Electronic Supporting Information (ESI)

Montmorillonite clay catalyzed synthesis of functionalized pyrroles through domino four-component coupling of amines, aldehydes, 1,3-dicarbonyl compounds and nitroalkanes

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S1. Fe-PILC catalyst preparation and characterization

S1a. Preparation of Fe-PILC

Ferric chloride ($FeCl_3$) was used in Fe-PILC synthesis. A base-hydrolyzed $FeCl_3$ pillaring solution was prepared using OH/Fe molar ratio of 2.0. The hydrolysis was carried out at room temperature for 16 h under continuous stirring. Montmorillonite clay K10 powder was added gradually to Fe pillared solution, providing a required mmol of Fe per gram of clay. Fe Pillared clay suspension was stirred for 3 h at room temperature to allow ion exchange between exchangeable cations of the clay and pillar precursors. The formed PILCs were centrifuged, washed, dried in air, and calcined in air at 425 °C for 3 h.

S1b. Characterization of Fe-PILC

Synthesized Fe-PILC catalyst was characterized using specific surface area determination, temperature programmed reduction (TPR), temperature programmed desorption (TPD) and scanning electron microscopy (SEM). The specific surface areas (m^2g^{-1}) of samples were estimated with the N_2 adsorption at the liquid nitrogen temperature on the Quantachrom Chem-BET 3000.

Temperature programmed reduction (TPR):

Temperature programmed reduction (TPR) profiles of catalyst precursors were collected on the Quantachrom Chem-BET 3000 apparatus equipped with a thermal conductivity detector (TCD). 50 mg samples placed in a quartz U-shaped tube were reduced in 5%H_2/N_2 flow (80 mL min^{-1}) from room temperature to 700 °C at a temperature rise of 5 °C min^{-1}. Samples were pretreated in N_2 flow (50 mL min^{-1}) at 300 °C for 2 h to remove the adsorbed water and other contaminants prior to each TPR experiment.

H_2-Temperature-programmed reduction (TPR) profiles of the Fe – PILC catalyst are shown in Figure S1. The reduction of iron oxides takes place in three steps. In the first step, Fe_2O_3 was reduced to Fe_3O_4 and the second step involved the reduction of Fe_3O_4 to FeO which was consequently reduced to Fe. Generally FeO is not expected to appear in the TPR spectra as it has been shown that FeO is unstable compared to Fe and Fe_3O_4. For the Fe - PILC, reduction of

Fe_2O_3 to Fe_3O_4 took place at 415 °C. The reduction of Fe_3O_4 to Fe occurred at 470 °C while the broad peak appearing between 500 to 750 was assigned to the reduction of small metal particles and mixed oxides which are difficult to reduce.

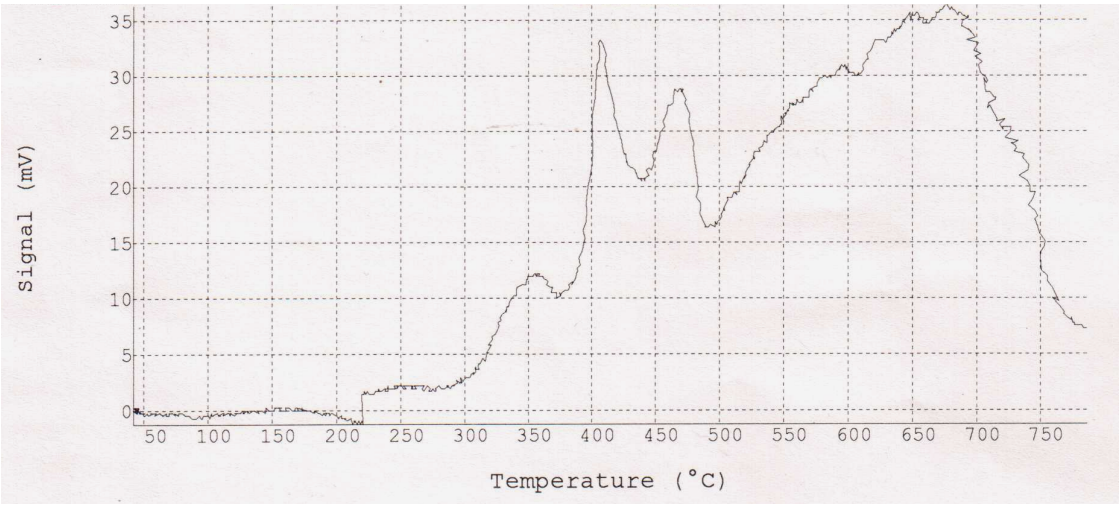


Figure S1. TPR profile of FE-PILC **B** catalyst

Ammonia TPD experiment:

The total acidity and acid distribution of the pillared clays was determined by ammonia TPD with the help of a CHEM BET-3000 (Quantachrome, USA) instrument in the temperature range of 30–800 °C. About 0.1 g of powdered sample was taken inside a quartz U tube and degassed at 350 °C for 1 h with ultrapure helium gas. After the sample was cooled to room temperature, NH_3 gas of 1000 ppm with N_2 gas was passed through the sample for 1 h. Then the ammonia adsorbed sample was purged with helium gas at 40 °C to remove any weakly adsorbed NH_3 on the surface. The temperature-programmed desorption of ammonia was performed between 80 and 800 °C at 10 °C /min.

Acidity was estimated as being the total amount of NH_3 released through thermal programmed desorption (TPD) per gram of dry clay sample. The number of desorbed molecules is supposed to be equal to that of the adsorption sites present on the clay surface. The acid strength is proportional to the temperature required to release the probe gas molecules. The strength distributions were expressed in terms of various amounts of ammonia desorbed under controlled temperature increase, and was estimated by TPD pattern deconvolution.

The acidity of PILC with respect to the type of pillar was observed by NH_3 TPD. The PILC contained enormously high surface acidity compared to the original clay montmorillonite. This simply indicates that the acidity of the clay is enhanced by pillaring the clay. The concentration and strength of the acidic sites of Fe – PILC catalyst have been determined by NH_3 TPD and showed in Table S1. Total acidity of the catalyst was found to be 7.91 mmol NH_3/g catalyst, which was distributed on the surface of the clay support as 47% (3.75 mmol NH_3/g catalyst), 18% (1.40 mmol NH_3/g catalyst) and 35% (2.76 mmol NH_3/g catalyst) of weak, medium and strong acidic sites.

Table S1. Distribution of activity in Fe-PILC **B** catalyst

Acidic sites	**mmol NH_3/g catalyst**	**%age**
Weak acidity	3.75	47.40
Medium acidity	1.40	17.70
Strong acidity	2.76	34.90
Total acidity	7.91	100

Morphology of the catalyst:

The morphology of Fe-PILC **B** catalyst was studied using JEOL.JEM100CXII electron microscope with ASID accelerating voltage of 40 KV. Figure depicts the representative SEM image of calcined Fe –PILC catalyst. The image shows that materials are randomly distributed over the support surface with flake formation. Result are supported by dispersion analysis (up to 99.4%) and average crystallite size as 11.60 A^o (CHEMBET- 3000). Fe particles are constituted by several aggregates and not by continuous film. Higher dispersed catalytic materials are able to adsorb the substrate and /or reagent to a high extent.

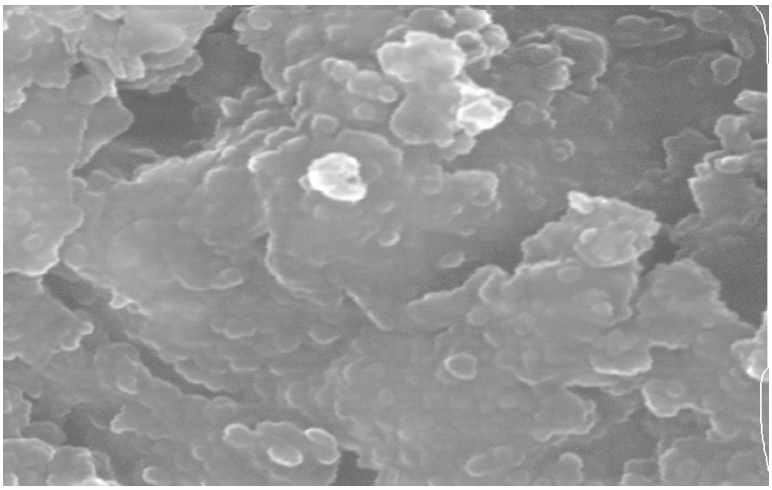
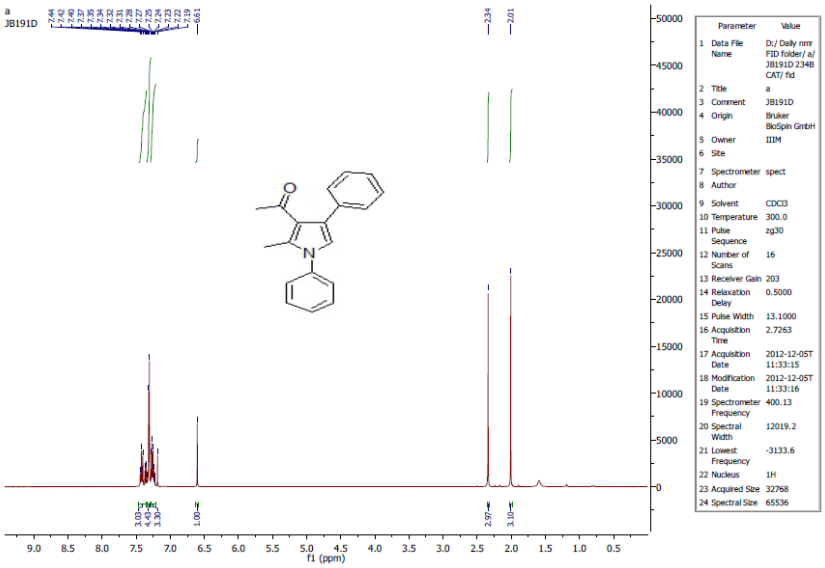
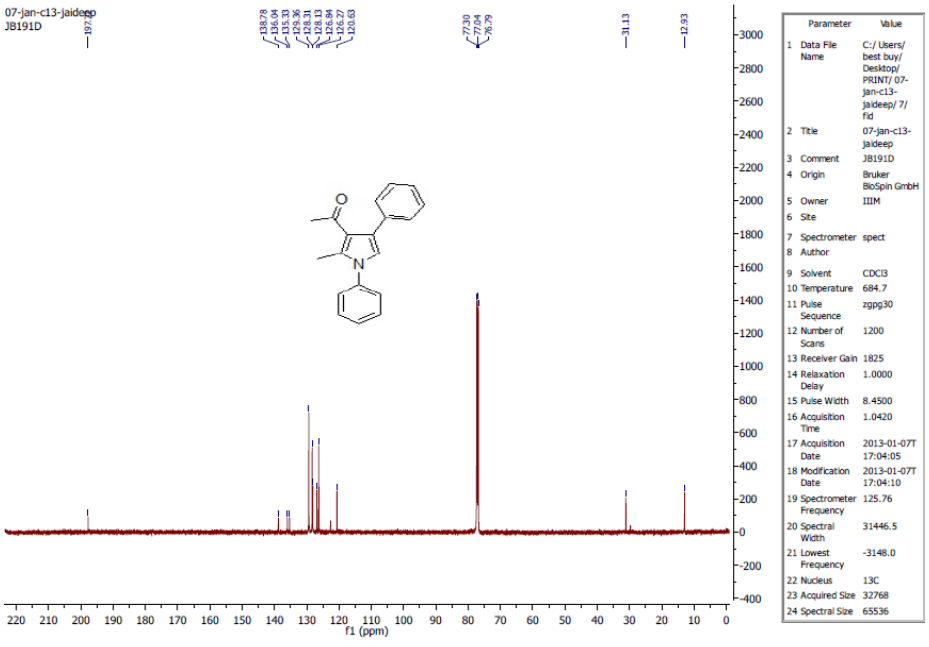
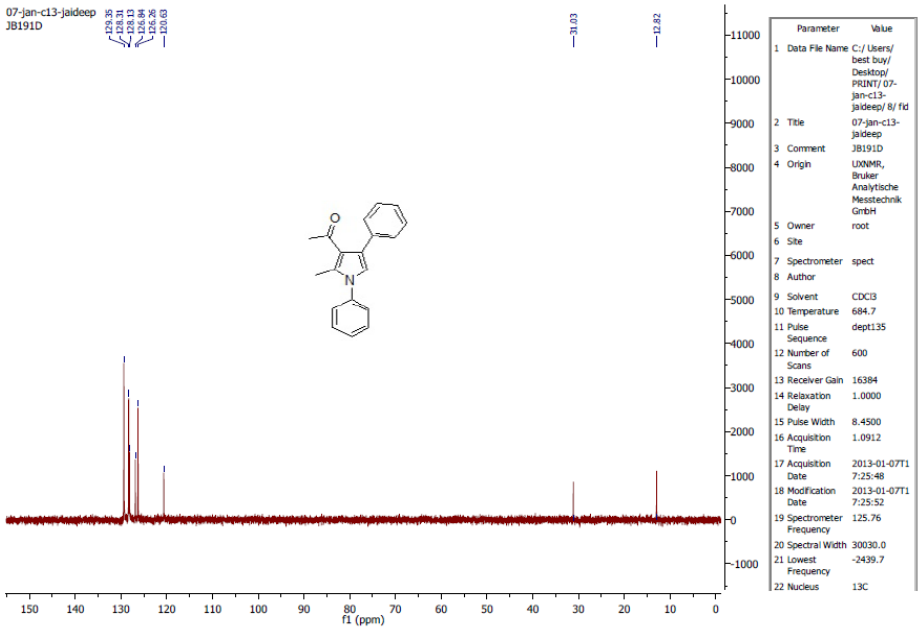


Figure S2. SEM image of Fe-PILC **B** catalyst

S2.a. ^{1}H, ^{13}C and DEPT-135 NMR of 1-(2-methyl-1,4-diphenyl-1H-pyrrol-3-yl) ethanone (1a):



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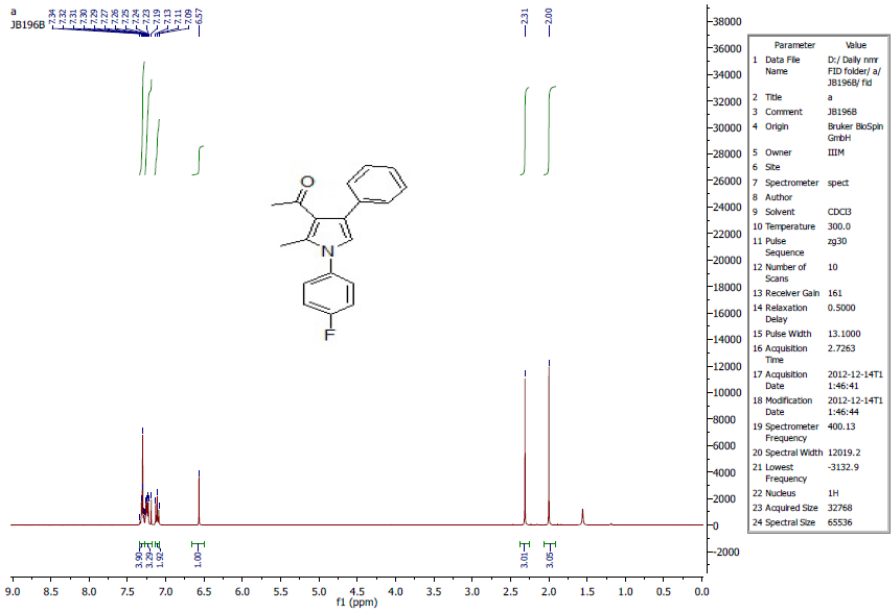
S2.b. ^{1}H, ^{13}C DEPT-135 NMR ,^{19}F of 1-(1-(4-fluorophenyl)-2-methyl-4-phenyl-1H-pyrrol-3-yl) ethanone (1b)



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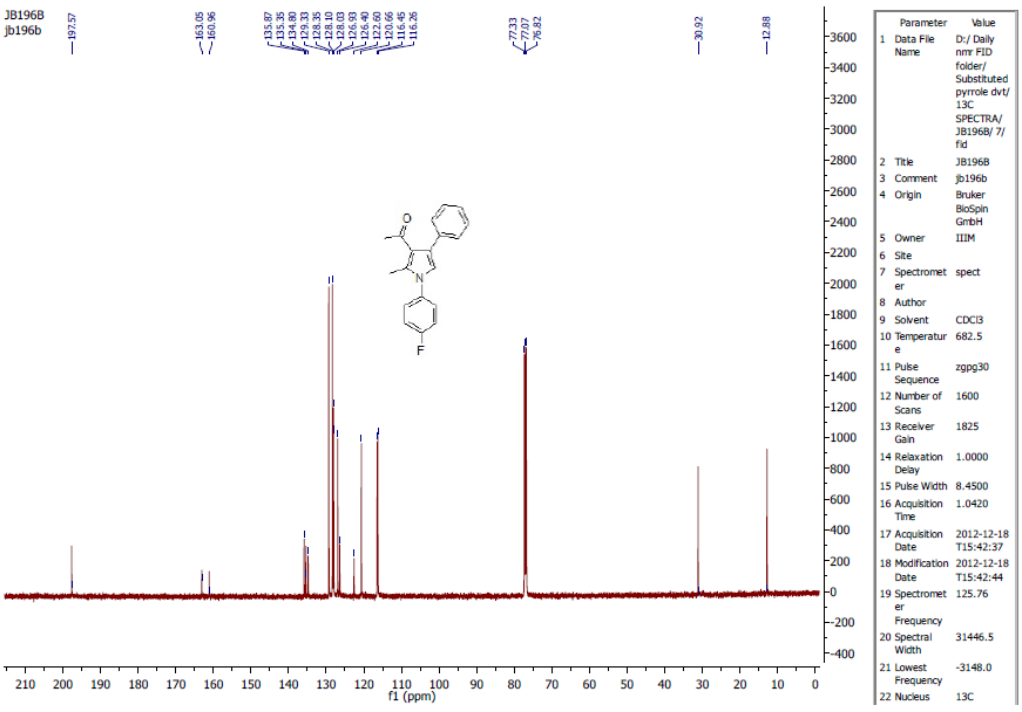

