Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
This journal is © The Royal Society of Chemistry 2015

Supporting Information

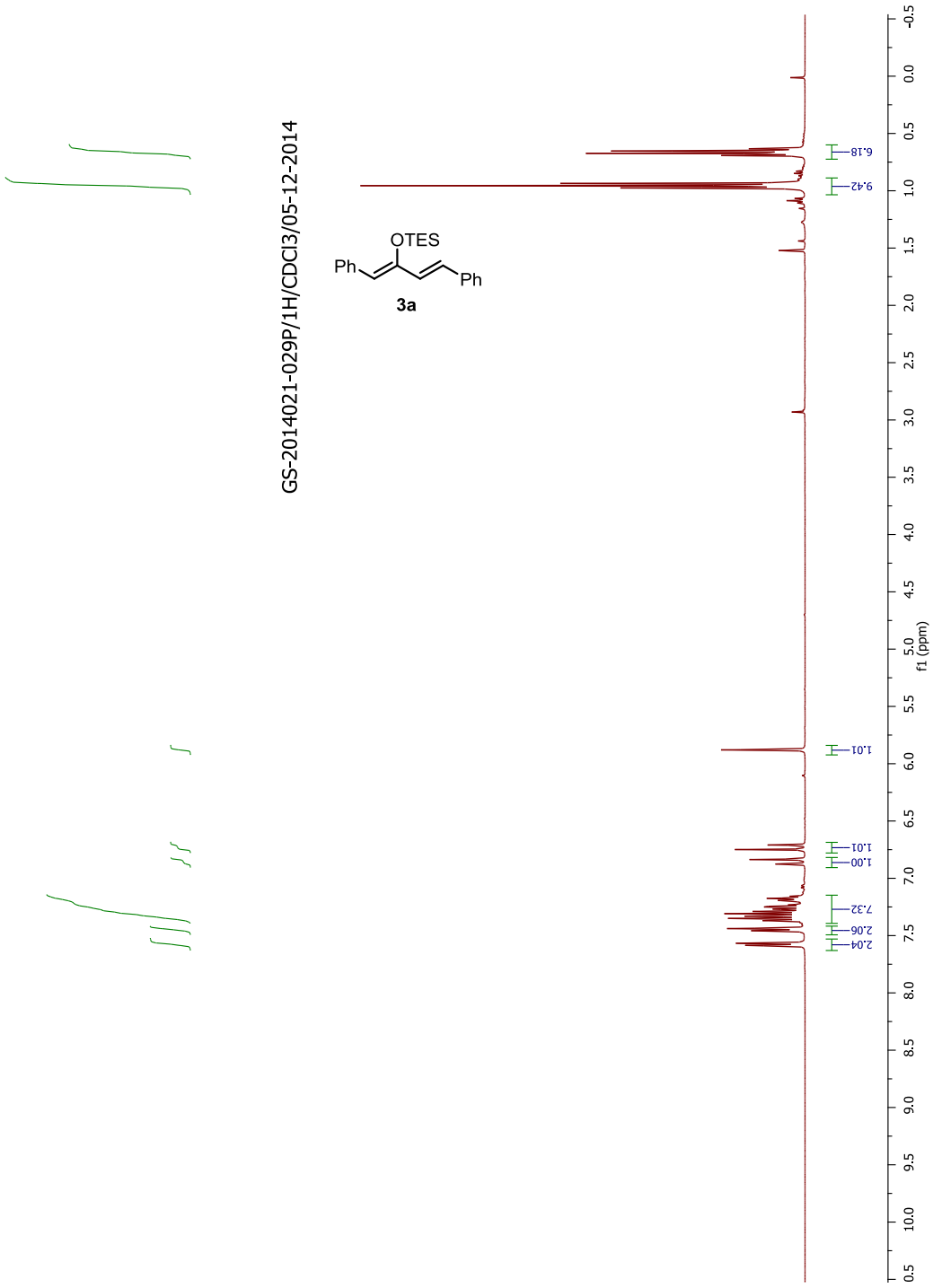
Palladium-catalyzed Synthesis of 2-Alkenyl-3-Arylindoles via Dual α-Arylation Strategy: Formal Synthesis of the Antilipemic Drug Fluvastatin

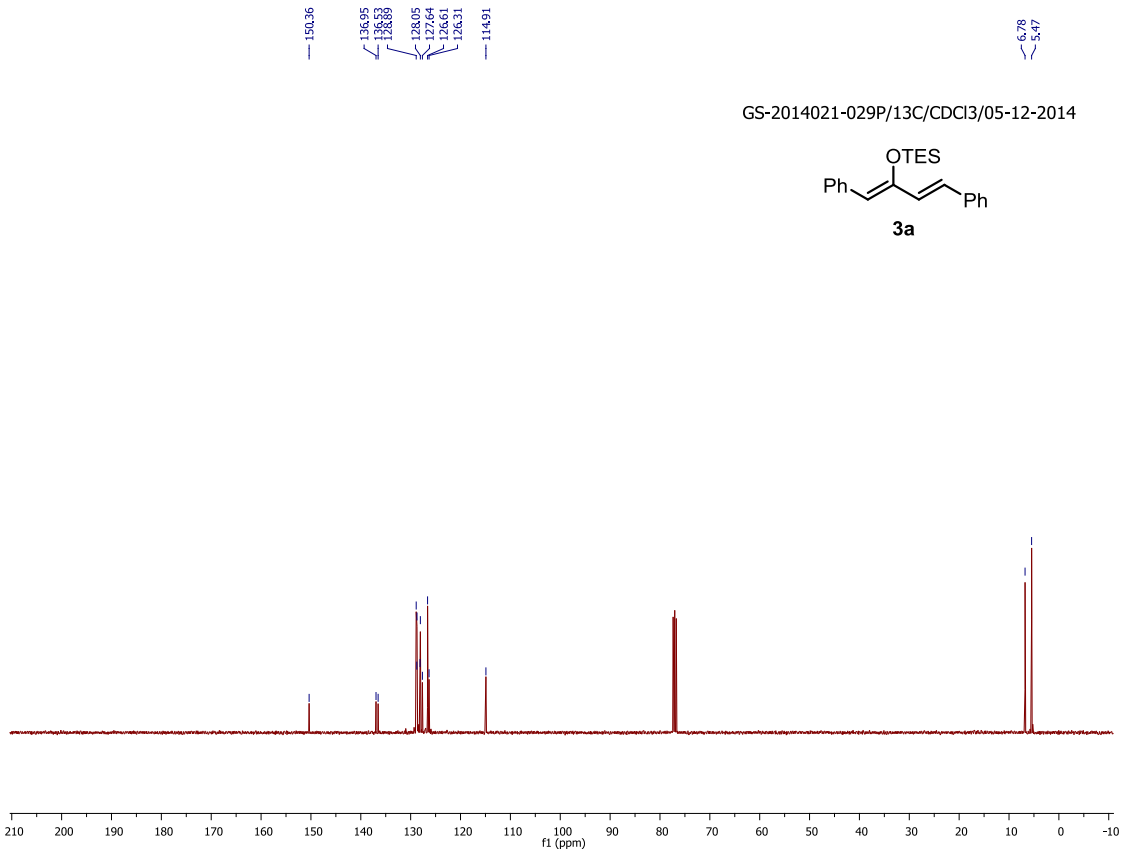
Ajit Prabhakar Kale, Gangam Srikanth Kumar and Manmohan Kapur *

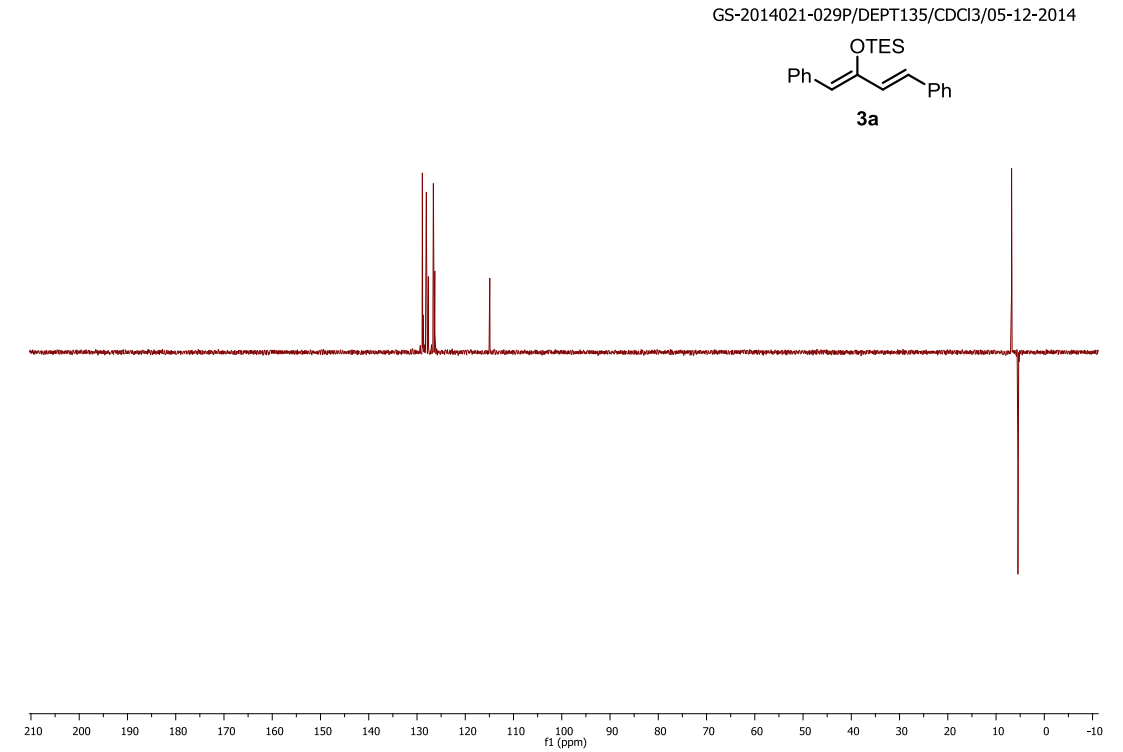
Department of Chemistry, Indian Institute of Science Education and Research Bhopal, Bhopal By-Pass Road, Bhopal-462066, INDIA

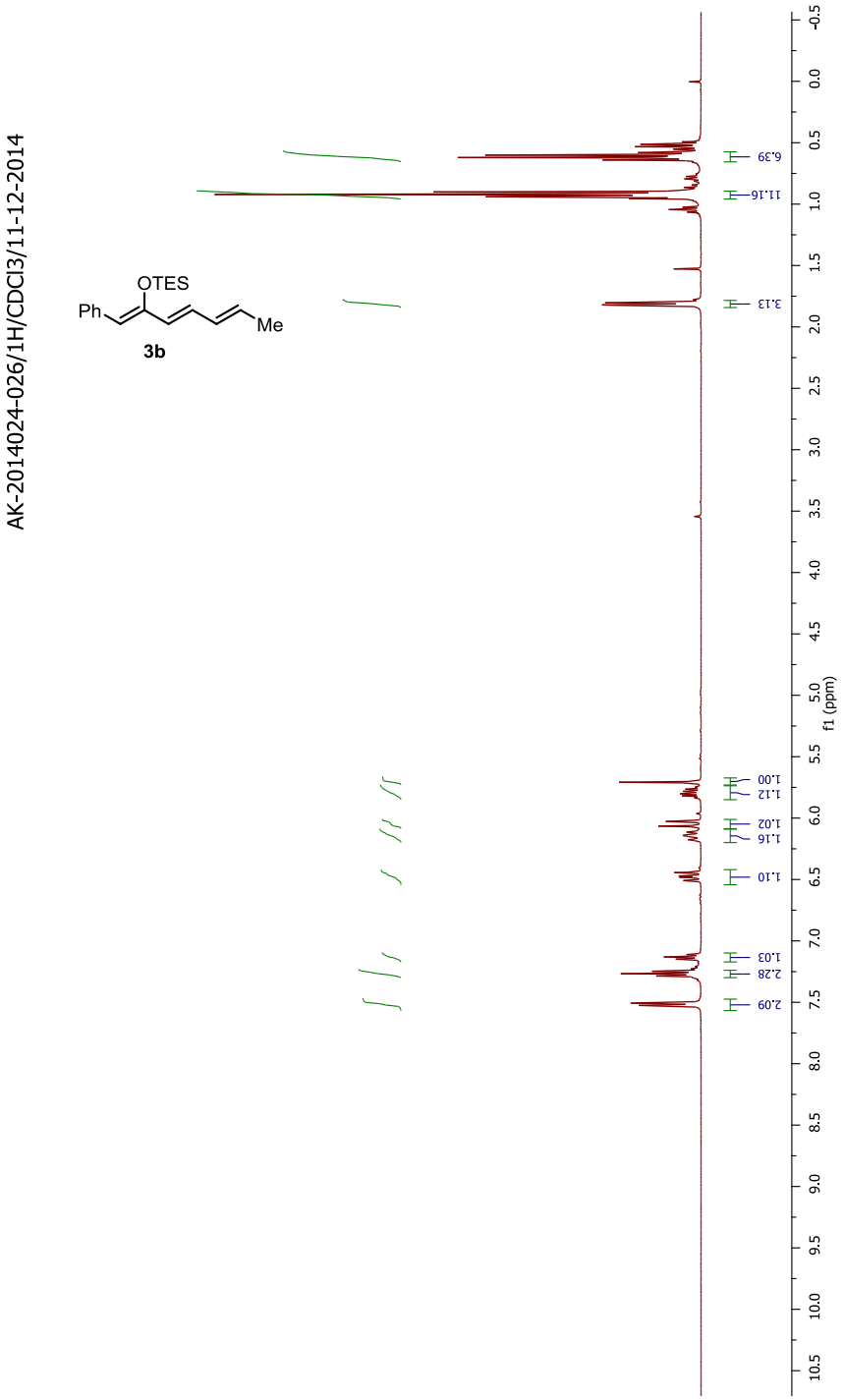
E-mail: mk@iiserb.ac.in

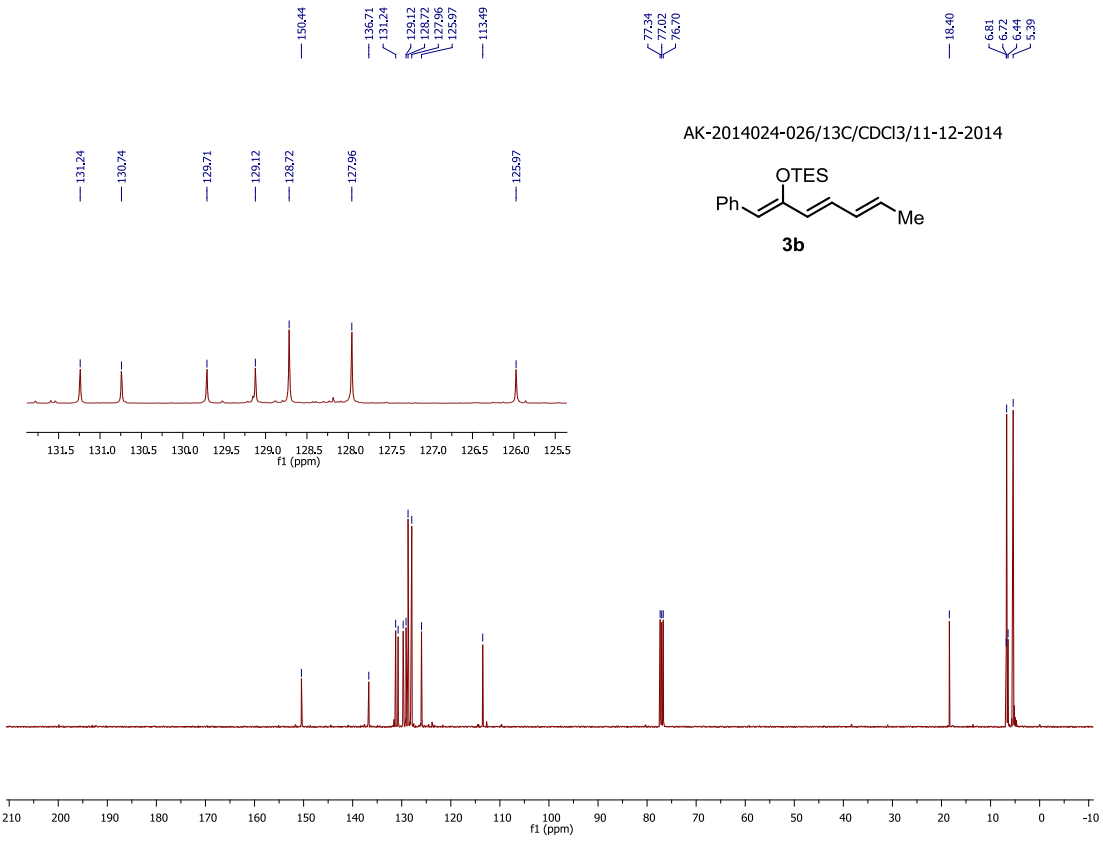
^{1}H- and ^{13}C-NMR & DEPT-135 spectra of new compounds Pg 2-51

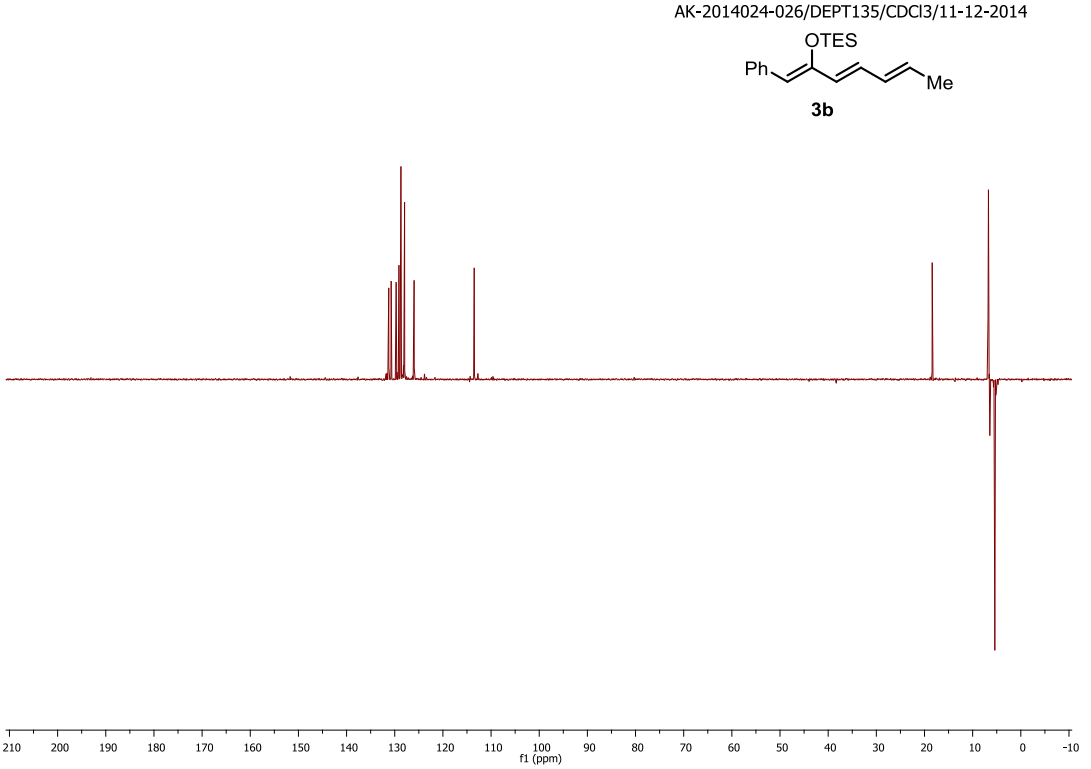

GS-2014021-029P/1H/CDCl3/05-12-2014
OTES
Ph
Ph
3a
6.18
9.42
1.01
1.01
1.00
7.32
2.06
2.04
f1 (ppm)

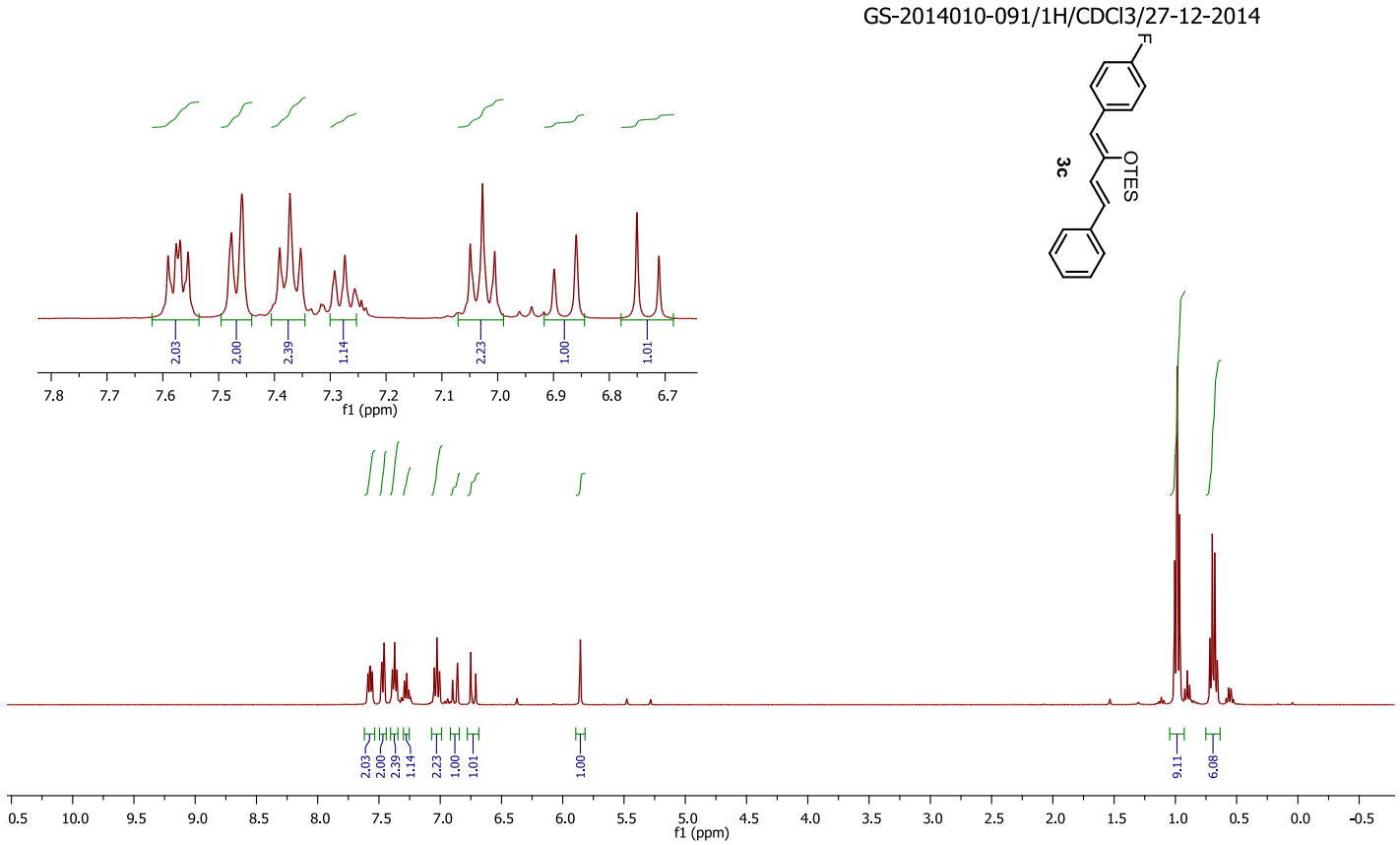

150.36
136.95
128.53
128.39
128.05
127.64
126.61
126.31
114.91
6.78
5.47
GS-2014021-029P/13C/CDCl3/05-12-2014
OTES
Ph
Ph
3a
f1 (ppm)

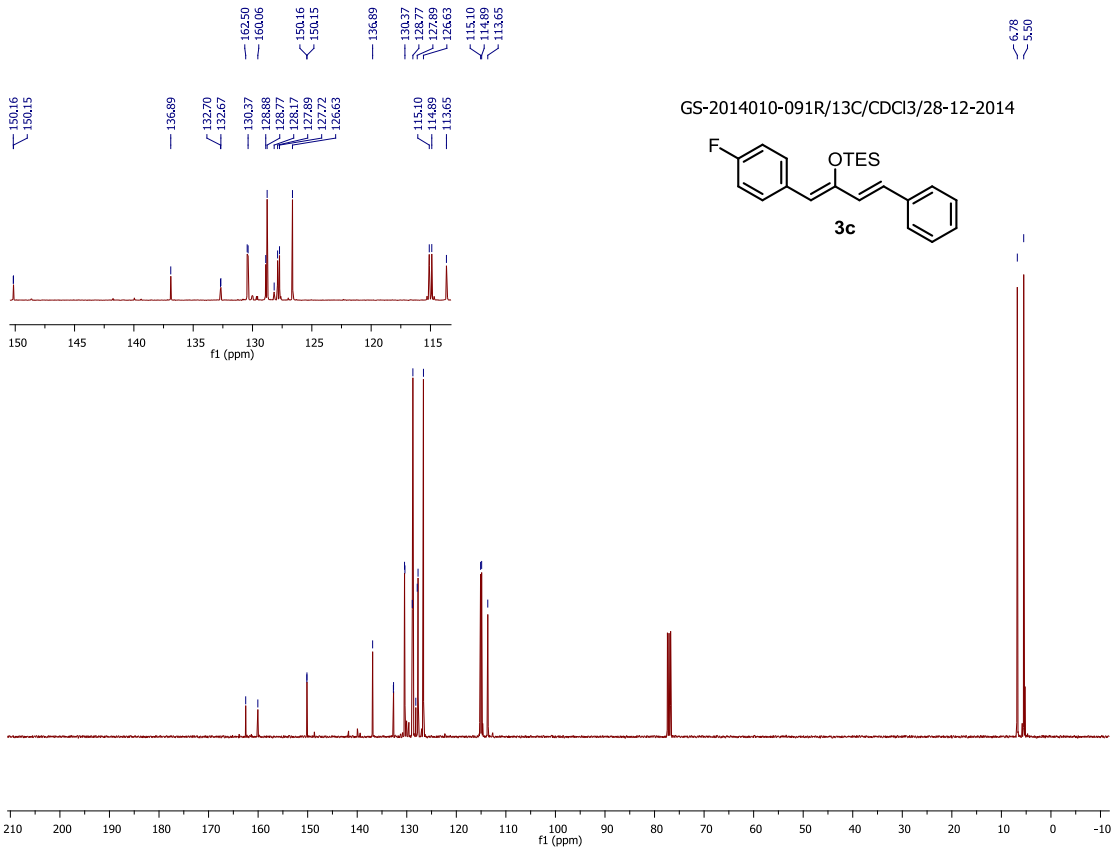

GS-2014021-029P/DEPT135/CDCl3/05-12-2014
OTES
Ph
Ph
3a
f1 (ppm)

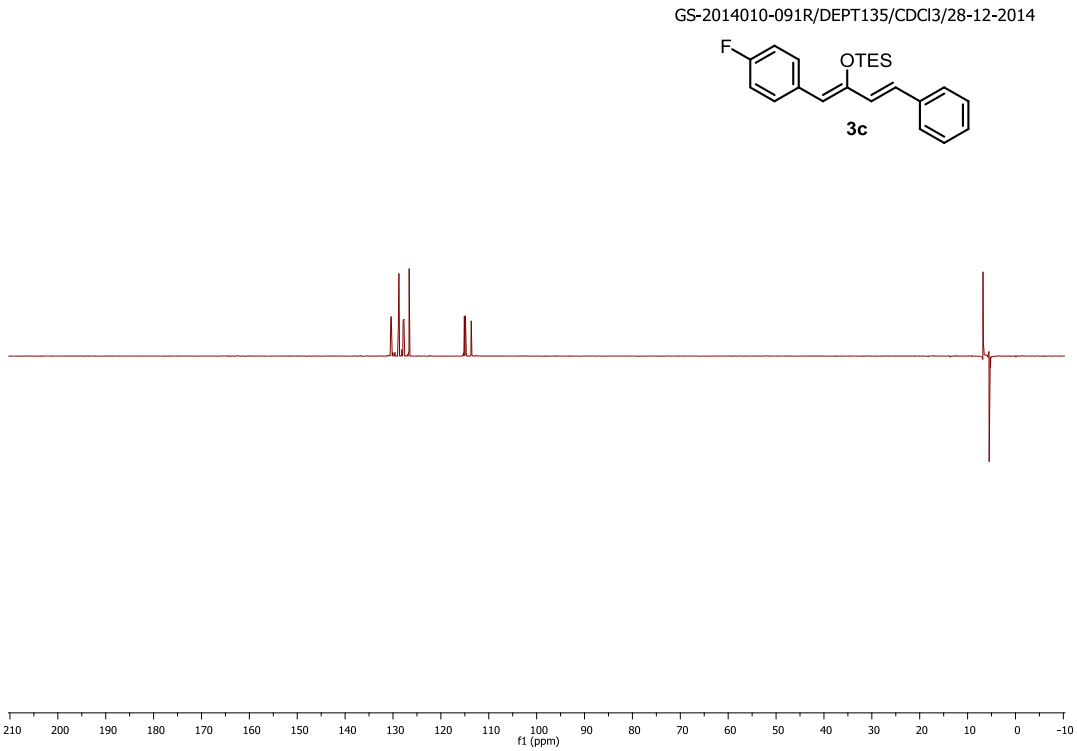

AK-2014024-026/1H/CDCl3/11-12-2014
OTES
Ph
Me
3b
6.39
11.16
3.13
1.00
1.12
1.02
1.16
1.10
1.03
2.28
2.09
f1 (ppm)

