Electronic Supporting Information (ESI)

Cu-Mn spinel oxide catalyzed synthesis of imidazo[1,2-a]pyridines through domino three-component coupling and 5-exo-dig cyclization in water ¤

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S1. Characterization of Cu-Mn catalysts

S1.a. XRD of Cu-Mn catalysts

The powder X-ray diffraction patterns of samples were recorded on X-ray diffractometer using Ni filter and Gobel Mirror parallel beam geometry (CuKα : λ = 0.15418 nm) in the 2θ range 10-750 in step scan mode (Step Size: 0.02o , Scan Speed: 2 s/step). The phases were identified by search match procedure with the help of DIFFRAC PLUS software using JCPDS databank.

It was found that kind of phase/s make the largest contribution to perform the main role of catalyst. The powder X-ray diffraction (XRD) of the catalysts shown in Fig 1 and the following phases were identified with the 2 theta values such as; Tenorite, (CuO): 35.490, 35.550, 38.730 and 48.760; Copper Manganese Oxide (Cu1.4Mn1.6O4): 30.420, 35.880, 43.560 and 57.600; Hausmannite, (Mn3O4): 18.000, 28.880, 32.31 and 36.080; Manganese Chloride Hydrate, ($MnCl_2.2H_2O$): 15.710, 20.170, 30.570 and 32.000 and Crednerite, ($CuMn_2O4$): 31.360, 33.020, 35.300, 36.960 and 51.780. Each phase marked in the Fig 1. XRD studies of the catalysts revealed that activity of the samples calcined at 425 oC might be due to the surface interaction of the two oxides because of formation of following bimetallic spinel such as $CuMn_2O_4$ and $CuxMn_3$-xO_4 (x = 1.4–1.6).

Table S1. Results of XRD for the Cu-Mn spinel oxide (A-C)

Catalyst	**Composition (Cu: Mn molar ratio)**	**Phases present**[a]
Cu-Mn catalyst **A**	2 : 0.25	Tenorite (CuO); Copper Manganese Oxide ($Cu1.4Mn1.6O_4$); Hausmannite, (Mn_3O_4); Manganese Chloride Hydrate, ($MnCl_2 \cdot 2H_2O$); Crednerite ($CuMn_2O_4$)
Cu-Mn catalyst **B**	1 : 0.25	Tenorite (CuO); Copper Manganese Oxide ($Cu1.4Mn1.6O_4$); Hausmannite, (Mn_3O_4); Manganese Chloride Hydrate, ($MnCl_2 \cdot 2H_2O$); Crednerite ($CuMn_2O_4$)
Cu-Mn catalyst **C**	3 : 0.25	Tenorite (CuO); Copper Manganese Oxide ($Cu1.4Mn1.6O_4$)

[a] Phases are identified by a search match procedure with the help of DIFFRACPLUS software using JCPDS databank.

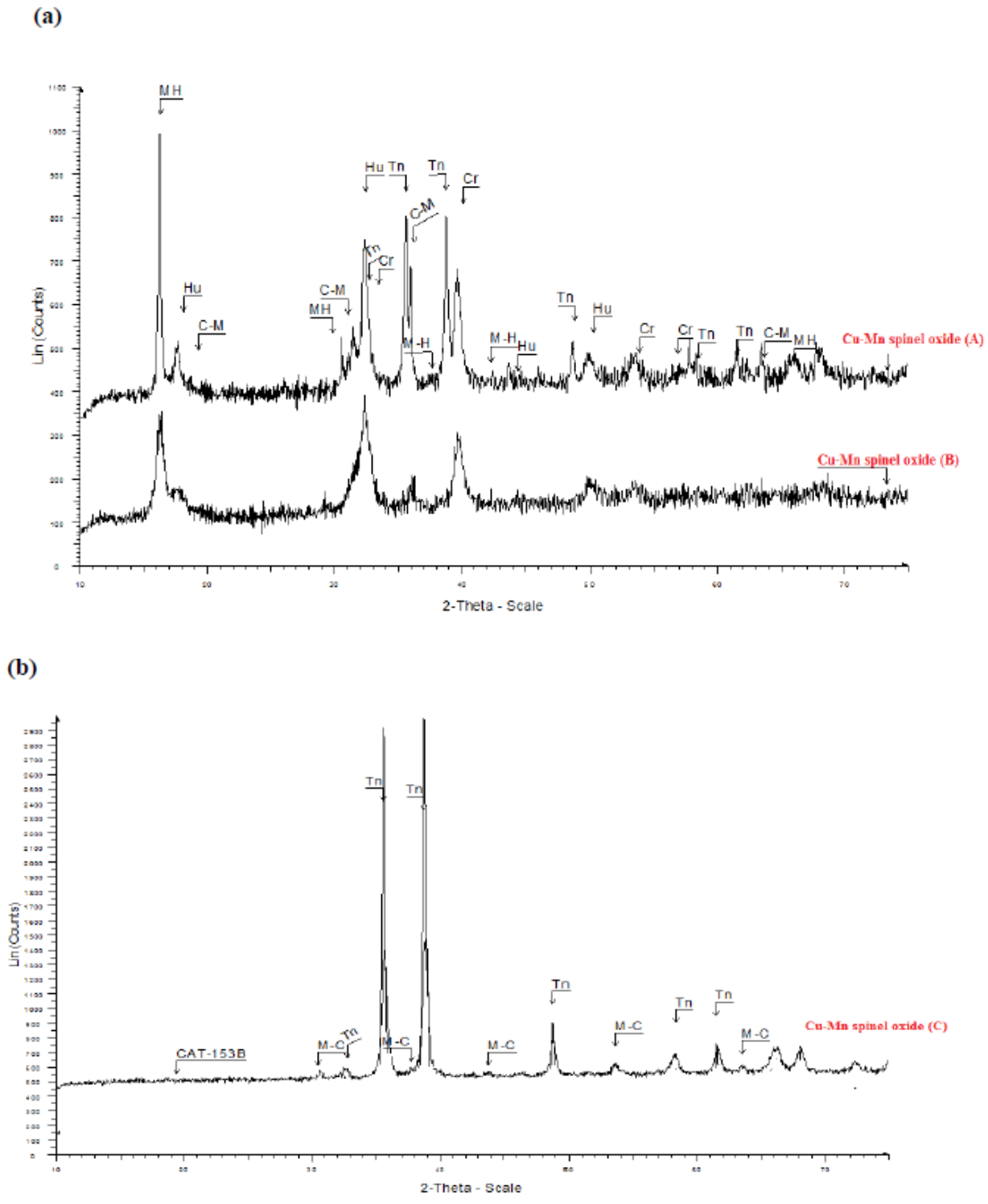


Figure S1. Powder X-ray diffraction (XRD) of the catalyst (a) Cu-Mn catalysts **A** and **B** (b) XRD of Cu-Mn catalyst **C**. (Tenorite: Tn, Copper Manganese Oxide: C-M, Hausmannite: Hu, Manganese Chloride Hydrate: M-H, Crednerite: Cr)

S1.b. Surface area of Cu-Mn catalysts

Specific surface areas of the Cu-Mn catalysts **A-C** were measured with N_2 adsorption using chemisorptions instrument and results are presented in Table S2.

Table S2. Specific surface area of Cu-Mn catalysts **A-C**

Catalysts	**Specific surface area (m^2/g)**
Cu-Mn catalyst **A**	42.07
Cu-Mn catalyst **B**	49.79
Cu-Mn catalyst **C**	46.62

S1.c. Scanning electron micrograph (SEM) of Cu-Mn catalysts

Scanning electron micrograph (SEM) of the samples was taken with an ASID attached to electron microscope at a magnification of about 15000 times. The accelerate voltage of 40 kv was applied. The image shows that the materials are composed of aggregates of near spherical nanoparticles and presented in a nanosize structure. This type of morphology showed the presence of a large number of adsorption sites in the materials which in part contribute to the high catalytic activity.[3] SEM patterns as shown in Fig 2 represents the before use and after use Cu-Mn spinel oxide (B). The SEM image of used catalyst was taken after third run and after each run catalyst (Cu-Mn spinel oxide B) was calcined at 425 °C. These nano-spherical particles have appeared almost same as fresh catalyst after regeneration. It can be seen that the morphology retained same as before test, this indicates that the catalyst maintains high structural stability during the reaction.

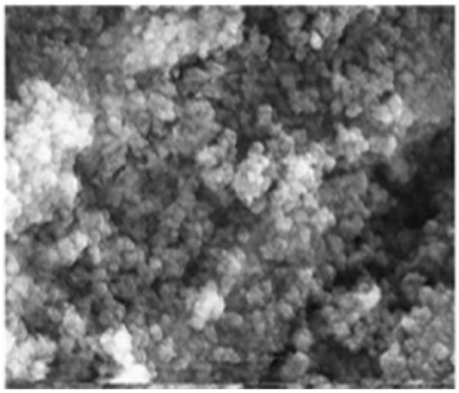


Figure S2. SEM image of Cu-Mn – B

S1.d. X-ray photoelectron spectra (XPS) for Cu-Mn catalyst B

The oxidation states of both metals in Cu-Mn catalyst B was determined by XPS analysis. Figure S3a shows the high resolution narrow scans of Mn 2p for Cu-Mn catalyst B. The observed spin-orbit splitting between the two main peak positions of Mn – Mn $2p_{3/2}$ and $Mn2p_{1/2}$ could be deconvoluted into three peaks each and the distance between them was ~ 12 eV.[8] The observed binding energy peaks are broad and asymmetric, which suggests the coexistence of Mn in multivalent states as Mn^{2+}, Mn^{3+} and Mn^{4+} ions. The asymmetric index β value was found to be 1.36, which is the evidence for the multiplet splitting of the Mn 2p level.[9] Figure S3b shows the high resolution narrow scans of Cu 2p for Cu-Mn catalyst B. The observed binding energy peaks at ~ 934 eV and ~ 955 eV are due to Cu $2p_{3/2}$ and Cu $2p_{1/2}$, respectively and can be attributed to Cu in +2 oxidation state. Thus, the XPS analysis indicated that the Cu exists in Cu^{2+} oxidation state and Mn in the multi-states (Mn^{2+}, Mn^{3+} and Mn^{4+}). Thus, the improved efficiency of Cu and Mn metals when combined in the form of bimetallic catalyst, over individual metals could be attributed to the existence of these metals in multiple oxidation states (Cu^{+2}, Mn^{+2}, Mn^{+3} and Mn^{+4}) in bimetallic Cu-Mn catalyst.

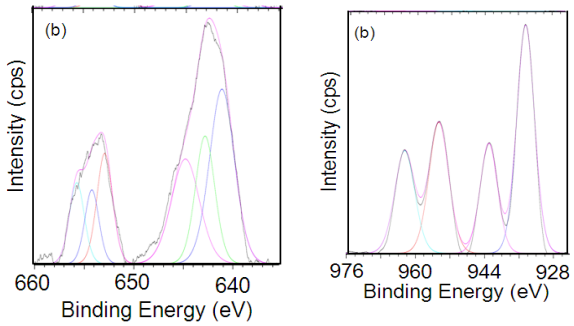
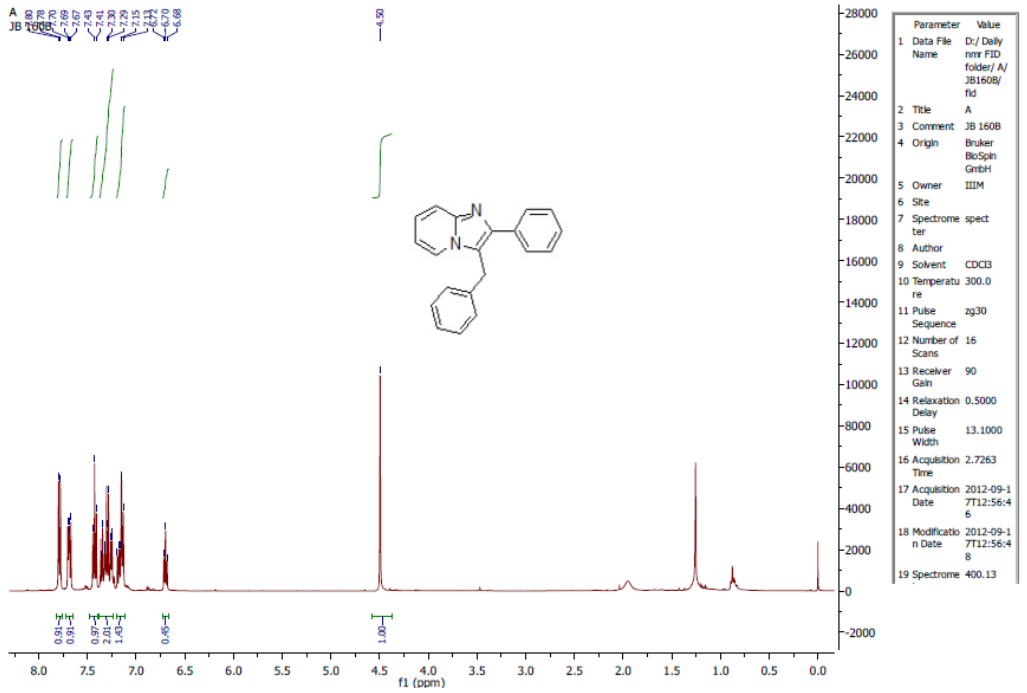
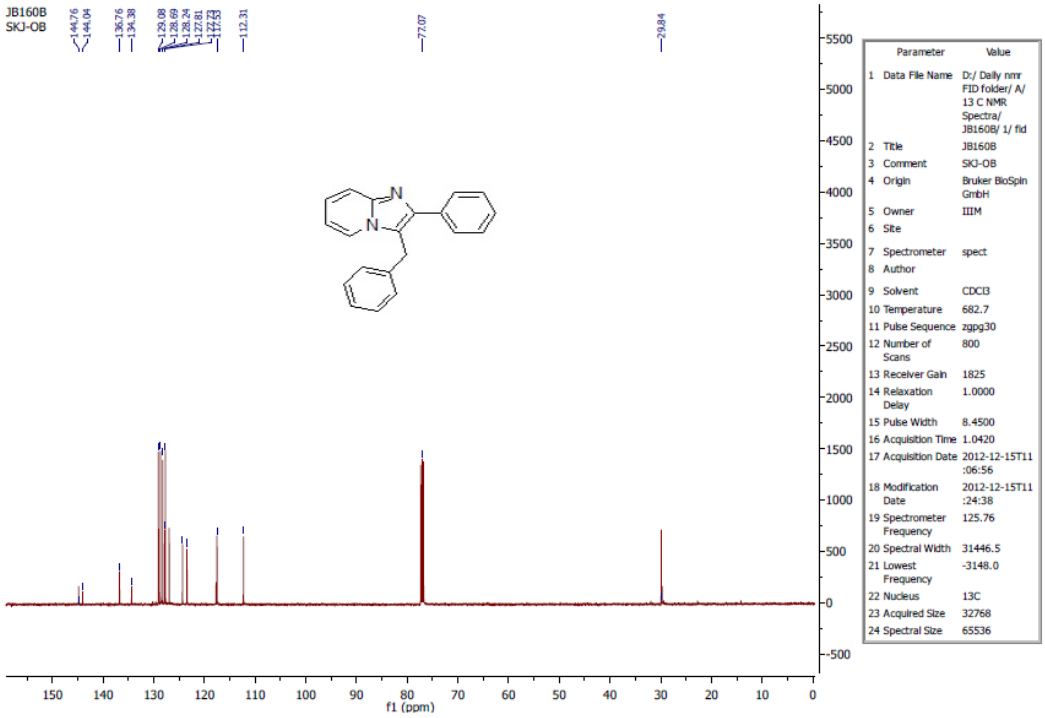


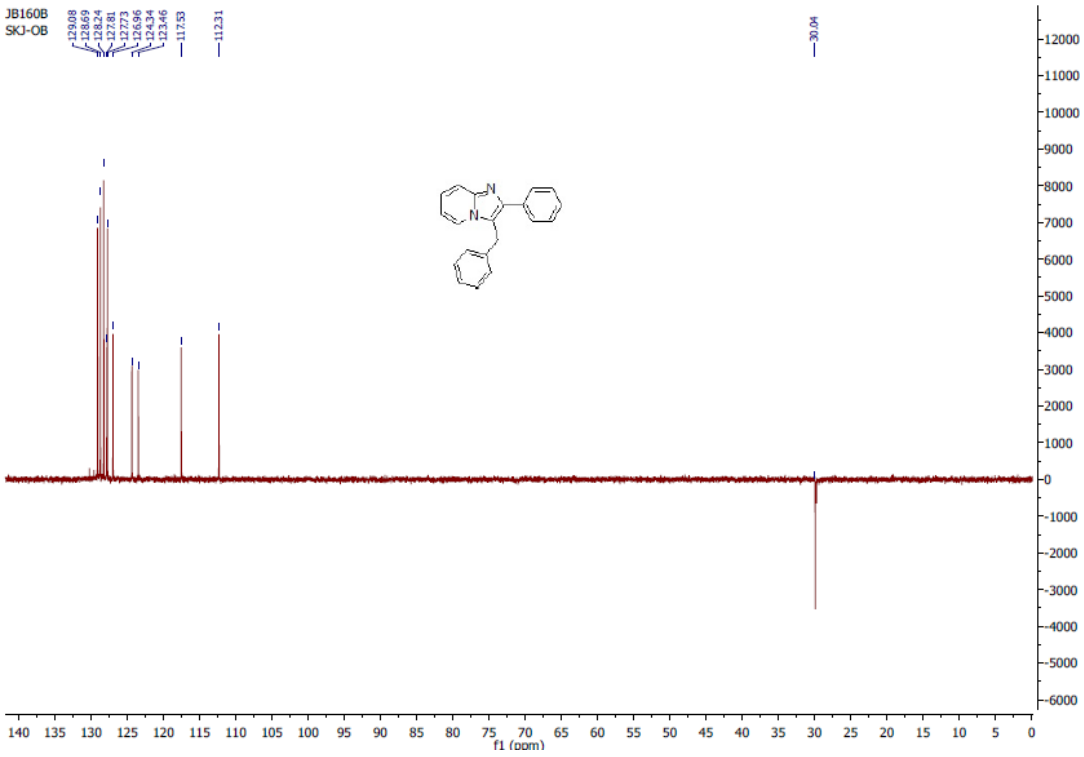
Figure S3. High resolution narrow X-ray photoelectron spectra (XPS) for Cu-Mn catalyst B

S2. SPECTRAL DATA SCANS OF IMIDAZO[1,2-A]PYRIDINES

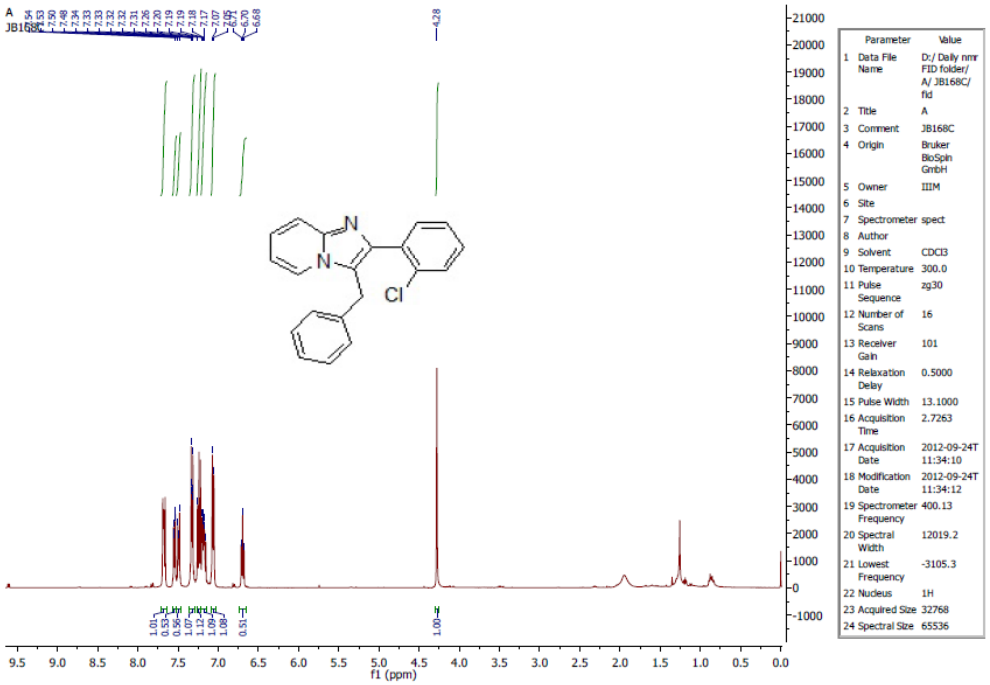
S2.a. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of 3-benzyl-2-phenyl-imidazo[1,2-a]pyridine (5a)

