Pentane/EA = 3:1 (Rf = 0.35), yellow oil (37.5 mg, 73% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.82 – 8.74 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.93 – 7.86 (m, 2H), 7.55 – 7.47 (m, 2H), 7.46 – 7.42 (m, 3H), 3.22 (d, *J* = 7.5 Hz, 2H), 2.68 (t, *J* = 8.0 Hz, 2H), 2.09 – 1.87 (m, 2H), 1.55 – 1.45 (m, 1H), 1.33 (s, 9H), 1.29 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 199.6, 171.9, 156.5, 148.0, 138.4, 136.3, 134.7, 134.3, 128.0, 127.9, 127.4, 125.4, 121.5, 121.3, 116.4, 83.1, 41.0, 37.7, 35.0, 31.1, 26.7, 24.8, 24.8.

^{11}B NMR (96 MHz, $CDCl_3$) δ 33.02.

HRMS (ESI): calcd for $[M+H]^+$ $C_{29}H_{35}BN_2O_4$ 515.3081, found: 515.3088.



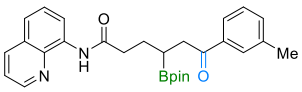
6-(3,4-Dimethylphenyl)-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanamide (3f)

Pentane/EA = 3:1 (Rf = 0.35), yellow oil (27.0 mg, 56% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.84 – 8.71 (m, 2H), 8.14 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.74 – 7.65 (m, 2H), 7.55 – 7.46 (m, 2H), 7.44 (dd, *J* = 8.5, 4.0 Hz, 1H), 7.20 – 7.14 (m, 1H), 3.21 (d, *J* = 6.5 Hz, 2H), 2.68 (t, *J* = 8.0 Hz, 2H), 2.29 (d, *J* = 2.5 Hz, 6H), 2.09 – 1.87 (m, 2H), 1.55 – 1.44 (m, 1H), 1.29 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 199.9, 171.9, 148.0, 142.2, 138.4, 136.7, 136.2, 134.8, 134.6, 129.6, 129.1, 127.9, 127.4, 125.8, 121.5, 121.2, 116.4, 83.1, 40.9, 37.7, 26.6, 24.8, 24.8, 20.0, 19.7.

HRMS (ESI): calcd for $[M+H]^+$ $C_{29}H_{35}BN_2O_4$ 487.2768, found: 487.2776.



6-Oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(m-tolyl)hexanamide (3g)

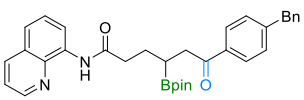
Pentane/EA = 3:1 (Rf = 0.35), yellow oil (19.2 mg, 41% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.84 – 8.74 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.80 – 7.72 (m, 2H), 7.56 – 7.47 (m, 2H), 7.44 (dd, *J* = 8.5, 4.0 Hz, 1H), 7.37 – 7.28 (m, 2H), 3.22 (d, *J* = 7.0 Hz, 2H), 2.68 (dd, *J* = 8.5, 7.5 Hz, 2H), 2.39 (q, *J* = 0.5 Hz, 3H), 2.10 – 1.88 (m, 2H), 1.50 (dq, *J* = 9.0, 7.0 Hz, 1H), 1.29 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.2, 171.8, 148.0, 138.4, 138.2, 136.9, 136.3, 134.6, 133.6, 128.5, 128.3, 127.9, 127.4, 125.2, 121.5, 121.3, 116.4, 83.2, 41.1, 37.7, 26.6, 24.8, 24.8, 21.3.

^{11}B NMR (128 MHz, $CDCl_3$) δ 32.9.

HRMS (ESI): calcd for $[M+H]^+$ $C_{28}H_{33}BN_2O_4$ 473.2611, found: 473.2617.



6-(4-Benzylphenyl)-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanamide (3h)

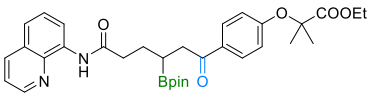
Pentane/EA = 3:1 (Rf = 0.35), yellow oil (31.2 mg, 57% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.87 – 8.70 (m, 2H), 8.14 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.92 – 7.84 (m, 2H), 7.56 – 7.46 (m, 2H), 7.44 (dd, *J* = 8.5, 4.5 Hz, 1H), 7.34 – 7.26 (m, 2H), 7.26 – 7.14 (m, 5H), 4.02 (s, 2H), 3.20 (d, *J* = 7.5 Hz, 2H), 2.68 (t, *J* = 8.0 Hz, 2H), 2.10 – 1.88 (m, 2H), 1.55 – 1.43 (m, 1H), 1.28 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 199.6, 171.8, 148.0, 146.5, 140.1, 138.4, 136.3, 135.0, 134.6, 129.0, 128.9, 128.6, 128.3, 127.9, 127.4, 126.3, 121.5, 121.3, 116.4, 83.2, 41.9, 41.0, 37.7, 26.6, 24.8, 24.7.

^{11}B NMR (96 MHz, $CDCl_3$) δ 33.5.

HRMS (ESI): calcd for $[M+H]^+$ $C_{34}H_{37}BN_2O_4$ 549.2925, found: 549.2935.



Ethyl 2-methyl-2-(4-(6-oxo-6-(quinolin-8-ylamino)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanoyl)phenoxy)propanoate (3i)

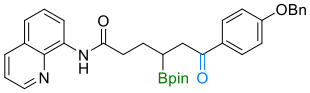
Pentane/EA = 3:1 (Rf = 0.30), yellow oil (35.9 mg, 61% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.84 – 8.70 (m, 2H), 8.14 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.91 – 7.84 (m, 2H), 7.55 – 7.46 (m, 2H), 7.43 (dd, *J* = 8.5, 4.0 Hz, 1H), 6.83 – 6.77 (m, 2H), 4.22 (q, *J* = 7.0 Hz, 2H), 3.25 – 3.08 (m, 2H), 2.67 (t, *J* = 8.0 Hz, 2H), 2.07 – 1.84 (m, 2H), 1.64 (s, 6H), 1.51 – 1.41 (m, 1H), 1.28 (s, 6H), 1.27 (s, 6H), 1.21 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 198.5, 173.7, 171.8, 159.5, 148.0, 138.4, 136.2, 134.6, 130.5, 129.8, 127.9, 127.4, 121.5, 121.2, 117.3, 116.4, 83.1, 79.2, 61.6, 40.8, 37.7, 26.7, 25.3, 24.8, 24.7, 14.0.

^{11}B NMR (96 MHz, $CDCl_3$) δ 32.8.

HRMS (ESI): calcd for $[M+H]^+$ $C_{33}H_{41}BN_2O_7$ 589.3085, found: 589.3087.



6-(4-(Benzyloxy)phenyl)-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanamide (3j)

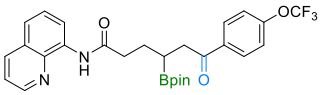
Pentane/EA = 2:1 (Rf = 0.30), yellow oil (38.9 mg, 69% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.84 – 8.72 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.97 – 7.89 (m, 2H), 7.57 – 7.46 (m, 2H), 7.46 – 7.31 (m, 6H), 7.01 – 6.94 (m, 2H), 5.12 (s, 2H), 3.18 (dd, *J* = 7.0, 1.5 Hz, 2H), 2.68 (dd, *J* = 8.5, 7.0 Hz, 2H), 2.10 – 1.86 (m, 2H), 1.55 – 1.42 (m, 1H), 1.29 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.5, 171.9, 162.4, 148.1, 138.4, 136.3, 136.3, 134.7, 130.3, 130.2, 128.7, 128.2, 127.9, 127.5, 127.4, 121.5, 121.3, 116.4, 114.4, 83.2, 70.1, 40.8, 37.8, 26.7, 24.9, 24.8.

^{11}B NMR (128 MHz, $CDCl_3$) δ 32.8.

HRMS (ESI): calcd for $[M+H]^+$ $C_{34}H_{37}BN_2O_5$ 565.2874, found: 565.2884.



6-Oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(4-(trifluoromethoxy)phenyl) hexanamide (3k)

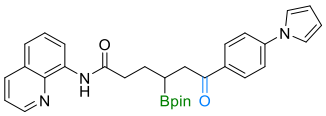
Pentane/EA = 3:1 (Rf = 0.42), colorless oil (22.8 mg, 42% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.83 – 8.73 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.02 – 7.96 (m, 2H), 7.55 – 7.47 (m, 2H), 7.45 (dd, *J* = 8.5, 4.0 Hz, 1H), 7.24 (dd, *J* = 9.0, 1.0 Hz, 2H), 3.21 (d, *J* = 7.0 Hz, 2H), 2.73 – 2.64 (m, 2H), 2.10 – 1.90 (m, 2H), 1.52 (dq, *J* = 9.0, 7.0 Hz, 1H), 1.28 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.5, 171.7, 152.4, 148.0, 138.4, 136.3, 135.1, 134.6, 130.0, 127.9, 127.4, 121.5, 121.3, 120.3, 120.3 (q, *J* = 258.0 Hz), 116.4, 83.3, 41.1, 37.6, 26.5, 24.8, 24.7.

^{19}F NMR (282 MHz, $CDCl_3$) δ -57.6 (s, 3F).

HRMS (ESI): calcd for $[M+H]^+$ $C_{28}H_{30}BN_2O_5F_3$ 543.2278, found: 543.2278.



6-(4-(1*H*-Pyrrol-1-yl)phenyl)-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanamide (3l)

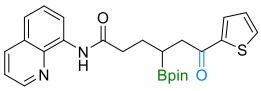
Pentane/EA = 3:1 (Rf = 0.20), yellow oil (32.0mg, 60% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.84 – 8.73 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.05 – 7.98 (m, 2H), 7.56 – 7.47 (m, 2H), 7.46 – 7.39 (m, 3H), 7.17 – 7.13 (m, 2H), 6.41 – 6.37 (m, 2H), 3.23 (d, *J* = 7.0 Hz, 2H), 2.69 (t, *J* = 8.0 Hz, 2H), 2.11 – 1.89 (m, 2H), 1.58 – 1.48 (m, 1H), 1.30 (s, 6H), 1.28 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 198.7, 171.8, 148.0, 143.8, 138.4, 136.3, 134.6, 133.8, 129.8, 127.9, 127.4, 121.5, 121.3, 119.3, 119.0, 116.4, 111.4, 83.2, 40.9, 37.7, 26.6, 24.8, 24.8.

^{11}B NMR (96 MHz, $CDCl_3$) δ 33.3.

HRMS (ESI): calcd for $[M+H]^+$ $C_{28}H_{30}BN_2O_5F_3$ 524.2720, found: 524.2728.



6-Oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(thiophen-2-yl)hexanamide (3m)

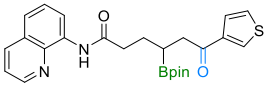
Pentane/EA = 3:1 (Rf = 0.35), yellow oil (37.5 mg, 81% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.86 – 8.69 (m, 2H), 8.14 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.72 (dd, *J* = 4.0, 1.0 Hz, 1H), 7.58 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.55 – 7.46 (m, 2H), 7.44 (dd, *J* = 8.5, 4.0 Hz, 1H), 7.09 (dd, *J* = 5.0, 4.0 Hz, 1H), 3.17 (d, *J* = 7.0 Hz, 2H), 2.67 (t, *J* = 8.0 Hz, 2H), 2.08 – 1.89 (m, 2H), 1.52 (dq, *J* = 8.5, 6.5 Hz, 1H), 1.28 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.8, 171.7, 148.0, 144.0, 138.4, 136.3, 134.6, 133.1, 131.7, 127.9, 127.9, 127.4, 121.5, 121.3, 116.4, 83.3, 41.4, 37.6, 26.6, 24.8, 24.7.

^{11}B NMR (96 MHz, $CDCl_3$) δ 32.8.

HRMS (ESI): calcd for $[M+Na]^+$ $C_{25}H_{29}BN_2O_4S$ 487.1833, found: 487.1831.



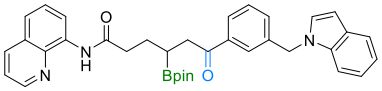
6-oxo-N-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(thiophen-3-yl)hexanamide (3n)

Pentane/EA = 3:1 (Rf = 0.35), yellow oil (35.0 mg, 75% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.84 – 8.74 (m, 2H), 8.14 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.04 (dd, *J* = 3.0, 1.5 Hz, 1H), 7.55 – 7.46 (m, 3H), 7.44 (dd, *J* = 8.5, 4.0 Hz, 1H), 7.31 – 7.24 (m, 1H), 3.14 (d, *J* = 7.0 Hz, 2H), 2.67 (dd, *J* = 8.5, 7.0 Hz, 2H), 2.13 – 1.88 (m, 2H), 1.49 (dq, *J* = 9.0, 7.0 Hz, 1H), 1.28 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 194.3, 171.8, 148.0, 142.1, 138.4, 136.3, 134.6, 131.7, 127.9, 127.4, 126.9, 126.0, 121.5, 121.3, 116.4, 83.2, 42.1, 37.7, 26.6, 24.8, 24.8.

HRMS (ESI): calcd for $[M+Na]^+$ $C_{25}H_{29}BN_2O_4S$ 487.1837, found: 487.1836.



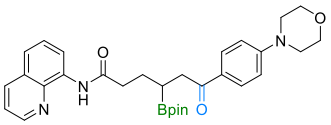
6-(3-((1*H*-Indol-1-yl)methyl)phenyl)-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanamide (3o)

Pentane/EA = 3:1 (Rf = 0.30), yellow oil (29.0 mg, 49% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.83 – 8.74 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.88 – 7.77 (m, 2H), 7.65 (ddd, *J* = 7.5, 1.5, 1.0 Hz, 1H), 7.56 – 7.47 (m, 2H), 7.44 (dd, *J* = 8.5, 4.0 Hz, 1H), 7.32 (t, *J* = 7.5 Hz, 1H), 7.27 – 7.24 (m, 1H), 7.20 – 7.08 (m, 4H), 6.57 (dd, *J* = 3.0, 1.0 Hz, 1H), 5.35 (s, 2H), 3.17 (d, *J* = 7.0 Hz, 2H), 2.67 (t, *J* = 8.0 Hz, 2H), 2.08 – 1.87 (m, 2H), 1.55 – 1.42 (m, 1H), 1.29 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.8, 171.8, 148.0, 138.4, 138.1, 137.3, 136.3, 136.1, 134.6, 131.0, 129.0, 128.7, 128.1, 127.9, 127.4, 127.4, 126.3, 121.8, 121.5, 121.3, 121.0, 119.6, 116.4, 109.5, 102.0, 83.2, 49.8, 41.1, 37.6, 26.5, 24.8, 24.7.

HRMS (ESI): calcd for $[M+H]^+$ $C_{36}H_{38}BN_3O_4$ 588.3033, found: 588.3036.



6-(4-Morpholinophenyl)-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanamide (3p)

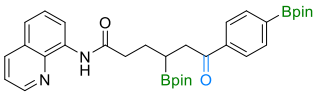
Pentane/EA = 1:1 (Rf = 0.5), yellow oil (37.9 mg, 70% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.84 – 8.72 (m, 2H), 8.14 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.93 – 7.86 (m, 2H), 7.56 – 7.46 (m, 2H), 7.44 (dd, *J* = 8.0, 4.0 Hz, 1H), 6.86 – 6.80 (m, 2H), 3.87 – 3.82 (m, 4H), 3.32 – 3.23 (m, 4H), 3.16 (dd, *J* = 7.0, 3.5 Hz, 2H), 2.67 (t, *J* = 8.0 Hz, 2H), 2.09 – 1.89 (m, 2H), 1.47 (m, 1H), 1.29 (s, 6H), 1.28 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 198.2, 171.9, 154.1, 148.0, 138.4, 136.2, 134.6, 130.0, 127.9, 127.8, 127.4, 121.5, 121.2, 116.4, 113.3, 83.0, 66.6, 47.6, 40.5, 37.8, 26.7, 24.8, 24.8.

^{11}B NMR (96 MHz, $CDCl_3$) δ 32.7.

HRMS (ESI): calcd for $[M+H]^+$ $C_{31}H_{38}BN_3O_5$ 544.2983, found: 544.2990.



6-Oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)hexanamide (3q)

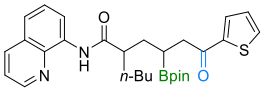
Pentane/EA = 3:1 (Rf = 0.32), yellow oil (xx mg, 68% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.84 – 8.74 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.95 – 7.89 (m, 2H), 7.88 – 7.83 (m, 2H), 7.56 – 7.47 (m, 2H), 7.44 (dd, *J* = 8.5, 4.0 Hz, 1H), 3.24 (d, *J* = 7.0 Hz, 2H), 2.68 (dd, *J* = 8.5, 7.0 Hz, 2H), 2.11 – 1.87 (m, 2H), 1.55 – 1.46 (m, 1H), 1.35 (s, 12H), 1.29 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.3, 171.8, 148.0, 138.8, 138.4, 136.3, 134.8, 134.6, 127.9, 127.4, 127.0, 121.5, 121.3, 116.4, 84.1, 83.2, 41.3, 37.7, 26.6, 24.9, 24.8, 24.7.

^{11}B NMR (96 MHz, $CDCl_3$) δ 30.3.

HRMS (ESI): calcd for $[M+Na]^+$ $C_{33}H_{42}B_2N_2O_6$ 585.3307, found: 585.3317.



2-Butyl-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(thiophen-2-yl)hexanamide (4a) (diasteromer 1:1)

Pentane/EA = 3:1 (Rf = 0.50), yellow oil (38.0 mg, 73% yield).

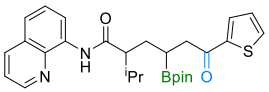
The reported dr was determined by ^{1}H NMR analysis of purified **4a** and is consistent with that of the crude reaction mixture. The following analytical data correspond to the mixture.

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.03 – 9.91 (m, 1H), 8.88 – 8.73 (m, 2H), 8.14 (dt, *J* = 8.5, 1.5 Hz, 1H), 7.71 – 7.63 (m, 1H), 7.59 – 7.46 (m, 3H), 7.45 – 7.41 (m, 1H), 7.05 (ddd, *J* = 6.5, 5.0, 4.0 Hz, 1H), 3.23 – 3.01 (m, 2H), 2.81 – 2.52 (m, 1H), 2.14 – 1.42 (m, 5H), 1.35 (td, *J* = 5.5, 3.5 Hz, 4H), 1.30 (d, *J* = 1.5 Hz, 6H), 1.26 (d, *J* = 7.0 Hz, 6H), 0.90 – 0.83 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.8, 175.2, 147.9, 143.9, 138.6, 136.1, 134.7, 133.0, 131.7, 127.9, 127.8, 127.4, 121.4, 121.3, 116.6, 83.2, 48.5, 42.4, 34.7, 33.6, 29.7, 24.9, 24.8, 22.7, 13.9.

^{11}B NMR (96 MHz, $CDCl_3$) δ 32.9.

HRMS (ESI): calcd for $[M+H]^+$ $C_{29}H_{37}BN_2O_4S$ 521.2645, found: 521.2656.



2-Isopropyl-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(thiophen-2-yl)hexanamide (4b) (diasteromer 1:1)

Pentane/EA = 3:1 (Rf = 0.50), yellow oil (31.4 mg, 62% yield).

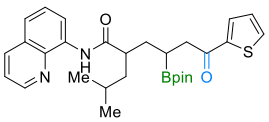
The reported dr was determined by ^{1}H NMR analysis of purified **4b** and is consistent with that of the crude reaction mixture. The following analytical data correspond to the mixture.

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.03 – 9.87 (m, 1H), 8.91 – 8.71 (m, 2H), 8.18 – 8.10 (m, 1H), 7.67 (ddd, *J* = 22.0, 4.0, 1.1 Hz, 1H), 7.59 – 7.46 (m, 3H), 7.43 (ddd, *J* = 8.5, 4.0, 1.6 Hz, 1H), 7.04 (dt, *J* = 5.0, 3.5 Hz, 1H), 3.26 – 3.03 (m, 2H), 2.50 – 2.28 (m, 1H), 2.13 – 1.76 (m, 3H), 1.48 (dd, *J* = 9.0, 5.5 Hz, 1H), 1.30 (d, *J* = 3.5 Hz, 6H), 1.21 (d, *J* = 9.0 Hz, 6H), 1.09 – 0.98 (m, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.9, 174.0, 148.0, 144.2, 138.5, 136.2, 134.5, 133.0, 131.8, 127.9, 127.8, 127.4, 121.4, 121.2, 116.5, 83.2, 54.9, 40.2, 31.6, 31.4, 24.9, 24.8, 21.1, 20.7.

^{11}B NMR (96 MHz, $CDCl_3$) δ 34.3.

HRMS (ESI): calcd for $[M+Na]^+$ $C_{28}H_{35}BN_2O_4S$ 529.2303, found: 529.2304.



2-Isobutyl-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(thiophen-2-yl)hexanamide (4c) (diasteromer 3:2)

Pentane/EA = 3:1 (Rf = 0.45), yellow oil (28.0 mg, 54% yield).

The reported dr was determined by ^{1}H NMR analysis of purified **4c** and is consistent with that of the crude reaction mixture. The following analytical data correspond to the mixture.

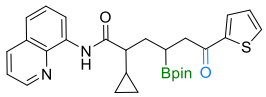
^{1}H NMR (300 MHz, $CDCl_3$) δ 10.09 – 9.94 (m, 1H), 8.90 – 8.71 (m, 2H), 8.14 (dt, *J* = 8.5, 1.5 Hz, 1H), 7.67 (ddd, *J* = 17.0, 4.0, 1.1 Hz, 1H), 7.58 – 7.46 (m, 3H), 7.43 (ddd, *J* = 8.5, 4.0, 1.0 Hz, 1H), 7.05 (dt, *J* = 5.0, 4.0 Hz,

1H), 3.24 – 3.01 (m, 2H), 2.93 – 2.66 (m, 1H), 2.05 – 1.69 (m, 3H), 1.59 – 1.33 (m, 3H), 1.32 (d, *J* = 3.0 Hz, 6H), 1.28 (d, *J* = 7.5 Hz, 6H), 0.96 (dd, *J* = 6.5, 4.0 Hz, 3H), 0.91 (dd, *J* = 6.5, 4.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.8, 175.2, 147.9, 143.9, 138.7, 136.1, 134.7, 133.0, 131.7, 127.9, 127.9, 127.4, 121.5, 121.3, 116.6, 83.2, 46.4, 43.1, 41.0, 35.0, 26.0, 25.0, 24.8, 23.2, 22.3.

^{11}B NMR (96 MHz, $CDCl_3$) δ 33.9.

HRMS (ESI): calcd for $[M+H]^+$ $C_{29}H_{37}BN_2O_4S$ 521.2645, found: 521.2650.



2-Cyclopropyl-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(thiophen-2-yl)hexanamide (4d) (diasteromer 2:1)

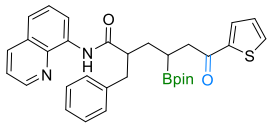
Pentane/EA = 5:1 (Rf = 0.30), brown oil (47.0 mg, 93% yield).

The reported dr was determined by ^{1}H NMR analysis of purified **4d** and is consistent with that of the crude reaction mixture. The following analytical data correspond to the mixture.

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.11 – 10.07 (m, 1H), 8.95 – 8.67 (m, 2H), 8.14 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.73 – 7.63 (m, 1H), 7.60 – 7.46 (m, 3H), 7.43 (dd, *J* = 8.5, 4.5 Hz, 1H), 7.11 – 7.02 (m, 1H), 3.32 – 2.98 (m, 2H), 2.33 – 1.83 (m, 3H), 1.56 – 1.36 (m, 1H), 1.25 (d, *J* = 10.0 Hz, 12H), 1.17 – 1.04 (m, 1H), 0.74 – 0.54 (m, 2H), 0.50 – 0.17 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.8, 174.5, 148.0, 144.0, 138.6, 136.2, 134.8, 132.9, 131.7, 127.8, 127.4, 121.4, 121.3, 116.5, 83.2, 53.3, 42.2, 34.1, 24.8, 14.8, 4.7, 4.0.

HRMS (ESI): calcd for $[M+H]^+$ $C_{28}H_{33}BN_2O_4S$ 505.2337, found: 505.2338.



2-Benzyl-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(thiophen-2-yl)hexanamide (4e) (diasteromer 1:1)

Pentane/EA = 3:1 (Rf = 0.45), brown oil (35.8 mg, 65% yield).

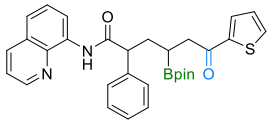
The reported dr was determined by ^{1}H NMR analysis of purified **4e** and is consistent with that of the crude reaction mixture. The following analytical data correspond to the mixture.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.94 – 9.75 (m, 1H), 8.84 – 8.65 (m, 2H), 8.12 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.73 – 7.44 (m, 4H), 7.41 (dt, *J* = 8.0, 4.0 Hz, 1H), 7.26 – 7.24 (m, 2H), 7.23 – 7.15 (m, 2H), 7.14 – 7.02 (m, 2H), 3.24 – 3.07 (m, 3H), 3.05 – 2.80 (m, 2H), 2.22 – 1.84 (m, 1H), 1.83 – 1.68 (m, 1H), 1.50 – 1.37 (m, 1H), 1.28 (s, 6H), 1.25 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.7, 173.7, 147.8, 144.0, 140.0, 138.4, 136.1, 134.5, 133.1, 131.8, 128.9, 128.3, 127.9, 127.8, 127.3, 126.1, 121.4, 116.6, 83.3, 50.1, 42.3, 39.7, 33.7, 24.8, 24.8.

^{11}B NMR (96 MHz, $CDCl_3$) δ 33.4.

HRMS (ESI): calcd for $[M+Na]^+$ $C_{32}H_{35}BN_2O_4S$ 577.2303, found: 577.2314.



6-Oxo-2-phenyl-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(thiophen-2-yl)hexanamide (4f) (diasteromer 1:1)

Pentane/EA = 3:1 (Rf = 0.50), yellow oil (32.4 mg, 60% yield).

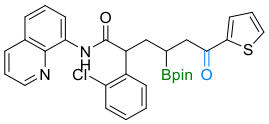
The reported dr was determined by ^{1}H NMR analysis of purified **4f** and is consistent with that of the crude reaction mixture. The following analytical data correspond to the mixture.

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.06 – 9.92 (m, 1H), 8.85 – 8.68 (m, 2H), 8.10 (ddd, *J* = 8.5, 3.5, 1.5 Hz, 1H), 7.65 (ddd, *J* = 8.0, 4.0, 1.0 Hz, 1H), 7.56 (ddd, *J* = 5.0, 2.5, 1.0 Hz, 1H), 7.53 – 7.42 (m, 4H), 7.42 – 7.30 (m, 3H), 7.29 – 7.21 (m, 1H), 7.06 (dd, *J* = 5.0, 4.0 Hz, 1H), 4.06 – 3.97 (m, 1H), 3.30 – 2.98 (m, 2H), 2.58 – 2.32 (m, 1H), 2.15 – 2.01 (m, 1H), 1.55 – 1.35 (m, 1H), 1.31 – 1.25 (m, 12H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.7, 172.2, 148.0, 143.9, 140.2, 139.7, 138.5, 136.1, 134.6, 133.0, 131.7, 128.7, 128.4, 127.9, 127.8, 127.3, 121.4, 121.3, 116.4, 83.2, 53.9, 41.7, 34.9, 24.9.

^{11}B NMR (96 MHz, $CDCl_3$) δ 33.4.

HRMS (ESI): calcd for $[M+H]^+$ $C_{31}H_{33}BN_2O_4S$ 541.2332, found: 541.2333.



2-(2-Chlorophenyl)-6-oxo-N-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(thiophen-2-yl)hexanamide (4g) (diasteromer 1:1)

Pentane/EA = 3:1 (Rf = 0.45), brown oil (32.8 mg, 57% yield).

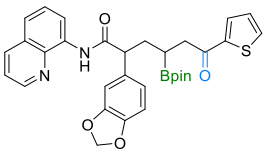
The reported dr was determined by ^{1}H NMR analysis of purified **4g** and is consistent with that of the crude reaction mixture. The following analytical data correspond to the mixture.

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.17 – 10.02 (m, 1H),), 8.84 – 8.65 (m, 2H), 8.11 (dt, *J* = 8.5, 1.5 Hz, 1H), 7.71 – 7.62 (m, 2H), 7.57 (ddd, *J* = 5.0, 2.5, 1.0 Hz, 1H), 7.52 – 7.44 (m, 2H), 7.44 – 7.34 (m, 2H), 7.31 – 7.24 (m, 1H), 7.17 (dddd, *J* = 8.0, 7.5, 2.5, 1.5 Hz, 1H), 7.10 – 7.05 (m, 1H), 4.70 – 4.57 (m, 1H), 3.29 – 3.05 (m, 2H), 2.65 – 2.35 (m, 1H), 2.14 – 2.00 (m, 1H), 1.56 – 1.40 (m, 1H), 1.33 – 1.26 (m, 12H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.6, 171.3, 148.1, 144.0, 137.4, 137.1, 136.1, 134.7, 134.3, 133.7, 133.1, 131.7, 129.6, 129.0, 128.3, 127.9, 127.8, 127.4, 127.3, 121.5, 116.4, 83.3, 48.8, 41.3, 33.1, 24.9.

^{11}B NMR (96 MHz, $CDCl_3$) δ 33.7.

HRMS (ESI): calcd for $[M+H]^+$ $C_{31}H_{32}BClN_2O_4S$ 575.1943, found: 575.1946.



2-(Benzo[d][1,3]dioxol-5-yl)-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(thiophen-2-yl)hexanamide (4h) (diasteromer 1:1)

Pentane/EA = 3:1 (Rf = 0.35), yellow oil (24.2 mg, 42% yield).

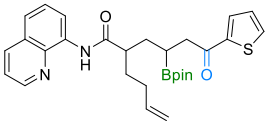
The reported dr was determined by ^{1}H NMR analysis of purified **4h** and is consistent with that of the crude reaction mixture. The following analytical data correspond to the mixture.

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.04 – 9.92 (m, 1H), 8.76 (ddt, *J* = 8.5, 4.5, 2.0 Hz, 2H), 8.11 (ddd, *J* = 8.5, 2.5, 1.5 Hz, 1H), 7.66 (ddd, *J* = 5.0, 3.5, 1.5 Hz, 1H), 7.63 – 7.53 (m, 1H), 7.53 – 7.36 (m, 3H), 7.14 – 6.99 (m, 2H), 6.99 – 6.90 (m, 1H), 6.77 (dd, *J* = 8.0, 6.0 Hz, 1H), 5.91 (dq, *J* = 3.5, 1.5 Hz, 2H), 4.04 – 3.83 (m, 1H), 3.32 – 2.96 (m, 2H), 2.51 – 2.27 (m,1H), 2.09 – 1.94 (m, 1H), 1.55 – 1.35 (m, 1H), 1.29 (dd, *J* = 4.0, 2.0 Hz, 12H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.7, 172.2, 148.0, 147.9, 146.7, 143.9, 138.5, 136.2, 134.6, 134.0, 133.4, 133.0, 131.7, 127.9, 127.3, 121.5, 121.2, 116.3, 108.5, 108.3, 100.9, 83.2, 53.4, 41.6, 34.8, 24.9, 24.8.

^{11}B NMR (96 MHz, $CDCl_3$) δ 32.5.

HRMS (ESI): calcd for $[M+Na]^+$ $C_{31}H_{32}BClN_2O_4S$ 607.2044, found: 607.2057.



2-(4-Oxo-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-4-(thiophen-2-yl)butyl)-*N*-(quinolin-8-yl)hex-5-enamide (4i) (diasteromer 1:1)

Pentane/EA = 3:1 (Rf = 0.45), brown oil (38.0 mg, 73% yield).

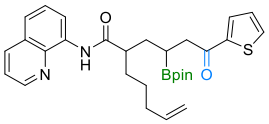
The reported dr was determined by ^{1}H NMR analysis of purified **4i** and is consistent with that of the crude reaction mixture. The following analytical data correspond to the mixture.

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.06 – 9.92 (m, 1H), 8.89 – 8.72 (m, 2H), 8.14 (dt, *J* = 8.5, 1.5 Hz, 1H), 7.67 (ddd, *J* = 17.0, 4.0, 1.1 Hz, 1H), 7.59 – 7.47 (m, 3H), 7.43 (ddd, *J* = 8.5, 4.0, 0.5 Hz, 1H), 7.06 (td, *J* = 4.5, 4.0 Hz, 1H), 5.88 – 5.74 (m, 1H), 5.10 – 4.91 (m, 2H), 3.24 – 3.02 (m, 2H), 2.86 – 2.60 (m, 1H), 2.26 – 2.05 (m, 2H), 1.99 – 1.74 (m, 2H), 1.72 – 1.55 (m, 2H), 1.54 – 1.38 (m, 1H), 1.30 (d, *J* = 3.0 Hz, 6H), 1.27 (d, *J* = 7.0 Hz, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.8, 174.8, 147.9, 143.9, 138.6, 138.0, 136.1, 134.7, 133.0, 131.7, 127.9, 127.9, 127.4, 121.4, 121.4, 116.6, 115.3, 83.2, 47.6, 42.4, 34.7, 32.9, 31.6, 24.9, 24.8.

^{11}B NMR (96 MHz, $CDCl_3$) δ 32.9.

HRMS (ESI): calcd for $[M+Na]^+$ $C_{29}H_{35}BN_2O_4S$ 541.2303, found: 541.2308.



2-(4-Oxo-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-4-(thiophen-2-yl)butyl)-*N*-(quinolin-8-yl)hept-6-enamide (4j) (diasteromer 1:1)

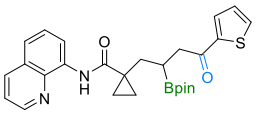
Pentane/EA = 3:1 (Rf = 0.45), yellow oil (38.3 mg, 72% yield).

The reported dr was determined by ^{1}H NMR analysis of purified **4j** and is consistent with that of the crude reaction mixture. The following analytical data correspond to the mixture.

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.04 – 9.92 (m, 1H), 8.90 – 8.67 (m, 2H), 8.14 (dt, *J* = 8.5, 1.5 Hz, 1H), 7.71 – 7.63 (m1H), 7.59 – 7.47 (m, 3H), 7.43 (ddd, *J* = 8.5, 4.5, 1.0 Hz, 1H), 7.06 (ddd, *J* = 6.5, 5.0, 4.0 Hz, 1H), 5.86 – 5.68 (m, 1H), 5.04 – 4.85 (m, 2H), 3.24 – 3.03 (m, 2H), 2.83 – 2.53 (m, 1H), 2.15 – 2.01 (m, 2H), 1.90 – 1.76 (m, 2H), 1.74 – 1.37 (m, 5H), 1.30 (s, 6H), 1.26 (d, *J* = 7.0 Hz, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.8, 175.0, 147.9, 143.9, 138.6, 136.2, 134.7, 133.0, 131.7, 127.9, 127.9, 127.4, 121.5, 121.4, 116.6, 114.6, 83.2, 48.4, 42.3, 34.6, 33.8, 32.2, 26.9, 24.9, 24.8.

HRMS (ESI): calcd for $[M+H]^+$ $C_{30}H_{37}BN_2O_4S$ 533.2651, found: 533.2649.



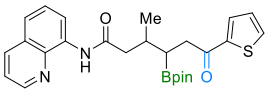
1-(4-Oxo-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-4-(thiophen-2-yl)butyl)-*N*-(quinolin-8-yl)cyclopropane-1-carboxamide (4k)

Pentane/EA = 3:1 (Rf = 0.40), yellow oil (20.7 mg, 42% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.29 (s, 1H), 8.77 (dd, *J* = 4.5, 1.5 Hz, 1H), 8.70 (dd, *J* = 7.0, 2.0 Hz, 1H), 8.13 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.64 (dd, *J* = 4.0, 1.5 Hz, 1H), 7.55 – 7.45 (m, 3H), 7.45 – 7.40 (m, 1H), 7.00 (dd, *J* = 5.0, 4.0 Hz, 1H), 3.56 – 3.15 (m, 2H), 2.19 (dd, *J* = 15.0, 6.5 Hz, 1H), 1.96 (dd, *J* = 15.5, 9.0 Hz, 1H), 1.85 – 1.71 (m, 1H), 1.25 (d, *J* = 2.5 Hz, 14H), 0.88 – 0.82 (m, 1H), 0.70 (ddd, *J* = 8.5, 5.5, 3.0 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.8, 172.7, 148.1, 143.9, 138.6, 136.2, 134.7, 133.0, 131.8, 127.9, 127.8, 127.4, 121.5, 121.1, 116.1, 83.2, 40.5, 34.6, 25.9, 24.9, 24.7, 15.7, 13.8.

HRMS (ESI): calcd for $[M+H]^+$ $C_{27}H_{31}BN_2O_4S$ 491.2176, found: 491.2182.



3-Methyl-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(thiophen-2-yl)hexanamide (4l) (diasteromer 1:1)

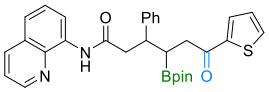
Pentane/EA = 3:1 (Rf = 0.38), yellow oil (30.5 mg, 64% yield).

The reported dr was determined by ^{1}H NMR analysis of purified **4l** and is consistent with that of the crude reaction mixture. The following analytical data correspond to the mixture.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.96 – 9.86 (m, 1H), 8.86 – 8.75 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.72 (dt, *J* = 4.0, 1.0 Hz, 1H), 7.58 (ddd, *J* = 5.0, 3.5, 1.0 Hz, 1H), 7.55 – 7.47 (m, 2H), 7.44 (dd, *J* = 8.5, 4.0 Hz, 1H), 7.09 (ddd, *J* = 5.0, 3.5, 1.0 Hz, 1H), 3.28 – 3.04 (m, 2H), 2.84 – 2.75 (m, 1H), 2.49 – 2.34 (m, 2H), 1.71 – 1.53 (m, 1H), 1.30 (d, *J* = 3.0 Hz, 6H), 1.27 (d, *J* = 11.5 Hz, 6H), 1.14 (dd, *J* = 11.5, 6.5 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 193.2, 171.3, 148.1, 144.1, 138.4, 136.3, 134.6, 133.0, 131.7, 127.9, 127.9, 127.4, 121.5, 121.3, 116.4, 83.3, 44.7, 39.0, 31.9, 24.9, 24.8, 19.6.

HRMS (ESI): calcd for $[M+Na]^+$ $C_{26}H_{31}BN_2O_4S$ 501.1989, found: 501.1998.



6-Oxo-3-phenyl-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(thiophen-2-yl)hexanamide (4m) (diasteromer >20:1)

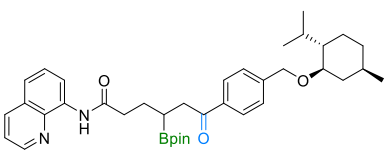
Pentane/EA = 3:1 (Rf = 0.38), yellow oil (25.9 mg, 48% yield).

The reported dr was determined by ^{1}H NMR analysis of purified 4m and is consistent with that of the crude reaction mixture.

^{1}H NMR (400 MHz,$CDCl_3$) δ 9.86 (s, 1H), 8.78 (dd, *J* = 4.5, 1.7 Hz, 1H), 8.72 (dd, *J* = 7.0, 2.0 Hz, 1H), 8.17 (d, *J* = 8.0 Hz, 1H), 7.67 (dd, *J* = 4.0, 1.0 Hz, 1H), 7.56 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.53 – 7.41 (m, 3H), 7.39 – 7.33 (m, 2H), 7.27 –7.23 (m, 2H), 7.18 – 7.10 (m, 1H), 7.07 (dd, *J* = 4.9, 3.8 Hz, 1H), 3.56 – 3.44 (m, 1H), 3.25 – 3.06 (m, 3H), 2.94 (dd, *J* = 14.5, 9.0 Hz, 1H), 2.10 – 2.01 (m, 1H), 1.14 (s, 6H), 1.08 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 192.7, 170.4, 147.9, 144.1, 143.3, 138.4, 136.2, 134.6, 133.0, 131.7, 128.3, 128.2, 127.8, 127.3, 126.6, 121.4, 121.3, 116.5, 83.3, 44.2, 43.9, 40.1, 24.8, 24.7.

HRMS (ESI): calcd for $[M+Na]^+$ $C_{31}H_{33}BN_2O_4S$ 563.2146, found: 563.2148.



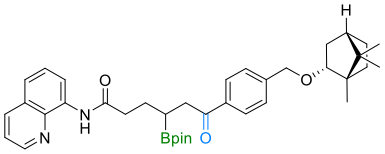
6-(4-((((1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl)oxy)methyl)phenyl)-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanamide (5a)

Pentane/EA = 3:1 (Rf = 0.38), yellow oil (42.2 mg, 67% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.82 – 8.74 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.96 – 7.89 (m, 2H), 7.55 – 7.47 (m, 2H), 7.46 – 7.38 (m, 3H), 4.70 (d, *J* = 12.5 Hz, 1H), 4.44 (d, *J* = 12.5 Hz, 1H), 3.26 – 3.13 (m, 3H), 2.68 (t, *J* = 8.0 Hz, 2H), 2.35 – 2.12 (m, 3H), 2.11 – 1.89 (m, 2H), 1.65 (ddd, *J* = 12.5, 6.5, 3.0 Hz, 2H), 1.57 – 1.44 (m, 1H), 1.29 (s, 6H), 1.27 (s, 6H), 0.95 – 0.90 (m, 10H), 0.73 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 199.7, 171.8, 148.0, 144.5, 138.4, 136.3, 136.0, 134.6, 128.1, 127.9, 127.4, 121.5, 121.3, 116.4, 83.2, 79.2, 69.7, 48.3, 41.1, 40.3, 37.7, 34.5, 31.5, 26.6, 25.6, 24.8, 24.7, 23.2, 22.3, 21.0, 16.1.

HRMS (ESI): calcd for $[M+H]^+$ $C_{38}H_{51}BN_2O_5$ 627.3969, found: 627.3972.



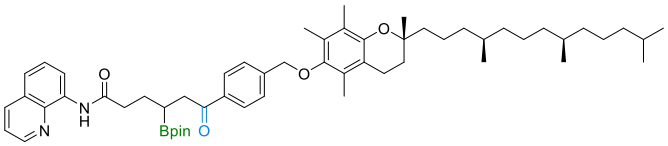
6-Oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(4-((((1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)methyl)phenyl)hexanamide (5b)

Pentane/EA = 3:1 (Rf = 0.35), yellow oil (28.0 mg, 45% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.83 – 8.74 (m, 2H), 8.15 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.95 – 7.90 (m, 2H), 7.54 – 7.47 (m, 2H), 7.44 (dd, *J* = 8.5, 4.0 Hz, 1H), 7.39 (d, *J* = 8.5 Hz, 2H), 4.61 (d, *J* = 13.0 Hz, 1H), 4.48 (d, *J* = 13.0 Hz, 1H), 3.69 (ddd, *J* = 9.5, 3.5, 2.0 Hz, 1H), 3.27 – 3.19 (m, 2H), 2.68 (dd, *J* = 8.5, 7.0 Hz, 2H), 2.17 – 2.02 (m, 3H), 2.01 – 1.90 (m, 1H), 1.79 – 1.64 (m, 3H), 1.55 – 1.46 (m, 1H), 1.29 (s, 6H), 1.27 (s, 6H), 1.16 – 1.03 (m, 2H), 0.91 (s, 3H), 0.85 (s, 3H), 0.83 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.7, 171.8, 148.0, 144.9, 138.4, 136.3, 135.8, 134.6, 128.1, 127.9, 127.4, 126.8, 121.5, 121.3, 116.4, 84.6, 83.2, 70.9, 49.3, 47.9, 45.0, 41.1, 37.7, 36.0, 28.2, 26.7, 26.6, 24.8, 24.7, 19.7, 18.9, 14.0.

HRMS (ESI): calcd for $[M+H]^+$ $C_{38}H_{49}BN_2O_5$ 625.3813, found: 625.3823.



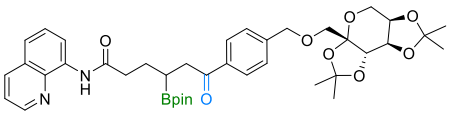
6-Oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(4-((((R)-2,5,7,8-tetramethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman-6-yl)oxy)methyl)phenyl)hexanamide (5c)

Pentane/EA = 3:1 (Rf = 0.38), yellow oil (46.2 mg, 51% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.88 (s, 1H), 8.83 – 8.76 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.01 – 7.96 (m, 2H), 7.58 – 7.54 (m, 2H), 7.53 – 7.47 (m, 2H), 7.45 (dd, *J* = 8.5, 4.0 Hz, 1H), 4.75 (s, 2H), 3.25 (d, *J* = 7.0 Hz, 2H), 2.70 (t, *J* = 8.0 Hz, 2H), 2.59 (t, *J* = 7.0 Hz, 2H), 2.20 (s, 3H), 2.15 (s, 3H), 2.10 (s, 3H), 2.10 – 2.01 (m, 2H), 2.00 – 1.91 (m, 1H), 1.86 – 1.74 (m, 2H), 1.57 – 1.48 (m, 4H), 1.46 – 1.34 (m, 5H), 1.30 (s, 6H), 1.28 (s, 7H), 1.25 (d, *J* = 3.5 Hz, 5H), 1.18 – 1.00 (m, 9H), 0.89 – 0.85 (m, 9H), 0.85 – 0.84 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.7, 171.8, 148.0, 148.0, 143.2, 138.4, 136.3, 136.2, 134.6, 128.2, 127.9, 127.8, 127.4, 127.1, 125.8, 123.0, 121.5, 121.3, 117.7, 116.4, 83.2, 74.9, 73.9, 41.1, 40.0, 39.4, 37.7, 37.4, 37.3, 32.8, 32.8, 32.7, 31.3, 31.2, 28.0, 26.6, 24.8, 24.8, 24.4, 23.9, 22.7, 22.6, 21.0, 20.7, 19.7, 19.7, 19.6, 12.8, 12.0, 11.8.

HRMS (ESI): calcd for $[M+H]^+$ $C_{57}H_{81}BN_2O_6$ 901.6266, found: 901.6267.



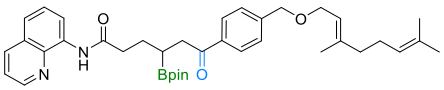
6-Oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6-(4-((((3a*S*,5a*R*,8a*R*,8b*S*)-2,2,7,7-tetramethyltetrahydro-3a*H*-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-3a-yl)methoxy)methyl)phenyl) hexanamide (5d)

Pentane/EA = 3:1 (Rf = 0.22), yellow oil (50.9 mg, 70% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.83 – 8.73 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.95 – 7.89 (m, 2H), 7.56 – 7.46 (m, 2H), 7.46 – 7.37 (m, 3H), 4.75 – 4.62 (m, 2H), 4.60 (dd, *J* = 5.5, 2.5 Hz, 1H), 4.44 (d, *J* = 2.5 Hz, 1H), 4.23 (ddd, *J* = 8.0, 2.0, 1.0 Hz, 1H), 3.92 (dd, *J* = 13.0, 2.0 Hz, 1H), 3.73 (dd, *J* = 13.0, 1.0 Hz, 1H), 3.63 (d, *J* = 1.0 Hz, 2H), 3.22 (d, *J* = 7.0 Hz, 2H), 2.68 (dd, *J* = 8.5, 7.0 Hz, 2H), 2.11 – 1.88 (m, 2H), 1.56 – 1.53 (m, 3H), 1.49 (dd, *J* = 6.5, 1.5 Hz, 1H), 1.42 (s, 3H), 1.41 (s, 3H), 1.33 (s, 3H), 1.29 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.6, 171.8, 148.0, 143.3, 138.4, 136.3, 136.1, 134.6, 128.1, 127.9, 127.4, 127.1, 121.5, 121.3, 116.4, 108.9, 108.6, 102.6, 83.2, 73.1, 71.8, 71.0, 70.1, 70.1, 61.0, 41.1, 37.7, 26.6, 26.5, 25.8, 25.4, 24.8, 24.7, 24.0.

HRMS (ESI): calcd for $[M+H]^+$ $C_{40}H_{51}BN_2O_{10}$ 731.3715, found: 731.3716.



(*E*)-6-(4-(((3,7-Dimethylocta-2,6-dien-1-yl)oxy)methyl)phenyl)-6-oxo-*N*-(quinolin-8-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanamide (5e)

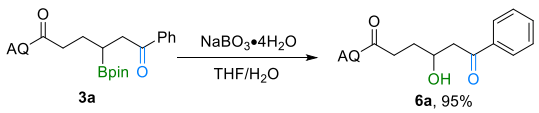
Pentane/EA = 3:1 (Rf = 0.35), yellow oil (26.6 mg, 43% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.88 – 8.69 (m, 2H), 8.15 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.98 – 7.89 (m, 2H), 7.55 – 7.47 (m, 2H), 7.44 (dd, *J* = 8.5, 4.0 Hz, 1H), 7.40 (d, *J* = 8.5 Hz, 2H), 5.41 (tq, *J* = 7.0, 1.5 Hz, 1H), 5.07 (dtt, *J* = 4.0, 2.5, 1.5 Hz, 1H), 4.53 (s, 2H), 4.02 (dd, *J* = 7.0, 1.0 Hz, 2H), 3.22 (d, *J* = 7.5 Hz, 2H), 2.68 (dd, *J* = 8.5, 7.0 Hz, 2H), 2.06 (d, *J* = 3.0 Hz, 5H), 1.99 – 1.91 (m, 1H), 1.76 (q, *J* = 1.0 Hz, 3H), 1.66 (d, *J* = 1.0 Hz, 3H), 1.58 (d, *J* = 1.0 Hz, 3H), 1.55 – 1.47 (m, 1H), 1.29 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.7, 171.8, 148.0, 143.9, 141.0, 138.4, 136.3, 136.1, 134.6, 132.0, 128.2, 127.9, 127.4, 127.3, 123.7, 121.5, 121.3, 116.4, 83.2, 71.4, 66.6, 41.1, 37.7, 32.2, 26.7, 26.6, 25.7, 24.8, 24.7, 23.5, 17.6.

HRMS (ESI): calcd for $[M+H]^+$ $C_{38}H_{49}BN_2O_5$ 625.3813, found: 625.3817.

6. Derivatization of *β*-Boryl ketones.



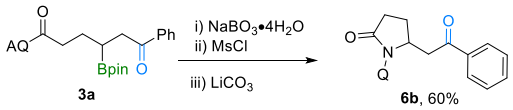
4-Hydroxy-6-oxo-6-phenyl-*N*-(quinolin-8-yl)hexanamide (6a)

The title compound was synthesized according to the following procedure:[1] To the boration product **3a** (229.0 mg, 0.5 mmol) in THF (2.5 mL) and water (2.5 mL) was added $NaBO_3 4H_2O$ (385 mg. 5 equiv). The reaction mixture was stirred vigorously for 0.5−1 h at room temperature. The reaction mixture was quenched with water and then extracted with ethyl acetate (5 mL). The combined organic layers were washed with brine (15 mL), dried over Na_2SO_4 and concentrated. The crude product was purified by column chromatography on silica gel to afford the corresponding product **6a** as white solid (165.2 mg, 95%)

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.93 (s, 1H), 8.85 – 8.71 (m, 2H), 8.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.00 – 7.91 (m, 2H), 7.61 – 7.42 (m, 6H), 4.44 – 4.28 (m, 1H), 3.79 (d, *J* = 2.5 Hz, 1H), 3.31 – 3.08 (m, 2H), 2.91 – 2.73 (m, 2H), 2.19 – 1.95 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 200.5, 171.7, 148.2, 138.3, 136.6, 136.3, 134.4, 133.5, 128.6, 128.1, 127.9, 127.3, 121.6, 121.5, 116.5, 67.1, 45.2, 34.2, 31.8.

HRMS (ESI): calcd for $[M+Na]^+$ $C_{21}H_{20}N_2O_3$ 371.1366, found: 371.1373.

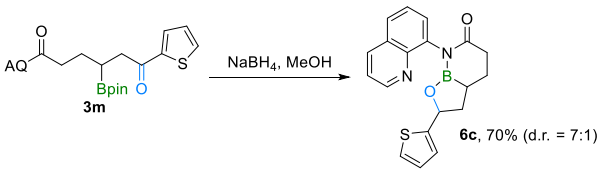


5-(2-Oxo-2-phenylethyl)-1-(quinolin-8-yl)pyrrolidin-2-one (6b)

In a Schlenk tube, a solution of **6b** (69.6 mg, 0.2 mmol) and triethylamine (42 µL, 0.3 mmol) in anhydrous DCM (2 mL) was cooled at 0 °C under argon. Then, methanesulfonyl chloride (20 µL, 1.3 equiv) was added dropwise, and the mixture was stirred for 1 h at 0 °C, warmed to room temperature and stirred for additional 3 h. The reaction mixture was extracted with DCM (3 x 15 mL), and the organic phases were combined, washed with 10% aqueous HCl solution and dried over magnesium sulfate. The solvent was evaporated under reduced pressure, and the product was transferred to a Schlenk tube containing Li_2CO_3 (30 mg, 2.0 equiv) and acetonitrile (5 mL). The reaction mixture was maintained at reflux under argon for 24 h. Then, the mixture was extracted with EtOAc (3 x 10 mL), dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel to afford the corresponding product **6b** as brown solid (41.6 mg, 63%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.91 (dd, *J* = 4.2, 1.8 Hz, 1H), 8.15 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.79 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.72 – 7.64 (m, 3H), 7.55 (dd, *J* = 8.2, 7.3 Hz, 1H), 7.51 – 7.44 (m, 1H), 7.41 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.36 – 7.29 (m, 2H), 5.36 – 5.21 (m, 1H), 3.21 – 3.01 (m, 2H), 2.81 – 2.68 (m, 3H), 2.08 – 1.91 (m, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 197.5, 175.7, 150.4, 144.4, 136.5, 136.2, 134.6, 133.2, 130.1, 129.4, 128.5, 128.2, 127.8, 126.3, 121.6, 58.2, 43.2, 30.8, 26.0.



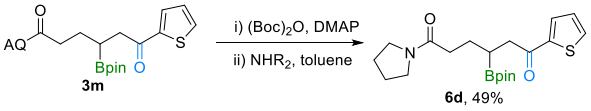
7-(Quinolin-8-yl)-2-(thiophen-2-yl)tetrahydro-2*H*-[1,2]oxaborolo[2,3-b][1,2]azaborinin-6(7*H*)-one

To the boration product **3m** (46.4 mg, 0.1 mmol) in MeOH (2.0 mL) was added $NaBH_4$ (5.7 mg. 1.5 equiv). The reaction mixture was stirred vigorously for 1 h at room temperature. The reaction mixture was quenched with water and then extracted with ethyl acetate (5 mL). The combined organic layers were washed with brine (15 mL), dried over Na_2SO_4 and concentrated. The crude product was purified by column chromatography on silica gel to afford the corresponding product **6c** as bright yellow solid (24.4 mg, 70%)

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.7, 149.6, 140.3, 139.9, 139.8, 137.0, 132.1, 127.3, 126.3, 123.7, 122.7, 122.4, 118.1, 117.4, 75.6, 42.4, 33.4, 28.4.

^{11}B NMR (96 MHz, $CDCl_3$) δ 12.1.

HRMS (ESI): calcd for $[M+H]^+$ $C_{19}H_{19}BN_2O_3S$ 349.1185, found: 349.1182.



6-(Pyrrolidin-1-yl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1-(thiophen-2-yl)hexane-1,6-dione (6d)

The title compound was synthesized according to the following procedure:[2] To a 25-mL round-bottom flask containing a Teflon-coated magnetic stir bar, were added 3m (46.4 mg, 0.1 mmol), DMAP (10 mol%), and Boc anhydride (2 equiv). The reaction flask was evacuated and backfilled with N_2, followed by addition of anhydrous MeCN (0.1 M). The reaction mixture was heated at 60 ºC for 2 h. After cooling to room temperature, the reaction was concentrated under vacuum and purified by column chromatography (pentane:EtOAc = 1:1) to afford the Bocprotected amide. The Boc amide was then dissolved in toluene (0.5 M), followed by addition of pyrrolidine (1.5 equiv). The reaction mixture was heated under N_2 atmosphere at 60 ºC overnight. Upon completion, the organic mixture was concentrated under vacuum and purified by column chromatography (pentane:EtOAc = 1:1) to afford pure product.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 3.8, 1.1 Hz, 1H), 7.56 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.07 (dd, *J* = 5.0, 3.8 Hz, 1H), 3.45 – 3.34 (m, 4H), 3.08 (d, *J* = 7.1 Hz, 2H), 2.42 – 2.23 (m, 2H), 1.96 – 1.71 (m, 6H), 1.47 – 1.32 (m, 1H), 1.21 (s, 6H), 1.20 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 193.0, 171.5, 144.0, 133.0, 131.7, 127.9, 83.0, 46.5, 45.5, 41.5, 34.1, 26.0, 25.8, 24.7, 24.7, 24.3.

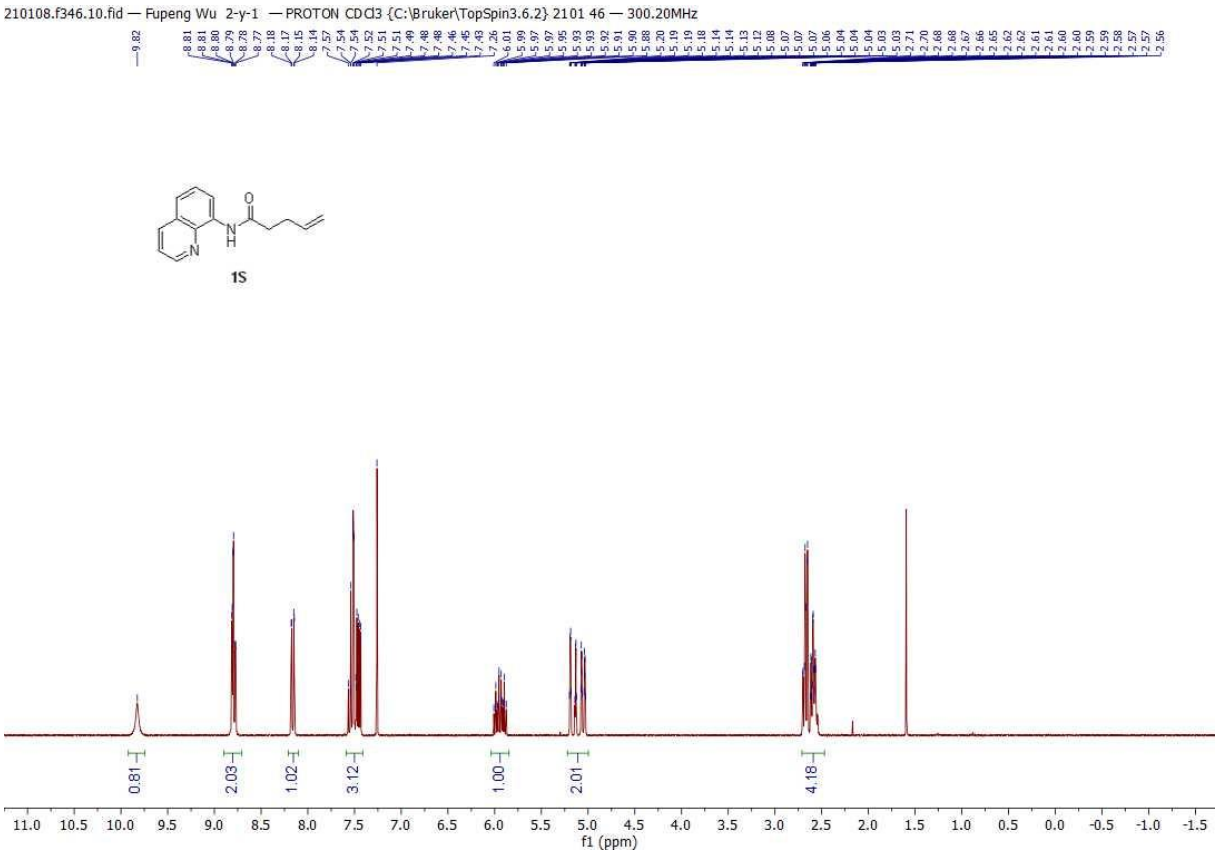
HRMS (ESI): calcd for $[M+H]^+$ $C_{20}H_{30}BNO_4S$ 392.2070, found: 392.2069.

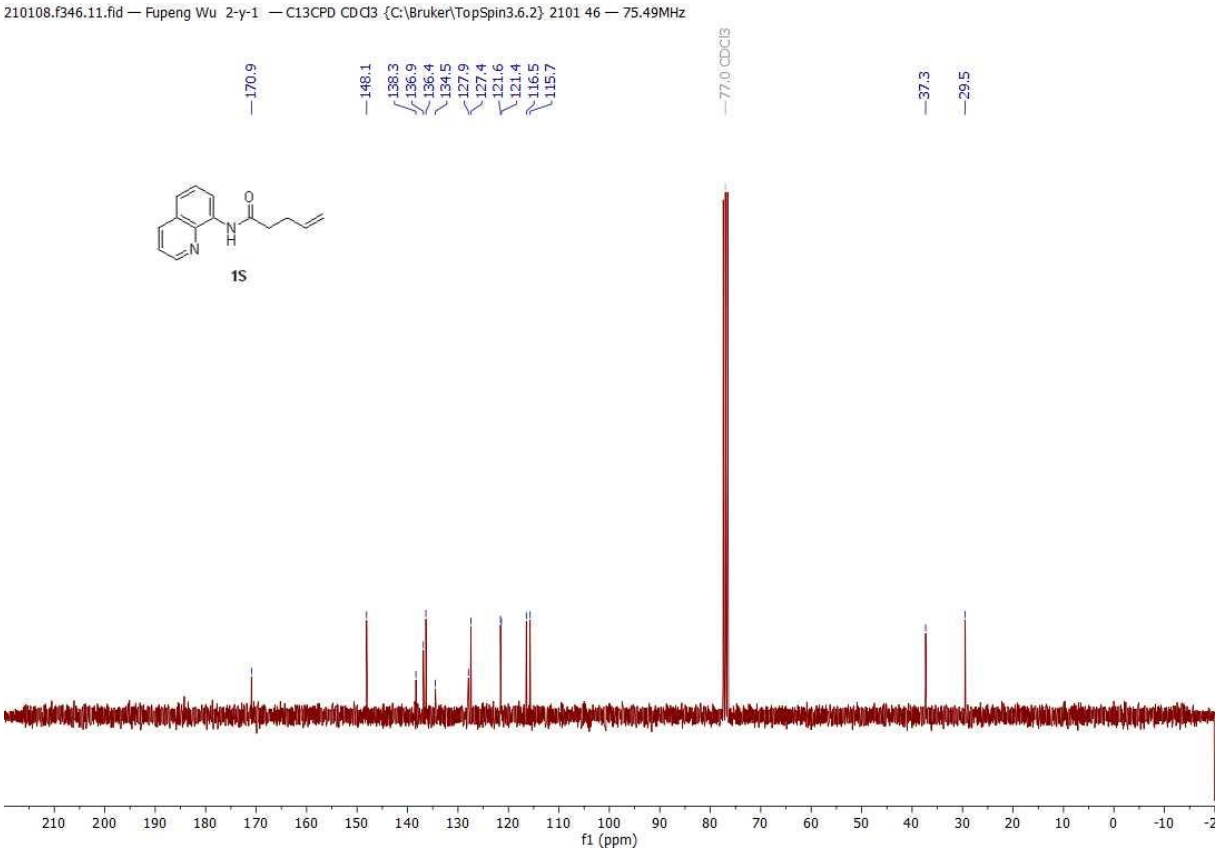
7. References

[1] J.-E. Lee, J. Yun, *Angew. Chem. Int. Ed.* **2008**, *47*, 145.
[2] O. Verho, M. P. Lati, M. Oshmann, *J. Org. Chem.* **2018**, *83*, 4464.
[3] J. Jeon, H. Ryu, C. Lee, D. Cho, M.-H. Baik, S. Hong, *J. Am. Chem. Soc.* **2019**, *141*, 10048.
[4] M. J. Kier, R. M. Leon, N. F. O'Rourke, A. L. Rheingold, G. C. Micalizio, *J. Am. Chem. Soc.* **2017**, *139*, 12374.
[5] J.-C. Wu, L. -B. Gong, Y. Xia, R.-J. Song, Y.-X. Xie, J.-H. Li, *Angew. Chem. Int. Ed.* **2012**, *51*, 9909.

