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Supporting Information

Synthesis and Stability Study of Isocyano Aryl Boronate Esters and their Synthetic Applications

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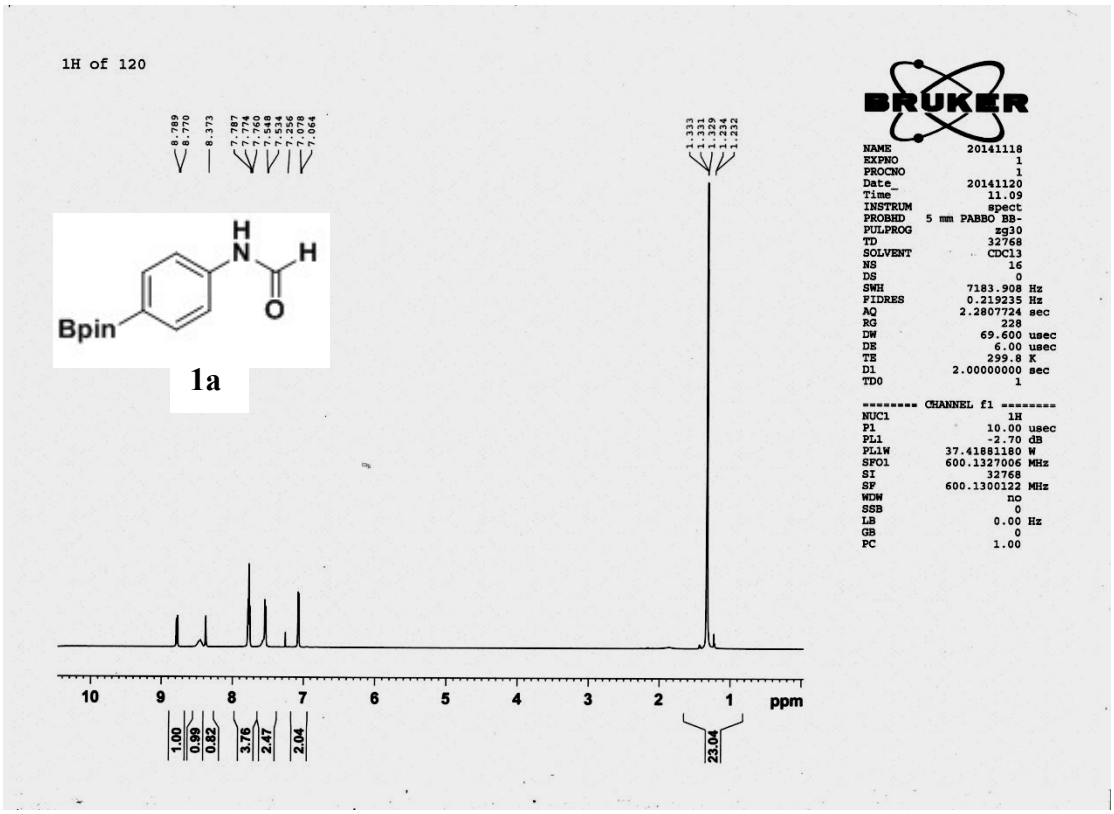
Department of Chemistry, Tamkang University

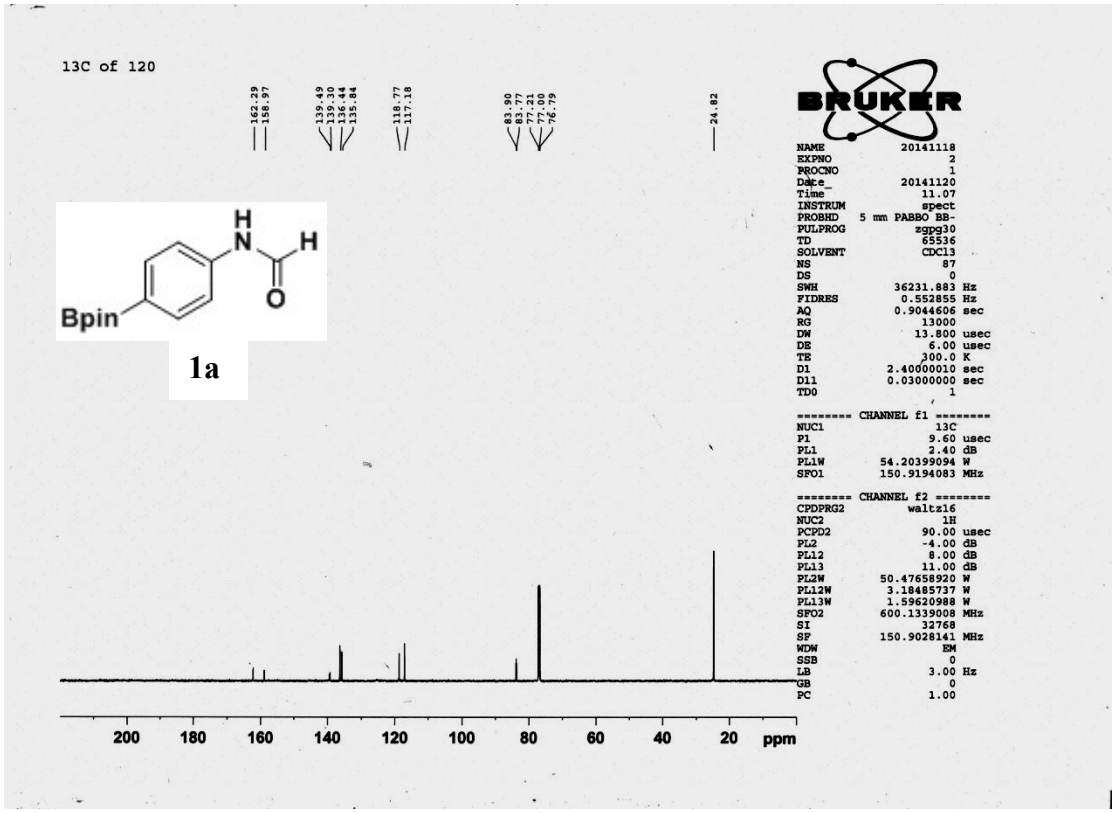
Content

N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)formamide **(1a)**

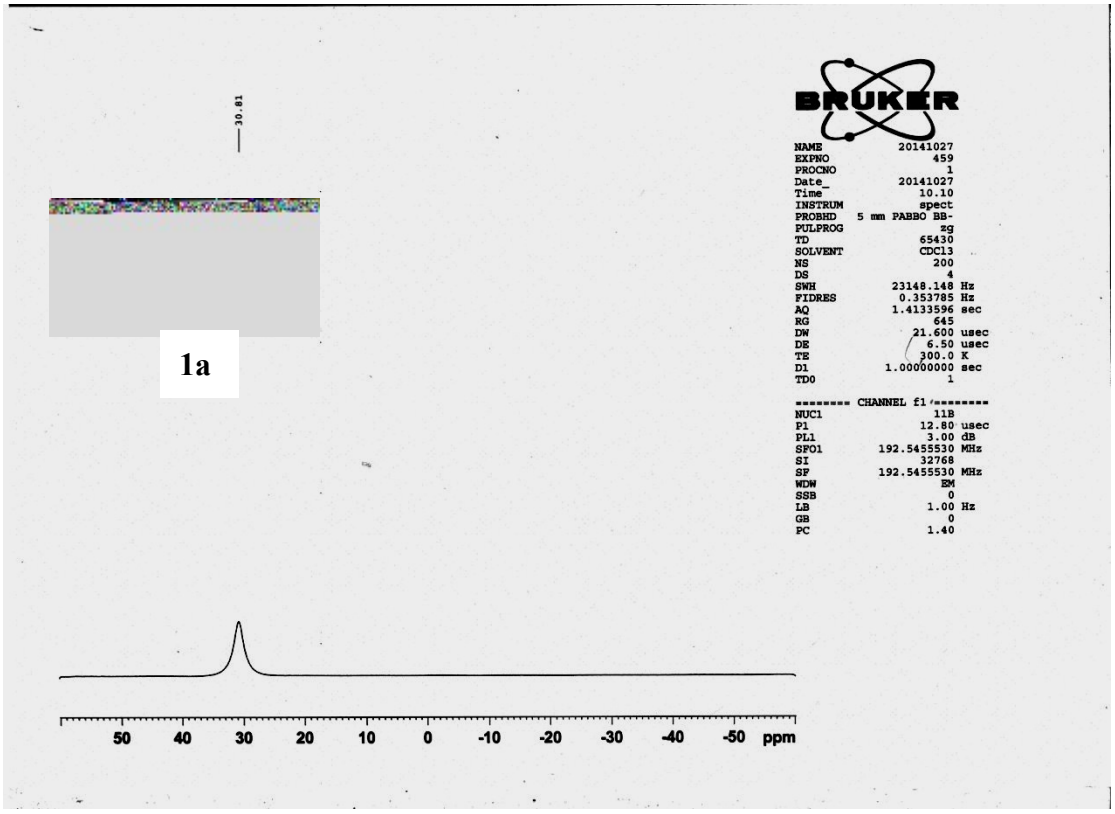
^{1}H-NMR (600 MHz, $CDCl_3$)



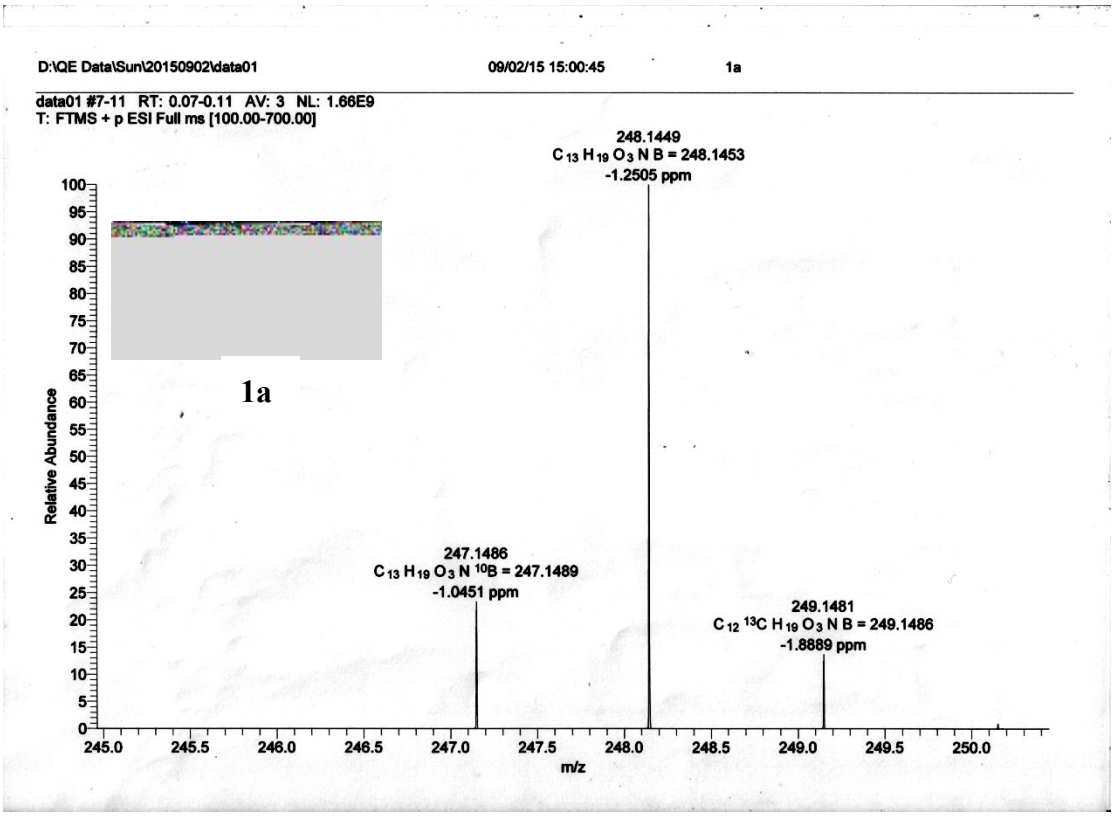
^{13}C-NMR (150 MHz, $CDCl_3$)



^{11}B-NMR (193 MHz, $CDCl_3$)

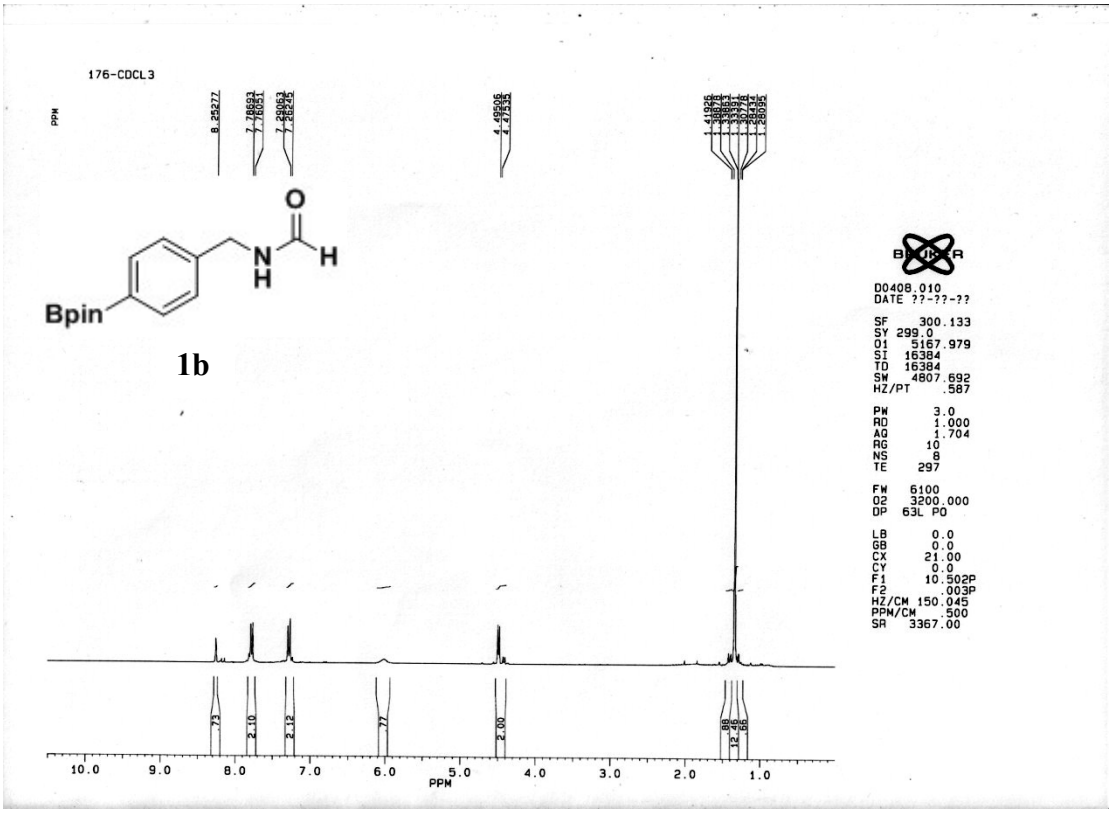


HRMS

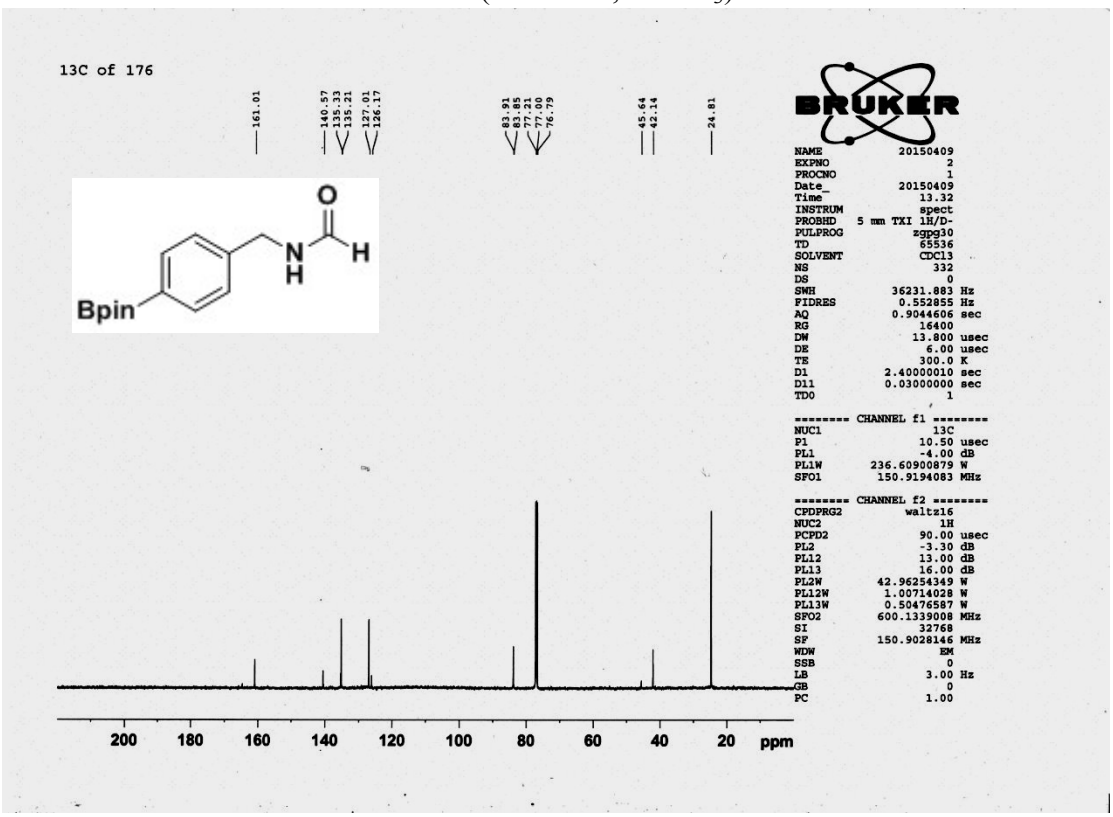


N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)formamide **(1b)**

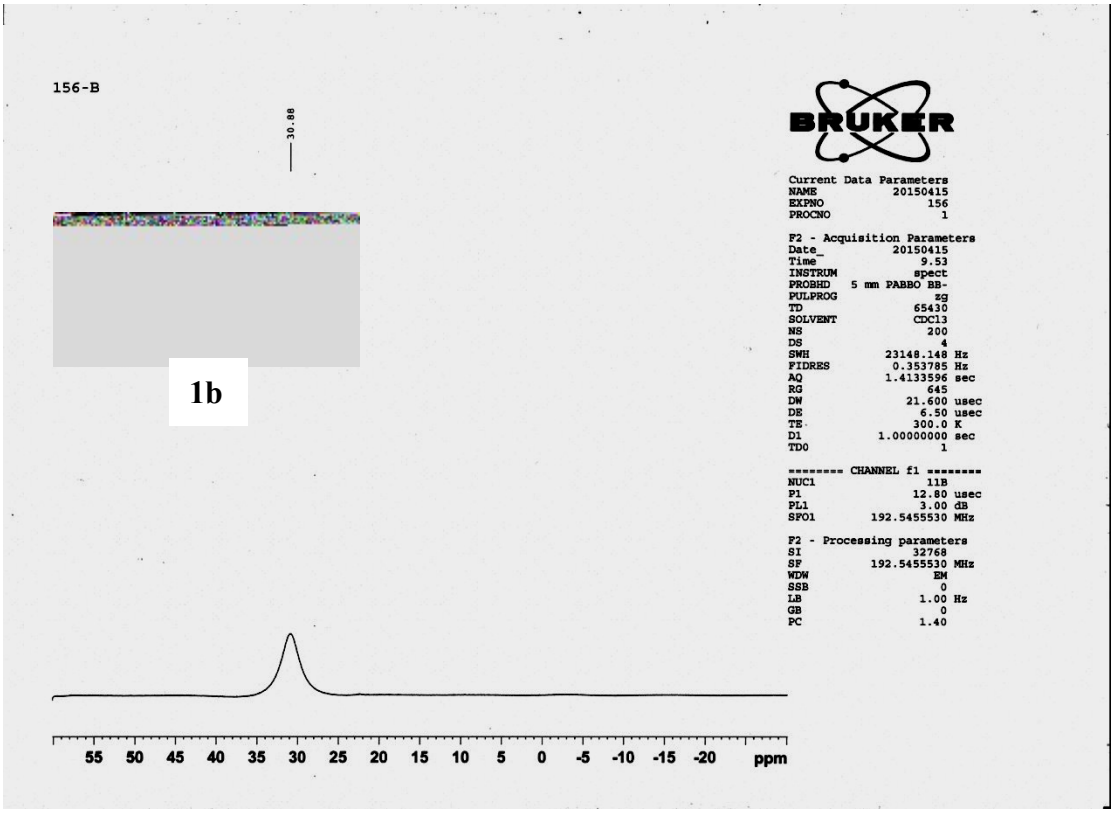
^{1}H-NMR (300 MHz, $CDCl_3$)



^{13}C-NMR (150 MHz, $CDCL_3$)



^{11}B-NMR (193 MHz, $CDCl_3$)



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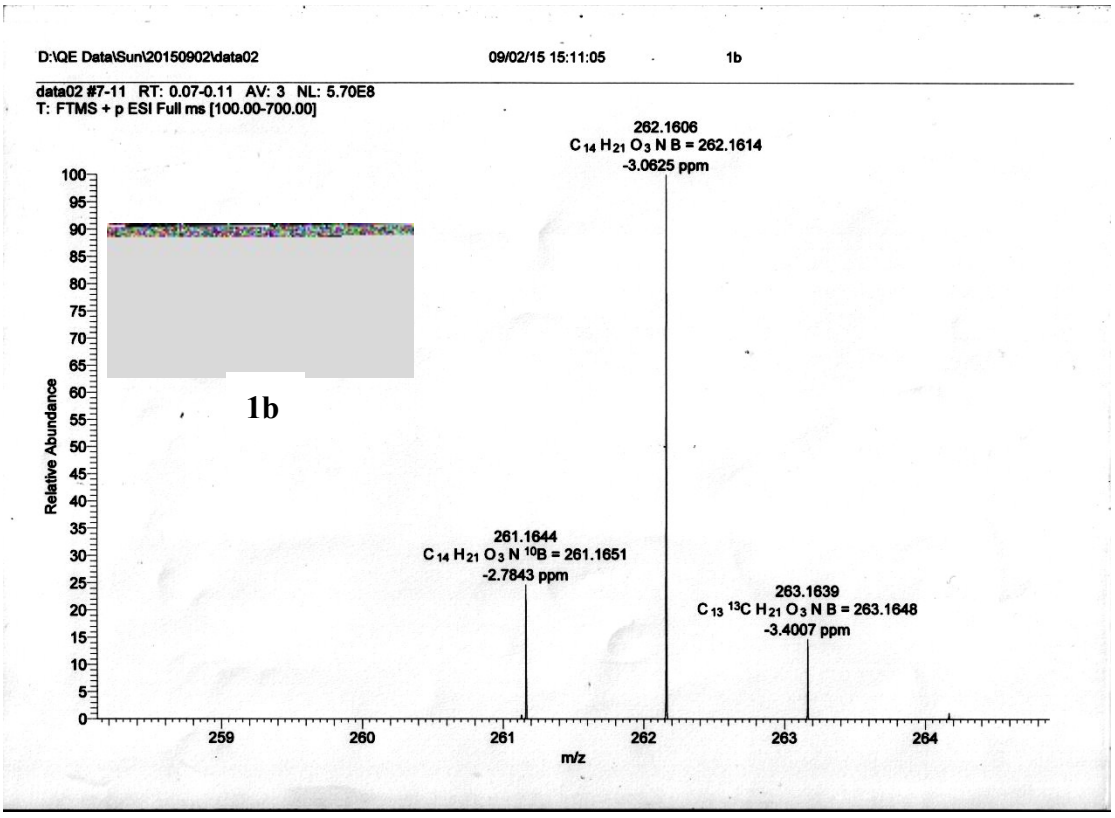
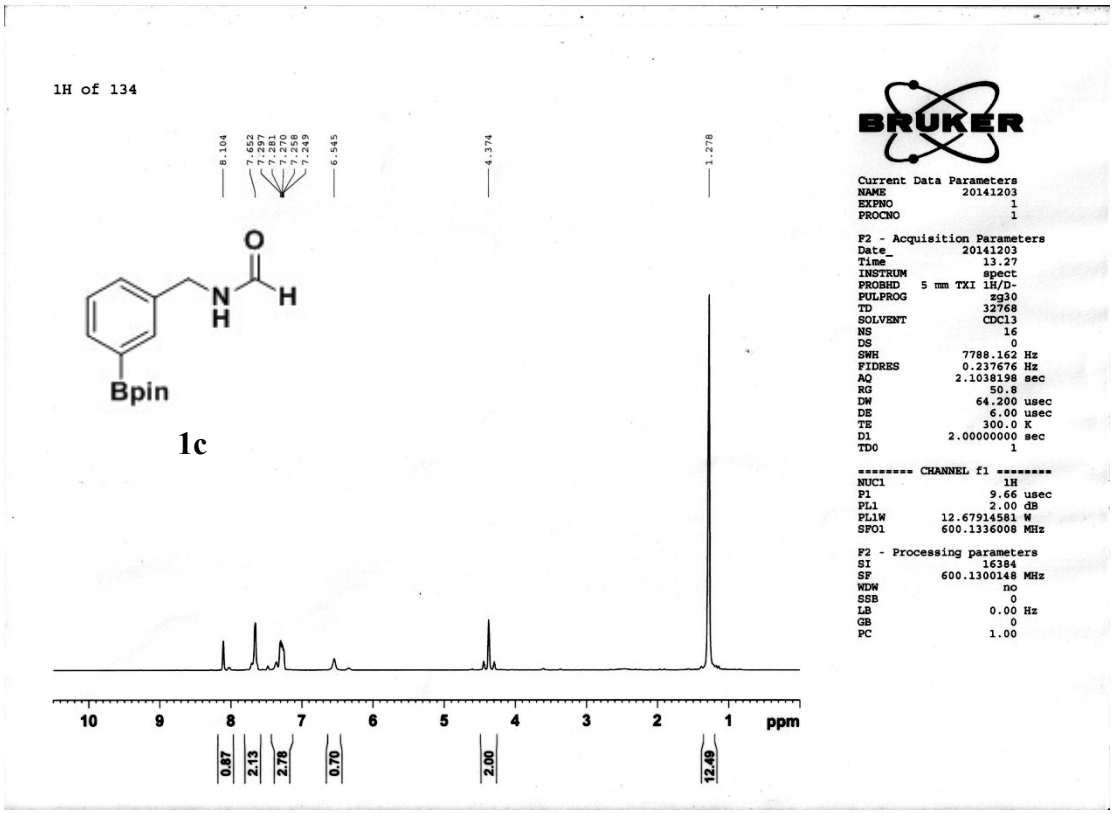
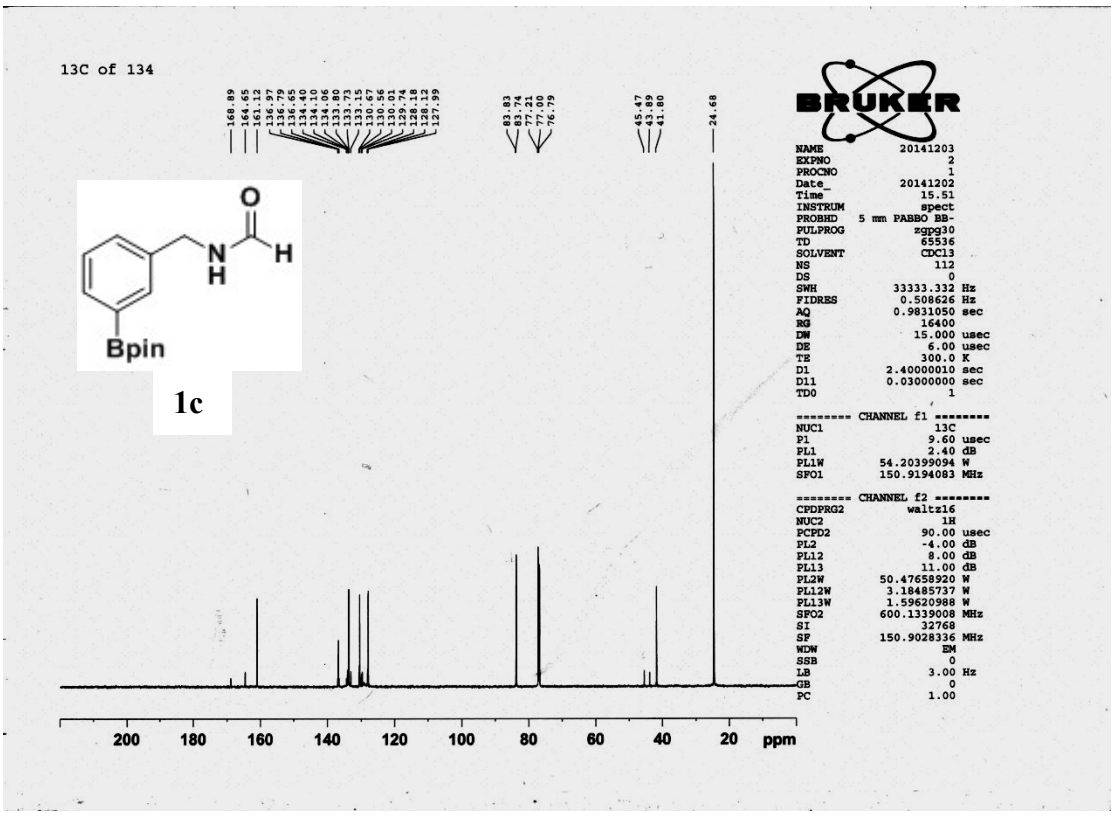


N-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)formamide **(1c)**

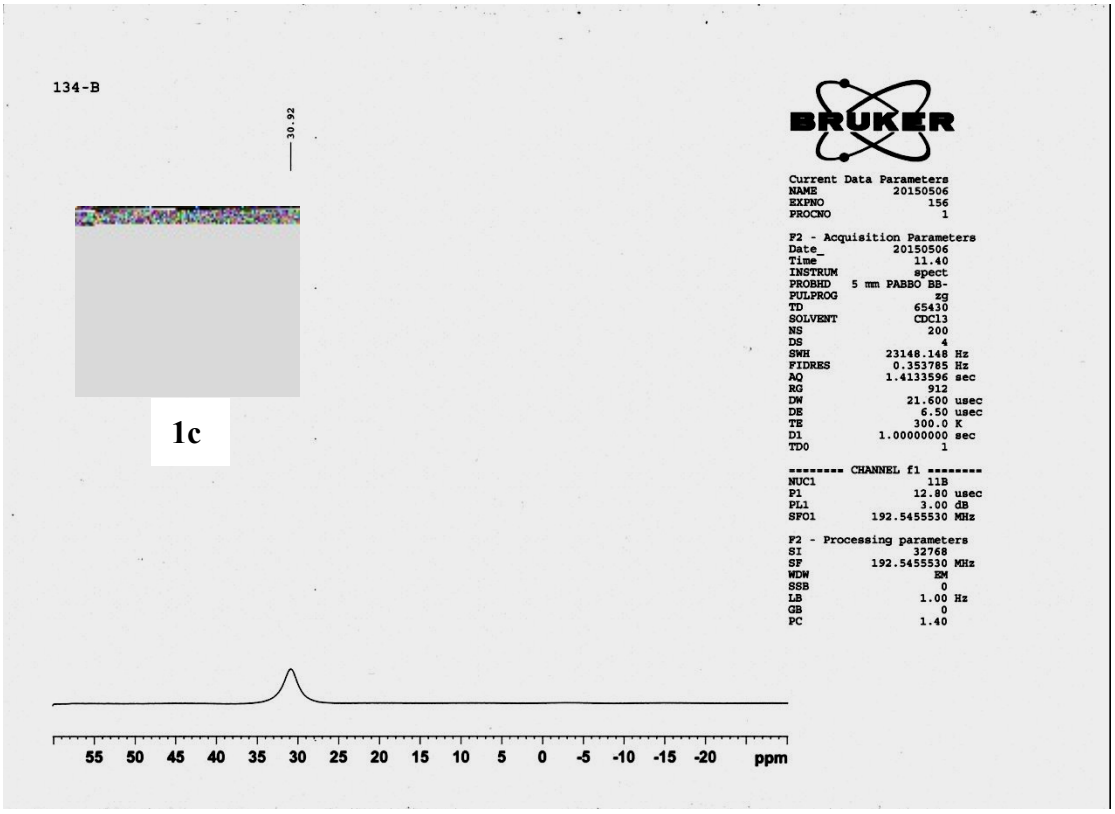
^{1}H-NMR (600 MHz, $CDCl_3$)



^{13}C-NMR (150 MHz, $CDCl_3$)



^{11}B-NMR (193 MHz, $CDCl_3$)