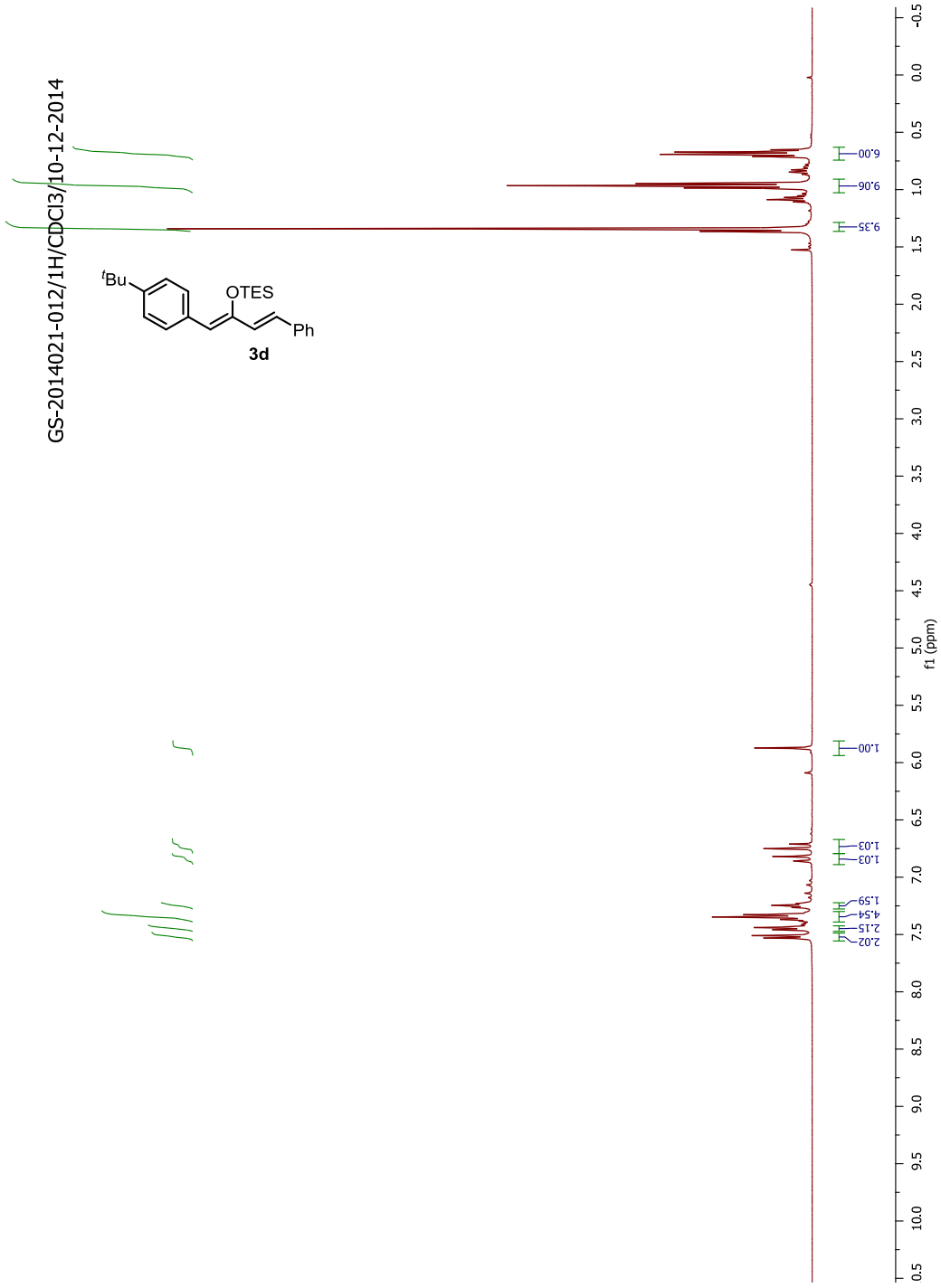

150.44
136.71
131.24
129.12
128.72
127.96
125.97
113.49
77.34
77.02
76.70
18.40
6.81
6.72
6.44
5.39
AK-2014024-026/13C/CDCl3/11-12-2014
OTES
Ph
Me
3b
131.24
130.74
129.71
129.12
128.72
127.96
125.97
f1 (ppm)


AK-2014024-026/DEPT135/CDCl3/11-12-2014
OTES
Ph
Me
3b
f1 (ppm)

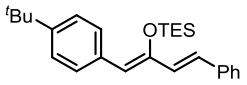

GS-2014010-091/1H/CDCl3/27-12-2014
F
OTES
3c
2.03
2.00
2.39
1.14
2.23
1.00
1.01
9.11
6.08
f1 (ppm)


GS-2014010-091R/13C/CDCl3/28-12-2014
F
OTES
3c
f1 (ppm)

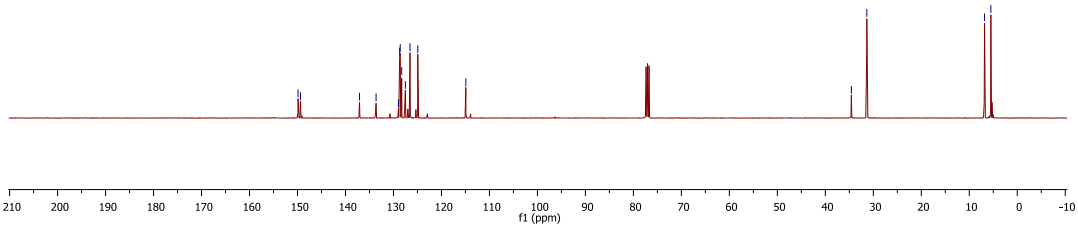

GS-2014010-091R/DEPT135/CDCl3/28-12-2014
F
OTES
3c
f1 (ppm)


GS-2014021-012/1H/CDCl3/10-12-2014
tBu
OTES
Ph
3d
6.00
9.06
9.35
1.00
1.03
1.03
1.59
4.54
2.15
2.02
f1 (ppm)

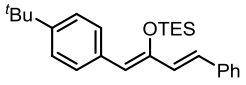
GS-2014021-012/13C/CDCl3/11-12-2014



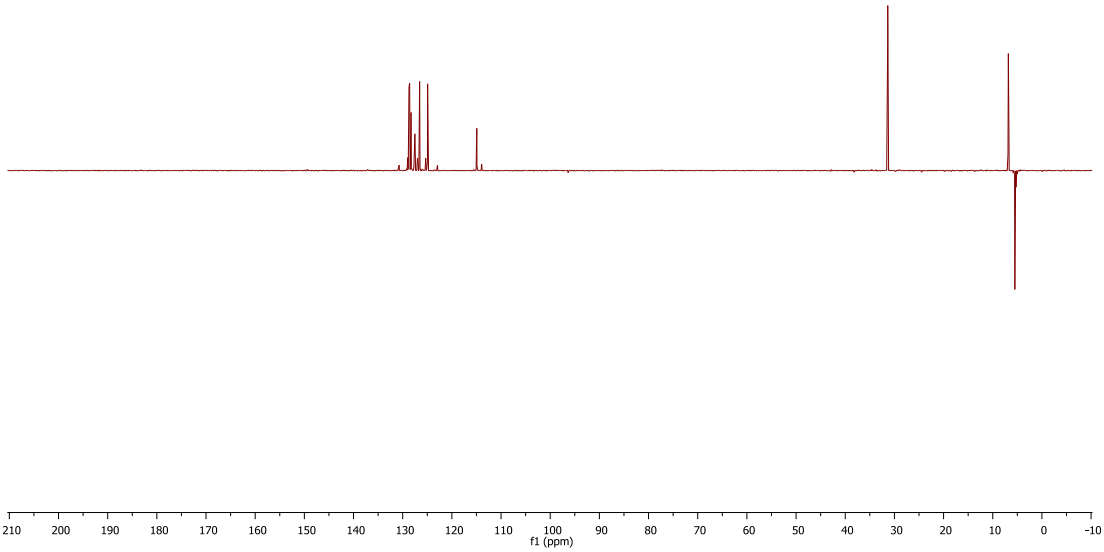
3d

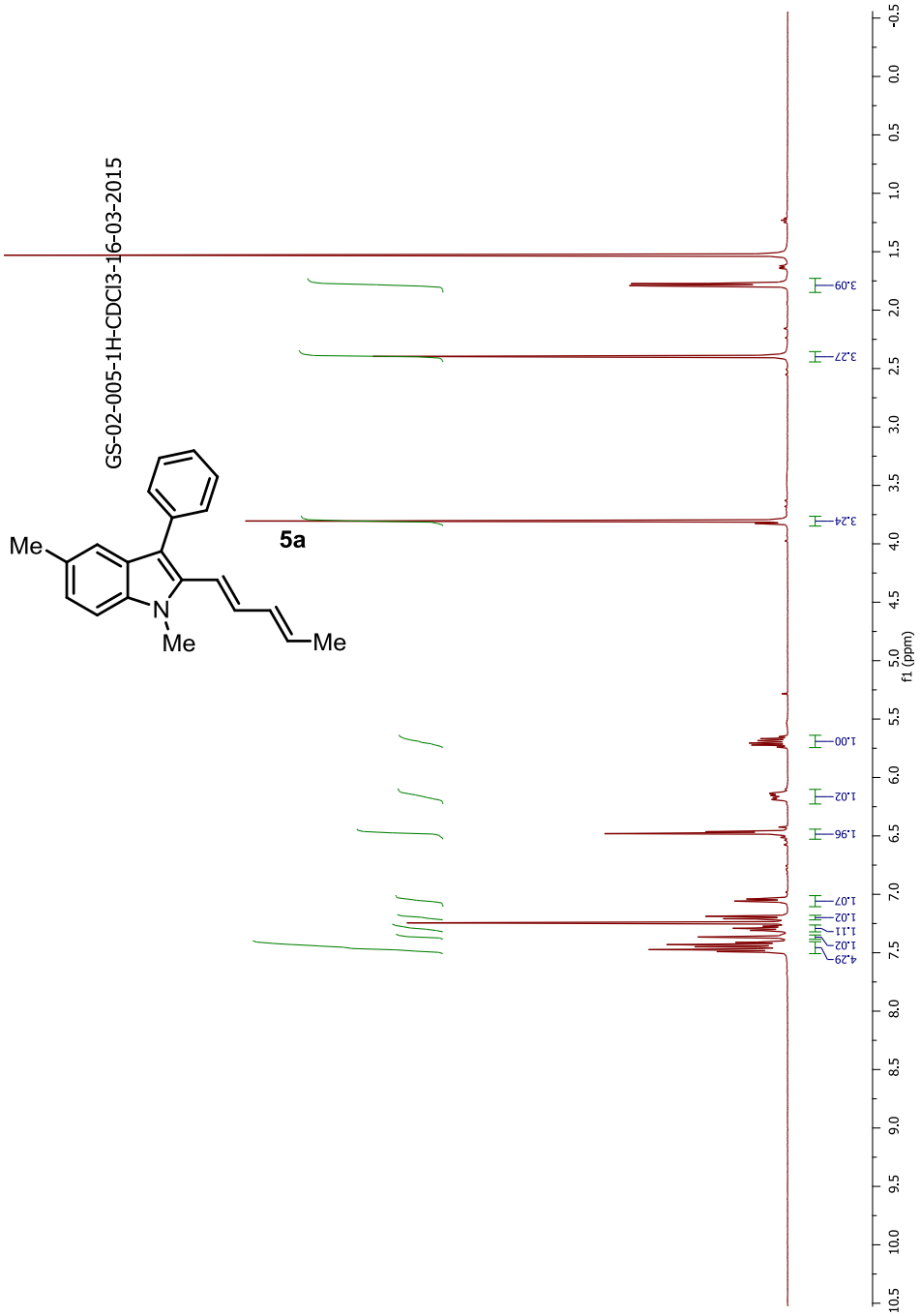


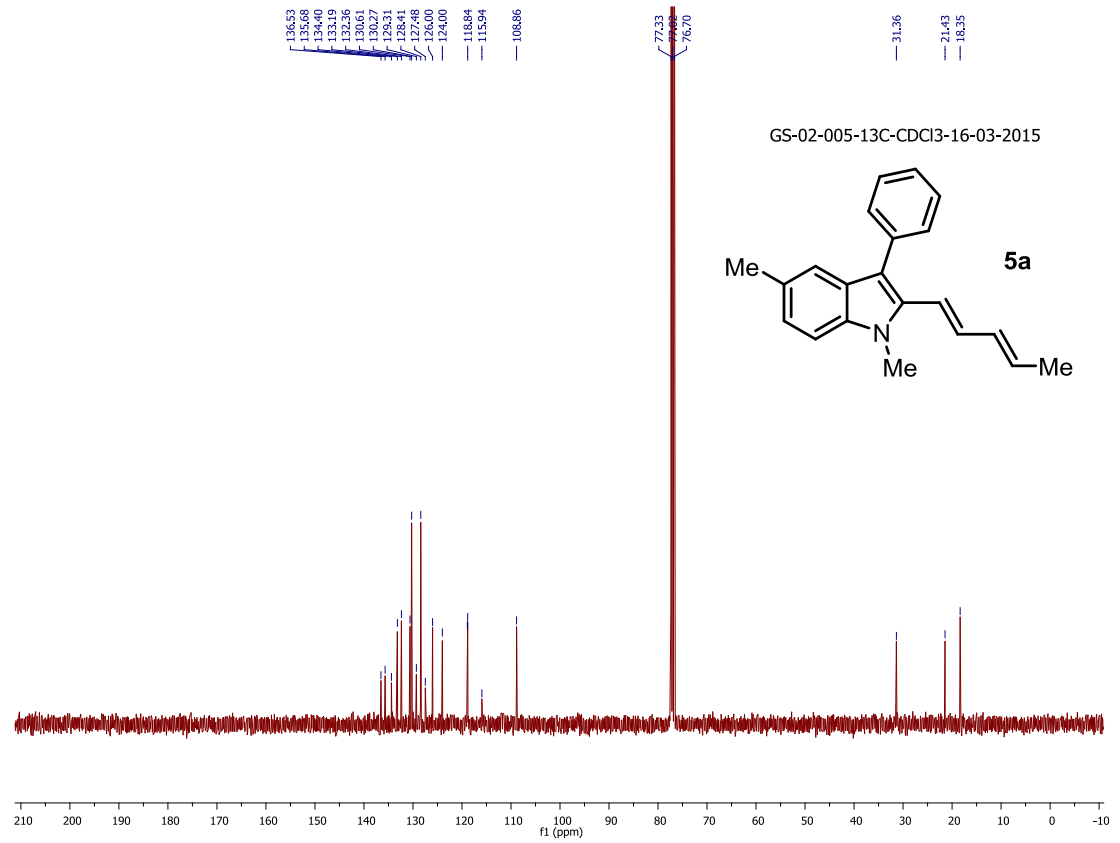
GS-2014021-012/DEPT135/CDCl3/11-12-2014

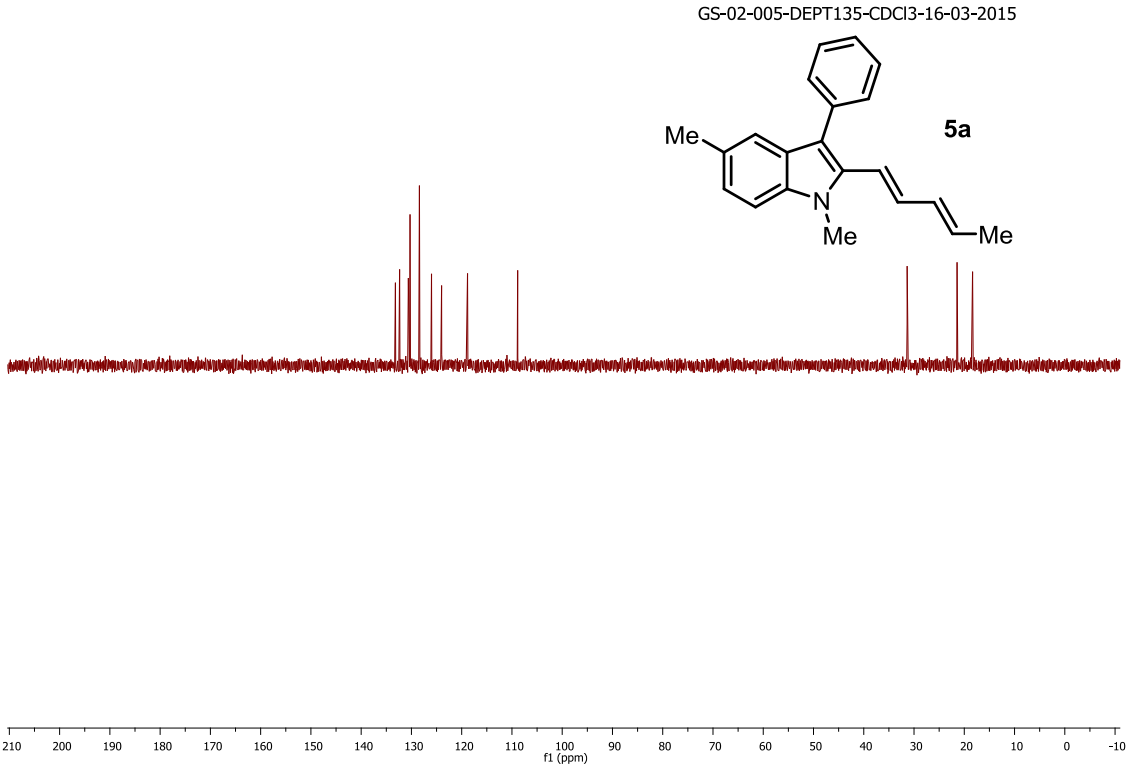


3d

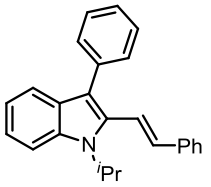



GS-02-005-1H-CDCl3-16-03-2015
5a
Me
N
Me
Me
3.09
3.27
3.24
1.00
1.02
1.96
1.07
1.02
1.11
1.02
4.29
f1 (ppm)

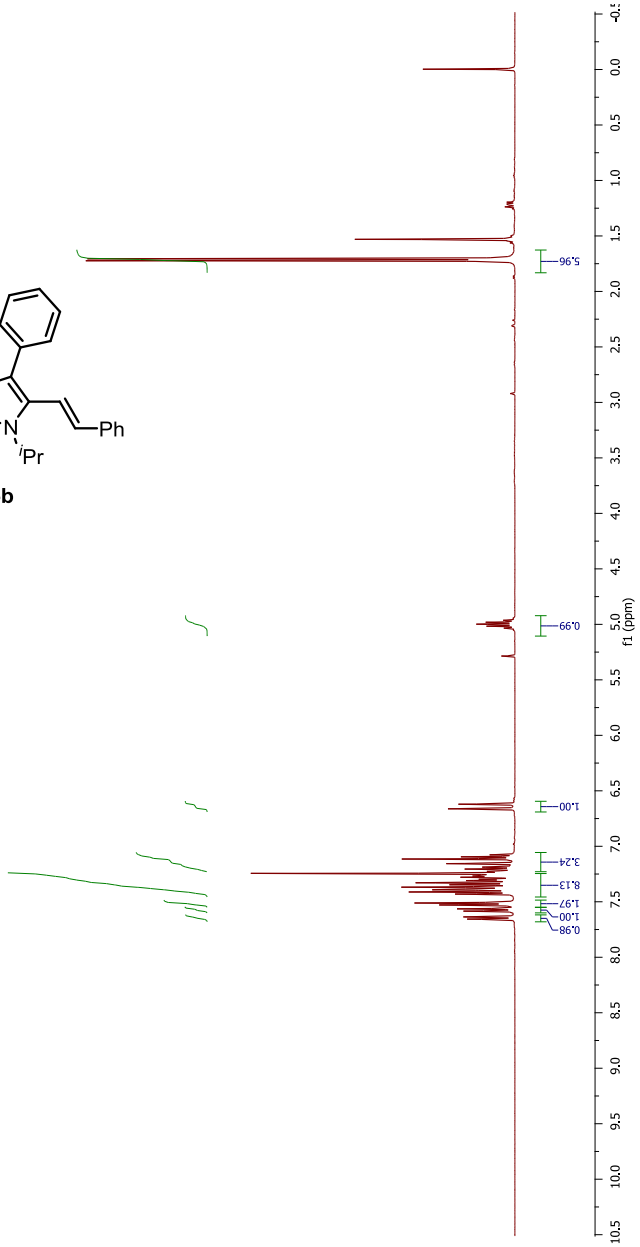

136.53
135.68
134.40
133.19
132.36
130.61
130.27
129.31
128.41
127.48
126.00
124.00
118.84
115.94
108.86
77.33
77.02
76.70
31.36
21.43
18.35
GS-02-005-13C-CDCl3-16-03-2015
Me
5a
N
Me
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

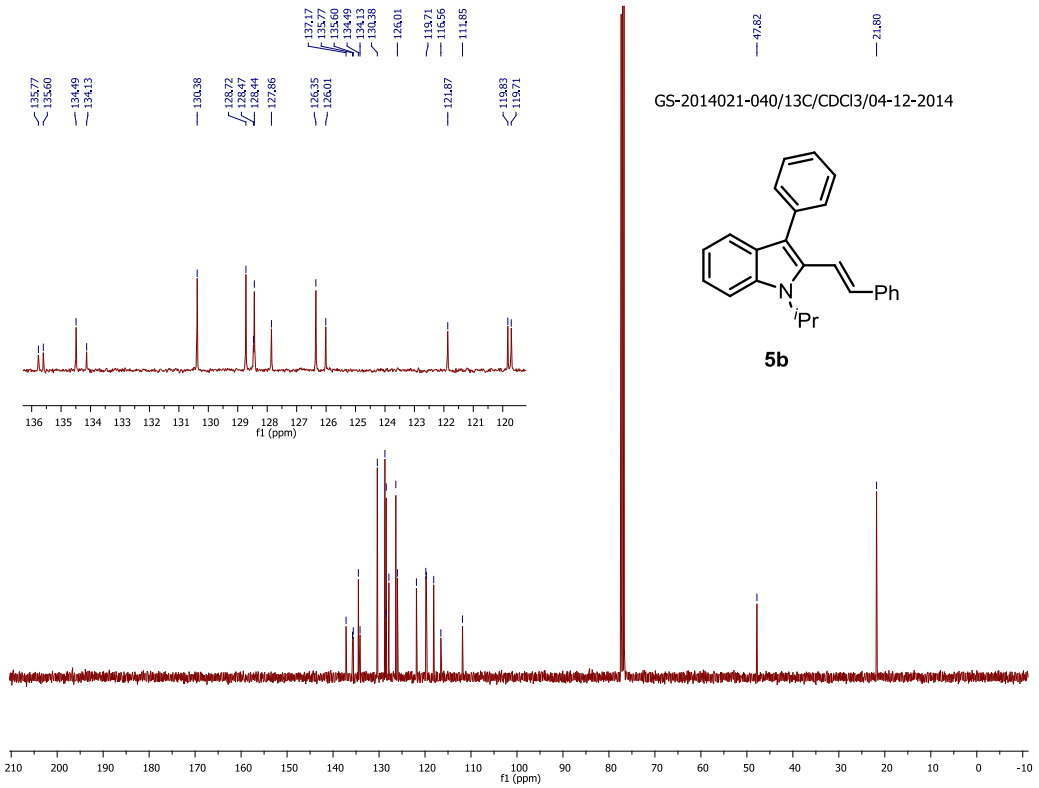

GS-02-005-DEPT135-CDCl3-16-03-2015
Me
5a
N
Me
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

