

Supporting Information

Oxidant-Controlled C-sp²/sp³ – H Cross-dehydrogenative Coupling of *N*-Heterocycles with Benzylamines

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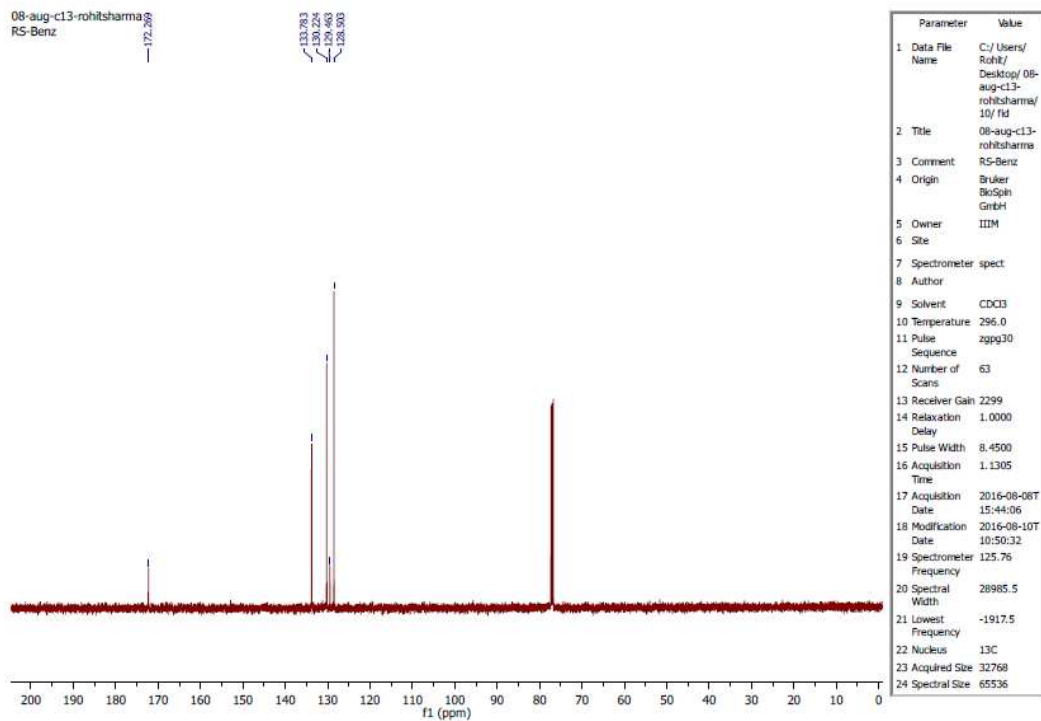
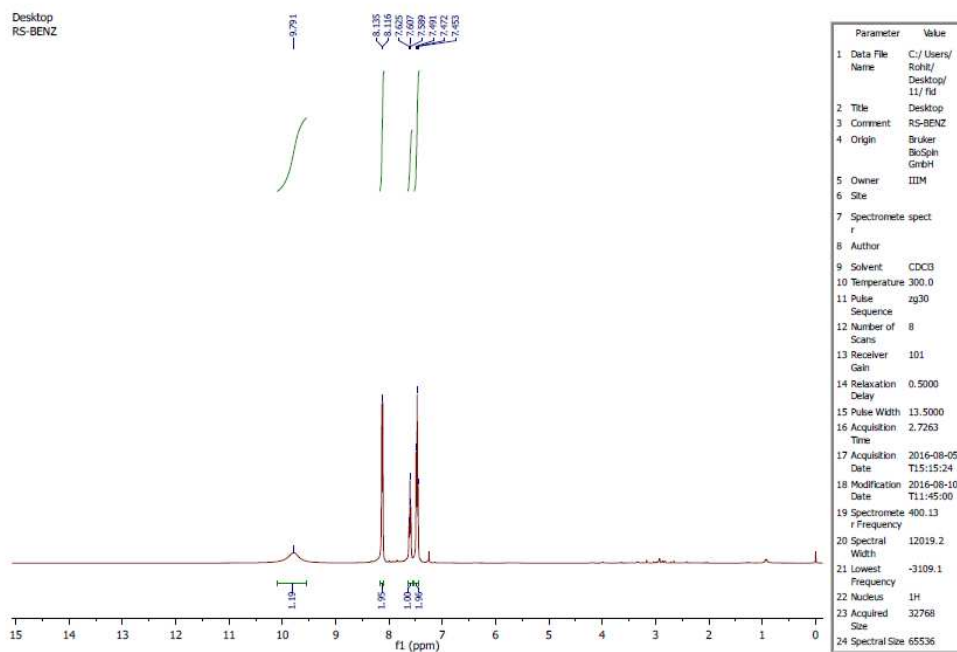
Corresponding Author

**Tel: +91-191-2586333; Tel: +91-191-2585006 (Extn. 345). E-mail: sbharate@iiim.ac.in, sandipbharate@gmail.com (S.B.B.)*

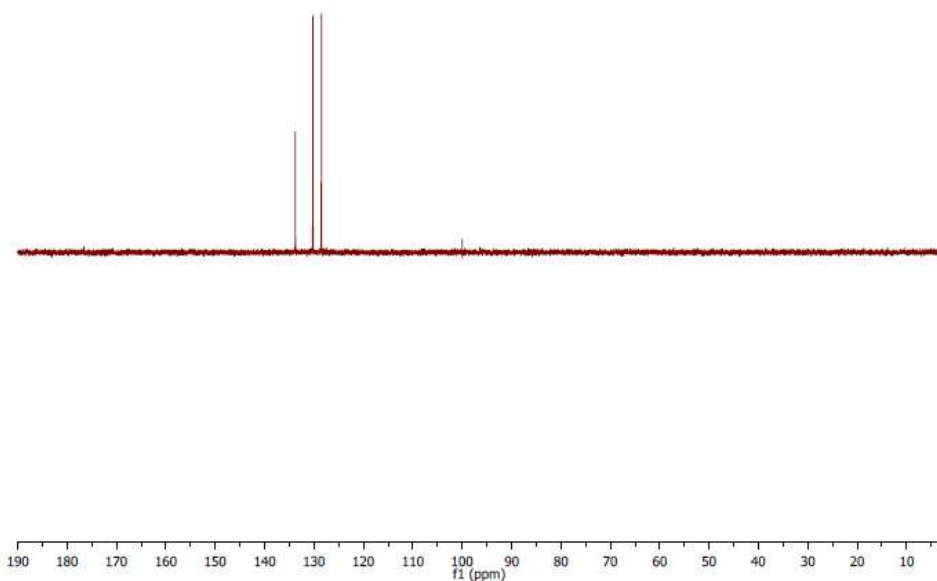
ORCID: 0000-0001-6081-5787

SCANNED COPIES OF ^1H NMR AND ^{13}C NMR SPECTRA OF COMPOUNDS

^1H NMR and ^{13}C NMR and DEPT135 spectra of benzoic acid (3aa).



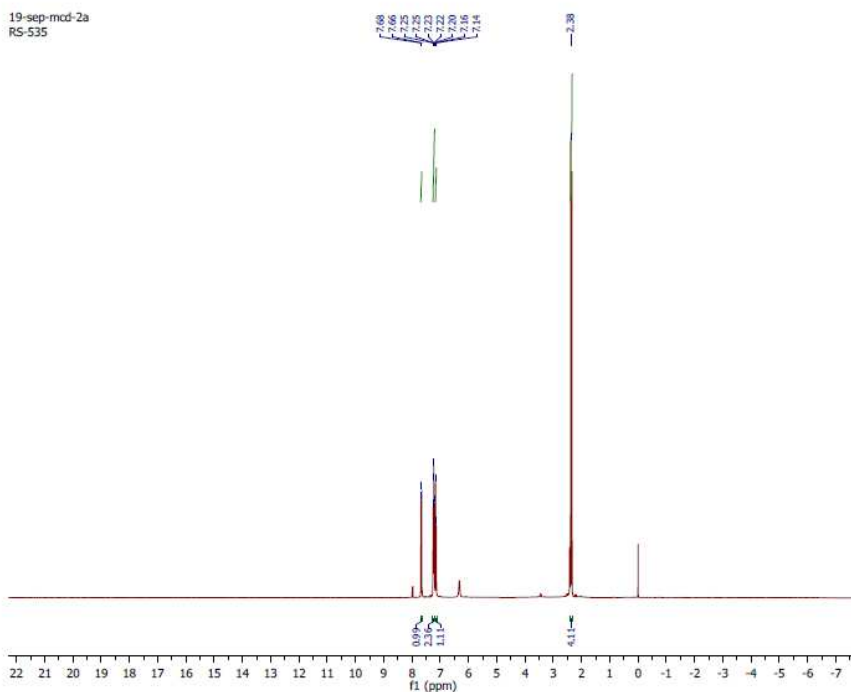
08-aug-c13-rohitsharma
RS-Benz



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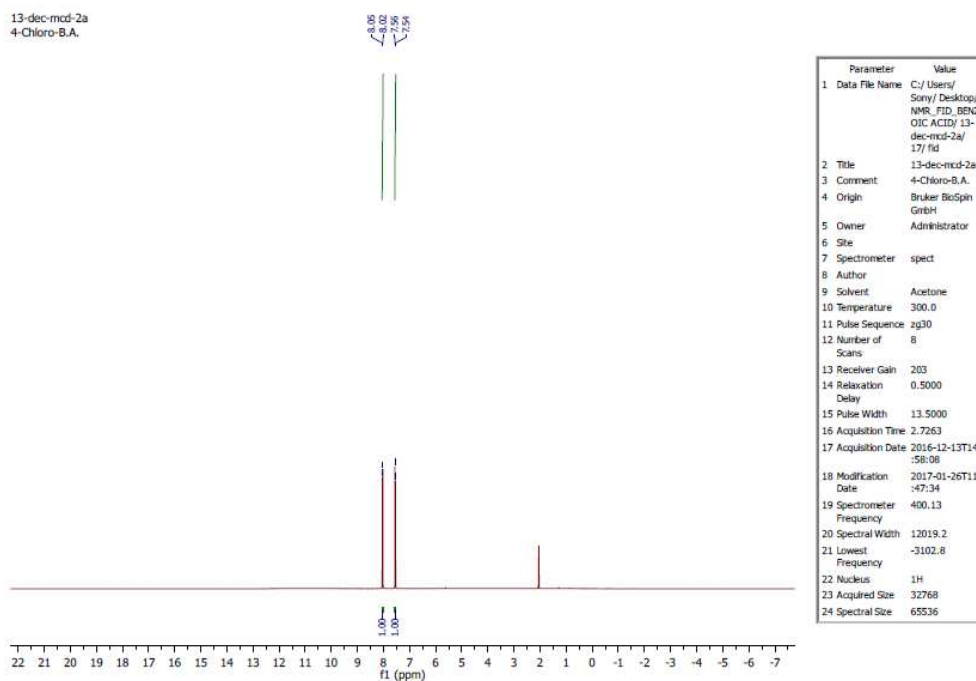
¹H NMR spectra of 4-methylbenzoic acid (3ab).

19-sep-mcd-2a
RS-535

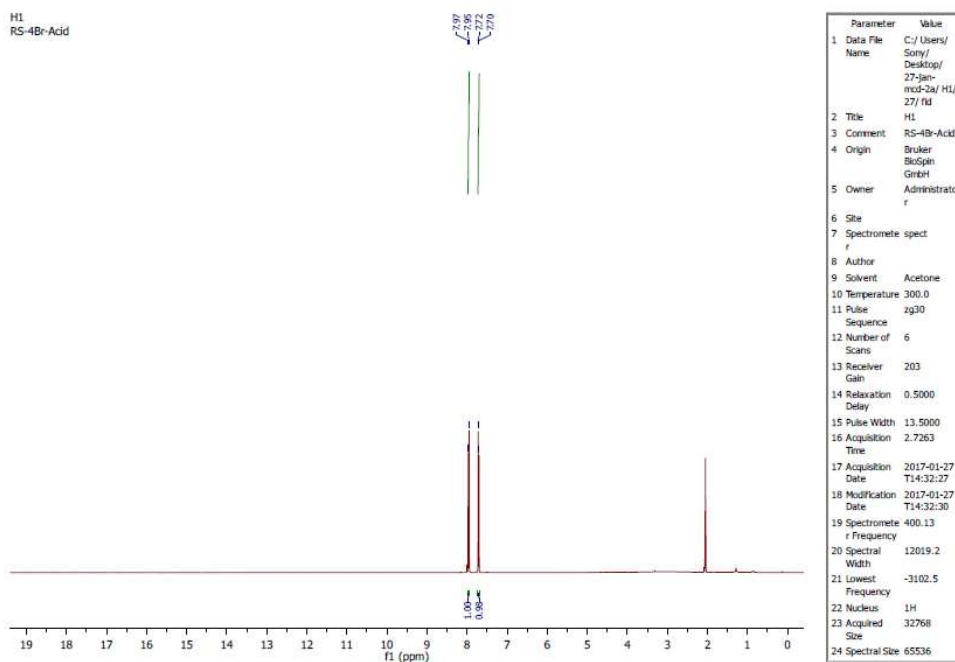


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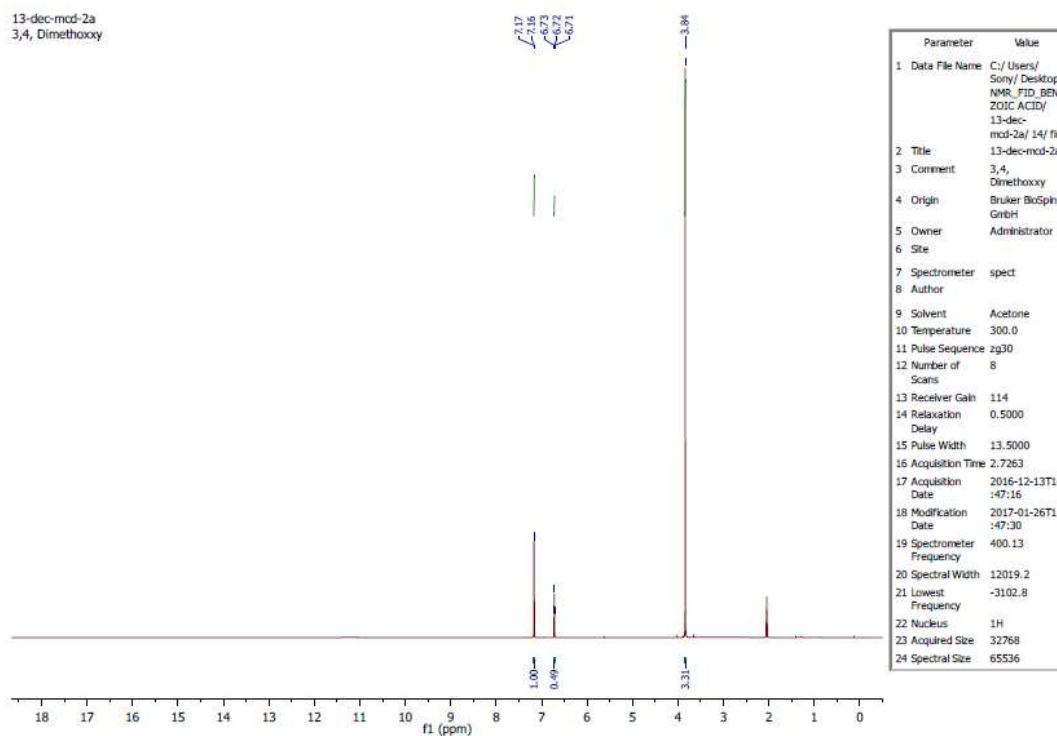
¹H NMR spectra of 4-chlorobenzoic acid (3ac).



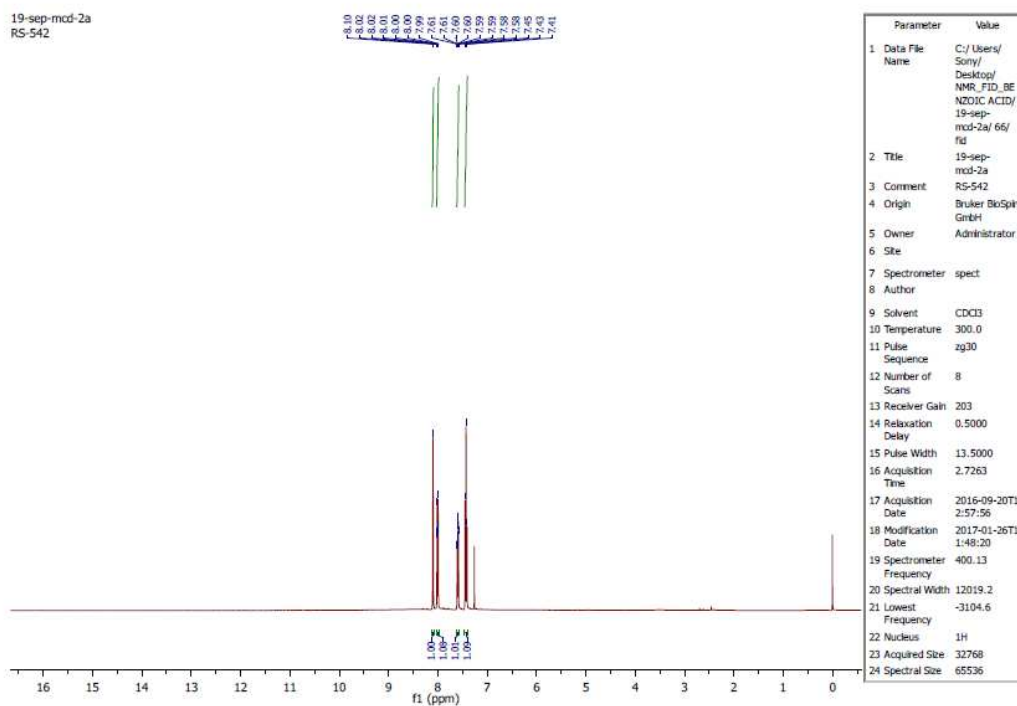
¹H NMR spectra of 4-bromobenzoic acid (3ad).



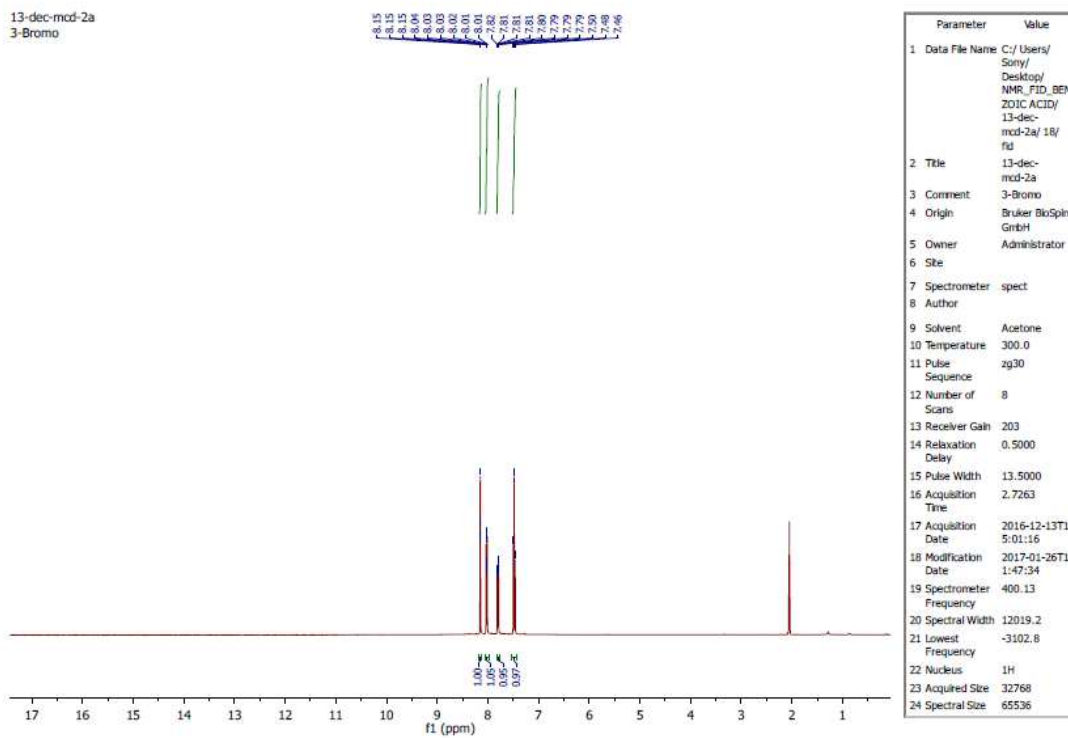
¹H NMR spectra of 3,5-dimethoxybenzoic acid (3ae).



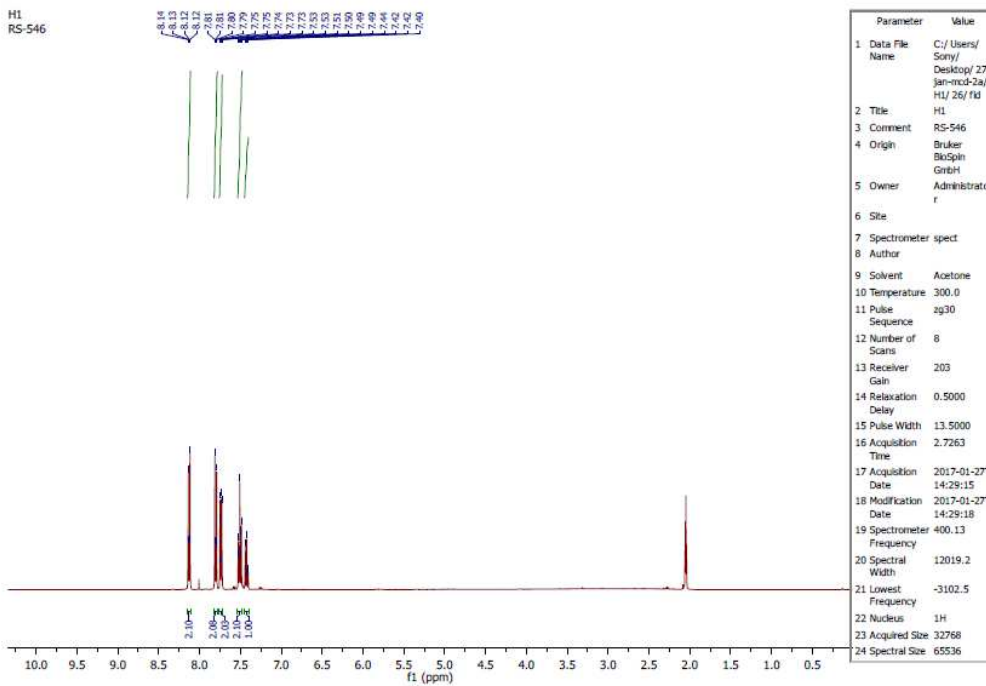
¹H NMR spectra of 3-chlorobenzoic acid (3af).



