Electronic Supplementary Information

Sterically Controlled Naphthalene Homo-Oligoamides with Novel Structural Architectures

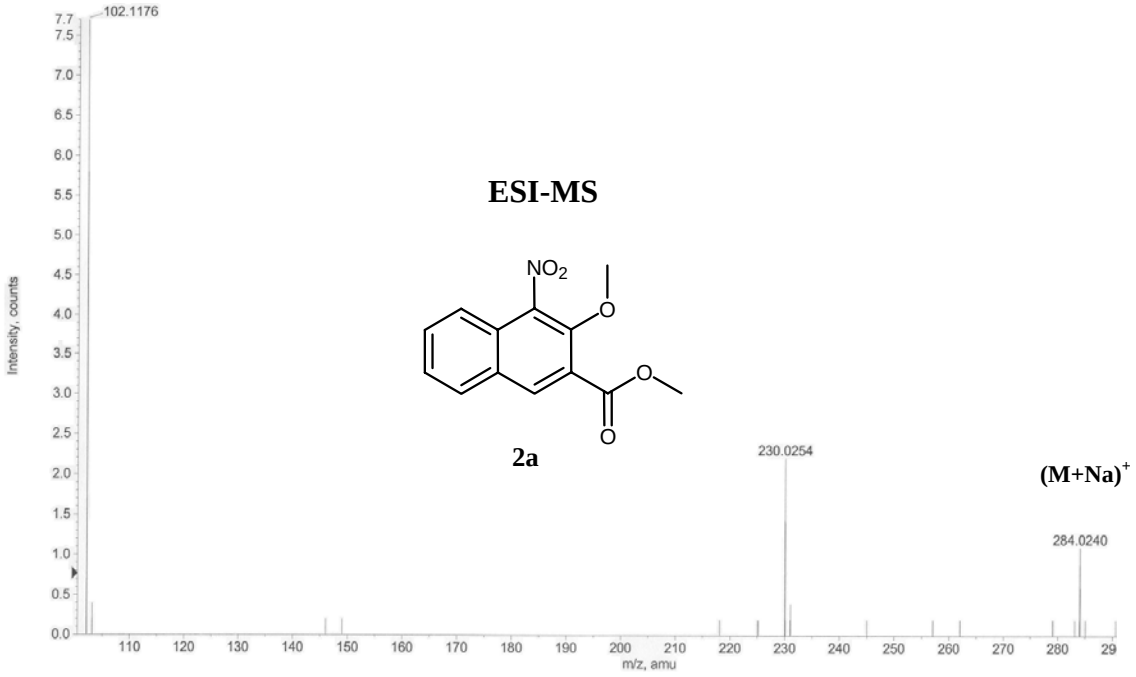
Panchami Prabhakaran,[a] Vedavati G. Puranik,[b] Jima N. C,[c] P. R. Rajamohanan,[,c] Hans-Jörg Hofmann*[,d] and Gangadhar J. Sanjayan*[,a,]*

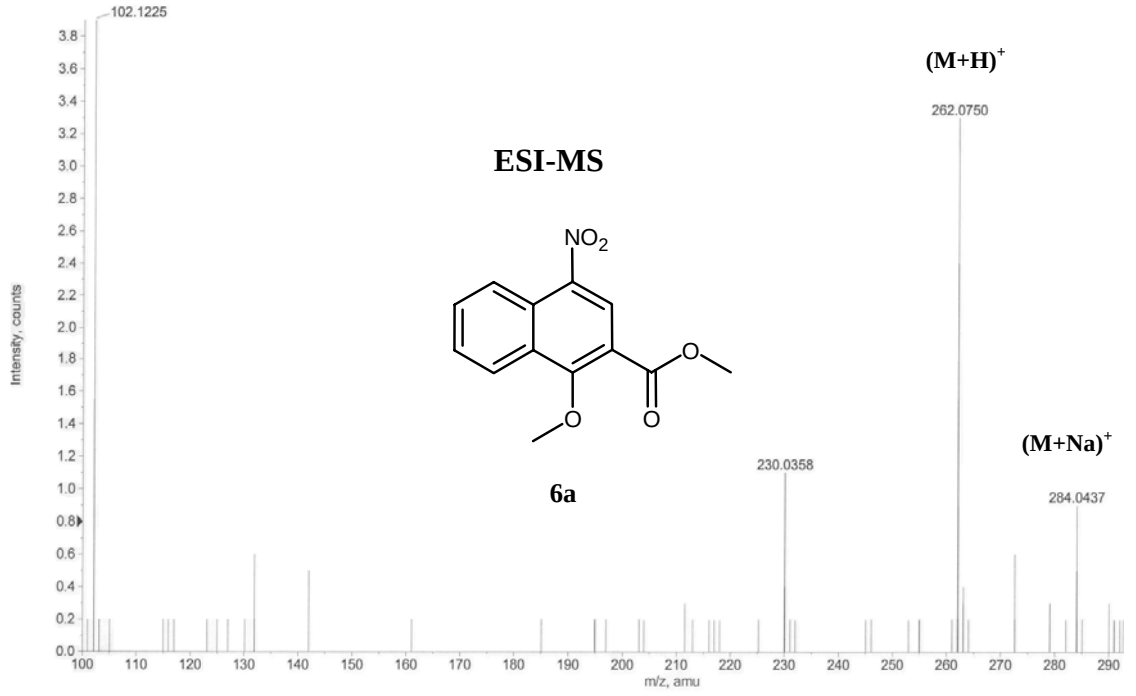
[a]Division of Organic Chemistry, [b]Center for Materials Characterization, [c]Central NMR Facility, National Chemical Laboratory, Dr. Homi Bhabha Road, Pune 411 008, India

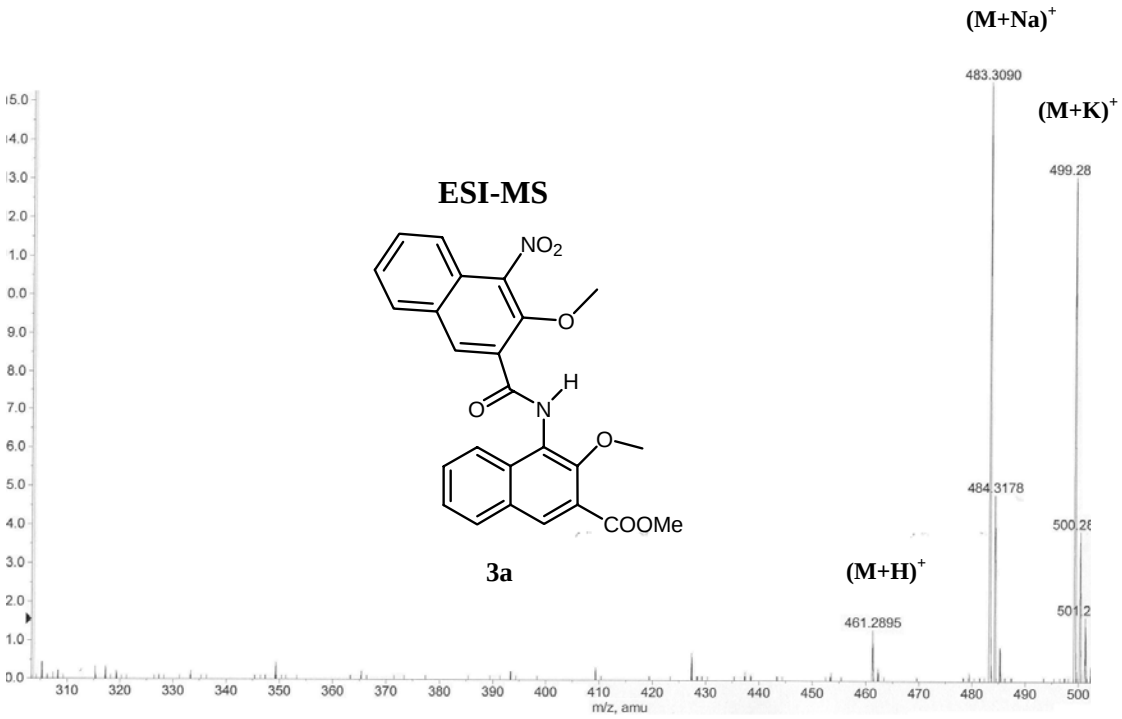
[d]Universität Leipzig, Fakultät für Biowissenschaften, Pharmazie und Psychologie, Institut für Biochemie, Brüderstraße 34, D-04103 Leipzig, Germany

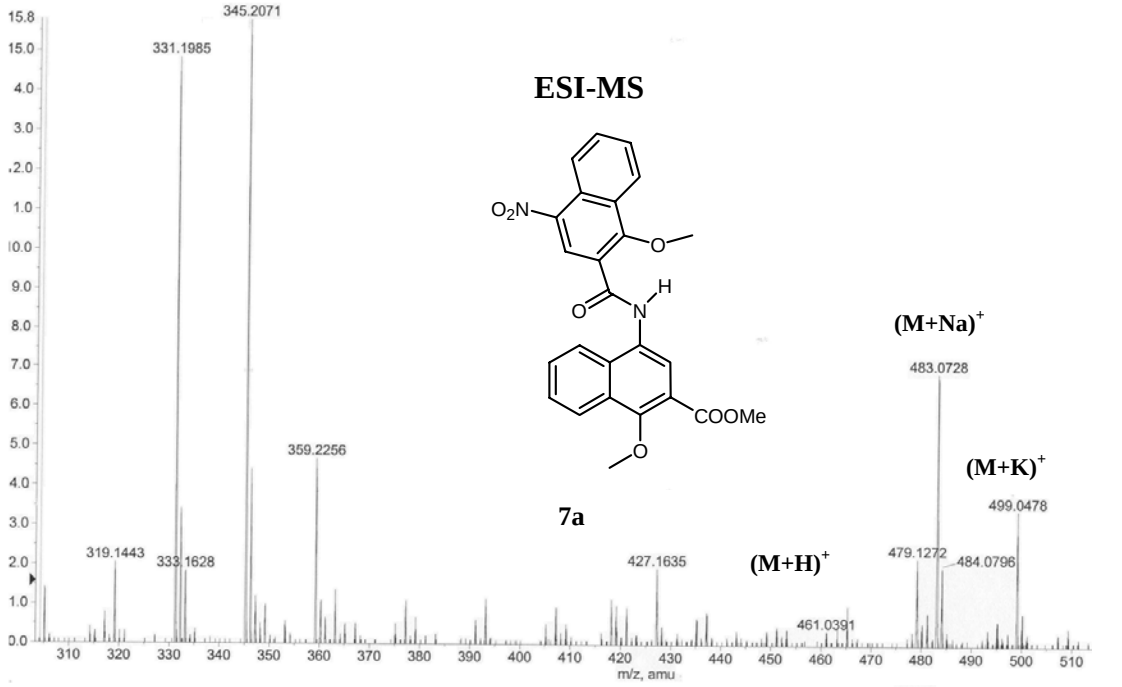
General Methods

Unless otherwise stated, all the chemicals and reagents were obtained commercially. Dichloromethane was dried by distilling over P_2O_5 and kept over 4 Å mol sieves. Analytical thin layer chromatography was done on precoated silica gel plates (Kieselgel $60F_{254}$, Merck). Column chromatographic purifications were done with 100-200 Mesh Silica gel. NMR spectra were recorded in $CDCl_3$ on AV 200 MHz, AV 400 MHz or AV-500 MHz Bruker NMR spectrometers. All chemical shifts are reported in δ ppm downfield to TMS and peak multiplicities as singlet (s), doublet (d), quartet (q), broad (b) broad singlet (bs), and multiplet (m). Elemental analyses were performed on an Elmentar-Vario-EL (Heraeus Company Ltd., Germany). IR spectra were recorded in $CHCl_3$ using Shimadzu FTIR-8400 spectrophotometer. Melting points were determined on a Buchi Melting Point B-540. Electron Scattered Ionization (ESI) Mass Spectrometric measurements were done with API QSTAR Pulsar mass Spectrometer. The quantum chemical calculations were done employing the Gaussian 03 program package (Gaussian, Inc, Wallingford, CT 06492, USA).


ESI-MS
NO2
O
O
O
2a
102.1176
230.0254
284.0240
(M+Na)+
Intensity, counts
m/z, amu


ESI-MS
NO2
O
O
O
6a
102.1225
(M+H)+
262.0750
230.0358
284.0437
(M+Na)+
Intensity, counts
m/z, amu


ESI-MS
NO2
O
H
N
O
O
COOMe
3a
(M+Na)+
483.3090
(M+K)+
499.28
484.3178
500.28
501.2
(M+H)+
461.2895
m/z, amu


ESI-MS
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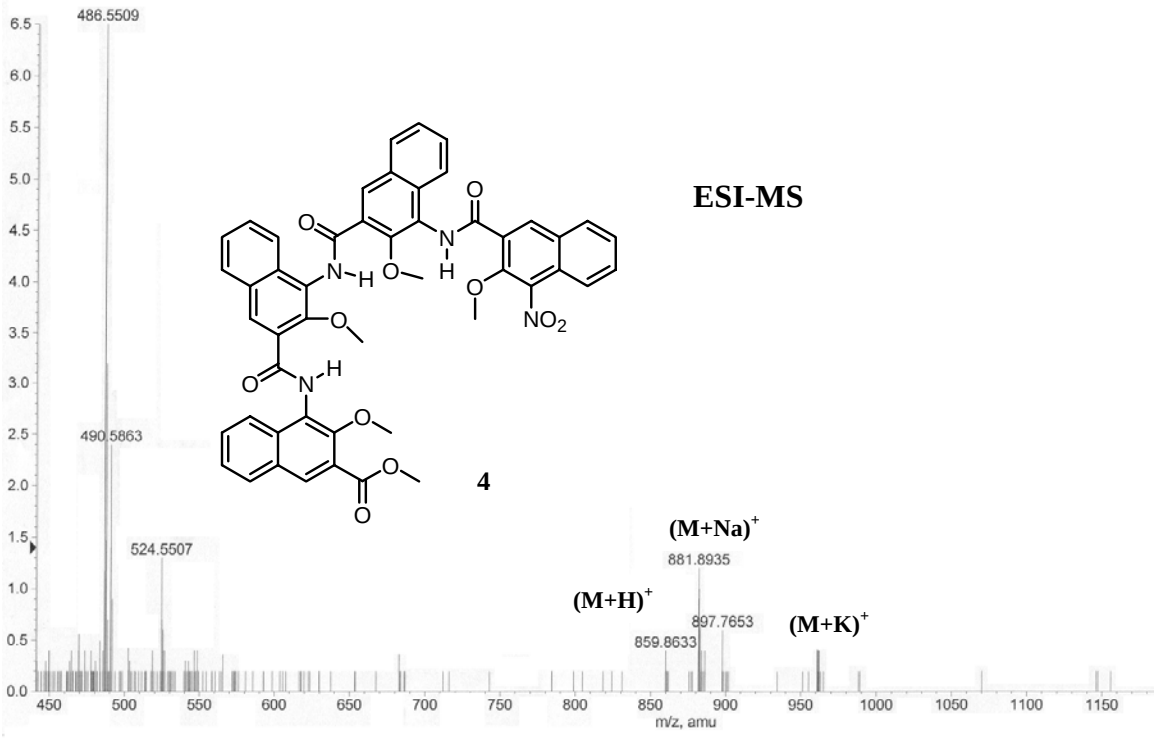
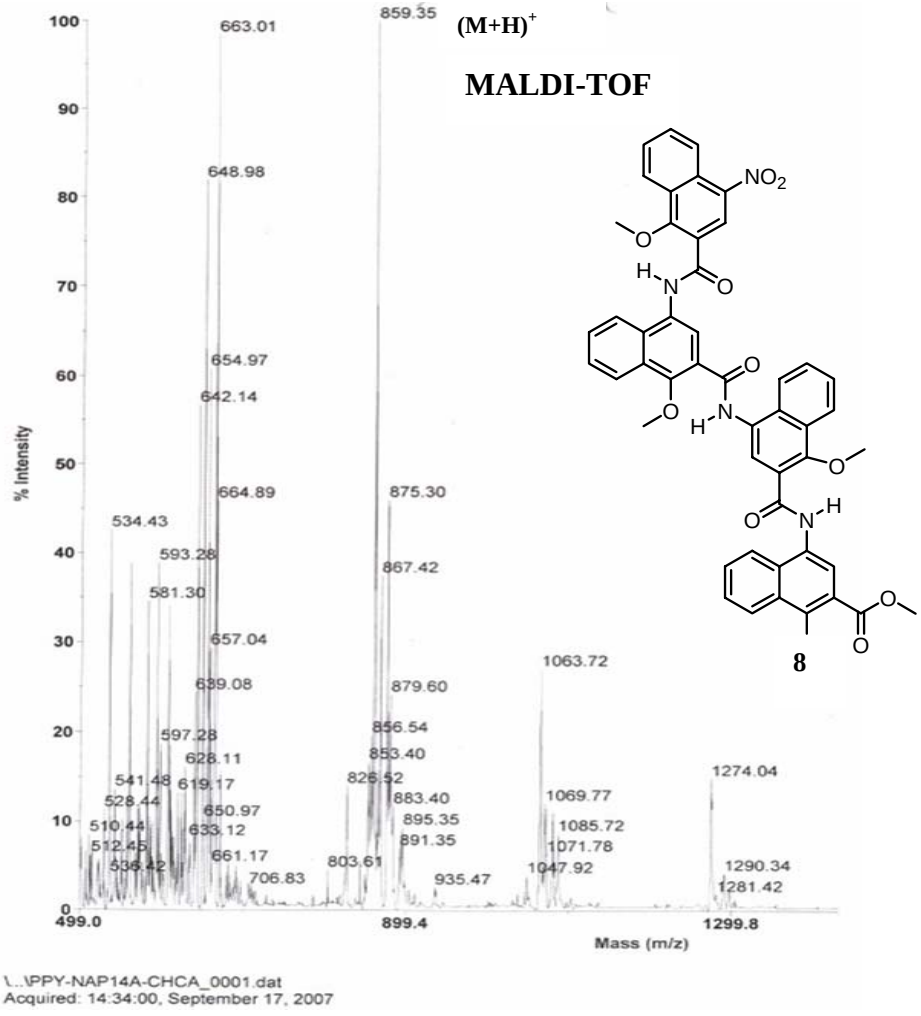
331.1985
O2N
O
H
N
O
COOMe
O
7a
(M+Na)+
483.0728
359.2256
(M+K)+
499.0478
319.1443
333.1628
427.1635
(M+H)+
479.1272
484.0796
461.0391
m/z, amu