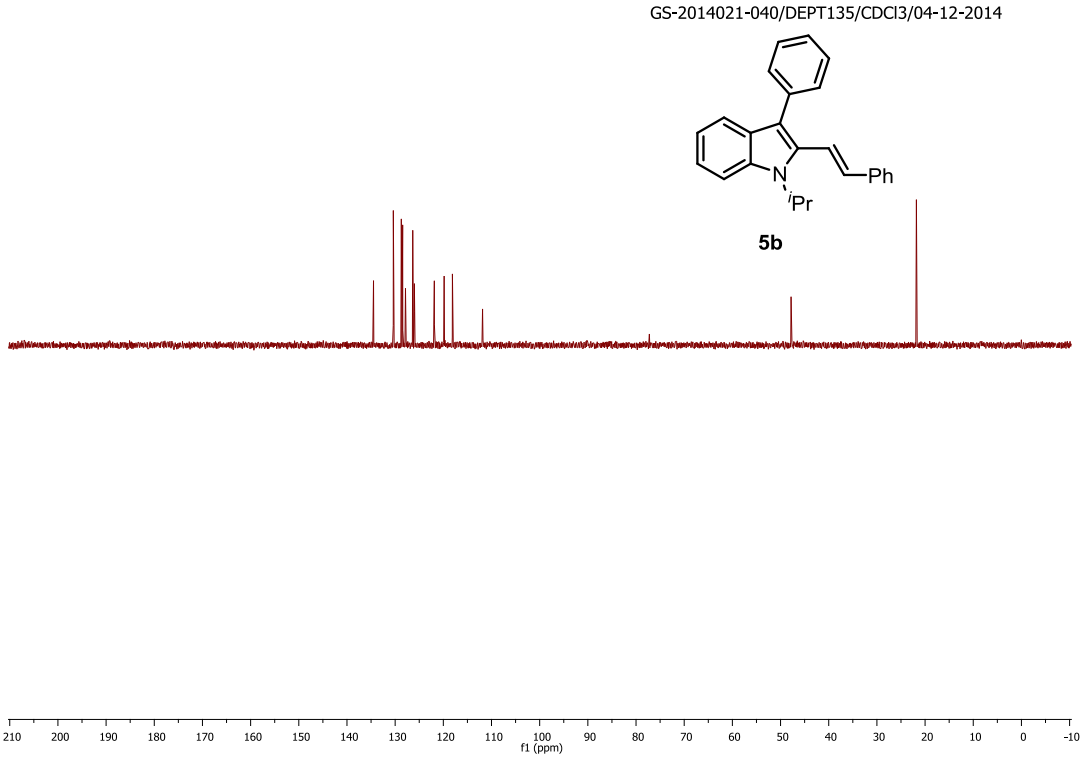
GS-2014021-040/1H/CDCl3/04-12-2014

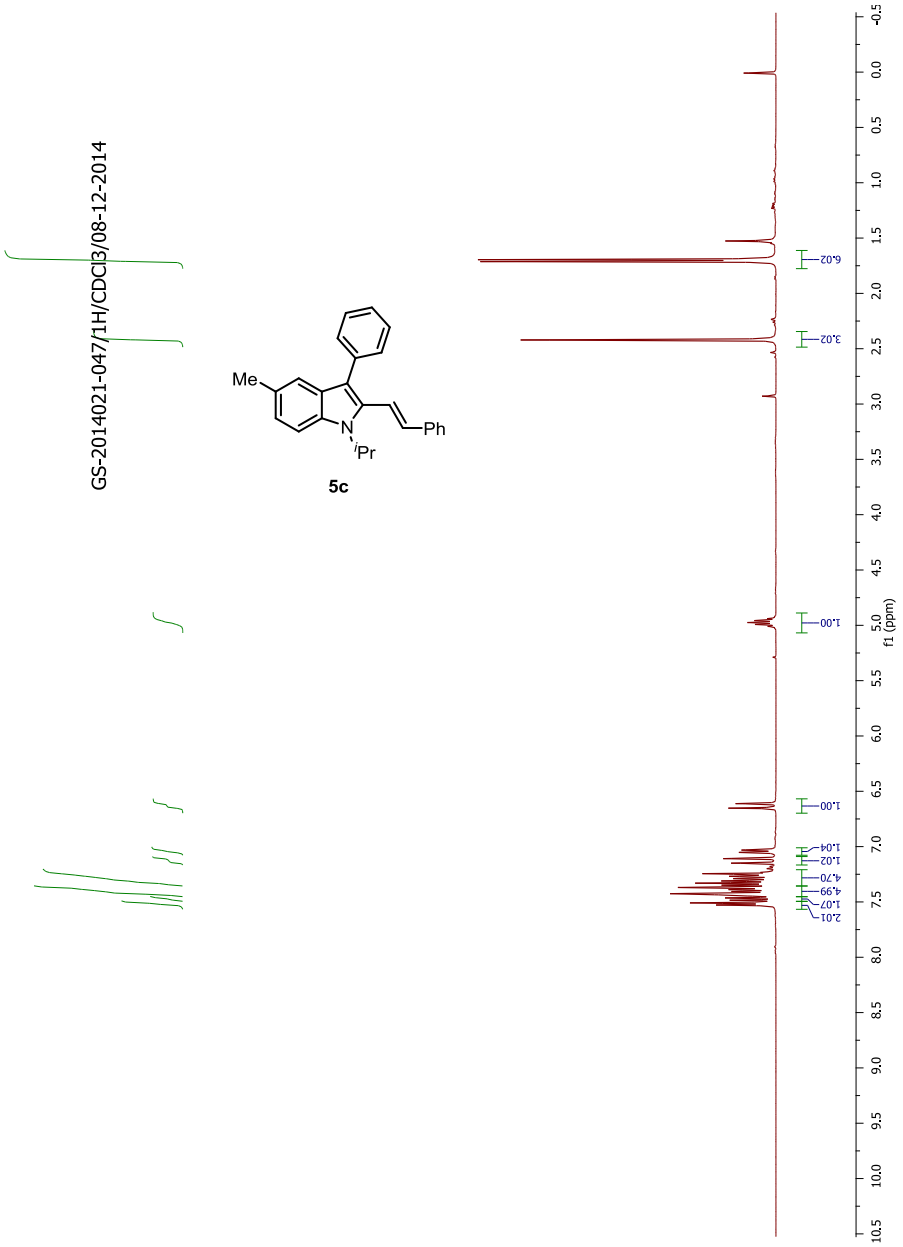


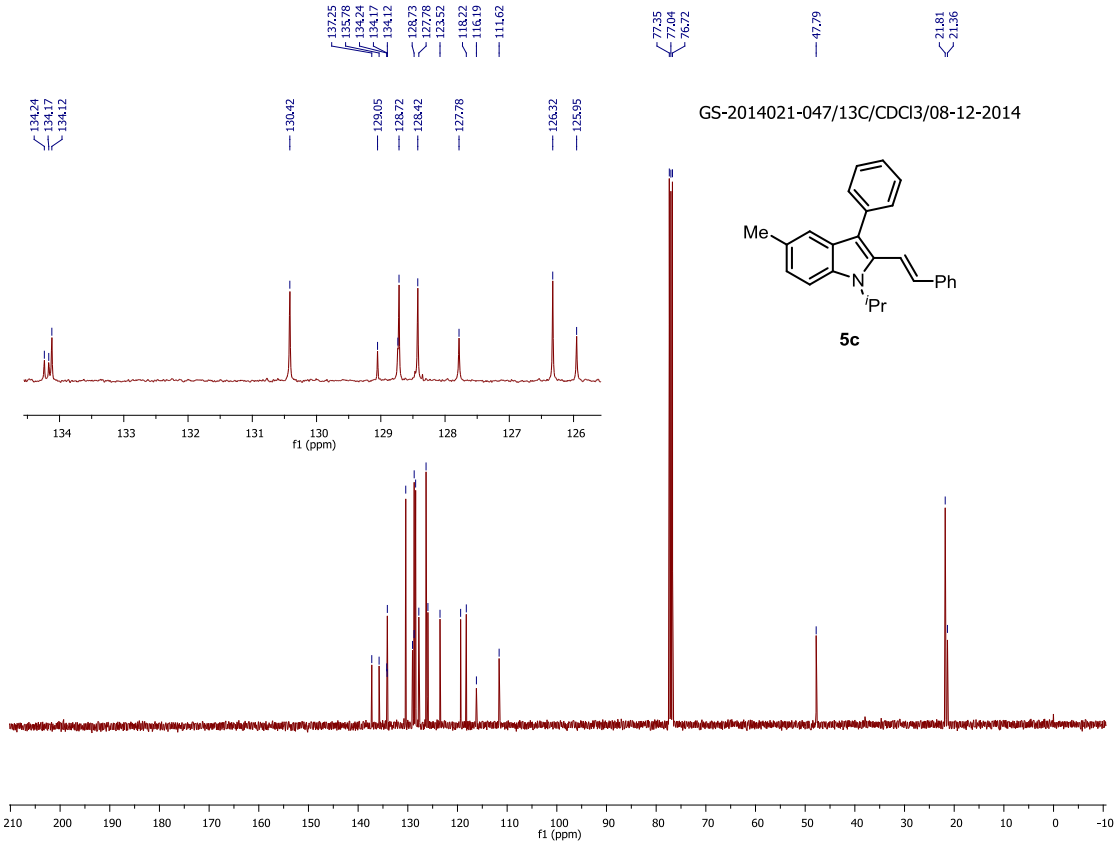
5b

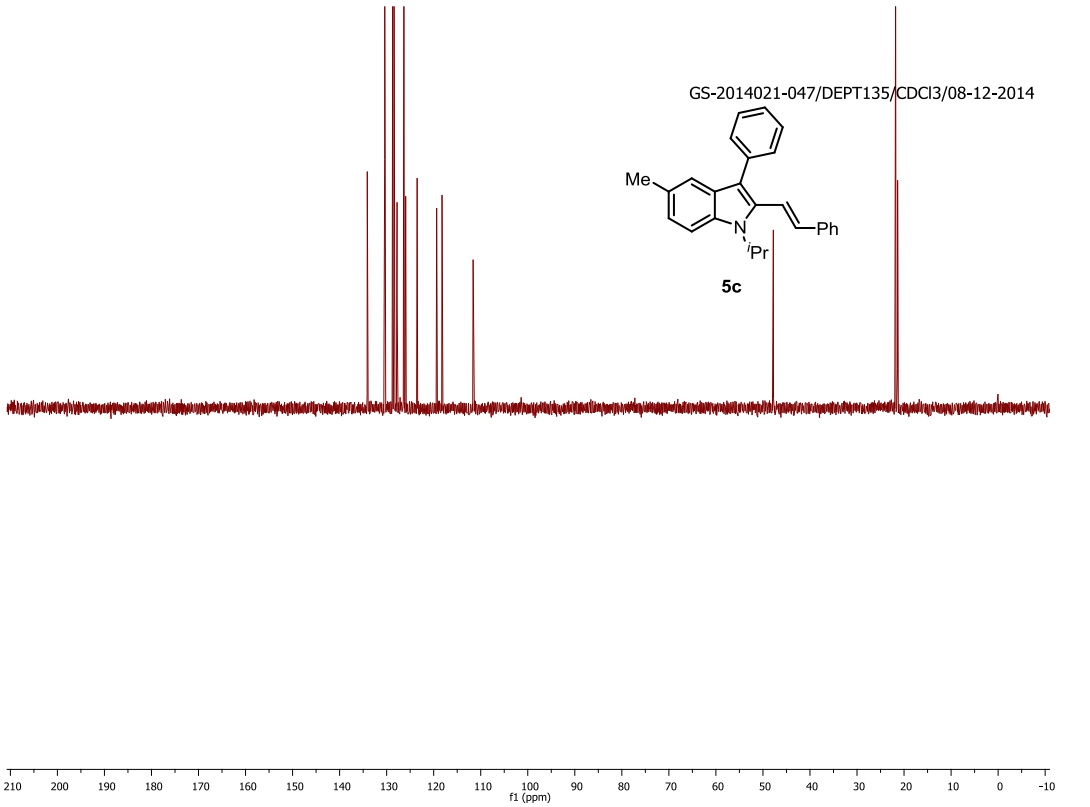


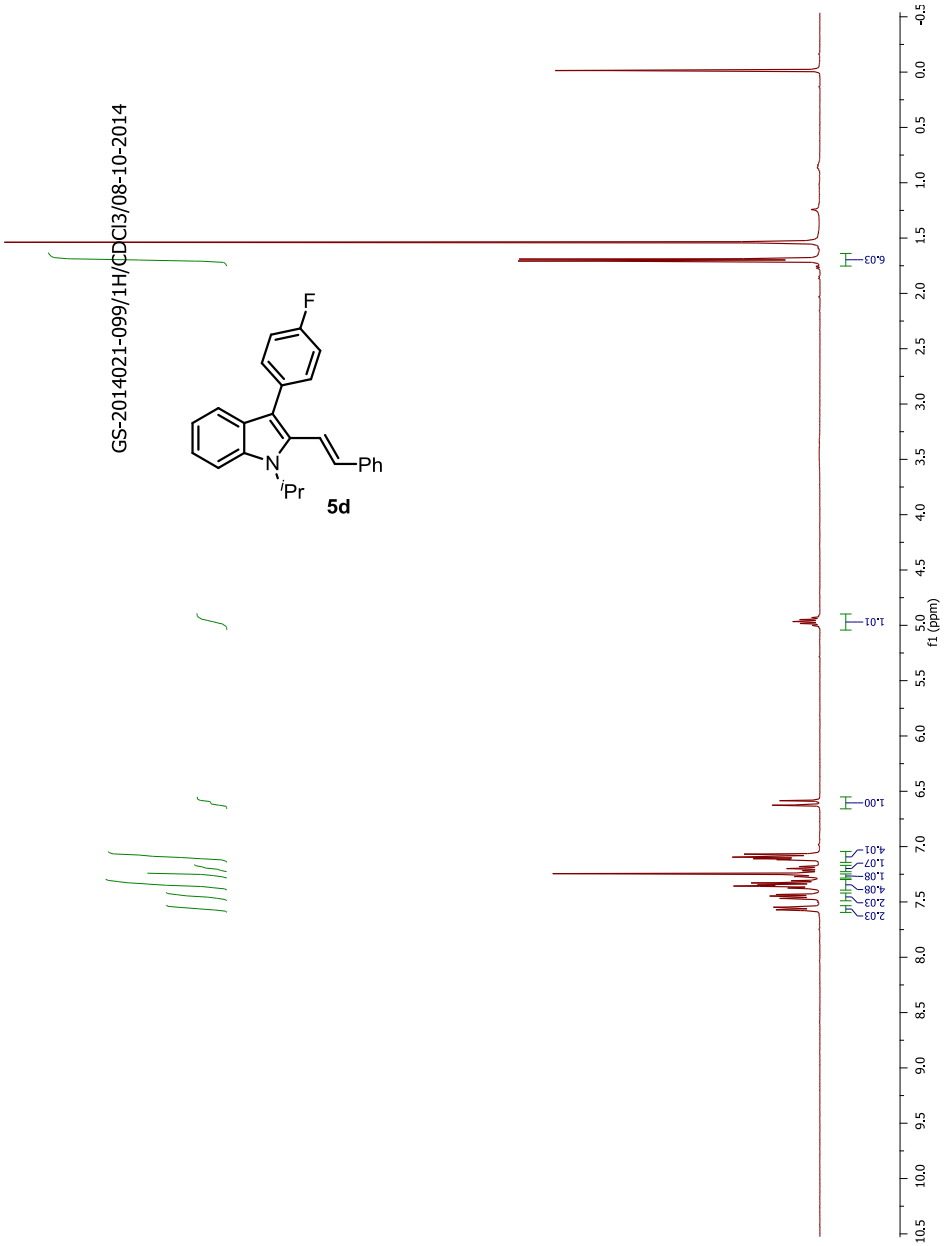

137.17
135.77
135.60
134.49
134.13
134.38
126.01
119.71
116.56
111.85
47.82
21.80
135.77
135.60
134.49
134.13
130.38
128.72
128.47
128.44
127.86
126.35
126.01
121.87
119.83
119.71
GS-2014021-040/13C/CDCl3/04-12-2014
Ph
N
iPr
5b
f1 (ppm)

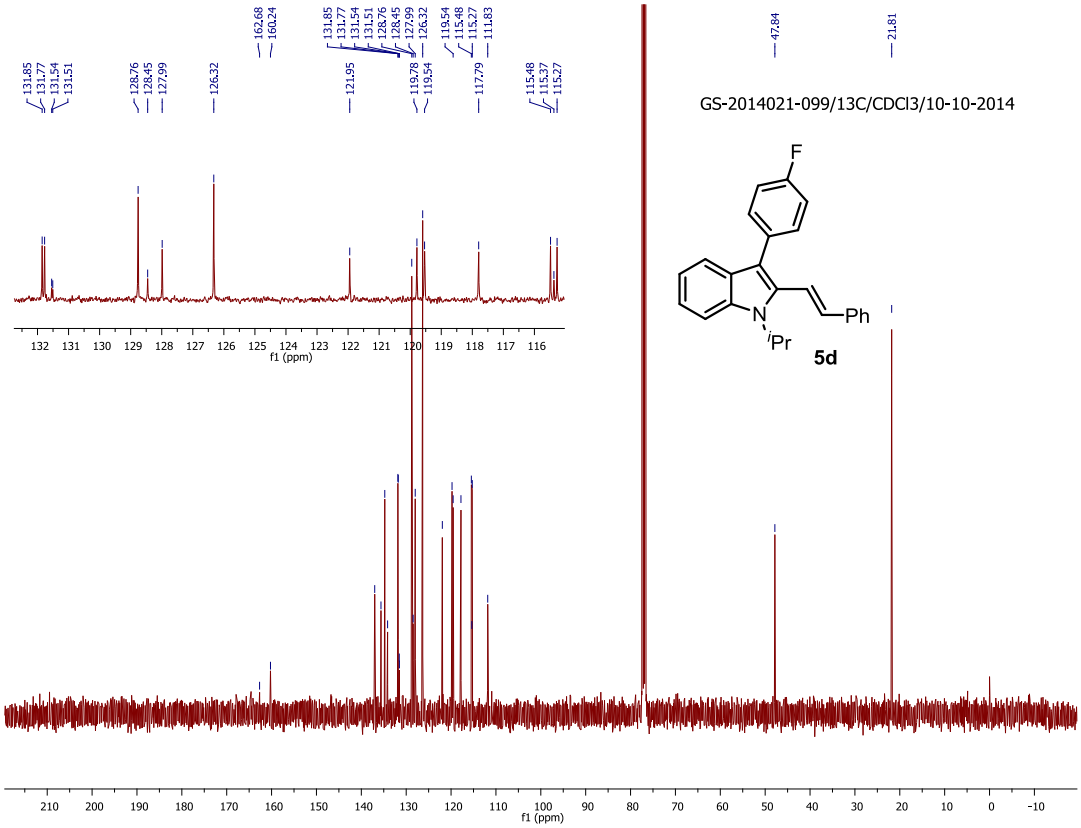

GS-2014021-040/DEPT135/CDCl3/04-12-2014
Ph
N
iPr
5b
f1 (ppm)

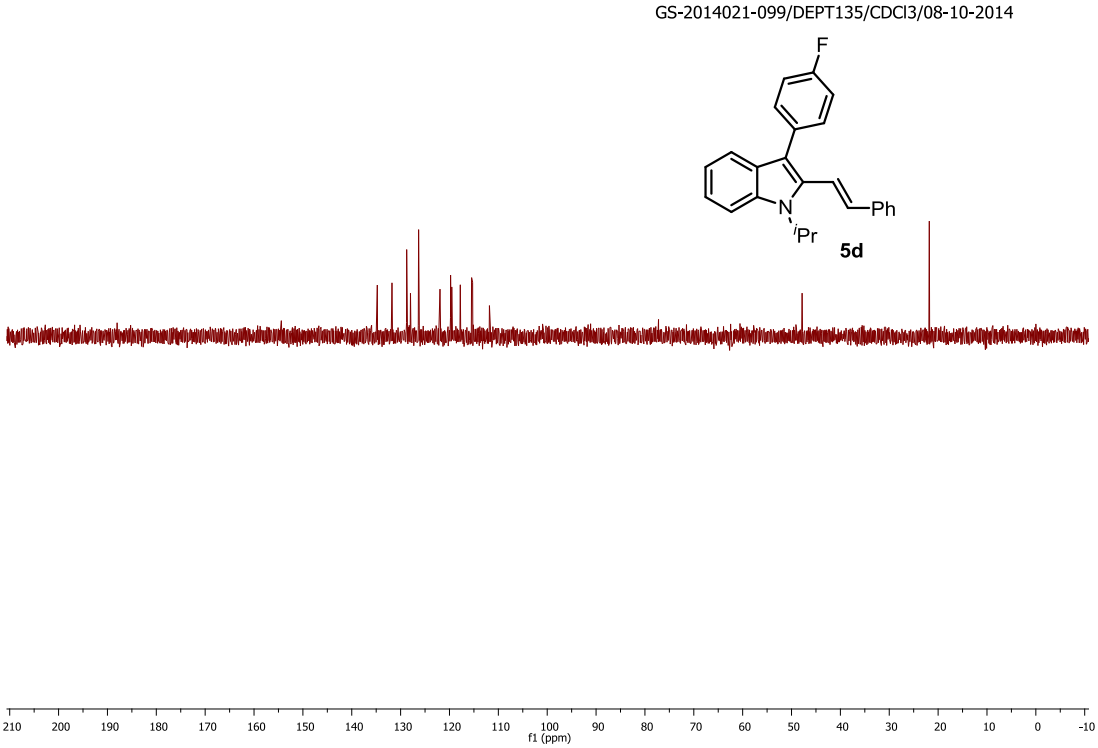

GS-2014021-047/1H/CDCl3/08-12-2014
Me
N
iPr
Ph
5c
6.02
3.02
1.00
1.00
1.04
1.02
4.70
4.99
1.07
2.01
f1 (ppm)

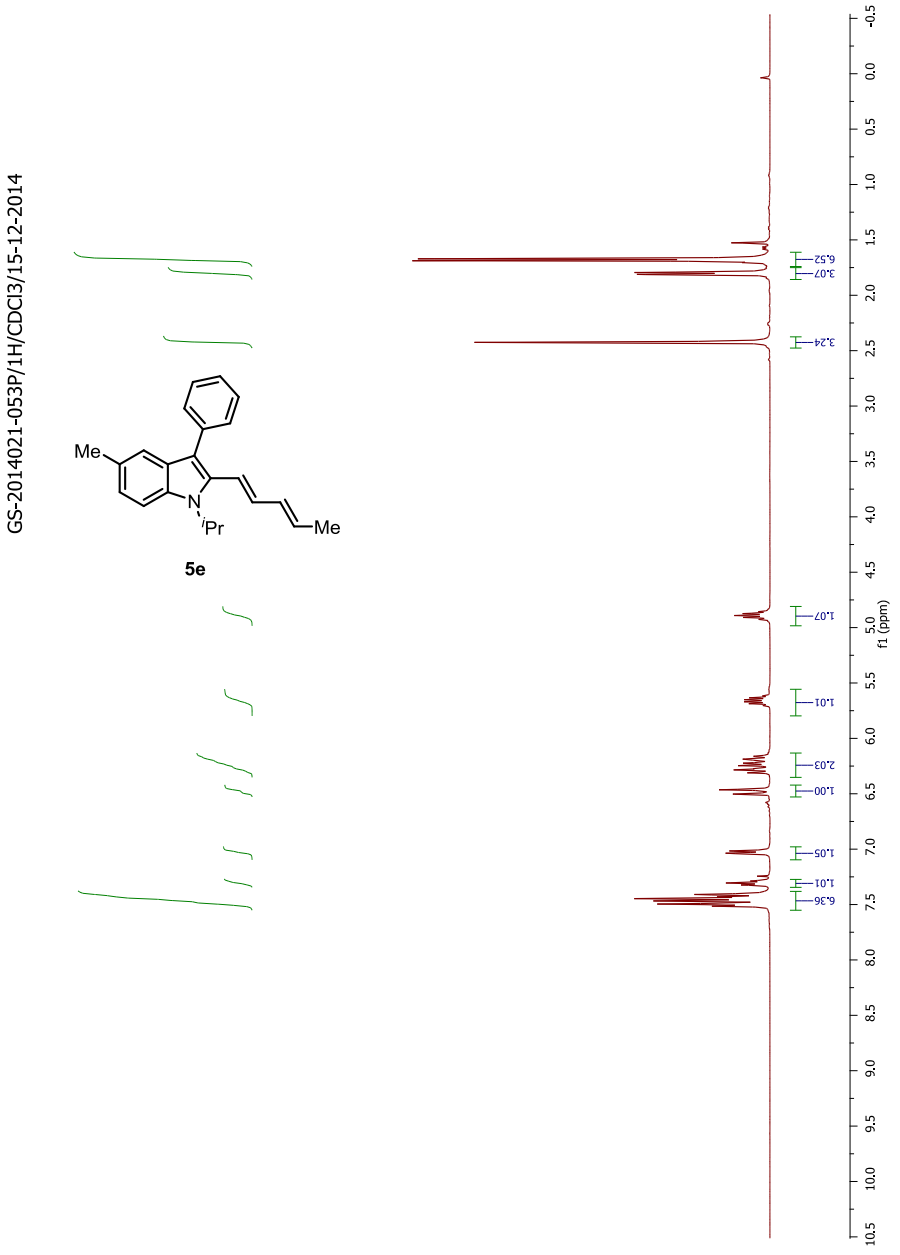

137.25
135.78
134.24
134.17
134.12
128.73
127.78
125.52
118.22
116.19
111.62
77.35
77.04
76.72
47.79
21.81
21.36
134.24
134.17
134.12
130.42
129.05
128.72
128.42
127.78
126.32
125.95
GS-2014021-047/13C/CDCl3/08-12-2014
Me
N
iPr
Ph
5c
f1 (ppm)

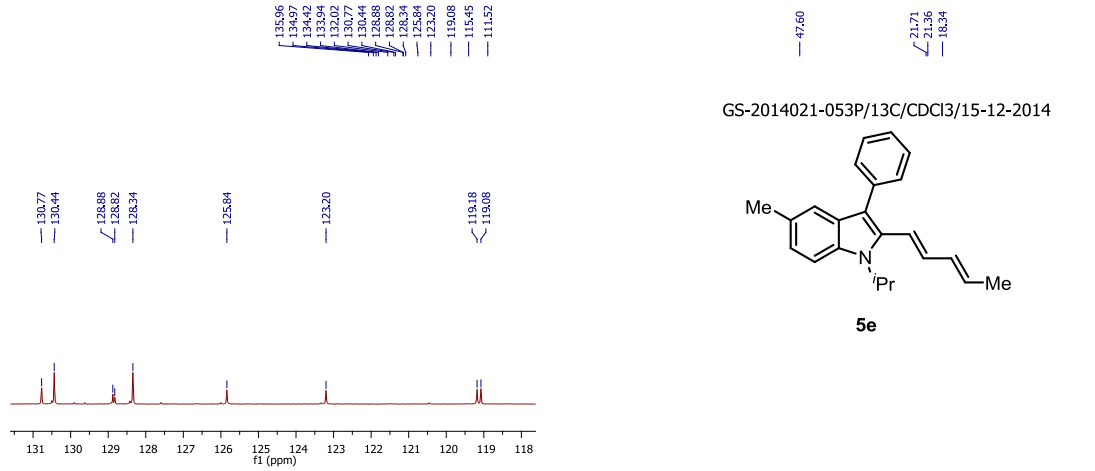

GS-2014021-047/DEPT135/CDCl3/08-12-2014
Me
N
iPr
Ph
5c
f1 (ppm)

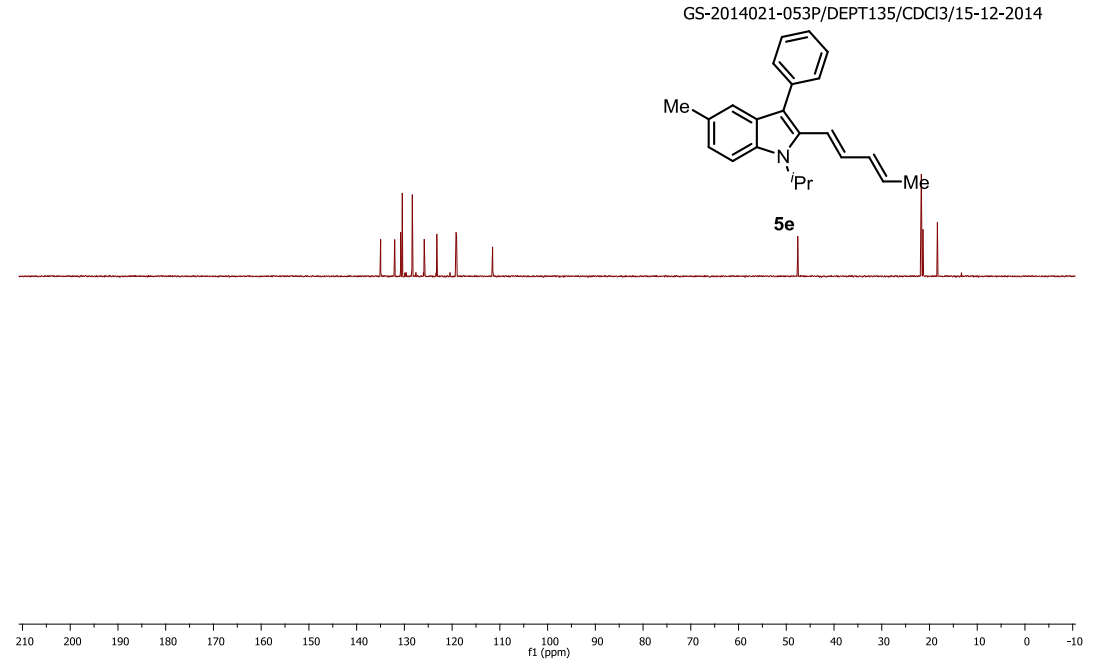

GS-2014021-099/1H/CDCl3/08-10-2014
F
Ph
N
iPr
5d
6.03
1.01
1.00
4.01
1.07
1.08
4.08
2.03
2.03
f1 (ppm)

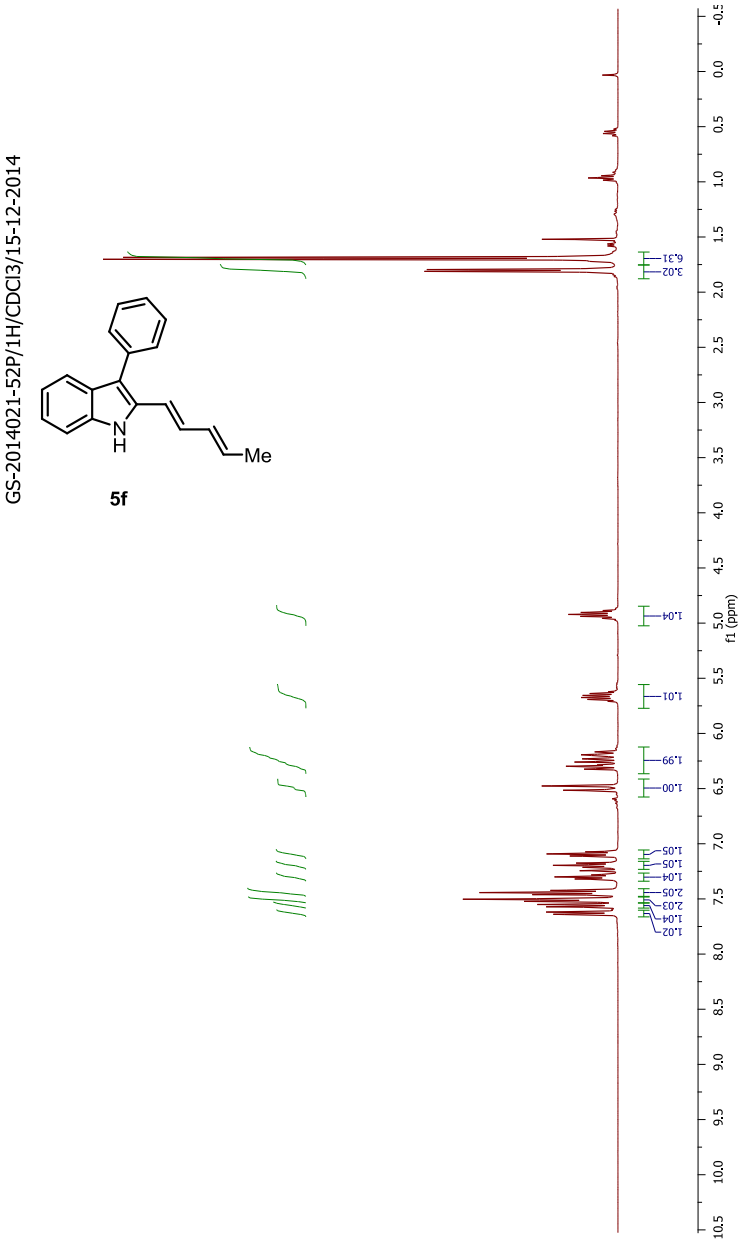

GS-2014021-099/13C/CDCl3/10-10-2014
F
Ph
N
iPr
5d
f1 (ppm)

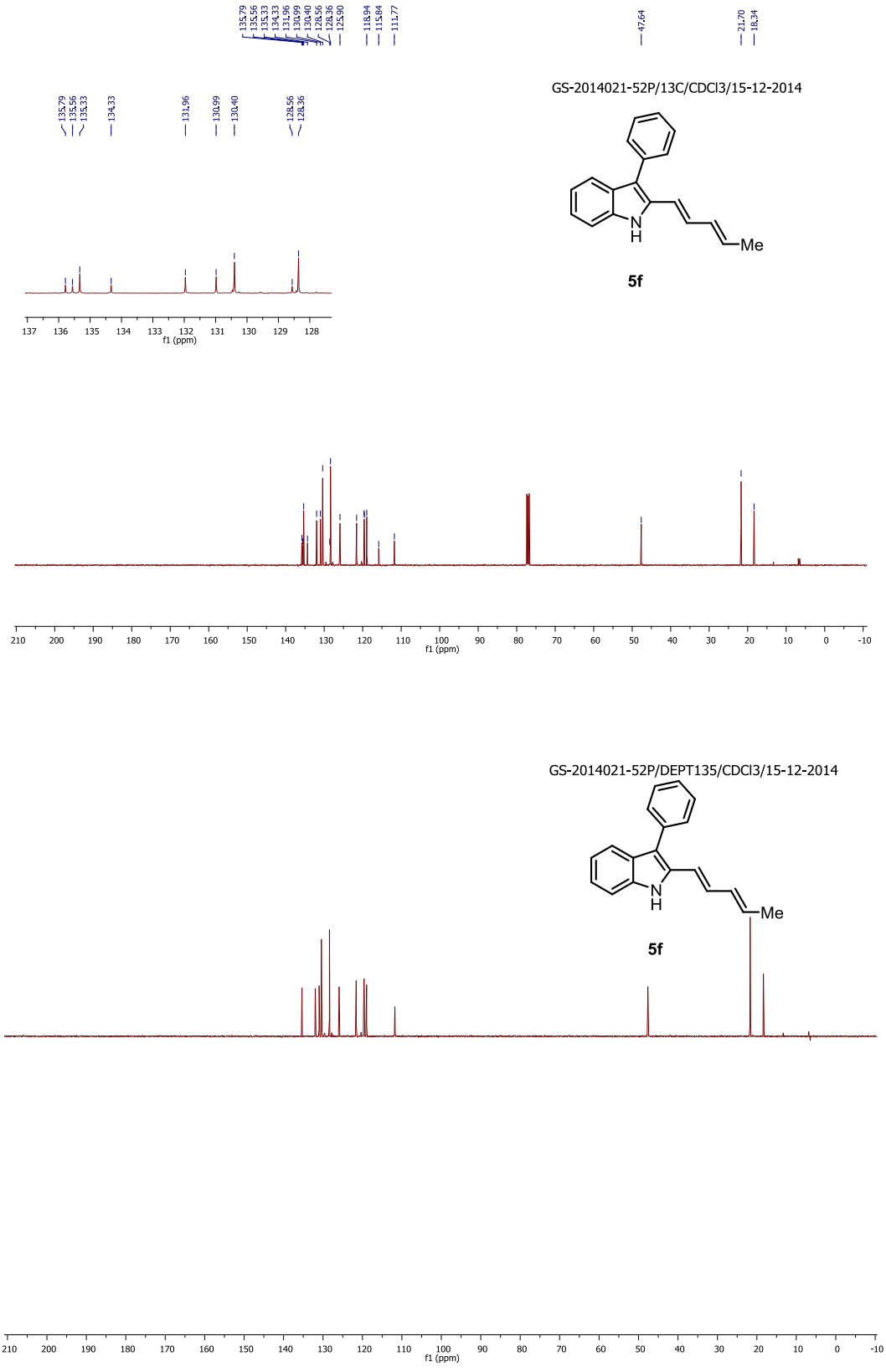

GS-2014021-099/DEPT135/CDCl3/08-10-2014
F
Ph
N
iPr
5d
f1 (ppm)