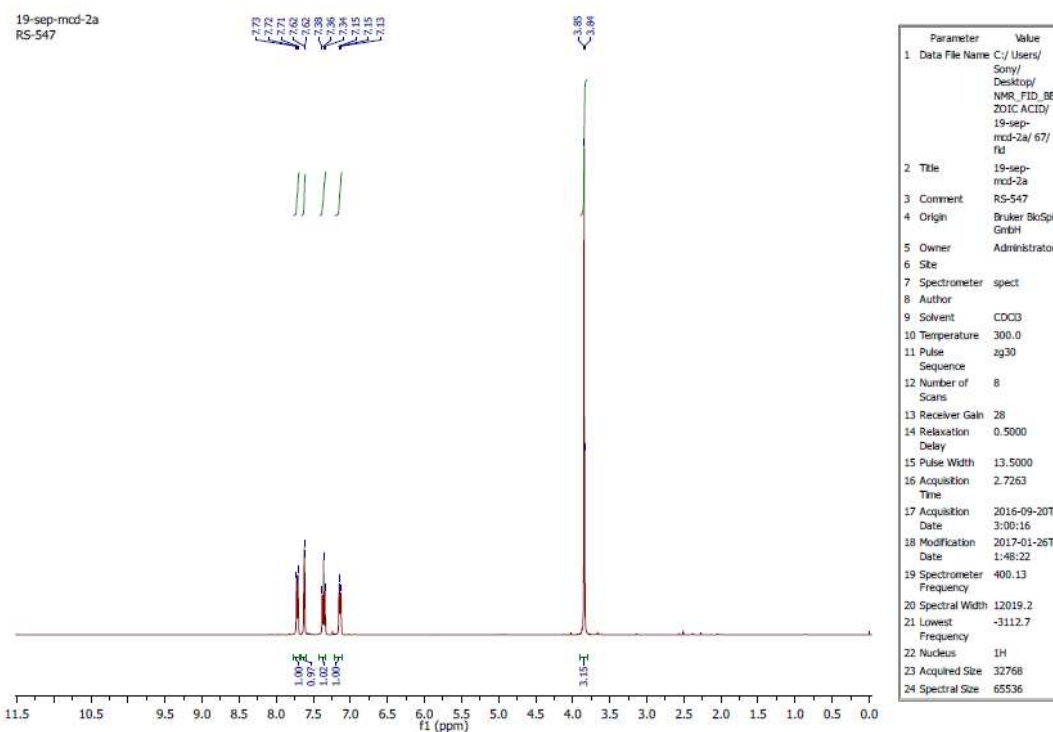
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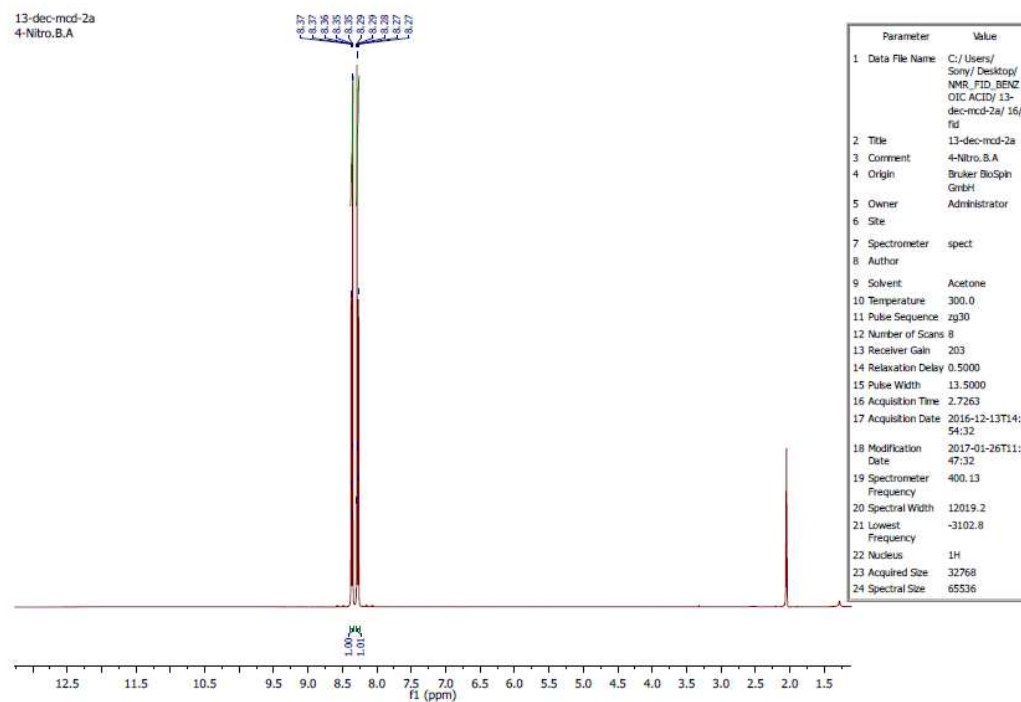
¹H NMR spectra of [1,1'-biphenyl]-4-carboxylic acid (3ah).



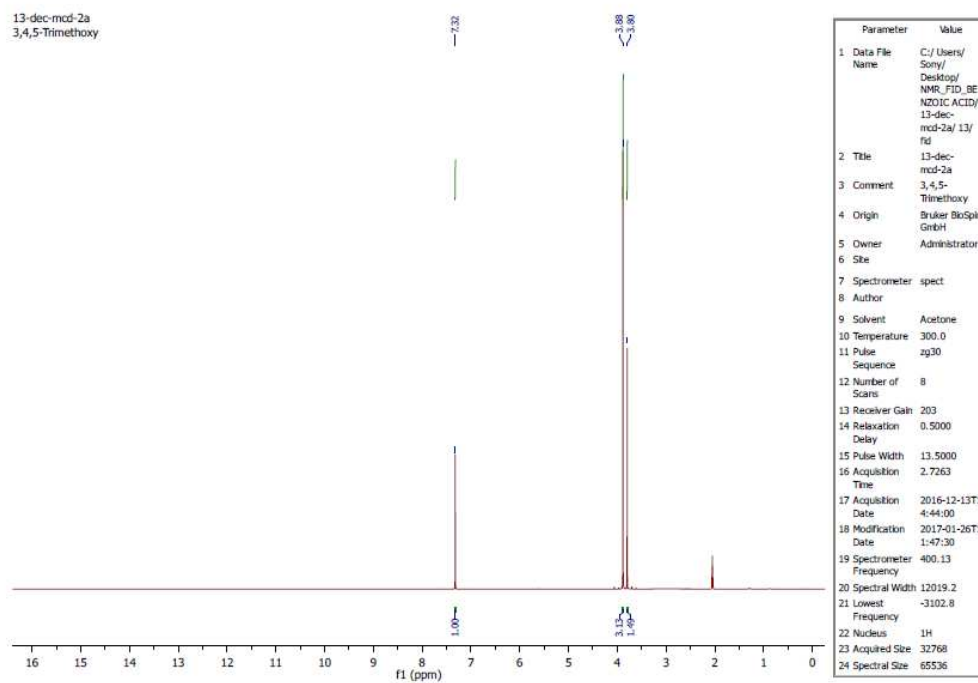
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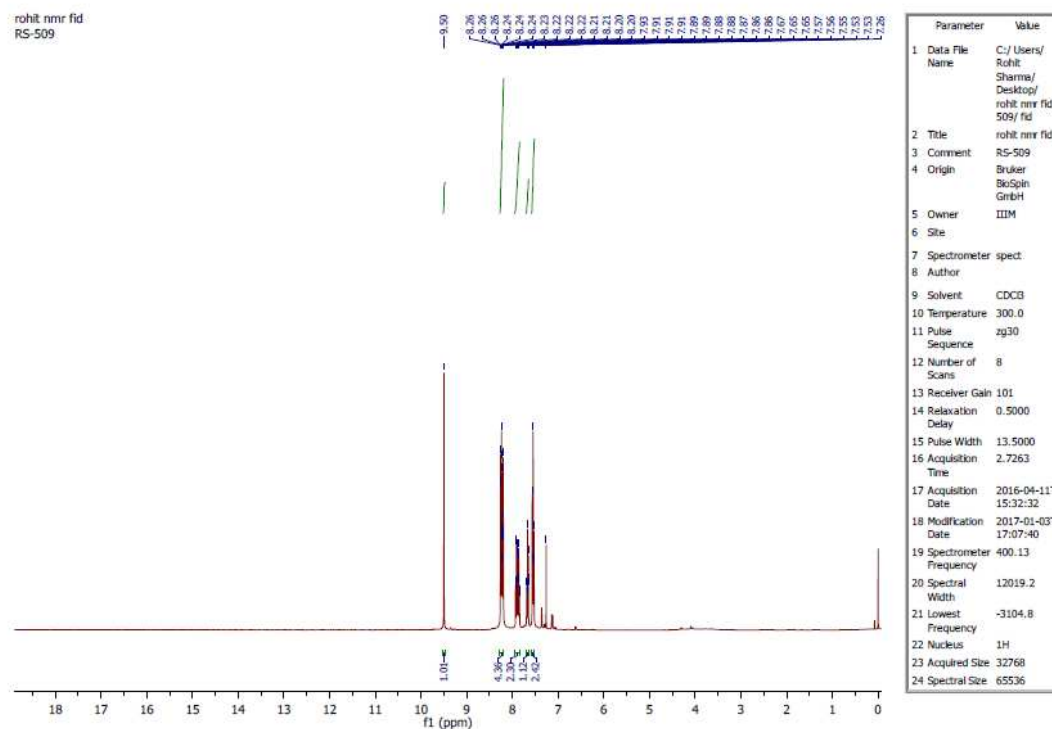
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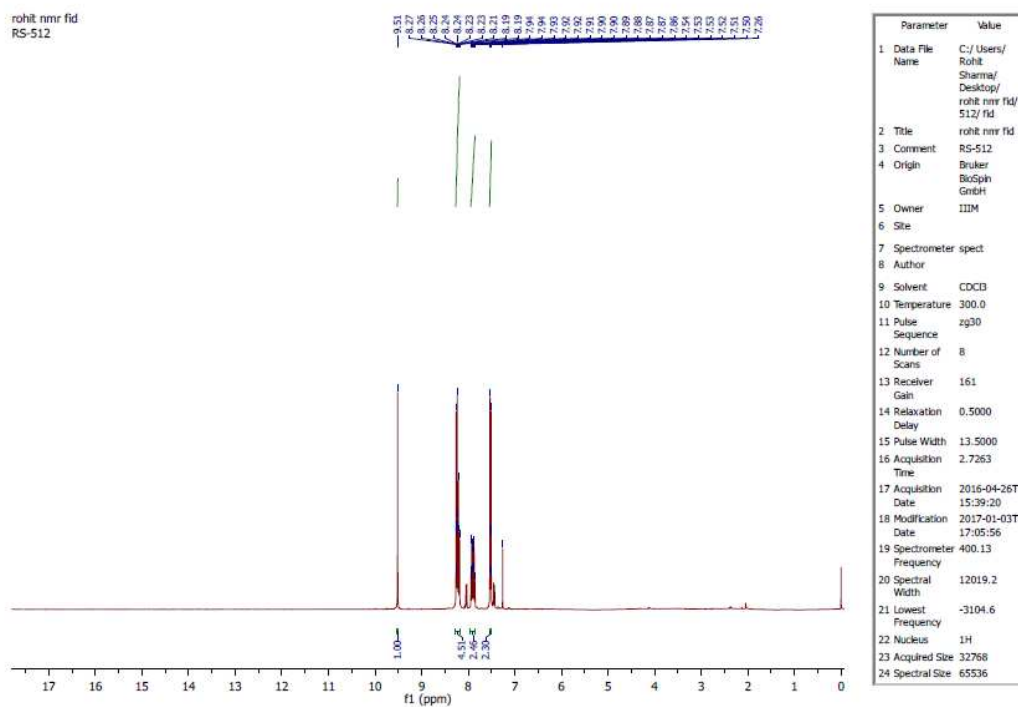
¹H NMR spectra of 3, 4, 5-trimethoxybenzoic acid (3ak).



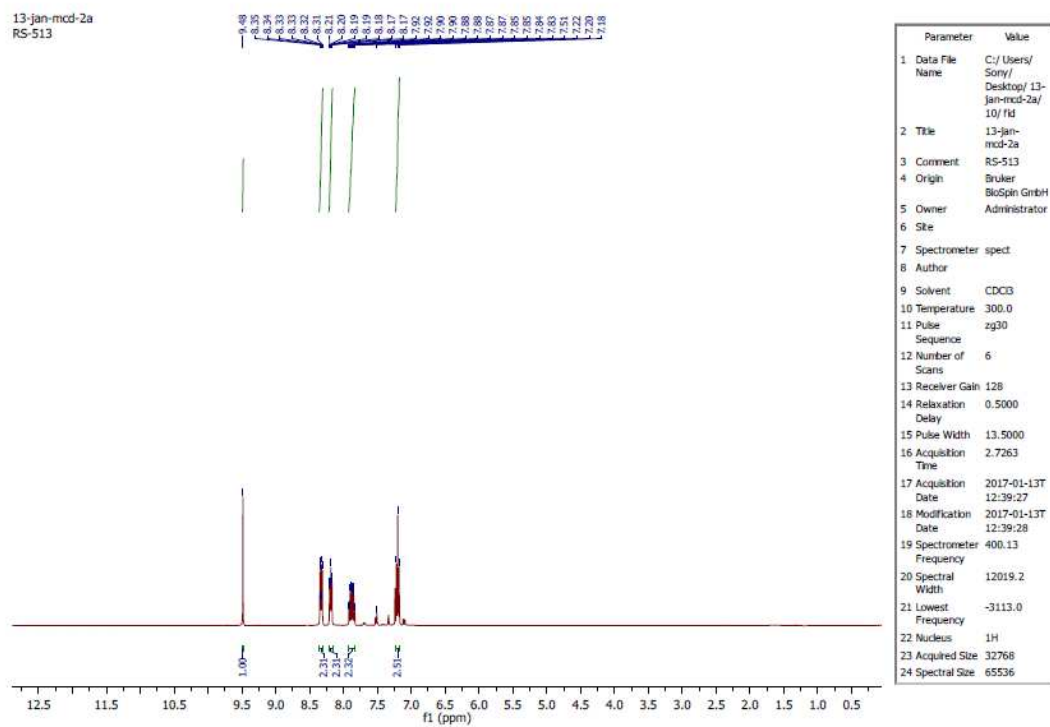
¹H NMR spectra of phenyl(quinoxalin-2-yl)methanone (1a).

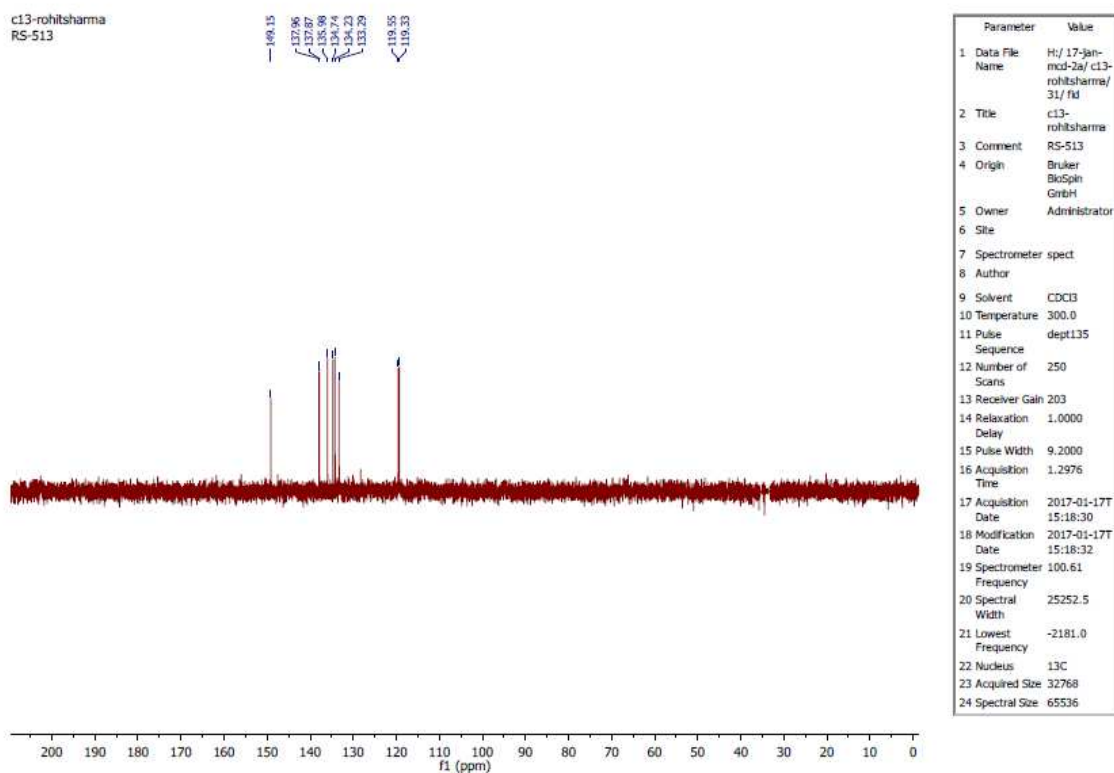
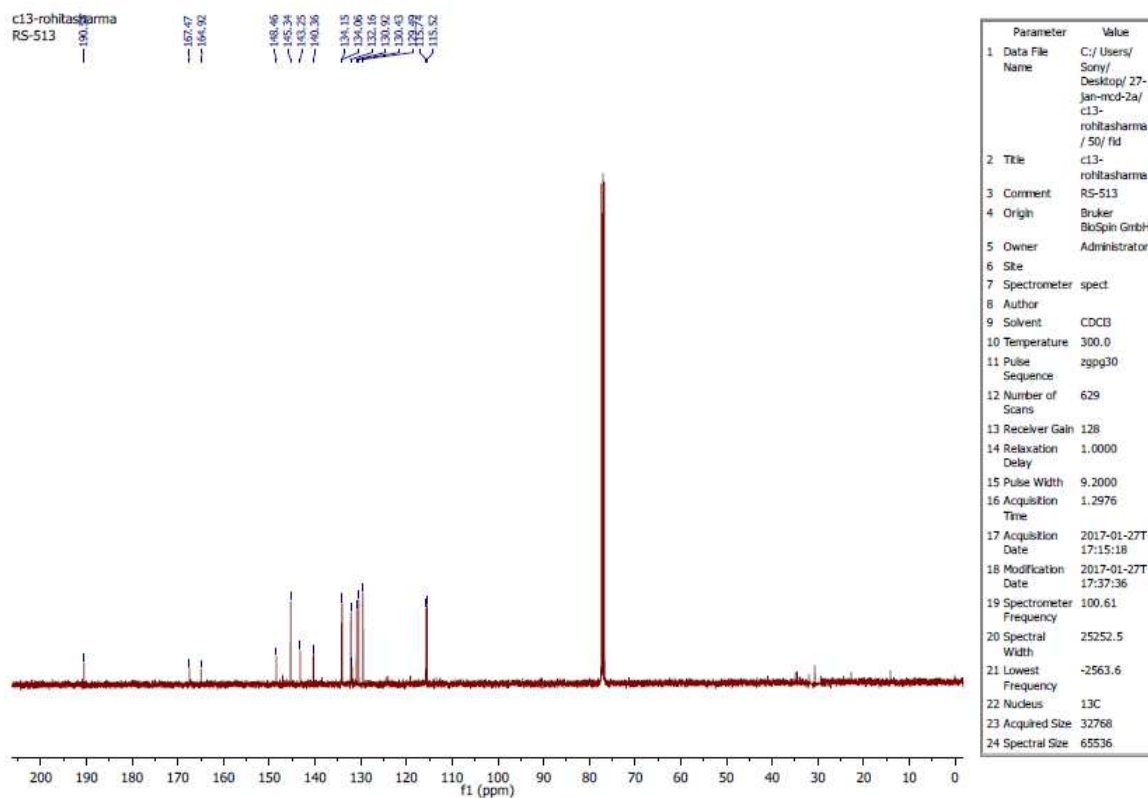


¹H NMR spectra of (4-chlorophenyl)(quinoxalin-2-yl)methanone (1b).

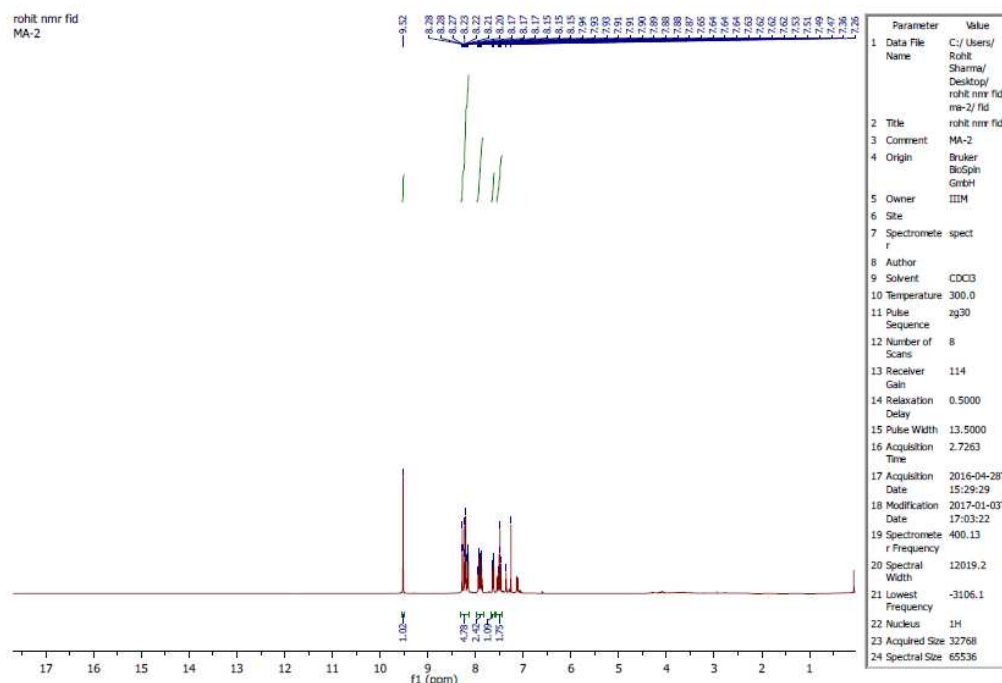


¹H, ¹³C and DEPT135 spectra of (4-fluorophenyl)(quinoxalin-2-yl)methanone (1c).

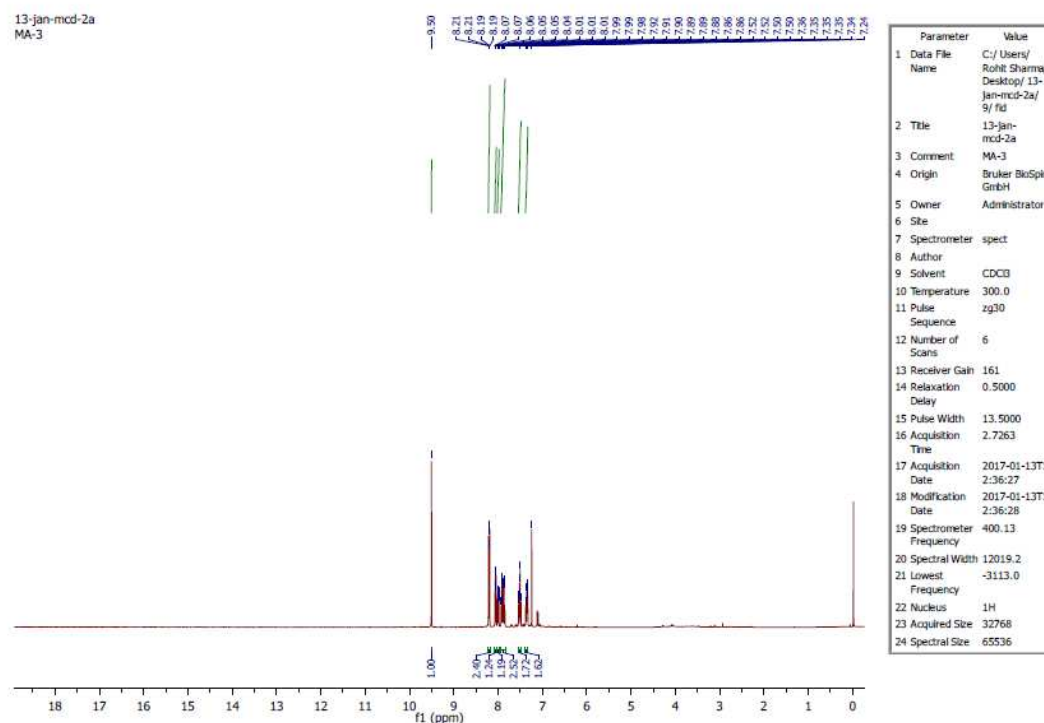


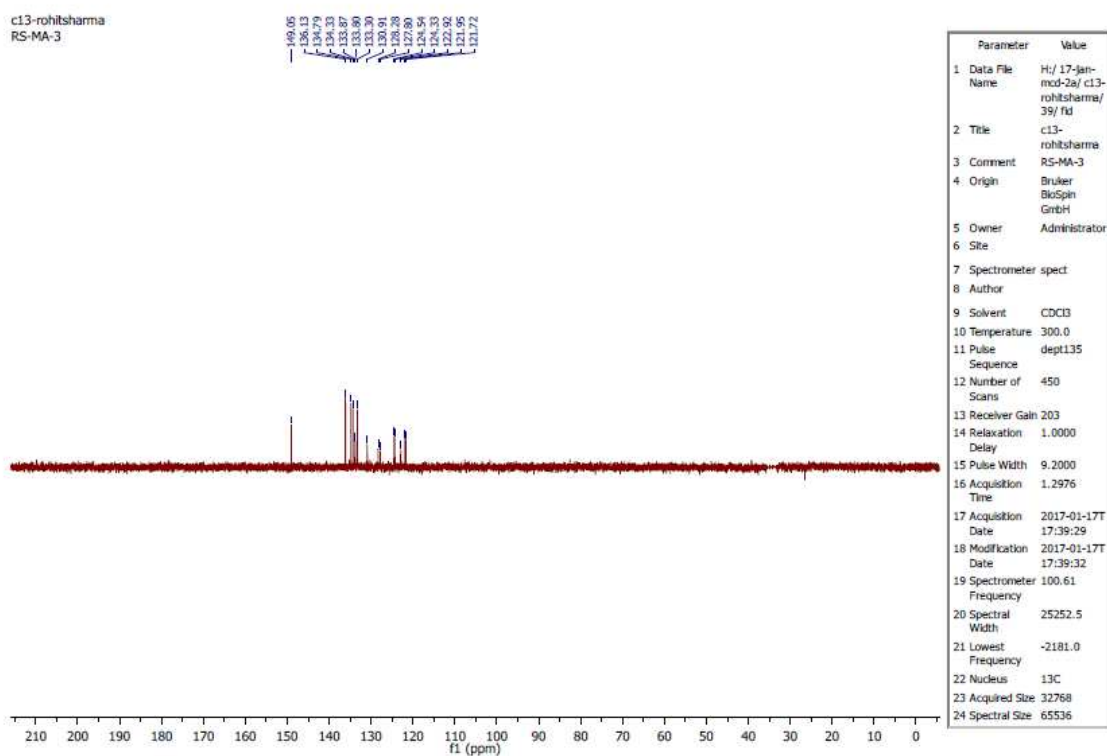
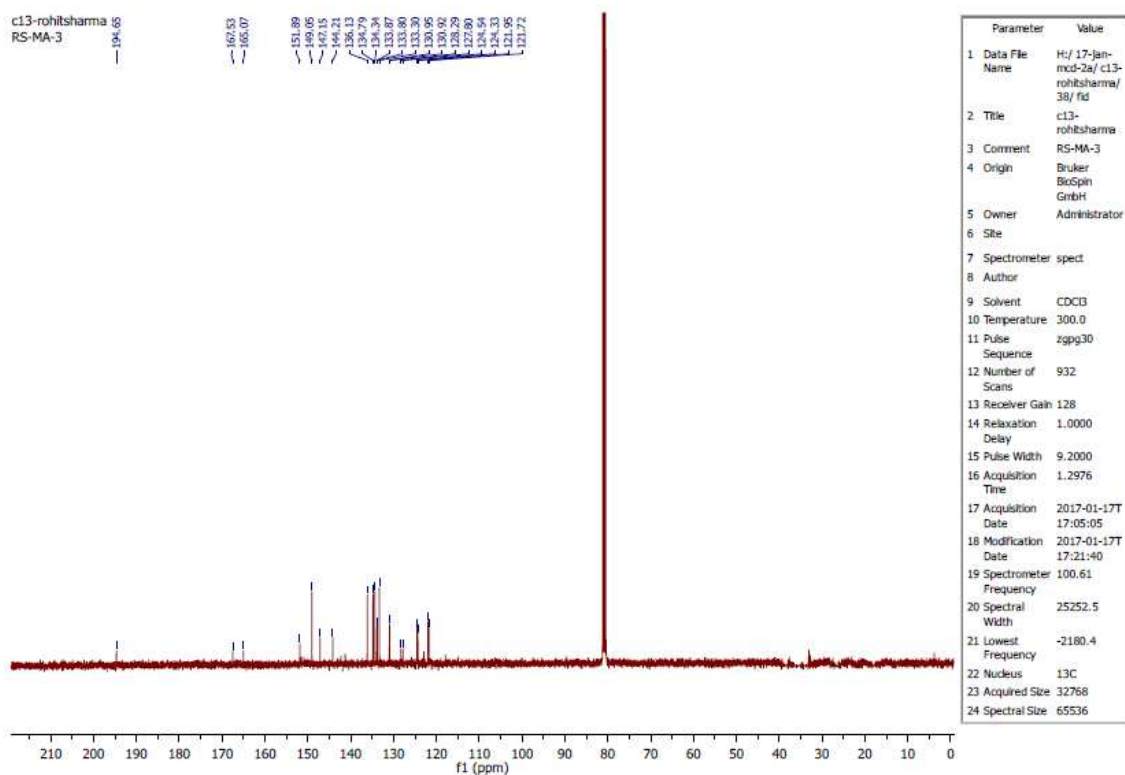


¹H NMR spectra of (3-chlorophenyl)(quinoxalin-2-yl)methanone (1d).

