Supporting Information

A Short Designed Semi-Aromatic Organic Nanotube

- synthesis, chiroptical characterization, and host properties

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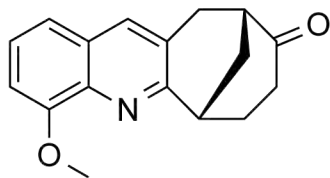and Kenneth Wärnmark[a*]

Table of Contents

NAME   TW938a
EXPNO   1
PROCNO   1
Date_   20121002
Time   15.03
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zg30
TD   57690
SOLVENT   CDCl3
NS   32
DS   2
SWH   7211.539 Hz
FIDRES   0.125005 Hz
AQ   3.9998901 sec
RG   161
DW   69.333 usec
DE   6.00 usec
TE   294.5 K
D1   0.00100000 sec
TD0   1

Compound 7

======== CHANNEL f1 ========
NUC1   1H
P1   10.00 usec
PL1   −4.00 dB
PL1W   21.45254898 W
SFO1   400.1334011 MHz
SI   131072
SF   400.1300067 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   4.00

7.857
7.416
7.396
7.377
7.316
7.295
7.267
7.010
6.990

4.080
3.669
3.373
3.356
3.328
3.311
3.033
2.989
2.318
2.275
2.208
2.198
2.186
2.175
2.164
2.154
2.142
2.132
2.122
1.982
1.965
1.947
1.929
1.911
1.893

1.00 1.03 1.01 1.00   3.11   1.01 1.03 2.04   4.17 1.13 1.11

S3

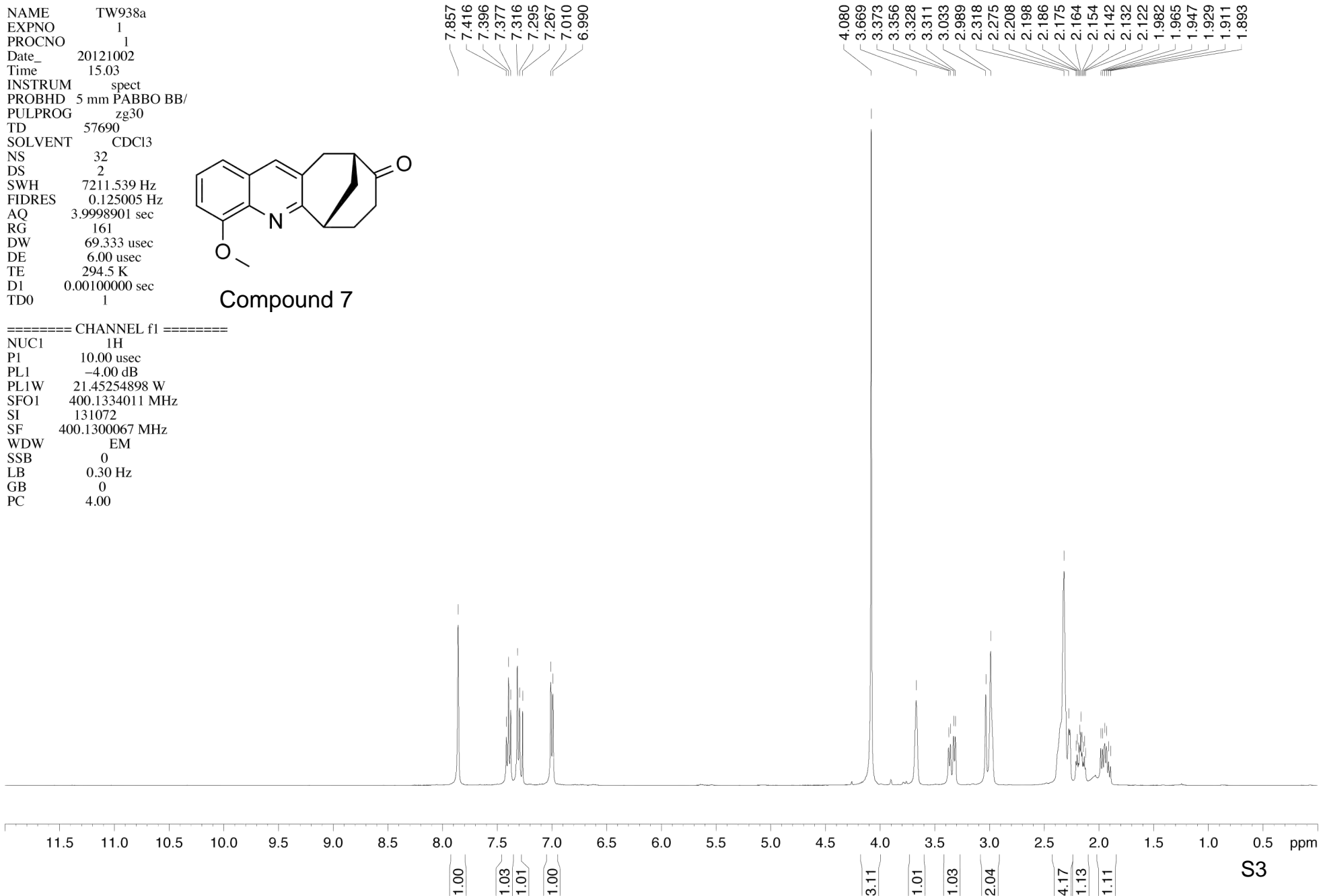NAME   TW938a
EXPNO   2
PROCNO   1
Date_   20121002
Time   21.15
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgdc30
TD   48074
SOLVENT   CDCl3
NS   4000
DS   4
SWH   24038.461 Hz
FIDRES   0.500030 Hz
AQ   0.9999892 sec
RG   57
DW   20.800 usec
DE   6.00 usec
TE   295.9 K
D1   0.00100000 sec
D11   0.03000000 sec
TD0   1

======= CHANNEL f1 =======
NUC1   13C
P1   8.50 usec
PL1   −3.00 dB
PL1W   58.63890457 W
SFO1   100.6228298 MHz

======= CHANNEL f2 =======
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 usec
PL2   −4.00 dB
PL12   14.06 dB
PL2W   21.45254898 W
PL12W   0.33533499 W
SFO2   400.1316005 MHz
SI   32768
SF   100.6127612 MHz

Compound 7

S4

NAME TW1099_2b
EXPNO 2
PROCNO 1
Date_ 20130802
Time 19.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 57690
SOLVENT CD2Cl2
NS 32
DS 2
SWH 7211.539 Hz
FIDRES 0.125005 Hz
AQ 3.9998901 sec
RG 362
DW 69.333 usec
DE 6.00 usec
TE 300.0 K
D1 0.00100000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.10 usec
PL1 −5.00 dB
PL1W 27.00716019 W
SFO1 400.1334011 MHz
SI 131072
SF 400.1300155 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1H NMR of compound 7 in CD2Cl2 displaying residual amounts of CHCl3.

7.874
7.424
7.404
7.385
7.341
7.338
7.328
7.320
7.317
7.016
7.013
6.997
6.994
5.323
5.320
5.317

7.341
7.338
7.328
7.320
7.317

S5

NAME   TW938c
EXPNO   2
PROCNO   1
Date_   20121004
Time   15.49
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zg30
TD   57690
SOLVENT   CDCl3
NS   8
DS   2
SWH   7211.539 Hz
FIDRES   0.125005 Hz
AQ   3.9998901 sec
RG   228
DW   69.333 usec
DE   6.00 usec
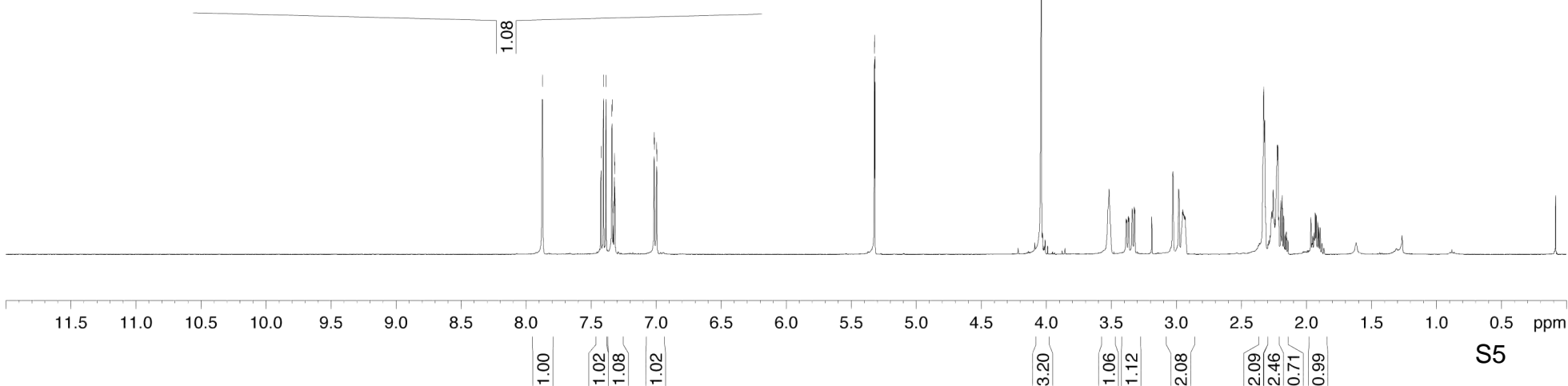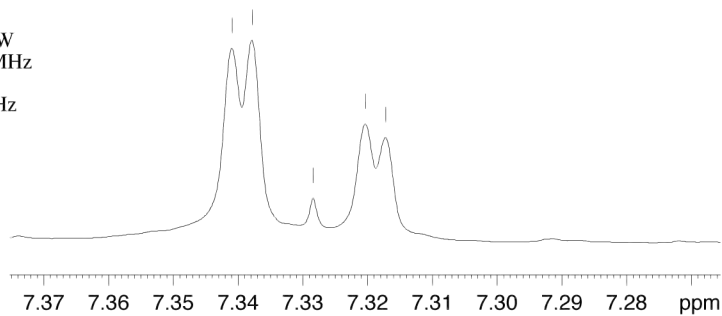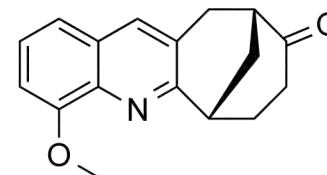TE   294.5 K
D1   0.00100000 sec
TD0   1

======= CHANNEL f1 ========
NUC1   1H
P1   10.00 usec
PL1   −4.00 dB
PL1W   21.45254898 W
SFO1   400.1334011 MHz
SI   131072
SF   400.1300059 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   4.00

Compound 8

7.645 7.305 7.285 7.270 7.265 7.165 7.162 7.144 7.142 6.937 6.919

4.080 3.946 3.939 3.526 3.514 3.484 3.472 3.391 3.349

2.523

2.021

2.00 1.58 0.58 2.02 2.03

6.26 2.07 2.11 2.03

2.05

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

S6
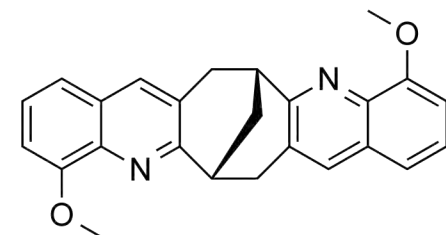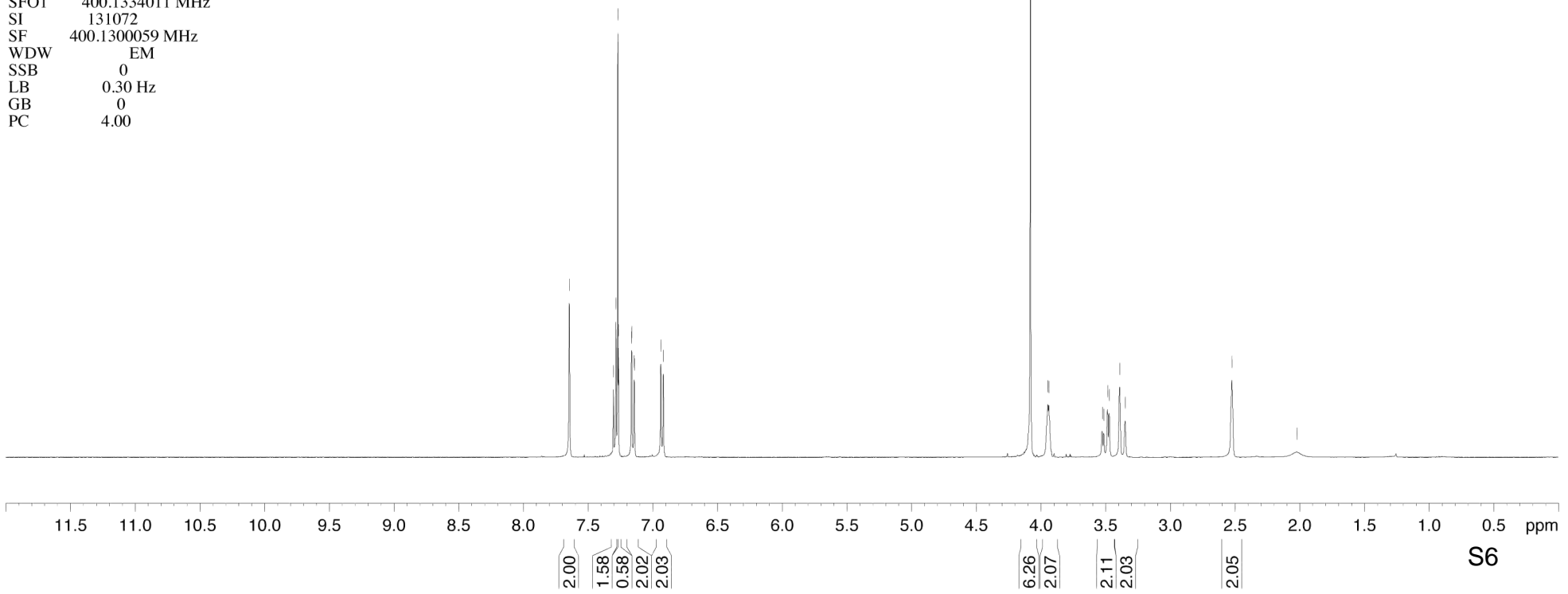
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EXPNO   3
PROCNO   1
Date_   20121004
Time   15.59
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgdc30
TD   48074
SOLVENT   CDCl3
NS   512
DS   4
SWH   24038.461 Hz
FIDRES   0.500030 Hz
AQ   0.9999892 sec
RG   57
DW   20.800 usec
DE   6.00 usec
TE   295.5 K
D1   0.00100000 sec
D11   0.03000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   8.50 usec
PL1   −3.00 dB
PL1W   58.63890457 W
SFO1   100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 usec
PL2   −4.00 dB
PL12   14.06 dB
PL2W   21.45254898 W
PL12W   0.33533499 W
SFO2   400.1316005 MHz
SI   32768
SF   100.6127592 MHz

160.600
154.948
139.192
136.100
129.175
128.687
125.871
119.066
106.880
77.477
77.159
76.841
56.174
38.541
36.362
29.138

Compound 8

S7

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Compound 9 displaying residual CHCl3

9.583
9.581
9.306

7.406
7.160
7.132
7.108
7.088
7.069
6.961
6.959
6.941
6.938
6.570
6.567
6.551
6.548
6.269

3.699
3.694
3.690
3.681
3.574
3.524
3.515
3.330
3.285
3.180
3.137
3.060
3.057
3.046
3.043
3.018
3.015
3.005
3.001
2.916
2.912
2.902
2.898
2.873
2.868
2.859
2.854

