Electronic Supporting Information

An Efficient Method for the Synthesis of Selenium Modified Nucleosides: Its application to the synthesis of *Se*-adenosyl-L-selenomethionine (SeAM)

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1. Single Crystal X-Ray Diffraction Data for Compound 6

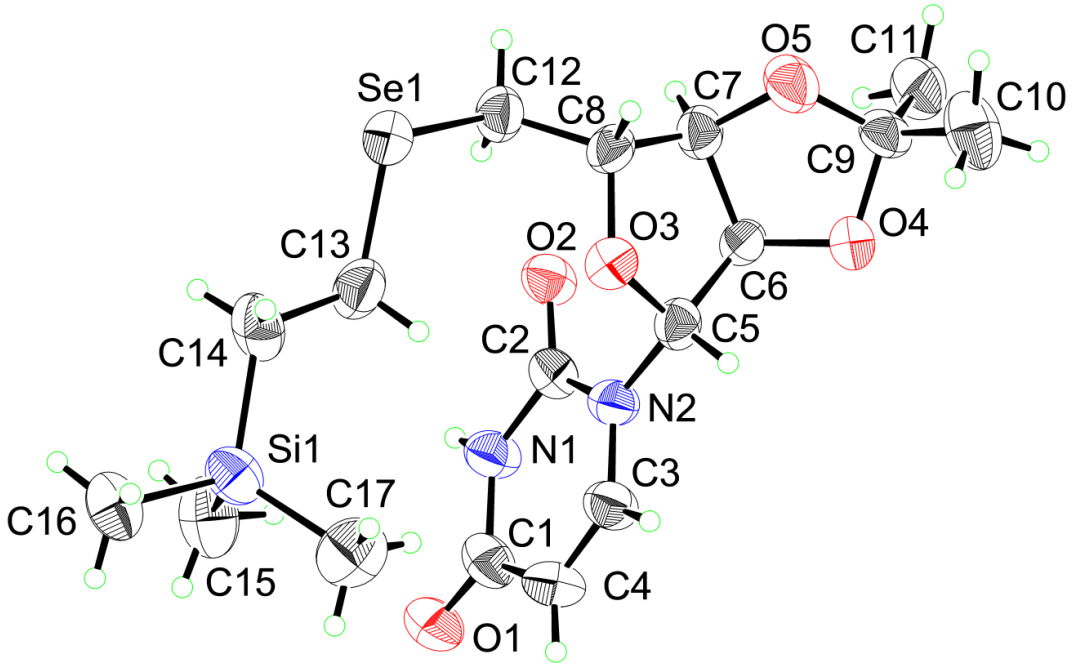


Figure S1: ORTEP diagram of the compound **6** crystallized from ethylacetate.

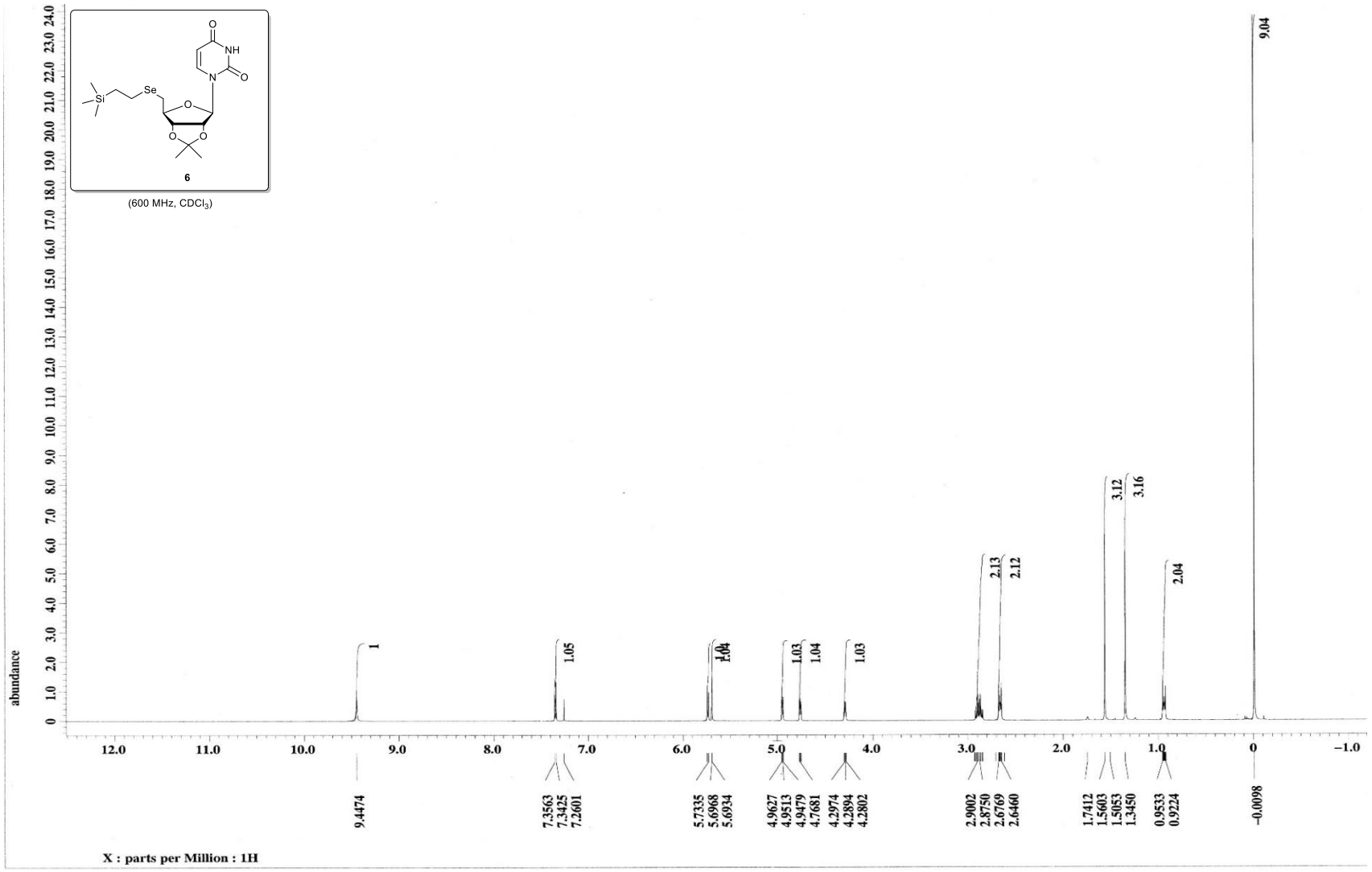
Single crystal X-ray diffraction data for compound **6** was collected on a Rigaku AFC-7R Mercury CCD diffractometer with graphite-monochromated Mo-Kα radiation (λ = 0.71075 Å). This data (CCDC 1058755) can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Crystal data and structure refinement for compound **6**.

Identification code	compound **6**
Empirical formula	$C_{17}H_{28}N_2O_5SeSi$
Formula weight	447.46
Temperature	293(2) K
Wavelength	0.71075 Å
Crystal system	orthorhombic
Space group	$P\ 2_12_12_1$
Unit cell dimensions	a = 7.621(2) Å

	b = 13.163(4) Å
	c = 23.299(7) Å
Volume	2337.2(12) Å^3
Z	4
Density (calculated)	1.272 Mg/m^3
Absorption coefficient	1.683 mm^{-1}
F(000)	928
Crystal size	0.20 x 0.20 x 0.20 mm^3
Theta range for data collection	3.05 to 27.50°.
Index ranges	-6<=*h*<=9, -16<=*k*<=17, -19<=*l*<=30
Reflections collected	14655
Independent reflections	5298 [*R*(int) = 0.0611]
Completeness to theta = 27.50°	98.4 %
Max. and min. transmission	0.7295 and 0.7295
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5298 / 0 / 240
Goodness-of-fit on F^2	1.058
Final *R* indices [$I>2\sigma(I)$]	*R*1 = 0.1050, *wR*2 = 0.2720
R indices (all data)	*R*1 = 0.1652, *wR*2 = 0.3186
Absolute structure parameter	-0.01(3)
Largest diff. peak and hole	0.746 and -0.857 e.Å^{-3}

2. Copies of ^{1}H, ^{13}C and ^{77}Se Spectra for All New Compounds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(600 MHz, CDCl3)
abundance
X : parts per Million : 1H
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3.16
2.13
2.12
2.04
1.05
1.03
1.04
1.03
1
9.4474
7.3563
7.3425
7.2601
5.7335
5.6968
5.6934
4.9627
4.9513
4.9479
4.7681
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4.2894
4.2802
2.9002
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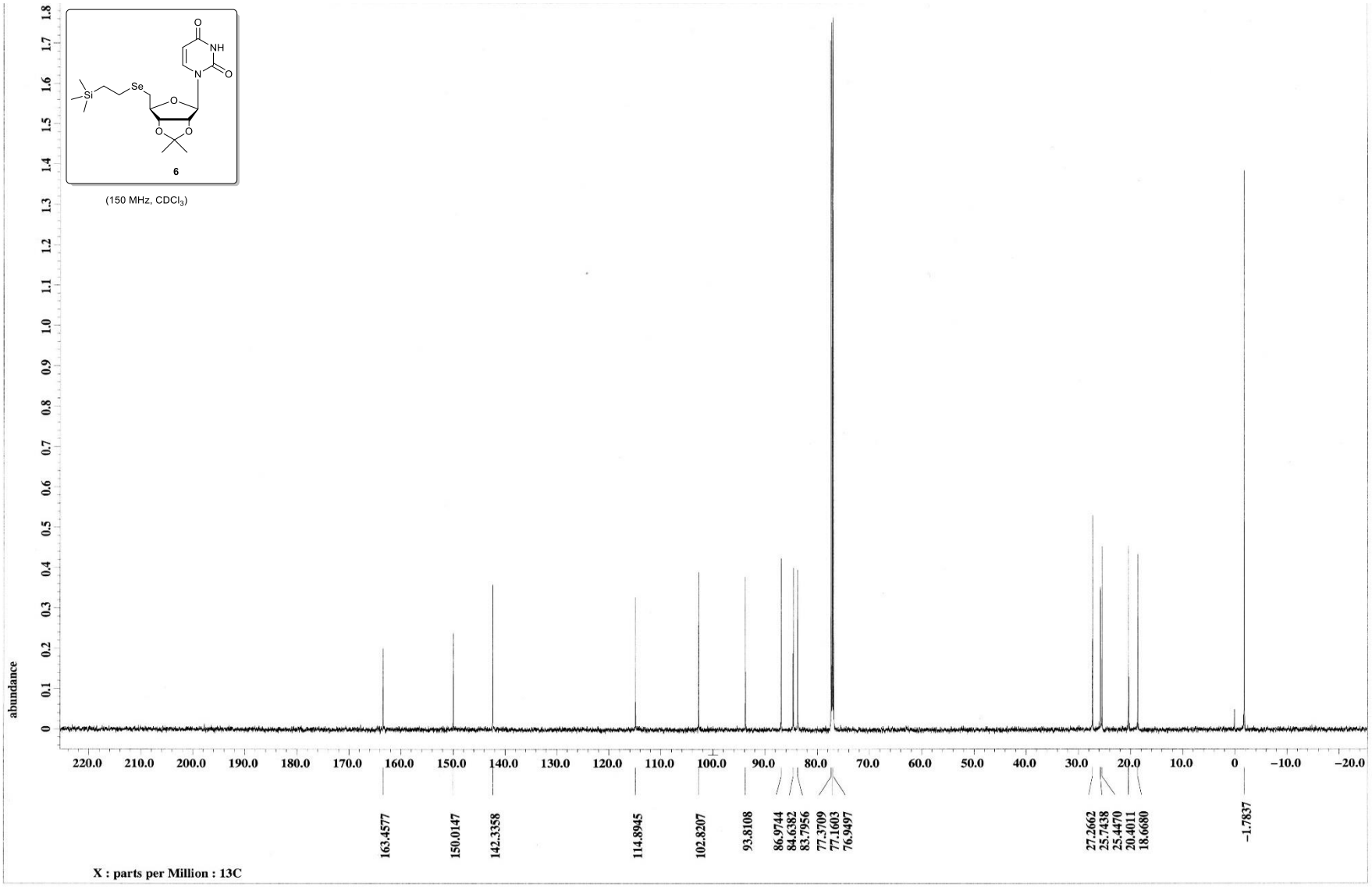
1.3450
0.9533
0.9224
−0.0098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X : parts per Million : 13C
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142.3358
114.8945
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93.8108
86.9744
84.6382
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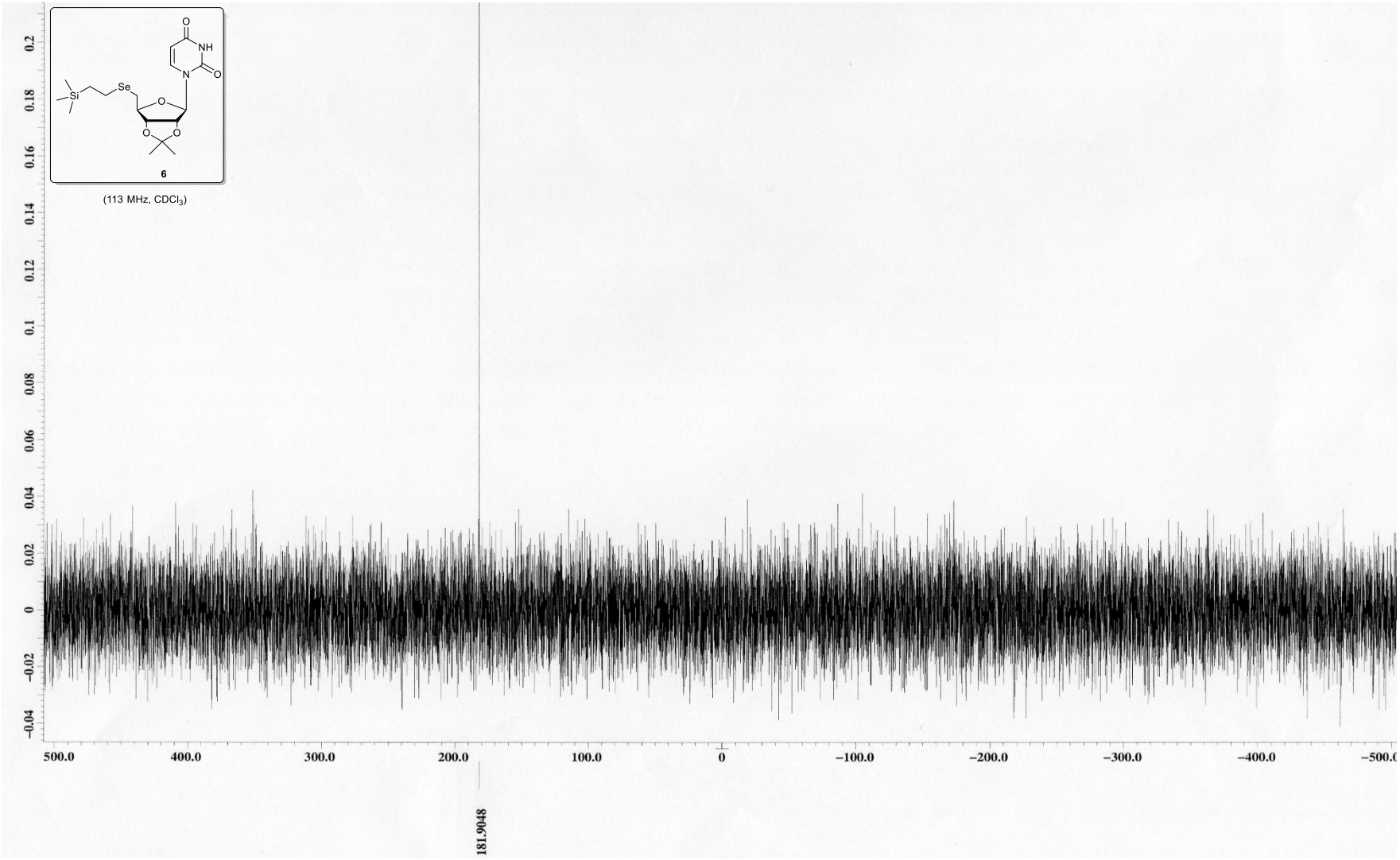
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0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
−0.02
−0.04
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0
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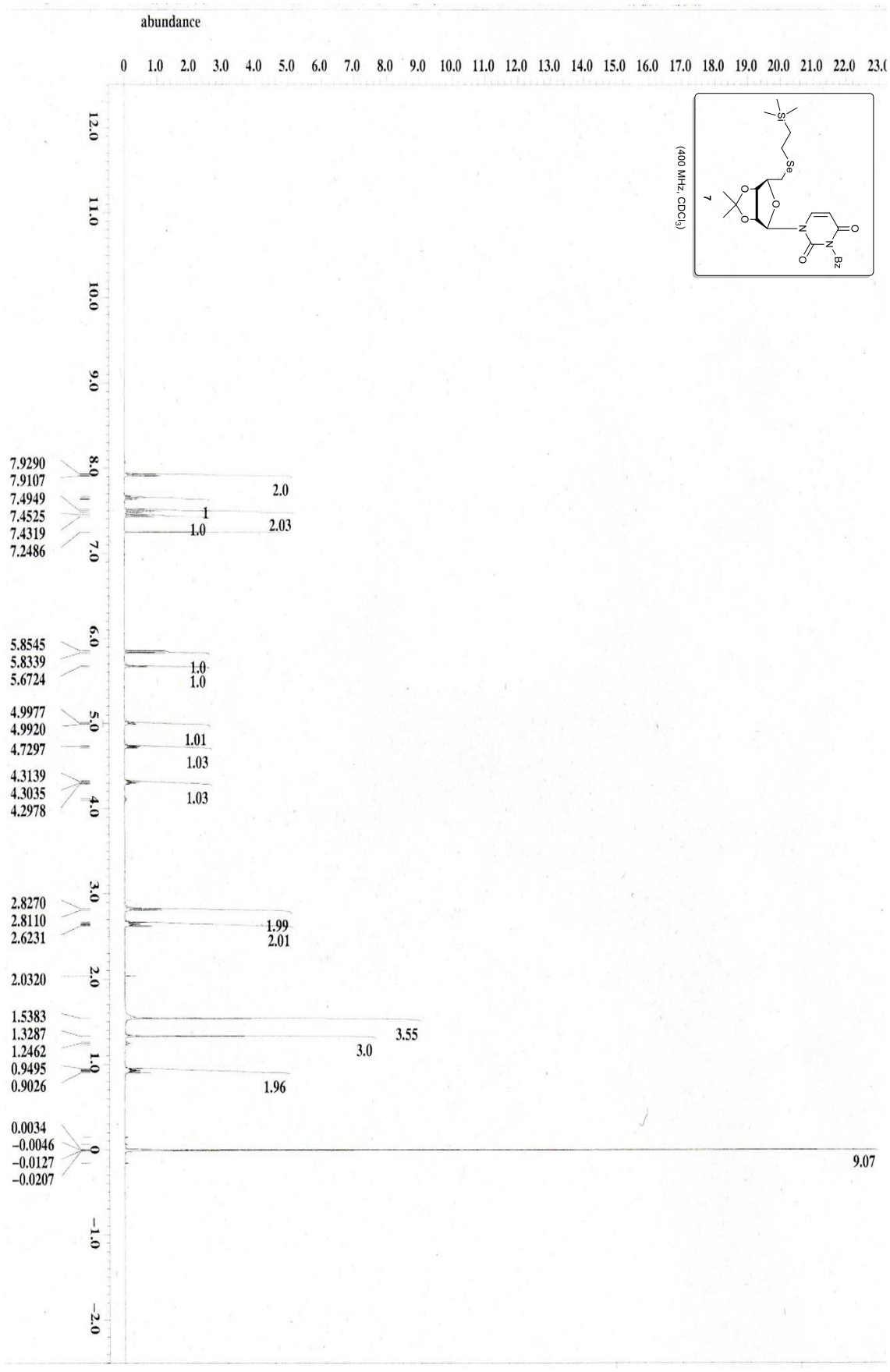
−400.0
181.9048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(400 MHz, CDCl3)
7
Si
Se
O
O
O
N
N
O
O
Bz
7.9290
7.9107
7.4949
7.4525
7.4319
7.2486
2.0
1
1.0
2.03
5.8545
5.8339
5.6724
1.0
1.0
4.9977
4.9920
4.7297
1.01
1.03
4.3139
4.3035
4.2978
1.03
2.8270
2.8110
2.6231
1.99
2.01
2.0320
1.5383
1.3287
1.2462
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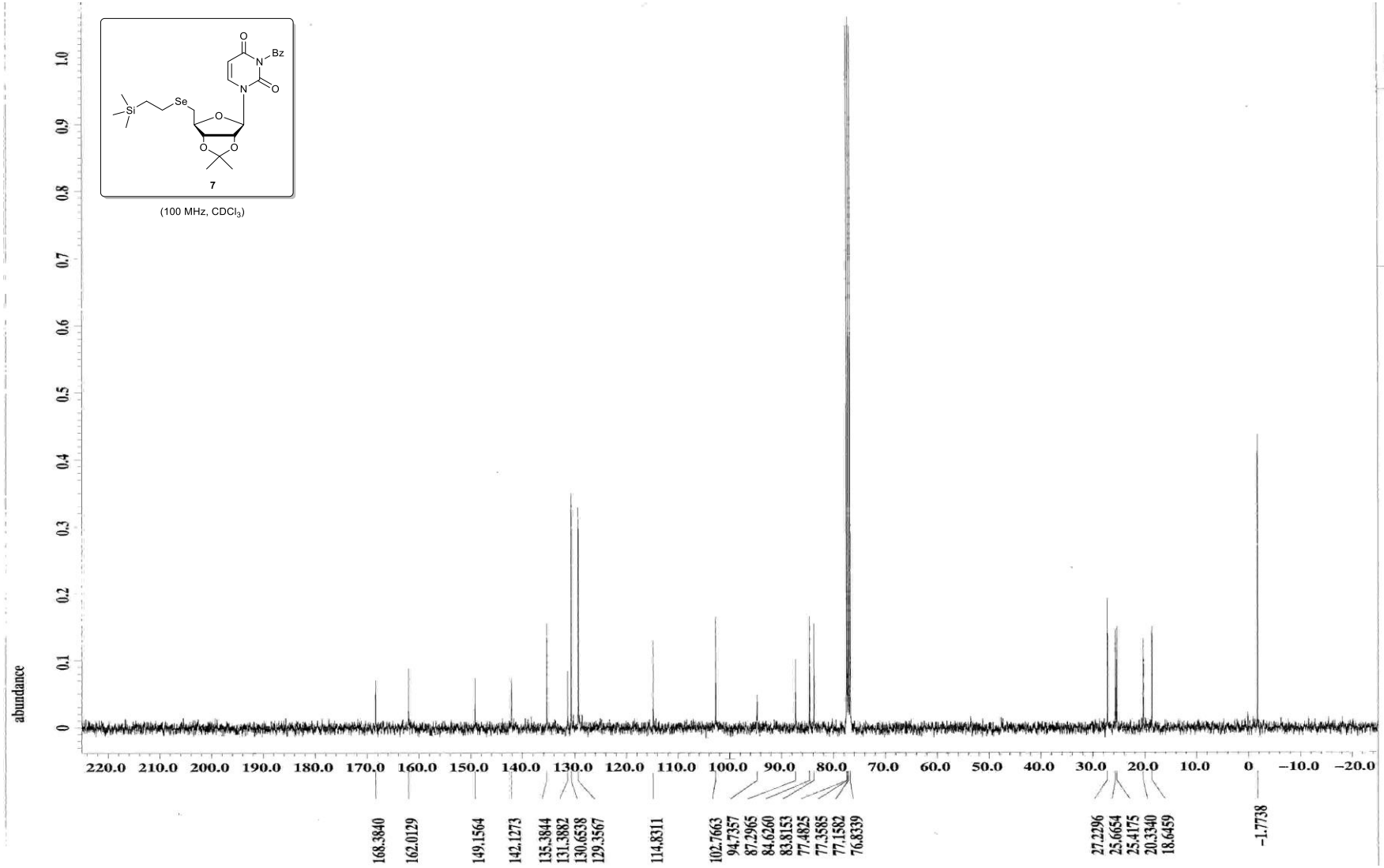
7
(100 MHz, CDCl3)
abundance
168.3840
162.0129
149.1564
142.1273
135.3844
131.3882
130.6538
129.3567
114.8311
102.7663
94.7357
87.2965
84.6260
83.8153
77.4825
77.3585
77.1582
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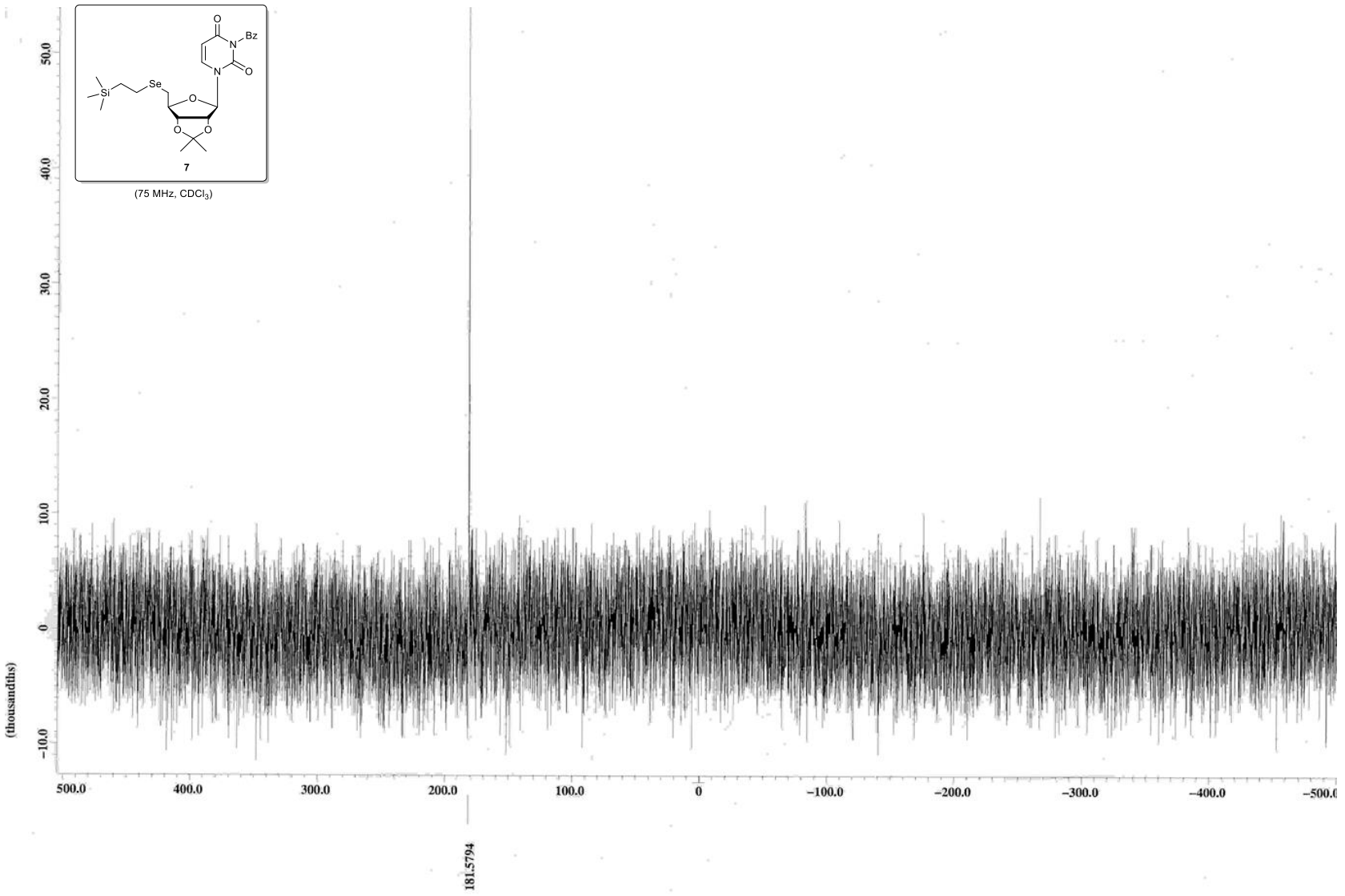
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(75 MHz, CDCl3)
(thousandths)
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20.0
10.0
0
−10.0
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300.0
200.0
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0
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−400.0
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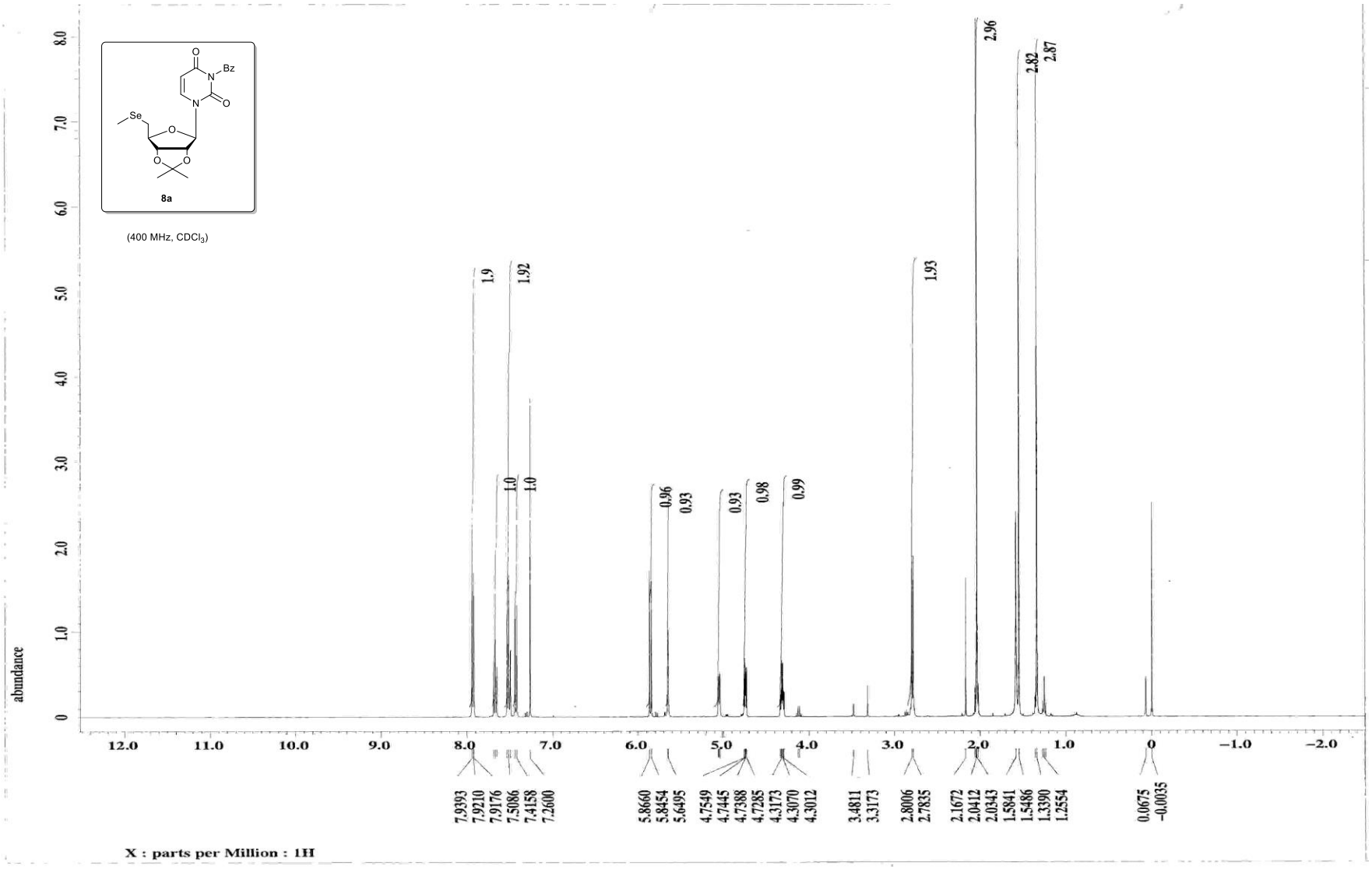
8a
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
1.9
1.92
1.0
1.0
1.0
0.96
0.93
0.93
0.98
0.99
1.93
2.96
2.82
2.87
7.9393
7.9210
7.9176
7.5086
7.4158
7.2600
5.8660
5.8454
5.6495
4.7549
4.7445
4.7388
4.7285
4.3173
4.3070
4.3012
3.4811
3.3173
2.8006
2.7835
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2.0412
2.0343
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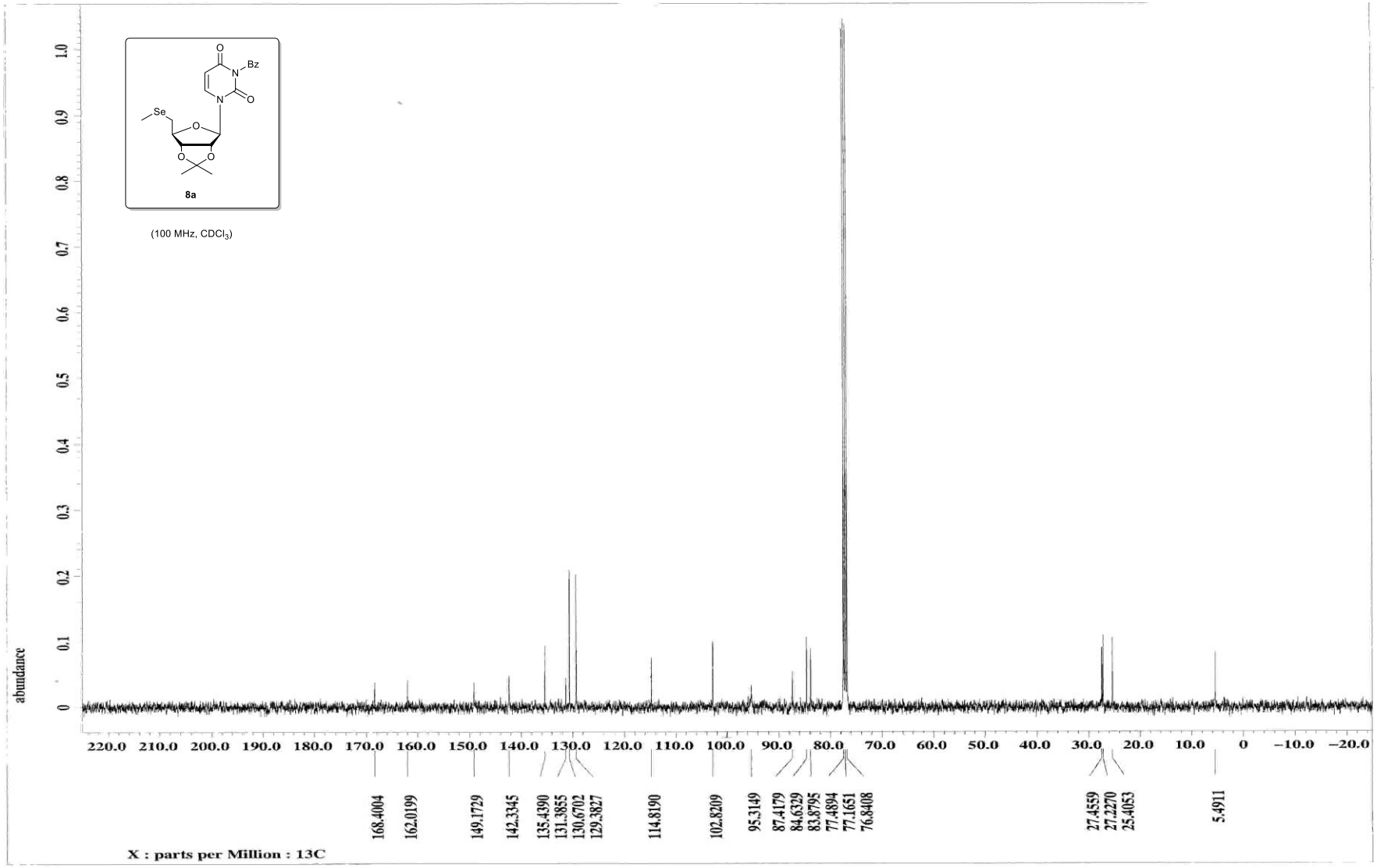
1.3390
1.2554
0.0675
-0.0035


