

Supporting Information for **Modeling, Synthesis and Biological Evaluation of Potential Retinoid-X-Receptor (RXR) Selective Agonists: Analogs of 4-[1-(3,5,5,8,8-Pentamethyl-5,6,7,8-tetrahydro-2-naphthyl)ethynyl]benzoic Acid (Bexarotene) and 6-(Ethyl(4-isobutoxy-3-isopropylphenyl)amino)nicotinic Acid (NEt-4IB):**

¹H- and ¹³C-NMR for all reported compounds

Representative HPLC Method for compound **33**

HPLC Traces for compounds **25-36, 37a** and **37b**

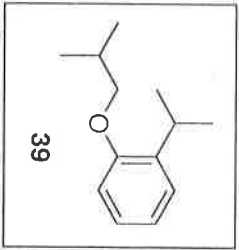
CWV-195

7.226
7.183
7.179
7.162
7.160
7.144
7.140
6.950
6.931
6.912
6.850
6.830

3.767
3.751
3.442
3.424
3.407
3.390
3.372
3.355
3.338
2.215
2.198
2.181
2.165
2.148
2.132
2.115
2.099
2.082
1.269
1.267
1.252
1.250
1.093
1.091
1.077
1.075



39



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

0.96
0.97
0.97
0.98

2.00
0.97

0.97

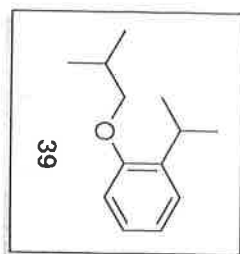
6.23
6.04

NAME CWV-195
EXPNO 1
PROCNO 1
Date_ 20141227
Time 15.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 0.50 dB
PL1W 12.76071072 W
SF01 400.1324710 MHz
SI 32768
SE 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-195

156.30
136.98
126.46
125.93
120.23
110.93
77.32
77.00
76.68
74.20
28.51
26.90
22.62
19.42



200 180 160 140 120 100 80 60 40 20 0 ppm



NAME CWV-195
EXPNO 2
PROCNO 1
Date 20141227
Time 15.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 51
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.363198 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

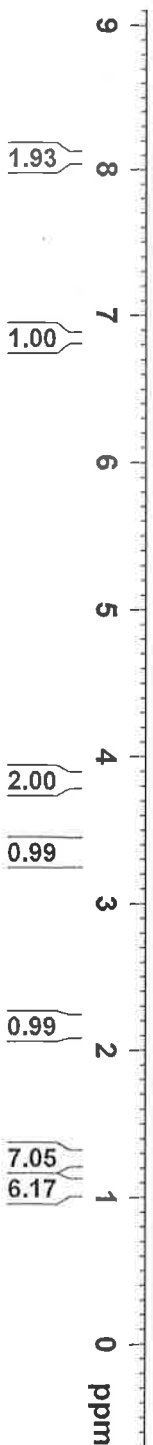
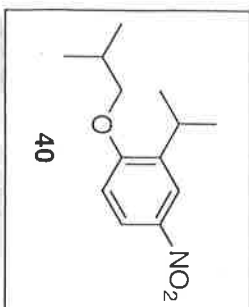
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CWV-197 bottom spot

8.097
8.091
8.082
8.075
8.060
8.053
7.260
6.856
6.833

3.840
3.824
3.398
3.380
3.363
3.346
3.329
3.311
3.294
2.214
2.198
2.181
2.164
2.148
2.132
2.115
1.260
1.243
1.082
1.065

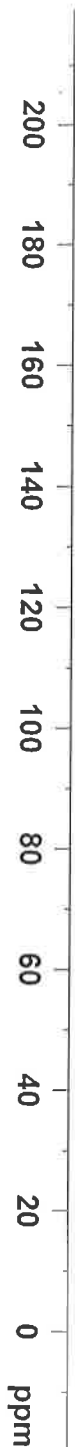
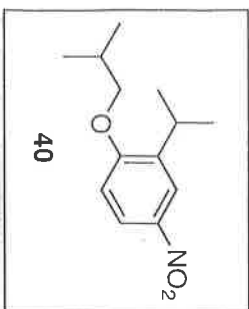


NAME CWV-197
EXPNO 7
PROCNO 1
Date_ 20150108
Time_ 9.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
FIDRES 0.125483 Hz
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
AQ 3.9846387 sec
RG 4
DE 60.800 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 0.50 dB
PL1W 12.76071072 W
SF01 400.1324710 MHz
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-197 bottom spot

161.48
141.21
138.04
123.30
121.98
110.23
77.32
77.00
76.68
74.94
28.30
27.05
22.16
19.23



NAME CWV-197
EXPNO 8
PROCNO 1
Date_ 20150108
Time_ 9.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 63
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
RW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

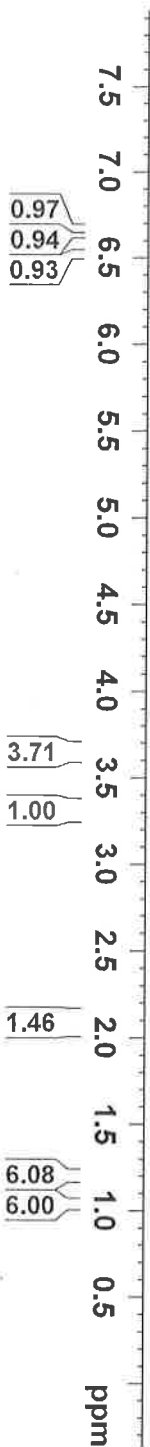
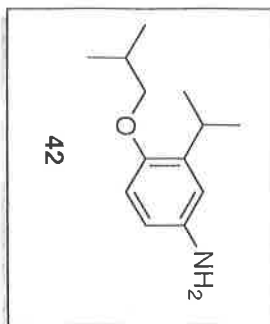
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CWV-199

7.260
6.675
6.654
6.632
6.625
6.526
6.519
6.505
6.498

3.664
3.648
3.358
3.341
3.324
3.307
3.289
3.272
3.255
2.149
2.132
2.115
2.099
2.082
2.066
2.052
2.033
1.210
1.193
1.046
1.029



NAME CWV-199
EXPNO 1
PROCNO 1
Date_ 20150112
Time_ 15.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DE 60.800 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

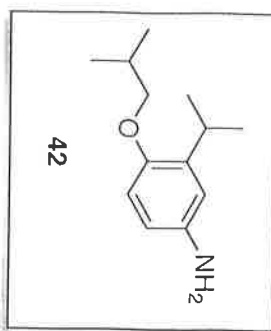
CWV-199

149.88
138.97
138.27

114.30
113.19
112.65

77.32
77.00
76.68
75.20

28.58
26.82
22.68
19.41



150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

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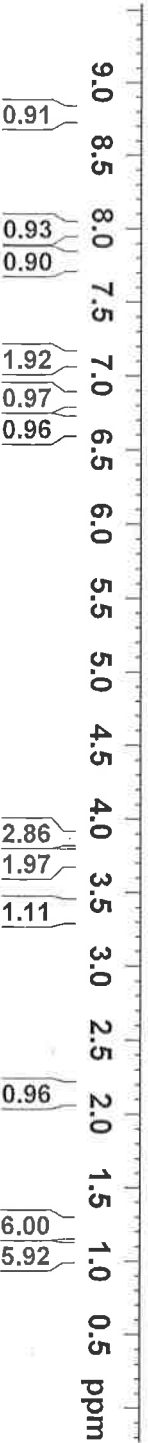
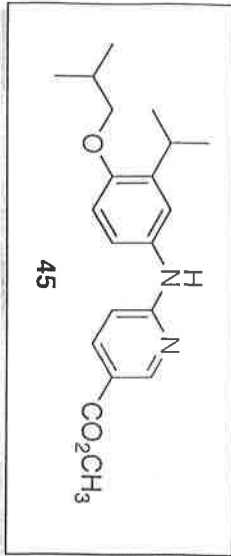
NAME CWV-199
EXPNO 2
PROCNO 1
Date_ 20150112
Time 15.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgig30
TD 65536
SOLVENT CDCl3
NS 160
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DM 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
Dl1 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
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CWV-219

- 8.764
- 8.762
- 8.006
- 8.000
- 7.983
- 7.978
- 7.770
- 7.260
- 7.117
- 7.098
- 7.091
- 6.837
- 6.834
- 6.818
- 6.815
- 6.669
- 6.667
- 6.646
- 6.645
- 3.865
- 3.753
- 3.737
- 3.414
- 3.397
- 3.380
- 3.363
- 3.345
- 3.328
- 3.311
- 2.199
- 2.183
- 2.166
- 2.150
- 2.133
- 2.117
- 2.100
- 2.084
- 2.067
- 1.238
- 1.221
- 1.076
- 1.059

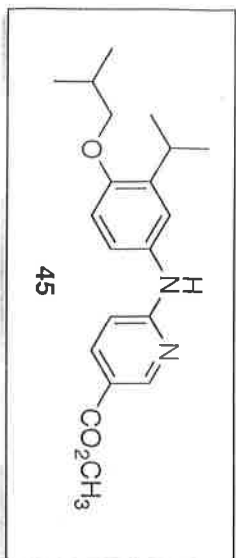


NAME CWV-219
 EXPNO 1
 PROCNO 1
 Date 20150331
 Time 12.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 4
 DW 60.800 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.50 usec
 PL1 0.50 dB
 PL1W 12.76071072 W
 SFO1 400.1324710 MHz
 SI 32768
 SF 400.1300096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

CWV-219

166.11
160.16
154.11
151.11
138.96
138.44
131.03
122.29
121.97
115.99
111.66
105.59
77.31
76.99
76.68
74.59
51.66
28.47
26.94
22.52
19.37



200
180
160
140
120
100
80
60
40
20
0
ppm



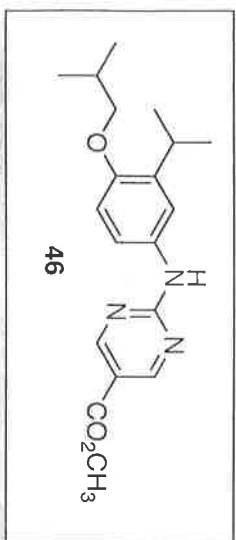
NAME CWV-219
EXPNO 2
PROCNO 1
Date 20150331
Time 12.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CWV-201

8.923
8.366
7.463
7.457
7.442
7.435
7.273
7.267
7.260
6.846
6.824
3.892
3.750
3.735
3.420
3.403
3.385
3.368
3.351
3.334
3.317
2.191
2.175
2.158
2.142
2.125
2.109
2.092
2.076
2.059
1.253
1.236
1.067
1.051



NAME CWV-201
EXPNO 1
PROCNO 1
Date 20150116
Time 16.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DM 60.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-201

164.78
161.72
160.07
153.58

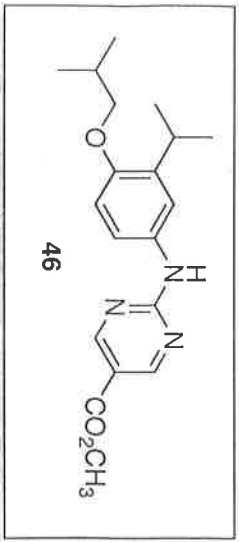
137.73
130.43

120.19
120.11
114.42
111.33

77.31
77.00
76.68
74.57

51.84

28.46
26.96
22.52
19.37



NAME CWV-201

EXPNO 2

PROCNO 1

Date 20150116

Time 17.07

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 208

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DM 20.800 usec

DE 6.50 usec

TE 298.2 K

DI 2.00000000 sec

D11 0.03000000 sec

TDO 1

===== CHANNEL f1 =====

NUC1 13C

PL 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

100.6127736 MHz

EM

1.00 Hz

0

1.40

0

1.00 Hz

0

1.40

0

1.40

0

1.40

0

1.40

0

1.40

0

1.40

0

1.40

0

1.40

0

1.40

0

1.40



CWV-215

7.836
7.815
7.794
7.773
7.752
7.260
7.017
6.973
6.966
6.875
6.869
6.853
6.847
6.827
6.816
6.805
6.795
6.763
6.757
6.730
6.725
6.552
6.531
6.496
6.462
3.964
3.899
3.863
3.765
3.750
3.732
3.368
3.350
3.333
3.316
2.164
2.148
2.131
2.115
2.098
1.223
1.206
1.076
1.059



NAME CWV-215

EXPNO 1

PROCNO 1

Date 20150331

Time 13.42

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zg30

TD 65536

SOLVENT CDCl3

NS 16

DS 2

SWH 8223.685 Hz

FIDRES 0.125483 Hz

AQ 3.9846387 sec

RG 4

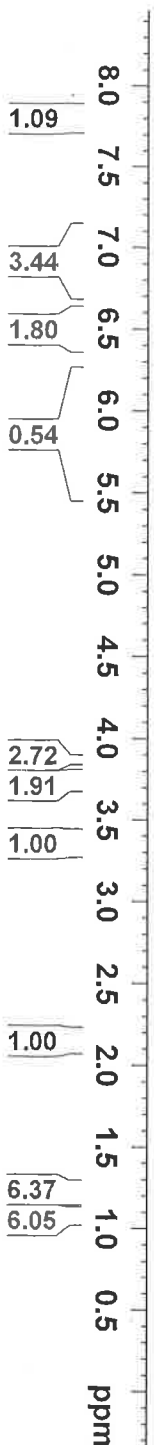
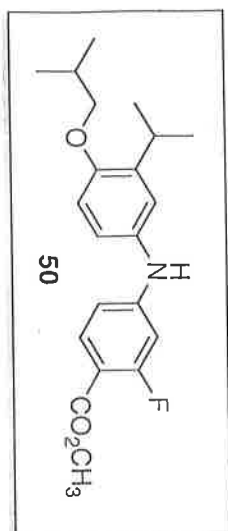
DM 60.800 usec

DE 6.50 usec

TE 298.0 K

D1 1.00000000 sec

TD0 1



===== CHANNEL f1 =====

NUC1 1H

PI 14.50 usec

PL1 0.50 dB

PL1W 12.76071072 W

SFO1 400.1324710 MHz

SI 32768

SF 400.1300096 MHz

WDW EM

SSB 0

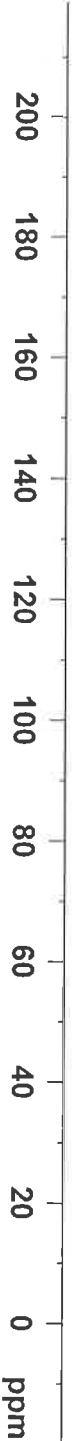
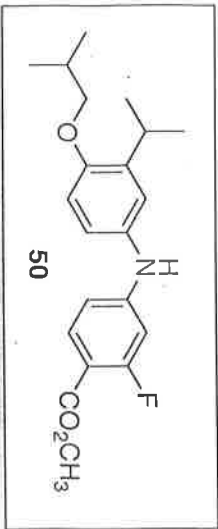
LB 0.30 Hz

GB 0

PC 1.00

CWV-215

165.30
164.99
164.95
164.52
164.48
164.23
162.74
161.65
155.23
153.91
152.05
151.94
139.43
138.50
136.90
133.60
133.03
131.98
128.94
128.37
125.72
125.52
122.18
121.78
116.95
112.11
112.01
111.91
111.71
109.75
109.49
109.37
107.45
107.34
100.63
100.33
77.32
77.00
76.68
74.61
51.67
28.48
26.93
22.53
22.43
19.38



NAME CWV-215
EXPNO 4
PROCNO 1
Date_ 20150401
Time_ 8.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

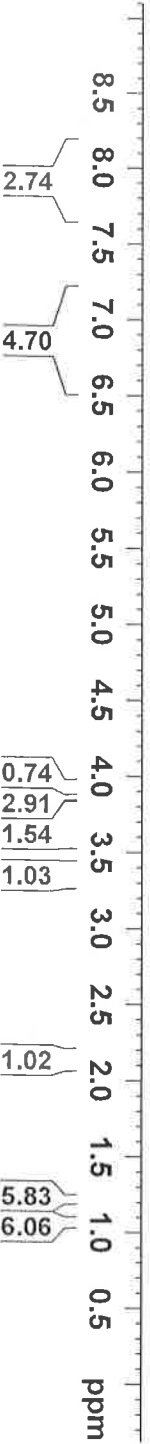
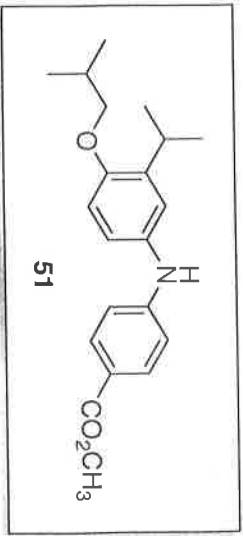
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CWV-217

8.147
8.126
7.901
7.895
7.883
7.878
7.872
7.705
7.684
7.260
7.077
7.055
6.811
6.790

3.955
3.887
3.861
3.755
3.739
3.408
3.390
3.373
3.356
3.339
3.321
3.303
2.197
2.181
2.164
2.148
2.131
2.115
2.098
2.082
2.065
1.227
1.209
1.078
1.061

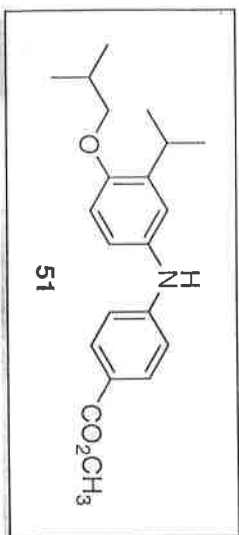


NAME CWV-217
EXPNO 1
PROCNO 1
Date 20150325
Time 17.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DE 60.800 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SF01 400.1324710 MHz
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-217

167.08
151.23
131.59
131.53
131.48
131.41
130.86
130.20
129.70
127.23
121.47
113.16
77.32
77.00
76.69
74.64
51.57
28.51
26.93
22.57
19.39



200 180 160 140 120 100 80 60 40 20 0 ppm



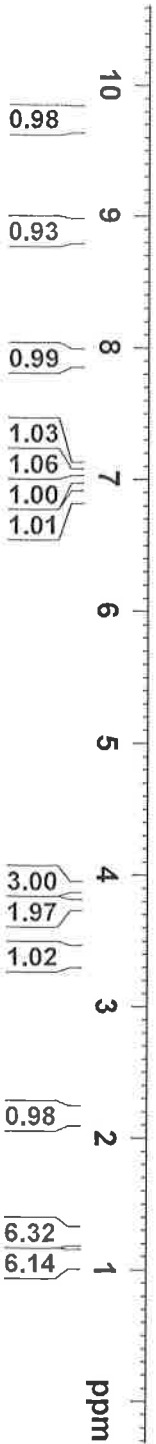
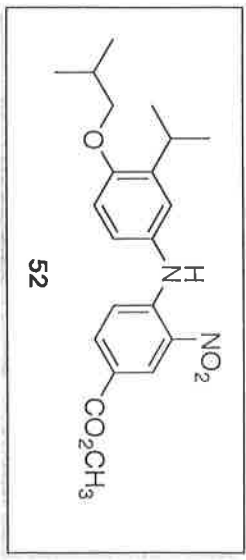
NAME CWV-217
EXPNO 2
PROCNO 1
Date 20150325
Time 18.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 365
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CWV-231

9.711
8.902
8.897
7.924
7.923
7.919
7.918
7.901
7.900
7.896
7.895
7.260
7.095
7.088
7.059
7.053
7.038
7.031
7.011
6.989
6.877
6.856
3.895
3.777
3.761
3.423
3.406
3.388
3.371
3.354
3.337
3.319
2.200
2.184
2.168
2.151
2.134
2.118
2.102
2.085
1.236
1.219
1.088
1.071

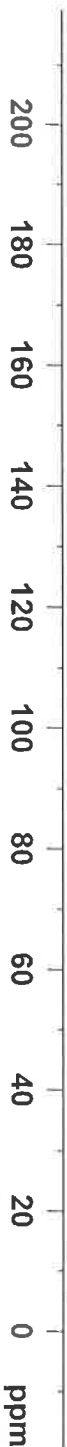
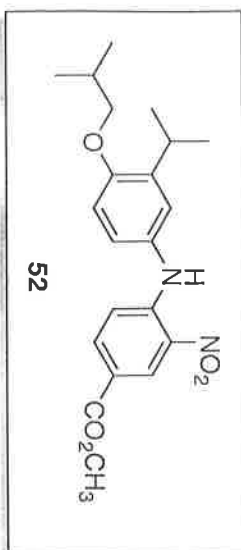


NAME CWV-231
EXPNO 1
PROCNO 1
Date_ 20150706
Time_ 9.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DE 60.800 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-231

165.46
155.26
147.23
138.93
135.73
131.51
129.58
129.27
128.92
128.35
124.00
123.93
118.27
115.54
111.77
77.31
77.00
76.68
74.56
52.07
28.45
26.97
22.47
19.35



NAME CWV-231
EXPNO 2
PROCNO 1
Date 20150706
Time 9.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 158
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DE 20.800 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

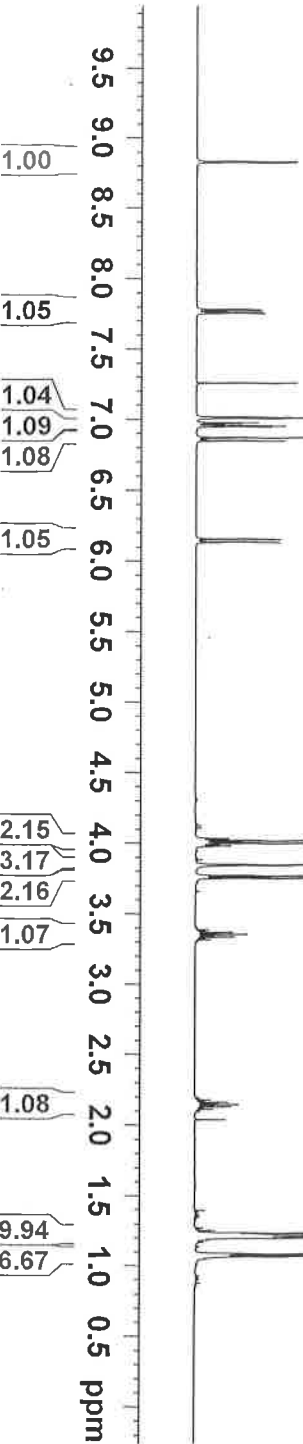
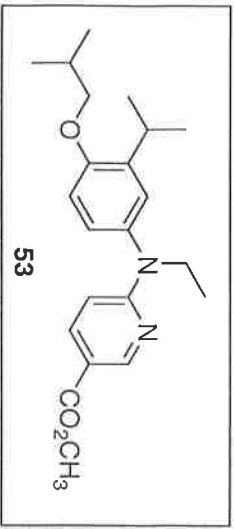
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CWV-221



8.834
8.833
8.829
8.827
7.783
7.777
7.761
7.755
7.260
7.019
7.013
6.979
6.973
6.958
6.952
6.873
6.852
6.157
6.136
6.135
4.036
4.018
4.001
3.983
3.848
3.772
3.756
3.389
3.372
3.355
3.337
3.320
2.180
2.164
2.147
2.131
2.114
1.236
1.225
1.219
1.208
1.201
1.087
1.070

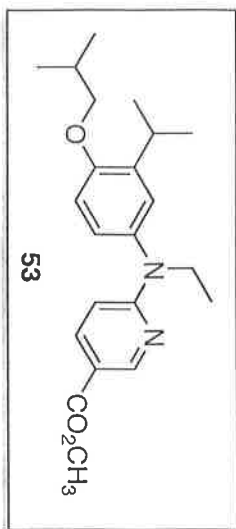


NAME CWV-221
EXPNO 1
PROCNO 1
Date_ 20150420
Time_ 13.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DM 60.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-221

166.63
160.74
155.32
150.97
139.09
137.34
135.94
126.12
126.05
114.04
111.91
107.24
74.46
51.52
45.44
28.49
27.05
22.51
19.39
12.98



200 180 160 140 120 100 80 60 40 20 0 ppm

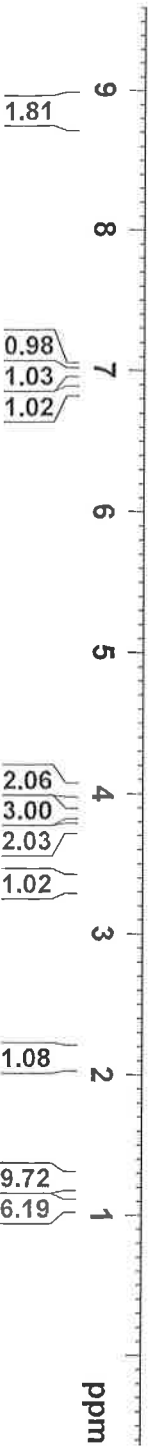
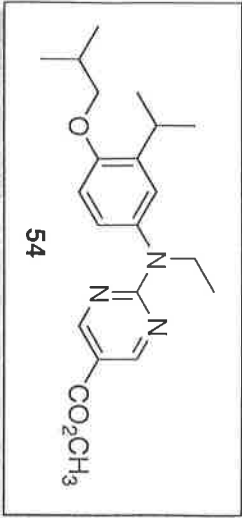
NAME CWV-221
EXPNO 2
PROCNO 1
Date 20150420
Time 13.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 464
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DM 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL F1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL F2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127714 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CWV-223

