Supporting Information

Structure-based Design of Novel Benzoxazinorifamycins with Potent Binding Affinity to Wild-type and Rifampin-resistant Mutant *Mycobacterium Tuberculosis* RNA Polymerases

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Figure 1aSI (compound 2a)

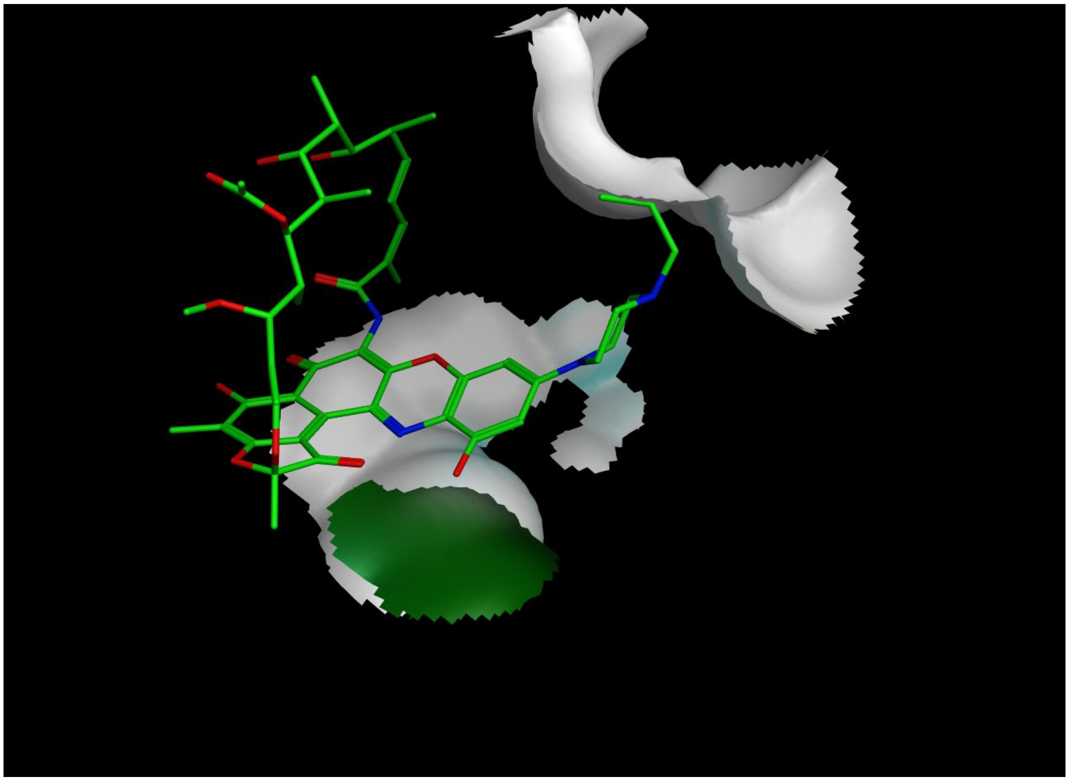


Figure 1bSI (compound 2c)

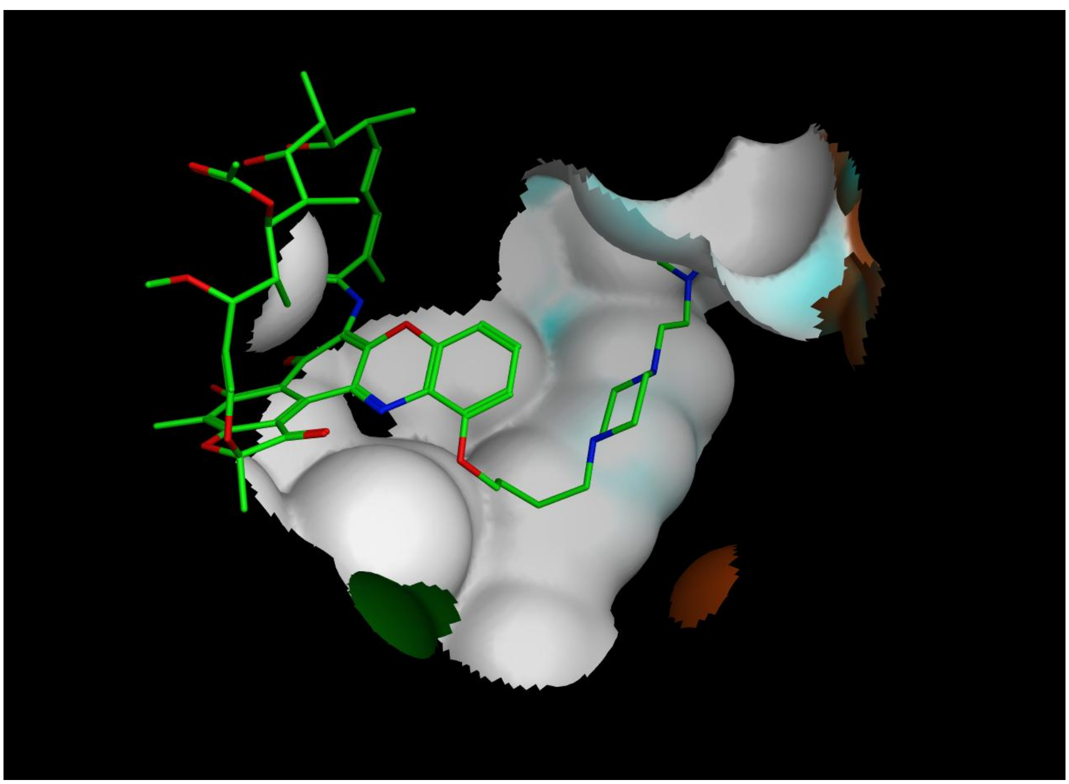


Figure 1cSI (compound 2d)

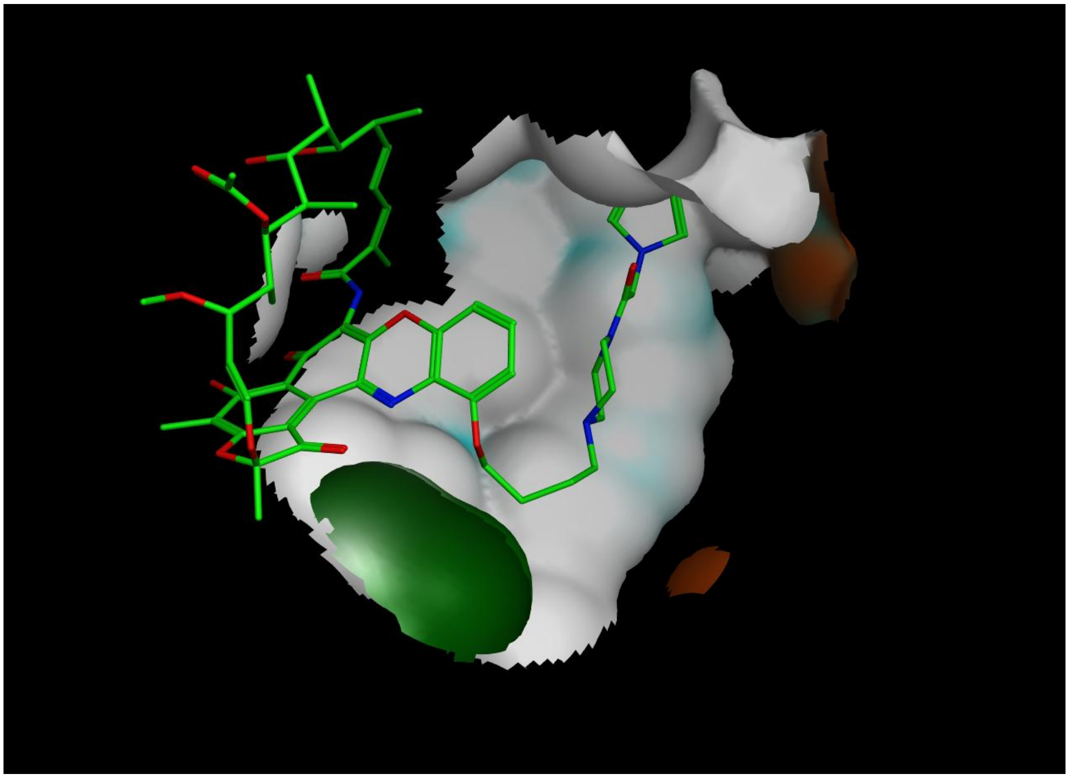


Figure 1a-cSI. Interaction surfaces at 4.5 Å between the compound tail and surrounding RNAP for benzoxazinorifamycins **2a** and **2c-d** in the same coloring scheme as Figure 2

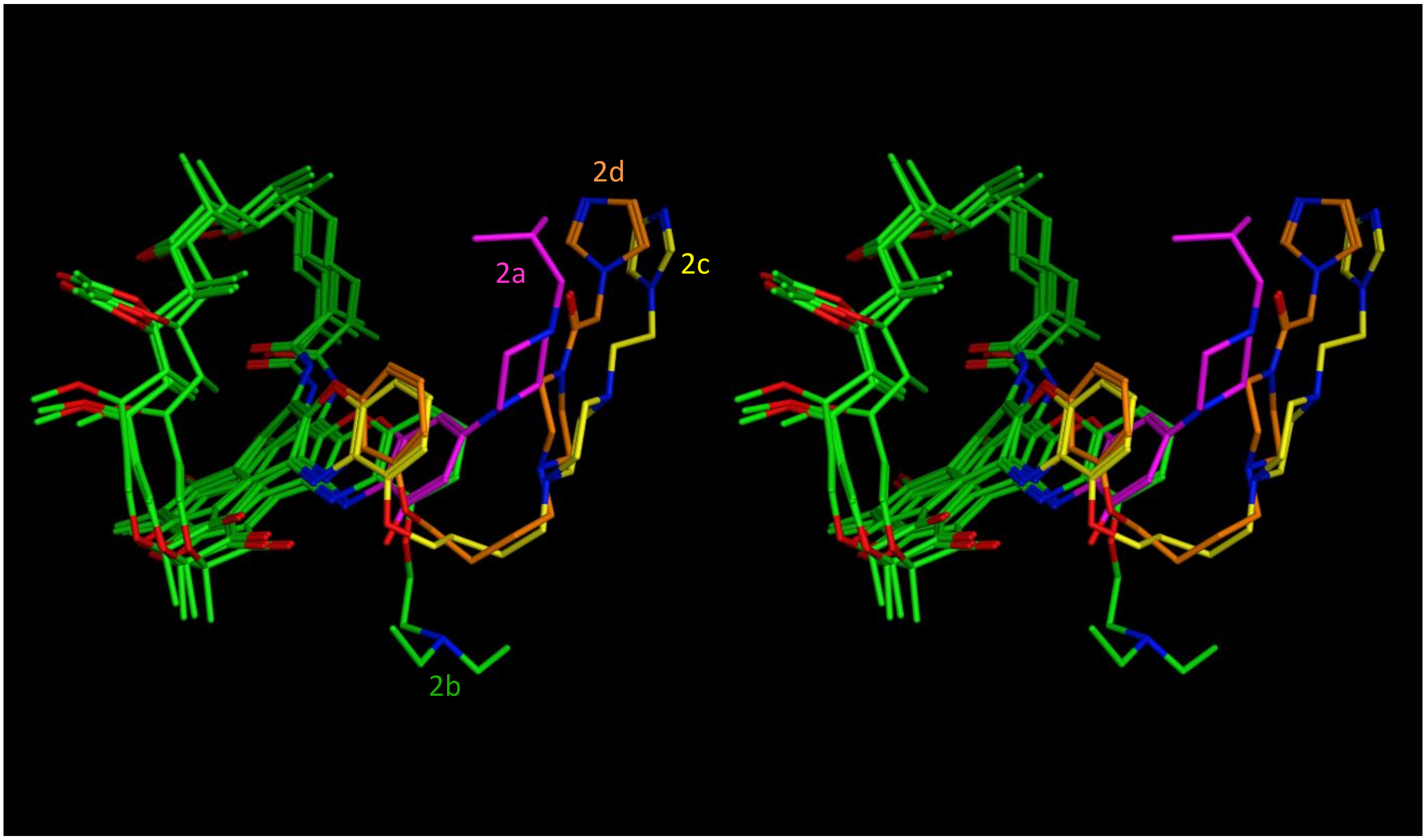
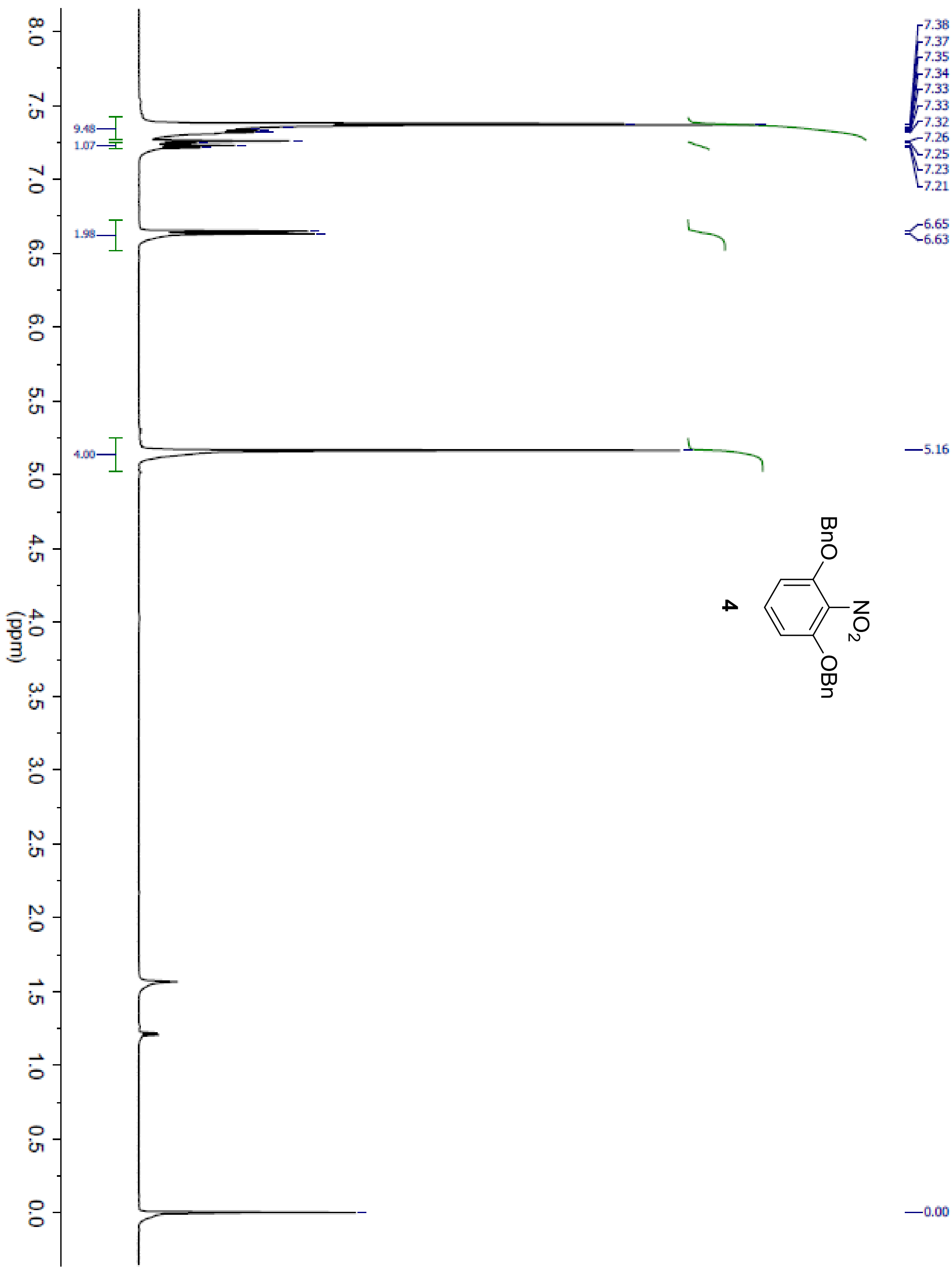


Figure 1dSI. Stereo view of superimposed compounds **2a-2d** in Figures 3 and 1a-cSI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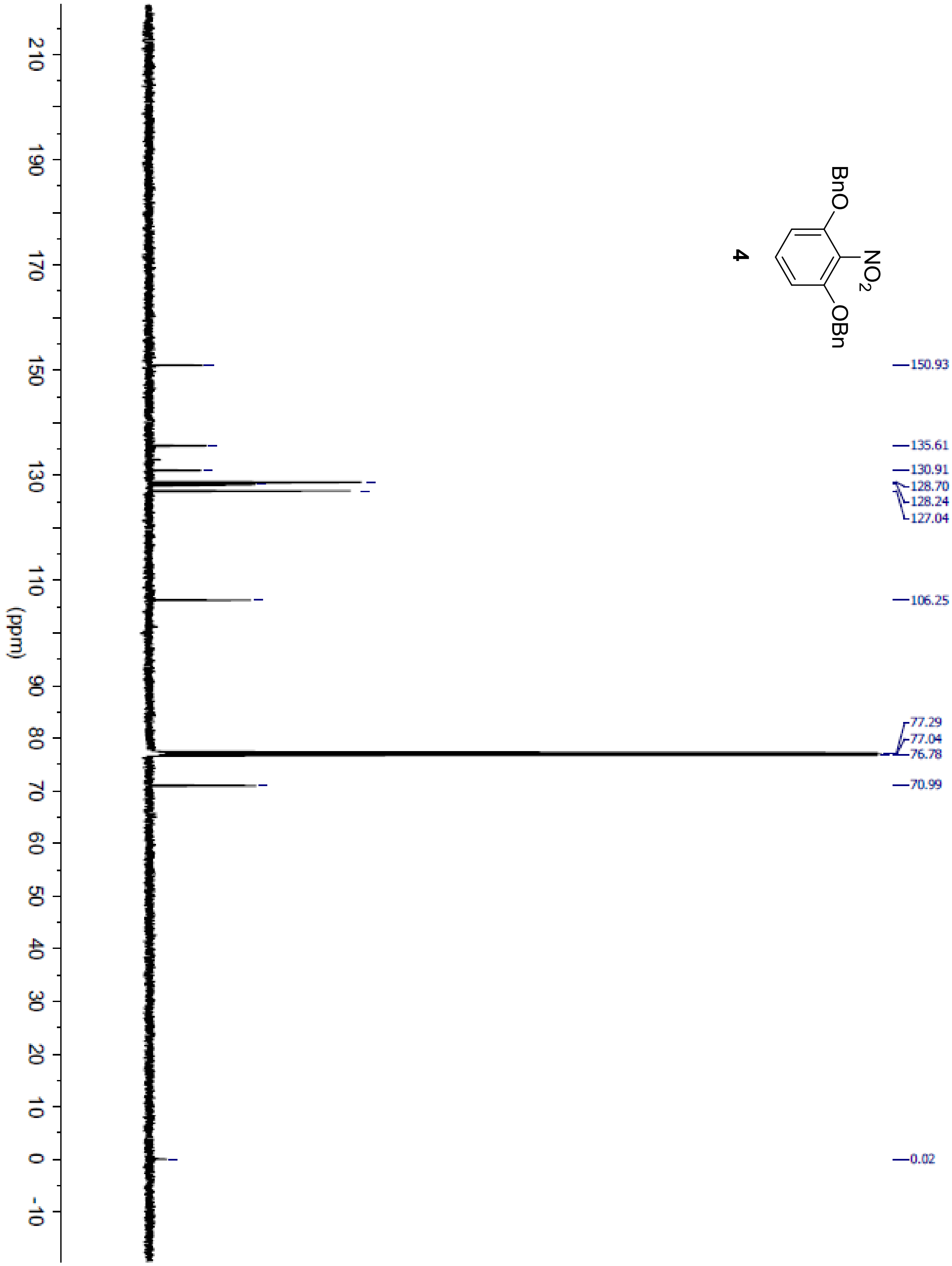
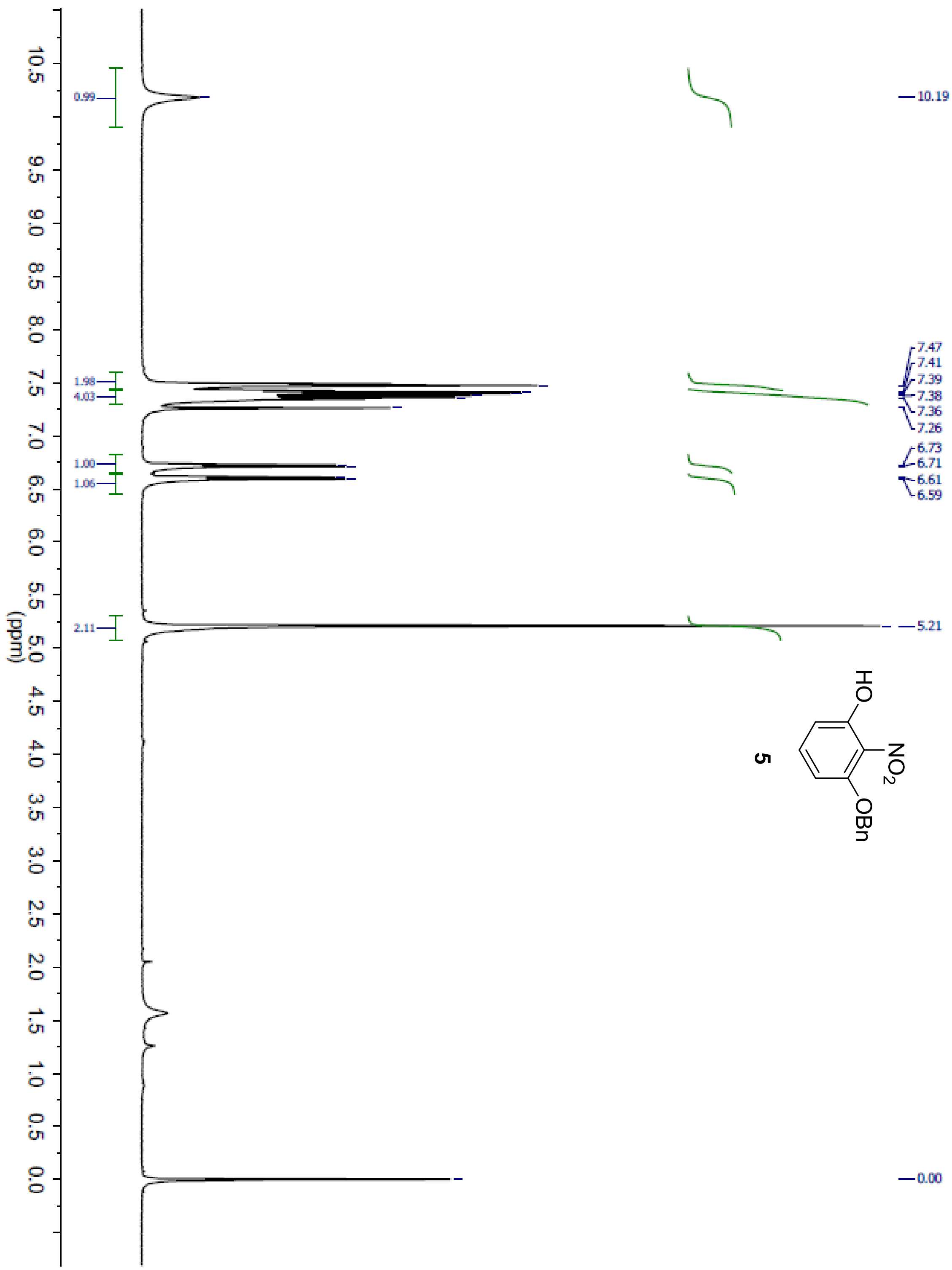
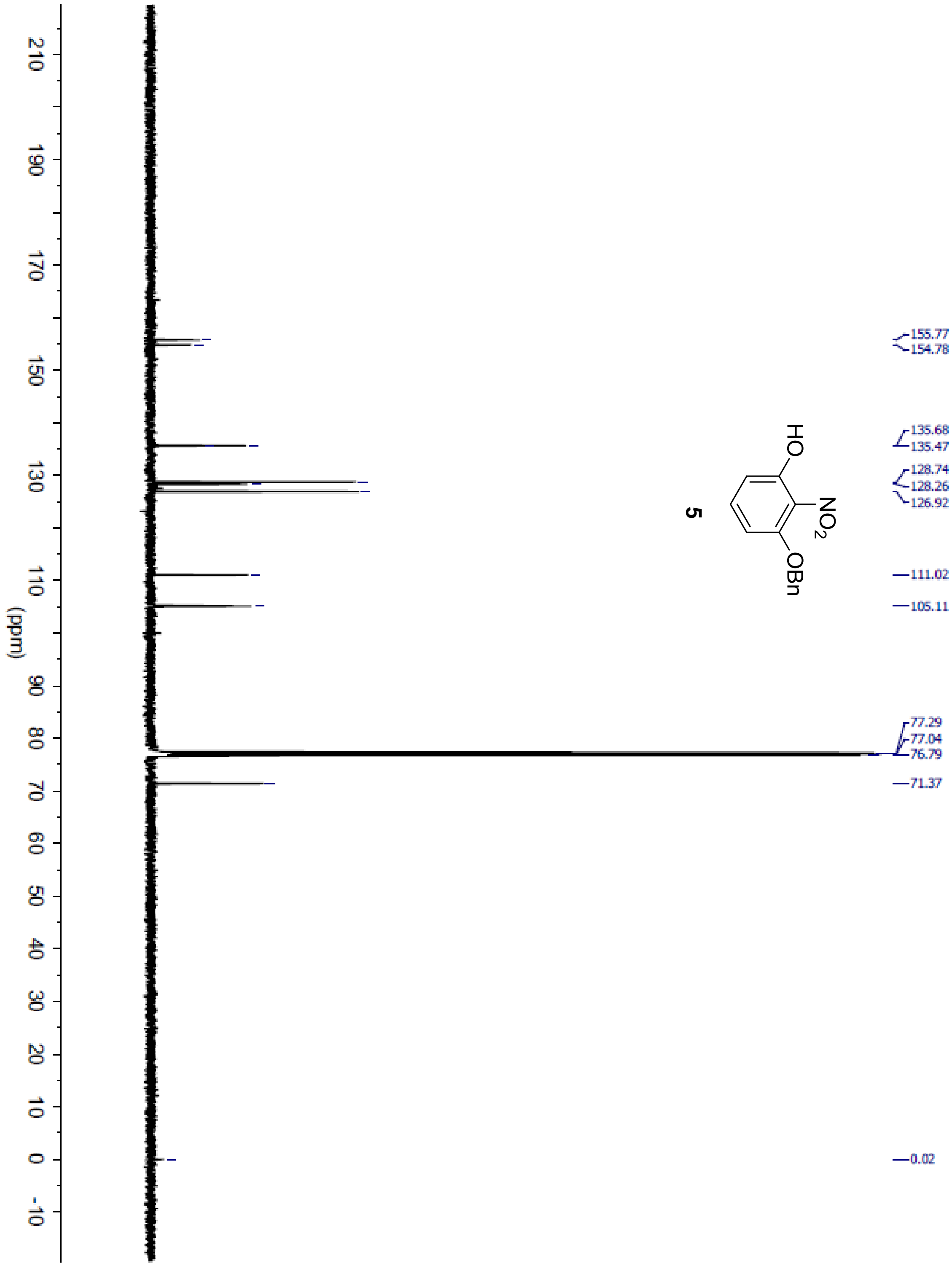
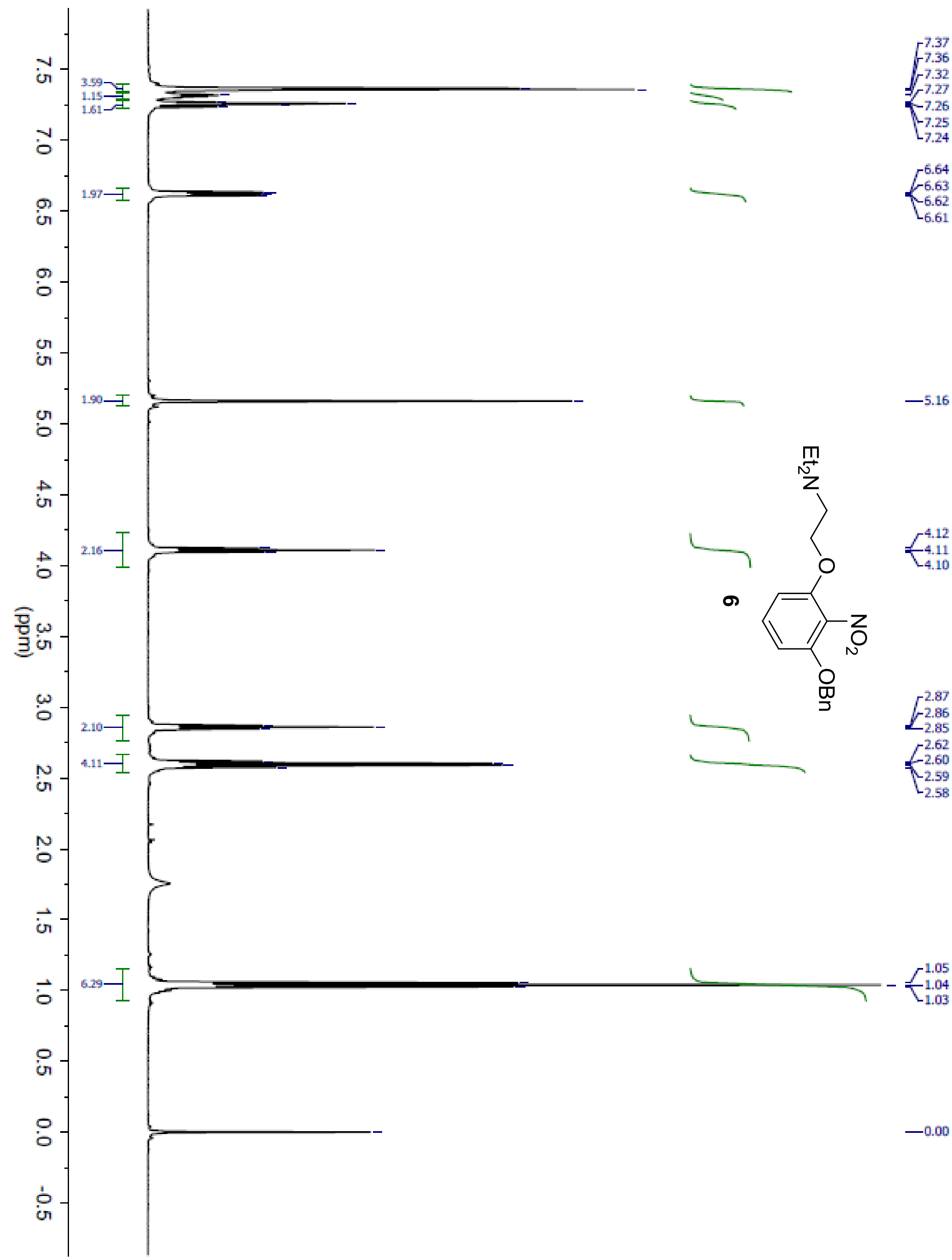
7.37
7.35
7.34
7.33
7.33
7.32
7.26
7.25
7.23
7.21
6.65
6.63
5.16
0.00
9.48
1.07
1.98
4.00
(ppm)
BnO
NO_2
OBn
4