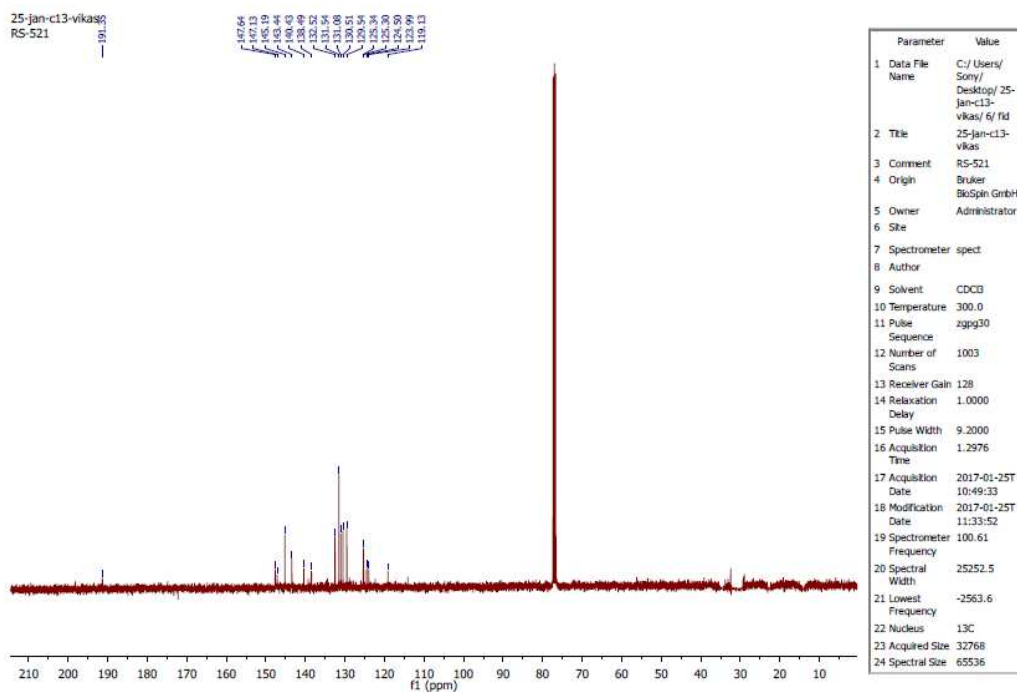
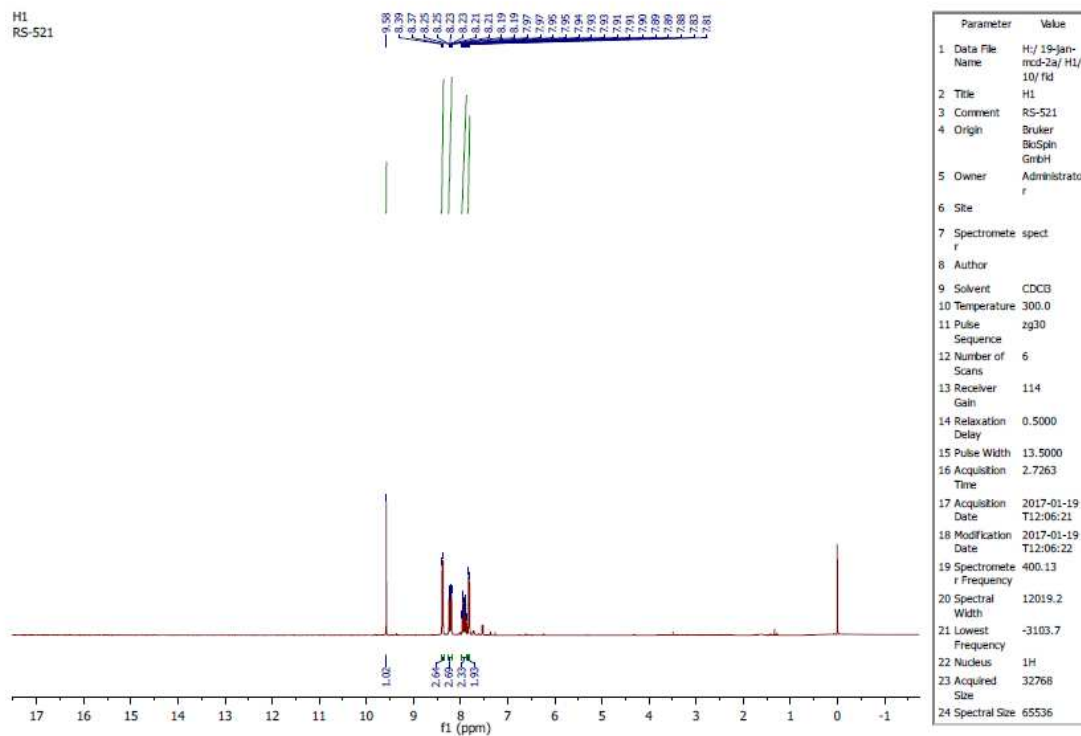


¹H, ¹³C and DEPT135 spectra of (3-fluorophenyl)(quinoxalin-2-yl)methanone (1e).

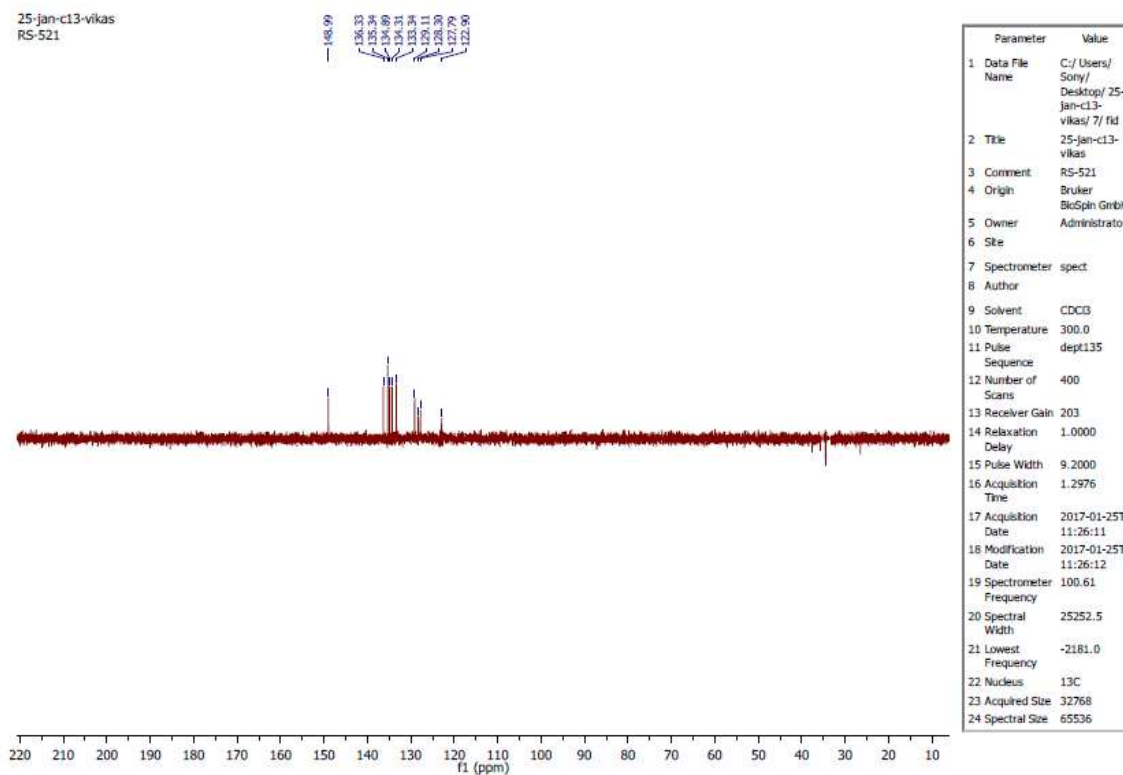




^1H NMR, ^{13}C NMR and DEPT135 spectra of (quinoxalin-2-yl(4-(trifluoromethyl)phenyl)methanone (1f).

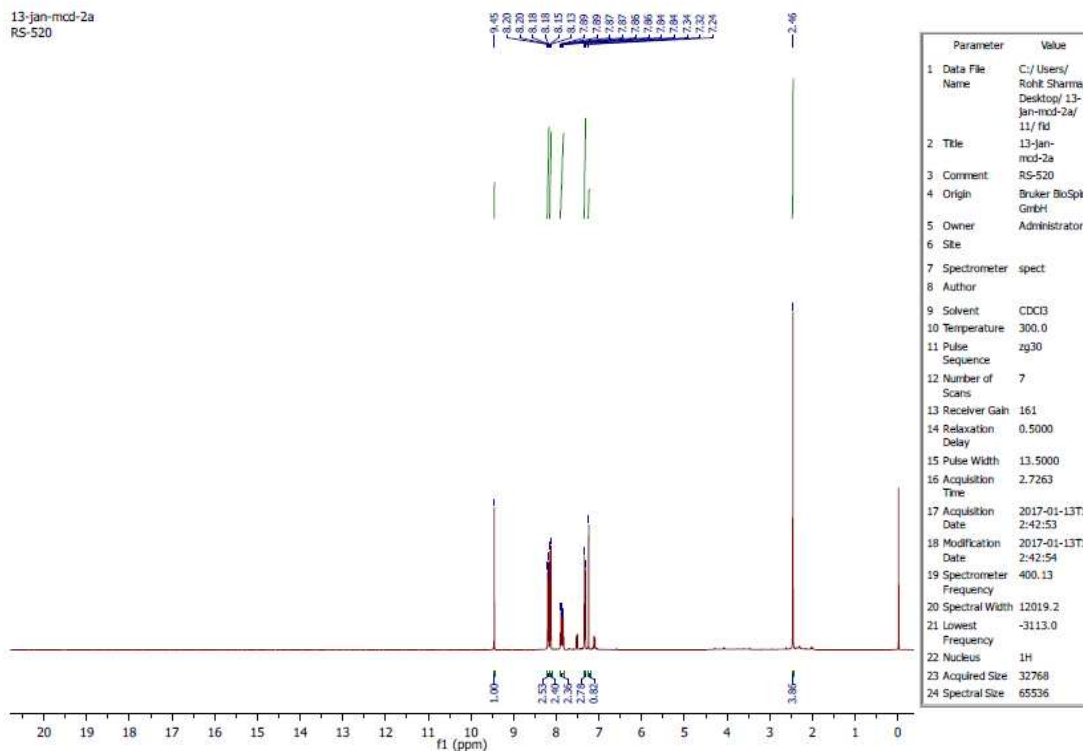


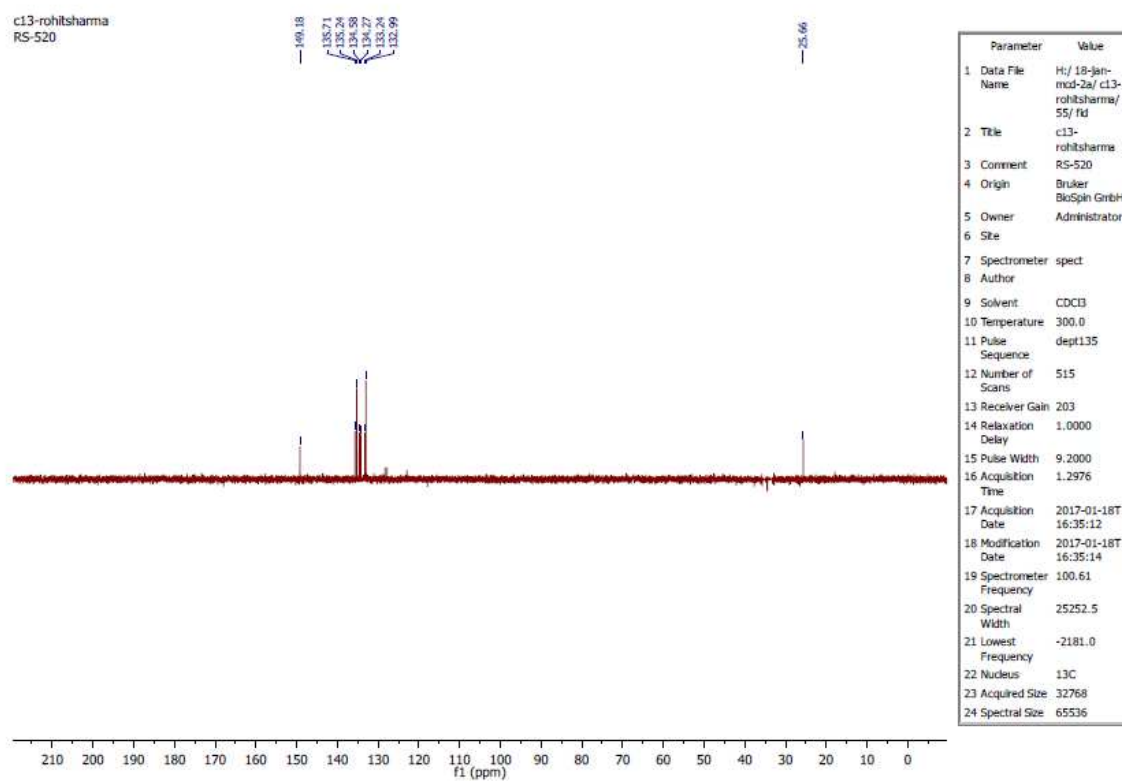
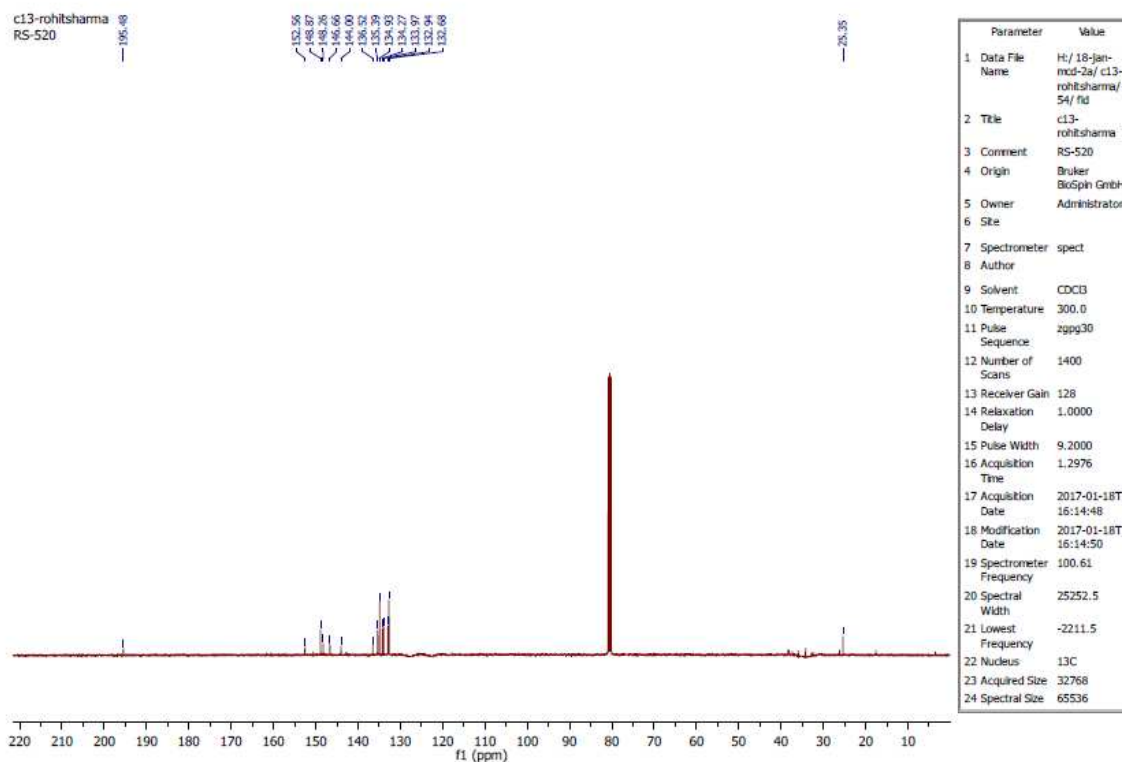
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RS-521



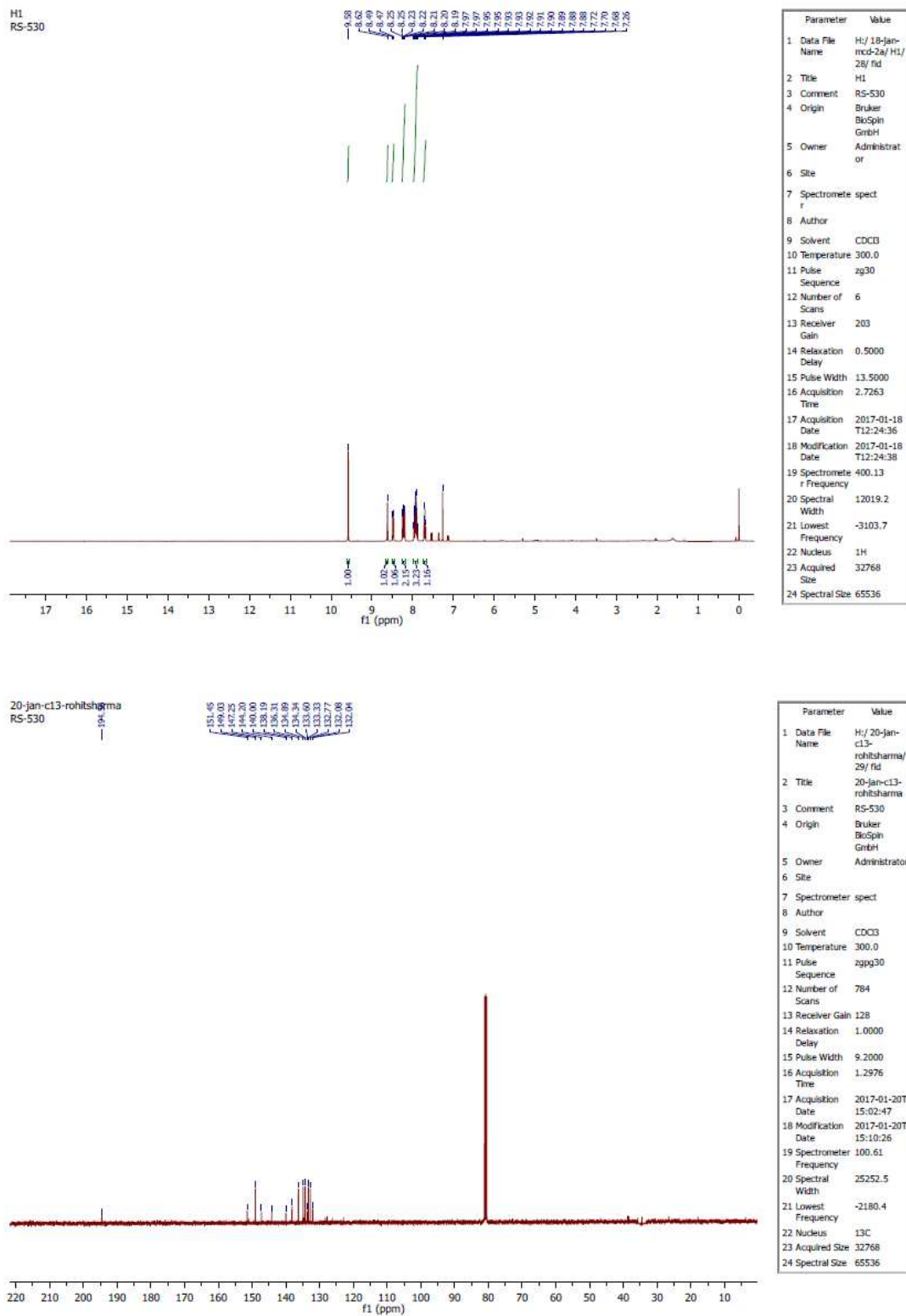
¹H NMR, ¹³C NMR and DEPT135 spectra of quinoxalin-2-yl(p-tolyl)methanone (1g).

13-jan-mcd-2a
RS-520

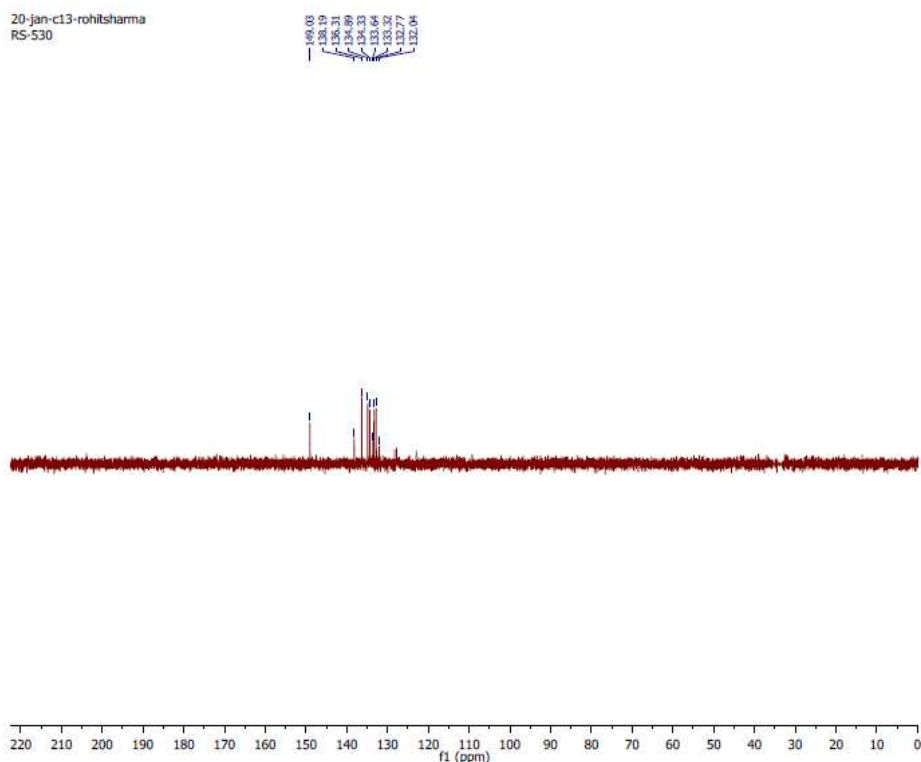




^1H NMR, ^{13}C NMR and DEPT135 spectra of quinoxalin-2-yl(3-(trifluoromethyl)phenyl)methanone (1h).