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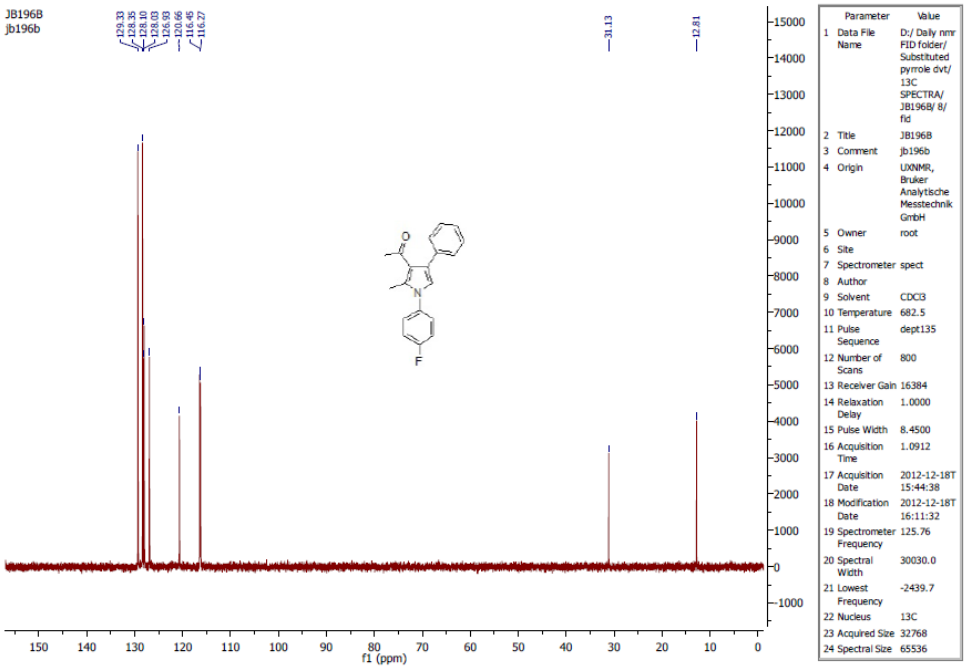
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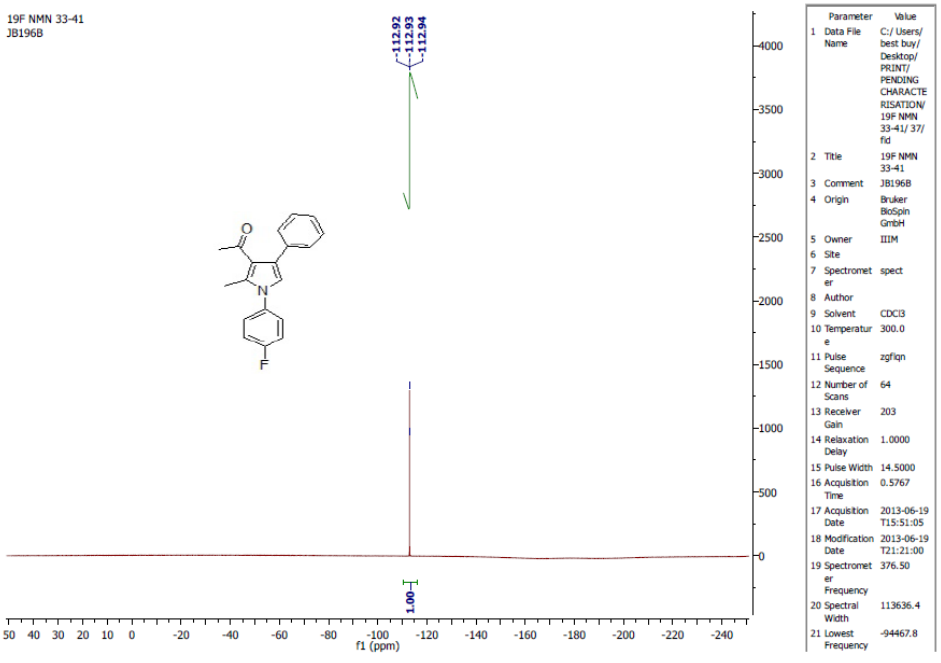
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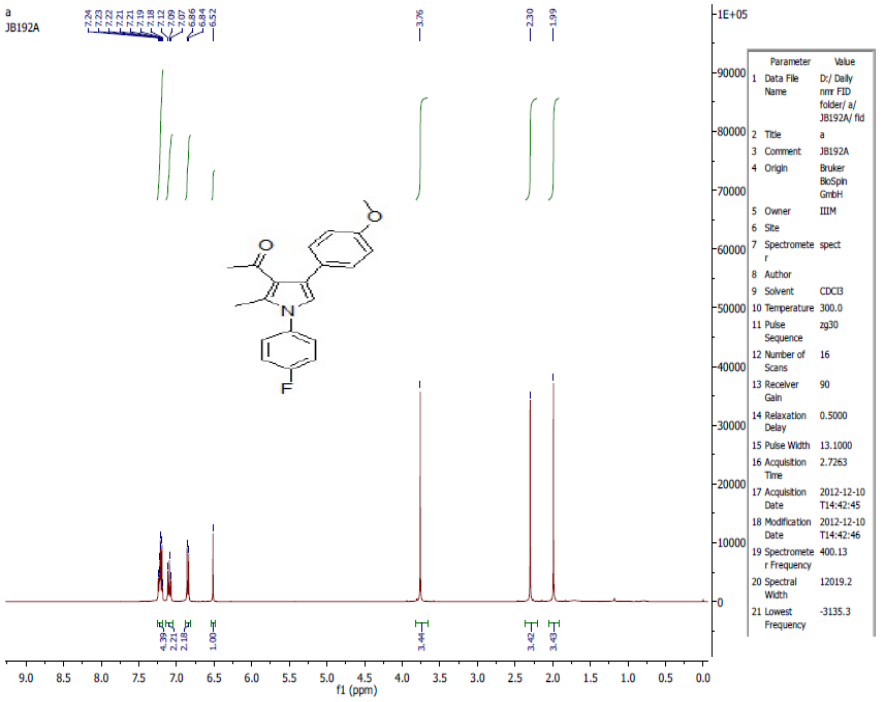
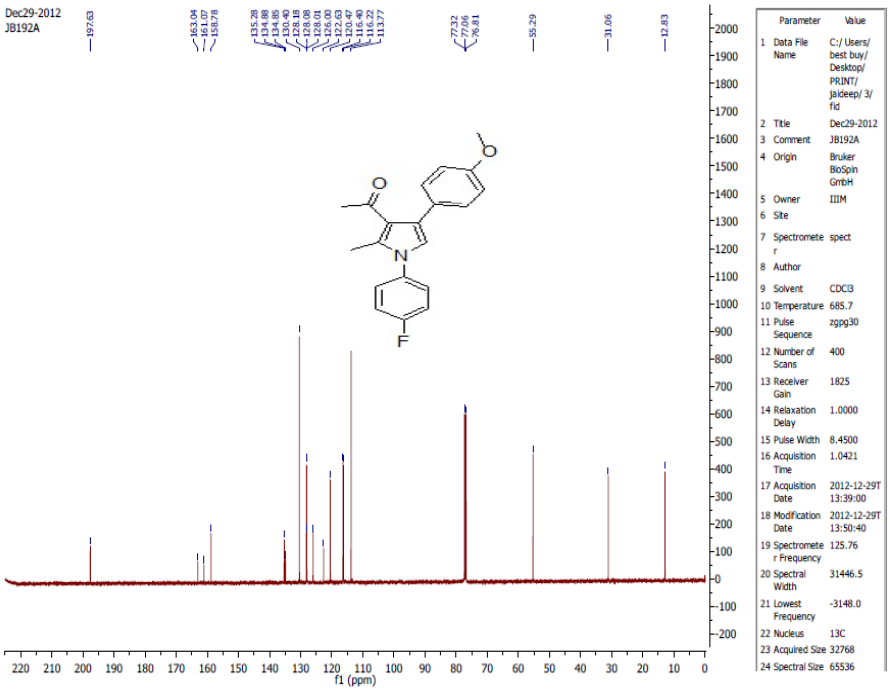
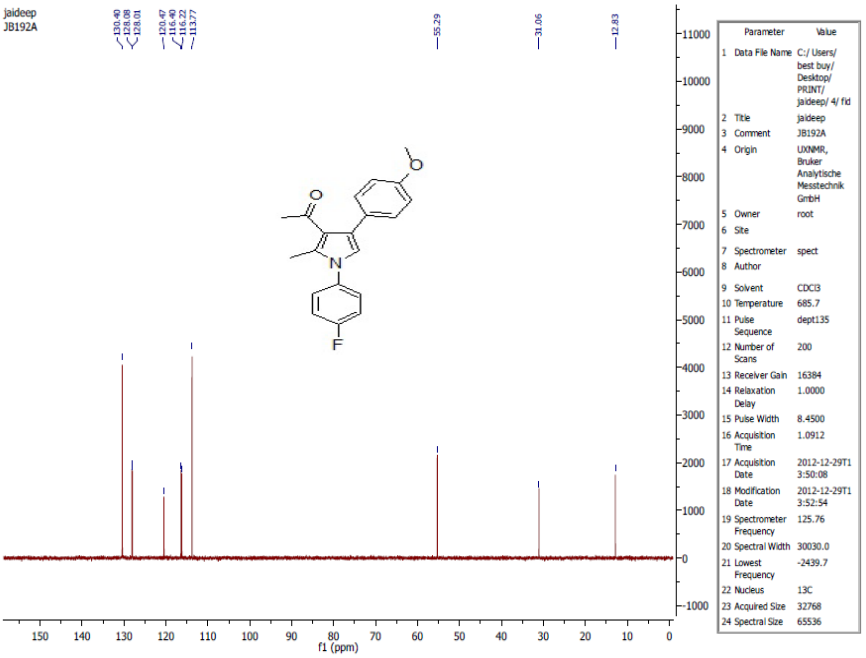
S2.c. ^{1}H, ^{13}C ,DEPT-135 NMR and ^{19}F of 1-(1-(4-fluorophenyl)-4-(4-methoxyphenyl)-2-methyl-1H-pyrrol-3-yl)ethanone (1c)



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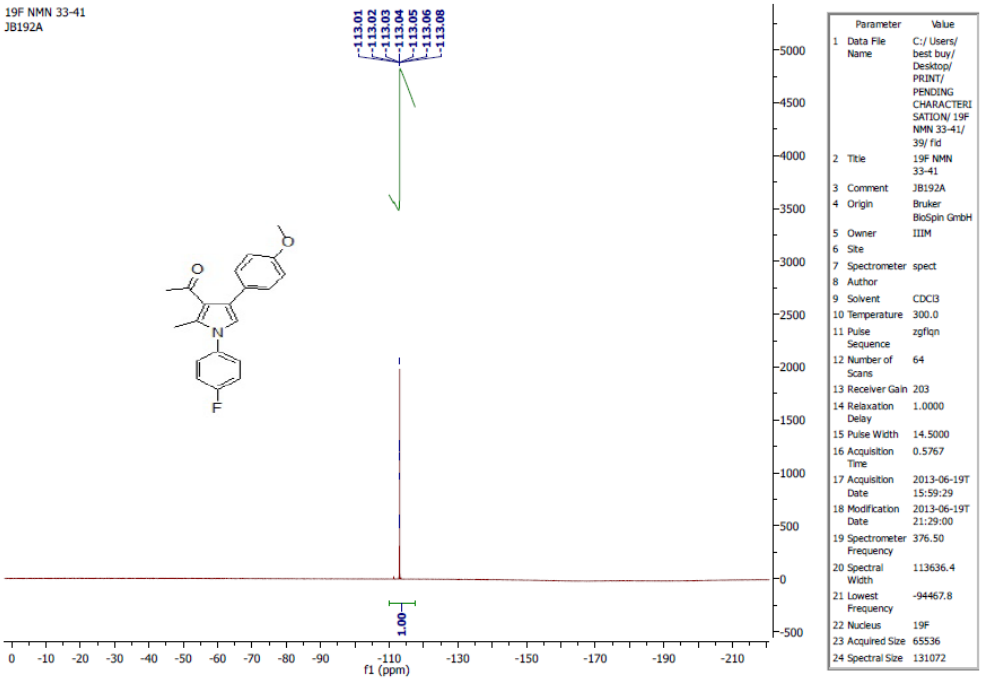
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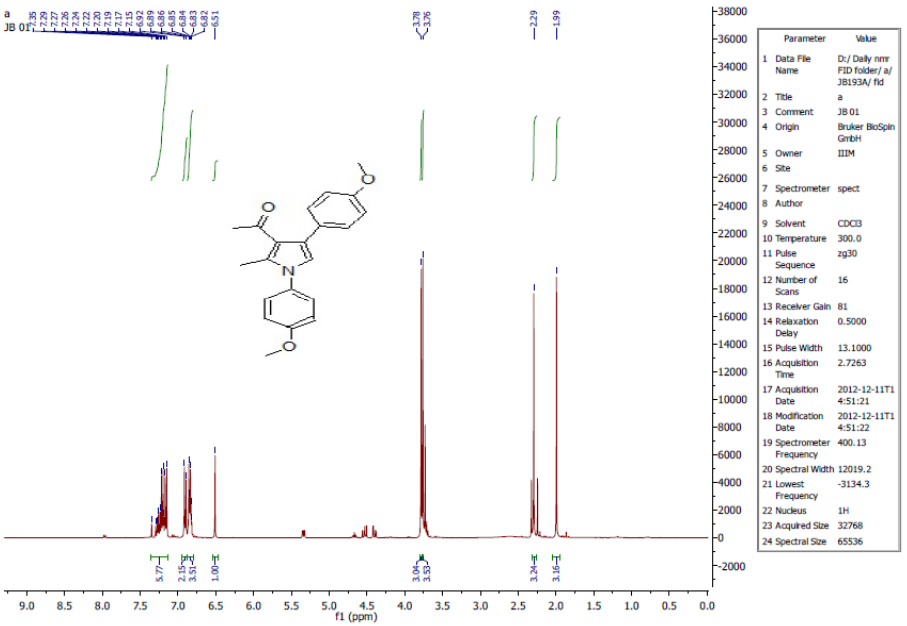
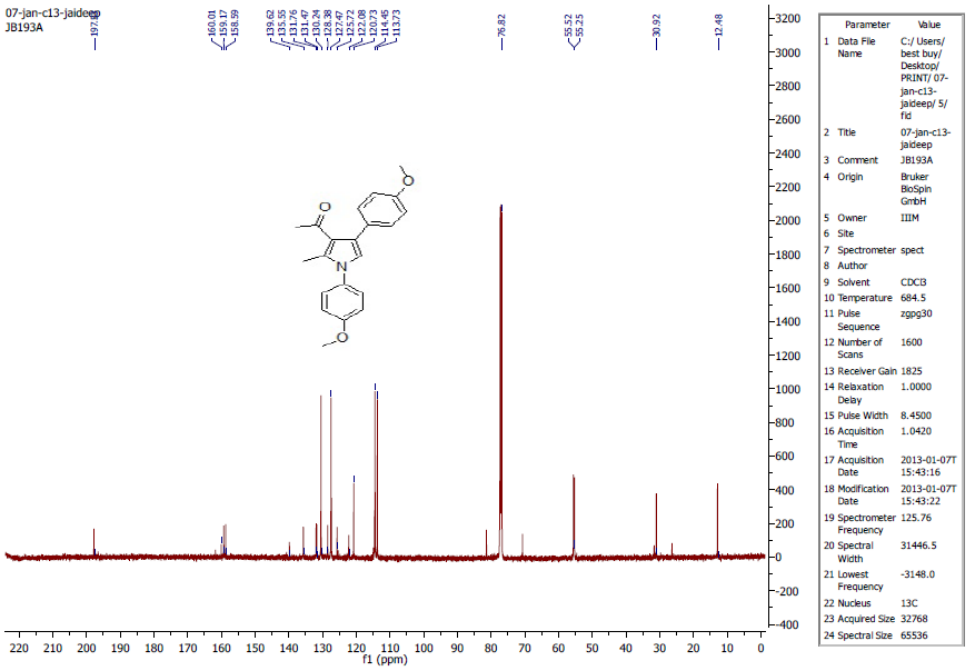
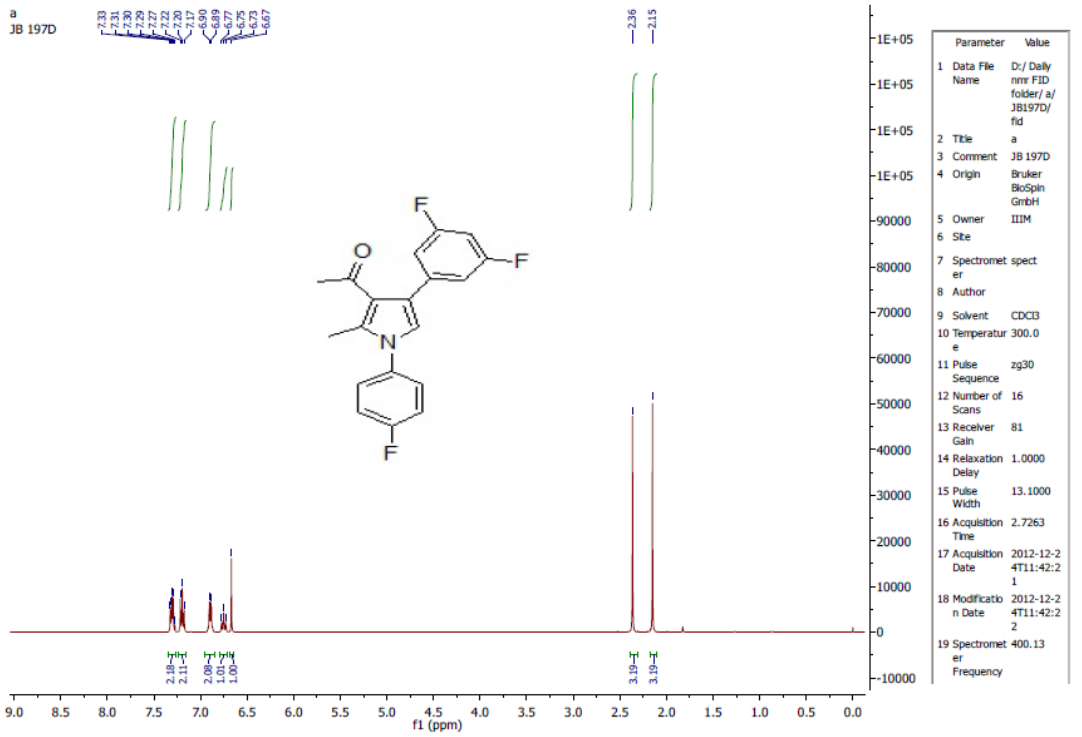
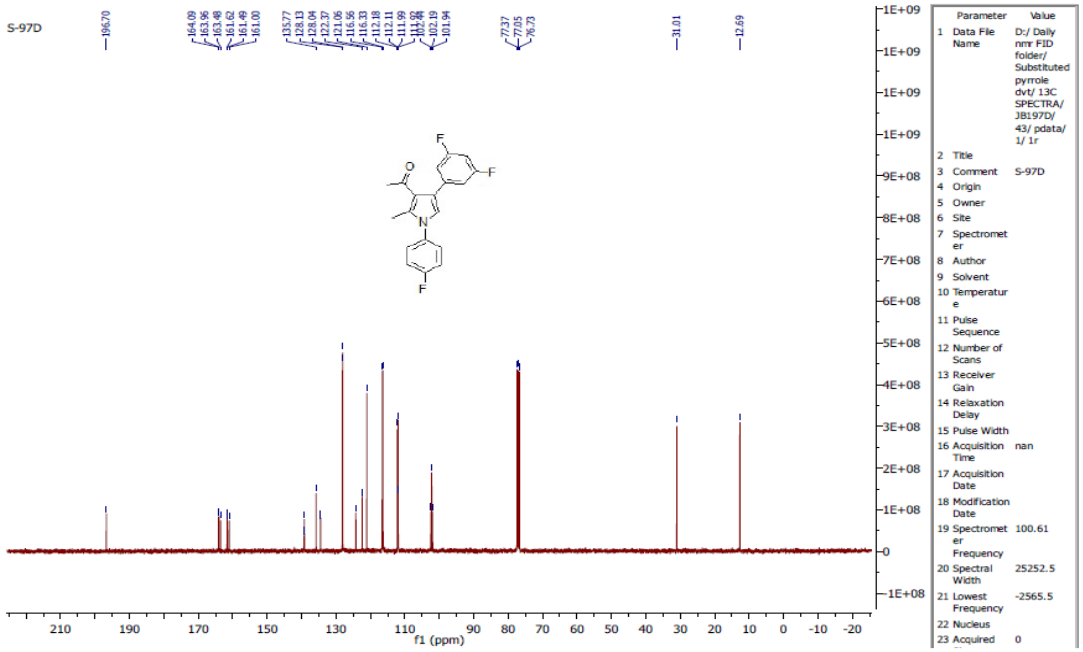
S2.d. ^{1}H, ^{13}C and DEPT-135 NMR of 1-(1,4-bis(4-methoxyphenyl)-2-methyl-1H-pyrrol-3-yl)ethanone (1d)