ESI-MS
4
(M+Na)+
(M+H)+
(M+K)+
486.5509
490.5863
524.5507
881.8935
897.7653
859.8633
m/z, amu


(M+H)+
MALDI-TOF
8
% Intensity
Mass (m/z)
859.35
663.01
648.98
654.97
642.14
664.89
875.30
534.43
593.28
867.42
581.30
657.04
1063.72
639.08
879.60
597.28
856.54
628.11
853.40
619.17
826.52
1274.04
541.48
528.44
883.40
1069.77
650.97
895.35
510.44
633.12
1085.72
891.35
512.45
661.17
1071.78
803.61
1290.34
706.83
935.47
1047.92
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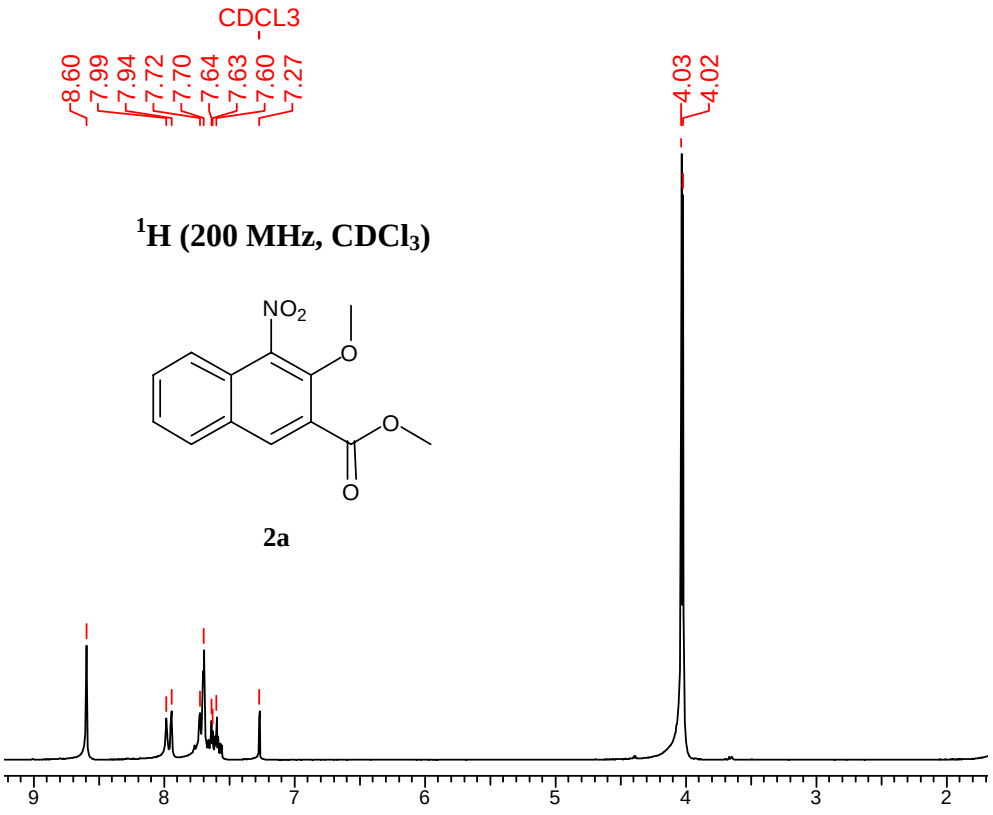
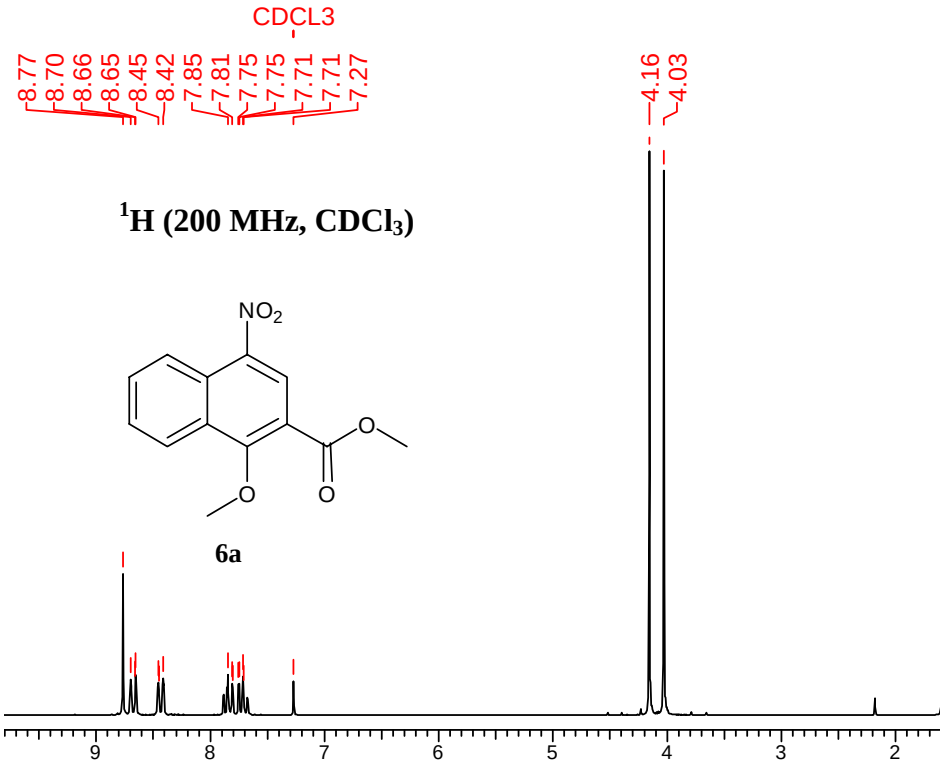


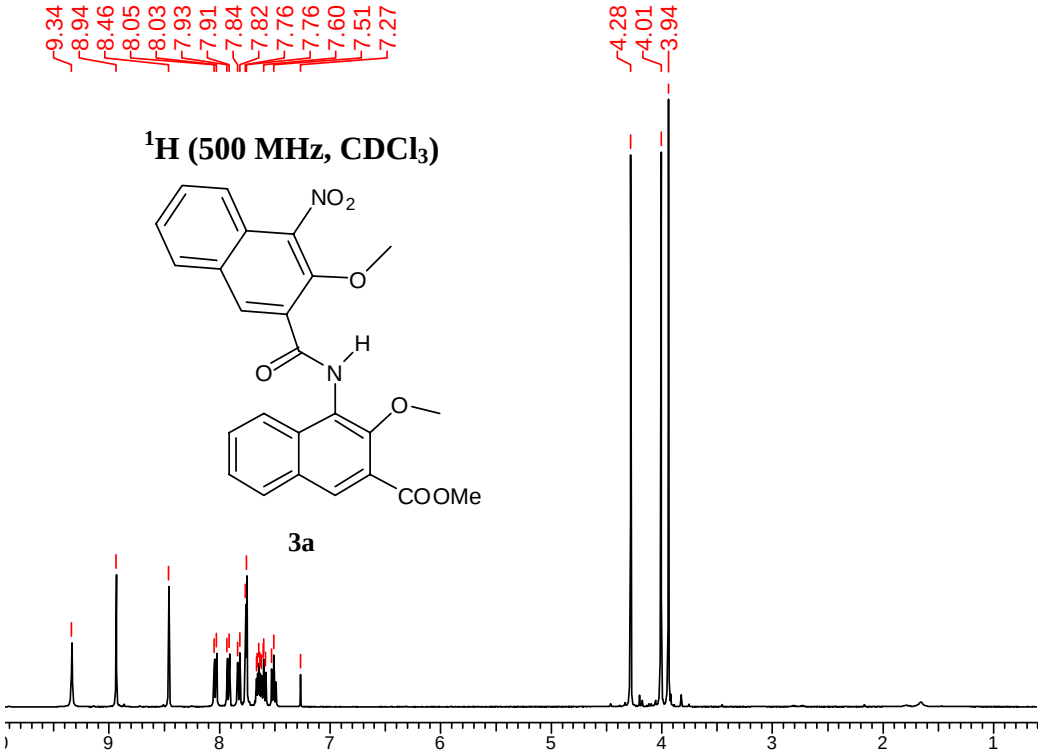
^{1}H (200 MHz, $CDCl_3$)

2a



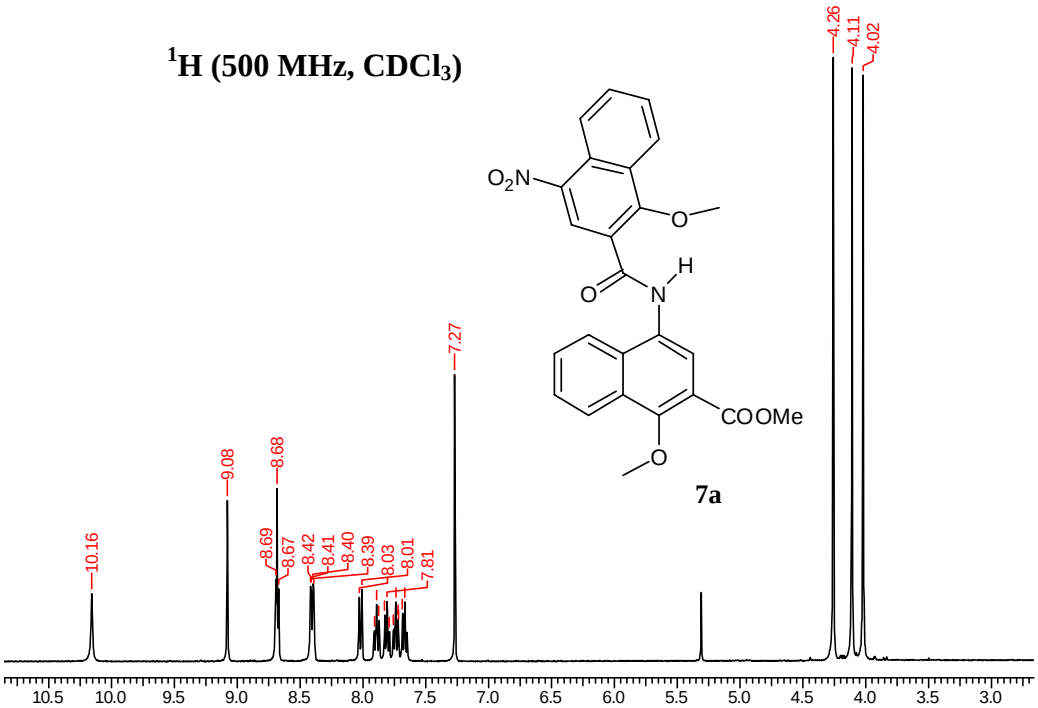
^{1}H (200 MHz, $CDCl_3$)

6a



^{1}H (500 MHz, $CDCl_3$)

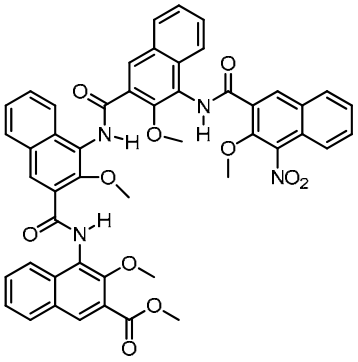
3a



^{1}H (500 MHz, $CDCl_3$)

7a

^{1}H (500 MHz, $CDCl_3$)



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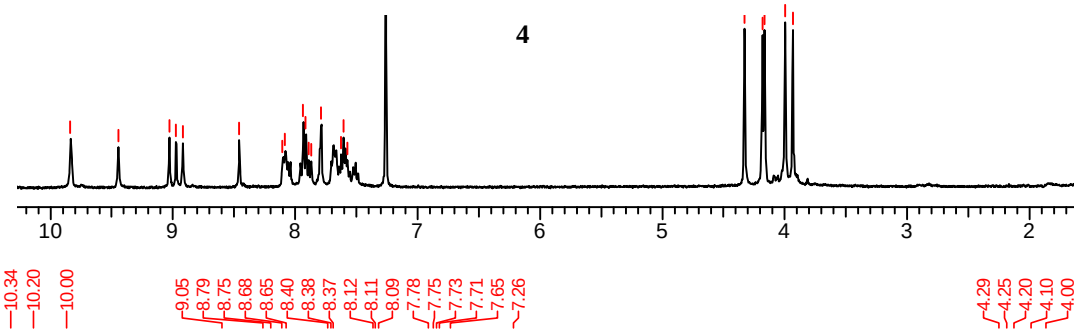
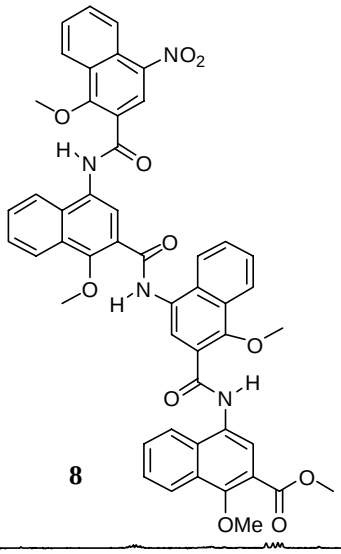