8.837
7.260
7.031
7.024
7.009
7.002
6.988
6.981
6.864
6.843
4.056
4.038
4.020
4.003
3.861
3.762
3.746
3.401
3.384
3.366
3.349
3.332
3.314
3.297
2.196
2.179
2.163
2.146
2.130
2.113
2.097
2.080
2.064
1.259
1.238
1.221
1.070
1.053



NAME CWV-223
EXPNO 1
PROCNO 1
Date_ 20150413
Time_ 12.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DE 60.800 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-223

165.38
162.80
159.78
155.17

138.17
135.35

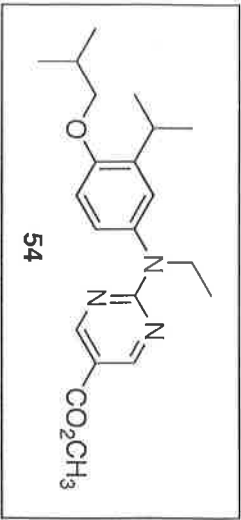
125.48
125.39

112.76
111.25

77.32
77.00
76.68
74.23

51.67
46.47

28.48
27.10
22.44
19.40
12.77



NAME CWV-223

EXPNO 2

PROCNO 1

Date 20150413

Time 12.37

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 284

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 298.6 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL12W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127714 MHz

WDW EM

SSB 0

LB 1.00 Hz

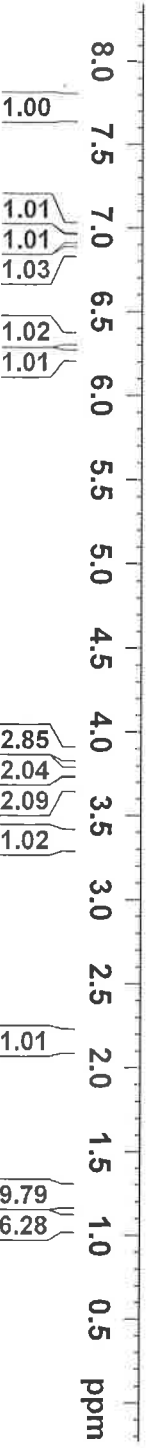
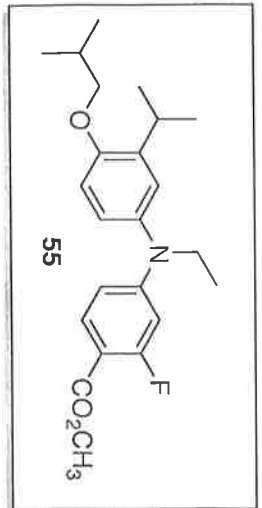
GB 0

PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

CWV-229

- 7.728
- 7.706
- 7.684
- 7.260
- 6.989
- 6.983
- 6.947
- 6.941
- 6.926
- 6.919
- 6.858
- 6.836
- 6.341
- 6.335
- 6.319
- 6.312
- 6.252
- 6.246
- 6.214
- 6.208
- 3.848
- 3.770
- 3.755
- 3.716
- 3.698
- 3.680
- 3.663
- 3.385
- 3.368
- 3.350
- 3.333
- 3.316
- 2.181
- 2.164
- 2.148
- 2.131
- 2.115
- 1.245
- 1.227
- 1.222
- 1.209
- 1.205
- 1.089
- 1.073



NAME EXPNO 1
 PROCNO 1
 Date 20150420
 Time 11.56
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 4
 DW 60.800 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.50 usec
 PL1 0.50 dB
 PL1W 12.76071072 W
 SFO1 400.1324710 MHz
 SI 32768
 SF 400.1300096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

CWV-229

165.19
165.15
162.60
155.09
154.14
154.02

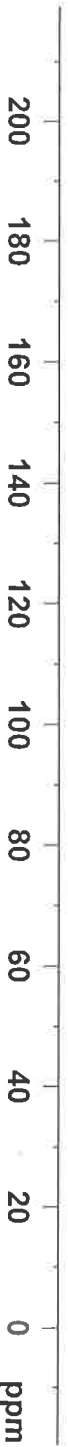
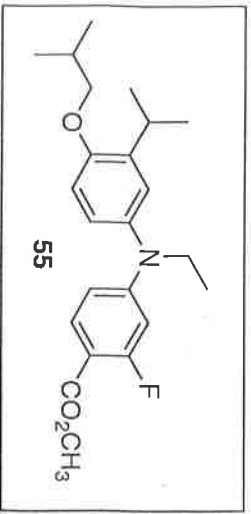
139.04
137.24
133.12
133.08
126.00
125.95

111.91
108.11
105.22
105.12
99.87
99.60

77.32
77.00
76.69
74.47

51.53
46.97

28.50
27.05
22.52
19.40
12.29



NAME CWV-229

EXPNO 2

PROCNO 1

Date 20150420

Time 12.14

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 376

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 298.5 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127714 MHz

WDW EM

SSB 0

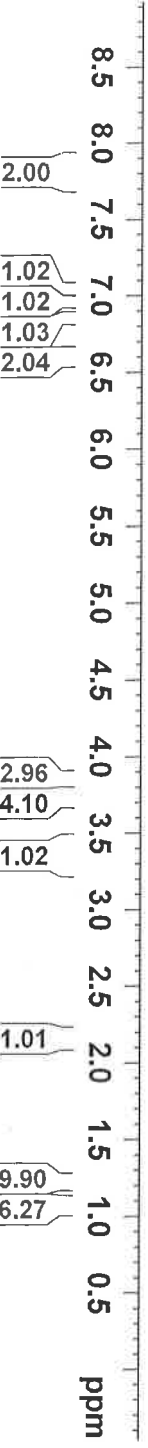
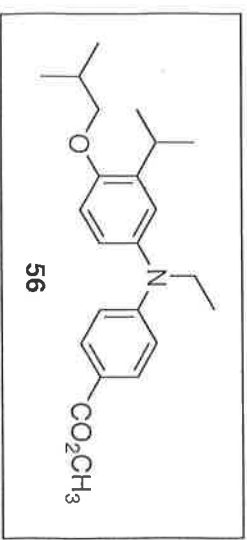
LB 1.00 Hz

GB 0

PC 1.40

CWV-227

- 7.822
- 7.817
- 7.805
- 7.799
- 7.260
- 7.021
- 7.014
- 6.970
- 6.963
- 6.948
- 6.942
- 6.857
- 6.836
- 6.596
- 6.591
- 6.578
- 6.573
- 3.840
- 3.770
- 3.755
- 3.740
- 3.722
- 3.704
- 3.405
- 3.388
- 3.371
- 3.354
- 3.336
- 3.319
- 3.302
- 2.207
- 2.197
- 2.180
- 2.164
- 2.147
- 2.131
- 2.114
- 2.098
- 1.253
- 1.236
- 1.222
- 1.204
- 1.091
- 1.074

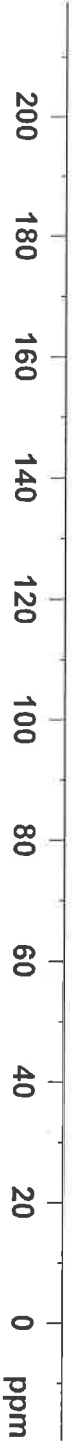
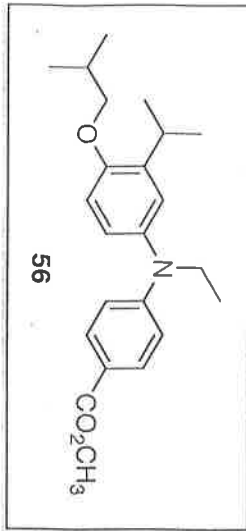


NAME CWV-227
 EXPNO 1
 PROCNO 1
 Date 20150420
 Time 12.27
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 4
 DW 60.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.50 usec
 PL1 0.50 dB
 PL1W 12.76071072 W
 SF01 400.1324710 MHz
 SI 32768
 SF 400.1300096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

CWV-227

167.33
154.74
152.29
138.84
137.98
131.09
126.01
125.93
117.34
112.03
111.84
77.32
77.00
76.68
74.45
51.42
46.79
28.51
27.04
22.54
19.41
12.33



```

NAME CWV-227
EXPNO 2
PROCNO 1
Date_ 20150420
Time 12.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 267
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DE 20.800 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

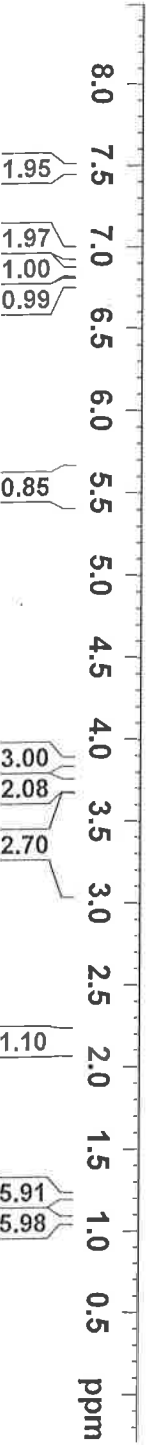
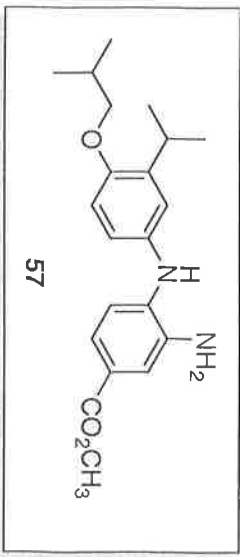
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
```

CWV-235

7.473
7.468
7.459
7.454
7.260
6.969
6.947
6.940
6.855
6.848
6.833
6.827
6.791
6.769

3.858
3.730
3.714
3.402
3.385
3.368
3.350
3.333
3.316
3.299
2.187
2.171
2.154
2.138
2.121
2.104
2.088
2.072
1.259
1.219
1.202
1.071
1.054

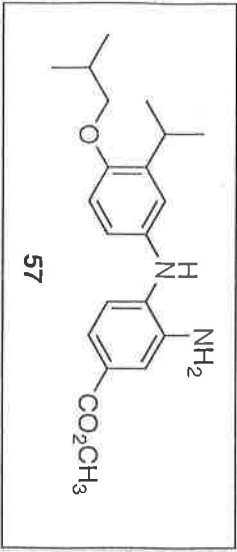


NAME CWV-235
EXPNO 1
PROCNO 1
Date 20150706
Time 15.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DM 60.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-235

167.26
152.45
139.36
138.37
134.71
134.28
122.95
121.67
119.68
118.86
118.26
114.15
111.93
77.32
77.00
76.68
74.74
60.37
51.68
28.52
26.92
22.59
21.01
19.40
14.16



NAME CWV-235

EXPNO 2

PROCNO 1

Date 20150706

Time 15.59

INSTRUM spect

PROBHD 5 mm PARBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 118

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 298.5 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127729 MHz

WDW EM

SSB 0

LB 1.00 Hz

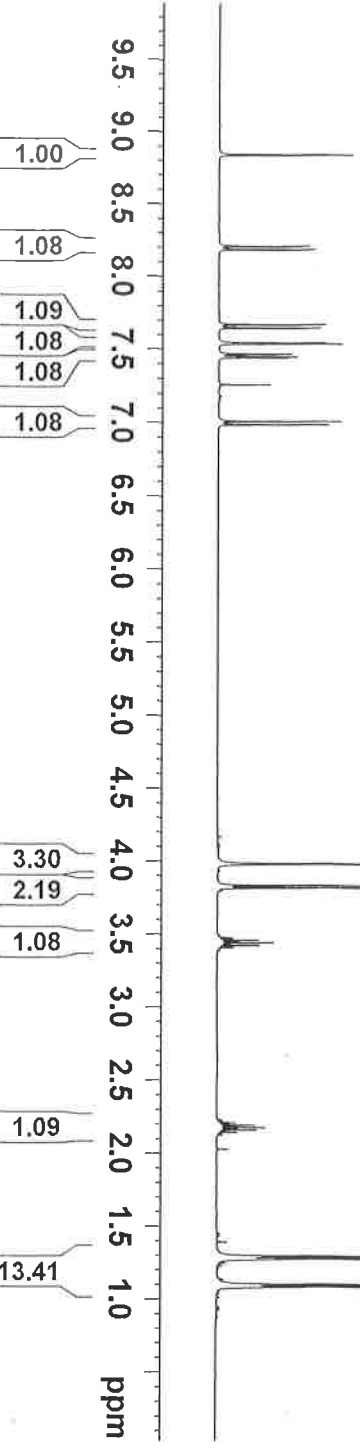
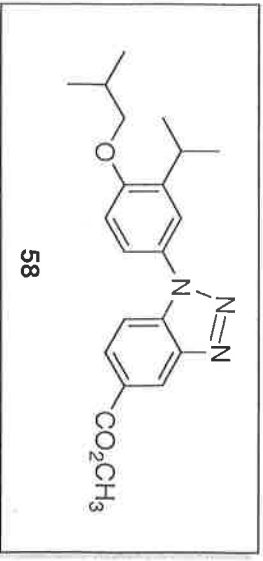
GB 0

PC 1.40

CWV-237

8.839
8.837
8.210
8.206
8.188
8.184
7.671
7.670
7.649
7.648
7.546
7.539
7.472
7.465
7.450
7.444
7.260
7.010
6.988