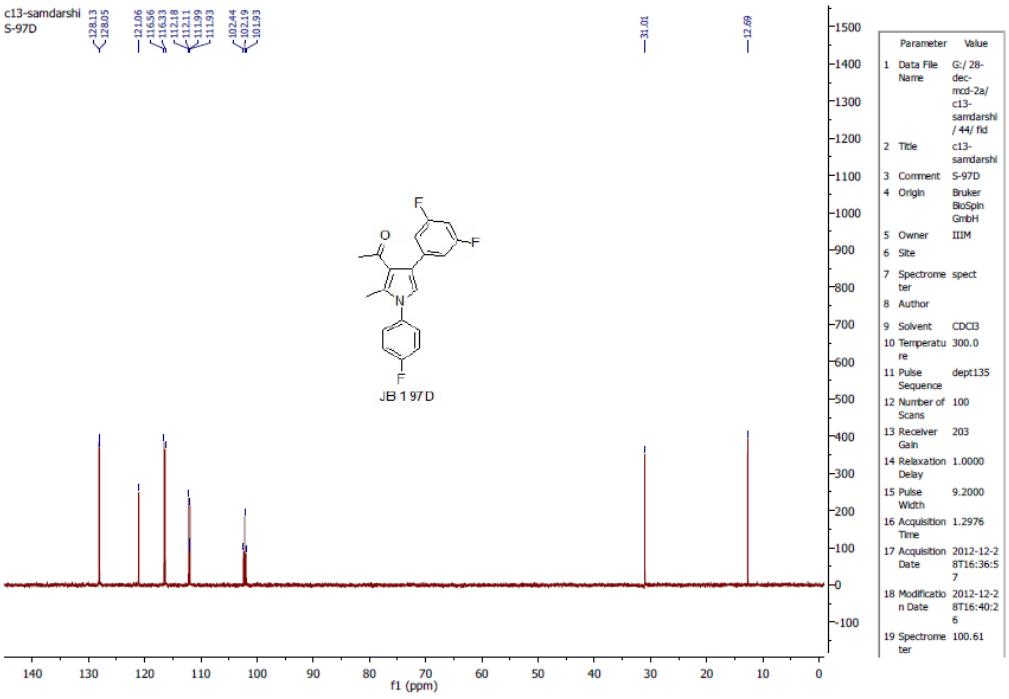




S2.e. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR of 1-(4-(3,5-difluorophenyl)-1-(4-fluorophenyl)-2-methyl-1H-pyrrol-3-yl)ethanone (1e)



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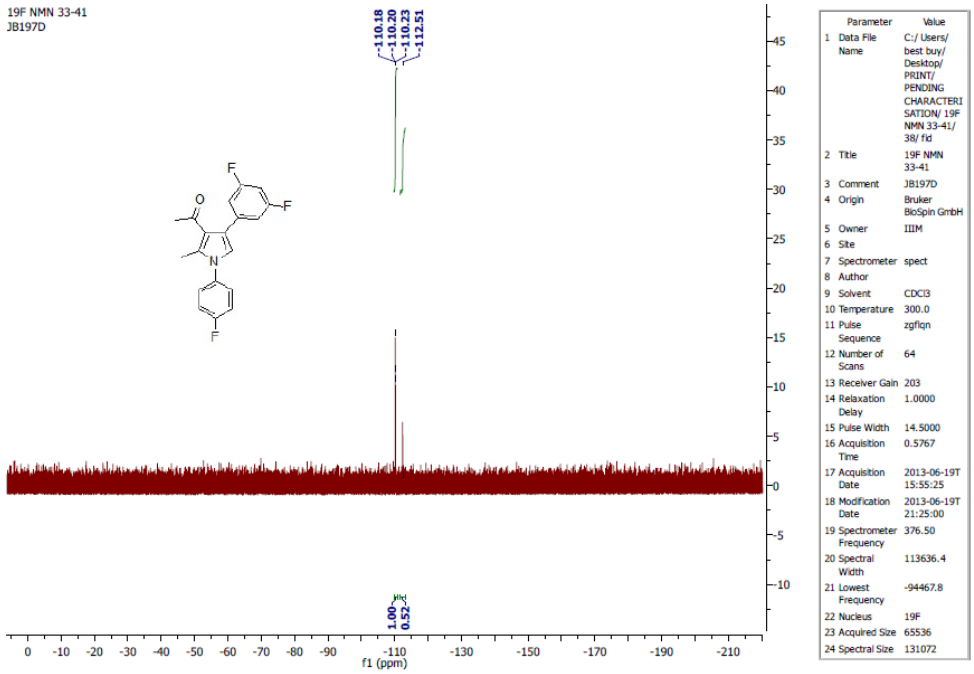
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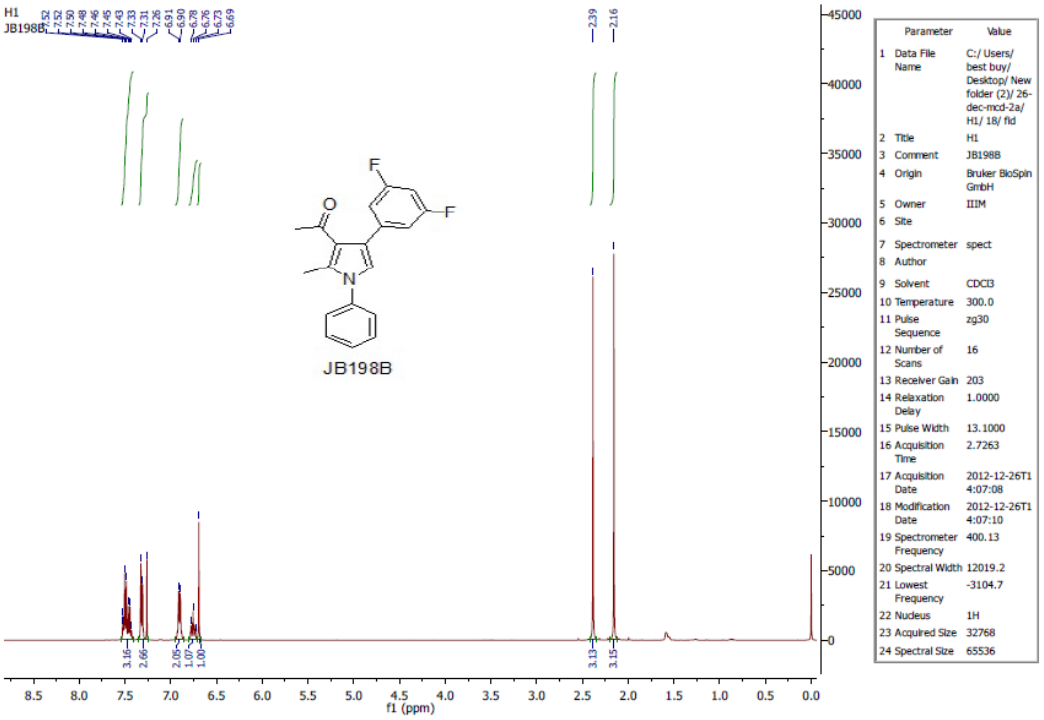
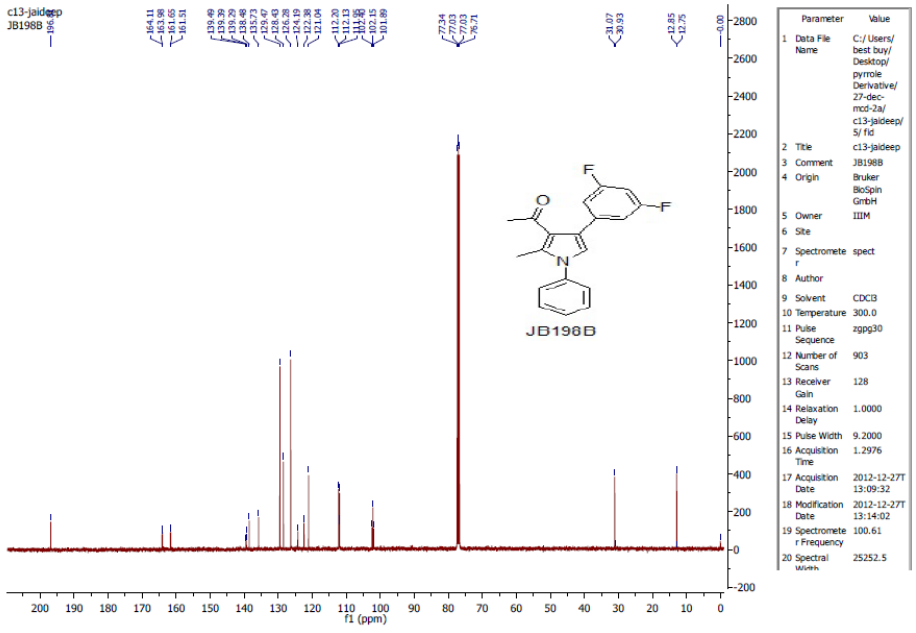
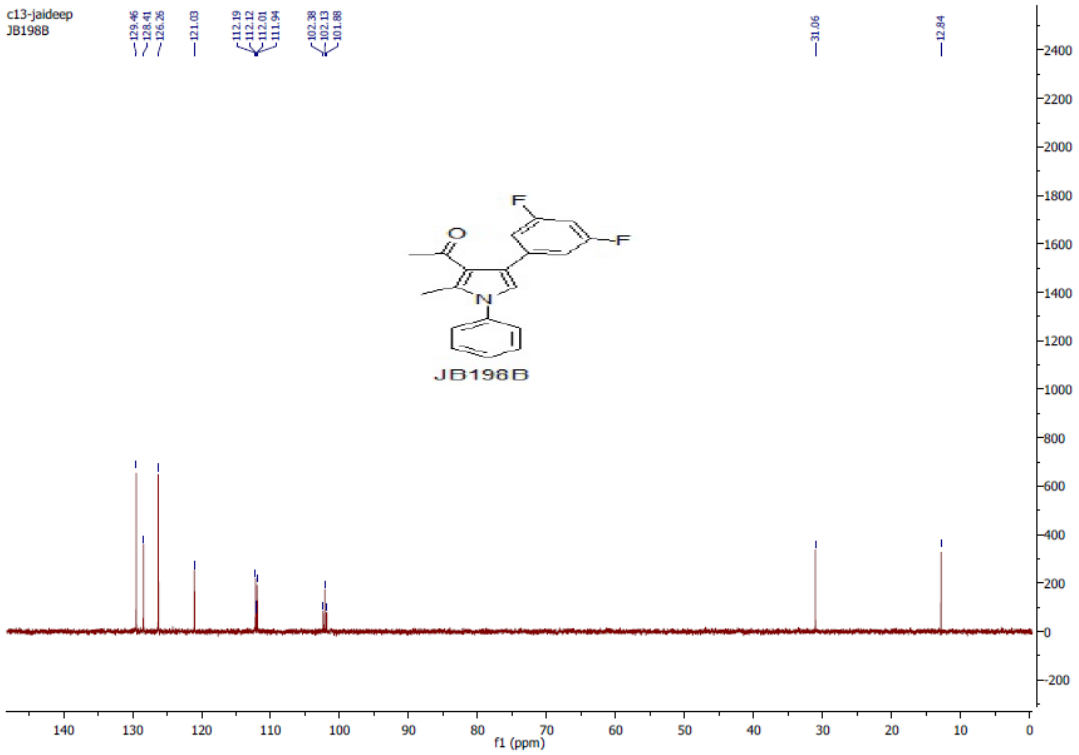
S2.f. ^{1}H, ^{13}C,DEPT-135 and ^{19}F NMR of 1-(4-(3,5-difluorophenyl)-2-methyl-1-phenyl-1H-pyrrol-3-yl)ethanone (1f)



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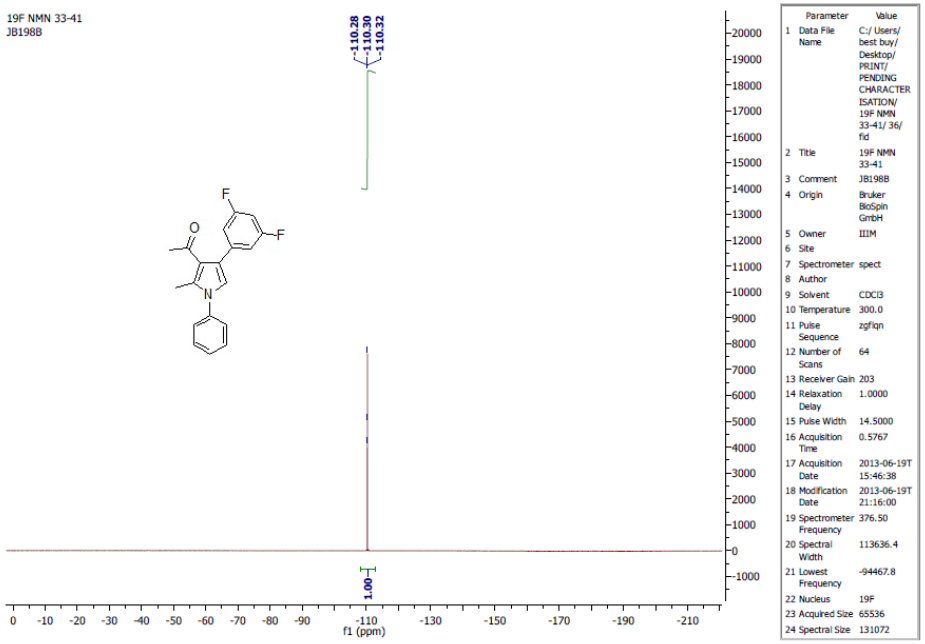
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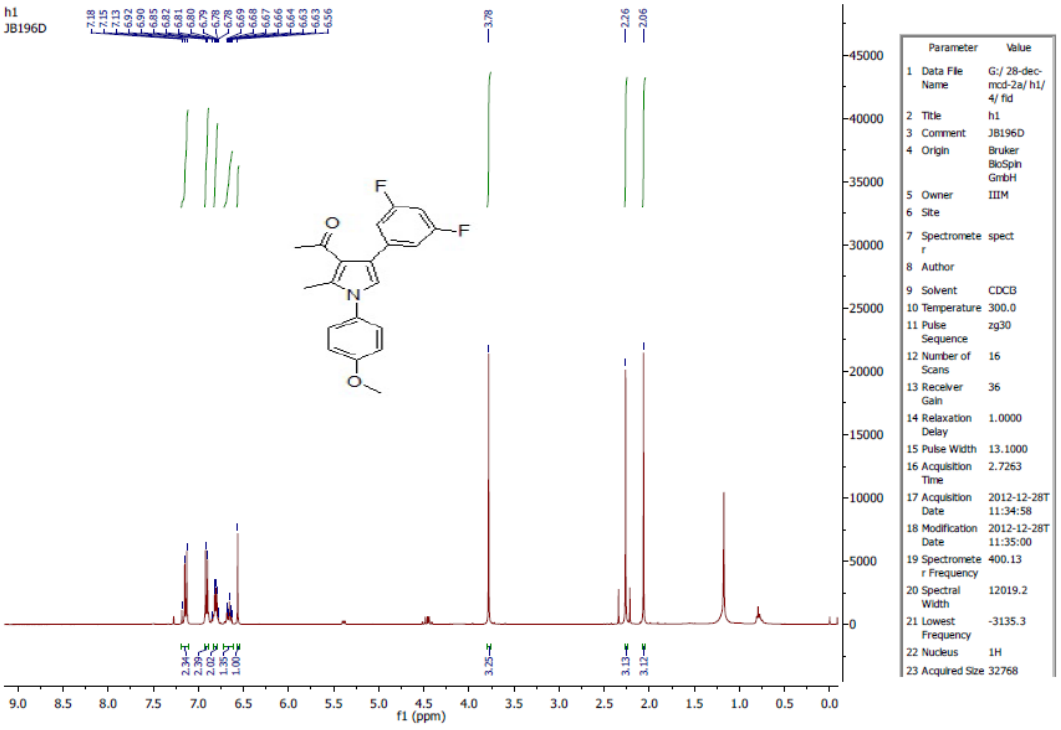
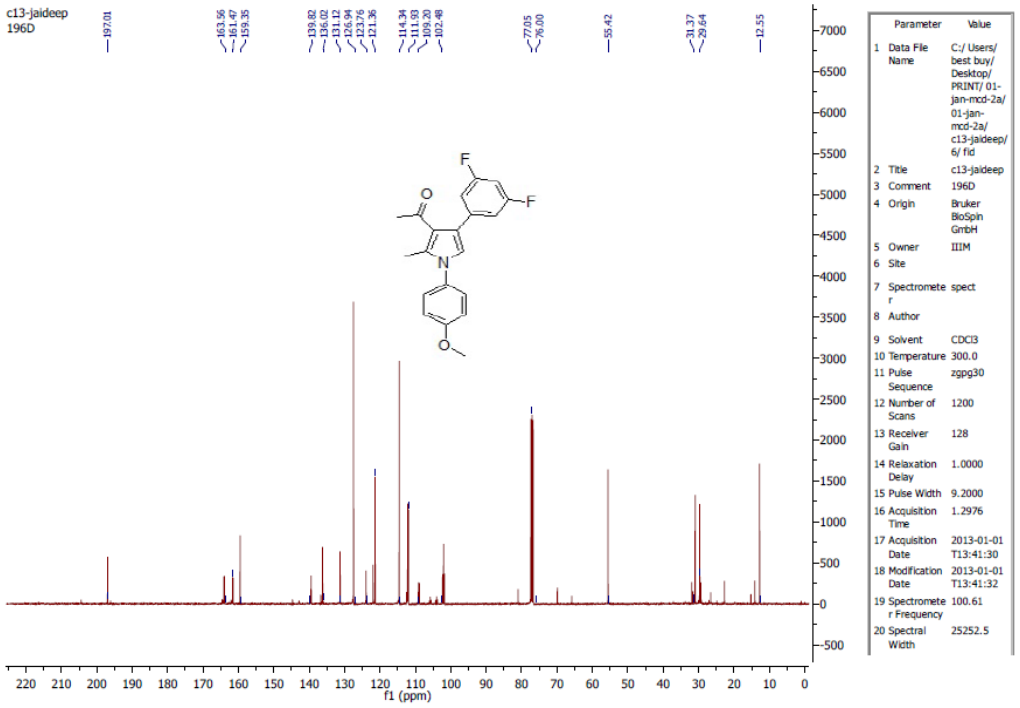
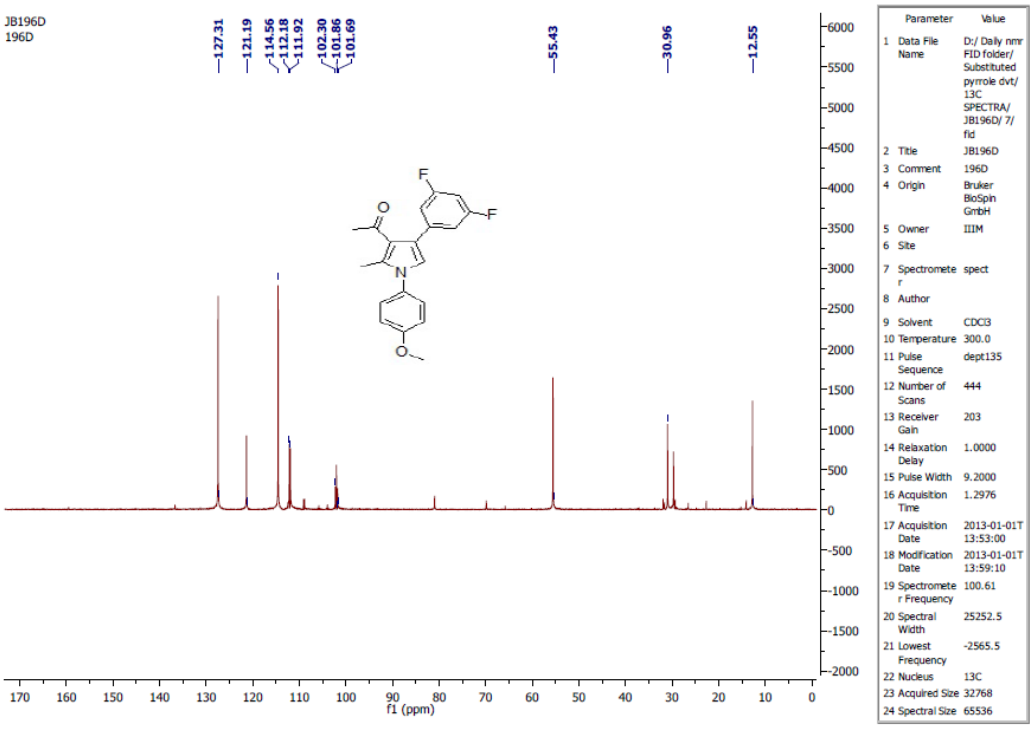
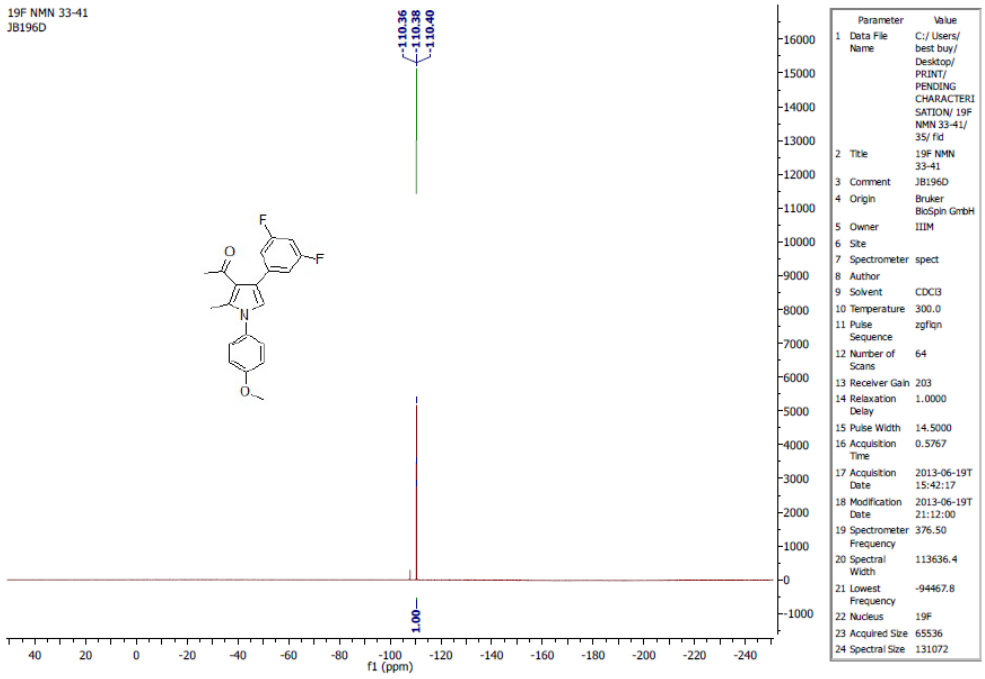
20 Spectral Width 113636.4
21 Lowest Frequency -94467.8
22 Nucleus 19F
23 Acquired Size 65536
24 Spectral Size 131072

