Supporting Information

Iridium-Catalyzed *Anti*-Stereoselective Asymmetric Ring Opening Reactions of Azabenzonorbornadienes with Carboxylic Acids

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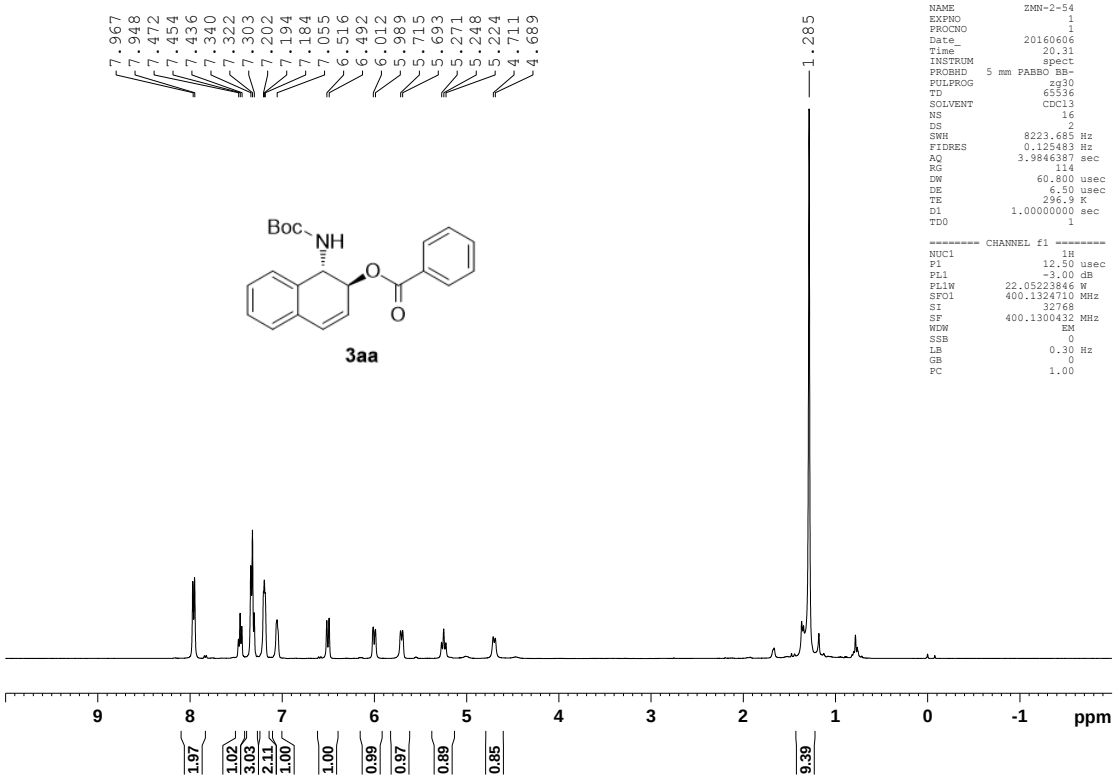
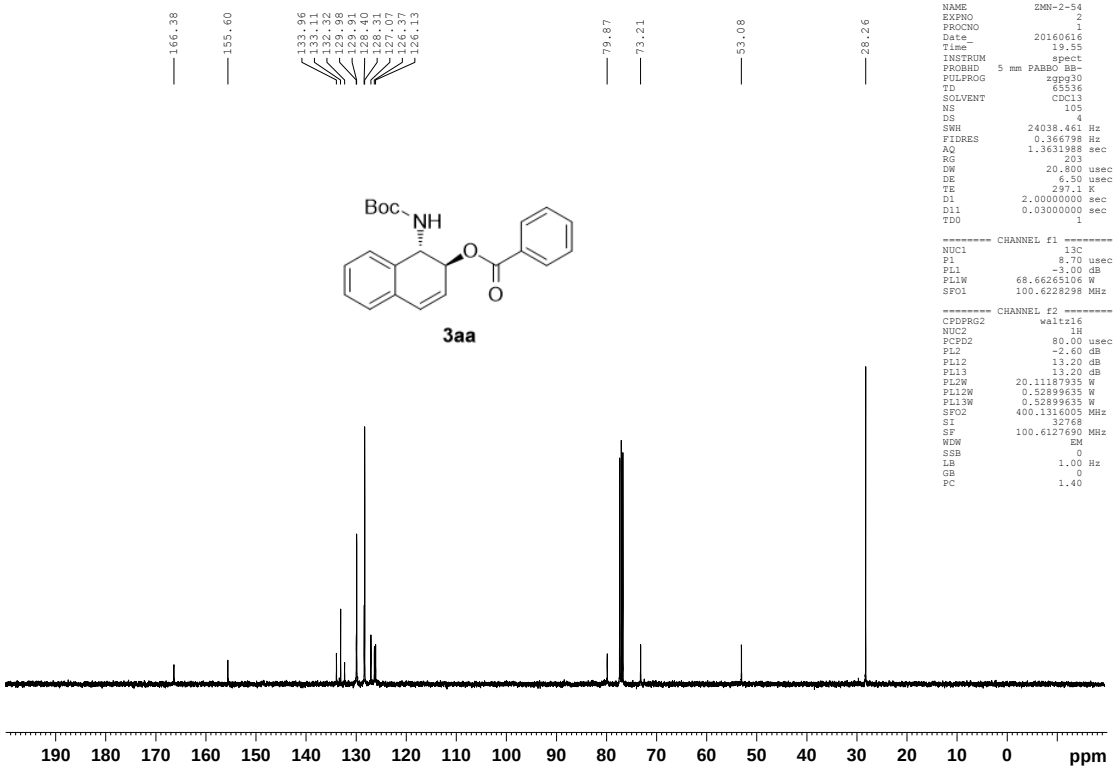
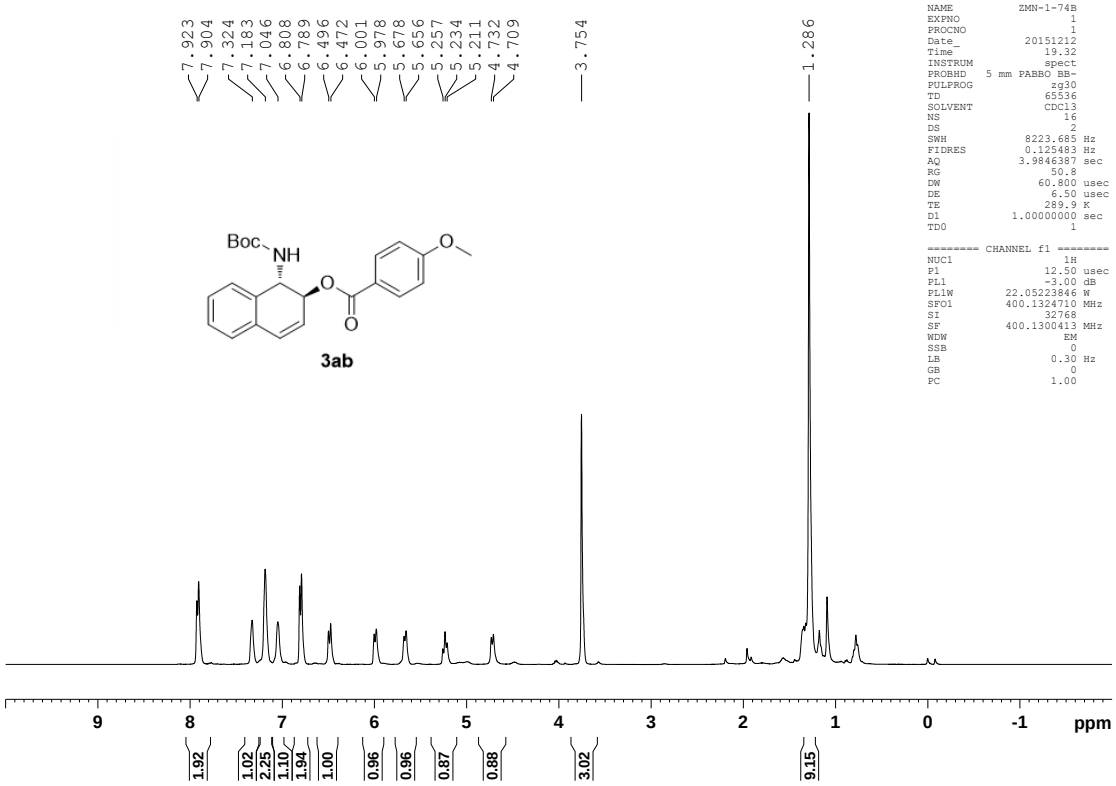
Table of contents