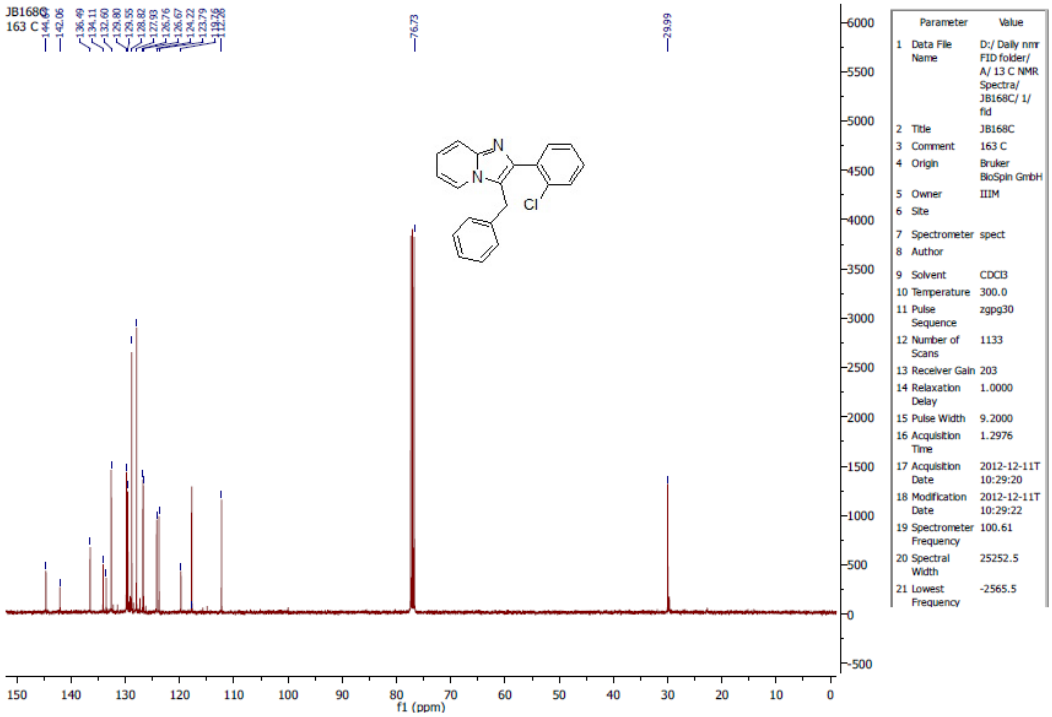


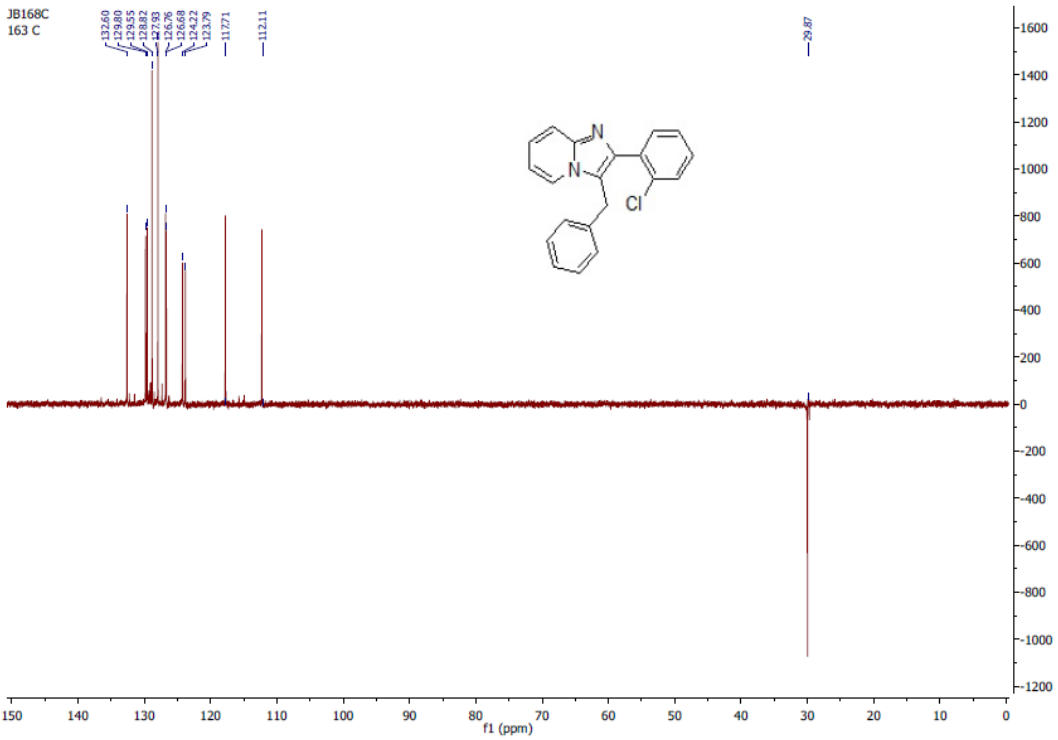




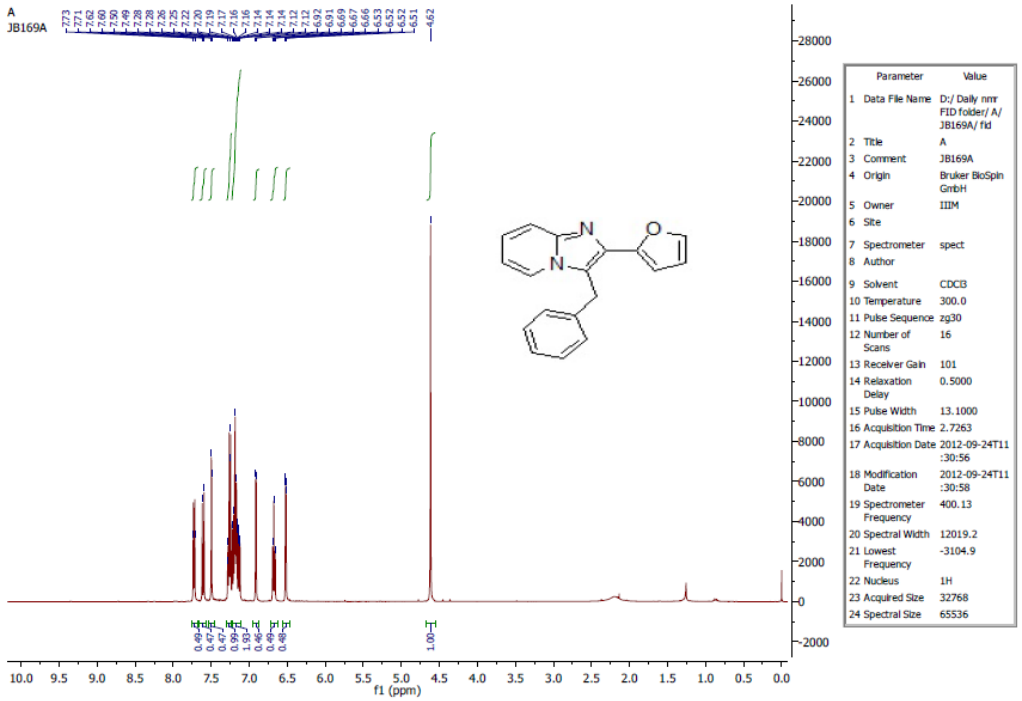
S2.b. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of 3-benzyl-2-(2-chlorophenyl)-imidazo[1,2-a]pyridine (5b)

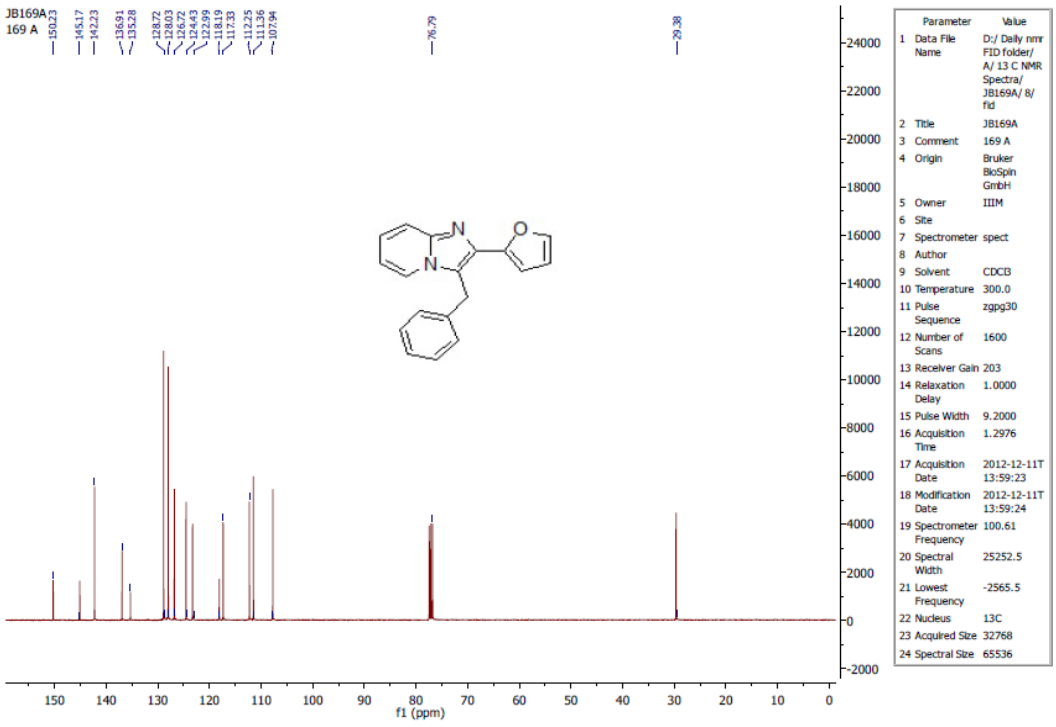


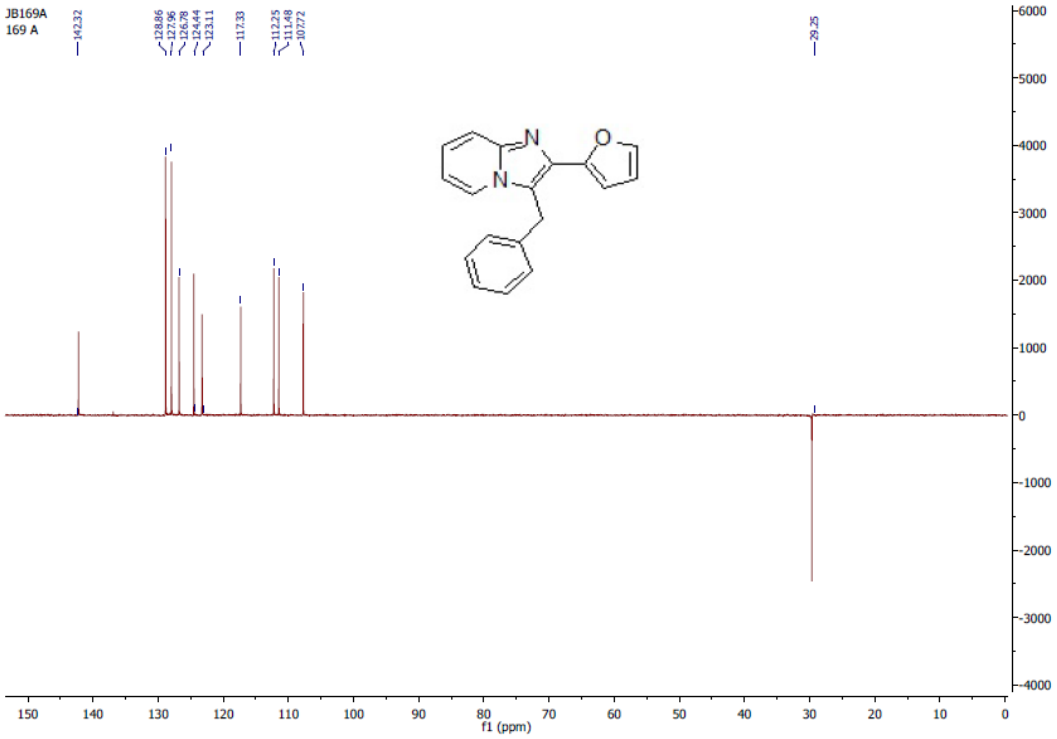




S2.c. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of 3-benzyl-2-(furan-2-yl)-imidazo[1,2-a]pyridine (5c)



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29.25
N
N
O
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5000
4000
3000
2000
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-3000
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150
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130
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110
100
90
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70
60
50
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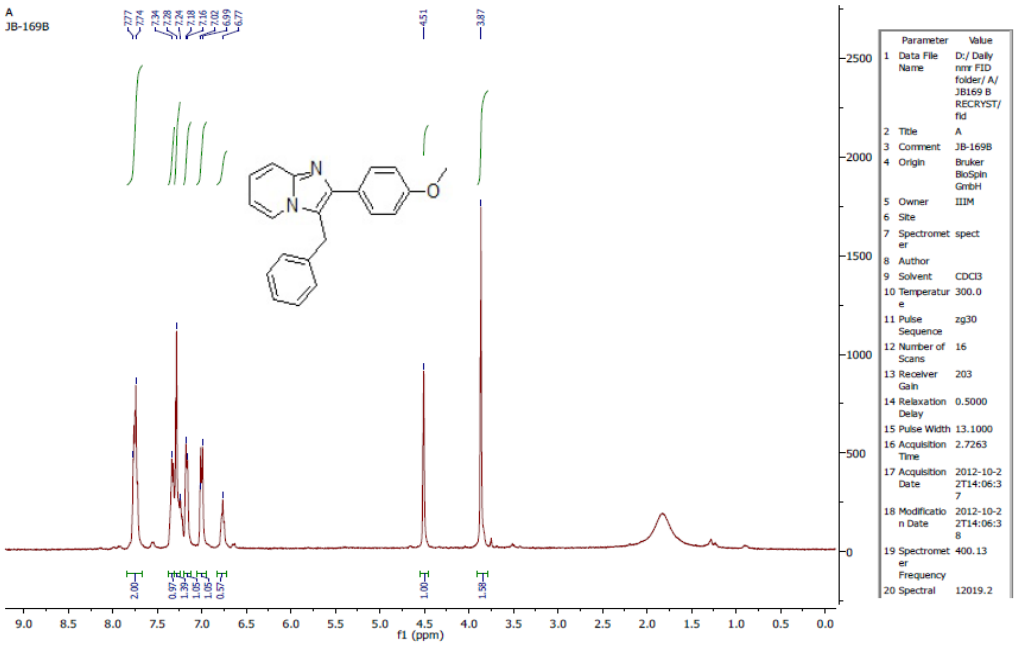
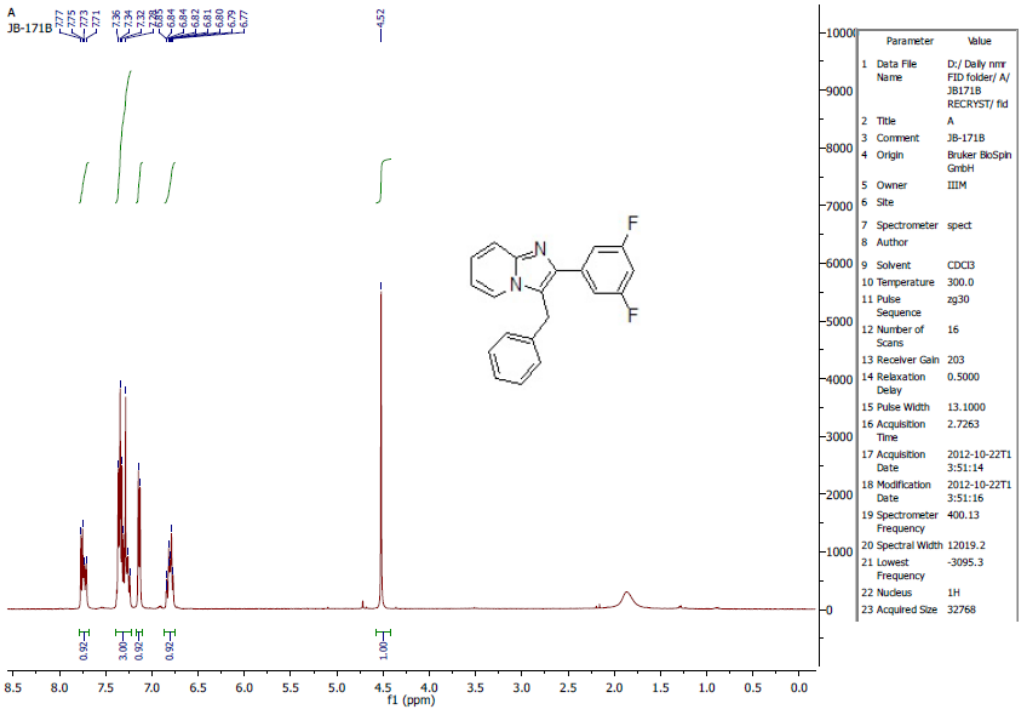
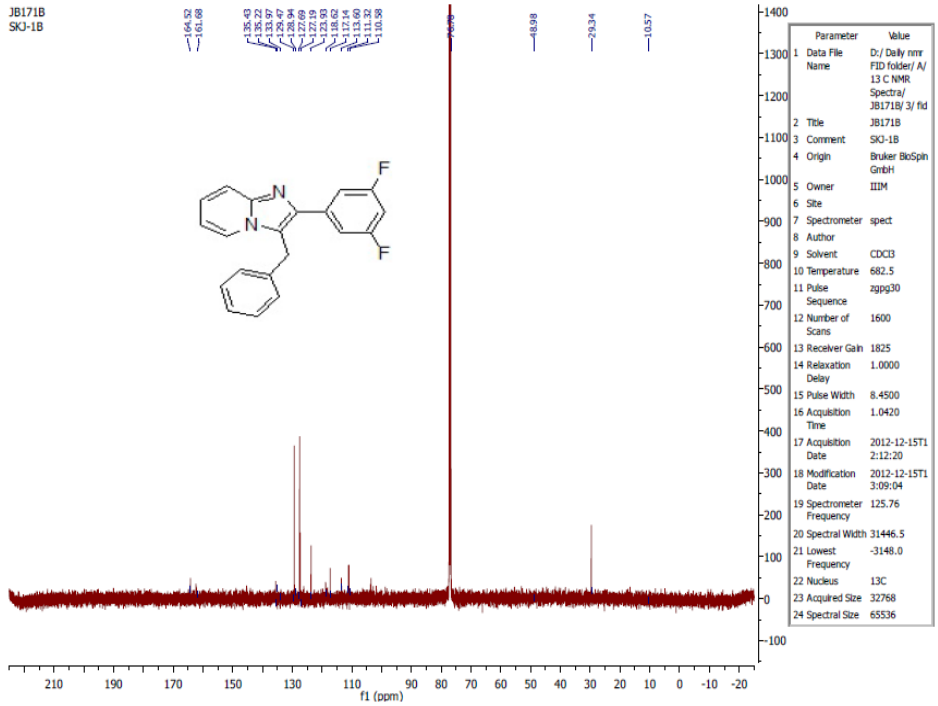
f1 (ppm)

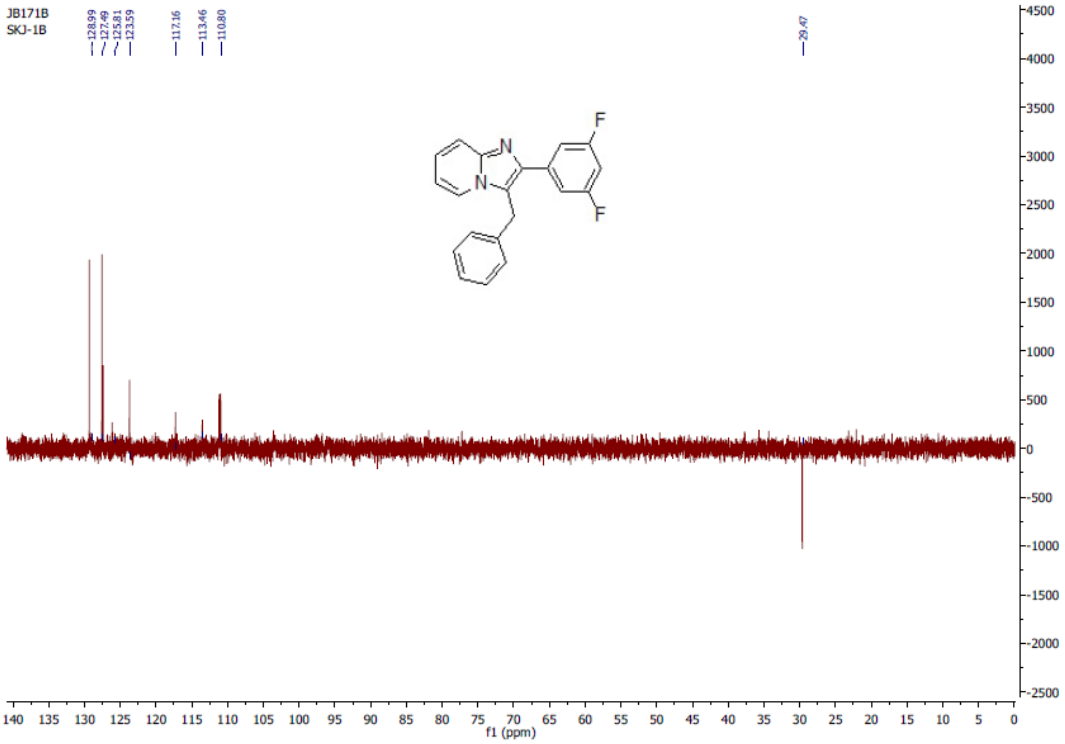
S2.d. ^{1}H NMR NMR spectrum of 3-benzyl-2-(4-methoxyphenyl)-imidazo[1,2-a]pyridine (5d)

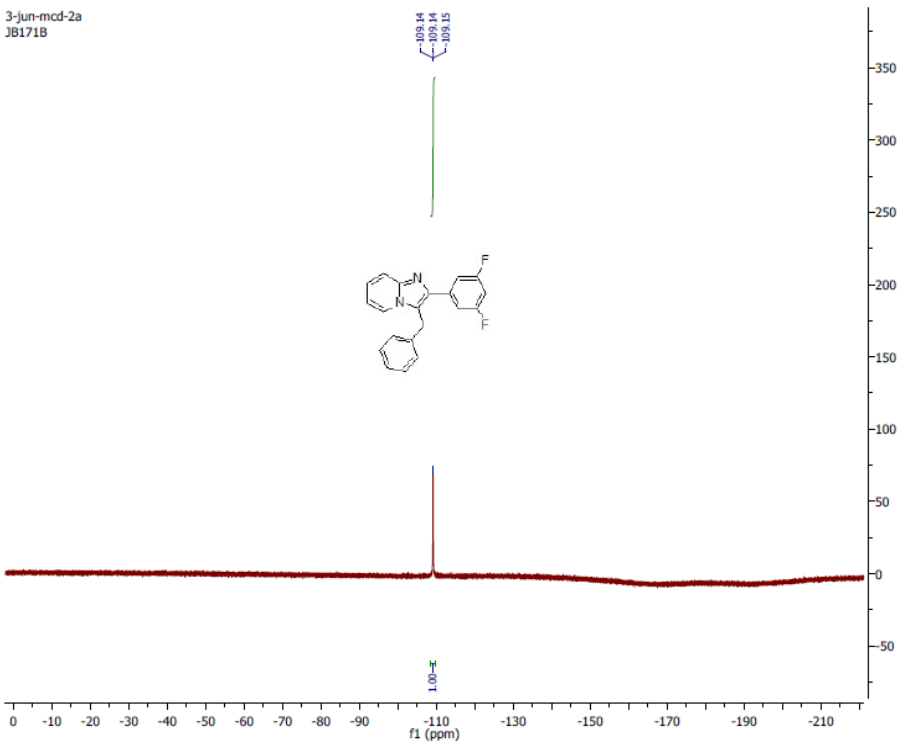


S2.e. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR spectrum of 3-benzyl-2-(3,5-difluorophenyl)-imidazo[1,2-a]pyridine (5e)