^{1}H (400 MHz, $CDCl_3$)



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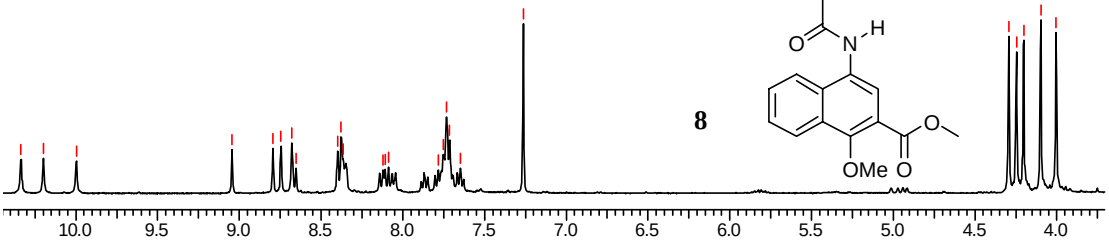
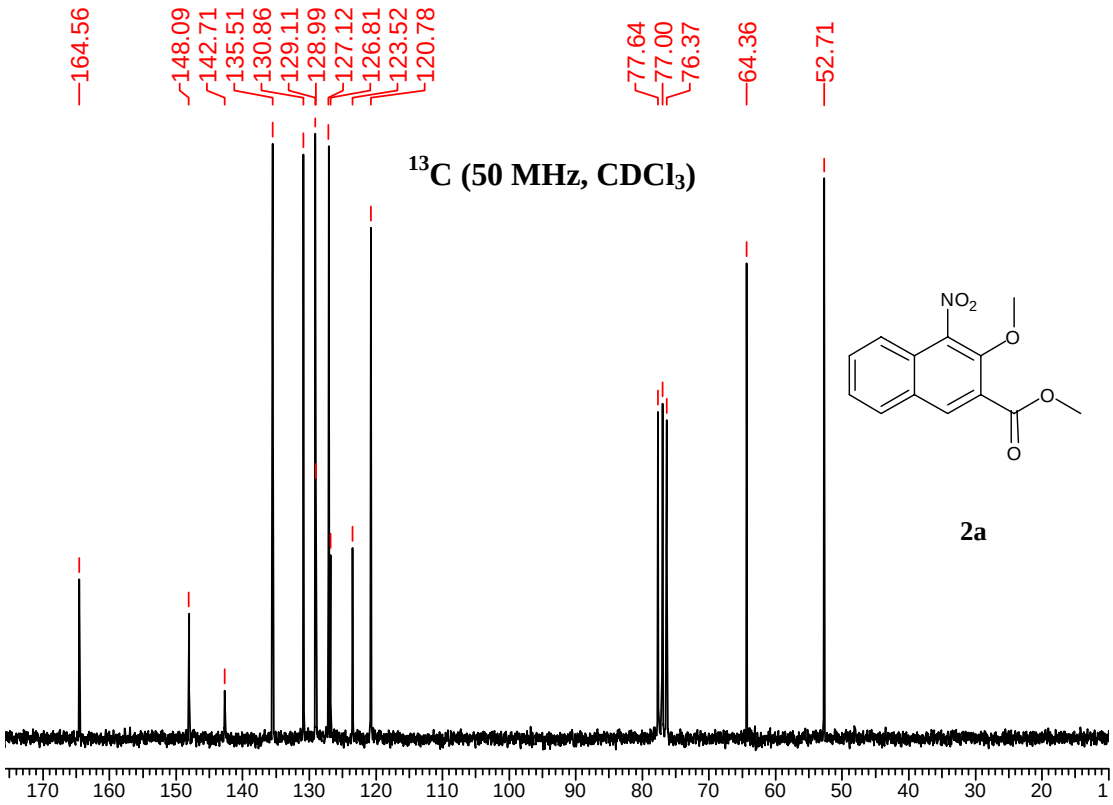
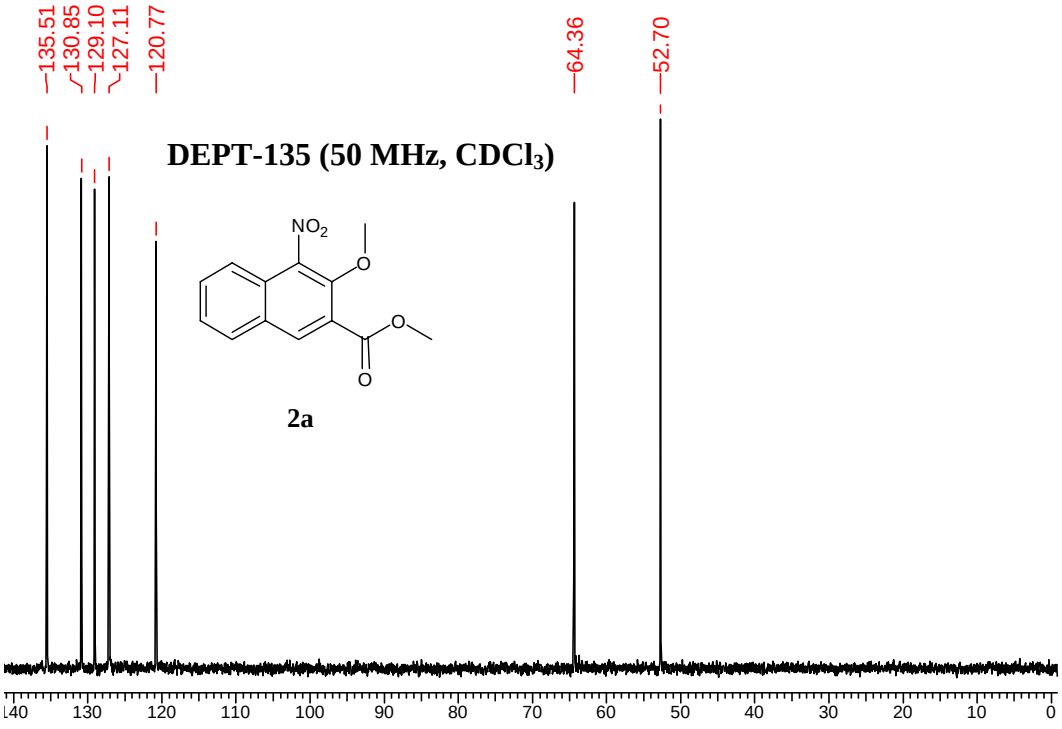
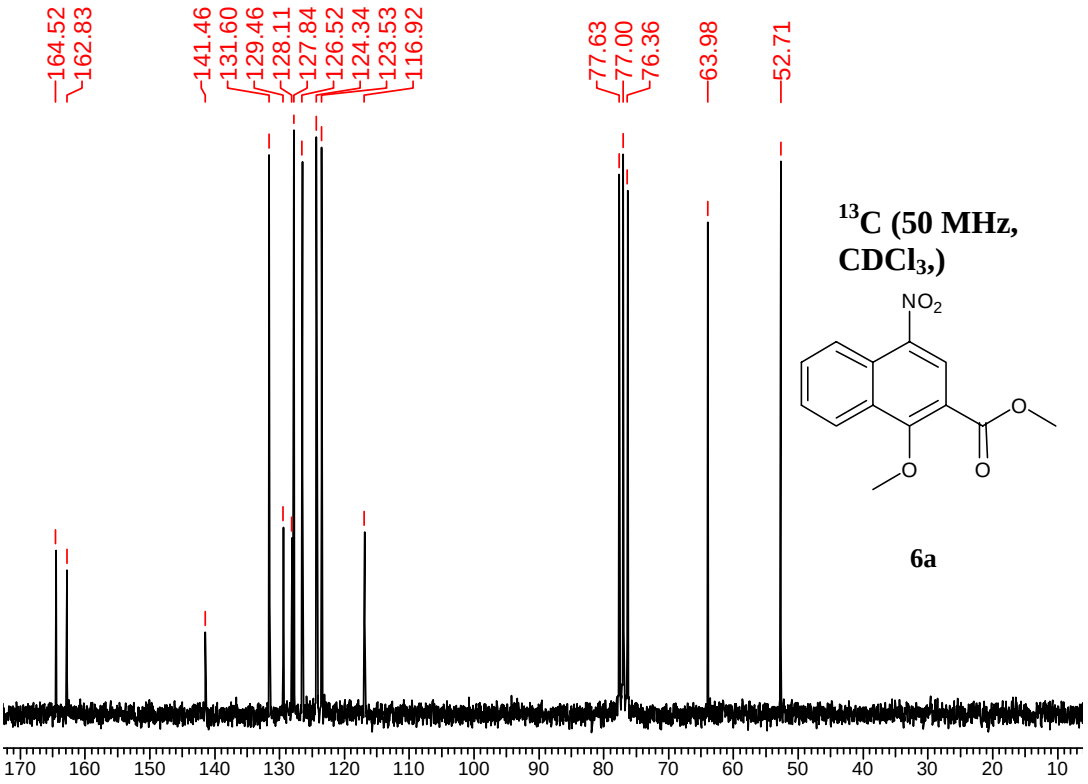


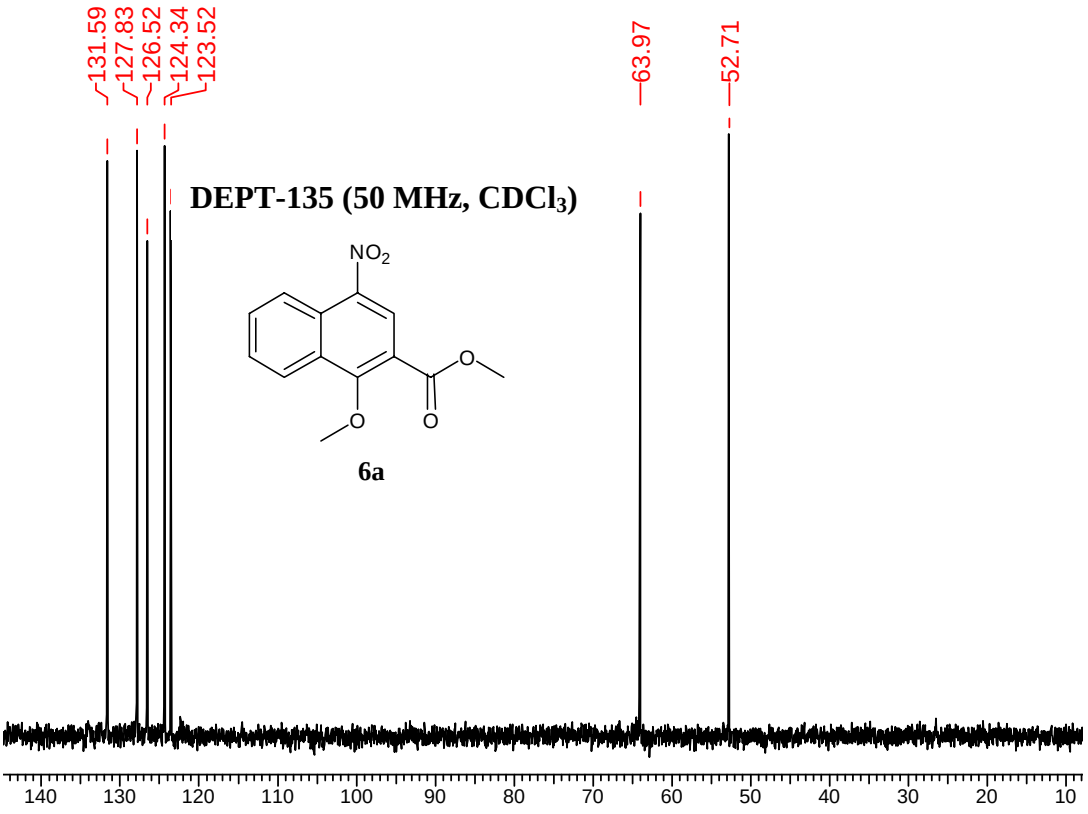

164.56
148.09
142.71
135.51
130.86
129.11
128.99
127.12
126.81
123.52
120.78
77.64
77.00
76.37
64.36
52.71
13C (50 MHz, CDCl3)
NO2
O
O
O
2a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
1


135.51
130.85
129.10
127.11
120.77
64.36
52.70
DEPT-135 (50 MHz, CDCl3)
NO2
O
O
O
2a
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



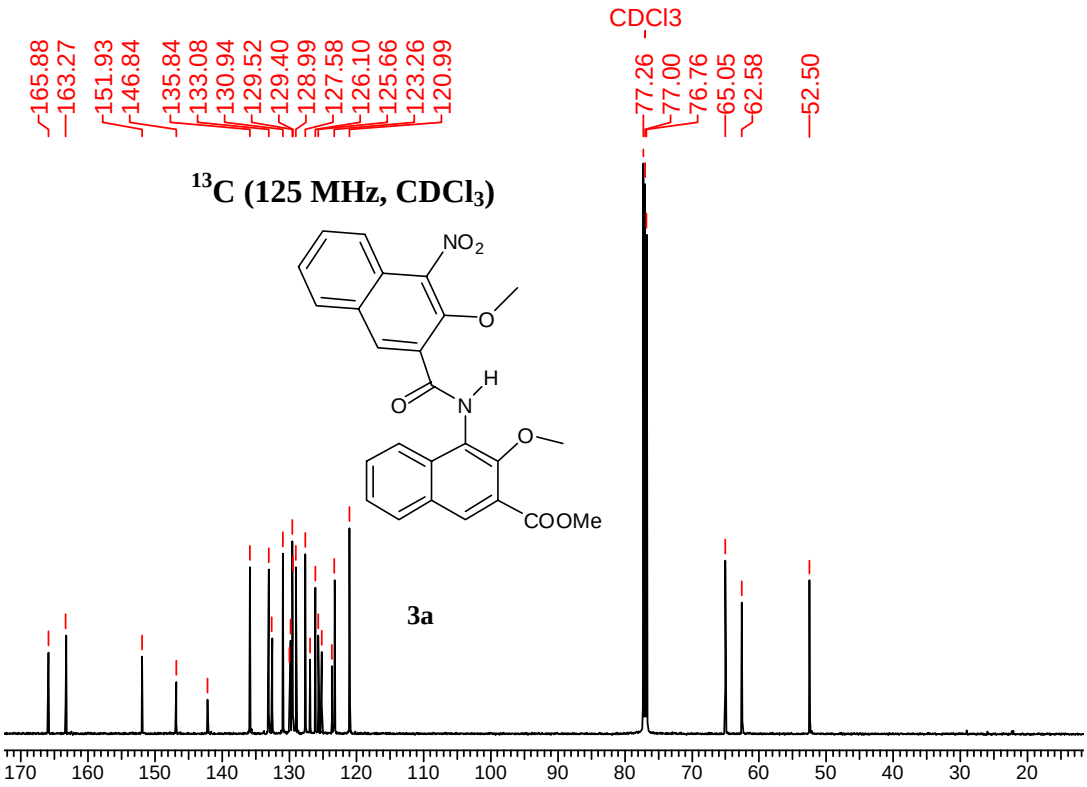
^{13}C (50 MHz, $CDCl_3$,)