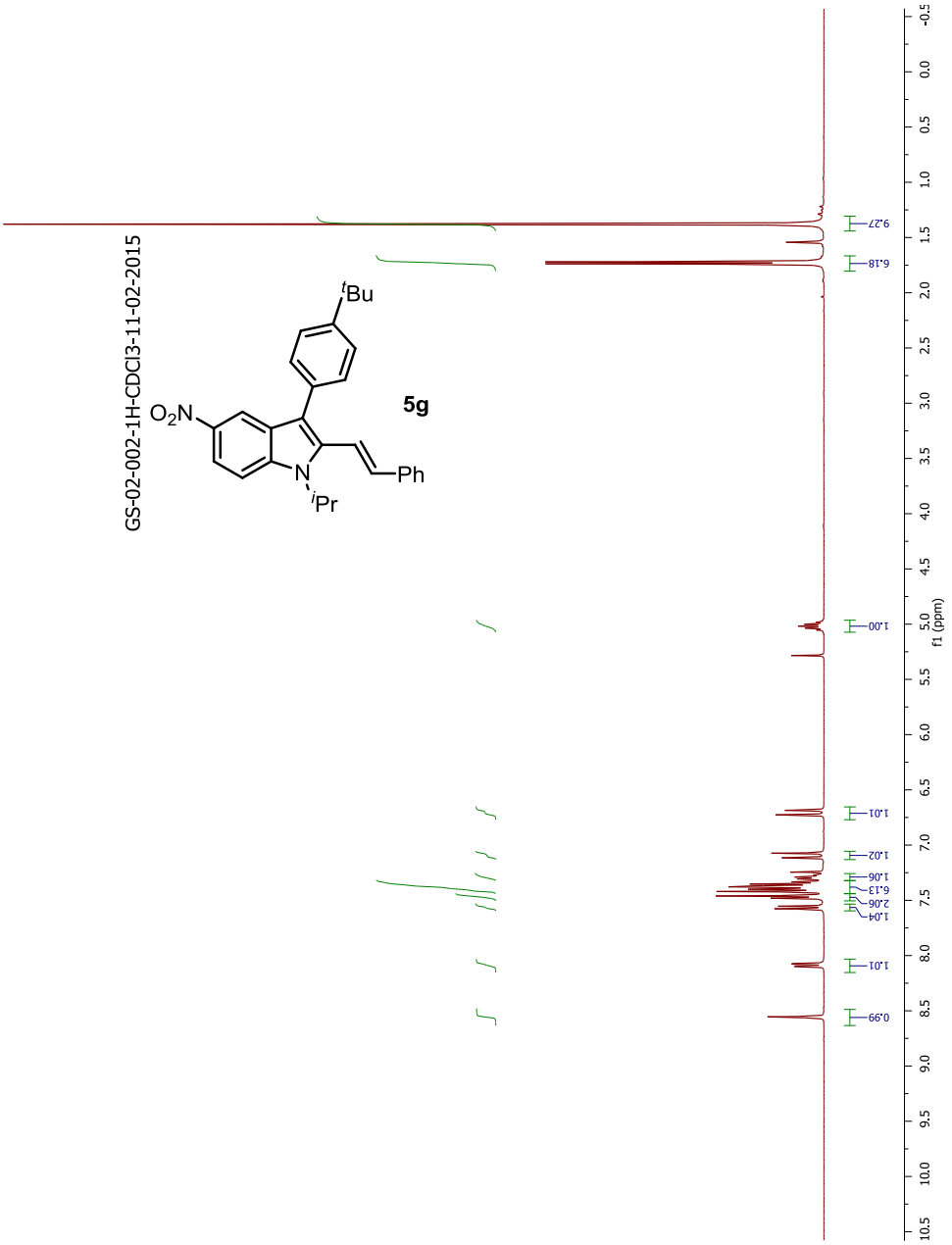

GS-2014021-053P/1H/CDCl3/15-12-2014
Me
N
iPr
Me
5e
6.52
3.07
3.24
1.07
1.01
2.03
1.00
1.05
1.01
6.36
f1 (ppm)

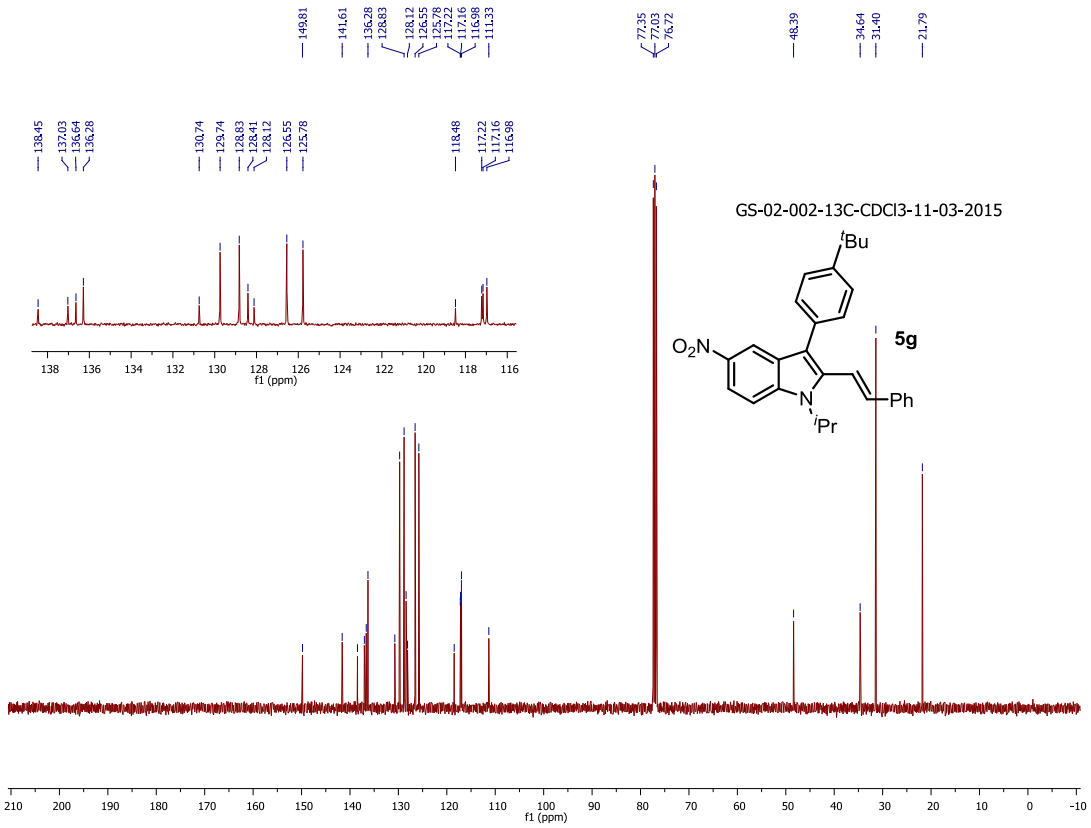

135.96
134.97
134.42
133.94
132.02
130.77
130.44
128.88
128.82
128.34
125.84
123.84
123.20
119.08
115.45
111.52
47.60
21.71
21.36
18.34
GS-2014021-053P/13C/CDCl3/15-12-2014
Me
N
iPr
Me
5e
130.77
130.44
128.88
128.82
128.34
125.84
123.20
119.18
119.08
131 130 129 128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

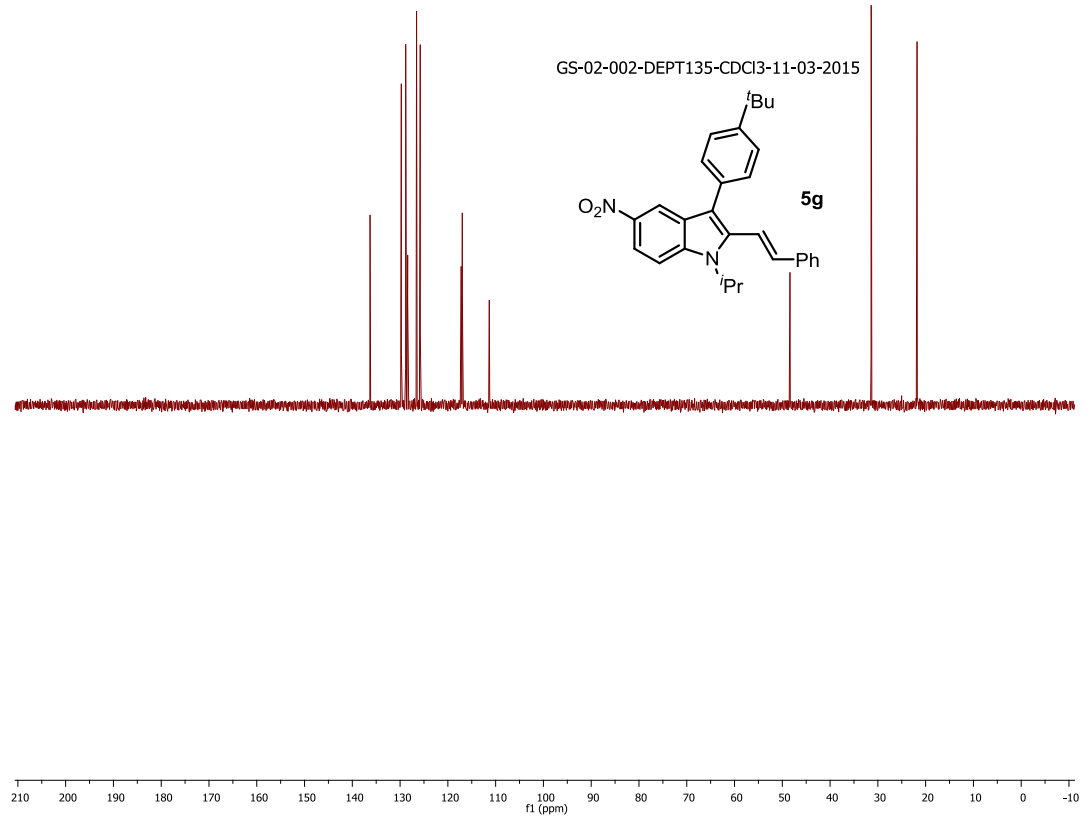

GS-2014021-053P/DEPT135/CDCl3/15-12-2014
Me
N
iPr
Me
5e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

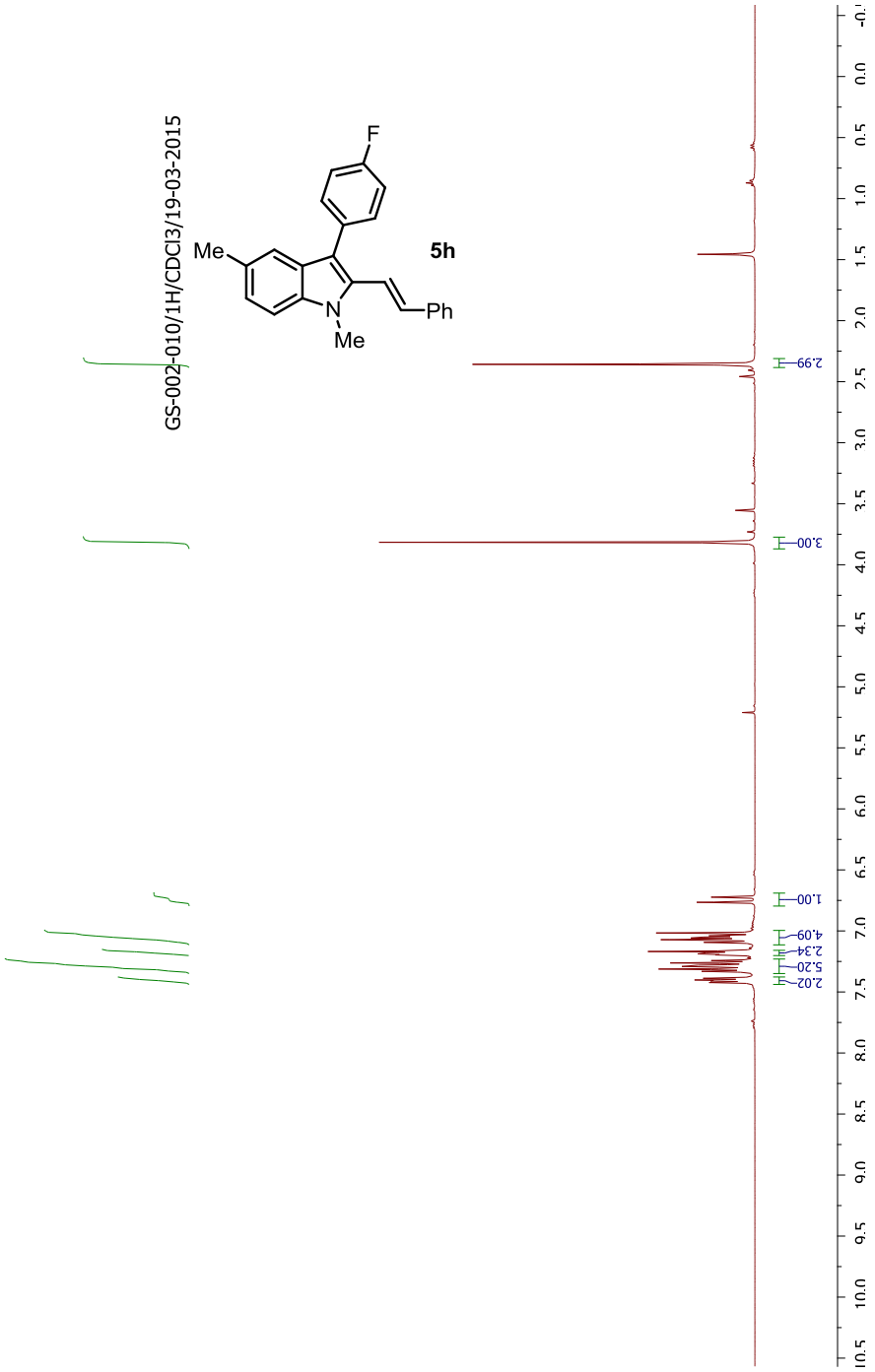

GS-2014021-52P/1H/CDCl3/15-12-2014
Me
5f
6.31
3.02
1.04
1.01
1.99
1.00
1.05
1.05
1.04
2.05
2.03
1.04
1.02
f1 (ppm)

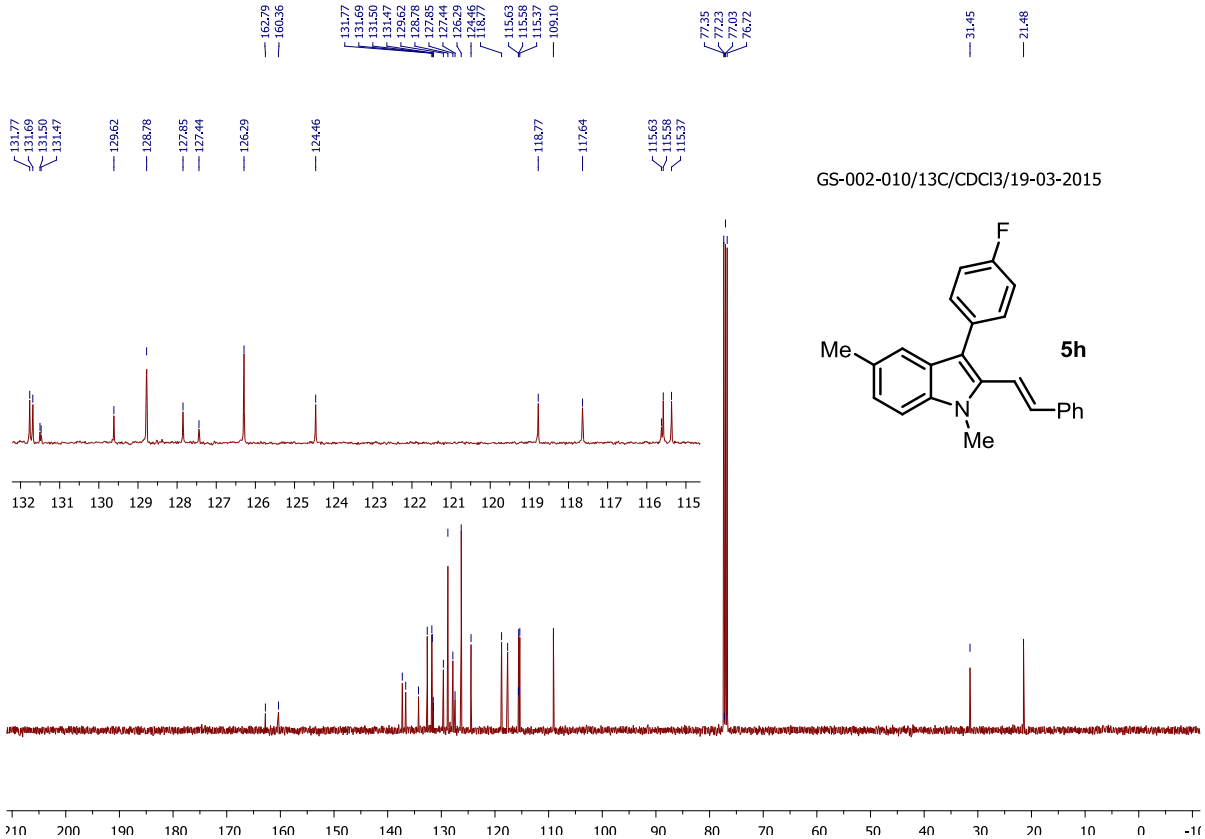

135.79
135.56
135.33
134.33
131.96
130.99
130.40
128.56
128.36
125.90
118.94
115.84
111.77
47.64
21.70
18.34
GS-2014021-52P/13C/CDCl3/15-12-2014
N
H
Me
5f
f1 (ppm)
GS-2014021-52P/DEPT135/CDCl3/15-12-2014
N
H
Me
5f
f1 (ppm)

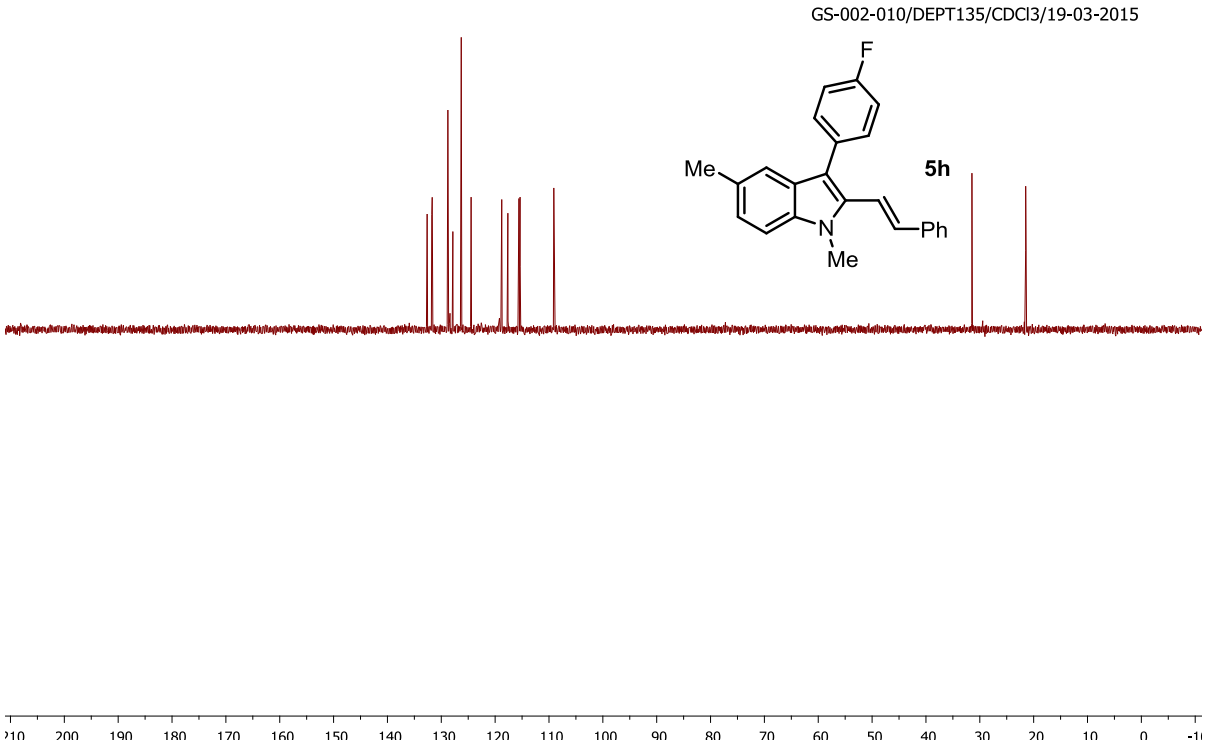

GS-02-002-1H-CDCl3-11-02-2015
tBu
O2N
N
iPr
Ph
5g
9.27
6.18
1.00
1.01
1.02
1.06
6.13
2.06
1.04
1.01
0.99
f1 (ppm)

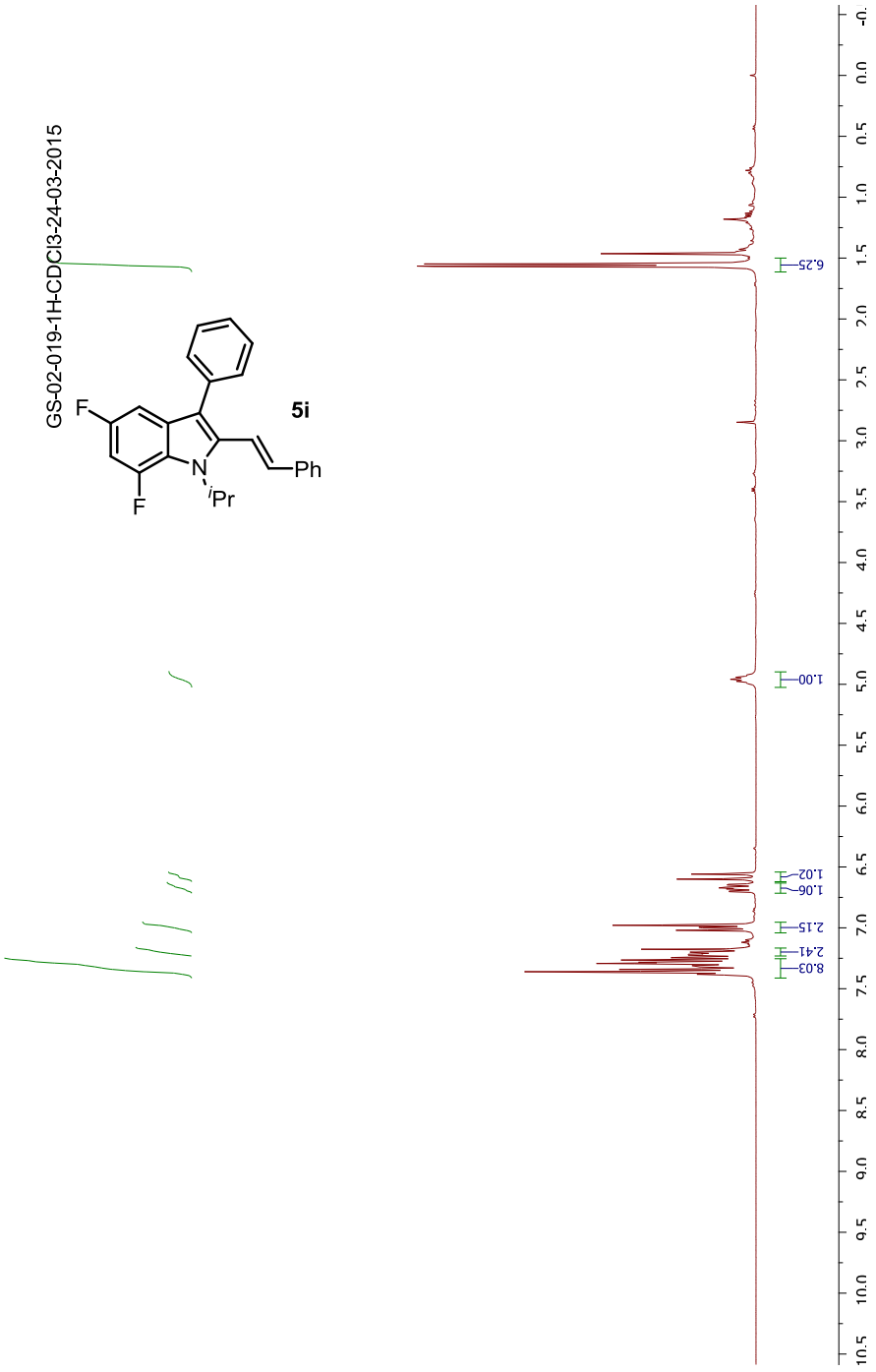

149.81
141.61
136.28
128.83
128.12
126.55
125.78
117.22
117.16
116.98
111.33
77.35
77.03
76.72
48.39
34.64
31.40
21.79
138.45
137.03
136.64
136.28
130.74
129.74
128.83
128.41
128.12
126.55
125.78
118.48
117.22
117.16
116.98
f1 (ppm)
GS-02-002-13C-CDCl3-11-03-2015
tBu
O2N
5g
N
iPr
Ph
f1 (ppm)

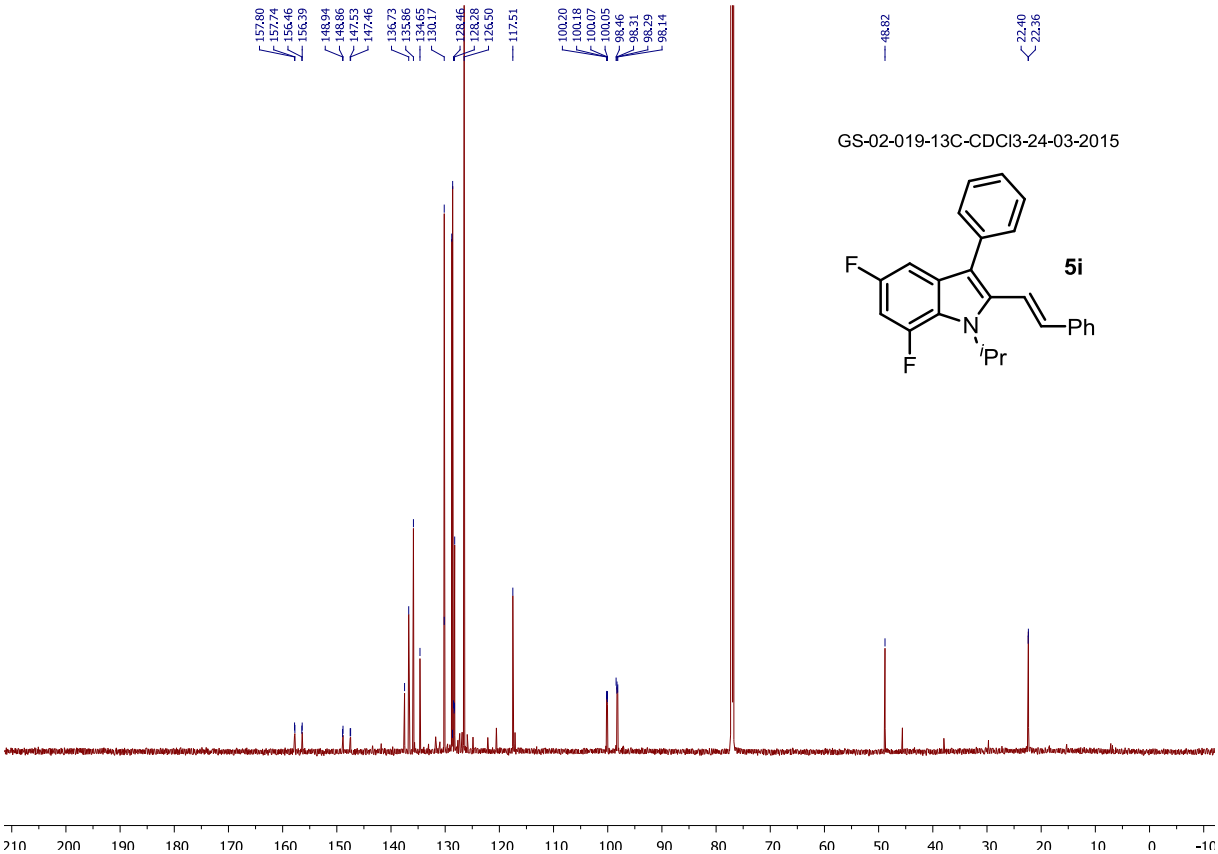

GS-02-002-DEPT135-CDCl3-11-03-2015
tBu
O2N
5g
N
iPr
Ph
f1 (ppm)