BnO
NO2
OBn
4
150.93
135.61
130.91
128.70
128.24
127.04
106.25
77.29
77.04
76.78
70.99
0.02
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
(ppm)


10.19
7.47
7.41
7.39
7.38
7.36
7.26
6.73
6.71
6.61
6.59
5.21
0.00
0.99
1.98
4.03
1.00
1.06
2.11
(ppm)
HO
NO2
OBn
5


155.77
154.78
135.68
135.47
128.74
128.26
126.92
111.02
105.11
77.29
77.04
76.79
71.37
0.02
HO
NO_2
OBn
5
(ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10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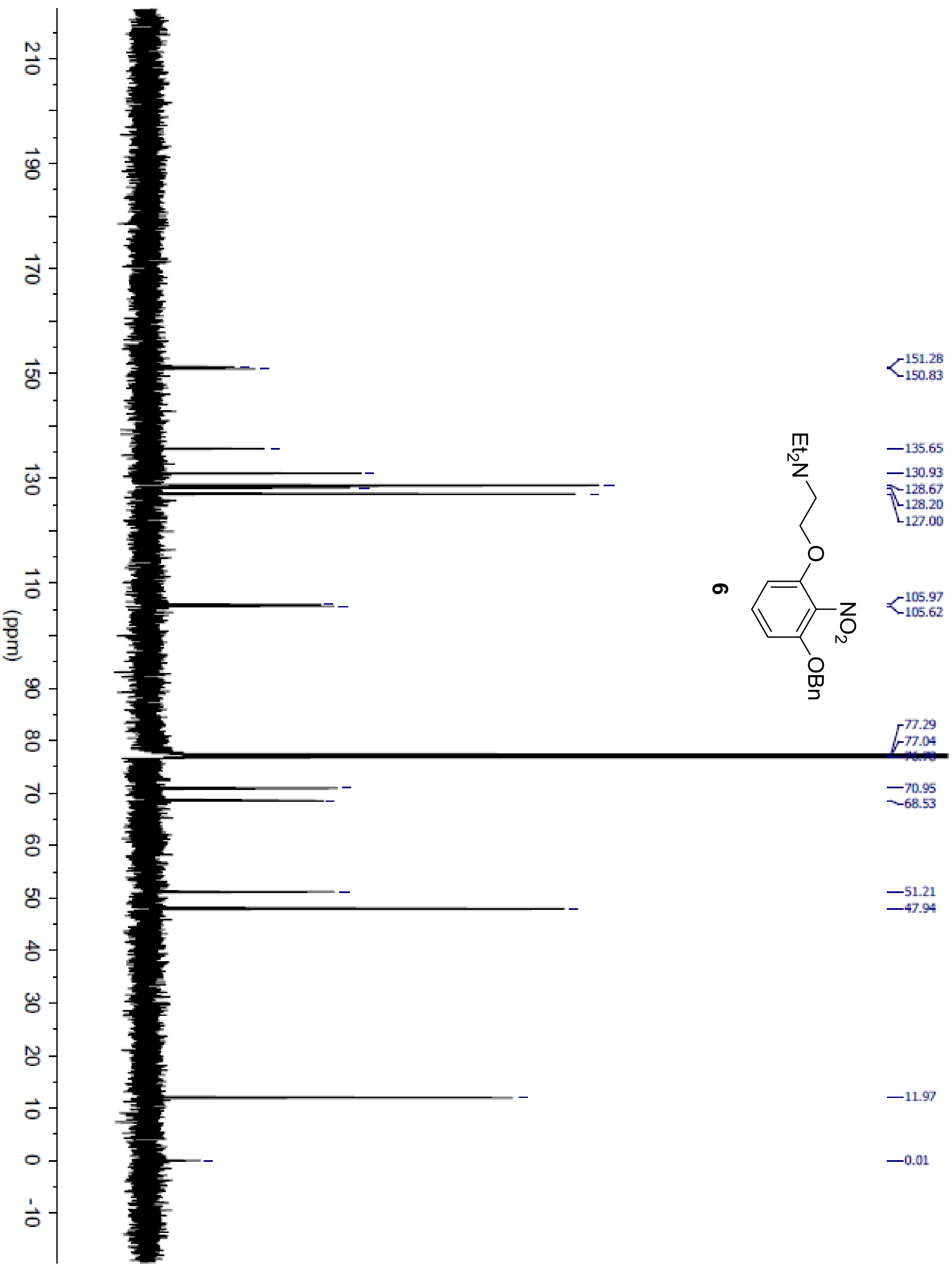
7.36
7.32
7.27
7.26
7.25
7.24
6.64
6.63
6.62
6.61
5.16
4.12
4.11
4.10
2.87
2.86
2.85
2.62
2.60
2.59
2.58
1.05
1.04
1.03
0.00
NO2
Et2N
O
OBn
6
3.59
1.15
1.61
1.97
1.90
2.16
2.10
4.11
6.29
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
(ppm)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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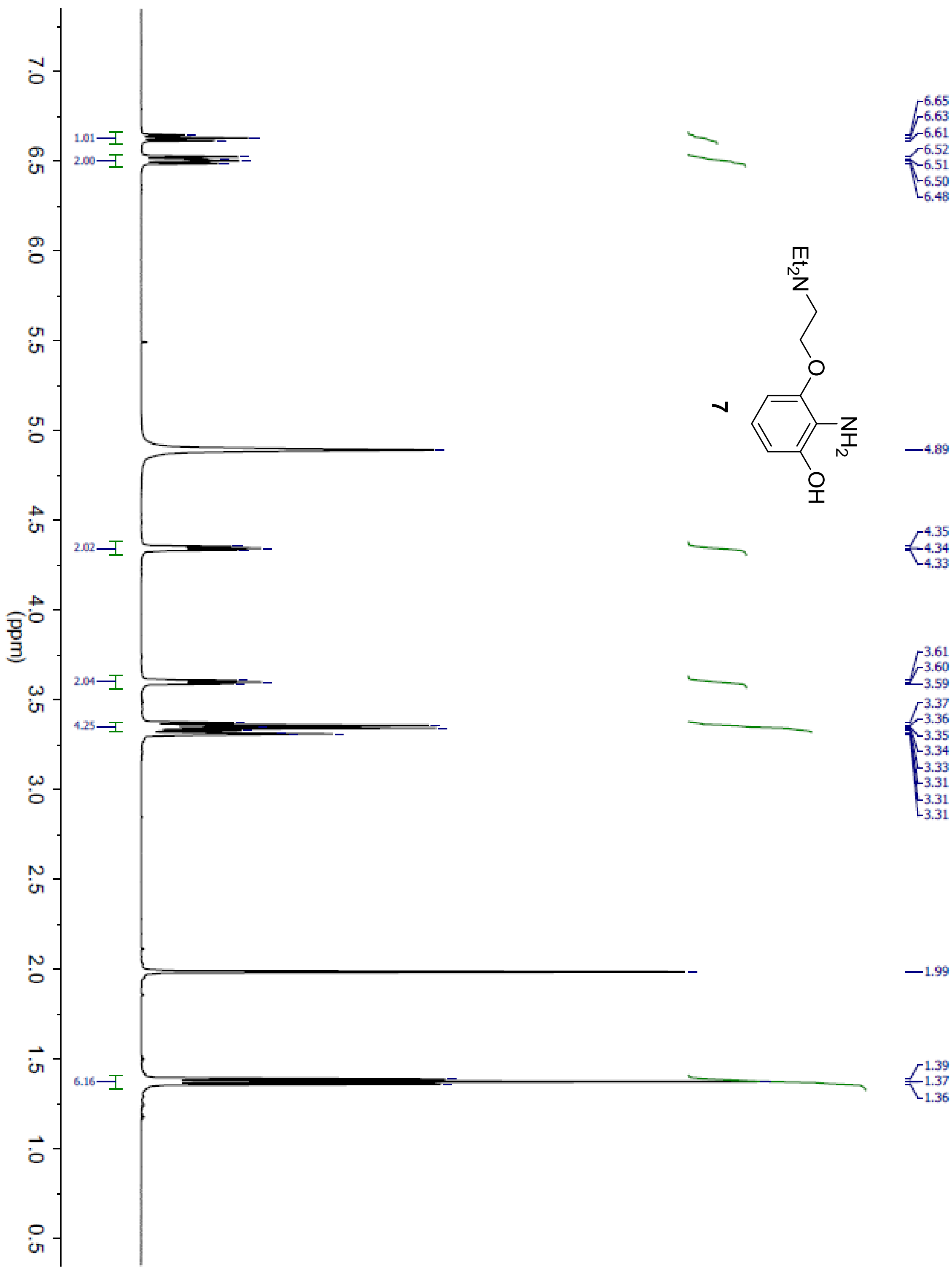
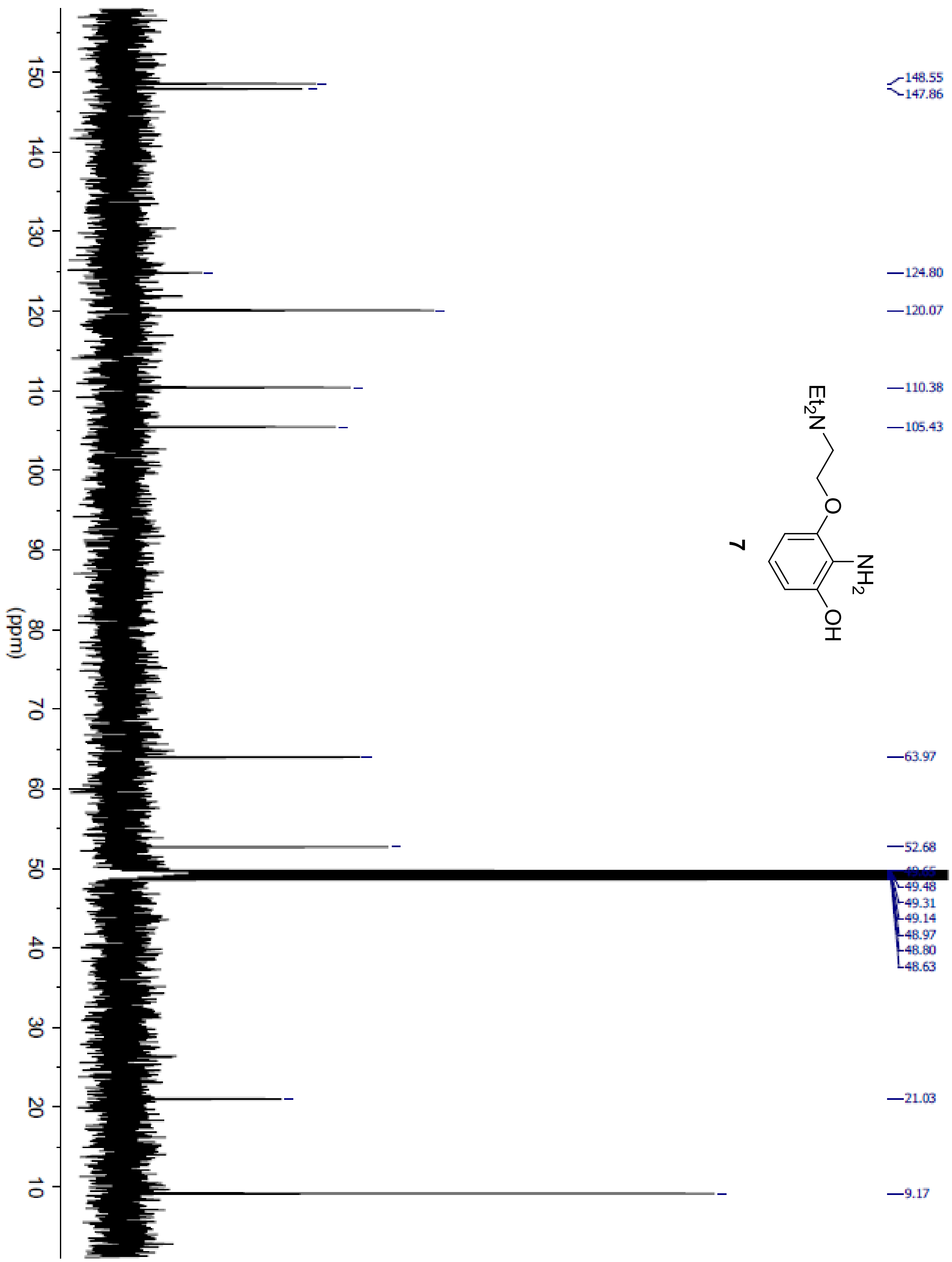
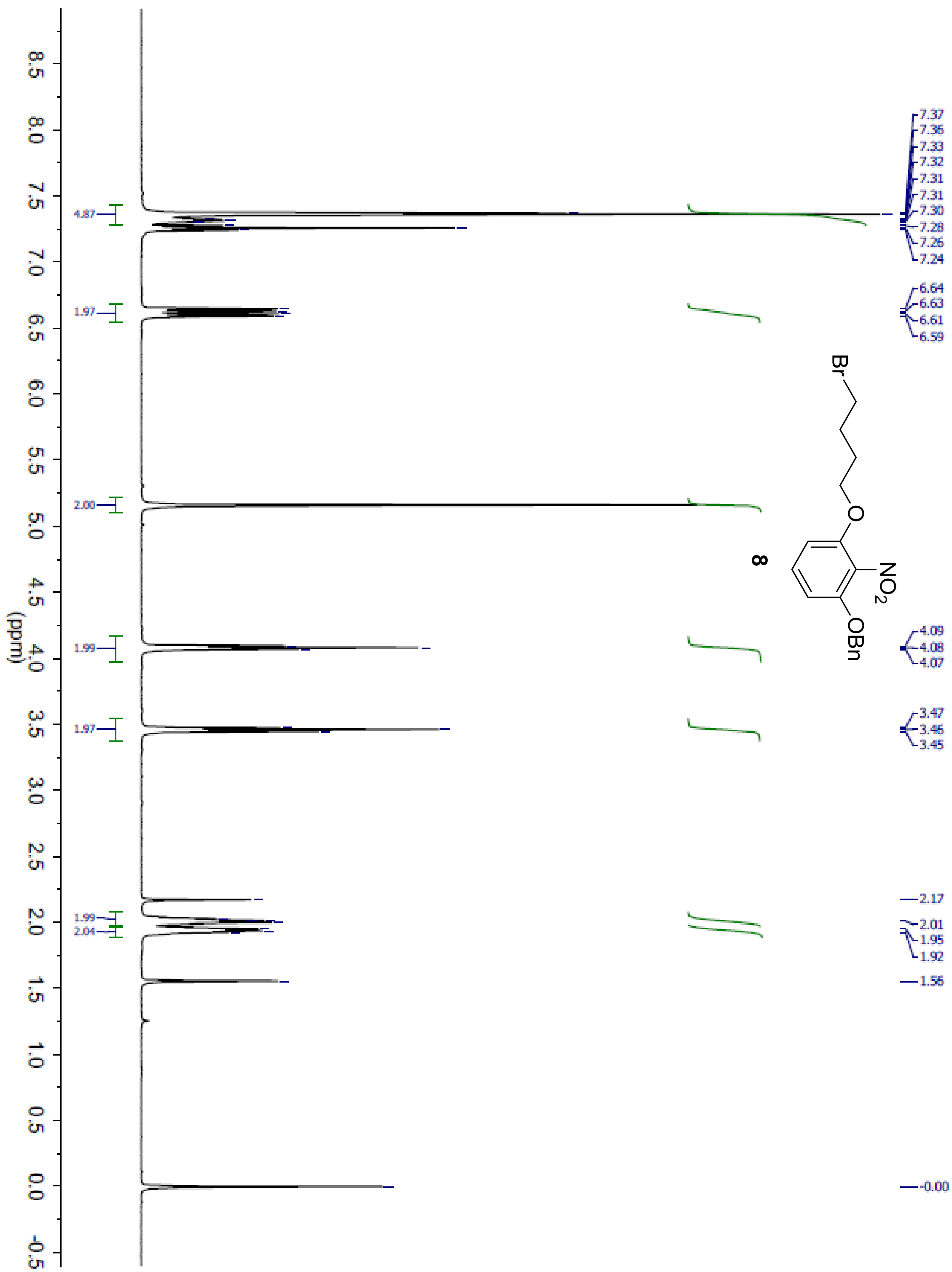
150.83
135.65
130.93
128.67
128.20
127.00
105.97
105.62
77.29
77.04
70.95
68.53
51.21
47.94
11.97
0.01
Et_2N
NO_2
OBn
O
6
(ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10


7
Et_2N
O
NH_2
OH
(ppm)
6.65
6.63
6.61
6.52
6.51
6.50
6.48
4.89
4.35
4.34
4.33
3.61
3.60
3.59
3.37
3.36
3.35
3.34
3.33
3.31
3.31
3.31
1.99
1.39
1.37
1.36
1.01
2.00
2.02
2.04
4.25
6.16



148.55
147.86
124.80
120.07
110.38
105.43
63.97
52.68
49.48
49.31
49.14
48.97
48.80
48.63
21.03
9.17
(ppm)
7