6a



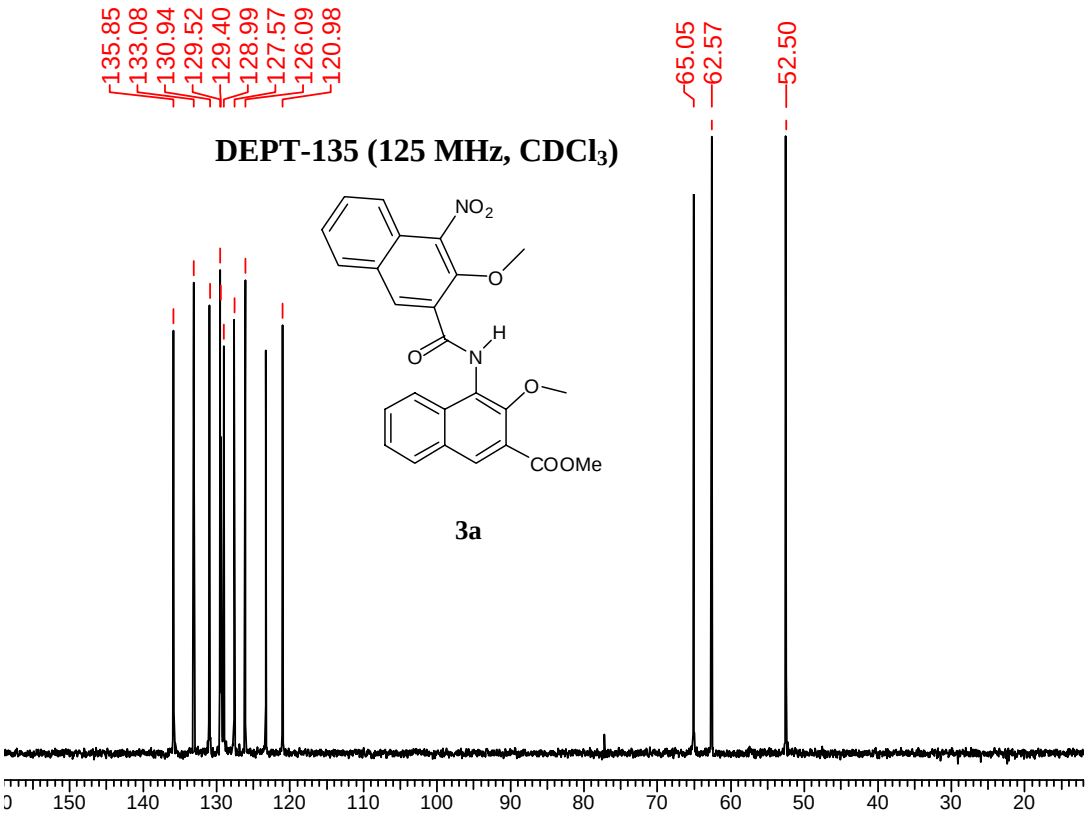
DEPT-135 (50 MHz, $CDCl_3$)

6a



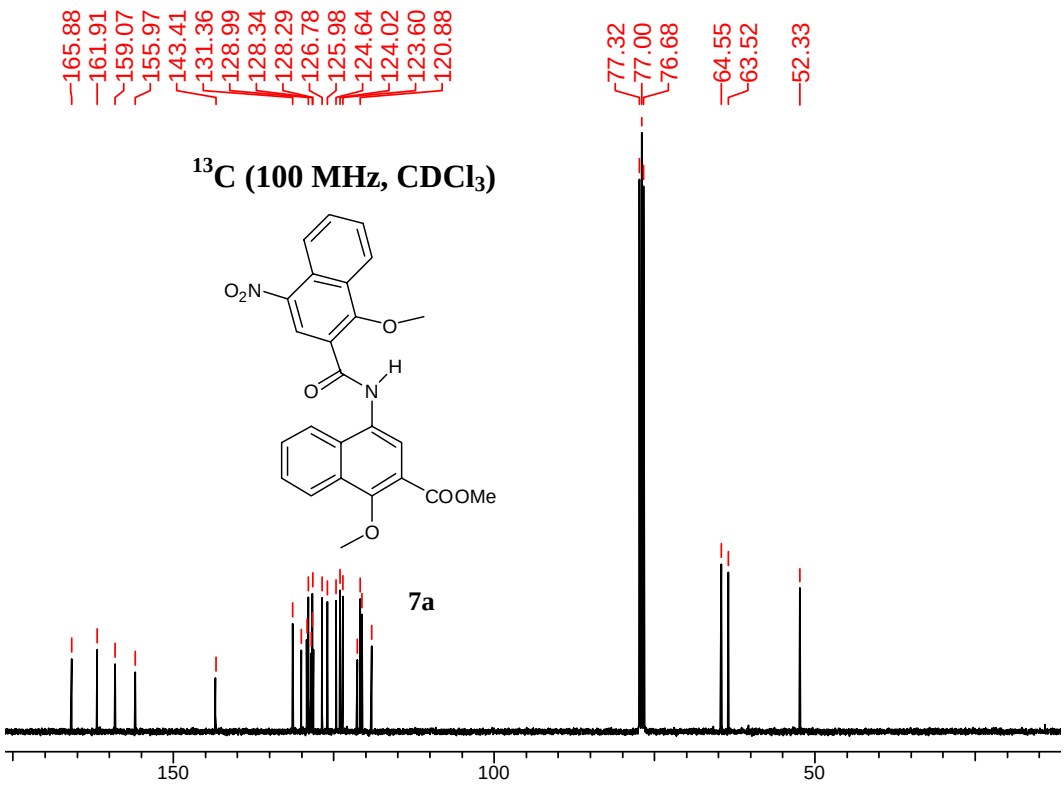
^{13}C (125 MHz, $CDCl_3$)

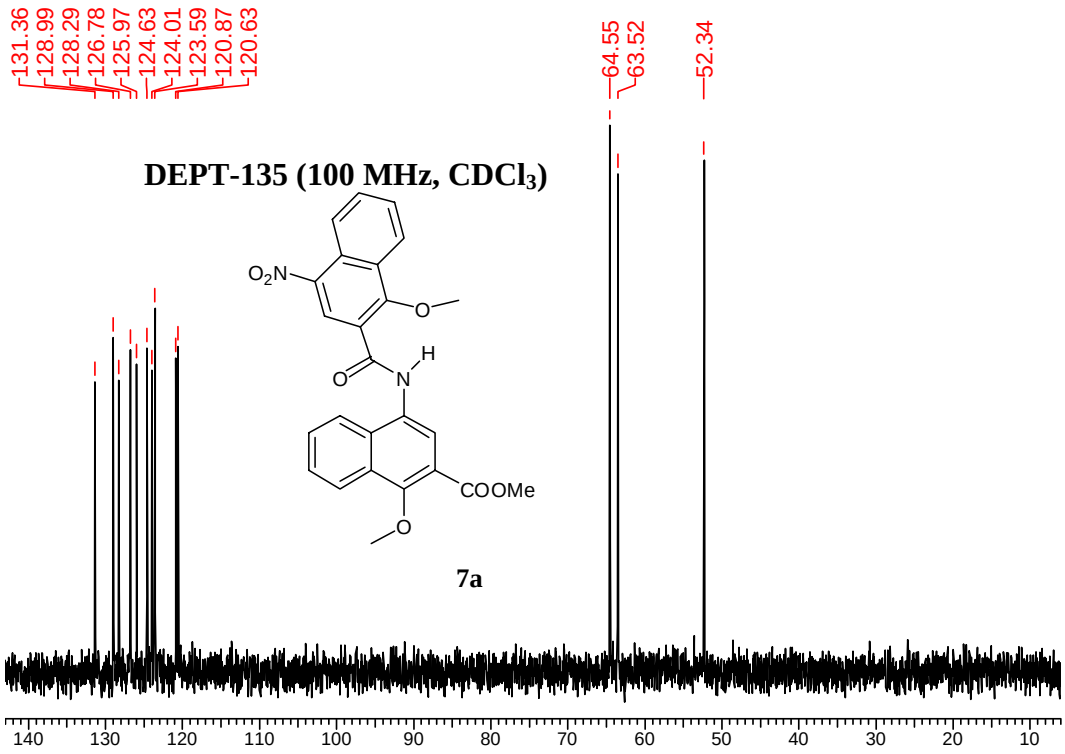
3a

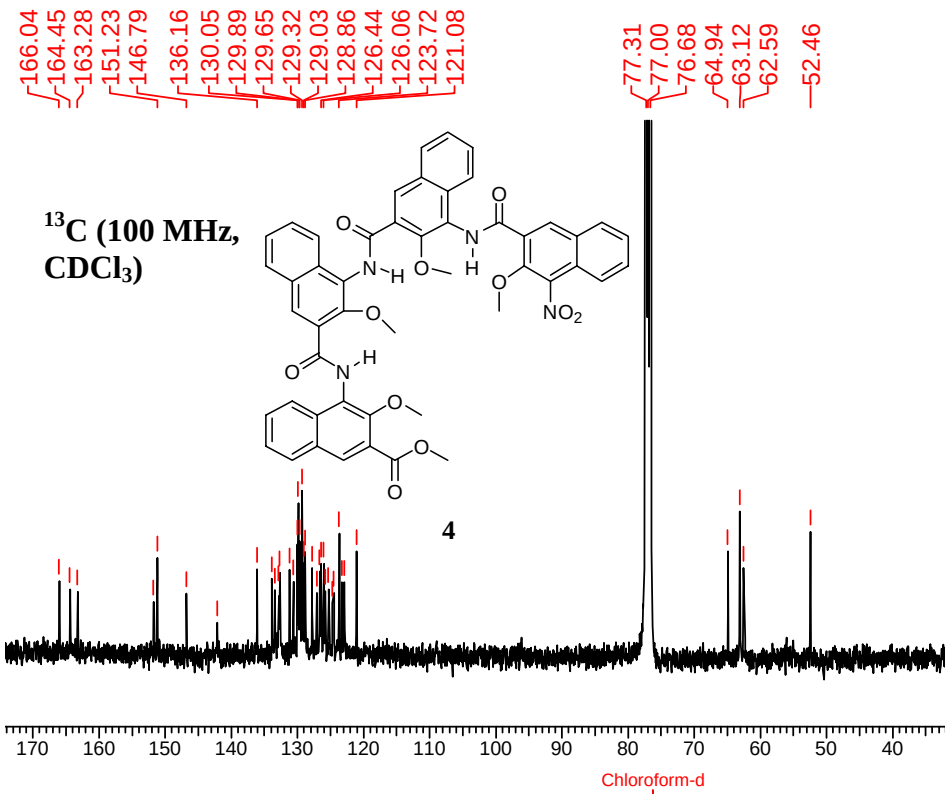


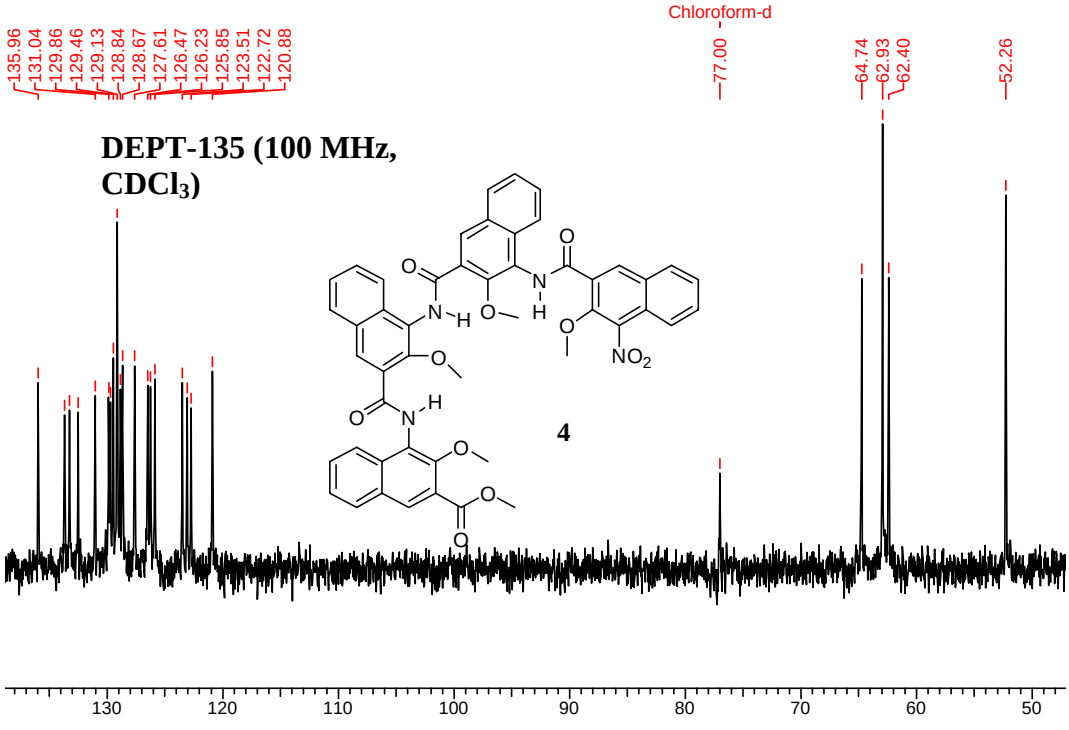
DEPT-135 (125 MHz, $CDCl_3$)

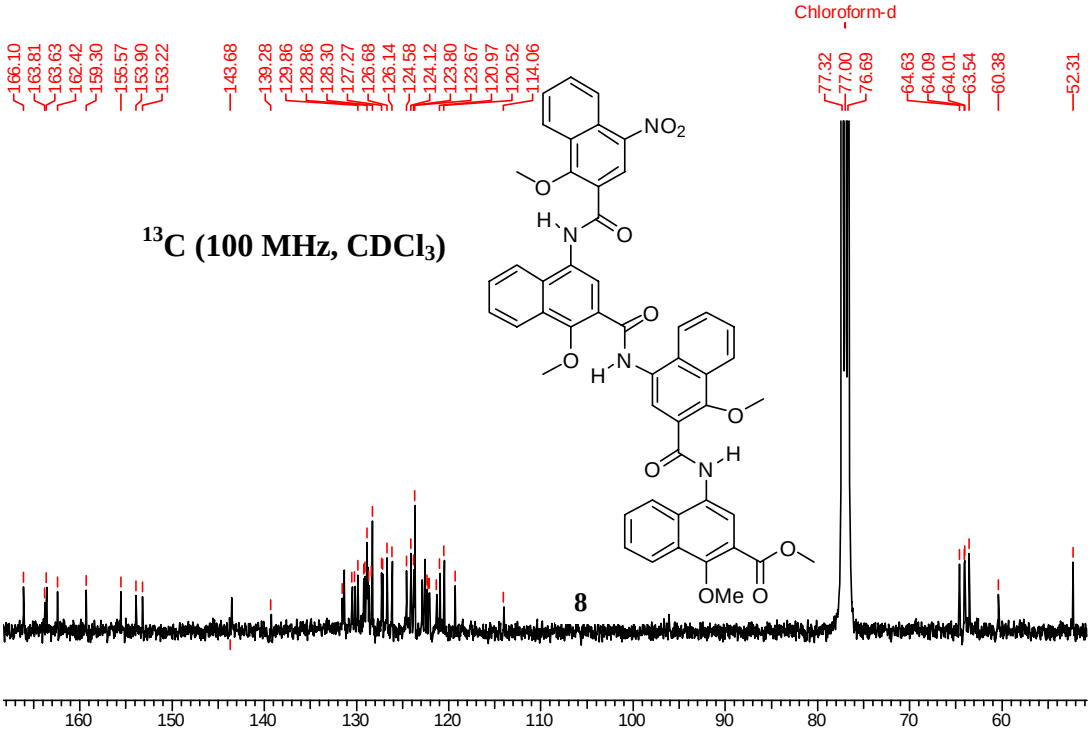
3a


165.88
161.91
159.07
155.97
143.41
131.36
128.99
128.34
128.29
126.78
125.98
124.64
124.02
123.60
120.88
77.32
77.00
76.68
64.55
63.52
52.33
13C (100 MHz, CDCl3)
O2N
O
H
N
O
COOMe
O
7a
150
100
50


131.36
128.99
128.29
126.78
125.97
124.63
124.01
123.59
120.87
120.63
64.55
63.52
52.34
DEPT-135 (100 MHz, CDCl3)
O2N
O
H
N
O
COOMe
O
7a
140
130
120
110
100
90
80
70
60
50
40
30
20
10