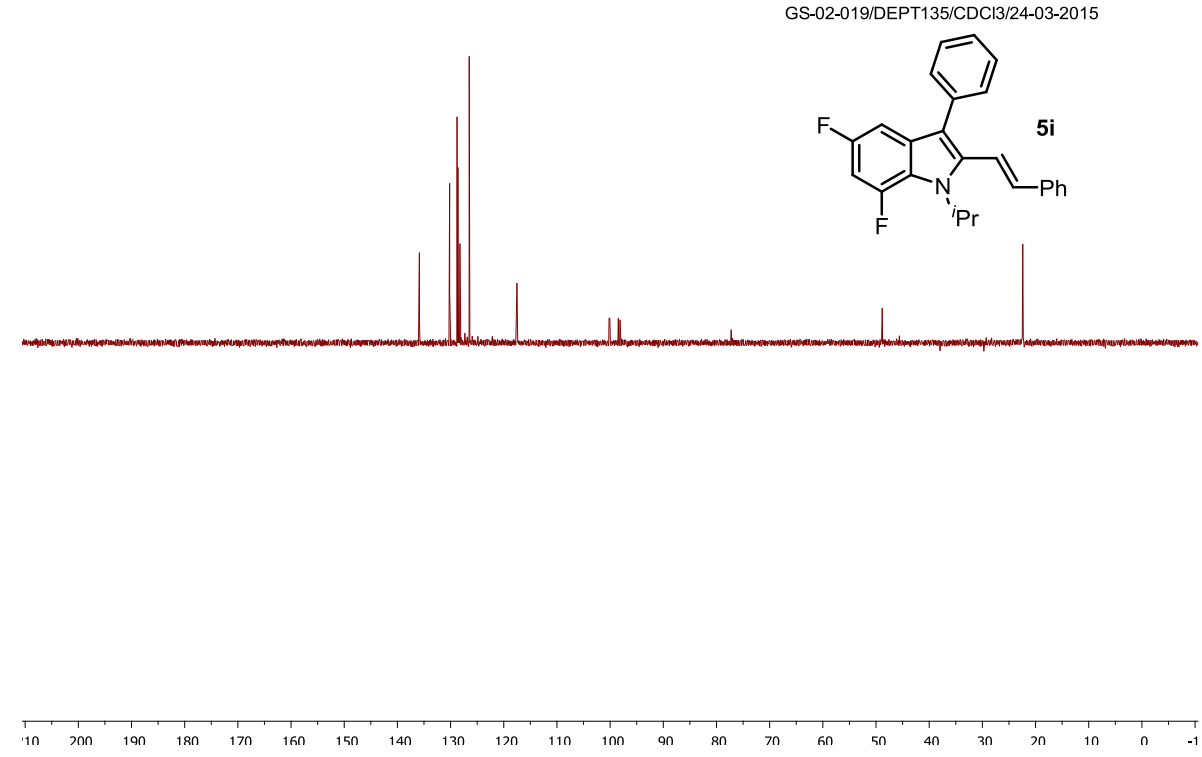

GS-002-010/1H/CDCl3/19-03-2015
F
Me
5h
N
Me
Ph
2.99
3.00
1.00
4.09
2.34
5.20
2.02

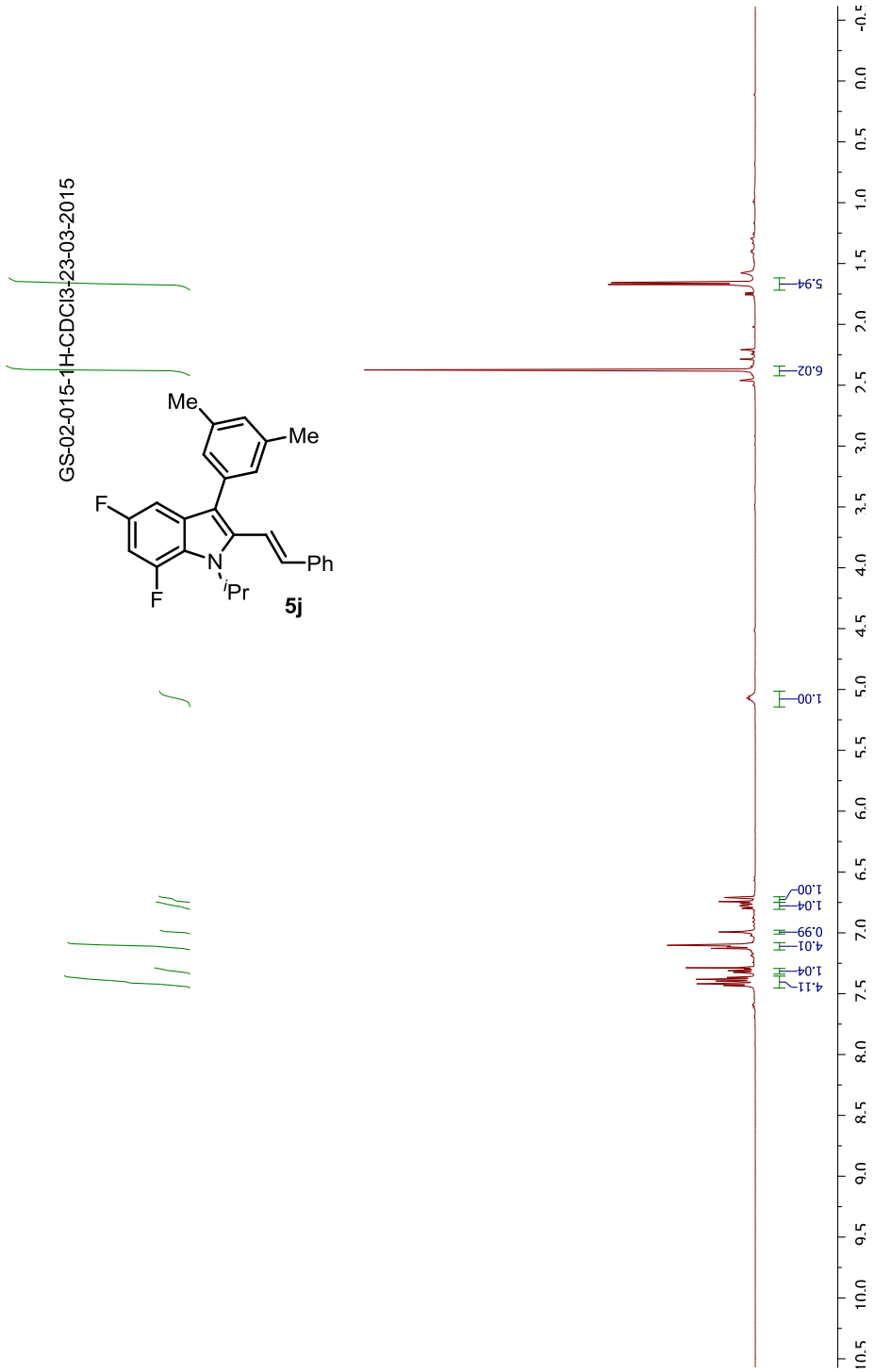

GS-002-010/13C/CDCl3/19-03-2015
5h
Me
F
Ph
N
Me

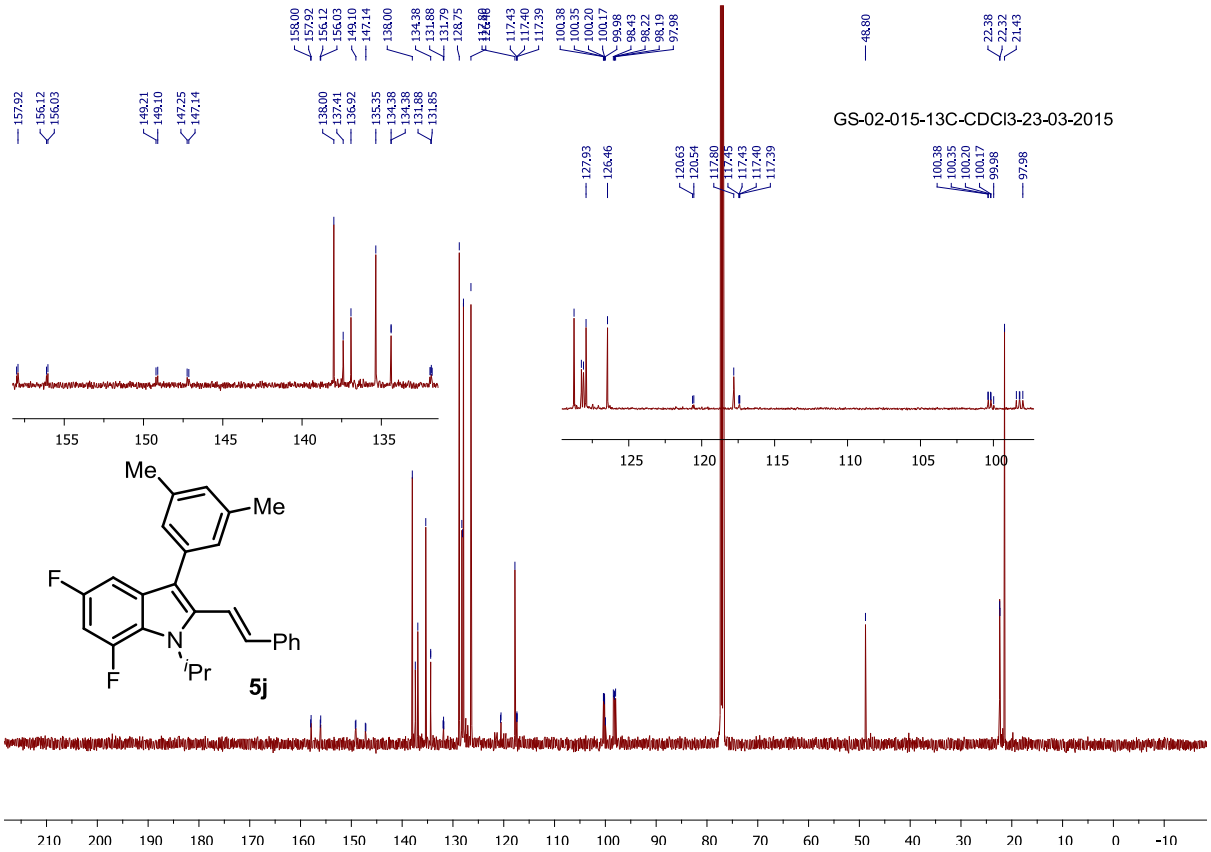

GS-002-010/DEPT135/CDCl3/19-03-2015
5h
Me
F
Ph
N
Me

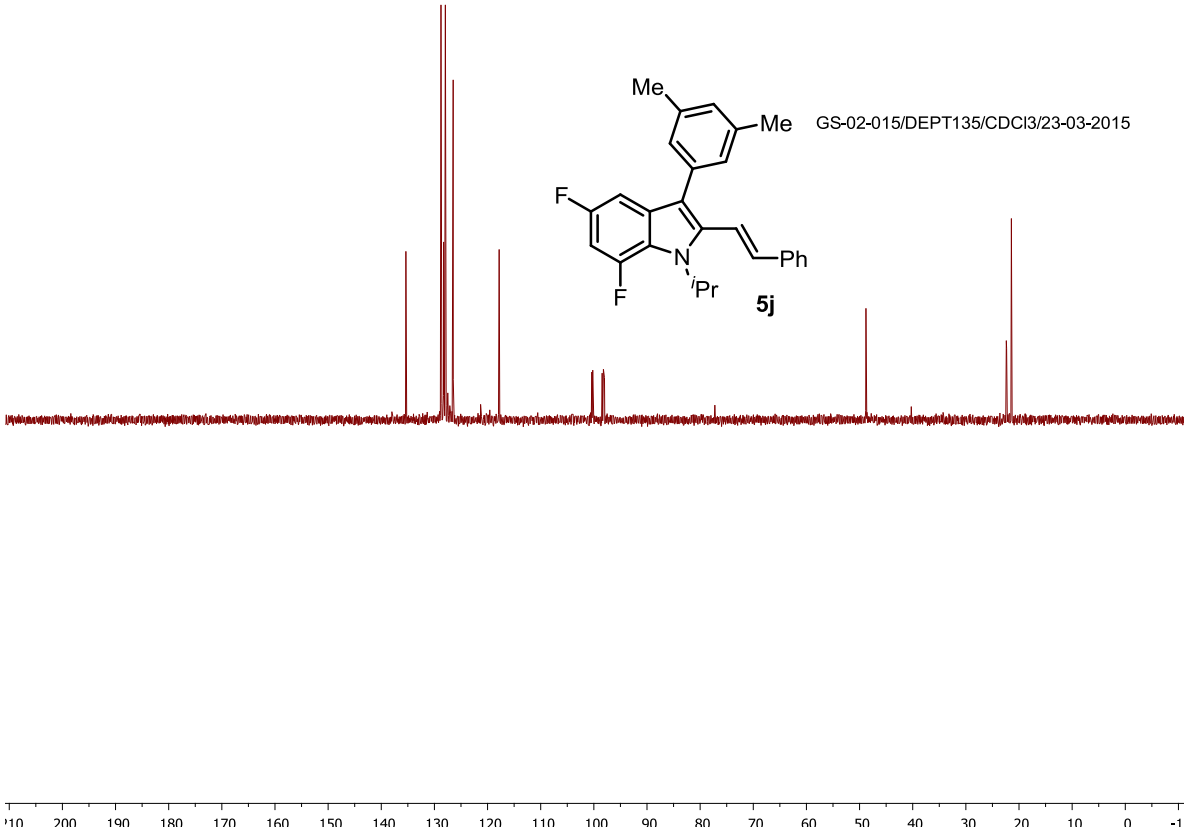

GS-02-019-1H-CDCl3-24-03-2015
F
F
N
iPr
Ph
5i
6.25
1.00
1.02
1.06
2.15
2.41
8.03

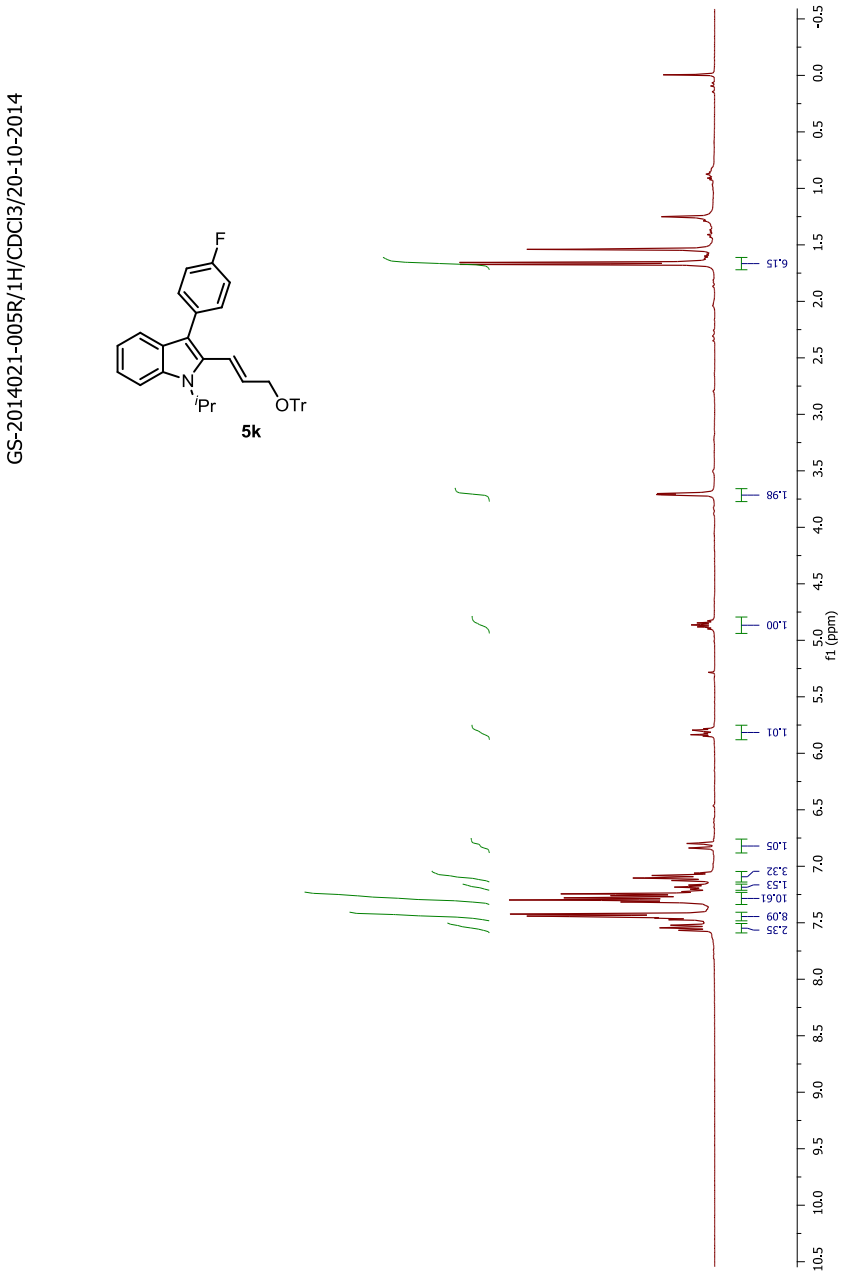

157.80
157.74
156.46
156.39
148.94
148.86
147.53
147.46
136.73
135.86
134.65
130.17
128.46
128.28
126.50
117.51
100.20
100.18
100.07
100.05
98.46
98.31
98.29
98.14
48.82
22.40
22.36
GS-02-019-13C-CDCl3-24-03-2015
5i
F
N
iPr
F
Ph

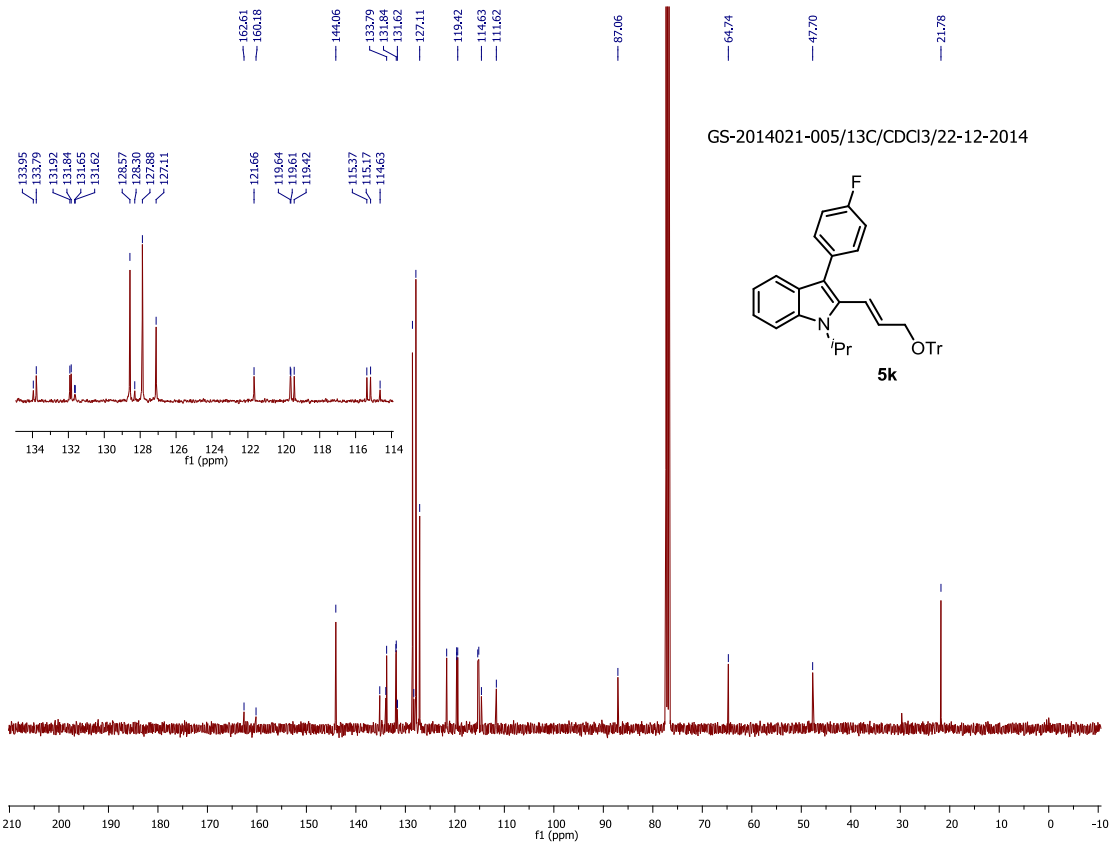

GS-02-019/DEPT135/CDCl3/24-03-2015
5i
F
N
iPr
F
Ph

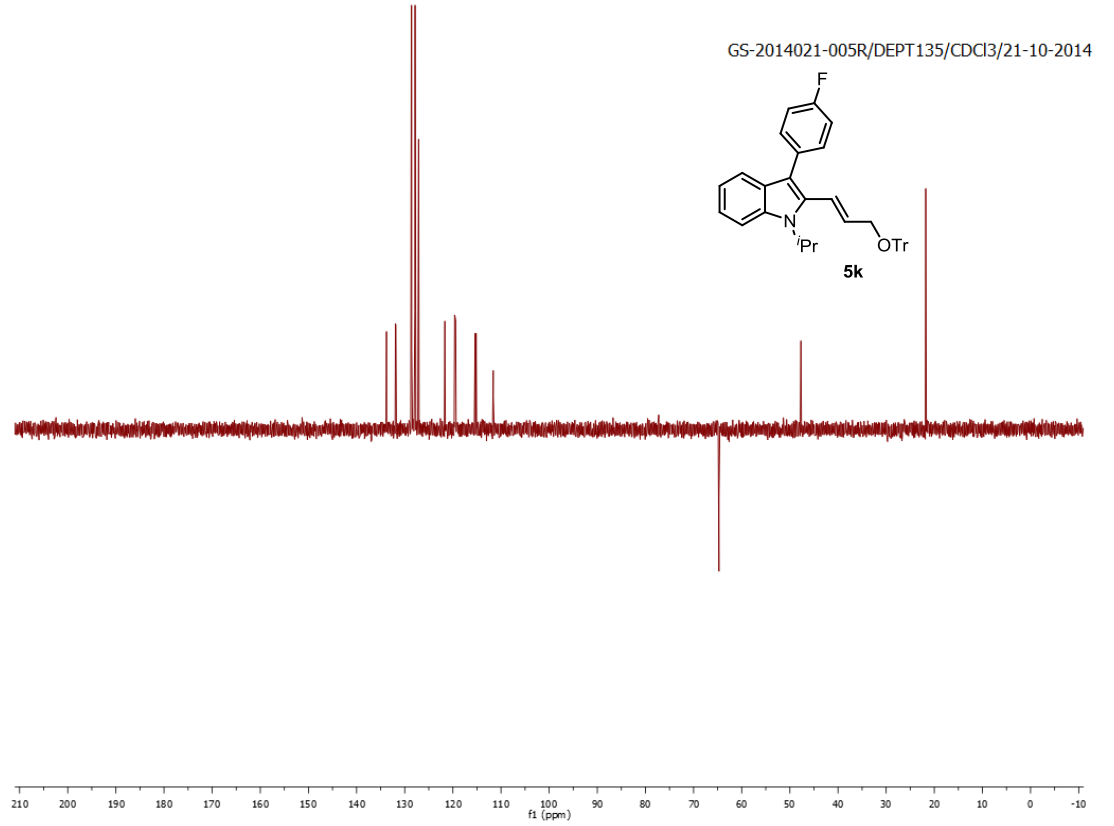

GS-02-015-1H-CDCl3-23-03-2015
Me
Me
F
N
iPr
F
Ph
5j
5.94
6.02
1.00
1.00
1.04
0.99
4.01
1.04
4.11

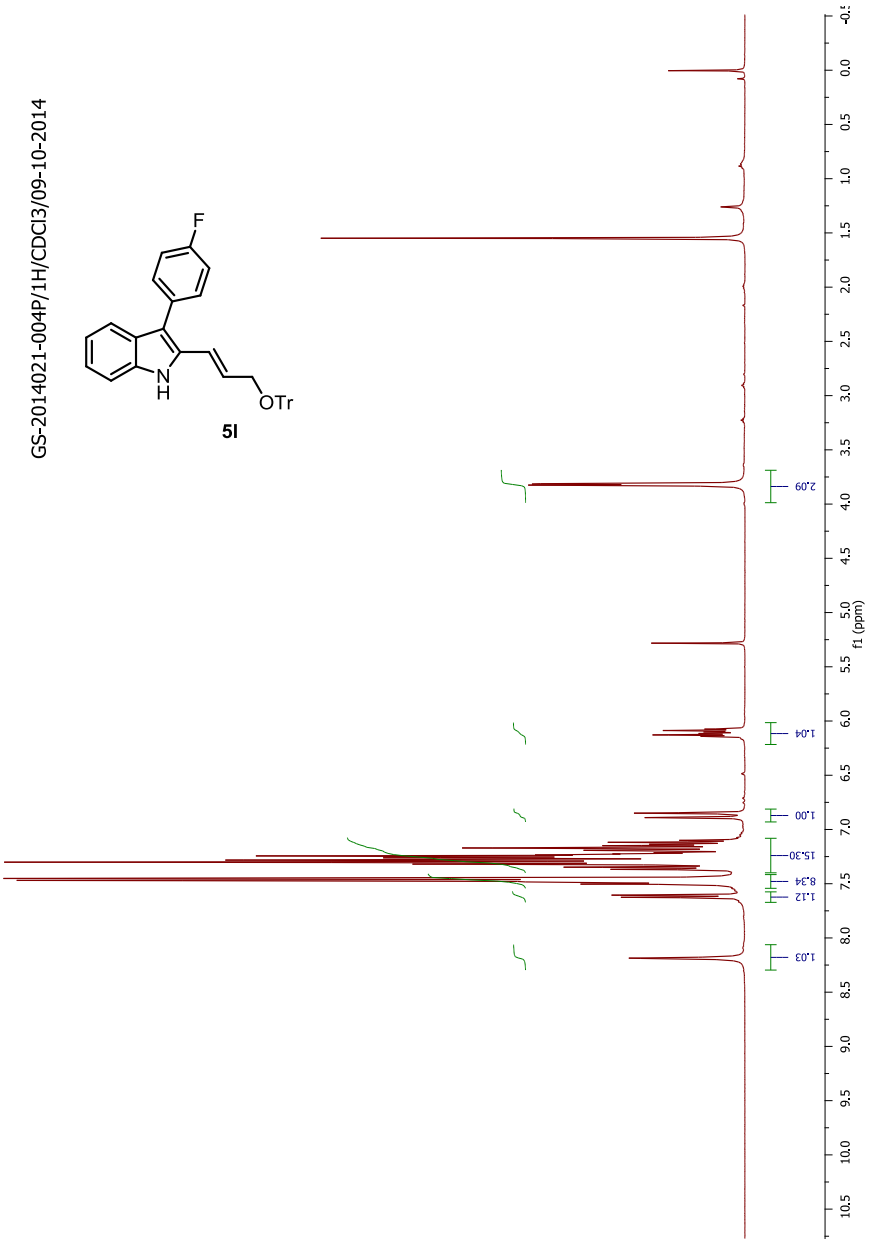

GS-02-015-13C-CDCl3-23-03-2015
Me
Me
F
F
N
iPr
Ph
5j

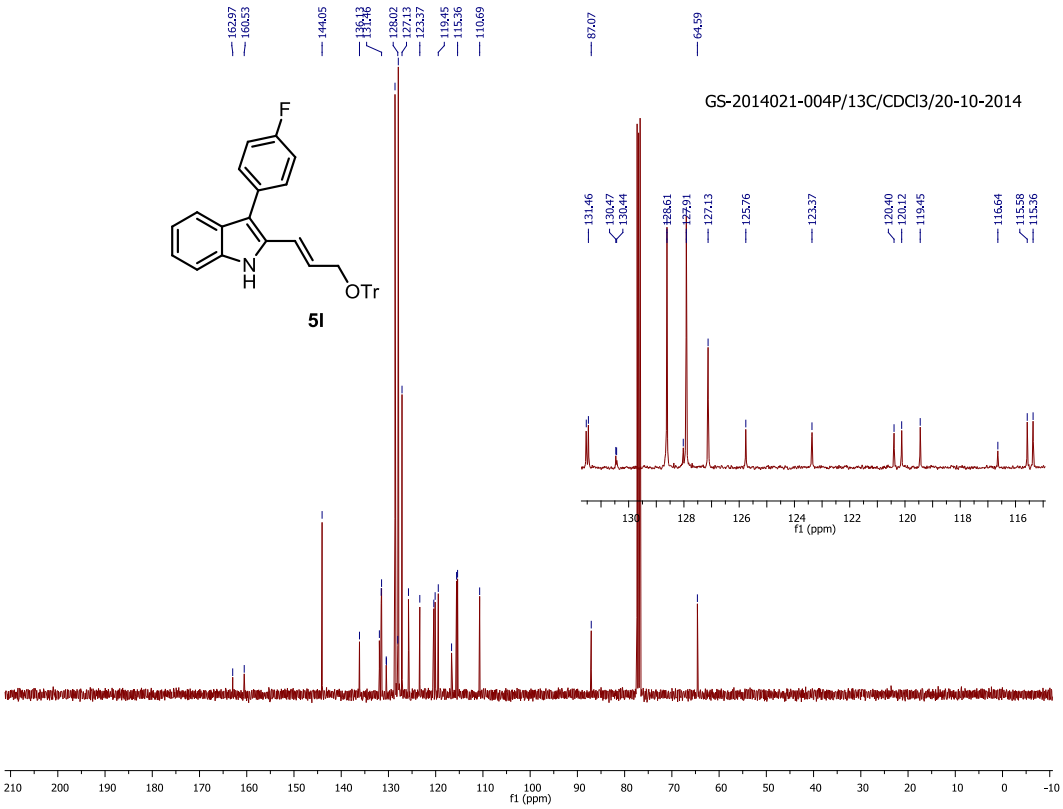

GS-02-015/DEPT135/CDCl3/23-03-2015
Me
Me
F
F
N
iPr
Ph
5j

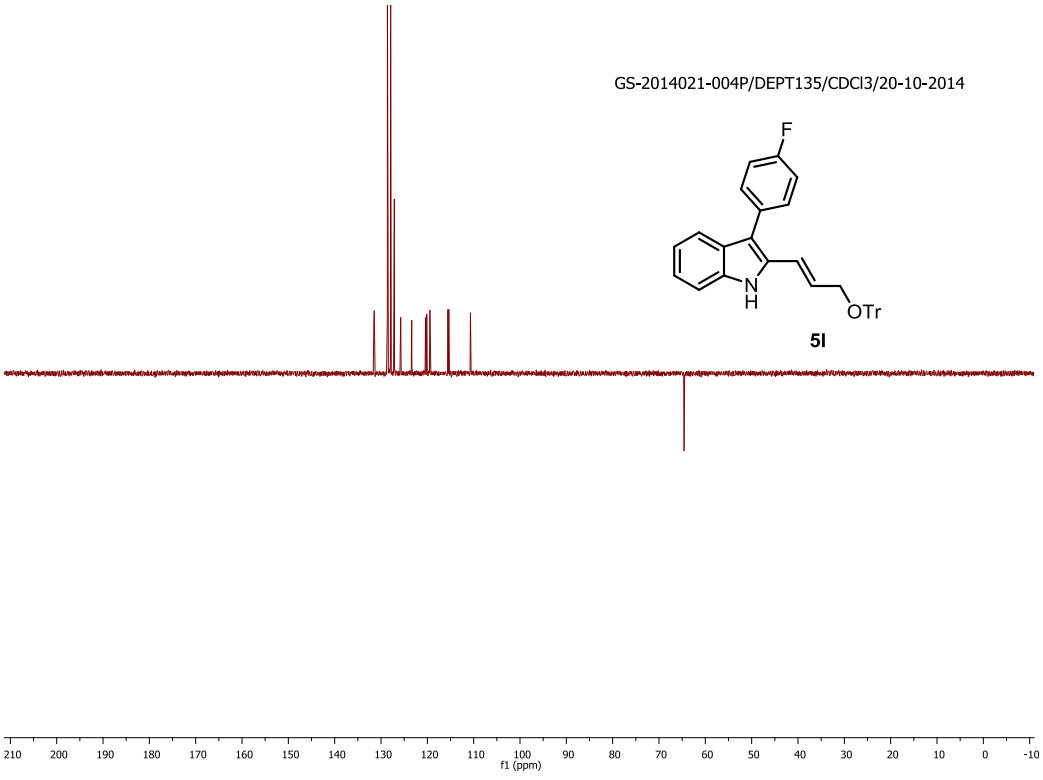

GS-2014021-005R/1H/CDCl3/20-10-2014
F
N
iPr
OTr
5k
6.15
1.98
1.00
1.01
1.05
3.32
1.53
10.61
8.09
2.35
f1 (ppm)