8a
(100 MHz, CDCl3)
abundance
X : parts per Million : 13C
168.4004
162.0199
149.1729
142.3345
135.4390
131.3855
130.6702
129.3827
114.8190
102.8209
95.3149
87.4179
84.6329
83.8795
77.4894
77.1651
76.8408
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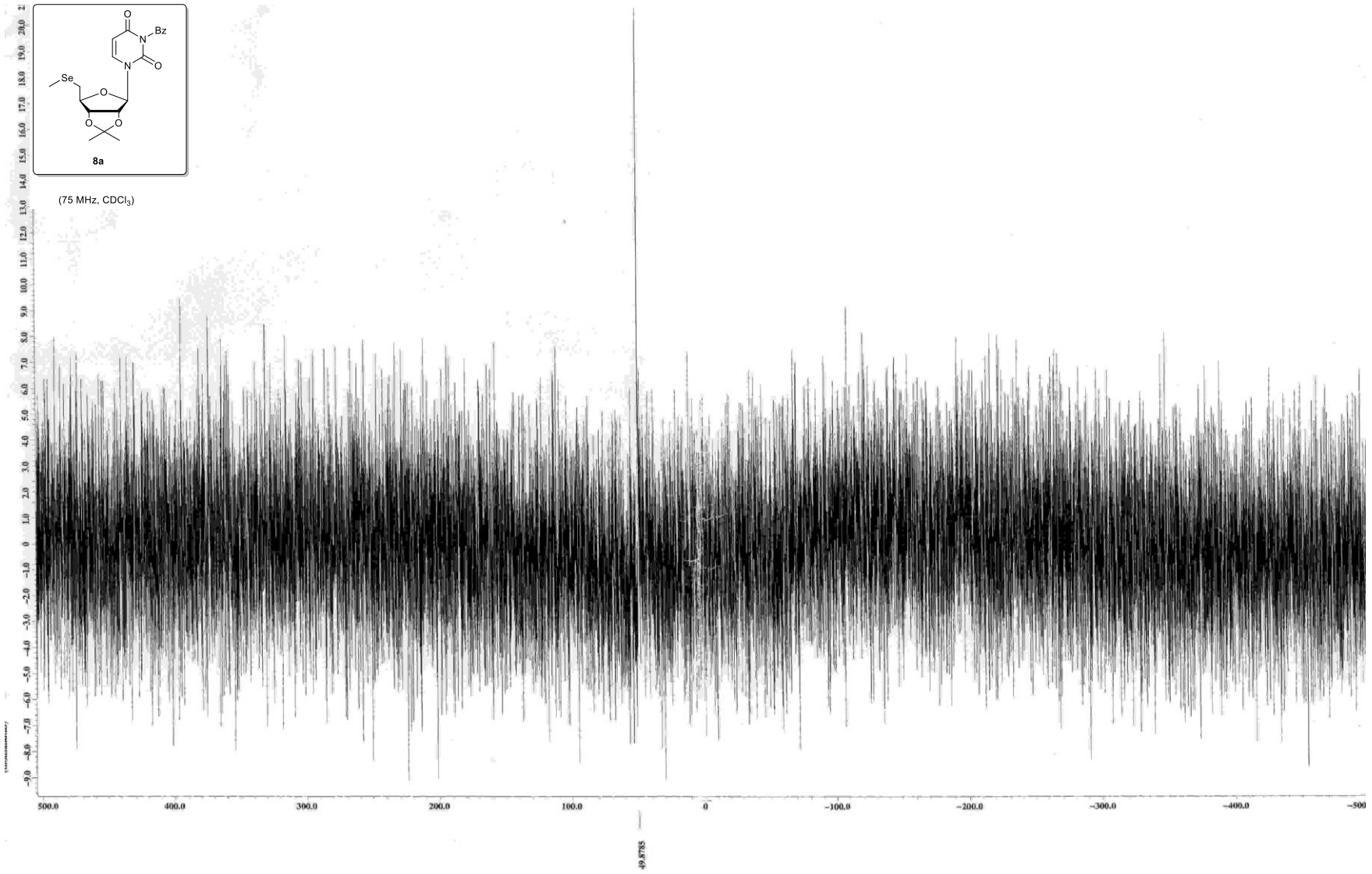
27.2270
25.4053
5.4911


Bz
Se
8a
(75 MHz, CDCl3)
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200.0
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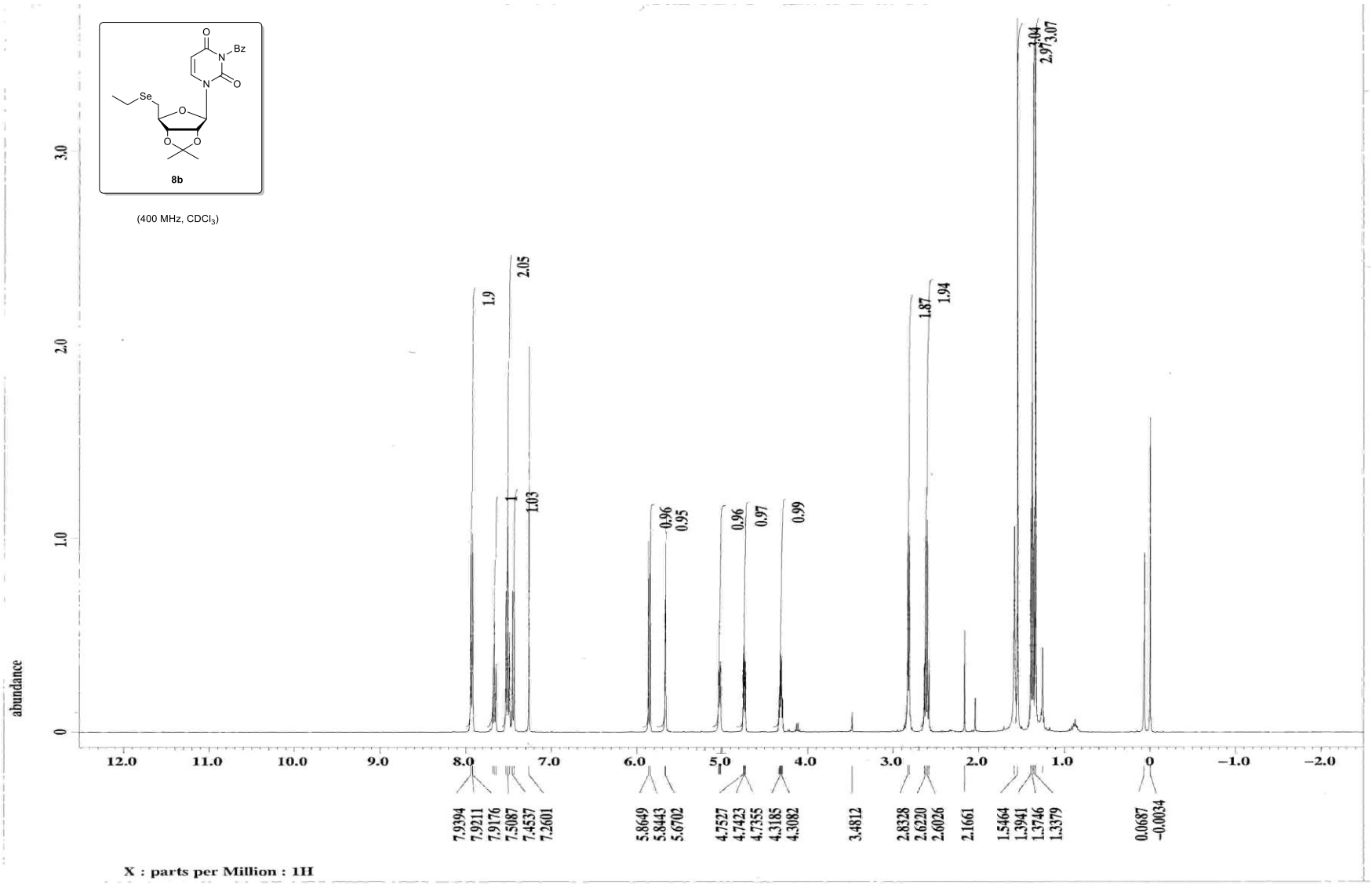
8b
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
7.9394
7.9211
7.9176
7.5087
7.4537
7.2601
5.8649
5.8443
5.6702
4.7527
4.7423
4.7355
4.3185
4.3082
3.4812
2.8328
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2.6026
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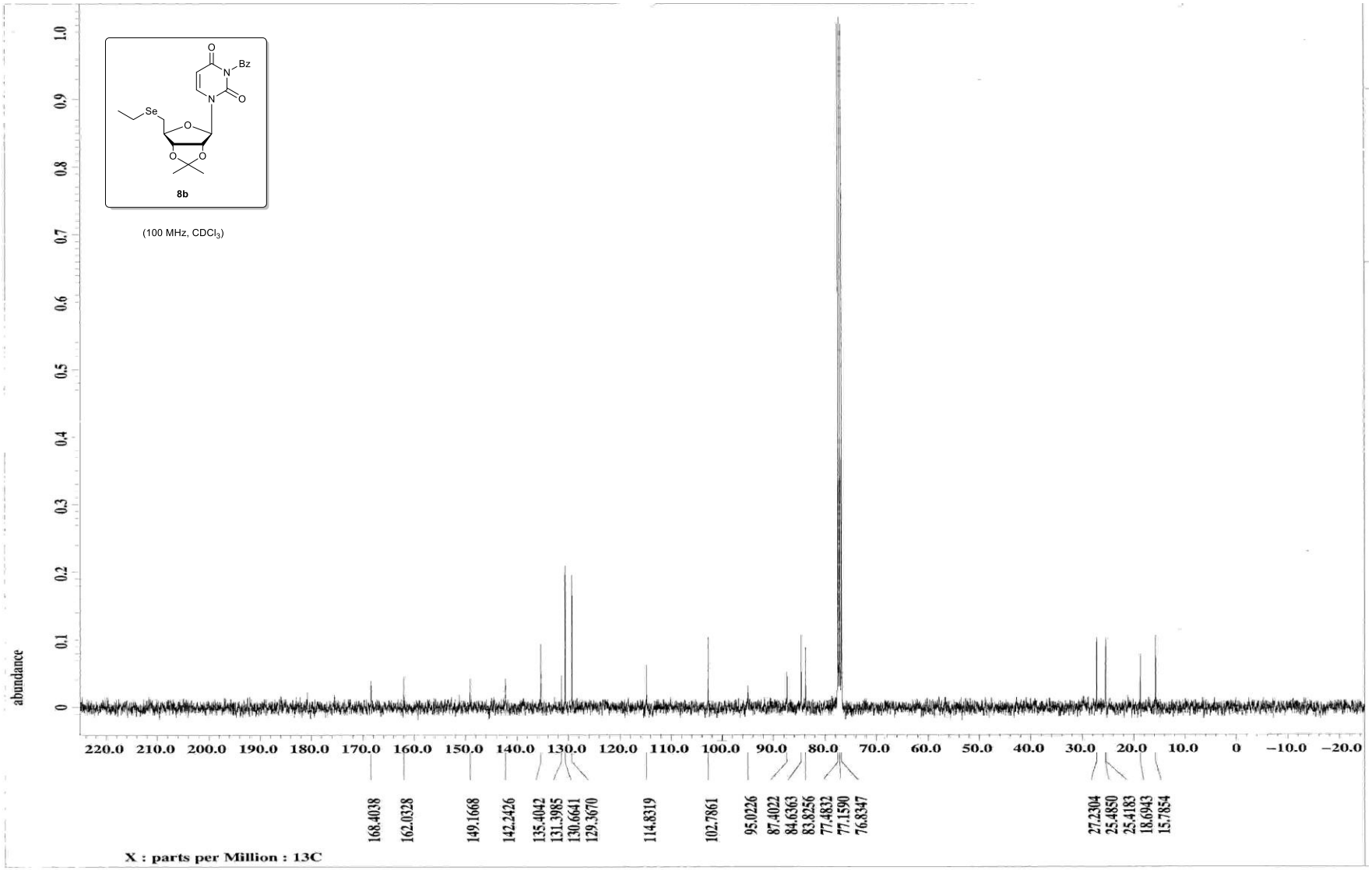
1.3746
1.3379
0.0687
-0.0034


8b
(100 MHz, CDCl3)
abundance
X : parts per Million : 13C
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162.0328
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142.2426
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131.3985
130.6641
129.3670
114.8319
102.7861
95.0226
87.4022
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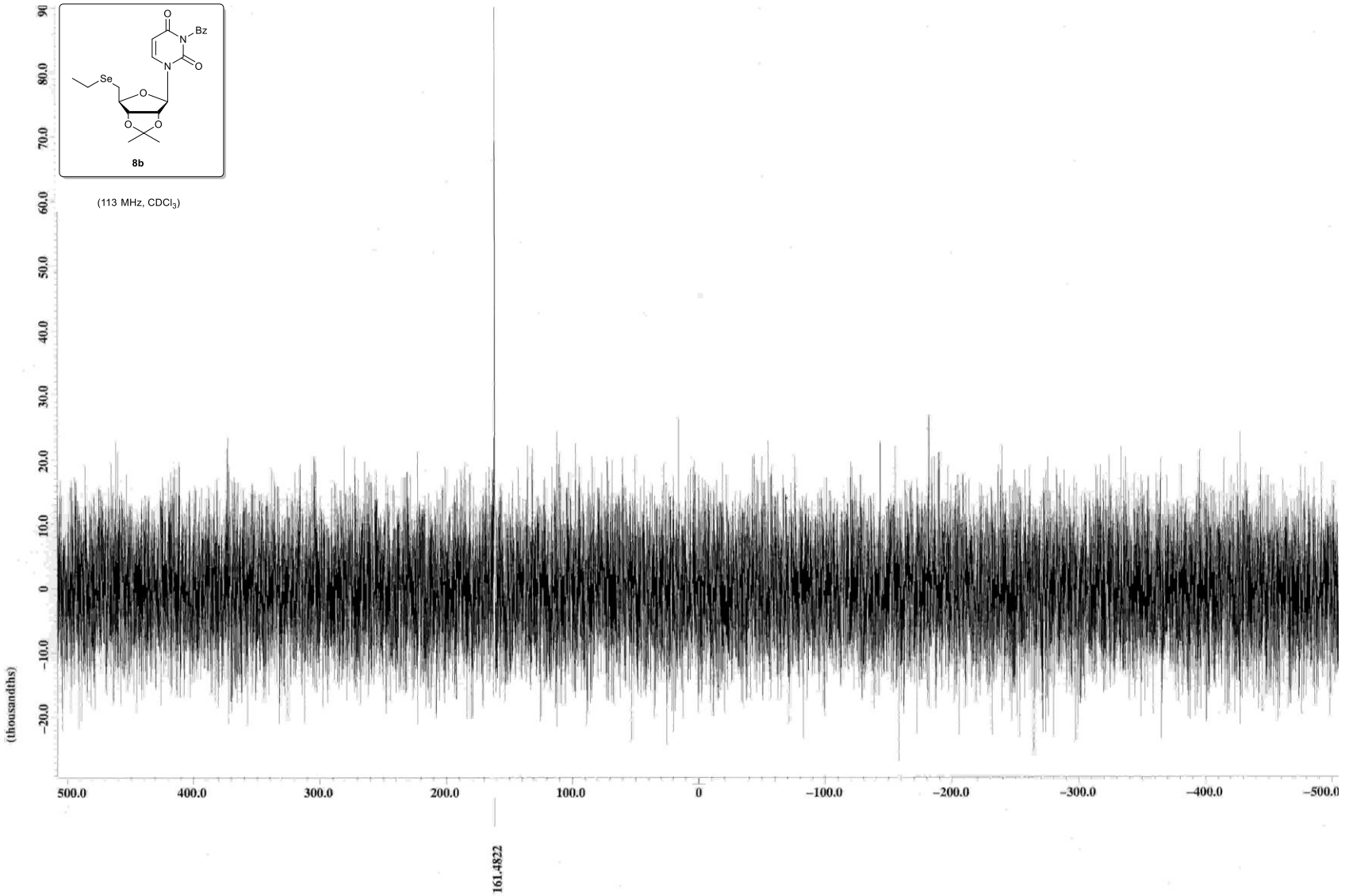
15.7854


8b
(113 MHz, CDCl3)
(thousandths)
90
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
−20.0
500.0
400.0
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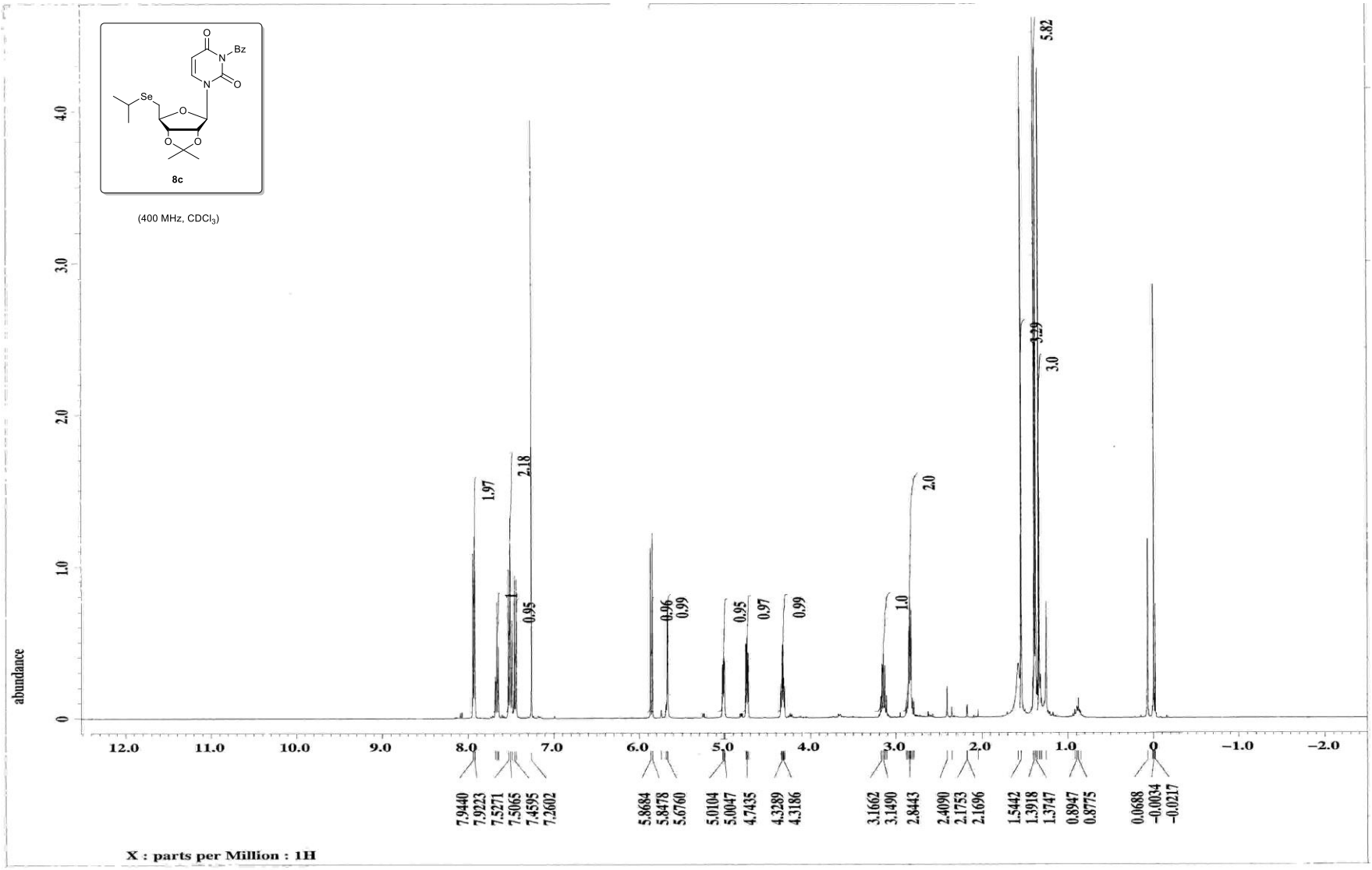
−500.0
161.4822


8c
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
7.9440
7.9223
7.5271
7.5065
7.4595
7.2602
5.8684
5.8478
5.6760
5.0104
5.0047
4.7435
4.3289
4.3186
3.1662
3.1490
2.8443
2.4090
2.1753
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1.3747
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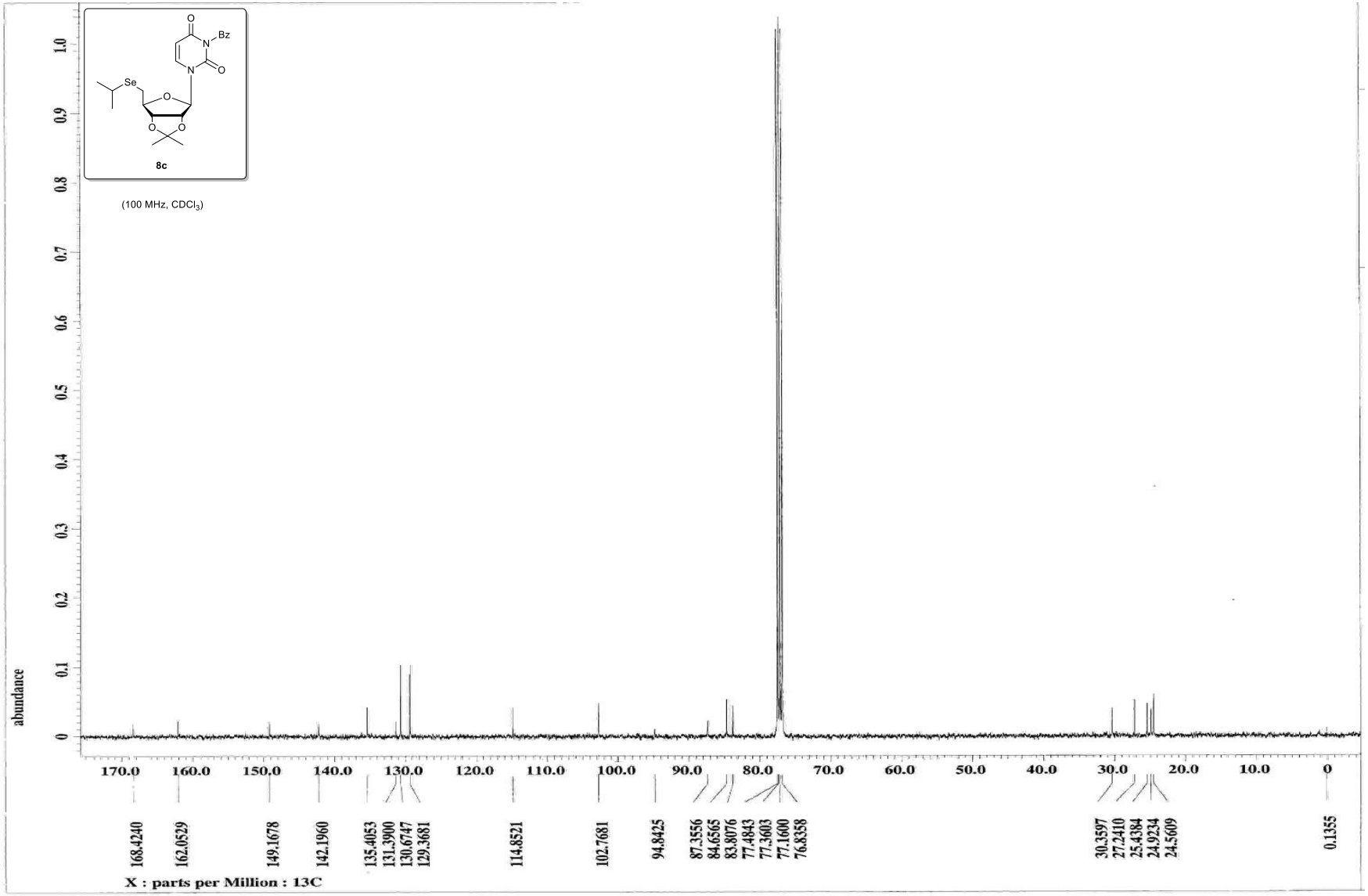
8c
(100 MHz, CDCl3)
abundance
X : parts per Million : 13C
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131.3900
130.6747
129.3681
114.8521
102.7681
94.8425
87.3556
84.6565
83.8076
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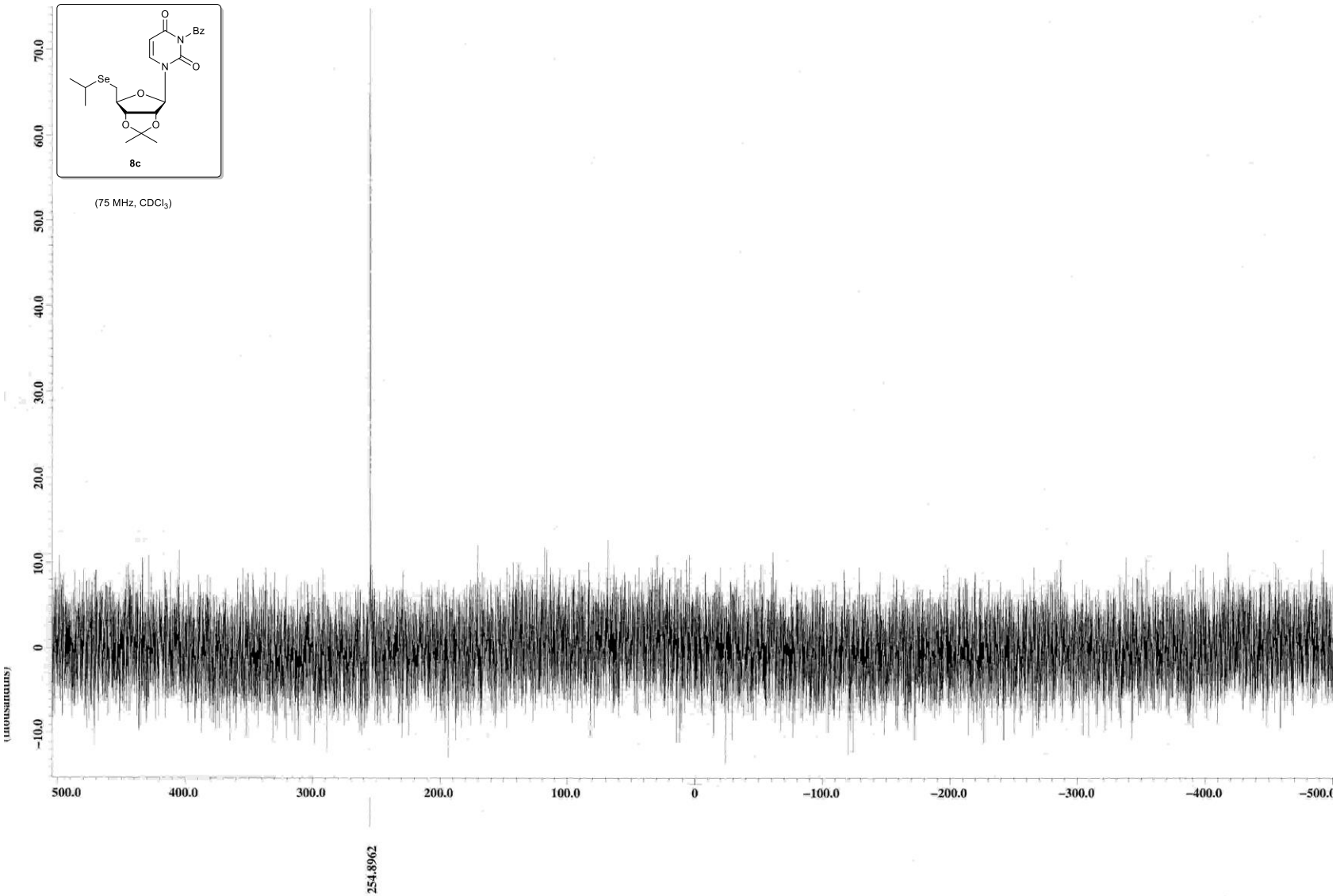
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40.0
30.0
20.0
10.0
0
−10.0
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400.0
300.0
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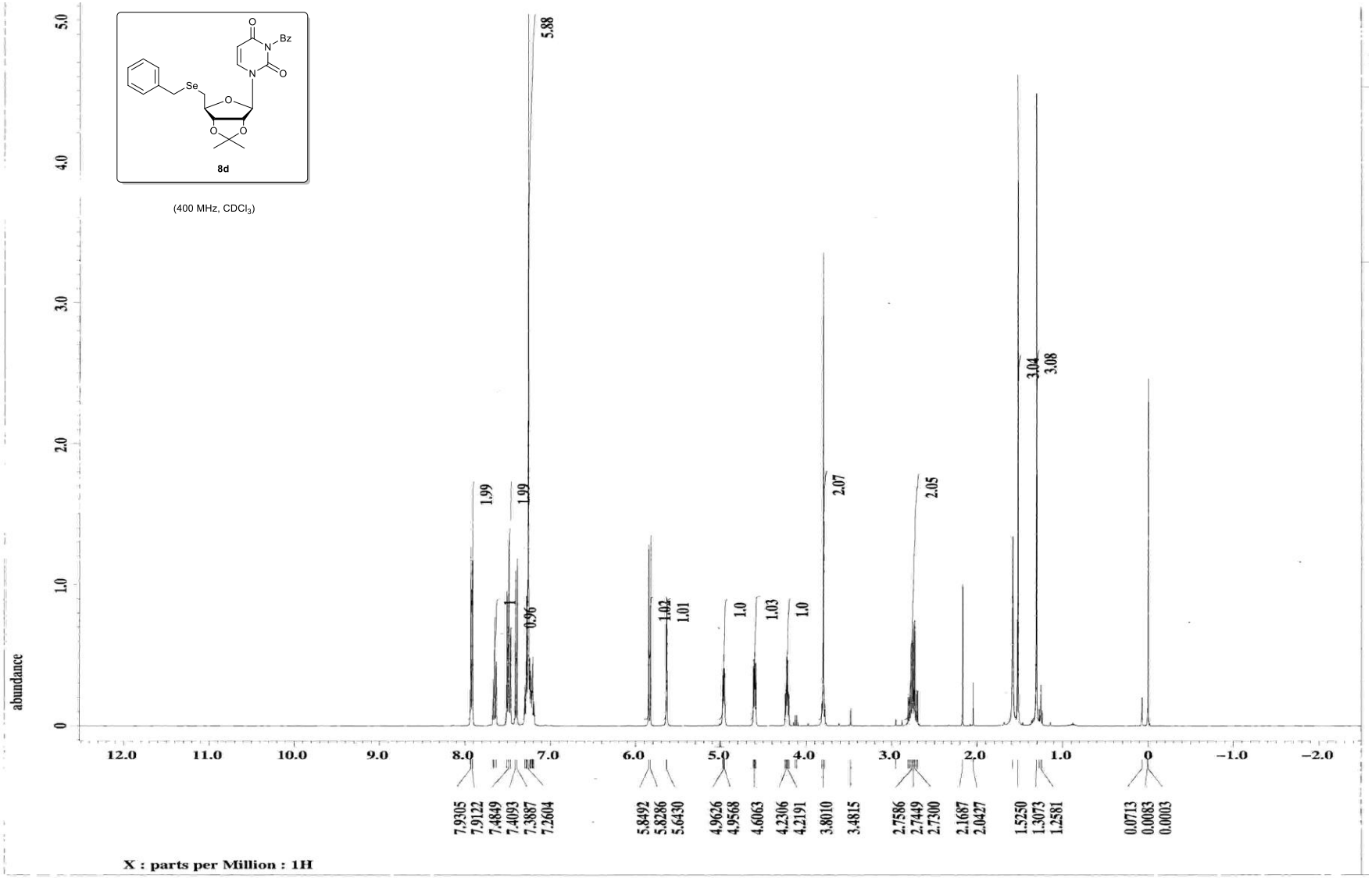
8d
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
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7.4093
7.3887
7.2604
5.8492
5.8286
5.6430
4.9626
4.9568
4.6063
4.2306
4.2191
3.8010
3.4815
2.7586
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1.3073
1.2581
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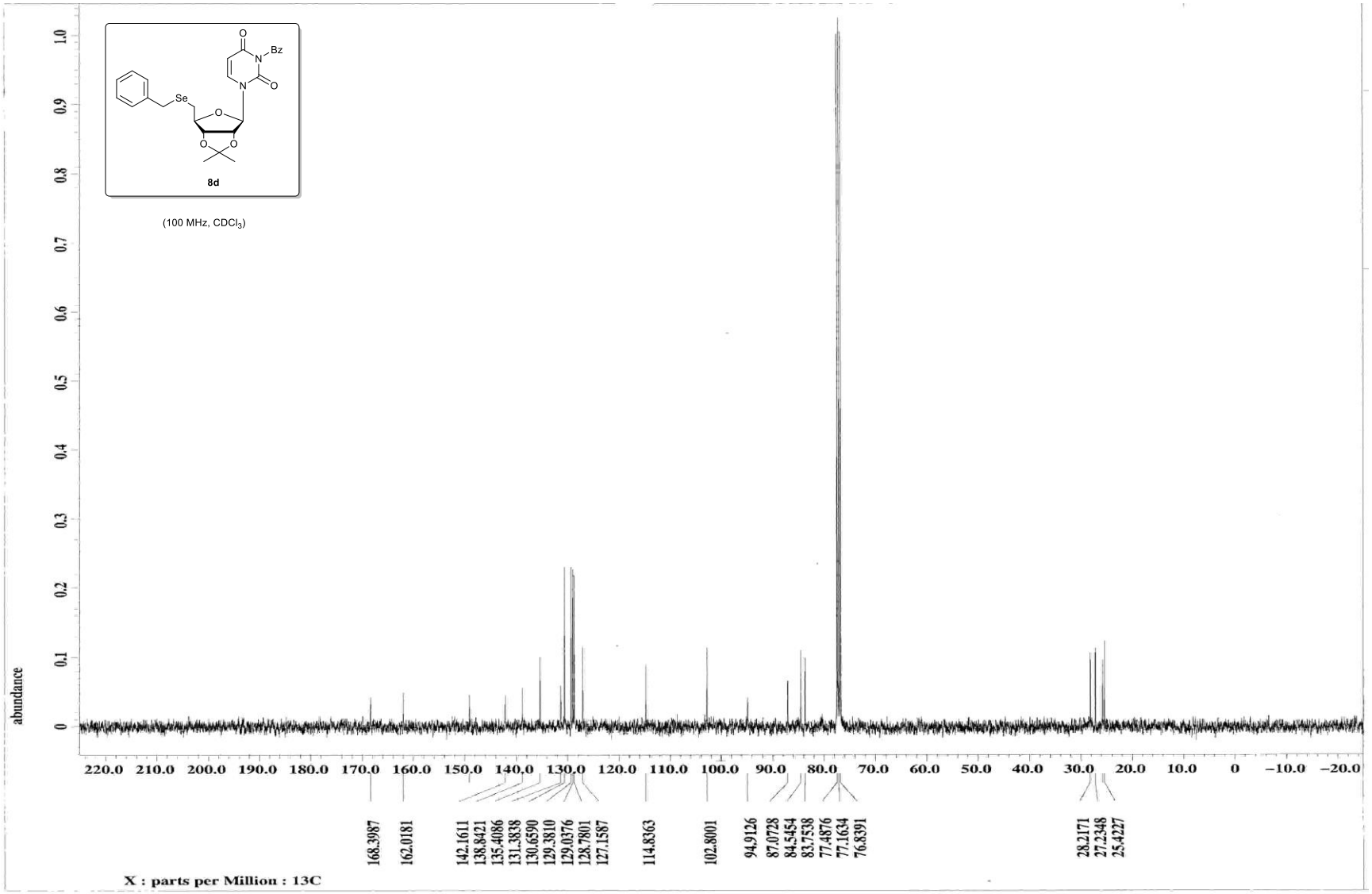
0.0083
0.0003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abundance
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131.3838
130.6590
129.3810
129.0376
128.7801
127.1587
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102.8001
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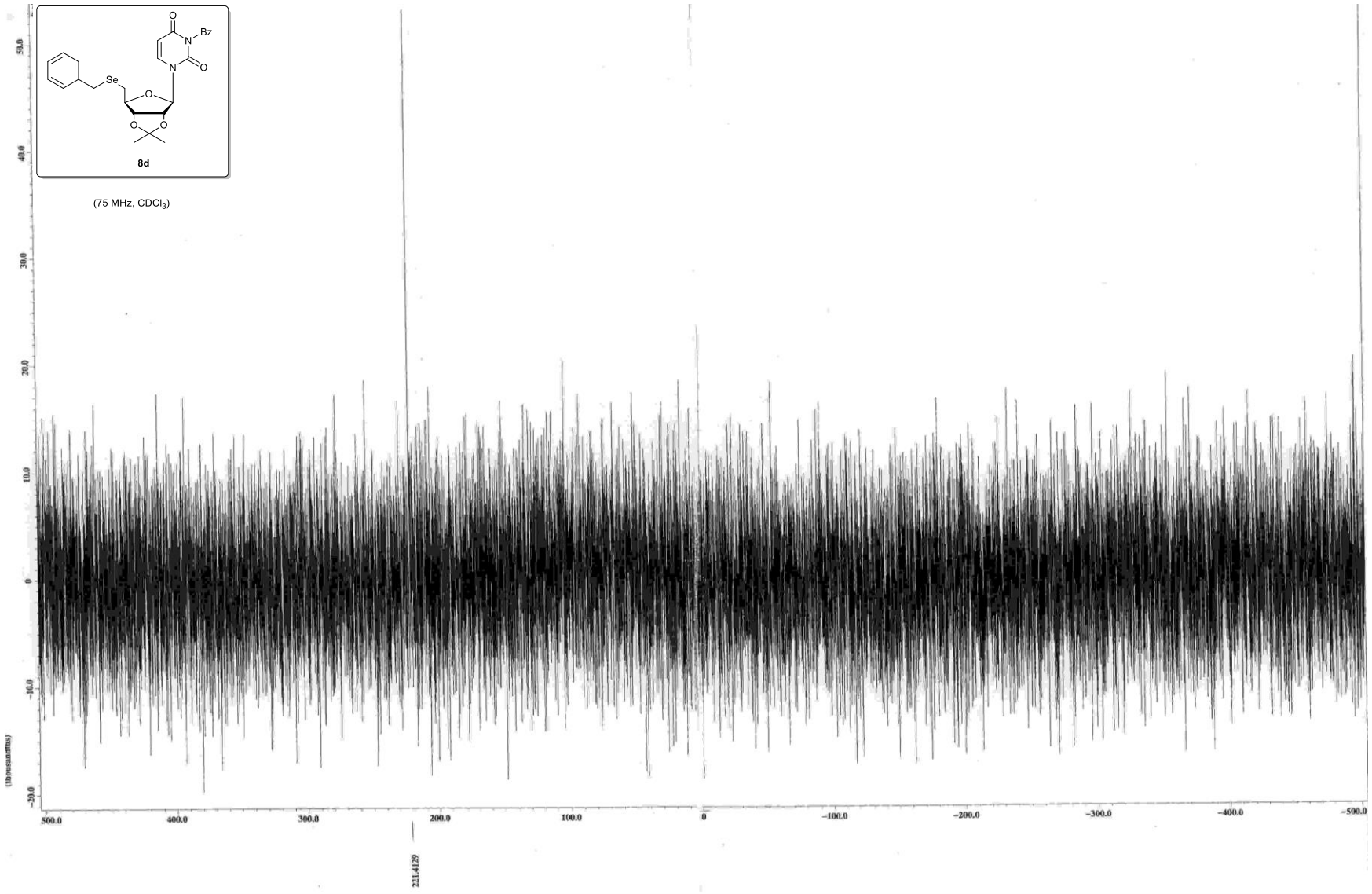
8d
(75 MHz, CDCl3)
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
(thousandths)
500.0
400.0
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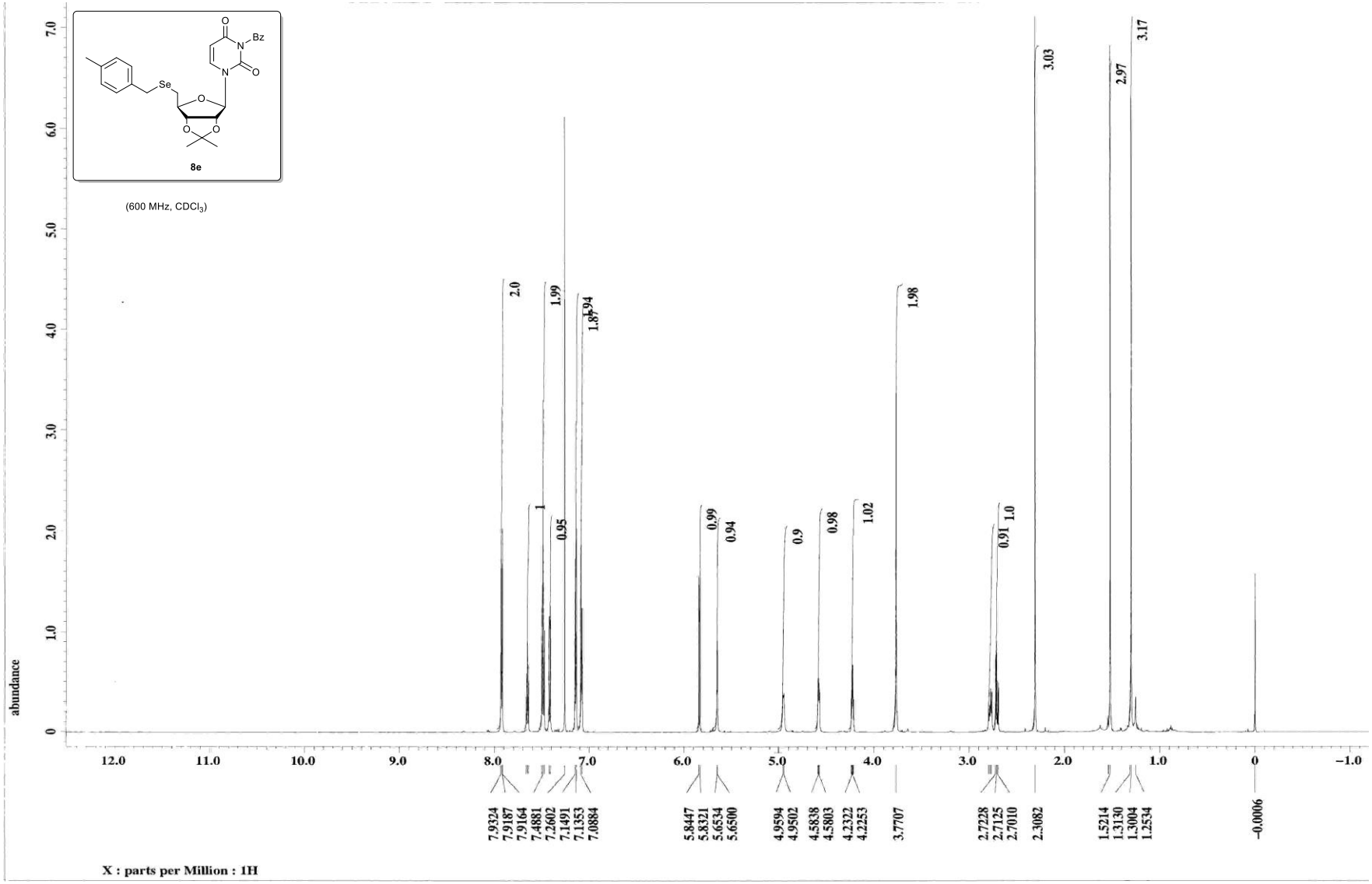
8e
(600 MHz, CDCl3)
abundance
X : parts per Million : 1H
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1
1.99
0.95
1.94
1.87
0.99
0.94
0.9
0.98
1.02
1.98
0.91
1.0
3.03
2.97
3.17
7.9324
7.9187
7.9164
7.4881
7.2602
7.1491
7.1353
7.0884
5.8447
5.8321
5.6534
5.6500
4.9594
4.9502
4.5838
4.5803
4.2322
4.2253
3.7707
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2.7125
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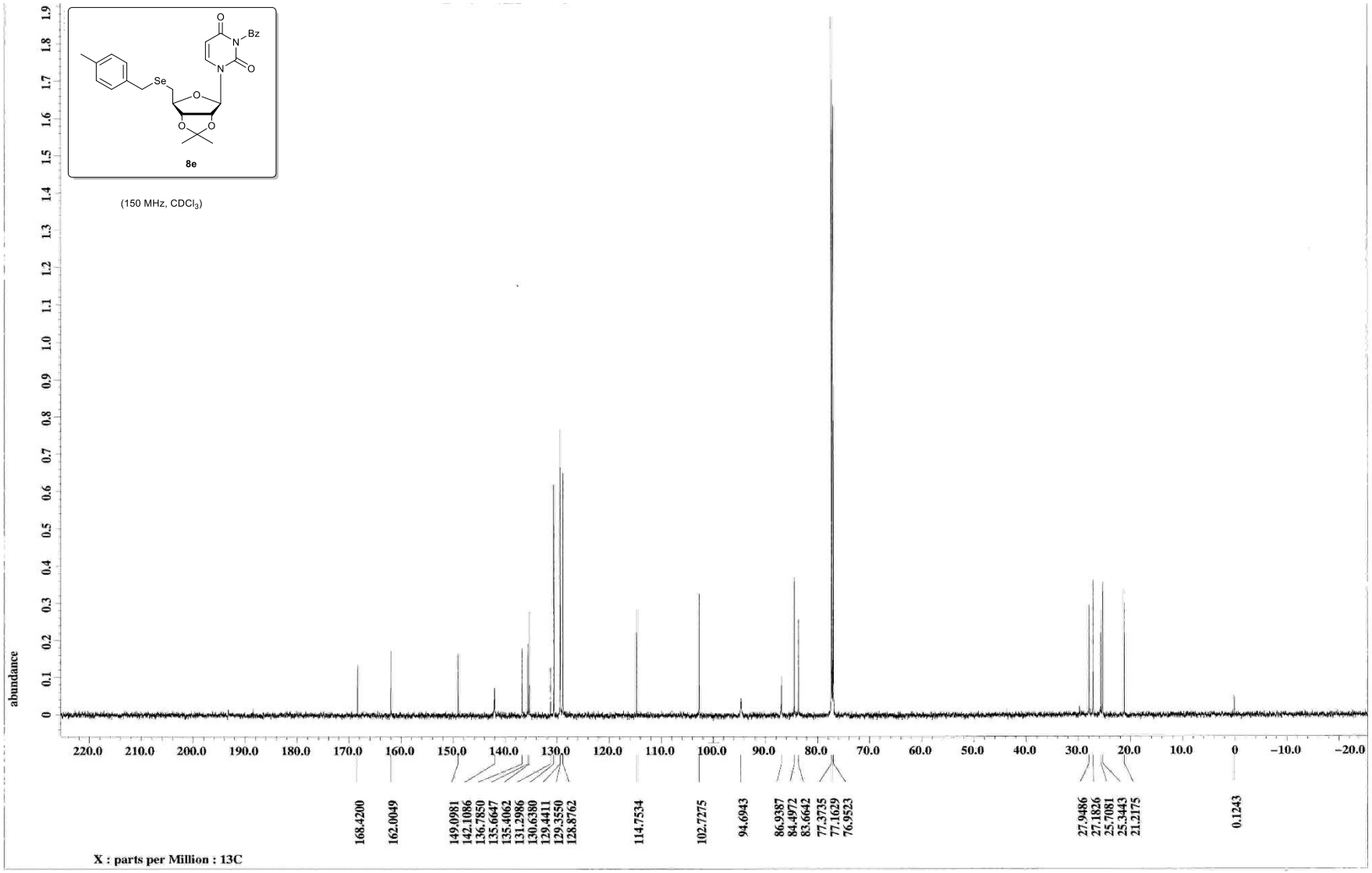
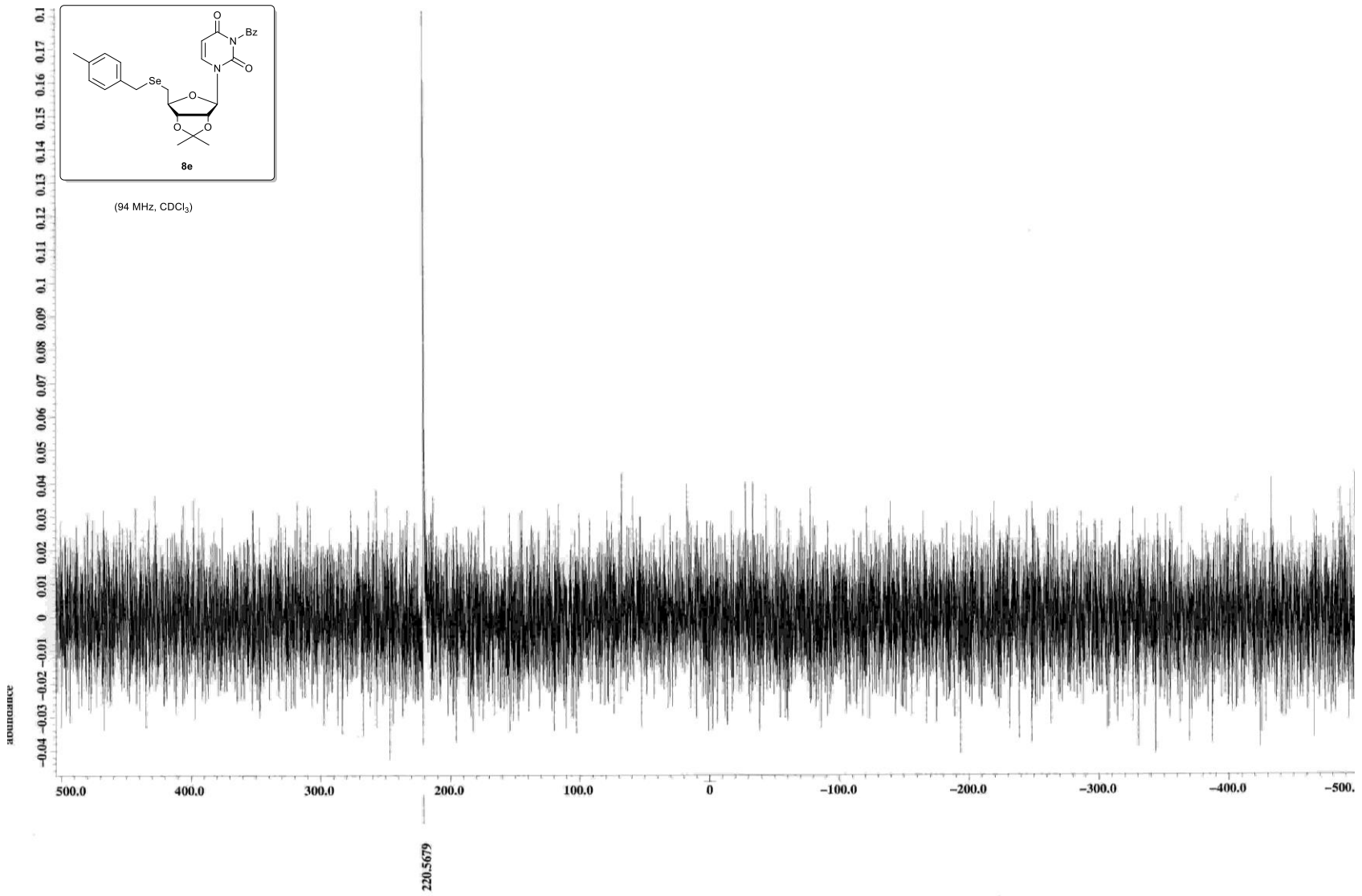
1.3130
1.3004
1.2534
-0.0006