3.983
3.834
3.819
3.478
3.461
3.443
3.426
3.409
2.229
2.212
2.196
2.179
2.163
2.146
2.130
1.294
1.277
1.101
1.085



```

NAME          CWV-237
EXPNO         1
PROCNO        1
Date_         20150805
Time_         16.05
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG            4
DE            60.800 usec
TE            298.1 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            14.50 usec
PL1           0.50 dB
PL1W          12.76071072 W
SFO1          400.1324710 MHz
SI            32768
SF            400.1300096 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

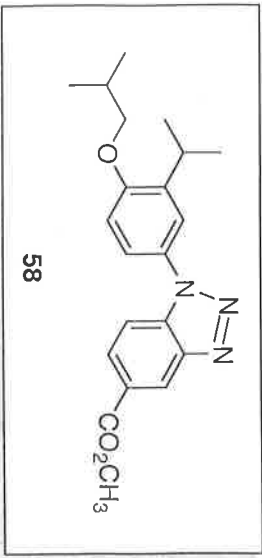
CWI-237

166.46
156.87
145.93
138.98
134.88
129.04
128.66
126.47
122.97
121.59
121.46
111.49
110.20

77.31
77.00
76.68
74.66

52.40

28.40
27.13
22.38
19.33



200
180
160
140
120
100
80
60
40
20
0
ppm

NAME CWI-237
EXPNO 2
PROCNO 1
Date 20150805
Time 16.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 63
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

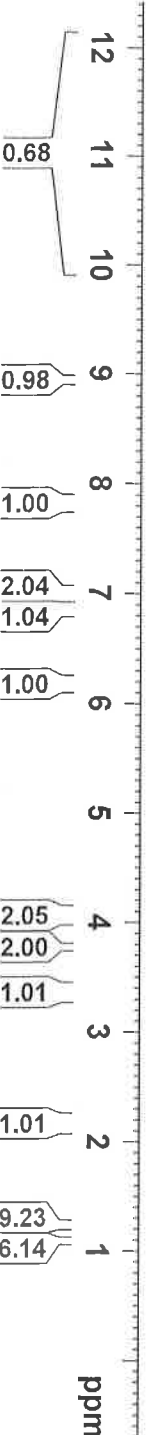
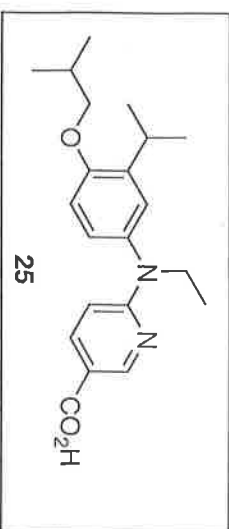
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127744 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CWV-253



- 8.927
- 8.922
- 8.921
- 7.842
- 7.836
- 7.819
- 7.813
- 7.260
- 7.030
- 7.024
- 6.991
- 6.985
- 6.970
- 6.964
- 6.886
- 6.865
- 6.187
- 6.164
- 4.064
- 4.046
- 4.029
- 4.011
- 3.779
- 3.763
- 3.397
- 3.380
- 3.362
- 3.345
- 3.328
- 3.311
- 2.202
- 2.186
- 2.169
- 2.153
- 2.136
- 2.120
- 2.103
- 1.258
- 1.240
- 1.235
- 1.222
- 1.217
- 1.091
- 1.075



NAME CWV-253
 EXPNO 1
 PROCNO 1
 Date 20150930
 Time 10.46
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 4
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 4
 DW 60.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TPD0 1

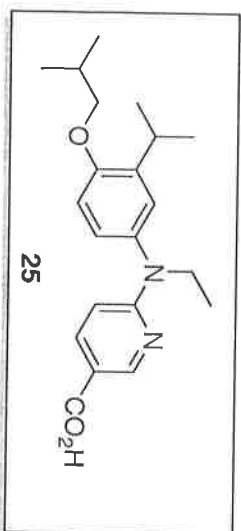
===== CHANNEL f1 =====
 NUC1 1H
 P1 14.50 usec
 PL1 0.50 dB
 PL1W 12.76071072 W
 SF01 400.1324710 MHz
 SI 32768
 SF 400.1300099 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

171.41
160.92
155.47
151.67
139.19
137.91
135.67
126.08
125.95
113.30
111.96
107.53

77.32
77.00
76.68
74.47

45.69

28.48
27.08
22.50
19.39
12.94



200
180
160
140
120
100
80
60
40
20
0
ppm



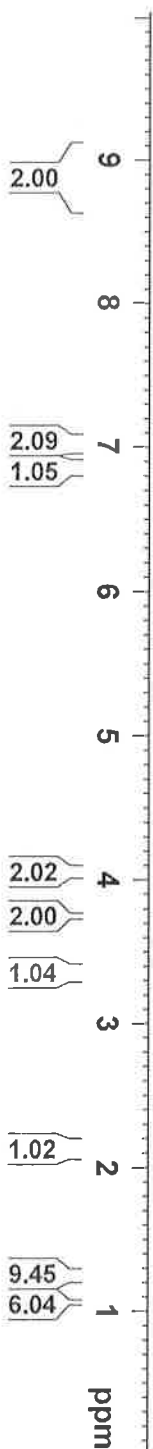
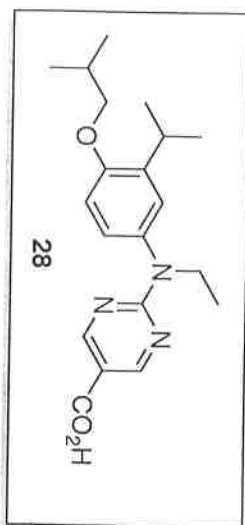
NAME CWV-253
EXPNO 2
PROCNO 1
Date_ 20150930
Time_ 10.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 377
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DM 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CWV-259

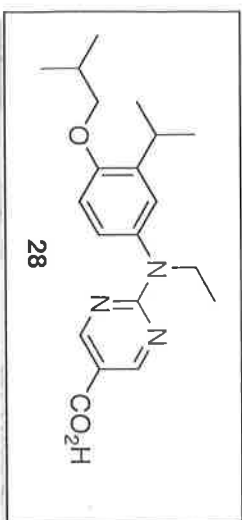
8.887
7.260
7.037
7.031
7.018
7.012
6.997
6.991
6.872
6.851
4.079
4.061
4.044
4.026
3.756
3.741
3.402
3.385
3.368
3.351
3.333
3.316
3.299
2.196
2.179
2.163
2.146
2.130
2.113
2.097
2.080
2.064
1.278
1.261



NAME CWV-259
EXPNO 1
PROCNO 1
Date 20150930
Time 11.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
FIDRES 0.125483 Hz
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DE 60.800 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-259

169.88
162.74
160.44
158.35
138.31
135.05
125.50
125.32
112.02
111.34
77.32
77.00
76.68
74.25
46.67
28.47
27.13
22.43
19.40
12.73



200 180 160 140 120 100 80 60 40 20 0 ppm



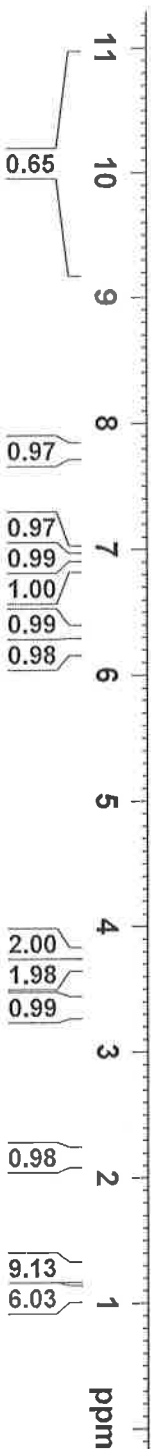
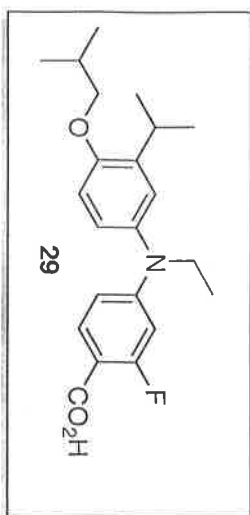
NAME CWV-259
EXPNO 2
PROCNO 1
Date 20150930
Time 11.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DM 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CMV-265

7.799
7.777
7.754
7.260
6.996
6.990
6.955
6.949
6.934
6.927
6.868
6.846
6.354
6.348
6.331
6.325
6.261
6.255
6.223
6.217
3.777
3.761
3.731
3.714
3.696
3.678
3.391
3.374
3.357
3.340
3.322
2.186
2.170
2.153
2.137
2.120
2.104
1.259
1.241
1.231
1.224
1.214
1.094
1.077

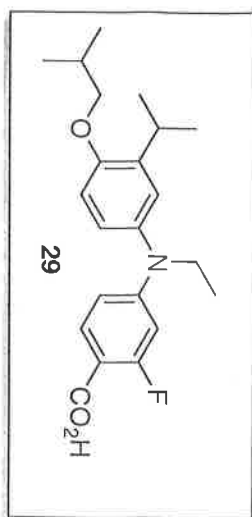


NAME
EXPNO 1
PROCNO 1
Date 20150930
Time 12.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-265

169.76
165.89
163.33
155.21
154.87
154.75
139.11
137.02
133.78
126.02
125.92
111.94
108.17
104.15
104.05
99.80
99.53
77.32
77.00
76.68
74.48
47.06
28.49
27.07
22.51
19.39
12.28



200
180
160
140
120
100
80
60
40
20
0
ppm



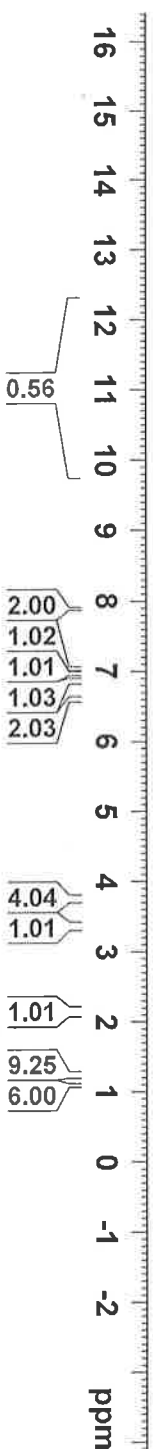
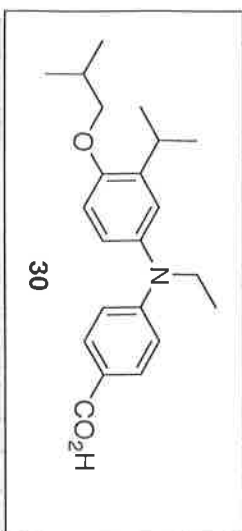
NAME CWV-265
EXPNO 2
PROCNO 1
Date_ 20150930
Time_ 12.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 207
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DM 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CWV-263

7.901
7.879
7.260
7.038
7.031
6.987
6.981
6.966
6.959
6.873
6.852
6.618
6.595
3.783
3.767
3.762
3.744
3.726
3.418
3.401
3.384
3.367
3.350
3.332
3.315
2.224
2.208
2.191
2.175
2.158
2.142
2.125
2.109
2.092
1.275
1.257

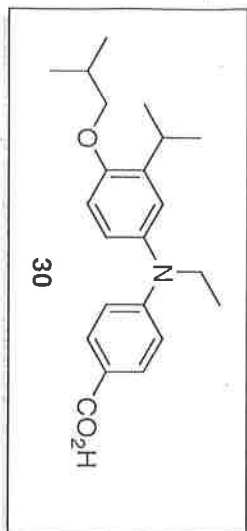


NAME CWV-263
EXPNO 1
PROCNO 1
Date_ 20150930
Time_ 11.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DM 60.800 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-263

172.44
154.88
152.90
138.92
137.77
131.89
126.00
116.37
112.01
111.88
77.32
77.00
76.68
74.46
46.89
28.51
27.07
22.54
19.41
12.32



200 180 160 140 120 100 80 60 40 20 0 ppm



NAME CWV-263

EXPNO 3

PROCNO 1

Date_ 20150930

Time_ 12.13

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 155

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DM 20.800 usec

DE 6.50 usec

TE 298.2 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127729 MHz

WDW EM

SSB 0

LB 1.00 Hz

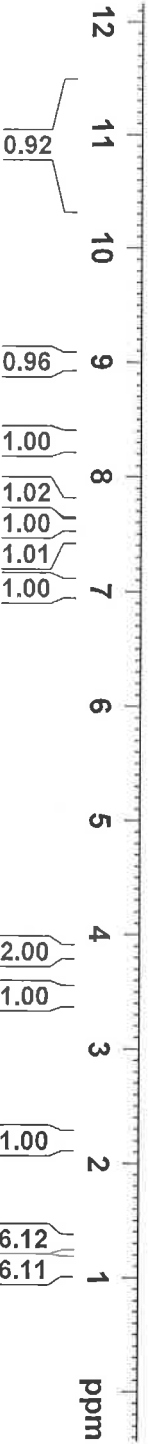
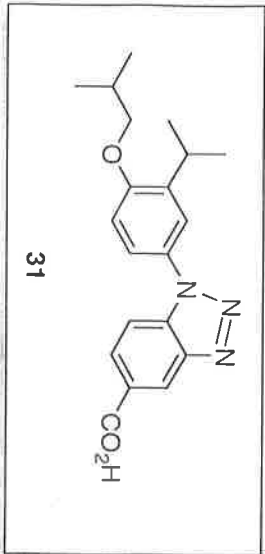
GB 0

PC 1.40

CWV-267



10.905
8.988
8.986
8.984
8.299
8.295
8.277
8.273
7.722
7.721
7.700
7.699
7.565
7.559
7.487
7.481
7.466
7.459
7.260
7.028
7.006
3.850
3.834
3.510
3.493
3.476
3.458
3.441
3.424
3.407
2.259
2.242
2.226
2.209
2.193
2.176
2.160
2.143
2.127
1.310
1.293



NAME CWV-267
EXPNO 1
PROCNO 1
Date_ 20150930
Time_ 12.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

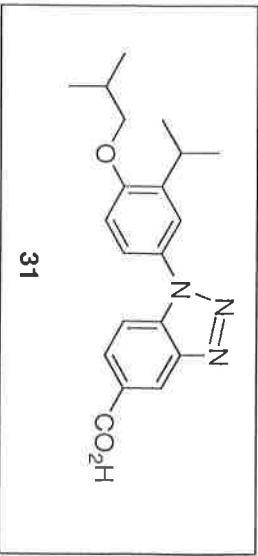
===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-267

171.37
156.98
145.87
139.07
135.35
129.01
128.95
125.74
124.04
121.67
121.54
111.54
110.43

77.32
77.00
76.68
74.70

28.43
27.17
22.41
19.36



CWV-267

NAME
EXPNO 2
PROCNO 1
Date_ 20150930
Time_ 12.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 148
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DM 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

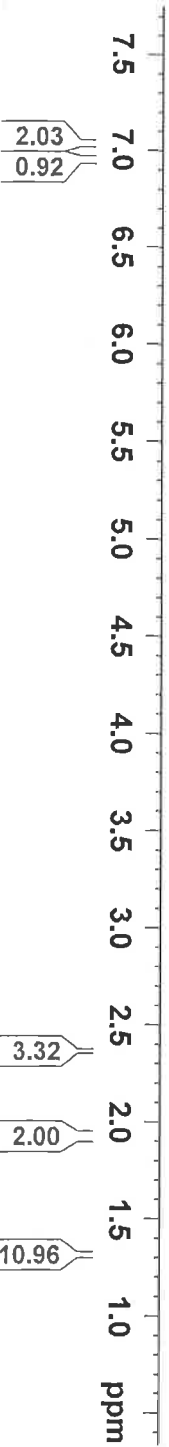
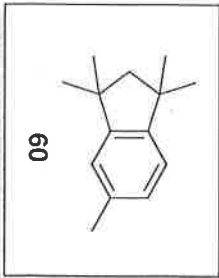
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
BC 1.40



CWV-247

7.042
7.039
6.952



2.367
1.927
1.321
1.316



NAME CWV-247
EXPNO 1
PROCNO 1
Date_ 20150723
Time_ 12.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SF01 400.1324710 MHz
SI 32768
SE 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-249 f7-11

9.420

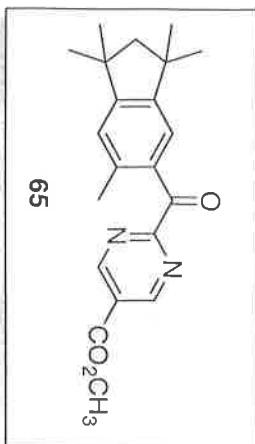
7.260
7.174
7.033

4.028

2.445

1.920

1.314
1.239

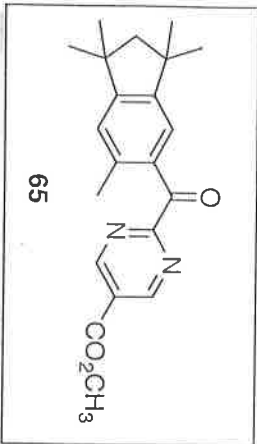


NAME CWV-249
EXPNO 1
PROCNO 1
Date_ 20150730
Time_ 10.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SMH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DM 60.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-249 f7-11

193.28
166.02
163.53
158.51
156.67
148.65
138.91
133.59
126.11
126.06
124.12
77.32
77.00
76.68
56.51
52.97
42.80
42.22
31.34
31.11
21.37



CWV-249

NAME

EXPNO

PROCNO

Date_

Time_

INSTRUM

PROBHD

PULPROG

TD

SOLVENT

NS

DS

SWH

FIDRES

AQ

RG

DW

DE

TE

D1

D11

TD0

1

=====

CHANNEL f1

NUC1

P1

PL1

PL1W

SFO1

=====

CHANNEL f2

CPDPRG2

NUC2

PCPD2

PL2

PL12

PL2W

PL12W

SFO2

SI

SF

WDW

SSB

LB

GB

PC

200 180 160 140 120 100 80 60 40 20 0 ppm

20150730
10.40
spect
5 mm PABBO BB-
zgpg30
65536
CDC13
110
4
24038.461 Hz
0.366798 Hz
1.3631988 sec
2050
20.800 usec
6.50 usec
298.4 K
2.00000000 sec
0.03000000 sec
1
=====

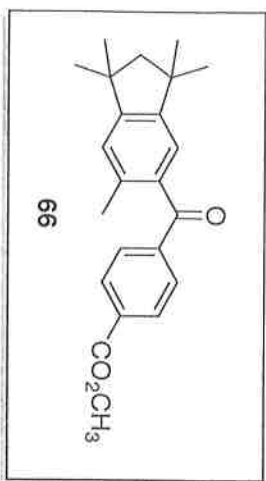
13C
8.50 usec
-2.10 dB
60.29227829 W
100.6228298 MHz

=====

waltz16
1H
90.00 usec
-1.80 dB
17.28 dB
21.67079544 W
0.26783961 W
400.1316005 MHz
32768
100.6127729 MHz
EM
0
1.00 Hz
0
1.40

CWVI-027 F4

8.119
8.114
8.110
7.877
7.872
7.860
7.855
7.260
7.059
7.030

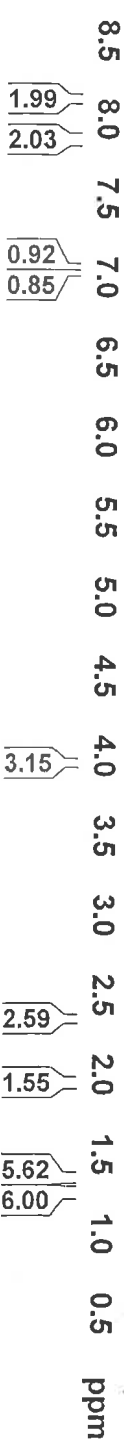


— 3.957

— 2.354

— 1.943

1.341
1.263



NAME CWVI-027
EXPNO 1
PROCNO 1
Date 20160520
Time 12.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DE 60.800 usec
TE 673.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-027 F4

198.18
166.34
154.57
148.42
141.87
136.35
136.28
133.44
129.93
129.52
125.37
123.74

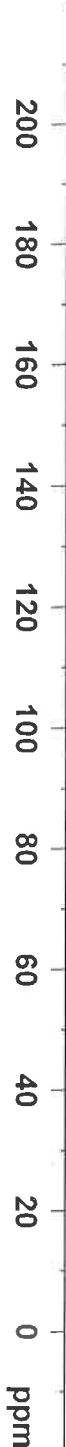
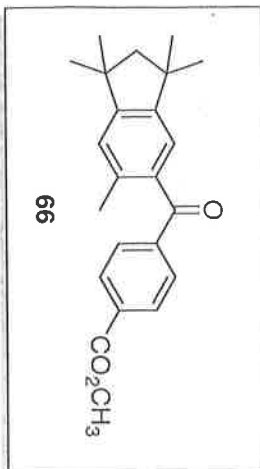
77.32
77.00
76.68

56.53
52.43

42.69
42.26

31.39
31.27

20.38



NAME CWVI-027

EXPNO 2

PROCNO 1

Date_ 20160520

Time_ 12.15

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 141

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 673.2 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127751 MHz

WDW EM

SSB 0

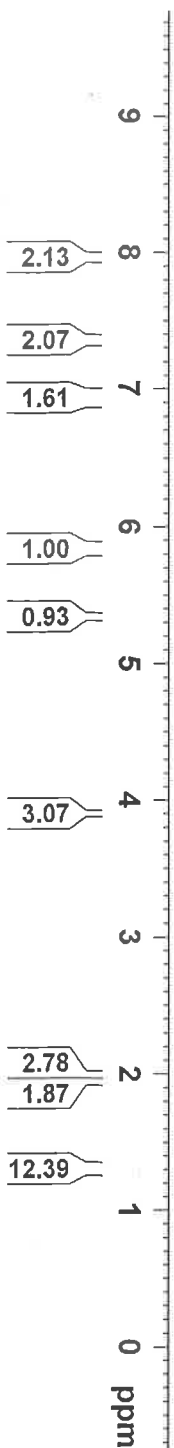
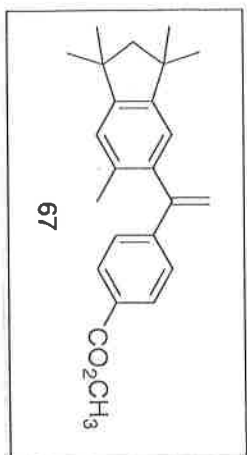
LB 1.00 Hz

GB 0

PC 1.40

CWVI-031

7.975
7.954
7.365
7.343
6.956
6.917
5.839
5.835
5.339
5.336
3.911
1.993
1.944
1.342
1.319

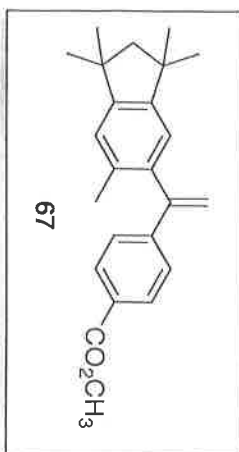


NAME CWVI-031
EXPNO 1
PROCNO 1
Date 20160718
Time 12.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DE 60.800 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SF01 400.1324710 MHz
SI 32768
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-031

166.96
150.91
149.45
148.92
145.55
139.30
134.22
129.65
129.62
128.91
126.50
123.99
116.82
77.32
77.00
76.68
56.87
52.03
42.39
42.30
31.58
31.54
20.23



NAME CWVI-031

EXPNO 2

PROCNO 1

Date 20160718

Time 12.40

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 209

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 295.1 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127736 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

CWVI-035

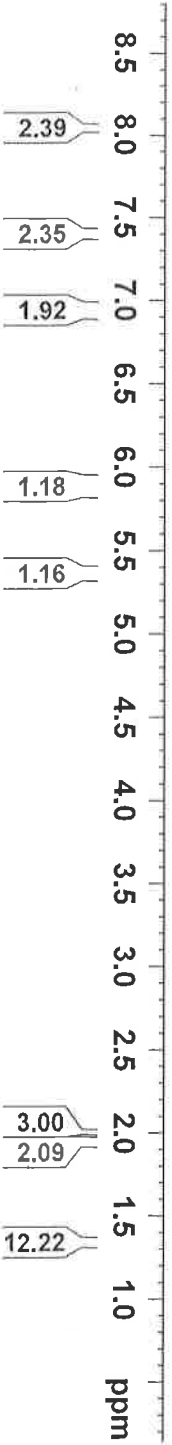
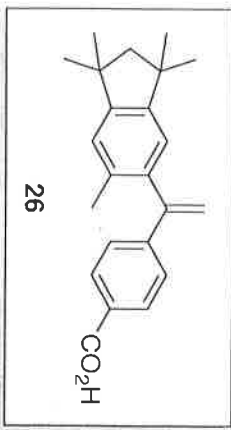
8.053
8.048
8.031
8.027
7.400
7.378
7.260
6.959
6.922

5.866
5.862

5.366
5.364

2.001
1.944

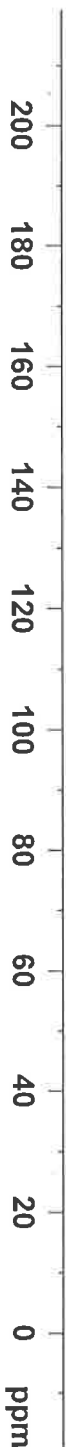
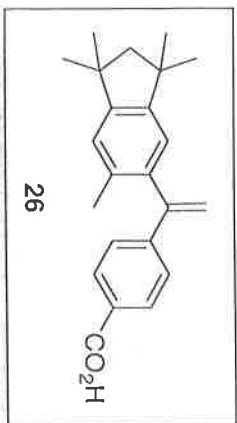
1.342
1.321



NAME CWVI-035
EXPNO 1
PROCNO 1
Date 20160729
Time 12.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DE 60.800 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SF01 400.1324710 MHz
SI 32768
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-035



```

NAME CWVI-035
EXPNO 2
PROCNO 1
Date_ 20160729
Time_ 13.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 731
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DE 20.800 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL12W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127714 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
```


CWV-251

9.251

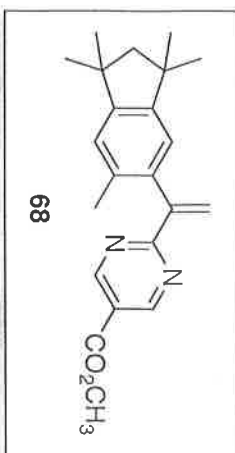
7.260
6.981
6.947
6.849
6.844

5.816
5.811

3.969

2.023
1.927

1.336
1.313



1.91

0.91
1.02
0.98

1.00

3.13

3.04
2.01

12.05

10
9
8
7
6
5
4
3
2
1
ppm



NAME CWV-251
EXPNO 1
PROCNO 1
Date 20150902
Time 11.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SF01 400.1324710 MHz
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CMV-251

168.71
164.37
158.21
150.97
148.80
148.70
137.62
134.20
126.68
123.93
123.84
121.18

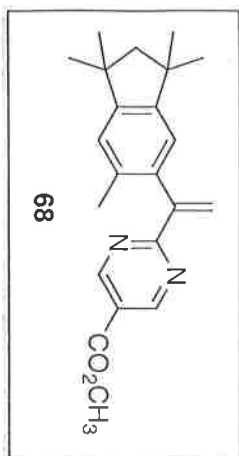
77.32
77.00
76.69

56.92
52.53

42.42
42.32

31.56
31.51

20.34



NAME CMV-251

EXPNO 2

PROCNO 1

Date 20150902

Time 11.50

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 139

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 300.0 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127714 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

CWVI-007

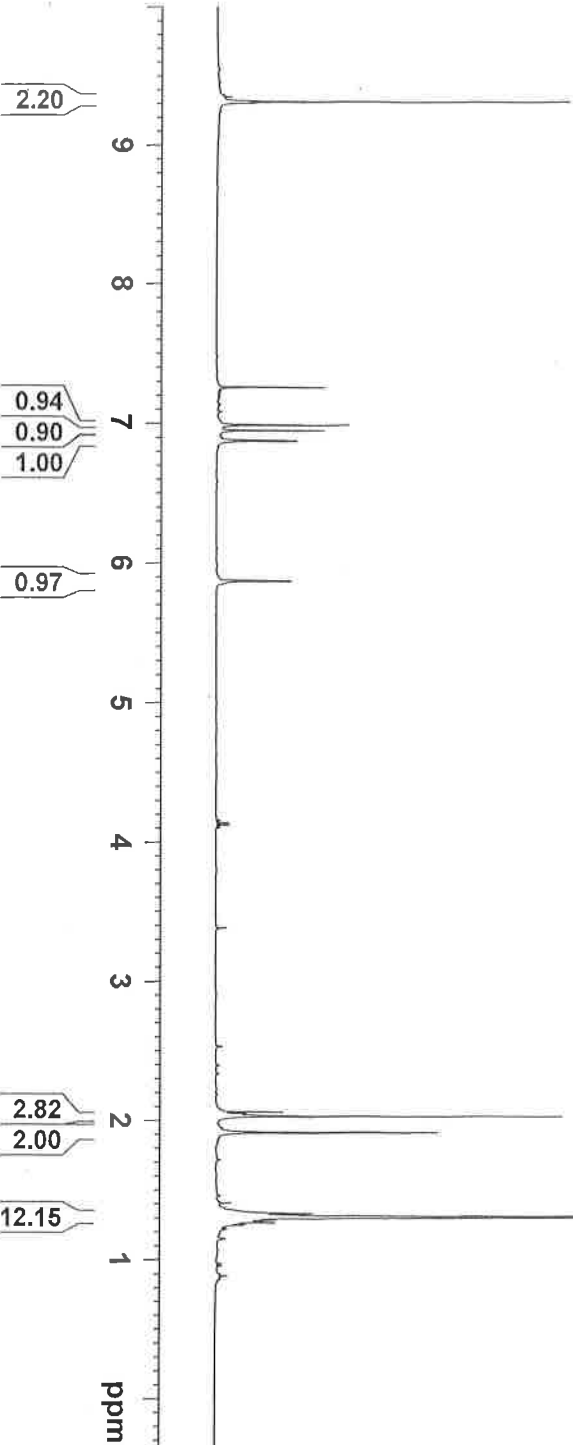
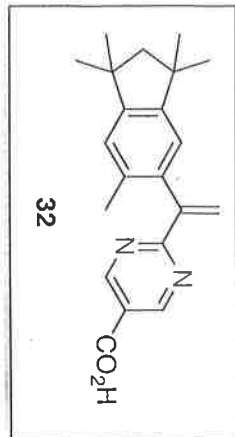
9.319

7.260
6.989
6.950
6.879
6.874

5.872
5.868

2.030
1.913

1.309
1.305



NAME CWVI-007
EXPNO 1
PROCNO 1
Date_ 20160328
Time_ 10.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SMH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SF01 400.1324710 MHz
SI 32768
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-007

169.04
168.04
158.84
151.17
148.91
148.33
137.24
134.24
127.50
124.00
123.90
120.76

77.32
77.00
76.68

56.81

42.42
42.32

31.56
31.49

20.34



NAME CWVI-007

EXPNO 2

PROCNO 1

Date 20160328

Time 11.08

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 3620

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 673.2 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127729 MHz

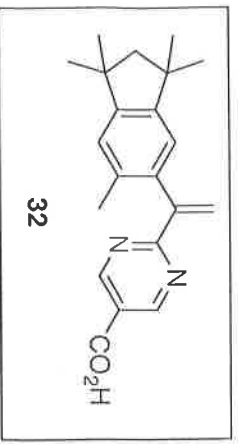
WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40



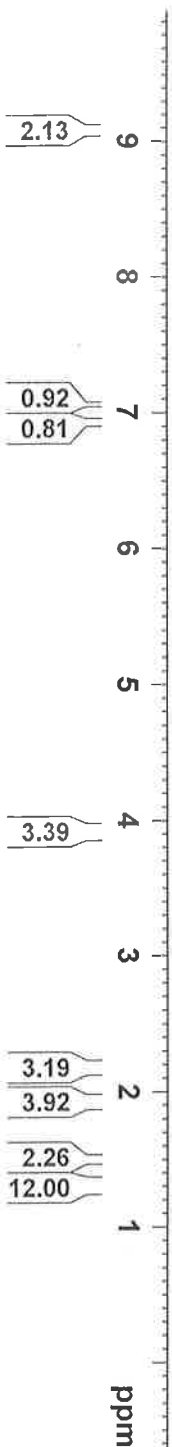
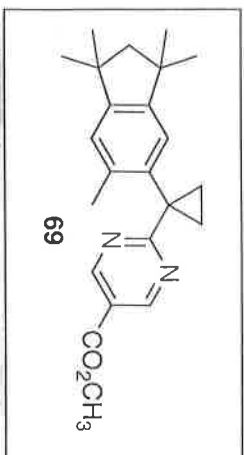
CMV-271

9.089
9.082
9.073
9.072

7.260
7.060
6.928

3.924

2.167
1.911
1.904
1.507
1.499
1.491
1.323
1.298

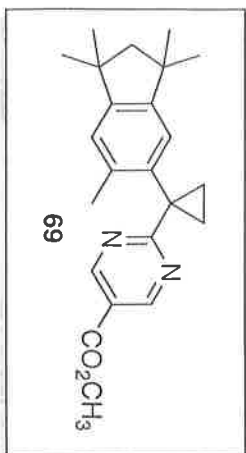


NAME CMV-271
EXPNO 1
PROCNO 1
Date 20151009
Time 10.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SF01 400.1324710 MHz
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-271

176.88
164.67
157.81
149.84
148.59
138.29
137.37
124.54
123.85
119.97
77.32
77.00
76.68
56.96
52.34
42.32
42.29
32.00
31.59
31.52
23.89
21.82
19.84



NAME CWV-271

EXPNO 2

PROCNO 1

Date 20151009

Time 11.00

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 282

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 298.4 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL F1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL F2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL12W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127714 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

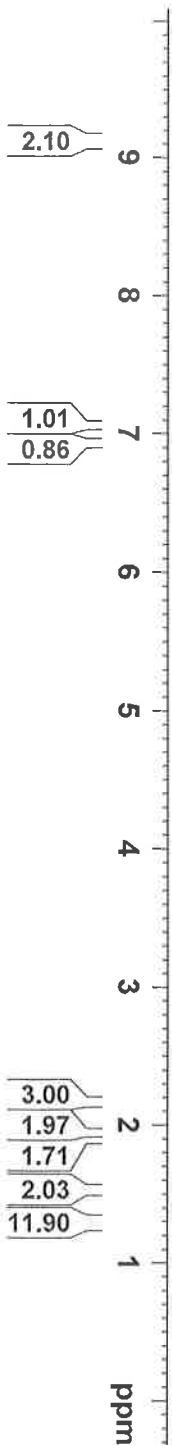
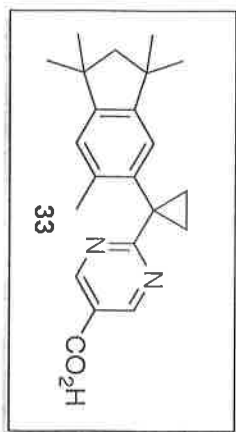
PC 1.40

CWVI-003

9.124

7.260
7.059
6.928

2.169
1.943
1.935
1.895
1.539
1.531
1.322
1.298
1.287
1.261

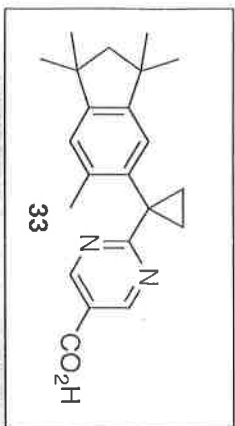


NAME CWVI-003
EXPNO 1
PROCNO 1
Date_ 20160328
Time_ 10.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-003

177.10
167.31
159.01
158.48
158.42
150.42
148.93
137.38
124.76
124.17
119.72
77.35
77.03
76.72
56.88
42.38
42.35
32.08
31.61
31.52
31.40
23.92
22.85
19.86



NAME CWVI-003

EXPNO 2

PROCNO 1

Date 20160330

Time 14.39

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 19951

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DM 20.800 usec

DE 6.50 usec

TE 673.2 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

PL 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127690 MHz

WDW EM

SSB 0

LB 1.00 Hz

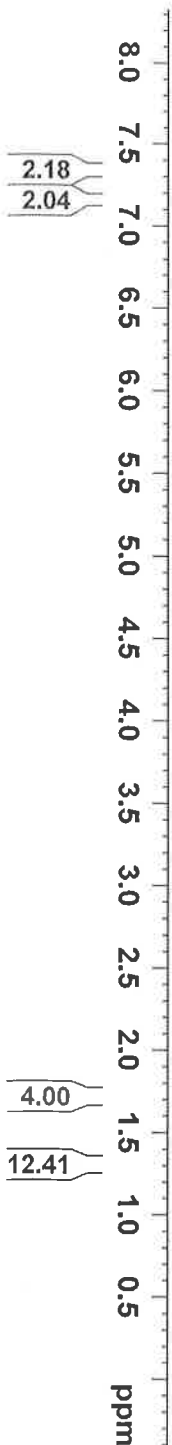
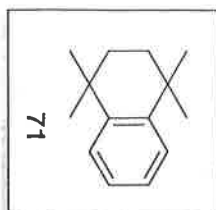
GB 0

PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

CWIII-121

7.359
7.350
7.344
7.335
7.327
7.260
7.176
7.167
7.161
7.152



— 1.726
— 1.323



