Stereospecific Synthesis of 23-Hydroxyundecylprodiginines and Analogues, and Conversion to Antimalarial Premarineosins via a Rieske Oxygenase Catalyzed Bicyclization

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*and Kevin A. Reynolds**

Supporting Information

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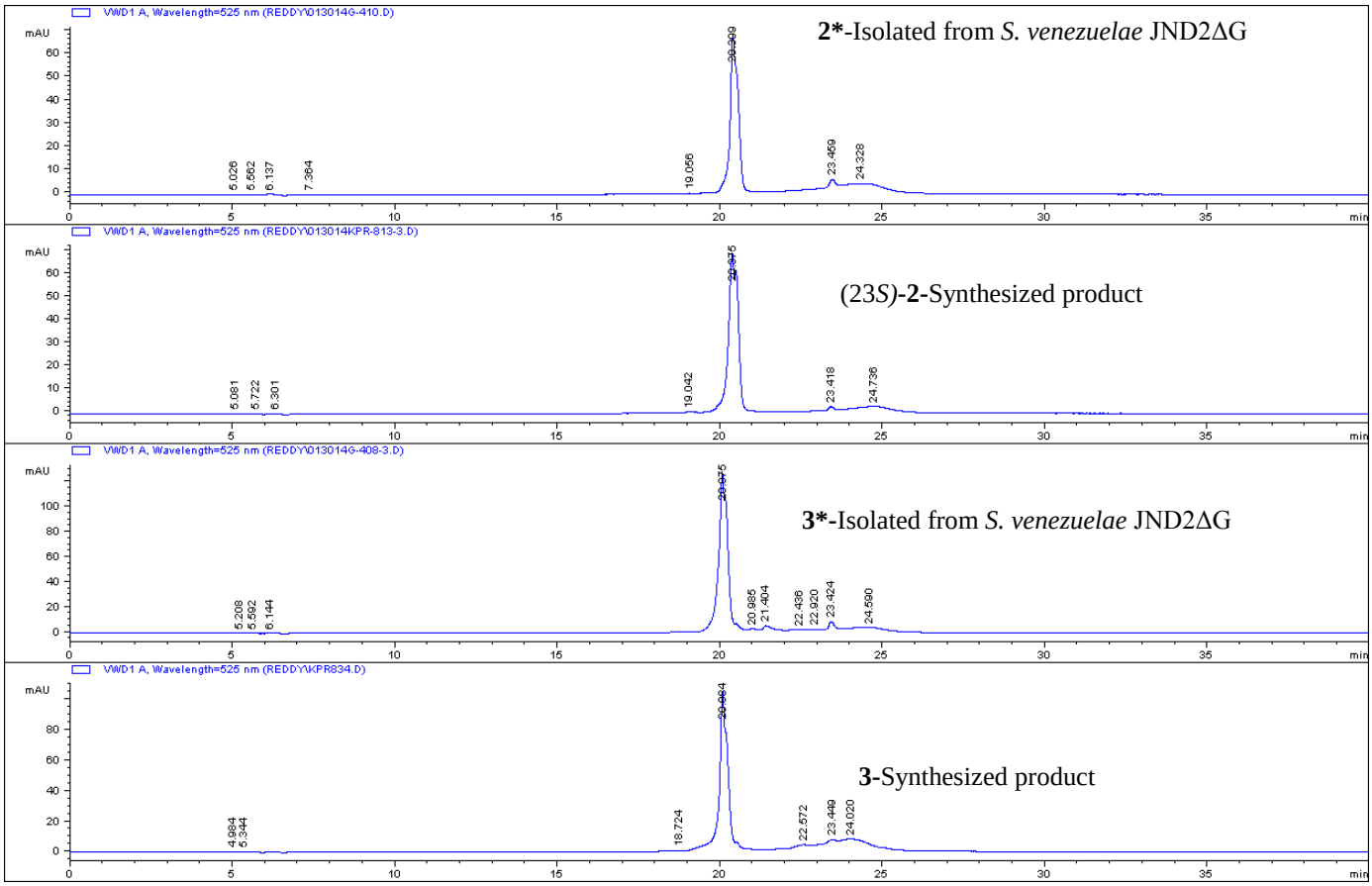


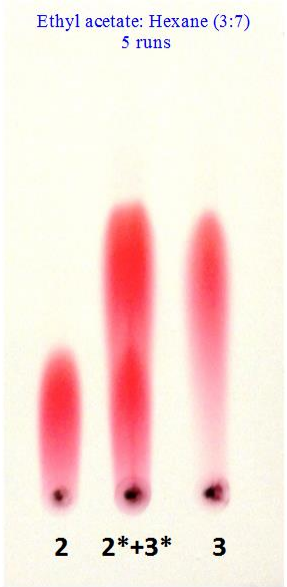


Figure S1. HPLC and TLC comparisons between synthetic [(23*S*)-**2**, and **3**], and natural prodiginines (**2***, and **3***)

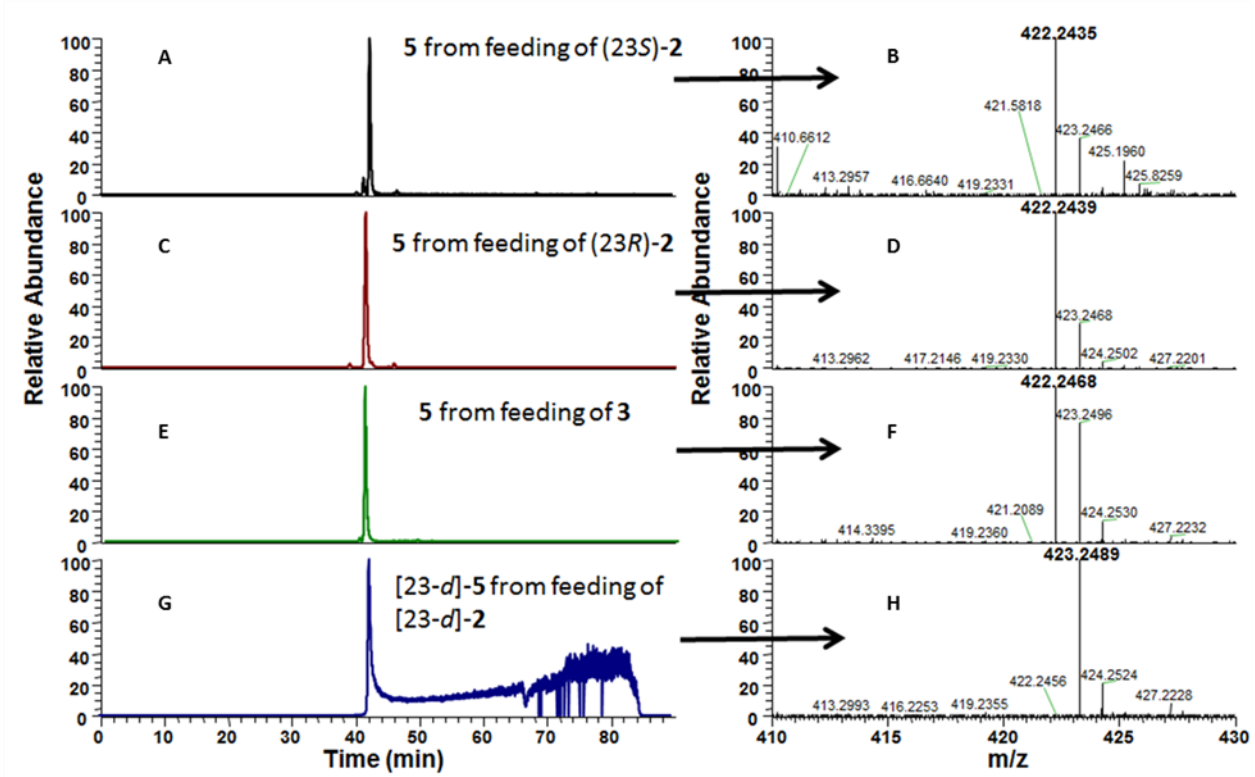


Figure S2. **LC-MS (EIC) profiles of 5 and [23-*d*]-5 from feeding of (23*S*)-2, (23*R*)-2, 3 and [23-*d*]-2 to *S. venezuelae* MarG**. (A) EIC for *m/z* 422.24-422.25, corresponding to $[M + H]^+$ for **5**, from LC-MS analysis of extracts of *S. venezuelae* MarG fed with (23*S*)-**2**. (B) MS spectrometry of **5** from extracts of *S. venezuelae* MarG fed with (23*S*)-**2**. (C) EIC for *m/z* 422.24-422.25, corresponding to $[M + H]^+$ for **5**, from LC-MS analysis of extracts of *S. venezuelae* MarG fed with (23*R*)-**2**. (D) MS spectrometry of **5** from extracts of *S. venezuelae* MarG fed with (23*R*)-**2**. (E) EIC for *m/z* 422.24-422.25, corresponding to $[M + H]^+$ for **5**, from LC-MS analysis of extracts of *S. venezuelae* MarG fed with **3**. (F) MS spectrometry of **5** from extracts of *S. venezuelae* MarG fed with **3**. (G) EIC for *m/z* 423.24-423.25, corresponding to $[M + H]^+$ for [23-*d*]-**5**, from LC-MS analysis of extracts of *S. venezuelae* MarG fed with [23-*d*]-**2**. (H) MS spectrometry of [23-*d*]-**5** from extracts of *S. venezuelae* MarG fed with [23-*d*]-**2**.

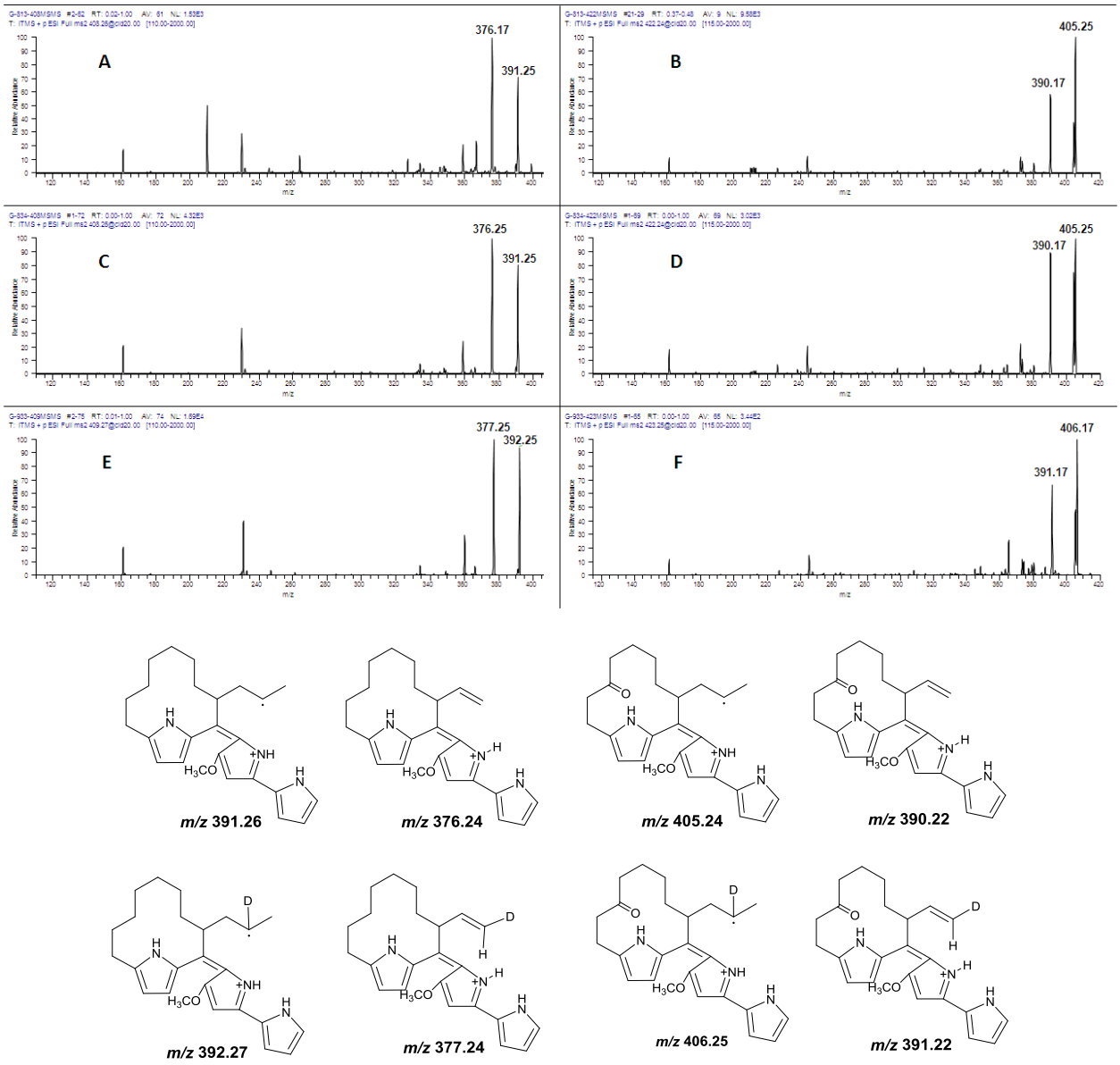


Figure S3. ESI-CID-MS^2 profile of 4, [23-*d*]-4, 5, and [23-*d*]-5 from feeding experiments with *S. venezuelae* MarG: A. The MS/MS profile of **4** from *S. venezuelae* marG fed with (23*S*)-**2**; **B.** The MS/MS profile of **5** from *S. venezuelae* marG fed with (23*S*)-**2**; **C**. The MS/MS profile of **4** from *S. venezuelae* marG fed with **3**; **D**. The MS/MS profile of **5** from *S. venezuelae* marG fed with **3**; **E**. The MS/MS profile of [23-*d*]-**4** from *S. venezuelae* marG fed with [23-*d*]-**2**; **F**. The MS/MS profile of [23-*d*]-**5** from *S. venezuelae* marG fed with [23-*d*]-**2**.

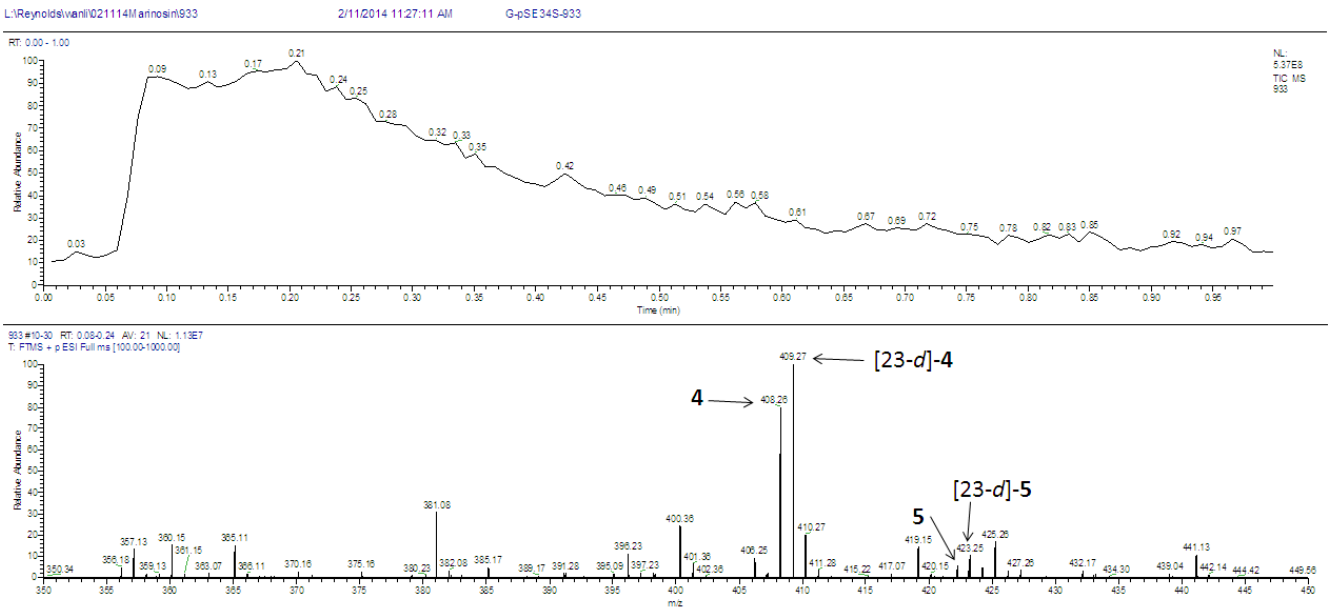


Figure S4. MS profile of [23-*d*]-**4**, and **4** (~1.2:1 ratio), and [23-*d*]-**5**, and **5** from feeding of [23-*d*]-**2** to *S. venezuelae* MarG

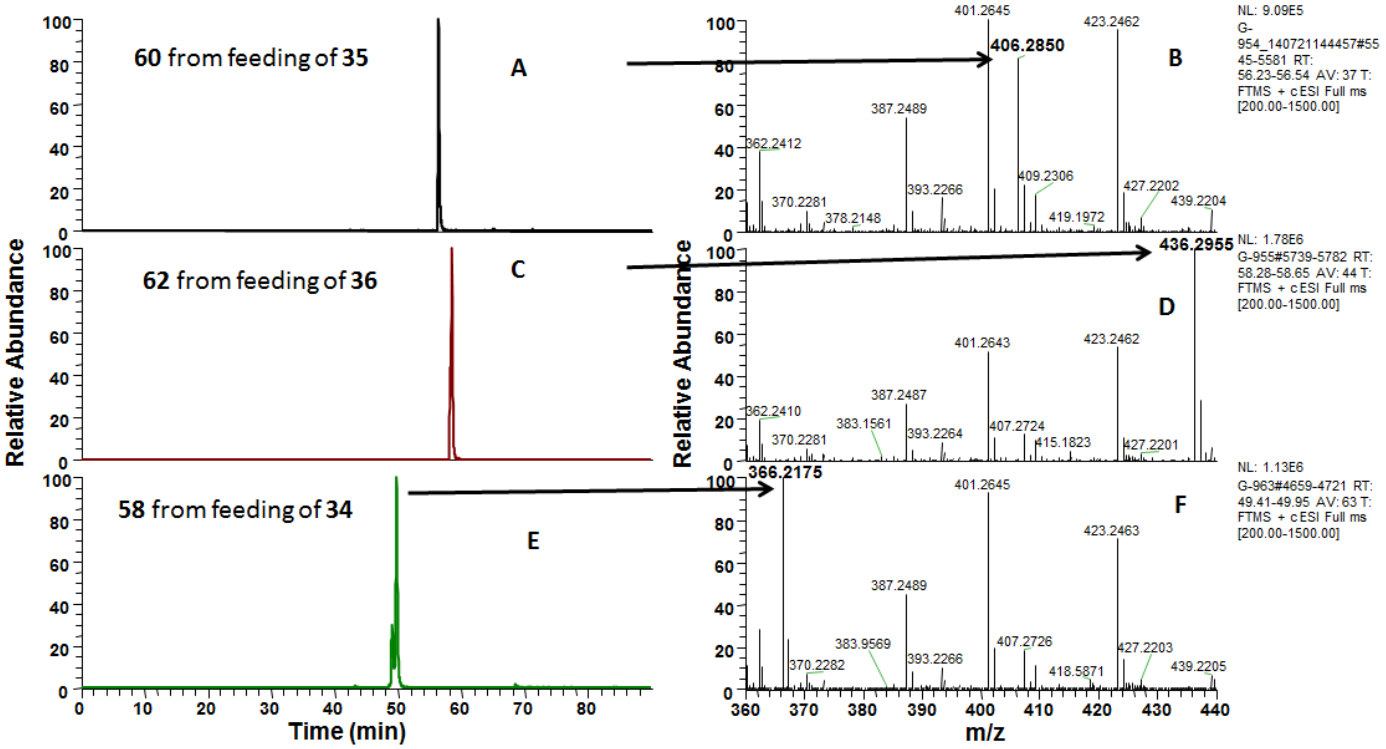


Figure S5. LC-MS (EIC) profiles of **58**, **60**, and **62** from feeding of **34**–**36** to *S. venezuelae* MarG. (A) EIC for *m/z* 406.28-406.29, corresponding to $[M + H]^+$ for **60**, from LC-MS analysis of extracts of *S. venezuelae* MarG fed with **35**. (B) MS spectrometry of **60** from extracts of *S. venezuelae* MarG fed with **35**. (C) EIC for *m/z* 436.29-436.30, corresponding to $[M + H]^+$ for **62**, from LC-MS analysis of extracts of *S. venezuelae* MarG fed with **36**. (D) MS spectrometry of **62** from extracts of *S. venezuelae* MarG fed with **36**. (E) EIC for *m/z* 366.21-366.22, corresponding to $[M + H]^+$ for **58**, from LC-MS analysis of extracts of *S. venezuelae* MarG fed with **34**. (F) MS spectrometry of **58** from extracts of *S. venezuelae* MarG fed with **34**.

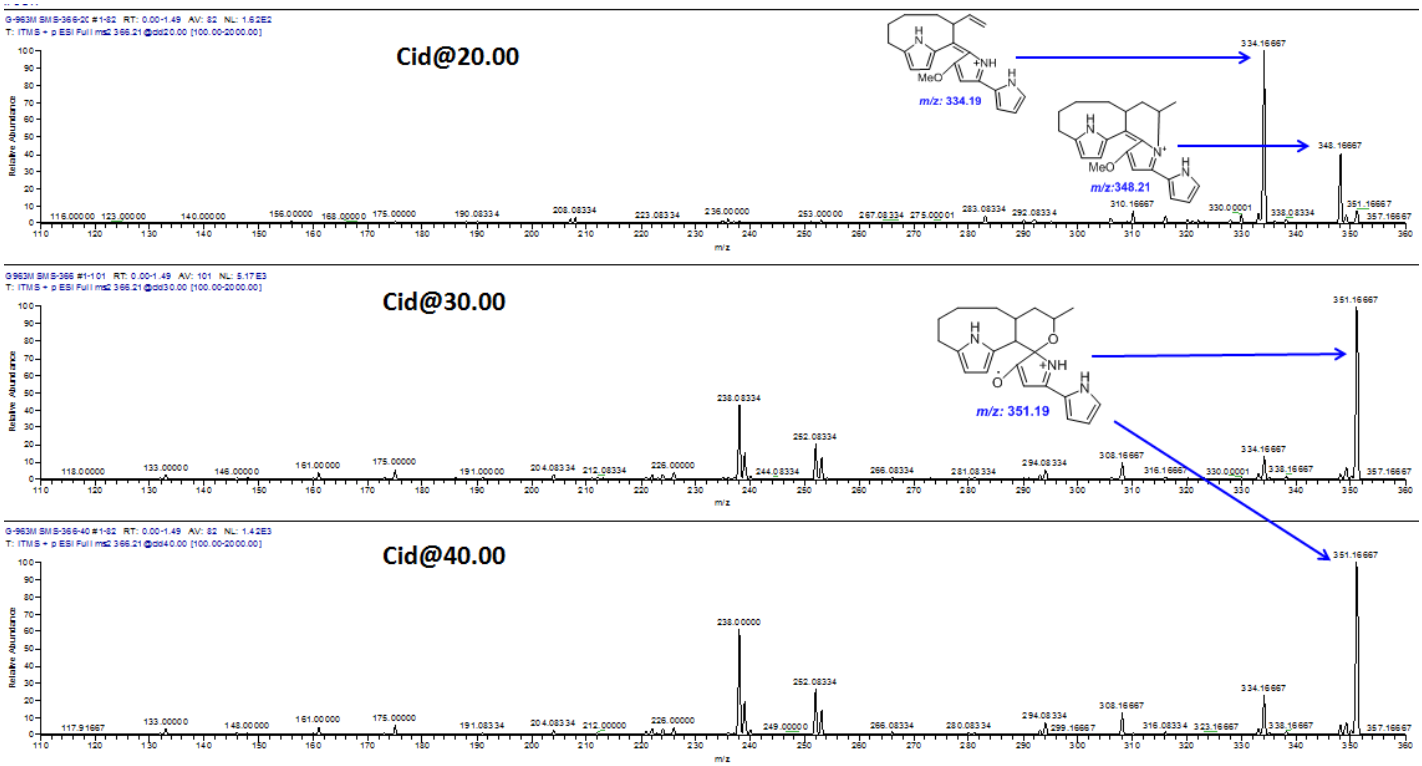


Figure S6. ESI-CID@20, 30, 40-MS^2 profiles of **58** from *S. venezuelae* marG fed with **34**.

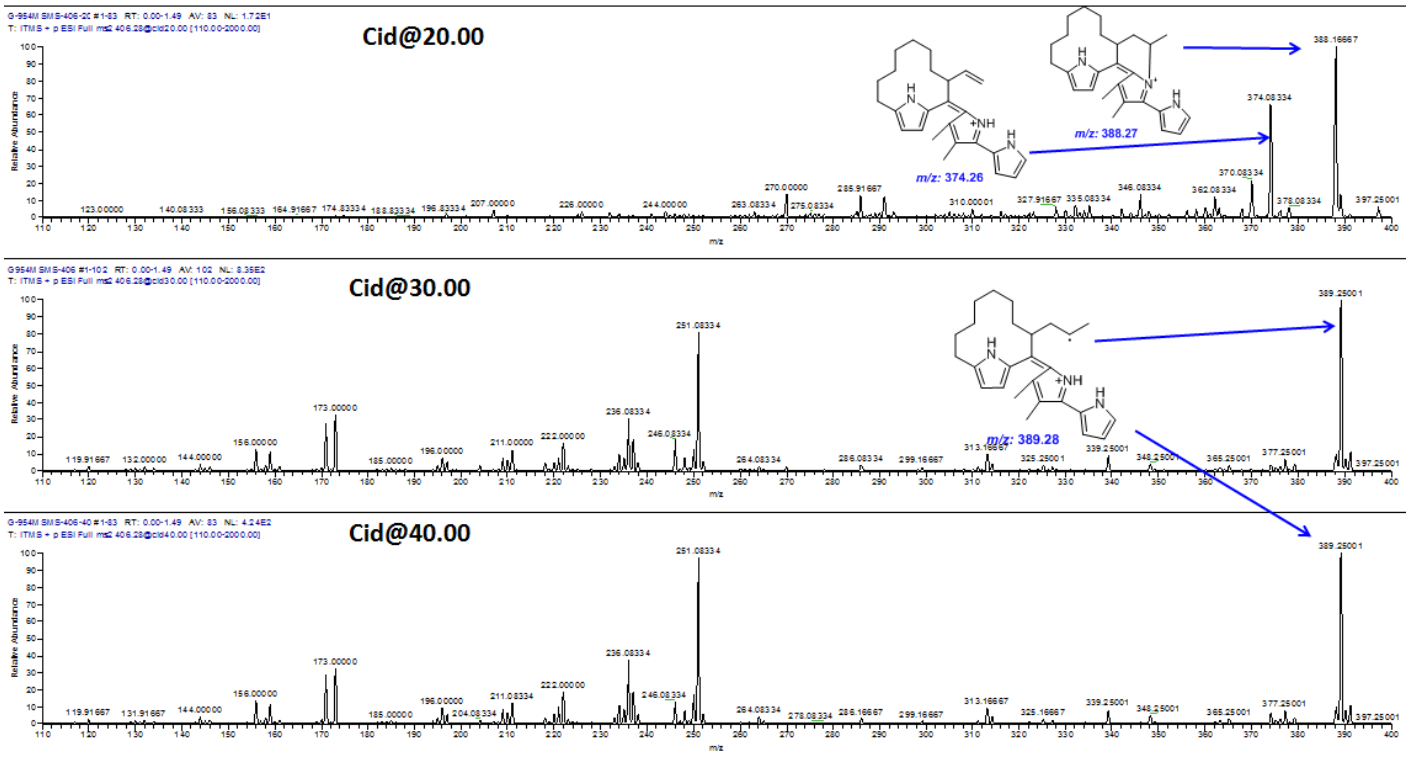


Figure S7. ESI-CID@20, 30, 40-MS^2 profiles of **60** from *S. venezuelae* marG fed with **35**.

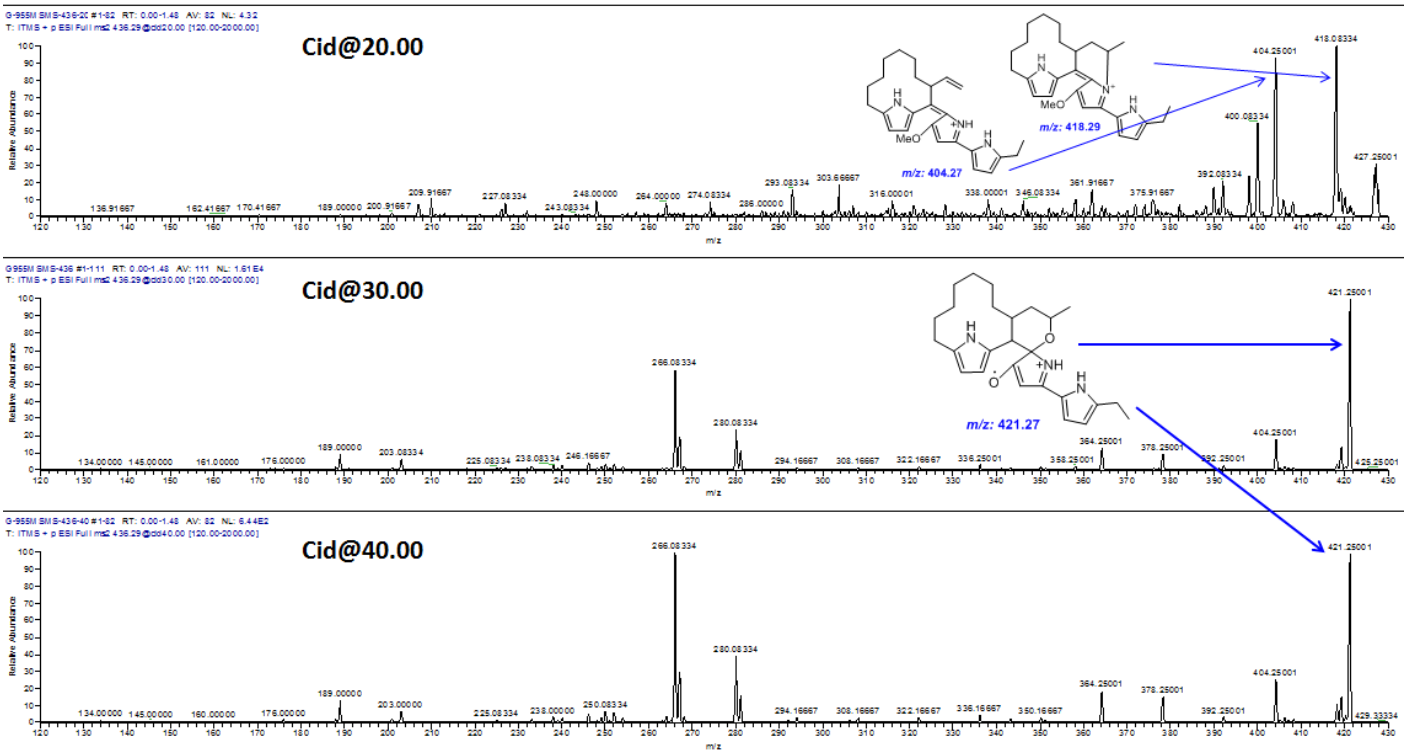


Figure S8. ESI-CID@20, 30, 40-MS^2 profiles of **62** from *S. venezuelae* marG fed with **36**.

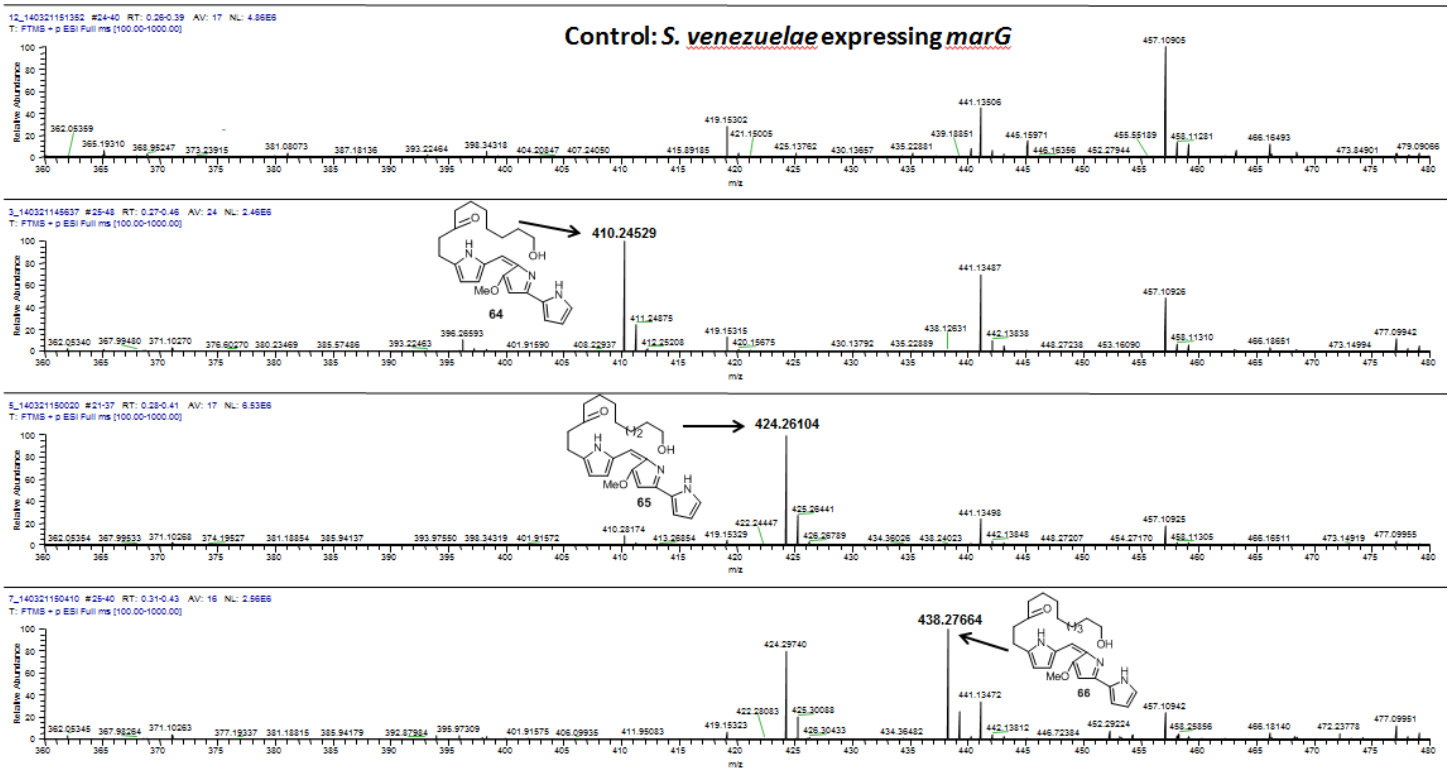


Figure S9. MS profile of **64**–**66** from feeding of **39**–**41** to *S. venezuelae* MarG

Table S1. Strains, plasmids and cosmid used in this study

Strains	Relevant genotype/comments	Source/ Reference
Escherichia coli One Shot TOP10	*F¯ mcrA Δ(mrr-hsdRMS-mcrBC) ϕ80lacZΔM15 ΔlacX74 recA1araD139 Δ(araleu) 7697 galU galK rpsL (StrR) endA1 nupG*	Invitrogen
E. coli ET12567(pUZ8002)	*dam dcm hsdS,* pUZ8002	1
Streptomyces venezuelae ATCC 15439	Wild-type pikromycin, methymycin, and neomethymycin producer	2
S. venezuelae MarG	*S. venezuelae* host the *marG* gene under the control of *ermE** promoter	This study
Plasmids and cosmid		
pCR8-GW-TOPO	High copy number PCR cloning vector containing T7 and SP6 RNA polymerase promoters flanking a multiple cloning region within the alpha-peptide coding region of the enzyme beta-galactosidase; *bla*.	Invitrogen
pET15b	T7 promoter, RBS, N terminal 6x His Tag, *bla*, pBR322 origin	Novagene
pSE34	pWHM3 with *ermE** promoter, *bla*, *tsr*	Pfizer Inc.
pIJ778	pBluescript KS (+) containing the spectinomycin/streptomycin resistance gene *aadA* and the *oriT* of plasmid RP4, flanked by FRT sites	3
pMarG-topo	1.4 kbp DNA fragment containing *marG* gene in pCR8-GW-TOPO	This study
pMarG-15b	pET15b with 1.4 kbp NdeI-BamHI *marG* ORF	This study
pMarG-34	pSE34 with 1.4 kbp XbaI-HindIII *marG* ORF along with RBS	This study
pMarG-34S	*bla* in pMarG-34 replaced with *aadA-oriT cassette*	This study
8A7	A SuperCos1 cosmid carrying the mar gene cluster together with 6 kbp of primary metabolic genes	4

Table S2. Primers used in this study

Primer	Sequence
marG-15bF	5′-**CATATG**CTCGGCGGGAAACTCGAAAG-3′
marG-15bR	5′-**GGATCC**TCAGGACCGCGCCGCCGCGC-3′
Amp-SpF	5′- *TGATAAATGCTTCAATAATATTGAAAAAGGAAGAGTATG*ATTCCGGGGATCCGTCGACC-3′
Amp-SpR	5′- *AATCTAAAGTATATATGAGTAAACTTGGTCTGACAGTTA*TGTAGGCTGGAGCTGCTTC-3′

Table S3. HPLC gradient used for synthetic [(23*S*)-**2** and **3**], and natural prodiginines (**2*** and **3***)

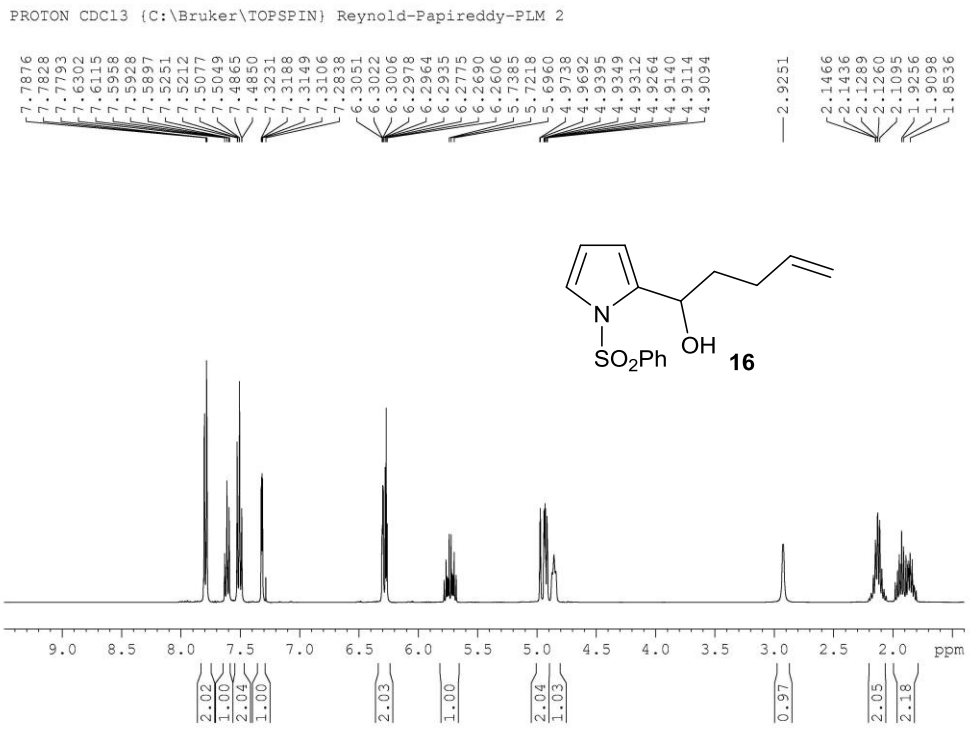
Time (min)	Flow rate (ml/min)	% A[a]	% B[b]
0	0.3	100	0
10	0.3	25	75
15	0.3	0	100
20	0.3	15	85
25	0.3	25	75
40	0.3	100	0

[a]Buffer A: water/acetonitrile/methanol/TFA (50:10:40:0.1)
[b]Buffer B: 100% methanol/0.1% TFA

Table S4. LC-MS gradient used for analysis of *S. venezuelae* MarG fed with synthesized hydroxyundecylprodiginines

Time (min)	Flow rate (mL/min)	%Water[a]	%Methanol[a]
0	0.25	90	10
5	0.25	90	10
70	0.25	0	100
80	0.25	0	100
81	0.25	90	10
90	0.25	90	10

[a] Contained 0.05% HCOOH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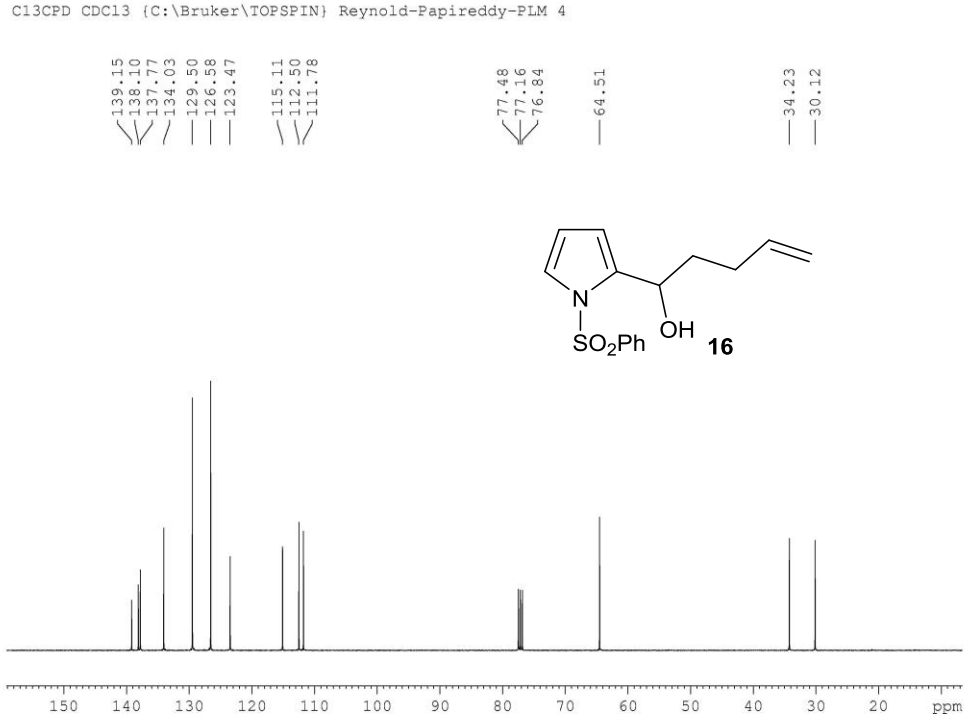
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111.78
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64.51
34.23
30.12
N
SO2Ph
OH
16
150
140
130
120
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ppm

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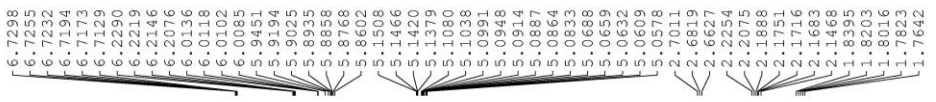

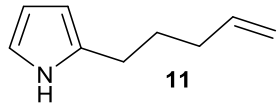

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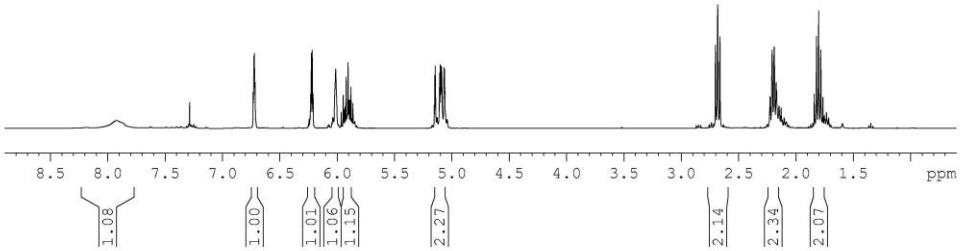

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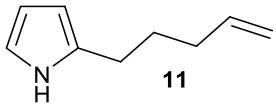

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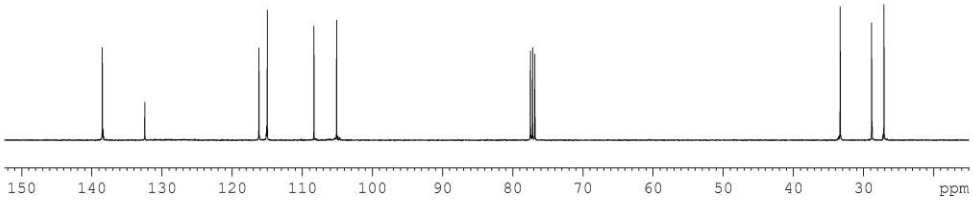

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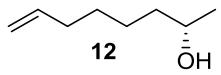

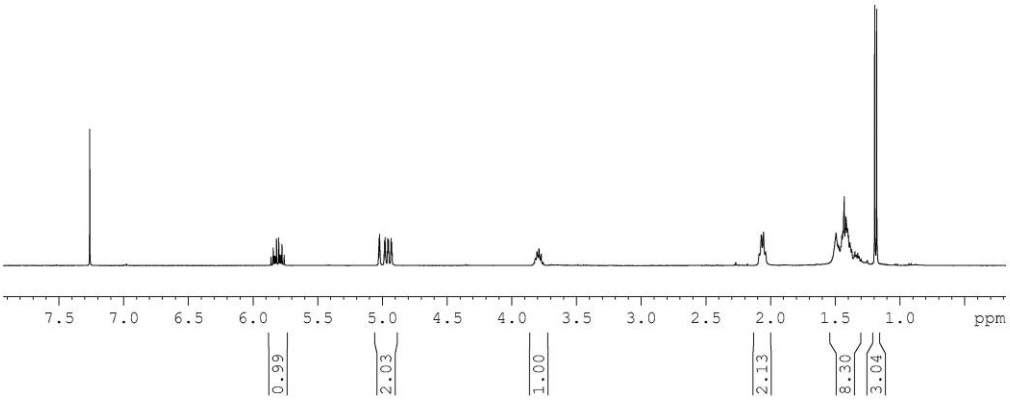

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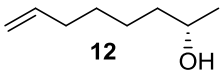

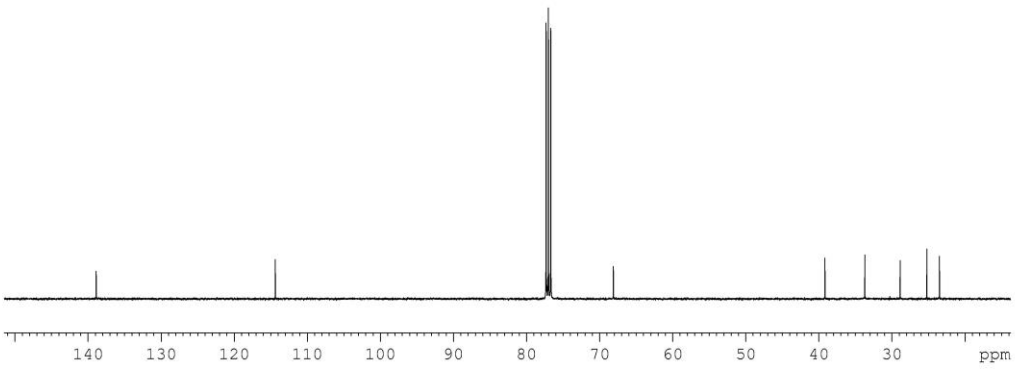

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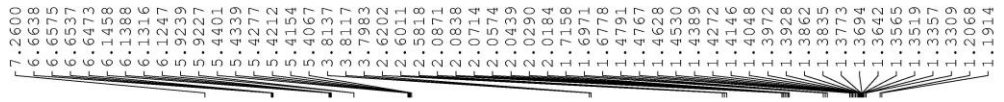

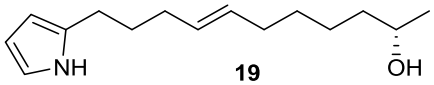

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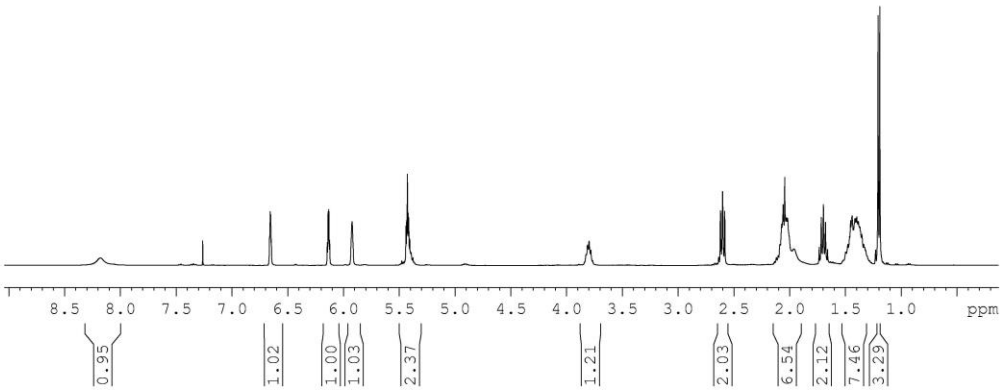

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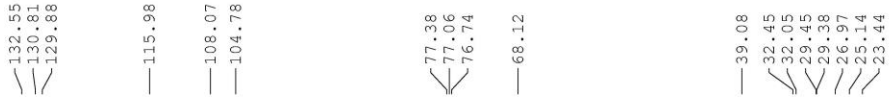

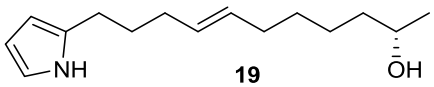

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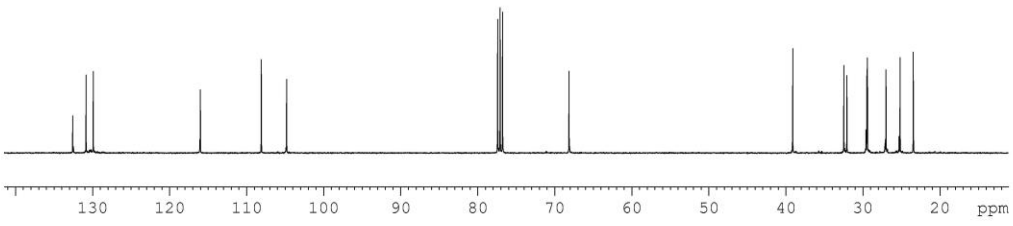

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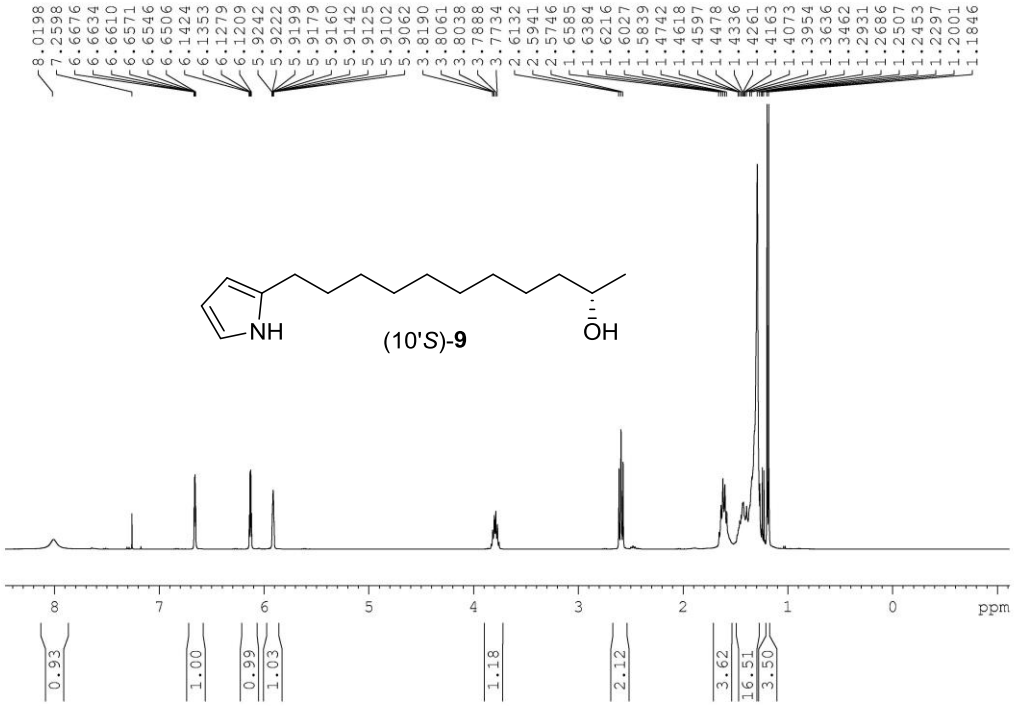