Br
O
NO2
OBn
8
(ppm)
7.37
7.36
7.33
7.32
7.31
7.31
7.30
7.28
7.26
7.24
6.64
6.63
6.61
6.59
4.09
4.08
4.07
3.47
3.46
3.45
2.17
2.01
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1.92
1.56
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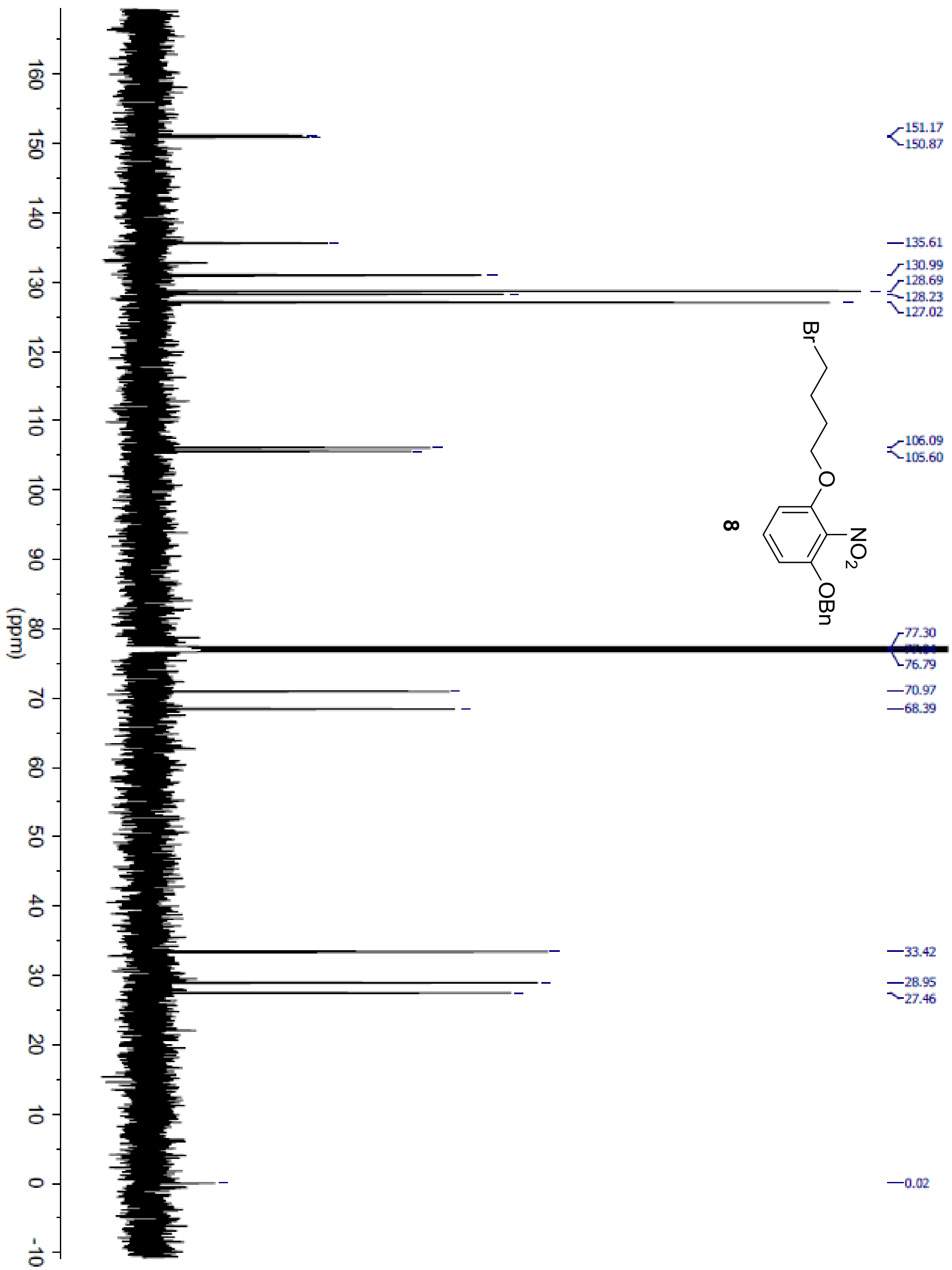
4.87
1.97
2.00
1.99
1.97
1.99
2.04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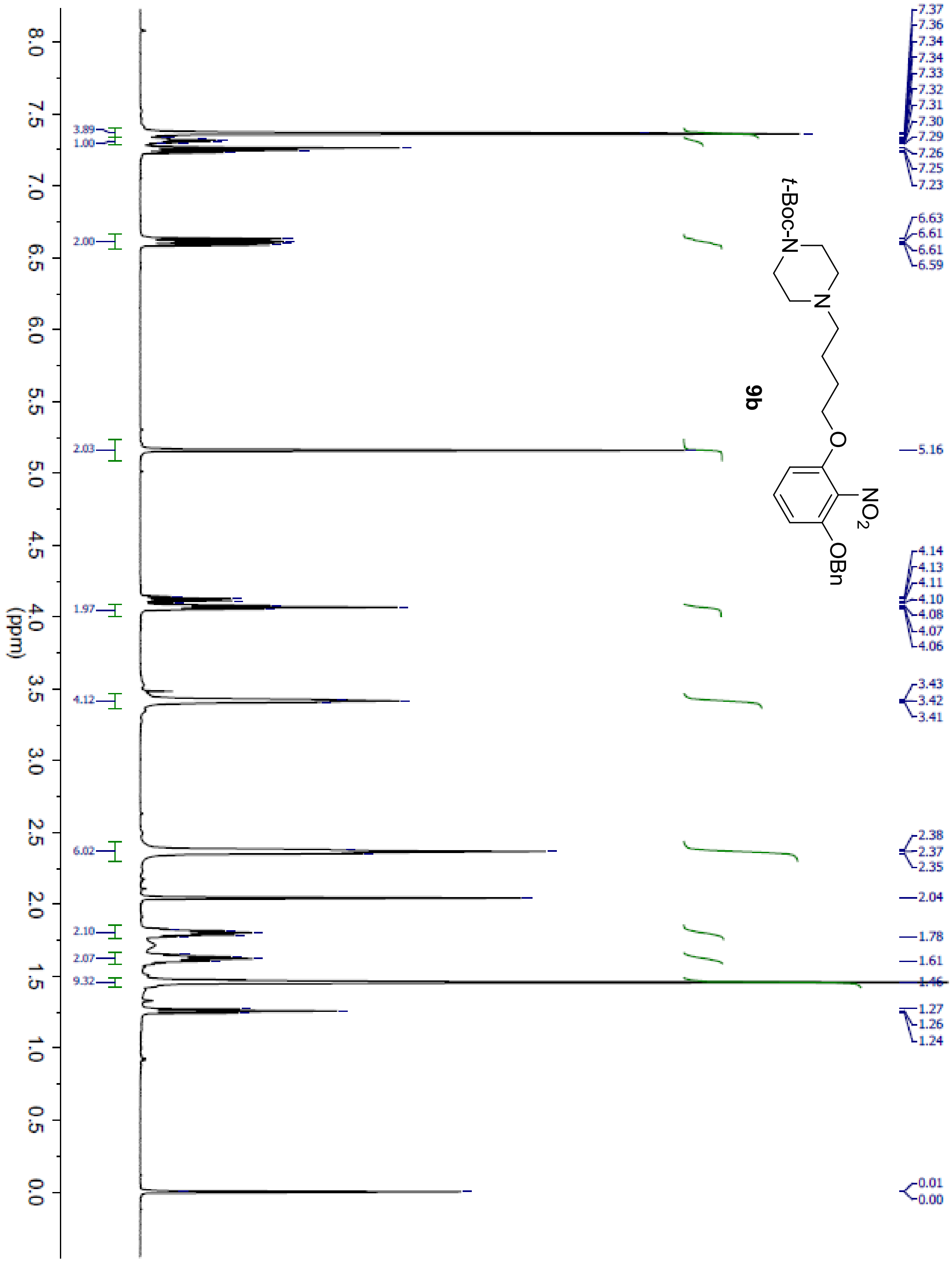
150.87
135.61
130.99
128.69
128.23
127.02
106.09
105.60
77.30
76.79
70.97
68.39
33.42
28.95
27.46
0.02
(ppm)
Br
O
NO2
OBn
8


9b
t-Boc-N
N
O
NO2
OBn
(ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
3.89
1.00
2.00
2.03
1.97
4.12
6.02
2.10
2.07
9.32
7.37
7.36
7.34
7.34
7.33
7.32
7.31
7.30
7.29
7.26
7.25
7.23
6.63
6.61
6.61
6.59
5.16
4.14
4.13
4.11
4.10
4.08
4.07
4.06
3.43
3.42
3.41
2.38
2.37
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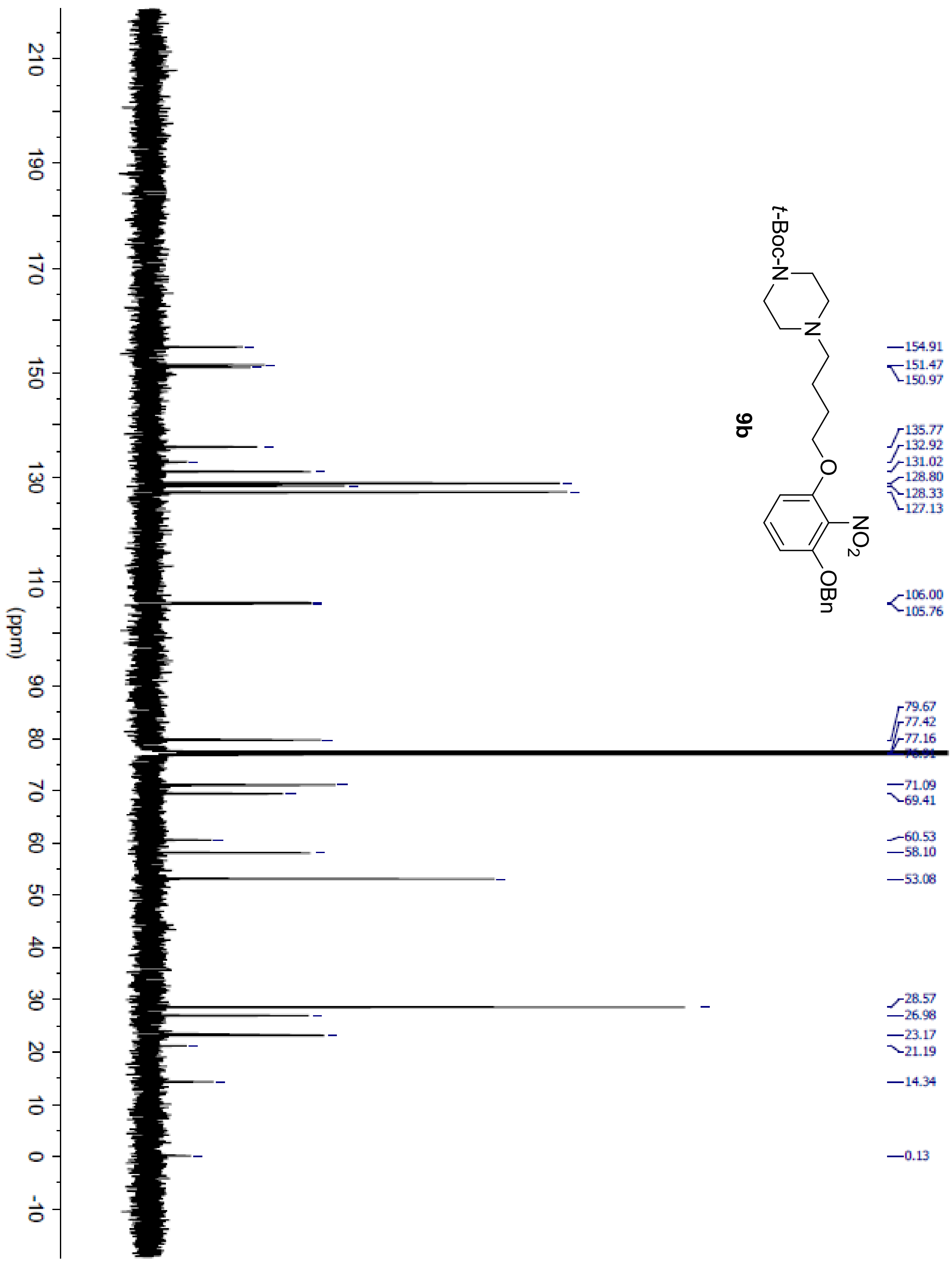
2.04
1.78
1.61
1.46
1.27
1.26
1.24
0.01
0.00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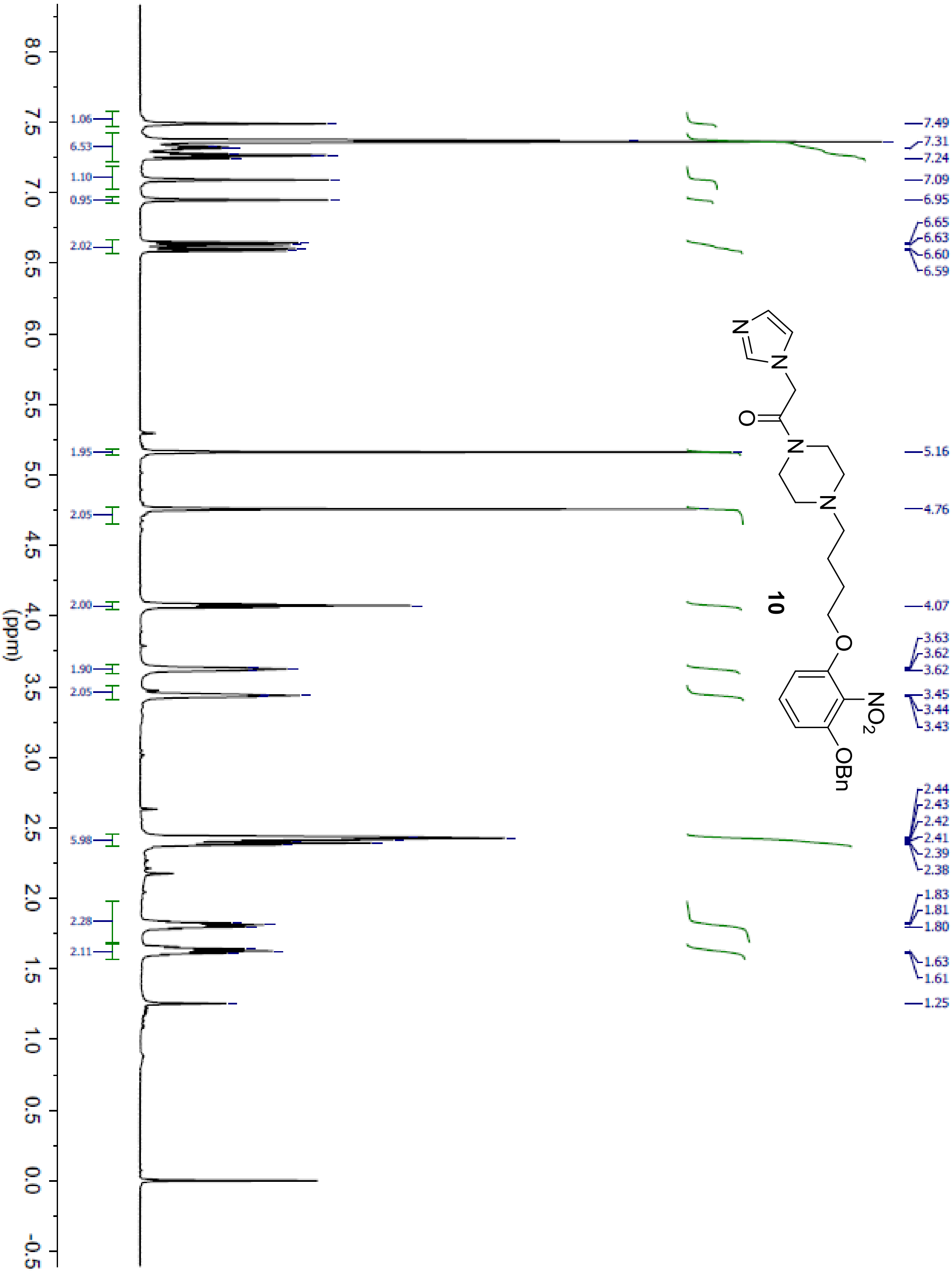
N
O
NO2
OBn
9b
154.91
151.47
150.97
135.77
132.92
131.02
128.80
128.33
127.13
106.00
105.76
79.67
77.42
77.16
71.09
69.41
60.53
58.10
53.08
28.57
26.98
23.17
21.19
14.34
0.13
(ppm)


10
(ppm)
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7.31
7.24
7.09
6.95
6.65
6.63
6.60
6.59
5.16
4.76
4.07
3.63
3.62
3.62
3.45
3.44
3.43
2.44
2.43
2.42
2.41
2.39
2.38
1.83
1.81
1.80
1.63
1.61
1.25
1.06
6.53
1.10
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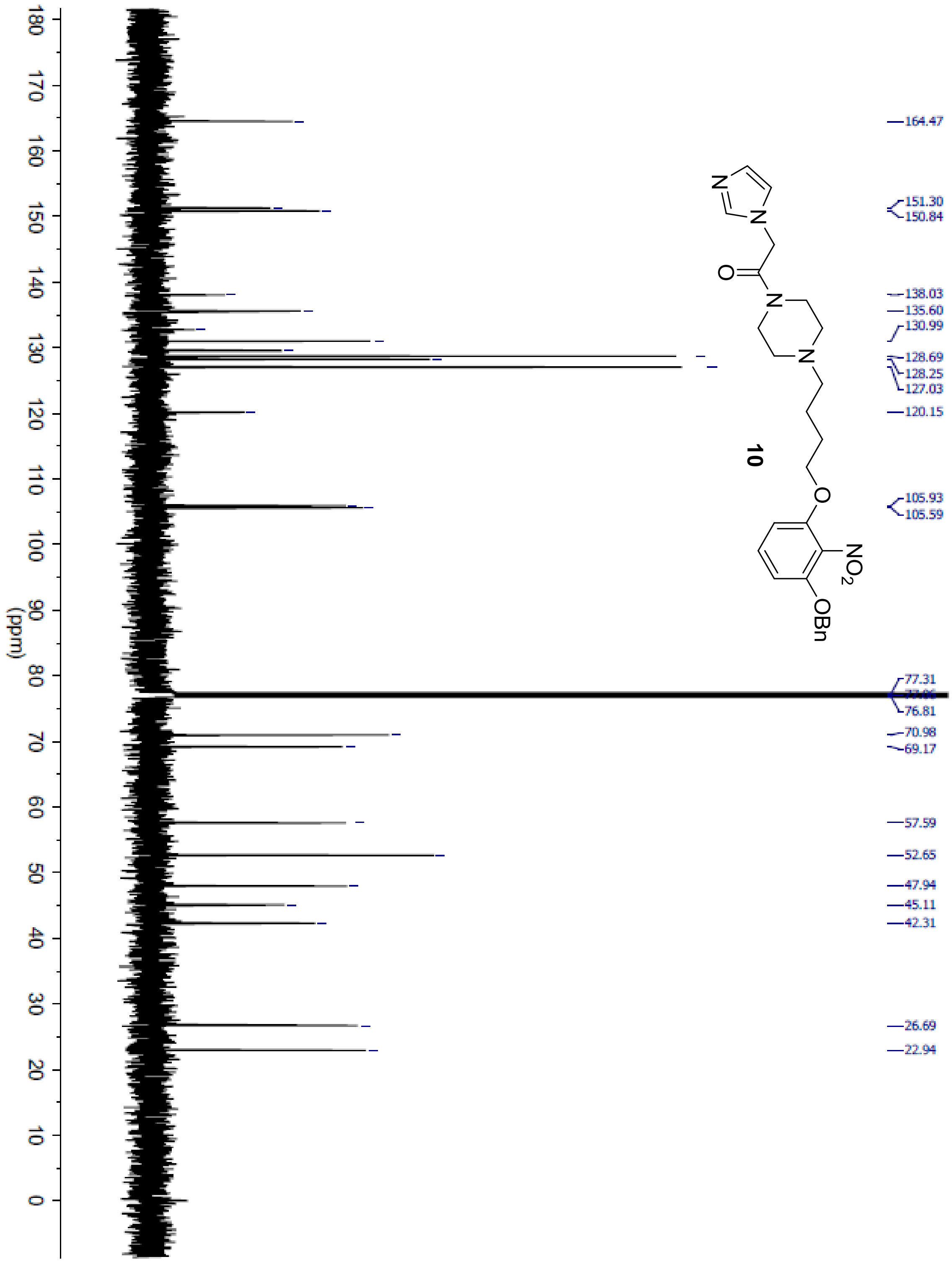
2.02
1.95
2.05
2.00
1.90
2.05
5.98
2.28
2.11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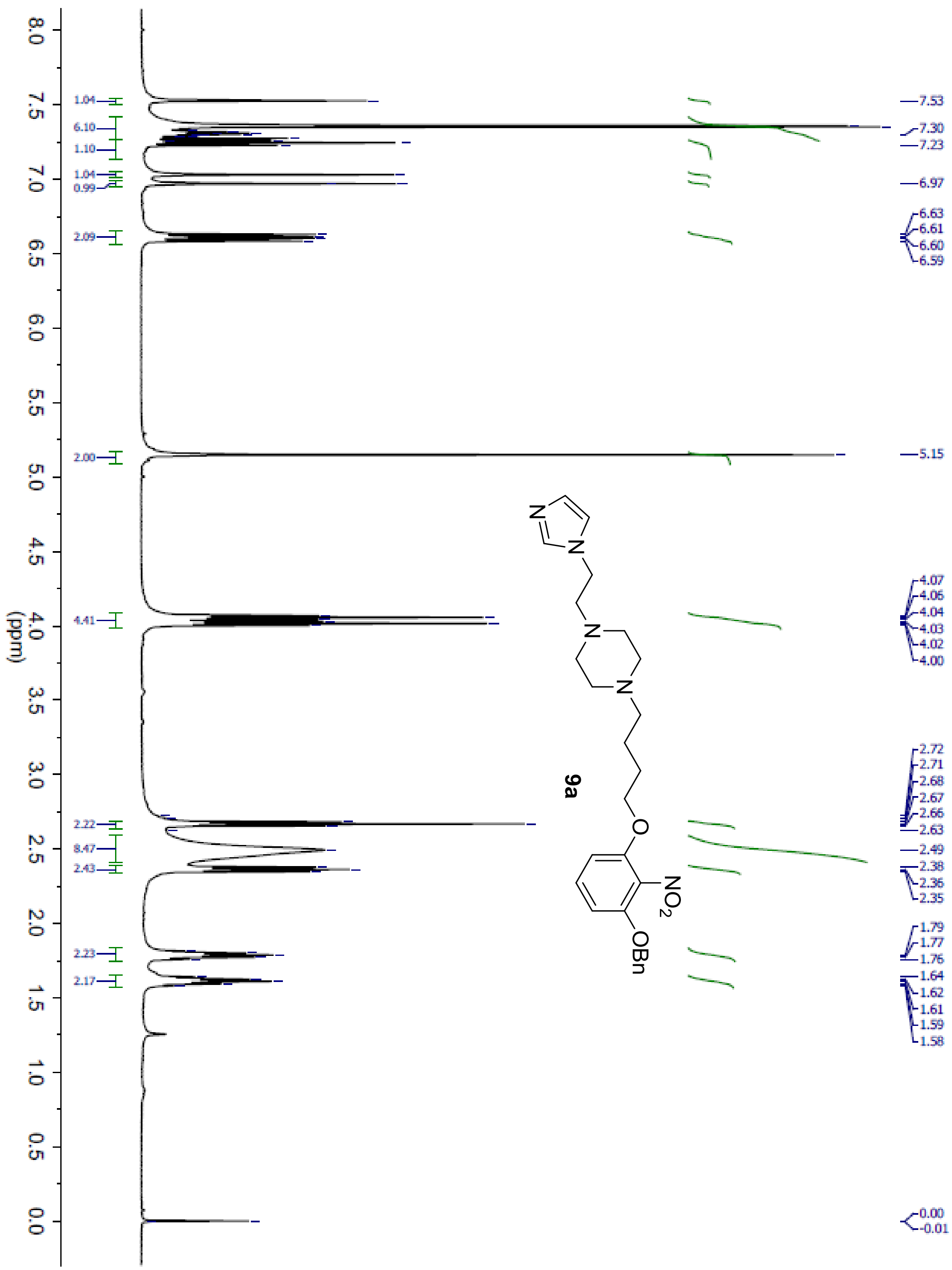
135.60
130.99
128.69
128.25
127.03
120.15
105.93
105.59
77.31
76.81
70.98
69.17
57.59
52.65
47.94
45.11
42.31
26.69
22.94
(ppm)
N
O
NO2
OBn
10


9a
(ppm)
7.53
7.30
7.23
6.97
6.63
6.61
6.60
6.59
5.15
4.07
4.06
4.04
4.03
4.02
4.00
2.72
2.71
2.68
2.67
2.66
2.63
2.49
2.38
2.36
2.35
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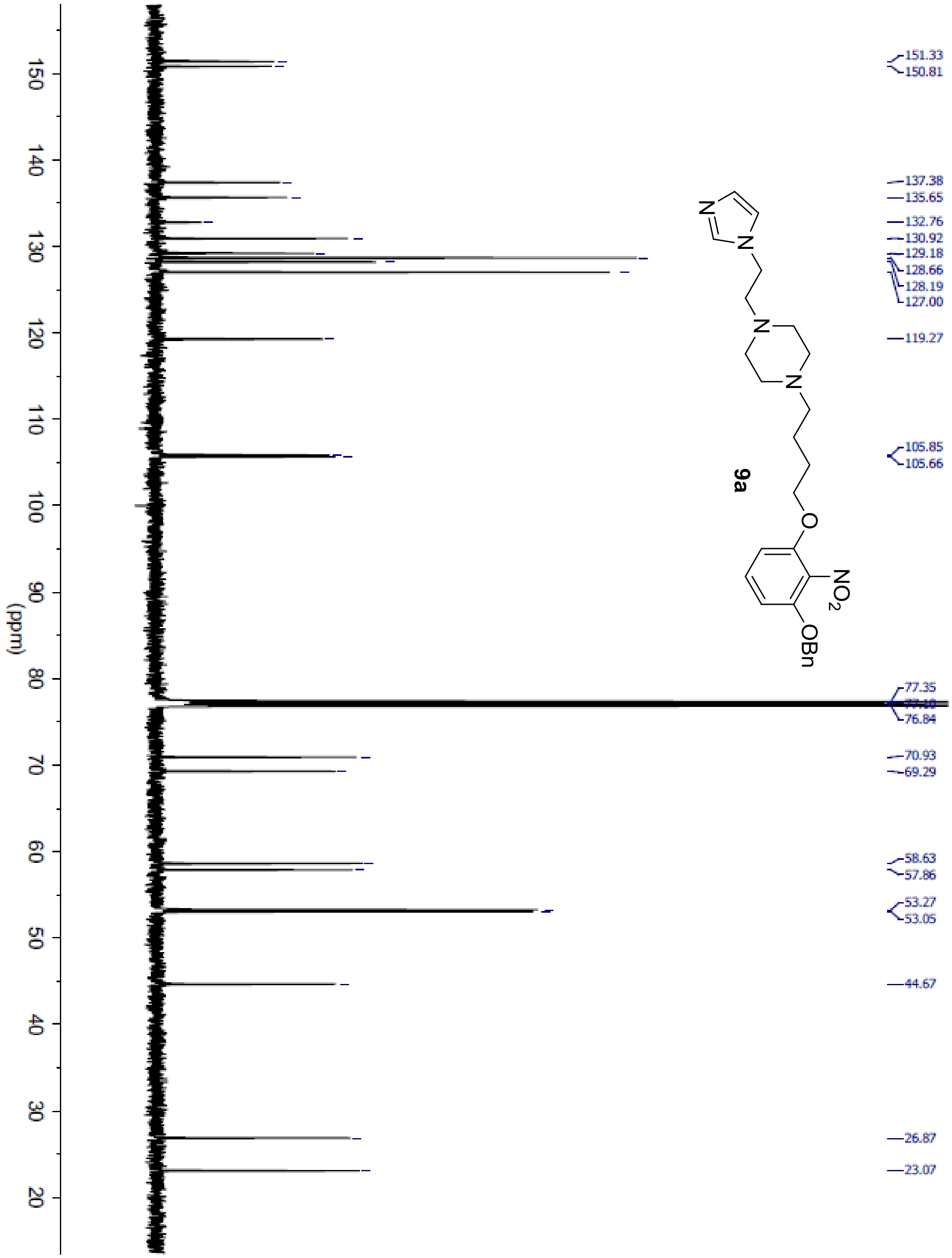
1.77
1.76
1.64
1.62
1.61
1.59
1.58
0.00
-0.01


