Multidimensional Reaction Screening for Photochemical Transformations as a Tool for Discovering New Chemotypes

Supporting Information

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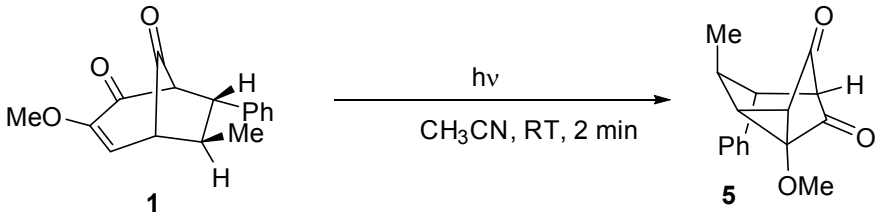
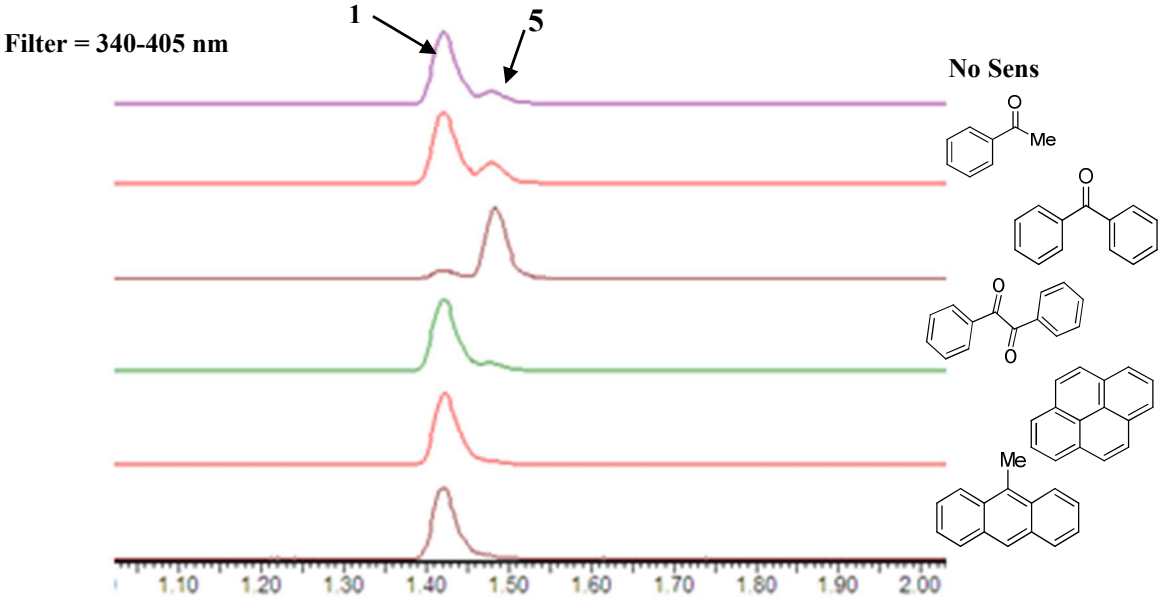
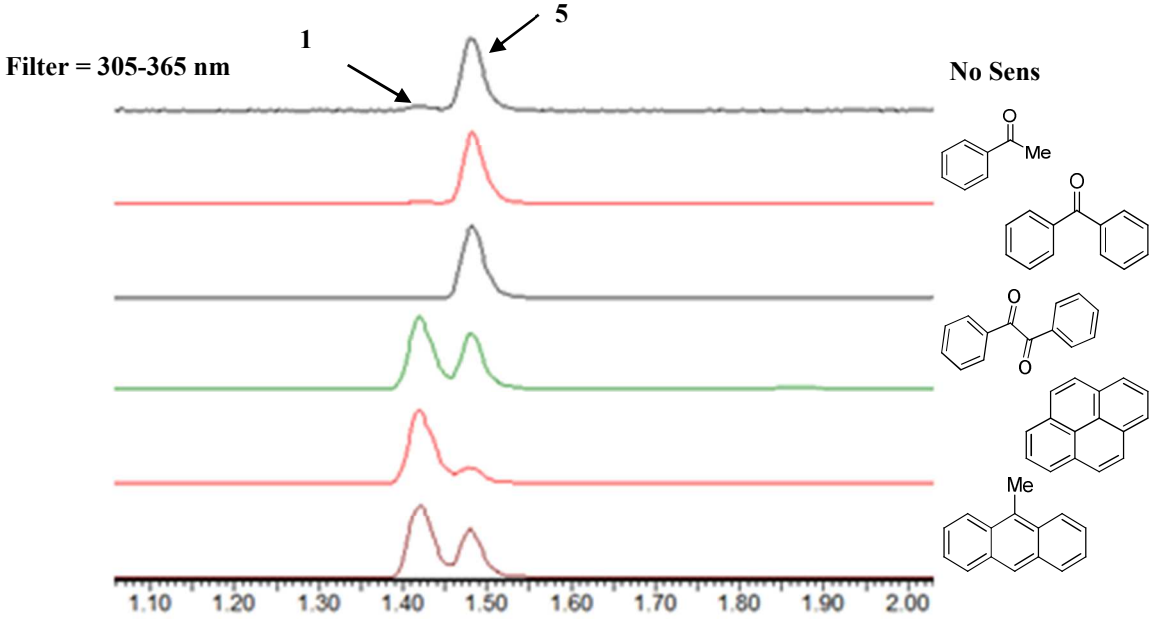
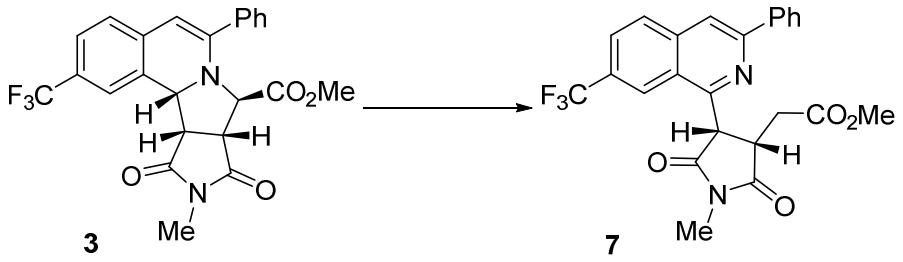
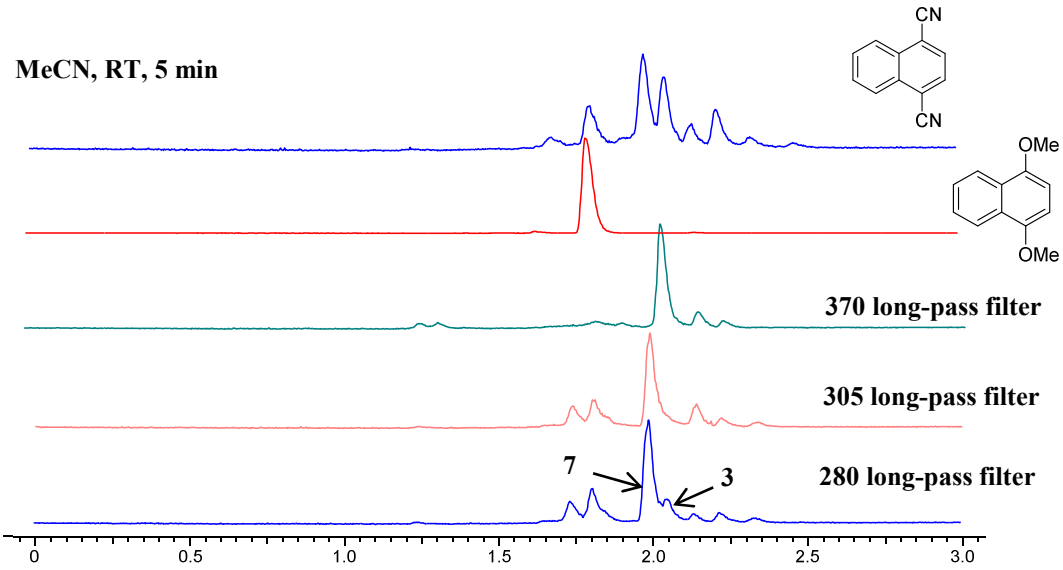
I. Analytical Reaction Screening and Selected Reaction Profiles

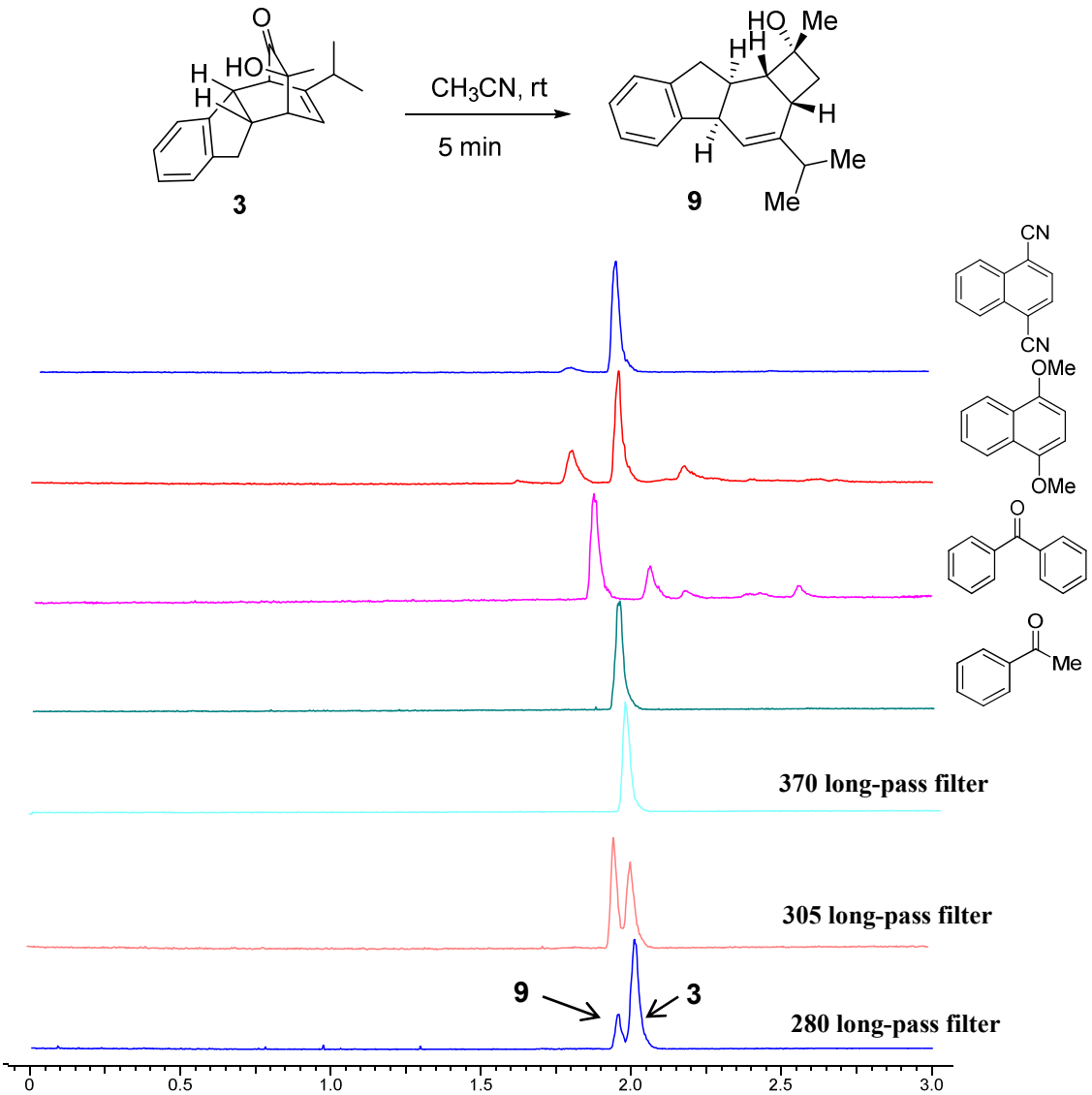


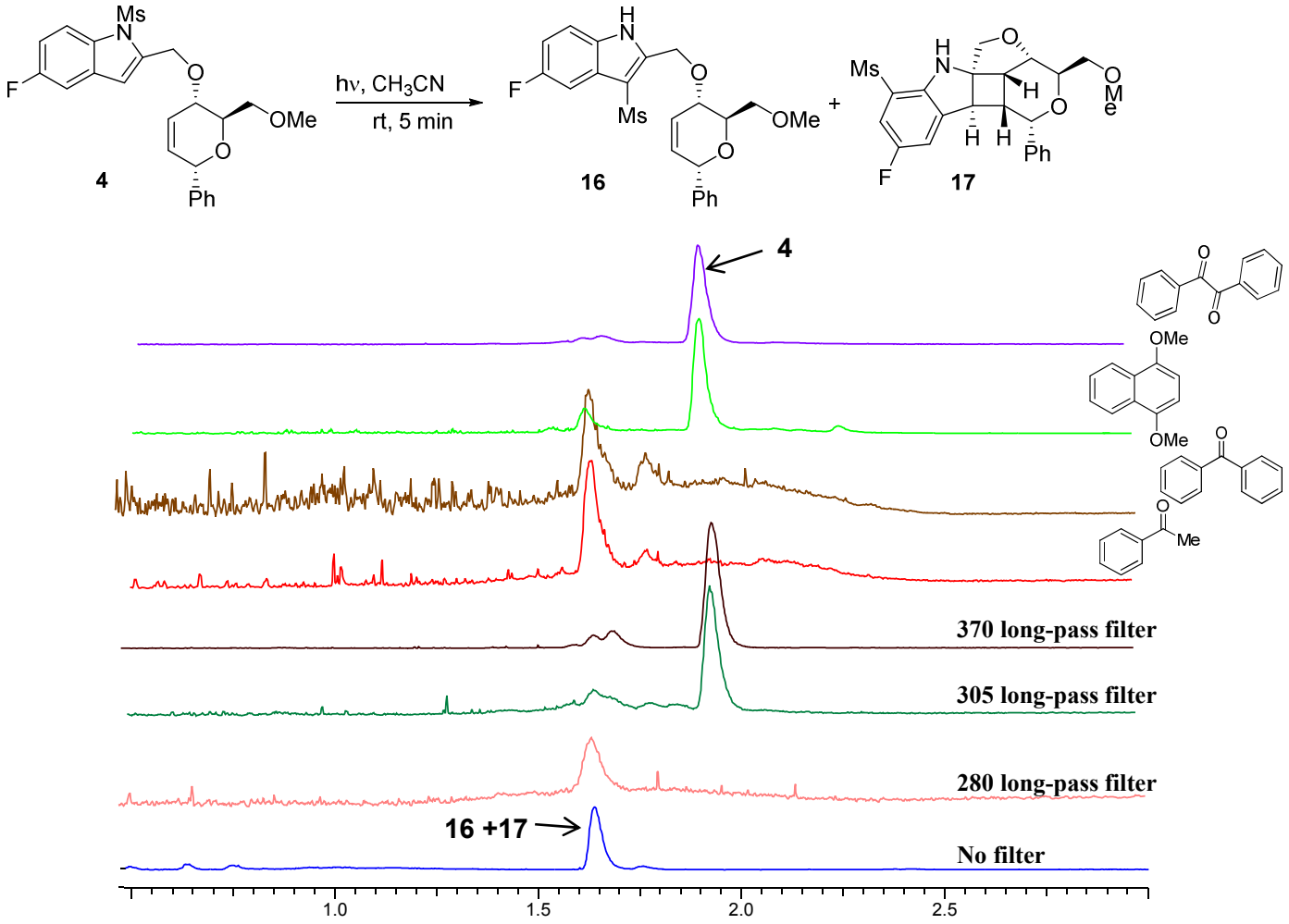


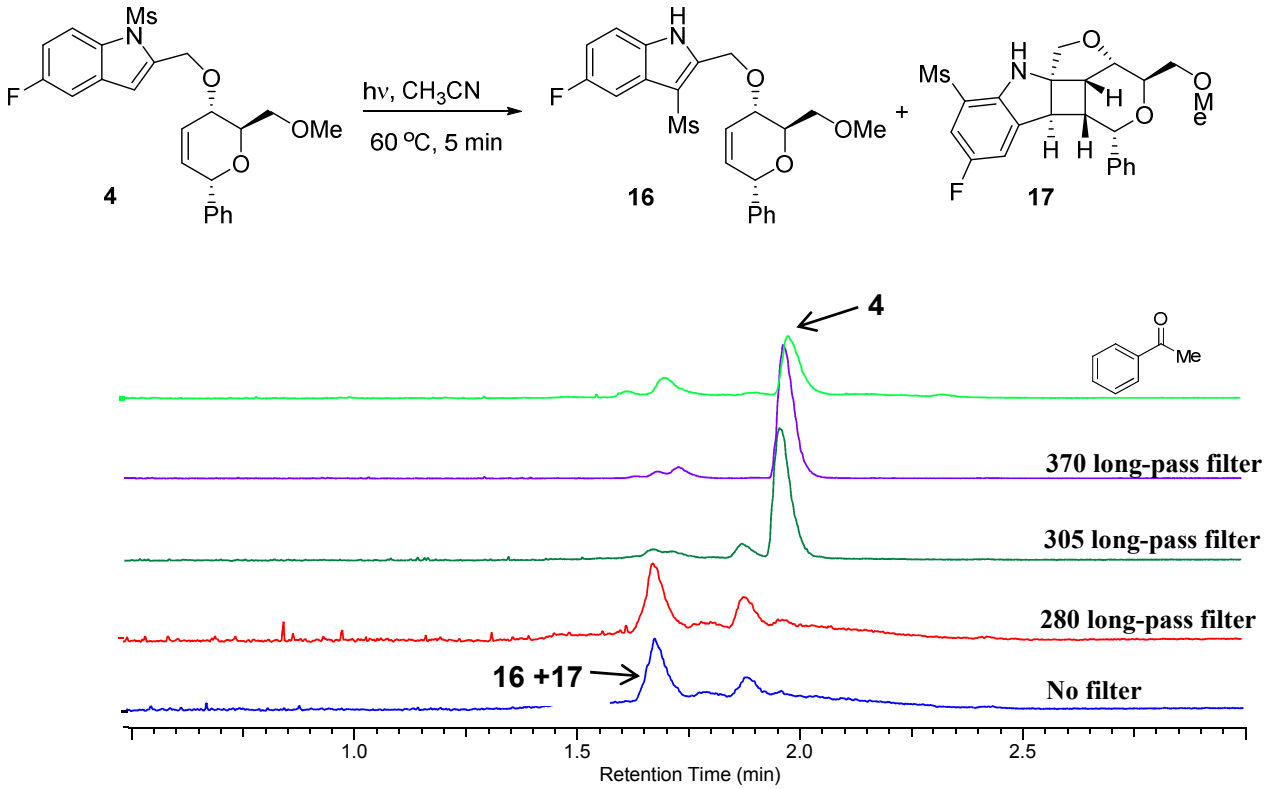


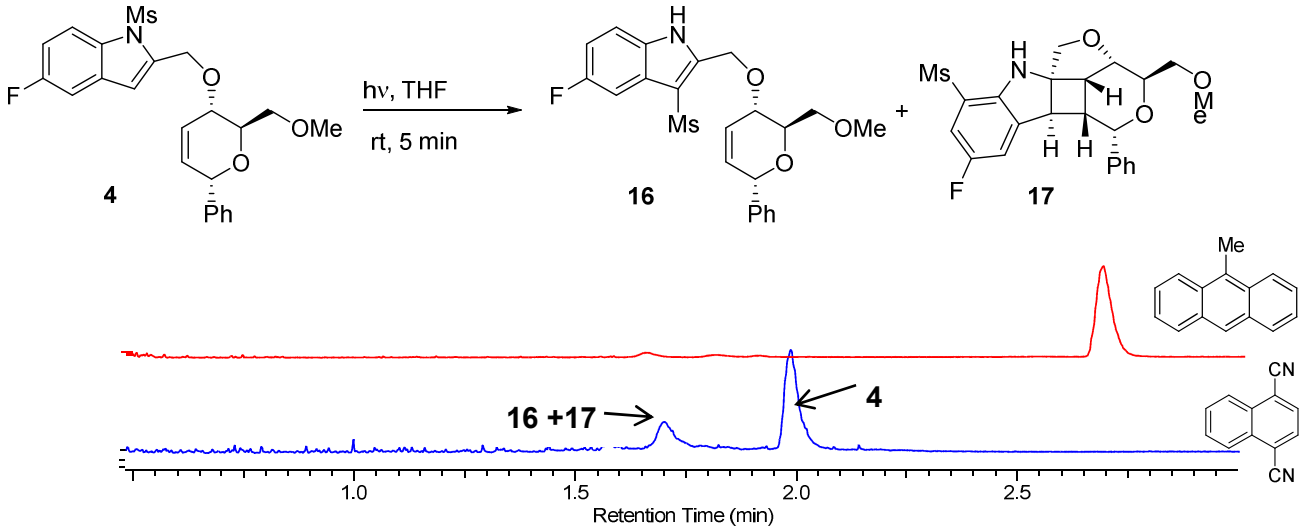

Ph
N
F_3C
CO_2Me
H
H
H
O
N
O
Me
3
Ph
N
F_3C
CO_2Me
H
H
O
N
O
Me
7


MeCN, RT, 5 min
CN
CN
OMe
OMe
370 long-pass filter
305 long-pass filter
280 long-pass filter
7
3
0
0.5
1.0
1.5
2.0
2.5
3.0