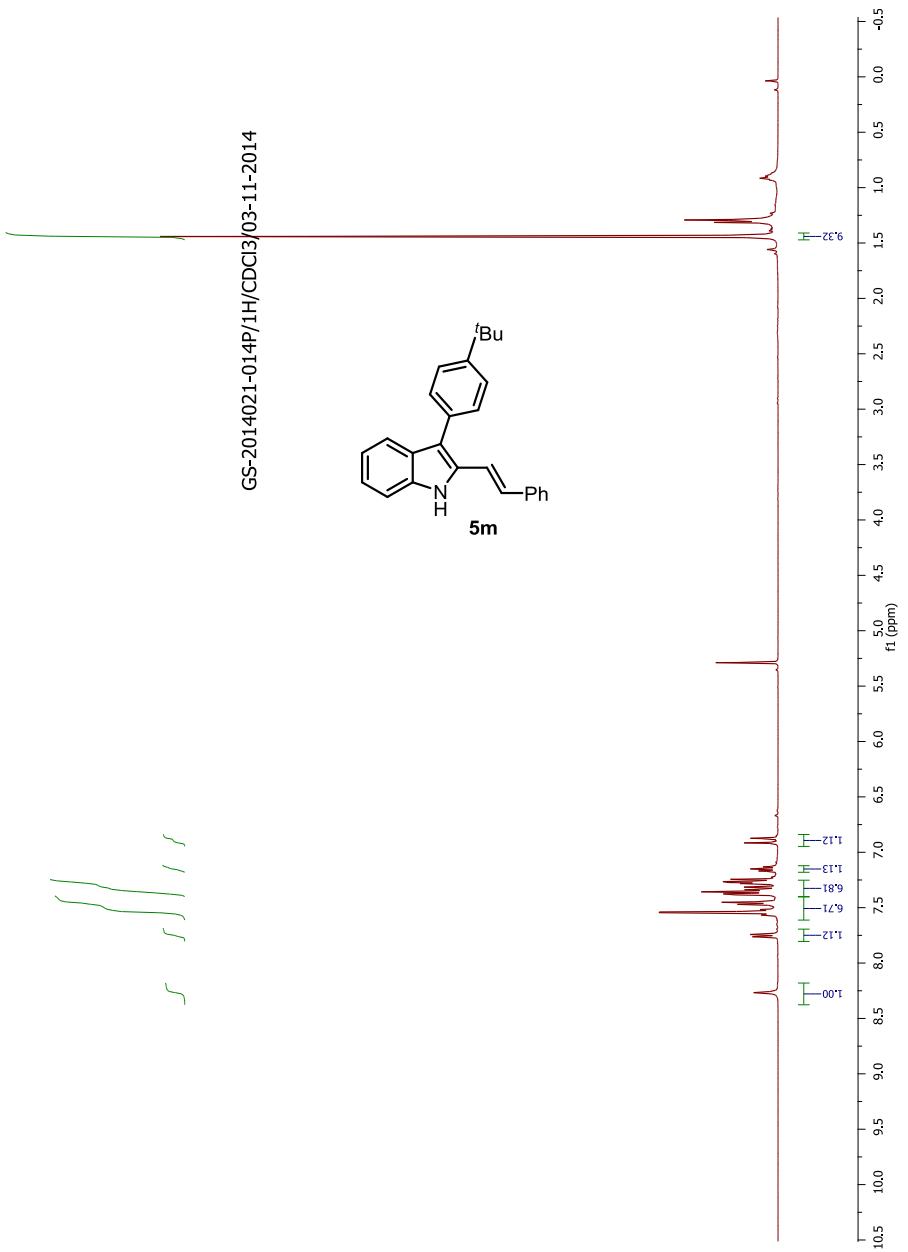

GS-2014021-005/13C/CDCl3/22-12-2014
5k
f1 (ppm)

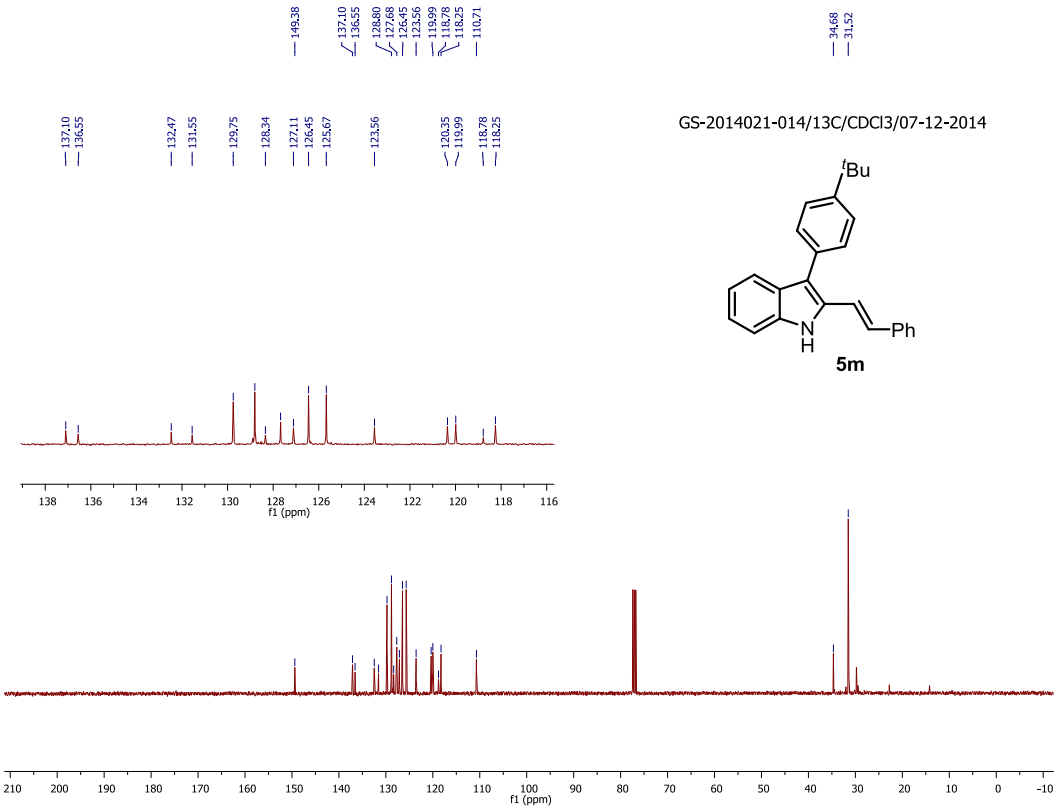

GS-2014021-005R/DEPT135/CDCl3/21-10-2014
5k
f1 (ppm)

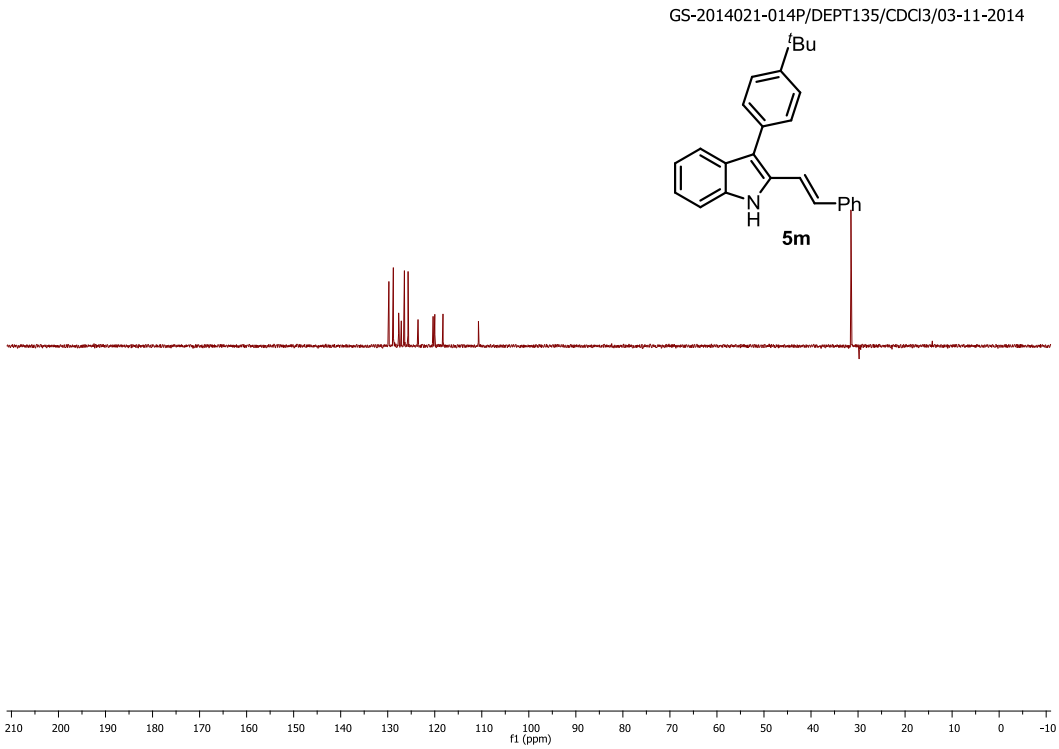

GS-2014021-004P/1H/CDCl3/09-10-2014
F
N
H
OTr
5l
2.09
1.04
1.00
15.30
8.34
1.12
1.03
f1 (ppm)

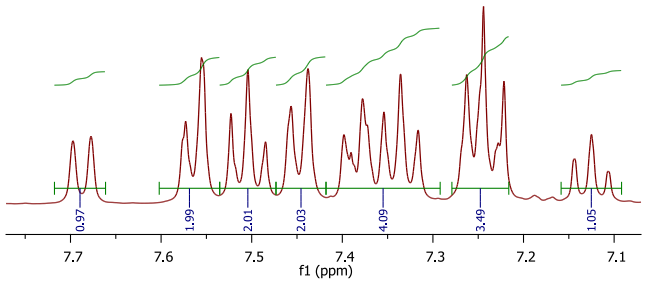

GS-2014021-004P/13C/CDCl3/20-10-2014
162.97
160.53
144.05
136.13
135.48
128.02
127.13
123.37
119.45
115.36
110.69
87.07
64.59
F
N
H
OTr
5l
131.46
130.47
130.44
128.61
127.91
127.13
125.76
123.37
120.40
120.12
119.45
116.64
115.58
115.36
130
128
126
124
122
120
118
116
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


GS-2014021-004P/DEPT135/CDCl3/20-10-2014
F
N
H
OTr
5l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

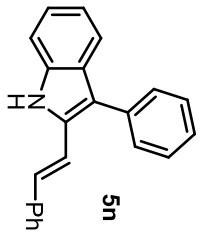

GS-2014021-014P/1H/CDCl3/03-11-2014
tBu
Ph
N
H
5m
9.32
1.12
1.13
6.81
6.71
1.12
1.00
f1 (ppm)


149.38
137.10
136.55
128.80
127.68
126.45
123.56
119.99
118.78
118.25
110.71
34.68
31.52
137.10
136.55
132.47
131.55
129.75
128.34
127.11
126.45
125.67
123.56
120.35
119.99
118.78
118.25
GS-2014021-014/13C/CDCl3/07-12-2014
tBu
Ph
N
H
5m
f1 (ppm)

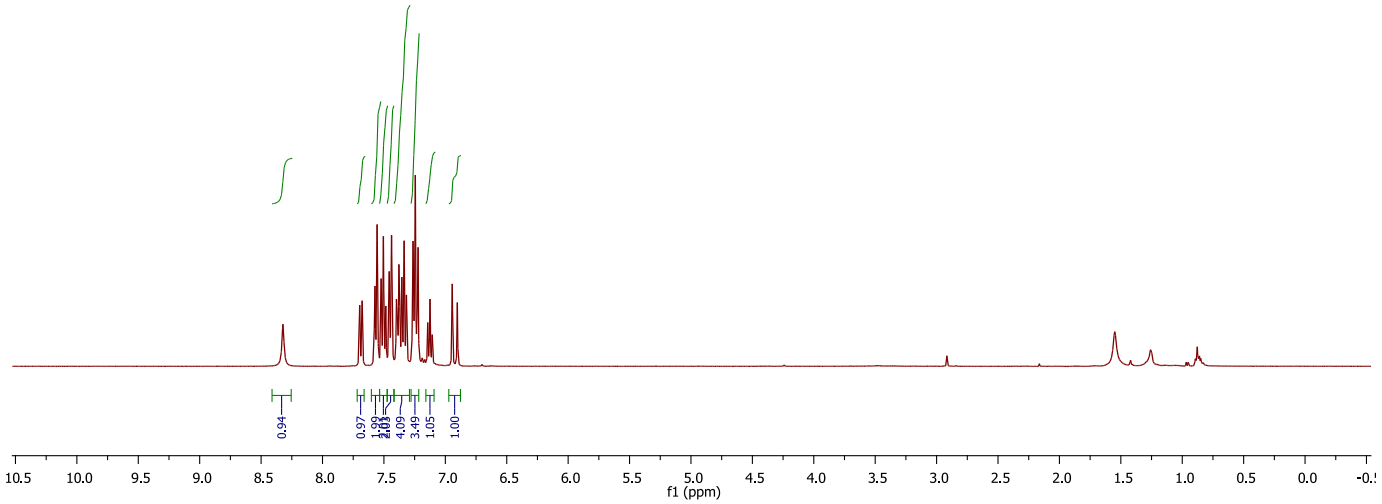

GS-2014021-014P/DEPT135/CDCl3/03-11-2014
tBu
Ph
N
H
5m
f1 (ppm)

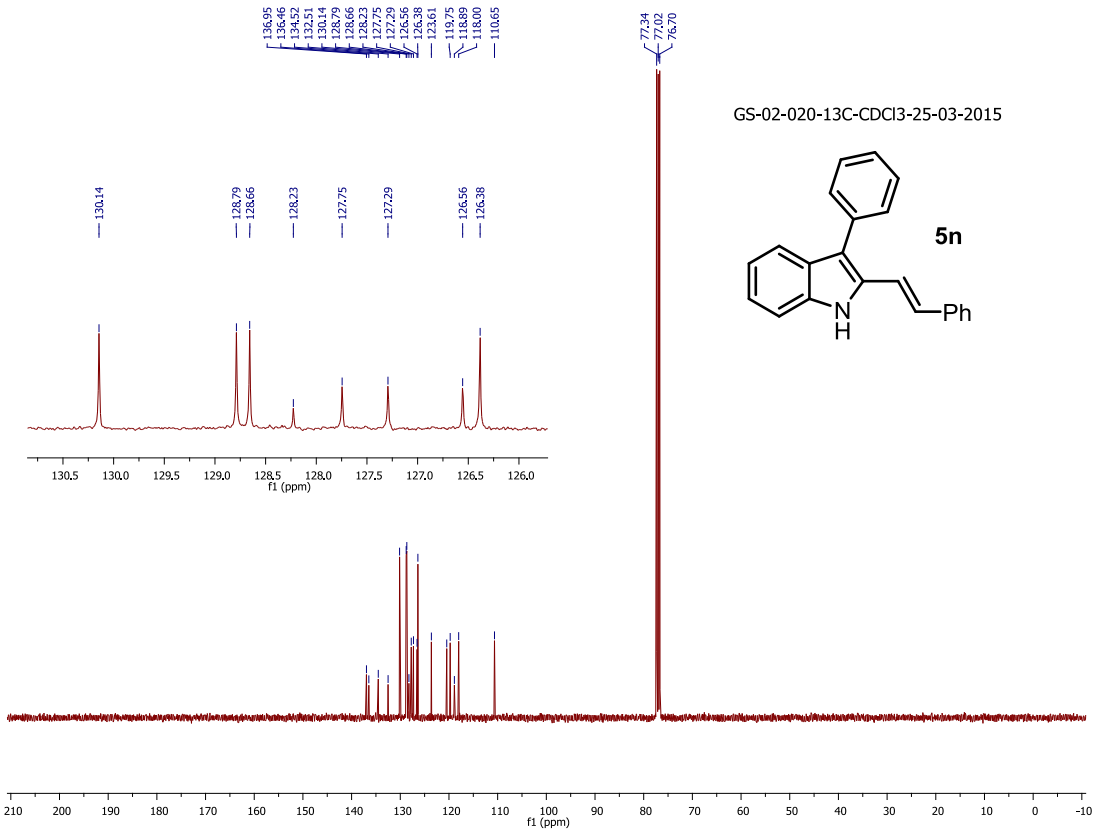


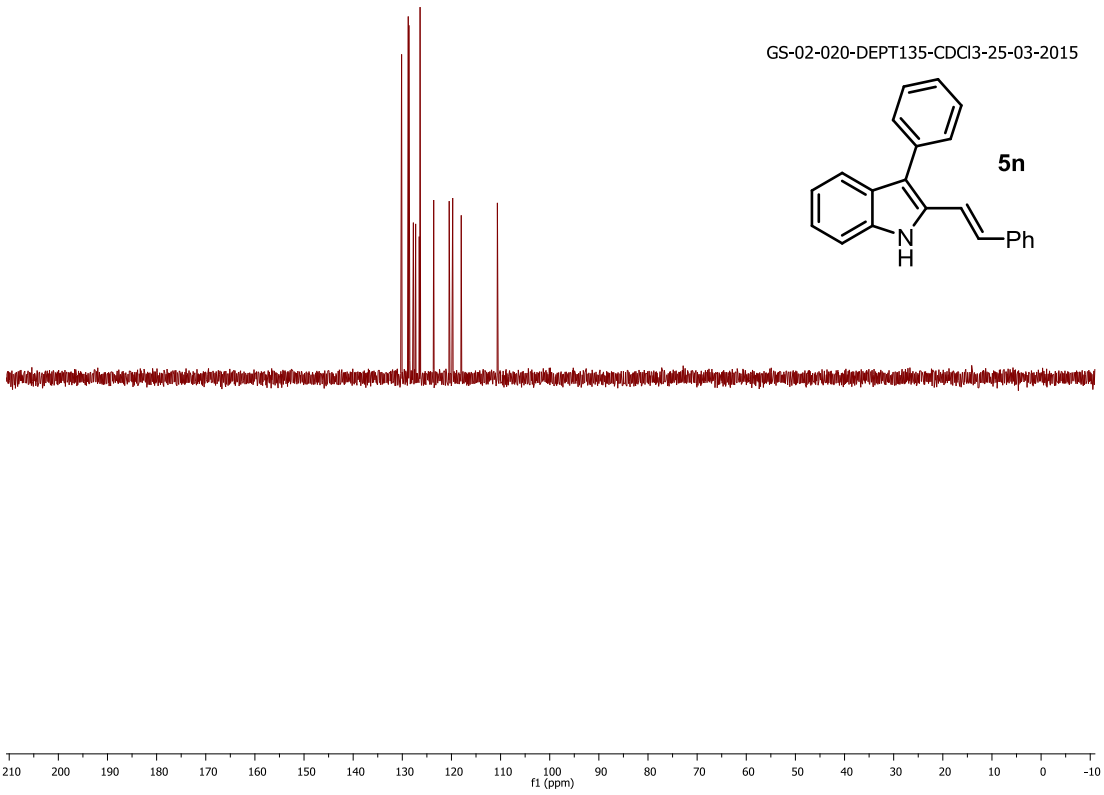
GS-02-020-1H-CDCl3-25-03-2015

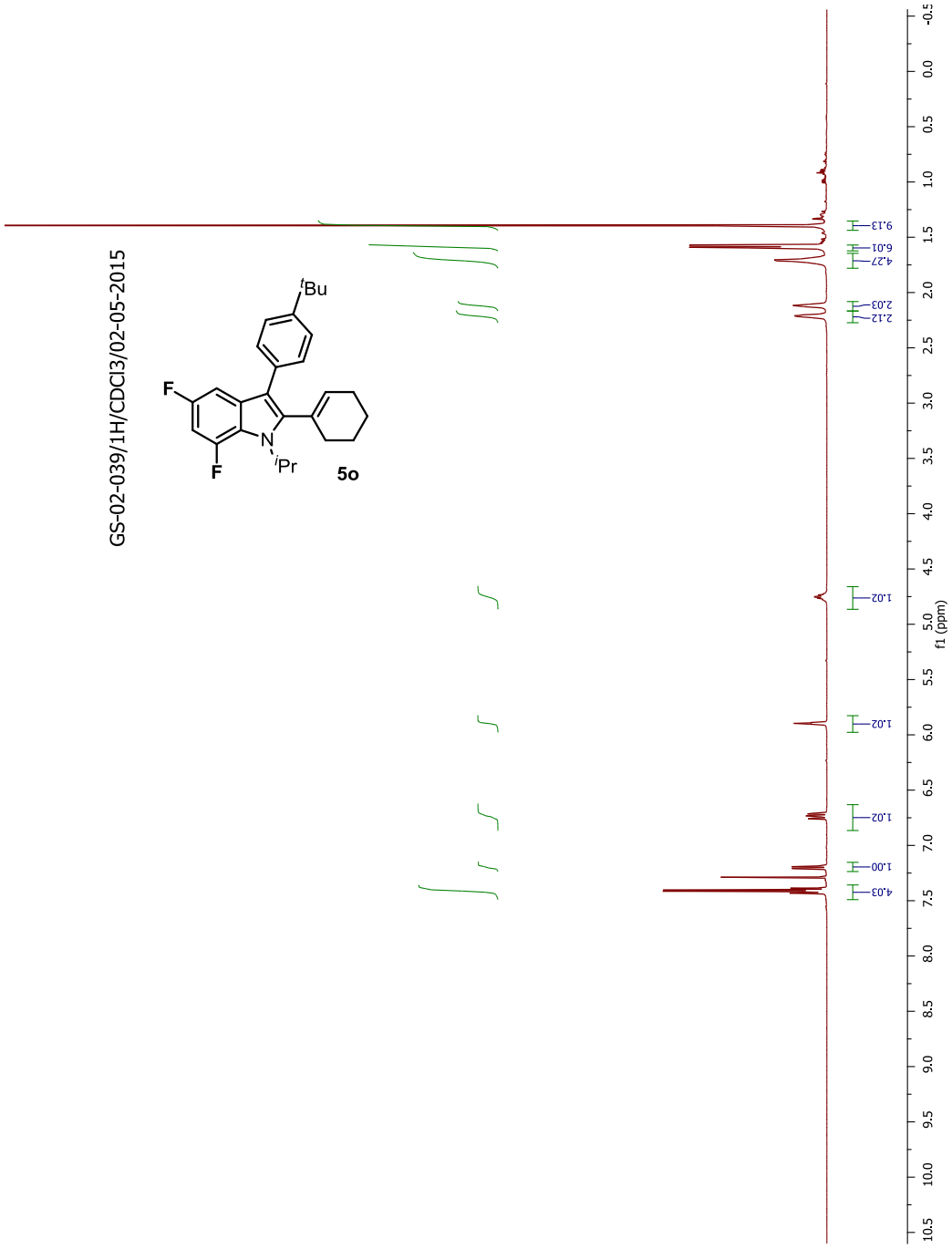


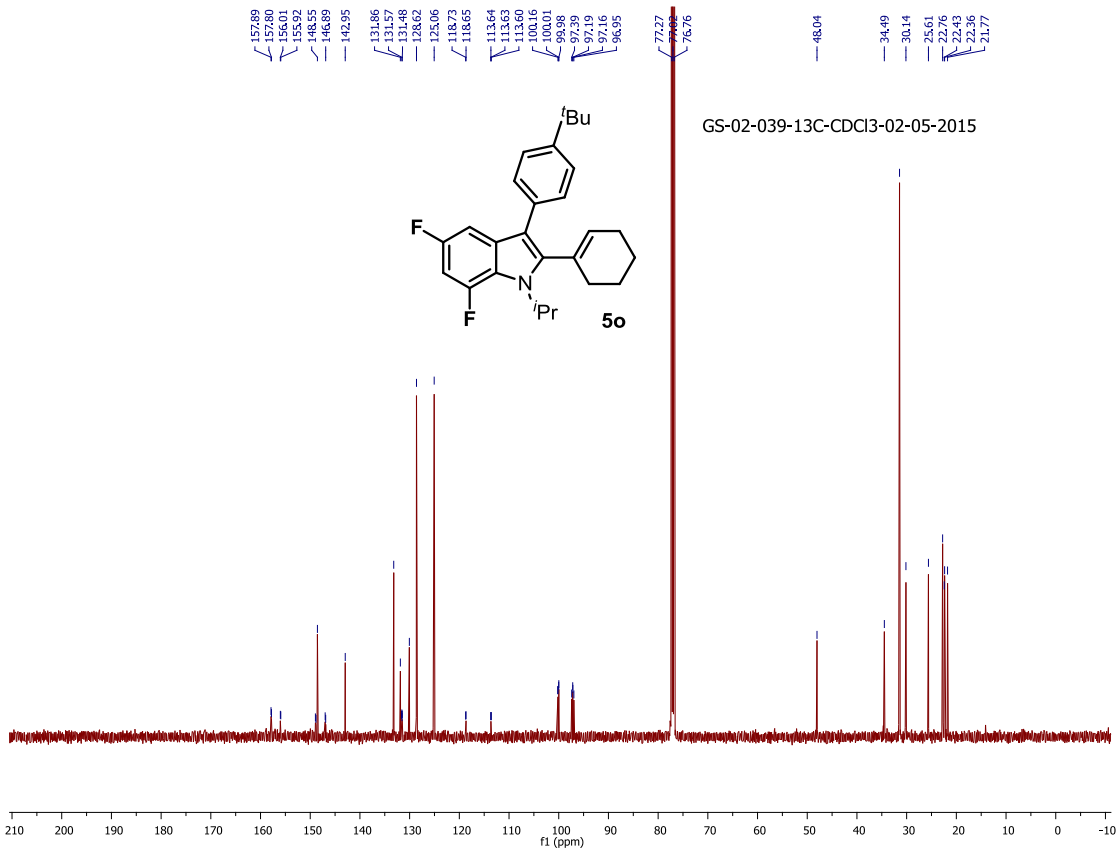
5n

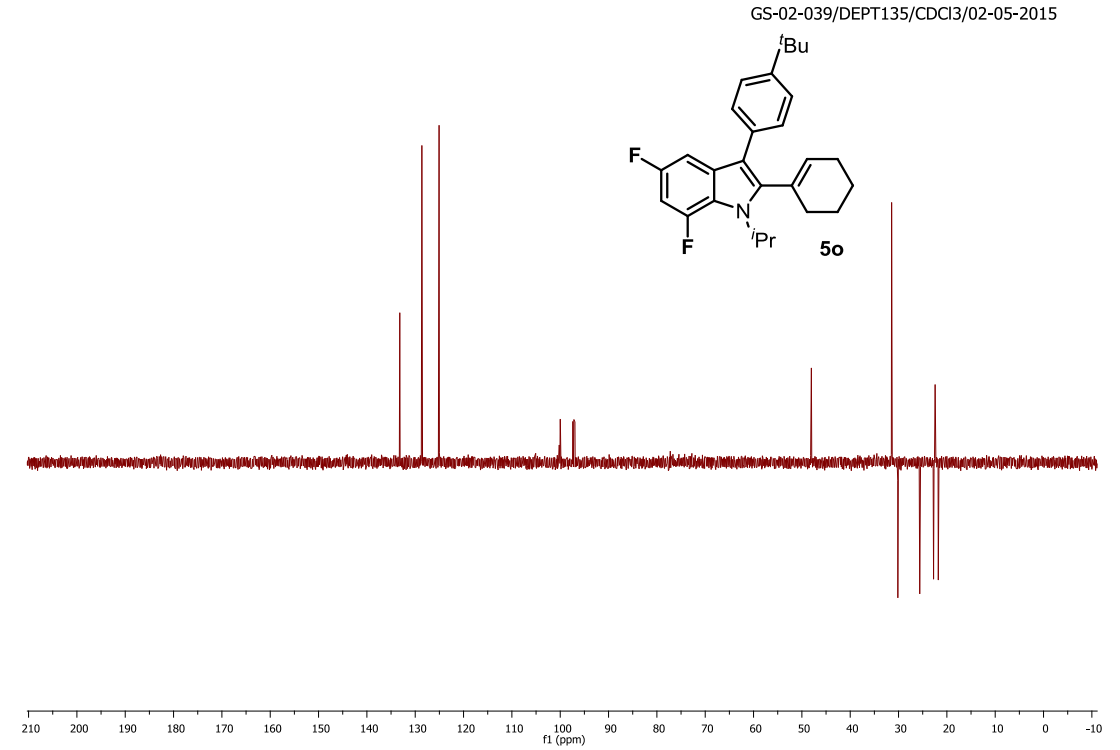


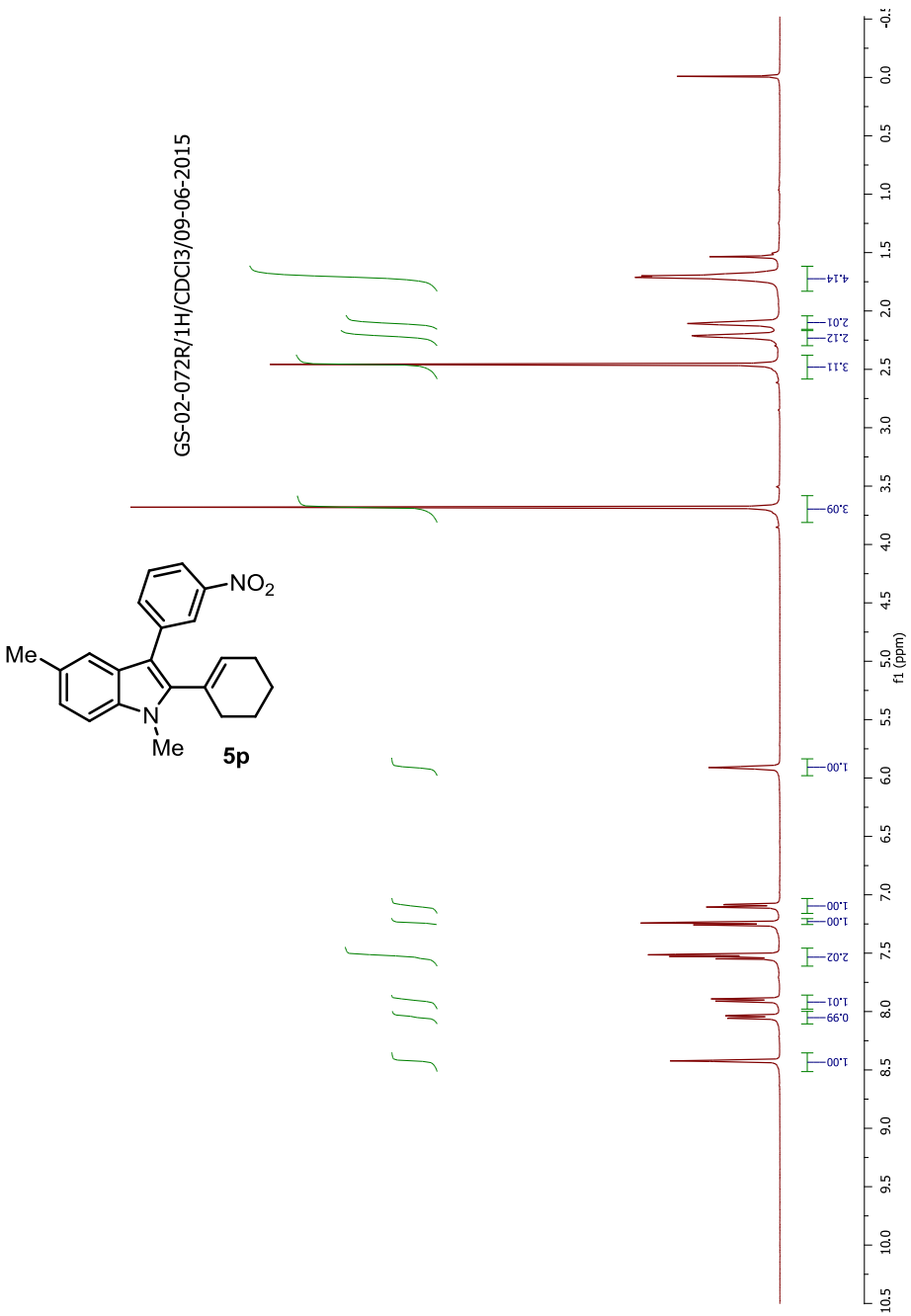

136.95
136.46
134.52
132.51
130.14
128.79
128.66
128.23
127.75
127.29
126.56
126.38
123.61
119.75
118.89
118.00
110.65
77.34
77.02
76.70
130.14
128.79
128.66
128.23
127.75
127.29
126.56
126.38
f1 (ppm)
GS-02-020-13C-CDCl3-25-03-2015
5n
N
H
Ph
f1 (ppm)