9a
NO2
OBn
(ppm)
151.33
150.81
137.38
135.65
132.76
130.92
129.18
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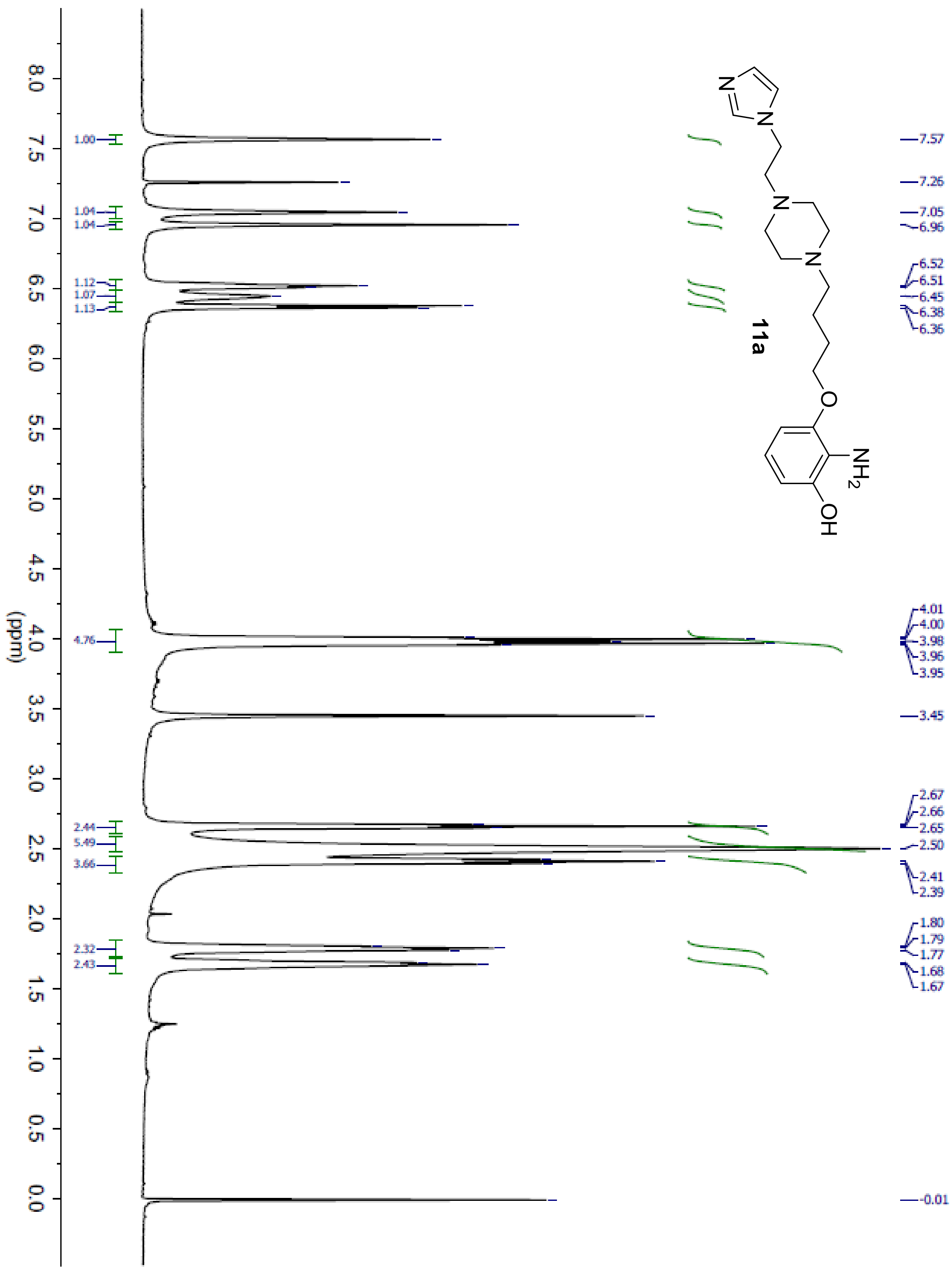
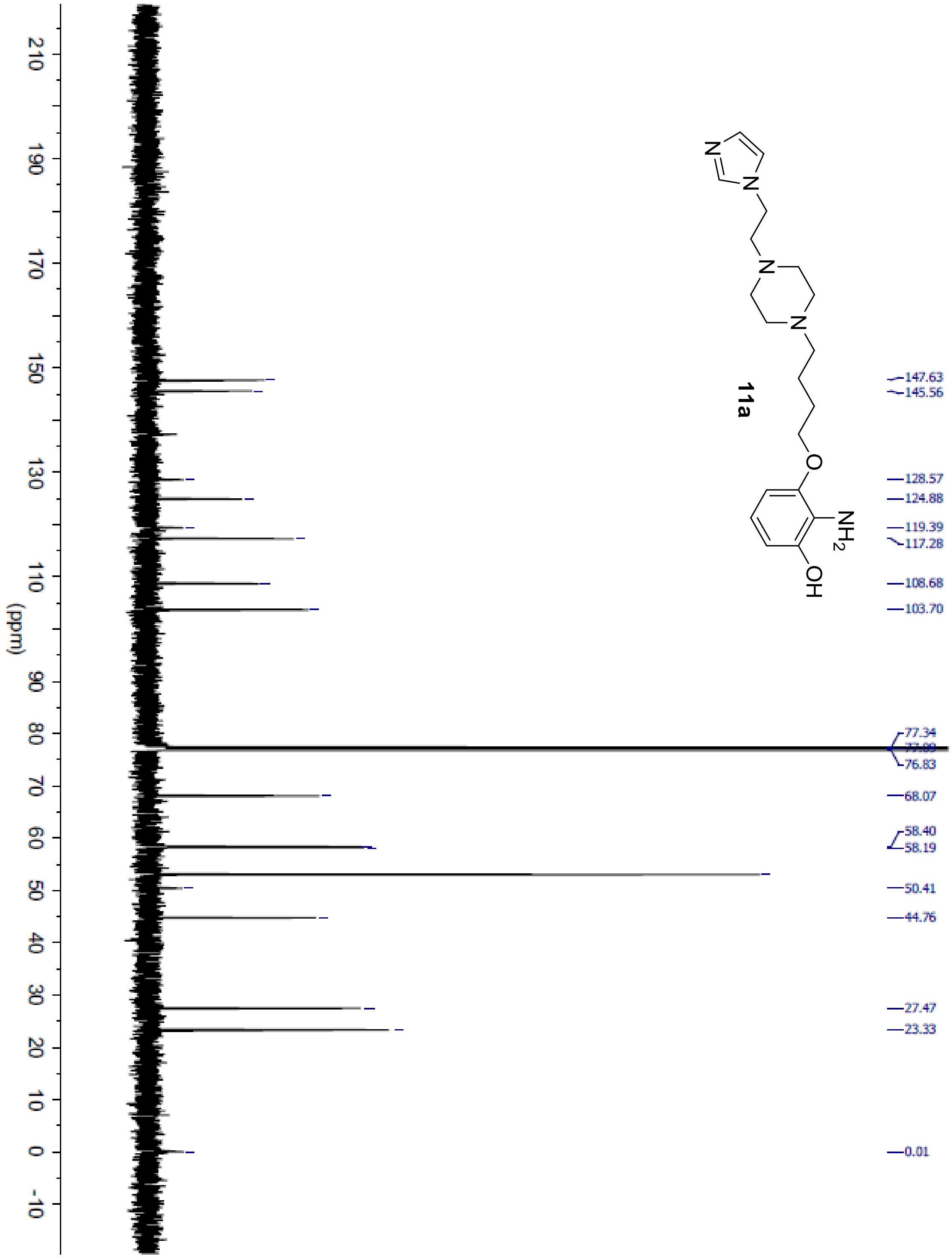
128.19
127.00
119.27
105.85
105.66
77.35
76.84
70.93
69.29
58.63
57.86
53.27
53.05
44.67
26.87
23.07




11a
147.63
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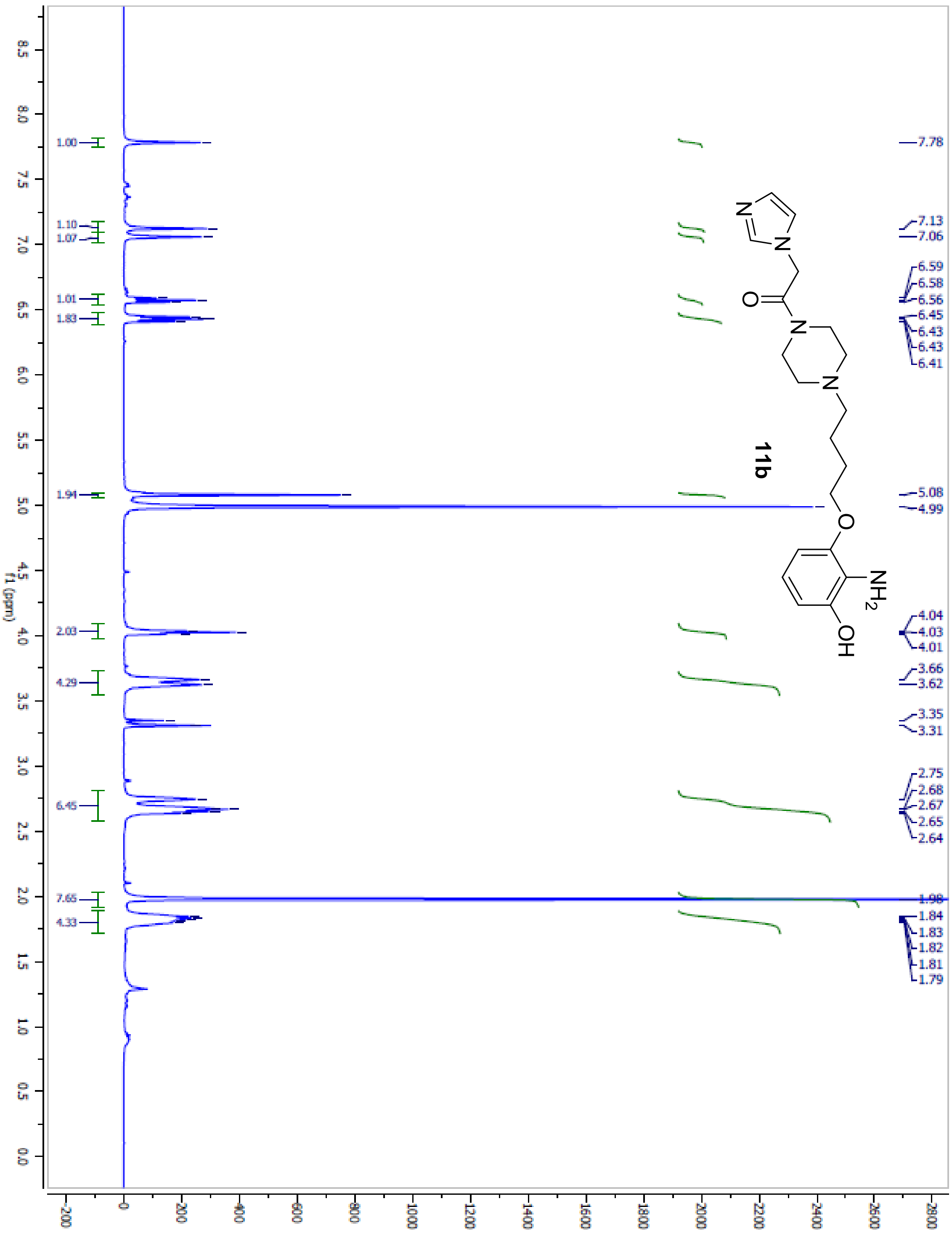
128.57
124.88
119.39
117.28
108.68
103.70
77.34
76.83
68.07
58.40
58.19
50.41
44.76
27.47
23.33
0.01
(ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10


11b
f1 (ppm)
NH2
OH
O
N

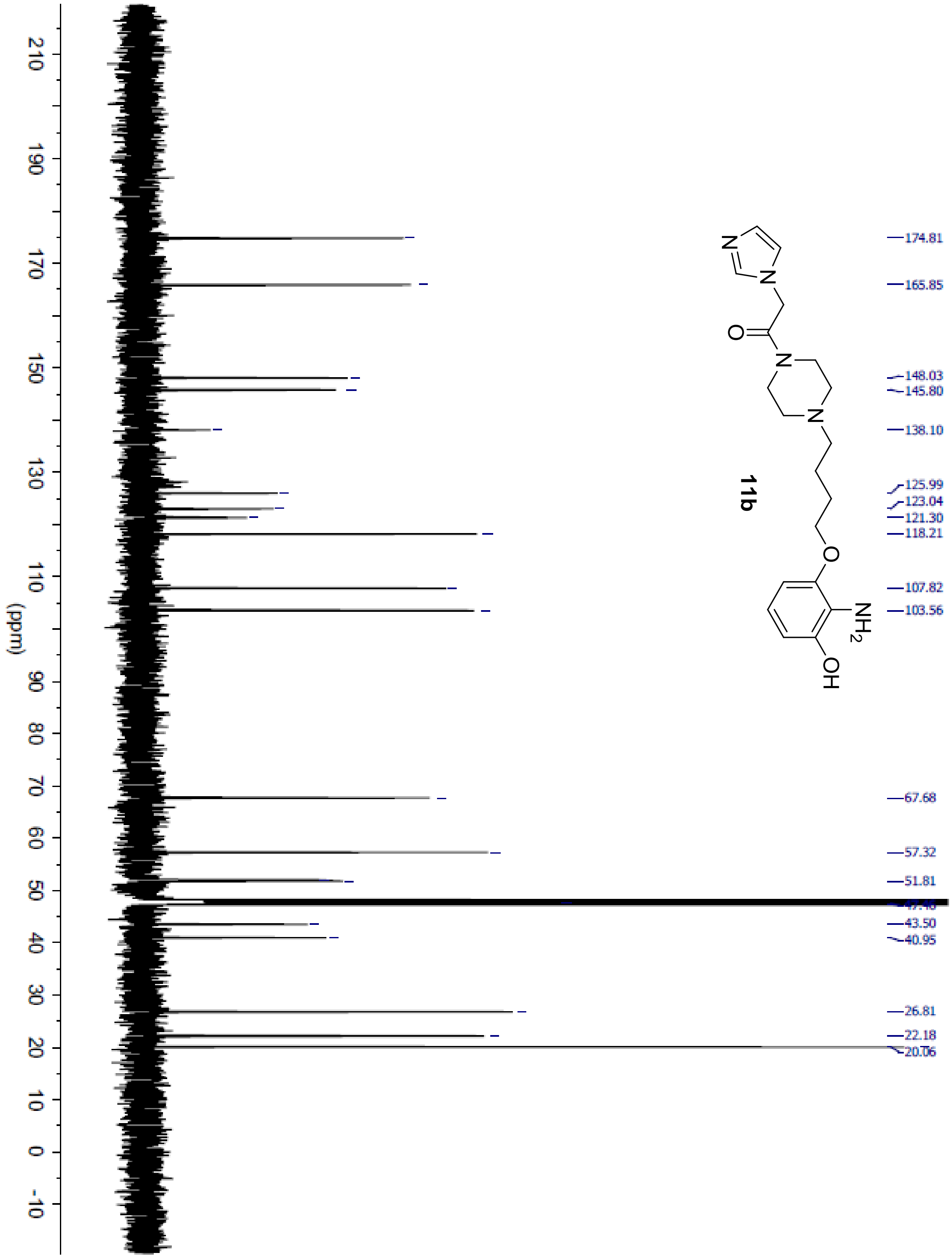
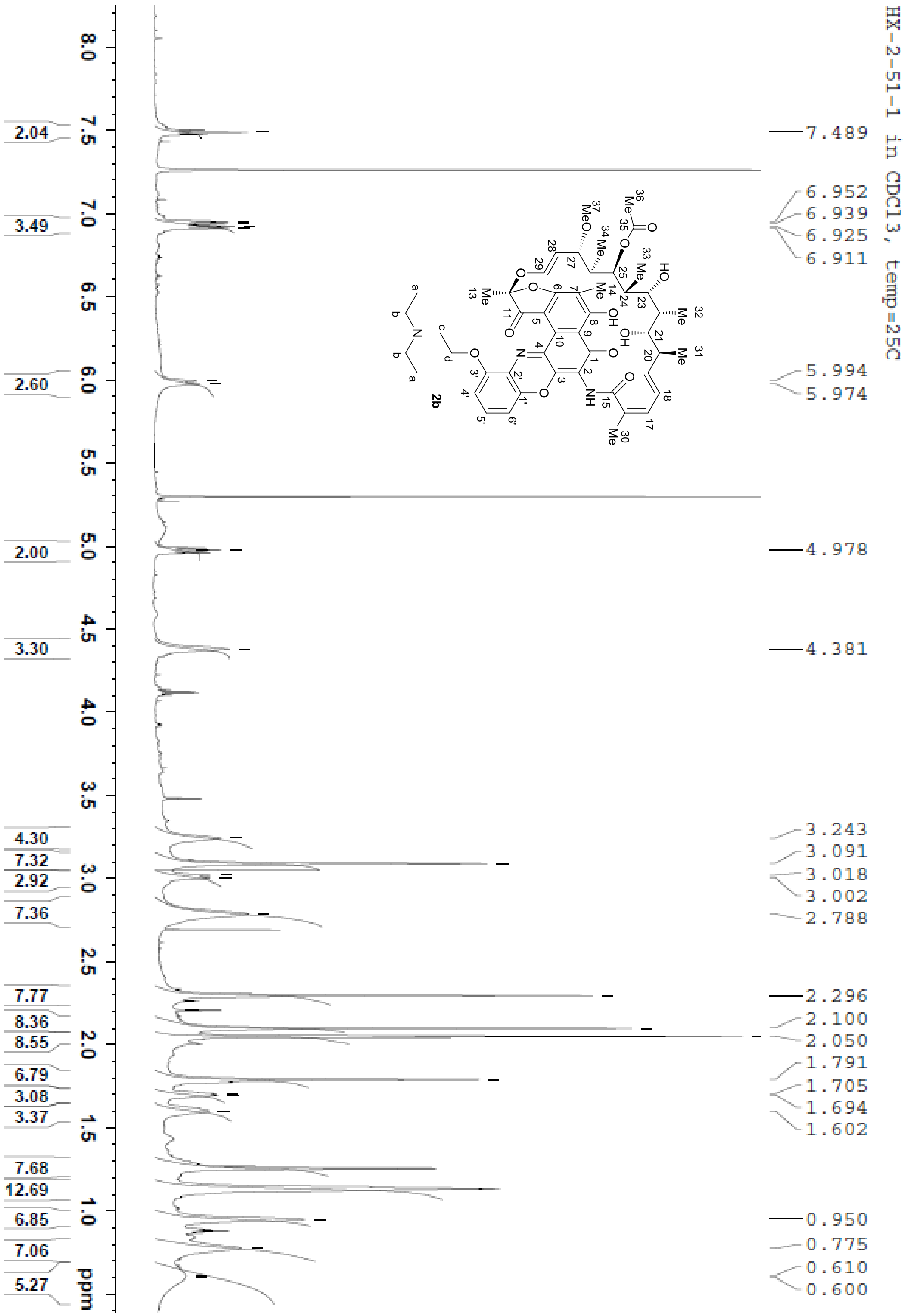
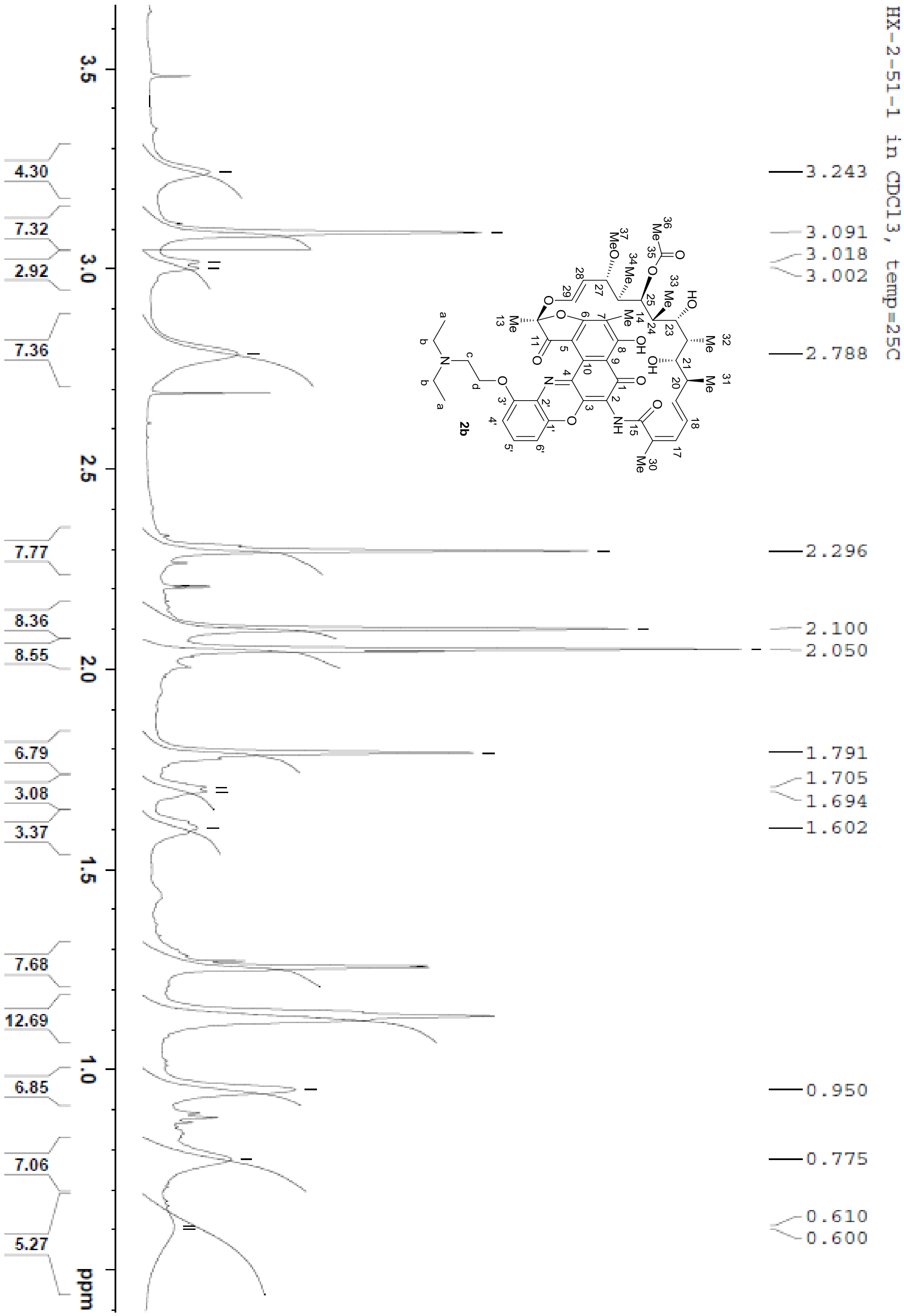
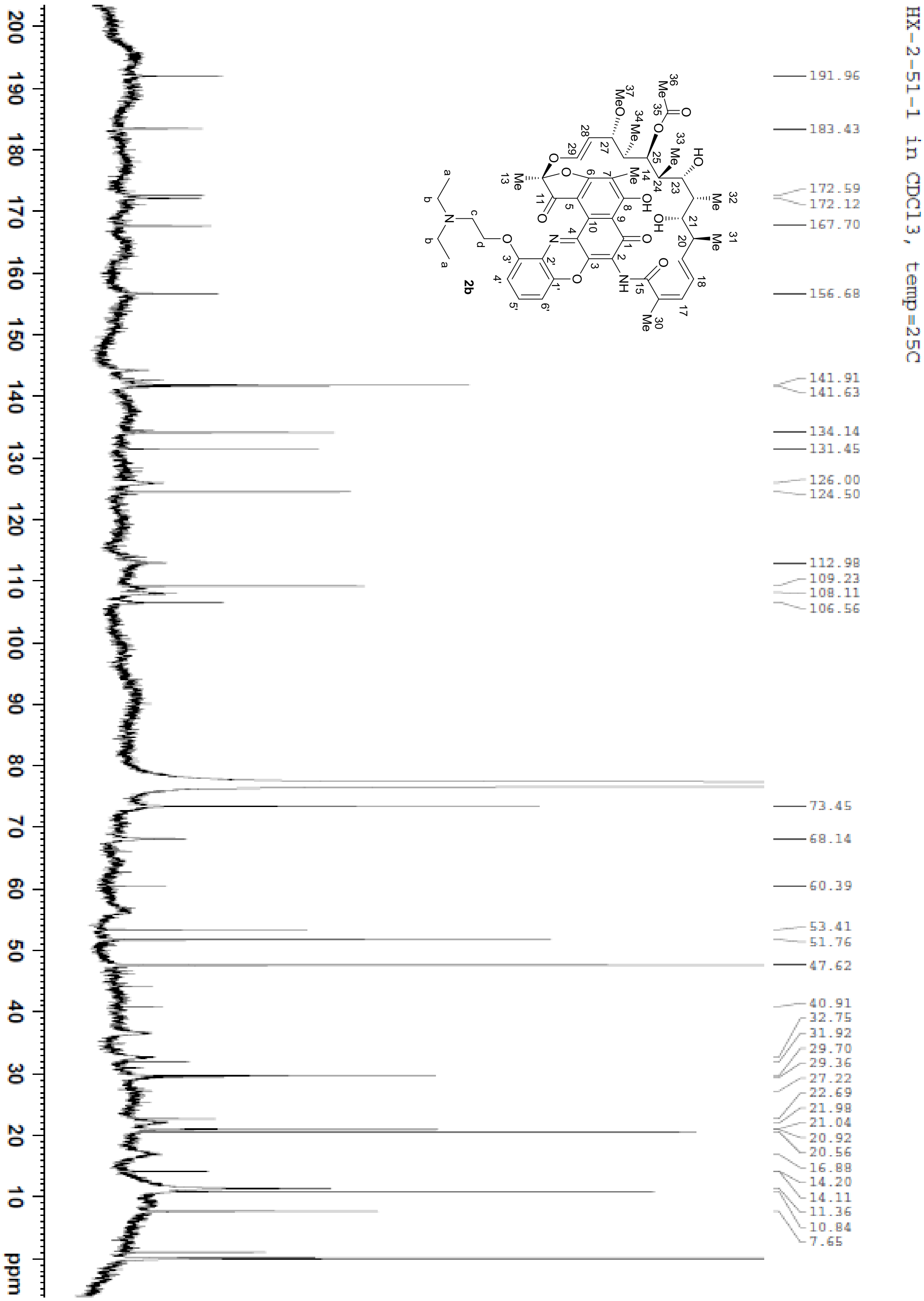