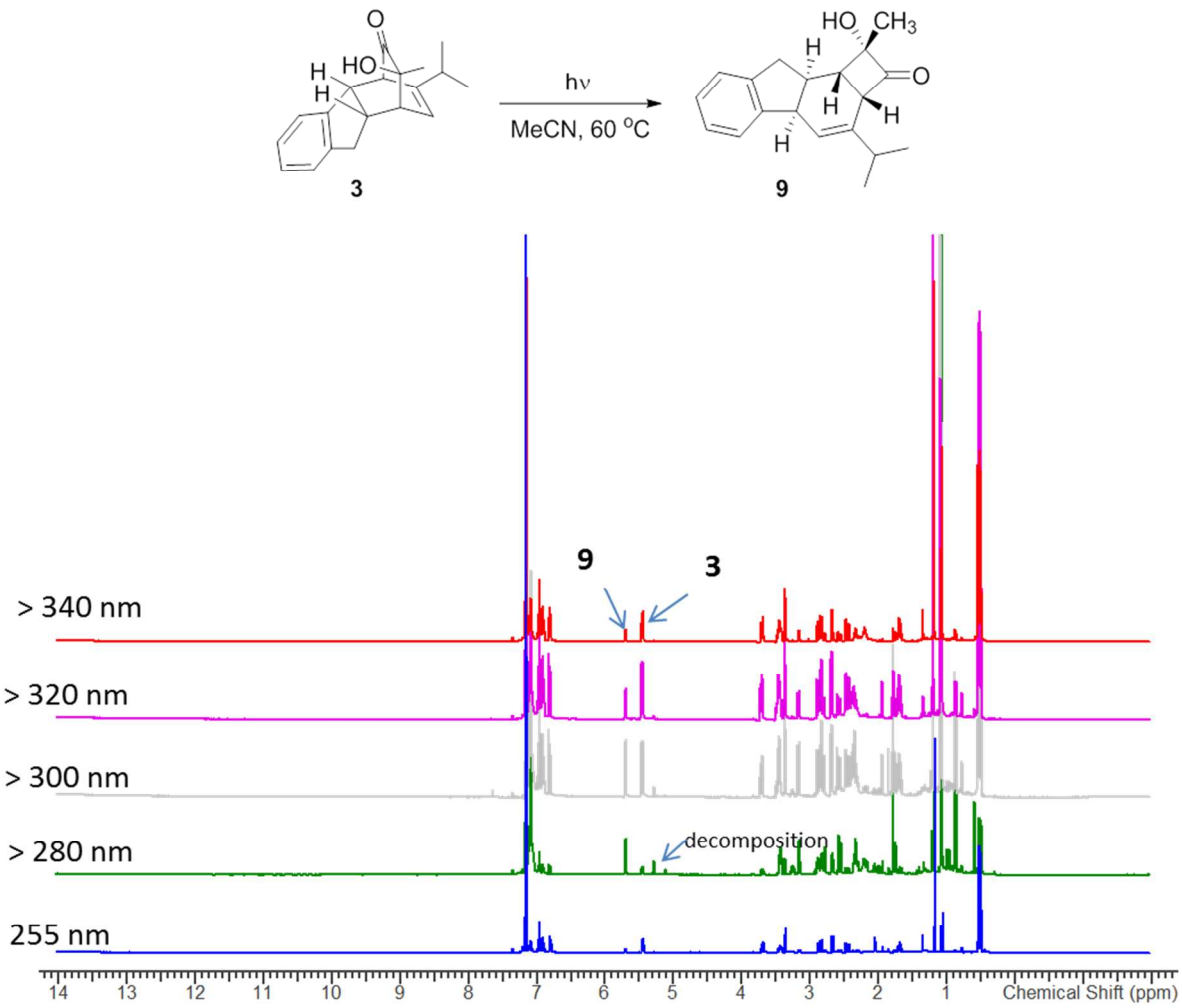

O
H
HO
H
3
CH3CN, rt
5 min
HO
Me
H
H
H
H
Me
Me
9
CN
CN
OMe
OMe
O
O
Me
370 long-pass filter
305 long-pass filter
280 long-pass filter
9
3
0
0.5
1.0
1.5
2.0
2.5
3.0


Ms
N
F
O
OMe
O
Ph
4
hν, CH3CN
rt, 5 min
H
N
F
Ms
O
OMe
O
Ph
16
+
Ms
H
N
O
H
O
O
Me
H
H
Ph
F
17
4
OMe
OMe
O
Me
370 long-pass filter
305 long-pass filter
280 long-pass filter
16 +17
No filter
1.0
1.5
2.0
2.5


hν, CH3CN
60 °C, 5 min
4
16
17
370 long-pass filter
305 long-pass filter
280 long-pass filter
No filter
16 +17
Retention Time (min)


hν, THF
rt, 5 min
4
16
17
16 +17
Retention Time (min)

IV. NMR profiles for the wavelength for wavelength optimization of cyclobutanone 9.



V. NMR Spectra

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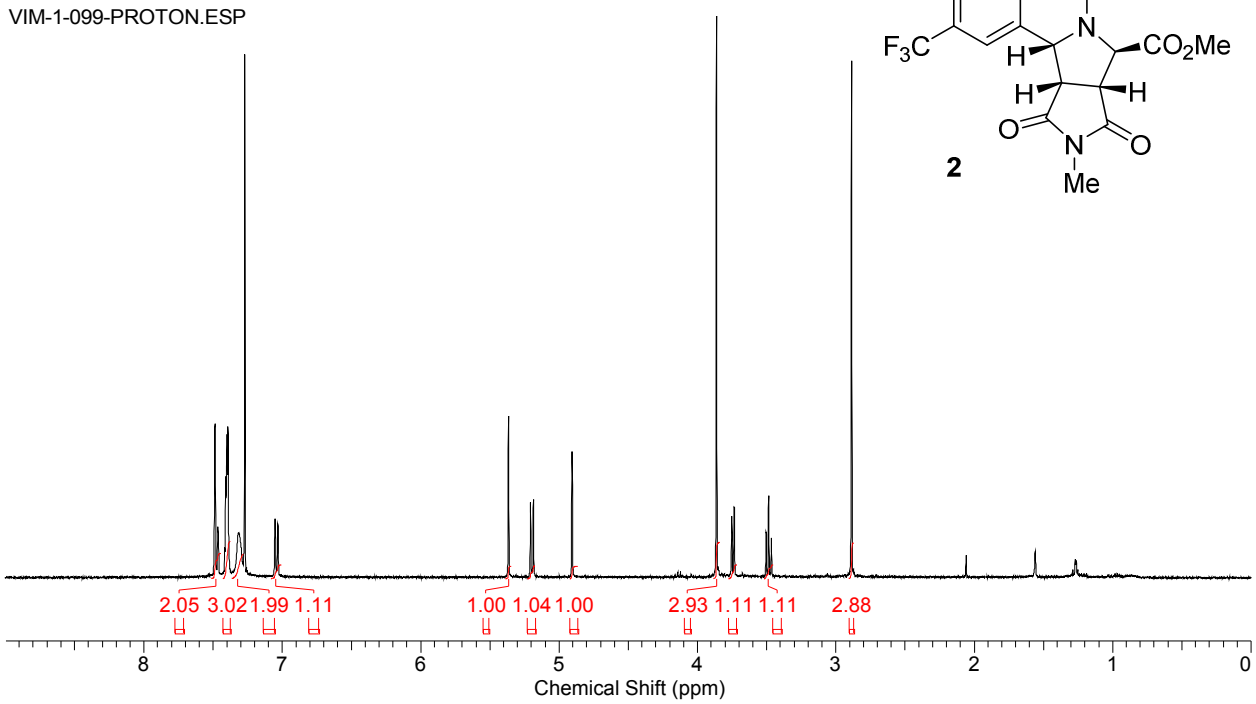
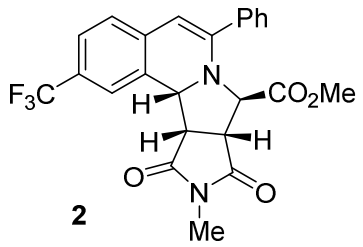
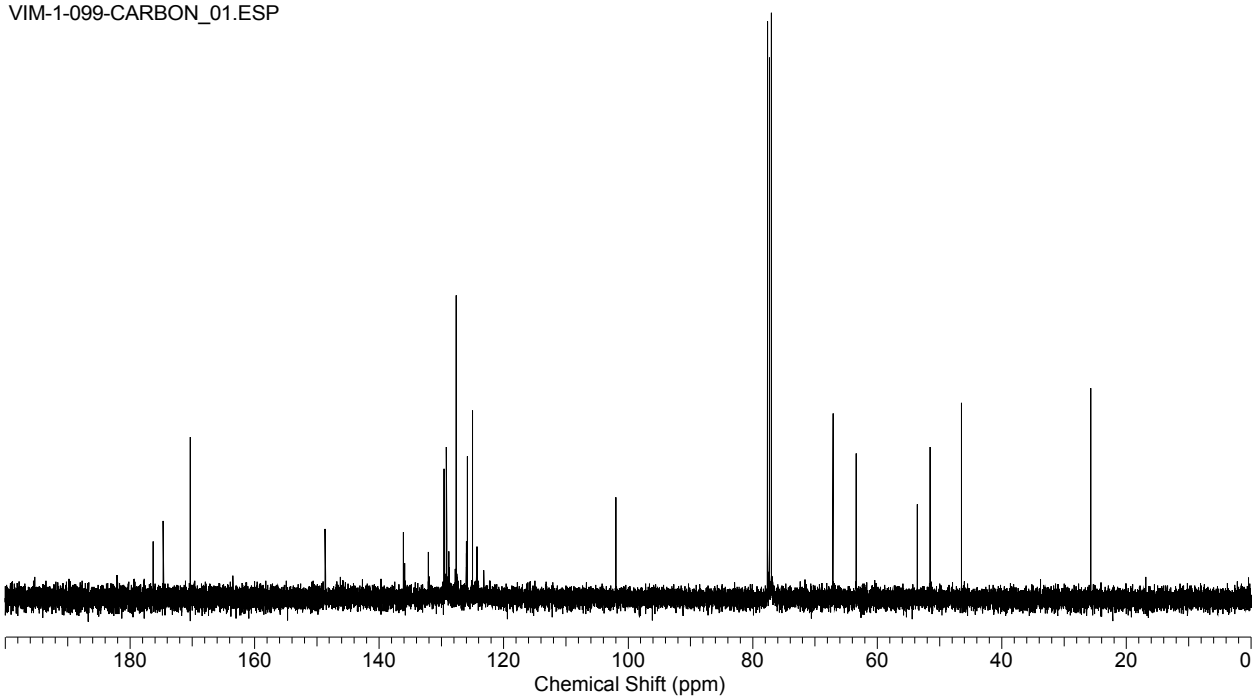
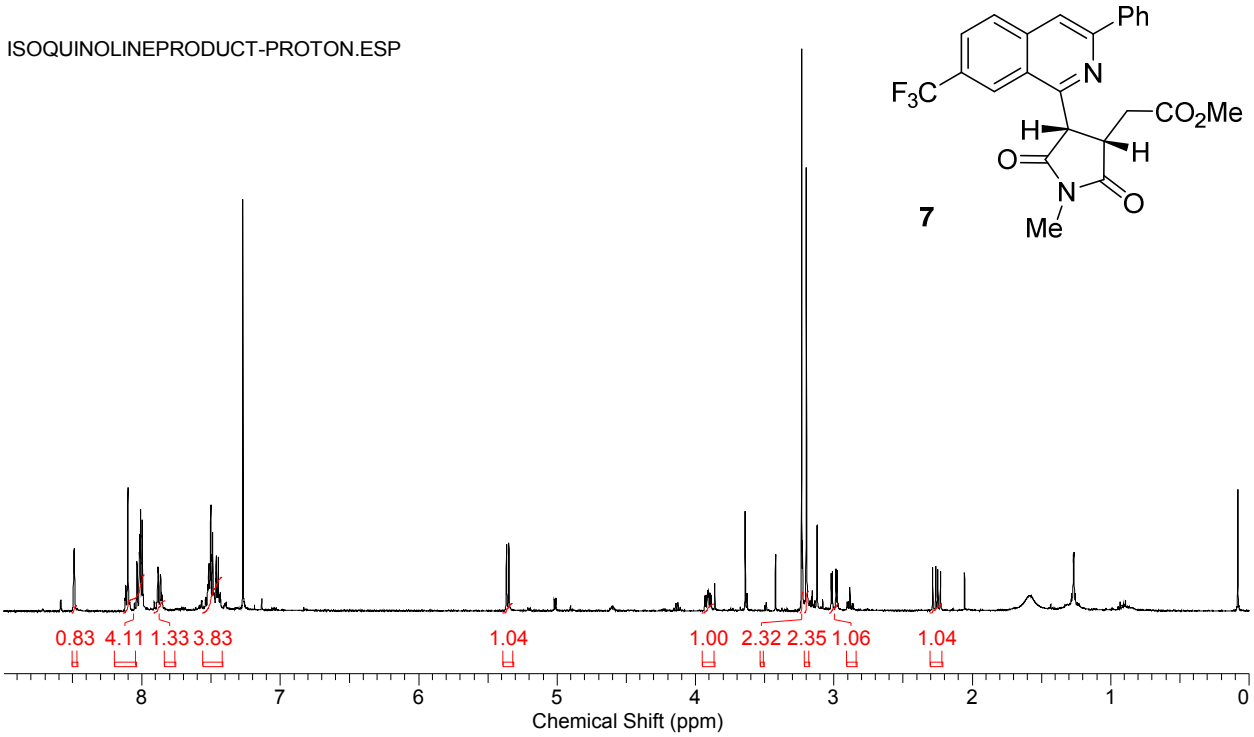