8e
(150 MHz, CDCl3)
abundance
X : parts per Million : 13C
168.4200
162.0049
149.0981
142.1086
136.7850
135.6647
135.4062
131.2986
130.6380
129.4411
129.3550
128.8762
114.7534
102.7275
94.6943
86.9387
84.4972
83.6642
77.3735
77.1629
76.9523
27.9486
27.1826
25.7081
25.3443
21.2175
0.1243


8e
(94 MHz, CDCl3)
abundance
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300.0
200.0
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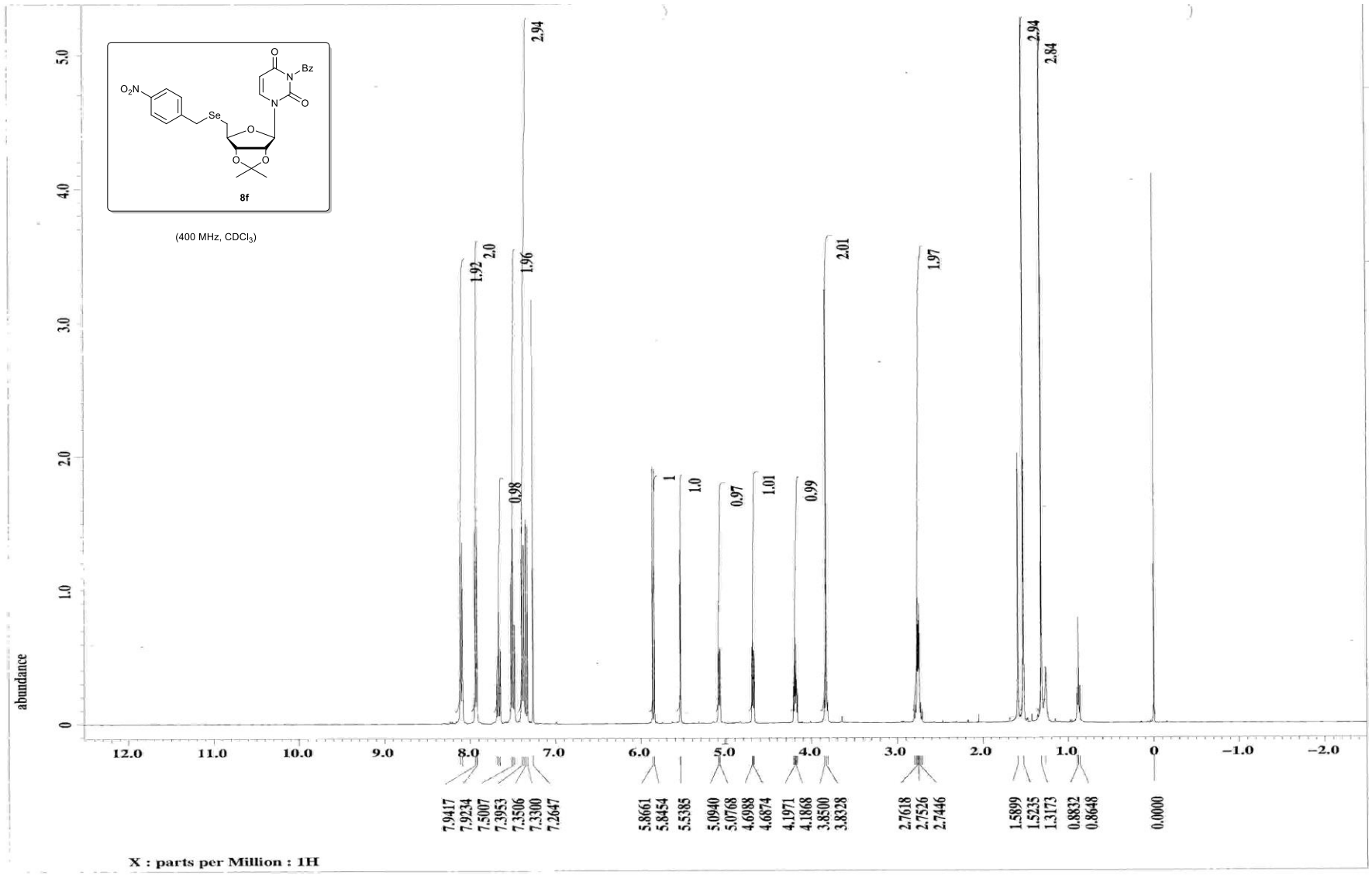
0
−100.0
−200.0
−300.0
−400.0
−500.


8f
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
7.9417
7.9234
7.5007
7.3953
7.3506
7.3300
7.2647
5.8661
5.8454
5.5385
5.0940
5.0768
4.6988
4.6874
4.1971
4.1868
3.8500
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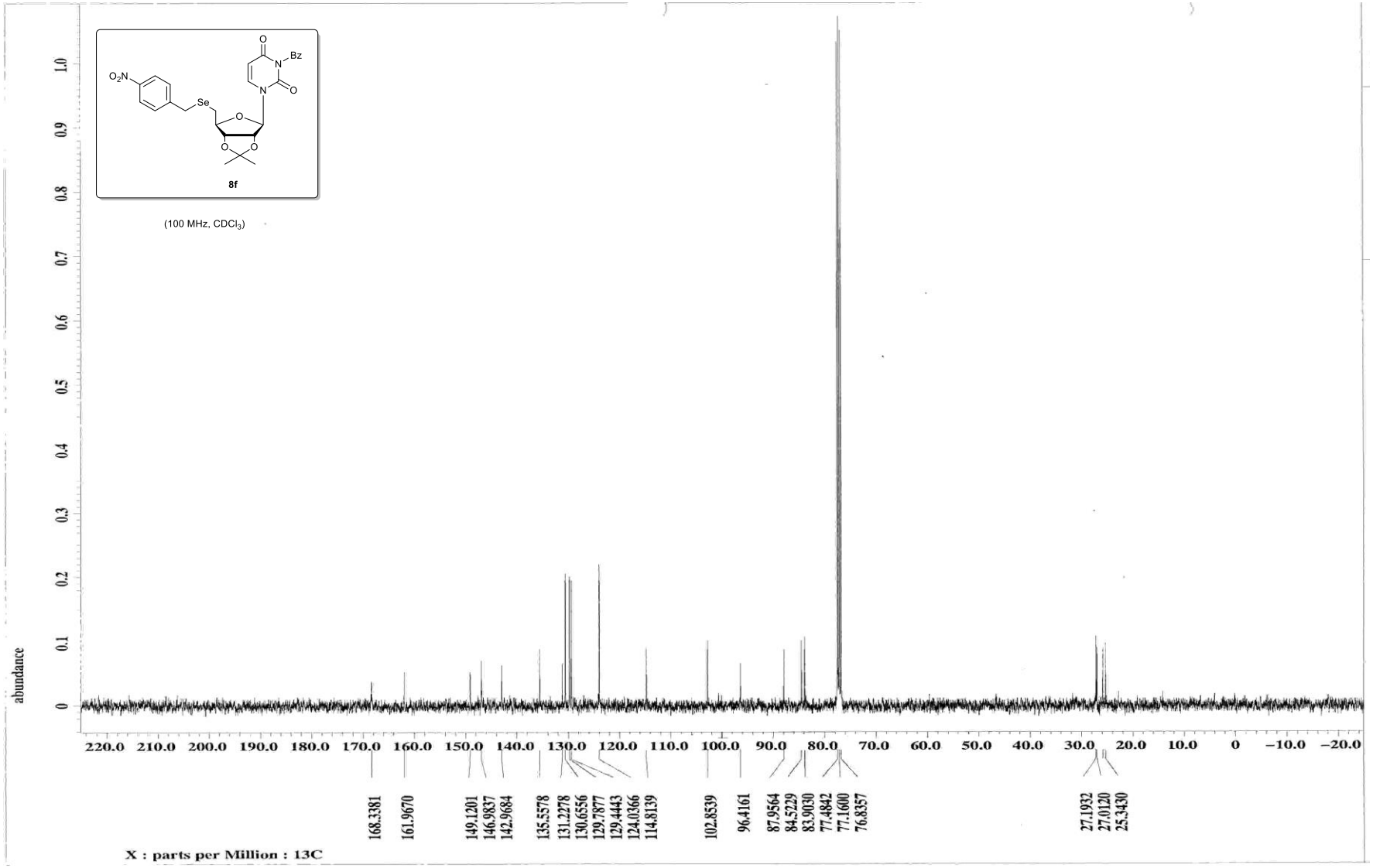
8f
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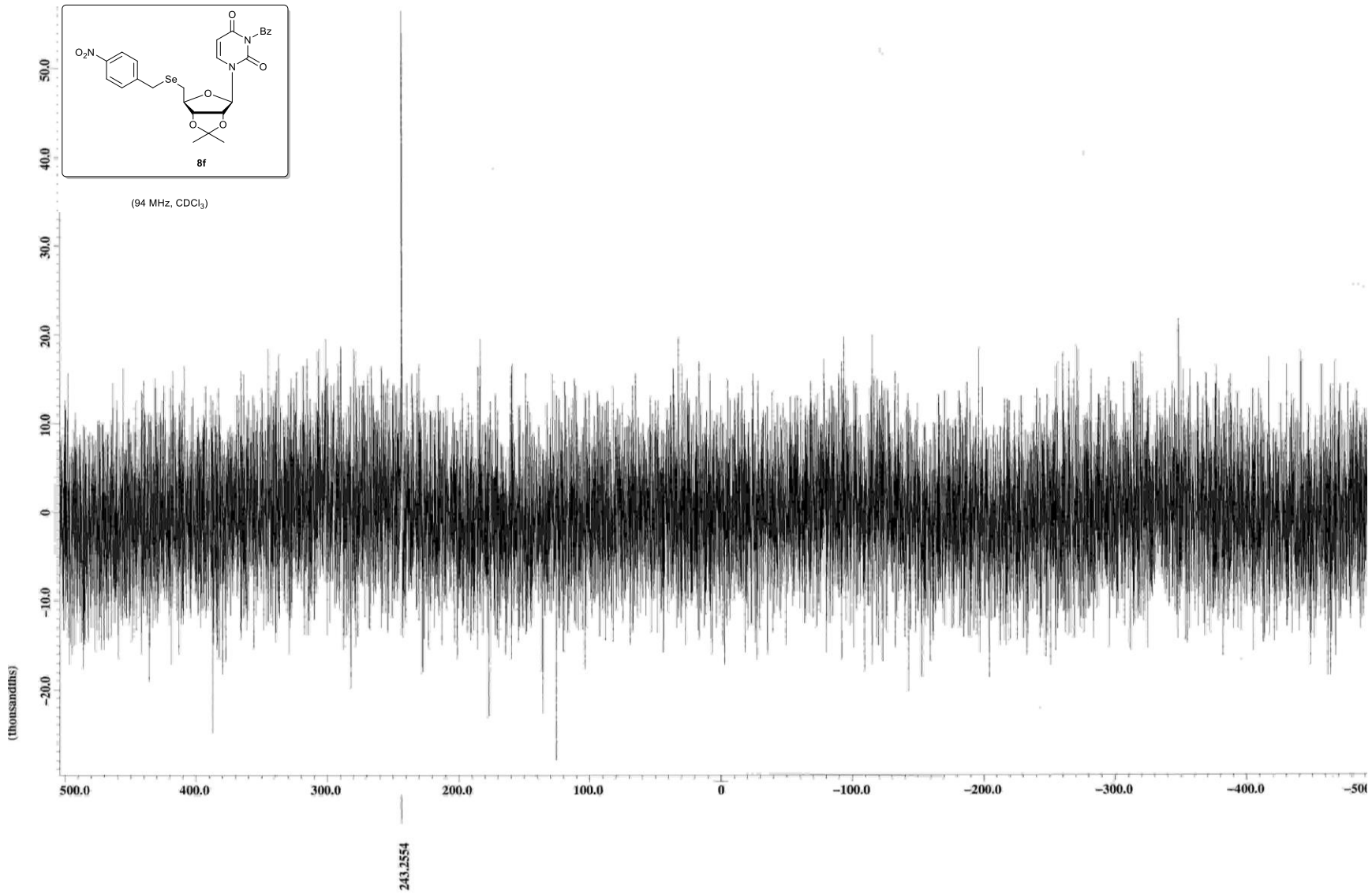
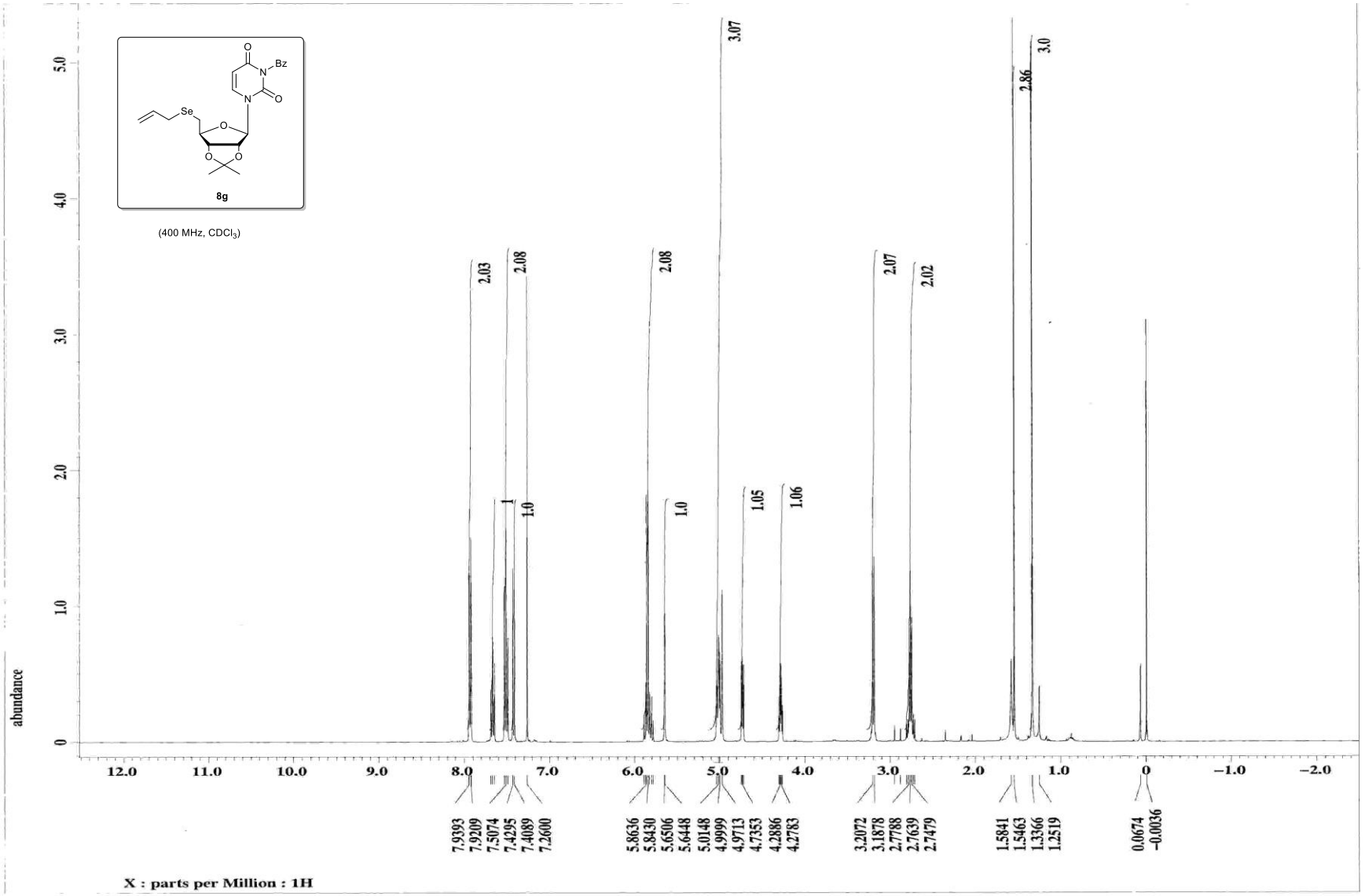
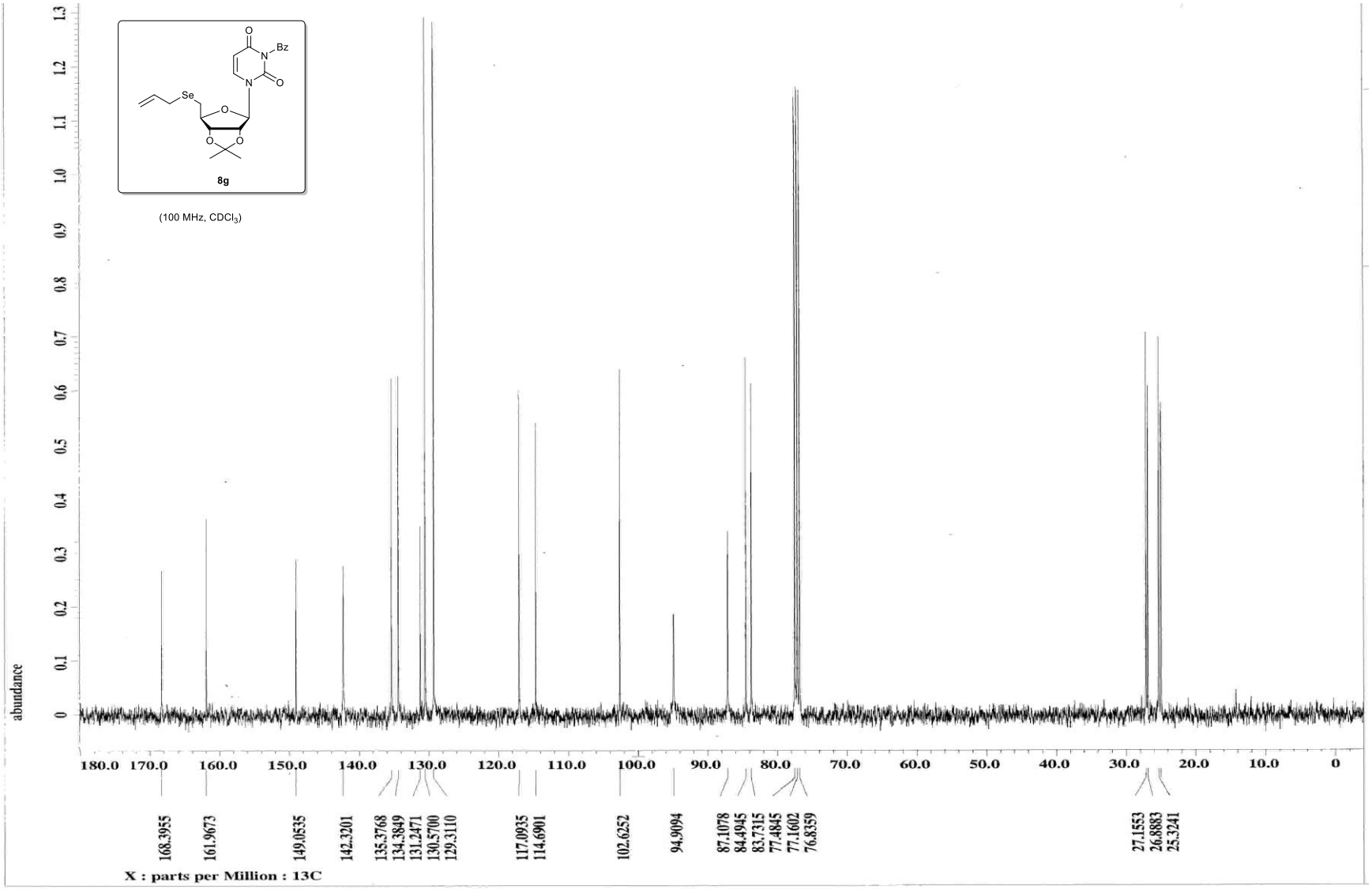
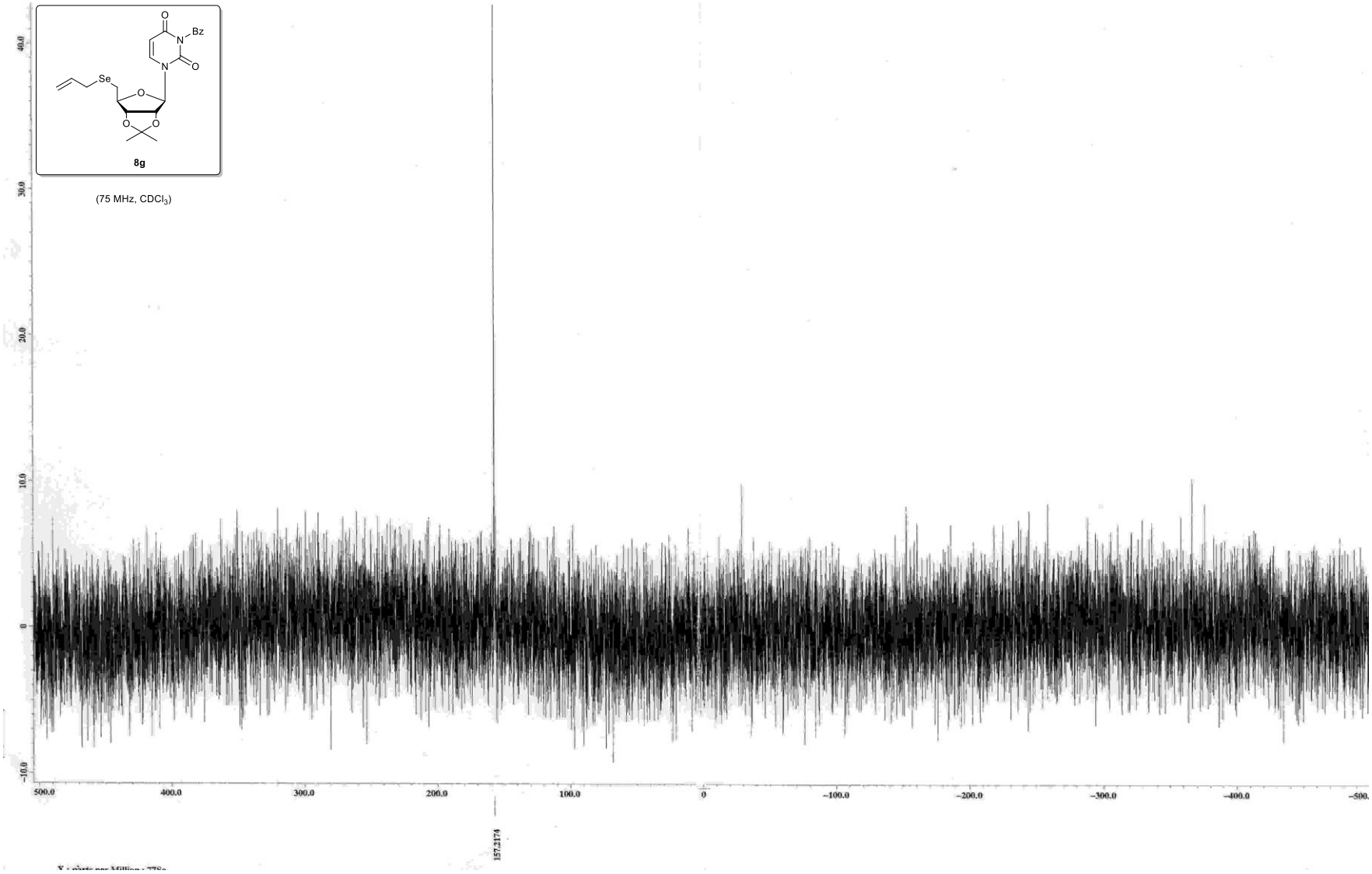
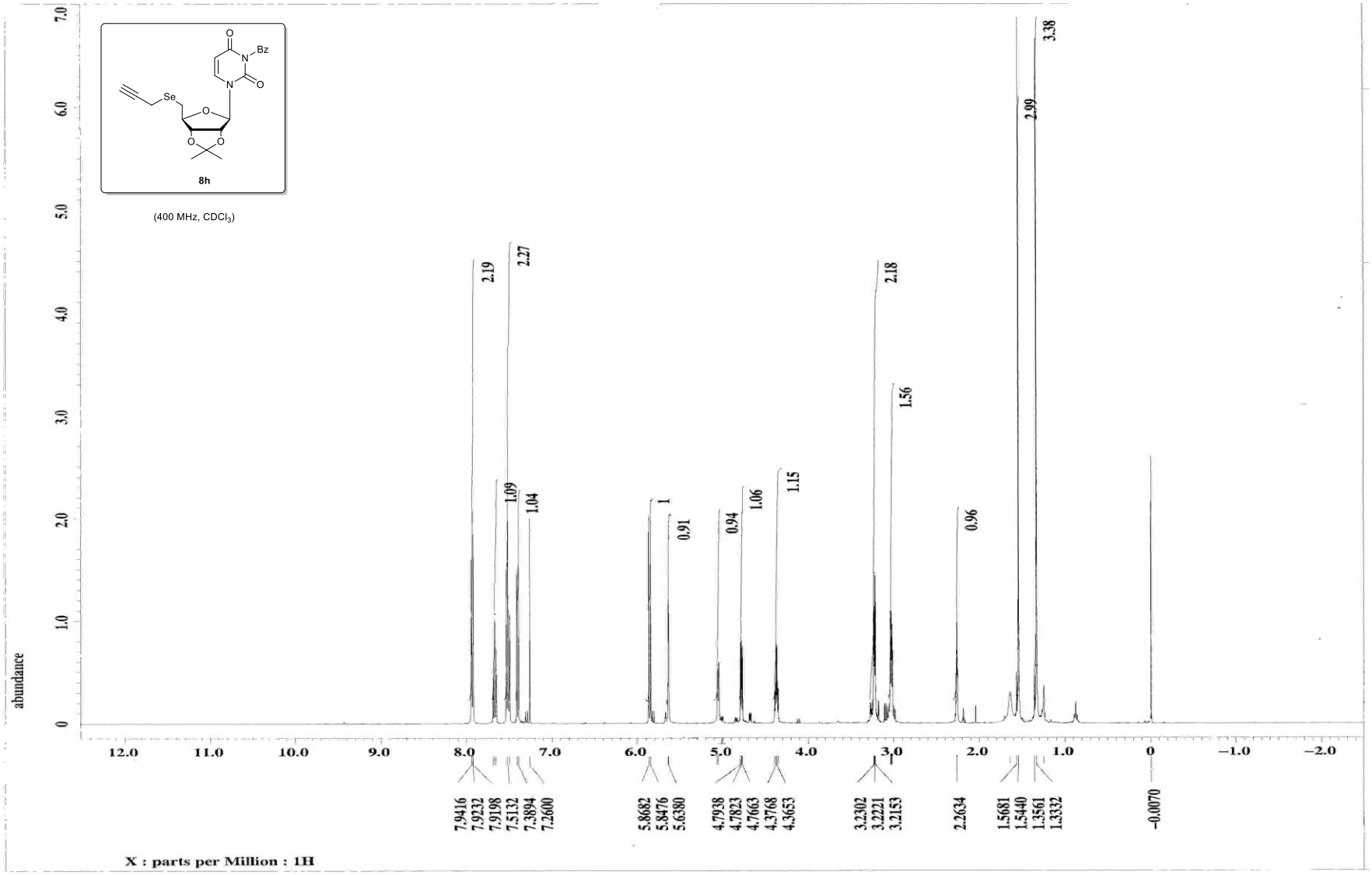
abundance
168.3381
161.9670
149.1201
146.9837
142.9684
135.5578
131.2278
130.6556
129.7877
129.4443
124.0366
114.8139
102.8539
96.4161
87.9564
84.5229
83.9030
77.4842
77.1600
76.8357
27.1932
27.0120
25.3430
X : parts per Million : 13C