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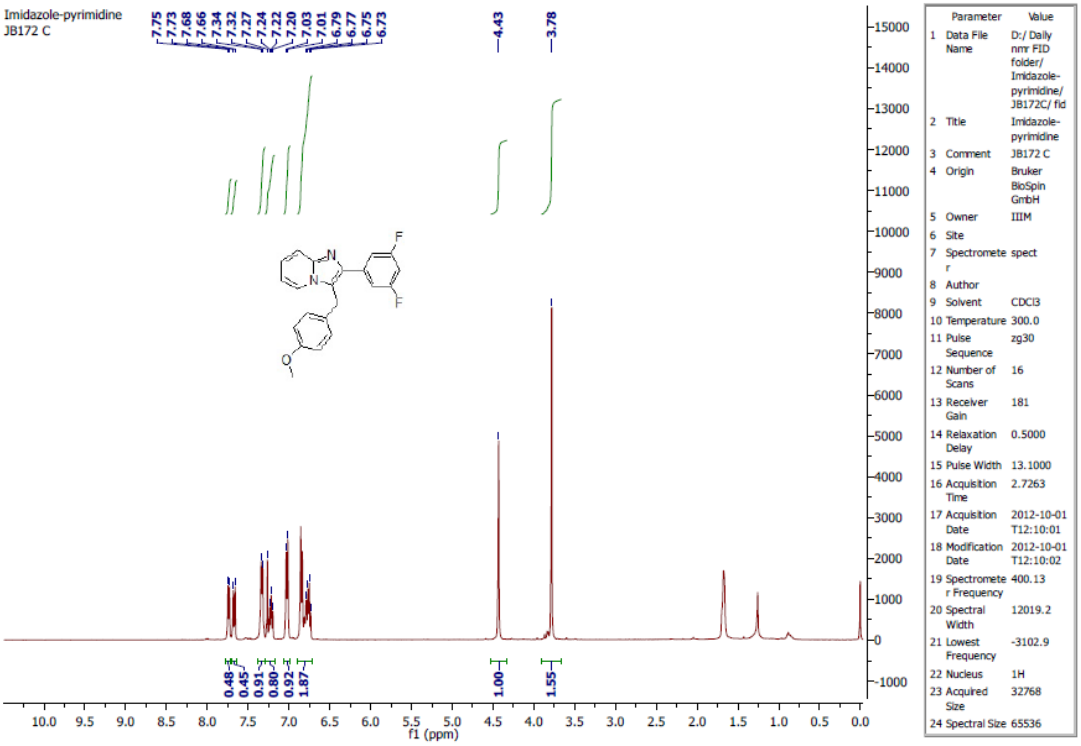
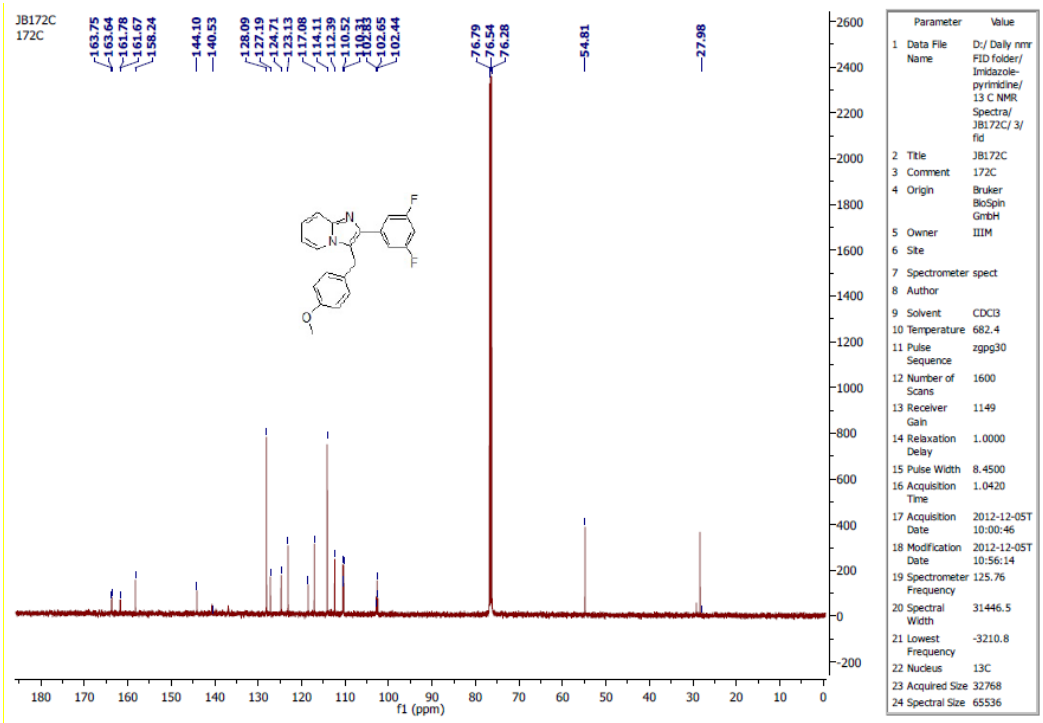
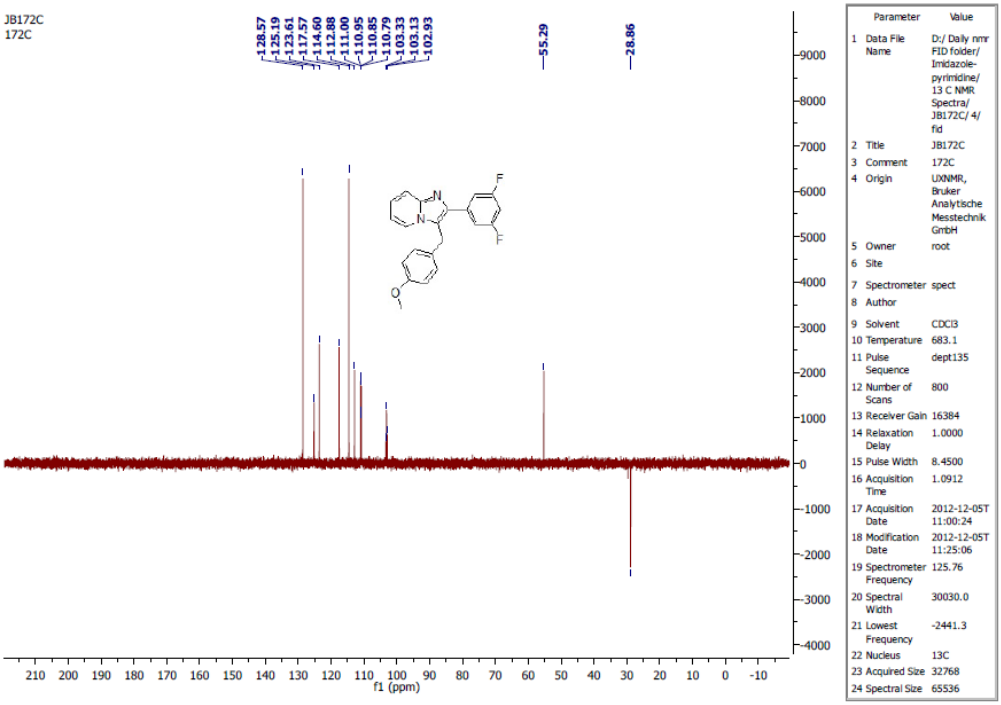
S2.f. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR spectrum of 3-(4-methoxybenzyl)-2-(3,5-difluorophenyl)-imidazo[1,2-a]pyridine (5g)







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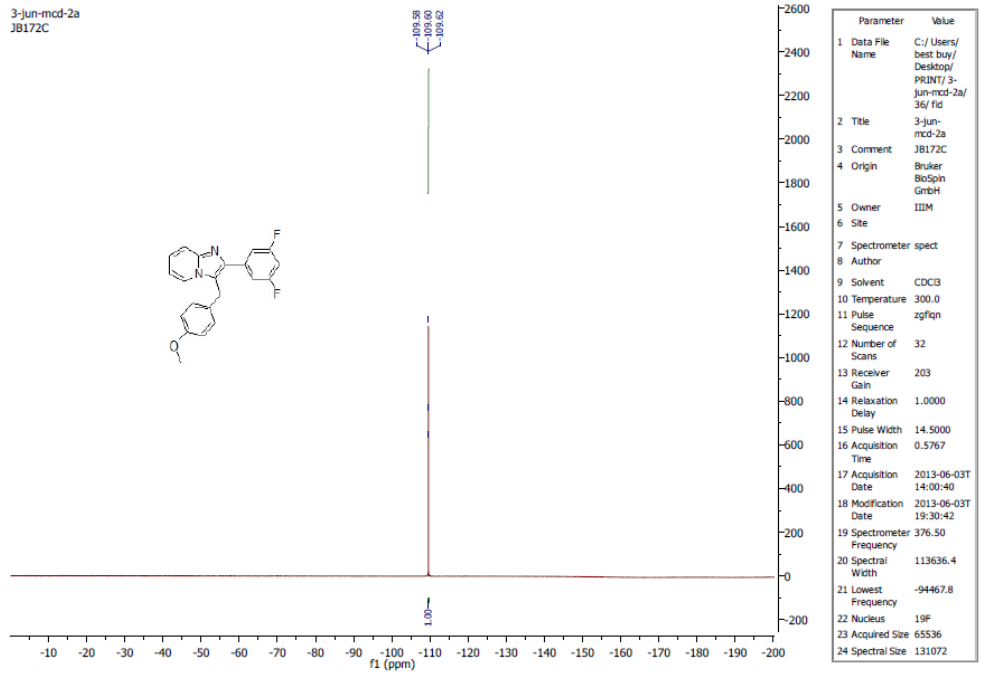

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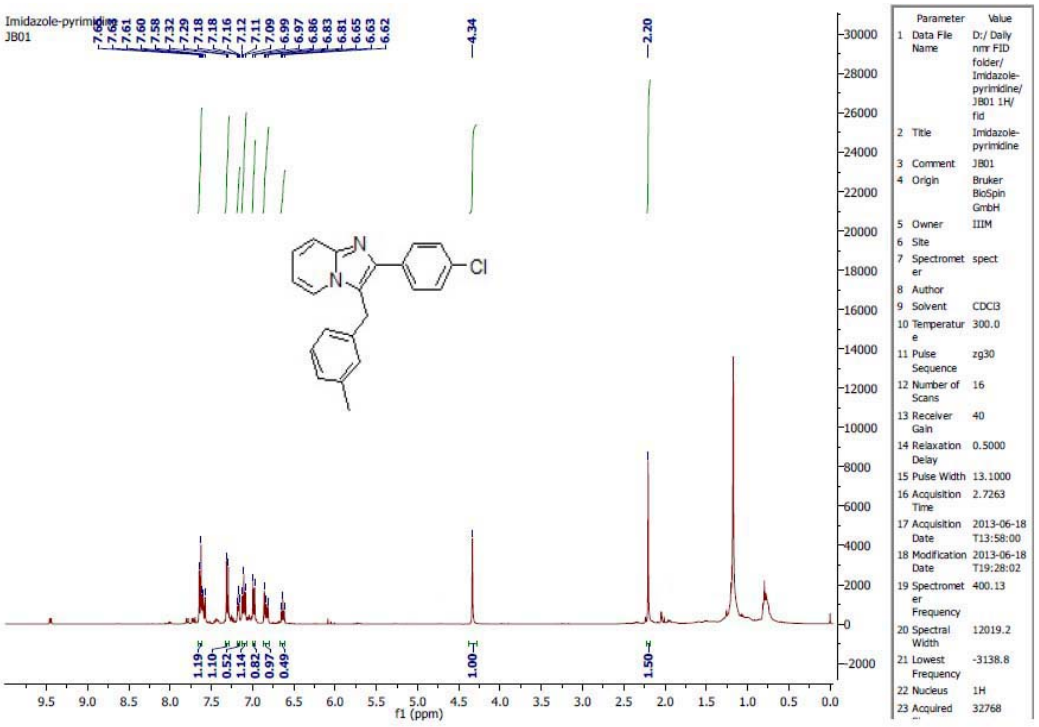
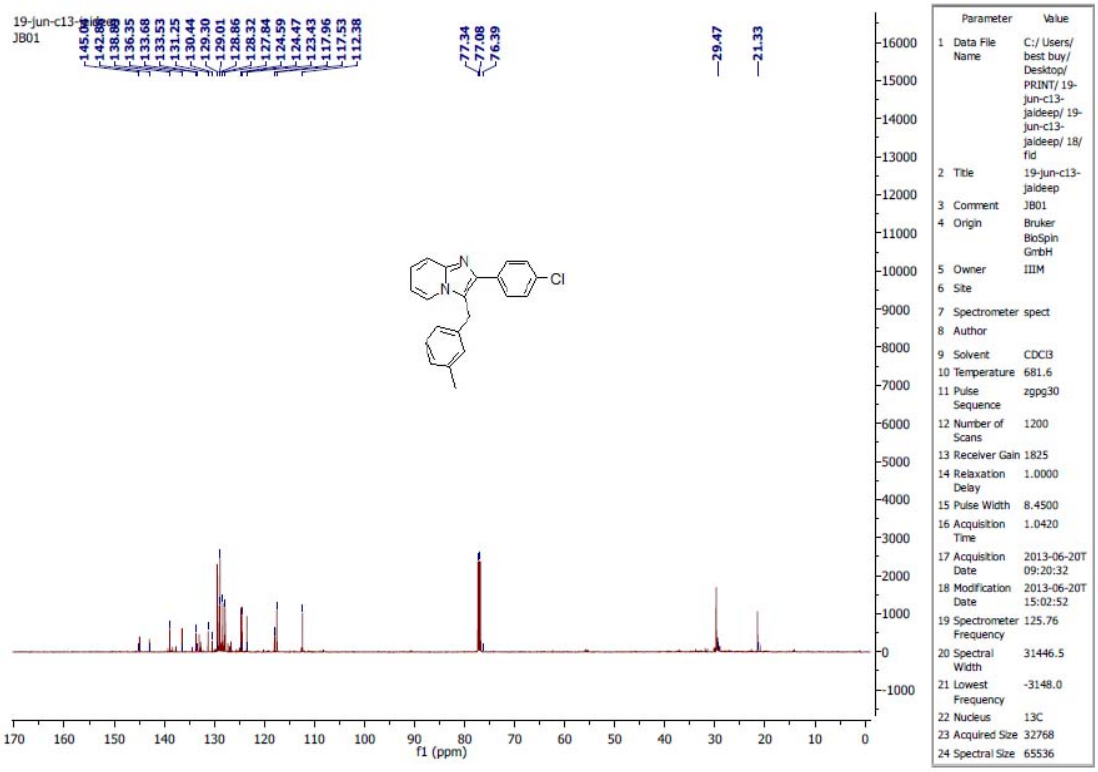
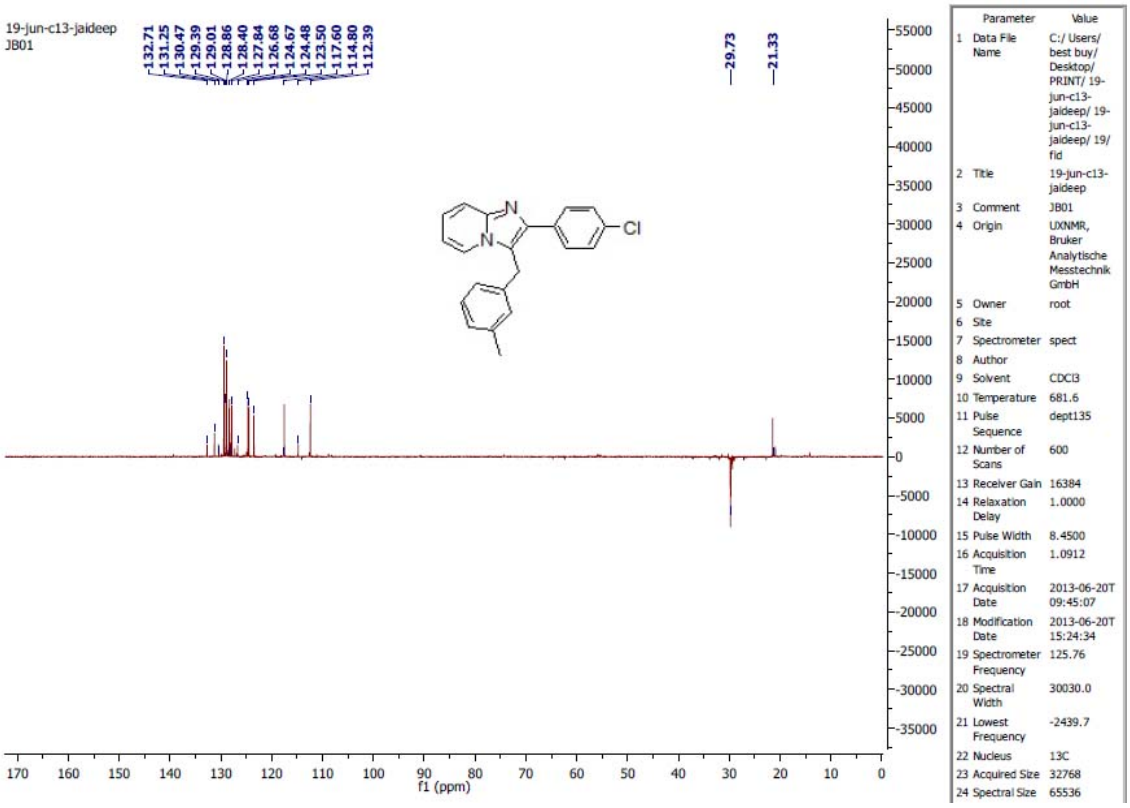
S2.g. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of 3-(3-methylbenzyl)-2-(4-chlorophenyl)H-imidazo[1,2-a]pyridine (5h)







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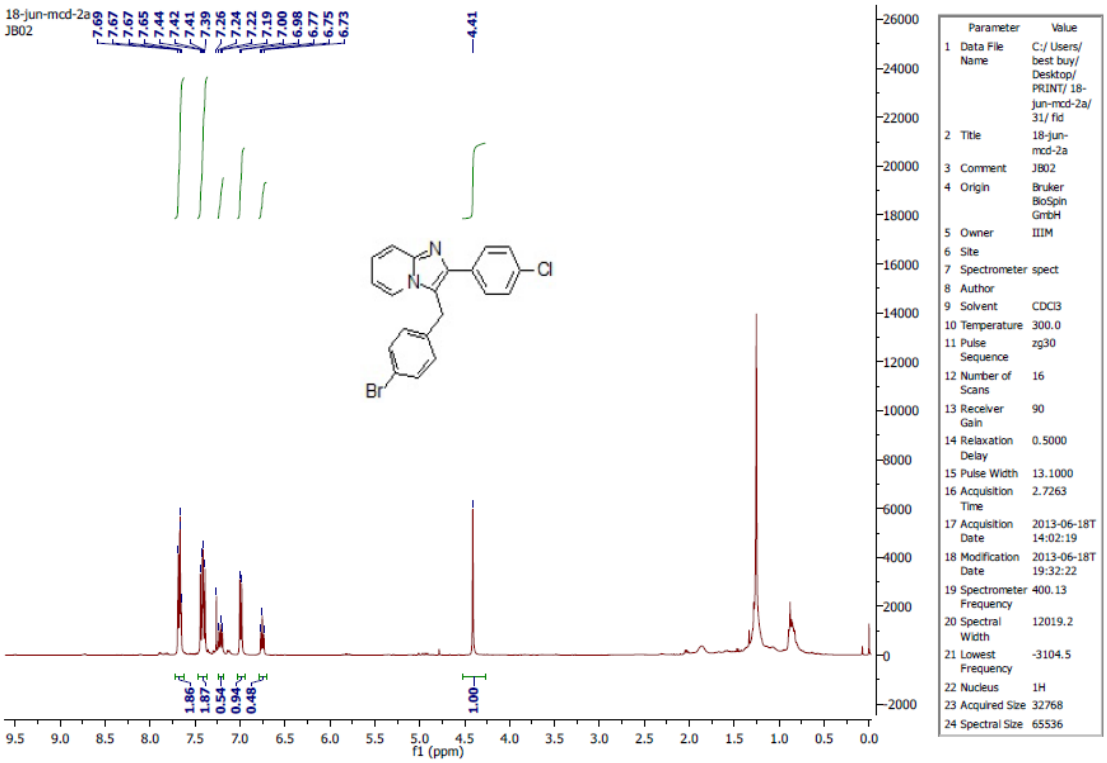
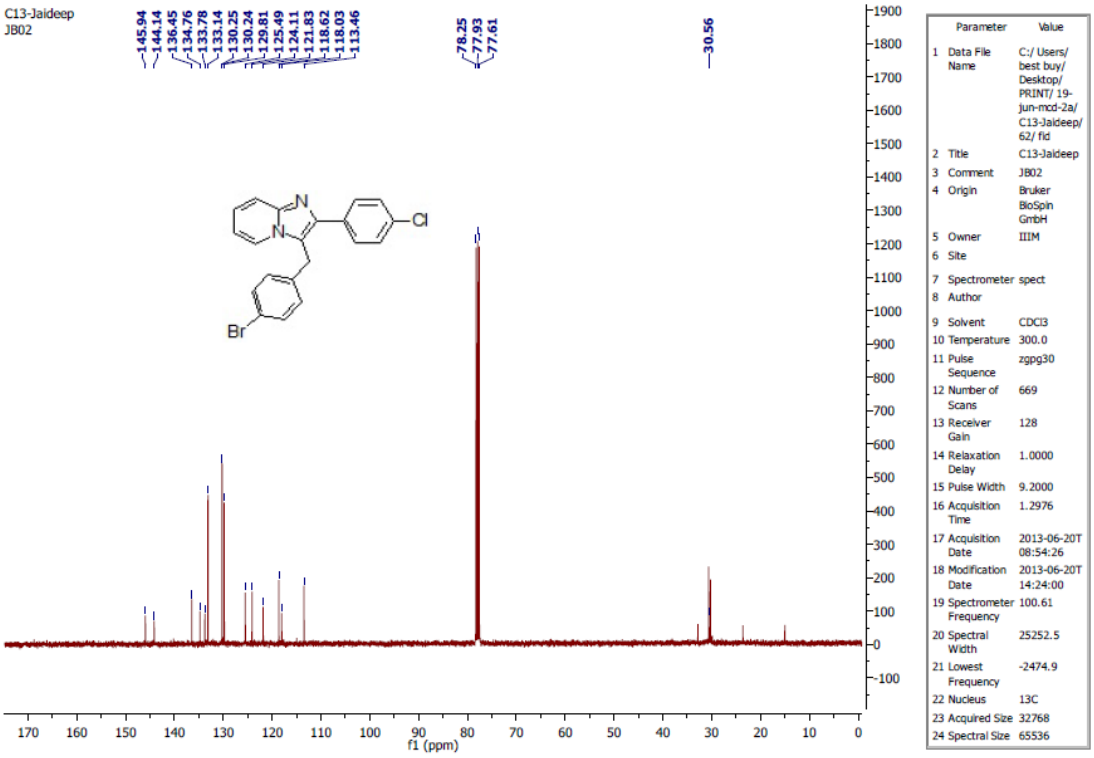
S2.h. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of 3-(4-bromobenzyl)-2-(4-chlorophenyl)H-imidazo[1,2-a]pyridine (5i)