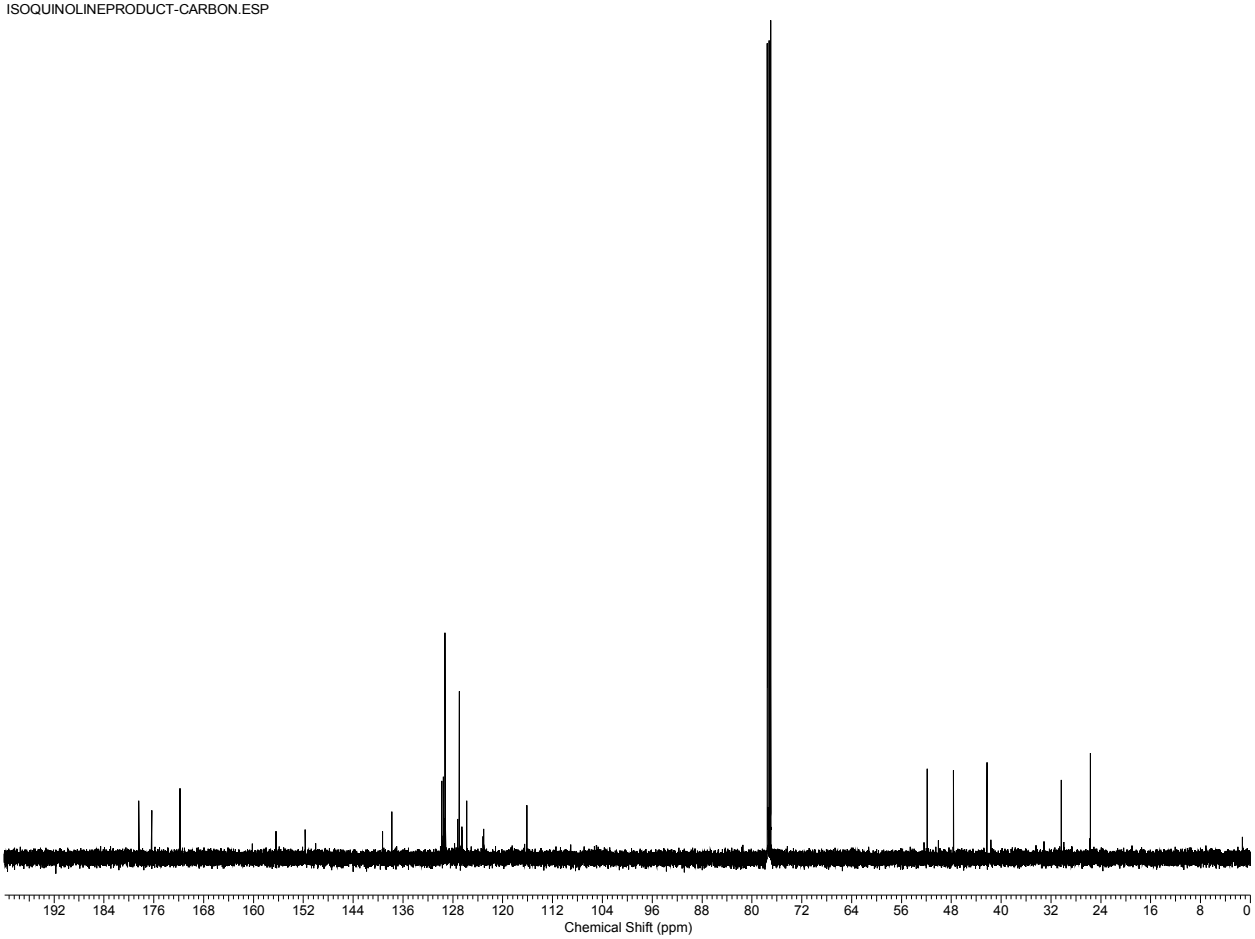
VIM-1-099-CARBON_01.ESP

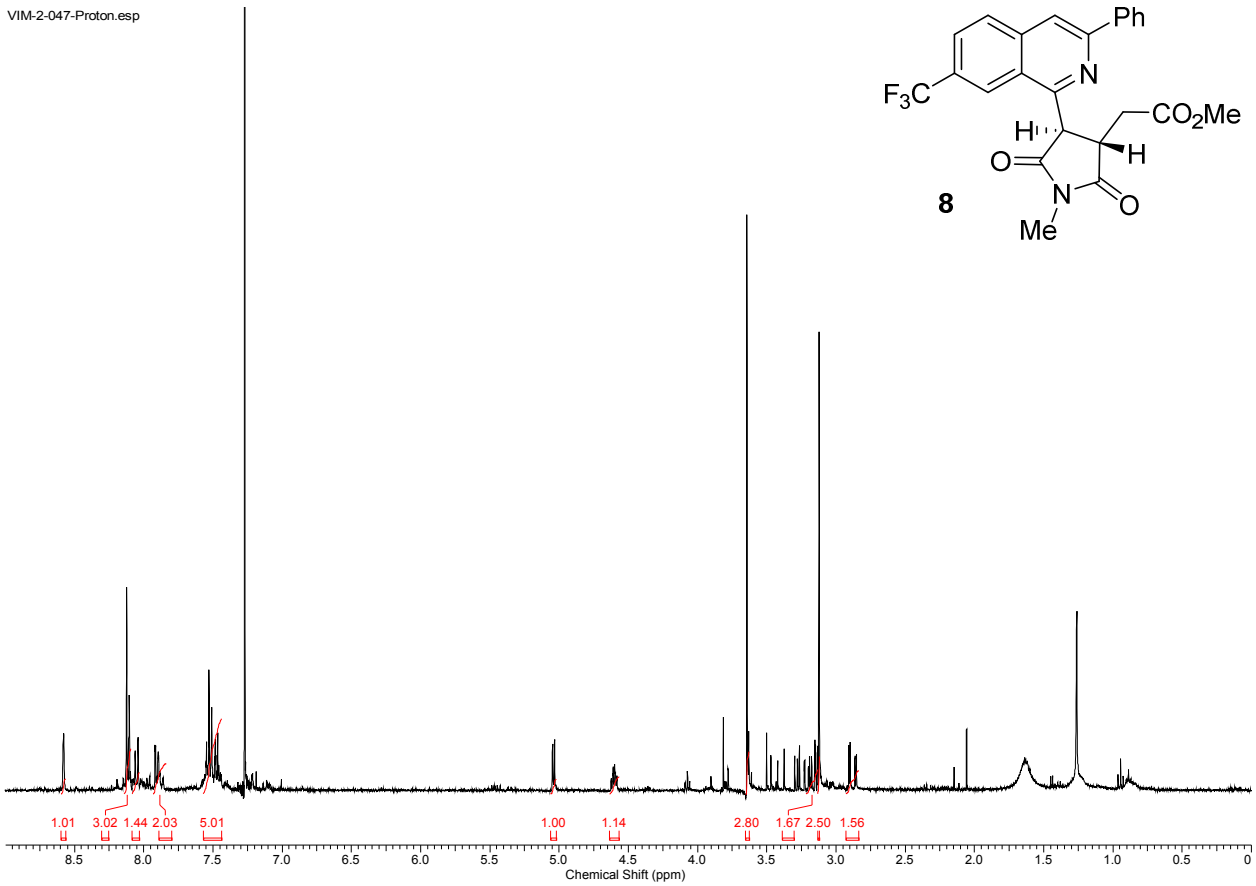


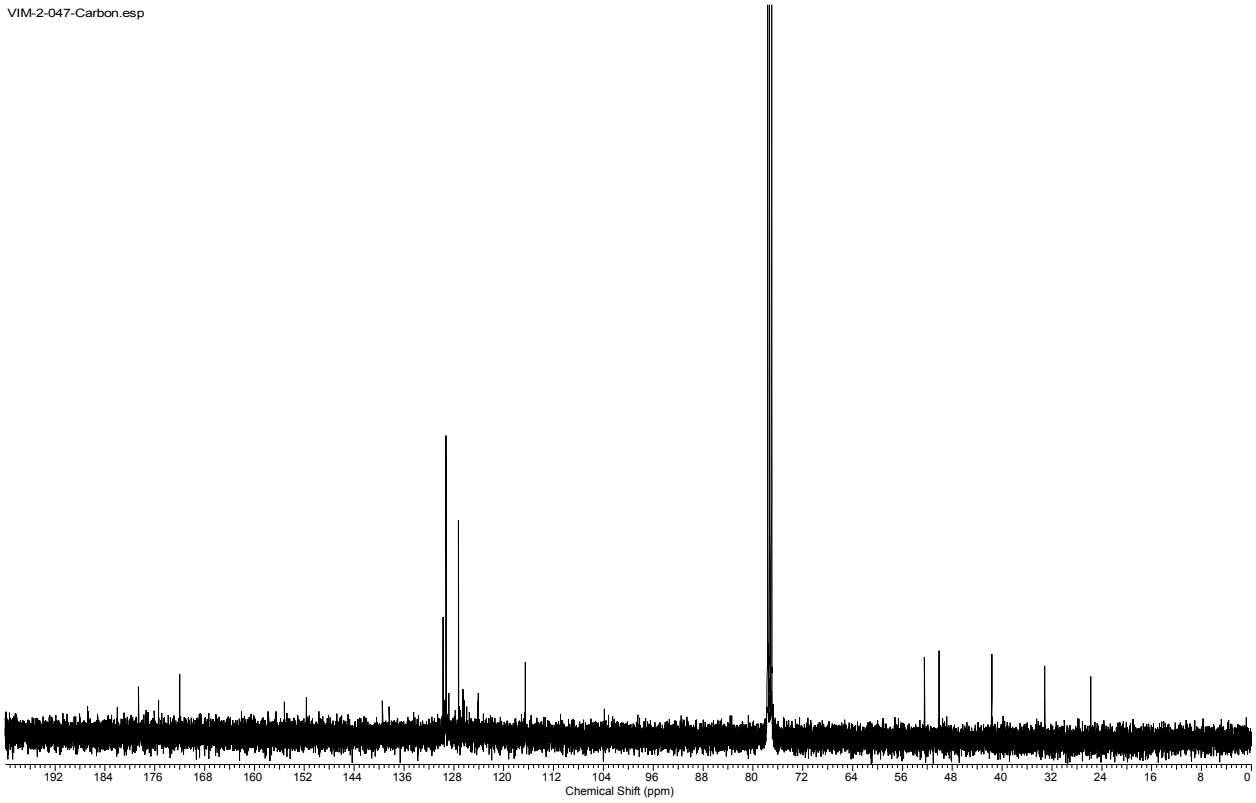
ISOQUINOLINEPRODUCT-PROTON.ESP

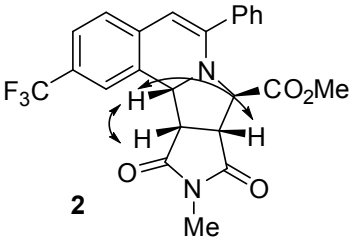


ISOQUINOLINEPRODUCT-CARBON.ESP

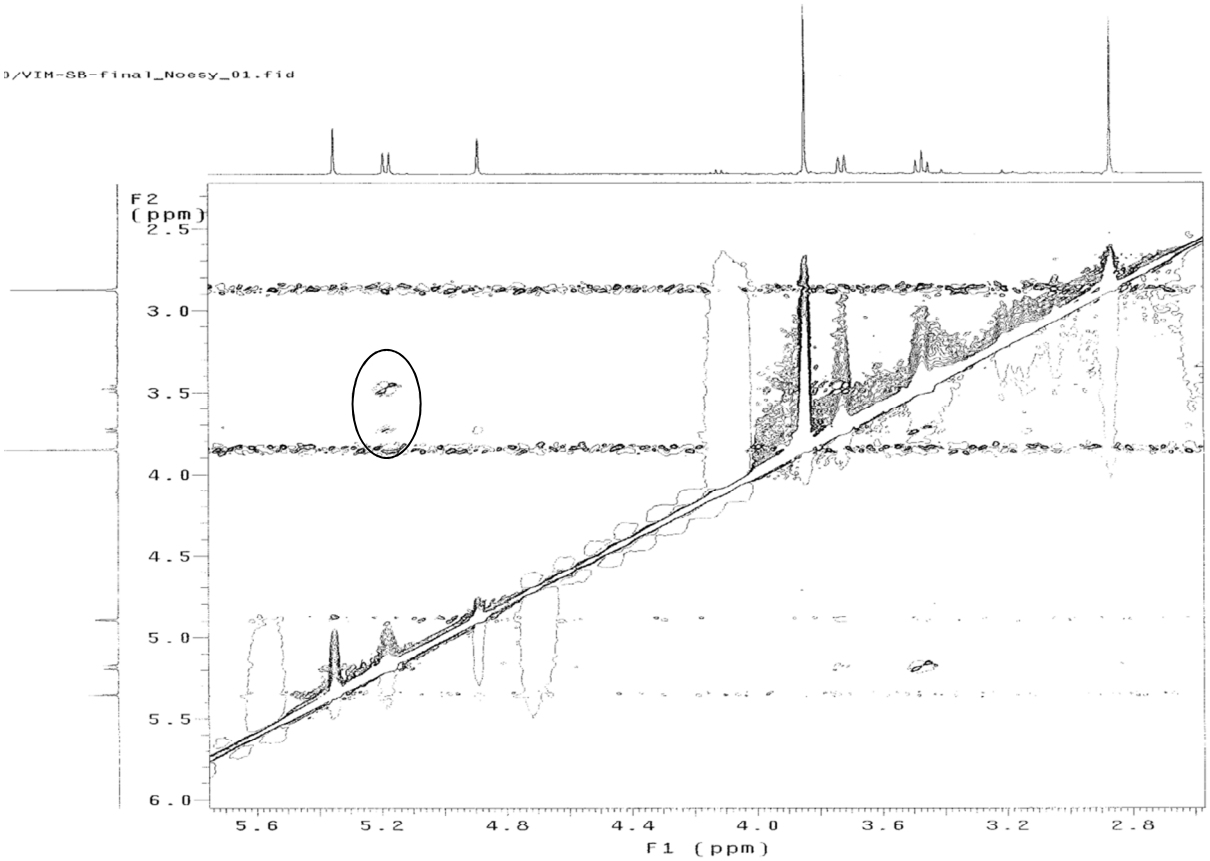


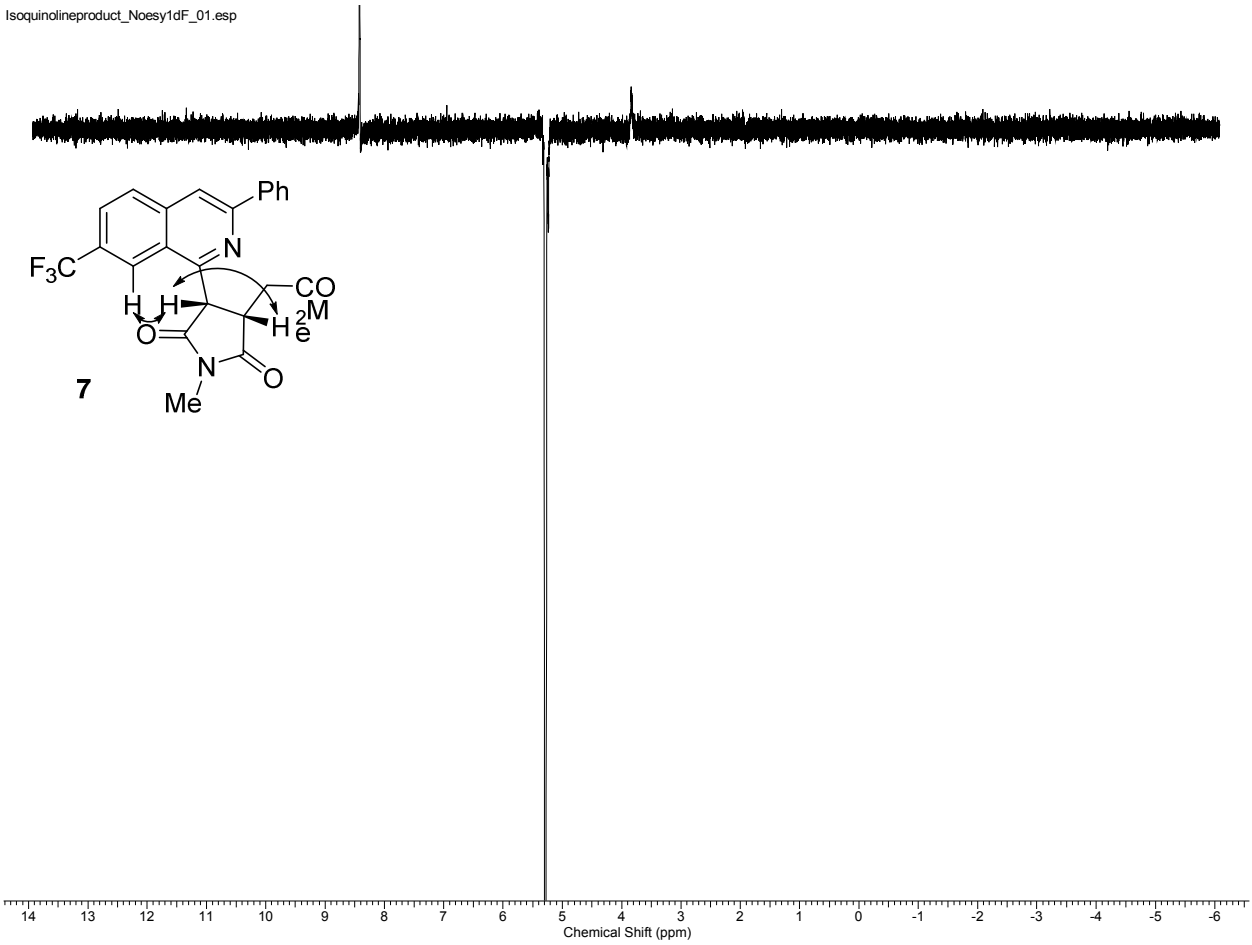

VIM-2-047-Proton.esp
Ph
N
F3C
CO2Me
H
H
O
N
O
Me
8
1.01
3.02
1.44
2.03
5.01
1.00
1.14
2.80
1.67
2.50
1.56
Chemical Shift (ppm)


VIM-2-047-Carbon.esp
Chemical Shift (ppm)

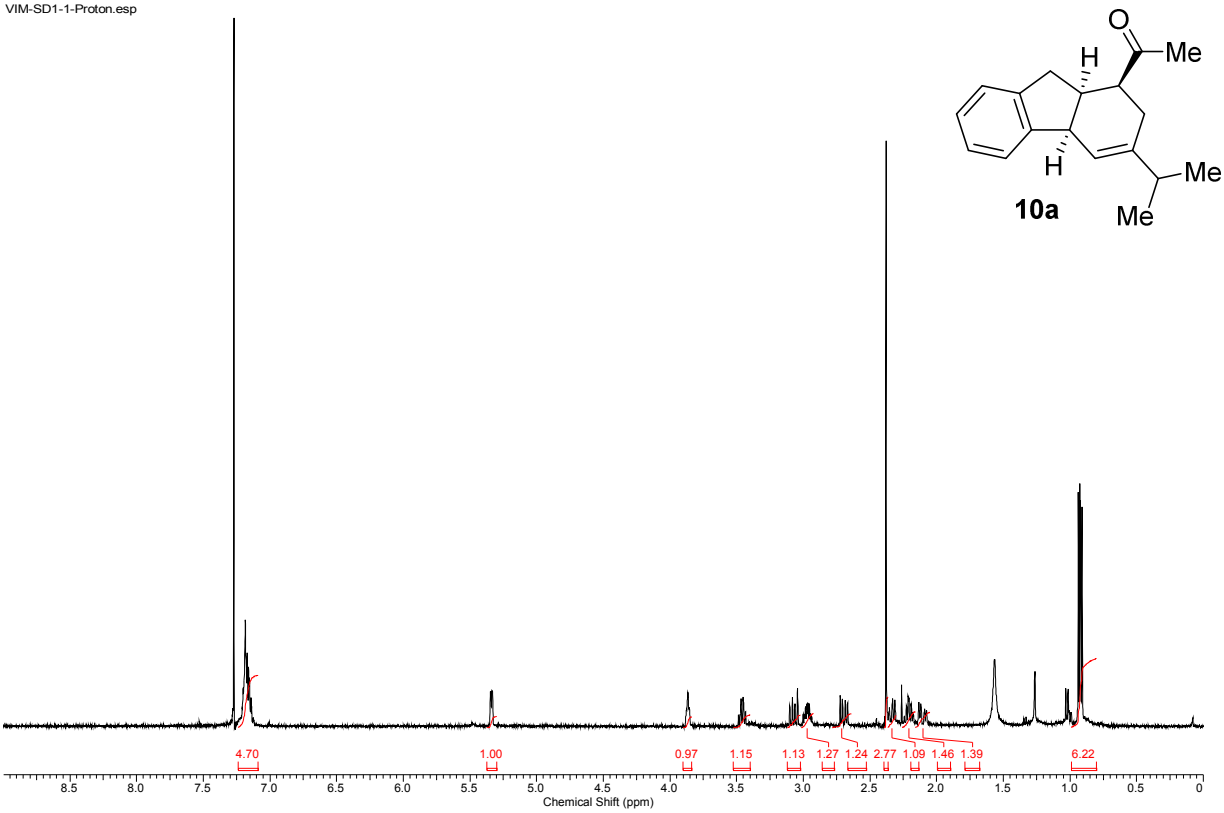

Ph
N
F_3C
CO_2Me
H
H
H
O
N
O
Me

2


3/VIM-SB-final_Noesy_01.fid
F2 (ppm)
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
F1 (ppm)


Isoquinolineproduct_Noesy1dF_01.esp
Ph
N
F3C
CO2Me
H
H
H
O
N
O
Me
7
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
Chemical Shift (ppm)

VIM-SD1-1-Proton.esp



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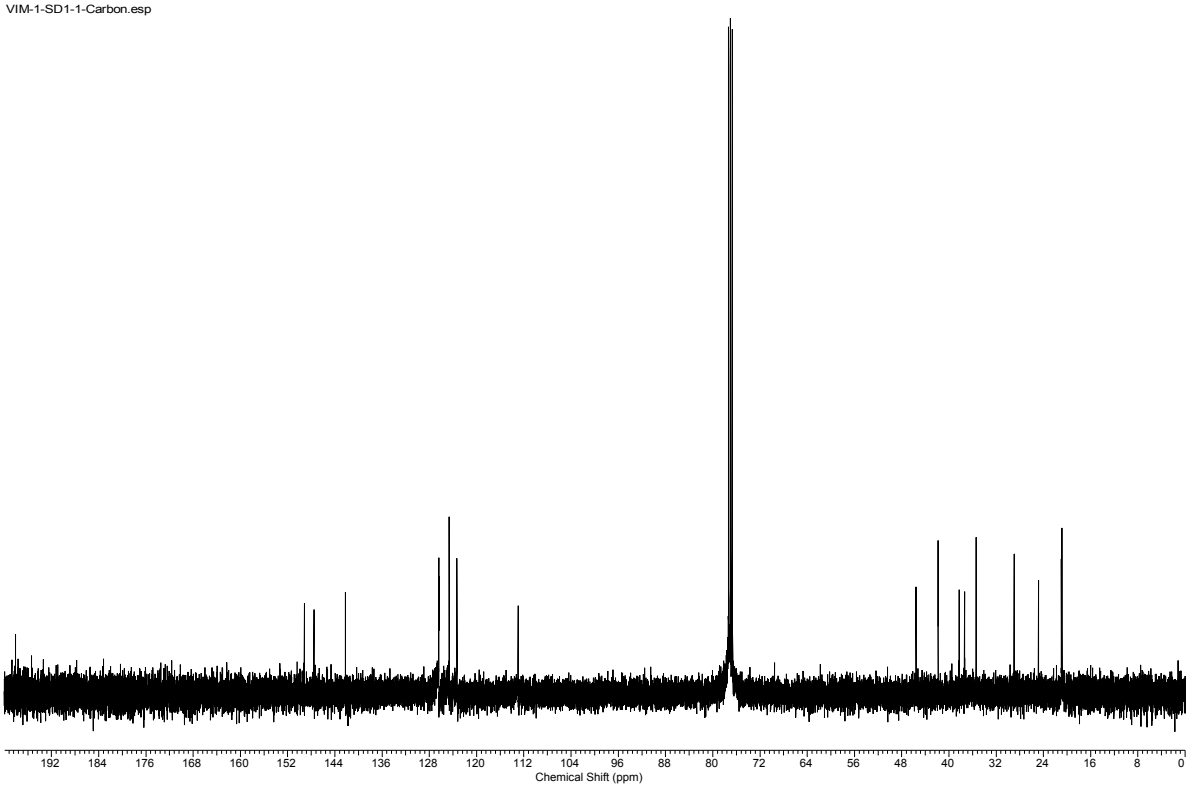

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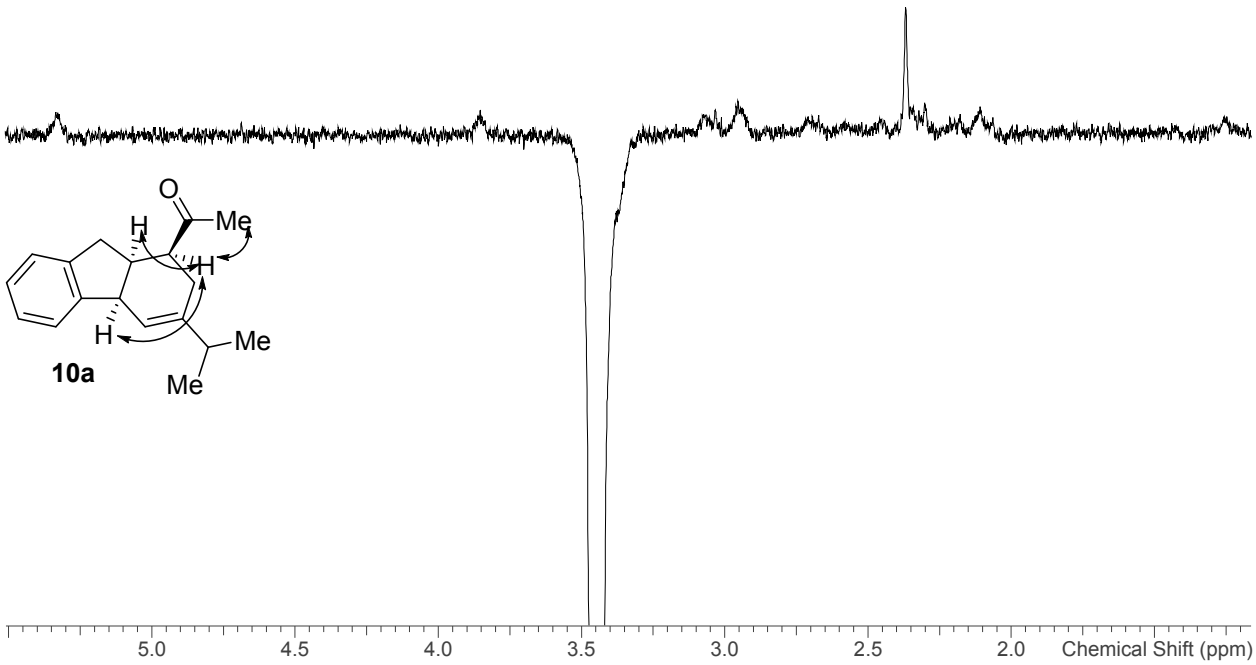
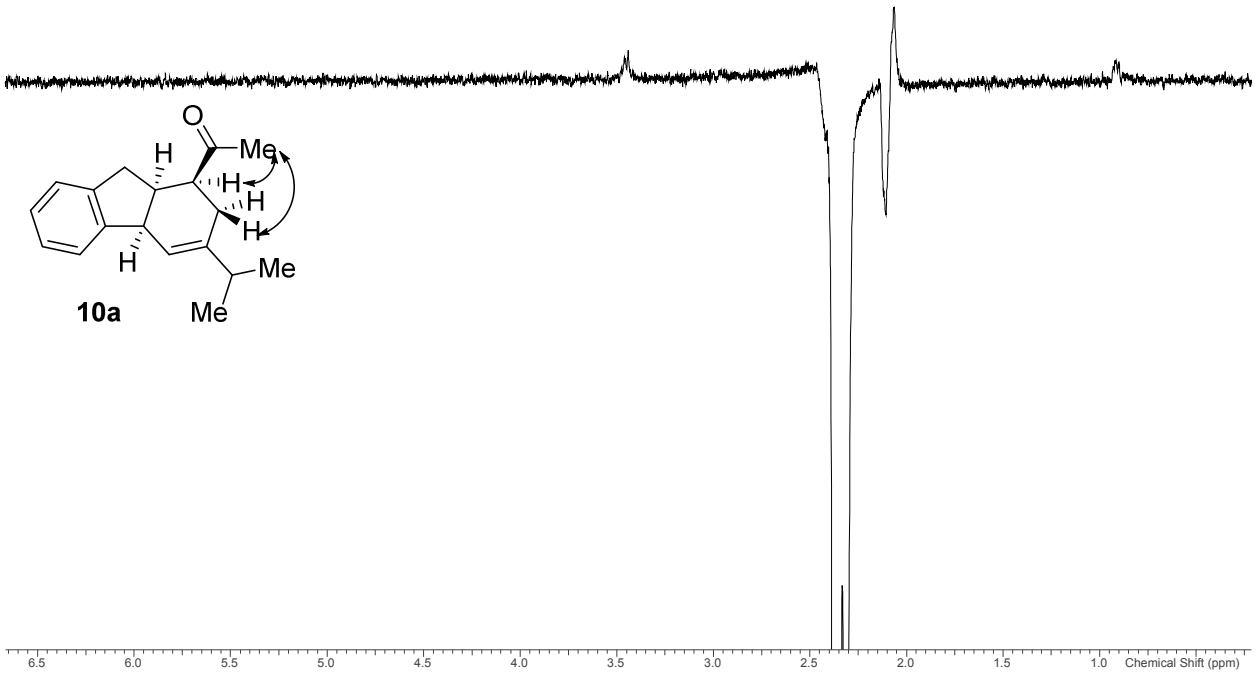
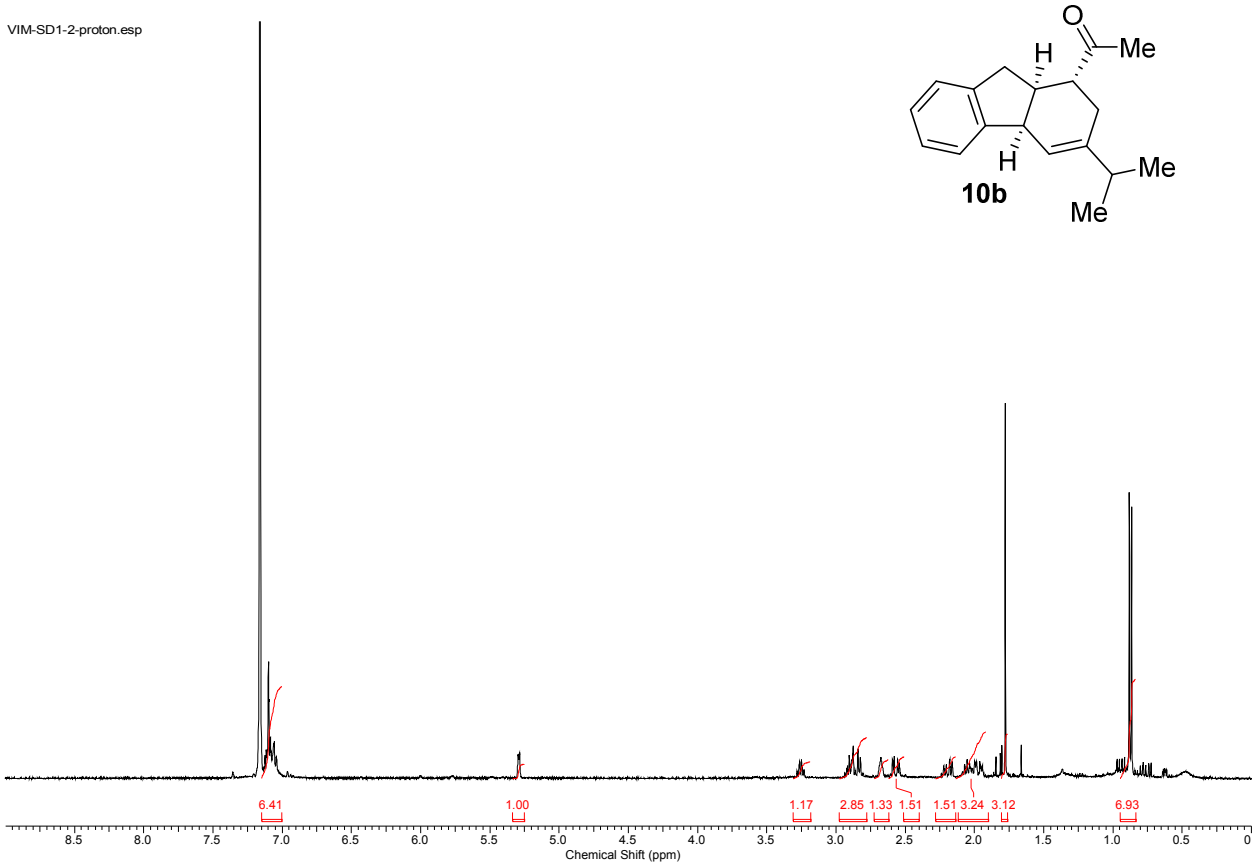
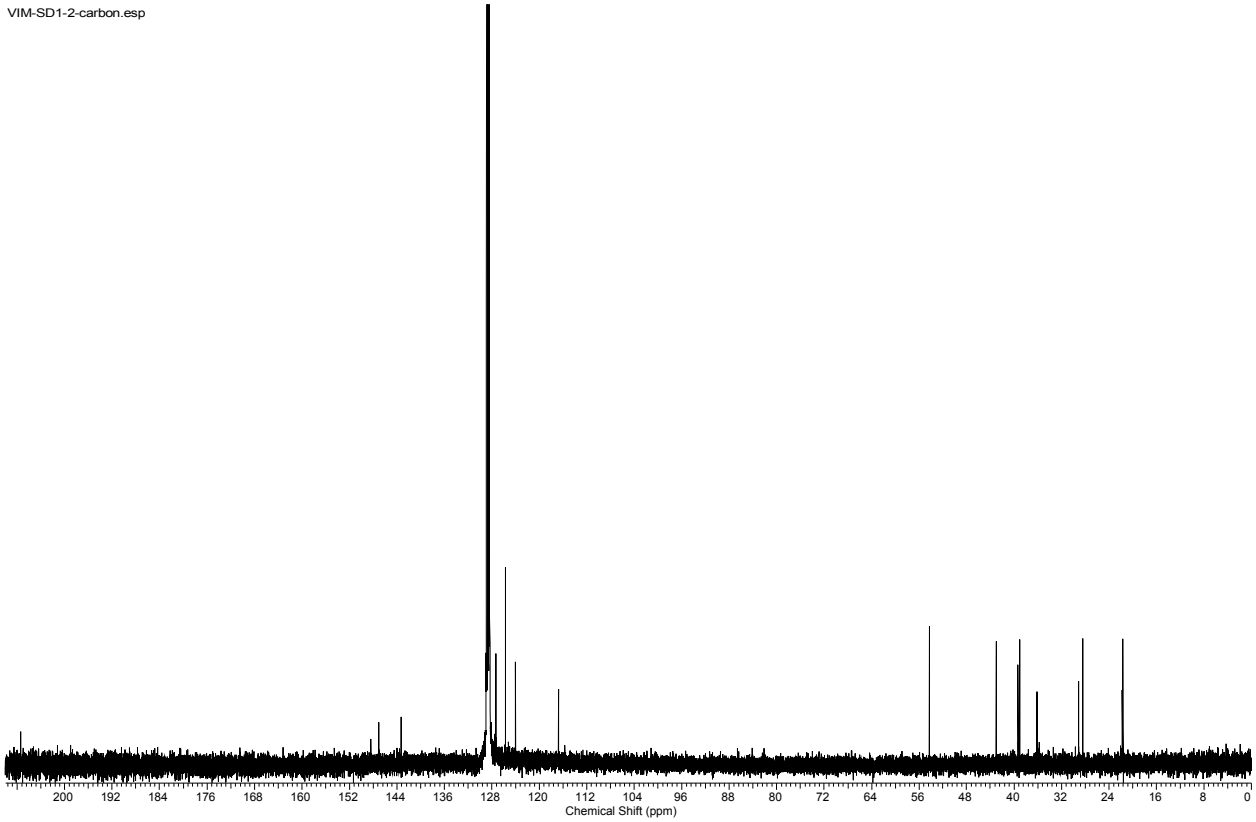