S2.g. ^{1}H, ^{13}C,DEPT-135 and ^{19}F NMR of 1-(4-(3,5-difluorophenyl)-1-(4-methoxyphenyl)-2-methyl-1H-pyrrol-3-yl)ethanone (1g)






JB196D
196D
127.31
121.19
114.56
112.18
111.92
102.30
101.86
101.69
55.43
30.96
12.55
f1 (ppm)
Parameter Value
1 Data File Name D:/ Daily nmr FID folder/ Substituted pyrrole dvt/ 13C SPECTRA/ JB196D/ 7/ fid
2 Title JB196D
3 Comment 196D
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 444
13 Receiver Gain 203
14 Relaxation Delay 1.0000
15 Pulse Width 9.2000
16 Acquisition Time 1.2976
17 Acquisition Date 2013-01-01T 13:53:00
18 Modification Date 2013-01-01T 13:59:10
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


19F NMN 33-41
JB196D
110.36
110.38
110.40
1.00
f1 (ppm)
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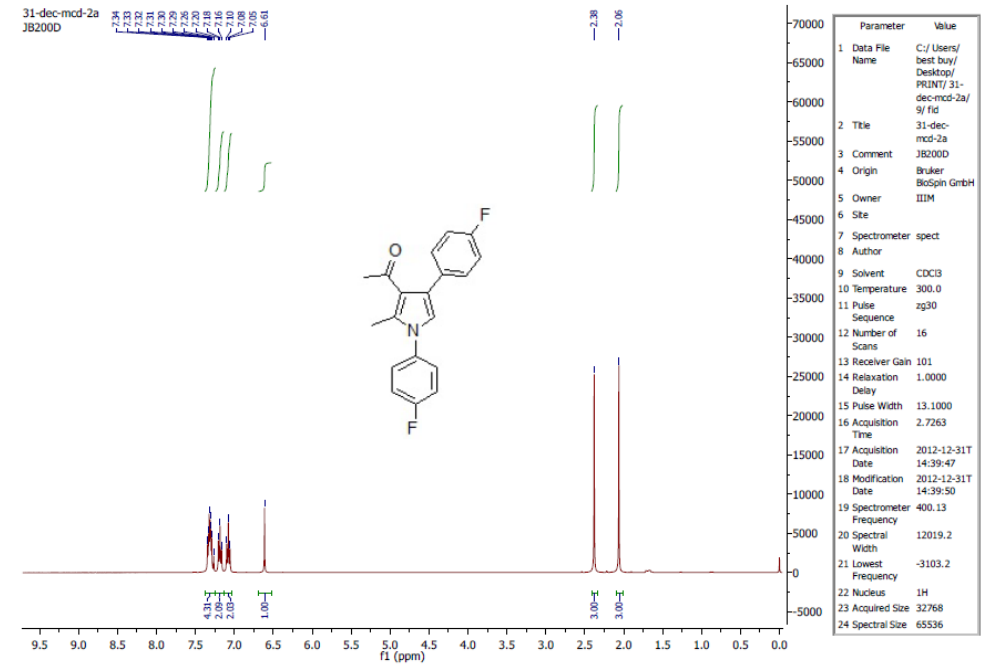
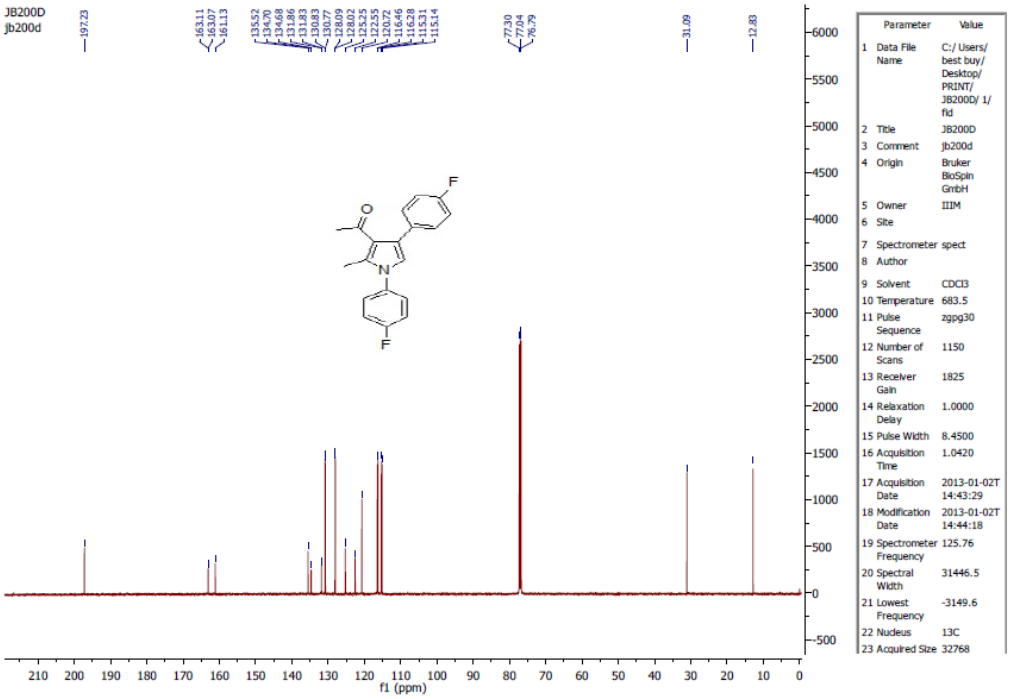
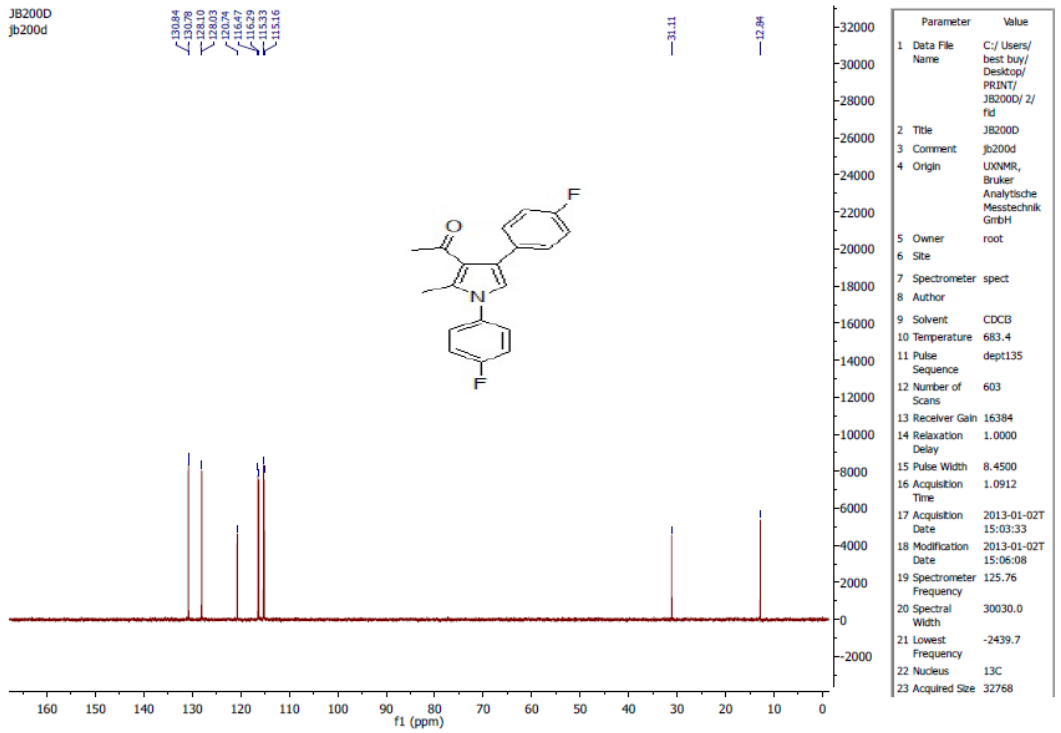
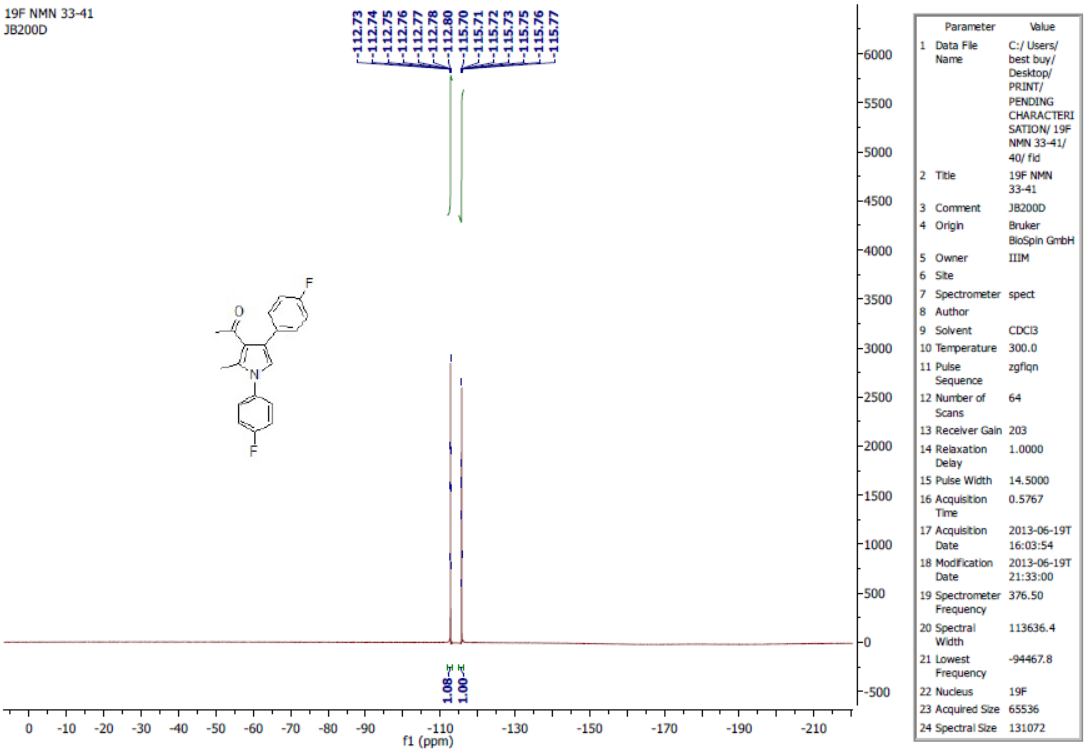
2 Title 19F NMN 33-41
3 Comment JB196D
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 300.0
11 Pulse Sequence zgflqn
12 Number of Scans 64
13 Receiver Gain 203
14 Relaxation Delay 1.0000
15 Pulse Width 14.5000
16 Acquisition Time 0.5767
17 Acquisition Date 2013-06-19T 15:42:17
18 Modification Date 2013-06-19T 21:12:00
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.h. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR of 1-(1,4-bis(4-fluorophenyl)-2-methyl-1H-pyrrol-3-yl)ethanone (1h)

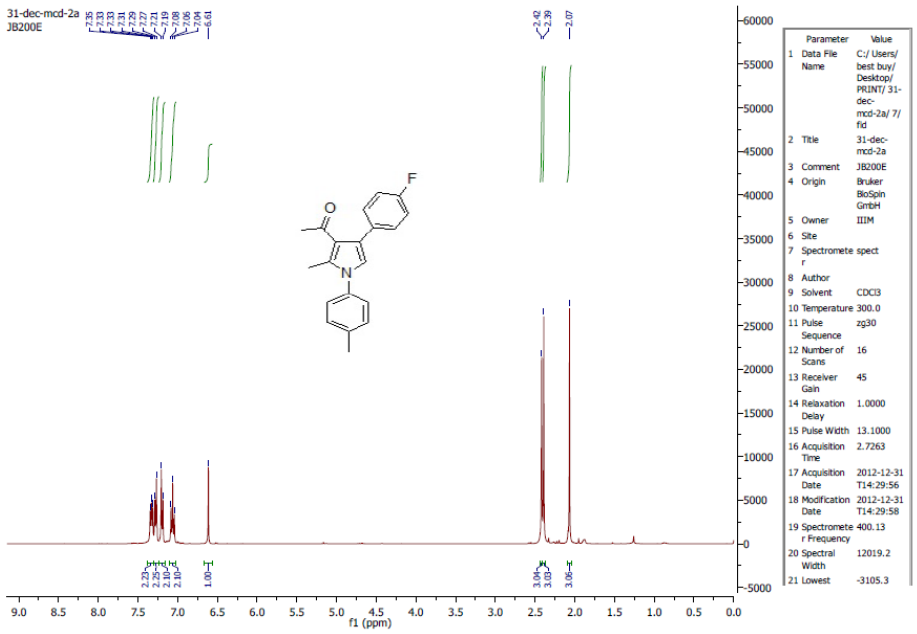


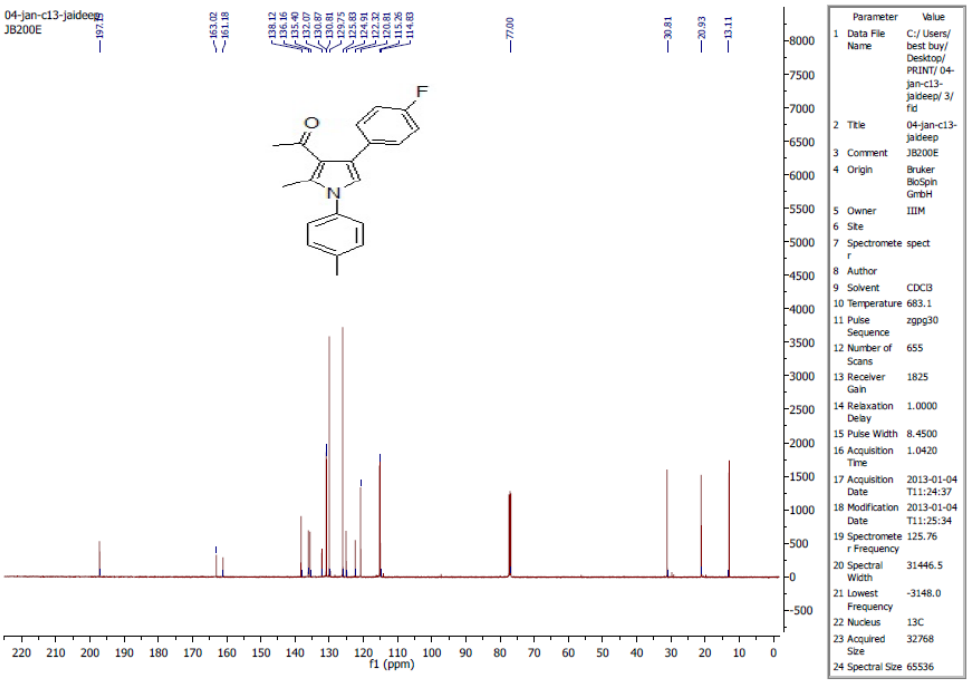


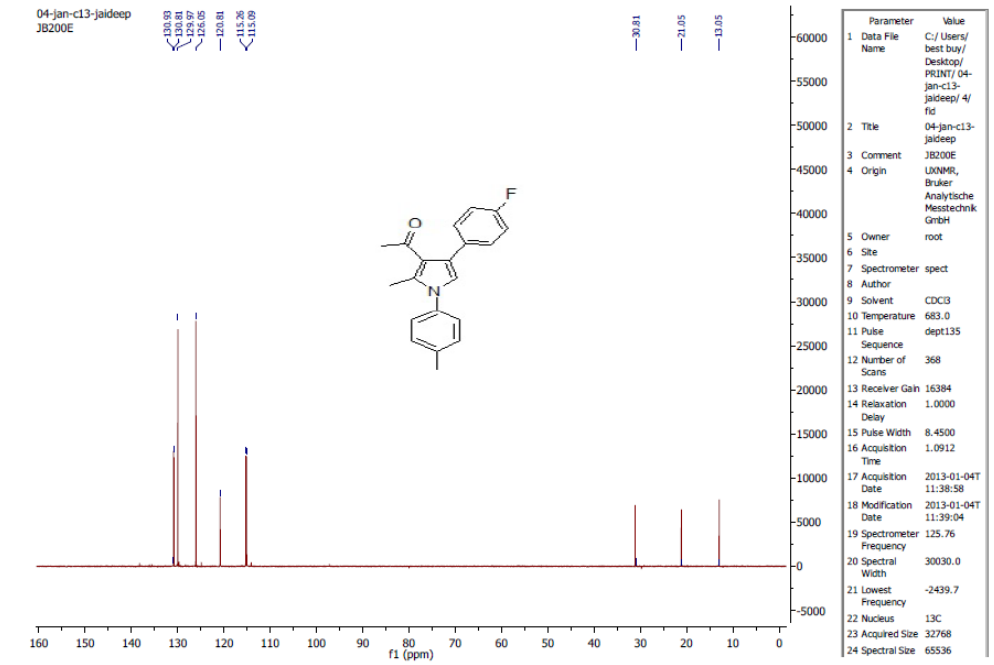

JB200D
jb200d
130.84
130.78
128.10
128.03
120.74
116.47
116.29
115.33
115.16
31.11
12.84
f1 (ppm)
Parameter Value
1 Data File Name C:/ Users/ best buy/ Desktop/ PRINT/ JB200D/ 2/ fid
2 Title JB200D
3 Comment jb200d
4 Origin UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner root
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 683.4
11 Pulse Sequence dept135
12 Number of Scans 603
13 Receiver Gain 16384
14 Relaxation Delay 1.0000
15 Pulse Width 8.4500
16 Acquisition Time 1.0912
17 Acquisition Date 2013-01-02T 15:03:33
18 Modification Date 2013-01-02T 15:06:08
19 Spectrometer Frequency 125.76
20 Spectral Width 30030.0
21 Lowest Frequency -2439.7
22 Nucleus 13C
23 Acquired Size 32768