Figure 2SI. ^{1}H and ^{13}C NMR spectra of 2-aminoresorcinol ethers (**7**, **11a**, **11b**) and precursors


HX-2-51-1 in CDCl3, temp=25C
7.489
6.952
6.939
6.925
6.911
5.994
5.974
4.978
4.381
3.243
3.091
3.018
3.002
2.788
2.296
2.100
2.050
1.791
1.705
1.694
1.602
0.950
0.775
0.610
0.600
2.04
3.49
2.60
2.00
3.30
4.30
7.32
2.92
7.36
7.77
8.36
8.55
6.79
3.08
3.37
7.68
12.69
6.85
7.06
5.27
ppm
2b


HX-2-51-1 in CDCl3, temp=25C
3.243
3.091
3.018
3.002
2.788
2.296
2.100
2.050
1.791
1.705
1.694
1.602
0.950
0.775
0.610
0.600
4.30
7.32
2.92
7.36
7.77
8.36
8.55
6.79
3.08
3.37
7.68
12.69
6.85
7.06
5.27
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2b


HX-2-51-1 in CDCl13, temp=25C
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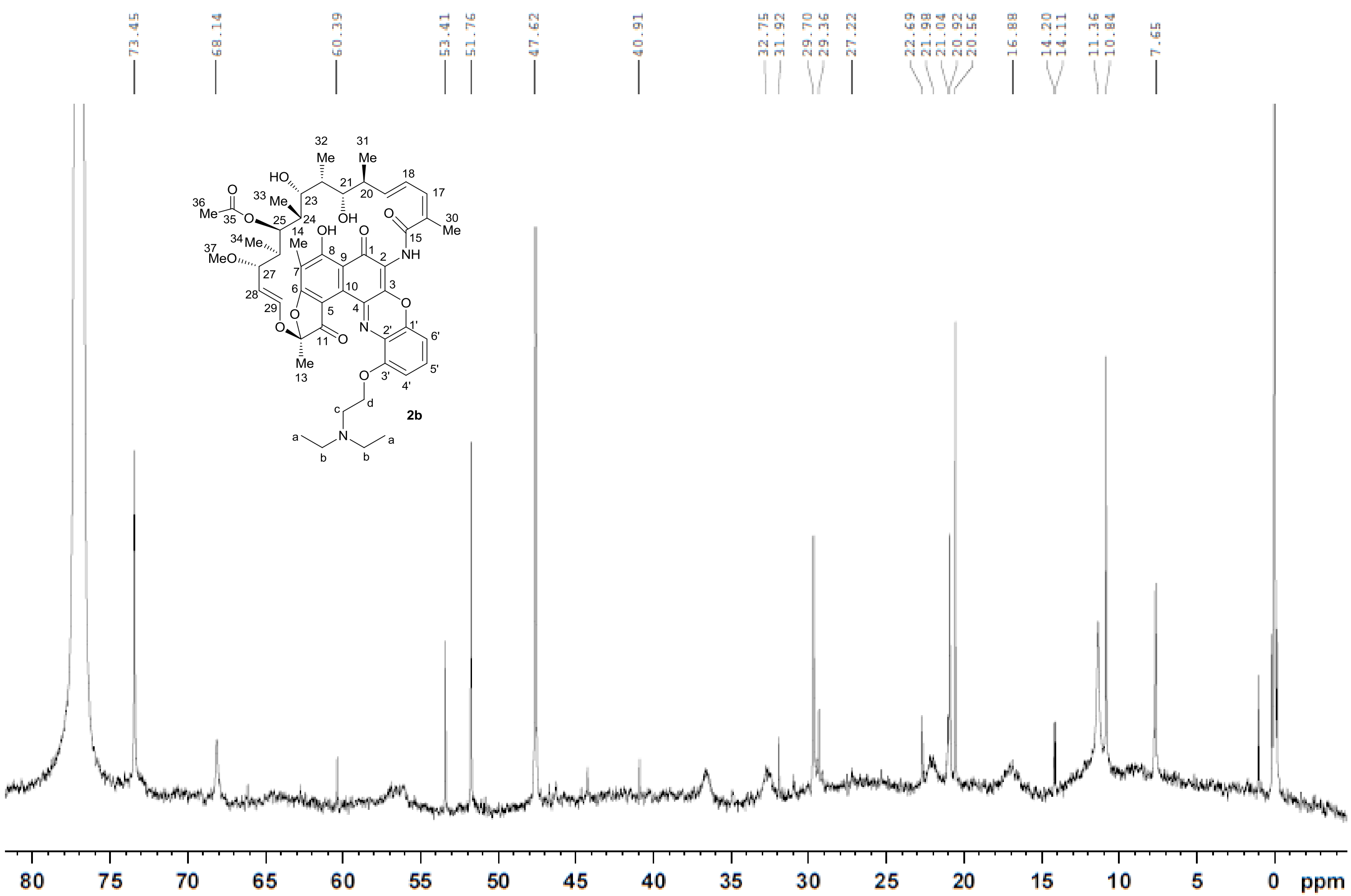
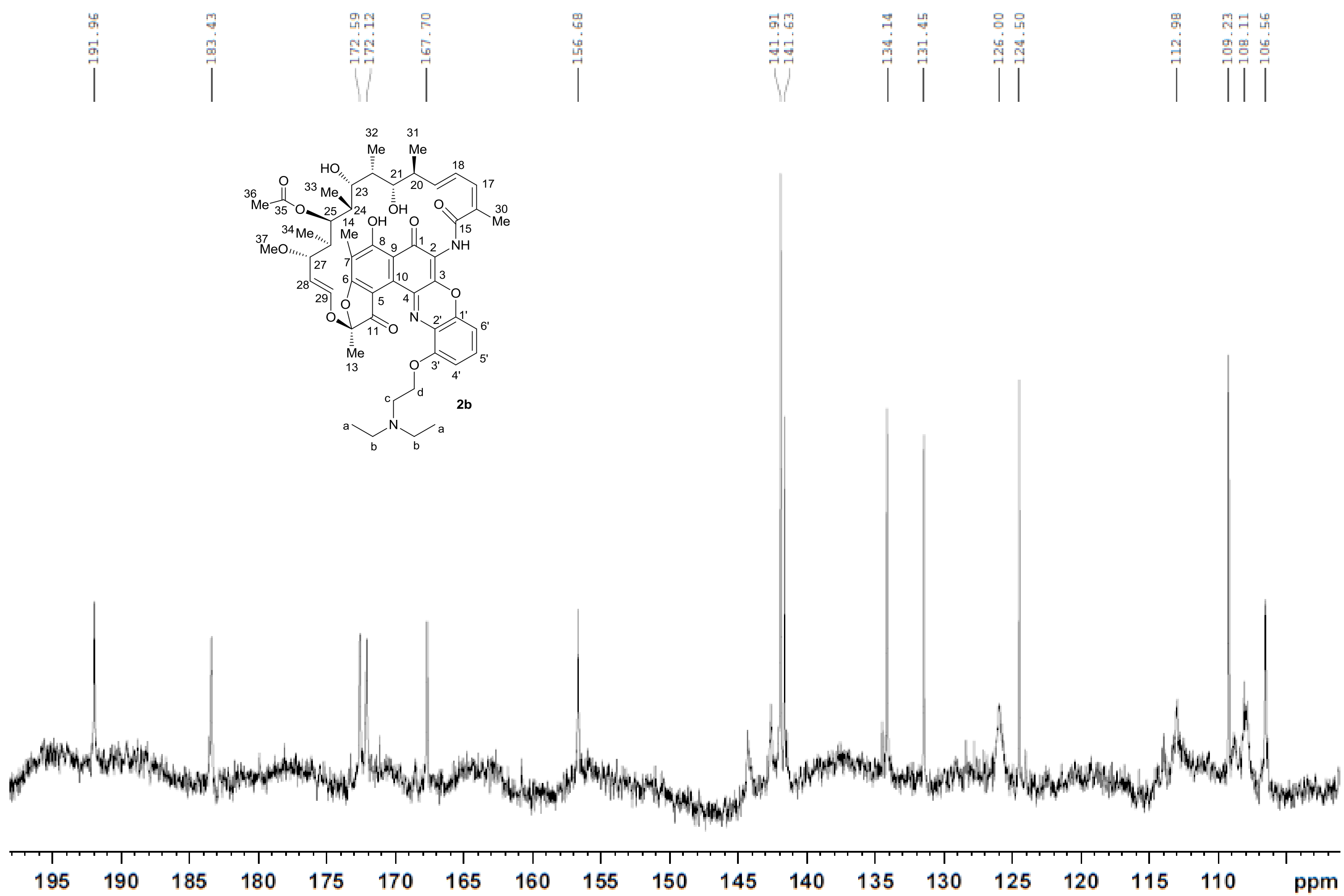
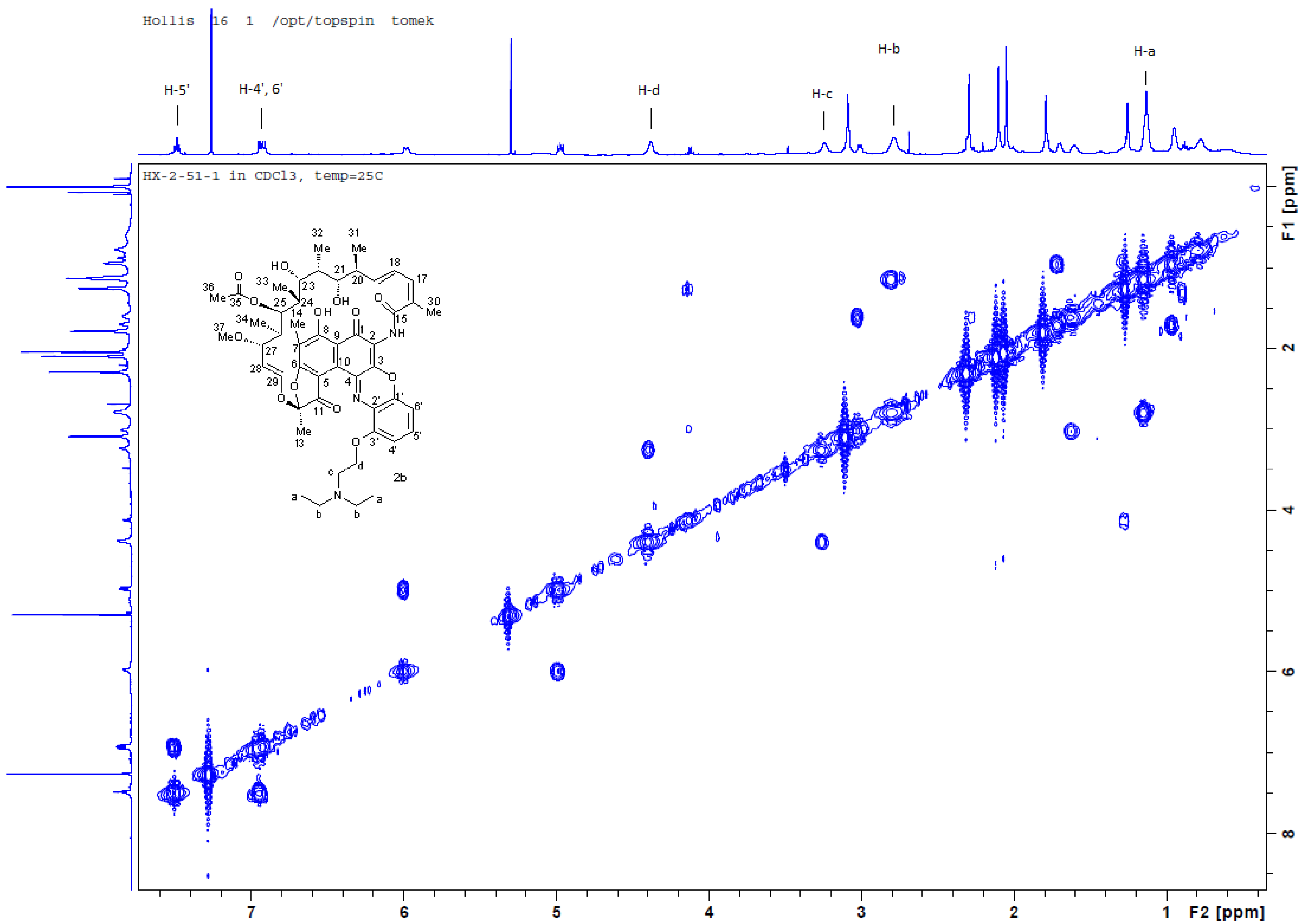
183.43
172.59
172.12
167.70
156.68
141.91
141.63
134.14
131.45
126.00
124.50
112.98
109.23
108.11
106.56
73.45
68.14
60.39
53.41
51.76
47.62
40.91
32.75
31.92
29.70
29.36
27.22
22.69
21.98
21.04
20.92
20.56
16.88
14.20
14.11
11.36
10.84
7.65
2b
ppm
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

HX-2-51-1 in CDCl3, temp=25C

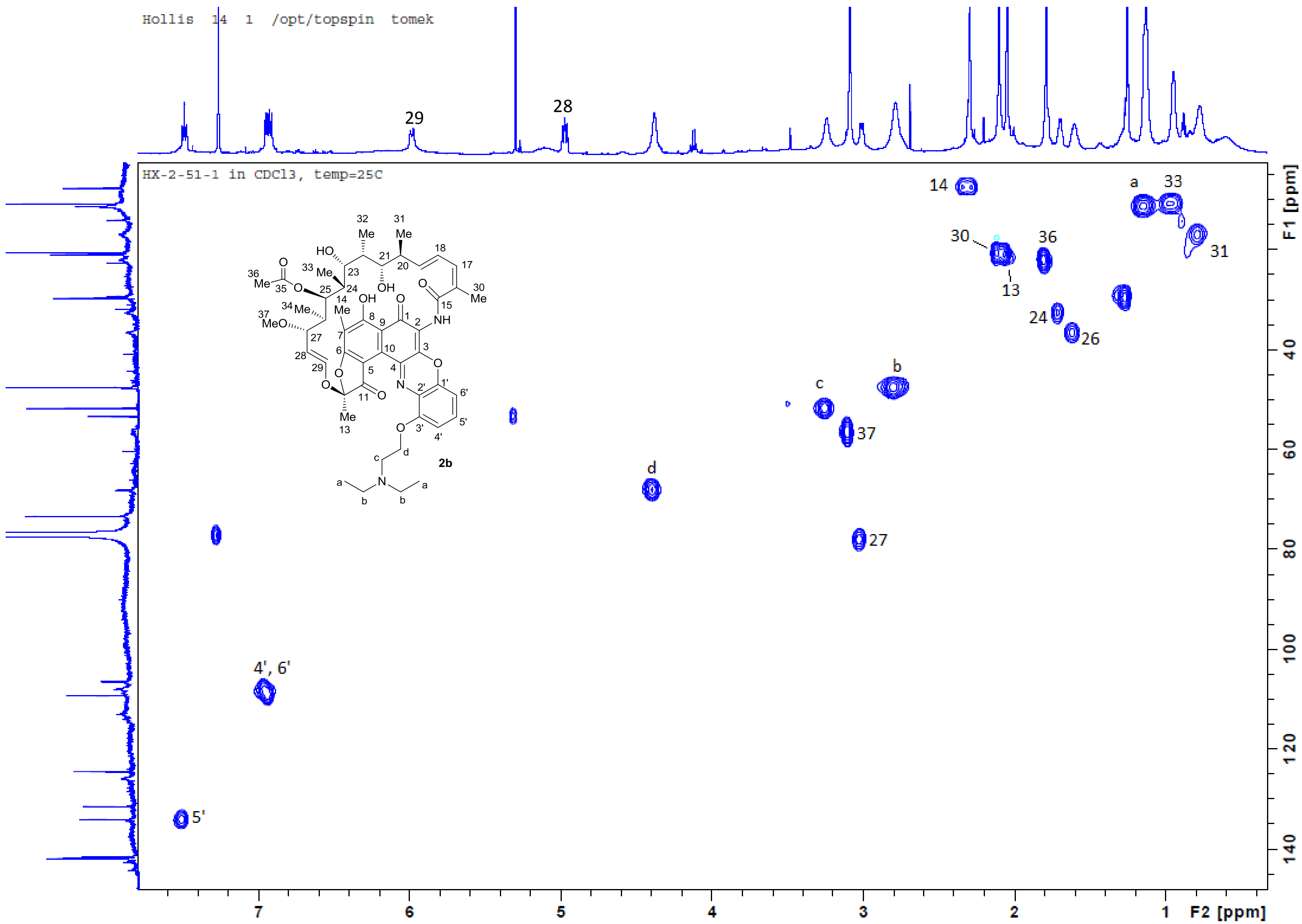


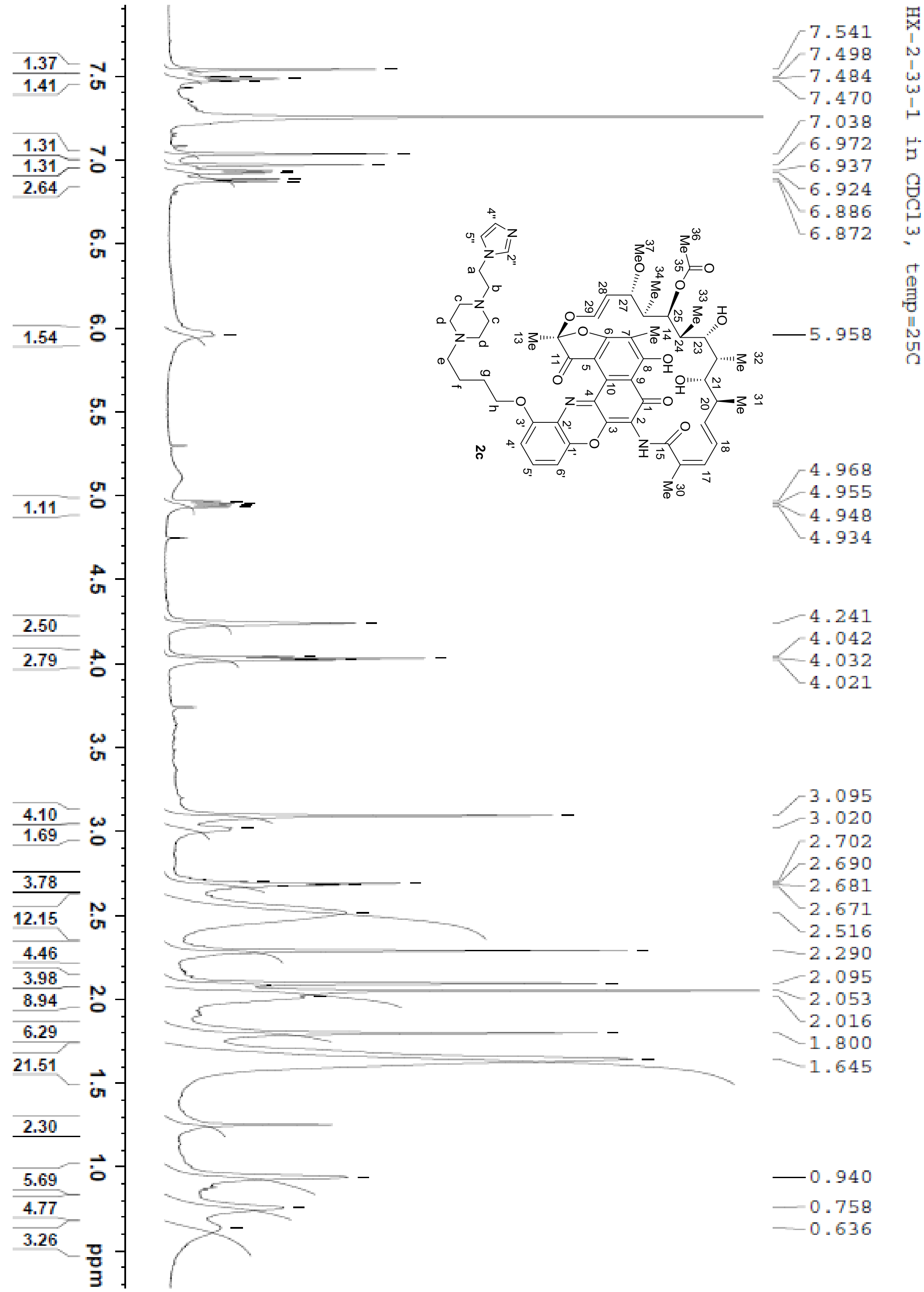
HX-2-51-1 in CDCl3, temp=25C



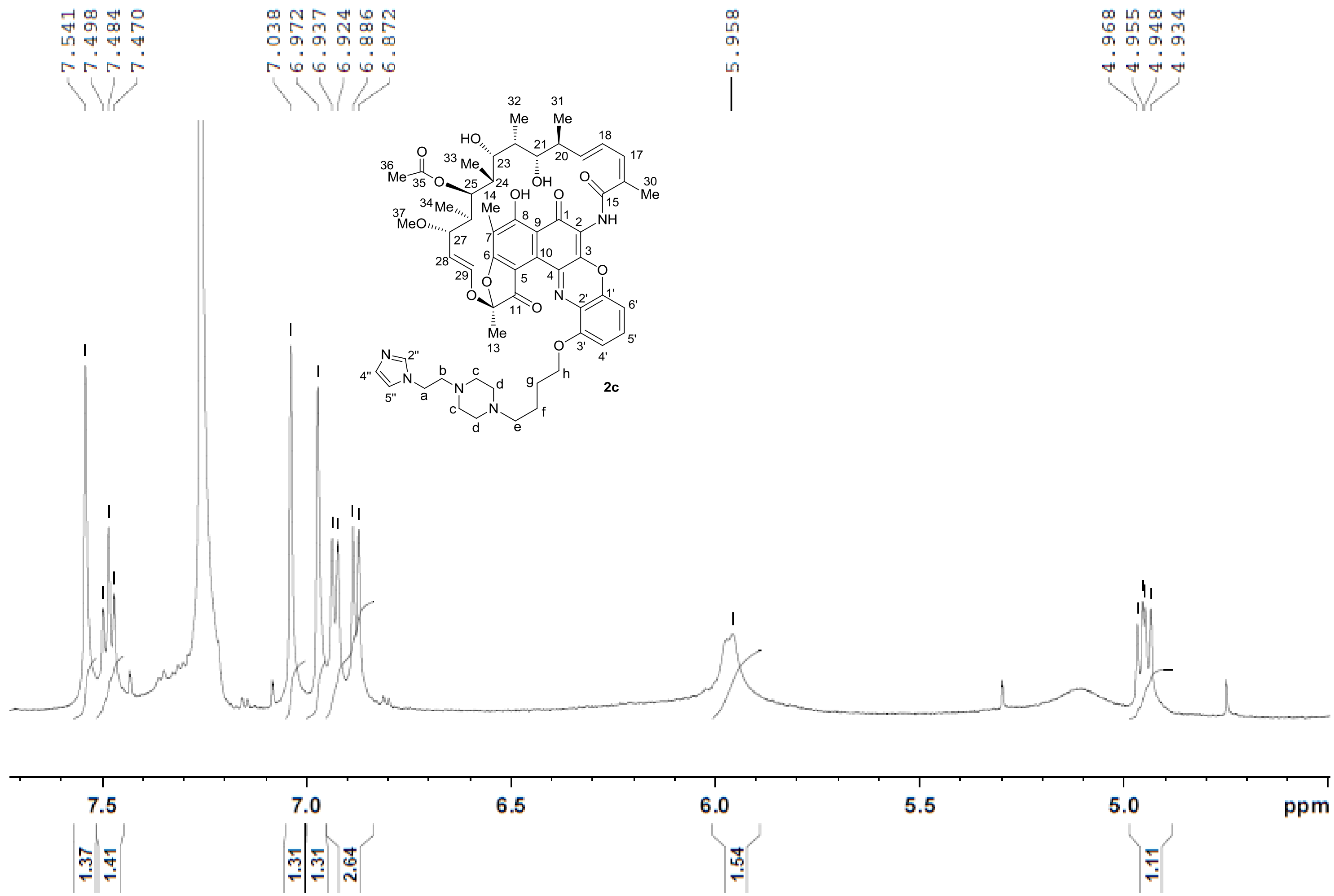


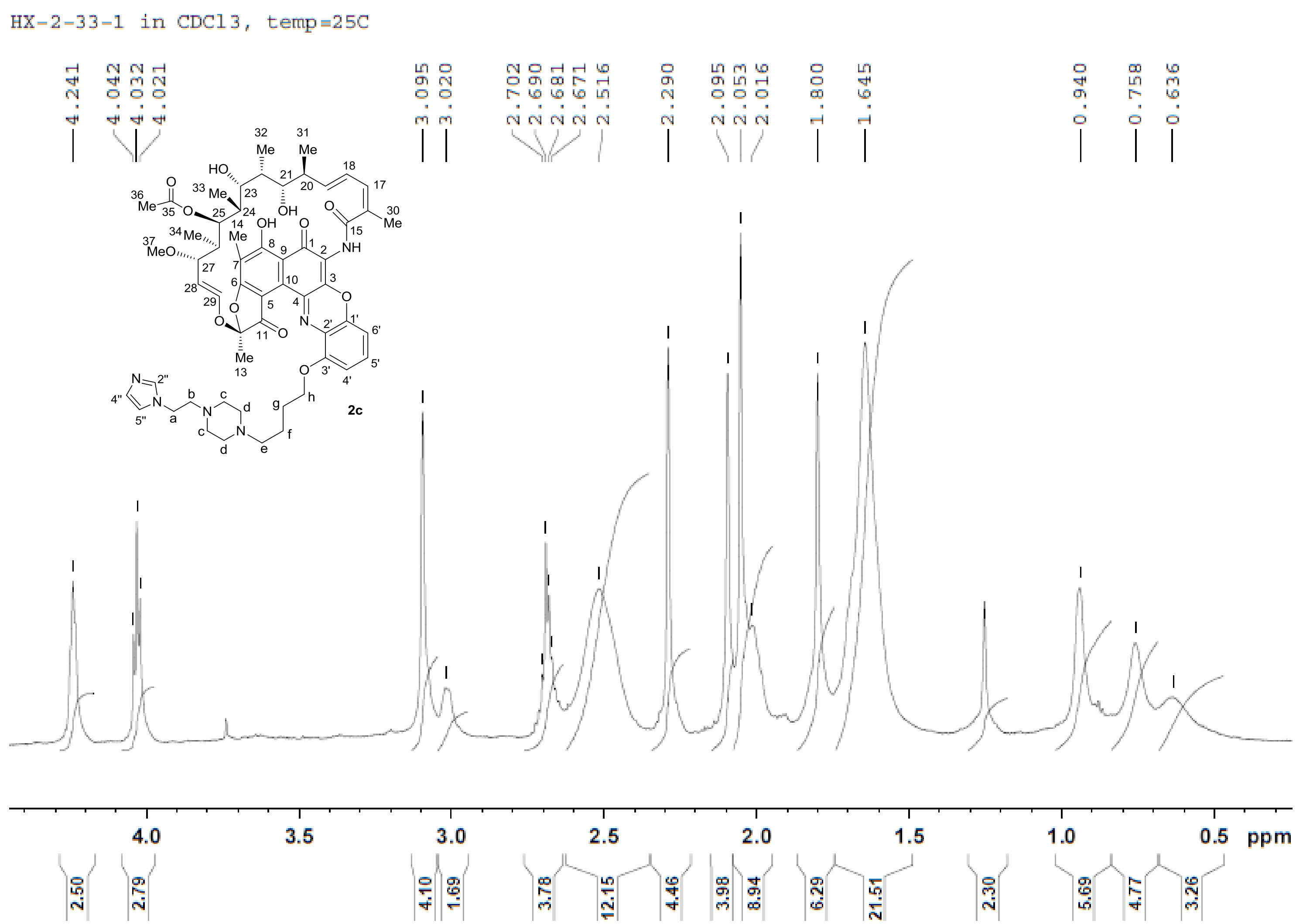
Hollis 16 1 /opt/topspin tomek
H-5'
H-4', 6'
H-d
H-c
H-b
H-a
HX-2-51-1 in CDCl3, temp=25C
2b
F1 [ppm]
F2 [ppm]