166.04
164.45
163.28
151.23
146.79
136.16
130.05
129.89
129.65
129.32
129.03
128.86
126.44
126.06
123.72
121.08
77.31
77.00
76.68
64.94
63.12
62.59
52.46
^{13}C (100 MHz, CDCl$_3$)
4
170
160
150
140
130
120
110
100
90
80
70
60
50
40


Chloroform-d
135.96
131.04
129.86
129.46
129.13
128.84
128.67
127.61
126.47
126.23
125.85
123.51
122.72
120.88
77.00
64.74
62.93
62.40
52.26
DEPT-135 (100 MHz, CDCl$_3$)
4
130
120
110
100
90
80
70
60
50


Chloroform-d
166.10
163.81
163.63
162.42
159.30
155.57
153.90
153.22
143.68
139.28
129.86
128.86
128.30
127.27
126.68
126.14
124.58
124.12
123.80
123.67
120.97
120.52
114.06
77.32
77.00
76.69
64.63
64.09
64.01
63.54
60.38
52.31
^{13}C (100 MHz, CDCl$_3$)
NO$_2$
OMe O
8
160
150
140
130
120
110
100
90
80
70
60

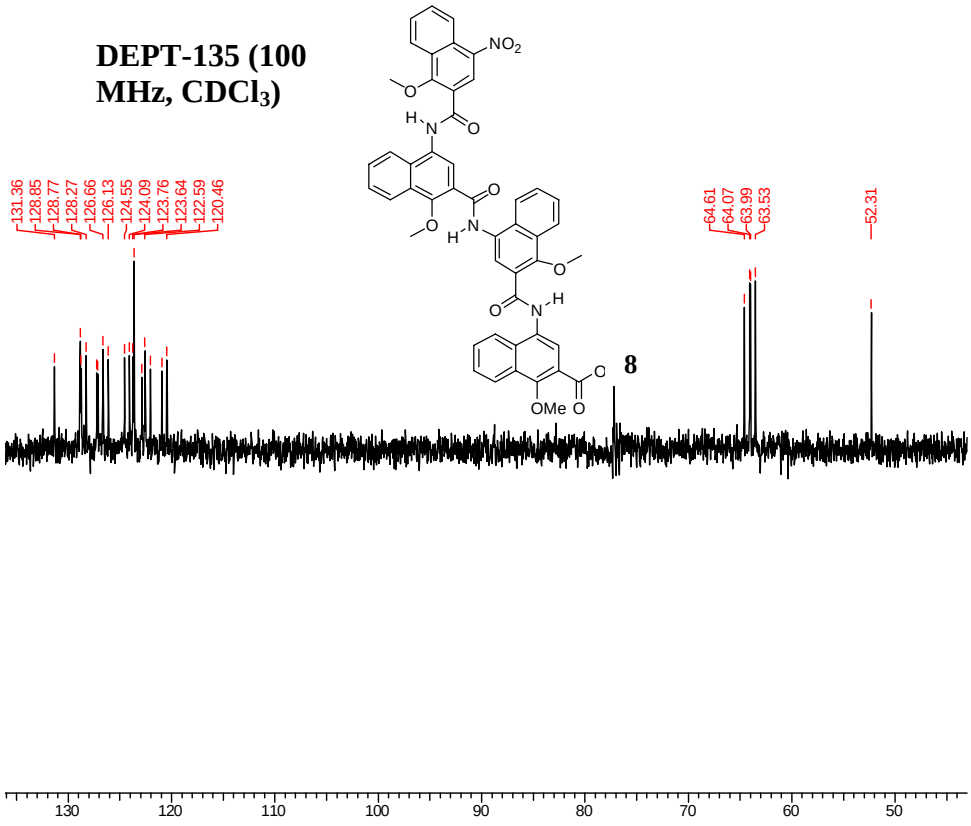

DEPT-135 (100 MHz, CDCl$_3$)
131.36
128.85
128.77
128.27
126.66
126.13
124.55
124.09
123.76
123.64
122.59
120.46
64.61
64.07
63.99
63.53
52.31
NO$_2$
OMe O
8
130
120
110
100
90
80
70
60
50

Table S1. Dilution study of **3a** (400 MHz, $CDCl_3$)

No	Concentration (in mmol)	δ_{NH}
1	120	9.34
2	100	9.34
3	80	9.34
4	60	9.34
5	40	9.34
6	20	9.34
7	10	9.35
8	5	9.35
9	4	9.35
10	2	9.35

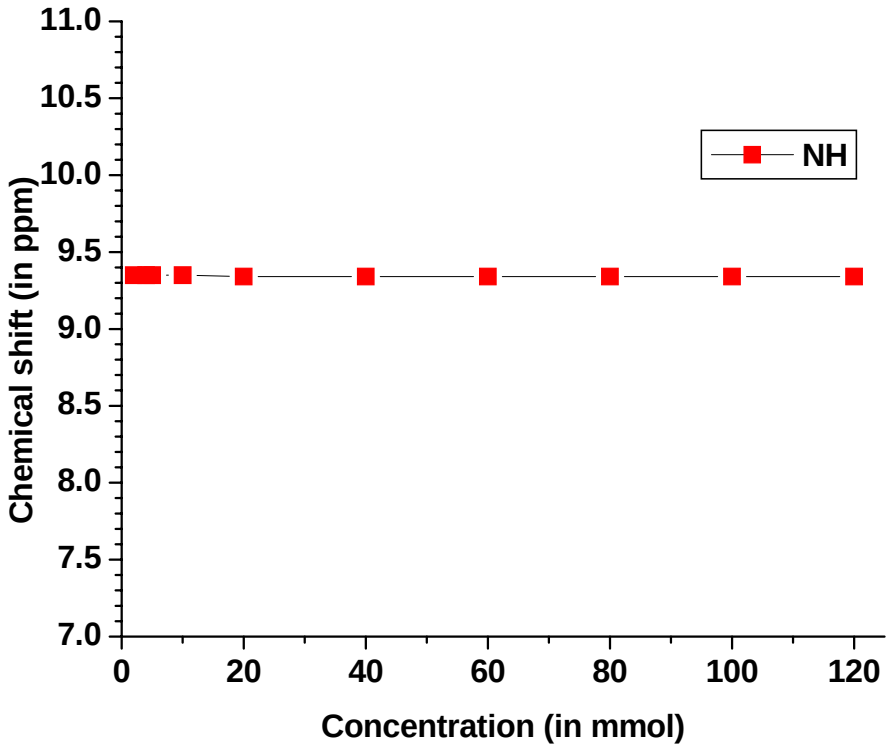


Figure S1. Dilution plot for **3a** (400 MHz, $CDCl_3$)

Table S2. Titration study of **3a** in $CDCl_3$ ($V_{DMSO\text{-}d6\ added}$ = 0-50 μ lit)

No	$V_{DMSO\text{-}d6}$ (in μL)	δ_{NH}
1	0	9.34
2	5	9.26
3	10	9.31
4	15	9.33
5	20	9.35
6	25	9.37
7	30	9.41
8	35	9.44
9	40	9.47
10	45	9.48
11	50	9.50

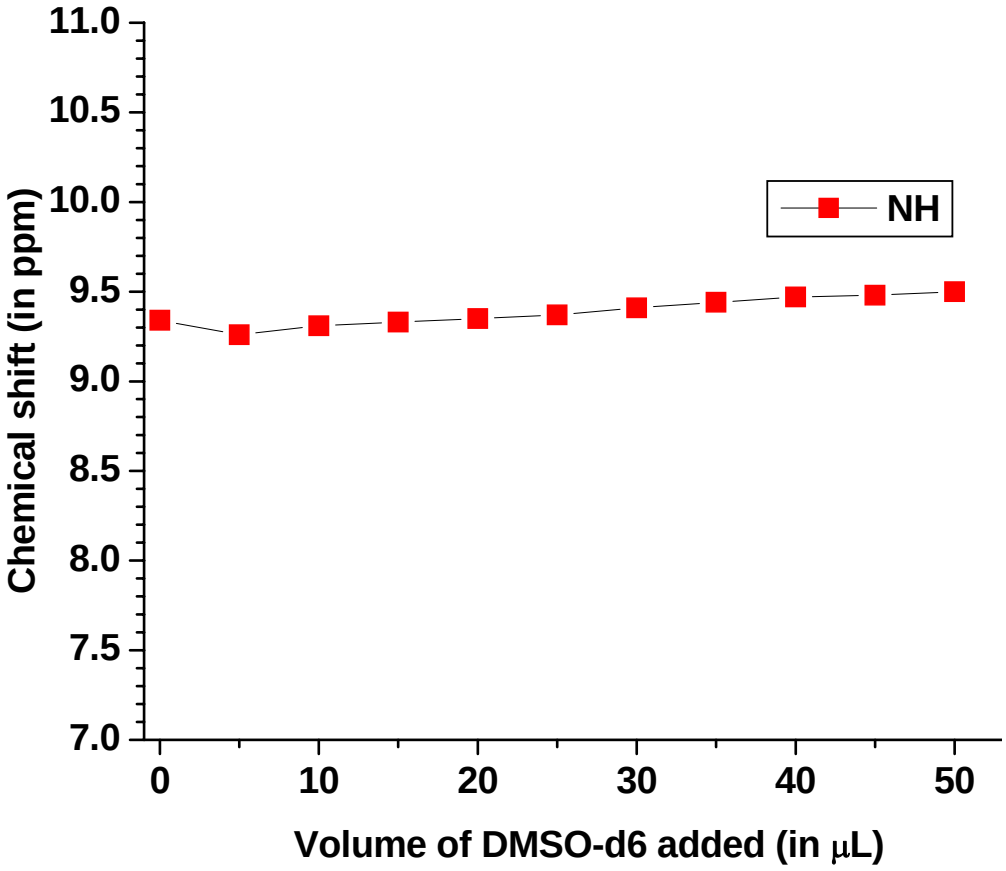


Figure S2. Titration plot for **3a** in $CDCl_3$ (400 MHz)

Table S3. Dilution study of **7a** (400 MHz, $CDCl_3$)

No	Concentration (in mmol)	δ_{NH}
1	120	10.14
2	100	10.14
3	80	10.15
4	60	10.15
5	40	10.15
6	20	10.15
7	10	10.15
8	5	10.16
9	4	10.16
10	2	10.16

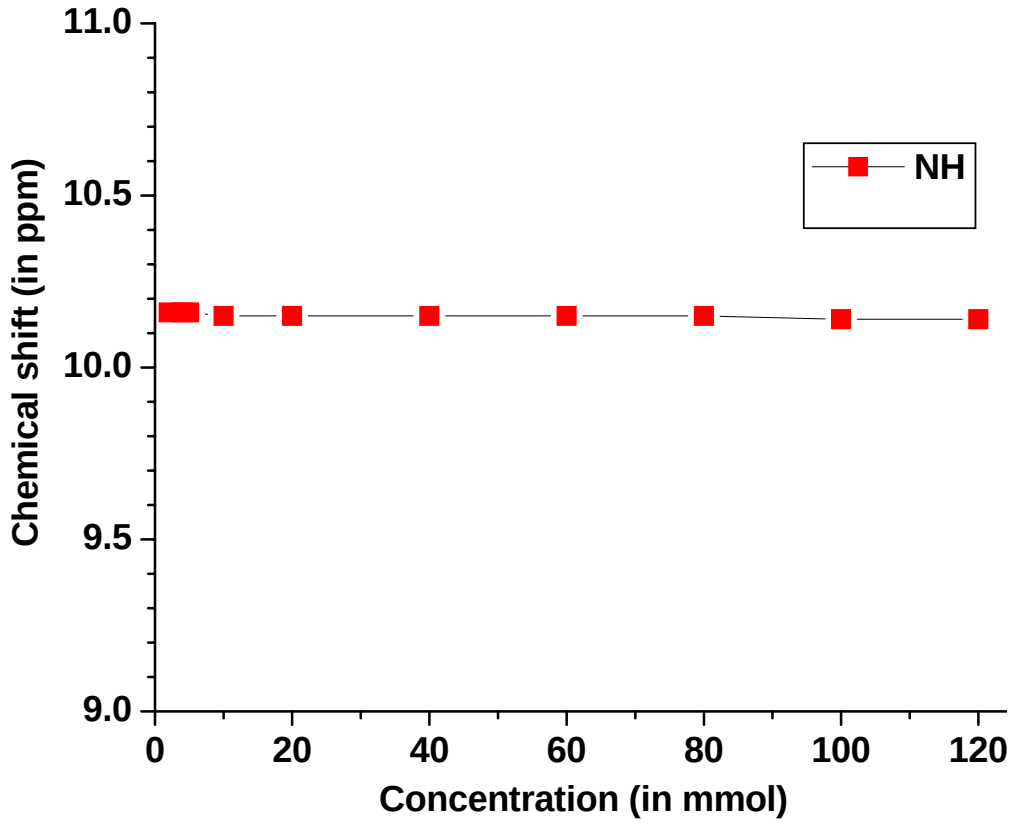


Figure S3. Dilution plot for **7a** ($CDCl_3$, 400 MHz)

Table S4. Titration study of **7a** in $CDCl_3$ (400 MHz)

No	$V_{DMSO-d6}$ (in µL)	δ_{NH}
1	0	10.16
2	5	10.08
3	10	10.10
4	15	10.13
5	20	10.14
6	25	10.15
7	30	10.17
8	35	10.18
9	40	10.19
10	45	10.21
11	50	10.23

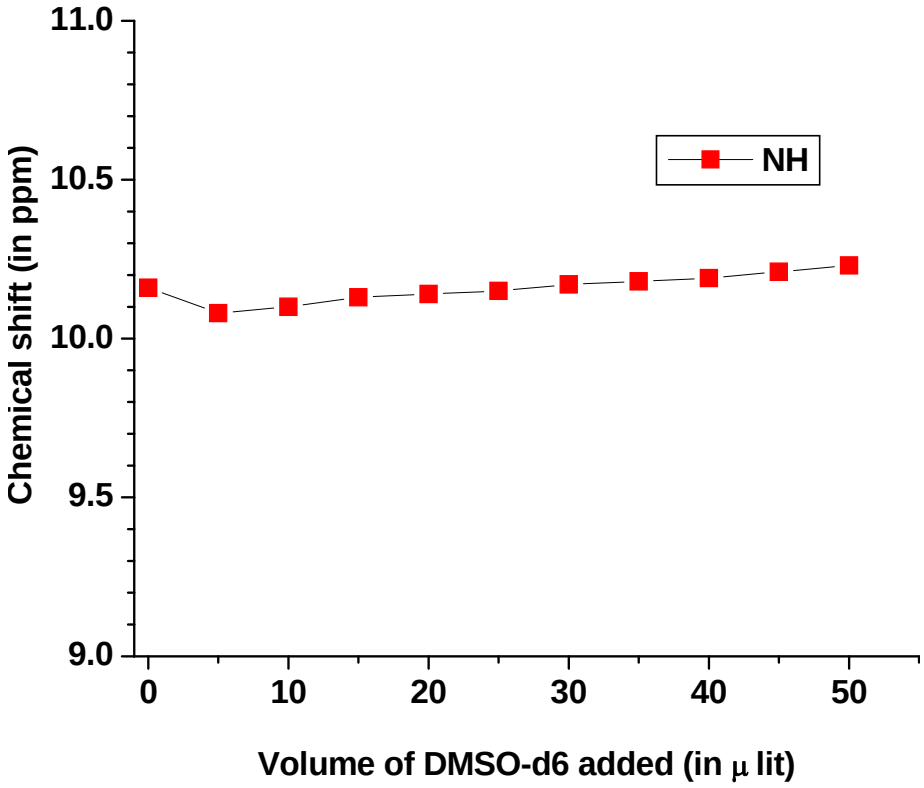
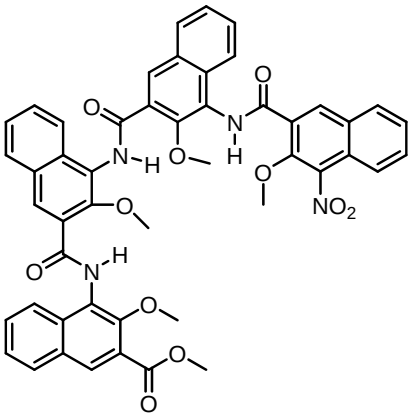