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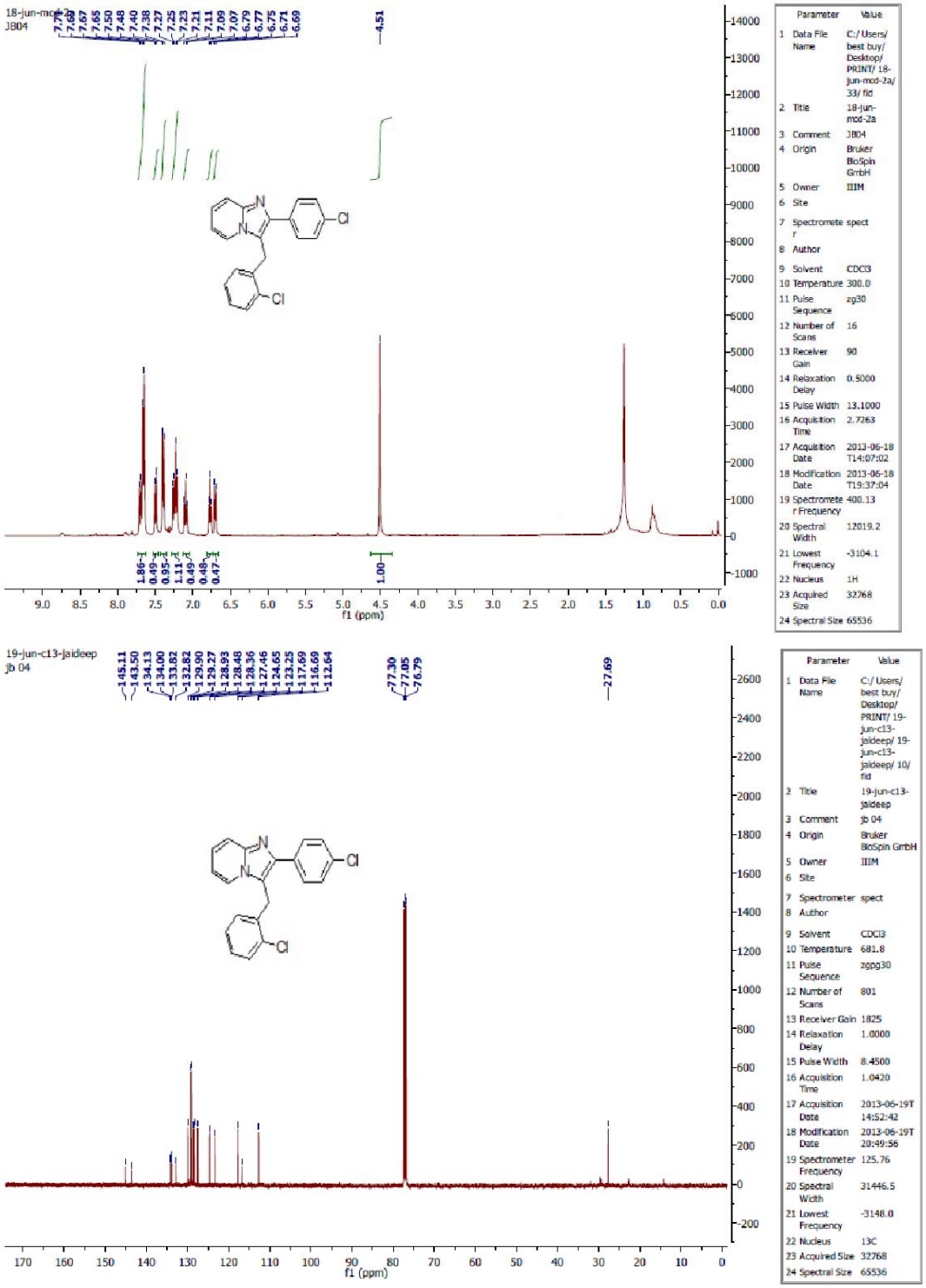

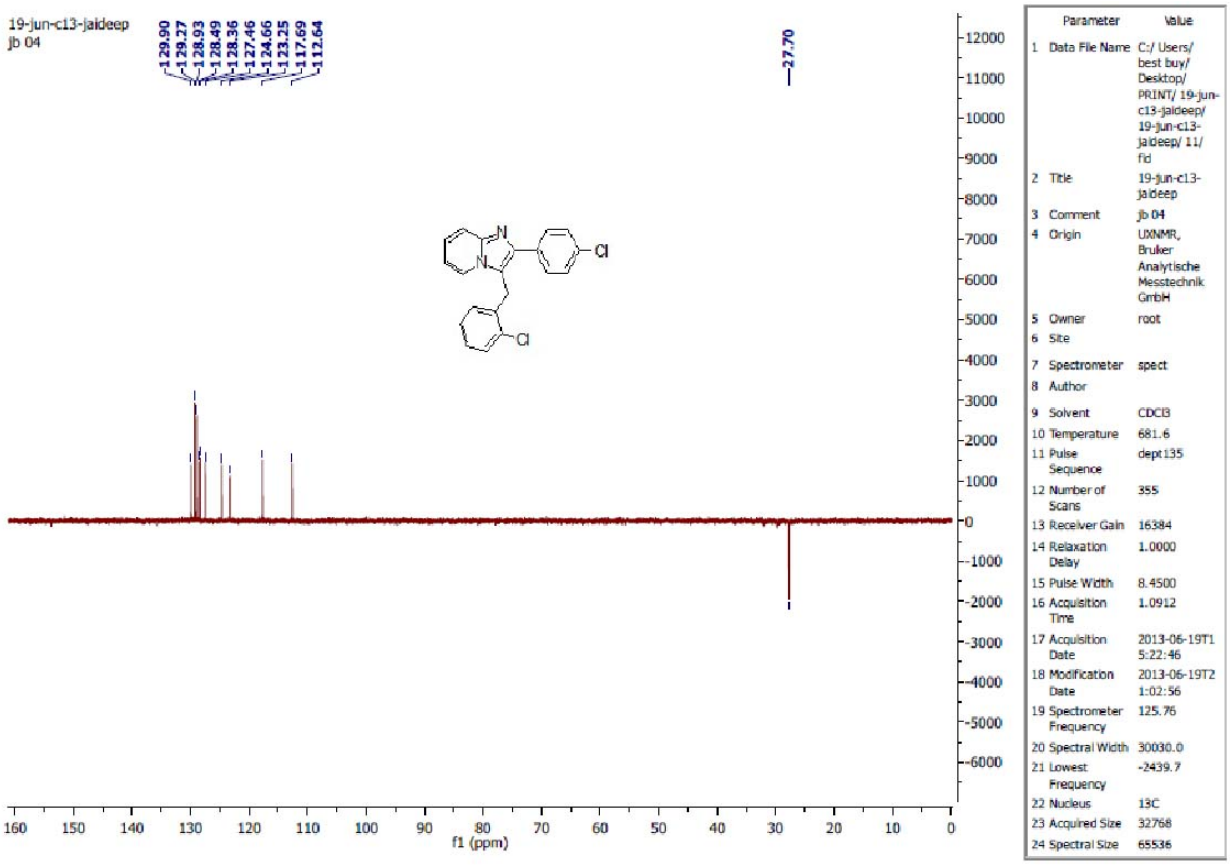

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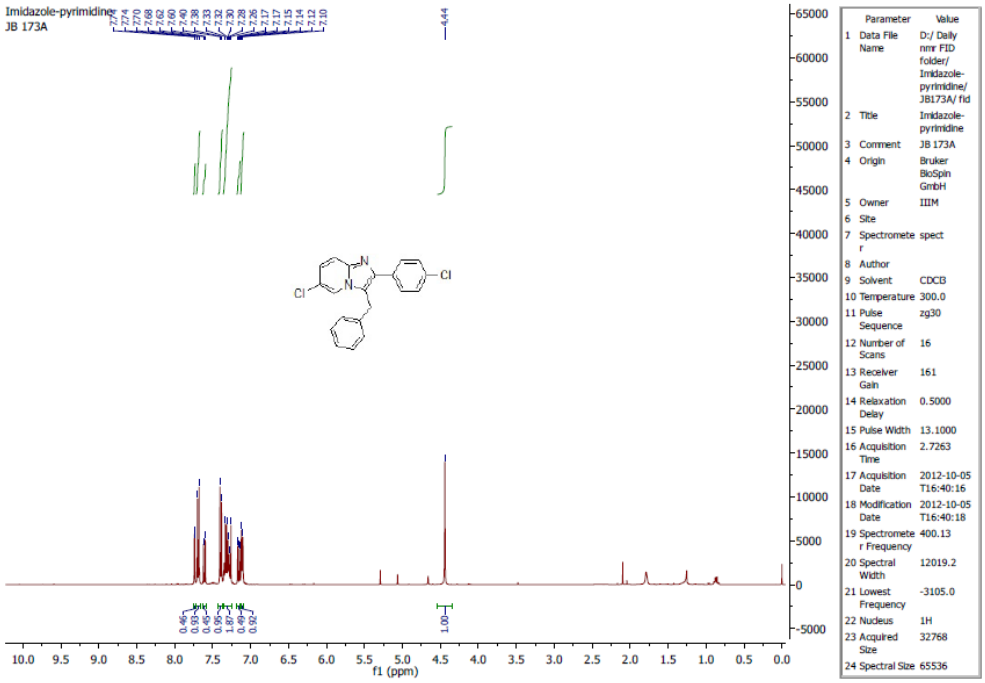
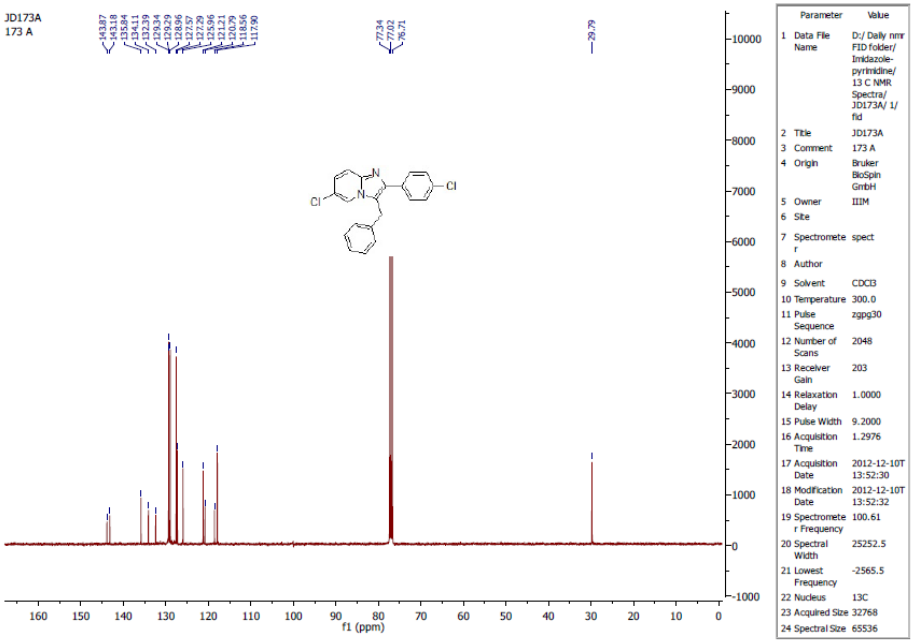
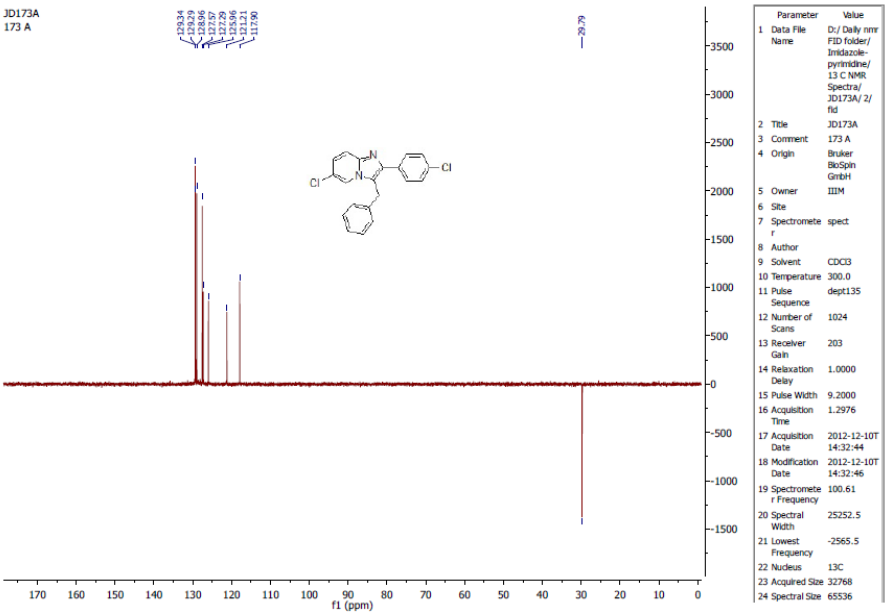
S2.j. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of 3-benzyl-6-chloro-2-(4-chlorophenyl)-imidazo[1,2-a]pyridine (5k)

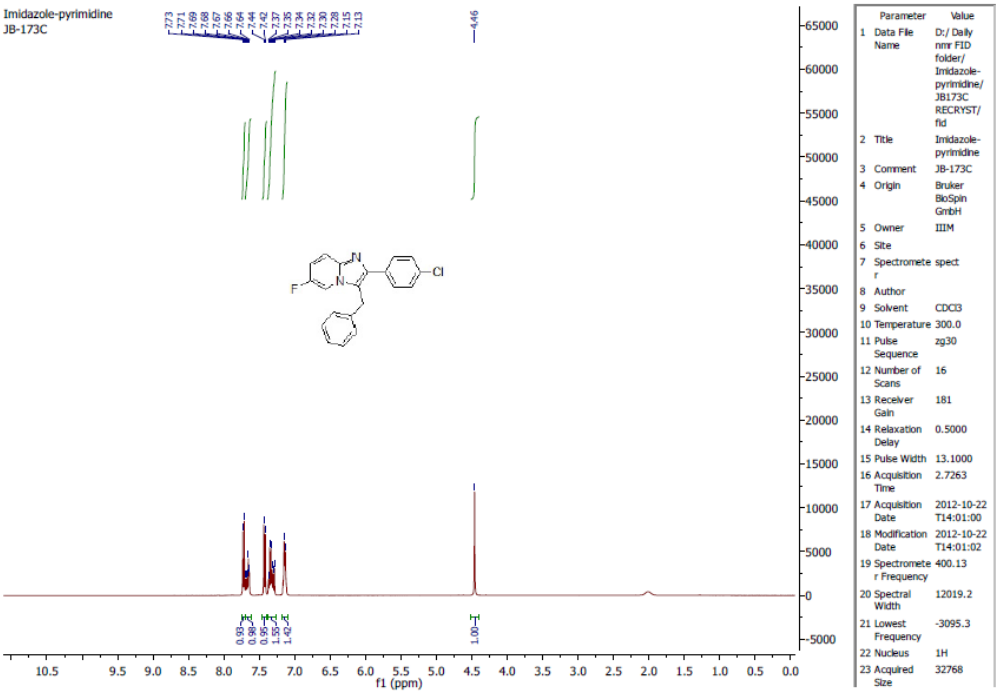




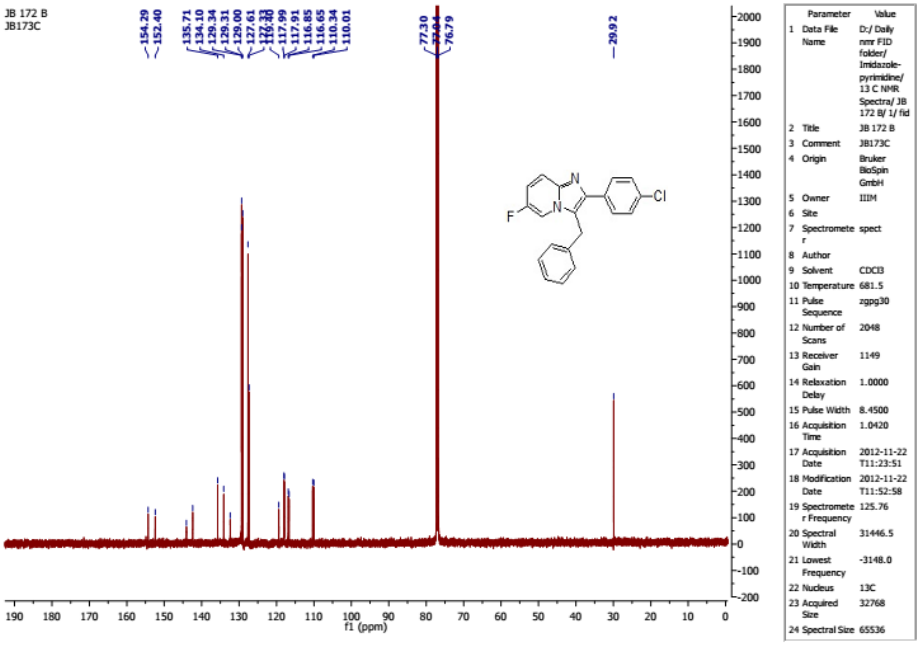


	Parameter	Value
1	Data File Name	D:/ Daily nmr FID folder/ Imidazole-pyrimidine/ 13 C NMR Spectra/ JD173A/ 2/ fid
2	Title	JD173A
3	Comment	173 A
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	dept135
12	Number of Scans	1024
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	9.2000
16	Acquisition Time	1.2976
17	Acquisition Date	2012-12-10T 14:32:44
18	Modification Date	2012-12-10T 14:32:46
19	Spectrometer Frequency	100.61
20	Spectral Width	25252.5
21	Lowest Frequency	-2565.5
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

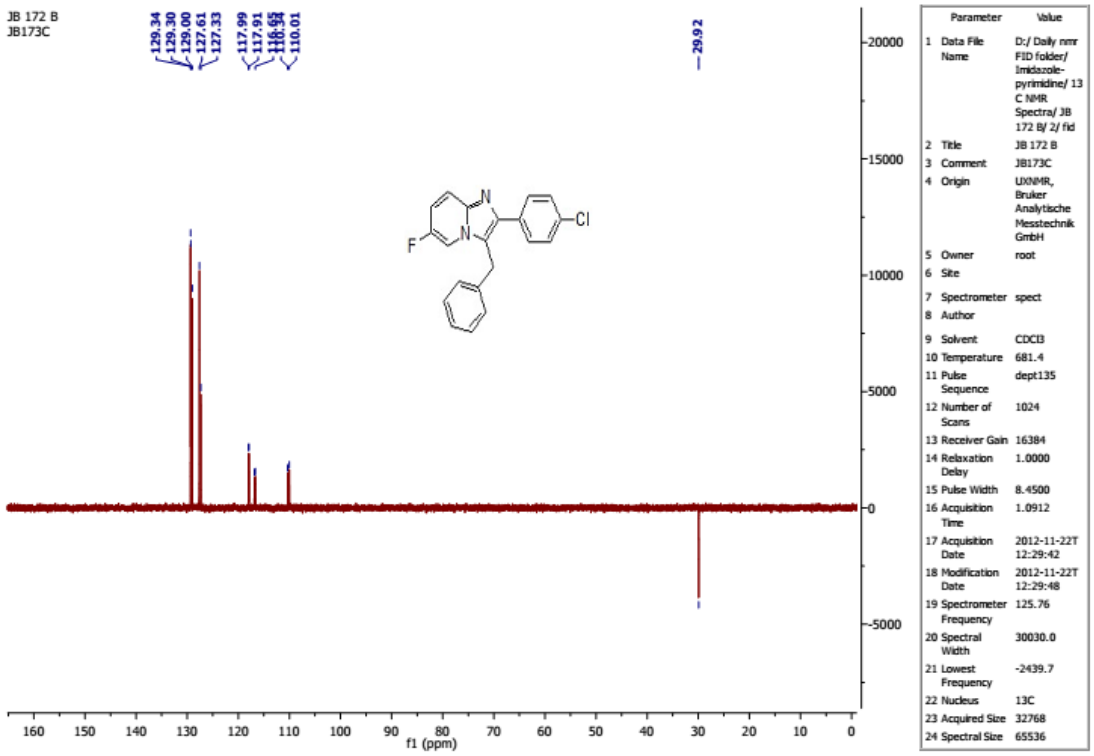
S2.k. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR spectrum of 3-benzyl-2-(4-chlorophenyl)-6-fluoro-imidazo[1,2-a]pyridine (5l)



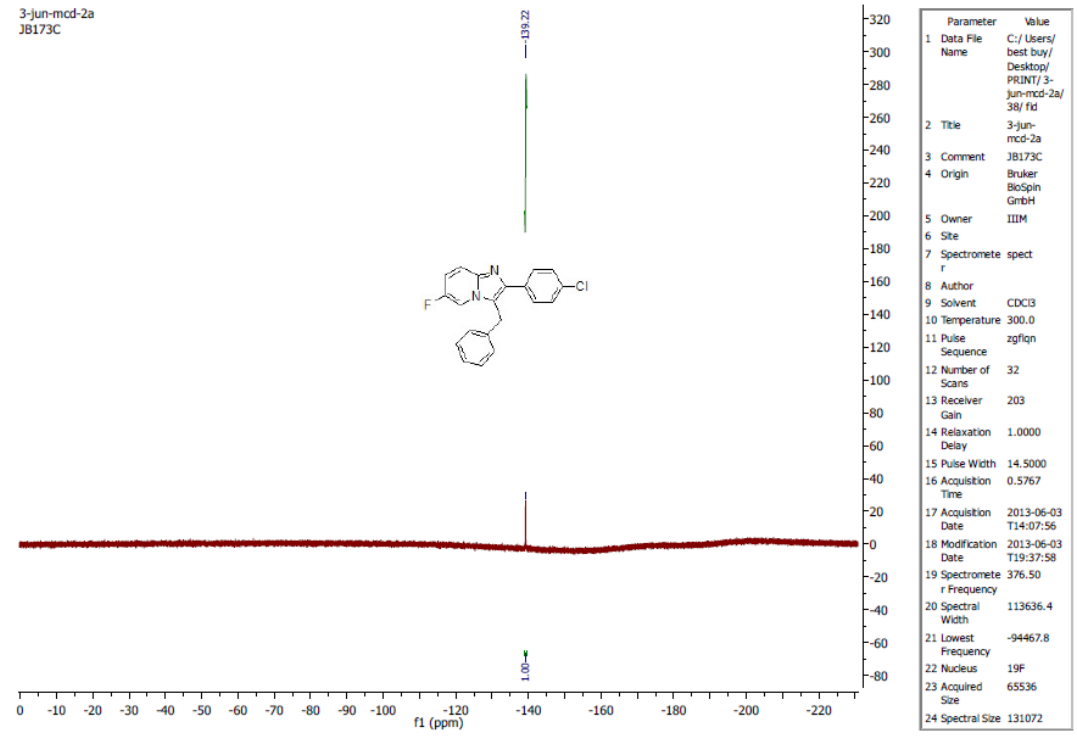
	Parameter	Value
1	Data File Name	D:/ Daily nmr FID folder/ Imidazole-pyrimidine/ JB173C RECRYST/ fid
2	Title	Imidazole-pyrimidine
3	Comment	JB-173C
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect r
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	181
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2012-10-22 T14:01:00
18	Modification Date	2012-10-22 T14:01:02
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3095.3
22	Nucleus	1H
23	Acquired Size	32768