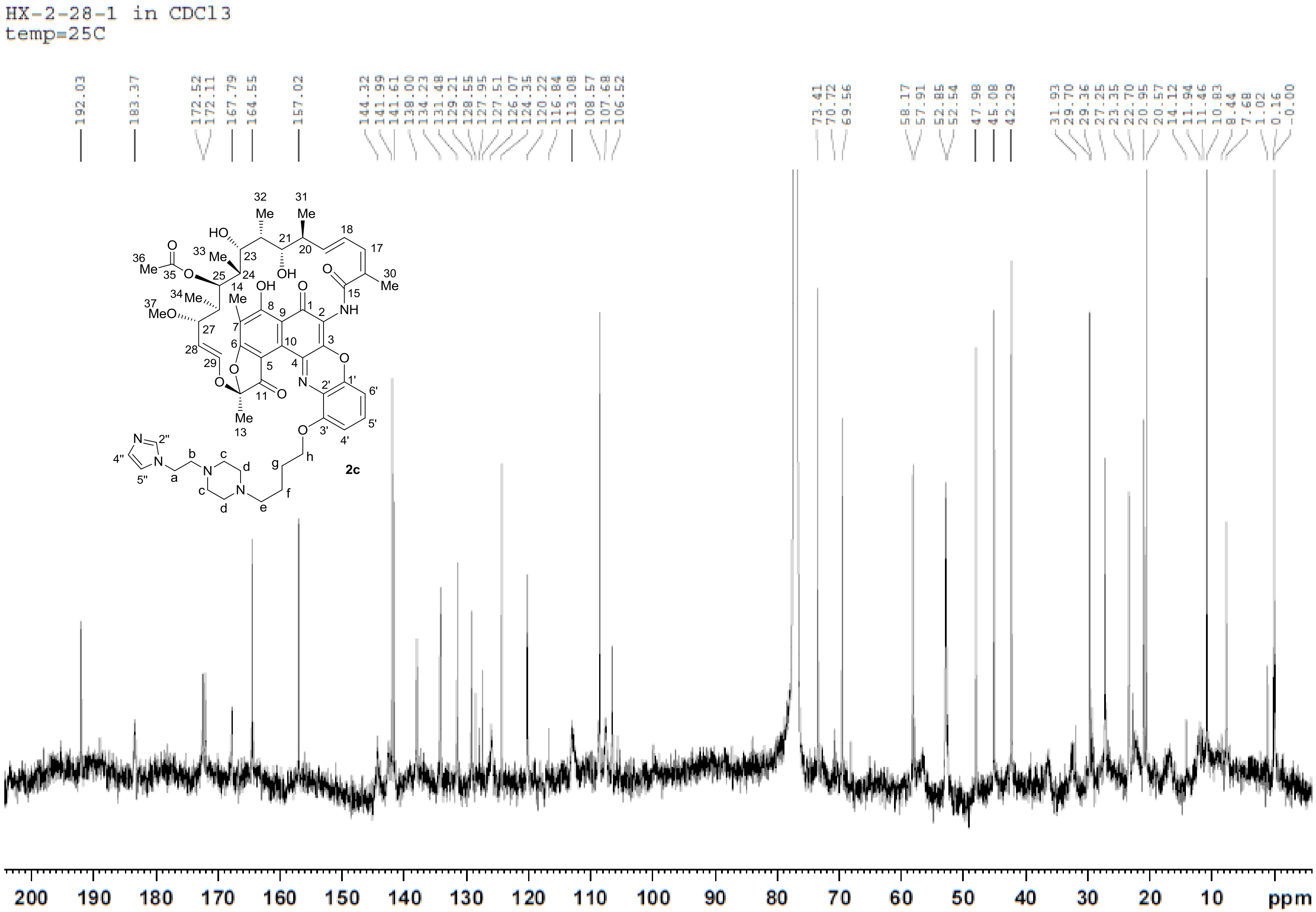

Hollis 14 1 /opt/topspin tomek
HX-2-51-1 in CDCl3, temp=25C
2b
29
28
14
a
33
30
13
36
31
24
26
b
c
37
d
27
4', 6'
5'
F2 [ppm]
F1 [ppm]

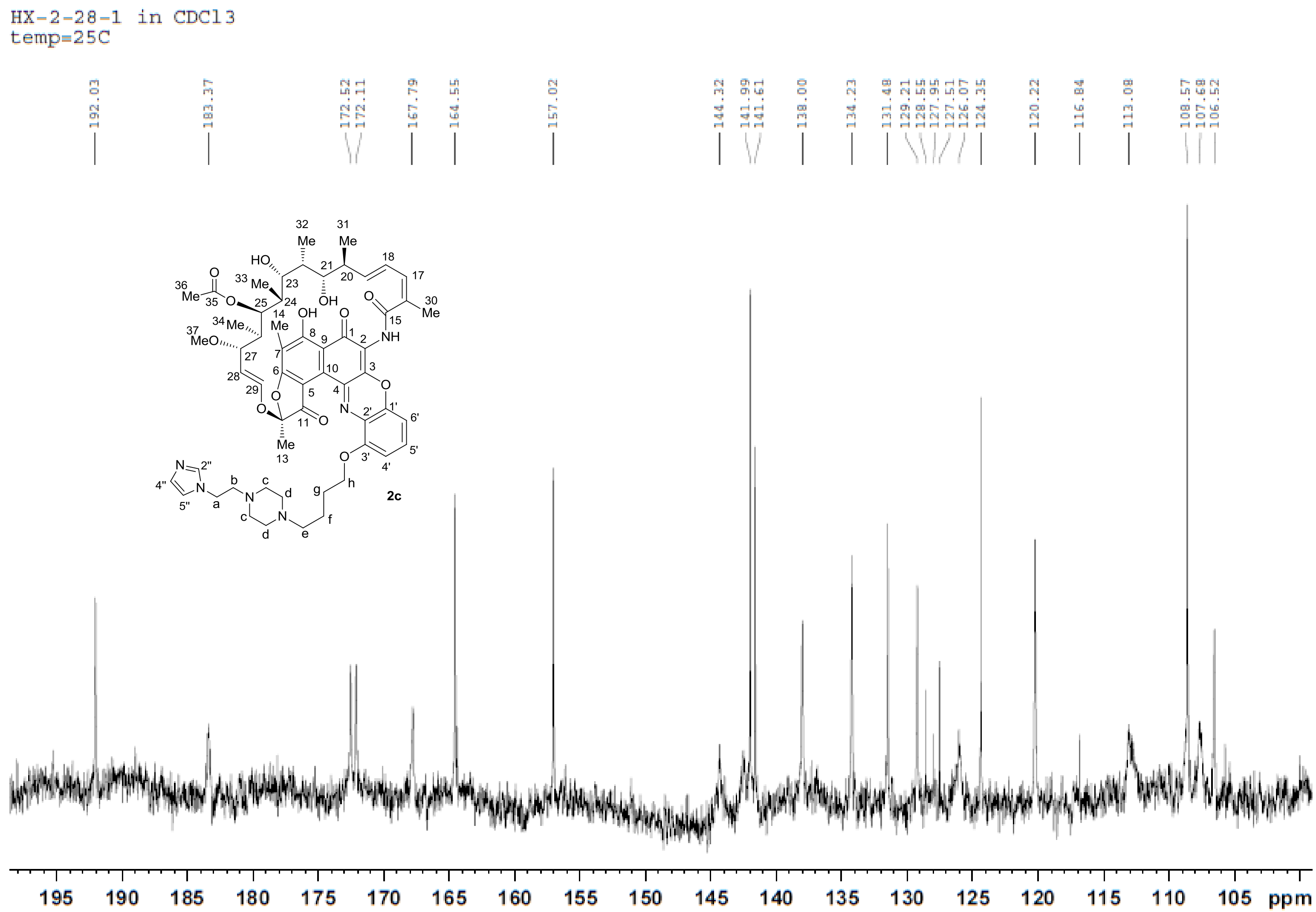

HX-2-33-1 in CDCl13, temp=25C
2c
7.541
7.498
7.484
7.470
7.038
6.972
6.937
6.924
6.886
6.872
5.958
4.968
4.955
4.948
4.934
4.241
4.042
4.032
4.021
3.095
3.020
2.702
2.690
2.681
2.671
2.516
2.290
2.095
2.053
2.016
1.800
1.645
0.940
0.758
0.636
ppm

HX-2-33-1 in CDCl3, temp=25C



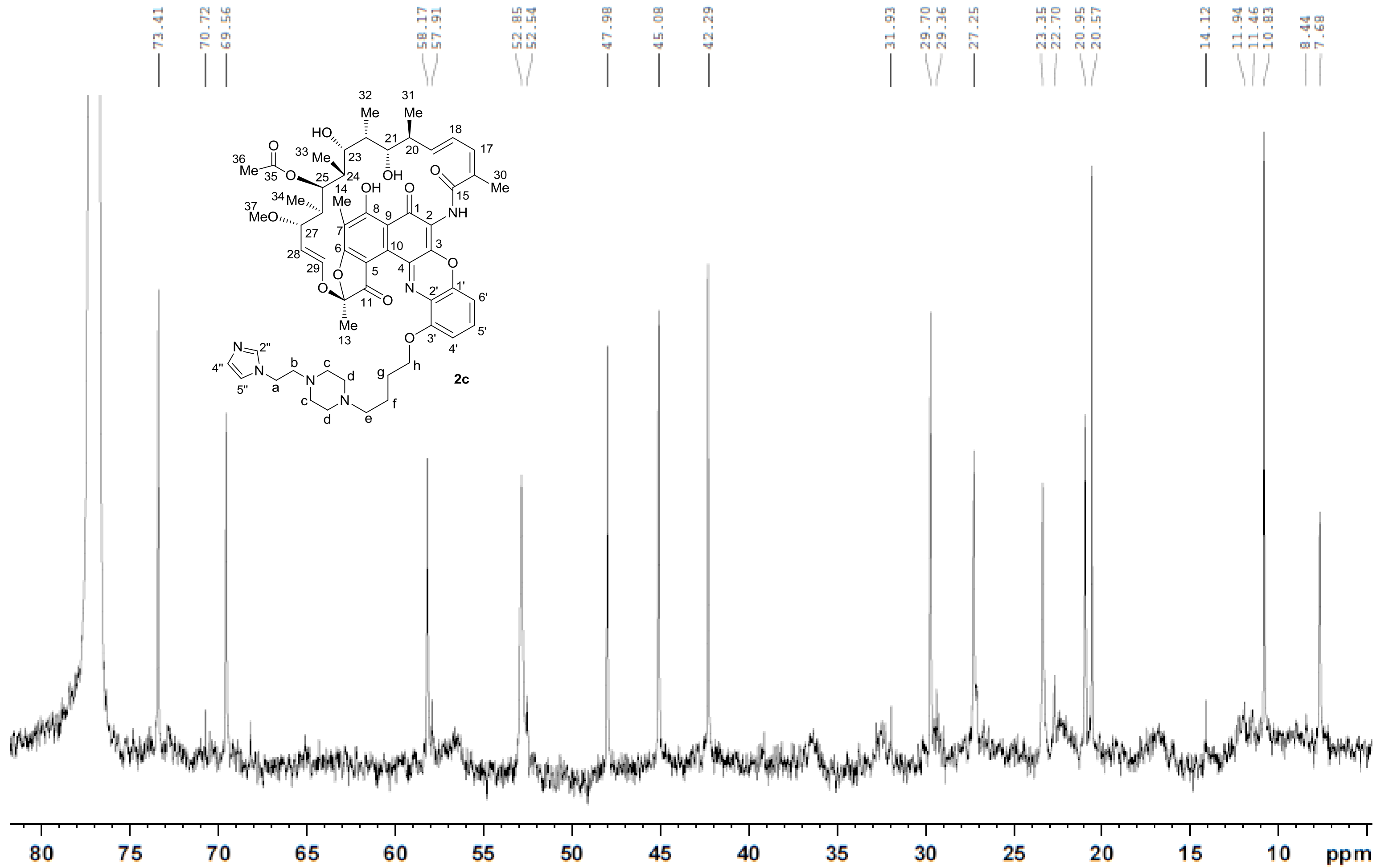

HX-2-33-1 in CDCl3, temp=25C
4.241
4.042
4.032
4.021
3.095
3.020
2.702
2.690
2.681
2.671
2.516
2.290
2.095
2.053
2.016
1.800
1.645
0.940
0.758
0.636
2c
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.50
2.79
4.10
1.69
3.78
12.15
4.46
3.98
8.94
6.29
21.51
2.30
5.69
4.77
3.26


HX-2-28-1 in CDCl3
temp=25C
192.03
183.37
172.52
172.11
167.79
164.55
157.02
144.32
141.99
141.61
138.00
134.23
131.48
129.21
128.55
127.95
127.51
126.07
124.35
120.22
116.84
113.08
108.57
107.68
106.52
73.41
70.72
69.56
58.17
57.91
52.85
52.54
47.98
45.08
42.29
31.93
29.70
29.36
27.25
23.35
22.70
20.95
20.57
14.12
11.94
11.46
10.83
8.44
7.68
1.02
0.16
-0.00
2c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

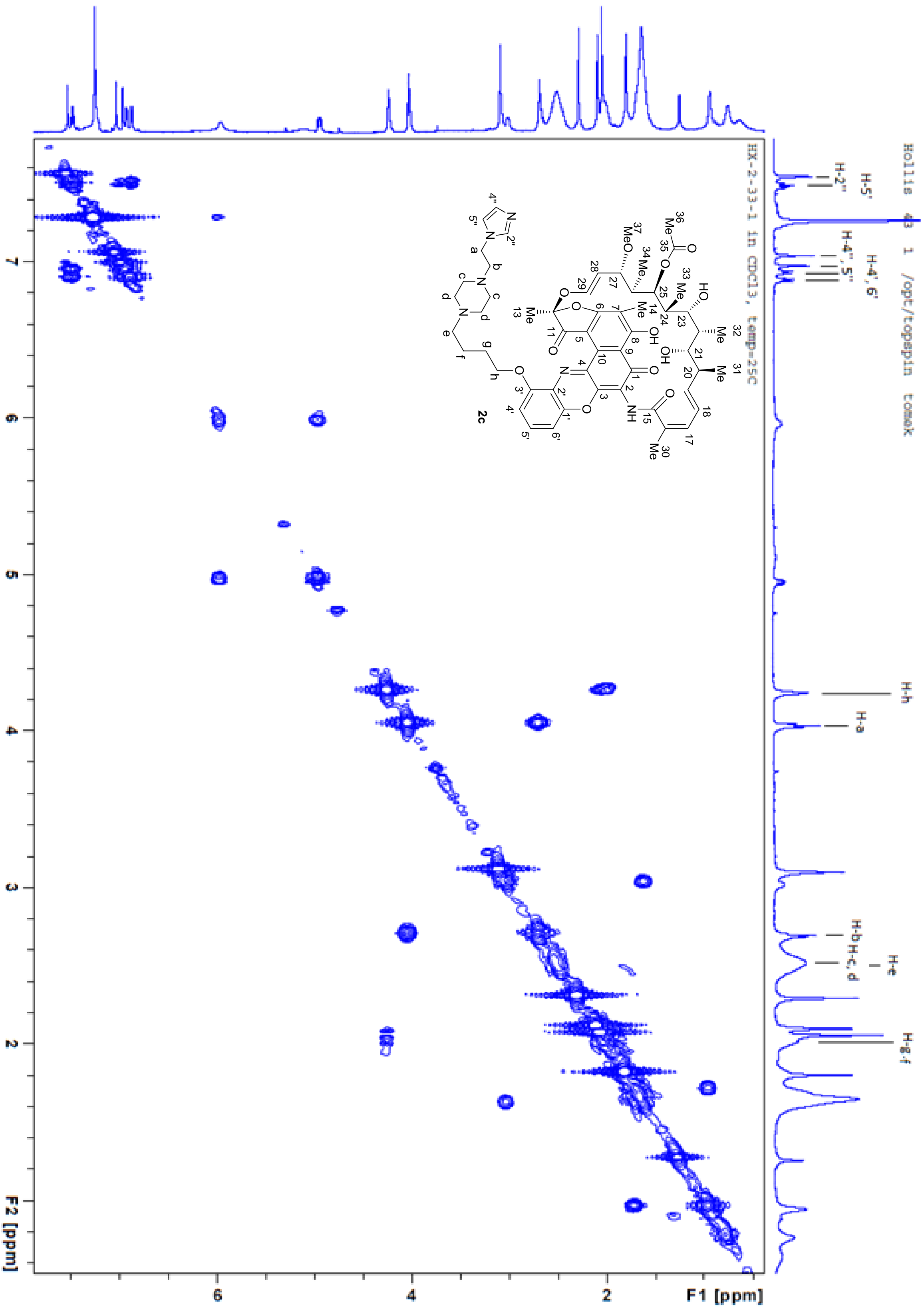

HX-2-28-1 in CDCl3
temp=25C
192.03
183.37
172.52
172.11
167.79
164.55
157.02
144.32
141.99
141.61
138.00
134.23
131.48
129.21
128.55
127.95
127.51
126.07
124.35
120.22
116.84
113.08
108.57
107.68
106.52
195
190
185
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
ppm

