Electronic Supporting Information (ESI)

Synthesis, antioxidant, neuroprotective and P-glycoprotein induction activity of 4-arylquinoline-2-carboxylates¤

Jaideep B. Bharate,[a,b] Abubakar Wani,[c] Sadhana Sharma,[c] Shahi Imam Reja,[d] Manoj Kumar,[d] Ram A. Vishwakarma[a,b,*] Ajay Kumar,[c,*] and Sandip B. Bharate[a,b,*]

[a]Medicinal Chemistry Division, Indian Institute of Integrative Medicine (CSIR), Canal Road, Jammu-180001, India

[b]Academy of Scientific & Innovative Research (AcSIR), Indian Institute of Integrative Medicine (CSIR), Canal Road, Jammu-180001, India

[c]Cancer Pharmacology Division, Indian Institute of Integrative Medicine (CSIR), Canal Road, Jammu-180001, India

[d]Department of Chemistry, Guru Nanak Dev University (GNDU), Amritsar- 143005, India.

*E-mail: sbharate@iiim.res.in (SBB);

ajaykmahajan@hotmail.com (AK);

ram@iiim.res.in (RAV)

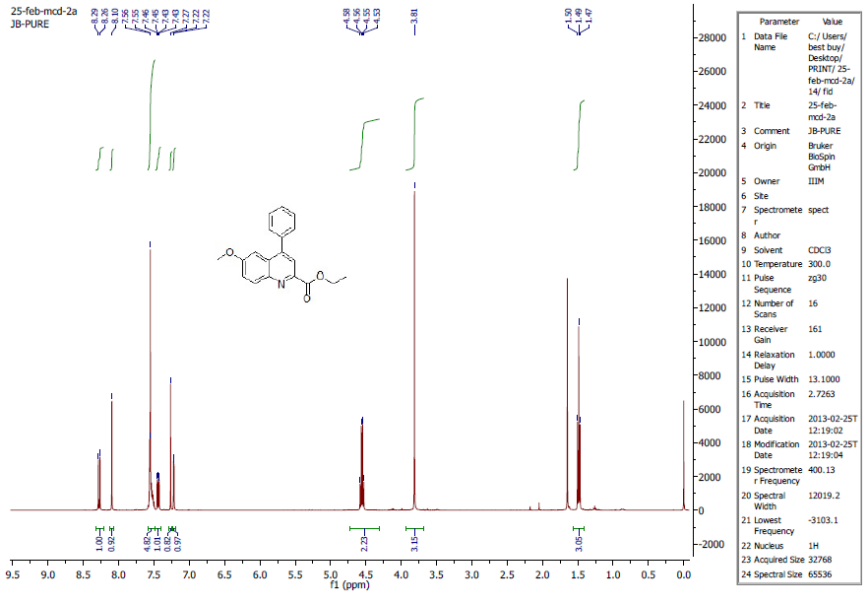
Fax: +91-191-2569333; Tel: +91-191-2569111

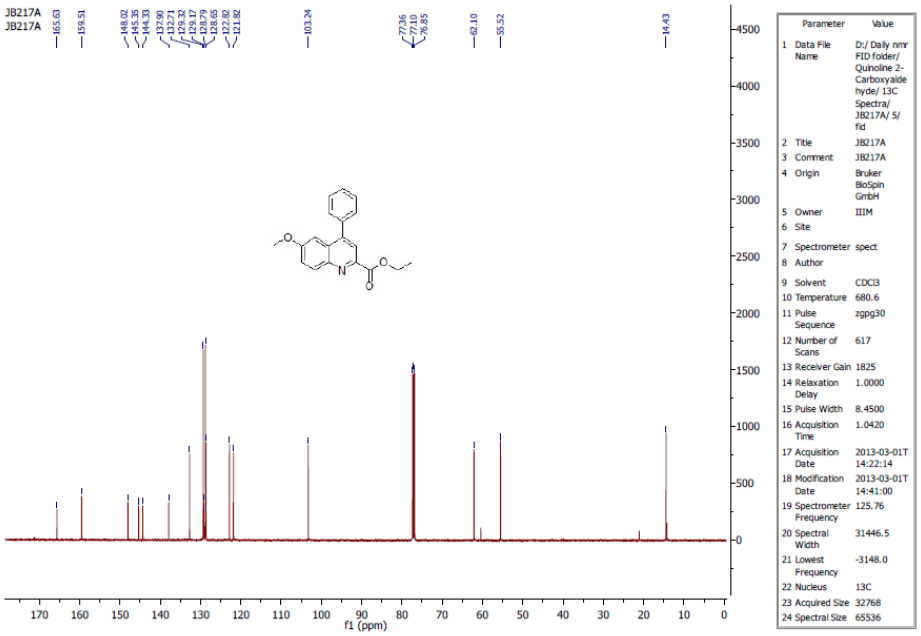
¤ IIIM Publication number IIIM/1669/2014

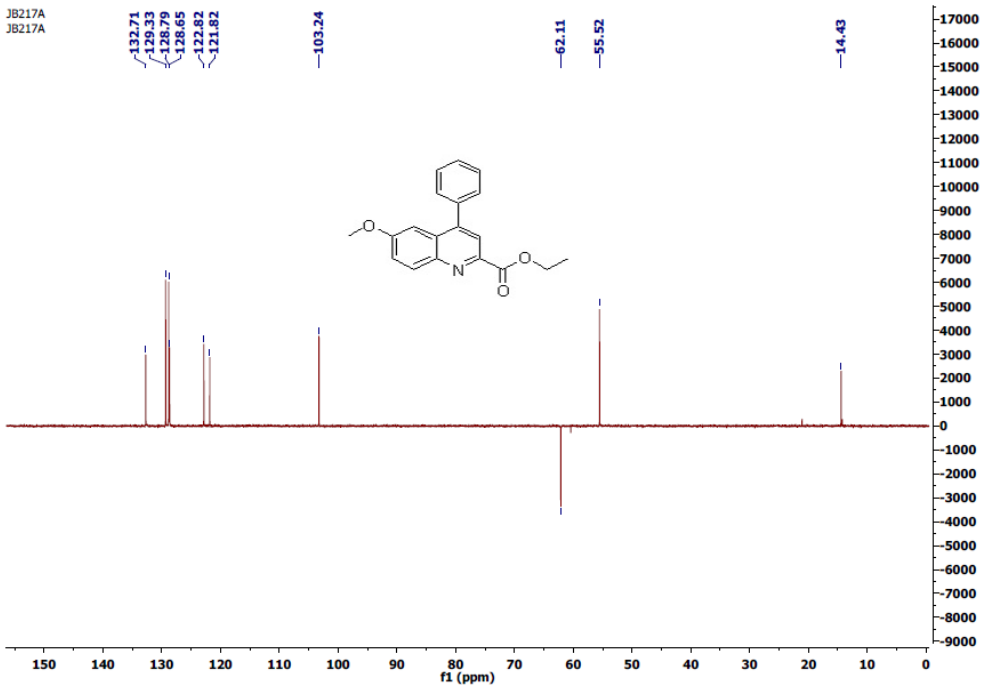
CONTENTS

S1. SPECTRAL DATA SCANS OF ALL COMPOUNDS

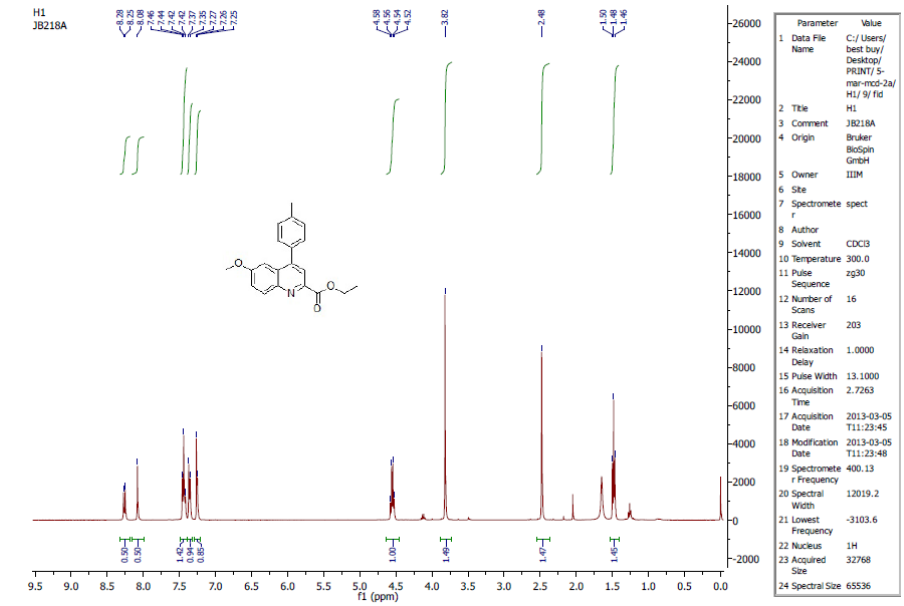
S1.a. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 6-methoxy-4-phenylquinoline-2-carboxylate (**1a**)

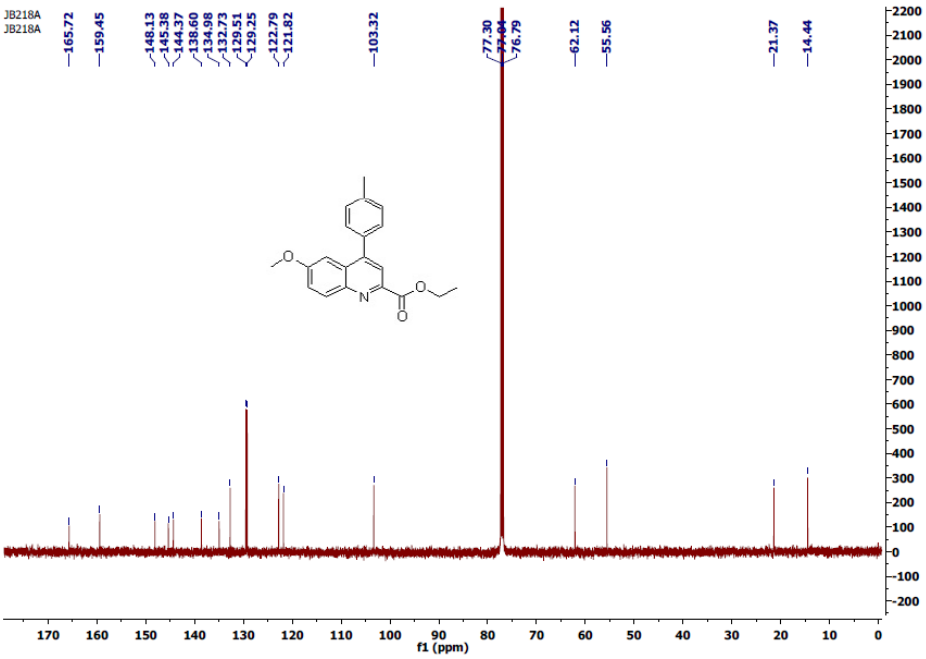


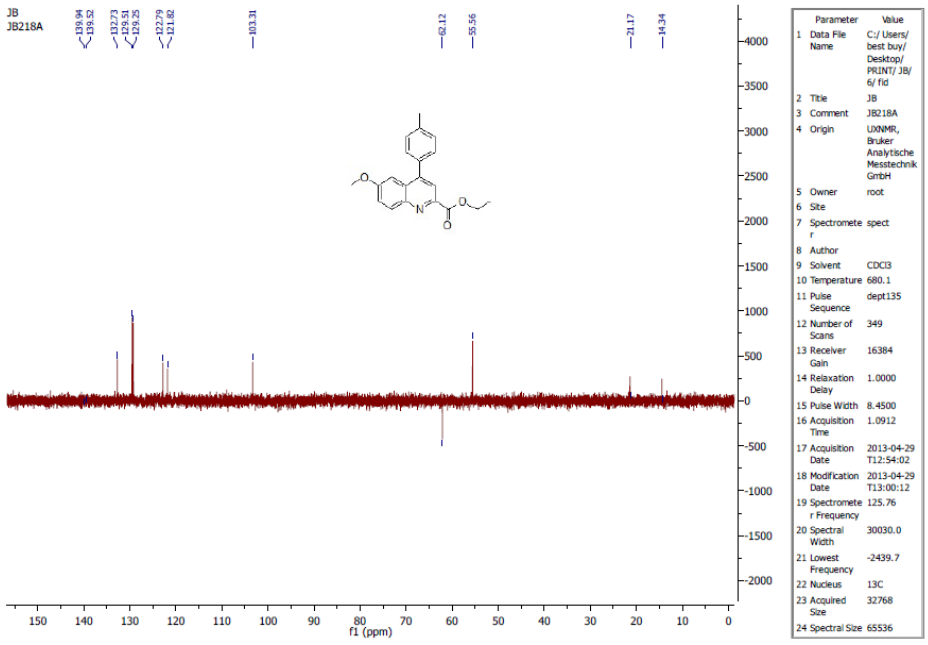



JB217A
JB217A
132.71
129.33
128.79
128.65
122.82
121.82
103.24
62.11
55.52
14.43
O
N
O
O
f1 (ppm)

S1.b. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 6-methoxy-4-p-tolylquinoline-2-carboxylate (**1b**)

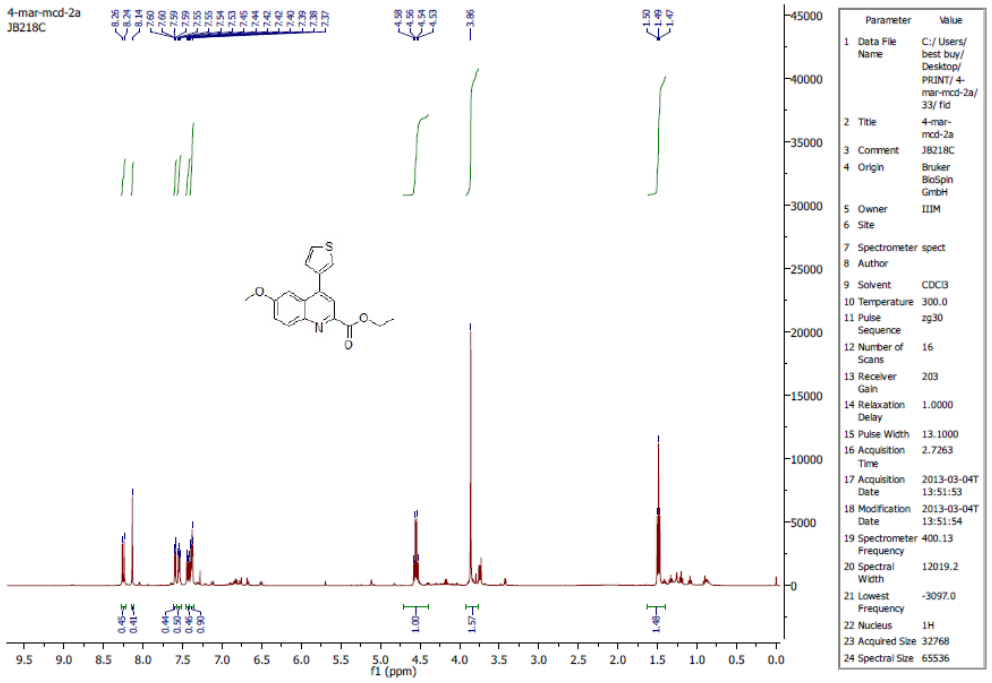




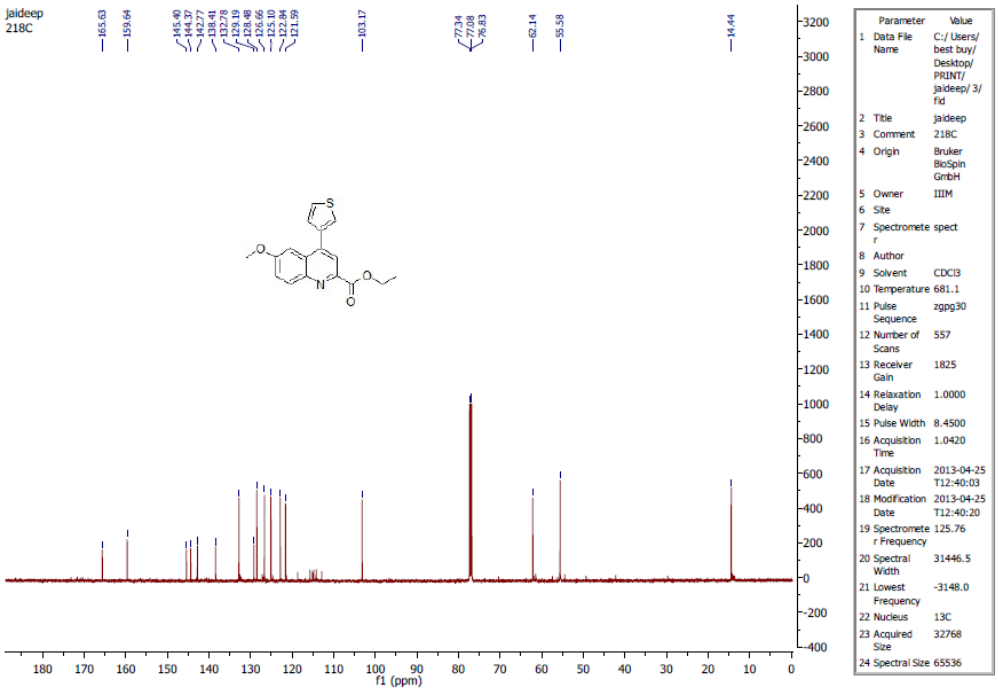


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ JB/ 6/ fid
2	Title	JB
3	Comment	JB218A
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.1
11	Pulse Sequence	dept135
12	Number of Scans	349
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2013-04-29 T12:54:02
18	Modification Date	2013-04-29 T13:00:12
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

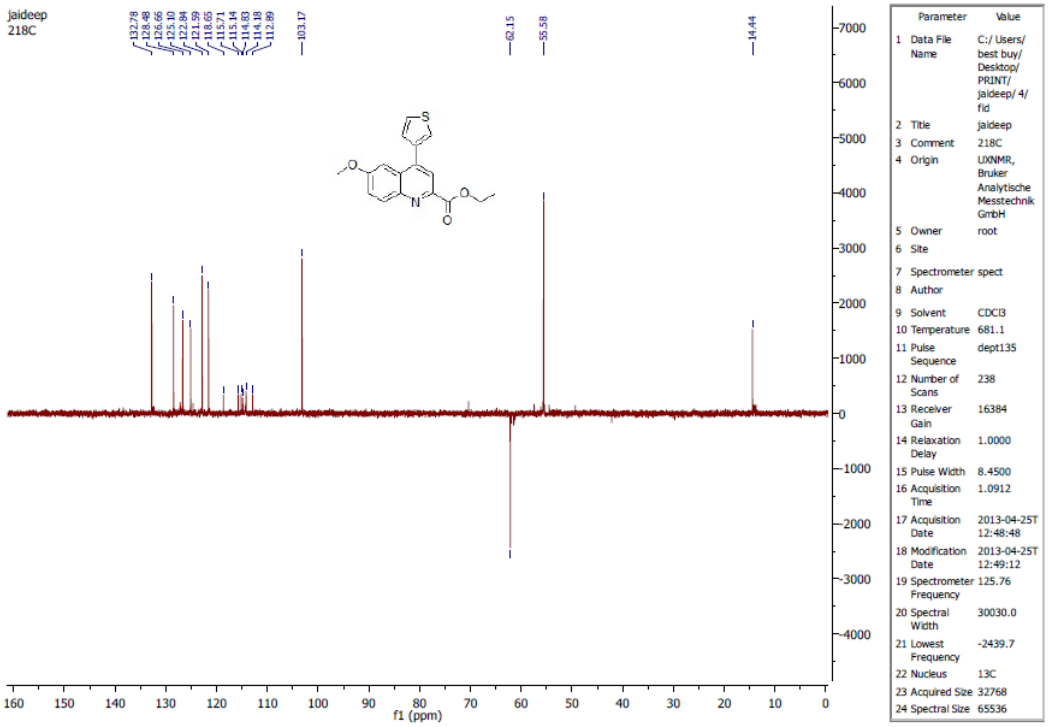
S1.c. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 6-methoxy-4-(thiophen-3-yl)quinoline-2-carboxylate (**1c**)



	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 4-mar-mcd-2a/ 33/ fid
2	Title	4-mar-mcd-2a
3	Comment	JB218C
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	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2013-03-04T 13:51:53
18	Modification Date	2013-03-04T 13:51:54
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3097.0
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