1.950
1.945
1.940
1.935
1.929
1.918
1.913
1.907
1.902
1.897
1.867
1.861

1.00	1.00		1.02	1.03	1.05	1.07	1.06			1.12

S8
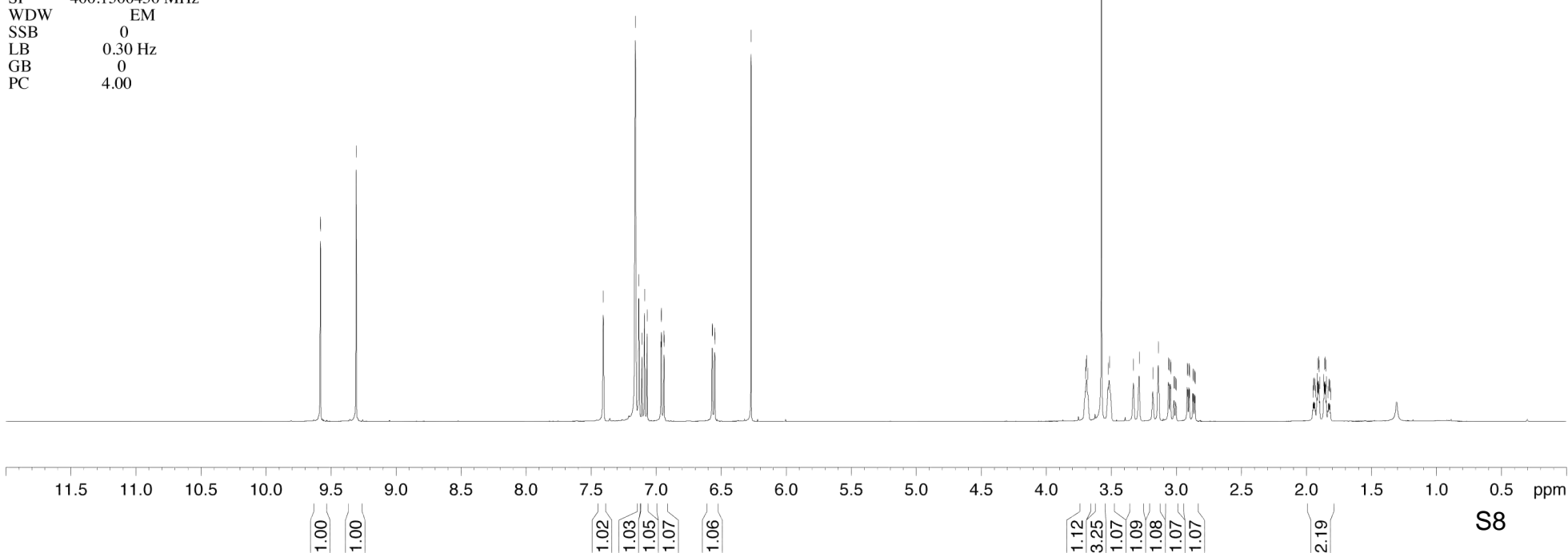
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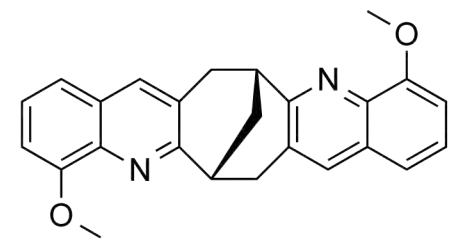EXPNO   4
PROCNO   1
Date_   20130629
Time_   2.34
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgdc30
TD   48074
SOLVENT   C6D6
NS   4000
DS   4
SWH   24038.461 Hz
FIDRES   0.500030 Hz
AQ   0.9999892 sec
RG   57
DW   20.800 usec
DE   6.00 usec
TE   295.6 K
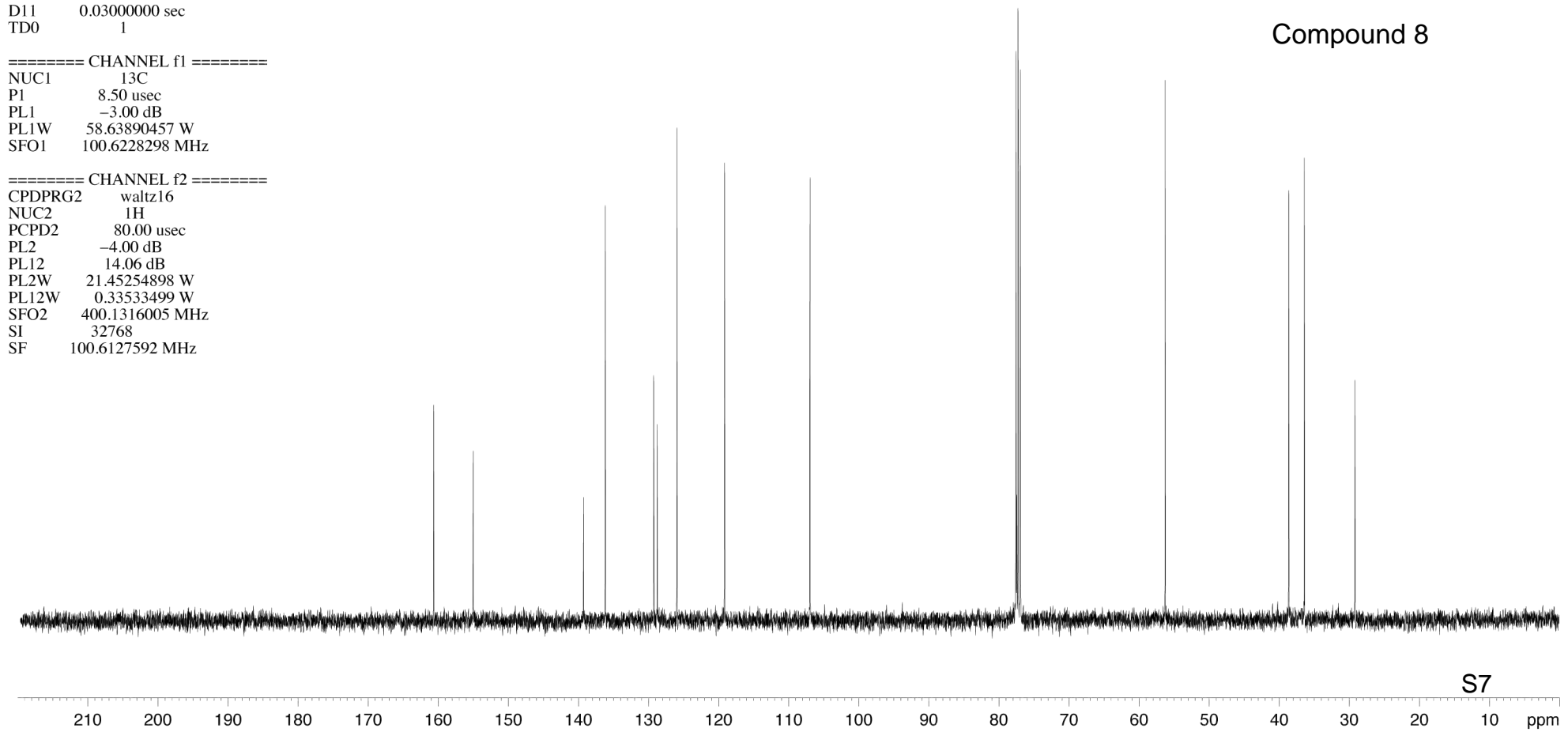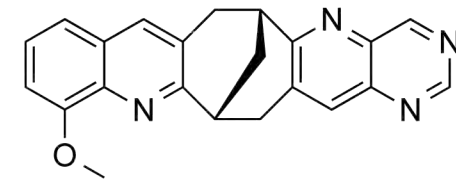D1   0.00100000 sec
D11   0.03000000 sec
TD0   1

======= CHANNEL f1 ========
NUC1   13C
P1   8.00 usec
PL1   −4.00 dB
PL1W   73.82200623 W
SFO1   100.6228298 MHz

======= CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 usec
PL2   −5.00 dB
PL12   13.88 dB
PL2W   27.00716019 W
PL12W   0.34952554 W
SFO2   400.1316005 MHz
SI   131072
SF   100.6127443 MHz

Compound 9

S9

Compound 10

S10
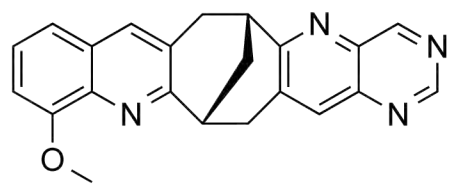
Compound 10

NAME   TW955
EXPNO   2
PROCNO   1
Date_   20130110
Time   17.27
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgdc30
TD   48074
SOLVENT   CDCl3
NS   512
DS   4
SWH   24038.461 Hz
FIDRES   0.500030 Hz
AQ   0.9999892 sec
RG   57
DW   20.800 usec
DE   6.00 usec
TE   295.7 K
D1   0.00100000 sec
D11   0.03000000 sec
TD0   1

======= CHANNEL f1 =======
NUC1   13C
P1   8.50 usec
PL1   −3.00 dB
PL1W   58.63890457 W
SFO1   100.6228298 MHz

======= CHANNEL f2 =======
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 usec
PL2   −4.00 dB
PL12   14.06 dB
PL2W   21.45254898 W
PL12W   0.33533499 W
SFO2   400.1316005 MHz
SI   32768
SF   100.6127621 MHz

195.767
160.246
154.829
149.720
144.814
139.067
137.097
136.343
133.529
129.034
128.685
126.024
124.367
119.038
106.980
77.480
77.162
76.844
56.108
38.498
37.761
35.824
34.707
29.148

S11

1H NMR of compound 10 in CD2Cl2
displaying residual amount of CHCl3
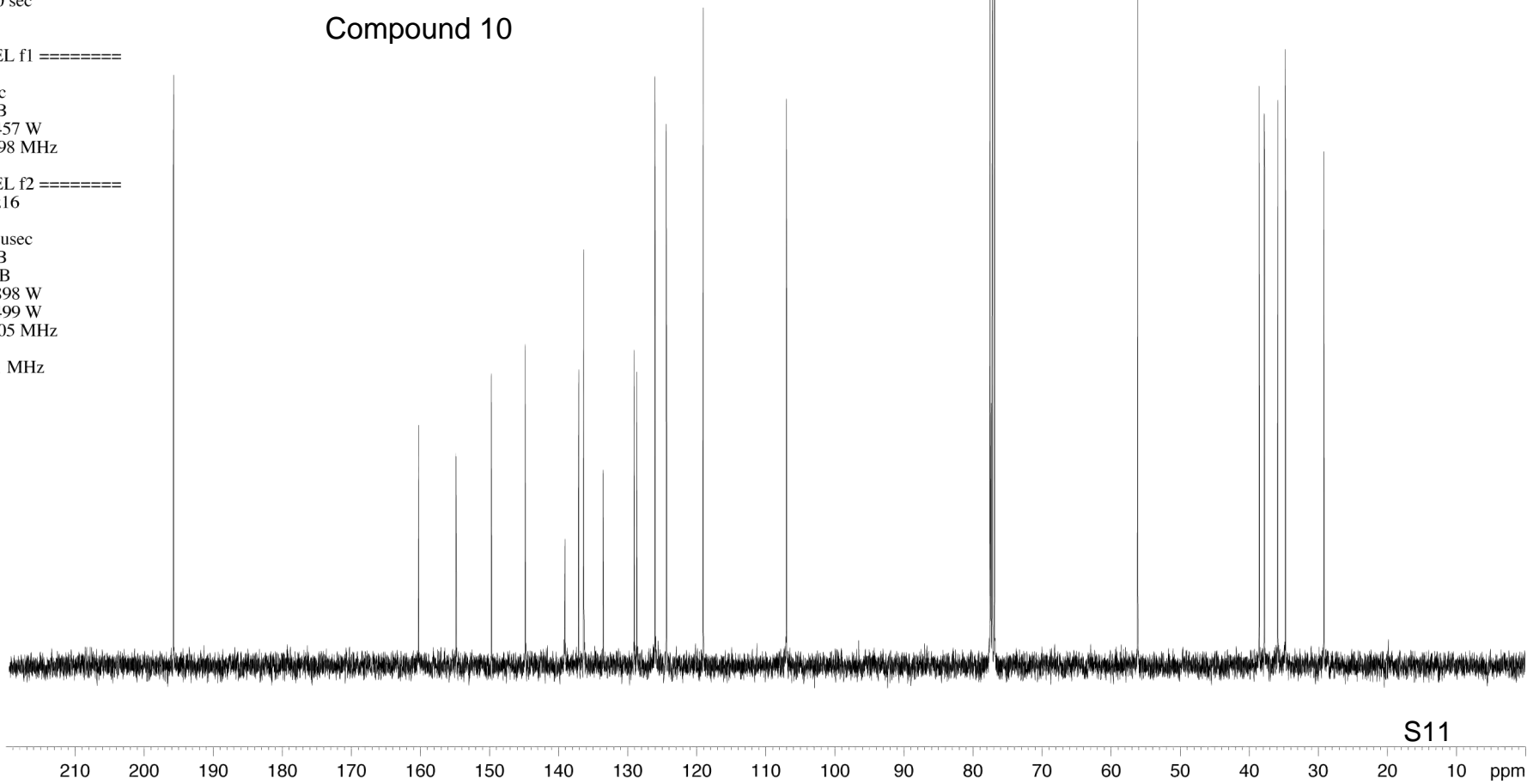
NAME   TW1007a
EXPNO   6
PROCNO   1
Date_   20130802
Time   19.53
INSTRUM   spect
PROBHD 5 mm PABBO BB/
PULPROG   zg30
TD   57690
SOLVENT   CD2Cl2
NS   32
DS   2
SWH   7211.539 Hz
FIDRES   0.125005 Hz
AQ   3.9998901 sec
RG   406
DW   69.333 usec
DE   6.00 usec
TE   300.0 K
D1   0.00100000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   9.10 usec
PL1   −5.00 dB
PL1W   27.00716019 W
SFO1   400.1334011 MHz
SI   131072
SF   400.1300156 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   4.00

9.948
9.947

7.711
7.343
7.325
7.303
7.227
7.224
7.207
7.204
6.954
6.951
6.934
6.932
6.604
5.734
5.332
5.322
5.320
5.317
4.036
4.018
3.681
3.487
3.483
3.429
3.426
3.416
3.413
3.388
3.385
3.375
3.372
3.335
3.332
3.321
3.318
3.292
3.289
3.278
3.275
3.205
3.164
3.079
3.035
2.465
2.459
2.454
2.449
2.444
2.432
2.427
2.422
2.417
2.408
2.403
2.398
2.392
2.381
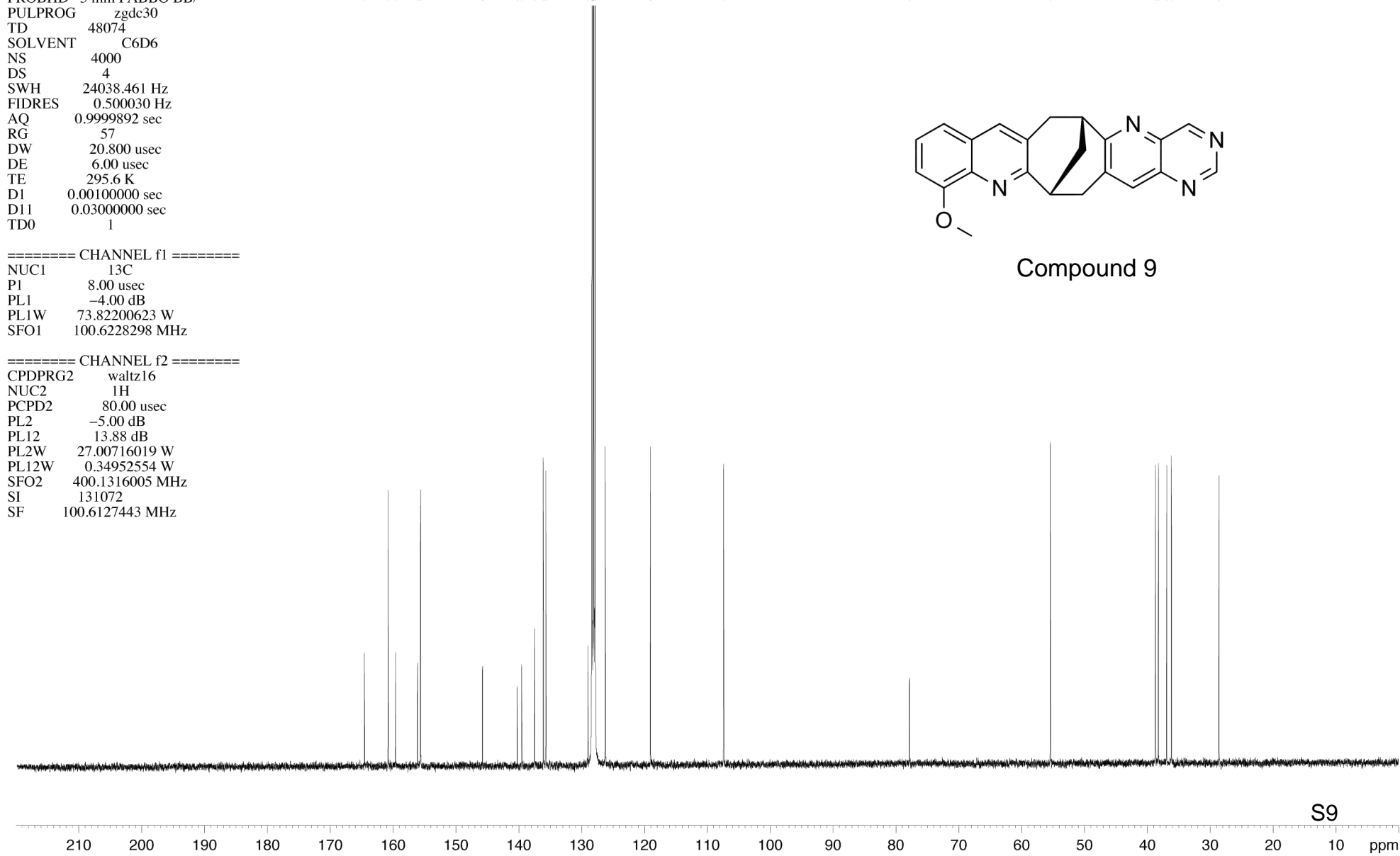
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EXPNO   2
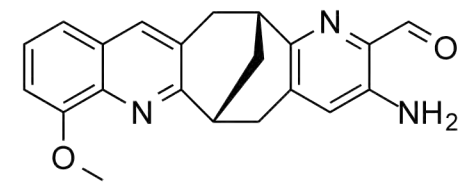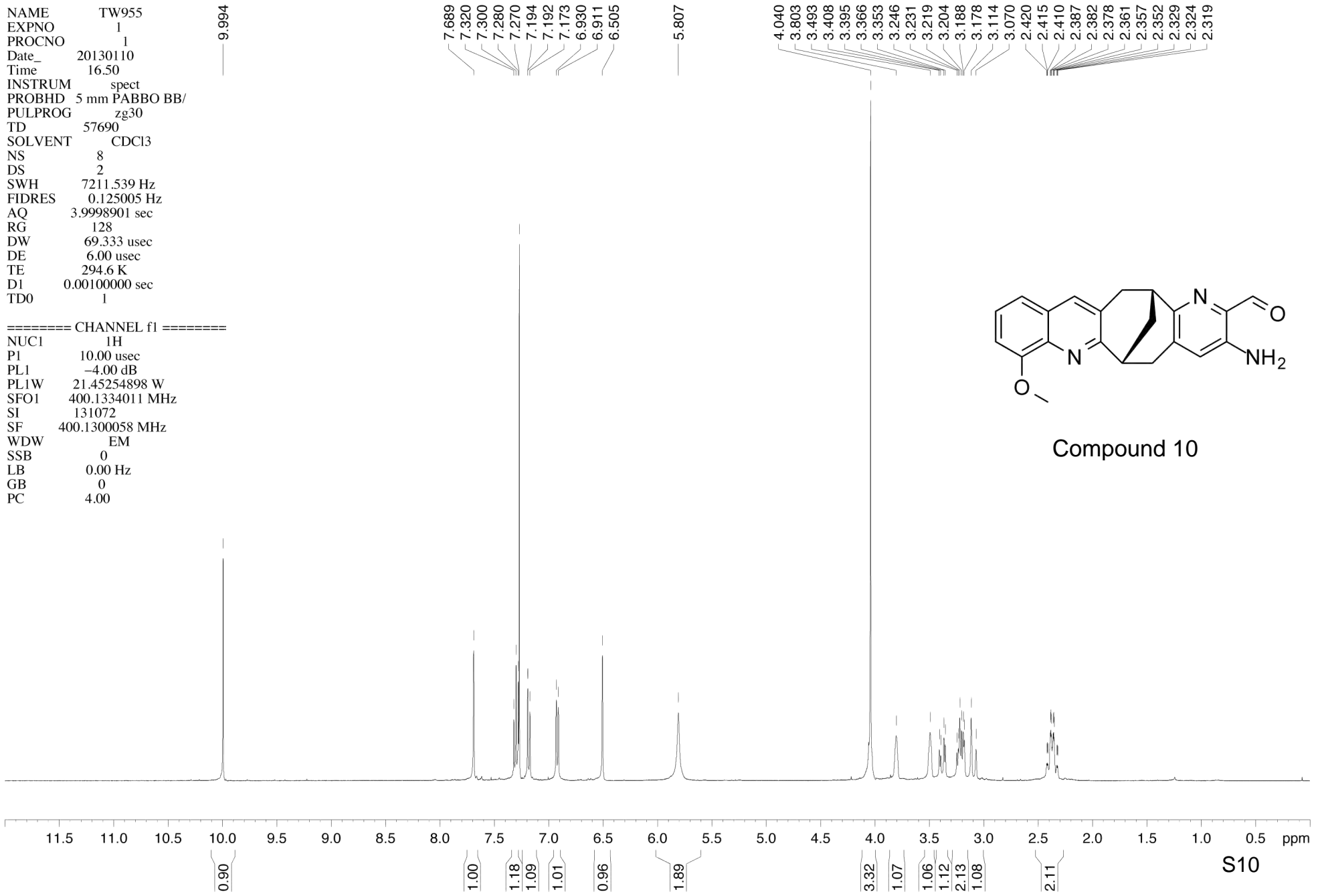PROCNO   1
Date_   20130218
Time   18.27
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zg30
TD   57690
SOLVENT   CDCl3
NS   32
DS   2
SWH   7211.539 Hz
FIDRES   0.125005 Hz
AQ   3.9998901 sec
RG   456
DW   69.333 usec
DE   6.00 usec
TE   294.4 K
D1   0.00100000 sec
TD0   1