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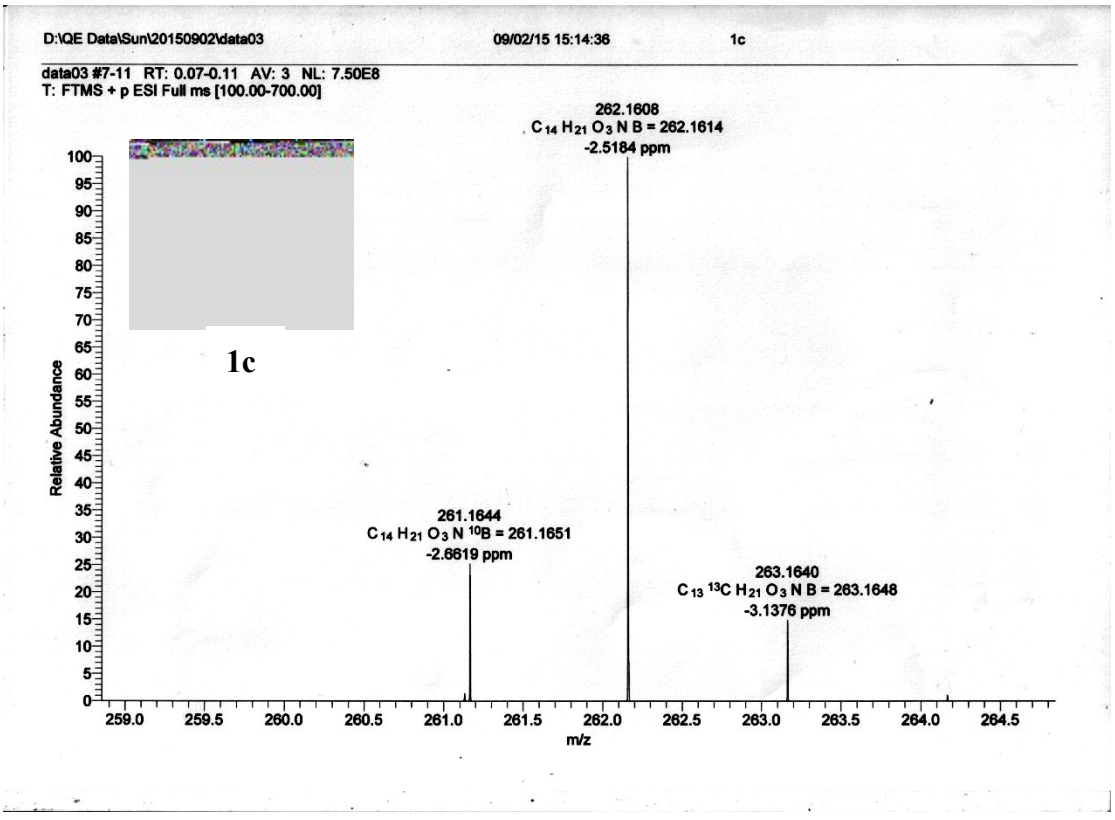
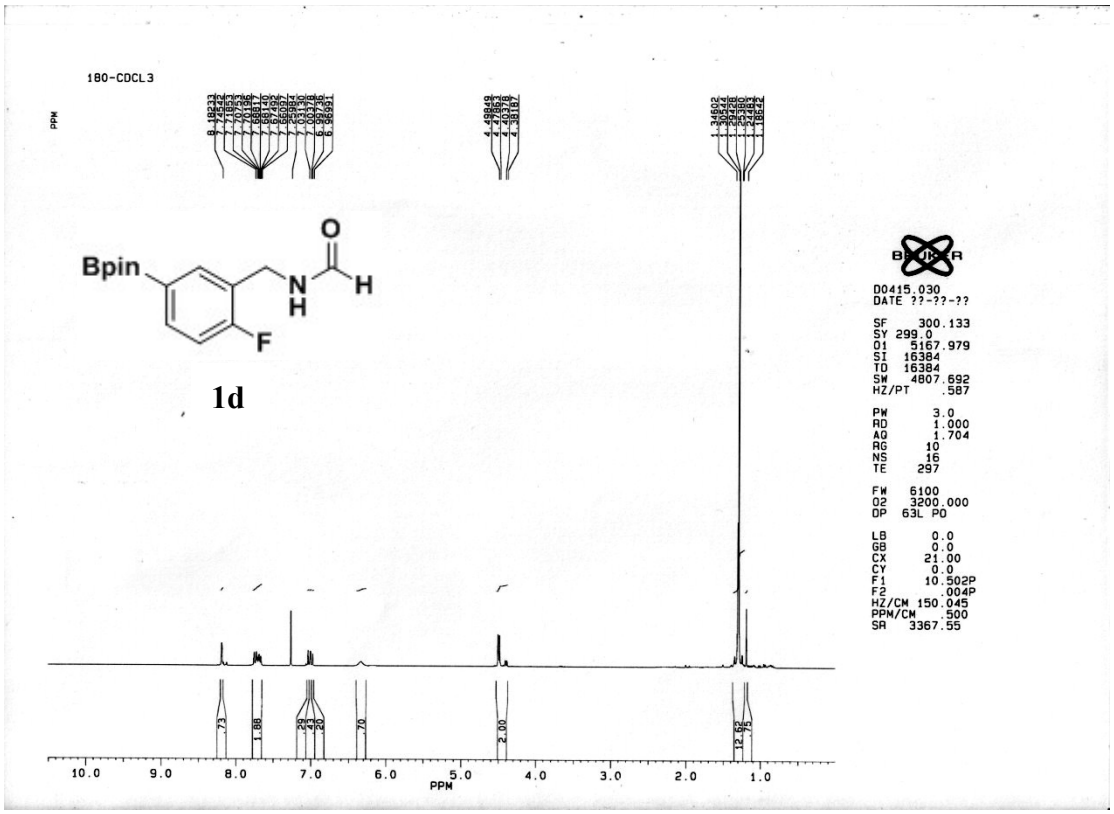
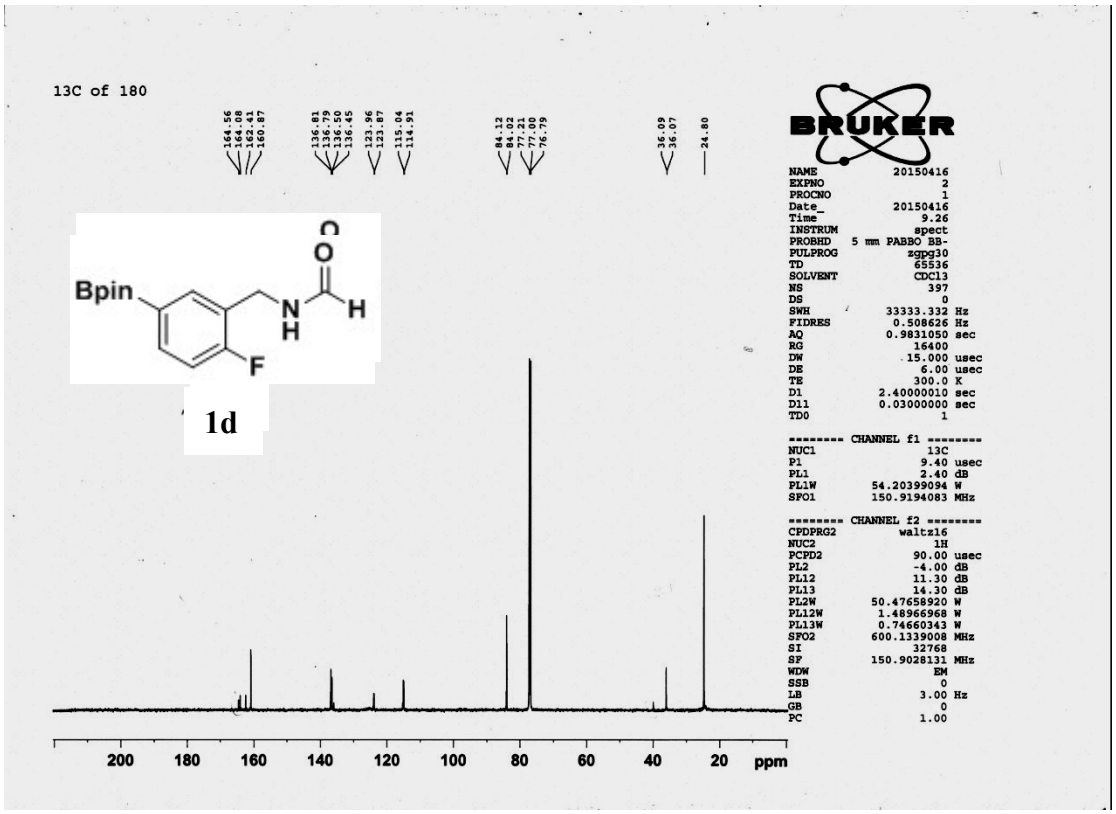


N-(2-fluoro-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)formamide **(1d)**

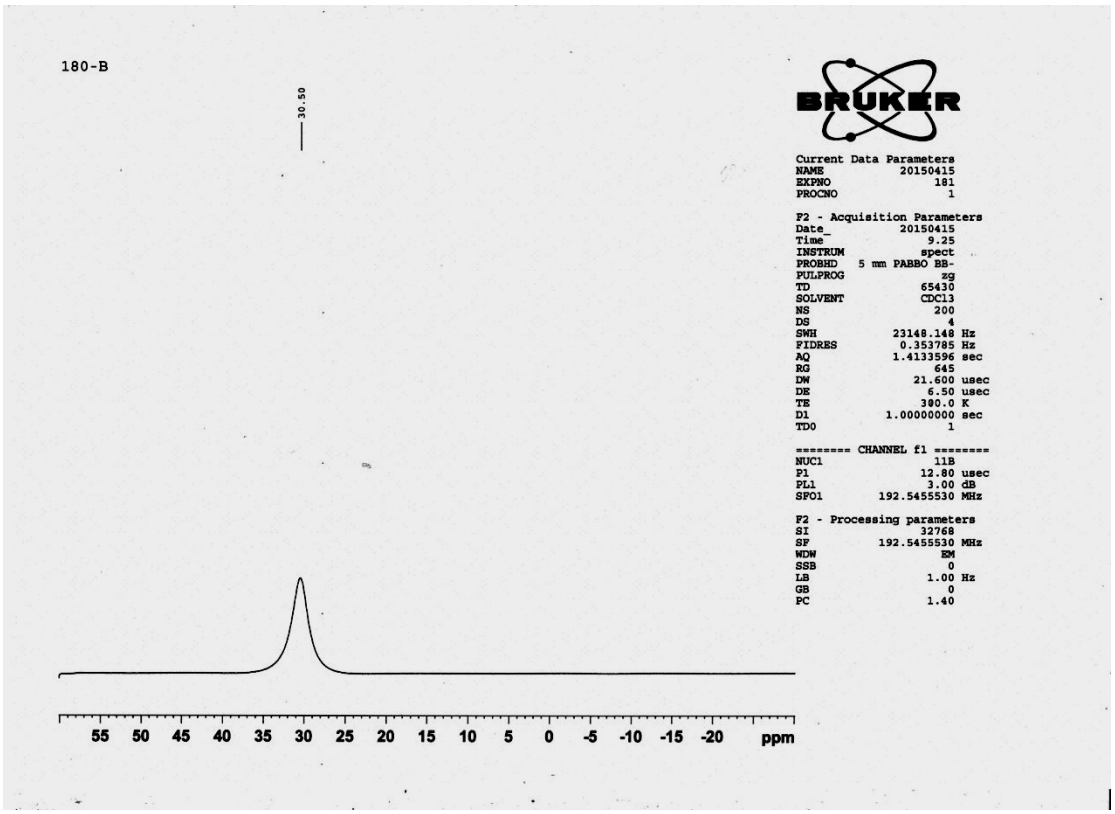
^{1}H-NMR (300 MHz, $CDCl_3$)



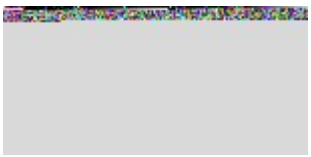
^{13}C-NMR (150 MHz, $CDCl_3$)



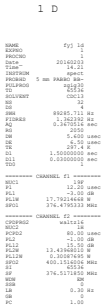
^{11}B-NMR (193 MHz, $CDCl_3$)

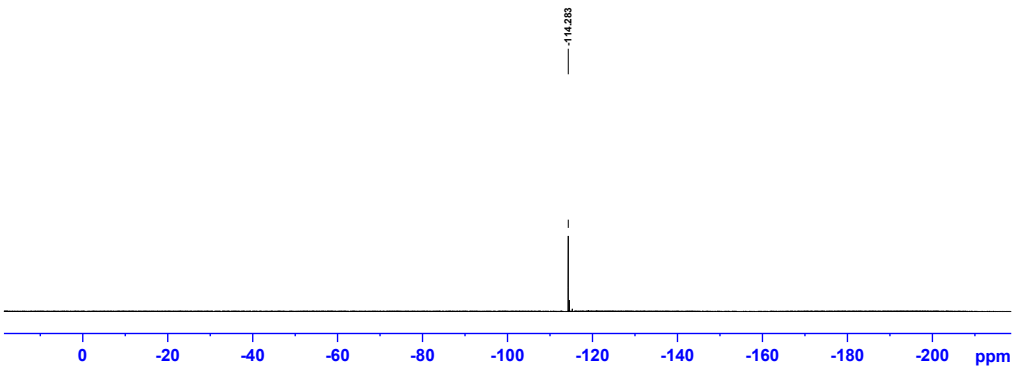


^{19}F-NMR

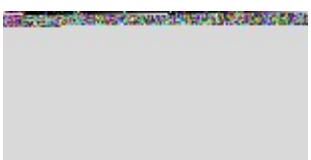


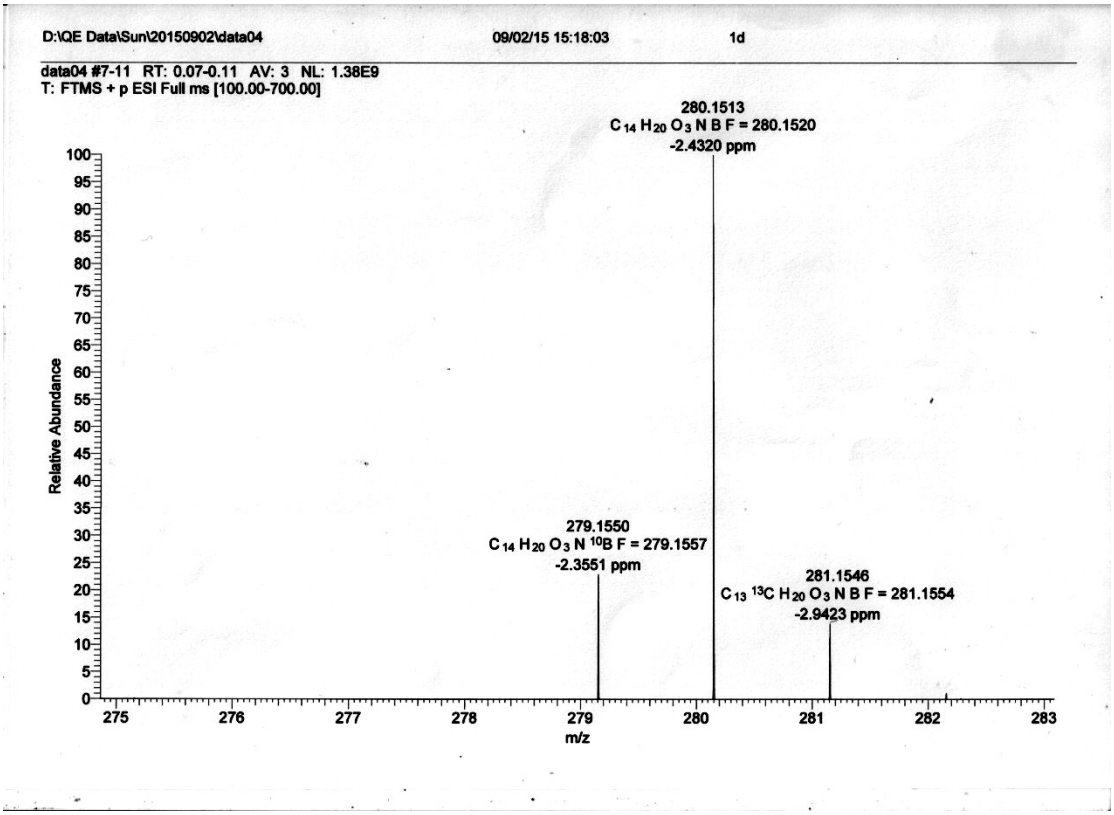
1d





HRMS

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1d
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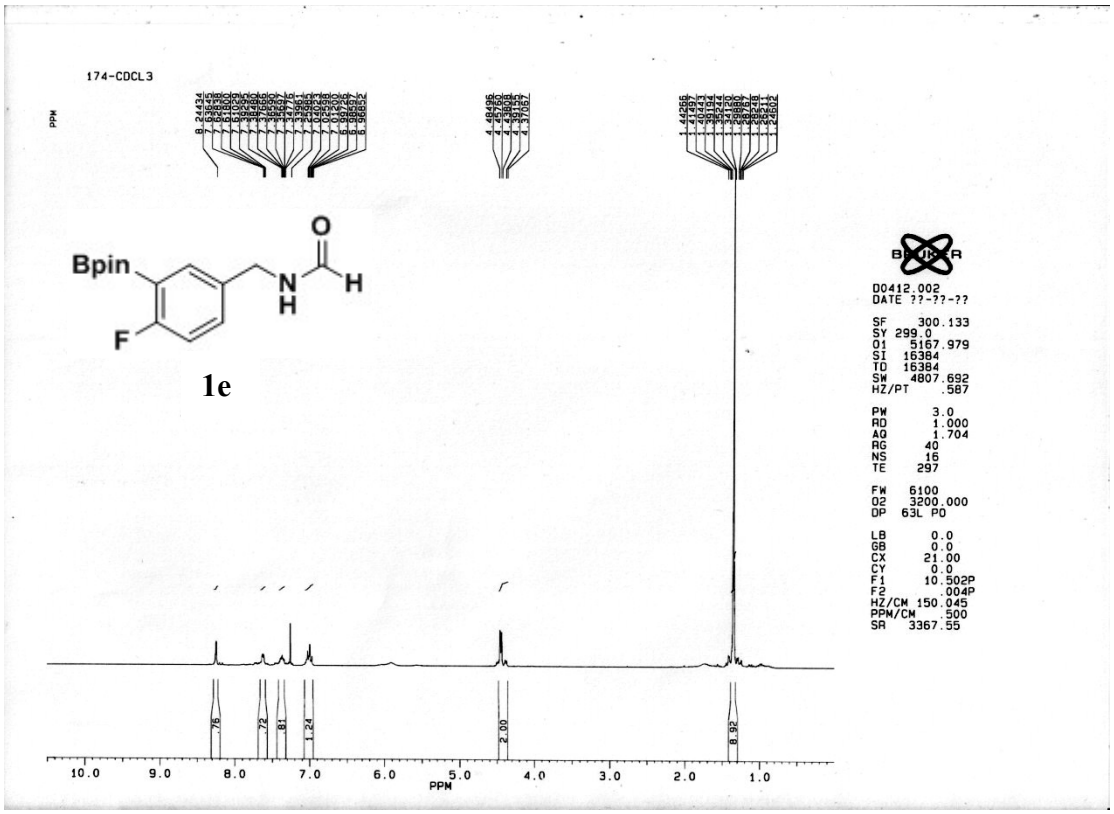
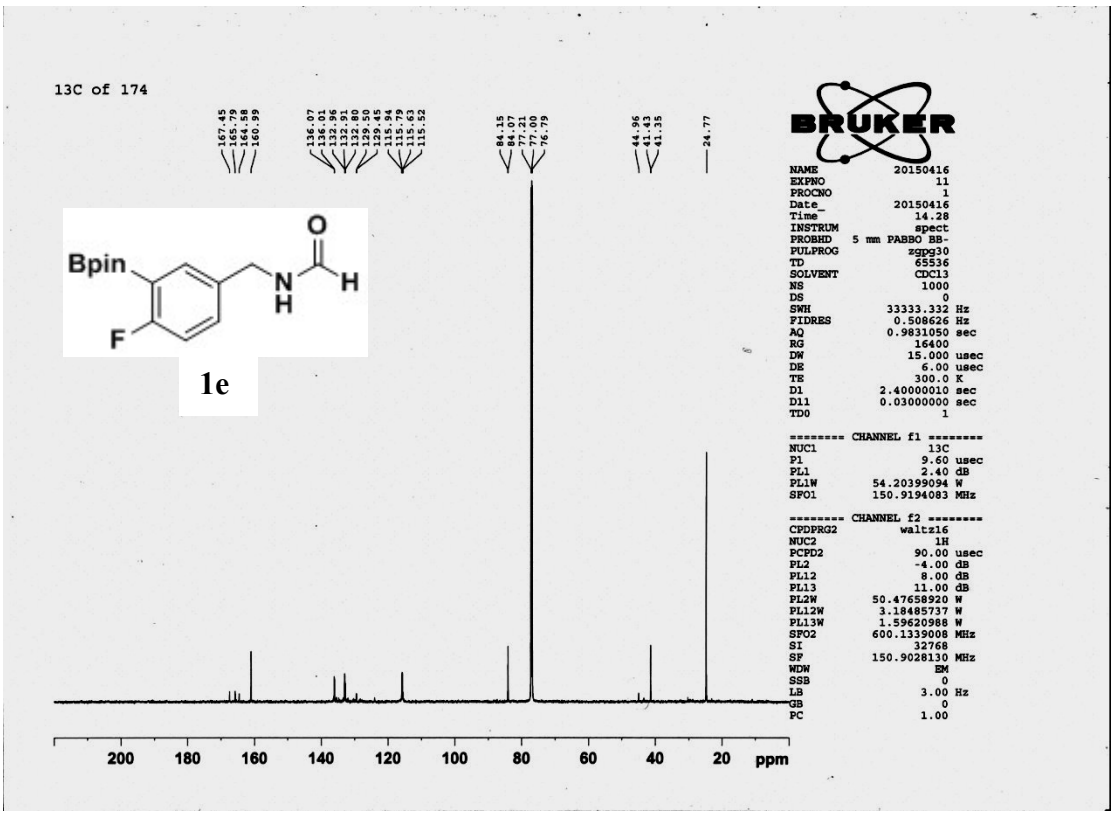
T: FTMS + p ESI Full ms [100.00-700.00]
280.1513
C 14 H 20 O 3 N B F = 280.1520
-2.4320 ppm
279.1550
C 14 H 20 O 3 N 10B F = 279.1557
-2.3551 ppm
281.1546
C 13 13C H 20 O 3 N B F = 281.1554
-2.9423 ppm
Relative Abundance
m/z

N-(4-fluoro-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)formamide **(1e)**

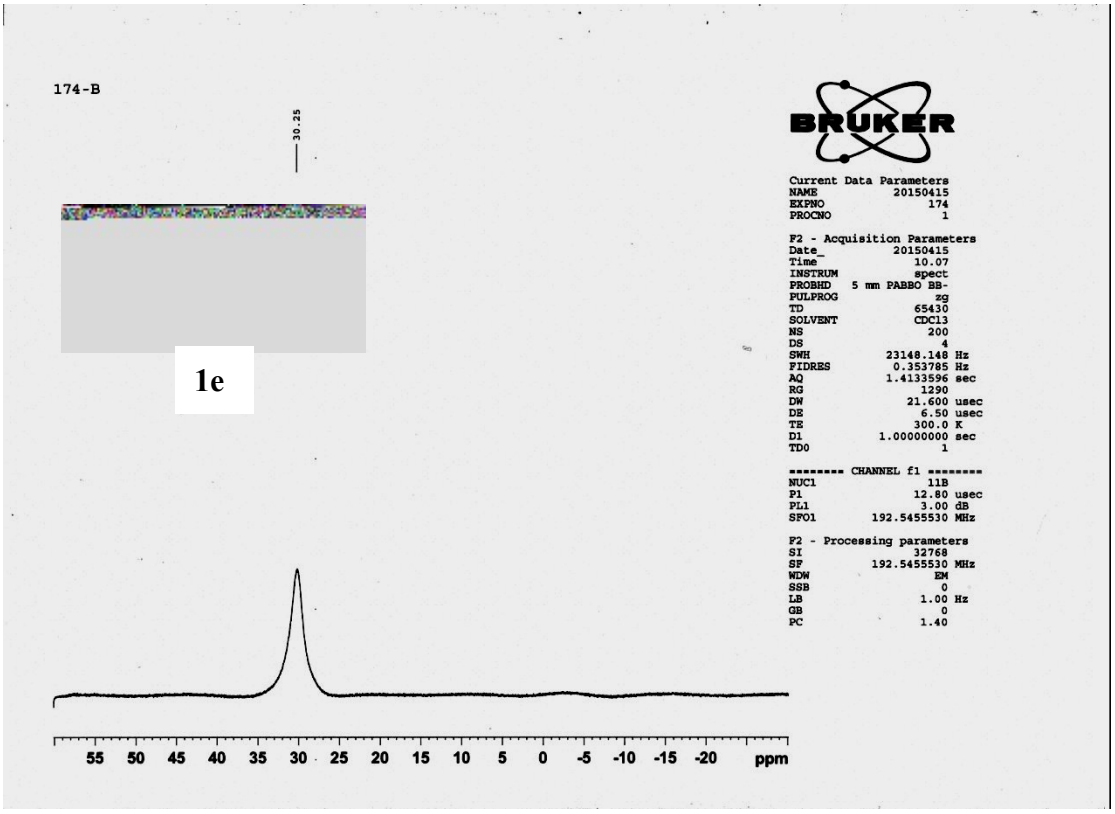
^{1}H-NMR (300 MHz, $CDCl_3$)



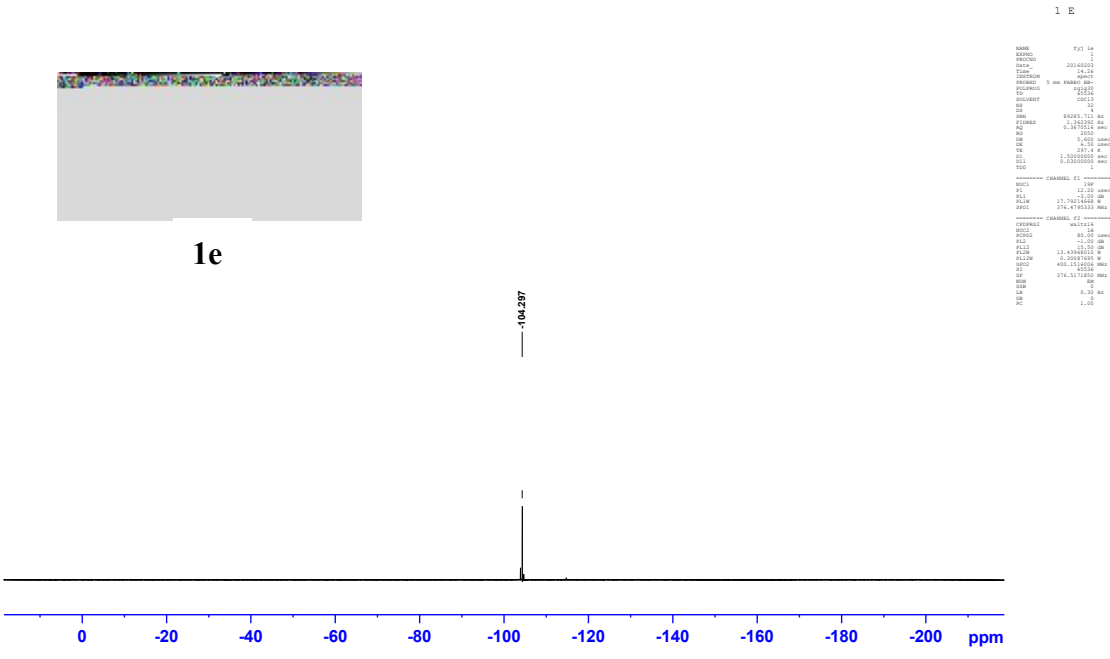
^{13}C-NMR (150 MHz, $CDCl_3$)



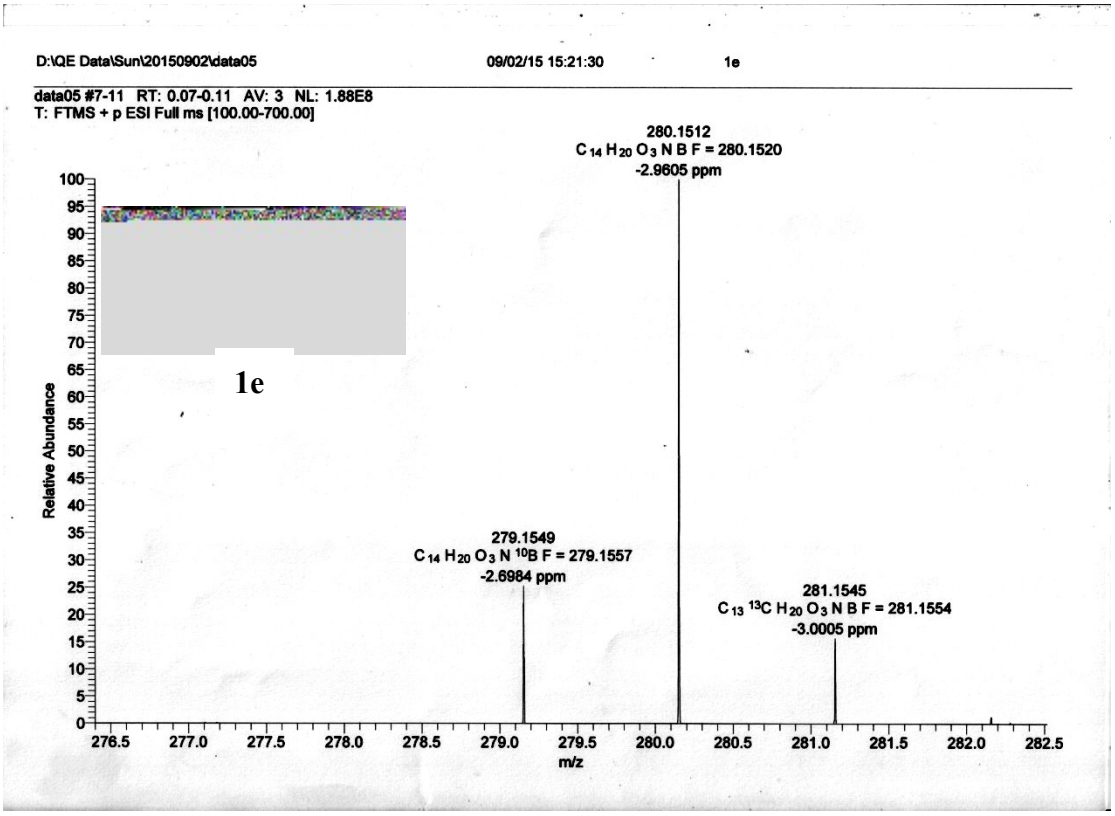
^{11}B-NMR (193 MHz, $CDCl_3$)



^{19}F-NMR



HRMS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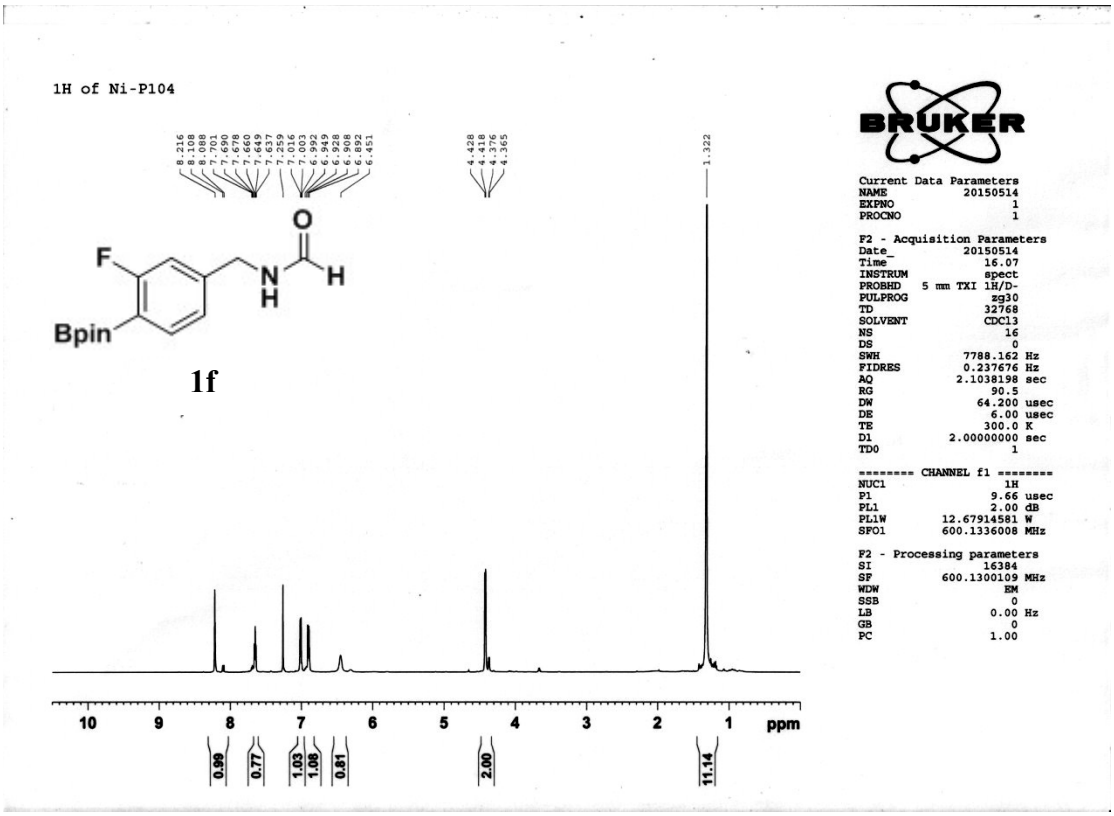
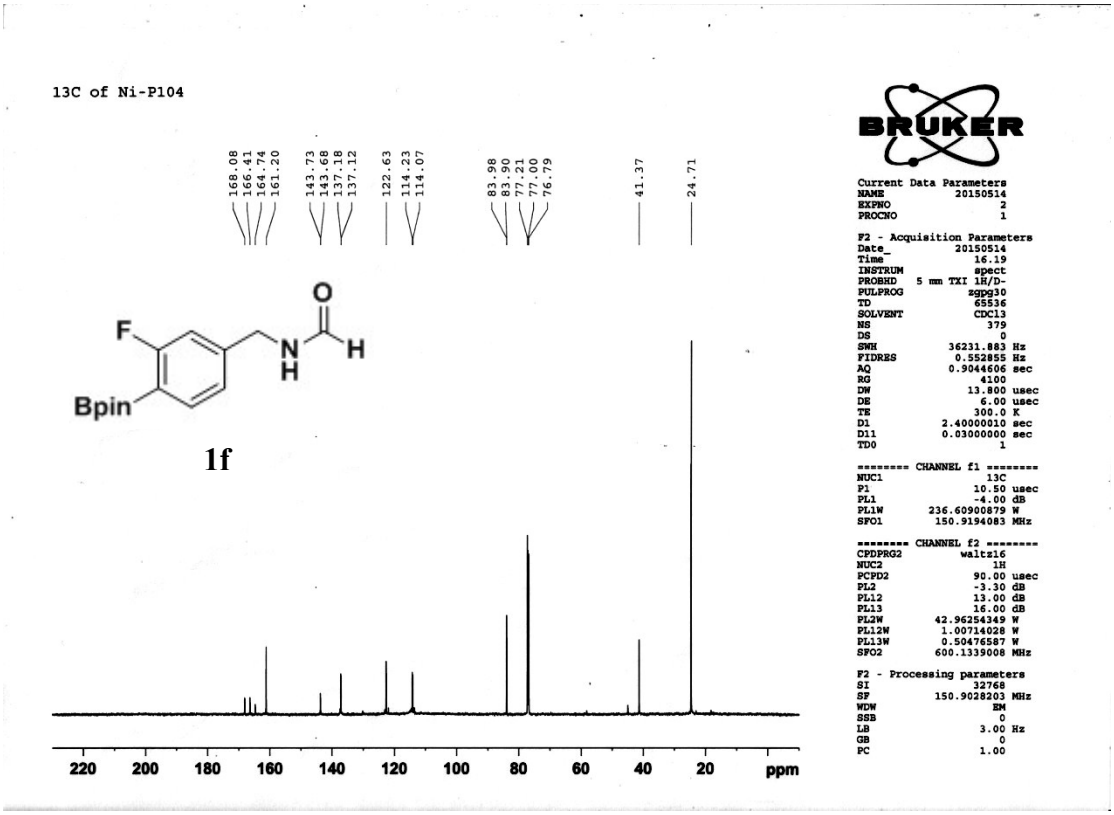
1e
data05 #7-11 RT: 0.07-0.11 AV: 3 NL: 1.88E8
T: FTMS + p ESI Full ms [100.00-700.00]
280.1512
C 14 H 20 O 3 N B F = 280.1520
-2.9605 ppm
279.1549
C 14 H 20 O 3 N 10B F = 279.1557
-2.6984 ppm
281.1545
C 13 13C H 20 O 3 N B F = 281.1554
-3.0005 ppm
1e
Relative Abundance
m/z