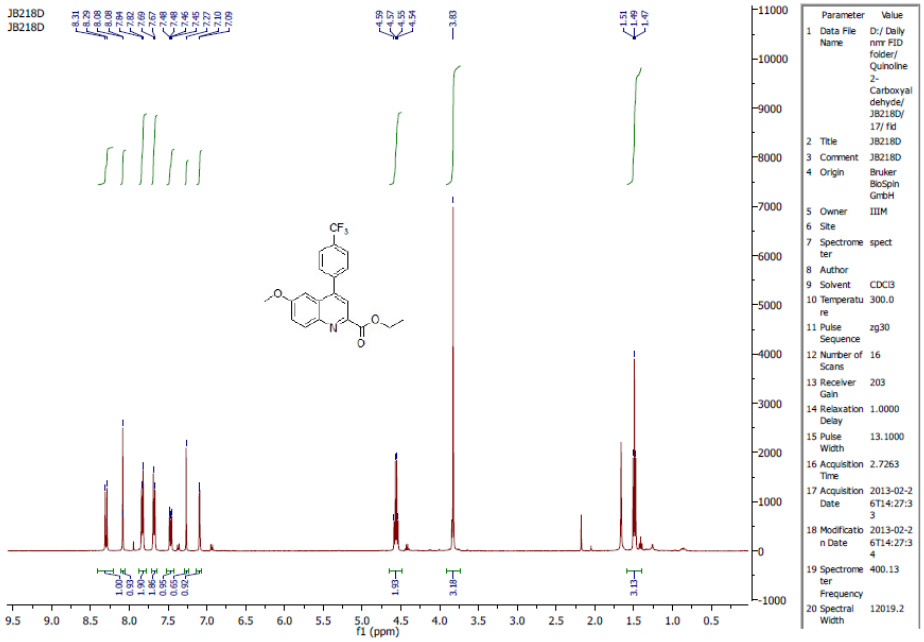


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ jaideep/ 3/ fid
2	Title	jaideep
3	Comment	218C
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect r
8	Author	
9	Solvent	CDCl3
10	Temperature	681.1
11	Pulse Sequence	zgpg30
12	Number of Scans	557
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2013-04-25 T12:40:03
18	Modification Date	2013-04-25 T12:40:20
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

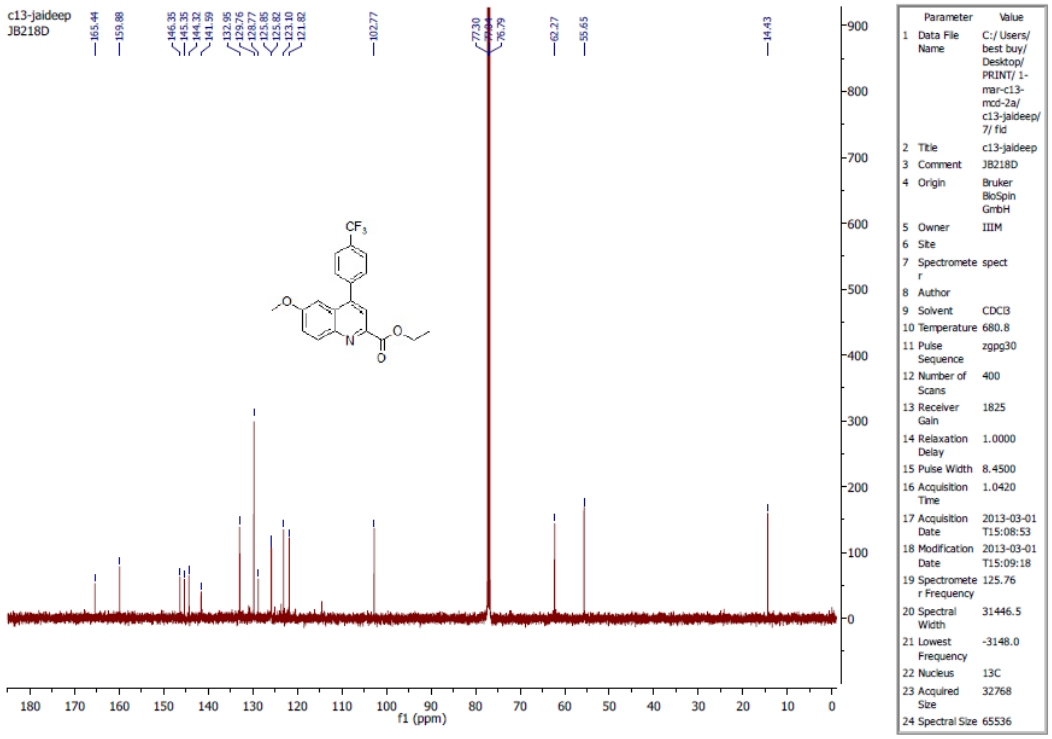


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ jaideep/ 4/ fid
2	Title	jaideep
3	Comment	218C
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	681.1
11	Pulse Sequence	dept135
12	Number of Scans	238
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2013-04-25T 12:48:48
18	Modification Date	2013-04-25T 12:49:12
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

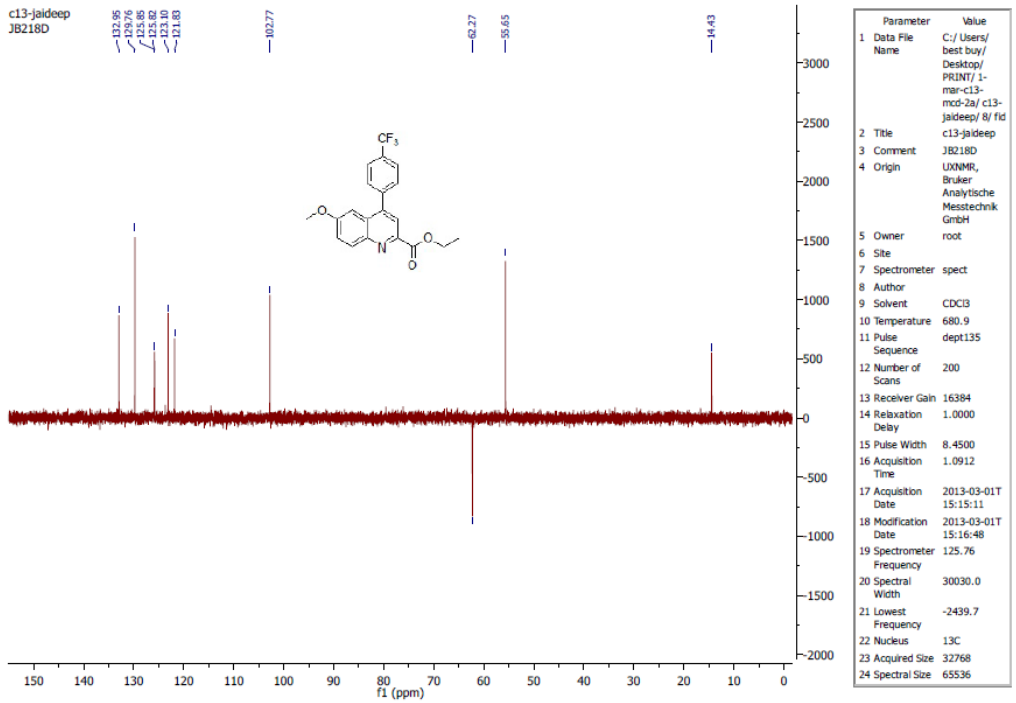
S1.d. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR spectrum of ethyl 4-(4-(trifluoromethyl)phenyl)-6-methoxyquinoline-2-carboxylate (**1d**)



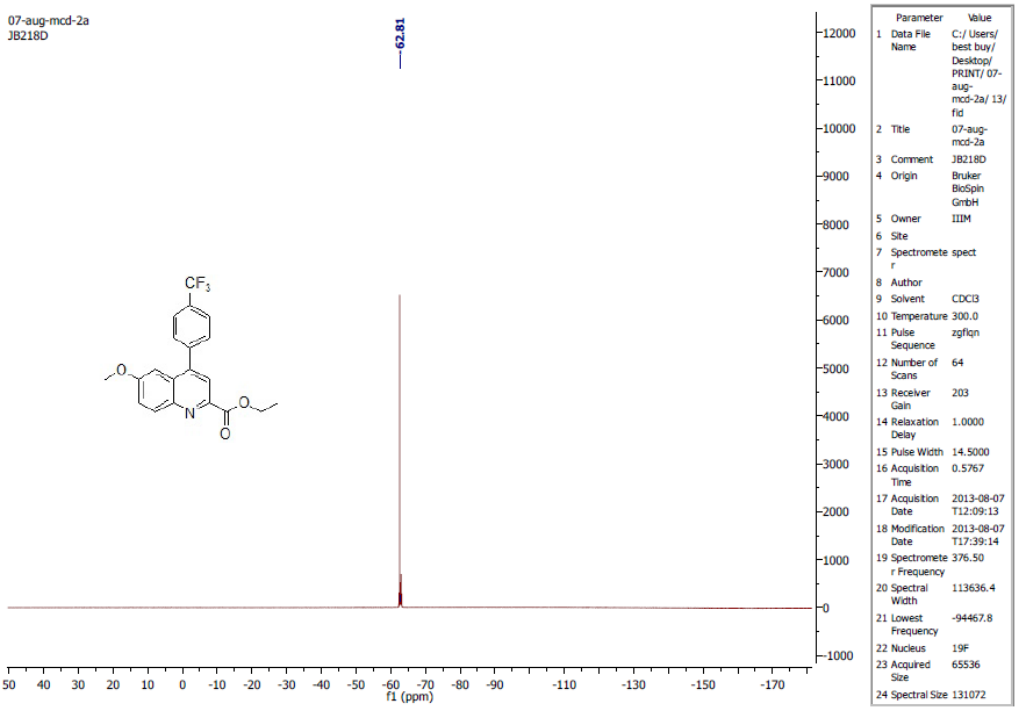
	Parameter	Value
1	Data File Name	D:/ Daily nmr FID folder/ Quinoline 2-Carboxyaldehyde/ JB218D/ 17/ fid
2	Title	JB218D
3	Comment	JB218D
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2013-02-26T14:27:33
18	Modification Date	2013-02-26T14:27:34
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2



	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 1-mar-c13-mcd-2a/ c13-jaideep/ 7/ fid
2	Title	c13-jaideep
3	Comment	JB218D
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.8
11	Pulse Sequence	zgpg30
12	Number of Scans	400
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2013-03-01T15:08:53
18	Modification Date	2013-03-01T15:09:18
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

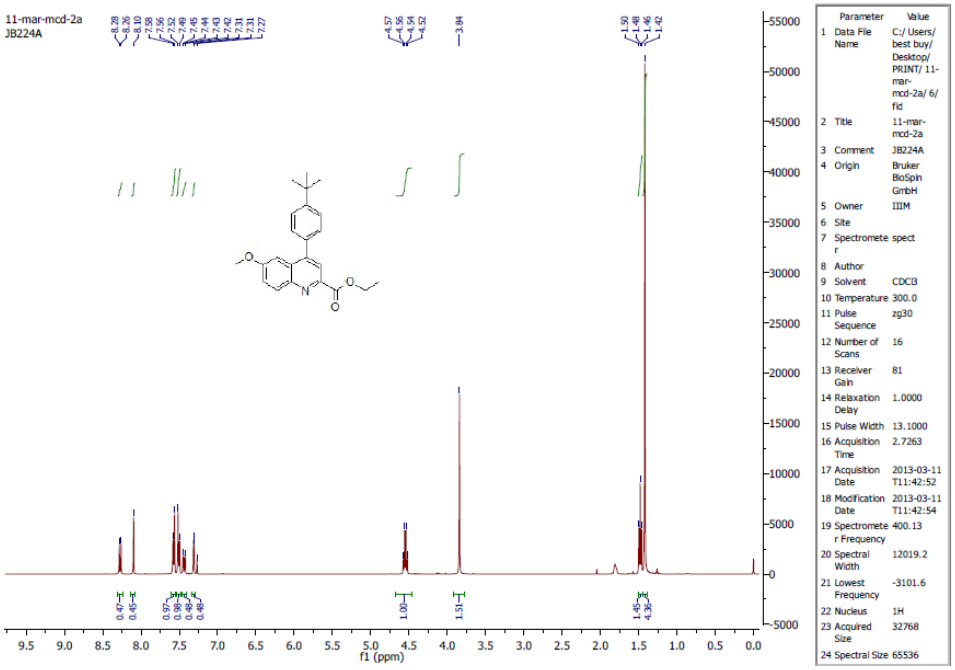


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 1-mar-c13-mcd-2a/ c13-jaideep/ 8/ fid
2	Title	c13-jaideep
3	Comment	JB218D
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.9
11	Pulse Sequence	dept135
12	Number of Scans	200
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2013-03-01T 15:15:11
18	Modification Date	2013-03-01T 15:16:48
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

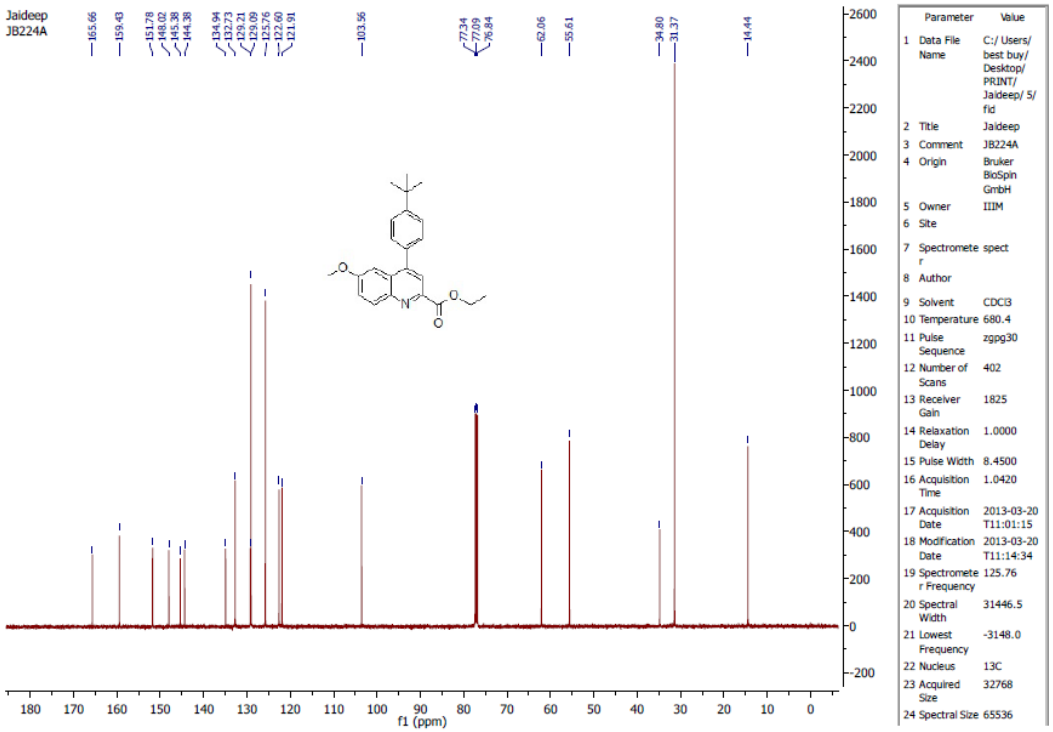


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 07-aug-mcd-2a/ 13/ fid
2	Title	07-aug-mcd-2a
3	Comment	JB218D
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgflqn
12	Number of Scans	64
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	14.5000
16	Acquisition Time	0.5767
17	Acquisition Date	2013-08-07 T12:09:13
18	Modification Date	2013-08-07 T17:39:14
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

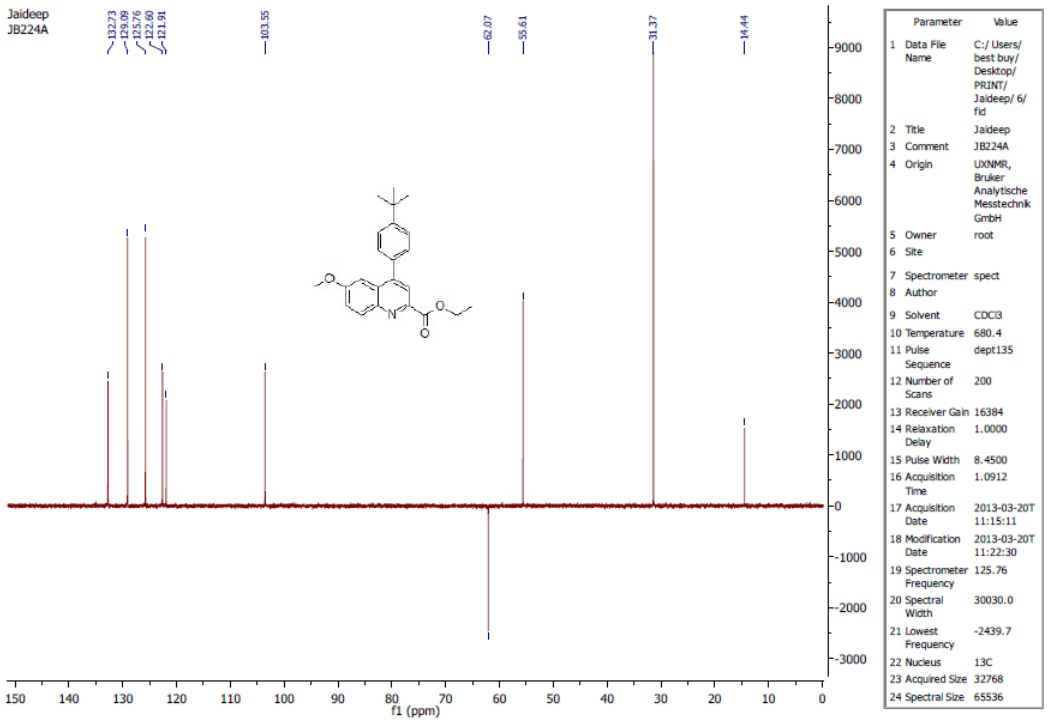
S1.e. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 4-(4-tert-butylphenyl)-6-methoxyquinoline-2-carboxylate (**1e**)



	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 11-mar-mcd-2a/ 6/ fid
2	Title	11-mar-mcd-2a
3	Comment	JB224A
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	81
14	Relaxation Delay	1.0000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2013-03-11 T11:42:52
18	Modification Date	2013-03-11 T11:42:54
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3101.6
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

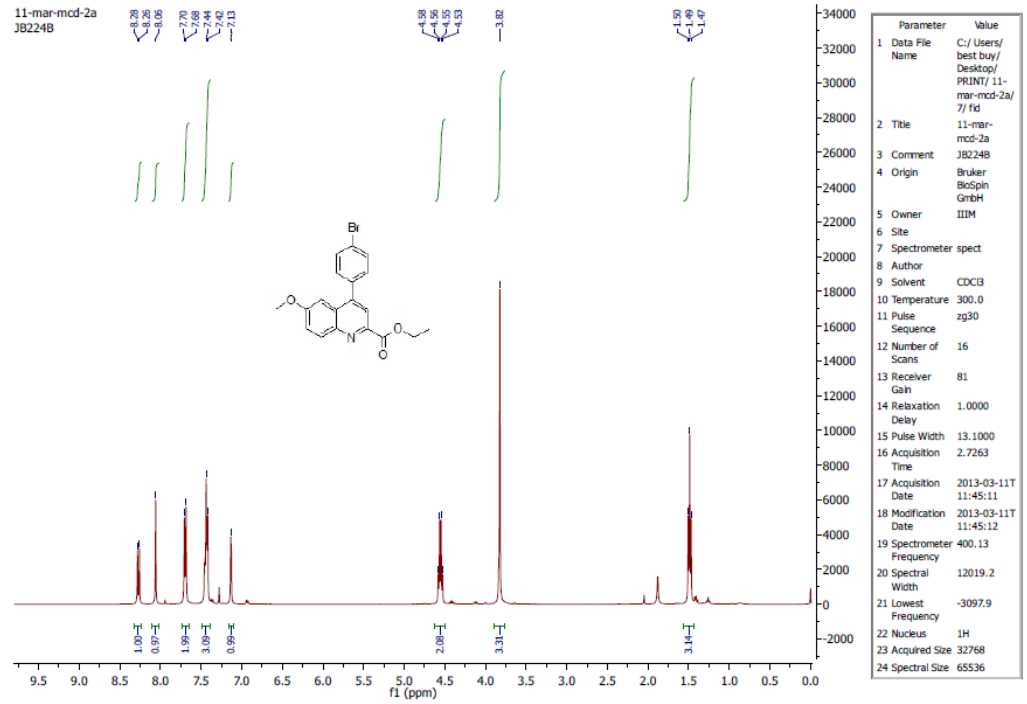


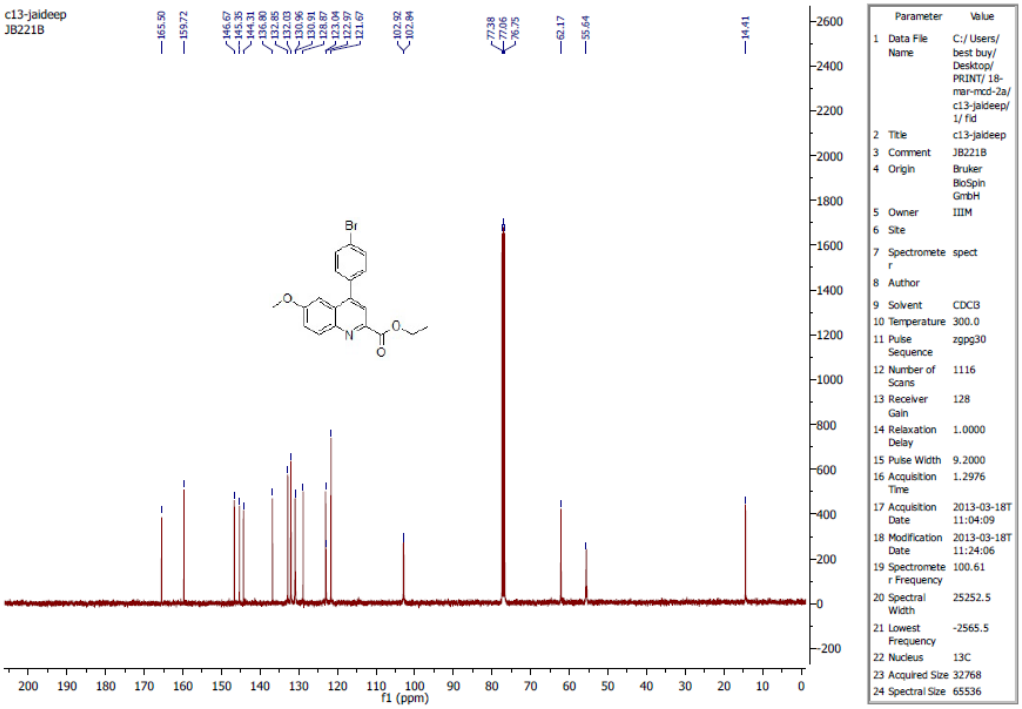
	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ Jaideep/ 5/ fid
2	Title	Jaideep
3	Comment	JB224A
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect r
8	Author	
9	Solvent	CDCl3
10	Temperature	680.4
11	Pulse Sequence	zgpg30
12	Number of Scans	402
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2013-03-20 T11:01:15
18	Modification Date	2013-03-20 T11:14:34
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