======= CHANNEL f1 ========
NUC1   1H
P1   10.00 usec
PL1   −4.00 dB
PL1W   21.45254898 W
SFO1   400.1334011 MHz
SI   131072
SF   400.1300058 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   4.00

Compound 12

9.518
9.212
7.864
7.782
7.524
7.294
7.270
7.255
7.081
7.062
6.942
6.923
4.155
4.137
4.119
4.101
4.083
3.945
3.860
3.785
3.737
3.650
3.637
3.607
3.594
3.563
3.520
3.495
3.482
3.456
3.414
3.388
3.349
3.307
3.183
3.142
2.618
2.585
2.556
2.523
2.053
1.664
1.284
1.266
1.248

Integrals: 1.00, 1.01, 2.13, 1.14, 1.13, 1.17, 1.13, 3.86, 1.22, 1.22, 2.31, 8.27, 1.11, 4.50

S13
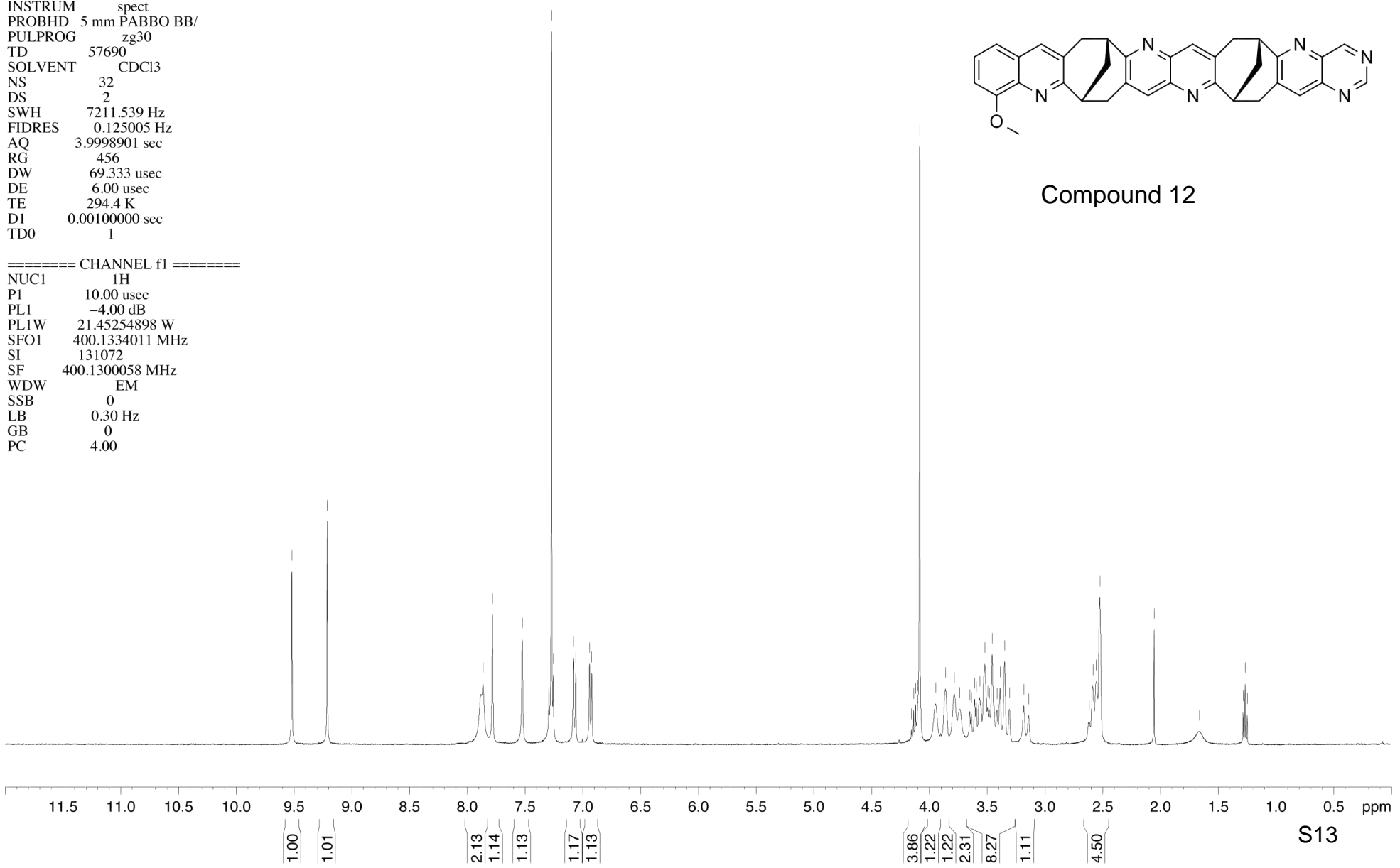
NAME   TW1020a
EXPNO   2
PROCNO   1
Date_   20130303
Time   18.31
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgdc30
TD   48074
SOLVENT   CDCl3
NS   2048
DS   4
SWH   24038.461 Hz
FIDRES   0.500030 Hz
AQ   0.9999892 sec
RG   57
DW   20.800 usec
DE   6.00 usec
TE   295.7 K
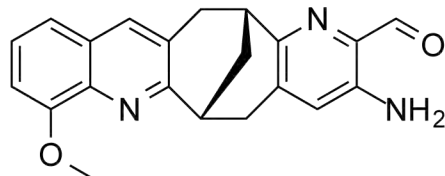D1   0.00100000 sec
D11   0.03000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   8.50 usec
PL1   −3.00 dB
PL1W   58.63890457 W
SFO1   100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 usec
PL2   −4.00 dB
PL12   14.06 dB
PL2W   21.45254898 W
PL12W   0.33533499 W
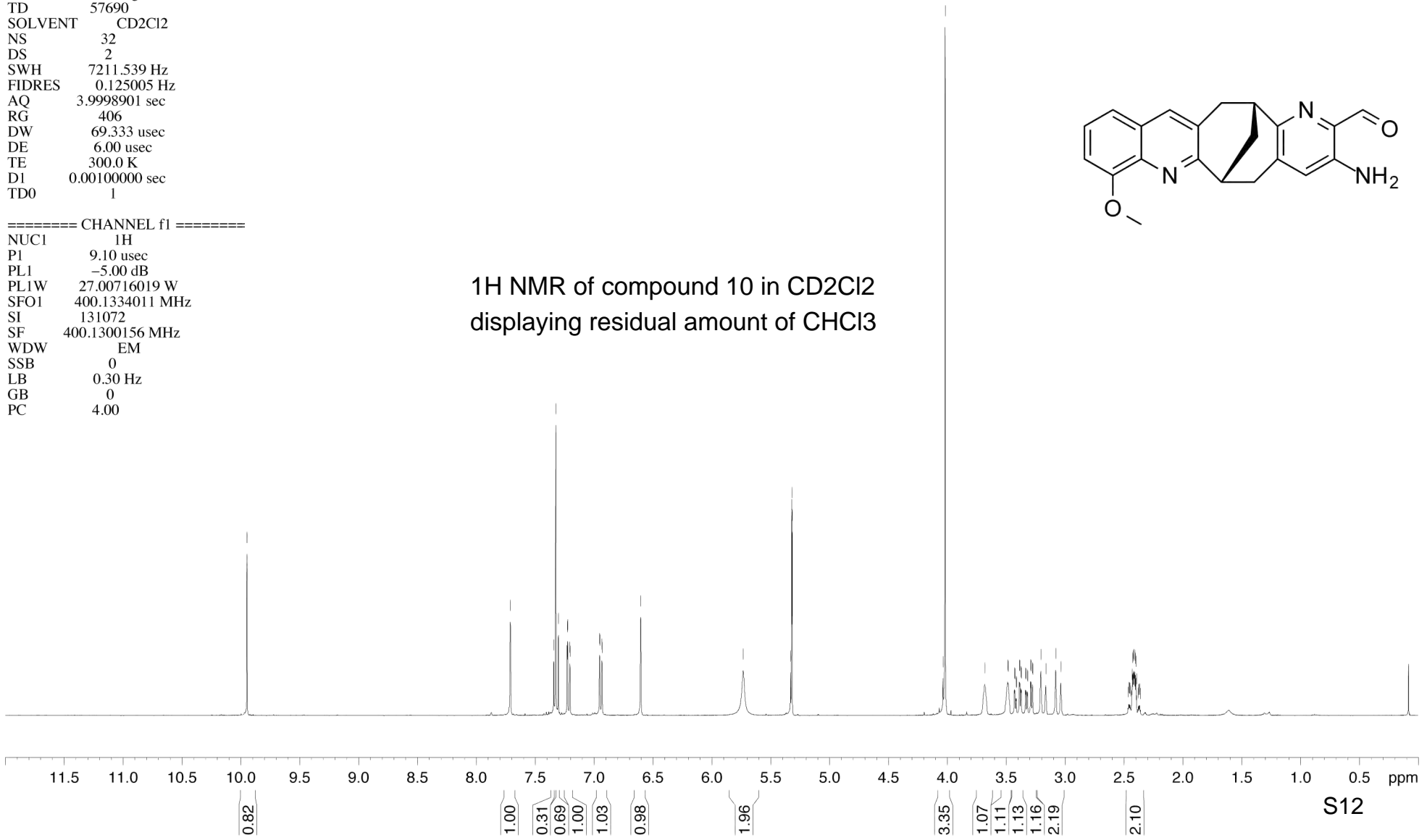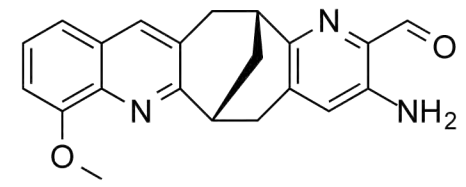SFO2   400.1316005 MHz
SI   32768
SF   100.6127604 MHz

Compound 12

S14

Compound 13

S15

195.827

162.135
161.624
160.141
154.945
149.410
144.672
141.553
139.269
136.660
136.316
136.075
136.061
135.981
133.706
131.997
131.731
128.683
128.589
126.007
124.220
118.969
106.997

77.482
77.163
76.847

38.708
38.376
38.334
38.001
36.407
36.111
35.931
34.520
29.123
29.039

Compound 13

S16
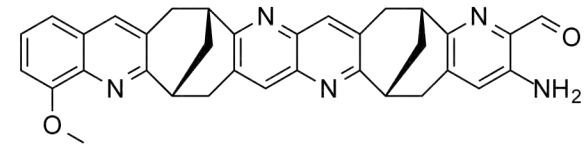
Compound 14
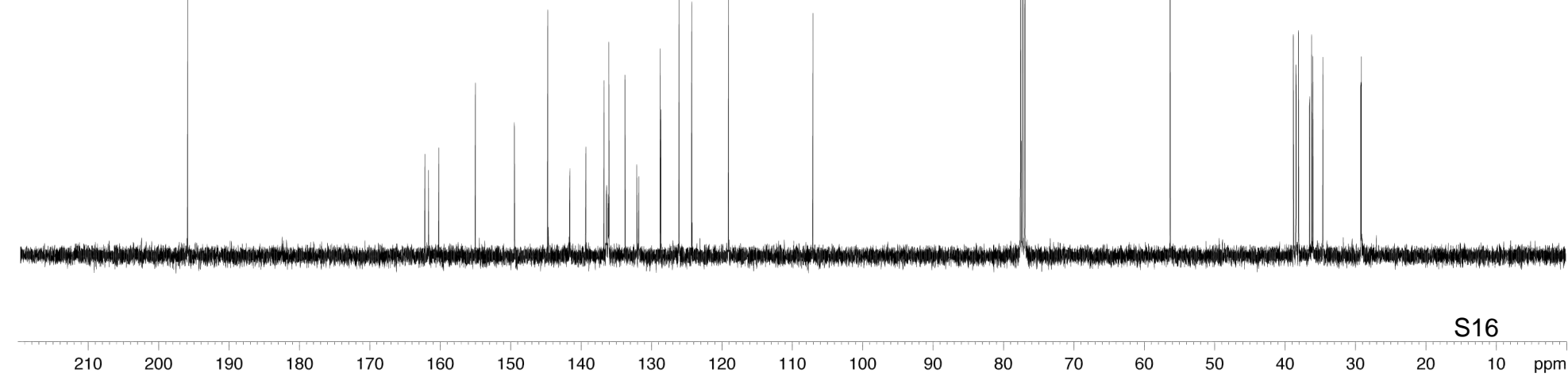
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EXPNO   1
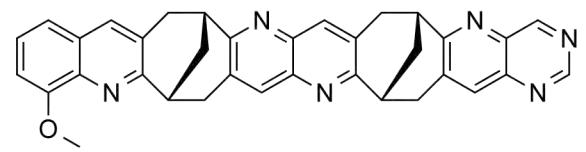PROCNO   1
Date_   20130516
Time   12.58
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zg30
TD   57690
SOLVENT   CDCl3
NS   16
DS   2
SWH   7211.539 Hz
FIDRES   0.125005 Hz
AQ   3.9998901 sec
RG   181
DW   69.333 usec
DE   6.00 usec
TE   295.0 K
D1   0.00100000 sec
TD0   1

======= CHANNEL f1 =======
NUC1   1H
P1   9.10 usec
PL1   −5.00 dB
PL1W   27.00716019 W
SFO1   400.1334011 MHz
SI   131072
SF   400.1300058 MHz
WDW   EM
SSB   0
LB   0.00 Hz
GB   0
PC   4.00

Peaks: 9.531, 9.529, 9.270

7.839, 7.803, 7.760, 7.696, 7.685, 7.549, 7.362, 7.342, 7.322, 7.270, 7.238, 7.235, 7.217, 7.215, 6.957, 6.955, 6.938, 6.936

4.080, 3.909, 3.835, 3.700, 3.654, 3.611, 3.569, 3.555, 3.520, 3.510, 3.481, 3.467, 3.444, 3.430, 3.415, 3.391, 3.365, 3.322, 3.248, 3.203, 3.183, 3.164, 3.140, 3.079, 3.038, 2.539, 2.507, 2.482

Integrals: 0.42, 0.43, 0.48, 0.45, 0.46, 0.87, 0.45, 0.45, 0.48, 0.47, 1.47, 0.51, 0.49, 1.94, 0.57, 3.43, 1.49, 0.52, 3.02

S17
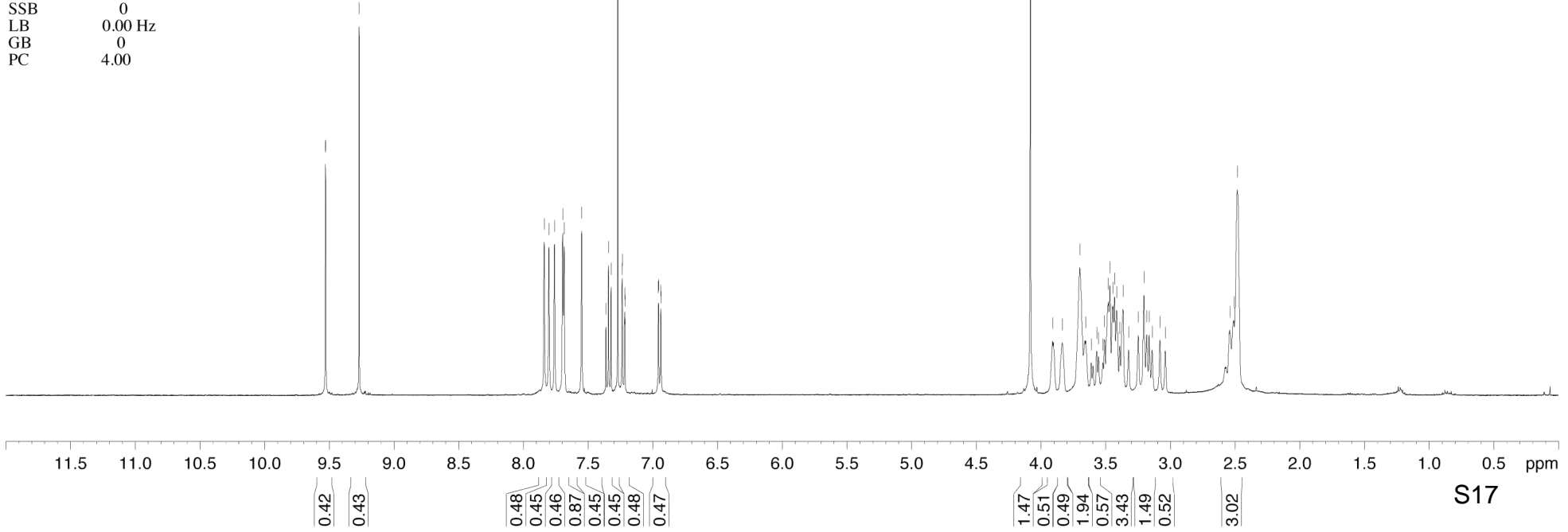
NAME   TW1092c
EXPNO   2
PROCNO   1
Date_   20130517
Time   2.05
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgdc30
TD   48074
SOLVENT   CDCl3
NS   7000
DS   4
SWH   24038.461 Hz
FIDRES   0.500030 Hz
AQ   0.9999892 sec
RG   57
DW   20.800 usec
DE   6.00 usec
TE   295.9 K
D1   0.00100000 sec
D11   0.03000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   8.00 usec
PL1   −4.00 dB
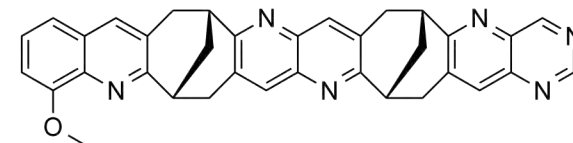PL1W   73.82200623 W
SFO1   100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 usec
PL2   −5.00 dB
PL12   13.88 dB
PL2W   27.00716019 W
PL12W   0.34952554 W
SFO2   400.1316005 MHz
SI   32768
SF   100.6127598 MHz