N-(3-fluoro-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)formamide **(1f)**

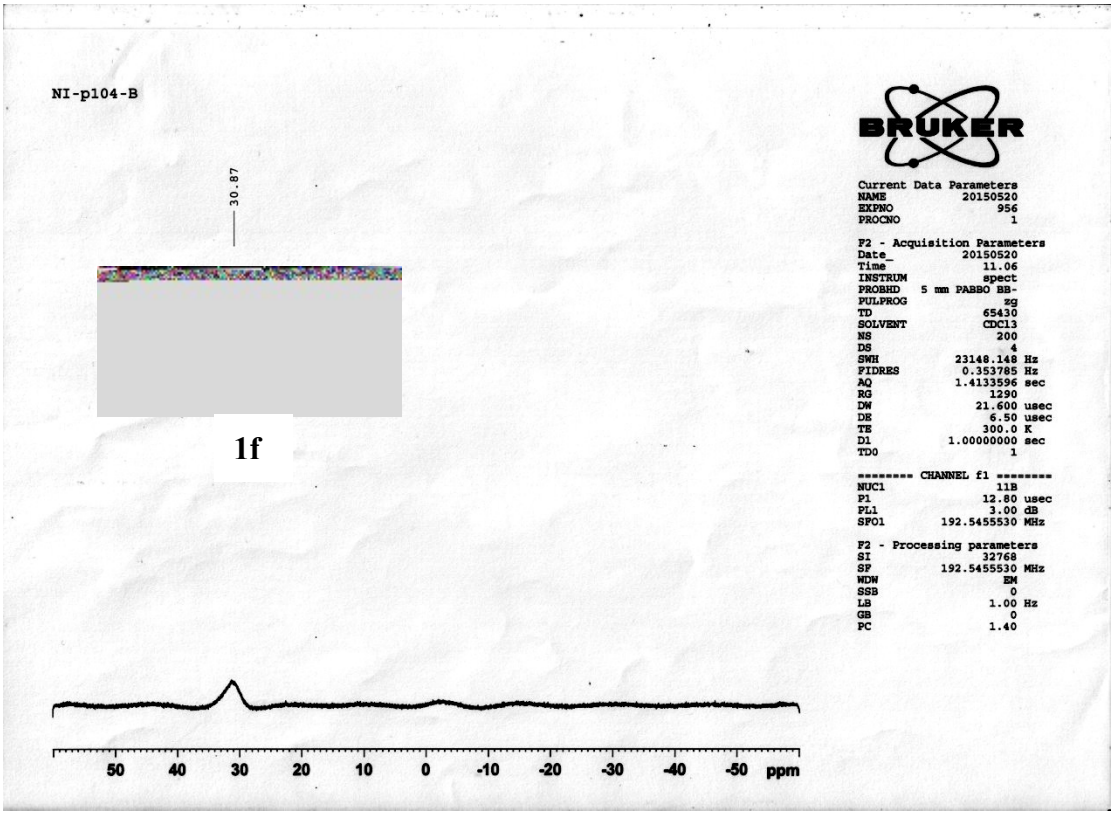
^{1}H-NMR (600 MHz, $CDCl_3$)



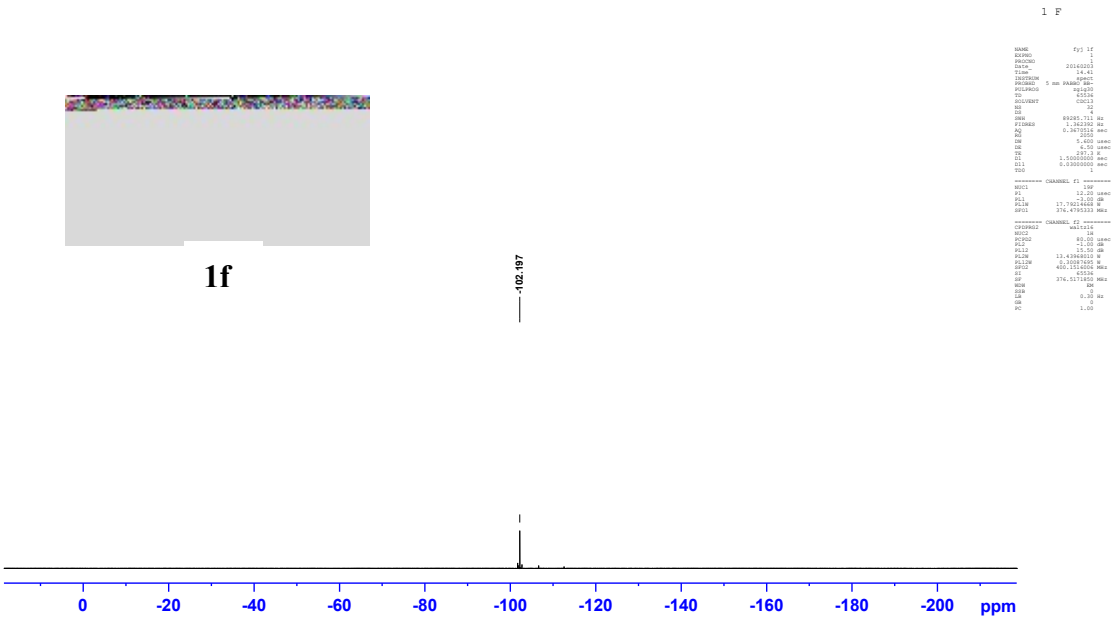
^{13}C-NMR (150 MHz, $CDCl_3$)



^{11}B-NMR (193 MHz, $CDCl_3$)



^{19}F-NMR



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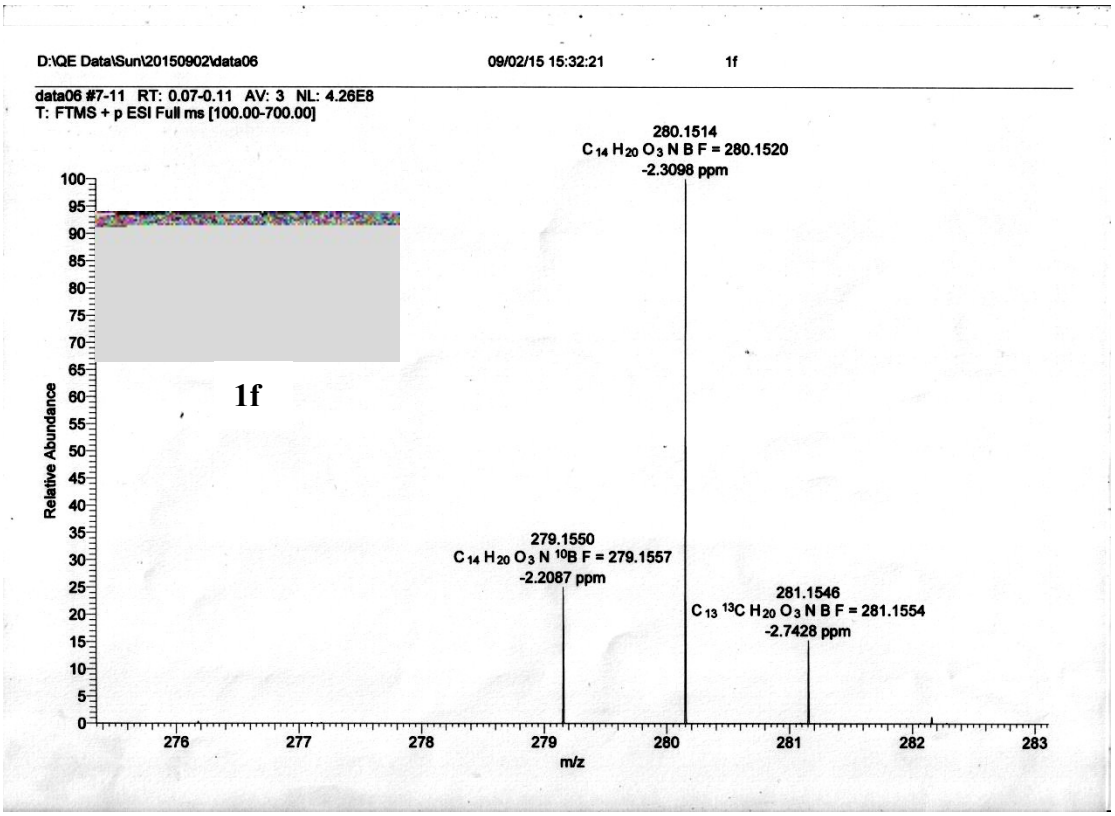
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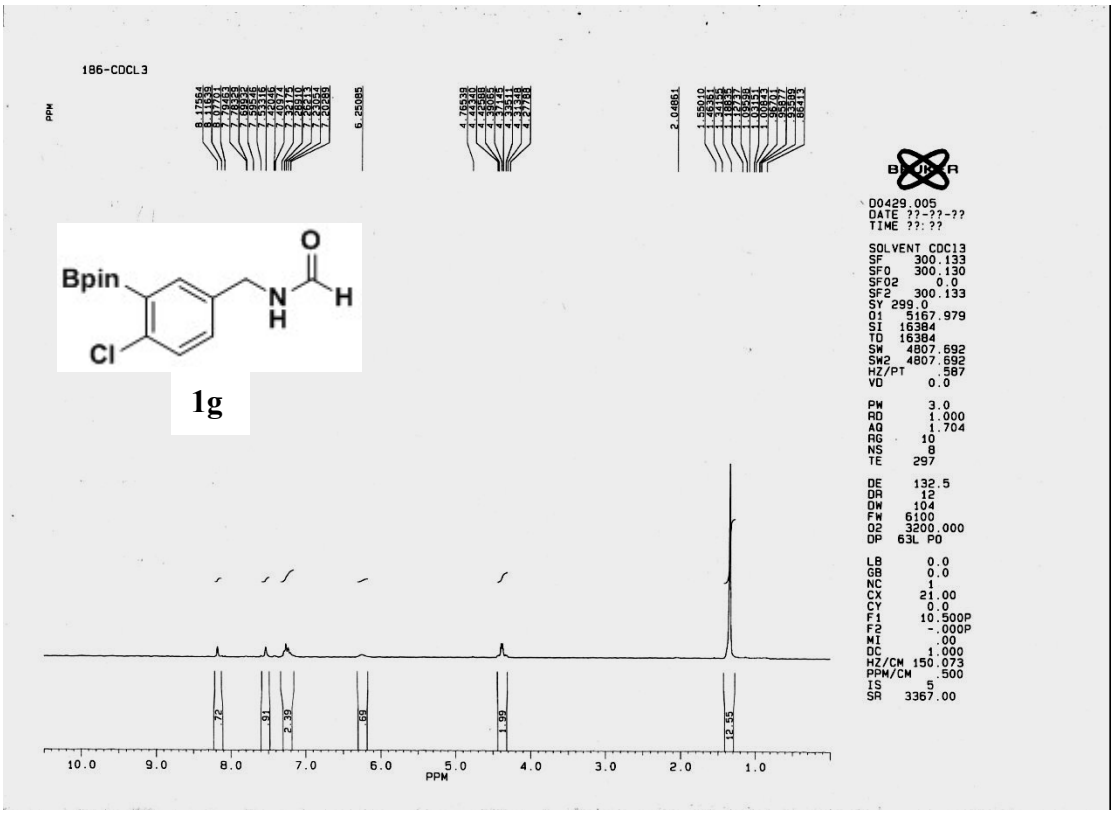
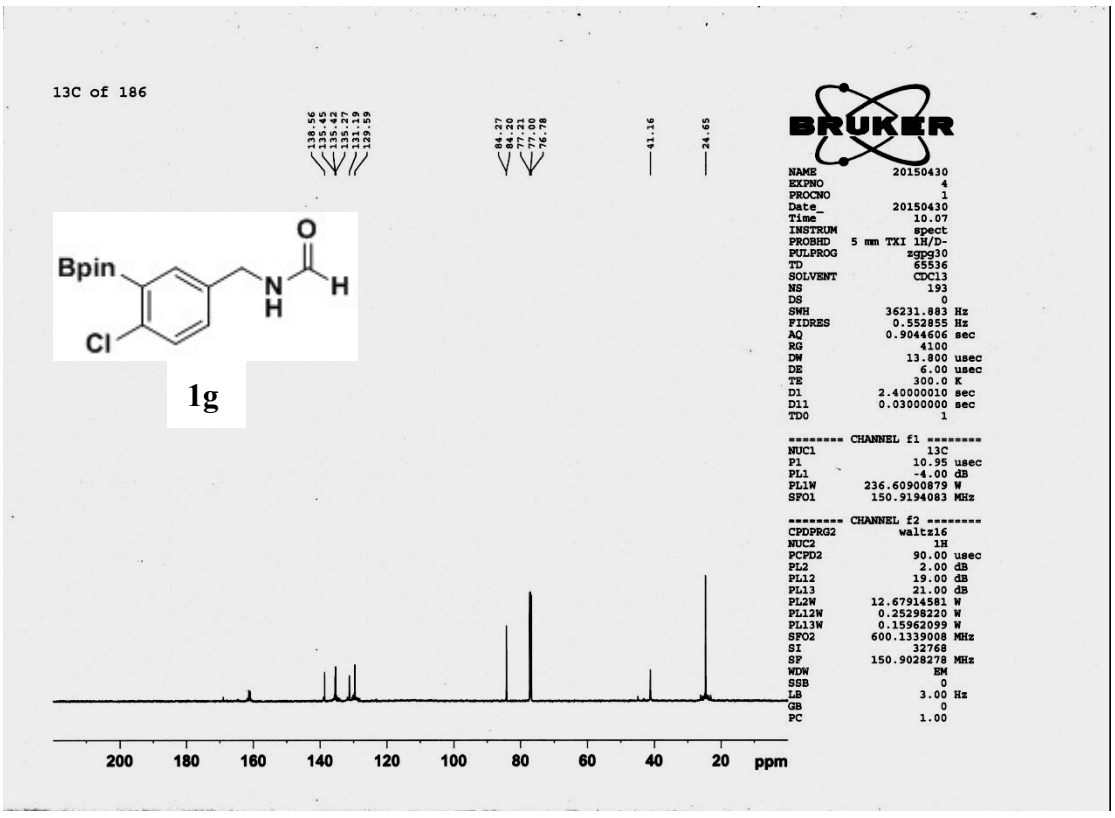
09/02/15 15:32:21
1f
data06 #7-11 RT: 0.07-0.11 AV: 3 NL: 4.26E8
T: FTMS + p ESI Full ms [100.00-700.00]
280.1514
C 14 H 20 O 3 N B F = 280.1520
-2.3098 ppm
1f
279.1550
C 14 H 20 O 3 N 10B F = 279.1557
-2.2087 ppm
281.1546
C 13 13C H 20 O 3 N B F = 281.1554
-2.7428 ppm
Relative Abundance
m/z

N-(4-chloro-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)formamide **(1g)**

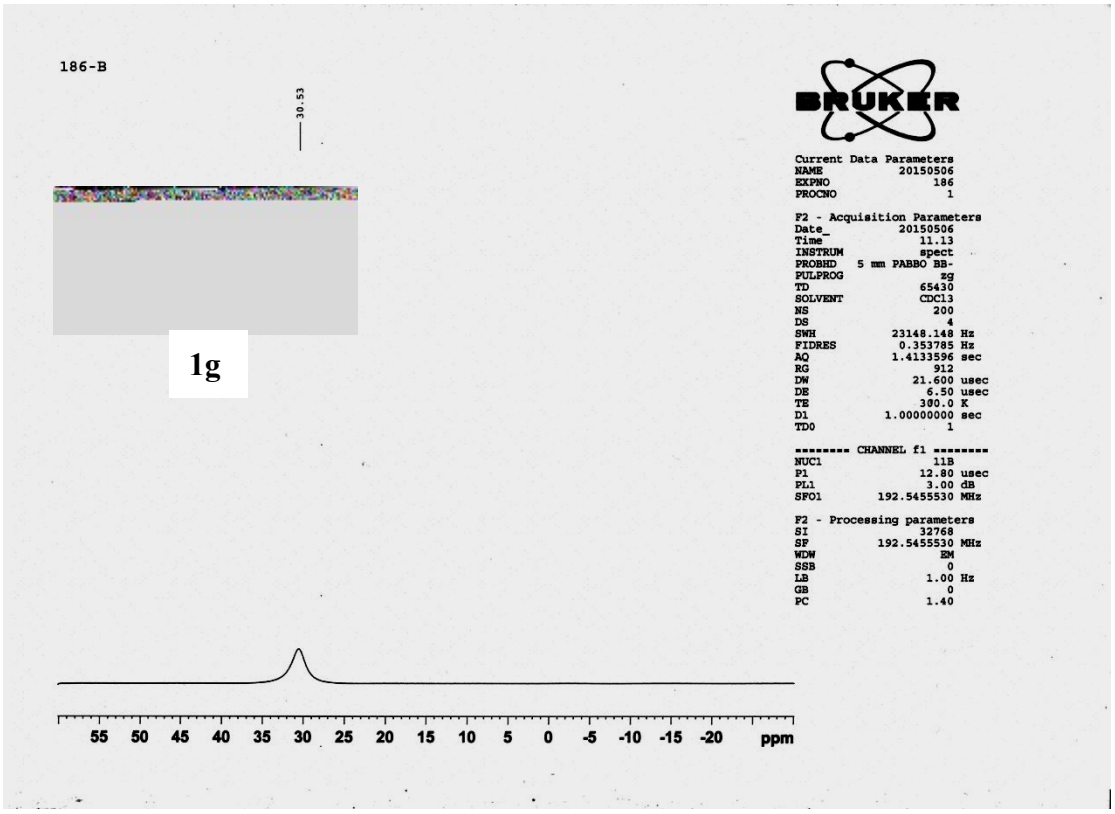
^{1}H-NMR (300 MHz, $CDCl_3$)



^{13}C-NMR (150 MHz, $CDCl_3$)

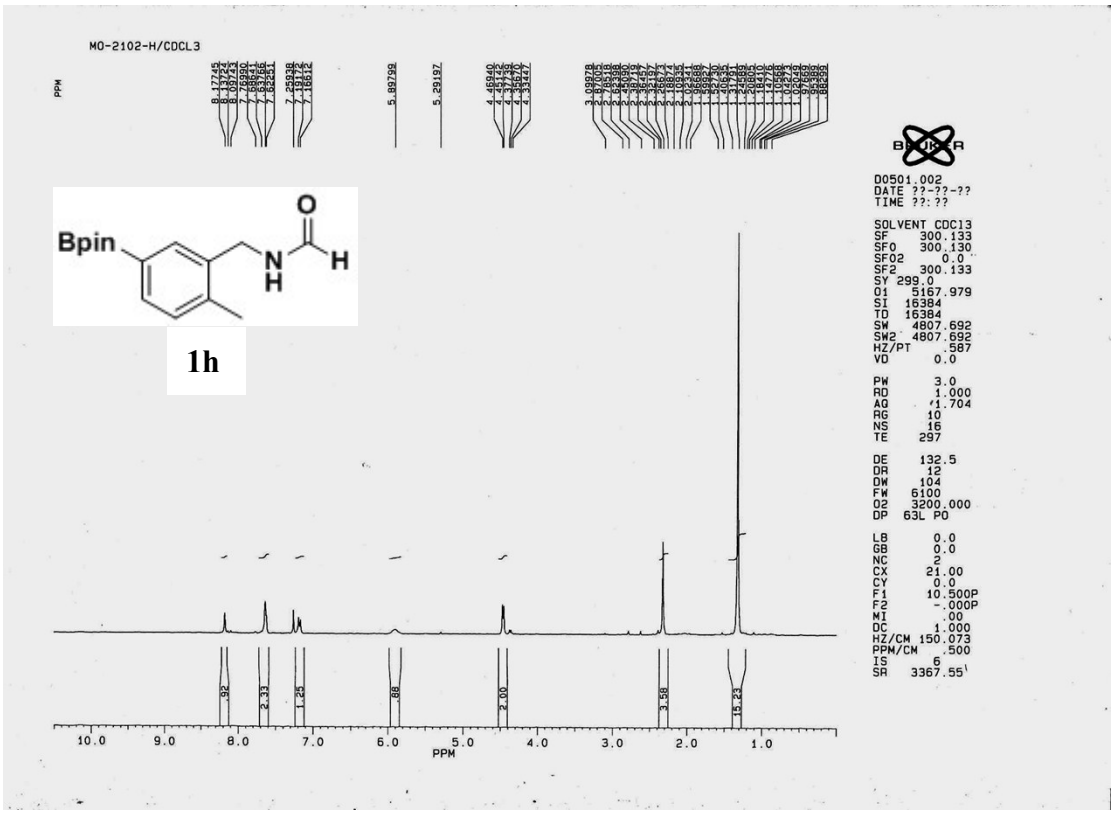


^{11}B-NMR (193 MHz, $CDCl_3$)

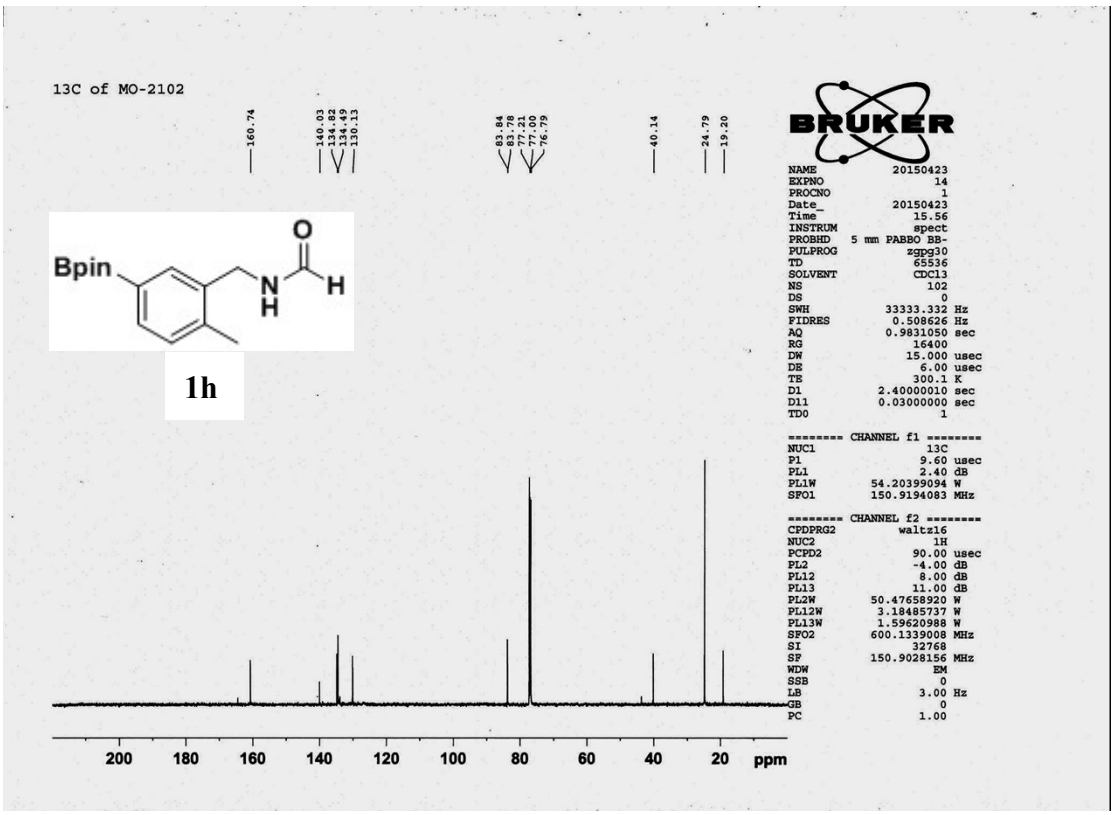


N-(2-methyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)formamide **(1h)**

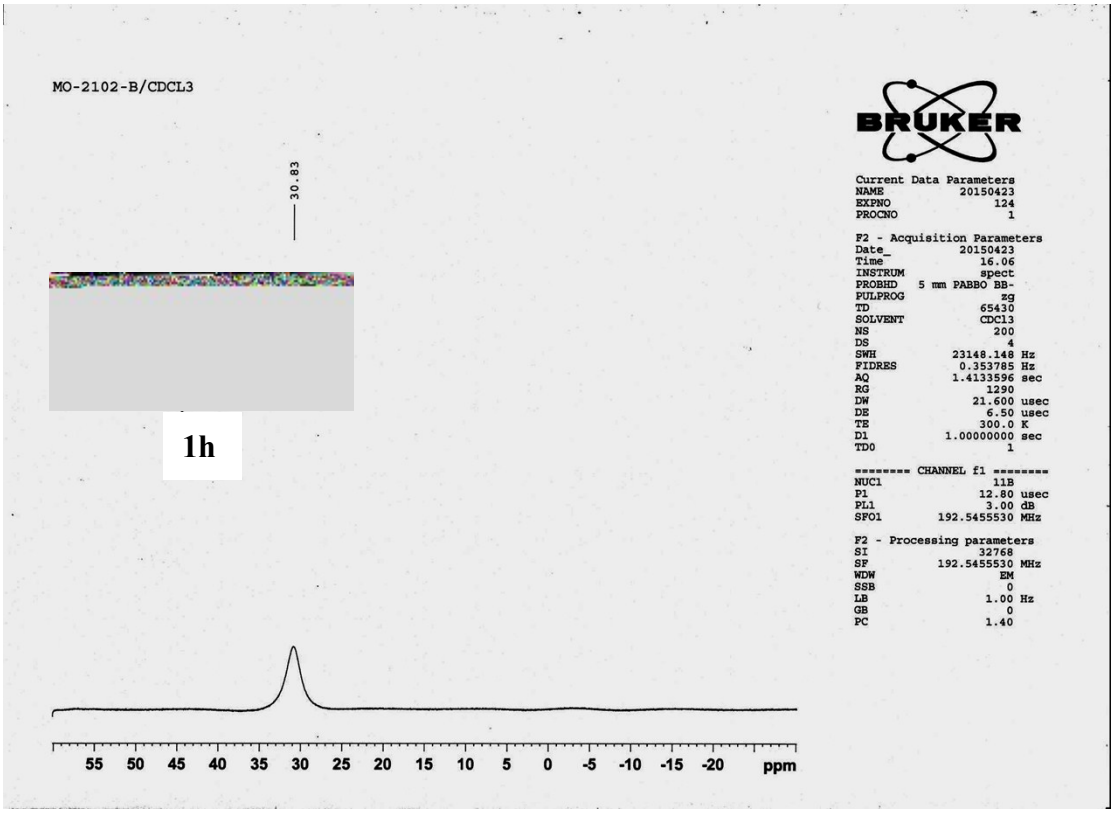
^{1}H-NMR (300 MHz, $CDCl_3$)



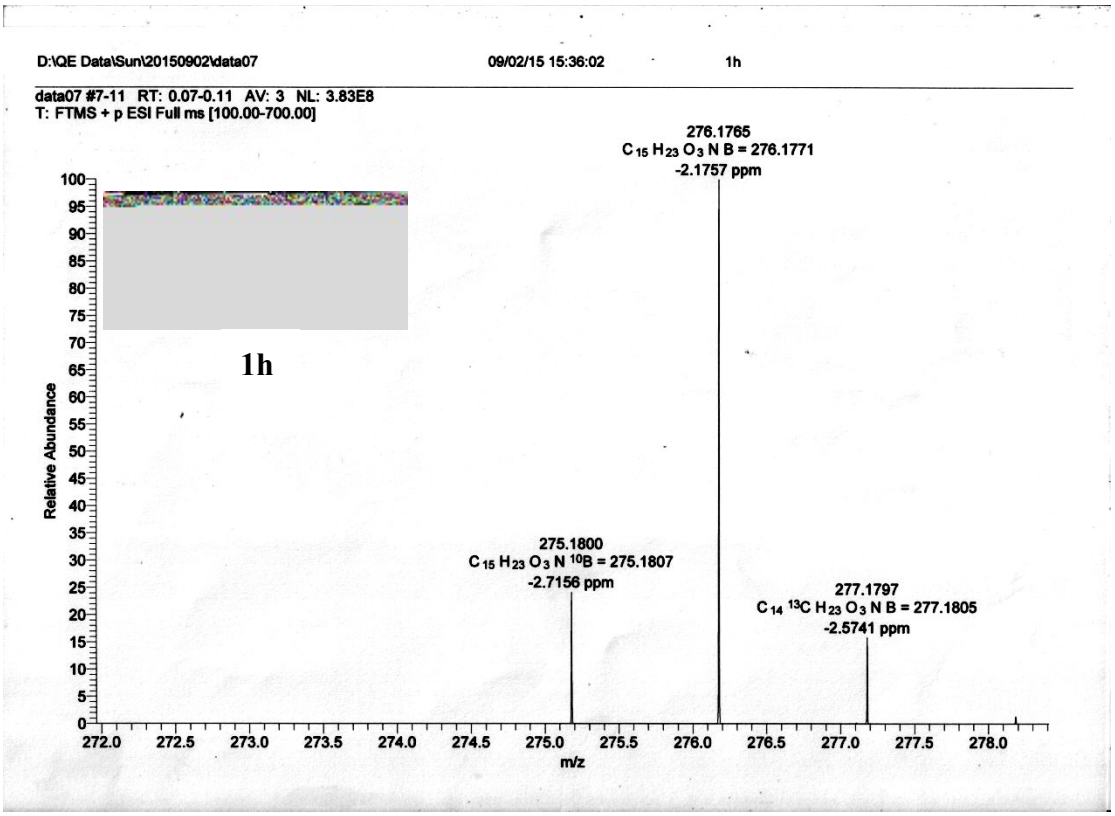
^{13}C-NMR (150 MHz, $CDCl_3$)



^{11}B-NMR (193 MHz, $CDCl_3$)

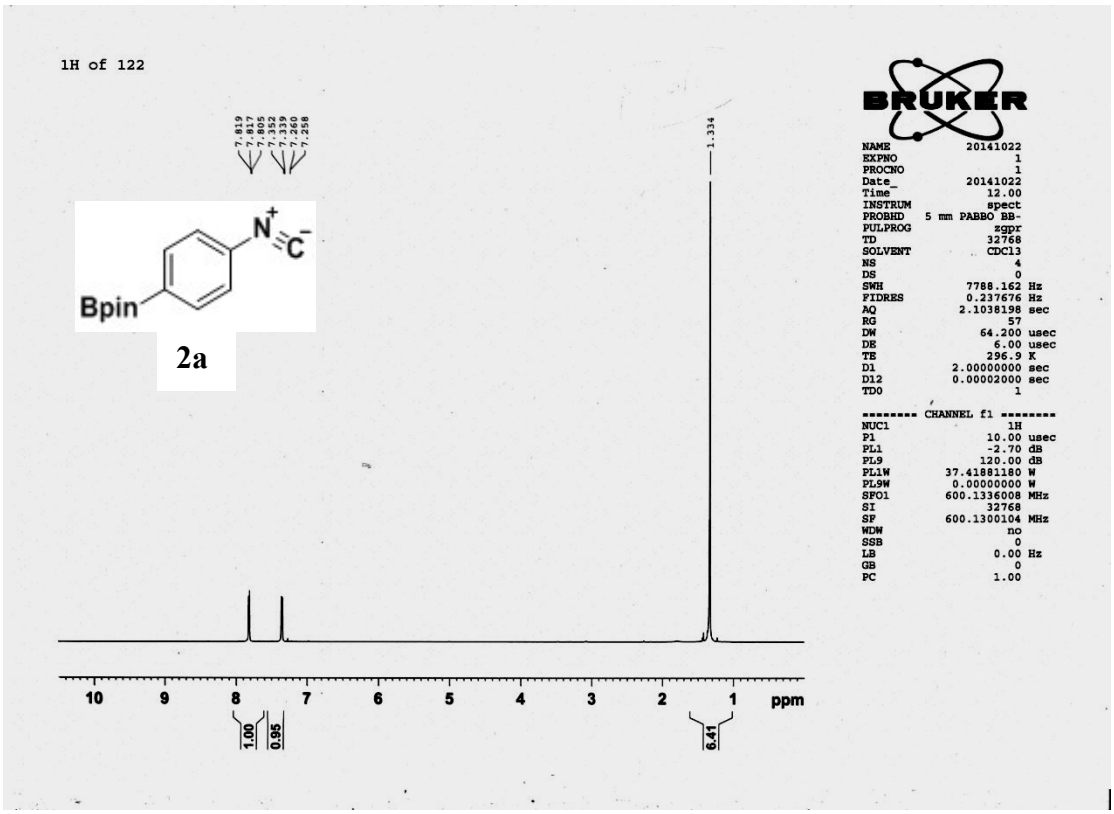


HRMS

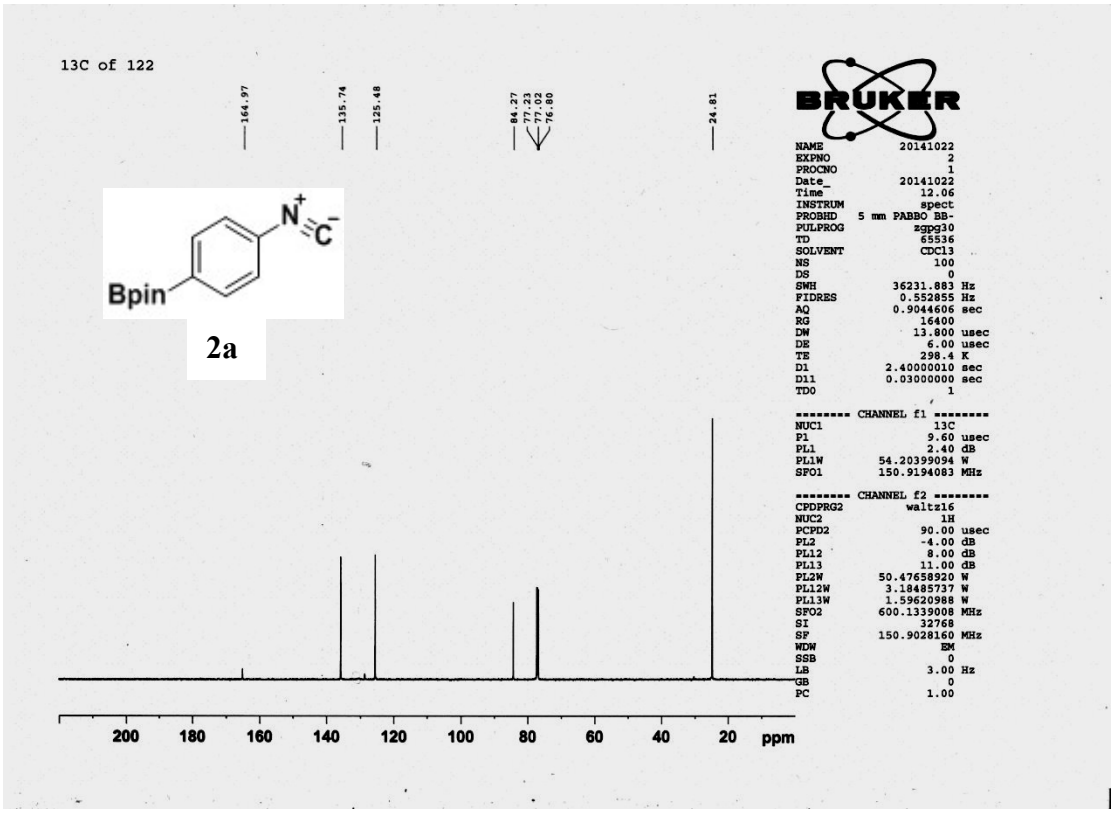


2-(4-isocyanophenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **(2a)**

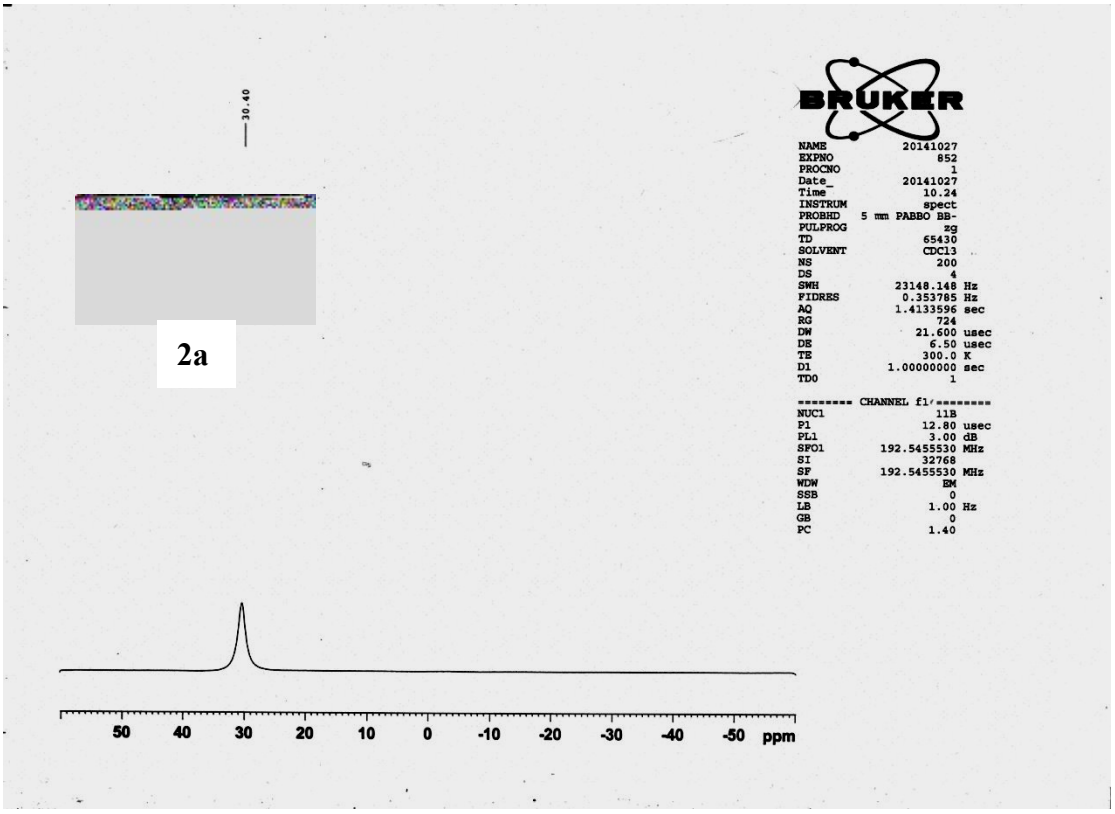
^{1}H-NMR (600 MHz, $CDCl_3$)