Part I NMR spectra



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6.001
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5.257
5.234
5.211
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4.709
3.754
1.286
Boc
NH
O
O
O
3ab
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EXPNO 1
PROCNO 1
Date_ 20151212
Time 19.32
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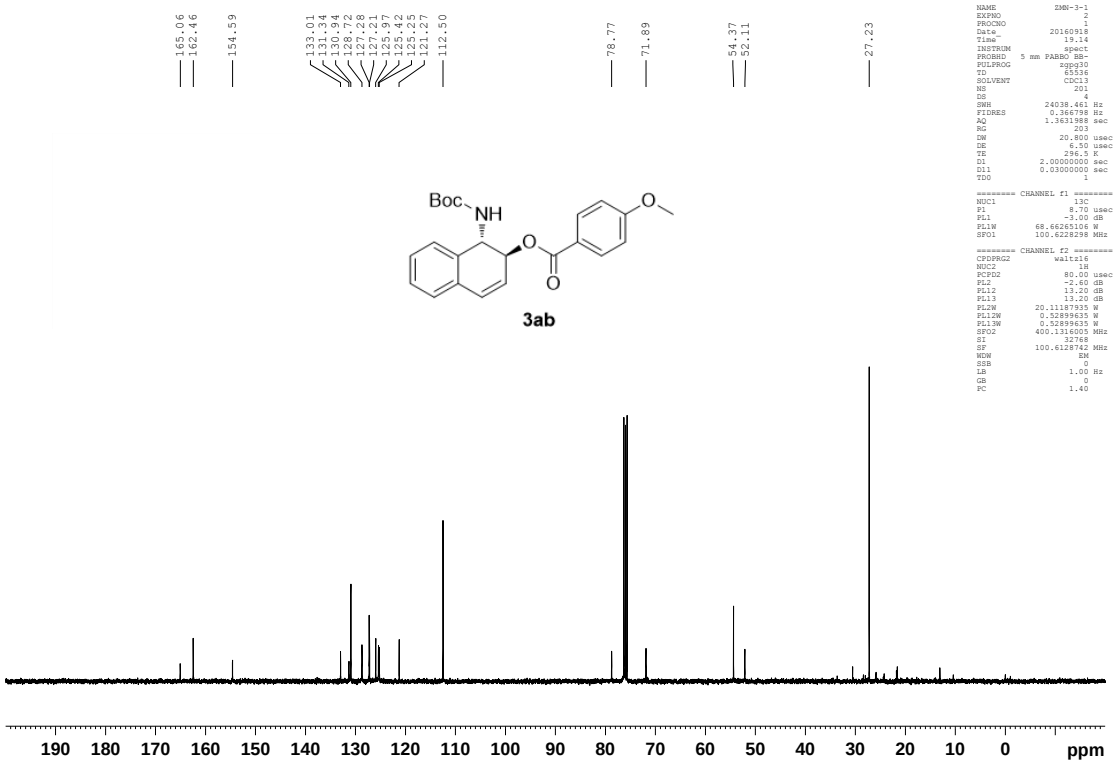
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 50.8
DW 60.800 usec
DE 6.50 usec
TE 289.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PL1W 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300413 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 0 -1 ppm
1.92
1.02
2.25
1.10
1.94
1.00
0.96
0.96
0.87
0.88
3.02
9.15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154.59
133.01
131.34
130.94
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128.28
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125.97
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112.50
78.77
71.89
54.37
52.11
27.23
Boc
NH
O
O
O
3ab
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EXPNO 2
PROCNO 1
Date_ 20160918
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PULPROG zgpg30
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SOLVENT CDCl3
NS 201
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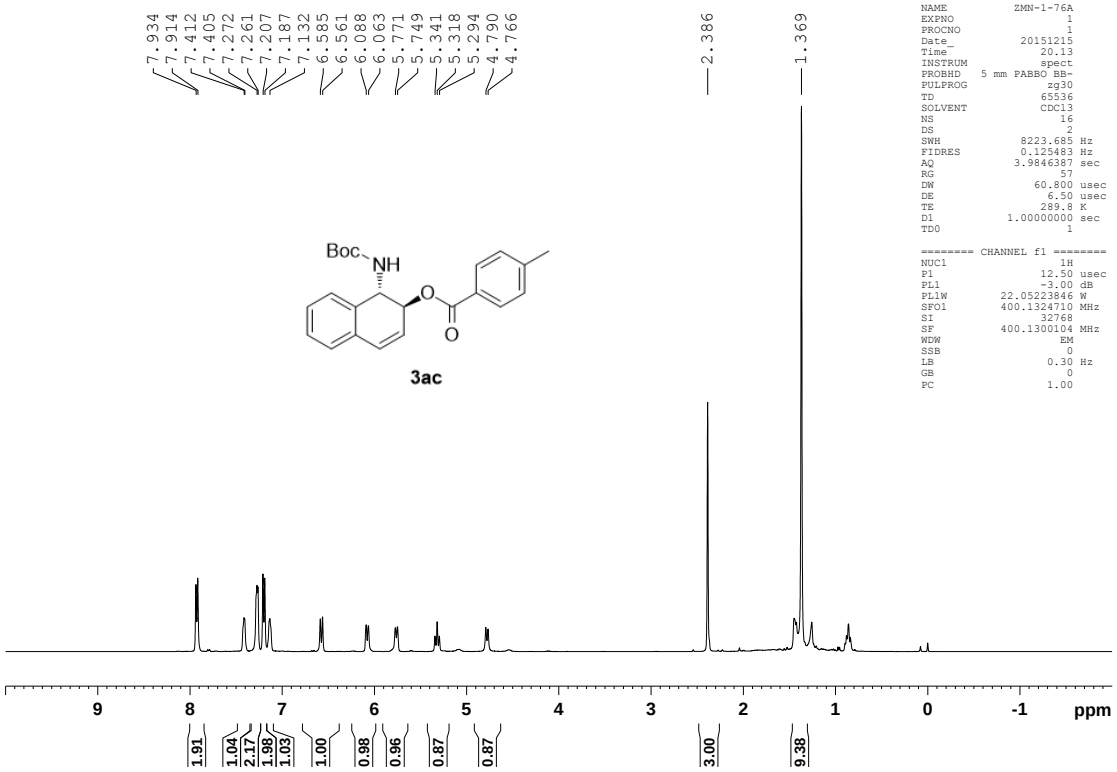
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.70 usec
PL1 -3.00 dB
PL1W 68.66265106 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.60 dB
PL12 13.20 dB
PL13 13.20 dB
PL2W 20.11187935 W
PL12W 0.52899635 W
PL13W 0.52899635 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128742 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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7.405
7.272
7.261
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6.585
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6.088
6.063
5.771
5.749
5.341
5.318
5.294
4.790
4.766
2.386
1.369
Boc
NH
O
O
3ac
NAME ZMN-1-76A
EXPNO 1
PROCNO 1
Date_ 20151215
Time 20.13
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 57
DW 60.800 usec
DE 6.50 usec
TE 289.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PL1W 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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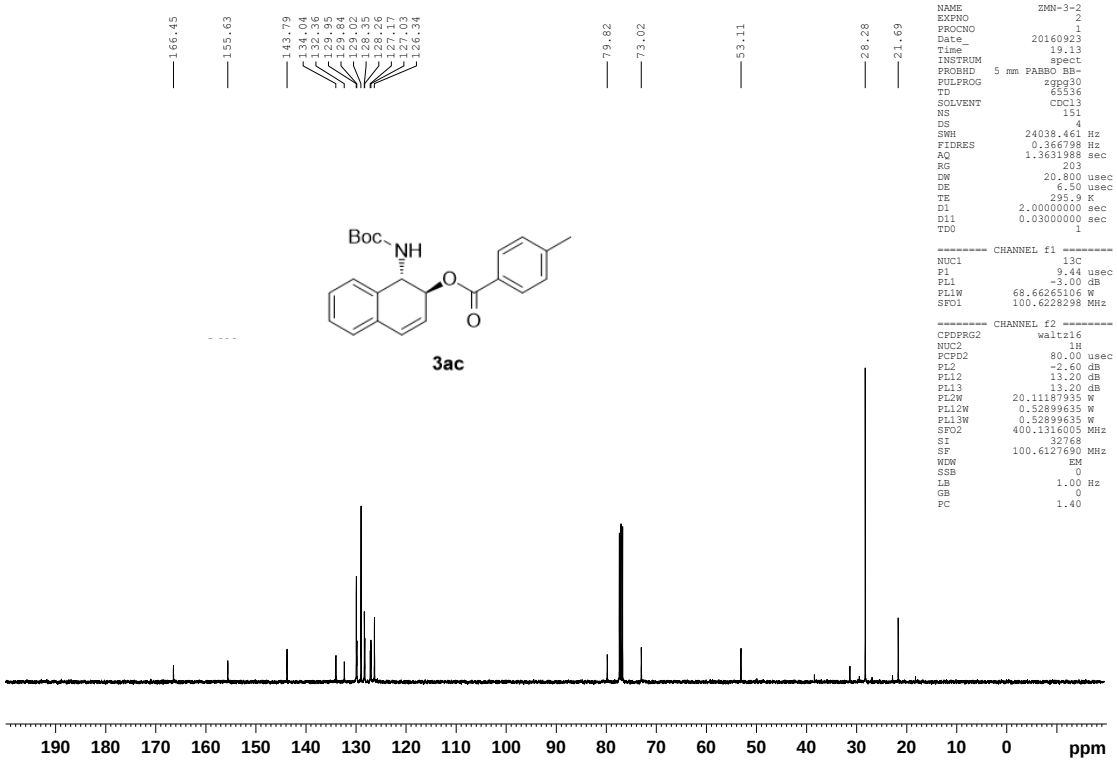
1.91 1.04 2.17 1.98 1.03 1.00 0.98 0.96 0.87 0.87 3.00 9.38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128.26
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127.03
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79.82
73.02
53.11
28.28
21.69
Boc
NH
O
O
3ac
NAME ZMN-3-2
EXPNO 2
PROCNO 1
Date_ 20160923
Time 19.13
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 151
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.44 usec
PL1 -3.00 dB
PL1W 68.66265106 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.60 dB
PL12 13.20 dB
PL13 13.20 dB
PL2W 20.11187935 W
PL12W 0.52899635 W
PL13W 0.52899635 W
SFO2 400.1316005 MHz
SI 32768
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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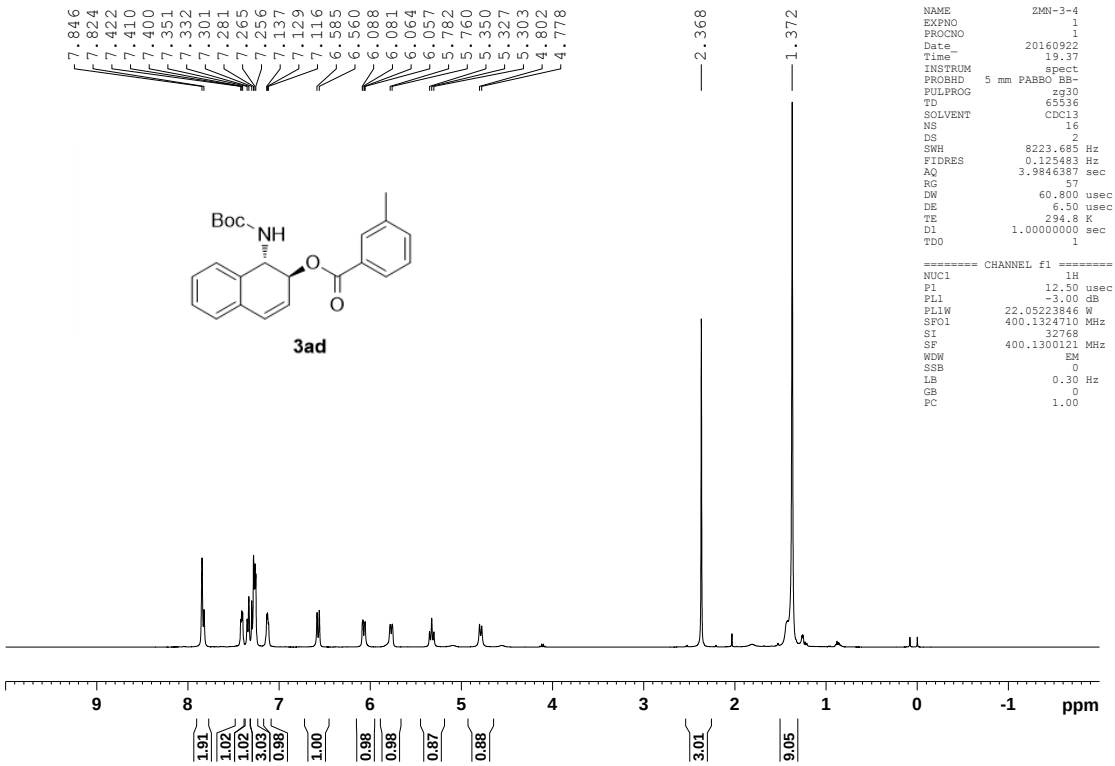
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7.137
7.129
7.116
6.585
6.560
6.088
6.081
6.064
6.057
5.782
5.760
5.350
5.327
5.303
4.802
4.778
2.368
1.372
Boc
NH
O
O
3ad
NAME ZMN-3-4
EXPNO 1
PROCNO 1
Date_ 20160922
Time_ 19.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 57
DW 60.800 usec
DE 6.50 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PL1W 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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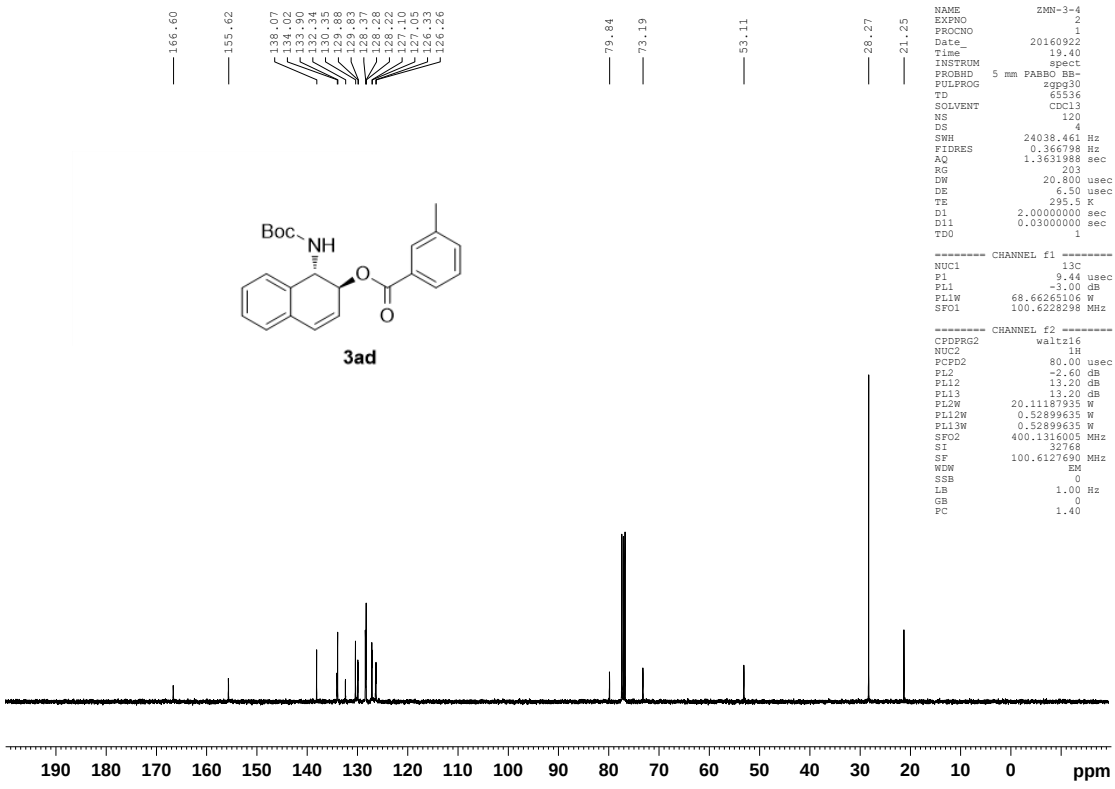
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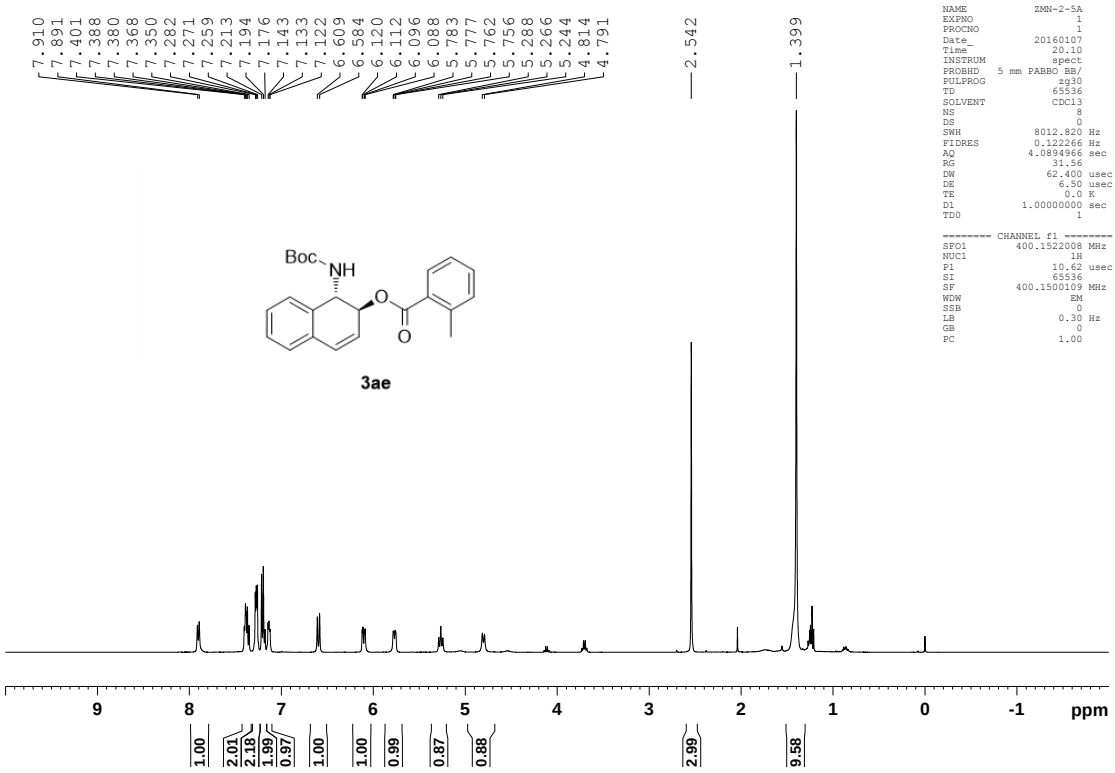
138.07
134.02
133.90
132.34
130.35
129.88
129.83
128.37
128.28
128.22
127.10
127.05
126.33
126.26
79.84
73.19
53.11
28.27
21.25
Boc
NH
O
O
3ad
NAME ZMN-3-4
EXPNO 2
PROCNO 1
Date_ 20160922
Time 19.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 120
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.44 usec
PL1 -3.00 dB
PL1W 68.66265106 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.60 dB
PL12 13.20 dB
PL13 13.20 dB
PL2W 20.11187935 W
PL12W 0.52899635 W
PL13W 0.52899635 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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7.259
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7.176
7.143
7.133
7.122
6.609
6.584
6.120
6.112
6.096
6.088
5.783
5.777
5.762
5.756
5.288
5.266
5.244
4.814
4.791
2.542
1.399
Boc
NH
O
O
3ae
NAME ZMN-2-5A
EXPNO 1
PROCNO 1
Date_ 20160107
Time_ 20.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 31.56
DW 62.400 usec
DE 6.50 usec
TE 0.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1522008 MHz
NUC1 1H
P1 10.62 usec
SI 65536
SF 400.1500109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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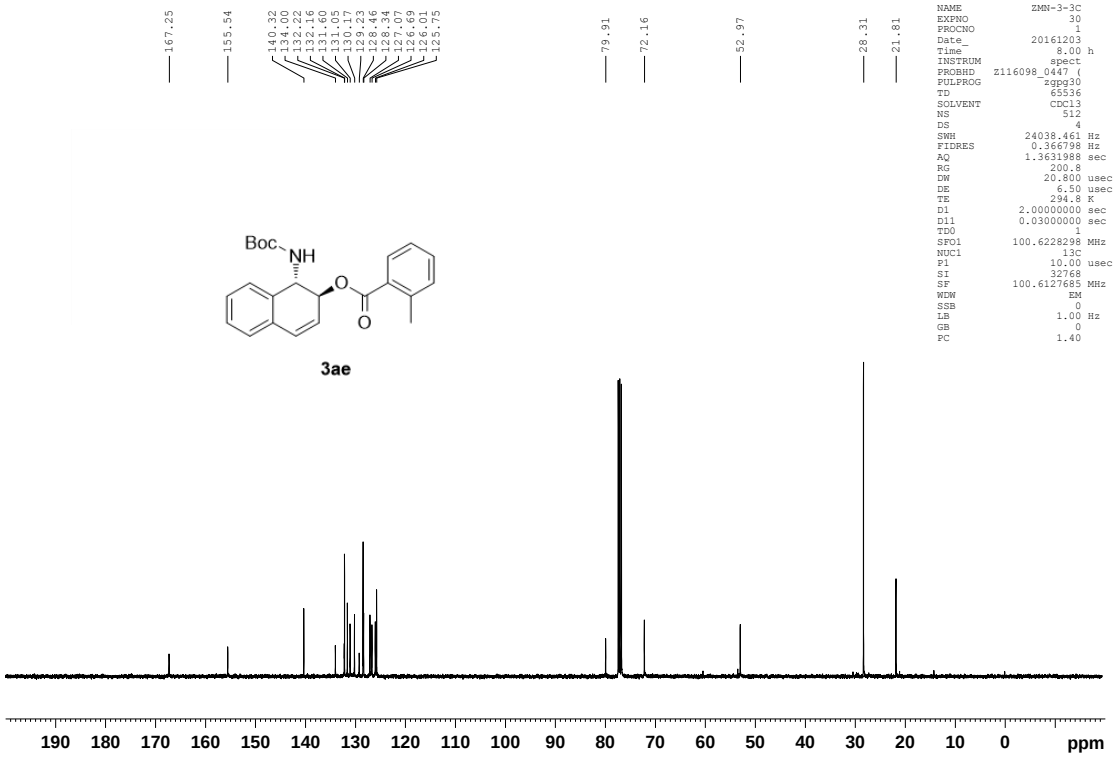
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132.16
131.60
131.55
130.17
129.23
128.46
128.34
127.07
126.69
126.01
125.75
79.91
72.16
52.97
28.31
21.81
Boc
NH
O
O
3ae
NAME ZMN-3-3C
EXPNO 30
PROCNO 1
Date_ 20161203
Time_ 8.00 h
INSTRUM spect
PROBHD Z116098_0447 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 200.8
DW 20.800 usec
DE 6.50 usec
TE 294.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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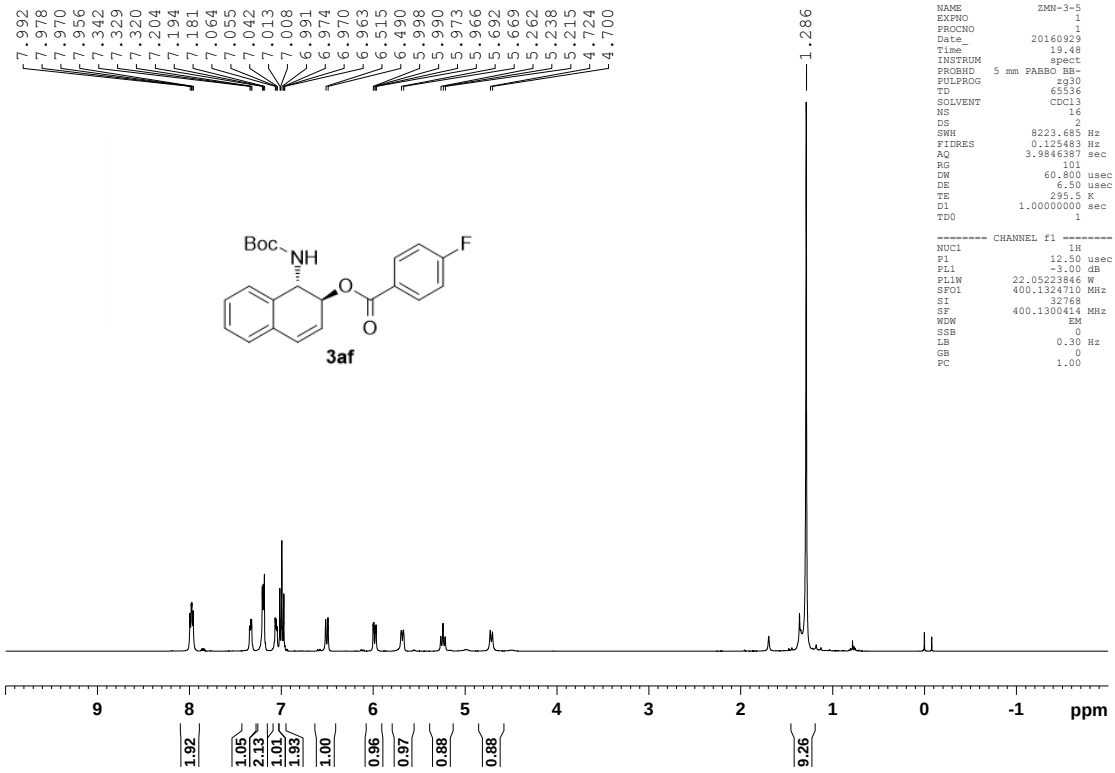
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7.042
7.013
7.008
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6.970
6.963
6.515
6.490
5.998
5.990
5.973
5.966
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5.215
4.724
4.700
1.286
Boc
NH
O
O
F
3af
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EXPNO 1
PROCNO 1
Date_ 20160929
Time 19.48
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 101
DW 60.800 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PL1W 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300414 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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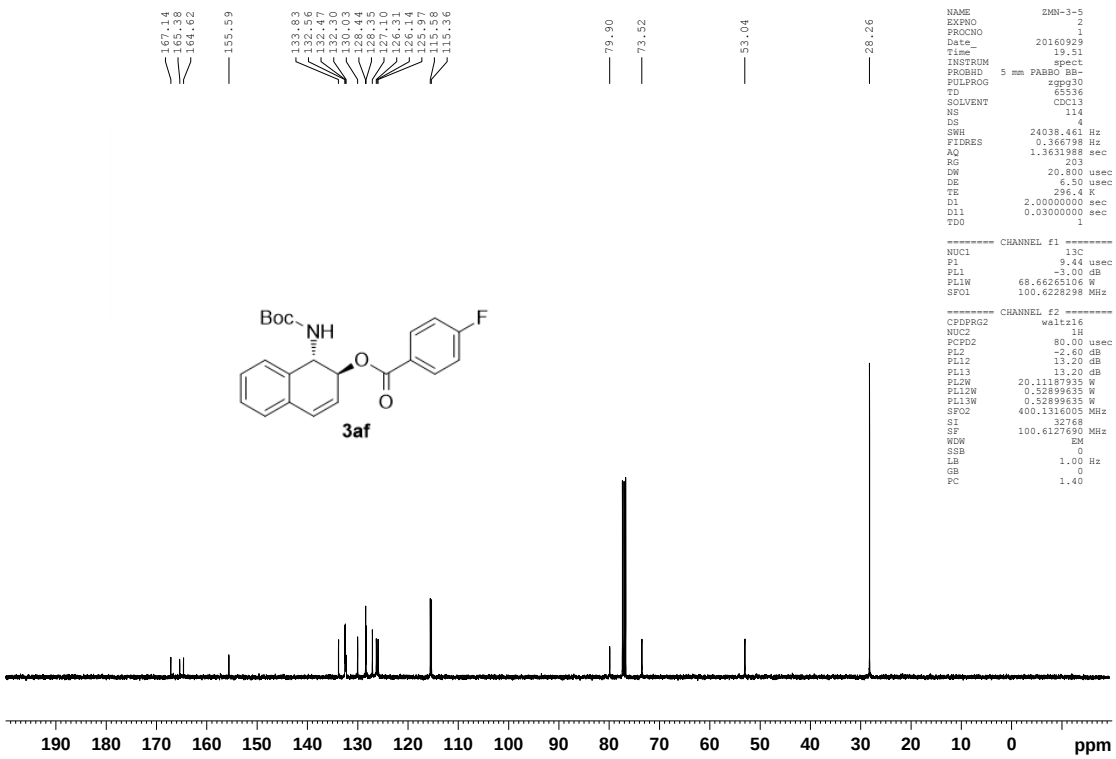
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164.62
155.59
133.83
132.56
132.47
132.30
130.03
128.44
128.35
127.10
126.31
126.14
125.97
115.58
115.36
79.90
73.52
53.04
28.26
Boc
NH
O
O
F
3af
NAME ZMN-3-5
EXPNO 2
PROCNO 1
Date_ 20160929
Time 19.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 114
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.44 usec
PL1 -3.00 dB
PL1W 68.66265106 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.60 dB
PL12 13.20 dB
PL13 13.20 dB
PL2W 20.11187935 W
PL12W 0.52899635 W
PL13W 0.52899635 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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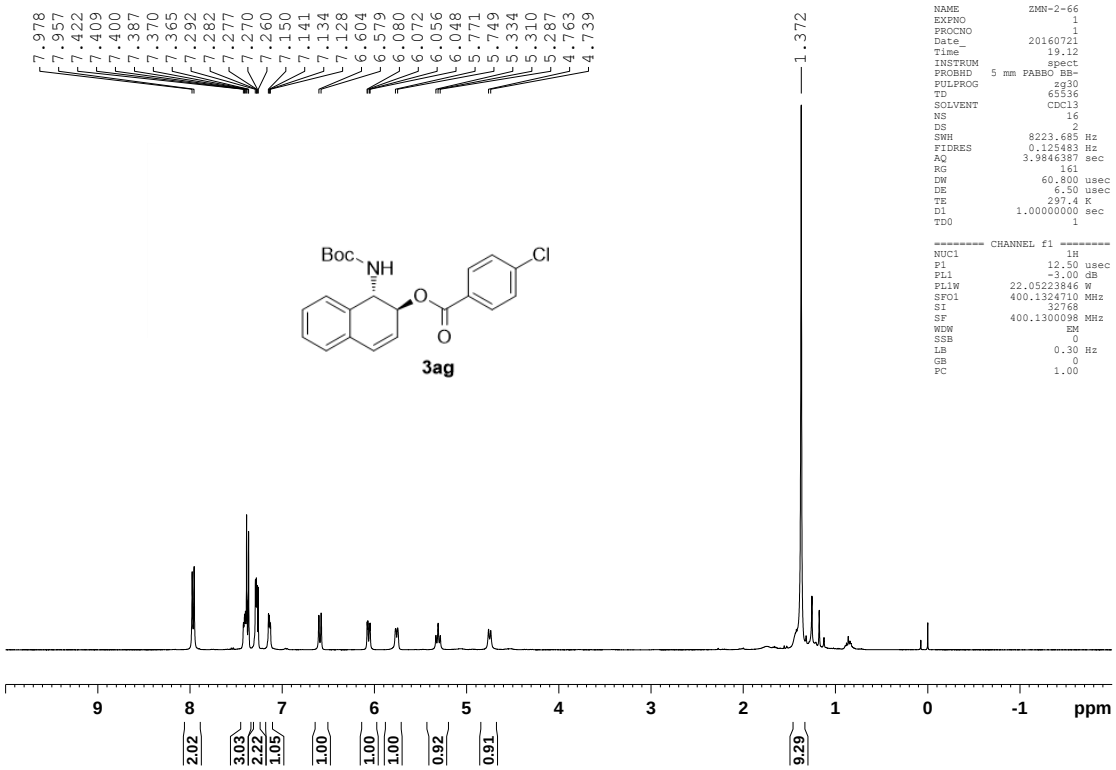
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7.422
7.409
7.400
7.387
7.370
7.365
7.292
7.282
7.277
7.270
7.260
7.150
7.141
7.134
7.128
6.604
6.579
6.080
6.072
6.056
6.048
5.771
5.749
5.334
5.310
5.287
4.763
4.739
1.372
Boc
NH
O
O
Cl
3ag
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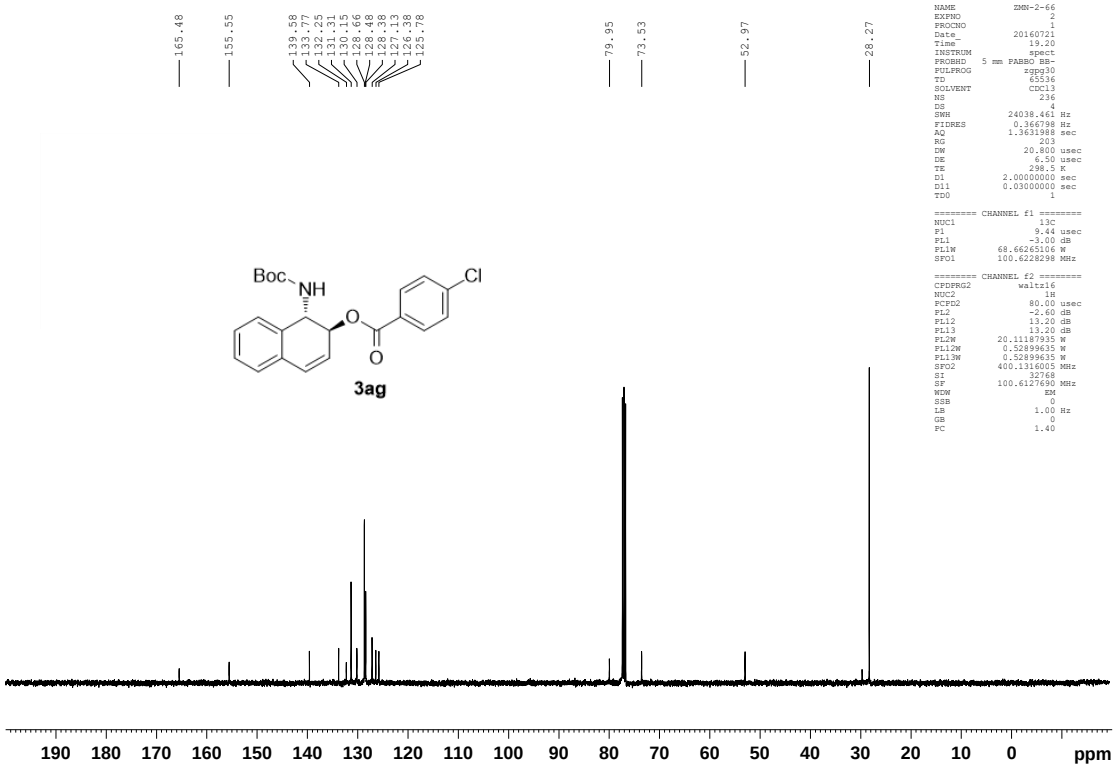
EXPNO 1
PROCNO 1
Date_ 20160721
Time 19.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PL1W 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 0 -1 ppm
2.02 3.03 2.22 1.05 1.00 1.00 1.00 0.92 0.91 9.29