VIM-SD1-1-Me_Noesy1d_01




VIM-SD1-2-proton.esp
O
Me
H
H
Me
Me
10b
6.41
1.00
1.17
2.85
1.33
1.51
1.51
3.24
3.12
6.93
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)


VIM-SD1-2-carbon.esp
200
192
184
176
168
160
152
144
136
128
120
112
104
96
88
80
72
64
56
48
40
32
24
16
8
0
Chemical Shift (ppm)

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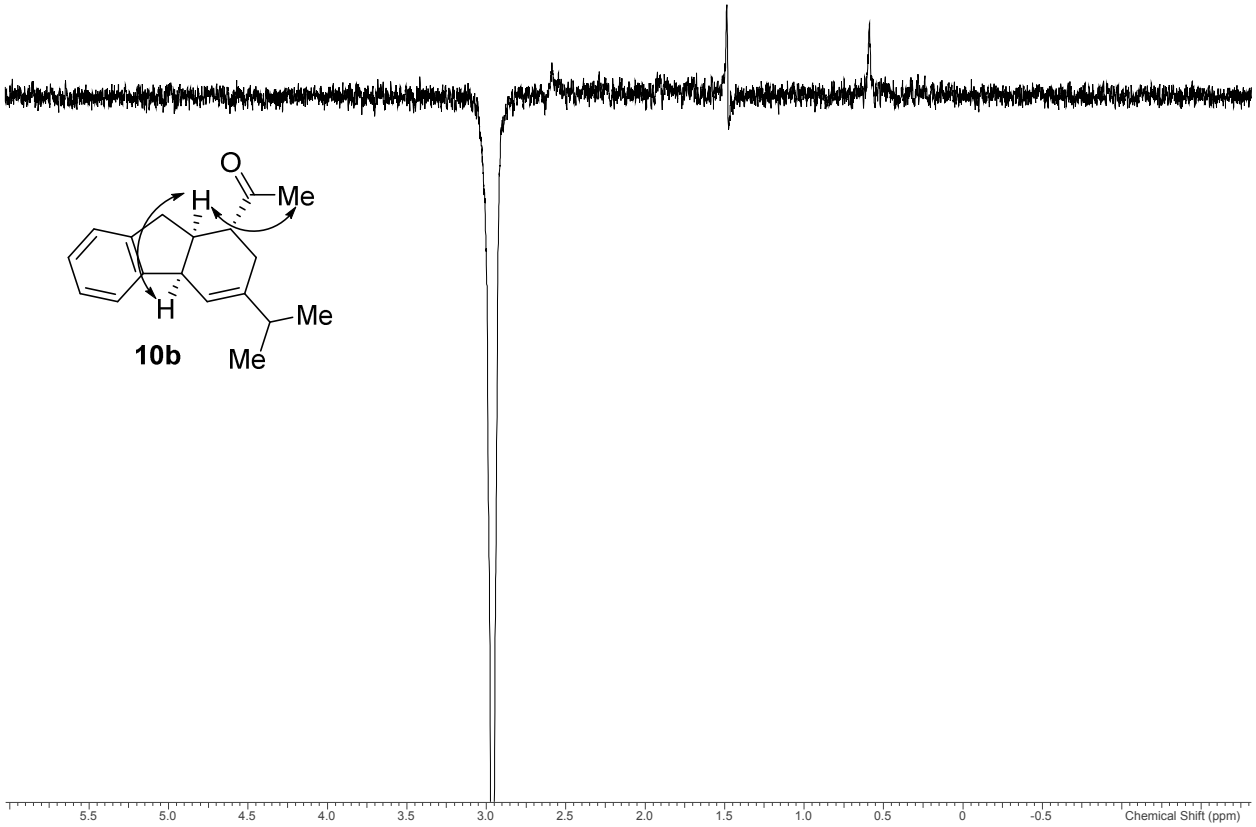

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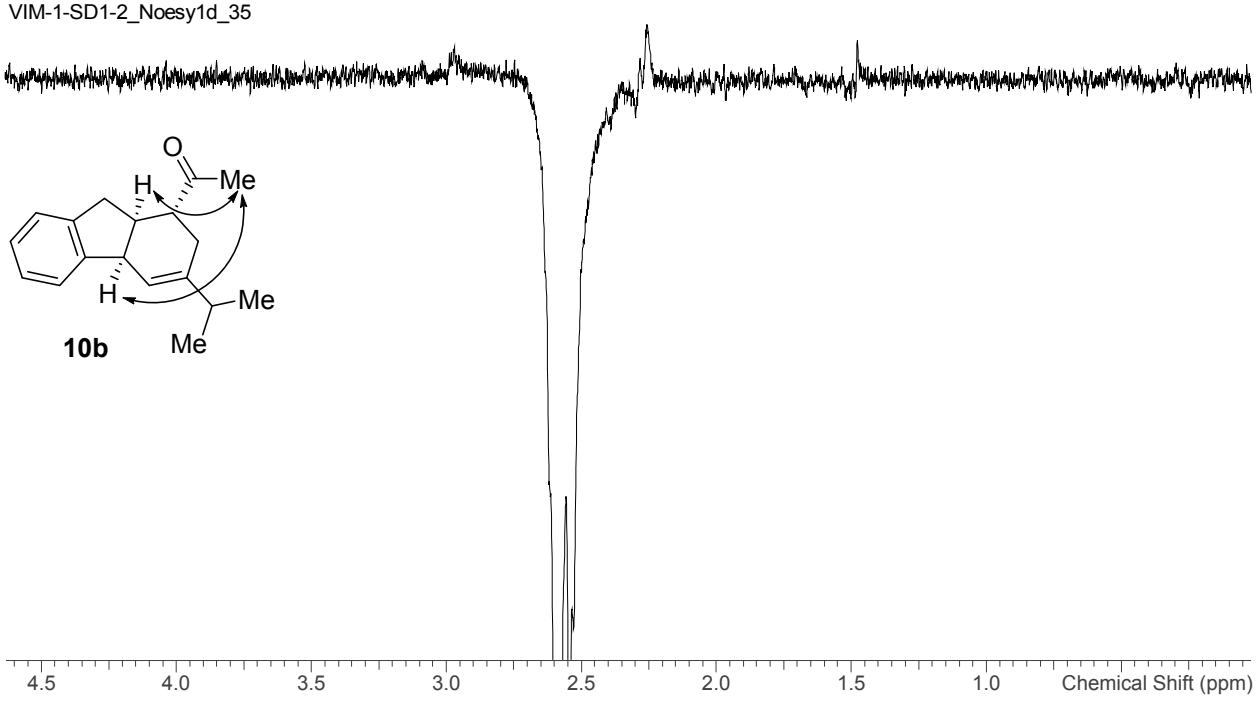
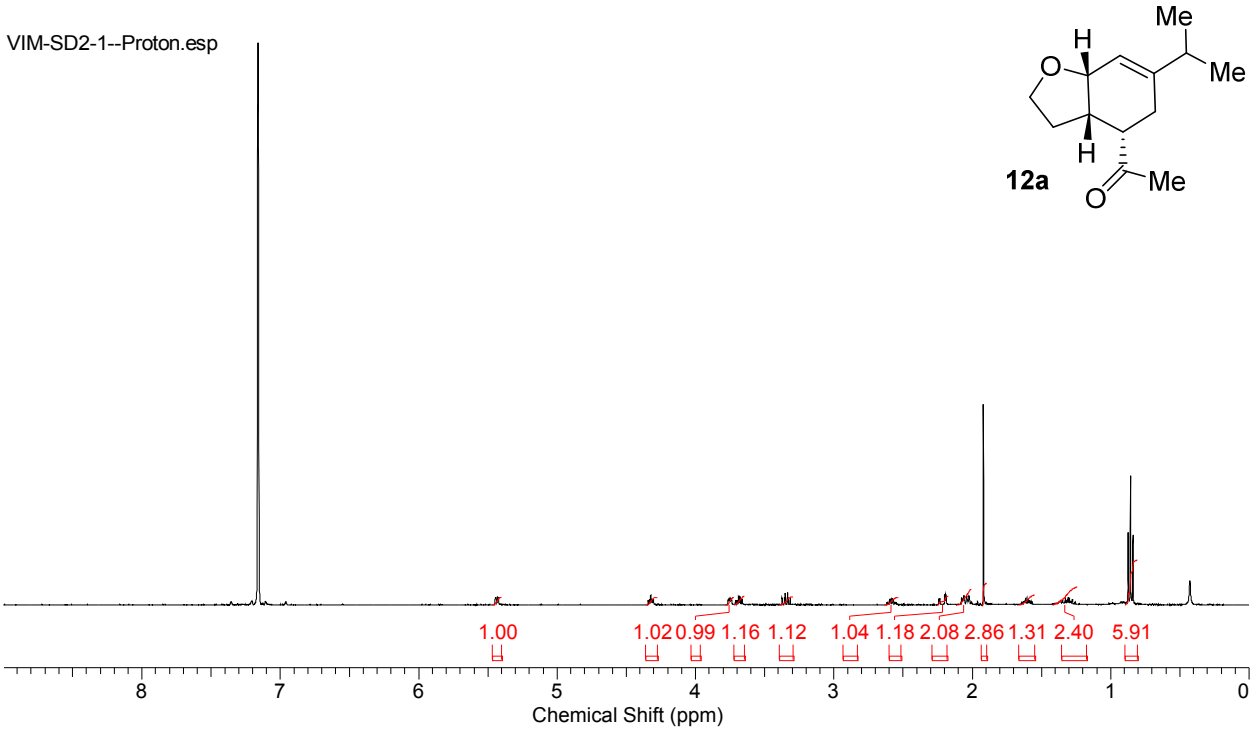
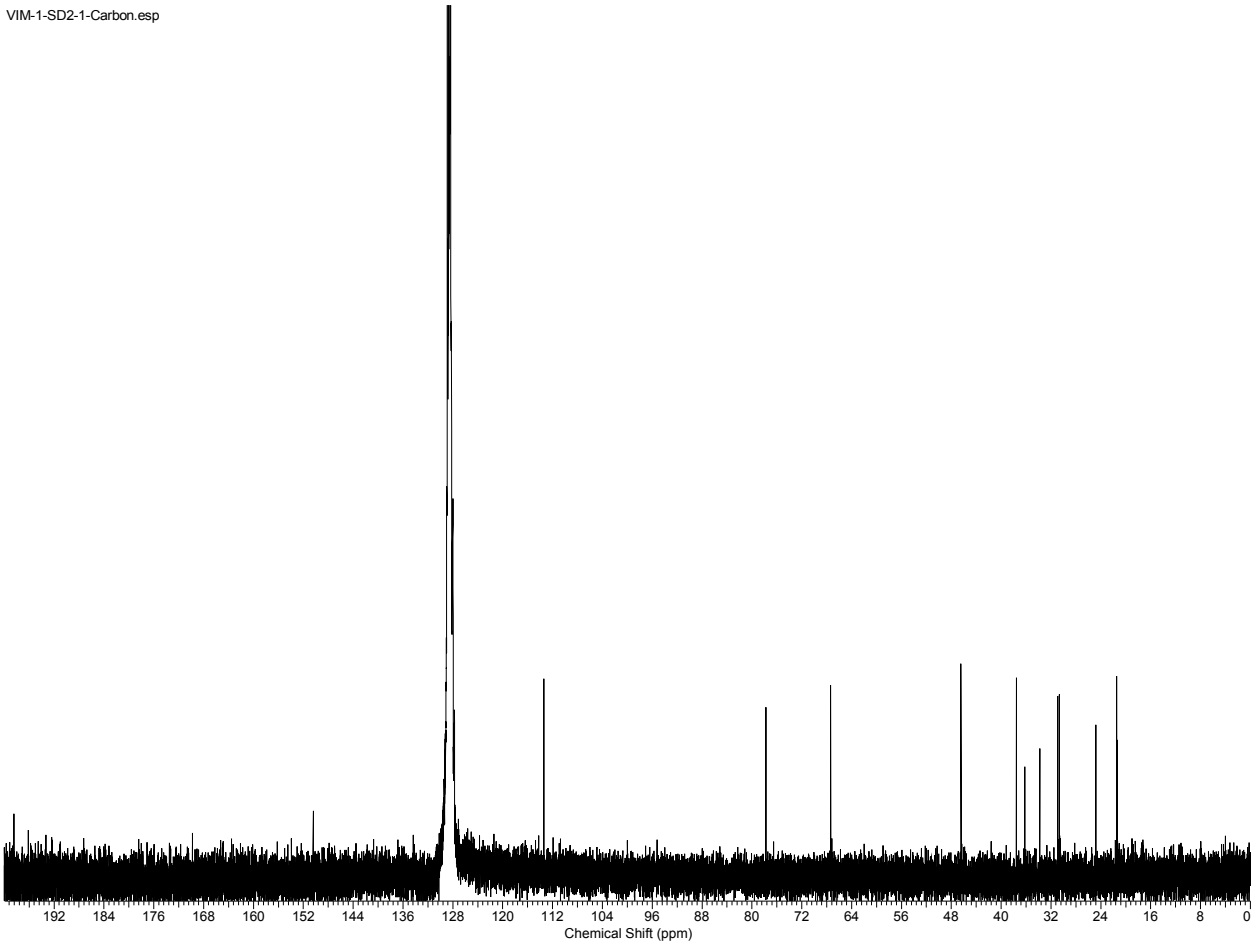



VIM-SD2-1--Proton.esp
Me
H
O
Me
H
12a
O
Me
1.00
1.02
0.99
1.16
1.12
1.04
1.18
2.08
2.86
1.31
2.40
5.91
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


VIM-1-SD2-1-Carbon.esp
192
184
176
168
160
152
144
136
128
120
112
104
96
88
80
72
64
56
48
40
32
24
16
8
0
Chemical Shift (ppm)

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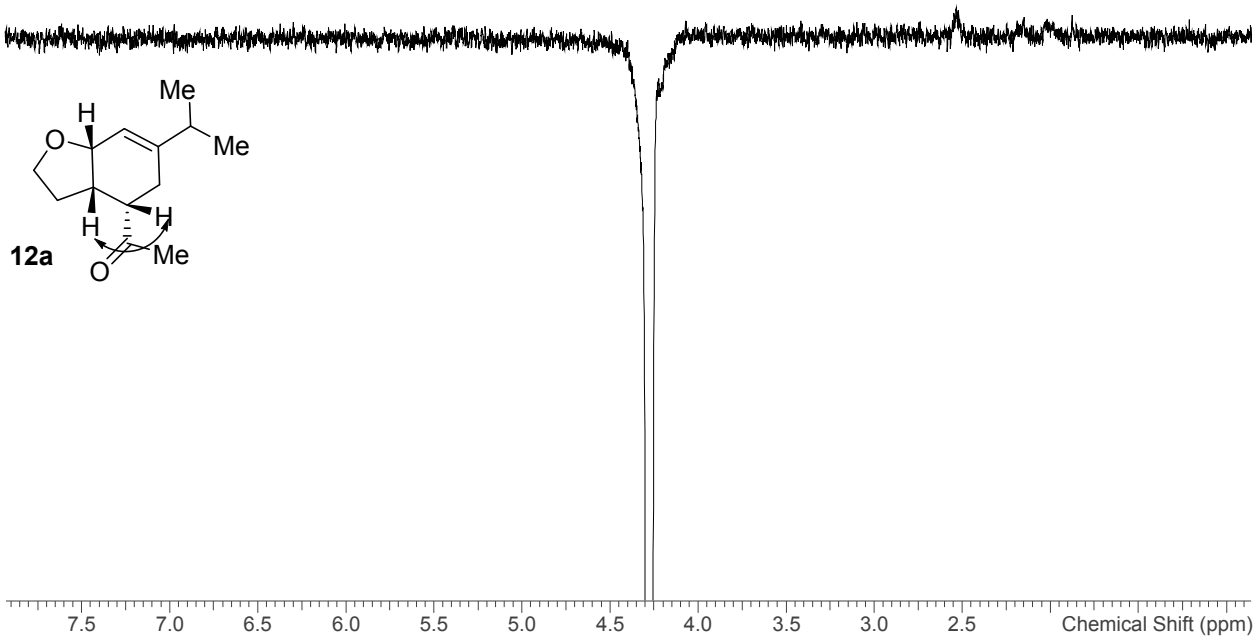

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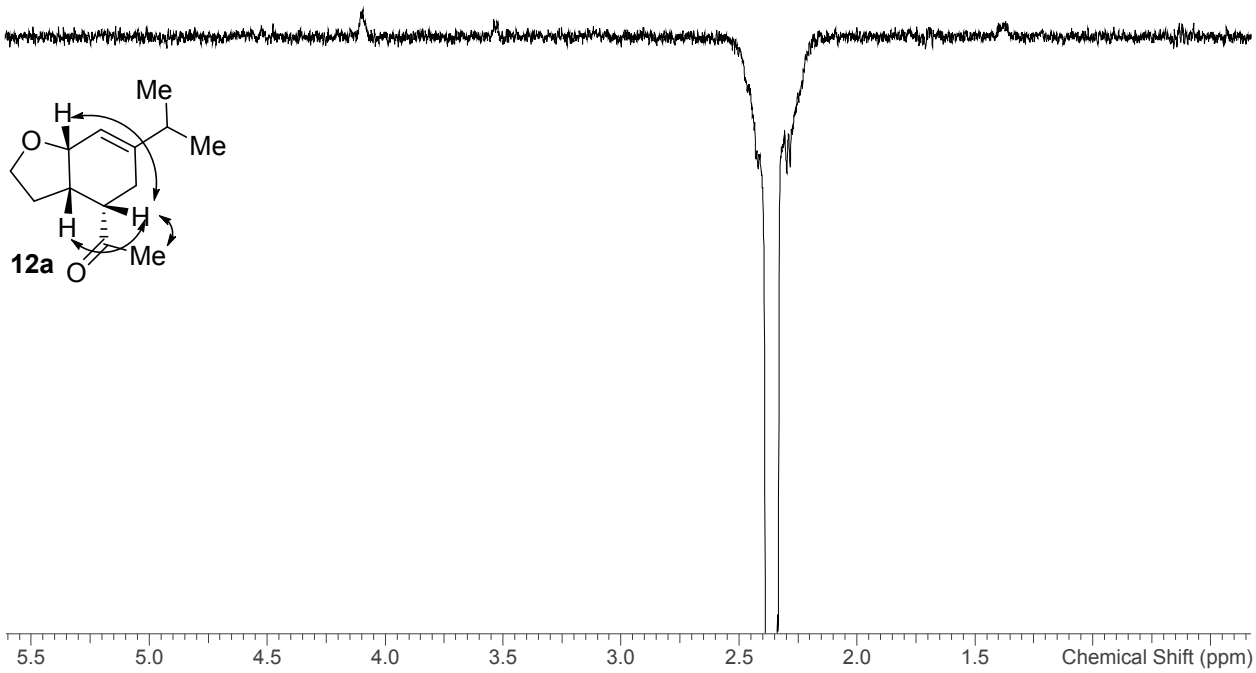

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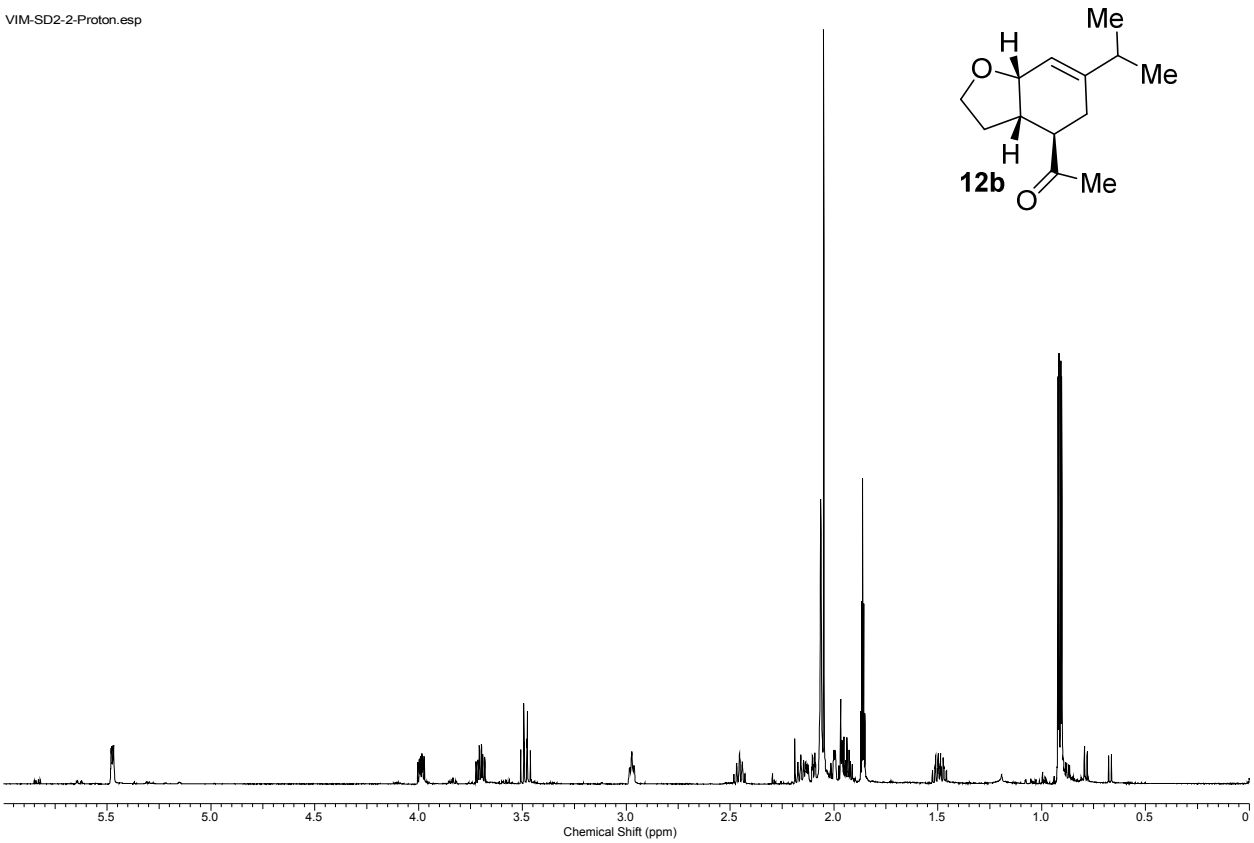