```

NAME CWIII-121
EXPNO 1
PROCNO 1
Date_ 20100609
Time_ 11.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 291.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -1.80 dB
PL1W 21.67079544 W
SF01 400.1324710 MHz
SI 32768
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
  
```

CWIII-121

144.74

126.45
125.50

77.31
77.00
76.68

35.06
34.18
31.86



NAME CWIII-121

EXPNO 2

PROCNO 1

Date 20100609

Time 11.43

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 41

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 291.4 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -1.50 dB

PL1W 52.51238251 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL12W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127766 MHz

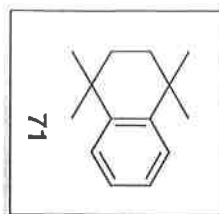
WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40



200 180 160 140 120 100 80 60 40 20 0 ppm

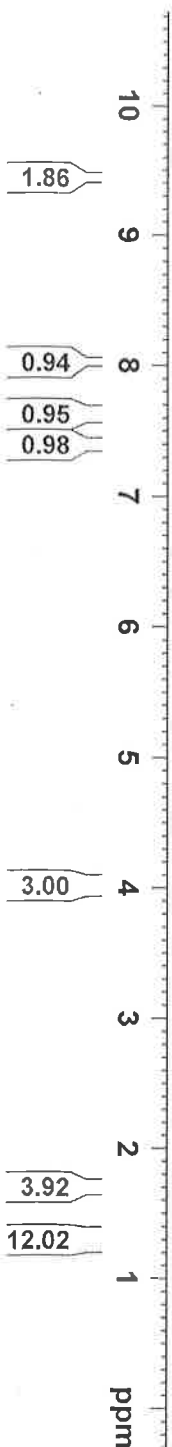
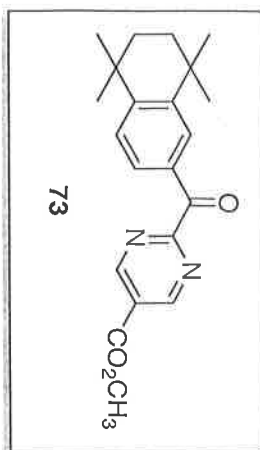
CWV-297

— 9.438

8.026
8.022
7.647
7.642
7.626
7.621
7.408
7.388
7.260

— 4.033

— 1.704
1.294
1.292



```

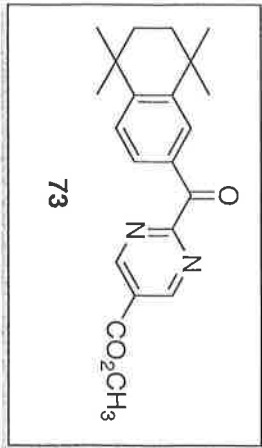
NAME CWV-297
EXPNO 1
PROCNO 1
Date_ 20151224
Time_ 15.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DE 60.800 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
  
```

CWV-297

190.36

165.38
163.52
158.34
152.11
145.52
131.95
129.34
128.05
126.78
124.19



77.32
77.00
76.68

52.98

34.83
34.74
34.65
34.41
31.70
31.50



NAME CWV-297

EXPNO 2

PROCNO 1

Date_ 20151224

Time_ 15.15

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 64

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 298.2 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127736 MHz

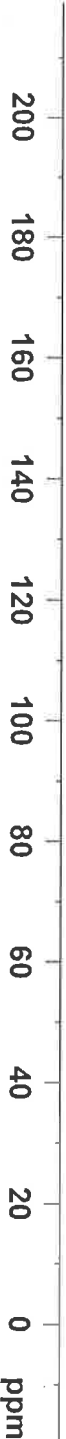
WDW EM

SSB 0

LB 1.00 Hz

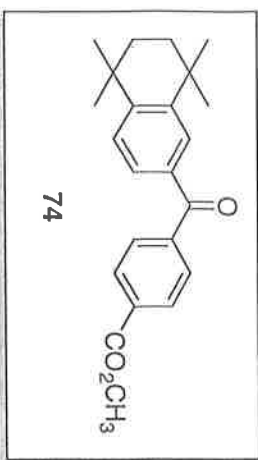
GB 0

PC 1.40



CWVI-017

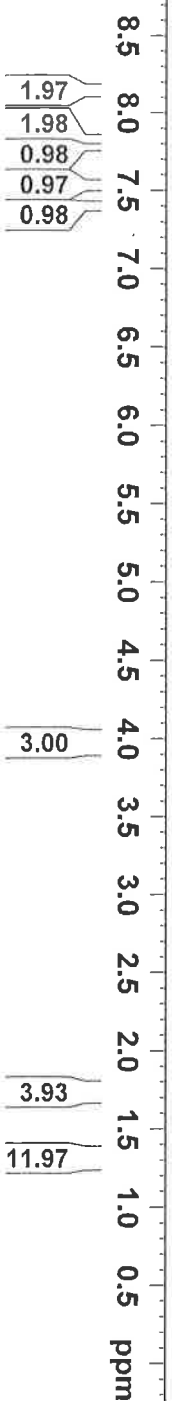
7.845
7.841
7.837
7.825
7.820
7.816
7.789
7.784
7.546
7.542
7.526
7.521
7.417
7.396
7.260



3.965

1.720

1.318
1.290

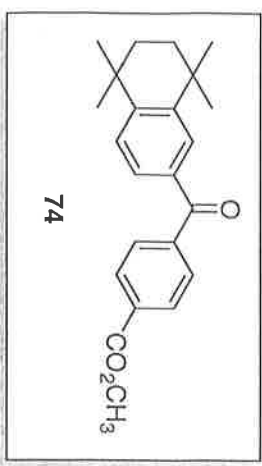


NAME CWVI-017
EXPNO 1
PROCNO 1
Date 20160728
Time 14.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
FIDRES 0.125483 Hz
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
AQ 3.9846387 sec
RG 4
DM 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SF01 400.1324710 MHz
SI 32768
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-017

- 195.91
- 166.41
- 150.78
- 145.29
- 141.86
- 134.13
- 132.89
- 129.68
- 129.38
- 128.89
- 127.36
- 126.70
- 77.32
- 77.00
- 76.68
- 52.42
- 34.79
- 34.73
- 34.72
- 34.40
- 31.73
- 31.60

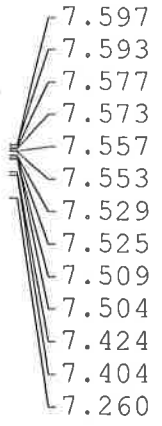


NAME CWVI-017
 EXPNO 2
 PROCNO 1
 Date_ 20160728
 Time_ 15.00
 INSTRUM spect
 PROBD 5 mm PABO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 157
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQC 1.3631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.50 usec
 TE 673.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.10 dB
 PL1W 60.29227829 W
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -1.80 dB
 PL12 17.28 dB
 PL12W 21.67079544 W
 PL12W 0.26783961 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127722 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

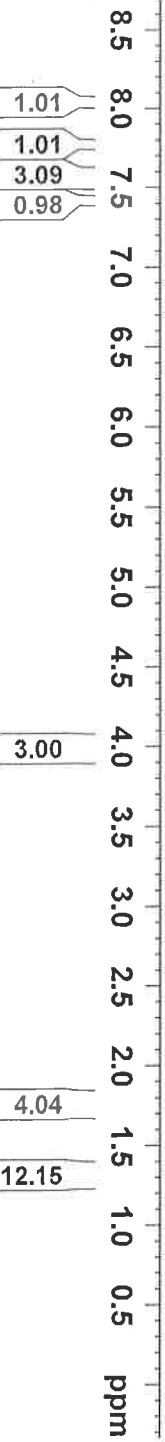
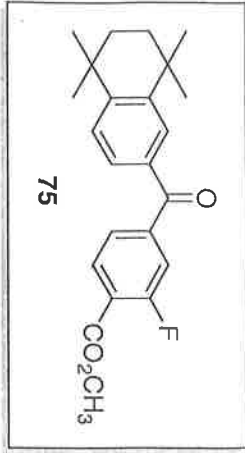
CWVI-015



— 3.974

— 1.720

1.316
1.293



NAME CWVI-015
EXPNO 1
PROCNO 1
Date 20160728
Time 14.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-015

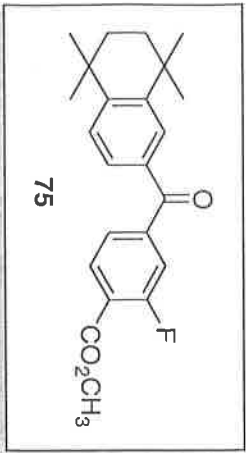
194.29
194.28

164.33
164.30
162.70
160.10
151.19
145.50
143.69
143.61
133.56
132.05
128.81
127.28
126.83
124.98
124.95
121.43
121.32
118.27
118.03

77.32
77.00
76.69

52.63

34.77
34.74
34.67
34.40
31.72
31.57



NAME CWVI-015

EXPNO 2

PROCNO 1

Date_ 20160728

Time_ 14.46

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDC13

NS 360

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AO 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 673.2 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127729 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40



CWVI-021

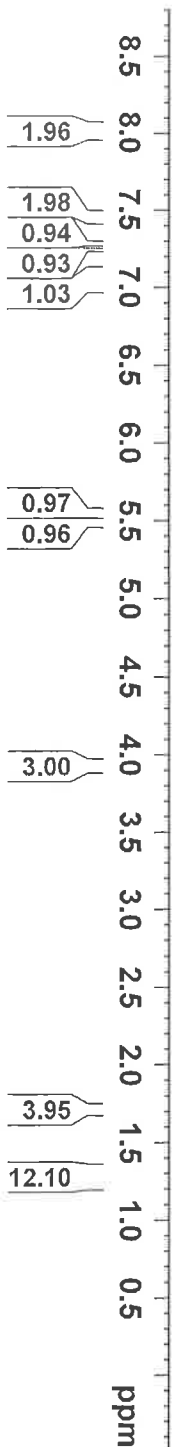
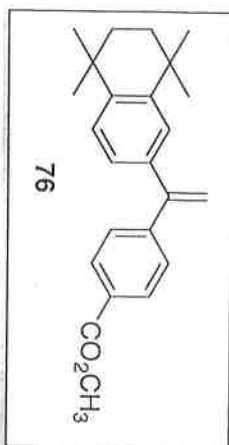
7.461
7.456
7.452
7.440
7.435
7.431
7.288
7.267
7.260
7.242
7.237
7.096
7.091
7.076
7.071
5.543
5.540
5.487
5.484

3.936

1.701

1.307

1.245

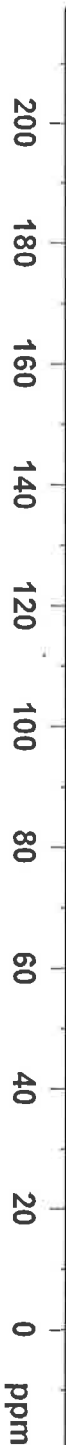
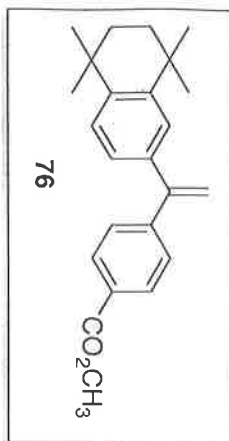


NAME CWVI-021
EXPNO 1
PROCNO 1
Date_ 20160728
Time_ 15.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-021

166.99
149.33
146.30
144.82
144.68
137.53
129.39
129.17
128.29
126.38
126.30
125.34
114.95
77.31
77.00
76.68
52.06
35.06
34.99
34.24
34.14
31.77



CWVI-021

NAME
EXPNO 2
PROCNO 1
Date 20160728
Time 15.33

INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30

TD 65536
SOLVENT CDCl3

NS 145
DS 4

SWH 24038.461 Hz
FIDRES 0.366798 Hz

AQ 1.3631988 sec
RG 2050

DW 20.800 usec
DE 6.50 usec

TE 295.7 K
D1 2.00000000 sec

D11 0.03000000 sec
TD0 1

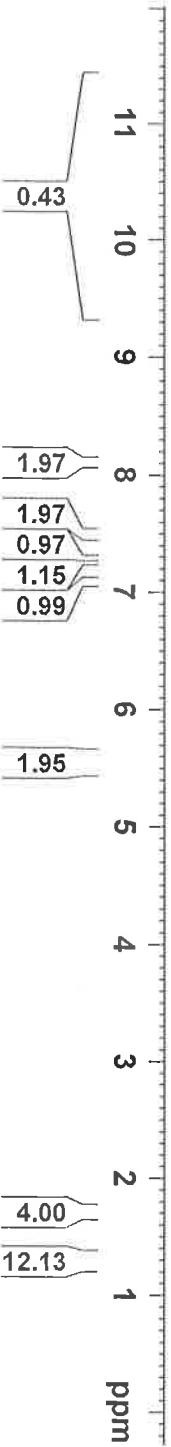
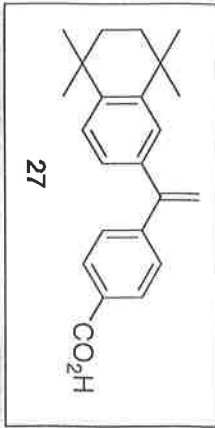
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL12W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127744 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CWVI-025

10.337
8.116
8.111
8.099
8.094
8.090
7.501
7.496
7.484
7.480
7.475
7.300
7.279
7.260
7.258
7.253
7.104
7.099
7.083
7.078
5.571
5.569
5.519
5.516

1.709
1.315
1.258



NAME CWVI-025
EXPNO 1
PROCNO 1
Date 20160729
Time 13.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1

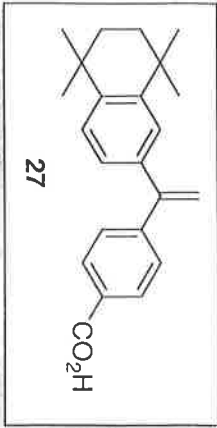
===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-025

172.14
149.30
147.28
144.90
144.76
137.46
130.09
128.42
128.31
126.44
126.33
125.37
115.29

77.32
77.00
76.68

35.08
35.01
34.27
34.17
31.80



CWVI-025

NAME

EXPNO

2

PROCNO

1

Date

20160729

Time

13.38

INSTRUM

spect

PROBHD

5 mm PABBO BB-

PULPROG

zgpg30

TD

65536

SOLVENT

CDCl3

NS

173

DS

4

SMH

24038.461 Hz

FIDRES

0.366798 Hz

AQ

1.3631988 sec

RG

2050

DW

20.800 usec

DE

6.50 usec

TE

296.0 K

D1

2.00000000 sec

D11

0.03000000 sec

TD0

1

===== CHANNEL f1 =====

NUC1

13C

P1

8.50 usec

PL1

-2.10 dB

PL1W

60.29227829 W

SFO1

100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2

waltz16

NUC2

1H

PCPD2

90.00 usec

PL2

-1.80 dB

PL12

17.28 dB

PL2W

21.67079544 W

PL12W

0.26783961 W

SFO2

400.1316005 MHz

SI

32768

SF

100.6127729 MHz

WDW

EM

SSB

0

LB

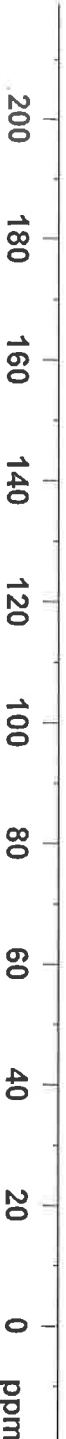
1.00 Hz

GB

0

PC

1.40



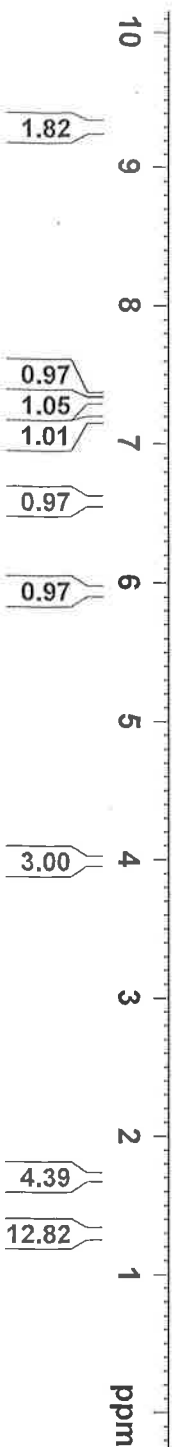
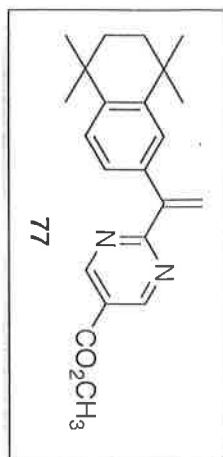
CWV-301

9.281

7.356
7.351
7.325
7.305
7.260
7.188
7.183
7.167
7.162
6.585
6.581
5.939
5.935

3.986

1.700
1.304
1.282



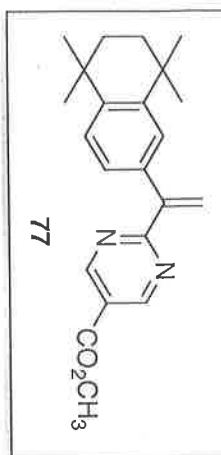
NAME CWV-301
EXPNO 2
PROCNO 1
Date_ 20151224
Time_ 16.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWV-301

168.98
164.33
158.07
147.78
144.78
144.45
135.53
126.87
126.26
125.83
124.41
121.52

52.57
36.60
35.09
35.03
34.26
34.16
31.81
31.78
24.65



NAME CWV-301

EXPNO 3

PROCNO 1

Date 20151224

Time 16.22

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 112

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 298.3 K

D1 2.0000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127729 MHz

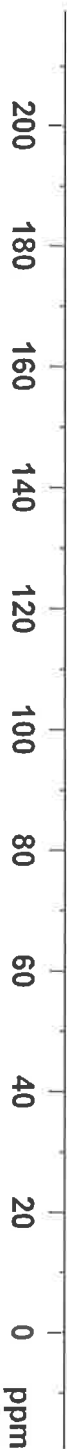
WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

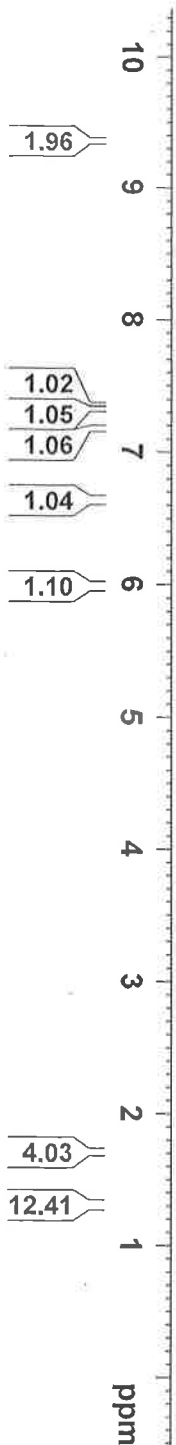
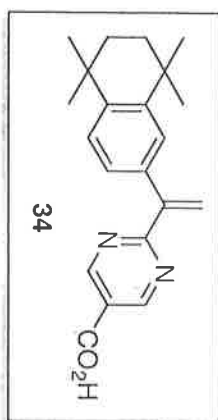


CWVI-009 from EtOAc



9.357
7.359
7.355
7.334
7.314
7.260
7.188
7.183
7.167
7.162
6.630
6.627
5.985
5.981

1.698
1.298
1.285



NAME CWVI-009
EXPNO 2
PROCNO 1
Date_ 20160331
Time_ 9.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
FIDRES 0.125483 Hz
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DE 60.800 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

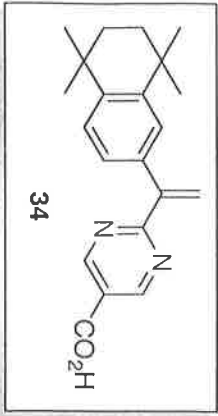
===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-009 From EtOAc

169.46
158.71
147.57
144.94
144.57
135.34
126.88
126.34
125.86
125.23
120.78

77.32
77.00
76.68

35.06
35.00
34.29
34.19
31.84
31.79



NAME CWVI-009

EXPNO 3

PROCNO 1

Date 20160401

Time 16.13

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 32372

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 673.2 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127722 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

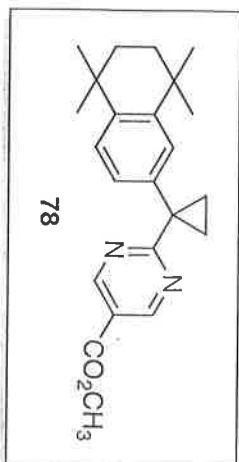
CWVI-011

9.088

7.303
7.299
7.288
7.268
7.260
7.160
7.155
7.140
7.135

3.928

1.807
1.797
1.790
1.781
1.683
1.515
1.506
1.498
1.488
1.291
1.265



1.93

0.97
0.93
1.03

2.83

1.97
4.00
2.09
12.59

ppm

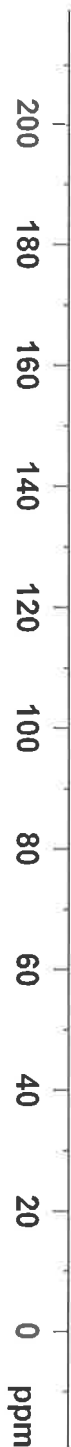
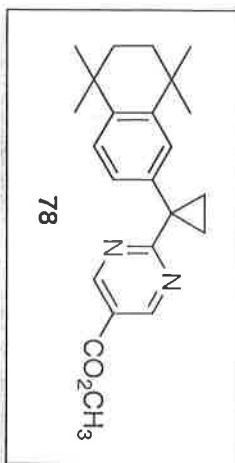


NAME CWVI-011
EXPNO 1
PROCNO 1
Date 20160317
Time 11.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
RW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-011

- 177.08
- 164.60
- 157.73
- 144.53
- 143.16
- 138.25
- 129.54
- 128.85
- 127.69
- 126.28
- 120.41
- 120.04
- 115.23
- 77.31
- 77.00
- 76.68
- 52.41
- 36.59
- 35.14
- 35.09
- 34.25
- 34.05
- 33.04
- 31.87
- 24.65
- 20.27



```

NAME CWVI-011
EXPNO 2
PROCNO 1
Date_ 20160317
Time_ 12.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DE 20.800 usec
TE 673.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

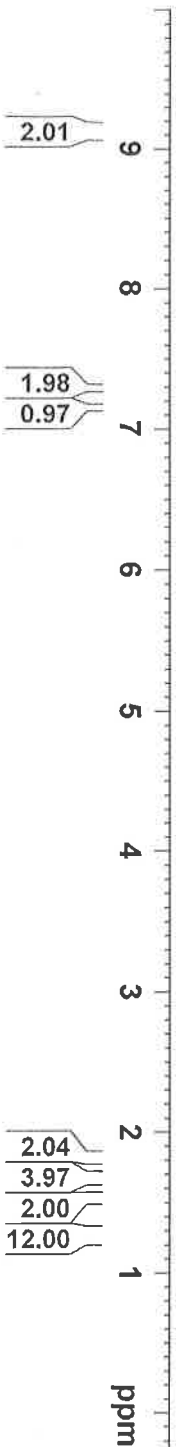
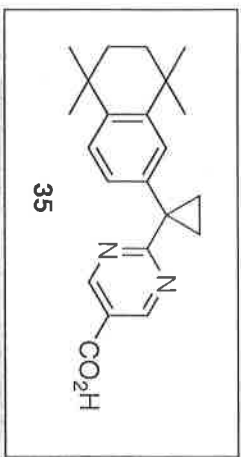
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
```

CWVI-013

9.130

7.304
7.300
7.290
7.269
7.260
7.161
7.156
7.141
7.136

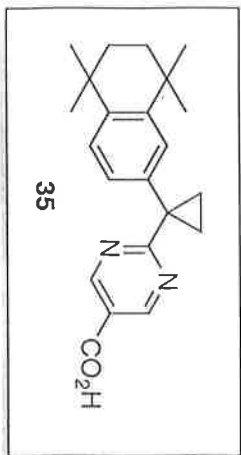
1.830
1.820
1.813
1.804
1.680
1.539
1.530
1.523
1.513
1.285
1.264



NAME CWVI-013
EXPNO 1
PROCNO 1
Date 20160323
Time 17.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SF01 400.1324710 MHz
SI 32768
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-013