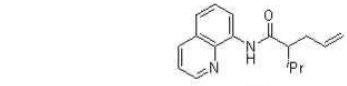
8. NMR Spectra of the Alkenes and *β*-boryl ketones

8.1 NMR spectra of the alkenes.

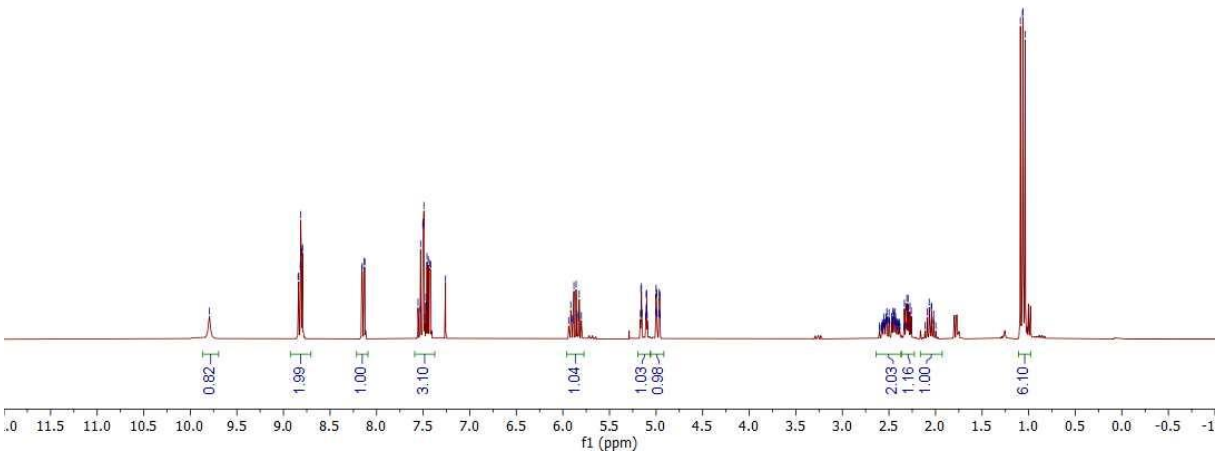




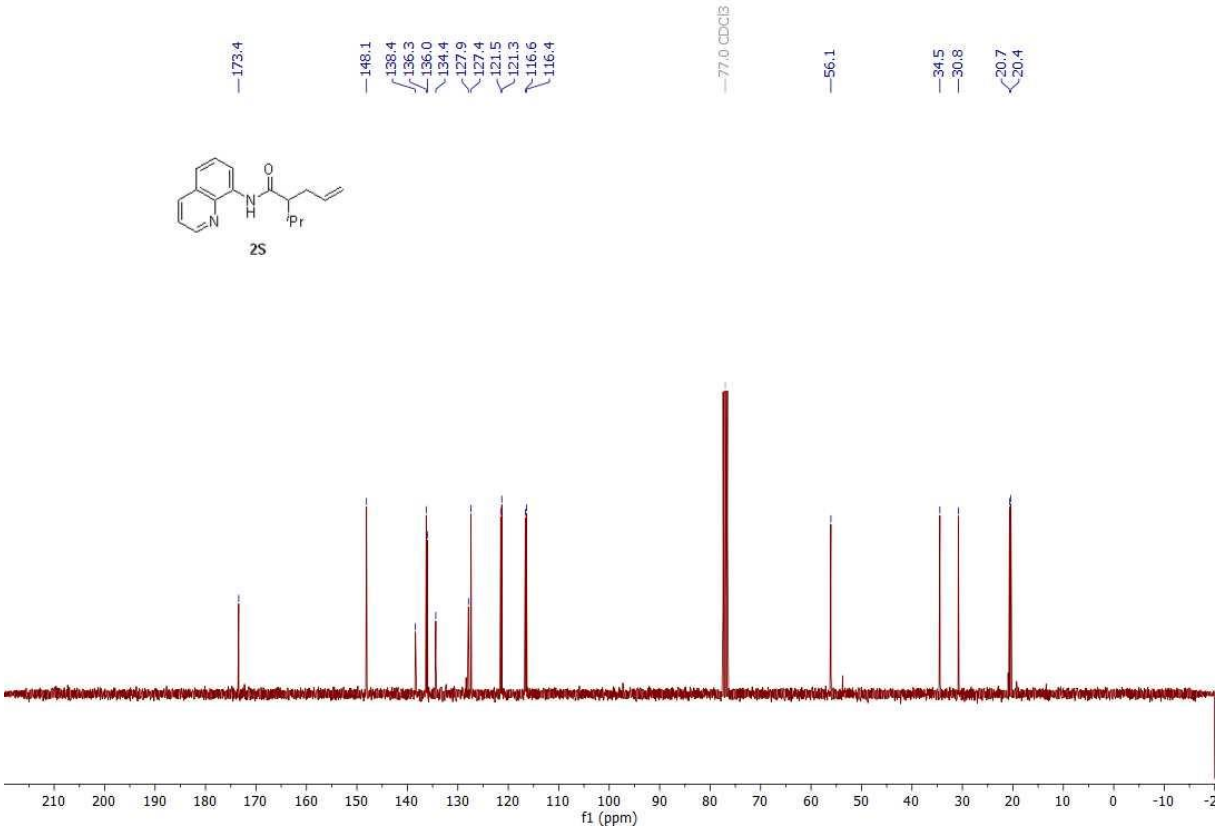
210308.f351.10.fid — Fupeng Wu Q-y-7 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 51 — 300.20MHz

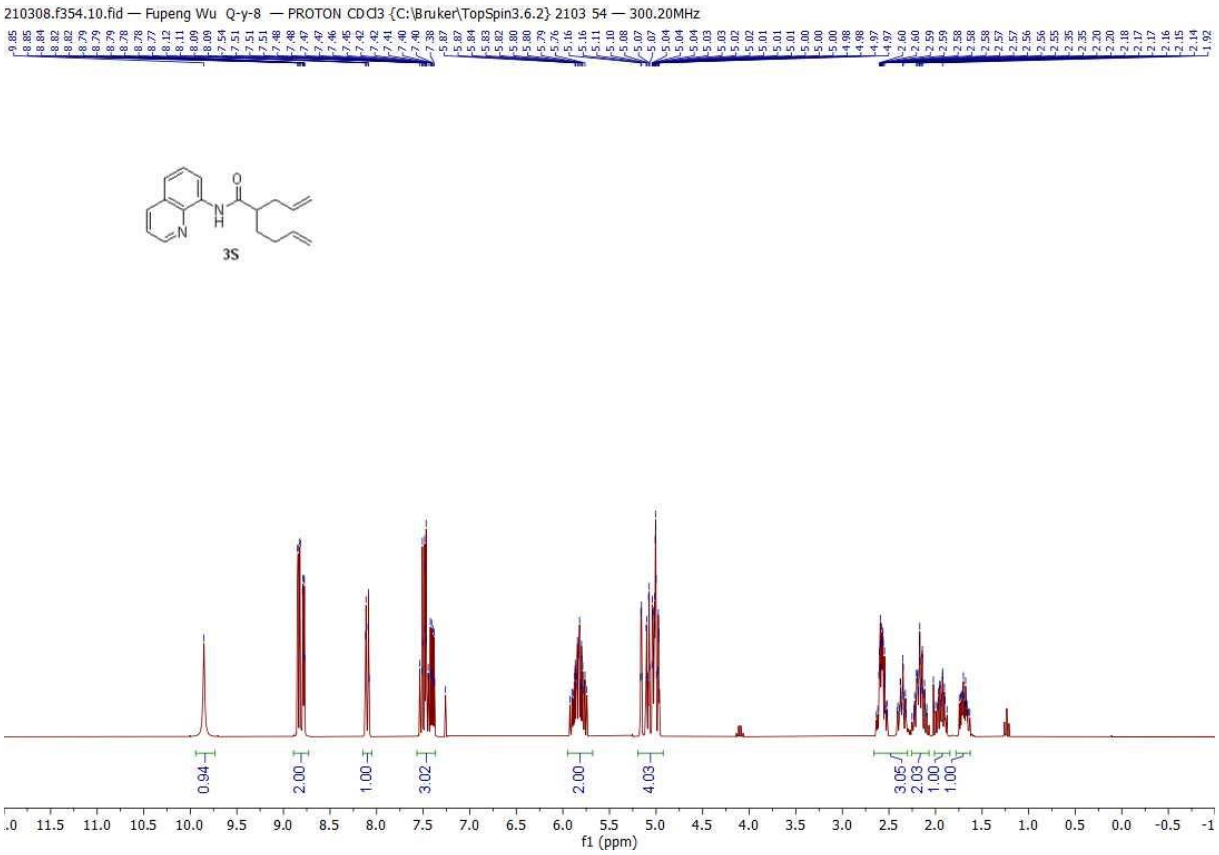


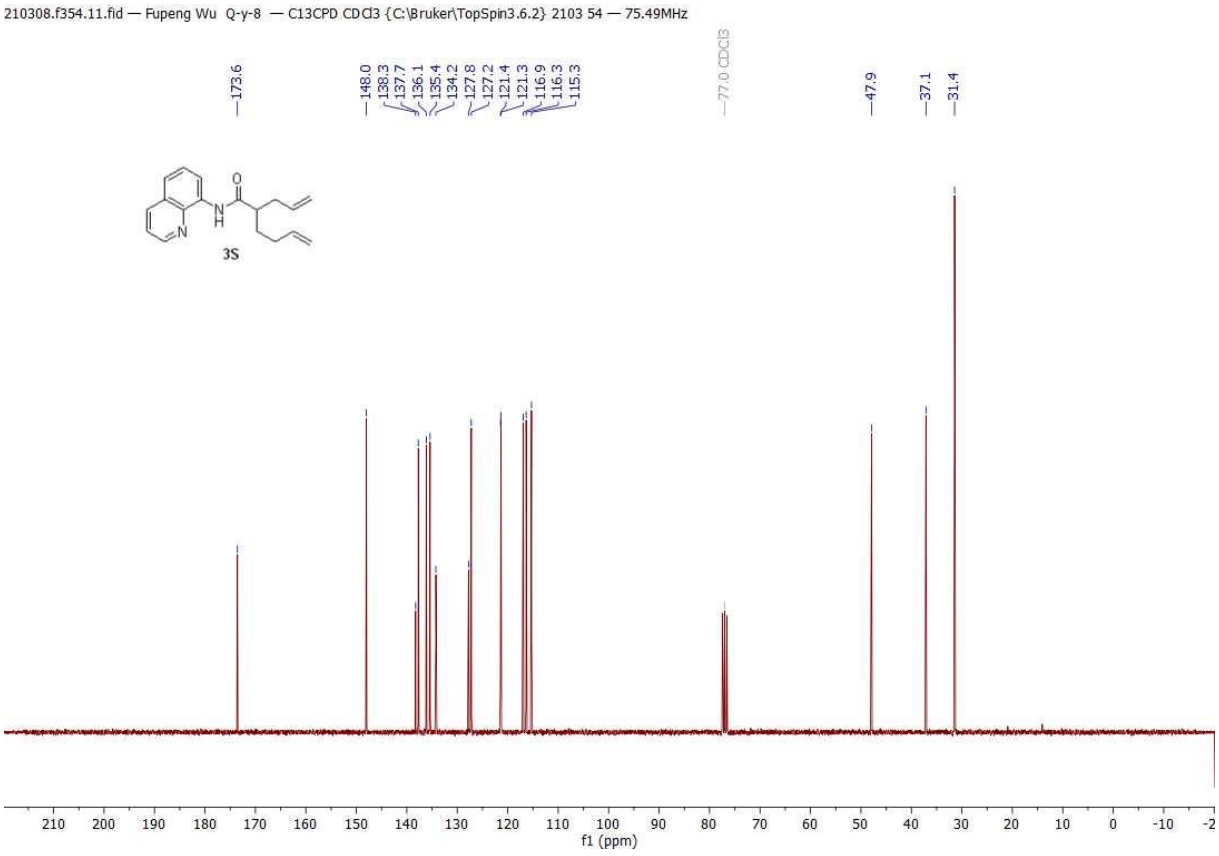
2S

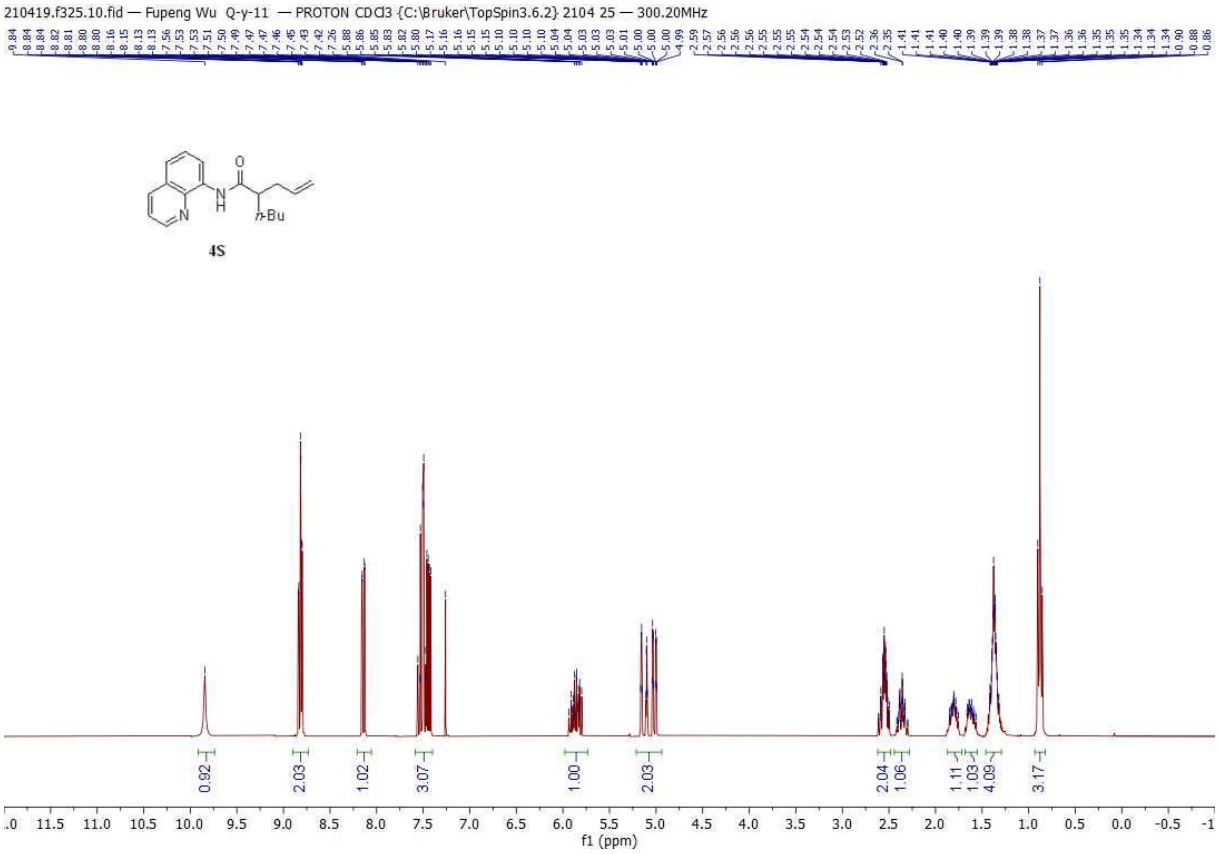


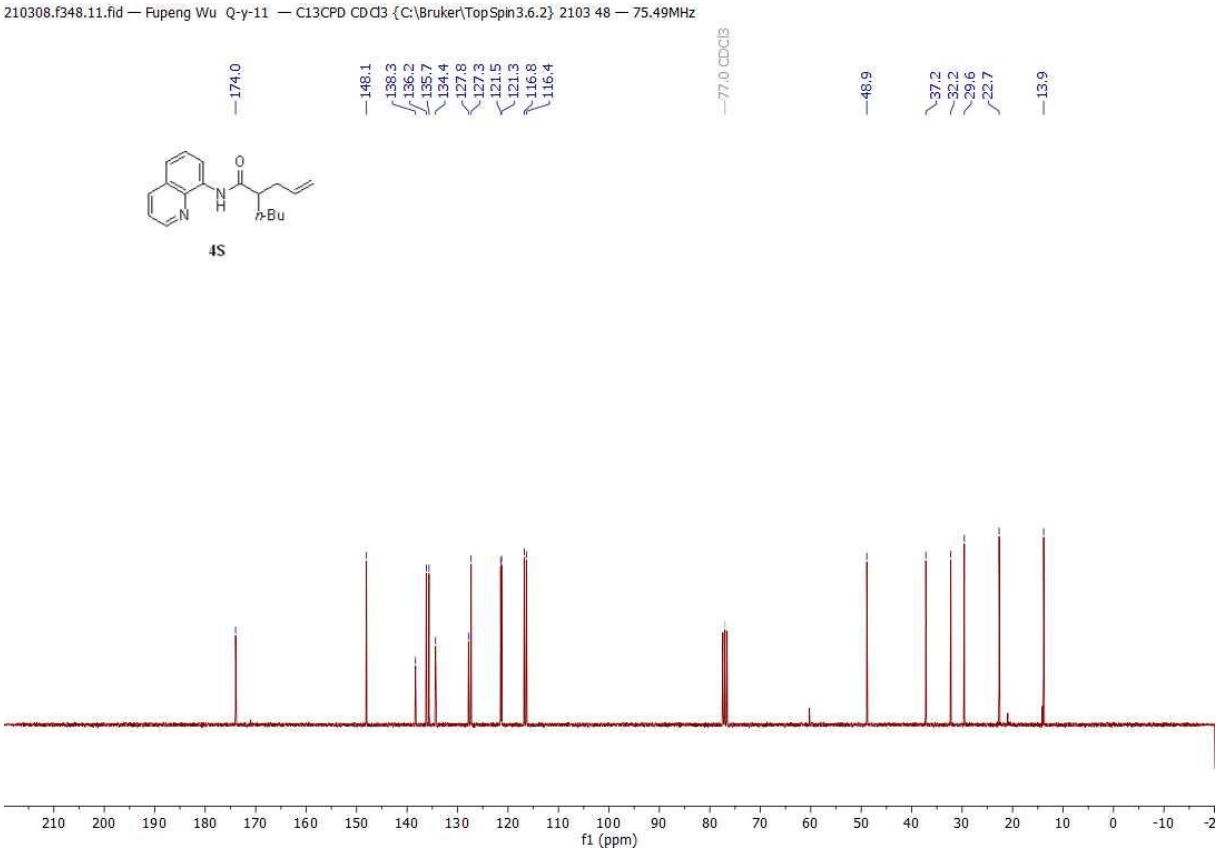
210308.f351.11.fid — Fupeng Wu Q-y-7 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 51 — 75.49MHz



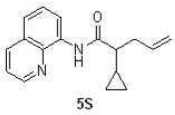

210308.f354.10.fid — Fupeng Wu Q-y-8 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 54 — 300.20MHz
3S
0.94
2.00
1.00
3.02
2.00
4.03
3.05
2.03
1.00
1.00
f1 (ppm)


210308.f354.11.fid — Fupeng Wu Q-y-8 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 54 — 75.49MHz
173.6
148.0
138.3
137.7
136.1
135.4
134.2
127.8
127.2
121.4
121.3
116.9
116.3
115.3
77.0 CDCl3
47.9
37.1
31.4
3S
f1 (ppm)

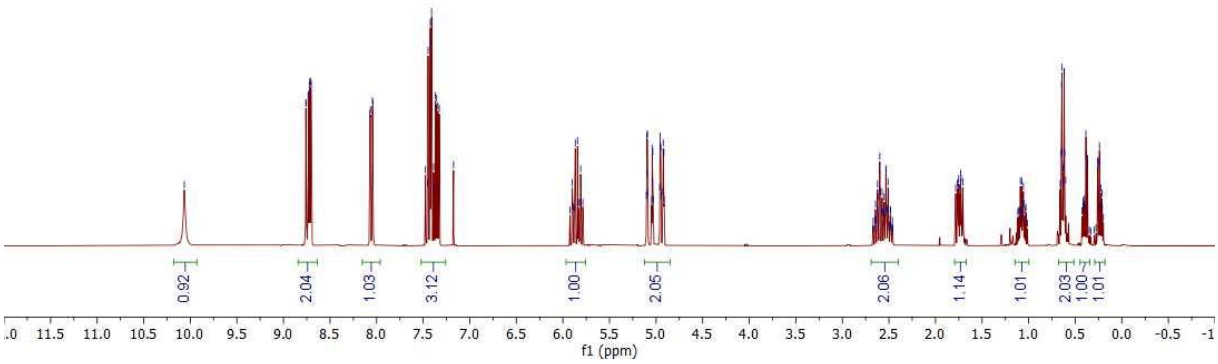

210419.f325.10.fid — Fupeng Wu Q-y-11 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2104 25 — 300.20MHz
4S
0.92
2.03
1.02
3.07
1.00
2.03
2.04
1.06
1.11
1.03
4.09
3.17
f1 (ppm)


210308.f348.11.fid — Fupeng Wu Q-y-11 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 48 — 75.49MHz
174.0
148.1
138.3
136.2
135.7
134.4
127.8
127.3
121.5
121.3
116.8
116.4
77.0 CDCl3
48.9
37.2
32.2
29.6
22.7
13.9
4S
f1 (ppm)

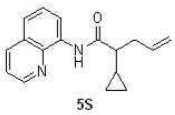
210318.f346.10.fid — Fupeng Wu Q-y-35 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 46 — 300.20MHz



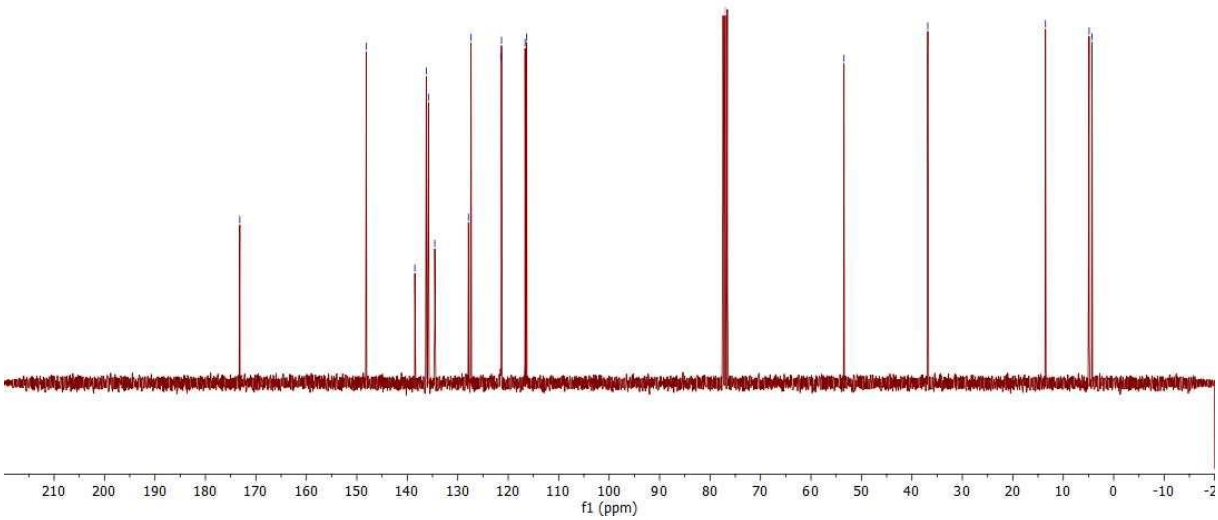
5S



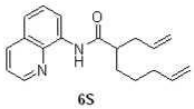
210318.f346.11.fid — Fupeng Wu Q-y-35 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 46 — 75.49MHz



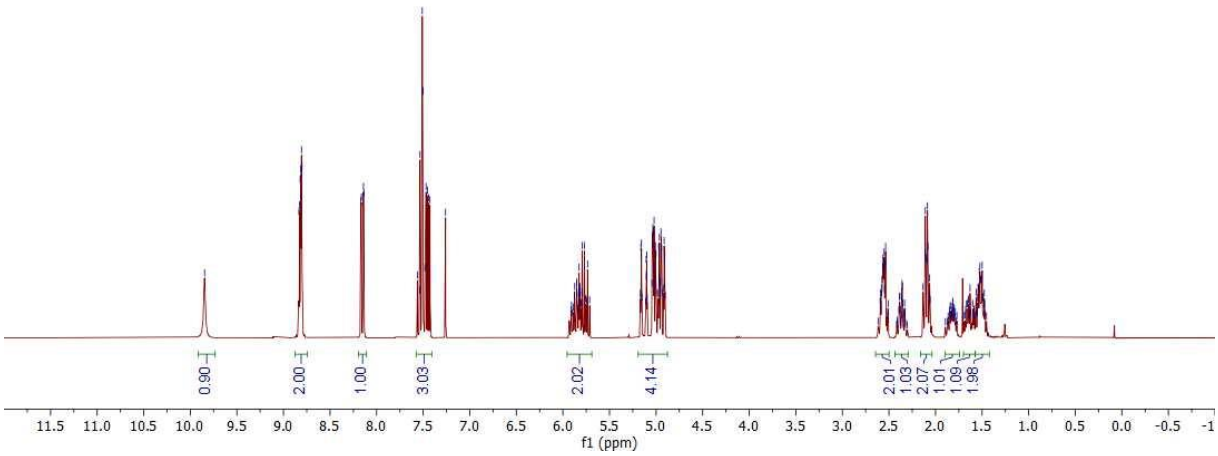
5S



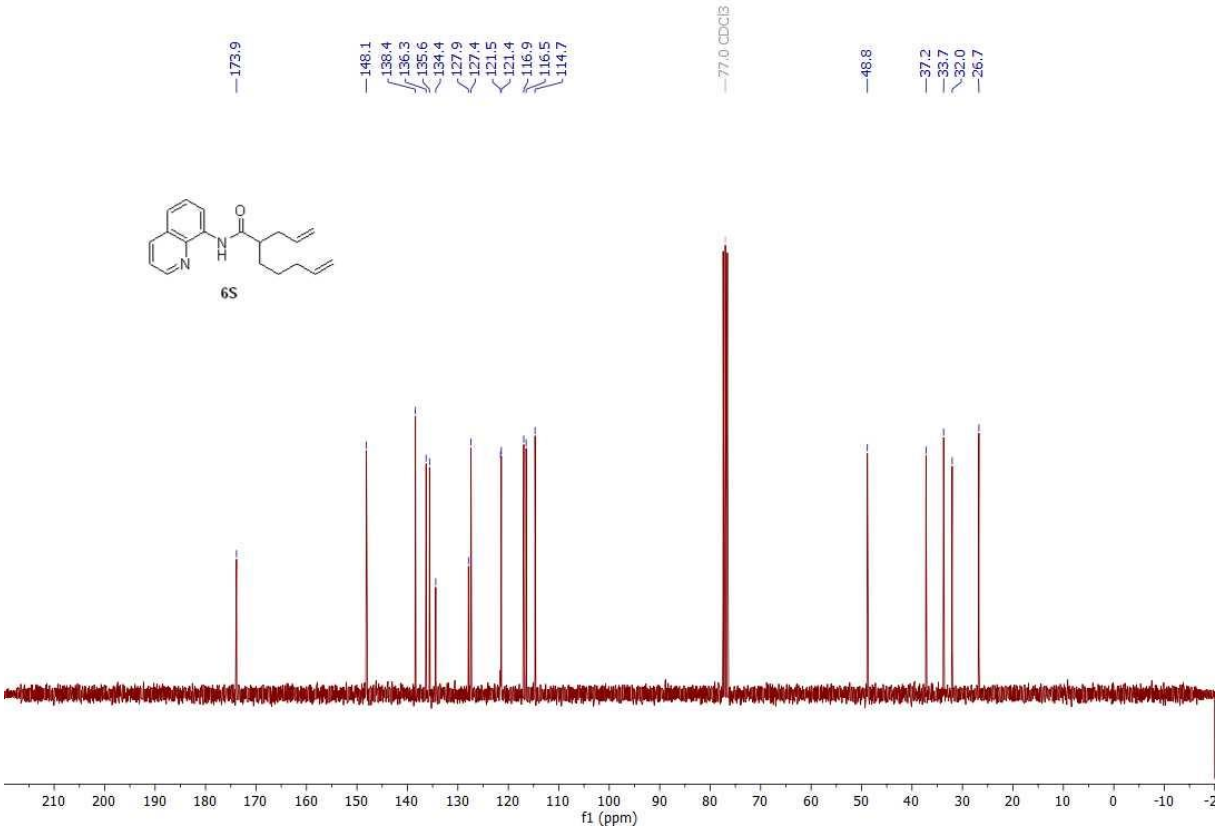
210318.f345.10.fid — Fupeng Wu Q-y-34 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 45 — 300.20MHz



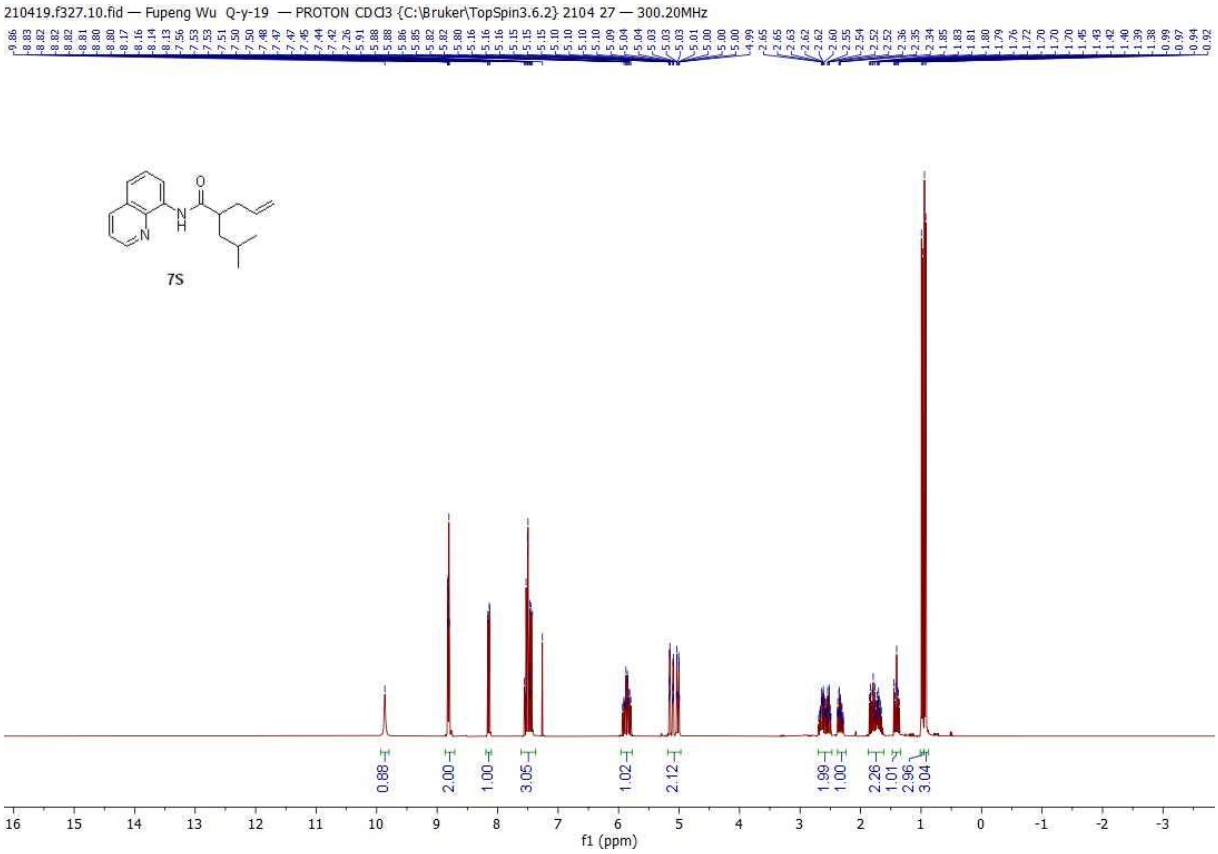
6S

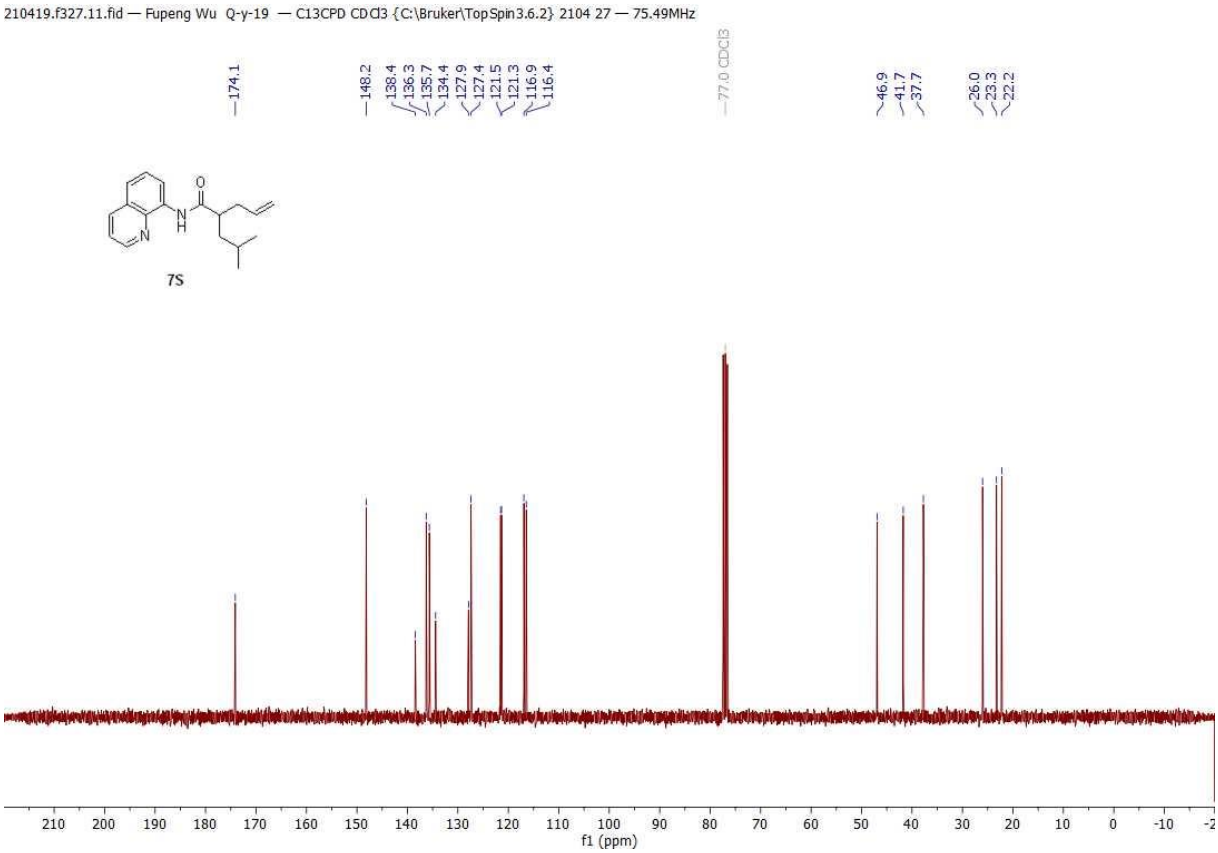


210318.f345.11.fid — Fupeng Wu Q-y-34 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 45 — 75.49MHz

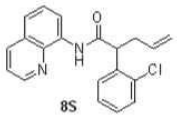


6S

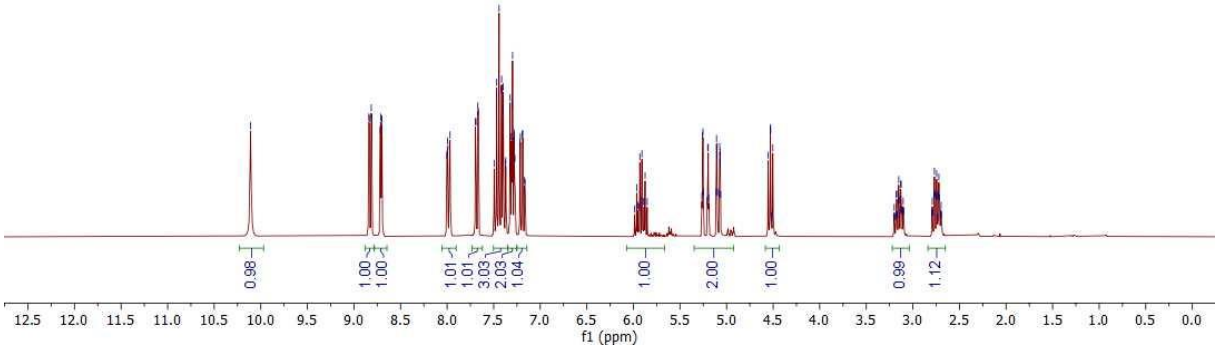

210419.f327.10.fid — Fupeng Wu Q-y-19 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2104 27 — 300.20MHz
7S
0.88
2.00
1.00
3.05
1.02
2.12
1.99
1.00
2.26
1.01
2.96
3.04
f1 (ppm)


210419.f327.11.fid — Fupeng Wu Q-y-19 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2104 27 — 75.49MHz
174.1
148.2
138.4
136.3
135.7
134.4
127.9
127.4
121.5
121.3
116.9
116.4
77.0 CDCl3
46.9
41.7
37.7
26.0
23.3
22.2
7S
f1 (ppm)

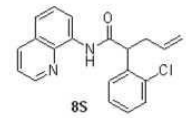
210303.f373.10.fid — Fupeng Wu Q-y-4 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 13 — 300.20MHz



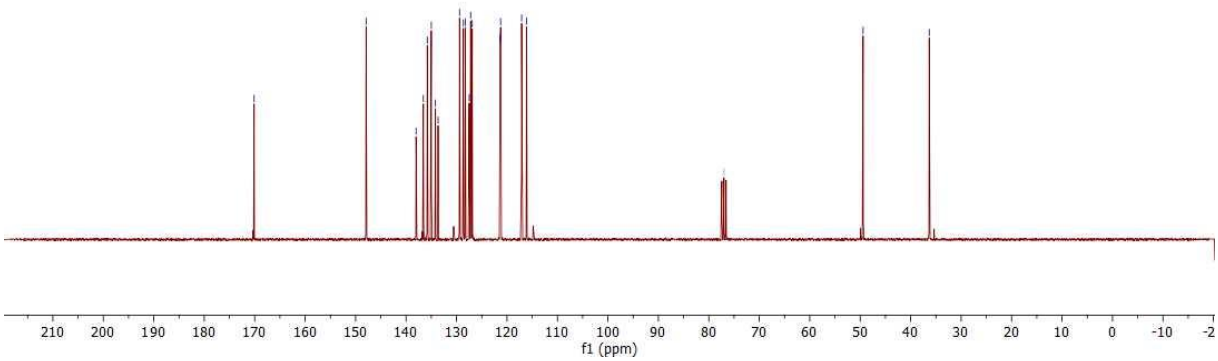
8S



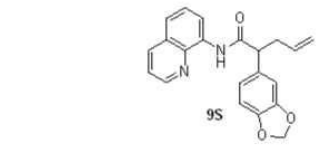
210303.f373.11.fid — Fupeng Wu Q-y-4 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 13 — 75.49MHz

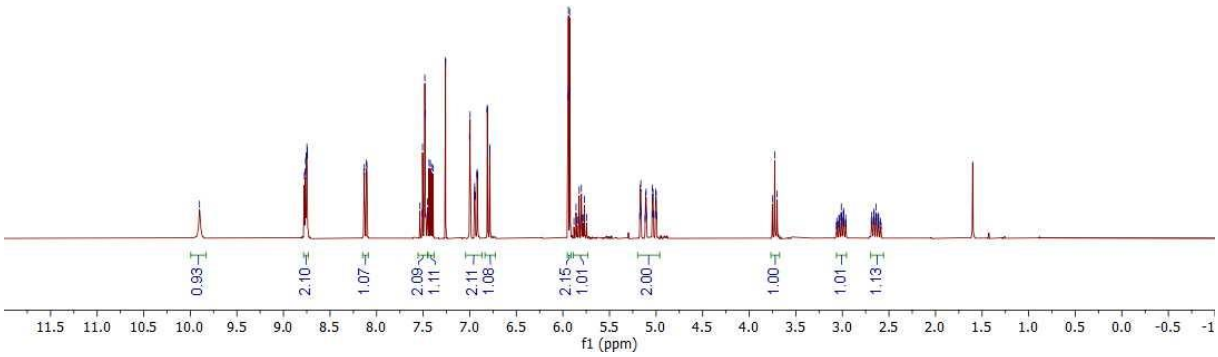


8S

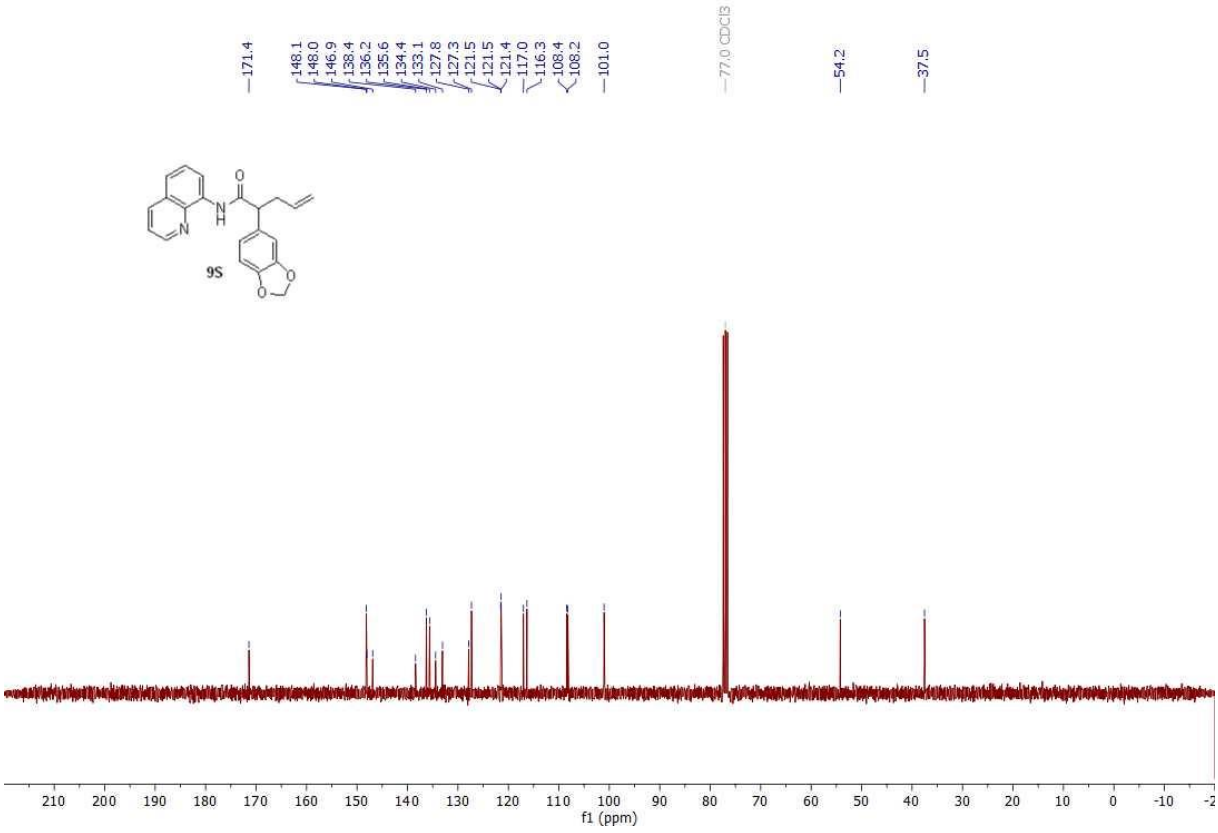


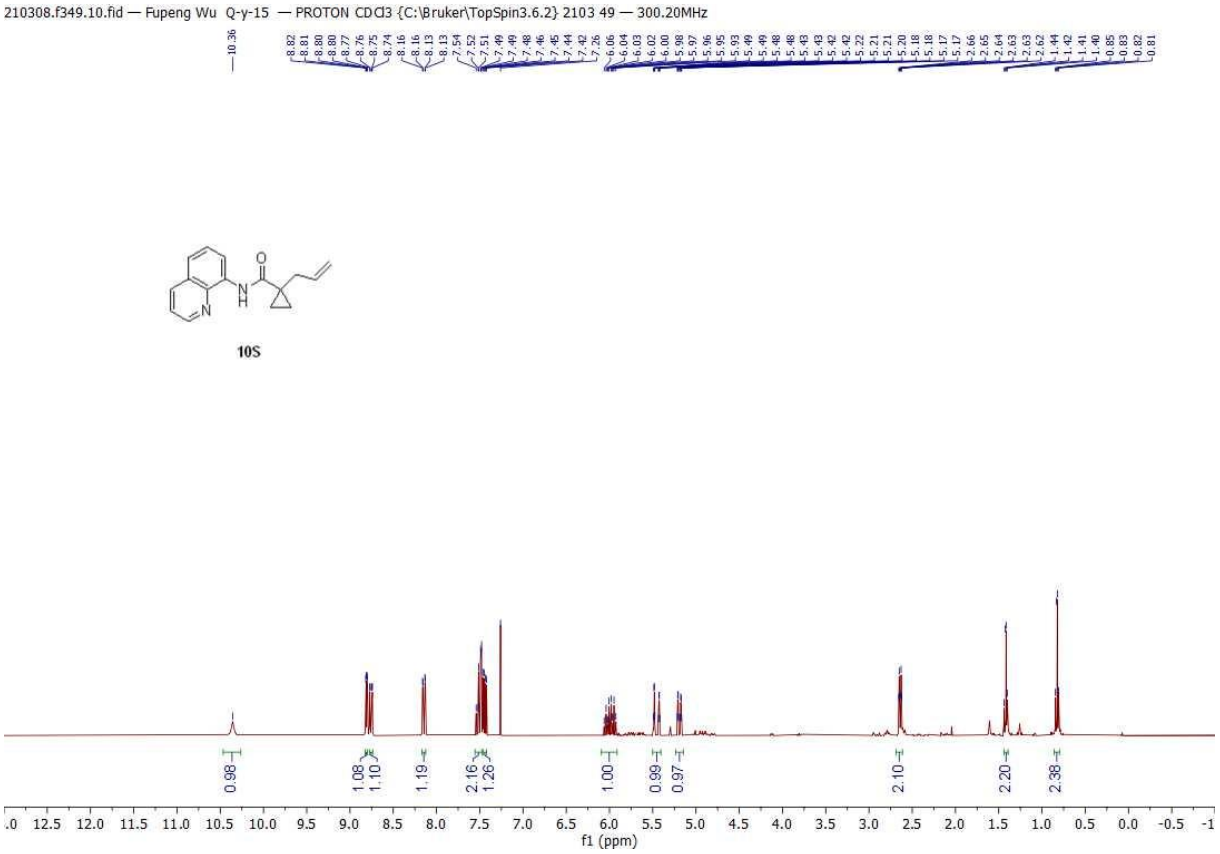
210419.f324.10.fid — Fupeng Wu Q-y-5 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2104 24 — 300.20MHz

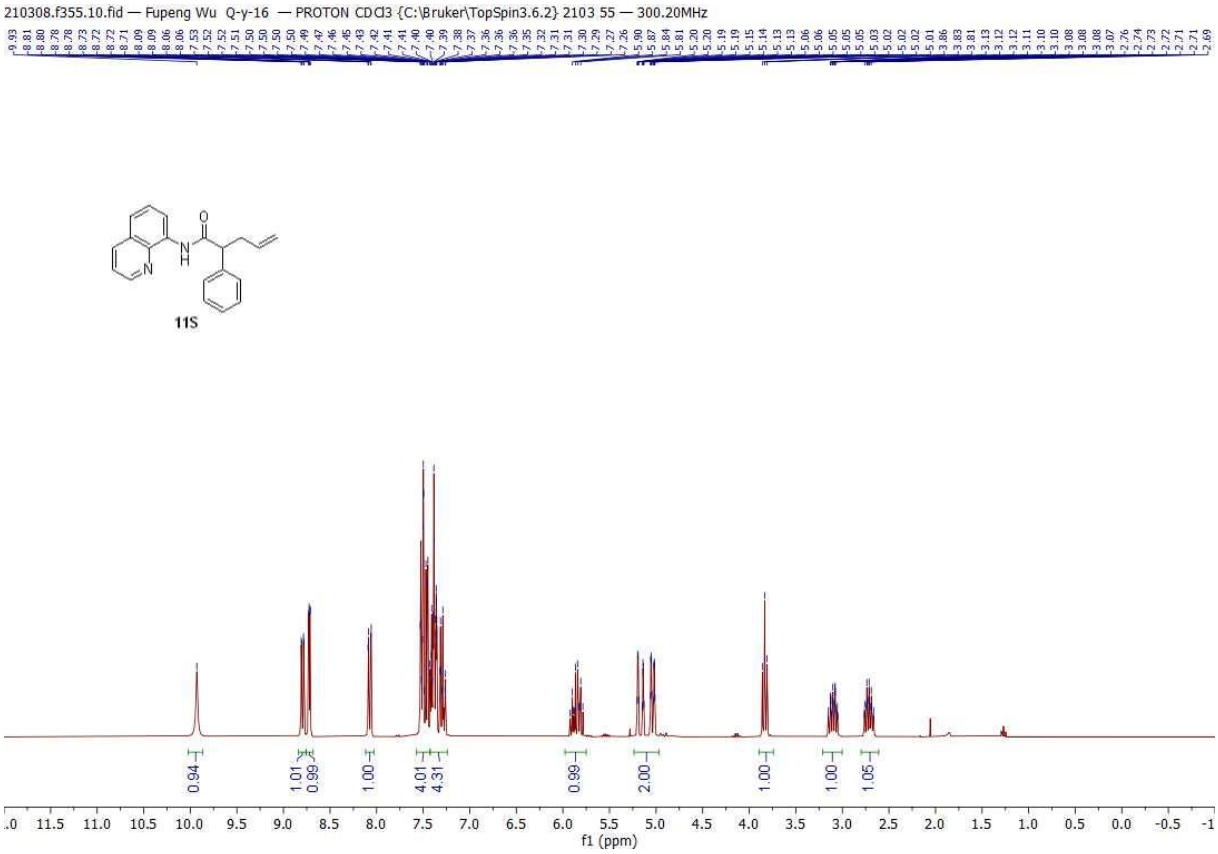


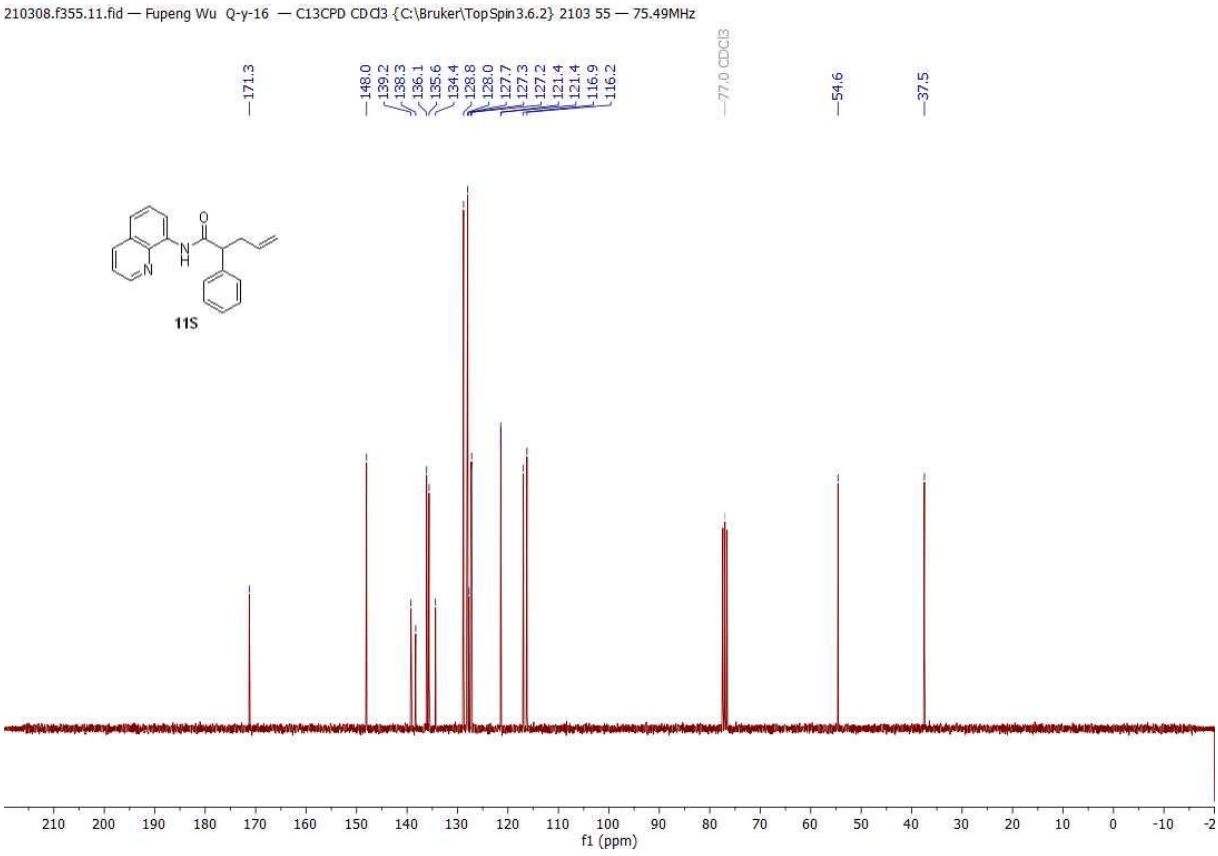


210308.f346.11.fid — Fupeng Wu Q-y-5 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 46 — 75.49MHz

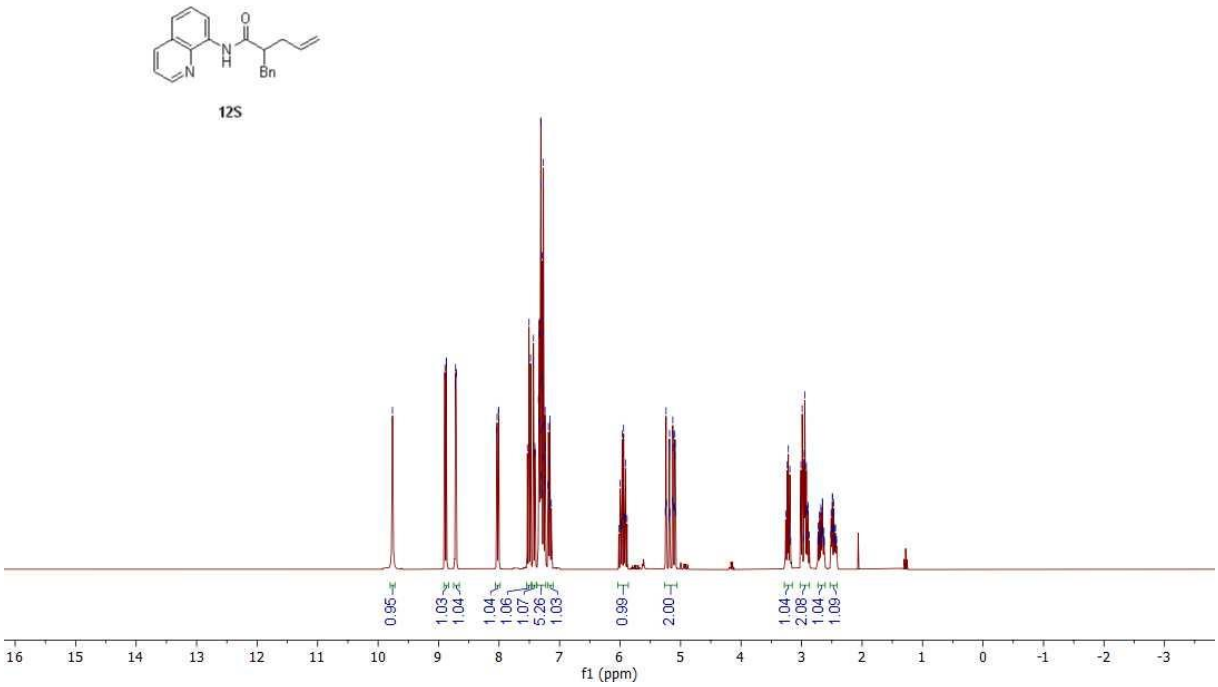



210308.f349.10.fid — Fupeng Wu Q-y-15 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 49 — 300.20MHz
10S
f1 (ppm)
210308.f349.11.fid — Fupeng Wu Q-y-15 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 49 — 75.49MHz
77.0 CDCl3
10S
f1 (ppm)

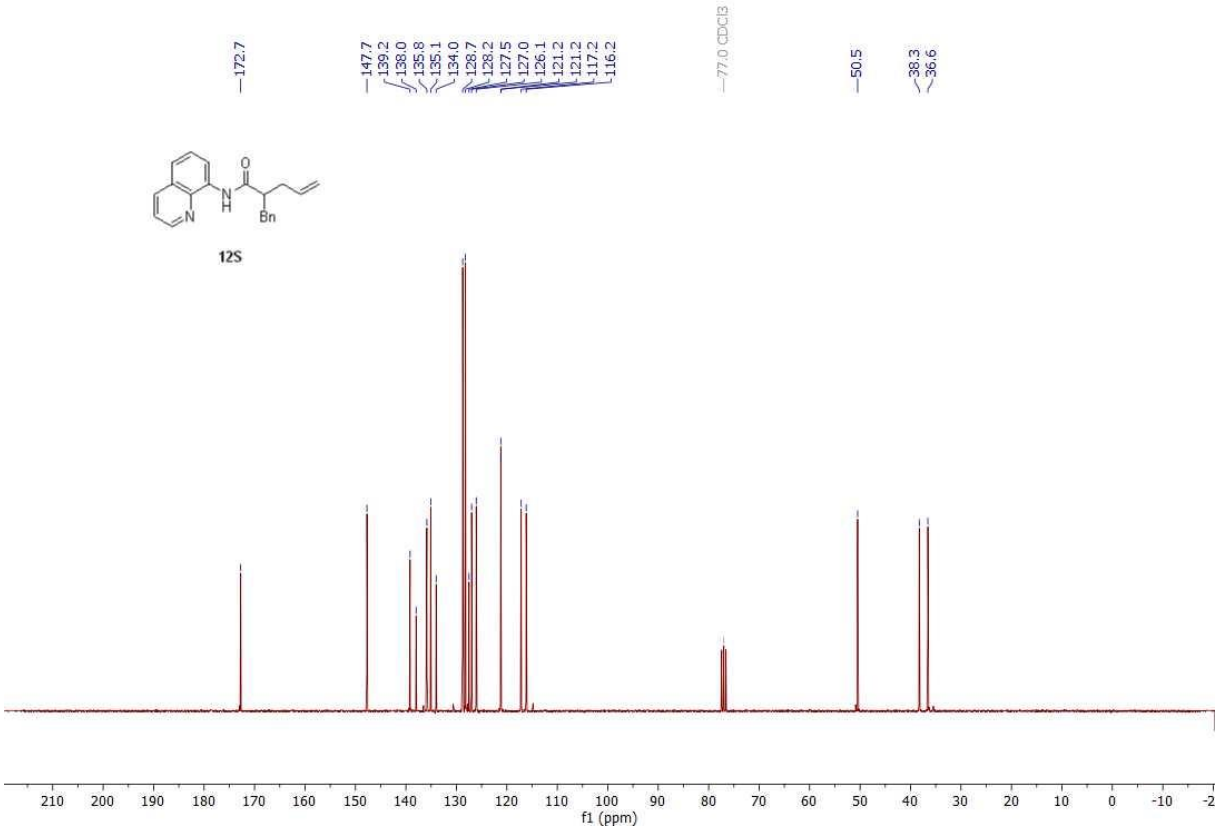

210308.f355.10.fid — Fupeng Wu Q-y-16 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 55 — 300.20MHz
11S
0.94
1.01
0.99
1.00
4.01
4.31
0.99
2.00
1.00
1.00
1.05
f1 (ppm)


210308.f355.11.fid — Fupeng Wu Q-y-16 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 55 — 75.49MHz
171.3
148.0
139.2
138.3
136.1
135.6
134.4
128.8
128.0
127.7
127.3
127.2
121.4
121.4
116.9
116.2
77.0 CDCl3
54.6
37.5
11S
f1 (ppm)

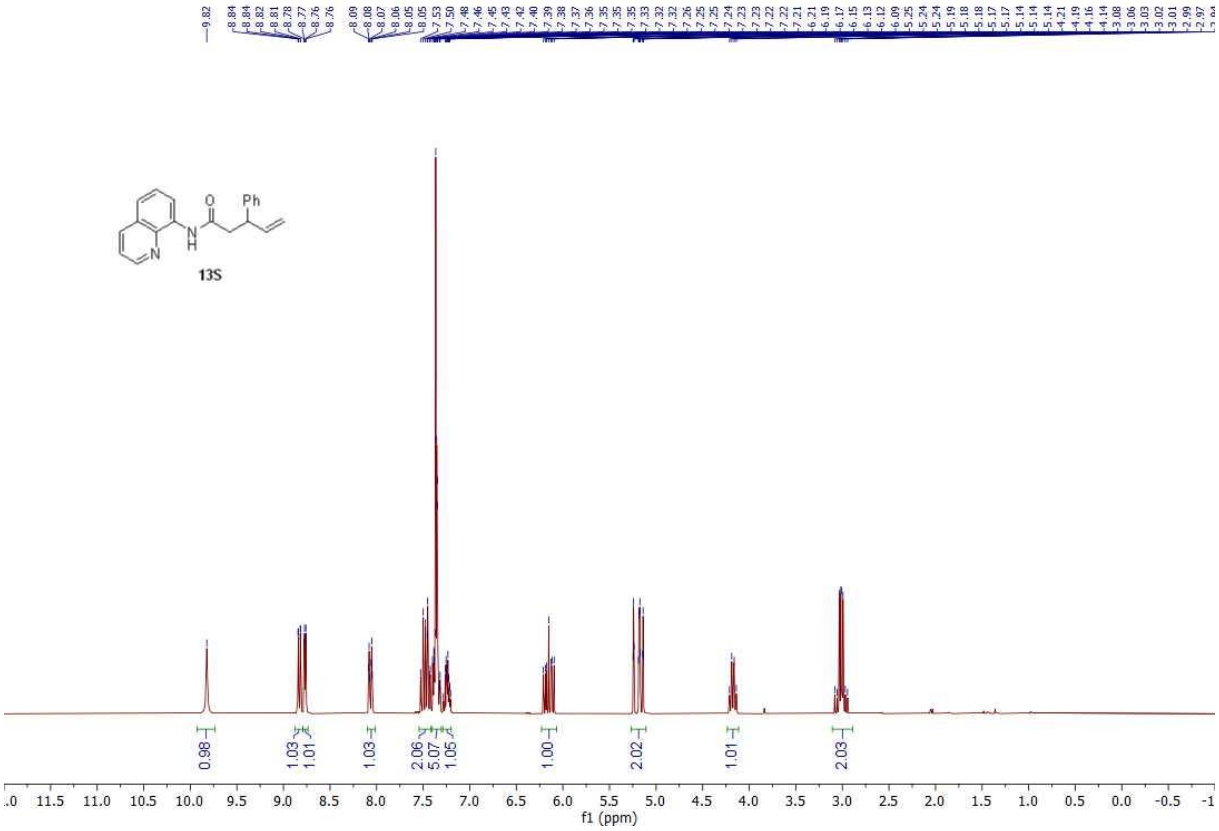
210308.f352.10.fid — Fupeng Wu Q-y-18 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 52 — 300.20MHz



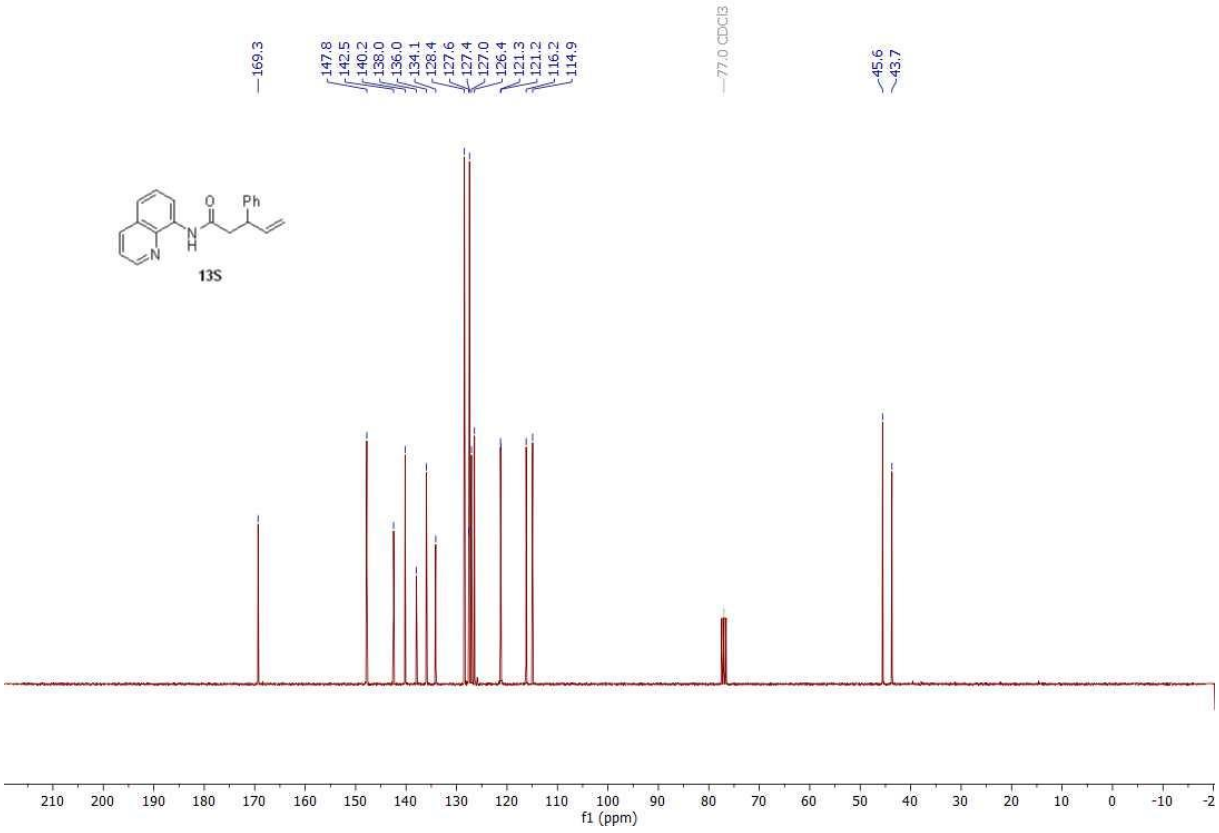
210308.f352.11.fid — Fupeng Wu Q-y-18 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 52 — 75.49MHz

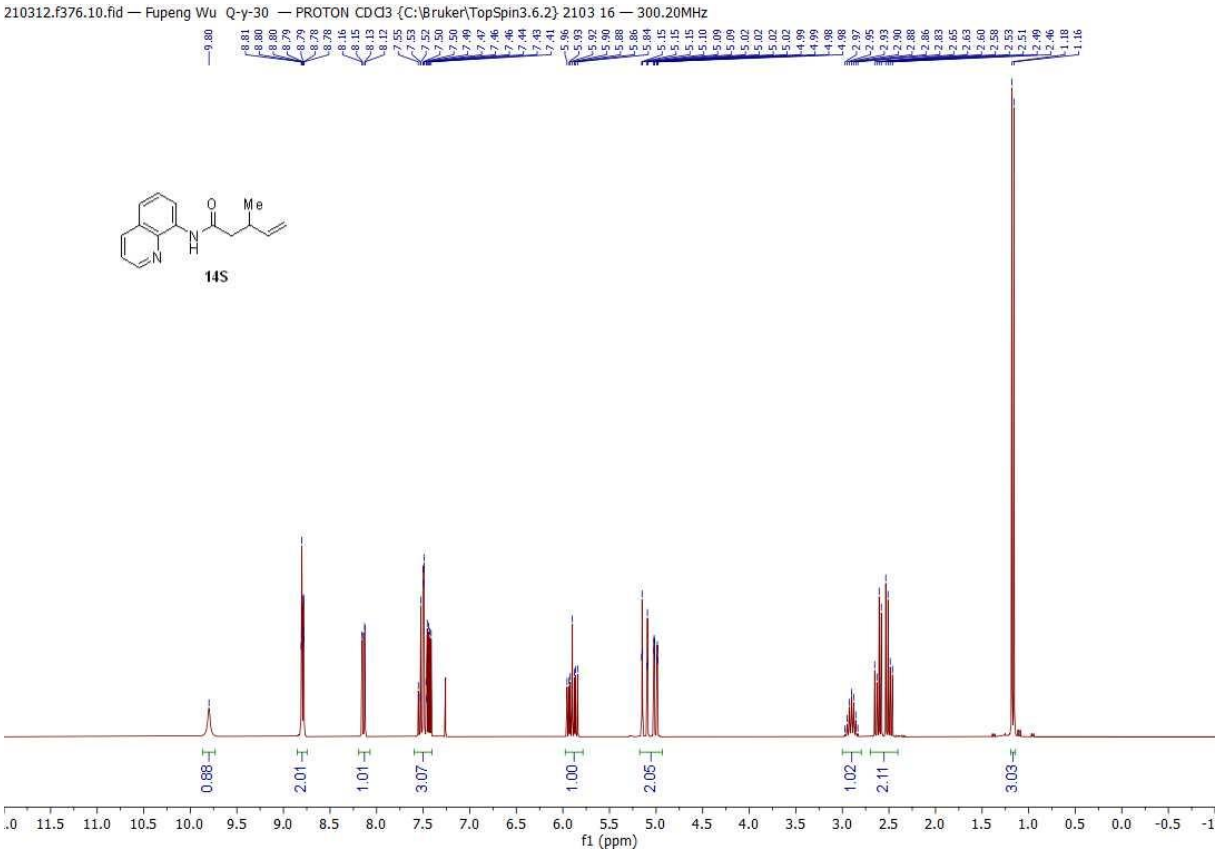


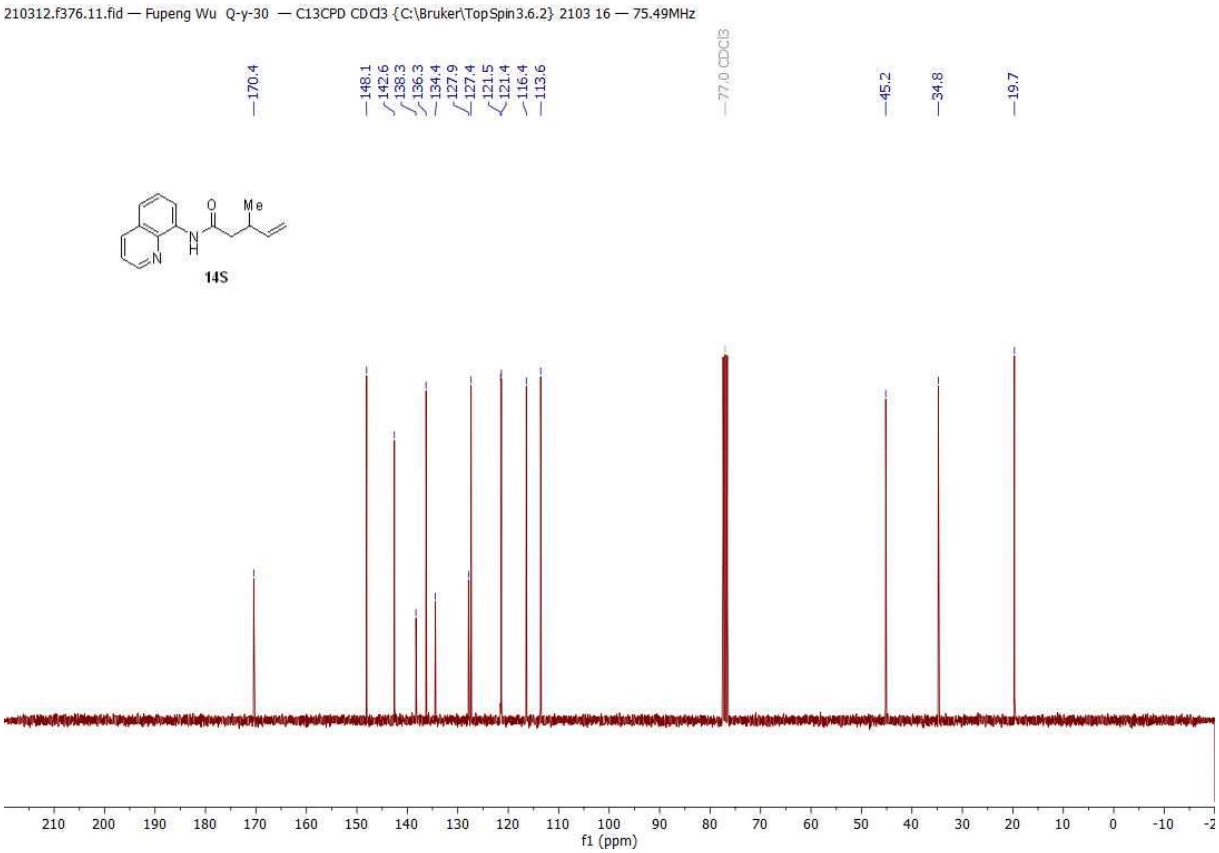
210312.f375.10.fid — Fupeng Wu Q-y-9 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 15 — 300.20MHz