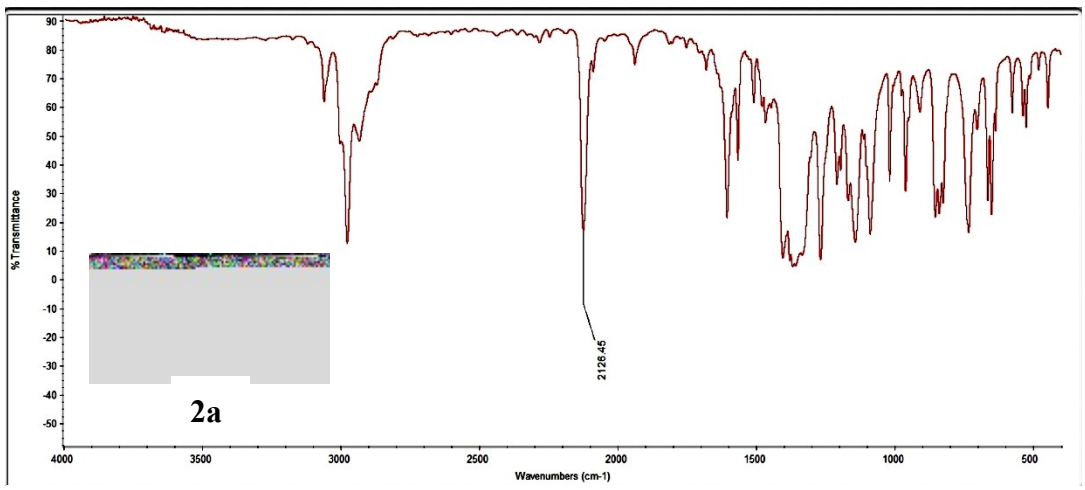
^{13}C-NMR (150 MHz, $CDCl_3$)



^{11}B-NMR (193 MHz, $CDCl_3$)



IR (KBr)



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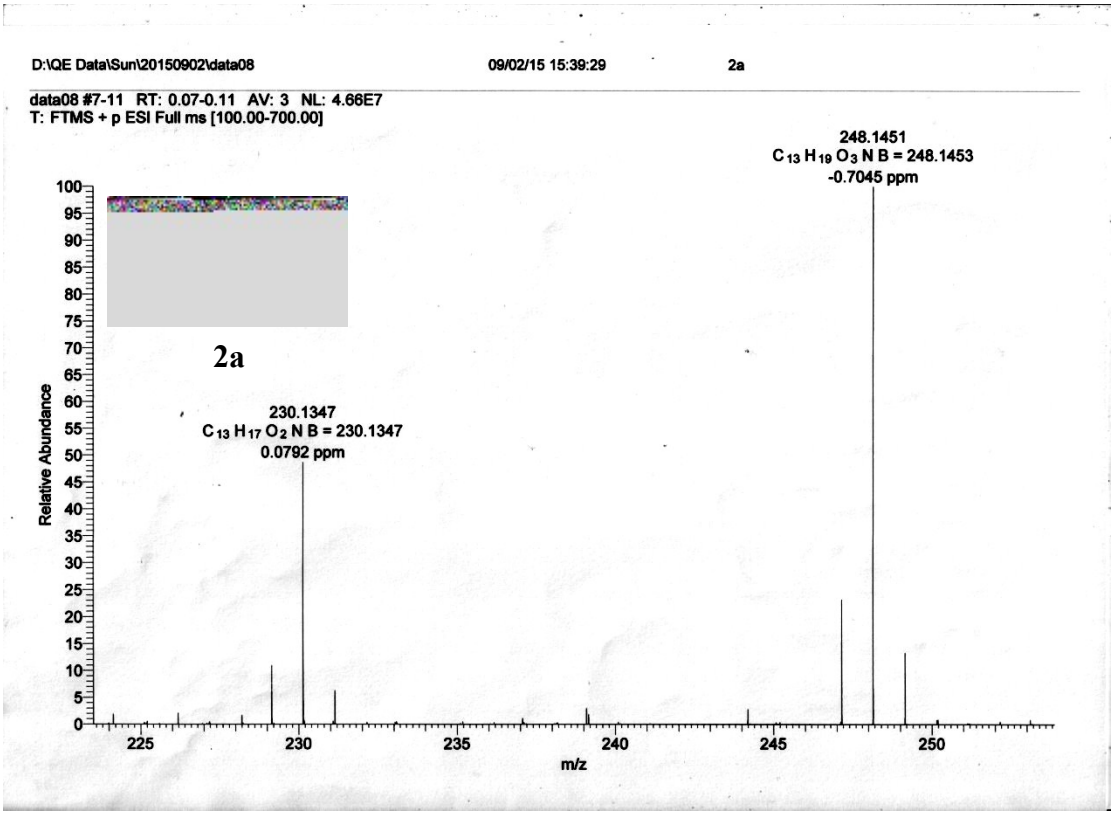
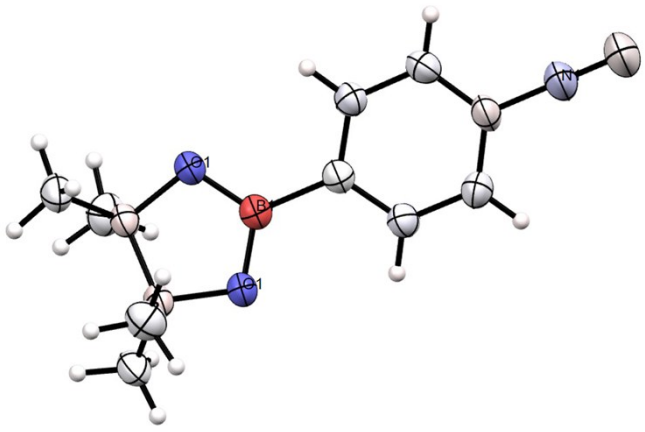


X-ray crystallographic analysis of 2-(4-isocyanophenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2a**), thermal ellipsoids drawn at the 50% probability level.



A clear light yellow columun-like specimen of $C_{13}H_{16}BNO_2$, approximate dimensions 0.72 mm x 0.28 mm x 0.19 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were collected.

Table 1. Crystal data and structure refinement for a17514.

Identification code	a17514	
Empirical formula	$C_{13}H_{16}BNO_2$	
Formula weight	229.08	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 11.0964(5) Å	□= 90°.
	b = 13.2916(6) Å	□= 119.655(2)°.
	c = 10.4278(7) Å	□ = 90°.
Volume	1336.54(12) $Å^3$	
Z	4	
Density (calculated)	1.138 Mg/m^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	488	
Crystal size	0.72 x 0.28 x 0.19 mm^3	
Theta range for data collection	4.07 to 25.00°.	
Index ranges	-12<=h<=13, -15<=k<=15, -12<=l<=12	
Reflections collected	3767	
Independent reflections	1136 [R(int) = 0.0239]	
Completeness to theta = 24.96°	96.3 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9859 and 0.9480	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1136 / 0 / 82	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.0925	
R indices (all data)	R1 = 0.0453, wR2 = 0.0996	
Largest diff. peak and hole	0.185 and -0.161 $e.Å^{-3}$	

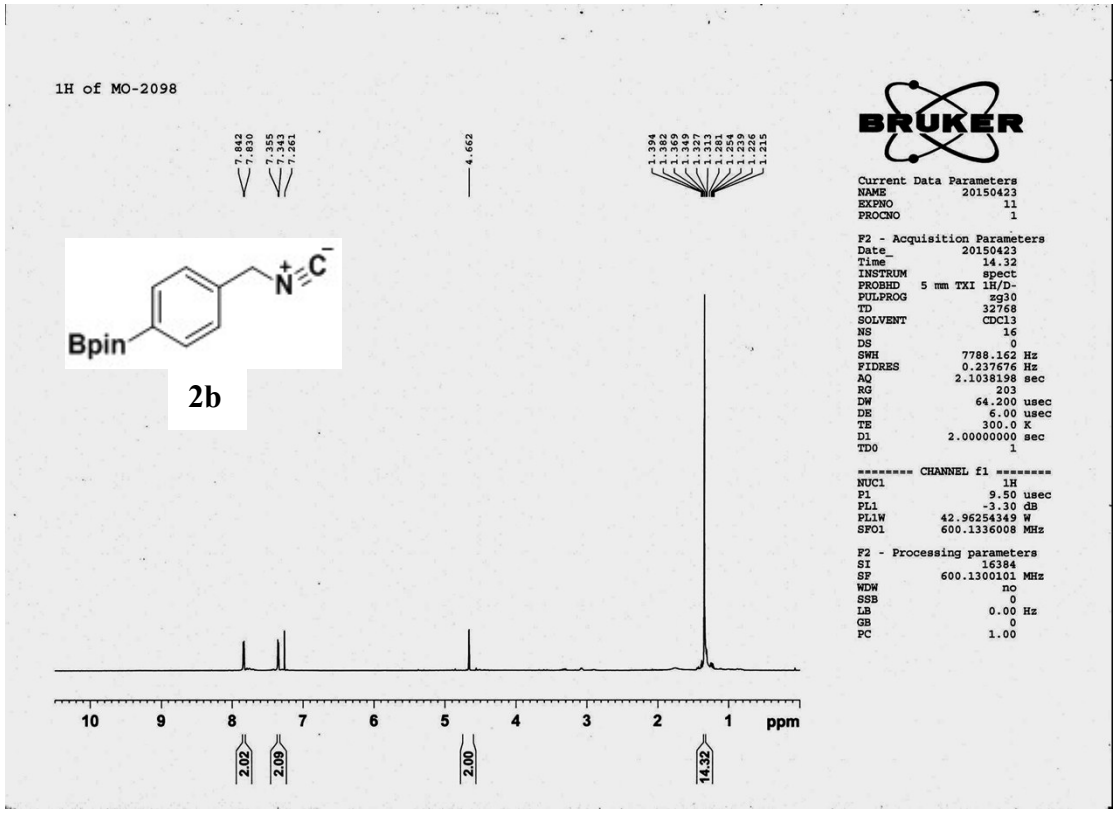
For the compound **2a**, the calculated absolute energy by DFT/B3LYP /6-31G(d,p) method was -735.174527 hatree (-461328.632263 kcal/mole), and the optimized atom coordinates of **2a** was collected in Table S1.

Table S1. The optimized atom coordinates of **2a** by DFT/B3LYP/6-31G(d,p) method.

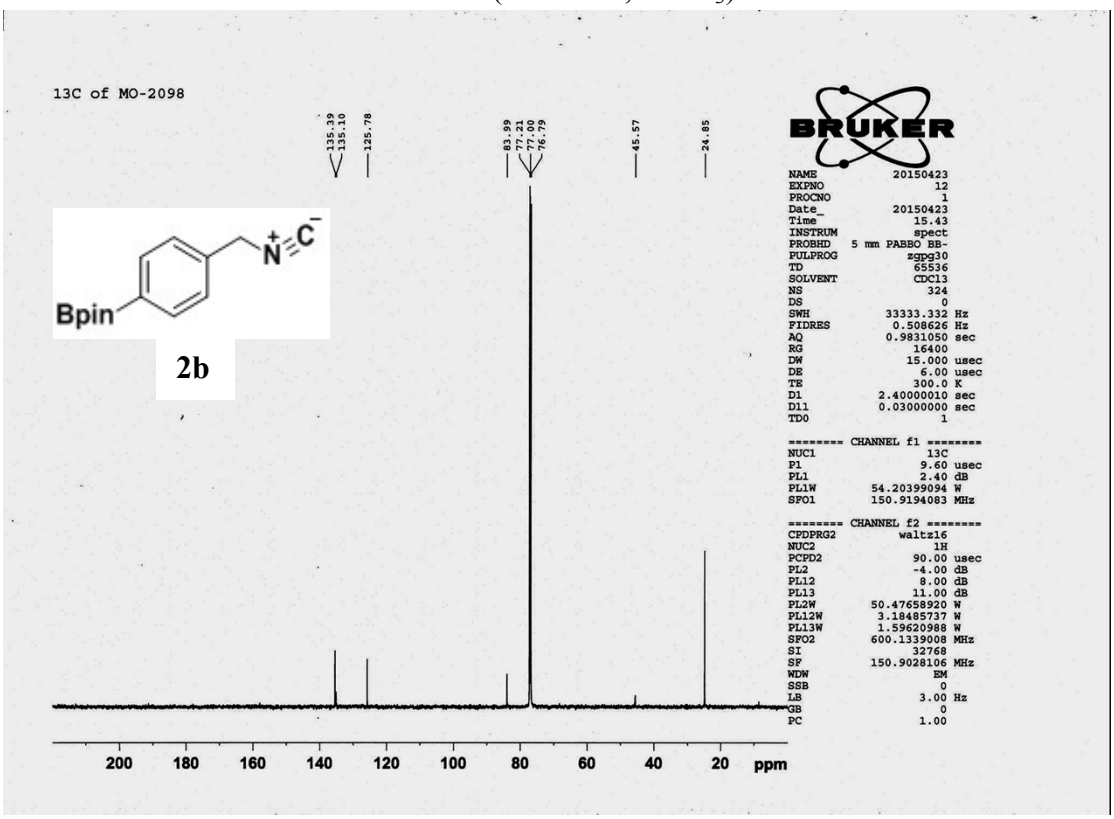
	Optimized Atom Coordinates of **2a**		
Atom	x	y	z
C	1.039562	-9E-06	-0.000154
C	1.762386	-1.19551	0.158532
C	3.153152	-1.20699	0.161158
C	3.846857	-4E-06	0.000006
C	3.153164	1.206974	-0.161223
C	1.762397	1.195494	-0.158747
H	1.22171	-2.12906	0.281753
H	3.711216	-2.12877	0.284297
H	3.711229	2.128764	-0.284307
H	1.221738	2.129042	-0.282029
N	5.232021	-7E-06	0.000082
C	6.413525	-1.1E-05	0.000144
B	-0.516824	-5.1E-05	-0.000212
O	-1.270261	-1.12853	0.205195
O	-1.270276	1.12848	-0.205407
C	-2.657529	0.78598	0.084366
C	-2.65766	-0.78589	-0.084316
C	-2.930555	1.24549	1.522035
H	-2.713745	2.314231	1.599273
H	-3.9747	1.084986	1.806056
H	-2.291649	0.719556	2.236772
C	-3.554668	1.544545	-0.890683
H	-3.283042	1.345092	-1.92847
H	-4.605176	1.272414	-0.745185
H	-3.457295	2.619874	-0.717193
C	-3.554563	-1.54447	0.890945
H	-4.605097	-1.27221	0.74585
H	-3.457379	-2.61978	0.717248
H	-3.282582	-1.34522	1.928672
C	-2.930964	-1.24549	-1.521887
H	-2.292326	-0.71952	-2.236839
H	-2.714056	-2.31421	-1.599132
H	-3.975206	-1.08512	-1.805647

2-(4-(isocyanomethyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **(2b)**

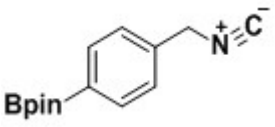
^{1}H-NMR (600 MHz, $CDCl_3$)

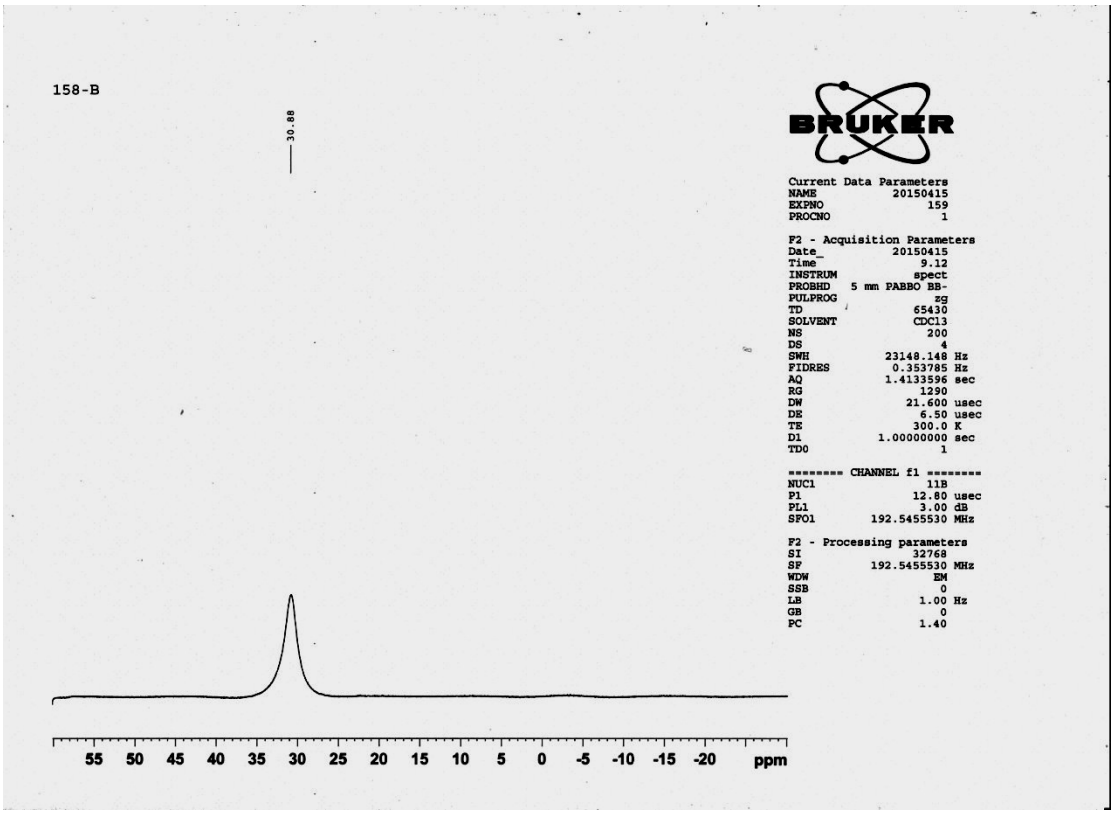


^{13}C-NMR (150 MHz, $CDCl_3$)

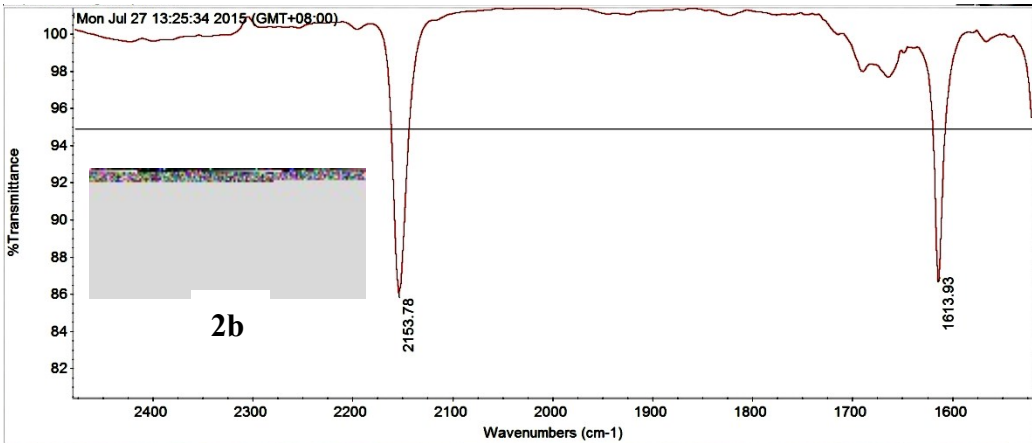


^{11}B-NMR (193 MHz, $CDCl_3$)

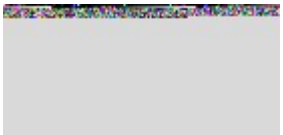


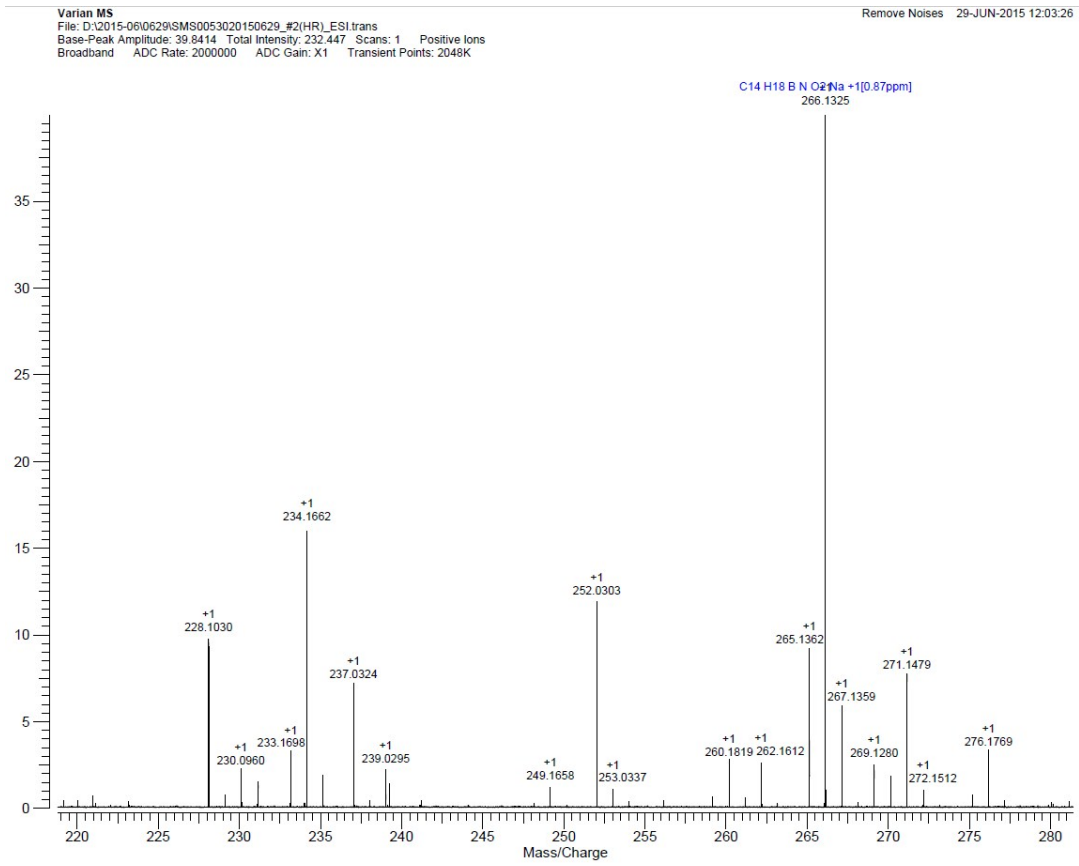

158-B
30.88
BRUKER
Current Data Parameters
NAME 20150415
EXPNO 159
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150415
Time 9.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 65430
SOLVENT CDCl3
NS 200
DS 4
SWH 23148.148 Hz
FIDRES 0.353785 Hz
AQ 1.4133596 sec
RG 1290
DW 21.600 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 12.80 usec
PL1 3.00 dB
SFO1 192.5455530 MHz
F2 - Processing parameters
SI 32768
SF 192.5455530 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 ppm

IR (KBr)


Mon Jul 27 13:25:34 2015 (GMT+08:00)
%Transmittance
100
98
96
94
92
90
88
86
84
82
2b
2153.78
1613.93
2400 2300 2200 2100 2000 1900 1800 1700 1600
Wavenumbers (cm-1)

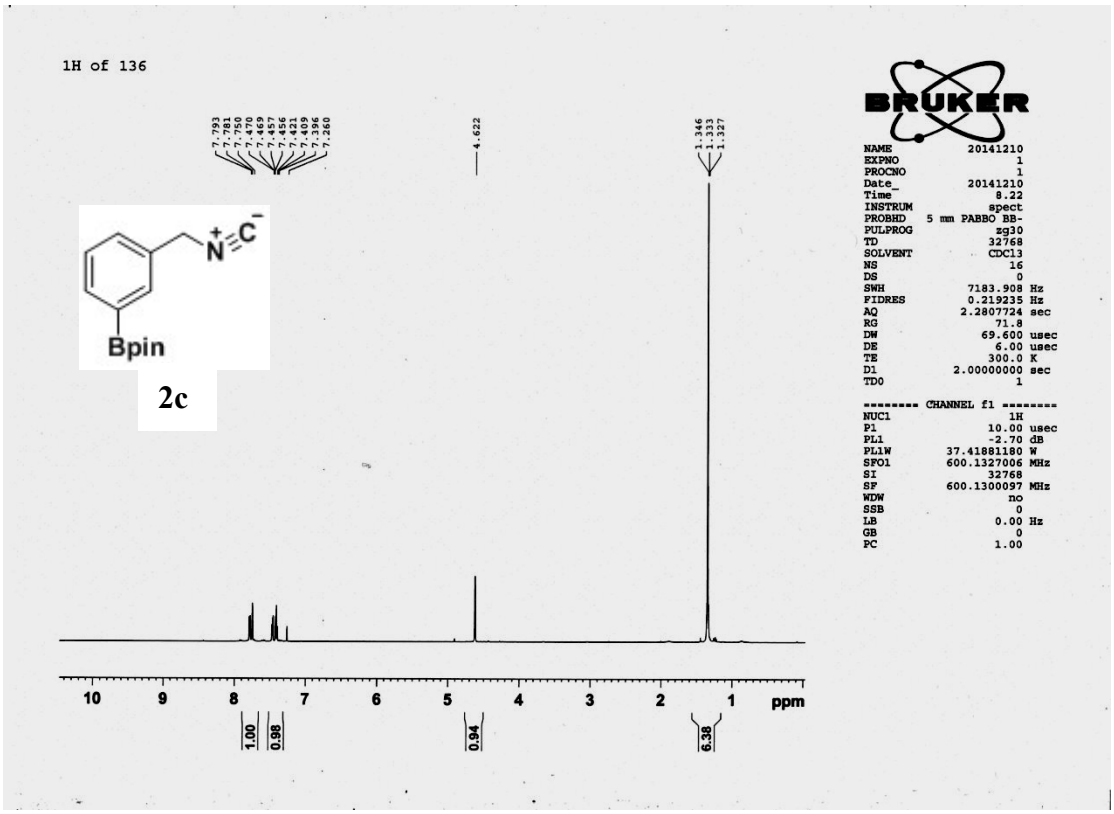
HRMS



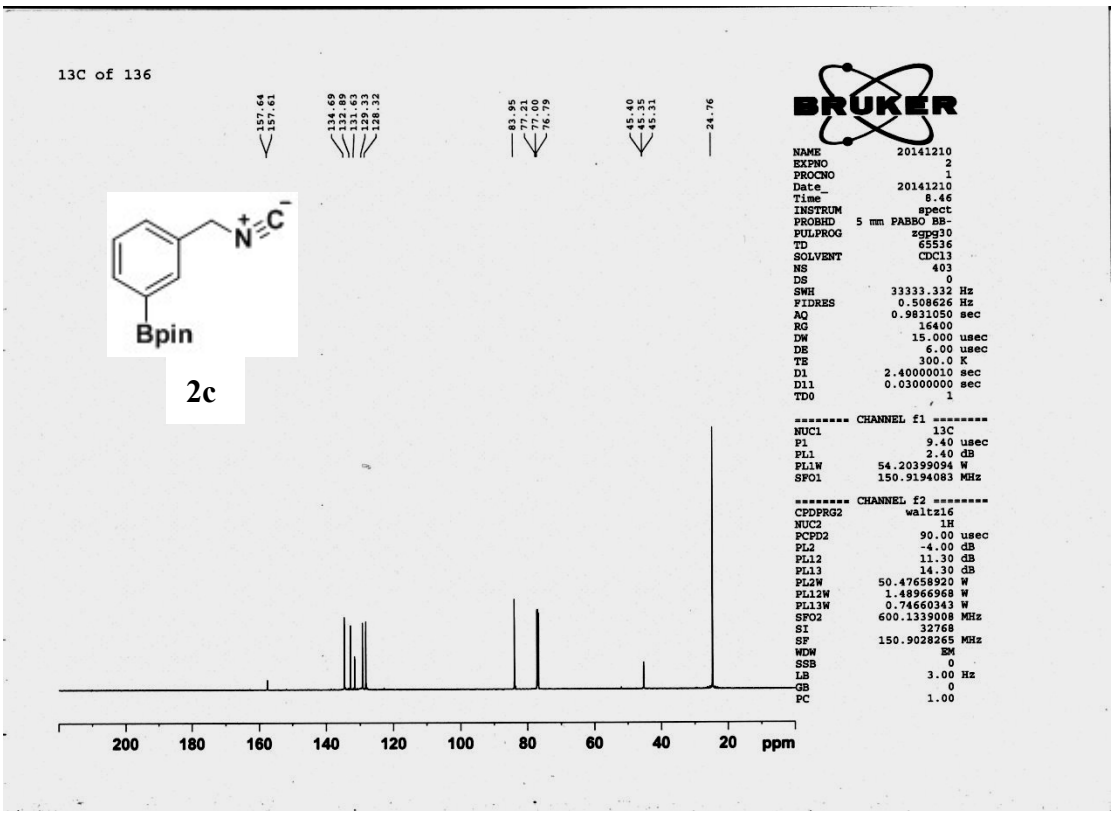

Varian MS
File: D:\2015-06\0629\SMS0053020150629_#2(HR)_ESI.trans
Base-Peak Amplitude: 39.8414 Total Intensity: 232.447 Scans: 1 Positive Ions
Broadband ADC Rate: 2000000 ADC Gain: X1 Transient Points: 2048K
Remove Noises 29-JUN-2015 12:03:26
C14 H18 B N O2 Na +1[0.87ppm]
266.1325
+1 234.1662
+1 228.1030
+1 252.0303
+1 237.0324
+1 265.1362
+1 271.1479
+1 267.1359
+1 233.1698
+1 230.0960
+1 239.0295
+1 249.1658
+1 253.0337
+1 260.1819
+1 262.1612
+1 269.1280
+1 276.1769
+1 272.1512
Mass/Charge