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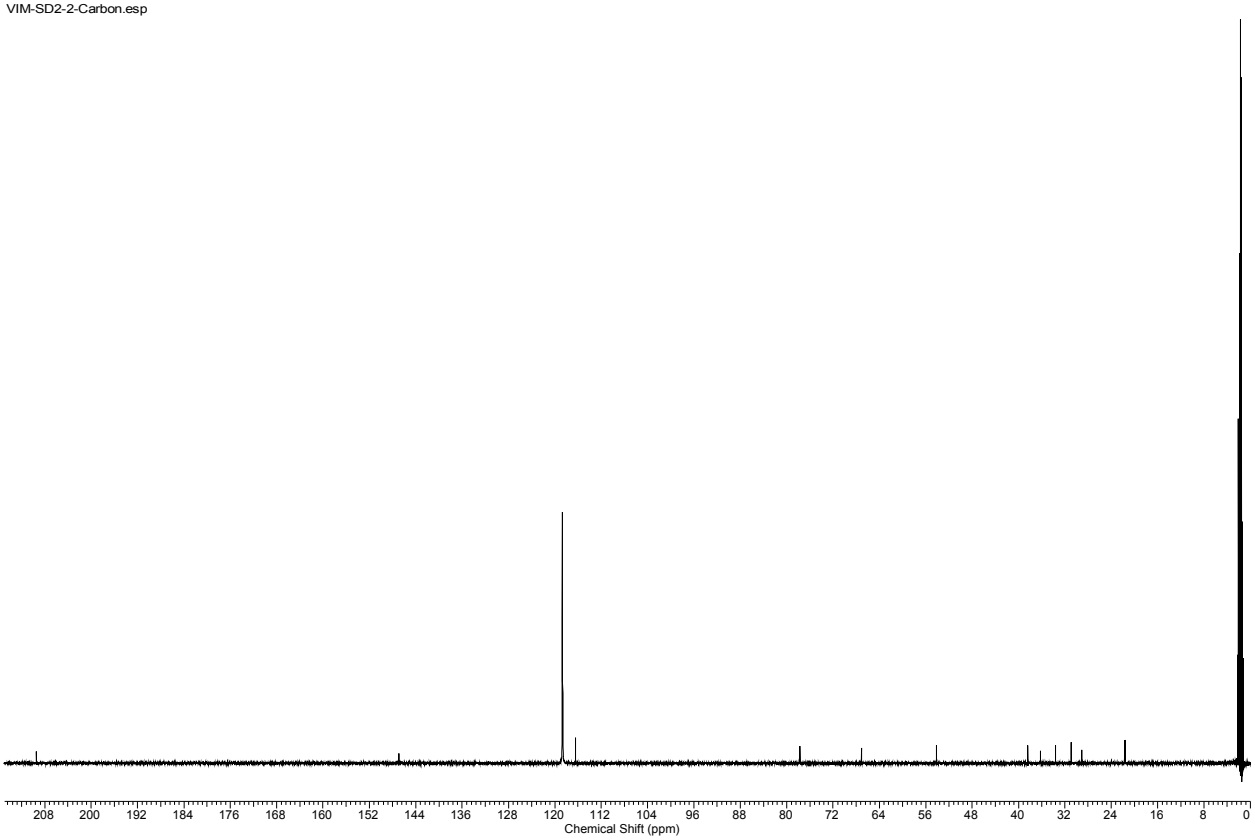
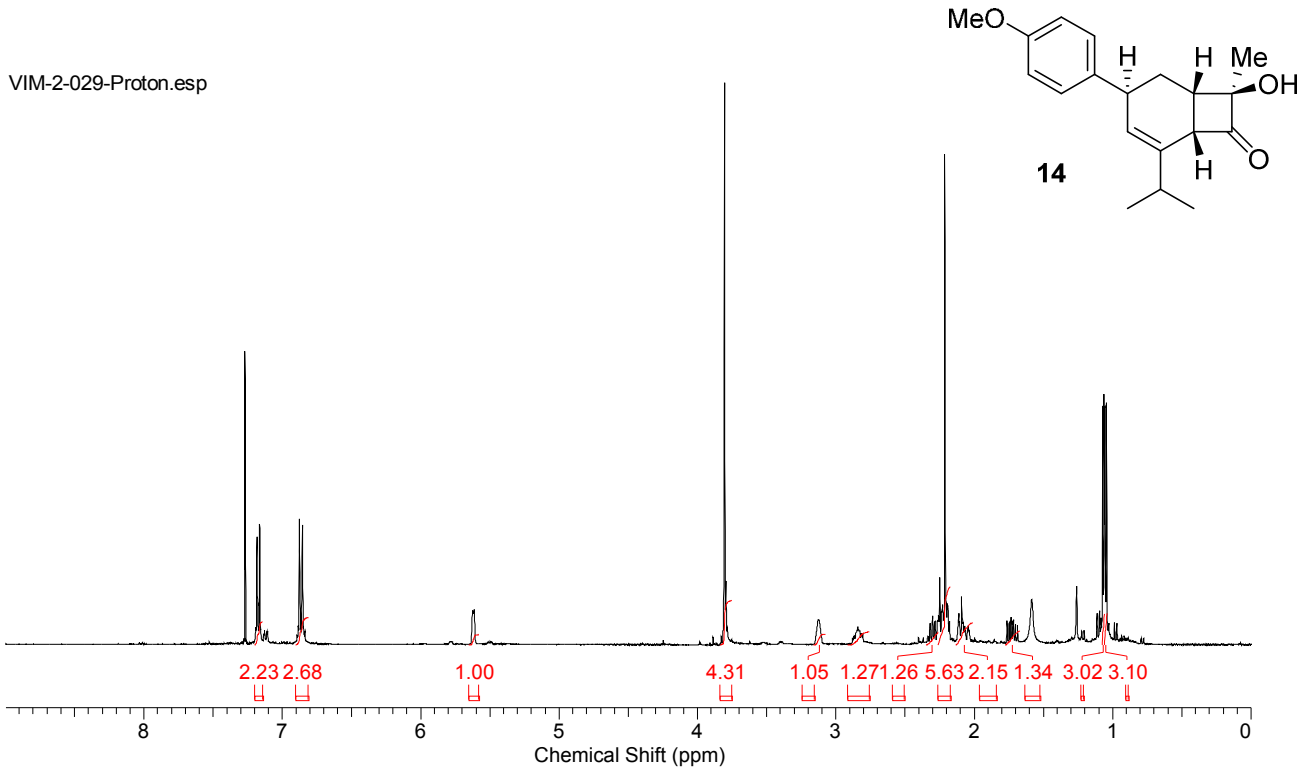
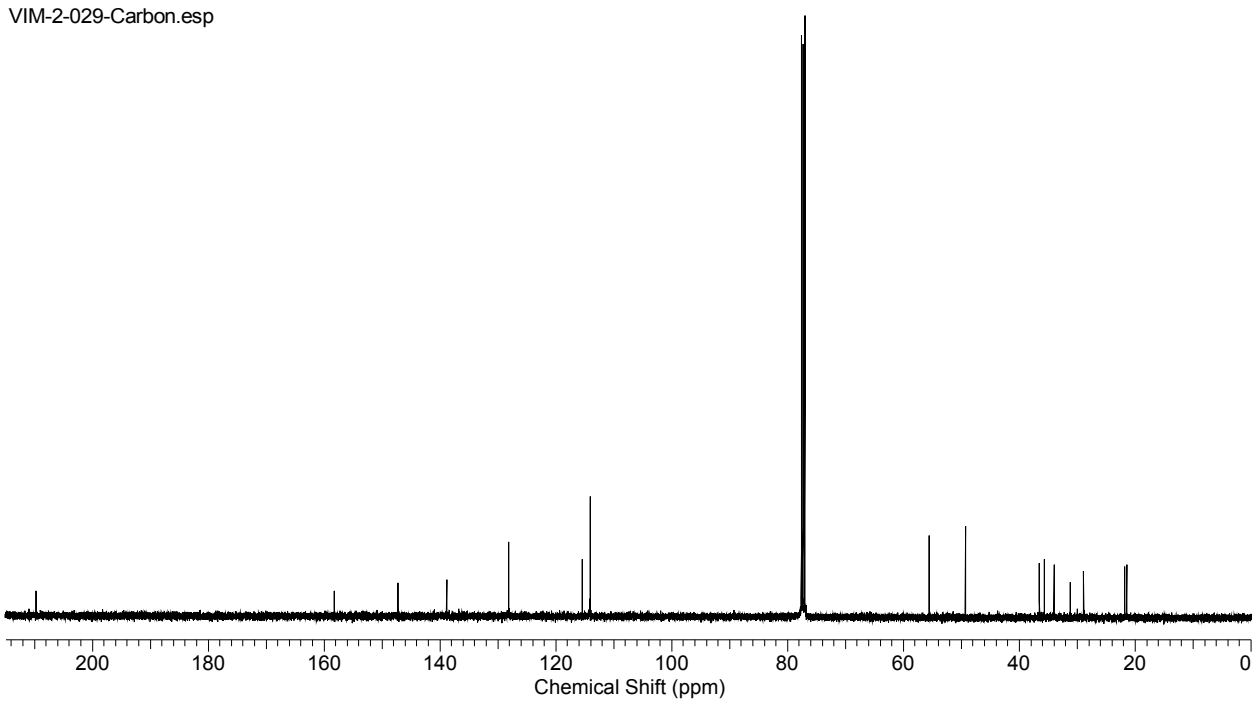



VIM-2-029-Proton.esp
MeO
H
H
Me
OH
O
H
14
2.23 2.68
1.00
4.31
1.05 1.27 1.26 5.63 2.15 1.34 3.02 3.10
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


VIM-2-029-Carbon.esp
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

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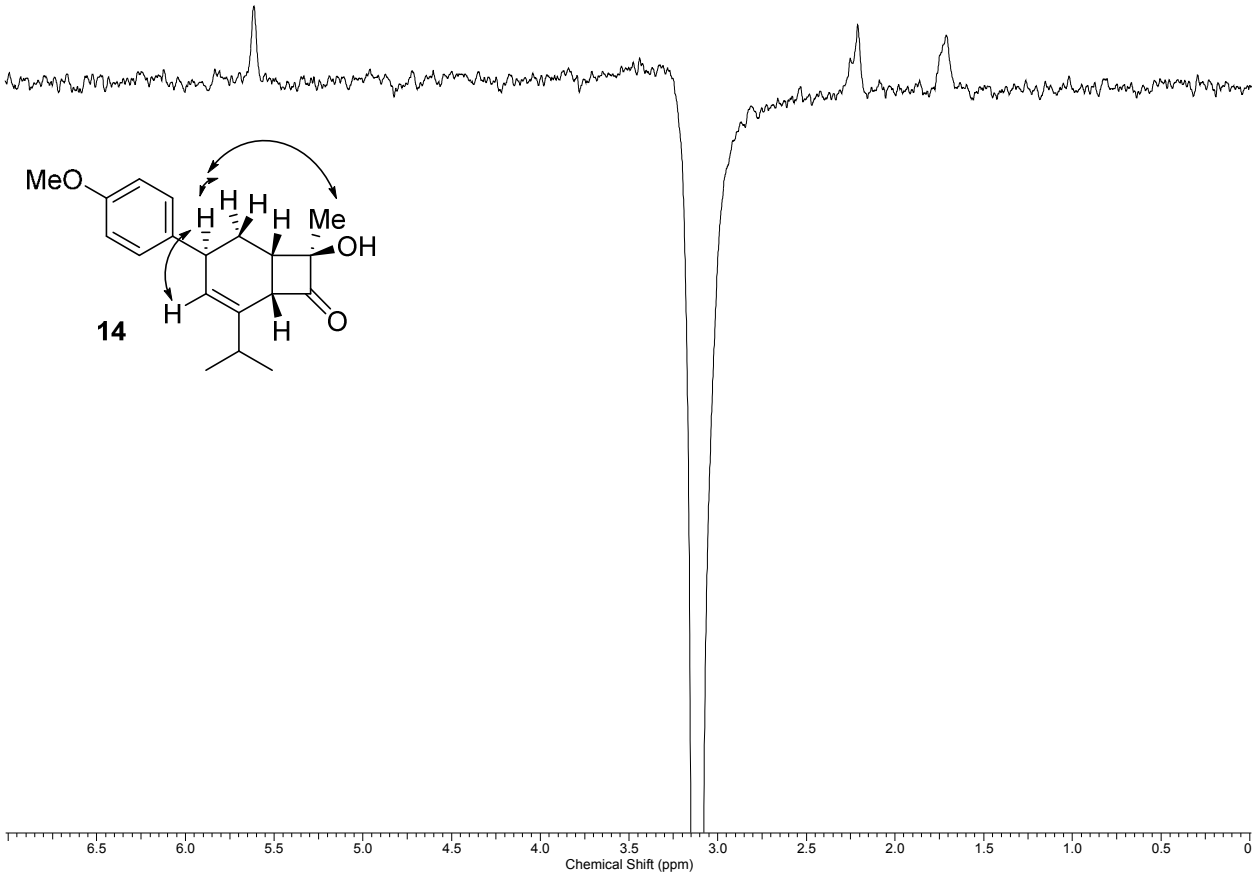

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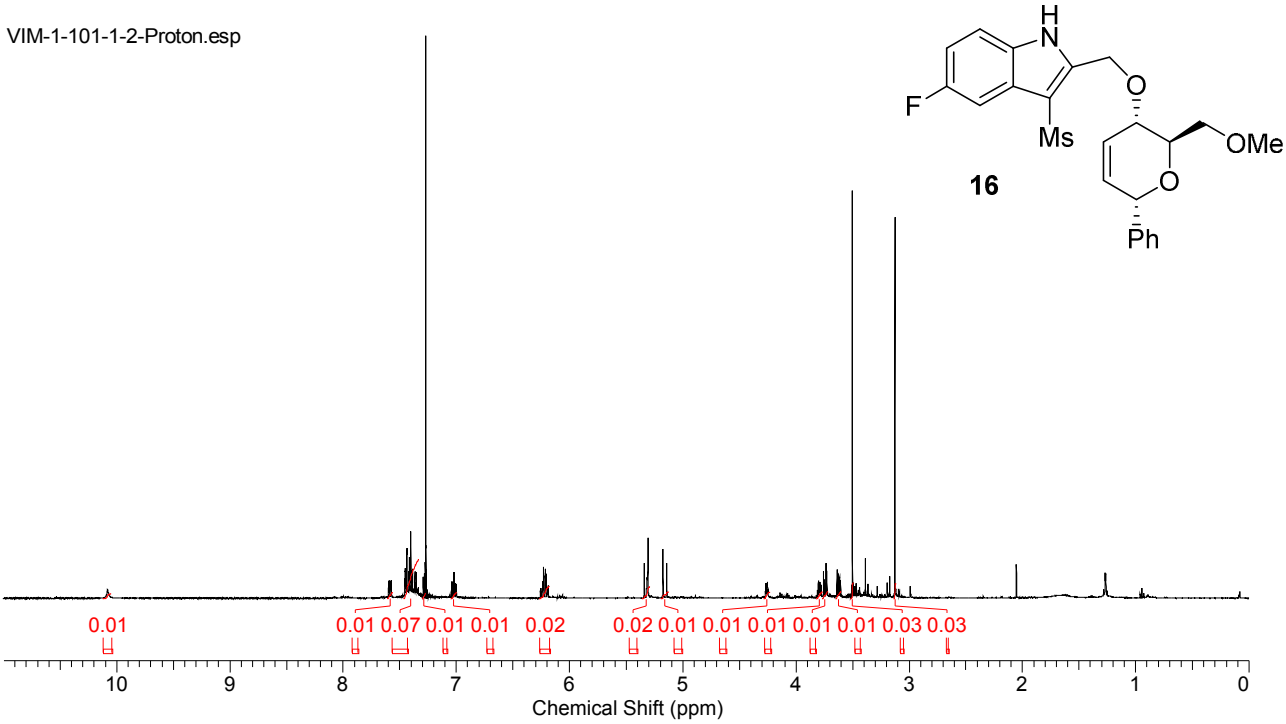

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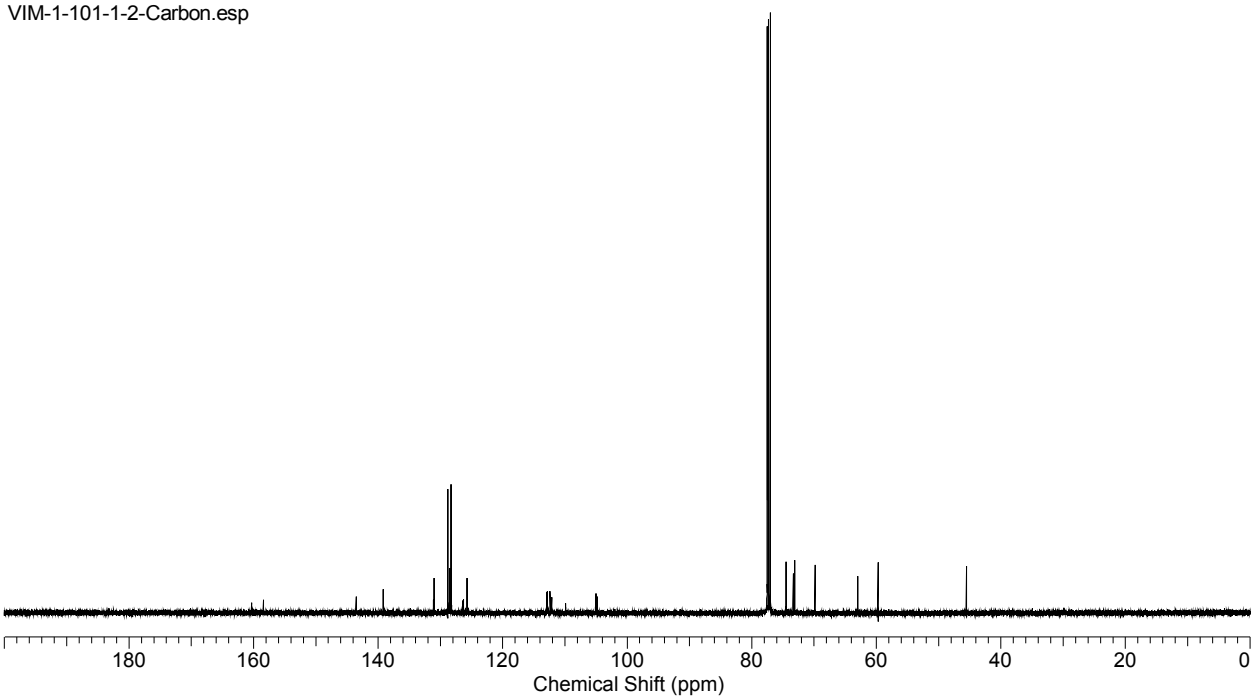

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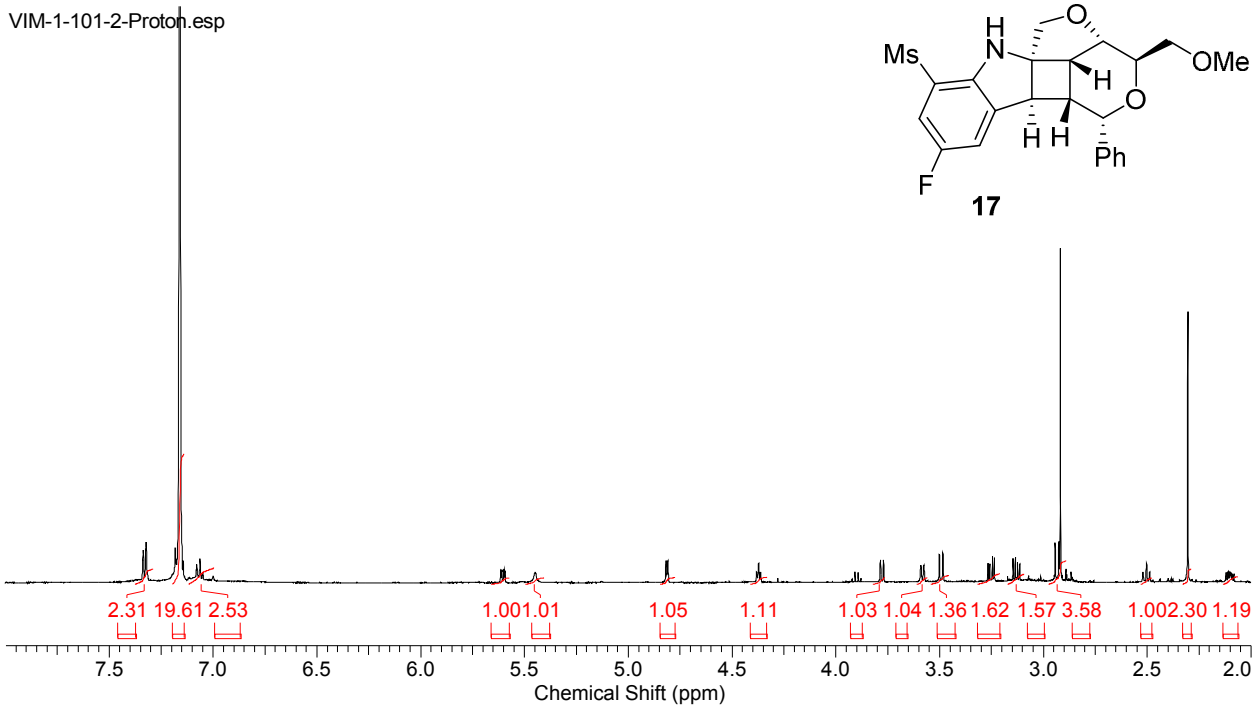