165.48
155.55
139.58
133.77
132.25
131.31
130.15
128.66
128.48
128.38
127.13
126.38
125.78
79.95
73.53
52.97
28.27
Boc
NH
O
O
Cl
3ag
NAME ZMN-2-66
EXPNO 2
PROCNO 1
Date_ 20160721
Time 19.20
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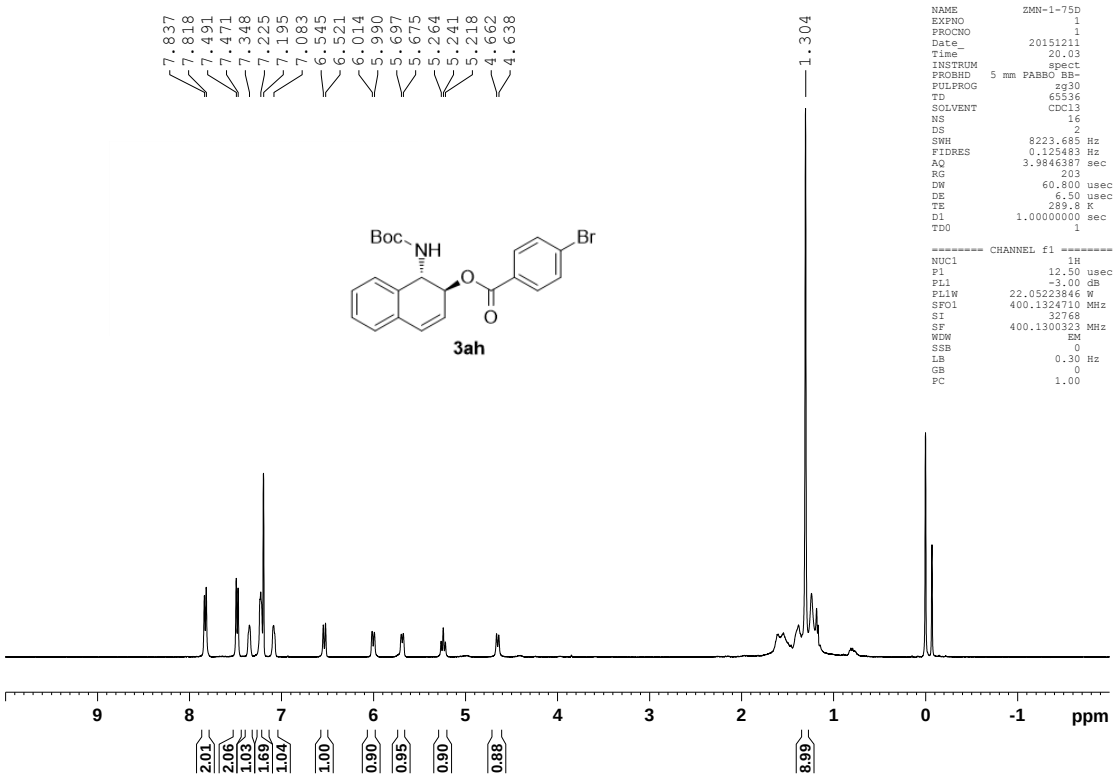
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 236
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.44 usec
PL1 -3.00 dB
PL1W 68.66265106 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.60 dB
PL12 13.20 dB
PL13 13.20 dB
PL2W 20.11187935 W
PL12W 0.52899635 W
PL13W 0.52899635 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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7.195
7.083
6.545
6.521
6.014
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5.675
5.264
5.241
5.218
4.662
4.638
1.304
Boc
NH
O
O
Br
3ah
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EXPNO 1
PROCNO 1
Date_ 20151211
Time 20.03
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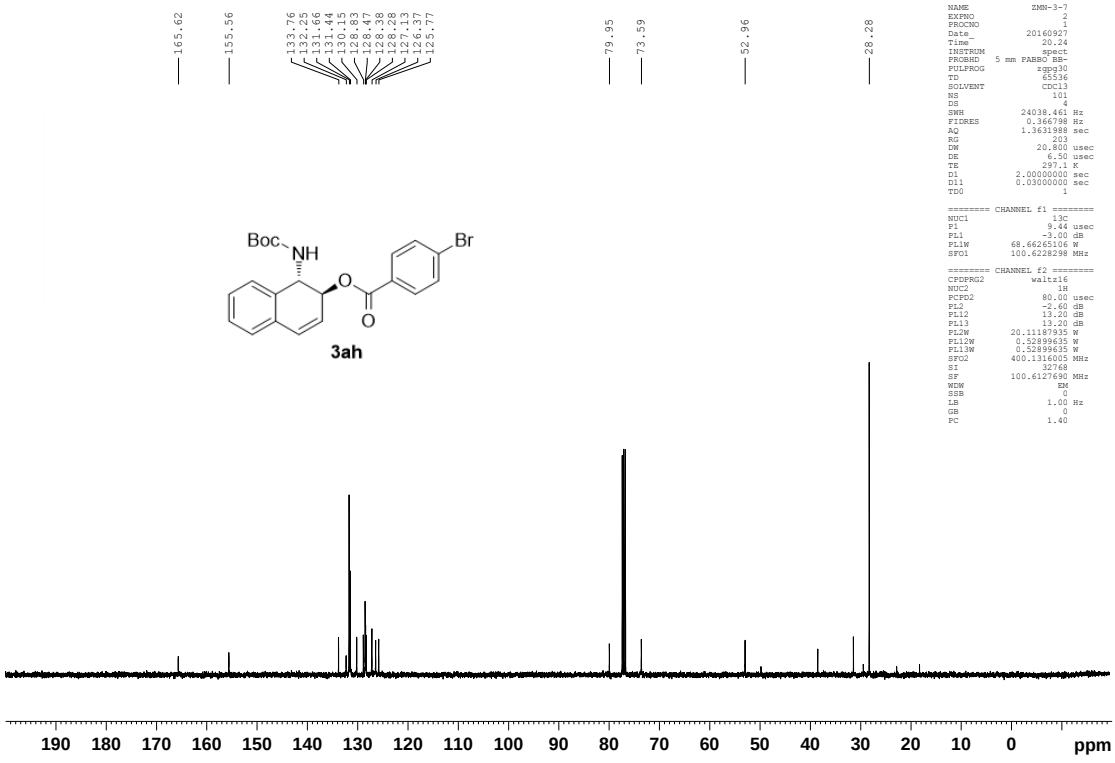
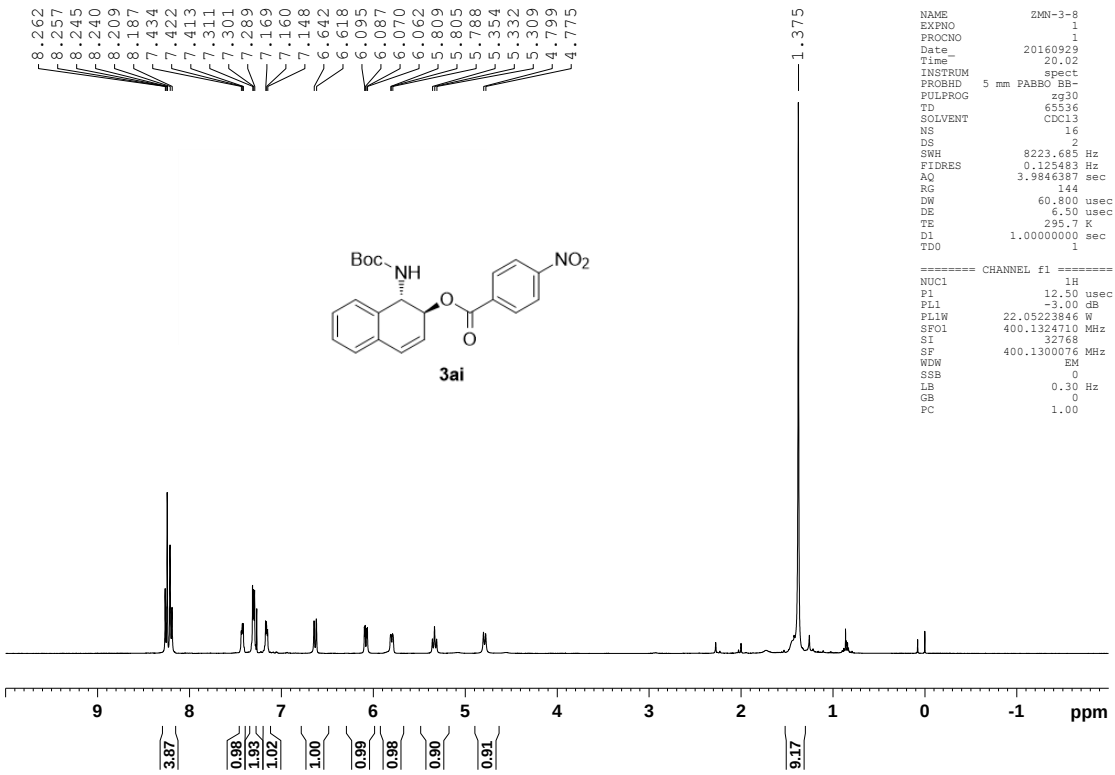
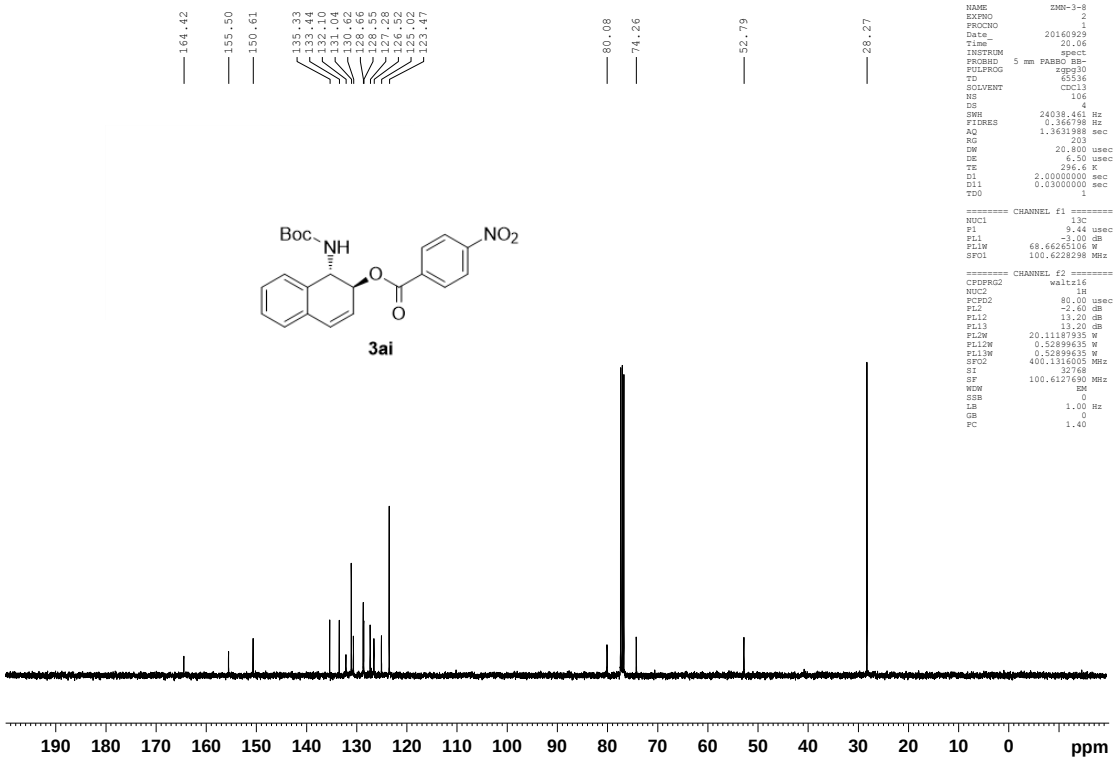
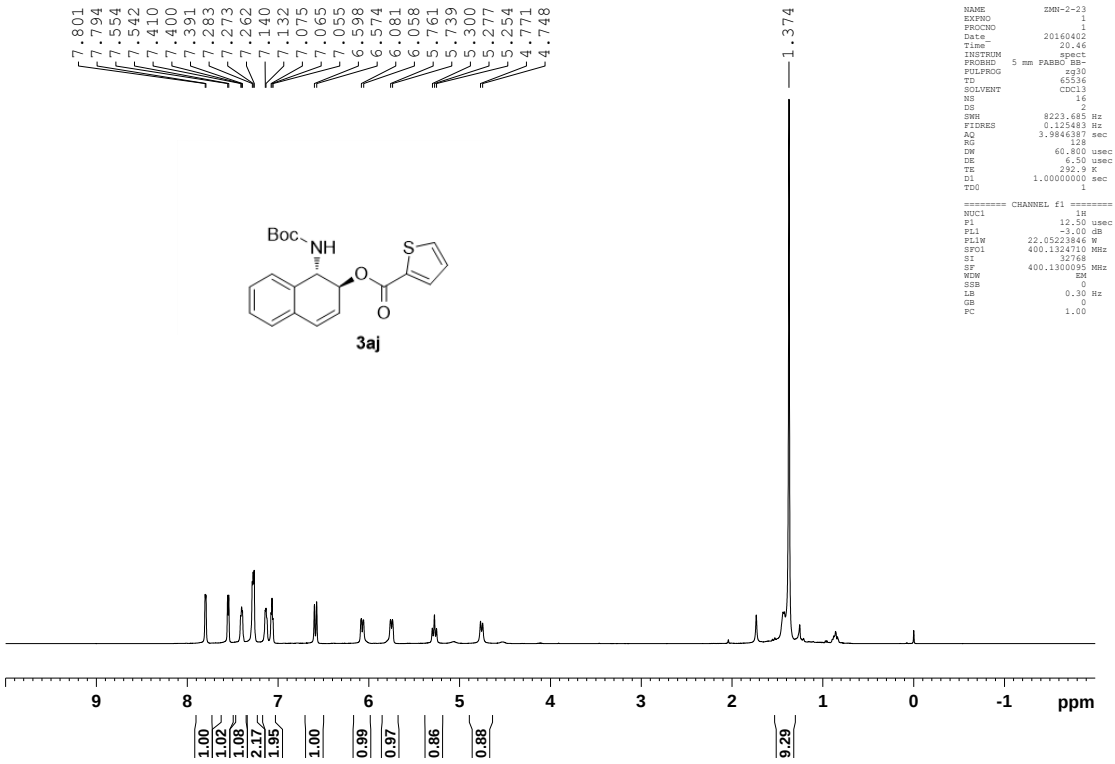
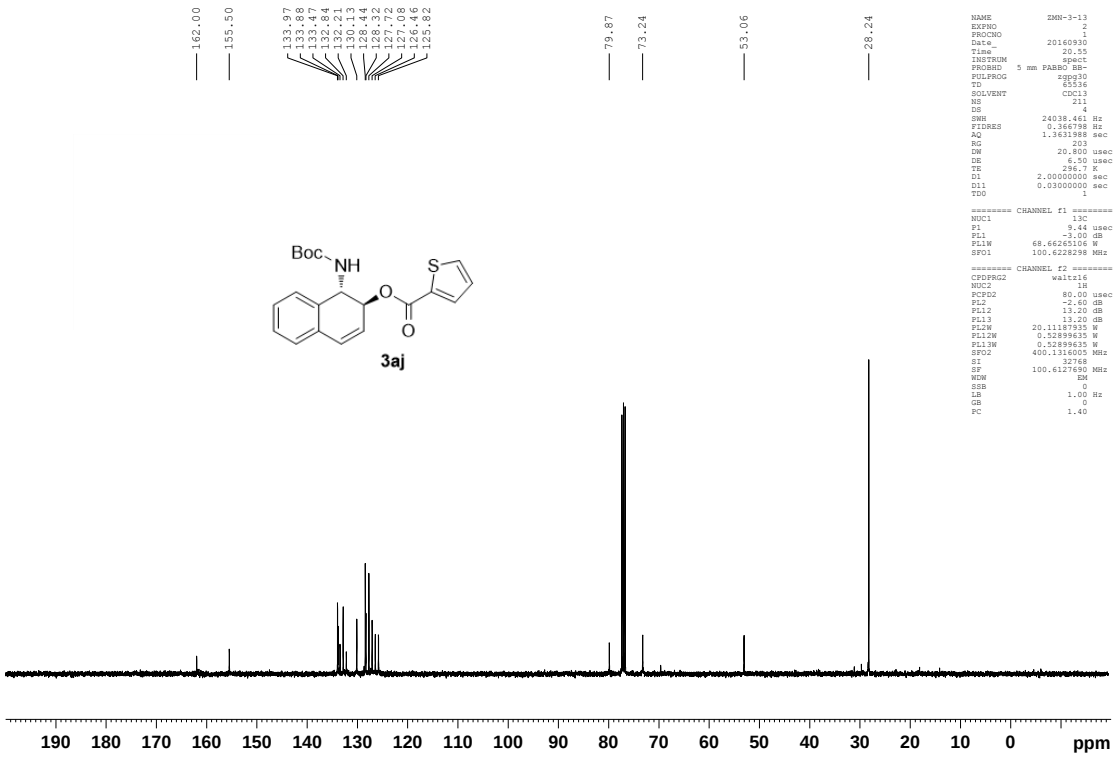
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 289.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PL1W 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300323 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
-1
ppm
2.01
2.06
1.03
1.69
1.04
1.00
0.90
0.95
0.90
0.88
8.99

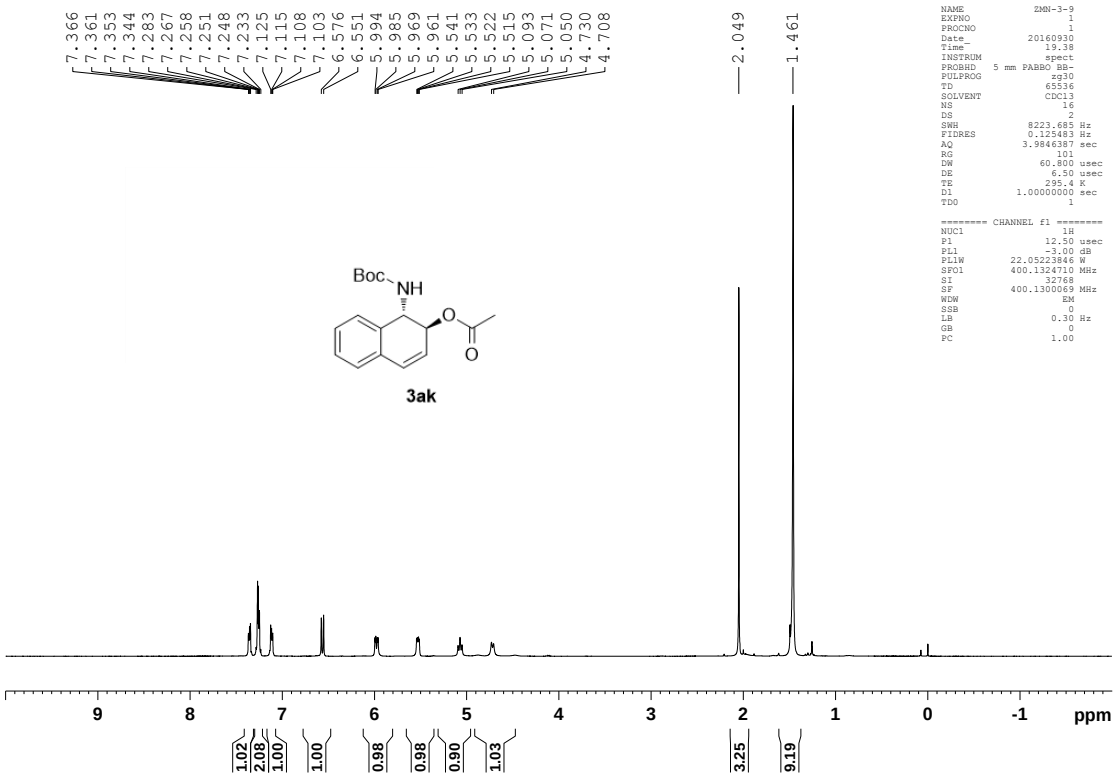

165.62
155.56
133.76
132.25
131.66
131.44
130.15
128.83
128.47
128.38
128.28
127.33
127.17
125.77
79.95
73.59
52.96
28.28
Boc
NH
O
O
Br
3ah
NAME ZMN-3-7
EXPNO 2
PROCNO 1
Date_ 20160927
Time 20.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 101
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.44 usec
PL1 -3.00 dB
PL1W 68.66265106 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.60 dB
PL12 13.20 dB
PL13 13.20 dB
PL2W 20.11187935 W
PL12W 0.52899635 W
PL13W 0.52899635 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

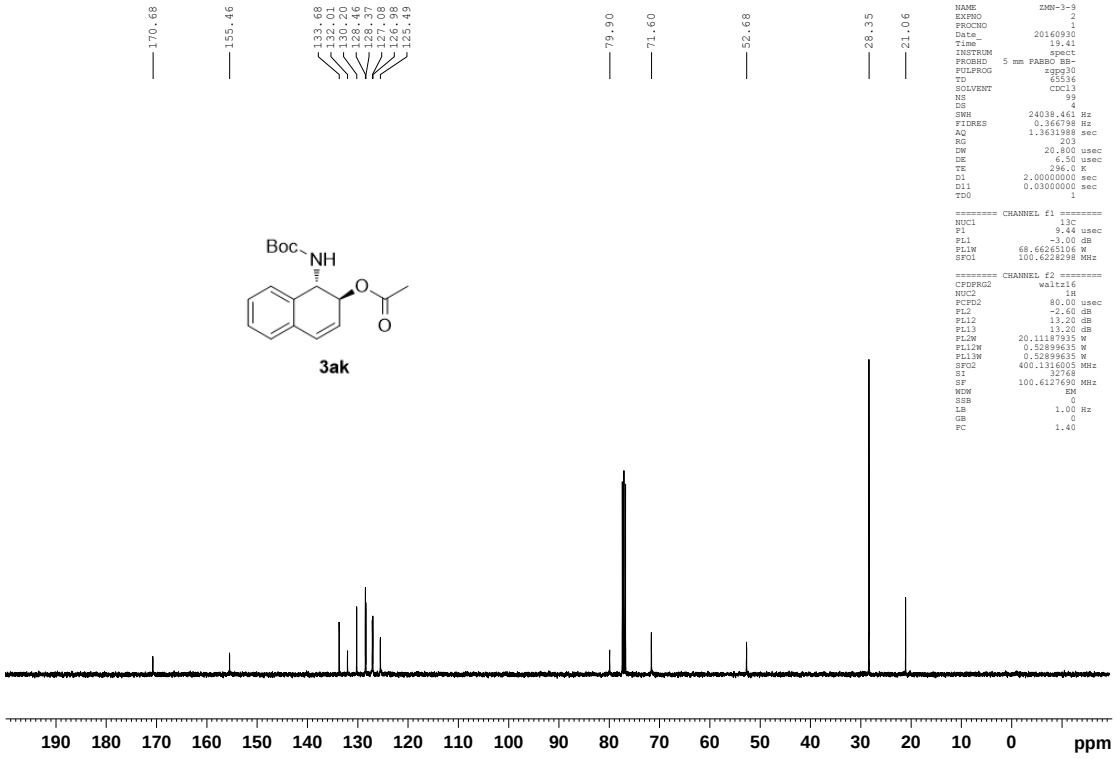

8.262
8.257
8.245
8.240
8.209
8.187
7.434
7.422
7.413
7.311
7.301
7.289
7.169
7.160
7.148
6.642
6.618
6.095
6.087
6.070
6.062
5.809
5.805
5.788
5.354
5.332
5.309
4.799
4.775
1.375
Boc
NH
O
O
NO2
3ai
NAME ZMN-3-8
EXPNO 1
PROCNO 1
Date 20160929
Time 20.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125493 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PL1W 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 0 -1 ppm
3.87 0.98 1.93 1.02 1.00 0.99 0.98 0.90 0.91 9.17