	Parameter	Value
1	Data File Name	D:/ Daily nmr FID folder/ Imidazole-pyrimidine/ 13 C NMR Spectra/ JB 172 B/ 1/ fid
2	Title	JB 172 B
3	Comment	JB173C
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect r
8	Author	
9	Solvent	CDCl3
10	Temperature	681.5
11	Pulse Sequence	zgpg30
12	Number of Scans	2048
13	Receiver Gain	1149
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2012-11-22 T11:23:51
18	Modification Date	2012-11-22 T11:52:58
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3148.0
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

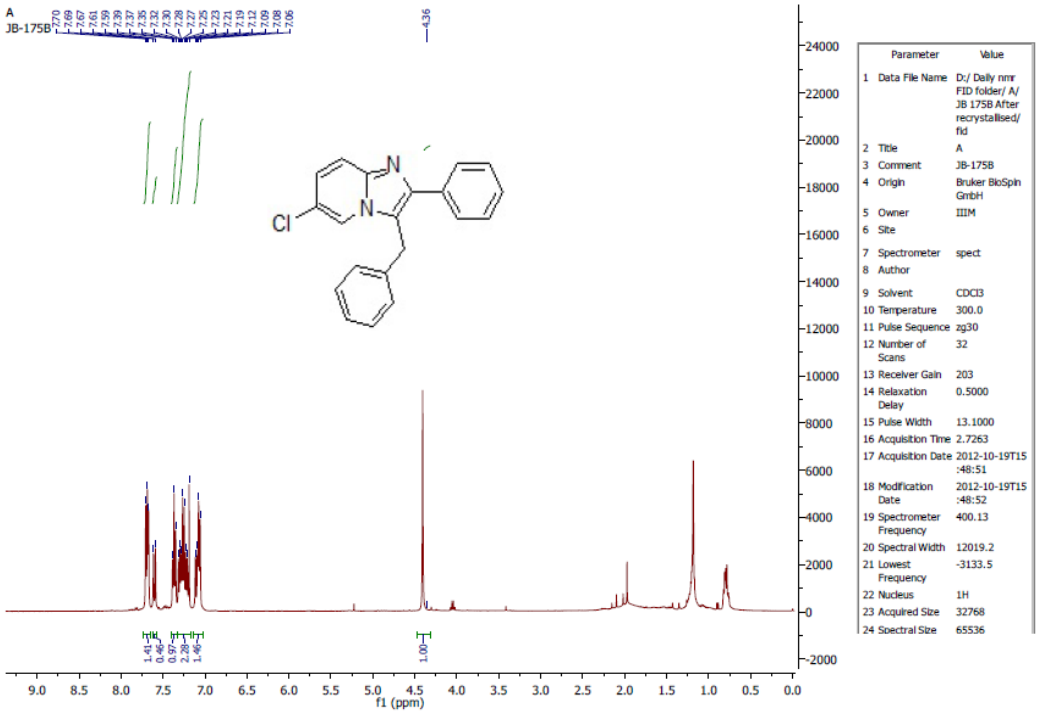


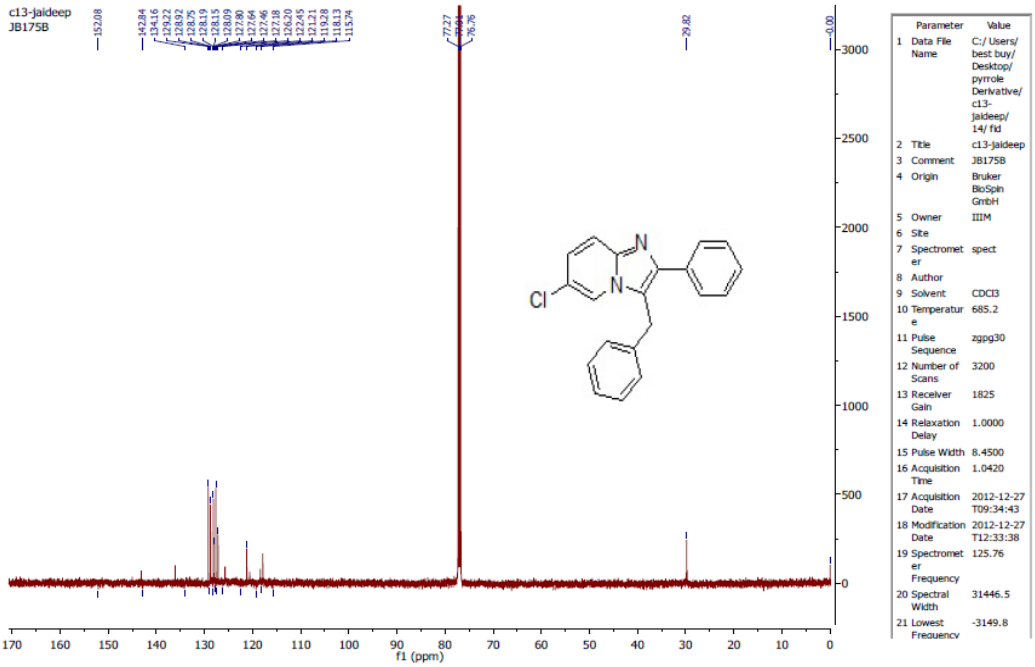
	Parameter	Value
1	Data File Name	D:/ Daily nmr FID folder/ Imidazole-pyrimidine/ 13 C NMR Spectra/ JB 172 B/ 2/ fid
2	Title	JB 172 B
3	Comment	JB173C
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	681.4
11	Pulse Sequence	dept135
12	Number of Scans	1024
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2012-11-22T 12:29:42
18	Modification Date	2012-11-22T 12:29:48
19	Spectrometer Frequency	125.76
20	Spectral Width	30030.0
21	Lowest Frequency	-2439.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

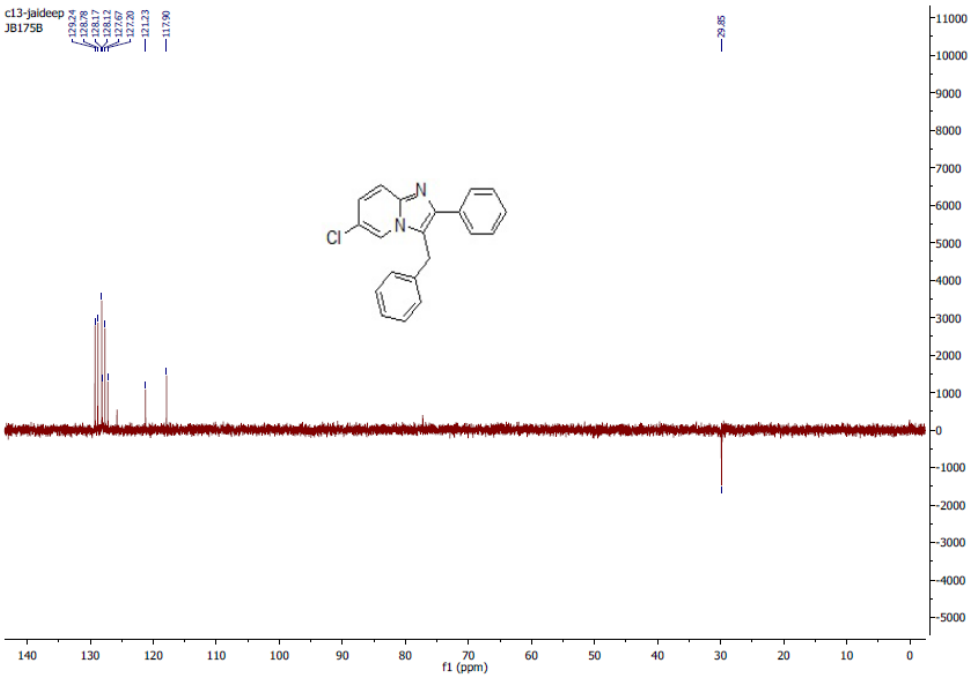


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 3-jun-mcd-2a/ 38/ fid
2	Title	3-jun-mcd-2a
3	Comment	JB173C
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgflqn
12	Number of Scans	32
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	14.5000
16	Acquisition Time	0.5767
17	Acquisition Date	2013-06-03 T14:07:56
18	Modification Date	2013-06-03 T19:37:58
19	Spectrometer Frequency	376.50
20	Spectral Width	113636.4
21	Lowest Frequency	-94467.8
22	Nucleus	19F
23	Acquired Size	65536
24	Spectral Size	131072

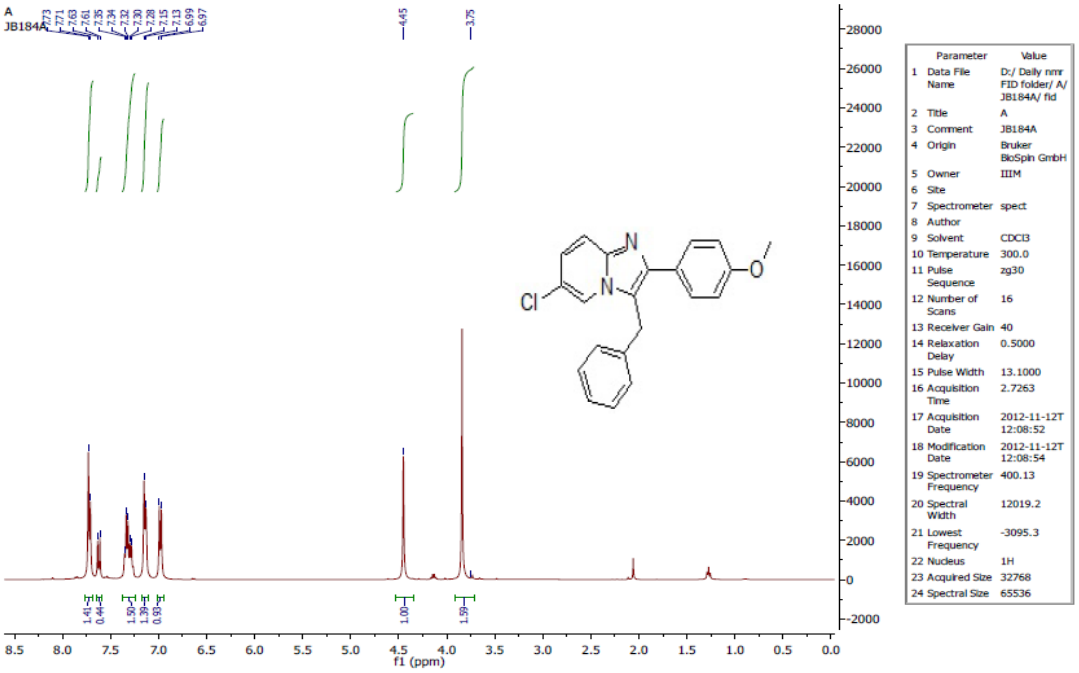
S2.l. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of 3-benzyl-6-chloro-2-phenyl-imidazo[1,2-a]pyridine (5m)

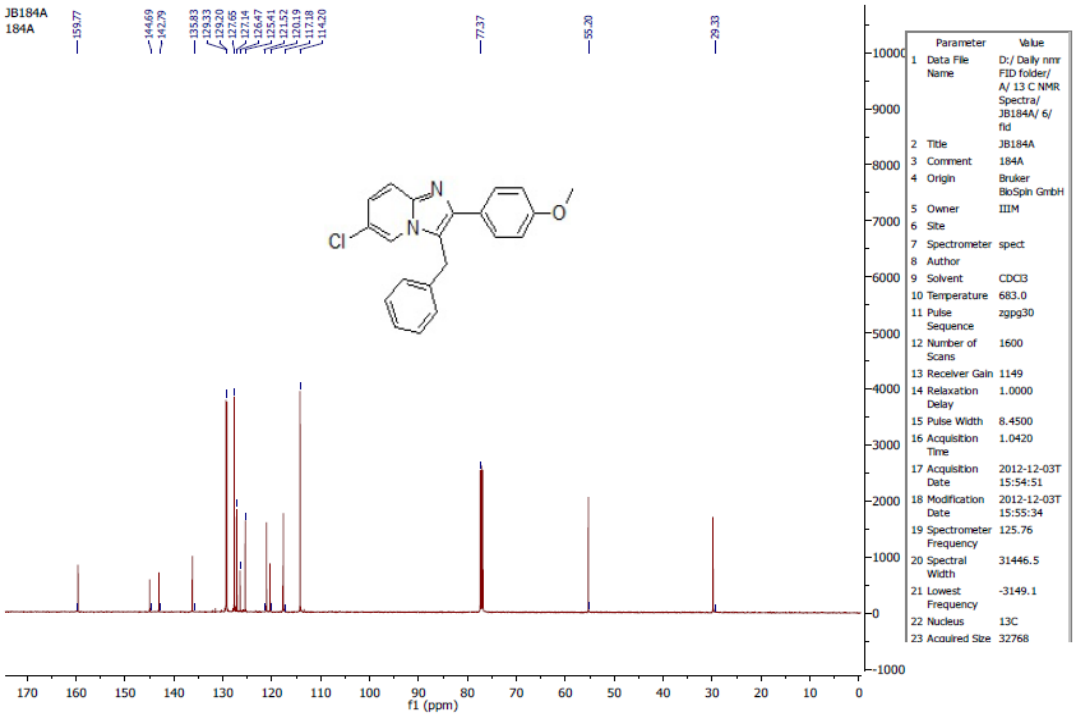


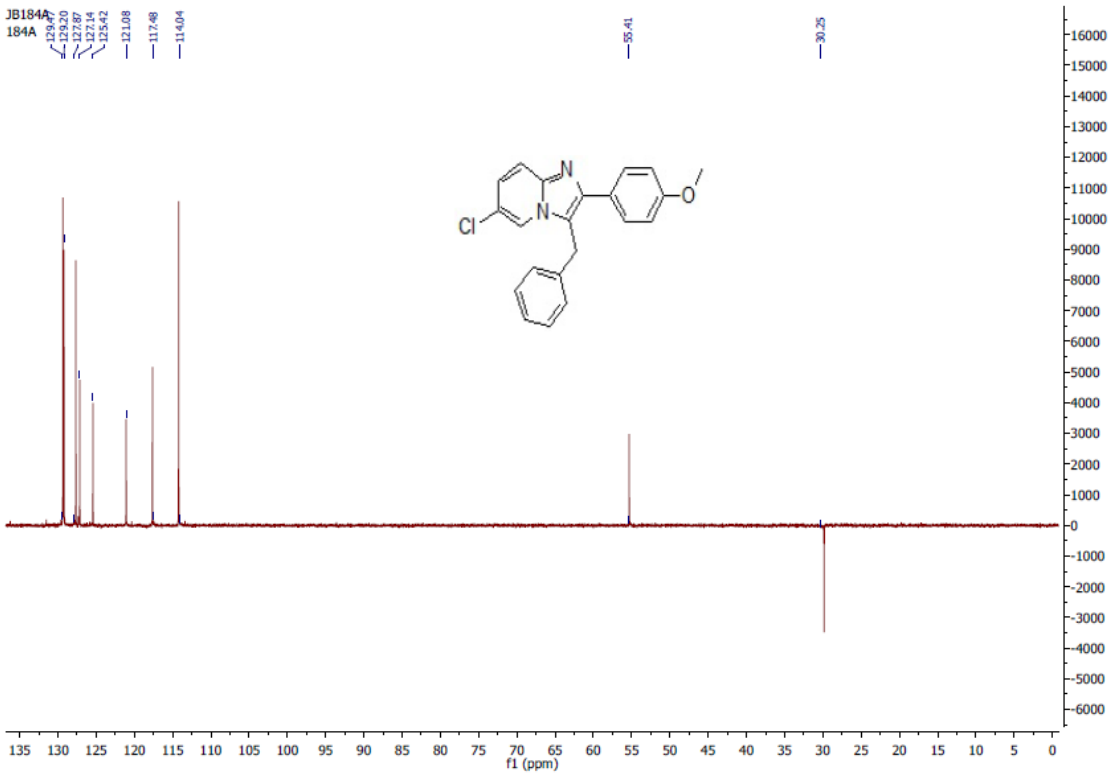



c13-jaideep
JB175B
129.24
128.78
128.17
128.12
127.67
127.20
121.23
117.90
29.85
N
N
Cl
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
-4000
-5000
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

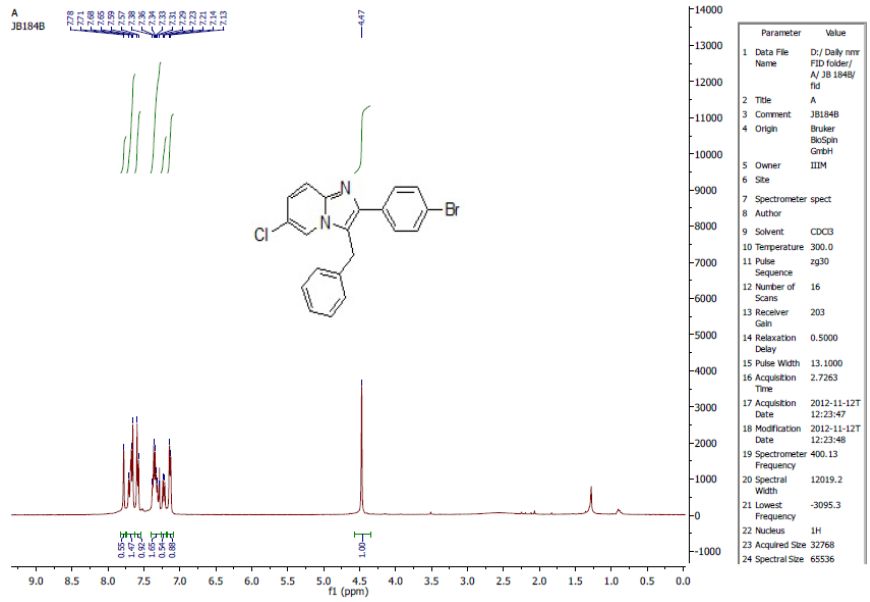
S2.m. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of 3-Benzyl-6-chloro-2-(4-methoxyphenyl)-imidazo[1,2-a]pyridine (5n):

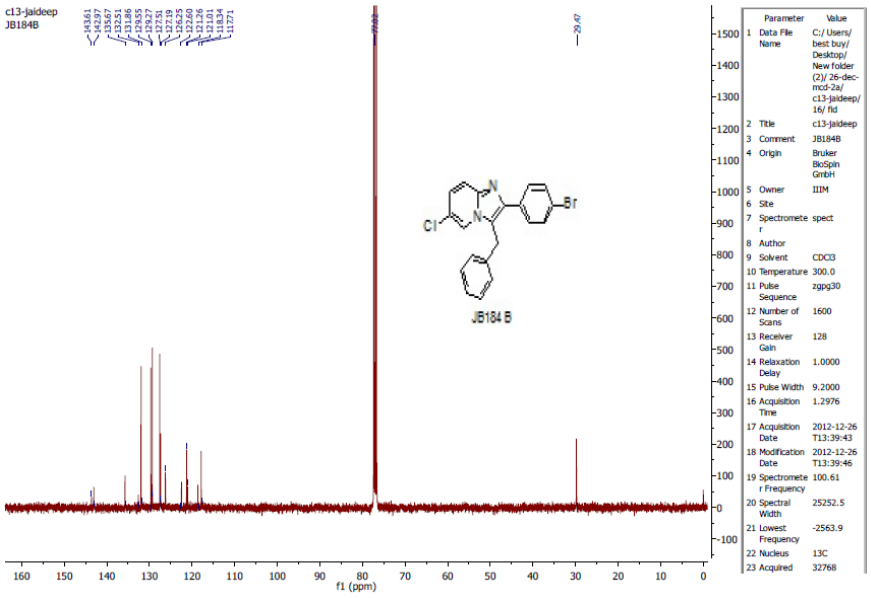


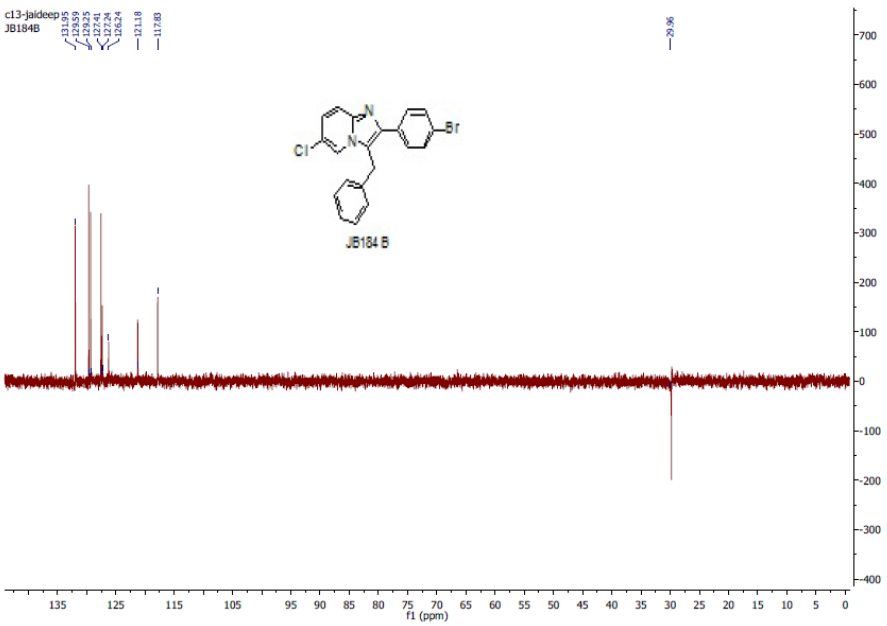




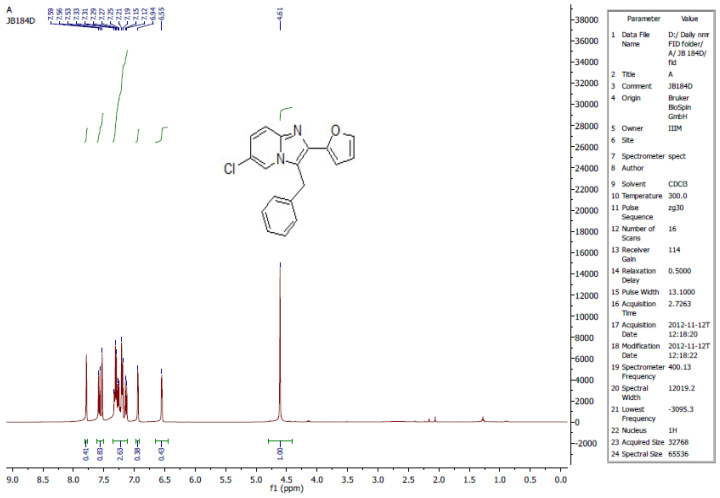
S2.n. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of 3-benzyl-2-(4-bromophenyl)-6-chloro-imidazo[1,2-a]pyridine (5o)