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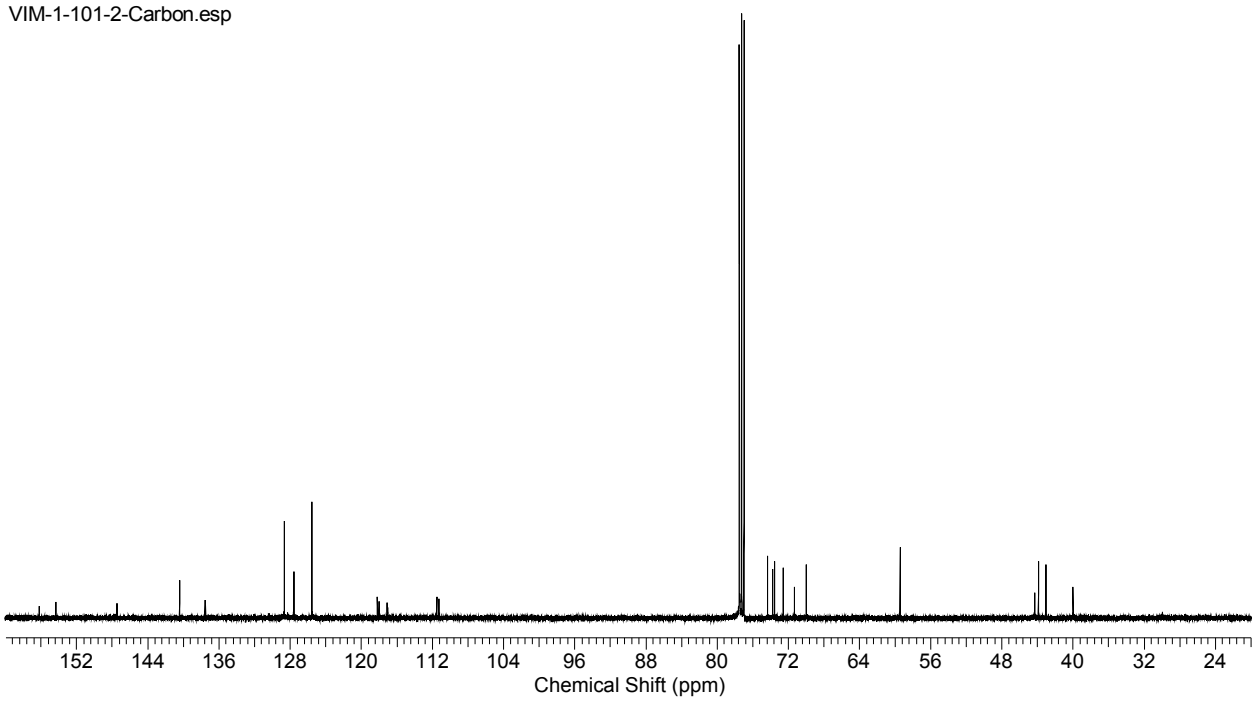
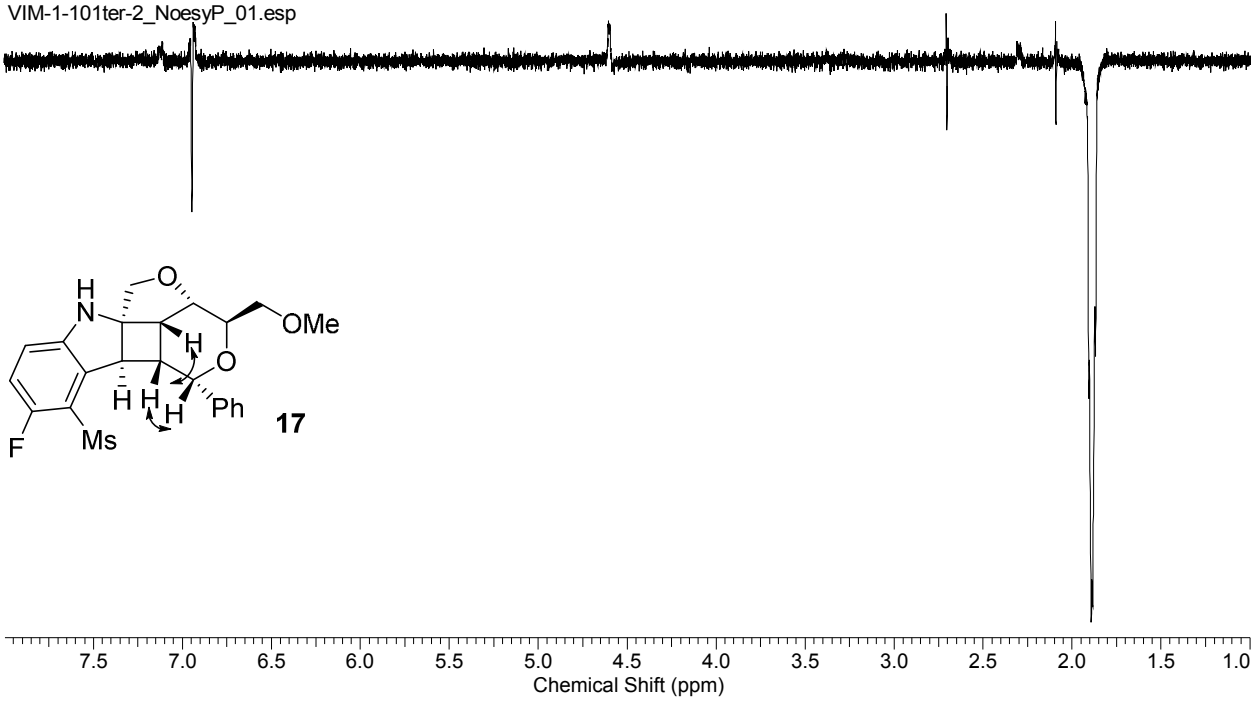
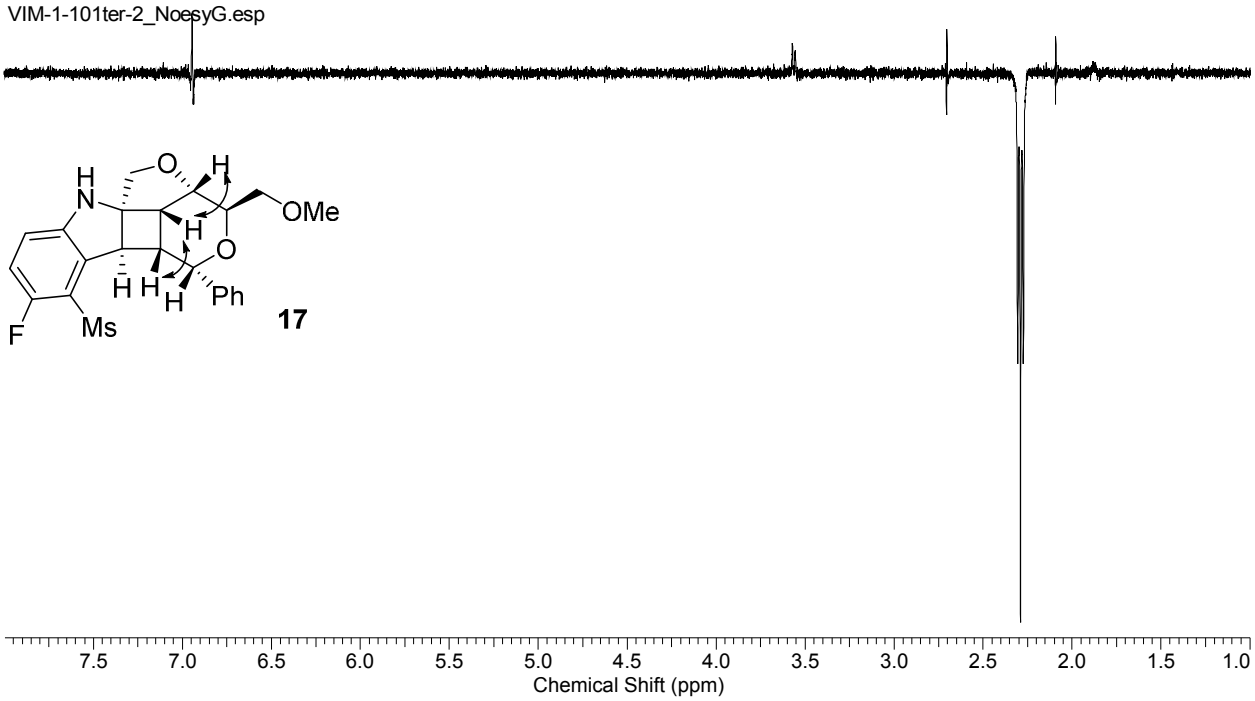
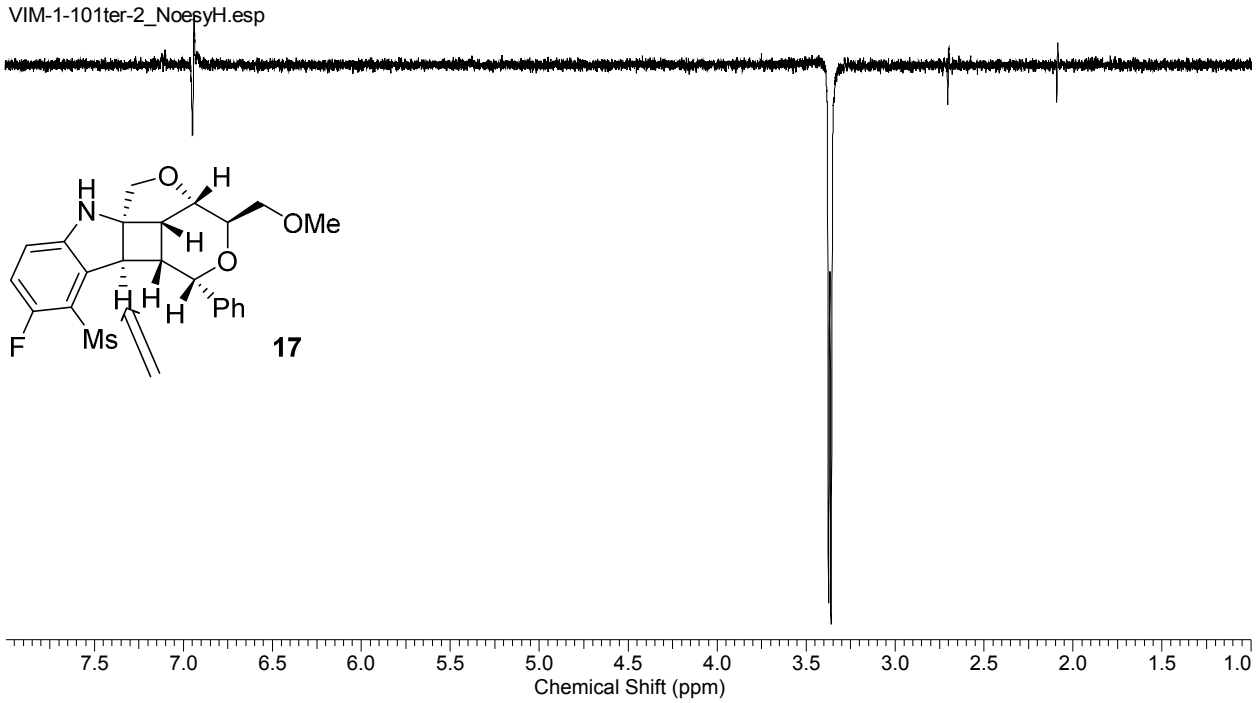


VIM-1-101ter-2_NoesyP_01.esp

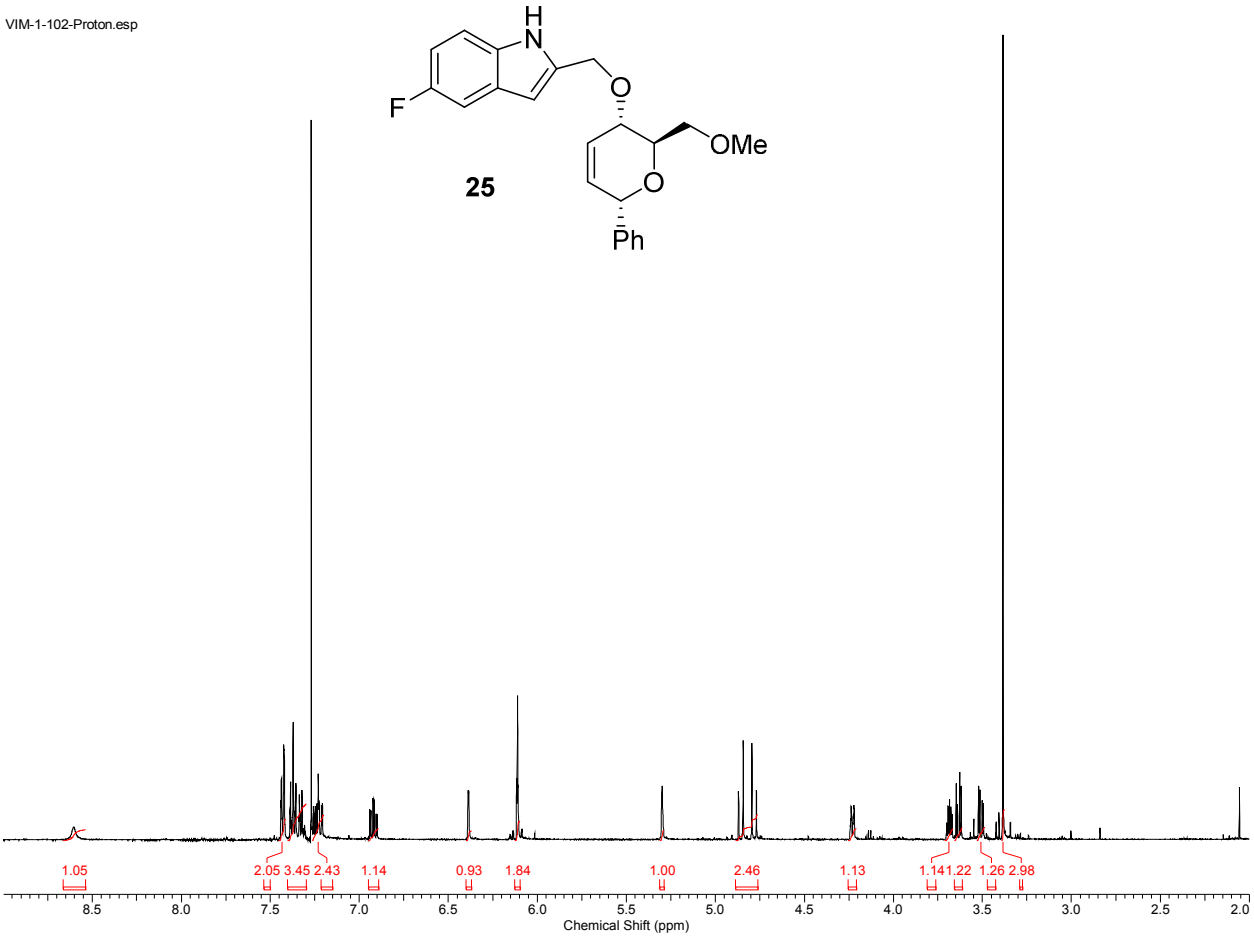


VIM-1-101ter-2_NoesyG.esp

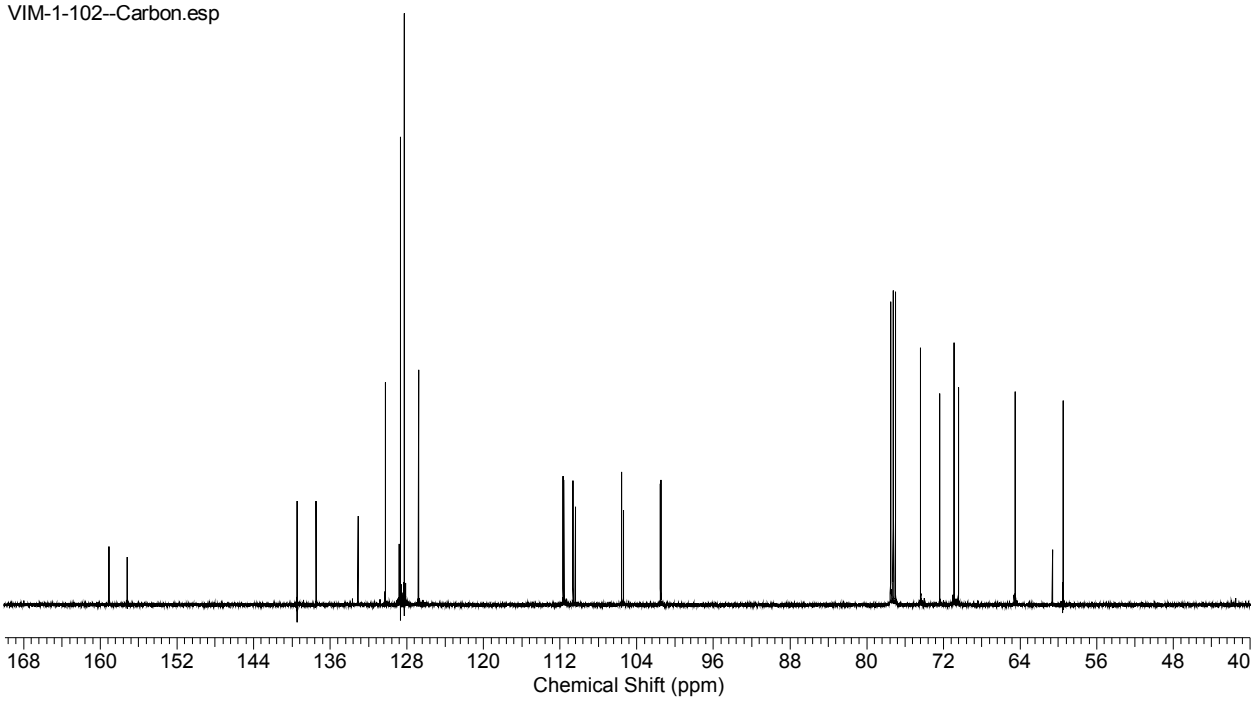



VIM-1-101ter-2_NoesyH.esp
H
N
O
H
OMe
H
O
H
H
H
Ph
F
Ms
17
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
Chemical Shift (ppm)