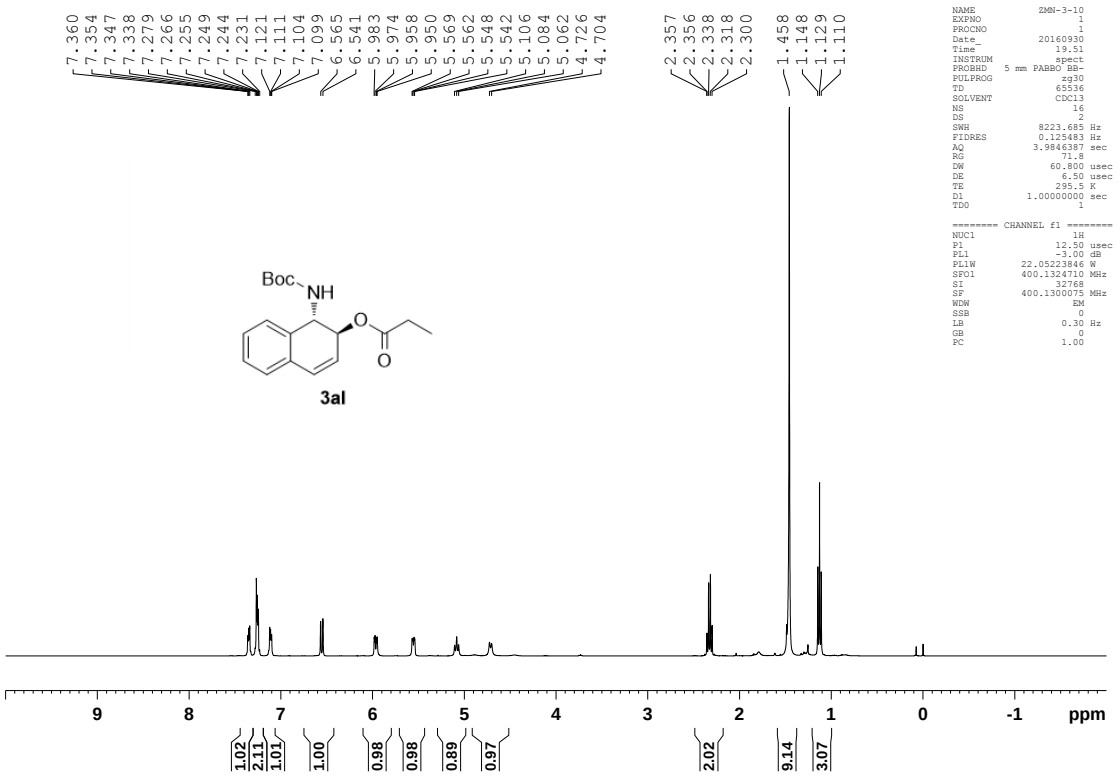

164.42
155.50
150.61
135.33
133.44
132.10
131.04
130.62
128.66
128.55
127.28
126.52
125.02
123.47
80.08
74.26
52.79
28.27
Boc
NH
O
O
NO2
3ai
NAME ZMN-3-8
EXPNO 2
PROCNO 1
Date 20160929
Time 20.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 106
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.44 usec
PL1 -3.00 dB
PL1W 68.66265106 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.60 dB
PL12 13.20 dB
PL13 13.20 dB
PL2W 20.11187935 W
PL12W 0.52899635 W
PL13W 0.52899635 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.801
7.794
7.554
7.542
7.410
7.400
7.391
7.283
7.273
7.262
7.140
7.132
7.075
7.065
7.055
6.598
6.574
6.081
6.058
5.761
5.739
5.300
5.277
5.254
4.771
4.748
1.374
Boc
NH
S
O
O
3aj
NAME ZMN-2-23
EXPNO 1
PROCNO 1
Date_ 20160402
Time 20.46
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 128
DW 60.800 usec
DE 6.50 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PL1W 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 0 -1 ppm
1.00 1.02 1.08 2.17 1.95 1.00 0.99 0.97 0.86 0.88 9.29


162.00
155.50
133.97
133.88
133.47
132.84
132.21
130.13
128.44
128.32
127.72
127.08
126.46
125.82
79.87
73.24
53.06
28.24
Boc
NH
S
O
O
3aj
NAME ZMN-3-13
EXPNO 2
PROCNO 1
Date_ 20160930
Time 20.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 211
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.44 usec
PL1 -3.00 dB
PL1W 68.66265106 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.60 dB
PL12 13.20 dB
PL13 13.20 dB
PL2W 20.11187935 W
PL12W 0.52899635 W
PL13W 0.52899635 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.366
7.361
7.353
7.344
7.283
7.267
7.258
7.251
7.248
7.233
7.125
7.115
7.108
7.103
6.576
6.551
5.994
5.985
5.969
5.961
5.541
5.533
5.522
5.515
5.093
5.071
5.050
4.730
4.708
2.049
1.461
Boc
NH
O
O
3ak
NAME ZMN-3-9
EXPNO 1
PROCNO 1
Date_ 20160930
Time 19.38
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 101
DW 60.800 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PLW 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300069 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 0 -1 ppm
1.02 2.08 1.00 1.00 0.98 0.98 0.90 1.03 3.25 9.19


170.68
155.46
133.68
132.01
130.20
128.46
128.37
127.08
126.98
125.49
79.90
71.60
52.68
28.35
21.06
Boc
NH
O
O
3ak
NAME ZMN-3-9
EXPNO 2
PROCNO 1
Date_ 20160930
Time 19.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 99
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
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 9.44 usec
PL1 -3.00 dB
PLW 68.66265106 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.60 dB
PL12 13.20 dB
PL13 13.20 dB
PL2W 20.11187935 W
PL12W 0.52899635 W
PL13W 0.52899635 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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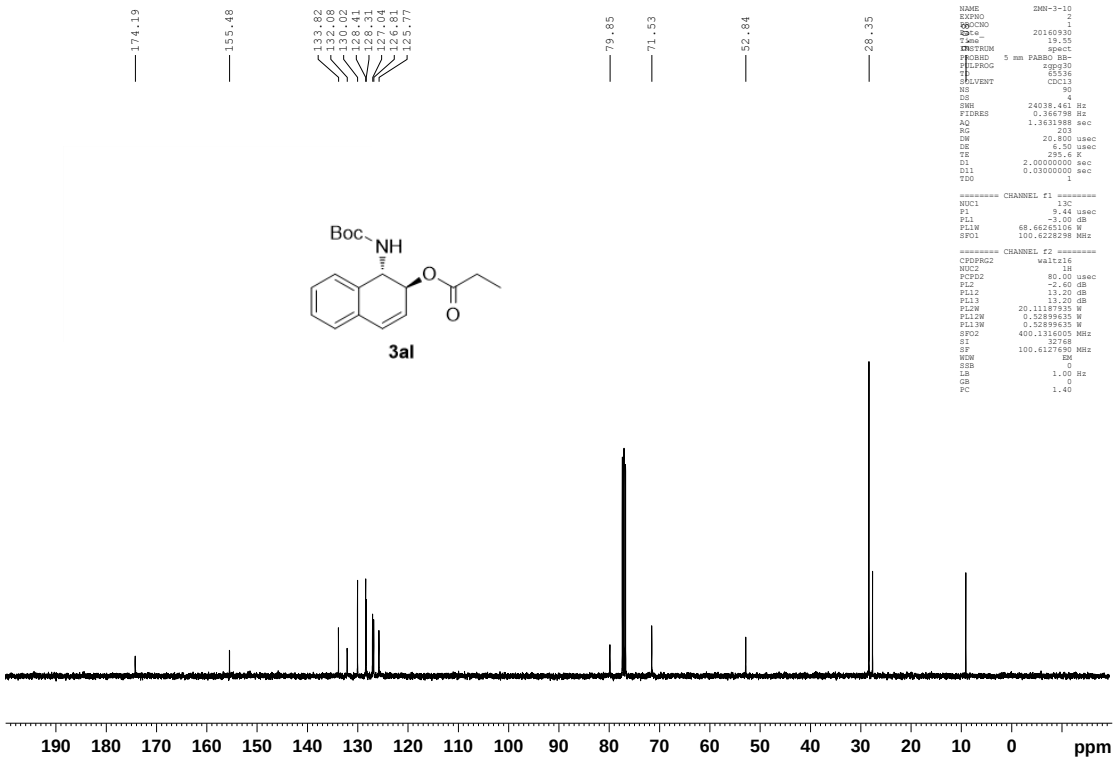
7.347
7.338
7.279
7.266
7.255
7.249
7.244
7.231
7.121
7.111
7.104
7.099
6.565
6.541
5.983
5.974
5.958
5.950
5.569
5.562
5.548
5.542
5.106
5.084
5.062
4.726
4.704
2.357
2.356
2.338
2.318
2.300
1.458
1.148
1.129
1.110
Boc
NH
O
O
3al
NAME ZMN-3-10
EXPNO 1
PROCNO 1
Date_ 20160930
Time 19.51
INSTRUM spect
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 71.8
DW 60.800 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PL1W 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
-1
ppm
1.02
2.11
1.01
1.00
0.98
0.98
0.89
0.97
2.02
9.14
3.07


174.19
155.48
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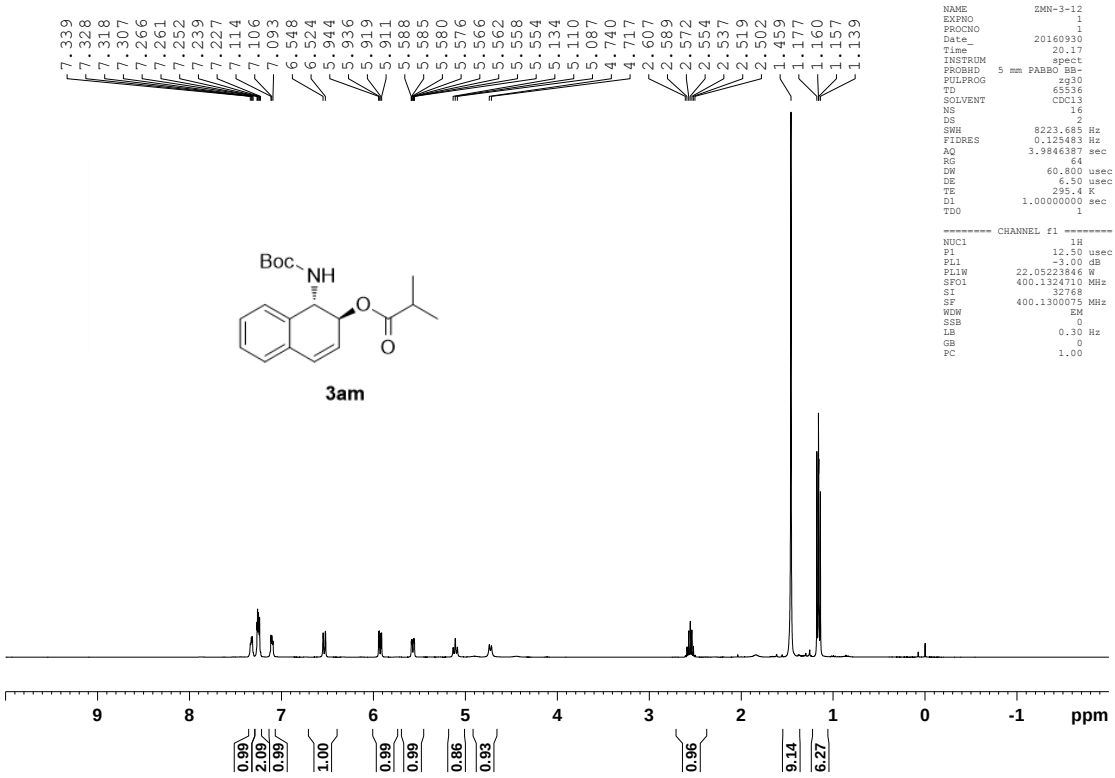
132.08
130.02
128.41
128.31
127.04
126.81
125.77
79.85
71.53
52.84
28.35
Boc
NH
O
O
3al
NAME ZMN-3-10
EXPNO 2
PROCNO 1
Date_ 20160930
Time 19.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 90
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.44 usec
PL1 -3.00 dB
PL1W 68.66265106 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.60 dB
PL12 13.20 dB
PL13 13.20 dB
PL2W 20.11187935 W
PL12W 0.52899635 W
PL13W 0.52899635 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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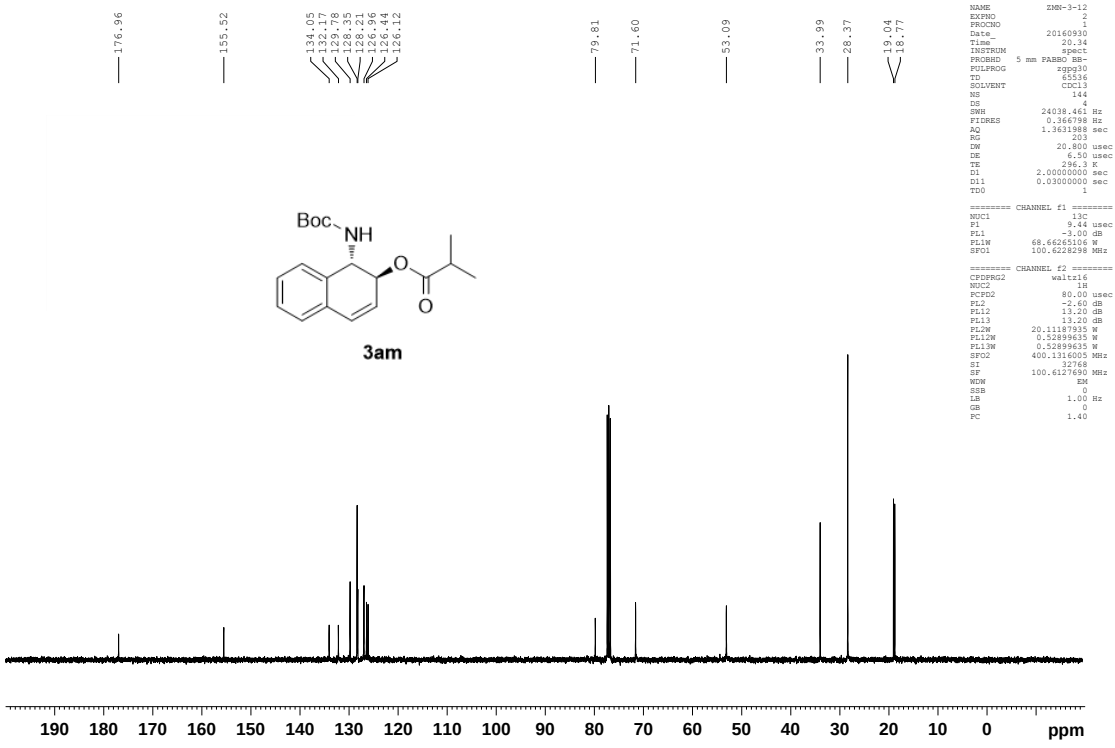
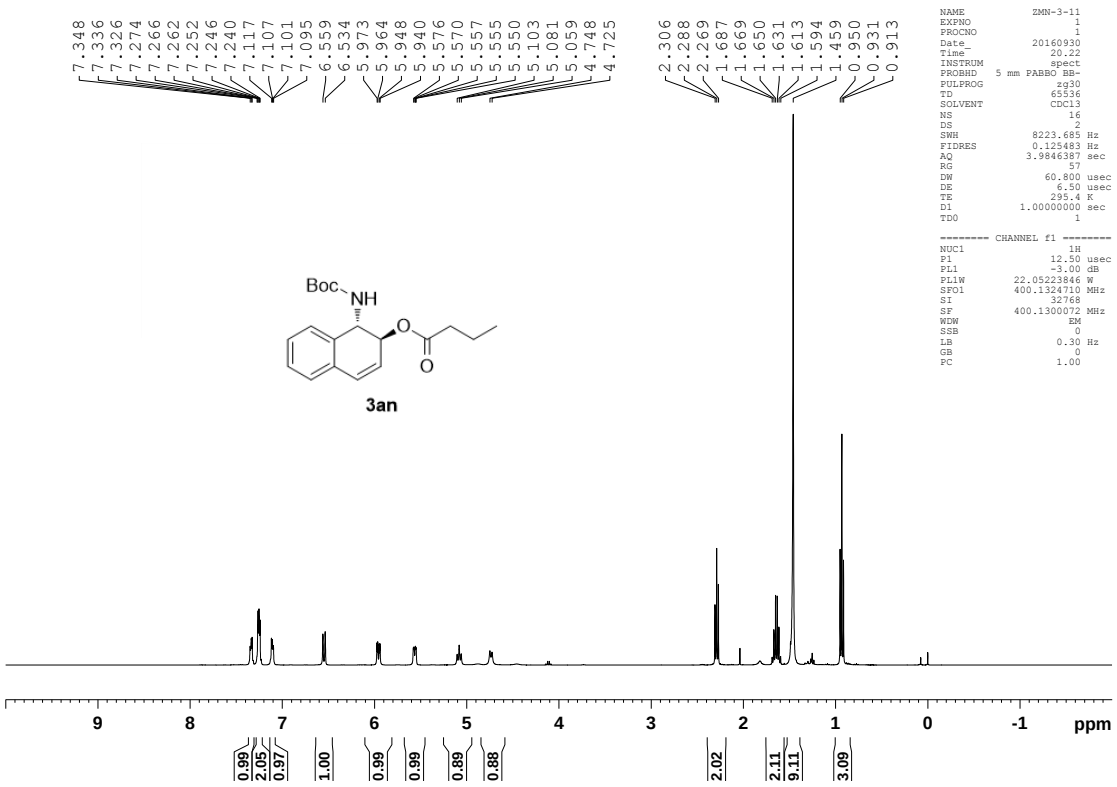
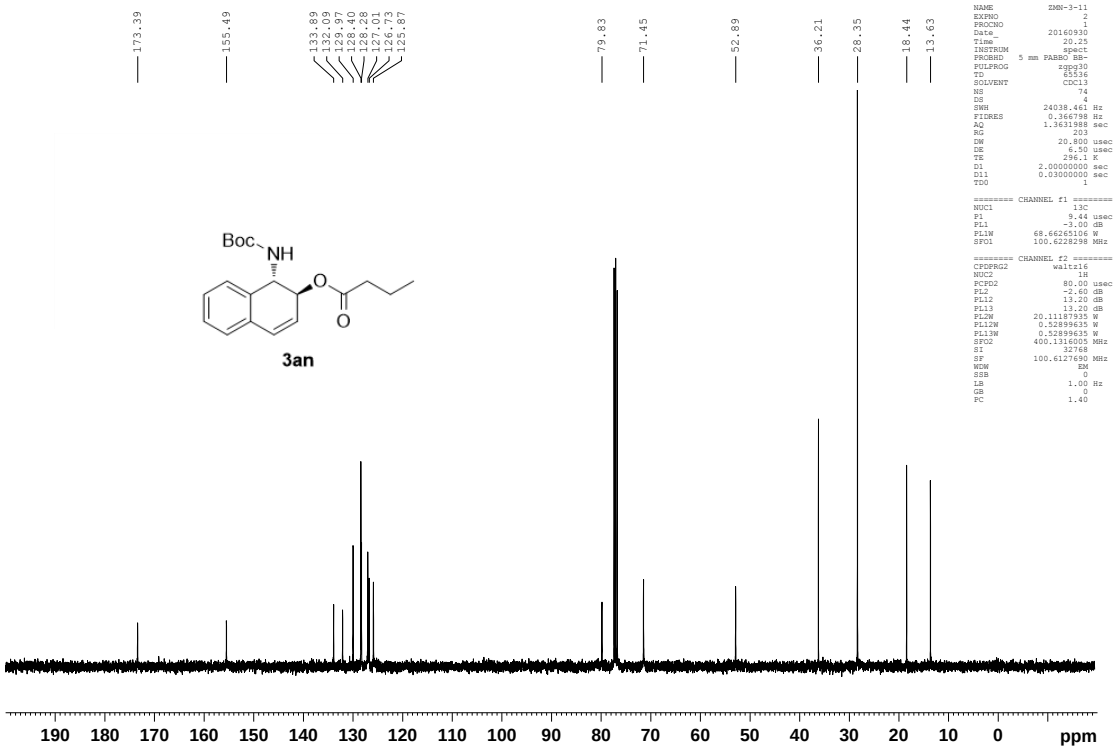
7.318
7.307
7.266
7.261
7.252
7.239
7.227
7.114
7.106
7.093
6.548
6.524
5.944
5.936
5.919
5.911
5.588
5.585
5.580
5.576
5.566
5.562
5.558
5.554
5.134
5.110
5.087
4.740
4.717
2.607
2.589
2.572
2.554
2.537
2.519
2.502
1.459
1.177
1.160
1.157
1.139
Boc
NH
O
O
3am
NAME ZMN-3-12
EXPNO 1
PROCNO 1
Date_ 20160930
Time 20.17
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 64
DW 60.800 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PL1W 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
-1
ppm
0.99
2.09
0.99
1.00
0.99
0.99
0.86
0.93
0.96
9.14
6.27


176.96
155.52
134.05
132.17
128.38
128.35
126.21
126.96
126.44
126.12
79.81
71.60
53.09
33.99
28.37
19.04
18.77
Boc
NH
O
O
3am
NAME ZMN-3-12
EXPNO 2
PROCNO 1
Date_ 20160930
Time 20.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 144
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.44 usec
PL1 -3.00 dB
PL1W 68.66265106 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.60 dB
PL12 13.20 dB
PL13 13.20 dB
PL2W 20.11197935 W
PL12W 0.52899635 W
PL13W 0.52899635 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.348
7.336
7.326
7.274
7.266
7.262
7.252
7.246
7.240
7.117
7.107
7.101
7.095
6.559
6.534
5.973
5.964
5.948
5.940
5.576
5.570
5.557
5.555
5.550
5.103
5.081
5.059
4.748
4.725
2.306
2.288
2.269
1.687
1.669
1.650
1.631
1.613
1.594
1.459
0.950
0.931
0.913
Boc
NH
O
O
3an
NAME ZMN-3-11
EXPNO 1
PROCNO 1
Date_ 20160930
Time_ 20.22
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 57
DW 60.800 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PL1W 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 0 -1 ppm
0.99 2.05 0.97 1.00 0.99 0.99 0.89 0.88 2.02 2.11 9.11 3.09