19F NMN 33-41
JB200D
-112.73
-112.74
-112.75
-112.76
-112.77
-112.78
-112.80
-115.70
-115.71
-115.72
-115.73
-115.75
-115.76
-115.77
1.00
1.00
f1 (ppm)
Parameter Value
1 Data File Name C:/ Users/ best buy/ Desktop/ PRINT/ PENDING CHARACTERISATION/ 19F NMN 33-41/ 40/ fid
2 Title 19F NMN 33-41
3 Comment JB200D
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 64
13 Receiver Gain 203
14 Relaxation Delay 1.0000
15 Pulse Width 14.5000
16 Acquisition Time 0.5767
17 Acquisition Date 2013-06-19T 16:03:54
18 Modification Date 2013-06-19T 21:33:00
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.i. ^{1}H, ^{13}C , DEPT-135 and ^{19}F NMR of 1-(4-(4-fluorophenyl)-2-methyl-1-p-tolyl-1H-pyrrol-3-yl)ethanone (1i)







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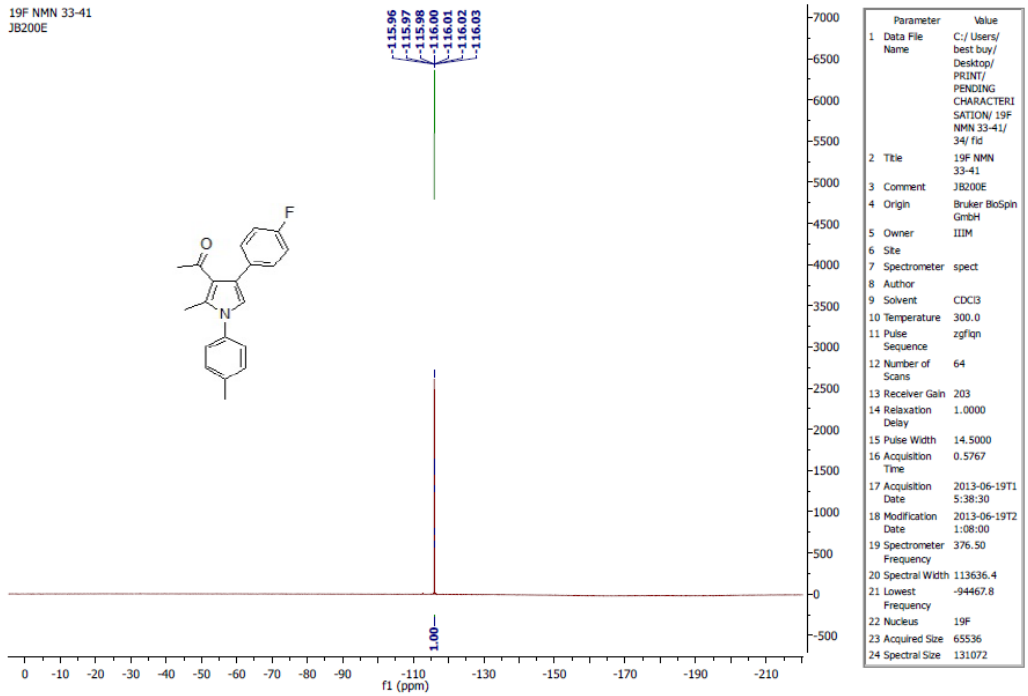
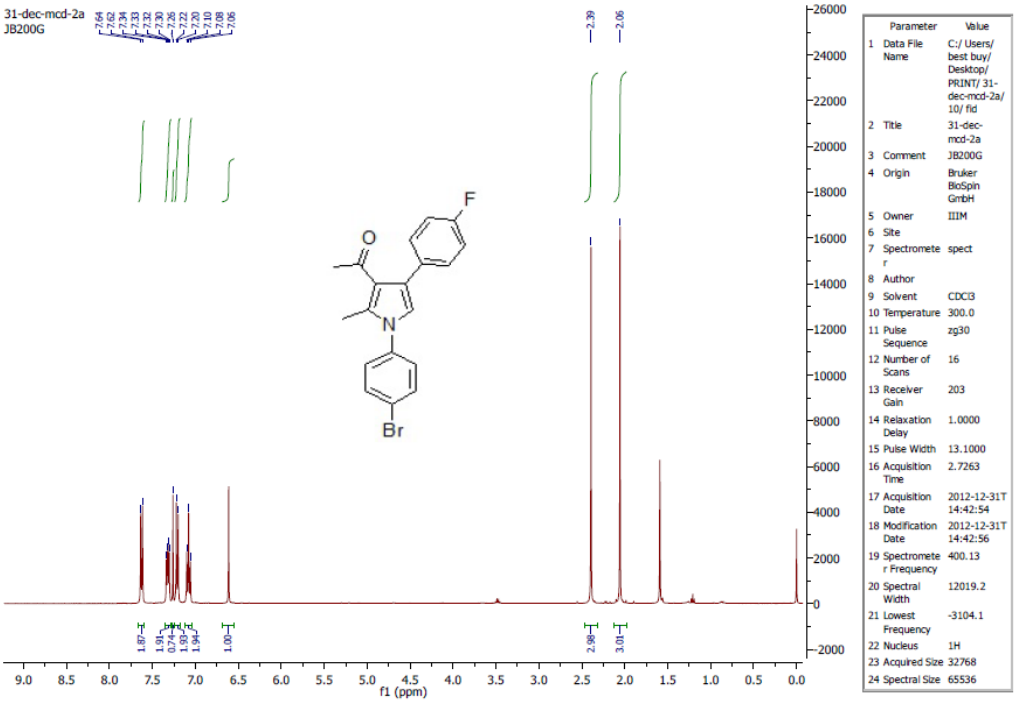
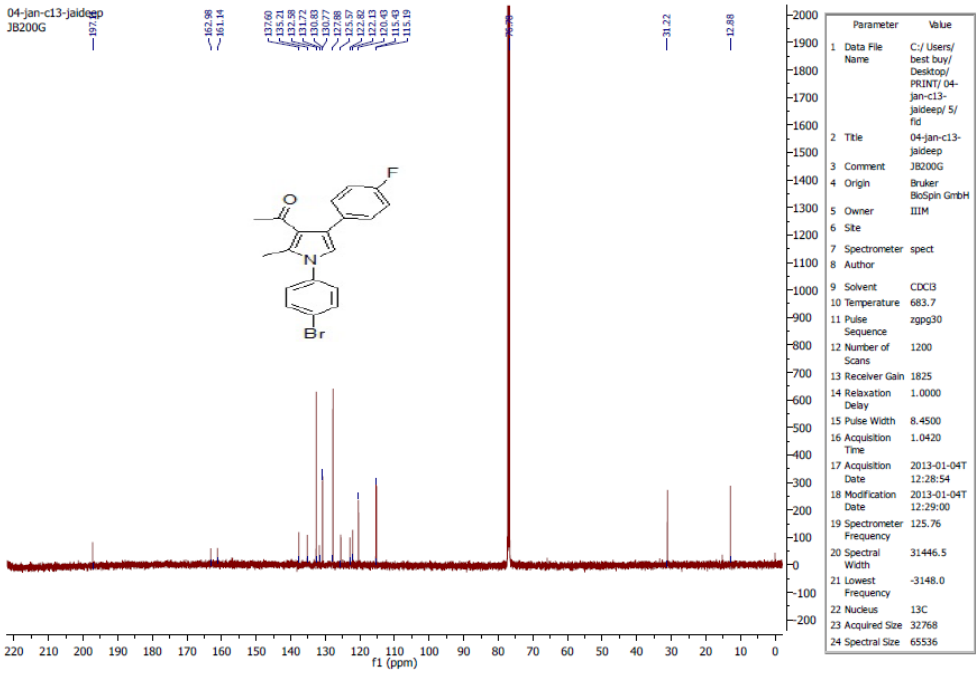
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 04-jan-c13-jaideep/ 4/ fid
2	Title	04-jan-c13-jaideep
3	Comment	JB200E
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	683.0
11	Pulse Sequence	dept135
12	Number of Scans	368
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2013-01-04T 11:38:58
18	Modification Date	2013-01-04T 11:39:04
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

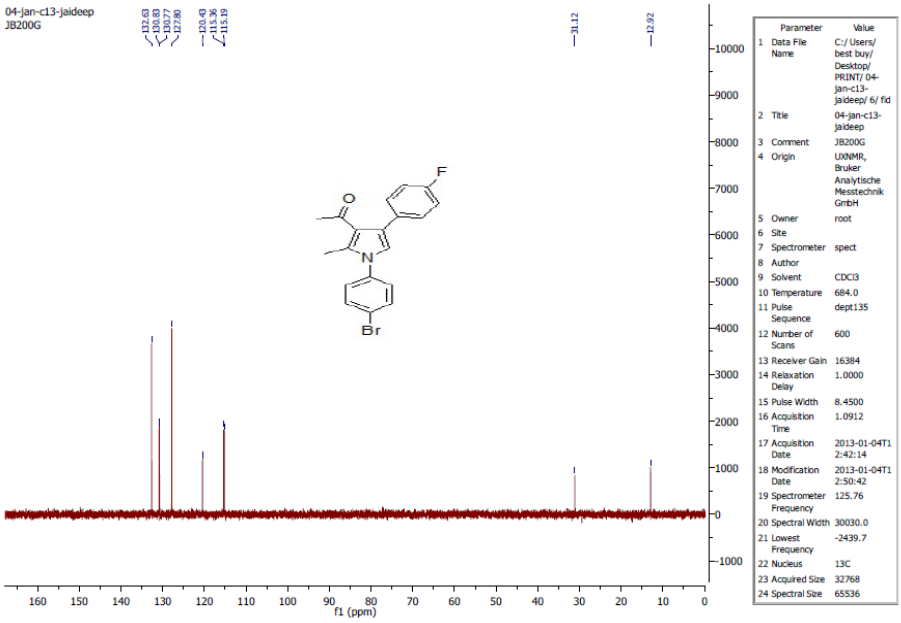


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ PENDING CHARACTERISATION/ 19F NMN 33-41/ 34/ fid
2	Title	19F NMN 33-41
3	Comment	JB200E
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgflqn
12	Number of Scans	64
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	14.5000
16	Acquisition Time	0.5767
17	Acquisition Date	2013-06-19T1 5:38:30
18	Modification Date	2013-06-19T2 1:08:00
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

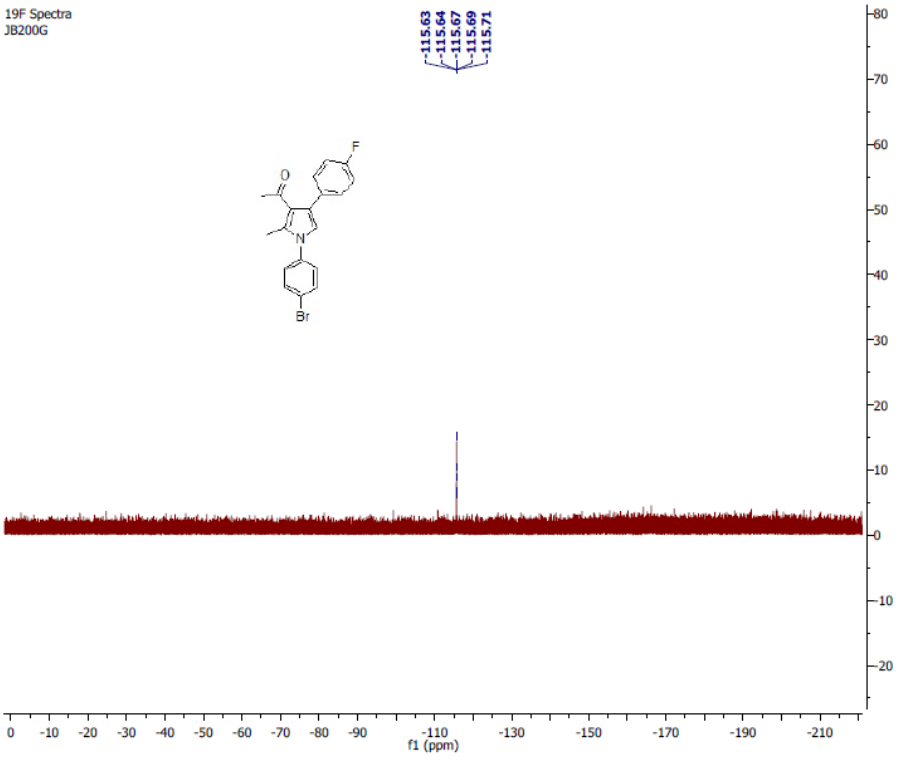
S2.j. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR of 1-(1-(4-bromophenyl)-4-(4-fluorophenyl)-2-methyl-1H-pyrrol-3-yl)ethanone (1j)







	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 04-jan-c13-jaideep/ 6/ fid
2	Title	04-jan-c13-jaideep
3	Comment	JB200G
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	684.0
11	Pulse Sequence	dept135
12	Number of Scans	600
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2013-01-04T12:42:14
18	Modification Date	2013-01-04T12:50:42
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



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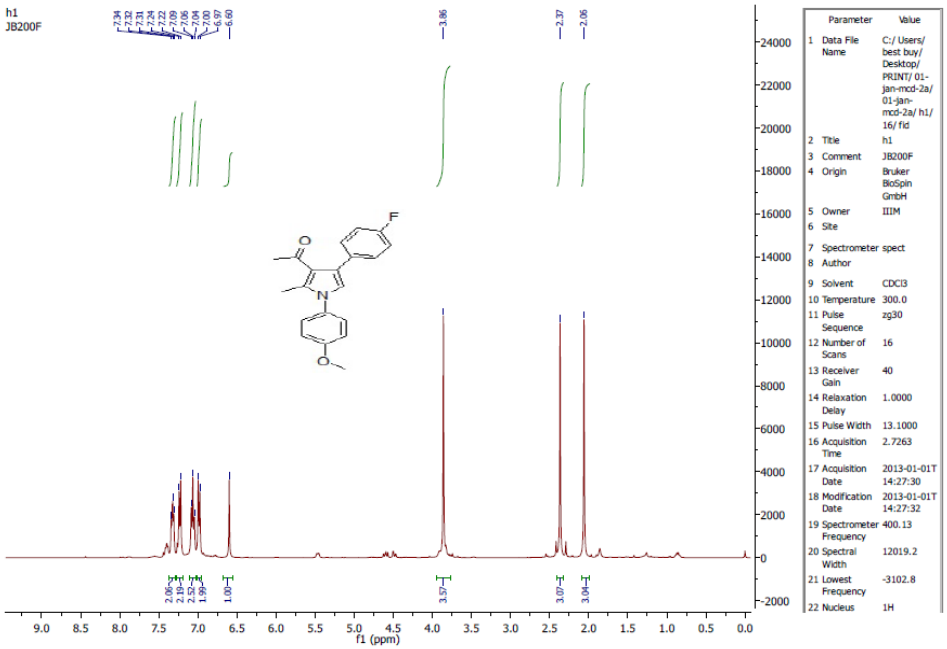
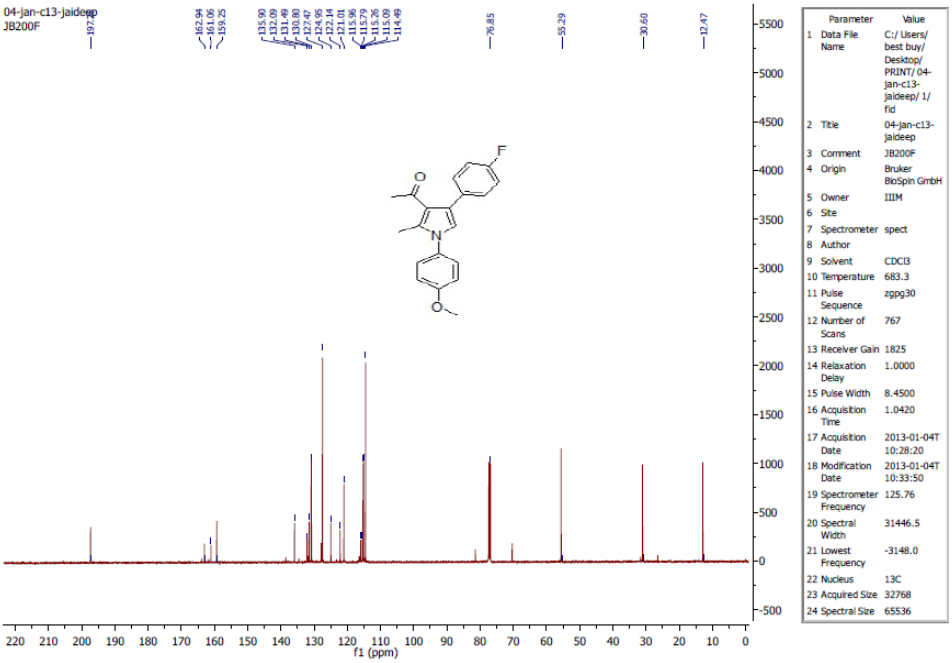
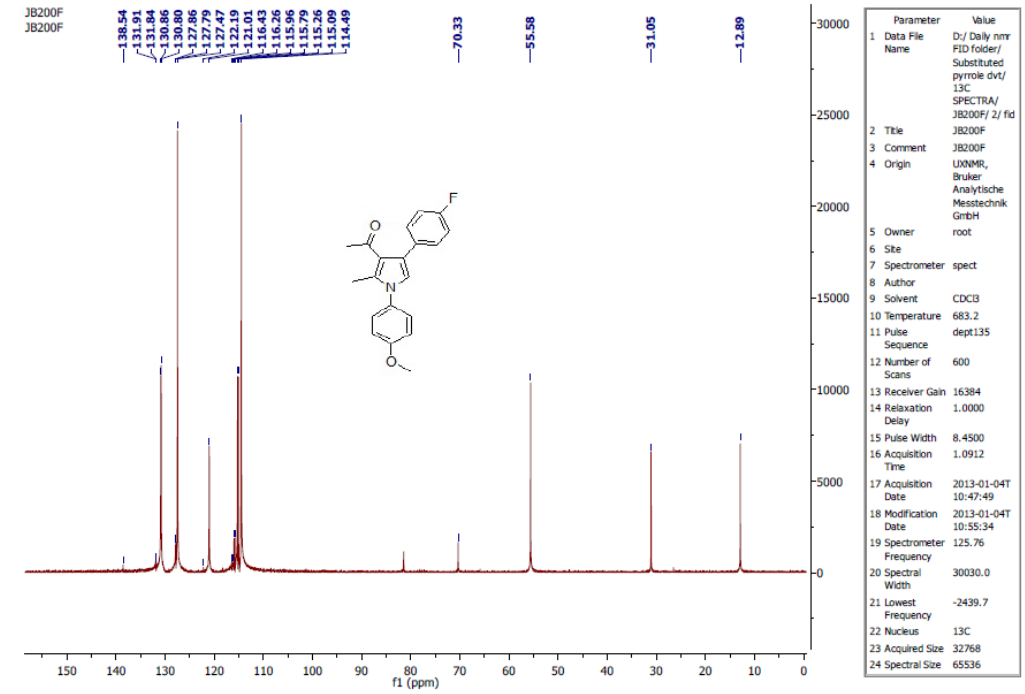
2	Title	19F Spectra
3	Comment	JB200G
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgflqn
12	Number of Scans	64
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	14.5000
16	Acquisition Time	0.5767
17	Acquisition Date	2013-06-20T15:36:47
18	Modification Date	2013-06-20T21:06:50
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.k. ^{1}H, ^{13}C,DEPT-135 and ^{19}F NMR of 1-(4-(4-fluorophenyl)-1-(4-methoxyphenyl)-2-methyl-1H-pyrrol-3-yl)ethanone (1k)