Peak labels: 164.545, 162.115, 161.949, 161.331, 160.862, 160.841, 159.986, 155.242, 154.899, 145.350, 141.665, 141.606, 141.476, 141.323, 139.225, 139.139, 137.464, 136.240, 136.089, 136.031, 135.883, 135.847, 132.006, 131.713, 131.163, 130.763, 128.628, 128.518, 126.056, 119.152, 107.037

77.475, 77.158, 76.840

56.211, 38.748, 38.631, 38.476, 38.328, 38.216, 36.422, 36.328, 36.163, 36.056, 36.025, 35.731, 28.950, 28.892, 28.591

Compound 14

S18

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
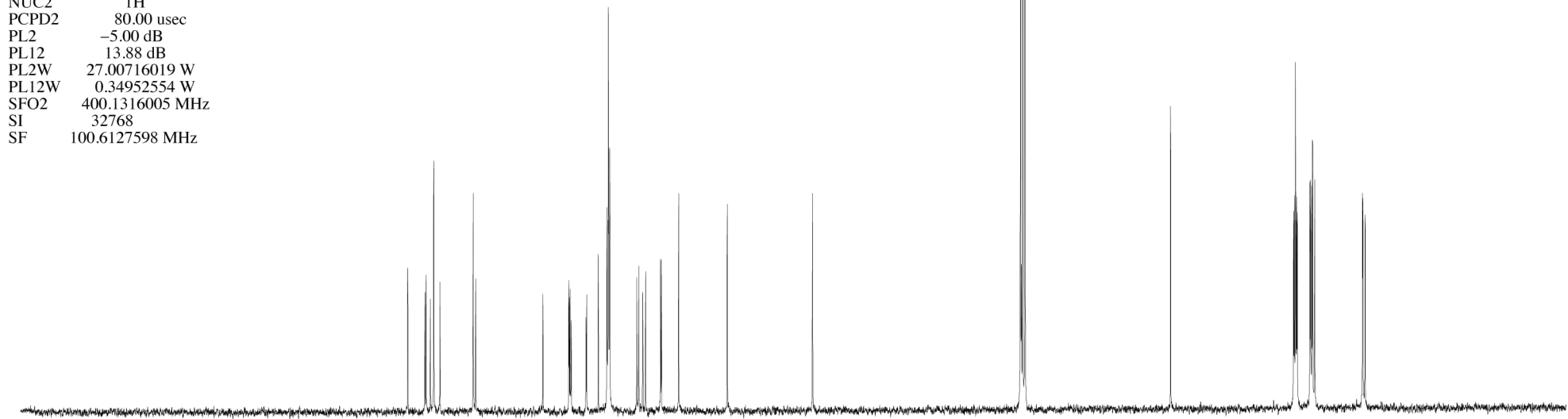
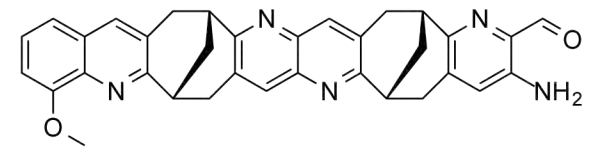NAME   TW1059a
EXPNO   1
PROCNO   1
Date_   20130326
Time   18.07
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zg30
TD   57690
SOLVENT   CDCl3
NS   16
DS   2
SWH   7211.539 Hz
FIDRES   0.125005 Hz
AQ   3.9998901 sec
RG   161
DW   69.333 usec
DE   6.00 usec
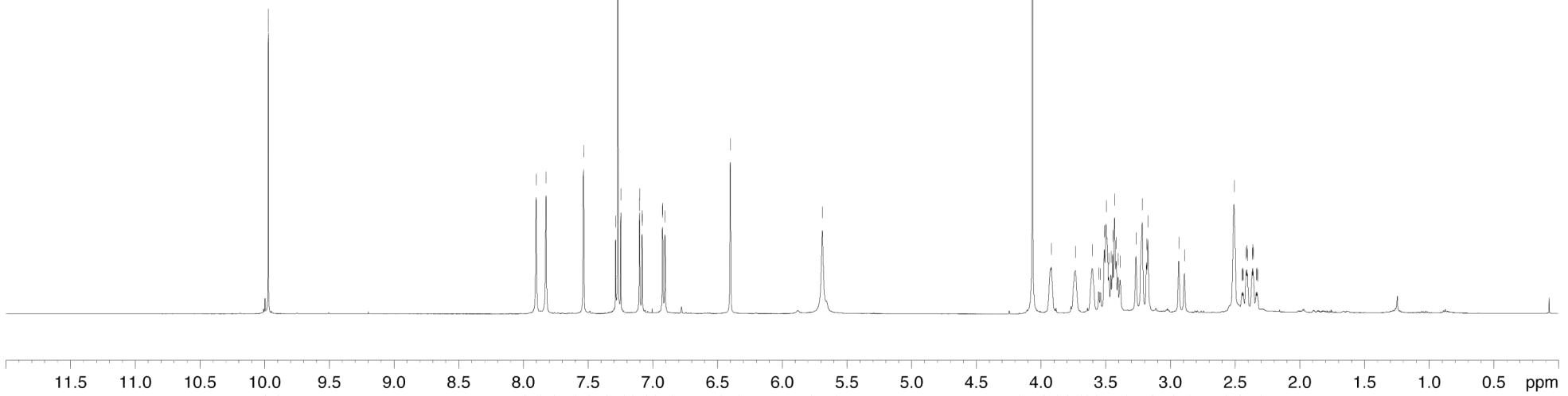TE   294.1 K
D1   0.00100000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   10.00 usec
PL1   −4.00 dB
PL1W   21.45254898 W
SFO1   400.1334011 MHz
SI   131072
SF   400.1300056 MHz
WDW   EM
SSB   0
LB   0.10 Hz
GB   0
PC   4.00

Compound 15

9.987

7.870
7.816
7.753
7.691
7.506
7.270
7.254
7.234
7.057
7.038
6.927
6.908
6.407

5.723

5.282
4.071
3.904
3.704
3.546
3.534
3.521
3.479
3.443
3.432
3.418
3.405
3.389
3.376
3.253
3.211
3.195
3.178
3.169
3.150
3.134
3.088
2.867
2.823
2.481
2.405
2.373
2.333
2.305
2.300

0.93

1.08
1.00
0.98
0.99
1.00
0.76
1.00
0.98

0.98

1.86

3.05
1.05
3.19
8.20
5.13
1.05
4.05
2.09

S19

NAME TW1059a
EXPNO 2
PROCNO 1
Date_ 20130327
Time 7.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgdc30
TD 48074
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.500030 Hz
AQ 0.9999892 sec
RG 57
DW 20.800 usec
DE 6.00 usec
TE 295.9 K
D1 0.00100000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 −3.00 dB
PL1W 58.63890457 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 −4.00 dB
PL12 14.06 dB
PL2W 21.45254898 W
PL12W 0.33533499 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127602 MHz

Peaks: 195.858

162.065 161.668 161.637 161.488 160.165 155.022 149.413 144.600 141.601 141.580 141.411 139.262 136.557 136.340 136.072 135.937 135.903 133.773 131.905 131.724 131.381 131.257 128.648 128.552 125.893 124.191 118.748 106.940

77.477 77.161 76.842

56.222 38.563 38.405 38.367 38.227 38.172 37.906 36.333 36.135 36.106 36.048 35.882 34.459 29.044 28.911 28.855

Compound 15

S20

Compound 15

Compound 16

Compound 16 with approximately 13% of compound 15 present.

S22
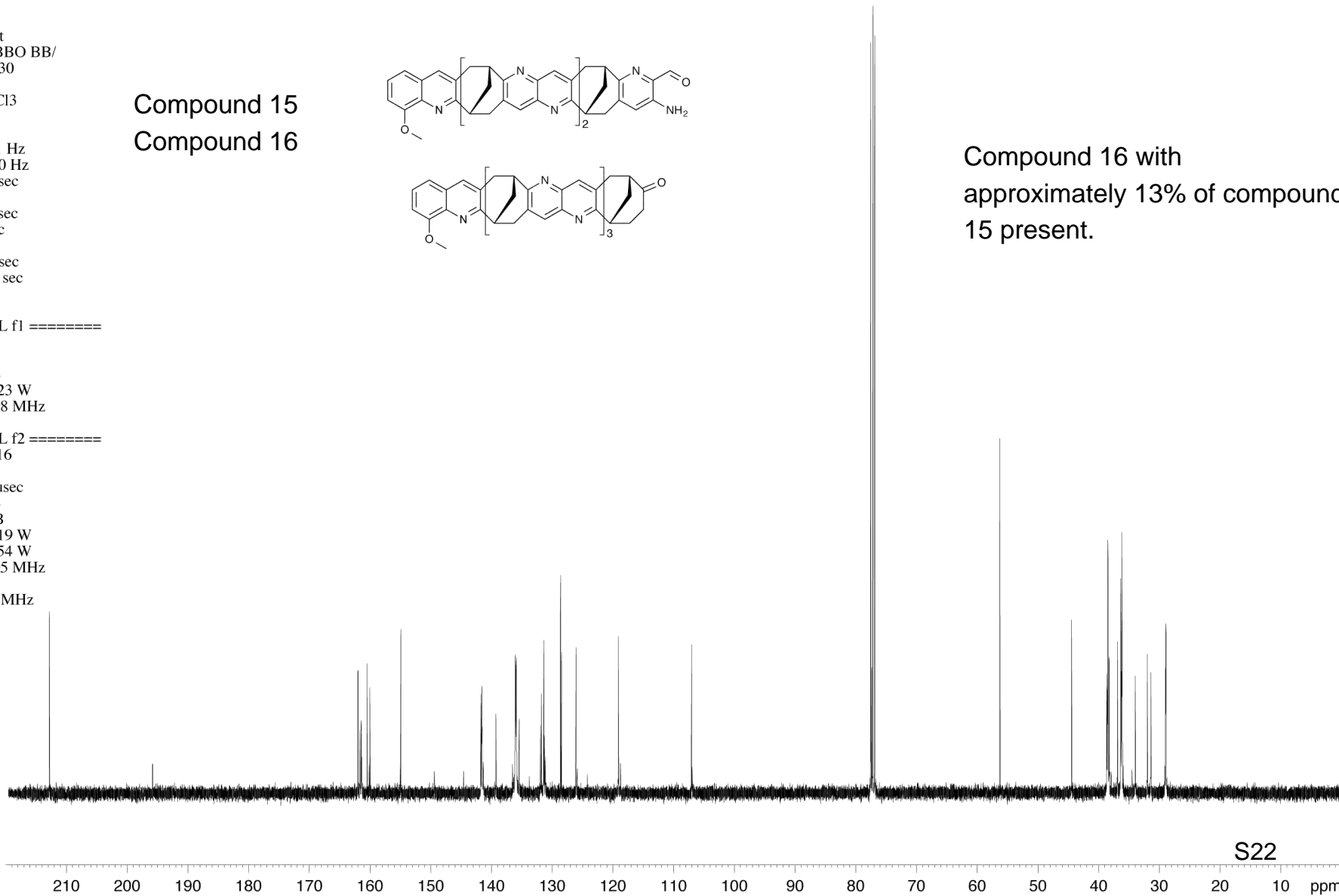
Compound 2 as a mixture of
2·TFA and 2·(TFA)2

•TFA

•(TFA)₂
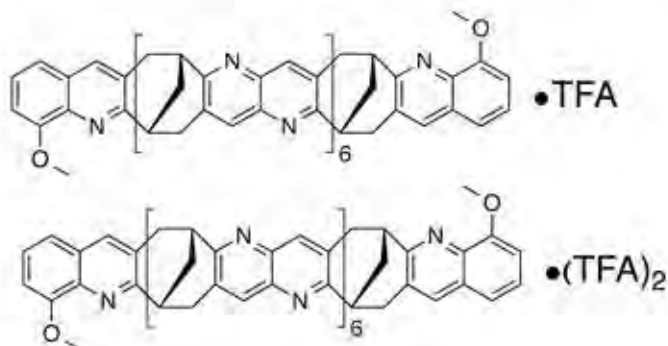
NAME   TW1103
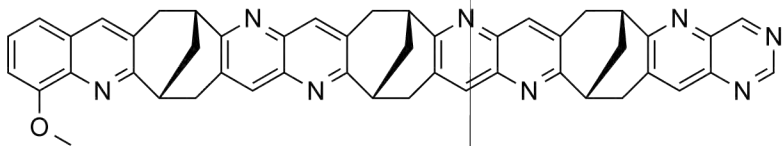EXPNO   3
PROCNO   1
Date_   20130528
Time   18.45
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgflqn
TD   131072
SOLVENT   CDCl3+MeOD
NS   128
DS   4
SWH   89285.711 Hz
FIDRES   0.681196 Hz
AQ   0.7340532 sec
RG   1820
DW   5.600 usec
DE   6.50 usec
TE   294.9 K
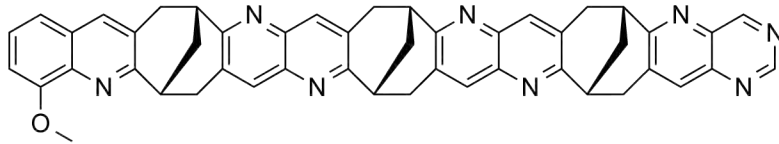D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   19F
P1   10.60 usec
PL1   -5.00 dB
PL1W   25.25963783 W
SFO1   376.4607164 MHz
SI   65536
SF   376.4983660 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

−66 −68 −70 −72 −74 −76 −78 −80 −82 −84 −86 −88 ppm

0.09   1.00

7.834
7.818
7.726
7.704
7.676
7.370
7.350
7.330
7.270
7.255
7.253
7.235
6.963
6.945

4.061
3.902
3.725
3.655
3.648
3.555
3.542
3.513
3.499
3.471
3.452
3.401
3.354
3.324
3.320
3.316
3.312
3.308
3.222
3.204
3.180
3.163
3.138
3.095
3.052
2.495
2.463

Compound 2

S24
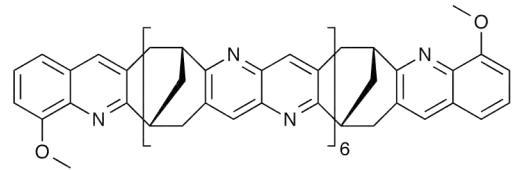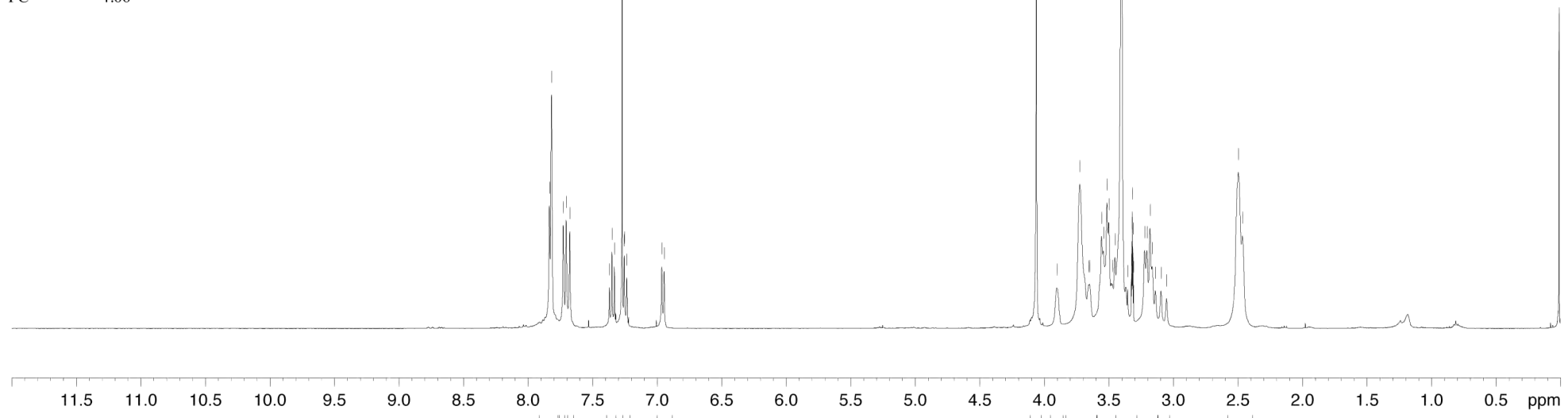
8.19
2.03
1.92
1.90
2.06
1.83
1.97

6.11
2.33
13.87
13.92
10.03
2.10
14.00

NAME TW1106
EXPNO 1
PROCNO 1
Date_ 20130528
Time 15.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 57690
SOLVENT CDCl3+MeOD
NS 128
DS 2
SWH 7211.539 Hz
FIDRES 0.125005 Hz
AQ 3.9998901 sec
RG 256
DW 69.333 usec
DE 6.00 usec
TE 294.9 K
D1 0.00100000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.10 usec
PL1 −5.00 dB
PL1W 27.00716019 W
SFO1 400.1334011 MHz
SI 131072
SF 400.1300213 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
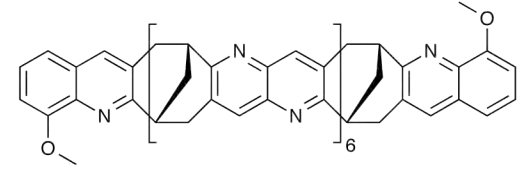
Compound 2 with TFA added to the NMR-sample.