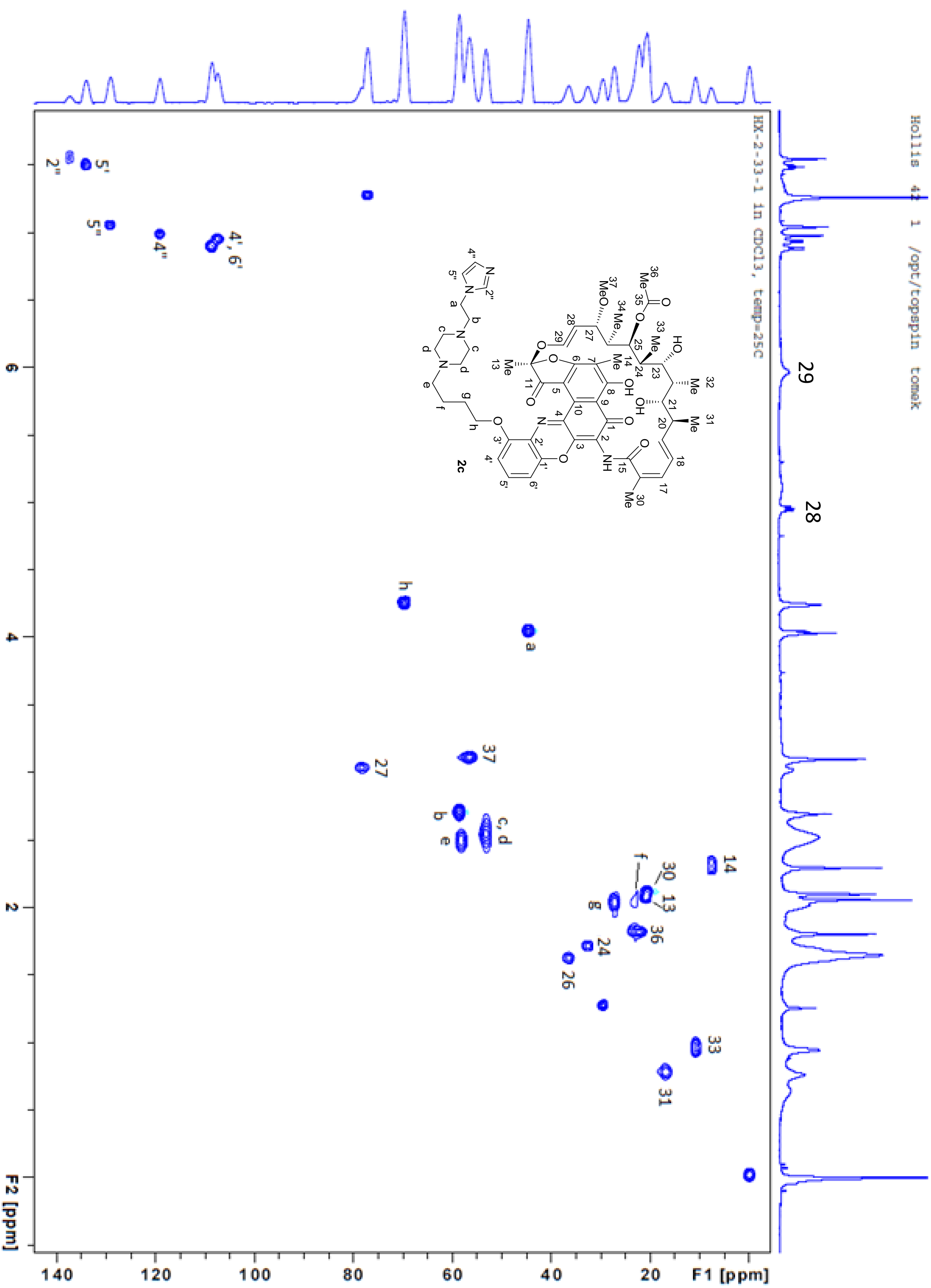
2c

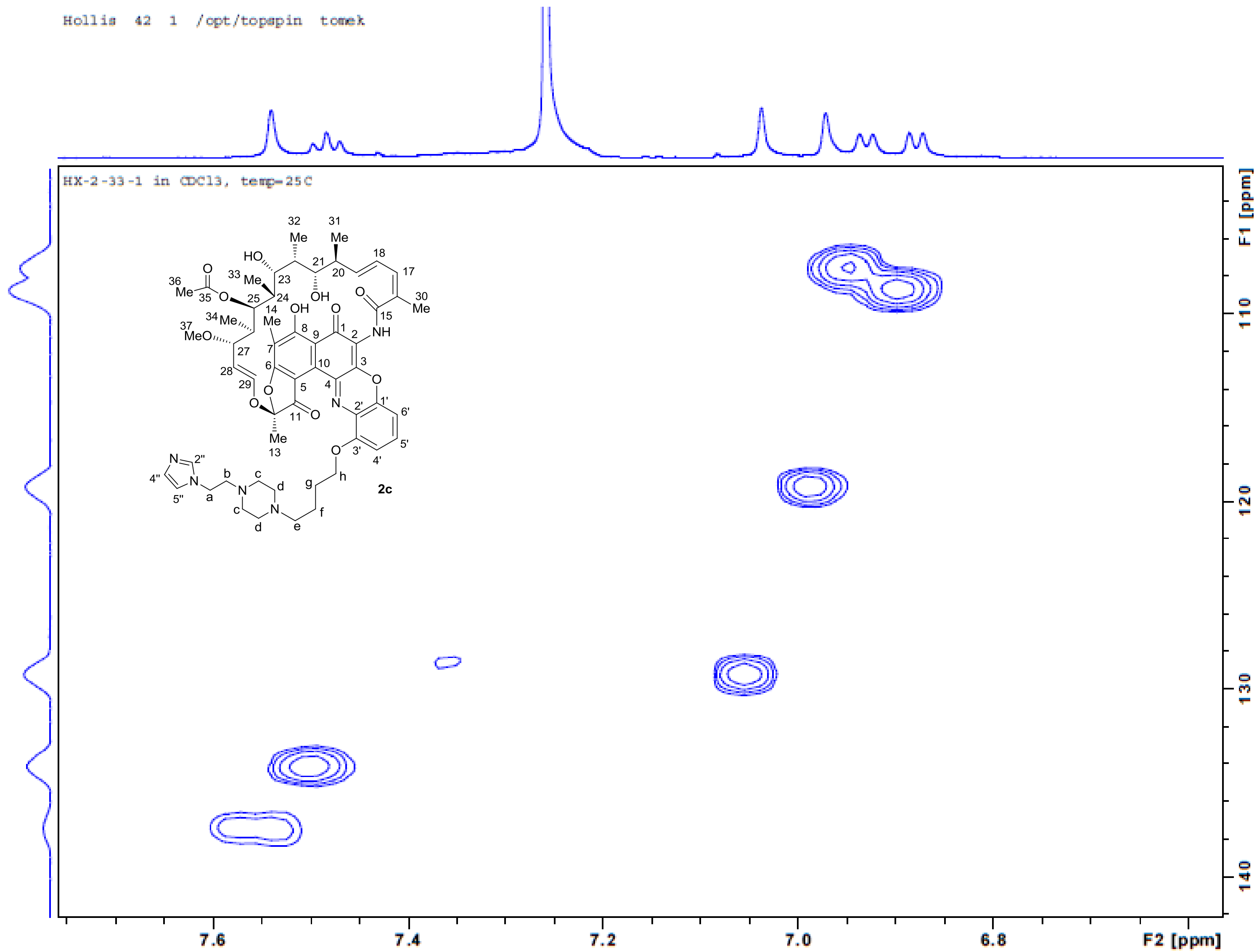
HX-2-28-1 in CDCl3
temp=25C

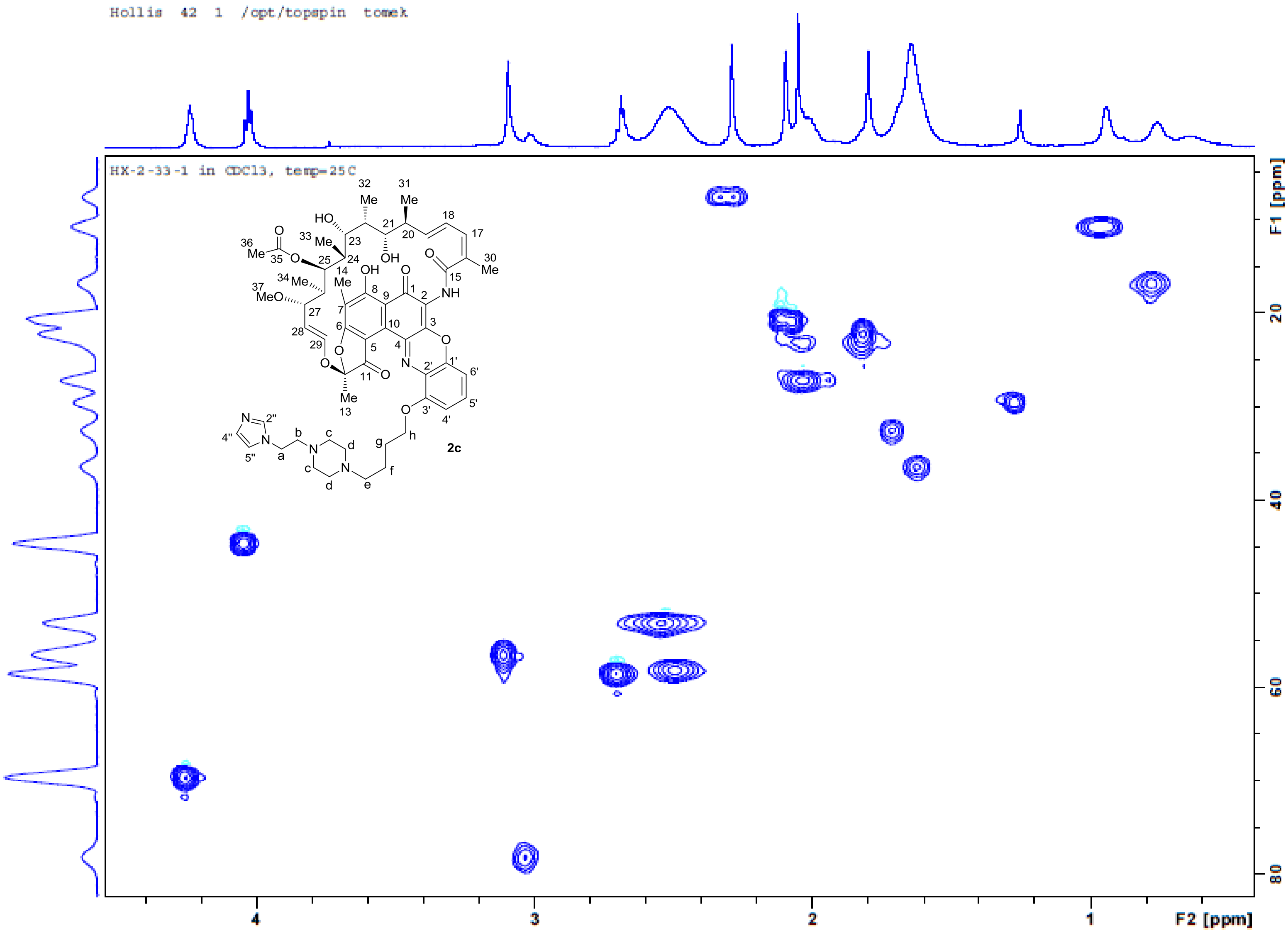


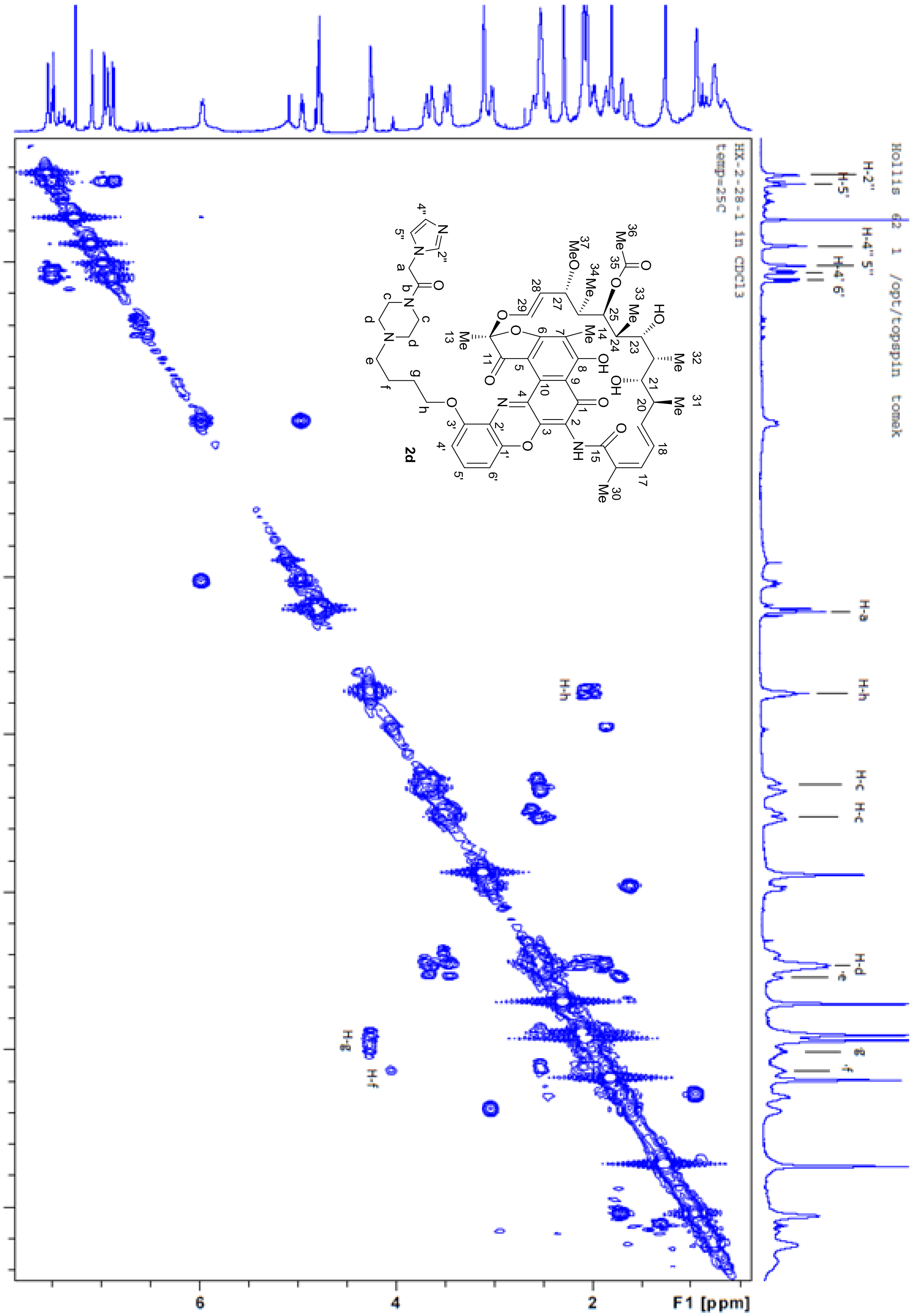
2c

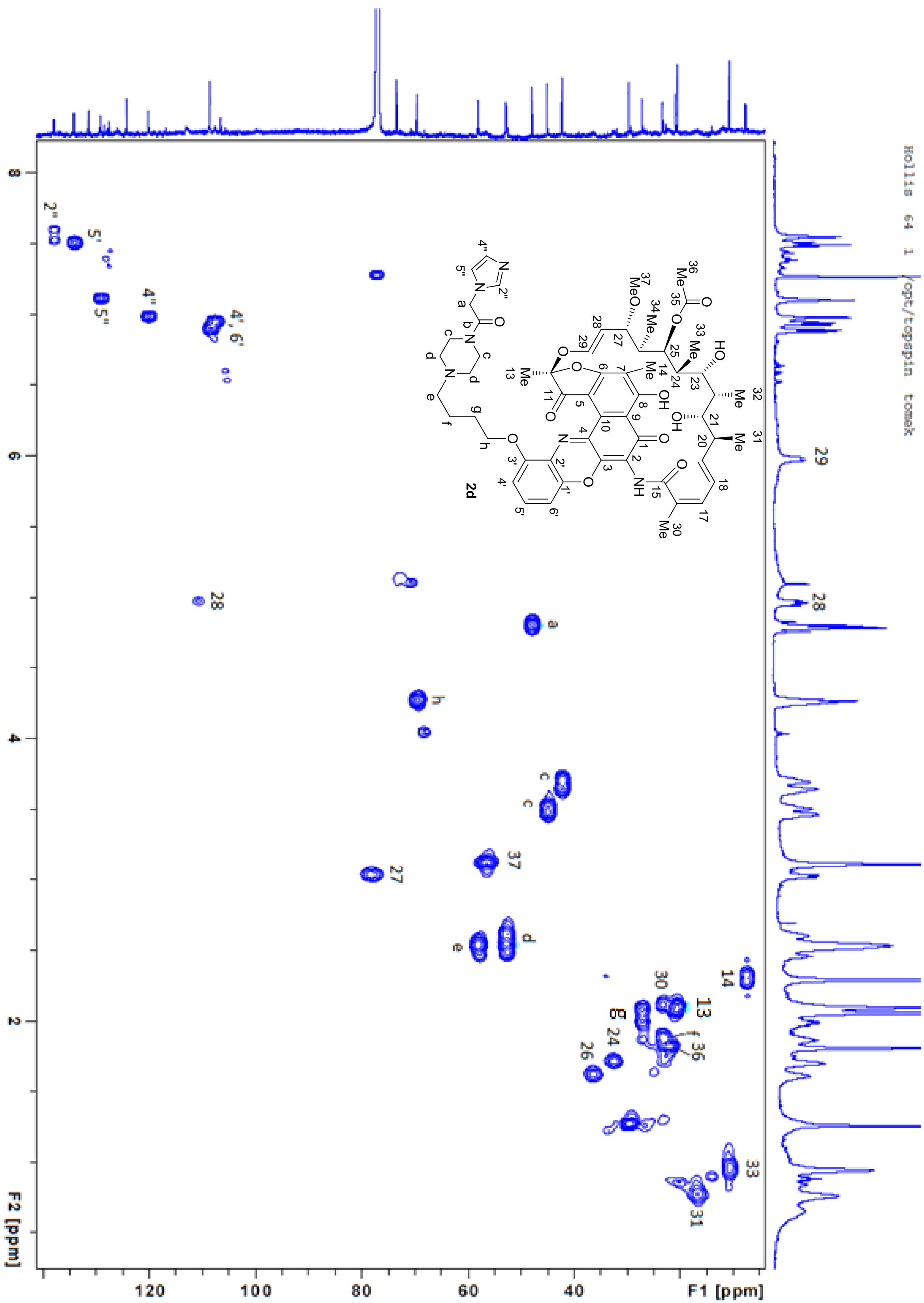

Hollis 43 1 /opt/topspin tomak
HX-2-33-1 in CDCl3, temp=25C
H-5'
H-2''
H-4', 6'
H-4'', 5''
H-h
H-a
H-b
H-c, d
H-e
H-g, f
2c
F1 [ppm]
F2 [ppm]

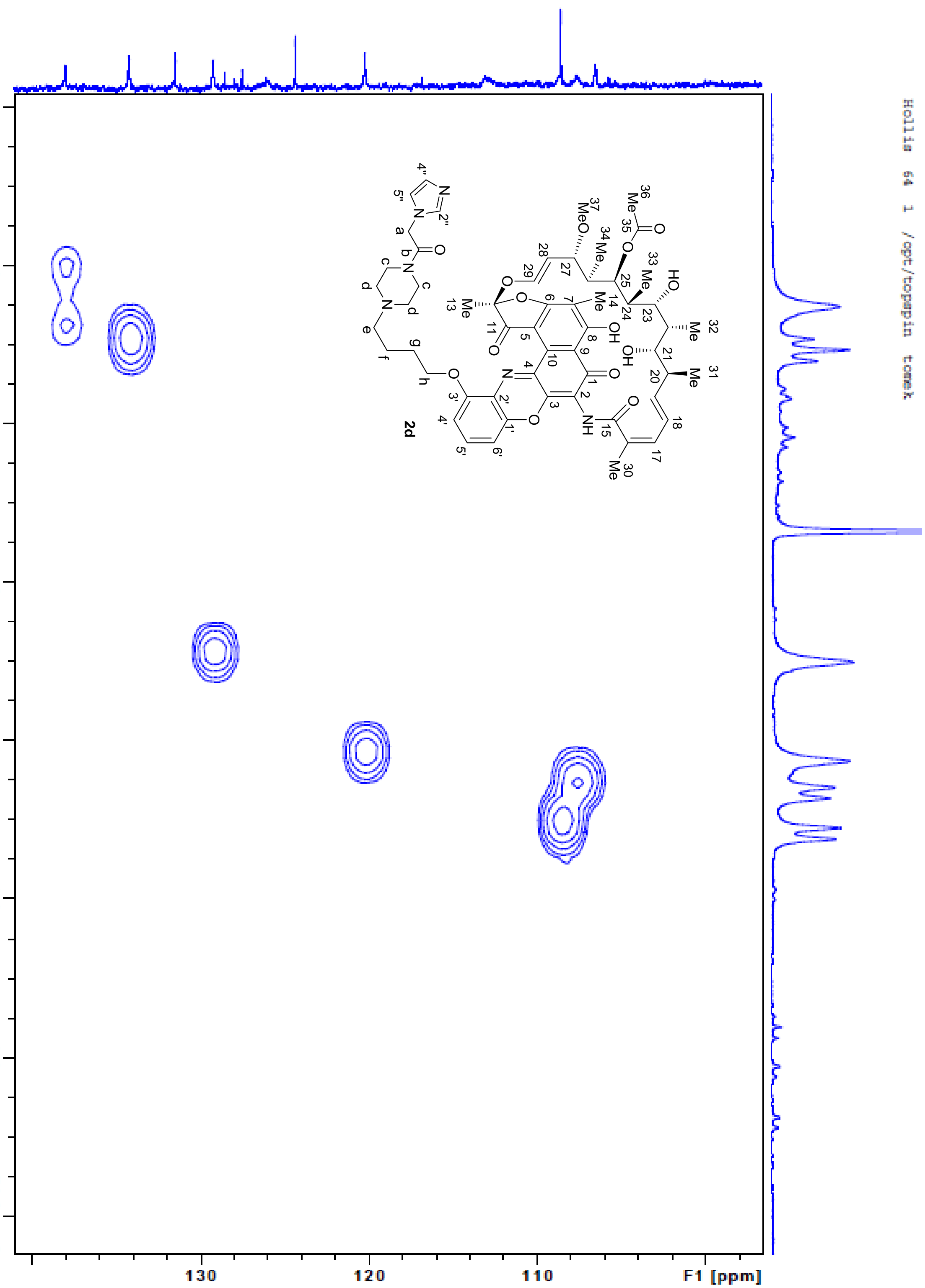

Hollis 42 1 /opt/topspin tomek
HX-2-33-1 in CDCl3, temp=25C
F1 [ppm]
F2 [ppm]
2c


Hollis 42 1 /opt/topspin tomek
HX-2-33-1 in CDCl3, temp=25C
2c
F1 [ppm]
F2 [ppm]
7.6
7.4
7.2
7.0
6.8
110
120
130
140


Hollis 42 1 /opt/topspin tomek
HX-2-33-1 in CDCl3, temp=25C
2c
F1 [ppm]
F2 [ppm]


Hollis d2 1 /opt/topspin tomak
HX-2-28-1 in CDCl3
temp=25C
2d
F1 [ppm]
F2 [ppm]


Hollis 64 1 /opt/topspin tomek
F1 [ppm]
F2 [ppm]
2d


Hollis 64 1 /opt/topspin tomek
2d
F2 [ppm]
F1 [ppm]
7.6
7.4
7.2
7.0
6.8
6.6
130
120
110

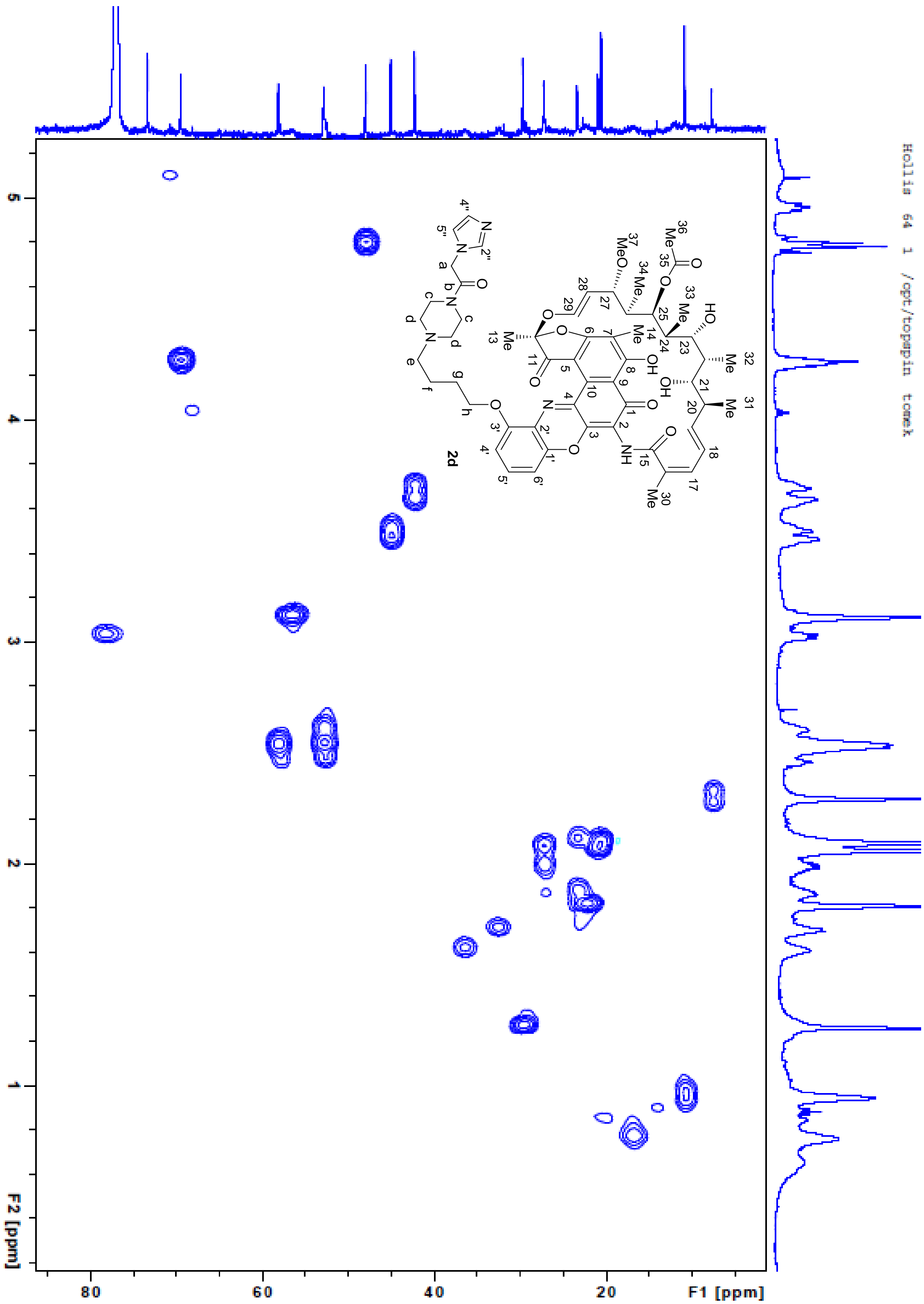
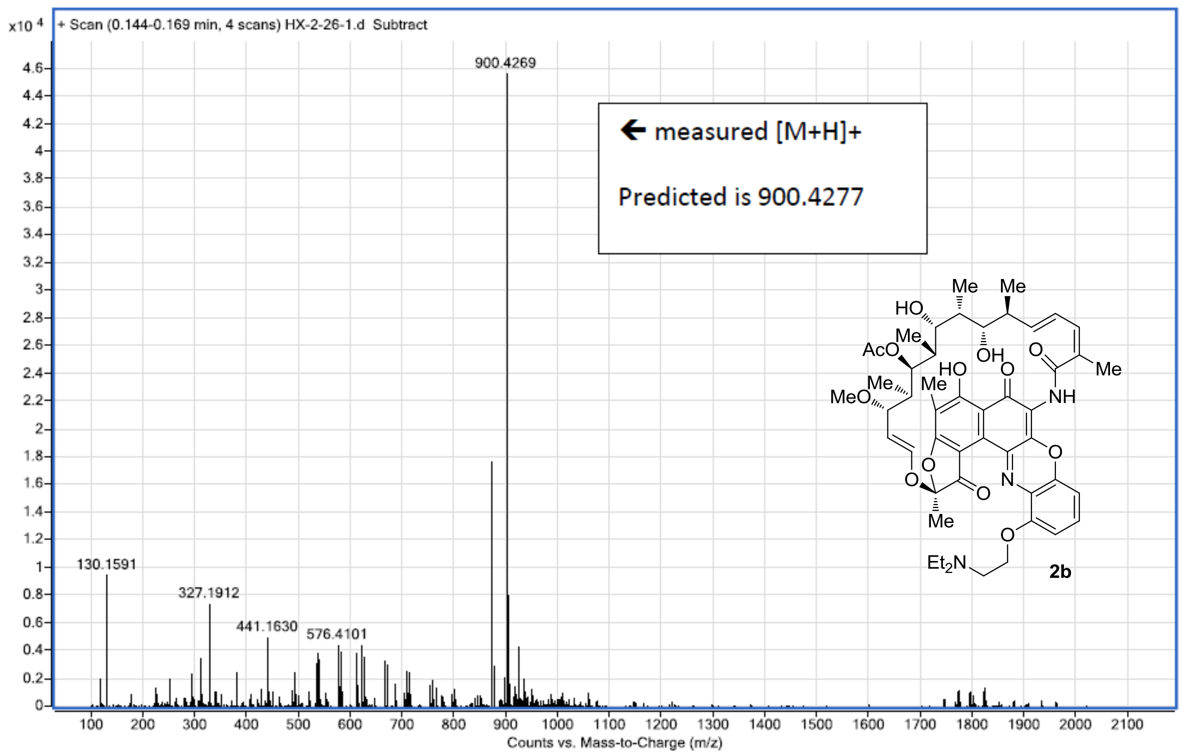
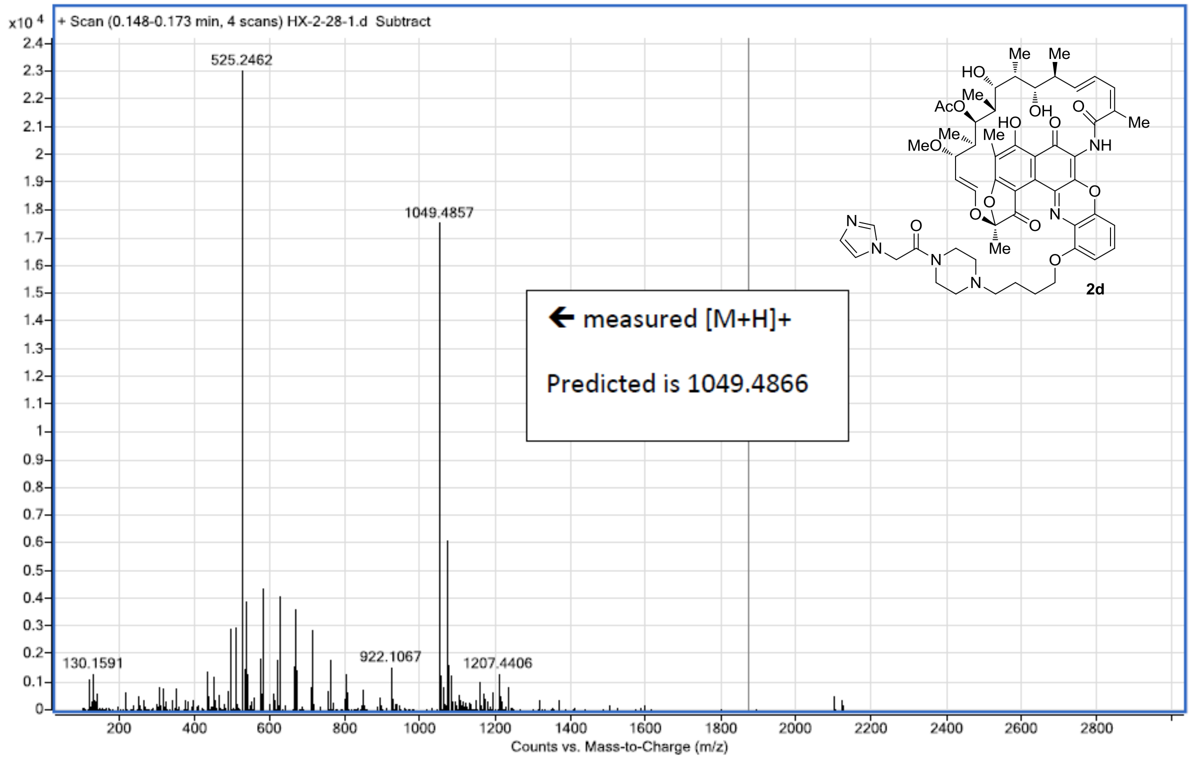