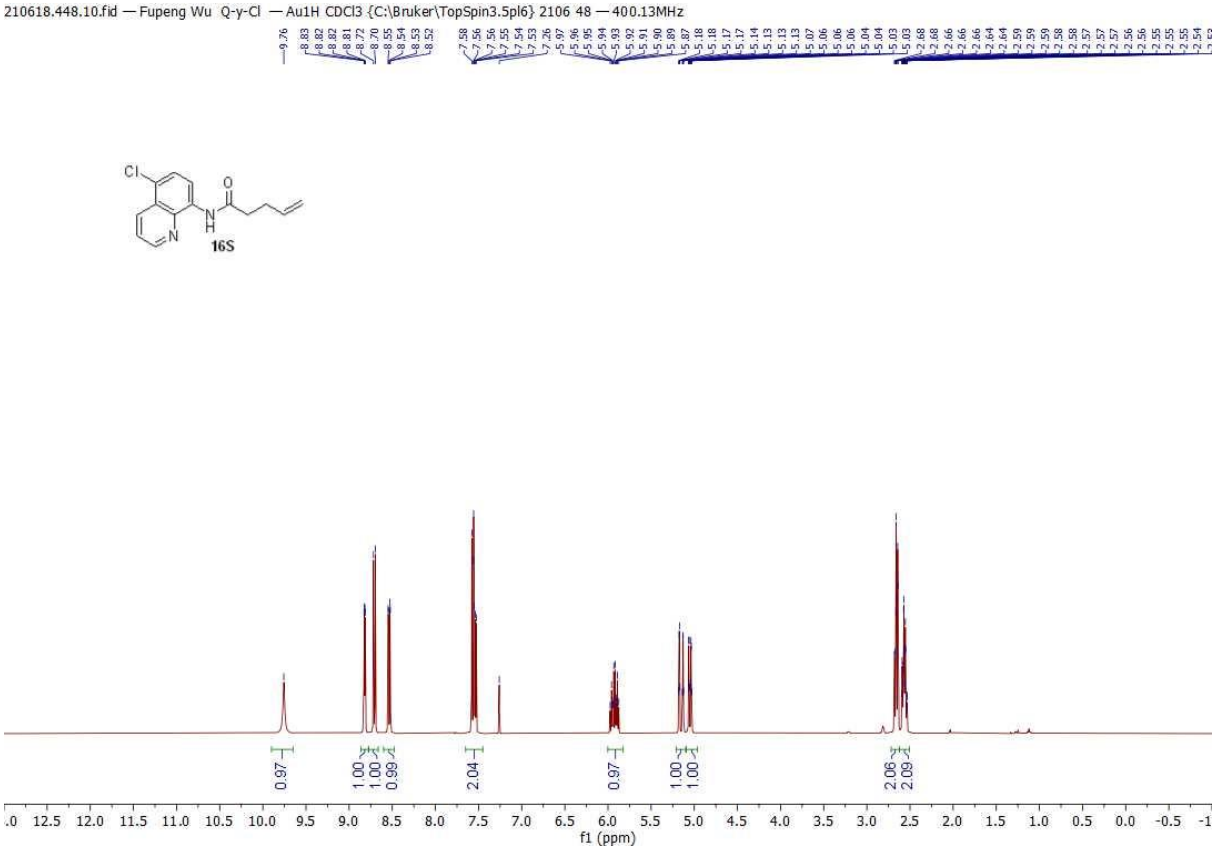


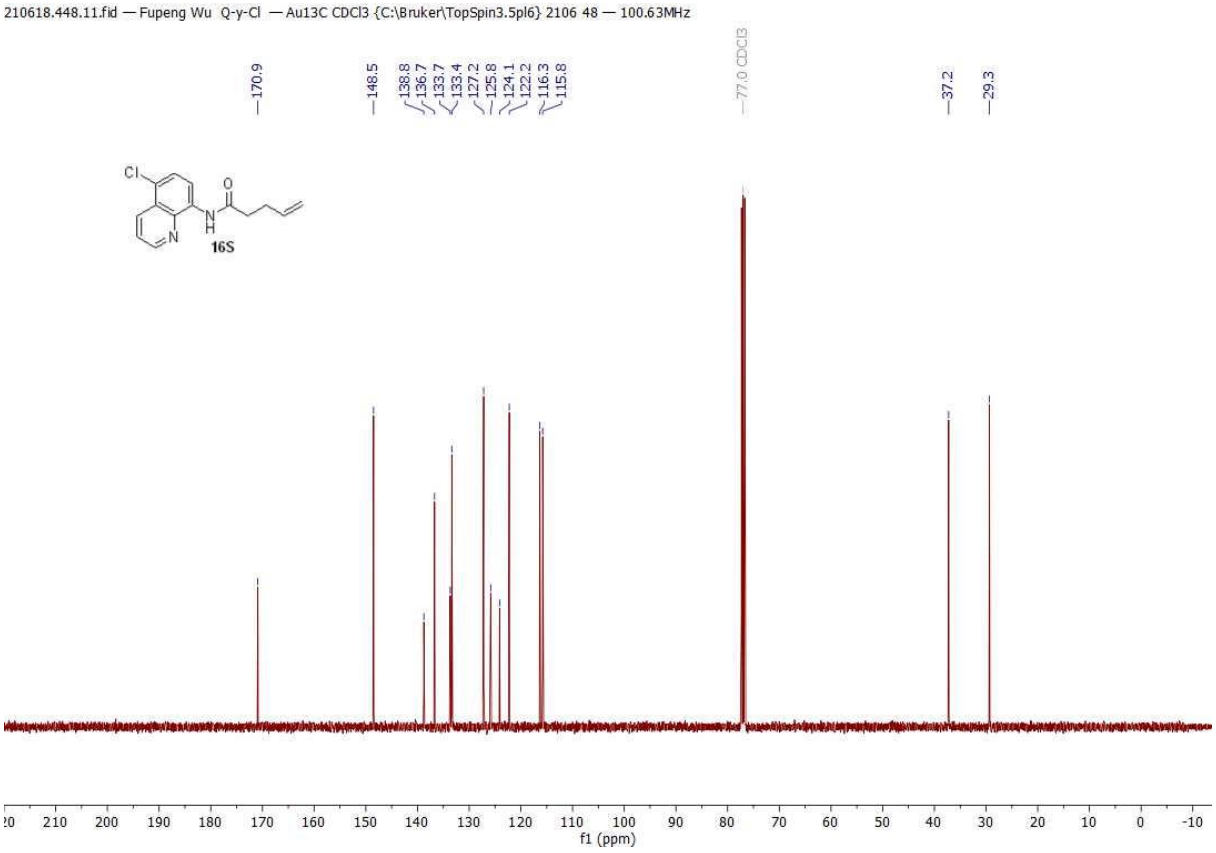
210312.f375.11.fid — Fupeng Wu Q-y-9 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 15 — 75.49MHz



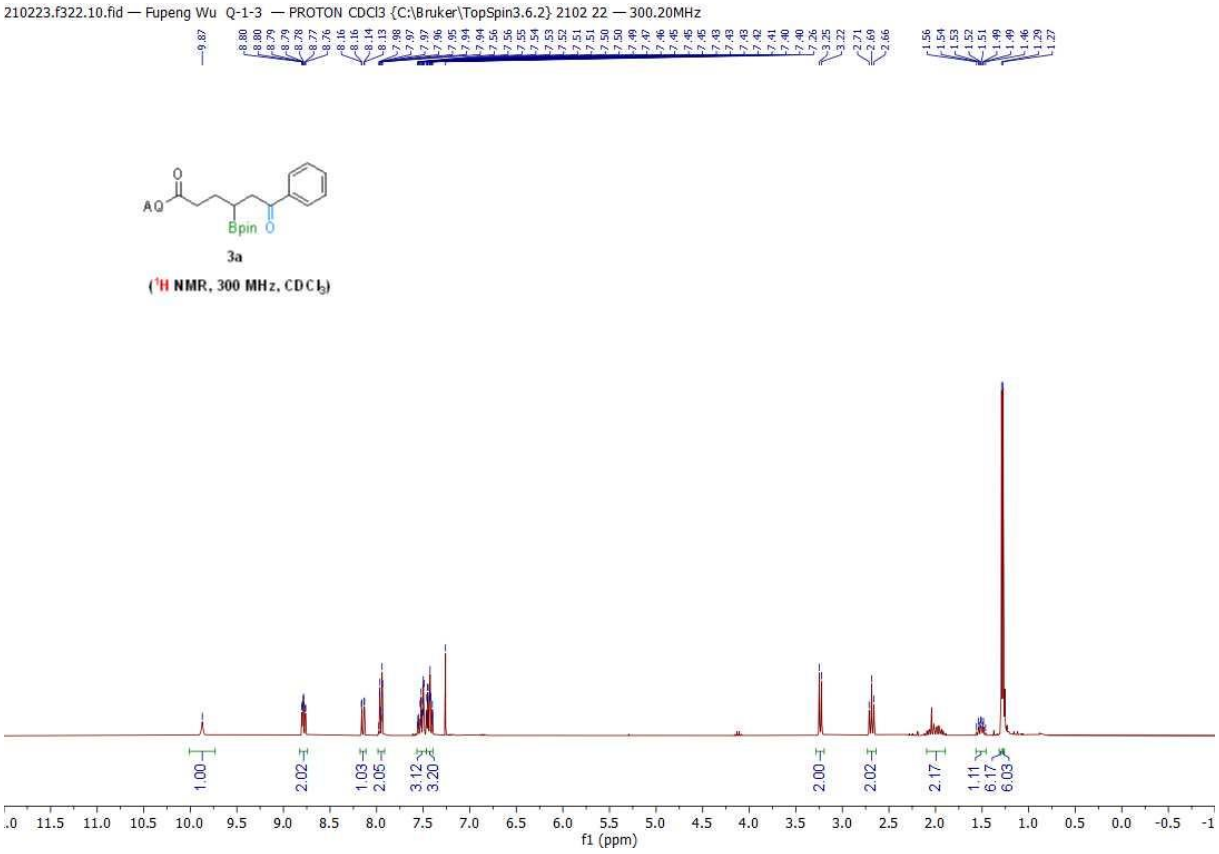

210312.f376.10.fid — Fupeng Wu Q-y-30 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 16 — 300.20MHz
Me
14S
0.88
2.01
1.01
3.07
1.00
2.05
1.02
2.11
3.03
f1 (ppm)

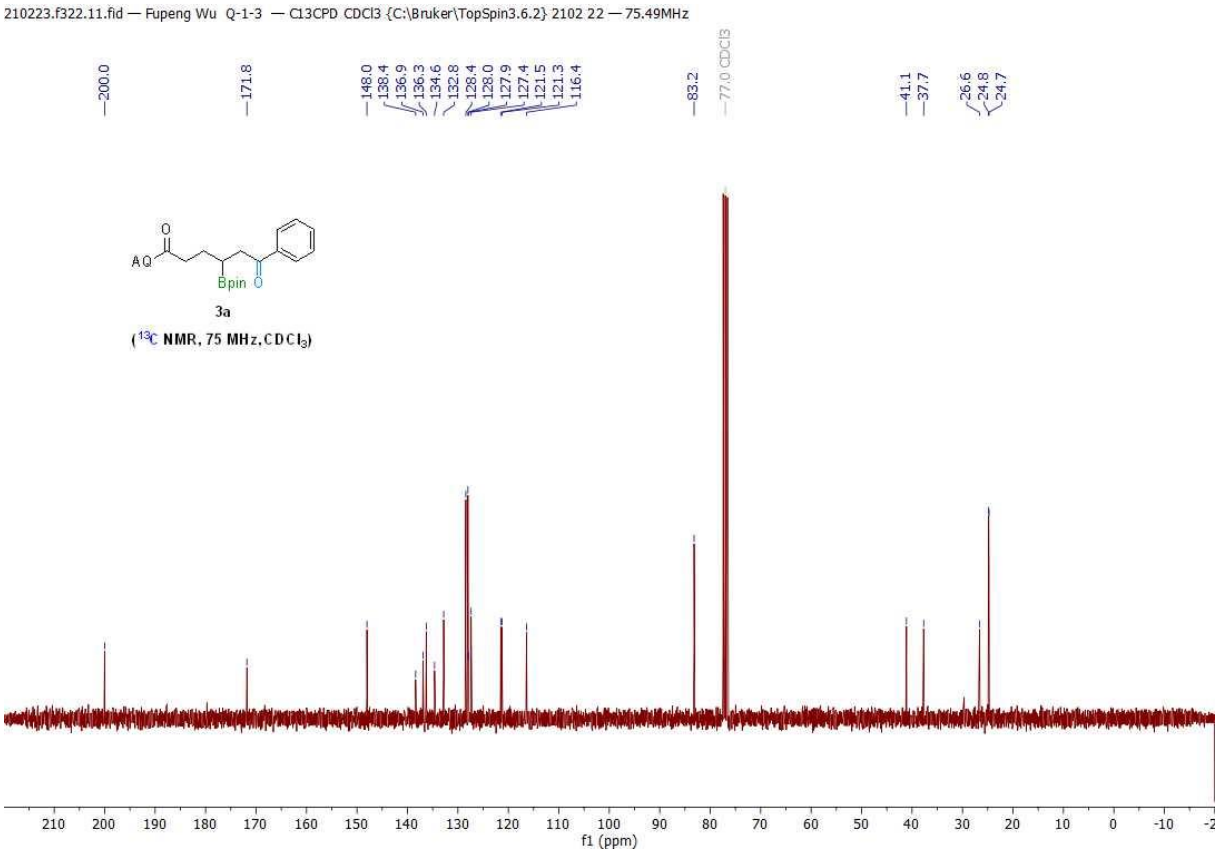

210312.f376.11.fid — Fupeng Wu Q-y-30 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 16 — 75.49MHz
170.4
148.1
142.6
138.3
136.3
134.4
127.9
127.4
121.5
121.4
116.4
113.6
77.0 CDCl3
45.2
34.8
19.7
Me
14S
f1 (ppm)


210618.448.10.fid — Fupeng Wu Q-y-Cl — Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2106 48 — 400.13MHz
16S
0.97
1.00
1.00
0.99
2.04
0.97
1.00
1.00
2.06
2.09
f1 (ppm)


210618.448.11.fid — Fupeng Wu Q-y-Cl — Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2106 48 — 100.63MHz
170.9
148.5
138.8
136.7
133.7
133.4
127.2
125.8
124.1
122.2
116.3
115.8
77.0 CDCl3
37.2
29.3
16S
f1 (ppm)

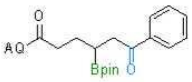
8.2 NMR spectra of the β-boryl ketones.





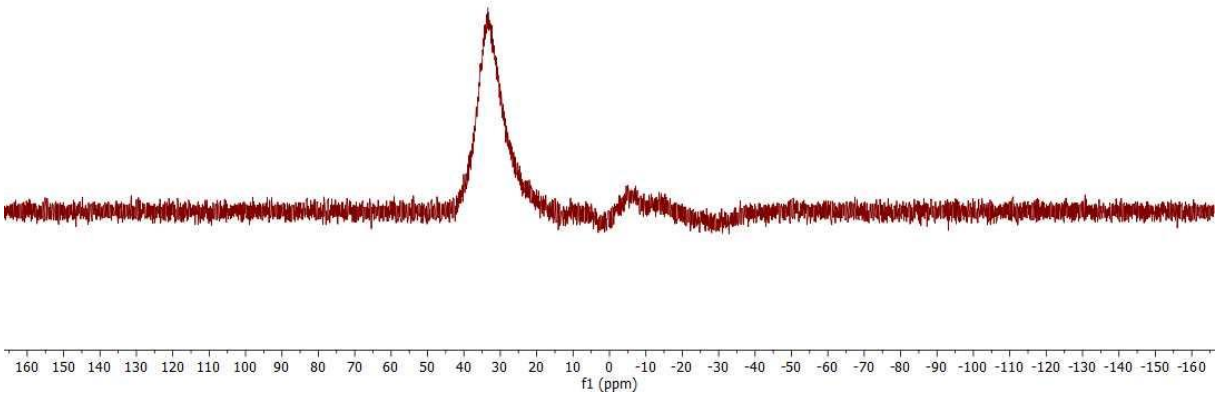
210223.f322.12.fid — Fupeng Wu Q-1-3 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 22 — 96.32MHz

33.4



3a

(^{11}B NMR, 96 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

File:21032201
Vial:1:B,1
Description:MeOH/0.1% HCOOH in H2O 90:10

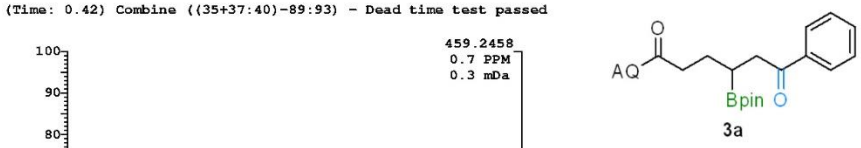
Sample Name:Q-1
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:11:36:29

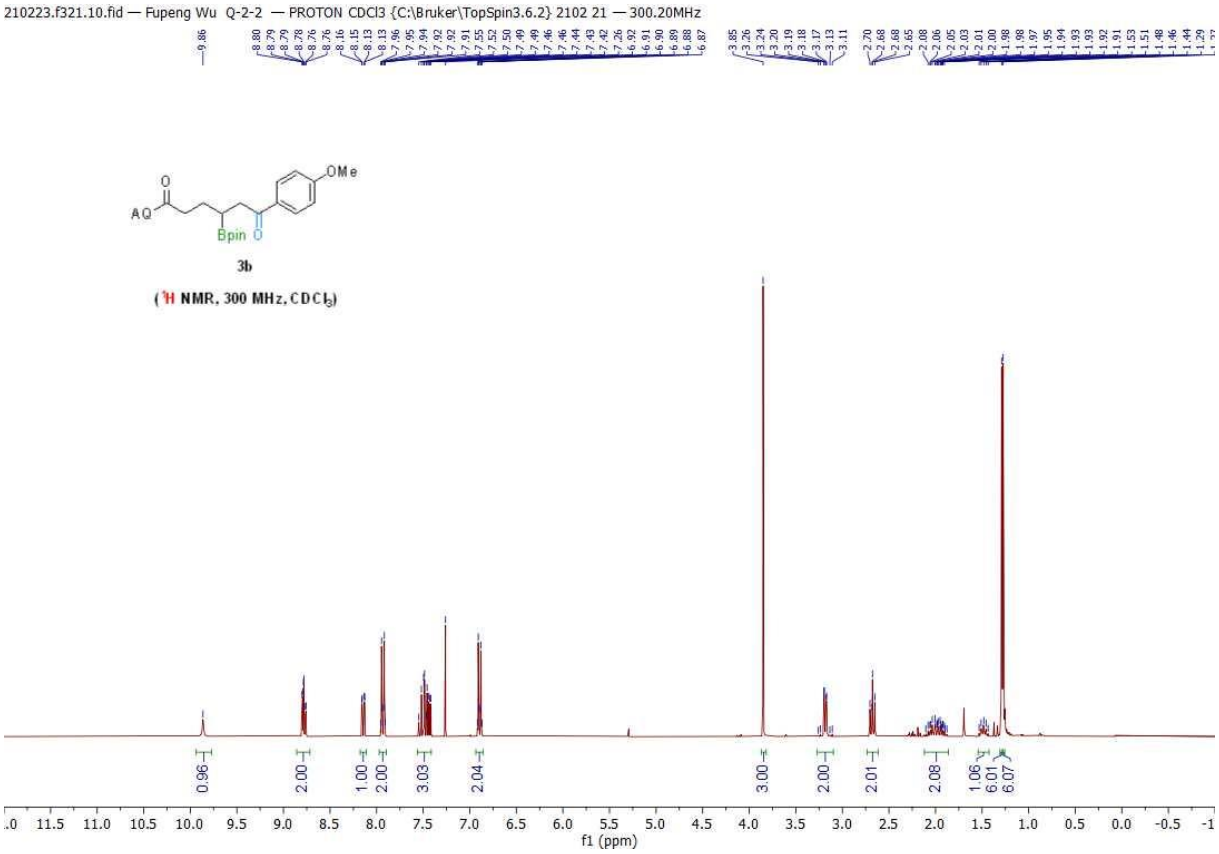
Sample Report:

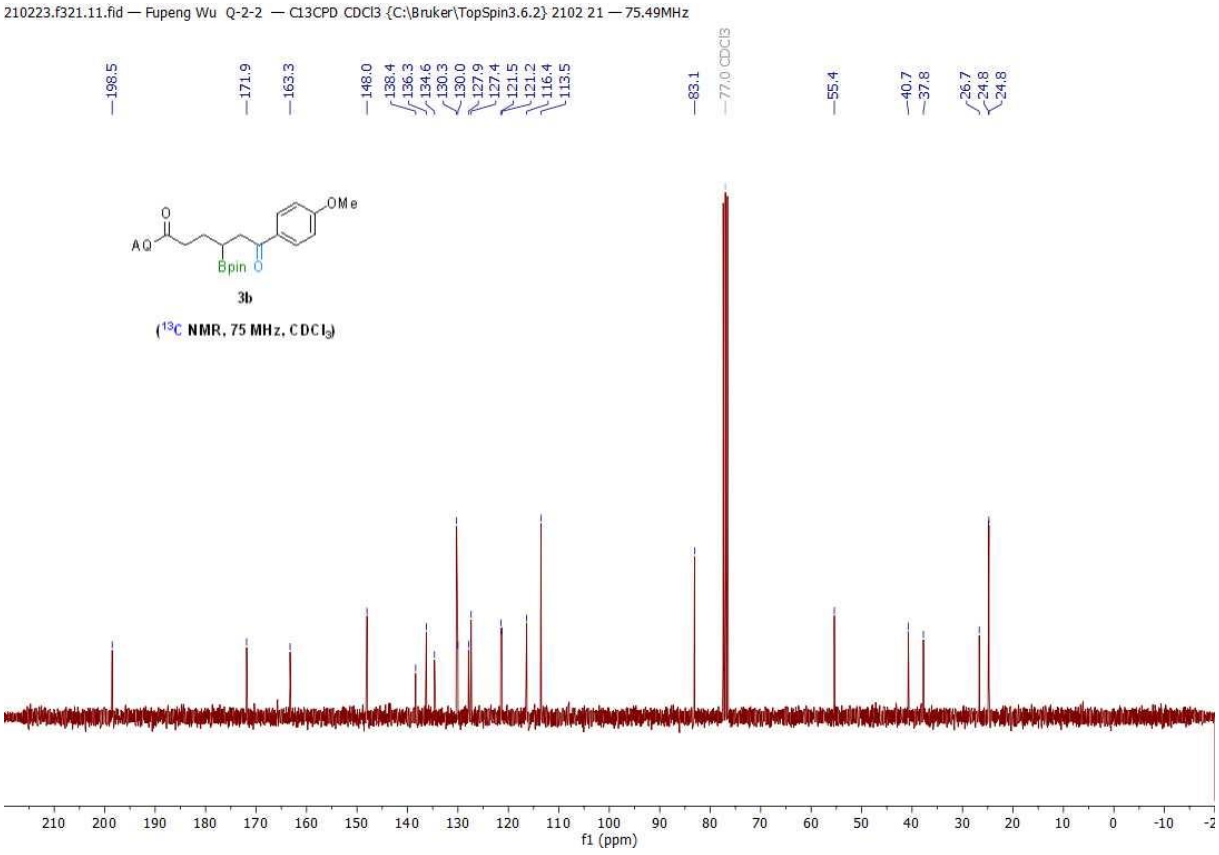
(Time: 0.42) Combine ((35+37:40)-89:93) - Dead time test passed

1:TOF MS ES+
3.9e+008



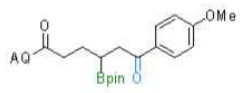
3a


210223.f321.10.fid — Fupeng Wu Q-2-2 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 21 — 300.20MHz
OMe
AQ
Bpin
3b
(1H NMR, 300 MHz, CDCl3)
0.96
2.00
1.00
2.00
3.03
2.04
3.00
2.00
2.01
2.08
1.06
6.01
6.07
f1 (ppm)


210223.f321.11.fid — Fupeng Wu Q-2-2 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 21 — 75.49MHz
198.5
171.9
163.3
148.0
138.4
136.3
134.6
130.3
130.0
127.9
127.4
121.5
121.2
116.4
113.5
83.1
77.0 CDCl3
55.4
40.7
37.8
26.7
24.8
24.8
OMe
AQ
Bpin
3b
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

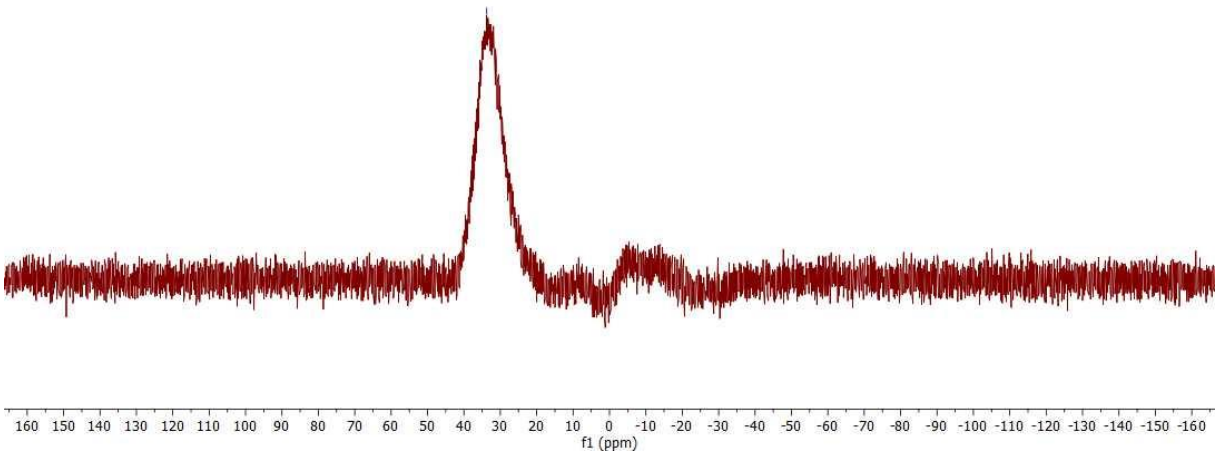
210223.f321.12.fid — Fupeng Wu Q-2-2 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 21 — 96.32MHz

33.7



3b

(^{11}B NMR, 96 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

File:21032223
Vial:1:B,2
Description:MeOH/0.1% HCOOH in H2O 90:10

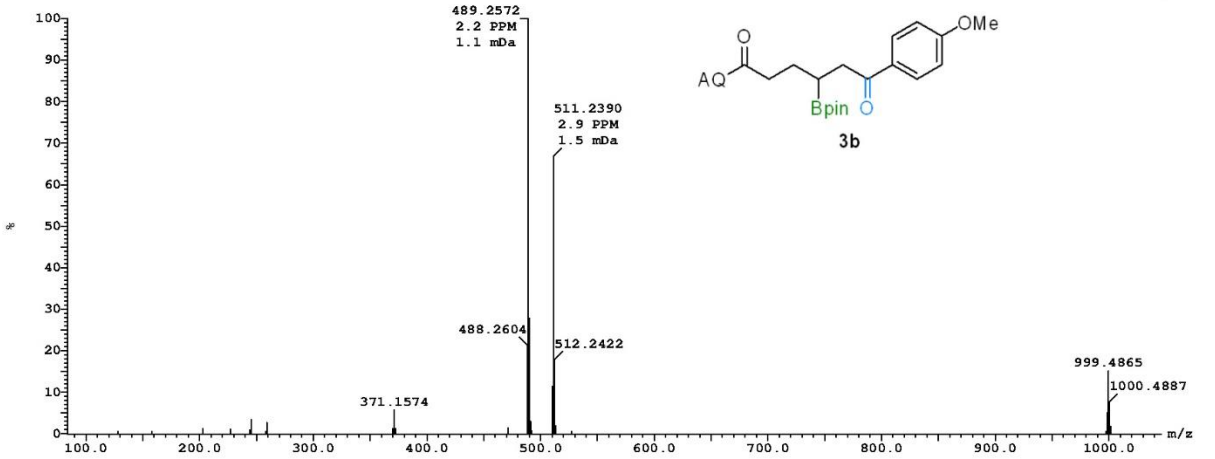
Sample Name:Q-2
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:15:35:09

Sample Report:

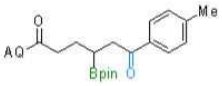
(Time: 0.41) Combine ((35+37:40)-88:92) - Dead time test passed

1:TOF MS ES+
3.6e+008

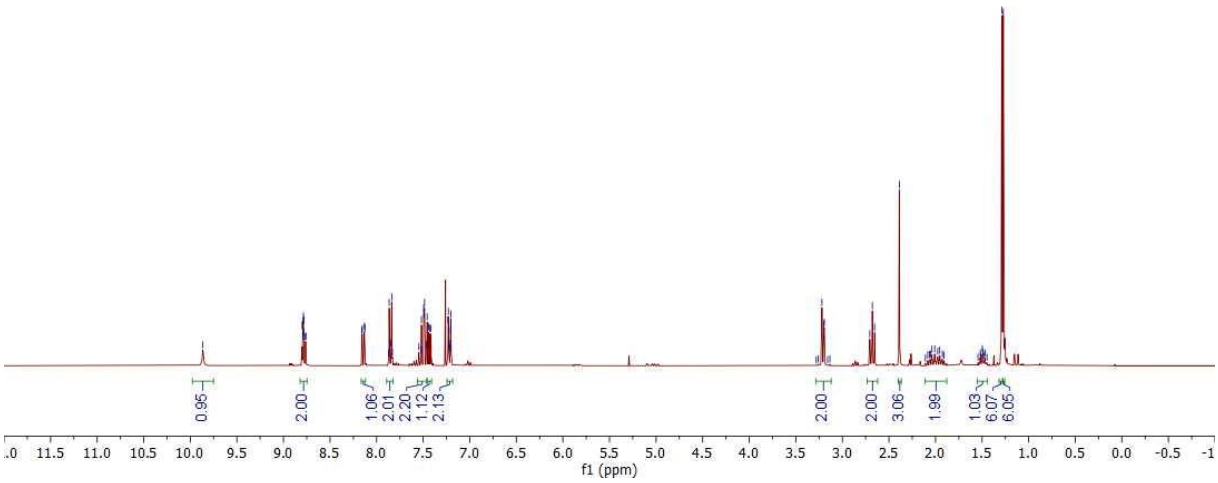


3b

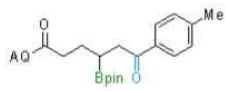
210226.f321.10.fid — Fupeng Wu Q-13 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 21 — 300.20MHz



3c
(¹H NMR, 300 MHz, CDCl₃)



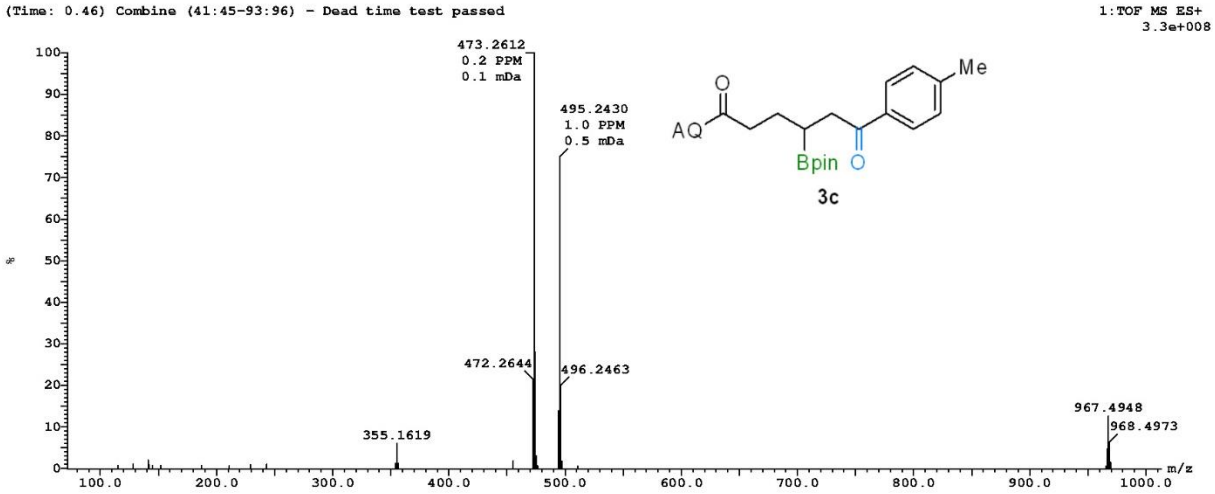
210226.f321.11.fid — Fupeng Wu Q-13 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 21 — 75.49MHz

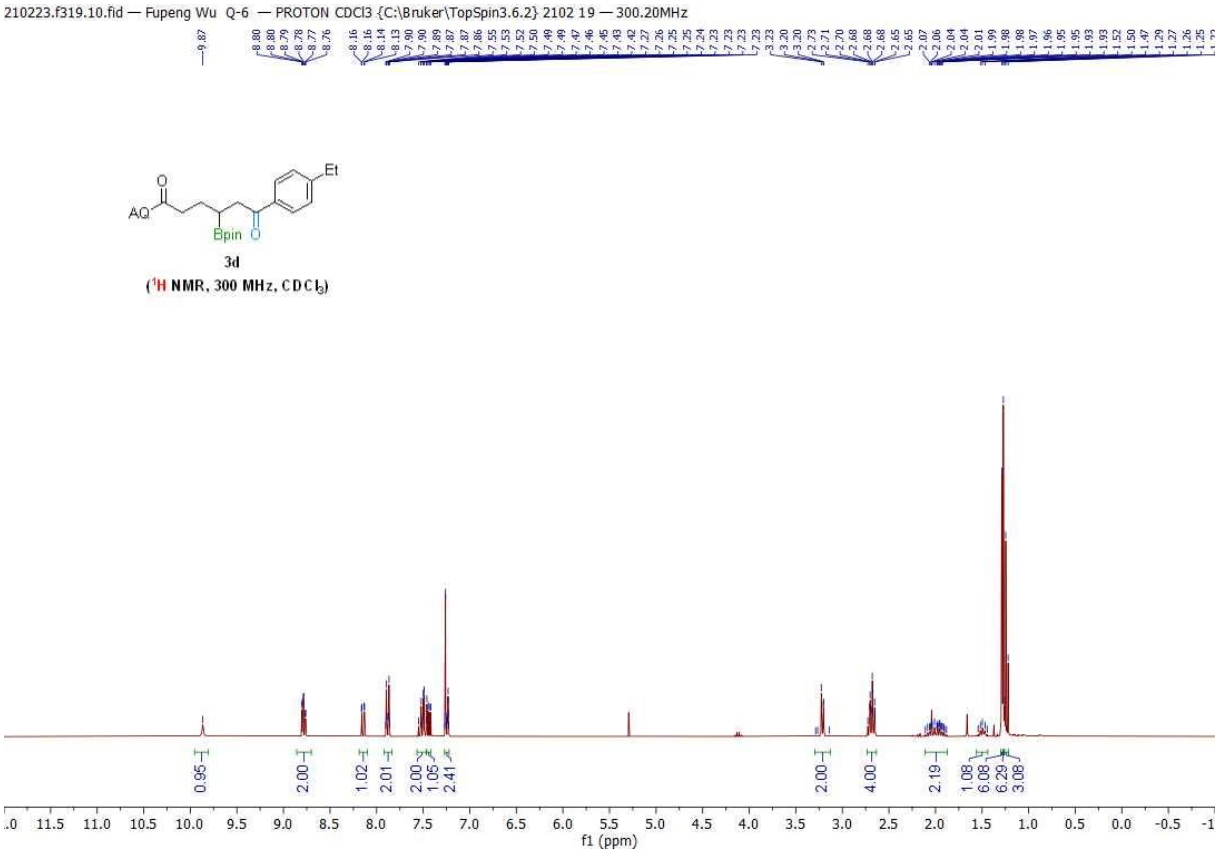


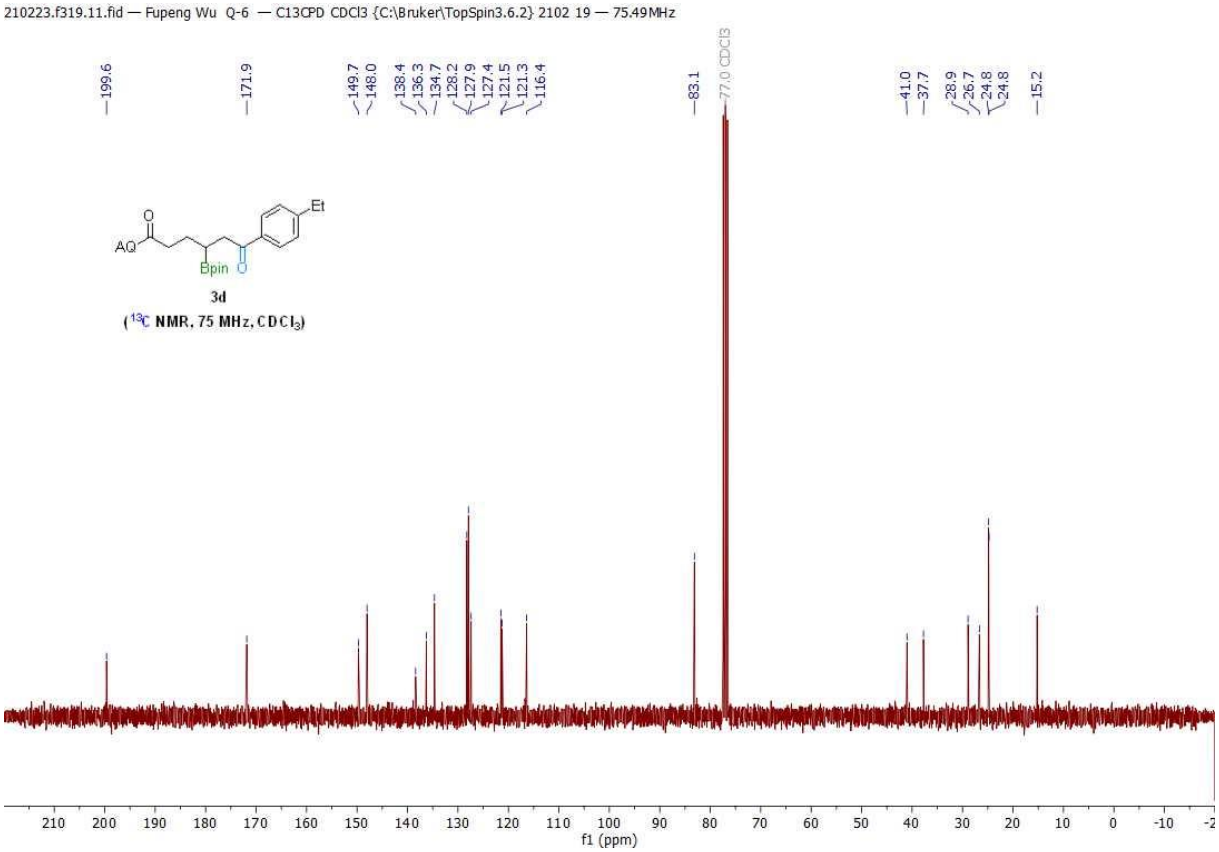
3c
(¹³C NMR, 75 MHz, CDCl₃)

File:21032210 Sample Name:Q-13 UserName:Fu-peng Wu
Vial:1:C,2 Date:22-Mar-2021 Time:12:17:14
Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Report:

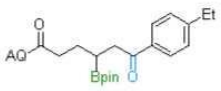



210223.f319.10.fid — Fupeng Wu Q-6 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 19 — 300.20MHz
AQ
Et
Bpin
3d
(1H NMR, 300 MHz, CDCl3)
0.95
2.00
1.02
2.01
2.00
1.05
2.41
2.00
4.00
2.19
1.08
6.08
6.29
3.08
f1 (ppm)


210223.f319.11.fid — Fupeng Wu Q-6 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 19 — 75.49MHz
199.6
171.9
149.7
148.0
138.4
136.3
134.7
128.2
127.9
127.4
121.5
121.3
116.4
83.1
77.0 CDCl3
41.0
37.7
28.9
26.7
24.8
24.8
15.2
AQ
Et
Bpin
3d
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

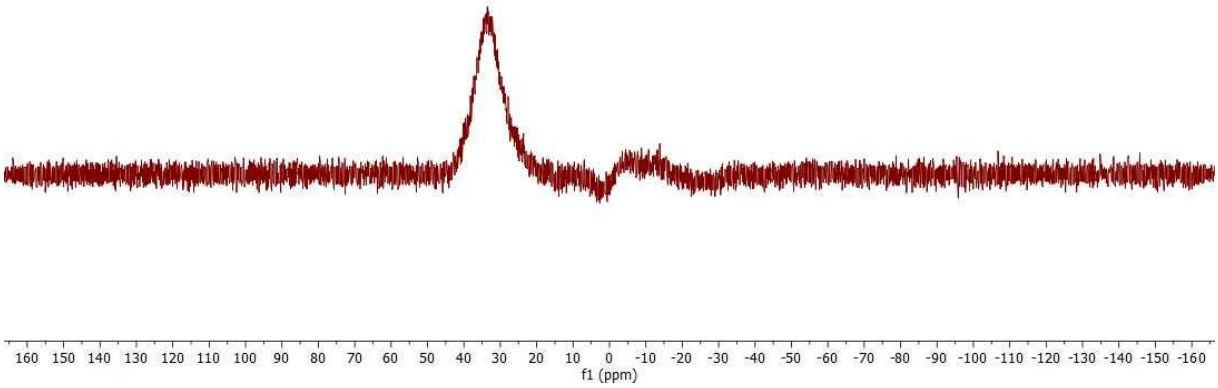
210223.f319.12.fid — Fupeng Wu Q-6 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 19 — 96.32MHz

33.6



3d

(^{11}B NMR, 96 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

Page 2

File:21032205
Vial:1:B,5
Description:MeOH/0.1% HCOOH in H2O 90:10

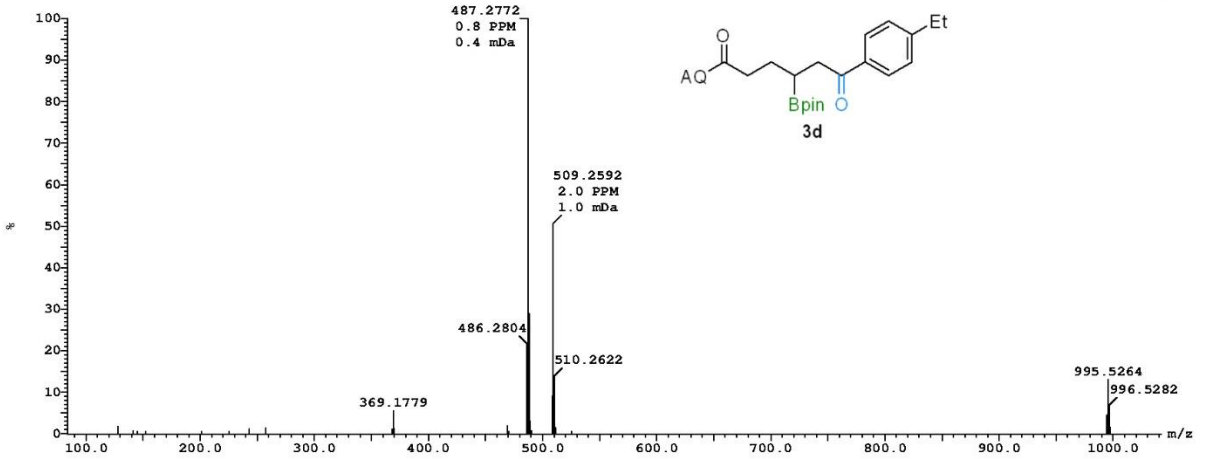
Sample Name:Q-6
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:11:54:25

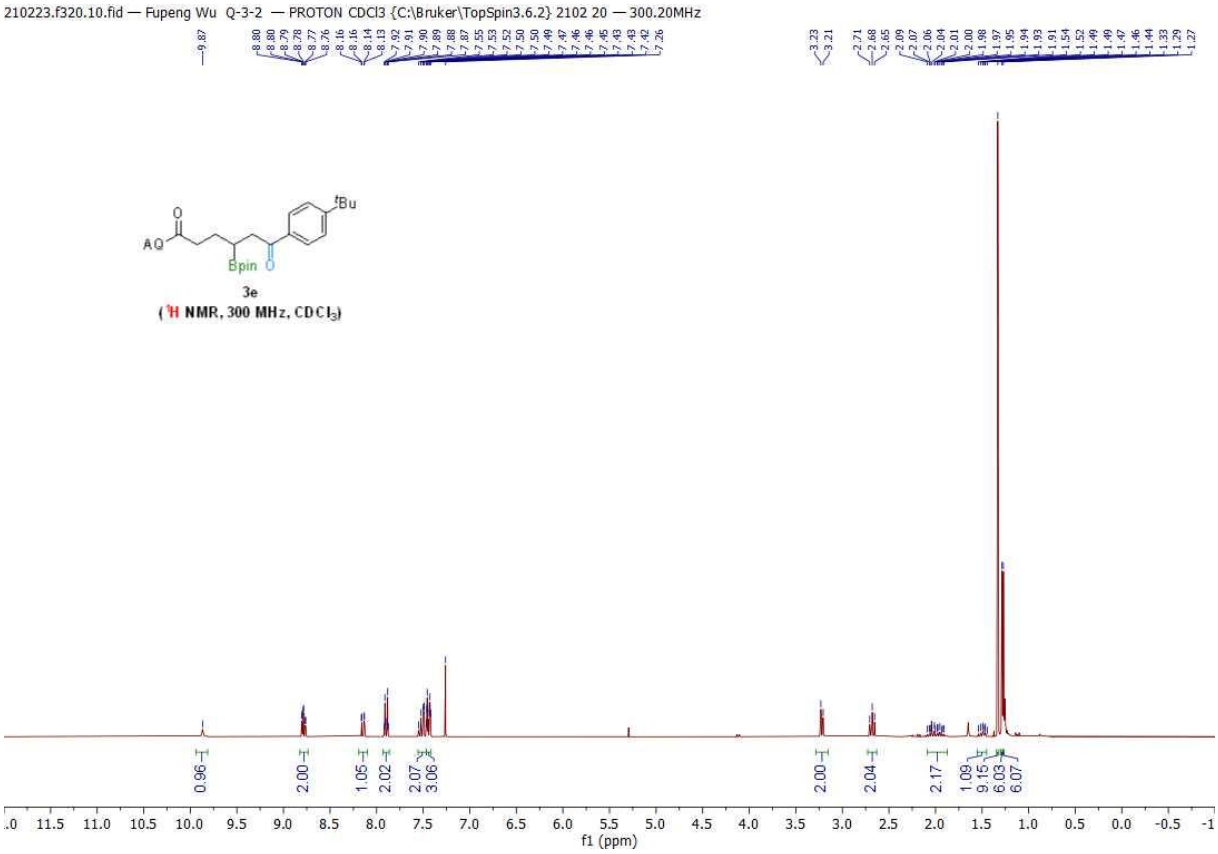
Sample Report:

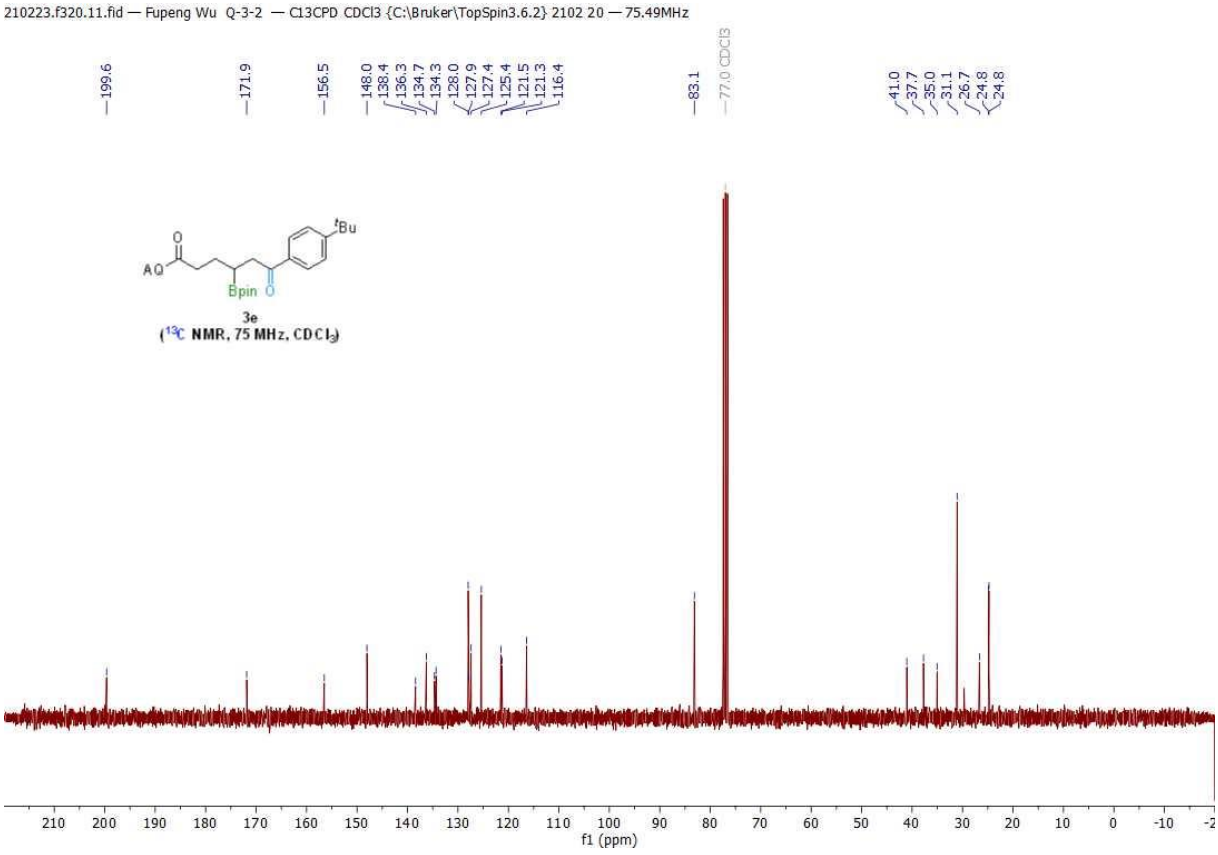
(Time: 0.50) Combine ((42:43+45:47)-96:99) - Dead time test passed

1:TOF MS ES+
4.0e+008



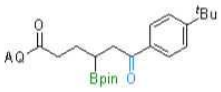
3d


210223.f320.10.fid — Fupeng Wu Q-3-2 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 20 — 300.20MHz
AQ
Bpin
tBu
3e
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)


210223.f320.11.fid — Fupeng Wu Q-3-2 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 20 — 75.49MHz
AQ
Bpin
tBu
3e
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

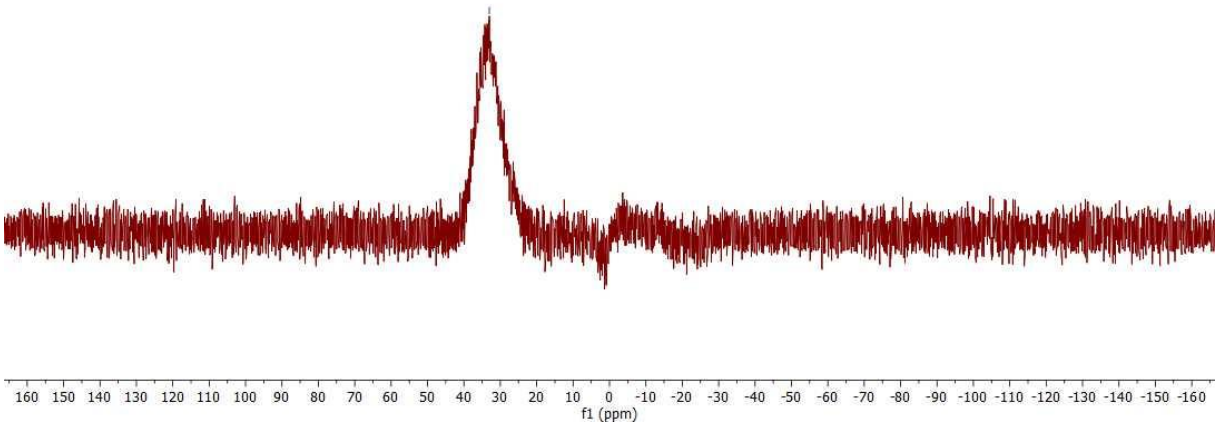
210223.f320.12.fid — Fupeng Wu Q-3-2 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 20 — 96.32MHz

33.0



3e

(^{11}B NMR, 96 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

File:21032203
Vial:1:B,3
Description:MeOH/0.1% HCOOH in H2O 90:10

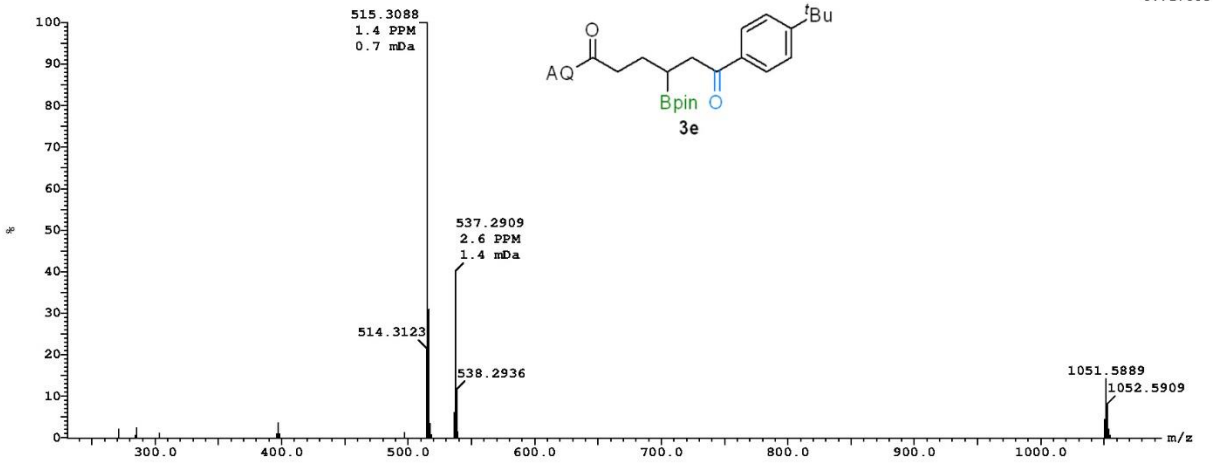
Sample Name:Q-3
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:11:45:27

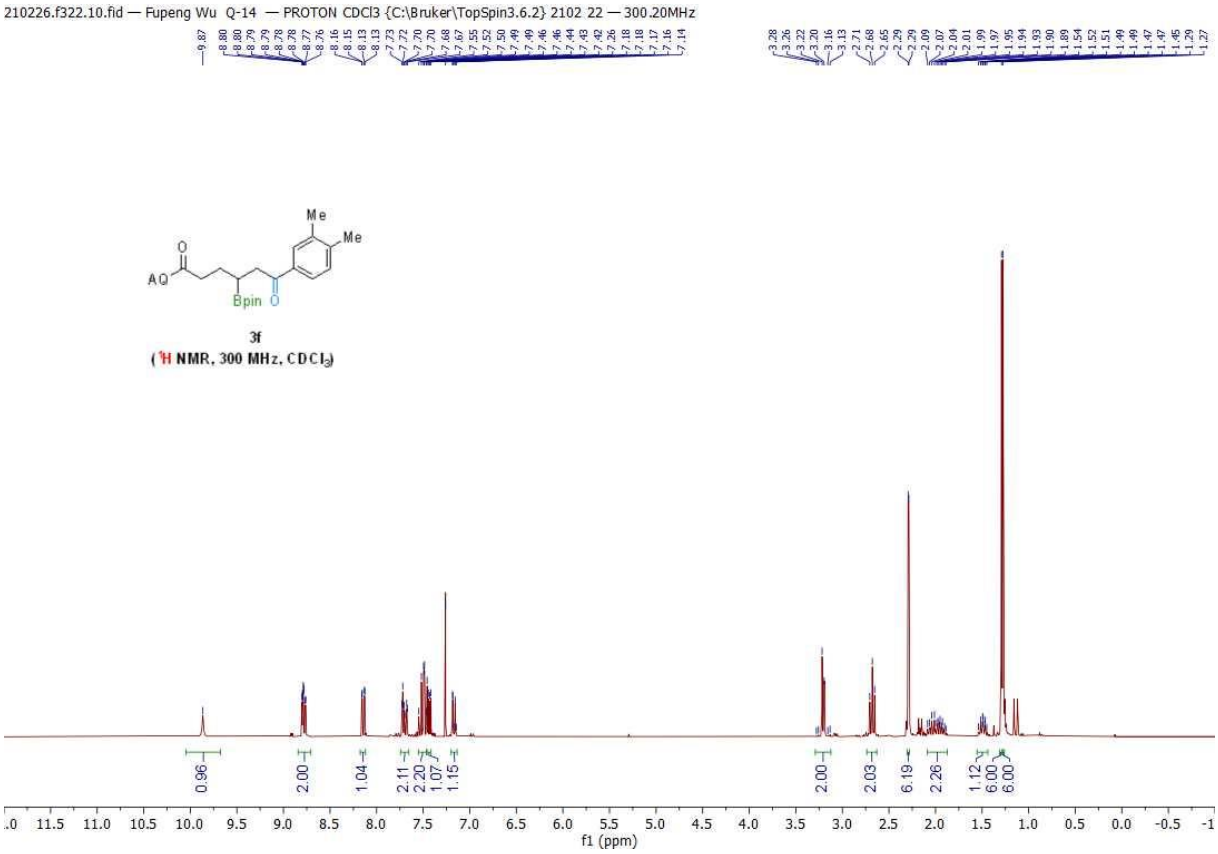
Sample Report:

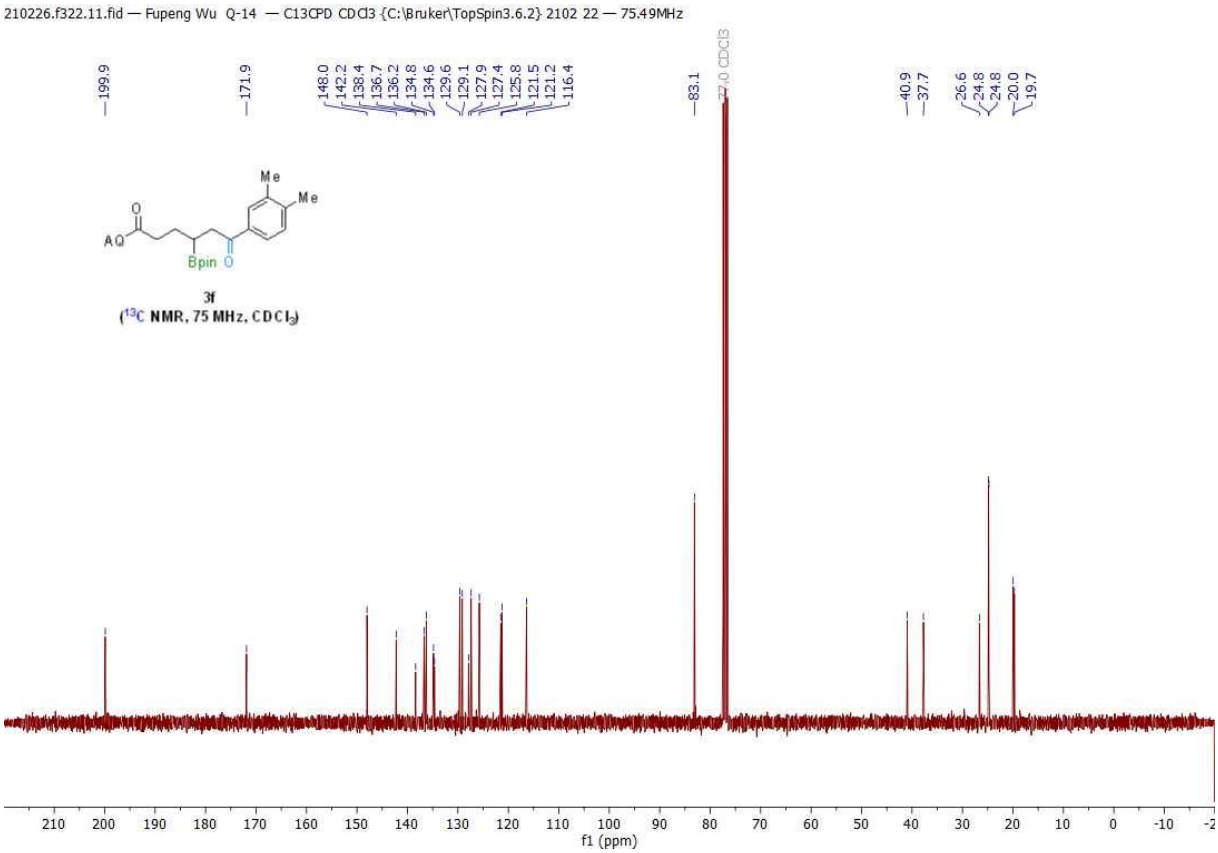
(Time: 0.58) Combine (51:55-(1:2+103:107)) - Dead time test passed

1:TOF MS ES+
4.7e+008



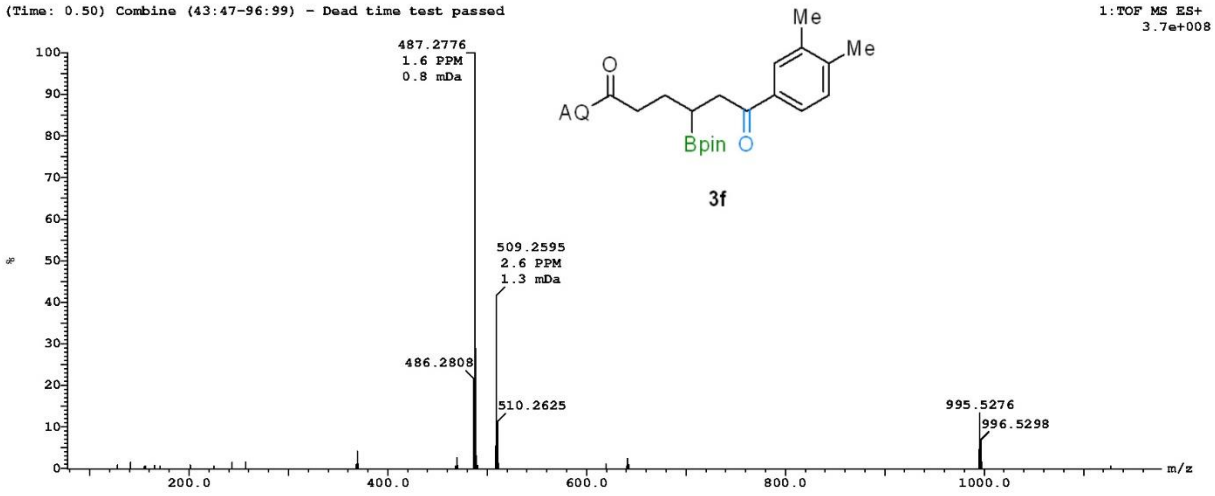
3e


210226.f322.10.fid — Fupeng Wu Q-14 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 22 — 300.20MHz
Me
Me
O
AQ
Bpin O
3f
(1H NMR, 300 MHz, CDCl3)
0.96
2.00
1.04
2.11
2.20
1.07
1.15
2.00
2.03
6.19
2.26
1.12
6.00
6.00
f1 (ppm)

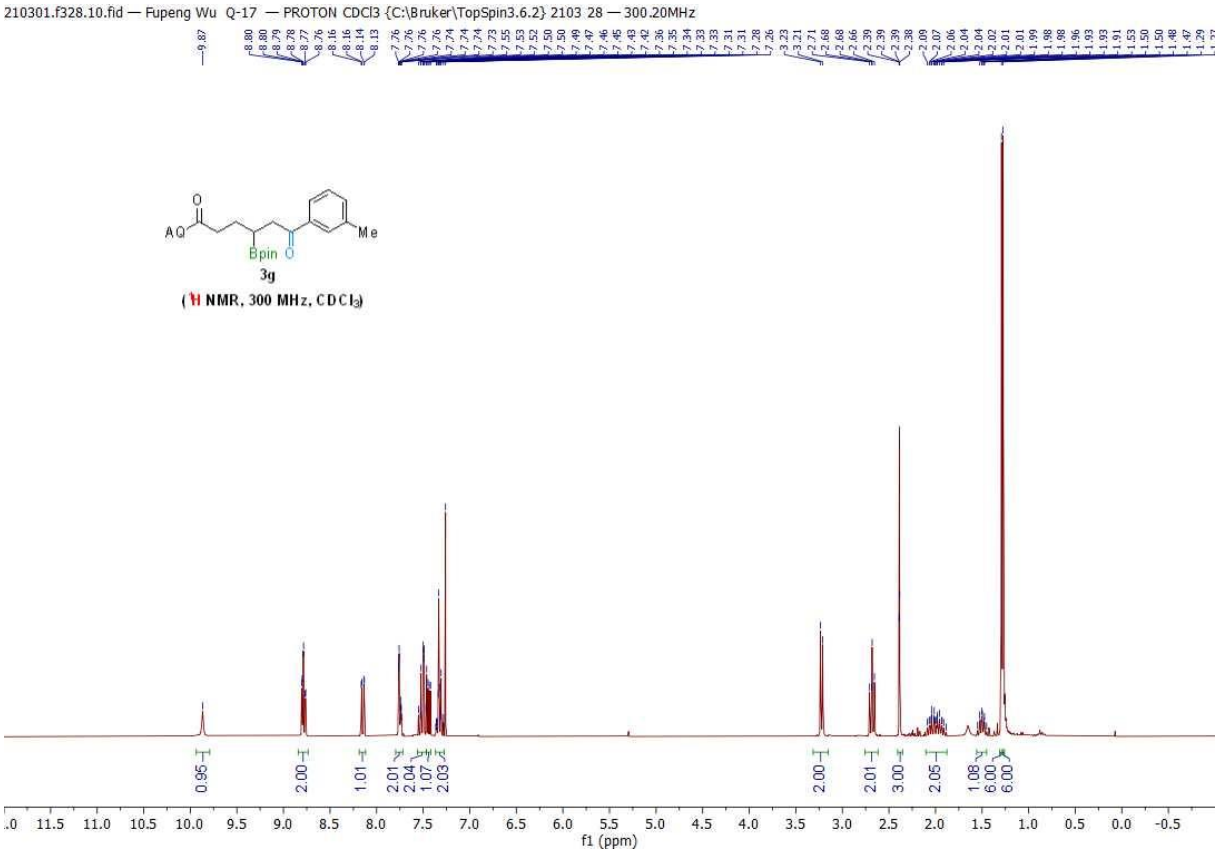

210226.f322.11.fid — Fupeng Wu Q-14 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 22 — 75.49MHz
199.9
171.9
148.0
142.2
138.4
136.7
136.2
134.8
134.6
129.6
129.1
127.9
127.4
125.8
121.5
121.2
116.4
83.1
77.0 CDCl3
40.9
37.7
26.6
24.8
24.8
20.0
19.7
Me
Me
O
AQ
Bpin O
3f
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