```

NAME CWVI-013
EXPNO 5
PROCNO 1
Date_ 20160329
Time 10.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 29547
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DM 20.800 usec
DE 6.50 usec
TE 673.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL2W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
```



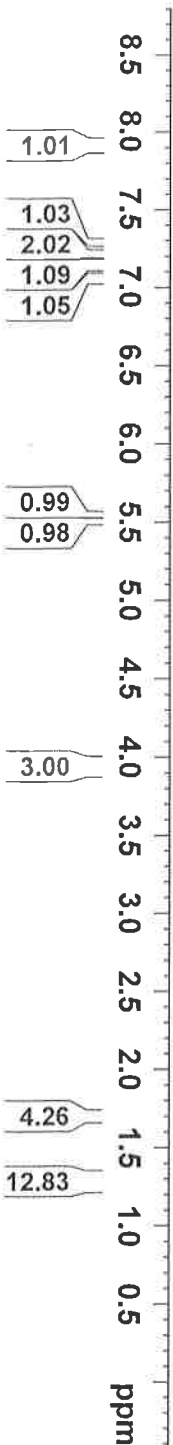
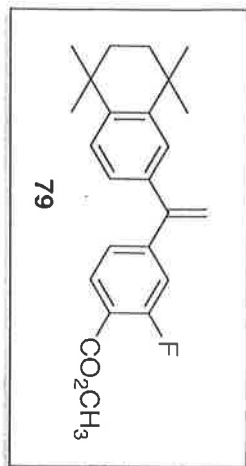
CWVI-019

7.271
7.260
7.229
7.225
7.220
7.215
7.209
7.205
7.165
7.161
7.134
7.130
7.070
7.065
7.049
7.044
5.549
5.547
5.508
5.506

3.945

1.698

1.303
1.248



NAME CWVI-019
EXPNO 1
PROCNO 1
Date_ 20160728
Time_ 15.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
FIDRES 0.125483 Hz
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DE 60.800 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SE 400.1300104 MHz
WDM EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

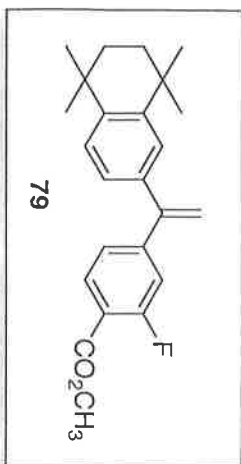
CWVI-019

164.83
164.79
163.06
160.48
148.53
148.44
148.32
148.29
145.09
144.85
136.92
131.81
126.52
126.29
125.33
123.78
123.74
117.37
117.27
116.72
116.49
115.79

77.31
77.00
76.68

52.28

35.02
34.96
34.25
34.17
31.77



CWVI-019

NAME

EXPNO 2

PROCNO 1

Date_ 20160728

Time_ 15.17

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 219

DS 4

SWH 24038.461 Hz

FTDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DM 20.800 usec

DE 6.50 usec

TE 673.2 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127736 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

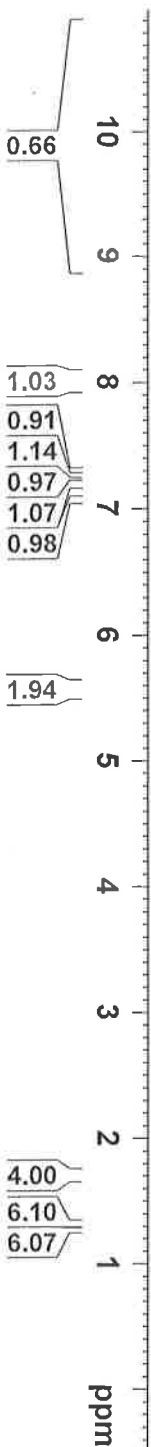
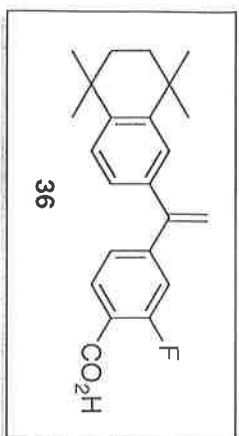
HC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

CWVI-023

9.911
8.033
8.014
7.994
7.306
7.285
7.275
7.271
7.260
7.254
7.250
7.238
7.233
7.207
7.203
7.177
7.173
7.079
7.074
7.058
7.053
5.581
5.580
5.545
5.544

1.709
1.313
1.263



NAME CWVI-023
EXPNO 1
PROCNO 1
Date 20160729
Time 13.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SMH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1

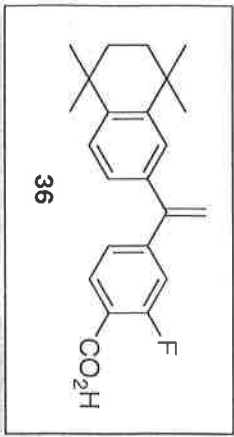
===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SF01 400.1324710 MHz
SI 32768
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-023

169.53
169.49
163.81
161.21
149.70
149.61
148.28
148.27
145.18
144.93
136.83
132.45
126.57
126.31
125.36
123.92
123.89
116.87
116.64
116.31
116.22
116.17

77.32
77.00
76.68

35.03
34.97
34.27
34.19
31.80
31.78



NAME CWVI-023

EXPNO 2

PROCNO 1

Date_ 20160729

Time_ 13.21

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 201

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 296.0 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127729 MHz

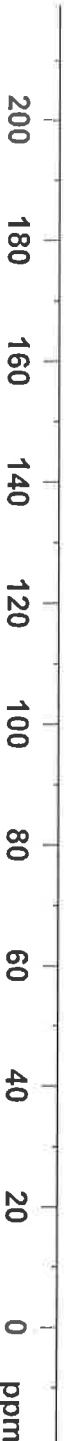
WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40



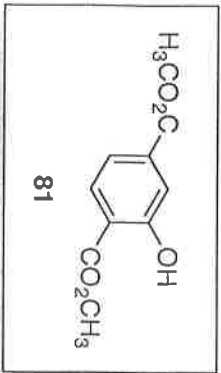
CWVI-053

— 10.749

7.903
7.882
7.629
7.625
7.525
7.521
7.504
7.500
7.260



NAME CWVI-053
EXPNO 1
PROCNO 1
Date_ 20161021
Time_ 10.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1



===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-053

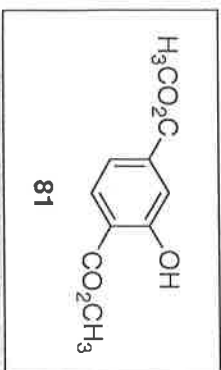
169.93
165.97
161.26

136.38
130.00

119.67
118.87
115.64

77.32
77.00
76.68

52.63
52.49



200
180
160
140
120
100
80
60
40
20
0
ppm



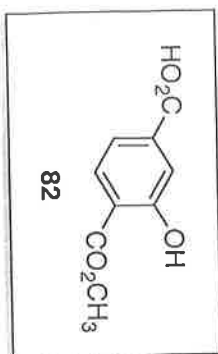
NAME CWVI-053
EXPNO 2
PROCNO 1
Date_ 20161021
Time_ 11.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 118
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 673.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL12W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CWVI-059 Middle Spot

10.792
7.953
7.933
7.709
7.705
7.593
7.589
7.572
7.569
7.260

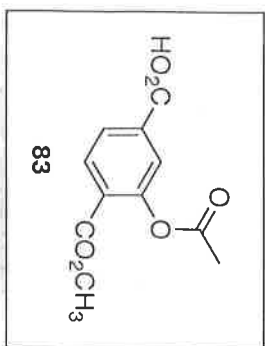


NAME CWVI-059
EXPNO 2
PROCNO 1
Date_ 20161107
Time_ 14.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

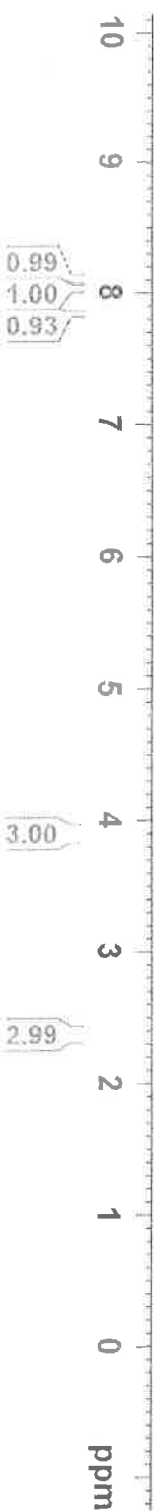
CWVI-061 f12-16

8.119
8.098
8.046
8.041
8.025
8.021
7.843
7.839
7.260



3.912

2.381



NAME CWVI-061
EXPNO 2
PROCNO 1
Date_ 20161122
Time_ 12.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-061 f12-16

169.84
169.50
164.17

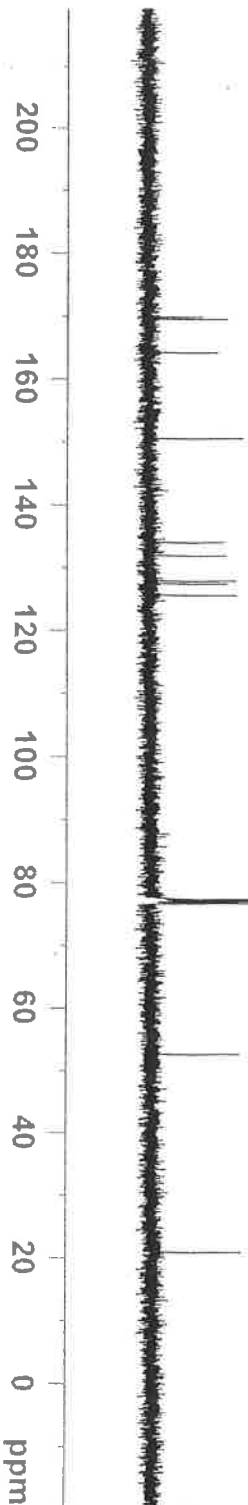
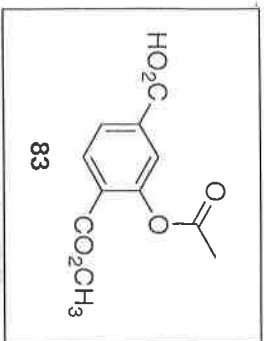
150.52

134.04
131.91
127.87
127.44
125.60

77.32
77.00
76.68

52.61

20.90



NAME CWVI-061

EXPNO 3

PROCNO 1

Date 20161122

Time 12.31

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 271

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 673.2 K

D1 2.0000000 sec

D11 0.0300000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127722 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

CWVI-069 F5-9

10.781

7.940
7.920
7.336
7.333
7.327
7.323
7.307
7.303
7.267
7.260
7.189

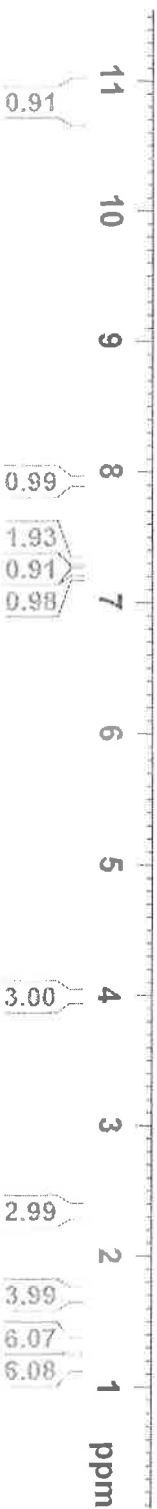
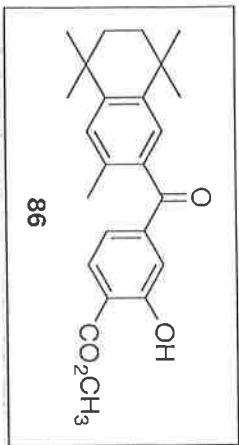
3.990

2.329

1.687

1.307

1.207



NAME CWVI-069
EXPNO 1
PROCNO 1
Date_ 20170210
Time_ 16.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

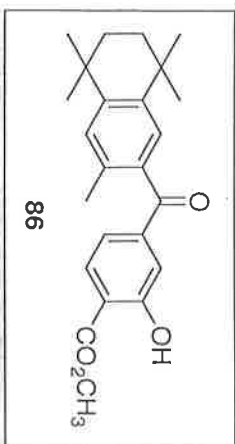
CWVI-069 F5-9

197.58
170.04
161.30
148.37
144.54
141.89
134.57
134.46
129.96
129.38
128.39
119.89
119.44
115.20

77.32
77.00
76.69

52.65

34.87
34.82
34.34
33.88
31.68
31.60
20.05



200
180
160
140
120
100
80
60
40
20
0
ppm

NAME CWVI-069
EXPNO 2
PROCNO 1
Date 20170210
Time 16.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 79
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 673.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.80 dB
PL12 17.28 dB
PL12W 21.67079544 W
PL12W 0.26783961 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

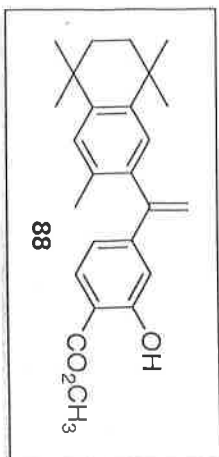


CWVI-071 F6B

— 10.745

7.771
7.750
7.409
7.399
7.393
7.386
7.260
7.114
7.069
6.902
6.897
6.881
6.877
6.846
6.841
5.816
5.813
5.333
5.330
— 3.941

1.960
1.699
1.306