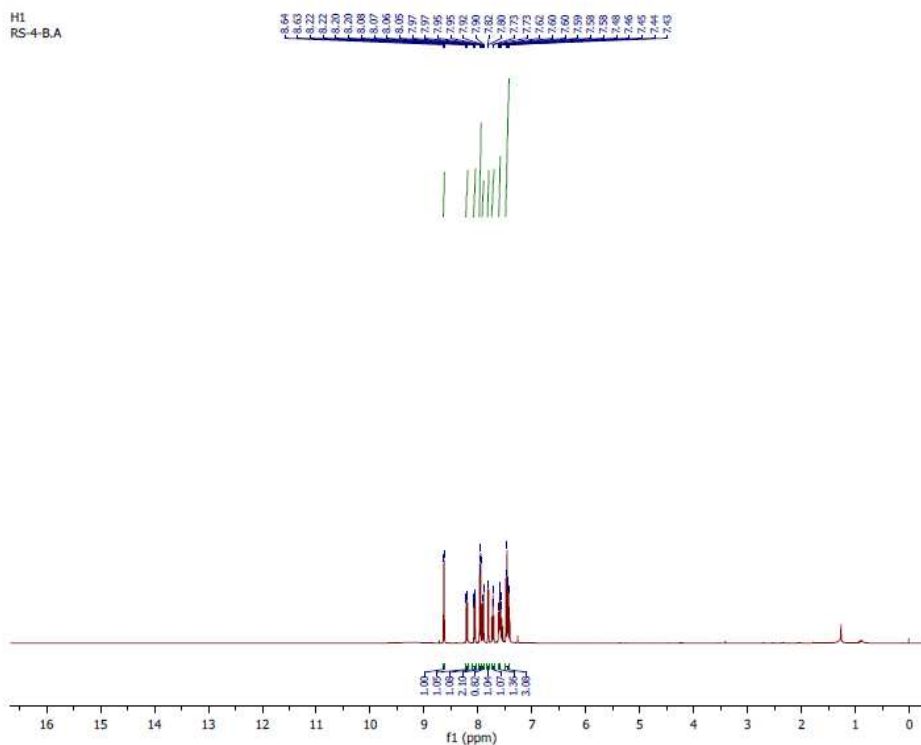
20-jan-c13-rohitsharma
RS-530



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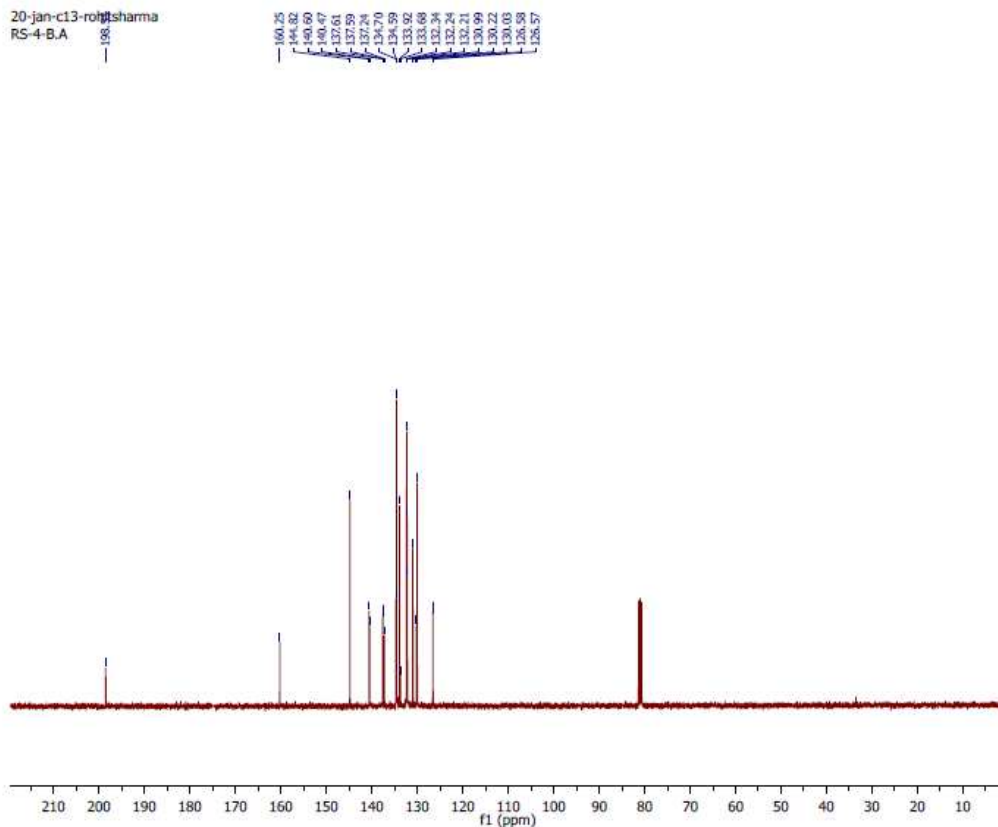
¹H NMR, ¹³C NMR and DEPT135 spectra of isoquinolin-1-yl(phenyl)methanone (5a).

H1
RS-4-B.A



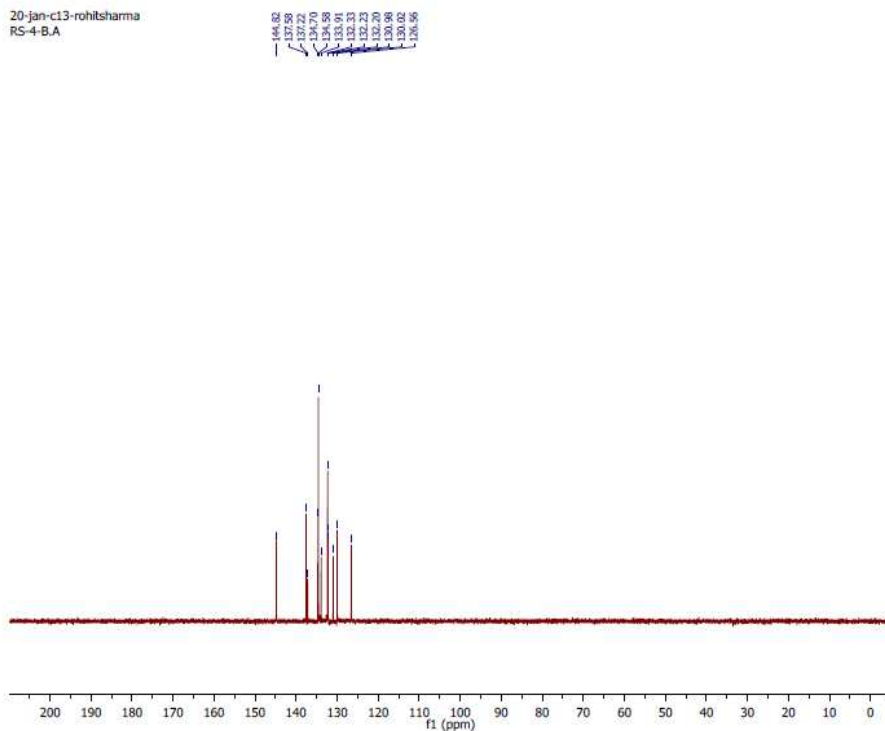
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20-jan-c13-rohitsharma
RS-4-B.A



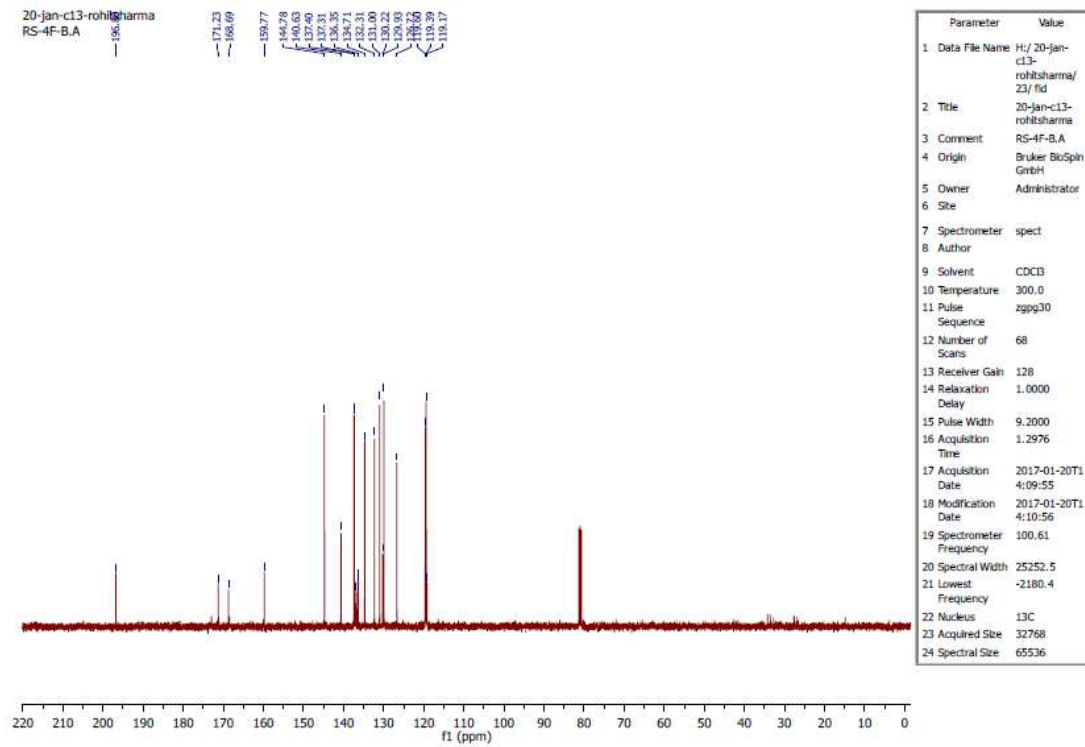
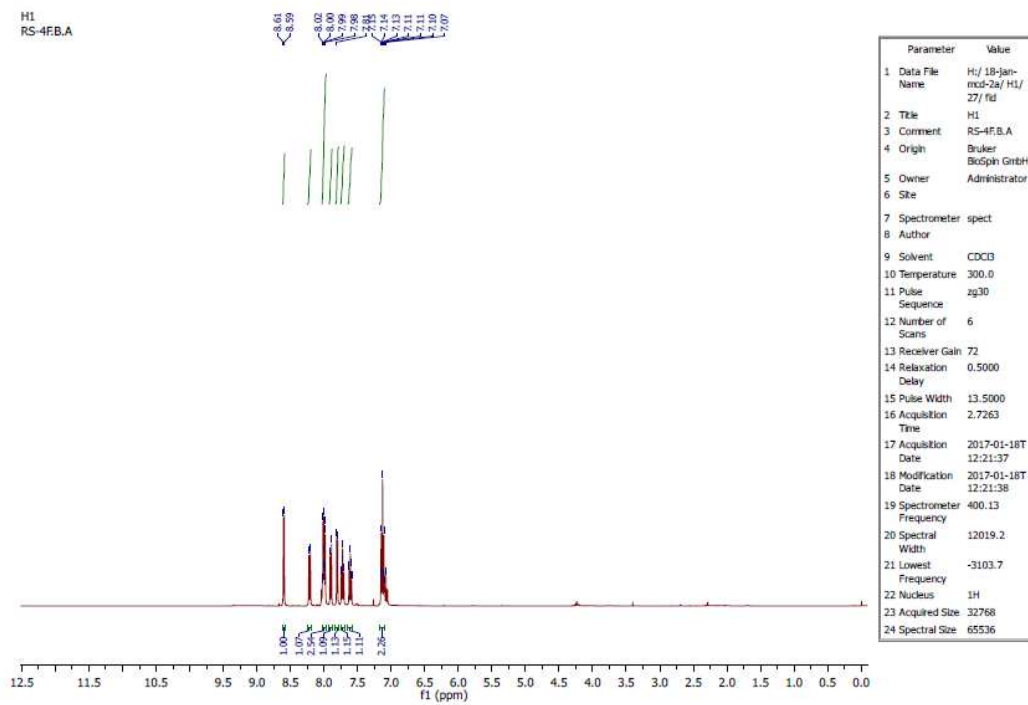
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RS-4-B.A

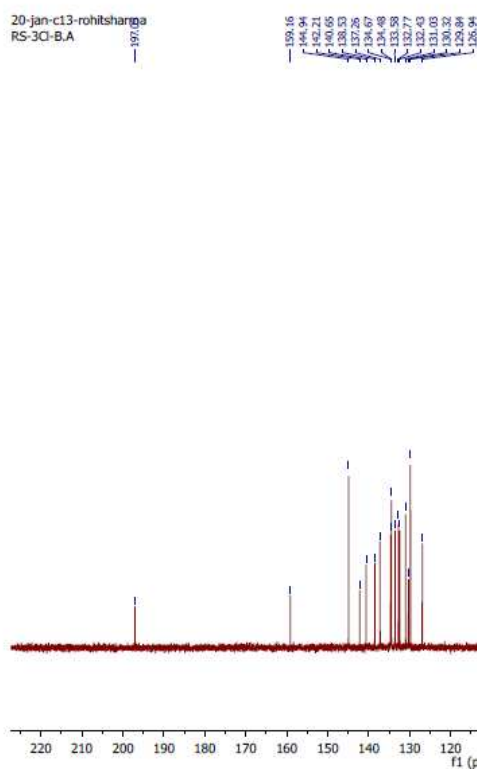


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¹H NMR, ¹³C NMR and DEPT135 spectra of (4-fluorophenyl)(isoquinolin-1-yl)methanone (5b).

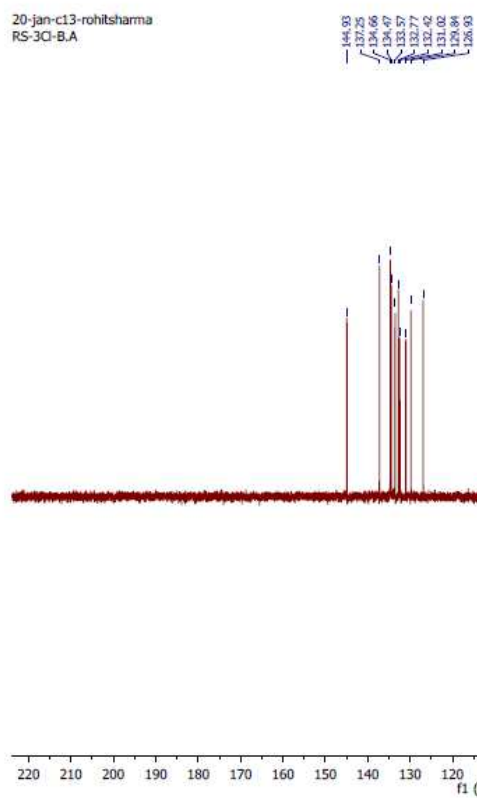


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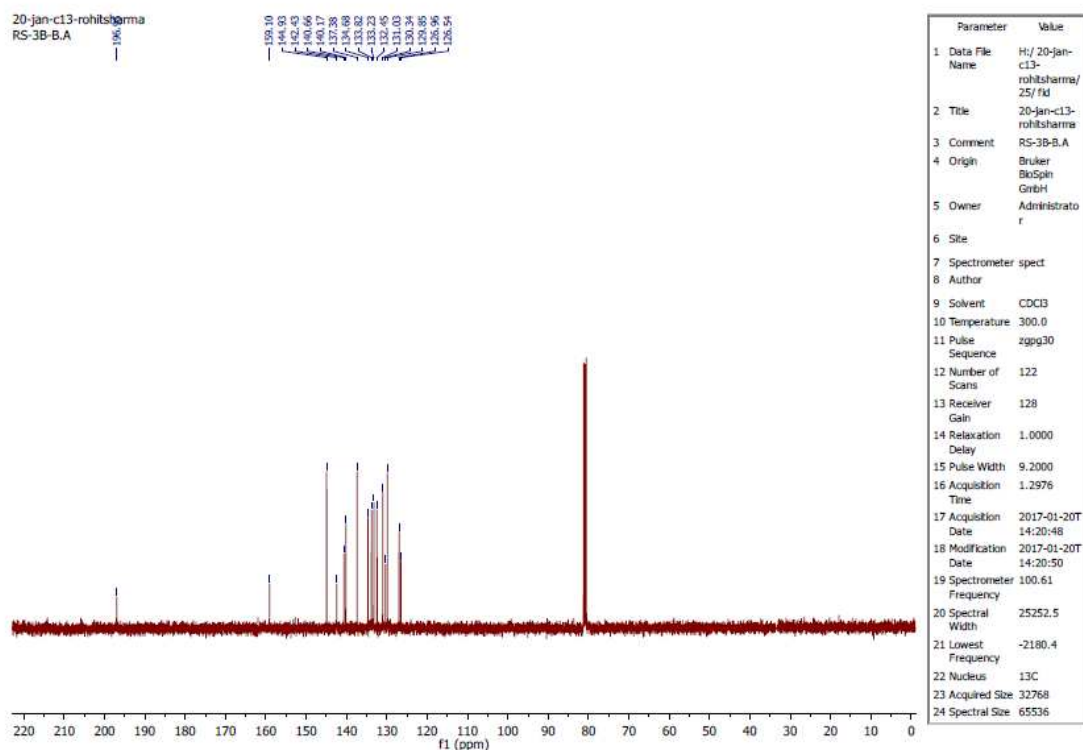
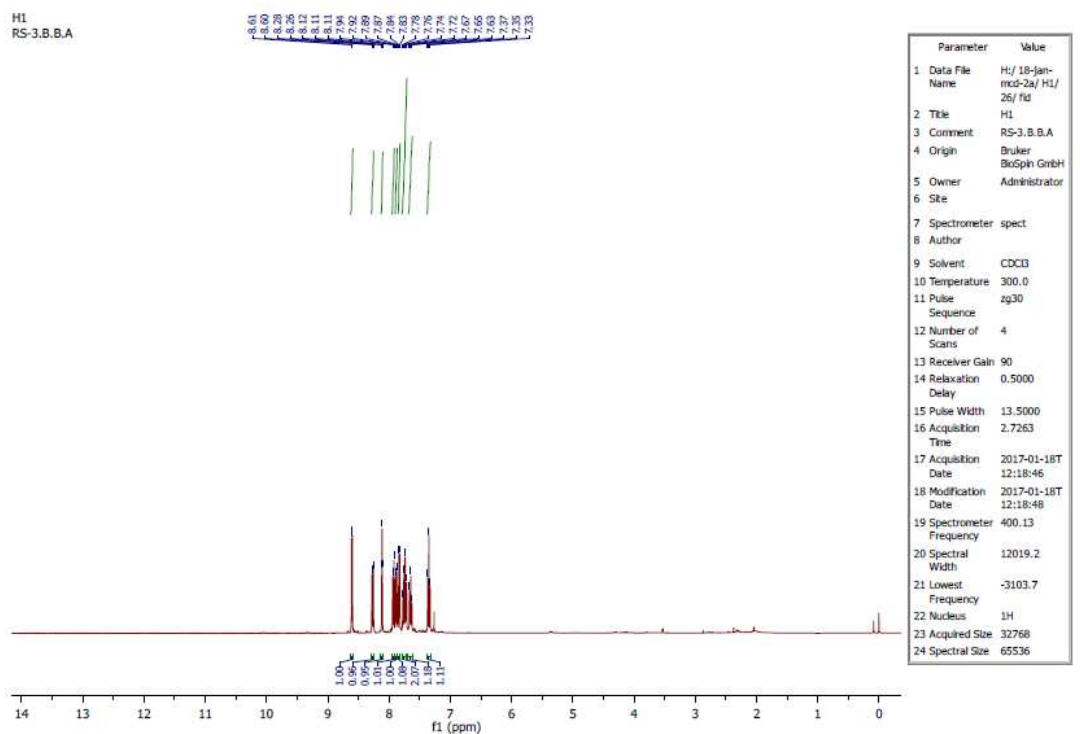
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20-jan-c13-rohitsharma
RS-3CI-B.A



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^1H NMR, ^{13}C NMR and DEPT135 spectra of (3-bromophenyl)(isoquinolin-1-yl)methanone (5d).



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504.507
RS-507

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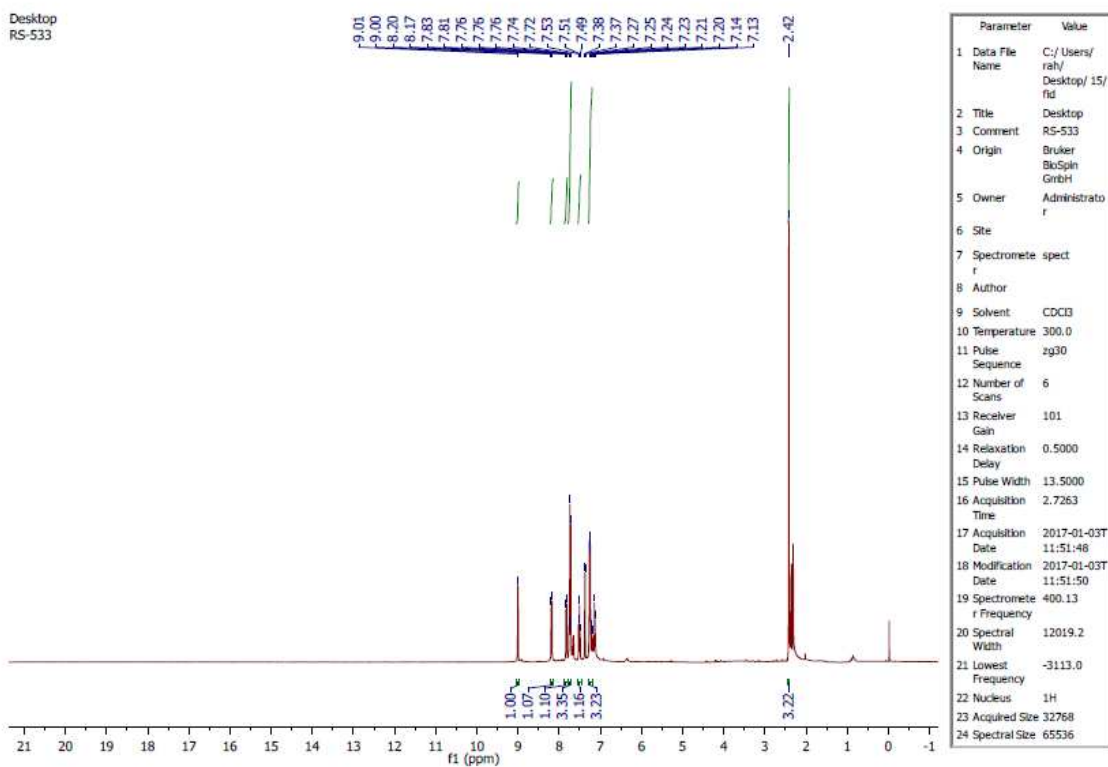
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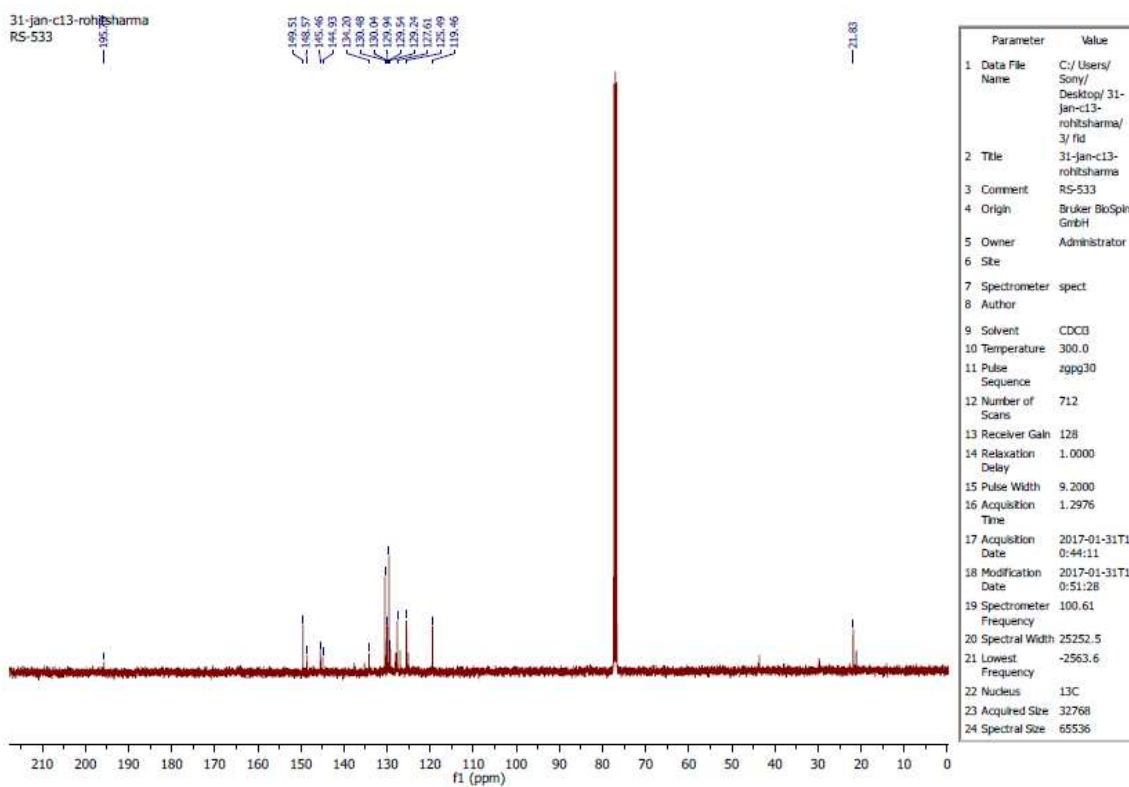
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Page S23