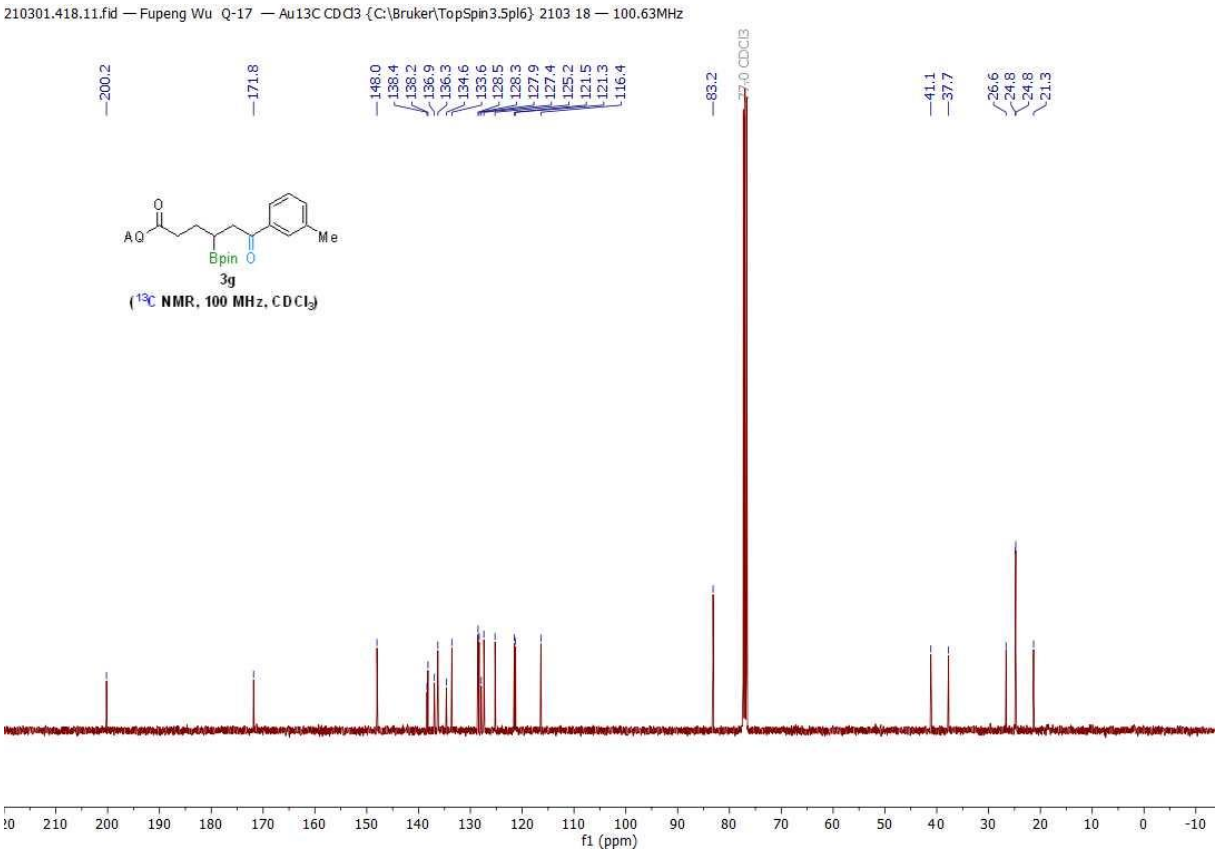
File:21032211 Sample Name:Q-14 UserName:Fu-peng Wu
Vial:1:C,3 Date:22-Mar-2021 Time:12:21:42
Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Report:



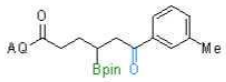
3f


210301.f328.10.fid — Fupeng Wu Q-17 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 28 — 300.20MHz
AQ
Bpin
Me
3g
(¹H NMR, 300 MHz, CDCl3)
f1 (ppm)


210301.418.11.fid — Fupeng Wu Q-17 — Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 18 — 100.63MHz
AQ
Bpin
Me
3g
(¹³C NMR, 100 MHz, CDCl3)
f1 (ppm)

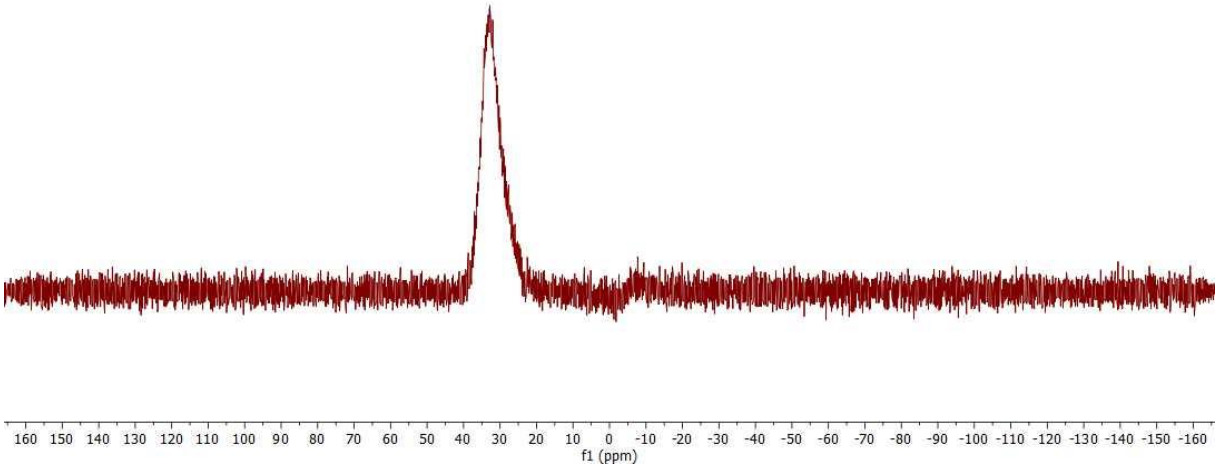
210301.418.10.fid — Fupeng Wu Q-17 — Au11B CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 18 — 128.38MHz

32.9



3g

(^{11}B NMR, 128 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

File:21032213
Vial:1:C,5
Description:MeOH/0.1% HCOOH in H2O 90:10

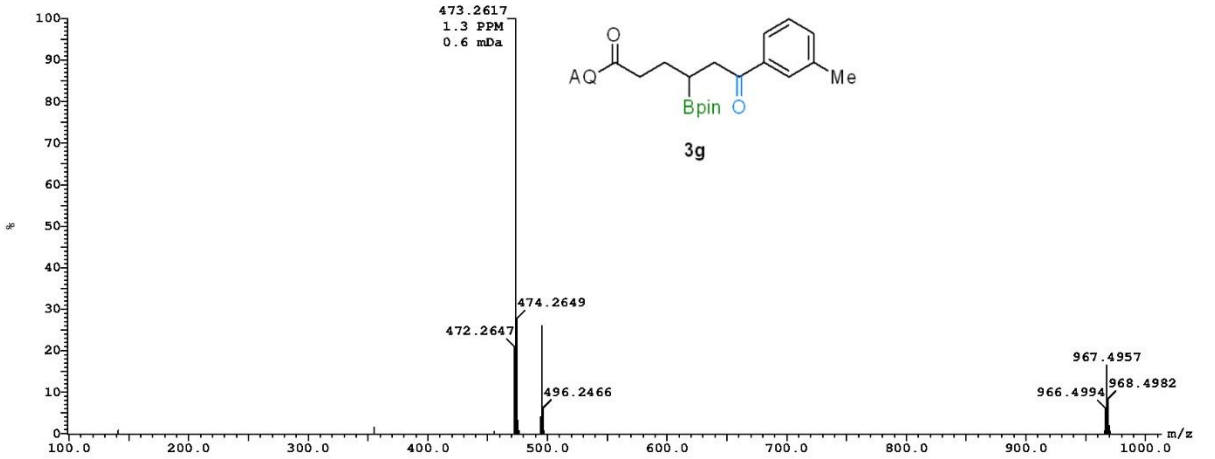
Sample Name:Q-17
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:12:30:38

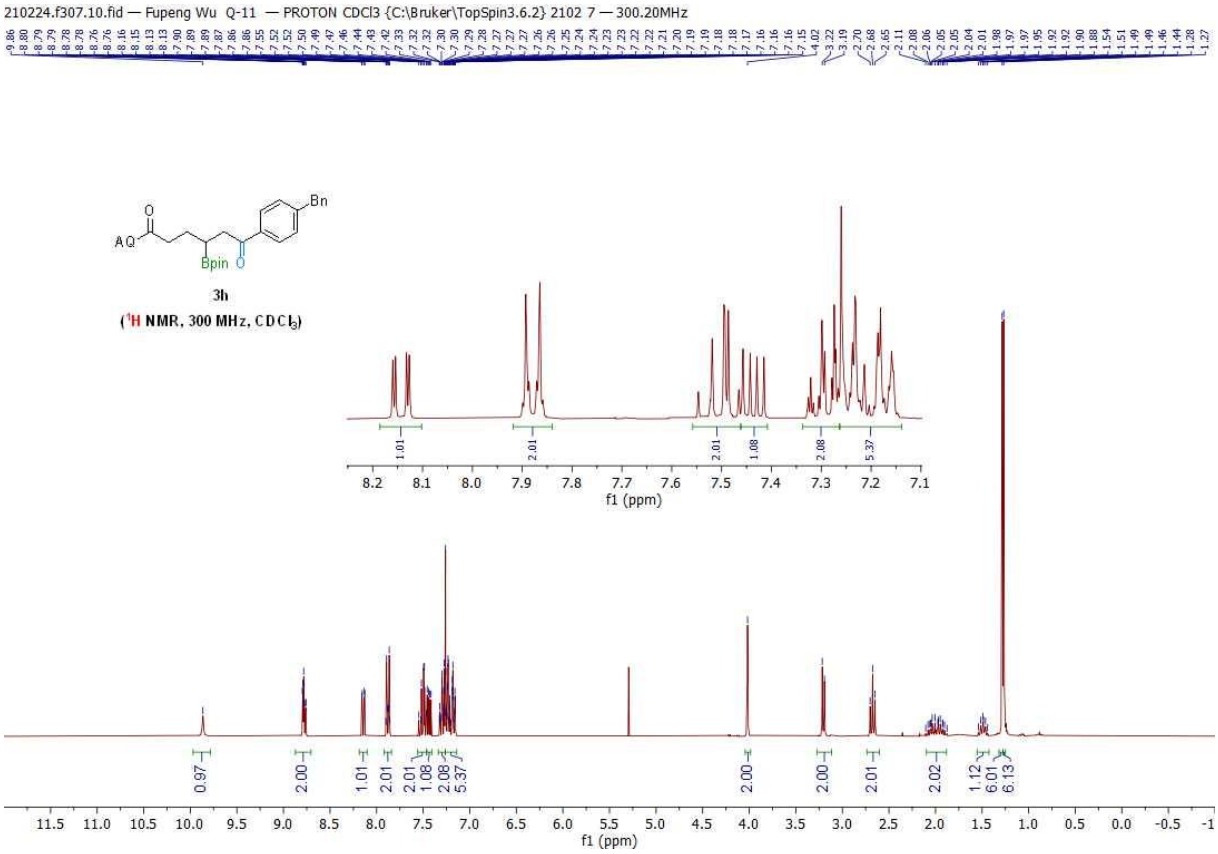
Sample Report:

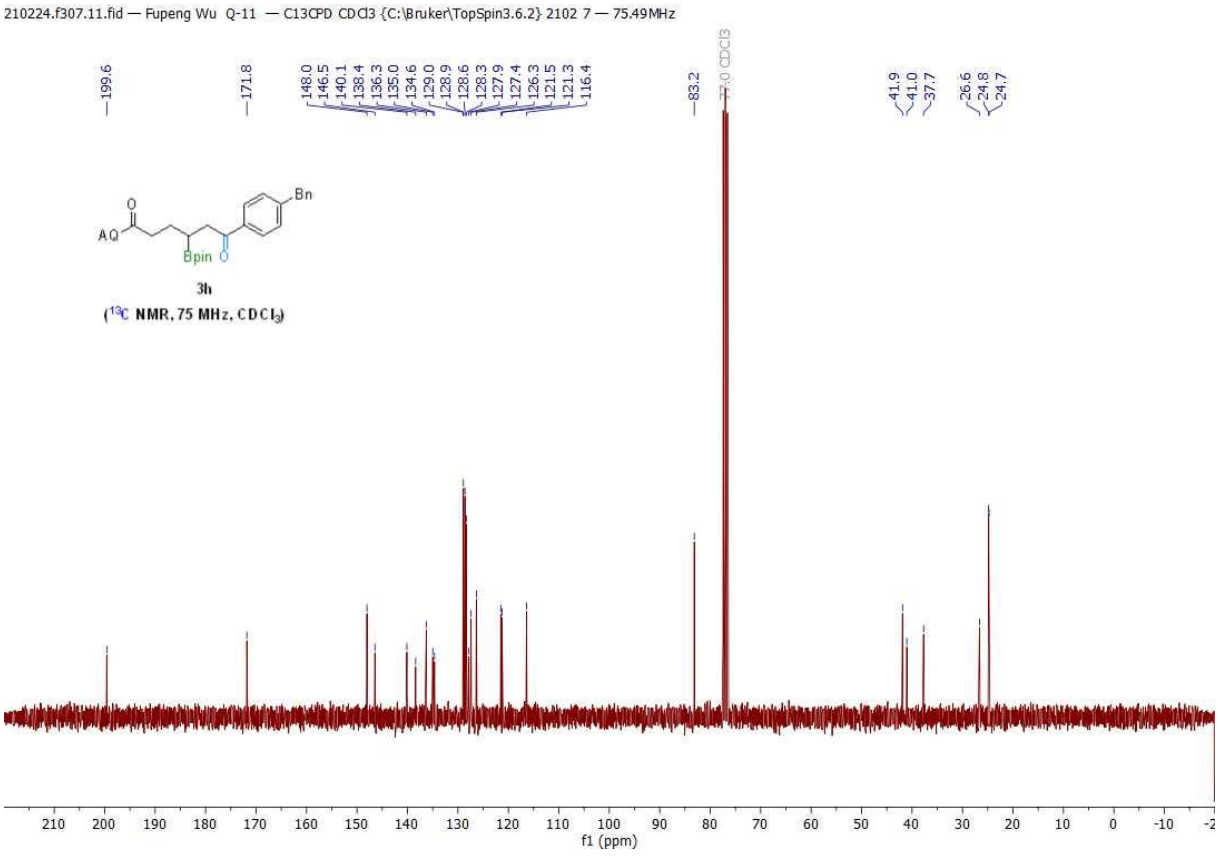
(Time: 0.45) Combine (39:43-92:96) - Dead time test passed

1:TOF MS ES+
2.9e+008



3g


210224.f307.10.fid — Fupeng Wu Q-11 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 7 — 300.20MHz
AQ
Bpin
Bn
3h
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)

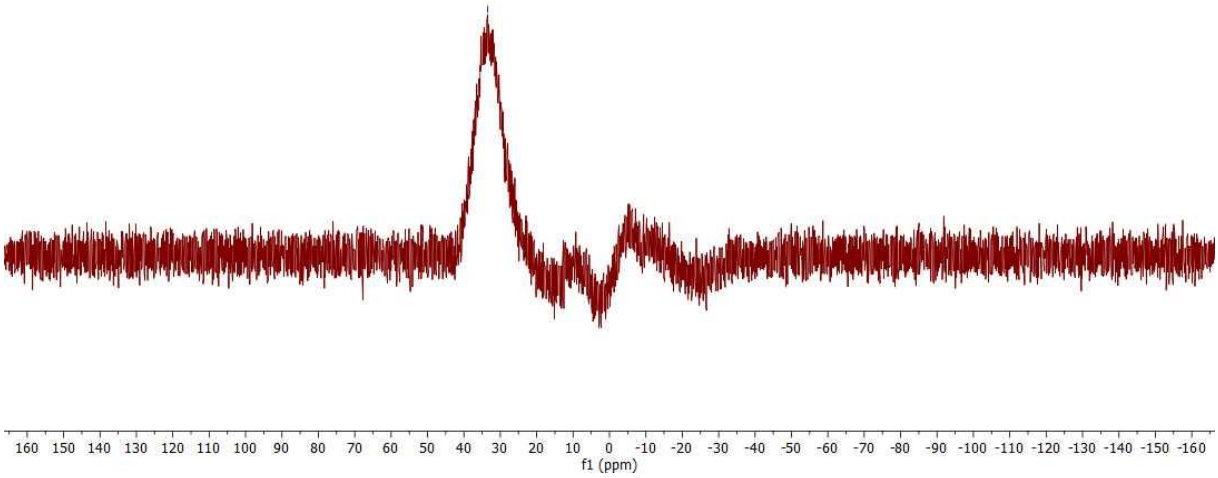

210224.f307.11.fid — Fupeng Wu Q-11 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 7 — 75.49MHz
AQ
Bpin
Bn
3h
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

210224.f307.12.fid — Fupeng Wu Q-11 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 7 — 96.32MHz

33.5

3h

(^{11}B NMR, 96 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

File:21032225
Vial:1:B,8
Description:MeOH/0.1% HCOOH in H2O 90:10

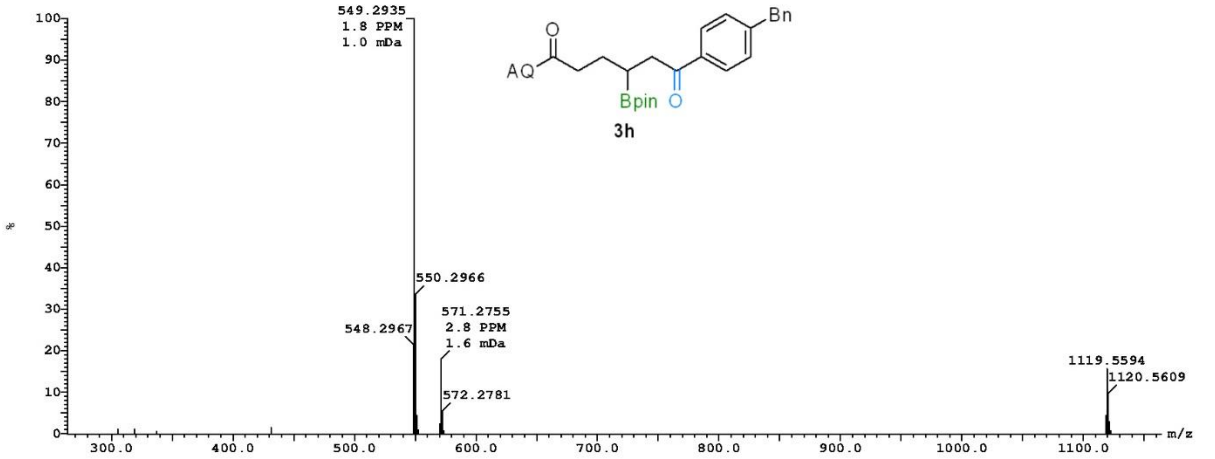
Sample Name:Q-11
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:15:10:47

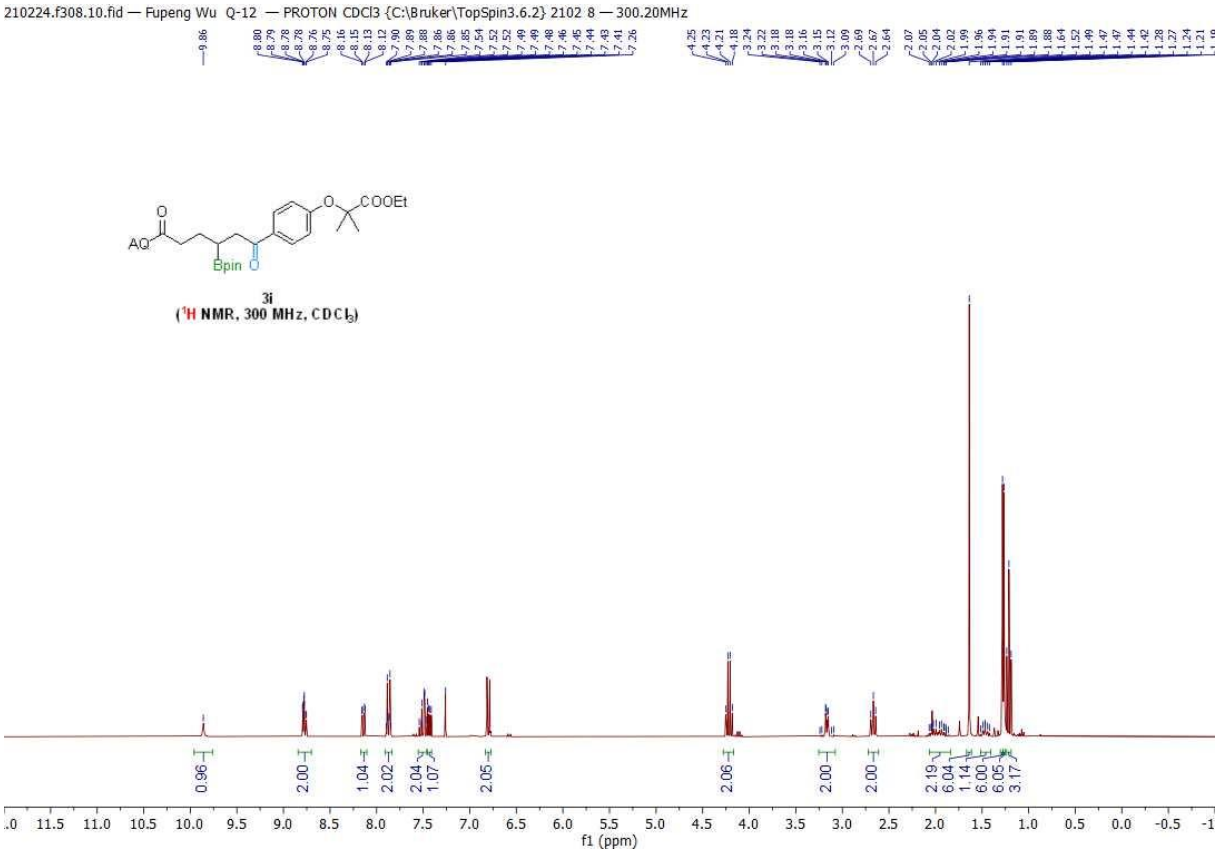
Sample Report:

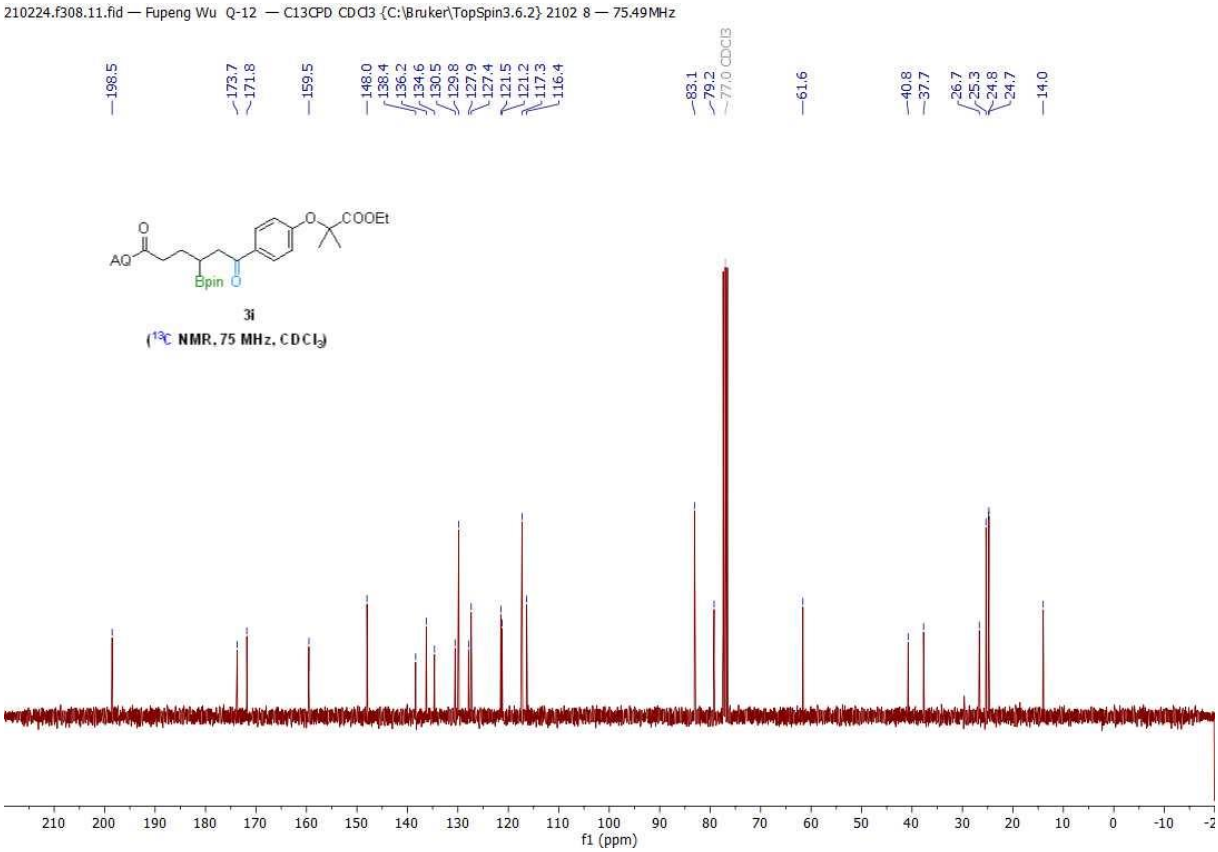
(Time: 0.56) Combine (49:53) - Dead time test passed

1:TOF MS ES+
4.4e+008



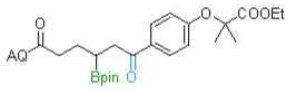
3h


210224.f308.10.fid — Fupeng Wu Q-12 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 8 — 300.20MHz
AQ
Bpin
COOEt
3i
(1H NMR, 300 MHz, CDCl3)
0.96
2.00
1.04
2.02
2.04
1.07
2.05
2.06
2.00
2.00
2.19
6.04
1.14
6.00
6.05
3.17
f1 (ppm)

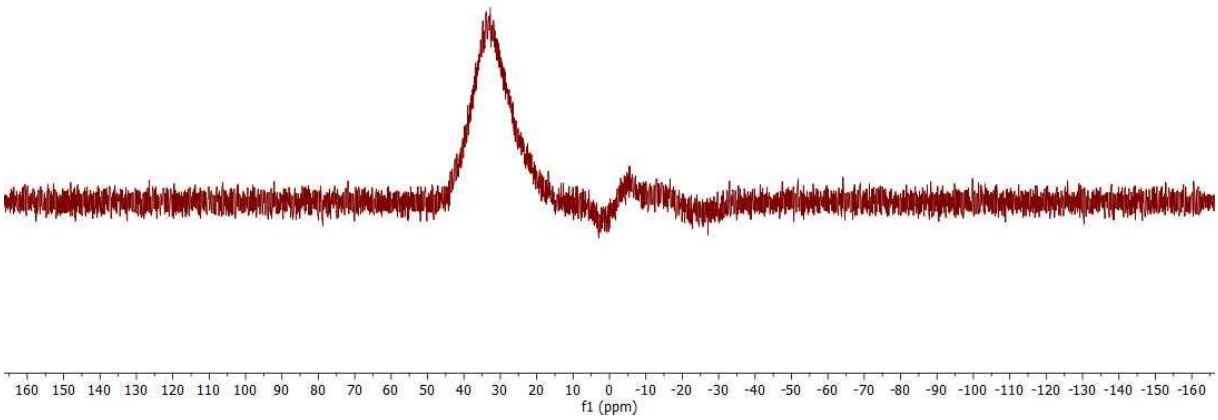

210224.f308.11.fid — Fupeng Wu Q-12 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 8 — 75.49MHz
198.5
173.7
171.8
159.5
148.0
138.4
136.2
134.6
130.5
129.8
127.9
127.4
121.5
121.2
117.3
116.4
83.1
79.2
77.0 CDCl3
61.6
40.8
37.7
26.7
25.3
24.8
24.7
14.0
AQ
Bpin
COOEt
3i
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

210224.f308.12.fid — Fupeng Wu Q-12 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 8 — 96.32MHz

32.8



3i
(^{11}B NMR, 96 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

File:21032209
Vial:1:C,1
Description:MeOH/0.1% HCOOH in H2O 90:10

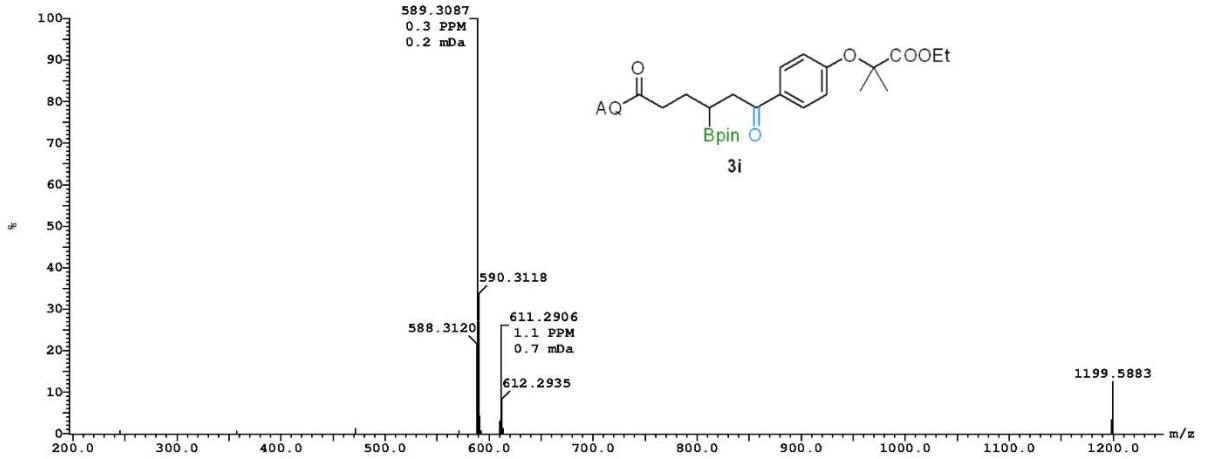
Sample Name:Q-12
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:12:12:46

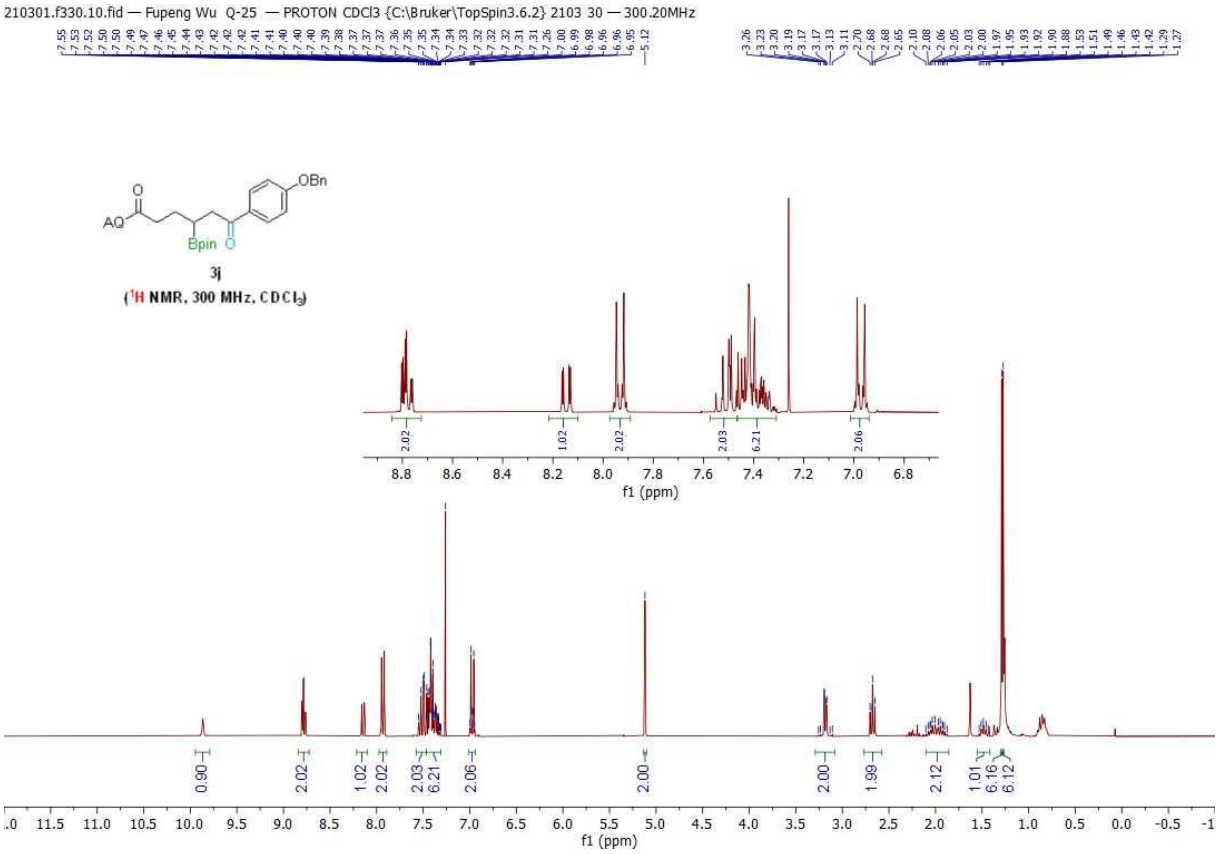
Sample Report:

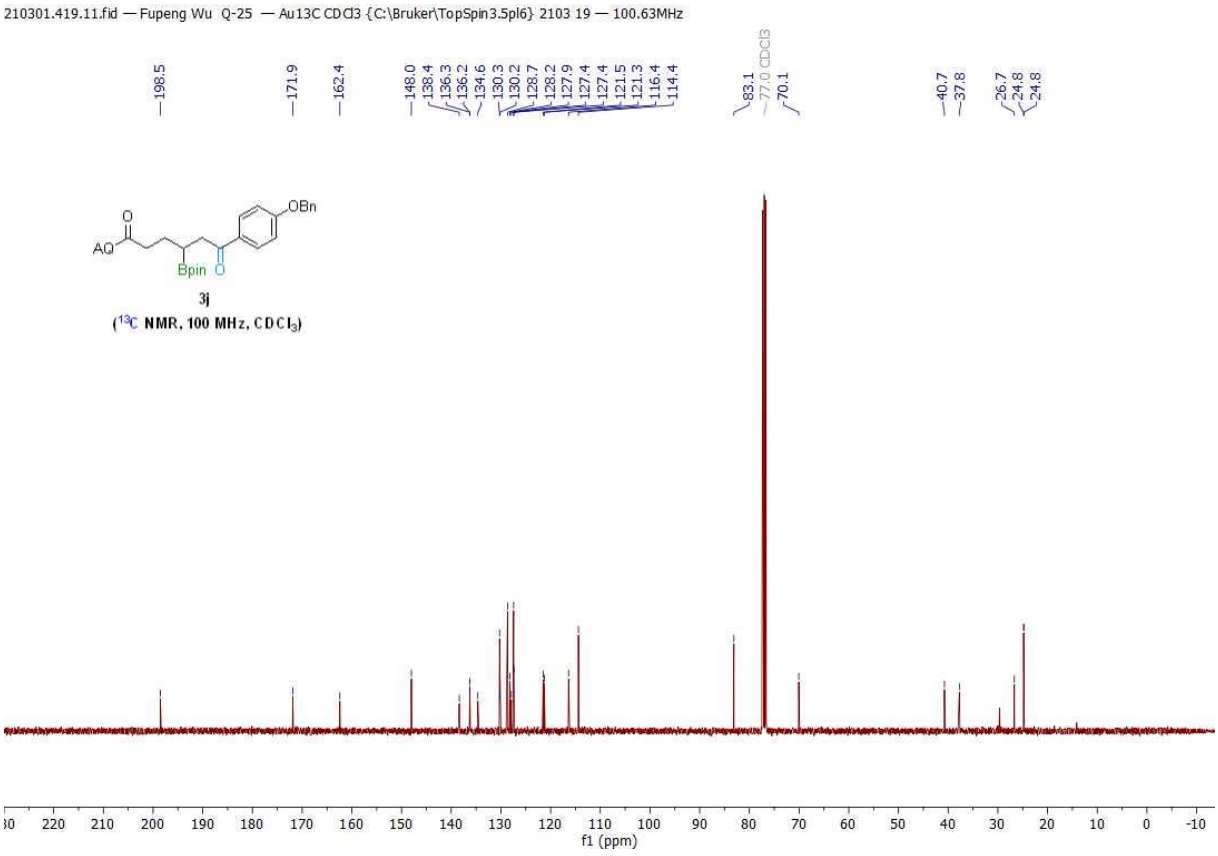
(Time: 0.44) Combine (38:42-91:95) - Dead time test passed

1:TOF MS ES+
6.1e+008



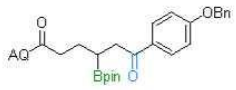
3i


210301.f330.10.fid — Fupeng Wu Q-25 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 30 — 300.20MHz
OBn
AQ
Bpin
3j
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)


210301.419.11.fid — Fupeng Wu Q-25 — Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 19 — 100.63MHz
OBn
AQ
Bpin
3j
(13C NMR, 100 MHz, CDCl3)
f1 (ppm)

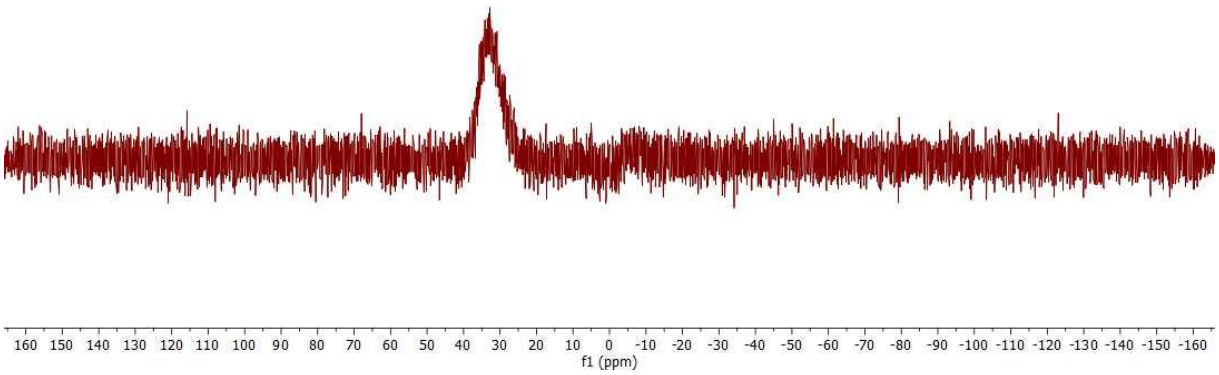
210301.419.10.fid — Fupeng Wu Q-25 — Au11B CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 19 — 128.38MHz

32.8



3j

(^{11}B NMR, 128 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

File:21032218
Vial:1:D,2
Description:MeOH/0.1% HCOOH in H2O 90:10

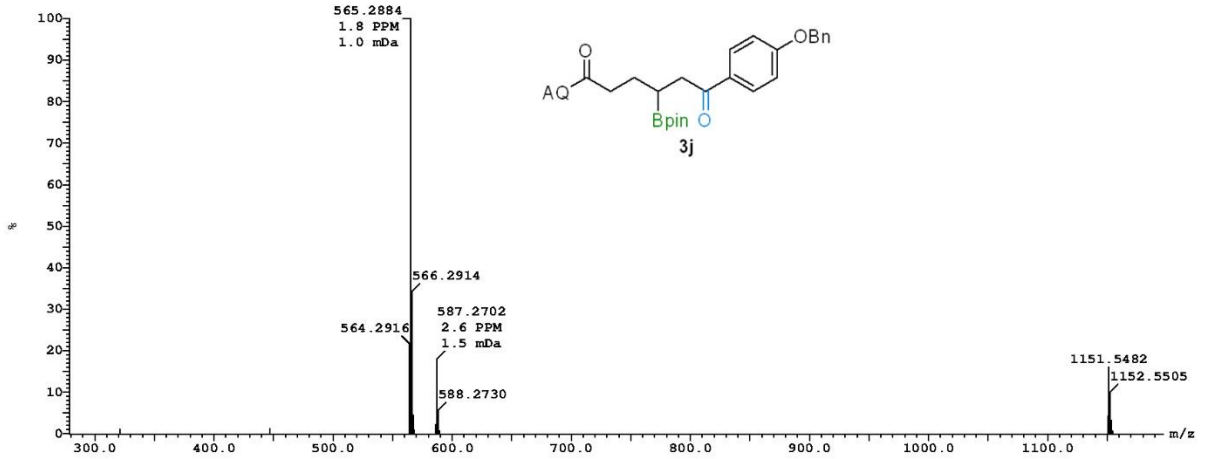
Sample Name:Q-25
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:12:53:04

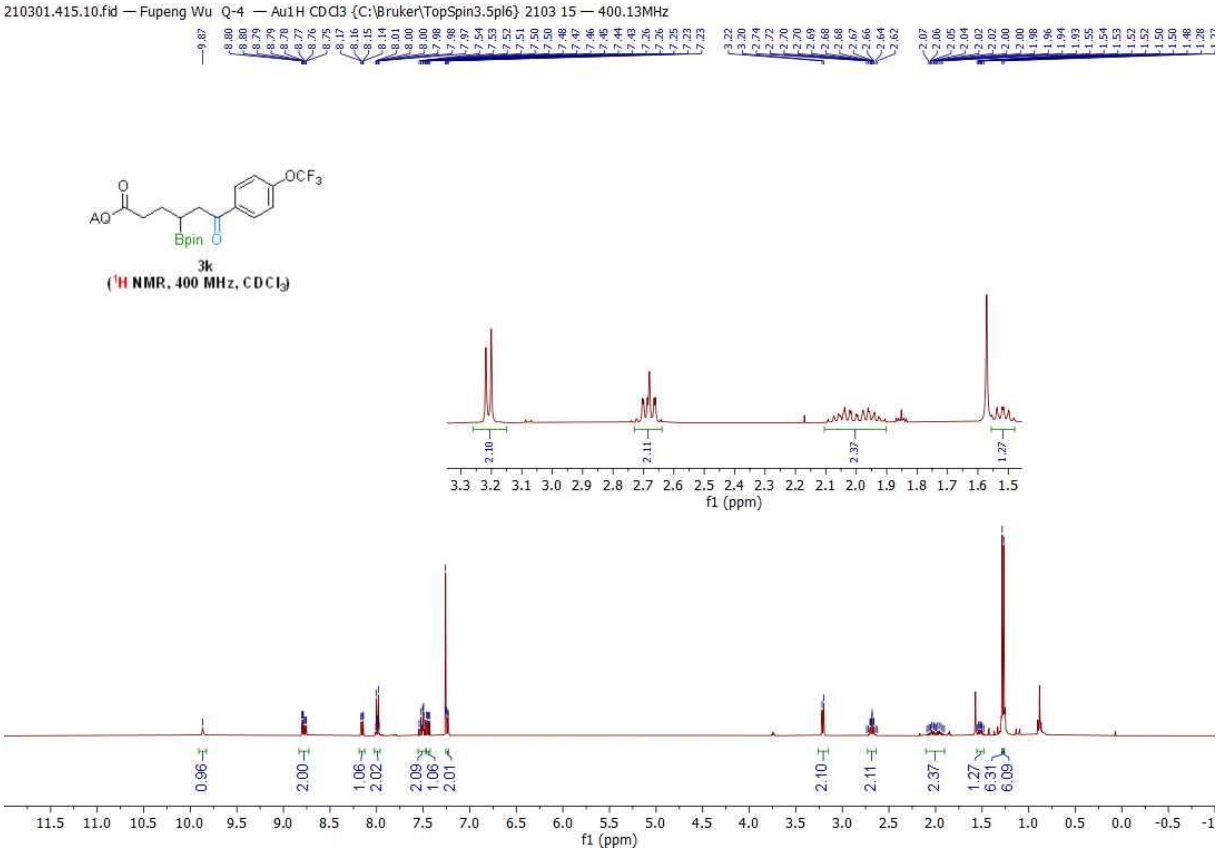
Sample Report:

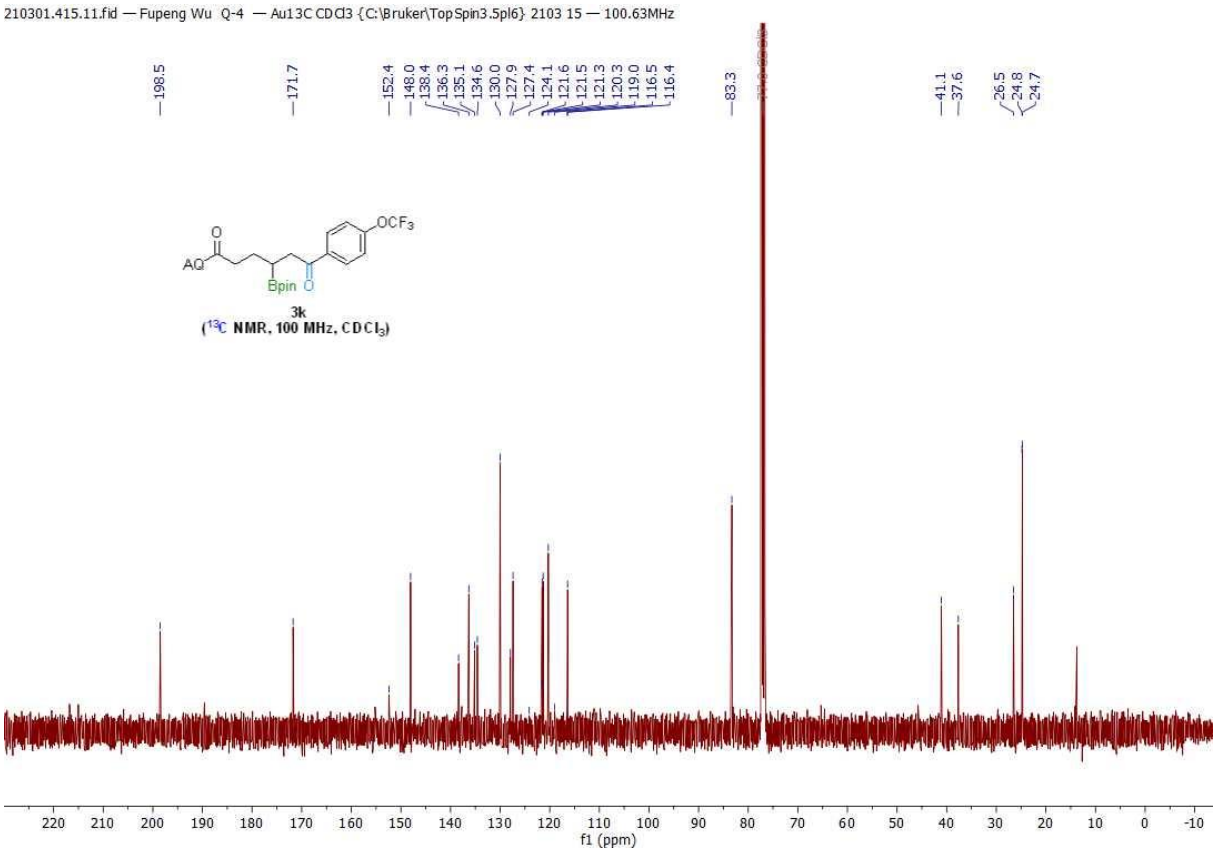
(Time: 0.51) Combine (44:48-97:100) - Dead time test passed

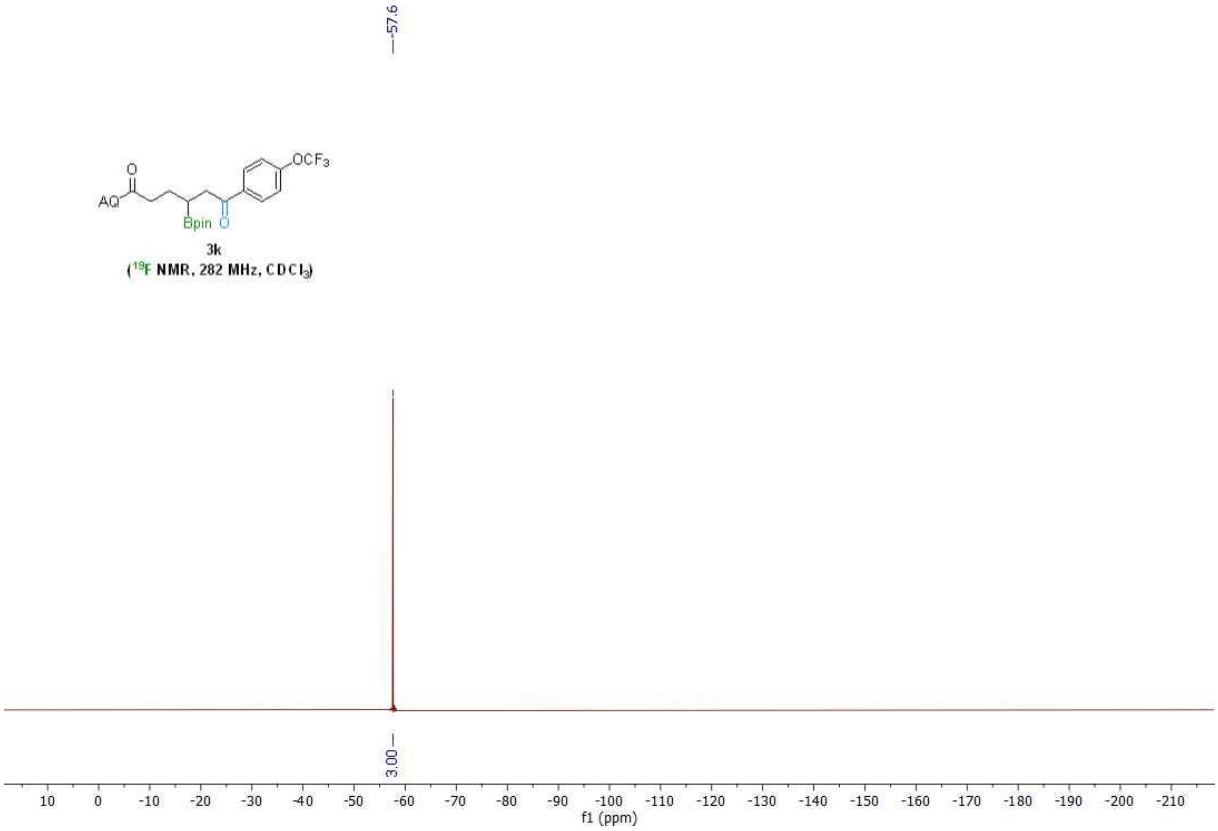
1:TOF MS ES+
5.2e+008



3j


210301.415.10.fid — Fupeng Wu Q-4 — Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 15 — 400.13MHz
OCF3
AQ
Bpin
3k
(1H NMR, 400 MHz, CDCl3)
f1 (ppm)


210301.415.11.fid — Fupeng Wu Q-4 — Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 15 — 100.63MHz
OCF3
AQ
Bpin
3k
(13C NMR, 100 MHz, CDCl3)
f1 (ppm)



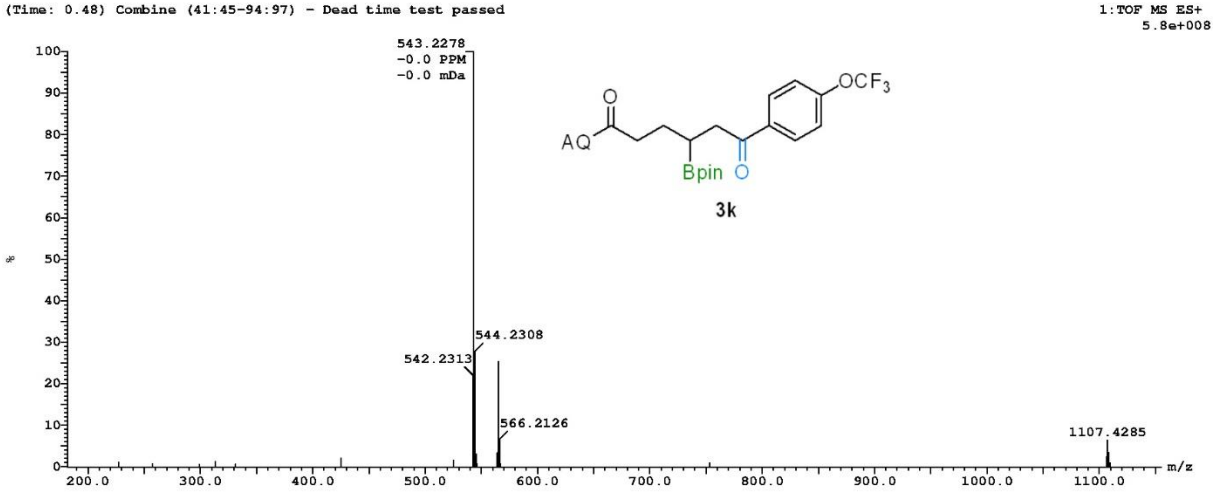
ESI-TOF Accurate Mass Report

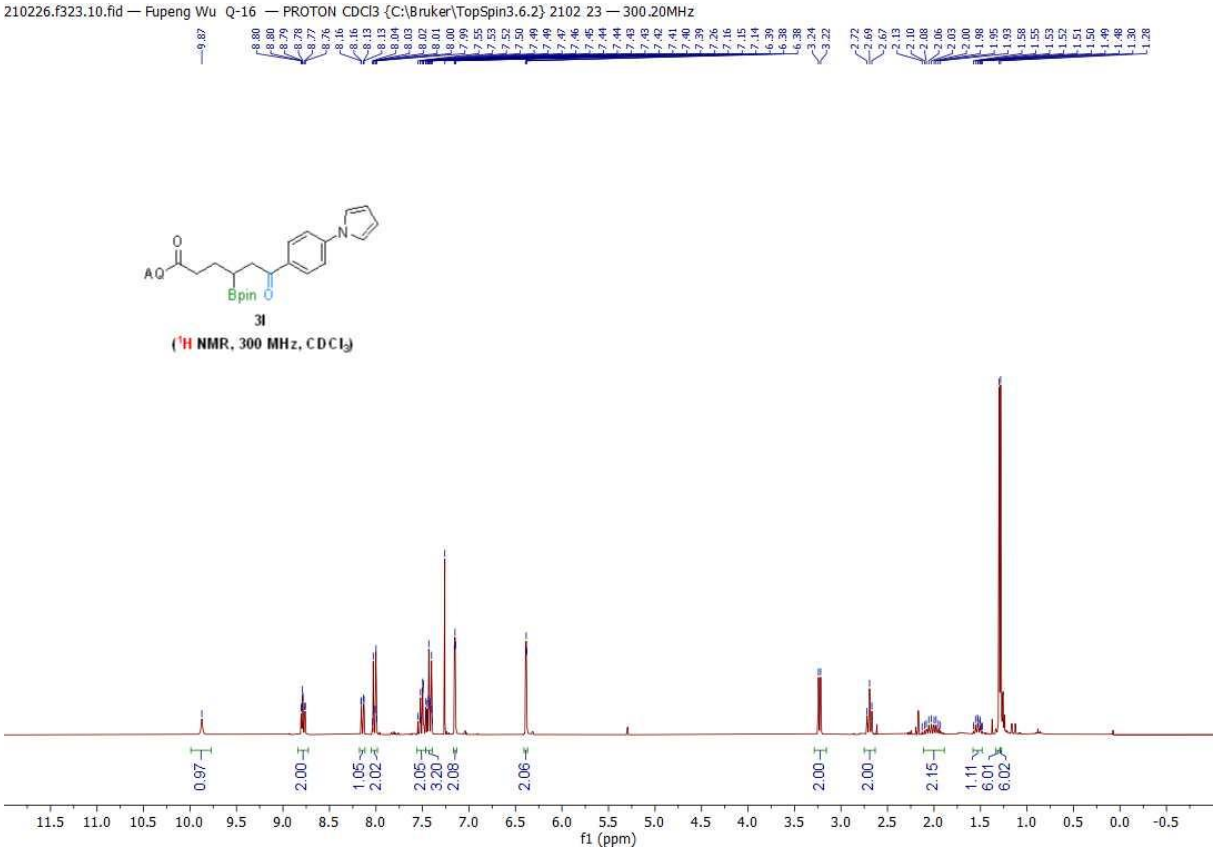
File:21032204
Vial:1:B,4
Description:MeOH/0.1% HCOOH in H2O 90:10

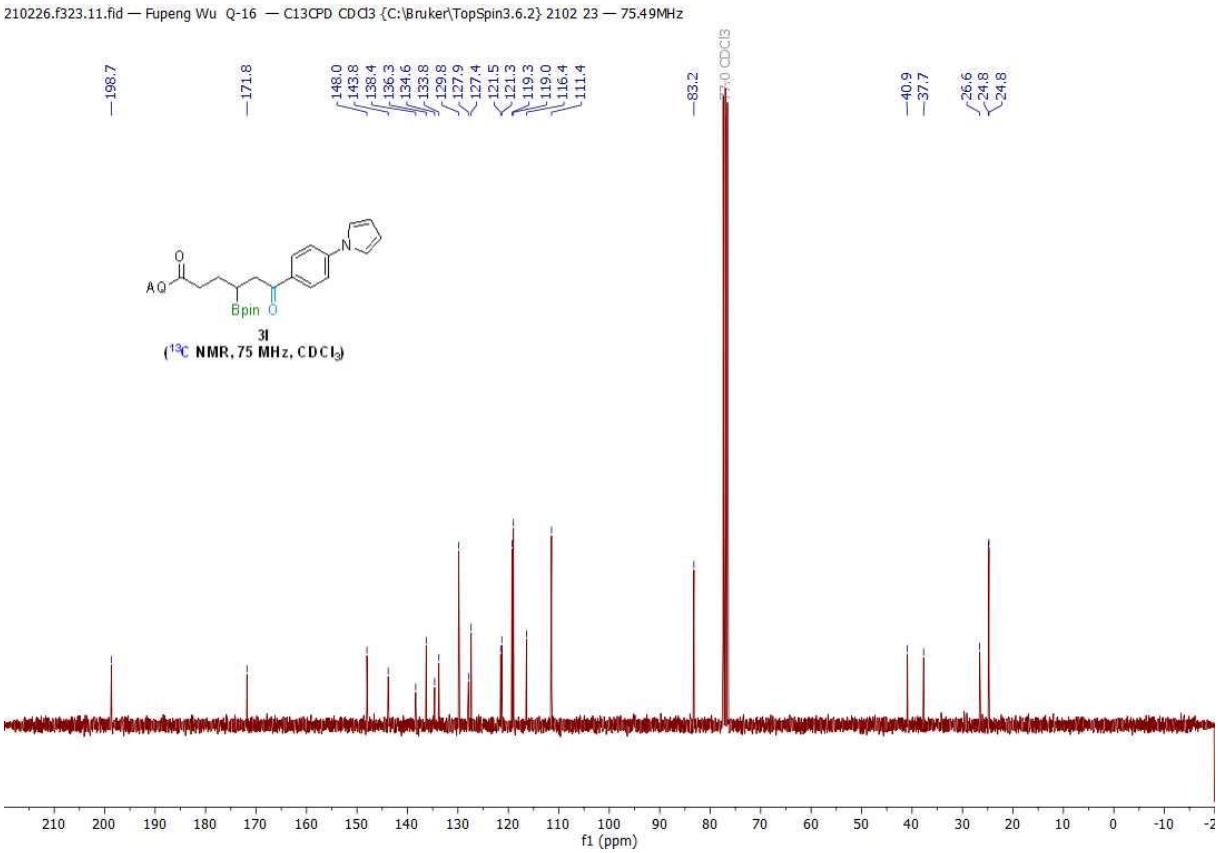
Sample Name:Q-4
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:11:49:55

Sample Report:

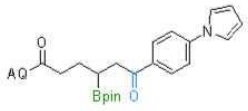



210226.f323.10.fid — Fupeng Wu Q-16 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 23 — 300.20MHz
AQ
Bpin
3l
(1H NMR, 300 MHz, CDCl3)
0.97
2.00
1.05
2.02
2.05
3.20
2.08
2.06
2.00
2.00
2.15
1.11
6.01
6.02
f1 (ppm)


210226.f323.11.fid — Fupeng Wu Q-16 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 23 — 75.49MHz
198.7
171.8
148.0
143.8
138.4
136.3
134.6
133.8
129.8
127.9
127.4
121.5
121.3
119.3
119.0
116.4
111.4
83.2
77.0 CDCl3
40.9
37.7
26.6
24.8
24.8
AQ
Bpin
3l
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

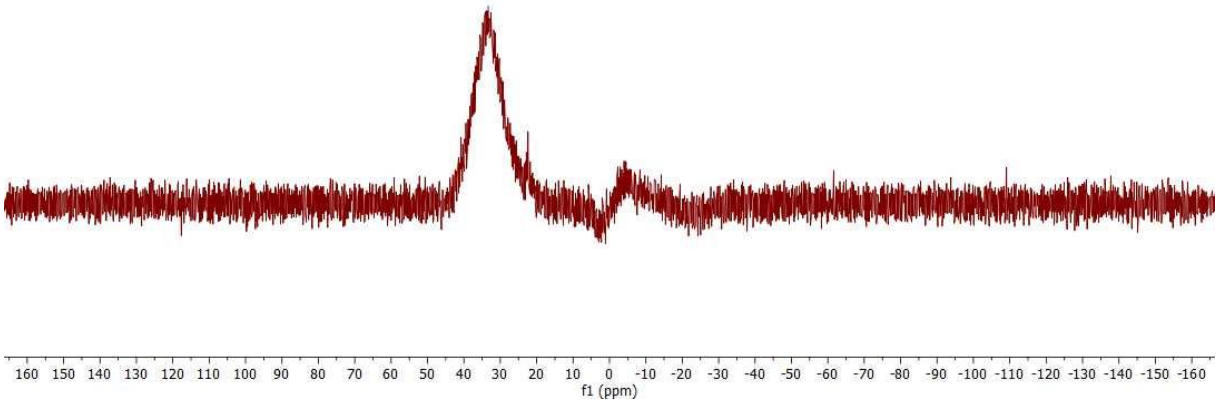
210226.f323.12.fid — Fupeng Wu Q-16 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 23 — 96.32MHz

33.3



3l

(^{11}B NMR, 96 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

File:21032212
Vial:1:C,4
Description:MeOH/0.1% HCOOH in H2O 90:10

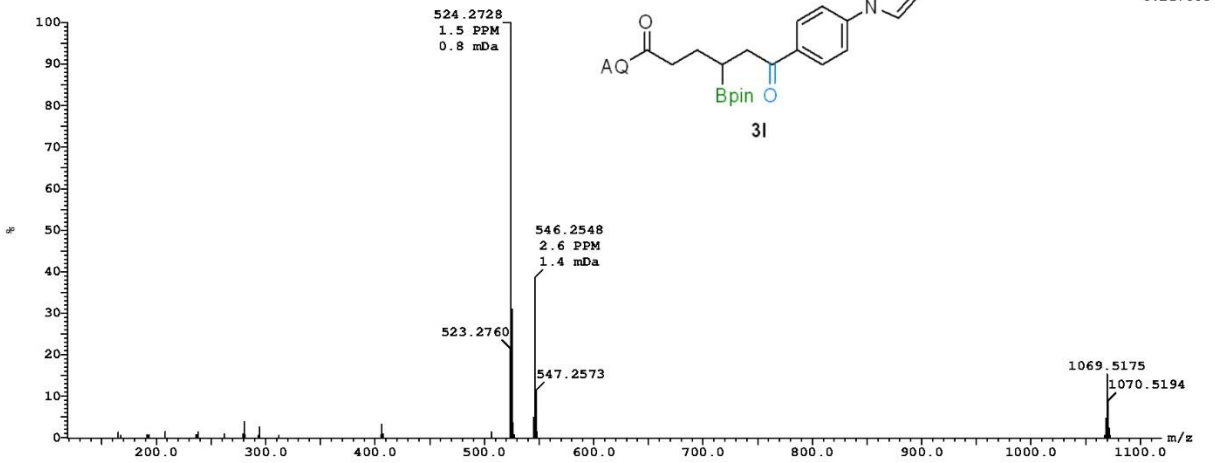
Sample Name:Q-16
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:12:26:10