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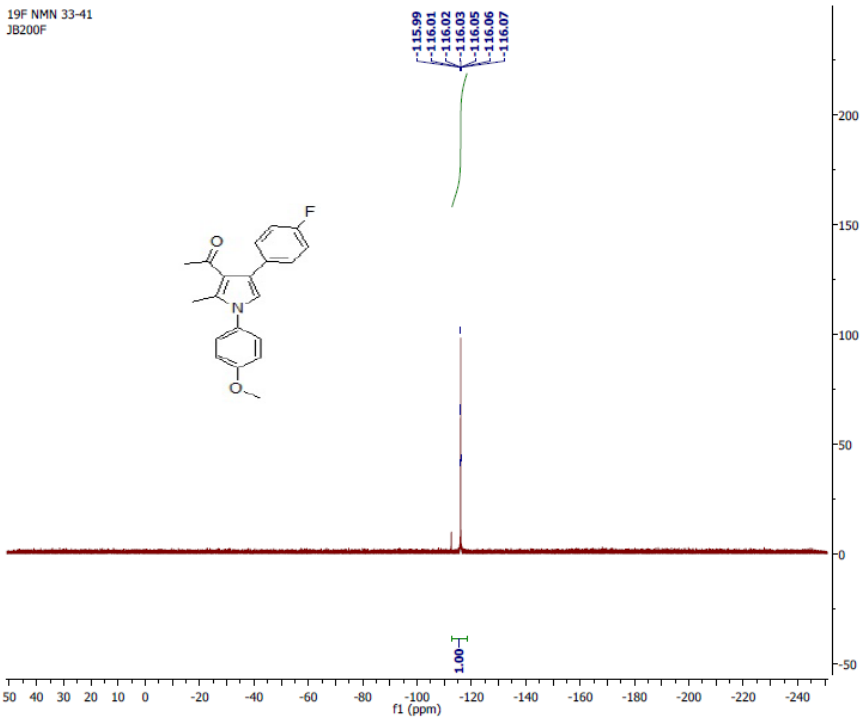
2	Title	JB200F
3	Comment	JB200F
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	683.2
11	Pulse Sequence	dept135
12	Number of Scans	600
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2013-01-04T 10:47:49
18	Modification Date	2013-01-04T 10:55:34
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



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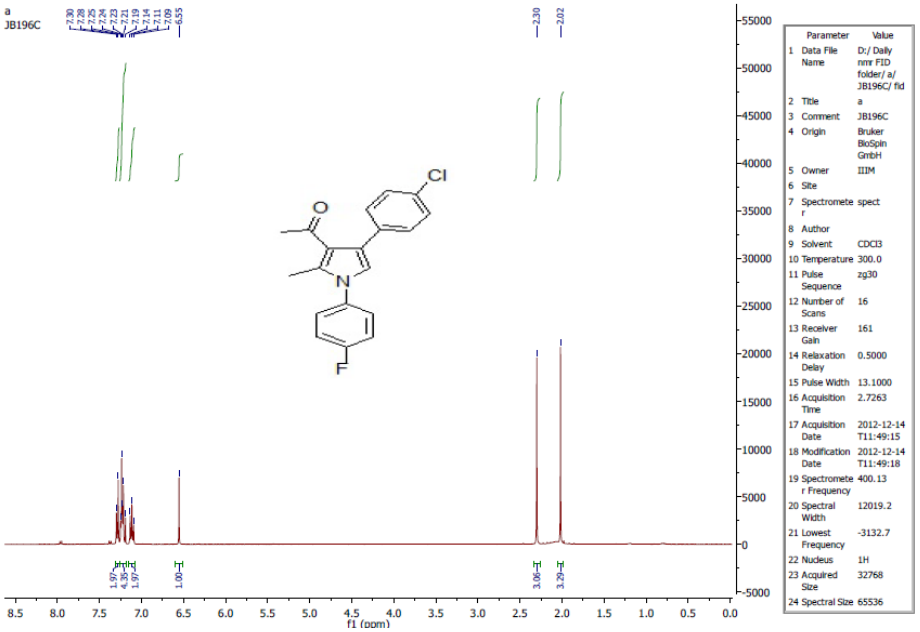
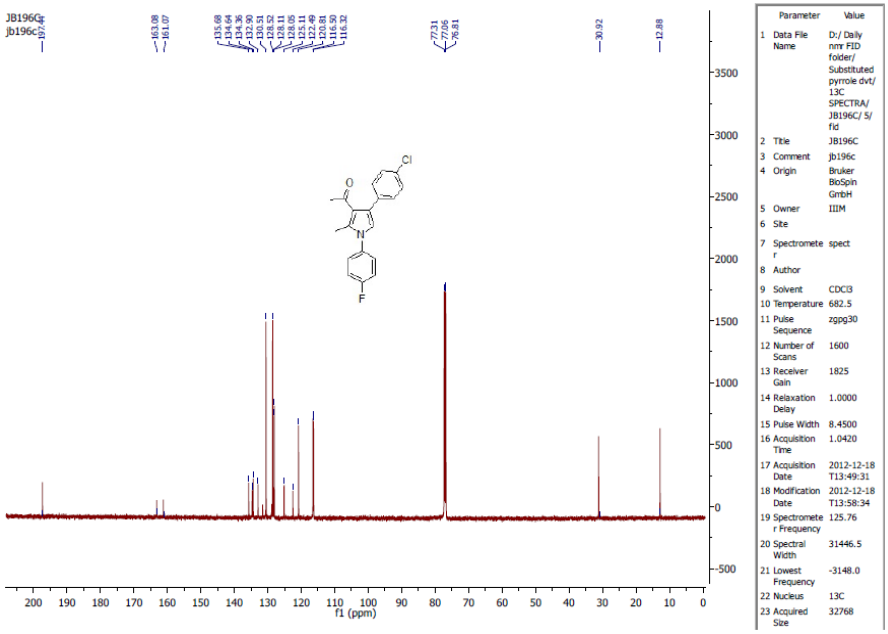
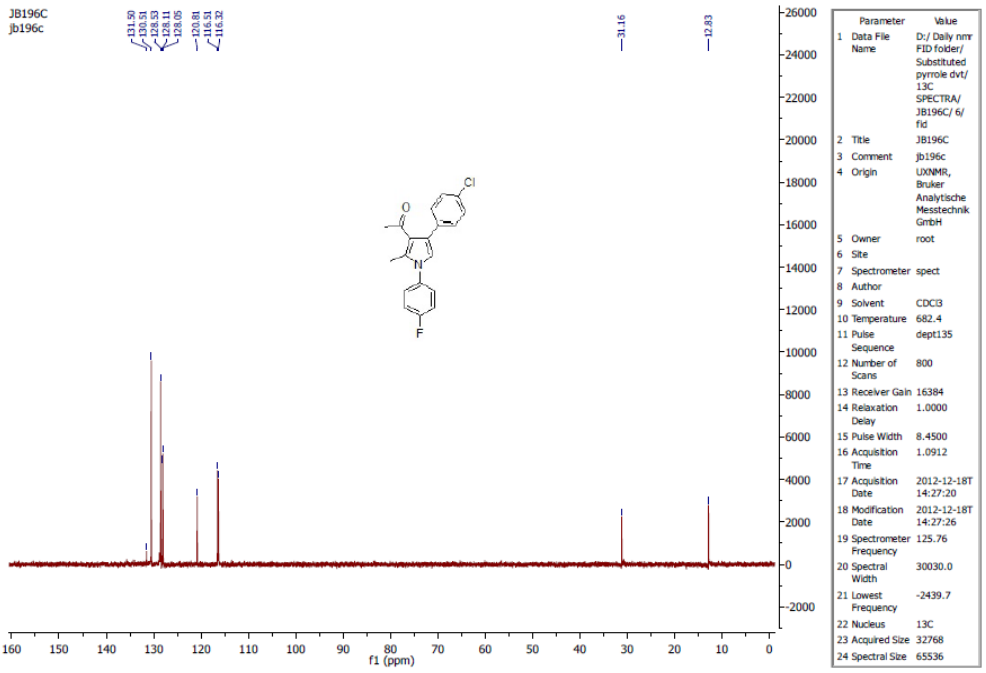
2	Title	19F NMN 33-41
3	Comment	JB200F
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgflqn
12	Number of Scans	40
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	14.5000
16	Acquisition Time	0.5767
17	Acquisition Date	2013-06-19T 15:34:16
18	Modification Date	2013-06-19T 21:04:00
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

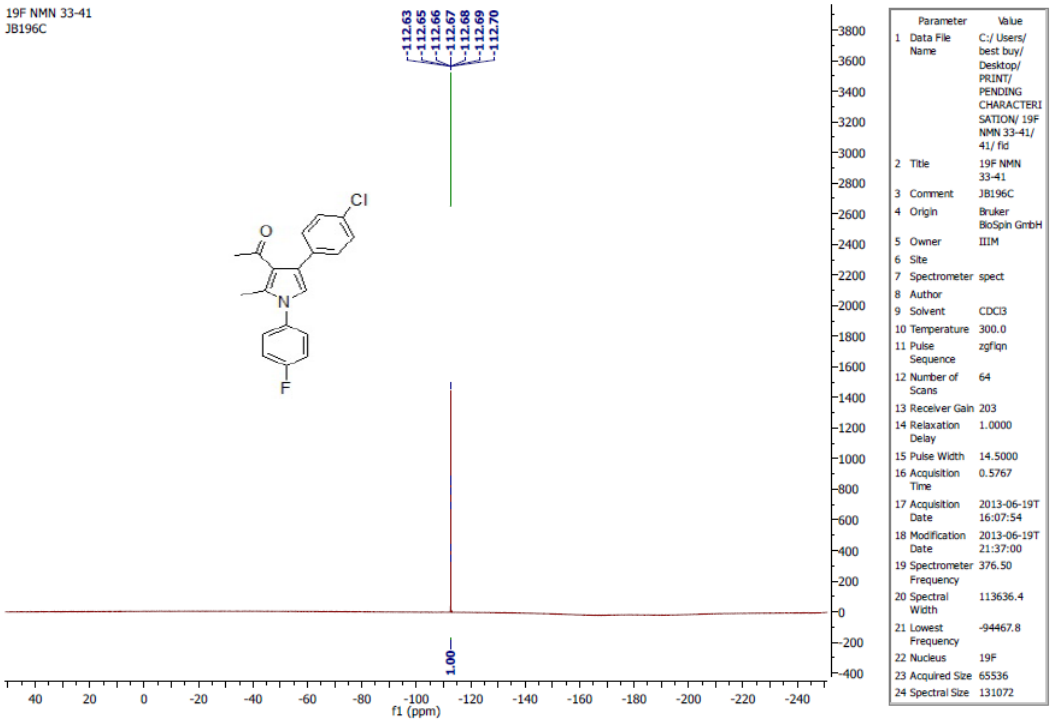
S2.l. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR of 1-(4-(4-chlorophenyl)-1-(4-fluorophenyl)-2-methyl-1H-pyrrol-3-yl)ethanone (1l)





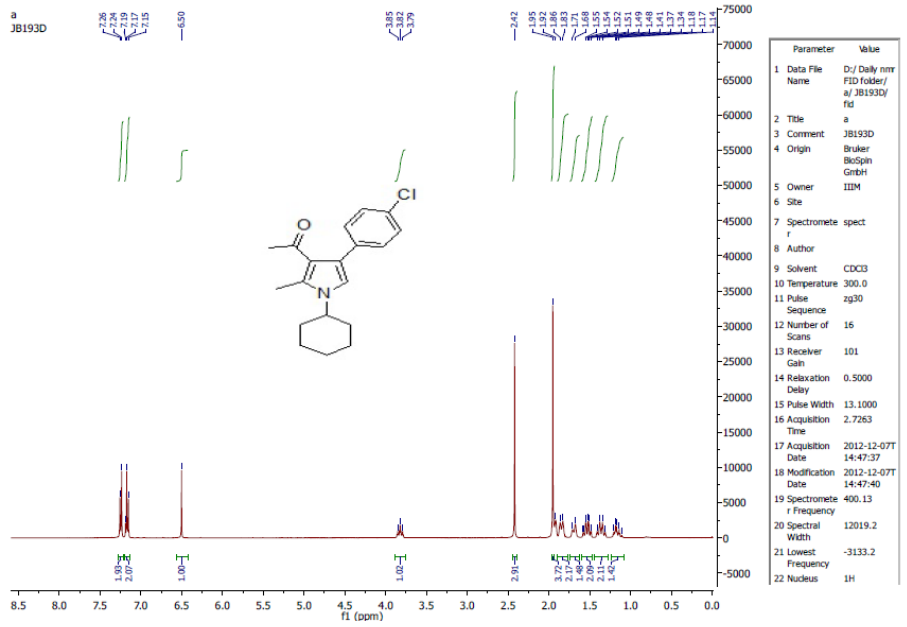


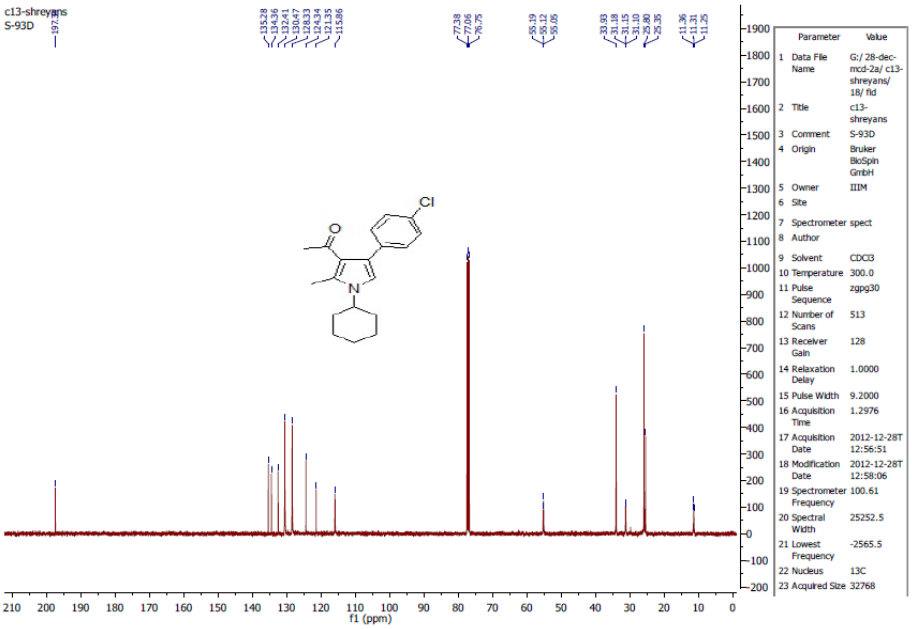
	Parameter	Value
1	Data File Name	D:/ Daily nmr FID folder/ Substituted pyrrole dvt/ 13C SPECTRA/ JB196C/ 6/ fid
2	Title	JB196C
3	Comment	jb196c
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	682.4
11	Pulse Sequence	dept135
12	Number of Scans	800
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2012-12-18T 14:27:20
18	Modification Date	2012-12-18T 14:27:26
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

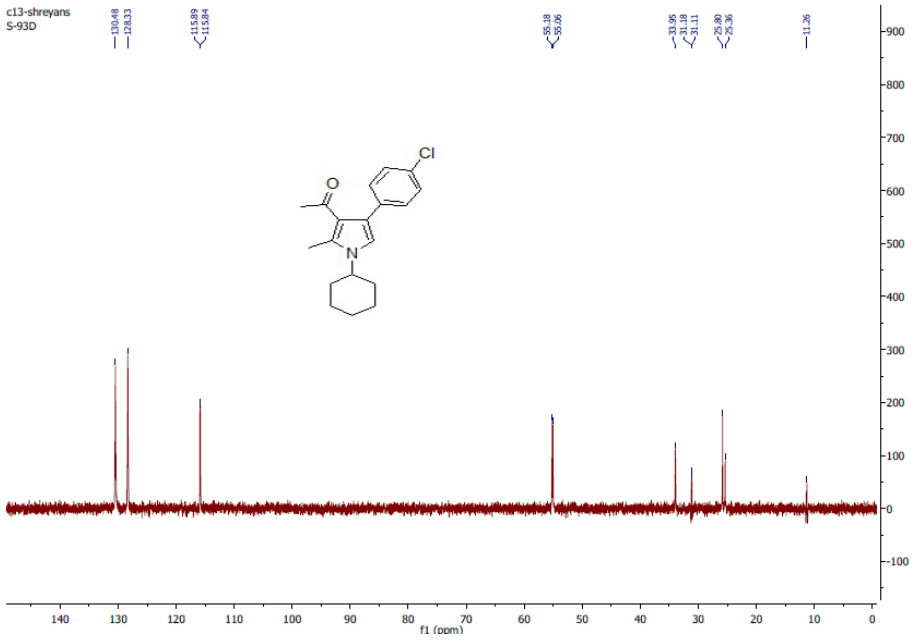


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ PENDING CHARACTERISATION/ 19F NMN 33-41/ 41/ fid
2	Title	19F NMN 33-41
3	Comment	JB196C
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgflqn
12	Number of Scans	64
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	14.5000
16	Acquisition Time	0.5767
17	Acquisition Date	2013-06-19T 16:07:54
18	Modification Date	2013-06-19T 21:37:00
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