2-(3-(isocyanomethyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **(2c)**

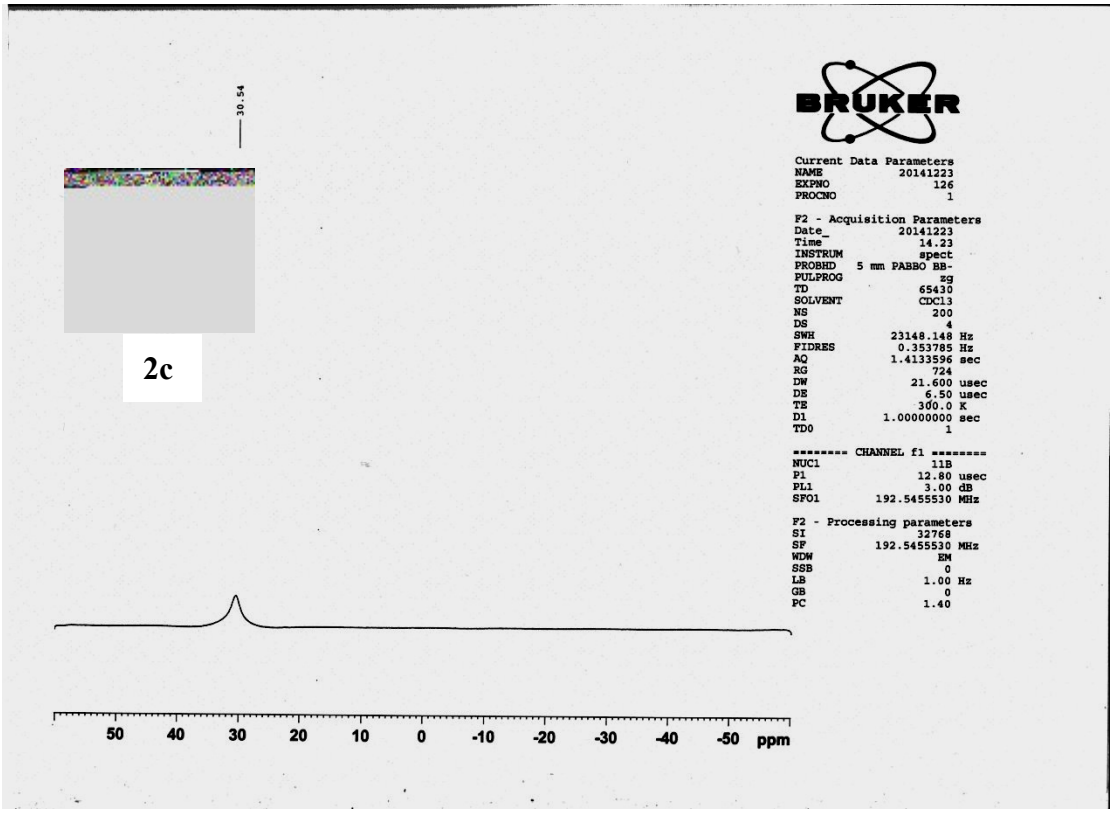
^{1}H-NMR (600 MHz, $CDCl_3$)



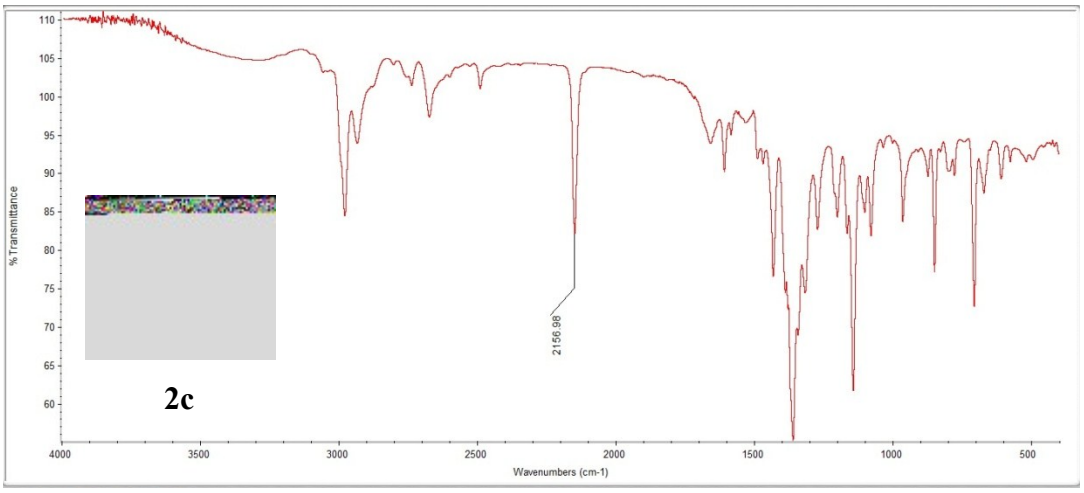
^{13}C-NMR (150 MHz, $CDCl_3$)



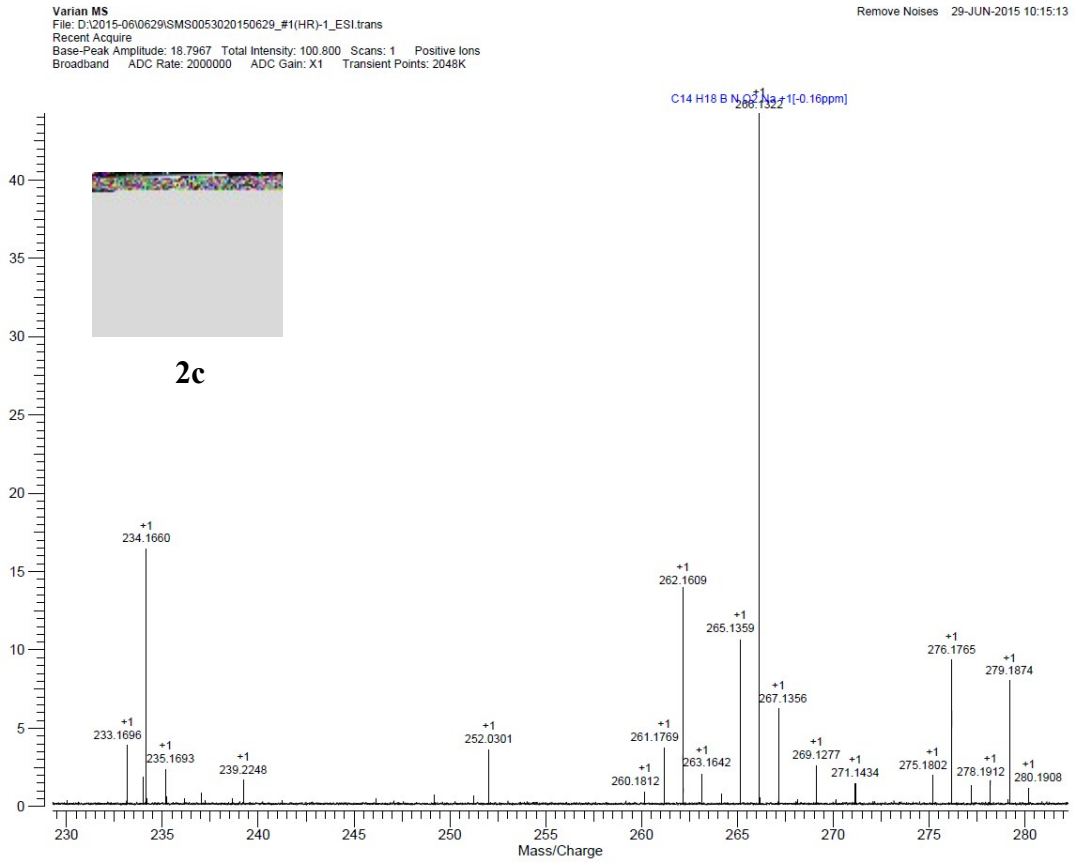
^{11}B-NMR (193 MHz, $CDCl_3$)



IR (KBr)

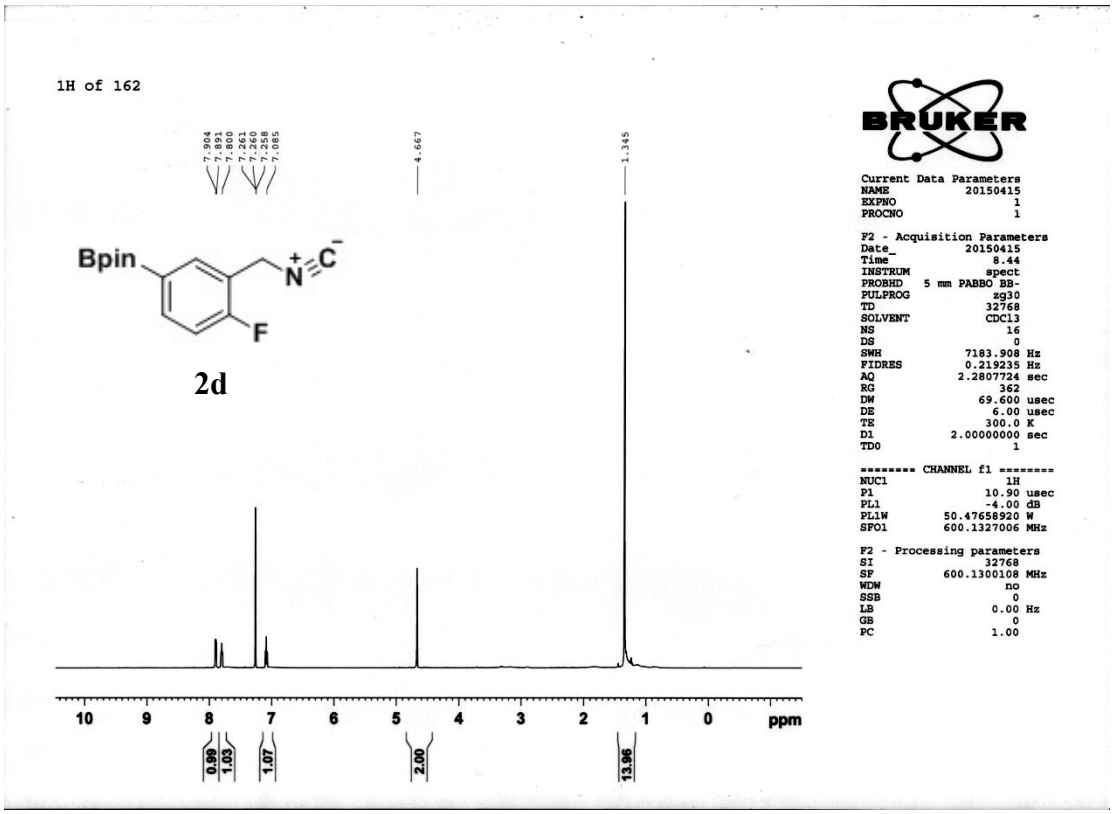


HRMS

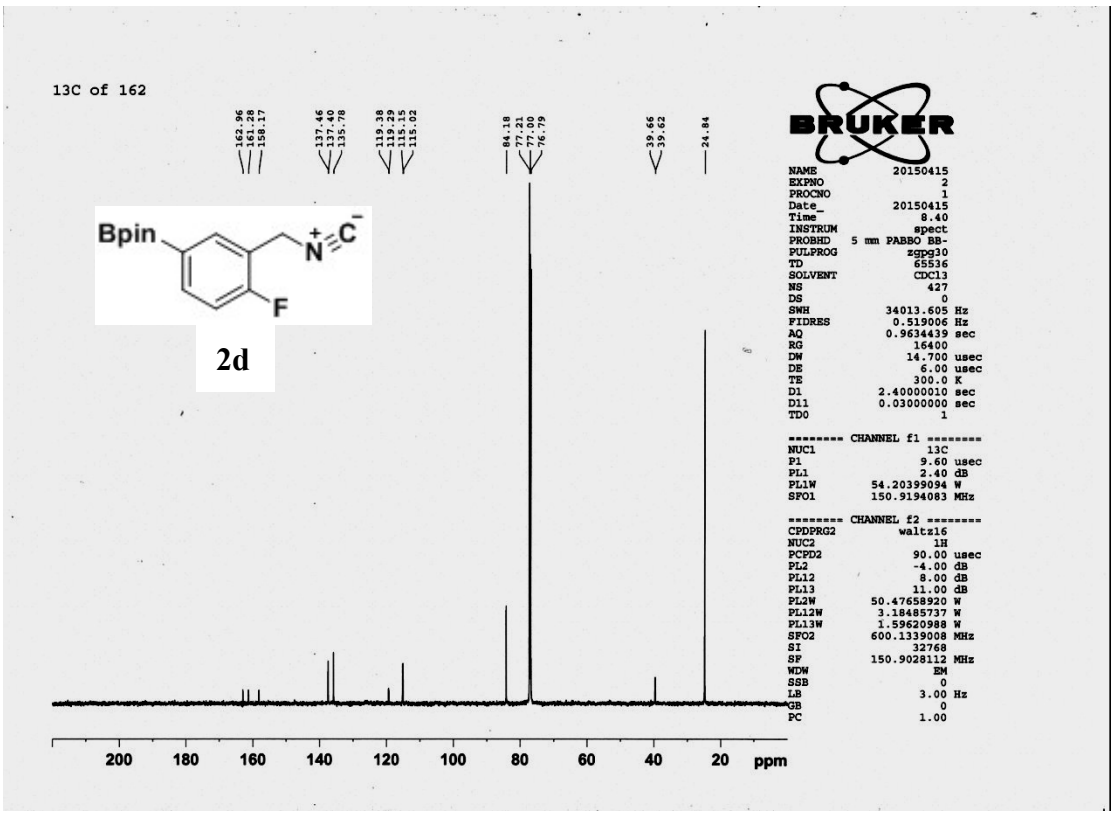

Varian MS
File: D:\2015-06\0629\SMS0053020150629_#1(HR)-1_ESI.trans
Recent Acquire
Base-Peak Amplitude: 18.7967 Total Intensity: 100.800 Scans: 1 Positive Ions
Broadband ADC Rate: 2000000 ADC Gain: X1 Transient Points: 2048K
Remove Noises 29-JUN-2015 10:15:13
2c
+1 234.1660
+1 233.1696
+1 235.1693
+1 239.2248
+1 252.0301
+1 260.1812
+1 261.1769
+1 262.1609
+1 263.1642
+1 265.1359
+1 267.1356
+1 269.1277
+1 271.1434
+1 275.1802
+1 276.1765
+1 278.1912
+1 279.1874
+1 280.1908
Mass/Charge

2-(4-fluoro-3-(isocyanomethyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **(2d)**

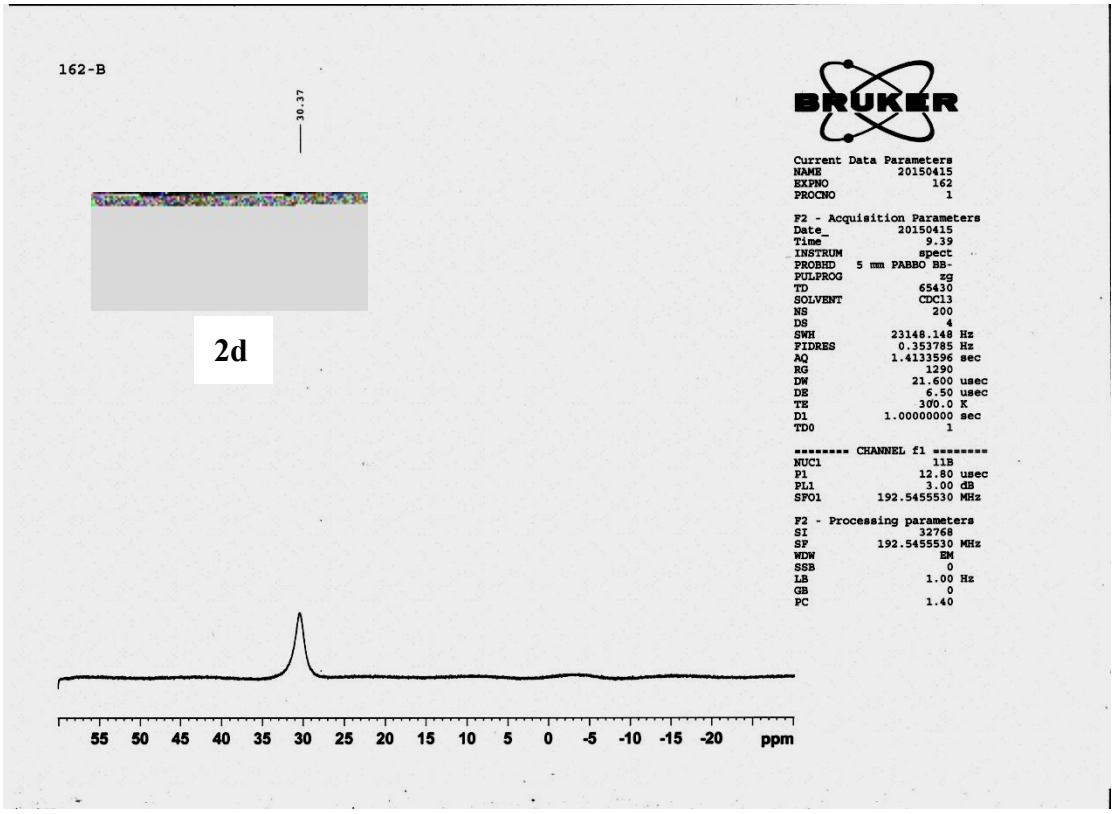
^{1}H-NMR (600 MHz, $CDCl_3$)



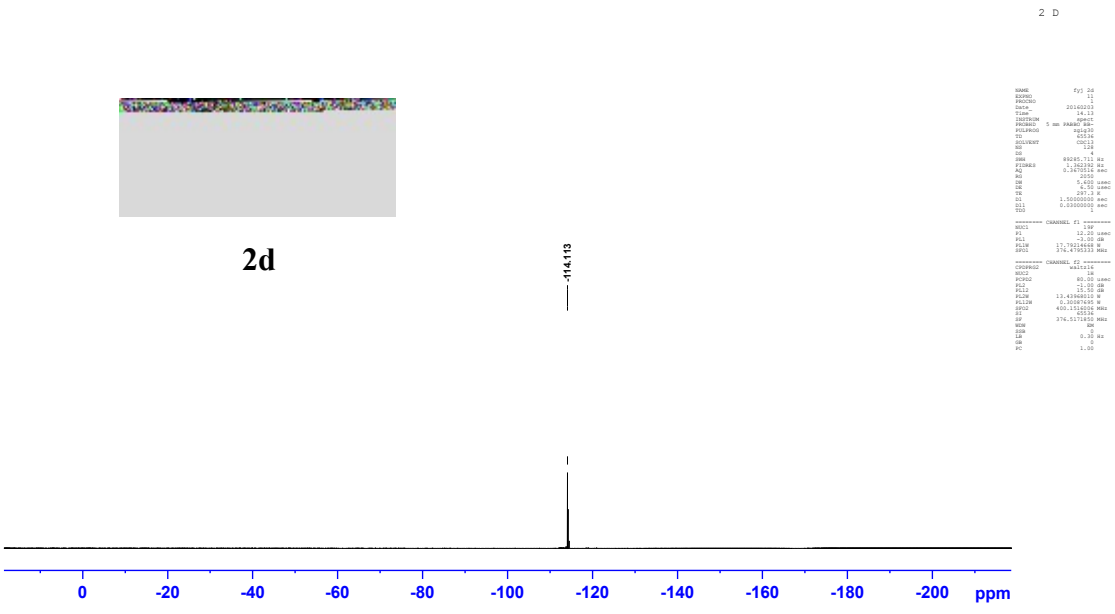
^{13}C-NMR (150 MHz, $CDCl_3$)



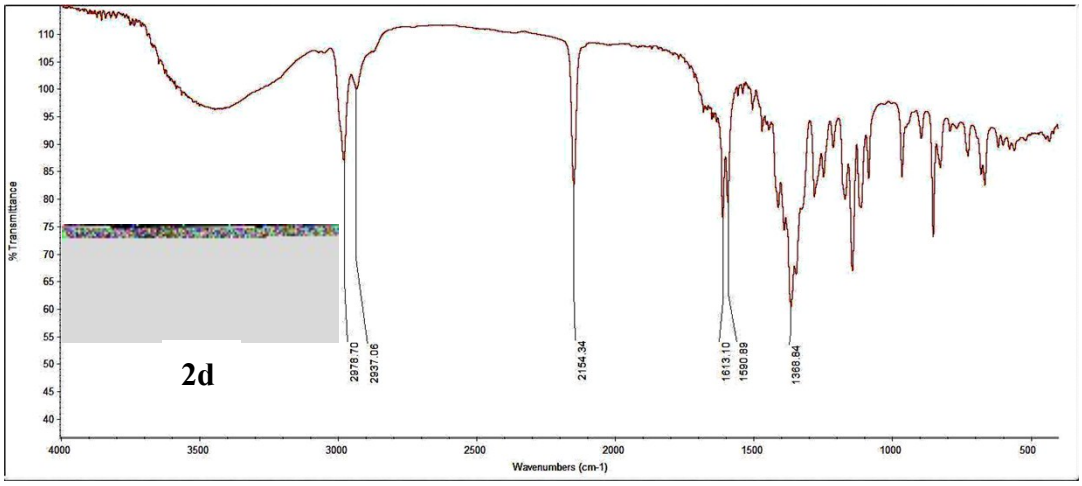
^{11}B-NMR (193 MHz, $CDCl_3$)



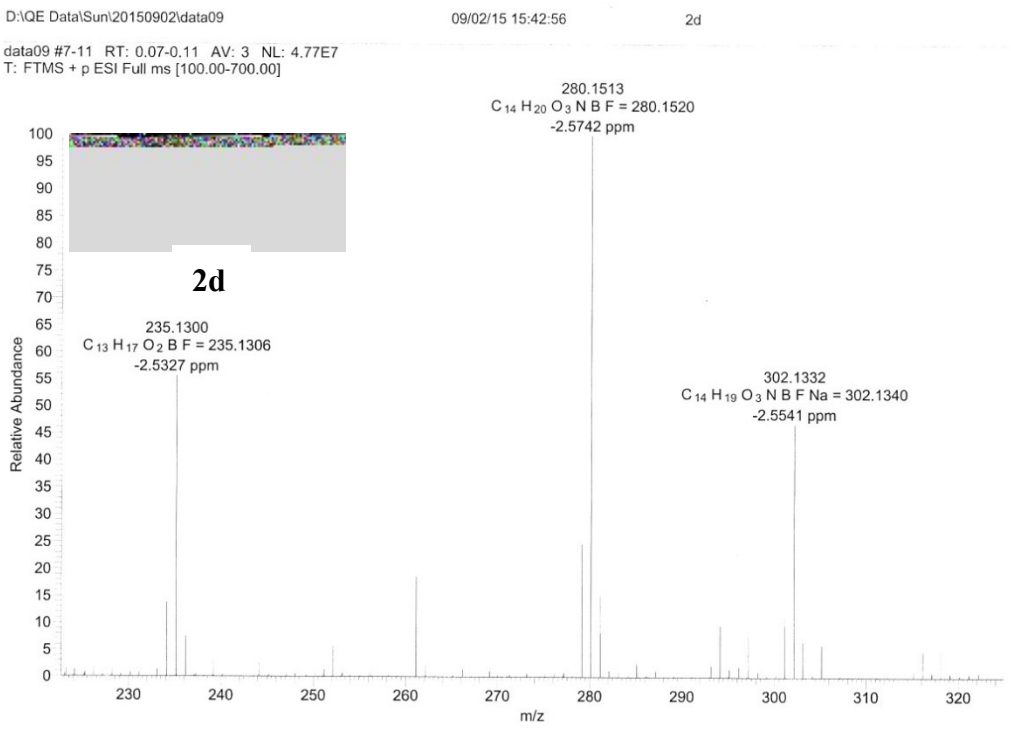
^{19}F-NMR



IR (KBr)

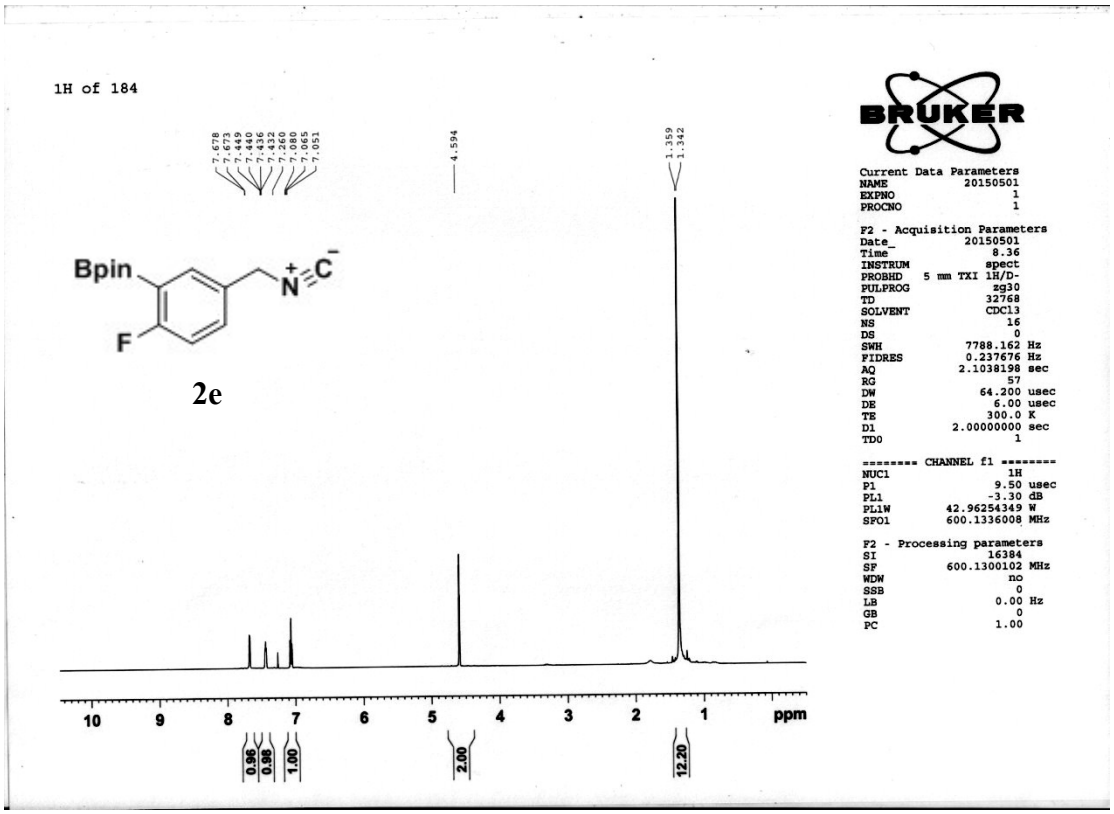

% Transmittance
Wavenumbers (cm-1)
2d
2978.70
2937.06
2154.34
1613.10
1590.89
1368.84

HRMS

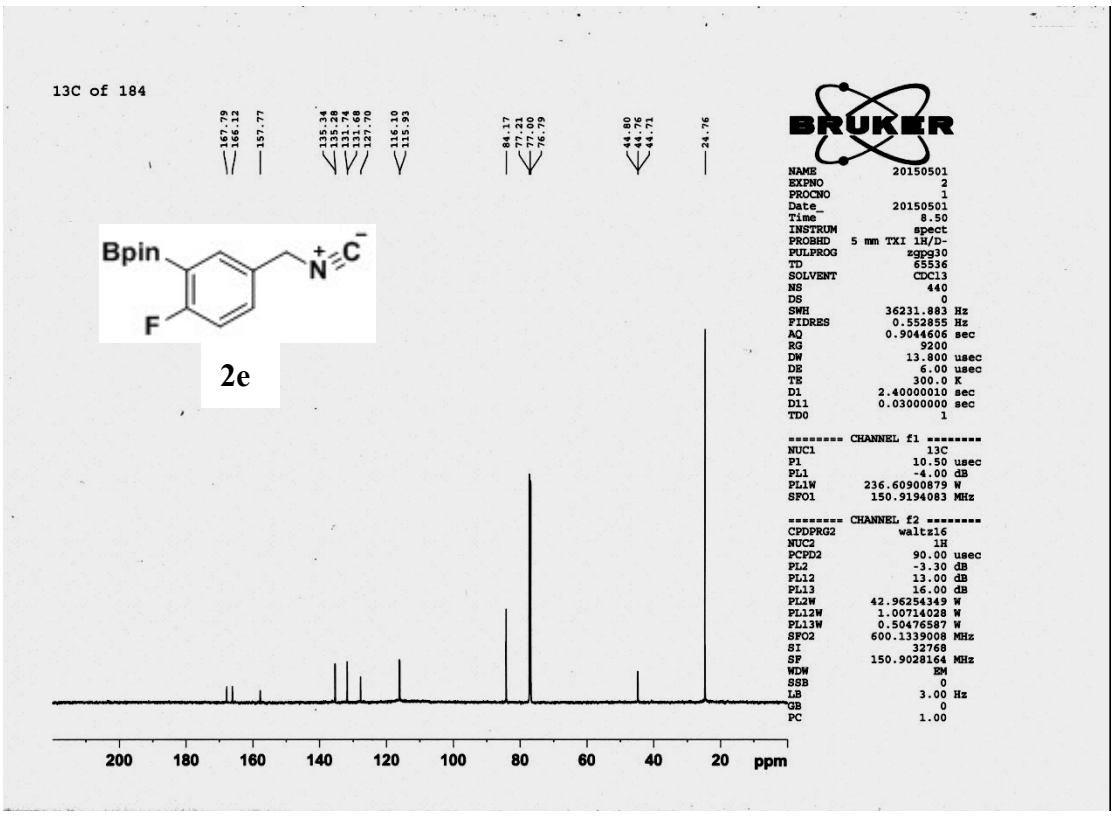

D:\QE Data\Sun\20150902\data09
09/02/15 15:42:56
2d
data09 #7-11 RT: 0.07-0.11 AV: 3 NL: 4.77E7
T: FTMS + p ESI Full ms [100.00-700.00]
2d
280.1513
C 14 H 20 O 3 N B F = 280.1520
-2.5742 ppm
235.1300
C 13 H 17 O 2 B F = 235.1306
-2.5327 ppm
302.1332
C 14 H 19 O 3 N B F Na = 302.1340
-2.5541 ppm
Relative Abundance
m/z

2-(2-fluoro-5-(isocyanomethyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **(2e)**

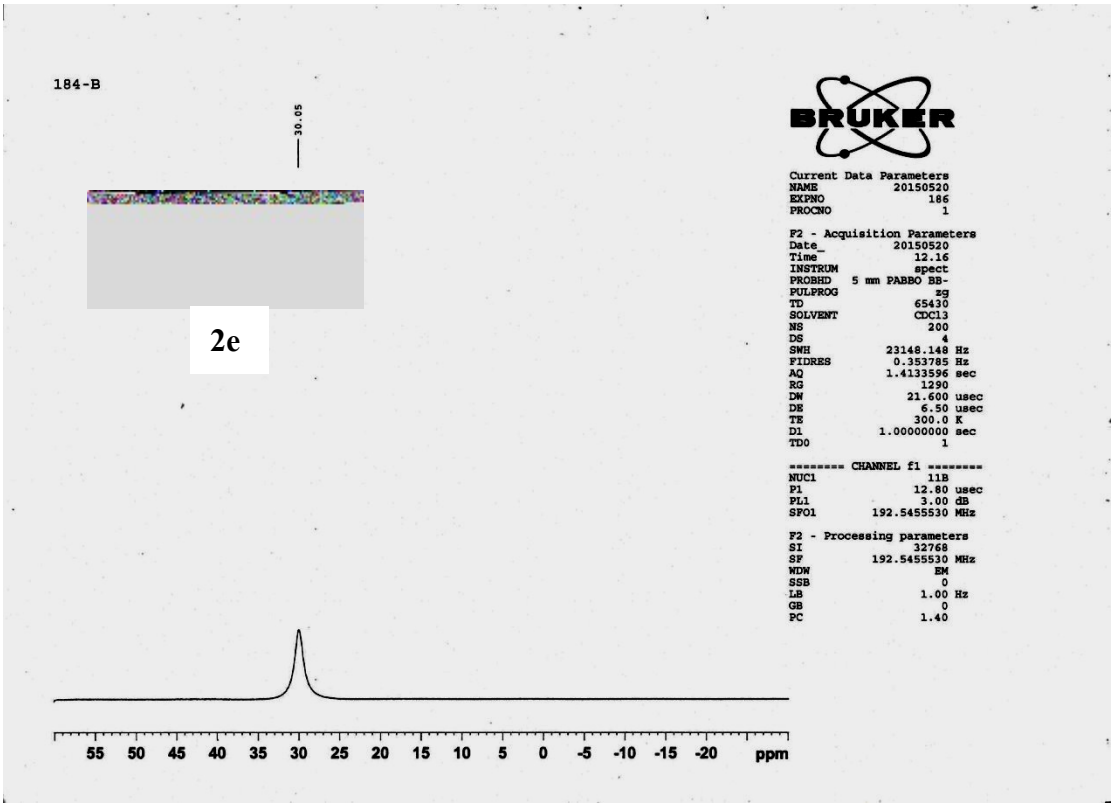
^{1}H-NMR (600 MHz, $CDCl_3$)



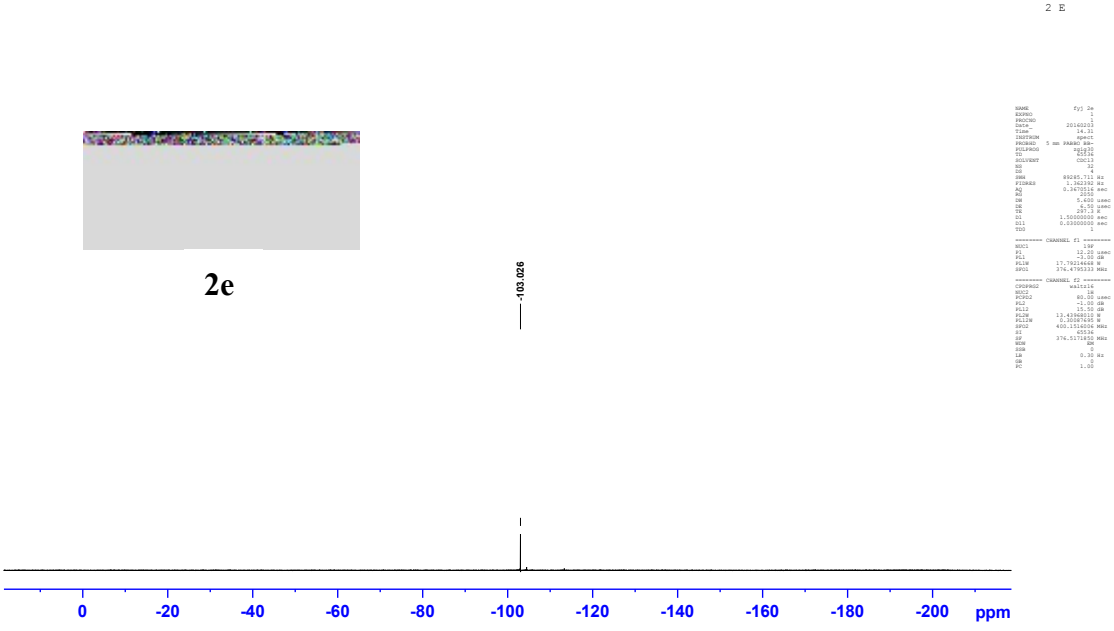
^{13}C-NMR (150 MHz, $CDCl_3$)