from TFA

S25

NAME   TW1112
EXPNO   3
PROCNO   1
Date_   20130614
Time   23.36
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgdc30
TD   48074
SOLVENT   CDCl3+MeOD
NS   12000
DS   4
SWH   24038.461 Hz
FIDRES   0.500030 Hz
AQ   0.9999892 sec
RG   57
DW   20.800 usec
DE   6.00 usec
TE   295.8 K
D1   0.00100000 sec
D11   0.03000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   8.00 usec
PL1   −4.00 dB
PL1W   73.82200623 W
SFO1   100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 usec
PL2   −5.00 dB
PL12   13.88 dB
PL2W   27.00716019 W
PL12W   0.34952554 W
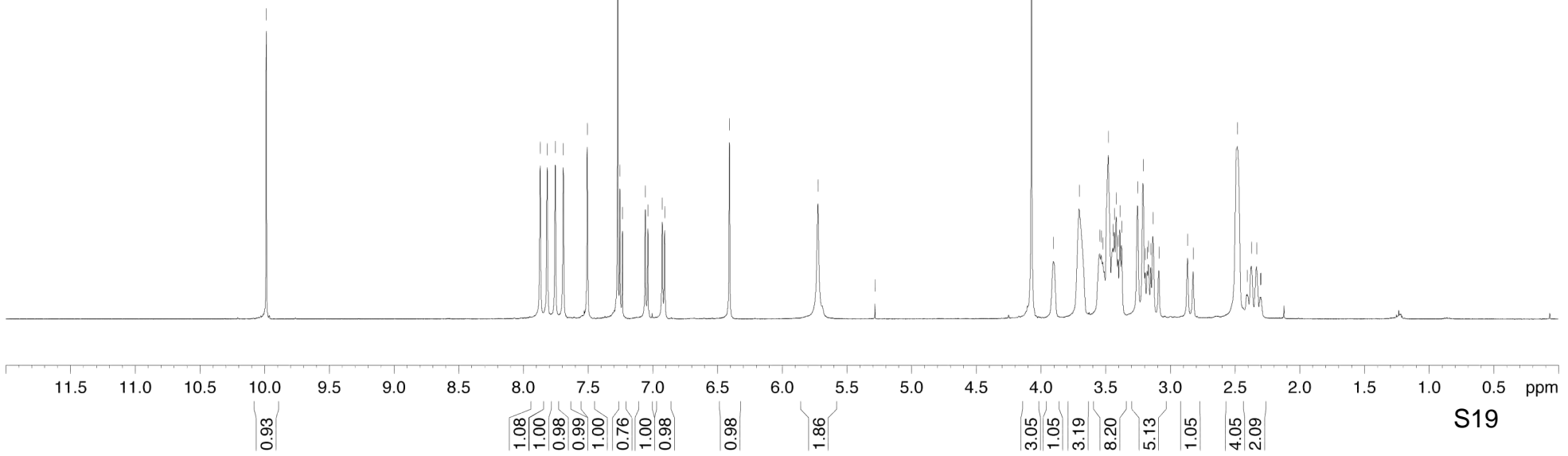SFO2   400.1316005 MHz
SI   32768
SF   100.6127670 MHz

Peak labels (left region): 162.316, 161.834, 161.797, 161.491, 159.953, 154.628, 141.345, 141.333, 141.301, 141.207, 141.171, 138.976, 136.248, 136.102, 136.040, 135.764, 135.683, 132.378, 131.575, 131.435, 131.356, 131.248, 128.566, 126.195, 118.987, 107.084

Peak labels (center): 77.478, 77.160, 76.840

Peak labels (right region): 38.462, 38.154, 37.921, 37.875, 36.111, 35.864, 35.828, 35.731, 35.485, 28.793, 28.510, 28.320
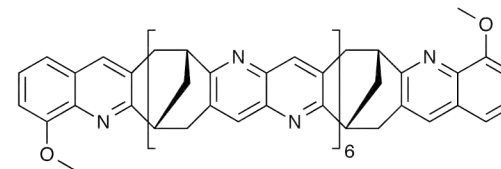
Compound 2

S26
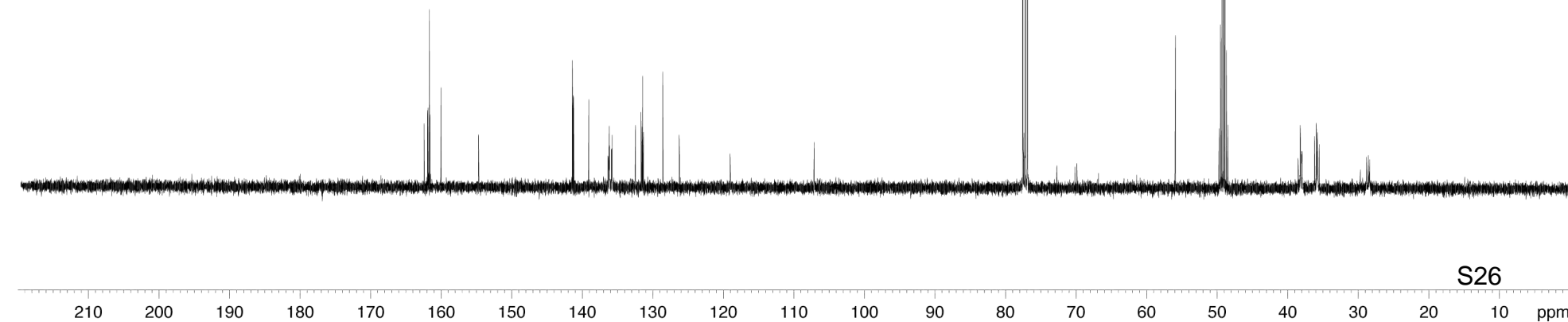
NAME   TW1163b
EXPNO   7
PROCNO   1
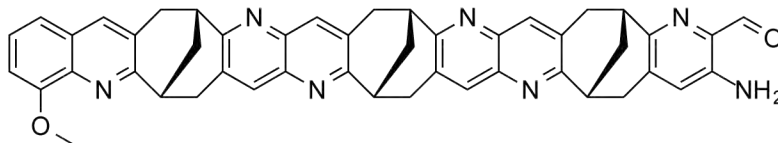Date_   20131103
Time   16.48
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgdc30
TD   48074
SOLVENT   CDCl3+MeOD
NS   32768
DS   4
SWH   24038.461 Hz
FIDRES   0.500030 Hz
AQ   0.9999892 sec
RG   57
DW   20.800 usec
DE   6.00 usec
TE   296.0 K
D1   0.00100000 sec
D11   0.03000000 sec
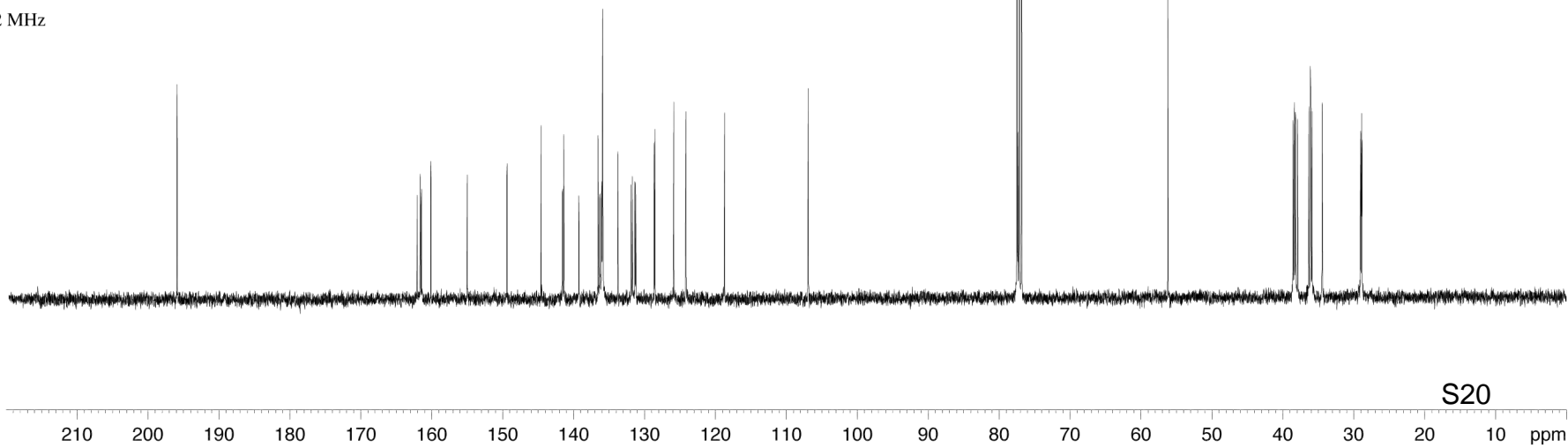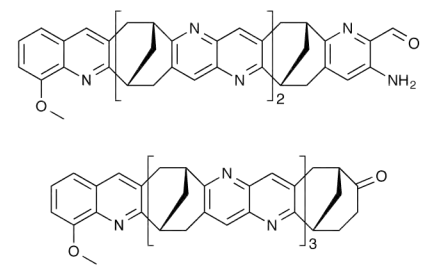TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   8.00 usec
PL1   −4.00 dB
PL1W   73.82200623 W
SFO1   100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 usec
PL2   −5.00 dB
PL12   13.88 dB
PL2W   27.00716019 W
PL12W   0.34952554 W
SFO2   400.1316005 MHz
SI   262144
SF   100.6127663 MHz

Peaks: 162.314, 161.861, 161.817, 161.639, 161.508, 159.968, 154.608, 141.373, 141.313, 141.238, 141.187, 138.912, 136.356, 136.154, 136.087, 135.781, 135.691, 132.375, 131.589, 131.446, 131.376, 131.352, 131.246, 128.614, 128.584, 126.252, 119.009, 107.153, 77.480, 77.161, 76.843, 55.936, 49.780, 49.566, 49.353, 49.139, 48.925, 48.712, 48.498, 38.486, 38.184, 37.928, 36.132, 35.901, 35.843, 35.745, 35.479, 28.798, 28.530, 28.393, 28.331
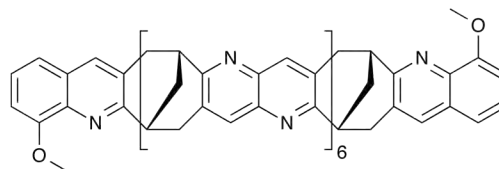
Compound 2
13C data in the paper is a
combination of this and the
previous 13C spectra

S27
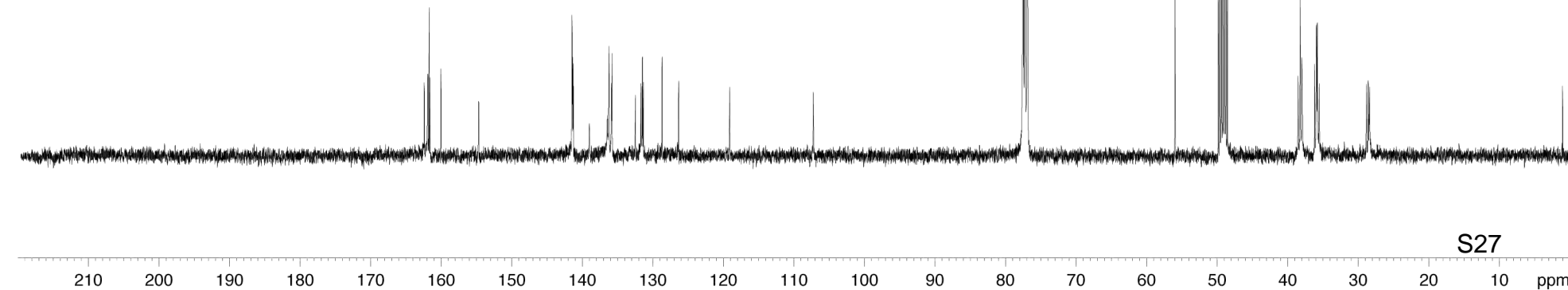
NMR Titrations

$[H]_0$ is the concentration of the host and it remains constant during the titration.

$[G]_0$ is the concentration of the stock solution of the guest.

The guest solution is prepared in the host solution. This solution is then added in portions (V_{add}) to the NMR sample. This solution also serves as the final data-point in each measurement. Noted as "Max conc." in the tables below.

$[G]$ is the concentration of the guest in the NMR sample in each measurement.

$\Delta\delta = \delta_{obs} - \delta_0$

δ_{obs} is the observed chemical shift of the host for each measurement in the presence of guest.

δ_0 is the observed chemical shift of the host without any guest present.

$\Delta\delta_{calc}$ is fitted to $\Delta\delta$ according to Eq. 1. using Kaleidagraph.

$$\Delta\delta_{calc} = \frac{\Delta\delta_{max}}{[H]_0}\left(\left(\frac{1}{2}[H]_0 + [G]_0 + \frac{1}{K_a}\right) - \sqrt{\frac{1}{4}\left([H]_0 + [G]_0 + \frac{1}{K_a}\right)^2 - [H]_0[G]_0}\right) \quad \text{Eq. 1}$$

$\Delta\delta_{max} = \delta_0 - \delta_{max}$; δ_{max} is the chemical shift at 100% complexation.

V_{add} and V_{tot} is the added volume of guest and the total volume in the NMR sample respectively.

The resonance used in the fit is from the proton shown in the structures below.

Solvent: MeOH-d_4 10%v/v in CDCl$_3$

Host: **1**   [H]$_0$: 0.8 mM

Guest: GndBPh$_4$ [G]$_0$: 68.5 mM

Initial Volume: 0.50 mL
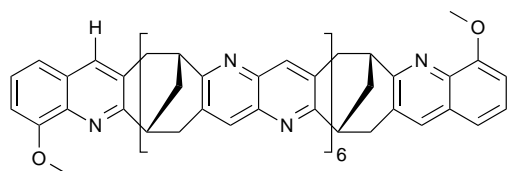
V$_{add}$ (mL)	V$_{tot}$ (mL)	[G] / M	$\Delta\delta$	$\Delta\delta_{calc}$	[HG]/[H]$_0$
0	0.5	0.000	0.000	0.000	0.0
0.02	0.52	0.003	-0.002	-0.002	1.2
0.03	0.55	0.006	-0.004	-0.004	2.7
0.05	0.6	0.011	-0.007	-0.007	4.9
0.07	0.67	0.017	-0.011	-0.010	7.2
0.1	0.77	0.024	-0.014	-0.014	9.7
0.15	0.92	0.031	-0.017	-0.018	12.3
0.25	1.17	0.039	-0.022	-0.022	15.0
0.4	1.57	0.047	-0.025	-0.025	17.3
	Max.	0.069	-0.034	-0.034	23.5
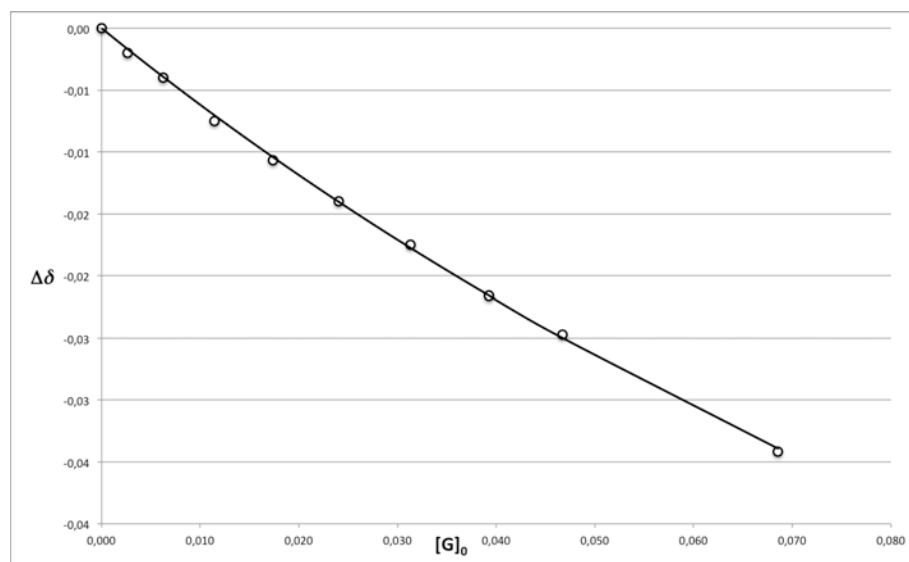
K_a: 5.0±0.5 M^{-1}
$\Delta\delta_{max}$: -0.13
R^2 = 0.999

Solvent: MeOH-d_4 10%v/v in CDCl₃

Host: **16**   [H]₀: 1.1 mM

Guest: GndBPh₄   [G]₀: 63.4 mM

Initial Volume: 0.50 mL
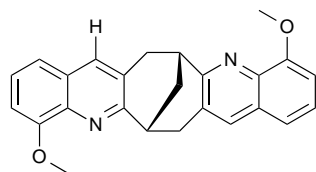
V_{add} (mL)	V_{tot} (mL)	[G] / M	$\Delta\delta$	$\Delta\delta_{calc}$	[HG]/[H]₀
0	0.5	0.000	0.000	0.000	0.0
0.02	0.52	0.002	-0.001	-0.001	2.0
0.03	0.55	0.006	-0.003	-0.002	4.6
0.05	0.6	0.011	-0.004	-0.004	8.1
0.07	0.67	0.016	-0.006	-0.006	11.8
0.1	0.77	0.022	-0.008	-0.008	15.6
0.15	0.92	0.029	-0.009	-0.009	19.3
0.25	1.17	0.036	-0.010	-0.011	23.1
	Max conc.	0.063	-0.017	-0.017	34.4
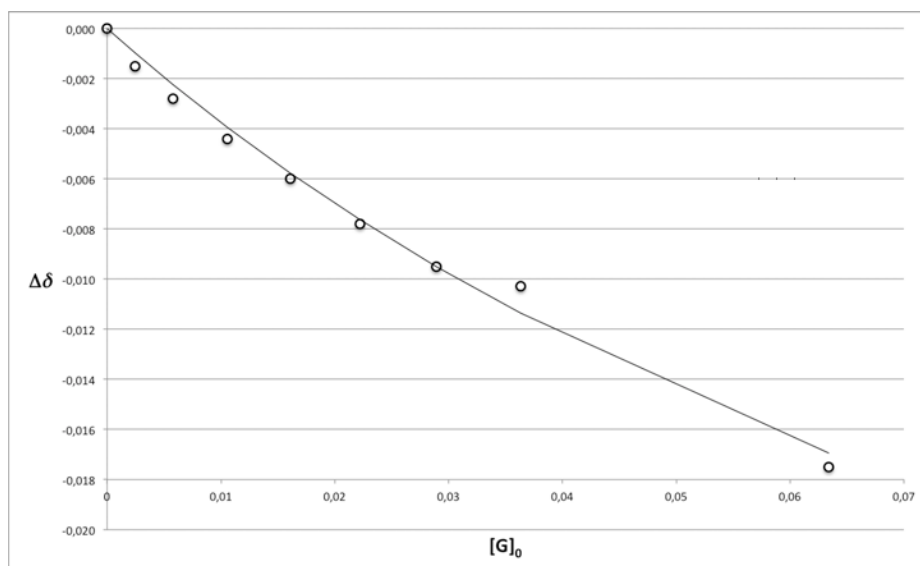
K_a: 8.1±2.2 M⁻¹
$\Delta\delta_{max}$: -0.05
$R^2 = 0.991$