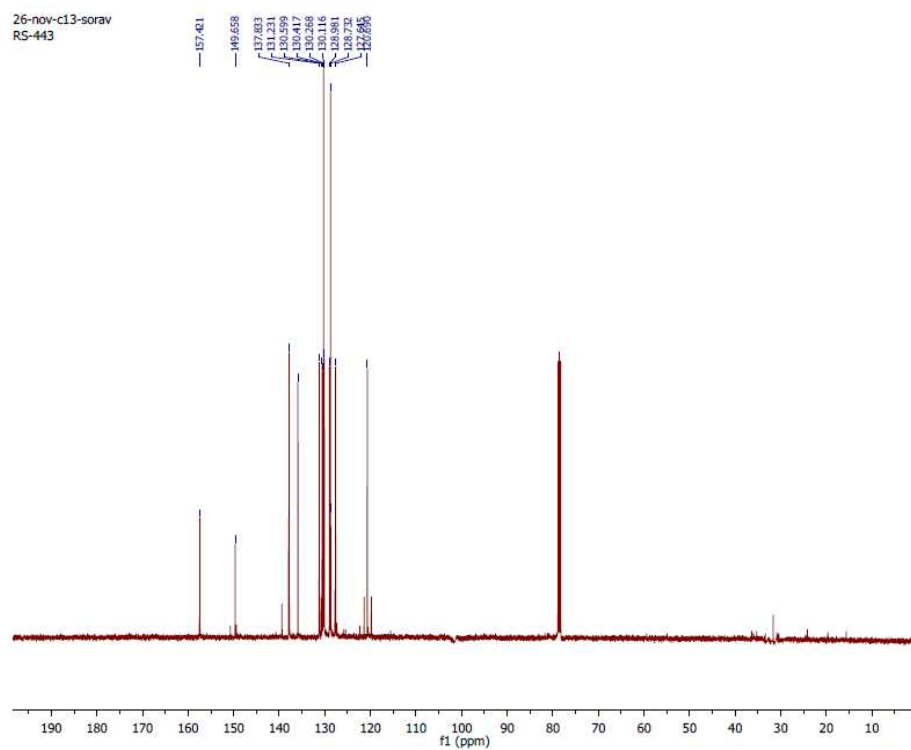
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RS-533



31-jan-c13-rohitsharma
RS-533

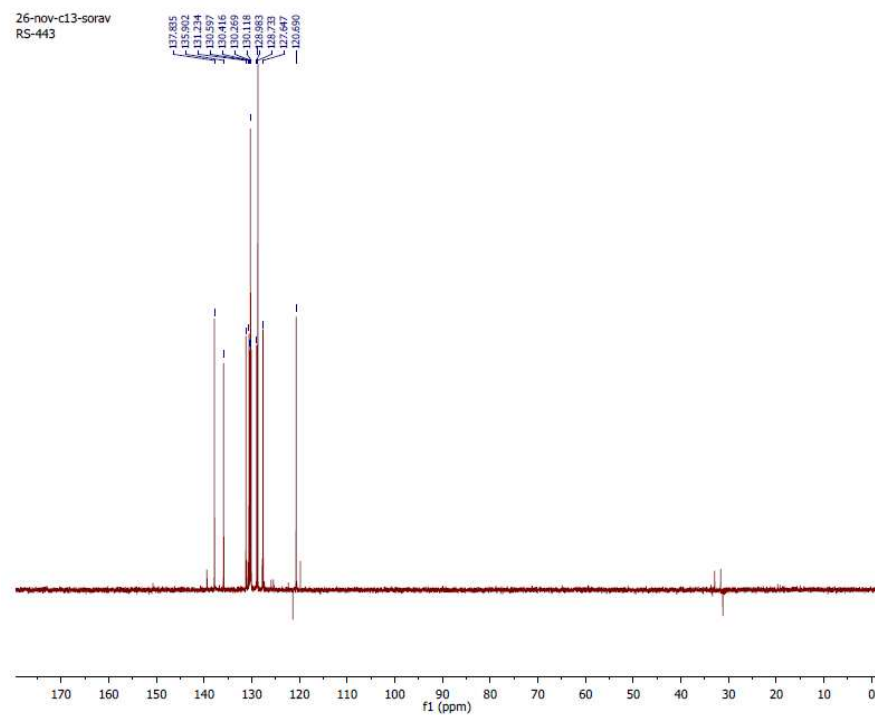


26-nov-c13-sorav
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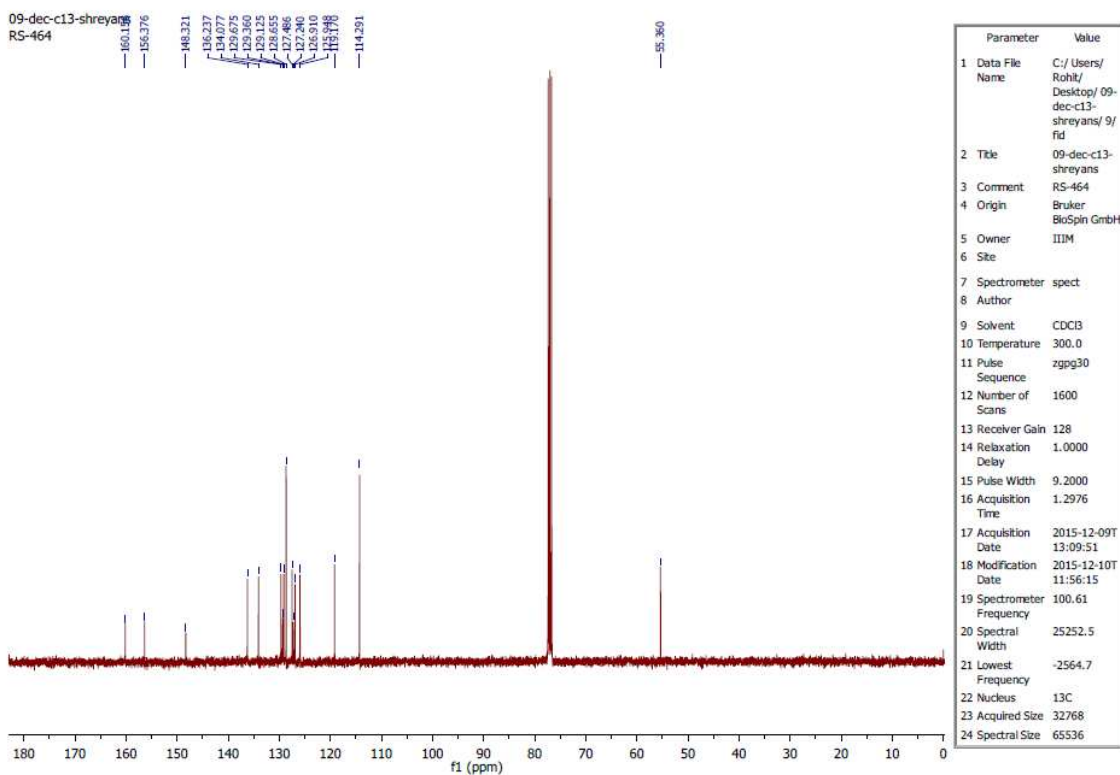
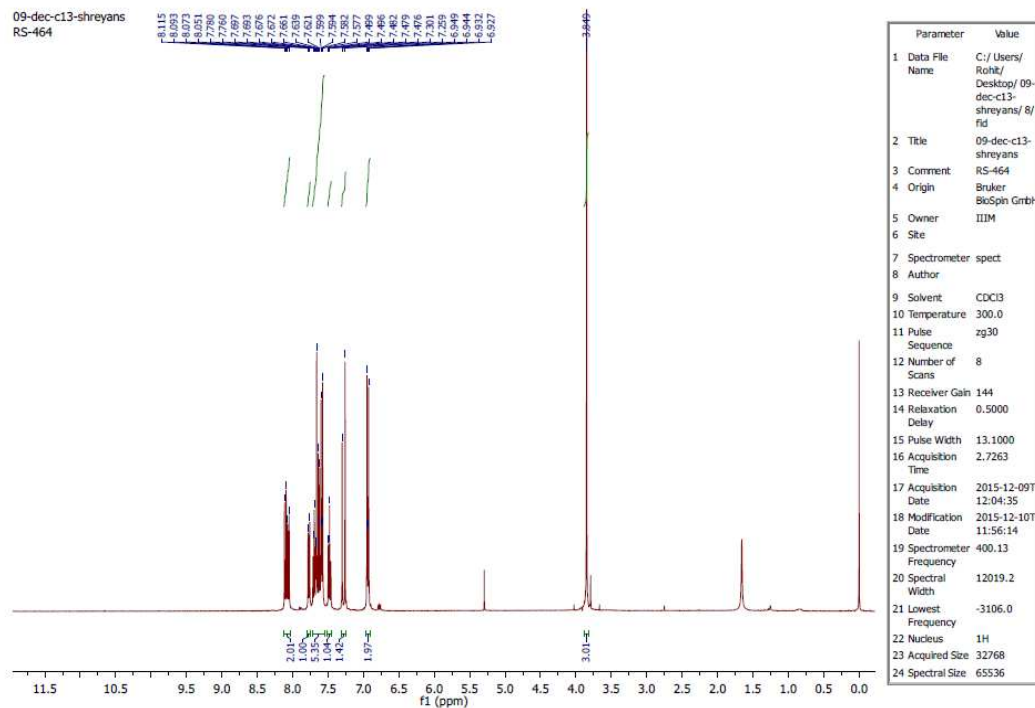
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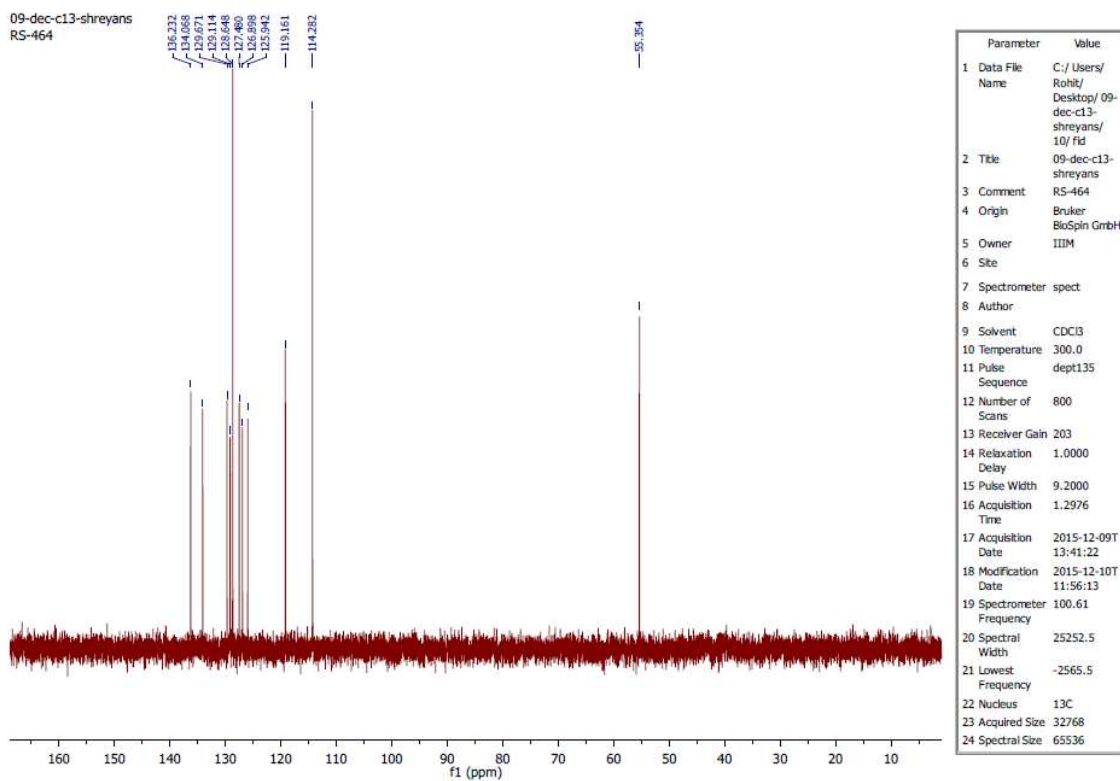
26-nov-c13-sorav
RS-443



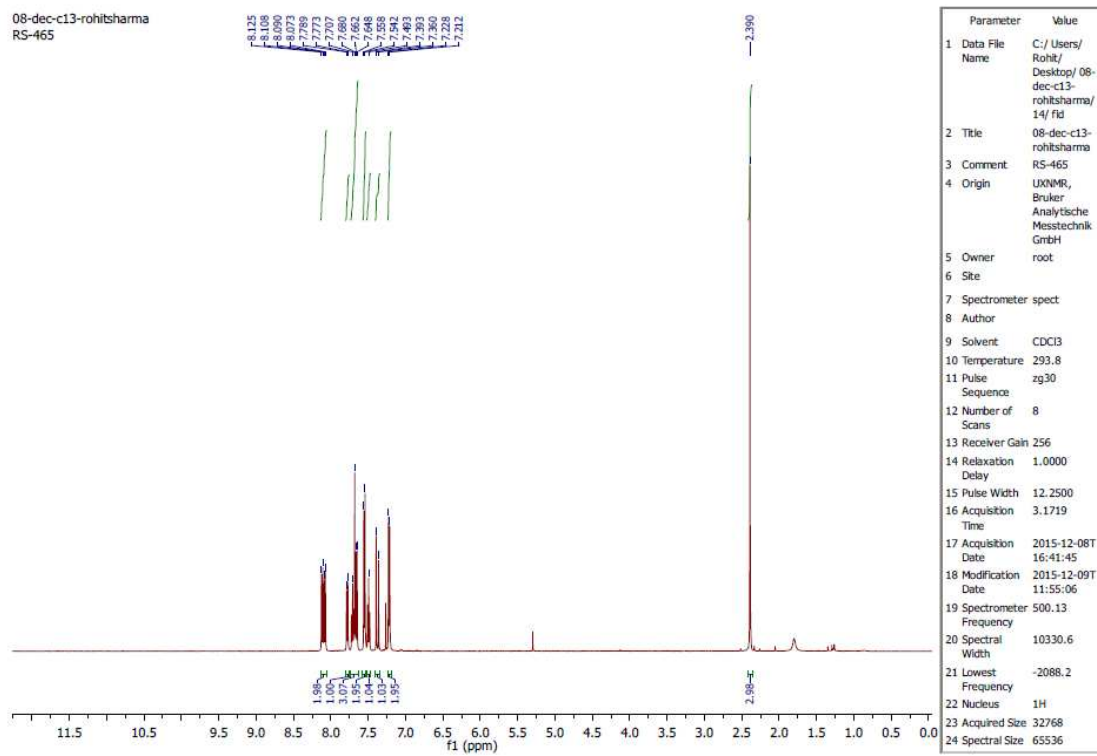
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3 Comment	RS-443
4 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner	root
6 Site	
7 Spectrometer spect	
8 Author	
9 Solvent	CDCl3
10 Temperature	292.6
11 Pulse Sequence	dept135
12 Number of Scans	300
13 Receiver Gain	16384
14 Relaxation Delay	1.0000
15 Pulse Width	8.4500
16 Acquisition Time	1.0420
17 Acquisition Date	2015-11-26T10:55:15
18 Modification Date	2015-12-03T11:03:41
19 Spectrometer Frequency	125.76
20 Spectral Width	31446.5
21 Lowest Frequency	-2969.4
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

^1H , ^{13}C and DEPT135 NMR spectra of (E)-2-(4-methoxystyryl)quinoline (9b).

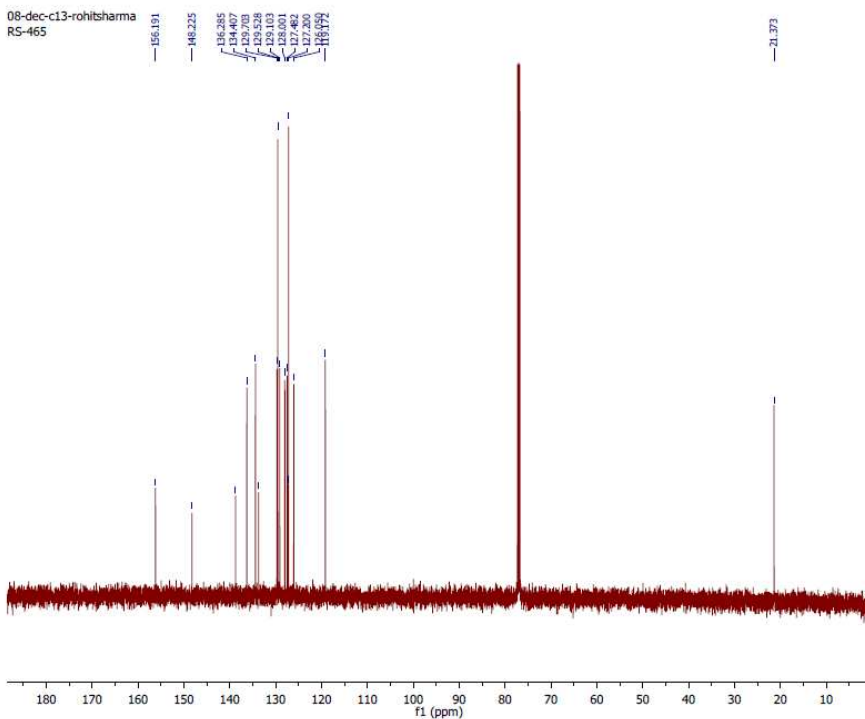




^1H , ^{13}C and DEPT135 NMR spectra of (E)-2-(4-methylstyryl)quinoline (9c).

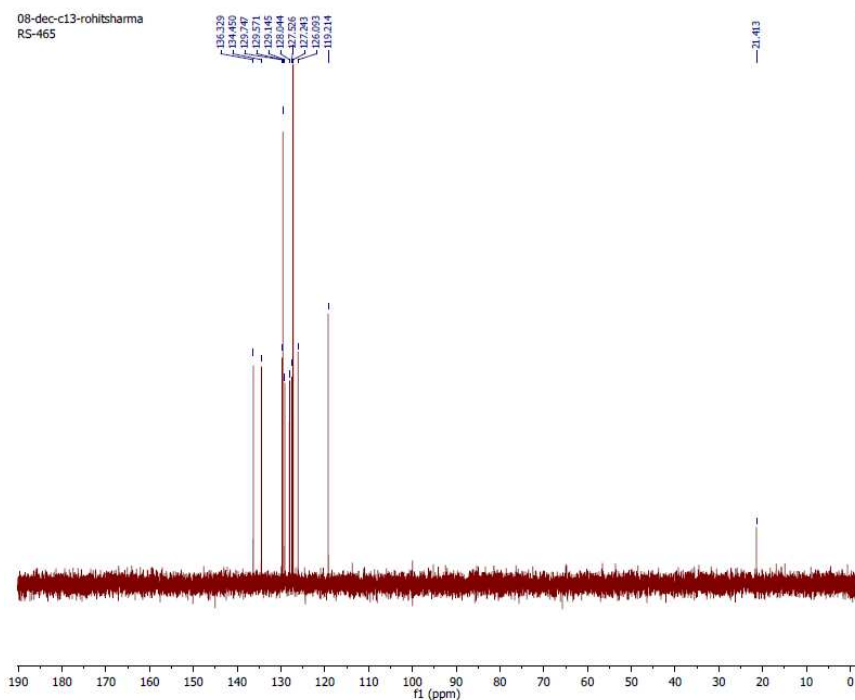


08-dec-c13-rohitsharma
RS-465



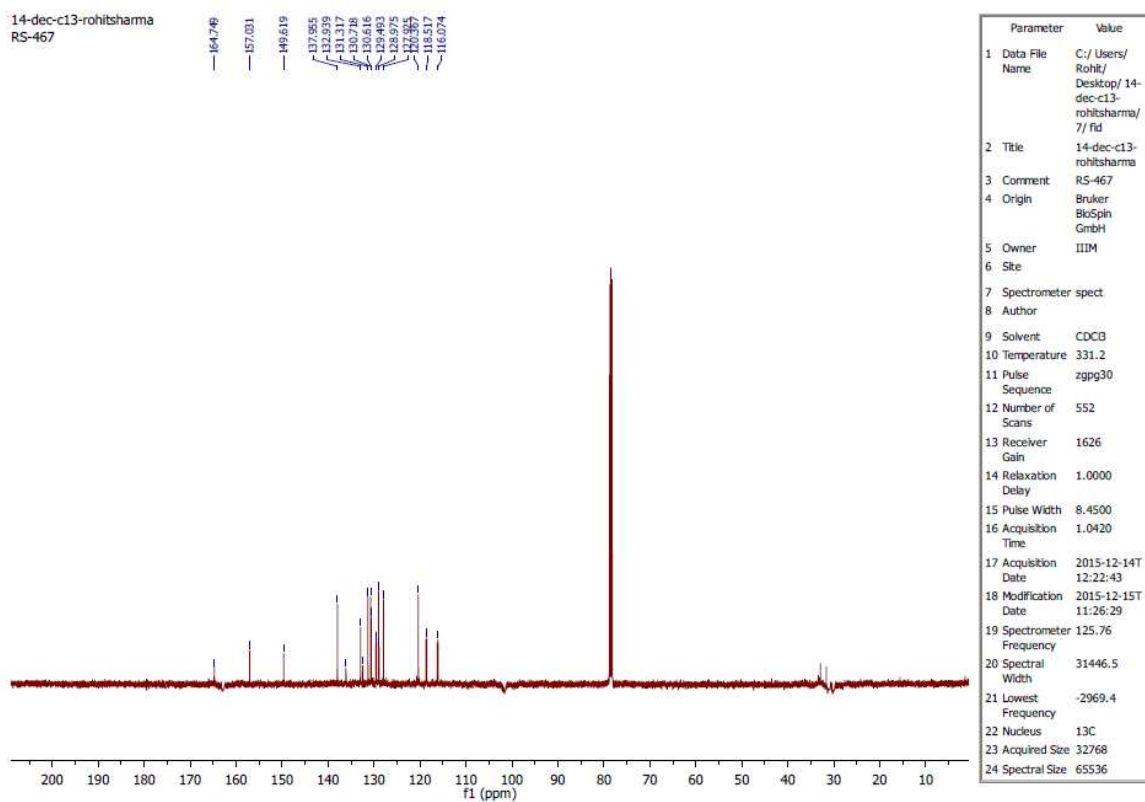
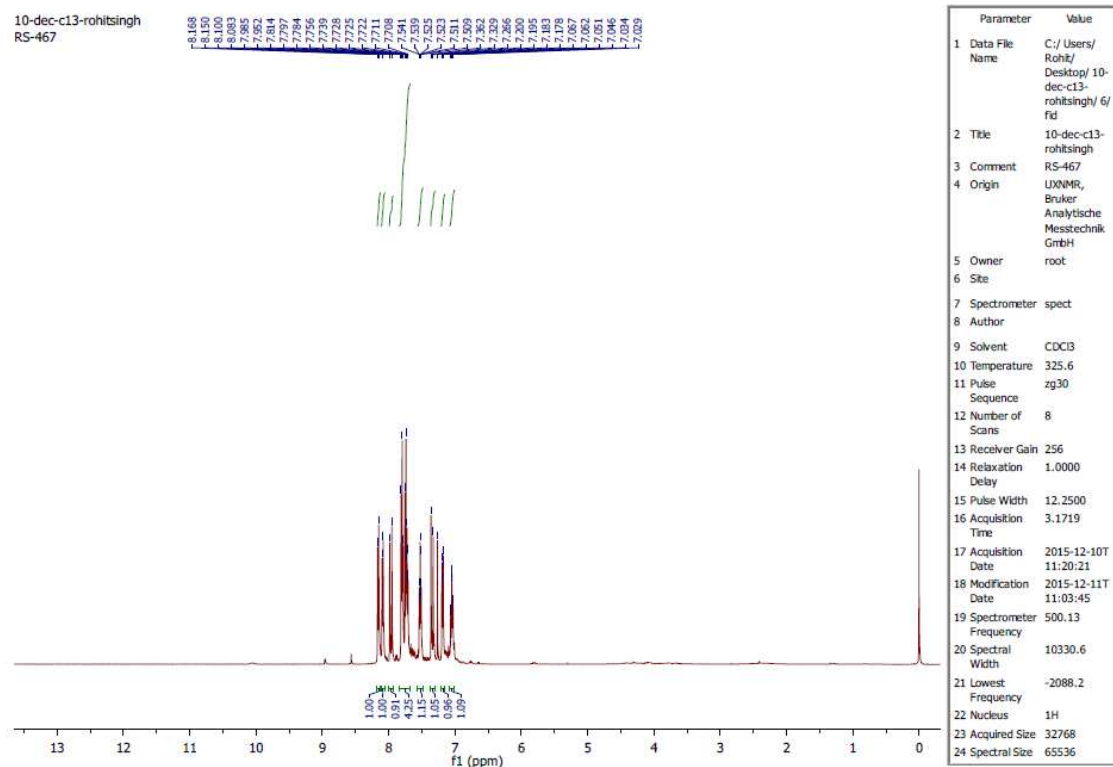
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1 Data File Name	C:/Users/Rohit/Desktop/08-dec-c13-rohitsharma/12/ fid
2 Title	08-dec-c13-rohitsharma
3 Comment	RS-465
4 Origin	Bruker BioSpin GmbH
5 Owner	IIIM
6 Site	
7 Spectrometer spect	
8 Author	
9 Solvent	CDCl3
10 Temperature	294.0
11 Pulse Sequence	zgpg30
12 Number of Scans	195
13 Receiver Gain	1626
14 Relaxation Delay	1.0000
15 Pulse Width	8.4500
16 Acquisition Time	1.0420
17 Acquisition Date	2015-12-08T16:30:48
18 Modification Date	2015-12-09T11:55:04
19 Spectrometer Frequency	125.76
20 Spectral Width	31446.5
21 Lowest Frequency	-3153.3
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