Figure 3SI. 1D- and 2D-NMR spectra for compounds **2b-2d**

Sample HX-2-26-1



Sample HX-2-28-1



Sample HX-2-33-1

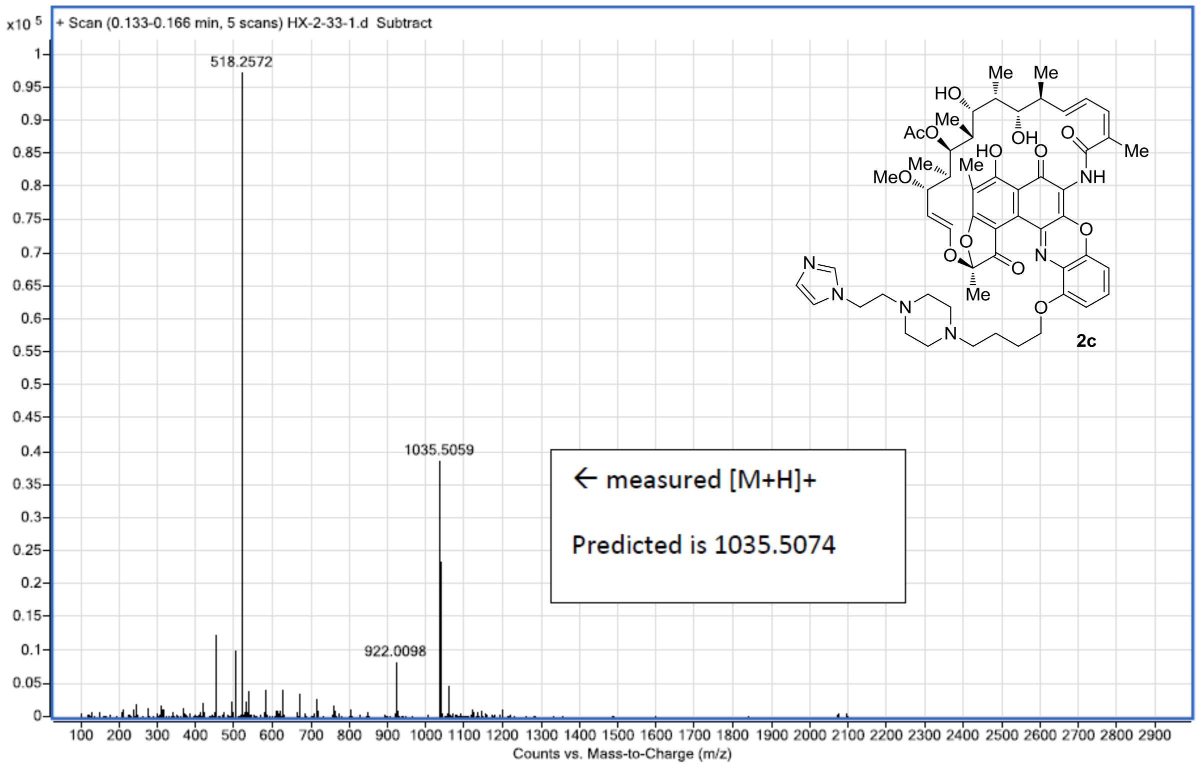
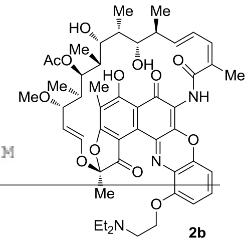


Figure 4SI. High resolution mass spectrometry traces for compounds **2b-2d**

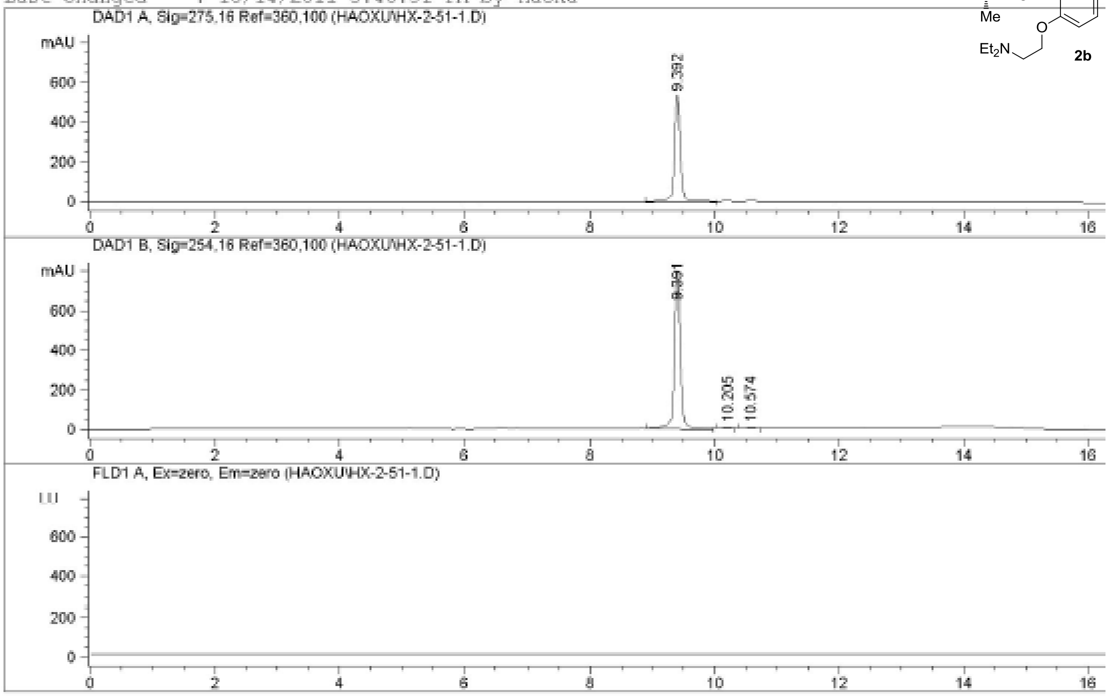
. File C:\CHEM32\1\DATA\HAOXU\HX-2-51-1.D
ple Name: HX-2-51-1

===

```
Acq. Operator   : hao xu                        Seq. Line :   1
Acq. Instrument : Instrument 1                   Location : Vial 41
Injection Date  : 2/19/2012 8:32:03 PM                Inj :   1
                                               Inj Volume : 20 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 10 µl
Method          : C:\CHEM32\HPLC METHOD FILE\HAOXU\HX20111010_OSELTAMIVIR.M
Last changed    : 10/14/2011 3:40:51 PM by HaoXu
```



2b



===

External Standard Report

===

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Sample Amount         :    300.00000  [wt%]    (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs
```

===

===

Area Percent Report

===

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Sample Amount         :    300.00000  [wt%]    (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs
```

. File C:\CHEM32\1\DATA\HAOXU\HX-2-51-1.D
ple Name: HX-2-51-1

ignal 1: DAD1 A, Sig=275,16 Ref=360,100

eak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.392	VV	0.1077	3836.46729	534.61926	100.0000

otals : 3836.46729 534.61926

ignal 2: DAD1 B, Sig=254,16 Ref=360,100

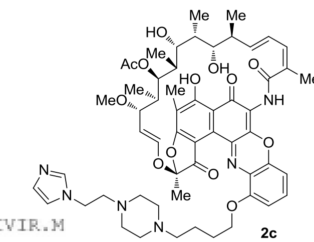
eak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.391	VB	0.1058	5639.96338	804.75433	98.1315
2	10.205	MM T	0.1600	54.09678	5.63606	0.9412
3	10.574	MM T	0.1521	53.29184	5.84105	0.9272

otals : 5747.35200 816.23145

ignal 3: FLD1 A, Ex=zero, Em=zero

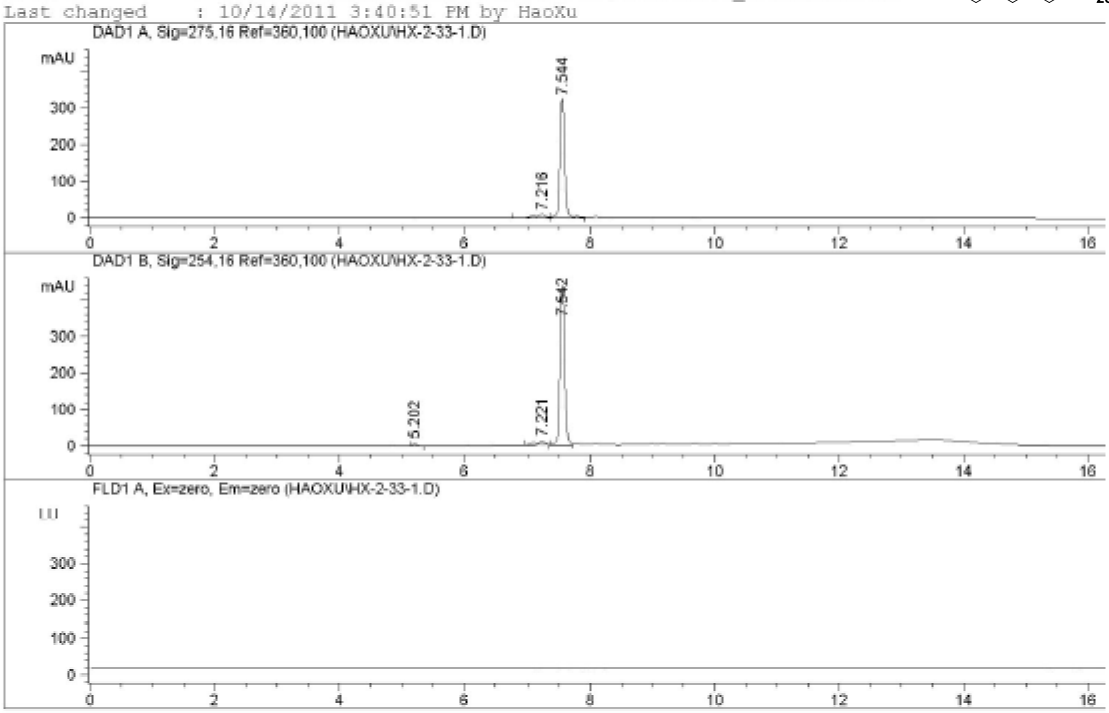
*** End of Report ***

. File C:\CHEM32\1\DATA\HAOXU\HX-2-33-1.D
ple Name: HX-2-33-1



===

```
Acq. Operator   : haoxu                          Seq. Line :    3
Acq. Instrument : Instrument 1                    Location : Vial 62
Injection Date  : 3/14/2012 9:35:00 PM                 Inj :    1
                                               Inj Volume : 20 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 10 µl
Method          : C:\CHEM32\HPLC METHOD FILE\HAOXU\HX20111010_OSELTAMIVIR.M
Last changed    : 10/14/2011 3:40:51 PM by HaoXu
```



===

External Standard Report

===

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Sample Amount         :    150.00000  [wt%]   (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs
```

===

===

Area Percent Report

===

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Sample Amount         :    150.00000  [wt%]   (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs
```

. File C:\CHEM32\1\DATA\HAOXU\HX-2-33-1.D
ple Name: HX-2-33-1

ignal 1: DAD1 A, Sig=275,16 Ref=360,100

eak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.216	VV	0.1776	131.26886	9.97083	7.1535
2	7.544	VV	0.0853	1703.76294	324.38193	92.8465

otals : 1835.03180 334.35275

ignal 2: DAD1 B, Sig=254,16 Ref=360,100

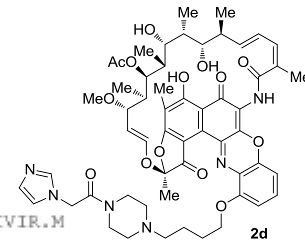
eak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.202	BB	0.0600	28.32638	7.18704	1.2048
2	7.221	MM T	0.1587	106.04414	11.13753	4.5105
3	7.542	VV	0.0771	2216.68555	437.60831	94.2847

otals : 2351.05607 455.93287

ignal 3: FLD1 A, Ex=zero, Em=zero

*** End of Report ***

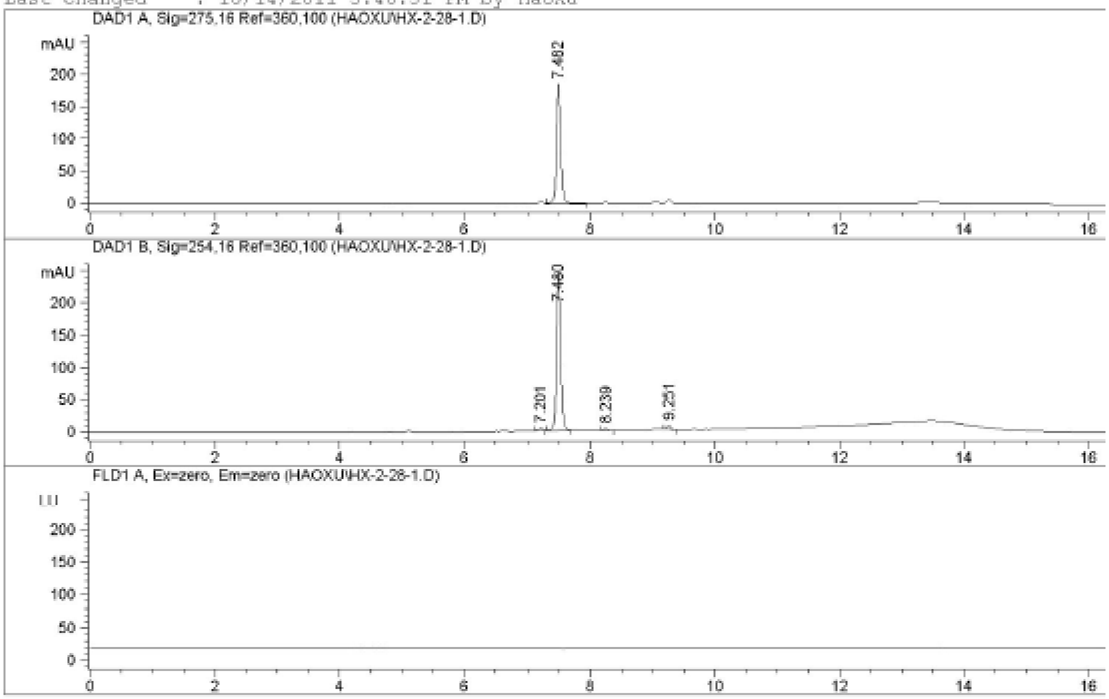
. File C:\CHEM32\1\DATA\HAOXU\HX-2-28-1.D
ple Name: HX-2-28-1



2d

===

Acq. Operator : haoxu Seq. Line : 2
Acq. Instrument : Instrument 1 Location : Vial 61
Injection Date : 3/14/2012 9:16:24 PM Inj : 1
Inj Volume : 20 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 10 µl
Method : C:\CHEM32\HPLC METHOD FILE\HAOXU\HX20111010_OSELTAMIVIR.M
Last changed : 10/14/2011 3:40:51 PM by HaoXu



===

External Standard Report

===

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount : 150.00000 [wt%] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

===

===

Area Percent Report

===

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount : 150.00000 [wt%] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

. File C:\CHEM32\1\DATA\HAOXU\HX-2-28-1.D
ple Name: HX-2-28-1

ignal 1: DAD1 A, Sig=275,16 Ref=360,100

eak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.482	VV	0.0823	928.80750	185.88354	100.0000
otals :				928.80750	185.88354	

ignal 2: DAD1 B, Sig=254,16 Ref=360,100

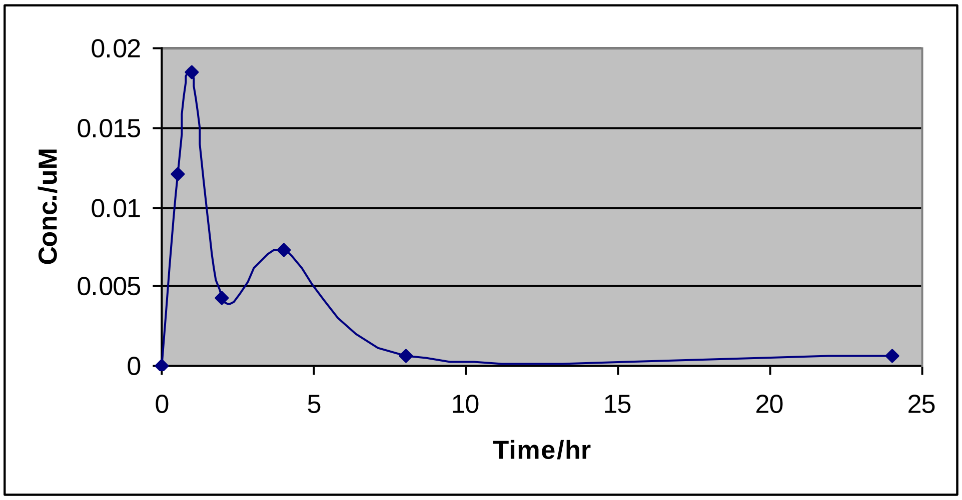
eak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.201	MM T	0.0684	16.75931	4.08280	1.3502
2	7.480	VV	0.0718	1180.38770	246.71176	95.0980
3	8.239	BB	0.0767	16.16008	3.21078	1.3019
4	9.251	MM T	0.0749	27.92550	6.21770	2.2498
otals :				1241.23258	260.22303	

ignal 3: FLD1 A, Ex=zero, Em=zero

*** End of Report ***

Figure 5SI. HPCL traces of benzoxazinorifamycins **2b-2d**

(a) Single dose



(b) Multiple dose

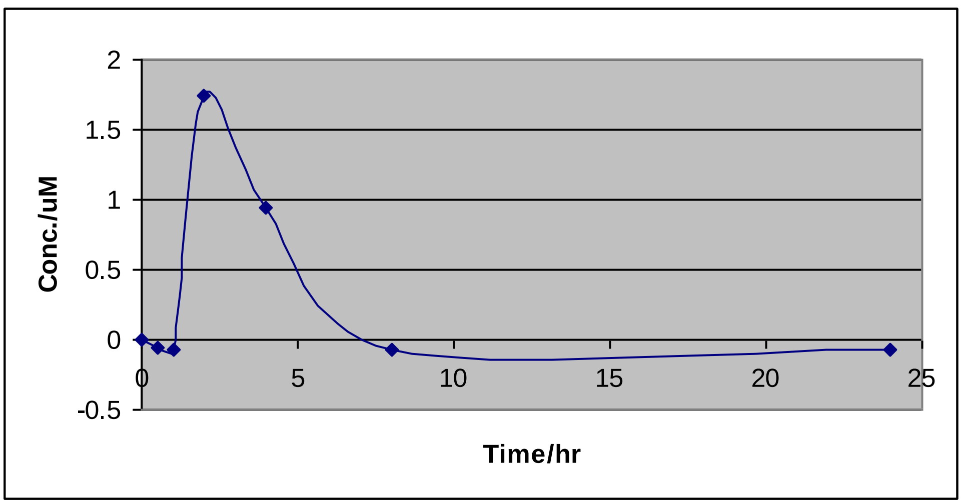


Figure 6SI. Linear plasma mean concentration vs. time profile for analog **2b** in (a) single dose and (b) multiple dose studies

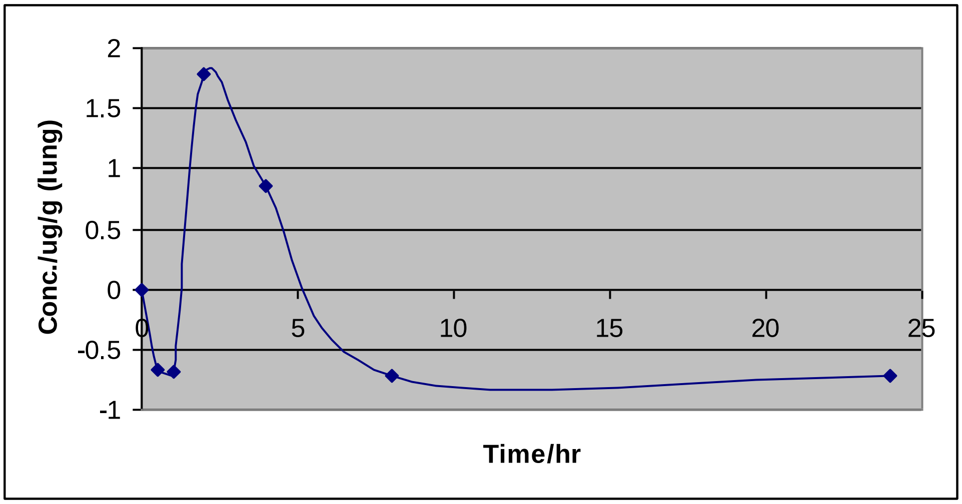


Figure 7SI. Linear lung tissue mean concentration vs. time profile for analog **2b** in a multiple dose study.

Table 1SI. ^{1}H-NMR chemical shifts of benzoxazinorifamycins

Proton atom	δ (ppm)		
	2b	**2c**	**2d**
H-13	2.05	2.05	2.05
H-14	2.30	2.29	2.28
H-24	1.70	1.7	1.71
H-26	1.60	1.6	1.61
H-27	3.01	3.02	3.02
H-28	4.98	4.95	4.95
H-29	5.98	5.96	5.97
H-30	2.10	2.10	2.09
H-31	0.77	0.75	0.76
H-33	0.95	0.94	0.94
H-34	0.60	0.63	0.65
H-36	1.79	1.80	1.80
H-37	3.09	3.09	3.10
H-4’	6.92	6.88	6.88
H-5’	7.49	7.48	7.49
H-6’	6.94	6.93	6.93
H-a	1.13	4.03	4.78
H-b	2.79	2.69	
H-c	3.24	2.51	3.68-3.45
H-d	4.38	2.51	2.53
H-e		2.51	2.45
H-f		2.02	1.87
H-g		2.02	1.99
H-h		4.24	4.26
H-2’’		7.54	7.54
H-4’’		6.97	6.97
H-5’’		7.04	7.10

Table 2SI. ^{13}C-NMR chemical shifts of benzoxazinorifamycins

	δ (ppm)		
Carbon atom	**2b**	**2c**	**2d**
C-13	21.0	20.7	20.6
C-14	7.6	7.5	7.7
C-24	32.7	32.4	32.5
C-26	36.8	36.5	36.4
C-27	78.1	78.1	78.5
C-28	113.0	113.6	113.7
C-29	142.5	142.9	142.0
C-30	20.5	21	20.9
C-31	16.7	16.8	16.8
C-33	10.6	10.8	10.8
C-34	N/A	N/A	N/A
C-36	22.0	22.4	22.0
C-37	56.5	56.5	56.9
C-4’	109.2	108.7	108.6
C-5’	134.1	134	134.2
C-6’	109.3	107.5	107.7
C-a	11.2	44.7	48.0
C-b	47.6	58.7	N/A
C-c	51.8	53.2	42.3, 44.9
C-d	68.1	53.2	52.8
C-e		58.2	58.2
C-f		23.2	22.7
C-g		27.3	27.2
C-h		69.8	69.6
C-2’’		137.4	138.0
C-4’’		119.1	120.2
C-5’’		129.2	129.2

Table 3SI. Log IC_{50}s and standard errors of the fits for RLZ (**2a**) and analogs (**2b** – **2d**) against RNAP

	2a (RLZ)	**2b**	**2c**	**2d**
WT RNAP (-σ^A)	-1.9407 (0.048, 1.09)	-2.5282 (0.026, 2.29)	-2.5103 (0.038, 2.38)	-2.4916 0.066, 1.22)
WT RNAP (+σ^A)	-2.4614 (0.068, 1.16)	-2.5442 (0.038, 1.65)	-2.5653 (0.055, 1.51)	-2.348 (0.096, 0.85)
D435V (+σ^A)	2.7331 (0.038, 2.02)	1.2946 (0.035, 0.95)	0.94796 (0.064, 0.87)	1.1085 (0.046, 0.88)
H445Y (+σ^A)	2.2355 (0.069, 0.71)	2.2337 (0.138, 0.41)	2.6407 (0.140, 0.64)	2.7592 (0.180, 0.53)
S450L (+σ^A)	2.0692 (0.157, 0.63)	1.2054 (0.056, 0.81)	-2.5103 (0.038, 2.38)	2.0881 (0.069, 0.67)

[a] The log IC_{50} values are such that the IC_{50} values will be in µM. Negative log IC_{50} values reflect IC_{50} values less than µM (e.g., in the nM range). Values were fit to a four parameter logistic regression model with the top and bottom limits set at 100 and 0 respectively. [b] The average error is ~10 %, which roughly translates to 20-25% in the IC_{50}. [c] The average Hill slope is 1.02.

Table 4SI. Mean relative fluorescence units (RFU)[a] for RMP (**1a**) and benzoxazinorifamycins (**2a** – **2d**) in the hPXR activation assay

Conc.	**1a** (RMP)	Conc.	**2a** (RLZ)	**2b**	**2c**	**2d**
20 µM	48427	100 µM	35250	11137	10881	11625
10 µM	59067	25 µM	63418	11591	12218	43077
5 µM	61839	6.25 µM	70784	43495	49297	66941
1 µM	64852	1.56 µM	73704	68860	60314	68172
0.5 µM	59756	0.39 µM	74950	69532	63570	68936
0.1 µM	63078	0.098 µM	72399	71149	65632	68628

[a] RFU is a measure of cell viability in the assay. For controls, 1% DMSO = 67021 RFU; Dosing media = 59992 RFU.