Solvent: MeOH-d_4 10%v/v in CDCl$_3$

Host: 8-Methoxyquinoline　　　　　　　[H]$_0$: 0.8 mM

Guest: GndBPh$_4$　　　　　　　　　　　[G]$_0$: 61.8 mM

Initial Volume: 0.50 mL
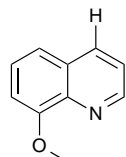
V_{add} (mL)	V_{tot} (mL)	[G] / M	$\Delta\delta$	$\Delta\delta_{calc}$	[HG]/[H]$_0$
0	0.5	0.000	0.000	0.000	0.0
0.02	0.52	0.002	-0.001	-0.001	3.5
0.03	0.55	0.006	-0.003	-0.003	7.9
0.05	0.6	0.010	-0.005	-0.005	13.6
0.07	0.67	0.016	-0.007	-0.008	19.3
0.1	0.77	0.022	-0.010	-0.010	24.9
0.15	0.92	0.028	-0.012	-0.012	30.1
0.25	1.17	0.035	-0.014	-0.014	35.1
0.4	1.57	0.042	-0.016	-0.016	39.2
	Max	0.062	-0.019	-0.019	48.6
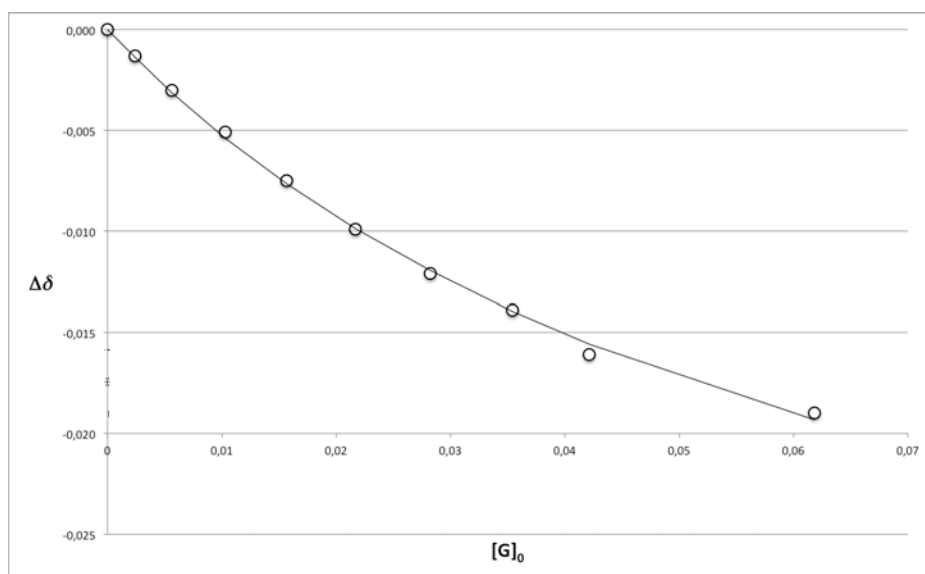
K_a: 15.6±1.2M^{-1}
$\Delta\delta_{max}$: -0.04
R^2 = 0.998

S3 Molecular Dynamics Simulations

S3.1 Host-Guest Interactions

S3.1.1 Initial Structures of Heptamer 2 - Guanidinium Complexes

The initial structures used as starting points for MD simulations (prepared as described in the Methods section of the article) are shown in Figure S1.

A   **B**   **C**
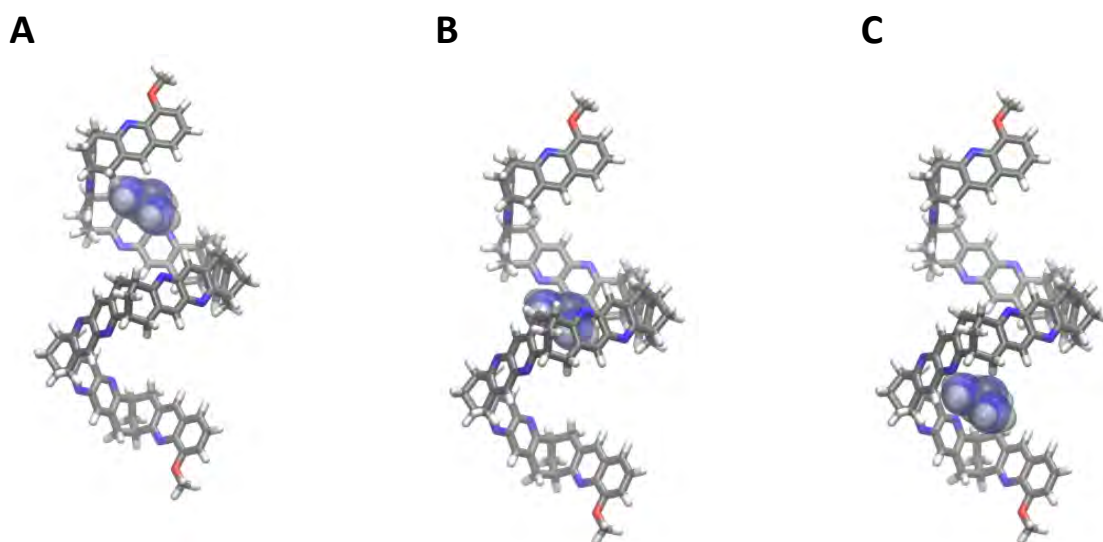
Figure S1. Initial geometry of 2•Gnd complexes A, B and C used as starting points for 250 ns MD simulations.

S3.1.2 Heptamer 2 - Acetylcholine Interatomic Distances in MD Simulations

MD time series for the minimum distances between any atom in acetylcholine (ACh) and heptamer **2** are shown in Figure S2.
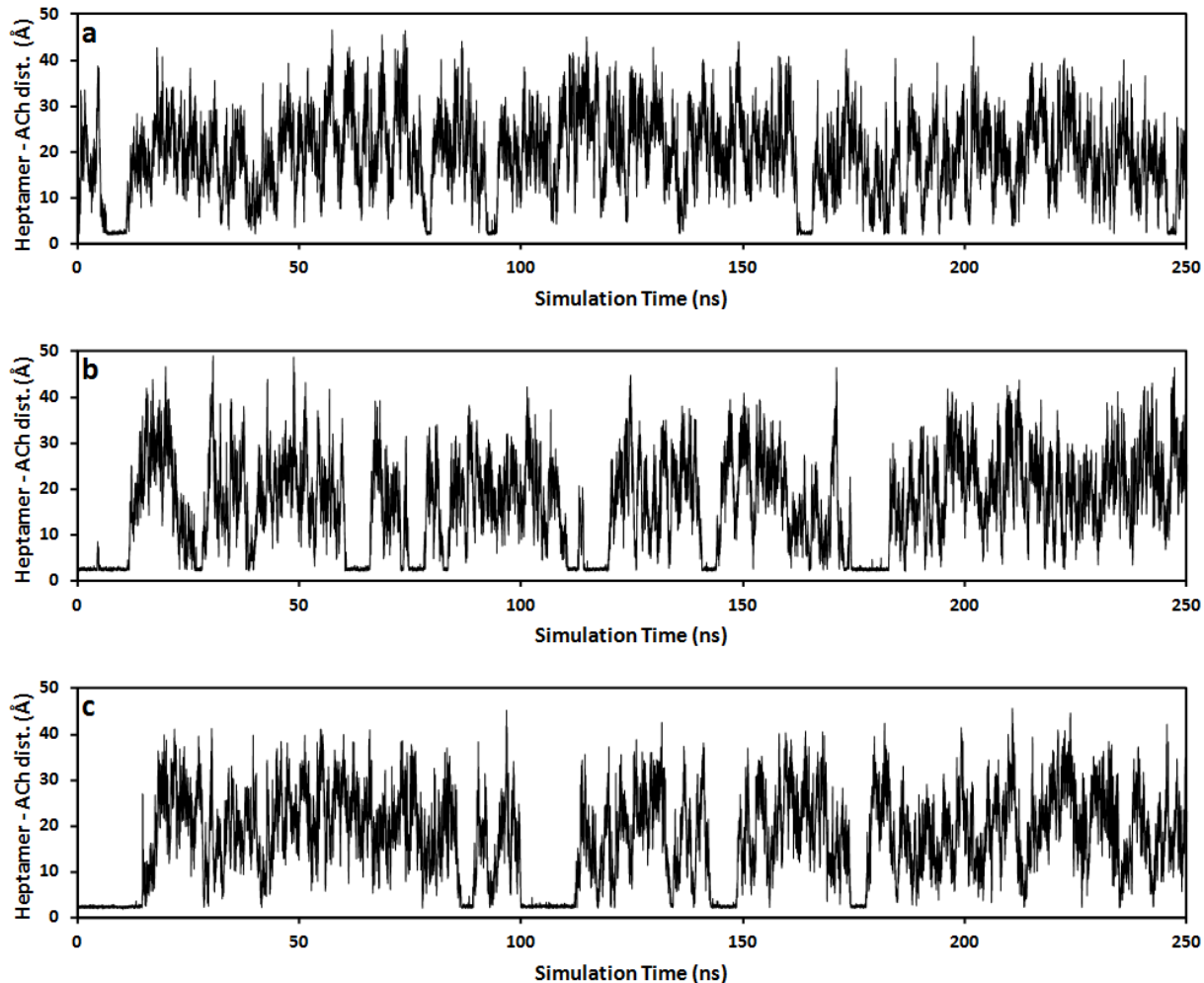
Figure S2. Minimum distance between any atom in heptamer 2 and acetylcholine (ACh) during three 250 ns MD simulations. Simulations were carried out in chloroform and started from different the geometries (A, B, C in Figure S1) corresponding to "top", "middle" or "bottom" initial positioning of Ach along the heptamer axis.

S3.1.3 Heptamer 2 - Guanidinium Interatomic Distances in MD Simulations

MD time series for the minimum distances between any atom in guanidinium (Gnd) and heptamer **2** are shown in Figure S3. Snapshots are shown in
Figure S4 - Figure S6.
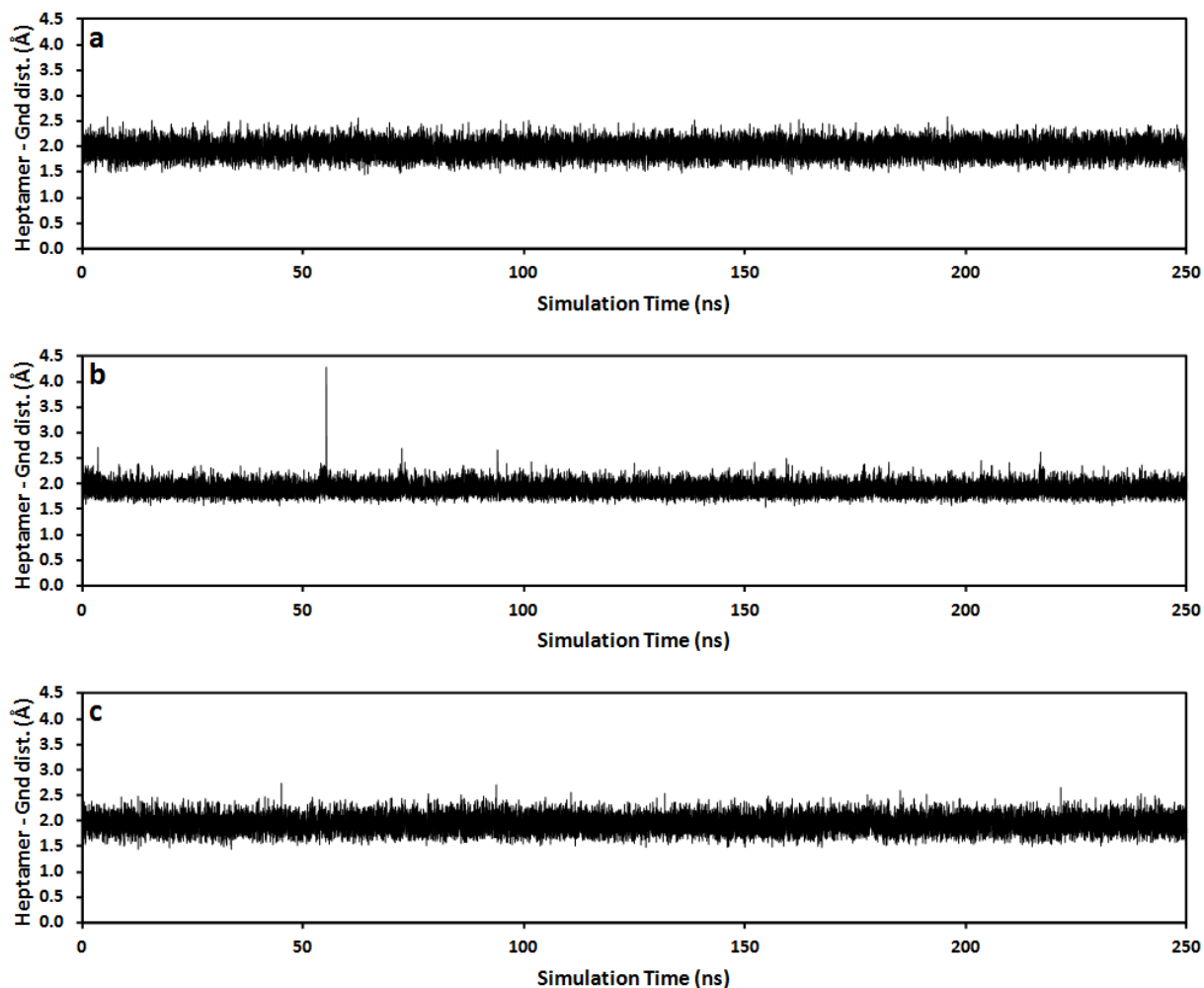
Figure S3. Minimum distance between any atom in heptamer 2 and guanidinium (Gnd) during three 250 ns MD. Simulations were carried out in chloroform started from different geometries (A, B, C), see Figure S1.