Figure S4. Titration plot for **7a** ($CDCl_3$, 400 MHz)

Table S5. Titration study of **4** in $CDCl_3$ ($V_{DMSO\text{-}d6\ added}$ = 0-50 μ lit)

V_{DMSO}-d_6 (in μl)	*Chemical shifts in ppm*		
	δ_{NH1}*	δ_{NH2}*	δ_{NH3}
0	9.84	9.83	9.45
5	9.84	9.84	9.46
10	9.84	9.84	9.47
15	9.85	9.85	9.50
20	9.86	9.86	9.51
25	9.89	9.86	9.60
30	9.94	9.88	9.71
35	9.94	9.88	9.73
40	9.97	9.90	9.78
45	9.98	9.90	9.79
50	9.98	9.90	9.79



*NHs could not be dispersed

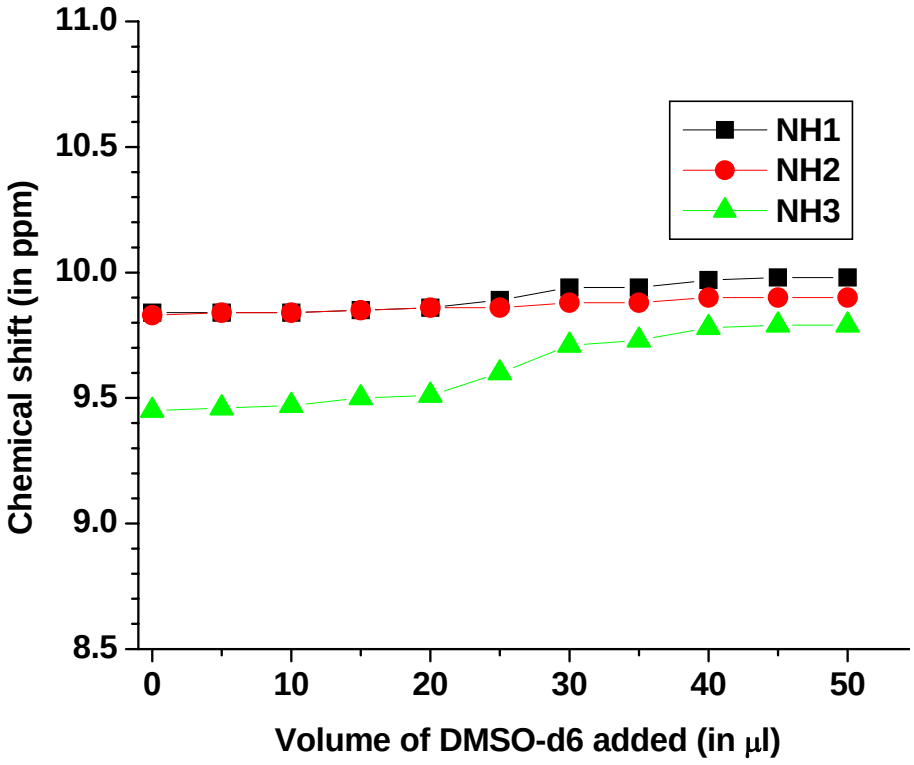
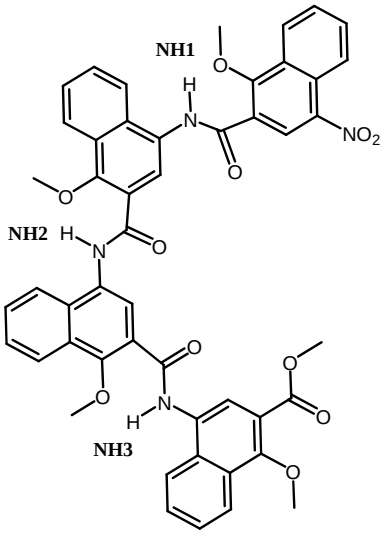


Figure S5. Titration plot for **4** in $CDCl_3$ (400 MHz)

Table S6. Titration study of **8** in $CDCl_3$ ($V_{DMSO\text{-}d6\ added}$ = 0-50 μ lit)

$V_{DMSO\text{-}d6}$ (in μl)	Chemical shifts in ppm		
	δ_{NH1}	δ_{NH2}	δ_{NH3}
0	10.34	10.20	10.0
5	10.34	10.20	10.0
10	10.34	10.20	10.0
15	10.34	10.21	10.02
20	10.37	10.27	10.12
25	10.38	10.28	10.14
30	10.39	10.30	10.16
35	10.40	10.31	10.19
40	10.40	10.32	10.20
45	10.41	10.34	10.23
50	10.42	10.35	10.24



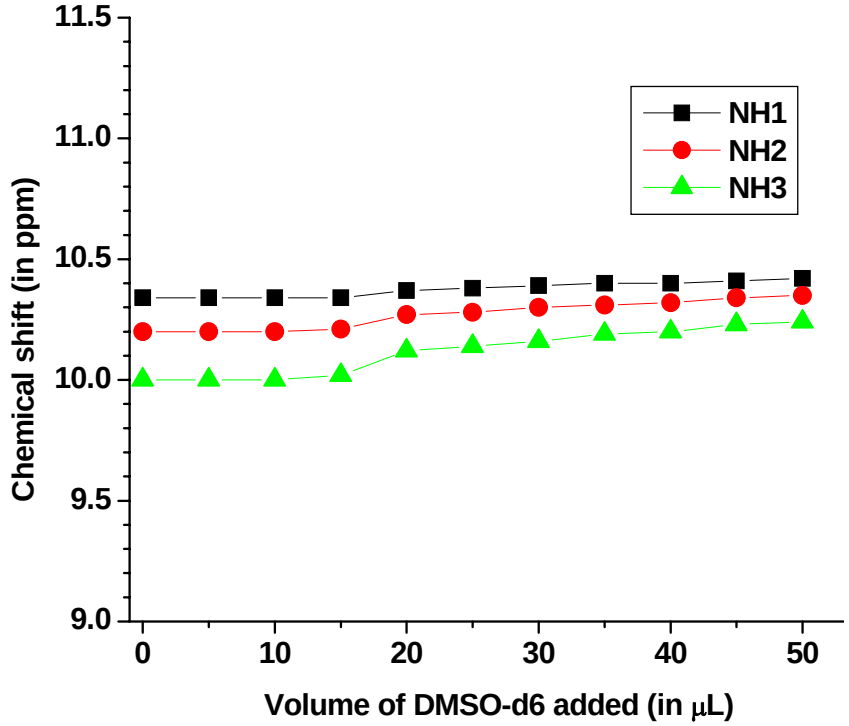


Figure S6. Titration plot for **8** in $CDCl_3$ (400 MHz)

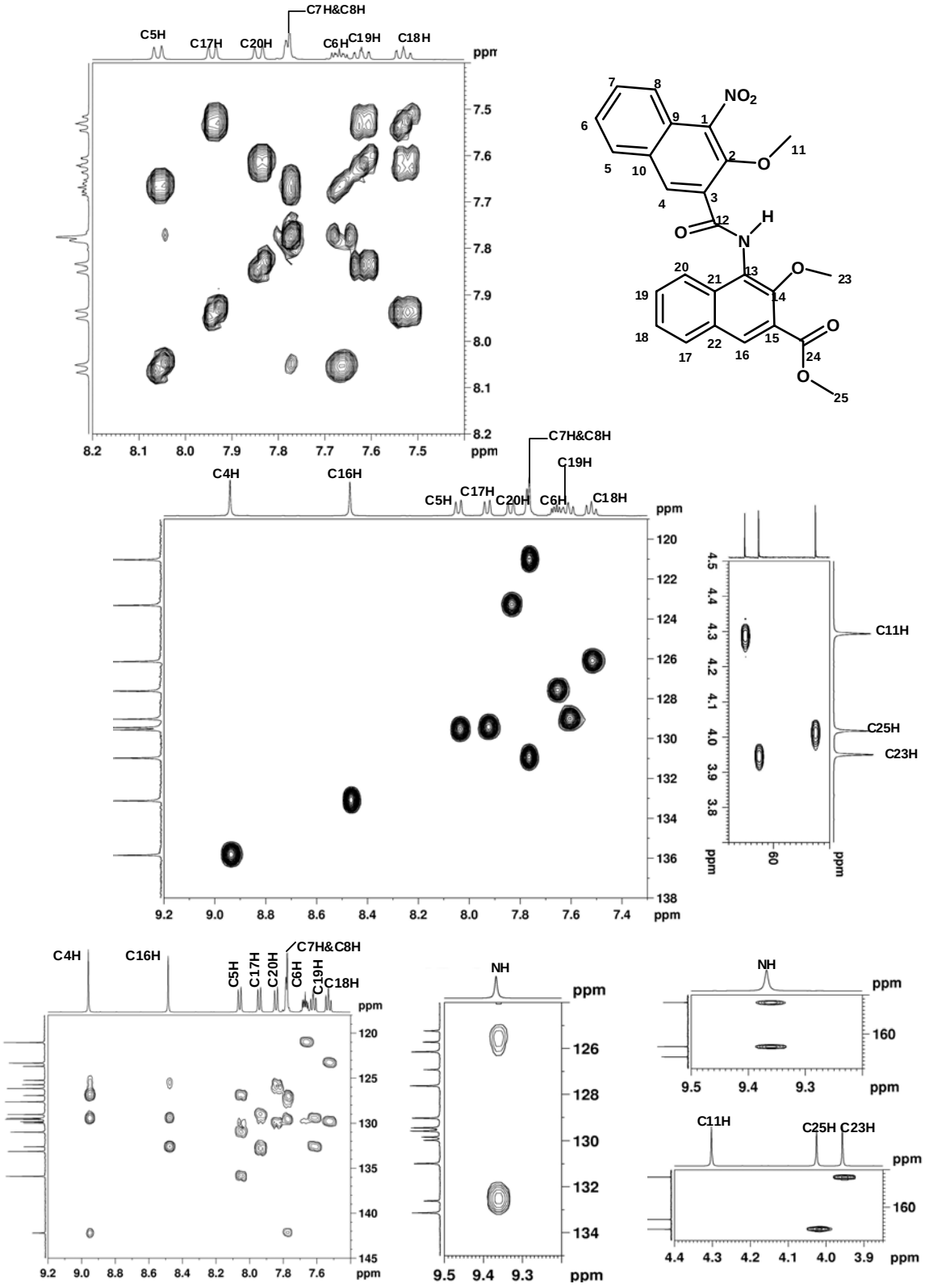


Figure S7. Partial 2D COSY, HSQC and HMBC spectra of **3a** (400 MHz, $CDCl_3$).

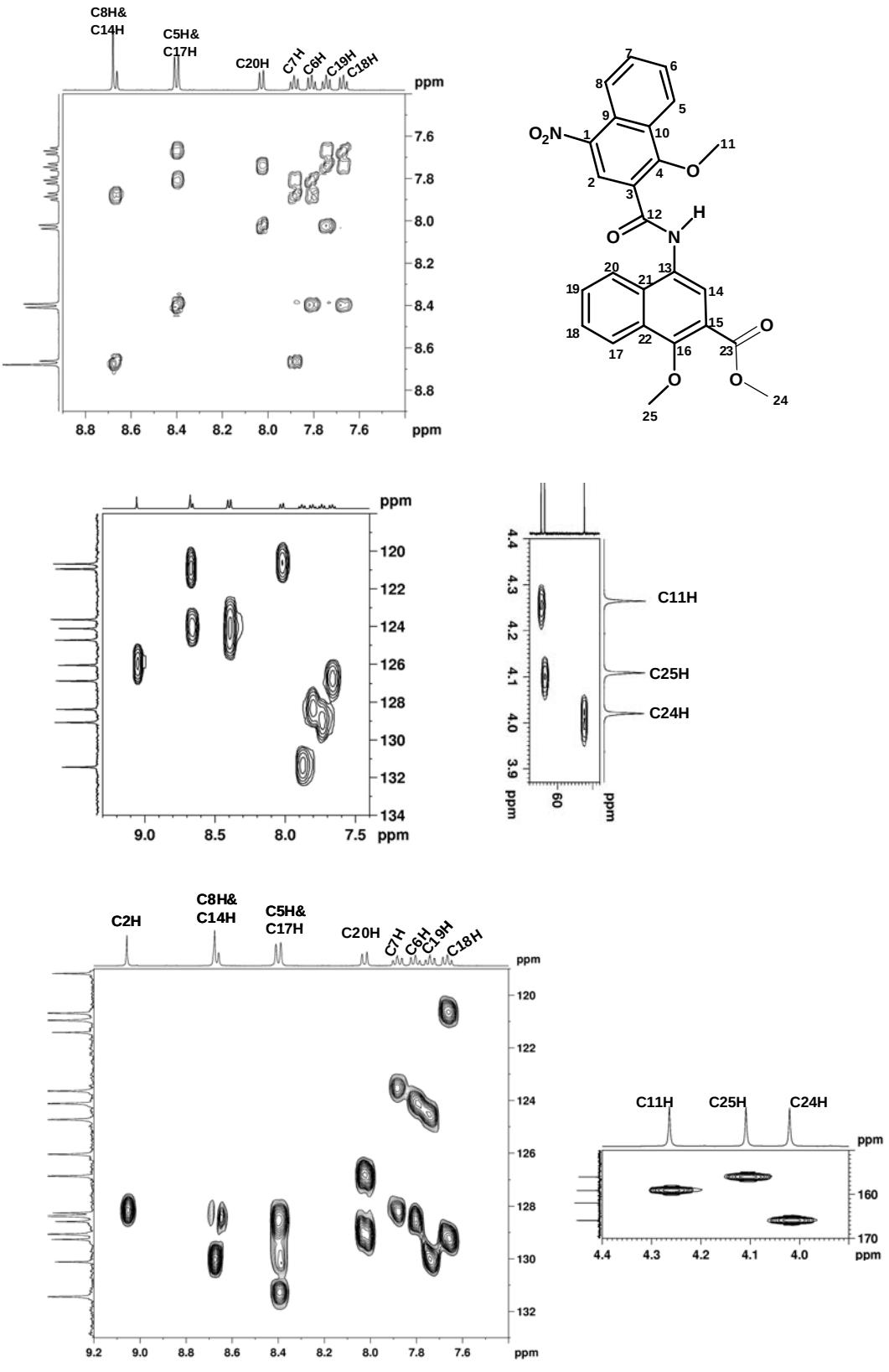


Figure S8. Partial 2D COSY, HSQC and HMBC spectra of **7a** (400 MHz, $CDCl_3$).