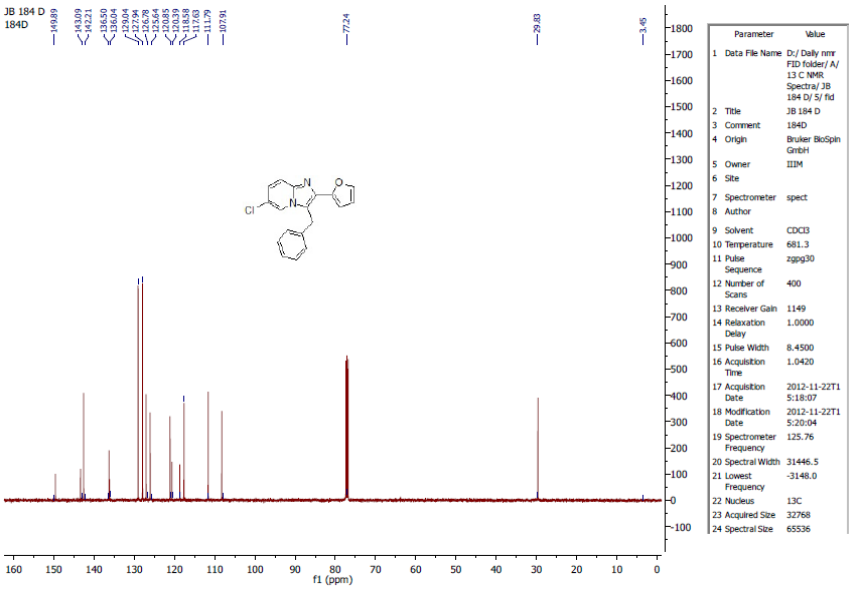


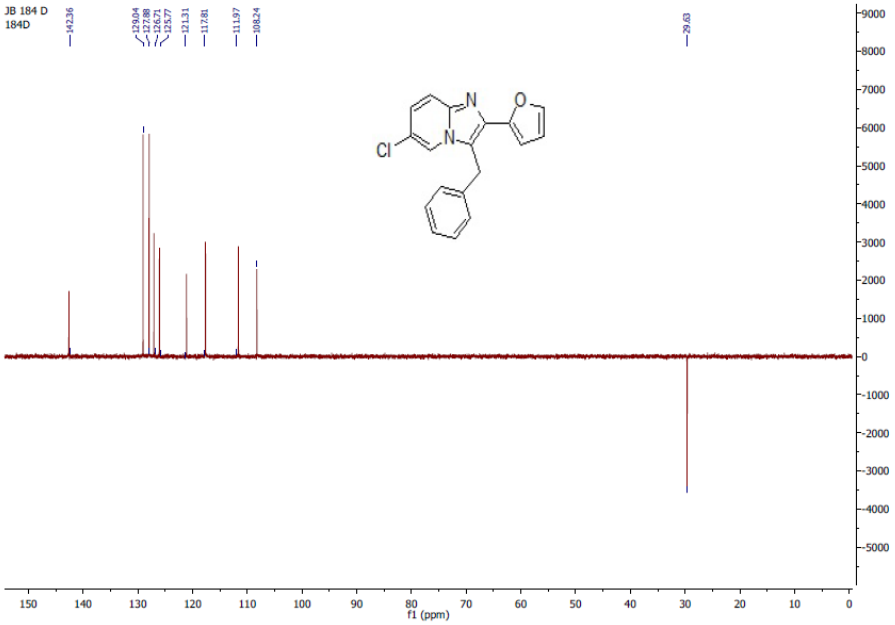



c13-jaideep
JB184B
131.95
129.59
129.25
127.41
127.24
126.84
121.18
117.83
29.96
N
N
Cl
Br
JB184 B
700
600
500
400
300
200
100
0
-100
-200
-300
-400
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

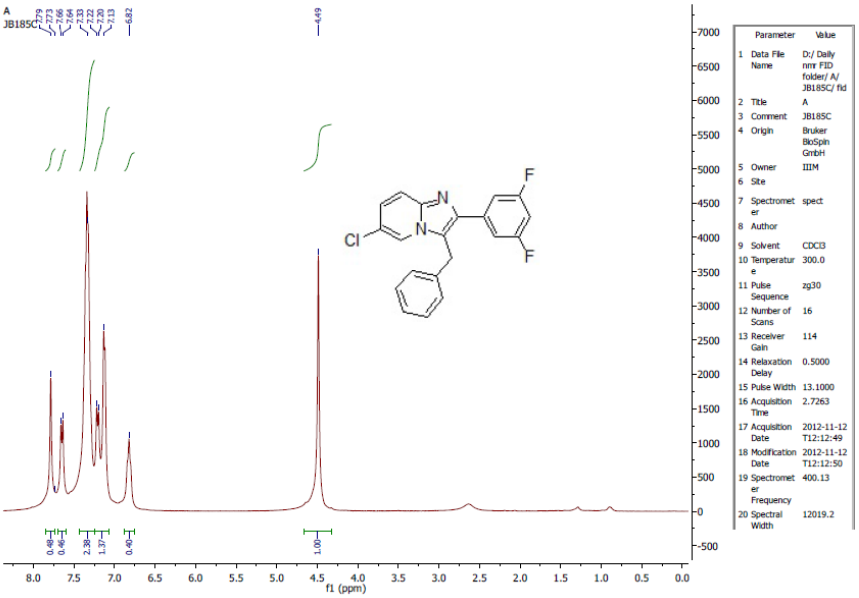
S2.o. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of 3-benzyl-6-chloro-2-(furan-2-yl)-imidazo[1,2-a]pyridine (5p)

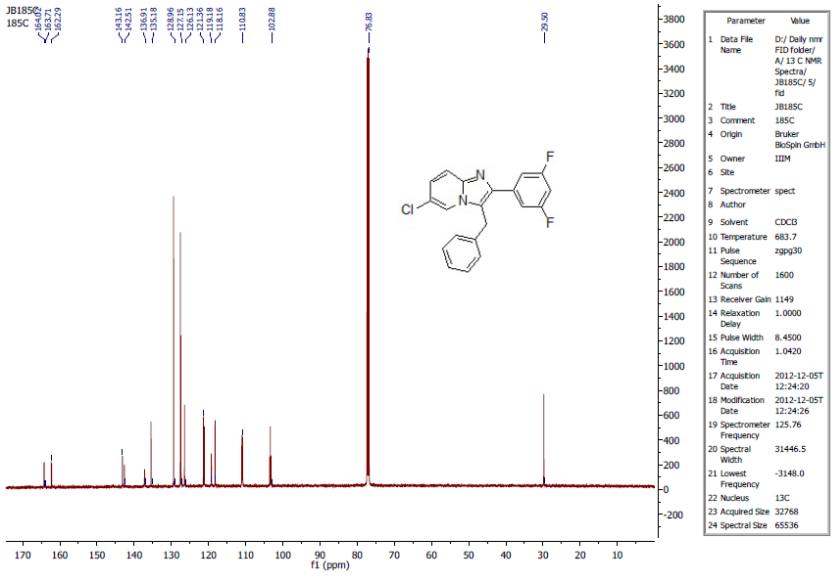


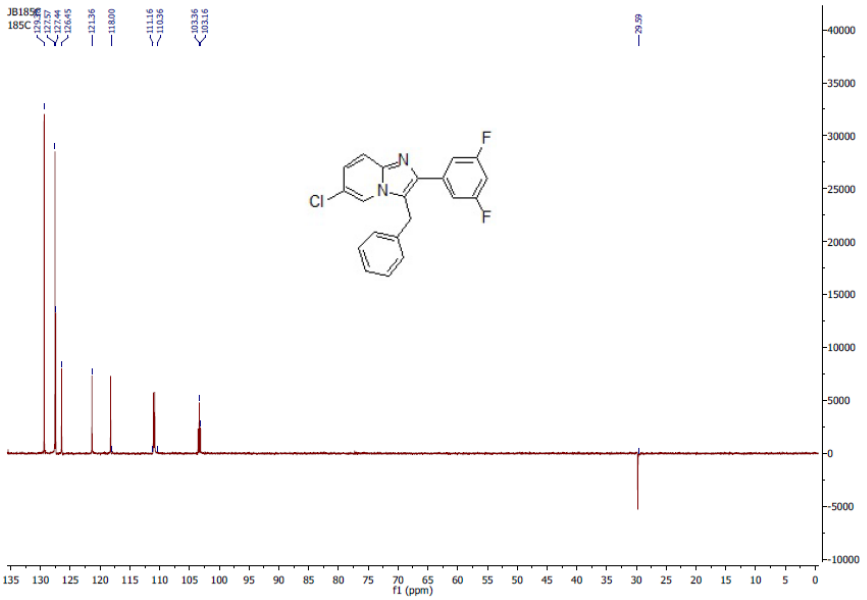


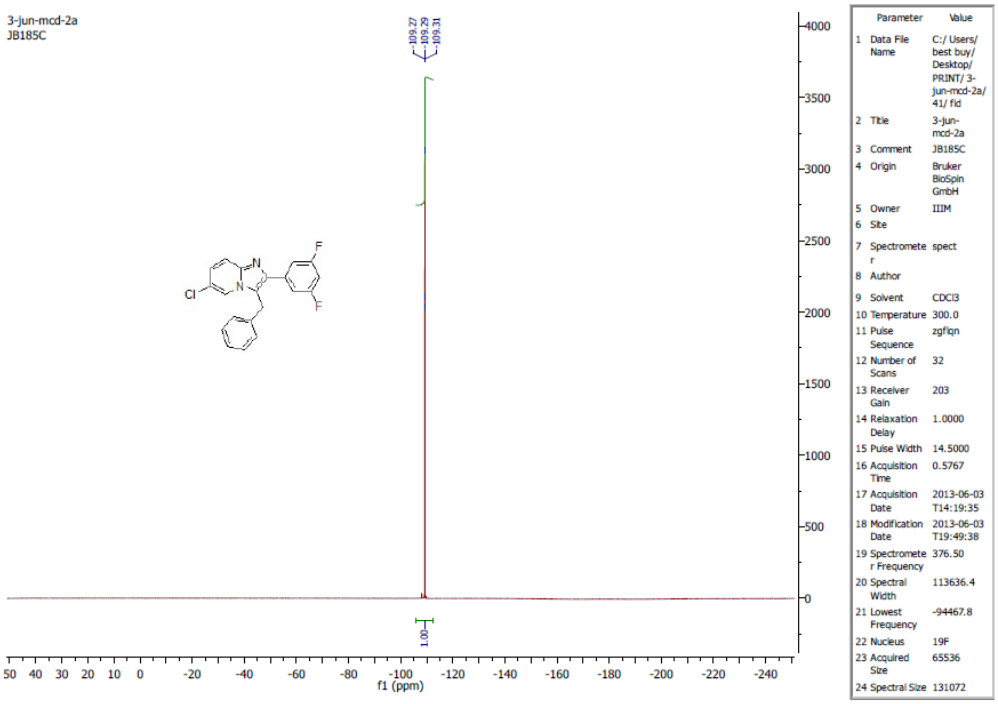


S2.p. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR spectrum of 3-Benzyl-6-chloro-2-(3,5-difluorophenyl)-imidazo[1,2-a]pyridine (5q)



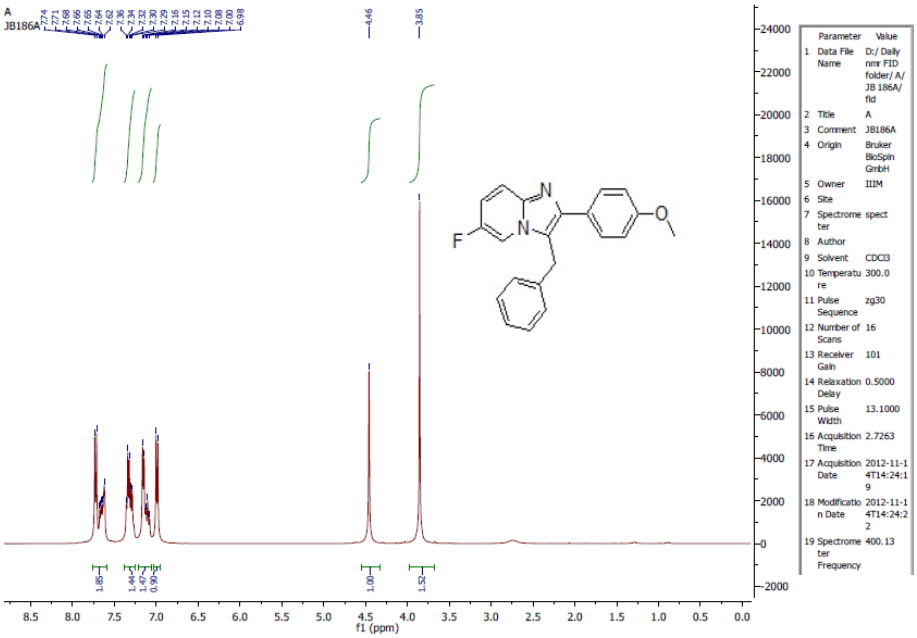


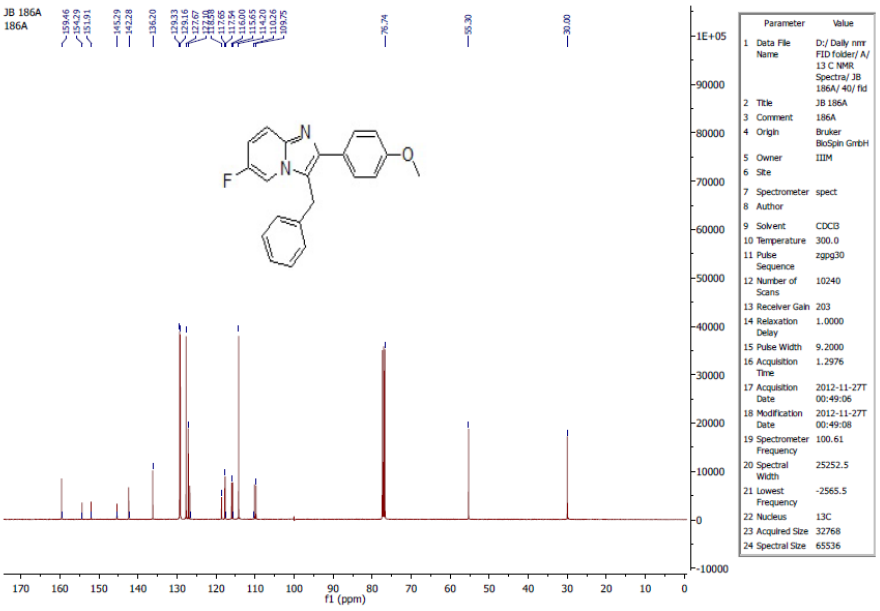


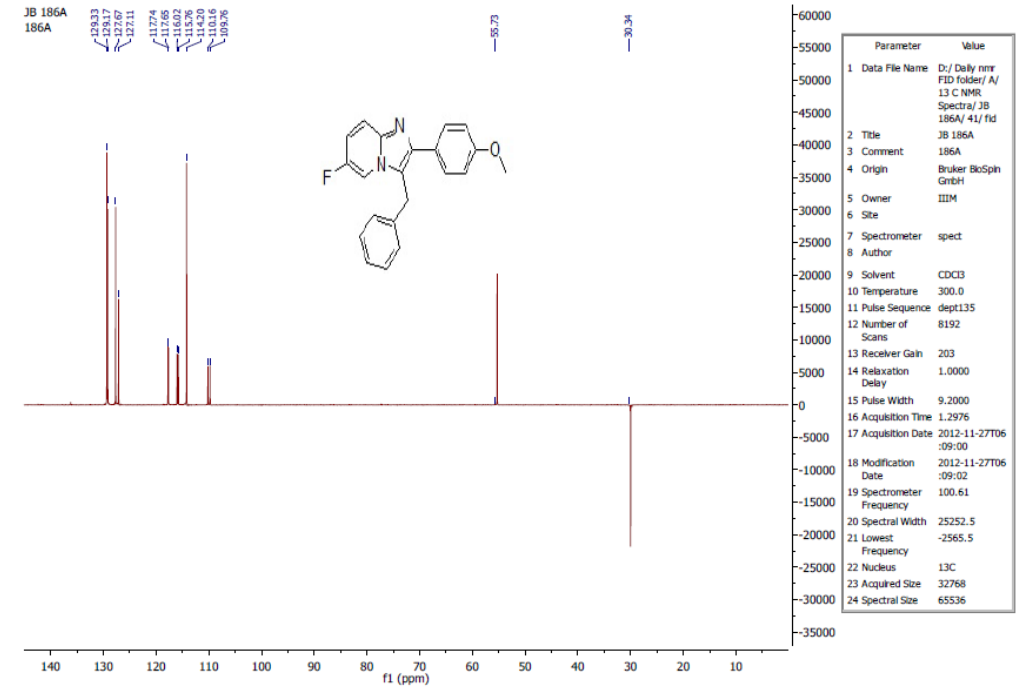


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 3-jun-mcd-2a/ 41/ fid
2	Title	3-jun-mcd-2a
3	Comment	JB185C
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgfiqn
12	Number of Scans	32
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	14.5000
16	Acquisition Time	0.5767
17	Acquisition Date	2013-06-03 T14:19:35
18	Modification Date	2013-06-03 T19:49:38
19	Spectrometer Frequency	376.50
20	Spectral Width	113636.4
21	Lowest Frequency	-94467.8
22	Nucleus	19F
23	Acquired Size	65536
24	Spectral Size	131072

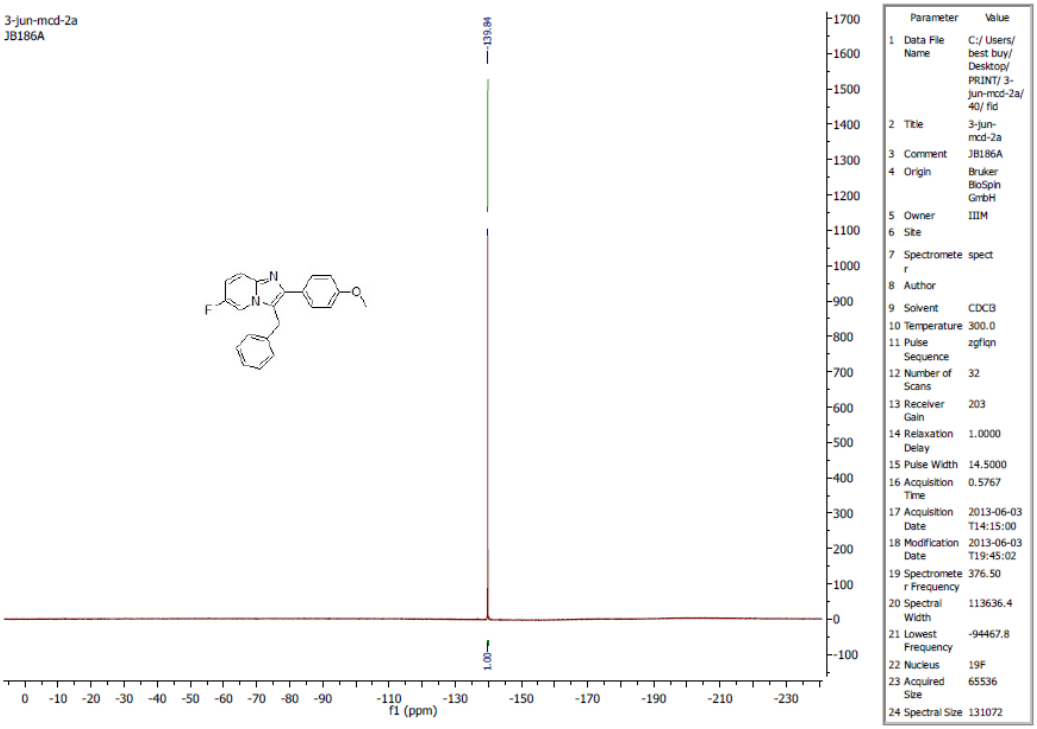
S2.q. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR spectrum of 3-Benzyl-6-fluoro-2-(4-methoxyphenyl)-imidazo[1,2-a]pyridine (5r)





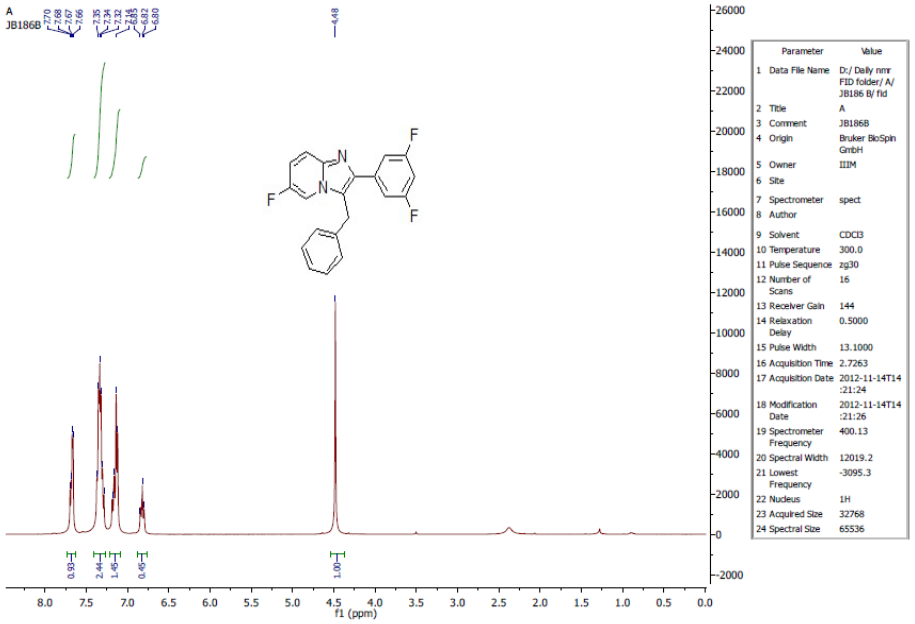


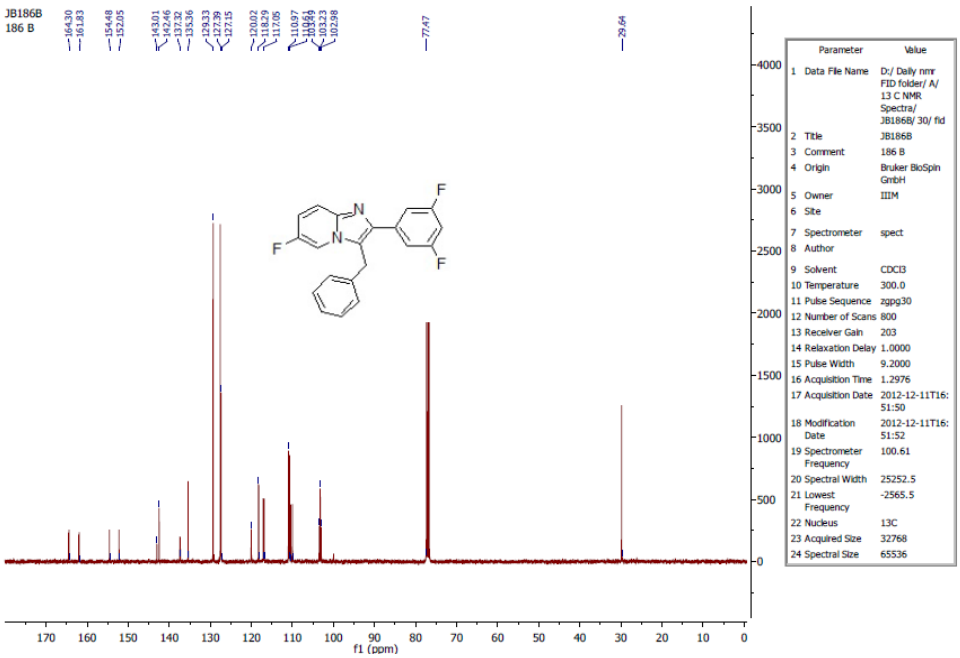
	Parameter	Value
1	Data File Name	D:/ Daily nmr FID folder/ A/ 13 C NMR Spectra/ JB 186A/ 41/ fid
2	Title	JB 186A
3	Comment	186A
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	dept135
12	Number of Scans	8192
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	9.2000
16	Acquisition Time	1.2976
17	Acquisition Date	2012-11-27T06 :09:00
18	Modification Date	2012-11-27T06 :09:02
19	Spectrometer Frequency	100.61
20	Spectral Width	25252.5
21	Lowest Frequency	-2565.5
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