S3.1.4. Snapshots from Heptamer 2 - Guanidinium Simulations
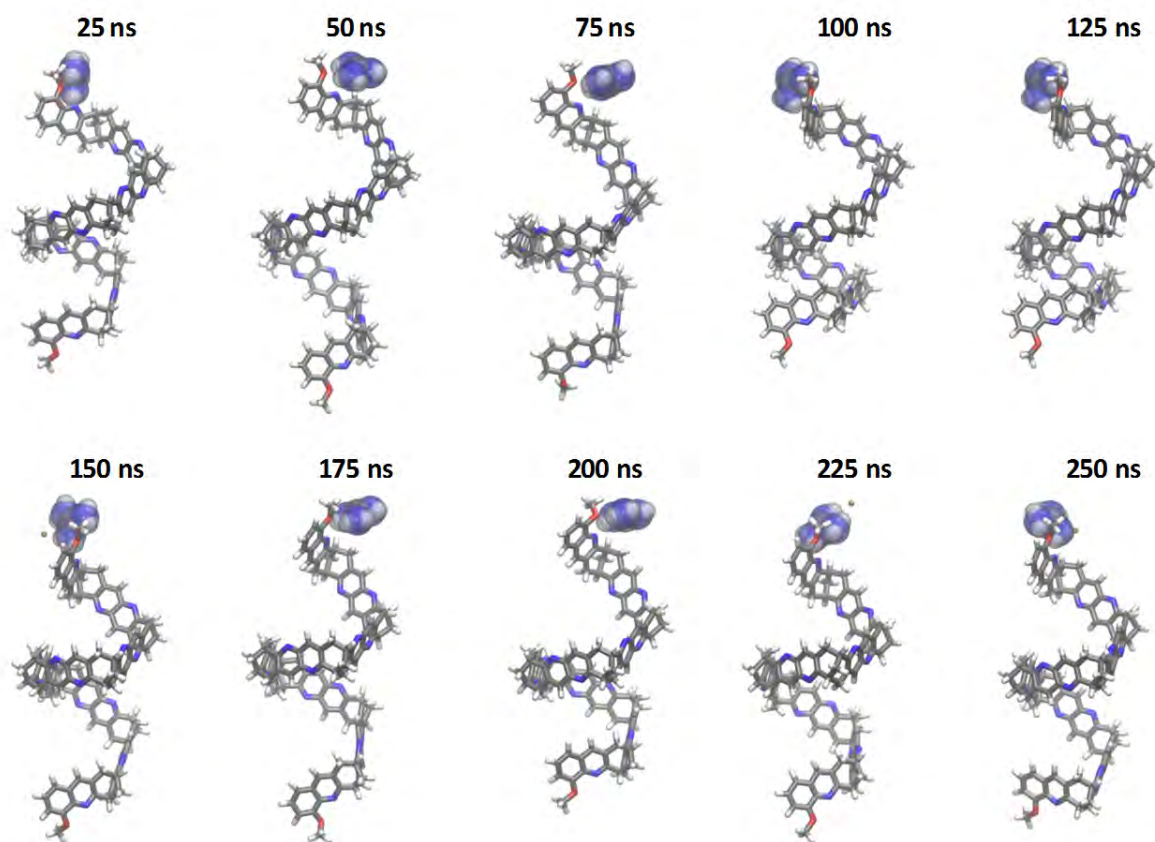
Figure S4. Snapshots extracted from the 250 ns MD simulation of heptamer 2 - guanidinium complex A.
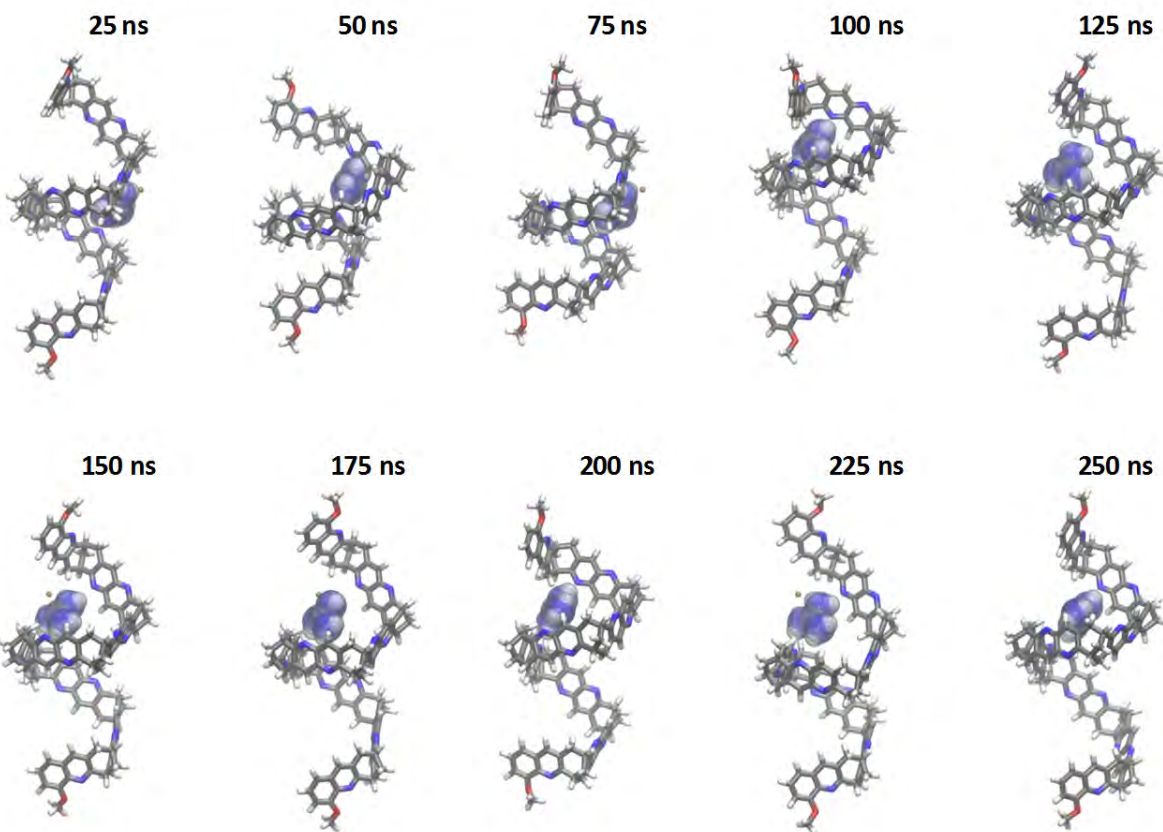
Figure S5. Snapshots extracted from the 250 ns MD simulation of heptamer 2 - guanidinium complex B.
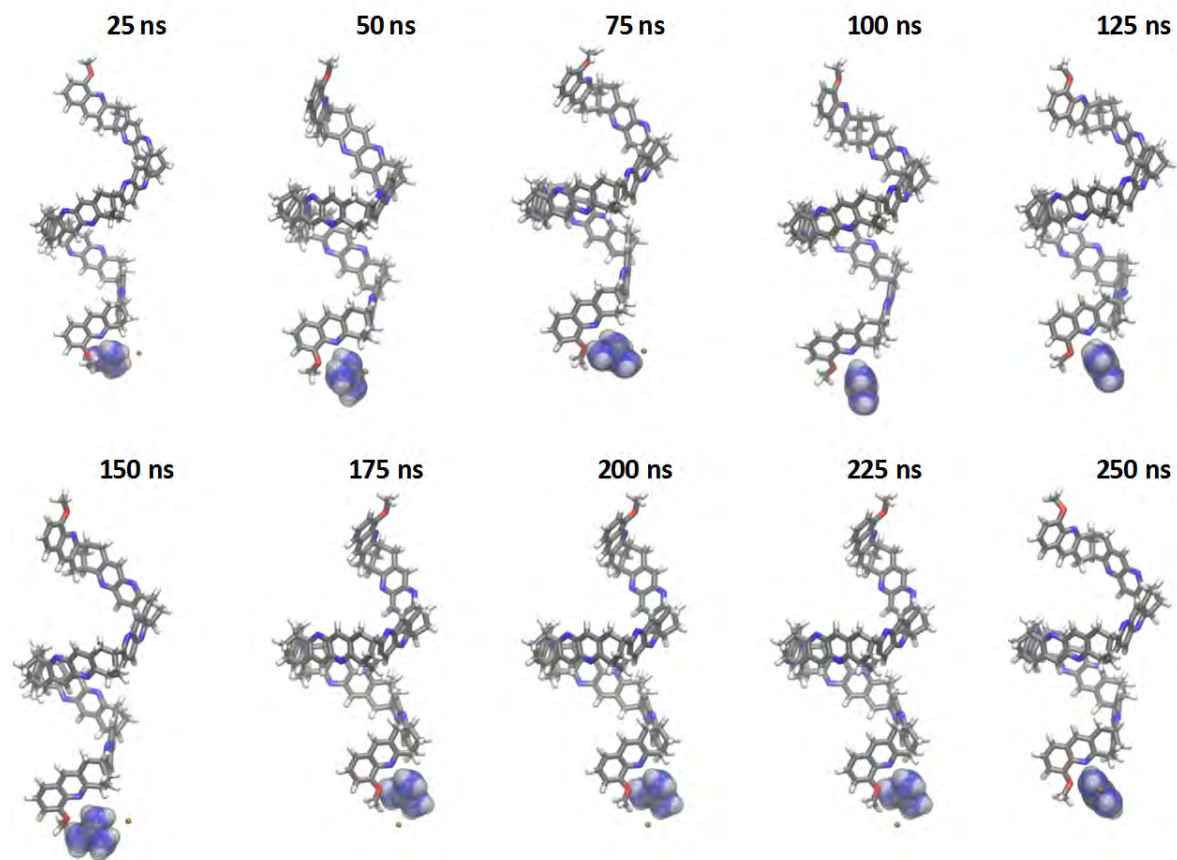
Figure S6. Snapshots extracted from the 250 ns MD simulation of heptamer 2 - guanidinium complex C.

S3.1.5 MD Snapshot of Heptamer 2 - Guanidinium Bridging Interaction

In the MD simulation started with Gnd positioned near the middle of heptamer **2**, i.e. geometry B (Figure S1b), Gnd occasionally bridged two 1,5-naphthyridine nitrogen atoms, which caused axial contraction of the heptamer, see Figure S7.
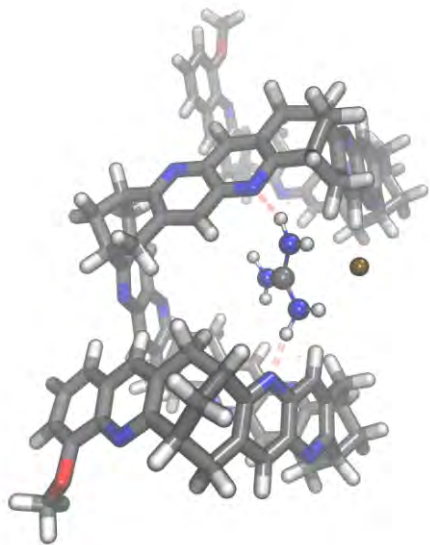
Figure S7. Snapshot from the MD simulation started from geometry B in Figure S1b, showing bridging of two 1,5-naphthyridine nitrogen atoms by guanidinium. The chloride counterion is shown as a yellow sphere.

S3.2 MD Simulations of the Free Heptamer 2

S3.2.1 Heptamer 2 MD Snapshots from 300 K and 400 K Simulations

Snapshots extracted at t = 0, 25, 50, 75 and 100 ns are shown in Figure S8 for the 300 K (top panel) and 400 K (bottom panel) simulations of the free heptamer **2** in explicit chloroform.

The simulations at 400 K caused visible perturbations of the heptamer, such as the longitudinal compression seen in Figure S8 at t = 50 ns. In contrast, the simulation at 300 K did not produce substantial perturbations. The structural conservation in this simulation was also evident from the high similarity between the averaged MD heptamer structure (Figure 4b) and the single OPLS_2005 optimized heptamer structure (Figure 4a).
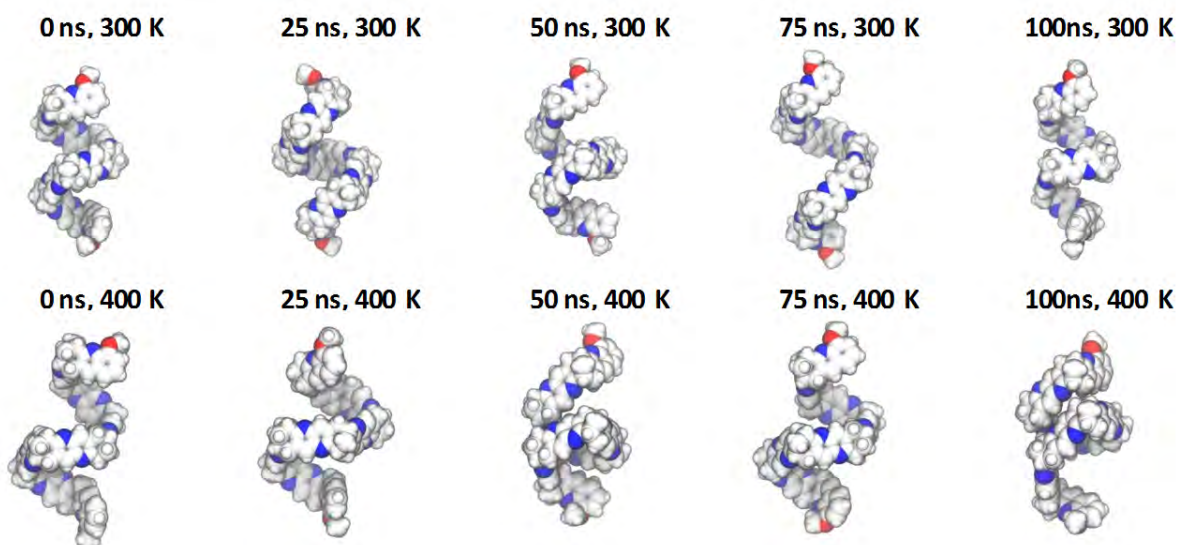
Figure S8. **Snapshots from the isolated heptamer 2 simulations extracted at 25 ns intervals at 300 K (top panel) and 400 K (bottom panel).**

S4 Heptamer 2 Molecular Models

S4.1 Heptamer 2 Molecular Model from B3LYP-D3/6-31G(d) Optimization
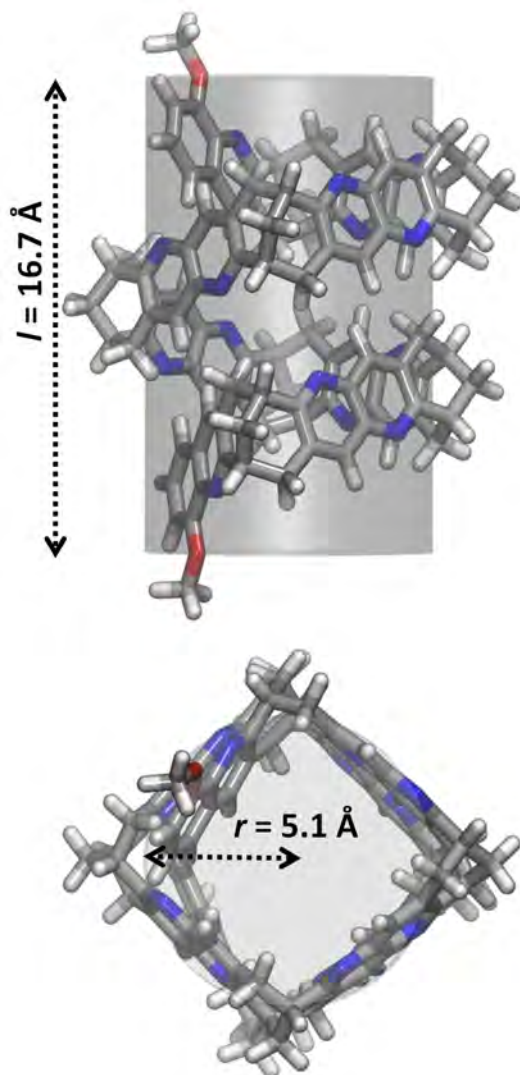
Figure S9. Heptamer 2 structure optimized at the B3LYP-D3/6-31G(d) level of theory. The structure deviated significantly from other models of the heptamer **2** (see Figure 4) and produced poor overlays with the crystal structure of **14**. For these reasons, the model was not considered further in the study.

S5 Calculated Heptamer ECD/UV Spectra

S5.1ECD/UV Spectra for Different Heptamer Models at Different Levels of Theory
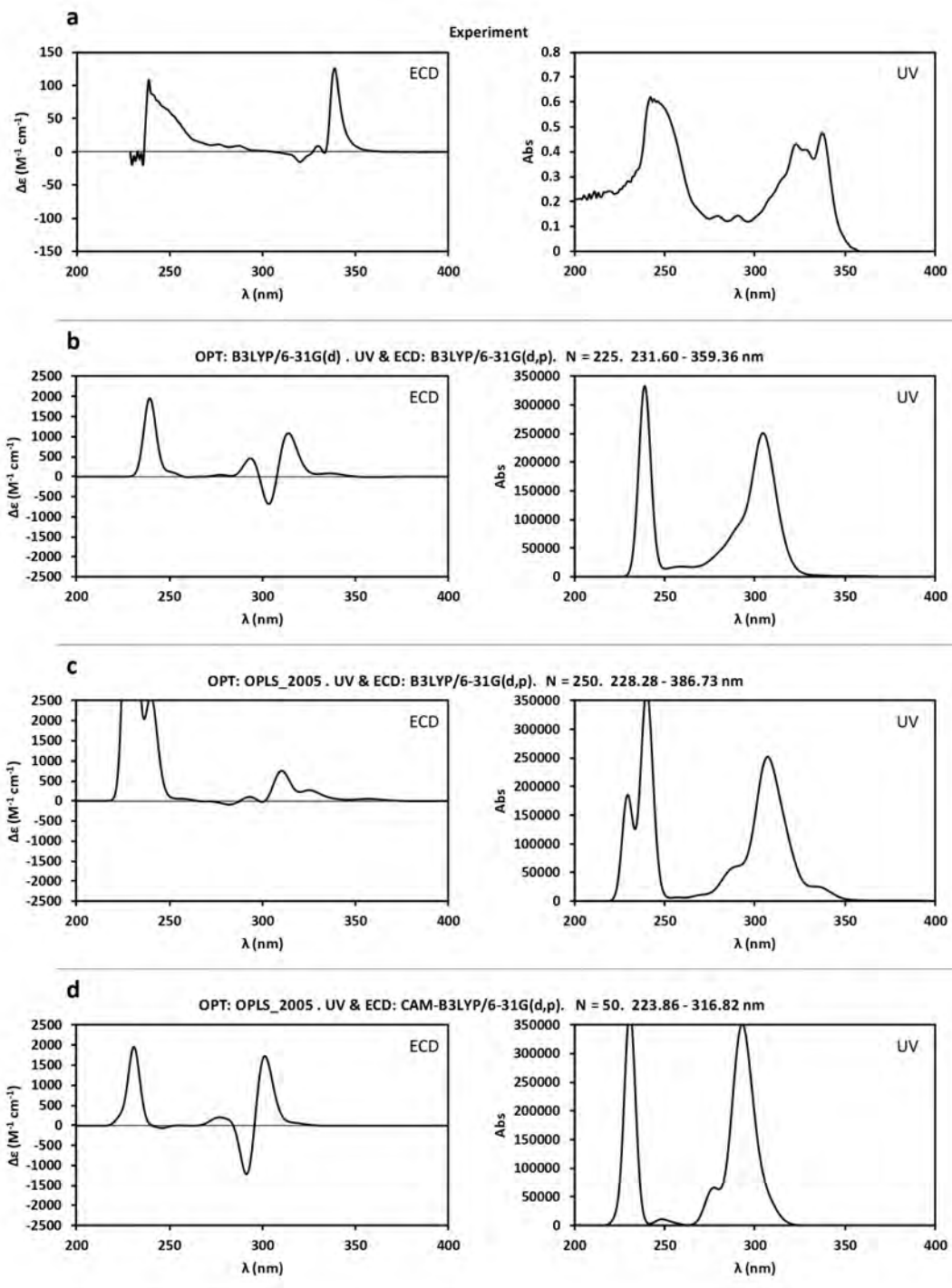
Figure S10. Calculated (b - d) and experimental (a) ECD/UV spectra for the heptamer 2. A bandwidth of 0.1 eV was used for calculated ECD curves. **a**, Experimental ECD and UV spectra. **b**, B3LYP/6-31G(d) geometry, B3LYP/6-31G(d,p) spectra. **c**. OPLS_2005 geometry, B3LYP/6-31G(d,p) spectra. **d**. OPLS_2005 geometry, CAM-B3LYP/6-31G(d,p) spectra.

S5.2 Heptamer ECD Spectra at Different Bandwidths

Calculated ECD spectra are influenced considerably by the choice of bandwidth (σ) as more spectral details are revealed at narrow bandwidths [13]. For the heptamer **2**, the spectra calculated at the B3LYP/6-31G(d,p) level for the B3LYP/6-31G(d) geometry (Figure S11 left panel, top), and at the CAM-B3LYP/6-31G(d,p) level for the OPLS_2005 geometry (Figure S11 left panel, bottom) contain approximately the same level of detail at $\sigma = 0.1$ eV. A bandwidth of $\sigma = 0.2$ eV causes peak attenuation and broadening, as shown in Figure S11, right panel.