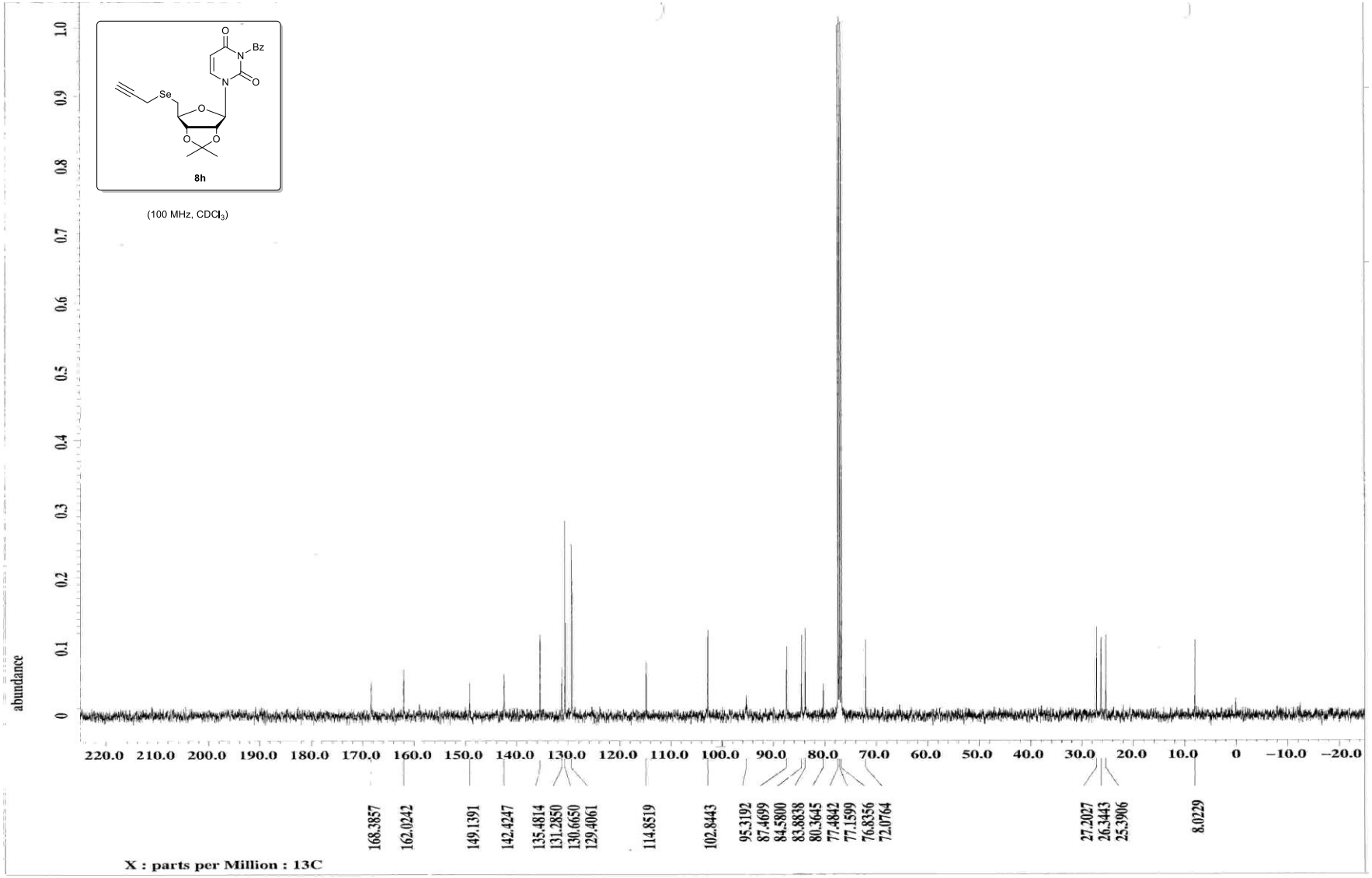

8f
(94 MHz, CDCl3)
(thousandths)
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
500.0
400.0
300.0
200.0
100.0
0
-100.0
-200.0
-300.0
-400.0
243.2554

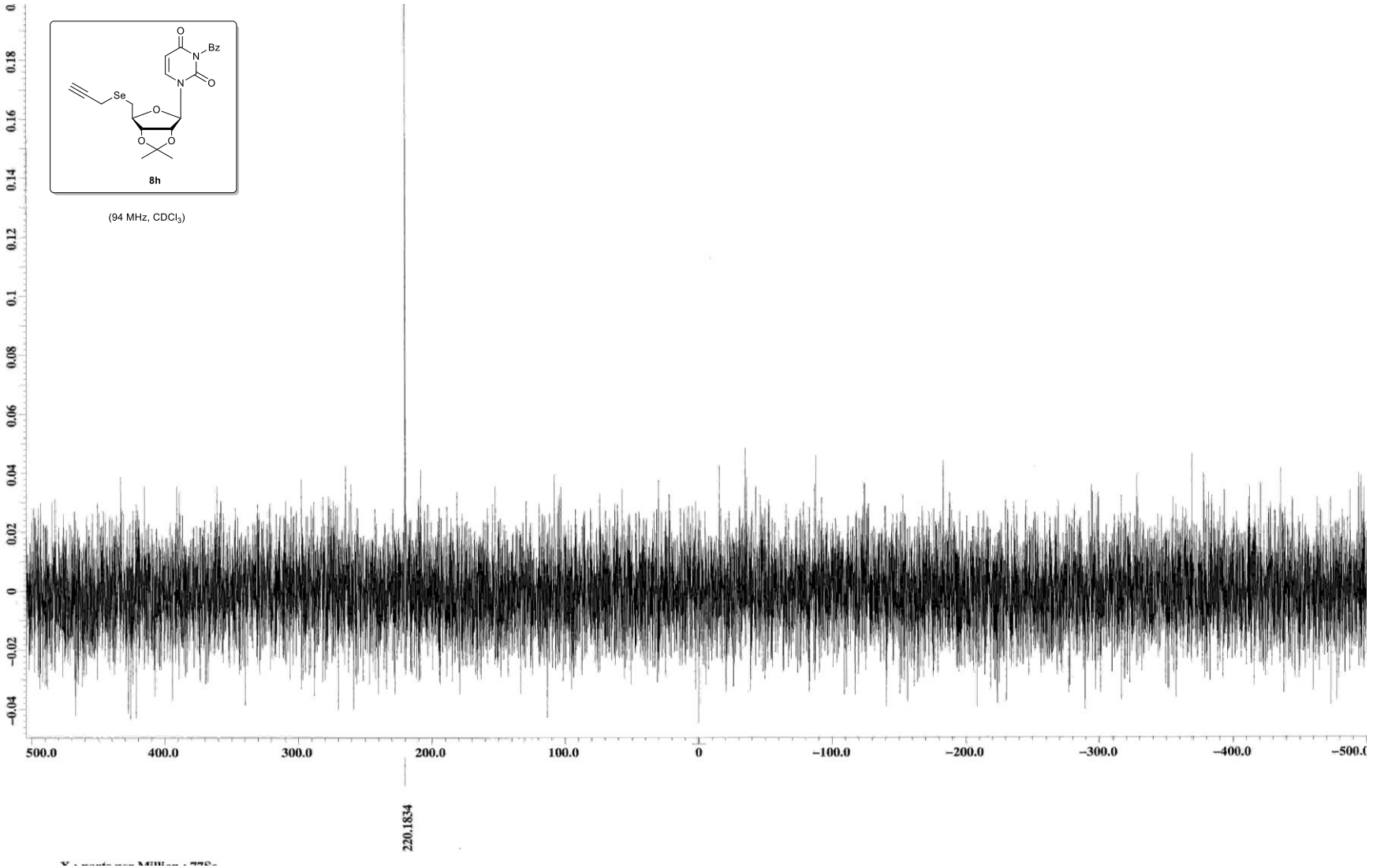

8g
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
2.03
2.08
1
1.0
2.08
1.0
3.07
1.05
1.06
2.07
2.02
2.86
3.0
7.9393
7.9209
7.5074
7.4295
7.4089
7.2600
5.8636
5.8430
5.6506
5.6448
5.0148
4.9999
4.9713
4.7353
4.2886
4.2783
3.2072
3.1878
2.7788
2.7639
2.7479
1.5841
1.5463
1.3366
1.2519
0.0674
−0.0036

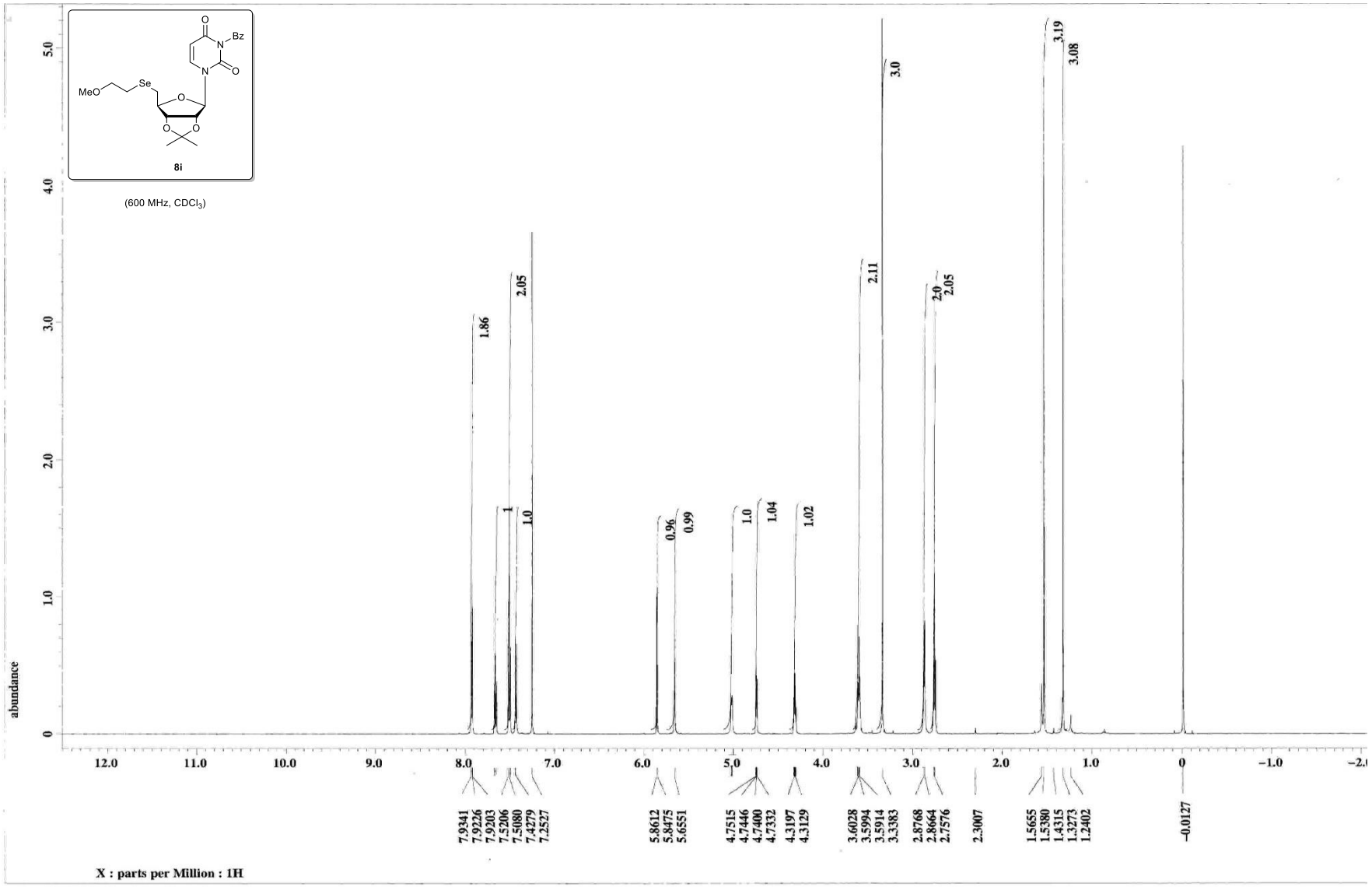

8g
(100 MHz, CDCl3)
abundance
180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
168.3955
161.9673
149.0535
142.3201
135.3768
134.3849
131.2471
130.5700
129.3110
117.0935
114.6901
102.6252
94.9094
87.1078
84.4945
83.7315
77.4845
77.1602
76.8359
27.1553
26.8883
25.3241
X : parts per Million : 13C

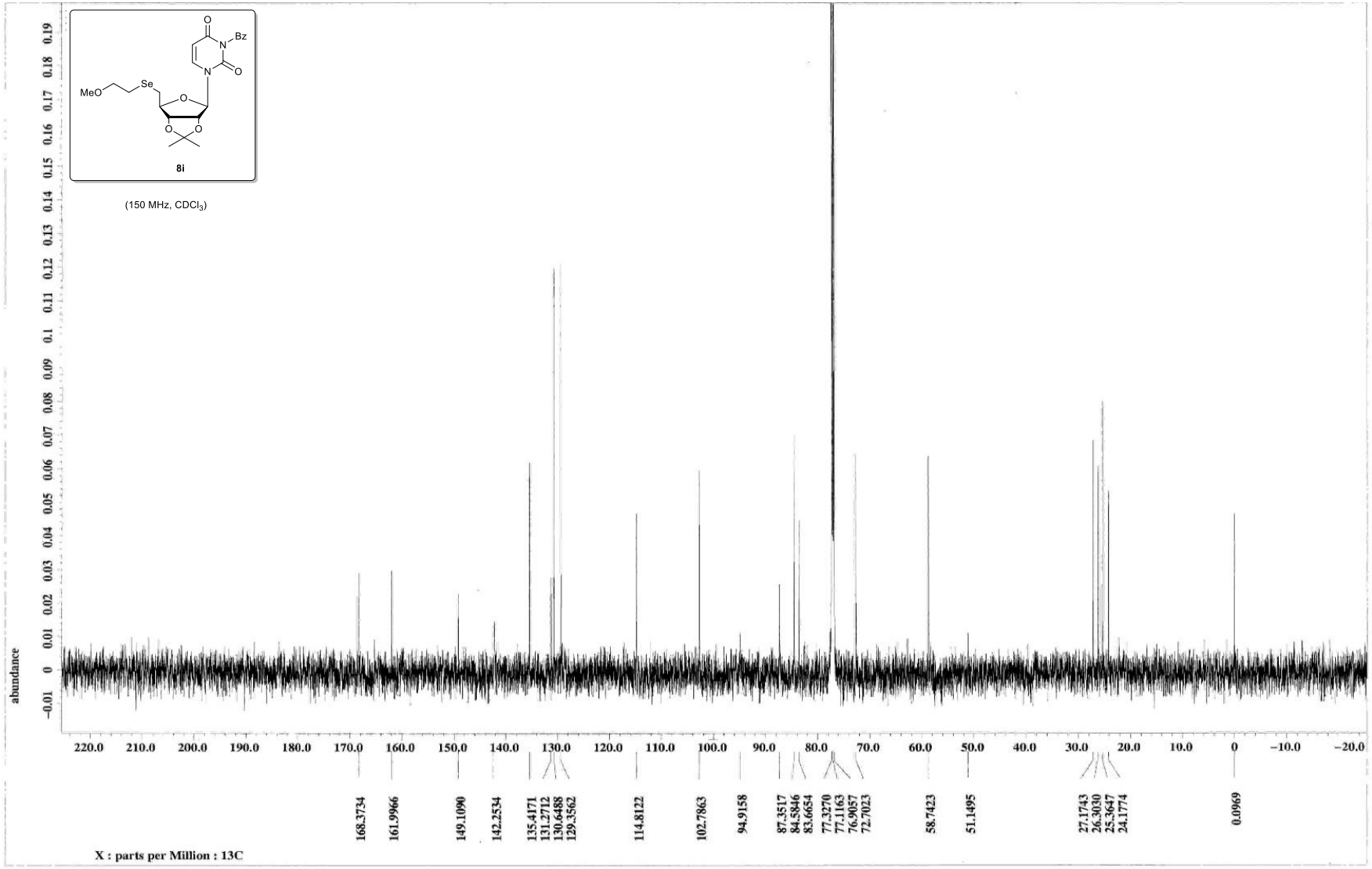

Bz
Se
8g
(75 MHz, CDCl3)
40.0
30.0
20.0
10.0
0
-10.0
500.0
400.0
300.0
200.0
100.0
0
-100.0
-200.0
-300.0
-400.0
157.2174

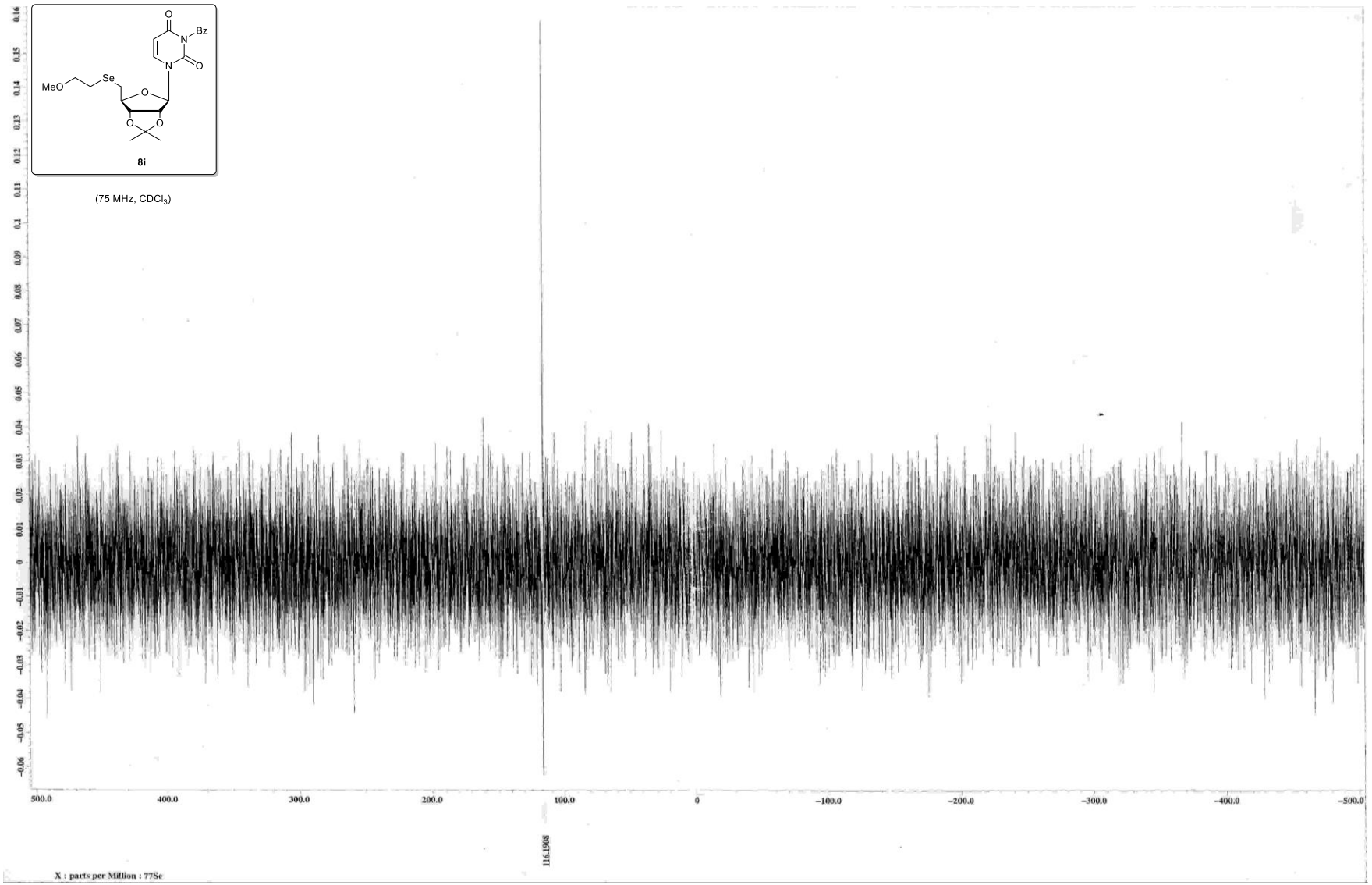

8h
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
2.19
2.27
1.09
1.04
1
0.91
0.94
1.06
1.15
2.18
1.56
0.96
2.99
3.38
7.9416
7.9232
7.9198
7.5132
7.3894
7.2600
5.8682
5.8476
5.6380
4.7938
4.7823
4.7663
4.3768
4.3653
3.2302
3.2221
3.2153
2.2634
1.5681
1.5440
1.3561
1.3332
-0.0070

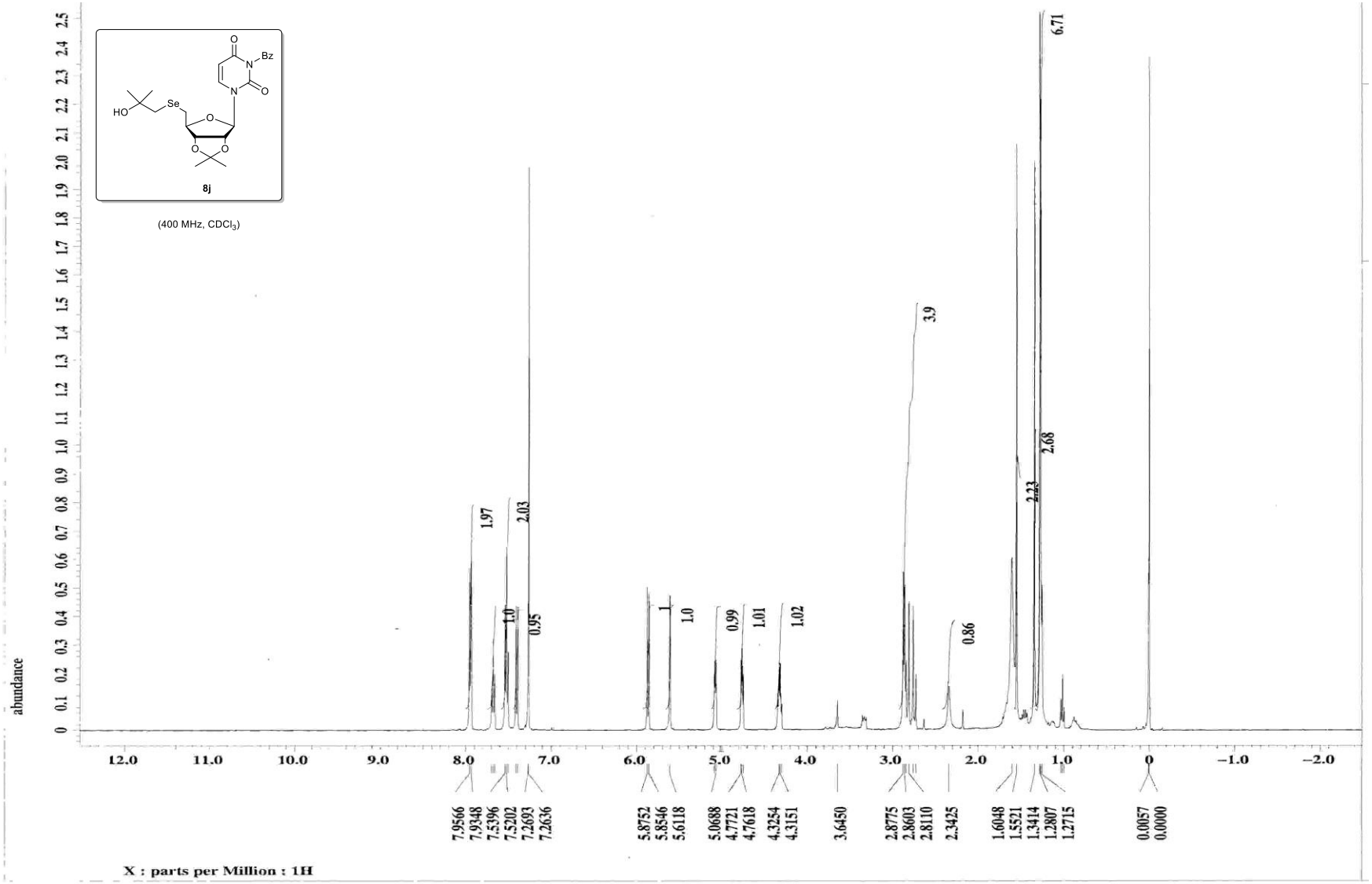

8h
(100 MHz, CDCl3)
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0 −20.0
168.3857
162.0242
149.1391
142.4247
135.4814
131.2850
130.6650
129.4061
114.8519
102.8443
95.3192
87.4699
84.5800
83.8838
80.3645
77.4842
77.1599
76.8356
72.0764
27.2027
26.3443
25.3906
8.0229
X : parts per Million : 13C

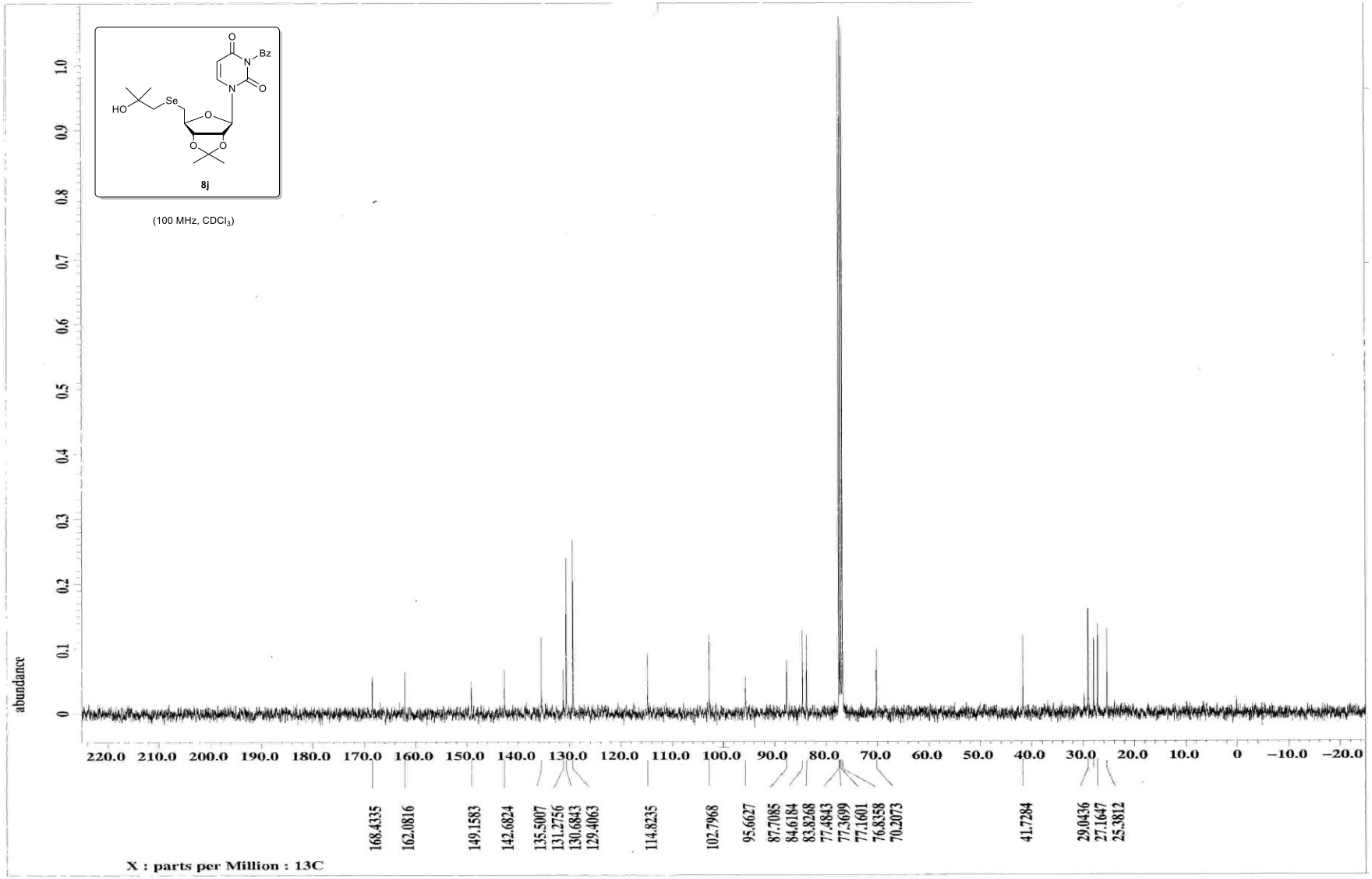

Bz
Se
8h
(94 MHz, CDCl3)
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
−0.02
−0.04
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
220.1834

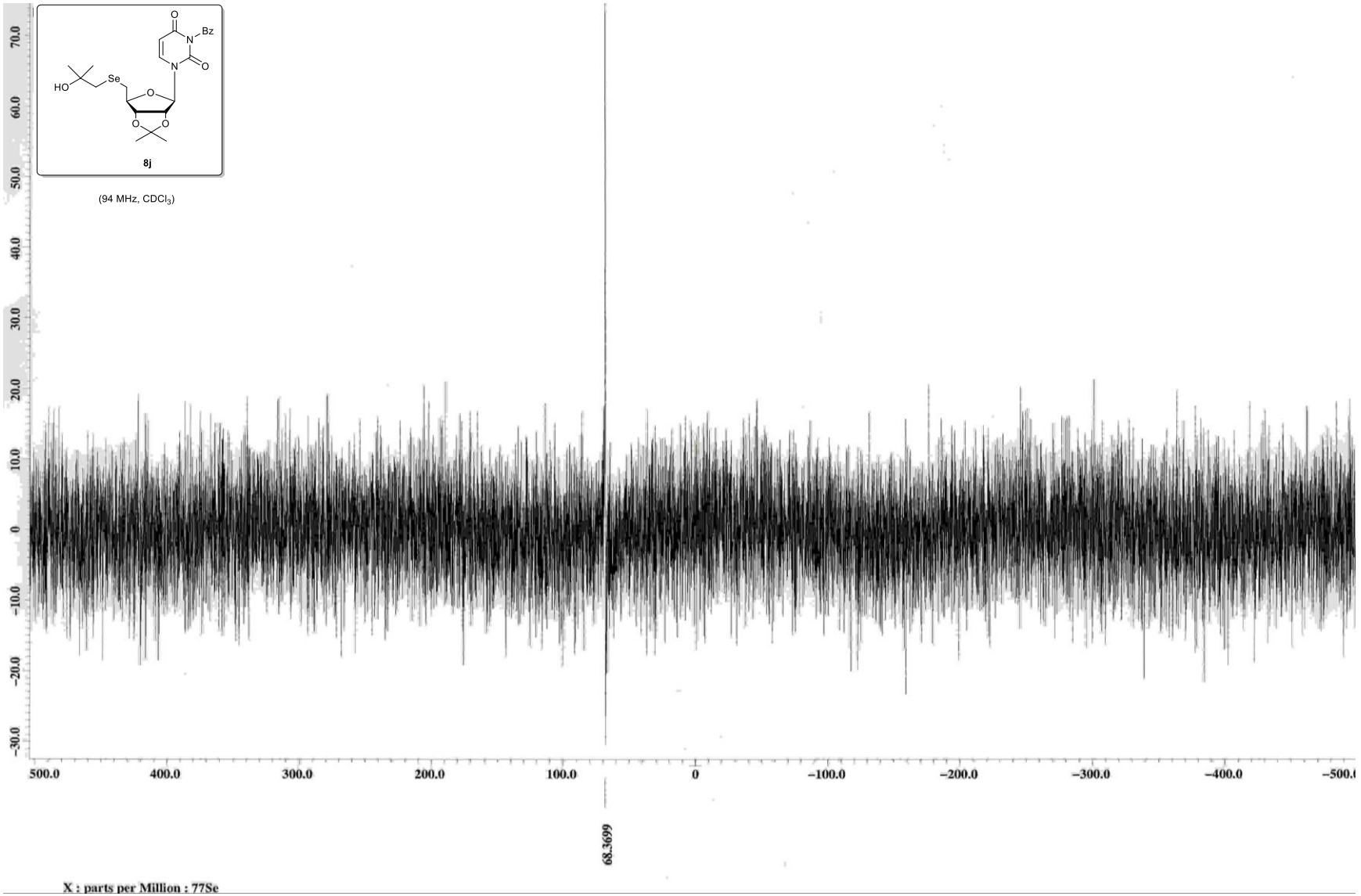

8i
(600 MHz, CDCl3)
abundance
X : parts per Million : 1H
7.9341
7.9226
7.9203
7.5206
7.5080
7.4279
7.2527
5.8612
5.8475
5.6551
4.7515
4.7446
4.7400
4.7332
4.3197
4.3129
3.6028
3.5994
3.5914
3.3383
2.8768
2.8664
2.7576
2.3007
1.5655
1.5380
1.4315
1.3273
1.2402
-0.0127