173.39
155.49
133.89
132.09
129.97
128.40
128.28
128.01
126.73
125.87
79.83
71.45
52.89
36.21
28.35
18.44
13.63
Boc
NH
O
O
3an
NAME ZMN-3-11
EXPNO 2
PROCNO 1
Date_ 20160930
Time 20.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 74
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.44 usec
PL1 -3.00 dB
PL1W 68.66265106 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.60 dB
PL12 13.20 dB
PL13 13.20 dB
PL2W 20.11187935 W
PL12W 0.52899635 W
PL13W 0.52899635 W
SFO2 400.1316005 MHz
SI 32768
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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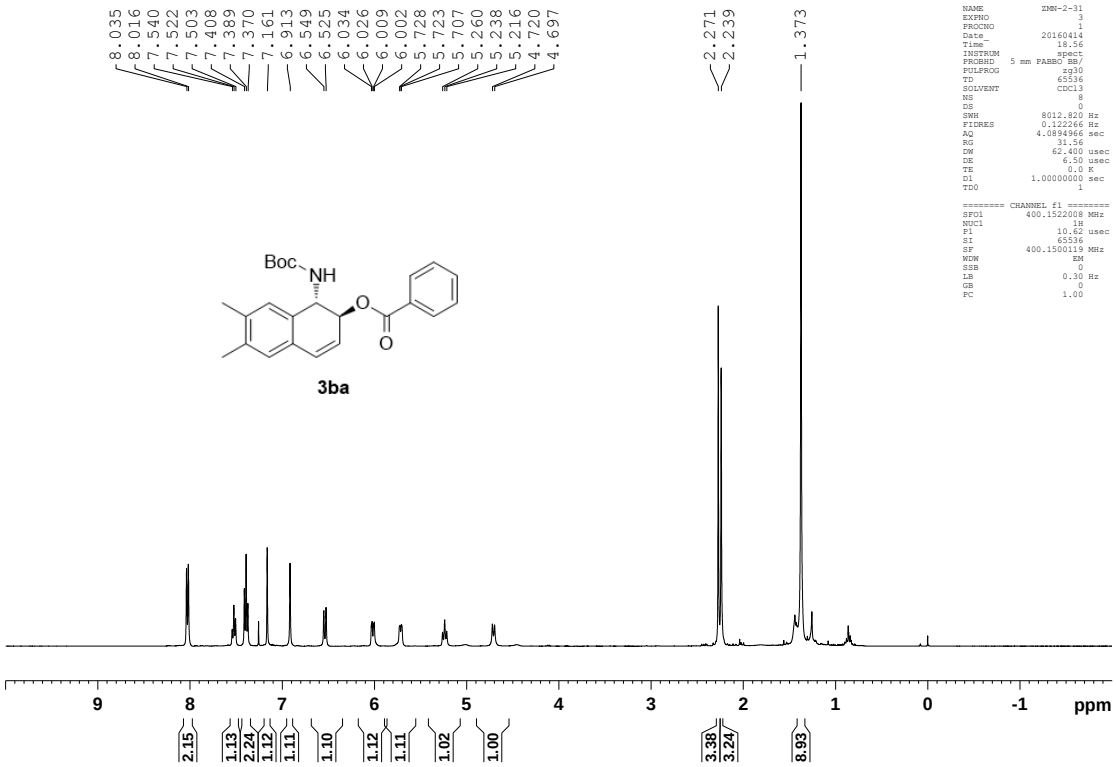
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4
3
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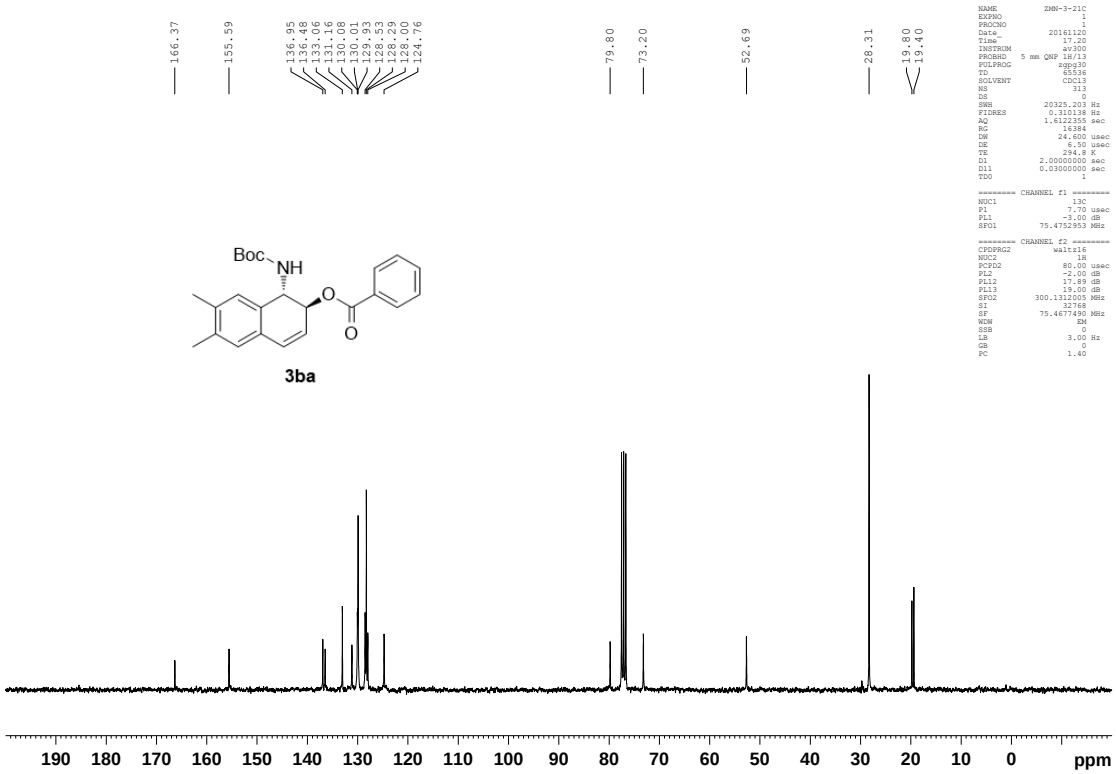
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19.80
19.40
Boc
NH
O
O
3ba
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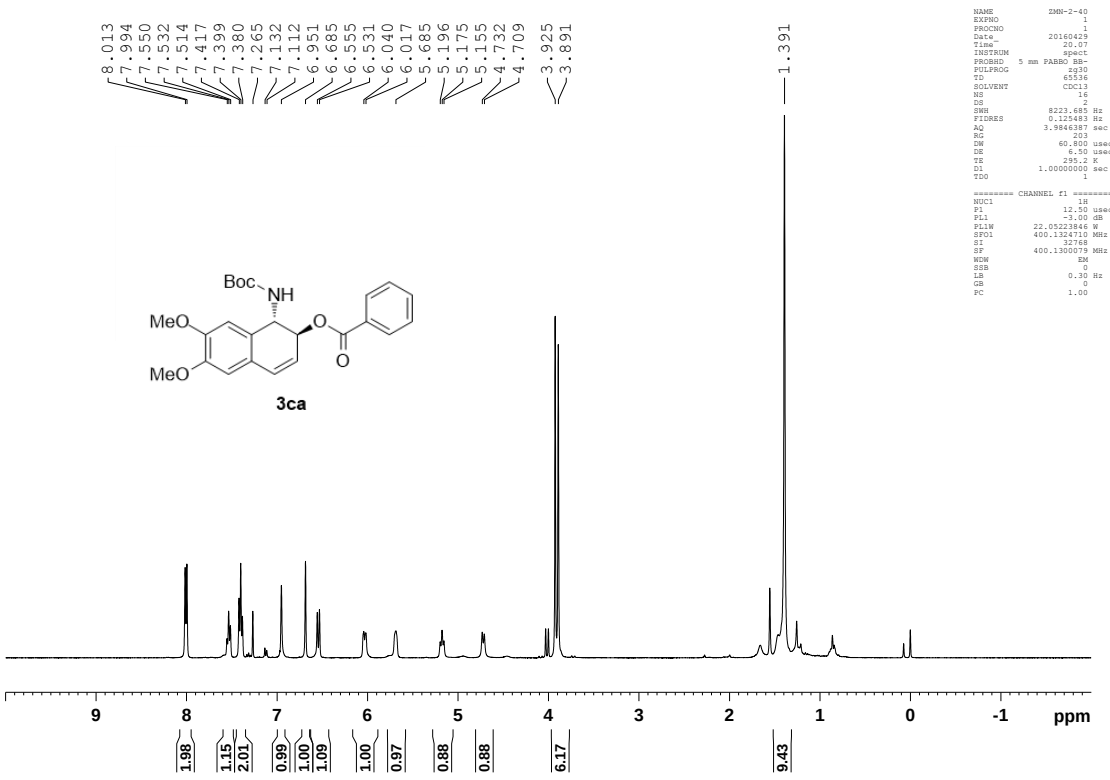
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Boc
NH
MeO
MeO
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O
3ca
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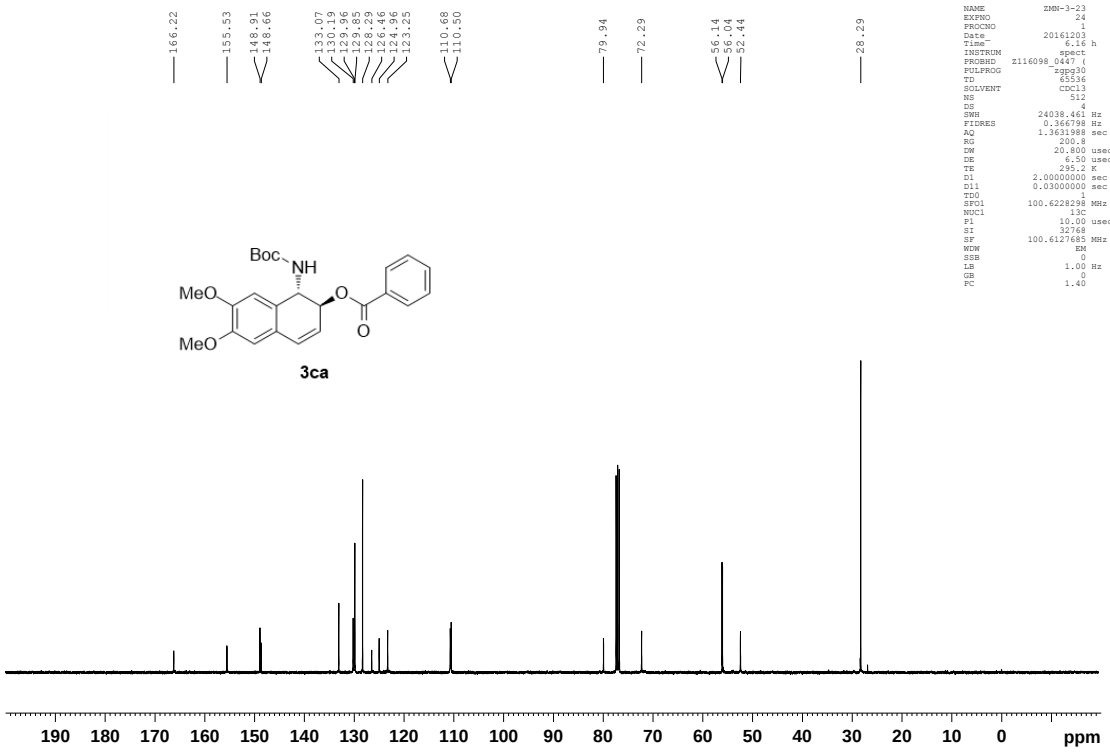
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NH
MeO
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O
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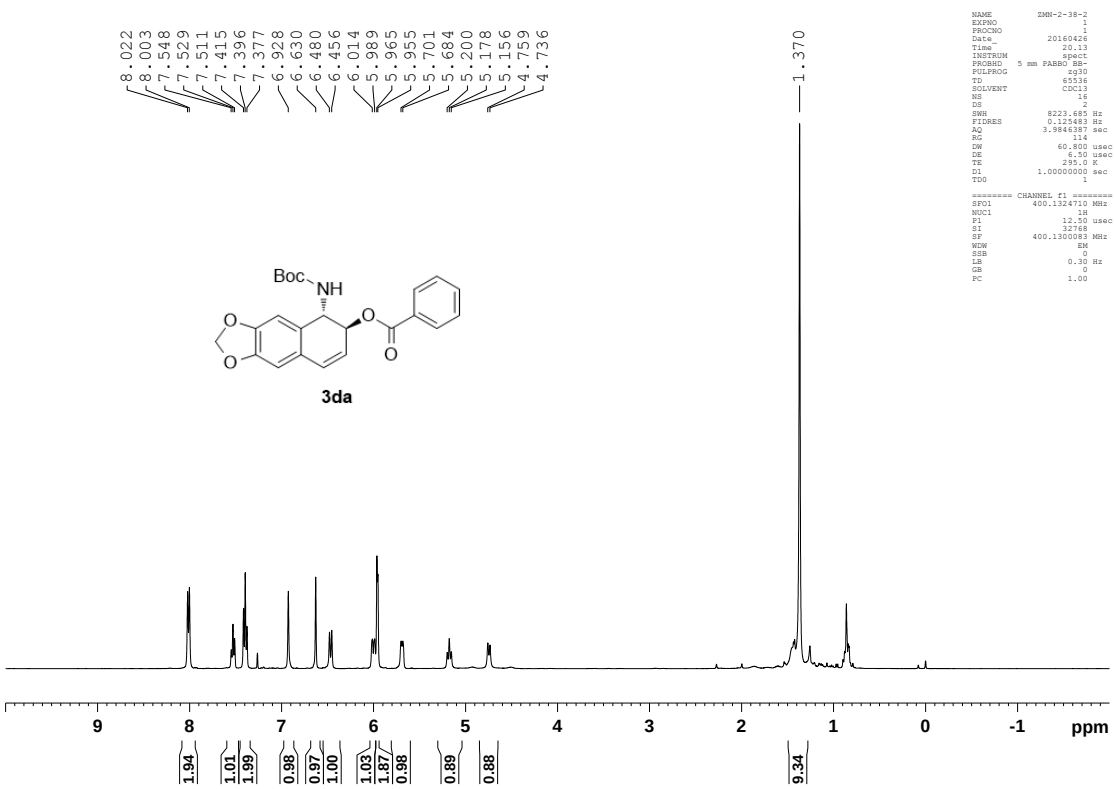
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5.156
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O
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5
4
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2
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-1
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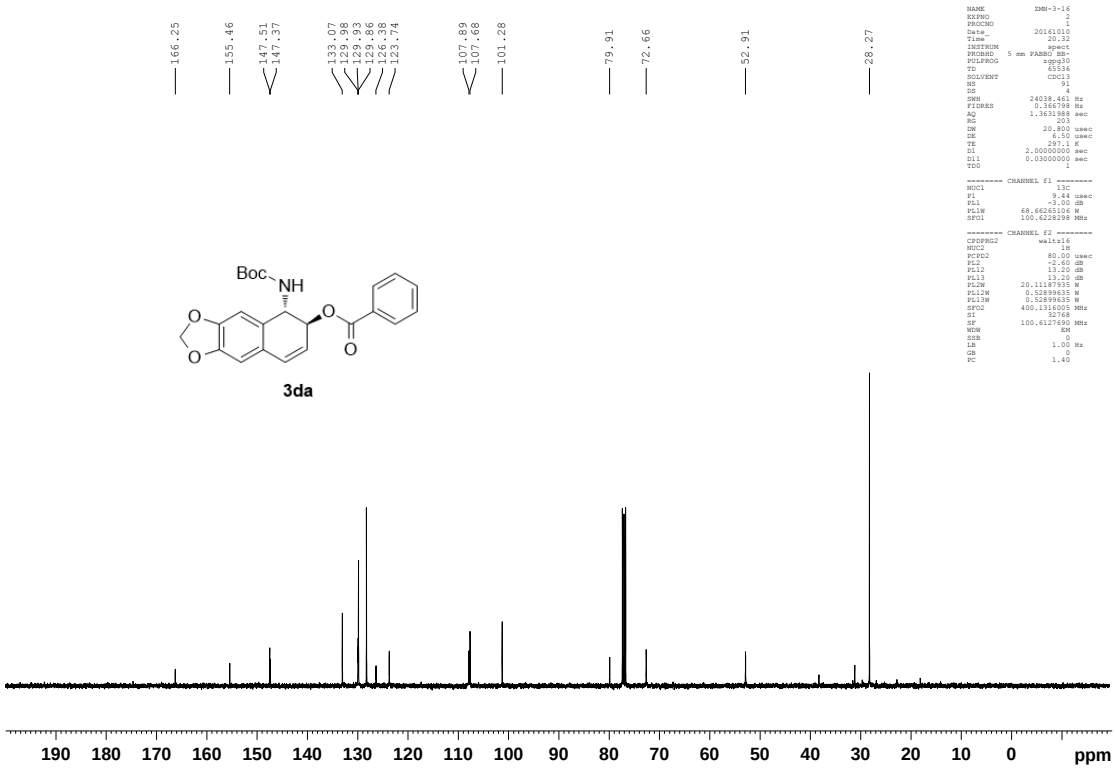
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52.91
28.27
Boc
NH
O
O
O
O
3da
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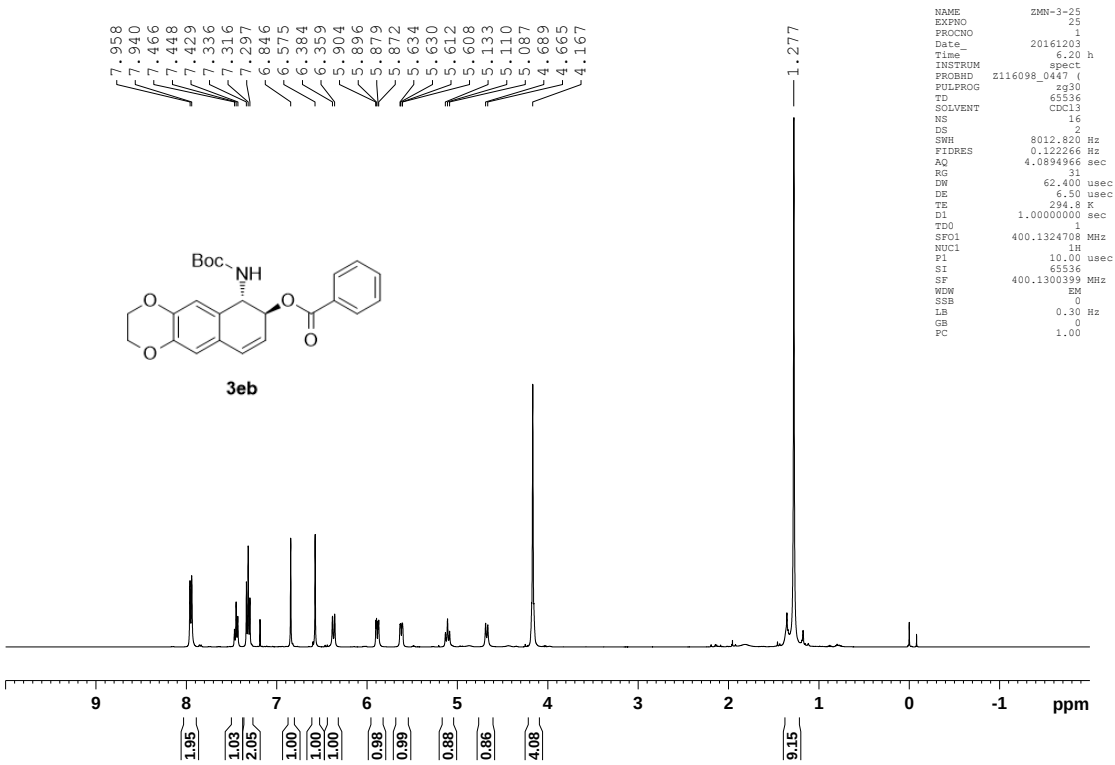
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5.608
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Boc
NH
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O
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5
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-1
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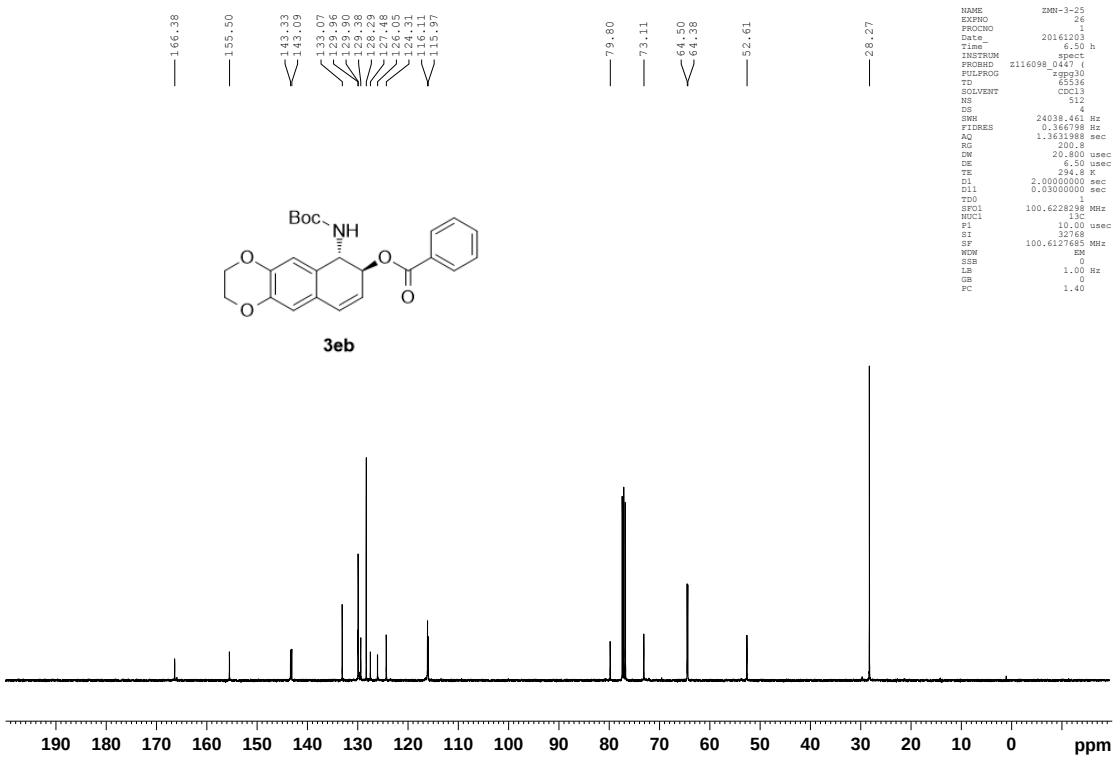
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O
O
O
3eb
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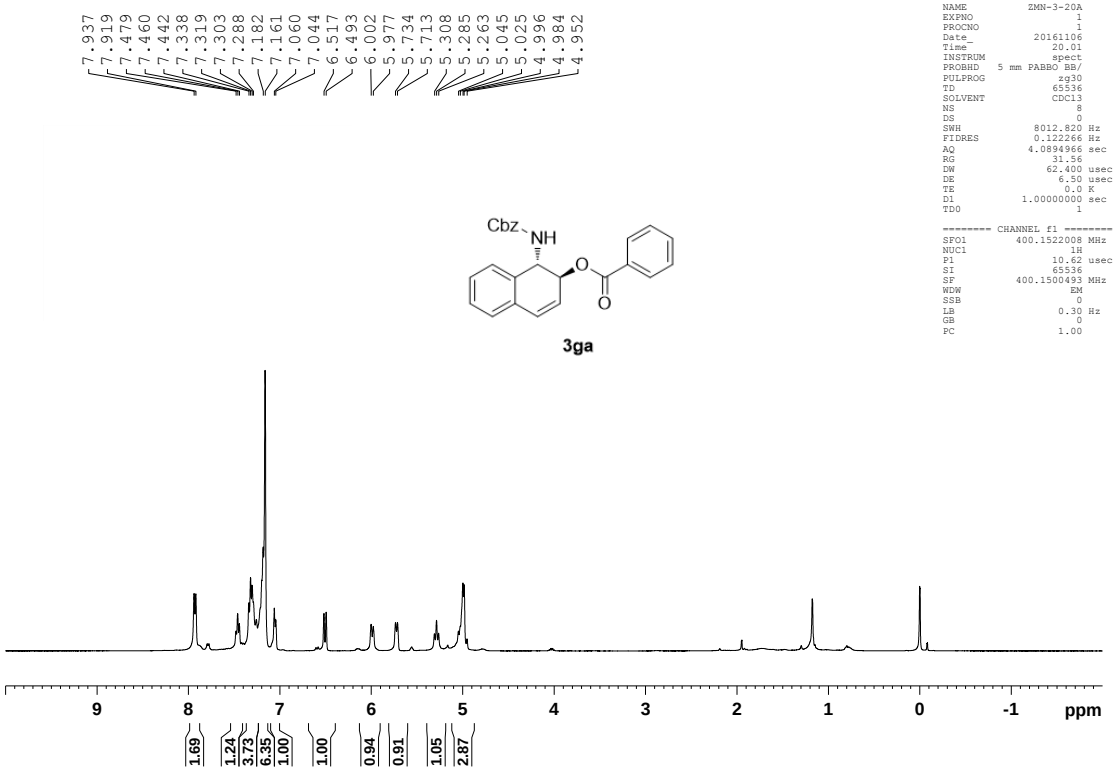
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Time_ 20.01
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SOLVENT CDCl3
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SWH 8012.820 Hz
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AQ 4.0894966 sec
RG 31.56
DW 62.400 usec
DE 6.50 usec
TE 0.0 K
D1 1.00000000 sec
TD0 1
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SFO1 400.1522008 MHz
NUC1 1H
P1 10.62 usec
SI 65536
SF 400.1500493 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Cbz
NH
O
O
3ga
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8
7
6
5
4
3
2
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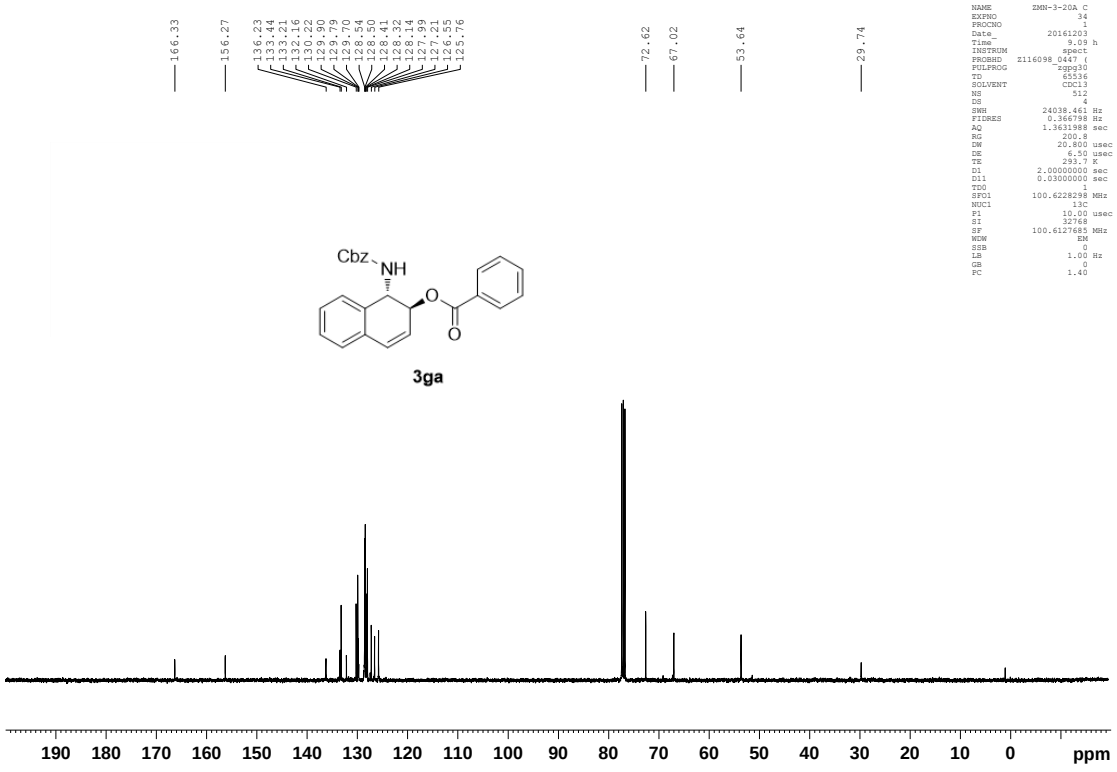
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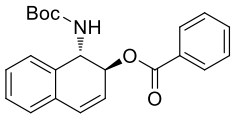
Part II HPLC spectra