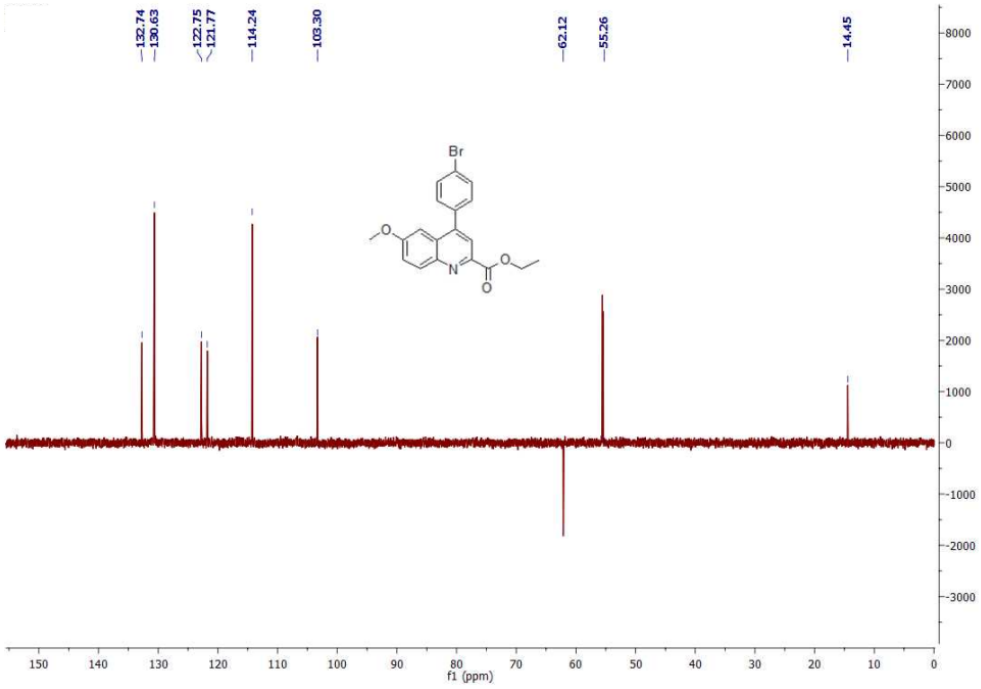


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ Jaideep/ 6/ fid
2	Title	Jaideep
3	Comment	JB224A
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.4
11	Pulse Sequence	dept135
12	Number of Scans	200
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2013-03-20T 11:15:11
18	Modification Date	2013-03-20T 11:22:30
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

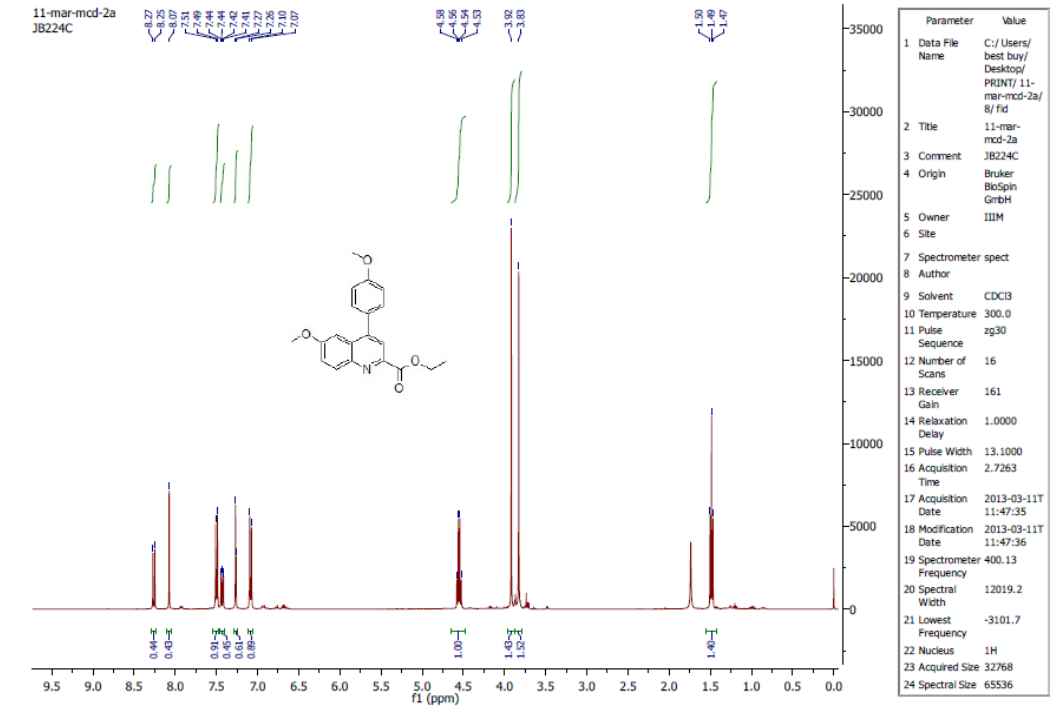
S1.f. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 4-(4-bromophenyl)-6-methoxyquinoline-2-carboxylate (**1f**)

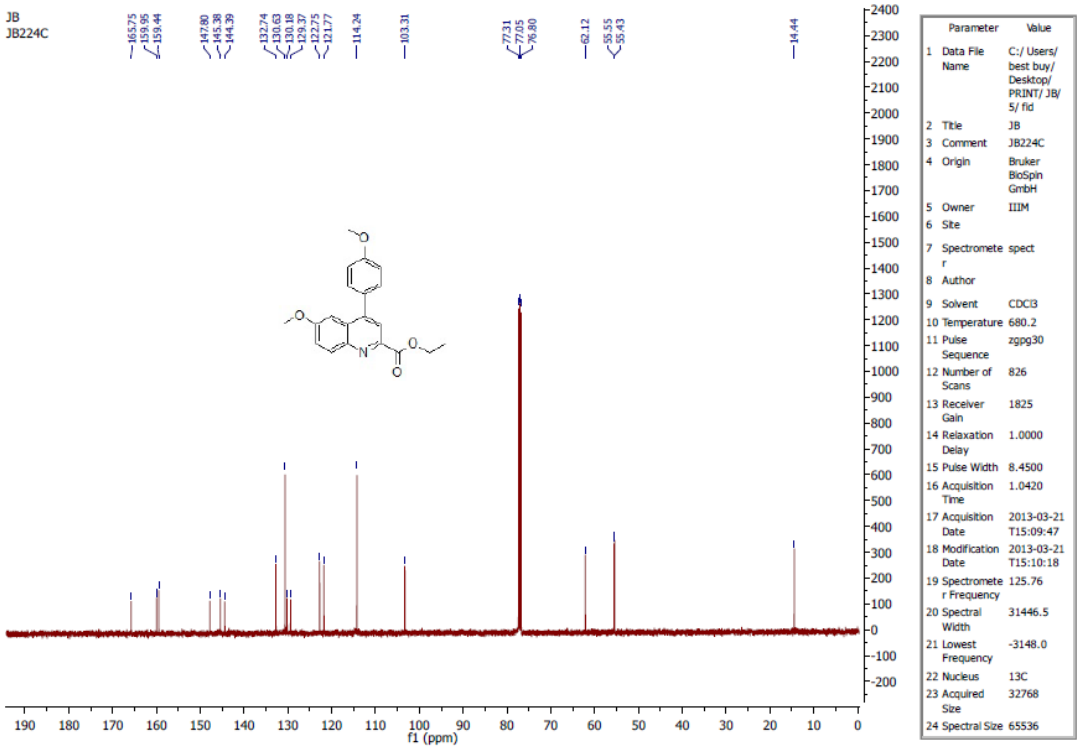


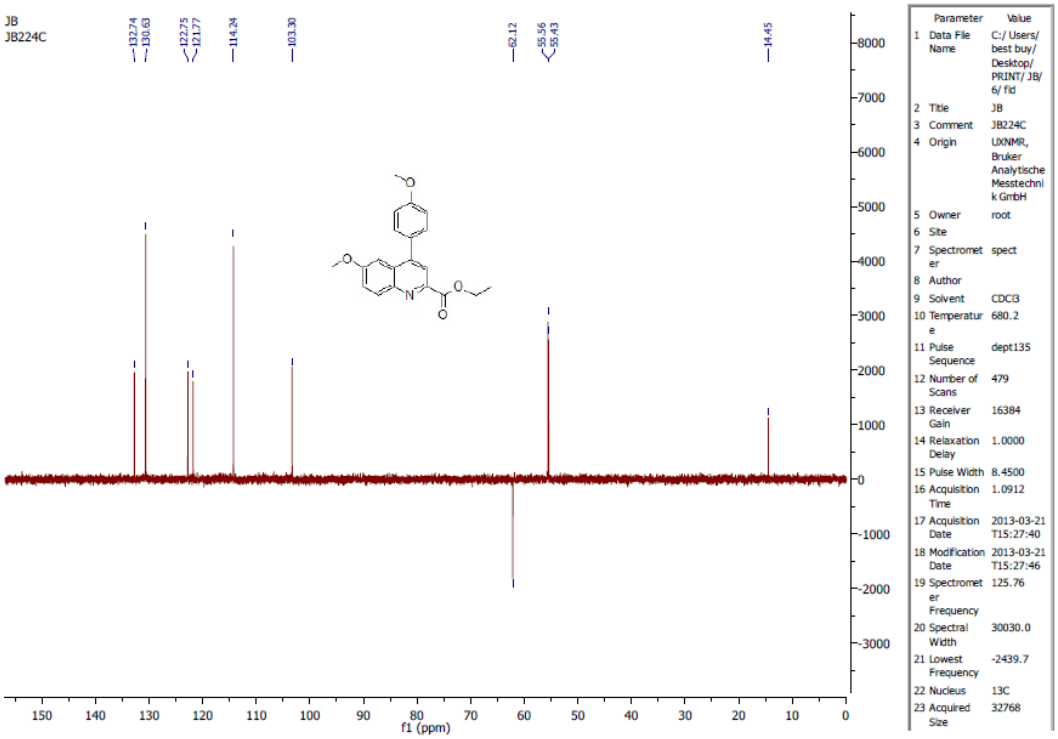



132.74
130.63
122.75
121.77
114.24
103.30
62.12
55.26
14.45
Br
O
N
O
O
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

S1.g. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 6-methoxy-4-(4-methoxyphenyl)quinoline-2-carboxylate (**1g**)

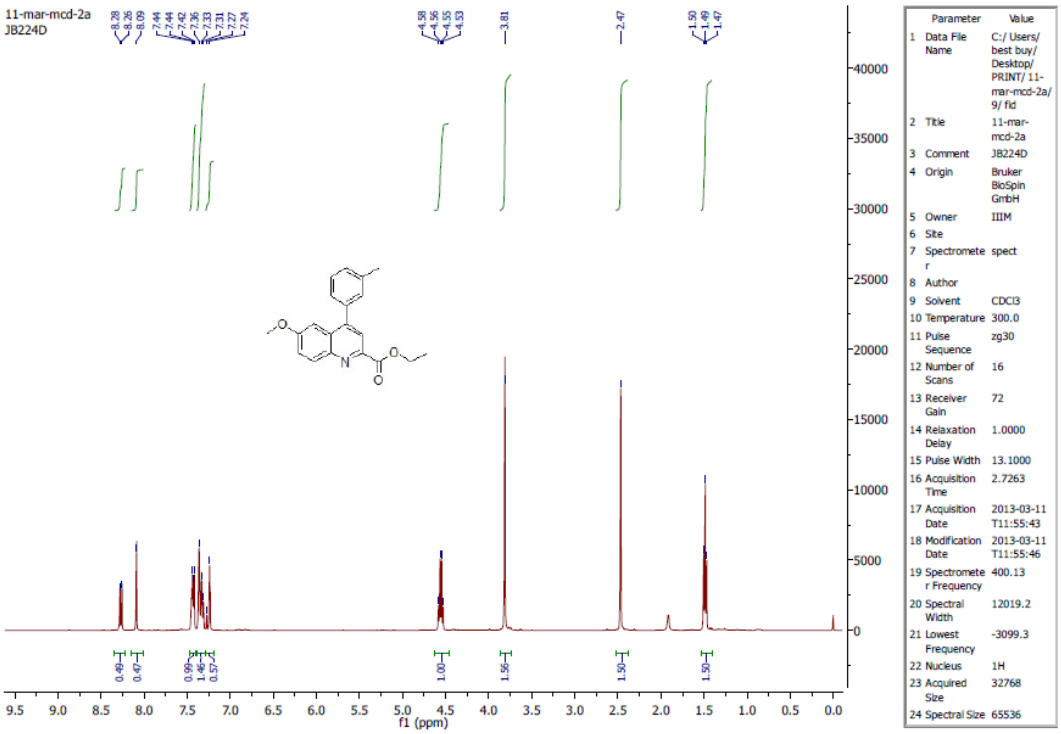


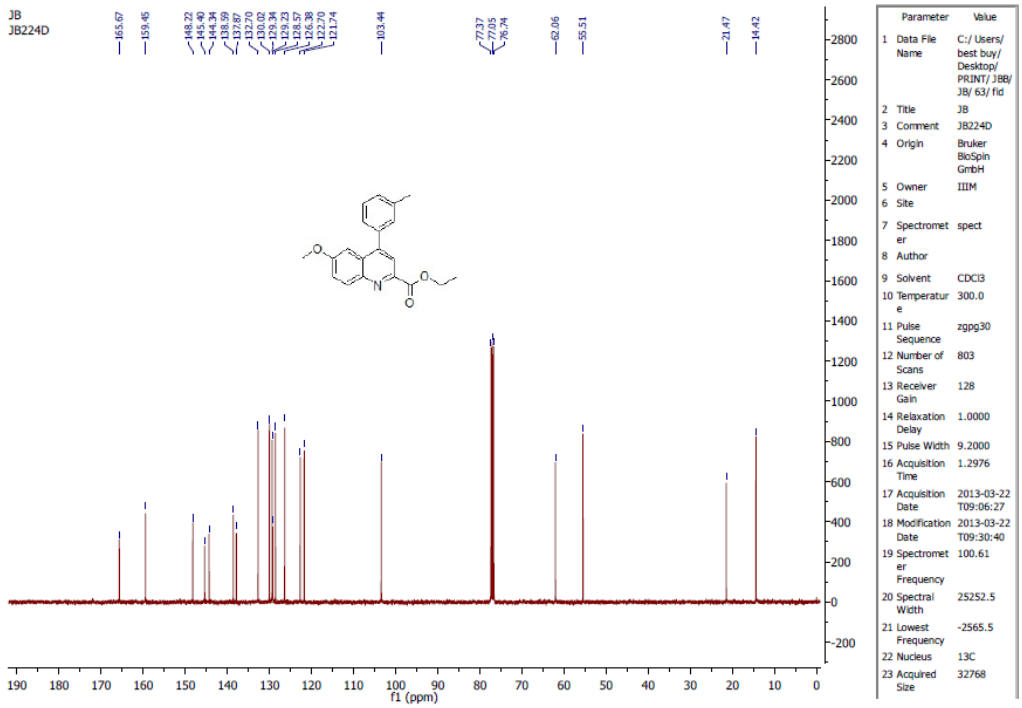


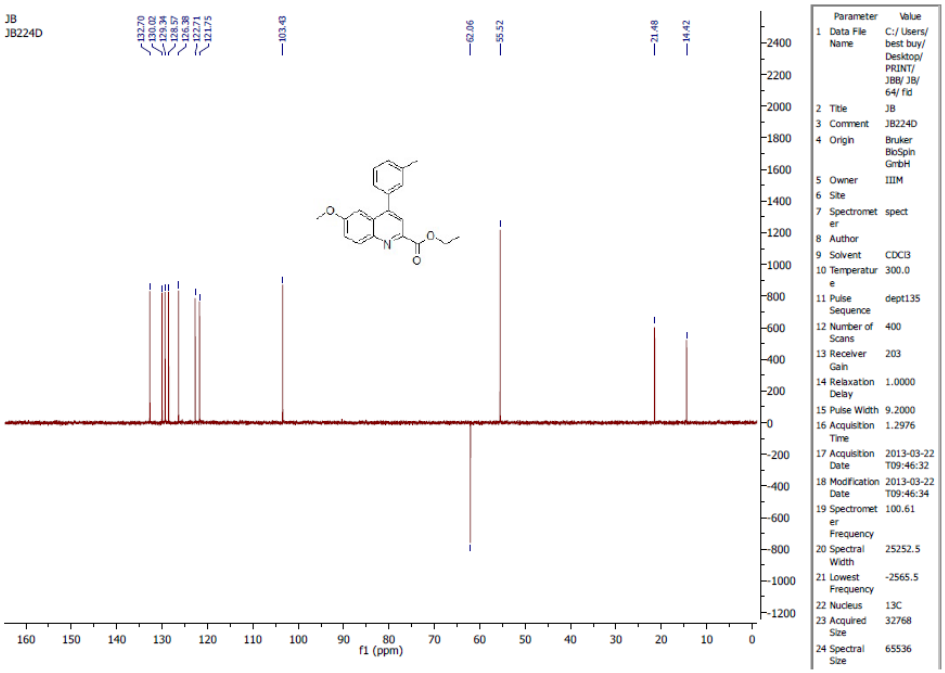


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ JB/ 6/ fid
2	Title	JB
3	Comment	JB224C
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.2
11	Pulse Sequence	dept135
12	Number of Scans	479
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2013-03-21 T15:27:40
18	Modification Date	2013-03-21 T15:27:46
19	Spectrometer Frequency	125.76
20	Spectral Width	30030.0
21	Lowest Frequency	-2439.7
22	Nucleus	13C
23	Acquired Size	32768

S1.h. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 6-methoxy-4-m-tolylquinoline-2-carboxylate (**1h**)