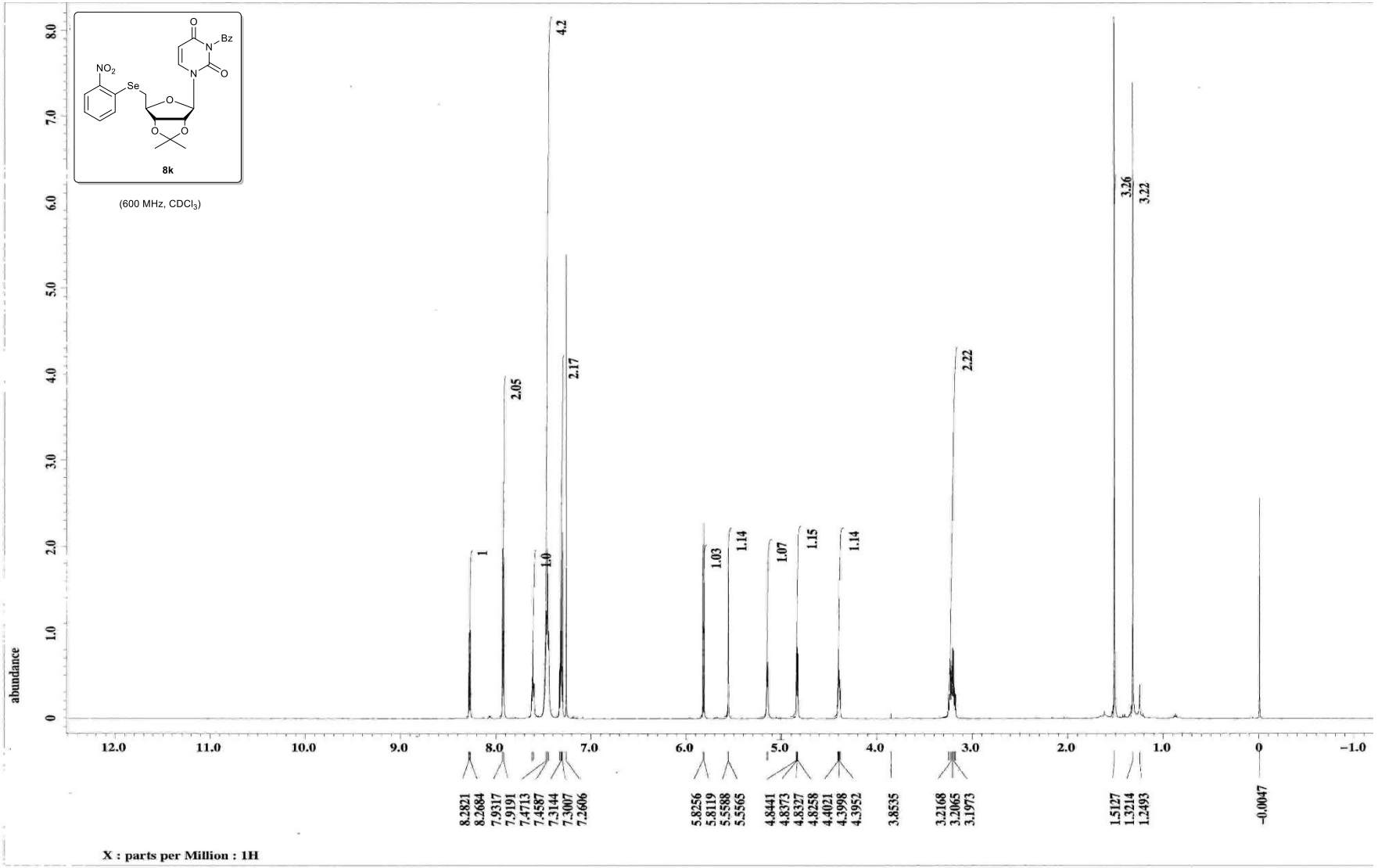

8i
(150 MHz, CDCl3)
abundance
X : parts per Million : 13C
168.3734
161.9966
149.1090
142.2534
135.4171
131.2712
130.6488
129.3562
114.8122
102.7863
94.9158
87.3517
84.5846
83.6654
77.3270
77.1163
76.9057
72.7023
58.7423
51.1495
27.1743
26.3030
25.3647
24.1774
0.0969

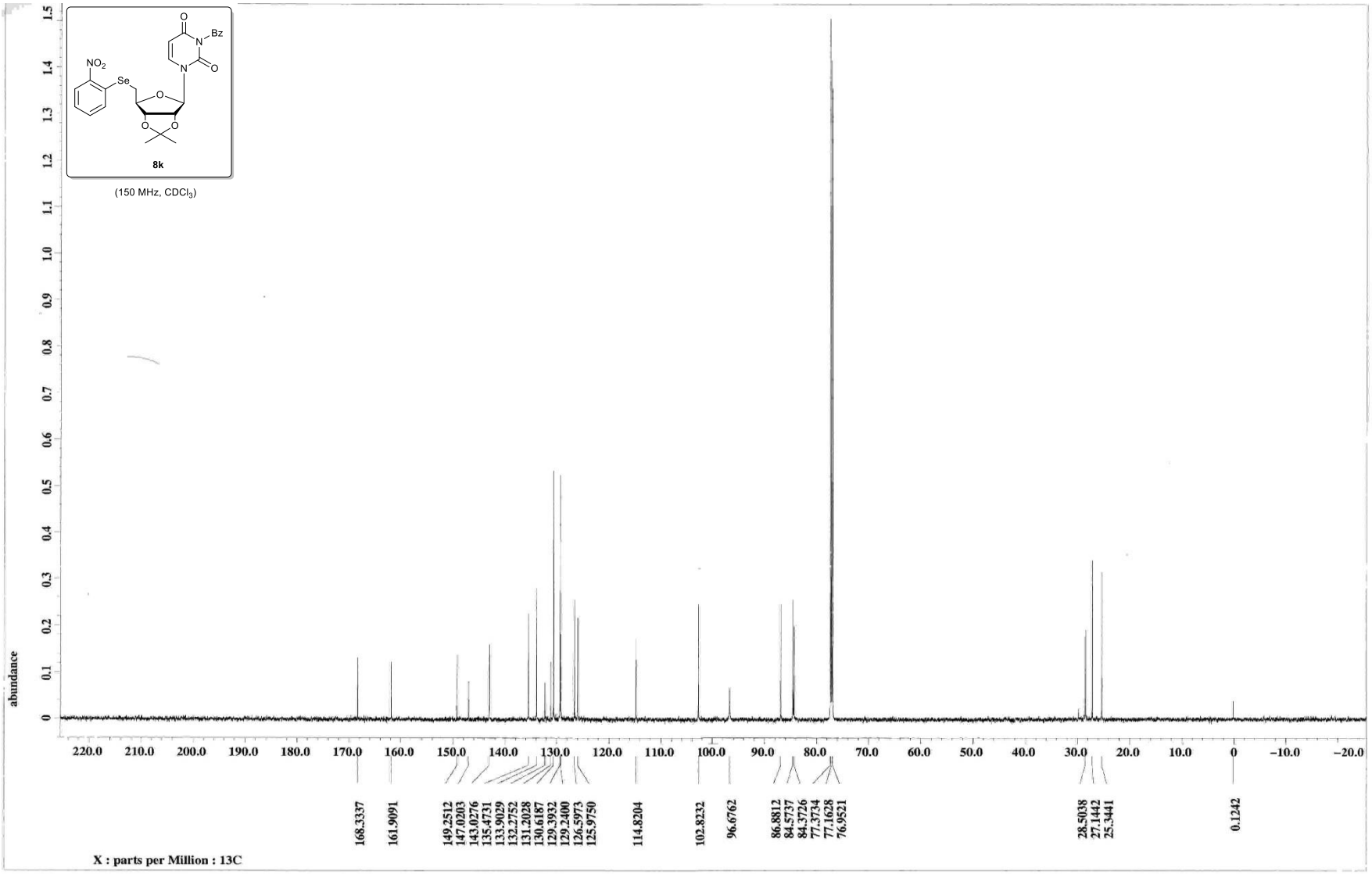

MeO
Se
O
N
Bz
O
O
O
O
8i
(75 MHz, CDCl3)
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
−500.0
116.1968
X : parts per Million : 77Se

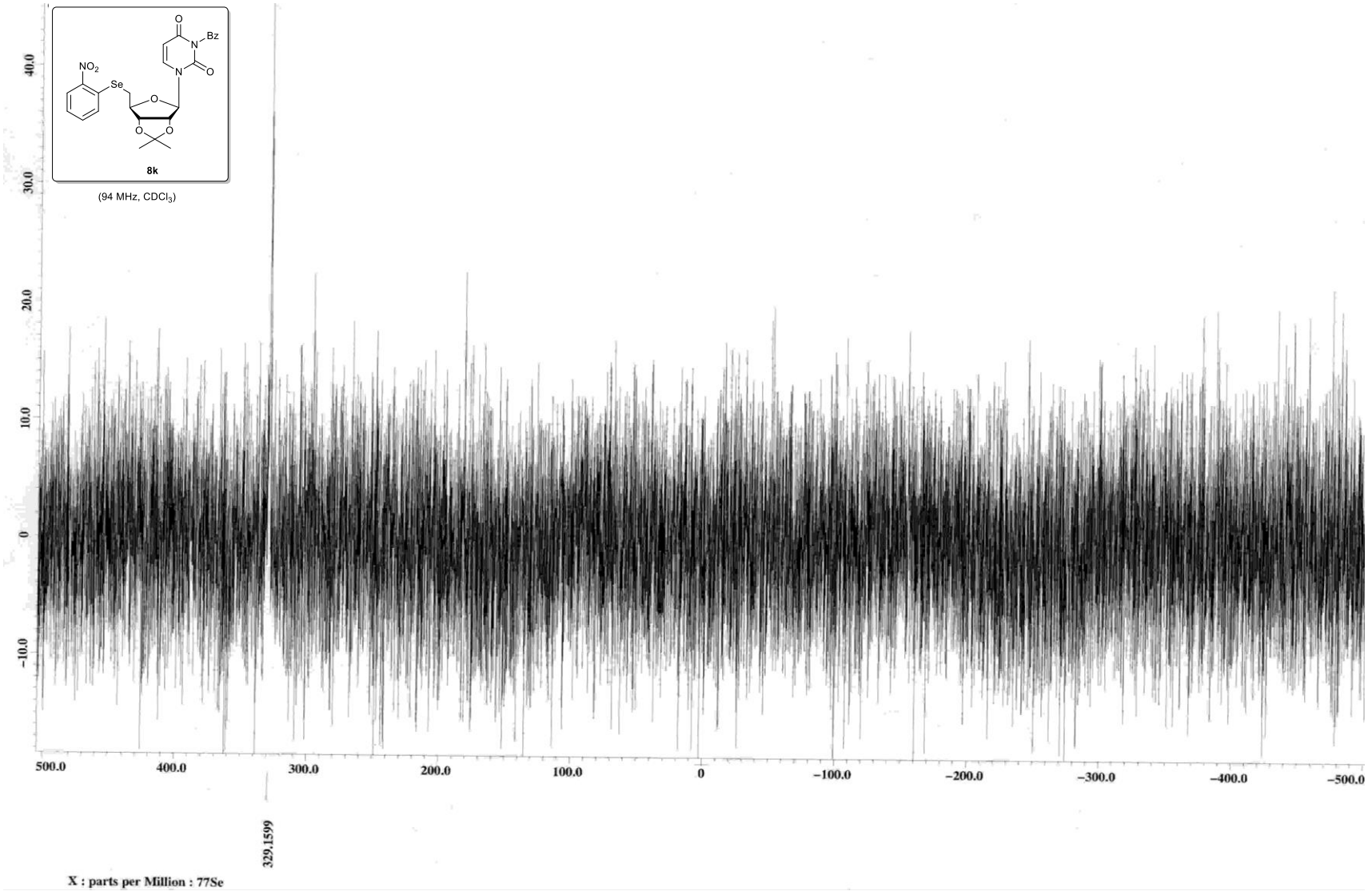

8j
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
1.97
2.03
1.0
0.95
1
1.0
0.99
1.01
1.02
0.86
3.9
2.23
2.68
6.71
7.9566
7.9348
7.5396
7.5202
7.2693
7.2636
5.8752
5.8546
5.6118
5.0688
4.7721
4.7618
4.3254
4.3151
3.6450
2.8775
2.8603
2.8110
2.3425
1.6048
1.5521
1.3414
1.2807
1.2715
0.0057
0.0000

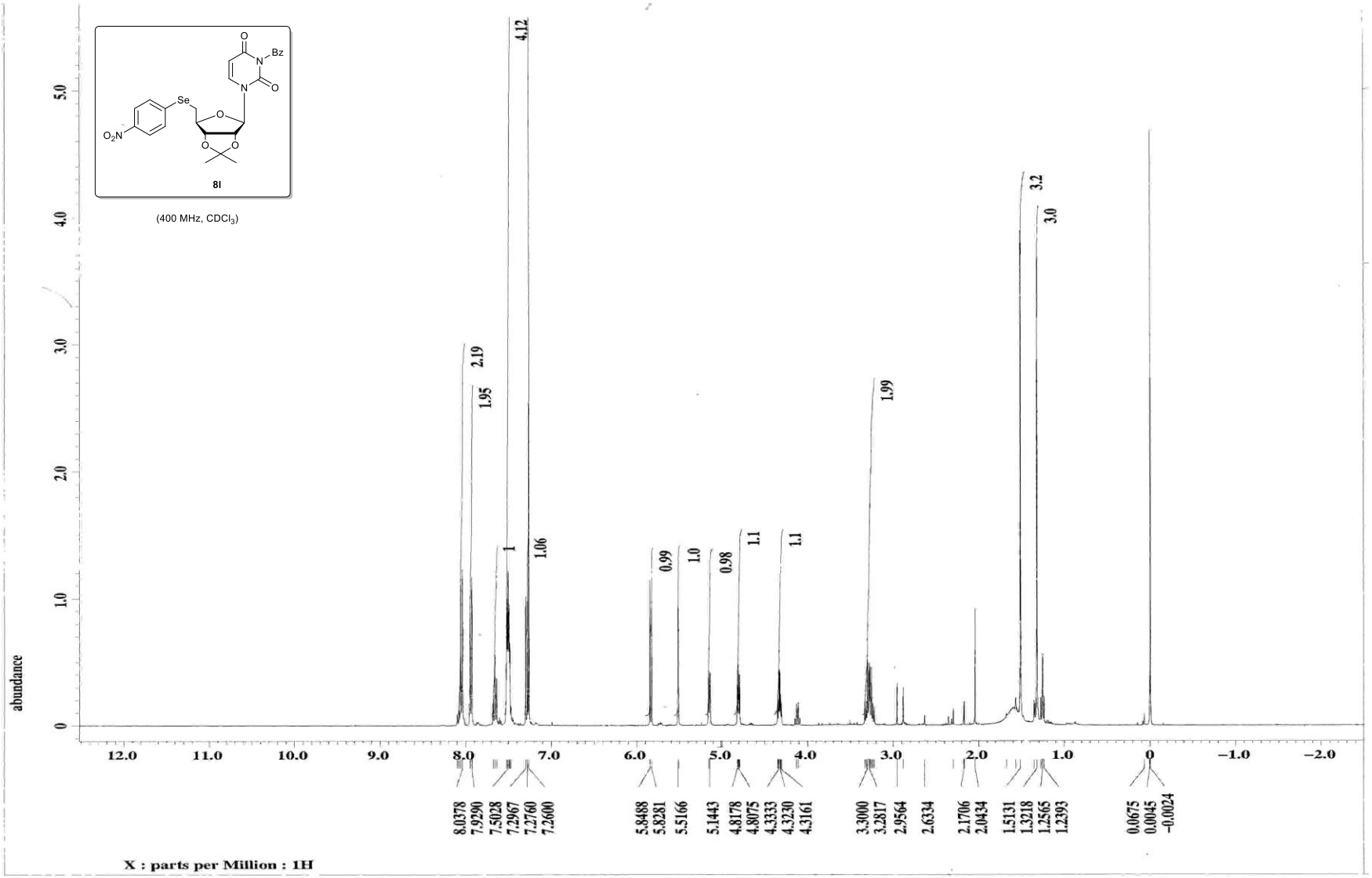

8j
(100 MHz, CDCl3)
abundance
X : parts per Million : 13C
168.4335
162.0816
149.1583
142.6824
135.5007
131.2756
130.6843
129.4063
114.8235
102.7968
95.6627
87.7085
84.6184
83.8268
77.4843
77.3699
77.1601
76.8358
70.2073
41.7284
29.0436
27.1647
25.3812

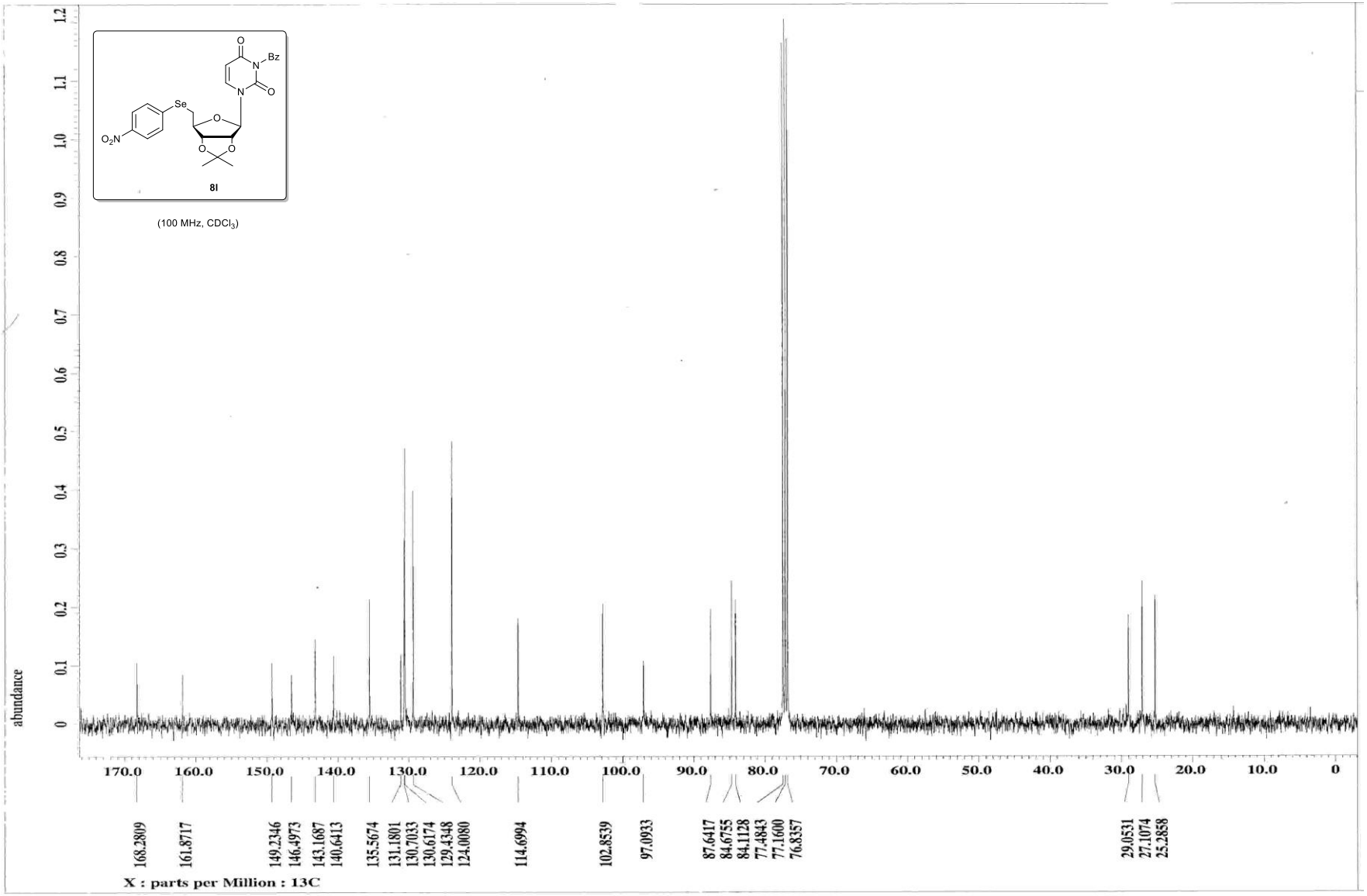

8j
(94 MHz, CDCl3)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
−20.0
−30.0
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
68.3699
X : parts per Million : 77Se

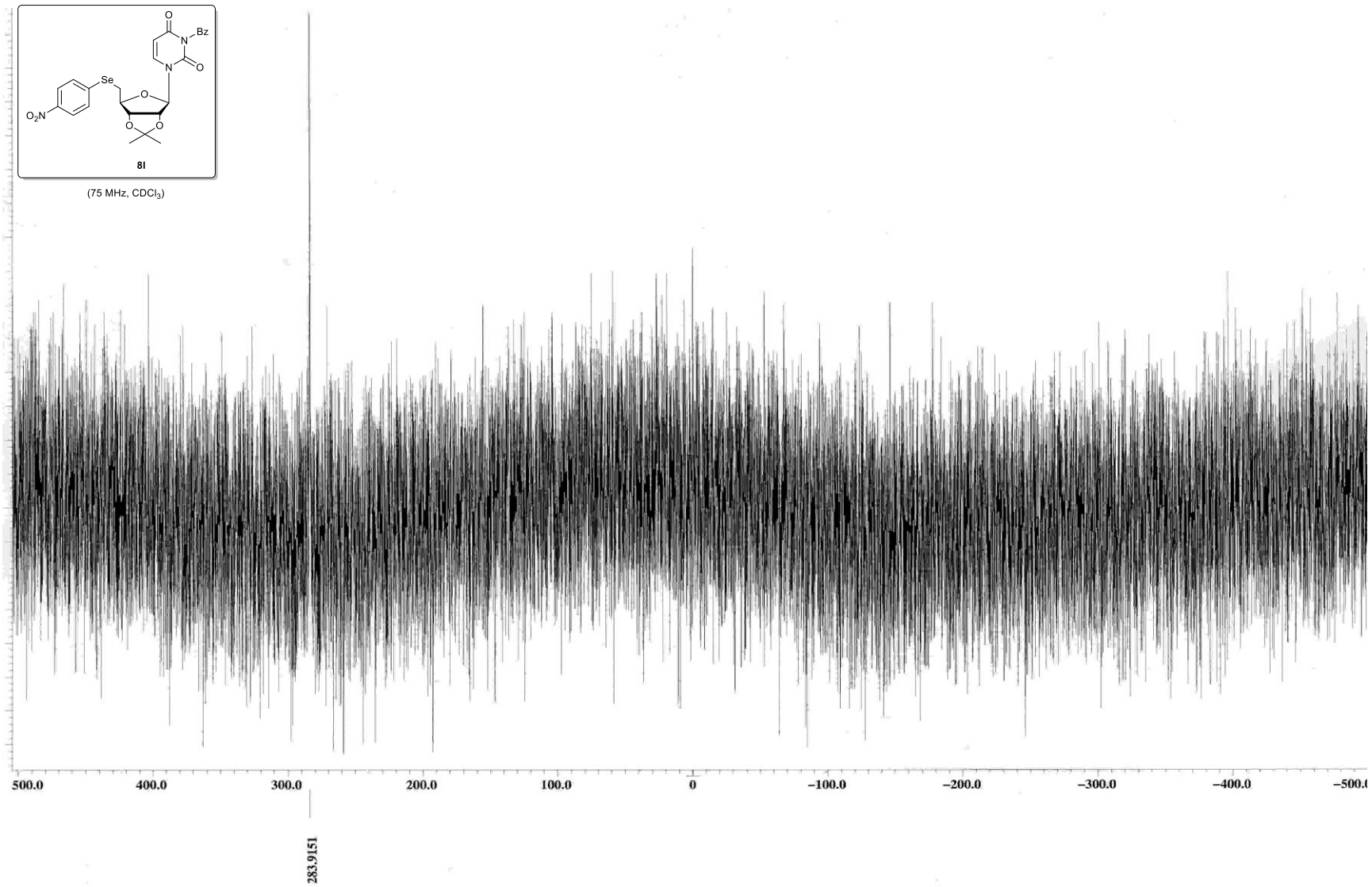

8k
(600 MHz, CDCl3)
abundance
X : parts per Million : 1H
8.2821
8.2684
7.9317
7.9191
7.4713
7.4587
7.3144
7.3007
7.2606
5.8256
5.8119
5.5588
5.5565
4.8441
4.8373
4.8327
4.8258
4.4021
4.3998
4.3952
3.8535
3.2168
3.2065
3.1973
1.5127
1.3214
1.2493
-0.0047

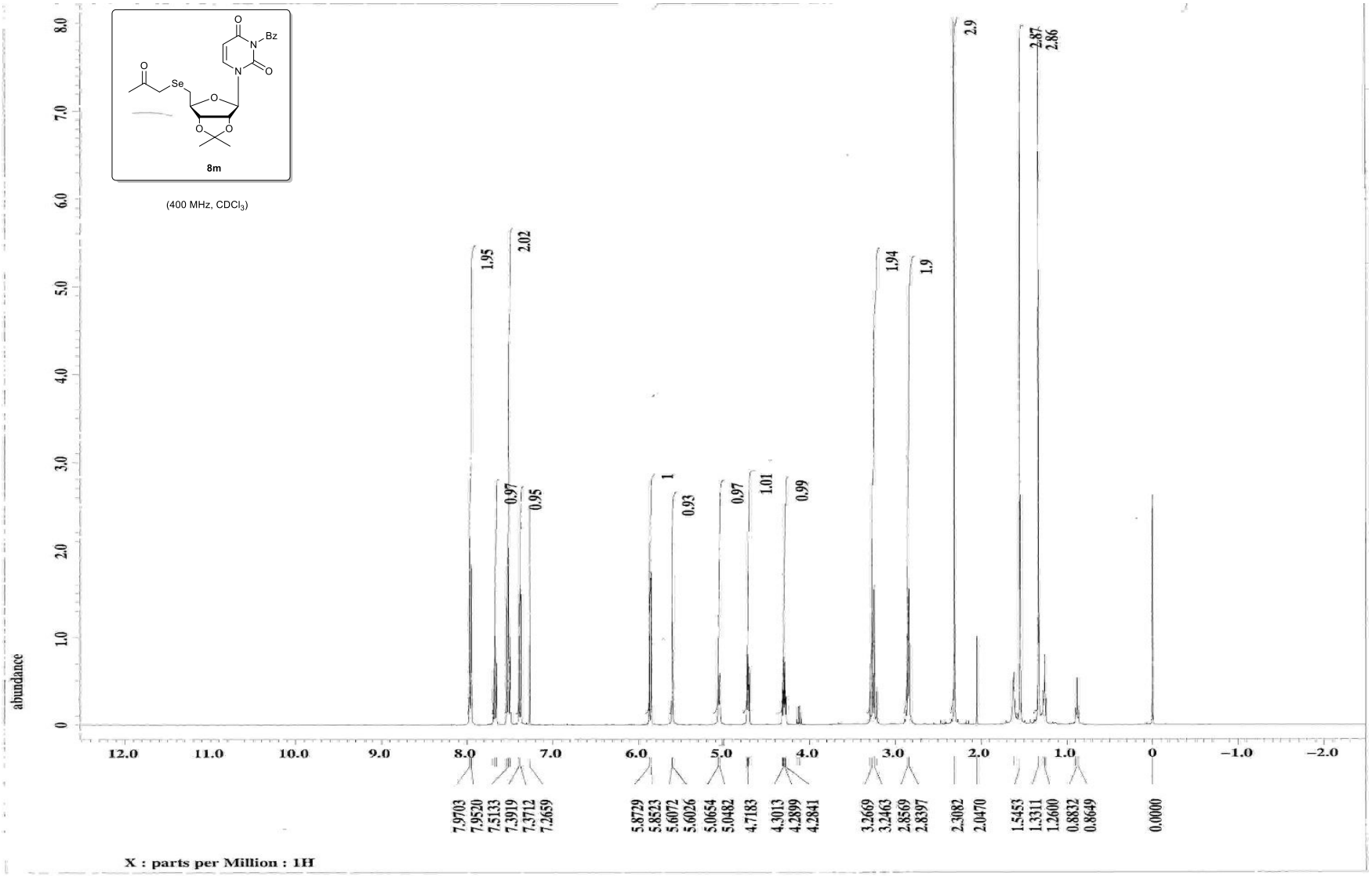

8k
(150 MHz, CDCl3)
abundance
X : parts per Million : 13C
168.3337
161.9091
149.2512
147.0203
143.0276
135.4731
133.9029
132.2752
131.2028
130.6187
129.3932
129.2400
126.5973
125.9750
114.8204
102.8232
96.6762
86.8812
84.5737
84.3726
77.3734
77.1628
76.9521
28.5038
27.1442
25.3441
0.1242

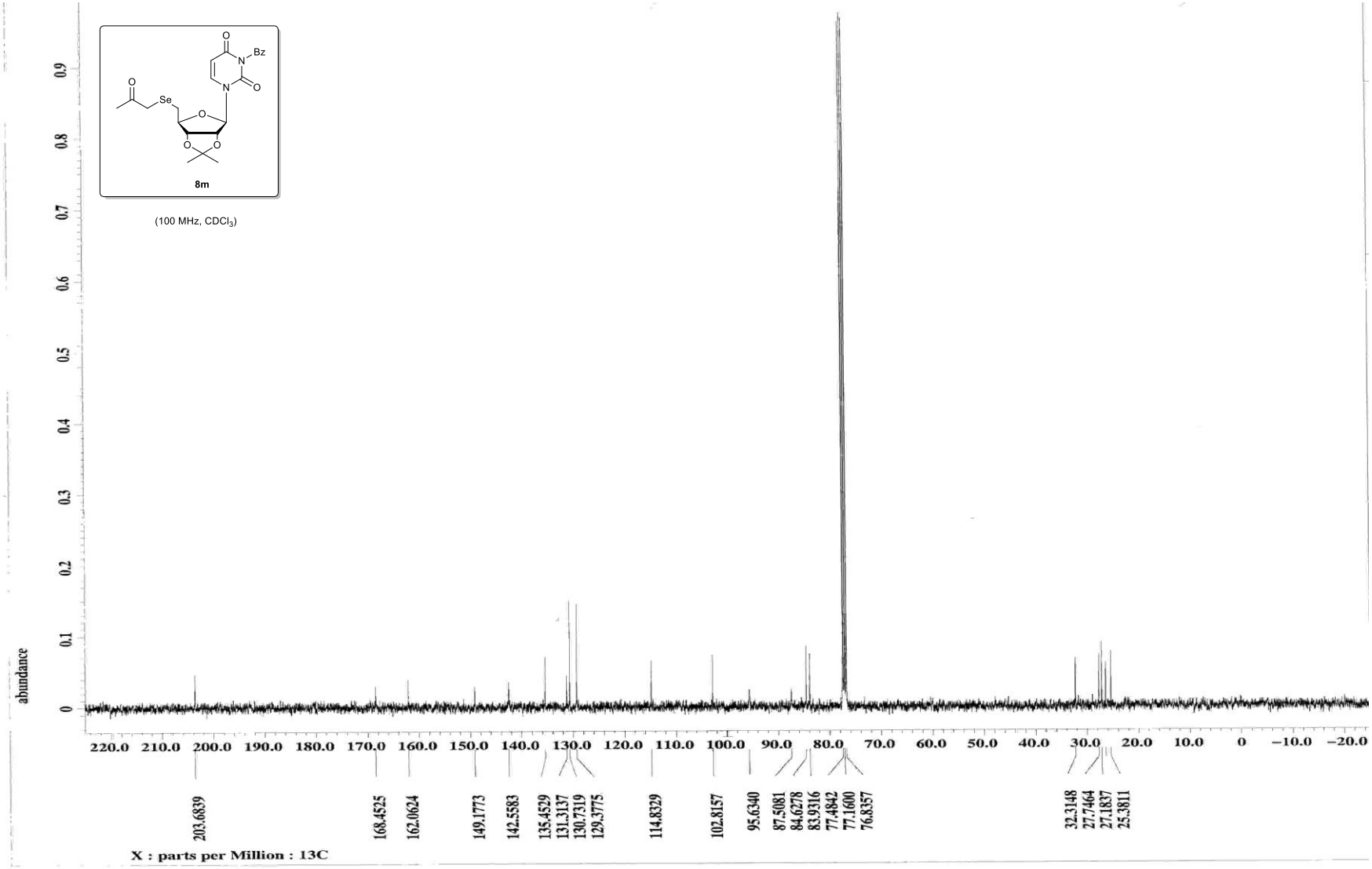

8k
(94 MHz, CDCl3)
40.0
30.0
20.0
10.0
0
−10.0
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
−500.0
329.1599
X : parts per Million : 77Se

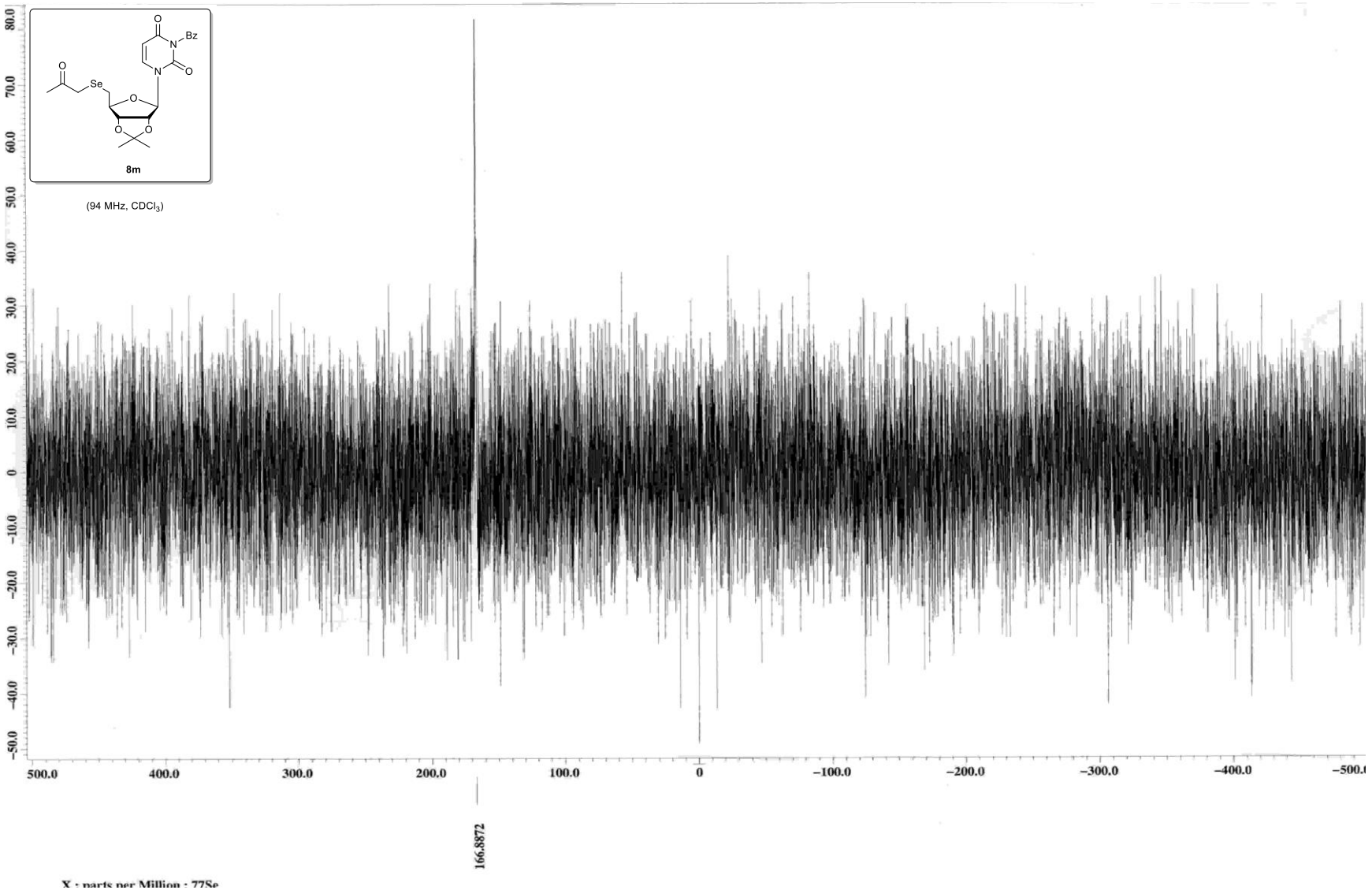

8l
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
4.12
2.19
1.95
1
1.06
0.99
1.0
0.98
1.1
1.1
1.99
3.2
3.0
8.0378
7.9290
7.5028
7.2967
7.2760
7.2600
5.8488
5.8281
5.5166
5.1443
4.8178
4.8075
4.3333
4.3230
4.3161
3.3000
3.2817
2.9564
2.6334
2.1706
2.0434
1.5131
1.3218
1.2565
1.2393
0.0675
0.0045
−0.0024

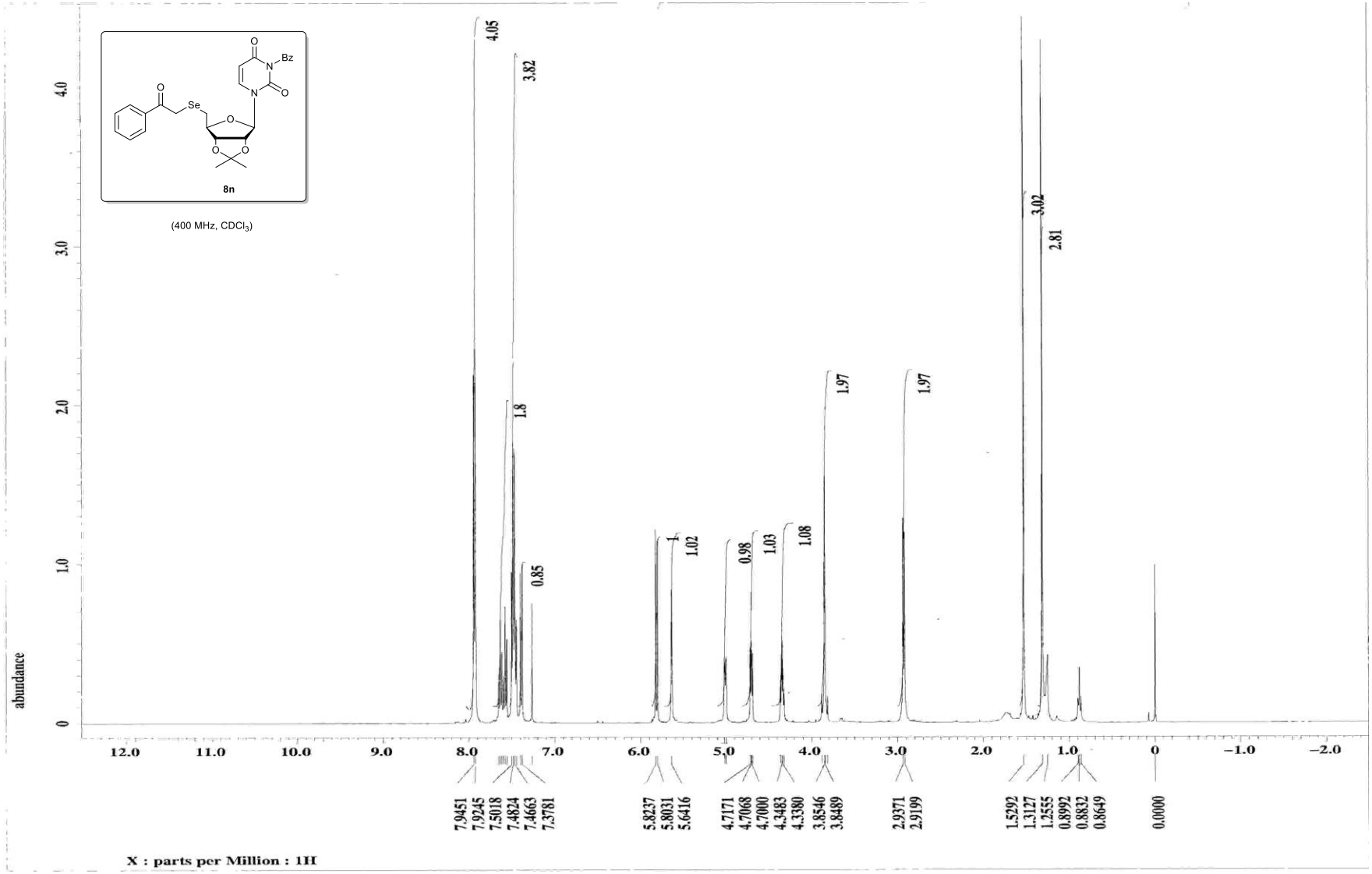

8l
(100 MHz, CDCl3)
abundance
X : parts per Million : 13C
168.2809
161.8717
149.2346
146.4973
143.1687
140.6413
135.5674
131.1801
130.7033
130.6174
129.4348
124.0080
114.6994
102.8539
97.0933
87.6417
84.6755
84.1128
77.4843
77.1600
76.8357
29.0531
27.1074
25.2858