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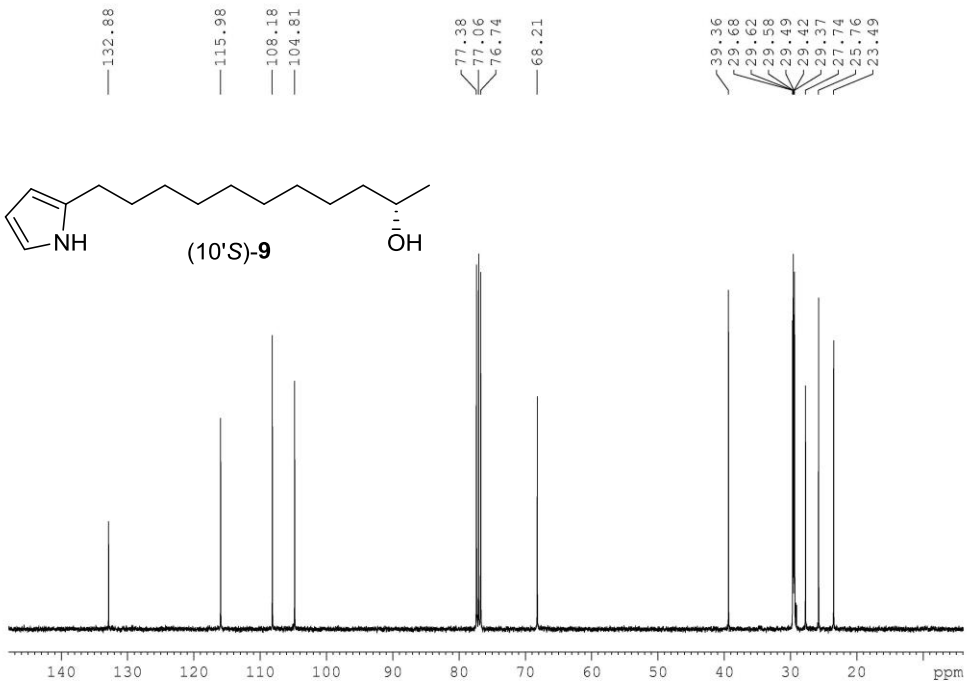

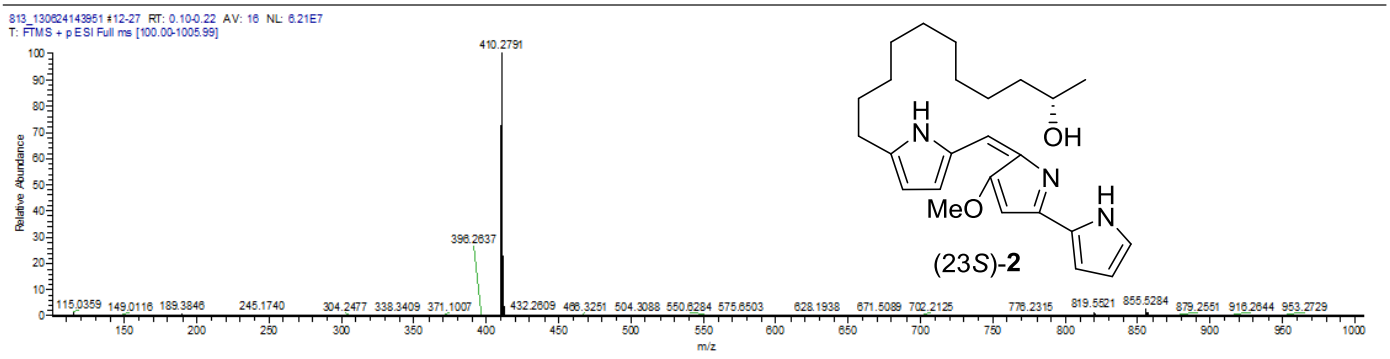
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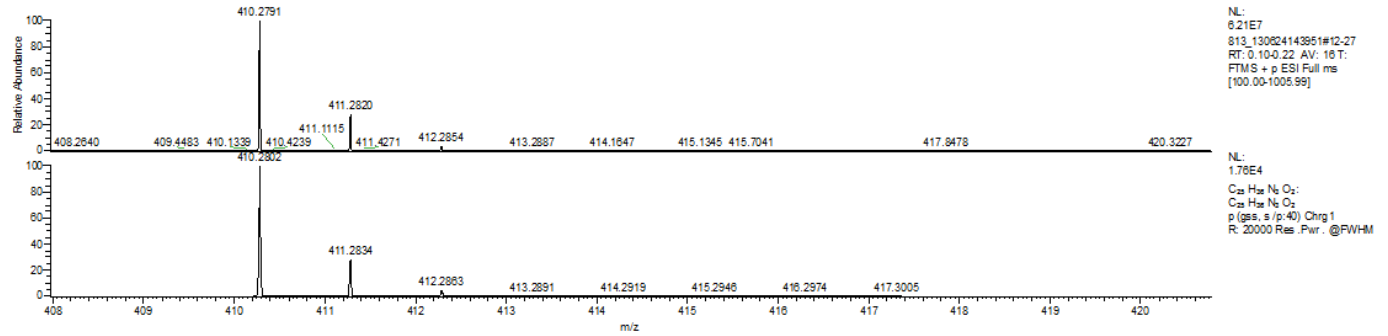
396.2637
Relative Abundance
m/z
(23S)-2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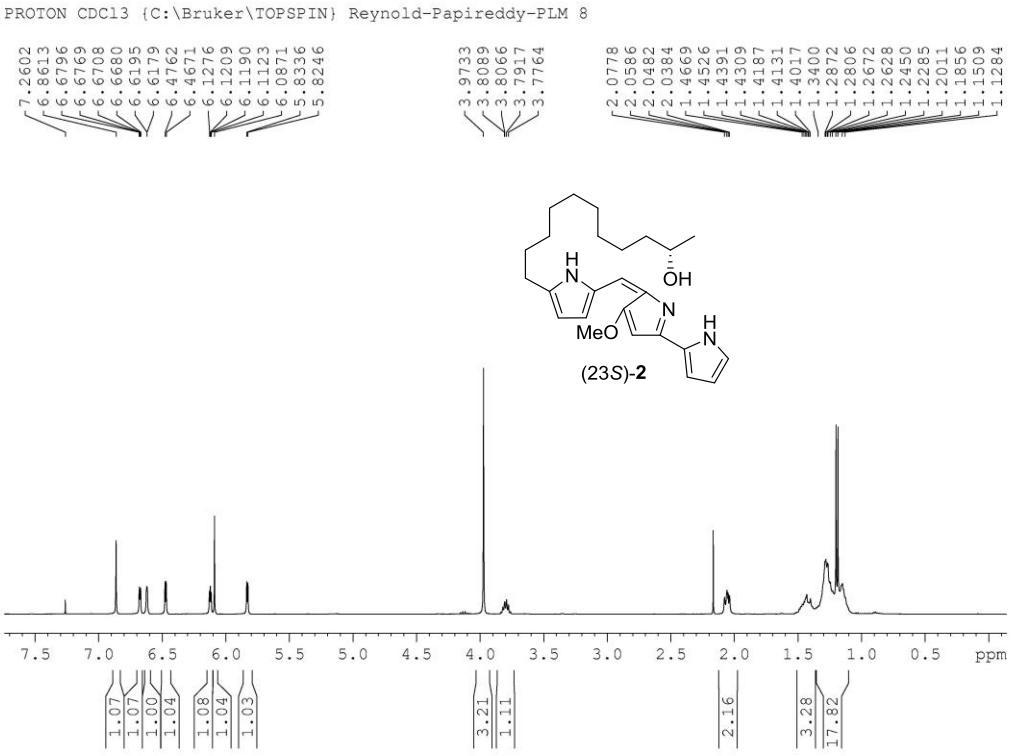
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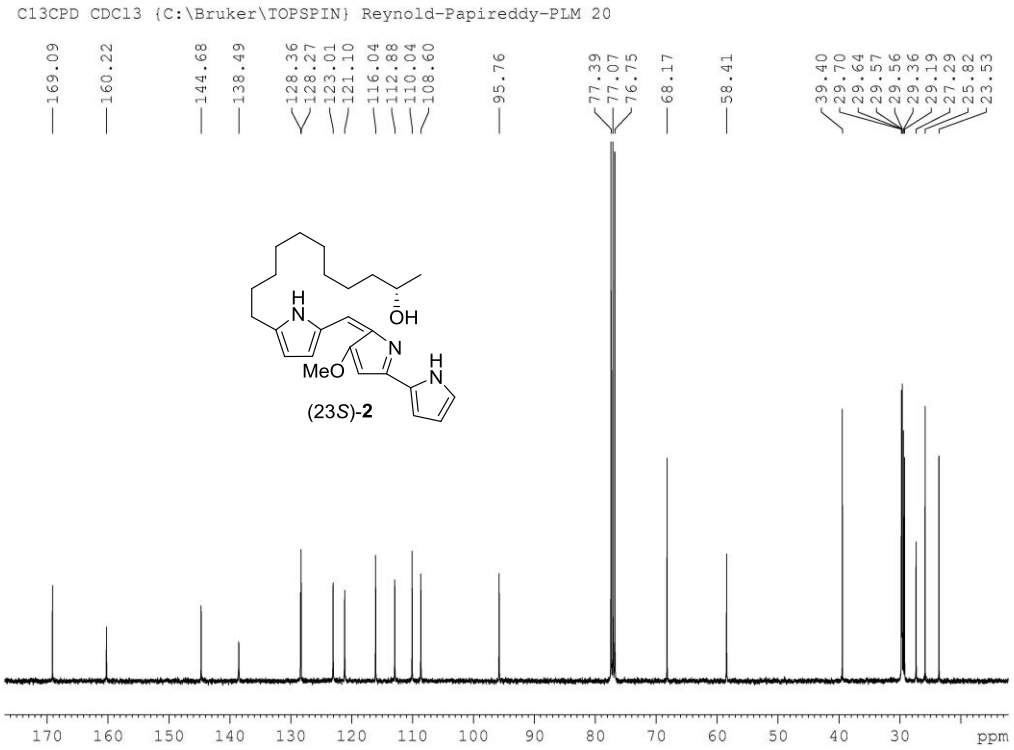
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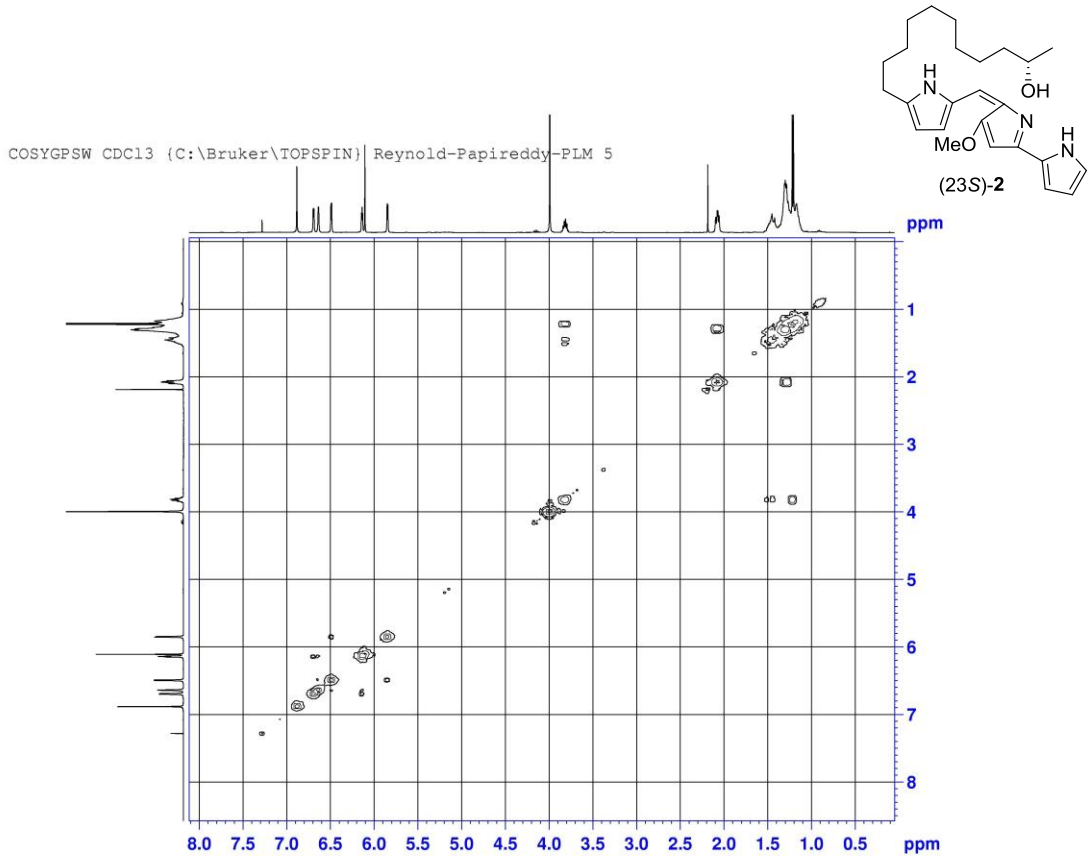
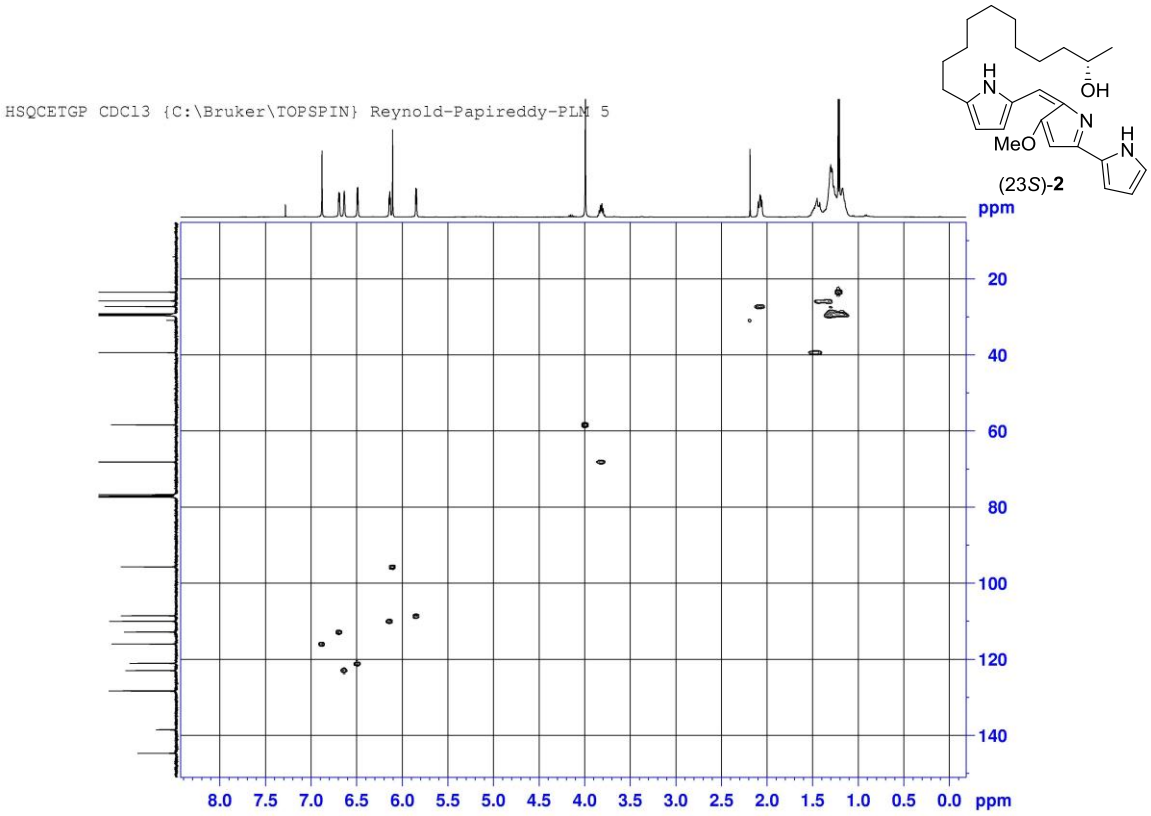
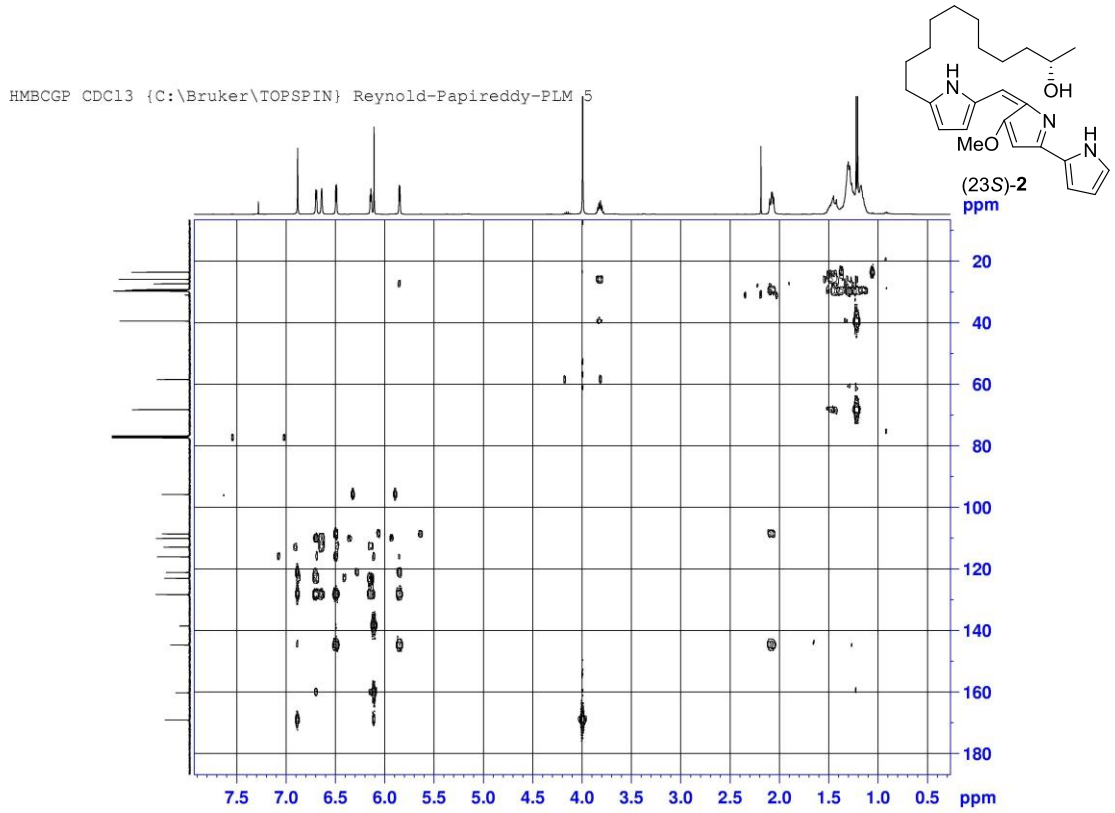
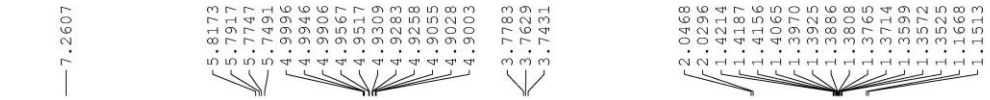
29.57
29.56
29.36
29.19
27.29
25.82
23.53
H
N
OH
N
MeO
H
N
(23S)-2
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

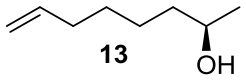

COSYGPSW CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5
H
N
OH
N
MeO
H
N
(23S)-2
ppm
1
2
3
4
5
6
7
8
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

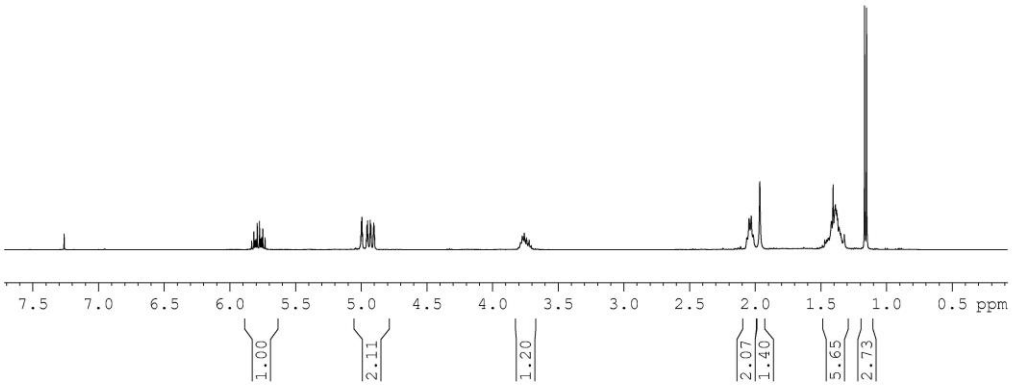

HSQCETGP CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5
H
N
OH
N
MeO
H
N
(23S)-2
ppm
20
40
60
80
100
120
140
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm


HMBCGP CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5
H
N
OH
N
MeO
H
N
(23S)-2
ppm
20
40
60
80
100
120
140
160
180
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 ppm

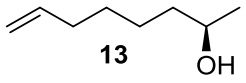
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 10

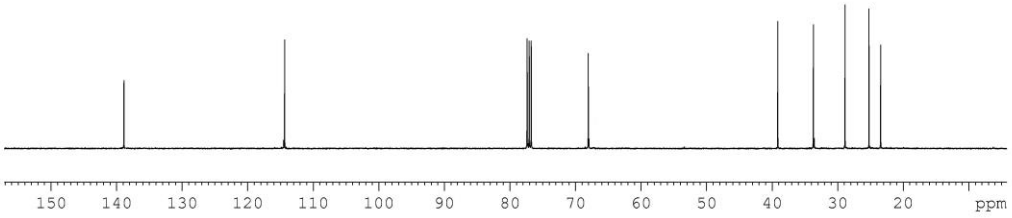


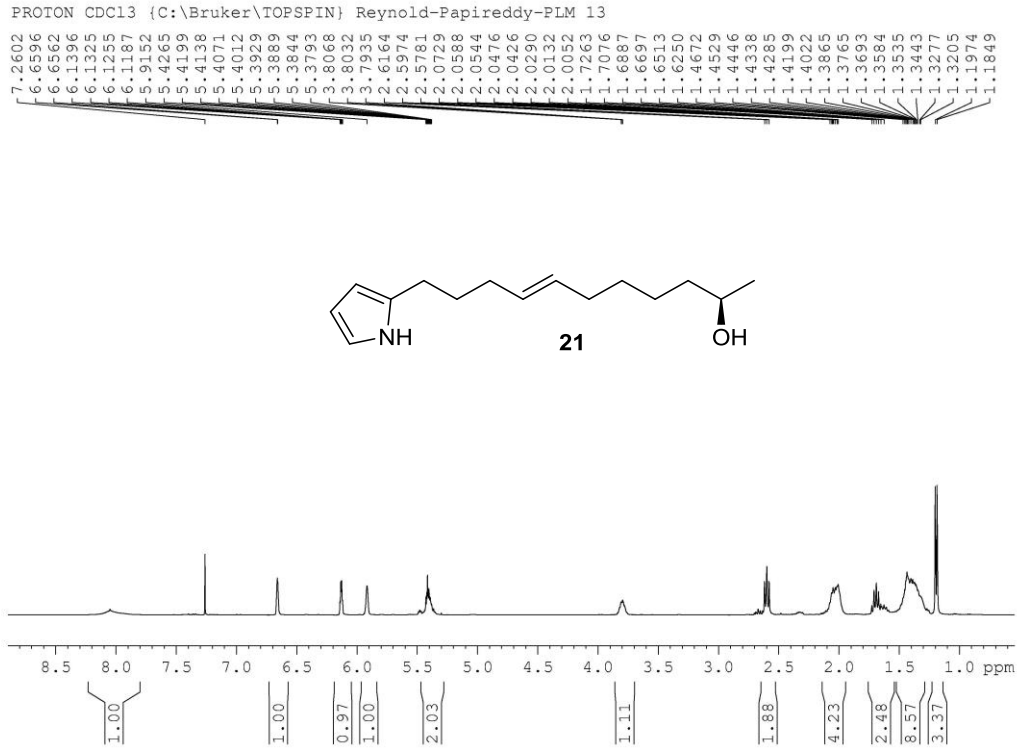


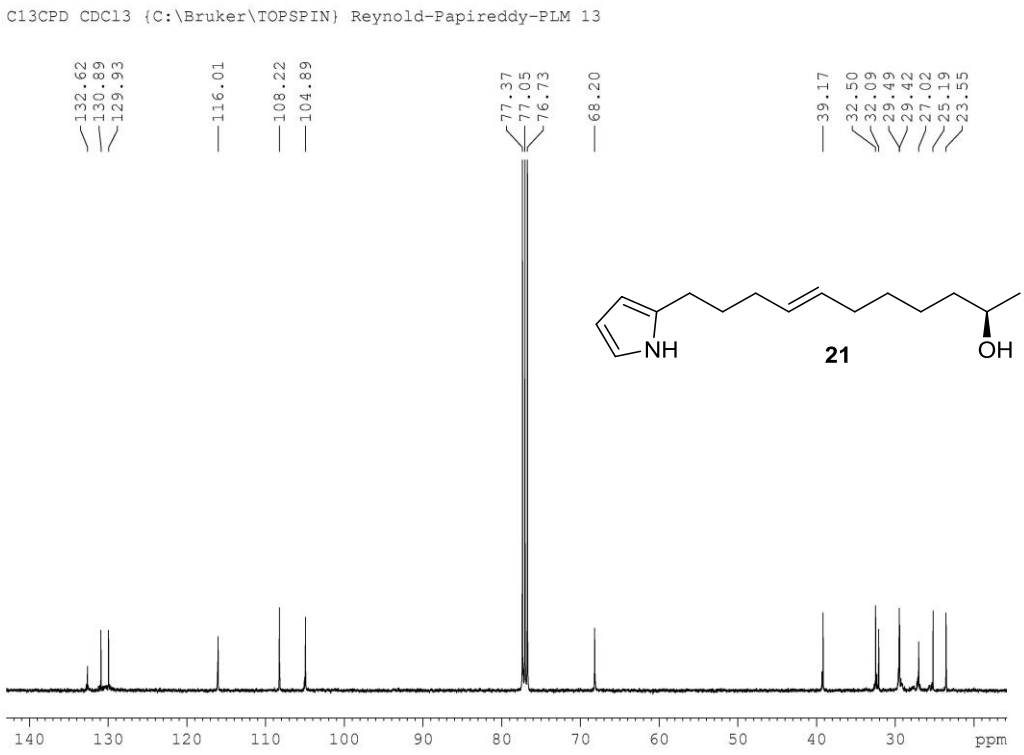


C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 10

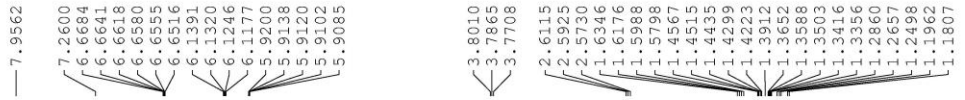


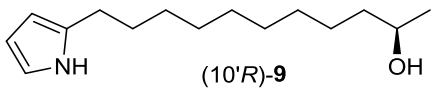



PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 13
7.2602
6.6596
6.6562
6.1396
6.1325
6.1255
6.1187
5.9152
5.4265
5.4199
5.4138
5.4071
5.4012
5.3929
5.3889
5.3844
5.3793
3.8068
3.8032
3.7935
2.6164
2.5974
2.5781
2.0729
2.0588
2.0544
2.0476
2.0426
2.0290
2.0132
2.0052
1.7263
1.7076
1.6887
1.6697
1.6513
1.6250
1.4672
1.4529
1.4446
1.4338
1.4285
1.4199
1.4022
1.3865
1.3765
1.3693
1.3584
1.3535
1.3443
1.3277
1.3205
1.1974
1.1849
NH
21
OH
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 ppm
1.00
1.00
0.97
1.00
2.03
1.11
1.88
4.23
2.48
8.57
3.37

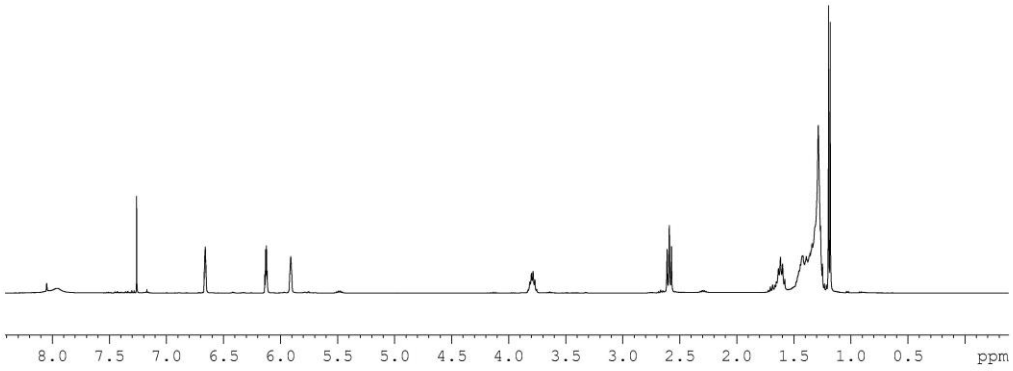

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 13
132.62
130.89
129.93
116.01
108.22
104.89
77.37
77.05
76.73
68.20
39.17
32.50
32.09
29.49
29.42
27.02
25.19
23.55
NH
21
OH
140
130
120
110
100
90
80
70
60
50
40
30
ppm

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 6

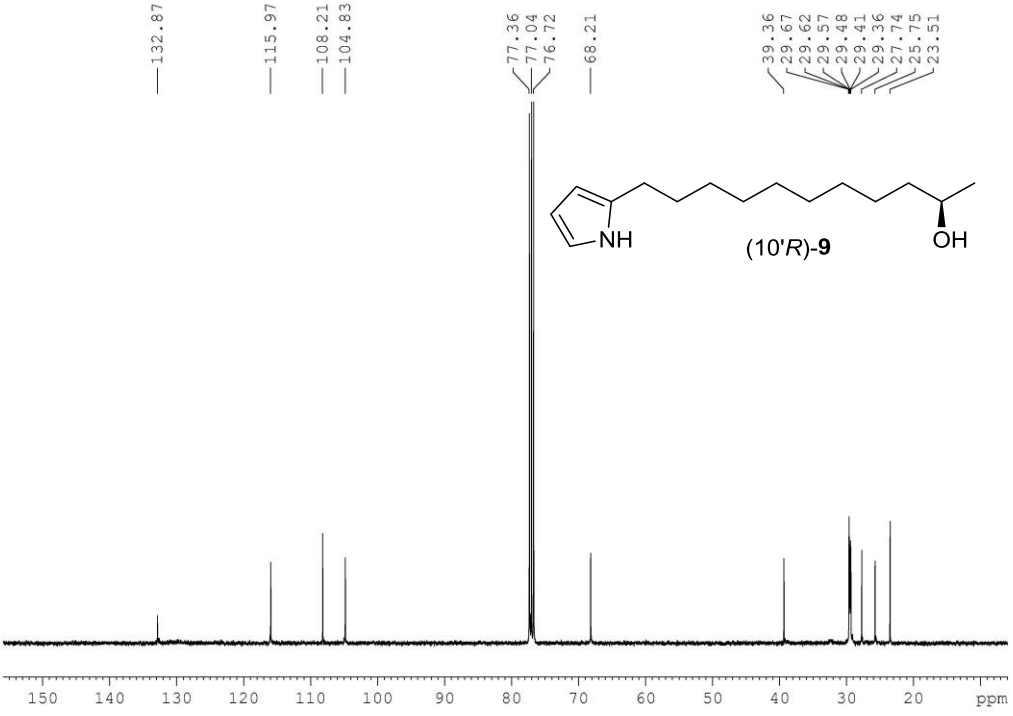




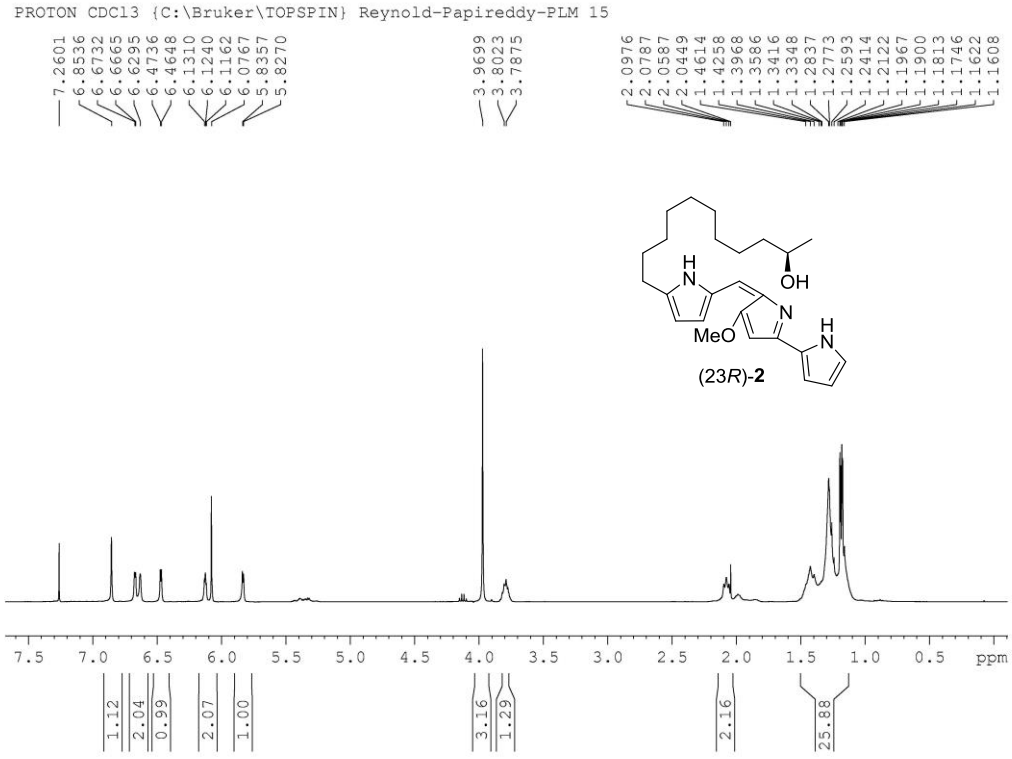
(10'*R*)-**9**

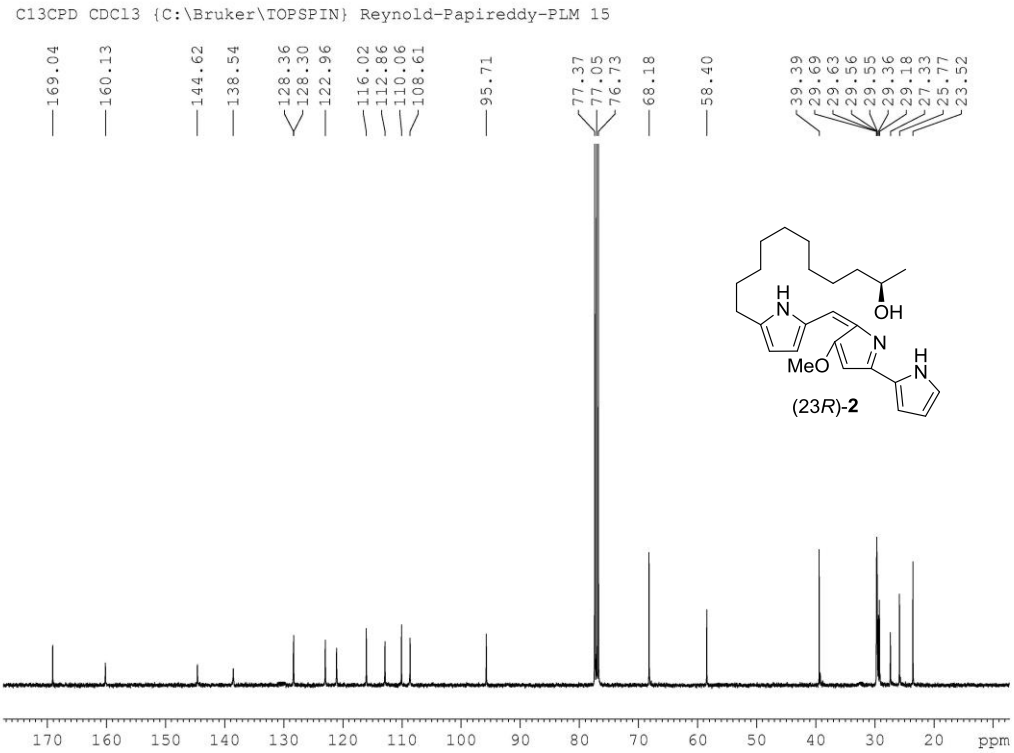


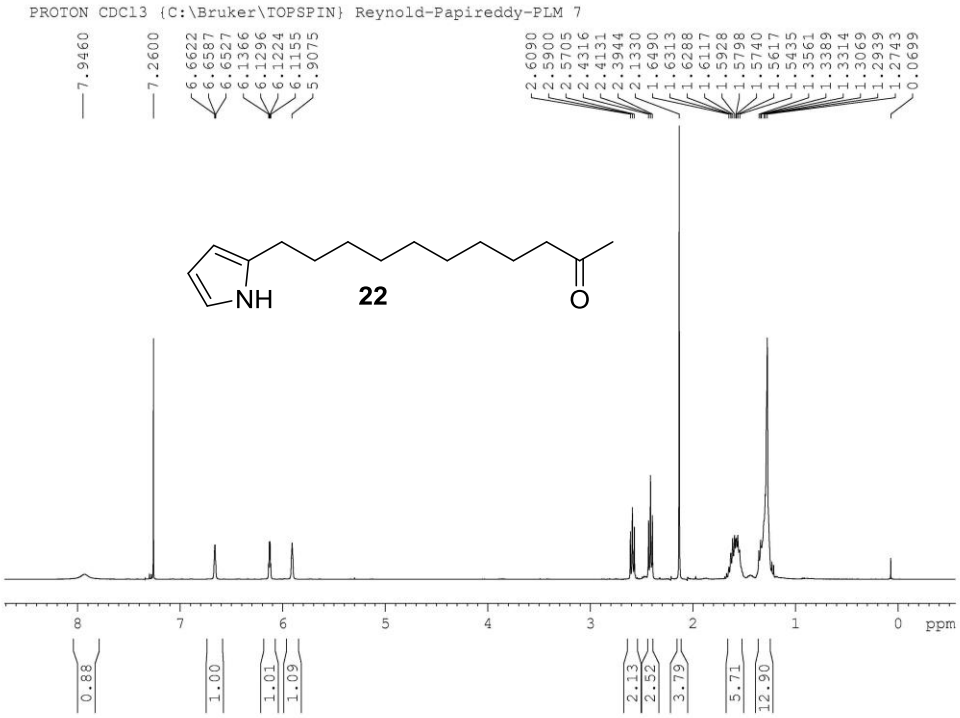
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 6

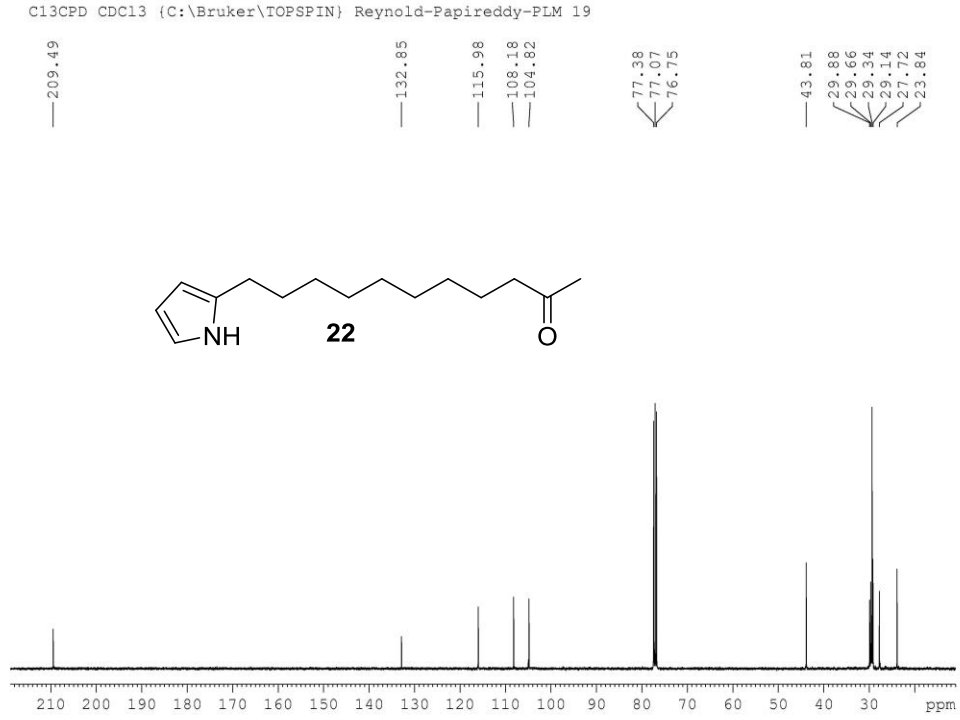


(10'*R*)-**9**

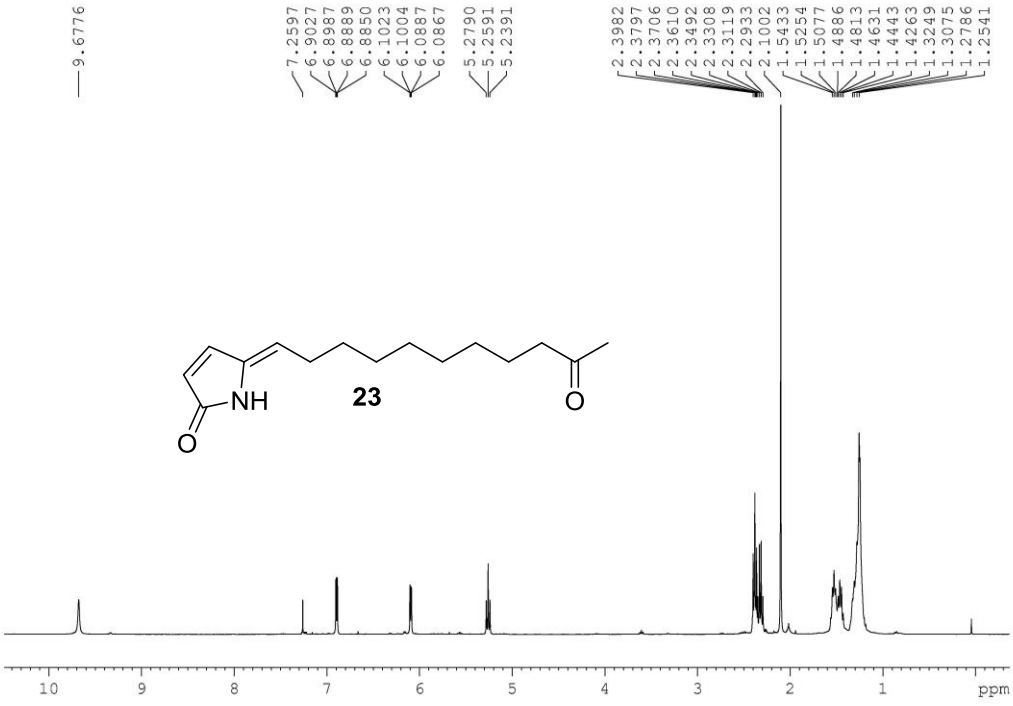

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 15
7.2601
6.8536
6.6732
6.6665
6.6295
6.4736
6.4648
6.1310
6.1240
6.1162
6.0767
5.8357
5.8270
3.9699
3.8023
3.7875
2.0976
2.0787
2.0587
2.0449
1.4614
1.4258
1.3968
1.3586
1.3416
1.3348
1.2837
1.2773
1.2593
1.2414
1.2122
1.1967
1.1900
1.1813
1.1746
1.1622
1.1608
H
N
OH
N
MeO
H
N
(23R)-2
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 ppm
1.12
2.04
0.99
2.07
1.00
3.16
1.29
2.16
25.88


C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 15
169.04
160.13
144.62
138.54
128.36
128.30
122.96
116.02
112.86
110.06
108.61
95.71
77.37
77.05
76.73
68.18
58.40
39.39
29.69
29.63
29.56
29.55
29.36
29.18
27.33
25.77
23.52
H
N
OH
N
MeO
H
N
(23R)-2
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

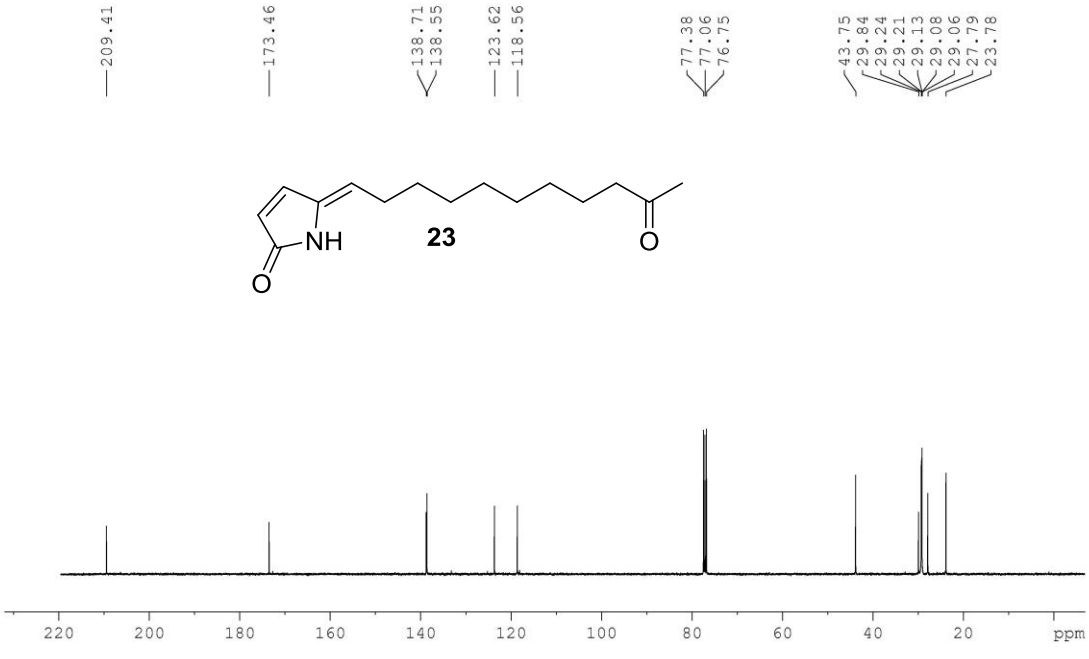

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 7
7.9460
7.2600
6.6622
6.6587
6.6527
6.1366
6.1296
6.1224
6.1155
5.9075
2.6090
2.5900
2.5705
2.4316
2.4131
2.3944
2.1330
1.6490
1.6313
1.6288
1.6117
1.5928
1.5798
1.5740
1.5617
1.5435
1.3561
1.3389
1.3314
1.3069
1.2939
1.2743
0.0699
NH
22
O
8
7
6
5
4
3
2
1
0
ppm
0.88
1.00
1.01
1.09
2.13
2.52
3.79
5.71
12.90

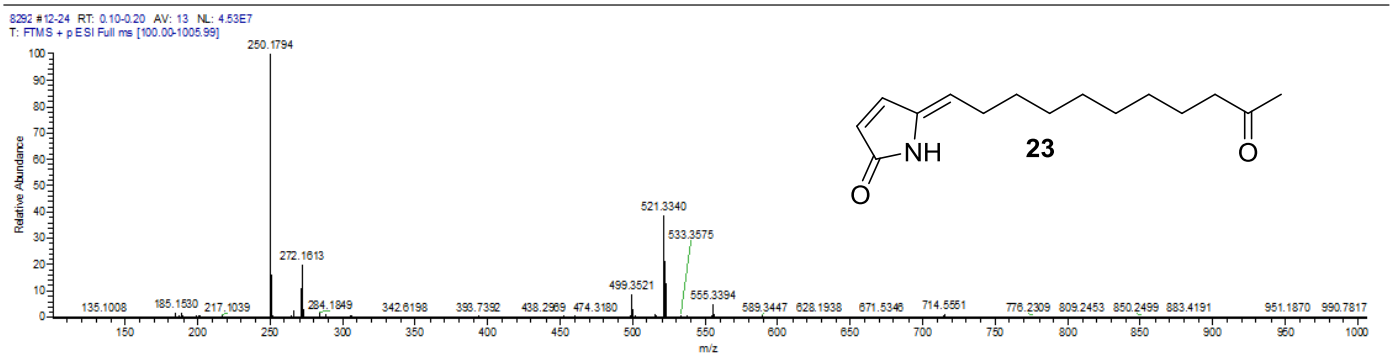

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 19
209.49
132.85
115.98
108.18
104.82
77.38
77.07
76.75
43.81
29.88
29.66
29.34
29.14
27.72
23.84
NH
22
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

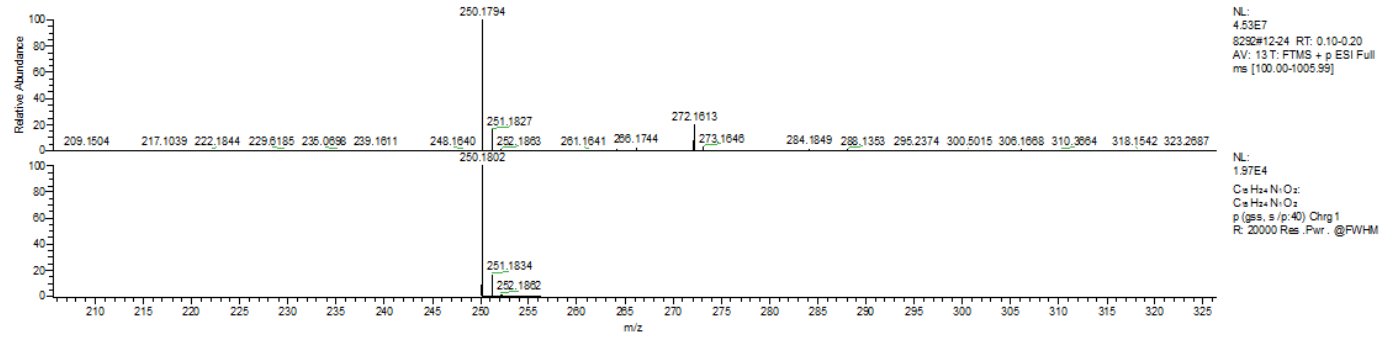
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 6

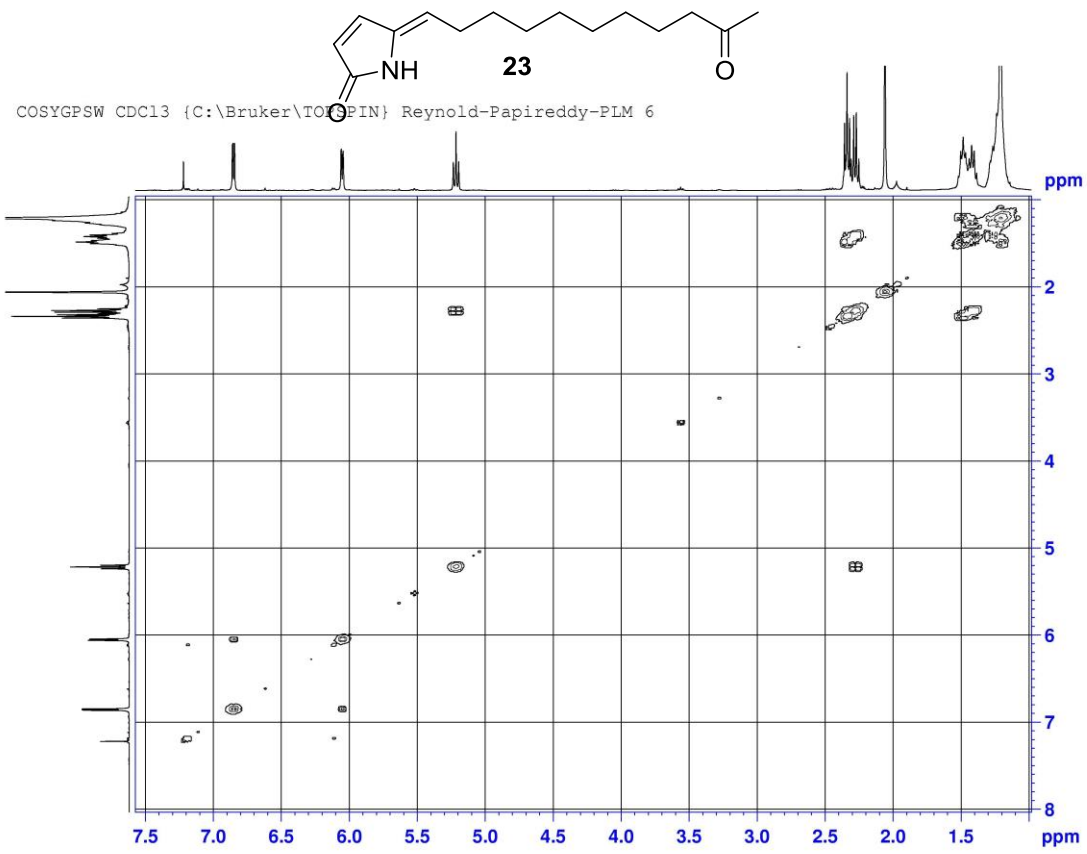


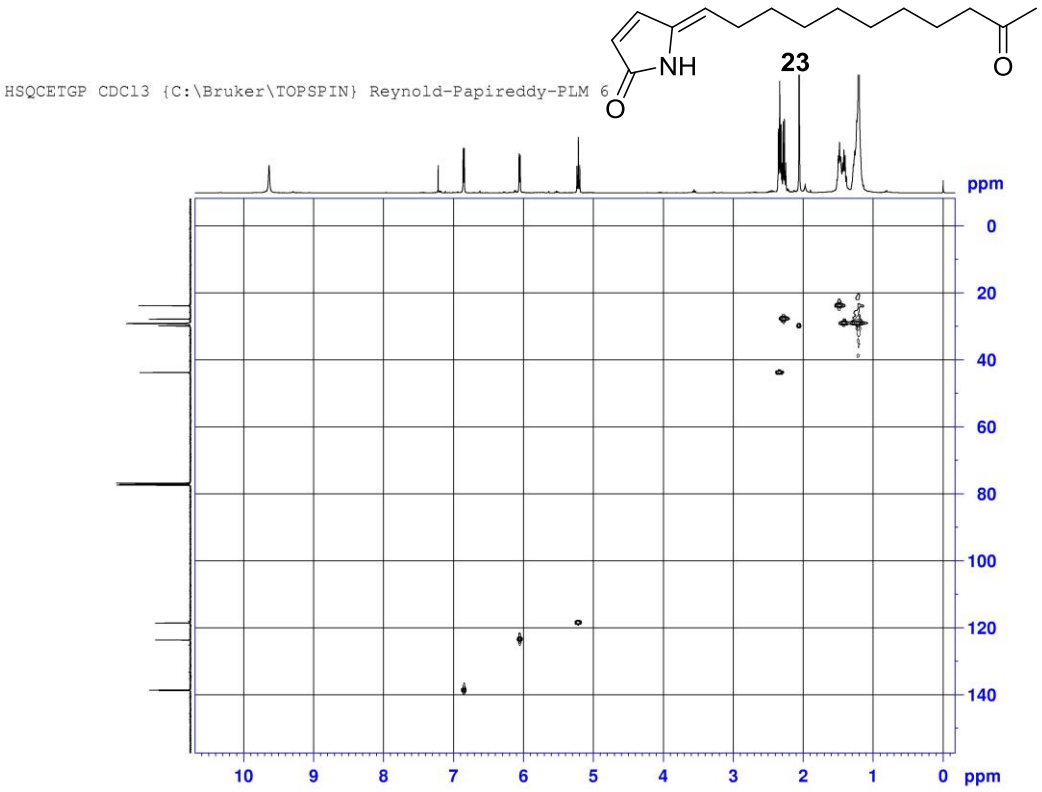
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 6