Table 7. ^{1}H, ^{13}C HSQC assignments for **3a**		
^{1}H (δ/ppm)		**^{13}C (δ/ppm)**
8.95 (C4H)		135.62
8.48 (C16H)		132.86
8.06 (C5H)		129.36
7.94 (C17H)		129.70
7.84 (C20H)		127.35
7.77 (2H)	C7H	123.04
	C8H	120.76
7.67 (C6H)		130.72
7.62 (C19H)		128.76
7.52 (C18H)		125.87
4.30 (3H, C11H)		64.83
4.02 (3H, C25H)		52.27
3.95 (3H, C23H)		62.37

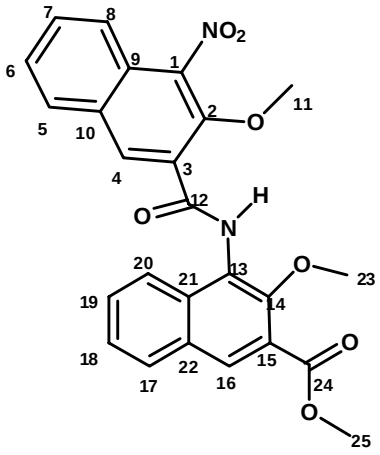


Table 8. ^{1}H, ^{13}C HMBC assignments for **3a**	
^{1}H (δ/ppm)	**^{13}C (δ/ppm)**
9.36 (NH)	163.03, 151.69, 132.32, 124.94
8.95 (C4H)	163.03, 146.61, 126.65, 124.94
8.48 (C16H)	165.64, 151.69, 132.32
8.06 (C5H)	126.65, 130.72, 141.91
7.94 (C17H)	132.32, 132.86, 128.76
7.84 (C20H)	129.70, 125.43, 125.87
7.67 (C6H)	132.32,
7.62 (C19H)	132.32, 129.17
7.52 (C18H)	129.70, 123.04,
4.30 (3H, C11H)	146.61
4.02 (3H, C25H)	165.64
3.95 (3H, C23H)	151.69

Table 9. ^{1}H, ^{13}C HSQC assignments for **7a**		
^{1}H (/ppm)		**^{13}C (/ppm)**
9.02 (C2H)		125.98
8.65 (C14H)		120.88
8.64 (C8H)		124.02
8.37	C5H	128.28, 126.78
	C17H	
8.01 (C20H)		120.64
7.85 (C7H)		131.36
7.78 (C6H)		128.99
7.72 (C19H)		120.64
7.64 (C18H)		126.78
4.24 (3H, C11H)		64.55
4.08 (3H, C25H)		63.52
4.00 (3H, C24H)		62.33

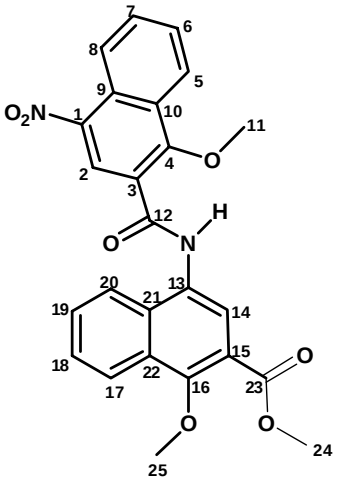


Table 10. ^{1}H, ^{13}C HMBC assignments for **7a**		
^{1}H (/ppm)		**^{13}C (/ppm)**
10.14 (NH)		161.91, 130.06, 120.88
9.02 (C2H)		161.91, 159.07, 128.17
8.65 (C14H)		165.88, 155.97, 130.06
8.64 (C8H)		121.35, 128.29, 128.34
8.37	C5H	159,07, 131.36, 128.17
	C17H	155.97, 130.06, 128.99
8.01 (C20H)		129.19, 126.78
7.85 (C7H)		128.17, 124.64
7.78 (C6H)		128.34, 124.02
7.72 (C19H)		130.06, 124.64
7.64 (C18H)		120.64, 129.19
4.24 (3H, C11H)		159.07
4.08 (3H, C25H)		155.97
4.00 (3H, C24H)		165.88

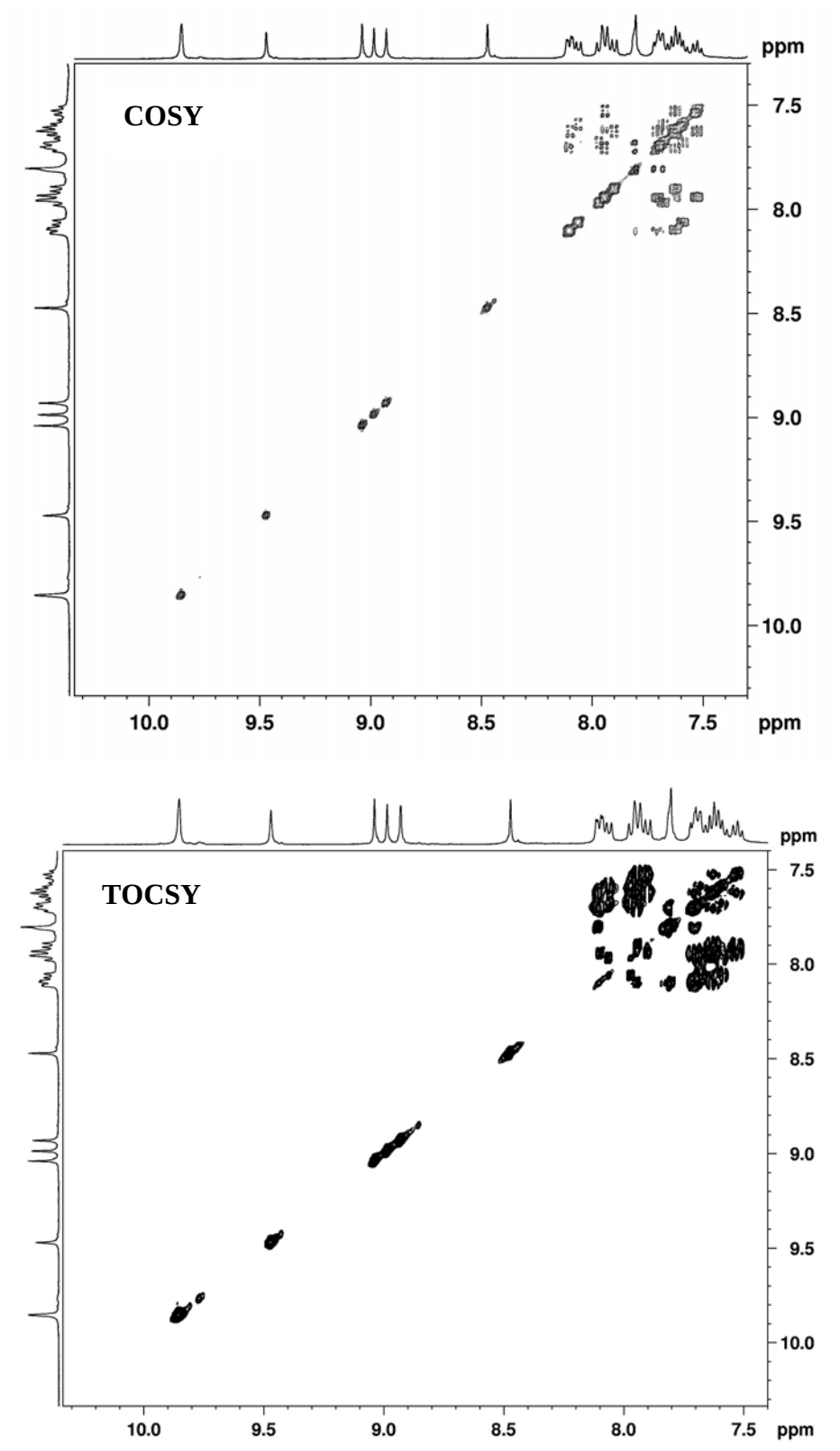


Figure S9. Partial 2D COSY and TOCSY spectra of **4** (400 MHz, $CDCl_3$).

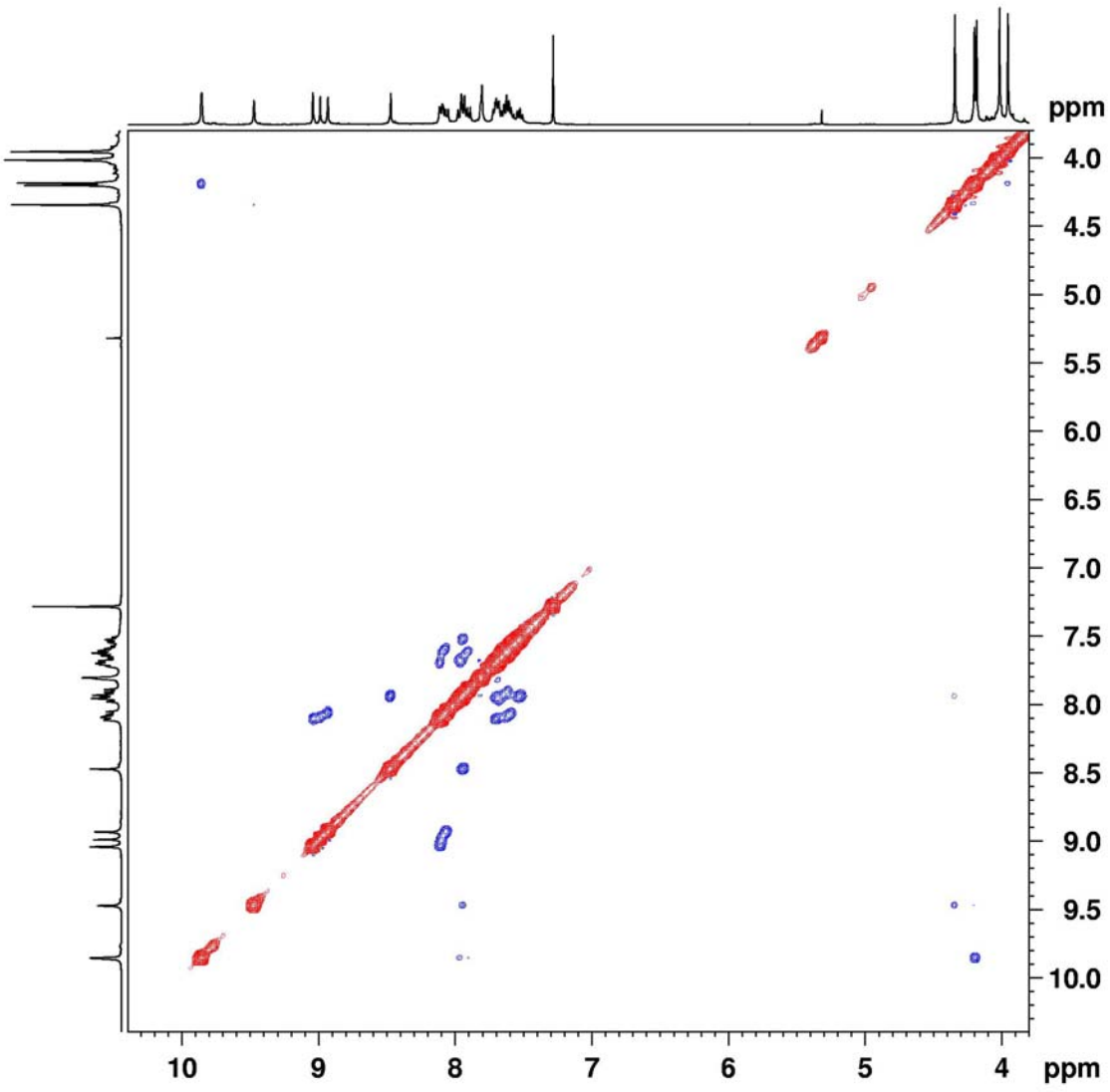


Figure S10. 2D NOESY spectrum of **4** (400 MHz, $CDCl_3$).

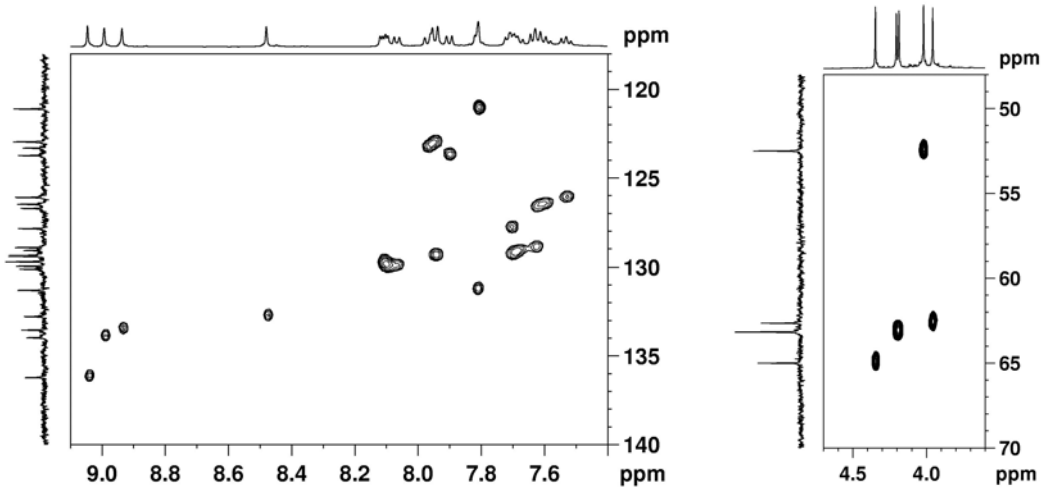


Figure S11. Partial HSQC spectra of **4** (400 MHz, $CDCl_3$).

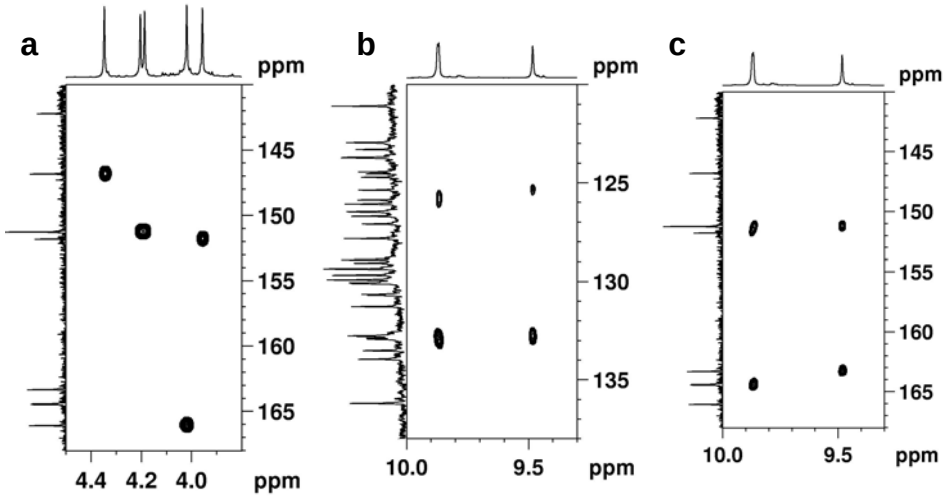


Figure S12. Partial HMBC spectra of **4** (400 MHz, $CDCl_3$).