1.279



NAME CWVI-071
EXPNO 1
PROCNO 1
Date_ 20170222
Time_ 14.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

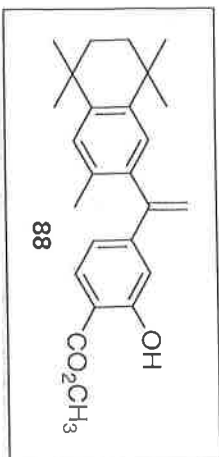
CWVI-071 F6B

170.40
161.43
148.98
148.50
144.32
142.24
137.72
133.85
133.67
132.70
132.35
132.24
129.71
129.59
128.80
128.76
128.68
128.00
117.62
117.32
115.53
111.14

77.32
77.00
76.68

52.22

35.13
33.95
33.84
31.90
31.85
19.85



200
180
160
140
120
100
80
60
40
20
0
ppm



NAME CWVI-071

EXPNO 2

PROCNO 1

Date 20170222

Time 14.16

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 98

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 673.2 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127751 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

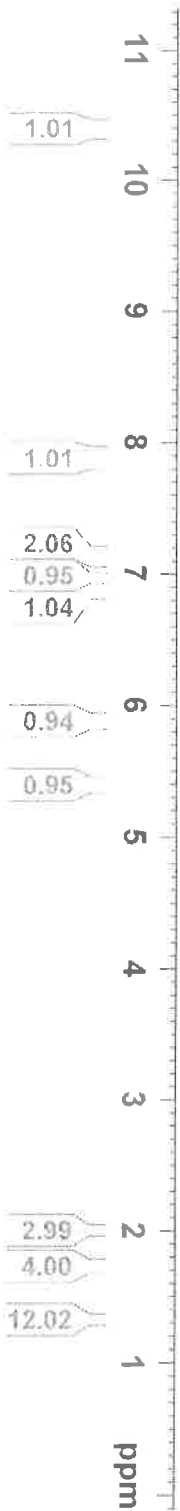
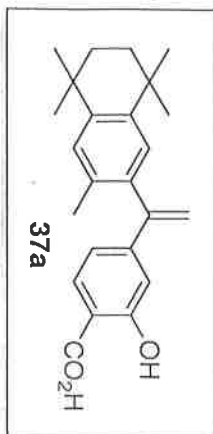
PC 1.40

CWVI-073

10.364

7.886
7.865
7.286
7.138
7.101
6.969
6.966
6.948
6.945
6.902
5.873
5.390

1.997
1.727
1.333
1.306



NAME CWVI-073

EXPNO 3

PROCNO 1

Date 20170227

Time 14.28

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zg30

TD 65536

SOLVENT CDCl3

NS 16

DS 2

SWH 8223.685 Hz

FIDRES 0.125483 Hz

AQ 3.9846387 sec

RG 4

DW 60.800 usec

DE 6.50 usec

TE 298.2 K

D1 1.00000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 1H

P1 14.75 usec

PL1 0.50 dB

PL1W 12.76071072 W

SFO1 400.1324710 MHz

SI 32768

SF 400.1300000 MHz

WDW EM

SSB 0

LB 0.30 Hz

GB 0

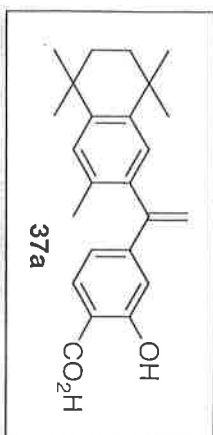
PC 1.00

CWVI-073

174.54
162.11
149.84
148.86
144.45
142.33
137.55
132.68
130.79
128.04
128.02
118.09
117.91
115.70
109.99

77.32
77.00
76.68

35.15
35.13
33.98
33.87
31.92
31.87
19.88



200
180
160
140
120
100
80
60
40
20
0
ppm



NAME CWVI-073

EXPNO 2

PROCNO 1

Date 20170227

Time 9.58

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 500

DS 4

SWH 24038.461 Hz

FTDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 673.2 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL F1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL F2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -1.80 dB

PL12 17.28 dB

PL2W 21.67079544 W

PL12W 0.26783961 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127729 MHz

WDM EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

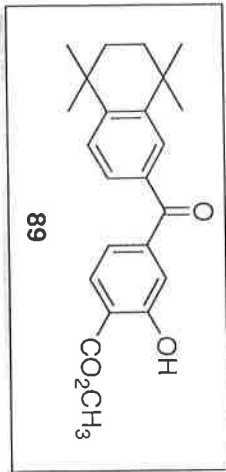
CWVI-099

10.820

7.955
7.934
7.811
7.807
7.546
7.541
7.525
7.521
7.404
7.384
7.329
7.326
7.264
7.260
7.244
7.240

3.995

1.715
1.312
1.294



12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

0.85

1.03
0.91
1.06
0.97
0.98
1.29

3.04

3.97
12.00



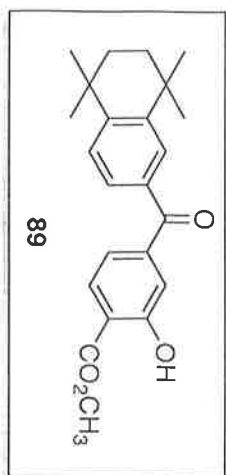
NAME CWVI-099
EXPNO 1
PROCNO 1
Date_ 20180305
Time_ 10.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 291.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.75 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-099

195.54
170.06
161.15
150.88
145.29
144.50
133.81
129.88
128.80
127.41
126.65
119.81
118.88
114.67

77.31
77.00
76.68
52.62
34.76
34.72
34.68
34.38
31.72
31.57



200
180
160
140
120
100
80
60
40
20
0
ppm



NAME CWVI-099

EXPNO 2

PROCNO 1

Date 20180305

Time 11.05

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 121

DS 4

SWH 24038.461 Hz

FIDRES 0.366798 Hz

AQ 1.3631988 sec

RG 2050

DW 20.800 usec

DE 6.50 usec

TE 292.1 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 -2.10 dB

PL1W 60.29227829 W

SFO1 100.6228298 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 0.50 dB

PL12 16.21 dB

PL2W 12.76071072 W

PL12W 0.34266910 W

SFO2 400.1316005 MHz

SI 32768

SF 100.6127744 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

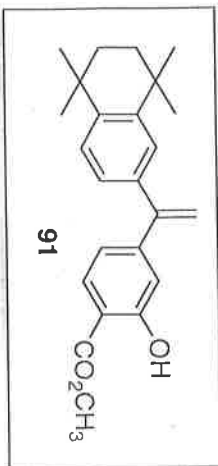
PC 1.40

CWVI-101

10.752

7.792
7.772
7.273
7.260
7.253
7.242
7.237
7.074
7.069
7.054
7.049
7.003
6.999
6.902
6.898
6.881
6.877
5.516
5.514
5.500
5.497
3.959

1.694
1.298
1.250



NAME: CWVI-101
EXPNO: 1
PROCNO: 1
Date_: 20180305
Time: 11.12
INSTRUM: spect
PROBHD: 5 mm PABBO BB-
PULPROG: zg30
TD: 65536
SOLVENT: CDCl3
NS: 16
DS: 2
SWH: 8223.685 Hz
FIDRES: 0.125483 Hz
AQ: 3.9846387 sec
RG: 4
DW: 60.800 usec
DE: 6.50 usec
TE: 291.9 K
D1: 1.00000000 sec
TD0: 1

===== CHANNEL f1 =====
NUC1: 1H
P1: 14.75 usec
PL1: 0.50 dB
PL1W: 12.76071072 W
SFO1: 400.1324710 MHz
SI: 32768
SF: 400.1300104 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

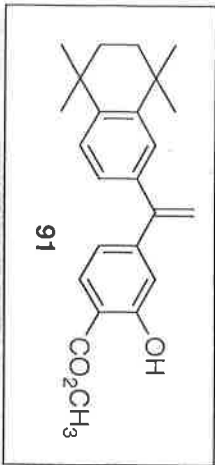
CWVI-101

170.42
161.36
149.26
149.13
144.78
144.66
137.30
129.43
126.36
126.35
125.40
119.41
117.18
115.32
111.37

77.32
77.00
76.68

52.25

35.05
34.98
34.24
34.14
31.79



200
180
160
140
120
100
80
60
40
20
0
ppm

NAME CWVI-101
EXPNO 2
PROCNO 1
Date 20180305
Time 11.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 115
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 292.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.50 dB
PL12 16.21 dB
PL2W 12.76071072 W
PL12W 0.34266910 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

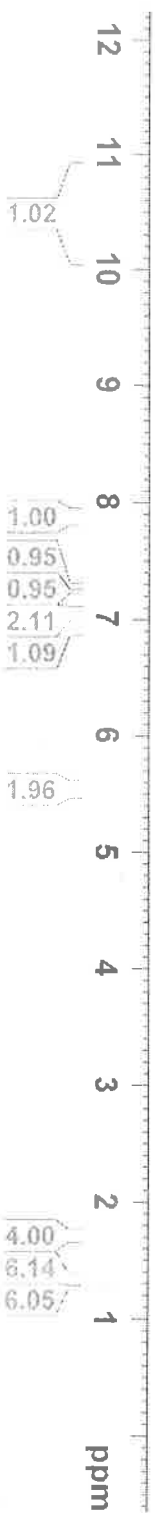
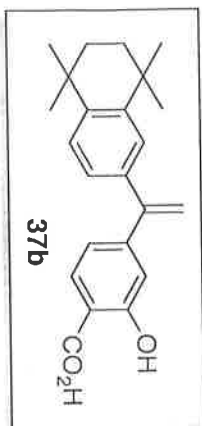


CWVI-103

10.377

7.897
7.876
7.287
7.266
7.260
7.254
7.249
7.079
7.074
7.058
7.053
7.034
7.031
6.967
6.963
6.946
6.943
5.549
5.535

1.702
1.305
1.263



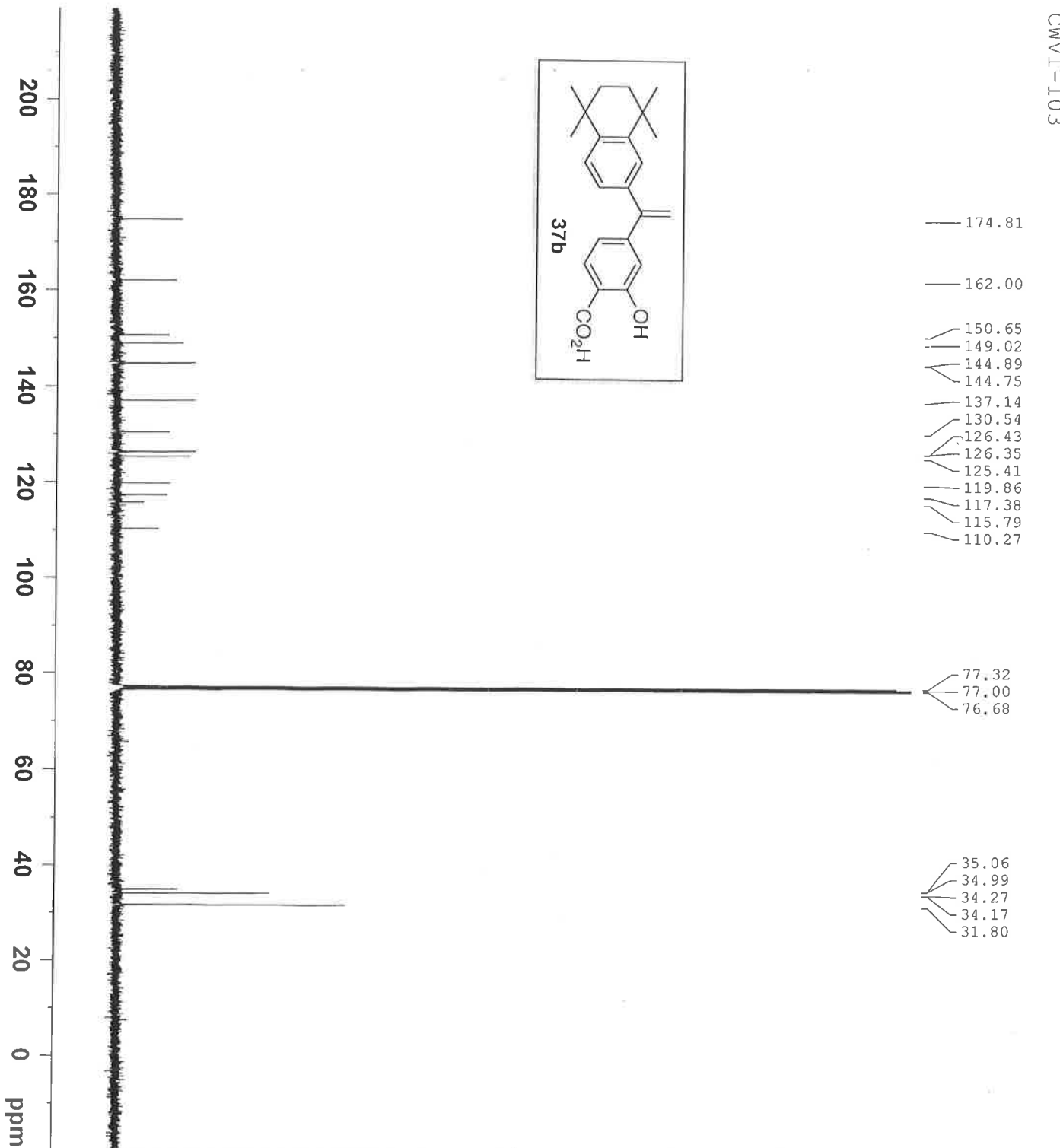
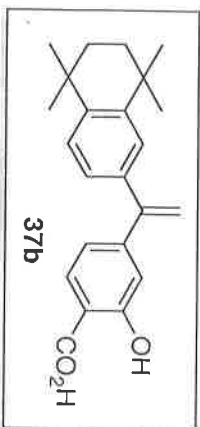
NAME CWVI-103
EXPNO 3
PROCNO 1
Date_ 20181025
Time_ 13.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 4
DW 60.800 usec
DE 6.50 usec
TE 292.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.75 usec
PL1 0.50 dB
PL1W 12.76071072 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CWVI-103

174.81
162.00
150.65
149.02
144.89
144.75
137.14
130.54
126.43
126.35
125.41
119.86
117.38
115.79
110.27

35.06
34.99
34.27
34.17
31.80



NAME CWVI-103
EXPNO 4
PROCNO 1
Date 20181025