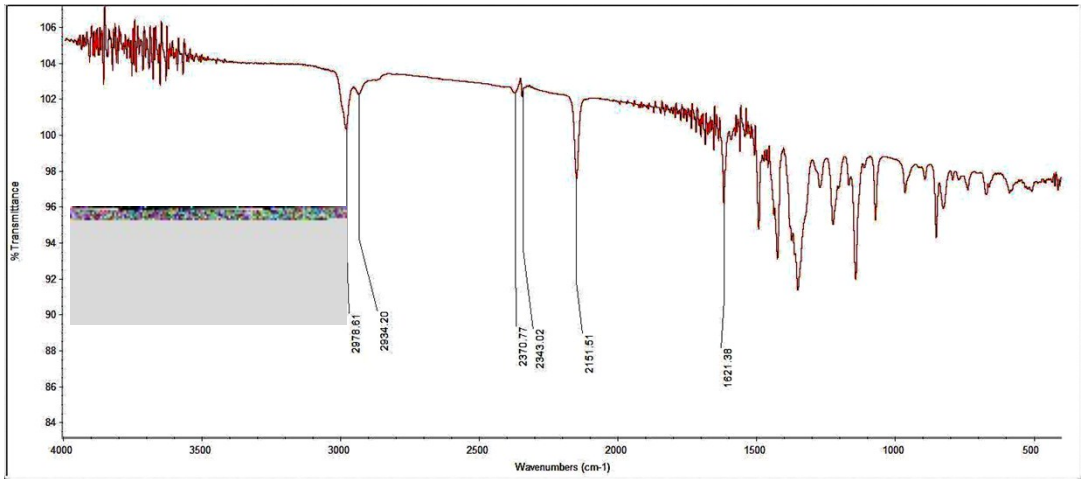
^{11}B-NMR (193 MHz, $CDCl_3$)



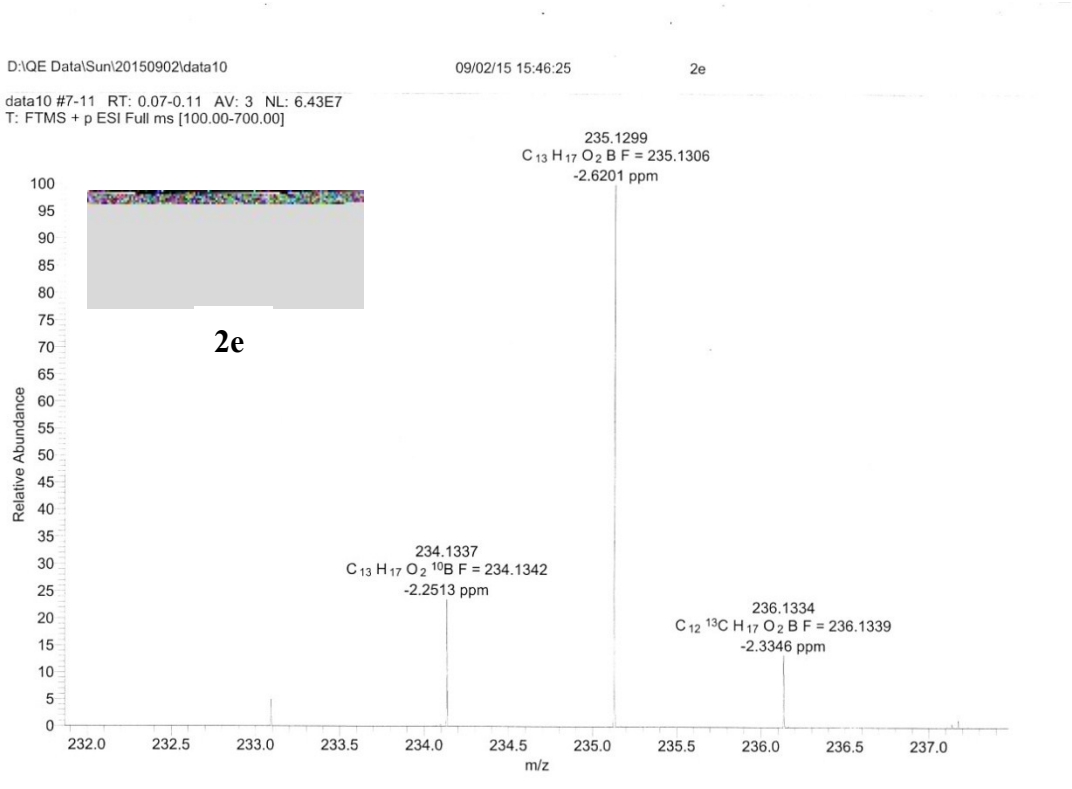
^{19}F-NMR



IR (KBr)

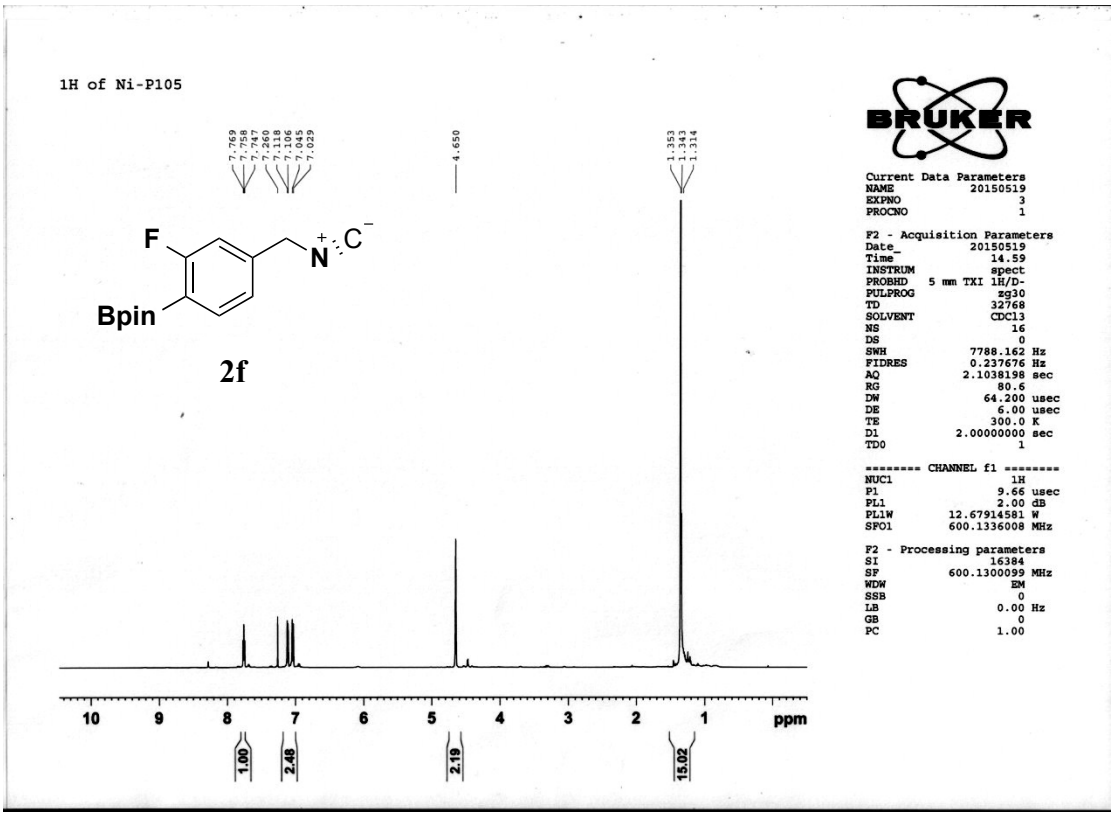

% Transmittance
Wavenumbers (cm-1)
2978.61
2934.20
2370.77
2343.02
2151.51
1621.38

HRMS

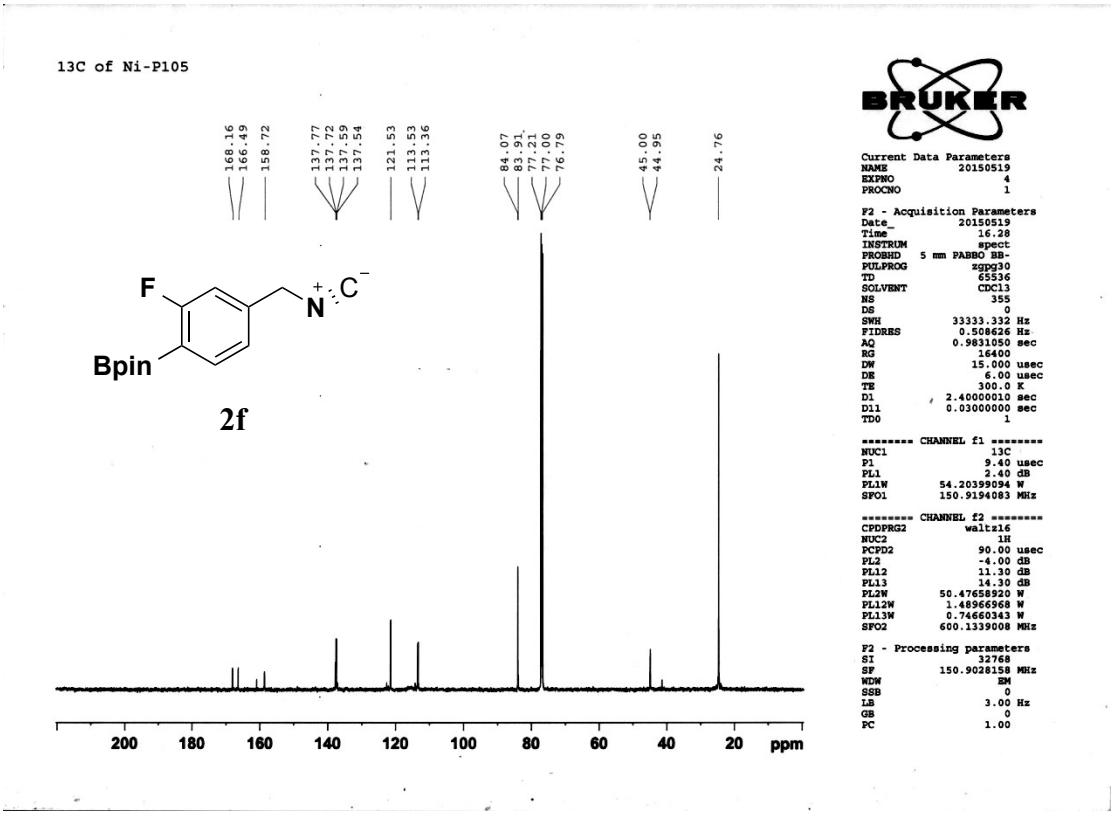

D:\QE Data\Sun\20150902\data10
09/02/15 15:46:25
2e
data10 #7-11 RT: 0.07-0.11 AV: 3 NL: 6.43E7
T: FTMS + p ESI Full ms [100.00-700.00]
235.1299
C 13 H 17 O 2 B F = 235.1306
-2.6201 ppm
2e
234.1337
C 13 H 17 O 2 10B F = 234.1342
-2.2513 ppm
236.1334
C 12 13C H 17 O 2 B F = 236.1339
-2.3346 ppm
Relative Abundance
m/z

2-(2-fluoro-4-(isocyanomethyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **(2f)**

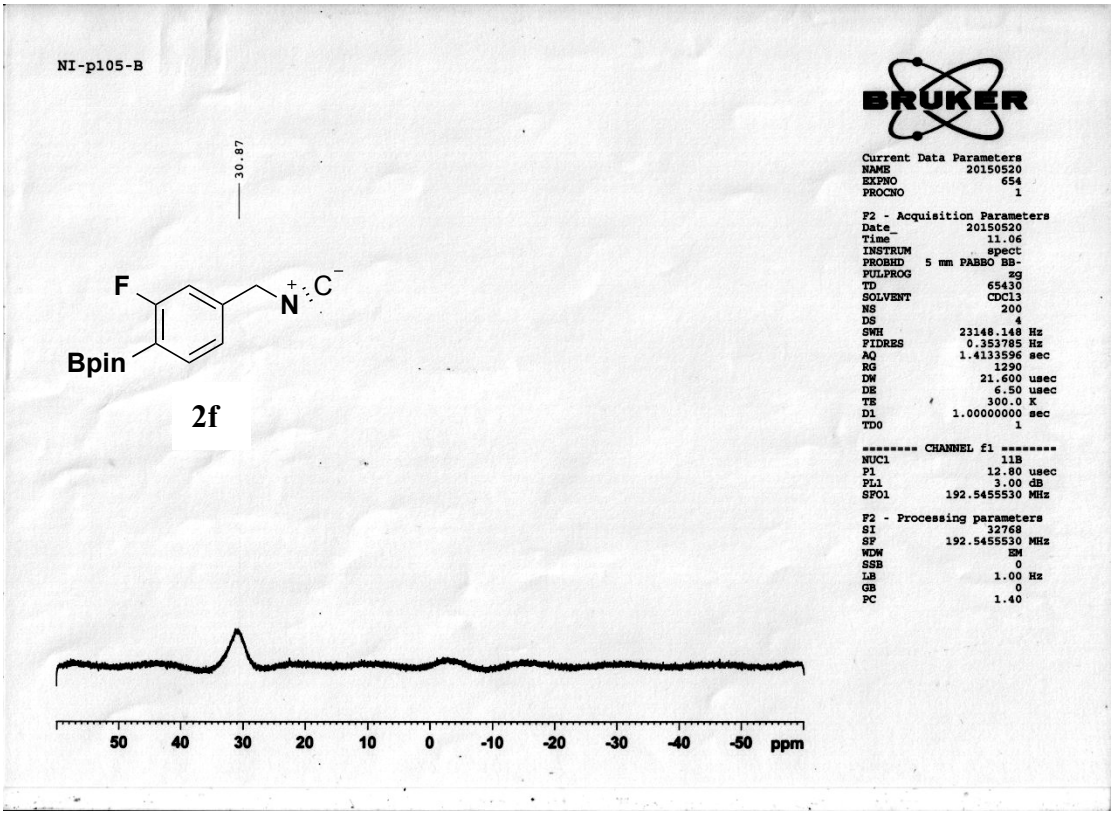
^{1}H-NMR (600 MHz, $CDCl_3$)



^{13}C-NMR (150 MHz, $CDCl_3$)

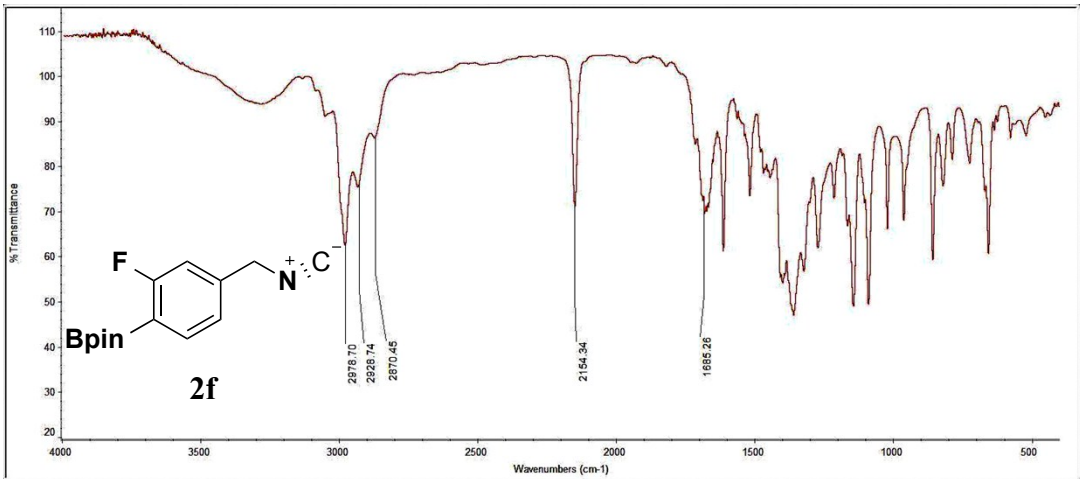


^{11}B-NMR (193 MHz, $CDCl_3$)

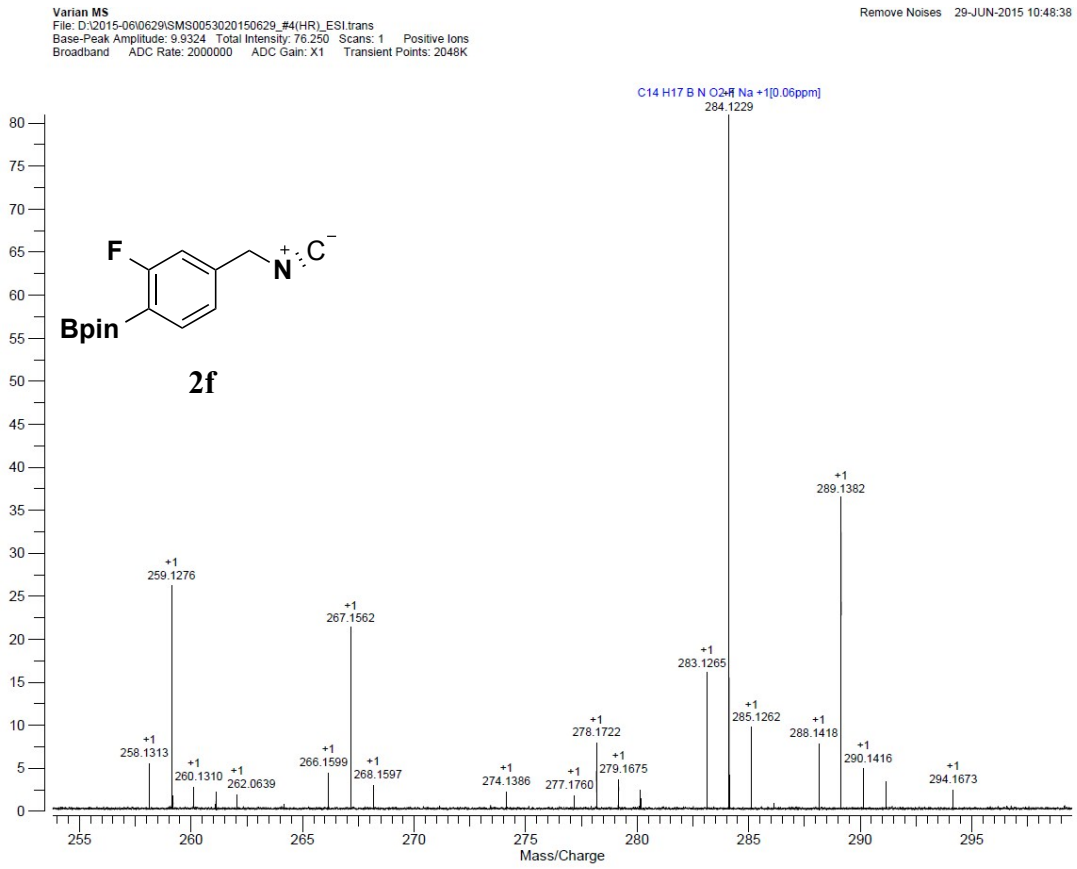


^{19}F-NMR

IR (KBr)

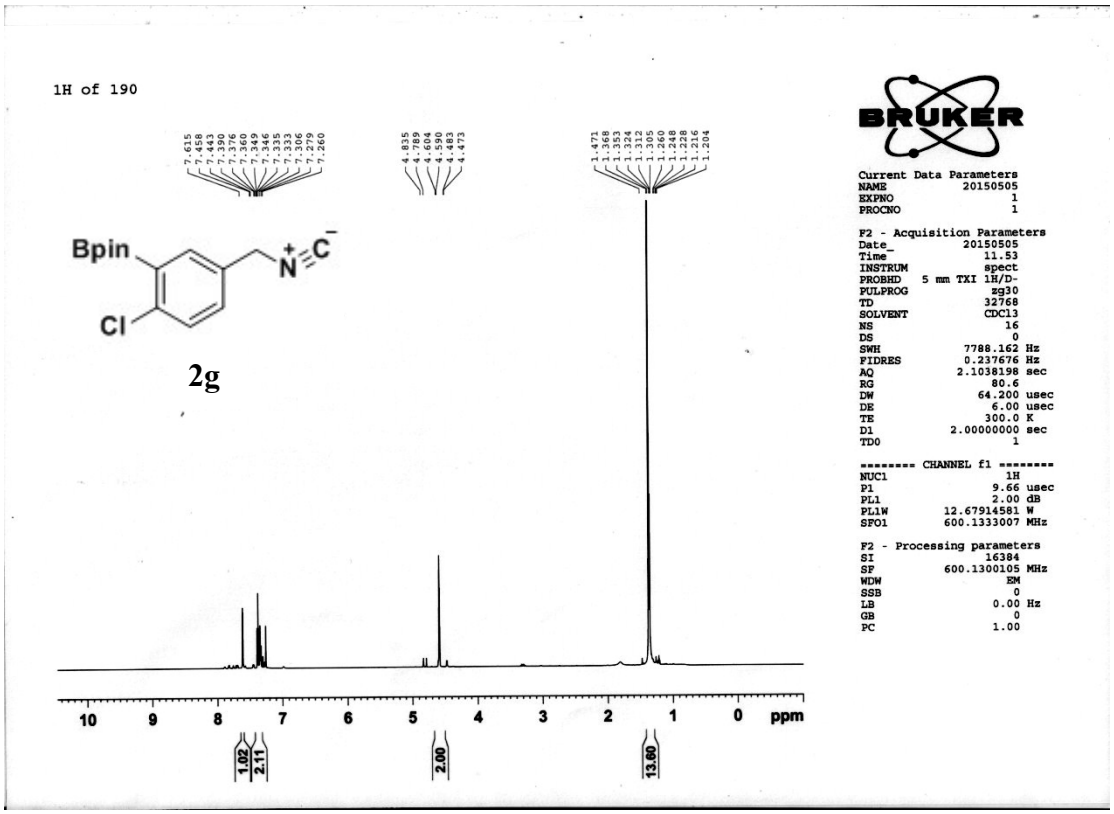

% Transmittance
Wavenumbers (cm-1)
2978.70
2928.74
2870.45
2154.34
1685.26
F
Bpin
N
C
2f

HRMS

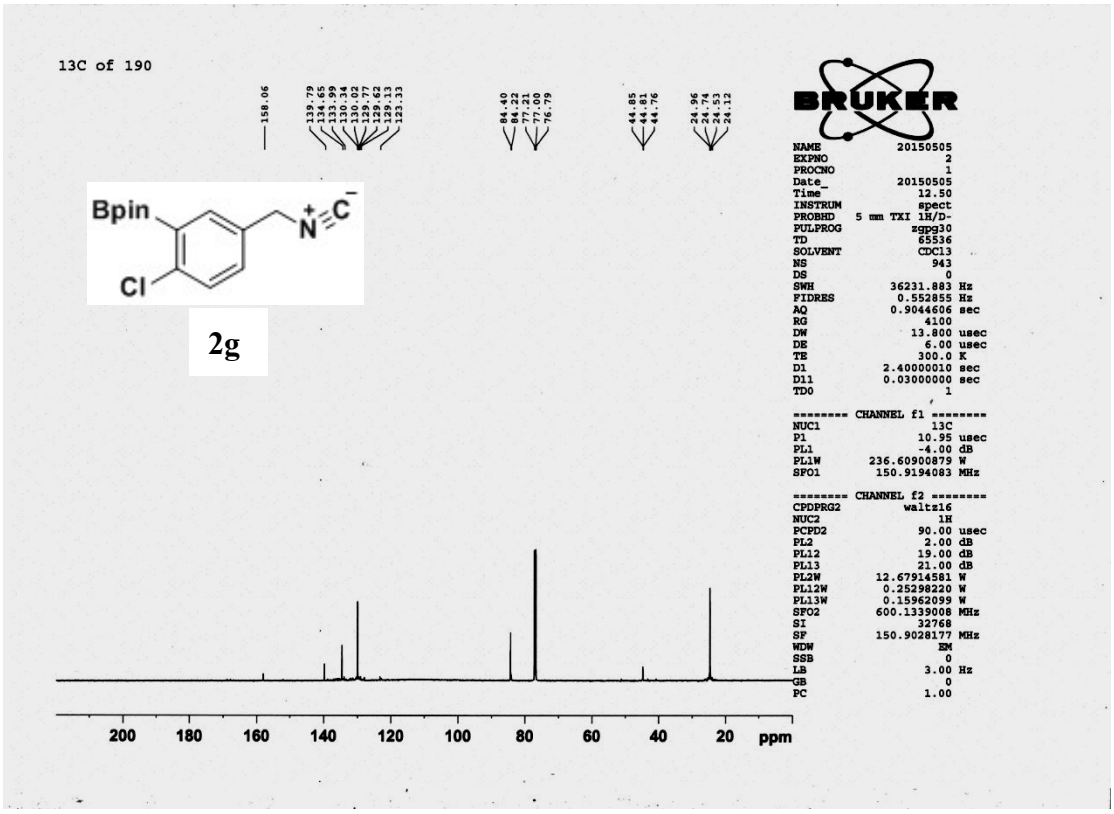

Varian MS
File: D:\2015-06\0629\SMS0053020150629_#4(HR)_ESI.trans
Base-Peak Amplitude: 9.9324 Total Intensity: 76.250 Scans: 1 Positive Ions
Broadband ADC Rate: 2000000 ADC Gain: X1 Transient Points: 2048K
Remove Noises 29-JUN-2015 10:48:38
C14 H17 B N O2 + Na +1[0.06ppm]
284.1229
289.1382
259.1276
267.1562
283.1265
285.1262
288.1418
278.1722
290.1416
258.1313
266.1599
268.1597
279.1675
260.1310
262.0639
274.1386
277.1760
294.1673
F
Bpin
N
C
2f
Mass/Charge

2-(2-chloro-5-(isocyanomethyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **(2g)**

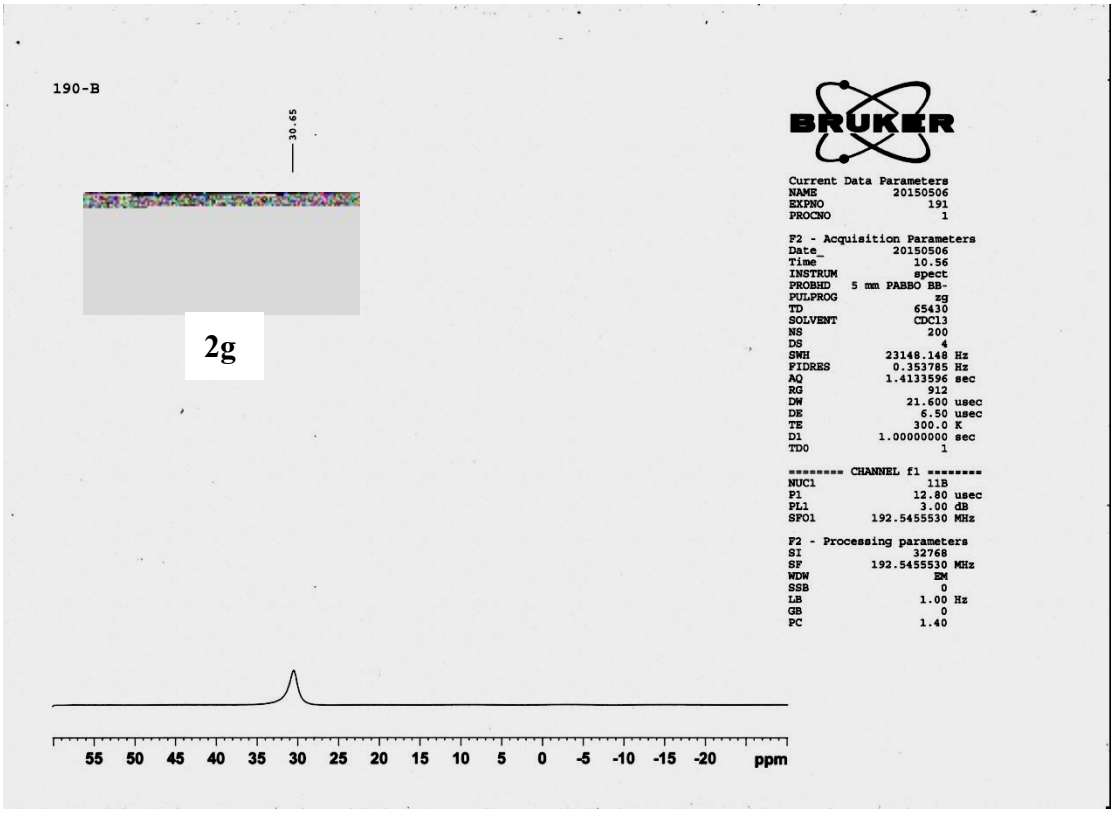
^{1}H-NMR (600 MHz, $CDCl_3$)



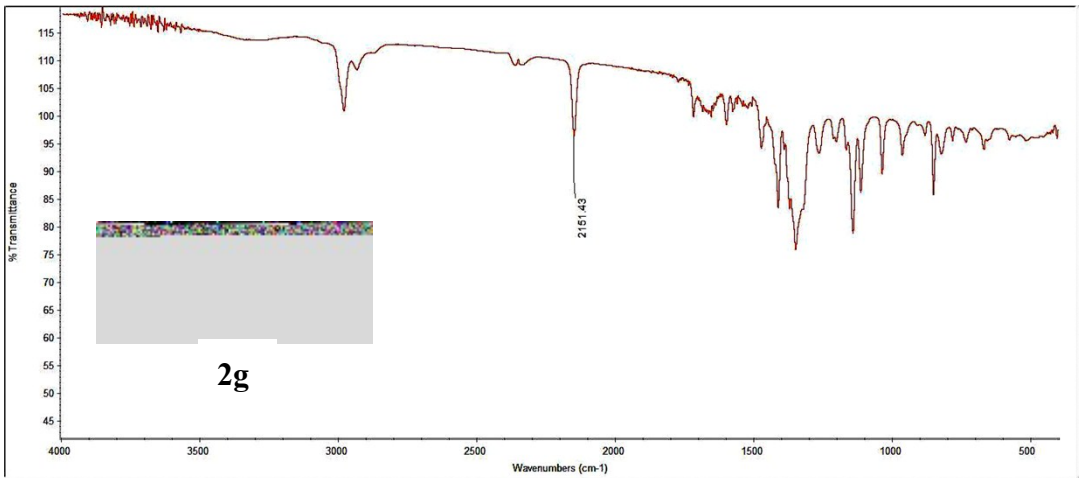
^{13}C-NMR (150 MHz, $CDCl_3$)



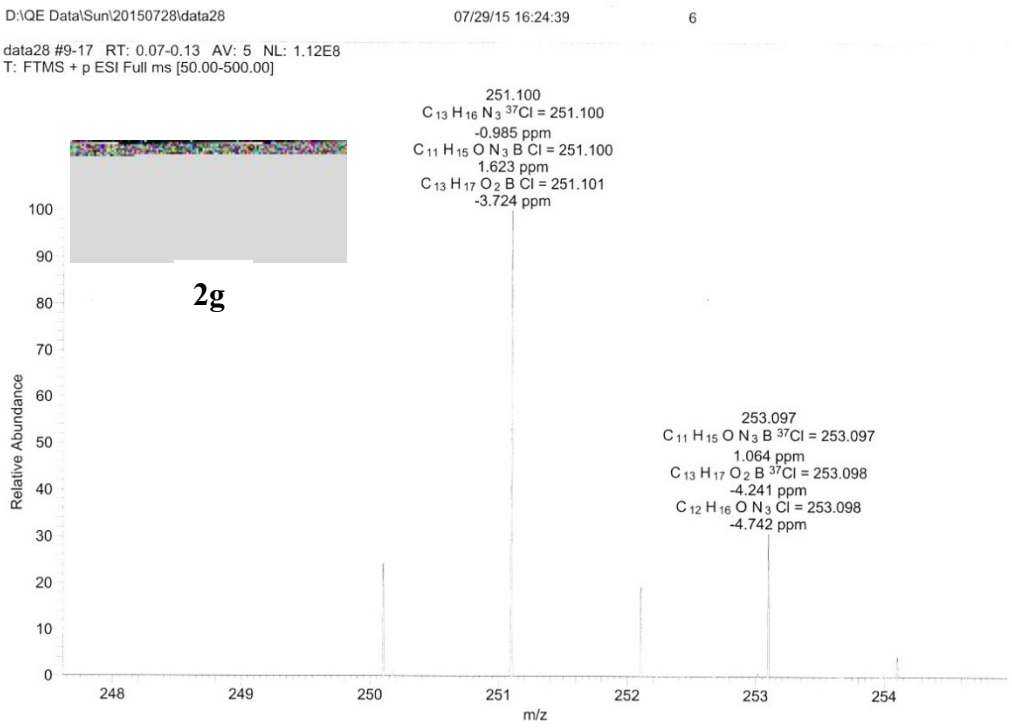
^{11}B-NMR (193 MHz, $CDCl_3$)



IR (KBr)