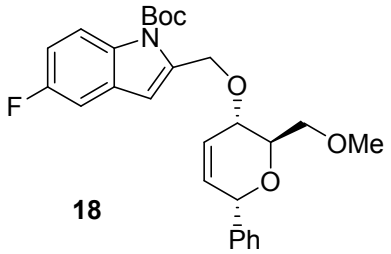
VIM-1-102-Proton.esp



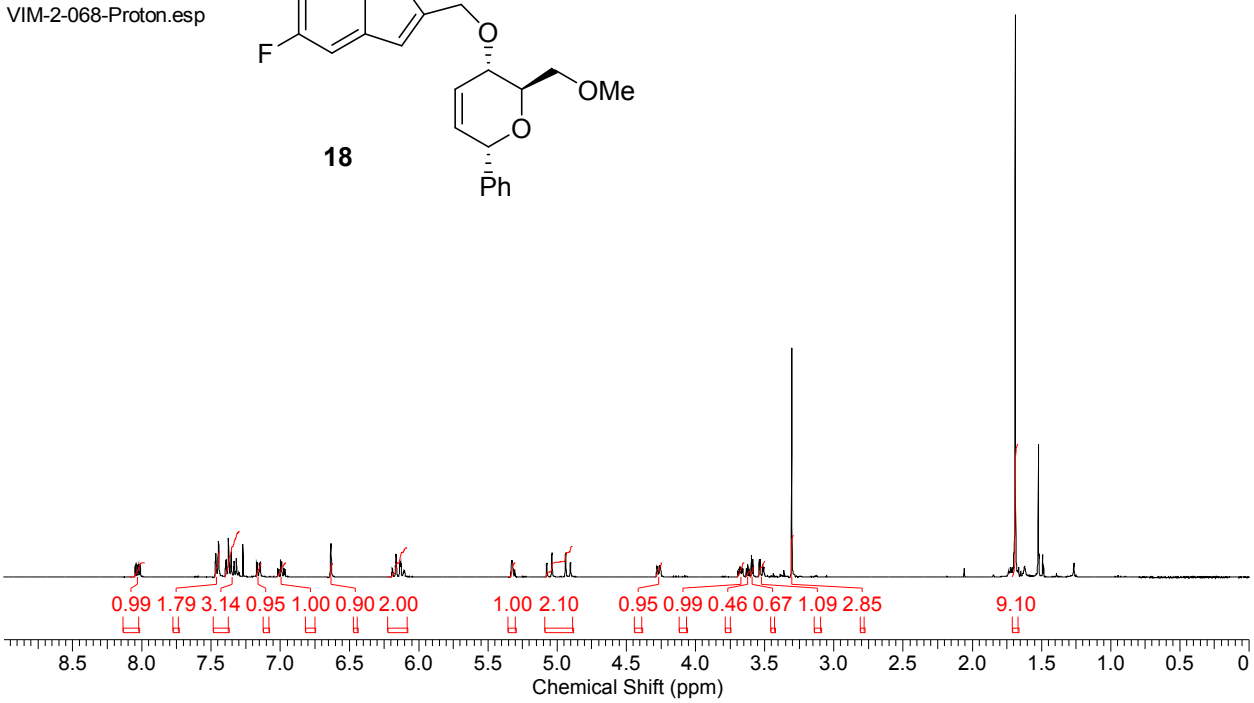
VIM-1-102--Carbon.esp



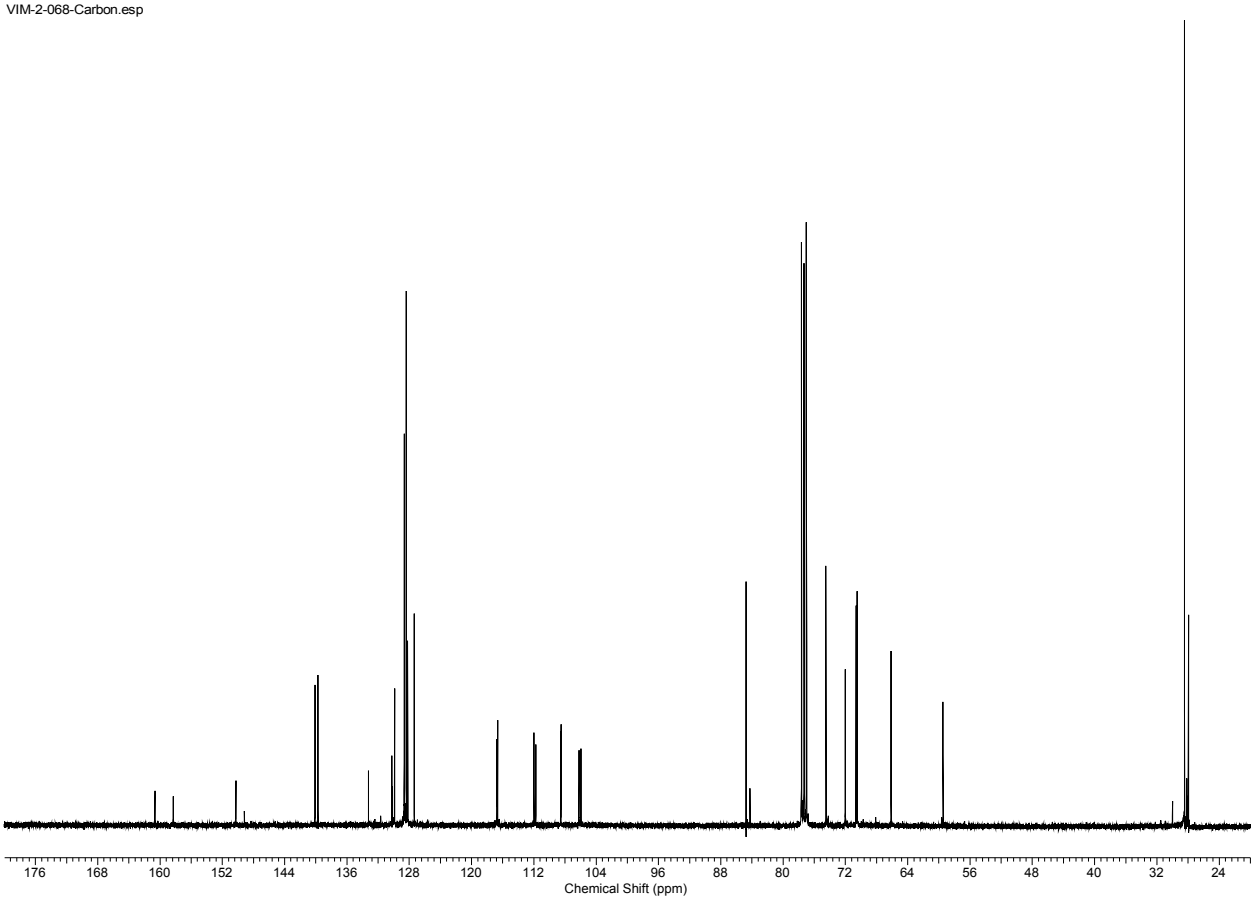
VIM-2-068-Proton.esp



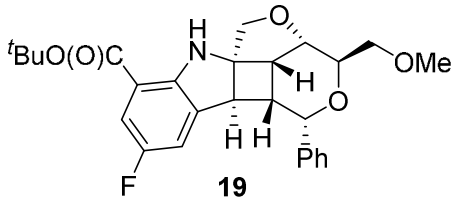
18

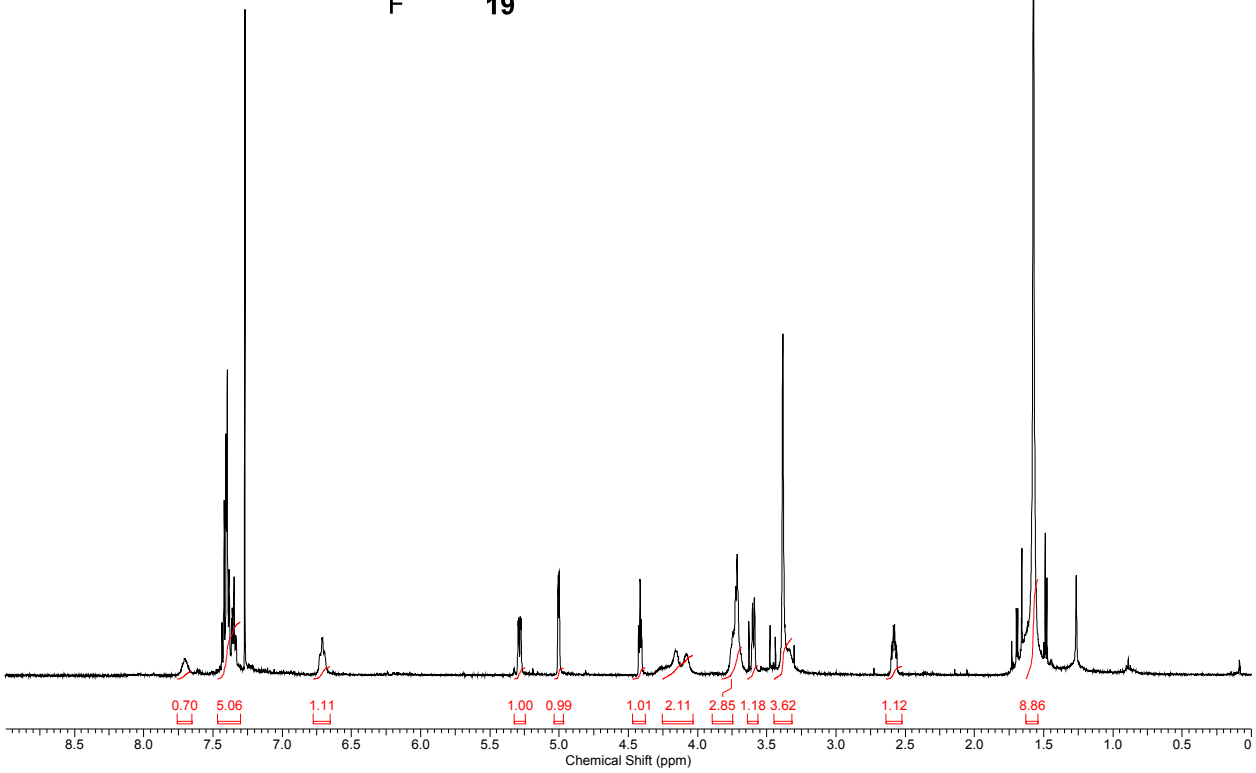


VIM-2-068-Carbon.esp

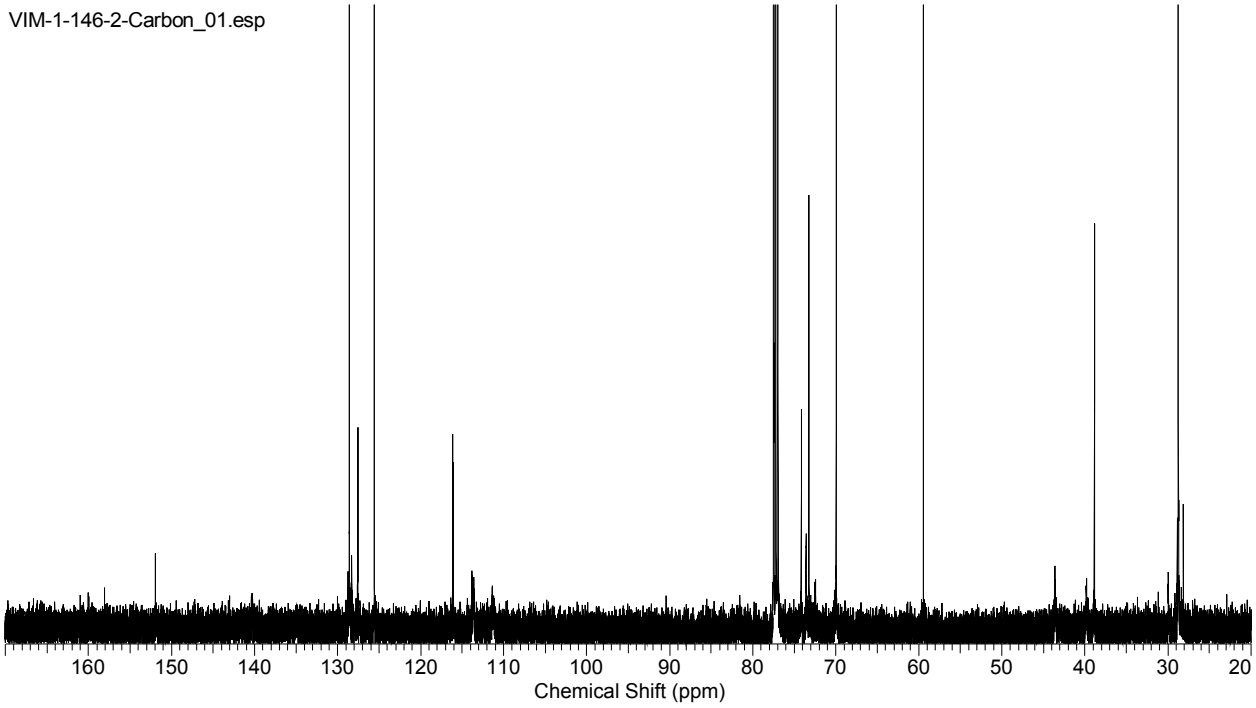


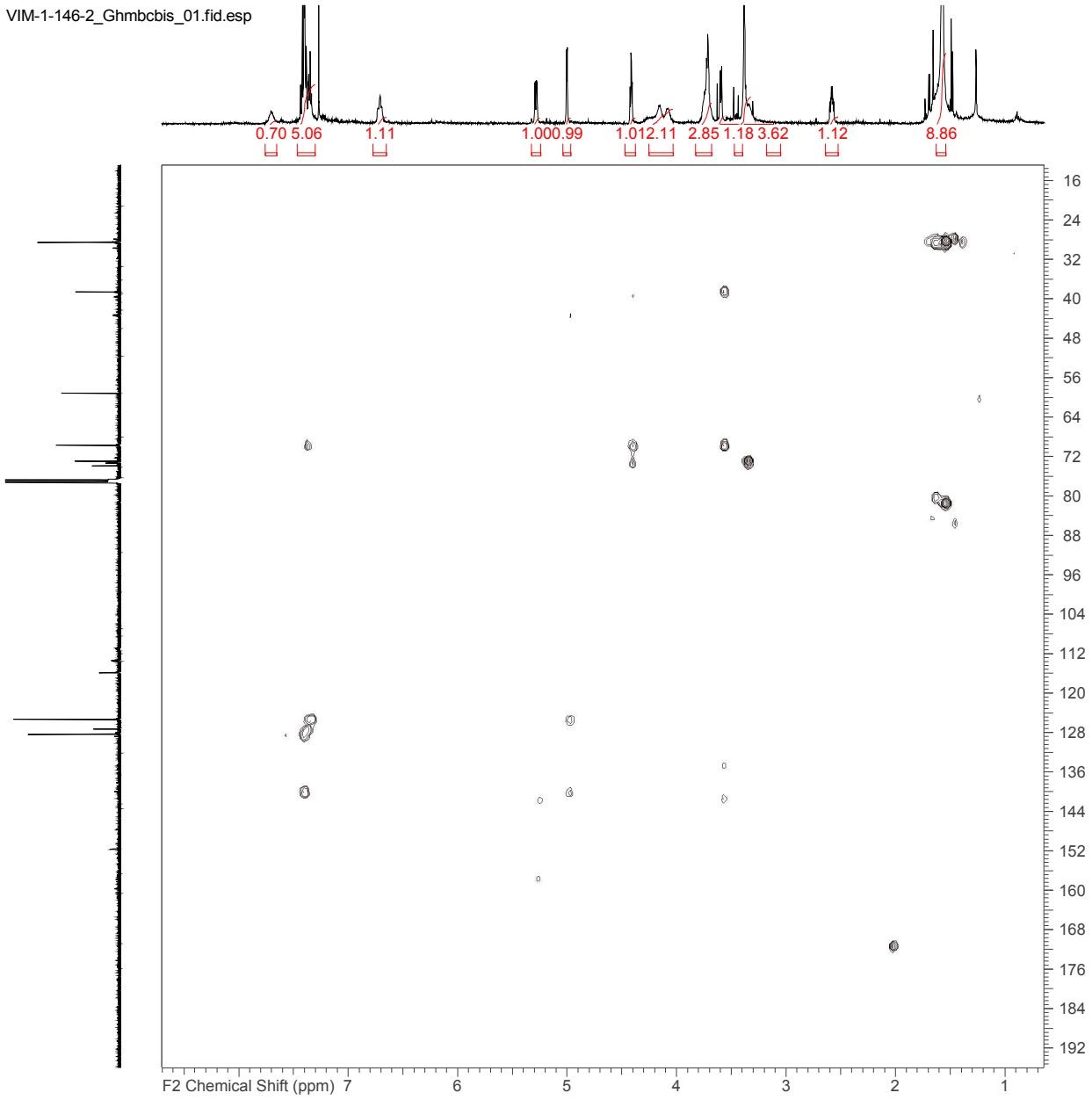
VIM-1-146-2-Proton.esp



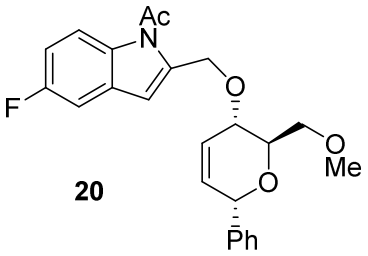


VIM-1-146-2-Carbon_01.esp

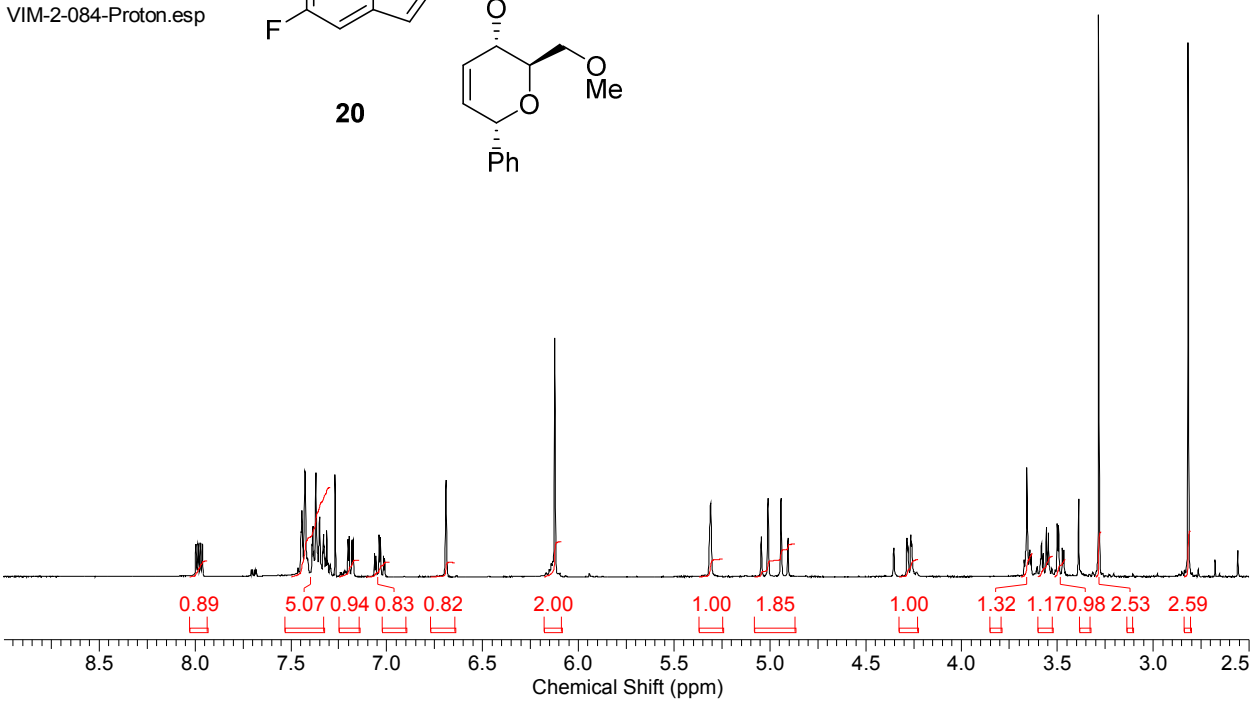



VIM-1-146-2_Ghmbcbis_01.fid.esp
0.70 5.06
1.11
1.00 0.99
1.01 2.11
2.85 1.18 3.62
1.12
8.86
F2 Chemical Shift (ppm)