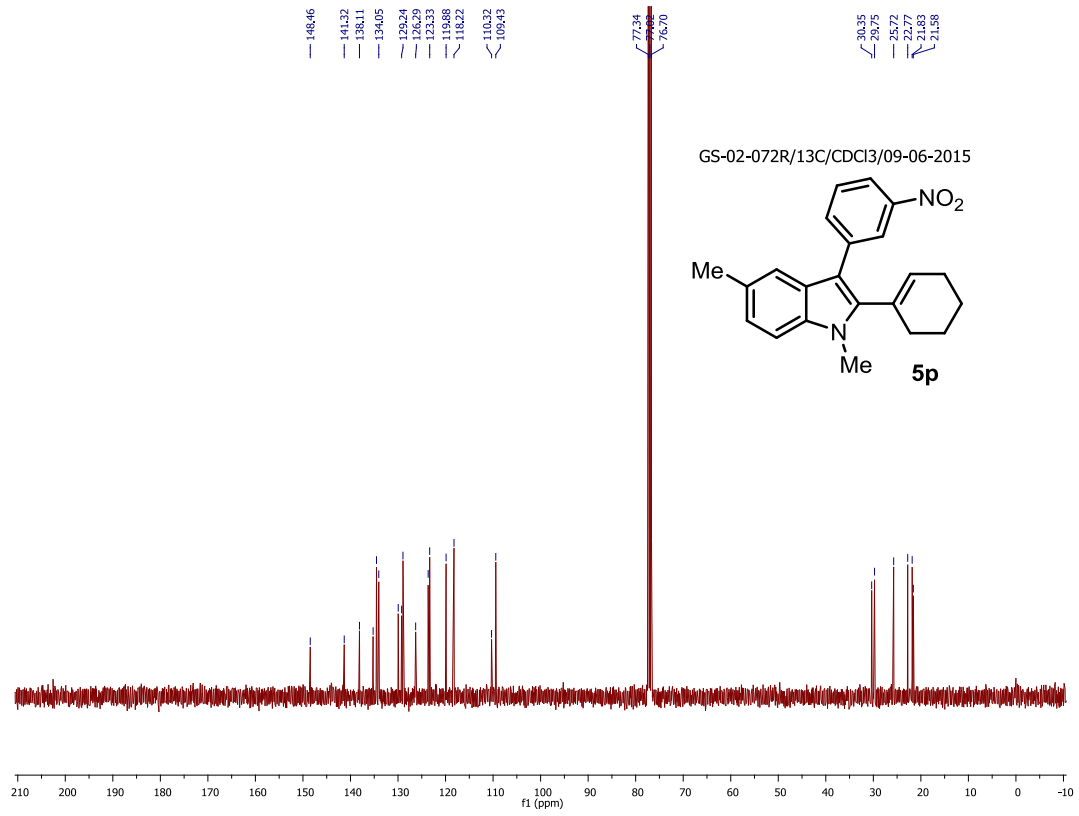

GS-02-020-DEPT135-CDCl3-25-03-2015
5n
N
H
Ph
f1 (ppm)

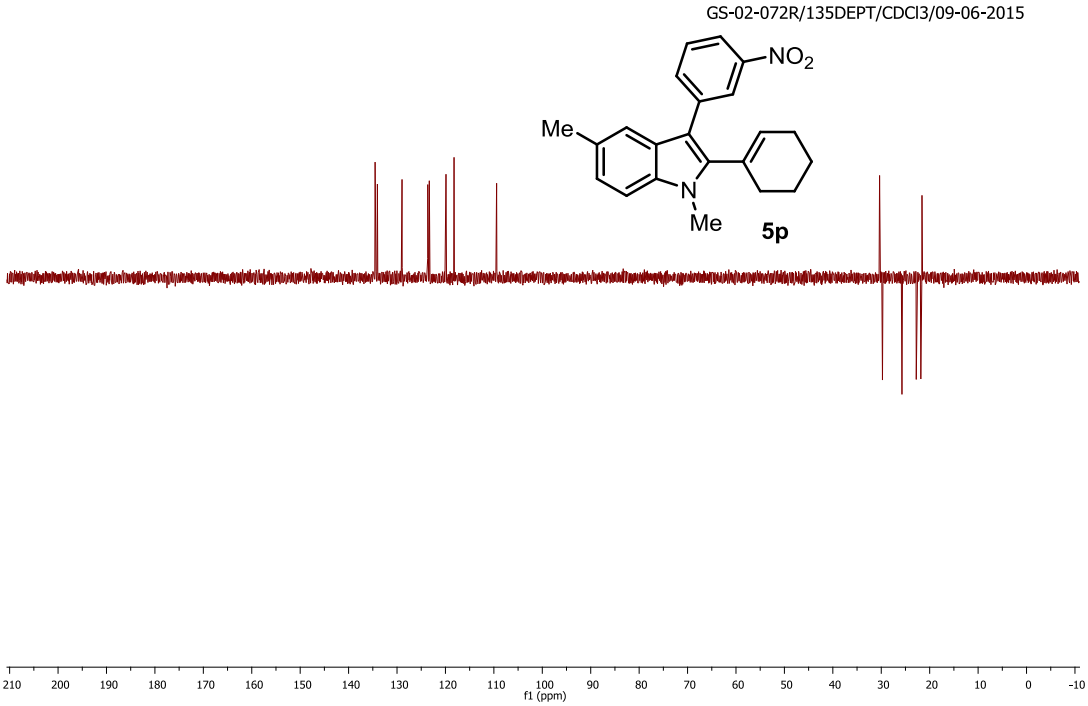

GS-02-039/1H/CDCl3/02-05-2015
tBu
F
F
N
iPr
5o
9.13
6.01
4.27
2.12
2.03
1.02
1.02
1.02
1.00
4.03
f1 (ppm)

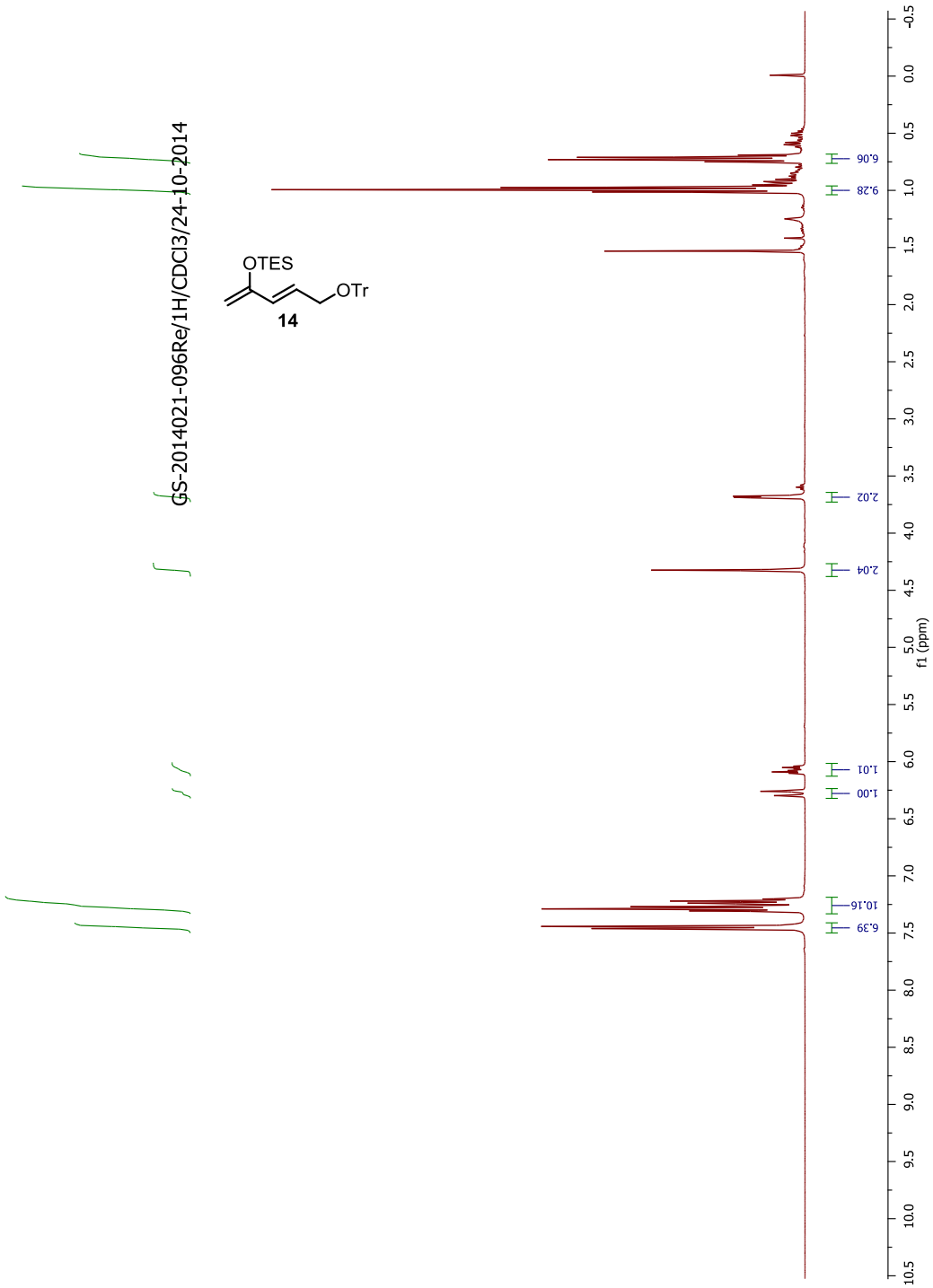

157.89
157.80
156.01
155.92
148.55
146.89
142.95
131.86
131.57
131.48
128.62
125.06
118.73
118.65
113.64
113.63
113.60
100.16
100.01
99.98
97.39
97.19
97.16
96.95
77.27
77.02
76.76
48.04
34.49
30.14
25.61
22.76
22.43
22.36
21.77
GS-02-039-13C-CDCl3-02-05-2015
tBu
F
N
iPr
F
5o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

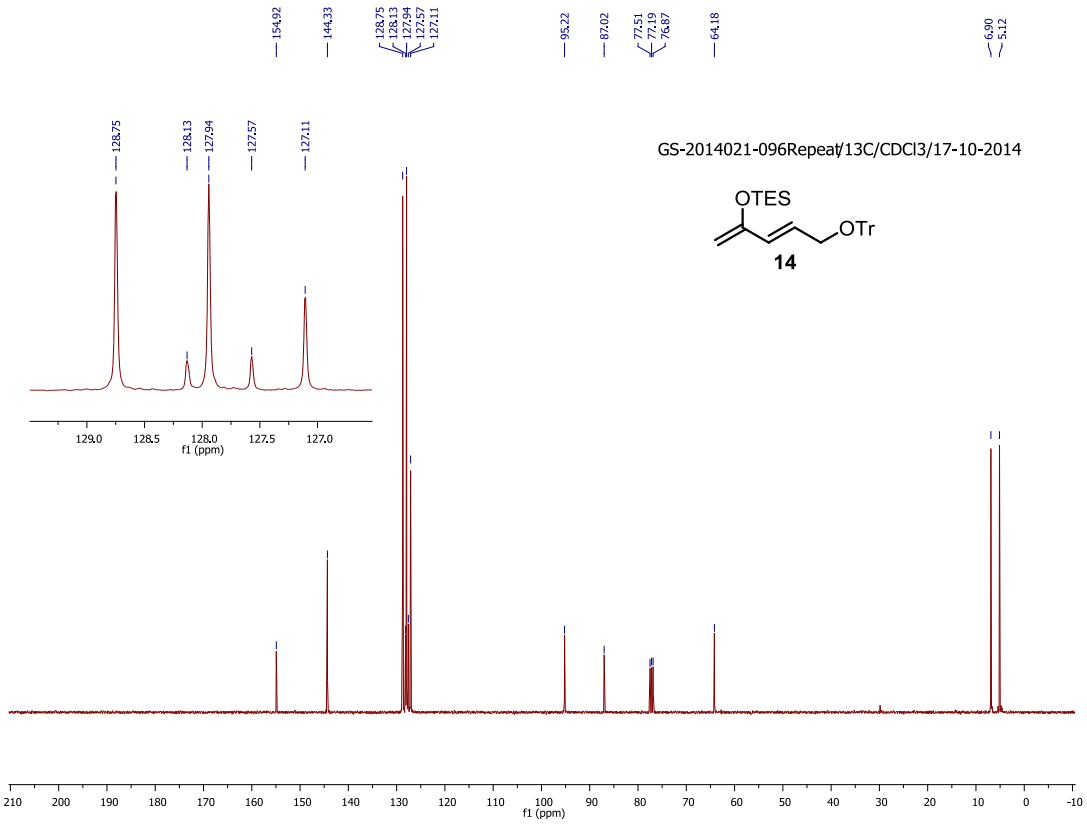

GS-02-039/DEPT135/CDCl3/02-05-2015
tBu
F
N
iPr
F
5o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

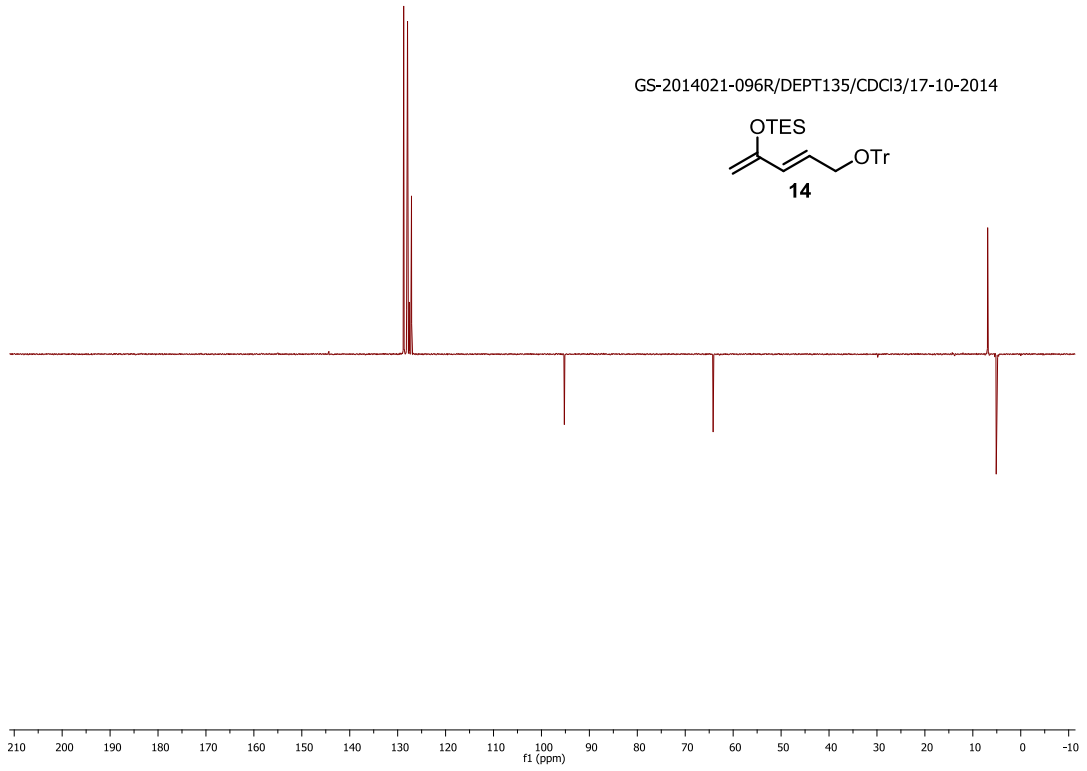

GS-02-072R/1H/CDCl3/09-06-2015
NO2
Me
N
Me
5p
4.14
2.01
2.12
3.11
3.09
1.00
1.00
1.00
2.02
1.01
0.99
1.00
f1 (ppm)

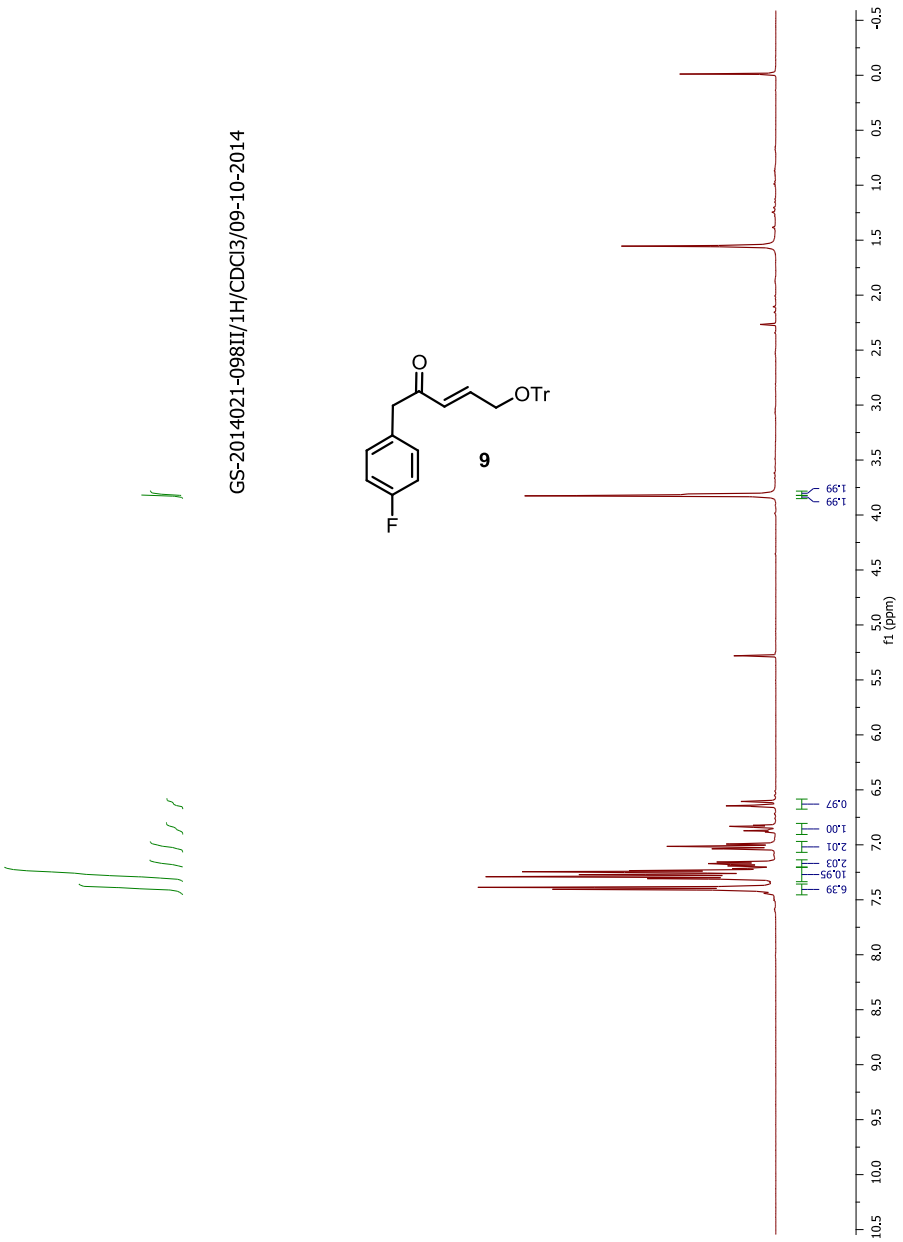

148.46
141.32
138.11
134.05
129.24
126.29
123.33
119.88
118.22
110.32
109.43
77.34
77.02
76.70
30.35
29.75
25.72
22.77
21.83
21.58
GS-02-072R/13C/CDCl3/09-06-2015
NO2
Me
N
Me
5p
f1 (ppm)

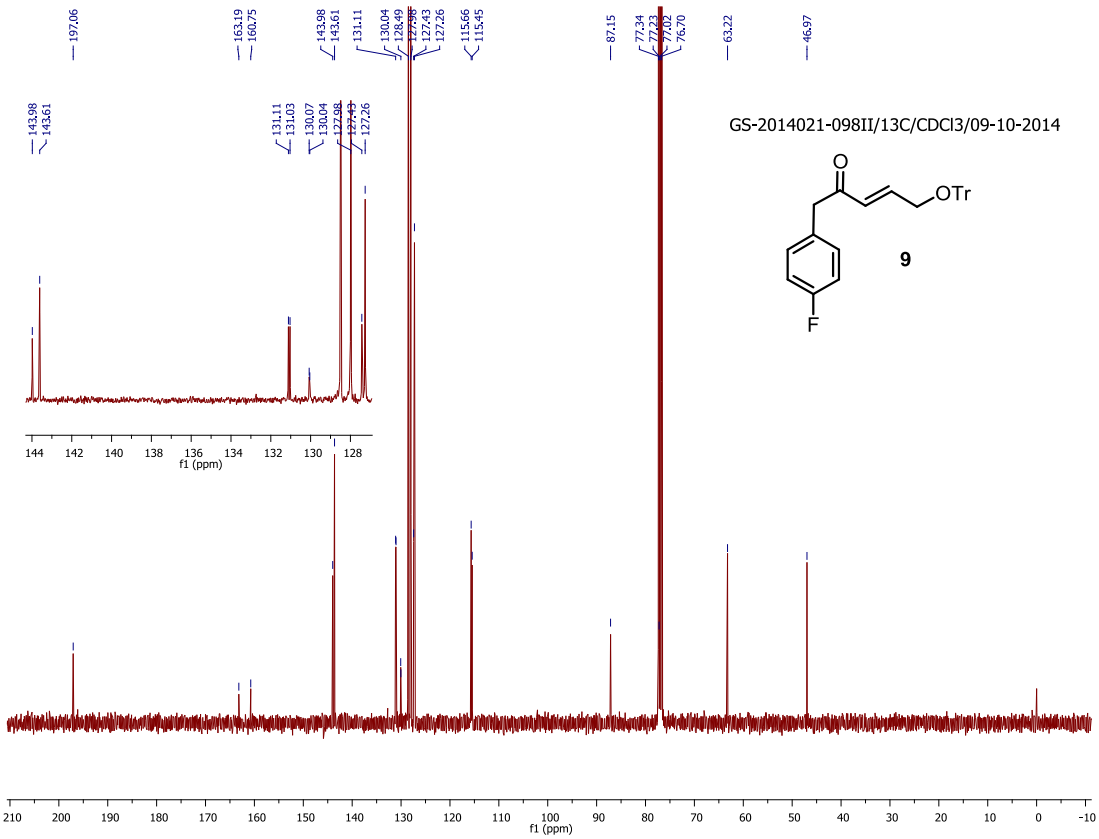

GS-02-072R/135DEPT/CDCl3/09-06-2015
NO2
Me
N
Me
5p
f1 (ppm)

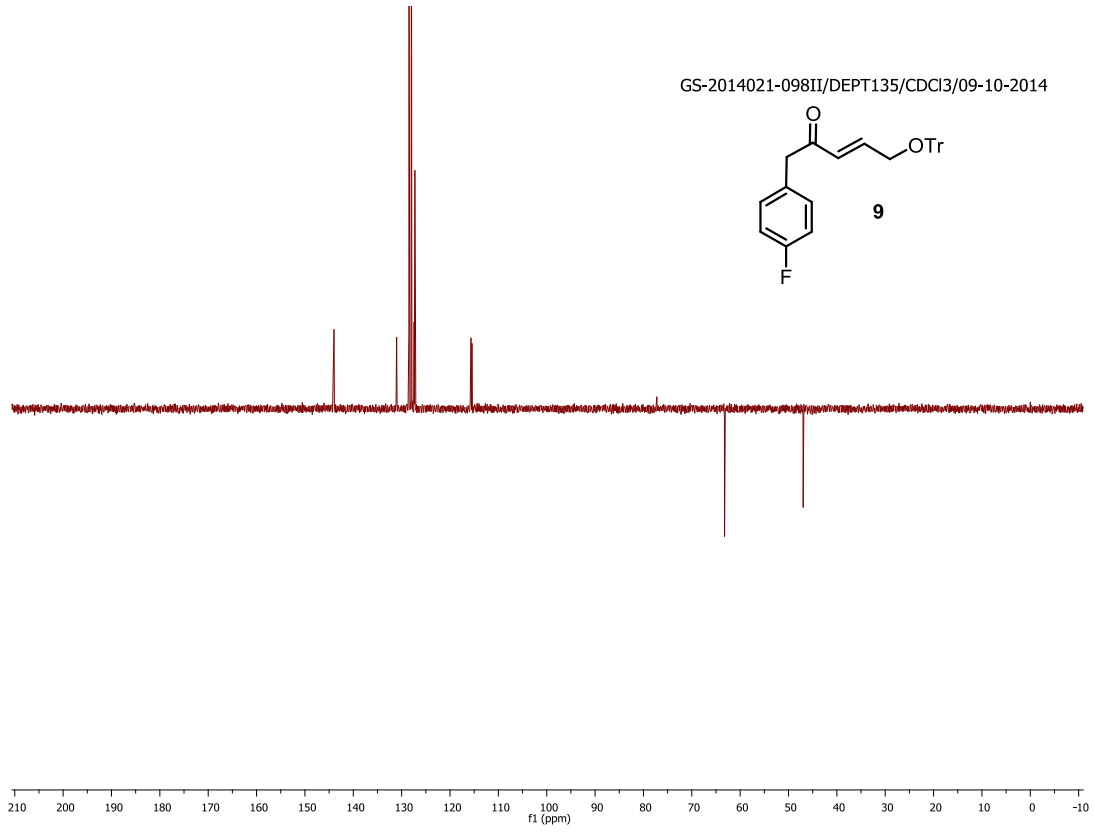

GS-2014021-096Re/1H/CDCl3/24-10-2014
OTES
OTr
14
6.06
9.28
2.02
2.04
1.01
1.00
10.16
6.39
f1 (ppm)