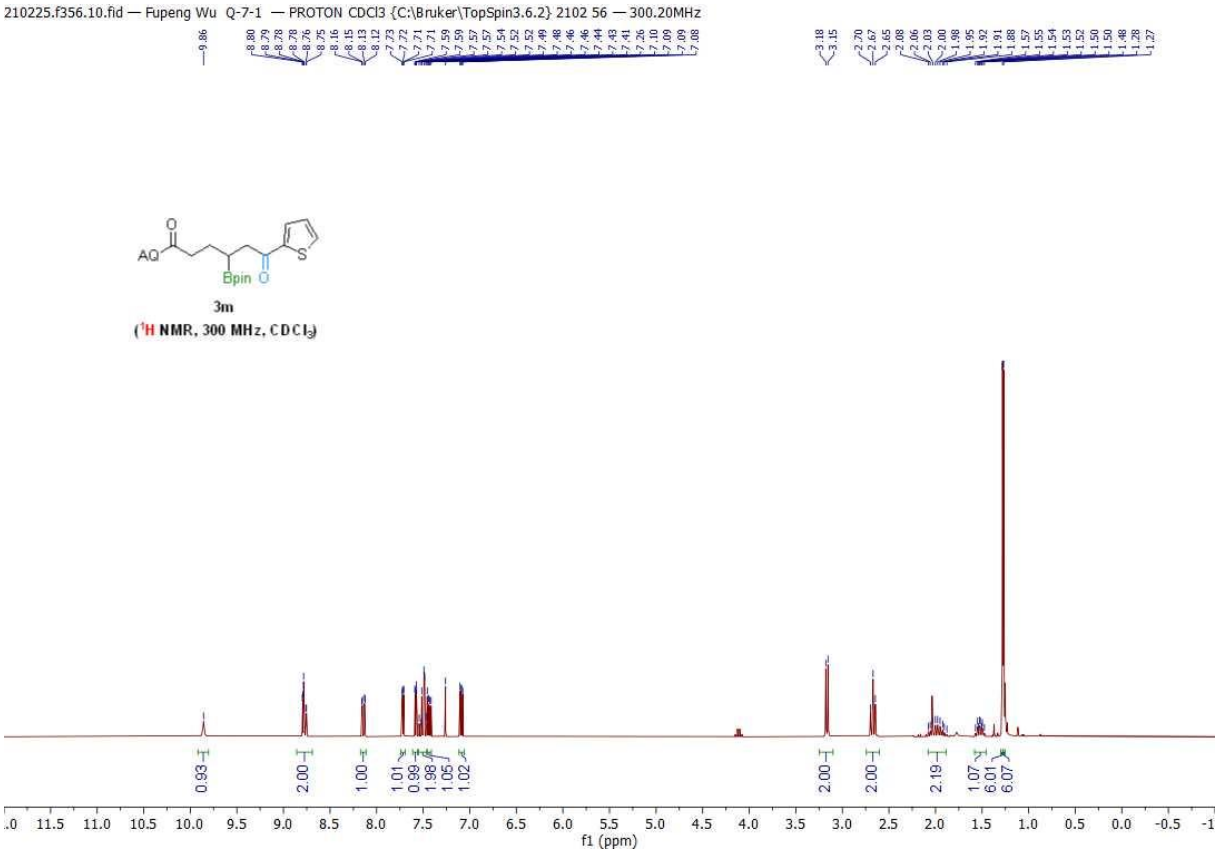
Sample Report:

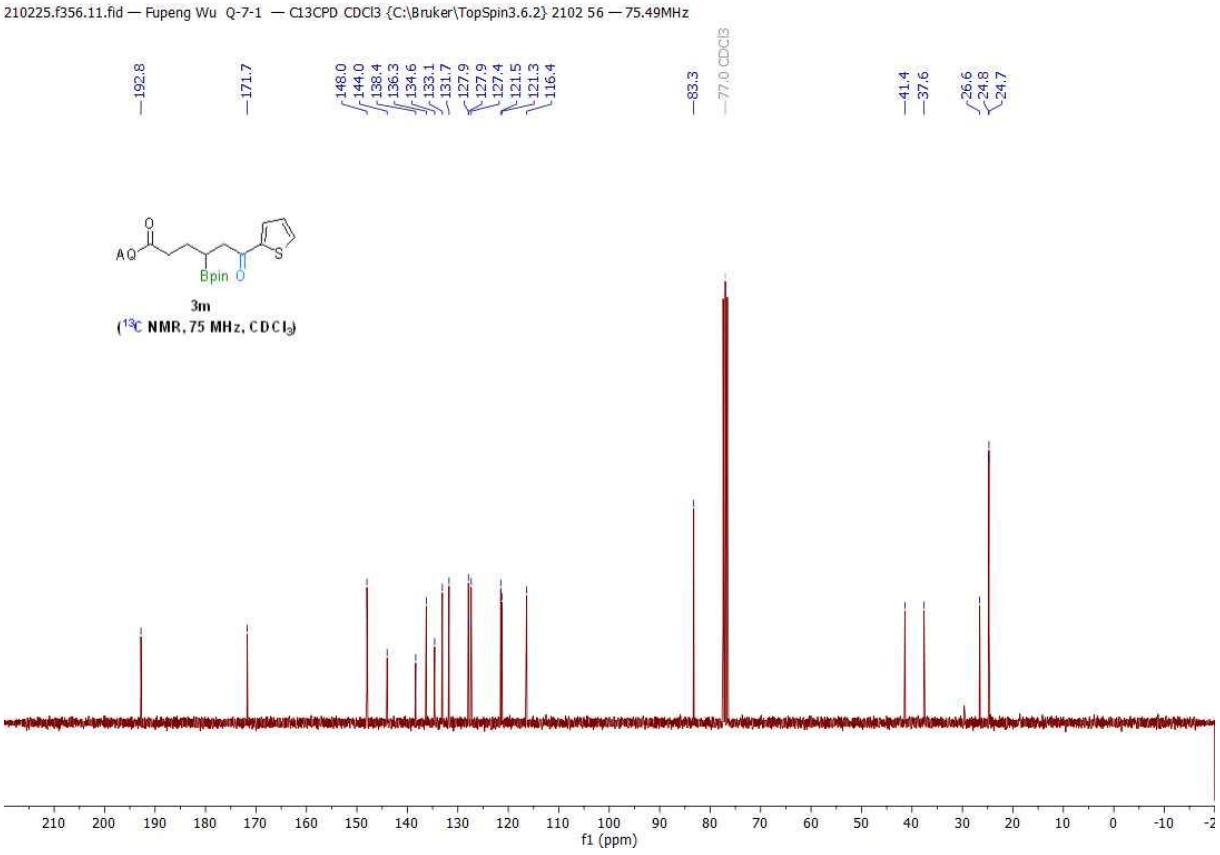
(Time: 0.46) Combine (39:43-93:96) - Dead time test passed

1:TOF MS ES+
4.2e+008



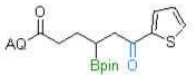
3l


210225.f356.10.fid — Fupeng Wu Q-7-1 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 56 — 300.20MHz
AQ
Bpin
3m
(1H NMR, 300 MHz, CDCl3)
0.93
2.00
1.00
1.01
0.99
1.98
1.05
1.02
2.00
2.00
2.19
1.07
6.01
6.07
f1 (ppm)


210225.f356.11.fid — Fupeng Wu Q-7-1 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 56 — 75.49MHz
192.8
171.7
148.0
144.0
138.4
136.3
134.6
133.1
131.7
127.9
127.9
127.4
121.5
121.3
116.4
83.3
77.0 CDCl3
41.4
37.6
26.6
24.8
24.7
AQ
Bpin
3m
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

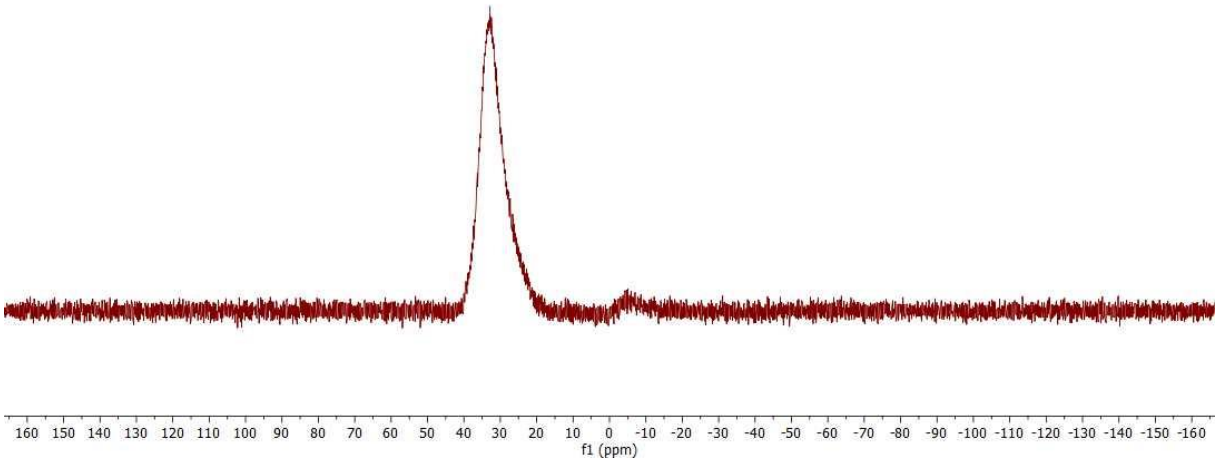
210225.f356.12.fid — Fupeng Wu Q-7-1 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 56 — 96.32MHz

32.8



3m

(^{11}B NMR, 96 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

File:21032224
Vial:1:B,6
Description:MeOH/0.1% HCOOH in H2O 90:10

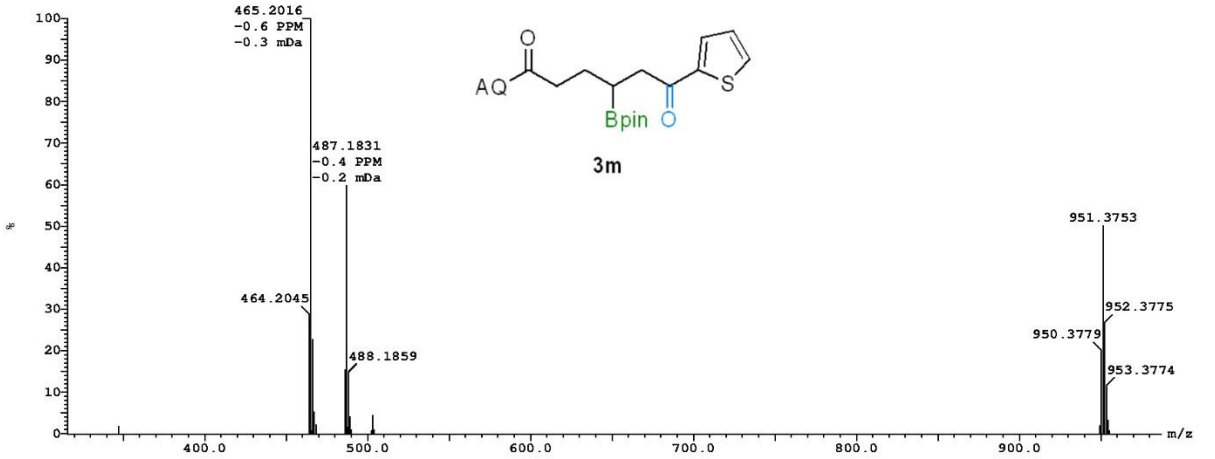
Sample Name:Q-7
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:15:08:12

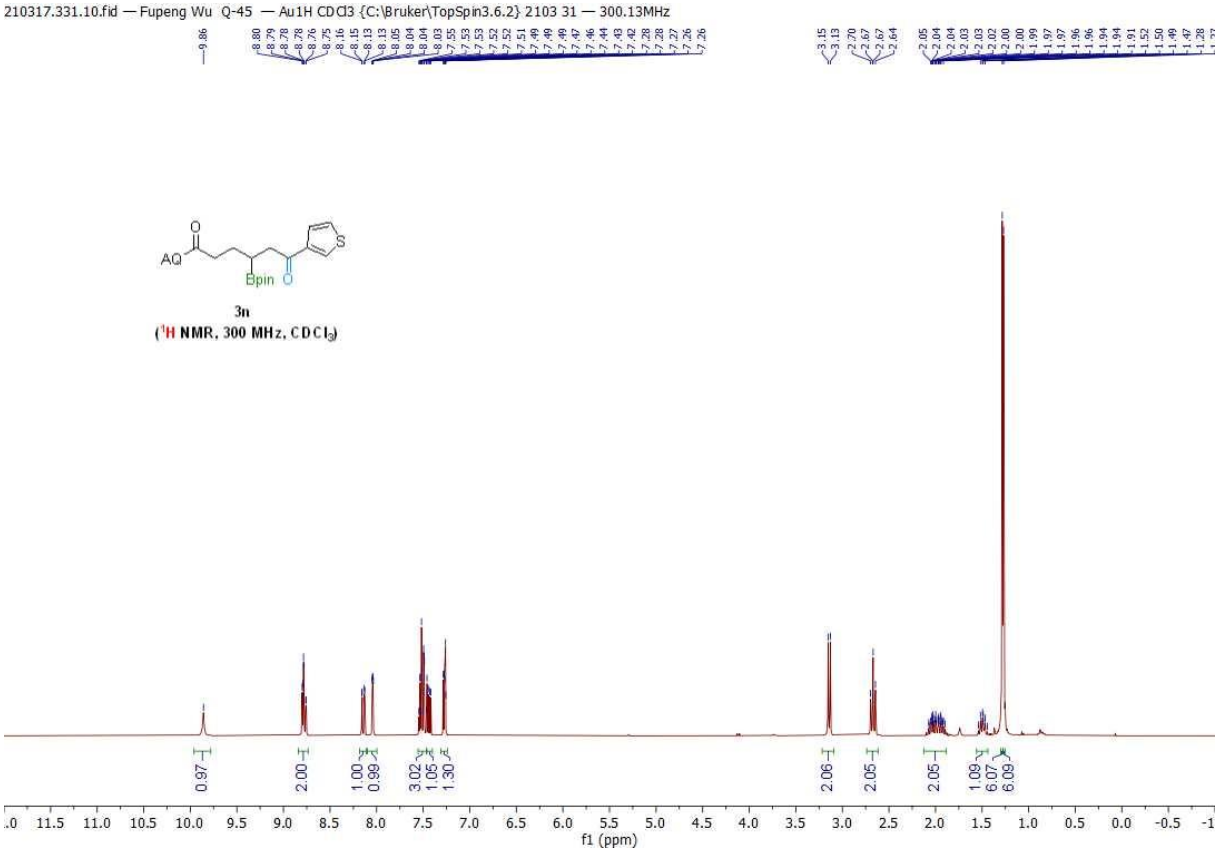
Sample Report:

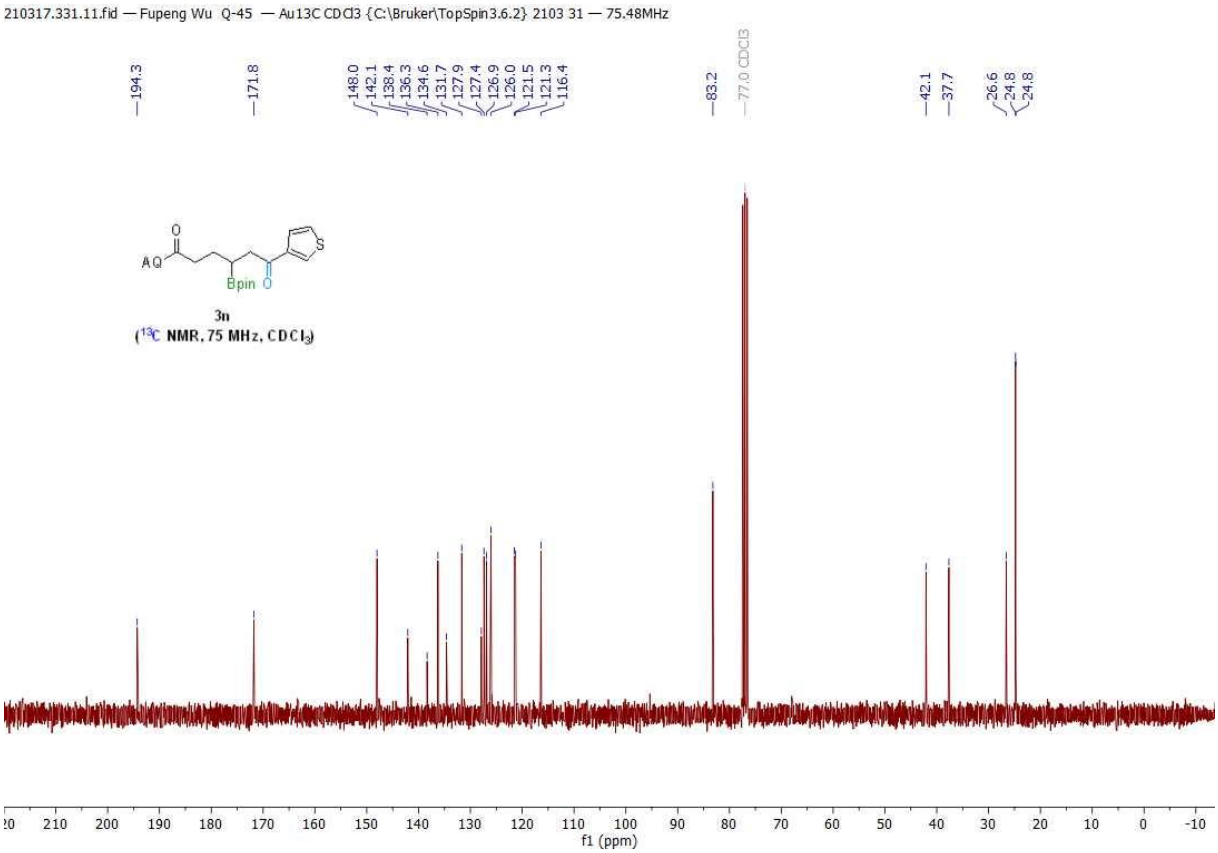
(Time: 0.39) Combine (33:37-86:90) - Dead time test passed

1:TOF MS ES+
3.4e+007



3m


210317.331.10.fid — Fupeng Wu Q-45 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 31 — 300.13MHz
AQ
Bpin
3n
(1H NMR, 300 MHz, CDCl3)
0.97
2.00
1.00
0.99
3.02
1.05
1.30
2.06
2.05
2.05
1.09
6.07
6.09
f1 (ppm)


210317.331.11.fid — Fupeng Wu Q-45 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 31 — 75.48MHz
194.3
171.8
148.0
142.1
138.4
136.3
134.6
131.7
127.9
127.4
126.9
126.0
121.5
121.3
116.4
83.2
77.0 CDCl3
42.1
37.7
26.6
24.8
24.8
AQ
Bpin
3n
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

ESI-TOF Accurate Mass Report
File:21040906
Vial:1:F,1
Description:MeOH/0.1% HCOOH in H2O 90:10

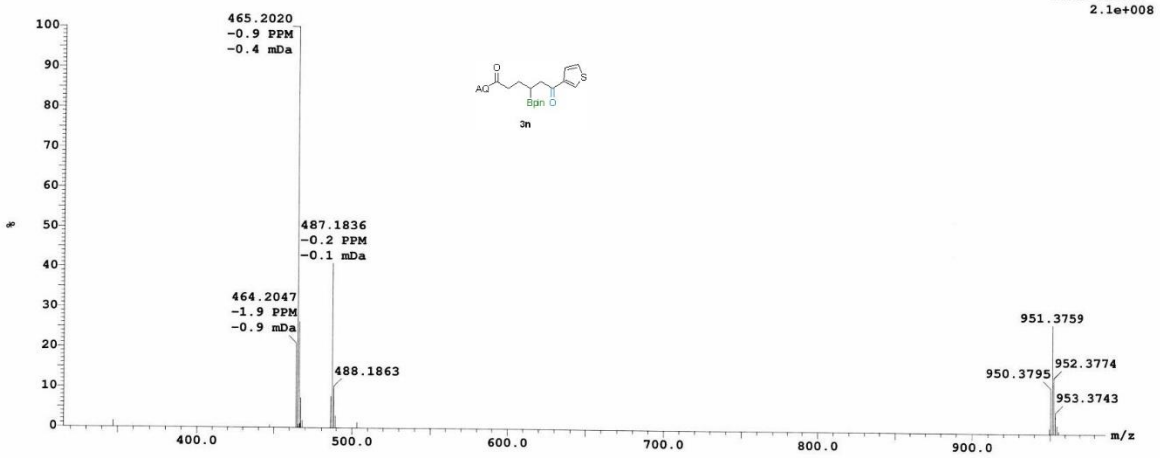
Sample Name:Q-45
Date:09-Apr-2021

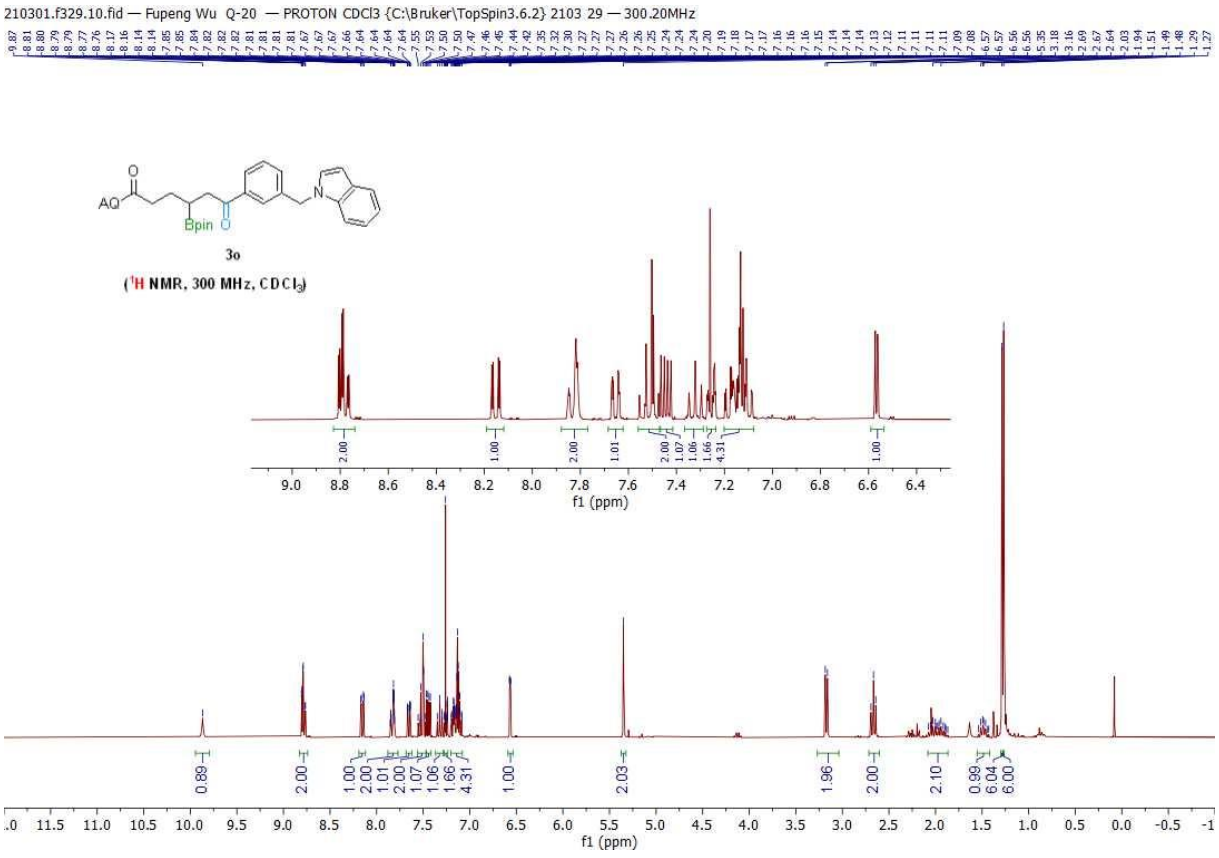
UserName:Fupeng Wu
Time:16:25:58

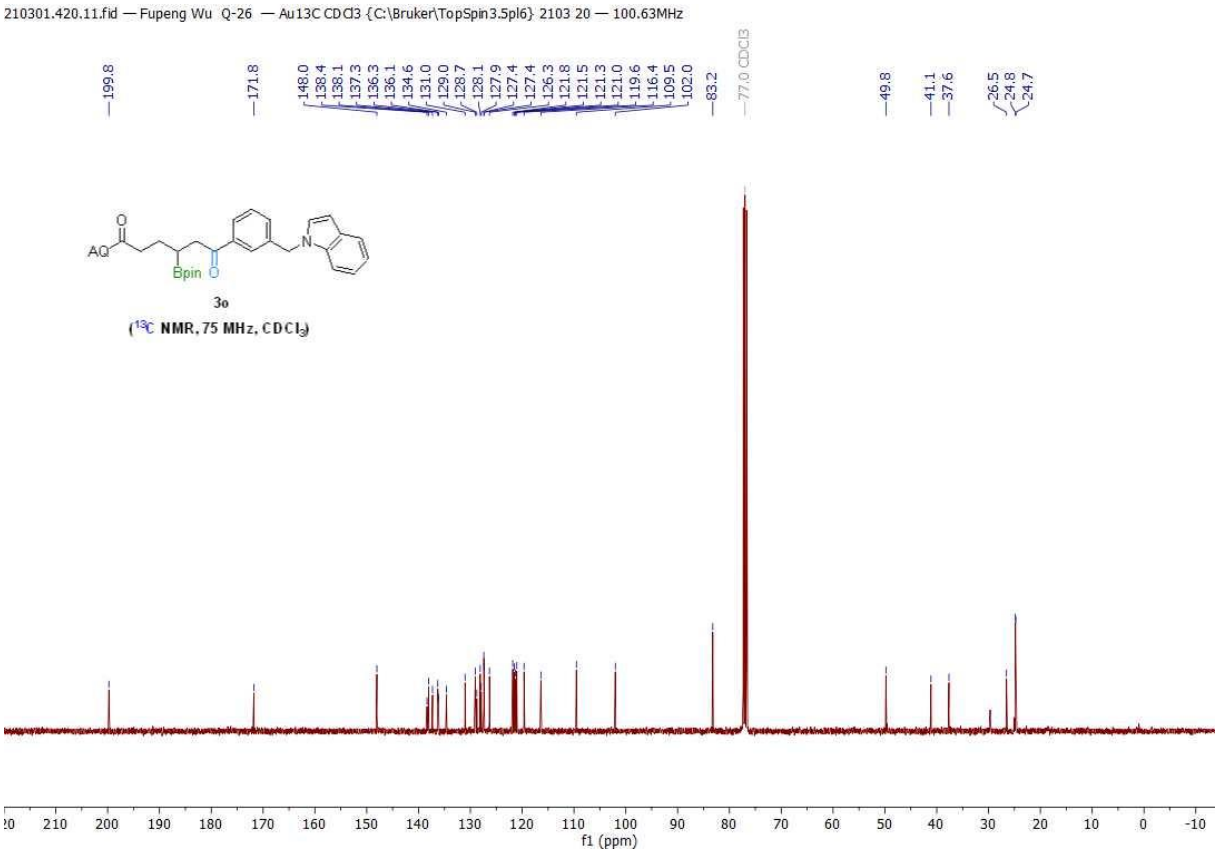
Sample Report:

(Time: 0.40) Combine (34:38-87:91) - Dead time test passed

1:TOF MS ES+
2.1e+008




210301.f329.10.fid — Fupeng Wu Q-20 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 29 — 300.20MHz
AQ
Bpin
3o
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)

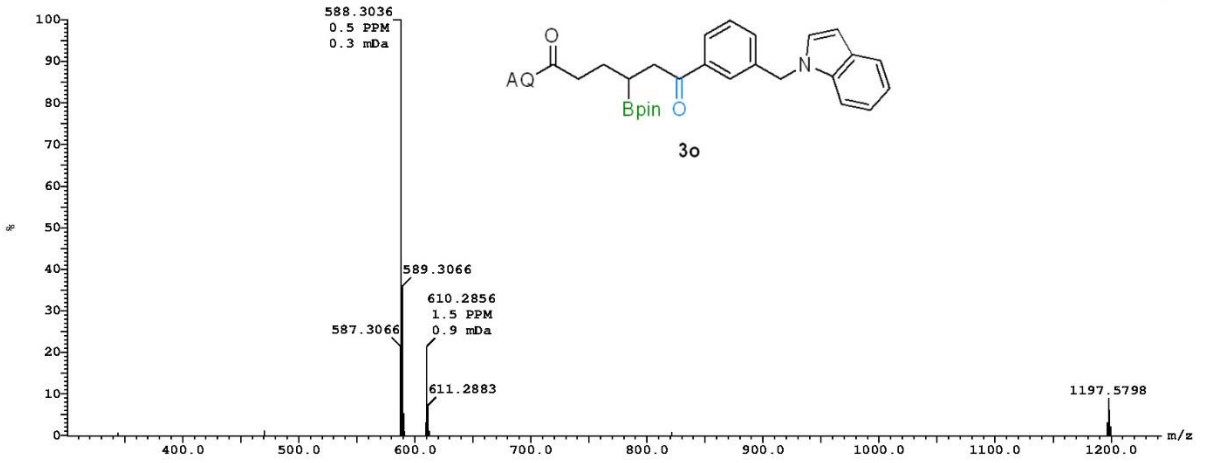

210301.420.11.fid — Fupeng Wu Q-26 — Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 20 — 100.63MHz
AQ
Bpin
3o
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

File:21032219 Sample Name:Q-26 UserName:Fu-peng Wu
Vial:1:D,3 Date:22-Mar-2021 Time:12:57:32
Description:MeOH/0.1% HCOOH in H2O 90:10

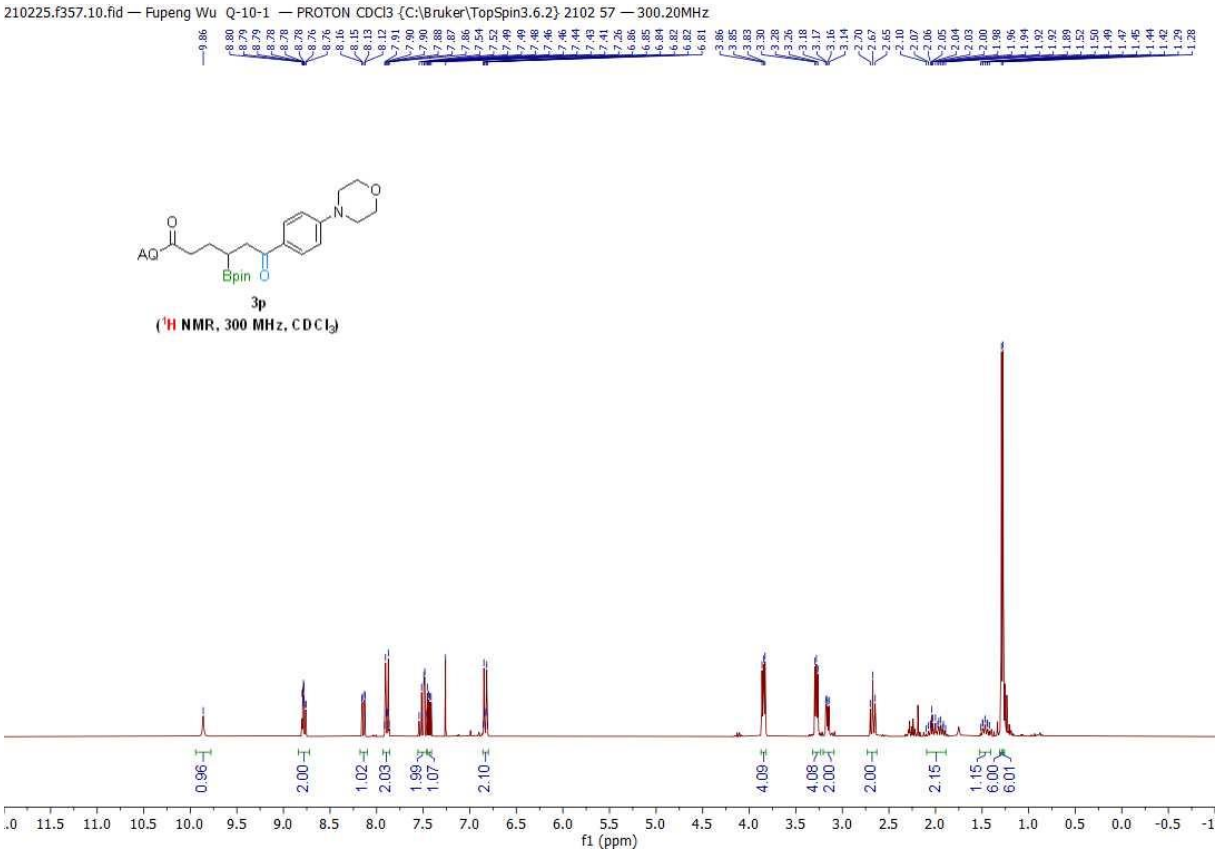
Sample Report:

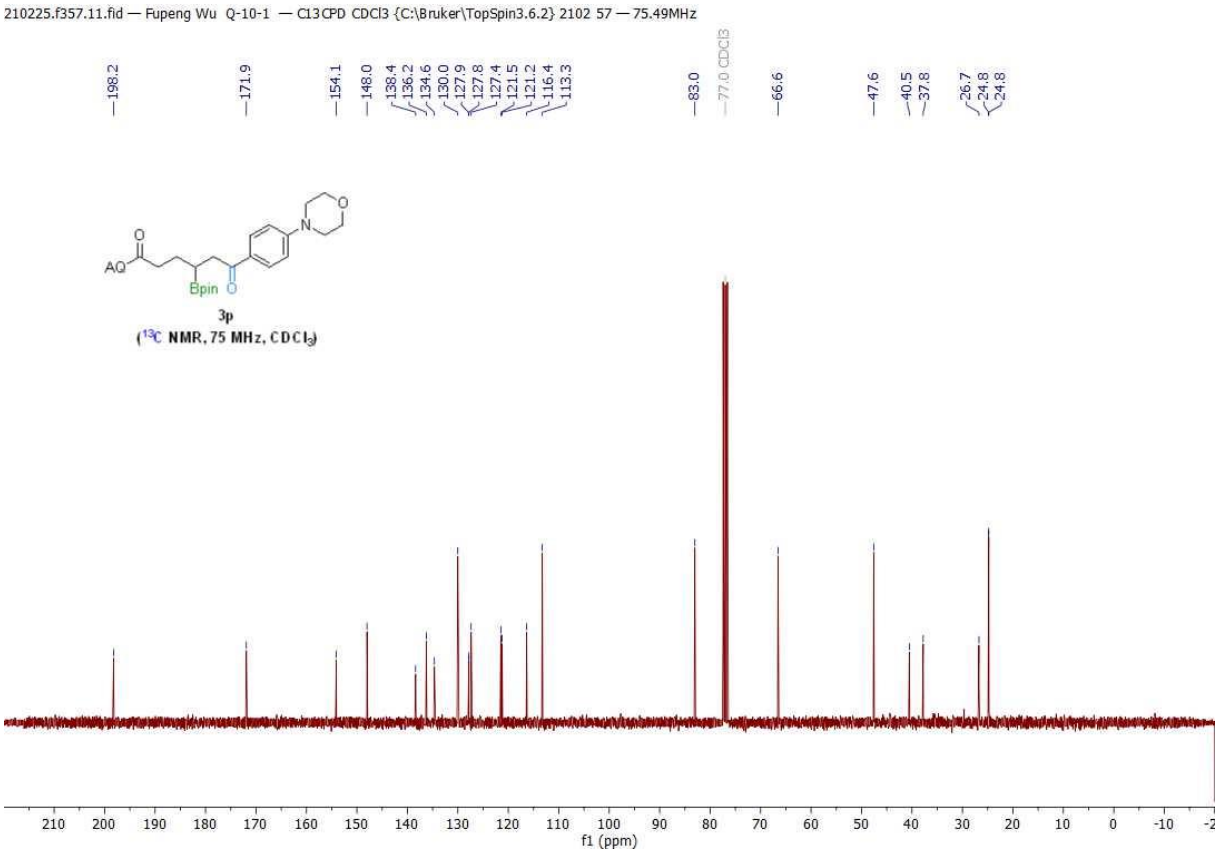
(Time: 0.51) Combine (43:47-97:100) - Dead time test passed

1:TOF MS ES+
4.6e+008



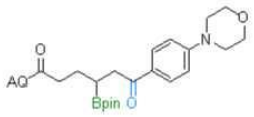
3o


210225.f357.10.fid — Fupeng Wu Q-10-1 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 57 — 300.20MHz
AQ
Bpin
3p
(1H NMR, 300 MHz, CDCl3)
0.96
2.00
1.02
2.03
1.99
1.07
2.10
4.09
4.08
2.00
2.00
2.15
1.15
6.00
6.01
f1 (ppm)


210225.f357.11.fid — Fupeng Wu Q-10-1 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 57 — 75.49MHz
198.2
171.9
154.1
148.0
138.4
136.2
134.6
130.0
127.9
127.8
127.4
121.5
121.2
116.4
113.3
83.0
77.0 CDCl3
66.6
47.6
40.5
37.8
26.7
24.8
24.8
AQ
Bpin
3p
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

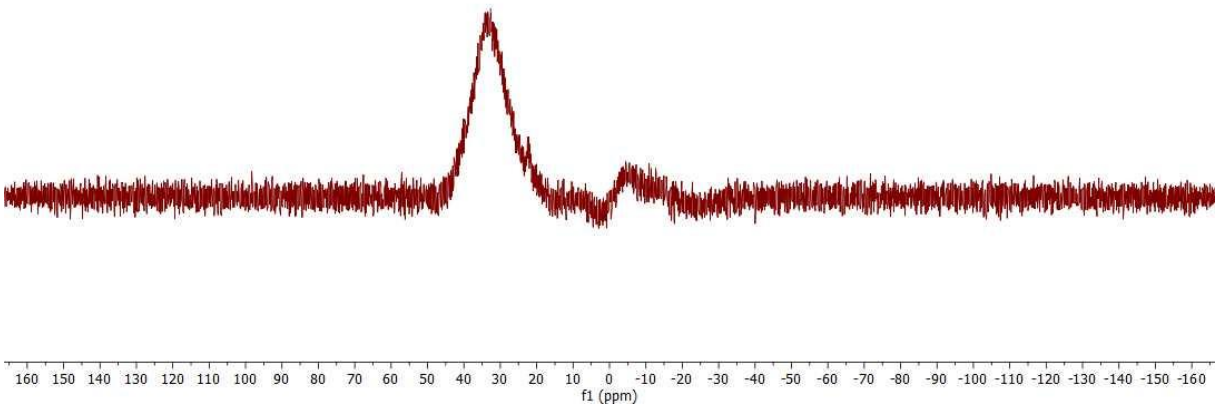
210225.f357.12.fid — Fupeng Wu Q-10-1 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 57 — 96.32MHz

32.7



3p

(^{11}B NMR, 96 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

Page 2

File:21032207
Vial:1:B,7
Description:MeOH/0.1% HCOOH in H2O 90:10

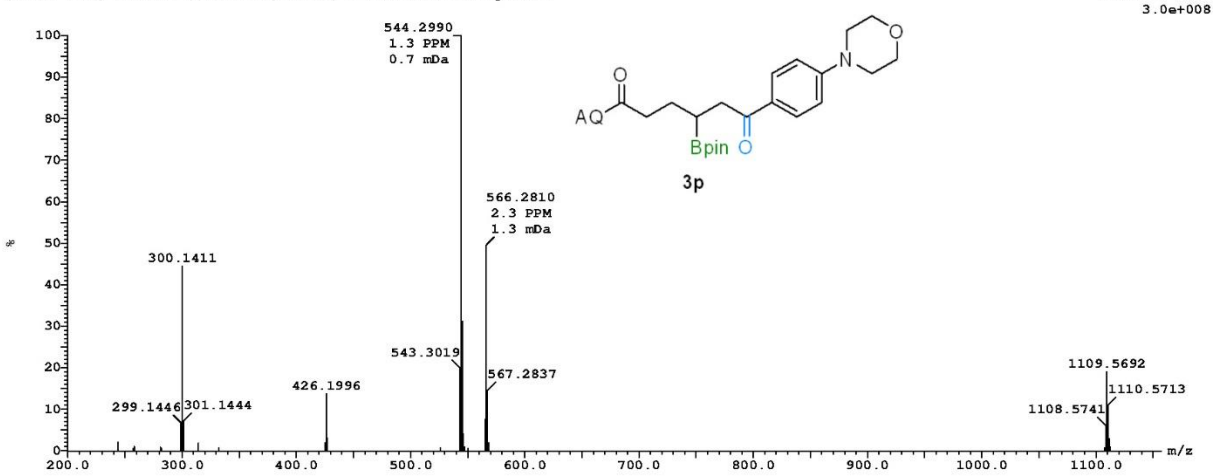
Sample Name:Q-10
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:12:03:24

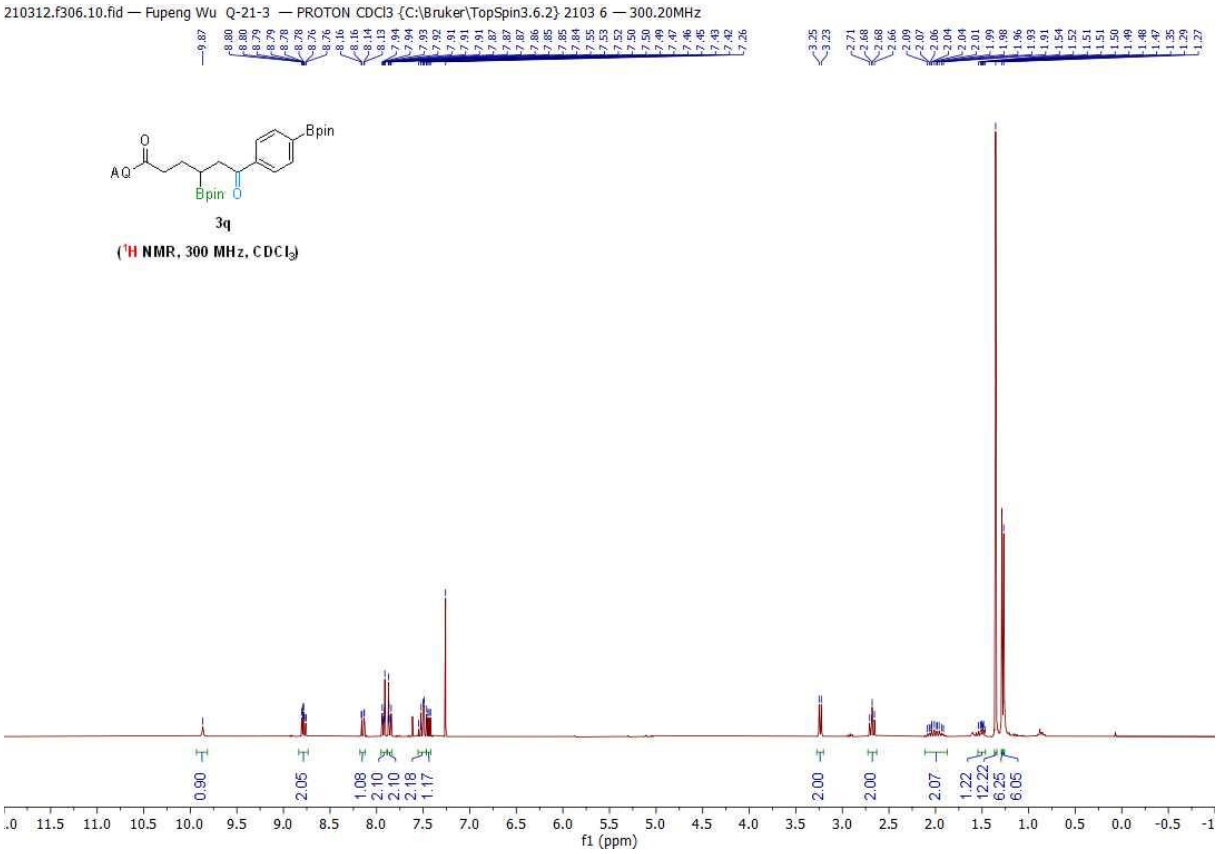
Sample Report:

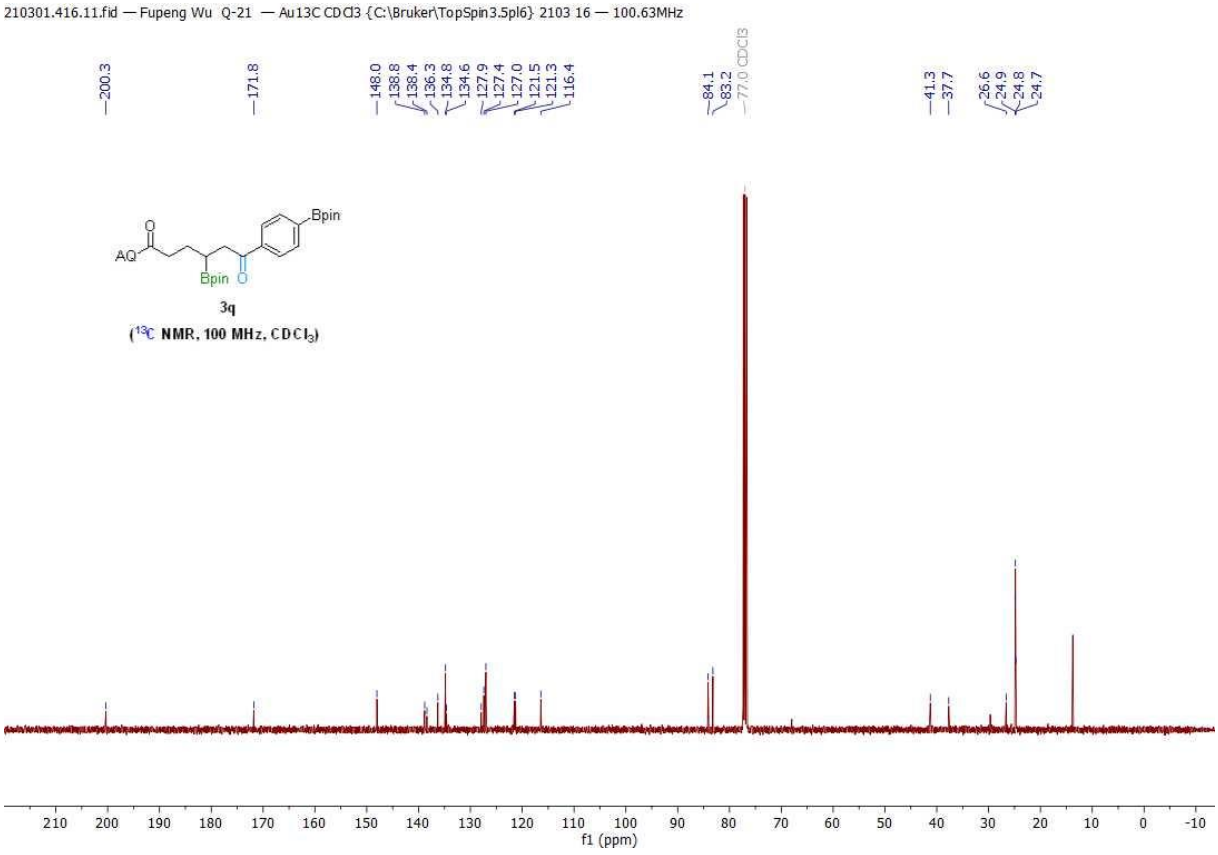
(Time: 0.40) Combine ((33+36:39)-87:91) - Dead time test passed

1:TOF MS ES+
3.0e+008



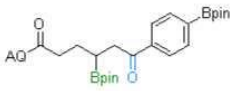
3p


210312.f306.10.fid — Fupeng Wu Q-21-3 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 6 — 300.20MHz
Bpin
AQ
Bpin
O
3q
(1H NMR, 300 MHz, CDCl3)
0.90
2.05
1.08
2.10
2.10
2.18
1.17
2.00
2.00
2.07
1.22
12.22
6.25
6.05
f1 (ppm)


210301.416.11.fid — Fupeng Wu Q-21 — Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 16 — 100.63MHz
200.3
171.8
148.0
138.8
138.4
136.3
134.8
134.6
127.9
127.4
127.0
121.5
121.3
116.4
84.1
83.2
77.0 CDCl3
41.3
37.7
26.6
24.9
24.8
24.7
Bpin
AQ
Bpin
O
3q
(13C NMR, 100 MHz, CDCl3)
f1 (ppm)

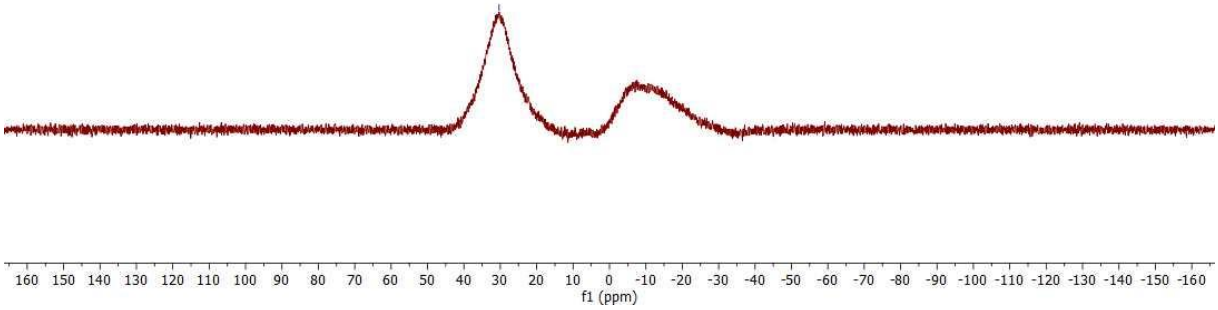
210226.f324.12.fid — Fupeng Wu Q-21 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2102 24 — 96.32MHz

30.3



3q

(^{11}B NMR, 96 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

File:21032215
Vial:1:C,7
Description:MeOH/0.1% HCOOH in H2O 90:10

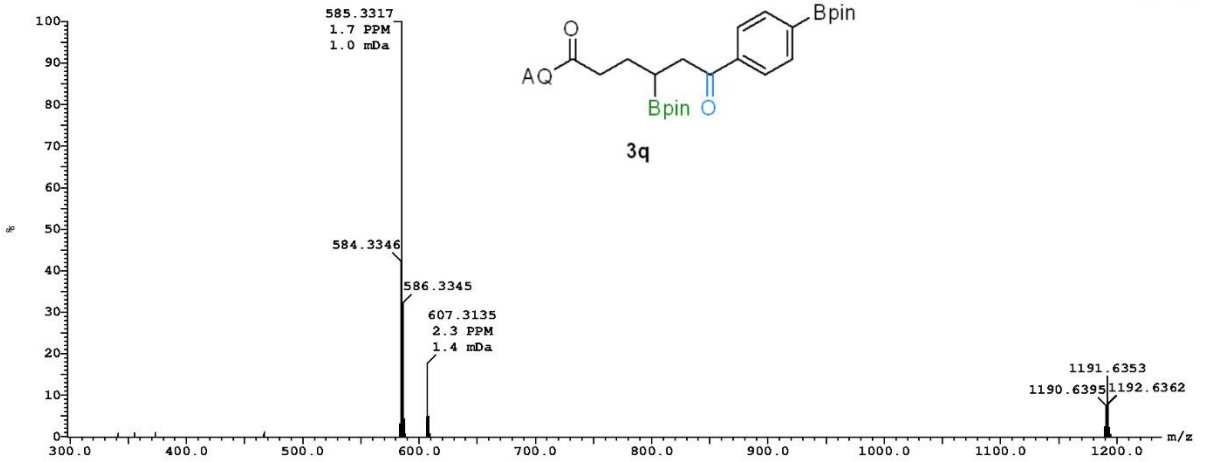
Sample Name:Q-21
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:12:39:34

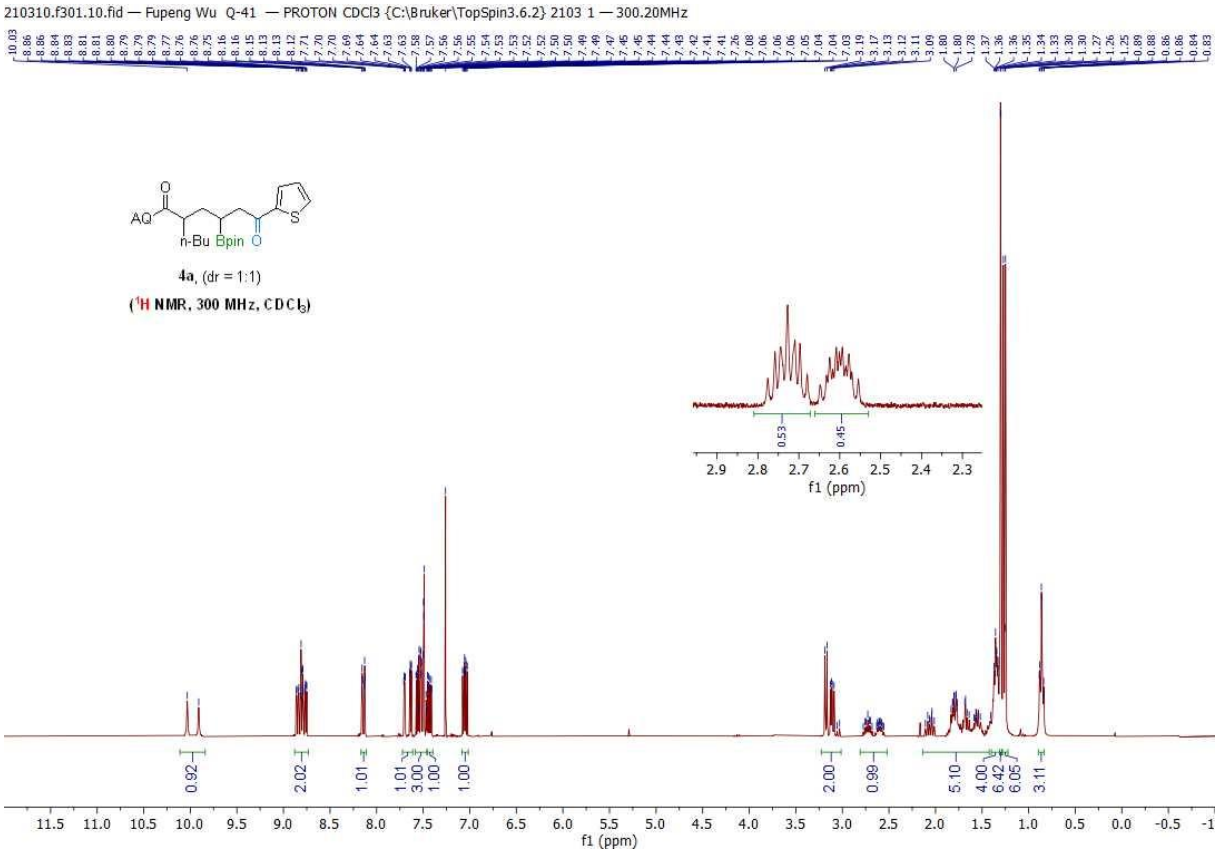
Sample Report:

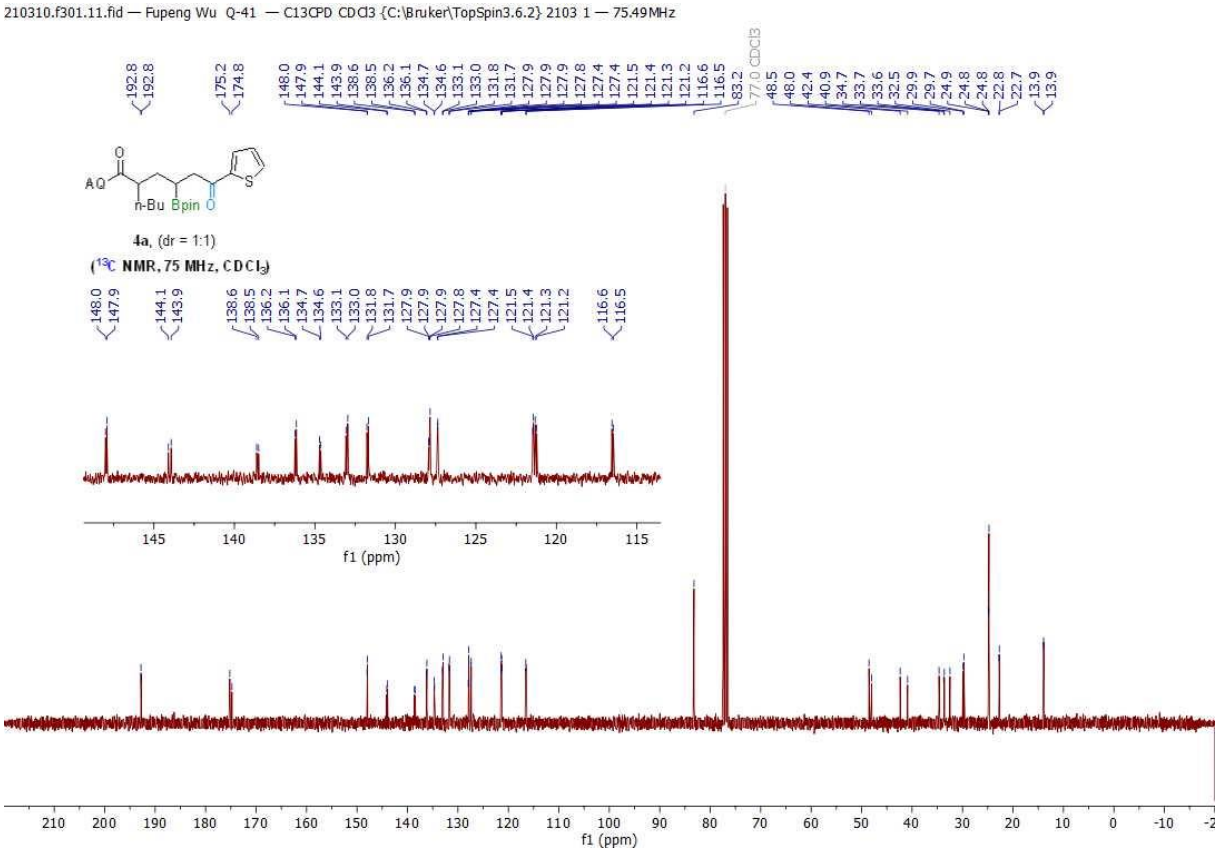
(Time: 0.55) Combine (48:52-100:104) - Dead time test passed

1:TOF MS ES+
4.1e+008



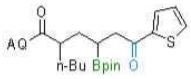
3q


210310.f301.10.fid — Fupeng Wu Q-41 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 1 — 300.20MHz
AQ
n-Bu Bpin
4a, (dr = 1:1)
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)

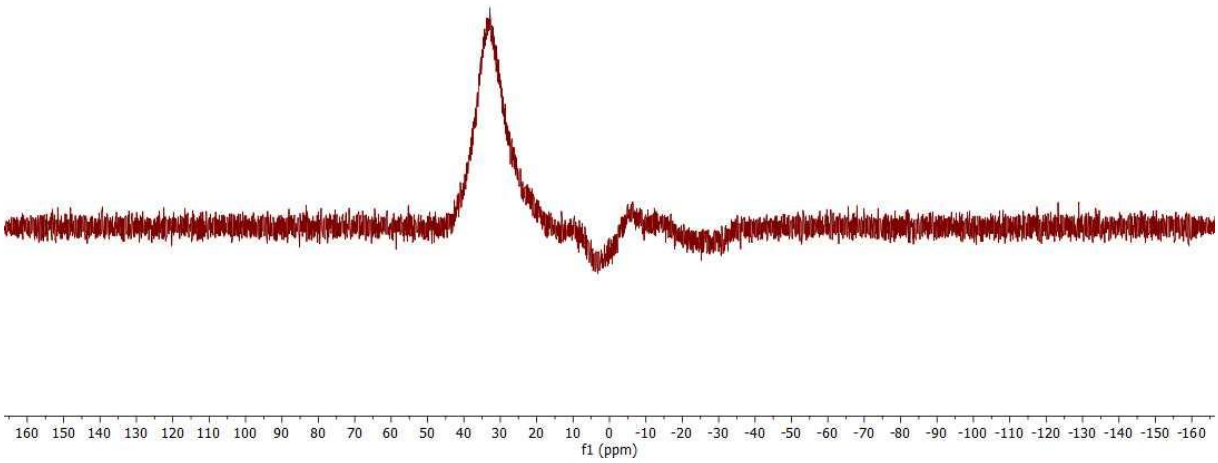

210310.f301.11.fid — Fupeng Wu Q-41 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 1 — 75.49MHz
AQ
n-Bu Bpin
4a, (dr = 1:1)
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

210310.f301.12.fid — Fupeng Wu Q-41 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 1 — 96.32MHz

32.9



4a, (dr = 1:1)
(**^{11}B NMR, 96 MHz, $CDCl_3$**)



ESI-TOF Accurate Mass Report

File:21032301
Vial:1:E,5
Description:MeOH/0.1% HCOOH in H2O 98:2

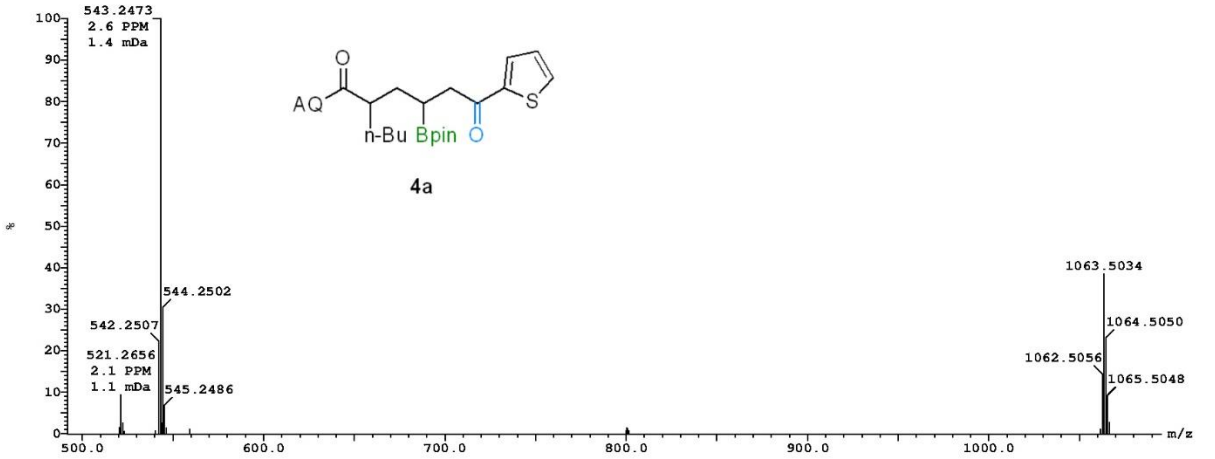
Sample Name:Q-41
Date:23-Mar-2021

UserName:Fu-peng Wu
Time:09:44:30

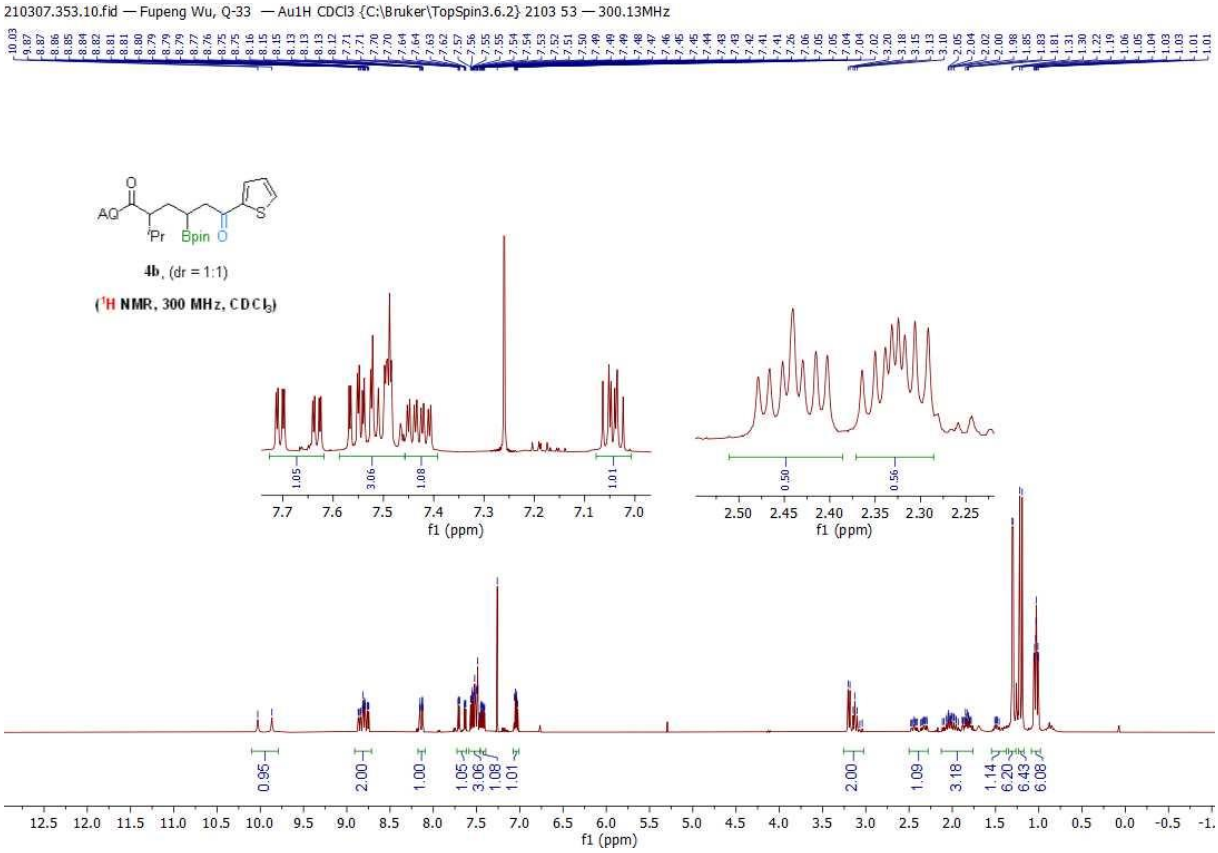
Sample Report:

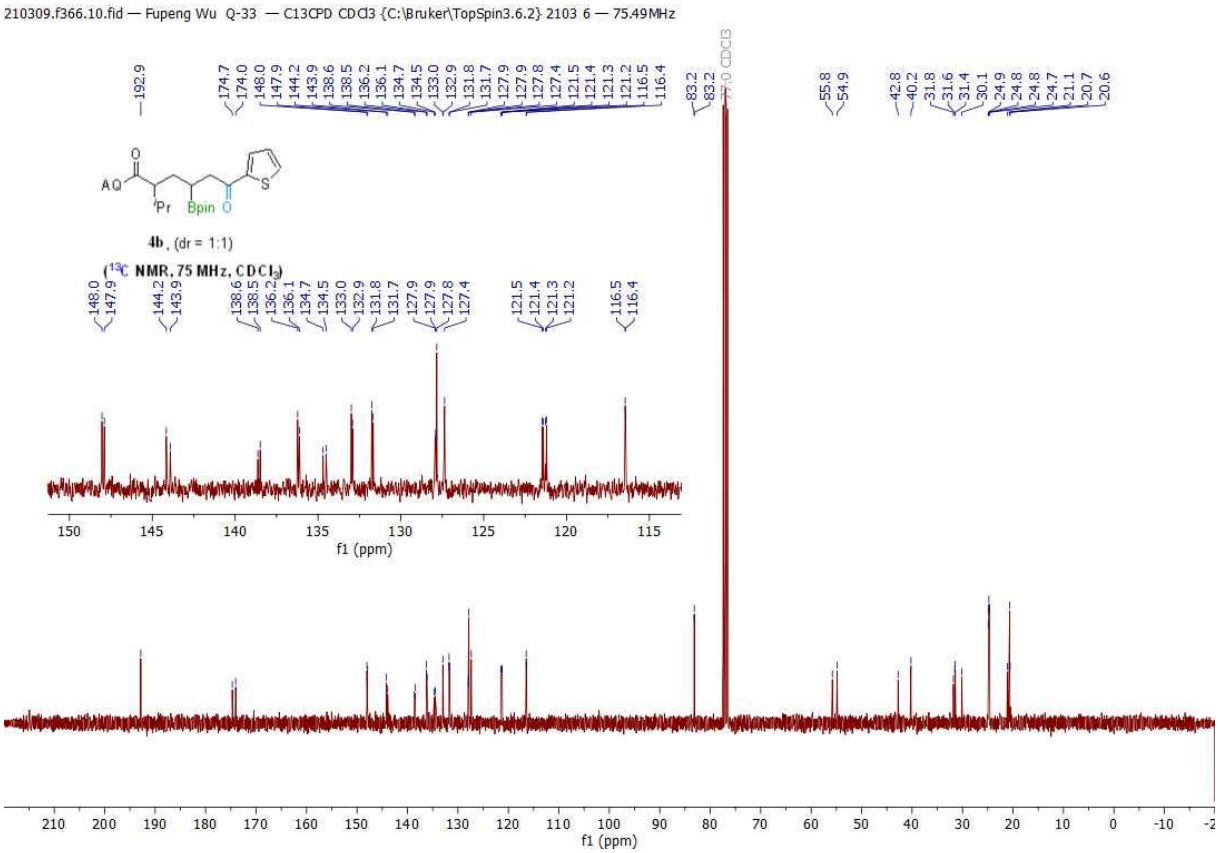
(Time: 0.34) Combine (29:33-81:85) - Dead time test passed