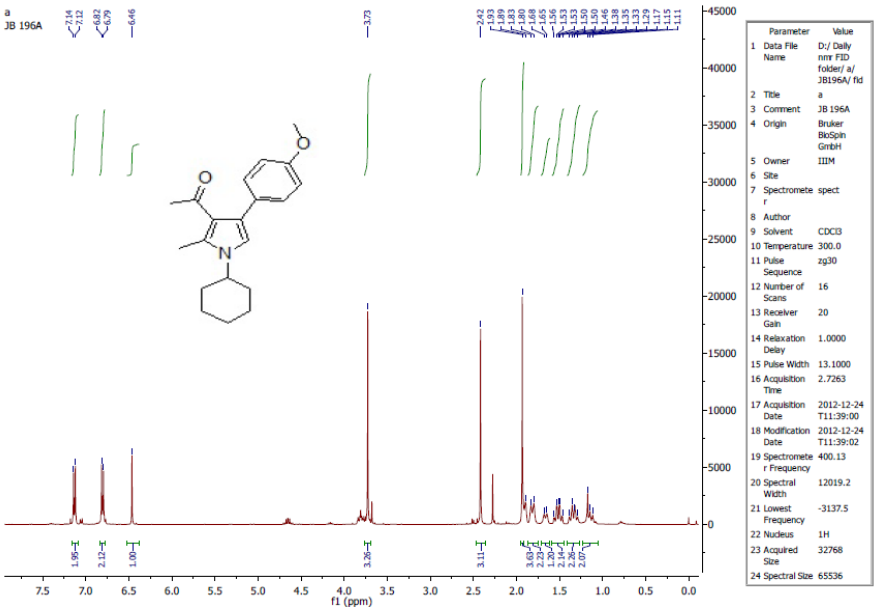
S2.m. ^{1}H, ^{13}C and DEPT-135 NMR of 1-(4-(4-chlorophenyl)-1-cyclohexyl-2-methyl-1H-pyrrol-3-yl)ethanone (1m)

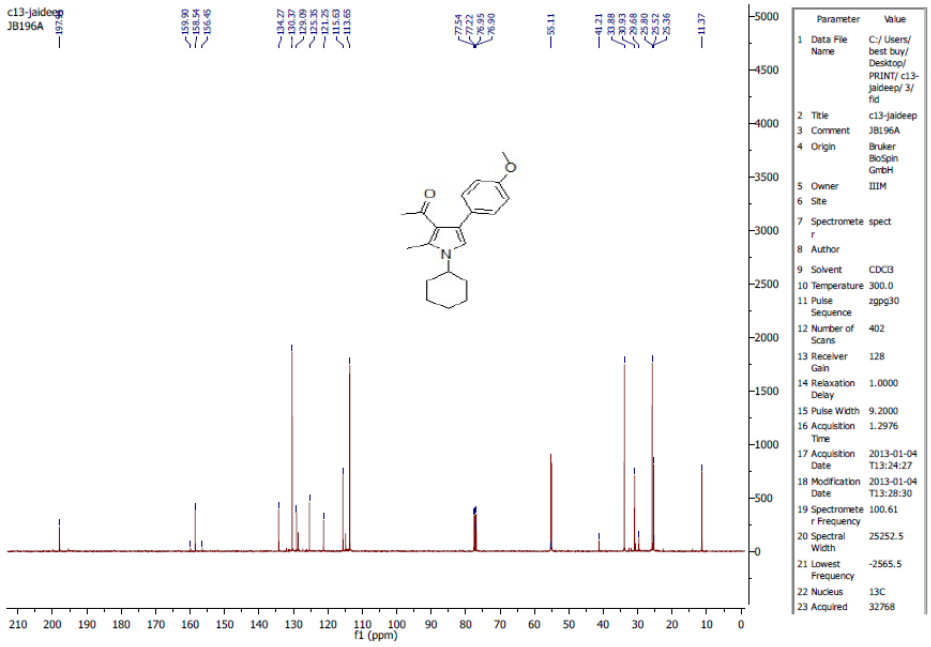






S2.n. ^{1}H, ^{13}C and DEPT-135 NMR of 1-(1-cyclohexyl-4-(4-methoxyphenyl)-2-methyl-1H-pyrrol-3-yl)ethanone (1n)





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5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Number of Scans	402
13	Receiver Gain	128
14	Relaxation Delay	1.0000
15	Pulse Width	9.2000
16	Acquisition Time	1.2976
17	Acquisition Date	2013-01-04 T13:24:27
18	Modification Date	2013-01-04 T13:28:30
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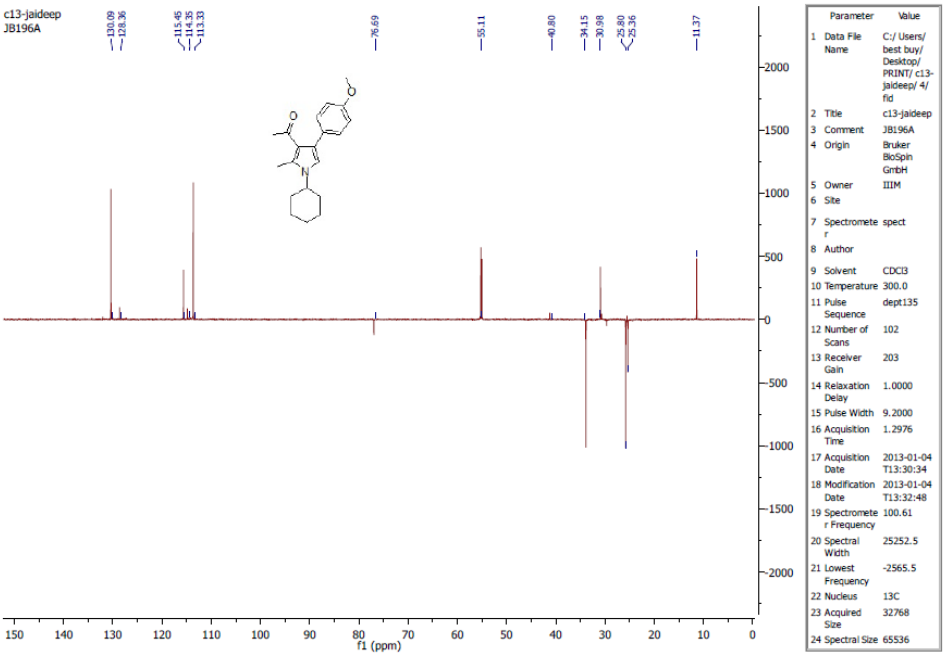
20	Spectral Width	25252.5
21	Lowest Frequency	-2565.5
22	Nucleus	13C
23	Acquired Size	32768



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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	102
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	9.2000
16	Acquisition Time	1.2976
17	Acquisition Date	2013-01-04 T13:30:34
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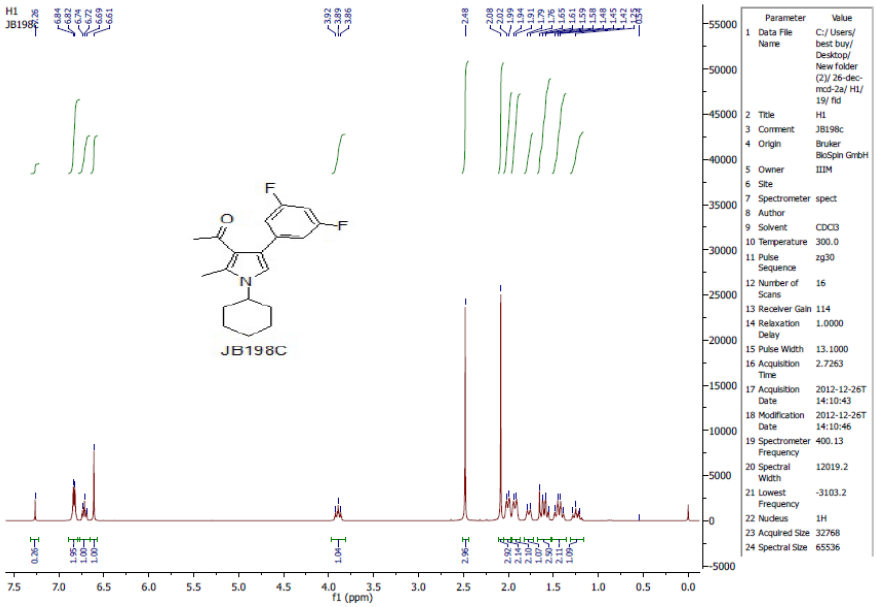
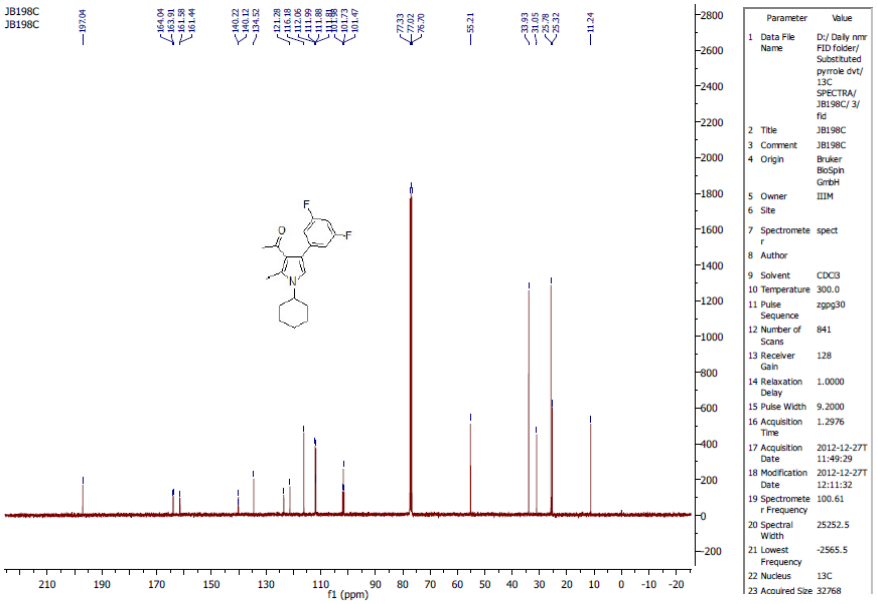
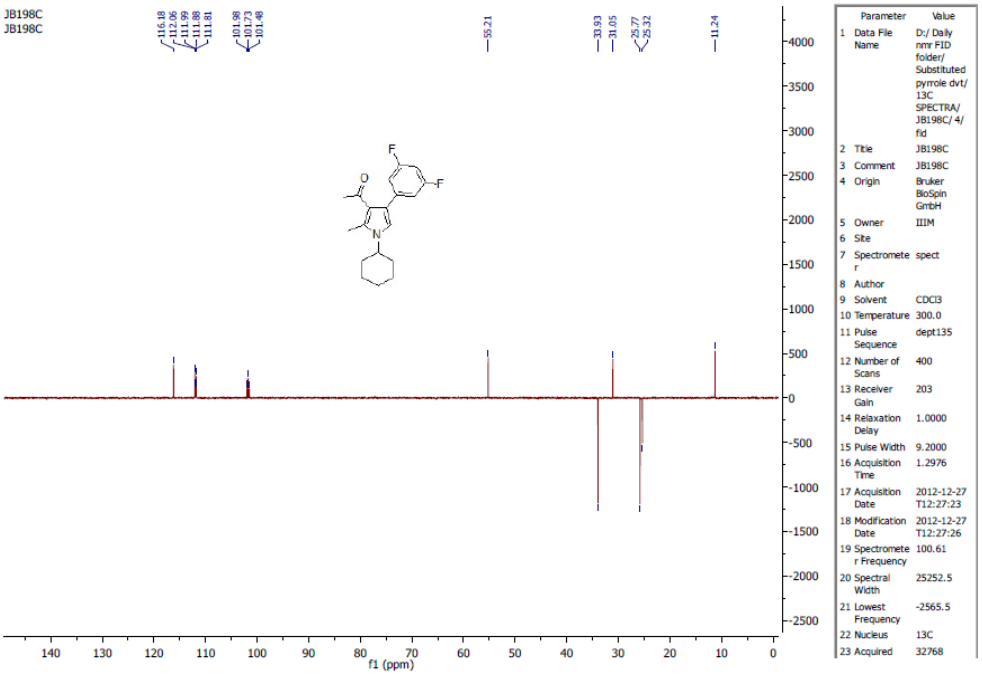
19	Spectrometer Frequency	100.61
20	Spectral Width	25252.5
21	Lowest Frequency	-2565.5
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

S2.o. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR of 1-(1-cyclohexyl-4-(3,5-difluorophenyl)-2-methyl-1H-pyrrol-3-yl)ethanone (1o)







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8	Author	
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10	Temperature	300.0
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14	Relaxation Delay	1.0000
15	Pulse Width	9.2000
16	Acquisition Time	1.2976
17	Acquisition Date	2012-12-27 T12:27:23
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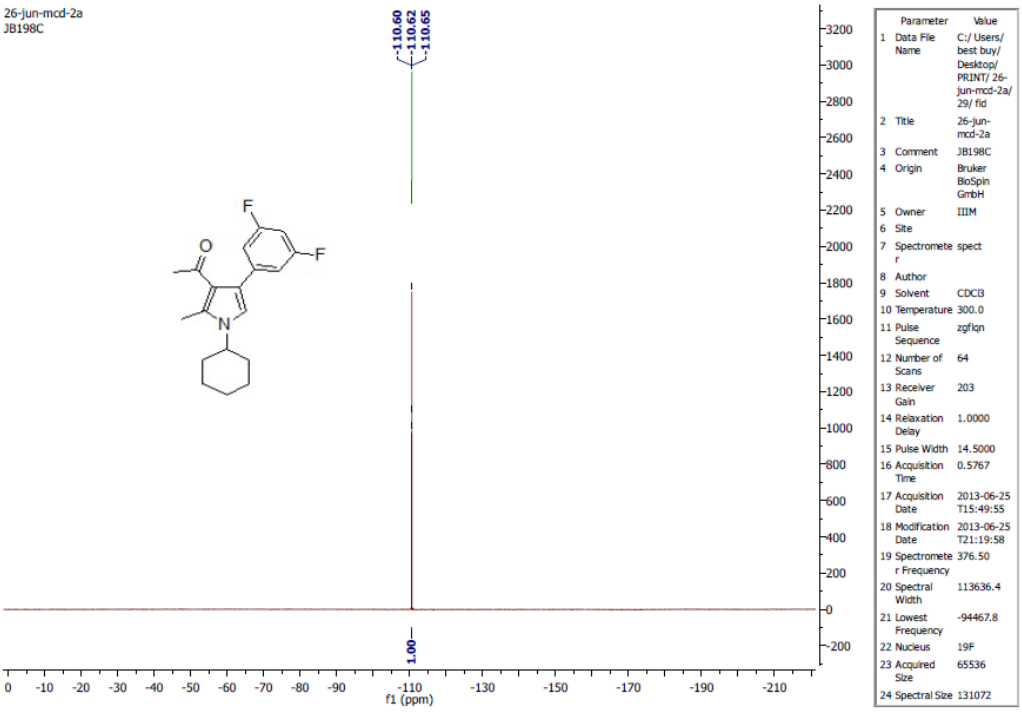
21	Lowest Frequency	-2565.5
22	Nucleus	13C
23	Acquired	32768



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5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgflqn
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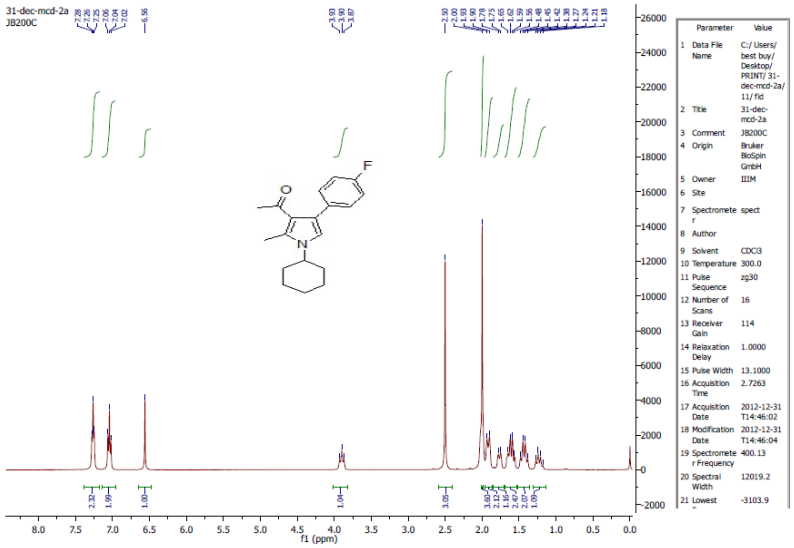
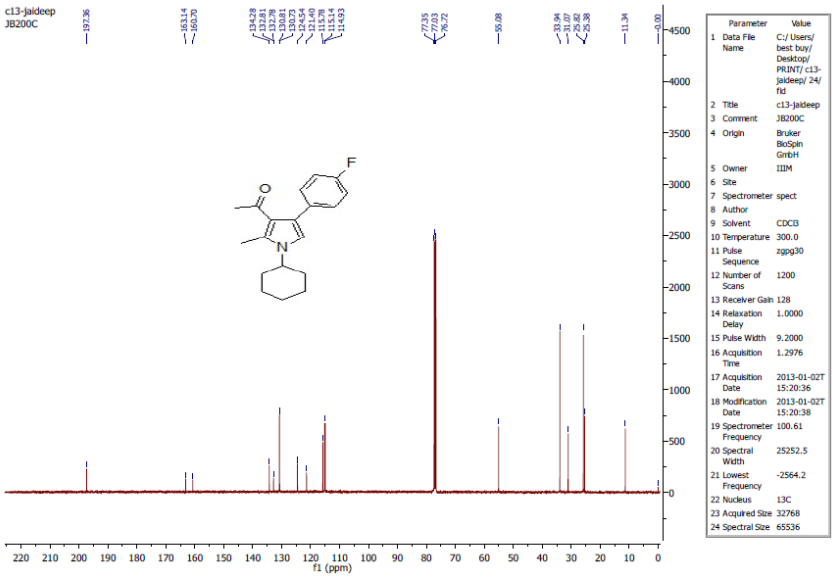
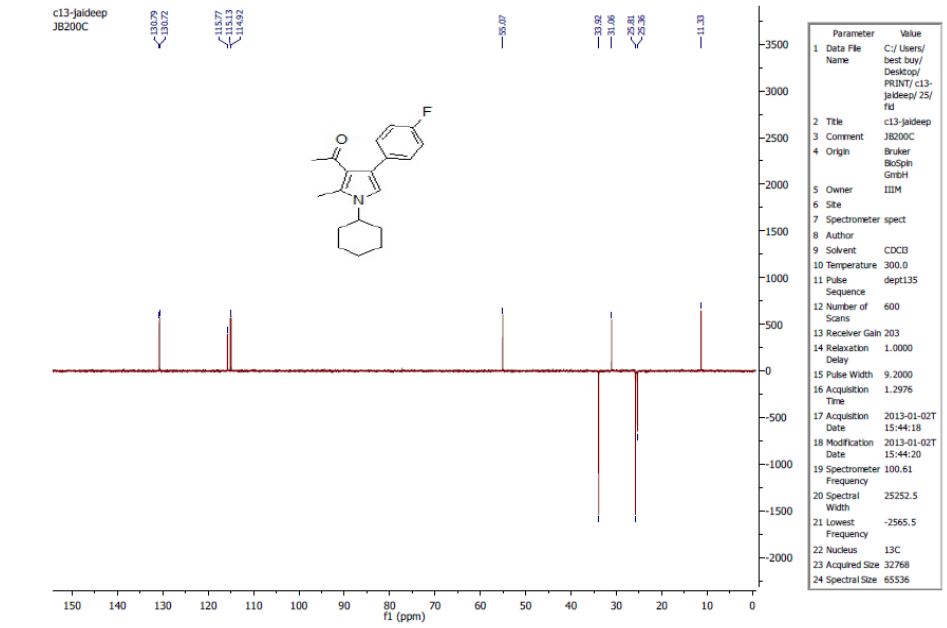
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	14.5000
16	Acquisition Time	0.5767
17	Acquisition Date	2013-06-25 T15:49:55
18	Modification Date	2013-06-25 T21:19:58
19	Spectrometer Frequency	376.50
20	Spectral Width	113636.4
21	Lowest Frequency	-94467.8
22	Nucleus	19F
23	Acquired Size	65536
24	Spectral Size	131072