08-dec-c13-rohitsharma
RS-465

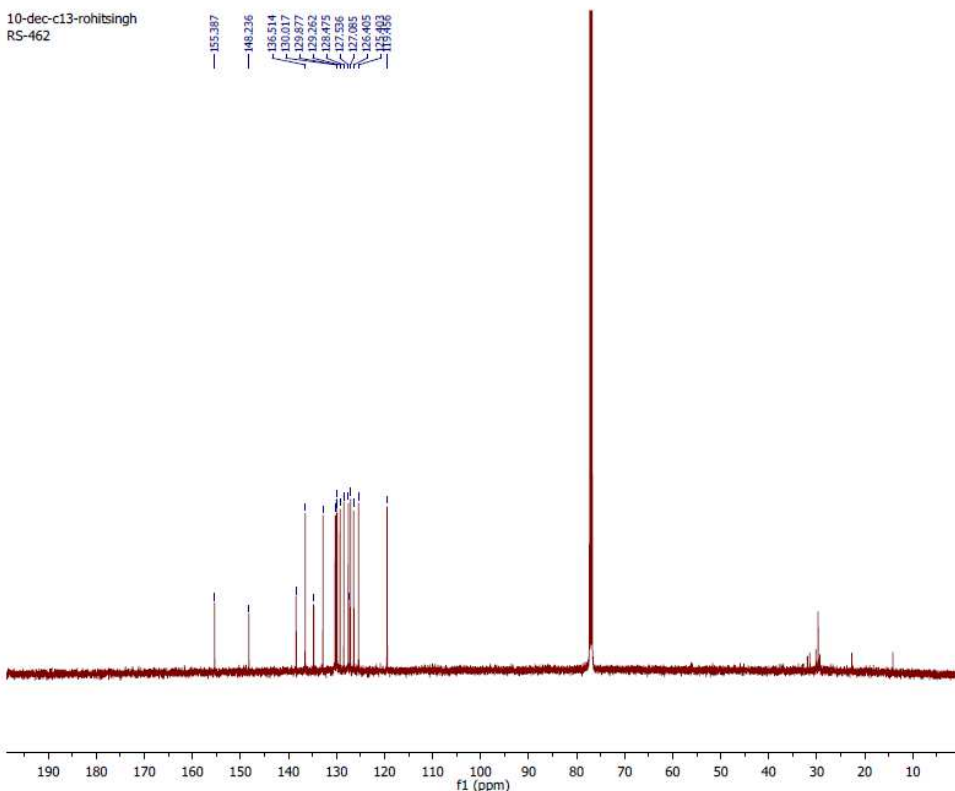


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2 Title	08-dec-c13-rohitsharma
3 Comment	RS-465
4 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner	root
6 Site	
7 Spectrometer spect	
8 Author	
9 Solvent	CDCl3
10 Temperature	294.0
11 Pulse Sequence	dept135
12 Number of Scans	87
13 Receiver Gain	16384
14 Relaxation Delay	1.0000
15 Pulse Width	8.4500
16 Acquisition Time	1.0420
17 Acquisition Date	2015-12-08T16:40:22
18 Modification Date	2015-12-09T11:55:05
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

^1H , ^{13}C and DEPT135 NMR spectra of (E)-2-(2-chloro-4-fluorostyryl)quinoline (9d).

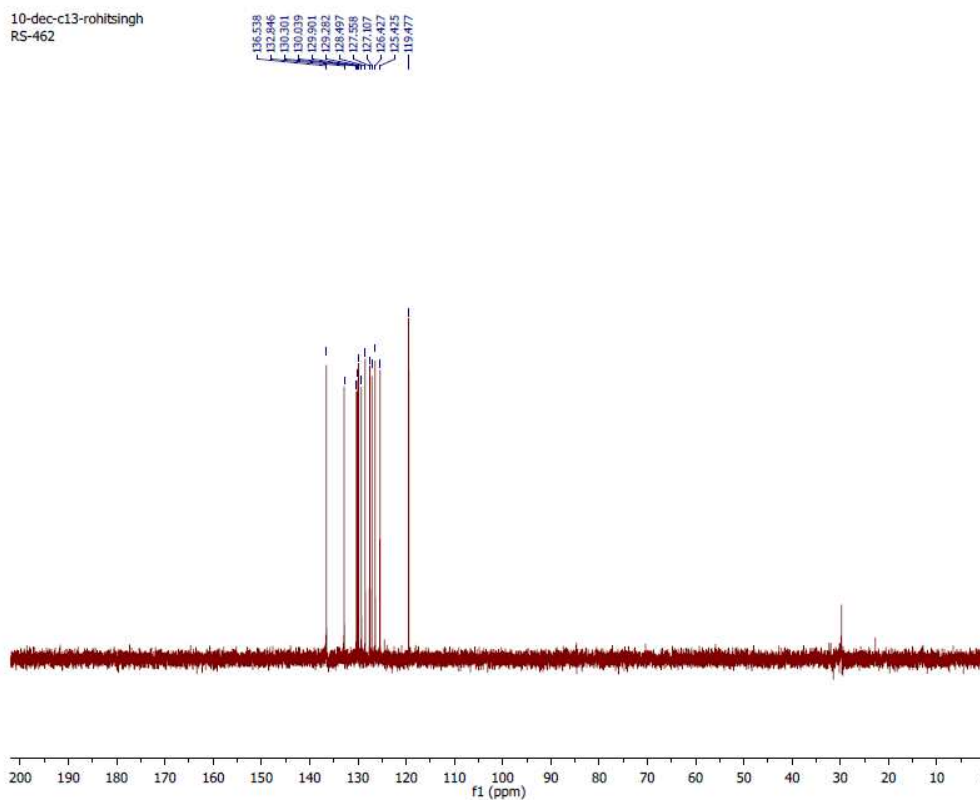


10-dec-c13-rohitsingh
RS-462



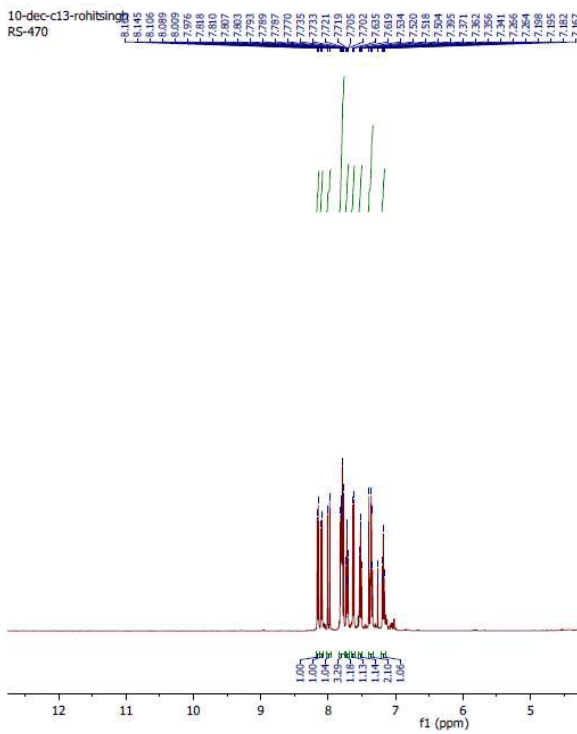
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2 Title	10-dec-c13-rohitsingh
3 Comment	RS-462
4 Origin	Bruker BioSpin GmbH
5 Owner	IIIM
6 Site	
7 Spectrometer spect	
8 Author	
9 Solvent	CDCI3
10 Temperature	326.0
11 Pulse Sequence	zgpg30
12 Number of Scans	1600
13 Receiver Gain	1626
14 Relaxation Delay	1.0000
15 Pulse Width	8.4500
16 Acquisition Time	1.0420
17 Acquisition Date	2015-12-10T12:34:11
18 Modification Date	2015-12-11T11:03:46
19 Spectrometer Frequency	125.76
20 Spectral Width	31446.5
21 Lowest Frequency	-3150.7
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

10-dec-c13-rohitsingh
RS-462

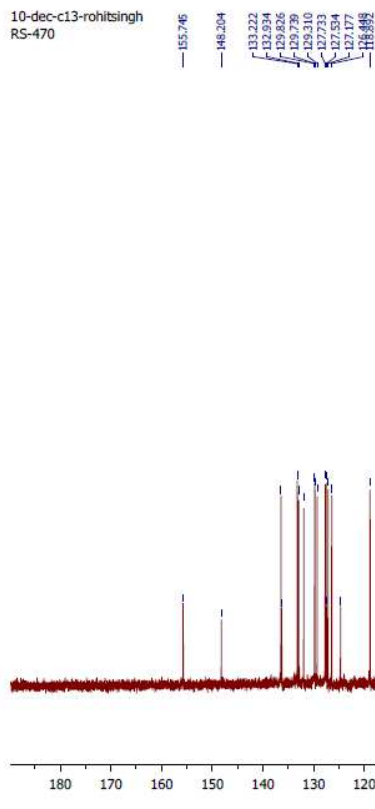


Parameter	Value
1 Data File Name	C:/Users/Rohit/Desktop/10-dec-c13-rohitsingh/10/fid
2 Title	10-dec-c13-rohitsingh
3 Comment	RS-462
4 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner	root
6 Site	
7 Spectrometer spect	
8 Author	
9 Solvent	CDCI3
10 Temperature	325.9
11 Pulse Sequence	dept135
12 Number of Scans	800
13 Receiver Gain	16384
14 Relaxation Delay	1.0000
15 Pulse Width	8.4500
16 Acquisition Time	1.0420
17 Acquisition Date	2015-12-10T13:57:50
18 Modification Date	2015-12-11T11:03:37
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

¹H, ¹³C and DEPT135 NMR spectra of (E)-2-(2-bromostyryl)quinoline (9f).

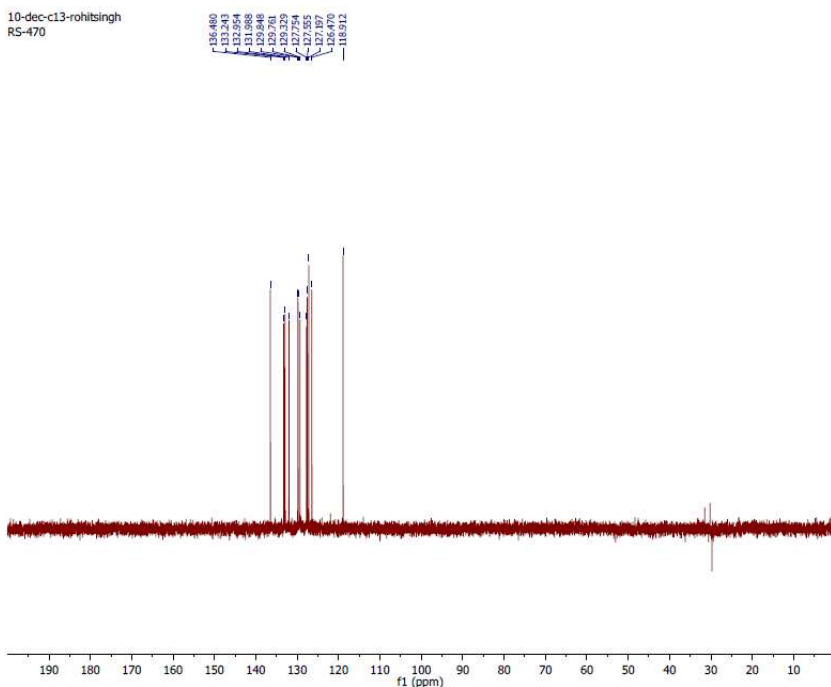


Parameter	Value
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3 Comment	RS-470
4 Origin	UXNMNR, Bruker, Analytische Messtechnik GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	325.4
11 Pulse Sequence	zg30
12 Number of Scans	8
13 Receiver Gain	181
14 Relaxation Delay	1.0000
15 Pulse Width	12.2500
16 Acquisition Time	3.1719
17 Acquisition Date	2015-12-10T15:37:42
18 Modification Date	2015-12-11T11:03:42
19 Spectrometer Frequency	500.13
20 Spectral Width	10330.6
21 Lowest Frequency	-2088.2
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/Users/Rohit/Desktop/10-dec-c13-rohitisinh/16/ f1d
2 Title	10-dec-c13 rohitisinh
3 Comment	RS-470
4 Origin	Bruker BioSpin GmbH
5 Owner	IIIM
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	326.6
11 Pulse Sequence	zgpg30
12 Number of Scans	434
13 Receiver Gain	1626
14 Relaxation Delay	1.0000
15 Pulse Width	8.4500
16 Acquisition Time	1.0420
17 Acquisition Date	2015-12-10T15:27:14
18 Modification Date	2015-12-11T1:03:40
19 Spectrometer Frequency	125.76
20 Spectral Width	31446.5
21 Lowest Frequency	-3150.7
22 Nucleus	¹³ C
23 Acquired Size	32768
24 Spectral Size	65536

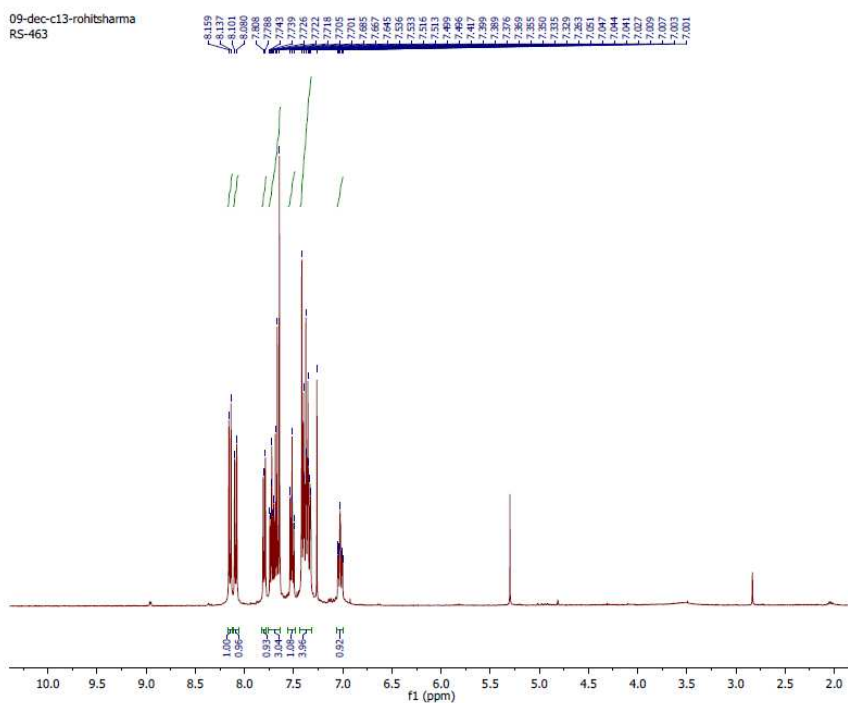
10-dec-c13-rohitsingh
RS-470



Parameter	Value
1 Data File Name	C:/Users/Rohit/Desktop/10-dec-c13-rohitsingh/17/fid
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3 Comment	RS-470
4 Origin	UNMR, Bruker Analytische Messtechnik GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	326.1
11 Pulse Sequence	dept135
12 Number of Scans	220
13 Receiver Gain	16384
14 Relaxation Delay	1.0000
15 Pulse Width	8.4500
16 Acquisition Time	1.0420
17 Acquisition Date	2015-12-10T15:35:57
18 Modification Date	2015-12-11T11:03:41
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

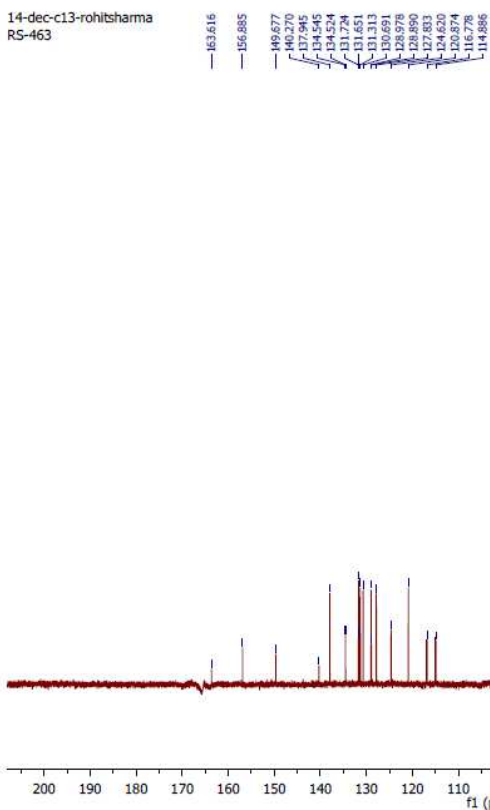
¹H, ¹³C and DEPT135 NMR spectra of (E)-2-(3-fluorostyryl)quinoline (9g).

09-dec-c13-rohitsharma
RS-463



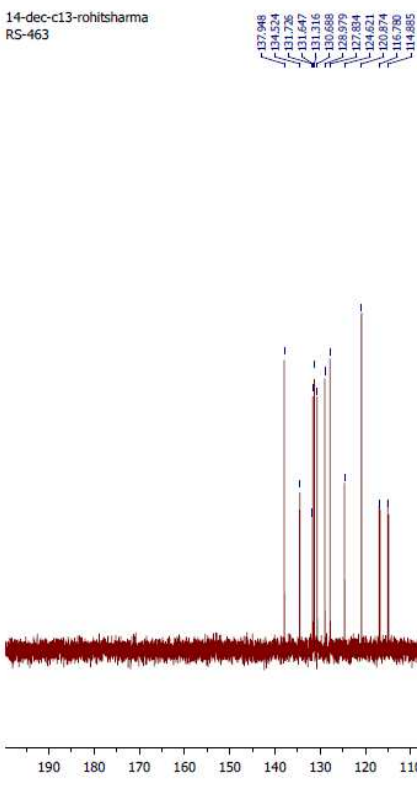
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1 Data File Name	C:/Users/Rohit/Desktop/09-dec-c13-rohitsharma/24/fid
2 Title	09-dec-c13-rohitsharma
3 Comment	RS-463
4 Origin	Bruker BioSpin GmbH
5 Owner	IIIM
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Number of Scans	8
13 Receiver Gain	203
14 Relaxation Delay	0.5000
15 Pulse Width	13.5000
16 Acquisition Time	2.7263
17 Acquisition Date	2015-12-10T08:56:22
18 Modification Date	2015-12-10T11:56:06
19 Spectrometer Frequency	400.13
20 Spectral Width	12019.2
21 Lowest Frequency	-3104.1
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

14-dec-c13-rohitsharma
RS-463



Parameter	Value
1 Data File Name	C:/Users/Rohit/Desktop/14-dec-c13-rohitsharma/11/ f1d
2 Title	14-dec-c13-rohitsharma
3 Comment	RS-463
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5 Owner	IIIM
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	331.0
11 Pulse Sequence	zgpg30
12 Number of Scans	1469
13 Receiver Gain	1626
14 Relaxation Delay	1.0000
15 Pulse Width	8.4500
16 Acquisition Time	1.0420
17 Acquisition Date	2015-12-14T15:01:10
18 Modification Date	2015-12-15T11:26:27
19 Spectrometer Frequency	125.76
20 Spectral Width	31446.5
21 Lowest Frequency	-2969.4
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

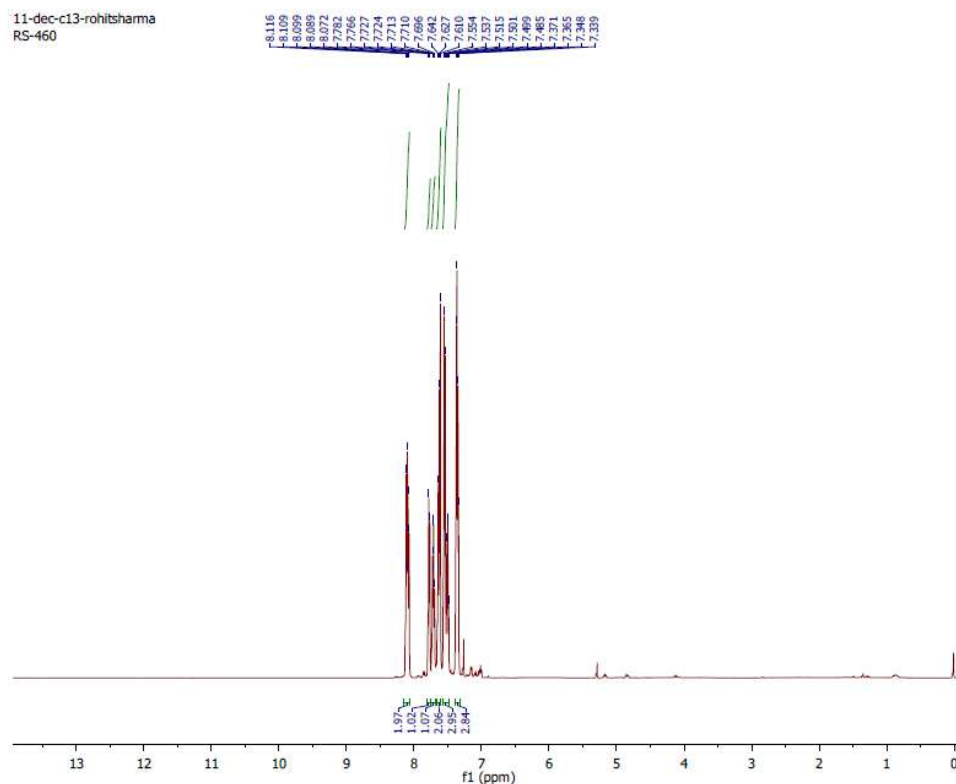
14-dec-c13-rohitsharma
RS-463



Parameter	Value
1 Data File Name	C:/Users/Rohit/Desktop/14-dec-c13-rohitsharma/12/ f1d
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3 Comment	RS-463
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5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	332.0
11 Pulse Sequence	dept135
12 Number of Scans	650
13 Receiver Gain	16384
14 Relaxation Delay	1.0000
15 Pulse Width	8.4500
16 Acquisition Time	1.0420
17 Acquisition Date	2015-12-14T16:14:55
18 Modification Date	2015-12-15T11:26:27
19 Spectrometer Frequency	125.76
20 Spectral Width	31446.5
21 Lowest Frequency	-2969.4
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

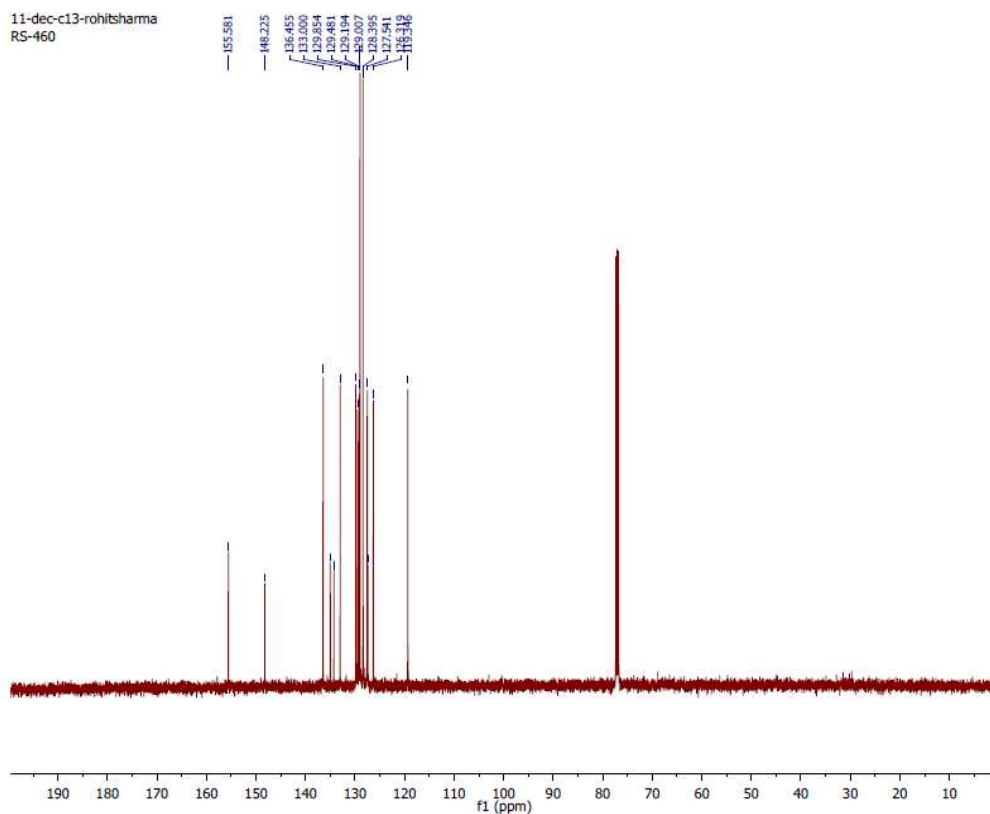
¹H, ¹³C and DEPT135 NMR spectra of (E)-2-(4-chlorostyryl)quinoline (9i).