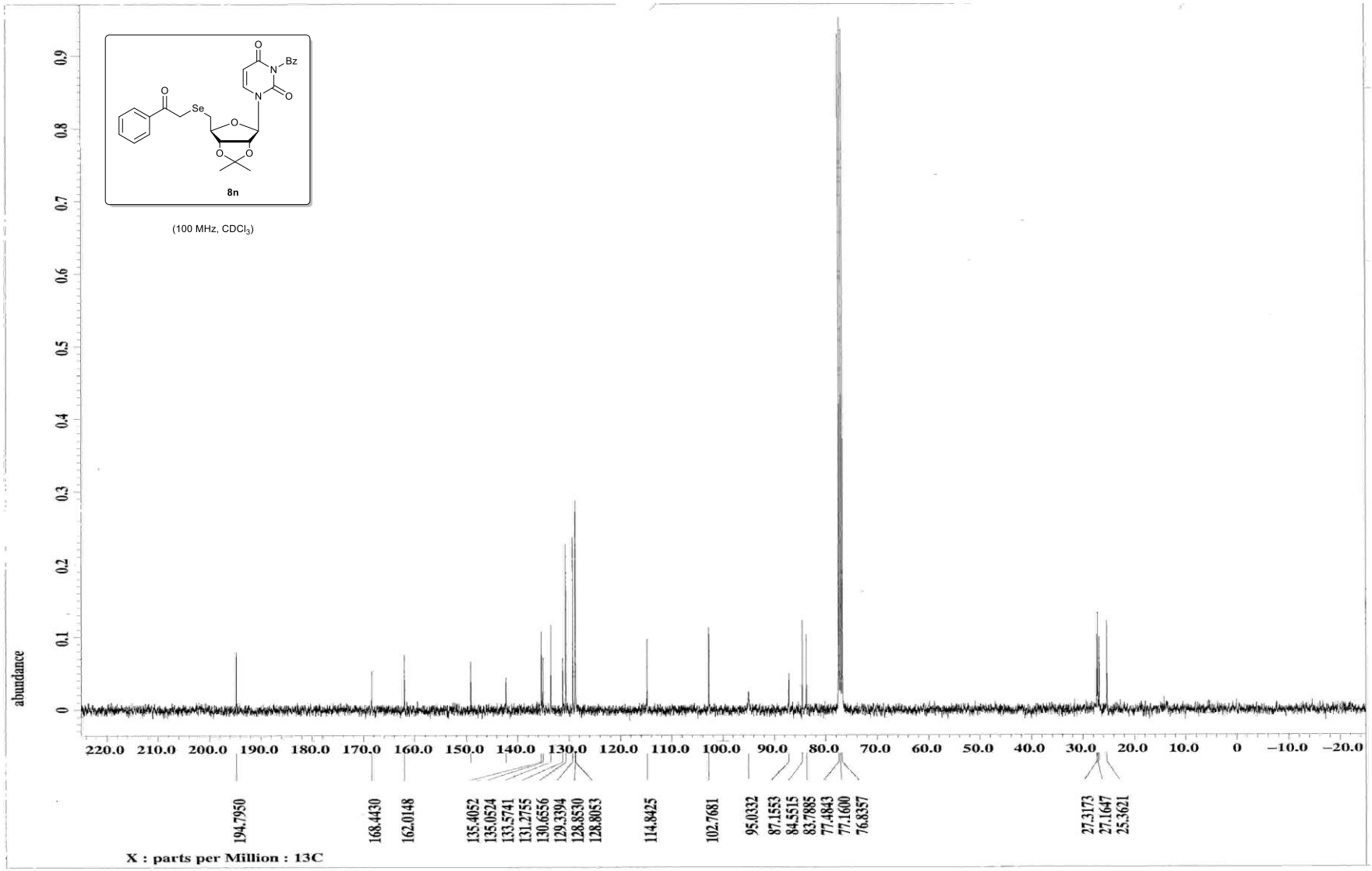

8l
(75 MHz, CDCl3)
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
283.9151

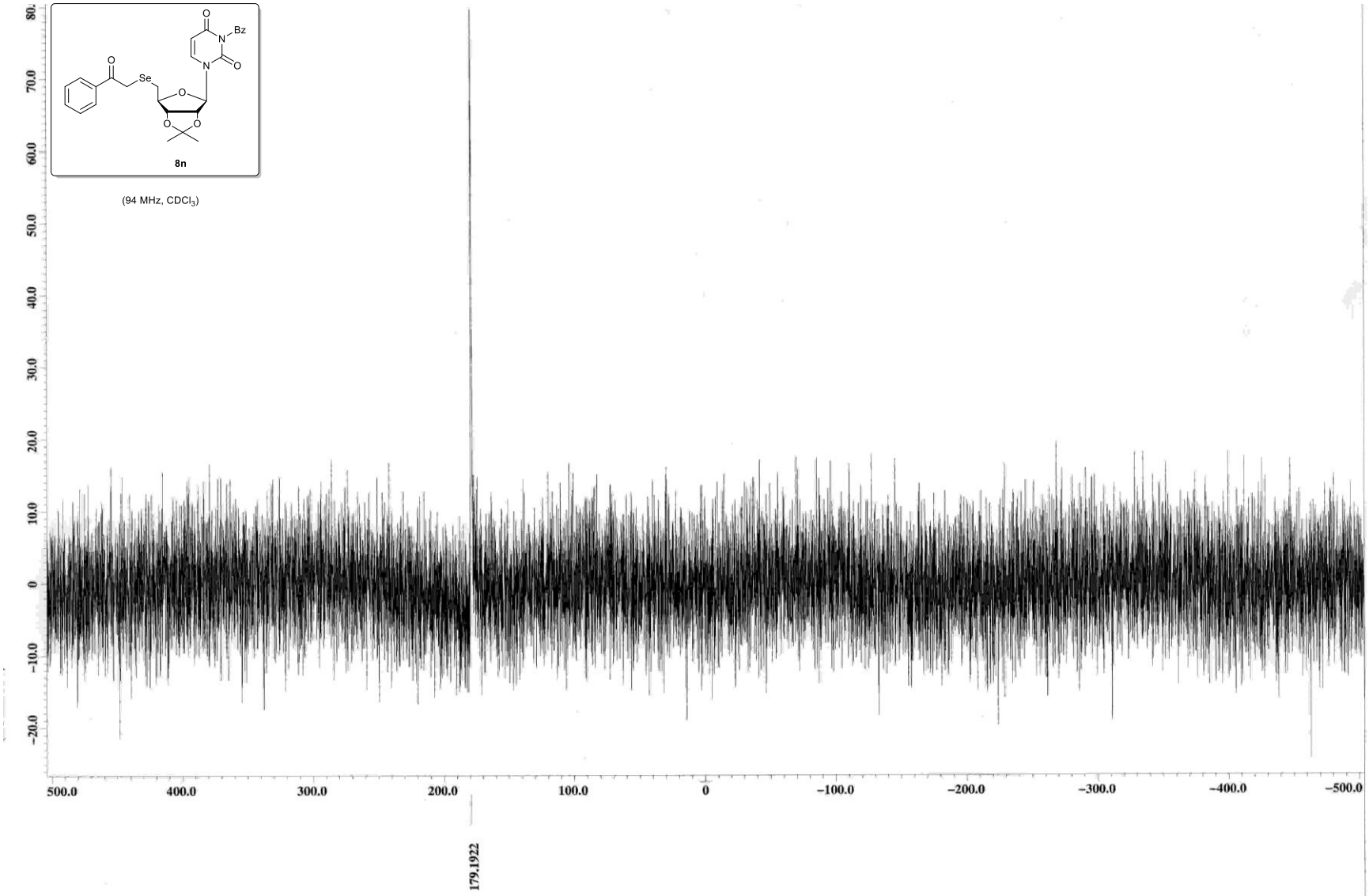

8m
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
1.95
2.02
0.97
0.95
1
0.93
0.97
1.01
0.99
1.94
1.9
2.9
2.87
2.86
7.9703
7.9520
7.5133
7.3919
7.3712
7.2659
5.8729
5.8523
5.6072
5.6026
5.0654
5.0482
4.7183
4.3013
4.2899
4.2841
3.2669
3.2463
2.8569
2.8397
2.3082
2.0470
1.5453
1.3311
1.2600
0.8832
0.8649
0.0000

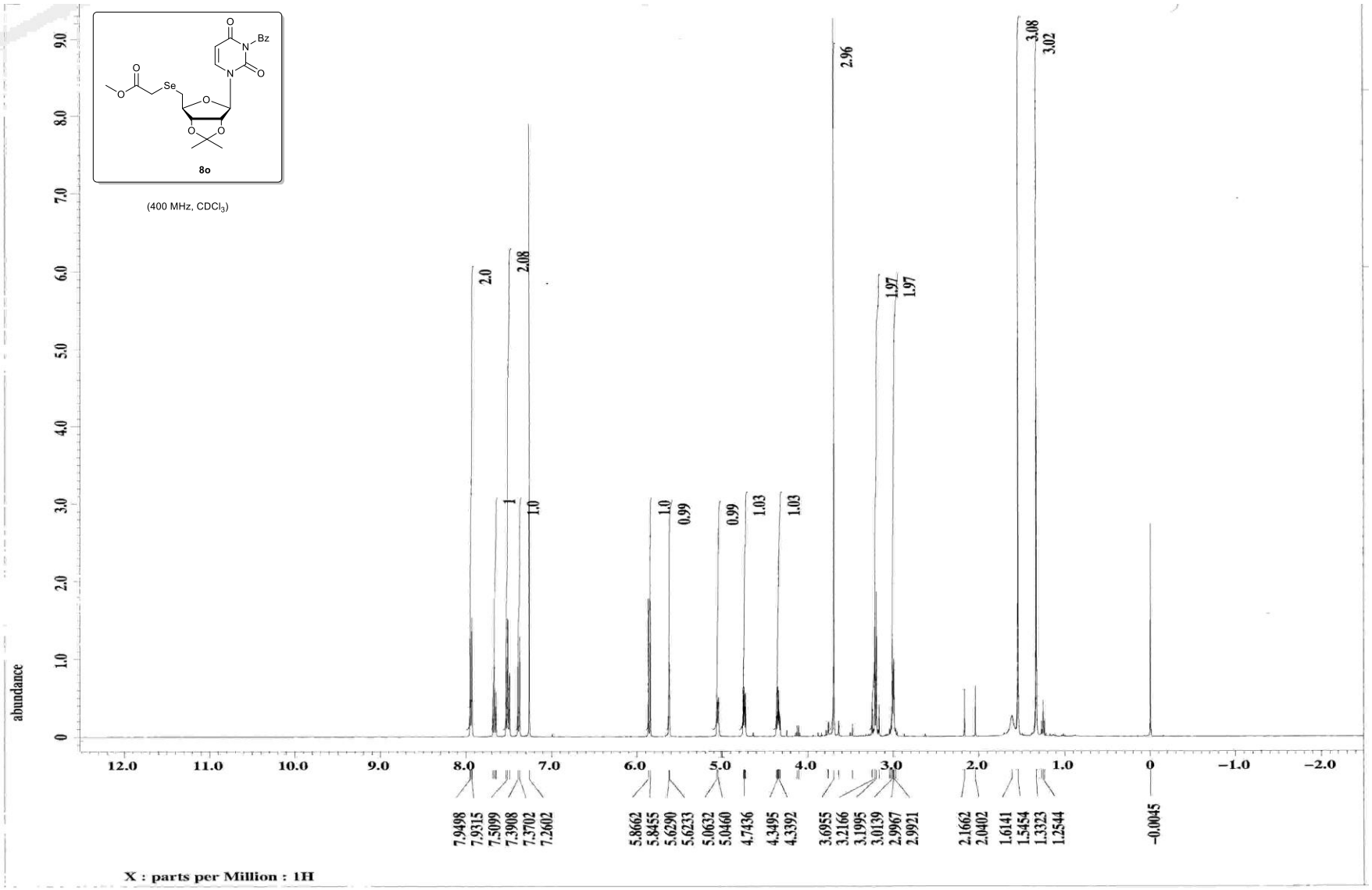

8m
(100 MHz, CDCl3)
abundance
X : parts per Million : 13C
203.6839
168.4525
162.0624
149.1773
142.5583
135.4529
131.3137
130.7319
129.3775
114.8329
102.8157
95.6340
87.5081
84.6278
83.9316
77.4842
77.1600
76.8357
32.3148
27.7464
27.1837
25.3811

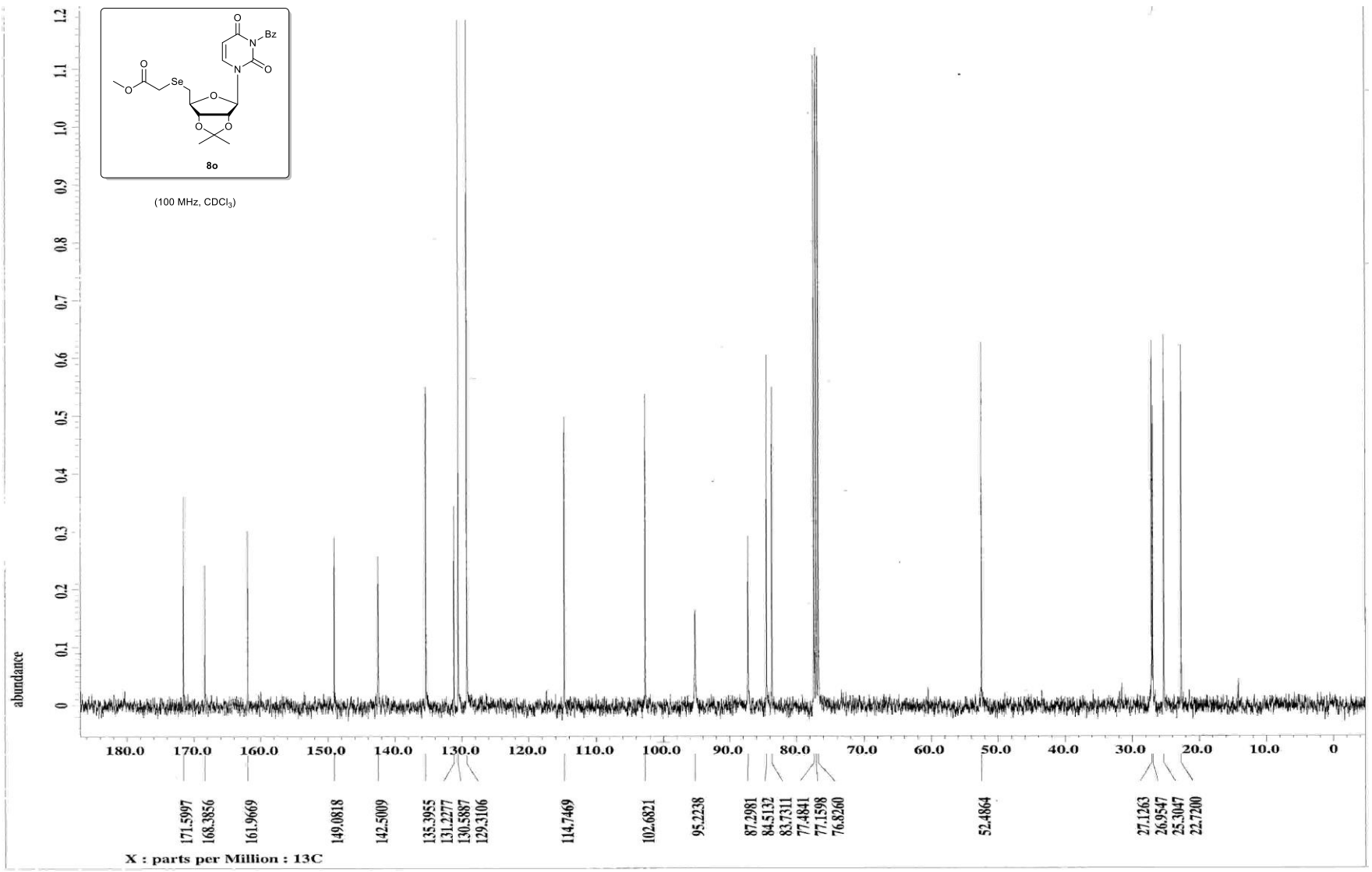

8m
(94 MHz, CDCl3)
166.8872
X : parts per Million : 77Se

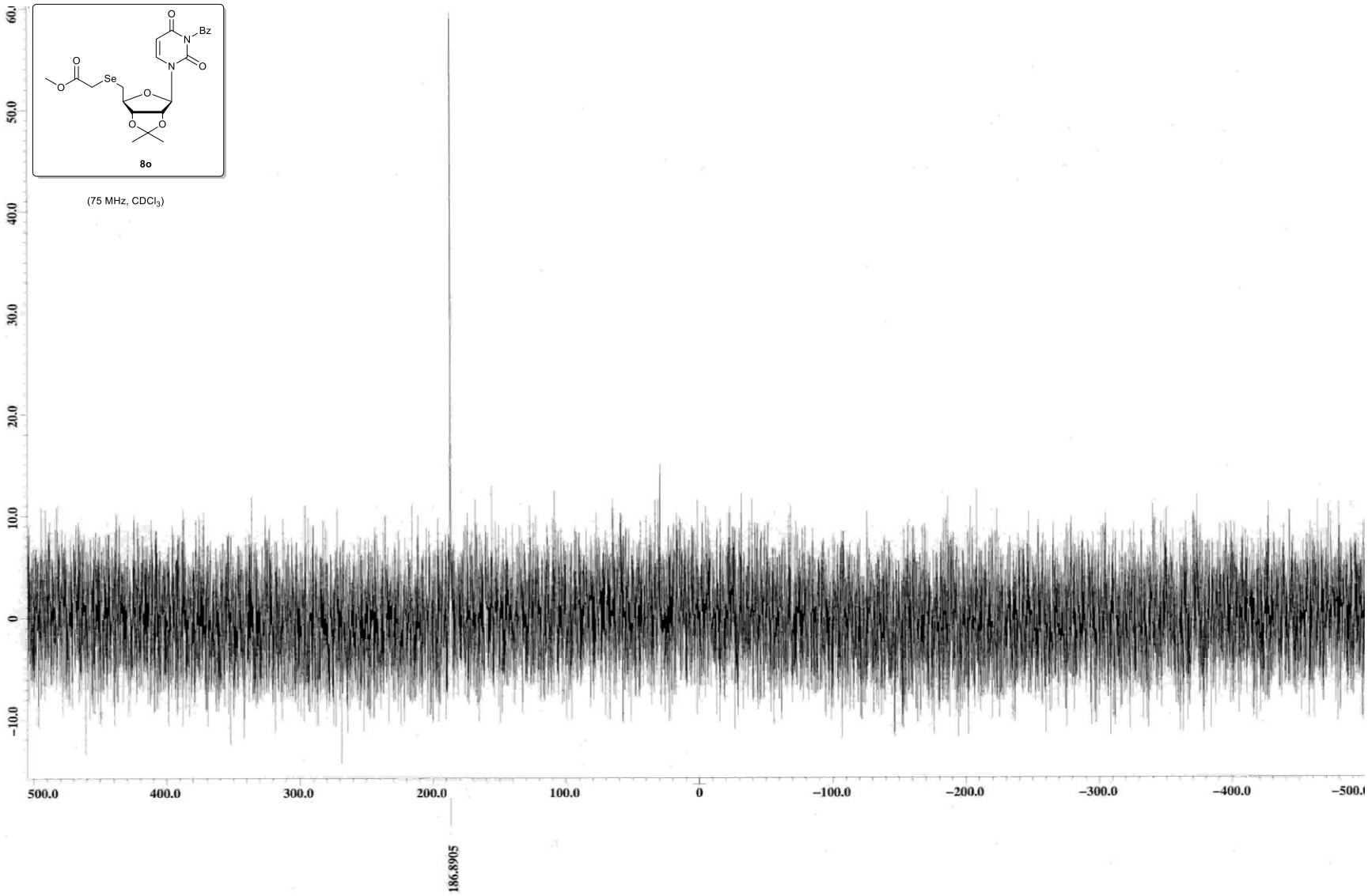

8n
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
4.05
3.82
1.8
0.85
1
1.02
0.98
1.03
1.08
1.97
1.97
3.02
2.81
7.9451
7.9245
7.5018
7.4824
7.4663
7.3781
5.8237
5.8031
5.6416
4.7171
4.7068
4.7000
4.3483
4.3380
3.8546
3.8489
2.9371
2.9199
1.5292
1.3127
1.2555
0.8992
0.8832
0.8649
0.0000

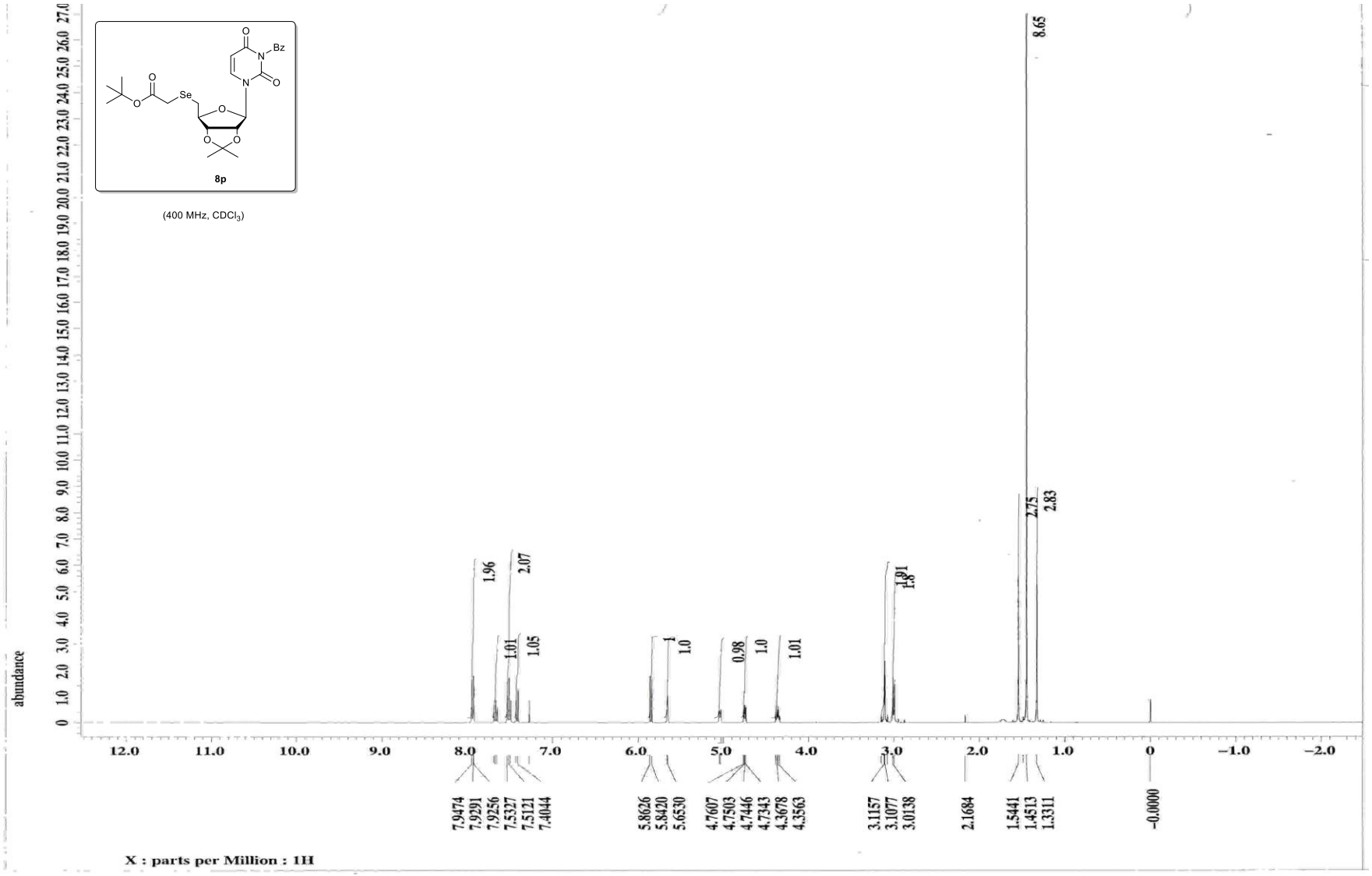

8n
(100 MHz, CDCl3)
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0 −20.0
194.7950
168.4430
162.0148
135.4052
135.0524
133.5741
131.2755
130.6556
129.3394
128.8530
128.8053
114.8425
102.7681
95.0332
87.1553
84.5515
83.7885
77.4843
77.1600
76.8357
27.3173
27.1647
25.3621
X : parts per Million : 13C

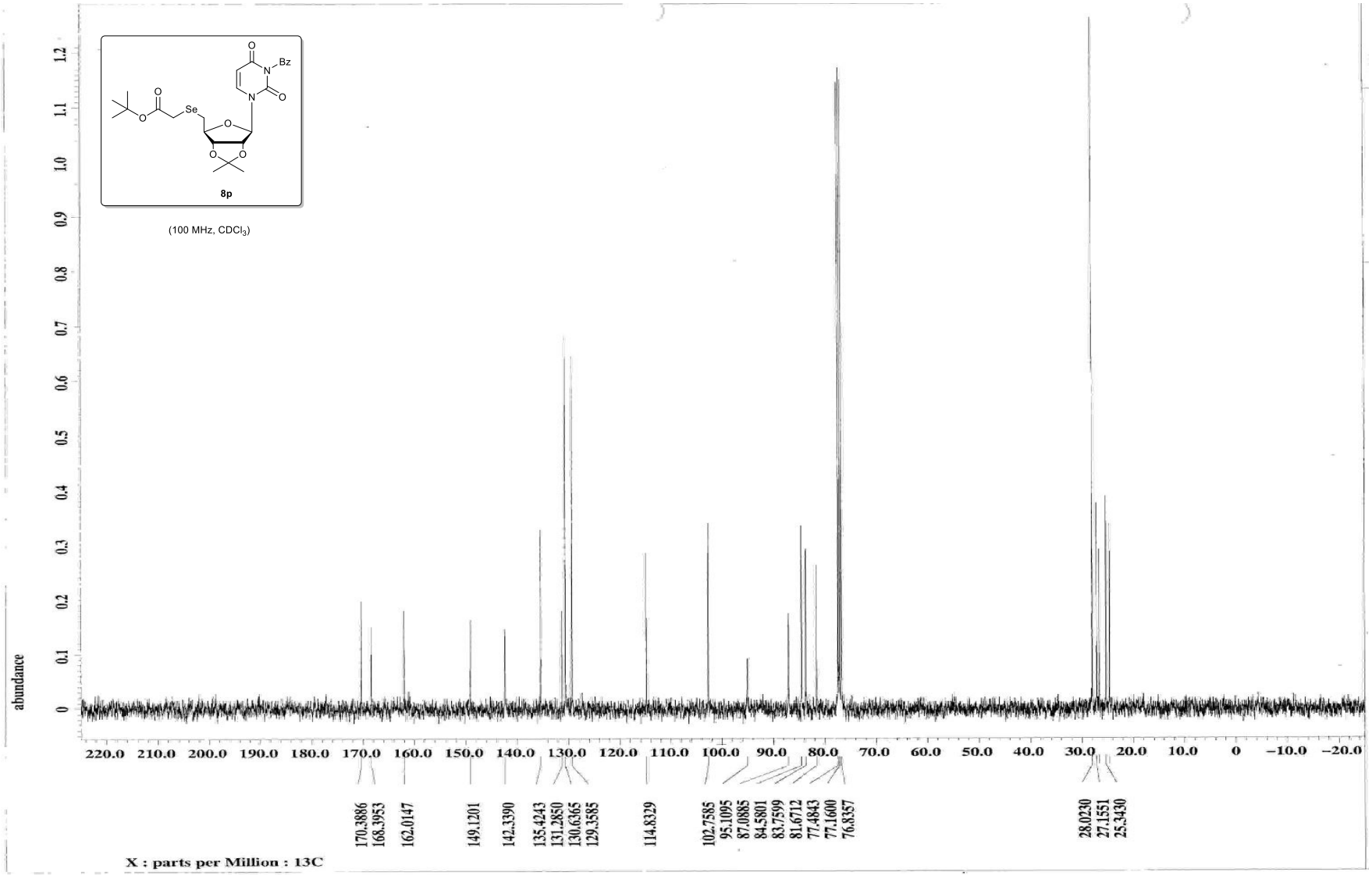

8n
(94 MHz, CDCl3)
80.
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
500.0
400.0
300.0
200.0
100.0
0
-100.0
-200.0
-300.0
-400.0
-500.0
179.1922

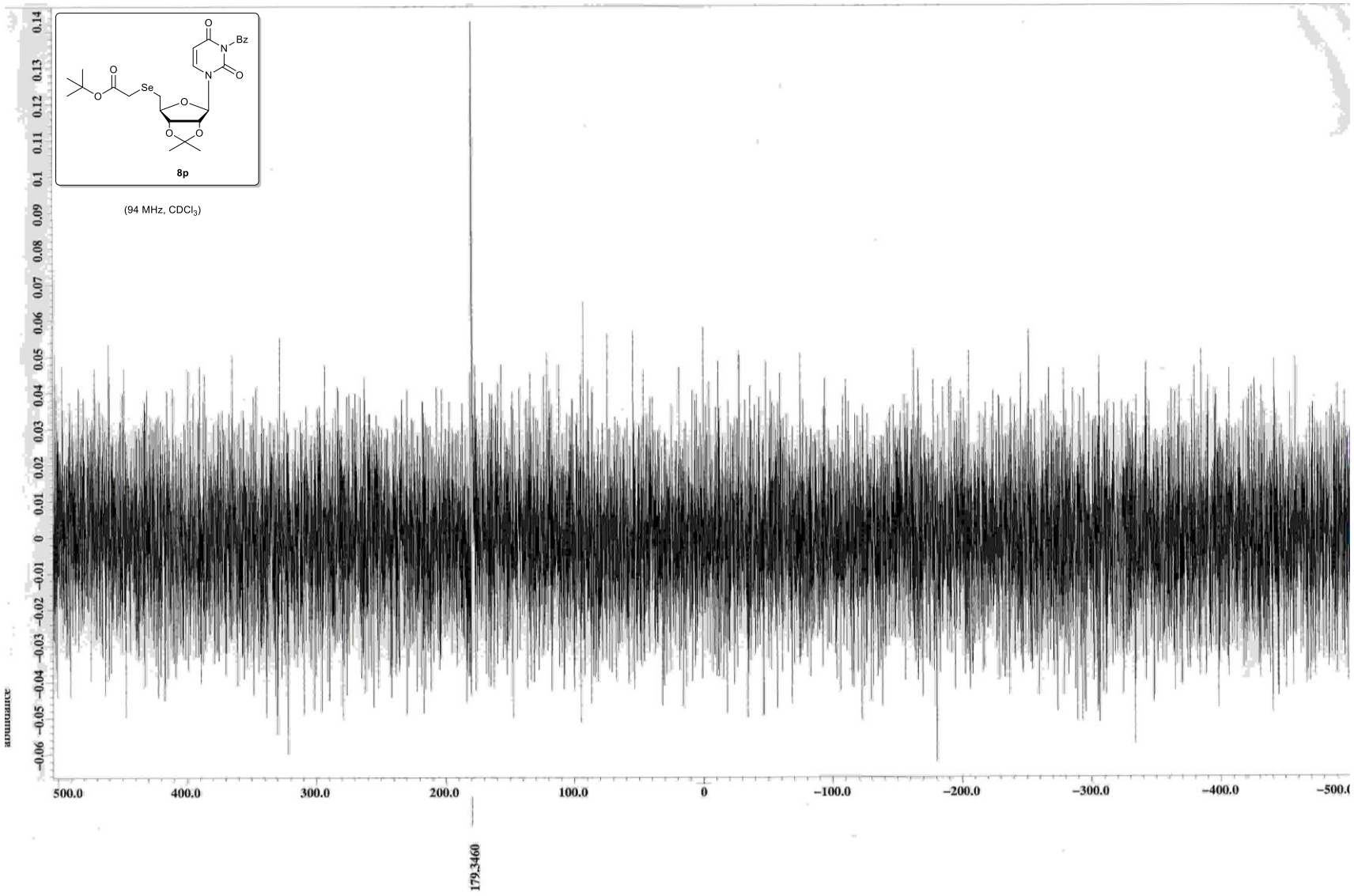

8o
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
2.0
2.08
1
1.0
1.0
0.99
0.99
1.03
1.03
2.96
1.97
1.97
3.08
3.02
7.9498
7.9315
7.5099
7.3908
7.3702
7.2602
5.8662
5.8455
5.6290
5.6233
5.0632
5.0460
4.7436
4.3495
4.3392
3.6955
3.2166
3.1995
3.0139
2.9967
2.9921
2.1662
2.0402
1.6141
1.5454
1.3323
1.2544
-0.0045

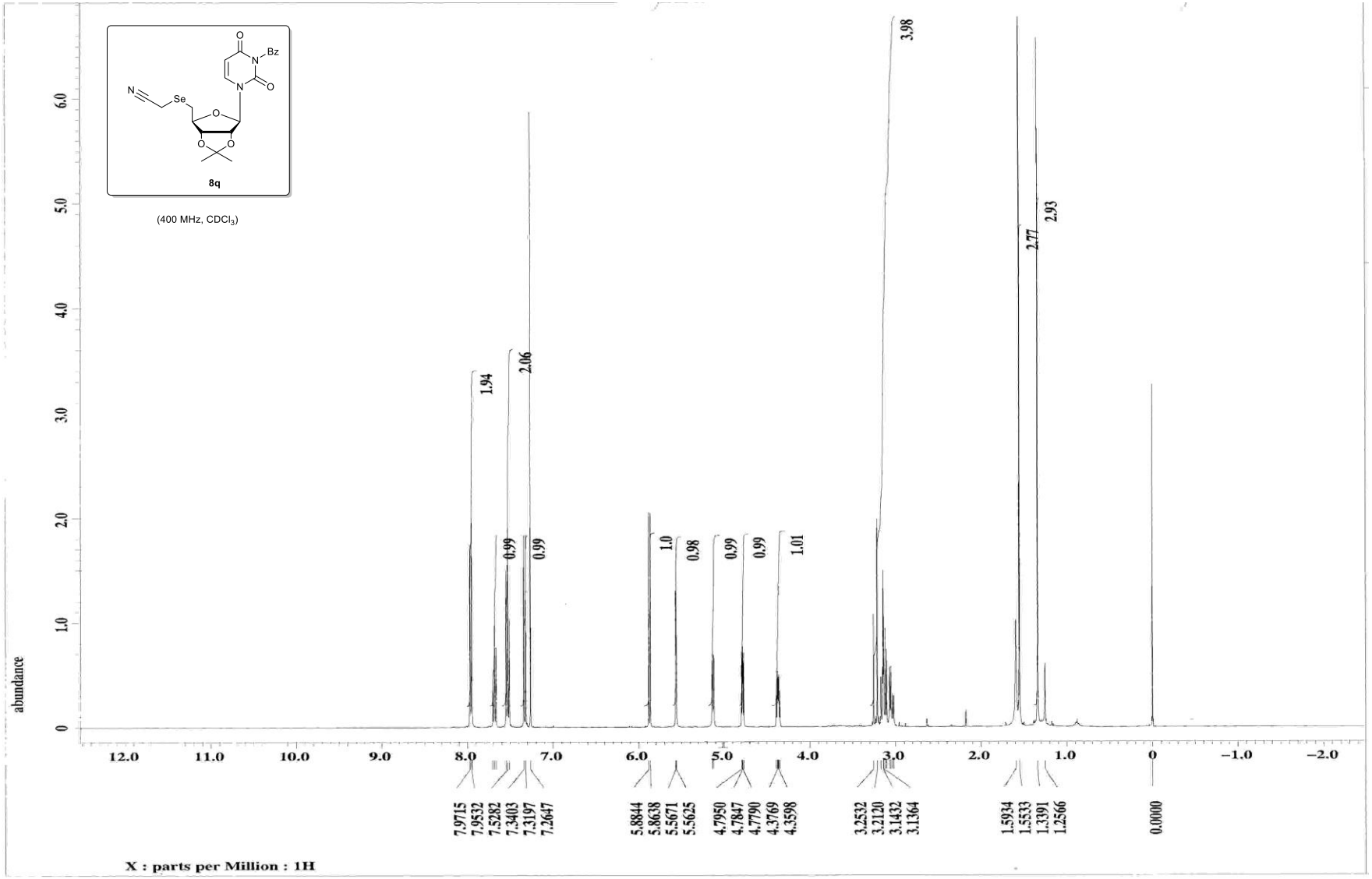

8o
(100 MHz, CDCl3)
abundance
X : parts per Million : 13C
171.5997
168.3856
161.9669
149.0818
142.5009
135.3955
131.2277
130.5887
129.3106
114.7469
102.6821
95.2238
87.2981
84.5132
83.7311
77.4841
77.1598
76.8260
52.4864
27.1263
26.9547
25.3047
22.7200