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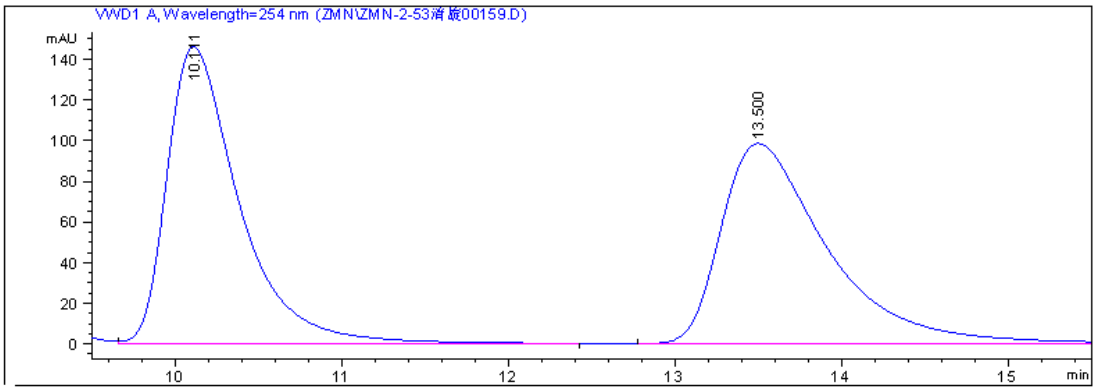
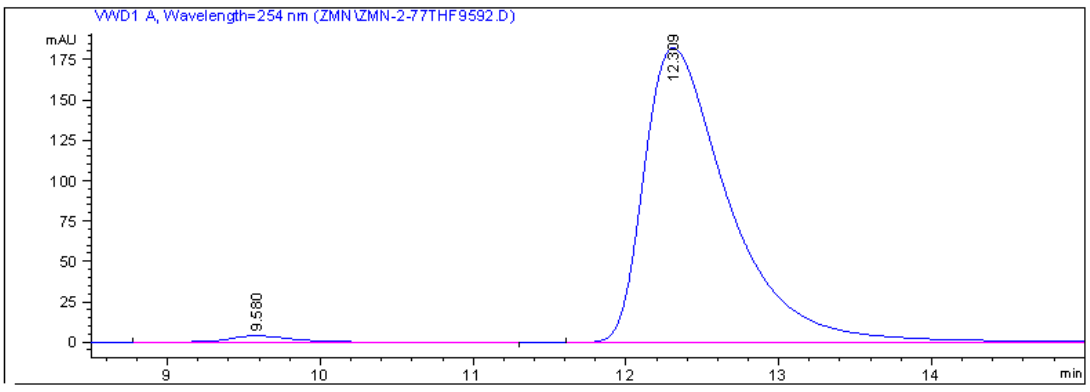
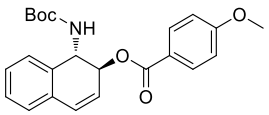


Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.111 VB	0.4527	4406.02979	146.15564	50.0647
2	13.500 BB	0.6659	4394.63867	98.43069	49.9353



Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.580 BB	0.4495	118.50734	3.91163	1.6547
2	12.309 BBA	0.5796	7043.33447	182.36887	98.3453



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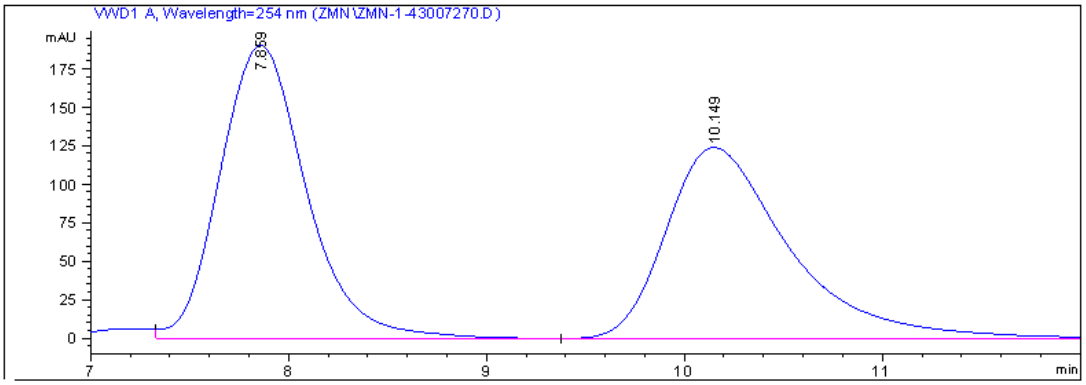
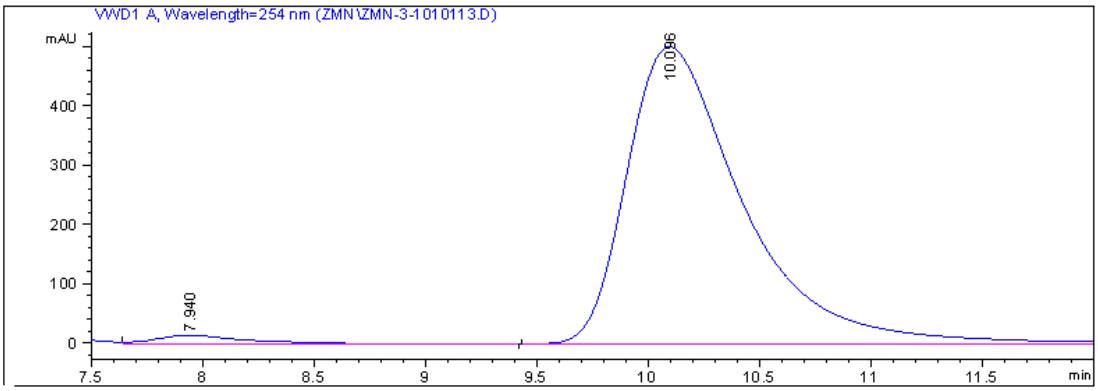
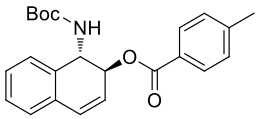


Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.859 VB	0.4725	5790.47705	190.55469	51.3996
2	10.149 BB	0.6587	5475.13525	124.34626	48.6004



Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.940 VB	0.4001	398.76794	14.30895	2.1199
2	10.096 BB	0.5516	1.84123e4	499.97595	97.8801



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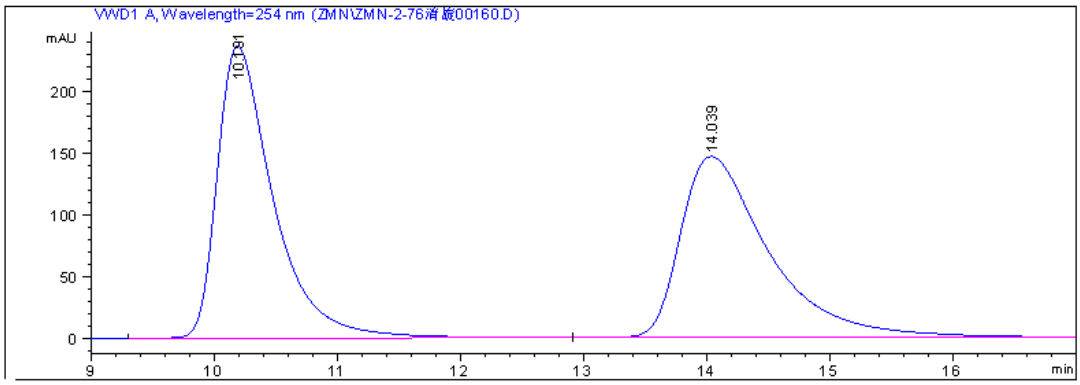
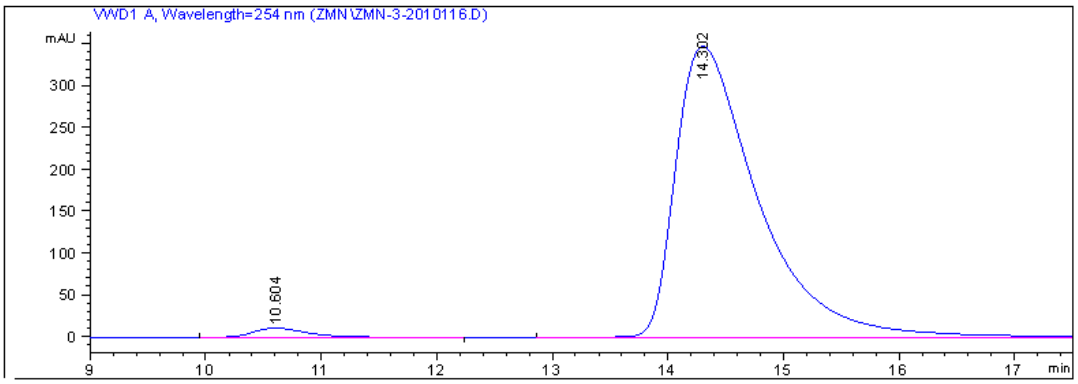
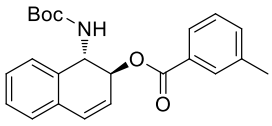


Peak #	RetTime Type [min]		Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.191	BB	0.4734	7500.10938	236.87837	50.2214
2	14.039	BB	0.7532	7433.96826	146.94327	49.7786



Peak #	RetTime Type [min]		Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.604	BB	0.4933	359.52988	10.94276	2.0236
2	14.302	BB	0.7473	1.74071e4	348.14319	97.9764



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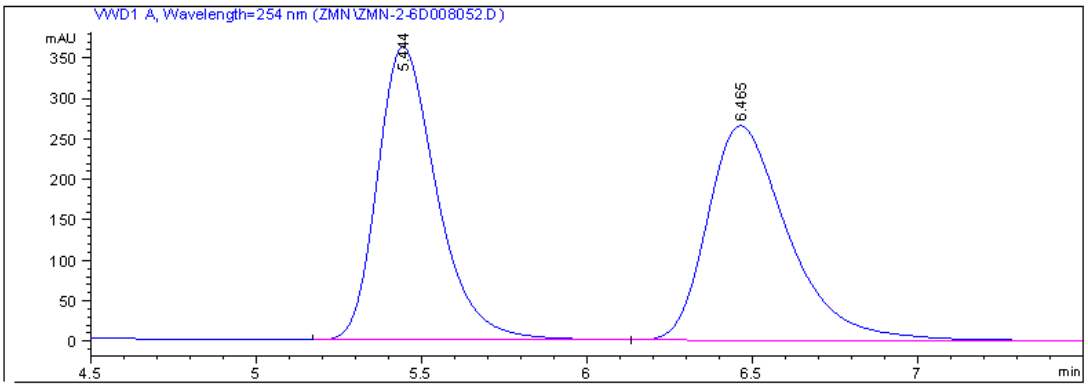
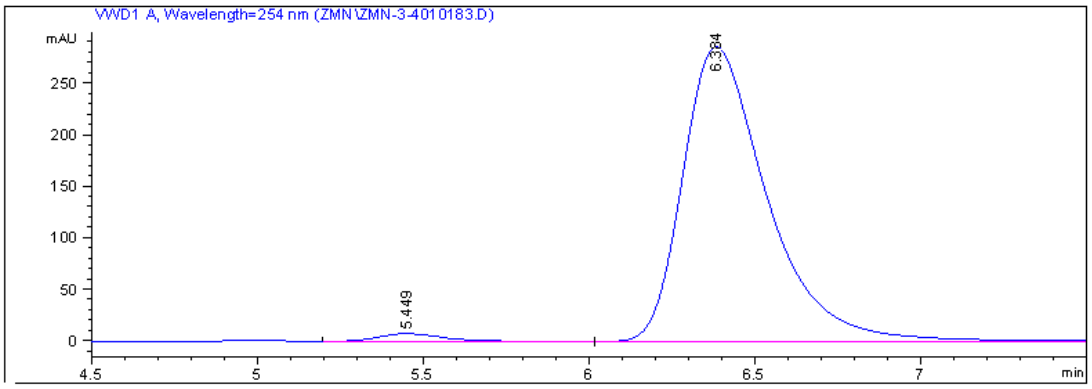
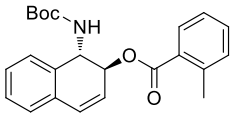


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.444	BB	0.1903	4514.91992	362.44409	50.0435
2	6.465	BBA	0.2585	4507.06641	264.96475	49.9565



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.449	VB	0.2095	104.02811	7.51323	2.0032
2	6.384	BB	0.2694	5088.97607	286.32828	97.9968



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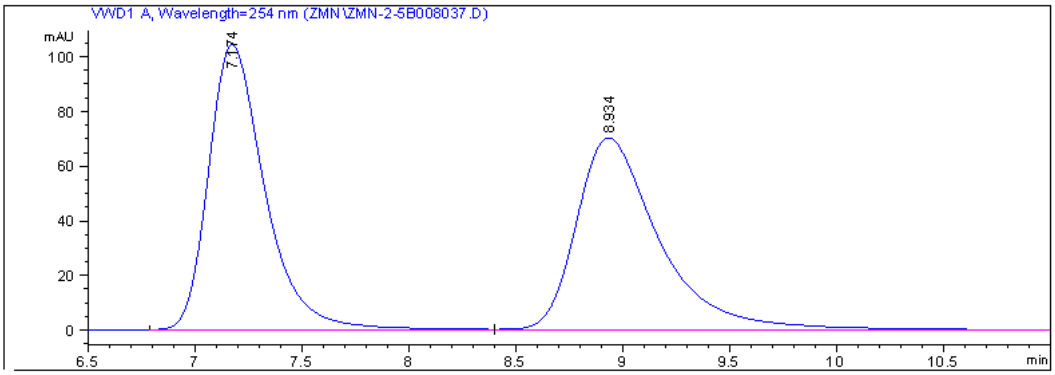
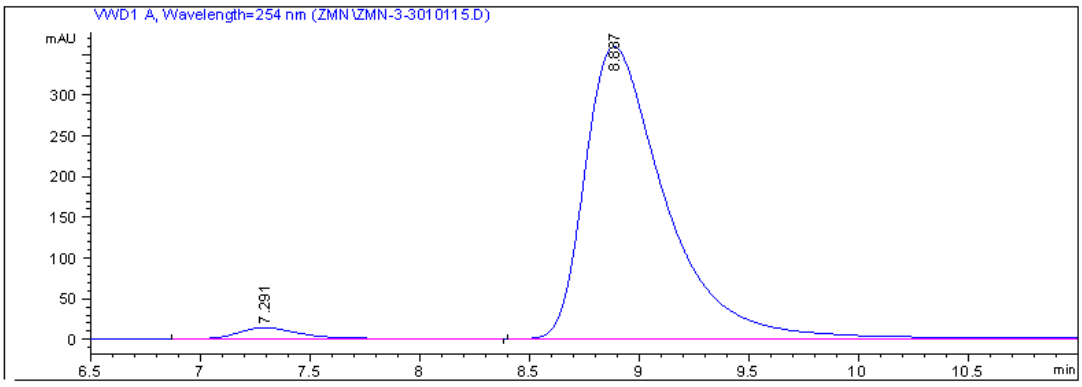
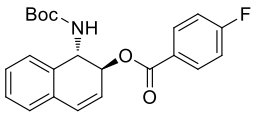


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.174	BB	0.2780	1902.11951	104.20311	50.1956
2	8.934	BB	0.4033	1887.29309	70.06568	49.8044



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.291	BB	0.2918	264.83719	13.74383	2.8092
2	8.887	BB	0.3830	9162.65625	358.70514	97.1908



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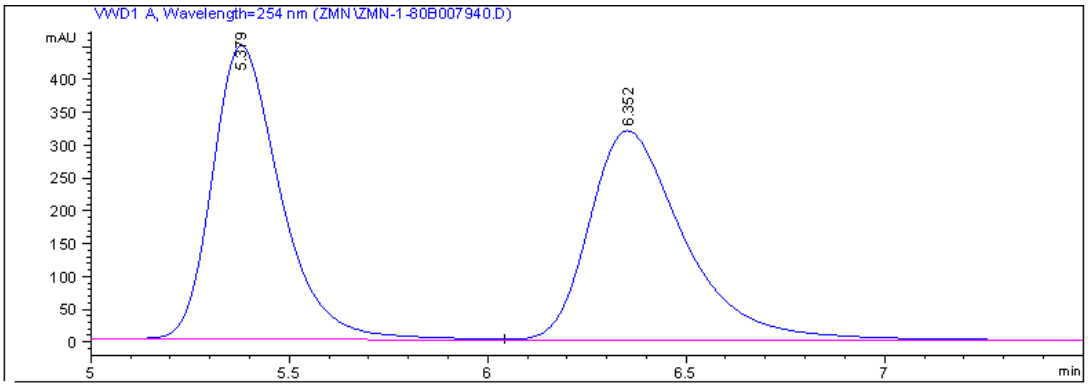
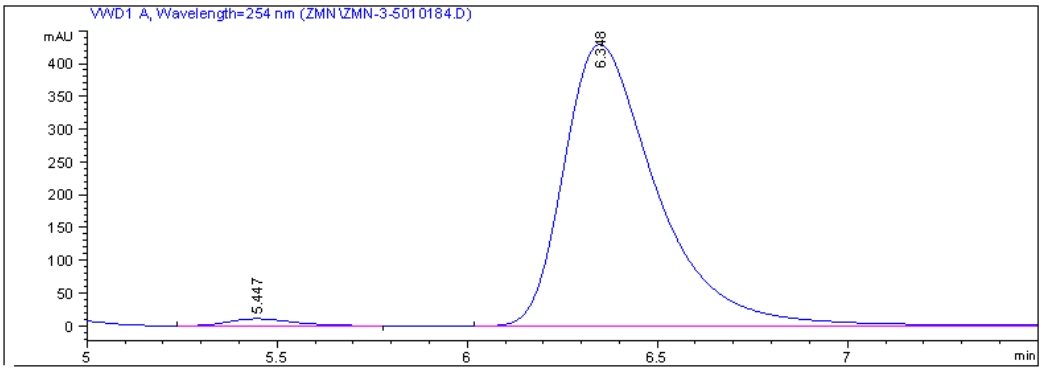
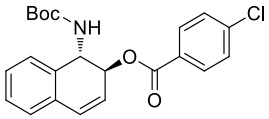