B3LYP/6-31G(d,p), 225 states, 0.1 eV **B3LYP/6-31G(d,p), 225 states, 0.2 eV**
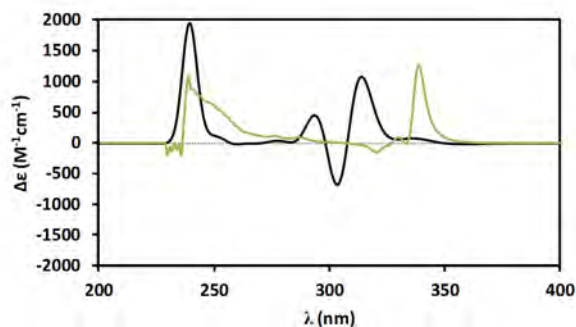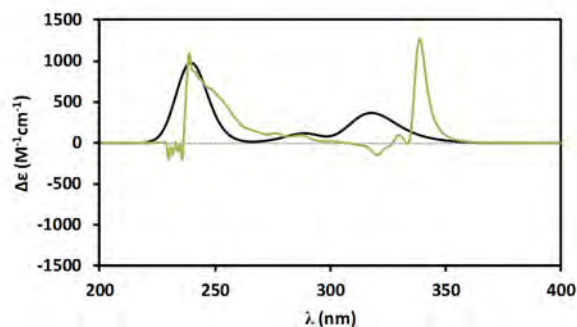
CAM-B3LYP/6-31G(d,p), 50 states, 0.1 eV **CAM-B3LYP/6-31G(d,p), 50 states, 0.2 eV**
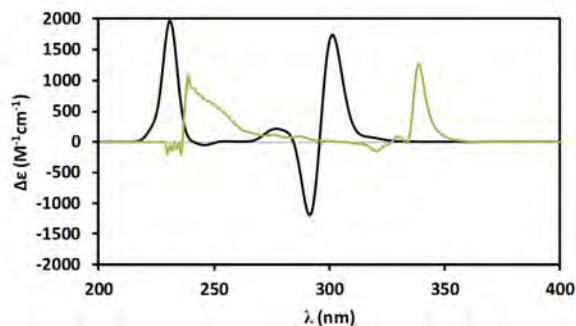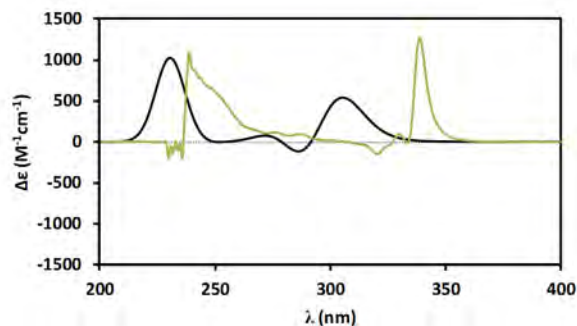
Figure S11. **Influence of bandwidth on calculated ECD spectra.** Simulated ECD spectra of heptamer **2** calculated at the B3LYP/6-31G(d,p) level (top panel) and the CAM-B3LYP/6-31G(d,p) level (bottom panel), using two different bandwidths (0.1 and 0.2 eV).

S6 Coordinates for Optimized Structures

S6.1B3LYP/6-31G(d) Optimized Geometry of Heptamer 2

```
C        3.27614600   -5.29972400    2.65349100
C        3.39768400   -4.85278500    1.17955500
C        4.78513500   -4.35513400    0.81915400
C        5.91549300   -4.65410100    1.64844900
C        5.74305000   -5.40620300    2.96234600
C        5.71879600   -4.42189500    4.15335500
C        4.44974400   -6.23289500    2.98242400
C        5.00512700   -3.62211800   -0.32765600
C        6.31234900   -3.19952500   -0.66416600
C        7.36552200   -3.56140800    0.22496400
N        7.14983600   -4.27385600    1.36390400
C        7.76140900   -2.10490300   -2.08707800
C        8.89543700   -2.42232100   -1.26897100
C        8.67398300   -3.14605900   -0.11651100
N        6.52567400   -2.47624500   -1.79651700
C       -7.50336600   -3.53372600    0.28292500
C       -6.47320400   -3.06017000    1.14624400
N       -7.26874200   -4.42769300   -0.71533100
C       -6.03709600   -4.87856500   -0.88467900
C       -4.92823200   -4.47355300   -0.07201000
C       -5.16794500   -3.56230000    0.93476600
C       -5.84285000   -5.84284800   -2.04849000
C       -5.76194000   -5.07226800   -3.38498900
C       -3.38536700   -5.72555300   -1.67870100
C       -3.54145600   -5.04612300   -0.29997300
C       -4.56735800   -6.68230500   -1.88927400
N       -6.70537500   -2.15704000    2.13698700
C       -7.93758200   -1.70837300    2.30827900
C       -9.04919900   -2.12248400    1.50265500
C       -8.80878800   -3.03166700    0.49452800
C       -3.05904900   -2.70690700   -4.70045700
C       -1.98166000   -3.12308500   -3.86561300
N       -2.92506500   -1.72812700   -5.63584500
C       -1.74534700   -1.14788000   -5.78013400
C       -0.59400300   -1.49276700   -4.99917900
C       -0.73541900   -2.47873700   -4.04565800
C       -1.67995700   -0.03475800   -6.81847800
C       -2.25805800    1.28037700   -6.24944400
C       -1.32651900    1.97112400   -5.27021300
C        0.06069100    1.61728400   -5.19650600
C        0.62764600    0.49155800   -6.05199900
C        0.74261400   -0.81382500   -5.23380300
C       -0.24158900    0.22249400   -7.28851500
C       -1.77896600    2.97649700   -4.44183300
C       -0.88611700    3.63077300   -3.56081400
C        0.47193300    3.19887600   -3.56847900
N        0.91984300    2.20252900   -4.37903100
N       -1.33243500    4.62898400   -2.75096900
C       -0.46903200    5.22447600   -1.94518900
C        0.91736100    4.86772000   -1.87038500
```

```
C         1.36499900    3.85131800   -2.68723300
C        -1.04572200    6.31431300   -1.04900600
C        -1.77387400    5.69850300    0.16645000
C        -0.82463100    5.15148000    1.21629900
C         0.56176400    5.51463400    1.22058600
C         1.13518800    6.42608700    0.14234900
C         1.86531500    5.60145500   -0.94002000
C         0.04350200    7.26627800   -0.53593800
C        -1.27070000    4.30411000    2.20827500
C        -0.37377700    3.81837000    3.18805500
C         0.98635600    4.23268300    3.09128900
N         1.42906100    5.07016900    2.11488400
N        -0.81822500    2.98600000    4.16789800
C         0.04833300    2.54284100    5.06332600
C         1.44034100    2.88539800    5.05276100
C         1.88712300    3.73146200    4.05994600
C        -0.51472500    1.58908200    6.11007400
C        -0.67646000    0.17001100    5.52259200
C         0.64427300   -0.55810400    5.35636000
C         1.82527800   -0.11166900    6.03523600
C         1.80591500    1.14880300    6.89162200
C         2.38633300    2.34921300    6.11112500
C         0.38515800    1.50561700    7.35106300
C         0.74340300   -1.68243800    4.56480300
C         1.97695900   -2.36376200    4.44561500
C         3.08751300   -1.83642900    5.16629100
N         2.99472200   -0.72243400    5.94185300
C         3.23696900   -4.09073900    3.57915000
C         4.41628900   -3.65094600    4.26533700
C         4.32044200   -2.52023800    5.04872200
N         2.07053300   -3.47346500    3.66451500
N        -2.11814600   -4.09473100   -2.92320700
C        -3.29556200   -4.68062600   -2.78404900
C        -4.44368500   -4.34485900   -3.57417700
C        -4.30450100   -3.35360700   -4.52245100
H         9.48875500   -3.41198500    0.55274100
H         2.31883400   -5.81887300    2.76697700
H         3.14920700   -5.71161800    0.53848400
H         2.65107600   -4.07984100    0.96534100
H         6.62142400   -6.04940300    3.07897700
H         6.56329500   -3.72782500    4.07581700
H         5.87260600   -4.99747300    5.07827600
H         4.31973800   -6.69451100    3.96962600
H         4.49341300   -7.04830900    2.24916000
H         4.19011600   -3.35265400   -0.99524500
H        -4.36939100   -3.20708200    1.58177700
H        -6.73097700   -6.48224200   -2.08471900
H        -5.89425000   -5.79207900   -4.20643200
H        -6.59648100   -4.36546300   -3.45390900
H        -2.43544800   -6.27019000   -1.67699200
H        -2.78535100   -4.26096300   -0.18774700
H        -3.33100000   -5.79482700    0.47815700
H        -4.64919900   -7.36402900   -1.03318600
H        -4.41737700   -7.30297700   -2.78185600
H        -9.60569300   -3.37988500   -0.15827500
H         5.17889400   -2.12877600    5.58937900
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H	0.09618700	-2.78245300	-3.41424200
H	-2.31582100	-0.34335000	-7.65474100
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H	-3.22598500	1.08257100	-5.77511100
H	1.63944300	0.79274000	-6.34250000
H	1.23517600	-0.60716100	-4.27694800
H	1.40204700	-1.50456300	-5.77996500
H	0.15250300	-0.64147600	-7.83859000
H	-0.22260000	1.07771300	-7.97612100
H	-2.82041400	3.28938200	-4.44442200
H	2.40314300	3.52791200	-2.67575900
H	-1.78910800	6.85442800	-1.64453700
H	-2.40121400	6.47836000	0.62309500
H	-2.45578200	4.91035300	-0.17245900
H	1.87642800	7.06771300	0.63008700
H	2.55034700	4.89193000	-0.46231400
H	2.48905300	6.28701000	-1.53276500
H	0.47951500	7.84561800	-1.35971100
H	-0.39369000	7.98625700	0.16760300
H	-2.30959100	3.98712000	2.26063100
H	2.93114600	4.02825200	3.99327900
H	-1.51175400	1.95759600	6.37309800
H	-1.32253300	-0.41056000	6.19771900
H	-1.20122200	0.22554800	4.56228200
H	2.45974500	0.96107800	7.74959100
H	3.34080200	2.06477000	5.65401800
H	2.61157100	3.15088600	6.83003500
H	0.39876400	2.46011900	7.89261200
H	-0.00655300	0.74900700	8.04282400
H	-0.11264500	-2.06891500	4.01687700
H	-5.13823900	-3.04450000	-5.14842700
C	7.91734600	-1.26255500	-3.34701600
C	7.53242700	0.20814300	-3.06951000
C	8.58293500	0.95514100	-2.26943700
C	9.91476700	0.45303200	-2.14679400
C	10.30476000	-0.89010000	-2.75195300
C	10.29476700	-1.99588500	-1.67330400
C	9.35458000	-1.30100900	-3.88525900
C	8.29795200	2.15370400	-1.65039200
C	9.29143000	2.86053800	-0.93322100
C	10.58932400	2.26580300	-0.88281800
N	10.86880400	1.08188900	-1.48122200
C	10.06792900	4.72554600	0.38965600
C	11.36469800	4.15715900	0.45224500
C	11.63422400	2.95002400	-0.16766600
C	9.04725100	4.10081700	-0.28369800
H	9.89160300	5.67459100	0.88897700
H	12.14042900	4.68467700	0.99481200
H	7.21142400	-1.65917200	-4.08416900
H	7.39065700	0.71379300	-4.03628800
H	6.56523700	0.24463400	-2.55521500
H	11.33173100	-0.78965300	-3.11787200
H	10.85563900	-1.65755400	-0.79483900
H	10.83273100	-2.87012100	-2.06937700
H	9.61338200	-2.30619500	-4.24207000
H	9.44808500	-0.62173200	-4.74221600

H	7.29391100	2.57173500	-1.70807500
C	-10.53500100	2.47114300	0.24770000
C	-9.21672700	3.02144100	0.25602400
N	-10.88768300	1.42013400	1.02776800
C	-9.98870300	0.88548600	1.83684300
C	-8.64386800	1.35719300	1.93537900
C	-8.28403000	2.41860600	1.13221100
C	-10.45760600	-0.32055100	2.64143000
C	-10.44690900	-1.59378500	1.76729400
C	-8.11288500	-0.66314600	3.40288500
C	-7.65973700	0.72693100	2.90260600
C	-9.57164800	-0.56449400	3.87151300
C	-8.89425000	4.11844800	-0.58788500
C	-9.85906900	4.64827900	-1.40885100
C	-11.17490100	4.12224900	-1.43304300
C	-11.52013800	3.05376400	-0.62489000
H	-7.26673100	2.80621600	1.16443600
H	-11.49385300	-0.12571100	2.93625500
H	-11.03075800	-2.37152400	2.28208400
H	-10.96115300	-1.39437400	0.82042500
H	-7.45433500	-0.95249100	4.22856400
H	-6.66955500	0.64694300	2.43962500
H	-7.54325000	1.38500600	3.77658300
H	-9.67312000	0.25244000	4.59740500
H	-9.88466400	-1.48620700	4.37856200
H	-9.62264200	5.48737100	-2.05778400
H	-11.90482800	4.57134100	-2.09641100
H	8.05382300	4.53925600	-0.32942900
H	-7.88608500	4.52406200	-0.57177900
O	12.84037000	2.32887500	-0.16263700
O	-12.75014600	2.48324600	-0.57846400
C	13.91033200	2.95559500	0.52406700
H	14.77109100	2.29624300	0.39900700
H	14.14167800	3.94095000	0.09755300
H	13.69200400	3.06986300	1.59442300
C	-13.76516400	3.01872700	-1.41046100
H	-14.65753200	2.42215800	-1.21279200
H	-13.97010400	4.07086400	-1.17089200
H	-13.50135600	2.93752700	-2.47357400

S6.2 OPLS_2005 Optimized Geometry of Heptamer 2

```
C        3.79006300   -3.50397400   -5.19691500
C        3.94357600   -1.98862700   -4.94065300
C        5.36799200   -1.56653000   -4.58599200
C        6.46184800   -2.44234800   -4.77301300
C        6.26201500   -3.86689500   -5.29550300
C        6.23697800   -4.89205600   -4.14066200
C        4.94949100   -3.97802500   -6.08873800
C        5.62188600   -0.27464500   -4.08177900
C        6.94164700    0.11815500   -3.77677600
C        7.97354600   -0.84383400   -4.00298900
N        7.73173100   -2.08575400   -4.48583800
C        8.45488100    1.71977400   -3.01536800
C        9.54838100    0.84389200   -3.20388800
C        9.29387600   -0.44956200   -3.70359400
N        7.18396600    1.36093400   -3.29613200
C       -7.97409000    0.80574800   -4.01023900
C       -6.94225600   -0.15425000   -3.77495600
N       -7.73195700    2.04312600   -4.50448000
C       -6.46182300    2.39687800   -4.79449800
C       -5.36821800    1.52276200   -4.59902200
C       -5.62237800    0.23549000   -4.08294600
C       -6.26171700    3.81640900   -5.33039600
C       -6.23690500    4.85243200   -4.18536200
C       -3.78978900    3.45412100   -5.22778400
C       -3.94355600    1.94137900   -4.95695300
C       -4.94901400    3.91962700   -6.12434100
N       -7.18502500   -1.39255800   -3.28311100
C       -8.45605900   -1.74856600   -2.99928200
C       -9.54931800   -0.87417300   -3.19585900
C       -9.29453800    0.41448600   -3.70744200
C       -3.58667900    5.66023600   -1.52063900
C       -2.47820300    4.98252100   -2.11519700
N       -3.49400700    6.34558400   -0.35625600
C       -2.30352200    6.40480600    0.27742600
C       -1.14440200    5.77185800   -0.22644400
C       -1.24460700    5.05347900   -1.43547100
C       -2.27663800    7.18571900    1.59316300
C       -2.79125600    6.32707400    2.76963800
C       -1.76597300    5.32420200    3.29532700
C       -0.40600600    5.39652300    2.91672900
C        0.09013800    6.45253200    1.92672700
C        0.19698000    5.87922800    0.49640600
C       -0.85154100    7.66772600    1.91054100
C       -2.15778600    4.31478000    4.19820500
C       -1.20163500    3.41093600    4.70602900
C        0.14625100    3.57396400    4.26100400
N        0.52343500    4.53844600    3.38843900
N       -1.57822500    2.44850300    5.58118500
C       -0.64502700    1.60362200    6.06893200
C        0.71636800    1.68081300    5.69621200
C        1.10485500    2.67872000    4.77918800
C       -1.14453000    0.53456700    7.04309600
```

C	-1.75527400	-0.67028200	6.29388400
C	-0.71516000	-1.62549000	5.71173500
C	0.64631400	-1.54492800	6.08310700
C	1.14638800	-0.46686300	7.04712300
C	1.75675900	0.73091000	6.28645100
C	0.00118700	0.03807500	7.94019900
C	-1.10403200	-2.63195600	4.80407900
C	-0.14560900	-3.53186900	4.29377400
C	1.20240200	-3.36470200	4.73673900
N	1.57933300	-2.39419400	5.60276500
N	-0.52304300	-4.50444300	3.43025800
C	0.40627100	-5.36688400	2.96627800
C	1.76631700	-5.29113600	3.34387300
C	2.15841500	-4.27302500	4.23697400
C	-0.09016400	-6.43240100	1.98650300
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S7 Crystallographic details of compound 14

The crystals show a curious habit where individual crystallites with tetragonal shape form hexagonal, snow-flake like aggregates. A single tetragonal crystal was chosen for the x-ray diffraction experiment. The crystal diffracts well, but due to the small size, quite weakly. The diffraction pattern can be indexed in a tetragonal unit cell, a=13.4835 b=23.3611 Å and the systematic absences are consistent with the symmetry $P4_12_12$. Given the relative sizes of the molecule (ca. 60 non-hydrogen atoms) and the volume of the unit cell ca. 4250Å^3, Z is expected to be 4, and therefore a sub group of P41212 is expected. Further, the molecule exhibits a pronounced pseudo symmetry, the violation of which would be consistent with lowering the symmetry from $P4_12_12$ to one of the two maximal subgroups that split the orbit of the 2-fold axes along [110], $P4_1$ or $P2_12_12_1$. The crystal structure was solved using direct methods (Shelxs-97, REF) and a solution featuring fragments of the expected molecule sitting on the diagonal 2-fold axis was chosen as a starting point for refinements. The structure was refined using JANA2006, and positions of non-hydrogen atoms were added with the help of direct inspection of electron density maps. The asymmetric methoxy group was clearly visible in the electron density, but had to be modelled as half occupied. The structure was completed by adding hydrogen positions constrained in a riding model, and because of numerical instabilities, all inter-atomic distances were constrained to standard values. In the final stage of the refinement, some solvent positions were identified. These were best understood in terms of an ethanol molecule encased in the fold of the molecule sandwiched between two water molecules. The agreement factors for observed reflections remained above 10%. Anisotropic thermal displacement parameters could not be refined.

In the next step, the symmetry of the model was reduced to either of the two maximal subgroups $P2_12_12_1$ and $P4_1$. Symmetry reduction was seeded by removing one of the half occupied methoxy groups. Both models contain a single, independent molecule in the unit cell and the fit is improved to $R_1=8\%$ in two more or less indistinguishable fits between model and data. Thermal parameters were constrained so that sites related by the pseudo 2-fold symmetry were kept equal. For both models twinning according to the original super group symmetry is important. This result is unsurprising given that the expected intramolecular interaction is very weak, and the crystallization basically represents a packing of objects with pseudo 2-fold symmetry. Indeed, it may even be assumed that the sample in question constitutes an intergrowth between the two structural models. To investigate this, a new compound model was constructed using the solutions from $P2_12_12_1$ and $P4_1$ and the same interatomic distances as for the individual models and thermal parameters were constrained to be equal for corresponding sites in the two models. This compound model refined to an R_1 of 6.11 for 2405 observed reflections (a total of 14987 independent reflections were measured) and 426 parameters. All data pertaining to the refinement of the individual structures are given in the respective cif files, as there is no agreed format for cif files for multiple structures from one data set.

S8 REFERENCES

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