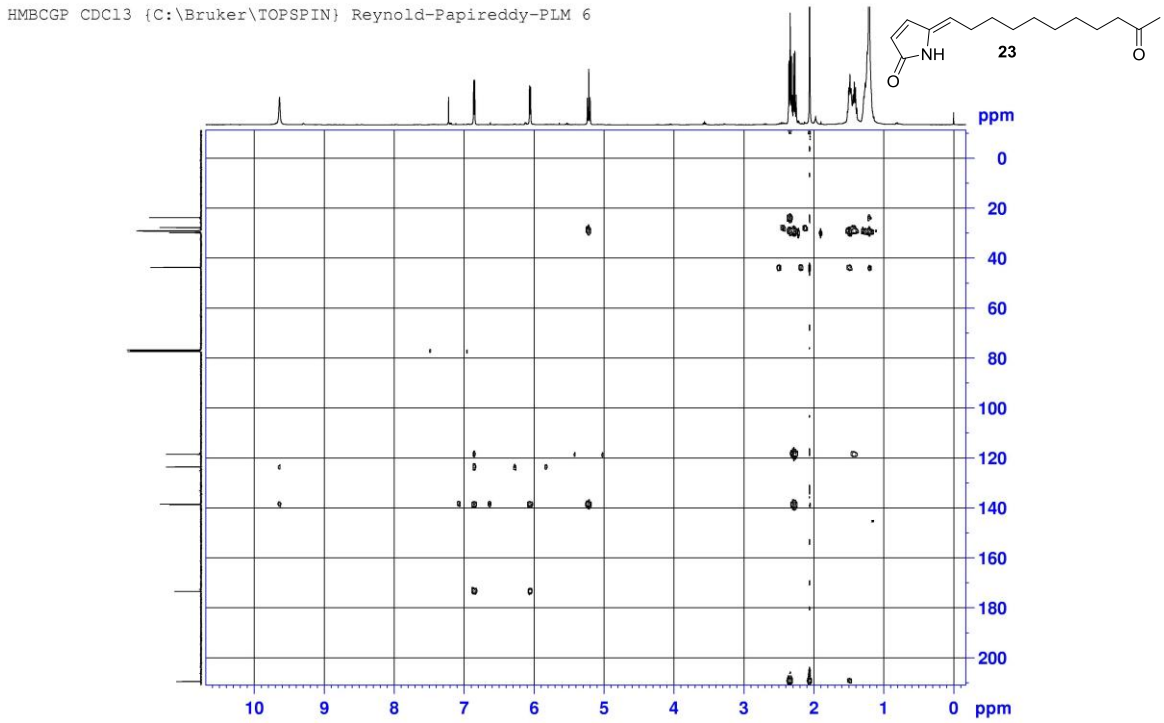


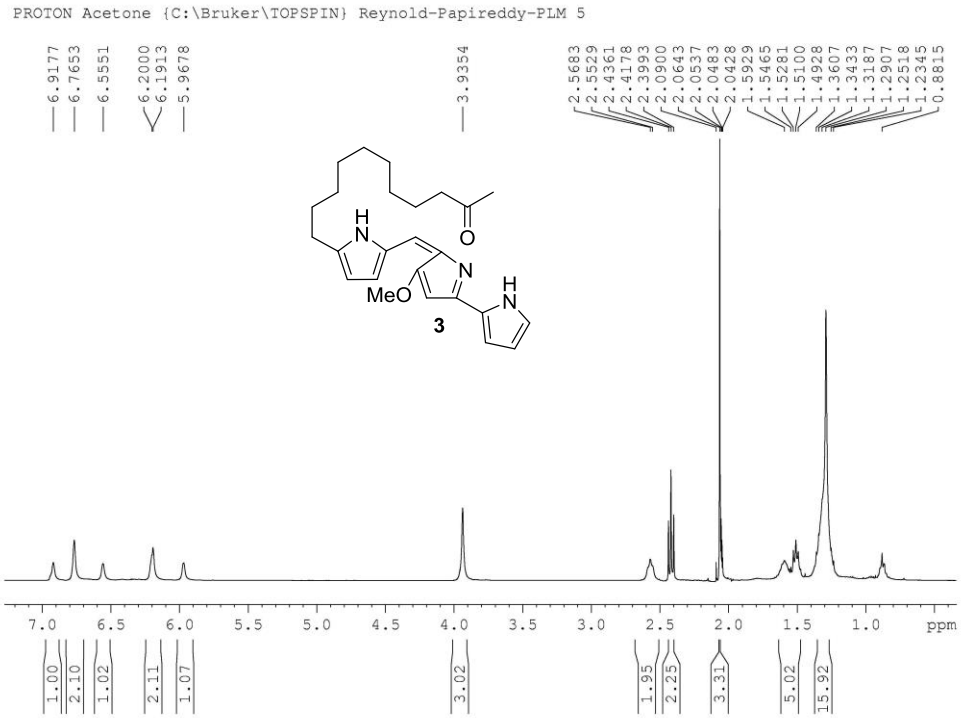

8292 #12-24 RT: 0.10-0.20 AV: 13 NL: 4.53E7
T: FTMS + p ESI Full ms [100.00-1005.99]
Relative Abundance
m/z
250.1794
272.1613
521.3340
533.3575
499.3521
555.3394
NH
O
O
23

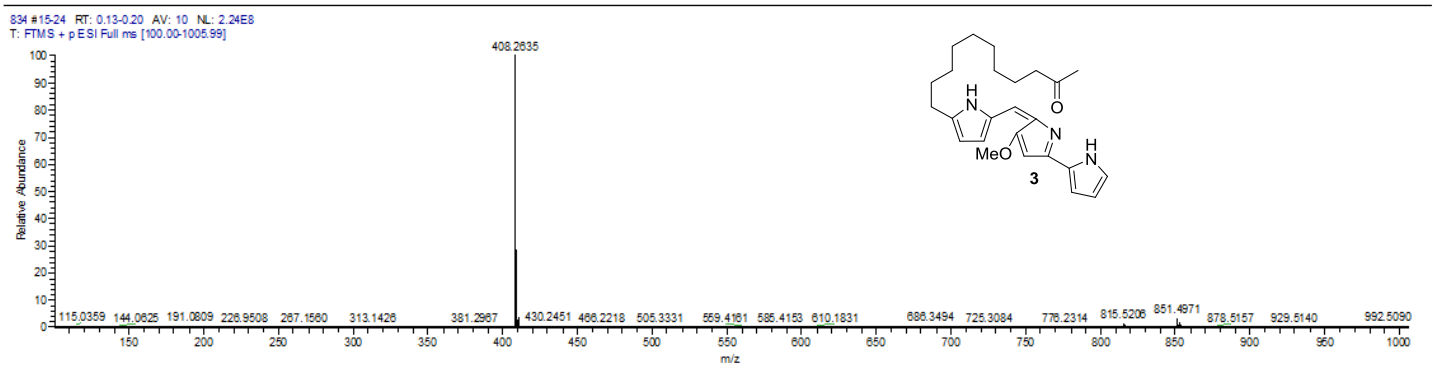

Relative Abundance
m/z
250.1794
251.1827
272.1613
250.1802
251.1834
NL:
4.53E7
8292#12-24 RT: 0.10-0.20
AV: 13 T: FTMS + p ESI Full
ms [100.00-1005.99]
NL:
1.97E4
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr . @FWHM

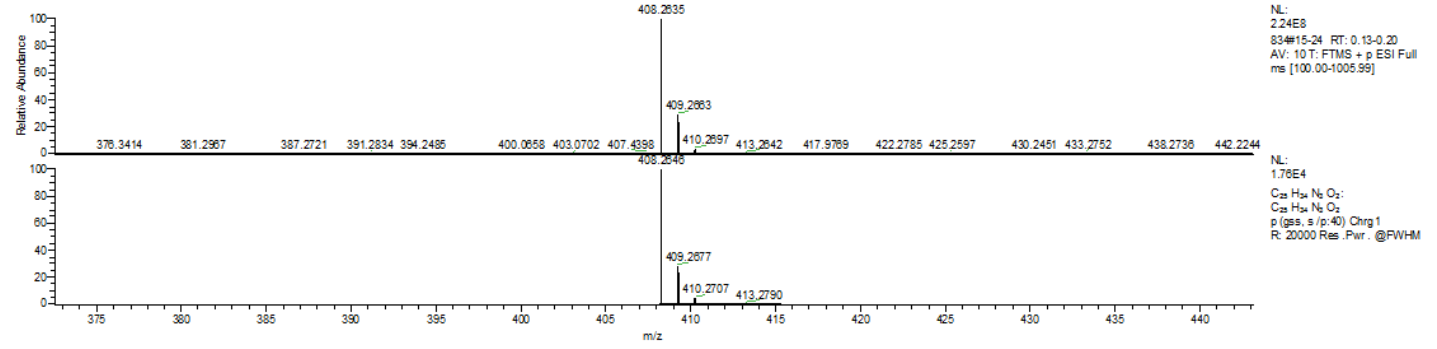

NH
23
O
O
COSYGPSW CDC13 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 6
ppm
ppm

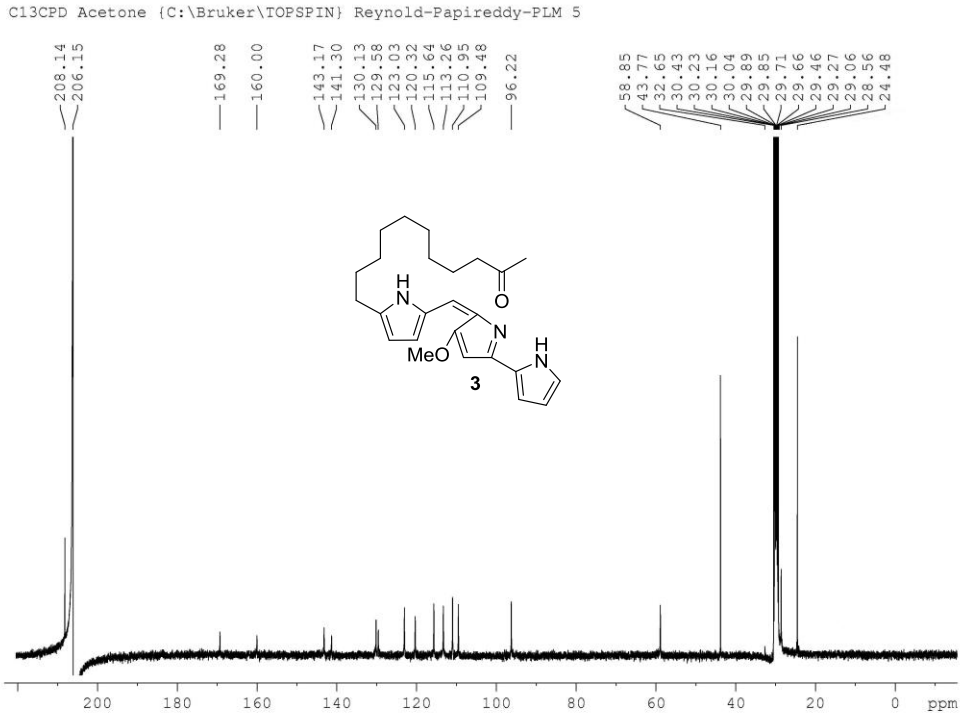

HSQCETGP CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 6
NH
O
23
O
ppm
0
20
40
60
80
100
120
140
10 9 8 7 6 5 4 3 2 1 0 ppm

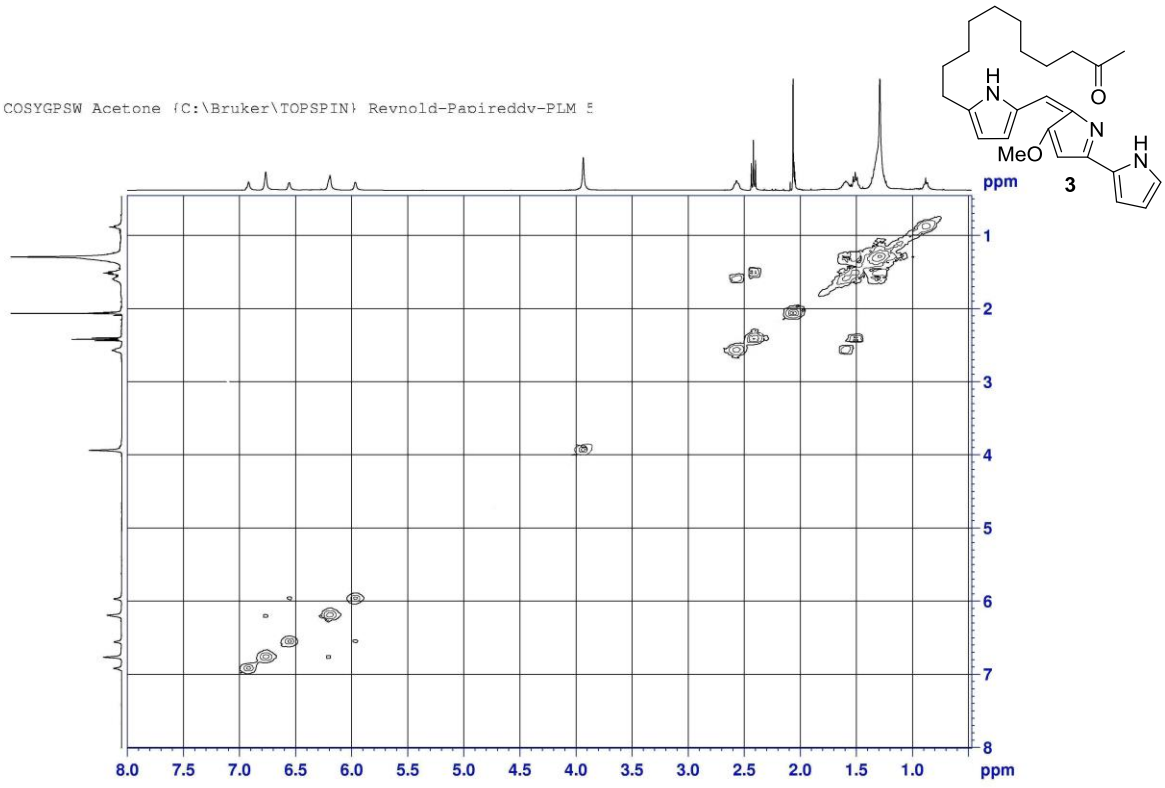

HMBCGP CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 6
NH
O
23
O
ppm
0
20
40
60
80
100
120
140
160
180
200
10 9 8 7 6 5 4 3 2 1 0 ppm

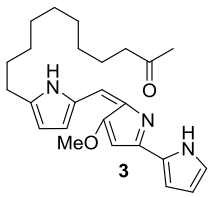

PROTON Acetone {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5
6.9177
6.7653
6.5551
6.2000
6.1913
5.9678
3.9354
2.5683
2.5529
2.4361
2.4178
2.3993
2.0900
2.0643
2.0537
2.0483
2.0428
1.5929
1.5465
1.5281
1.5100
1.4928
1.3607
1.3433
1.3187
1.2907
1.2518
1.2345
0.8815
MeO
3
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
2.10
1.02
2.11
1.07
3.02
1.95
2.25
3.31
5.02
15.92


834 #15-24 RT: 0.13-0.20 AV: 10 NL: 2.24E8
T: FTMS + p ESI Full ms [100.00-1005.99]
408.2635
Relative Abundance
115.0359
144.0625
191.0809
228.9508
267.1560
313.1426
381.2967
430.2451
466.2218
505.3331
559.4161
585.4153
610.1831
686.3494
725.3084
776.2314
815.5206
851.4971
878.5157
929.5140
992.5090
m/z
MeO
3

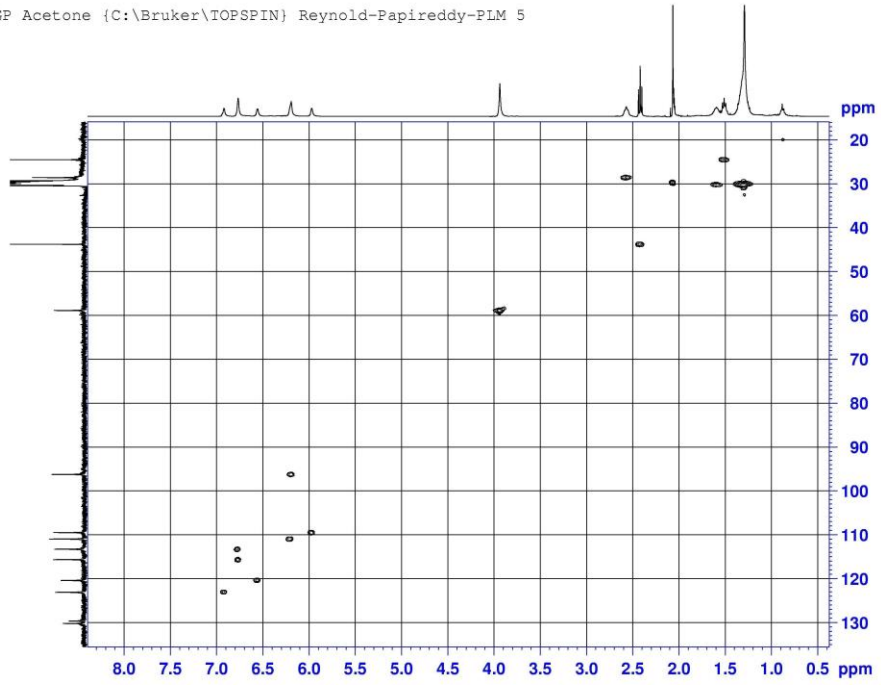

408.2635
409.2663
410.2697
Relative Abundance
376.3414
381.2967
387.2721
391.2834
394.2485
400.0658
403.0702
407.4398
413.2642
417.9769
422.2785
425.2597
430.2451
433.2752
438.2736
442.2244
NL:
2.24E8
834#15-24 RT: 0.13-0.20
AV: 10 T: FTMS + p ESI Full
ms [100.00-1005.99]
408.2646
409.2677
410.2707
413.2790
NL:
1.76E4
C28 H34 N6 O2:
C28 H34 N6 O2
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr . @FWHM
m/z


C13CPD Acetone {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5
208.14
206.15
169.28
160.00
143.17
141.30
130.13
129.58
123.03
120.32
115.64
113.26
110.95
109.48
96.22
58.85
43.77
32.65
30.43
30.23
30.16
30.04
29.89
29.85
29.71
29.66
29.46
29.27
29.06
28.56
24.48
MeO
3
200
180
160
140
120
100
80
60
40
20
0
ppm

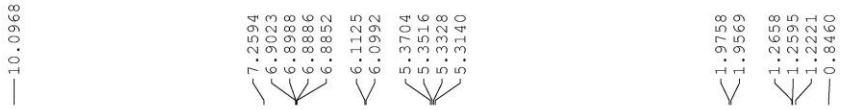

COSYGPSW Acetone {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5
MeO
3
ppm
1
2
3
4
5
6
7
8
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm

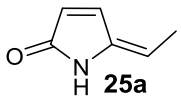


HSQCETGP Acetone {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5

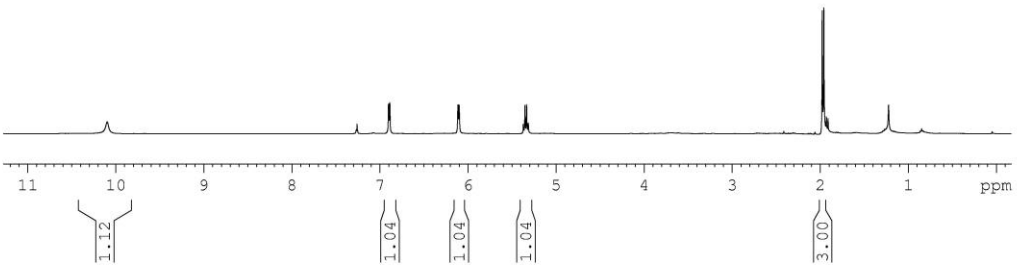


PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 15

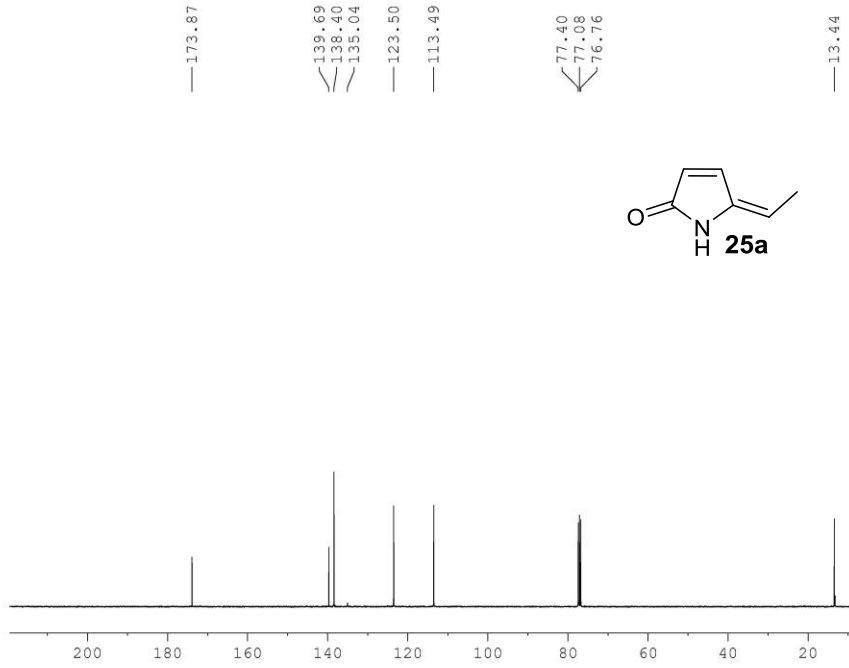




25a

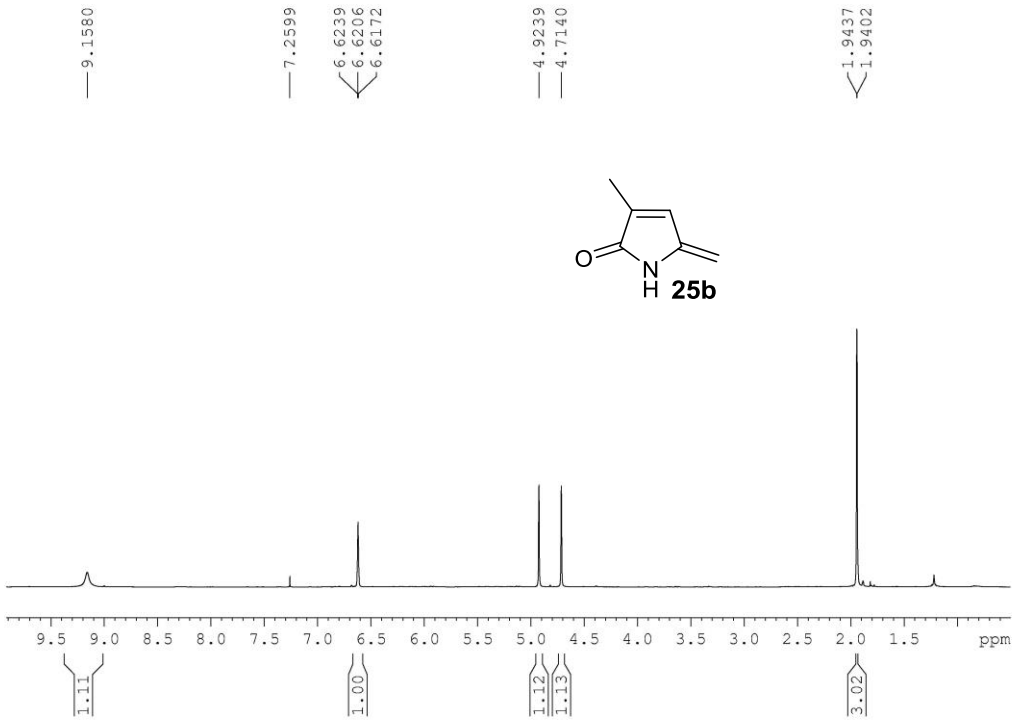


C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 7

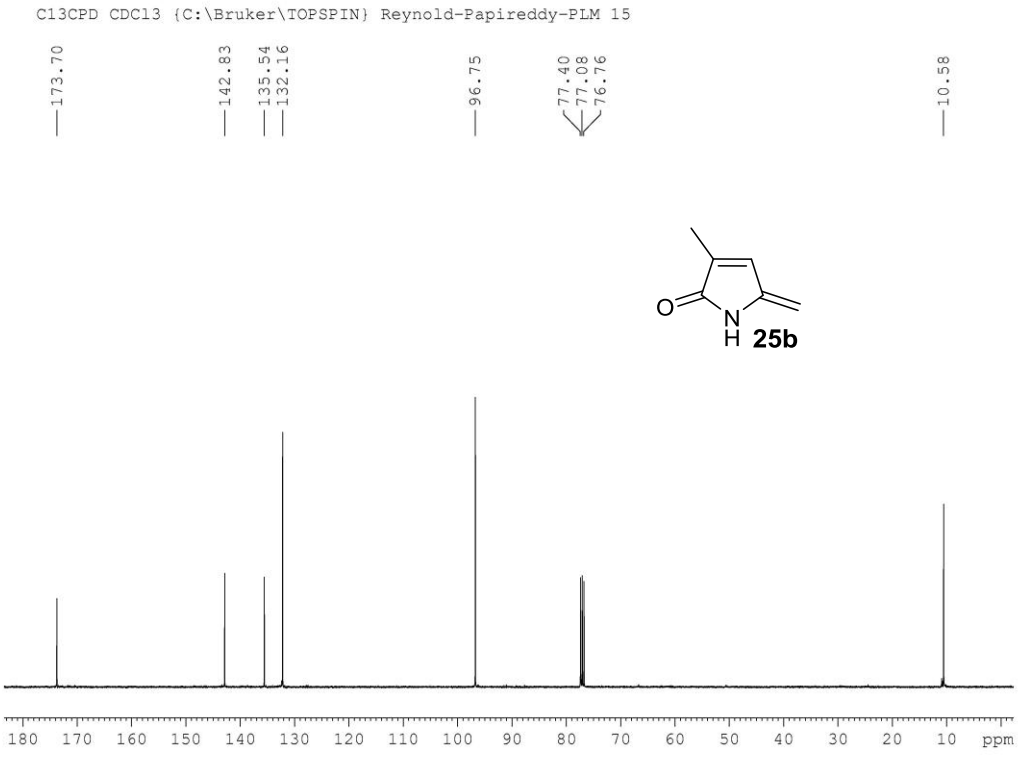


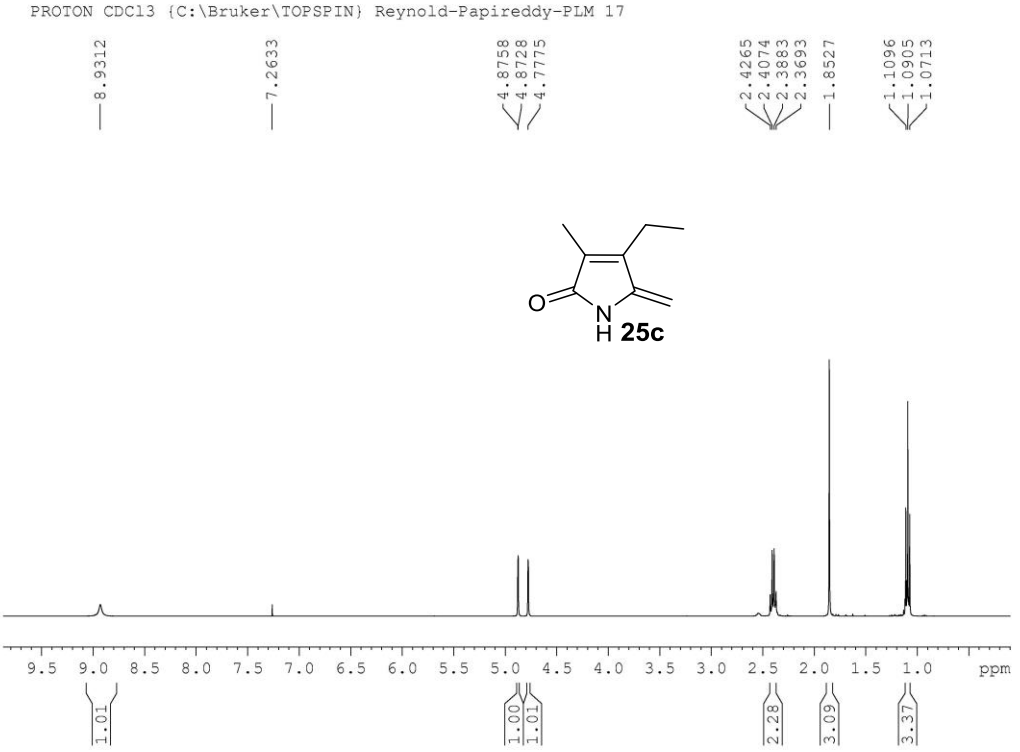
25a

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 10

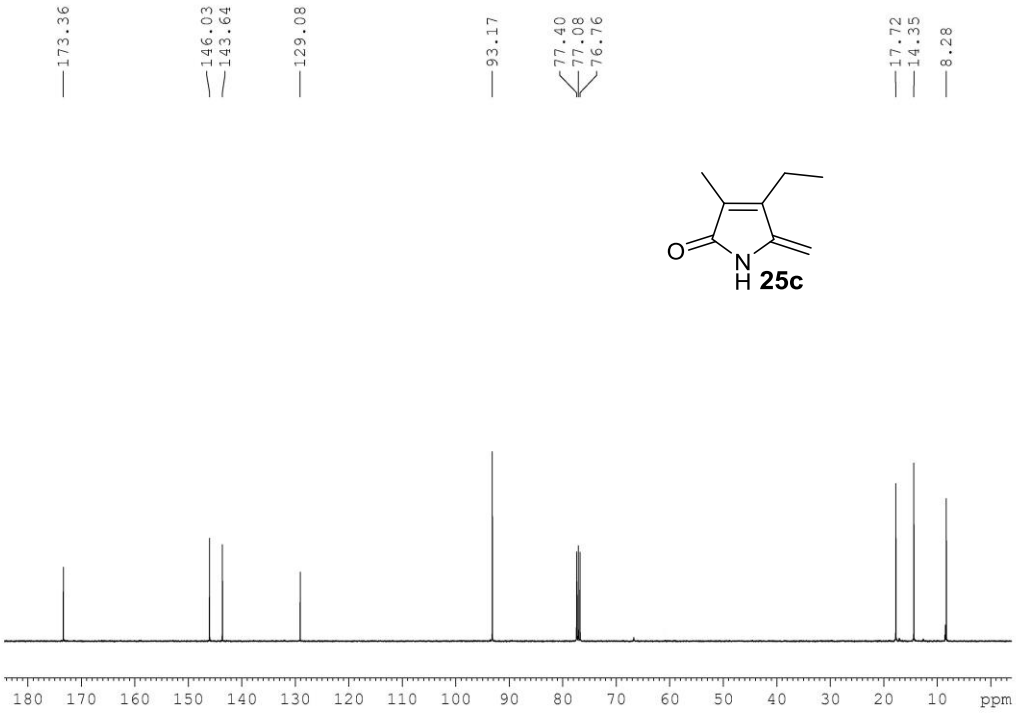


25b

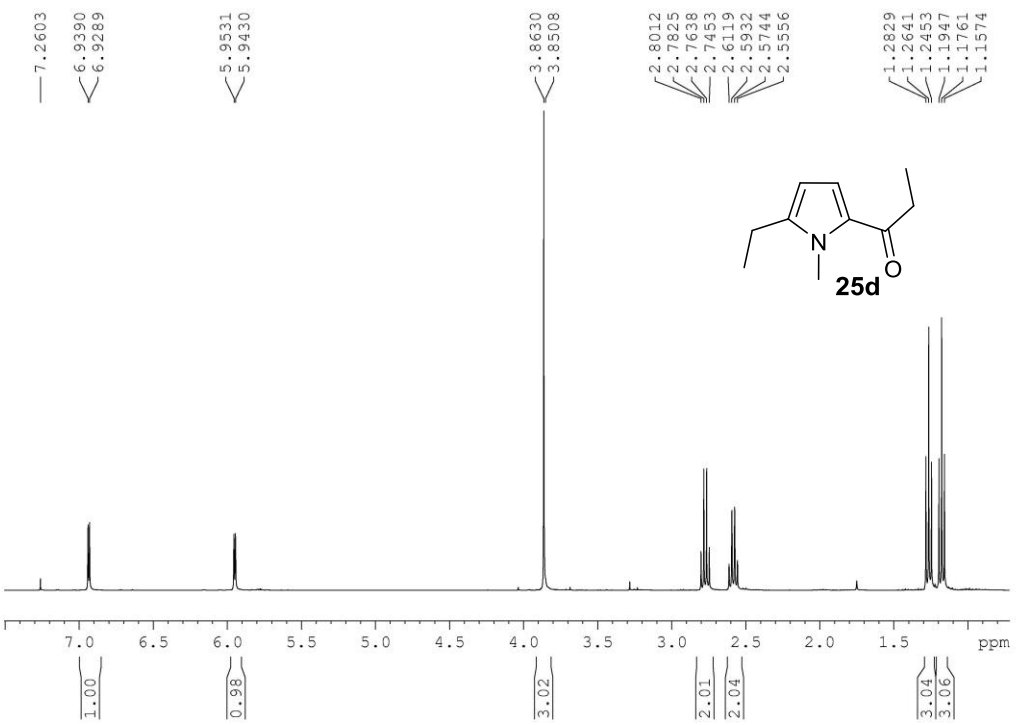

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 15
173.70
142.83
135.54
132.16
96.75
77.40
77.08
76.76
10.58
O
N
H
25b
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

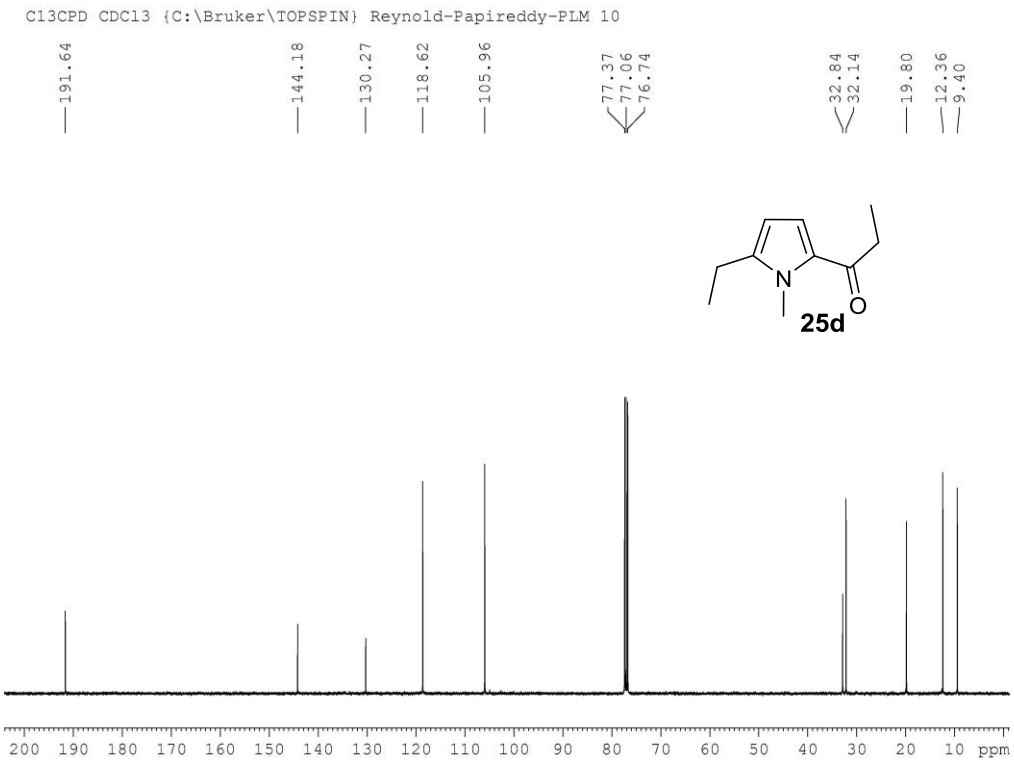

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 17
8.9312
7.2633
4.8758
4.8728
4.7775
2.4265
2.4074
2.3883
2.3693
1.8527
1.1096
1.0905
1.0713
O
N
H
25c
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.01
1.00
1.01
2.28
3.09
3.37

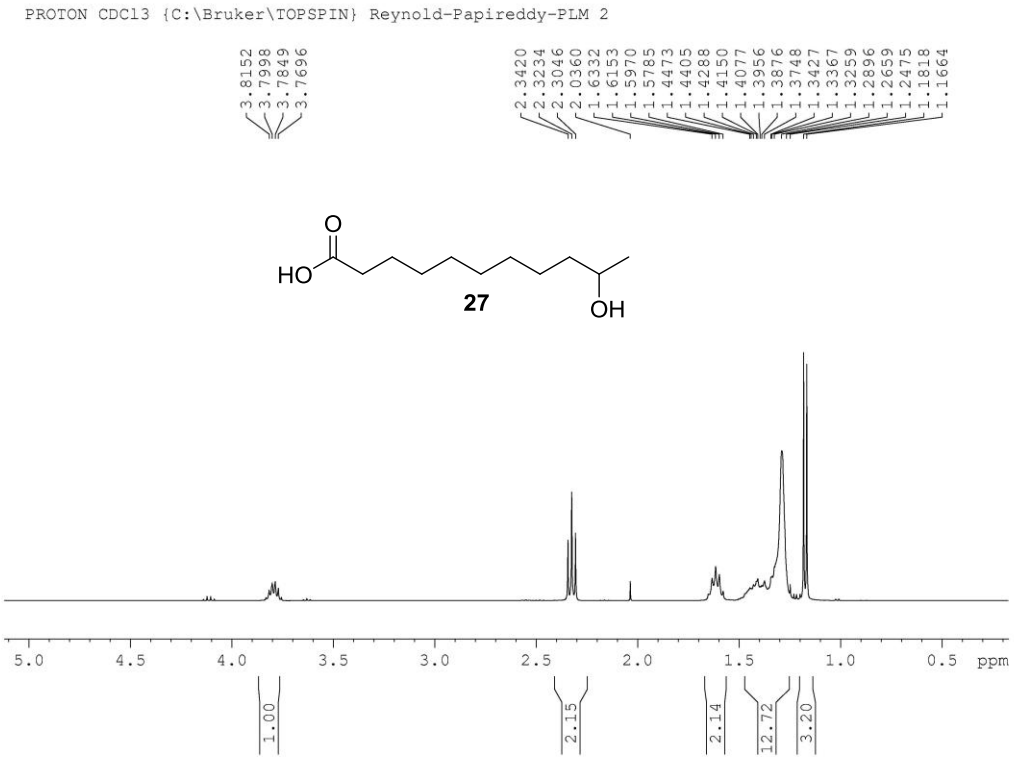
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 18



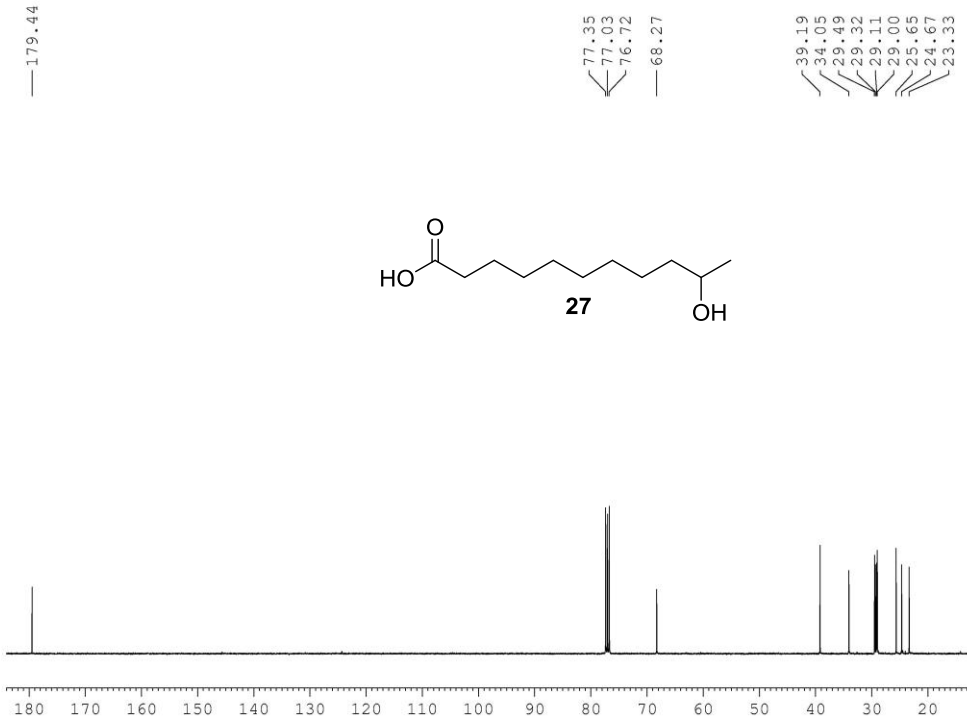
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 7



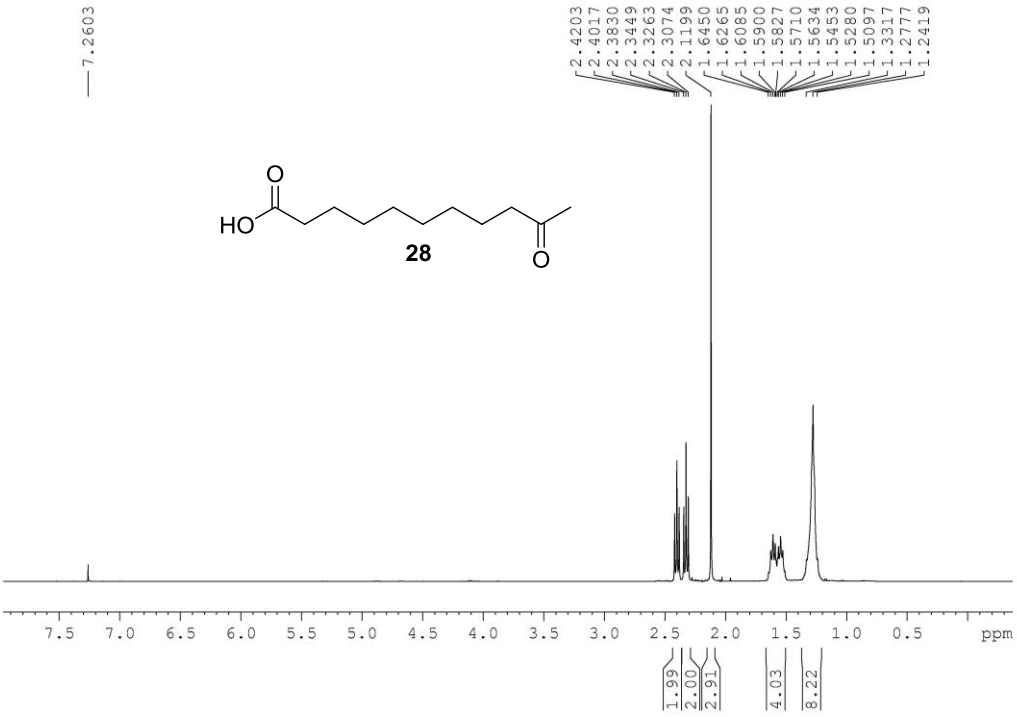

C13CPD CDC13 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 10
191.64
144.18
130.27
118.62
105.96
77.37
77.06
76.74
32.84
32.14
19.80
12.36
9.40
N
O
25d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


PROTON CDC13 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 2
3.8152
3.7998
3.7849
3.7696
2.3420
2.3234
2.3046
2.0360
1.6332
1.6153
1.5970
1.5785
1.4473
1.4405
1.4288
1.4150
1.4077
1.3956
1.3876
1.3748
1.3427
1.3367
1.3259
1.2896
1.2659
1.2475
1.1818
1.1664
O
HO
OH
27
5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
2.15
2.14
12.72
3.20

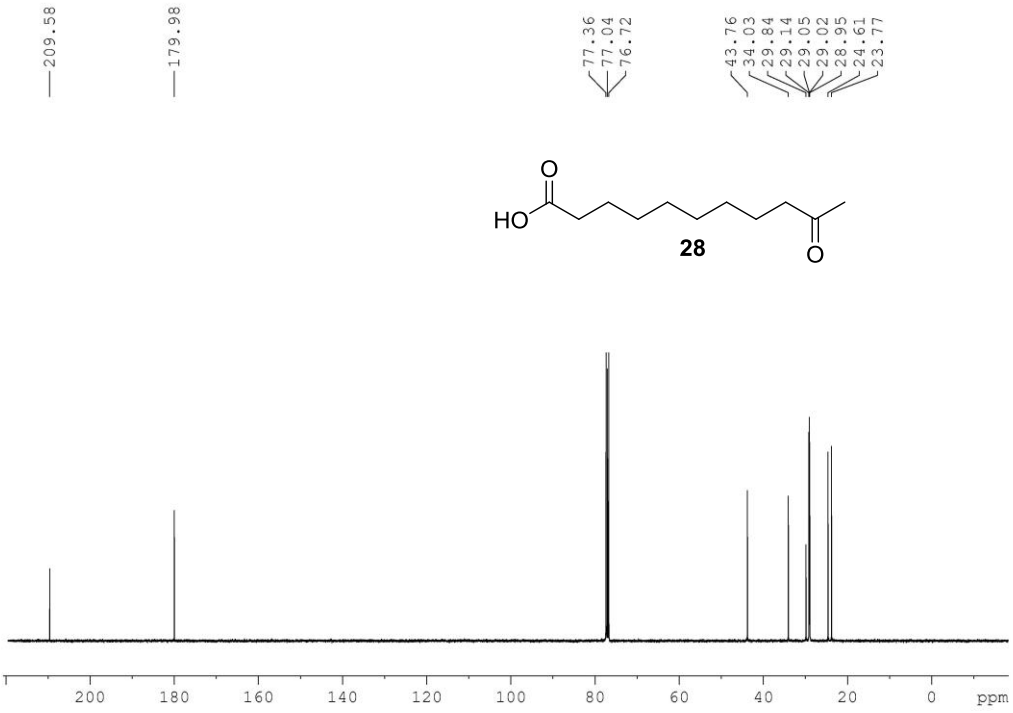
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 10



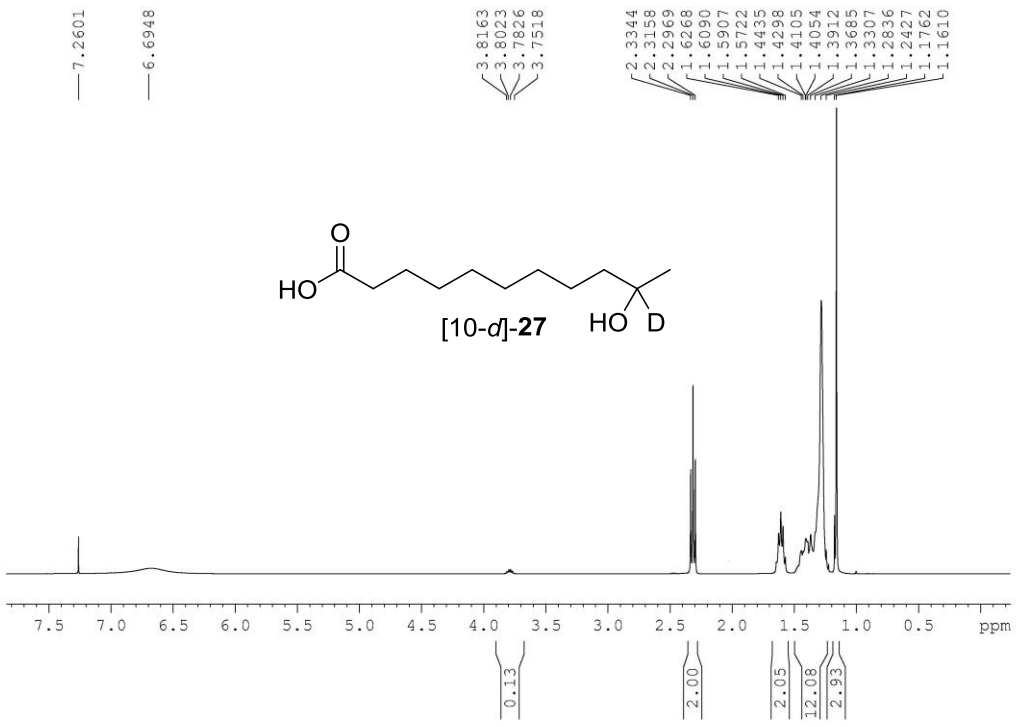
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 11



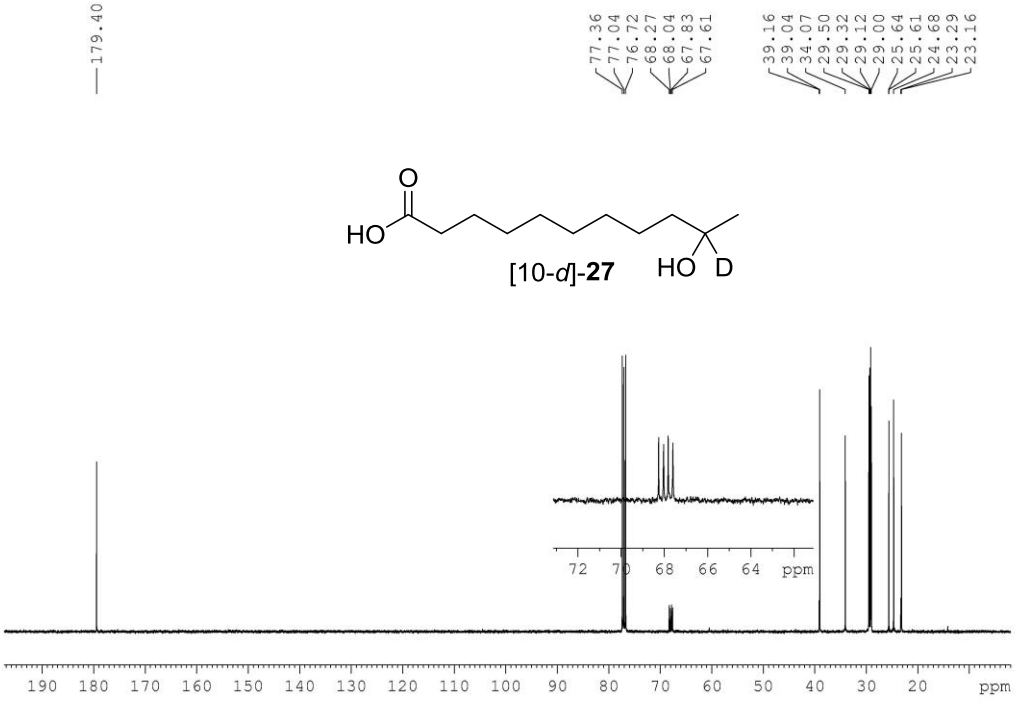
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 13



PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 19

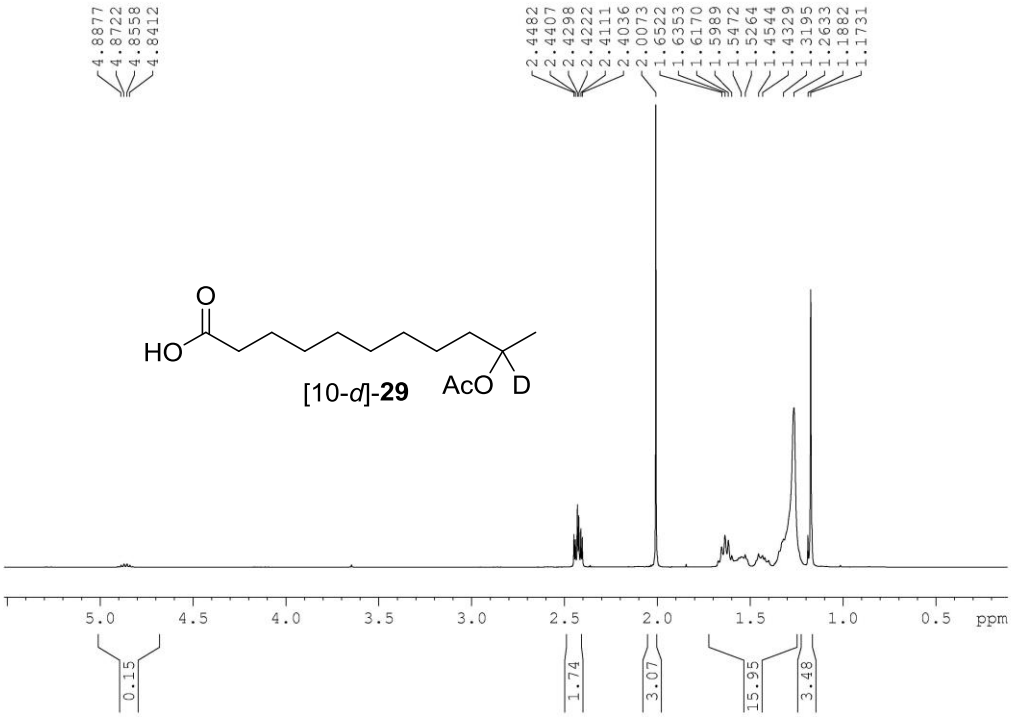


C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 19

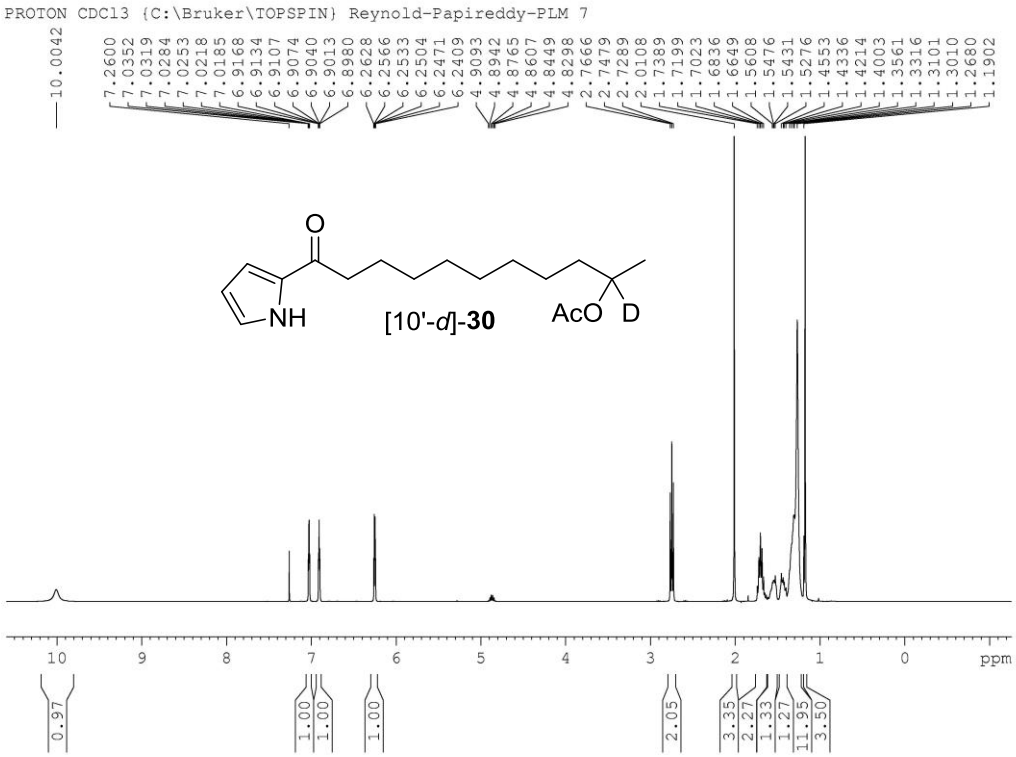


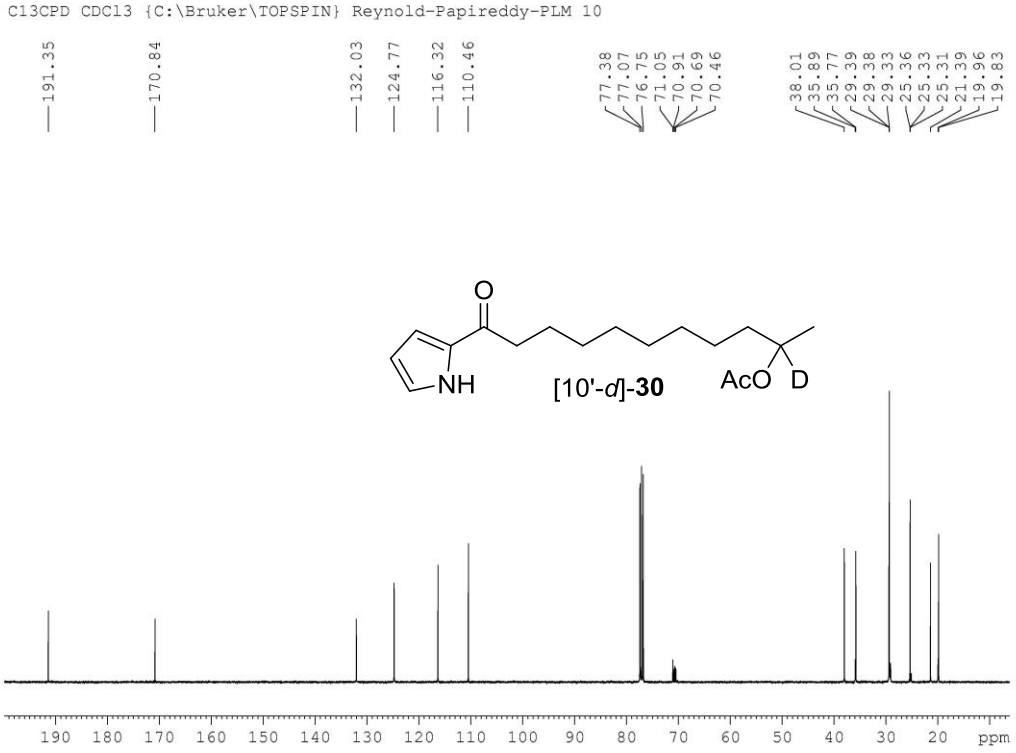
[10-*d*]-**27**

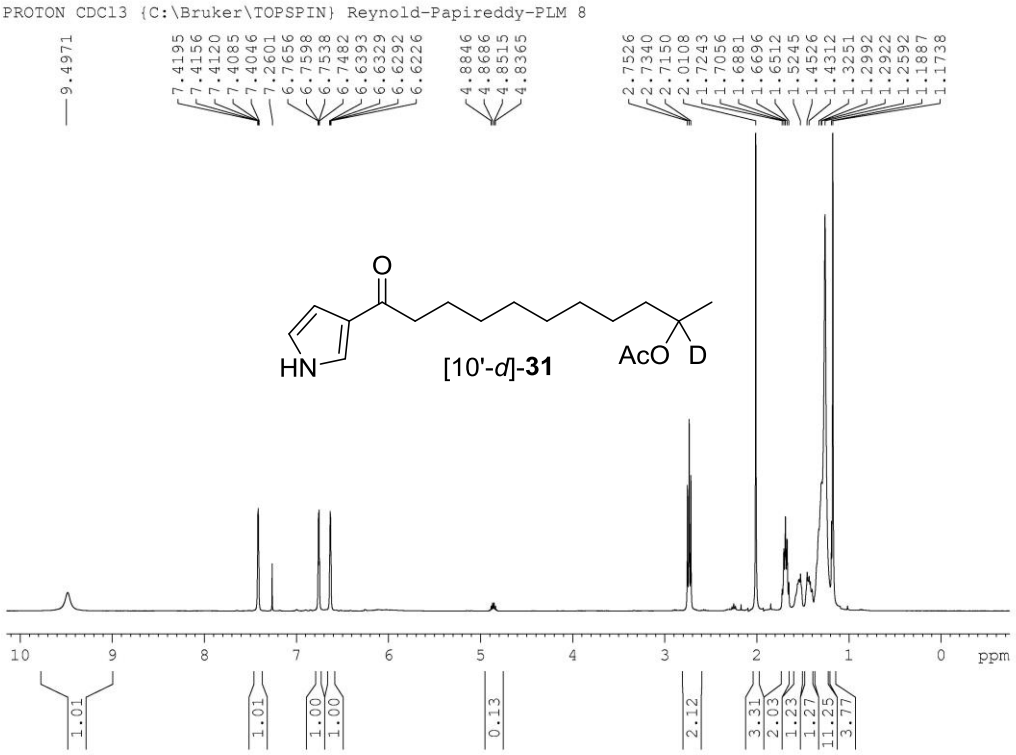
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 20

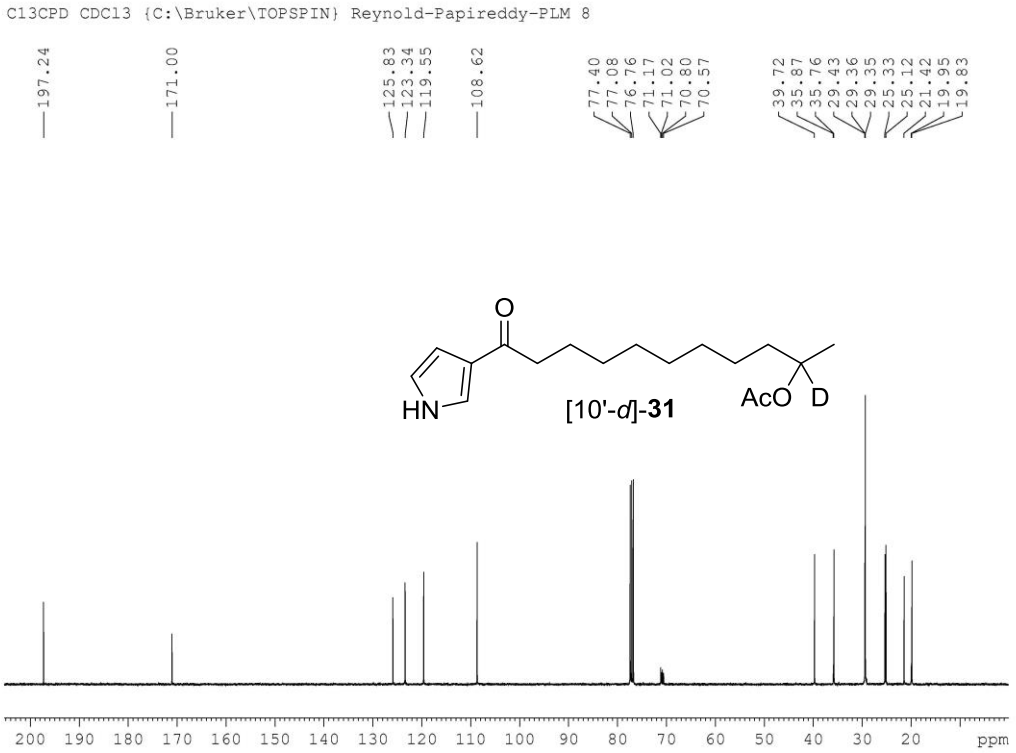


[10-*d*]-**29**

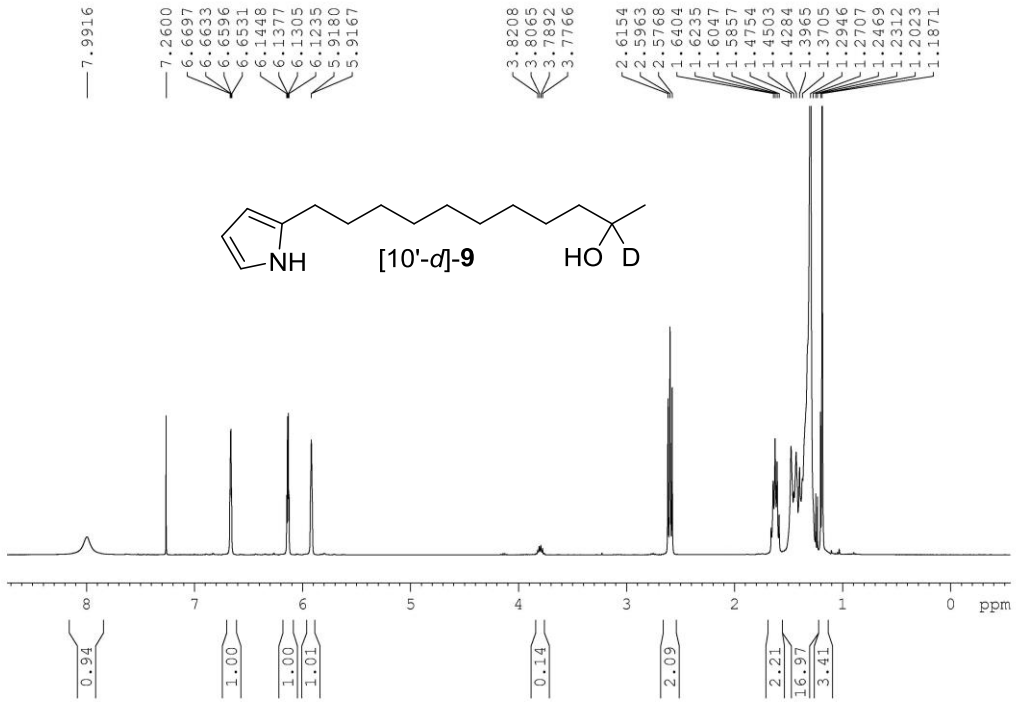

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 7
10.0042
7.2600
7.0352
7.0319
7.0284
7.0253
7.0218
7.0185
6.9168
6.9134
6.9107
6.9074
6.9040
6.9013
6.8980
6.2628
6.2566
6.2533
6.2504
6.2471
6.2409
4.9093
4.8942
4.8765
4.8607
4.8449
4.8298
2.7666
2.7479
2.7289
2.0108
1.7389
1.7199
1.7023
1.6836
1.6649
1.5608
1.5476
1.5431
1.5276
1.4553
1.4336
1.4214
1.4003
1.3561
1.3316
1.3101
1.3010
1.2680
1.1902
O
NH
[10'-d]-30
AcO
D
10
9
8
7
6
5
4
3
2
1
0
ppm
0.97
1.00
1.00
1.00
2.05
3.35
2.27
1.33
1.27
11.95
3.50


C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 10
191.35
170.84
132.03
124.77
116.32
110.46
77.38
77.07
76.75
71.05
70.91
70.69
70.46
38.01
35.89
35.77
29.39
29.38
29.33
25.36
25.33
25.31
21.39
19.96
19.83
O
NH
[10'-d]-30
AcO
D
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

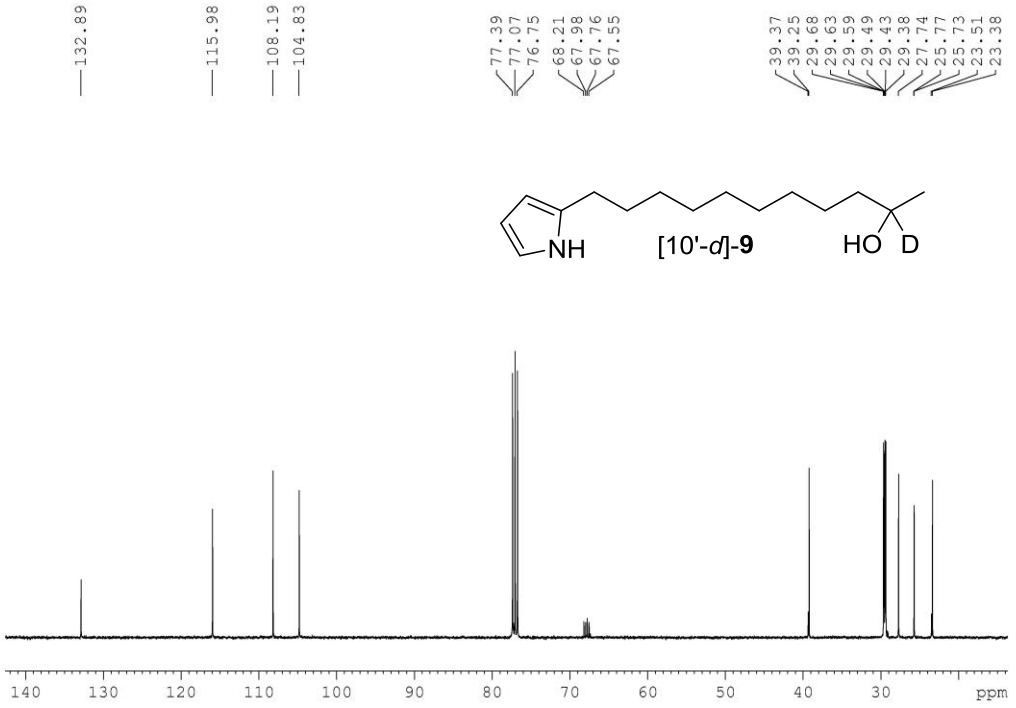

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 8
9.4971
7.4195
7.4156
7.4120
7.4085
7.4046
7.2601
6.7656
6.7598
6.7538
6.7482
6.6393
6.6329
6.6292
6.6226
4.8846
4.8686
4.8515
4.8365
2.7526
2.7340
2.7150
2.0108
1.7243
1.7056
1.6881
1.6696
1.6512
1.5245
1.4526
1.4312
1.3251
1.2992
1.2922
1.2592
1.1887
1.1738
O
HN
AcO D
[10'-d]-31
10 9 8 7 6 5 4 3 2 1 0 ppm
1.01
1.01
1.00
1.00
0.13
2.12
3.31
2.03
1.23
1.27
11.25
3.77

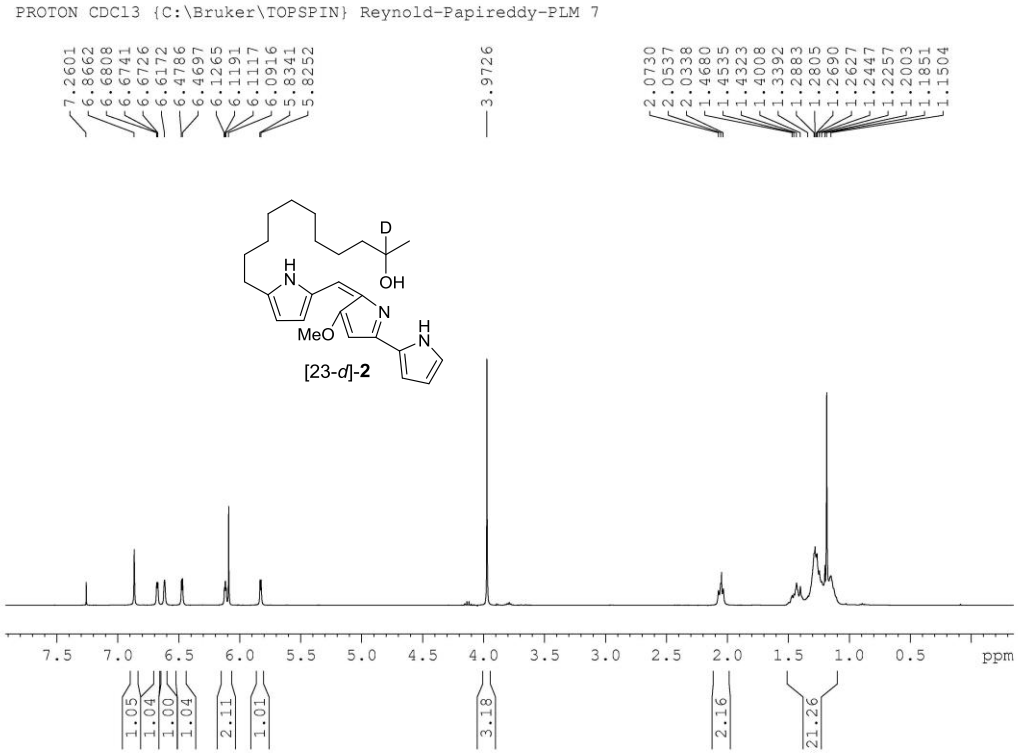

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 8
197.24
171.00
125.83
123.34
119.55
108.62
77.40
77.08
76.76
71.17
71.02
70.80
70.57
39.72
35.87
35.76
29.43
29.36
29.35
25.33
25.12
21.42
19.95
19.83
O
HN
AcO D
[10'-d]-31
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

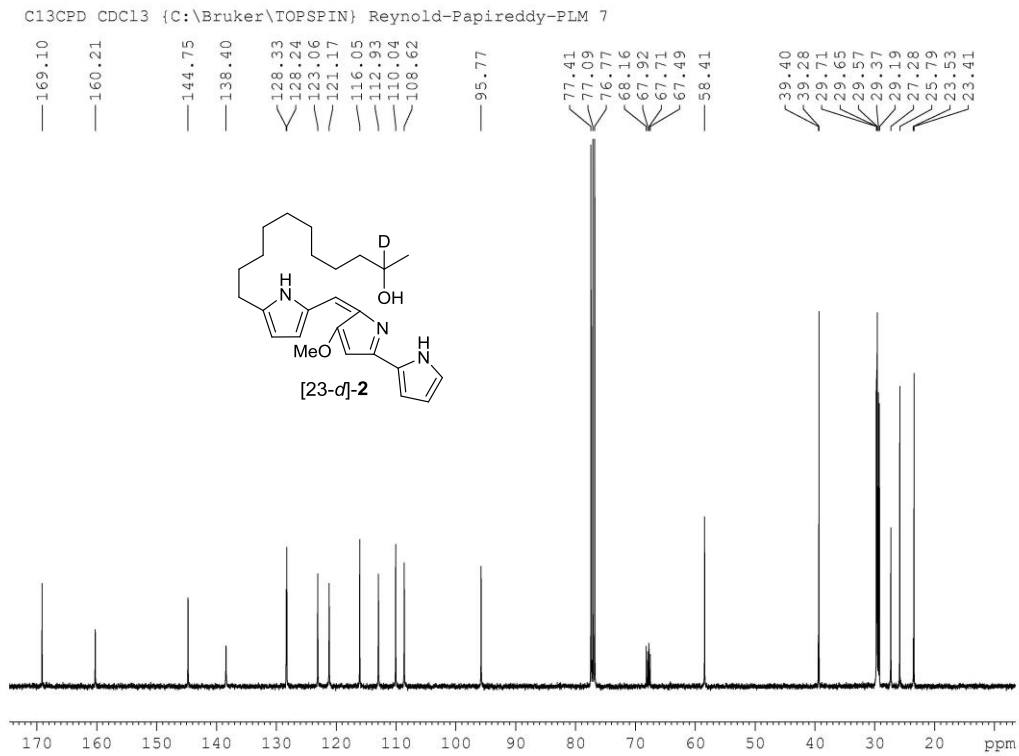
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 19

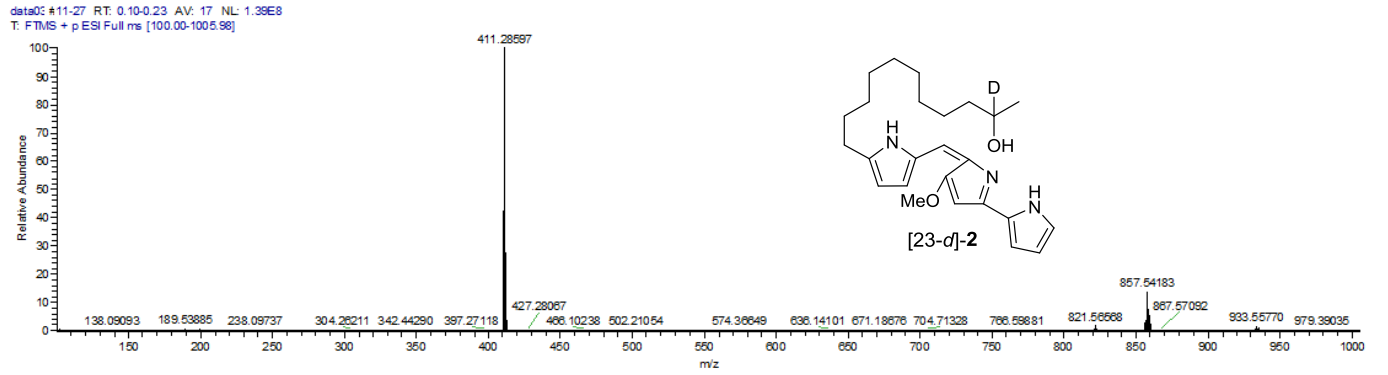


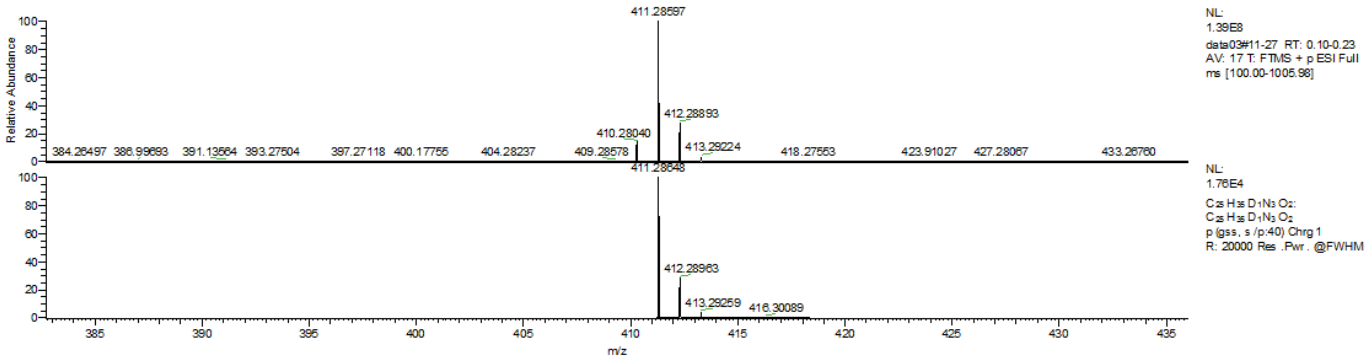
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 8

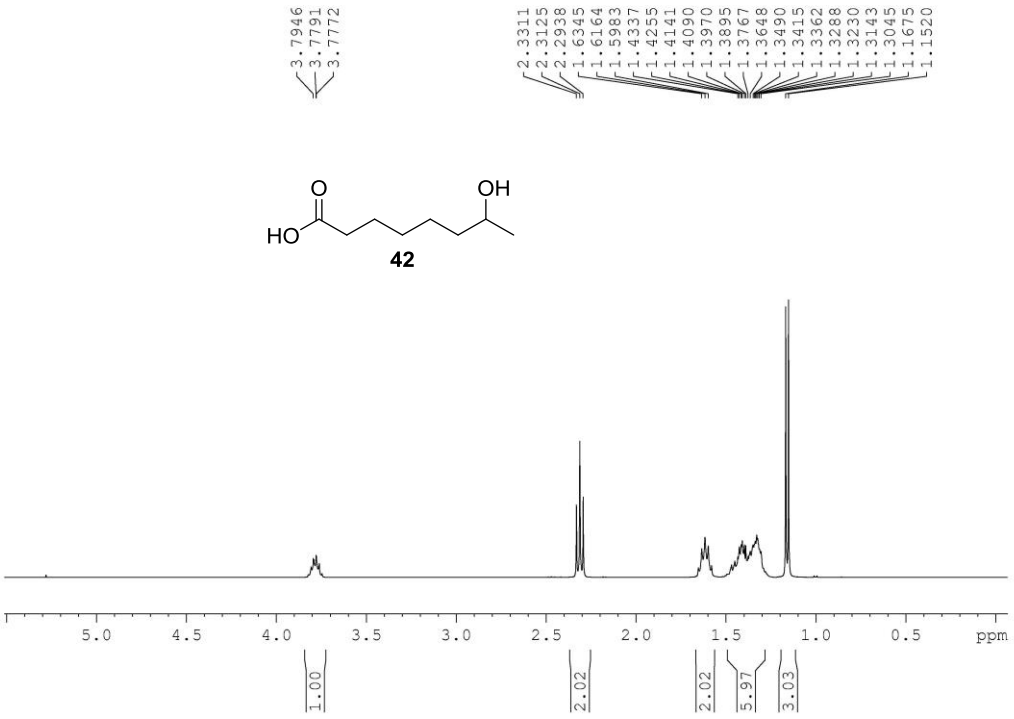



PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 7
7.2601
6.8662
6.6808
6.6741
6.6726
6.6172
6.4786
6.4697
6.1265
6.1191
6.1117
6.0916
5.8341
5.8252
3.9726
2.0730
2.0537
2.0338
1.4680
1.4535
1.4323
1.4008
1.3392
1.2883
1.2805
1.2690
1.2627
1.2447
1.2257
1.2003
1.1851
1.1504
D
OH
H
N
N
MeO
H
N
[23-d]-2
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 ppm
1.05
1.04
1.00
1.04
2.11
1.01
3.18
2.16
21.26

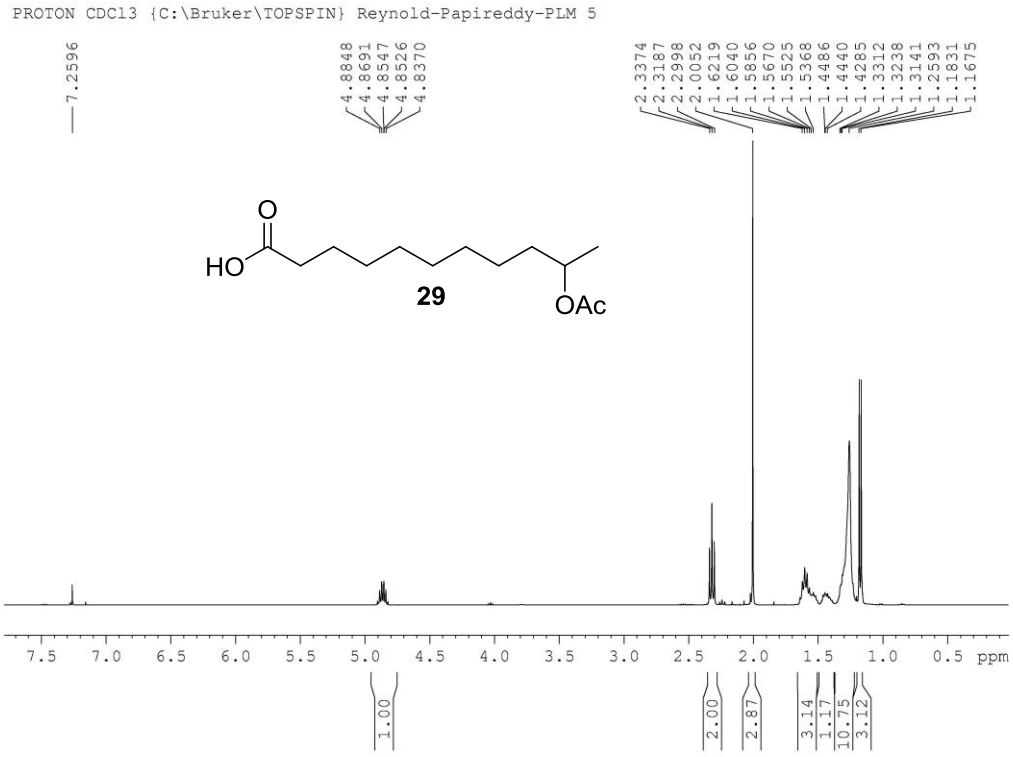

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 7
169.10
160.21
144.75
138.40
128.33
128.24
123.06
121.17
116.05
112.93
110.04
108.62
95.77
77.41
77.09
76.77
68.16
67.92
67.71
67.49
58.41
39.40
39.28
29.71
29.65
29.57
29.37
29.19
27.28
25.79
23.53
23.41
D
OH
H
N
N
MeO
H
N
[23-d]-2
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


data03 #11-27 RT: 0.10-0.23 AV: 17 NL: 1.39E8
T: FTMS + p ESI Full ms [100.00-1005.98]
411.28597
427.28067
857.54183
867.57092
Relative Abundance
m/z
[23-d]-2

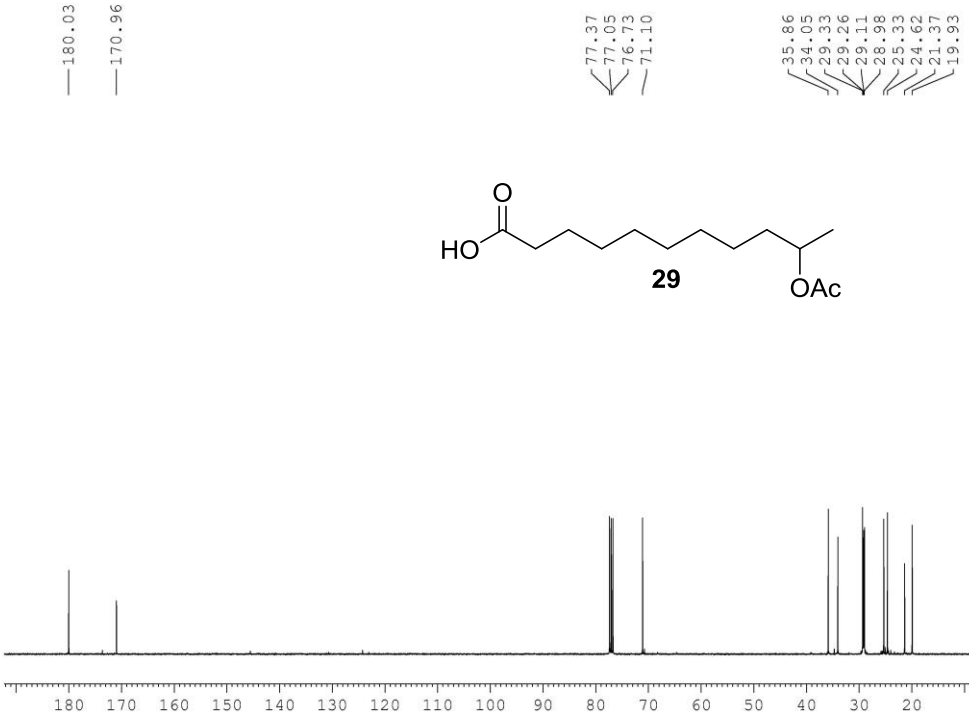

411.28597
412.28893
410.28040
413.29224
411.28648
412.28963
413.29259
416.30089
Relative Abundance
m/z
NL:
1.39E8
data03#11-27 RT: 0.10-0.23
AV: 17 T: FTMS + p ESI Full
ms [100.00-1005.98]
NL:
1.76E4
C25 H35 D1 N3 O2:
C25 H35 D1 N3 O2
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr. @FWHM


3.7946
3.7791
3.7772
2.3311
2.3125
2.2938
1.6345
1.6164
1.5983
1.4337
1.4255
1.4141
1.4090
1.3970
1.3895
1.3767
1.3648
1.3490
1.3415
1.3362
1.3288
1.3230
1.3143
1.3045
1.1675
1.1520
HO
O
OH
42
ppm
1.00
2.02
2.02
5.97
3.03

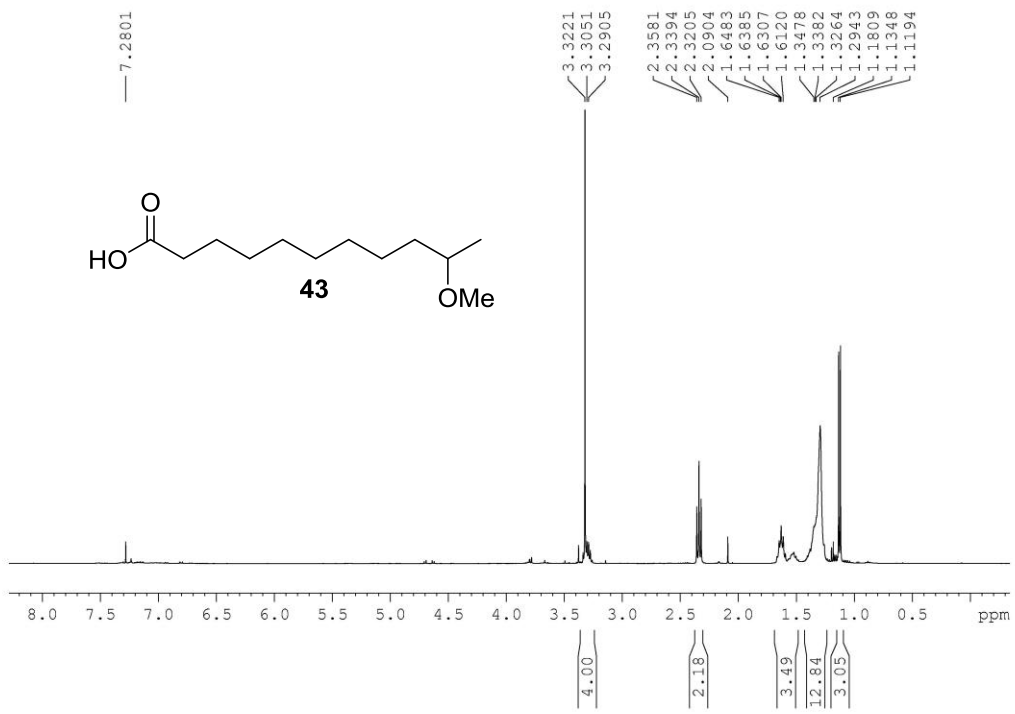

179.06
77.37
77.05
76.73
68.13
38.82
33.98
28.98
25.29
24.64
23.23
O
OH
HO
42
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5
7.2596
4.8848
4.8691
4.8547
4.8526
4.8370
2.3374
2.3187
2.2998
2.0052
1.6219
1.6040
1.5856
1.5670
1.5525
1.5368
1.4486
1.4440
1.4285
1.3312
1.3238
1.3141
1.2593
1.1831
1.1675
O
HO
29
OAc
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 ppm
1.00
2.00
2.87
3.14
1.17
10.75
3.12

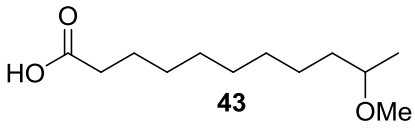
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5



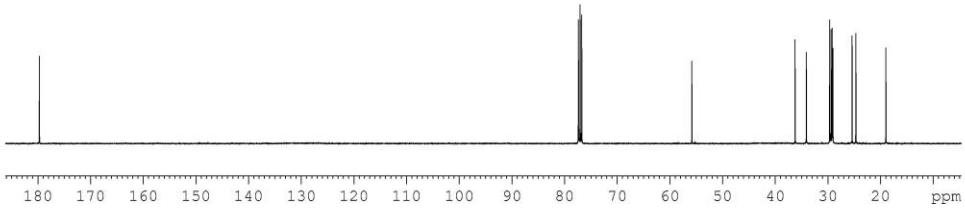
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 22



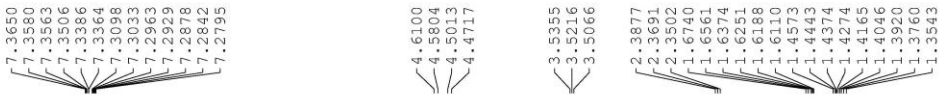
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 19

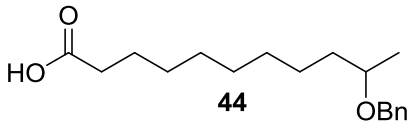


43

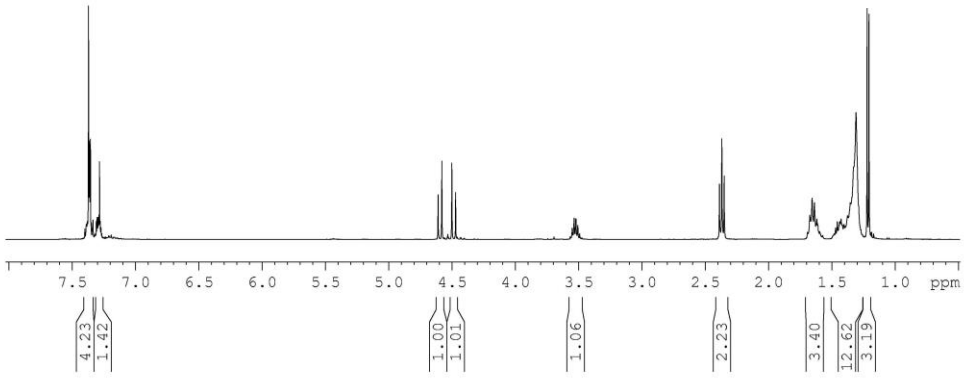


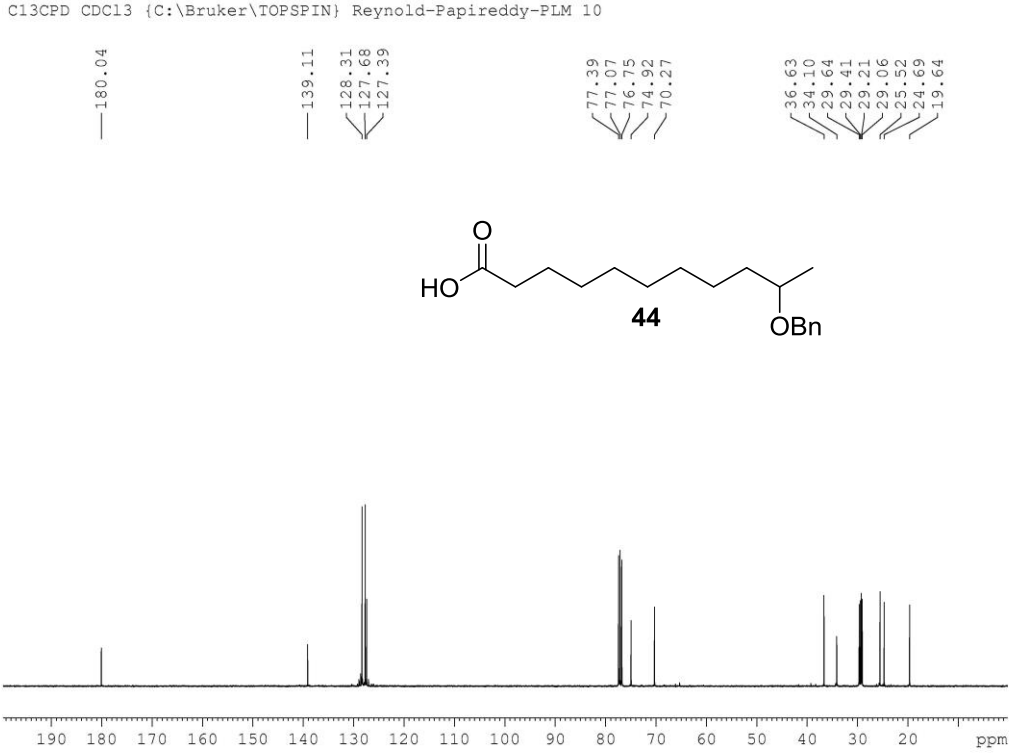
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 4

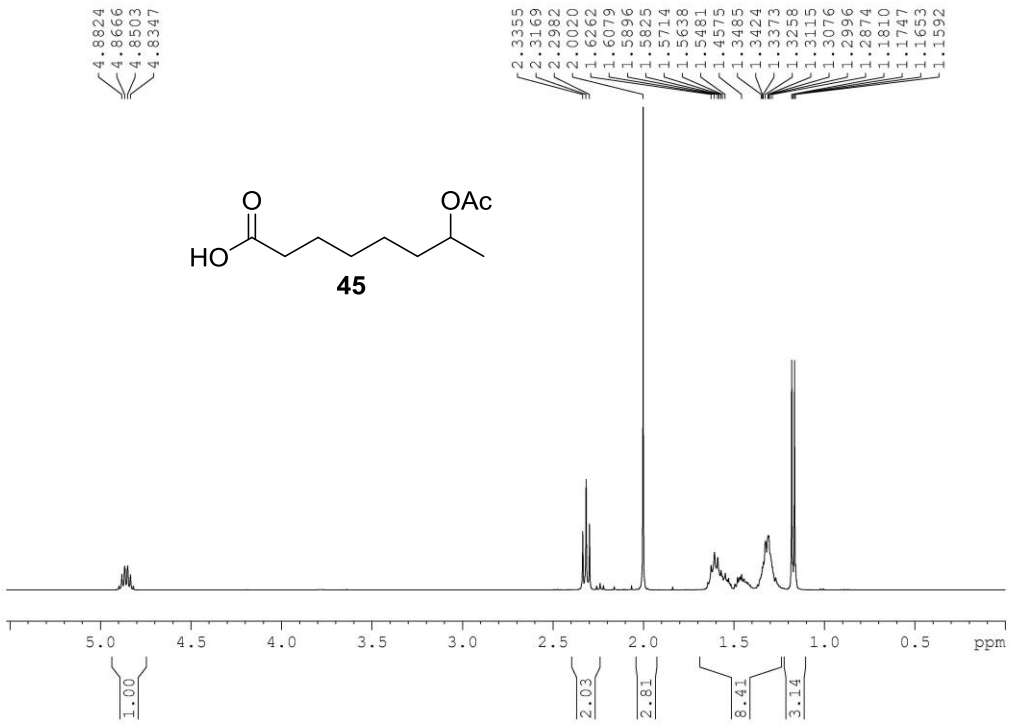


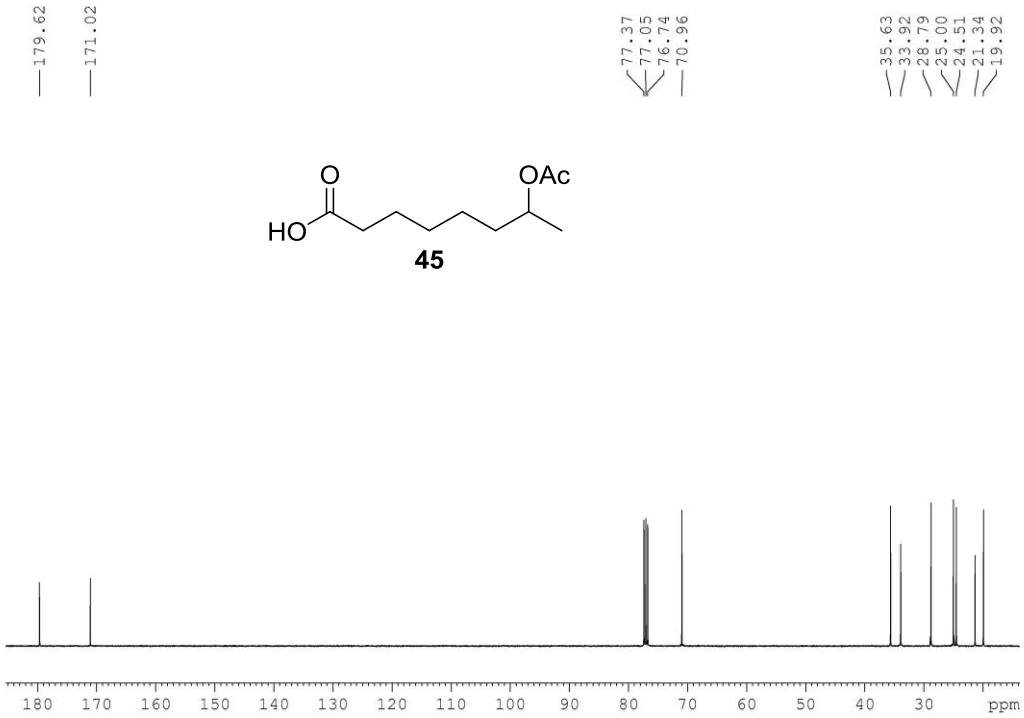


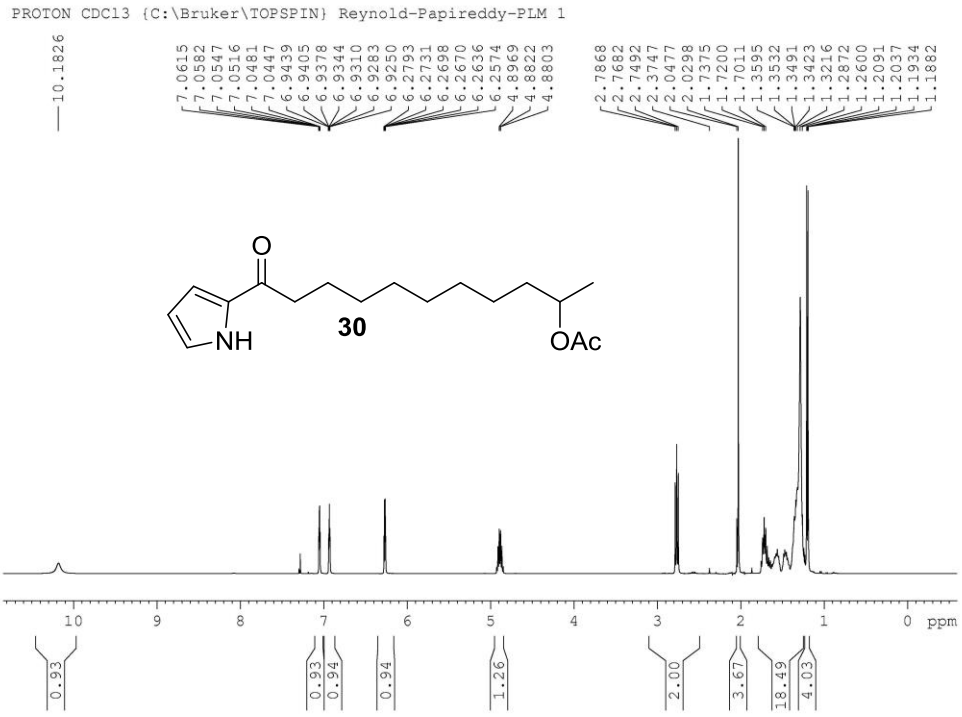
44

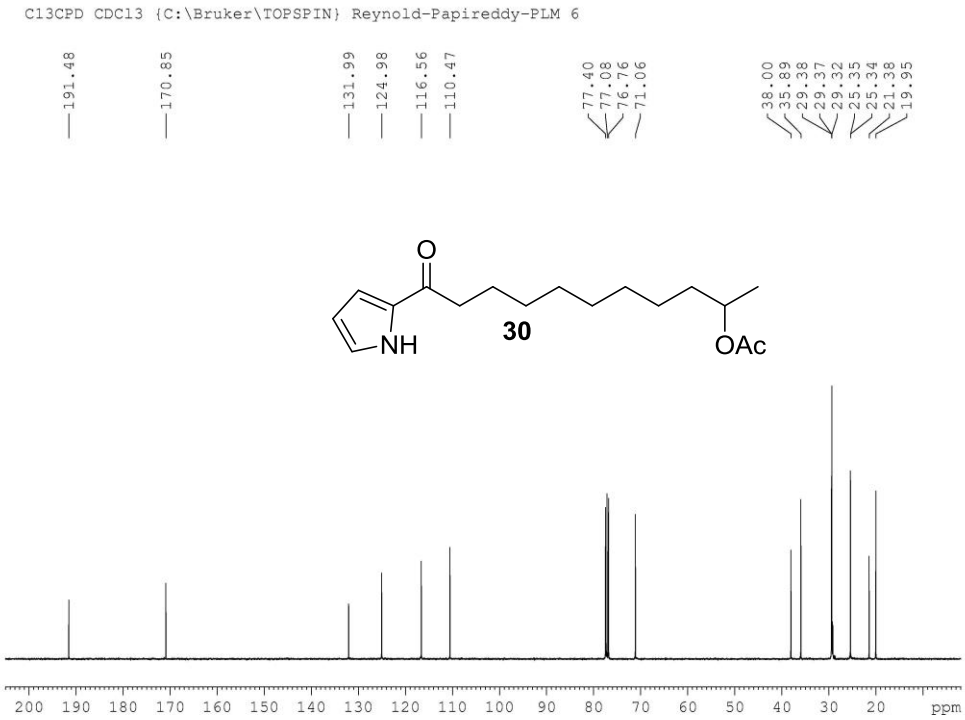


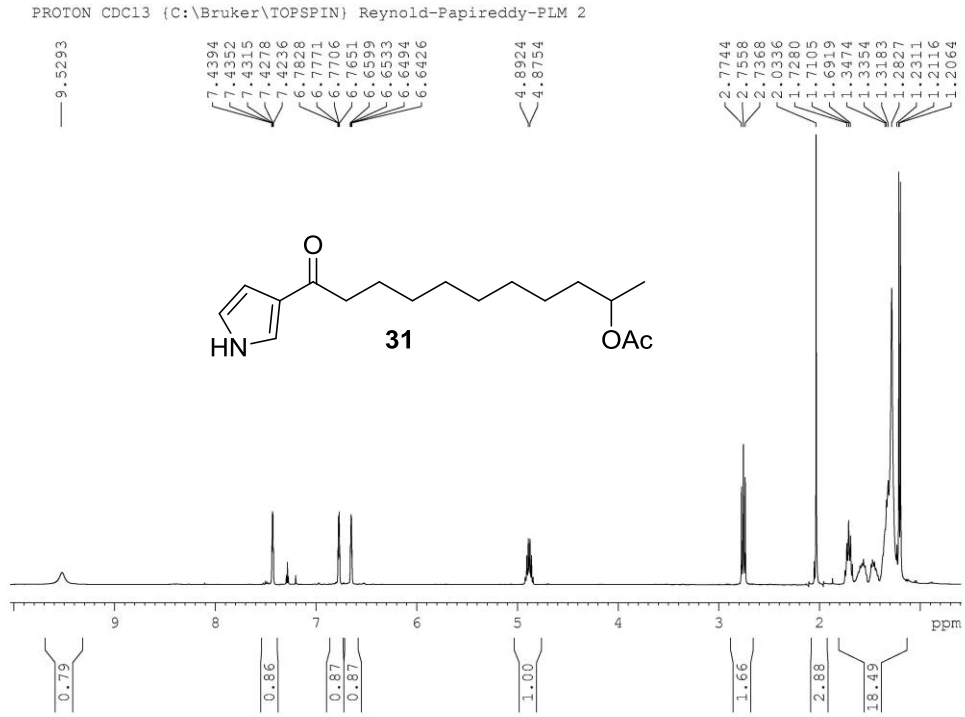

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 10
180.04
139.11
128.31
127.68
127.39
77.39
77.07
76.75
74.92
70.27
36.63
34.10
29.64
29.41
29.21
29.06
25.52
24.69
19.64
O
HO
OBn
44
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