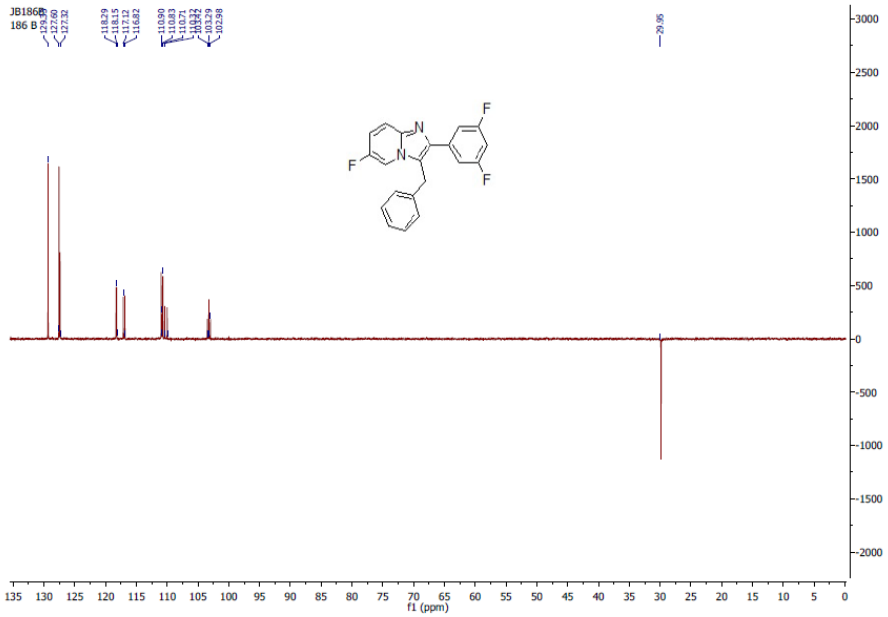


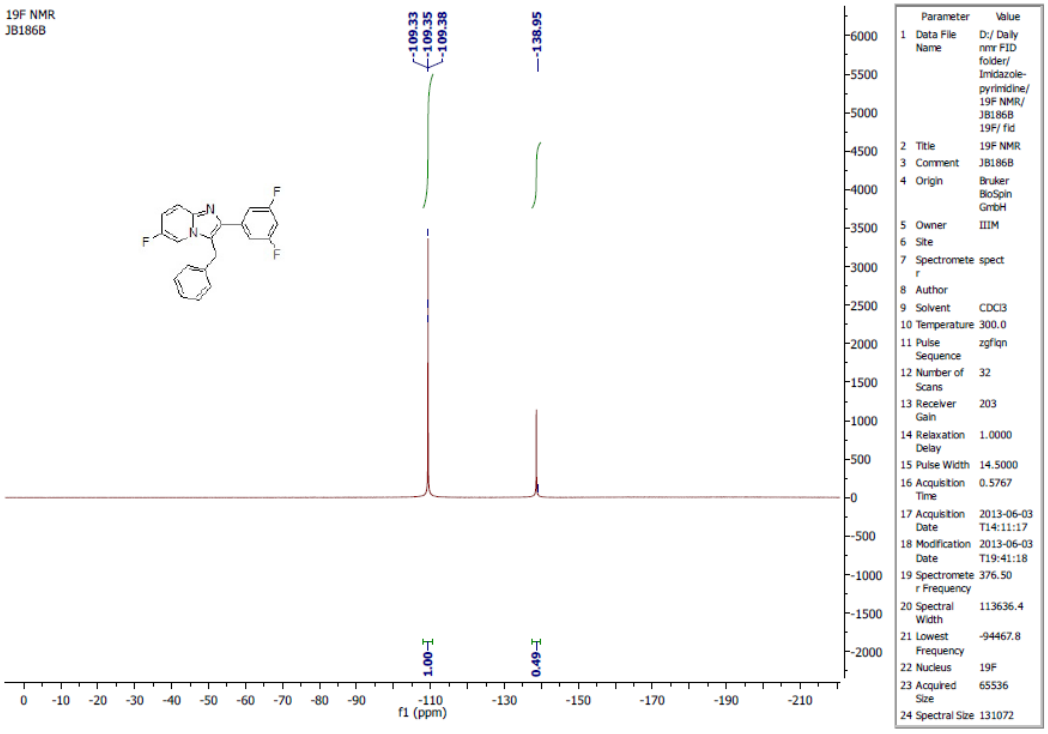
	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 3-jun-mcd-2a/ 40/ fid
2	Title	3-jun-mcd-2a
3	Comment	JB186A
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgflqn
12	Number of Scans	32
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	14.5000
16	Acquisition Time	0.5767
17	Acquisition Date	2013-06-03 T14:15:00
18	Modification Date	2013-06-03 T19:45:02
19	Spectrometer Frequency	376.50
20	Spectral Width	113636.4
21	Lowest Frequency	-94467.8
22	Nucleus	19F
23	Acquired Size	65536
24	Spectral Size	131072

S2.r. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR spectrum of 3-benzyl-6-fluoro-2-(3,5-difluorophenyl)-imidazo[1,2-a]pyridine (5s):

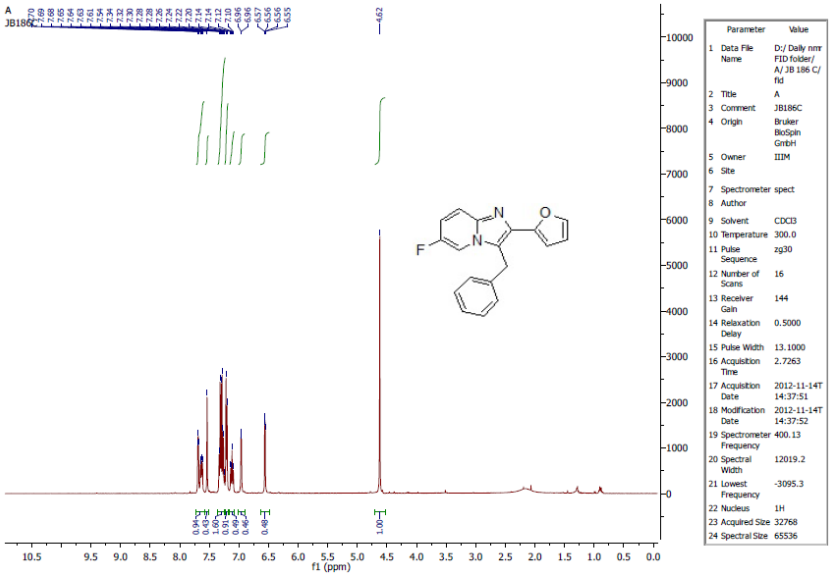


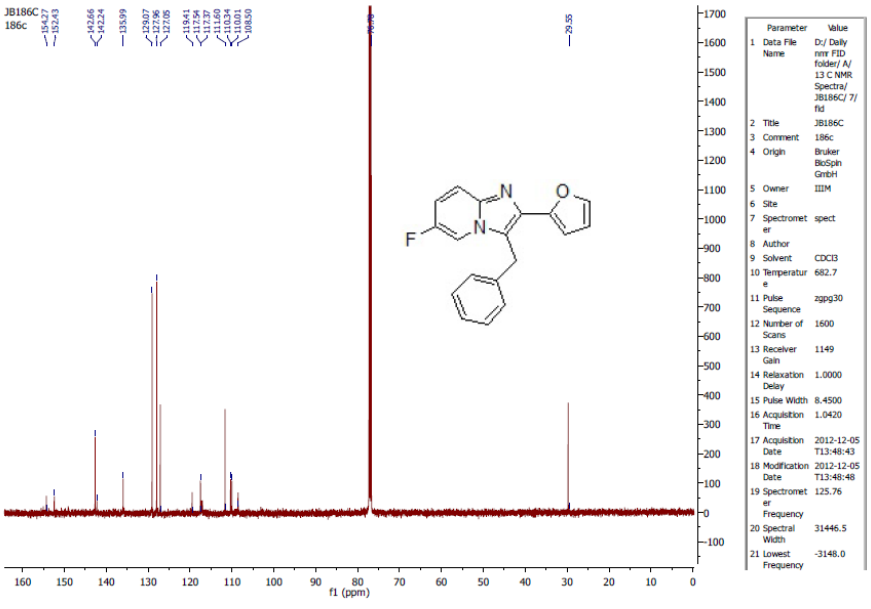


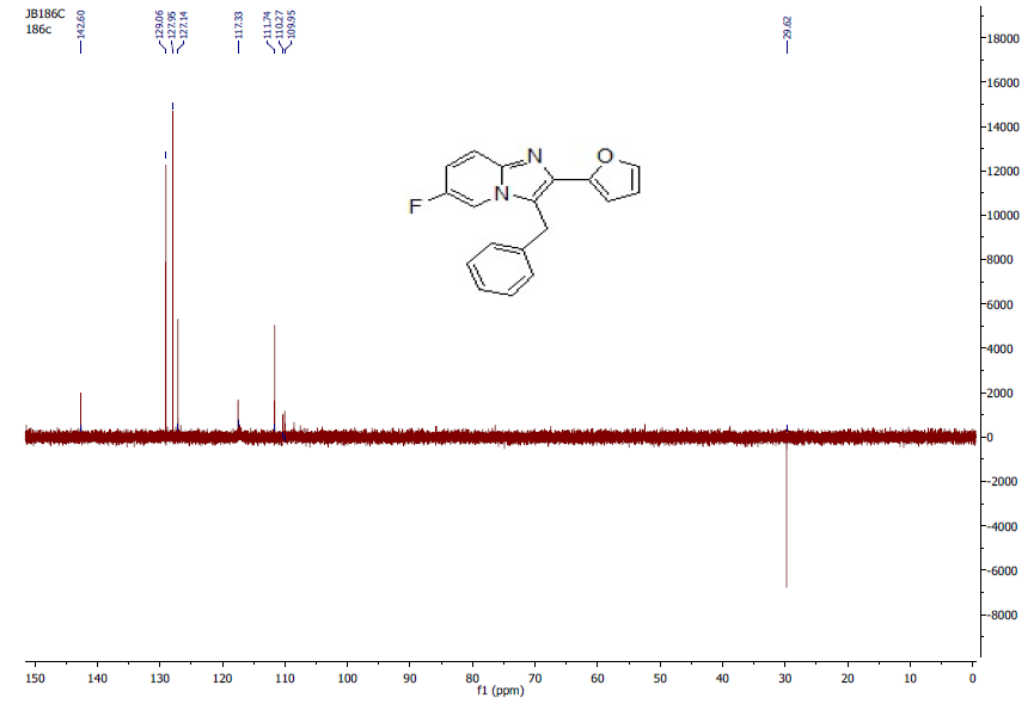

JB186B
186 B
129.89
127.60
127.32
118.29
118.15
117.12
116.82
110.90
110.83
110.71
103.22
103.29
102.98
29.95
F
N
F
F
3000
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

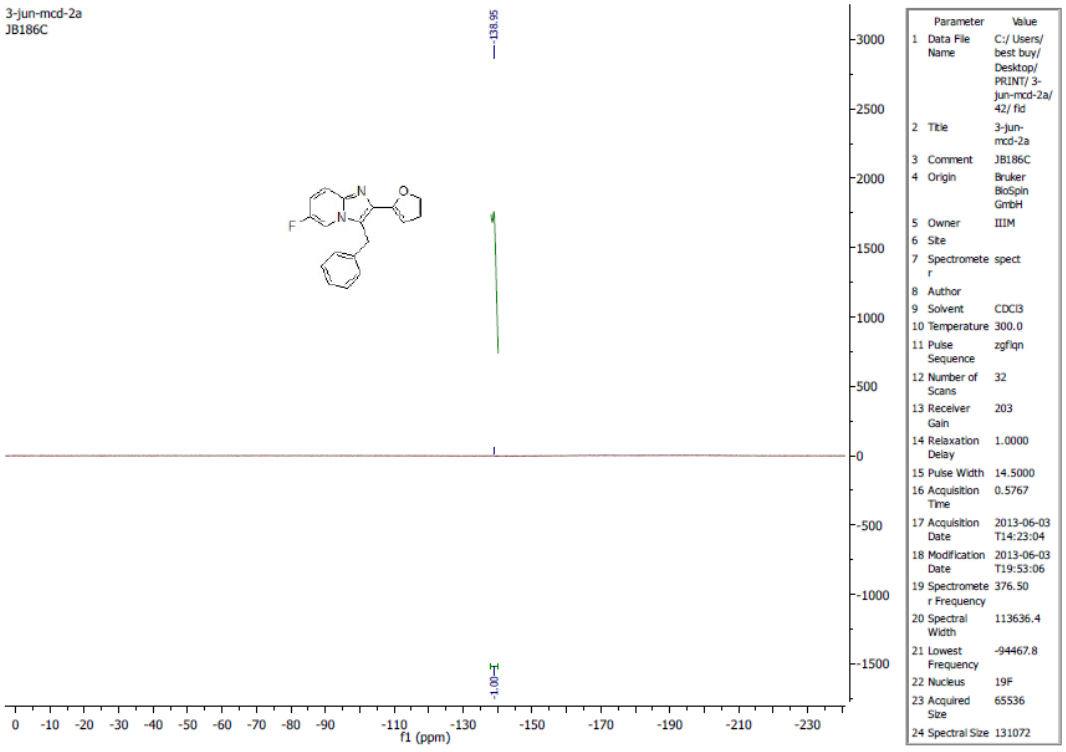

19F NMR
JB186B
-109.33
-109.35
-109.38
-138.95
F
N
F
F
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
1.00
0.49
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)
Parameter Value
1 Data File Name D:/ Daily nmr FID folder/ Imidazole-pyrimidine/ 19F NMR/ JB186B 19F/ fid
2 Title 19F NMR
3 Comment JB186B
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect r
8 Author
9 Solvent CDCl3
10 Temperature 300.0
11 Pulse Sequence zgflqn
12 Number of Scans 32
13 Receiver Gain 203
14 Relaxation Delay 1.0000
15 Pulse Width 14.5000
16 Acquisition Time 0.5767
17 Acquisition Date 2013-06-03 T14:11:17
18 Modification Date 2013-06-03 T19:41:18
19 Spectrometer Frequency 376.50
20 Spectral Width 113636.4
21 Lowest Frequency -94467.8
22 Nucleus 19F
23 Acquired Size 65536
24 Spectral Size 131072

S2.s. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR spectrum of 3-benzyl-6-fluoro-2-(furan-2-yl)-imidazo[1,2-a]pyridine (5t):






JB186C
186c
142.60
129.06
127.95
127.14
117.33
111.74
110.27
109.95
29.62
F
N
N
O
f1 (ppm)


3-jun-mcd-2a
JB186C
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-1.00
F
N
N
O
f1 (ppm)
Parameter Value
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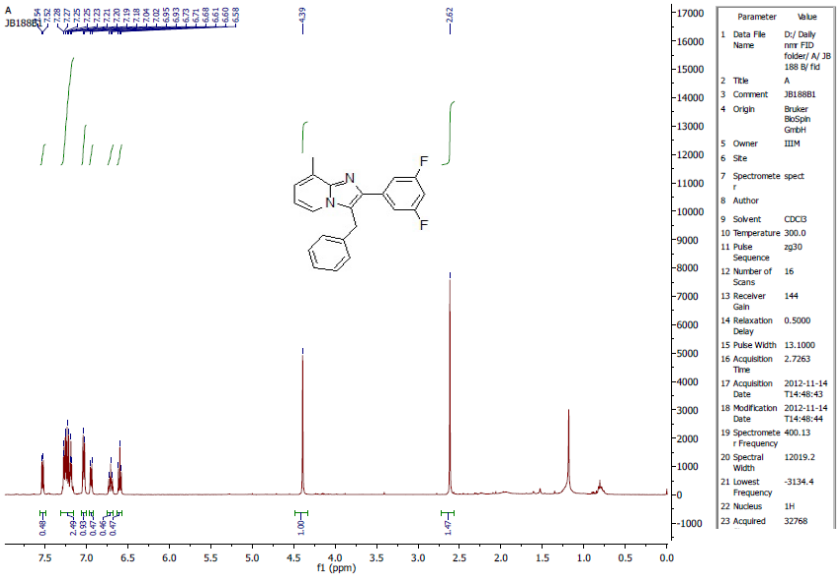
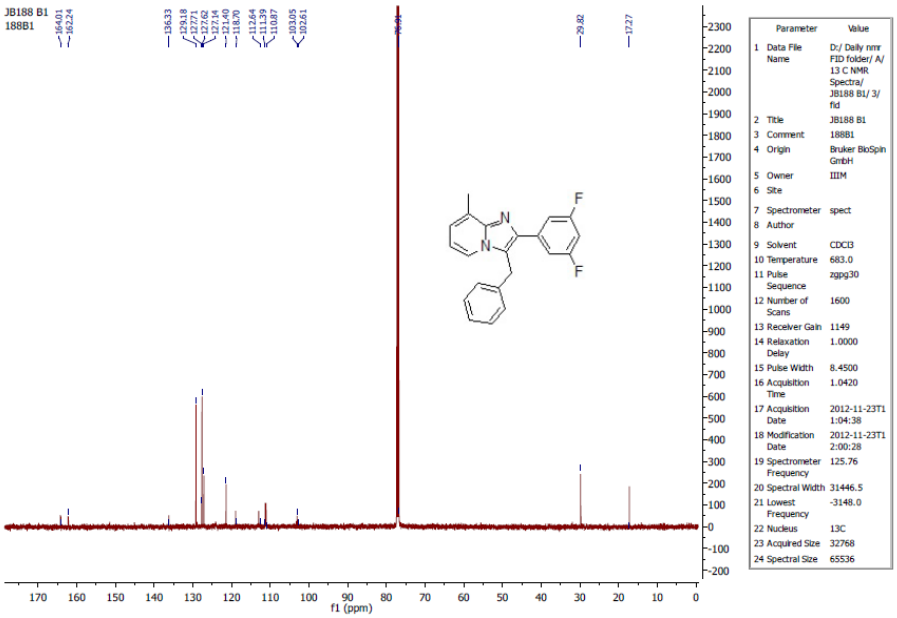
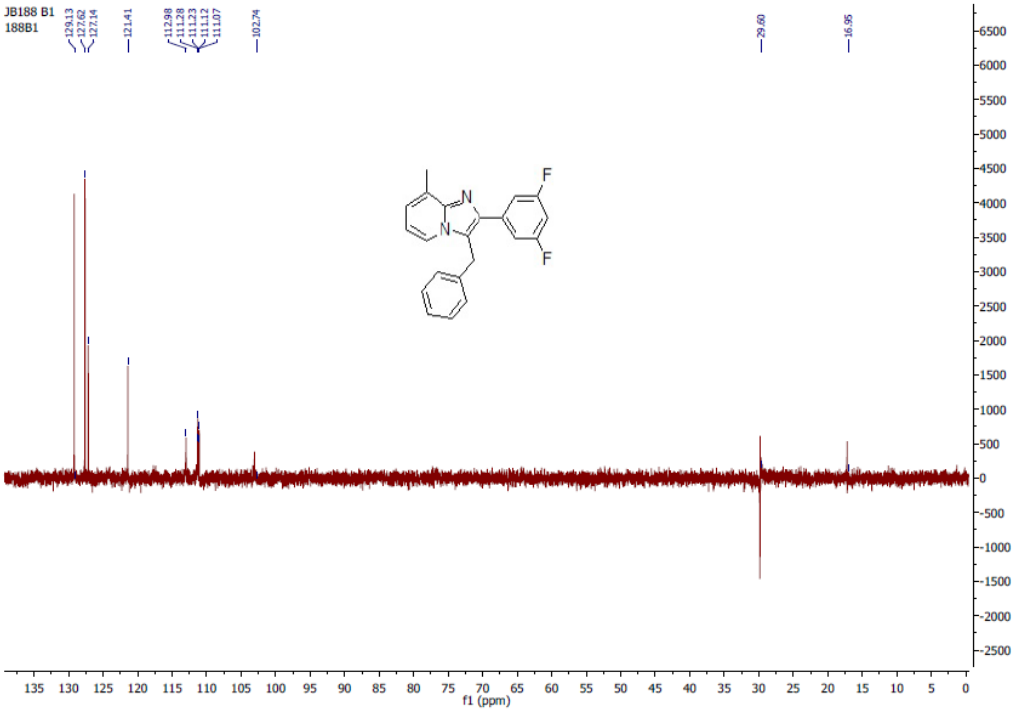
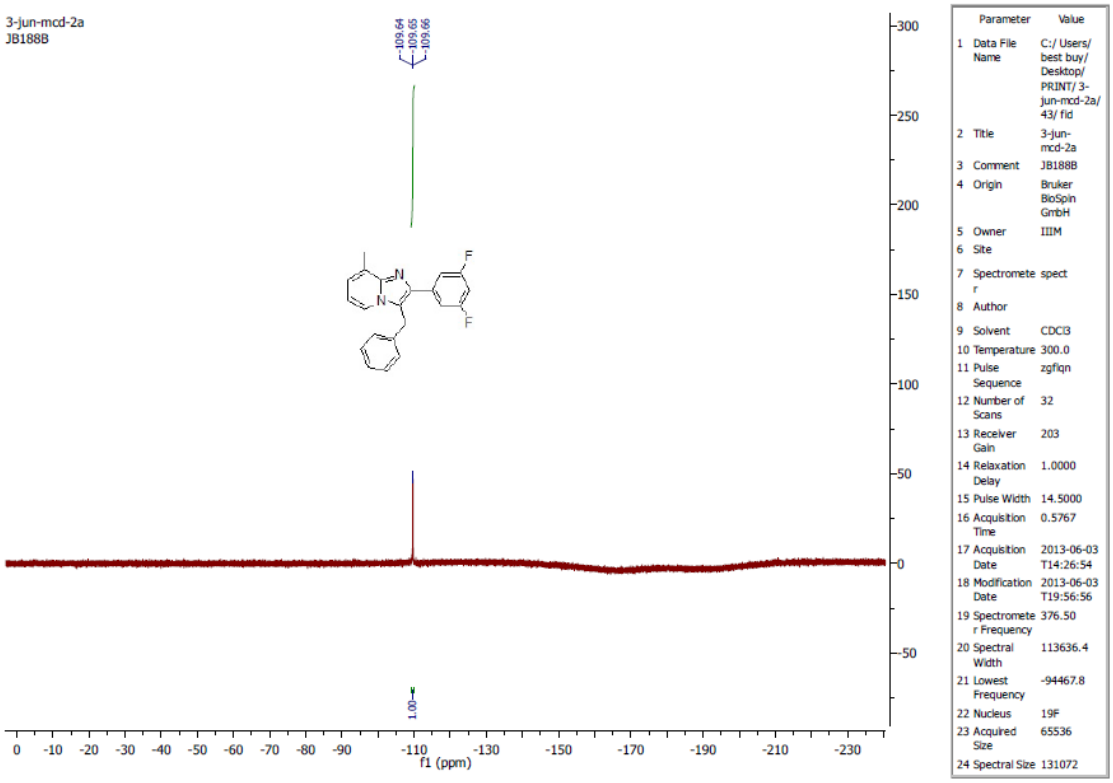
2 Title 3-jun-mcd-2a
3 Comment JB186C
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 300.0
11 Pulse Sequence zgflqn
12 Number of Scans 32
13 Receiver Gain 203
14 Relaxation Delay 1.0000
15 Pulse Width 14.5000
16 Acquisition Time 0.5767
17 Acquisition Date 2013-06-03 T14:23:04
18 Modification Date 2013-06-03 T19:53:06
19 Spectrometer Frequency 376.50
20 Spectral Width 113636.4
21 Lowest Frequency -94467.8
22 Nucleus 19F
23 Acquired Size 65536
24 Spectral Size 131072