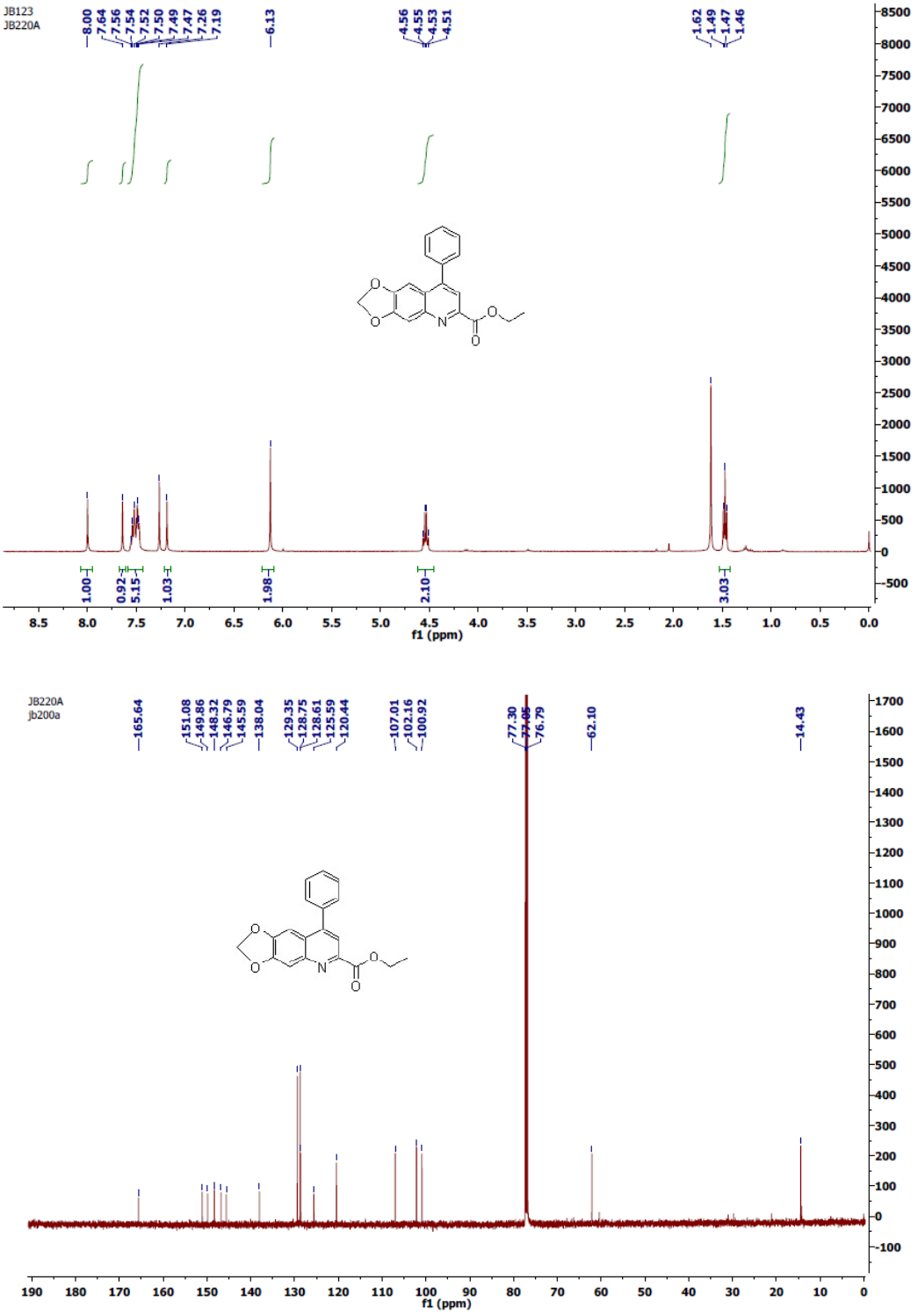


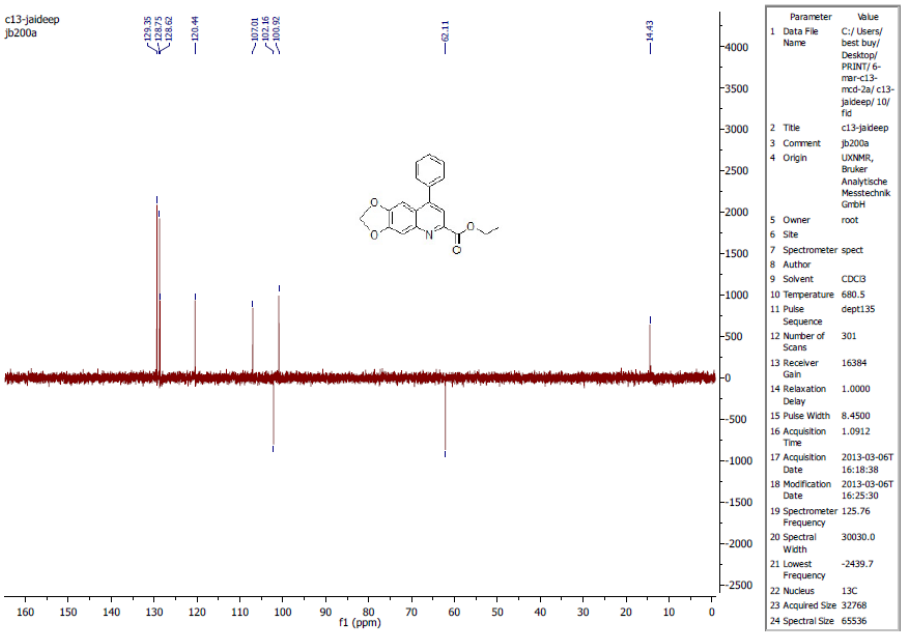




	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ JBB/ JB/ 64/ fid
2	Title	JB
3	Comment	JB224D
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	dept135
12	Number of Scans	400
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	9.2000
16	Acquisition Time	1.2976
17	Acquisition Date	2013-03-22 T09:46:32
18	Modification Date	2013-03-22 T09:46:34
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

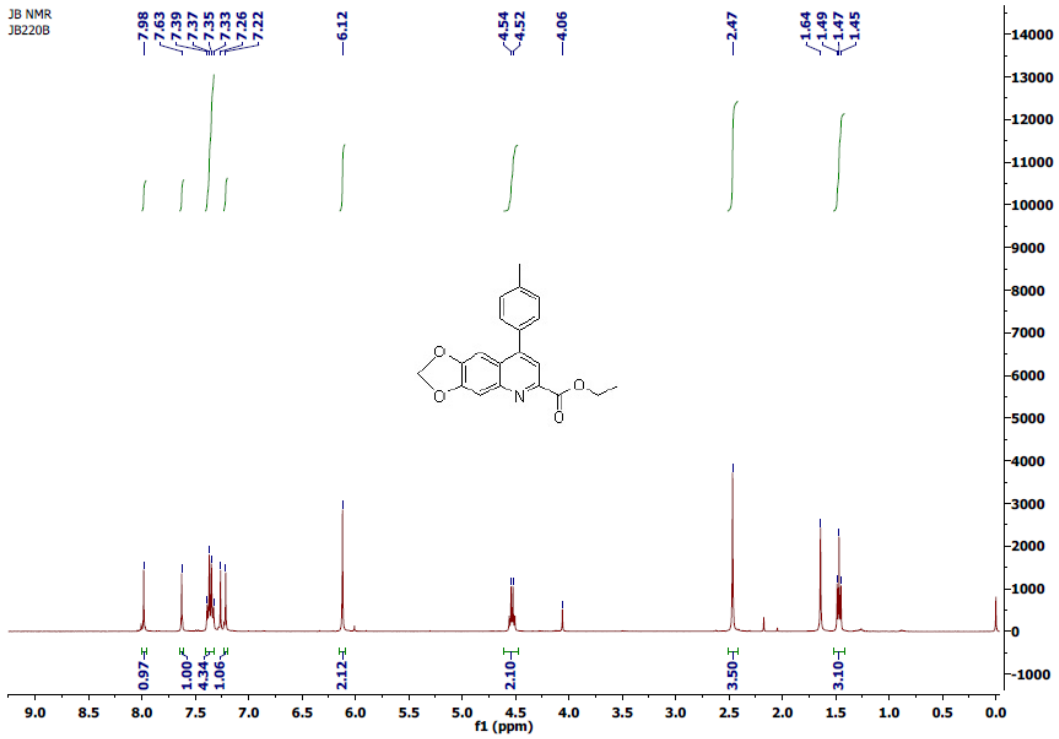
S2.i. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 8-phenyl-[1,3]dioxolo[4,5-g]quinoline-6-carboxylate (**1i**)

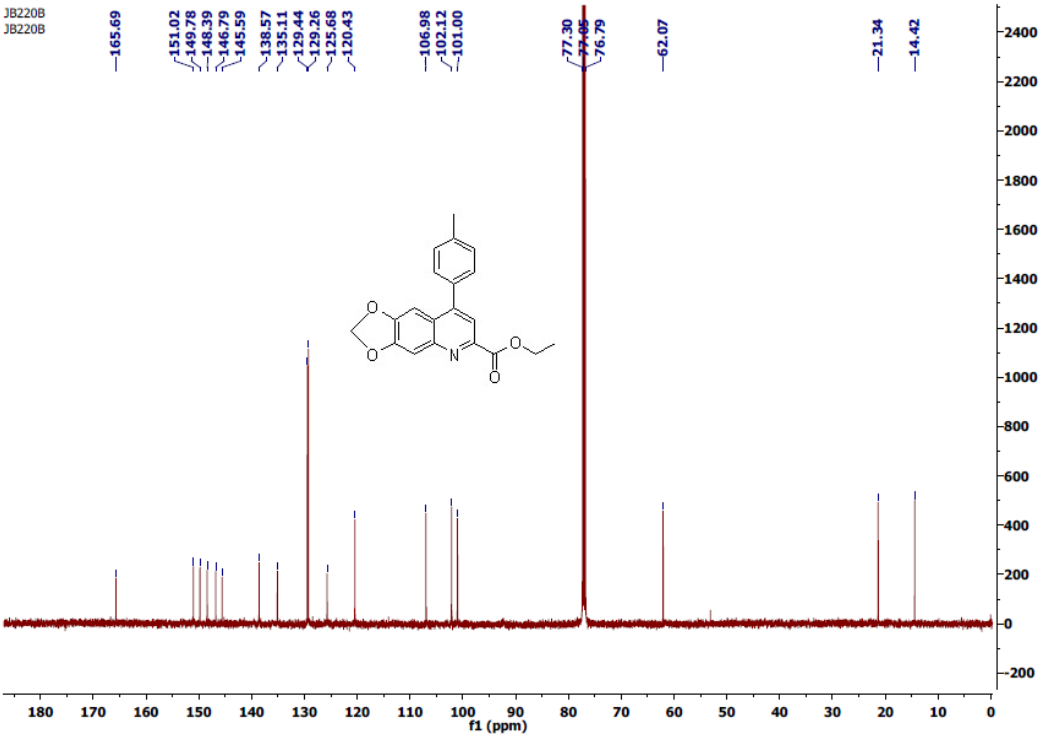


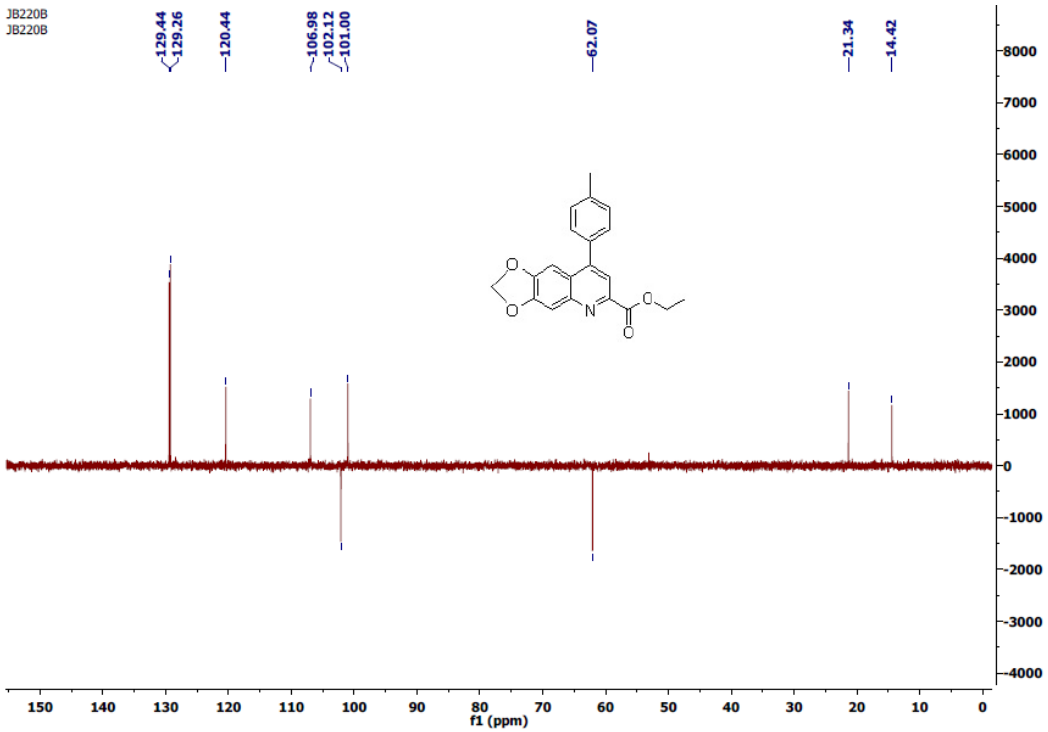


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 6-mar-c13-mcd-2a/ c13-jaideep/ 10/ fid
2	Title	c13-jaideep
3	Comment	jb200a
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.5
11	Pulse Sequence	dept135
12	Number of Scans	301
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2013-03-06T 16:18:38
18	Modification Date	2013-03-06T 16:25:30
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

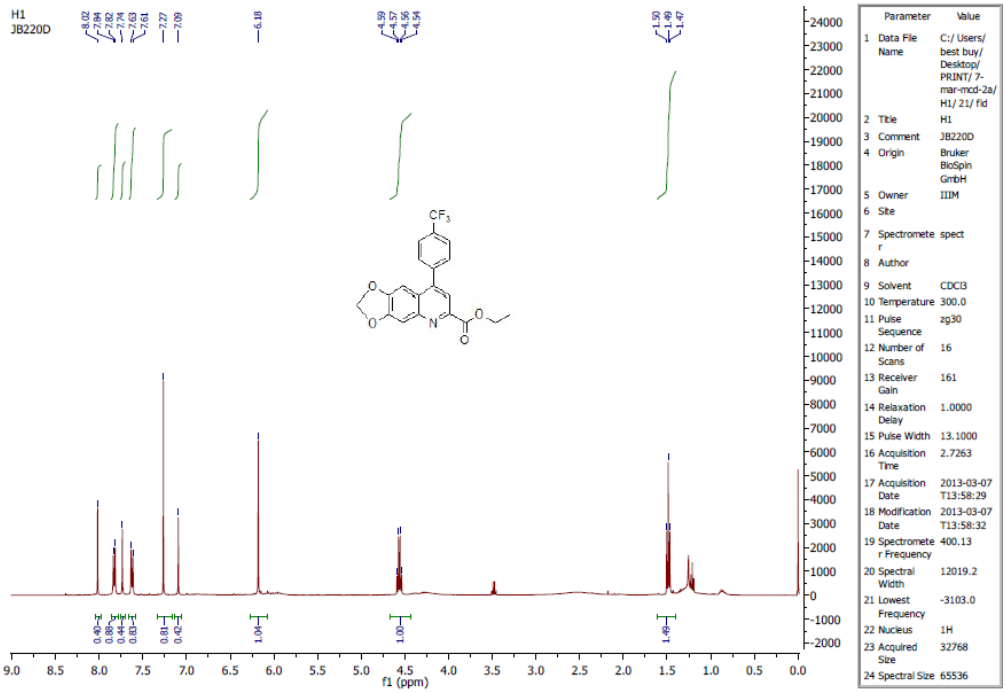
S2.j. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 8-p-tolyl-[1,3]dioxolo[4,5-g]quinoline-6-carboxylate (**1j**)

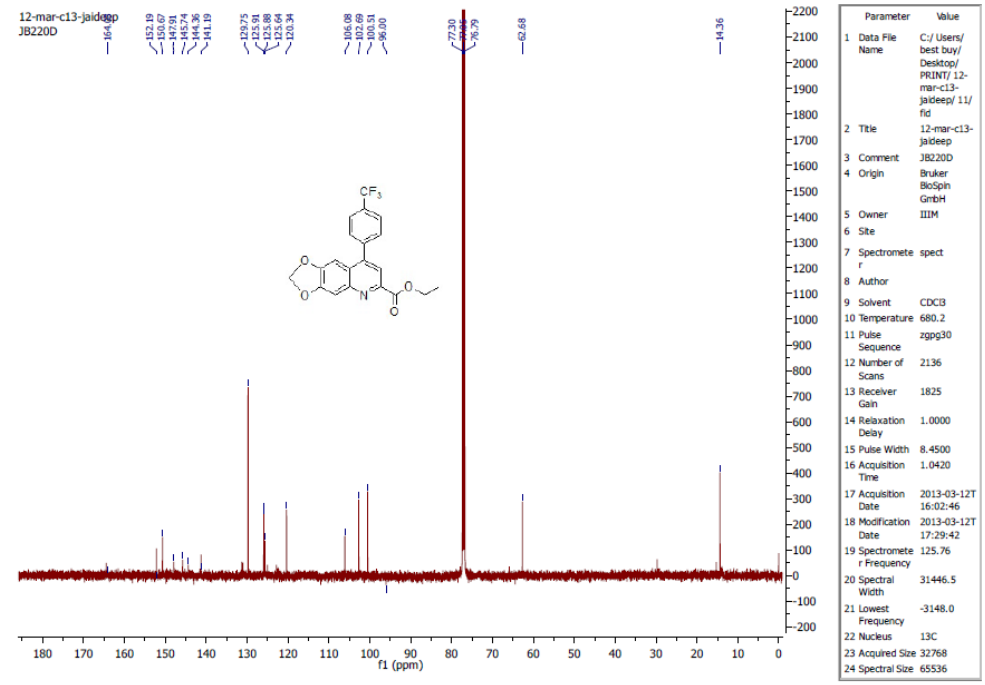


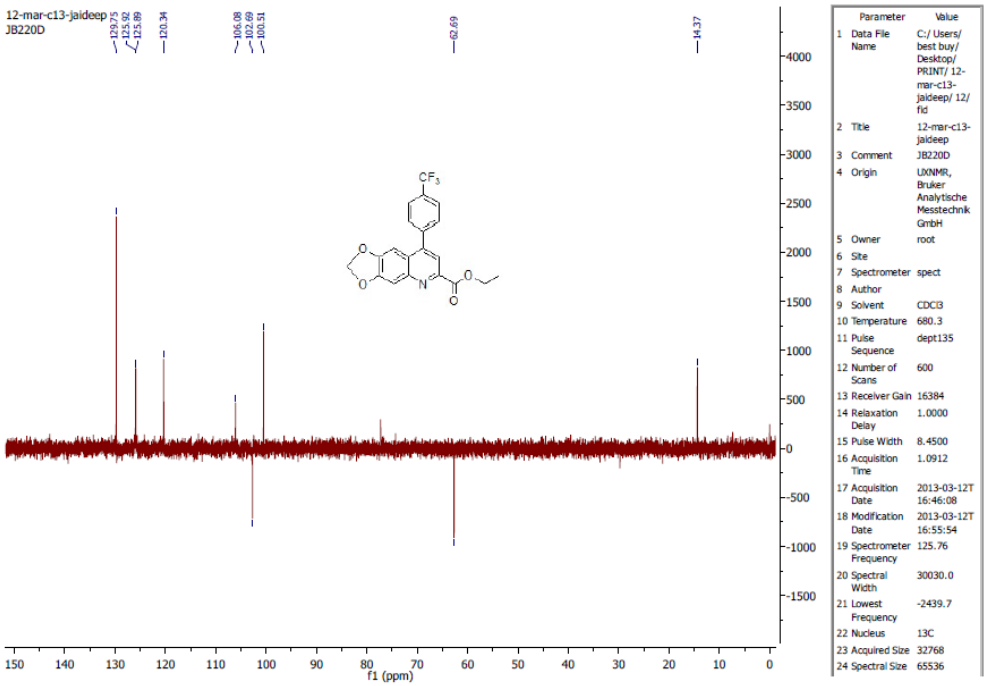



JB220B
JB220B
129.44
129.26
120.44
106.98
102.12
101.00
62.07
21.34
14.42
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
-4000
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
O
N
O
O

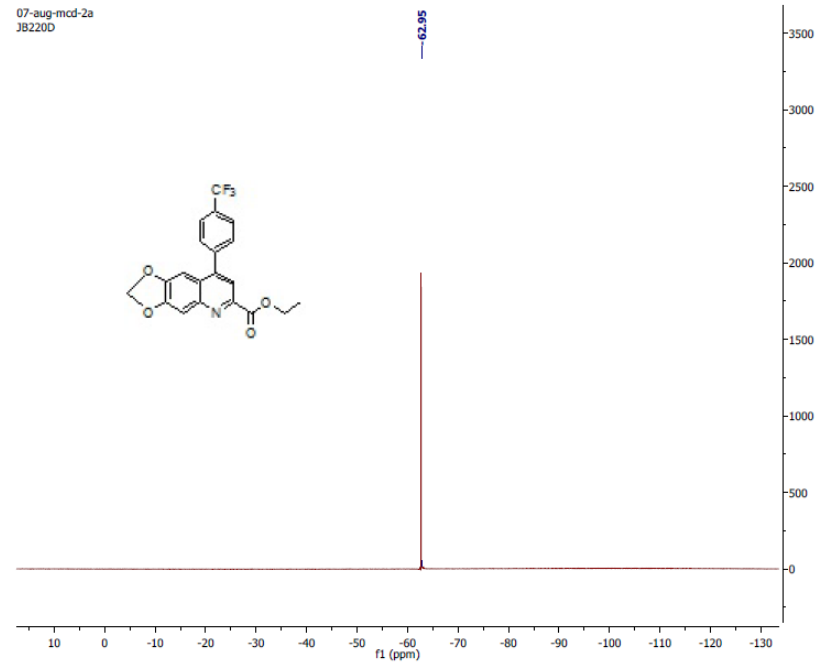
S2.k. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR spectrum of ethyl 8-(4-(trifluoromethyl)phenyl)-[1,3]dioxolo[4,5-g]quinoline-6-carboxylate (**1k**)