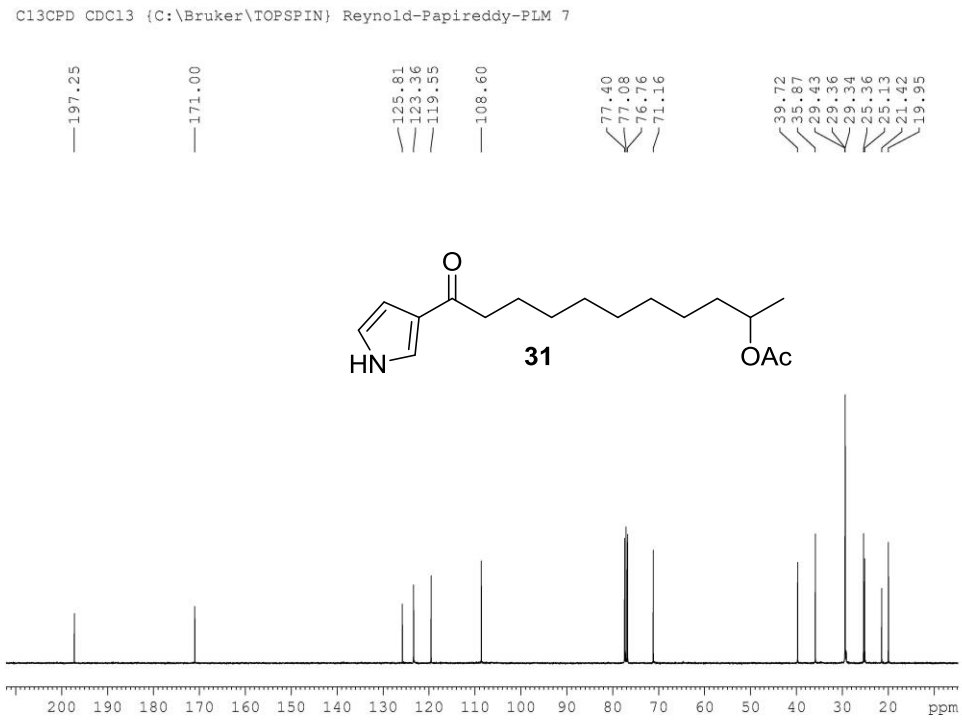

4.8824
4.8666
4.8503
4.8347
2.3355
2.3169
2.2982
2.0020
1.6262
1.6079
1.5896
1.5825
1.5714
1.5638
1.5481
1.4575
1.3485
1.3424
1.3373
1.3258
1.3115
1.3076
1.2996
1.2874
1.1810
1.1747
1.1653
1.1592
O
OAc
HO
45
5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
2.03
2.81
8.41
3.14

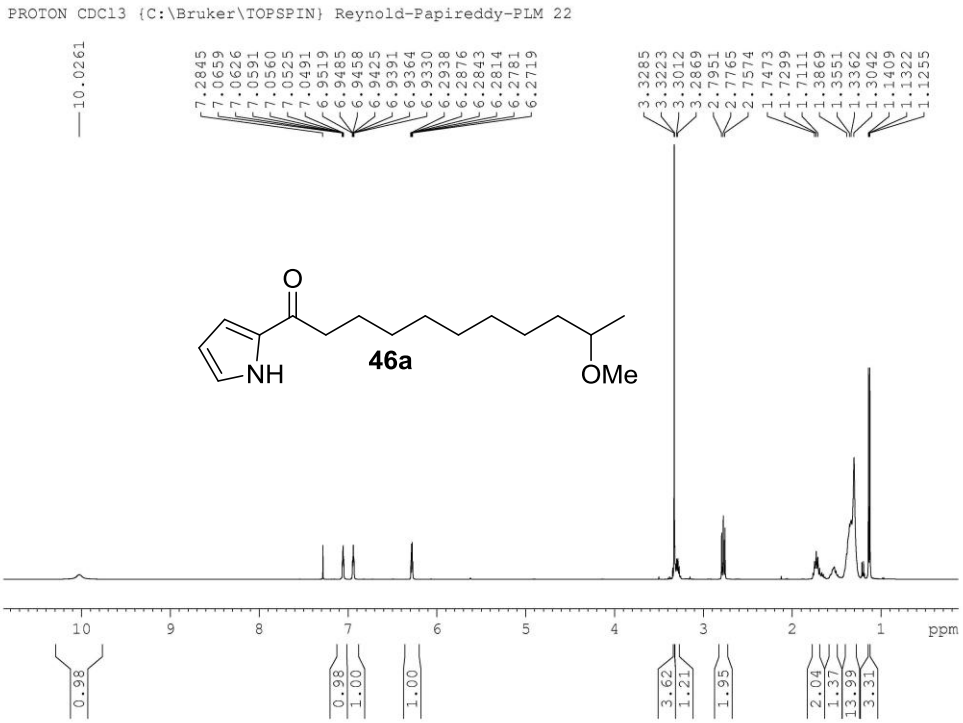

179.62
171.02
77.37
77.05
76.74
70.96
35.63
33.92
28.79
25.00
24.51
21.34
19.92
O
OAc
HO
45
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm


PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 1
10.1826
7.0615
7.0582
7.0547
7.0516
7.0481
7.0447
6.9439
6.9405
6.9378
6.9344
6.9310
6.9283
6.9250
6.2793
6.2731
6.2698
6.2670
6.2636
6.2574
4.8969
4.8822
4.8803
2.7868
2.7682
2.7492
2.3747
2.0477
2.0298
1.7375
1.7200
1.7011
1.3595
1.3532
1.3491
1.3423
1.3216
1.2872
1.2600
1.2091
1.2037
1.1934
1.1882
O
NH
30
OAc
10
9
8
7
6
5
4
3
2
1
0
ppm
0.93
0.93
0.94
0.94
1.26
2.00
3.67
18.49
4.03

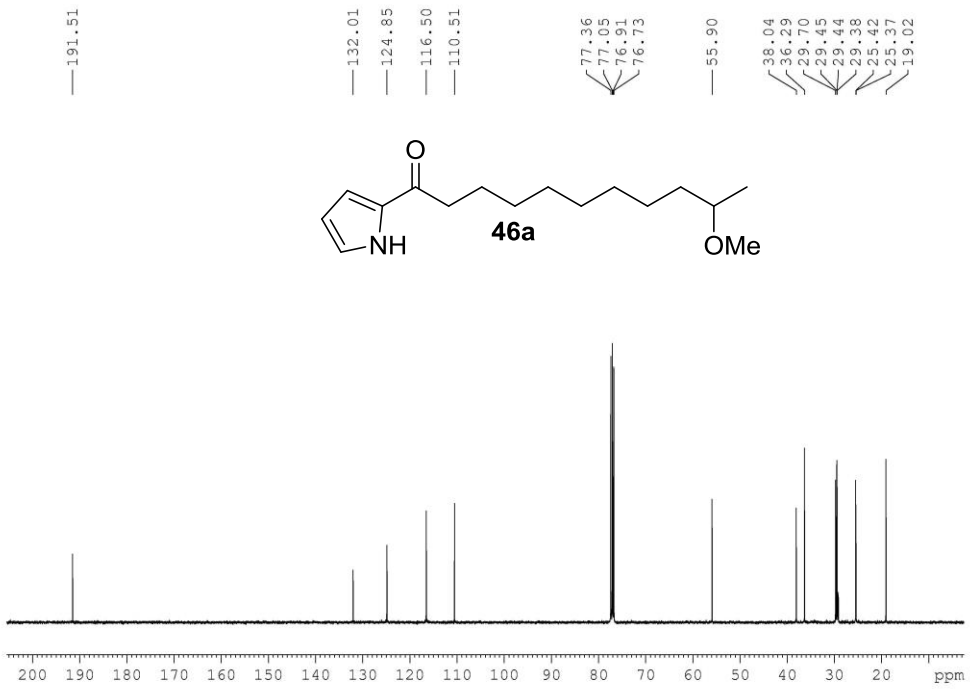

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 6
191.48
170.85
131.99
124.98
116.56
110.47
77.40
77.08
76.76
71.06
38.00
35.89
29.38
29.37
29.32
25.35
25.34
21.38
19.95
O
NH
30
OAc
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 2
9.5293
7.4394
7.4352
7.4315
7.4278
7.4236
6.7828
6.7771
6.7706
6.7651
6.6599
6.6533
6.6494
6.6426
4.8924
4.8754
2.7744
2.7558
2.7368
2.0336
1.7280
1.7105
1.6919
1.3474
1.3354
1.3183
1.2827
1.2311
1.2116
1.2064
O
HN
31
OAc
9 8 7 6 5 4 3 2 ppm
0.79
0.86
0.87
0.87
1.00
1.66
2.88
18.49

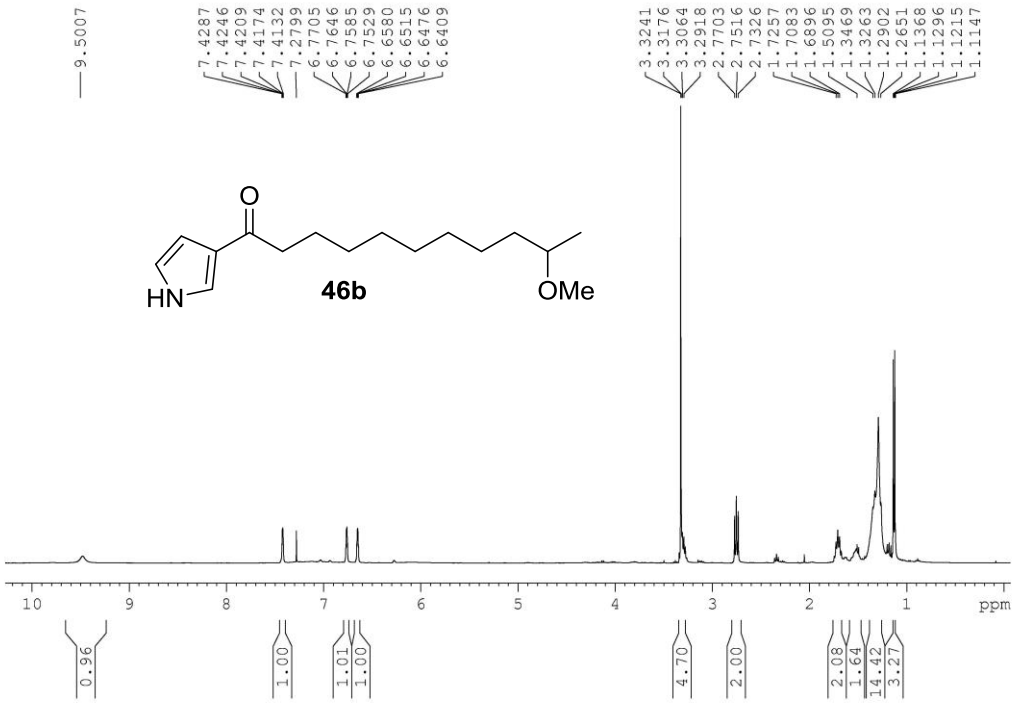

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 7
197.25
171.00
125.81
123.36
119.55
108.60
77.40
77.08
76.76
71.16
39.72
35.87
29.43
29.36
29.34
25.36
25.13
21.42
19.95
O
HN
31
OAc
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

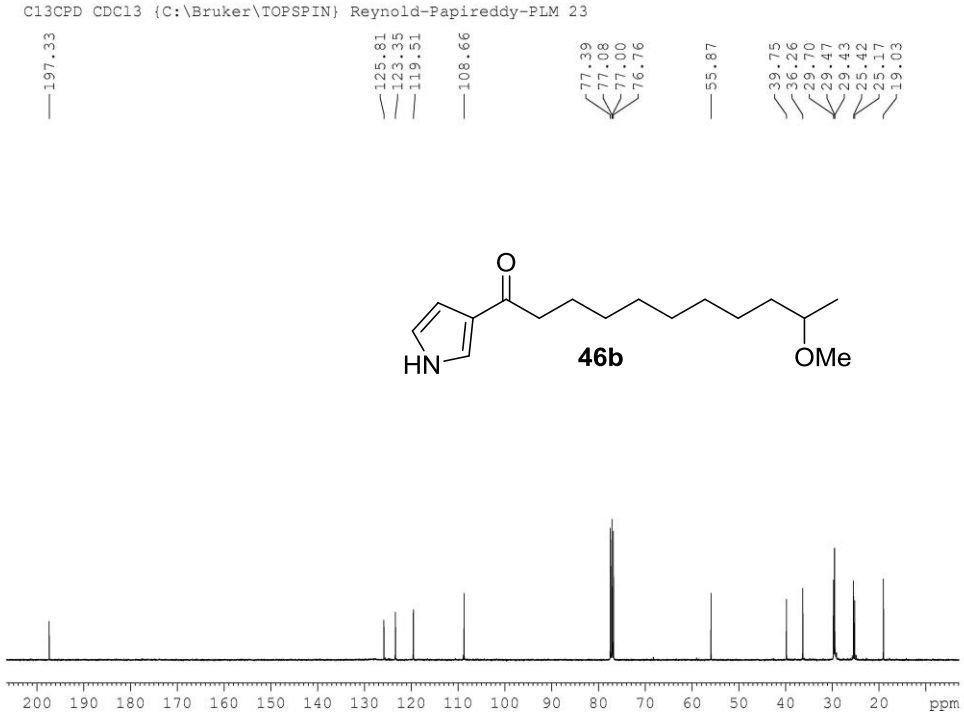

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 22
10.0261
7.2845
7.0659
7.0626
7.0591
7.0560
7.0525
7.0491
6.9519
6.9485
6.9458
6.9425
6.9391
6.9364
6.9330
6.2938
6.2876
6.2843
6.2814
6.2781
6.2719
3.3285
3.3223
3.3012
3.2869
2.7951
2.7765
2.7574
1.7473
1.7299
1.7111
1.3869
1.3551
1.3362
1.3042
1.1409
1.1322
1.1255
O
NH
46a
OMe
10 9 8 7 6 5 4 3 2 1 ppm
0.98
0.98
1.00
1.00
3.62
1.21
1.95
2.04
1.37
13.99
3.31

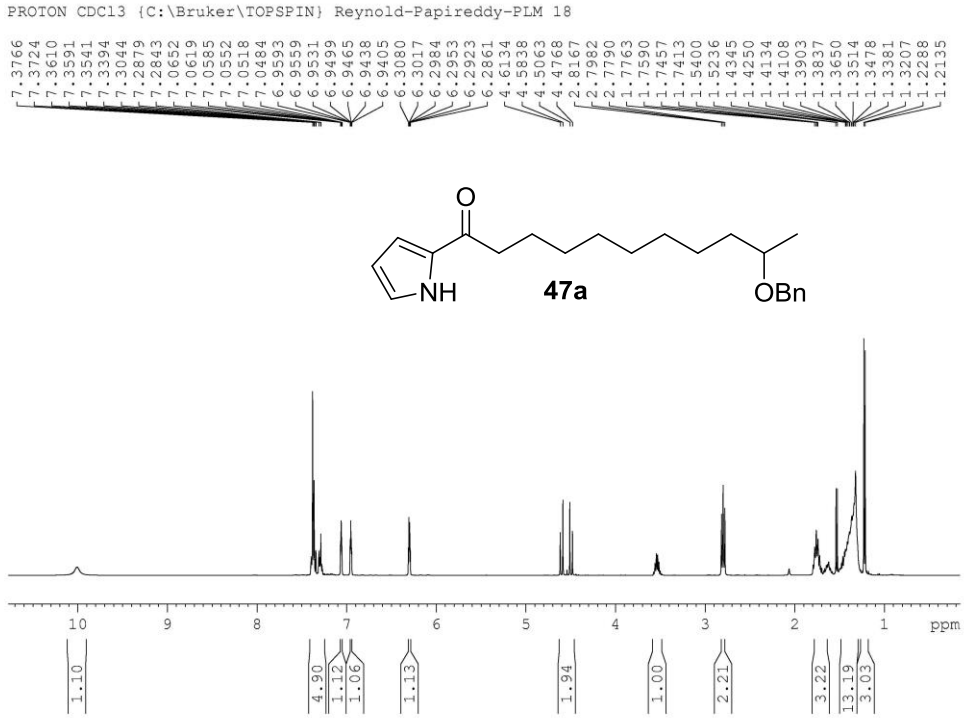
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 24



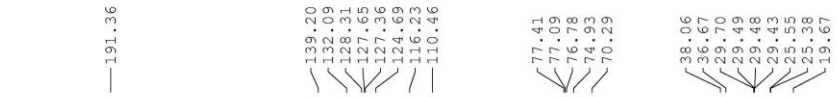
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 23

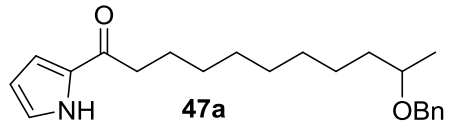


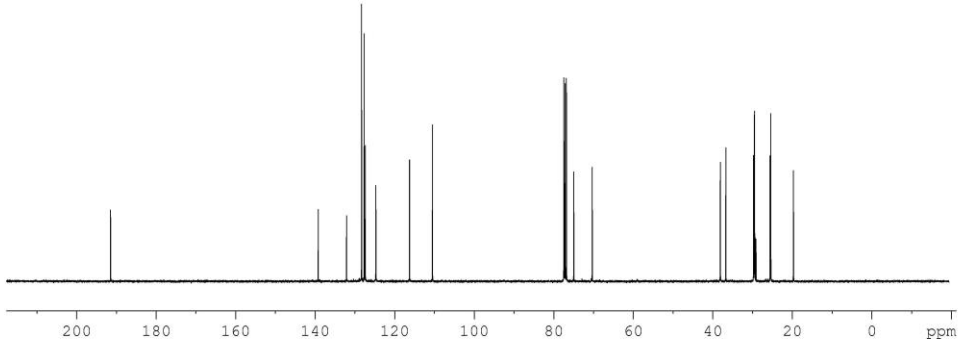

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 23
197.33
125.81
123.35
119.51
108.66
77.39
77.08
77.00
76.76
55.87
39.75
36.26
29.70
29.47
29.43
25.42
25.17
19.03
O
HN
46b
OMe
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 18
7.3766
7.3724
7.3610
7.3591
7.3541
7.3394
7.3044
7.2879
7.2843
7.0652
7.0619
7.0585
7.0552
7.0518
7.0484
6.9593
6.9559
6.9531
6.9499
6.9465
6.9438
6.9405
6.3080
6.3017
6.2984
6.2953
6.2923
6.2861
4.6134
4.5838
4.5063
4.4768
2.8167
2.7982
2.7790
2.7763
1.7590
1.7457
1.7413
1.5400
1.5236
1.4345
1.4250
1.4134
1.4108
1.3903
1.3837
1.3650
1.3514
1.3478
1.3381
1.3207
1.2288
1.2135
O
NH
47a
OBn
10 9 8 7 6 5 4 3 2 1 ppm
1.10
4.90
1.12
1.06
1.13
1.94
1.00
2.21
3.22
13.19
3.03

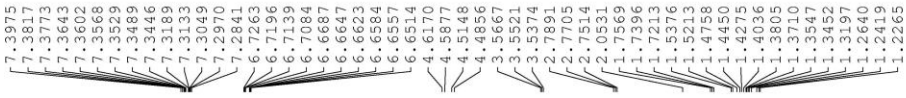
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 18

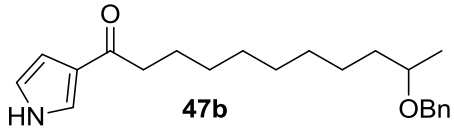


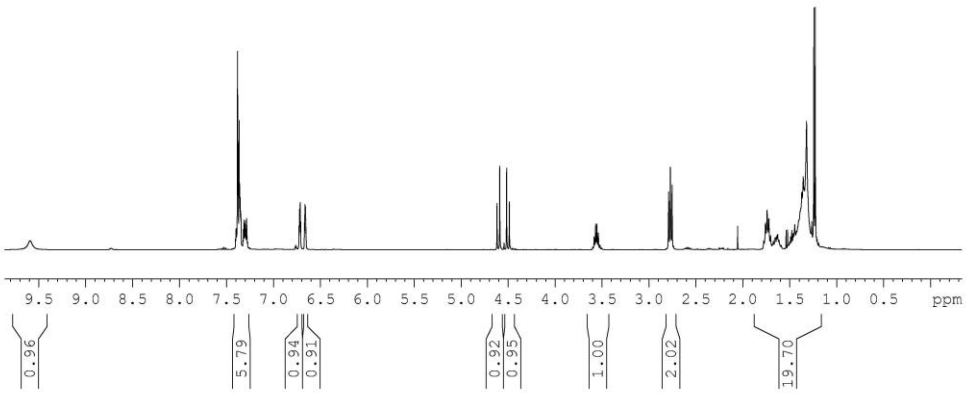


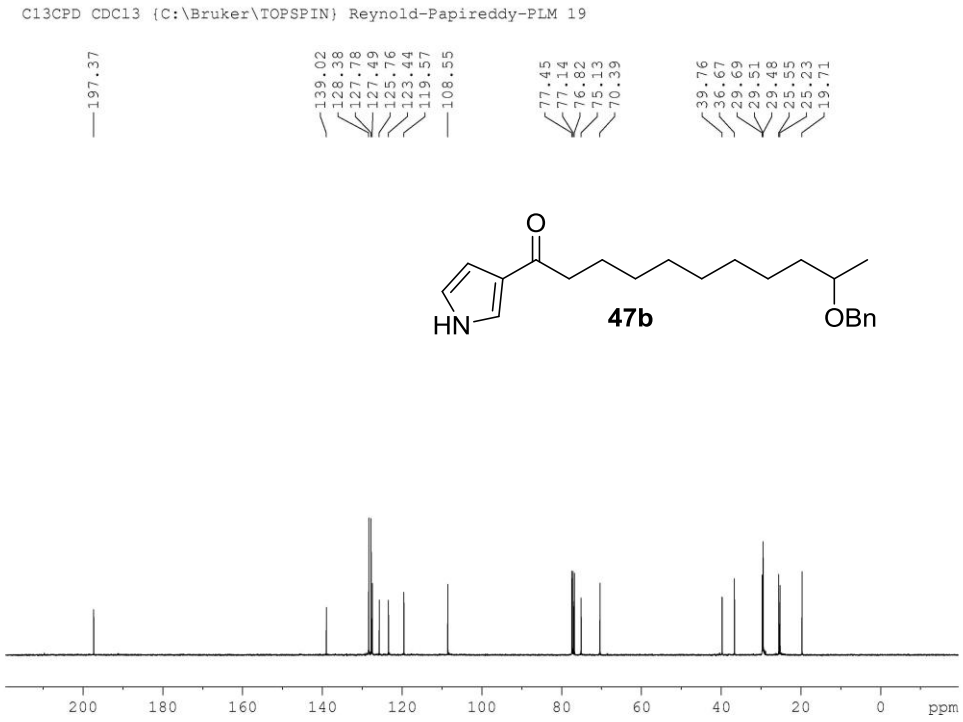


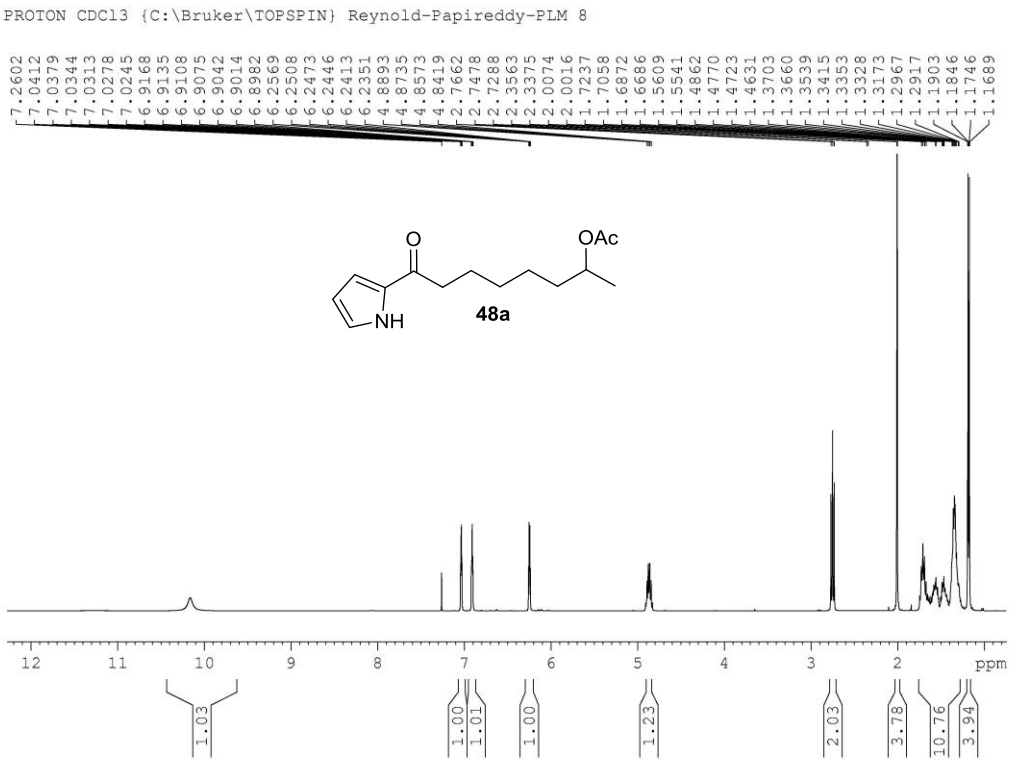
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 19



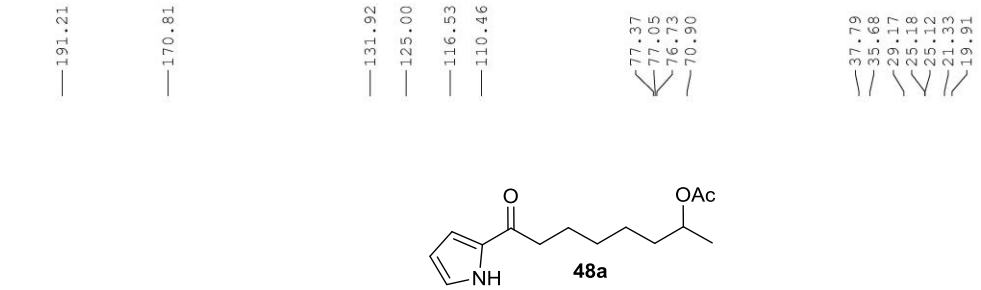




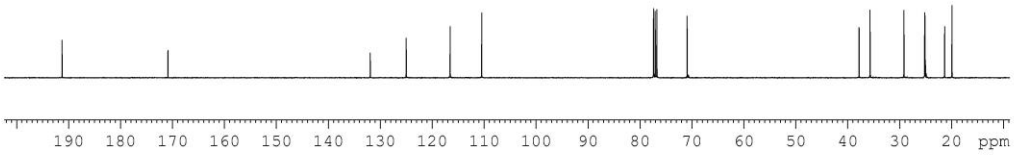

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 19
197.37
139.02
128.38
127.78
127.49
125.76
123.44
119.57
108.55
77.45
77.14
76.82
75.13
70.39
39.76
36.67
29.69
29.51
29.48
25.55
25.23
19.71
O
HN
47b
OBn
200
180
160
140
120
100
80
60
40
20
0
ppm


PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 8
7.2602
7.0412
7.0379
7.0344
7.0313
7.0278
7.0245
6.9168
6.9135
6.9108
6.9075
6.9042
6.9014
6.8982
6.2569
6.2508
6.2473
6.2446
6.2413
6.2351
4.8893
4.8735
4.8573
4.8419
2.7662
2.7478
2.7288
2.3563
2.3375
2.0074
2.0016
1.7237
1.7058
1.6872
1.6686
1.5609
1.5541
1.4862
1.4770
1.4723
1.4631
1.3703
1.3660
1.3539
1.3415
1.3353
1.3328
1.3173
1.2967
1.2917
1.1903
1.1846
1.1746
1.1689
O
OAc
NH
48a
12
11
10
9
8
7
6
5
4
3
2
ppm
1.03
1.00
1.01
1.00
1.23
2.03
3.78
10.76
3.94

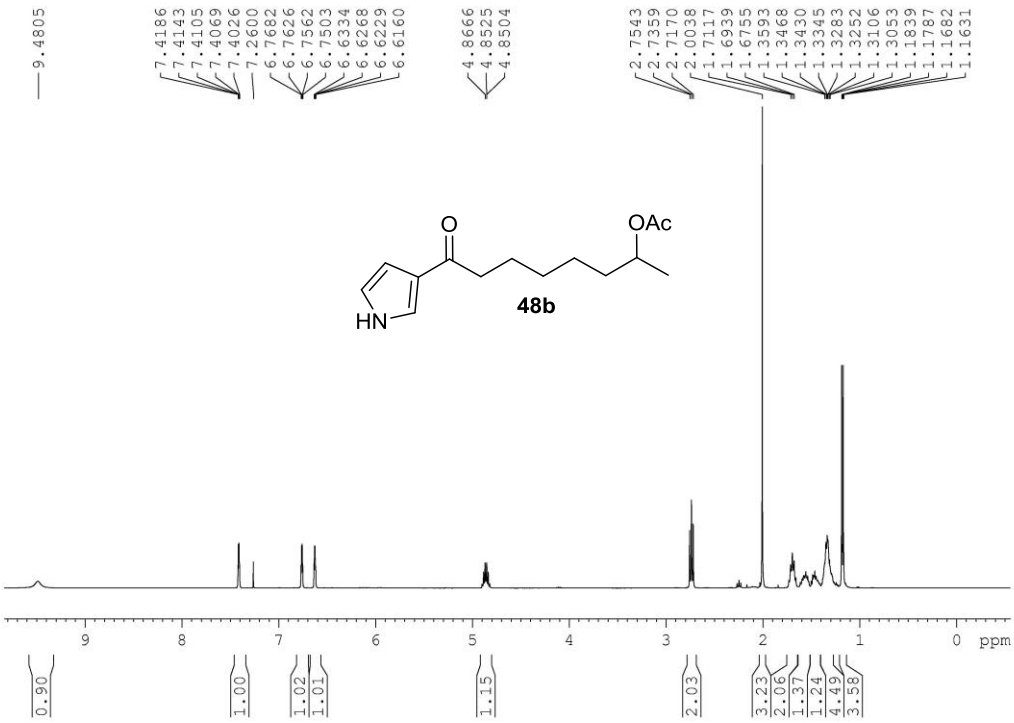
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 8



48a



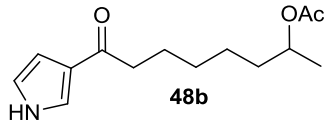
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 9



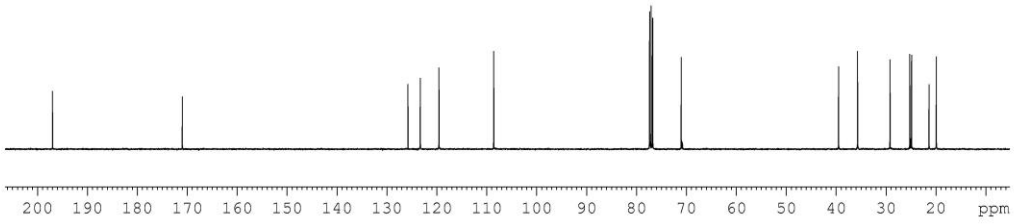
48b

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 9

196.97
170.96
125.76
123.30
119.54
108.58
77.36
77.04
76.73
71.02
39.50
35.69
29.20
25.23
24.86
21.37
19.91

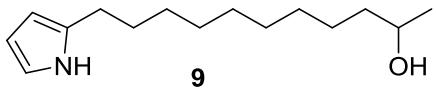


48b

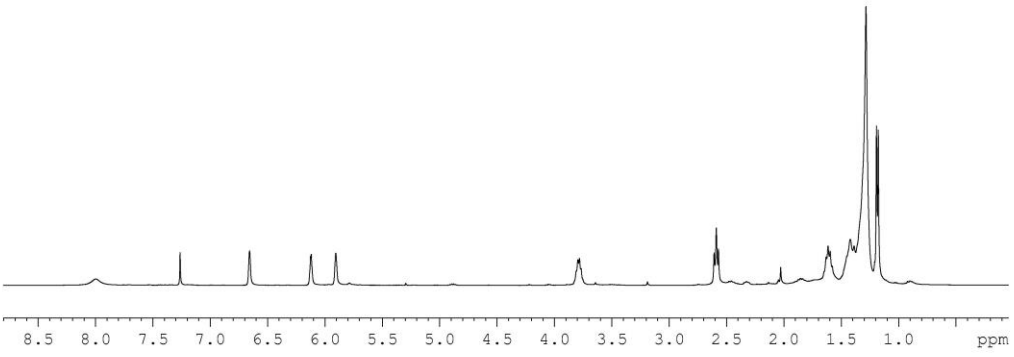


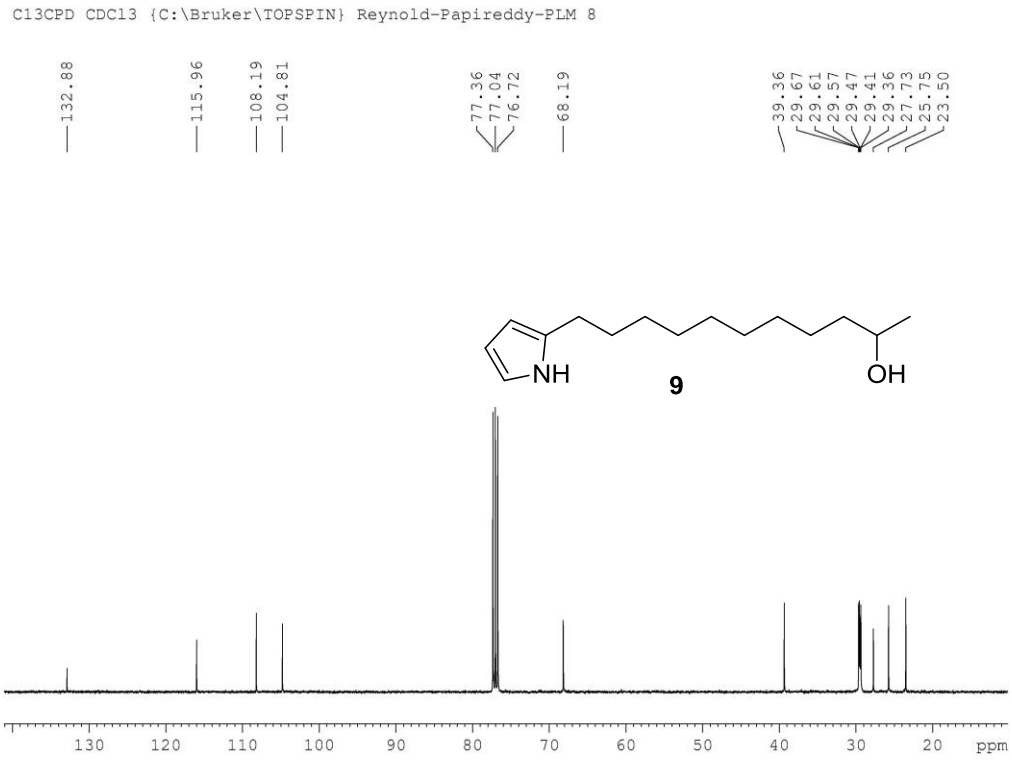
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 16

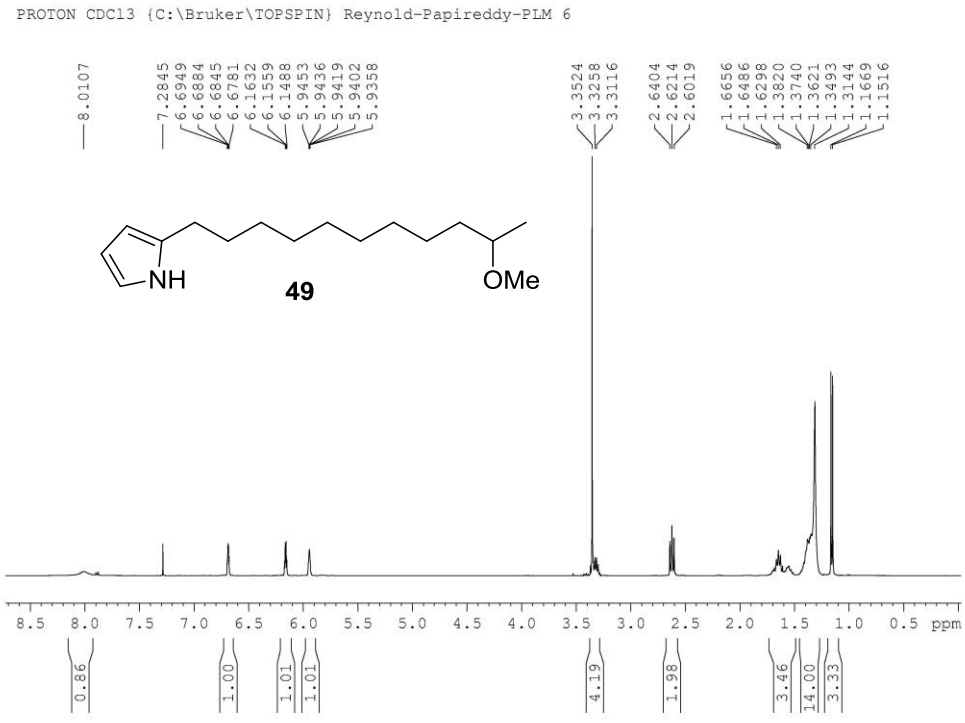
8.0000
7.2599
6.6537
6.1252
6.1189
5.9049
3.7950
3.7813
3.7665
2.6069
2.5881
2.5688
1.6305
1.6137
1.5954
1.5772
1.4189
1.3869
1.2829
1.1913
1.1759



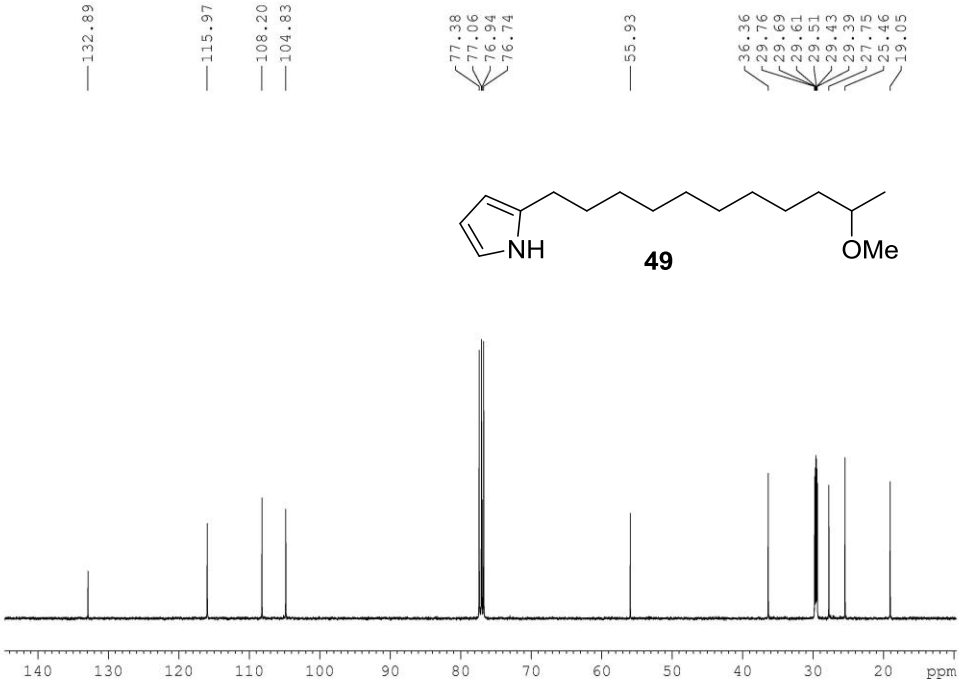
9



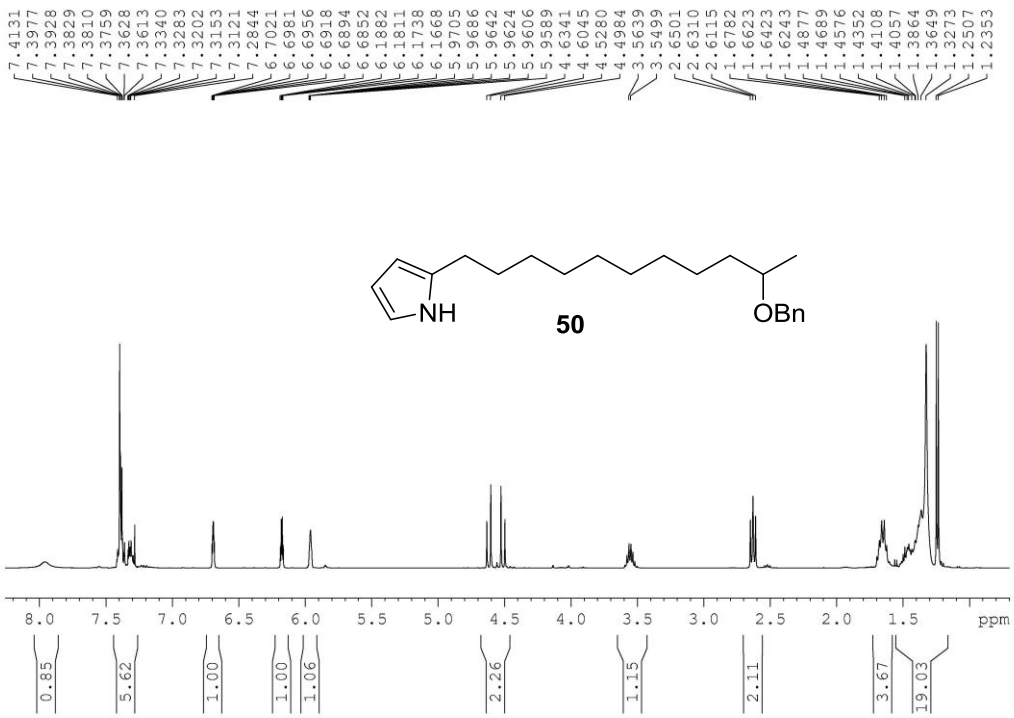

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 8
132.88
115.96
108.19
104.81
77.36
77.04
76.72
68.19
39.36
29.67
29.61
29.57
29.47
29.41
29.36
27.73
25.75
23.50
NH
OH
9
130
120
110
100
90
80
70
60
50
40
30
20
ppm

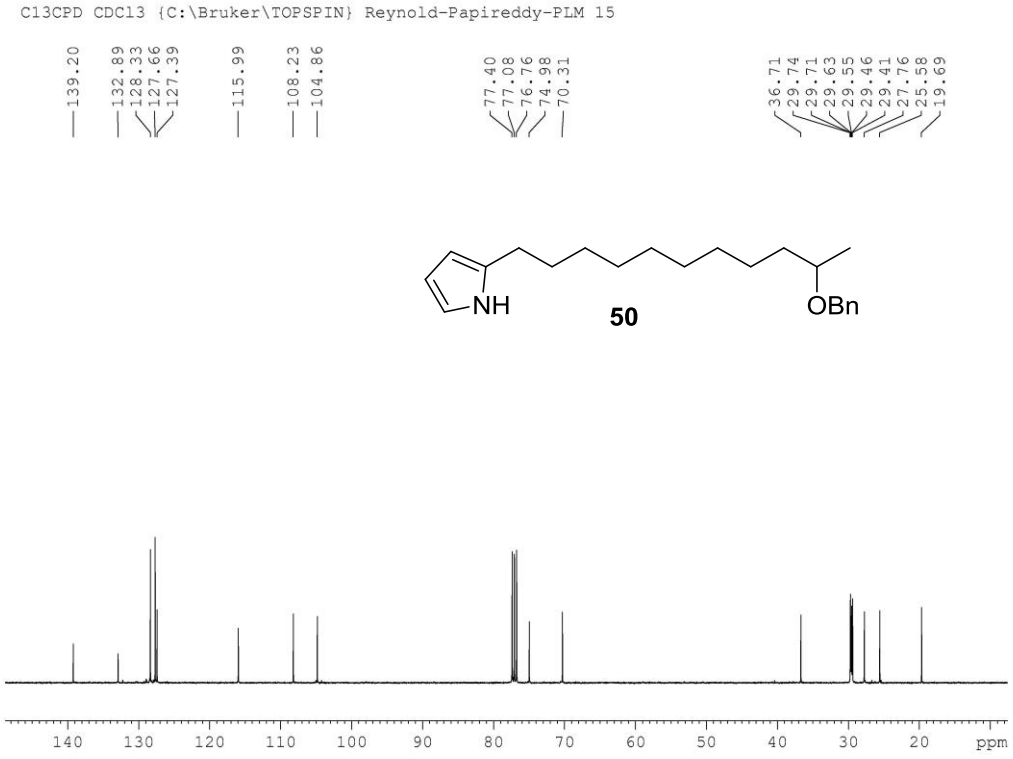

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 6
8.0107
7.2845
6.6949
6.6884
6.6845
6.6781
6.1632
6.1559
6.1488
5.9453
5.9436
5.9419
5.9402
5.9358
3.3524
3.3258
3.3116
2.6404
2.6214
2.6019
1.6656
1.6486
1.6298
1.3820
1.3740
1.3621
1.3493
1.3144
1.1669
1.1516
NH
OMe
49
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.86
1.00
1.01
1.01
4.19
1.98
3.46
14.00
3.33

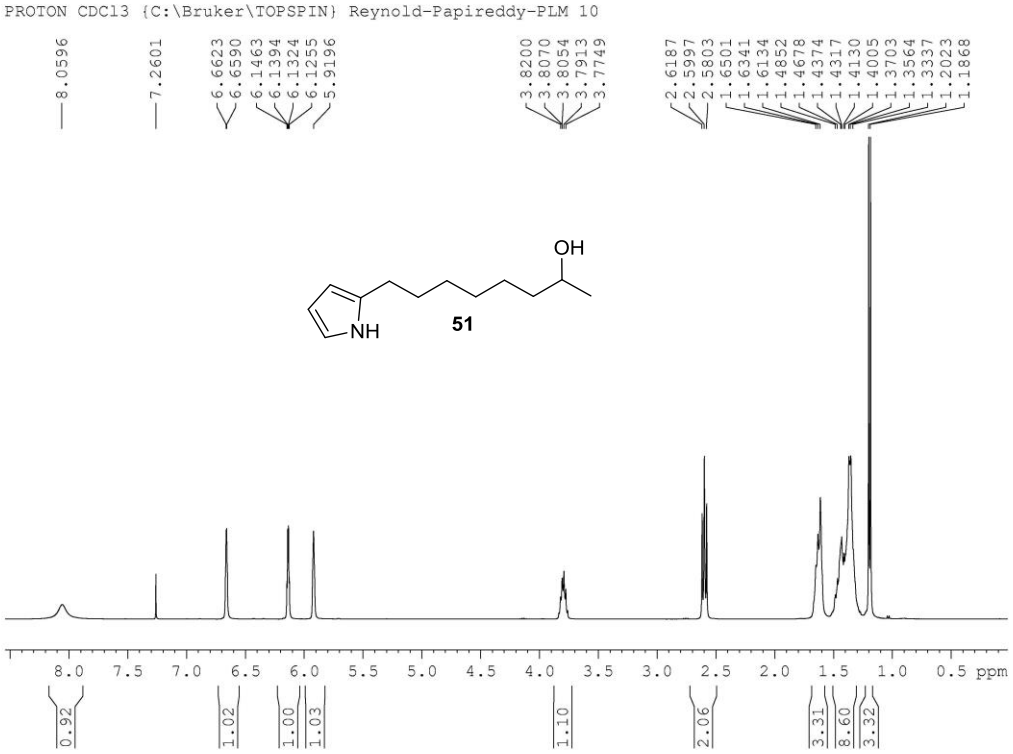
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 6



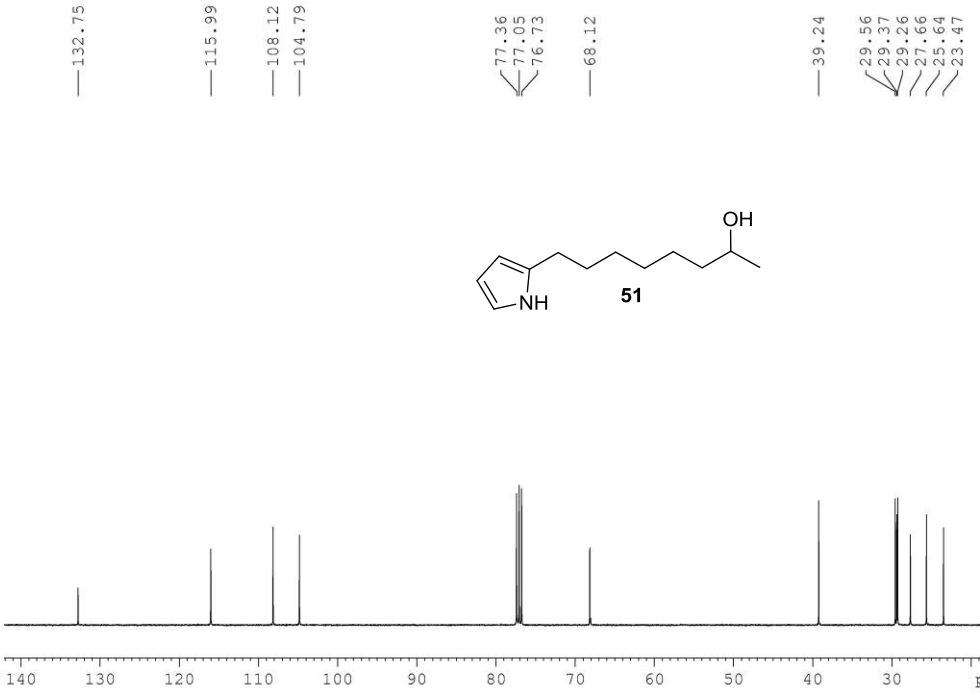
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 15