S2.t. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR spectrum of 3-benzyl-2-(3,5-difluorophenyl)-8-methyl-imidazo[1,2-a]pyridine (5u):









	Parameter	Value
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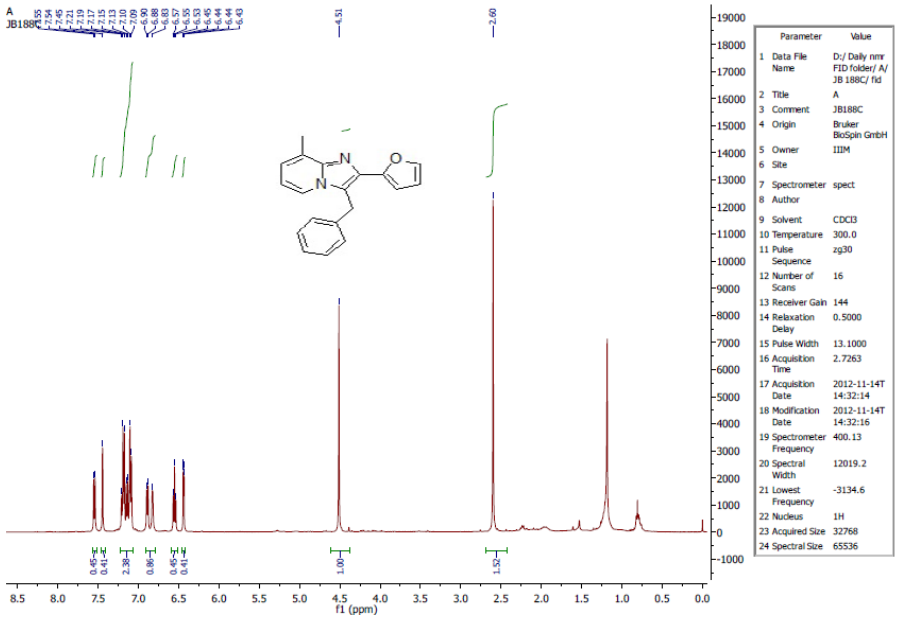
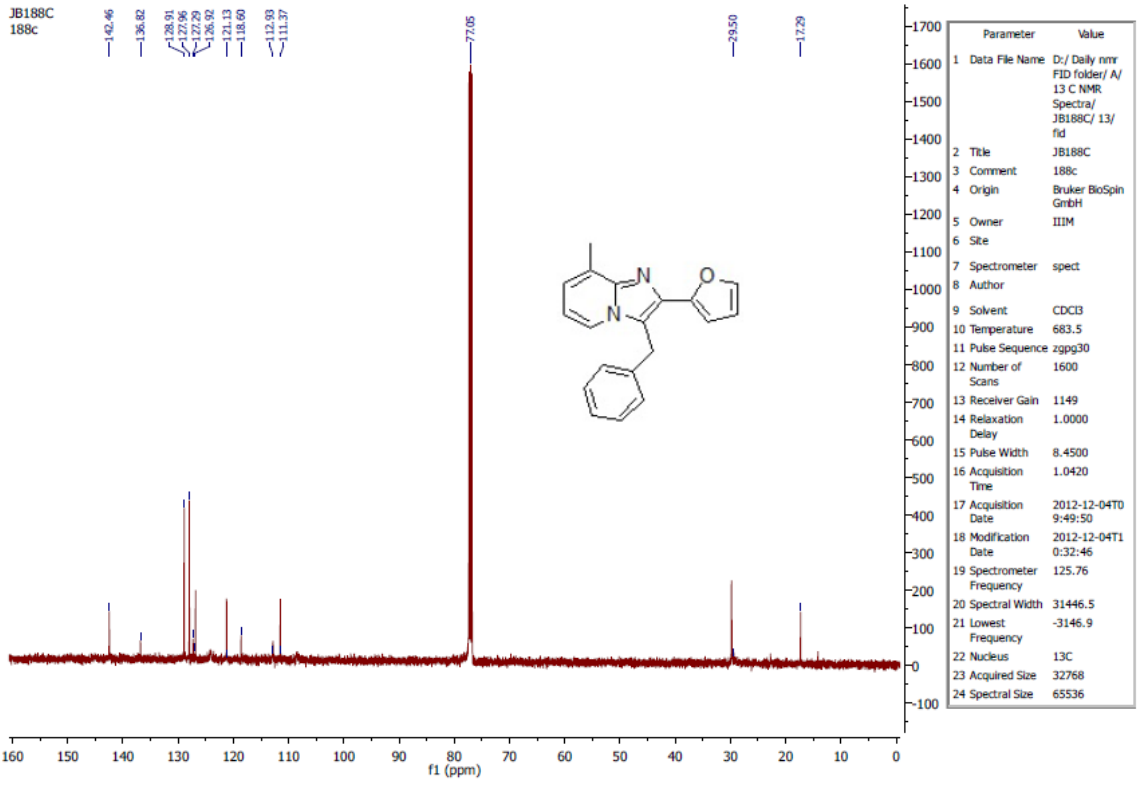
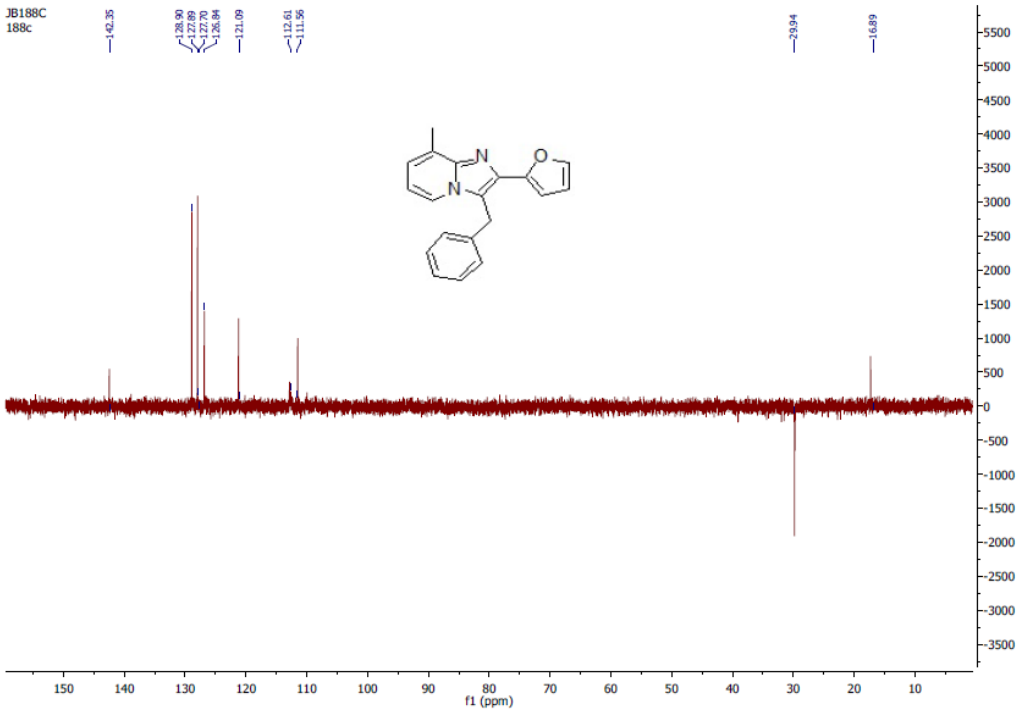
3	Comment	JB188B
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgflqn
12	Number of Scans	32
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	14.5000
16	Acquisition Time	0.5767
17	Acquisition Date	2013-06-03 T14:26:54
18	Modification Date	2013-06-03 T19:56:56
19	Spectrometer Frequency	376.50
20	Spectral Width	113636.4
21	Lowest Frequency	-94467.8
22	Nucleus	19F
23	Acquired Size	65536
24	Spectral Size	131072

S2.u. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of 3-benzyl-2-(furan-2-yl)-8-methyl-imidazo[1,2-a]pyridine (5v)






JB188C
188c
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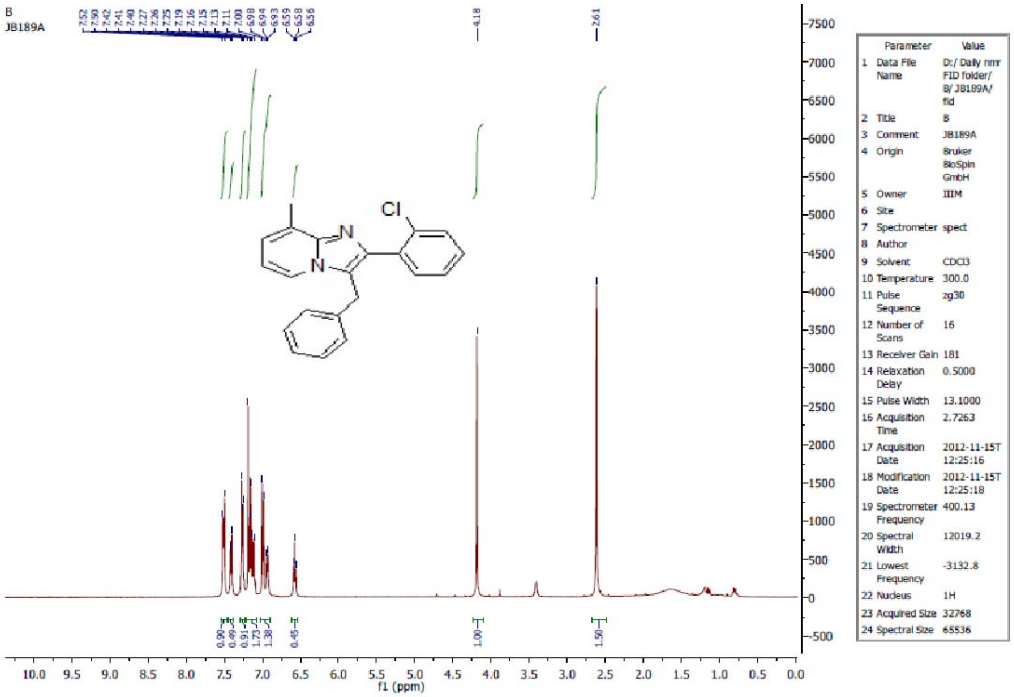
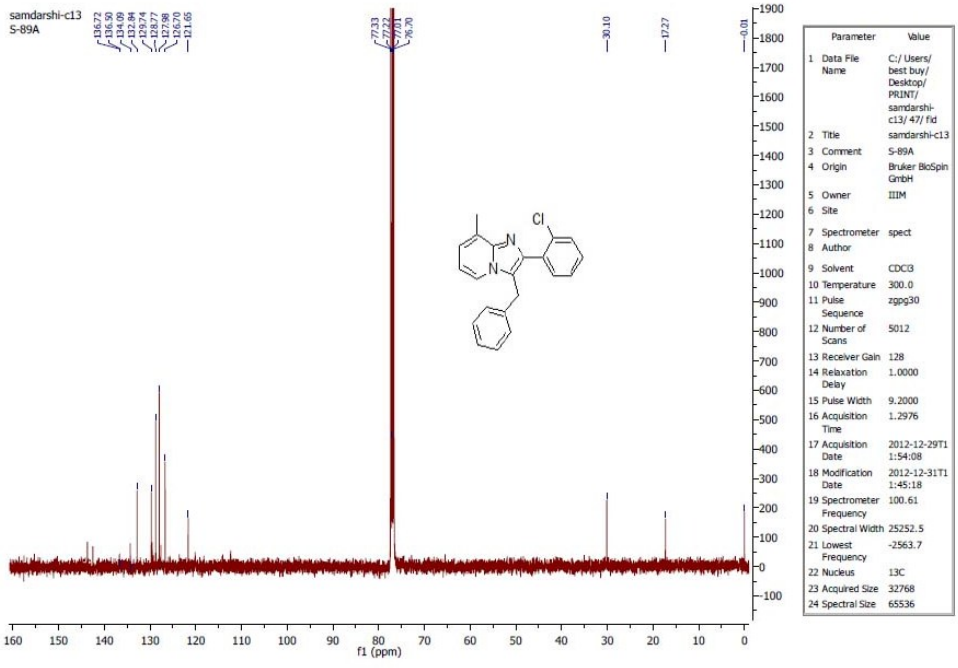
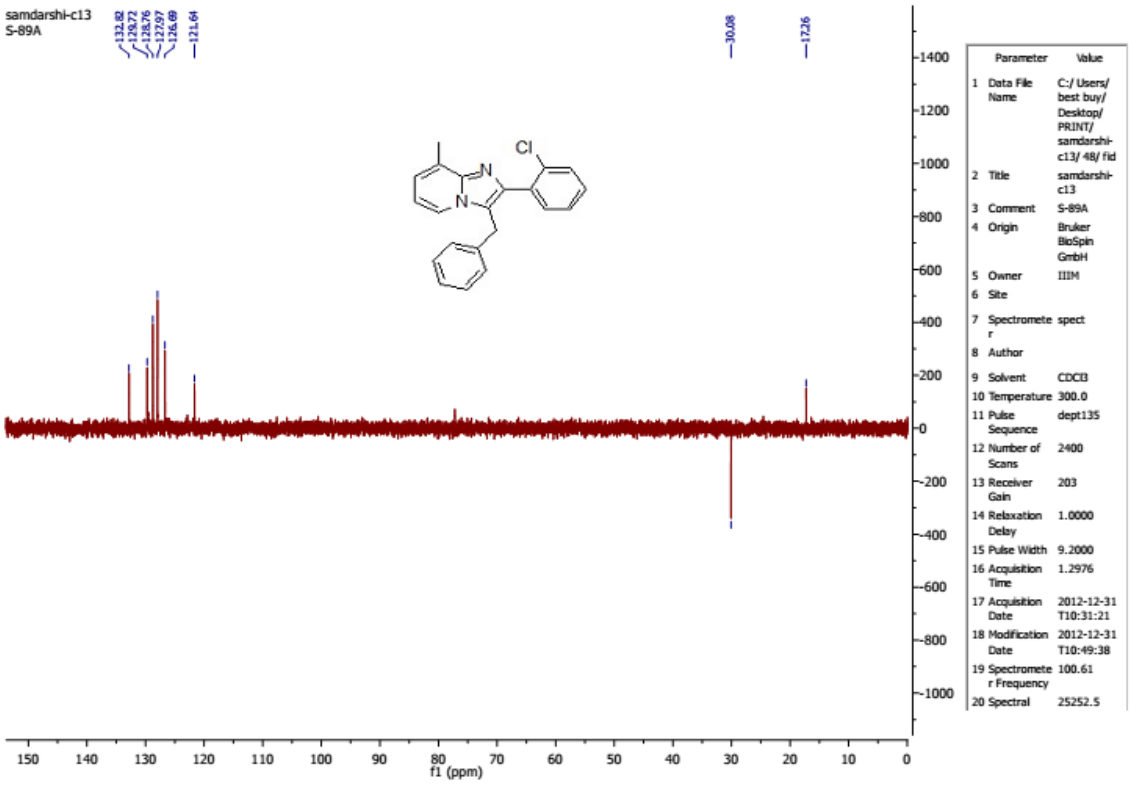
128.90
127.89
127.70
126.84
121.09
112.61
111.56
29.94
16.89
N
N
O
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
-2500
-3000
-3500
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

S2.v. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of 3-benzyl-2-(2-chlorophenyl)-8-methyl-imidazo[1,2-a]pyridine (5w)






samdarshi-c13
S-89A
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128.76
127.97
126.69
121.64
30.08
17.26
Cl
N
N
f1 (ppm)
Parameter Value
1 Data File Name C:/ Users/ best buy/ Desktop/ PRINT/ samdarshi-c13/ 48/ fid
2 Title samdarshi-c13
3 Comment S-89A
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 300.0
11 Pulse Sequence dept135
12 Number of Scans 2400
13 Receiver Gain 203
14 Relaxation Delay 1.0000
15 Pulse Width 9.2000
16 Acquisition Time 1.2976
17 Acquisition Date 2012-12-31 T10:31:21
18 Modification Date 2012-12-31 T10:49:38
19 Spectrometer Frequency 100.61
20 Spectral 25252.5

S3. Anticancer activity of imidazo[1,2-a]pyridines 5a-g and 5k-5w

Table S3. Anticancer activity of imidazo[1,2-a]pyridines **5a-g** and **5k-5w** (% growth inhibition) at 10 μM

Entry	MIAPaCa-2	PC-3	HL-60	A549
5a	12.11	29.71	21.11	17.88
5b	23.32	22.53	19.01	12.88
5c	9.11	7.05	8.99	10.98
5d	12.98	18.94	23.9	25.55
5e	27.99	**37.32**	21.1	**34.12**
5f	14.44	13.79	24.99	24
5g	0	0	15.98	10.98
5k	11.99	9.95	23.89	13.33
5l	8.90	0	12.11	7.76
5m	17.67	19.15	31.9	31.77
5n	**30.11**	**30.34**	**32.09**	**36.87**
5o	11	0	12.56	12
5p	13.23	18.41	21.41	17.88
5q	21.99	18.53	28.87	23
5r	**21.66**	**34.08**	21.77	28.99
5s	31.11	8.55	31.23	16.98
5t	21.22	**38.03**	21.00	23.44
5u	22.67	4.38	24.76	27.99
5v	15.52	1.25	15.67	11.21
5w	26.43	0	12.90	0

S4. Mechanism of the reaction

The possible mechanism for Cu-Mn catalyzed domino three-component coupling and 5-*exo-dig* cyclization is depicted in Figure S4. The reaction mechanism comprises a cascade of reactions involving initial condensation of 2-aminopyridine and aldehyde to form imine **I**. The nucleophilic attack by alkyne to the imine C=N bond of **I** produces propargyl amine **II**. Finally, the intramolecular nucleophilic attack of nitrogen in pyridine ring to the triple bond in a '*5-exo-dig*' fashion produces cyclized intermediate **III** which after protonation followed by isomerization leads to formation of imidazo[1,2-a]pyridine **5a**.

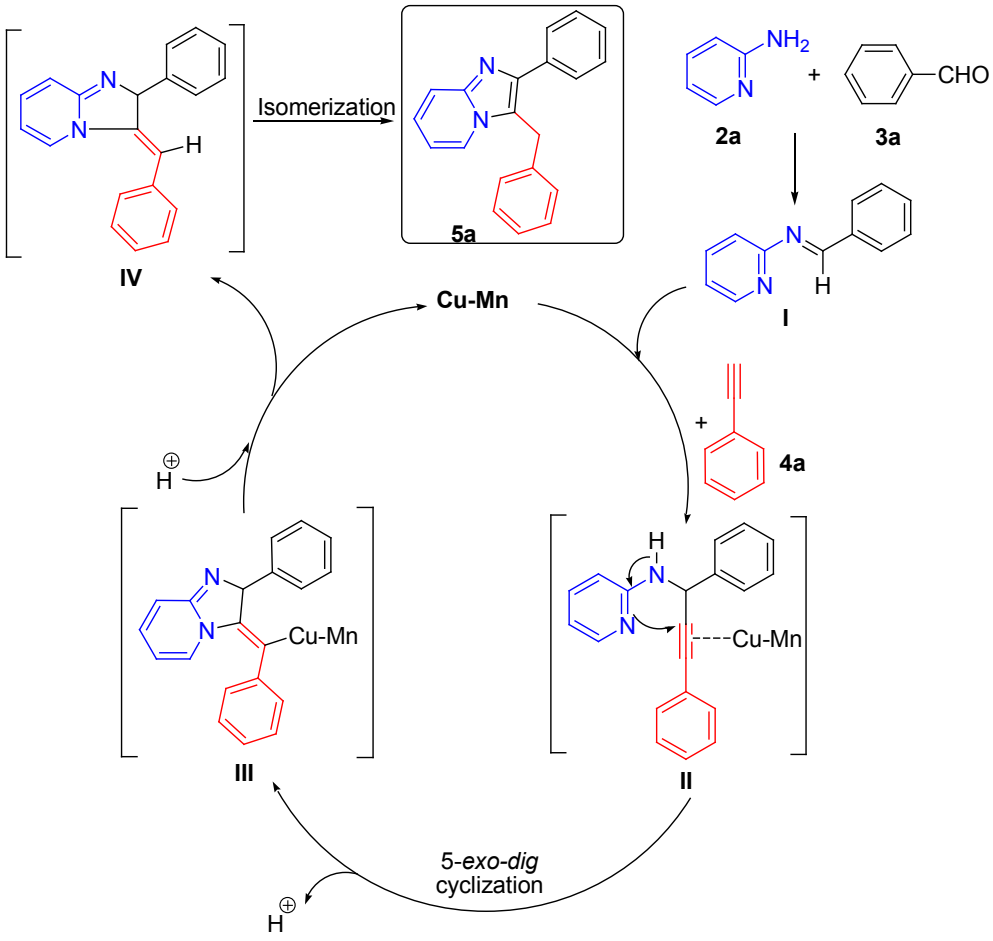

Figure S4. Proposed mechanism for Cu-Mn catalyzed MCR protocol for synthesis of imidazo[1,2-a]pyridine **5a**