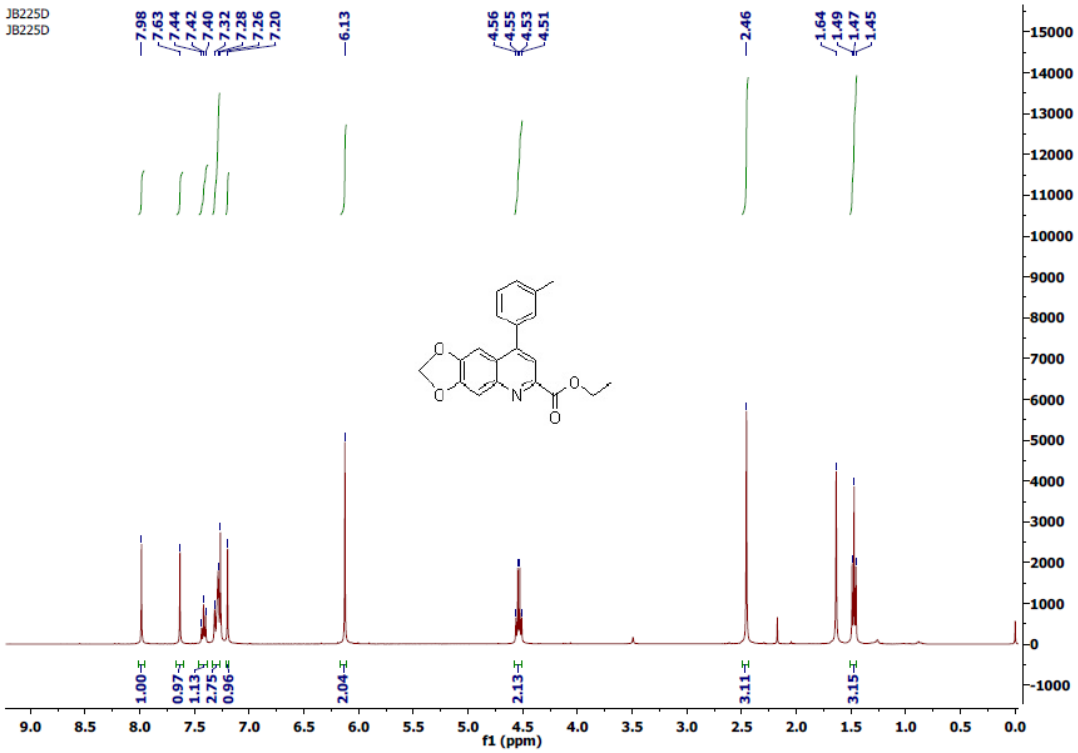


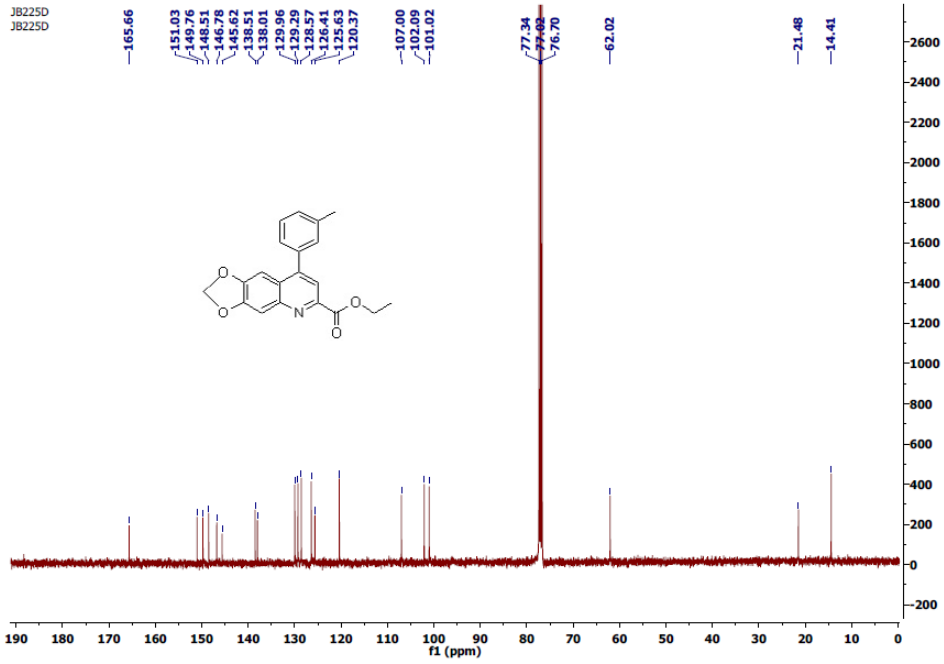
	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 12-mar-c13-jaideep/ 12/ fid
2	Title	12-mar-c13-jaideep
3	Comment	JB220D
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.3
11	Pulse Sequence	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	2013-03-12T 16:46:08
18	Modification Date	2013-03-12T 16:55:54
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

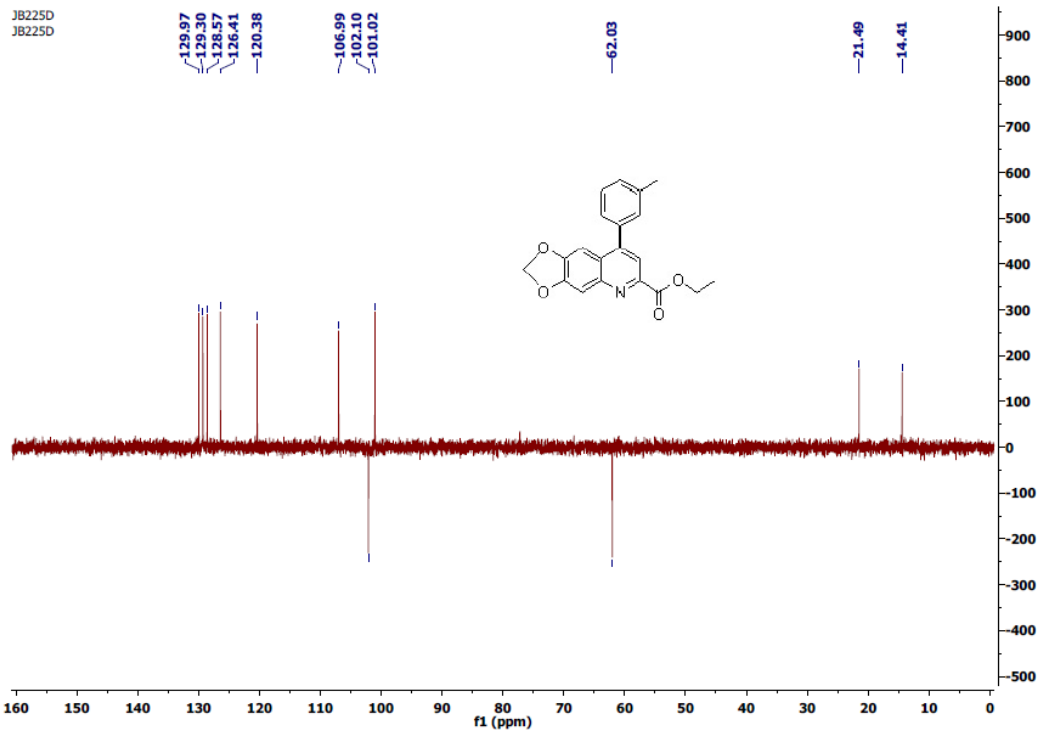


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 07-aug-mcd-2a/ 14/ fid
2	Title	07-aug-mcd-2a
3	Comment	JB220D
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgfiqn
12	Number of Scans	64
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	14.5000
16	Acquisition Time	0.5767
17	Acquisition Date	2013-08-07 T12:12:01
18	Modification Date	2013-08-07 T17:42:04
19	Spectrometer Frequency	376.50
20	Spectral Width	113636.4
21	Lowest Frequency	-94467.8
22	Nucleus	19F
23	Acquired Size	65536

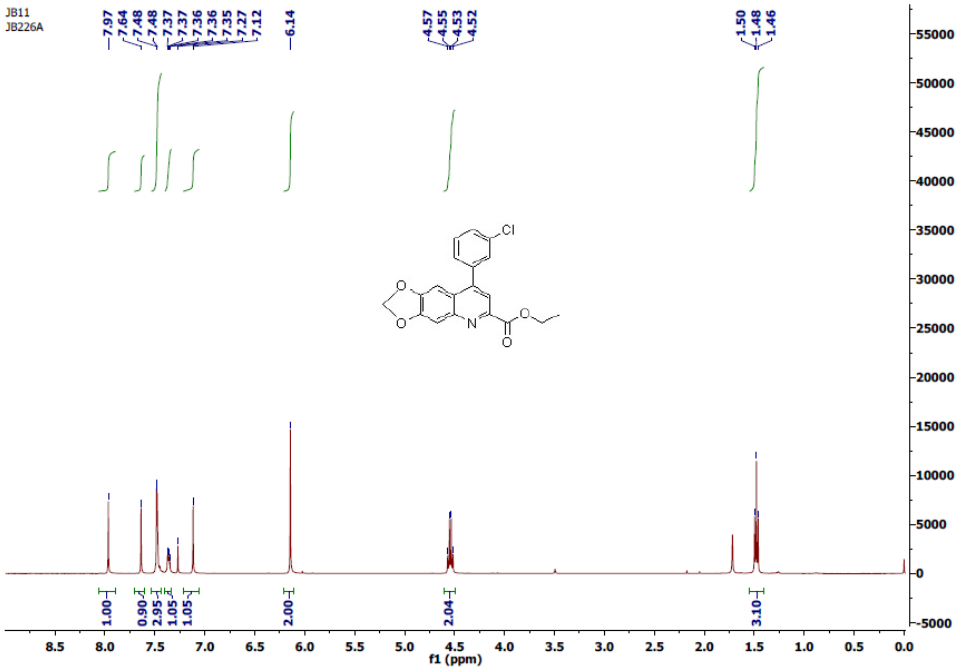
S2.l. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 8-m-tolyl-[1,3]dioxolo[4,5-g]quinoline-6-carboxylate (**11**)

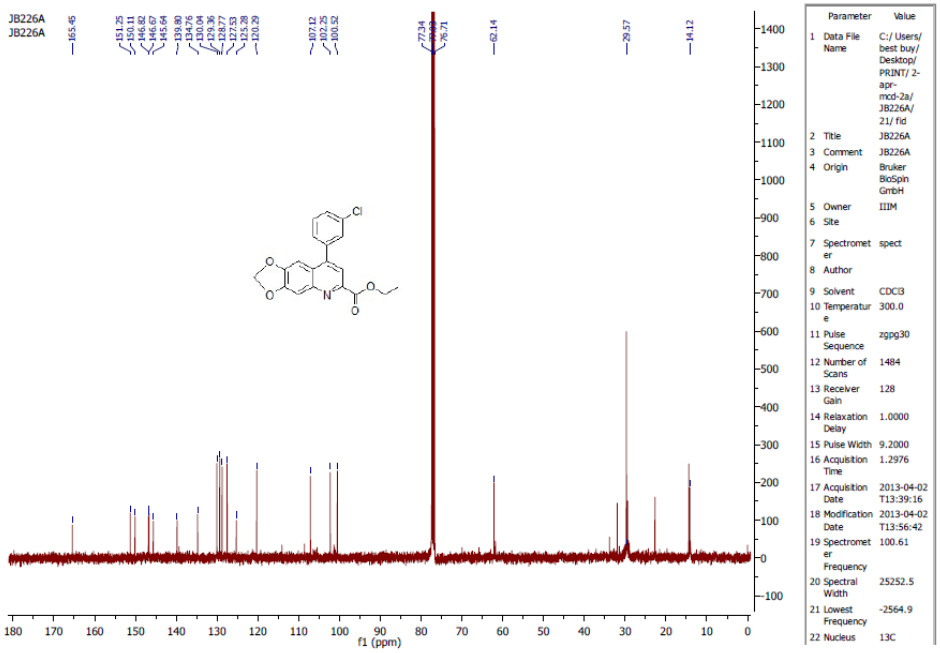


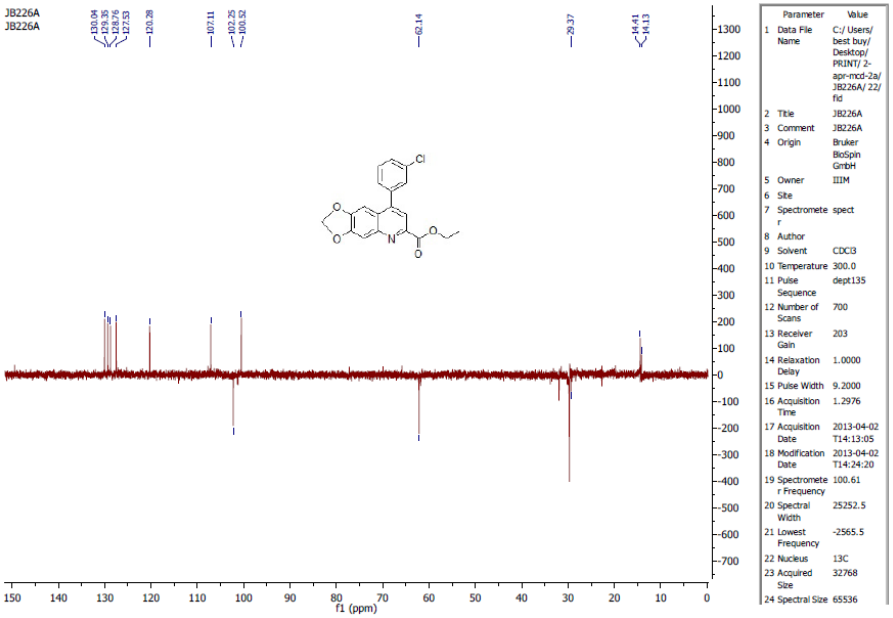



JB225D
JB225D
129.97
129.30
128.57
126.41
120.38
106.99
102.10
101.02
62.03
21.49
14.41
f1 (ppm)

S2.m. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 8-(3-chlorophenyl)-[1,3]dioxolo[4,5-g]quinoline-6-carboxylate (**1m**)

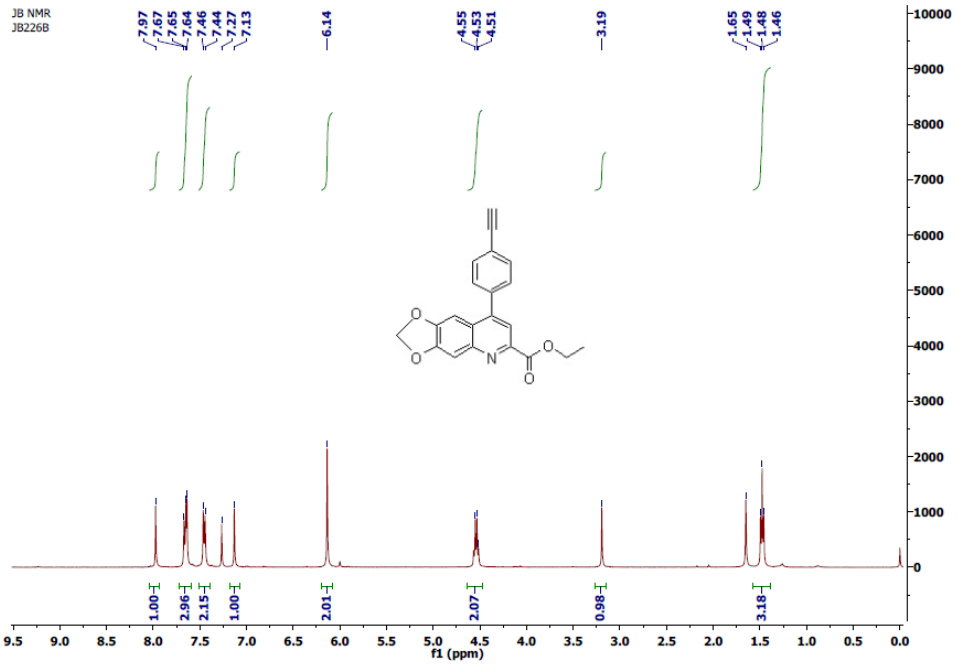


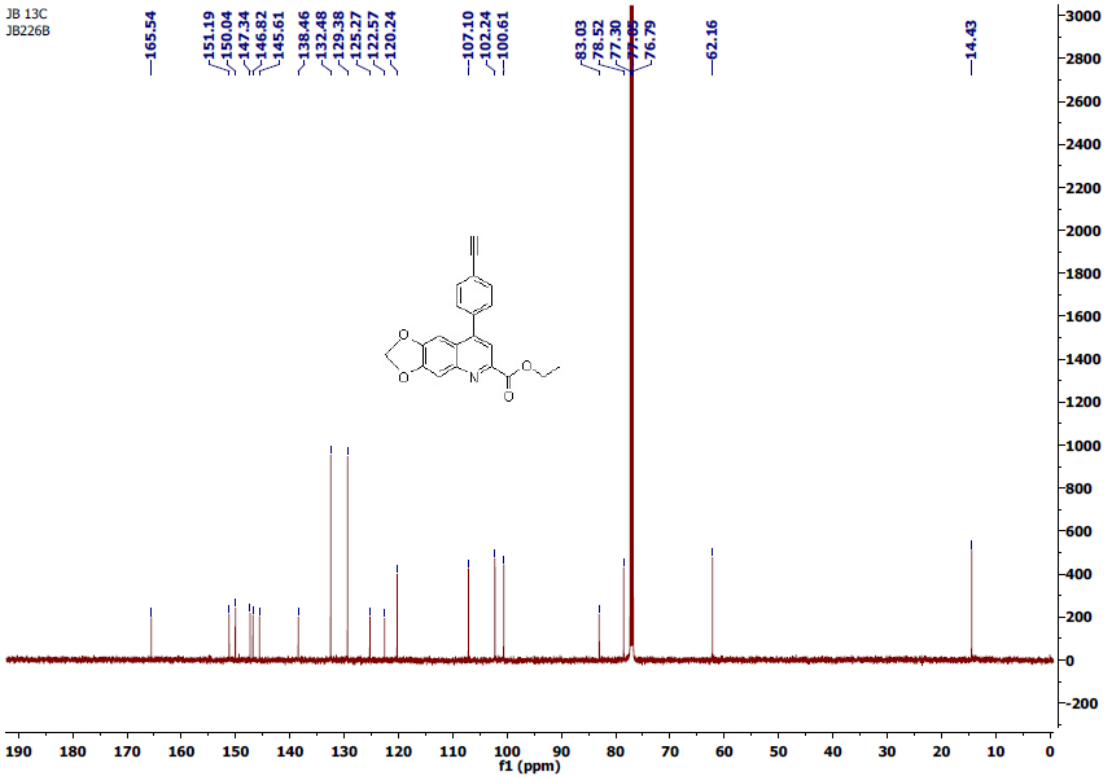


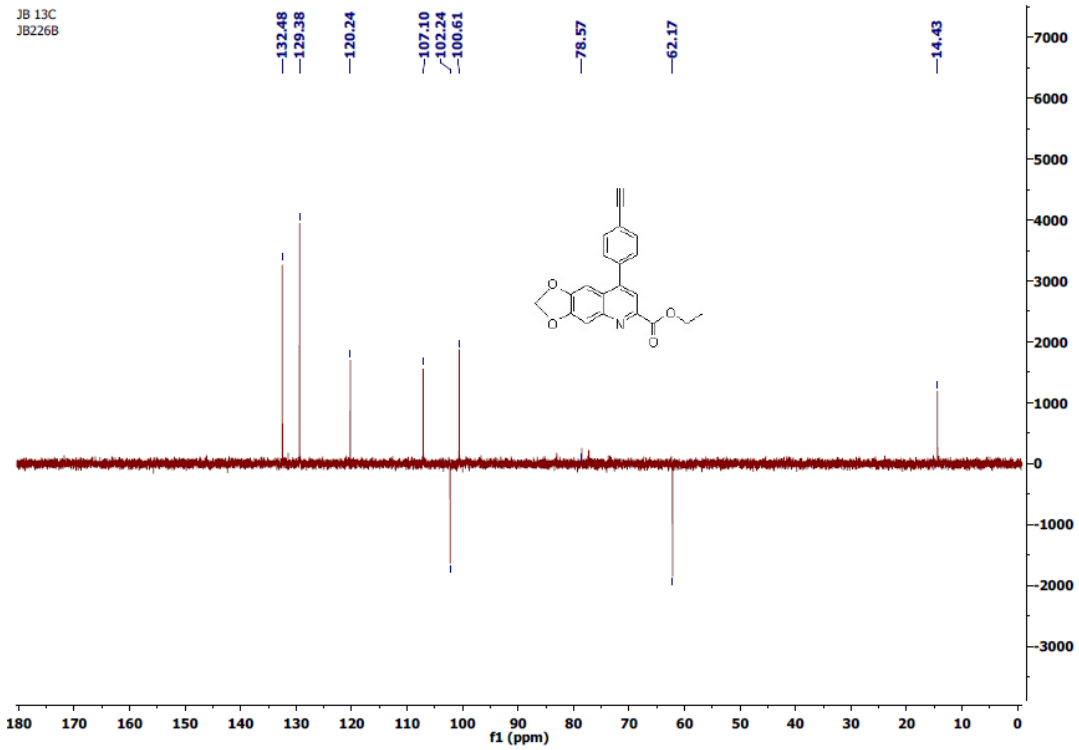


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 2-apr-mcd-2a/ JB226A/ 22/ fid
2	Title	JB226A
3	Comment	JB226A
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	dept135
12	Number of Scans	700
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	9.2000
16	Acquisition Time	1.2976
17	Acquisition Date	2013-04-02 T14:13:05
18	Modification Date	2013-04-02 T14:24:20
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