S2.p. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR of 1-(1-cyclohexyl-4-(4-fluorophenyl)-2-methyl-1H-pyrrol-3-yl)ethanone (1p)






c13-jaideep
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130.72
115.77
115.13
114.92
55.07
33.92
31.06
25.81
25.36
11.33
F
O
N
f1 (ppm)
Parameter Value
1 Data File Name C:/ Users/ best buy/ Desktop/ PRINT/ c13-jaideep/ 25/ fid
2 Title c13-jaideep
3 Comment JB200C
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 600
13 Receiver Gain 203
14 Relaxation Delay 1.0000
15 Pulse Width 9.2000
16 Acquisition Time 1.2976
17 Acquisition Date 2013-01-02T 15:44:18
18 Modification Date 2013-01-02T 15:44:20
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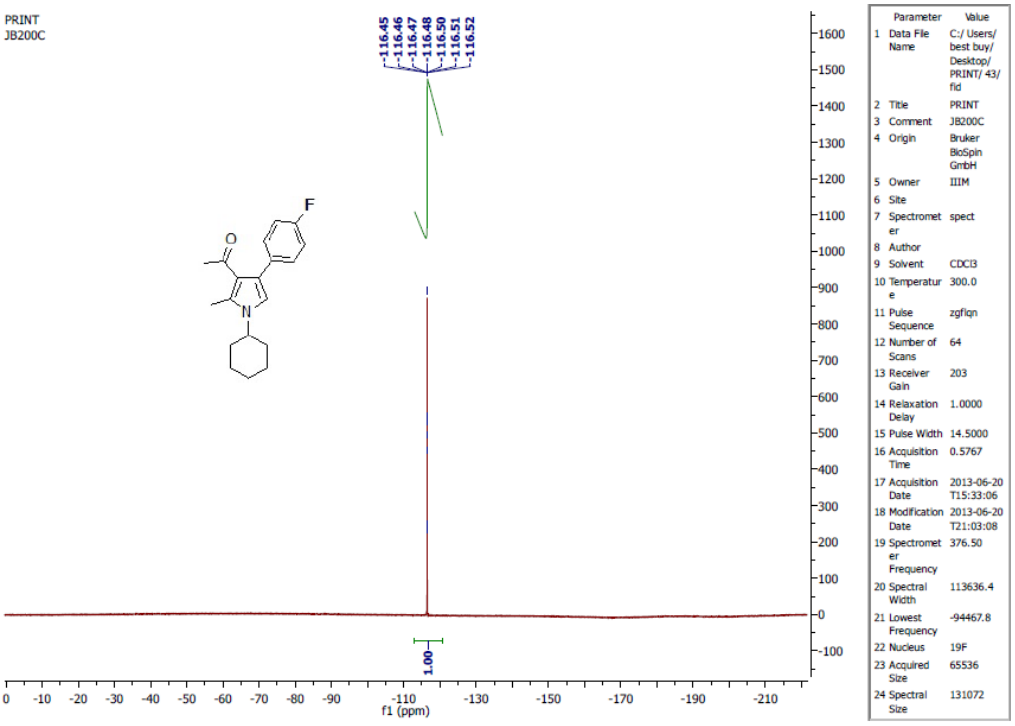
20 Spectral Width 25252.5
21 Lowest Frequency -2565.5
22 Nucleus 13C
23 Acquired Size 32768
24 Spectral Size 65536


PRINT
JB200C
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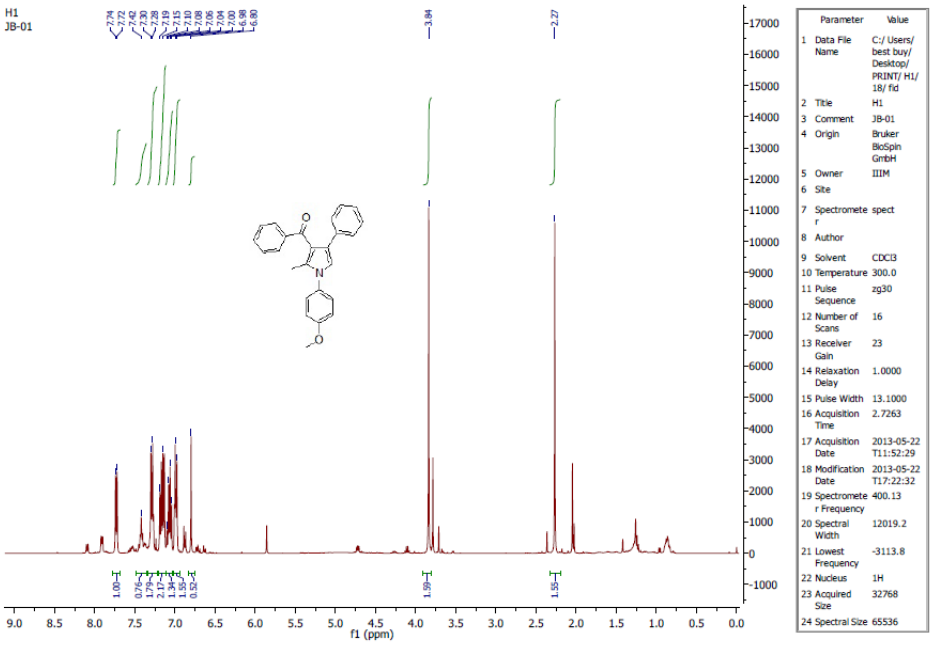
-116.46
-116.47
-116.48
-116.50
-116.51
-116.52
F
O
N
1.00
f1 (ppm)
Parameter Value
1 Data File Name C:/ Users/ best buy/ Desktop/ PRINT/ 43/ fid
2 Title PRINT
3 Comment JB200C
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 300.0
11 Pulse Sequence zgfigq
12 Number of Scans 64
13 Receiver Gain 203
14 Relaxation Delay 1.0000
15 Pulse Width 14.5000
16 Acquisition Time 0.5767
17 Acquisition Date 2013-06-20 T15:33:06
18 Modification Date 2013-06-20 T21:03:08
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 and DEPT-135 NMR of (1-(4-methoxyphenyl)-2-methyl-4-phenyl-1H-pyrrol-3-yl)(phenyl)methanone (1q)



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1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ H1/ 18/ fid
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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	23
14	Relaxation Delay	1.0000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2013-05-22 T11:52:29
18	Modification Date	2013-05-22 T17:22:32
19	Spectrometer Frequency	400.13
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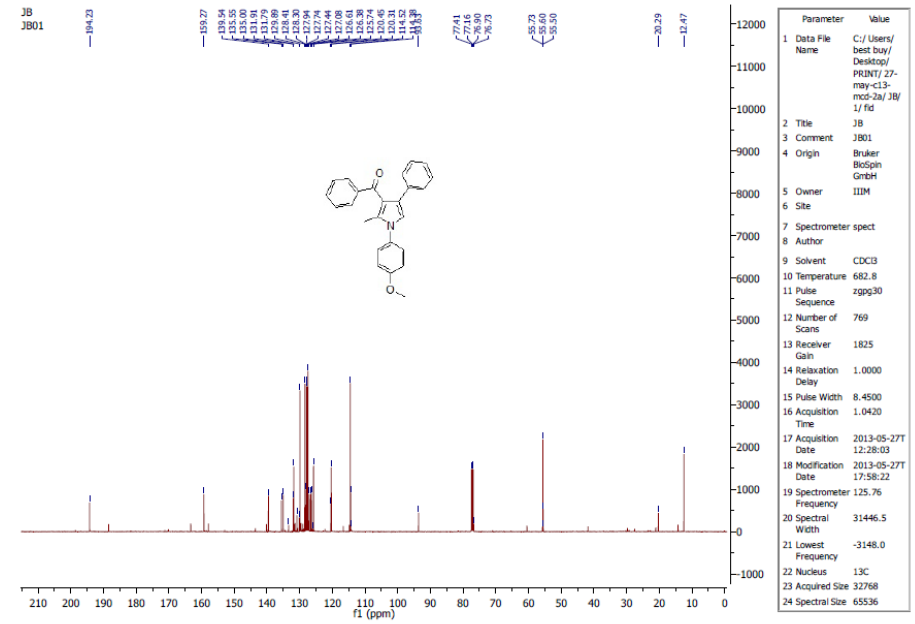
21	Lowest Frequency	-3113.8
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



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5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
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11	Pulse Sequence	zgpg30
12	Number of Scans	769
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2013-05-27T 12:28:03
18	Modification Date	2013-05-27T 17:58:22
19	Spectrometer Frequency	125.76
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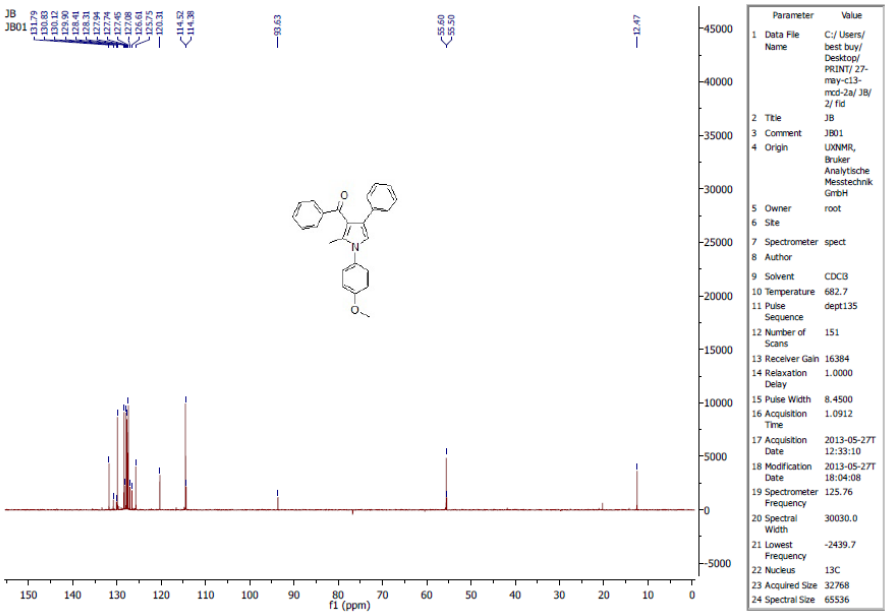
21	Lowest Frequency	-3148.0
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536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130.12
129.90
128.41
125.31
122.34
127.45
127.08
126.64
125.75
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114.52
114.38
93.63
55.60
55.50
12.47
O
N
O
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
Parameter
Value
1 Data File Name
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2 Title
JB
3 Comment
JB01
4 Origin
UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner
root
6 Site
7 Spectrometer
spect
8 Author
9 Solvent
CDCl3
10 Temperature
682.7
11 Pulse Sequence
dept135
12 Number of Scans
151
13 Receiver Gain
16384
14 Relaxation Delay
1.0000
15 Pulse Width
8.4500
16 Acquisition Time
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17 Acquisition Date
2013-05-27T 12:33:10
18 Modification Date
2013-05-27T 18:04:08
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

S3. X-ray crystallography of methyl 1-(1-(4-fluorophenyl)-2-methyl-4-phenyl-1H-pyrrol-3-yl) ethanone 1b:

Single crystals of 1-(1-(4-Fluorophenyl)-2-methyl-4-phenyl-1H-pyrrol-3-yl) ethanone were obtained by slow evaporation at room temperature, from a mixture of Methanol/water. The X-ray data was collected from a dry crystal mounted on an 'Xcalibur, Sapphire3', Oxford diffractometer. The crystal structure was solved by direct method using SHELXS-97 followed by Full matrix anisotropic least square refinement using SHELXL-97. All the hydrogen atoms were located from difference Fourier map and refined isotropically. All the relevant crystallographic data collection parameters and structure refinement details for **1b** is summarized in Table S2. Bond lengths and bond angles are given in Table S3.

Table S2. Crystal data and structure refinement for **1b**

Identification code	1	
Empirical formula	$C_{19}\ H_{16}\ F_1\ N_1\ O_1$	
Formula weight	293.33	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\ 2_1/n$	
Unit cell dimensions	a = 9.7980(13) Å	α= 90°
	b = 7.8015(9) Å	β= 98.077(13)°
	c = 20.558(2) Å	γ = 90°
Volume	1555.8(3) $Å^3$	
Z	4	
Density (calculated)	1.252 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	616	
Crystal size	0.4 x 0.2 x 0.2 mm^3	
Theta range for data collection	3.75 to 27.00°	
Index ranges	$-12 \leq h \leq 9, -9 \leq k \leq 5, -15 \leq l \leq 26$	
Reflections collected	6121	
Scan type	ω-scan	

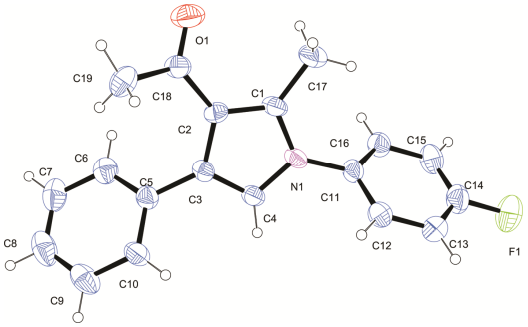
Unique reflections	3330 [R_{int} = 0.0276]
Observed reflection [|F| >4σ(F)]	1792
Completeness to theta = 26.74°	98.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3330 / 0 / 264
Goodness-of-fit (S)	1.019
Final R indices [I>2sigma(I)]	R_1 = 0.0510, wR_2 = 0.1129
R indices (all data)	R_1 = 0.1052, wR_2 = 0.1476
Largest diff. peak and hole	0.136 and -0.140 $eÅ^{-3}$
CCDC number	946744

Table S3. Bond lengths [Å] and angles [°] for **1b**

H(4) - C(12)	1.00(3)	H(5) - C(4)	0.94(3)
H(2) - C(15)	1.00(3)	H(6) - C(6)	1.01(2)
H(10) - C(10)	1.05(3)	H(15) - C(17)	0.99(3)
H(8) - C(8)	0.94(3)	H(9) - C(9)	0.98(3)
H(16) - C(17)	0.97(4)	H(14) - C(17)	1.02(3)
H(11) - C(19)	0.95(3)	H(1) - C(16)	0.94(3)
H(3) - C(13)	0.93(3)	H(7) - C(7)	1.01(3)
H(12) - C(19)	0.89(4)	H(13) - C(19)	0.90(4)
N(1) - C(1)	1.371(3)	N(1) - C(4)	1.377(3)
N(1) - C(11)	1.425(3)	O(1) - C(18)	1.215(3)
F(1) - C(14)	1.354(4)	C(1) - C(2)	1.383(3)
C(1) - C(17)	1.491(4)	C(2) - C(3)	1.442(3)
C(2) - C(18)	1.464(3)	C(3) - C(4)	1.348(3)
C(3) - C(5)	1.471(3)	C(5) - C(6)	1.385(3)
C(5) - C(10)	1.391(4)	C(6) - C(7)	1.381(4)
C(7) - C(8)	1.368(5)	C(8) - C(9)	1.367(5)
C(9) - C(10)	1.372(5)	C(11) - C(12)	1.379(4)
C(11) - C(16)	1.377(4)	C(12) - C(13)	1.372(4)
C(13) - C(14)	1.350(4)	C(14) - C(15)	1.366(4)
C(15) - C(16)	1.376(4)	C(18) - C(19)	1.496(4)

C(1)-N(1)-C(4)	109.3(2)	C(1)-N(1)-C(11)	127.2(2)

C(4)-N(1)-C(11)	123.4(2)	N(1)-C(1)-C(2)	107.4(2)
N(1)-C(1)-C(17)	121.8(2)	C(2)-C(1)-C(17)	130.6(2)
C(1)-C(2)-C(3)	107.2(2)	C(1)-C(2)-C(18)	123.3(2)
C(3)-C(2)-C(18)	129.0(2)	C(2)-C(3)-C(4)	106.8(2)
C(2)-C(3)-C(5)	128.5(2)	C(4)-C(3)-C(5)	124.2(2)
H(5)-C(4)-N(1)	119.2(12)	H(5)-C(4)-C(3)	131.5(12)
N(1)-C(4)-C(3)	109.2(2)	C(3)-C(5)-C(6)	120.9(2)
C(3)-C(5)-C(10)	120.9(2)	C(6)-C(5)-C(10)	118.1(3)
H(6)-C(6)-C(5)	118.8(11)	H(6)-C(6)-C(7)	120.6(11)
C(5)-C(6)-C(7)	120.6(3)	H(7)-C(7)-C(6)	114.1(14)
H(7)-C(7)-C(8)	125.7(14)	C(6)-C(7)-C(8)	120.3(3)
H(8)-C(8)-C(7)	119.4(16)	H(8)-C(8)-C(9)	120.8(16)
C(7)-C(8)-C(9)	119.9(3)	H(9)-C(9)-C(8)	122.0(15)
H(9)-C(9)-C(10)	117.5(15)	C(8)-C(9)-C(10)	120.5(3)
H(10)-C(10)-C(5)	119.3(14)	H(10)-C(10)-C(9)	120.0(14)
C(5)-C(10)-C(9)	120.7(3)	N(1)-C(11)-C(12)	119.0(2)
N(1)-C(11)-C(16)	120.8(2)	C(12)-C(11)-C(16)	120.1(3)
H(4)-C(12)-C(11)	121.7(12)	H(4)-C(12)-C(13)	118.3(12)
C(11)-C(12)-C(13)	120.1(3)	H(3)-C(13)-C(12)	121.5(18)
H(3)-C(13)-C(14)	119.9(18)	C(12)-C(13)-C(14)	118.6(3)
F(1)-C(14)-C(13)	118.9(3)	F(1)-C(14)-C(15)	118.0(3)
C(13)-C(14)-C(15)	123.0(3)	H(2)-C(15)-C(14)	121.2(14)
H(2)-C(15)-C(16)	120.4(14)	C(14)-C(15)-C(16)	118.4(3)
H(1)-C(16)-C(11)	118.3(14)	H(1)-C(16)-C(15)	121.9(14)
C(11)-C(16)-C(15)	119.8(3)	H(15)-C(17)-H(16)	105.5(23)
H(15)-C(17)-H(14)	116.0(21)	H(15)-C(17)-C(1)	111.3(15)
H(16)-C(17)-H(14)	104.8(23)	H(16)-C(17)-C(1)	111.2(17)
H(14)-C(17)-C(1)	107.8(16)	O(1)-C(18)-C(2)	121.8(3)
O(1)-C(18)-C(19)	119.0(3)	C(2)-C(18)-C(19)	119.1(3)
H(11)-C(19)-H(12)	106.1(28)	H(11)-C(19)-H(13)	107.8(27)
H(11)-C(19)-C(18)	114.4(18)	H(12)-C(19)-H(13)	113.8(31)
H(12)-C(19)-C(18)	110.6(23)	H(13)-C(19)-C(18)	104.4(20)



The ORTEP diagram showing numbering scheme and the molecular conformation of **1b** in crystals.