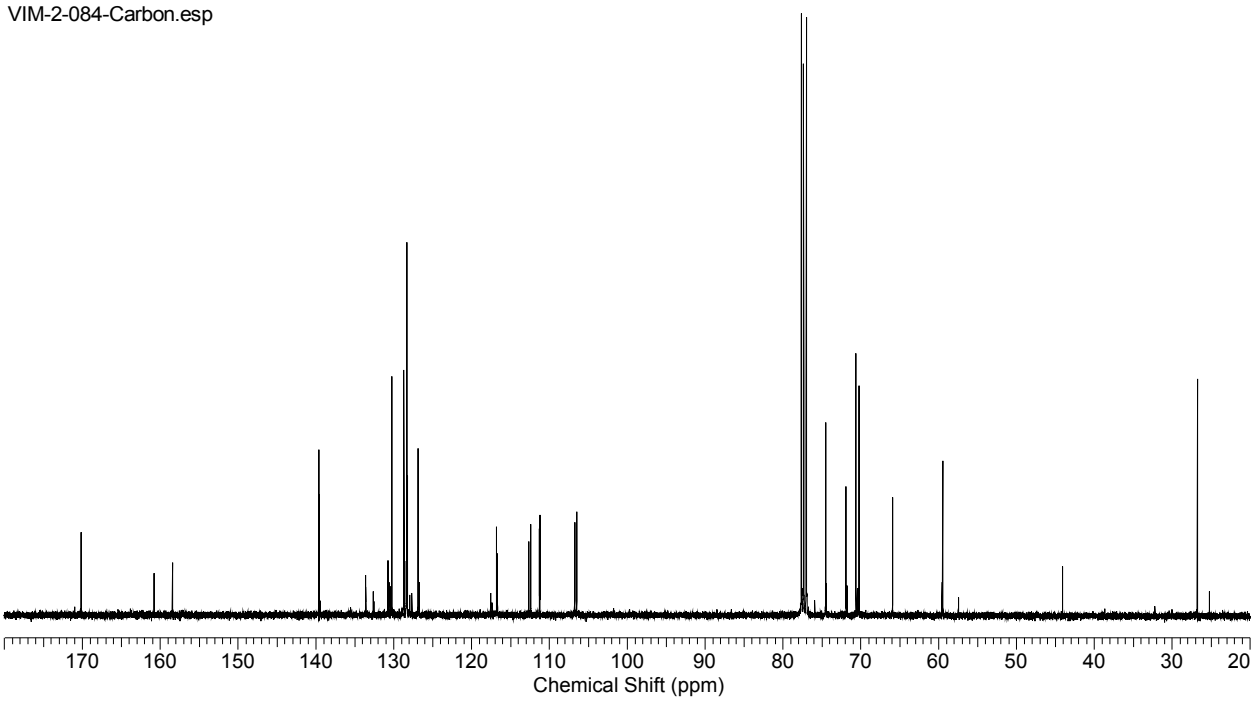
VIM-2-084-Proton.esp

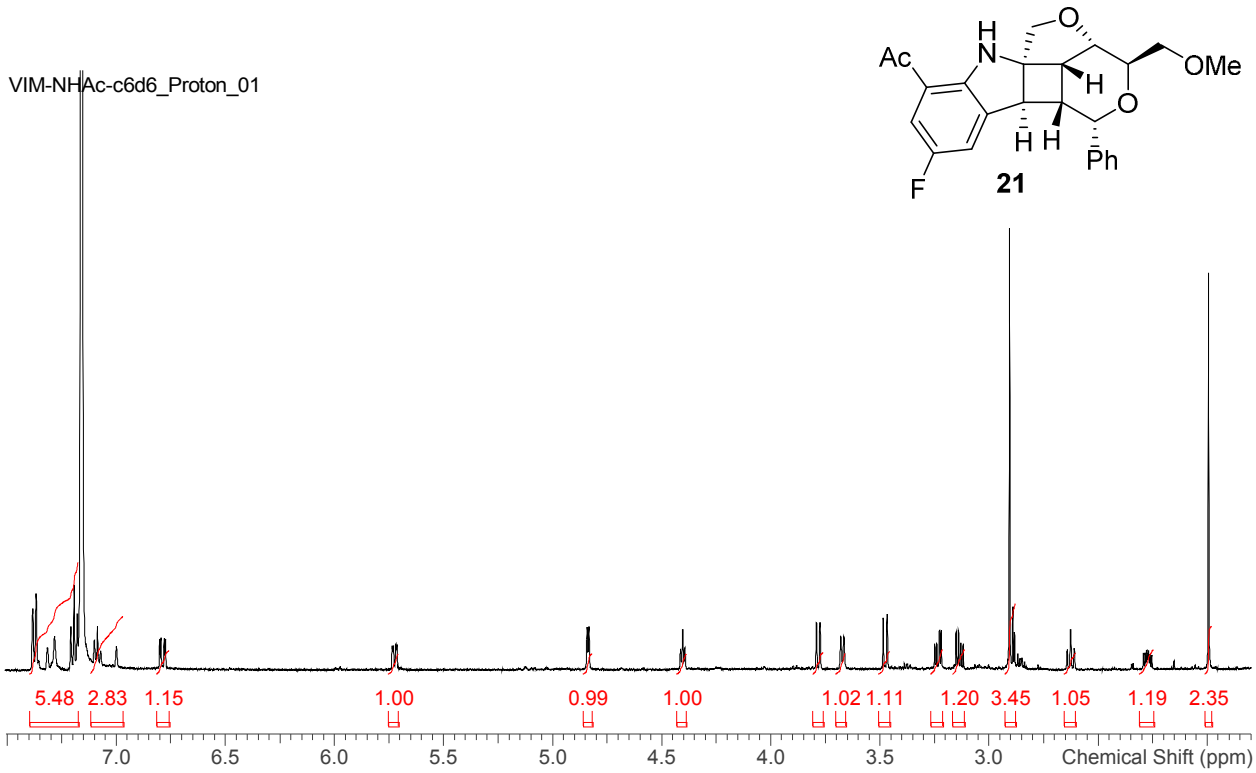


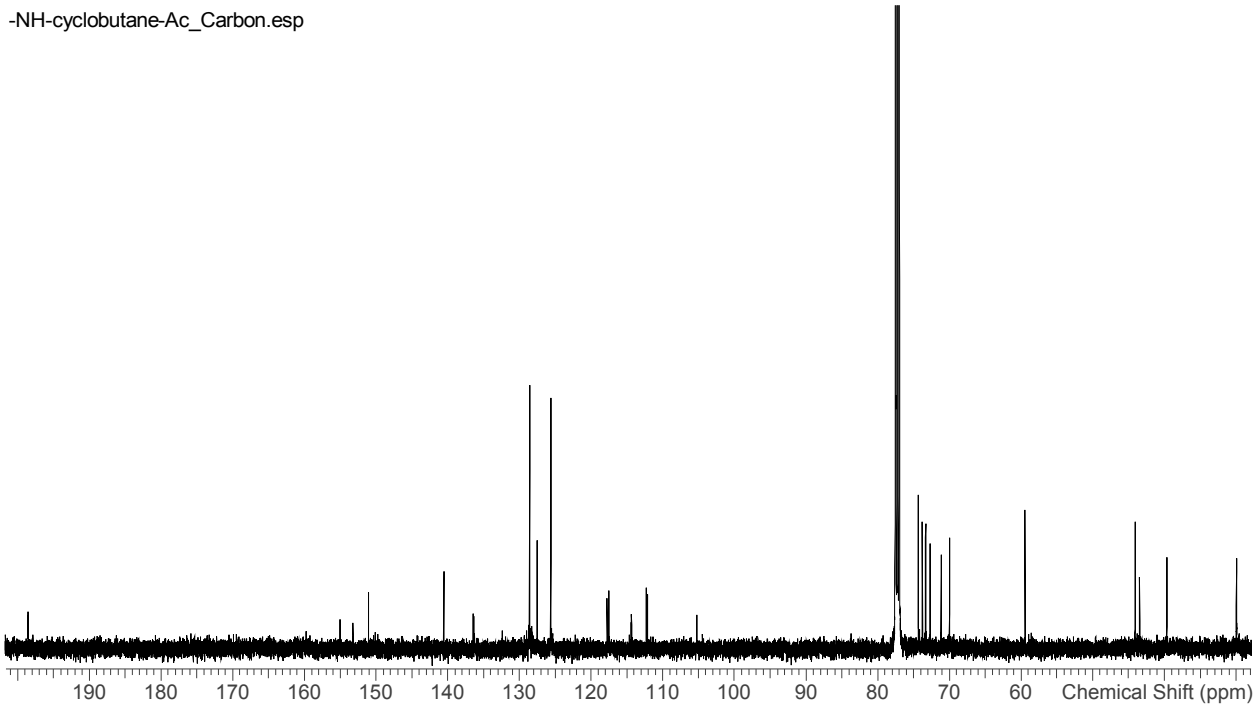
20



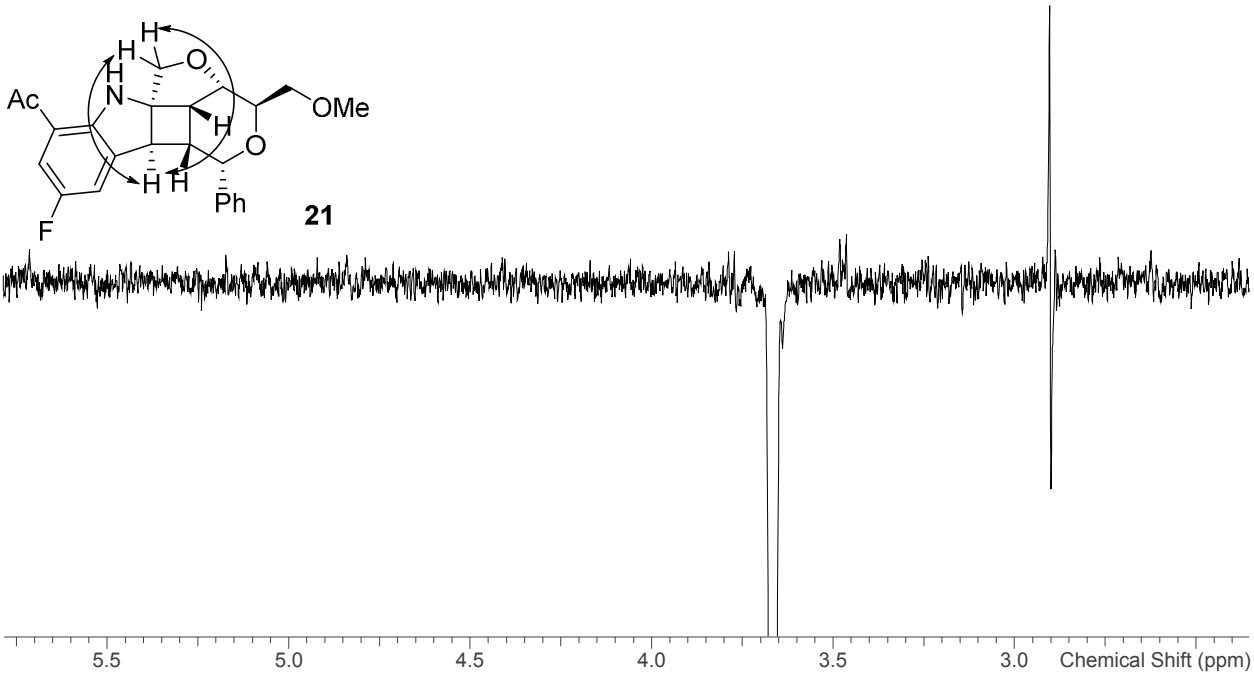
VIM-2-084-Carbon.esp



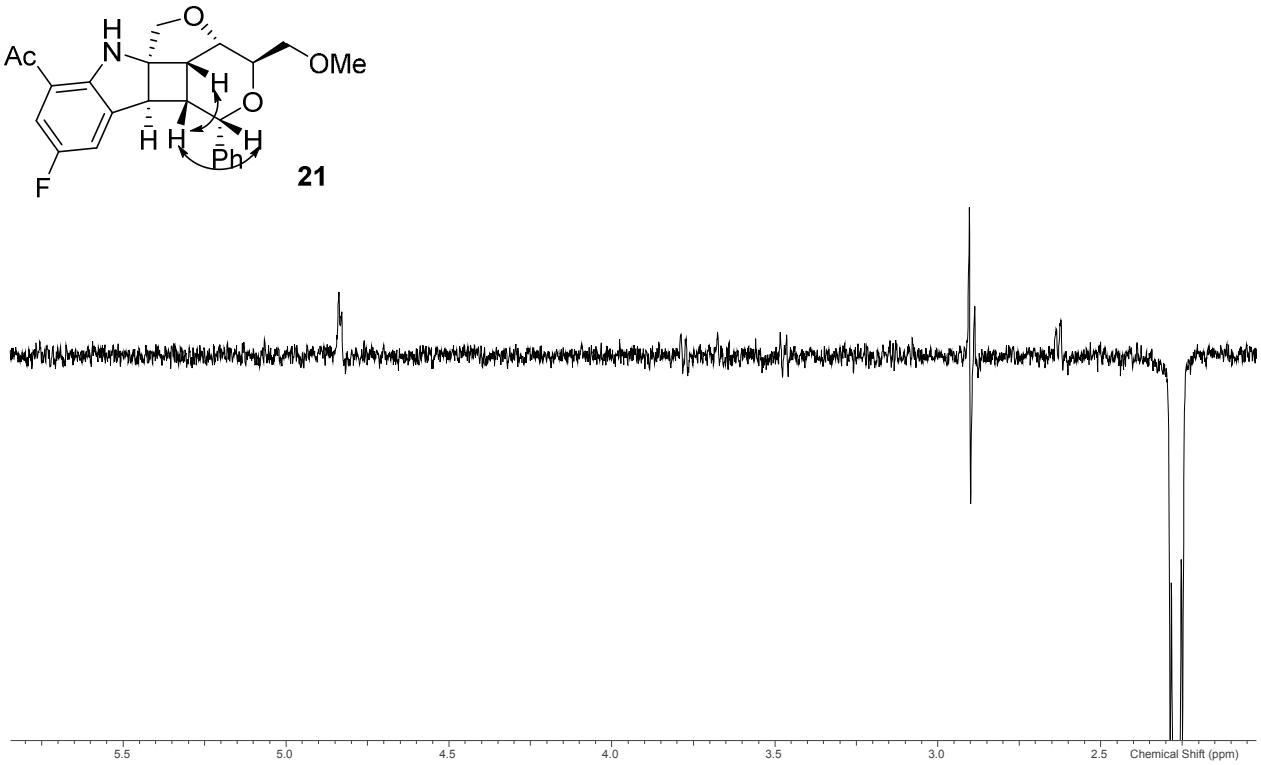

VIM-NHAc-c6d6_Proton_01
Ac
H
N
O
OMe
H
O
H H
Ph
F
21
5.48 2.83 1.15 1.00 0.99 1.00 1.02 1.11 1.20 3.45 1.05 1.19 2.35
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 Chemical Shift (ppm)

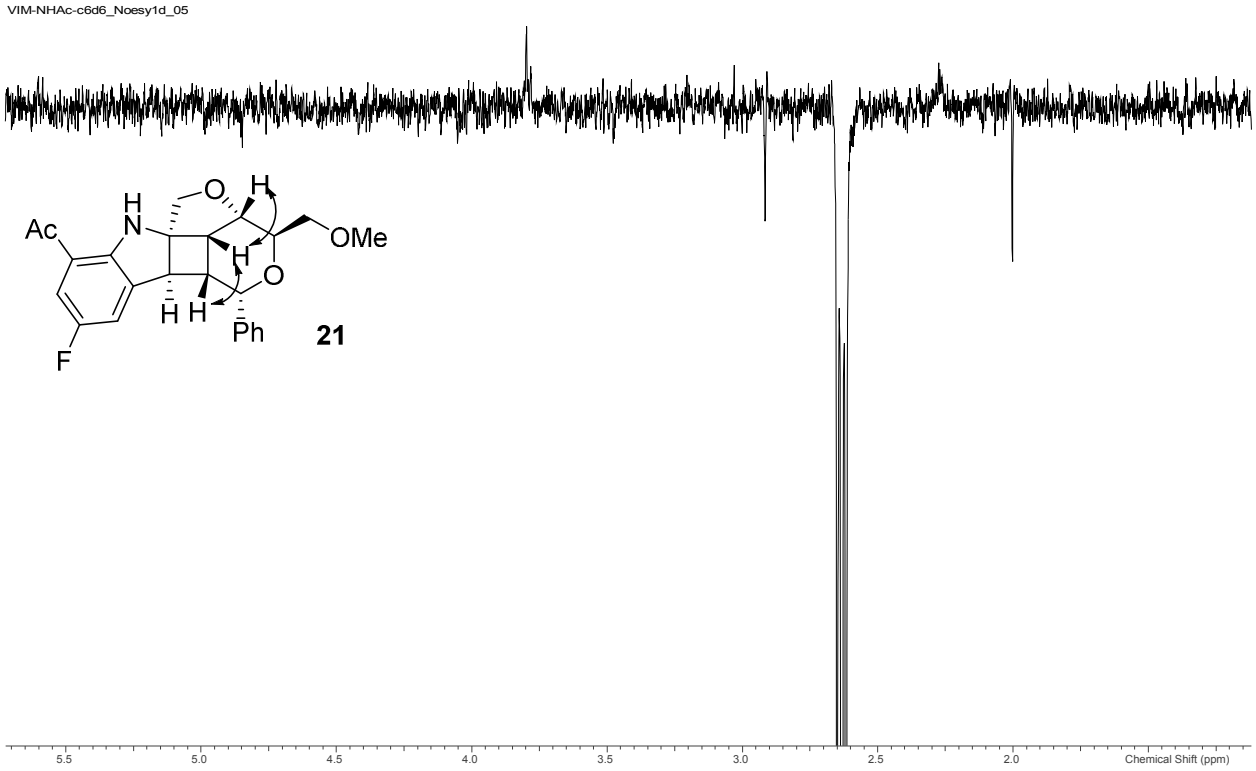

-NH-cyclobutane-Ac_Carbon.esp
190 180 170 160 150 140 130 120 110 100 90 80 70 60 Chemical Shift (ppm)

VIM-NHAc-c6d6_Noesy1d_04



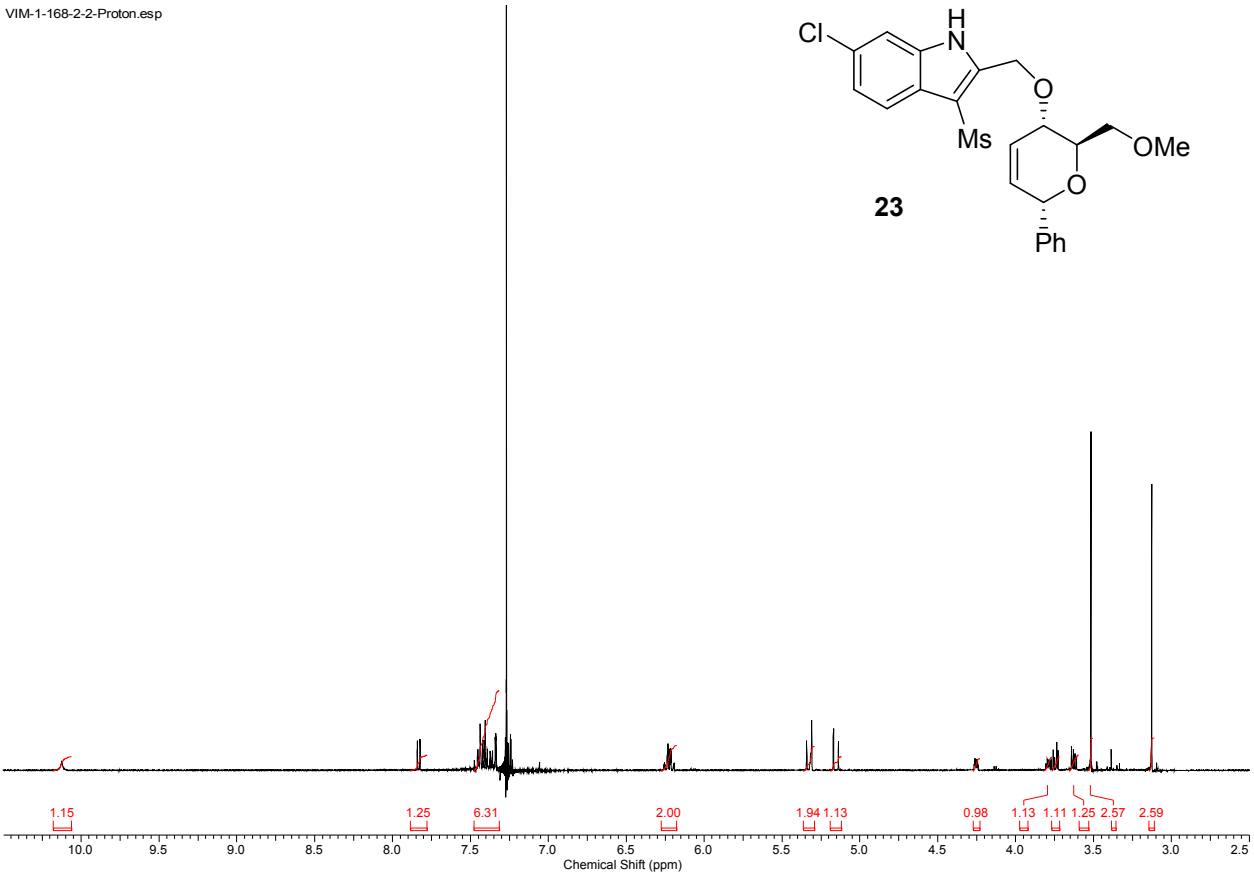
VIM-NHAc-c6d6_Noesy1d_03



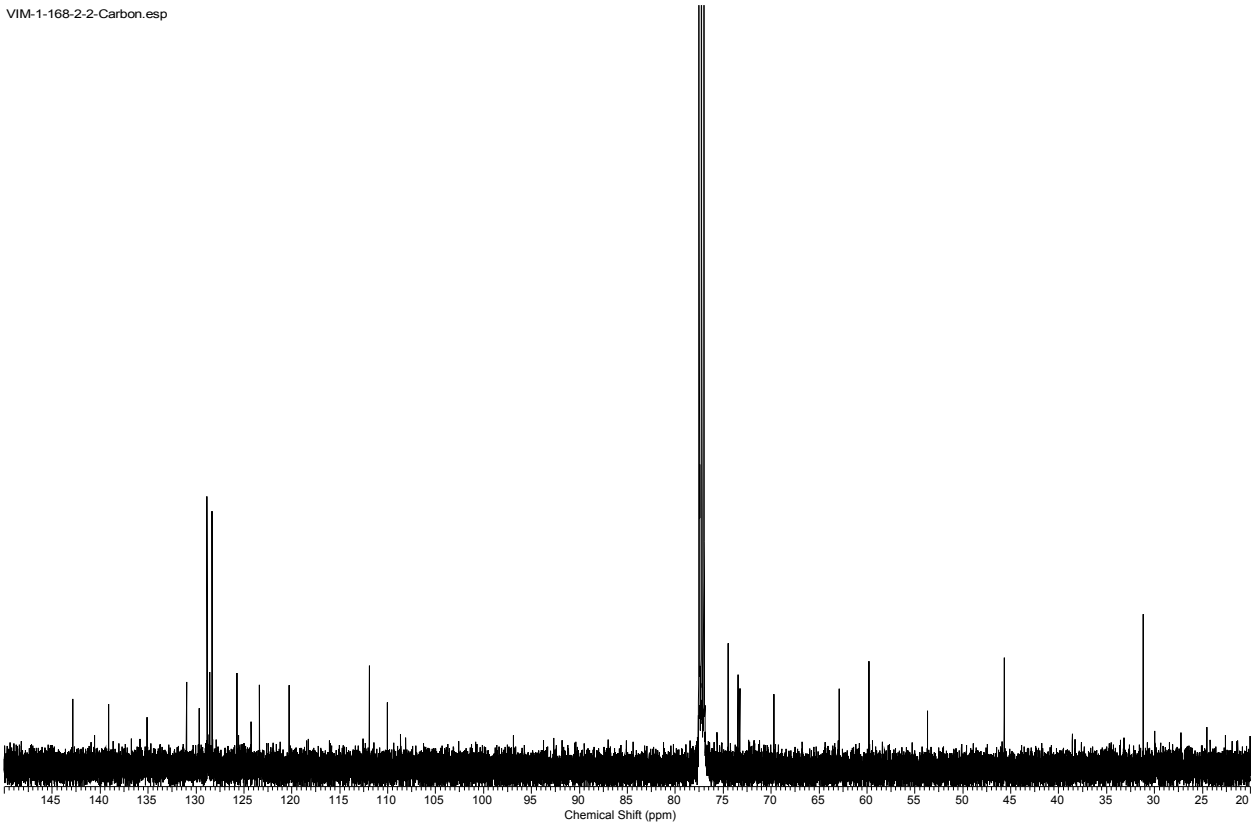

VIM-NHAc-c6d6_Noesy1d_05
Ac
H
N
O
H
OMe
H
O
H H
Ph
F
21
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
Chemical Shift (ppm)

VIM-1-168-2-2-Proton.esp

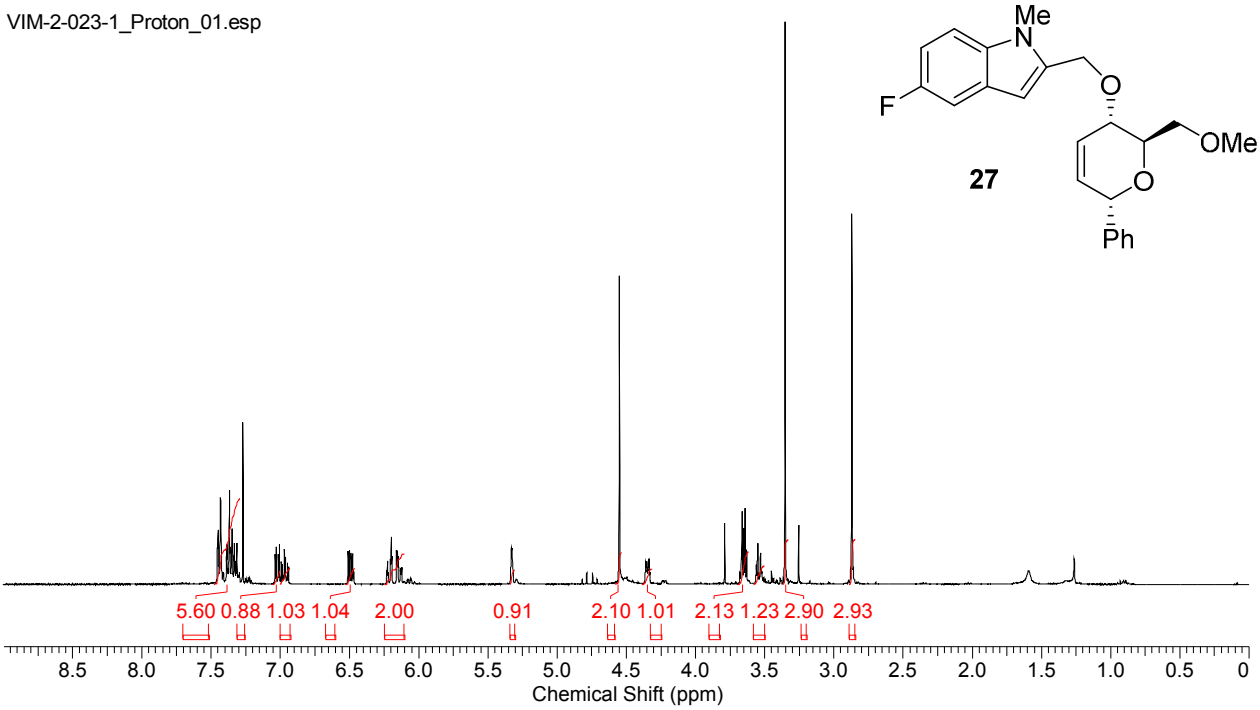
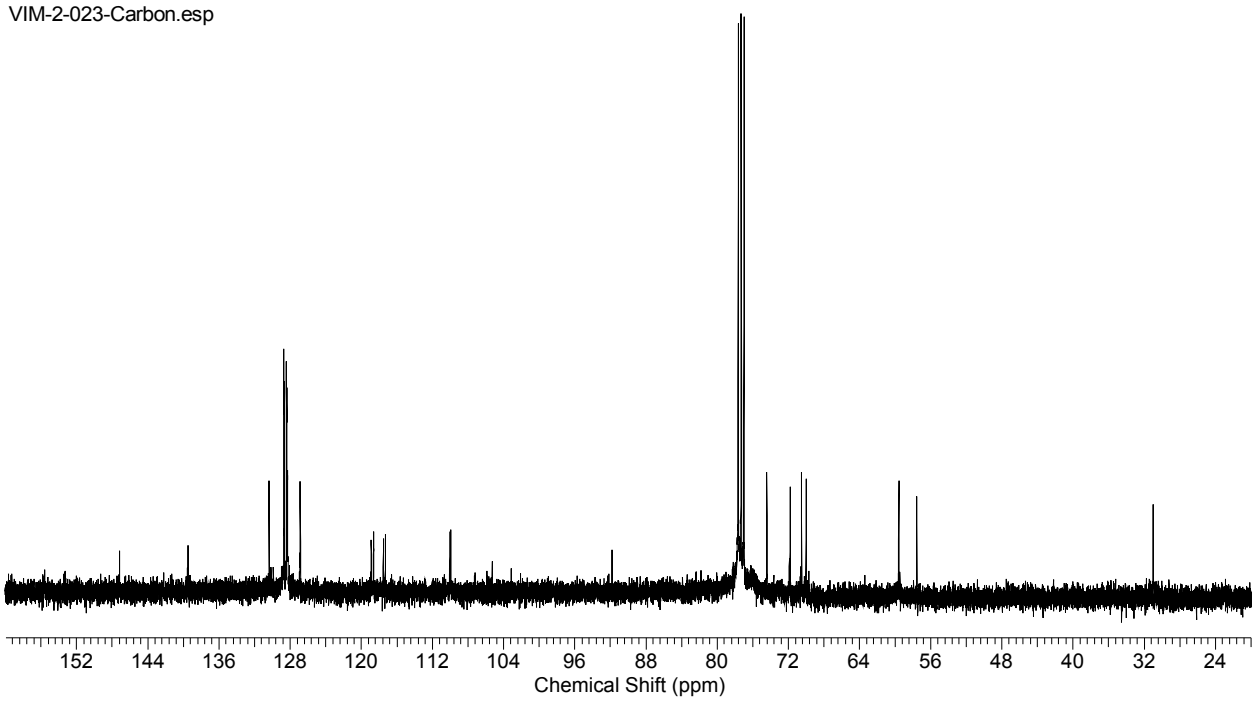
23



VIM-1-168-2-2-Carbon.esp



VIM-2-023-1_Proton_01.esp



VIM-2-023-Carbon.esp