11-dec-c13-rohitsharma
RS-460

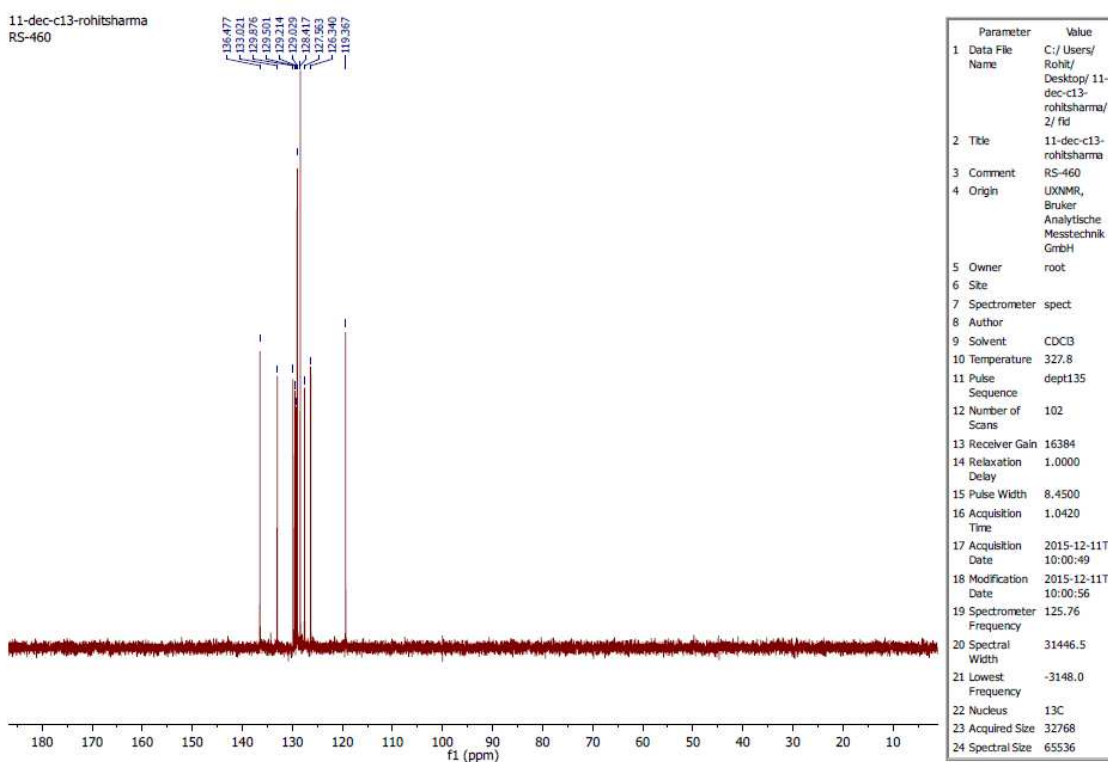


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3 Comment	RS-460
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5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCB
10 Temperature	328.2
11 Pulse Sequence	zg30
12 Number of Scans	8
13 Receiver Gain	144
14 Relaxation Delay	1.0000
15 Pulse Width	12.2500
16 Acquisition Time	3.1719
17 Acquisition Date	2015-12-11T 10:02:24
18 Modification Date	2015-12-11T 10:02:30
19 Spectrometer Frequency	500.13
20 Spectral Width	10330.6
21 Lowest Frequency	-2088.2
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

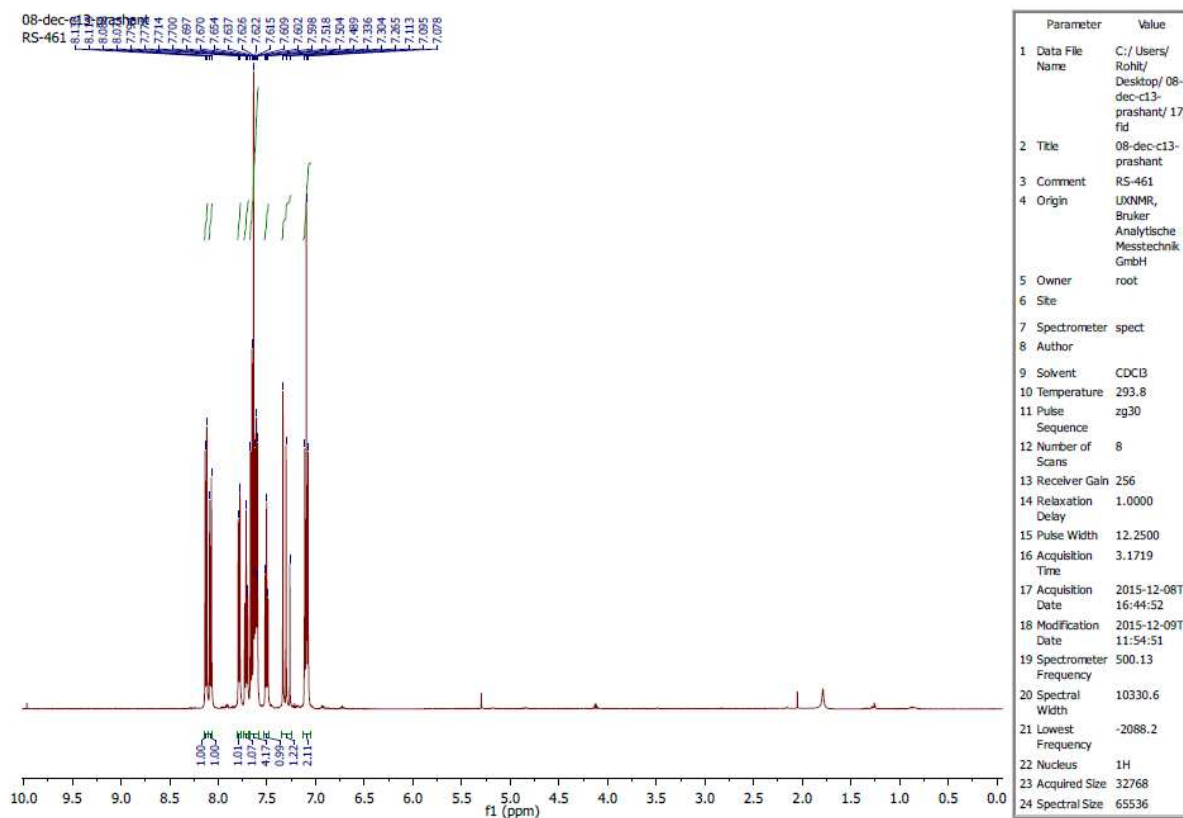
11-dec-c13-rohitsharma
RS-460

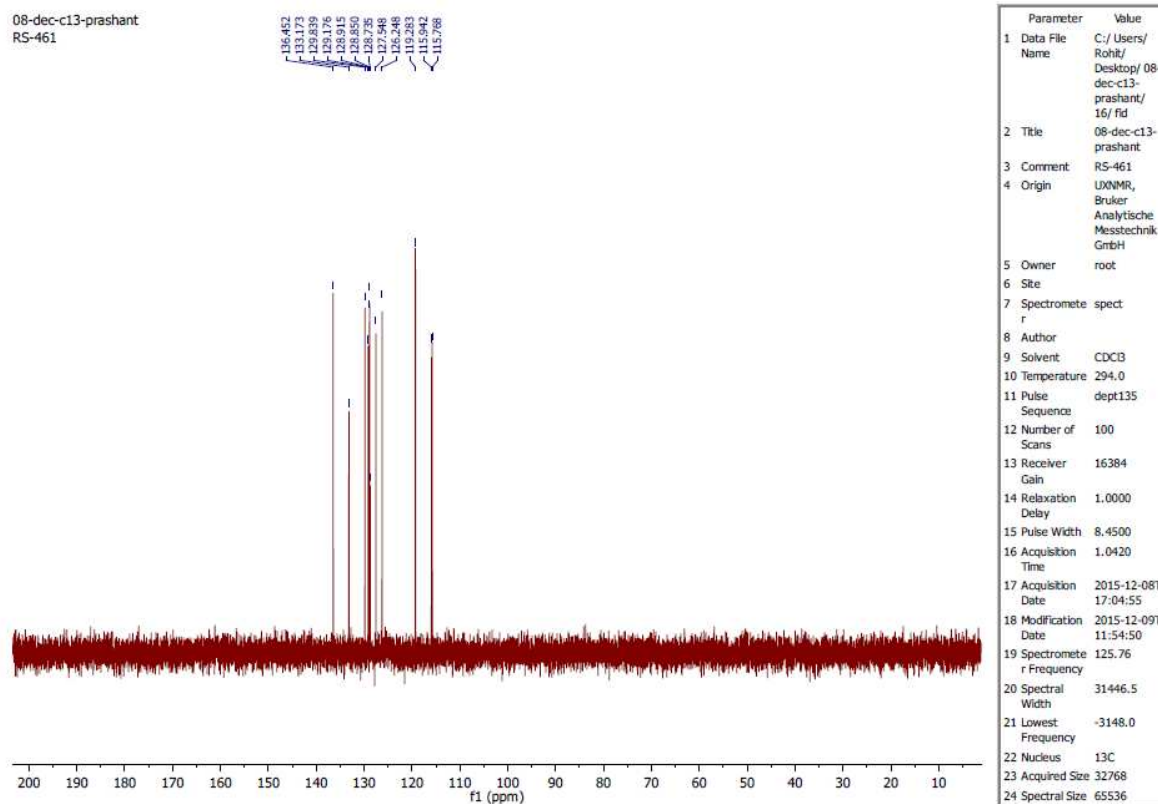
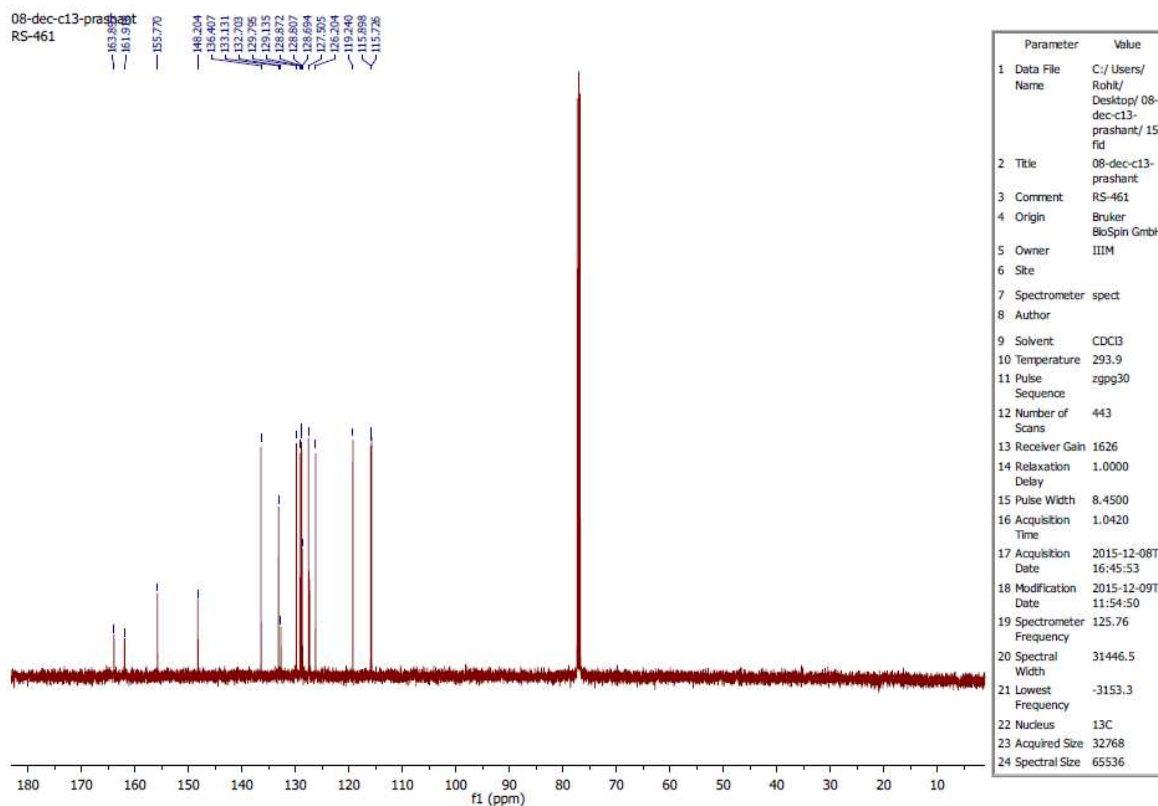


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3 Comment	RS-460
4 Origin	Bruker BioSpin GmbH
5 Owner	IIIM
6 Site	
7 Spectrometer spect	
8 Author	
9 Solvent	CDCB
10 Temperature	325.8
11 Pulse Sequence	zgpg30
12 Number of Scans	282
13 Receiver Gain	1626
14 Relaxation Delay	1.0000
15 Pulse Width	8.4500
16 Acquisition Time	1.0420
17 Acquisition Date	2015-12-11T 09:49:22
18 Modification Date	2015-12-11T 09:56:58
19 Spectrometer Frequency	125.76
20 Spectral Width	31446.5
21 Lowest Frequency	-3150.7
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

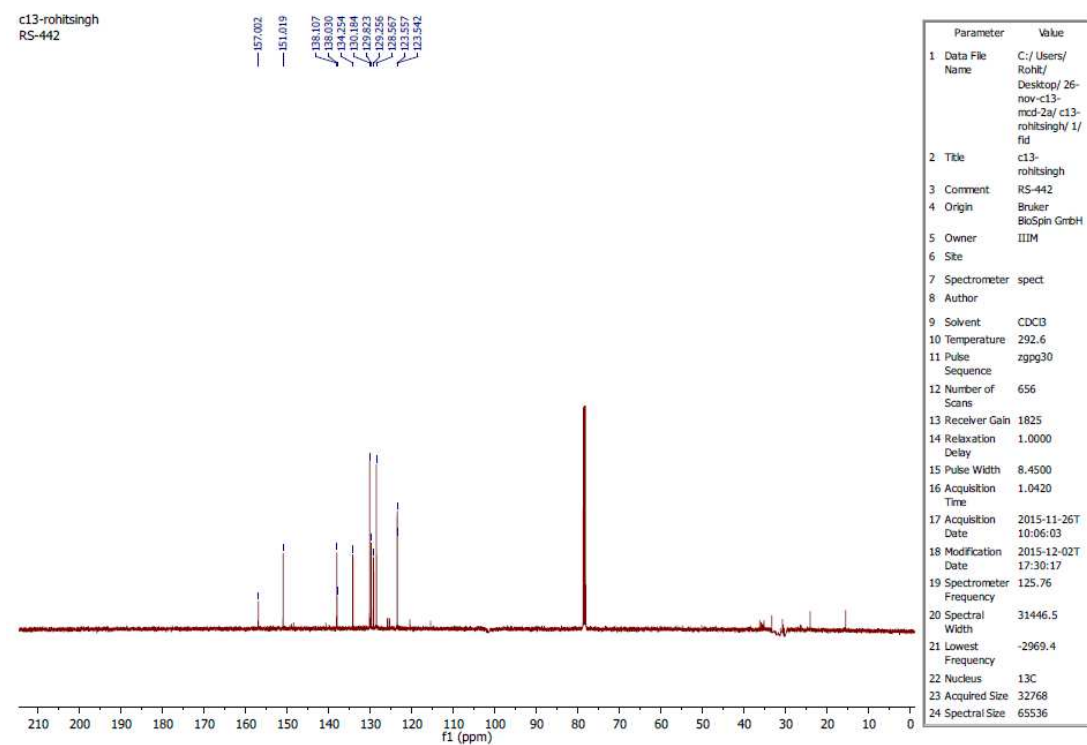
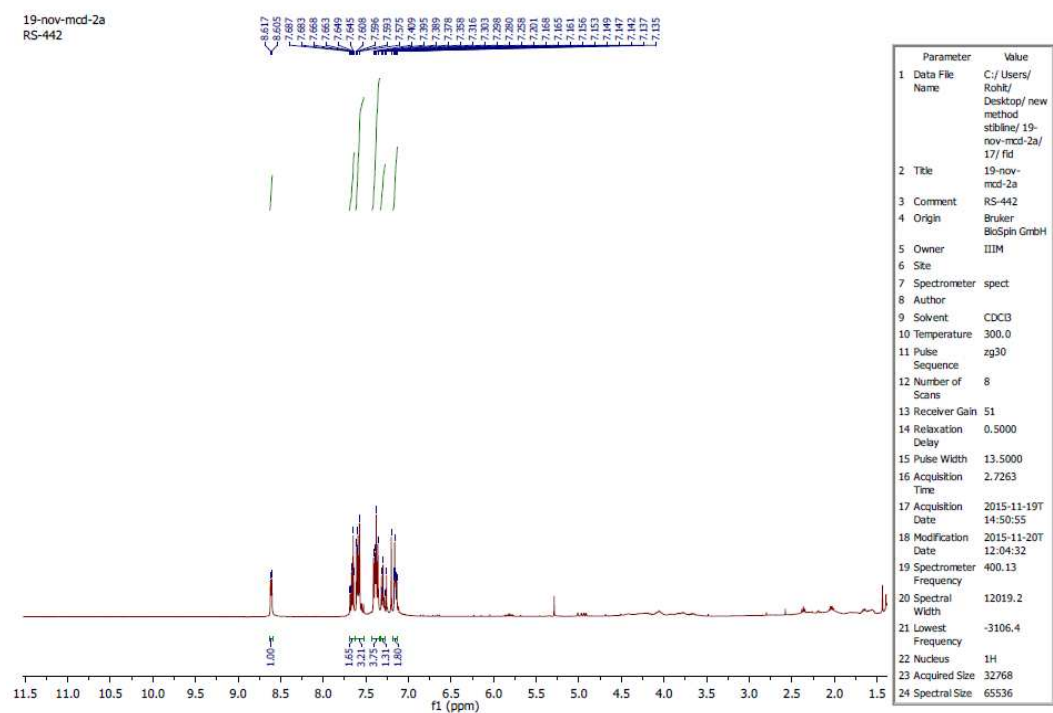


^1H , ^{13}C and DEPT135 NMR spectra of (E)-2-(4-fluorostyryl)quinoline (9i).

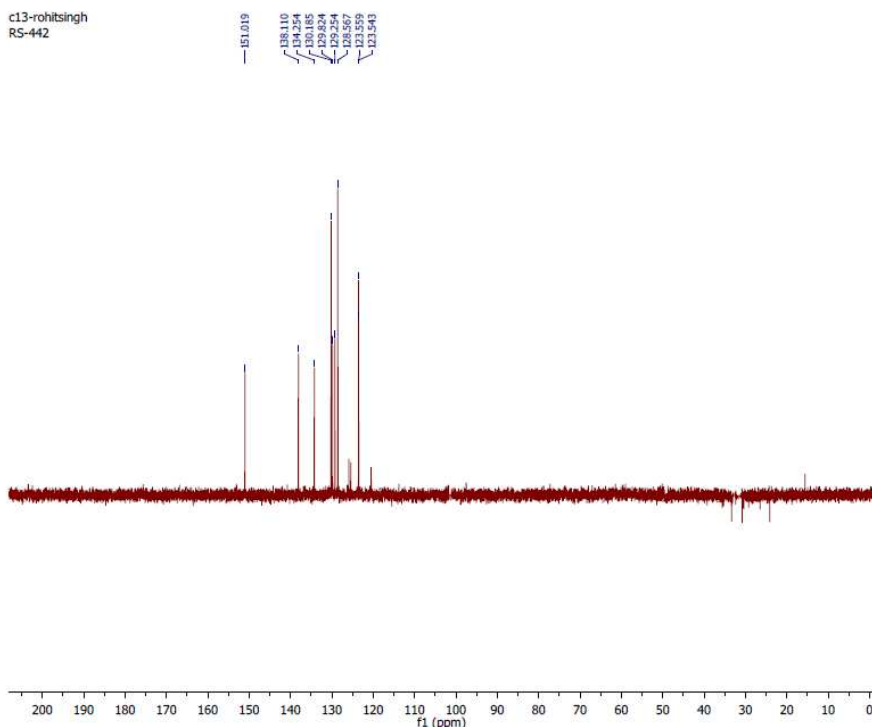




¹H, ¹³C and DEPT135 NMR spectra of (E)-2-styrylpyridine (11a).



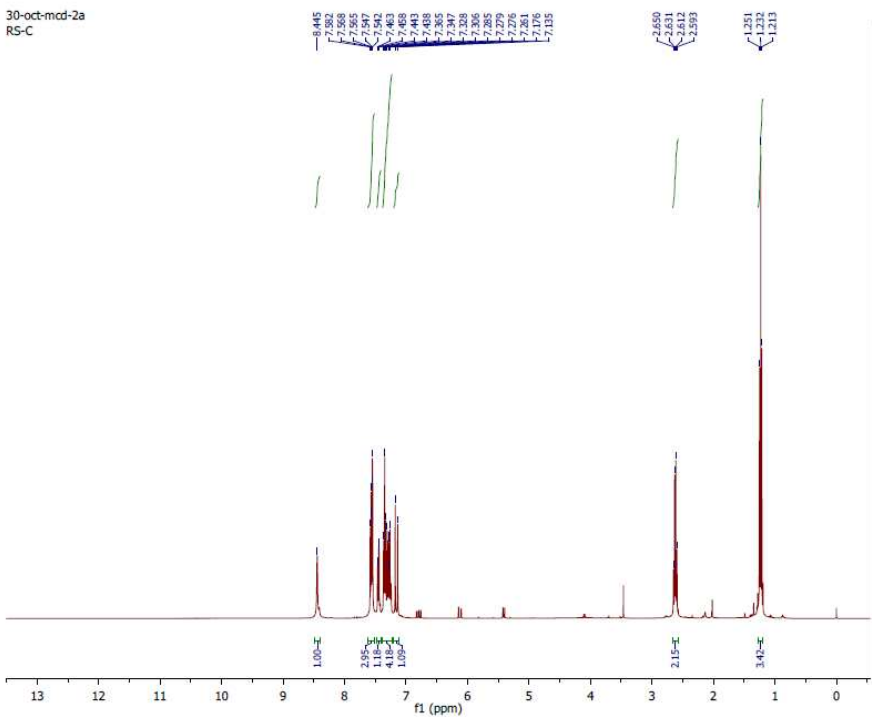
c13-rohitsingh
RS-442



Parameter	Value
1 Data File Name	C:/Users/Rohit/Desktop/26-nov-c13-mcd-2a/c13-rohitsingh/2/fid
2 Title	c13-rohitsingh
3 Comment	RS-442
4 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCB
10 Temperature	292.5
11 Pulse Sequence	dept135
12 Number of Scans	189
13 Receiver Gain	16384
14 Relaxation Delay	1.0000
15 Pulse Width	8.4500
16 Acquisition Time	1.0420
17 Acquisition Date	2015-11-26T10:19:43
18 Modification Date	2015-12-02T17:30:17
19 Spectrometer Frequency	125.76
20 Spectral Width	31446.5
21 Lowest Frequency	-2969.4
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

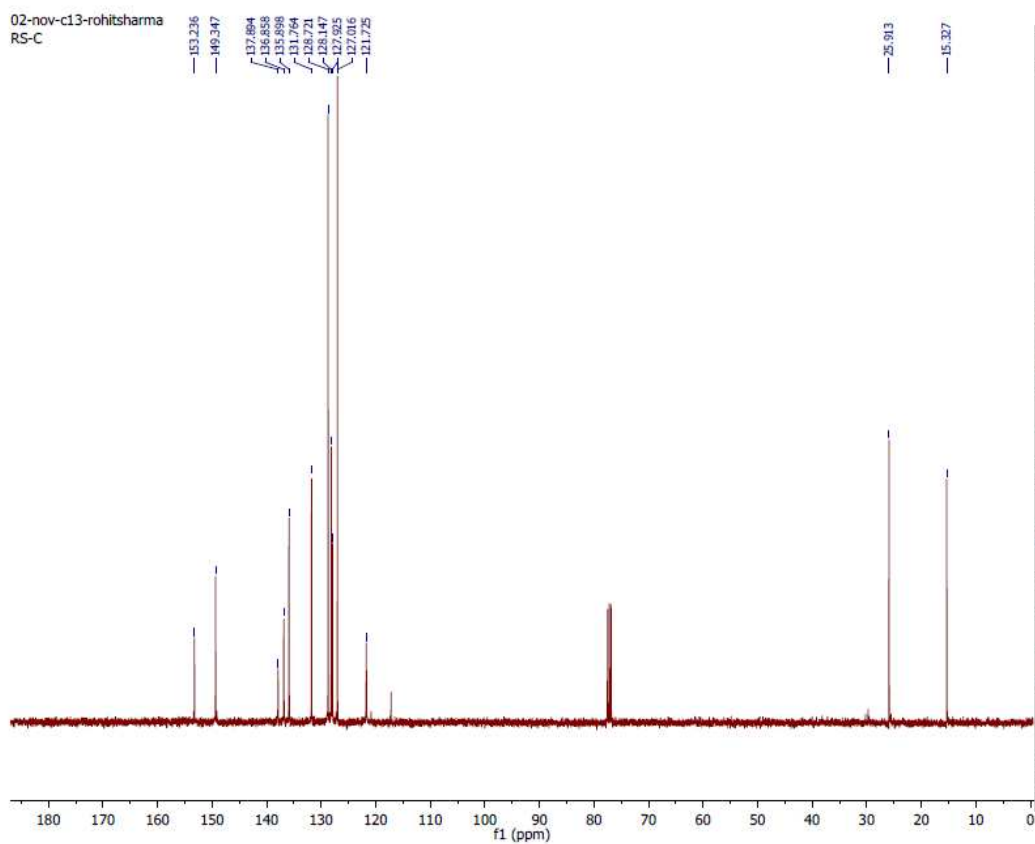
^1H , ^{13}C and DEPT135 NMR spectra of (E)-5-ethyl-2-styrylpyridine (11b).