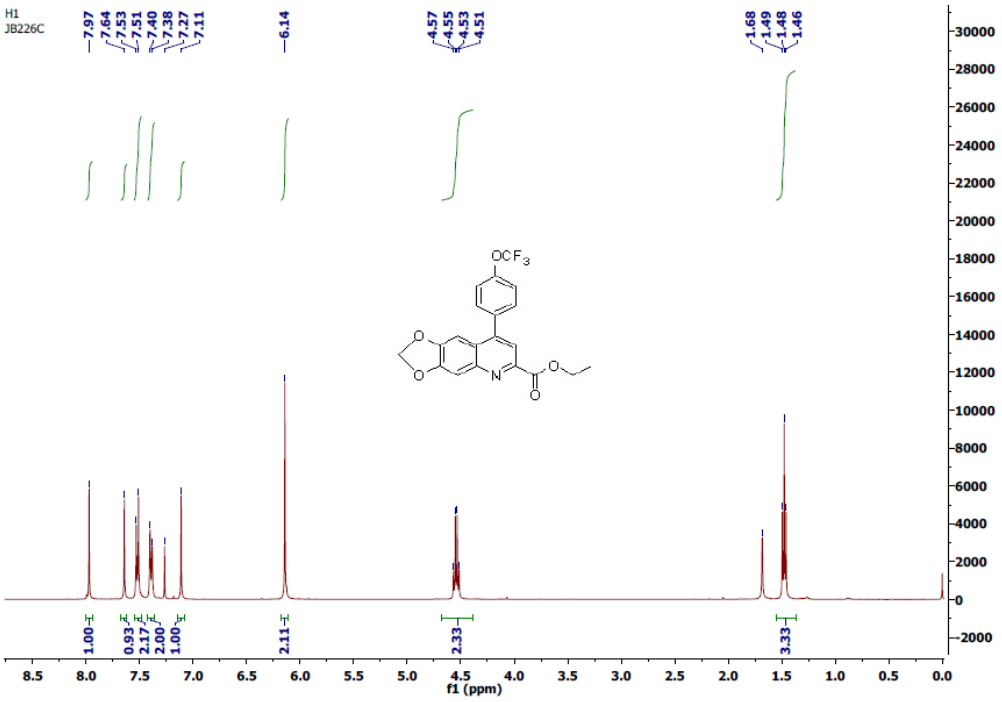
S2.n. ^{1}H, ^{13}C and DEPT-135 NMR Spectrum of ethyl 8-(4-ethynylphenyl)-[1,3]dioxolo[4,5-g]quinoline-6-carboxylate (**1n**)

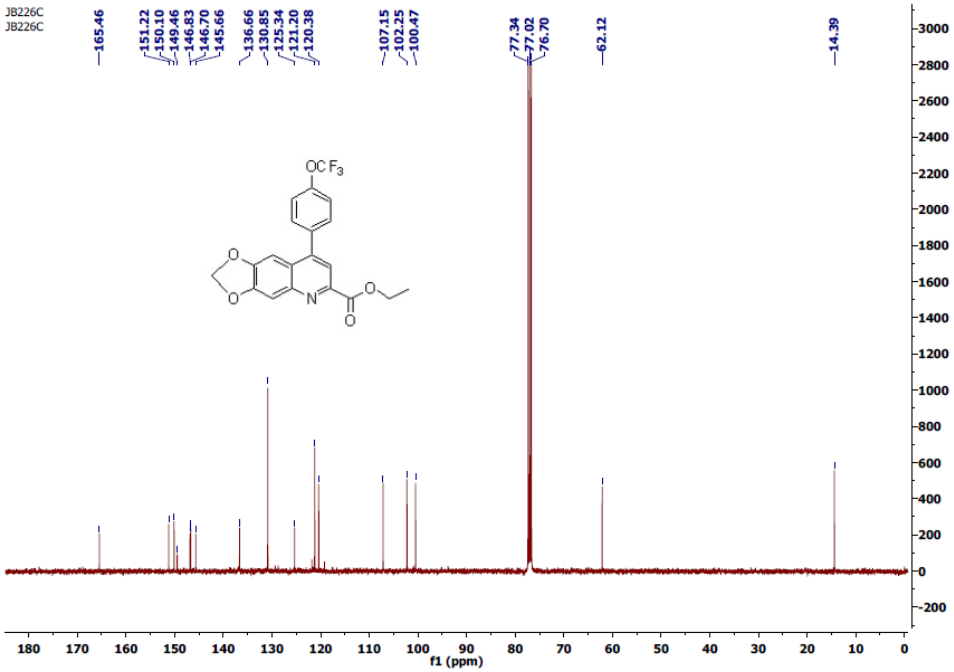


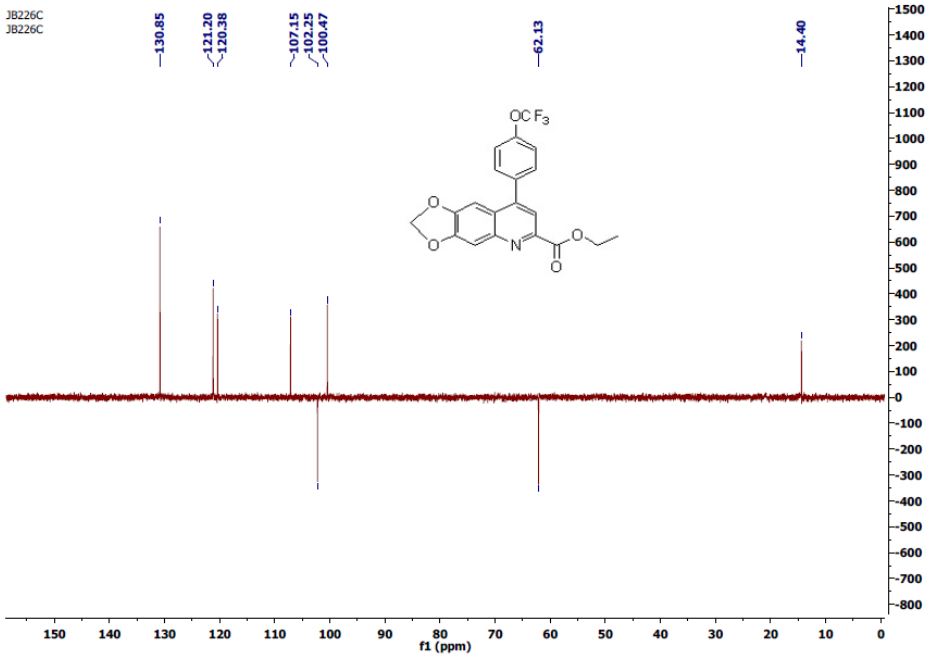


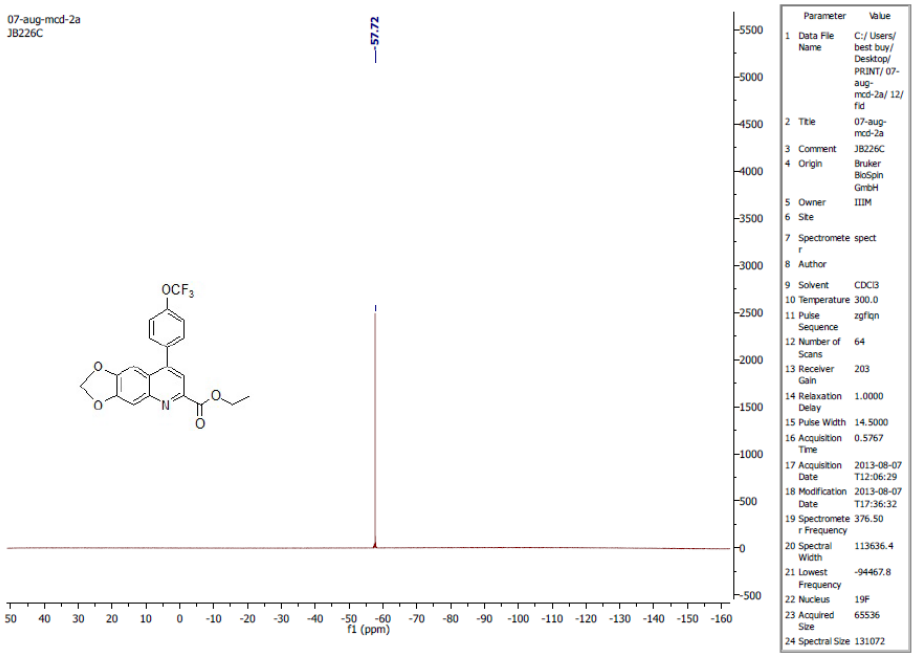

JB 13C
JB226B
132.48
129.38
120.24
107.10
102.24
100.61
78.57
62.17
14.43
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

S2.o. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR spectrum of ethyl 8-(4-(trifluoromethoxy)phenyl)-[1,3]dioxolo[4,5-g]quinoline-6-carboxylate (**1o**)

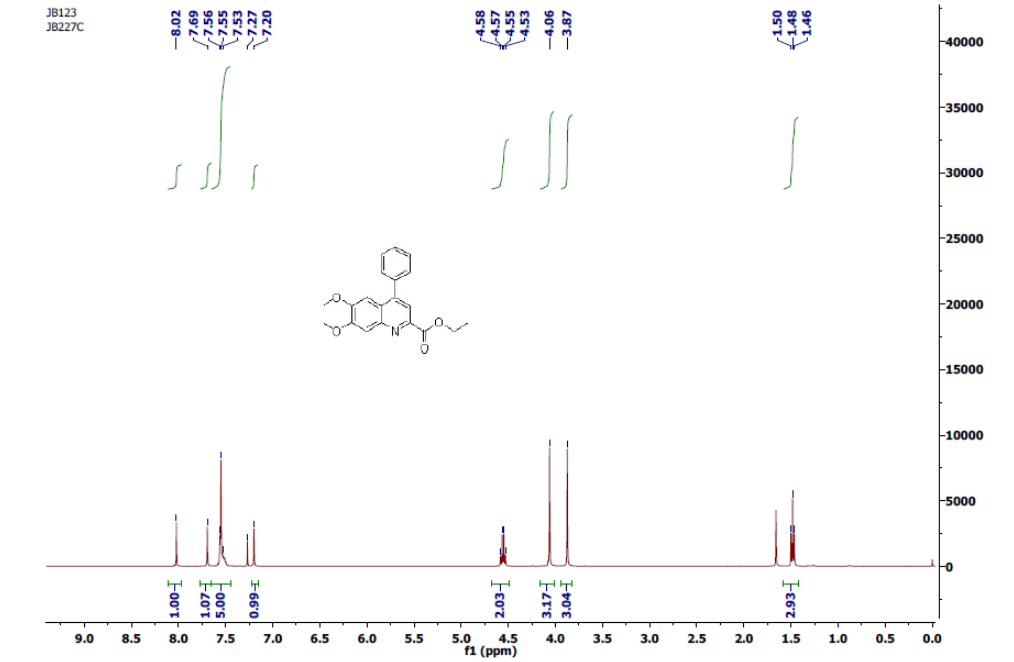


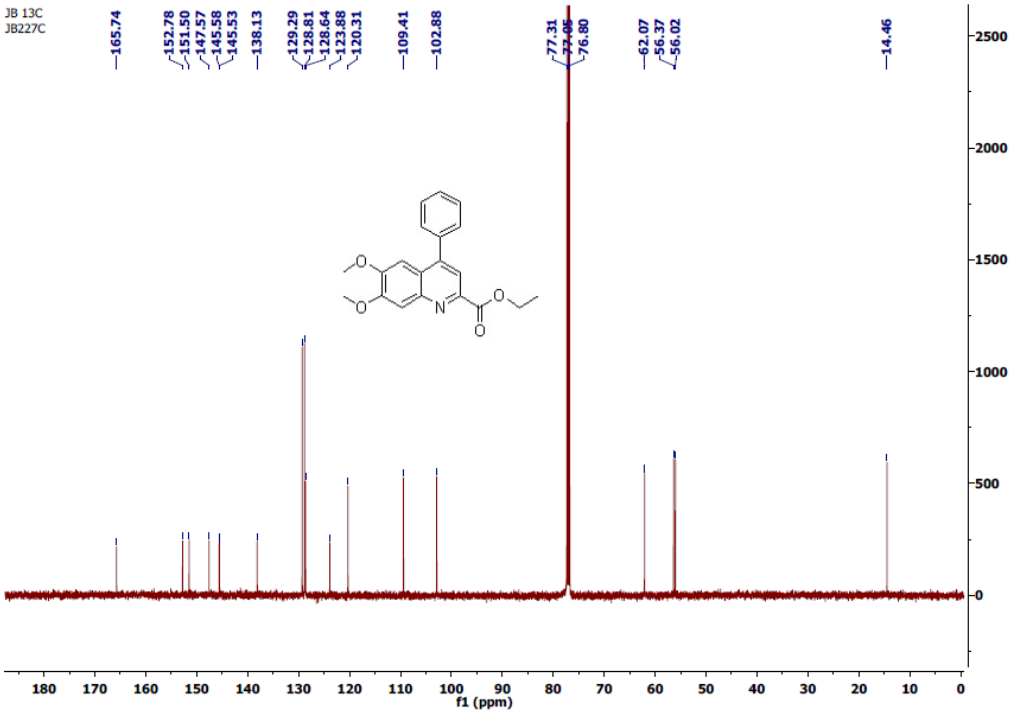


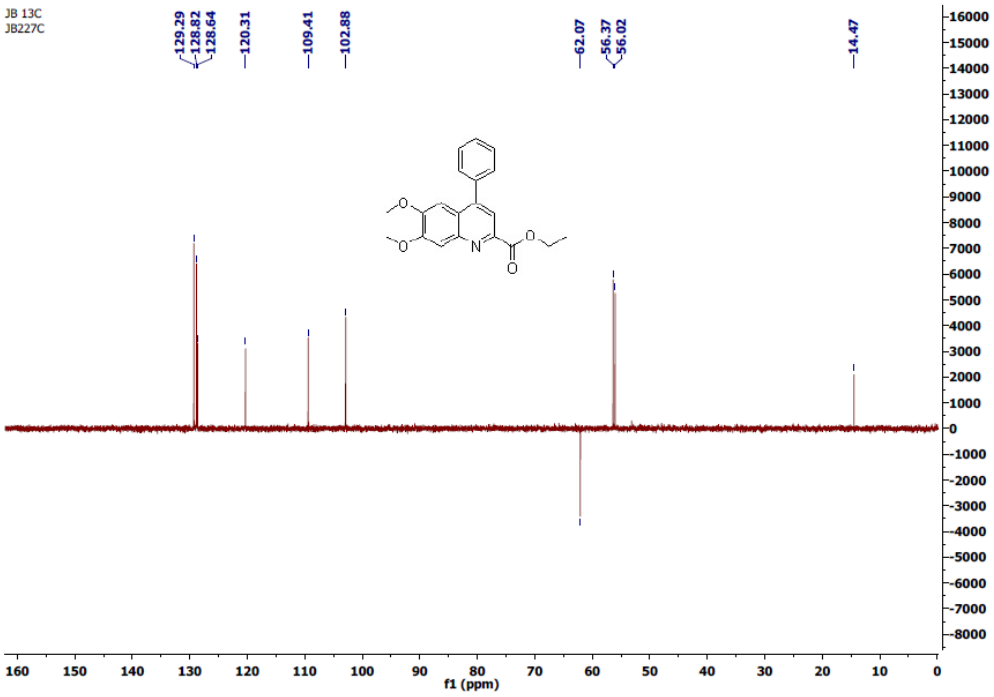

JB226C
JB226C
130.85
121.20
120.38
107.15
102.25
100.47
62.13
14.40
OCF3
O
O
N
O
O
f1 (ppm)


07-aug-mcd-2a
JB226C
57.72
OCF3
O
O
N
O
O
f1 (ppm)
Parameter Value
1 Data File Name C:/ Users/ best buy/ Desktop/ PRINT/ 07-aug-mcd-2a/ 12/ fid
2 Title 07-aug-mcd-2a
3 Comment JB226C
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 64
13 Receiver Gain 203
14 Relaxation Delay 1.0000
15 Pulse Width 14.5000
16 Acquisition Time 0.5767
17 Acquisition Date 2013-08-07 T12:06:29
18 Modification Date 2013-08-07 T17:36:32
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

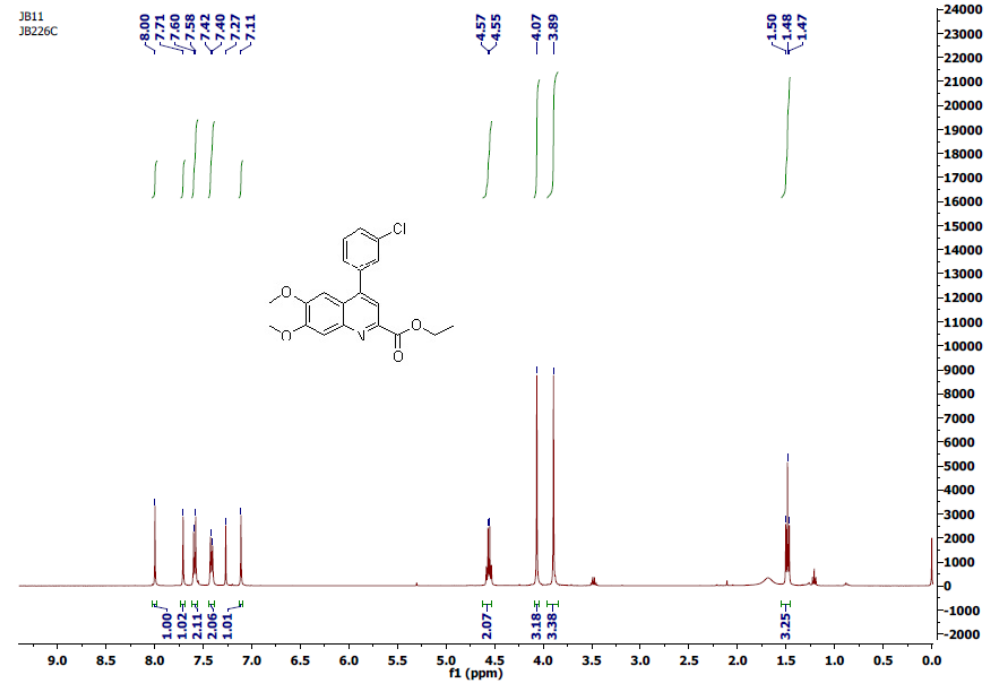
S3.p. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 6,7-dimethoxy-4-phenylquinoline-2-carboxylate (**1p**)

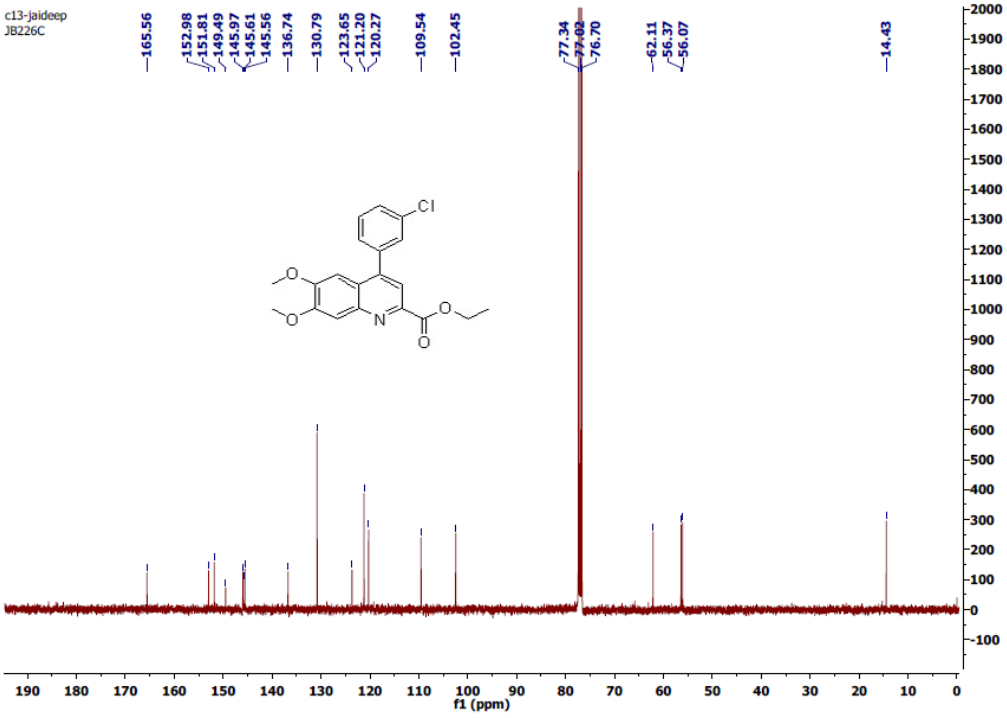


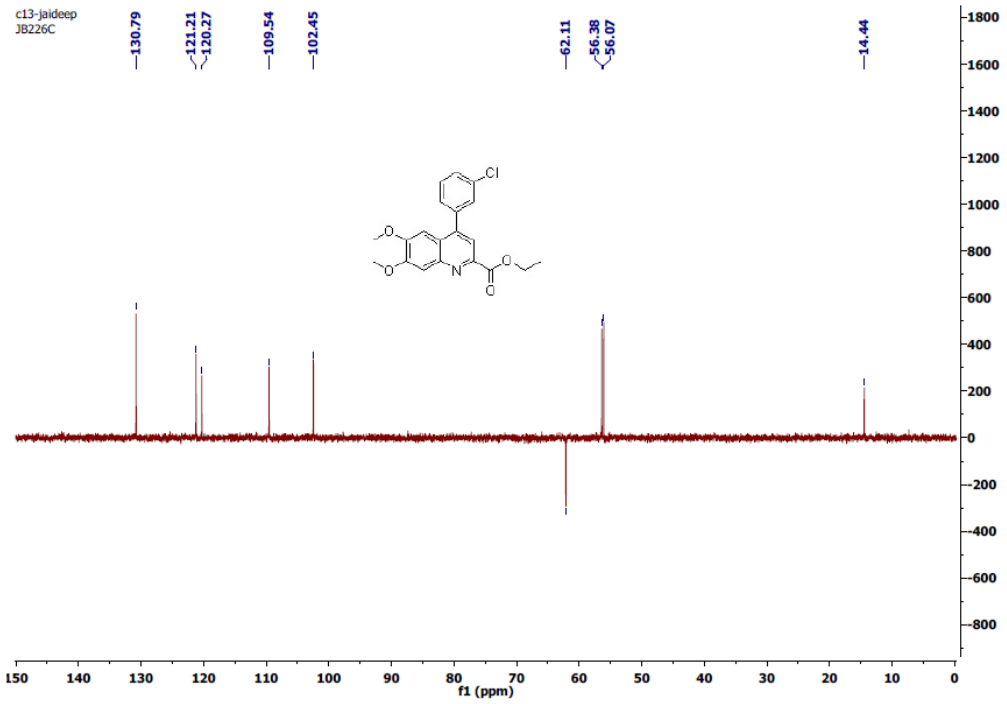



JB 13C
JB227C
129.29
128.82
128.64
120.31
109.41
102.88
62.07
56.37
56.02
14.47
f1 (ppm)