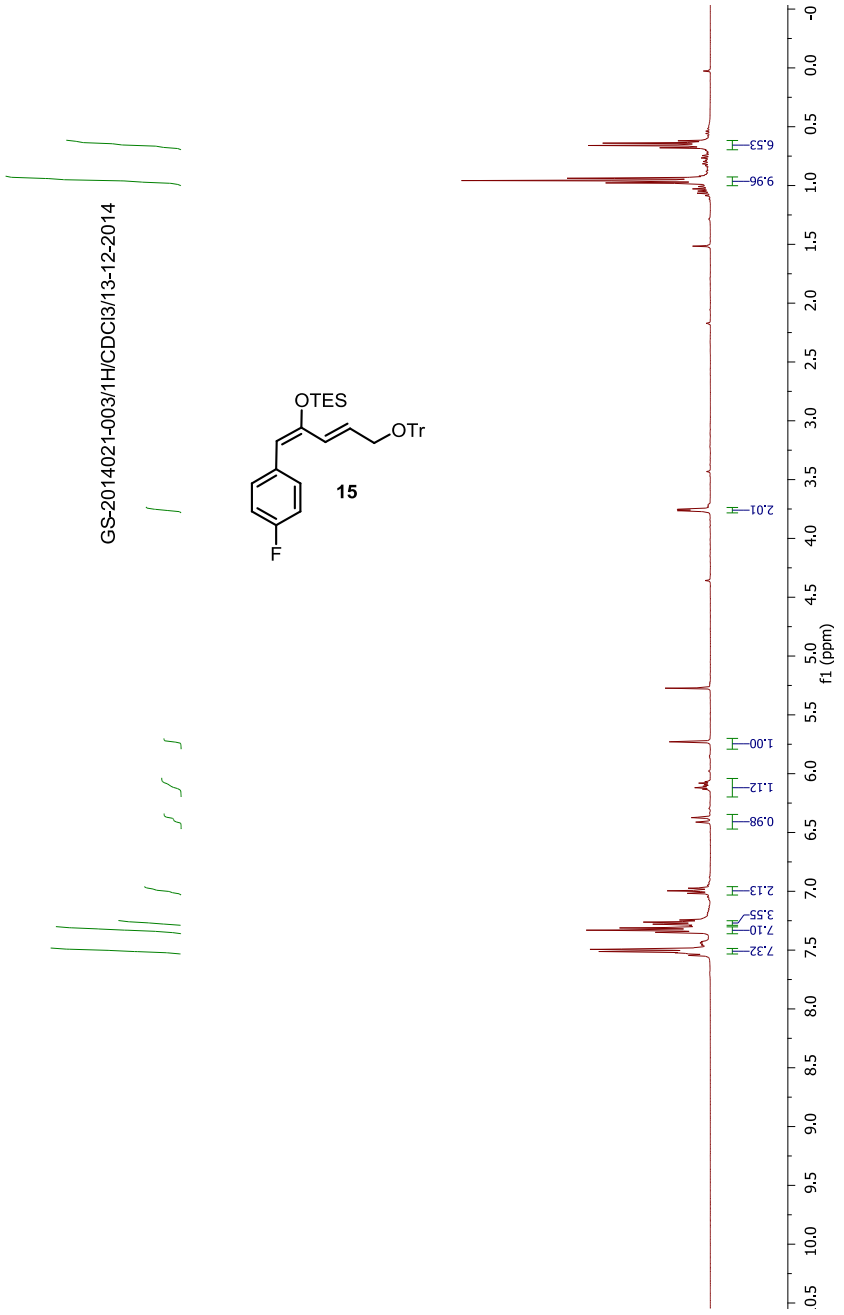

154.92
144.33
128.75
128.13
127.94
127.57
127.11
95.22
87.02
77.51
77.19
76.87
64.18
6.90
5.12
GS-2014021-096Repeat/13C/CDCl3/17-10-2014
OTES
OTr
14
f1 (ppm)

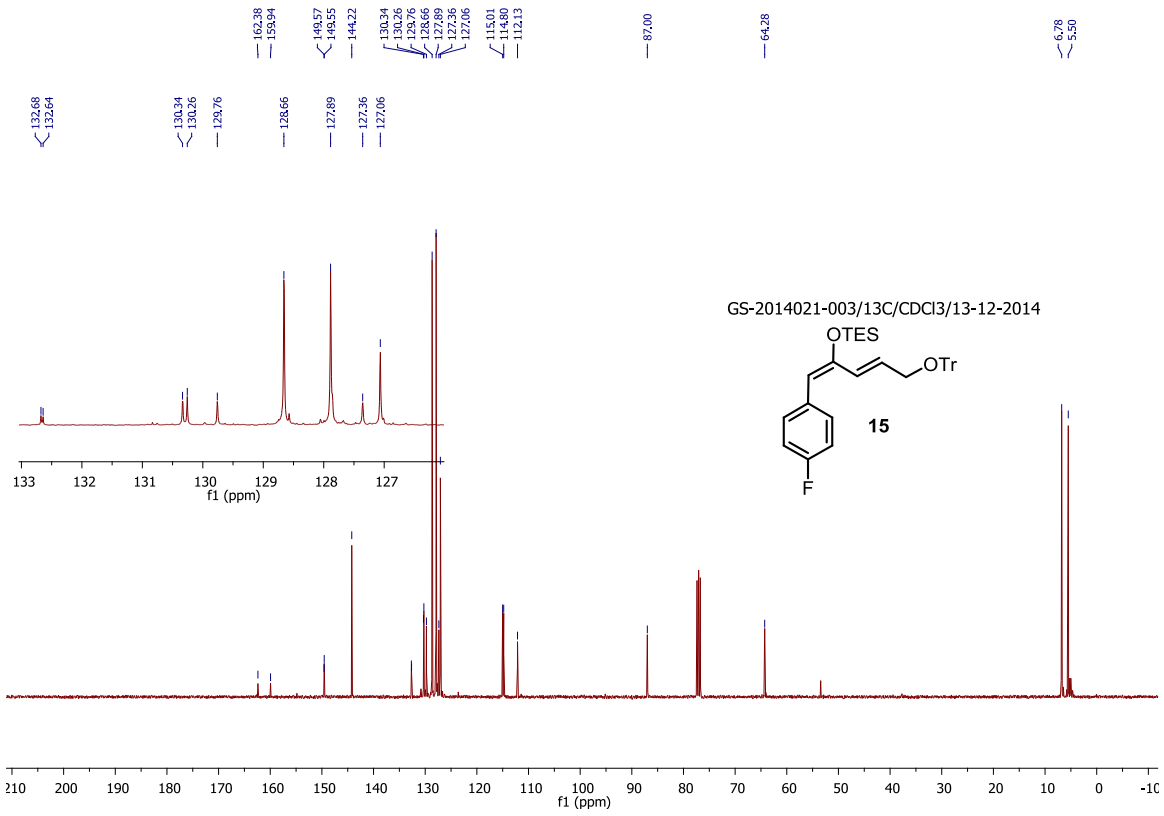

GS-2014021-096R/DEPT135/CDCl3/17-10-2014
OTES
OTr
14
f1 (ppm)

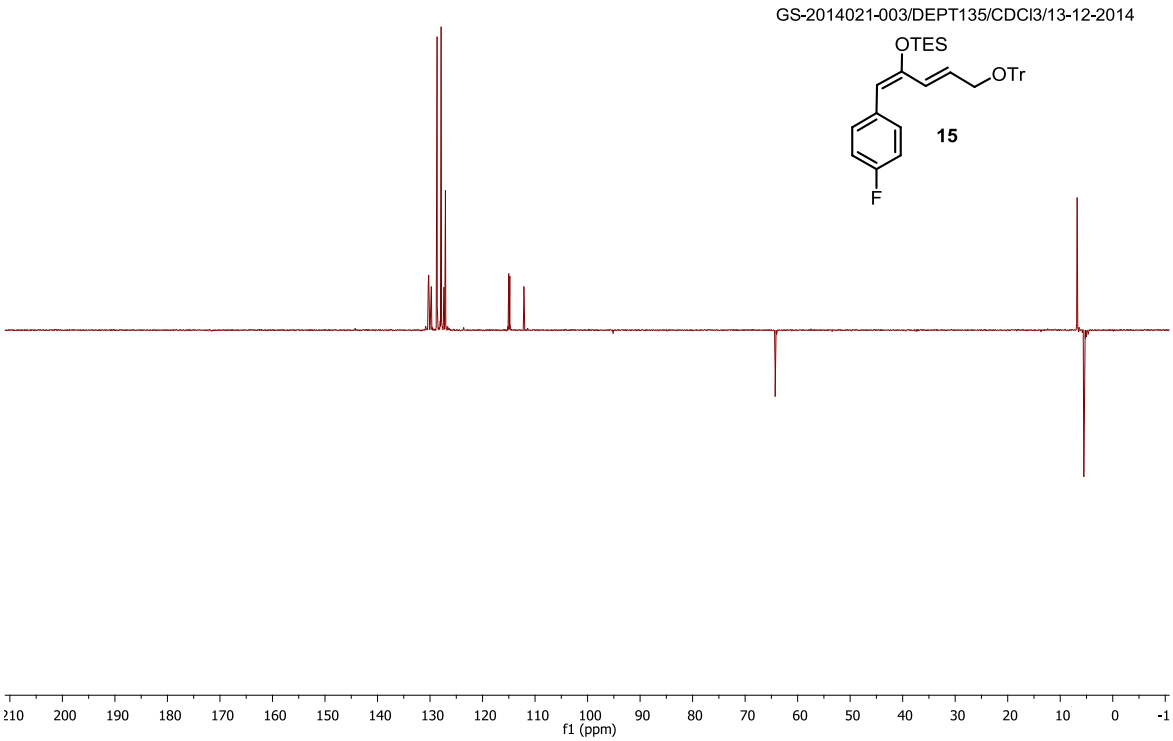

GS-20140210-098II/1H/CDCl3/09-10-2014
O
OTr
F
9
1.99
1.99
0.97
1.00
2.01
2.03
10.95
6.39
f1 (ppm)

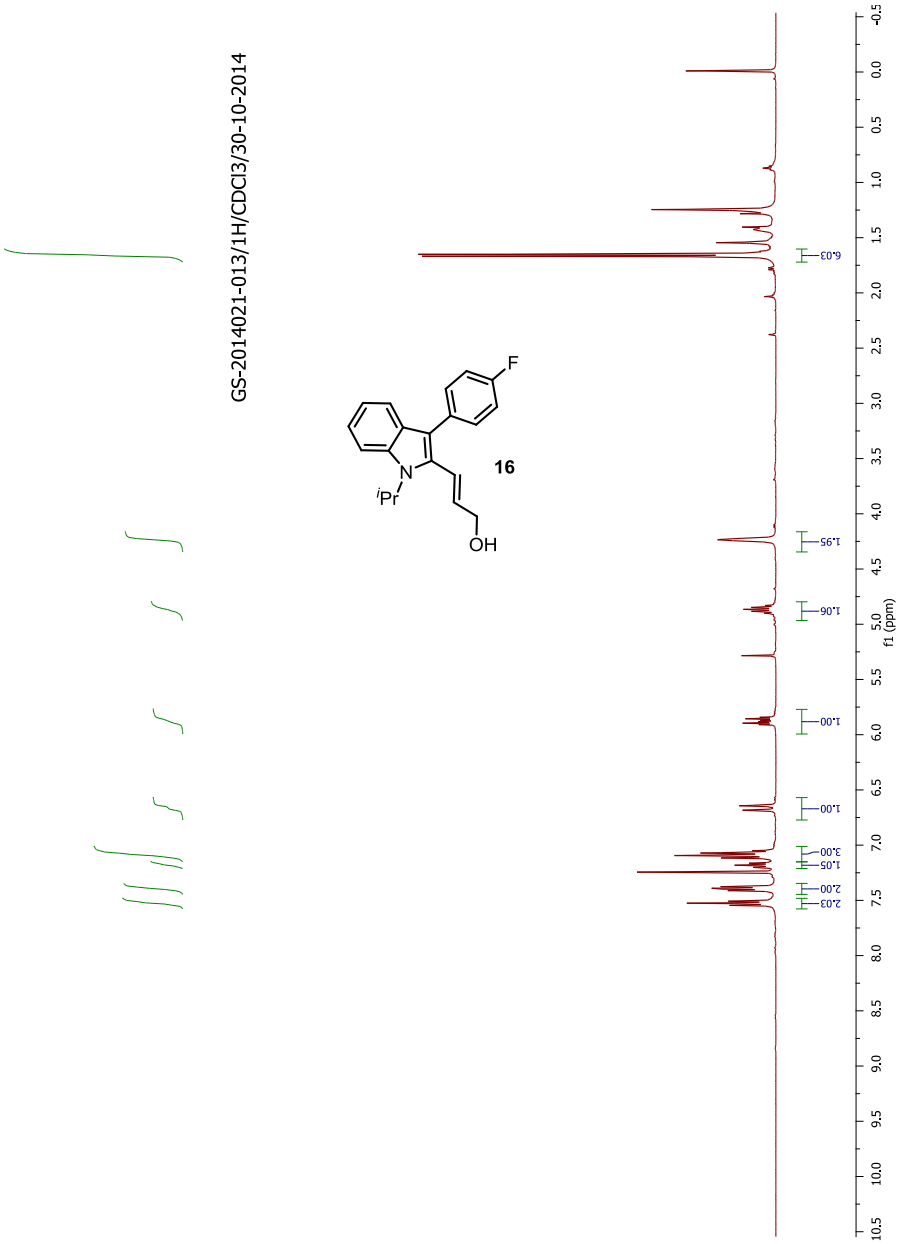

197.06
163.19
160.75
143.98
143.61
131.11
130.04
128.49
127.98
127.43
127.26
115.66
115.45
87.15
77.34
77.23
77.02
76.70
63.22
46.97
GS-2014021-098II/13C/CDCl3/09-10-2014
O
OTr
9
F
f1 (ppm)

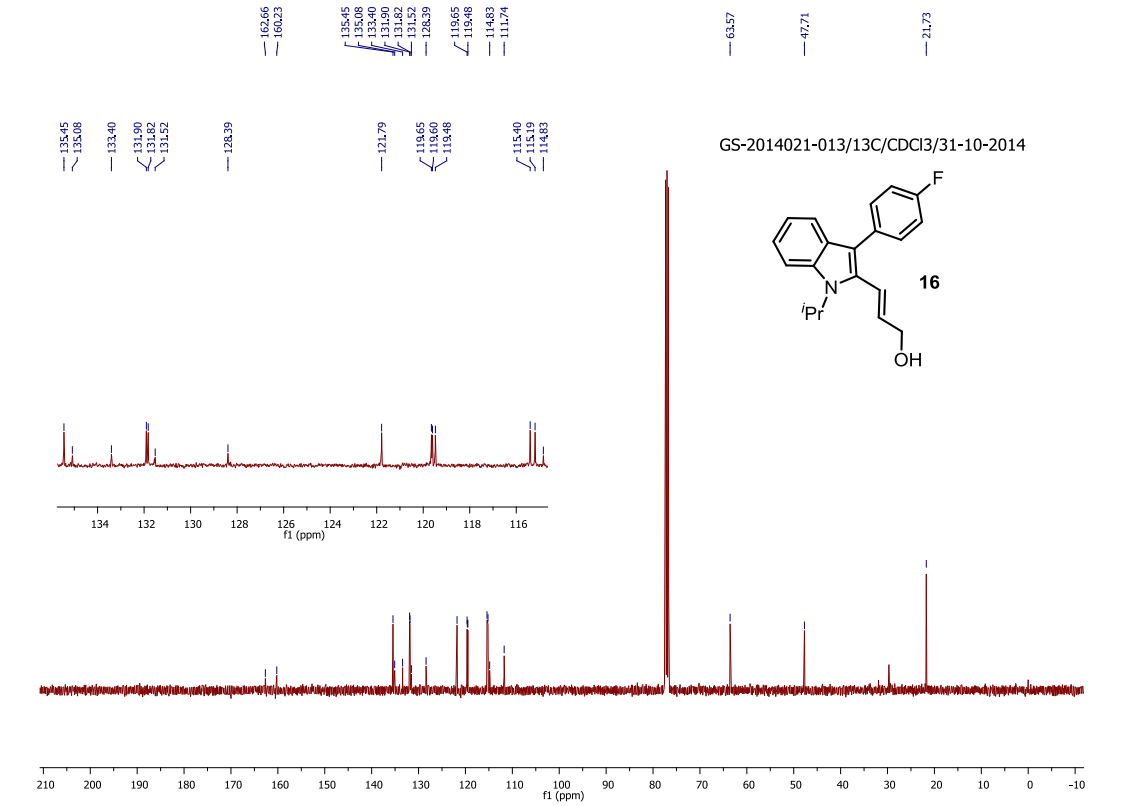

GS-2014021-098II/DEPT135/CDCl3/09-10-2014
O
OTr
9
F
f1 (ppm)

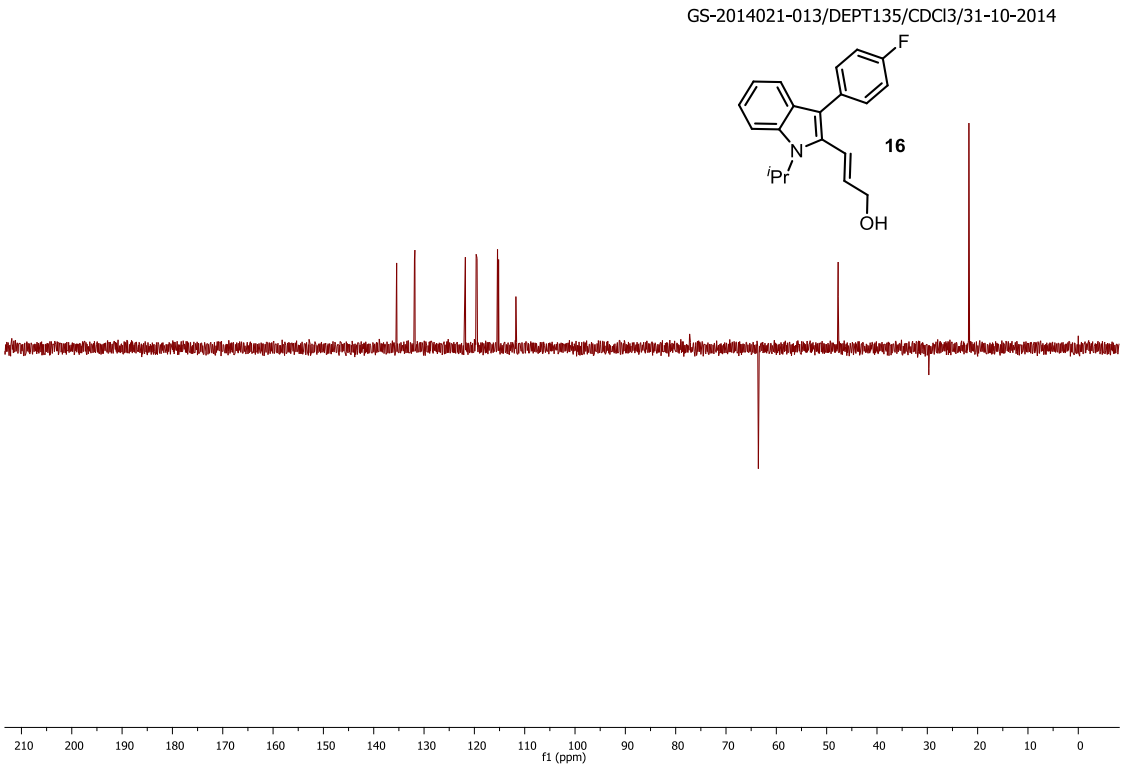

GS-2014021-003/1H/CDCl3/13-12-2014
OTES
OTr
15
F
6.53
9.96
2.01
1.00
1.12
0.98
2.13
3.55
7.10
7.32
f1 (ppm)

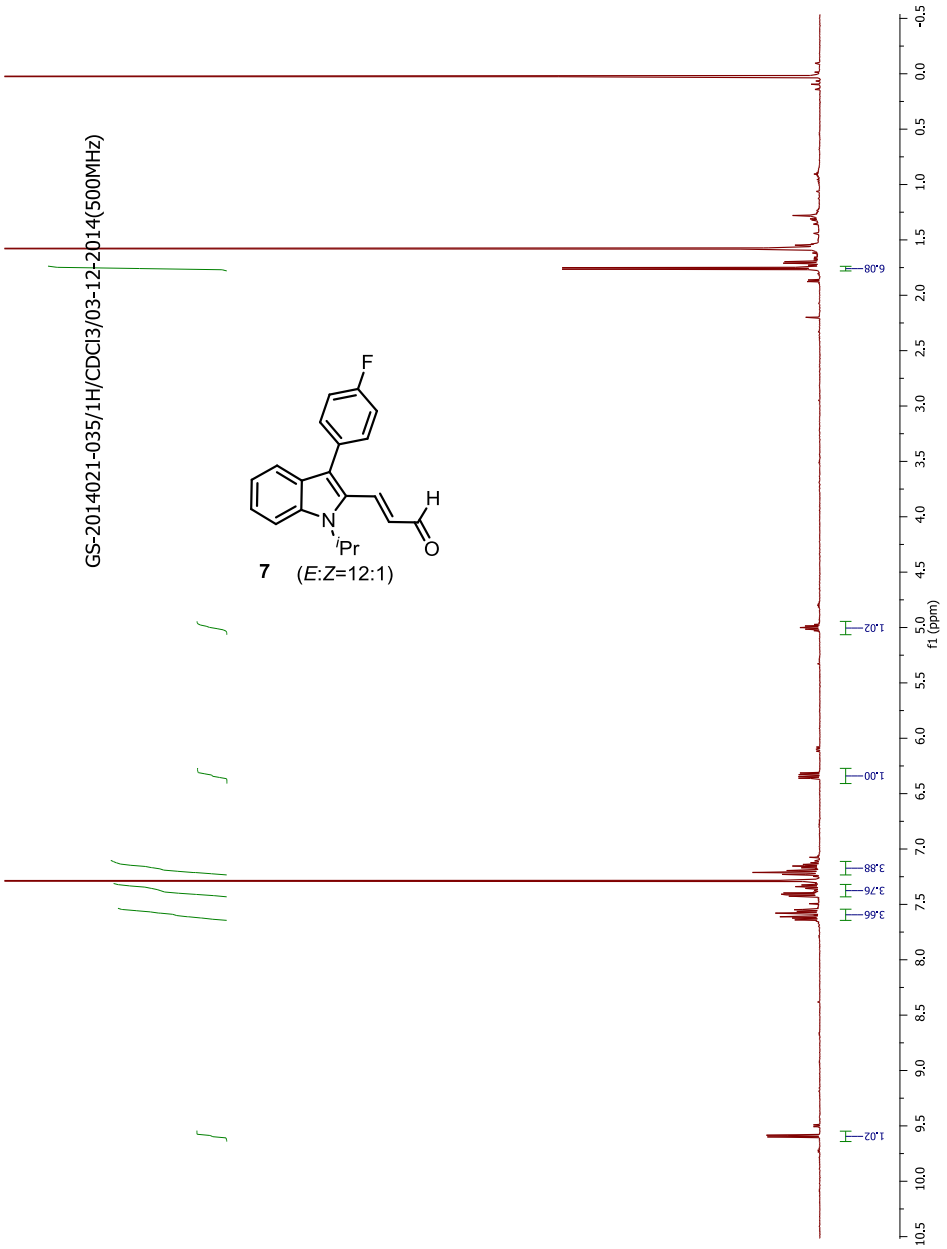

GS-2014021-003/13C/CDCl3/13-12-2014
OTES
OTr
15
F
f1 (ppm)

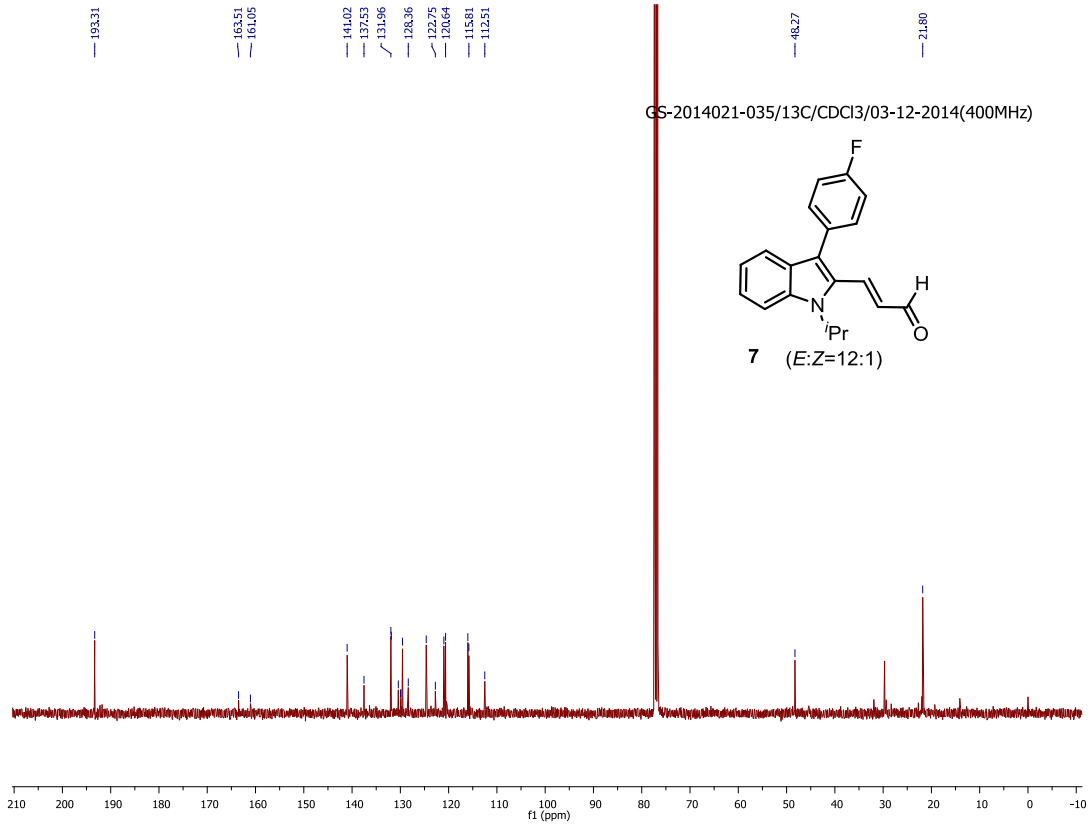

GS-2014021-003/DEPT135/CDCl3/13-12-2014
OTES
OTr
15
F
f1 (ppm)

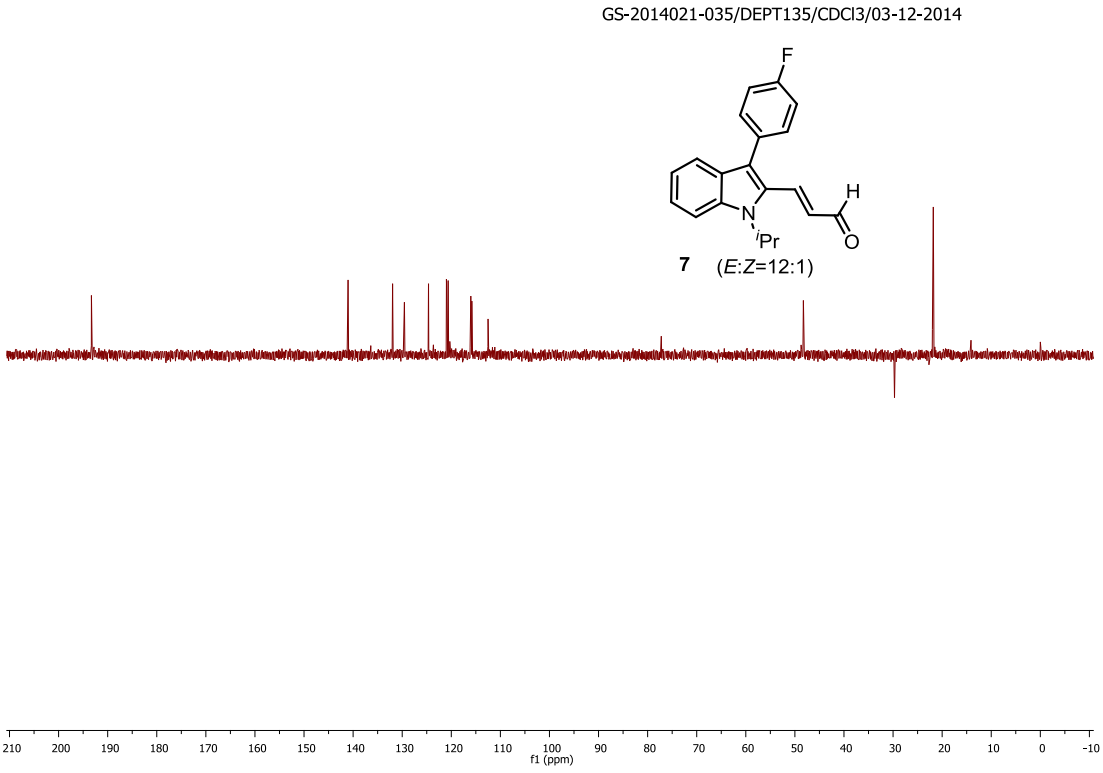

GS-2014021-013/1H/CDCl3/30-10-2014
F
N
iPr
OH
16
6.03
1.95
1.06
1.00
1.00
3.00
1.05
2.00
2.03
f1 (ppm)


GS-2014021-013/13C/CDCl3/31-10-2014
16
f1 (ppm)


GS-2014021-013/DEPT135/CDCl3/31-10-2014
16
f1 (ppm)


GS-2014021-035/1H/CDCl3/03-12-2014(500MHz)
F
H
O
N
iPr
7 (E:Z=12:1)
6.08
1.02
1.00
3.88
3.76
3.66
1.02
f1 (ppm)


193.31
163.51
161.05
141.02
137.53
131.96
128.36
122.75
120.64
115.81
112.51
48.27
21.80
GS-2014021-035/13C/CDCl3/03-12-2014(400MHz)
F
H
N
iPr
O
7 (E:Z=12:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


GS-2014021-035/DEPT135/CDCl3/03-12-2014
F
H
N
iPr
O
7 (E:Z=12:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)