Time 14.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 541
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 292.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.25 usec
PL1 -2.10 dB
PL1W 60.29227829 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.50 dB
PL12 16.21 dB
PL2W 12.76071072 W
PL12W 0.34266910 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Acquisition Experiment Report

File: c:\masslynx\july 21.pro\data\210826_cw-vi-003.raw

Header

Acquired File Name: 210826_CW-VI-003

Acquired Date: 26-Aug-2021

Acquired Time: 09:54:58

Job Code: July21

Task Code:

User Name:

Laboratory Name:

Instrument: ACQ-QDA#KAD3226

Conditions:

Submitter:

SampleID:

Bottle Number: 2:1

Description:

Instrument Calibration:

Calibration File: C:\MassLynx\IntelliStart.pro\AcquDB\AutoCal.cal

Parameters

MS1 Static:

Mass: 30 Da to 1250 Da.

Resolution: -0.1/-0.0

Ion Energy: -0.3

Reference File: Internal

Acquisition File:

MS1 Scanning:

Mass: 30 Da to 1250 Da.

Resolution: -0.1/-0.0

Ion Energy: -0.3

Reference File: Internal

Acquisition File:

MS1 Scan Speed Compensation:

Scan: 40 to 10000 amu/sec.

Resolution: -0.1/-0.0

Ion Energy: -0.3

Reference File: Internal

Acquisition File:

Calibration Time: 10:54

Calibration Date: 09/13/17

Coefficients

MS1 Static: $-0.000000000000 \times x^4 + 0.000000000656 \times x^3 +$
 $-0.000001077025 \times x^2 + 1.000599988917 \times x + -0.085640798905$

Function 1: $-0.000000000000 \times x^4 + 0.000000000433 \times x^3 +$
 $-0.000000811760 \times x^2 + 1.000482155999 \times x + -0.071926097790$

Function 2: None

Parameters for C:\MassLynx\July

21.PRO\ACQUDB\NEG_100-500_C_2Hz_5min.EXP

Prescan Statistics:

Initial Average Intensity 379.7862
Initial Average Std Dev 1.1247
Bunch Zero Level 0.0000
Bunch Std Dev 0.0000
Bunch Threshold 0.0000
Spike Removal Std Dev 1.1245
Ion Count Threshold: 25.0000

Data Processing:

Targeted Sampling Frequency 2
Actual Sampling Frequency 2.000
SIR Chromatogram Spike Removal ON
SIR Smoothing ON
Smoothing window size (scans) 3
Number of smooths 2

Method Events:

Initial Stop Flow: No Change
Initial Switch 1: No Change
Timed Events Enabled

| Event | Time(Sec) | Name | Action |
|-------|-----------|------|--------|
|-------|-----------|------|--------|

Instrument Parameters - Function 1:

Polarity ES-
Calibration Dynamic 2
Capillary (kV) 0.80
Cone (V) 5.00
Source Temperature (°C) 120
Probe Temperature (°C) 350
Calibration Temperature (°C) 0

Engineers Settings:

LM 1 Resolution -0.12
HM 1 Resolution -0.02
Low Mass Ion Energy 1 -0.26
High Mass Ion Energy 1 -0.12
Low Mass Position 0.69
High Mass Position -1.81
Low Mass Setup 0.63
High Mass Setup -6.13
Detector Gain Positive 1.0
Detector Gain Negative 1.0
Nominal Rod Polarity Negative

| | |
|-------------------------------------|-------|
| Dynamic Offset Positive Settings: | |
| Dynamic Offset Low Mass Resolution | 0.00 |
| Dynamic Offset High Mass Resolution | 0.00 |
| Dynamic Offset Low Mass Ion Energy | 0.00 |
| Dynamic Offset High Mass Ion Energy | -0.02 |

| | |
|-------------------------------------|-------|
| Dynamic Offset Negative Settings: | |
| Dynamic Offset Low Mass Resolution | -0.01 |
| Dynamic Offset High Mass Resolution | 0.21 |
| Dynamic Offset Low Mass Ion Energy | 0.00 |
| Dynamic Offset High Mass Ion Energy | 0.19 |

| | |
|-----------------------------------|-------|
| Dynamic Offset Settings: | |
| Dynamic Offset Low Mass Position | -0.71 |
| Dynamic Offset High Mass Position | -0.46 |
| Dynamic Offset Low Mass Setup | 0.55 |
| Dynamic Offset High Mass Setup | -0.04 |
| Dynamic Offset Linearity Gain | 4.80 |

| | |
|-------------------|-----|
| Set Detector Gain | 1.0 |
|-------------------|-----|

| | |
|------------------------------|-------|
| Instrument Readbacks | |
| Capillary (kV) | 0.80 |
| Cone (V) | -9.32 |
| Source Temperature (°C) | 120 |
| Multiplier | 355 |
| Probe Temperature (°C) | 350 |
| Calibration Temperature (°C) | 28 |

| | |
|--------------------|---------|
| Inter-scan delays: | |
| Automatic Mode | |
| MS Delay Table | |
| | R delay |
| <= 16.000 | 0.005 |
| > 16.000 | 0.006 |

Health Check Failures:
All Health Checks Passed

Health Checks all enabled unless shown below:
Resolution Setup Required
Recalibration Required
Service Due

ACE Experimental Record

Inlet Method File: c:\masslynx\july
21.pro\acqddb\col4_pfp_fa_acn_5mins

----- Run method parameters -----

-- PUMP --

Waters ACQUITY QSM

Solvent A Name: Water
Solvent B Name: Methanol
Solvent C Name: 0.1% FA
Solvent D Name: Acetonitrile
Low Pressure Limit: 0 psi
High Pressure Limit: 15000 psi
Seal Wash Period: 5.00 min
[Gradient Table]

| | Time(min) | Flow Rate(mL/min) | %A | %B | %C | %D | Curve |
|----|-----------|-------------------|-----|-----|------|------|---------|
| 1. | Initial | 0.500 | 0.0 | 0.0 | 95.0 | 5.0 | Initial |
| 2. | 2.00 | 0.500 | 0.0 | 0.0 | 5.0 | 95.0 | 6 |
| 3. | 3.50 | 0.500 | 0.0 | 0.0 | 95.0 | 5.0 | 11 |
| 4. | 5.00 | 0.500 | 0.0 | 0.0 | 95.0 | 5.0 | 11 |

Comment:

Flow Ramp Rate: 0.45 min
D Solvent Selection (if supported): No Change
System Pressure Data Channel: No
Flow Rate Data Channel: No
%A Data Channel: No
%B Data Channel: No
%C Data Channel: No
%D Data Channel: No
Primary Data Channel: No
Accumulator Data Channel: No
Degasser Data Channel: No
Gradient Start: At Injection
Gradient Start Volume: 0 uL
Gradient Start Time: 0.00 min
Participate in pre-analysis: No

-- END PUMP --

-- DETECTOR --

Waters Acquity CM

Target Column Temperature: 50.0 C
Temperature Alarm Band: 5.0 C
: No

Column Valve Position: Column 4
Equilibration Time: 0.1 min
External Valve 1: No Change
External Valve 2: No Change
External Valve 3: No Change