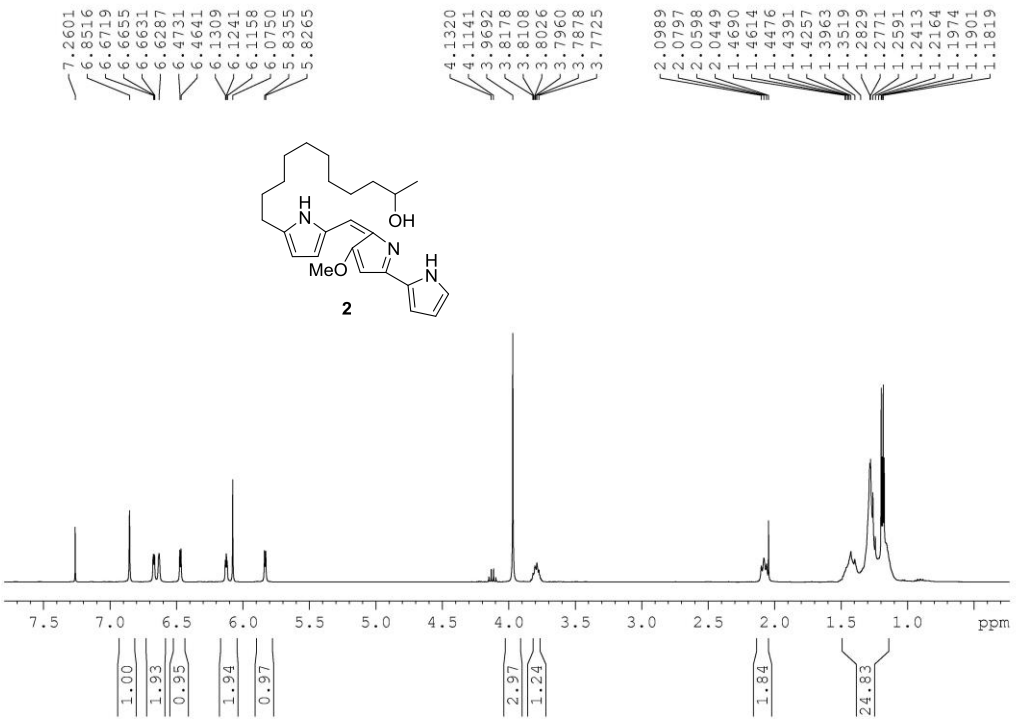

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 15
139.20
132.89
128.33
127.66
127.39
115.99
108.23
104.86
77.40
77.08
76.76
74.98
70.31
36.71
29.74
29.71
29.63
29.55
29.46
29.41
27.76
25.58
19.69
NH
OBn
50
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

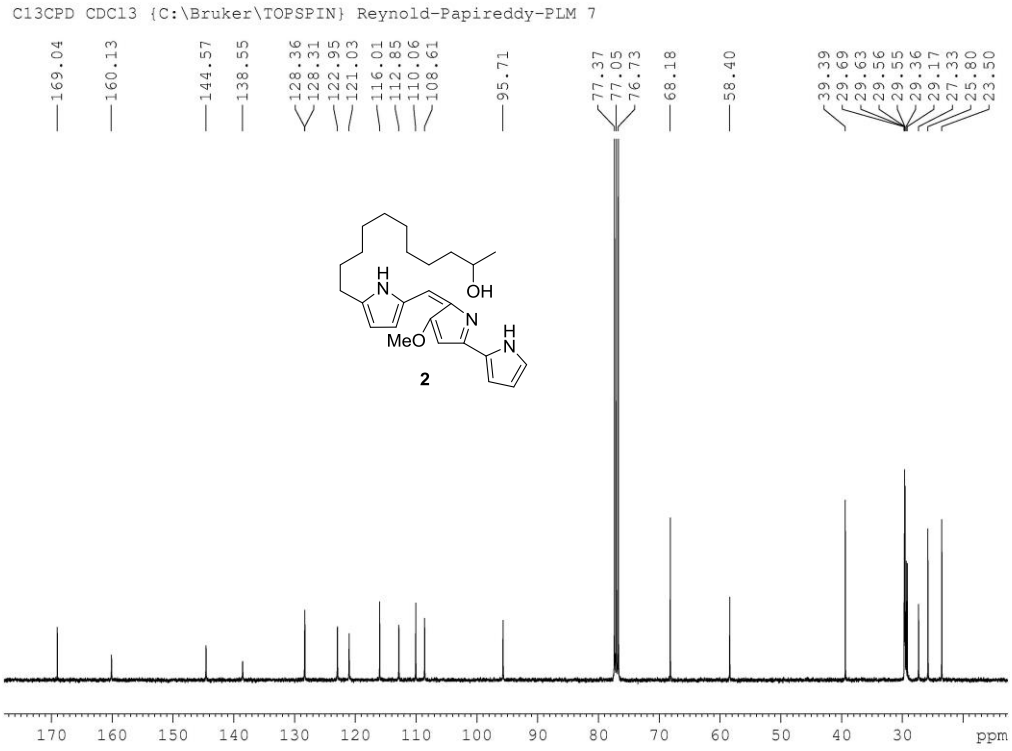

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 10
8.0596
7.2601
6.6623
6.6590
6.1463
6.1394
6.1324
6.1255
5.9196
3.8200
3.8070
3.8054
3.7913
3.7749
2.6187
2.5997
2.5803
1.6501
1.6341
1.6134
1.4852
1.4678
1.4374
1.4317
1.4130
1.4005
1.3703
1.3564
1.3337
1.2023
1.1868
OH
NH
51
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.92
1.02
1.00
1.03
1.10
2.06
3.31
8.60
3.32

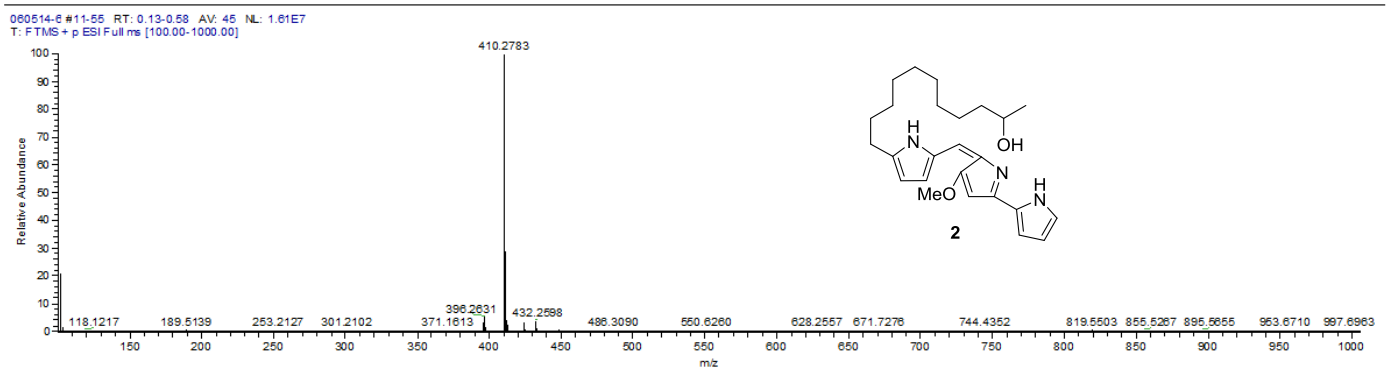
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 10

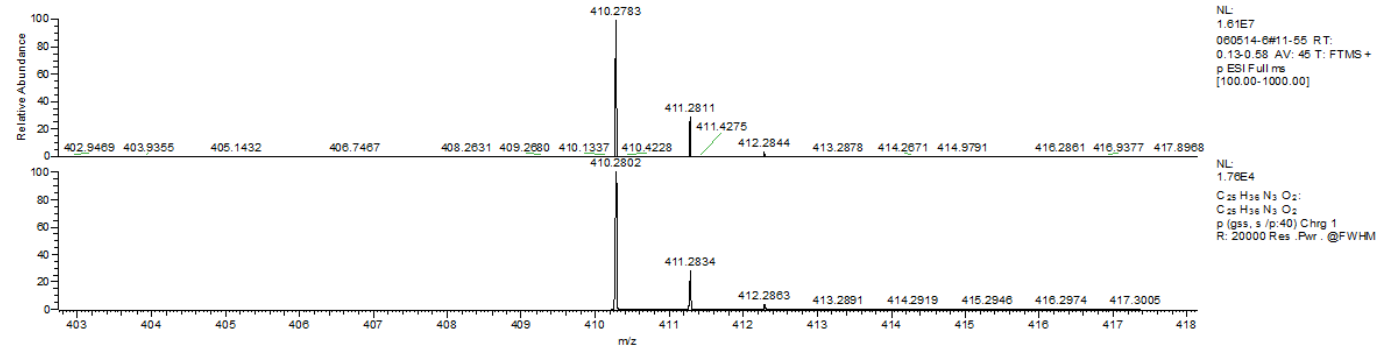


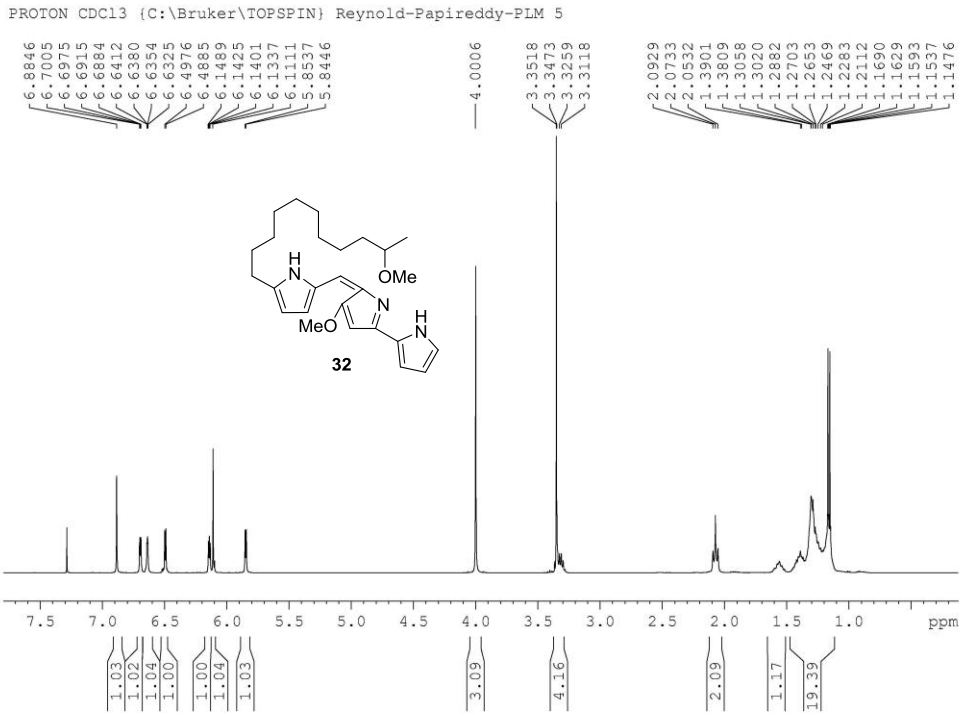
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 7

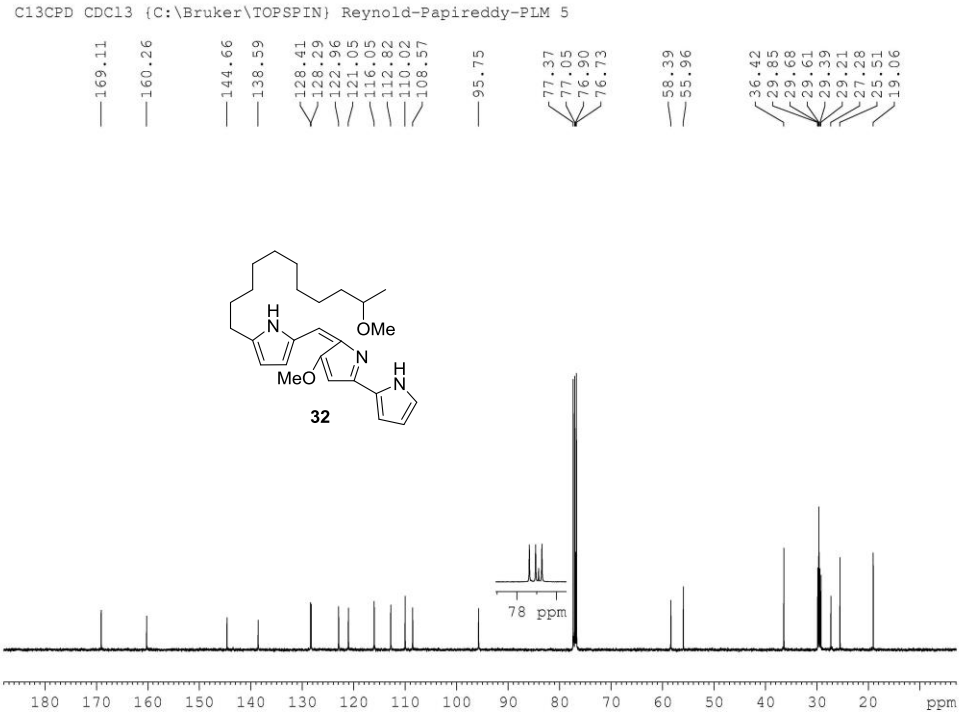


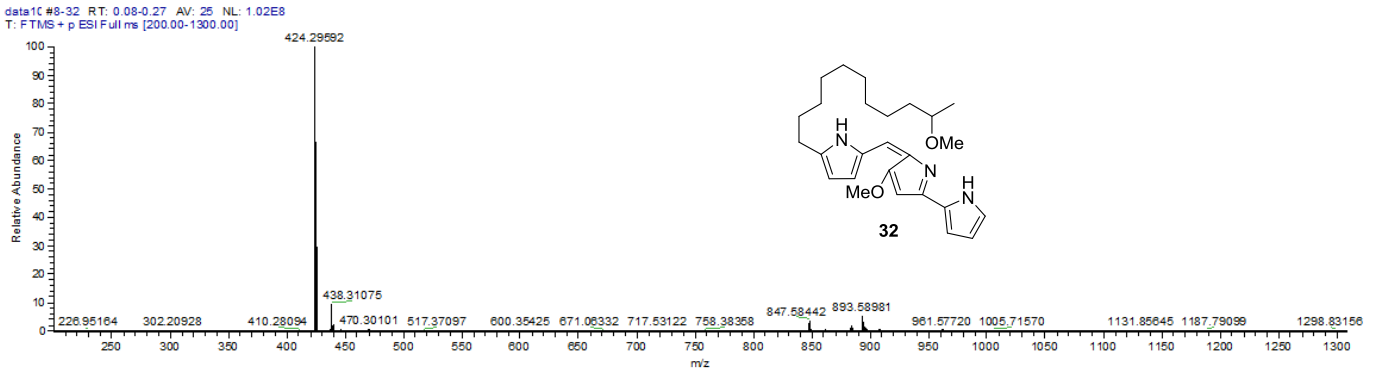

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 7
169.04
160.13
144.57
138.55
128.36
128.31
122.95
121.03
116.01
112.85
110.06
108.61
95.71
77.37
77.05
76.73
68.18
58.40
39.39
29.69
29.63
29.56
29.55
29.36
29.17
27.33
25.80
23.50
OH
H
N
N
MeO
H
N
2
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

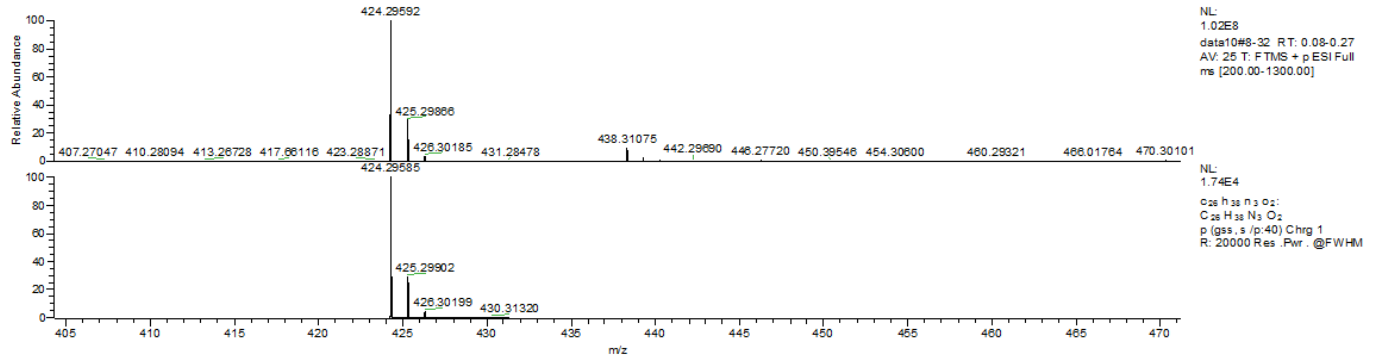

060514-6 #11-55 RT: 0.13-0.58 AV: 45 NL: 1.61E7
T: FTMS + p ESI Full ms [100.00-1000.00]
410.2783
Relative Abundance
118.1217
189.5139
253.2127
301.2102
371.1613
396.2631
432.2698
486.3090
550.6260
628.2557
671.7276
744.4352
819.5503
855.5267
895.5655
953.6710
997.6963
m/z
OH
H
N
N
MeO
H
N
2

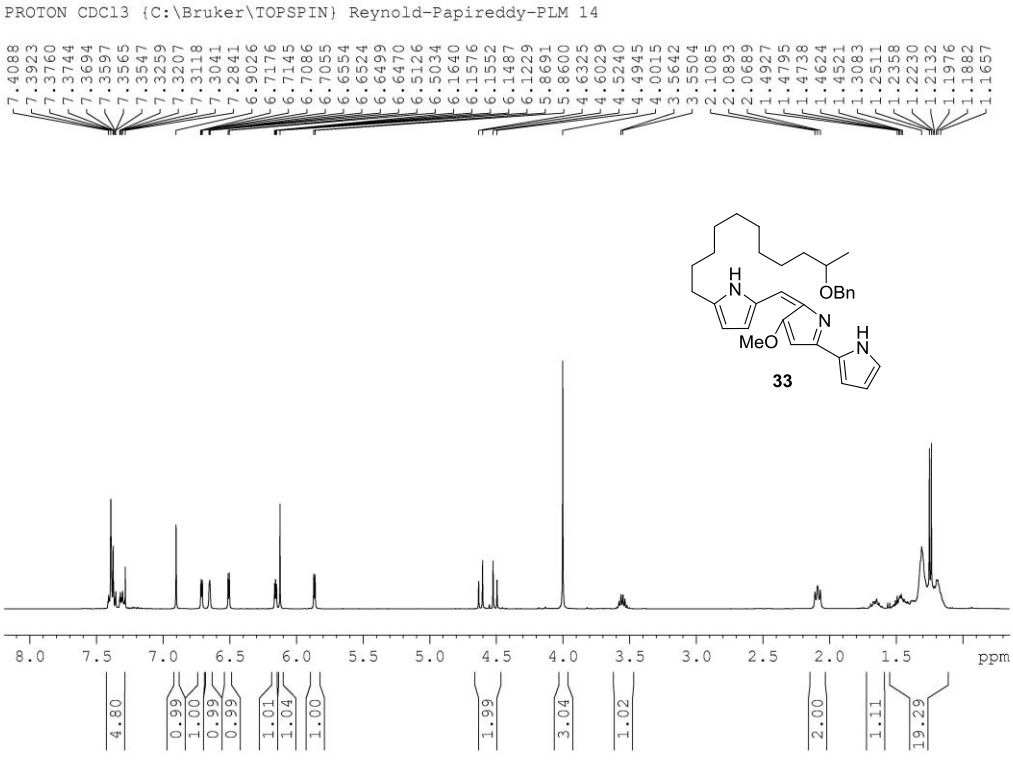

410.2783
411.2811
411.4275
412.2844
Relative Abundance
402.9469
403.9355
405.1432
406.7467
408.2631
409.2680
410.1337
410.4228
413.2878
414.2671
414.9791
416.2861
416.9377
417.8968
NL:
1.61E7
060514-6#11-55 RT:
0.13-0.58 AV: 45 T: FTMS +
p ESI Full ms
[100.00-1000.00]
410.2802
411.2834
412.2863
413.2891
414.2919
415.2946
416.2974
417.3005
NL:
1.76E4
C25 H36 N3 O2:
C25 H36 N3 O2
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr . @FWHM
m/z

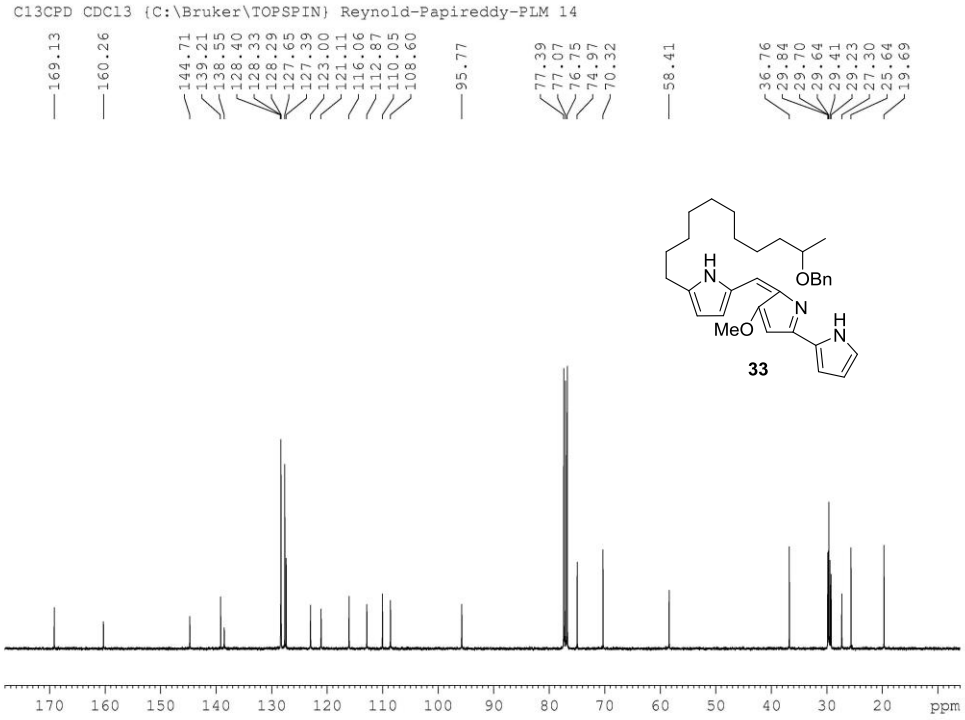

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5
6.8846
6.7005
6.6975
6.6915
6.6884
6.6412
6.6380
6.6354
6.6325
6.4976
6.4885
6.1489
6.1425
6.1401
6.1337
6.1111
5.8537
5.8446
4.0006
3.3518
3.3473
3.3259
3.3118
2.0929
2.0733
2.0532
1.3901
1.3809
1.3058
1.3020
1.2882
1.2703
1.2653
1.2469
1.2283
1.2112
1.1690
1.1629
1.1593
1.1537
1.1476
OMe
MeO
32
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
ppm
1.03
1.02
1.04
1.00
1.00
1.04
1.03
3.09
4.16
2.09
1.17
19.39

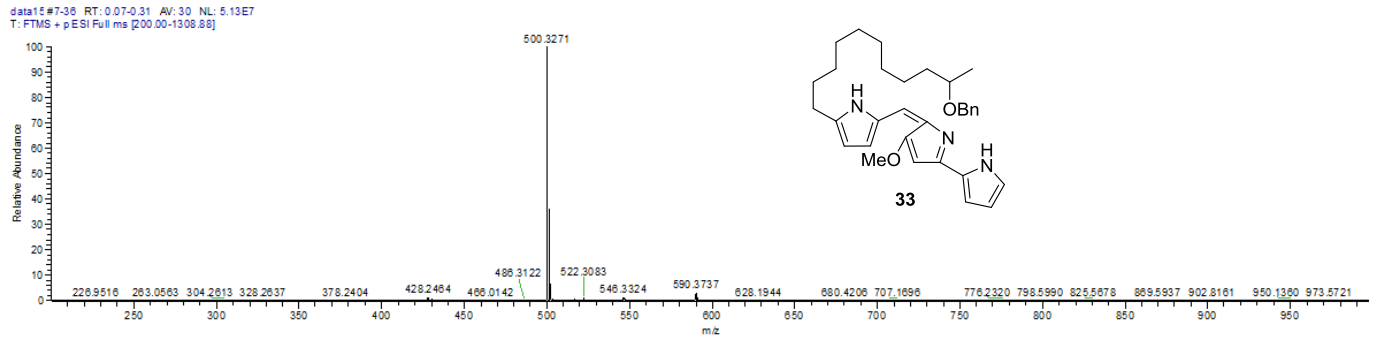

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5
169.11
160.26
144.66
138.59
128.41
128.29
122.96
121.05
116.05
112.82
110.02
108.57
95.75
77.37
77.05
76.90
76.73
58.39
55.96
36.42
29.85
29.68
29.61
29.39
29.21
27.28
25.51
19.06
OMe
MeO
32
78 ppm
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

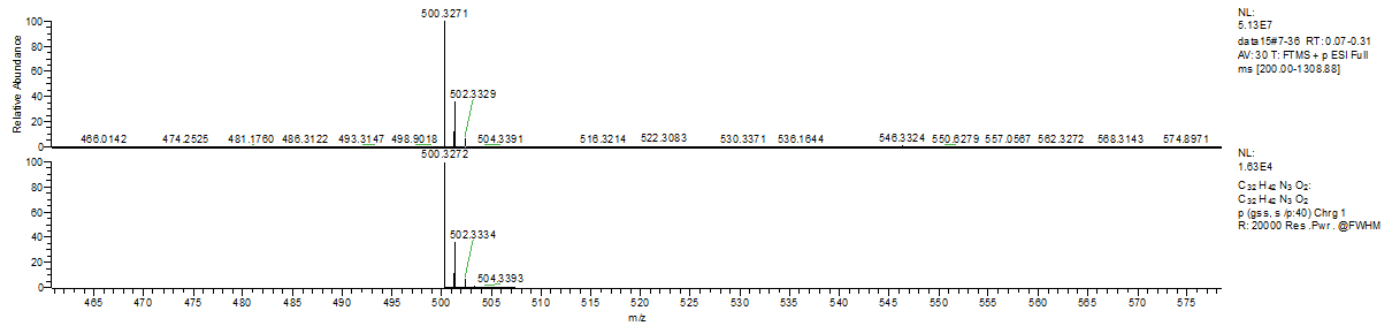

data10 #8-32 RT: 0.08-0.27 AV: 25 NL: 1.02E8
T: FTMS + p ESI Full ms [200.00-1300.00]
424.29592
438.31075
Relative Abundance
m/z
OMe
MeO
32


424.29592
425.29866
426.30185
438.31075
424.29585
425.29902
426.30199
430.31320
Relative Abundance
m/z
NL:
1.02E8
data10#8-32 RT: 0.08-0.27
AV: 25 T: FTMS + p ESI Full
ms [200.00-1300.00]
NL:
1.74E4
C28 H38 N3 O2:
C28 H38 N3 O2
p (gss, s /p:40) Chrg 1
R: 20000 Res. Pwr. @FWHM

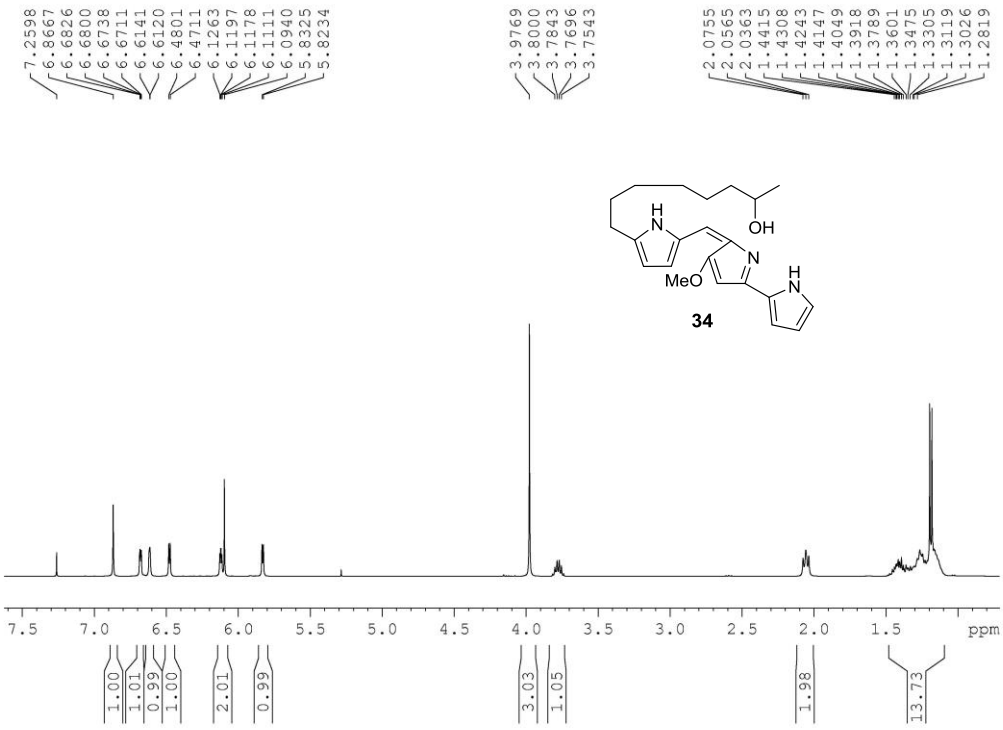

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 14
OBn
MeO
33
ppm
4.80
0.99
1.00
0.99
0.99
1.01
1.04
1.00
1.99
3.04
1.02
2.00
1.11
19.29


C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 14
169.13
160.26
144.71
139.21
138.55
128.40
128.33
128.29
127.65
127.39
123.00
121.11
116.06
112.87
110.05
108.60
95.77
77.39
77.07
76.75
74.97
70.32
58.41
36.76
29.84
29.70
29.64
29.41
29.23
27.30
25.64
19.69
OBn
MeO
33
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

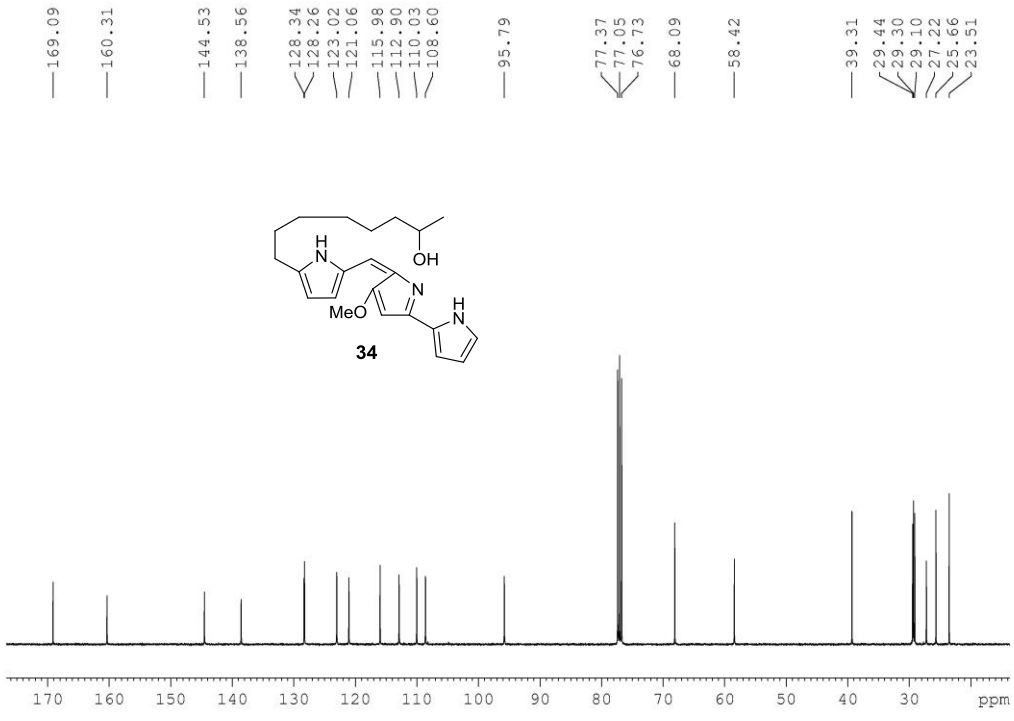

data15#7-36 RT: 0.07-0.31 AV: 30 NL: 5.13E7
T: FTMS + p ESI Full ms [200.00-1308.88]
500.3271
Relative Abundance
m/z
33

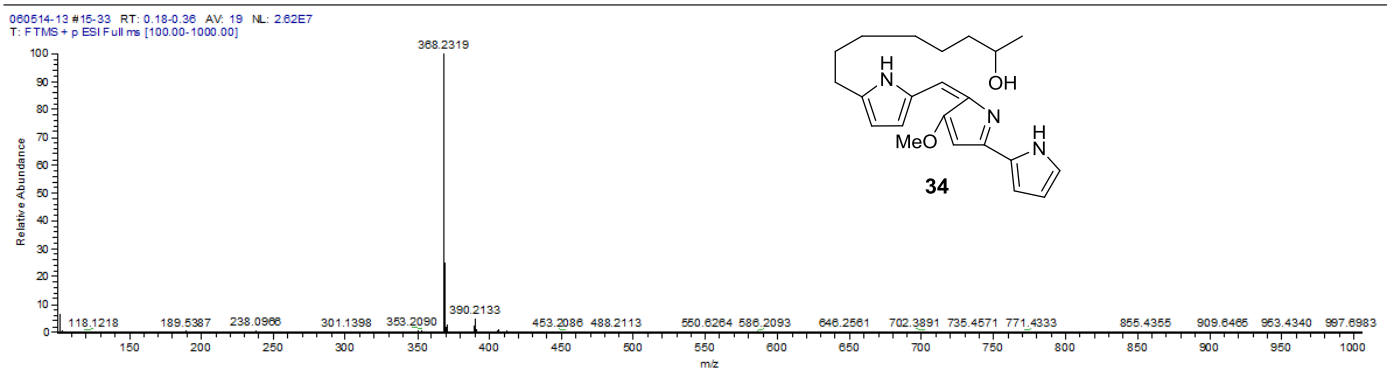

500.3271
502.3329
500.3272
502.3334
504.3393
Relative Abundance
m/z
NL:
5.13E7
data15#7-36 RT: 0.07-0.31
AV: 30 T: FTMS + p ESI Full
ms [200.00-1308.88]
NL:
1.63E4
C32 H42 N3 O2:
C32 H42 N3 O2
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr. @FWHM

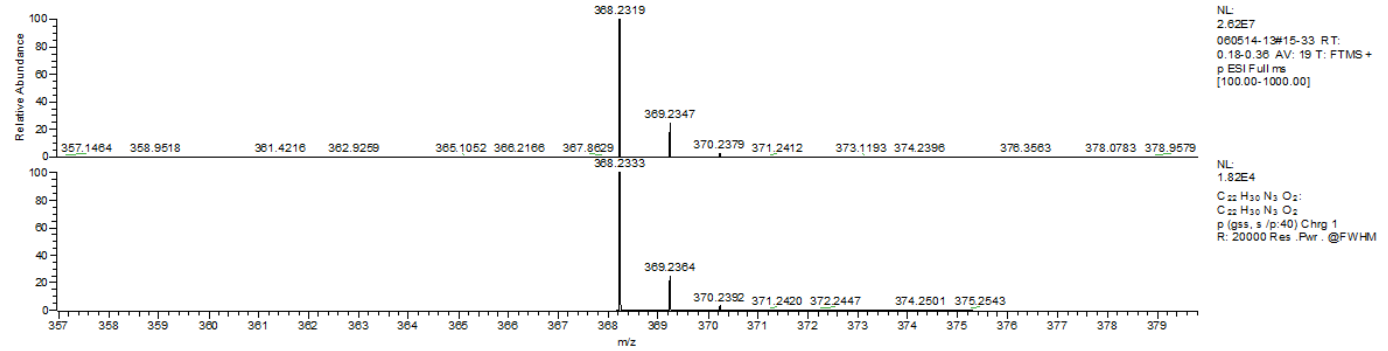
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 2

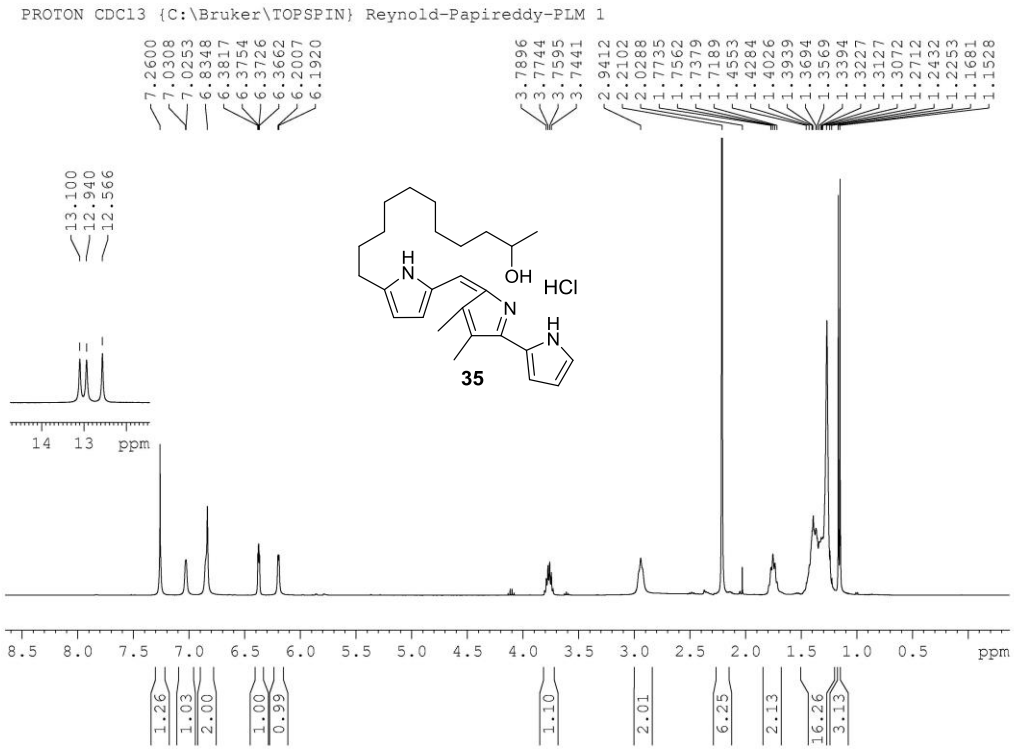


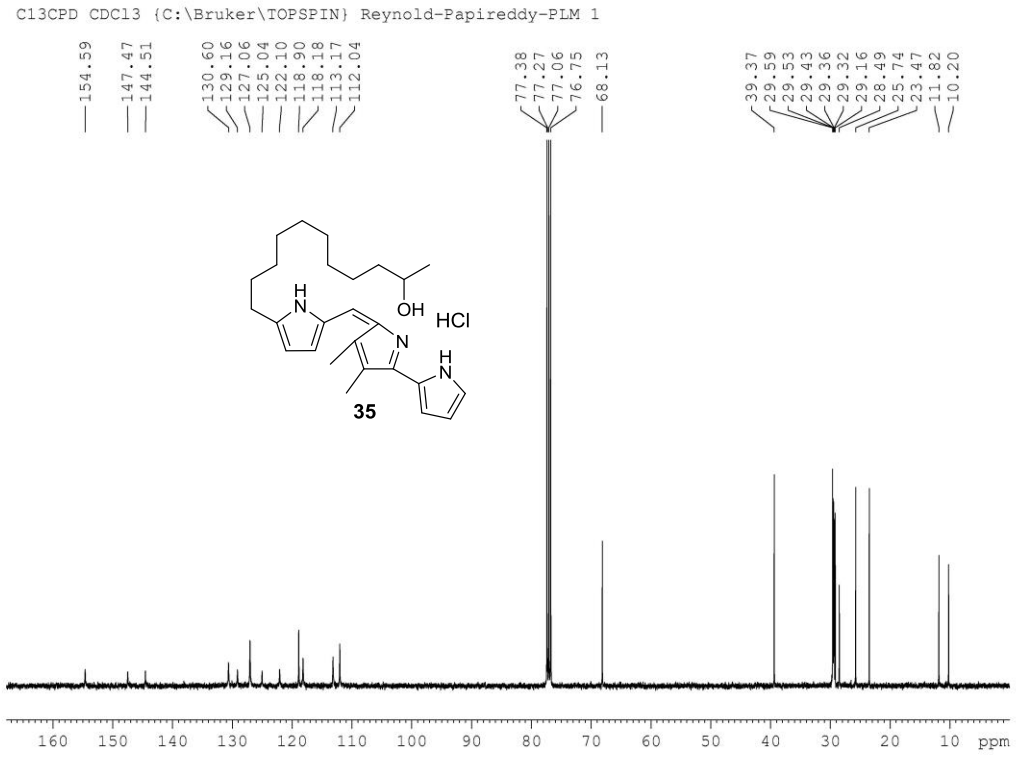
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 2

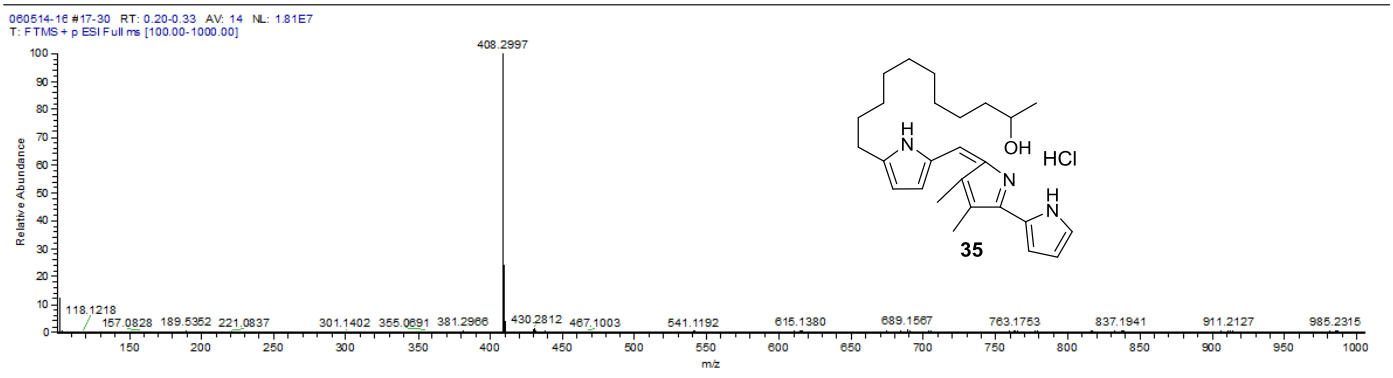


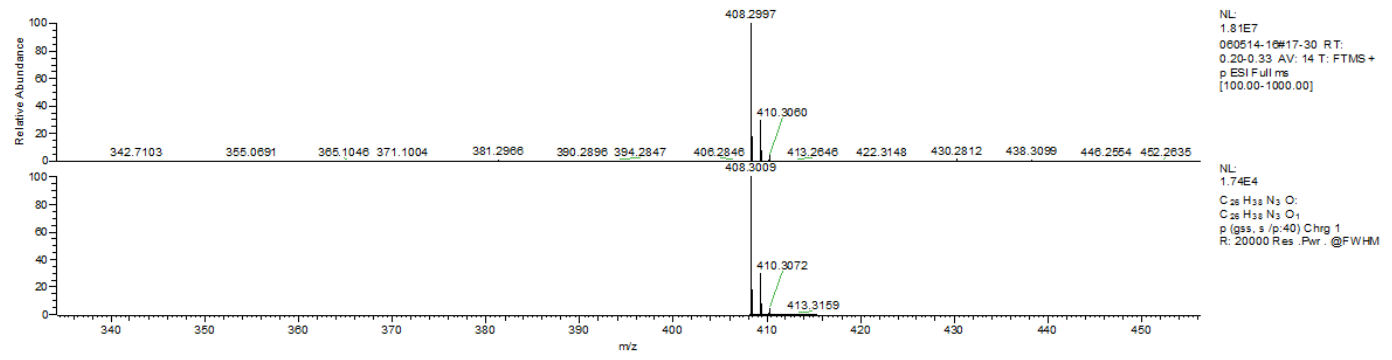

060514-13 #15-33 RT: 0.18-0.36 AV: 19 NL: 2.62E7
T: FTMS + p ESI Full ms [100.00-1000.00]
368.2319
390.2133
Relative Abundance
m/z
34

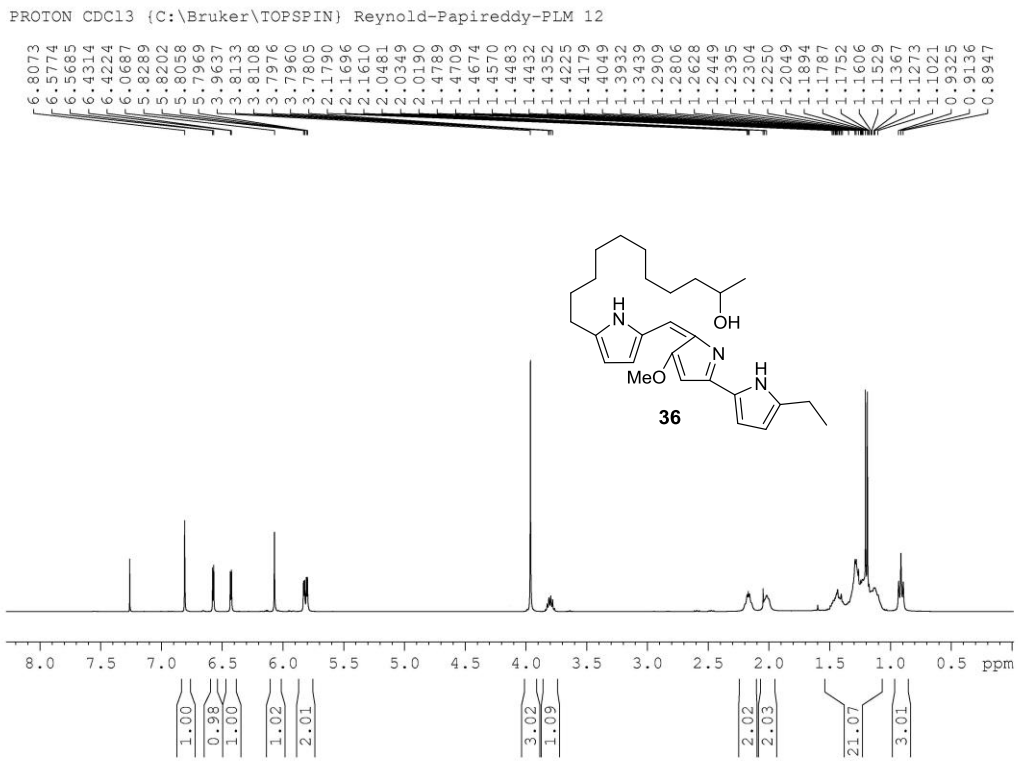

368.2319
369.2347
368.2333
369.2364
NL:
2.62E7
060514-13#15-33 RT:
0.18-0.36 AV: 19 T: FTMS +
p ESI Full ms
[100.00-1000.00]
NL:
1.82E4
C22 H30 N3 O2:
C22 H30 N3 O2
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr . @FWHM
Relative Abundance
m/z

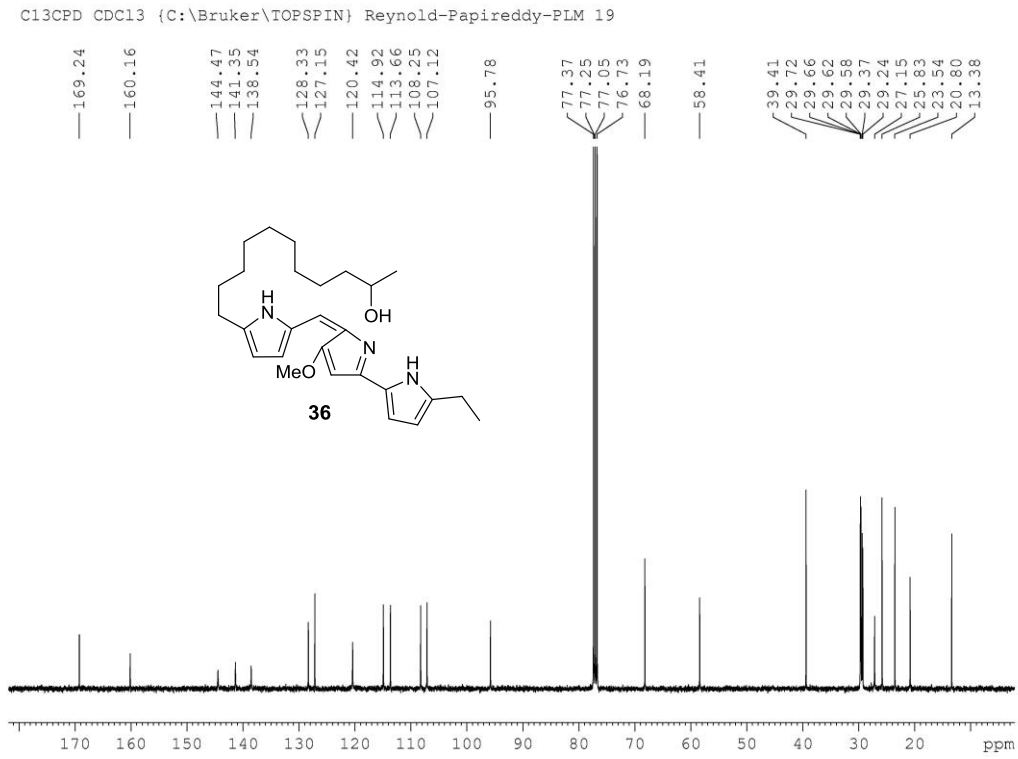

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 1
7.2600
7.0308
7.0253
6.8348
6.3817
6.3754
6.3726
6.3662
6.2007
6.1920
3.7896
3.7744
3.7595
3.7441
2.9412
2.2102
2.0288
1.7735
1.7562
1.7379
1.7189
1.4553
1.4284
1.4026
1.3939
1.3694
1.3569
1.3394
1.3227
1.3127
1.3072
1.2712
1.2432
1.2253
1.1681
1.1528
13.100
12.940
12.566
HCl
35
14 13 ppm
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 ppm
1.26
1.03
2.00
1.00
0.99
1.10
2.01
6.25
2.13
16.26
3.13

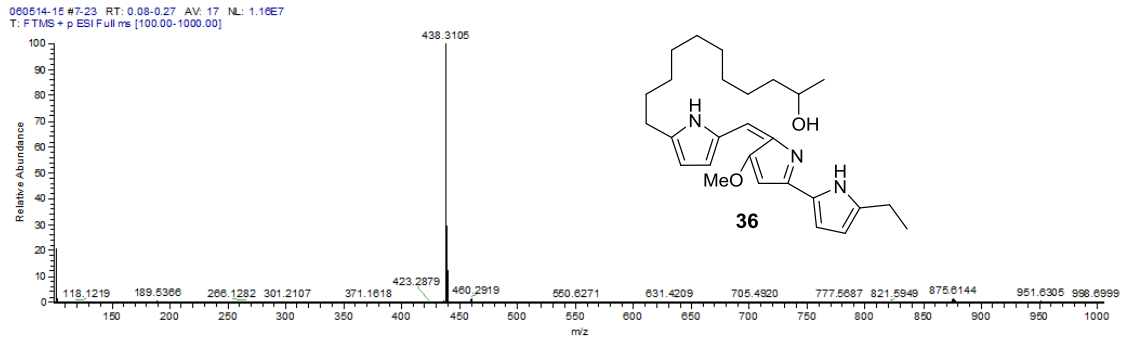

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 1
154.59
147.47
144.51
130.60
129.16
127.06
125.04
122.10
118.90
118.18
113.17
112.04
77.38
77.27
77.06
76.75
68.13
39.37
29.59
29.53
29.43
29.36
29.32
29.16
28.49
25.74
23.47
11.82
10.20
OH
HCl
35
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


060514-16 #17-30 RT: 0.20-0.33 AV: 14 NL: 1.81E7
T: FTMS + p ESI Full ms [100.00-1000.00]
408.2997
Relative Abundance
118.1218
157.0828
189.5352
221.0837
301.1402
355.0691
381.2966
430.2812
467.1003
541.1192
615.1380
689.1567
763.1753
837.1941
911.2127
985.2315
m/z
OH
HCl
35

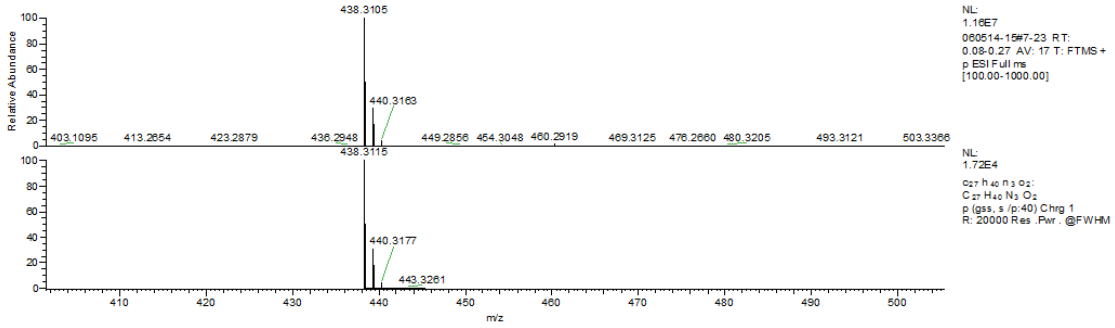

408.2997
410.3060
342.7103
355.0691
365.1046
371.1004
381.2966
390.2896
394.2847
406.2846
413.2646
422.3148
430.2812
438.3099
446.2554
452.2635
Relative Abundance
NL:
1.81E7
060514-16#17-30 RT:
0.20-0.33 AV: 14 T: FTMS +
p ESI Full ms
[100.00-1000.00]
408.3009
410.3072
413.3159
NL:
1.74E4
C25 H38 N3 O:
C25 H38 N3 O1
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr . @FWHM
m/z