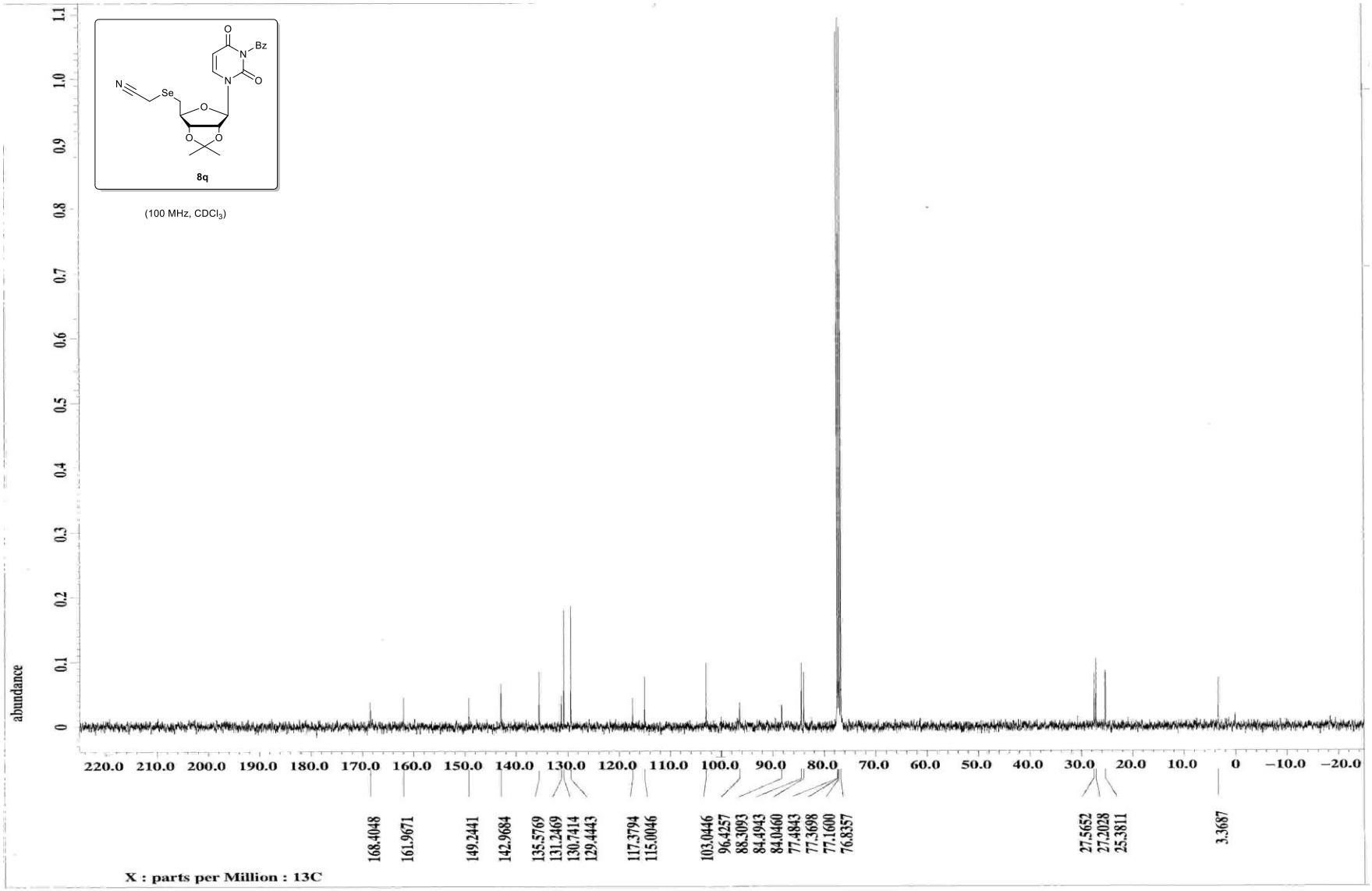

8o
(75 MHz, CDCl3)
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
186.8905

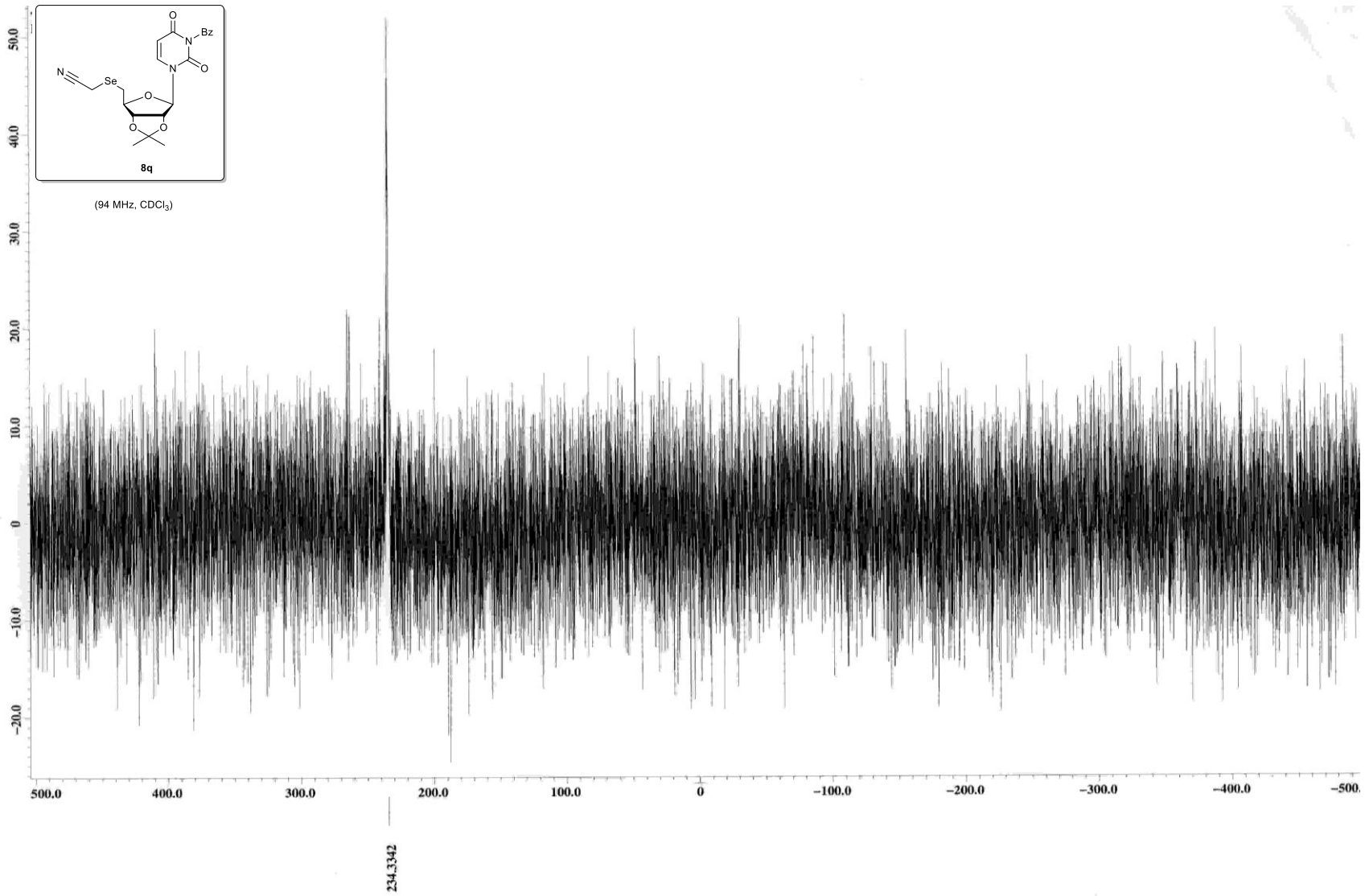

8p
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
8.65
2.83
2.75
2.07
1.96
1.91
1.8
1.05
1.01
1.01
1.0
1.0
0.98
7.9474
7.9291
7.9256
7.5327
7.5121
7.4044
5.8626
5.8420
5.6530
4.7607
4.7503
4.7446
4.7343
4.3678
4.3563
3.1157
3.1077
3.0138
2.1684
1.5441
1.4513
1.3311
-0.0000

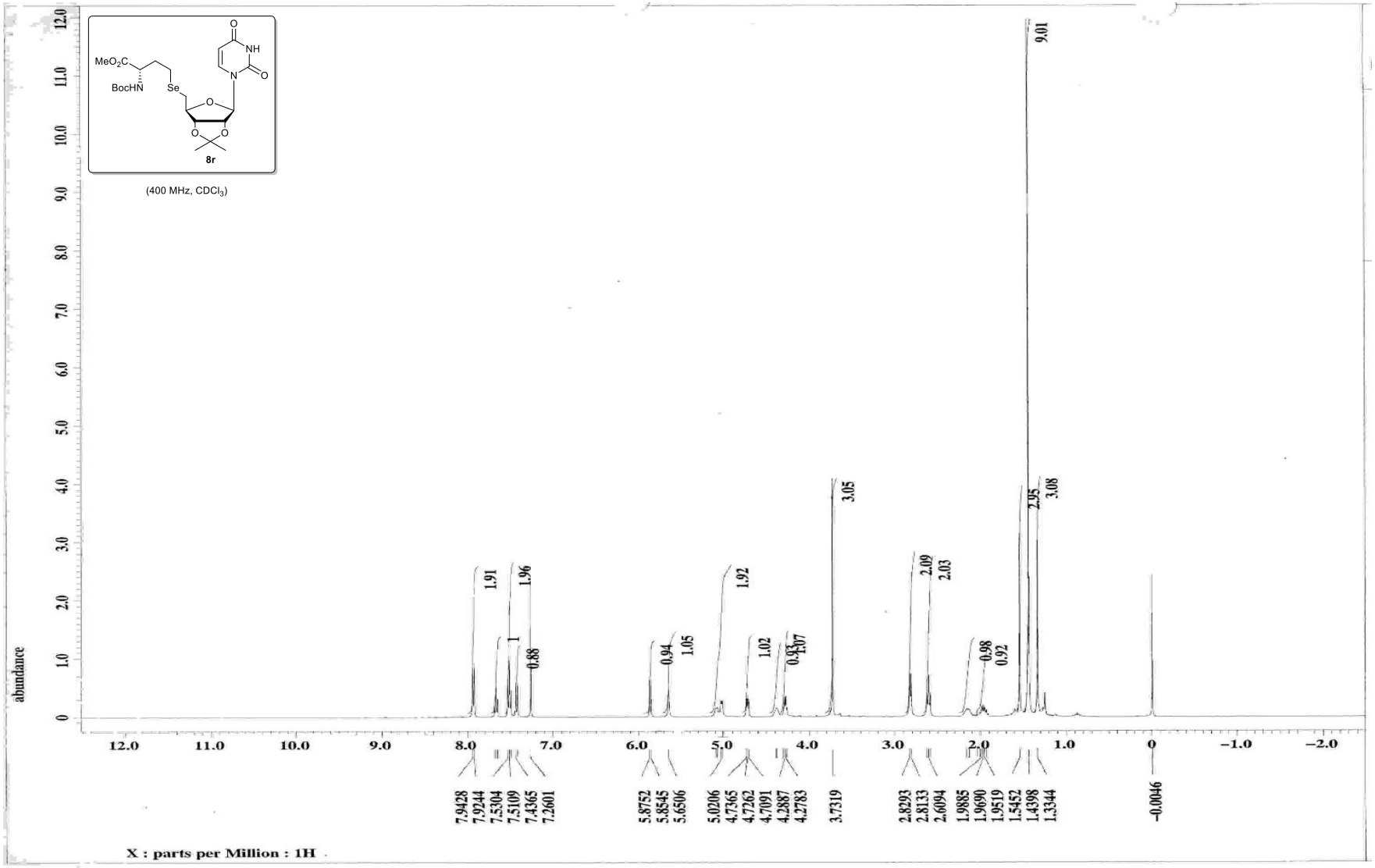

8p
(100 MHz, CDCl3)
abundance
X : parts per Million : 13C
170.3886
168.3953
162.0147
149.1201
142.3390
135.4243
131.2850
130.6365
129.3585
114.8329
102.7585
95.1095
87.0885
84.5801
83.7599
81.6712
77.4843
77.1600
76.8357
28.0230
27.1551
25.3430

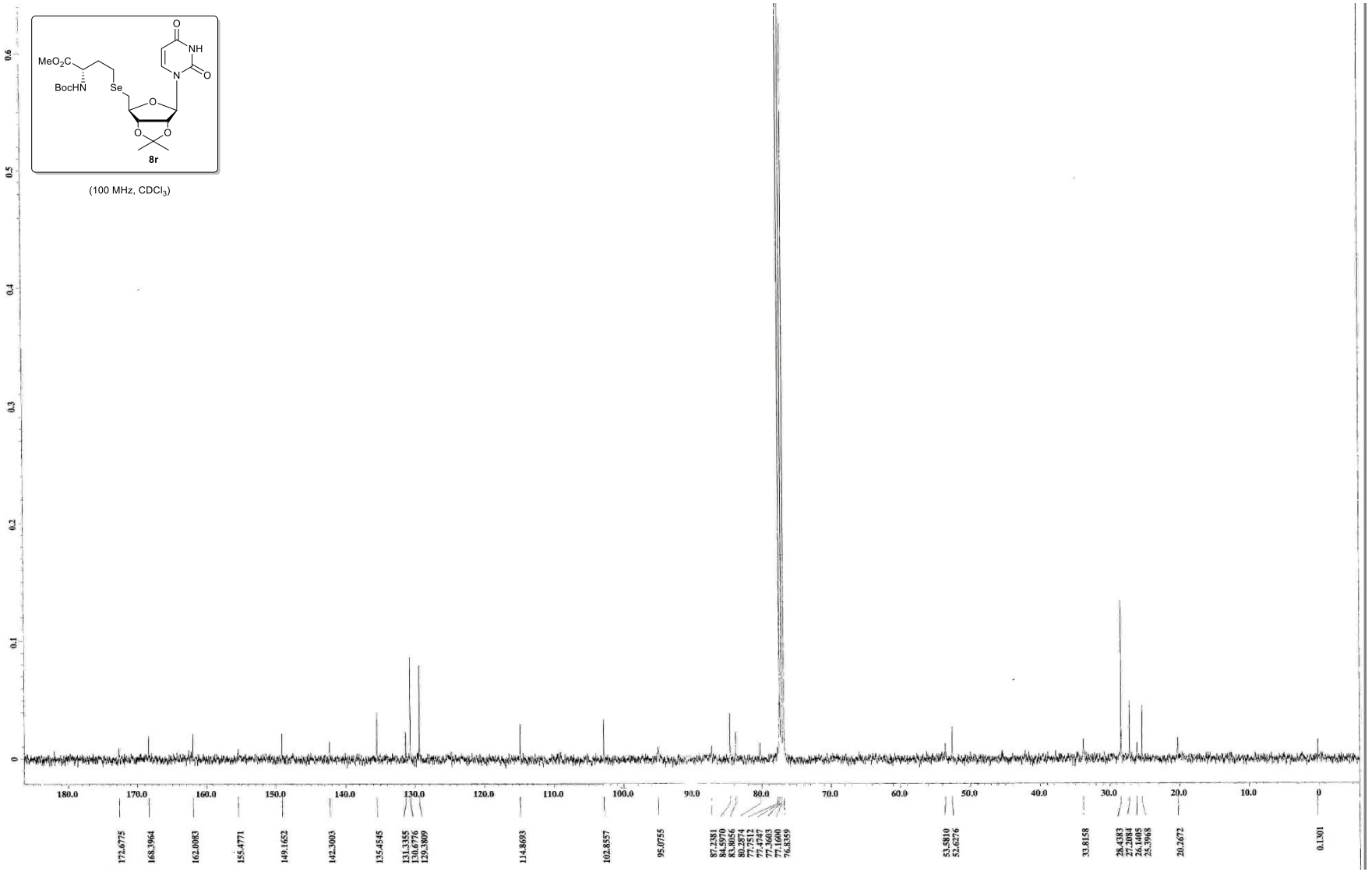

8p
(94 MHz, CDCl3)
179.3460

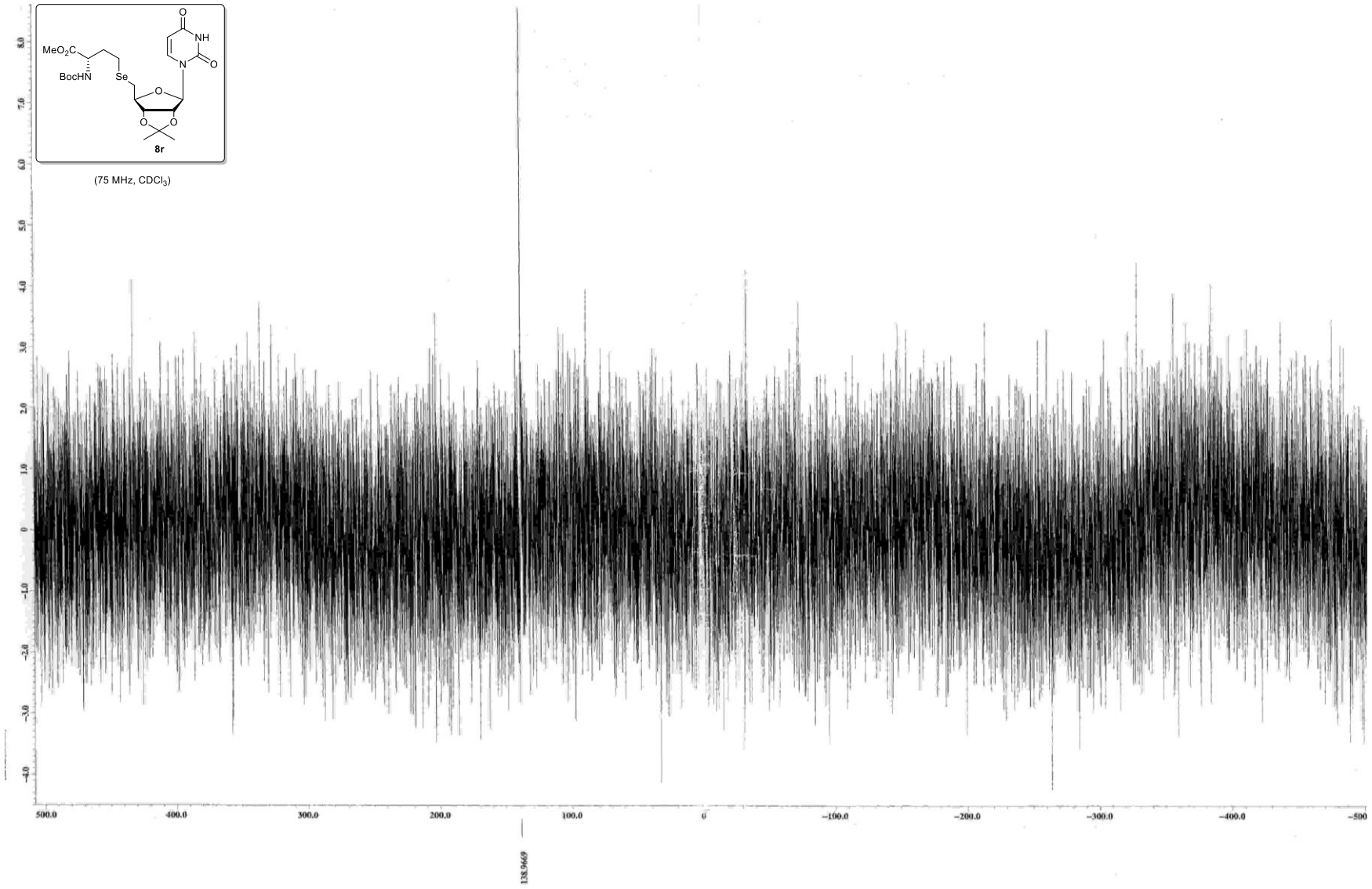

8q
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
1.94
2.06
0.99
0.99
1.0
0.98
0.99
0.99
1.01
3.98
2.77
2.93
7.9715
7.9532
7.5282
7.3403
7.3197
7.2647
5.8844
5.8638
5.5671
5.5625
4.7950
4.7847
4.7790
4.3769
4.3598
3.2532
3.2120
3.1432
3.1364
1.5934
1.5533
1.3391
1.2566
0.0000

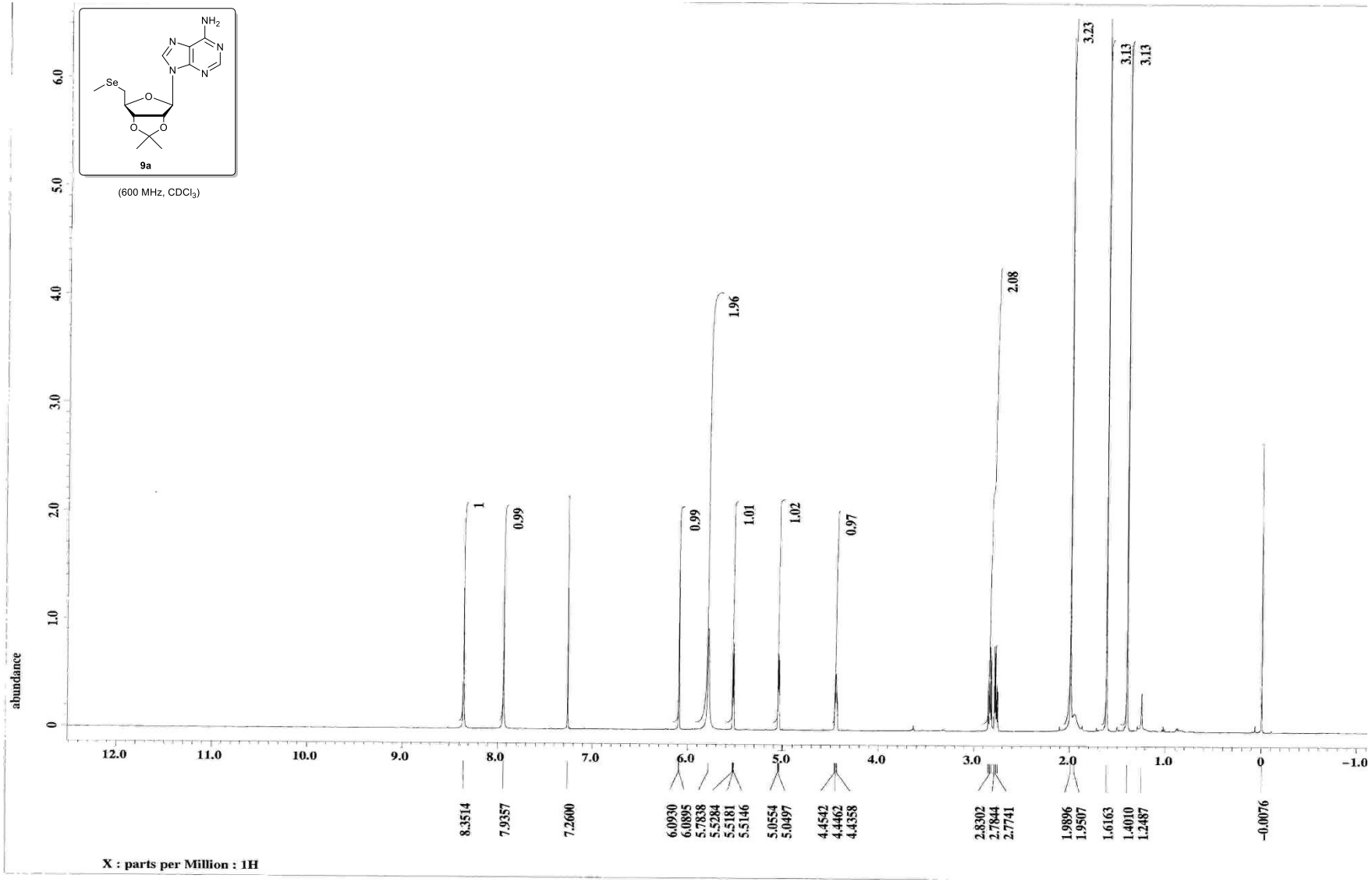

8q
(100 MHz, CDCl3)
abundance
X : parts per Million : 13C
168.4048
161.9671
149.2441
142.9684
135.5769
131.2469
130.7414
129.4443
117.3794
115.0046
103.0446
96.4257
88.3093
84.4943
84.0460
77.4843
77.3698
77.1600
76.8357
27.5652
27.2028
25.3811
3.3687

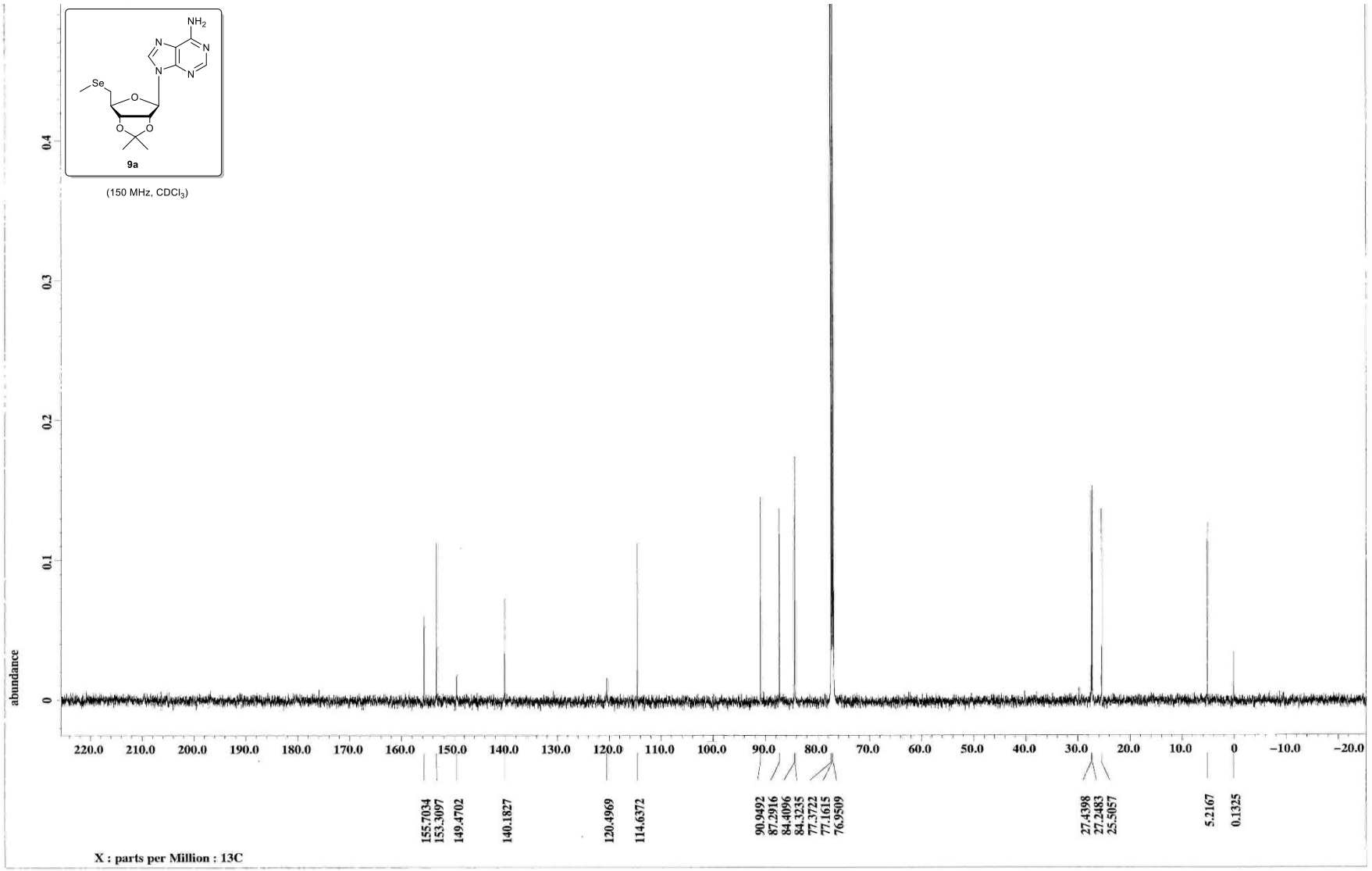

8q
(94 MHz, CDCl3)
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
500.0
400.0
300.0
200.0
100.0
0
-100.0
-200.0
-300.0
-400.0
234.3342

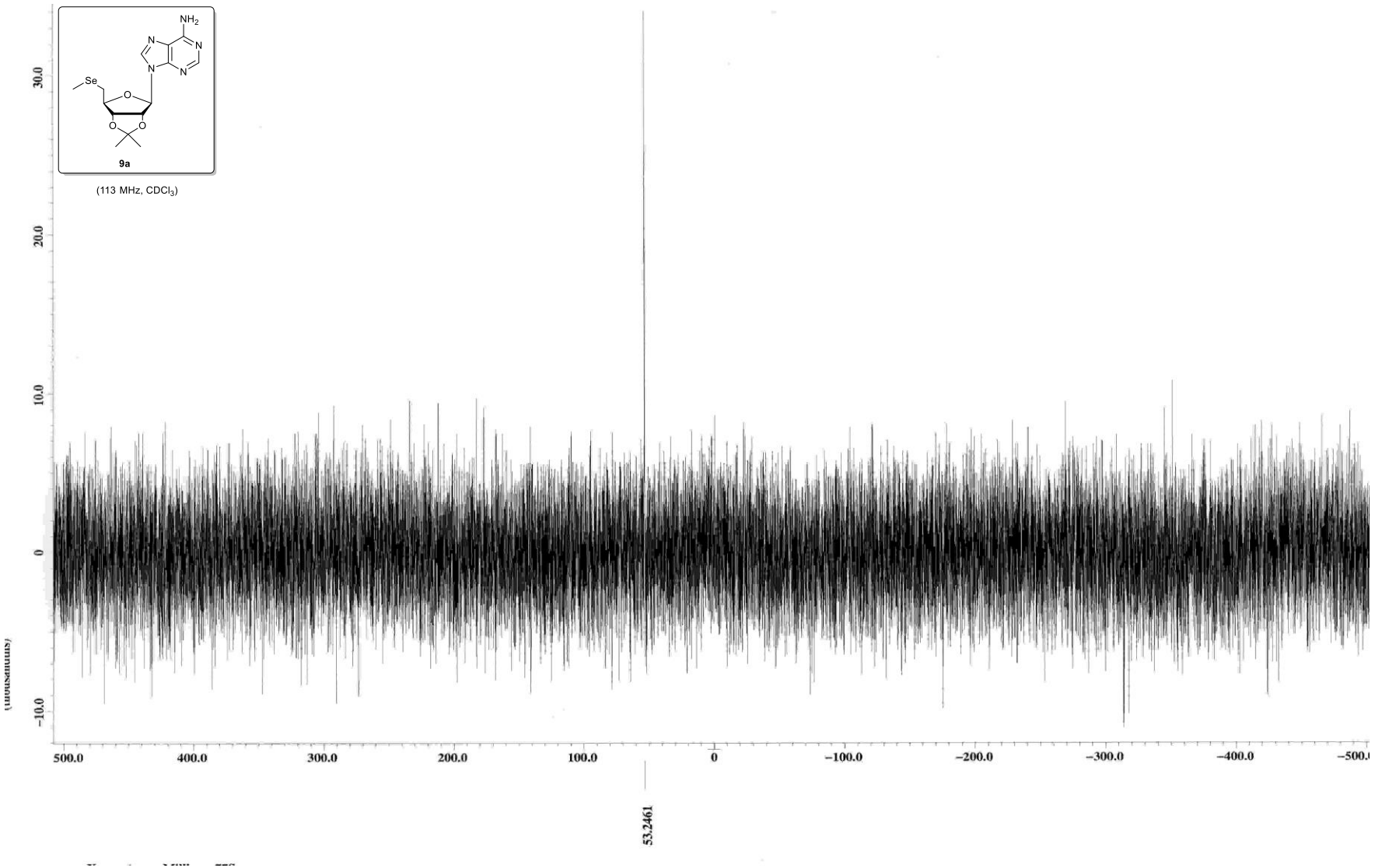

MeO2C
BocHN
Se
NH
O
N
O
8r
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
9.01
3.08
3.05
2.95
2.09
2.03
1.96
1.92
1.91
1.05
1.02
1.00
0.98
0.94
0.92
0.88
1
7.9428
7.9244
7.5304
7.5109
7.4365
7.2601
5.8752
5.8545
5.6506
5.0206
4.7365
4.7262
4.7091
4.2887
4.2783
3.7319
2.8293
2.8133
2.6094
1.9885
1.9690
1.9519
1.5452
1.4398
1.3344
-0.0046

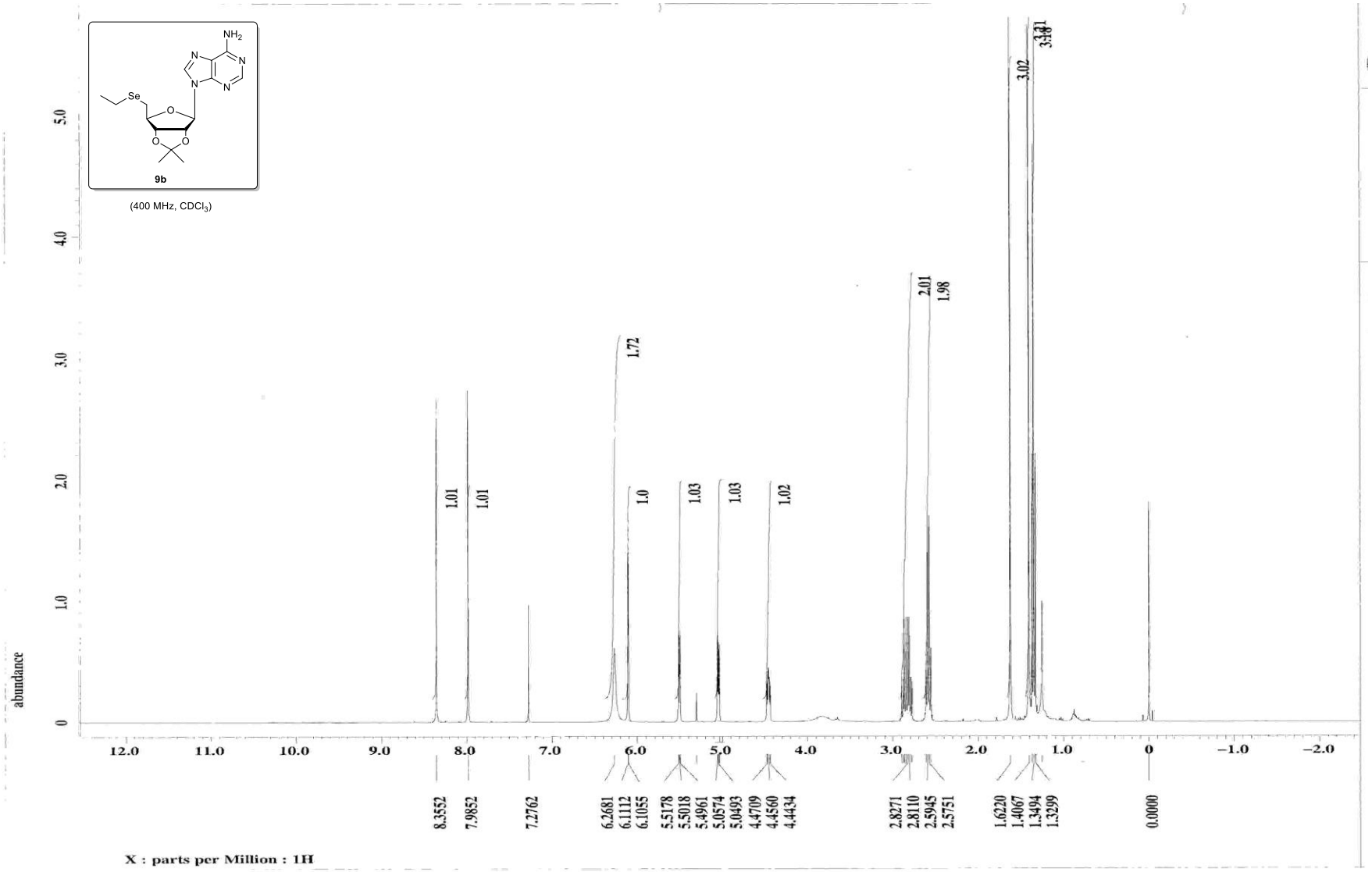

MeO2C
BocHN
Se
O
NH
N
O
O
O
O
8r
(100 MHz, CDCl3)
0.6
0.5
0.4
0.3
0.2
0.1
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
172.6775
168.3964
162.0083
155.4771
149.1652
142.3003
135.4545
131.3355
130.6776
129.3809
114.8693
102.8557
95.0755
87.2381
84.4570
83.8056
80.2874
77.7512
77.4747
77.3603
77.1690
76.8359
53.5810
52.6276
33.8158
28.4383
27.2084
26.1405
25.3968
20.2672
0.1301