1:TOF MS ES+
5.8e+008



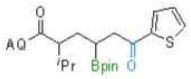
4a


210307.353.10.fid — Fupeng Wu, Q-33 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 53 — 300.13MHz
4b, (dr = 1:1)
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)


210309.f366.10.fid — Fupeng Wu Q-33 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 6 — 75.49MHz
4b, (dr = 1:1)
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

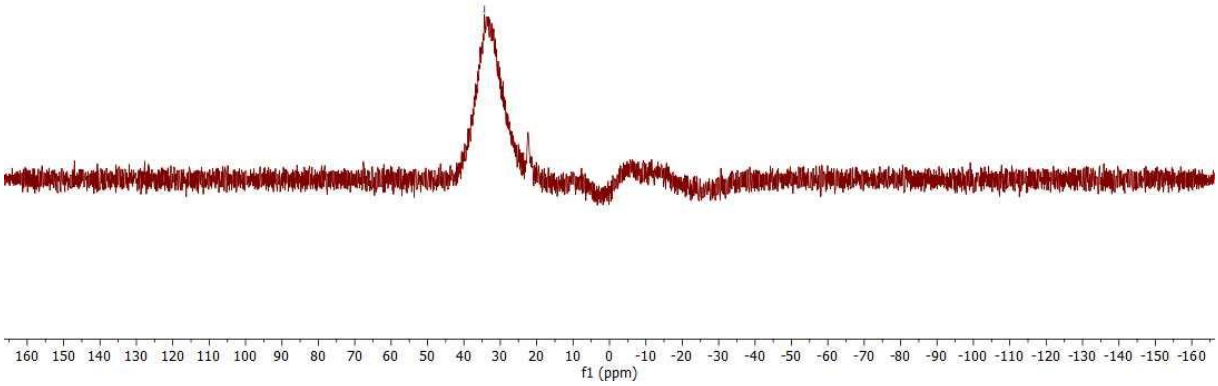
210309.f366.11.fid — Fupeng Wu Q-33 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 6 — 96.32MHz

34.3



4b, (dr = 1:1)

(**^{11}B NMR, 96 MHz, $CDCl_3$**)



ESI-TOF Accurate Mass Report

File:21032230
Vial:1:D,6
Description:MeOH/0.1% HCOOH in H2O 98:2

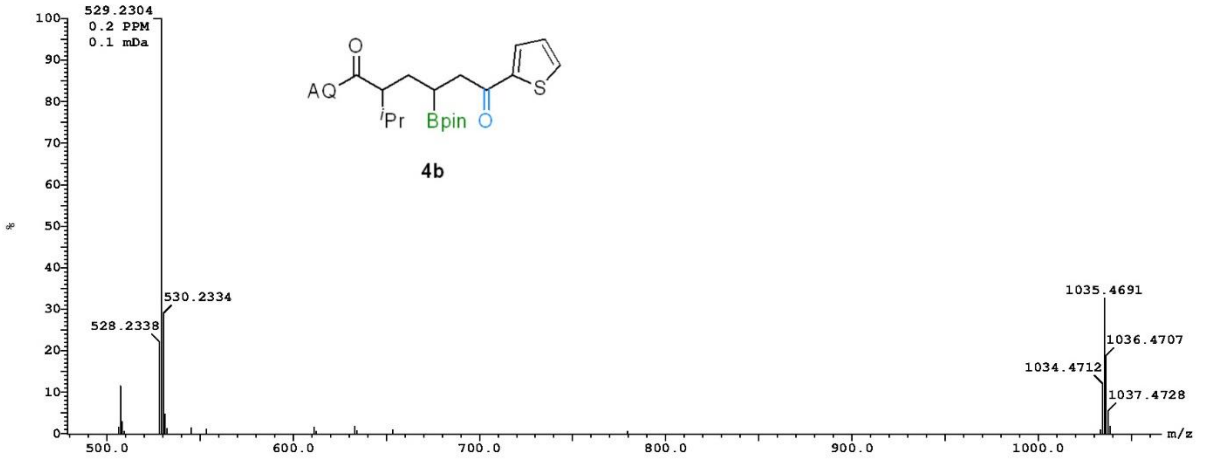
Sample Name:Q-33
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:15:53:18

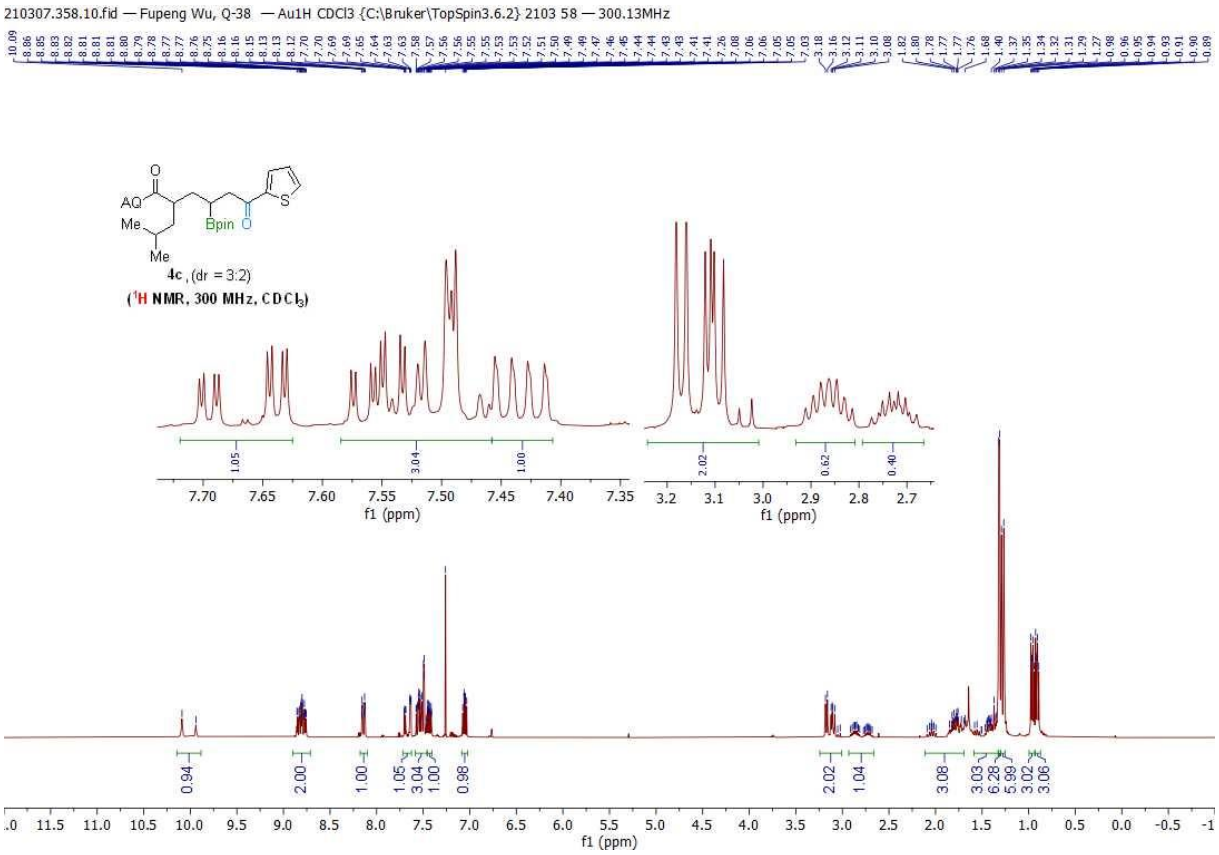
Sample Report:

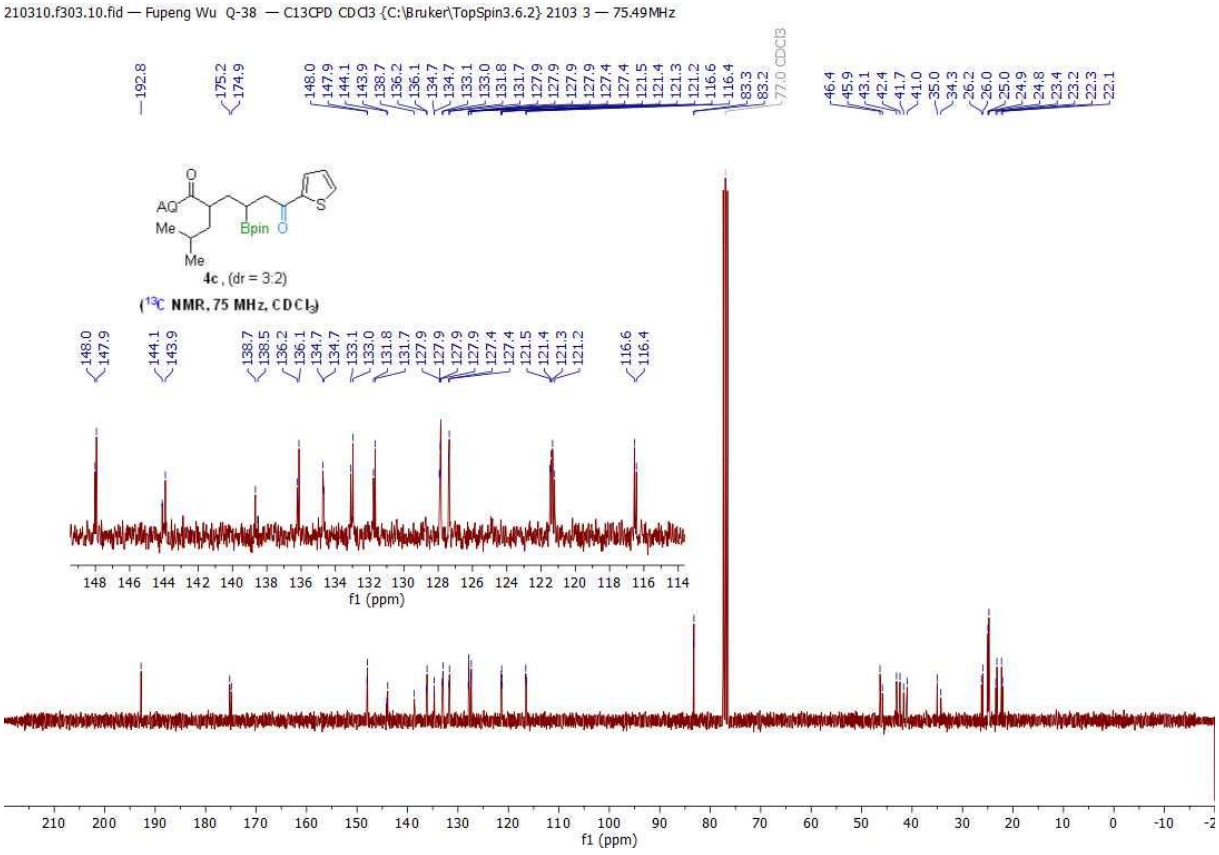
(Time: 0.34) Combine (29:33-81:85) - Dead time test passed

1:TOF MS ES+
4.7e+008



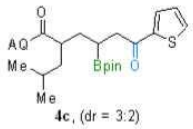
4b


210307.358.10.fid — Fupeng Wu, Q-38 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 58 — 300.13MHz
4c, (dr = 3:2)
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)


210310.f303.10.fid — Fupeng Wu Q-38 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 3 — 75.49MHz
4c, (dr = 3:2)
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

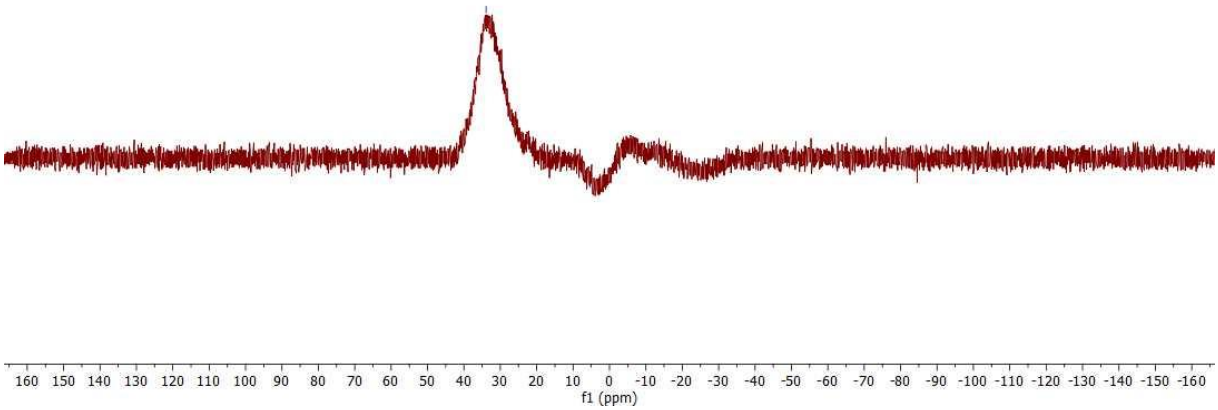
210310.f303.11.fid — Fupeng Wu Q-38 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 3 — 96.32MHz

33.9



4c, (dr = 3:2)

(**^{11}B NMR, 96 MHz, $CDCl_3$**)



ESI-TOF Accurate Mass Report

File:21032235
Vial:1:E,3
Description:MeOH/0.1% HCOOH in H2O 98:2

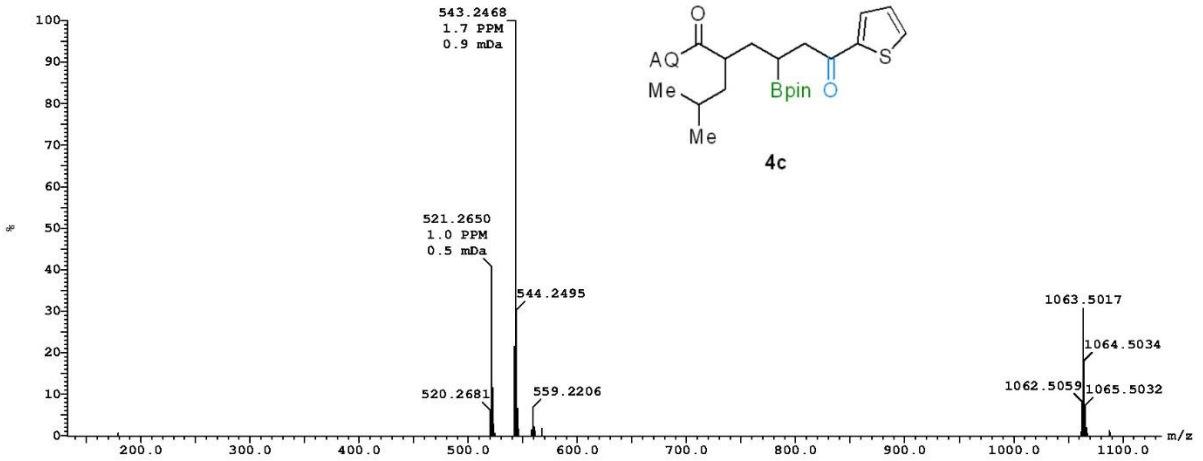
Sample Name:Q-38
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:16:11:20

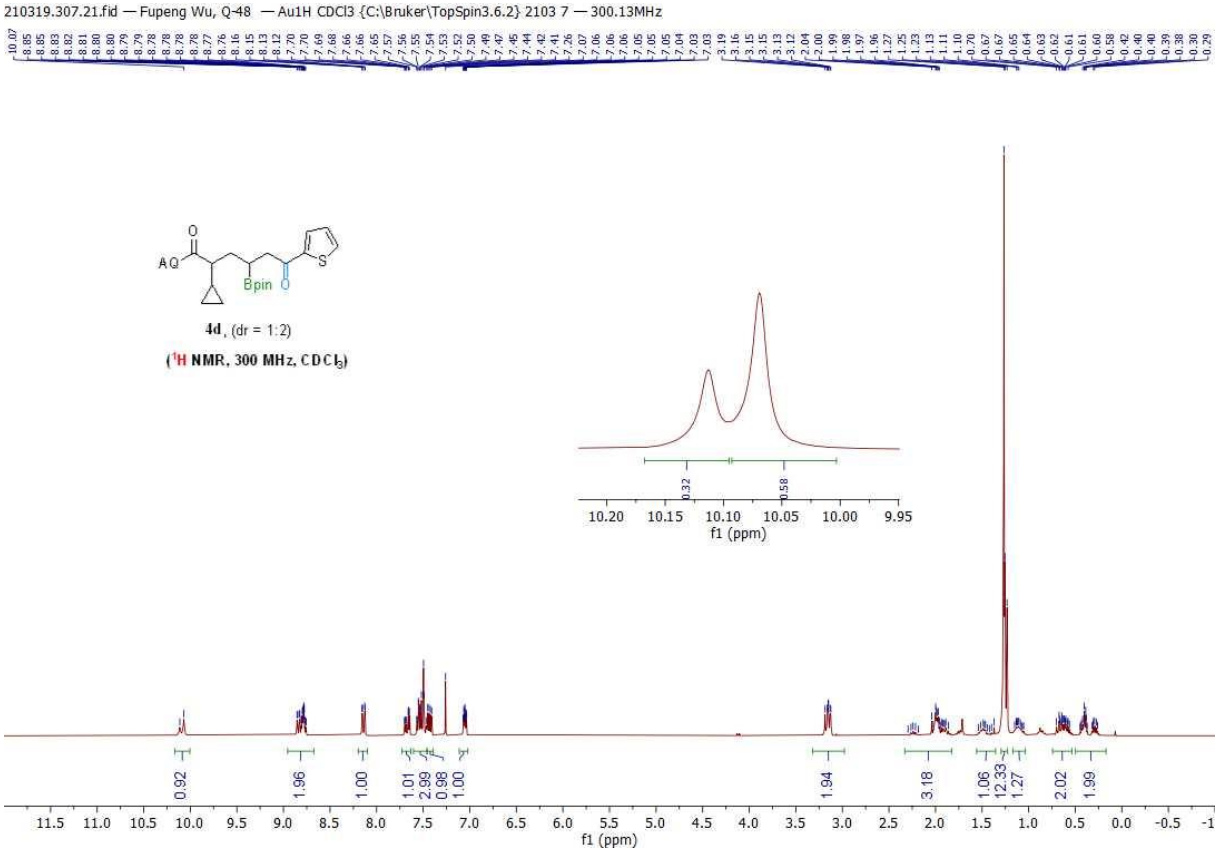
Sample Report:

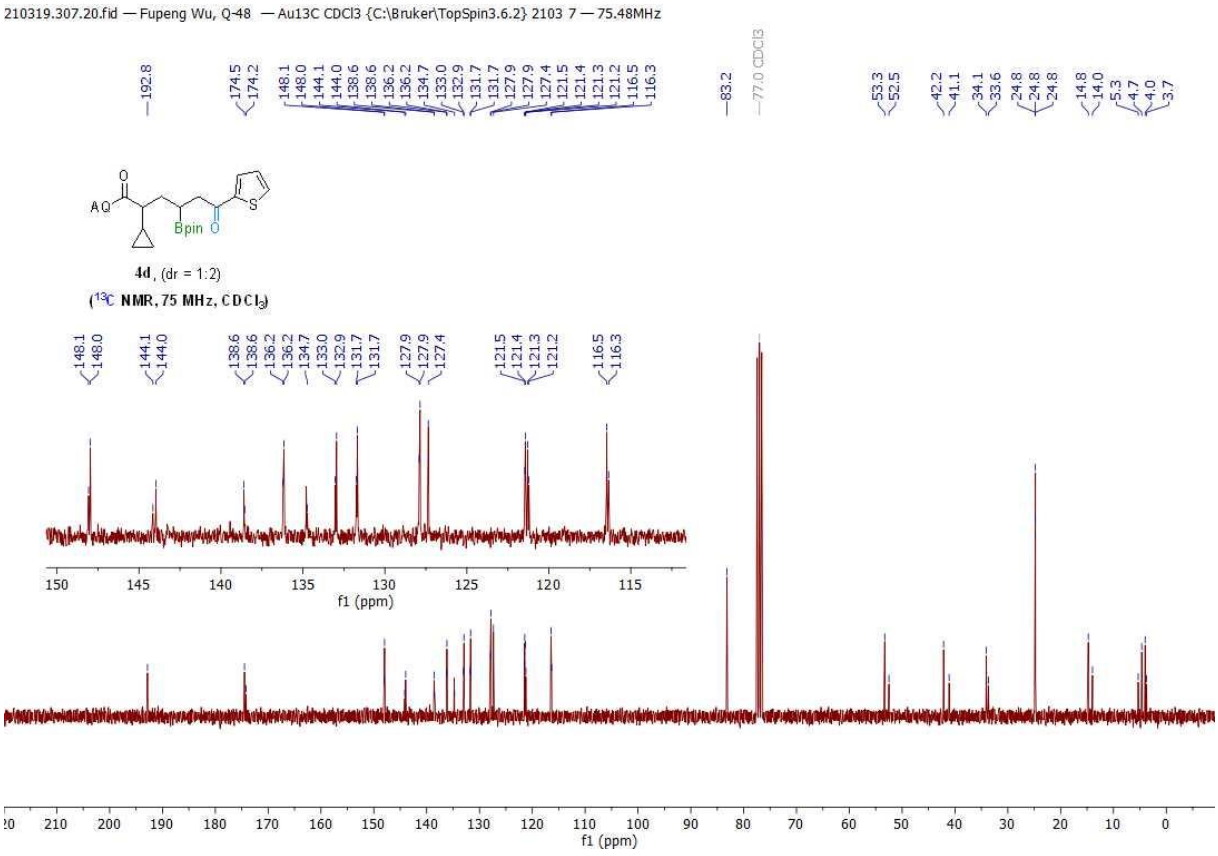
(Time: 0.34) Combine (29:33-81:85) - Dead time test passed

1:TOF MS ES+
2.9e+008



4c


210319.307.21.fid — Fupeng Wu, Q-48 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 7 — 300.13MHz
AQ
Bpin
4d, (dr = 1:2)
(1H NMR, 300 MHz, CDCl3)
0.92
1.96
1.00
1.01
2.99
0.98
1.00
1.94
3.18
1.06
12.33
1.27
2.02
1.99
f1 (ppm)

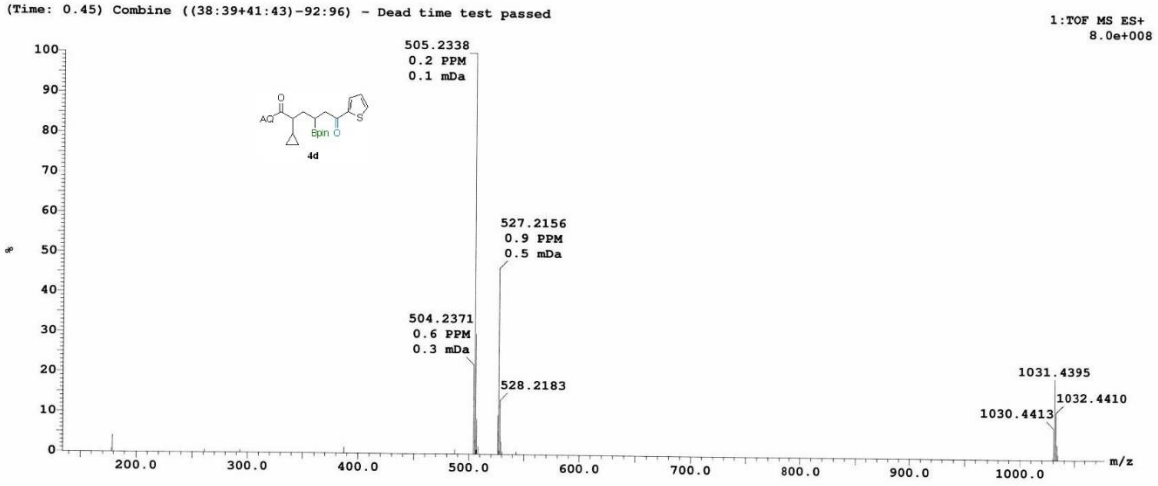

210319.307.20.fid — Fupeng Wu, Q-48 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 7 — 75.48MHz
77.0 CDCl3
AQ
Bpin
4d, (dr = 1:2)
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

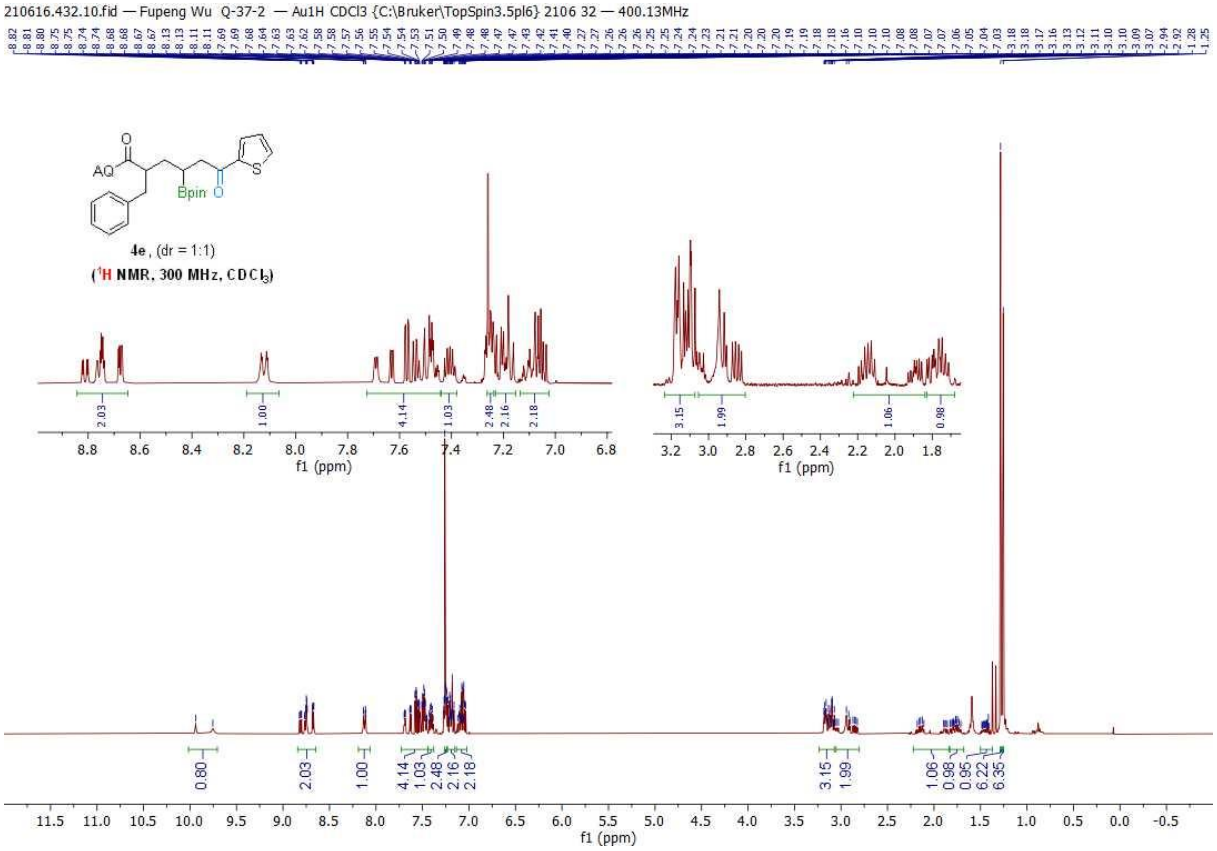
ESI-TOF Accurate Mass Report
File:21040907
Vial:1:F,2
Description:MeOH/0.1% HCOOH in H2O 90:10

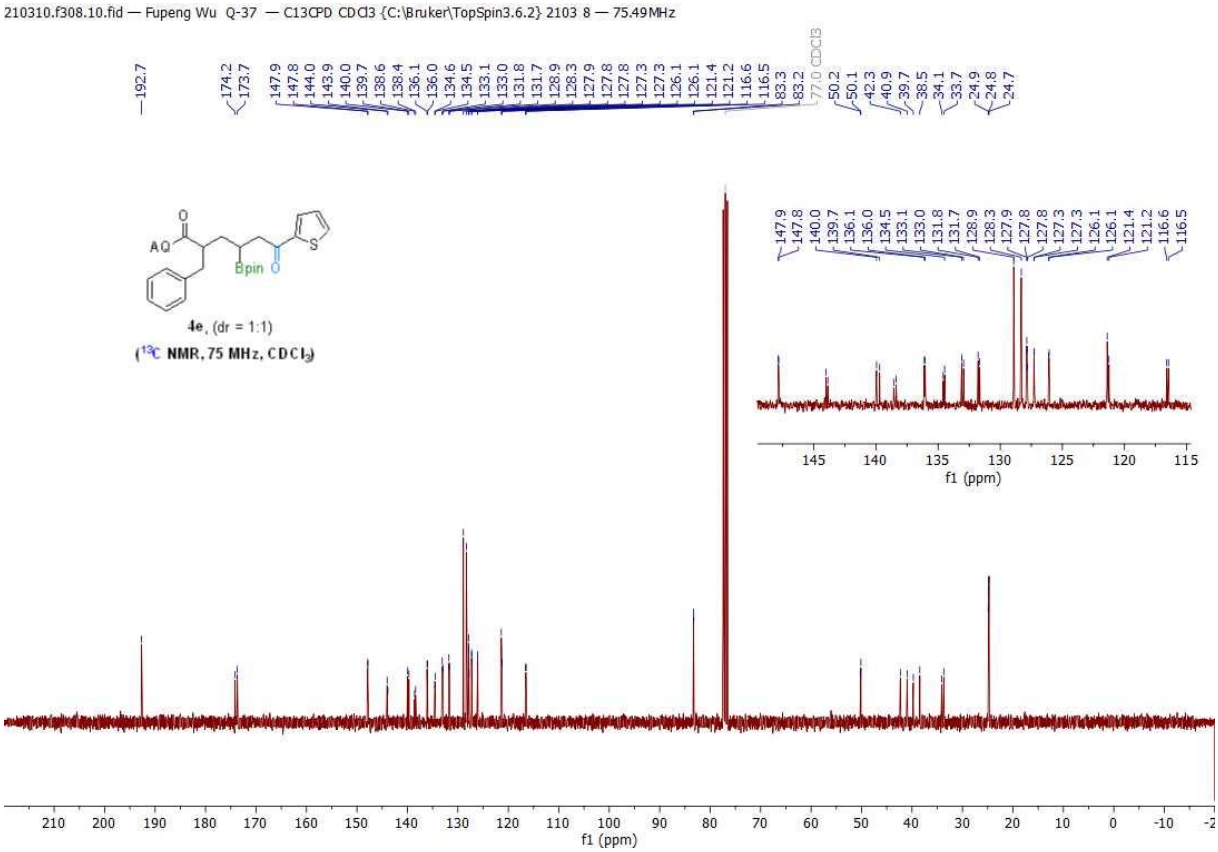
Sample Name:Q-48
Date:09-Apr-2021

UserName:Fupeng Wu
Time:15:16:02

Sample Report:

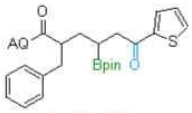



210616.432.10.fid — Fupeng Wu Q-37-2 — Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2106 32 — 400.13MHz
4e, (dr = 1:1)
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)


210310.f308.10.fid — Fupeng Wu Q-37 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 8 — 75.49MHz
4e, (dr = 1:1)
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

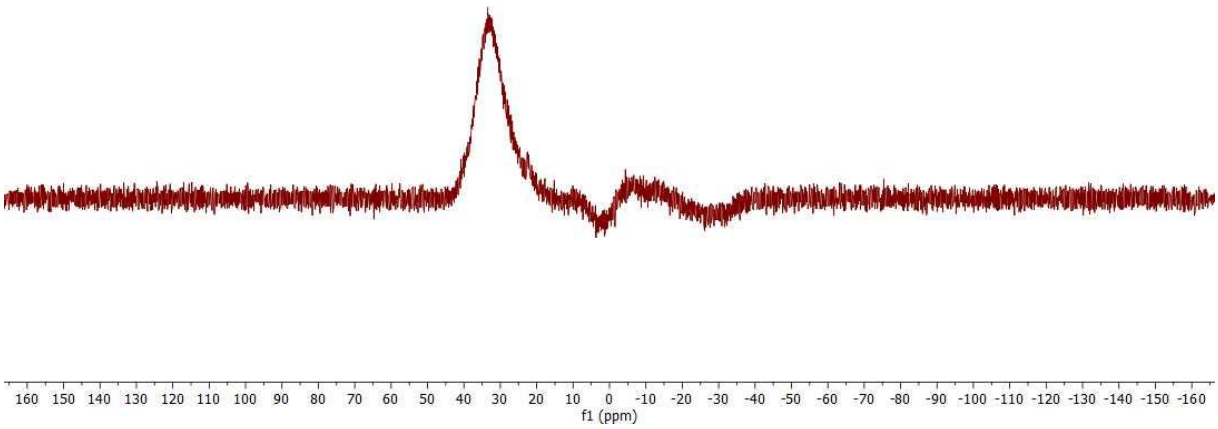
210310.f308.11.fid — Fupeng Wu Q-37 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 8 — 96.32MHz

33.4



4e, (dr = 1:1)

(**^{11}B NMR, 96 MHz, $CDCl_3$**)



ESI-TOF Accurate Mass Report

File:21032234
Vial:1:E,2
Description:MeOH/0.1% HCOOH in H2O 98:2

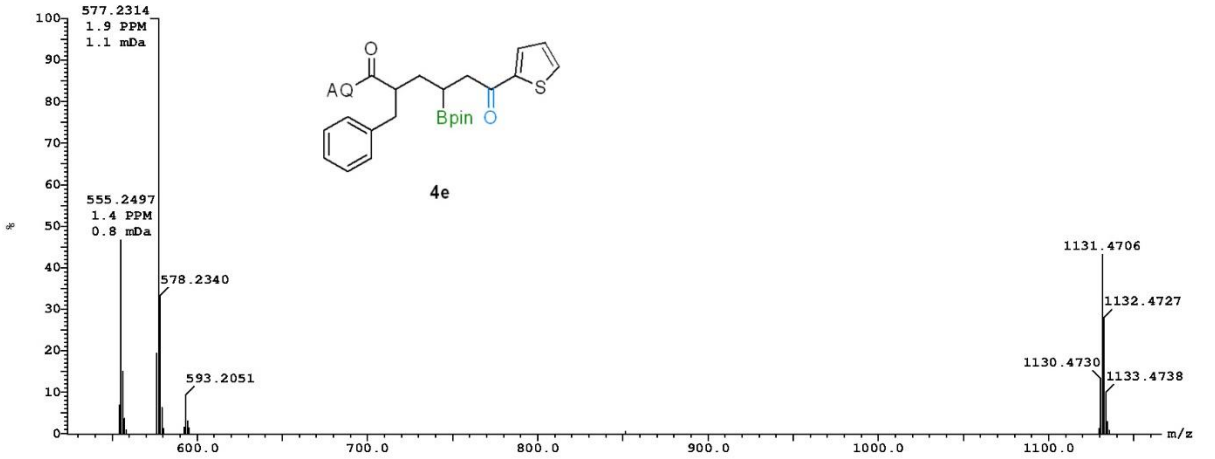
Sample Name:Q-37
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:16:08:45

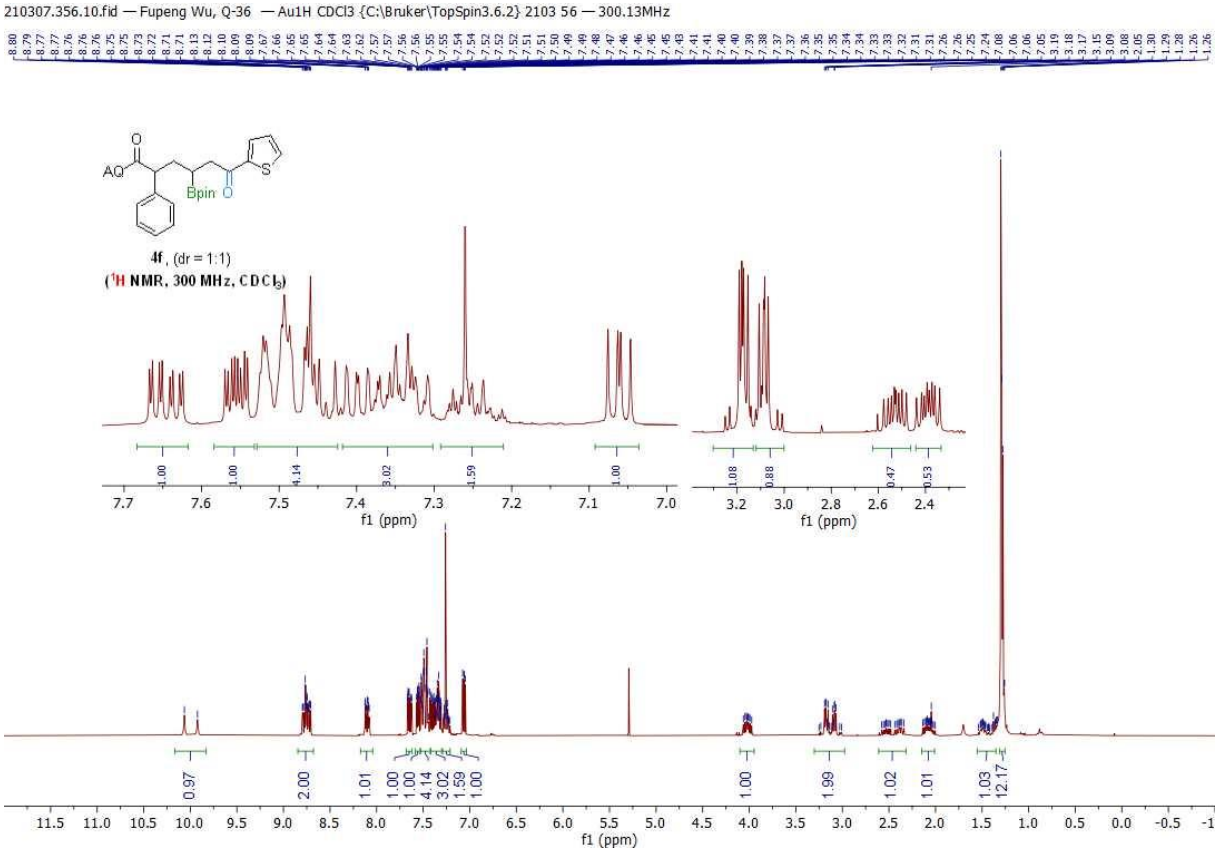
Sample Report:

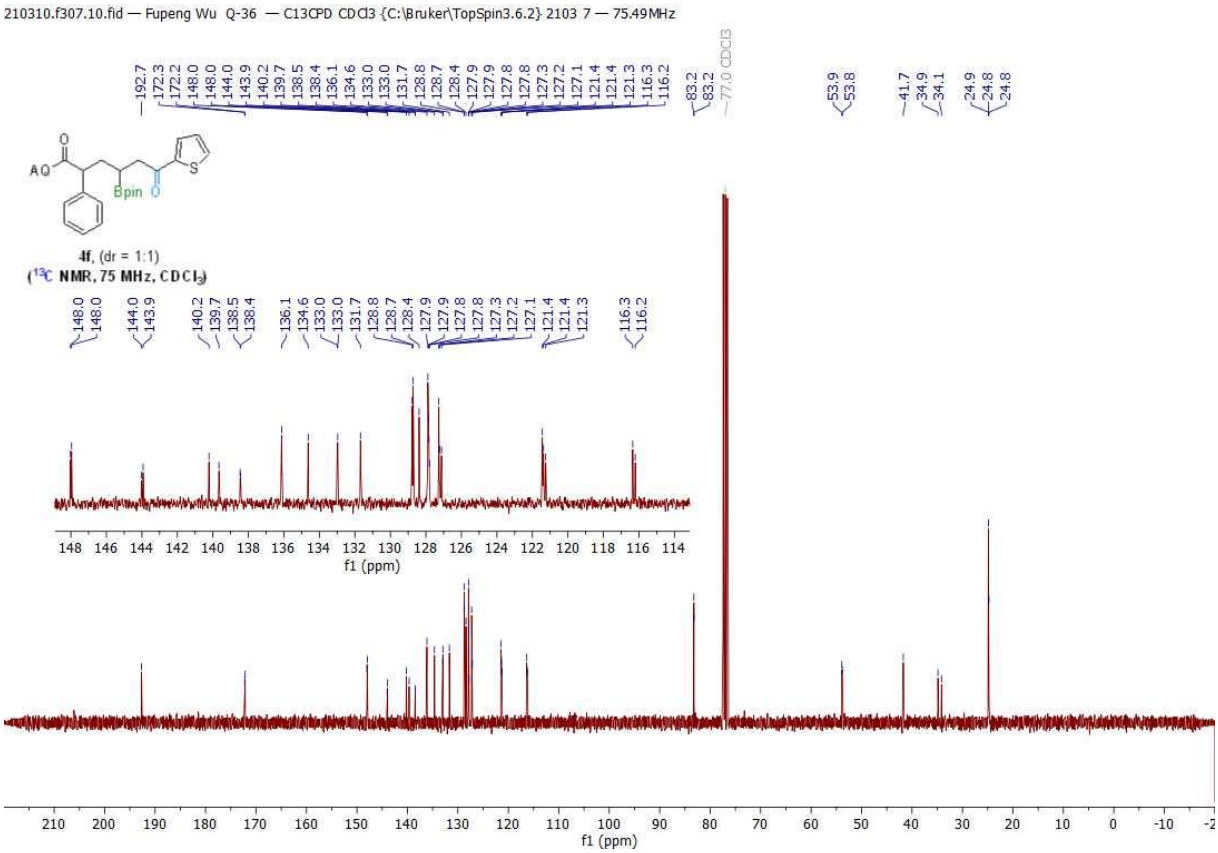
(Time: 0.33) Combine (28:32-80:84) - Dead time test passed

1:TOF MS ES+
3.1e+008



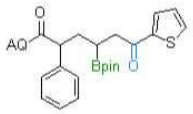
4e


210307.356.10.fid — Fupeng Wu, Q-36 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 56 — 300.13MHz
AQ
Bpin
4f, (dr = 1:1)
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)

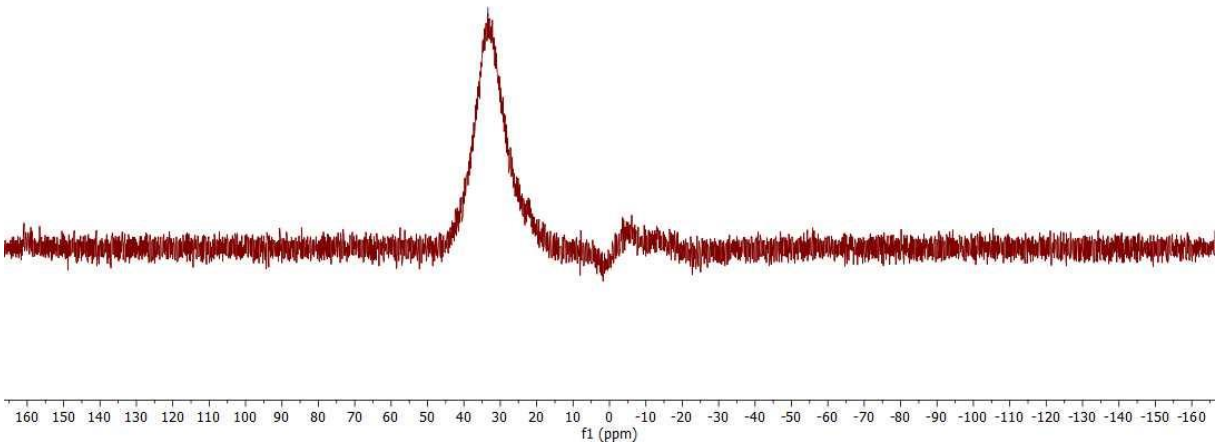

210310.f307.10.fid — Fupeng Wu Q-36 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 7 — 75.49MHz
AQ
Bpin
4f, (dr = 1:1)
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

210310.f307.11.fid — Fupeng Wu Q-36 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 7 — 96.32MHz

33.4



4f, (dr = 1:1)
(**^{11}B NMR, 96 MHz, $CDCl_3$**)



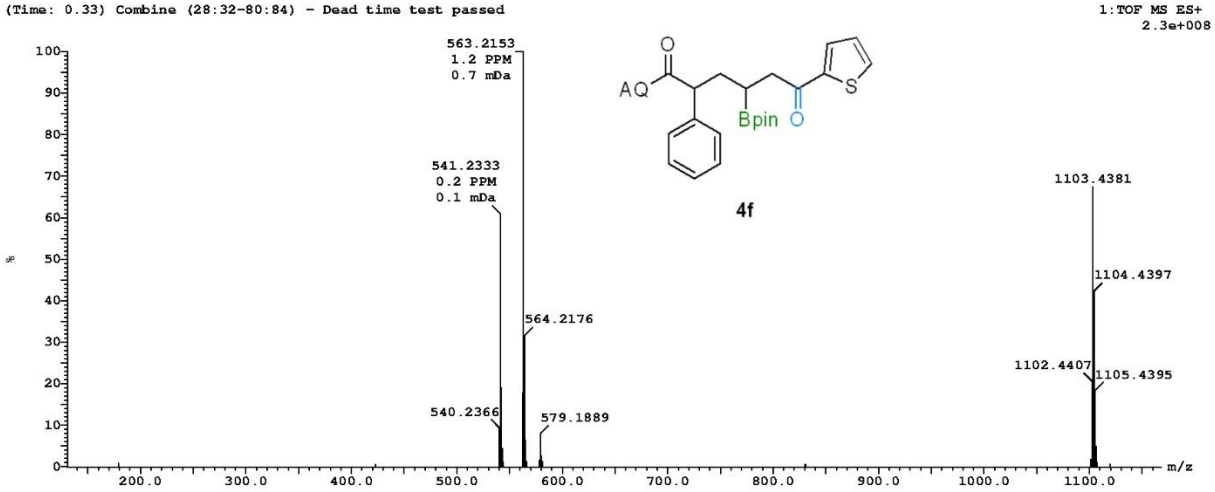
ESI-TOF Accurate Mass Report

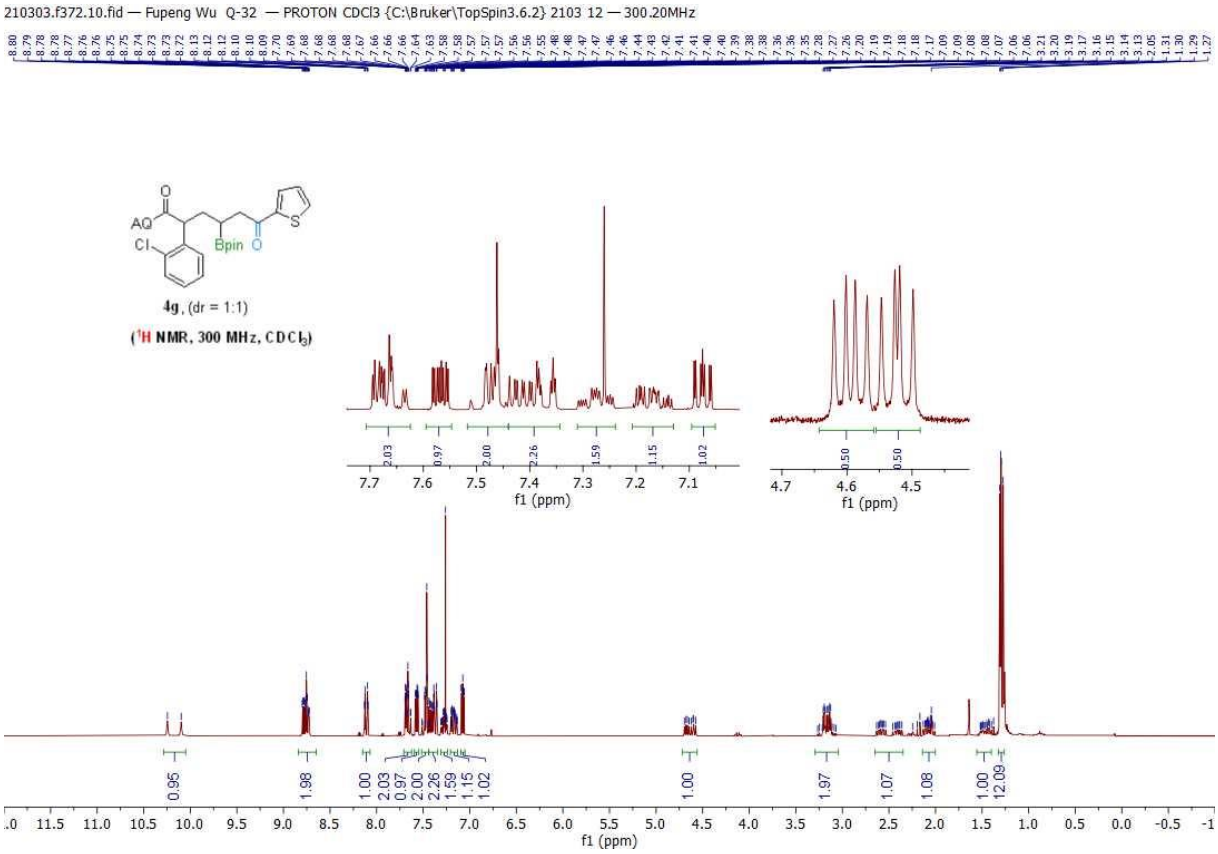
File:21032233
Vial:1:E,1
Description:MeOH/0.1% HCOOH in H2O 98:2

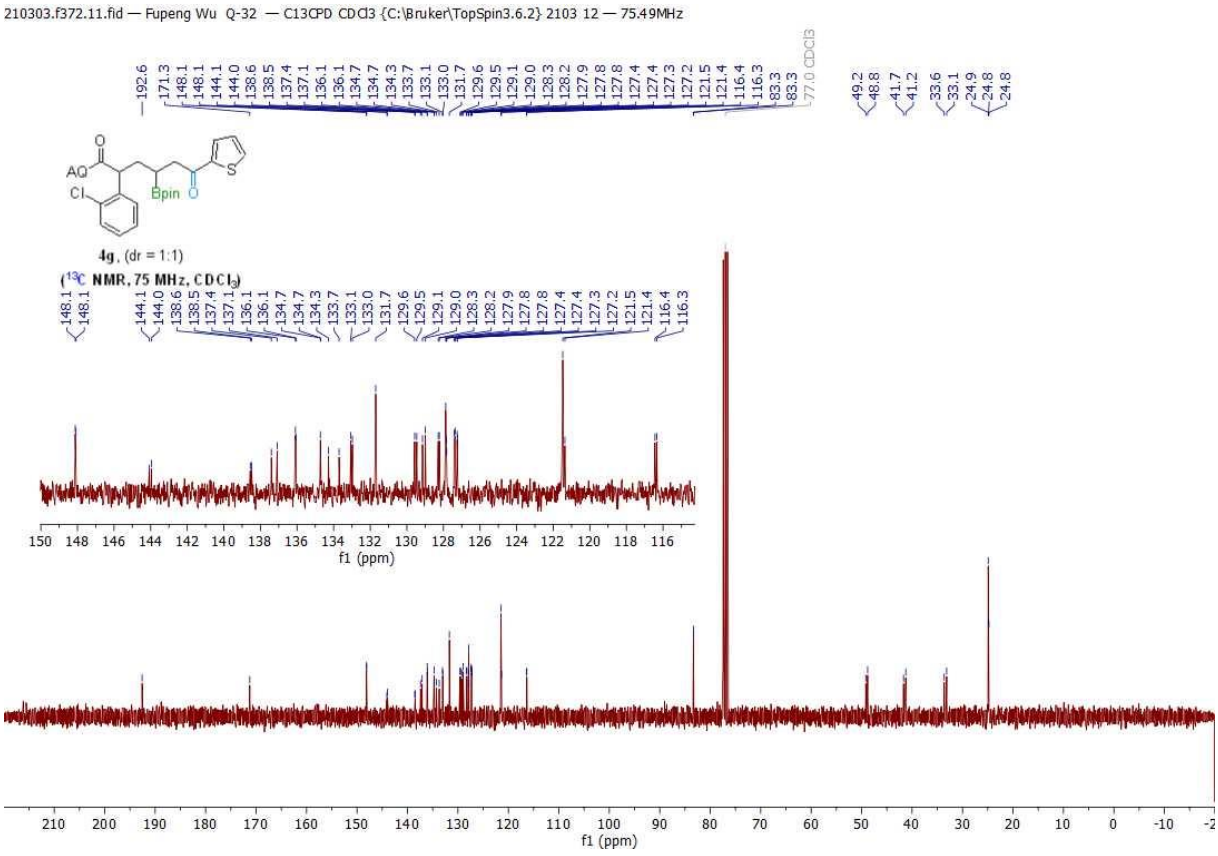
Sample Name:Q-36
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:16:06:10

Sample Report:

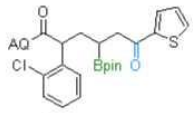



210303.f372.10.fid — Fupeng Wu Q-32 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 12 — 300.20MHz
4g, (dr = 1:1)
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)

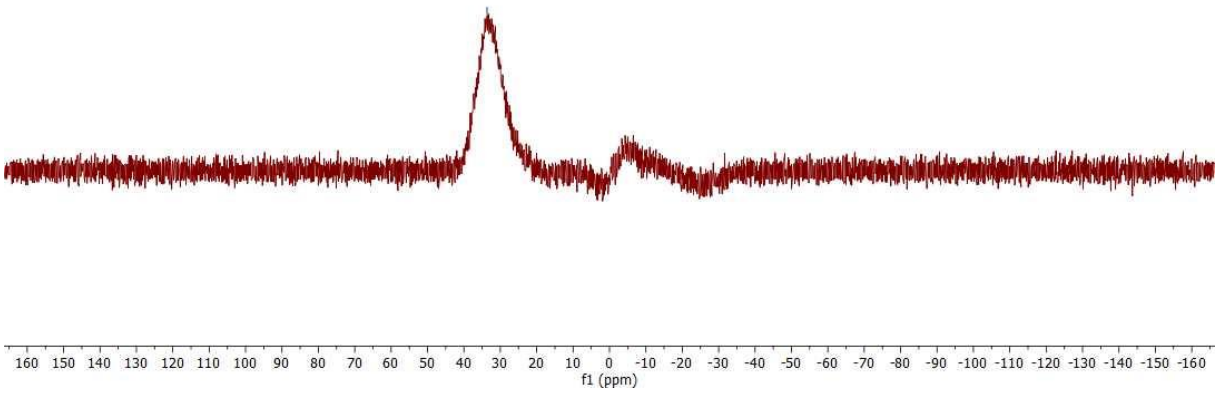

210303.f372.11.fid — Fupeng Wu Q-32 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 12 — 75.49MHz
4g, (dr = 1:1)
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

210303.f372.12.fid — Fupeng Wu Q-32 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 12 — 96.32MHz

33.6



4g, (dr = 1:1)
(**^{11}B NMR, 96 MHz, $CDCl_3$**)



ESI-TOF Accurate Mass Report

File:21032222
Vial:1:D,6
Description:MeOH/0.1% HCOOH in H2O 90:10

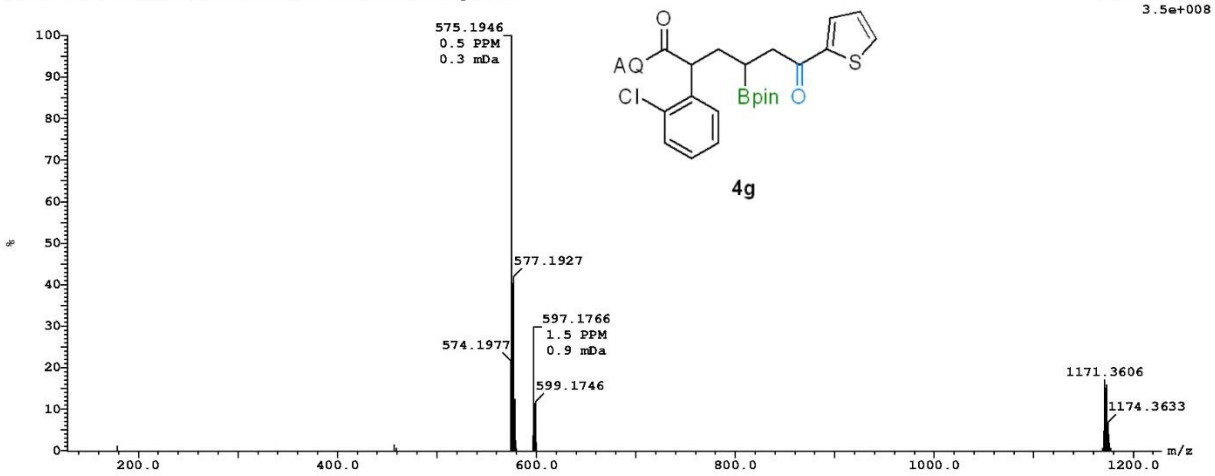
Sample Name:Q-32
Date:22-Mar-2021

UserName:Fu-peng Wu
Time:15:19:55

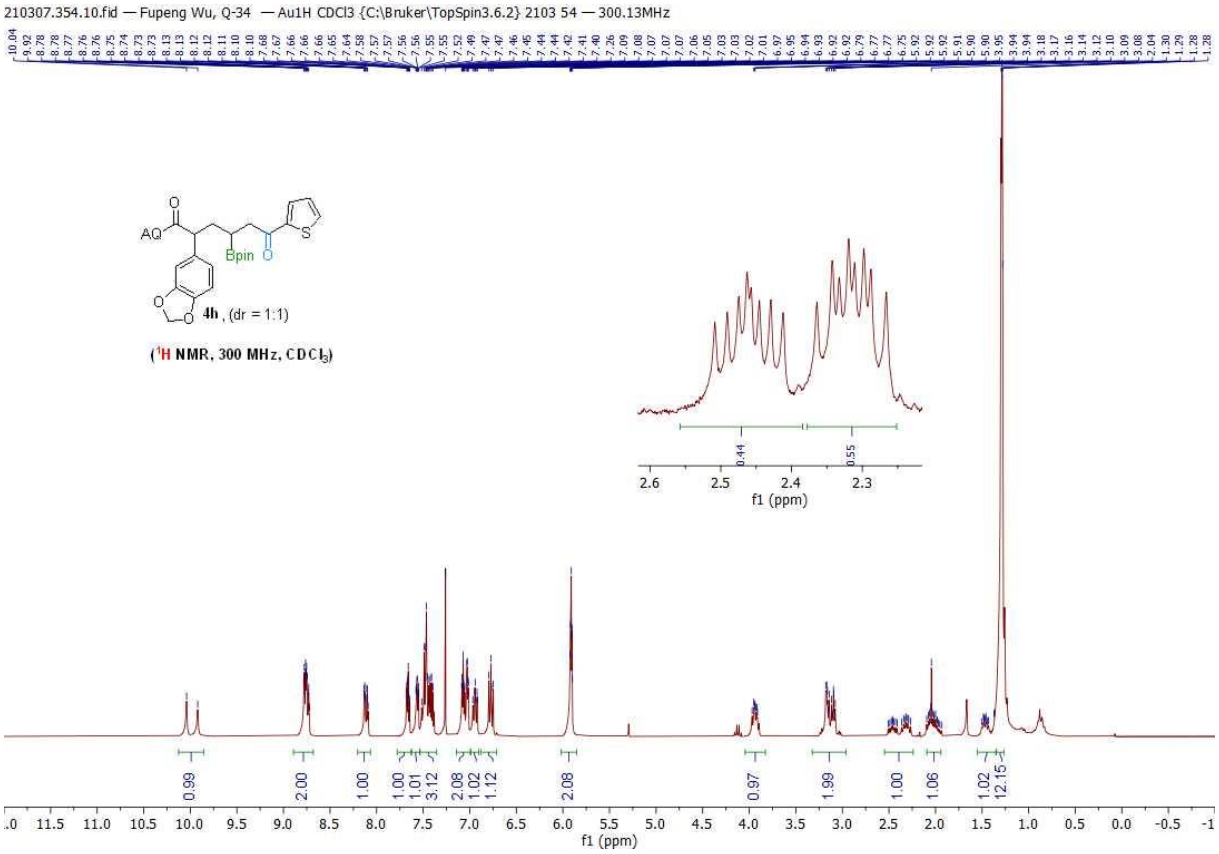
Sample Report:

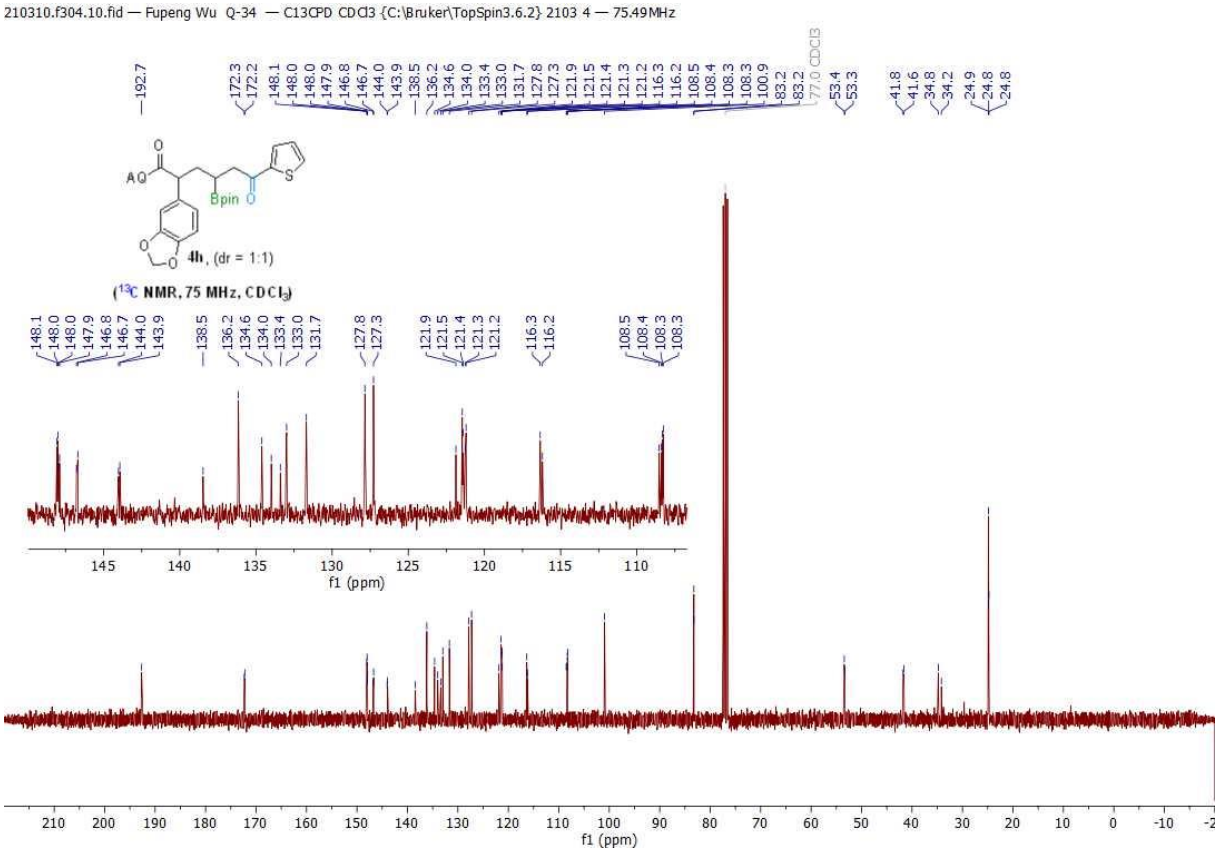
(Time: 0.53) Combine (45:49-98:102) - Dead time test passed

1:TOF MS ES+
3.5e+008



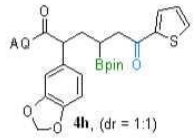
4g


210307.354.10.fid — Fupeng Wu, Q-34 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 54 — 300.13MHz
AQ
Bpin
4h, (dr = 1:1)
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)


210310.f304.10.fid — Fupeng Wu Q-34 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 4 — 75.49MHz
AQ
Bpin
4h, (dr = 1:1)
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

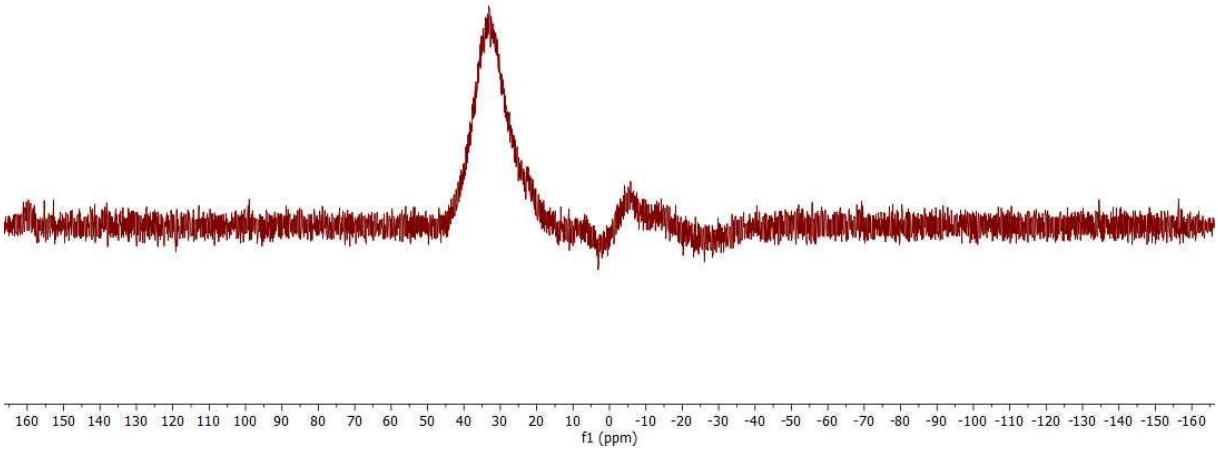
210310.f304.11.fid — Fupeng Wu Q-34 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 4 — 96.32MHz

32.5



4h, (dr = 1:1)