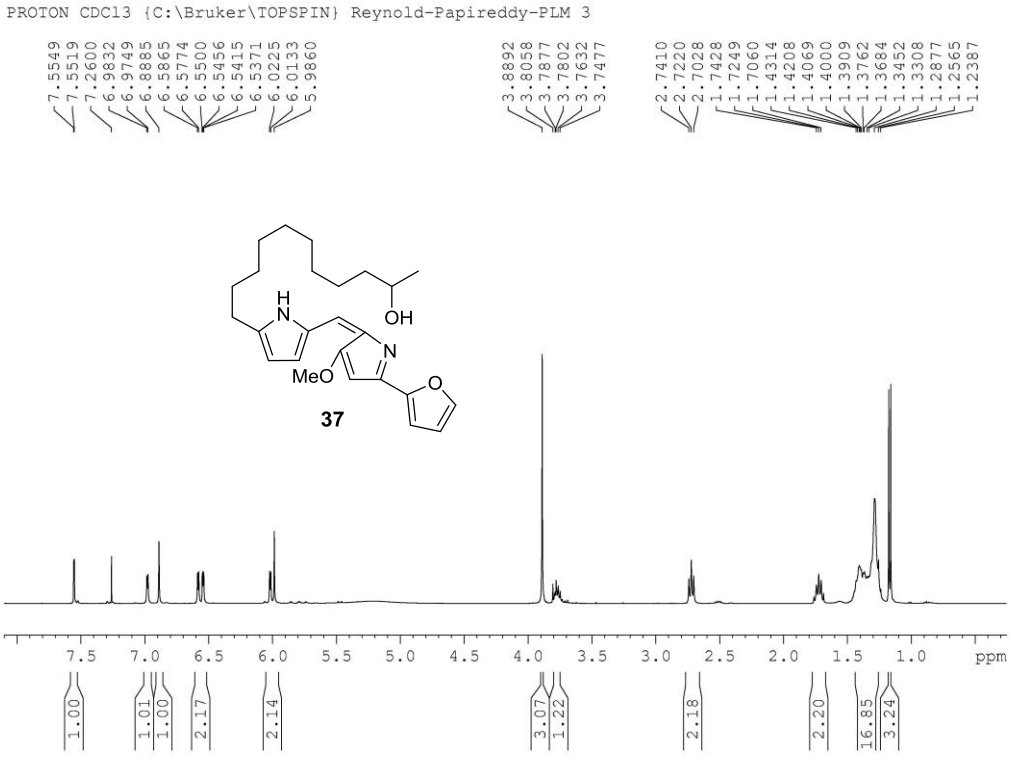

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 12
6.8073
6.5774
6.5685
6.4314
6.4224
6.0687
5.8289
5.8202
5.8058
5.7969
3.9637
3.8133
3.8108
3.7976
3.7960
3.7805
2.1790
2.1696
2.1610
2.0481
2.0349
2.0190
1.4789
1.4709
1.4674
1.4570
1.4483
1.4432
1.4352
1.4225
1.4179
1.4049
1.3932
1.3439
1.2909
1.2806
1.2628
1.2449
1.2395
1.2304
1.2250
1.2049
1.1894
1.1787
1.1752
1.1606
1.1529
1.1367
1.1273
1.1021
0.9325
0.9136
0.8947
H
N
OH
N
MeO
H
N
36
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
ppm
1.00
0.98
1.00
1.02
2.01
3.02
1.09
2.02
2.03
21.07
3.01


C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 19
169.24
160.16
144.47
141.35
138.54
128.33
127.15
120.42
114.92
113.66
108.25
107.12
95.78
77.37
77.25
77.05
76.73
68.19
58.41
39.41
29.72
29.66
29.62
29.58
29.37
29.24
27.15
25.83
23.54
20.80
13.38
H
N
OH
N
MeO
H
N
36
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

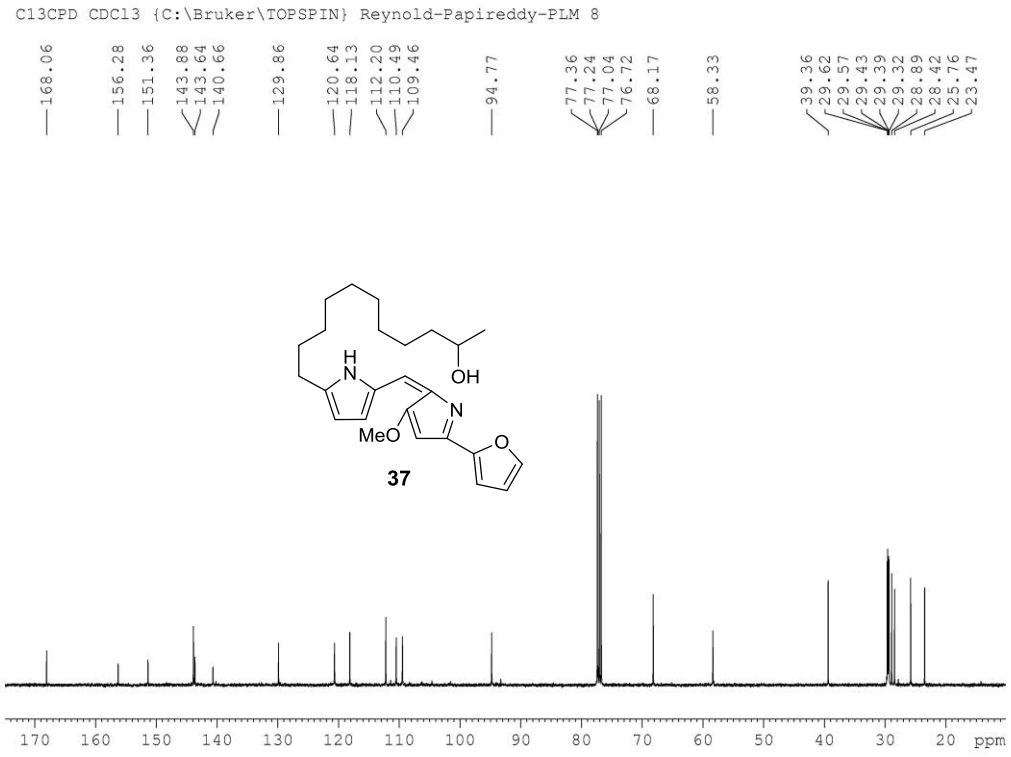

060514-15 #7-23 RT: 0.08-0.27 AV: 17 NL: 1.16E7
T: FTMS + p ESI Full ms [100.00-1000.00]
438.3105
423.2879
460.2919
Relative Abundance
m/z
OH
H
N
N
MeO
H
N

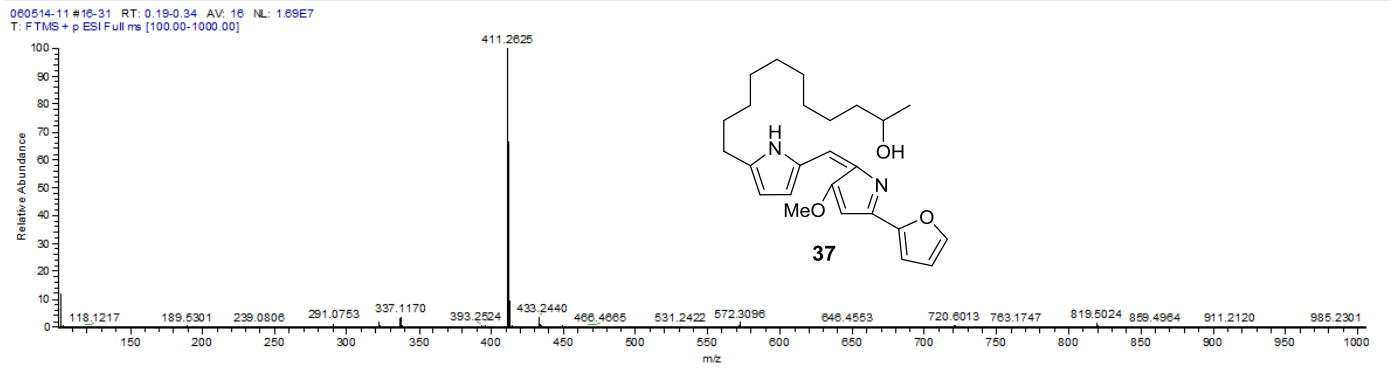
36

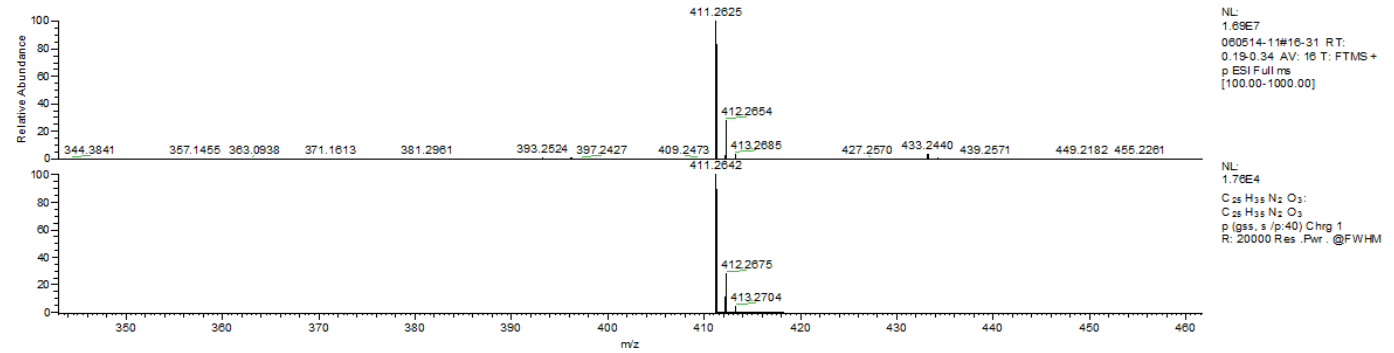

438.3105
440.3163
438.3115
440.3177
443.3261
Relative Abundance
m/z
NL:
1.16E7
060514-15#7-23 RT:
0.08-0.27 AV: 17 T: FTMS +
p ESI Full ms
[100.00-1000.00]
NL:
1.72E4
C27 H40 N3 O2:
C27 H40 N3 O2
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr . @FWHM


PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 3
7.5549
7.5519
7.2600
6.9832
6.9749
6.8885
6.5865
6.5774
6.5500
6.5456
6.5415
6.5371
6.0225
6.0133
5.9860
3.8892
3.8058
3.7877
3.7802
3.7632
3.7477
2.7410
2.7220
2.7028
1.7428
1.7249
1.7060
1.4314
1.4208
1.4069
1.4000
1.3909
1.3762
1.3684
1.3452
1.3308
1.2877
1.2565
1.2387
OH
H
N
N
MeO
O
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
ppm
1.00
1.01
1.00
2.17
2.14
3.07
1.22
2.18
2.20
16.85
3.24

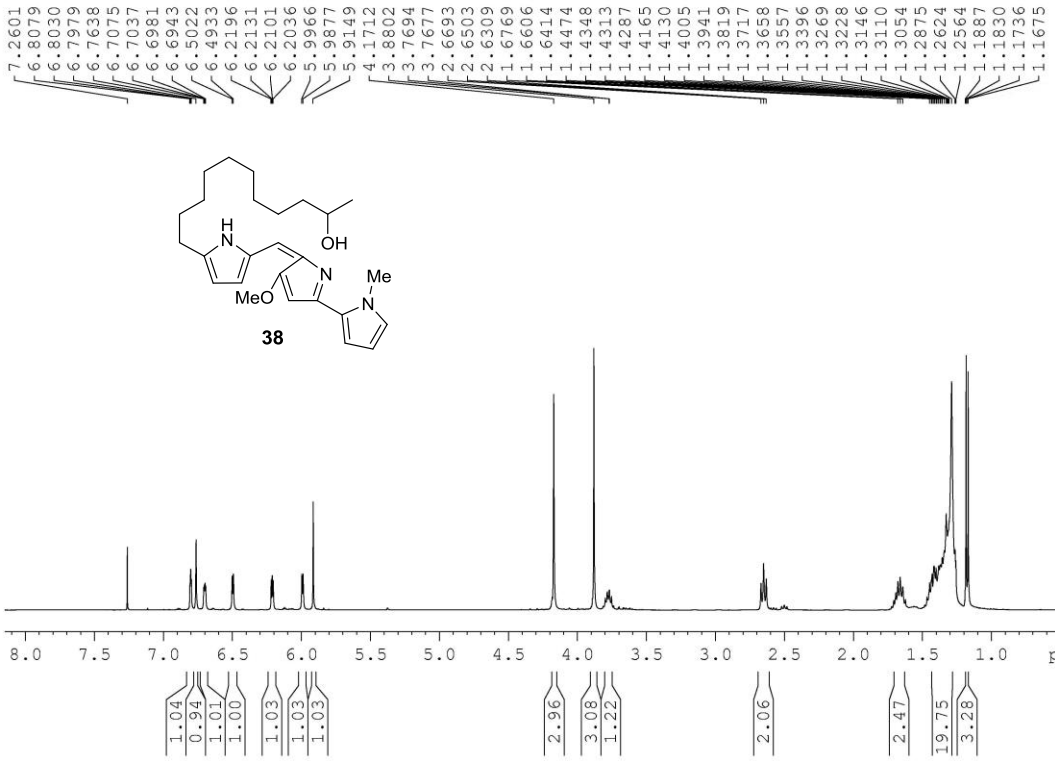
37


C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 8
168.06
156.28
151.36
143.88
143.64
140.66
129.86
120.64
118.13
112.20
110.49
109.46
94.77
77.36
77.24
77.04
76.72
68.17
58.33
39.36
29.62
29.57
29.43
29.39
29.32
28.89
28.42
25.76
23.47
H
N
OH
N
MeO
O
37
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

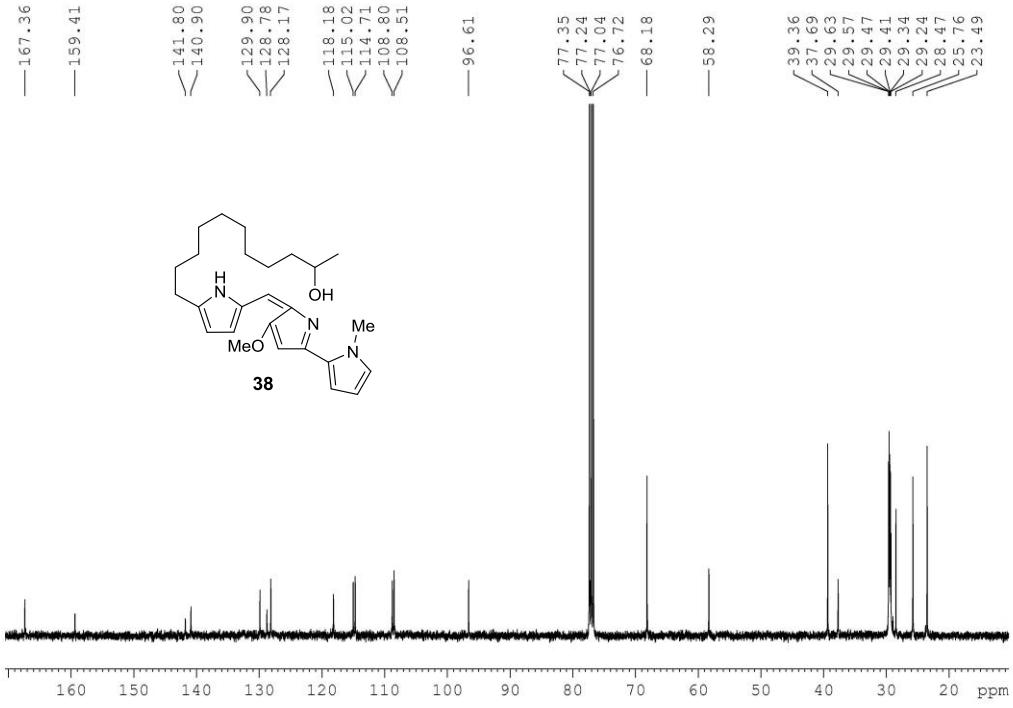

060514-11 #16-31 RT: 0.19-0.34 AV: 16 NL: 1.69E7
T: FTMS + p ESI Full ms [100.00-1000.00]
411.2625
Relative Abundance
m/z
H
N
OH
N
MeO
O
37

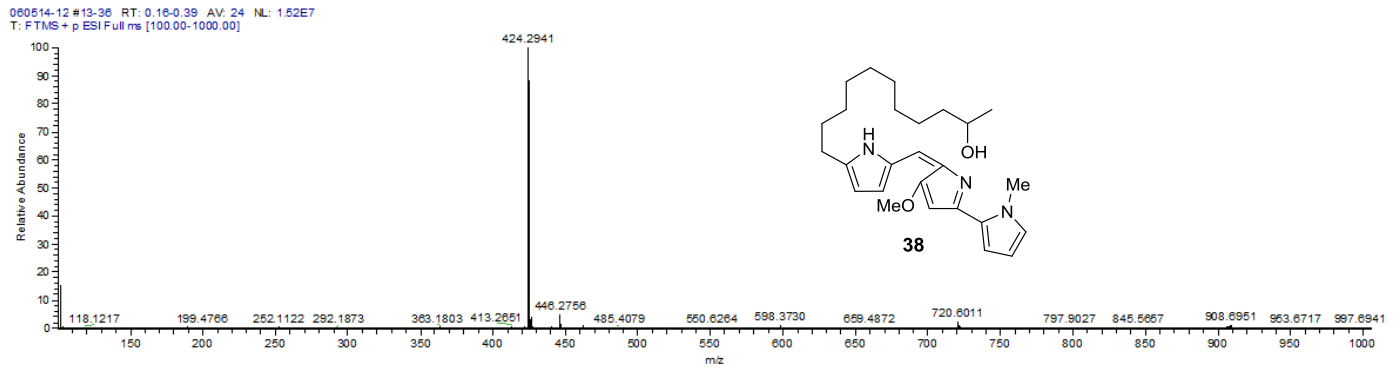

411.2625
412.2654
413.2685
411.2642
412.2675
413.2704
NL:
1.69E7
060514-11#16-31 RT:
0.19-0.34 AV: 16 T: FTMS +
p ESI Full ms
[100.00-1000.00]
NL:
1.76E4
C25 H35 N2 O3:
C25 H35 N2 O3
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr . @FWHM
Relative Abundance
m/z

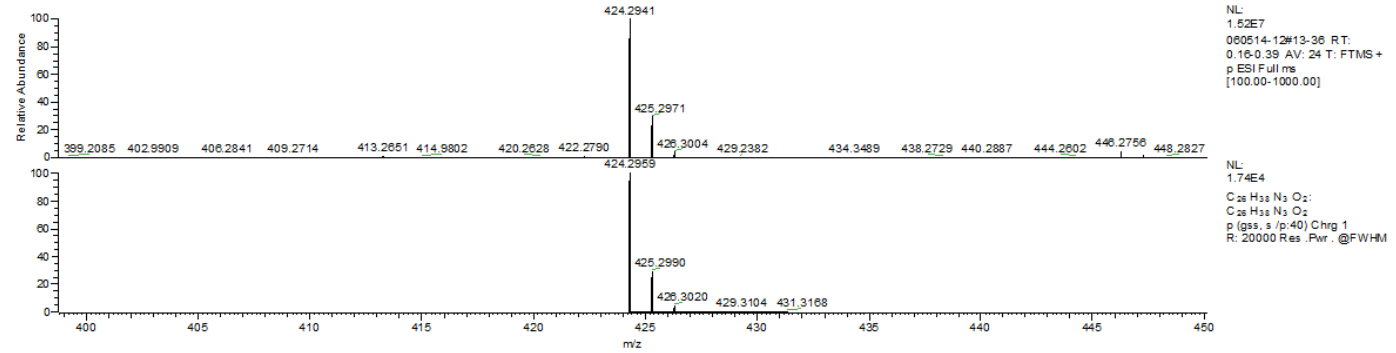
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 7

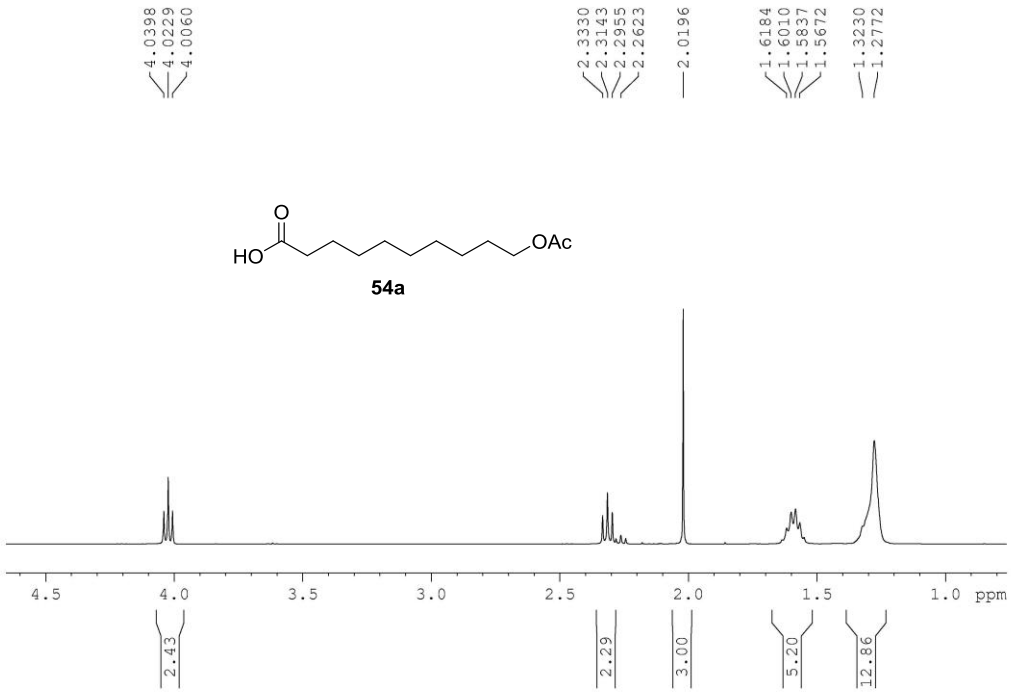


C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5



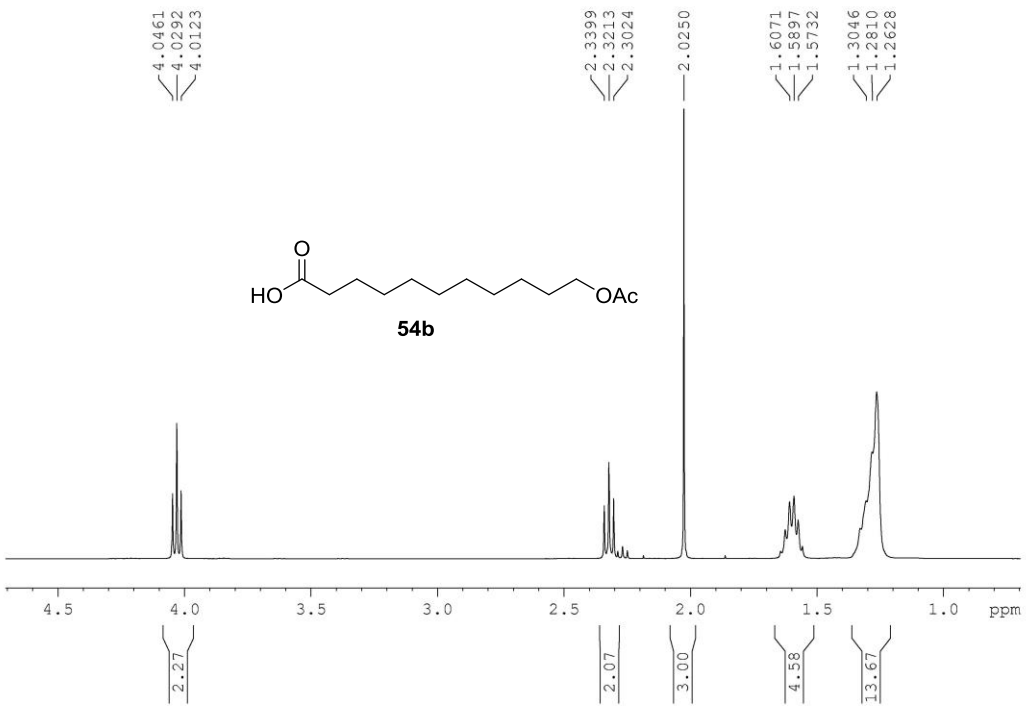

060514-12 #13-36 RT: 0.16-0.39 AV: 24 NL: 1.52E7
T: FTMS + p ESI Full ms [100.00-1000.00]
Relative Abundance
m/z
424.2941
446.2756
38


Relative Abundance
m/z
424.2941
425.2971
426.3004
424.2959
425.2990
426.3020
NL:
1.52E7
060514-12#13-36 RT:
0.16-0.39 AV: 24 T: FTMS +
p ESI Full ms
[100.00-1000.00]
NL:
1.74E4
C25 H38 N3 O2:
C25 H38 N3 O2
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr . @FWHM

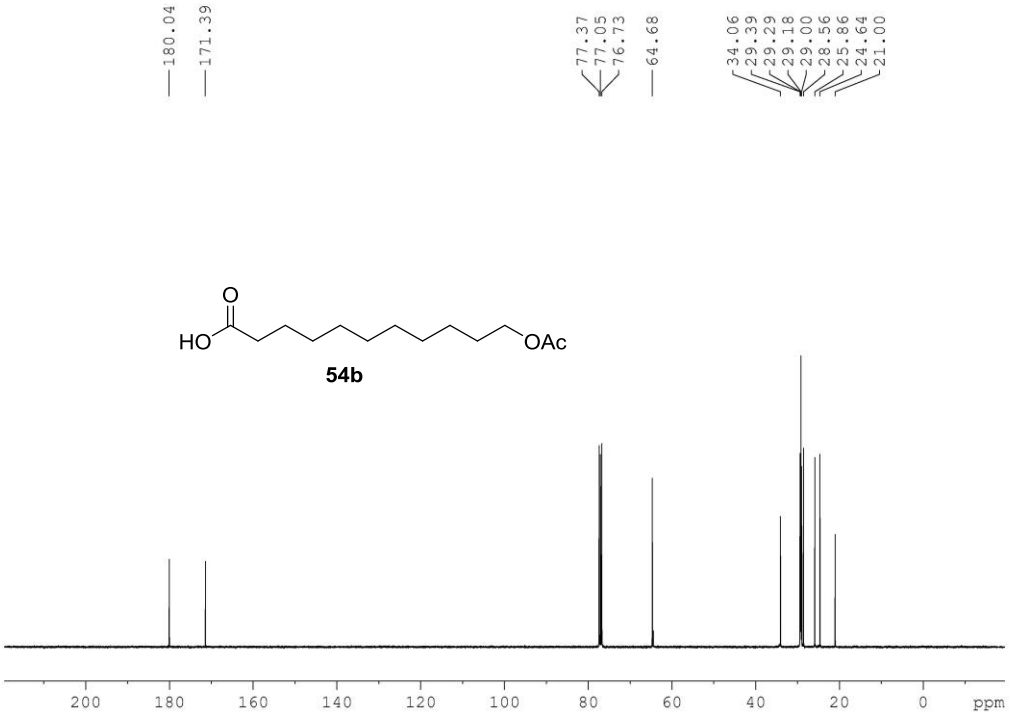

4.0398
4.0229
4.0060
2.3330
2.3143
2.2955
2.2623
2.0196
1.6184
1.6010
1.5837
1.5672
1.3230
1.2772
HO
OAc
54a
ppm
2.43
2.29
3.00
5.20
12.86


179.93
171.42
77.38
77.06
76.74
64.67
34.05
29.24
29.13
29.10
28.98
28.54
25.84
24.63
20.98
O
HO
OAc
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

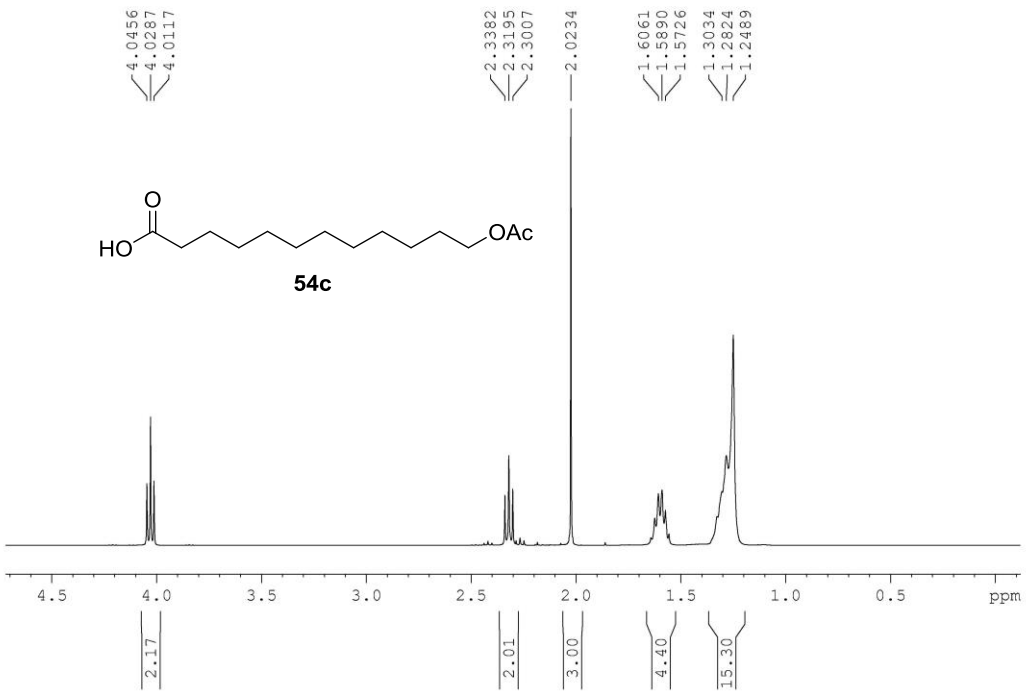
54a


4.0461
4.0292
4.0123
2.3399
2.3213
2.3024
2.0250
1.6071
1.5897
1.5732
1.3046
1.2810
1.2628
O
HO
OAc
4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.27
2.07
3.00
4.58
13.67

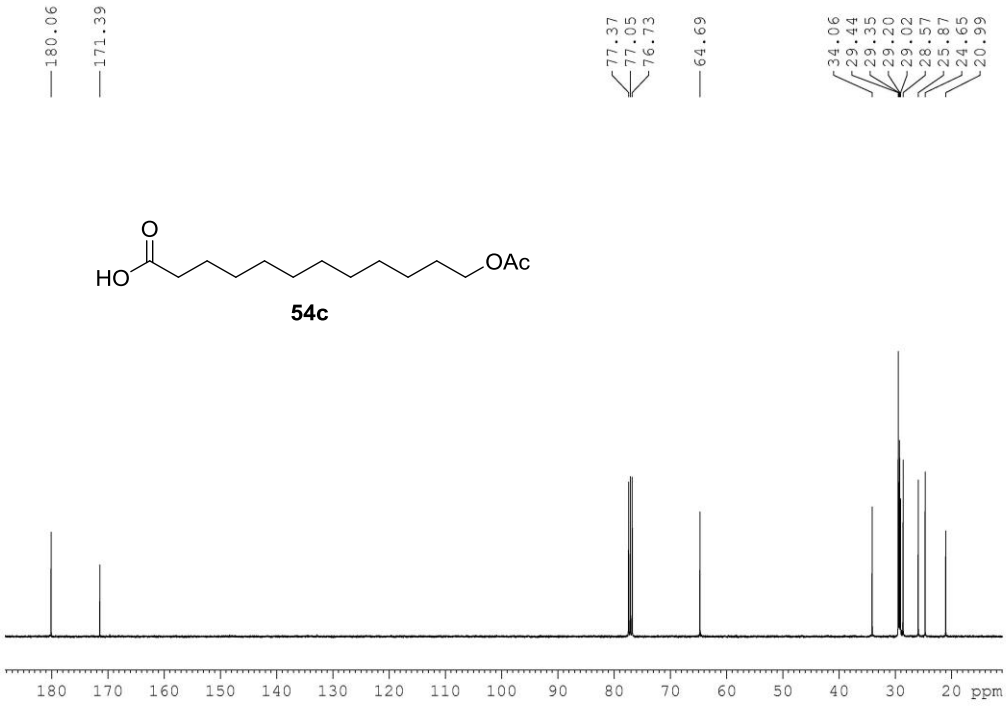
54b

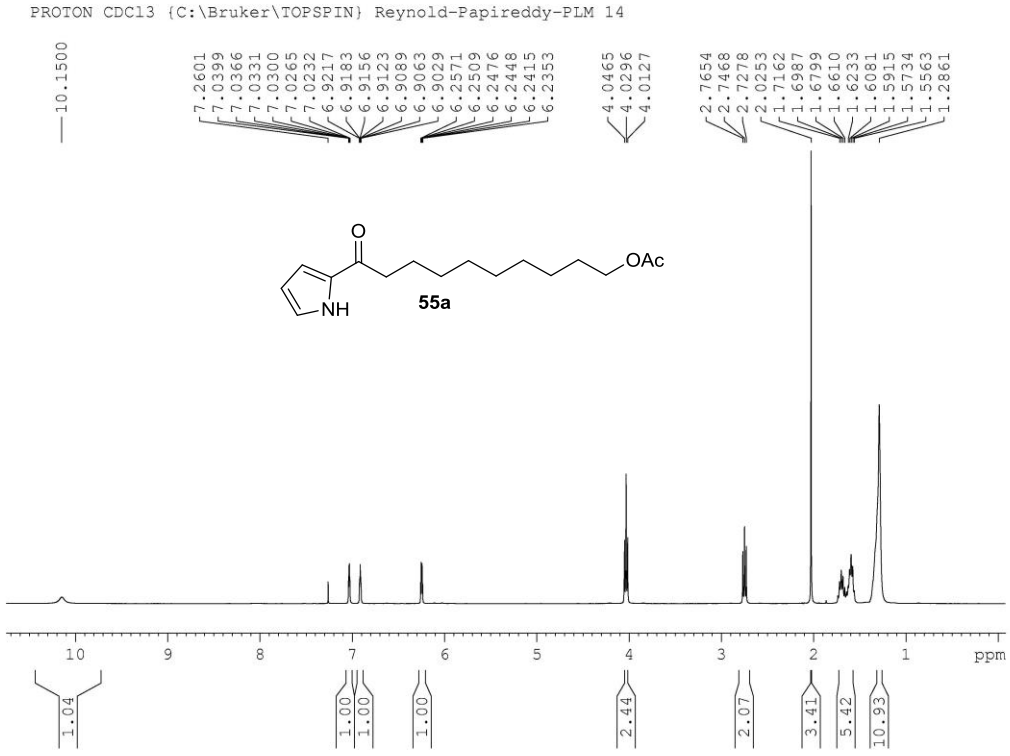

180.04
171.39
77.37
77.05
76.73
64.68
34.06
29.39
29.29
29.18
29.00
28.56
25.86
24.64
21.00
O
HO
OAc
200
180
160
140
120
100
80
60
40
20
0
ppm

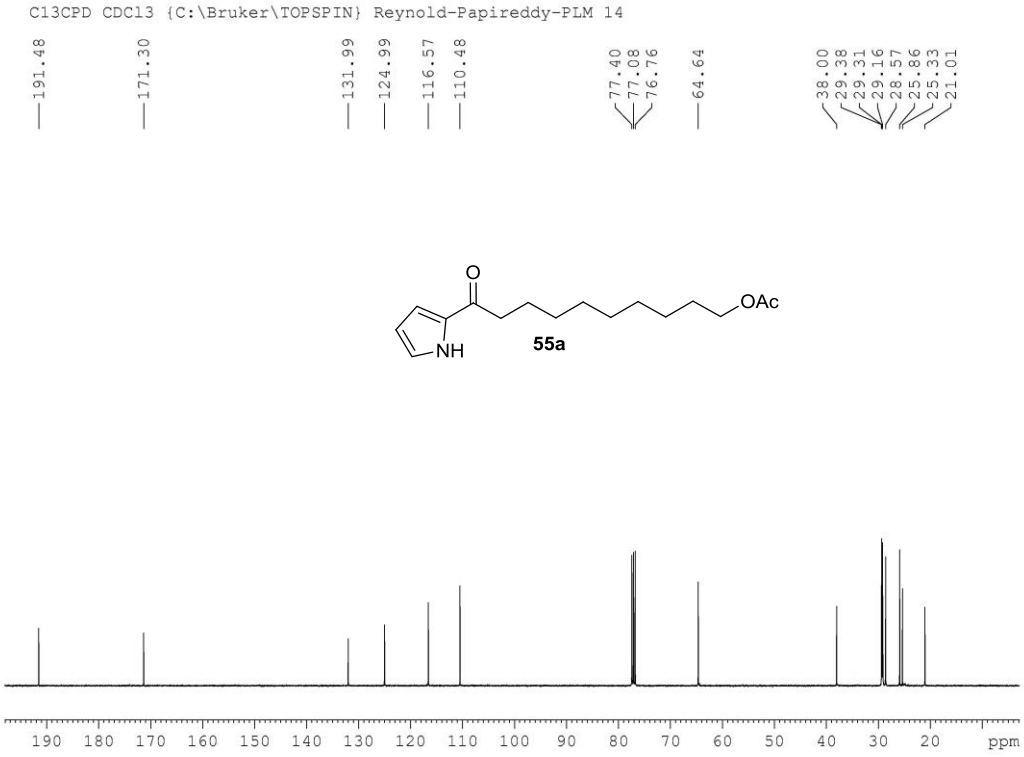
54b


4.0456
4.0287
4.0117
2.3382
2.3195
2.3007
2.0234
1.6061
1.5890
1.5726
1.3034
1.2824
1.2489
O
HO
OAc
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.17
2.01
3.00
4.40
15.30

54c

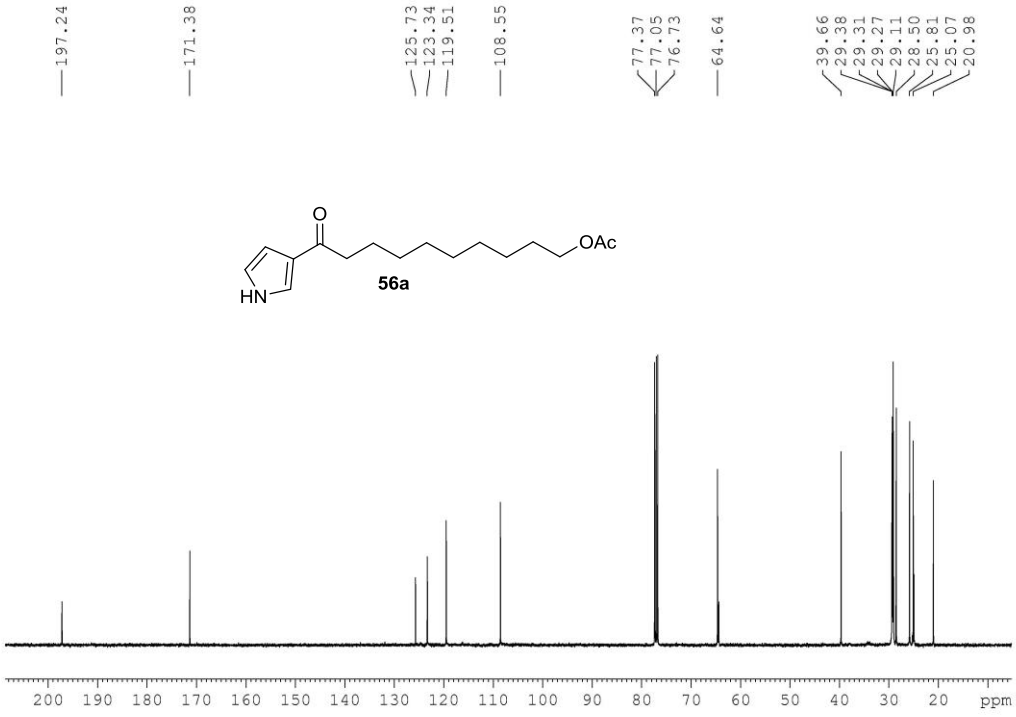

180.06
171.39
77.37
77.05
76.73
64.69
34.06
29.44
29.35
29.20
29.02
28.57
25.87
24.65
20.99
O
HO
OAc
54c
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 14
10.1500
7.2601
7.0399
7.0366
7.0331
7.0300
7.0265
7.0232
6.9217
6.9183
6.9156
6.9123
6.9089
6.9063
6.9029
6.2571
6.2509
6.2476
6.2448
6.2415
6.2353
4.0465
4.0296
4.0127
2.7654
2.7468
2.7278
2.0253
1.7162
1.6987
1.6799
1.6610
1.6233
1.6081
1.5915
1.5734
1.5563
1.2861
O
OAc
NH
55a
10 9 8 7 6 5 4 3 2 1 ppm
1.04
1.00
1.00
1.00
2.44
2.07
3.41
5.42
10.93

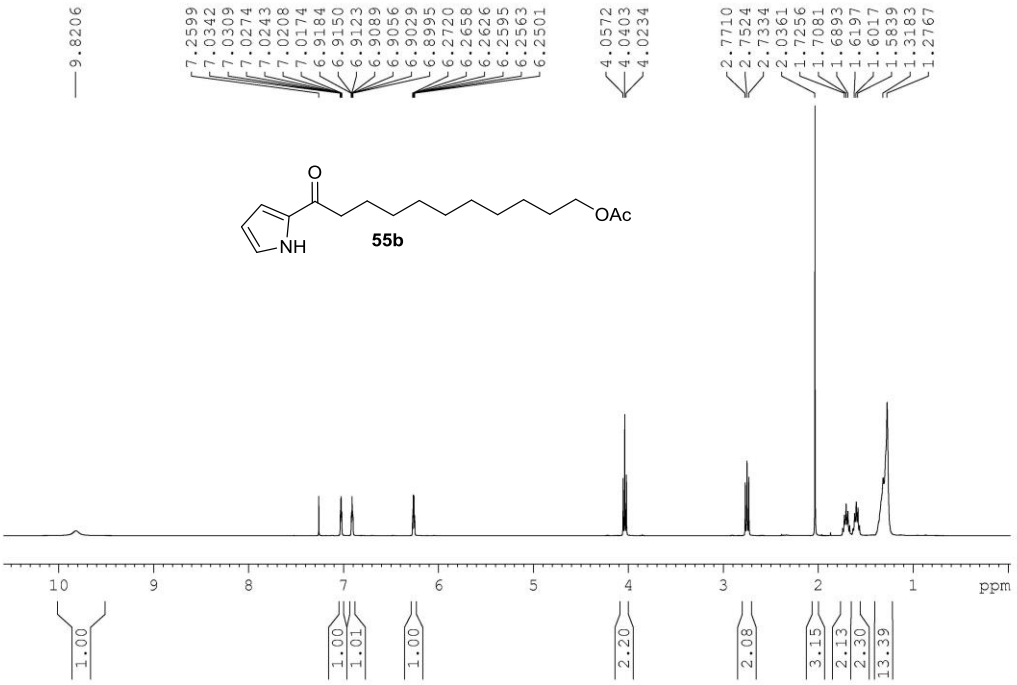

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 14
191.48
171.30
131.99
124.99
116.57
110.48
77.40
77.08
76.76
64.64
38.00
29.38
29.31
29.16
28.57
25.86
25.33
21.01
O
OAc
NH
55a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 15
9.5368
7.4088
7.4051
7.4017
7.3975
7.2604
6.7565
6.7494
6.7459
6.7441
6.7387
6.6279
6.6241
6.6215
6.6182
6.6152
4.0395
4.0226
4.0057
2.7468
2.7281
2.7093
2.0225
1.7177
1.6992
1.6817
1.6633
1.6447
1.6021
1.5856
1.5687
1.5520
1.2755
O
OAc
HN
56a
10 9 8 7 6 5 4 3 2 1 ppm
1.06
1.00
1.05
1.07
2.54
2.24
3.38
2.05
3.98
10.64

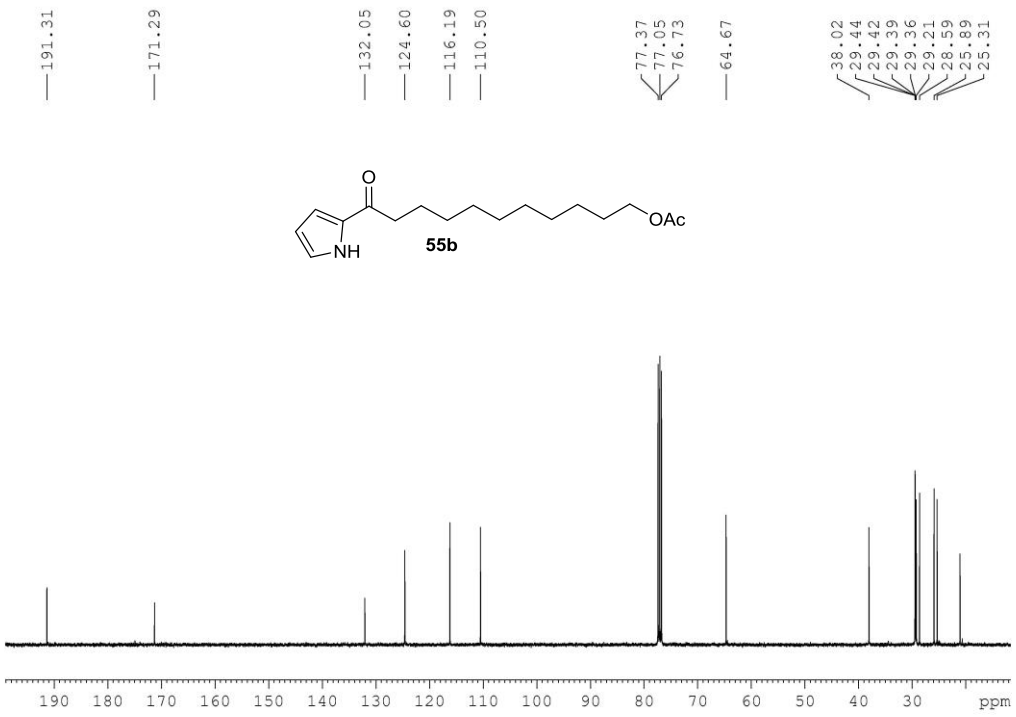
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 15



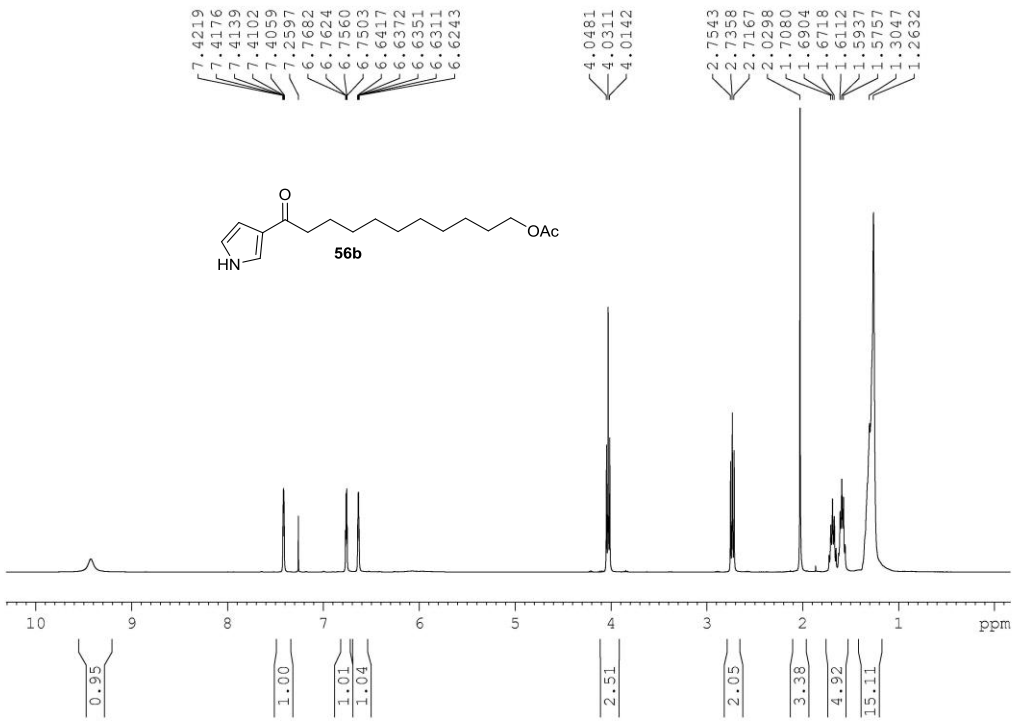
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 10

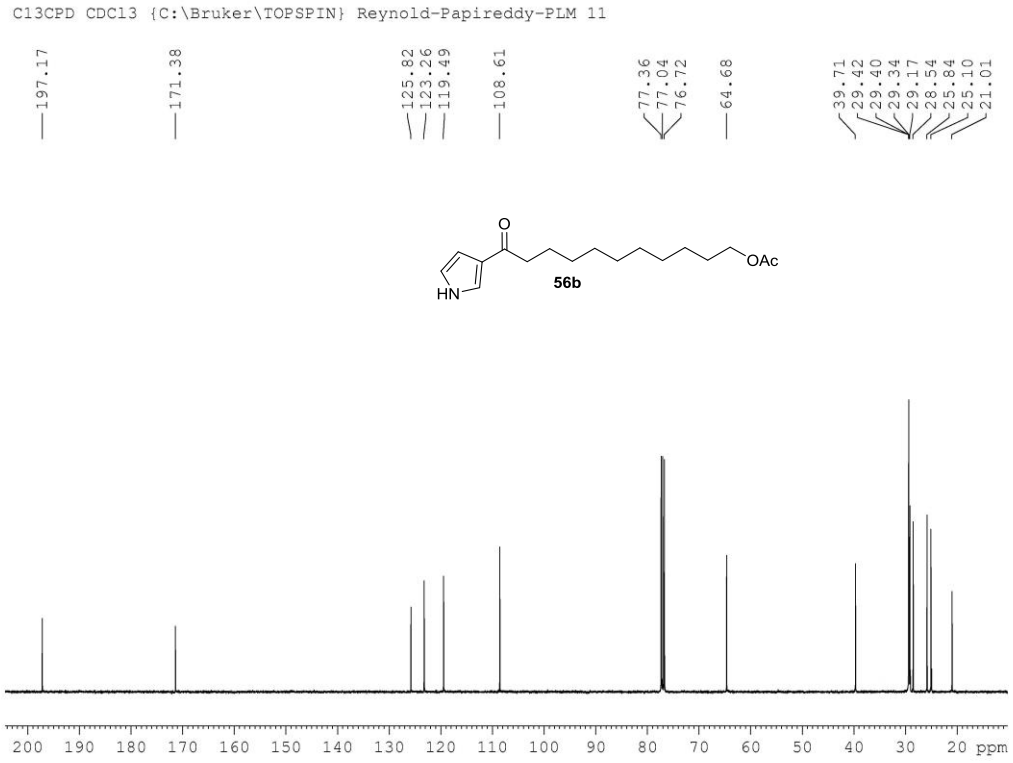


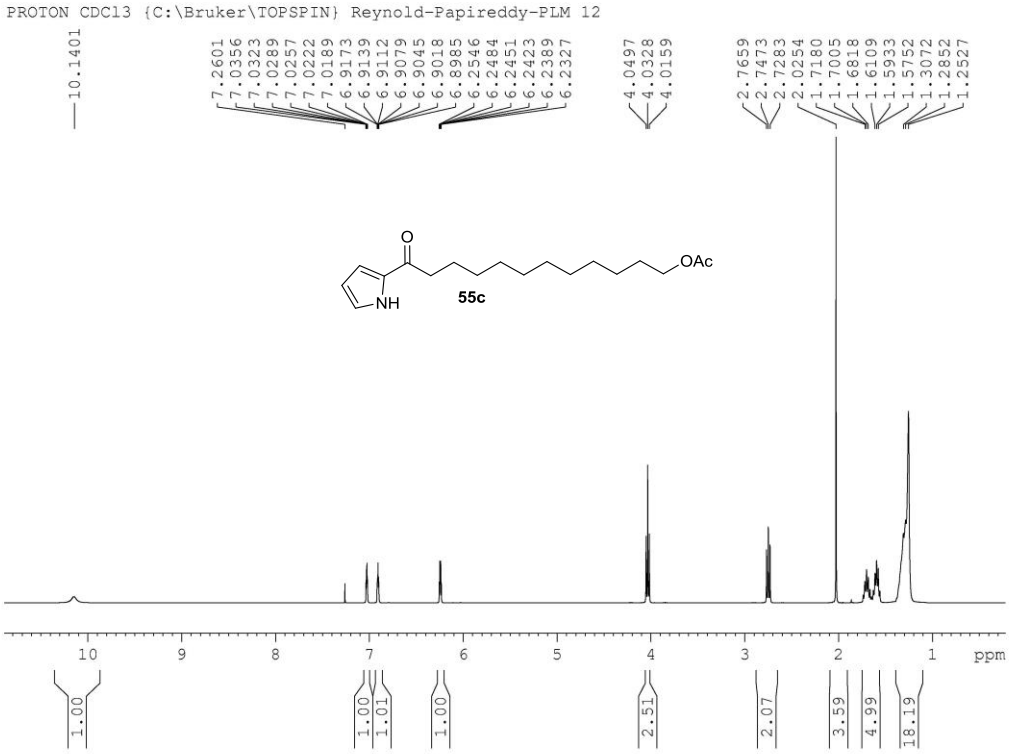
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 10