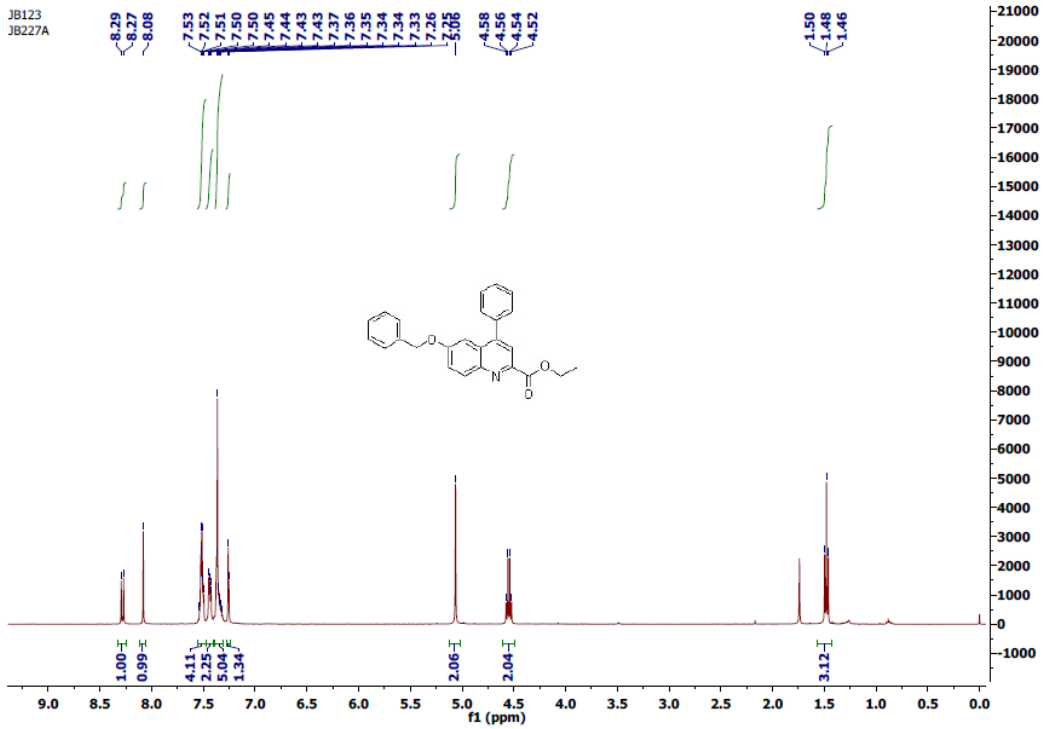
S3.q. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 4-(3-chlorophenyl)-6,7-dimethoxyquinoline-2-carboxylate (**1q**)

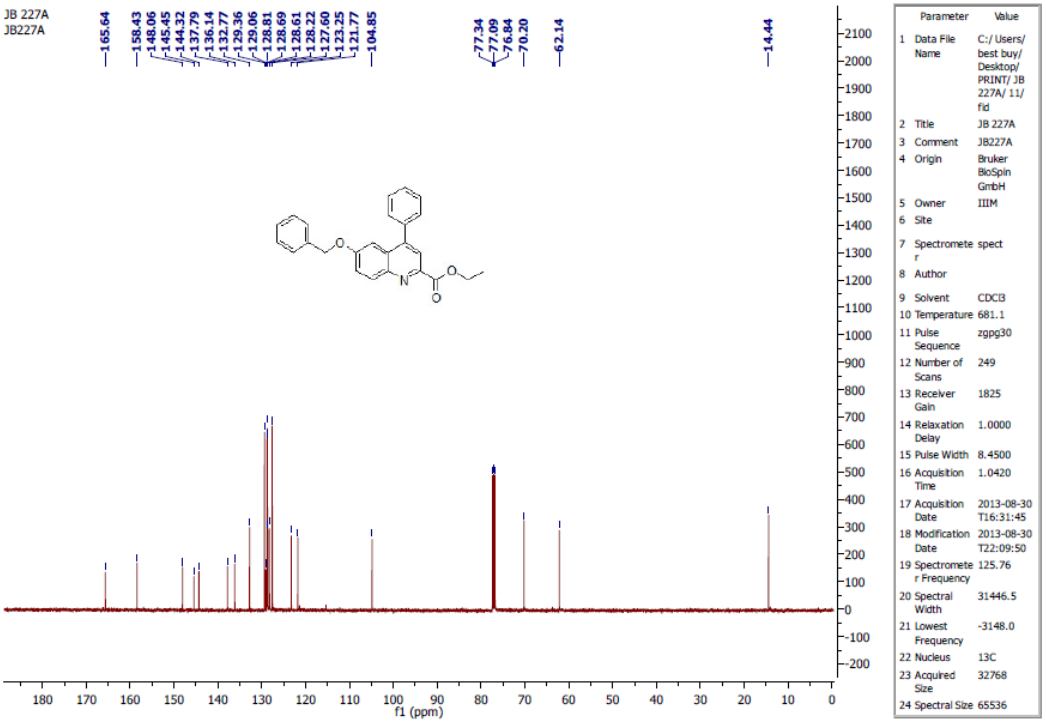


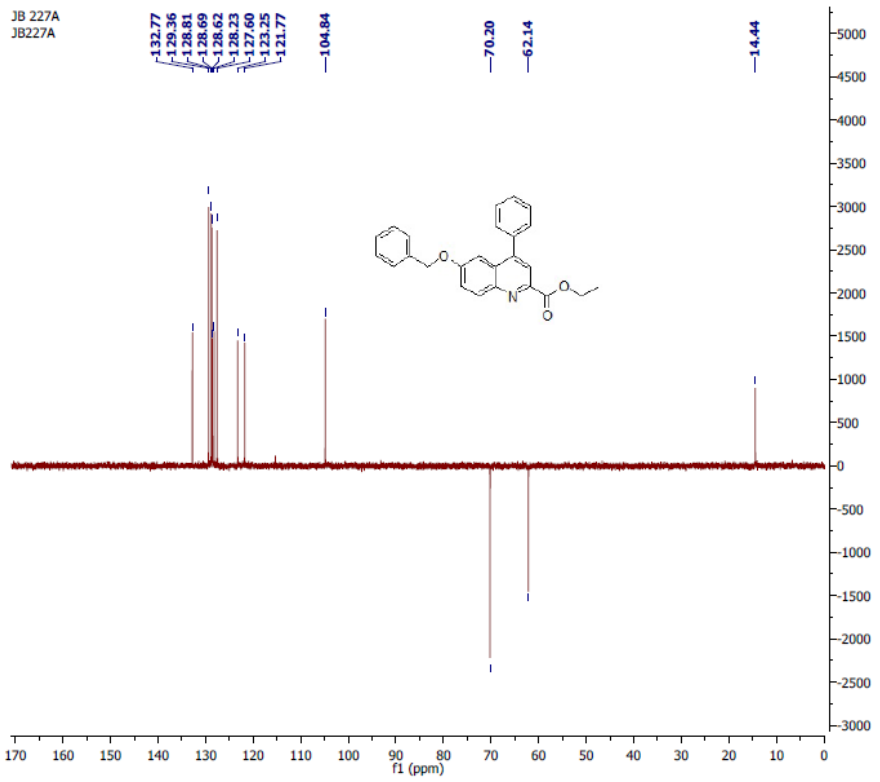



c13-jaideep
JB226C
130.79
121.21
120.27
109.54
102.45
62.11
56.38
56.07
14.44
Cl
O
O
N
O
O
f1 (ppm)

S4.r. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 6-(benzyloxy)-4-phenylquinoline-2-carboxylate (**1r**)

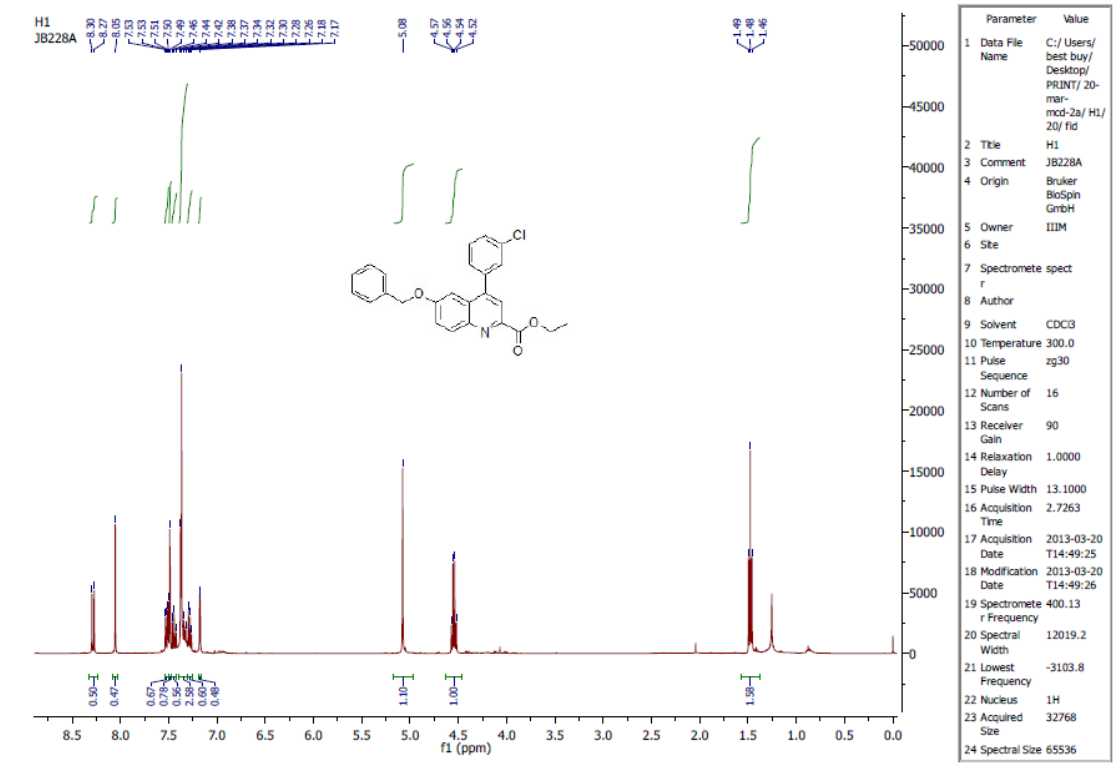


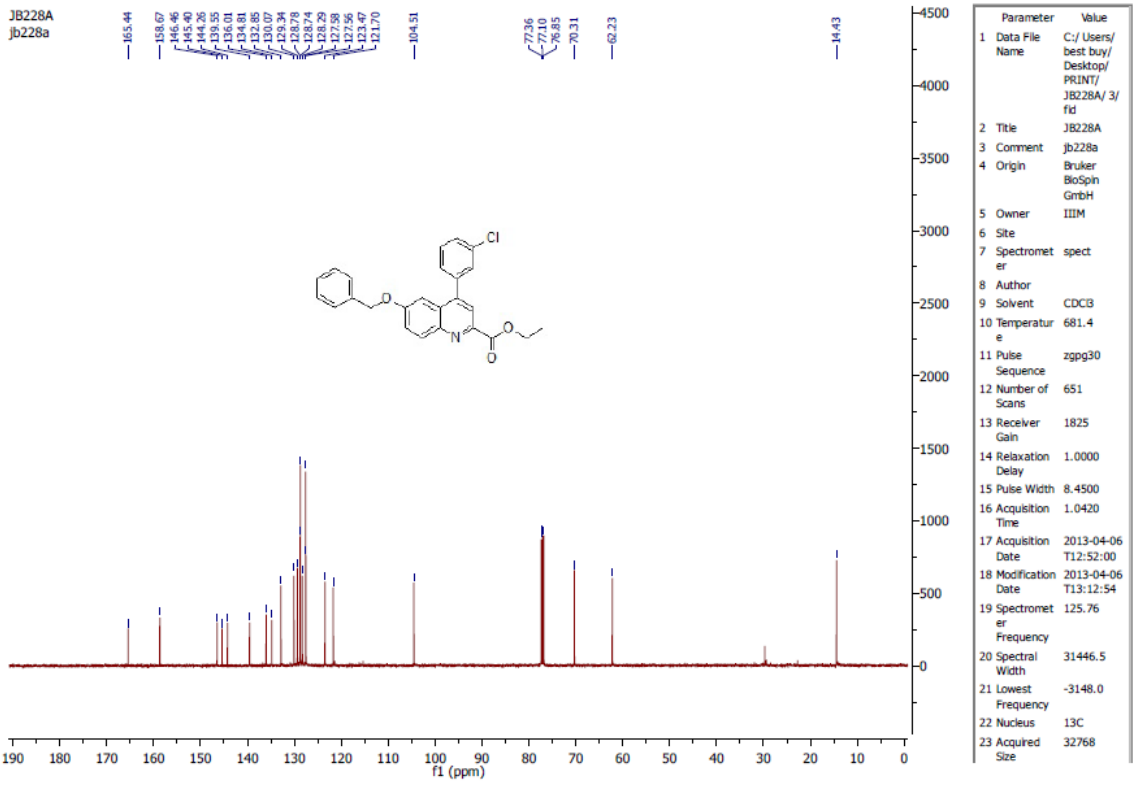


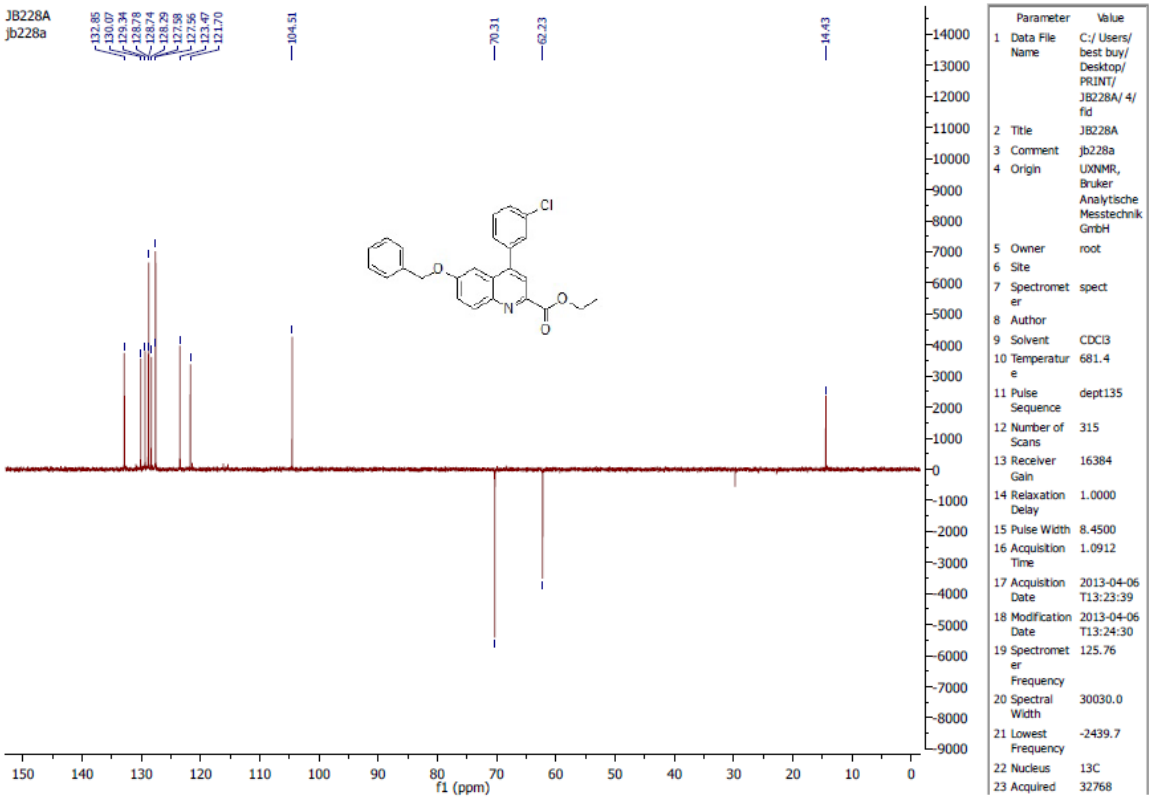


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ JB 227A/ 12/ fid
2	Title	JB 227A
3	Comment	JB227A
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	681.0
11	Pulse Sequence	dept135
12	Number of Scans	100
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2013-08-30T 16:43:43
18	Modification Date	2013-08-30T 22:13:50
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

S4.s. ^{1}H, ^{13}C and DEPT-135 NMR spectrum of ethyl 6-(benzyloxy)-4-(3-chlorophenyl)quinoline-2-carboxylate (**1s**)

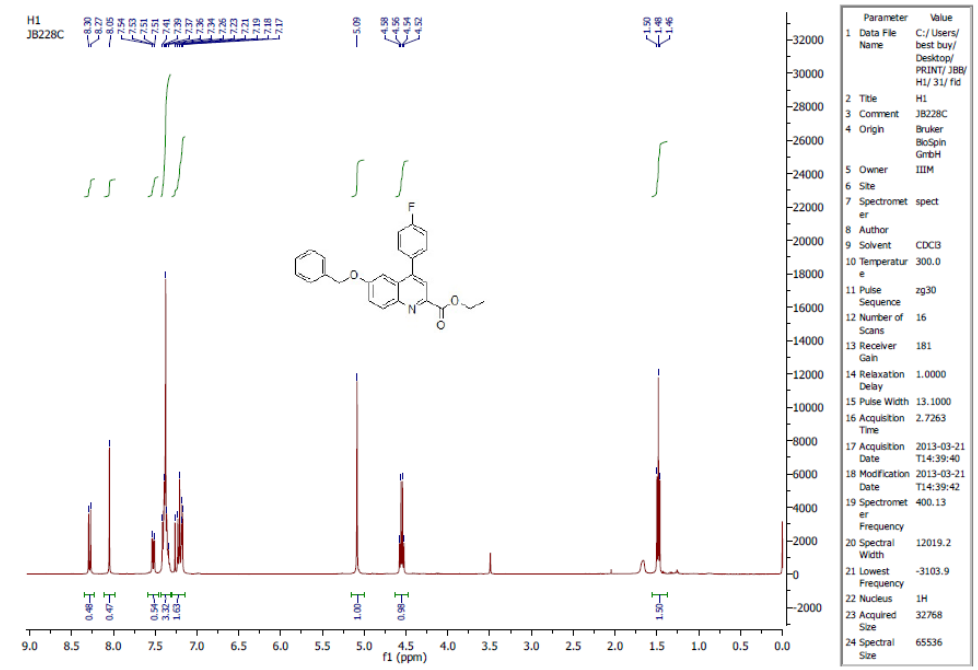


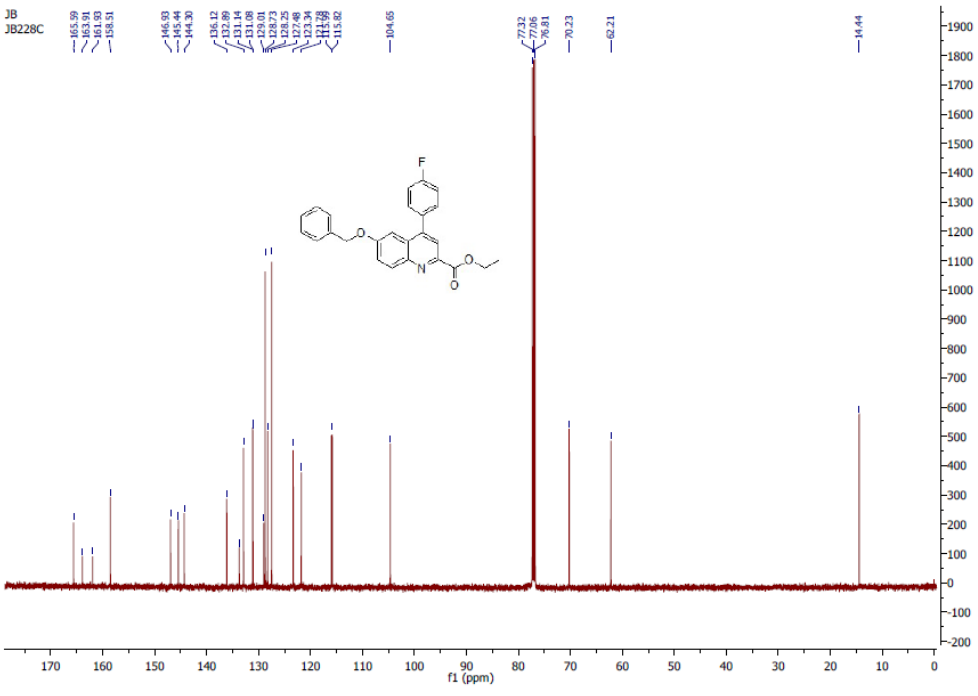


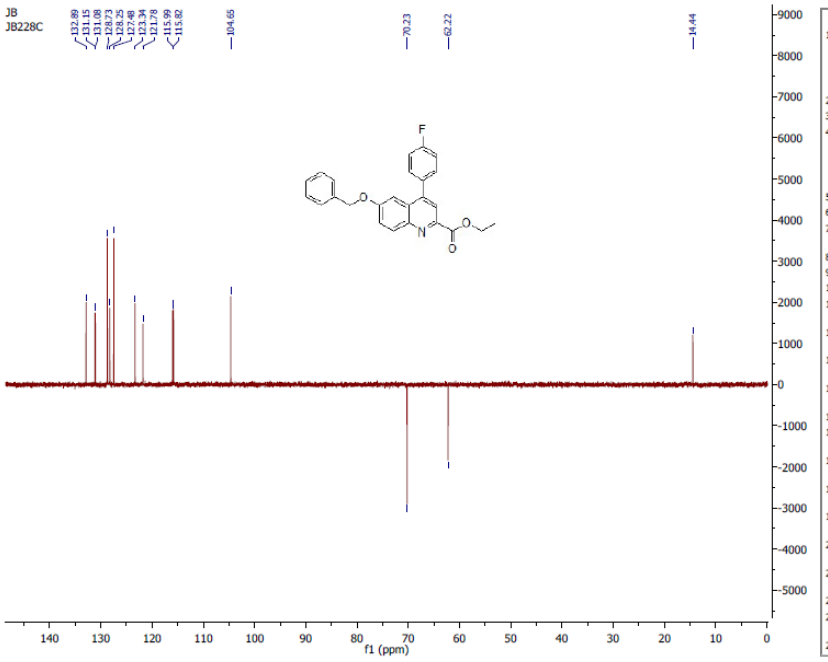


	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ JB228A/ 4/ fid
2	Title	JB228A
3	Comment	jb228a
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	681.4
11	Pulse Sequence	dept135
12	Number of Scans	315
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2013-04-06 T13:23:39
18	Modification Date	2013-04-06 T13:24:30
19	Spectrometer Frequency	125.76
20	Spectral Width	30030.0
21	Lowest Frequency	-2439.7
22	Nucleus	13C
23	Acquired	32768