(^{11}B NMR, 96 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

File:21032231
Vial:1:D,7
Description:MeOH/0.1% HCOOH in H2O 98:2

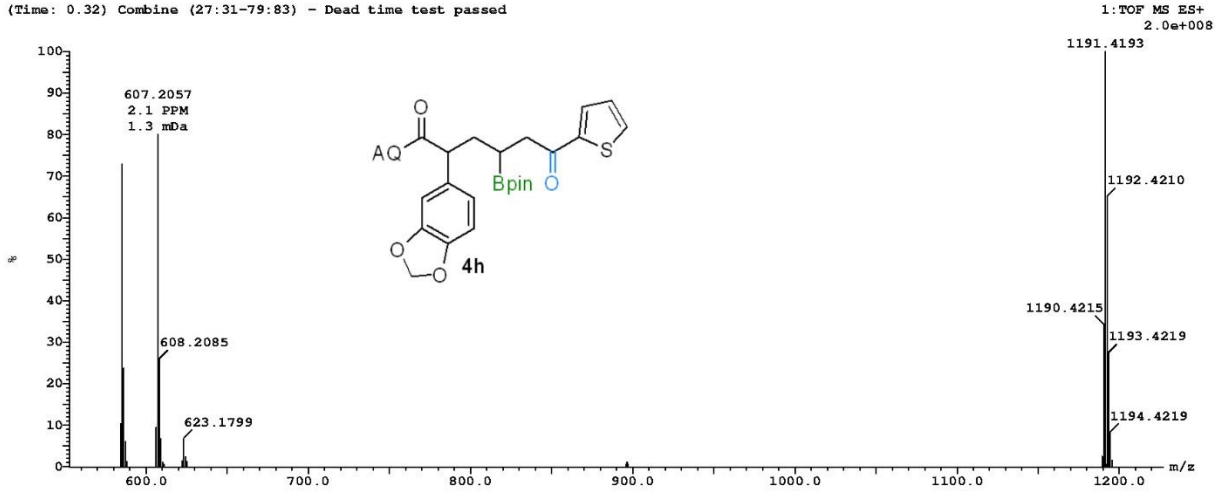
Sample Name:Q-34
Date:22-Mar-2021

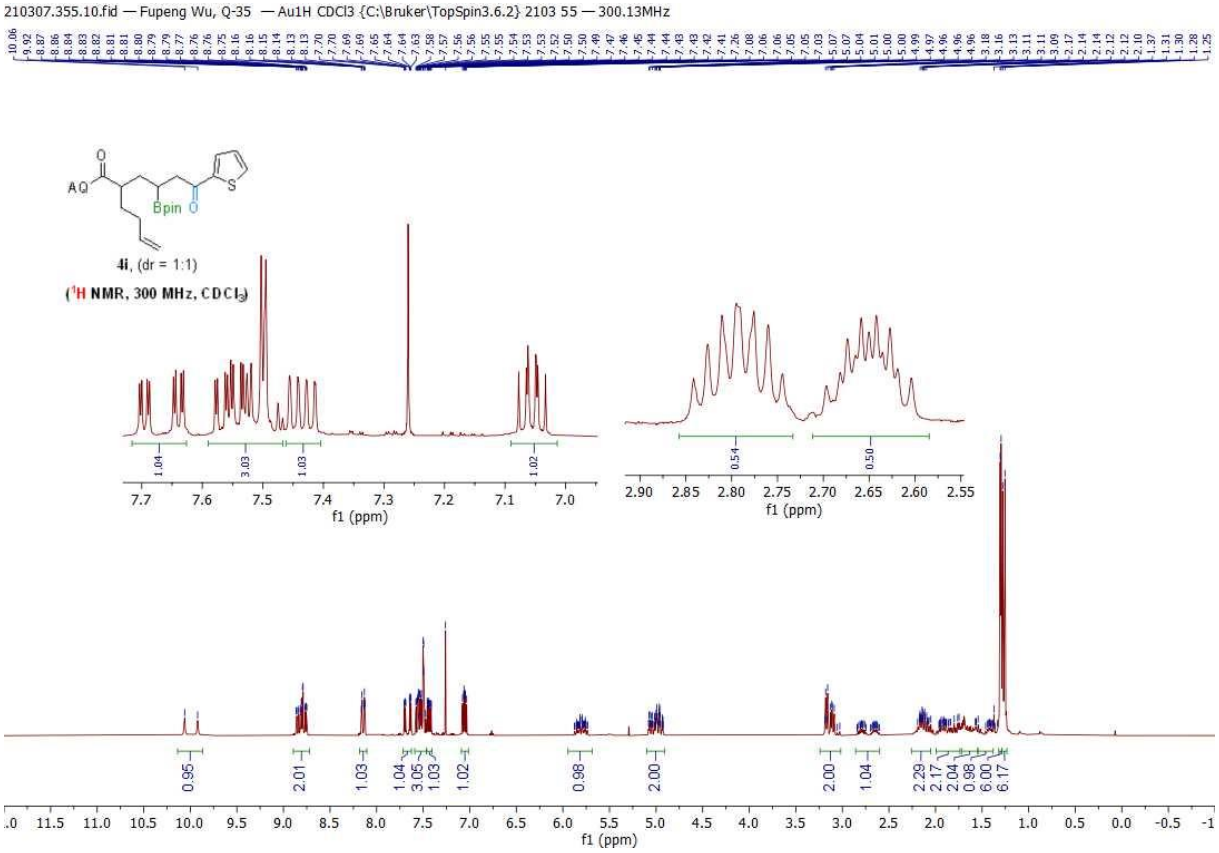
UserName:Fu-peng Wu
Time:16:01:07

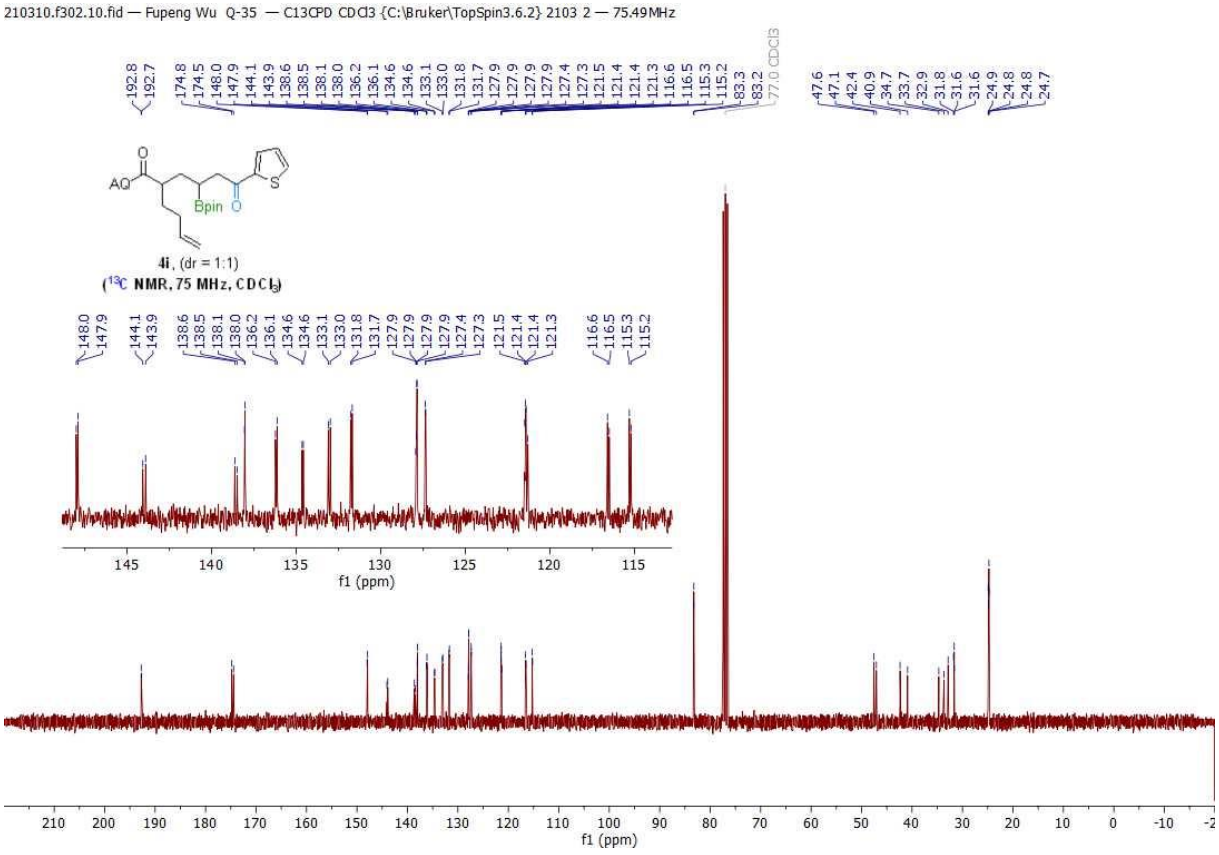
Sample Report:

(Time: 0.32) Combine (27:31-79:83) - Dead time test passed

1:TOF MS ES+
2.0e+008

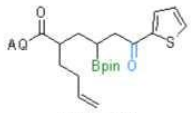



210307.355.10.fid — Fupeng Wu, Q-35 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 55 — 300.13MHz
AQ
Bpin
4i, (dr = 1:1)
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)

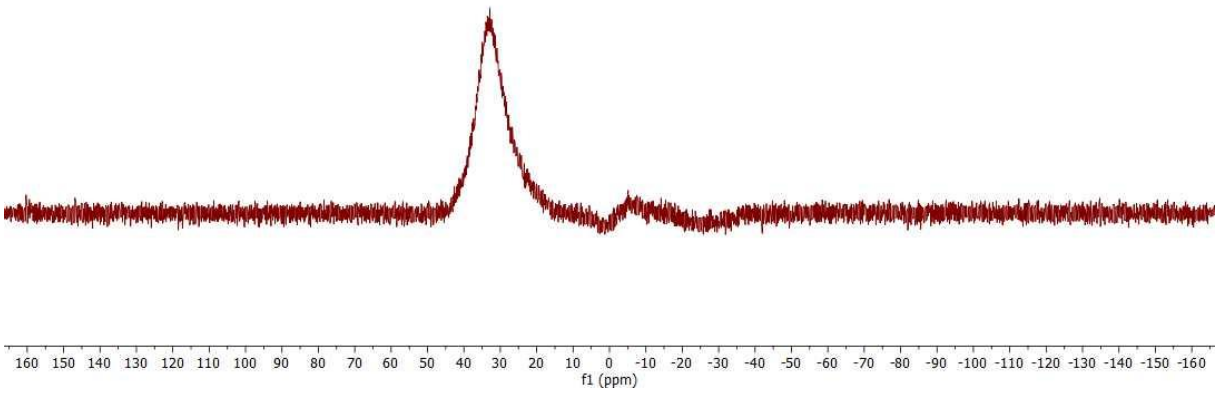

210310.f302.10.fid — Fupeng Wu Q-35 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 2 — 75.49MHz
AQ
Bpin
4i, (dr = 1:1)
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

210310.f302.11.fid — Fupeng Wu Q-35 — 11B CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 2 — 96.32MHz

32.9



4i, (dr = 1:1)
(**^{11}B NMR, 96 MHz, $CDCl_3$**)

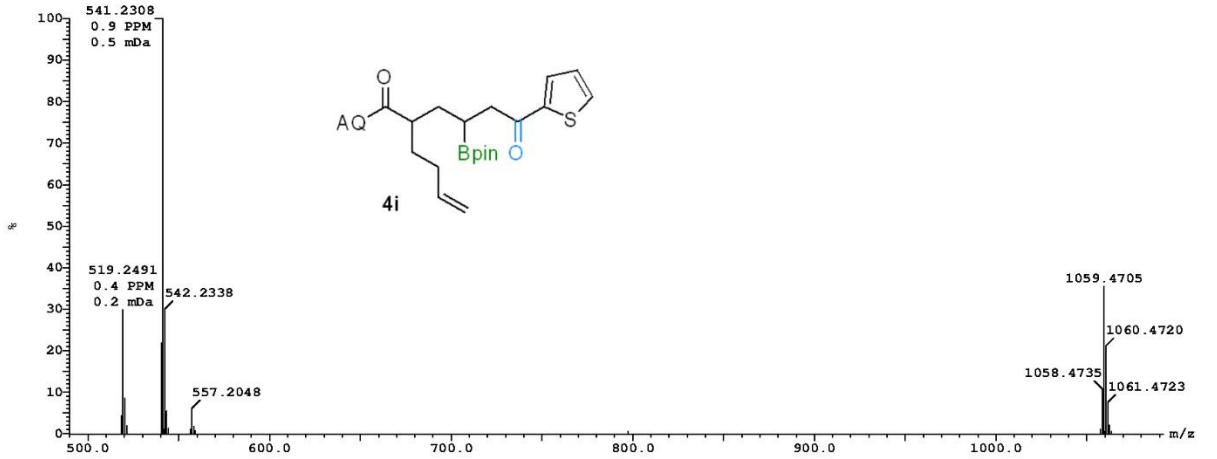


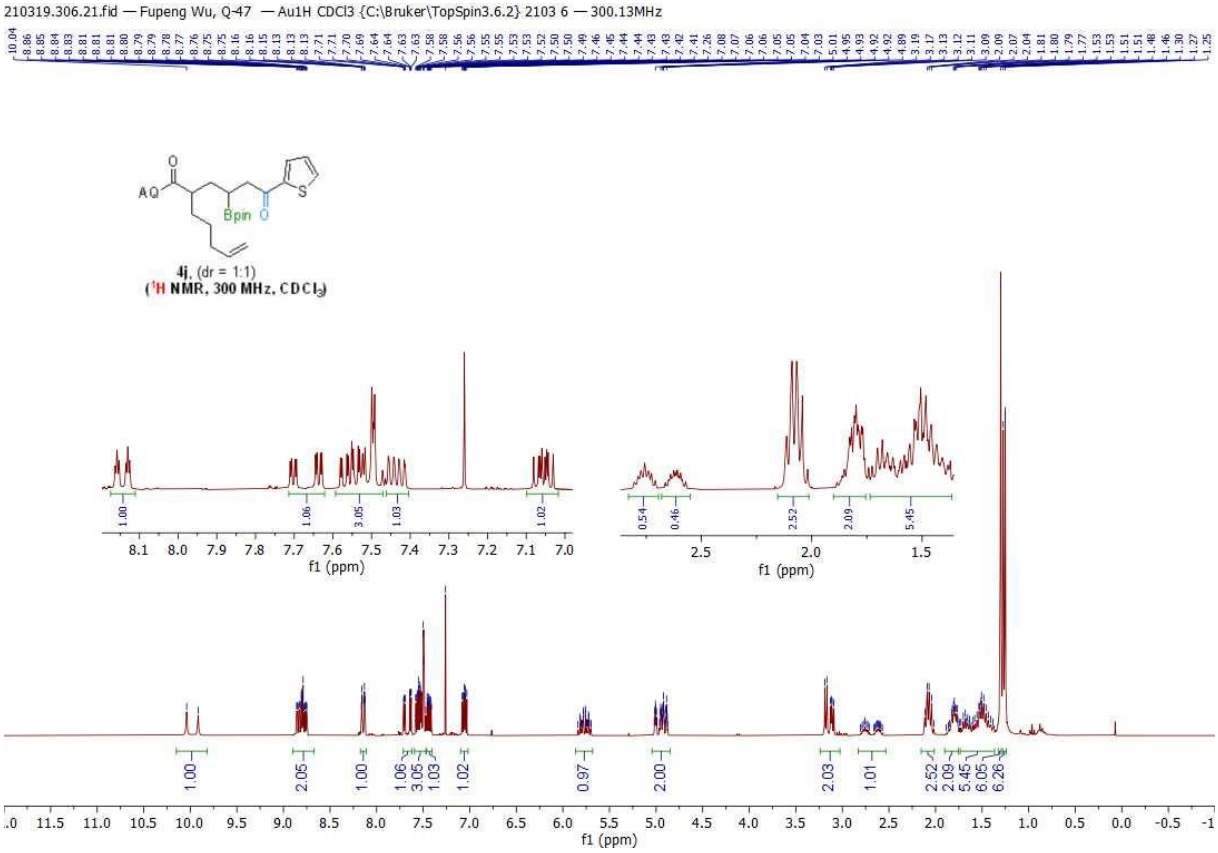
ESI-TOF Accurate Mass Report Page 2

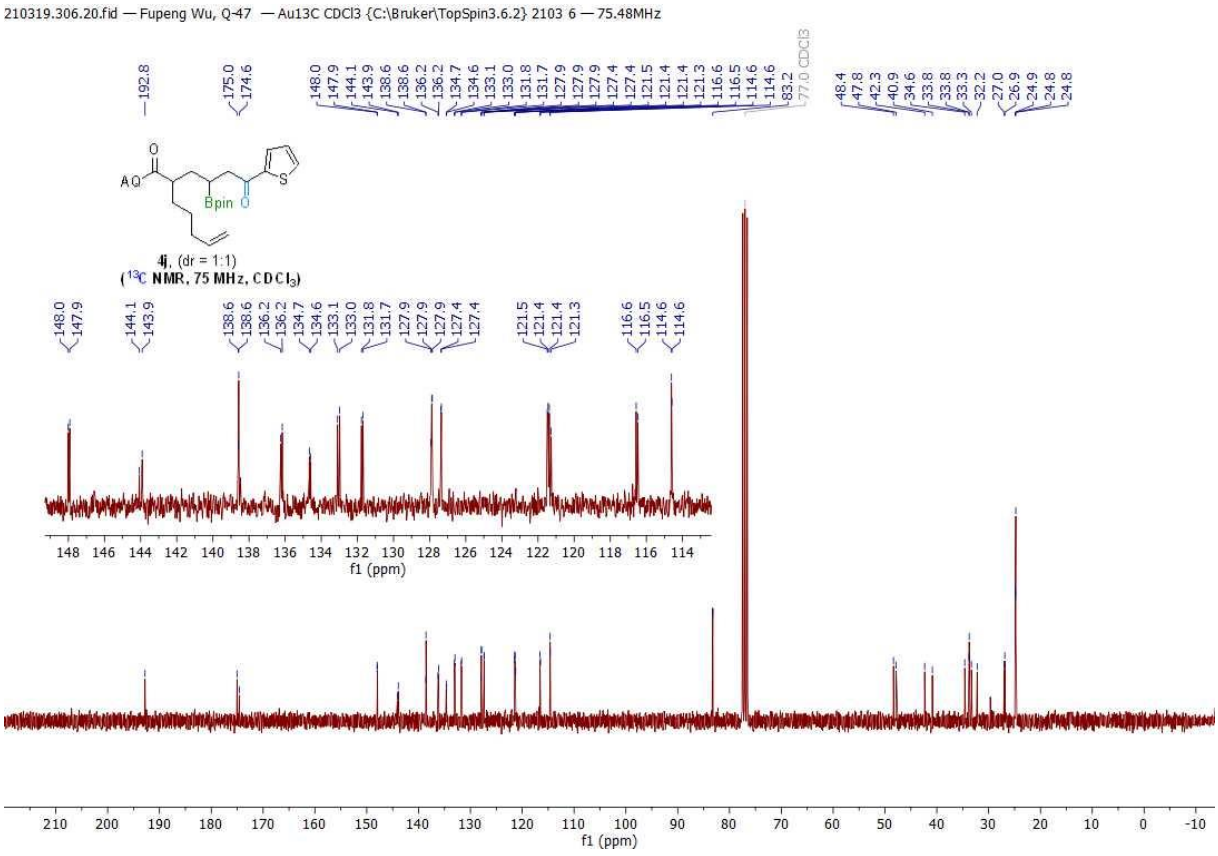
File:21032232 Sample Name:Q-35 UserName:Fu-peng Wu
Vial:1:D,8 Date:22-Mar-2021 Time:16:03:38
Description:MeOH/0.1% HCOOH in H2O 98:2

Sample Report:

(Time: 0.34) Combine ((28+30:33)-81:85) - Dead time test passed 1:TOF MS ES+ 3.7e+008




210319.306.21.fid — Fupeng Wu, Q-47 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 6 — 300.13MHz
4j, (dr = 1:1)
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)

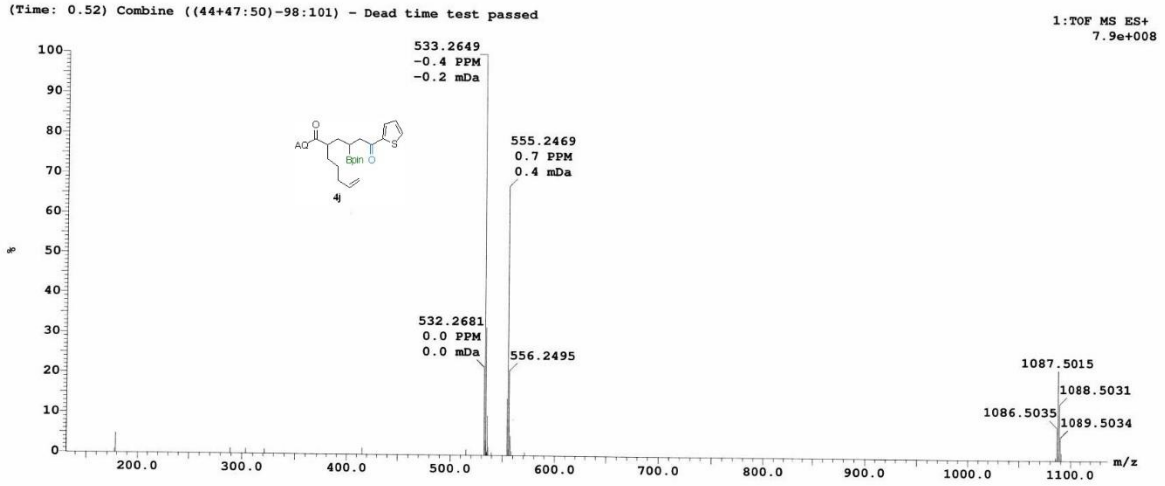

210319.306.20.fid — Fupeng Wu, Q-47 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 6 — 75.48MHz
4j, (dr = 1:1)
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

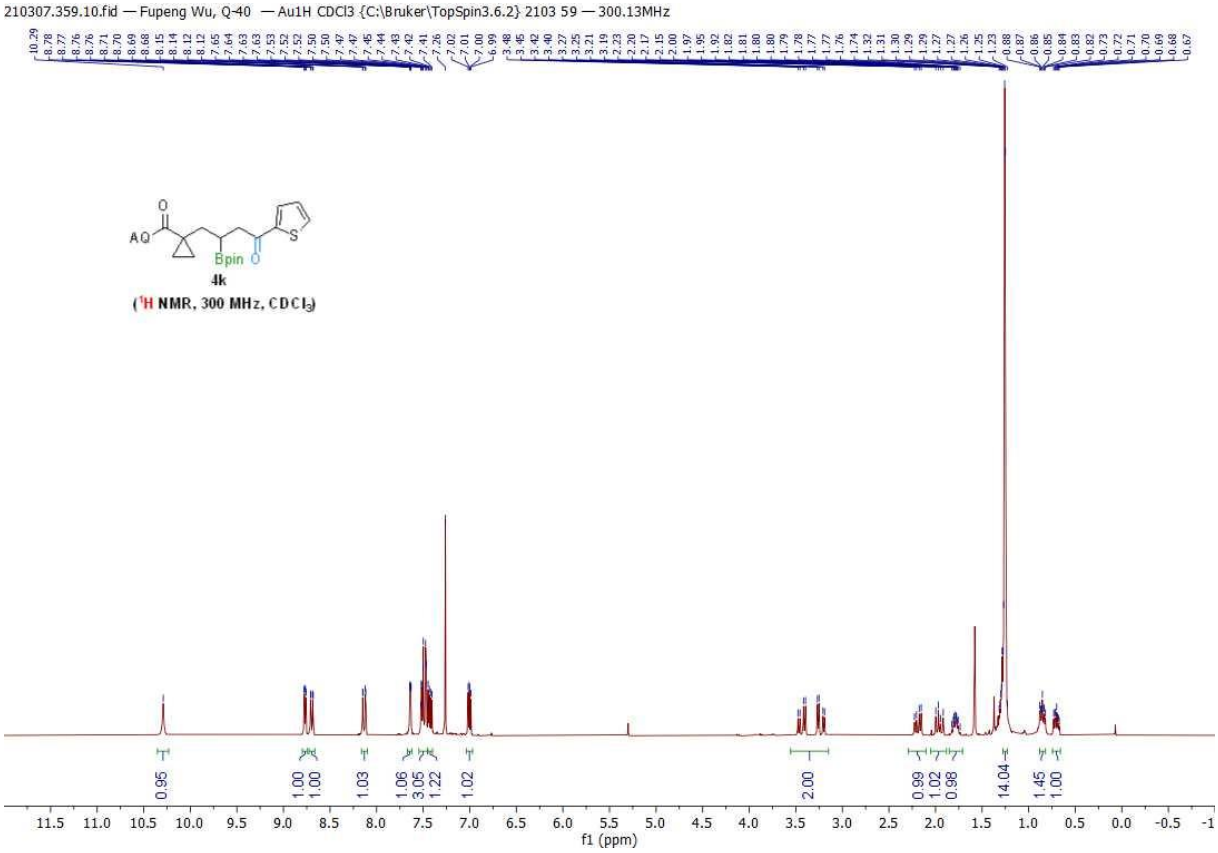
ESI-TOF Accurate Mass Report
File:21040908
Vial:1:F,3
Description:MeOH/0.1% HCOOH in H2O 90:10

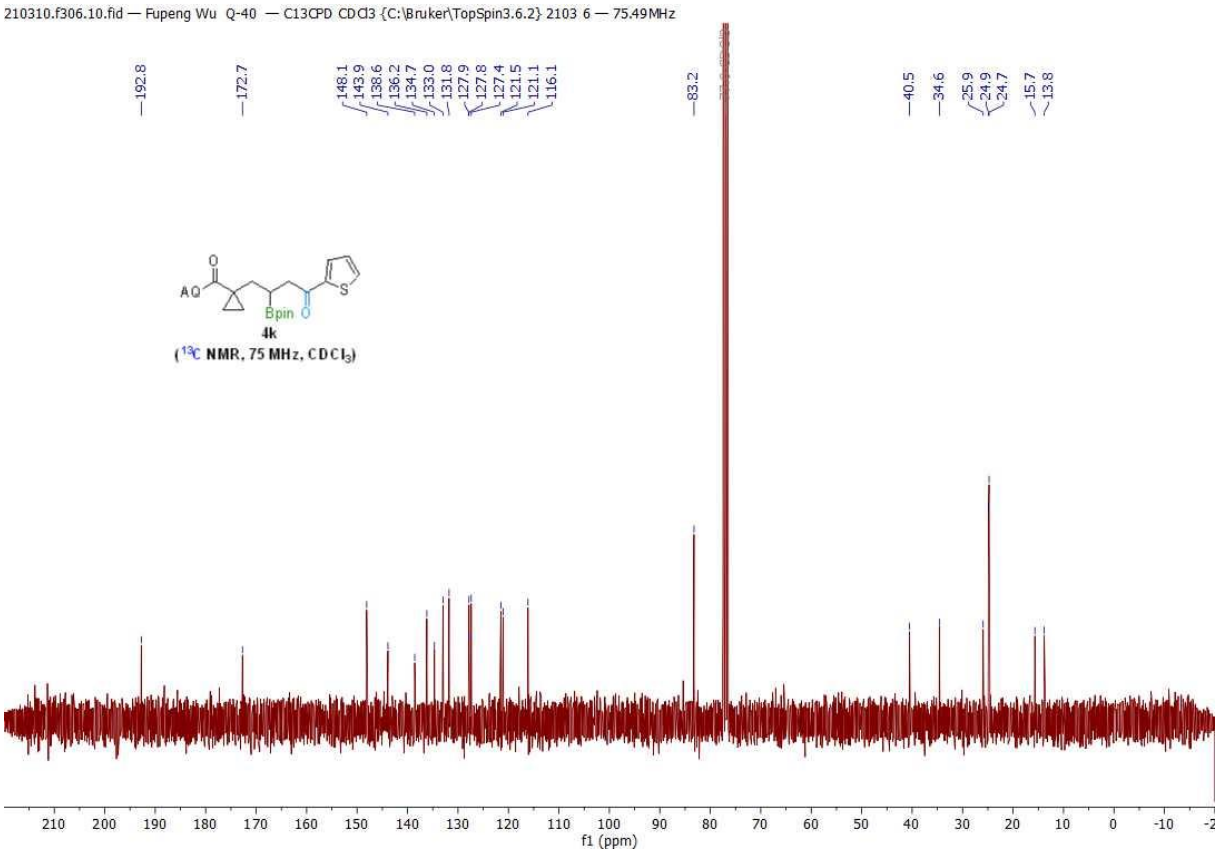
Sample Name:Q-47
Date:09-Apr-2021

UserName:Fupeng Wu
Time:15:18:37

Sample Report:

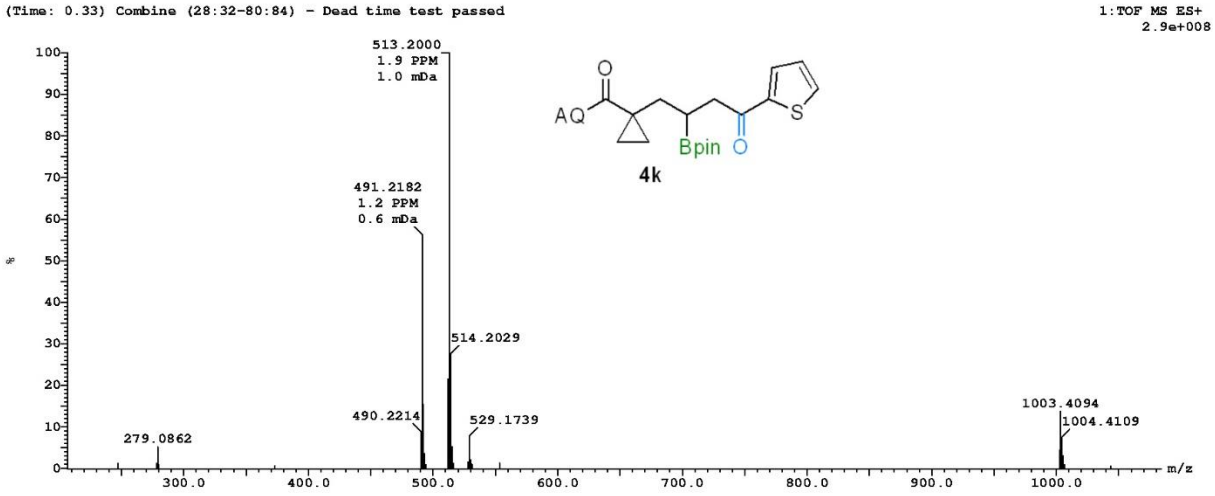


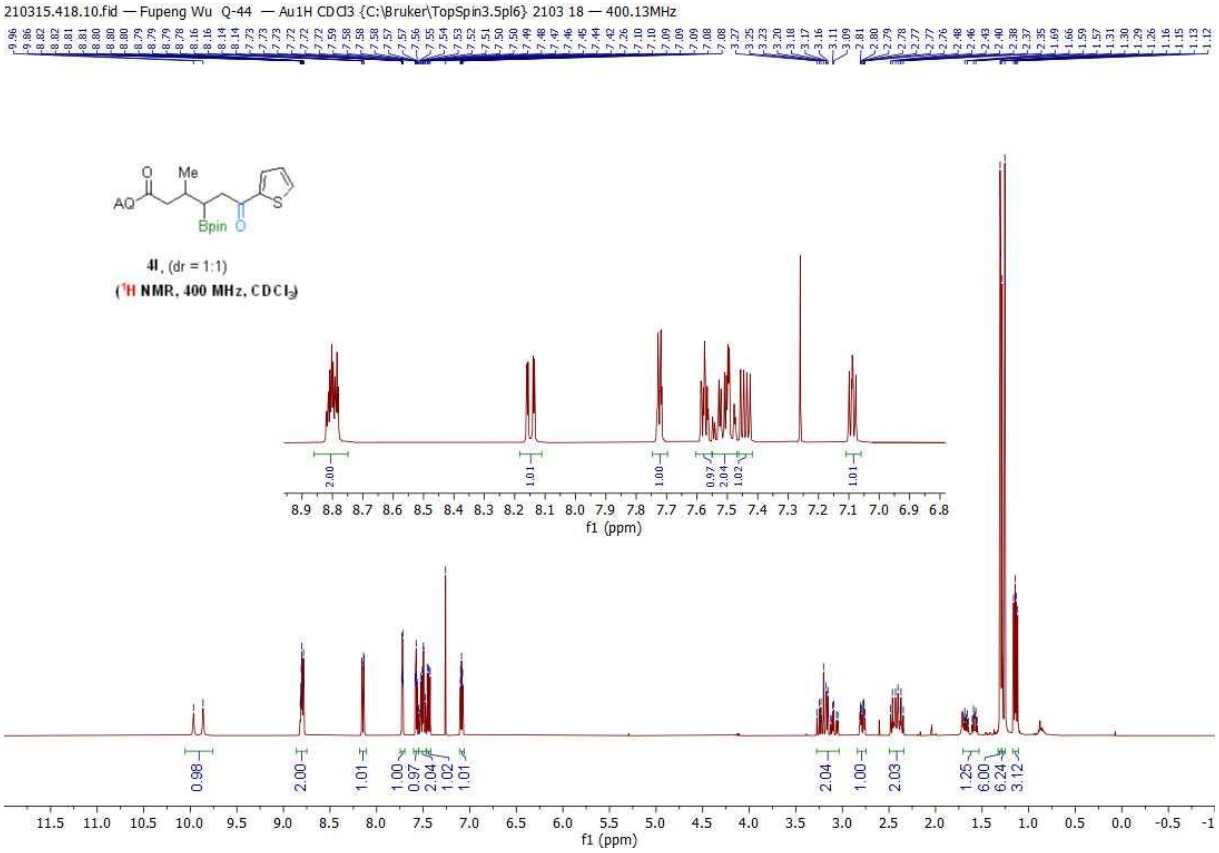

210307.359.10.fid — Fupeng Wu, Q-40 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 59 — 300.13MHz
AQ
Bpin
4k
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)

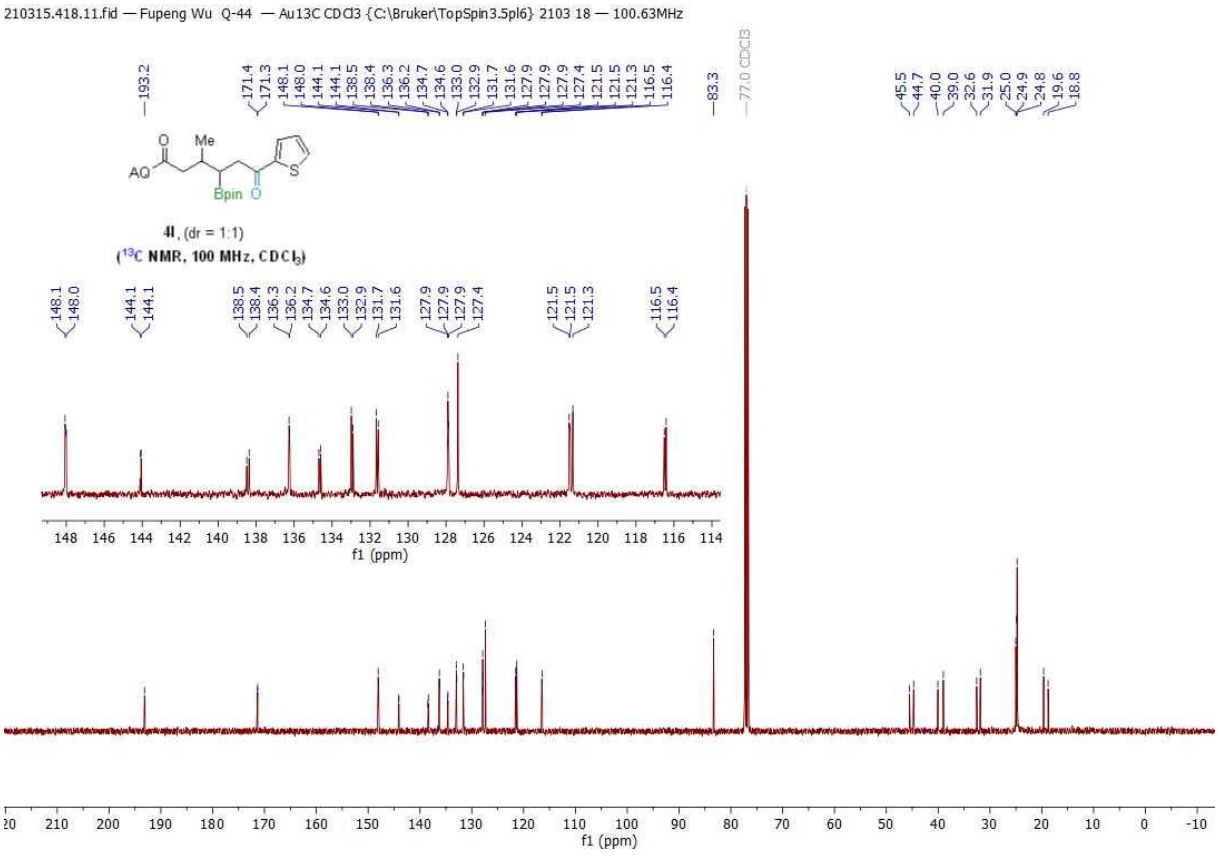

210310.f306.10.fid — Fupeng Wu Q-40 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 6 — 75.49MHz
AQ
Bpin
4k
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

File:21032236 Sample Name:Q-40 UserName:Fu-peng Wu
Vial:1:E,4 Date:22-Mar-2021 Time:16:13:54
Description:MeOH/0.1% HCOOH in H2O 98:2

Sample Report:




210315.418.10.fid — Fupeng Wu Q-44 — Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 18 — 400.13MHz
4l, (dr = 1:1)
(1H NMR, 400 MHz, CDCl3)
f1 (ppm)

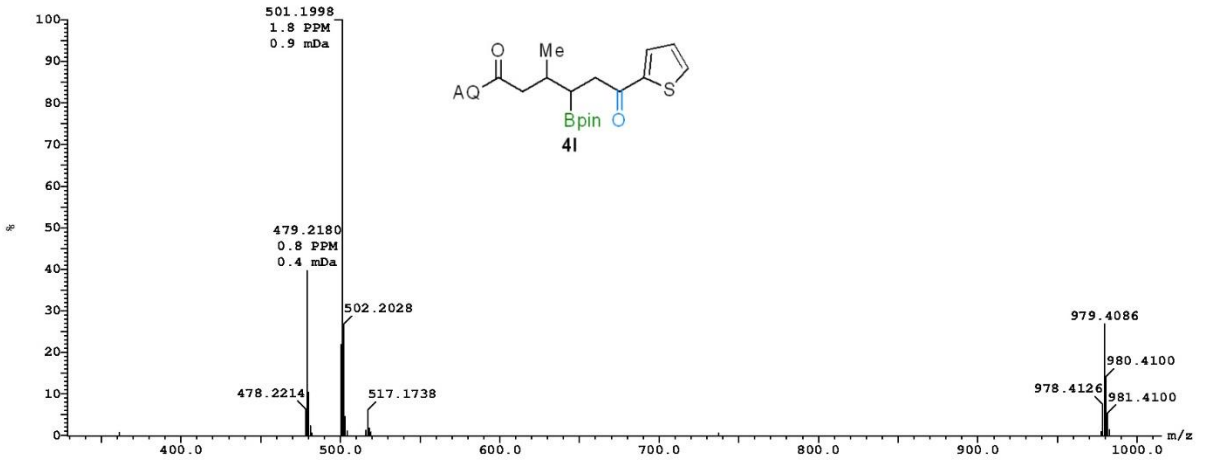

210315.418.11.fid — Fupeng Wu Q-44 — Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 18 — 100.63MHz
4l, (dr = 1:1)
(13C NMR, 100 MHz, CDCl3)
f1 (ppm)

File:21032239 Sample Name:Q-44 UserName:Fu-peng Wu
Vial:1:E,7 Date:22-Mar-2021 Time:16:21:39
Description:MeOH/0.1% HCOOH in H2O 98:2

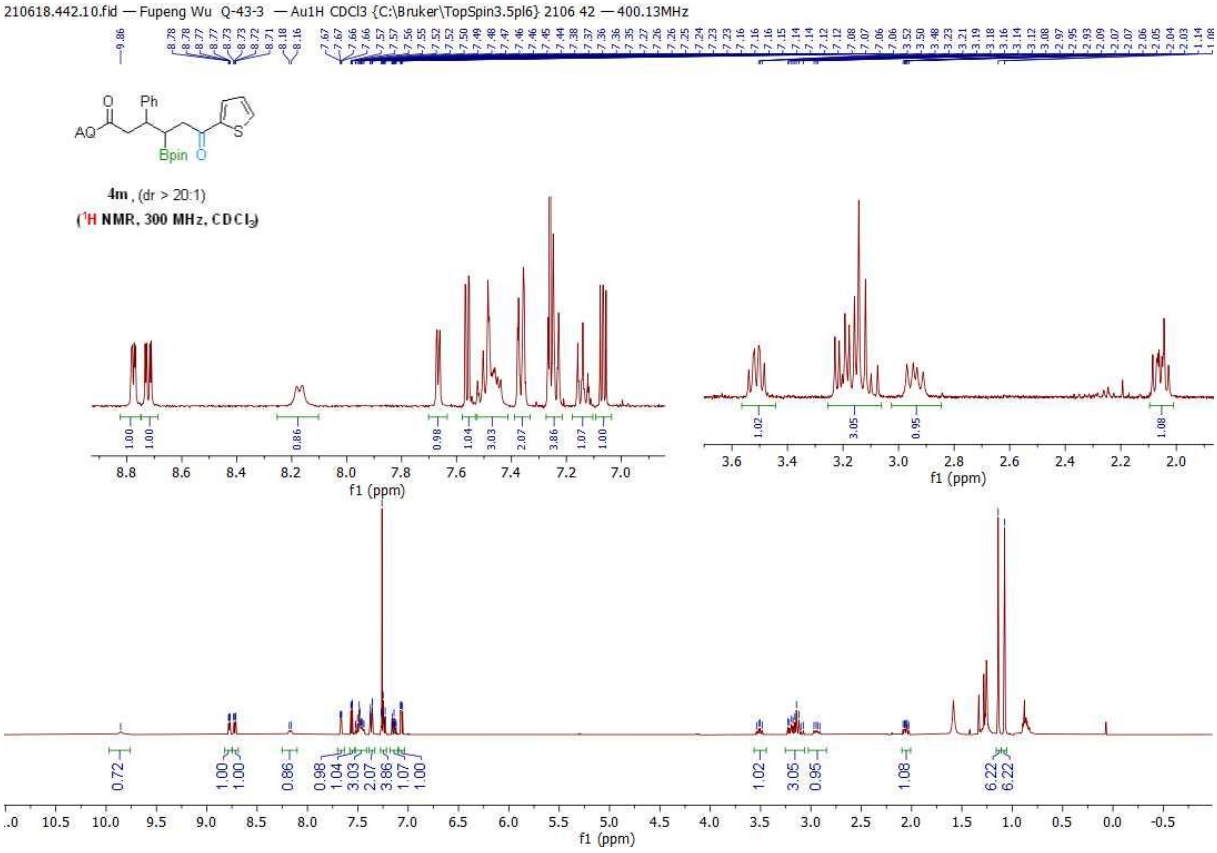
Sample Report:

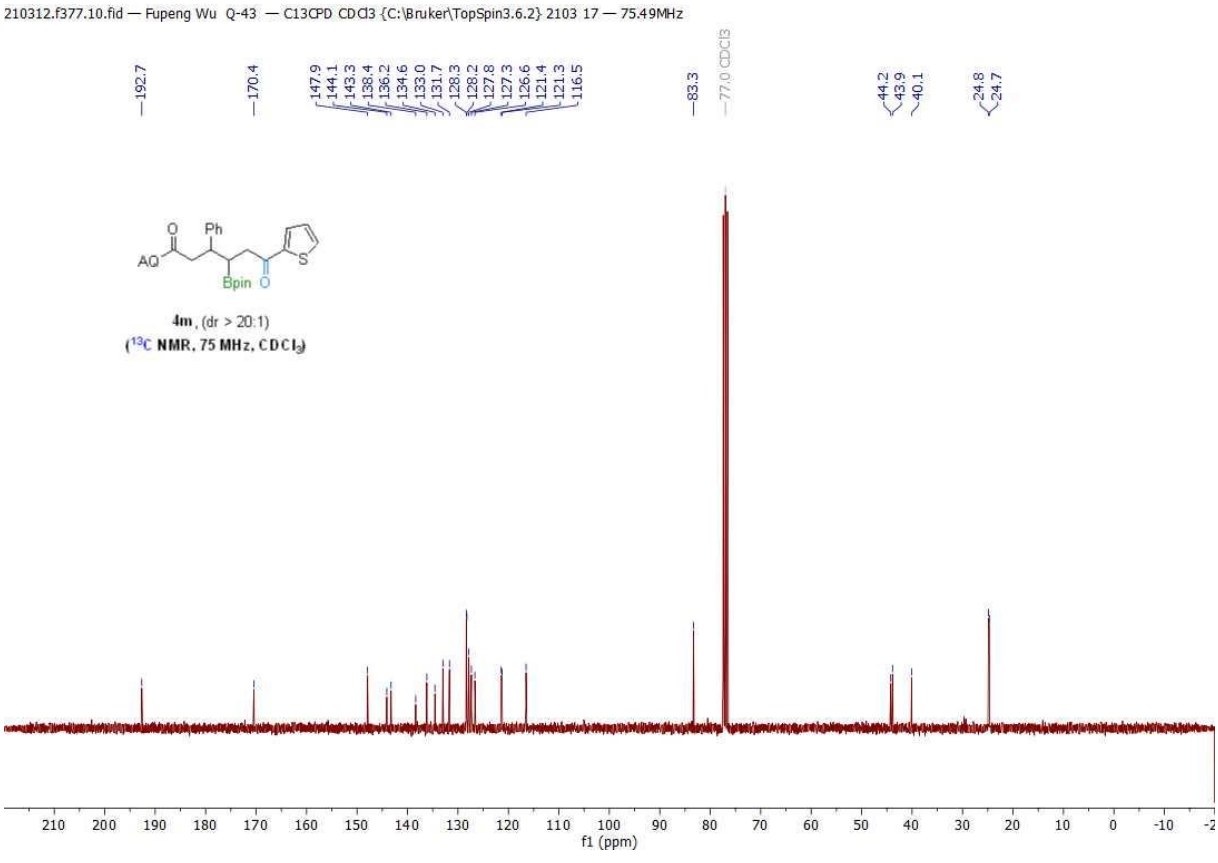
(Time: 0.33) Combine (29:33-80:84) - Dead time test passed

1:TOF MS ES+
3.5e+008



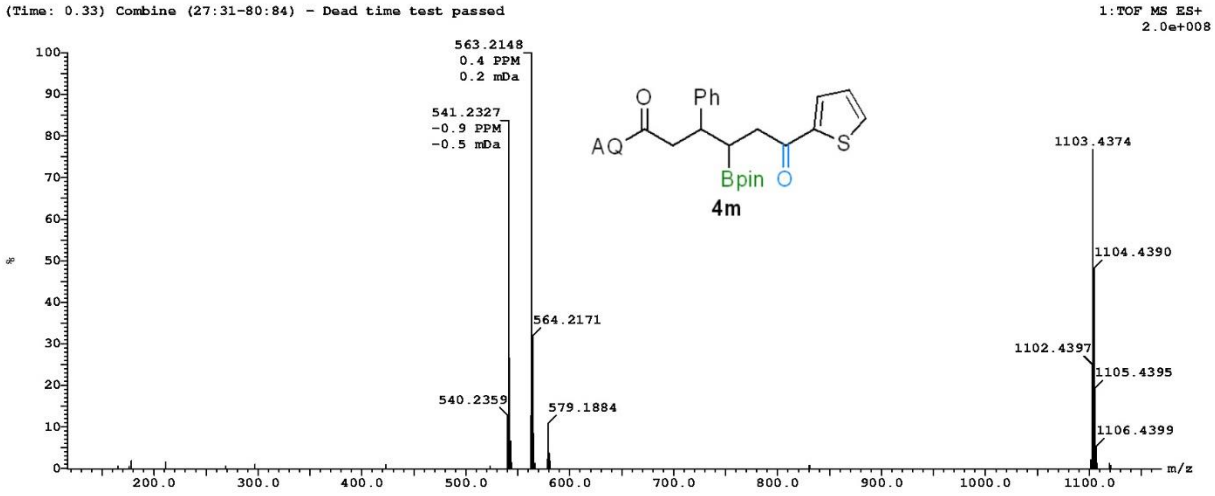
4l

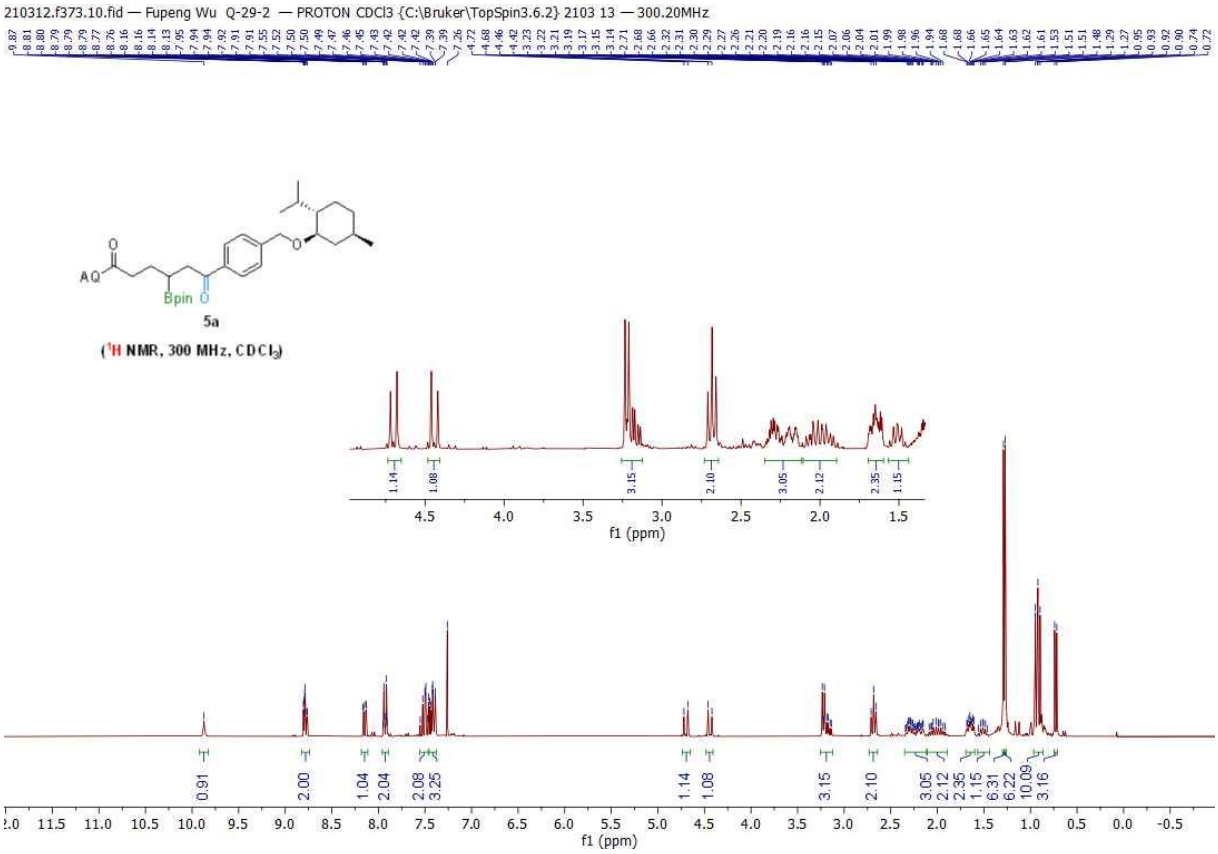

210618.442.10.fid — Fupeng Wu Q-43-3 — Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2106 42 — 400.13MHz
AQ
Ph
Bpin
O
S
4m, (dr > 20:1)
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)

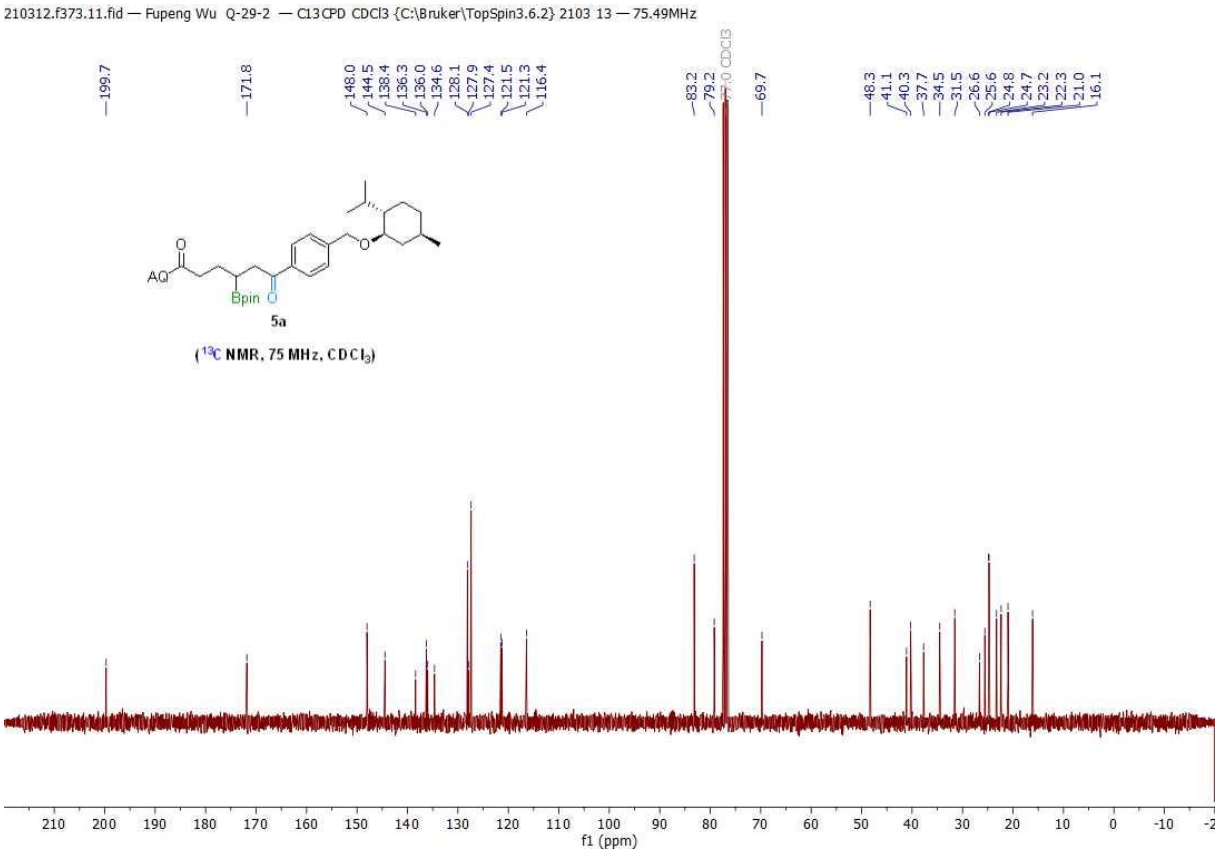

210312.f377.10.fid — Fupeng Wu Q-43 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 17 — 75.49MHz
77.0 CDCl3
AQ
Ph
Bpin
O
S
4m, (dr > 20:1)
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

File:21032238 Sample Name:Q-43 UserName:Fu-peng Wu
Vial:1:E,6 Date:22-Mar-2021 Time:16:19:04
Description:MeOH/0.1% HCOOH in H2O 98:2

Sample Report:

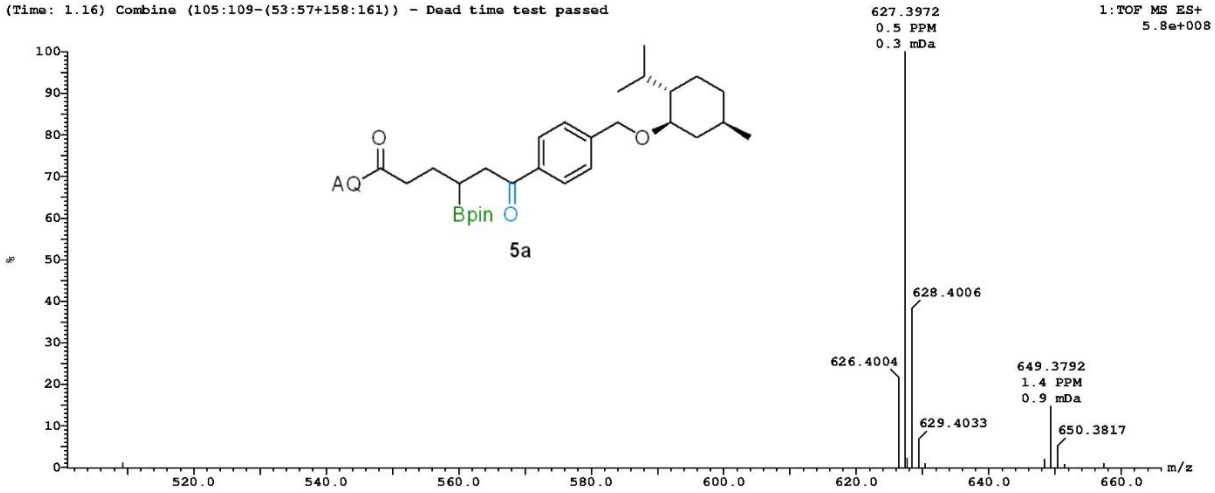


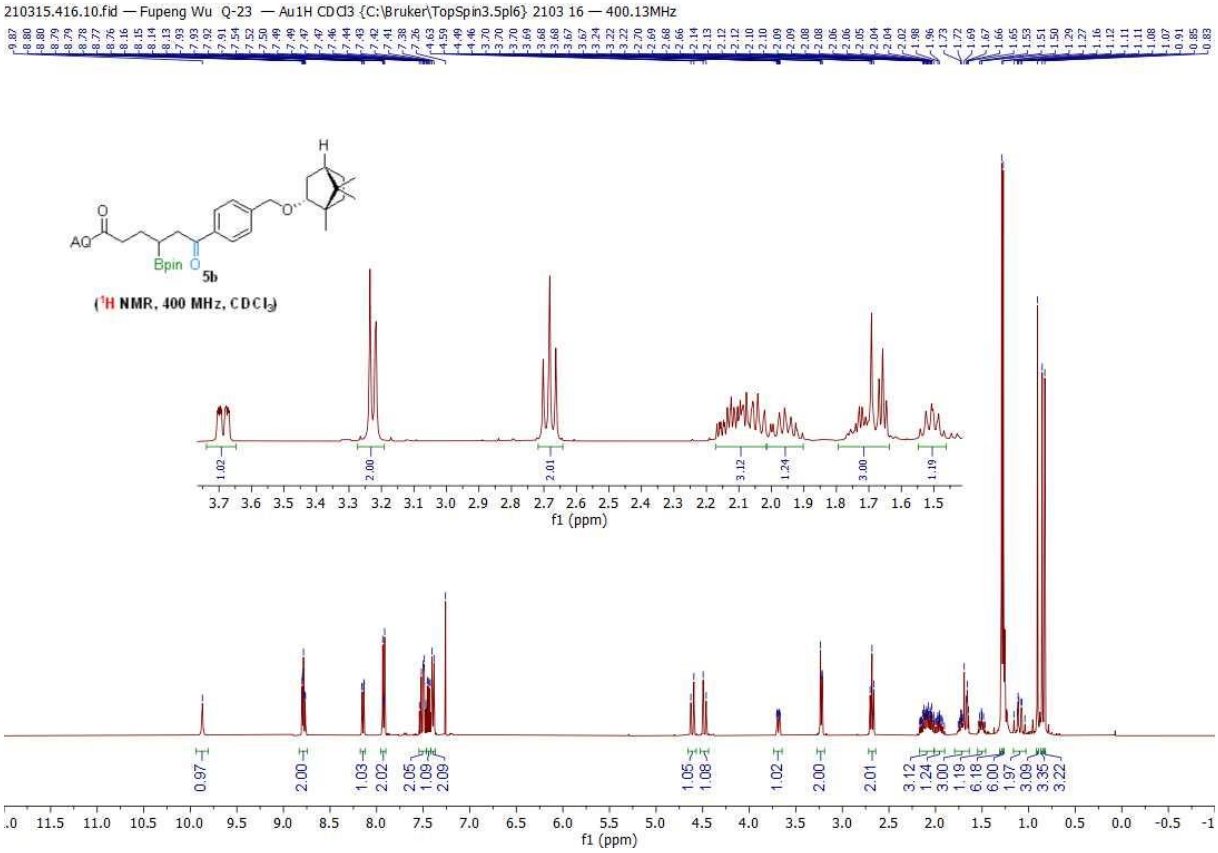

210312.f373.10.fid — Fupeng Wu Q-29-2 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 13 — 300.20MHz
AQ
Bpin
5a
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)

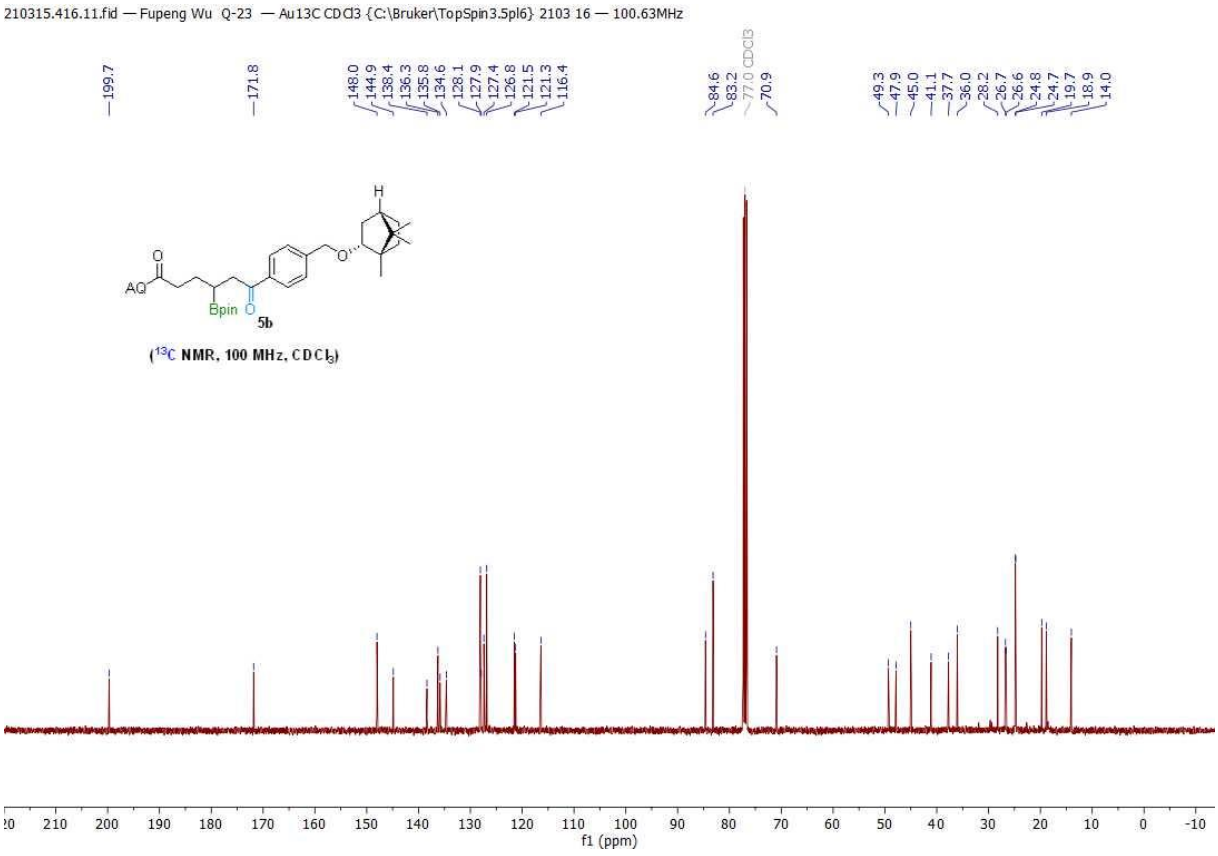

210312.f373.11.fid — Fupeng Wu Q-29-2 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 13 — 75.49MHz
AQ
Bpin
5a
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

File:21032220 Sample Name:Q-29 UserName:Fu-peng Wu
Vial:1:D,4 Date:22-Mar-2021 Time:13:02:26
Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Report:

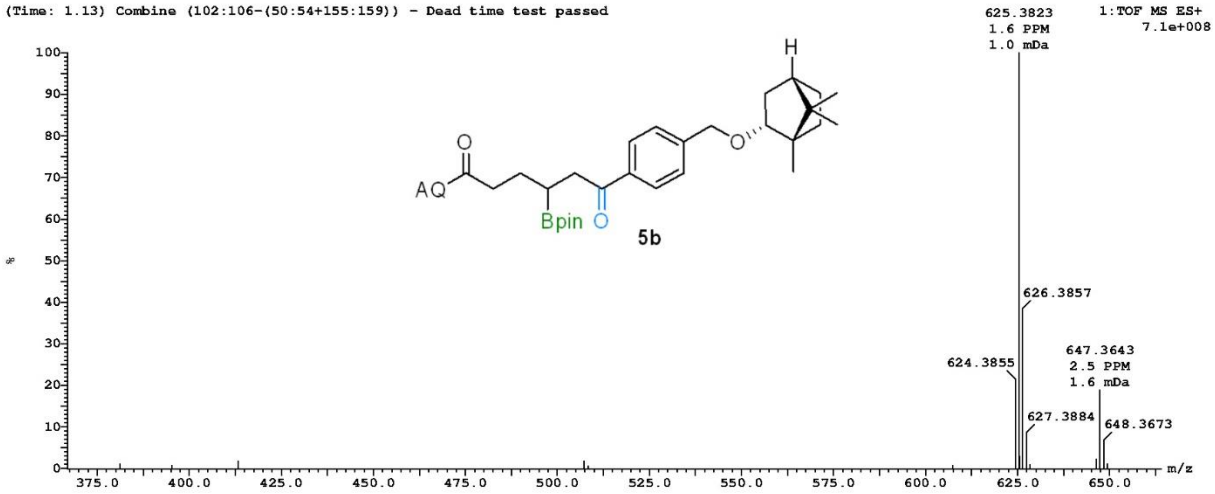


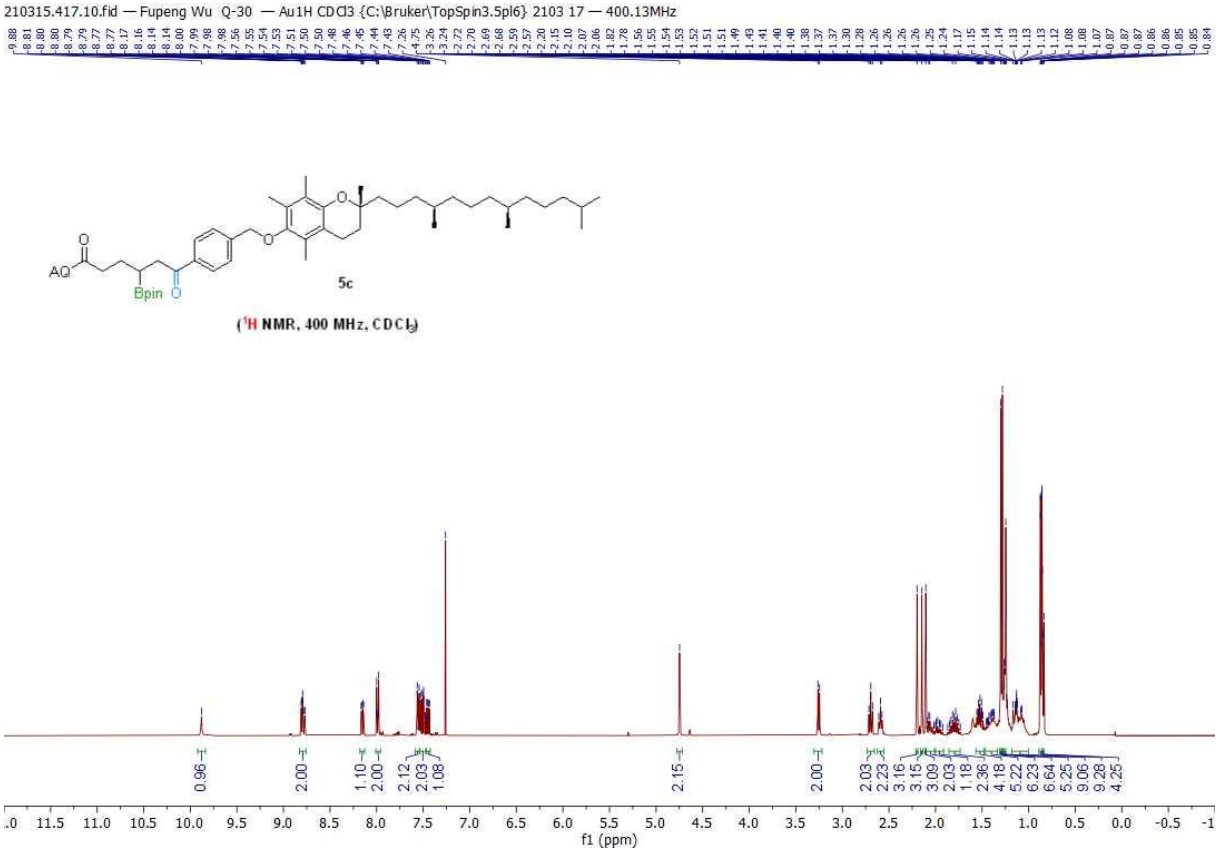

210315.416.10.fid — Fupeng Wu Q-23 — Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 16 — 400.13MHz
AQ
Bpin
O
5b
(1H NMR, 400 MHz, CDCl3)
f1 (ppm)