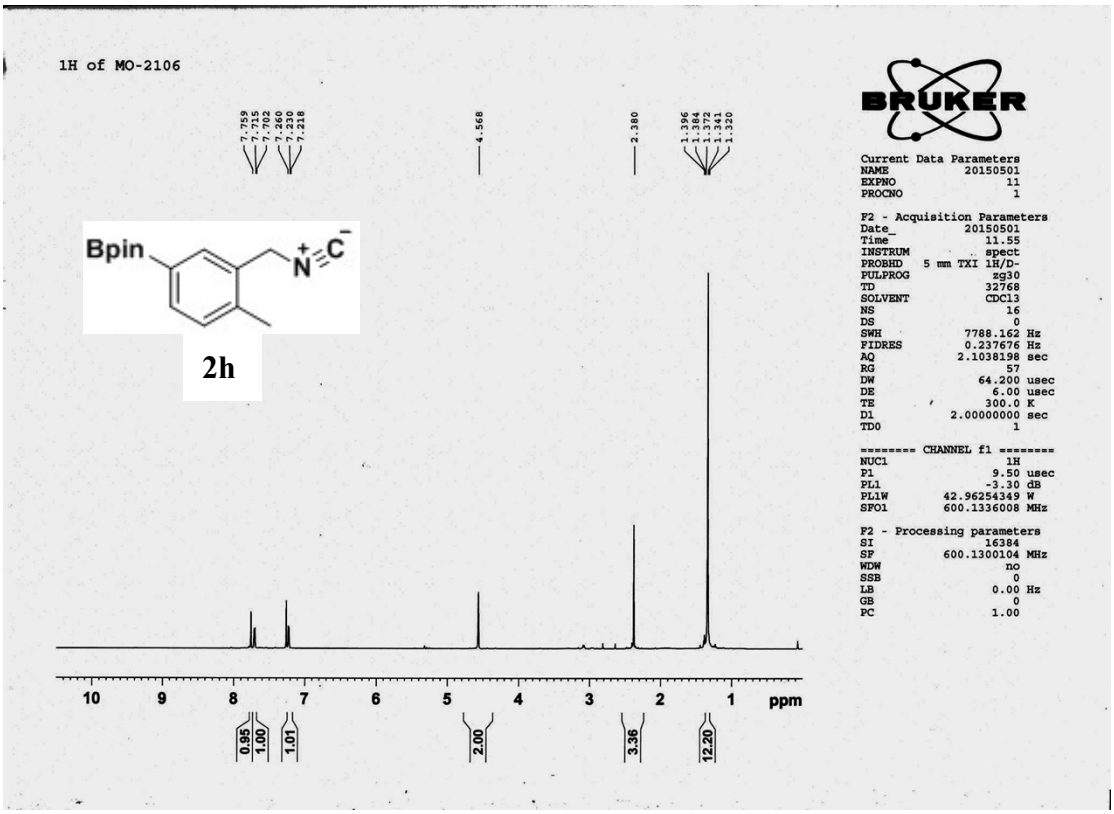


HRMS

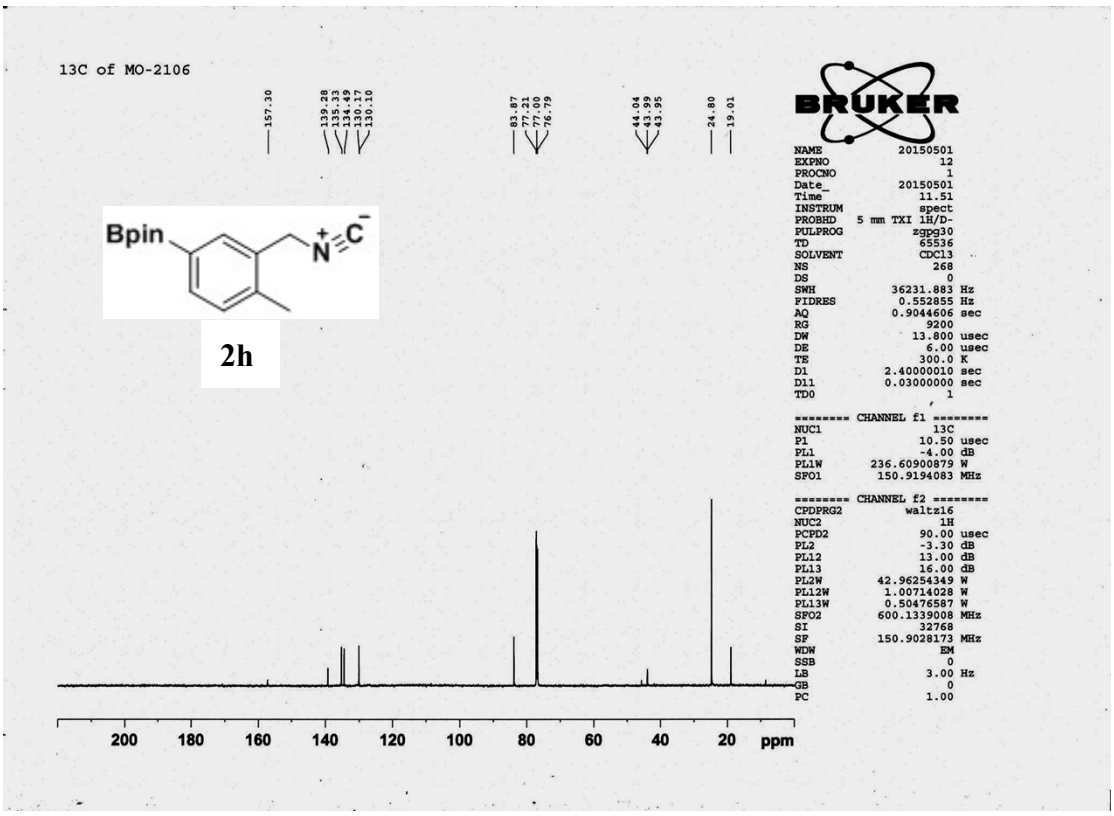

D:\QE Data\Sun\20150728\data28
07/29/15 16:24:39
6
data28 #9-17 RT: 0.07-0.13 AV: 5 NL: 1.12E8
T: FTMS + p ESI Full ms [50.00-500.00]
251.100
C 13 H 16 N 3 37Cl = 251.100
-0.985 ppm
C 11 H 15 O N 3 B Cl = 251.100
1.623 ppm
C 13 H 17 O 2 B Cl = 251.101
-3.724 ppm
2g
253.097
C 11 H 15 O N 3 B 37Cl = 253.097
1.064 ppm
C 13 H 17 O 2 B 37Cl = 253.098
-4.241 ppm
C 12 H 16 O N 3 Cl = 253.098
-4.742 ppm
Relative Abundance
m/z
100
90
80
70
60
50
40
30
20
10
0
248
249
250
251
252
253
254

2-(3-(isocyanomethyl)-4-methylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **(2h)**

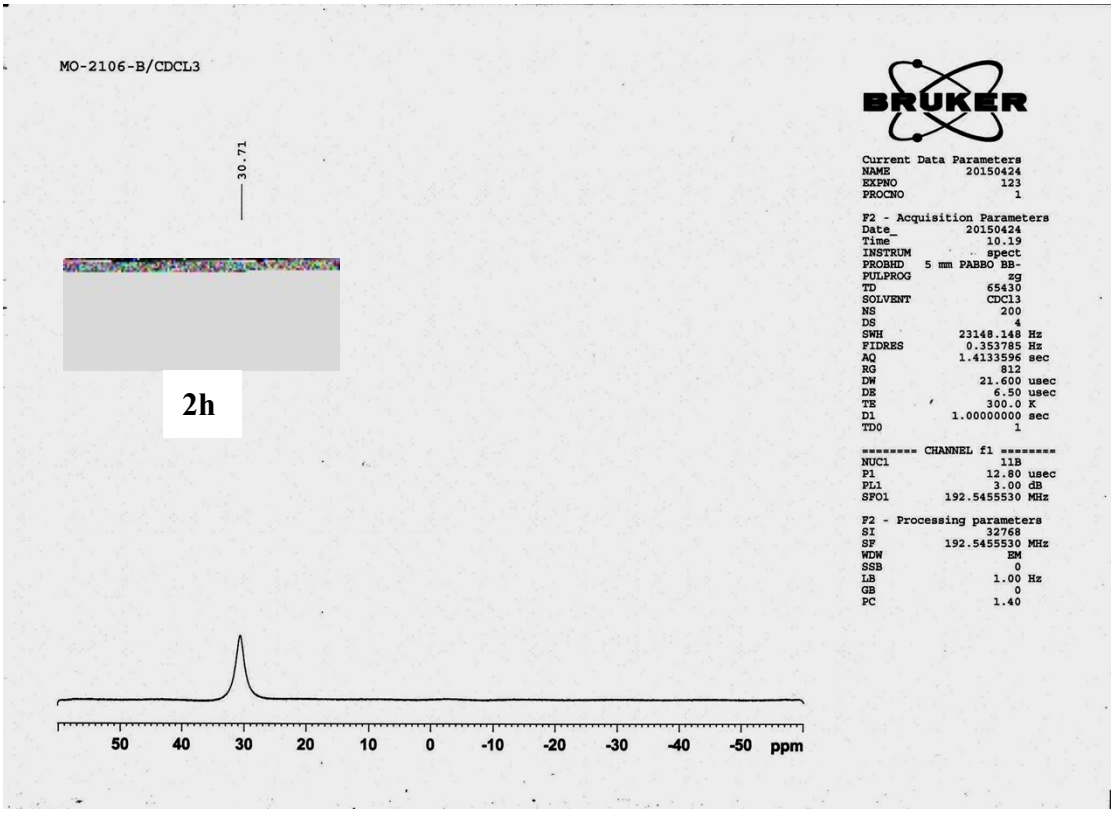
^{1}H-NMR (600 MHz, $CDCl_3$)



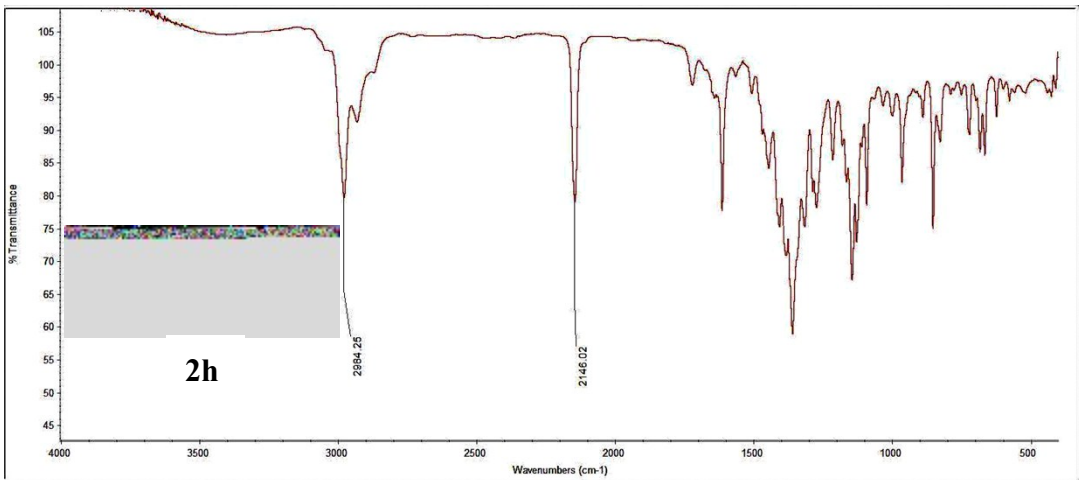
^{13}C-NMR (150 MHz, $CDCl_3$)



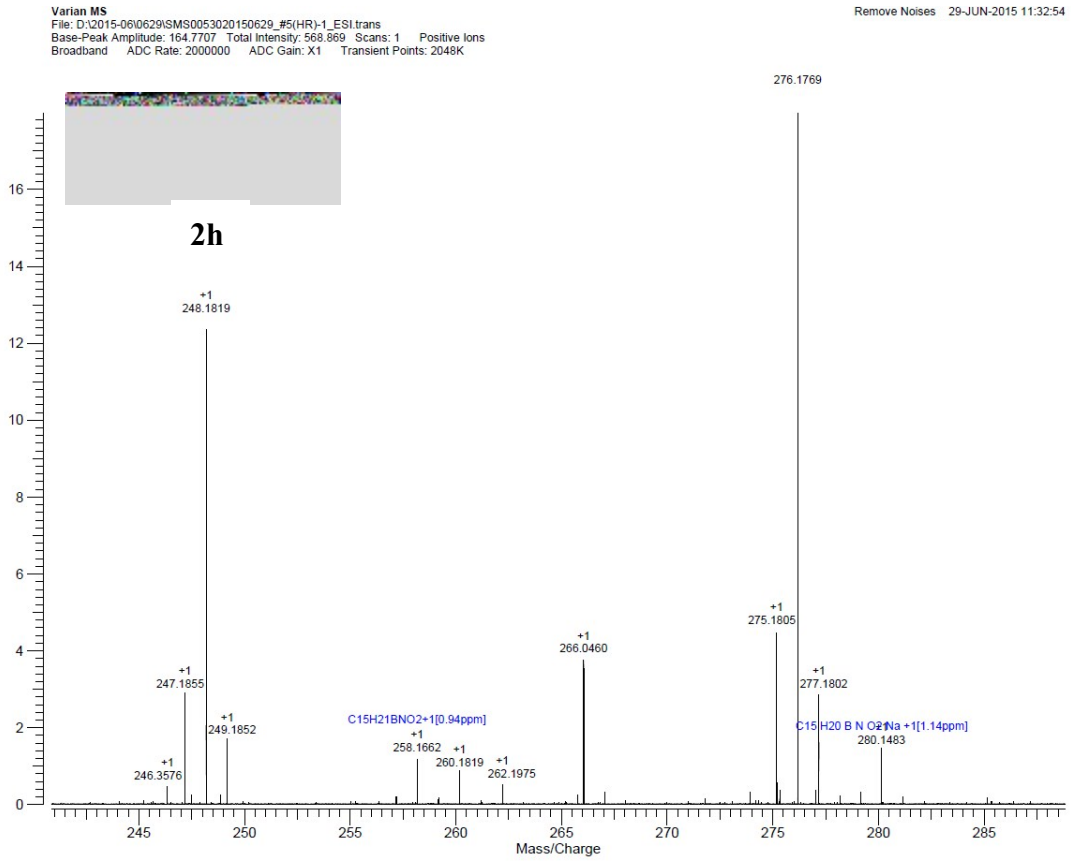
^{11}B-NMR (193 MHz, $CDCl_3$)



IR (KBr)

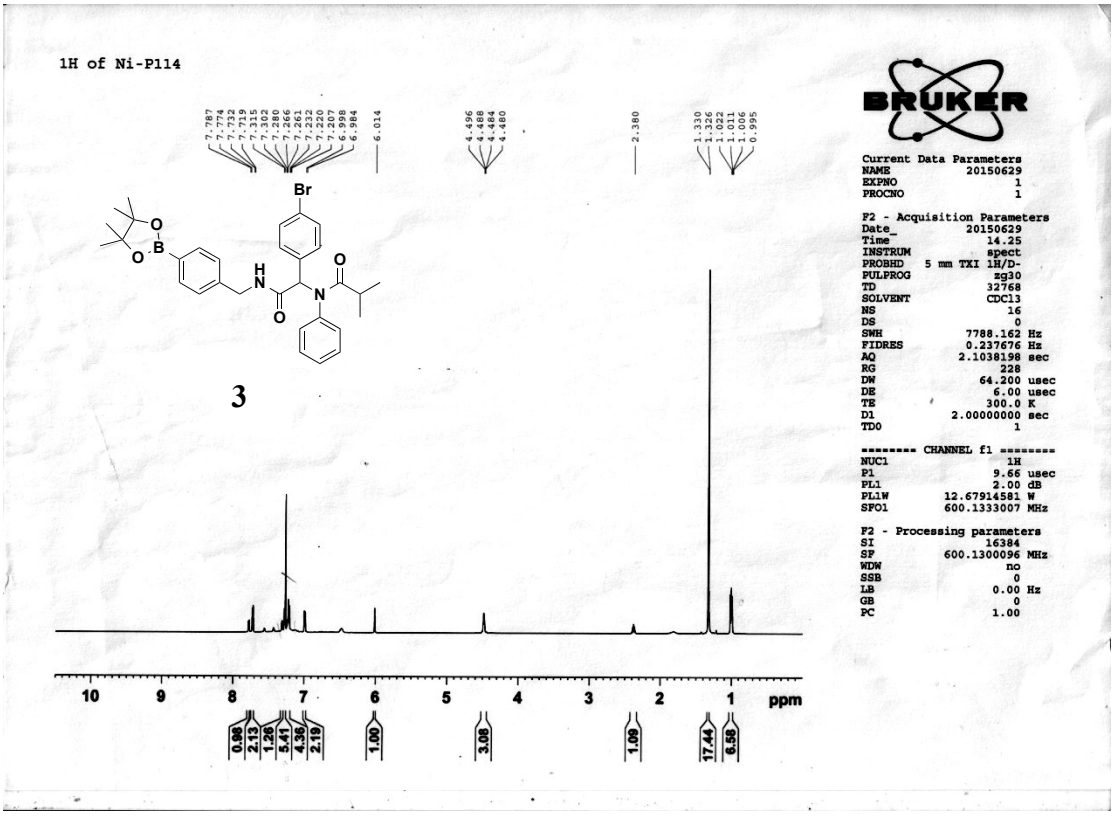


HRMS

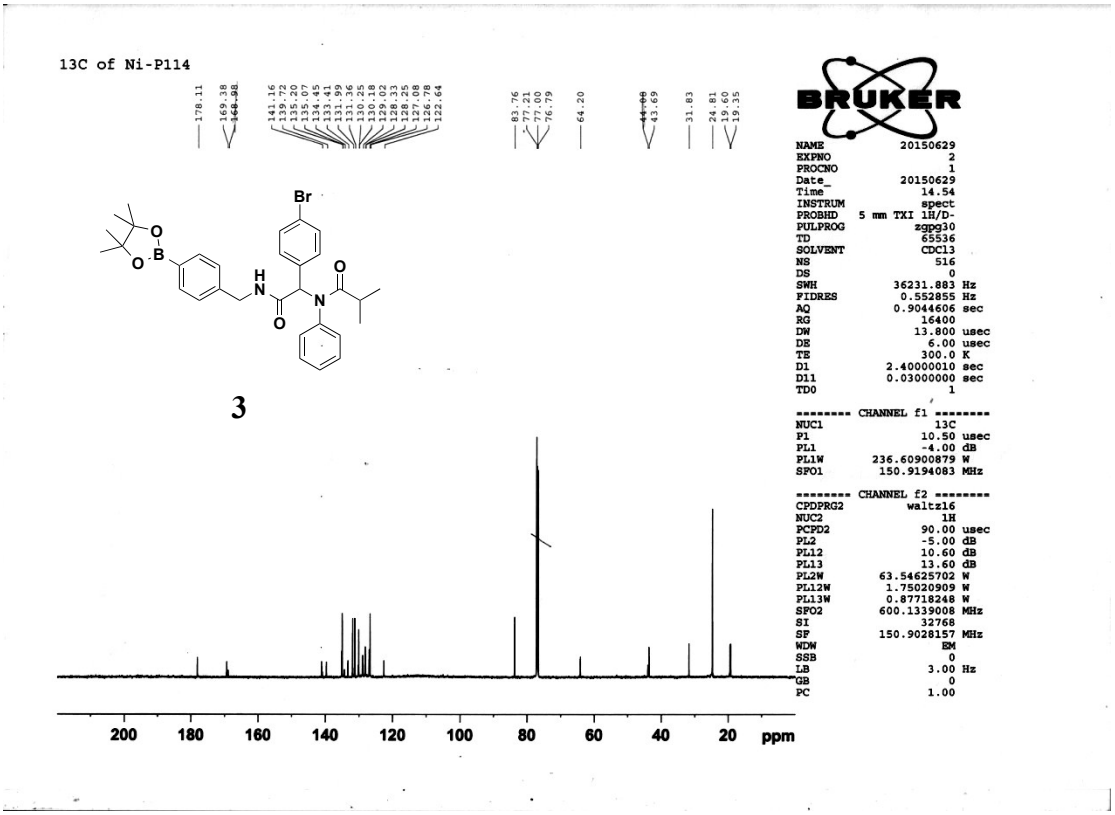

Varian MS
File: D:\2015-06\0629\SMS0053020150629_#5(HR)-1_ESI.trans
Base-Peak Amplitude: 164.7707 Total Intensity: 568.869 Scans: 1 Positive Ions
Broadband ADC Rate: 2000000 ADC Gain: X1 Transient Points: 2048K
Remove Noises 29-JUN-2015 11:32:54
2h
276.1769
+1 248.1819
+1 247.1855
+1 249.1852
+1 246.3576
+1 258.1662
+1 260.1819
+1 262.1975
+1 266.0460
+1 275.1805
+1 277.1802
+1 280.1483
C15H21BNO2+1[0.94ppm]
C15H20BNO2Na+1[1.14ppm]
Mass/Charge

N-(1-(4-bromophenyl)-2-oxo-2-((4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)amino)ethyl)-*N*-phenylisobutyramide **(3)**

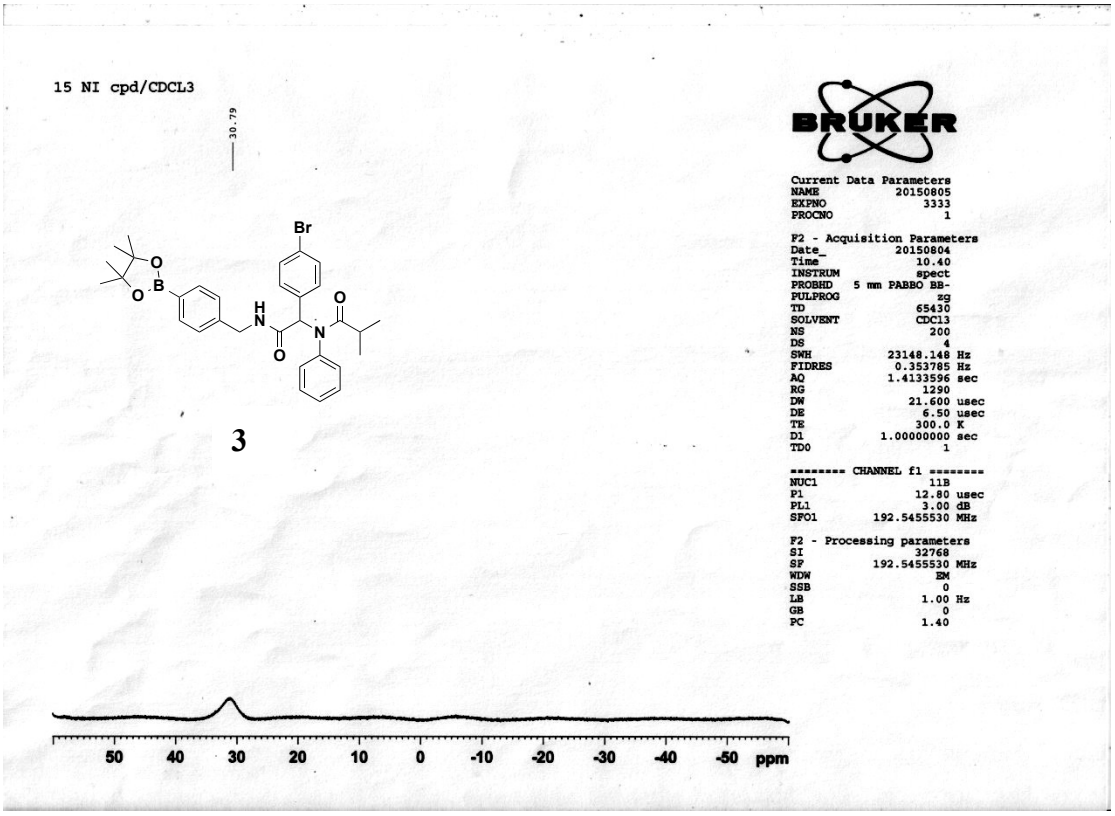
^{1}H-NMR (600 MHz, $CDCl_3$)



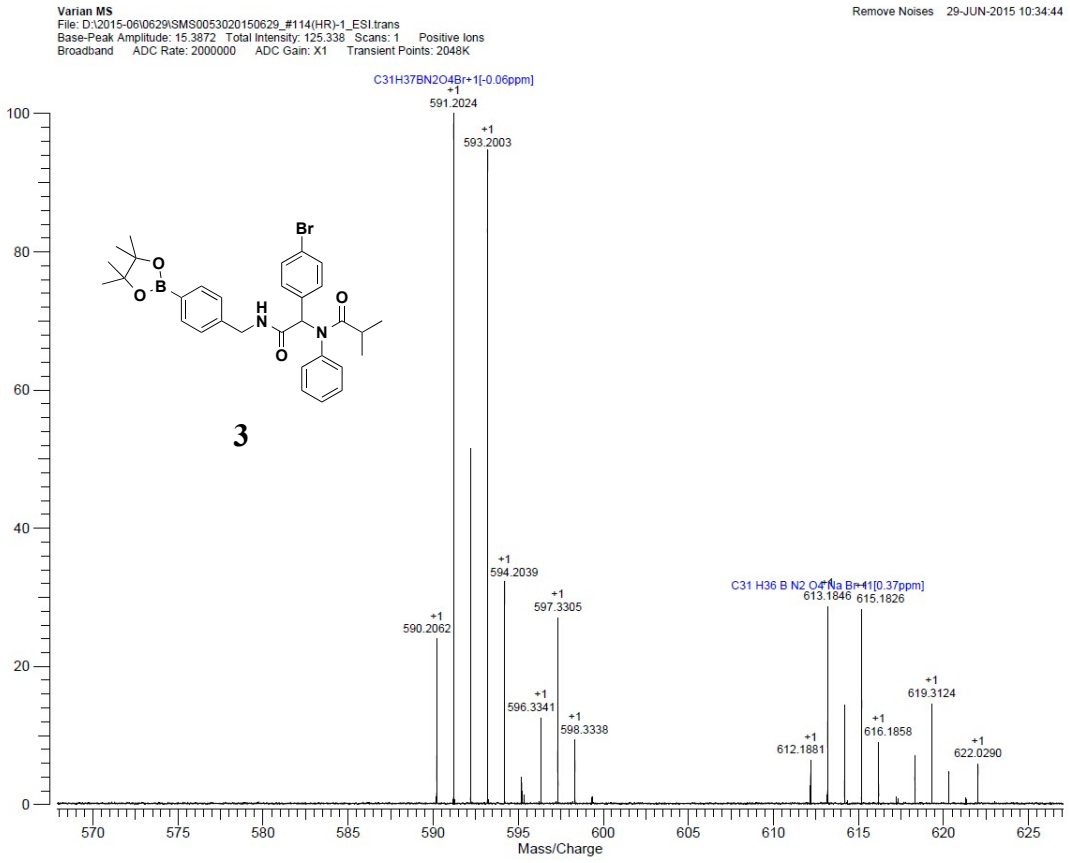
^{13}C-NMR (150 MHz, $CDCl_3$)



^{11}B-NMR (193 MHz, $CDCl_3$)

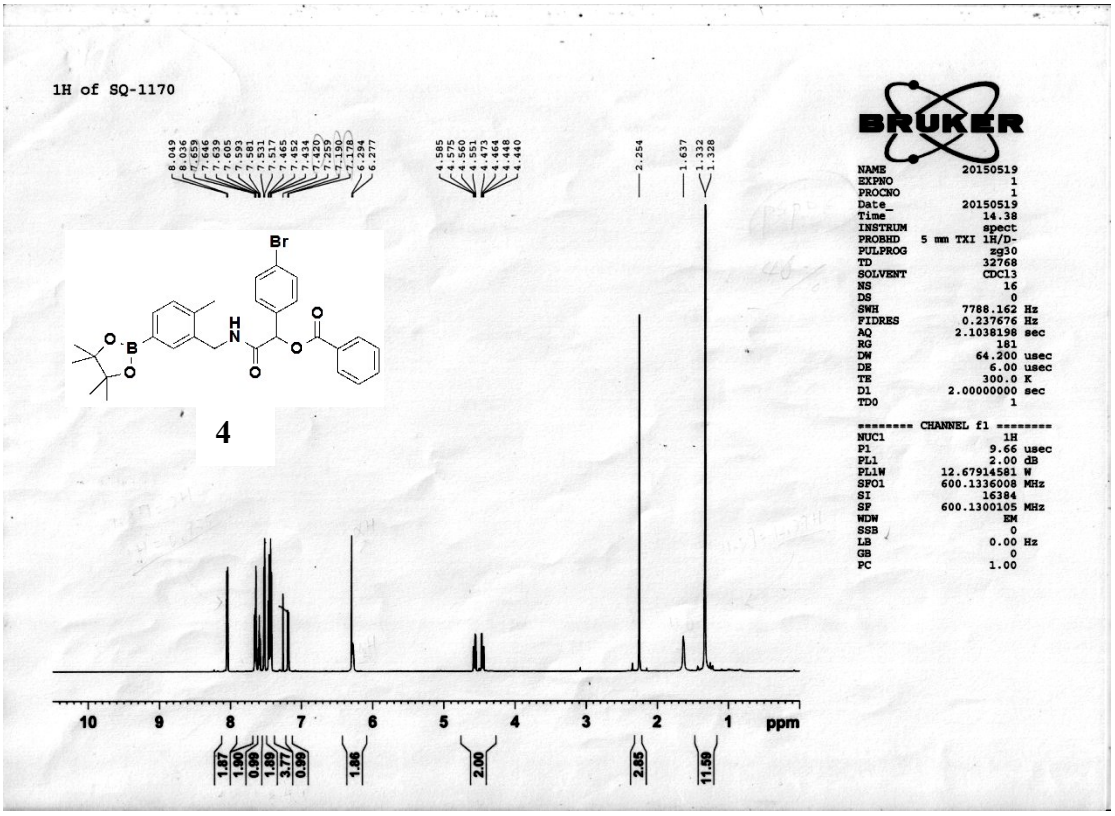


HRMS

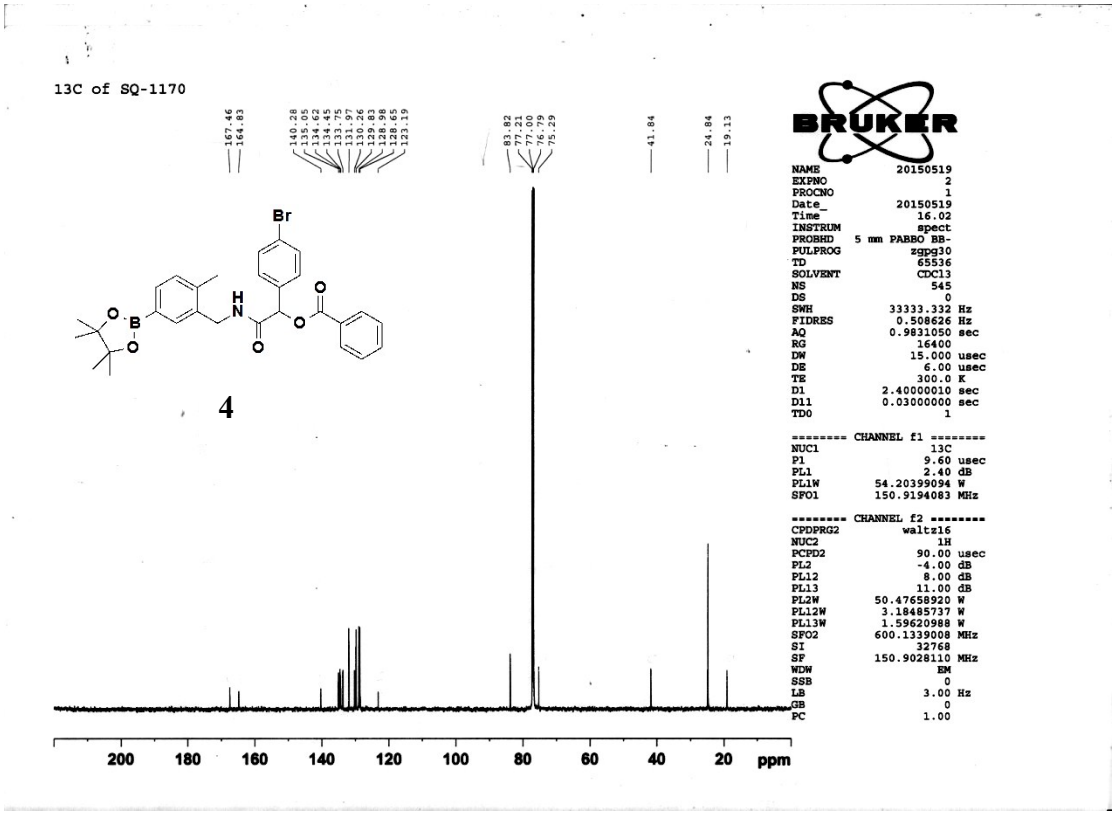


1-(4-bromophenyl)-2-((2-methyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benz yl)amino)-2-oxoethyl benzoate (**4**).