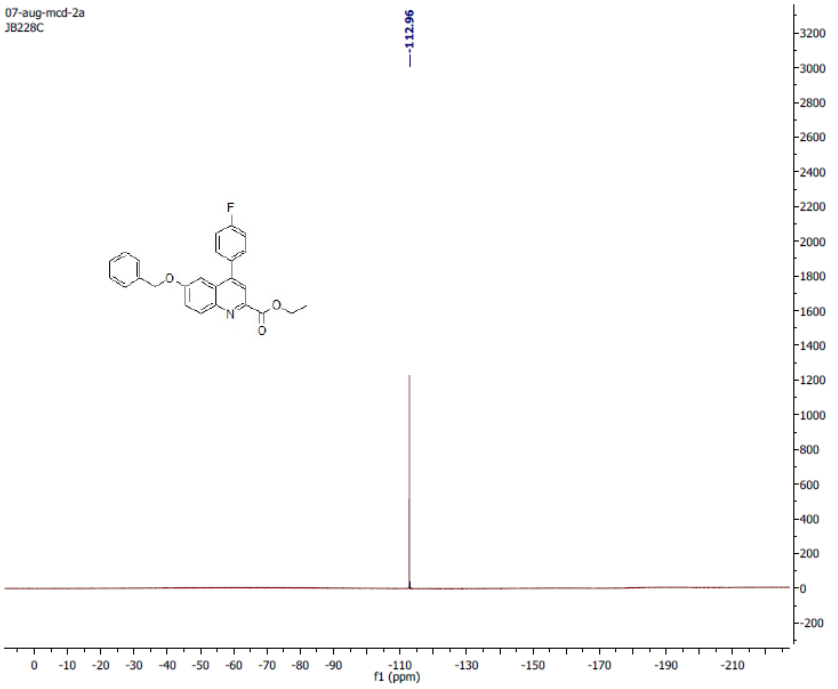
S4.t. ^{1}H, ^{13}C, DEPT-135 and ^{19}F NMR spectrum of ethyl 6-(benzyloxy)-4-(4-fluorophenyl)quinoline-2-carboxylate (**1t**)







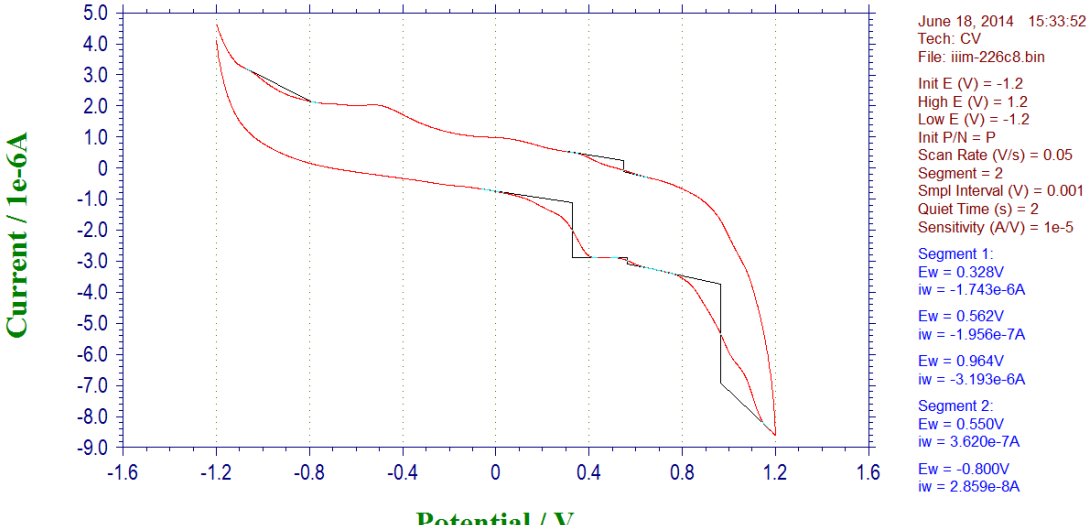
	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ JB/ 14/ fid
2	Title	JB
3	Comment	JB228C
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	679.7
11	Pulse Sequence	dept135
12	Number of Scans	241
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2013-03-25 T17:43:20
18	Modification Date	2013-03-25 T17:43:26
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

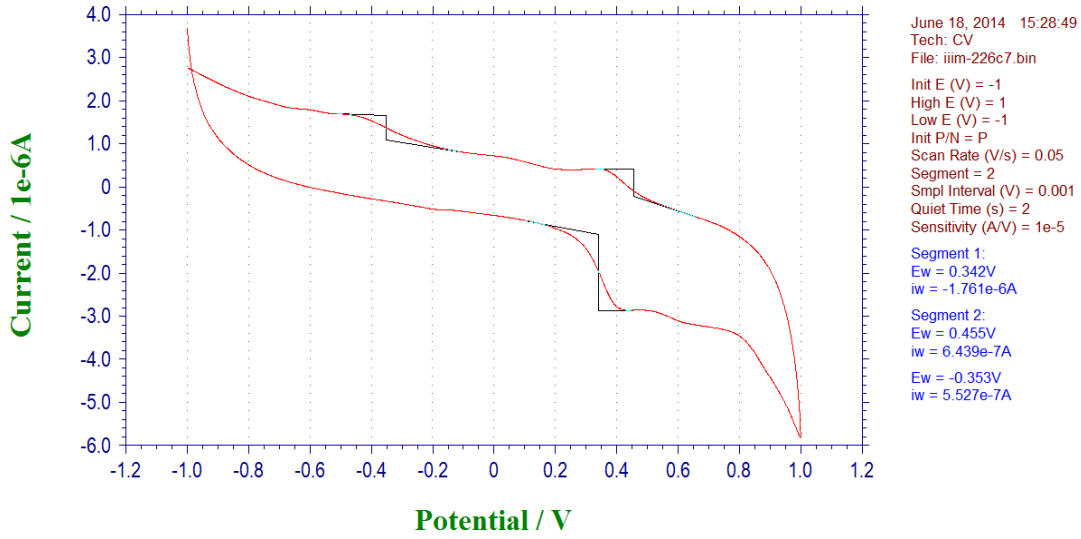


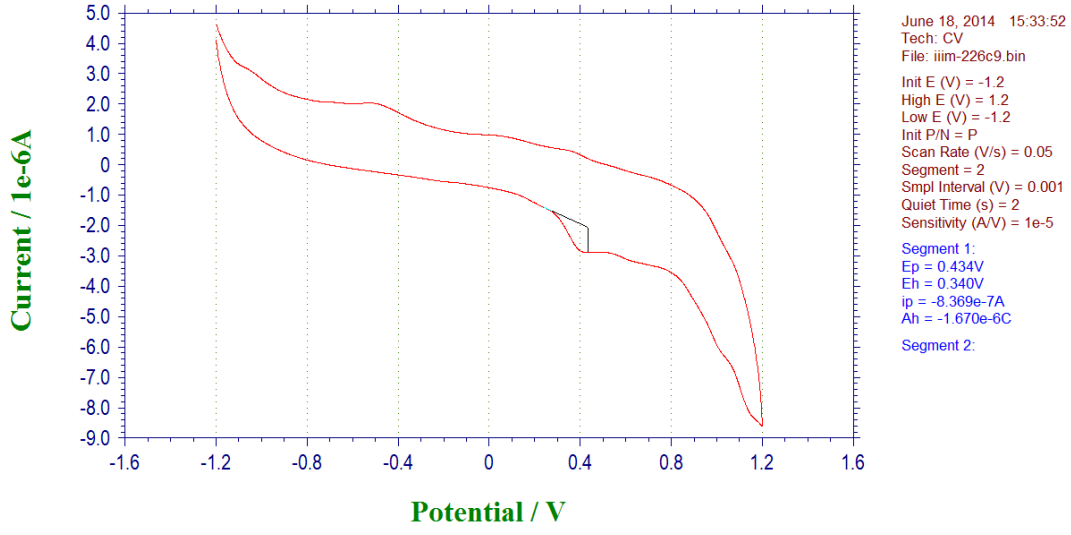
	Parameter	Value
1	Data File Name	C:/ Users/ best buy/ Desktop/ PRINT/ 07-aug-mcd-2a/ 11/ fid
2	Title	07-aug-mcd-2a
3	Comment	JB228C
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgflqn
12	Number of Scans	64
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	14.5000
16	Acquisition Time	0.5767
17	Acquisition Date	2013-08-07T 12:01:46
18	Modification Date	2013-08-07T 17:31:48
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. Redox potential measurement of compound 1o

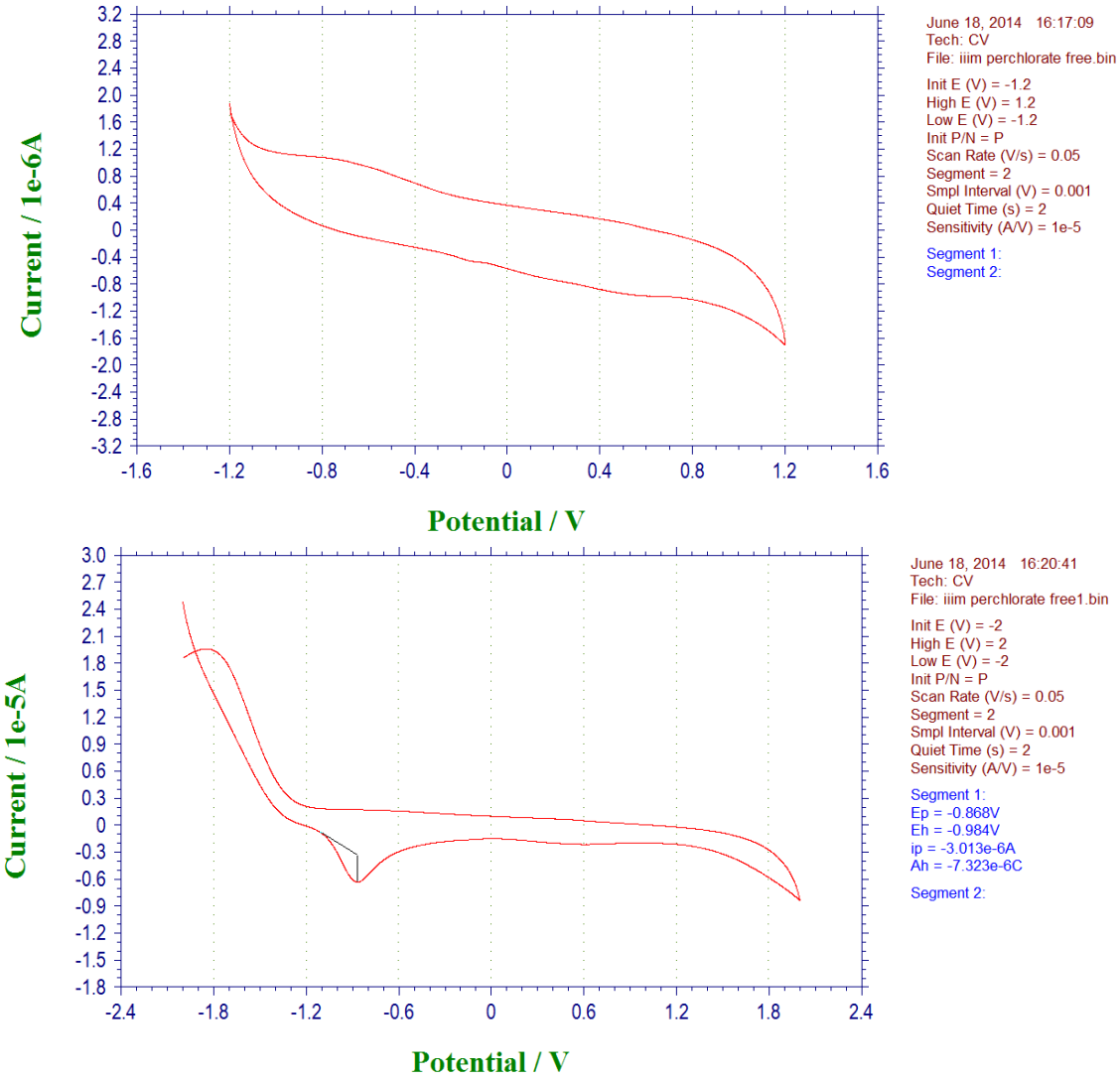
S2a. Cyclic voltammogram trace of compound **1o**





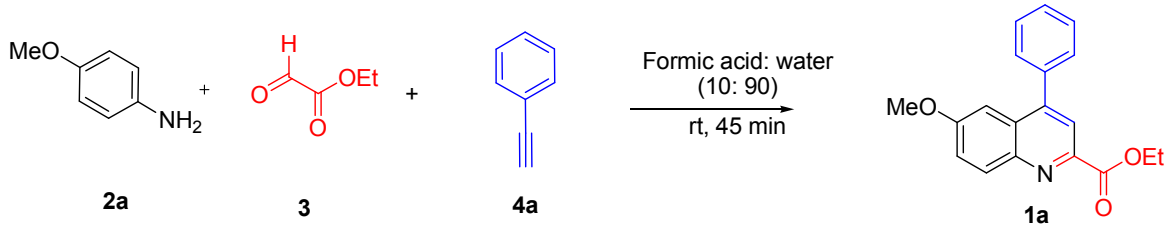


S2b. Cyclic voltammogram trace of tetrabutylammonium perchlorate (ACN)



S3. LCMS analysis of the reaction mixture

The reaction was carried out using optimized reaction conditions (Entry 16 of Table 1). The LCMS analysis was done after 45 min reaction time.

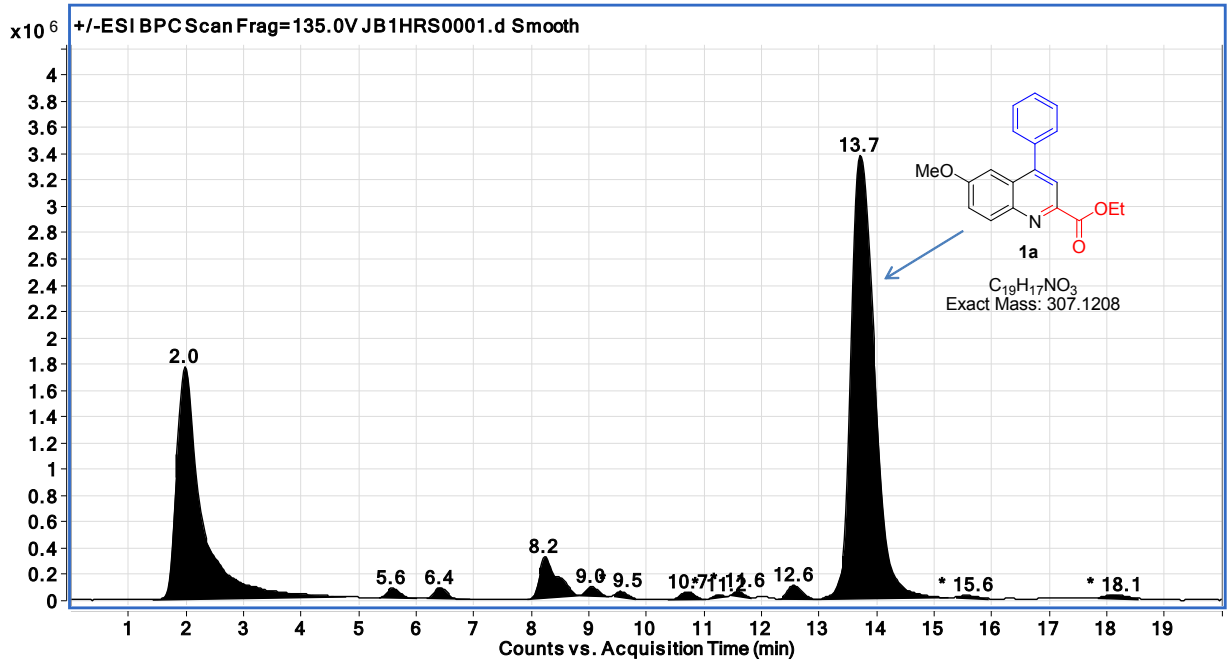


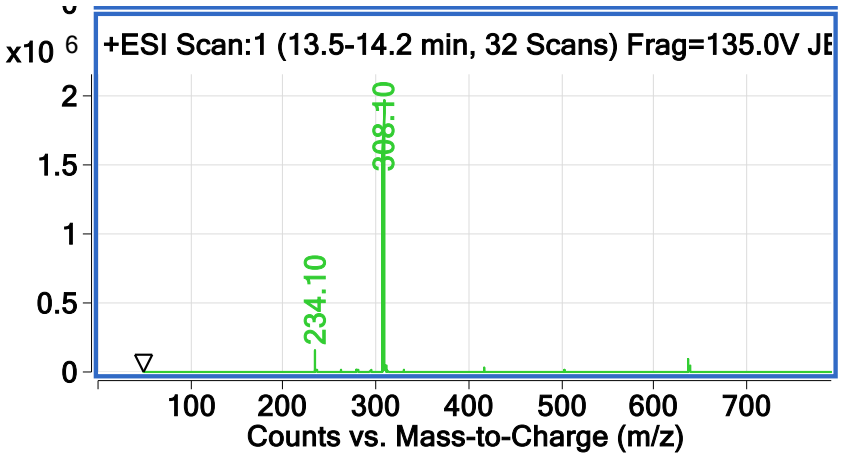
C_7H_9NO
Exact Mass: 123.0684

$C_4H_6O_3$
Exact Mass: 102.0317

C_8H_6
Exact Mass: 102.047

$C_{19}H_{17}NO_3$
Exact Mass: 307.1208





LC-ESI-MS/MS analysis was carried out on Agilent Triple-Quad LC-MS/MS system (model 6410). Liquid chromatography analyses were carried out using an Agilent 1260 Infinity (Agilent, USA) quaternary pump equipped with an autosampler, column heater and online degasser. A Chromolith C_{18} (Merck, Germany) column (55 x 4.6 mm) was used at 30 °C temperature and the injection volume was 10 µl. The elution was carried out with binary solvent system consisting of 0.1% formic acid in water (solvent A) and acetonitrile (solvent B) at a constant flow-rate of 0.5 ml/min. The gradient elution was used, as depicted in Table S1-a.

Table S1-a. Gradient details used in LC-ESI-MS/MS analysis

Time	**Solvent A (water)**	**Solvent B (acetonitrile)**	**Flow rate (ml/min)**
0	90	10	0.5
10	40	60	0.5
15	40	60	0.5
17	90	10	0.5
20	90	10	0.5

Table S1-b. Instrument parameters during LC-ESI-MS analysis

Source parameters		**Autosampler parameters**		**Quaternary pump parameters**	
Gas Temp.	300 °C	Injection volume	10 µl	Run time	20 min
Gas flow	12 L/min	Eject speed	200 µl/min	Flow rate	0.5 ml/min
Nebulizer pressure	50 psi	Draw speed	200 µl/min	Elution	Gradient*
Capillary voltage	4000 v				
Cell Acc (v)	7 v				

* Gradient system is provided in Table S1-a