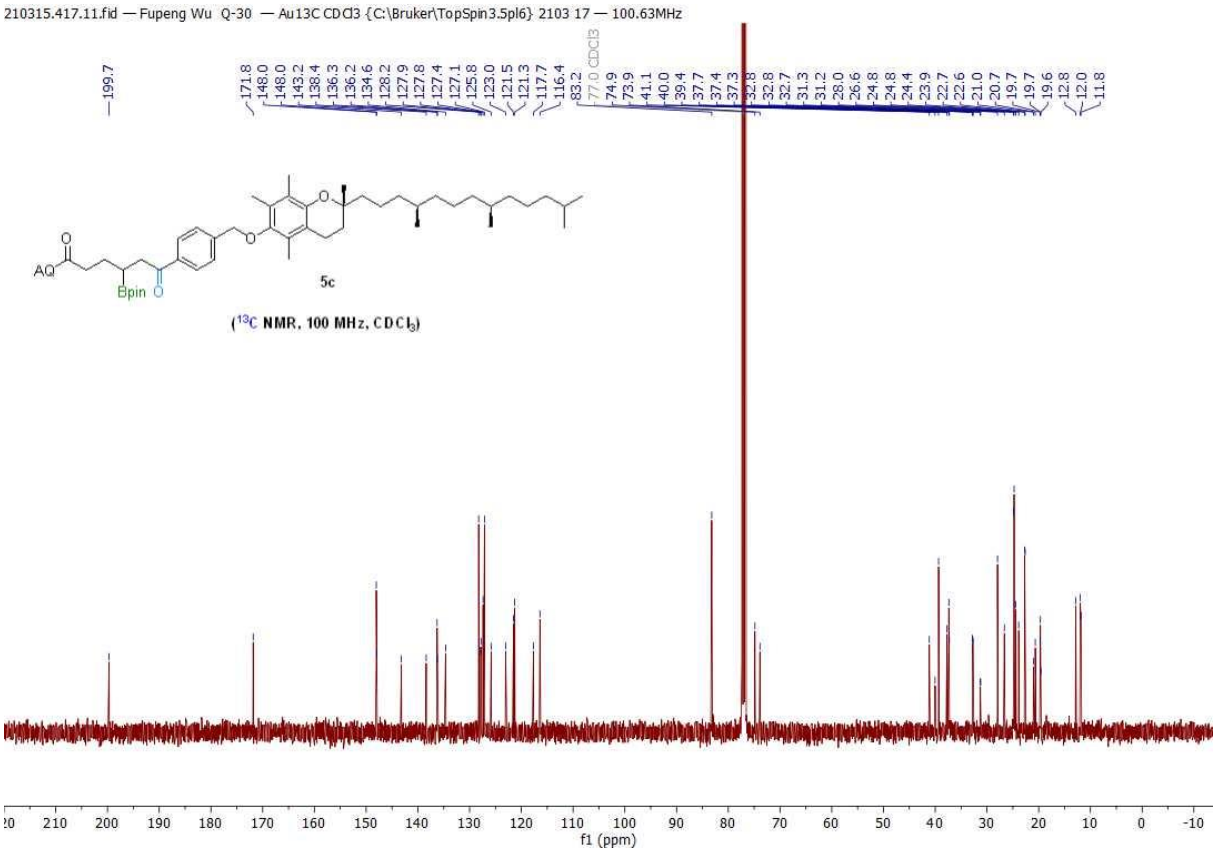

210315.416.11.fid — Fupeng Wu Q-23 — Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 16 — 100.63MHz
77.0 CDCl3
AQ
Bpin
O
5b
(13C NMR, 100 MHz, CDCl3)
f1 (ppm)

File:21032217 Sample Name:Q-23 UserName:Fu-peng Wu
Vial:1:D,1 Date:22-Mar-2021 Time:12:48:33
Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Report:

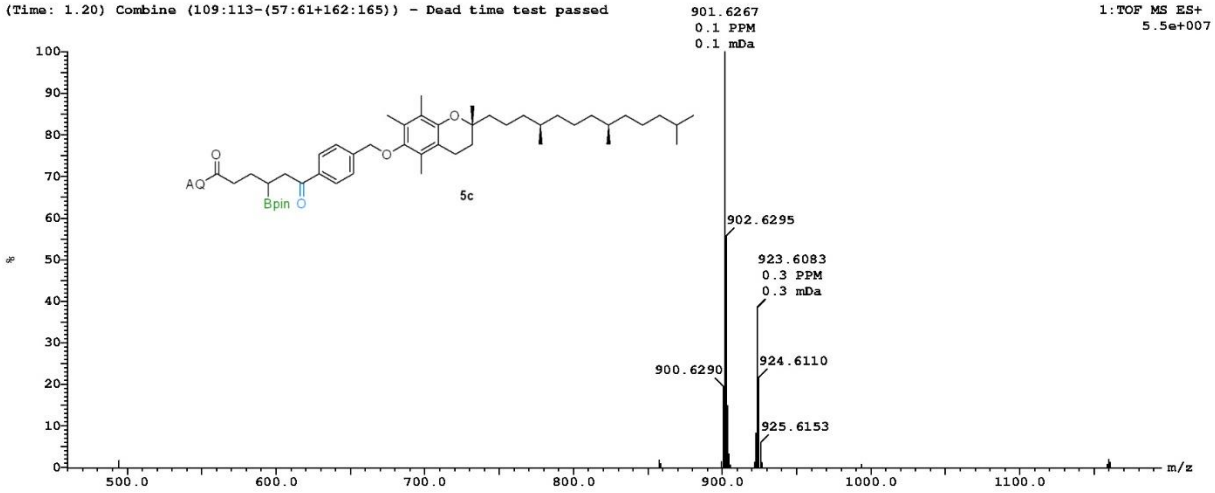



210315.417.10.fid — Fupeng Wu Q-30 — Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 17 — 400.13MHz
AQ
Bpin
5c
(1H NMR, 400 MHz, CDCl3)
f1 (ppm)

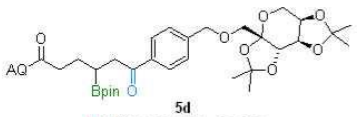

210315.417.11.fid — Fupeng Wu Q-30 — Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 17 — 100.63MHz
AQ
Bpin
5c
(13C NMR, 100 MHz, CDCl3)
f1 (ppm)

File:21032229 Sample Name:Q-30 UserName:Fu-peng Wu
Vial:1:D,5 Date:22-Mar-2021 Time:15:48:47
Description:MeOH/0.1% HCOOH in H2O 98:2

Sample Report:

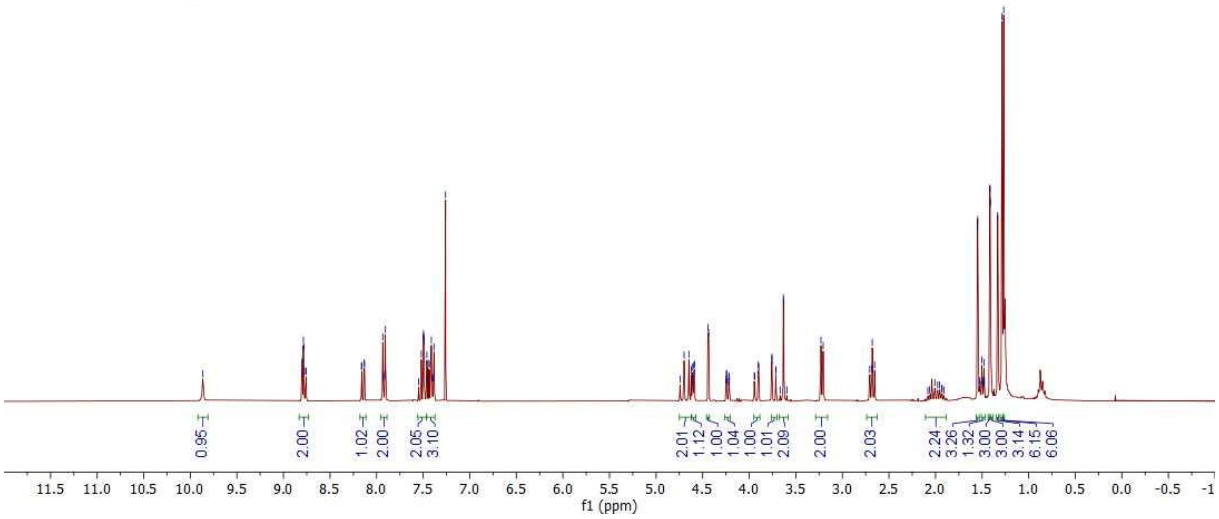


210316.f314.10.fid — Fupeng Wu Q-22-6 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 14 — 300.20MHz

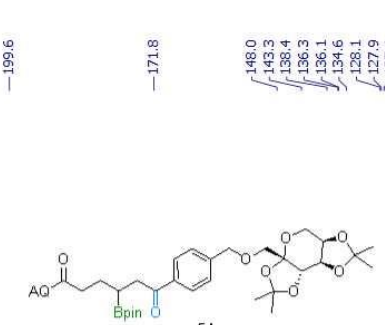


5d

(**^{1}H NMR, 300 MHz, $CDCl_3$**)



210315.415.11.fid — Fupeng Wu Q-22-5 — Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 15 — 100.63MHz

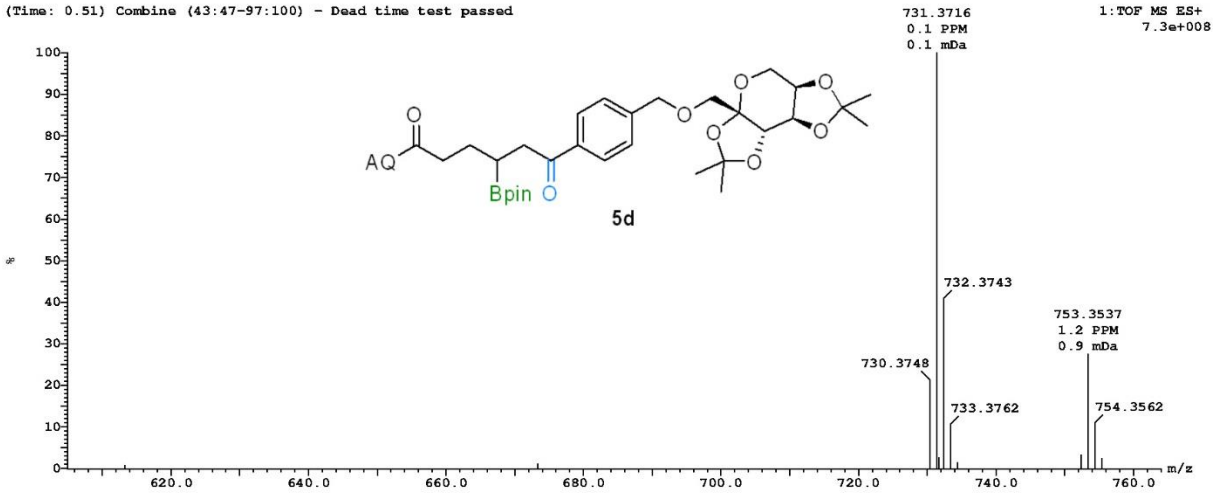


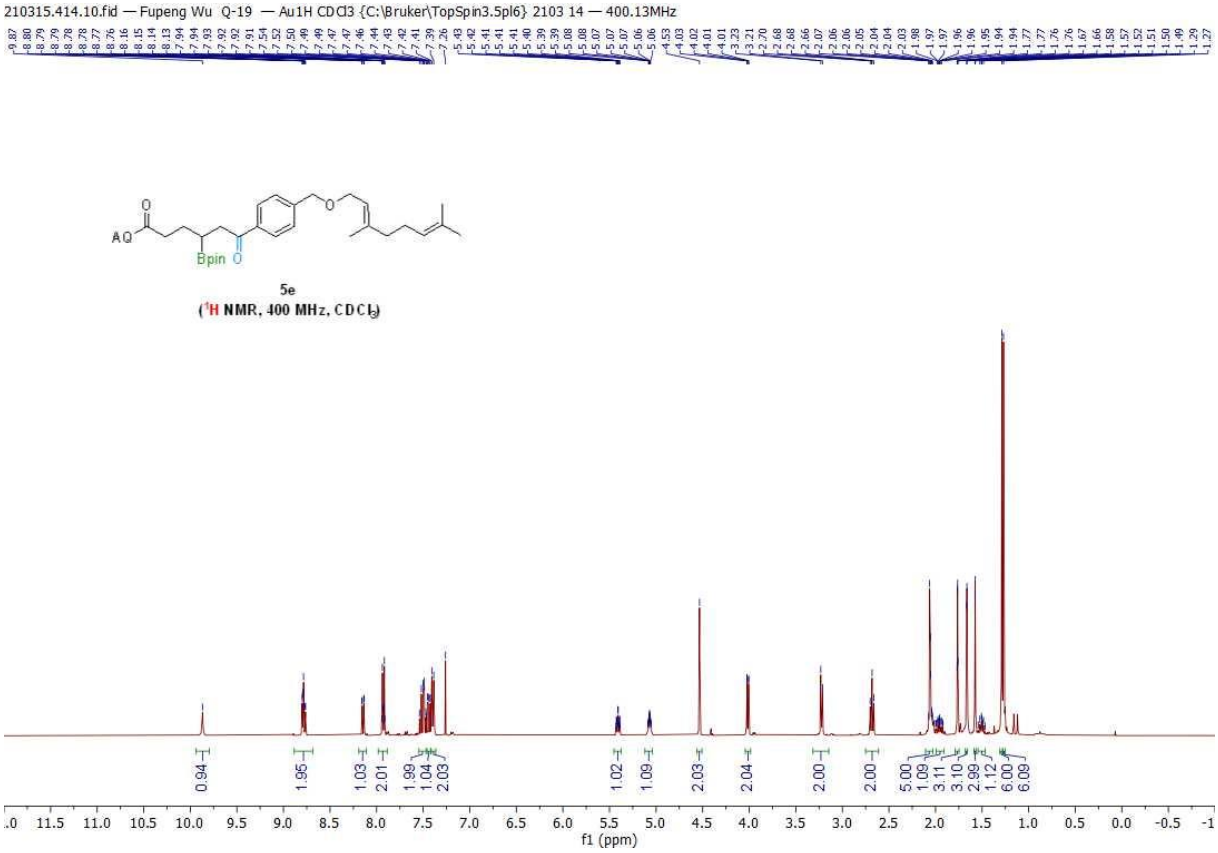
5d

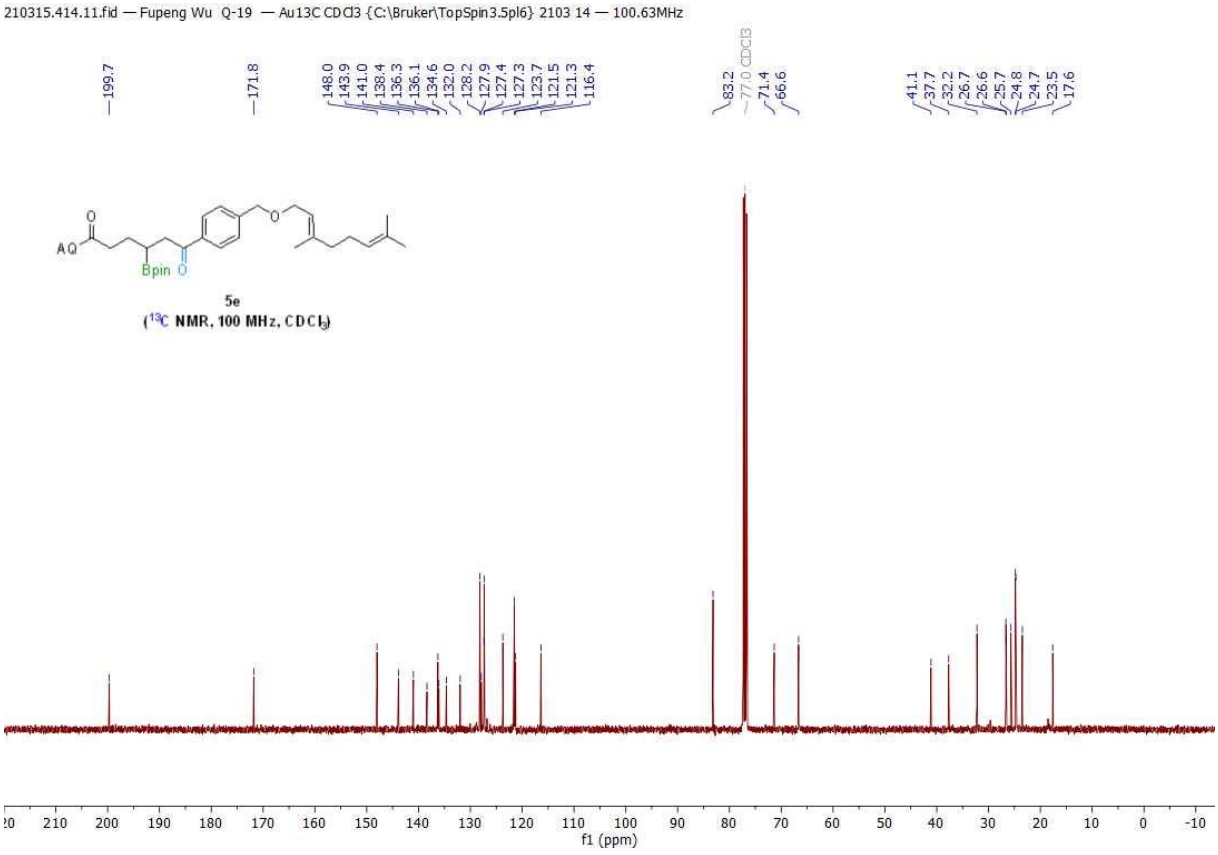
(**^{13}C NMR, 100 MHz, $CDCl_3$**)

File:21032216 Sample Name:Q-22 UserName:Fu-peng Wu
Vial:1:C,8 Date:22-Mar-2021 Time:12:44:02
Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Report:




210315.414.10.fid — Fupeng Wu Q-19 — Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 14 — 400.13MHz
AQ
Bpin
5e
(1H NMR, 400 MHz, CDCl3)
0.94
1.95
1.03
2.01
1.99
1.04
2.03
1.02
1.09
2.03
2.04
2.00
2.00
5.00
1.09
3.11
3.10
2.99
1.12
6.00
6.09
f1 (ppm)

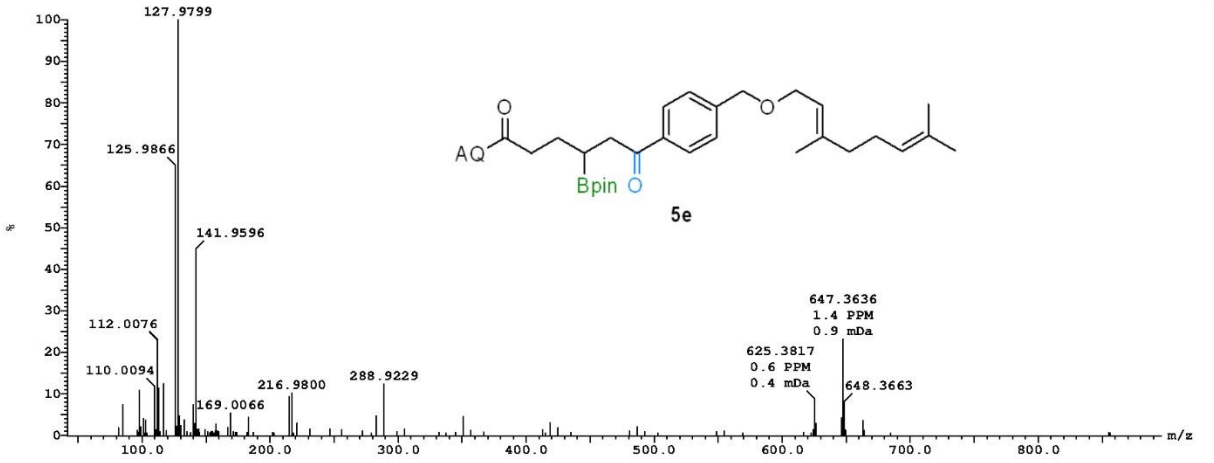

210315.414.11.fid — Fupeng Wu Q-19 — Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2103 14 — 100.63MHz
199.7
171.8
148.0
143.9
141.0
138.4
136.3
136.1
134.6
132.0
128.2
127.9
127.4
127.3
123.7
121.5
121.3
116.4
83.2
77.0 CDCl3
71.4
66.6
41.1
37.7
32.2
26.7
26.6
25.7
24.8
24.7
23.5
17.6
AQ
Bpin
5e
(13C NMR, 100 MHz, CDCl3)
f1 (ppm)

File:21032302 Sample Name:Q-19 UserName:Fu-peng Wu
Vial:1:B,1 Date:23-Mar-2021 Time:09:47:11
Description:MeOH/0.1% HCOOH in H2O 90:10

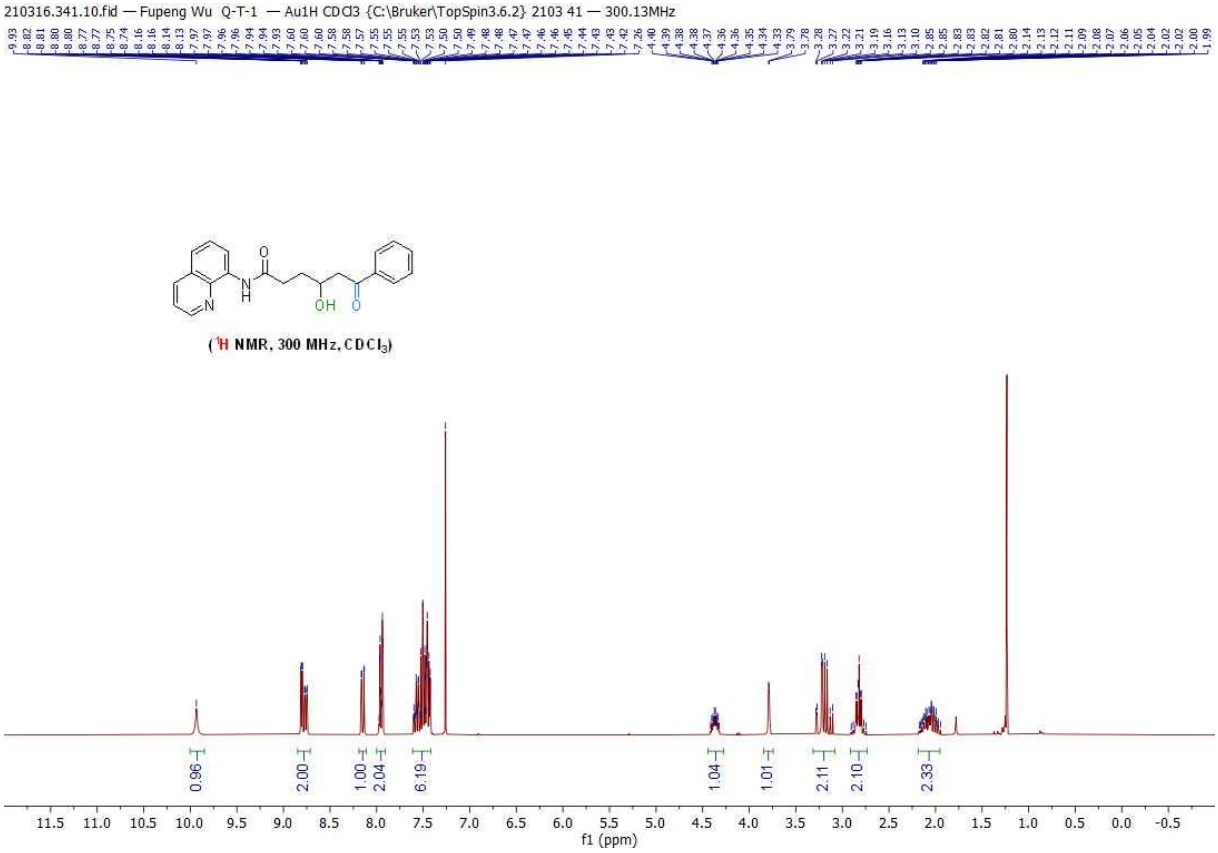
Sample Report:

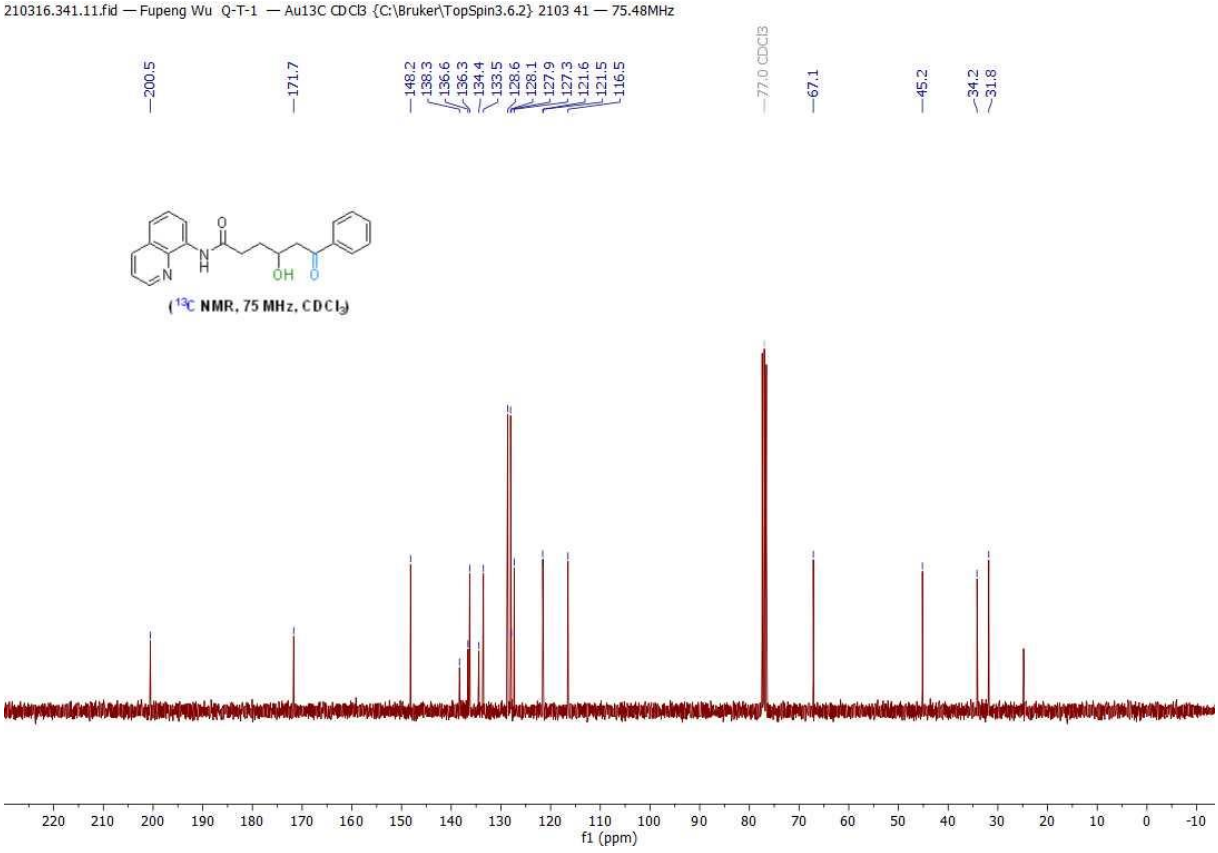
(Time: 0.37) Combine (32:36-84:88) - Dead time test passed

1:TOF MS ES+
4.4e+006



5e


210316.341.10.fid — Fupeng Wu Q-T-1 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 41 — 300.13MHz
(^{1}H NMR, 300 MHz, CDCl$_3$)
0.96
2.00
1.00
2.04
6.19
1.04
1.01
2.11
2.10
2.33
f1 (ppm)

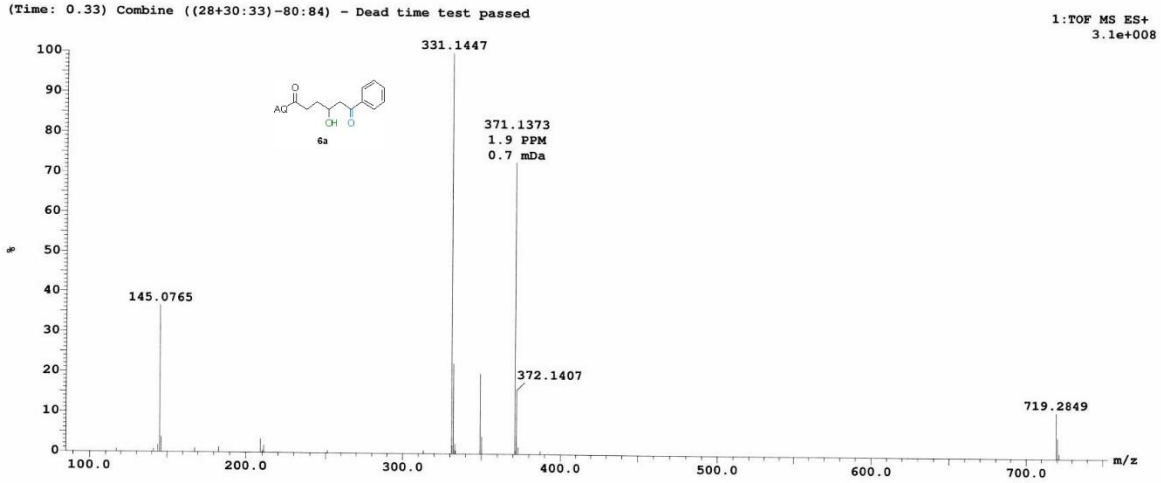

210316.341.11.fid — Fupeng Wu Q-T-1 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 41 — 75.48MHz
200.5
171.7
148.2
138.3
136.6
136.3
134.4
133.5
128.6
128.1
127.9
127.3
121.6
121.5
116.5
77.0 CDCl3
67.1
45.2
34.2
31.8
(^{13}C NMR, 75 MHz, CDCl$_3$)
f1 (ppm)

ESI-TOF Accurate Mass Report
File:21040909
Vial:1:F,4
Description:MeOH/0.1% HCOOH in H2O 90:10

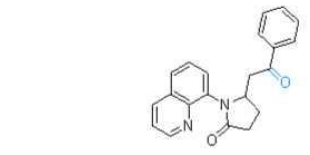
Sample Name:Q-T-1
Date:09-Apr-2021

UserName:Fupeng Wu
Time:16:28:32

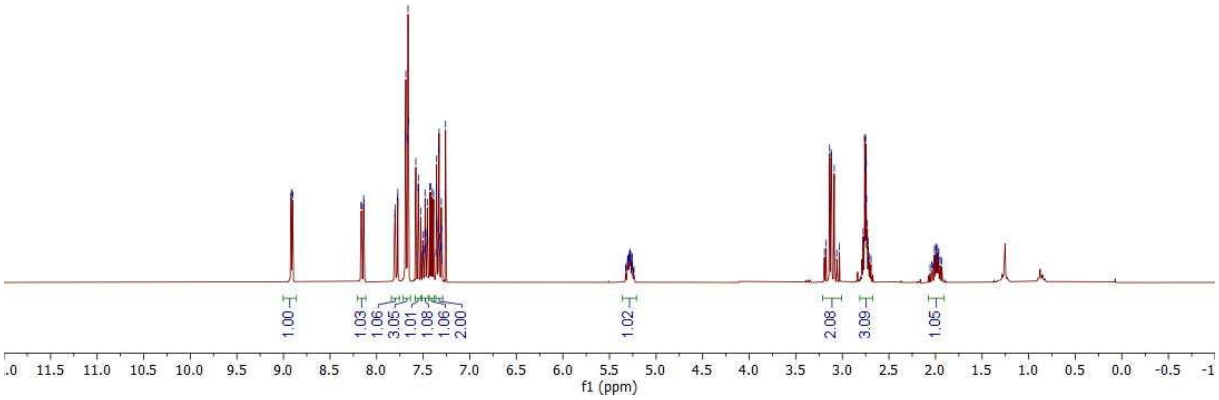
Sample Report:



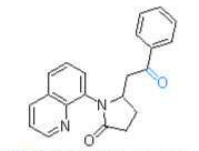
210319.305.21.fid — Fupeng Wu, Q-7-2 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 5 — 300.13MHz



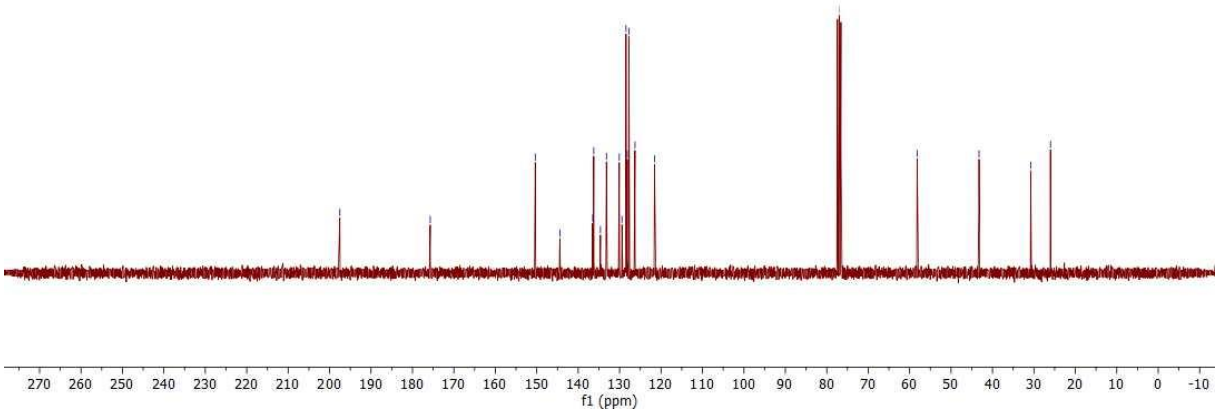
(^{1}H NMR, 300 MHz, $CDCl_3$)

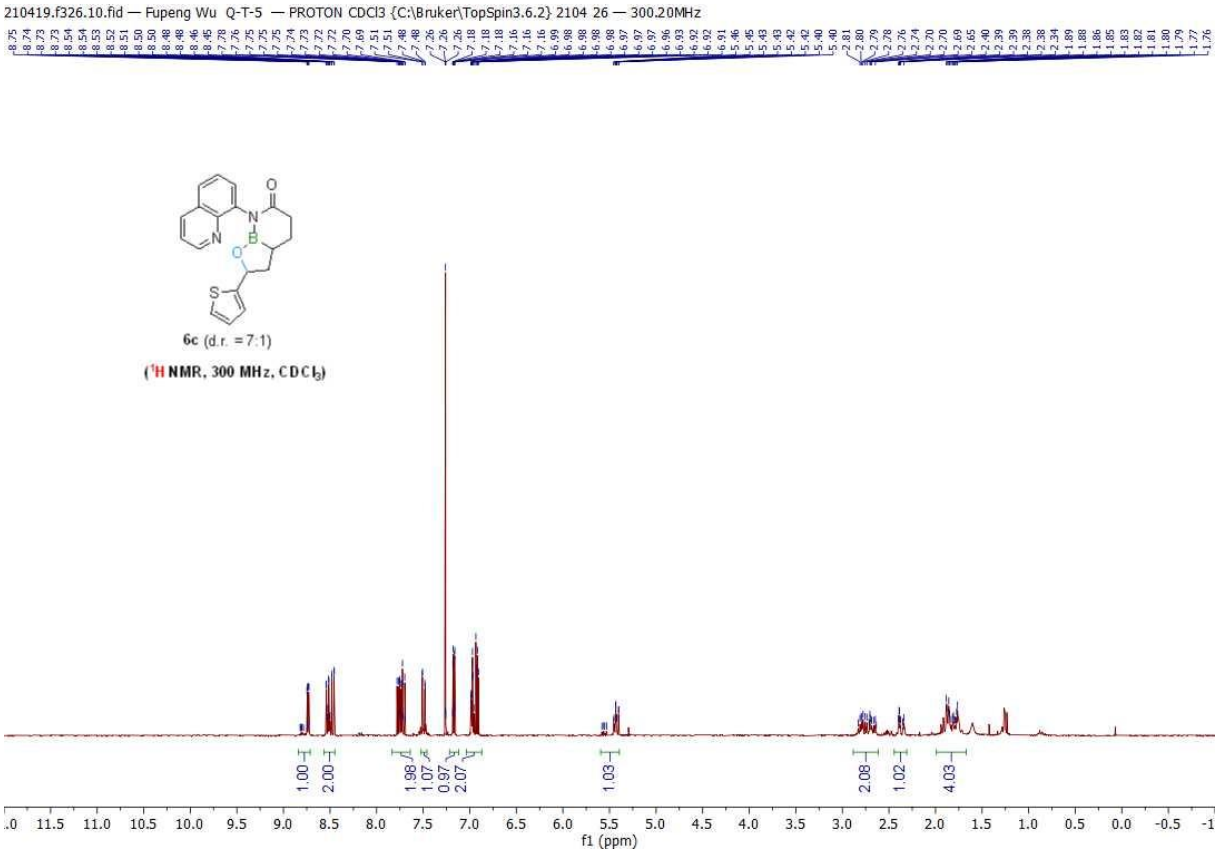


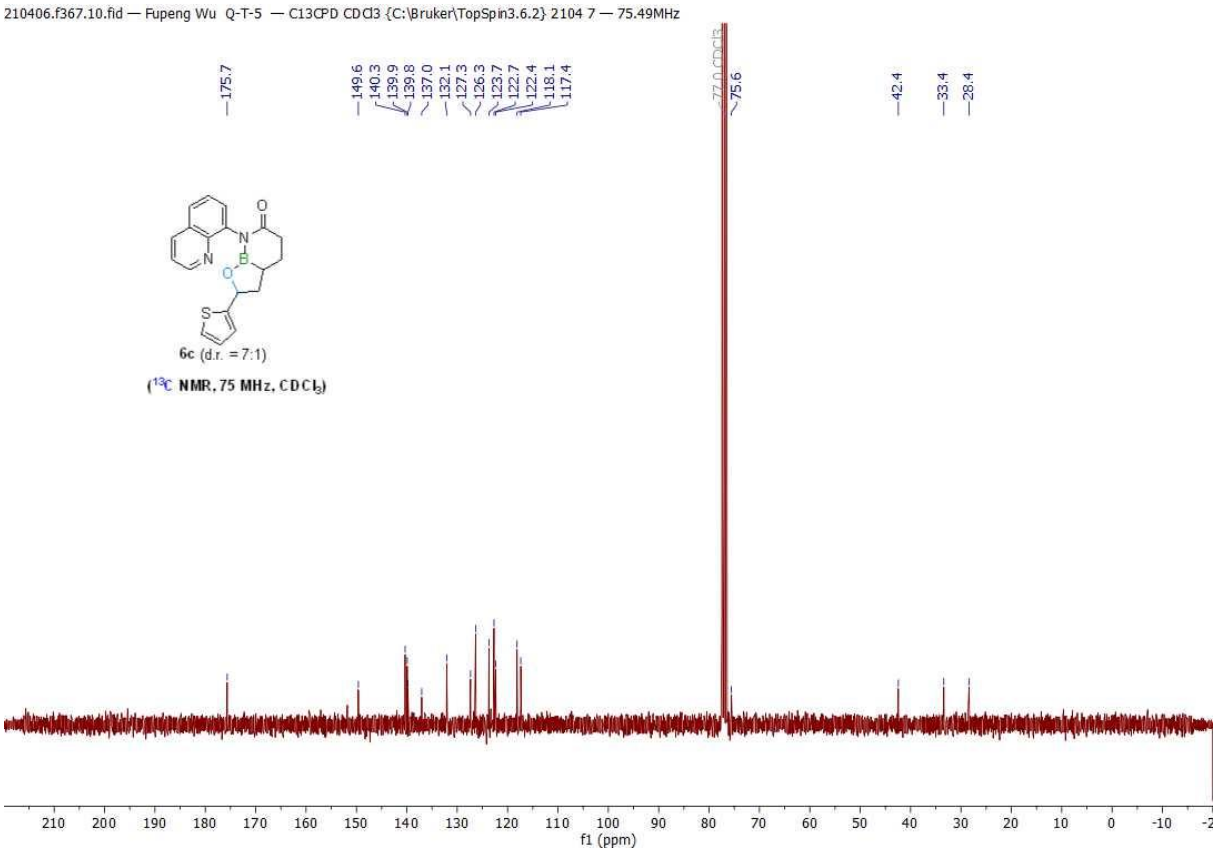
210319.305.20.fid — Fupeng Wu, Q-7-2 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 5 — 75.48MHz



(^{13}C NMR, 75 MHz, $CDCl_3$)

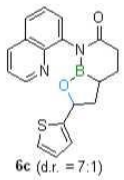



210419.f326.10.fid — Fupeng Wu Q-T-5 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2104 26 — 300.20MHz
6c (d.r. = 7:1)
(1H NMR, 300 MHz, CDCl3)
1.00
2.00
1.98
1.07
0.97
2.07
1.03
2.08
1.02
4.03
f1 (ppm)


210406.f367.10.fid — Fupeng Wu Q-T-5 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2104 7 — 75.49MHz
175.7
149.6
140.3
139.9
139.8
137.0
132.1
127.3
126.3
123.7
122.7
122.4
118.1
117.4
77.0 CDCl3
75.6
42.4
33.4
28.4
6c (d.r. = 7:1)
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)

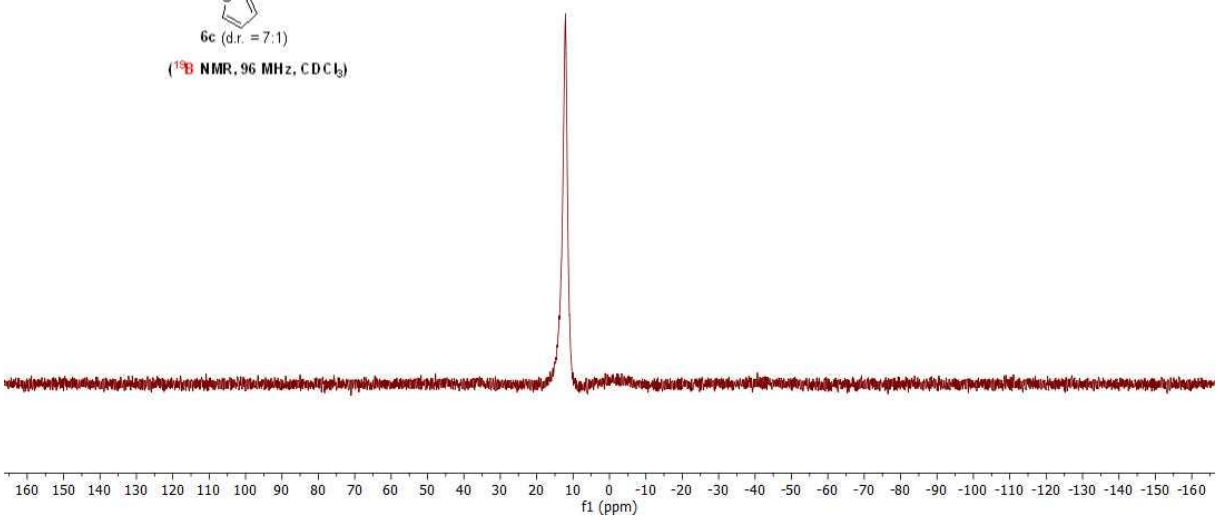
210326.f323.11.fid — Fupeng Wu / Q-T-4 — 11B(H-entk) CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 23 — 96.32MHz

12.1



6c (d.r. = 7:1)

(^{11}B NMR, 96 MHz, $CDCl_3$)



ESI-TOF Accurate Mass Report

File:21040911
Vial:1:F,6
Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:Q-T-3
Date:09-Apr-2021

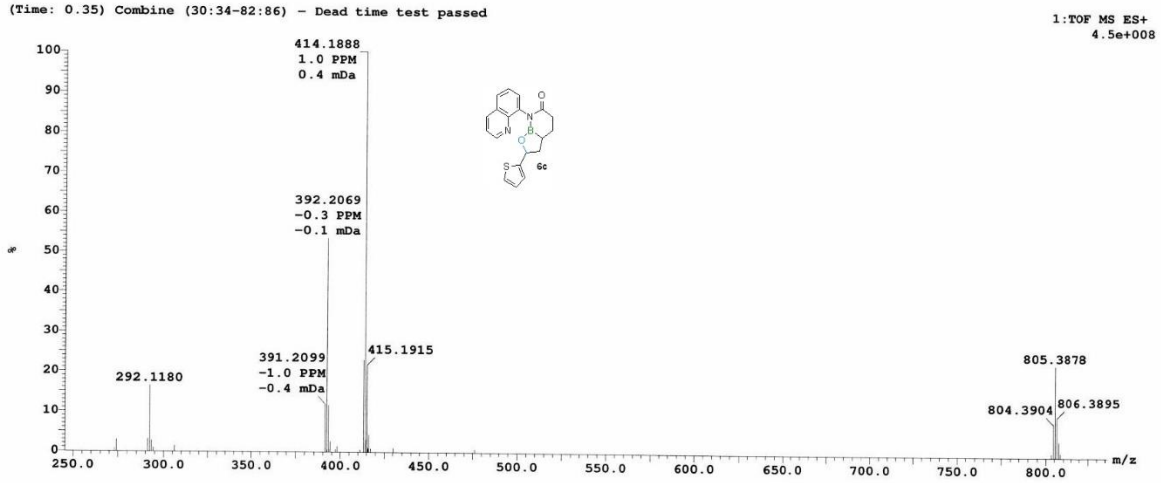
UserName:Fupeng Wu
Time:15:26:23

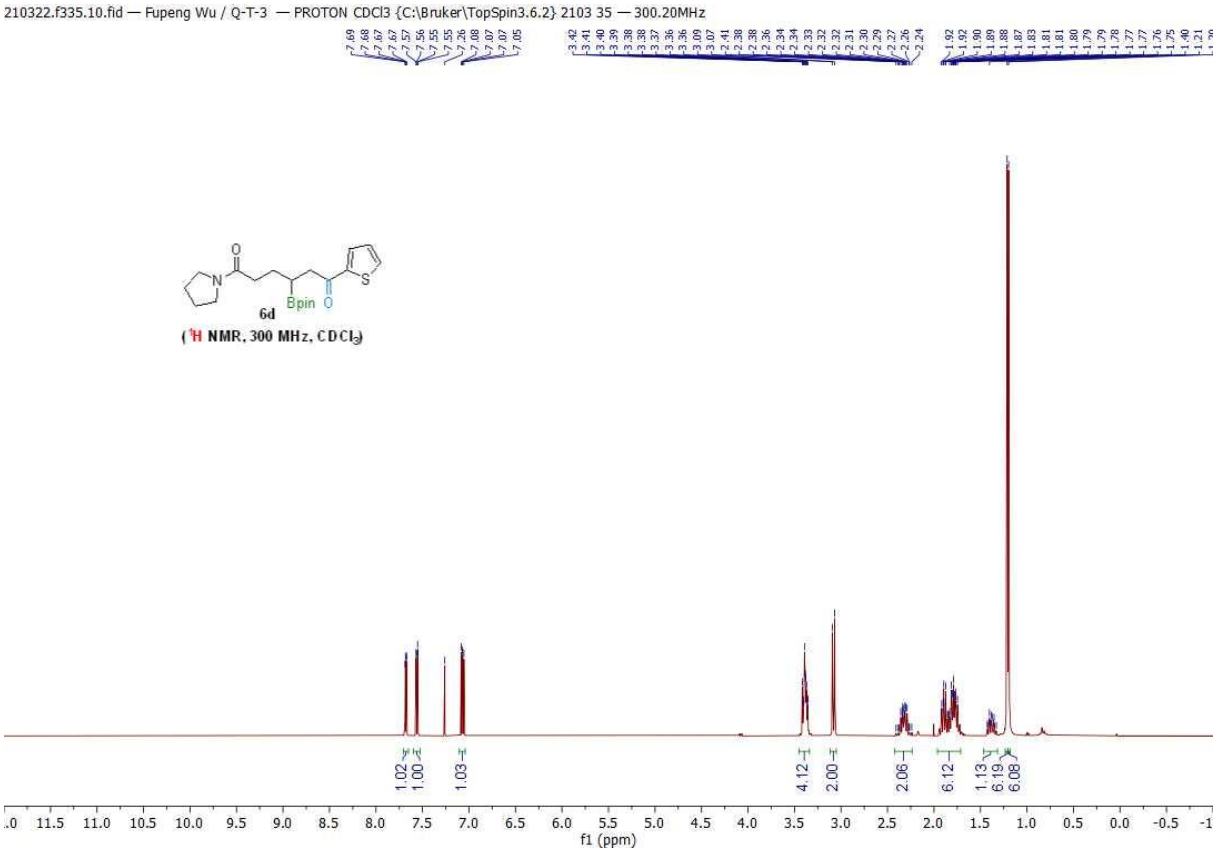
Page 2

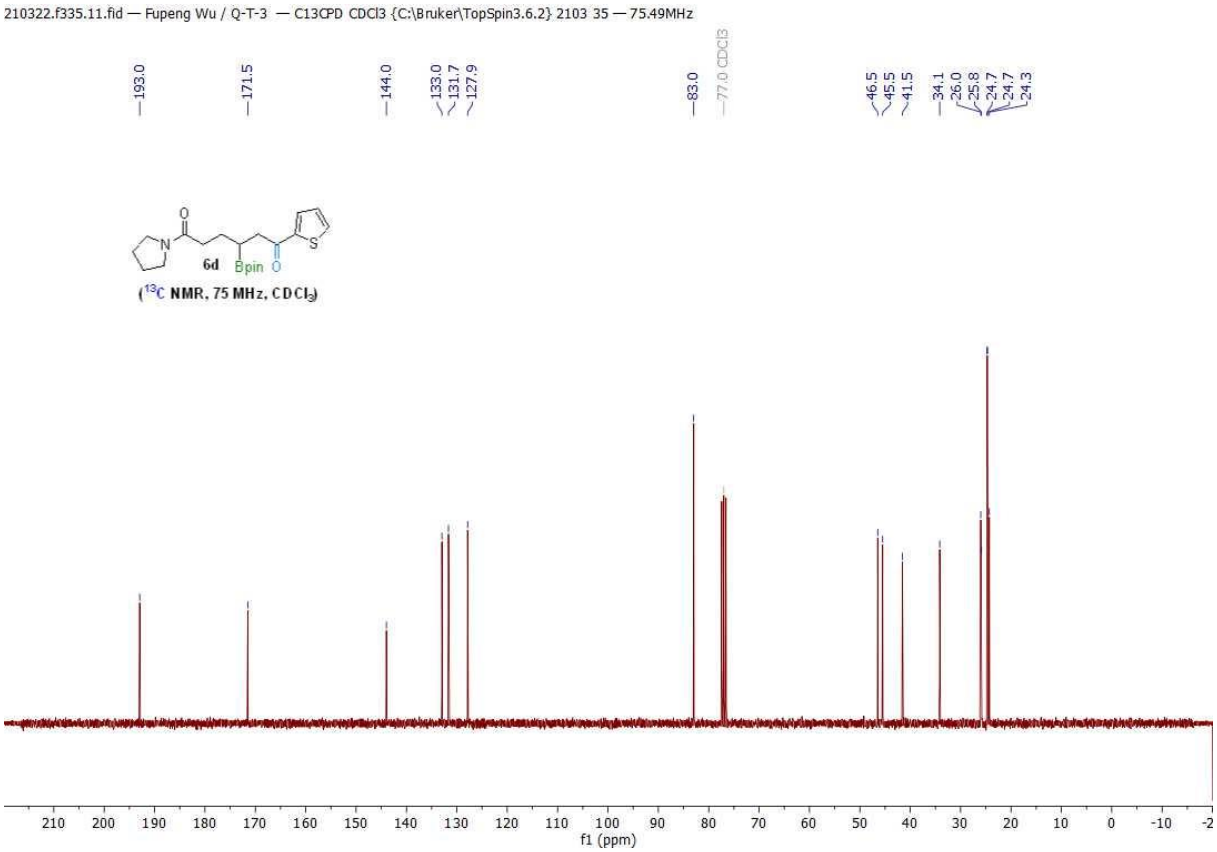
Sample Report:

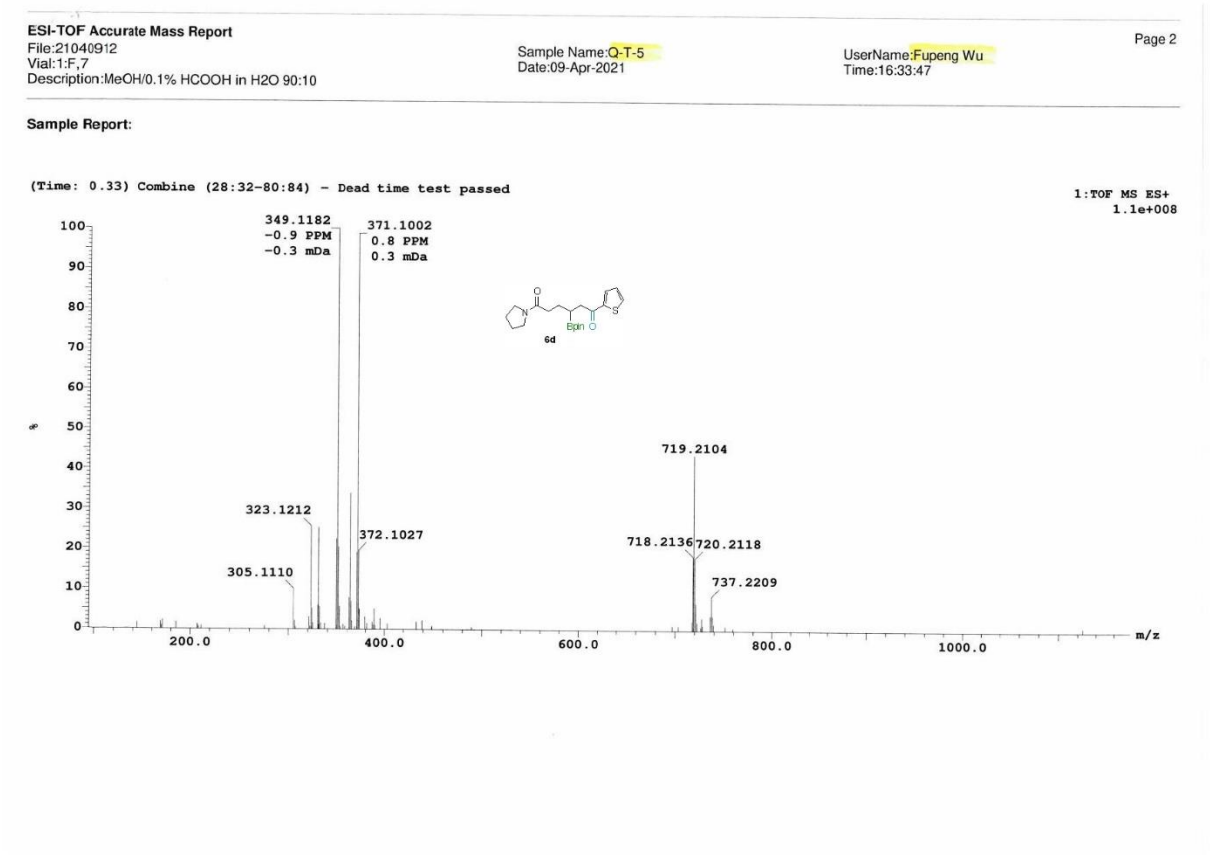
(Time: 0.35) Combine (30:34-82:86) - Dead time test passed

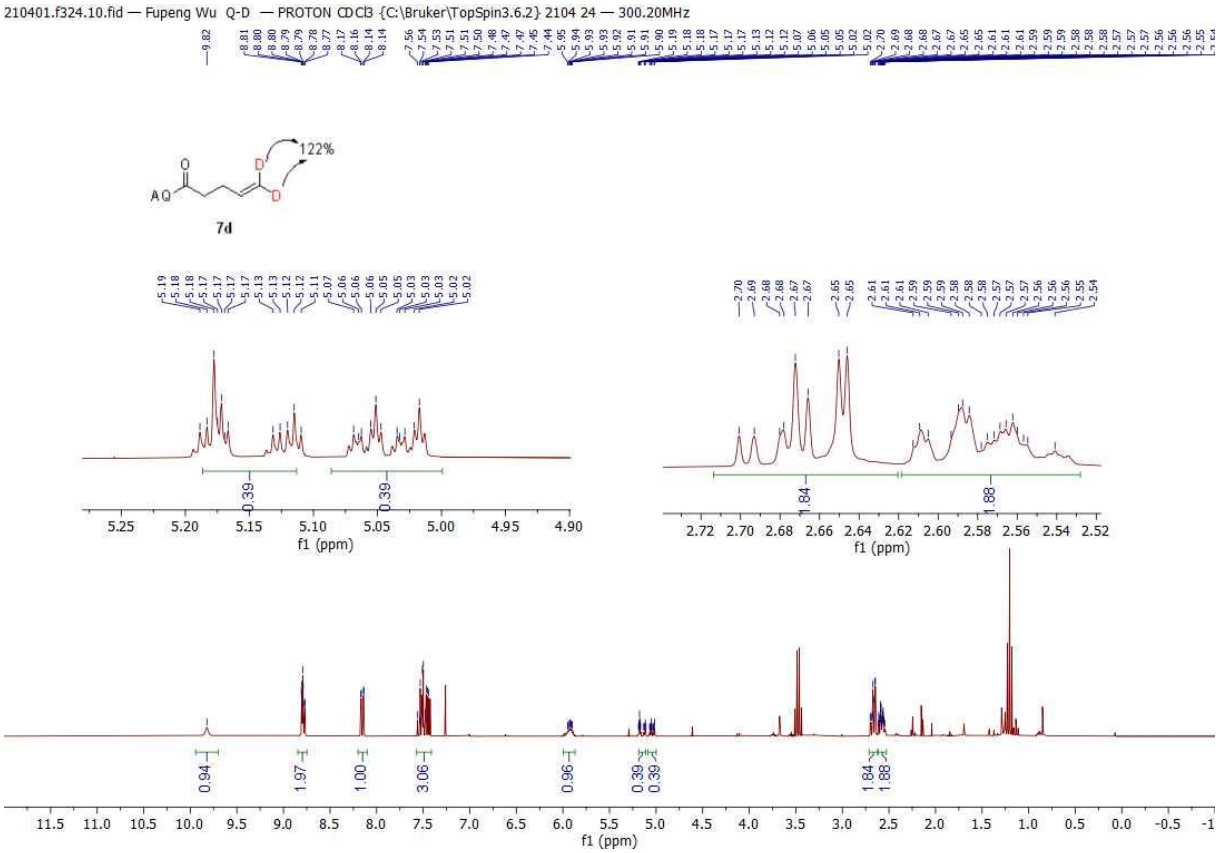
1:TOF MS ES+
4.5e+008

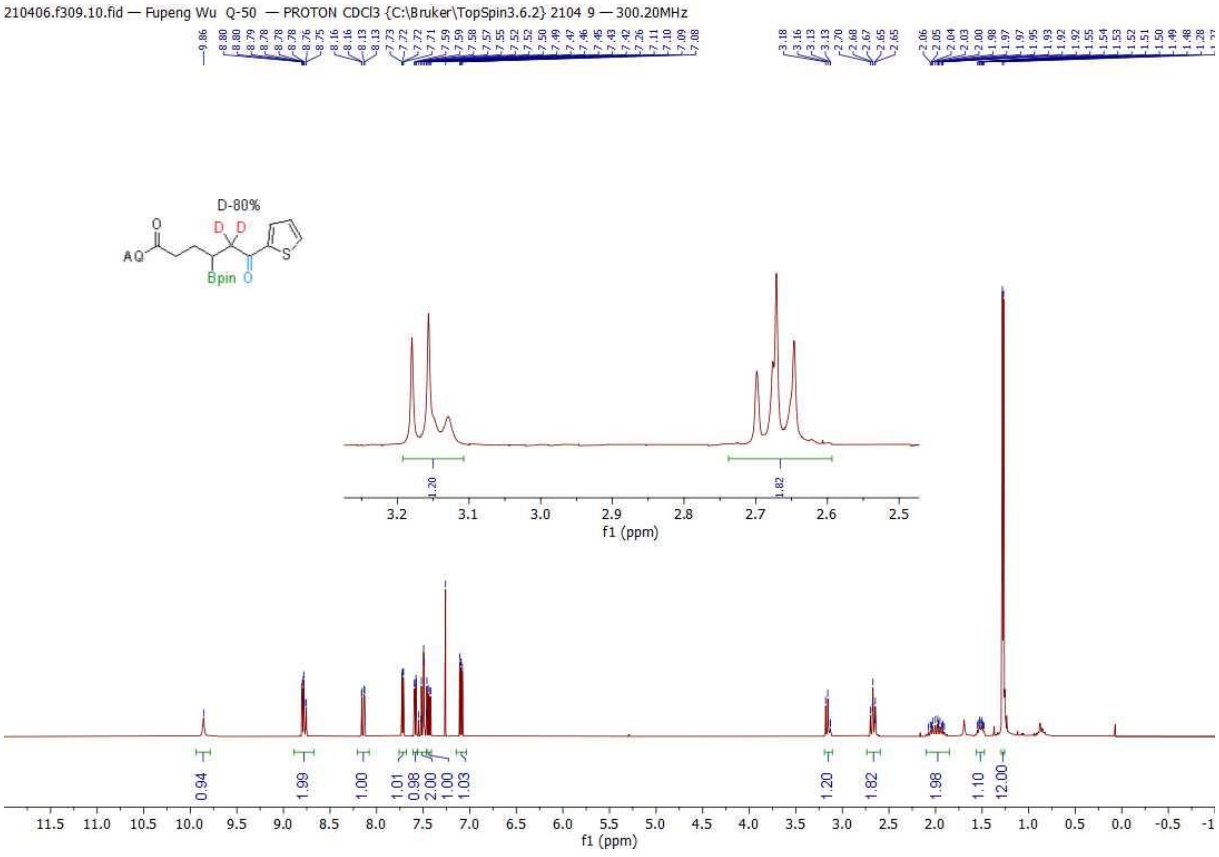


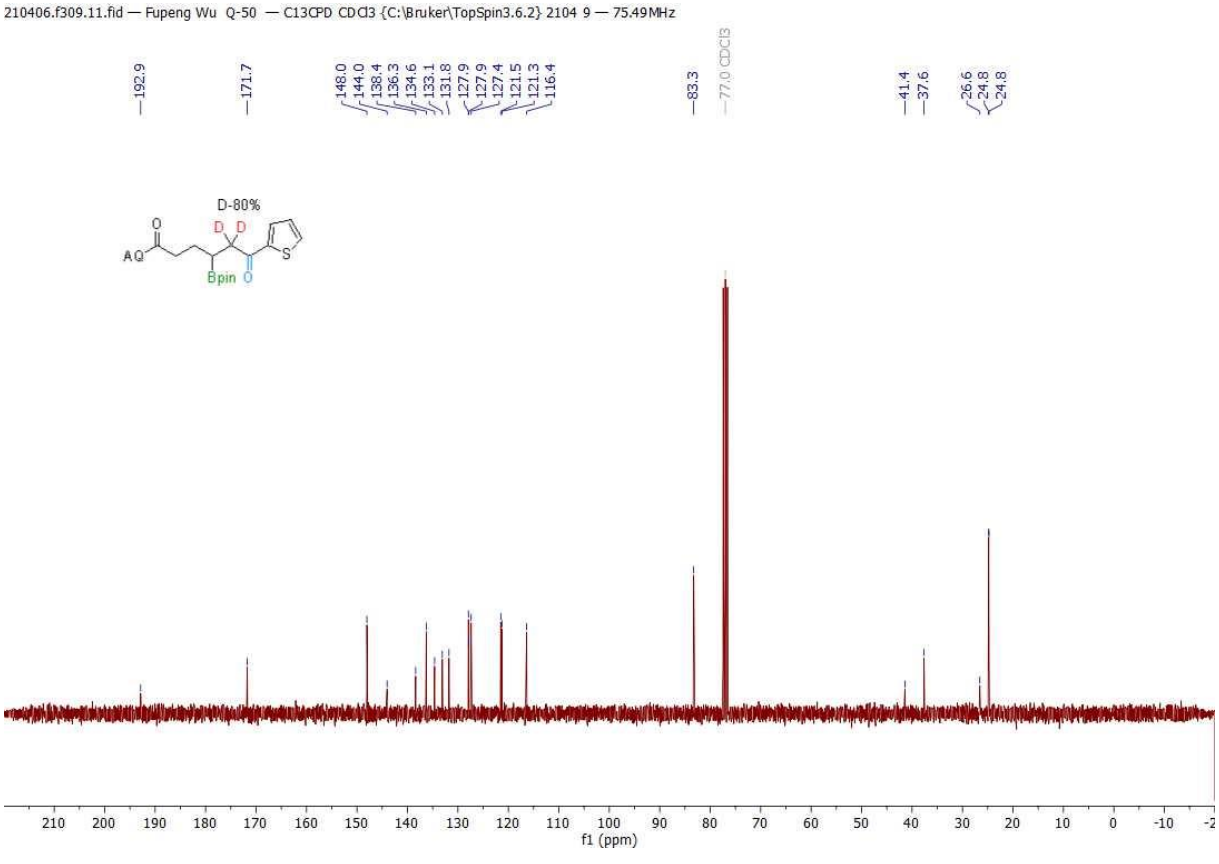

210322.f335.10.fid — Fupeng Wu / Q-T-3 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 35 — 300.20MHz
6d
(1H NMR, 300 MHz, CDCl3)
f1 (ppm)


210322.f335.11.fid — Fupeng Wu / Q-T-3 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2103 35 — 75.49MHz
6d
(13C NMR, 75 MHz, CDCl3)
f1 (ppm)


ESI-TOF Accurate Mass Report
File:21040912
Vial:1:F,7
Description:MeOH/0.1% HCOOH in H2O 90:10
Sample Name:Q-T-5
Date:09-Apr-2021
UserName:Fupeng Wu
Time:16:33:47
Page 2
Sample Report:
(Time: 0.33) Combine (28:32-80:84) - Dead time test passed
1:TOF MS ES+
1.1e+008
349.1182
-0.9 PPM
-0.3 mDa
371.1002
0.8 PPM
0.3 mDa
6d
719.2104
323.1212
372.1027
718.2136
720.2118
305.1110
737.2209
%
m/z


210401.f324.10.fid — Fupeng Wu Q-D — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2104 24 — 300.20MHz
122%
7d
0.39
0.39
1.84
1.88
f1 (ppm)
0.94
1.97
1.00
3.06
0.96
0.39
0.39
1.84
1.88
f1 (ppm)


210406.f309.10.fid — Fupeng Wu Q-50 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2104 9 — 300.20MHz
D-80%
f1 (ppm)


210406.f309.11.fid — Fupeng Wu Q-50 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2104 9 — 75.49MHz
D-80%
77.0 CDCl3
f1 (ppm)