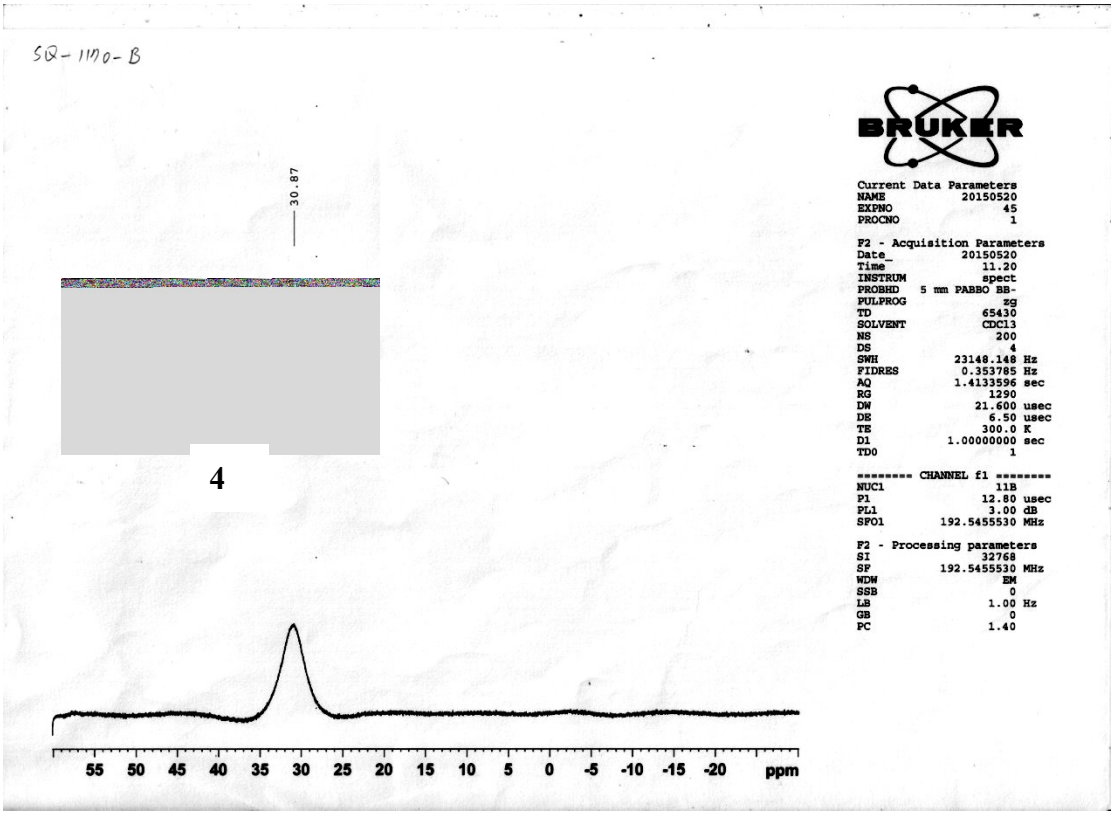
^{1}H-NMR (600 MHz, $CDCl_3$)



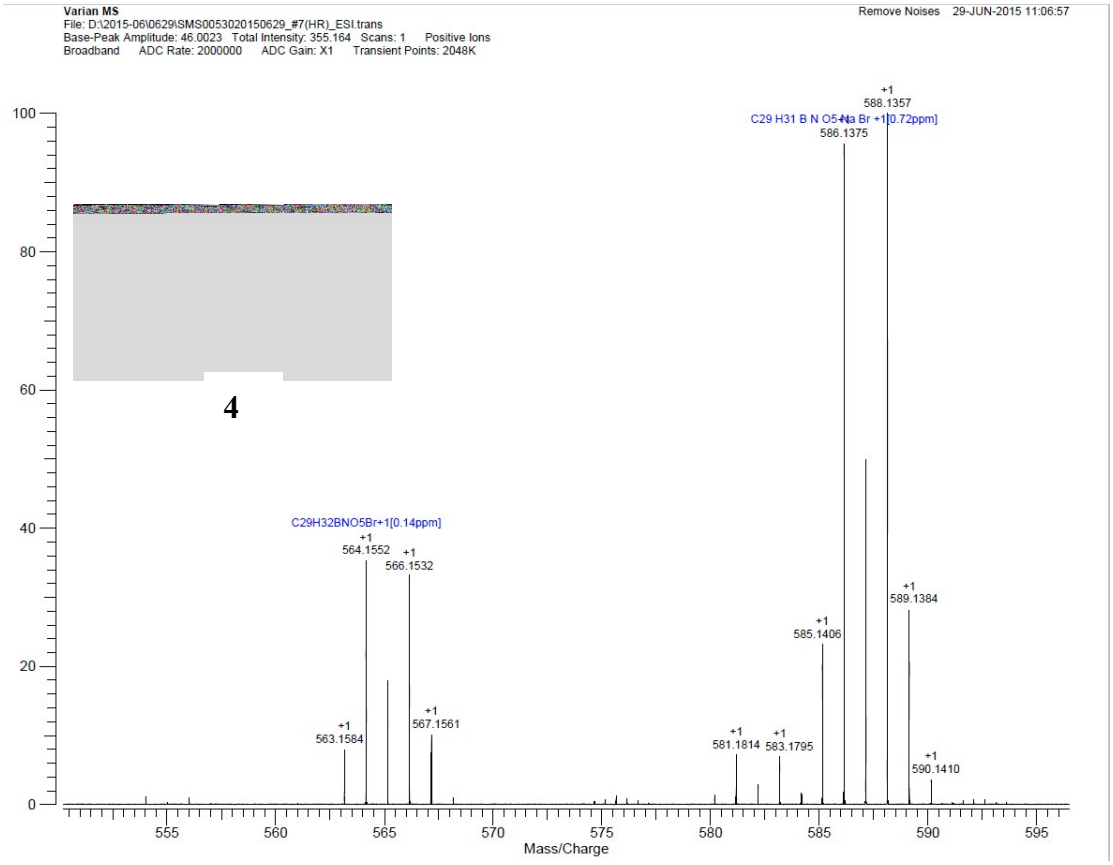
^{13}C-NMR (150 MHz, $CDCl_3$)



^{11}B-NMR (193 MHz, $CDCl_3$)

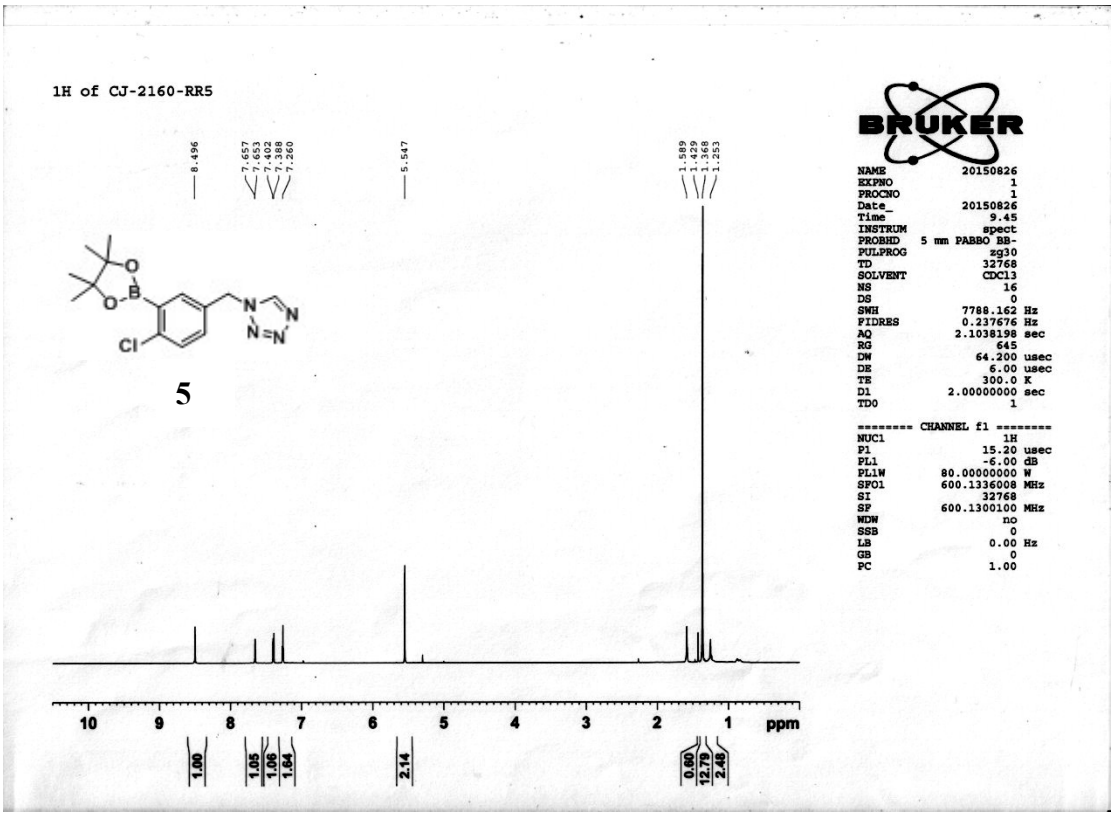


HRMS

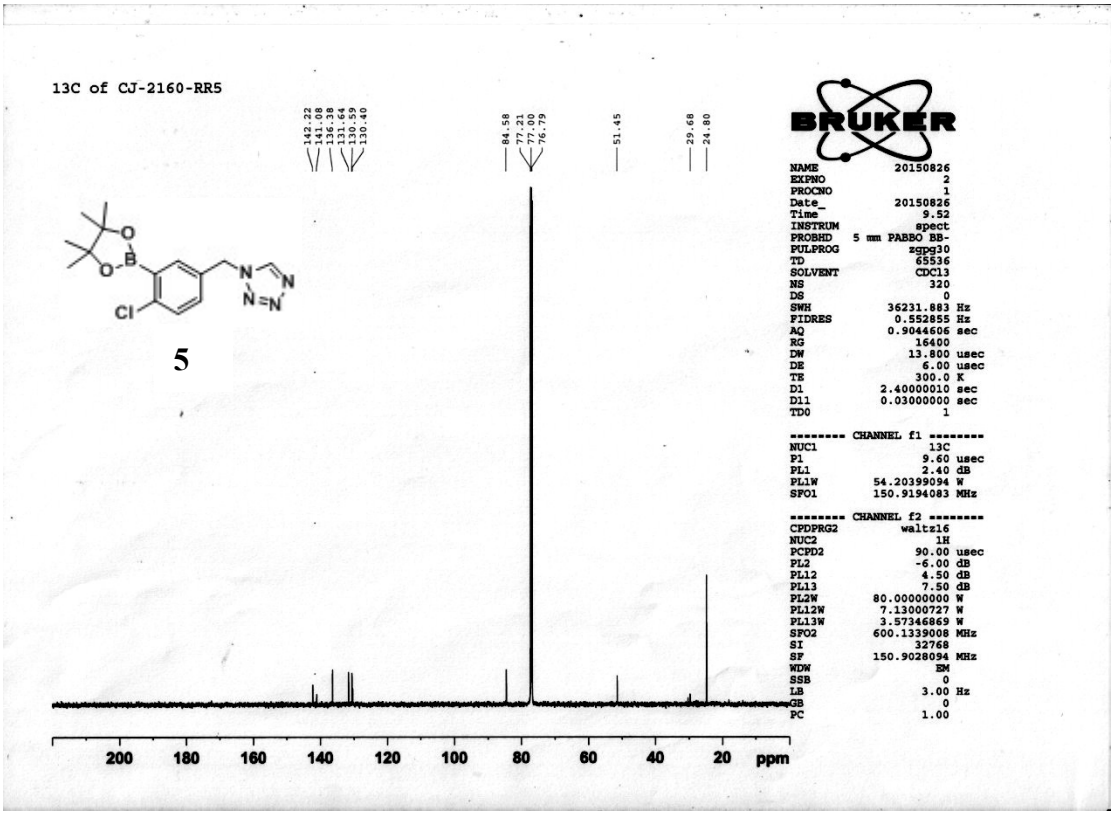


1-(4-chloro-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)-1*H*-tetrazole **(5)**

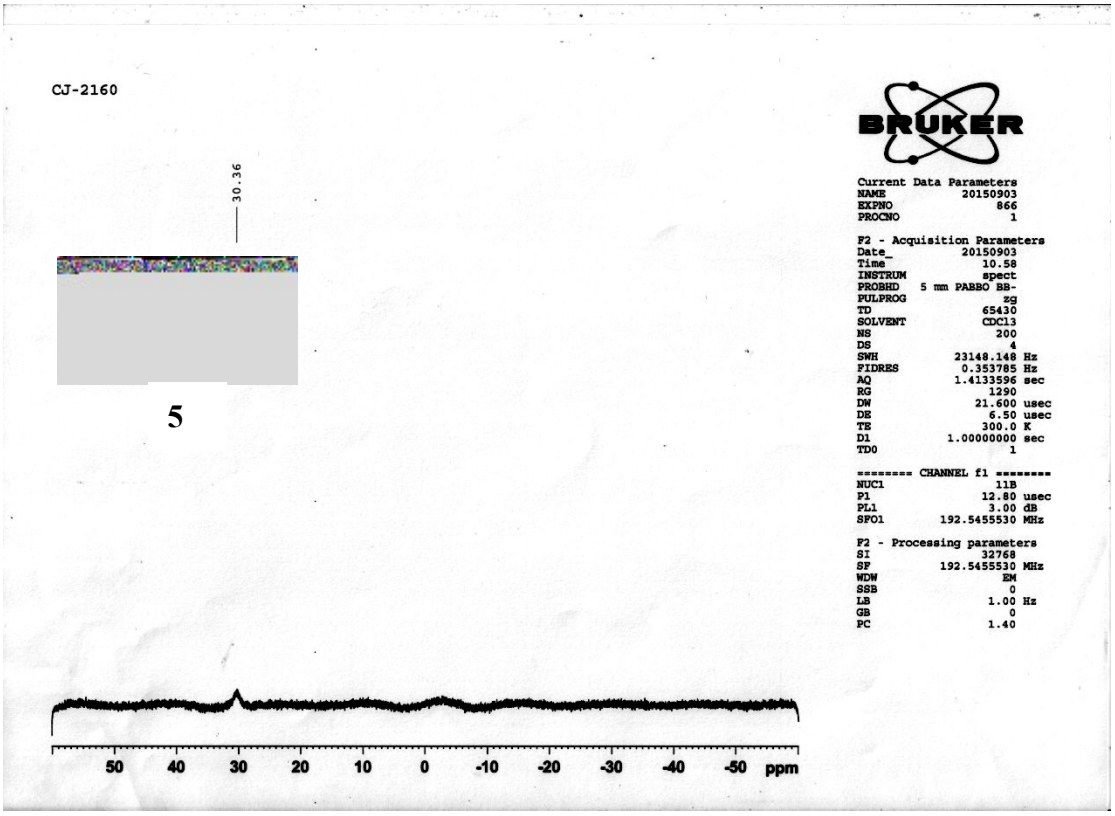
^{1}H-NMR (600 MHz, $CDCl_3$)



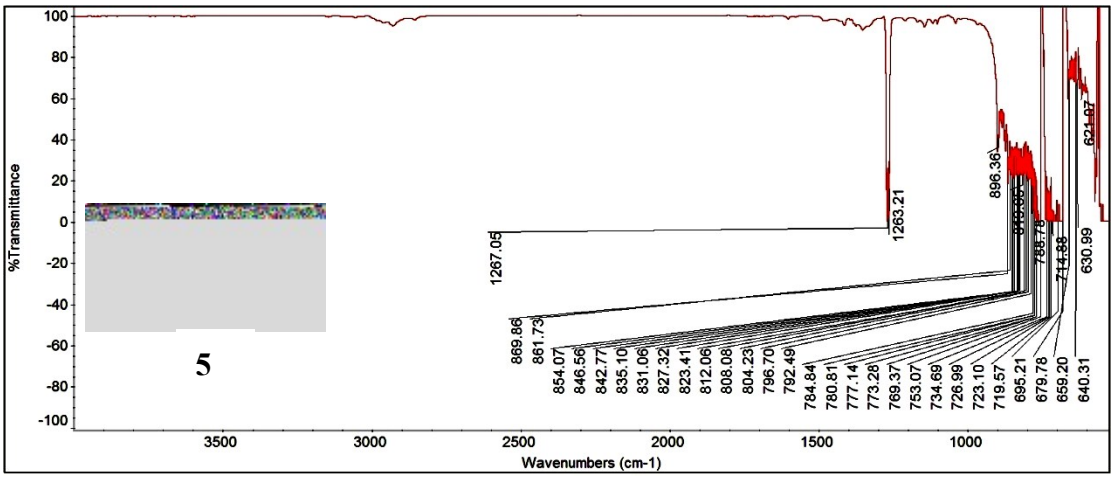
^{13}C-NMR (150 MHz, $CDCl_3$)



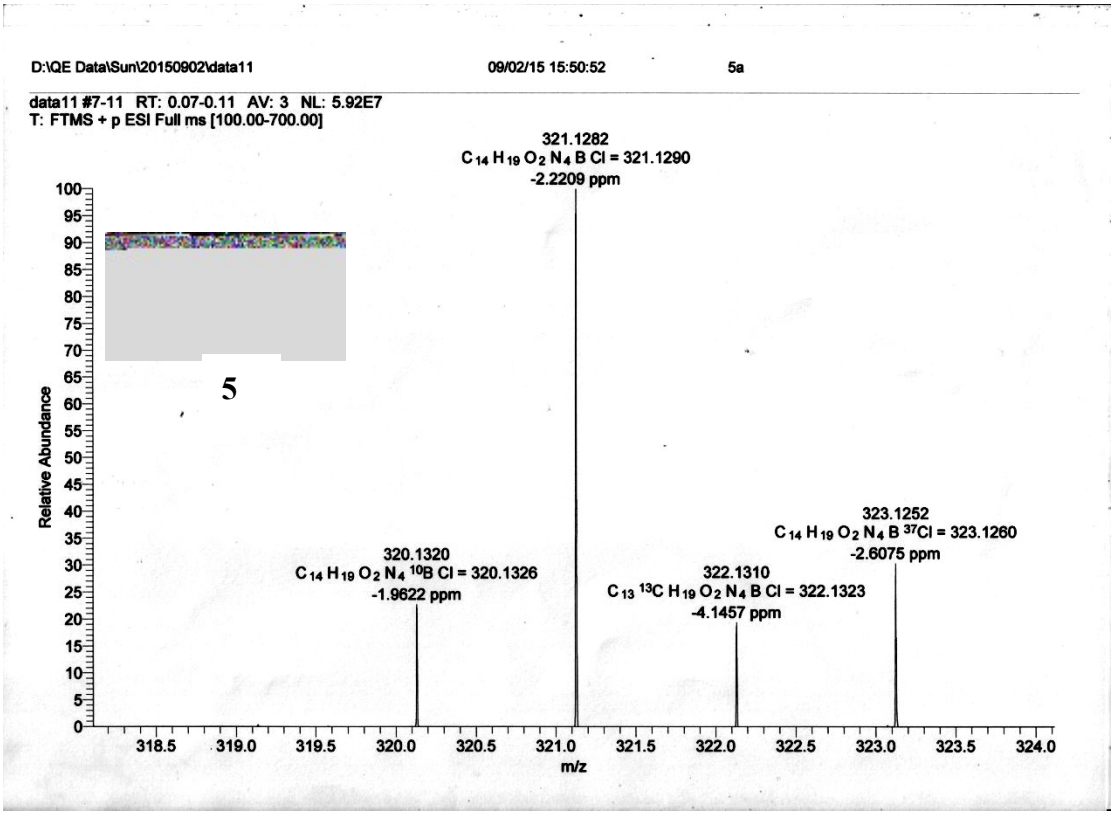
^{11}B-NMR (193 MHz, $CDCl_3$)



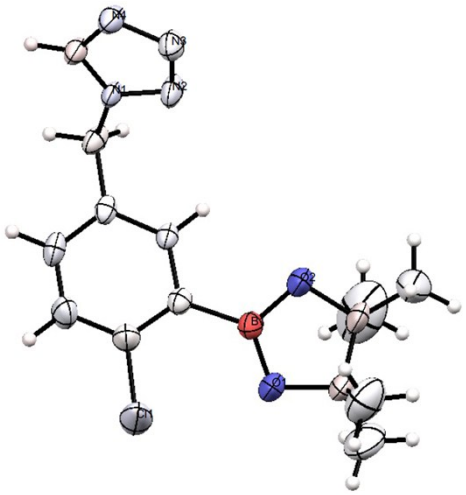
IR (KBr)



HRMS



X-ray crystallographic analysis of 1-(4-chloro-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl)-1*H*-tetrazole (**5**), thermal ellipsoids drawn at the 50% probability level.



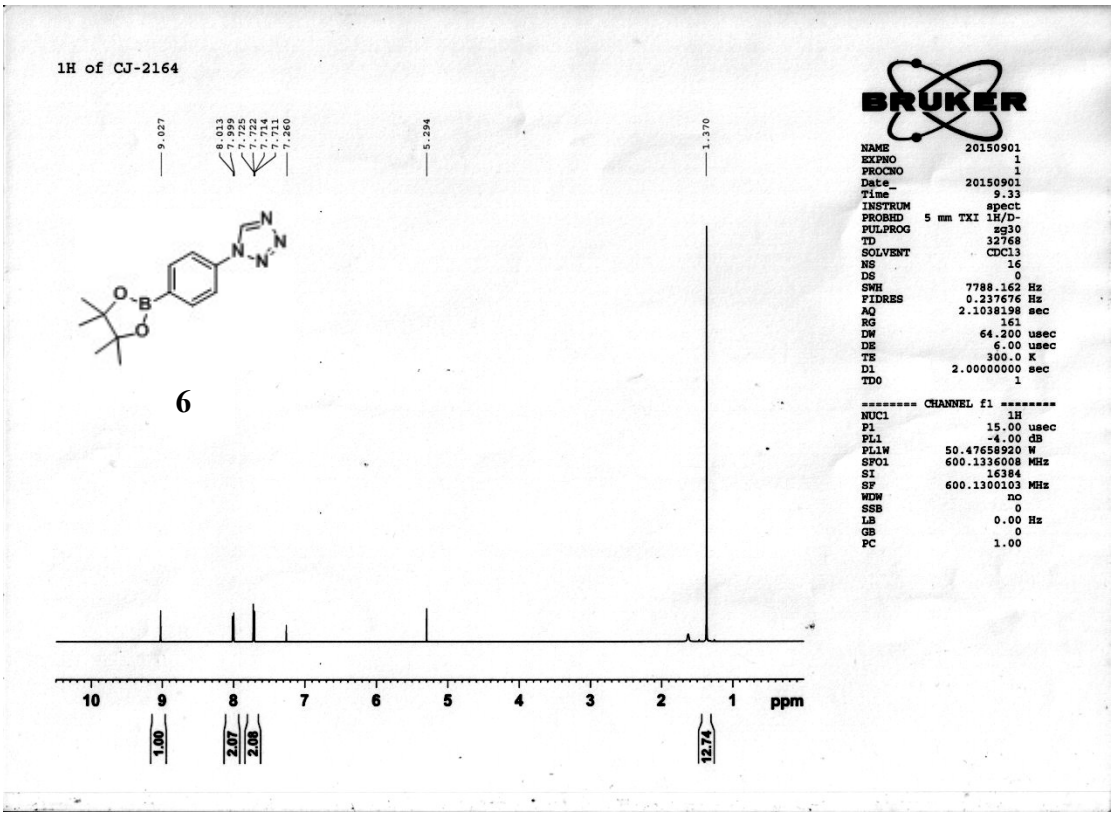
A clear pale-yellow columun-like specimen of $C_{14}H_{18}BClN_4O_2$, approximate dimensions 0.50 mm x 0.22 mm x 0.02 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were collected.

Table 1. Crystal data and structure refinement for 17399.

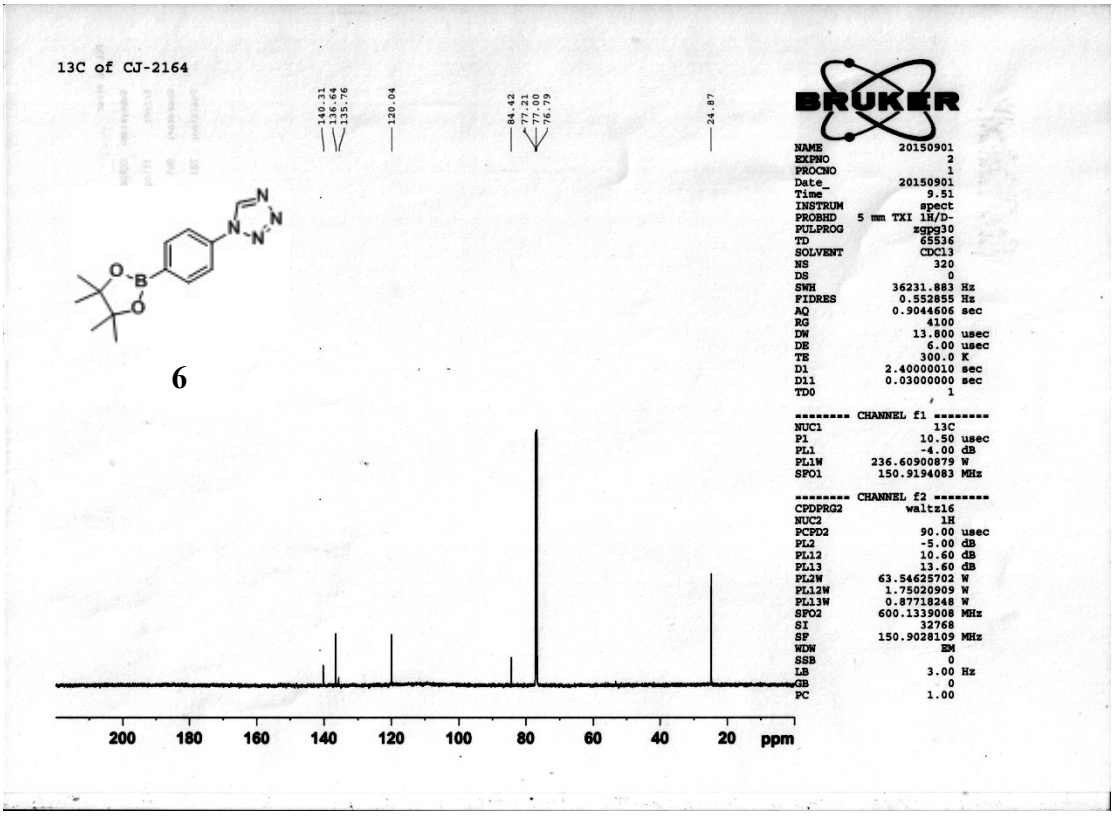
Identification code	17399	
Empirical formula	$C_{14}H_{18}BClN_4O_2$	
Formula weight	320.58	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 15.8491(11) Å	□= 90°.
	b = 10.2222(8) Å	□= 101.018(3)°.
	c = 10.1374(8) Å	□ = 90°.
Volume	1612.1(2) $Å^3$	
Z	4	
Density (calculated)	1.321 Mg/m^3	
Absorption coefficient	0.248 mm^{-1}	
F(000)	672	
Crystal size	0.50 x 0.22 x 0.02 mm^3	
Theta range for data collection	1.31 to 25.06°.	
Index ranges	-18<=h<=18, -8<=k<=12, -12<=l<=8	
Reflections collected	7566	
Independent reflections	2851 [R(int) = 0.0357]	
Completeness to theta = 25.06°	99.9 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9951 and 0.8860	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2851 / 0 / 199	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0626, wR2 = 0.1745	
R indices (all data)	R1 = 0.0896, wR2 = 0.2057	
Largest diff. peak and hole	0.681 and -0.379 $e.Å^{-3}$	

1-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1*H*-tetrazole **(6)**

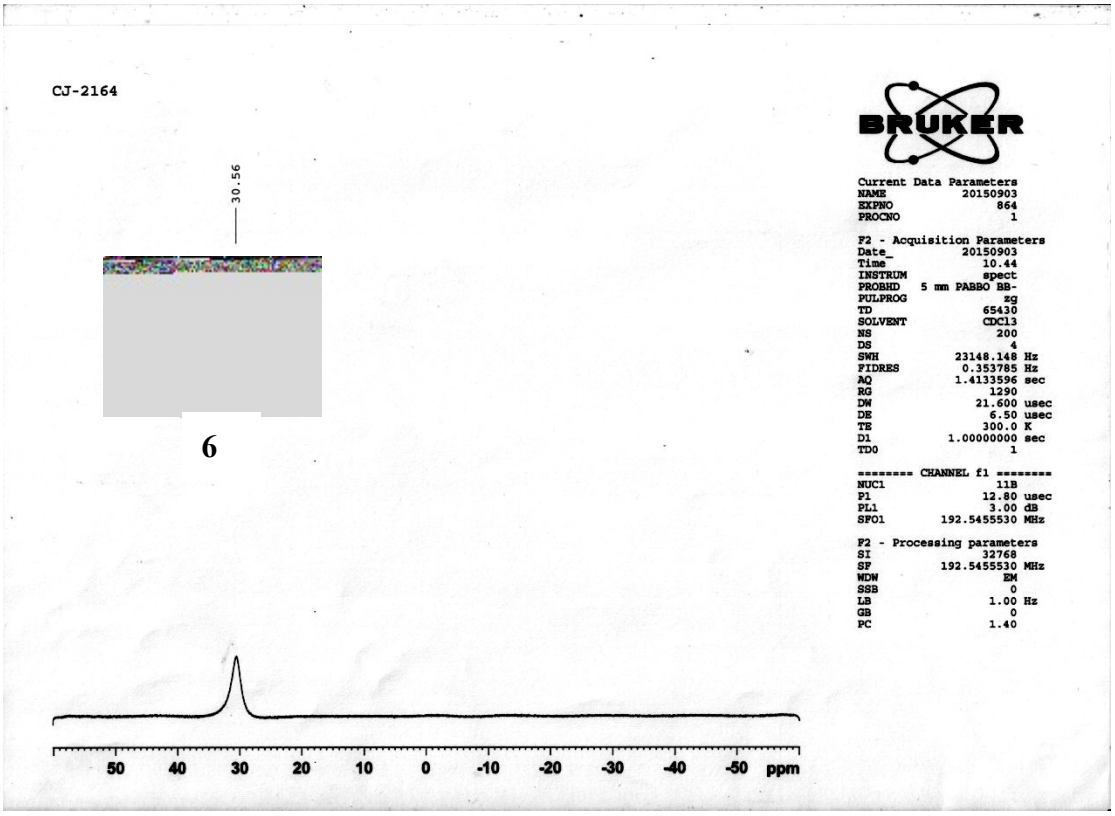
^{1}H-NMR (600 MHz, $CDCl_3$)



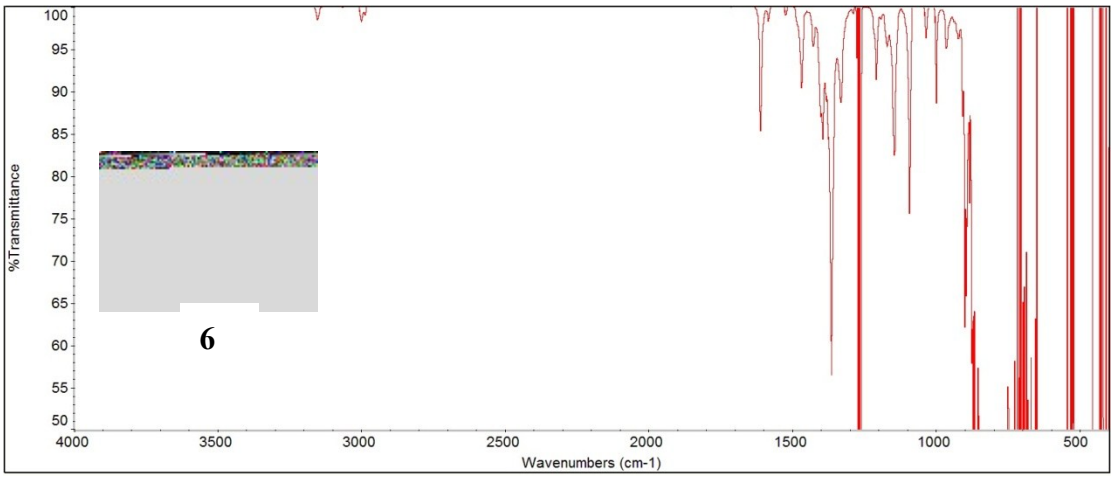
^{13}C-NMR (150 MHz, $CDCl_3$)



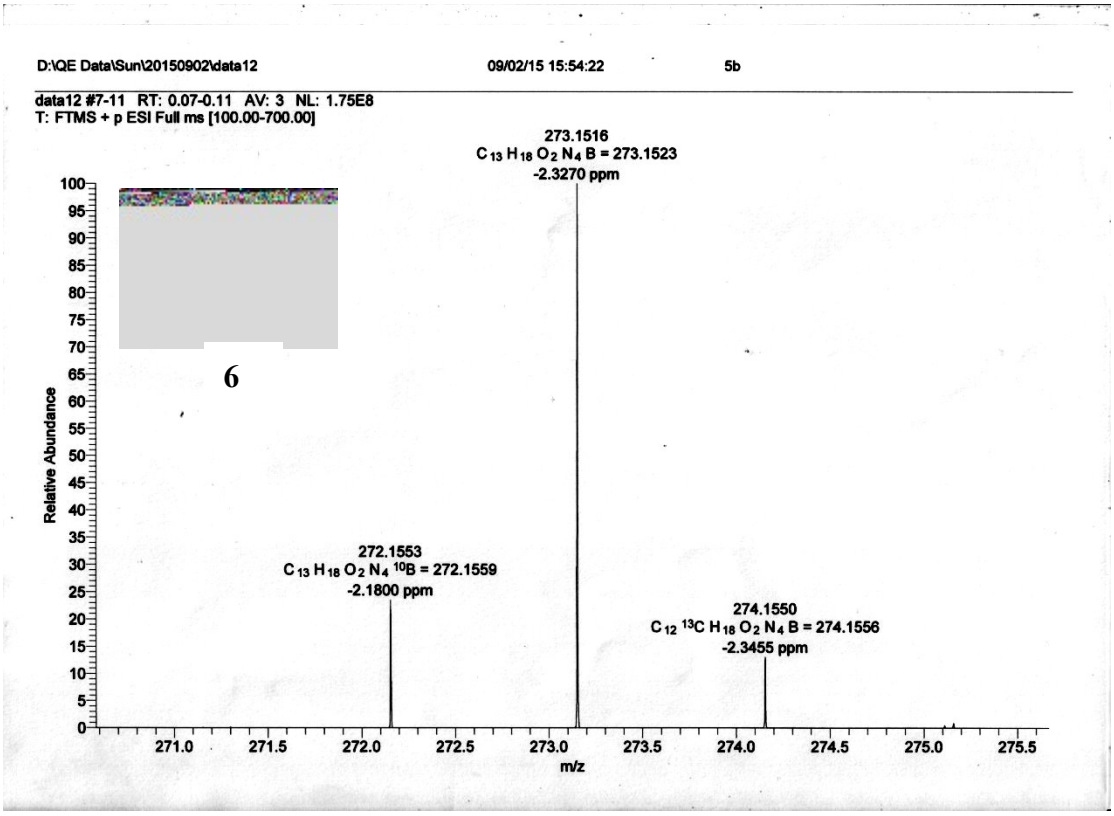
^{11}B-NMR (193 MHz, $CDCl_3$)



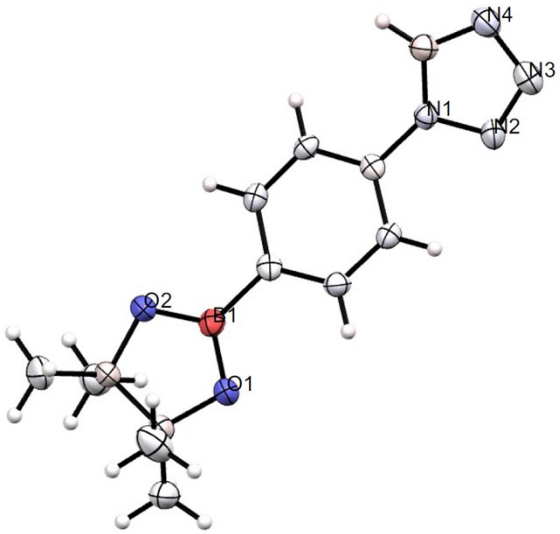
IR (KBr)



HRMS



X-ray crystallographic analysis of 1-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1*H*-tetrazole (**6**), thermal ellipsoids drawn at the 50% probability level.



A clear light-yellow columun-like specimen of $C_{13}H_{17}BN_4O_2$, approximate

dimensions 0.22 mm x 0.19 mm x 0.02 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were collected.

Table 1. Crystal data and structure refinement for a17398.

Identification code	a17398	
Empirical formula	C_{13} H_{17} BN_4O_2	
Formula weight	272.12	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 17.6880(11) Å	□= 90°.
	b = 6.9800(8) Å	□= 108.949(5)°.
	c = 11.9076(9) Å	□ = 90°.
Volume	1390.5(2) Å^3	
Z	4	
Density (calculated)	1.300 Mg/m^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	576	
Crystal size	0.22 x 0.19 x 0.02 mm^3	
Theta range for data collection	2.43 to 25.01°.	
Index ranges	-19<=h<=21, -7<=k<=8, -13<=l<=14	
Reflections collected	7550	
Independent reflections	2442 [R(int) = 0.0487]	
Completeness to theta = 25.01°	99.4 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9982 and 0.9806	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2442 / 0 / 181	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0503, wR2 = 0.1003	
R indices (all data)	R1 = 0.0966, wR2 = 0.1169	
Largest diff. peak and hole	0.182 and -0.179 e.Å^{-3}	

Calculation methods

All the calculation results were performed by Gaussion 09 software.[1] The optimized structure of 2a was obtained at DFT/B3LYP/6-31G(d,p) method.[2-4] Projected density of state (pDOS) analysis and related molecular diagrams of HOMO and LUMO were achieved by using the pop = full keyword under the calculation procedure of DFT/B3LYP/6-31G(d,p) method.

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3 B. Miehlich, A. Savin, H. Stoll, H. Preuss, *Chem. Phys. Lett.* 1989, **157**, 200.

4 C. Lee, W. Yang, R.G. Parr, *Phys. Rev. B.,* 1988, **37***,* 785.