30-oct-mcd-2a
RS-C



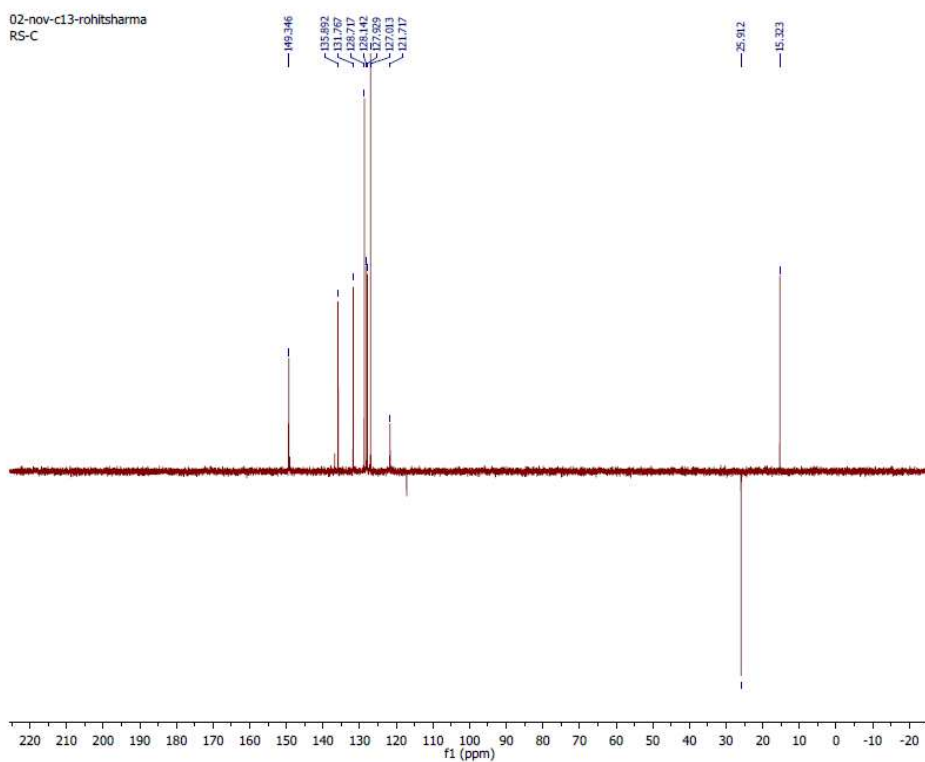
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2 Title	30-oct-mcd-2a
3 Comment	RS-C
4 Origin	Bruker BioSpin GmbH
5 Owner	IIIM
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCB
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	28
14 Relaxation Delay	0.5000
15 Pulse Width	13.1000
16 Acquisition Time	2.7263
17 Acquisition Date	2015-10-30T14:28:40
18 Modification Date	2015-10-30T19:20:19
19 Spectrometer Frequency	400.13
20 Spectral Width	12019.2
21 Lowest Frequency	-3109.4
22 Nucleus	^1H
23 Acquired Size	32768
24 Spectral Size	65536

02-nov-c13-rohitsharma
RS-C



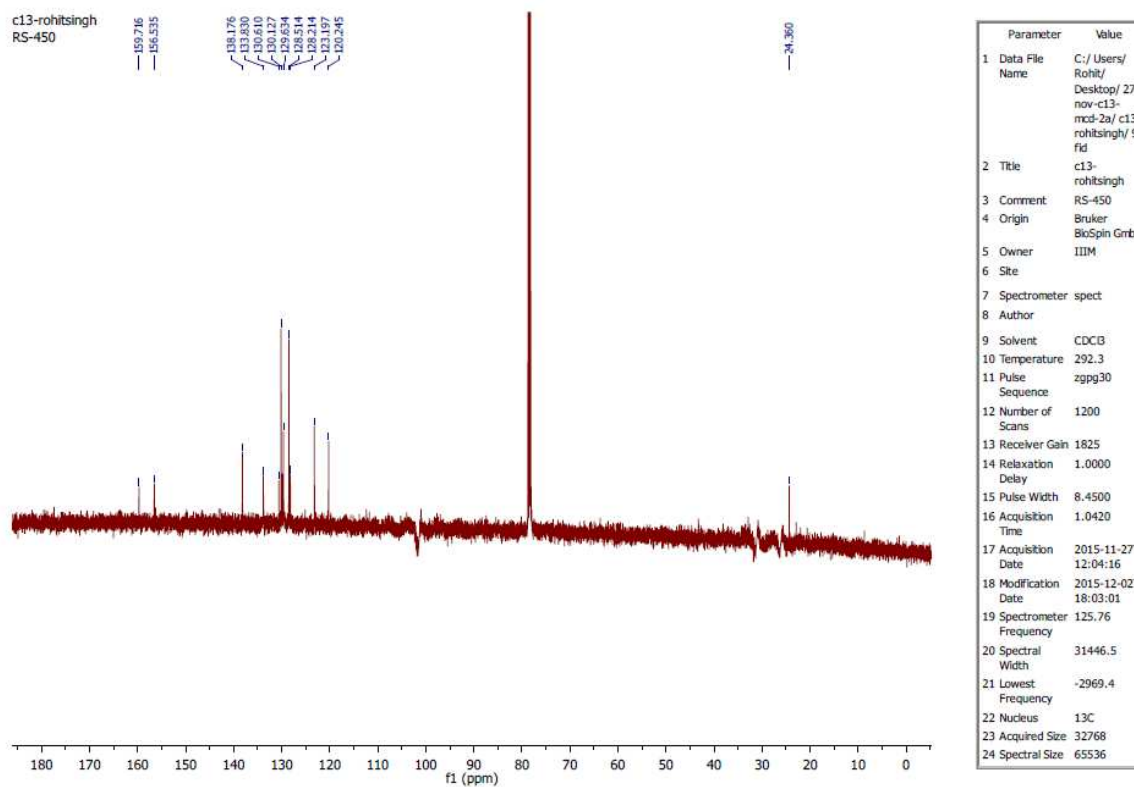
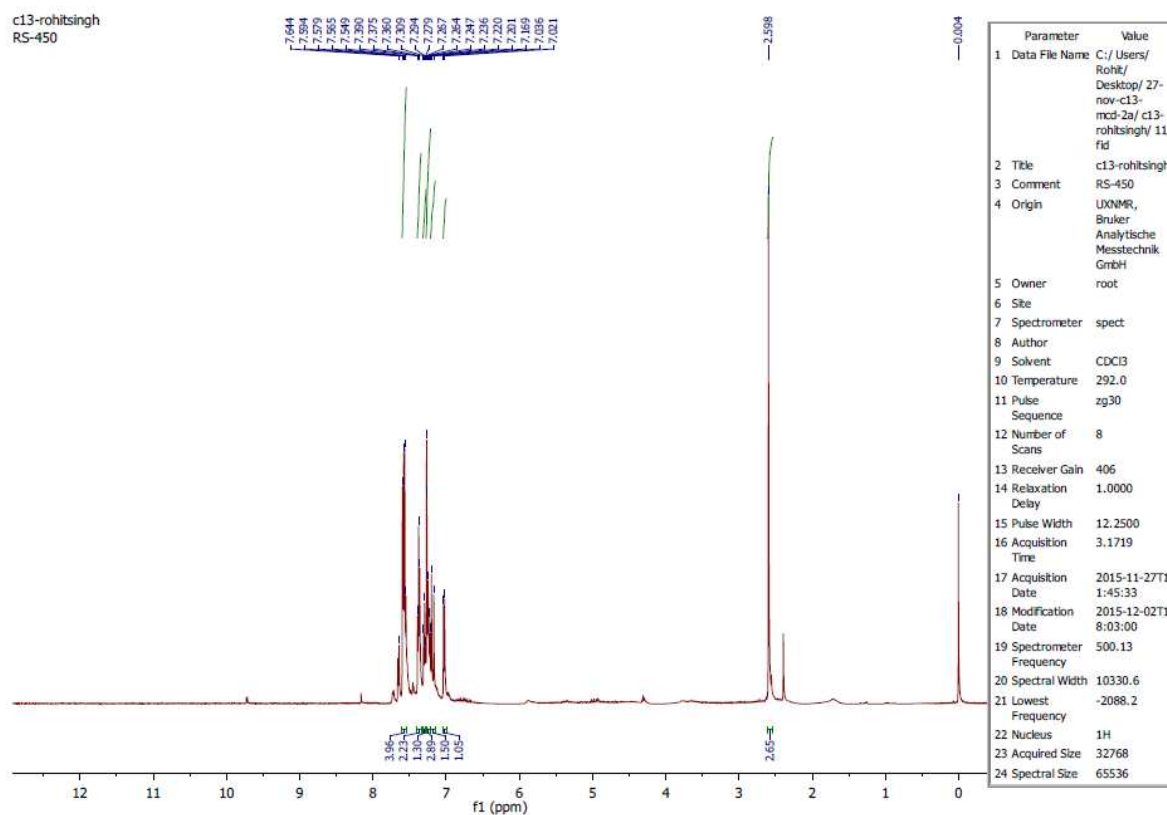
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2 Title	02-nov-c13-rohitsharma
3 Comment	RS-C
4 Origin	Bruker BioSpin GmbH
5 Owner	IIIM
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Number of Scans	120
13 Receiver Gain	128
14 Relaxation Delay	1.0000
15 Pulse Width	9.2000
16 Acquisition Time	1.2976
17 Acquisition Date	2015-11-03T09:12:25
18 Modification Date	2015-11-03T11:48:27
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

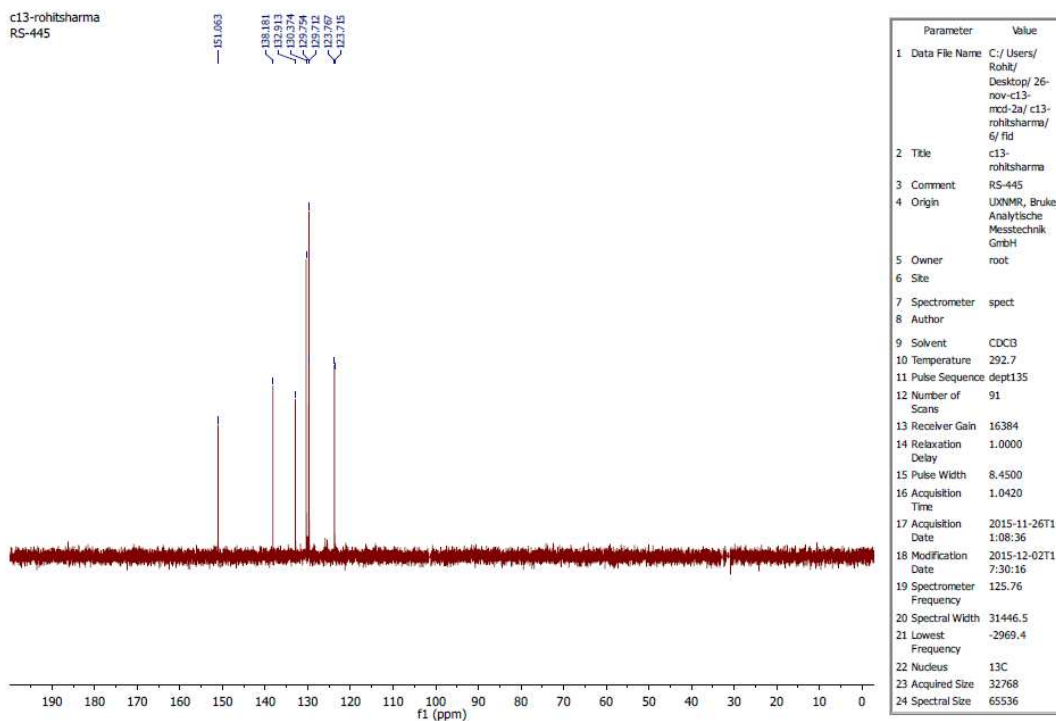
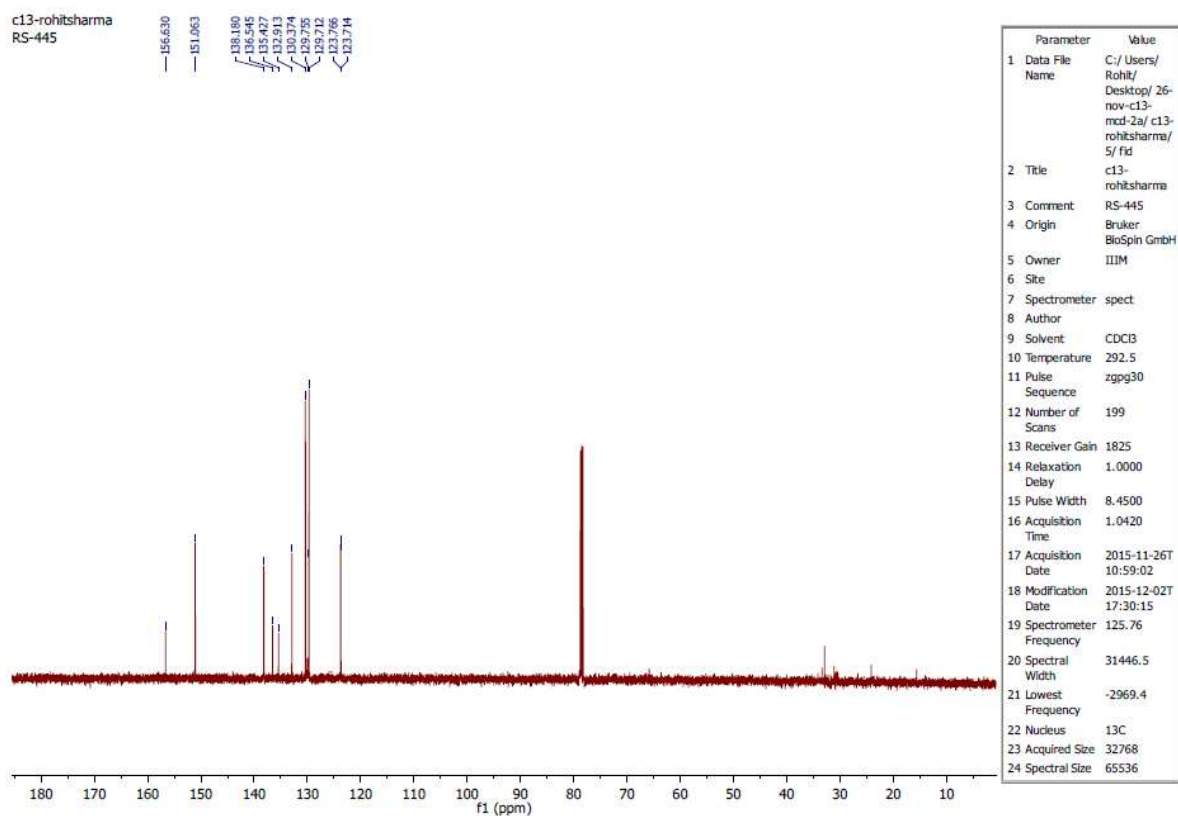
02-nov-c13-rohitsharma
RS-C



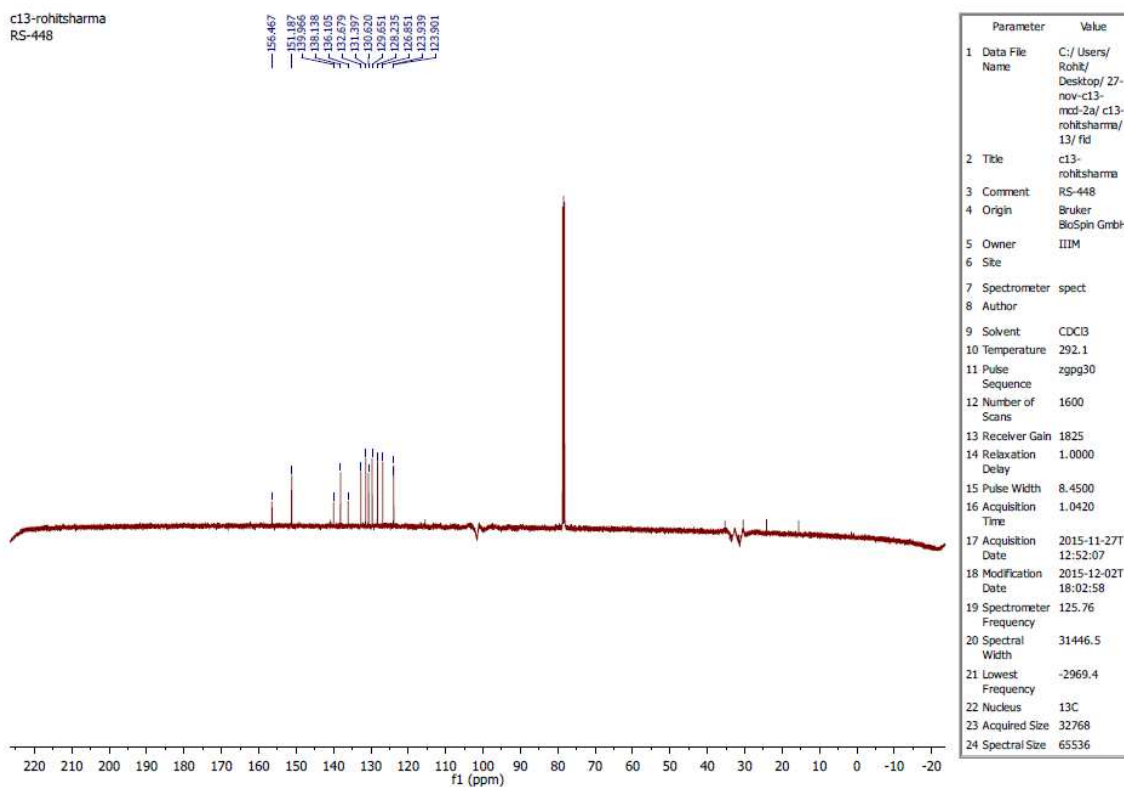
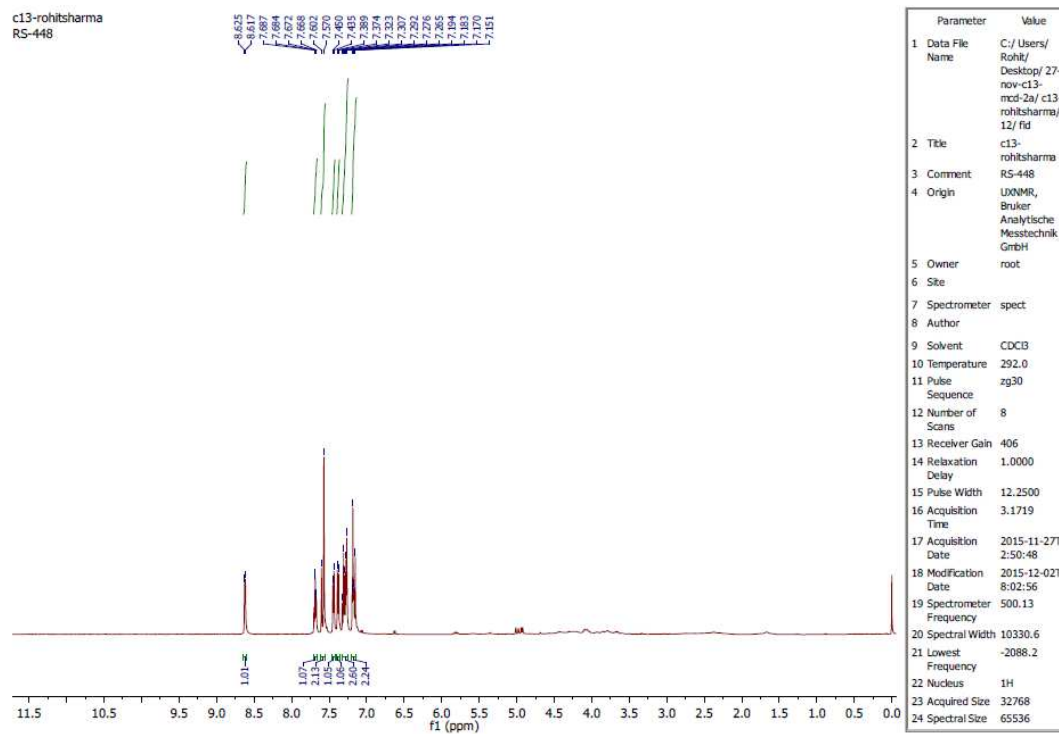
Parameter	Value
1 Data File Name	C:/Users/Rohit/Desktop/02-nov-c13-rohitsharma/43/ f1d
2 Title	02-nov-c13-rohitsharma
3 Comment	RS-C
4 Origin	Bruker BioSpin GmbH
5 Owner	IIIM
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	dept135
12 Number of Scans	50
13 Receiver Gain	203
14 Relaxation Delay	1.0000
15 Pulse Width	9.2000
16 Acquisition Time	1.2976
17 Acquisition Date	2015-11-03T09:15:06
18 Modification Date	2015-11-03T11:48:28
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

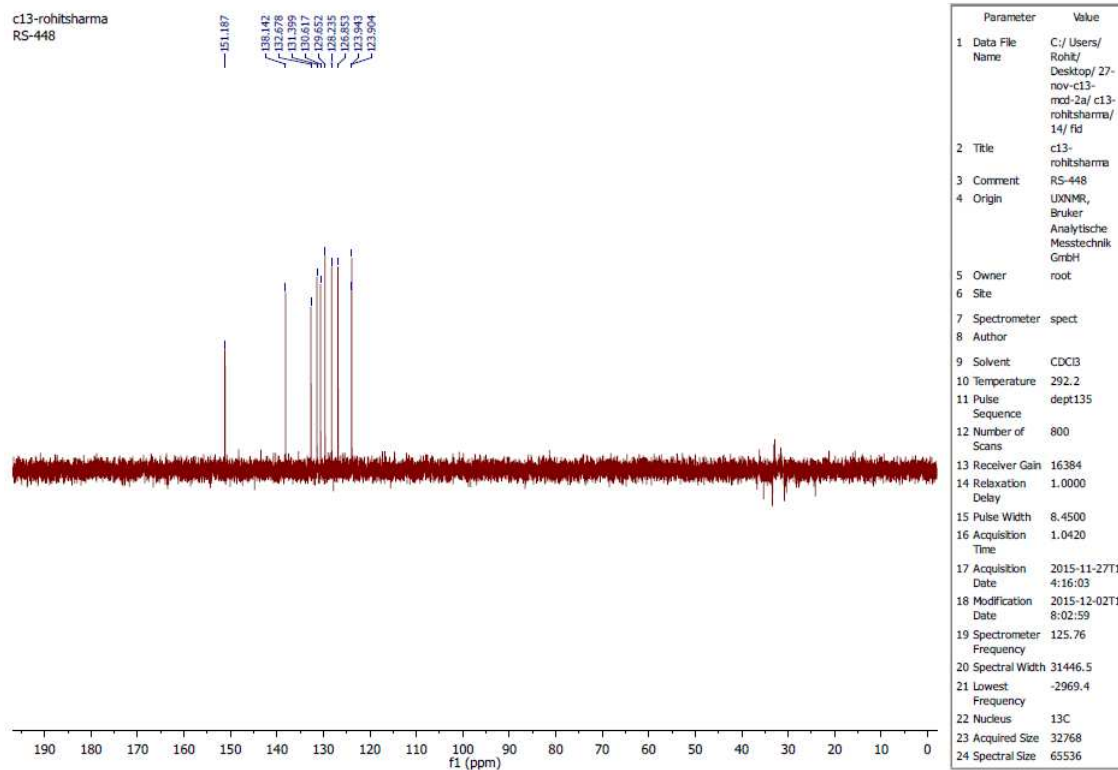
¹H, ¹³C and DEPT135 NMR spectra of (E)-2-methyl-6-styrylpyridine (11c).





¹H, ¹³C and DEPT135 NMR spectra of (E)-2-(3-chlorostyryl)pyridine (11e).





^1H , ^{13}C and DEPT135 NMR spectra of (E)-2-(4-chlorostyryl)-6-methylpyridine(11f).