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.379	BV	0.1815	5347.60400	447.31070	50.1636
2	6.352	VB	0.2526	5312.71973	318.45160	49.8364



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.447	VB	0.1813	125.70827	10.68456	1.6873
2	6.348	BB	0.2570	7324.67822	429.38684	98.3127



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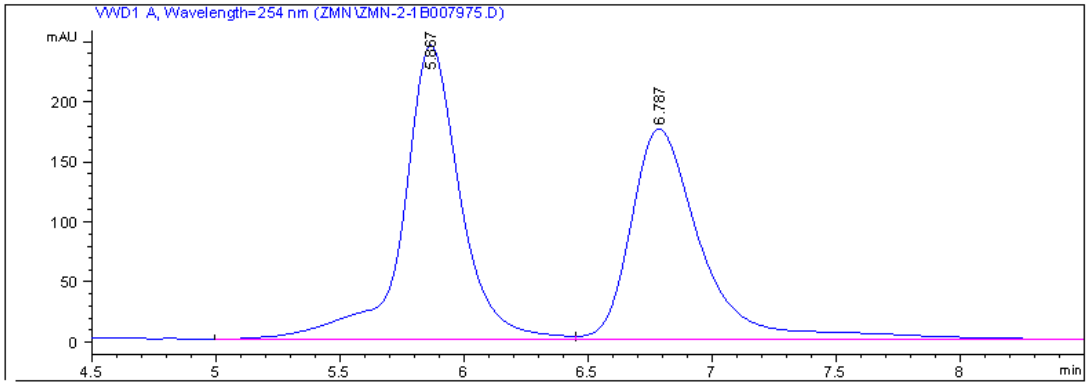
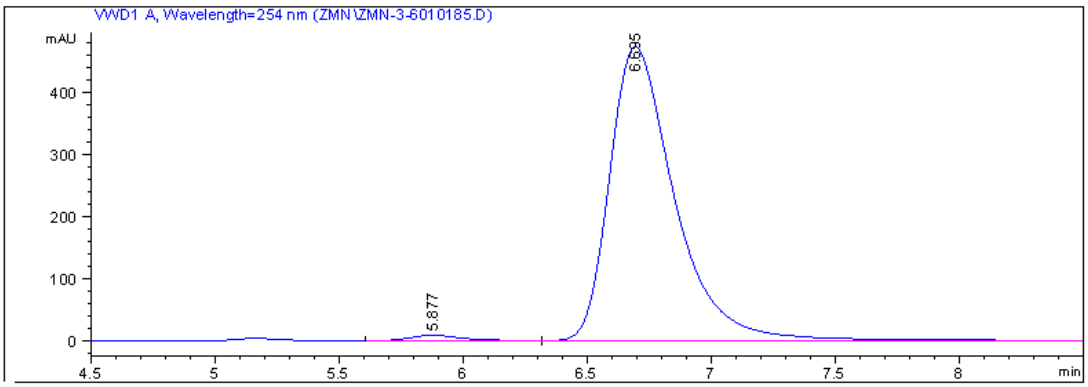
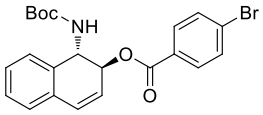


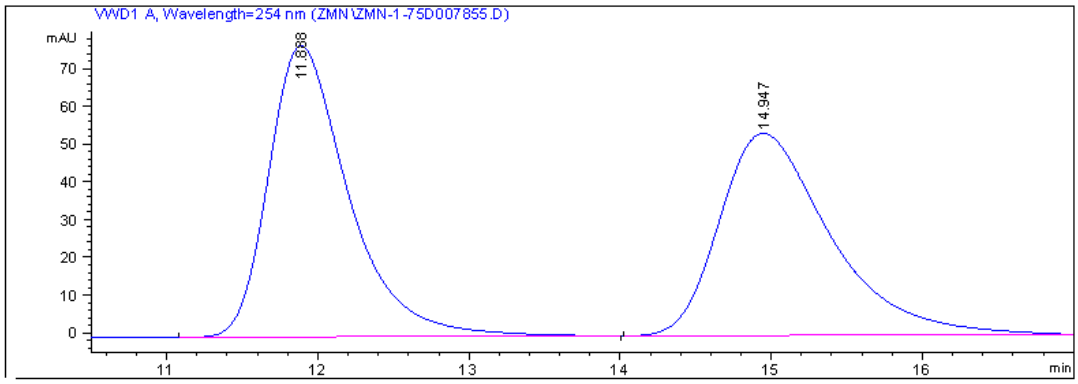
Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.867 BV	0.2379	3948.81348	245.16718	53.0429
2	6.787 VB	0.2976	3495.75659	175.35701	46.9571



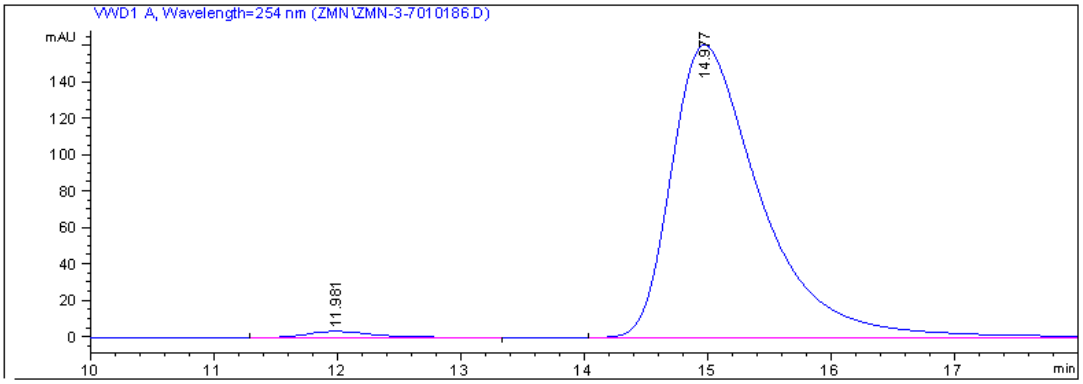
Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.877 VV	0.2199	121.22844	8.37205	1.3750
2	6.695 VB	0.2768	8695.07910	474.37961	98.6250



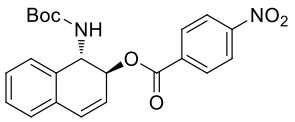
3ah



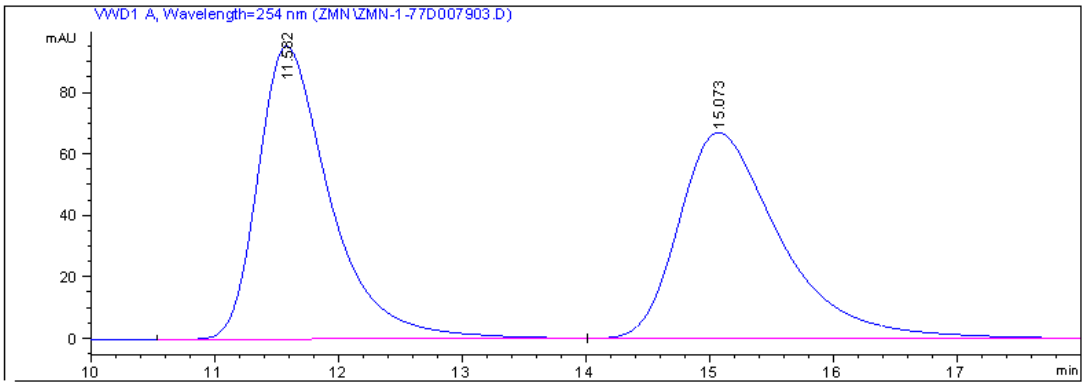
Peak #	RetTime Type [min]		Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.888	BB	0.5568	2838.98975	77.05785	50.9614
2	14.947	BBA	0.7685	2731.86938	53.51704	49.0386



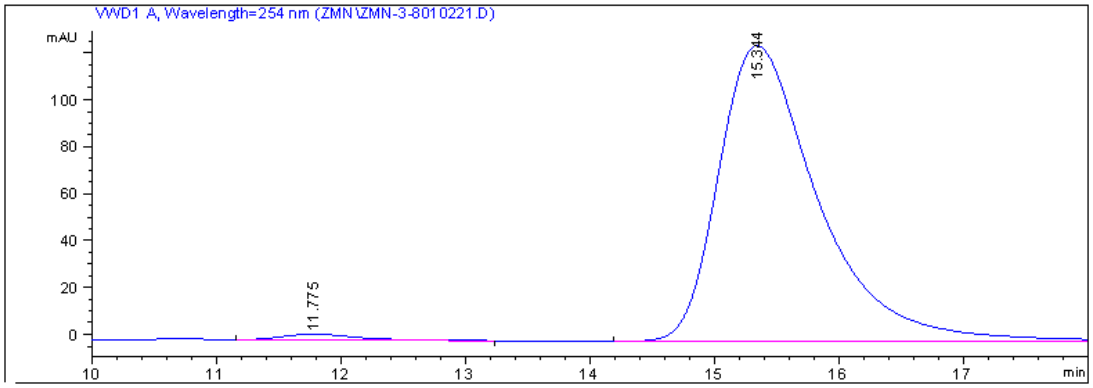
Peak #	RetTime Type [min]		Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.981	BB	0.5611	124.76105	3.32992	1.5107
2	14.977	BB	0.7589	8133.66943	160.59227	98.4893



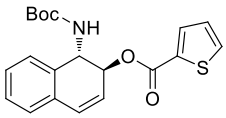
3ai



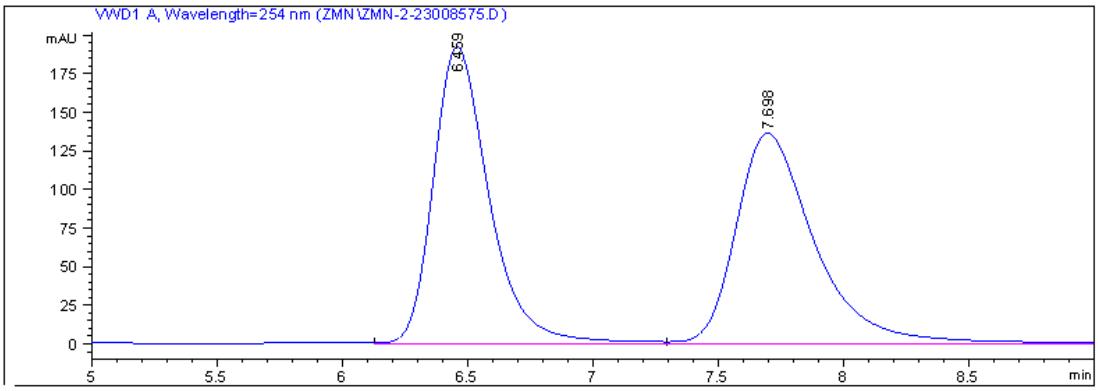
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.582	BB	0.6097	3866.84961	95.43839	50.1154
2	15.073	BBA	0.8605	3849.04785	67.07291	49.8846



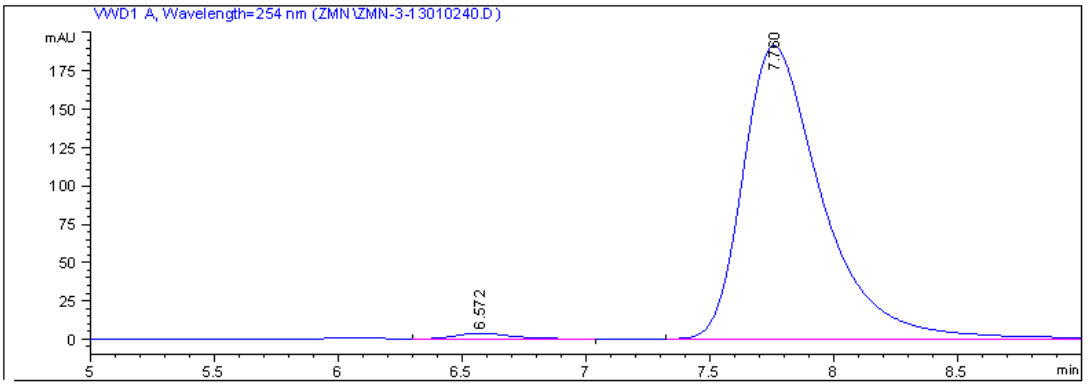
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.775	BB	0.6155	101.01411	2.42734	1.4195
2	15.344	BB	0.8387	7014.94141	125.96156	98.5805



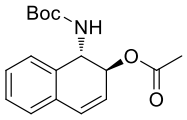
3aj



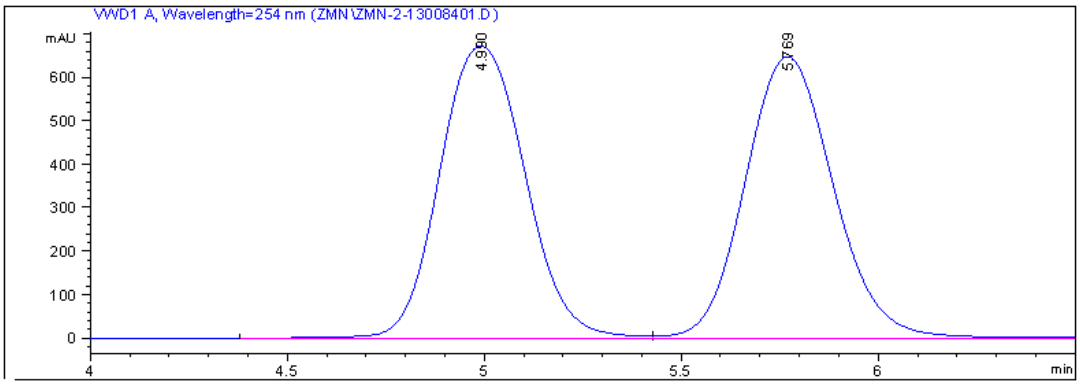
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.459	VV	0.2371	3003.41772	192.47223	49.0274
2	7.698	VBA	0.3410	3122.58472	136.44499	50.9726



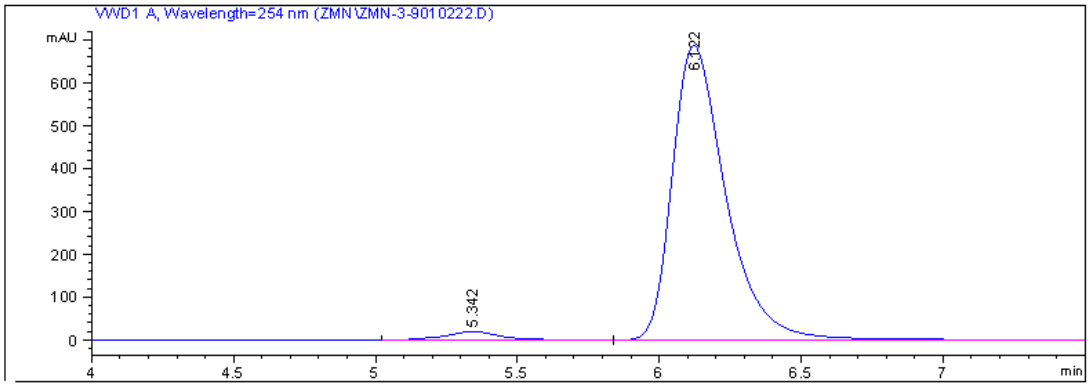
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.572	VB	0.2380	56.32539	3.63006	1.3040
2	7.760	BB	0.3350	4263.06738	191.28763	98.6960



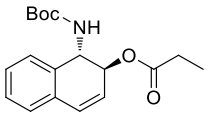
3ak



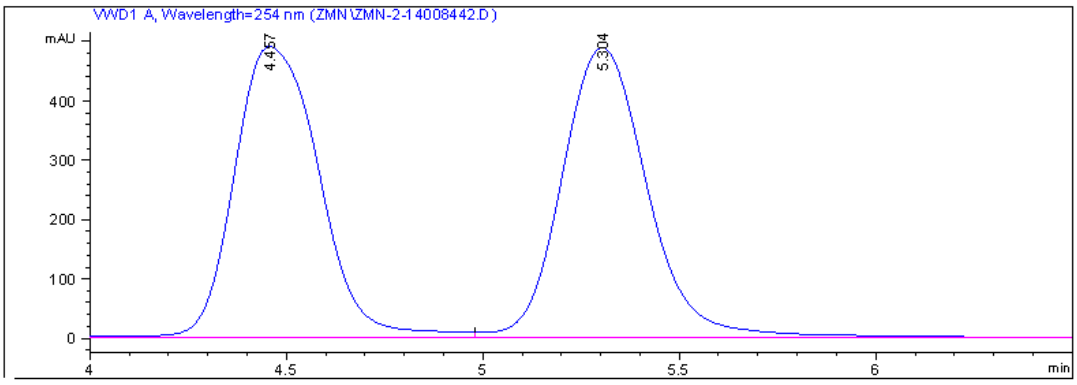
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.990	BV	0.2403	1.01580e4	672.17706	50.0818
2	5.769	VV	0.2443	1.01248e4	648.08630	49.9182



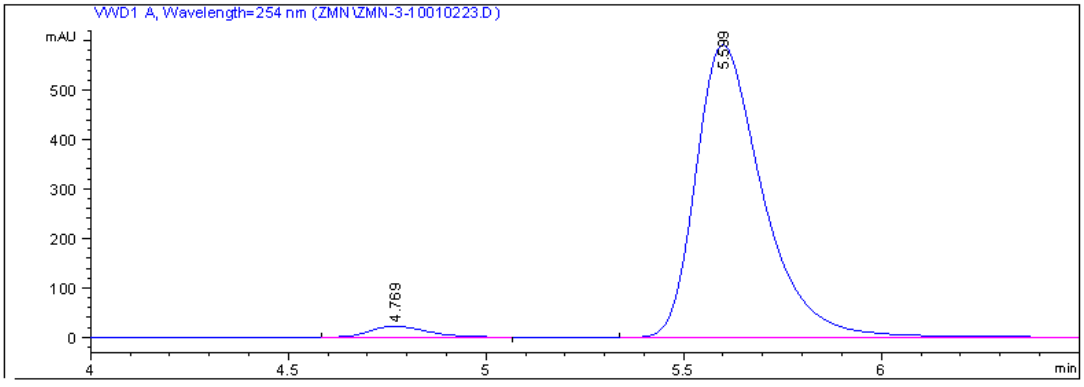
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.342	BV	0.1929	257.13596	19.37162	2.7717
2	6.122	VB	0.1992	9019.96387	686.78674	97.2283



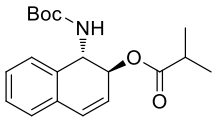
3al



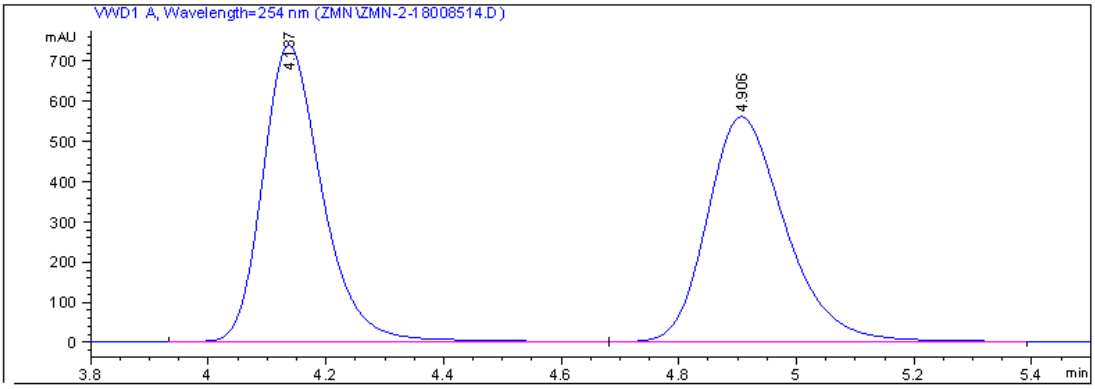
Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.457 BV	0.2401	7307.01807	489.63141	49.7531
2	5.304 VB	0.2365	7379.54004	487.78821	50.2469



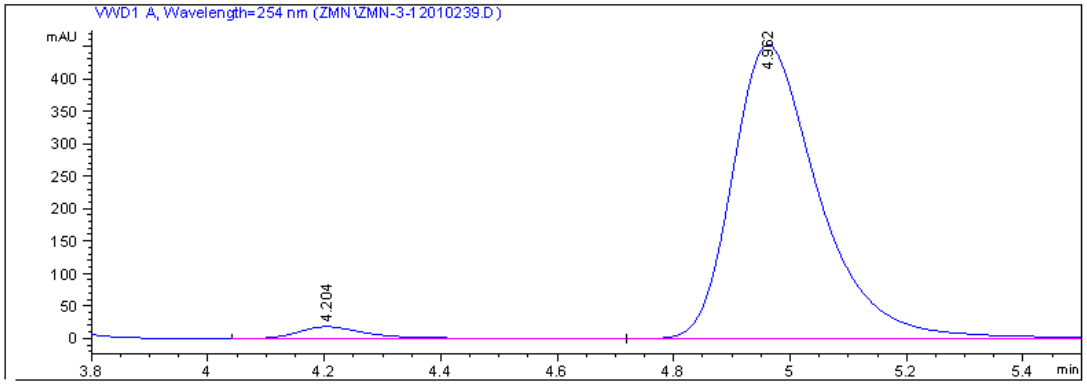
Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.769 VV	0.1586	233.08716	22.74498	3.2366
2	5.599 BB	0.1784	6968.43066	591.55780	96.7634