Comment:
Column Temperature Data Channel: No
Preheater Temperature Data Channel: No

-- END DETECTOR --

-- DETECTOR --

Waters Acquity PDA

Run Time: 5.00 min
PDA Detector Type: UPLC LG 500 nm
Lamp: On
Sampling Rate: 20 points/sec
Filter Time Constant: 0.2000 sec
Exposure Time: Auto msec
Interpolate 2nd order filter Region: No
Use UV Blocking Filter: Yes
3D Channel...
Range: 210 - 499
Resolution: 2.4 nm
Channel 1...
Data Mode: Absorbance at 214
Resolution: 2.4 nm
Channel 2...
Data Mode: Absorbance at 380
Resolution: 2.4 nm
Initial Switch 1: No Change
Initial Switch 2: No Change

-- END DETECTOR --

-- AUTOSAMPLER --

Waters ACQUITY FTN AutoSampler

Run Time: 5.00 min
Comment:
Load Ahead: Disabled
Loop Offline: Automatic min
Wash Solvent Name: Weak Wash
Pre-Inject Wash Time: 0.0 sec
Post-Inject Wash Time: 6.0 sec
Purge Solvent Name: Strong Wash

Maximum System Pressure: 5734.0 psi

Average System Pressure: 4515.0 psi

----- oOo -----

----- Waters ACQUITY FTN Postrun Report -----

Software Version: 1.60.1774

Firmware Version: 1.60.364 (Sep 20 2013)

Checksum: 0x35d5392b

Serial Number: D17SDI835G

Sample Syringe Size: 100.0

Extension Loop Size: 0.0

Needle Size: 30.0

Minimum Sample Temperature: 10.0

Maximum Sample Temperature: 10.2

Average Sample Temperature: 10.1

Minimum Column Temperature: -0.2

Maximum Column Temperature: 0.0

Average Column Temperature: -0.2

----- oOo -----

----- Waters Acquity CM Postrun Report -----

Software Version: 1.60.2072

Firmware Version: 1.65.142 (Apr 02 2015)

Checksum: 0x18bfb4ea

Serial Number: D17CMP604G

Valve Position: 4

Minimum Column Temperature: 50.0

Maximum Column Temperature: 50.0

Average Column Temperature: 50.0

----- o0o -----

----- Active eCord Data -----

Valve Current Position: 4

Failed to retrieve Active eCord ColumnData Data

----- o0o -----

----- Generic Instrument Postrun Report -----

Software Version: 1.60.1390

Firmware Version: 1.60.6169 (Aug 13 2013)

Checksum: 0xdcfe9340

Serial Number: B17UPD132A

Lamp On/Off Event: No

Lamp Life: 3223.00 hours

Lamp Serial Number: 000133684

Exposure Time: 50.000 msec

Lambda1: 187.360

Lambda512: 502.647

Flow Cell Type: Analytical LG

Flow Cell Path Length: 10.000 mm

Flow Cell Volume: 0.500 microliters

Flow Cell Serial Number: PDA10-15625

Flow Cell Part Number: 205015017

Optics Temperature Stabilization Setting: Normal Temperature

----- o0o -----

-----Failed to get IECordHost2 Interface -----

Function 1

| | |
|---------------------------|----------------|
| Scans in function: | 601 |
| Cycle time (secs): | Automatic |
| Scan duration (secs): | 0.495 |
| Inter Scan Delay (secs): | Automatic |
| Start and End Time(mins): | 0.000 to 5.000 |
| Ionization mode: | ES- |
| Data type: | Accurate Mass |
| Function type: | Scan |
| Mass range: | 100 to 500 |

Function 2

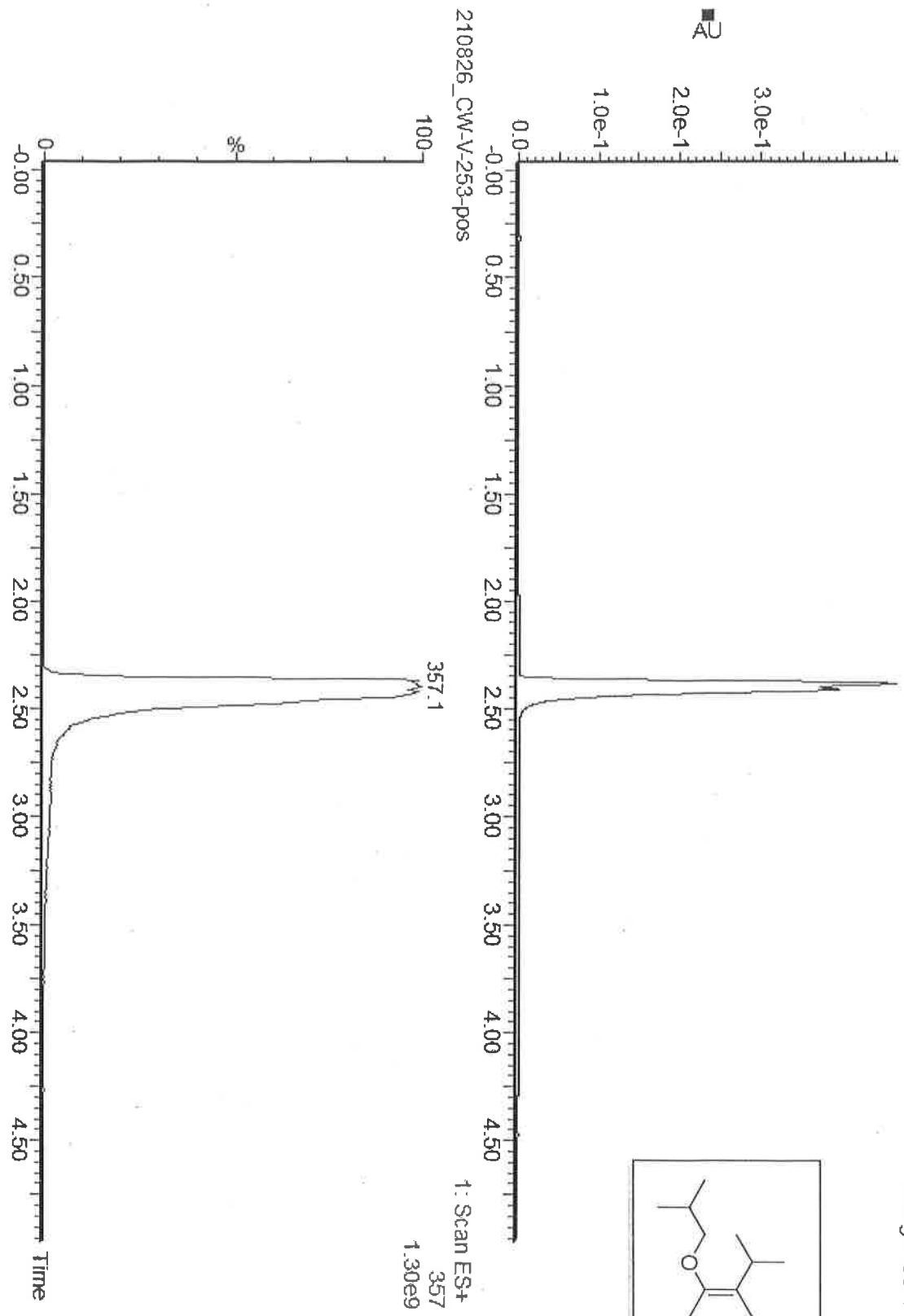
| | |
|------------------------|-------------|
| Scans in function: | 6001 |
| Function type: | Diode Array |
| Wavelength range (nm): | 210 to 499 |

mz not observed; see 426

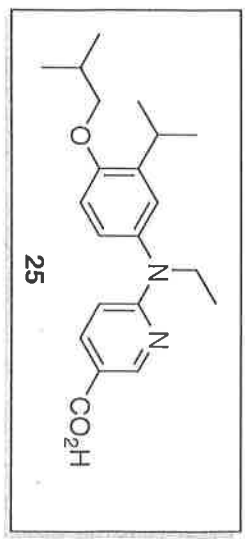
210826_CW-V-253-pos

(2) PDA Ch2 260nm@2.4nm

Range: 5e-1



1: Scan ES+
357
1.30e9



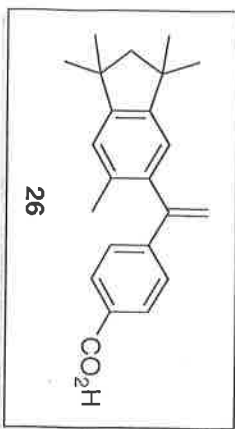
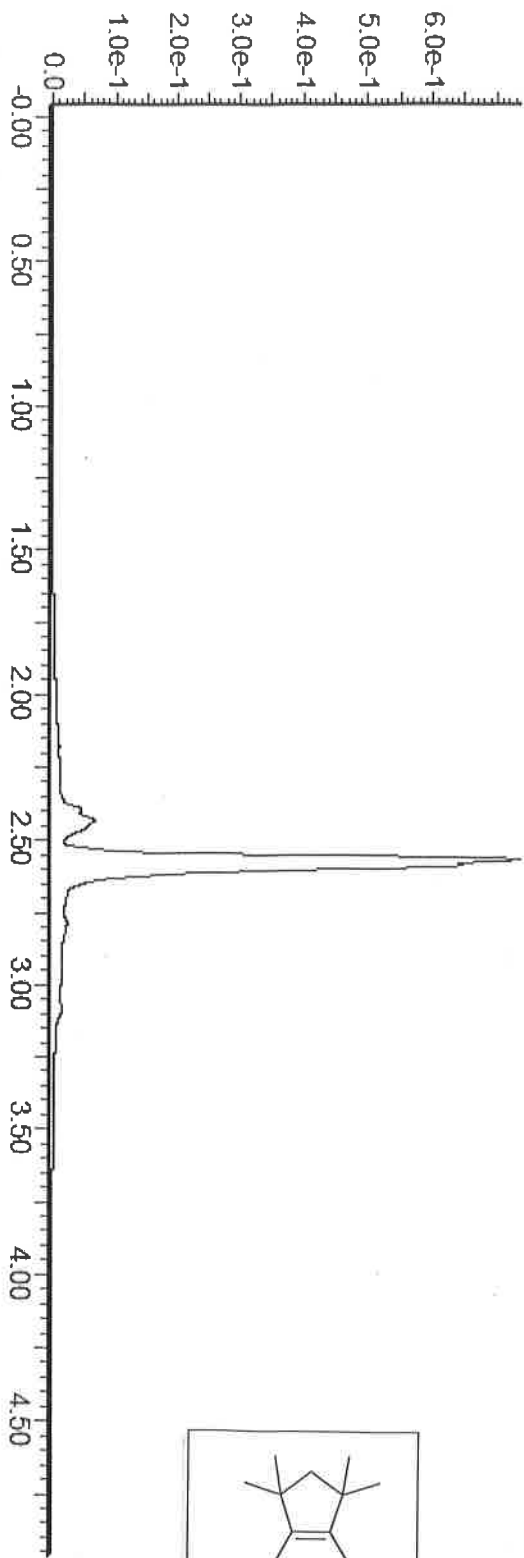
m/z not observed

210826_CW-VI-035_pos

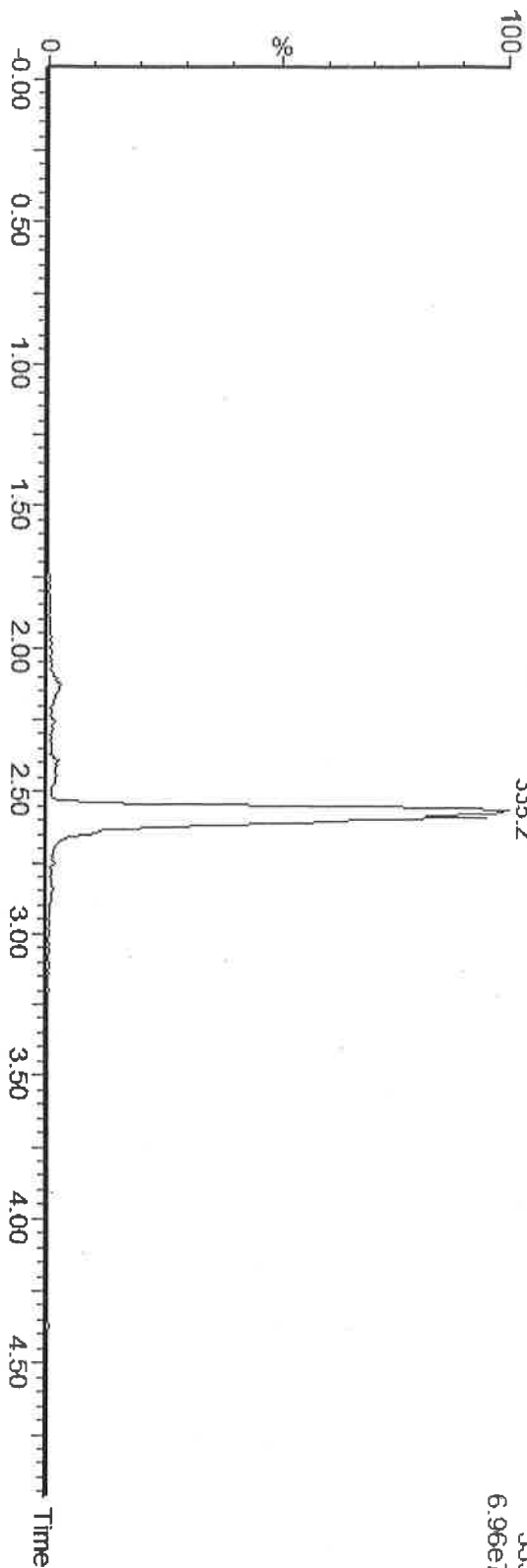
(2) PDA Ch2 260nm@2.4nm

Range: 7e-1

AU



210826_CW-VI-035_pos

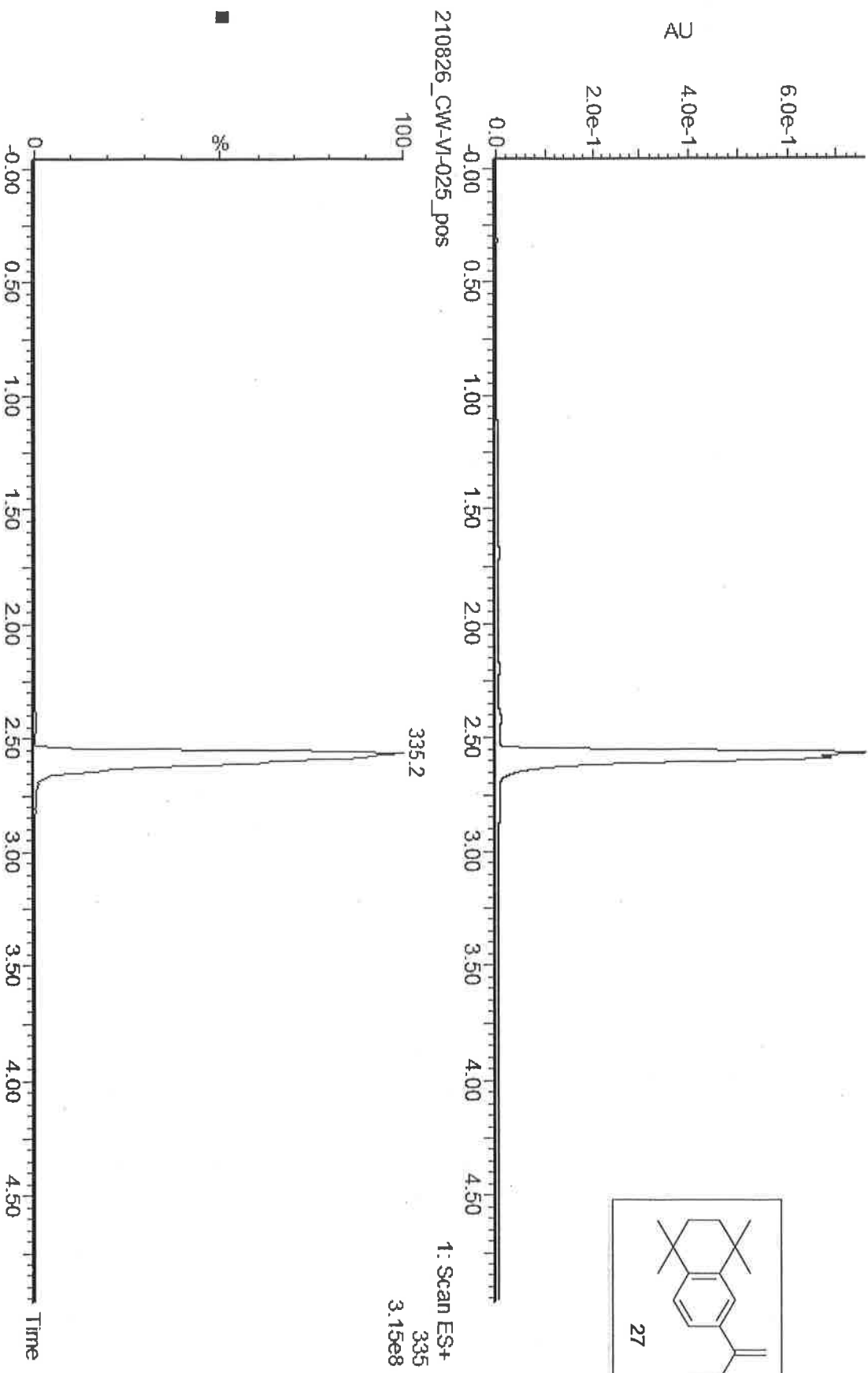
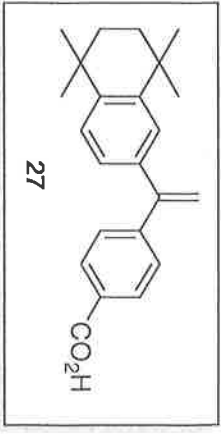


1: Scan ES+
335
6.96e7

mz not observed

210826_CW-VI-025_pos

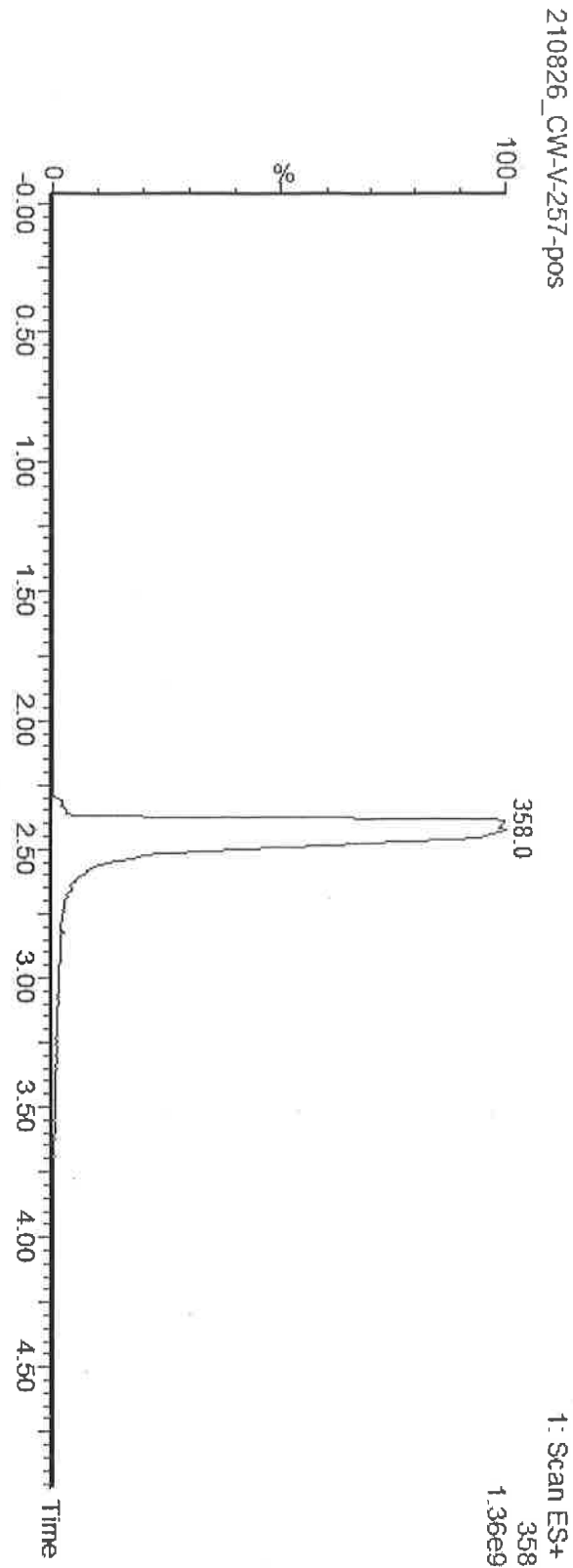
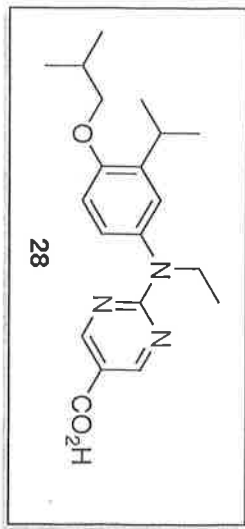
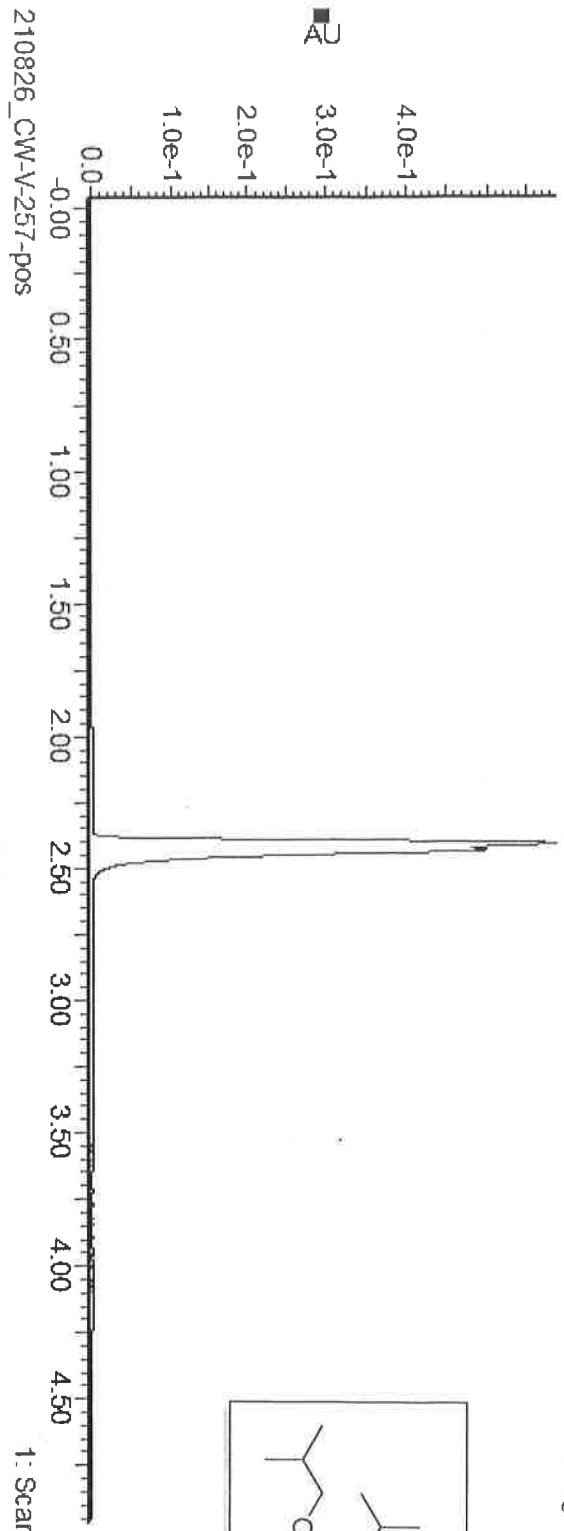
(2) PDA Ch2 260nm@2.4nm
Range: 8e-1



1: Scan ES+
335
3.15e8

Label - CW-V-259; weak; see 402
210826_CW-V-257-pos

(2) PDA Ch2 260nm@2.4nm
Range: 6e-1



1: Scan ES+
358
1.36e9

mz not observed

210826_CW-V-265-pos

(2) PDA Ch2 260nm@2.4nm
Range: 2e-1

1.5e-1
1.0e-1
5.0e-2

AU

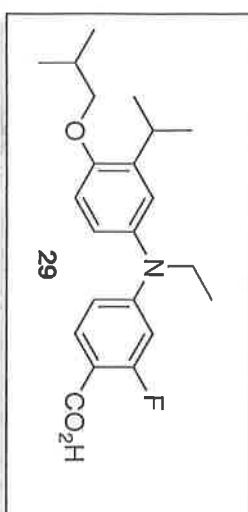
210826_CW-V-265-pos

100

374.1

1: Scan ES+
374
1.38e9

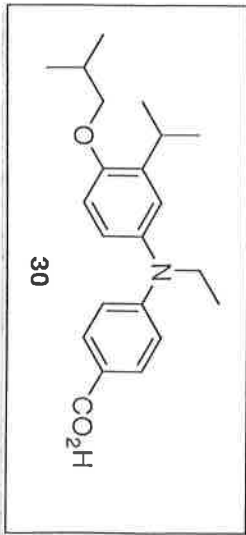
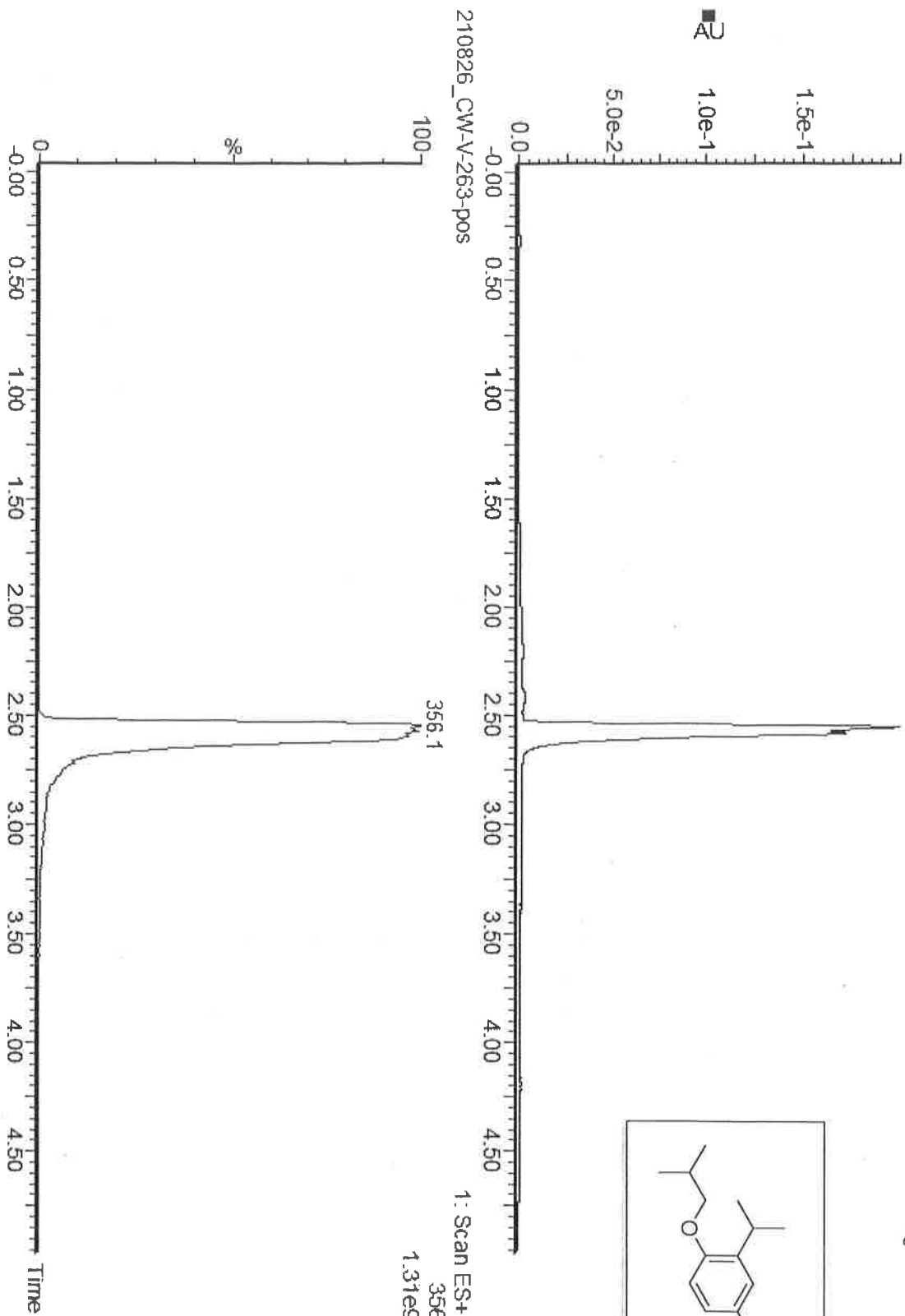
0
-0.00 0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50
Time



m/z not observed

210826_CW-V-263-pos

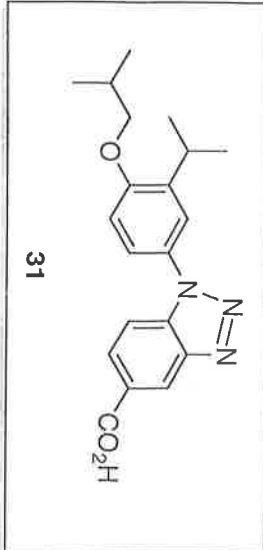
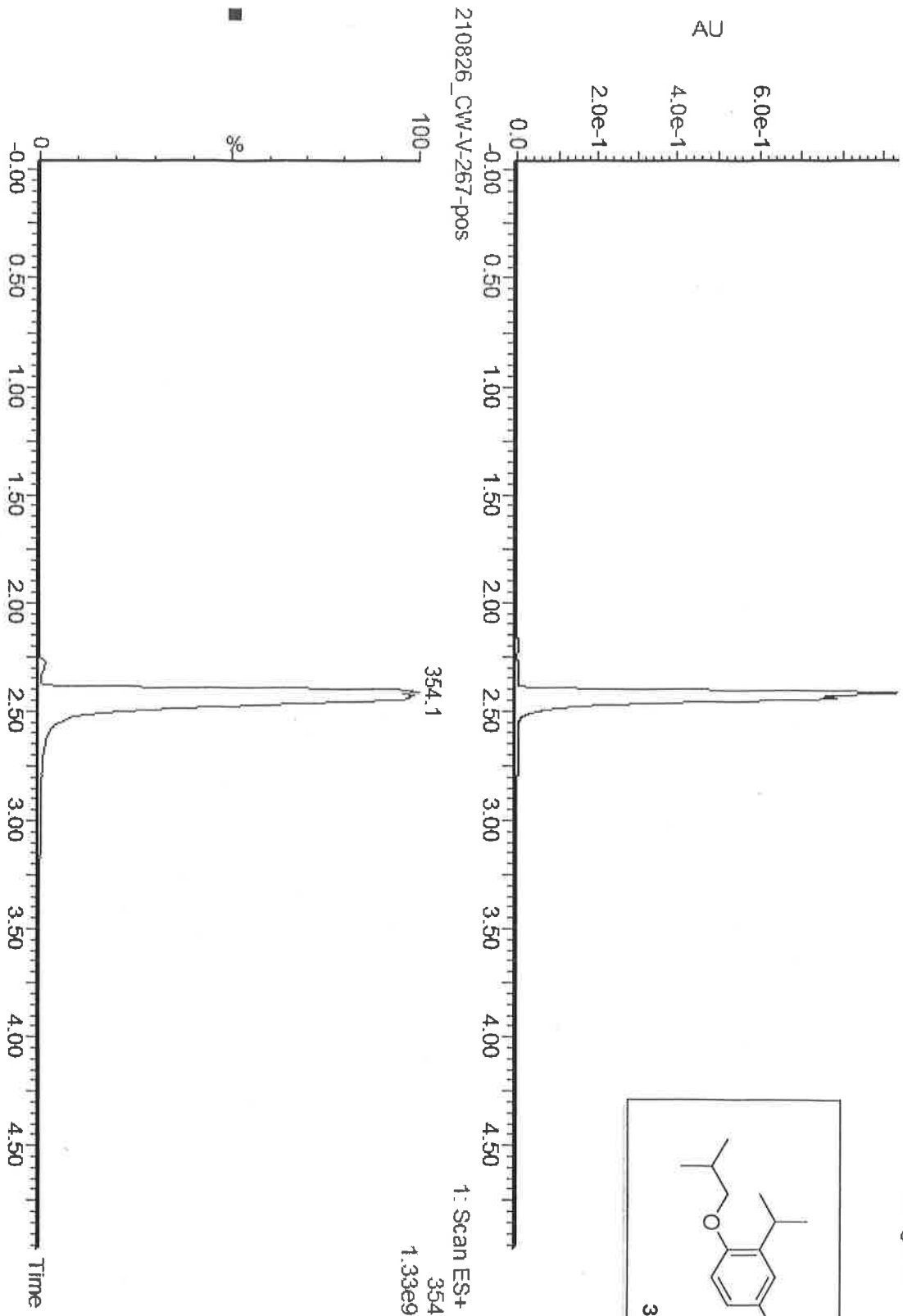
(2) PDA Ch2 260nm@2.4nm
Range: 2e-1



mz weak; see 398

210826_CW-V-267-pos

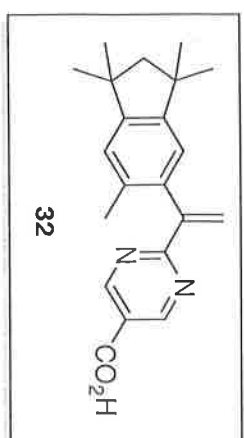
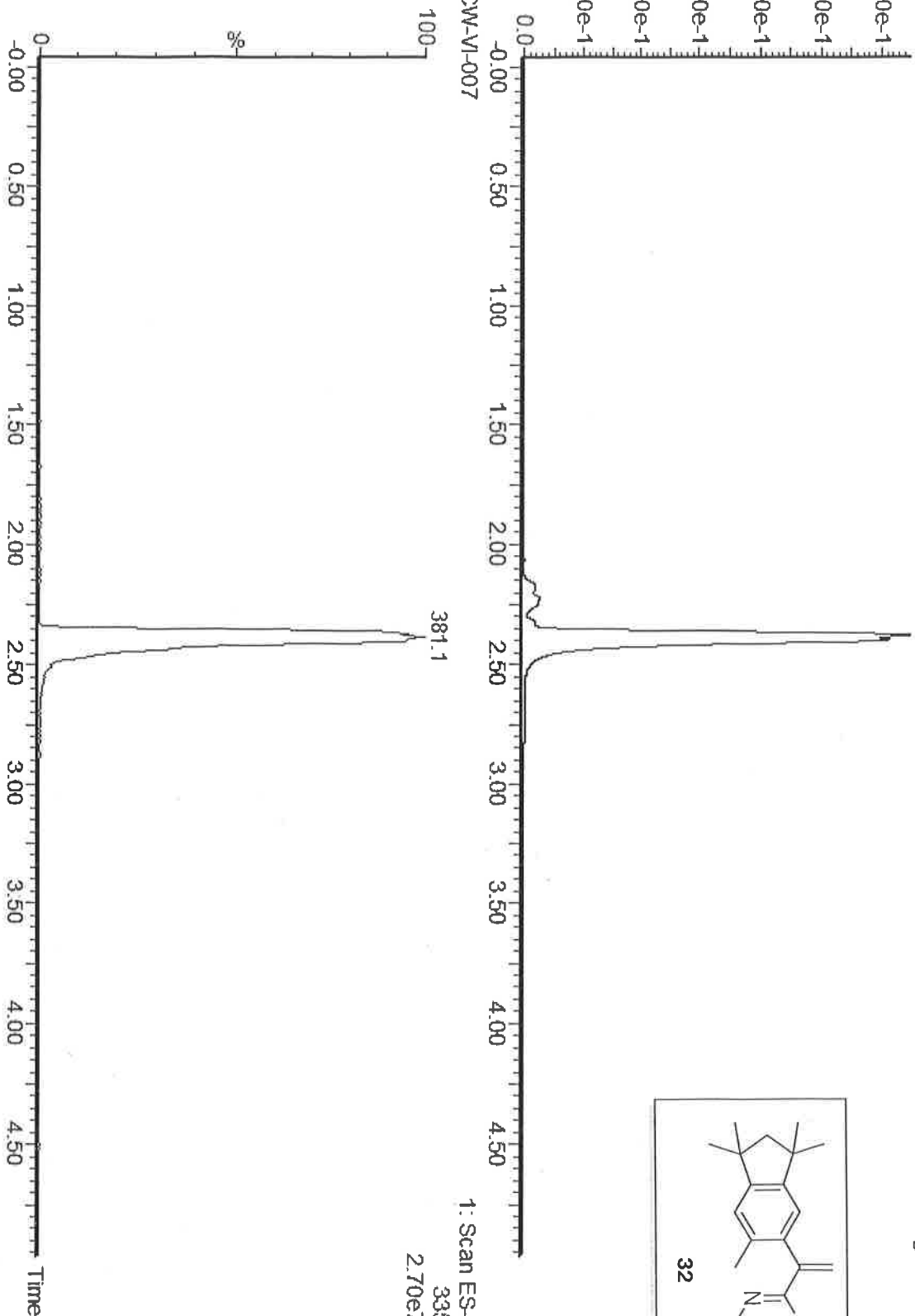
(2) PDA Ch2 260nm@2.4nm
Range: 9e-1



210826_CW-VI-007

(2) PDA Ch2 260nm@2.4nm
Range: 7e-1

AU



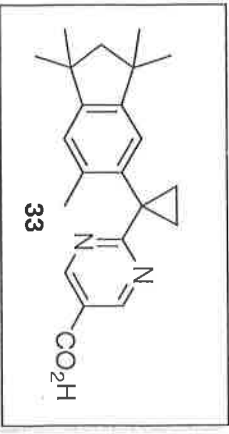
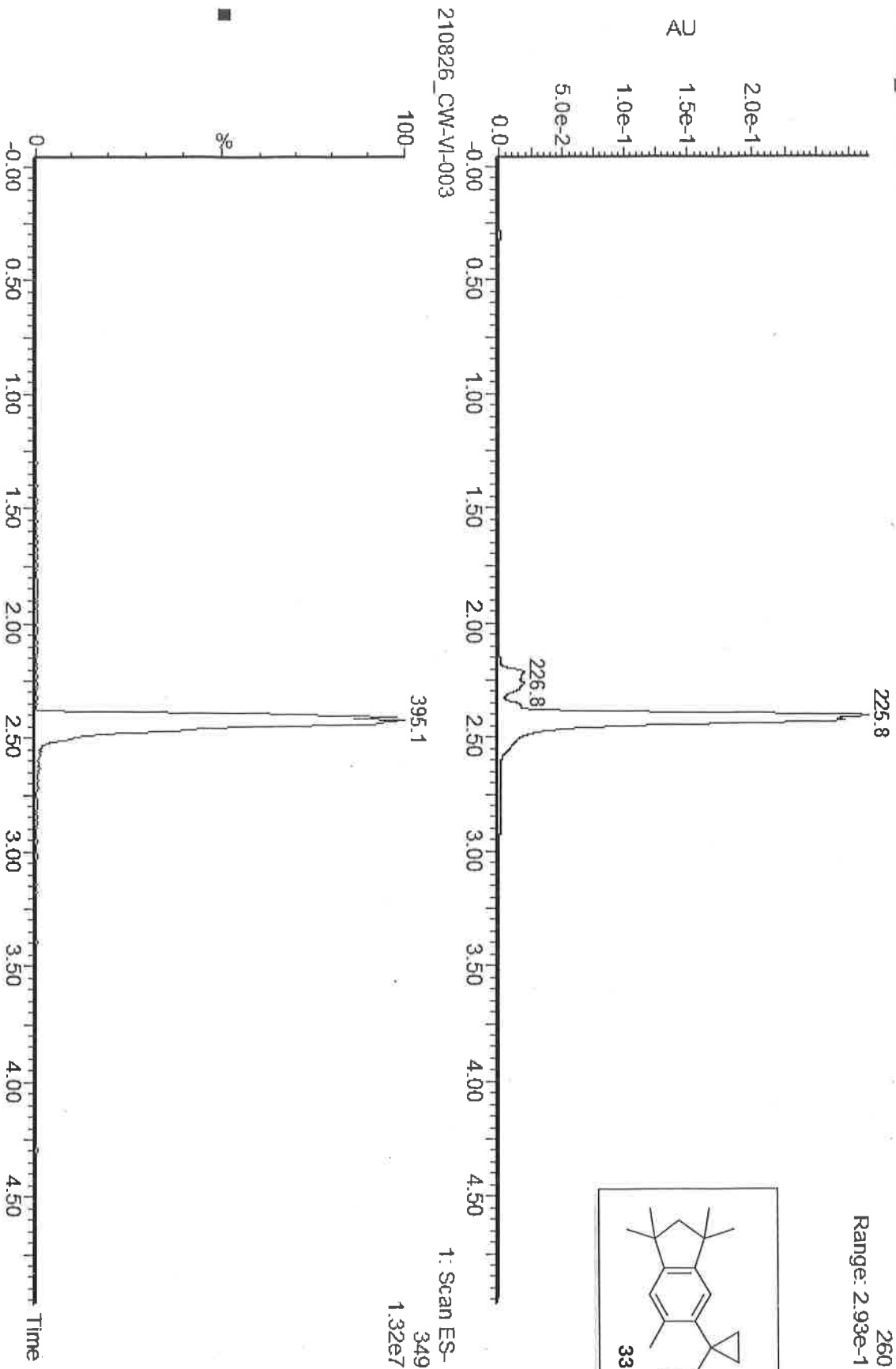
32

210826_CW-VI-007

1: Scan ES-
335
2.70e7

210826_CW-VI-003

2: Diode Array
260
Range: 2.93e-1



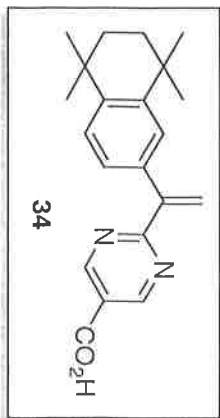
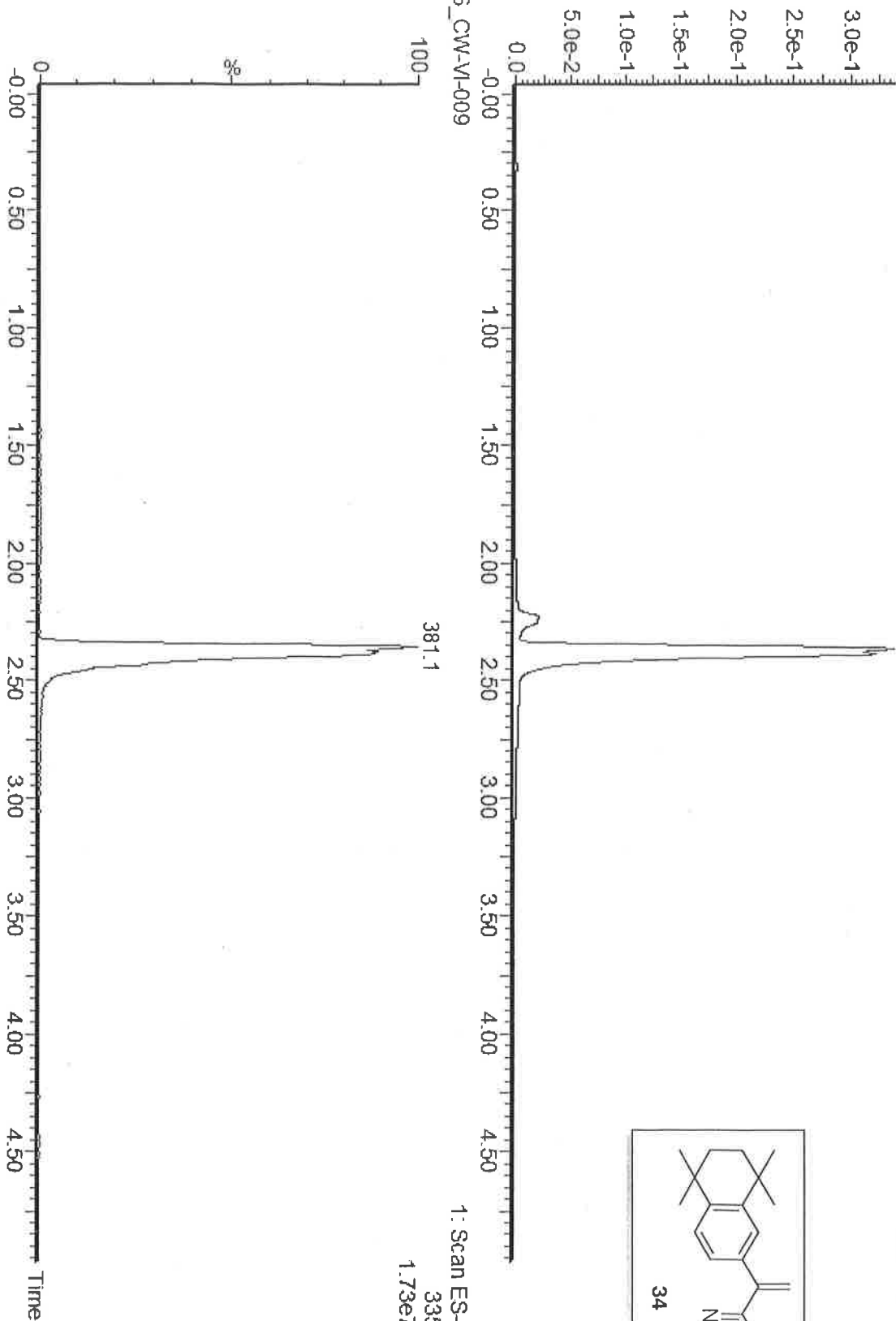
1: Scan ES-
349
1.32e7

210826_CW-VI-009

(2) PDA Ch2 260nm@2.4nm
Range: 3e-1

AU

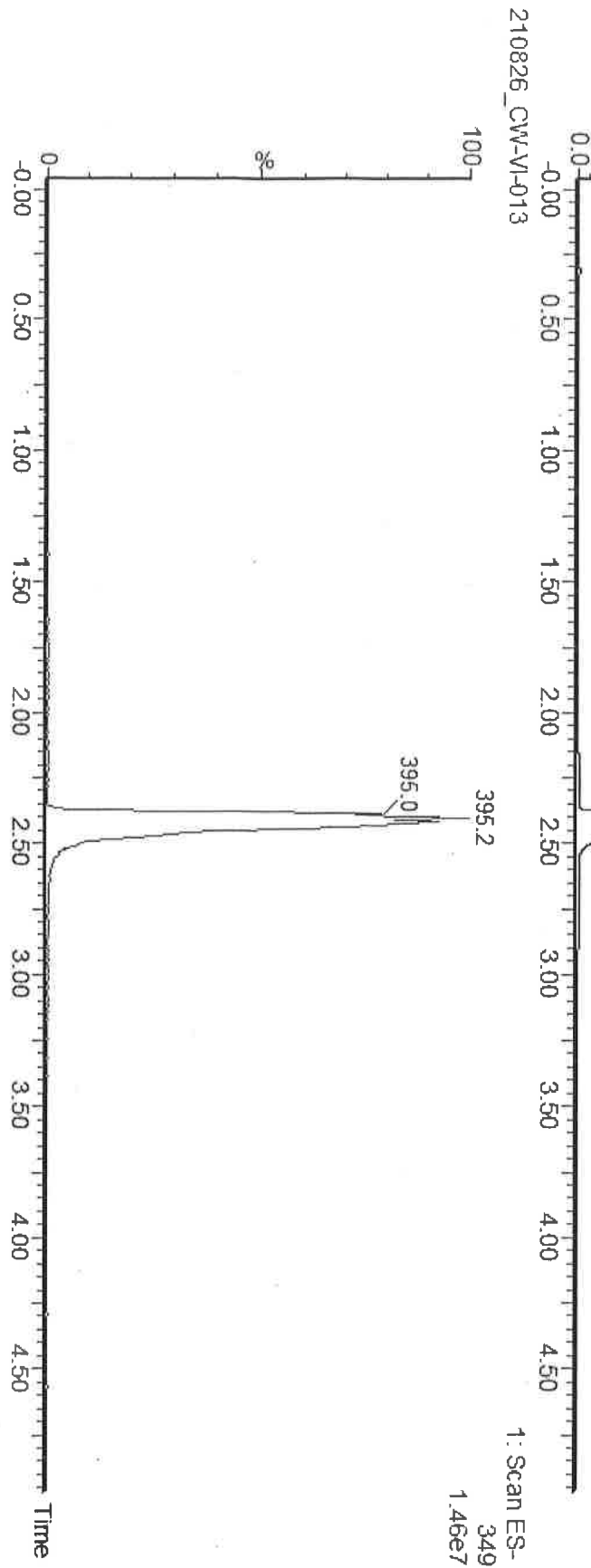
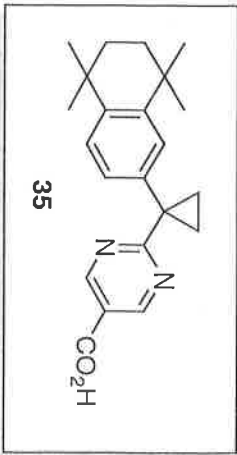
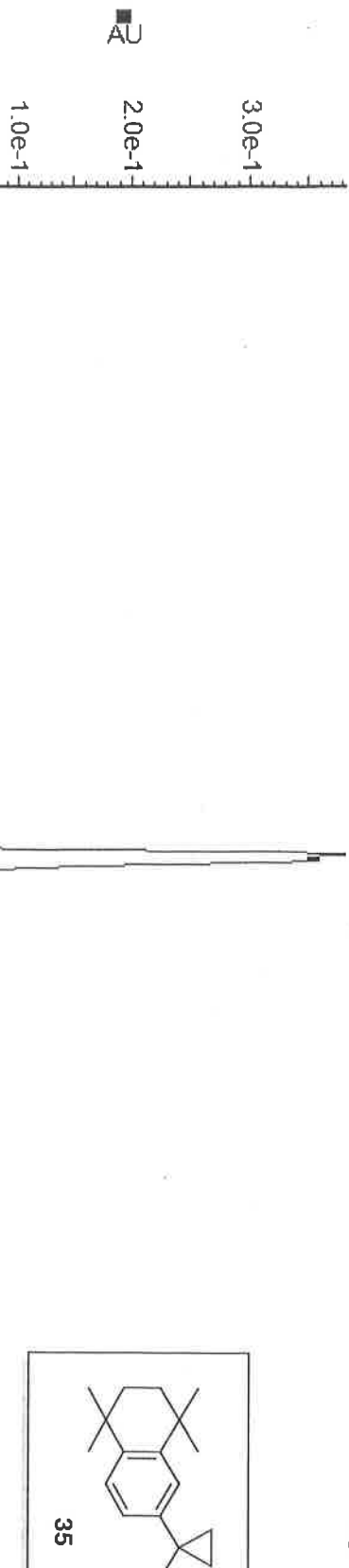
210826_CW-VI-009



1: Scan ES-
335
1.73e7

210826_CW-VI-013

(2) PDA Ch2 260nm@2.4nm
Range: 4e-1

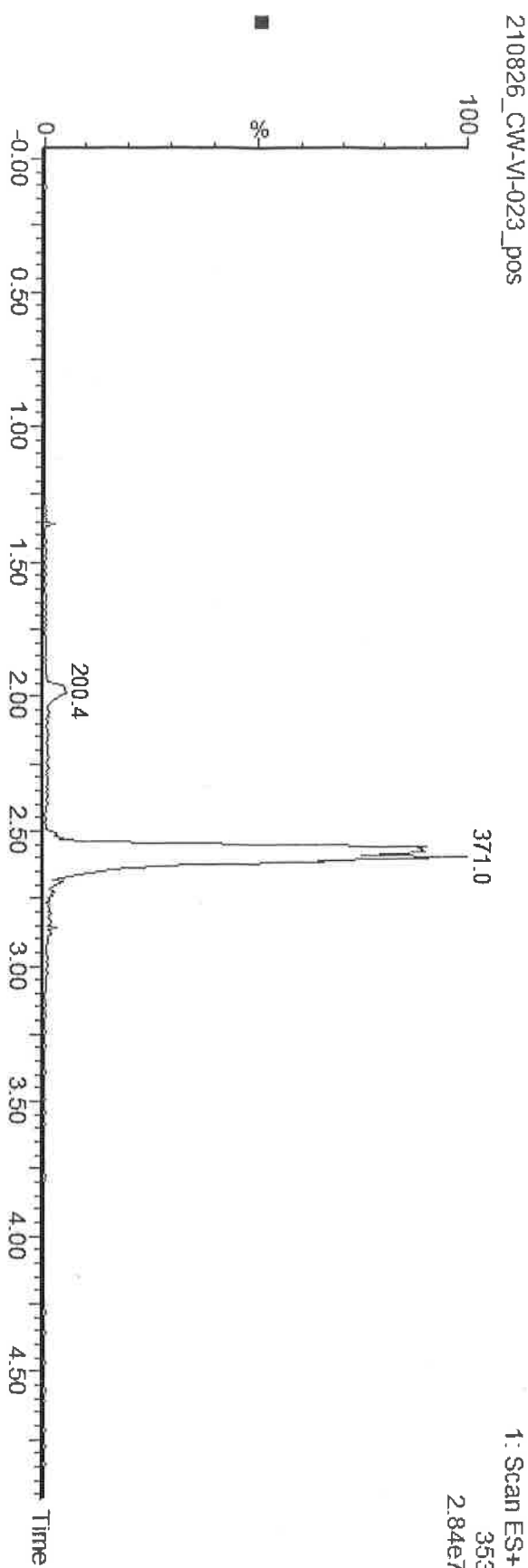
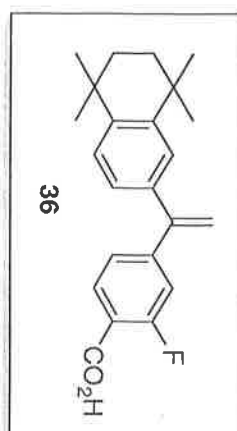
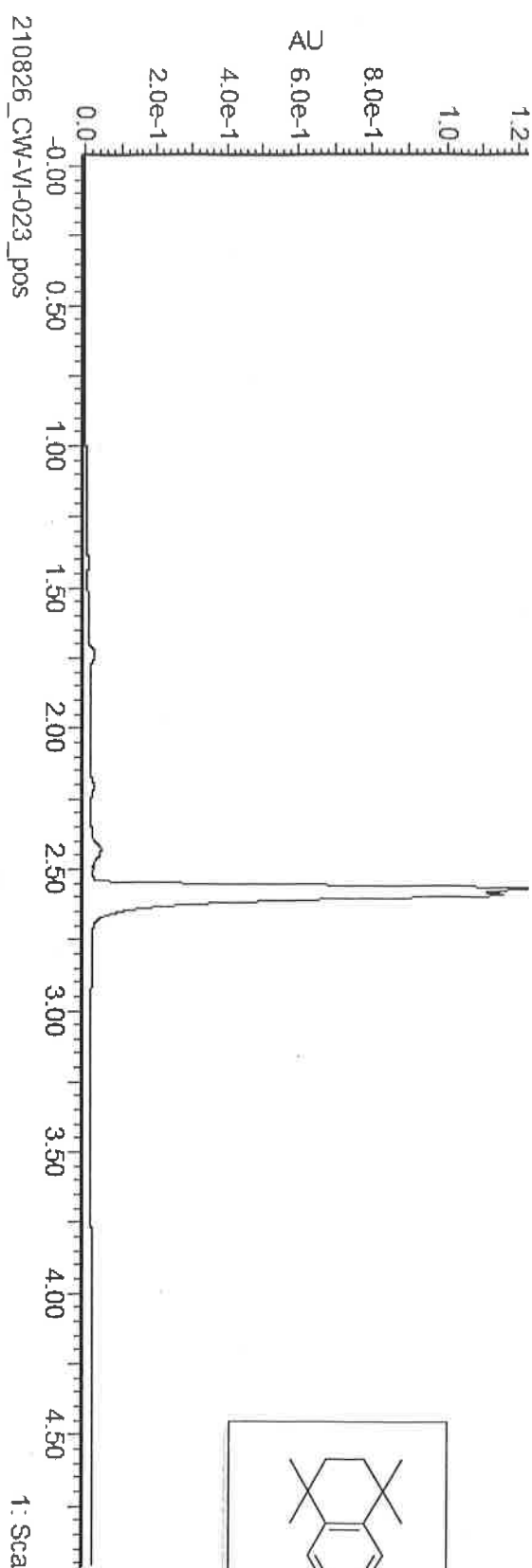


1: Scan ES-
349
1.46e7

weak

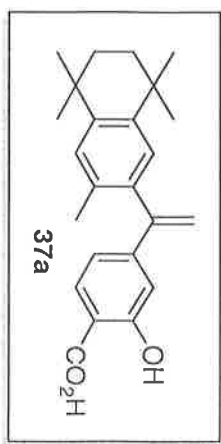
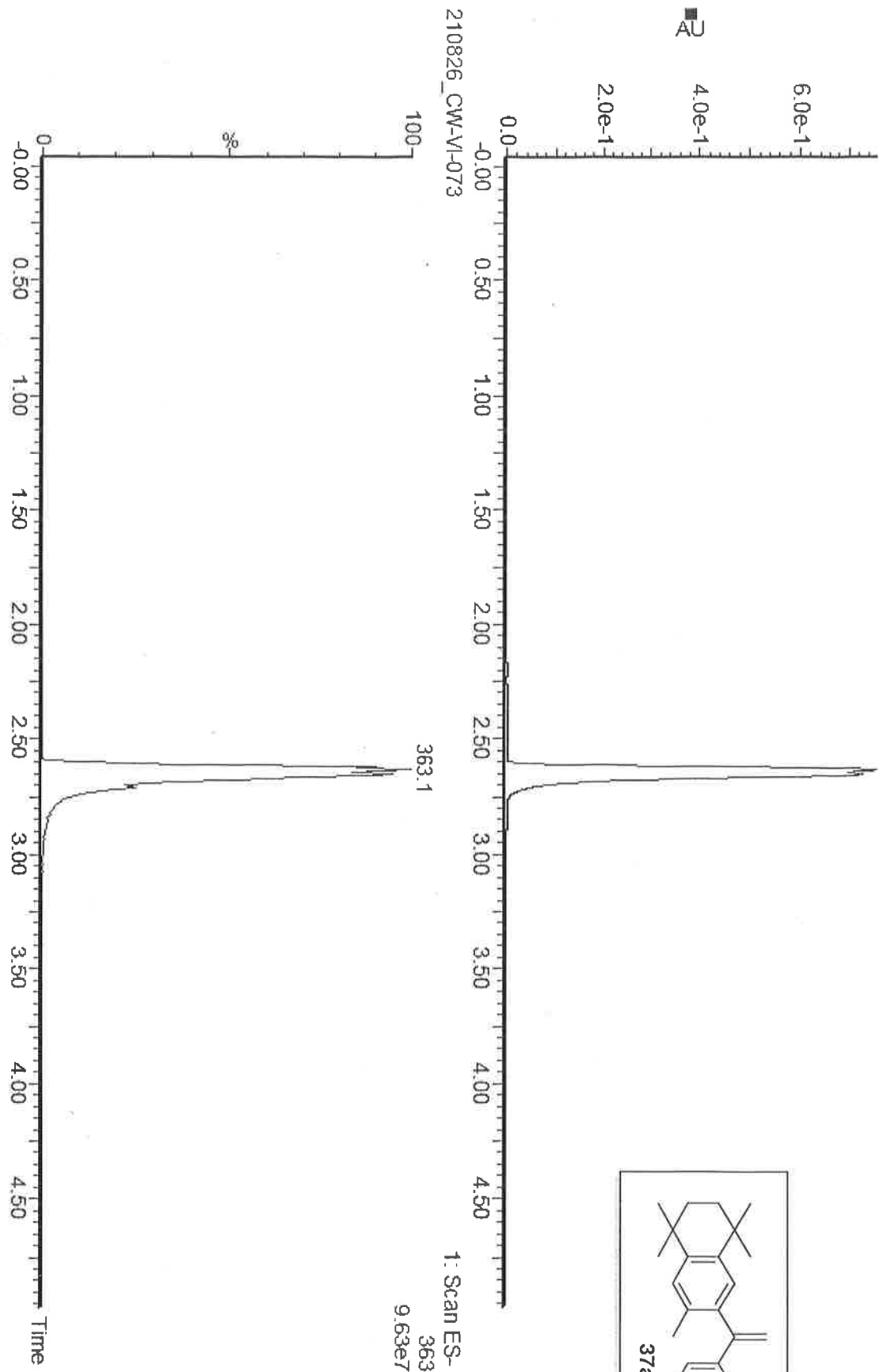
210826_CW-VI-023_pos

(2) PDA Ch2 260nm@2.4nm
Range: 1



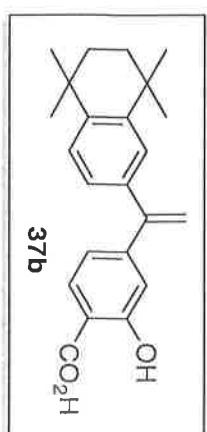
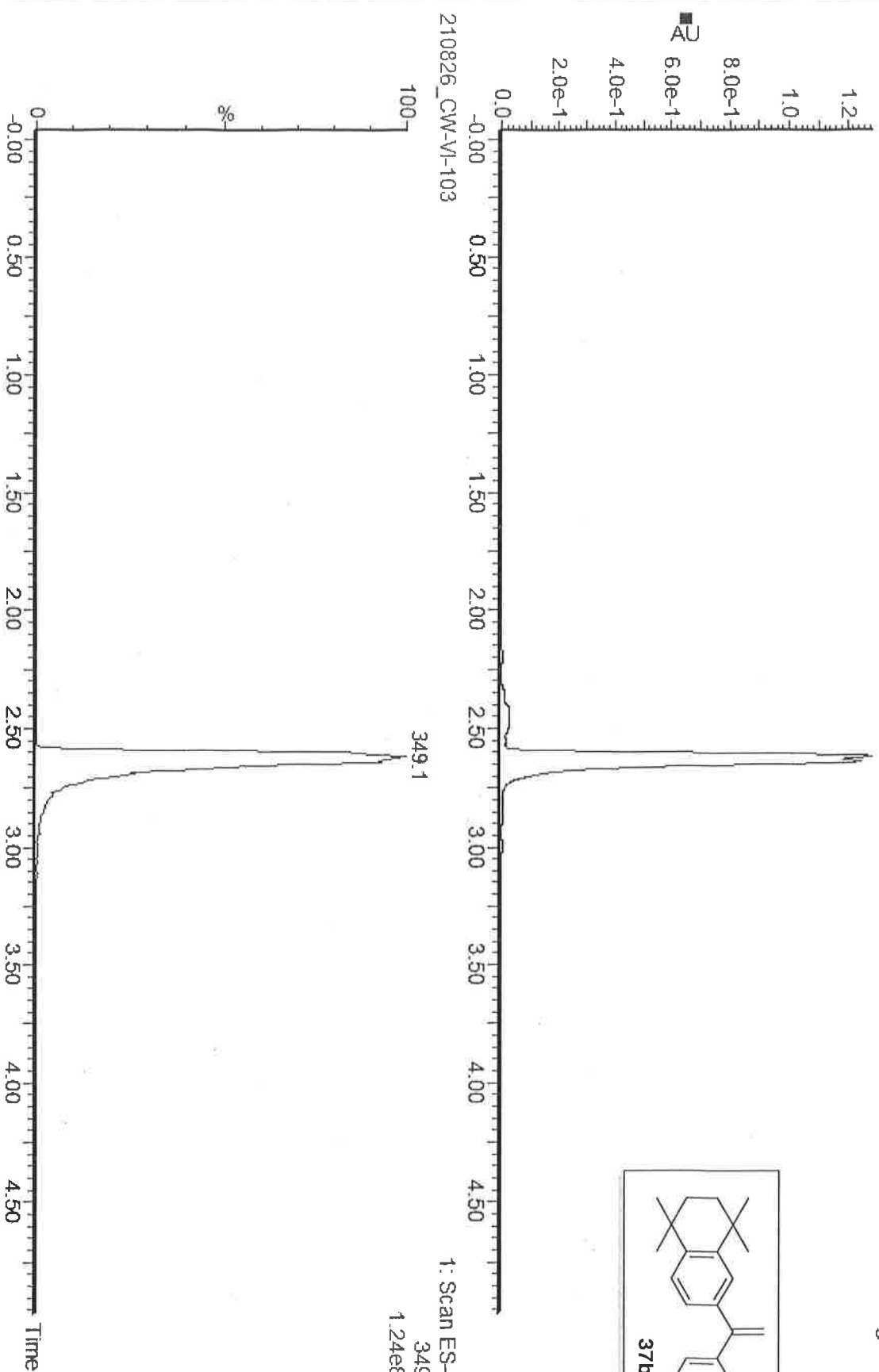
210826_CW-VI-073

(2) PDA Ch2 260nm@2.4nm
Range: 8e-1



210826_CW-VI-103

(2) PDA Ch2 260nm@2.4nm
Range: 1



1: Scan ES-
349
1.24e8