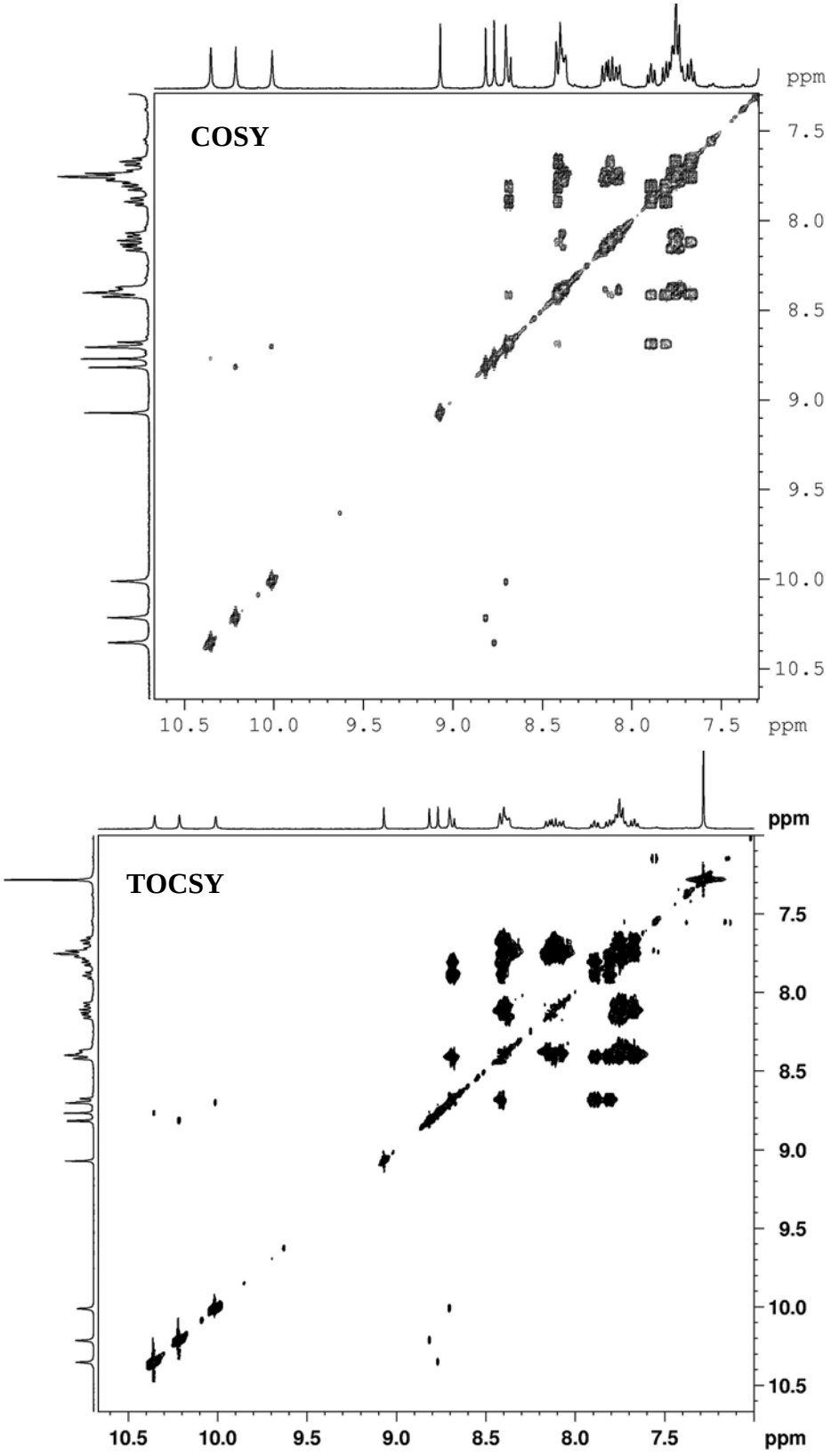


Figure S13. Partial 2D COSY and TOCSY spectra of **8** (400 MHz, $CDCl_3$).

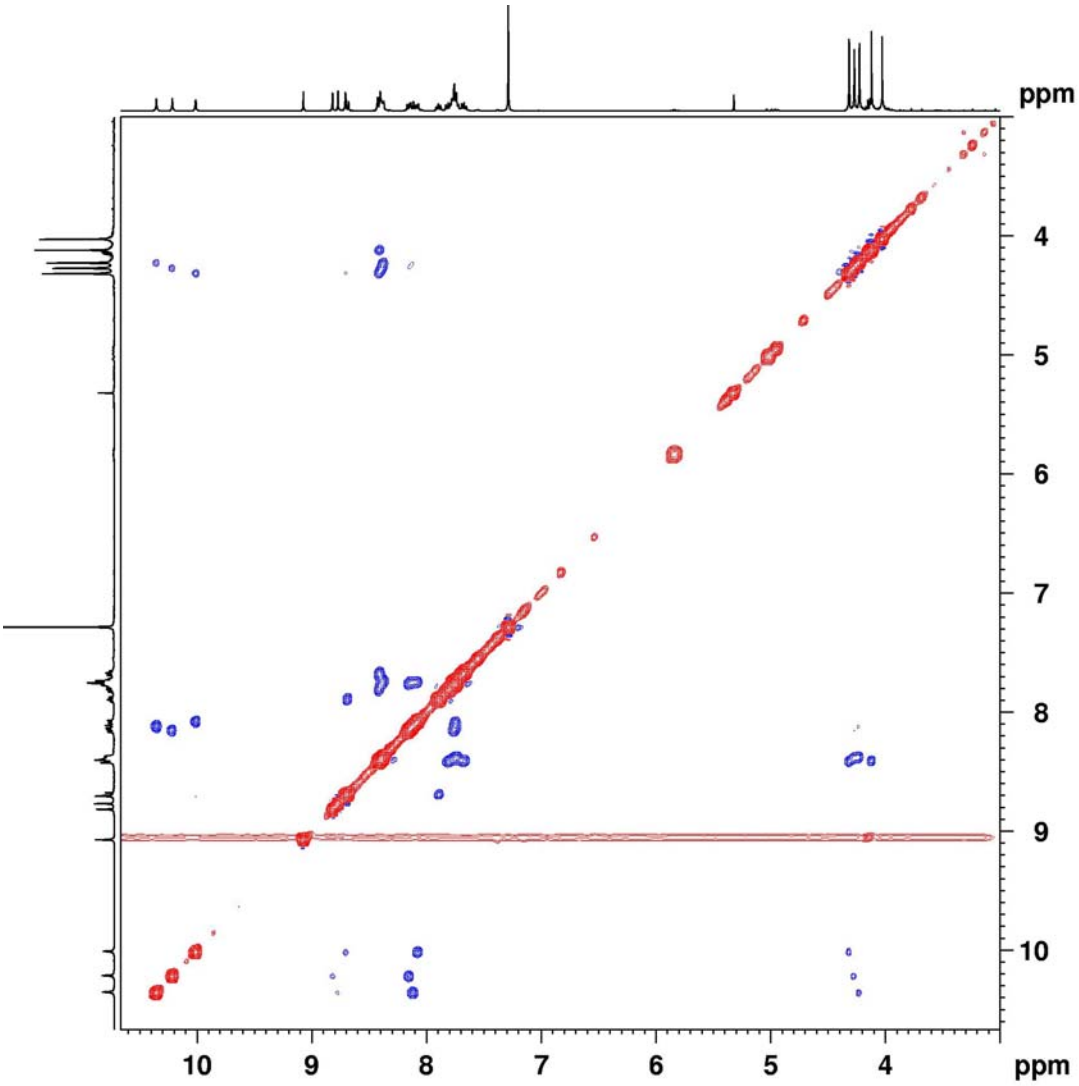


Figure S14. 2D NOESY spectrum of **8** (400 MHz, $CDCl_3$).

Quantum Chemical Calculations

The conformational structure of the oligomers **4** and **8** is considerably predetermined by the approximate anti-periplanar arrangement of the naphthyl rings and the hydrogen bonding between the amide NHs and the methoxy groups. Therefore, complete geometry optimization at the HF/6-31G* level of *ab initio* MO theory is straightforward and confirms these conformational features. Nevertheless, conformational alternatives without hydrogen bonding were considered, but proved to be lesser stable than the hydrogen-bonded conformers. Starting the geometry optimization from more planar arrangements leads always to the approximate anti-periplanar arrangement of the naphthyl rings.
The geometry of the oligomers **4** and **8** is given as pdb-files:

Oligomer **4** (E_T(HF/6-31G*) = -2918.876626 a.u.)

```
HEADER
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HETATM    4  N   UNK  0001       8.012   2.457  -1.334
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HETATM    7  C   UNK  0001      -6.871   4.608  -1.024
HETATM    8  C   UNK  0001      -6.574   3.454  -0.253
HETATM    9  C   UNK  0001      -5.670   2.498  -0.753
HETATM   10  C   UNK  0001      -5.079   2.723  -2.025
HETATM   11  C   UNK  0001      -7.163   3.244   1.018
HETATM   12  C   UNK  0001      -6.856   2.152   1.763
HETATM   13  C   UNK  0001      -5.977   1.162   1.241
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Oligomer **8** (E_T(HF/6-31G*) = -2918.899241 a.u.)

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HETATM    4  N   UNK  0001     -10.659   0.259   1.647
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HETATM   32  C   UNK  0001      -4.146  -0.997  -1.218
HETATM   33  C   UNK  0001      -4.083  -1.912  -2.313
HETATM   34  C   UNK  0001      -2.944  -2.730  -2.437
HETATM   35  C   UNK  0001      -1.892  -2.628  -1.476
HETATM   36  C   UNK  0001      -5.106  -2.019  -3.289
HETATM   37  C   UNK  0001      -4.987  -2.885  -4.329
HETATM   38  C   UNK  0001      -3.837  -3.696  -4.461
HETATM   39  C   UNK  0001      -2.843  -3.620  -3.539
HETATM   40  C   UNK  0001      -6.471  -0.535  -0.628
HETATM   41  C   UNK  0001      -0.944  -4.725  -0.990
HETATM   42  C   UNK  0001      -7.489   0.522  -0.271
HETATM   43  C   UNK  0001      -8.613   0.043   0.447
HETATM   44  C   UNK  0001      -9.581   0.880   0.883
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HETATM   45  C   UNK  0001      -9.543   2.289   0.638
HETATM   46  C   UNK  0001      -8.436   2.765  -0.098
HETATM   47  C   UNK  0001      -7.430   1.858  -0.554
HETATM   48  C   UNK  0001     -10.539   3.221   1.034
HETATM   49  C   UNK  0001     -10.407   4.541   0.733
HETATM   50  C   UNK  0001      -9.280   5.022   0.035
HETATM   51  C   UNK  0001      -8.319   4.153  -0.371
HETATM   52  C   UNK  0001      -6.587   2.439  -2.675
HETATM   53  C   UNK  0001      11.423   2.788  -1.096
HETATM   54  O   UNK  0001       4.336   0.692  -0.634
HETATM   55  O   UNK  0001      11.271  -0.179  -1.667
HETATM   56  O   UNK  0001       9.631  -1.644  -1.502
HETATM   57  O   UNK  0001       4.886  -0.585   3.298
HETATM   58  O   UNK  0001      -1.127  -0.739   1.511
HETATM   59  O   UNK  0001      -0.827  -3.466  -1.630
HETATM   60  O   UNK  0001      -6.754  -1.694  -0.512
HETATM   61  O   UNK  0001      -6.402   2.385  -1.267
HETATM   62  O   UNK  0001     -11.162   0.889   2.529
HETATM   63  O   UNK  0001     -10.961  -0.860   1.363
HETATM   64  O   UNK  0001      10.285   2.428  -1.856
HETATM   65  H   UNK  0001       5.501   5.273   0.461
HETATM   66  H   UNK  0001       7.444   6.112  -0.824
HETATM   67  H   UNK  0001       9.156   4.550  -1.605
HETATM   68  H   UNK  0001       5.262   2.898   0.922
HETATM   69  H   UNK  0001       7.851  -0.966  -0.108
HETATM   70  H   UNK  0001       6.128  -0.111   1.768
HETATM   71  H   UNK  0001       2.362  -0.556  -0.449
HETATM   72  H   UNK  0001       9.930  -3.573  -1.936
HETATM   73  H   UNK  0001      11.344  -2.761  -1.241
HETATM   74  H   UNK  0001      10.892  -2.453  -2.916
HETATM   75  H   UNK  0001       3.886  -1.960   5.037
HETATM   76  H   UNK  0001       2.191  -3.355   6.106
HETATM   77  H   UNK  0001       0.127  -3.956   4.877
HETATM   78  H   UNK  0001      -0.226  -3.165   2.605
HETATM   79  H   UNK  0001       0.512  -2.427  -0.507
HETATM   80  H   UNK  0001       3.907   0.555   4.715
HETATM   81  H   UNK  0001       4.658   1.464   3.397
HETATM   82  H   UNK  0001       5.667   0.700   4.632
HETATM   83  H   UNK  0001      -3.153  -0.212   0.467
HETATM   84  H   UNK  0001      -5.983  -1.411  -3.195
HETATM   85  H   UNK  0001      -5.771  -2.954  -5.062
HETATM   86  H   UNK  0001      -3.751  -4.367  -5.296
HETATM   87  H   UNK  0001      -1.958  -4.216  -3.646
HETATM   88  H   UNK  0001      -5.053   0.854  -0.992
HETATM   89  H   UNK  0001      -0.064  -5.288  -1.260
HETATM   90  H   UNK  0001      -1.830  -5.245  -1.329
HETATM   91  H   UNK  0001      -0.984  -4.603   0.085
HETATM   92  H   UNK  0001      -8.677  -1.007   0.641
HETATM   93  H   UNK  0001     -11.392   2.885   1.582
HETATM   94  H   UNK  0001     -11.171   5.231   1.043
HETATM   95  H   UNK  0001      -9.184   6.072  -0.170
HETATM   96  H   UNK  0001      -7.450   4.506  -0.889
HETATM   97  H   UNK  0001      -5.715   2.933  -3.075
HETATM   98  H   UNK  0001      -7.475   3.006  -2.921
HETATM   99  H   UNK  0001      -6.663   1.442  -3.086
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HETATM  100  H   UNK  0001      12.139   3.183  -1.801
HETATM  101  H   UNK  0001      11.841   1.926  -0.602
HETATM  102  H   UNK  0001      11.169   3.552  -0.370
CONECT    1   14   15   70
CONECT    2   20   29   79
CONECT    3   32   40   88
CONECT    4   44   62   63
CONECT    5    6   10   65
CONECT    6    5    7   66
CONECT    7    6    8   67
CONECT    8    7    9   11
CONECT    9    8   10   14
CONECT   10    5    9   68
CONECT   11    8   12   64
CONECT   12   11   13   22
CONECT   13   12   14   69
CONECT   14    1    9   13
CONECT   15    1   16   54
CONECT   16   15   17   21
CONECT   17   16   18   57
CONECT   18   17   19   24
CONECT   19   18   20   27
CONECT   20    2   19   21
CONECT   21   16   20   71
CONECT   22   12   55   56
CONECT   23   56   72   73   74
CONECT   24   18   25   75
CONECT   25   24   26   76
CONECT   26   25   27   77
CONECT   27   19   26   78
CONECT   28   57   80   81   82
CONECT   29    2   30   58
CONECT   30   29   31   35
CONECT   31   30   32   83
CONECT   32    3   31   33
CONECT   33   32   34   36
CONECT   34   33   35   39
CONECT   35   30   34   59
CONECT   36   33   37   84
CONECT   37   36   38   85
CONECT   38   37   39   86
CONECT   39   34   38   87
CONECT   40    3   42   60
CONECT   41   59   89   90   91
CONECT   42   40   43   47
CONECT   43   42   44   92
CONECT   44    4   43   45
CONECT   45   44   46   48
CONECT   46   45   47   51
CONECT   47   42   46   61
CONECT   48   45   49   93
CONECT   49   48   50   94
CONECT   50   49   51   95
CONECT   51   46   50   96
CONECT   52   61   97   98   99
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CONECT   53   64  100  101  102
CONECT   54   15
CONECT   55   22
CONECT   56   22   23
CONECT   57   17   28
CONECT   58   29
CONECT   59   35   41
CONECT   60   40
CONECT   61   47   52
CONECT   62    4
CONECT   63    4
CONECT   64   11   53
CONECT   65    5
CONECT   66    6
CONECT   67    7
CONECT   68   10
CONECT   69   13
CONECT   70    1
CONECT   71   21
CONECT   72   23
CONECT   73   23
CONECT   74   23
CONECT   75   24
CONECT   76   25
CONECT   77   26
CONECT   78   27
CONECT   79    2
CONECT   80   28
CONECT   81   28
CONECT   82   28
CONECT   83   31
CONECT   84   36
CONECT   85   37
CONECT   86   38
CONECT   87   39
CONECT   88    3
CONECT   89   41
CONECT   90   41
CONECT   91   41
CONECT   92   43
CONECT   93   48
CONECT   94   49
CONECT   95   50
CONECT   96   51
CONECT   97   52
CONECT   98   52
CONECT   99   52
CONECT  100   53
CONECT  101   53
CONECT  102   53
END
```