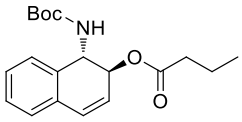
3am



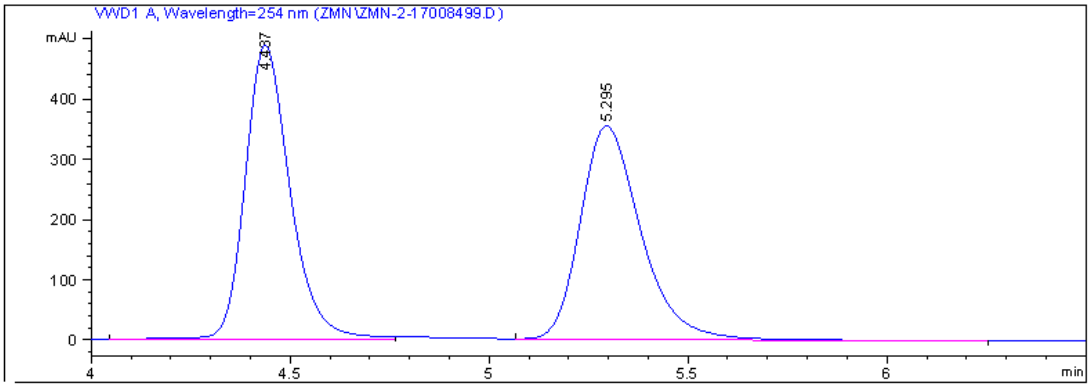
Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.137 VB	0.1073	5203.57129	737.97168	50.1187
2	4.906 BV	0.1409	5178.92725	559.88318	49.8813



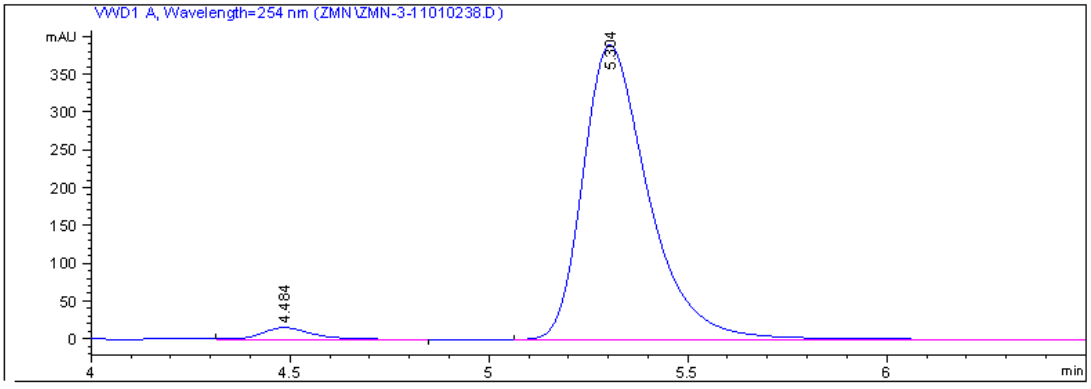
Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.204 BB	0.1212	145.01088	17.96815	3.0056
2	4.962 BB	0.1567	4679.71289	452.49139	96.9944



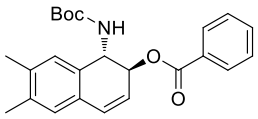
3an



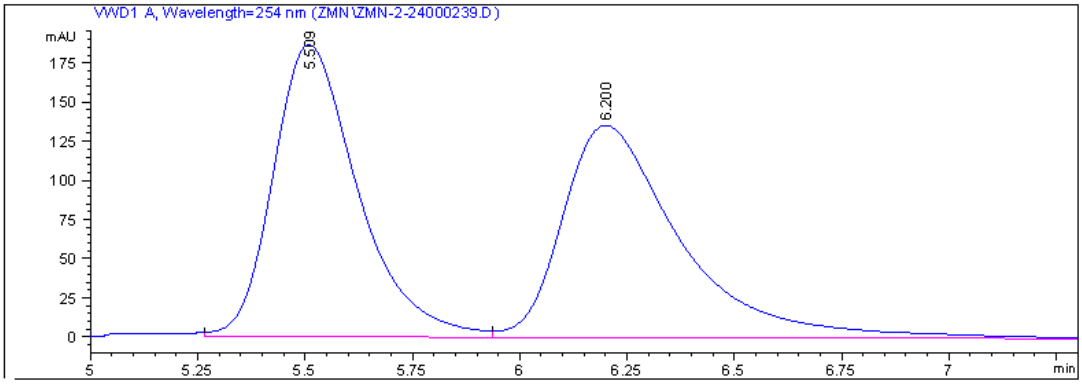
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.437	BV	0.1210	3852.90942	488.62445	50.4306
2	5.295	VB	0.1622	3787.11938	355.69980	49.5694



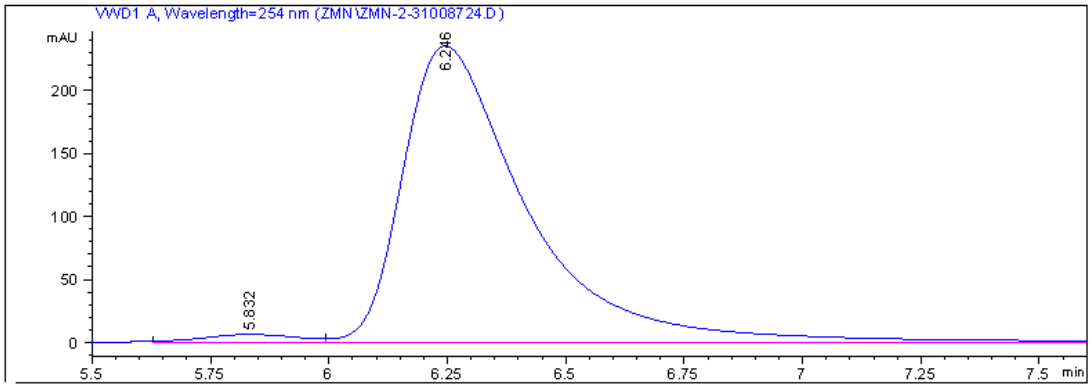
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.484	VB	0.1296	134.56712	15.60391	2.9239
2	5.304	VB	0.1728	4467.73682	389.55658	97.0761



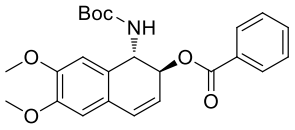
3ba



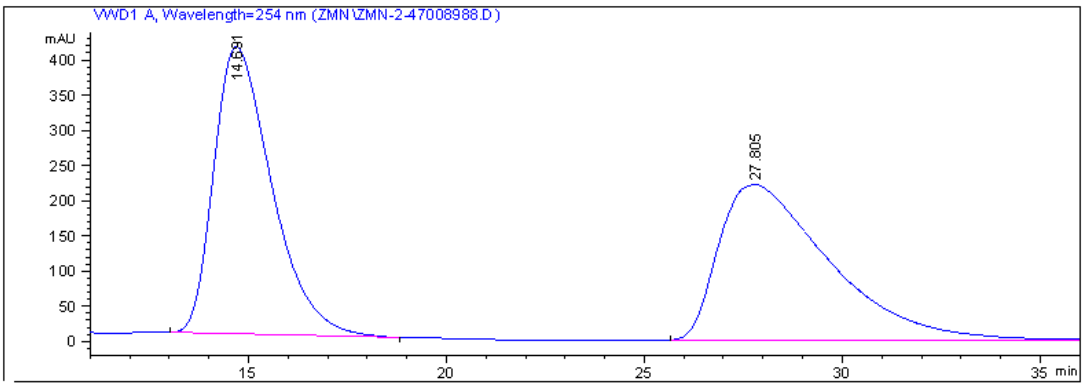
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.509	VV	0.2085	2568.13379	186.67397	49.5095
2	6.200	VB	0.2863	2619.01514	135.60257	50.4905



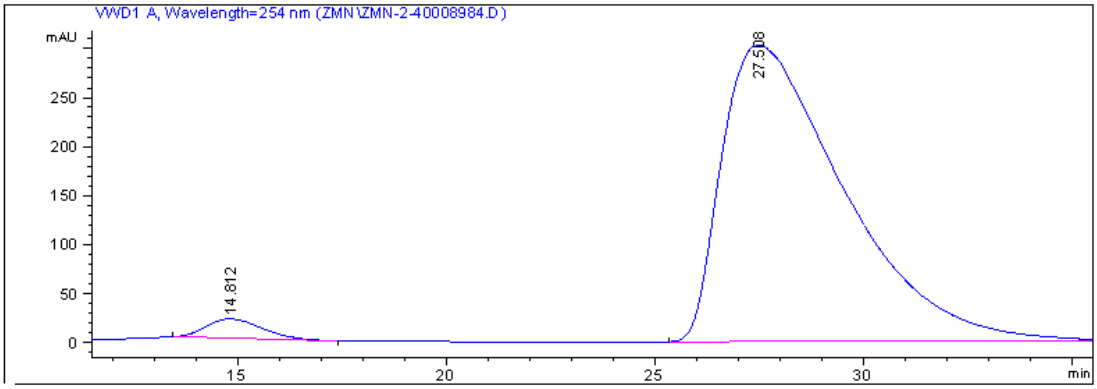
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.832	VV	0.2119	80.01855	5.87523	1.8130
2	6.246	VB	0.2717	4333.48242	235.50822	98.1870



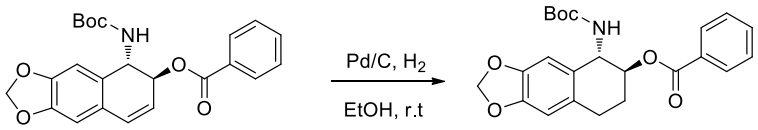
3ca



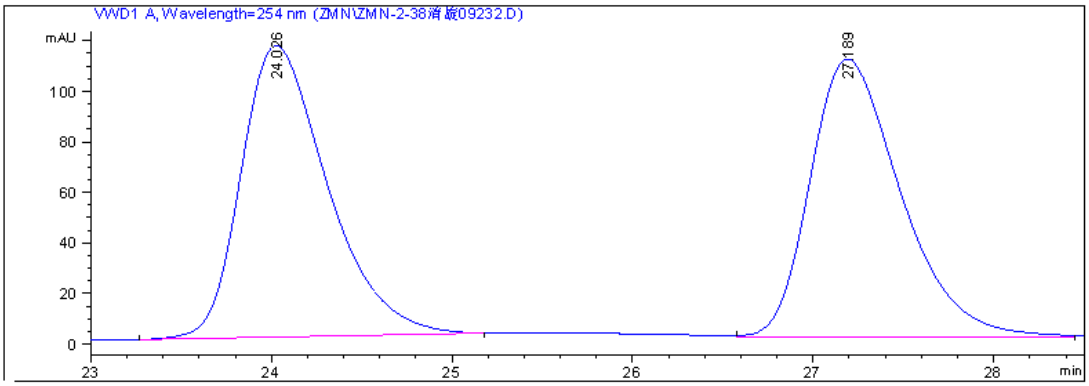
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.691	BB	1.5218	4.15486e4	407.74561	49.1554
2	27.805	BBA	2.4795	4.29765e4	220.53348	50.8446



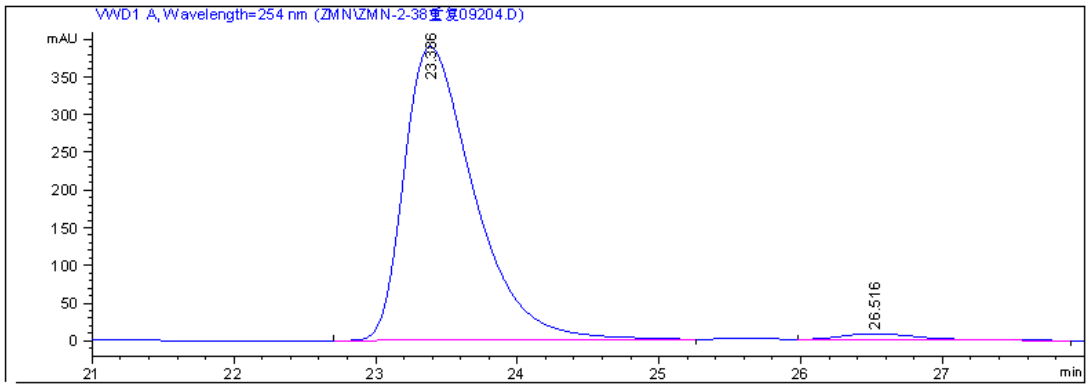
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.812	BB	1.3739	1808.91406	19.68779	2.8505
2	27.508	BBA	2.5974	6.16509e4	302.79507	97.1495



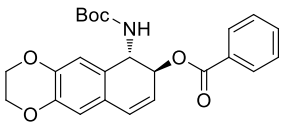
3da **3da-2** (95% yield)



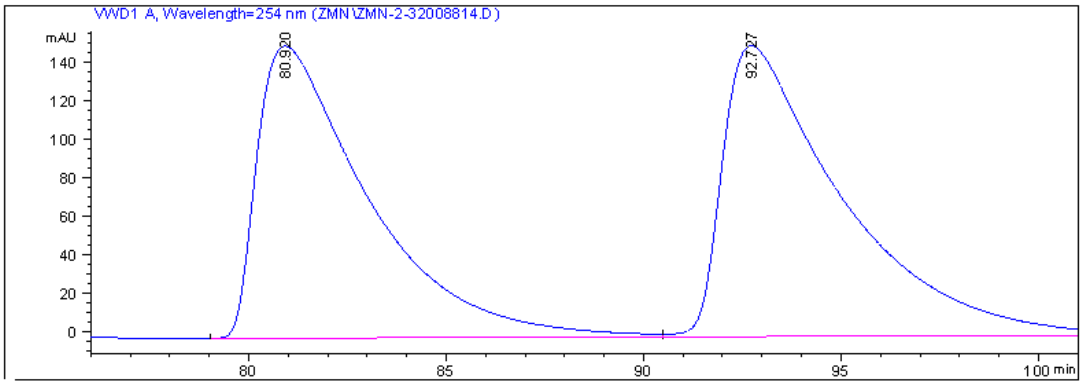
Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.026 BB	0.5102	3833.13550	115.19636	50.0058
2	27.189 VV	0.5344	3832.25391	110.02157	49.9942



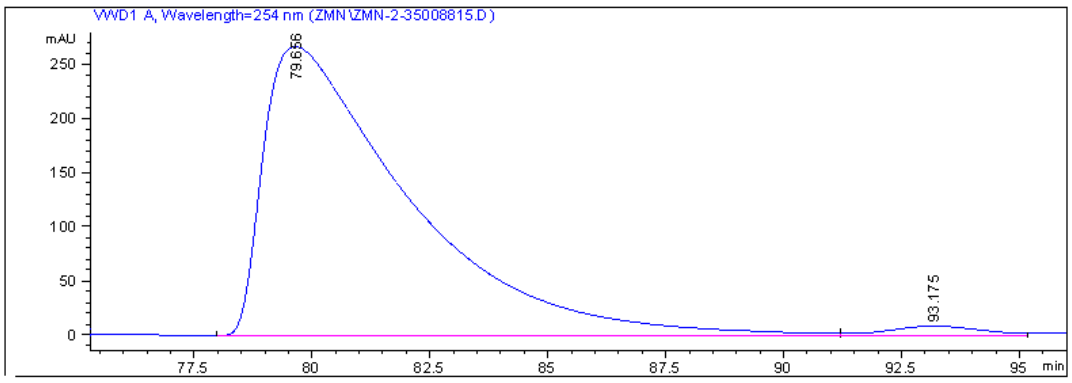
Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.386 BB	0.5242	1.33571e4	389.37451	97.7177
2	26.516 VB	0.5700	311.96478	8.29022	2.2823



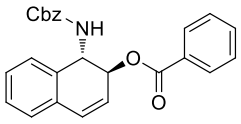
3ea



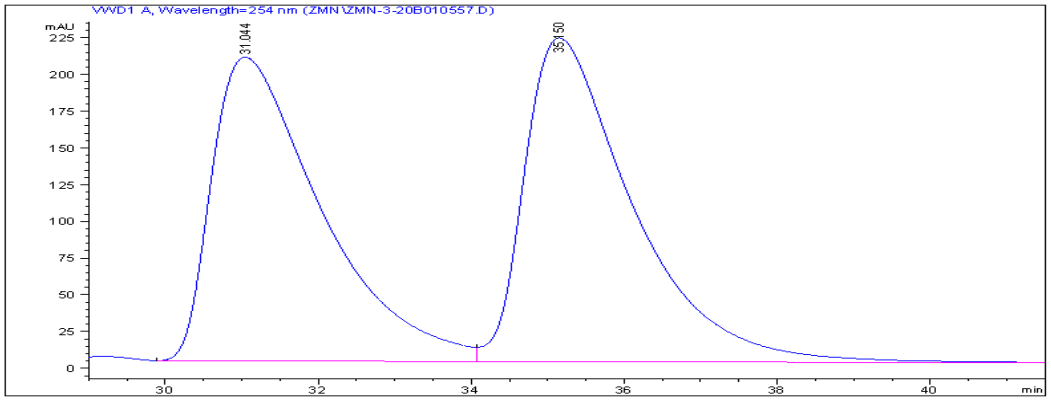
Peak #	RetTime Type [min]		Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	80.920	BV	2.8182	2.96618e4	151.36539	48.1329
2	92.727	VBA	2.9640	3.19630e4	150.85327	51.8671



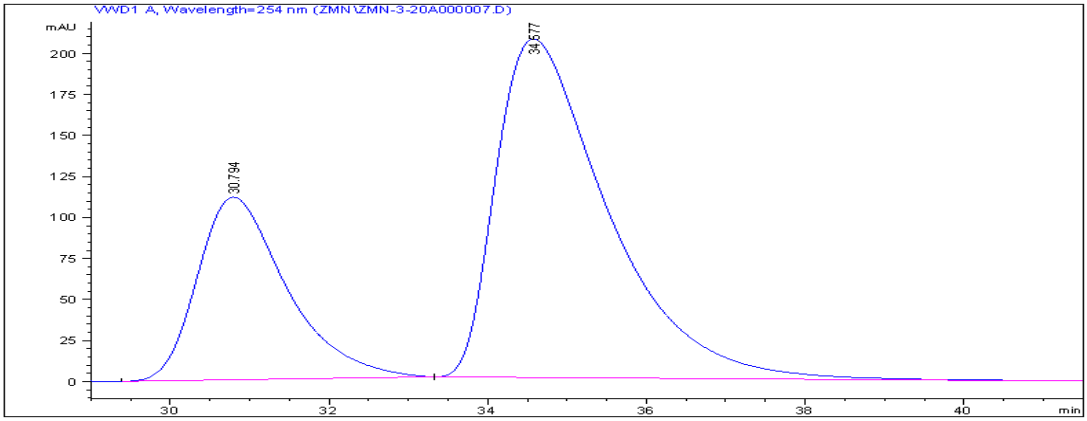
Peak #	RetTime Type [min]		Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	79.656	BV	3.0958	5.71477e4	266.28531	97.7899
2	93.175	VV	2.1302	1291.57166	9.13106	2.2101



3ga

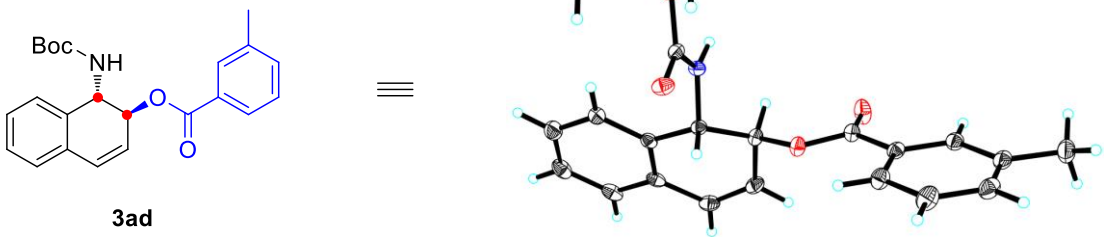


Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	31.044 BV	1.4777	2.05520e4	206.76195	48.6973
2	35.150 VB	1.4533	2.16516e4	220.35353	51.3027



Peak #	RetTime Type [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.794 BB	1.1732	8681.72949	111.27433	29.9883
2	34.577 BB	1.4669	2.02687e4	206.36736	70.0117

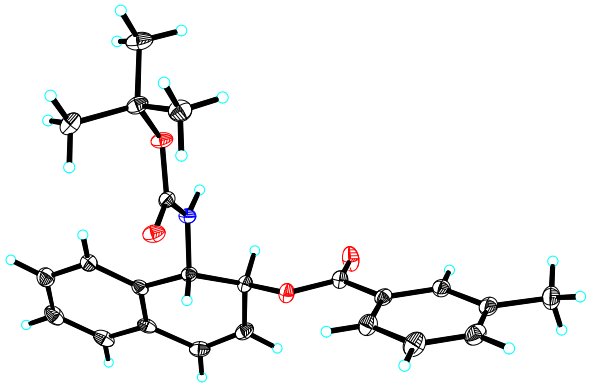
Part III Crystal structure data of 3ad



3ad

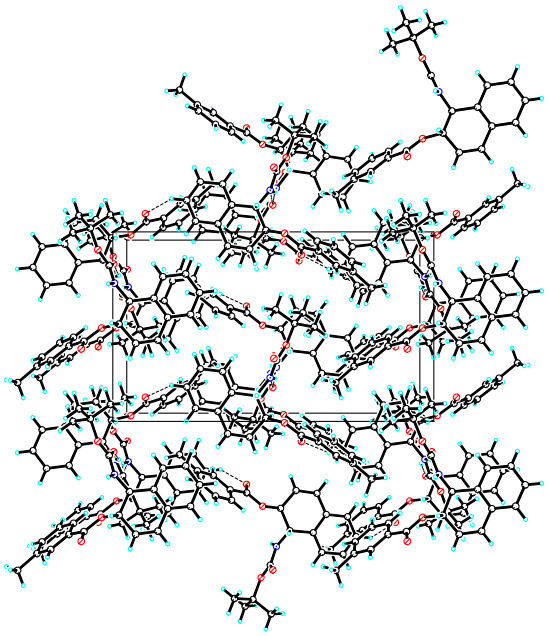
CCDC 1524577

Crystal data for cu_zmn34_0m: $C_{23}H_{25}NO_4$, M = 379.44, a = 9.6023(8) Å, b = 11.2451(9) Å, c = 19.0201(15) Å, α = 90 °, β = 90 °, γ = 90 °, V = 2053.8(3) Å^3, T = 100(2) K, space group $P212121$, Z = 4, μ(CuKα) = 0.676 mm^{-1}, 10276 reflections measured, 3449 independent reflections (R_{int} = 0.0511). The final R_1 values were 0.0458 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1287 ($I > 2\sigma(I)$). The final R_1 values were 0.0459 (all data). The final $wR(F^2)$ values were 0.1289 (all data). The goodness of fit on F^2 was 1.057. Flack parameter = 0.01(6).



View of a molecule of zmn34 with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the pack drawing of zmn34.

Hydrogen-bonds are shown as dashed lines.