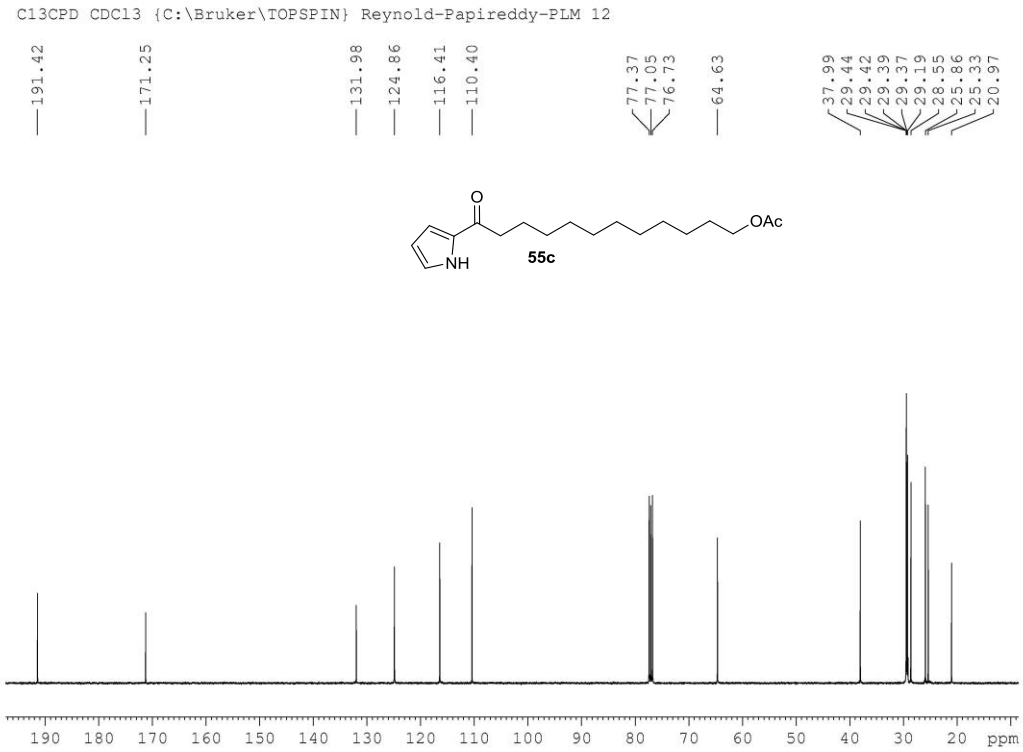


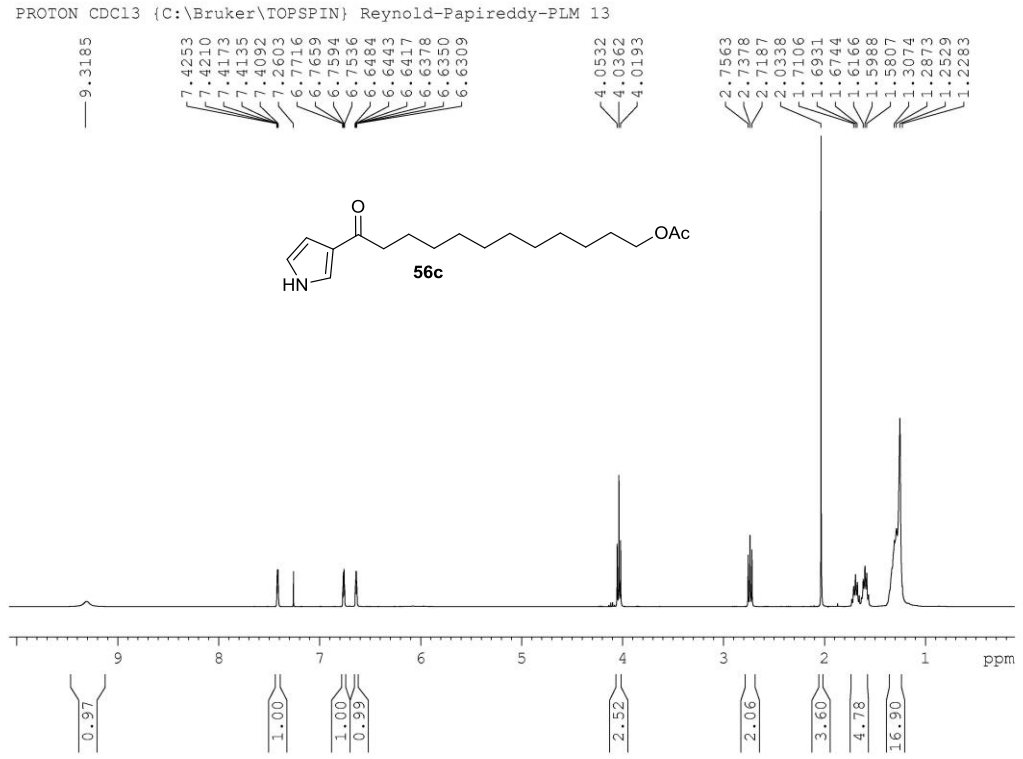
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 11

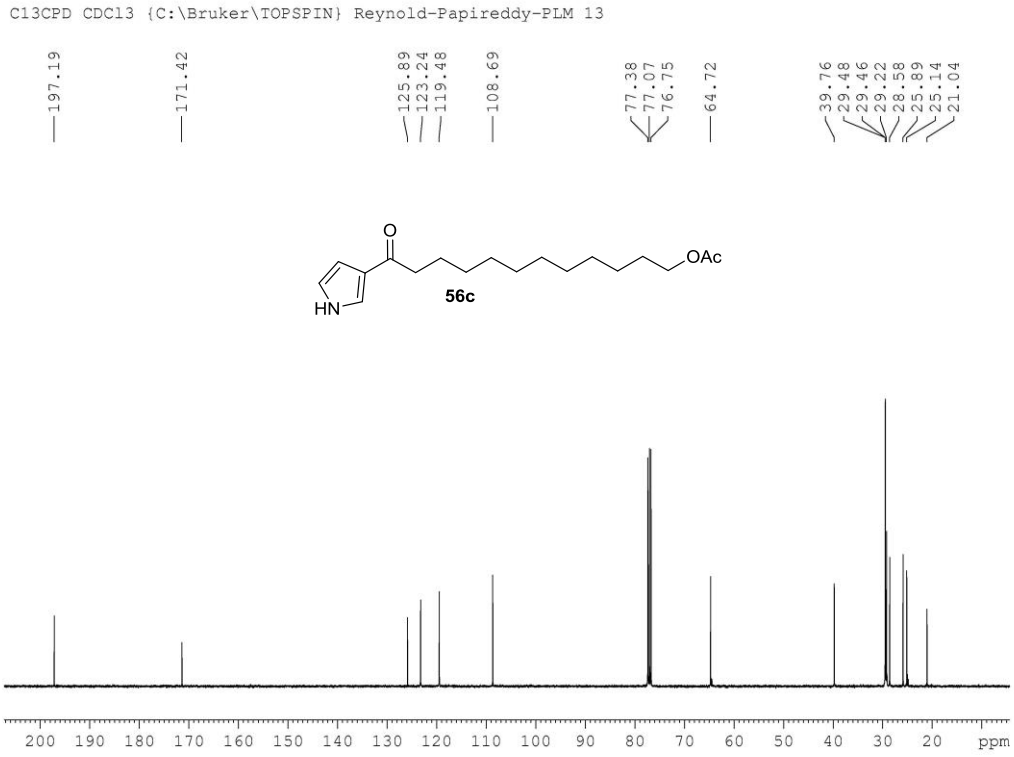


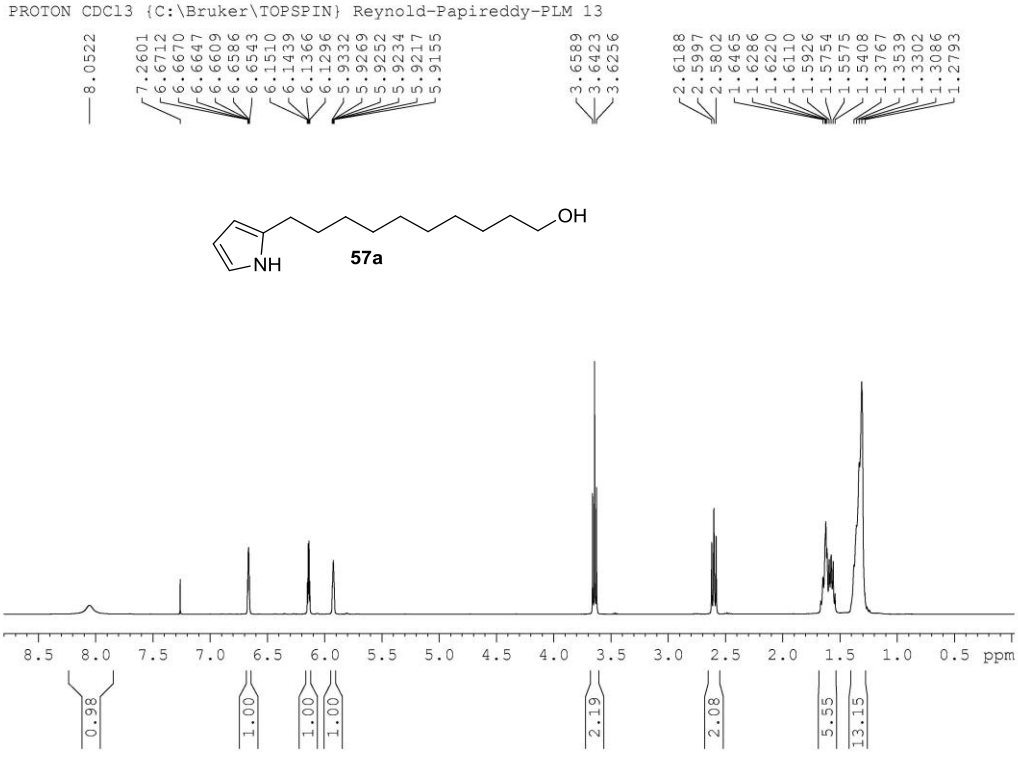

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 11
197.17
171.38
125.82
123.26
119.49
108.61
77.36
77.04
76.72
64.68
39.71
29.42
29.40
29.34
29.17
28.54
25.84
25.10
21.01
O
OAc
HN
56b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

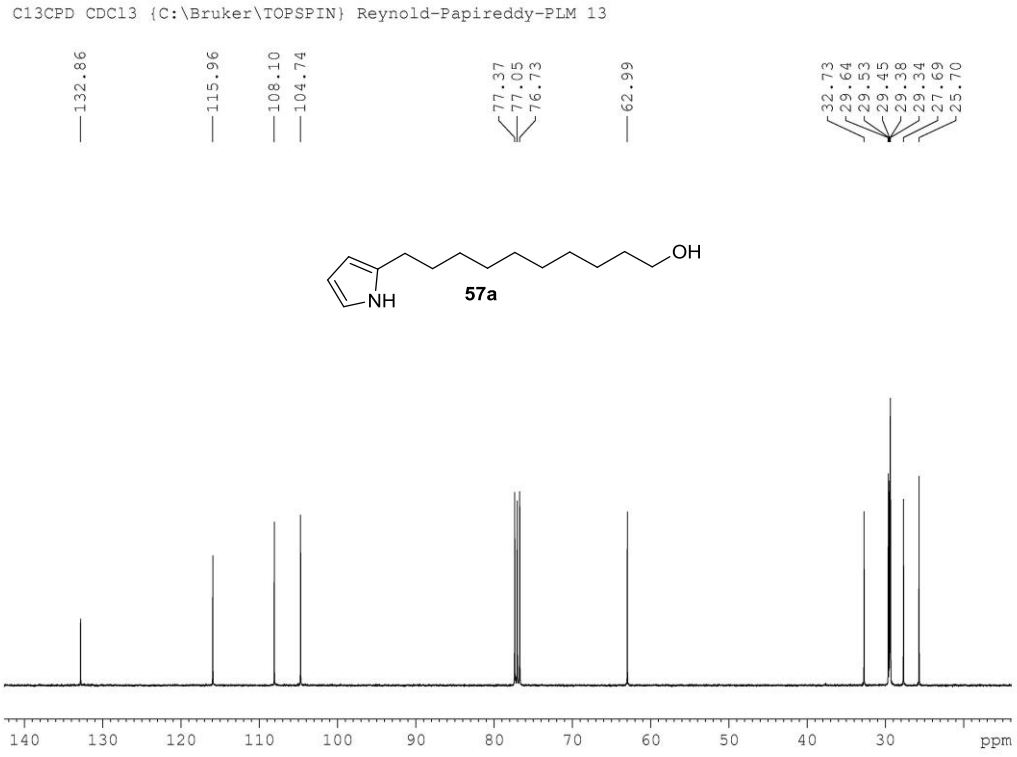

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 12
10.1401
7.2601
7.0356
7.0323
7.0289
7.0257
7.0222
7.0189
6.9173
6.9139
6.9112
6.9079
6.9045
6.9018
6.8985
6.2546
6.2484
6.2451
6.2423
6.2389
6.2327
4.0497
4.0328
4.0159
2.7659
2.7473
2.7283
2.0254
1.7180
1.7005
1.6818
1.6109
1.5933
1.5752
1.3072
1.2852
1.2527
O
OAc
NH
55c
10 9 8 7 6 5 4 3 2 1 ppm
1.00
1.00
1.01
1.00
2.51
2.07
3.59
4.99
18.19

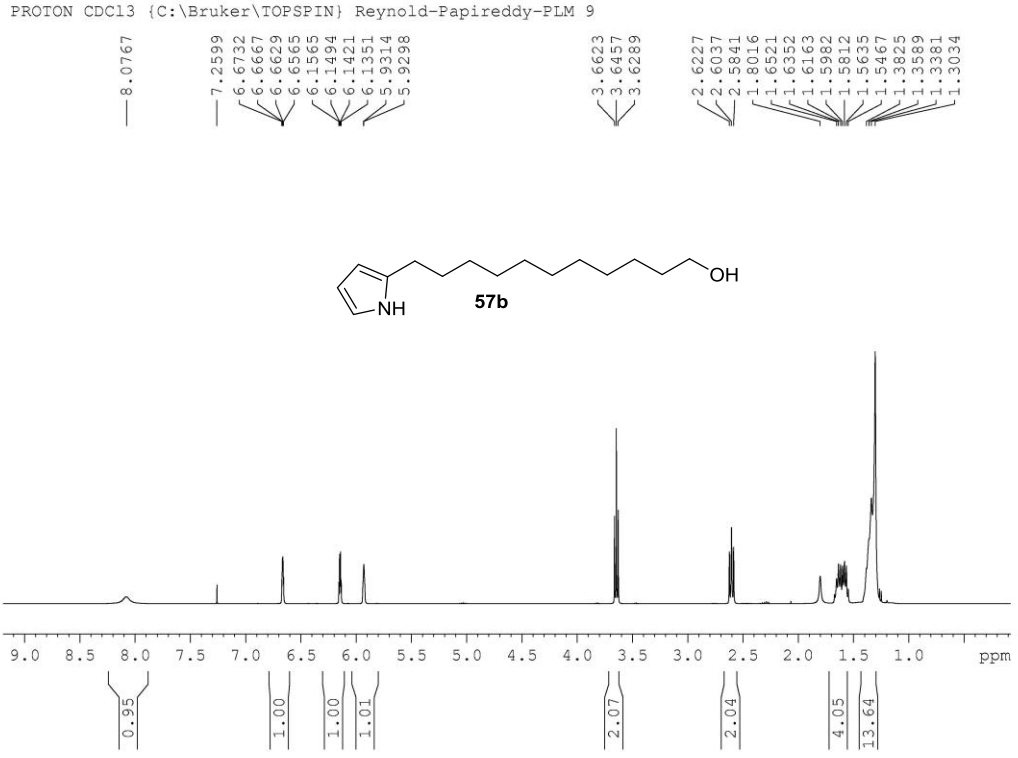

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 12
191.42
171.25
131.98
124.86
116.41
110.40
77.37
77.05
76.73
64.63
37.99
29.44
29.42
29.39
29.37
29.19
28.55
25.86
25.33
20.97
O
OAc
NH
55c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 13
9.3185
7.4253
7.4210
7.4173
7.4135
7.4092
7.2603
6.7716
6.7659
6.7594
6.7536
6.6484
6.6443
6.6417
6.6378
6.6350
6.6309
4.0532
4.0362
4.0193
2.7563
2.7378
2.7187
2.0338
1.7106
1.6931
1.6744
1.6166
1.5988
1.5807
1.3074
1.2873
1.2529
1.2283
O
OAc
HN
56c
9 8 7 6 5 4 3 2 1 ppm
0.97
1.00
1.00
0.99
2.52
2.06
3.60
4.78
16.90


C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 13
197.19
171.42
125.89
123.24
119.48
108.69
77.38
77.07
76.75
64.72
39.76
29.48
29.46
29.22
28.58
25.89
25.14
21.04
O
OAc
HN
56c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

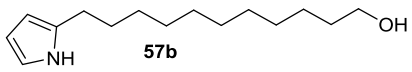

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 13
8.0522
7.2601
6.6712
6.6670
6.6647
6.6609
6.6586
6.6543
6.1510
6.1439
6.1366
6.1296
5.9332
5.9269
5.9252
5.9234
5.9217
5.9155
3.6589
3.6423
3.6256
2.6188
2.5997
2.5802
1.6465
1.6286
1.6220
1.6110
1.5926
1.5754
1.5575
1.5408
1.3767
1.3539
1.3302
1.3086
1.2793
OH
NH
57a
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 ppm
0.98
1.00
1.00
1.00
2.19
2.08
5.55
13.15


C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 13
132.86
115.96
108.10
104.74
77.37
77.05
76.73
62.99
32.73
29.64
29.53
29.45
29.38
29.34
27.69
25.70
OH
NH
57a
140
130
120
110
100
90
80
70
60
50
40
30
ppm

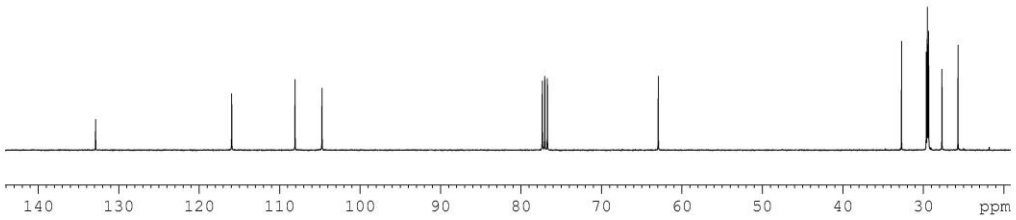

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 9
8.0767
7.2599
6.6732
6.6667
6.6629
6.6565
6.1565
6.1494
6.1421
6.1351
5.9314
5.9298
3.6623
3.6457
3.6289
2.6227
2.6037
2.5841
1.8016
1.6521
1.6352
1.6163
1.5982
1.5812
1.5635
1.5467
1.3825
1.3589
1.3381
1.3034
OH
NH
57b
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.95
1.00
1.00
1.01
2.07
2.04
4.05
13.64

C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 12

132.86
115.94
108.07
104.71
77.37
77.05
76.73
62.95
32.71
29.64
29.54
29.50
29.37
29.34
27.69
25.70

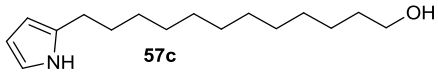


57b

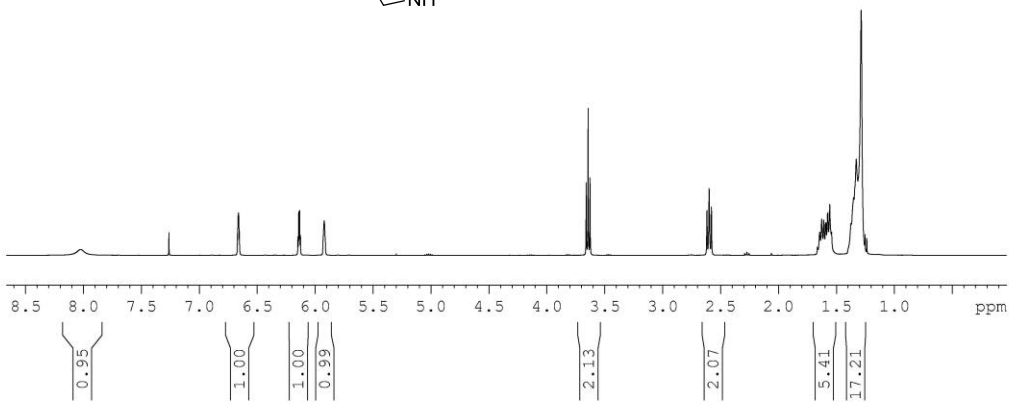


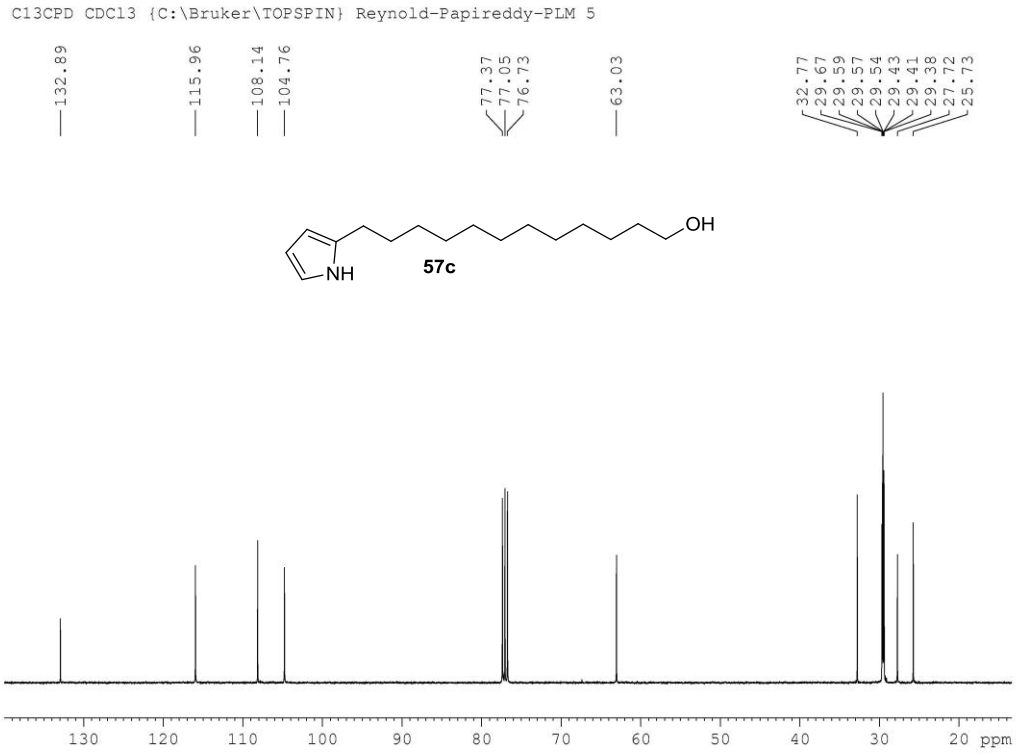
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5

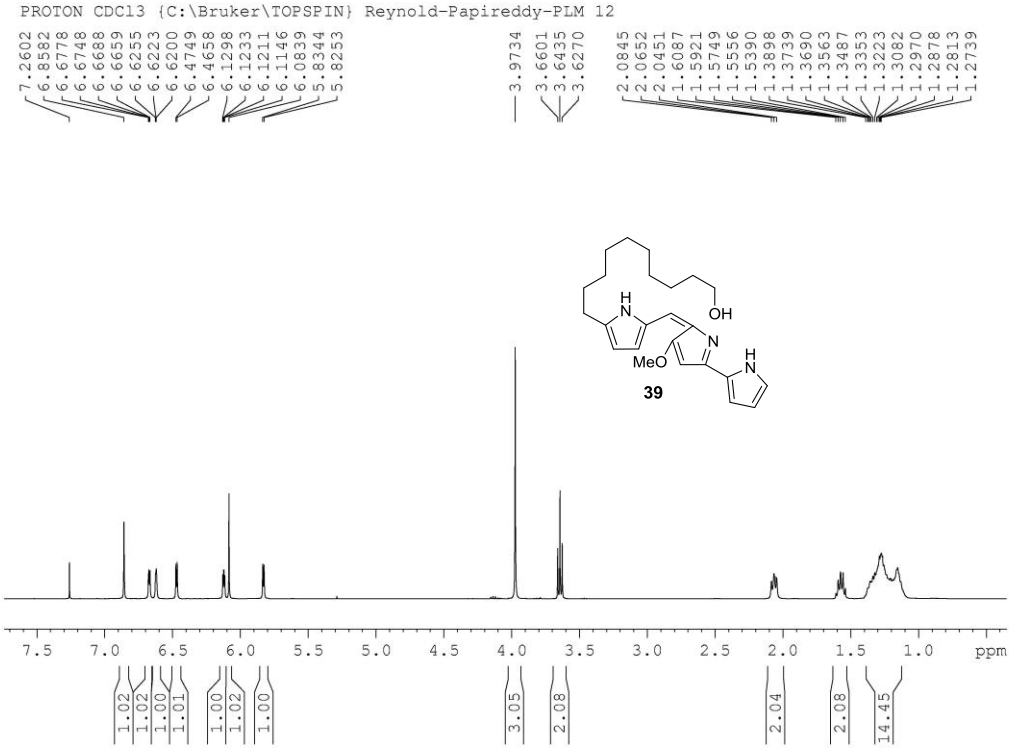
8.0235
7.2601
6.6709
6.6667
6.6645
6.6606
6.6541
6.1486
6.1415
6.1342
6.1272
5.9227
5.9210
3.6603
3.6437
3.6270
2.6177
2.5987
2.5791
1.6642
1.6443
1.6275
1.6088
1.5929
1.5903
1.5751
1.5575
1.5414
1.3736
1.3511
1.3287
1.2860
1.2526
1.2369

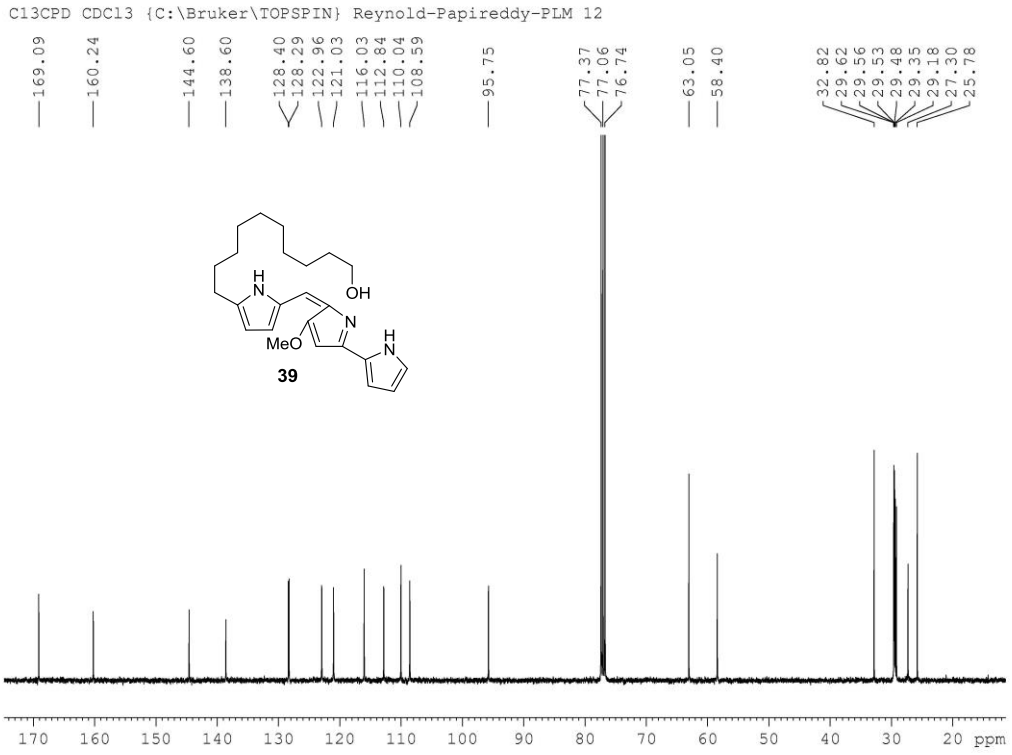


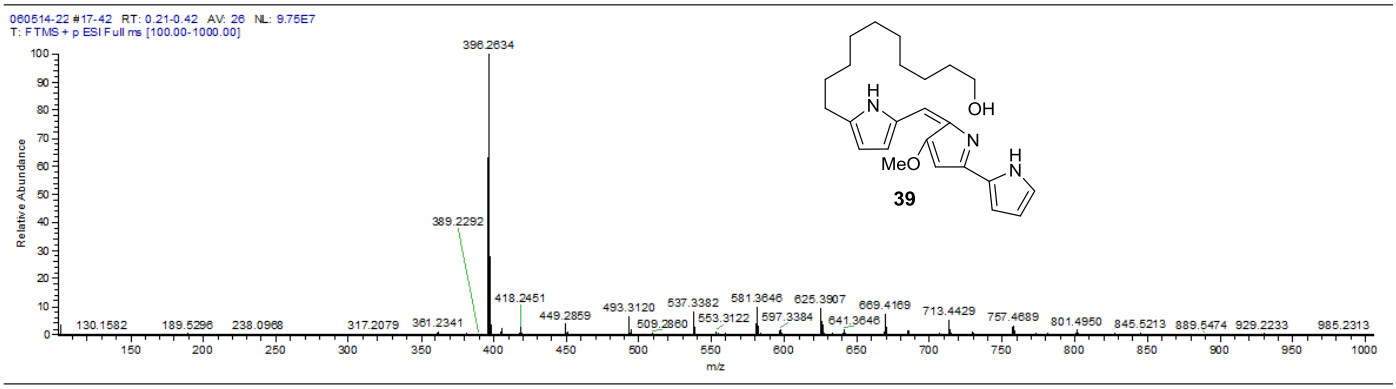
57c

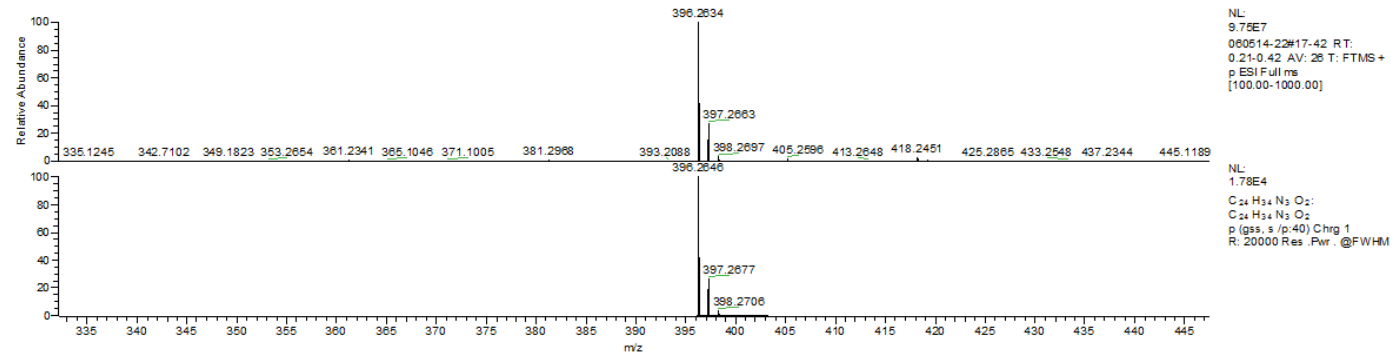



C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 5
132.89
115.96
108.14
104.76
77.37
77.05
76.73
63.03
32.77
29.67
29.59
29.57
29.54
29.43
29.41
29.38
27.72
25.73
OH
NH
57c
130
120
110
100
90
80
70
60
50
40
30
20 ppm

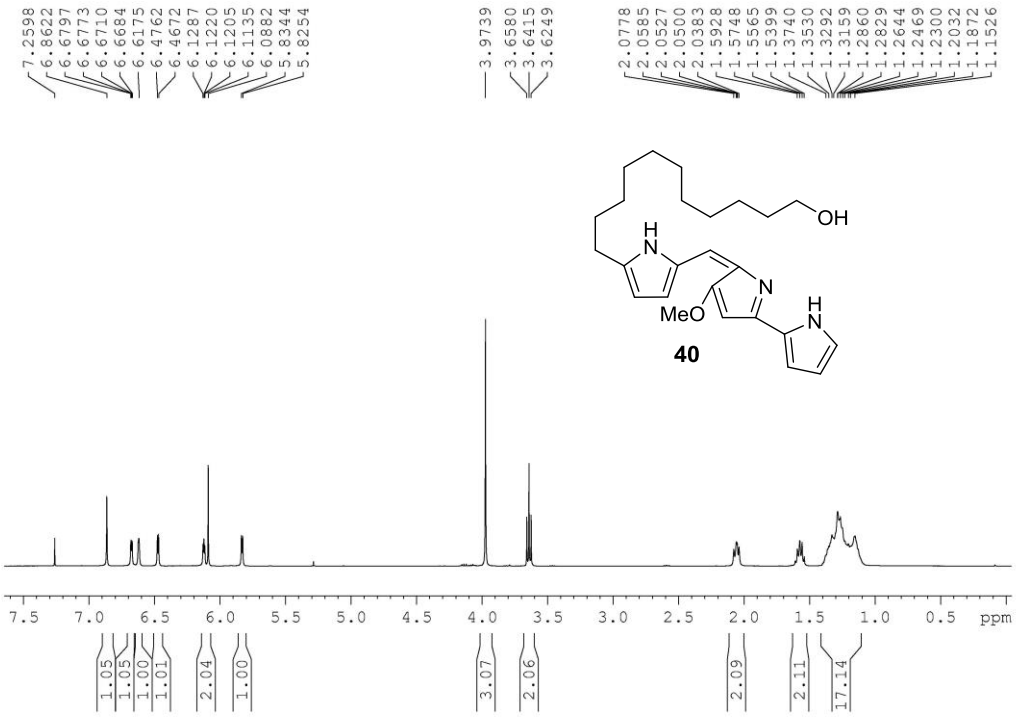

PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 12
7.2602
6.8582
6.6778
6.6748
6.6688
6.6659
6.6255
6.6223
6.6200
6.4749
6.4658
6.1298
6.1233
6.1211
6.1146
6.0839
5.8344
5.8253
3.9734
3.6601
3.6435
3.6270
2.0845
2.0652
2.0451
1.6087
1.5921
1.5749
1.5556
1.5390
1.3898
1.3739
1.3690
1.3563
1.3487
1.3353
1.3223
1.3082
1.2970
1.2878
1.2813
1.2739
OH
N
H
MeO
N
H
39
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
ppm
1.02
1.02
1.00
1.01
1.00
1.02
1.00
3.05
2.08
2.04
2.08
14.45


C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 12
169.09
160.24
144.60
138.60
128.40
128.29
122.96
121.03
116.03
112.84
110.04
108.59
95.75
77.37
77.06
76.74
63.05
58.40
32.82
29.62
29.56
29.53
29.48
29.35
29.18
27.30
25.78
H
N
OH
N
MeO
H
N
39
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

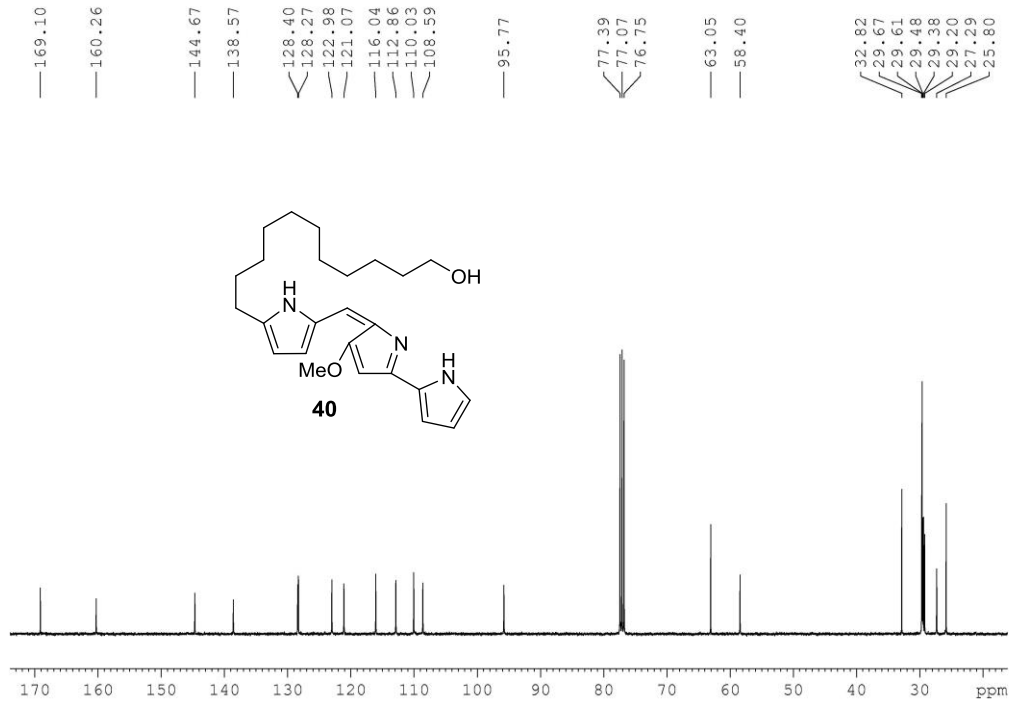

060514-22 #17-42 RT: 0.21-0.42 AV: 26 NL: 9.75E7
T: FTMS + p ESI Full ms [100.00-1000.00]
Relative Abundance
m/z
396.2634
389.2292
418.2451
130.1582
189.5296
238.0968
317.2079
361.2341
449.2859
493.3120
509.2860
537.3382
553.3122
581.3646
597.3384
625.3907
641.3646
669.4169
713.4429
757.4689
801.4950
845.5213
889.5474
929.2233
985.2313
H
N
OH
N
MeO
H
N
39

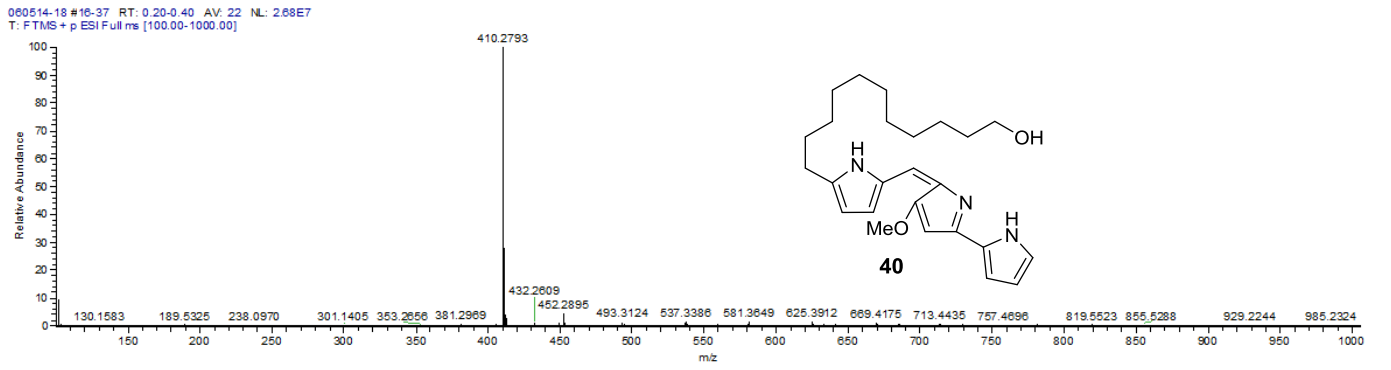

Relative Abundance
m/z
396.2634
397.2663
335.1245
342.7102
349.1823
353.2654
361.2341
365.1046
371.1005
381.2968
393.2088
398.2697
405.2596
413.2648
418.2451
425.2865
433.2548
437.2344
445.1189
NL:
9.75E7
060514-22#17-42 RT:
0.21-0.42 AV: 26 T: FTMS +
p ESI Full ms
[100.00-1000.00]
396.2646
397.2677
398.2706
NL:
1.78E4
C24 H34 N3 O2:
C24 H34 N3 O2
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr . @FWHM

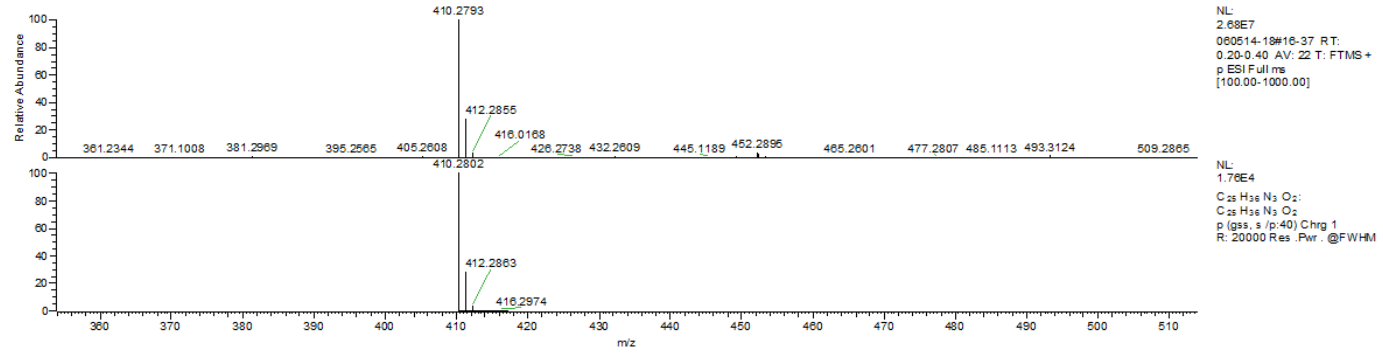
PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 10

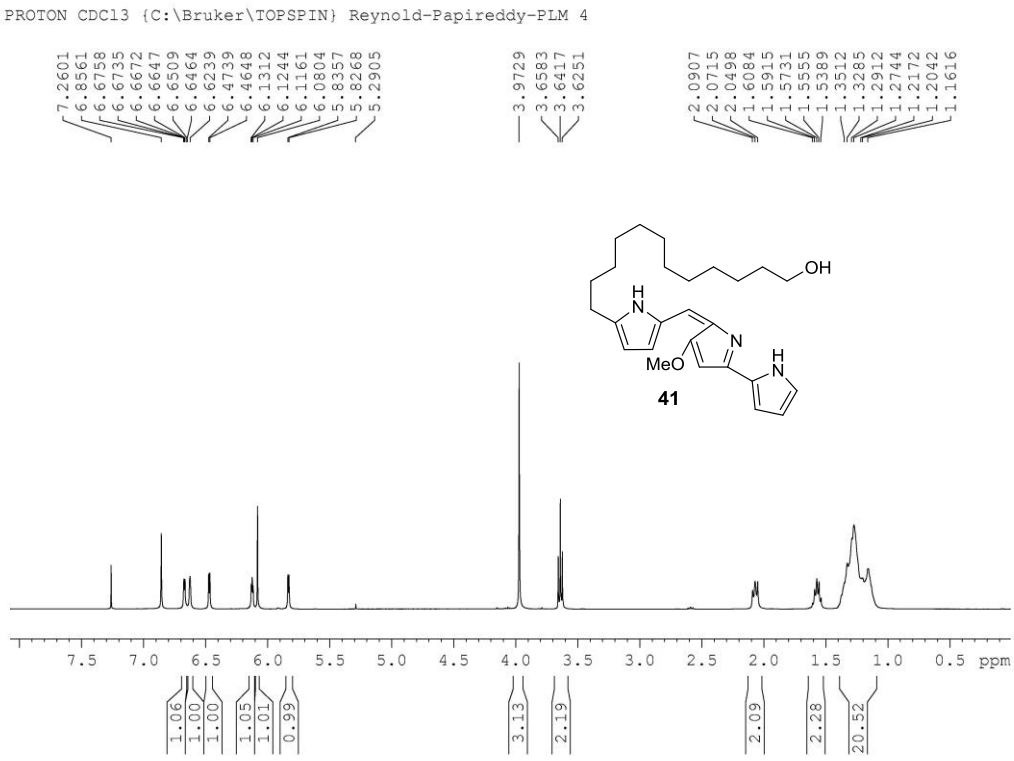


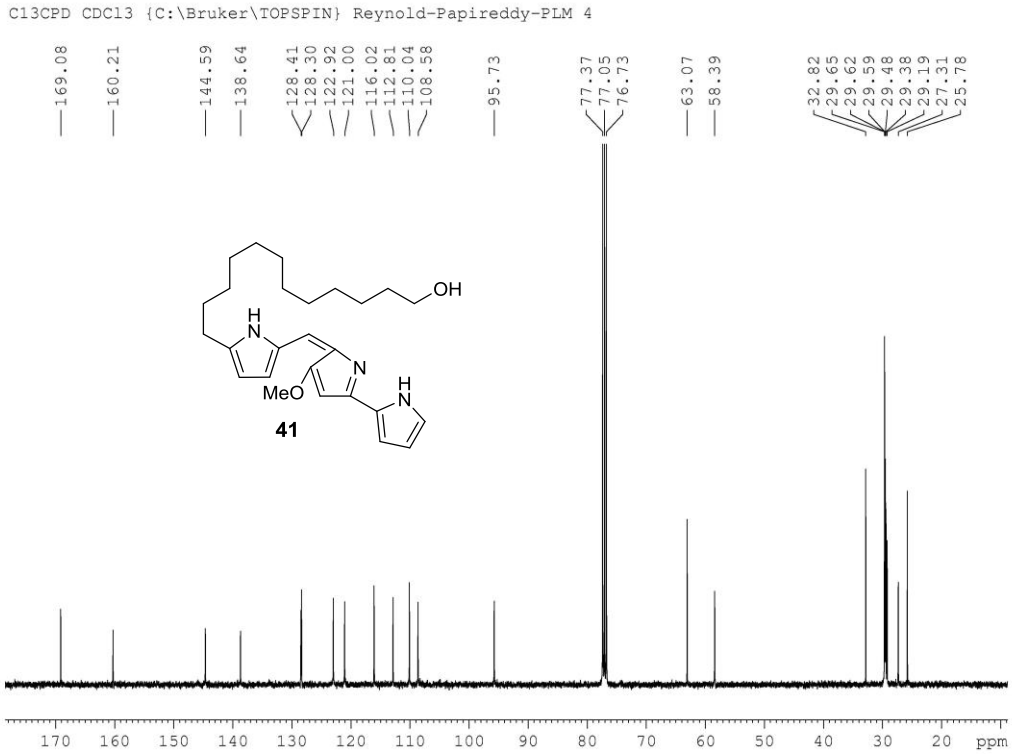
C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 13

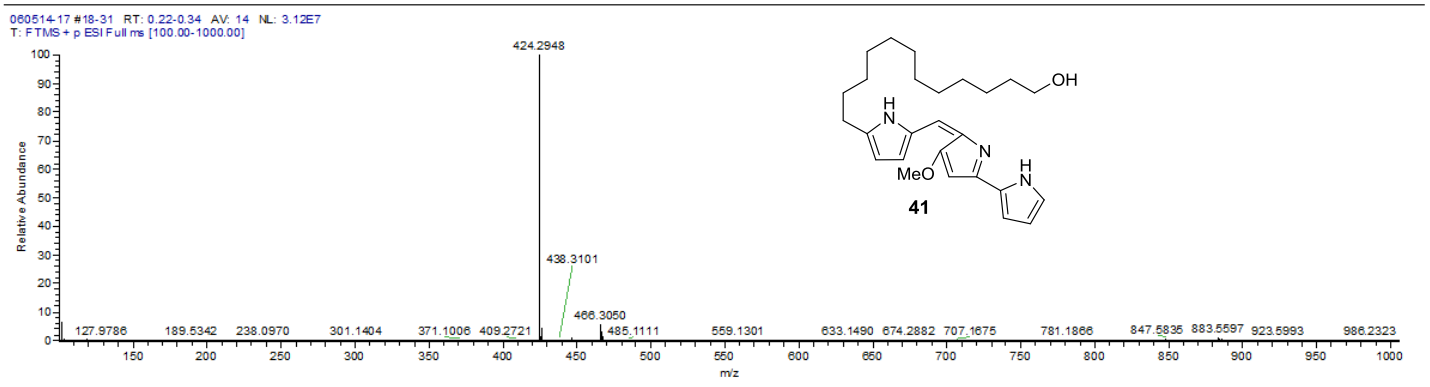


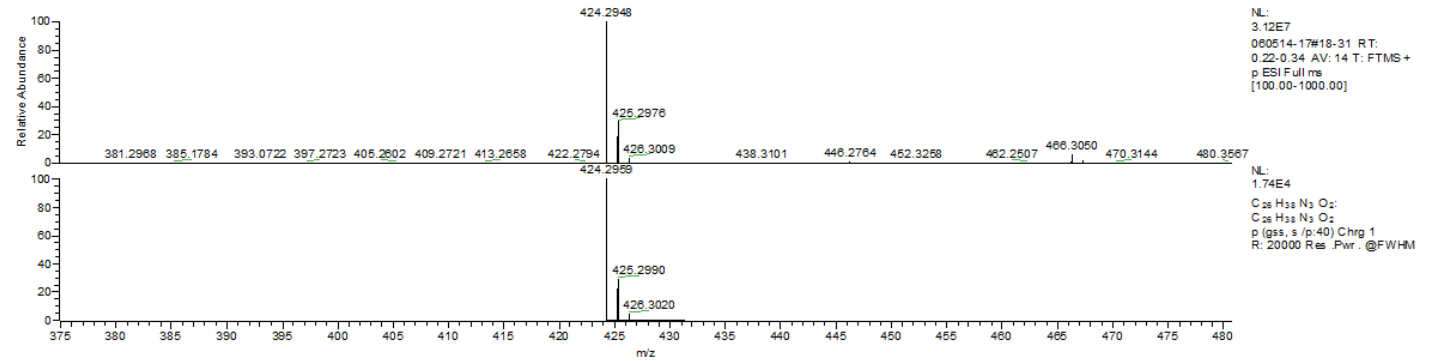

060514-18 #16-37 RT: 0.20-0.40 AV: 22 NL: 2.68E7
T: FTMS + p ESI Full ms [100.00-1000.00]
Relative Abundance
m/z
410.2793
432.2609
452.2895
OH
H
N
N
MeO
H
N
40


Relative Abundance
m/z
410.2793
412.2855
416.0168
410.2802
412.2863
416.2974
NL:
2.68E7
060514-18#16-37 RT:
0.20-0.40 AV: 22 T: FTMS +
p ESI Full ms
[100.00-1000.00]
NL:
1.76E4
C25 H36 N3 O2:
C25 H36 N3 O2
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr . @FWHM


PROTON CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 4
7.2601
6.8561
6.6758
6.6735
6.6672
6.6647
6.6509
6.6464
6.6239
6.4739
6.4648
6.1312
6.1244
6.1161
6.0804
5.8357
5.8268
5.2905
3.9729
3.6583
3.6417
3.6251
2.0907
2.0715
2.0498
1.6084
1.5915
1.5731
1.5555
1.5389
1.3512
1.3285
1.2912
1.2744
1.2172
1.2042
1.1616
OH
H
N
N
MeO
H
N
41
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
ppm
1.06
1.00
1.00
1.05
1.01
0.99
3.13
2.19
2.09
2.28
20.52


C13CPD CDCl3 {C:\Bruker\TOPSPIN} Reynold-Papireddy-PLM 4
169.08
160.21
144.59
138.64
128.41
128.30
122.92
121.00
116.02
112.81
110.04
108.58
95.73
77.37
77.05
76.73
63.07
58.39
32.82
29.65
29.62
29.59
29.48
29.38
29.19
27.31
25.78
OH
H
N
N
MeO
H
N
41
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


060514-17 #18-31 RT: 0.22-0.34 AV: 14 NL: 3.12E7
T: FTMS + p ESI Full ms [100.00-1000.00]
424.2948
438.3101
466.3050
OH
H
N
N
MeO
H
N
41
Relative Abundance
m/z


424.2948
425.2976
426.3009
424.2959
425.2990
426.3020
NL:
3.12E7
060514-17#18-31 RT:
0.22-0.34 AV: 14 T: FTMS +
p ESI Full ms
[100.00-1000.00]
NL:
1.74E4
C28 H38 N3 O2:
C28 H38 N3 O2
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr. @FWHM
Relative Abundance
m/z

References

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2. Xue, Y.; Zhao, L.; Liu, H. W.; Sherman, D. H. *Proc Natl Acad Sci U S A* **1998,** *95*, 12111–12116.
3. Gust, B.; Challis, G. L.; Fowler, K.; Kieser, T.; Chater, K. F. *Proc Natl Acad Sci U S A* **2003**, *100*, 1541–1546.
4. Salem, S. M.; Kancharla, P.; Florova, G.; Gupta, S.; Lu, W.; Reynolds, K. A. *J. Am. Chem. Soc.* **2014**, *136*, 4565−4574.