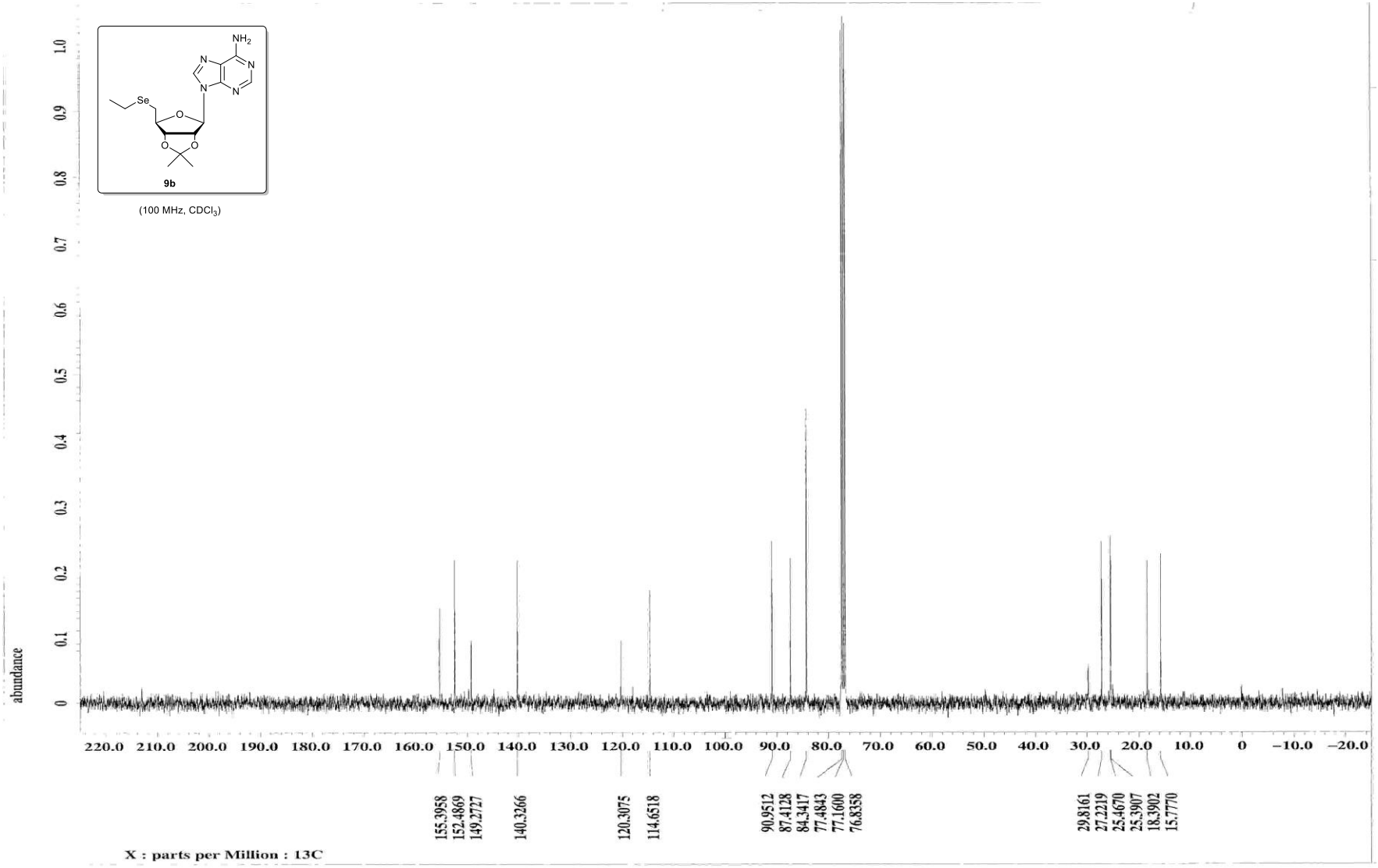

MeO2C
BocHN
Se
NH
O
O
O
O
O
8r
(75 MHz, CDCl3)
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
−500
138.9669

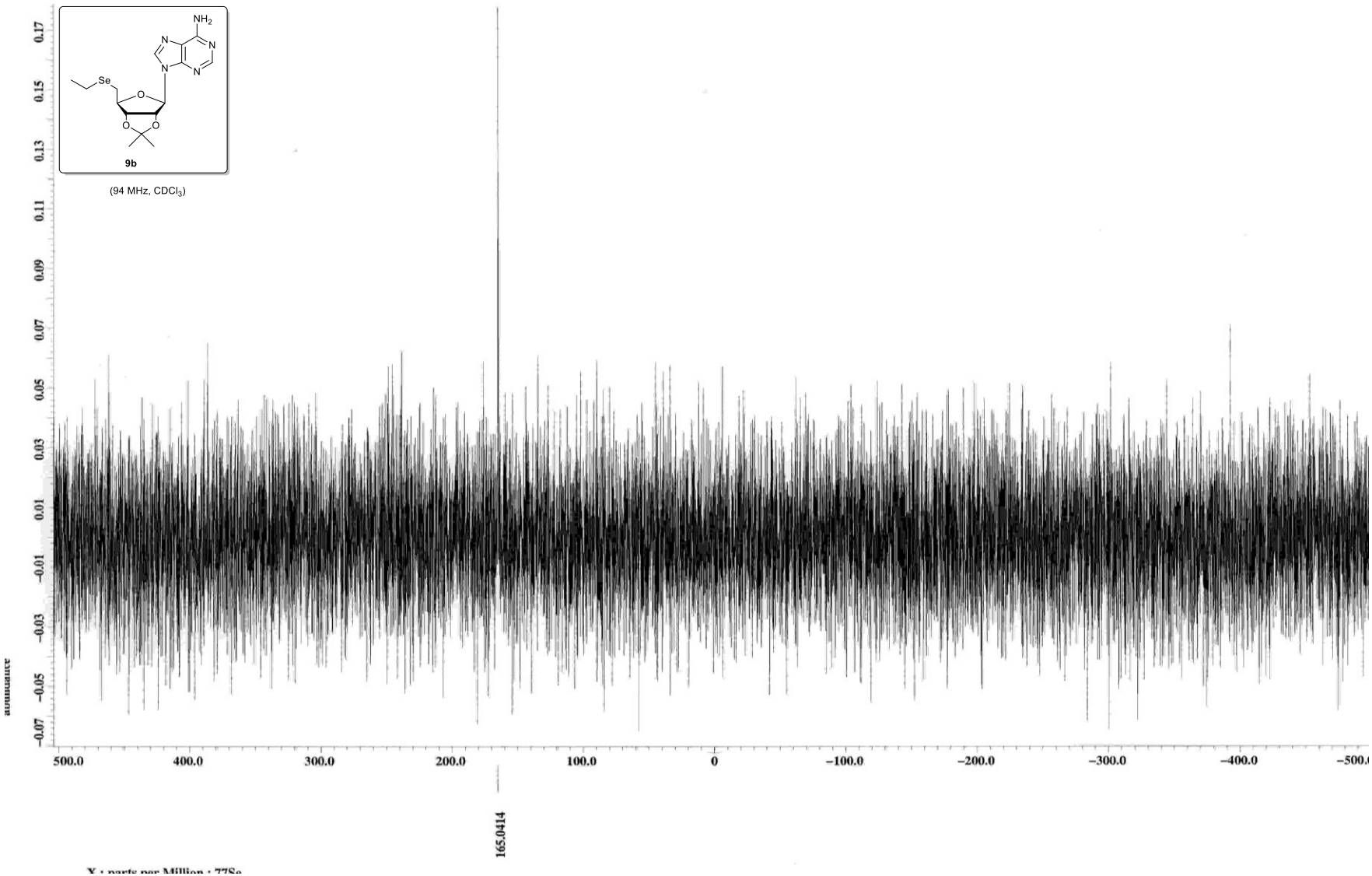

NH2
Se
9a
(600 MHz, CDCl3)
abundance
X : parts per Million : 1H
8.3514
7.9357
7.2600
6.0930
6.0895
5.7838
5.5284
5.5181
5.5146
5.0554
5.0497
4.4542
4.4462
4.4358
2.8302
2.7844
2.7741
1.9896
1.9507
1.6163
1.4010
1.2487
-0.0076
1
0.99
0.99
1.96
1.01
1.02
0.97
2.08
3.23
3.13
3.13

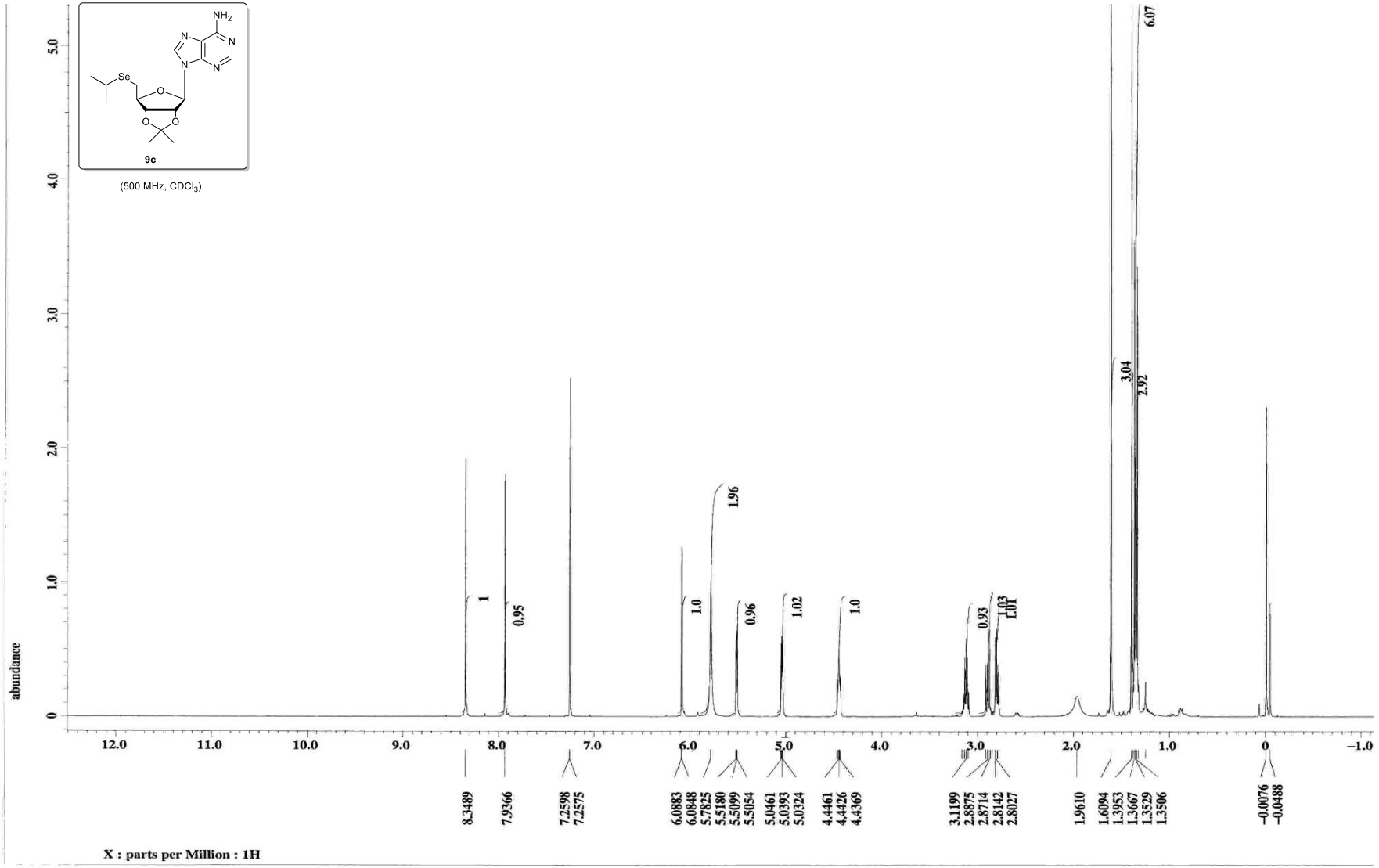

9a
(150 MHz, CDCl3)
abundance
0.4
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0 −20.0
155.7034
153.3097
149.4702
140.1827
120.4969
114.6372
90.9492
87.2916
84.4096
84.3235
77.3722
77.1615
76.9509
27.4398
27.2483
25.5057
5.2167
0.1325
X : parts per Million : 13C

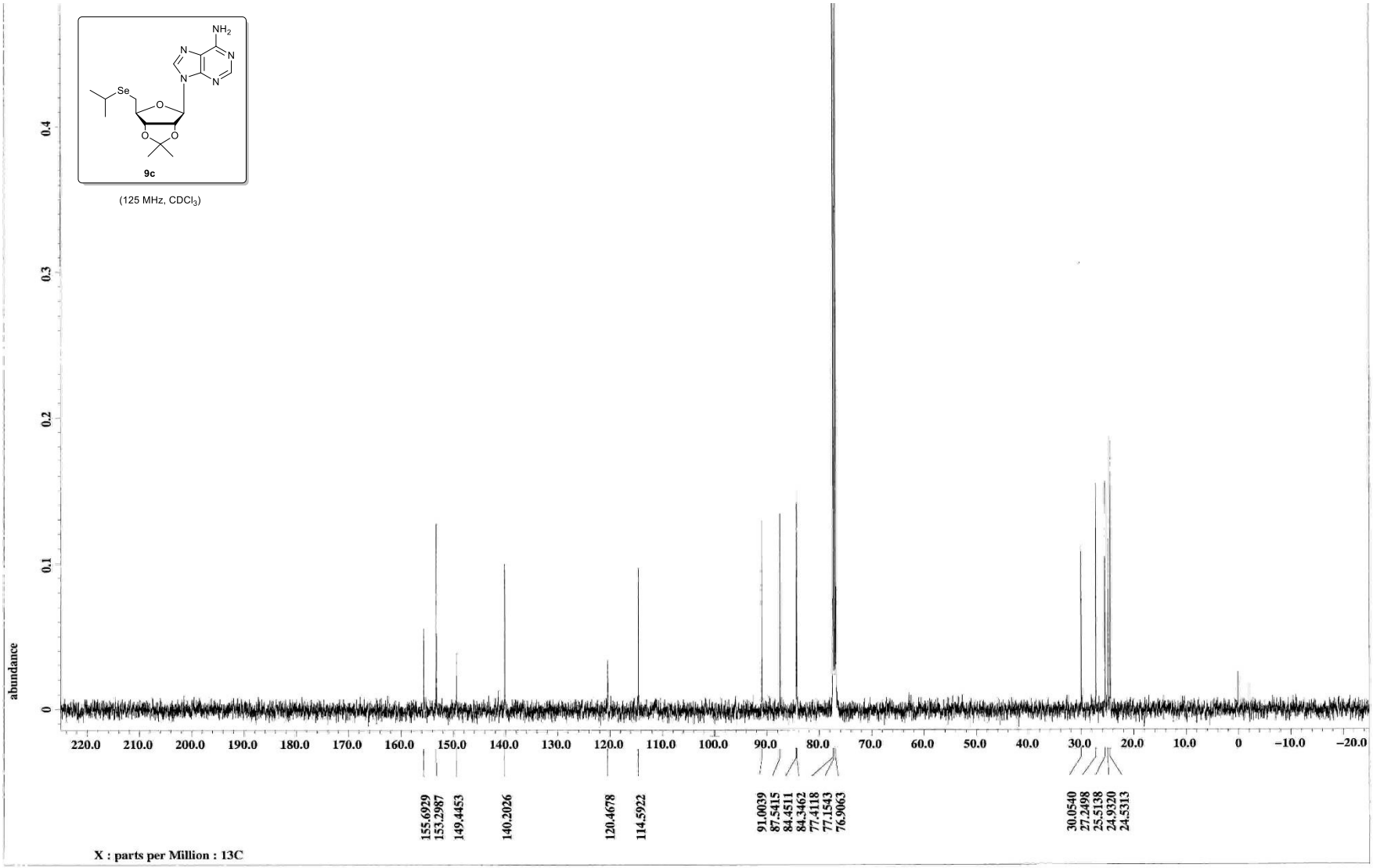

NH2
N
N
N
N
Se
O
O
O
9a
(113 MHz, CDCl3)
30.0
20.0
10.0
0
−10.0
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
53.2461

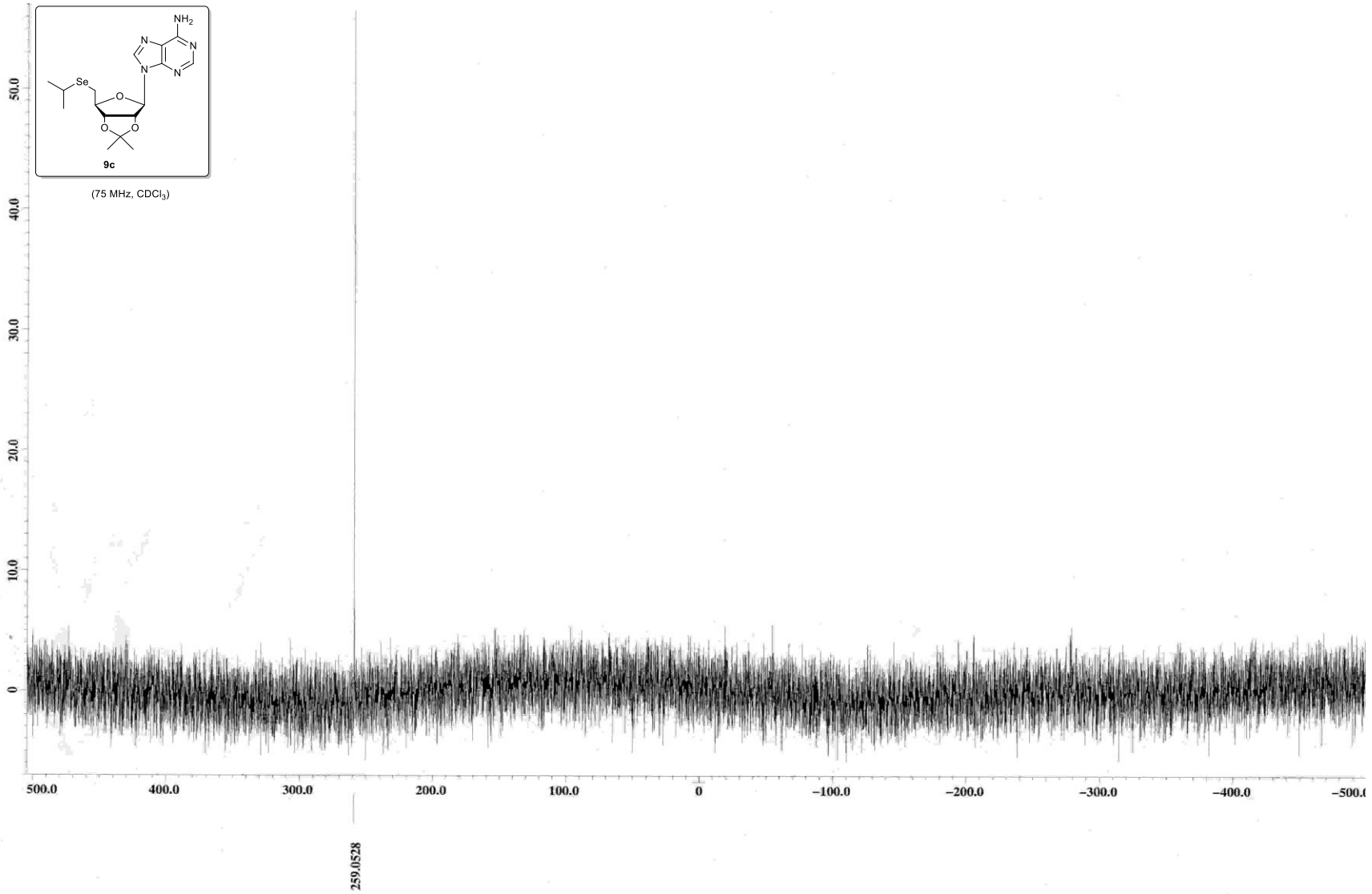

9b
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
1.01
1.01
1.72
1.0
1.03
1.03
1.02
2.01
1.98
3.02
8.3552
7.9852
7.2762
6.2681
6.1112
6.1055
5.5178
5.5018
5.4961
5.0574
5.0493
4.4709
4.4560
4.4434
2.8271
2.8110
2.5945
2.5751
1.6220
1.4067
1.3494
1.3299
0.0000

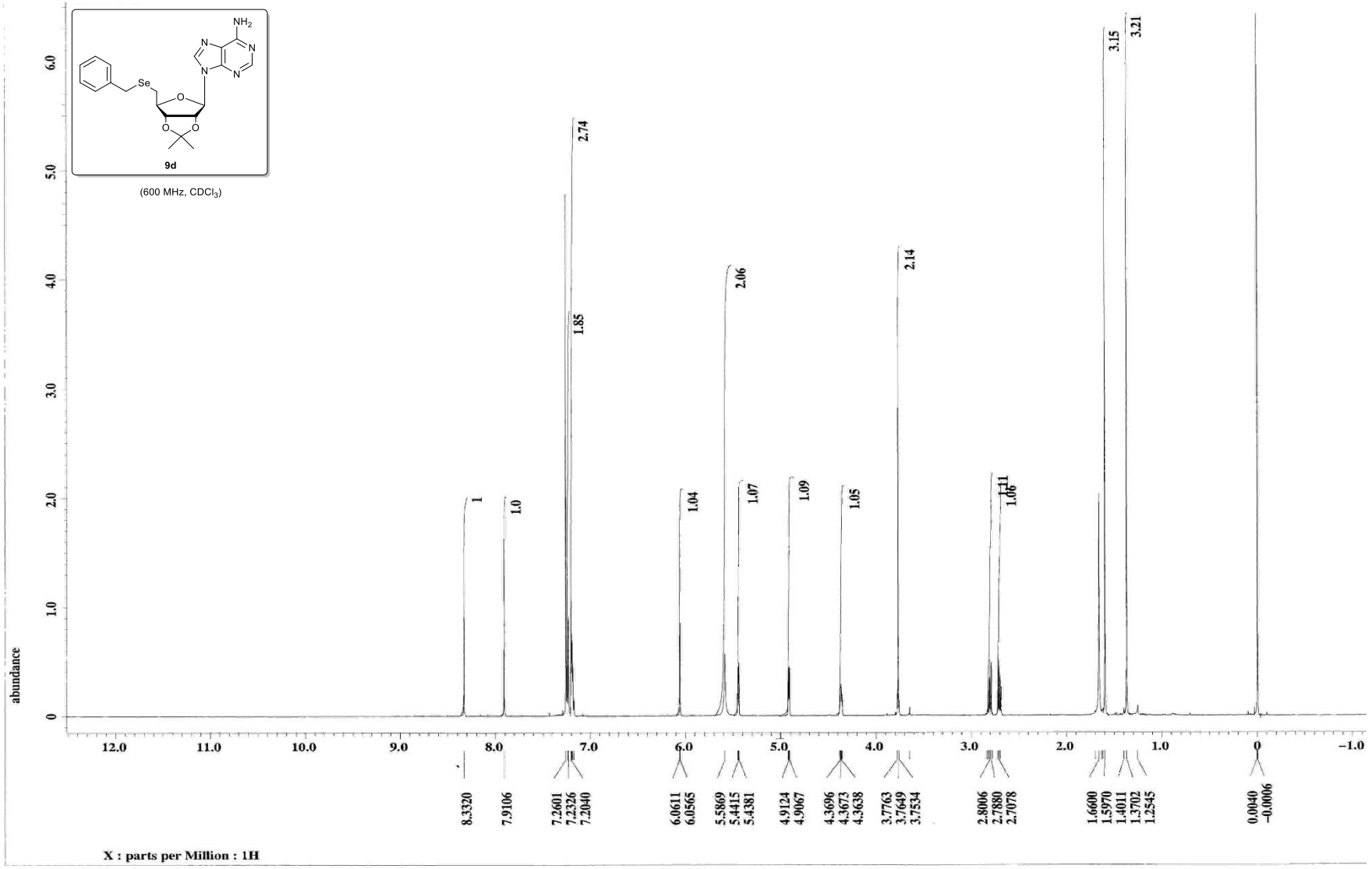

9b
(100 MHz, CDCl3)
abundance
X : parts per Million : 13C
155.3958
152.4869
149.2727
140.3266
120.3075
114.6518
90.9512
87.4128
84.3417
77.4843
77.1600
76.8358
29.8161
27.2219
25.4670
25.3907
18.3902
15.7770

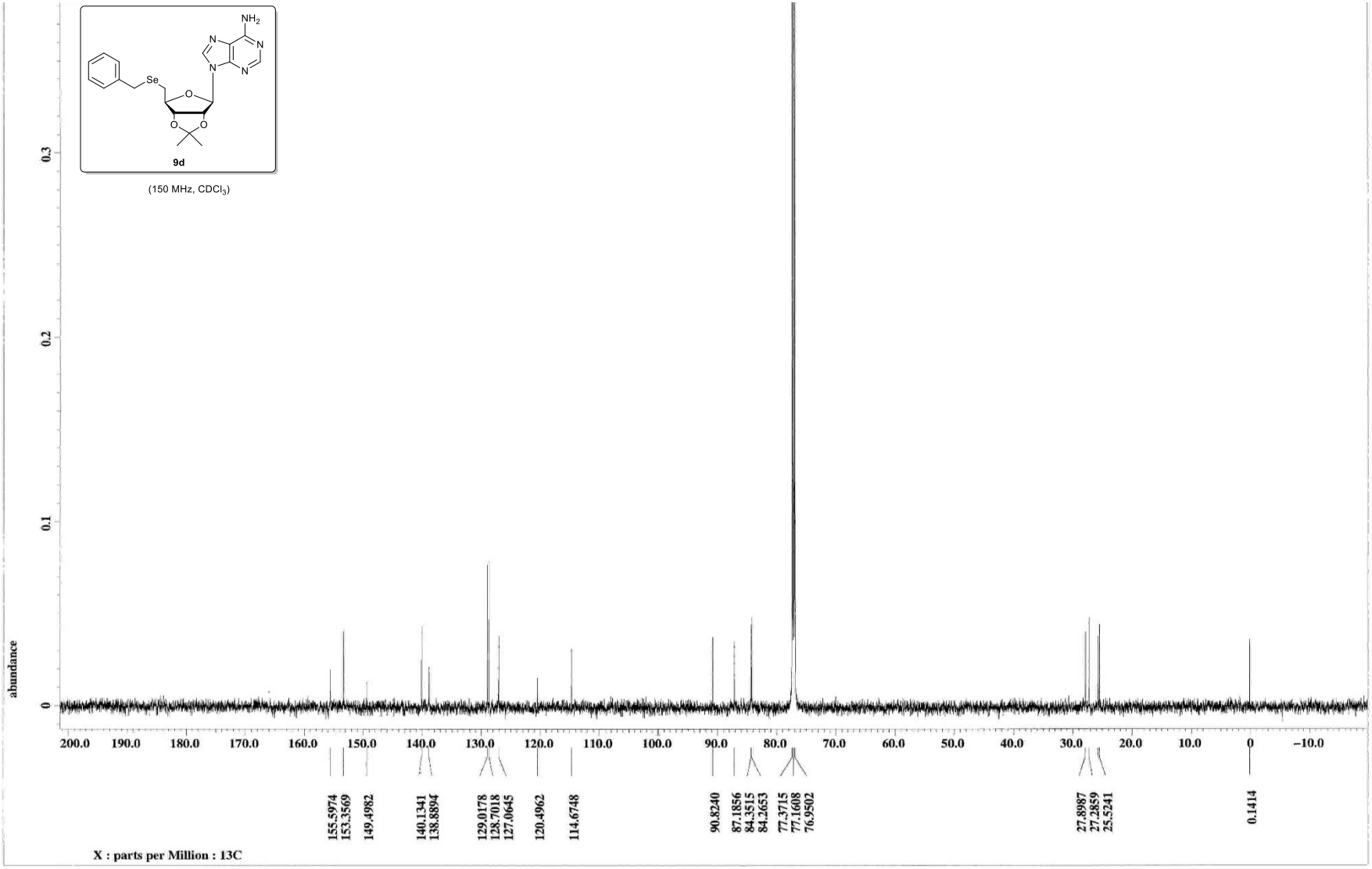

NH2
N
N
N
N
Se
O
O
O
9b
(94 MHz, CDCl3)
0.17
0.15
0.13
0.11
0.09
0.07
0.05
0.03
0.01
−0.01
−0.03
−0.05
−0.07
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
165.0414

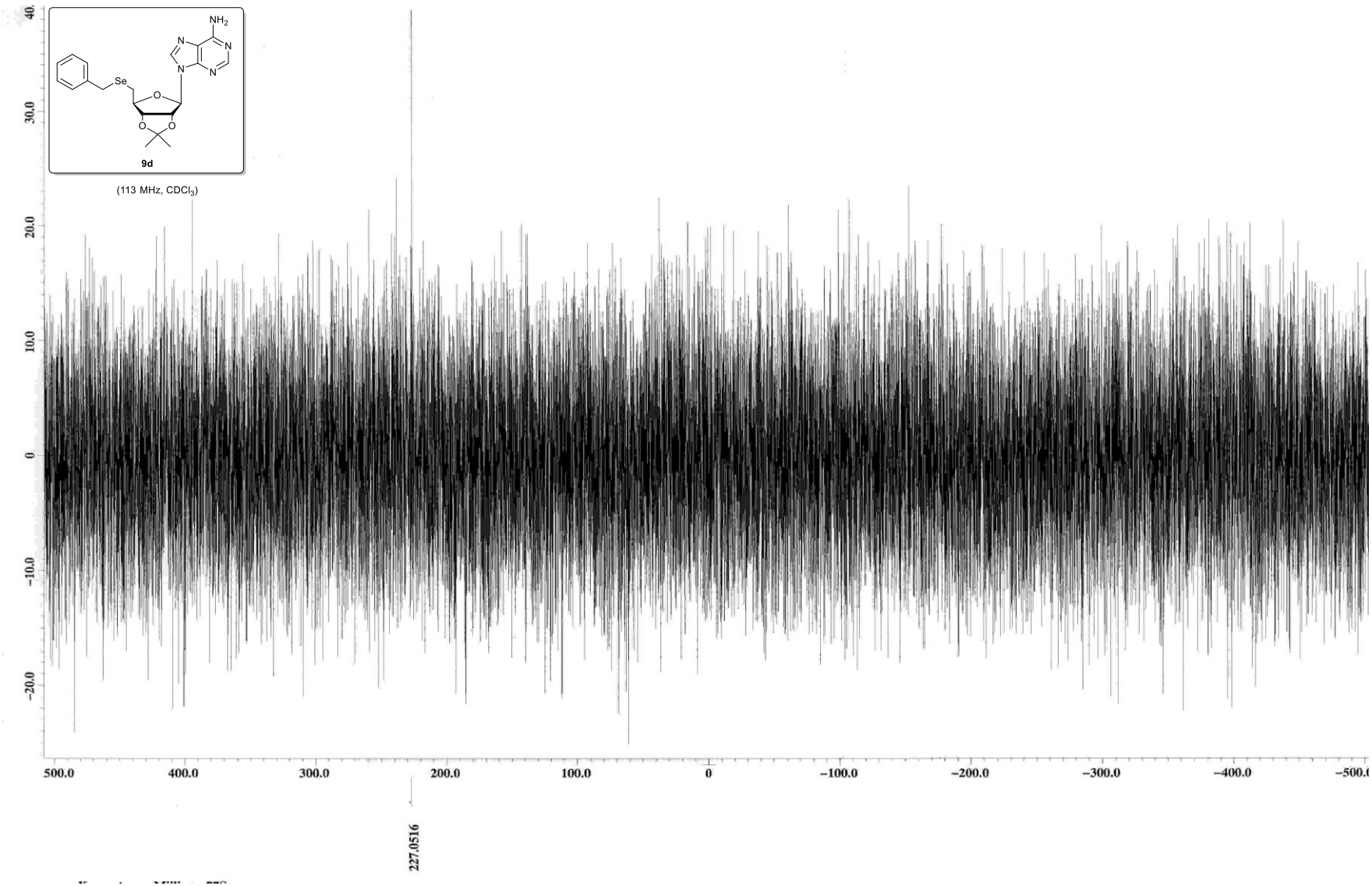

9c
(500 MHz, CDCl3)
abundance
X : parts per Million : 1H
8.3489
7.9366
7.2598
7.2575
6.0883
6.0848
5.7825
5.5180
5.5099
5.5054
5.0461
5.0393
5.0324
4.4461
4.4426
4.4369
3.1199
2.8875
2.8714
2.8142
2.8027
1.9610
1.6094
1.3953
1.3667
1.3529
1.3506
−0.0076
−0.0488

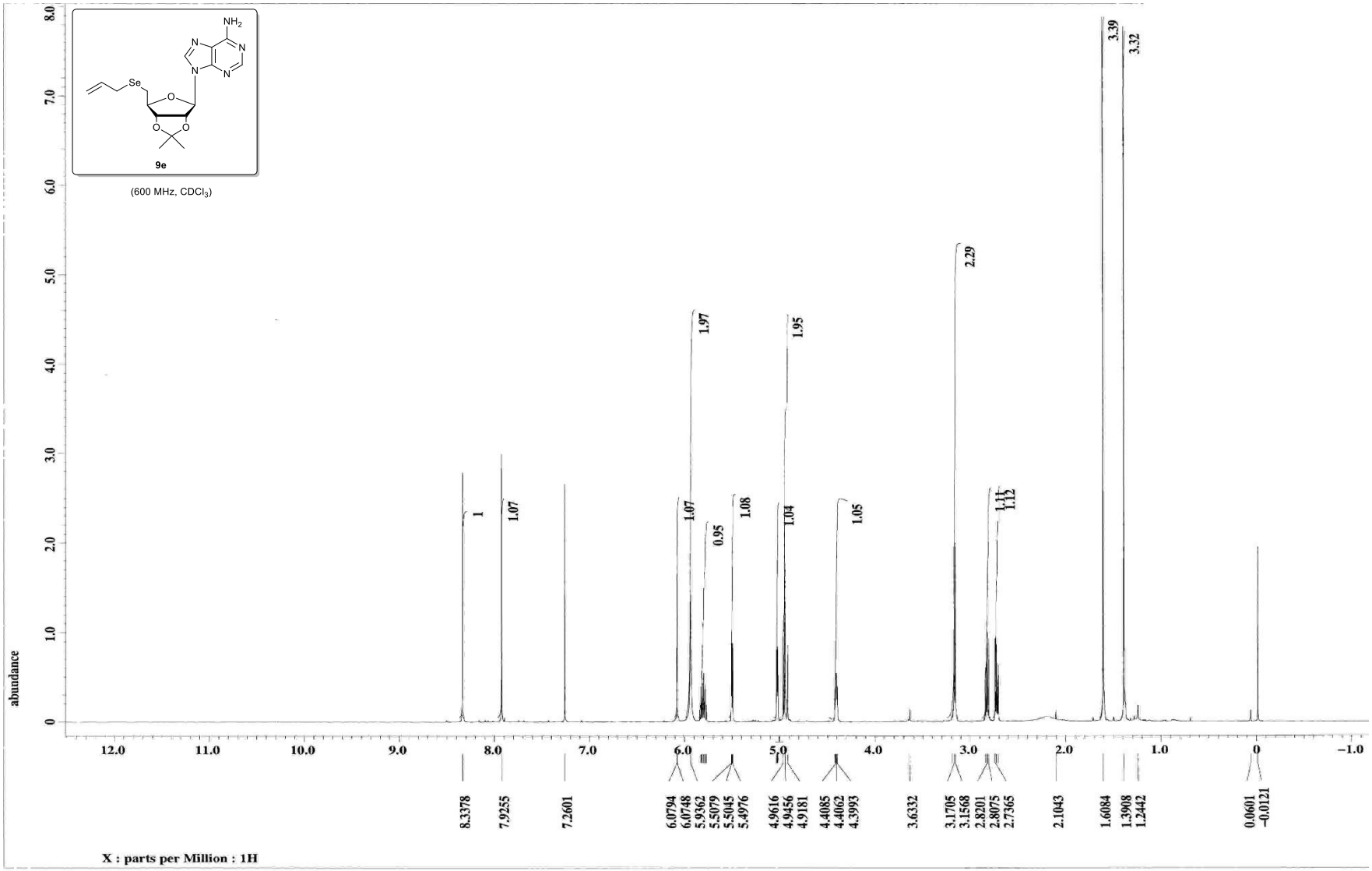

NH2
Se
O
O
O
9c
(125 MHz, CDCl3)
abundance
0
0.1
0.2
0.3
0.4
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
−20.0
155.6929
153.2987
149.4453
140.2026
120.4678
114.5922
91.0039
87.5415
84.4511
84.3462
77.4118
77.1543
76.9063
30.0540
27.2498
25.5138
24.9320
24.5313
X : parts per Million : 13C

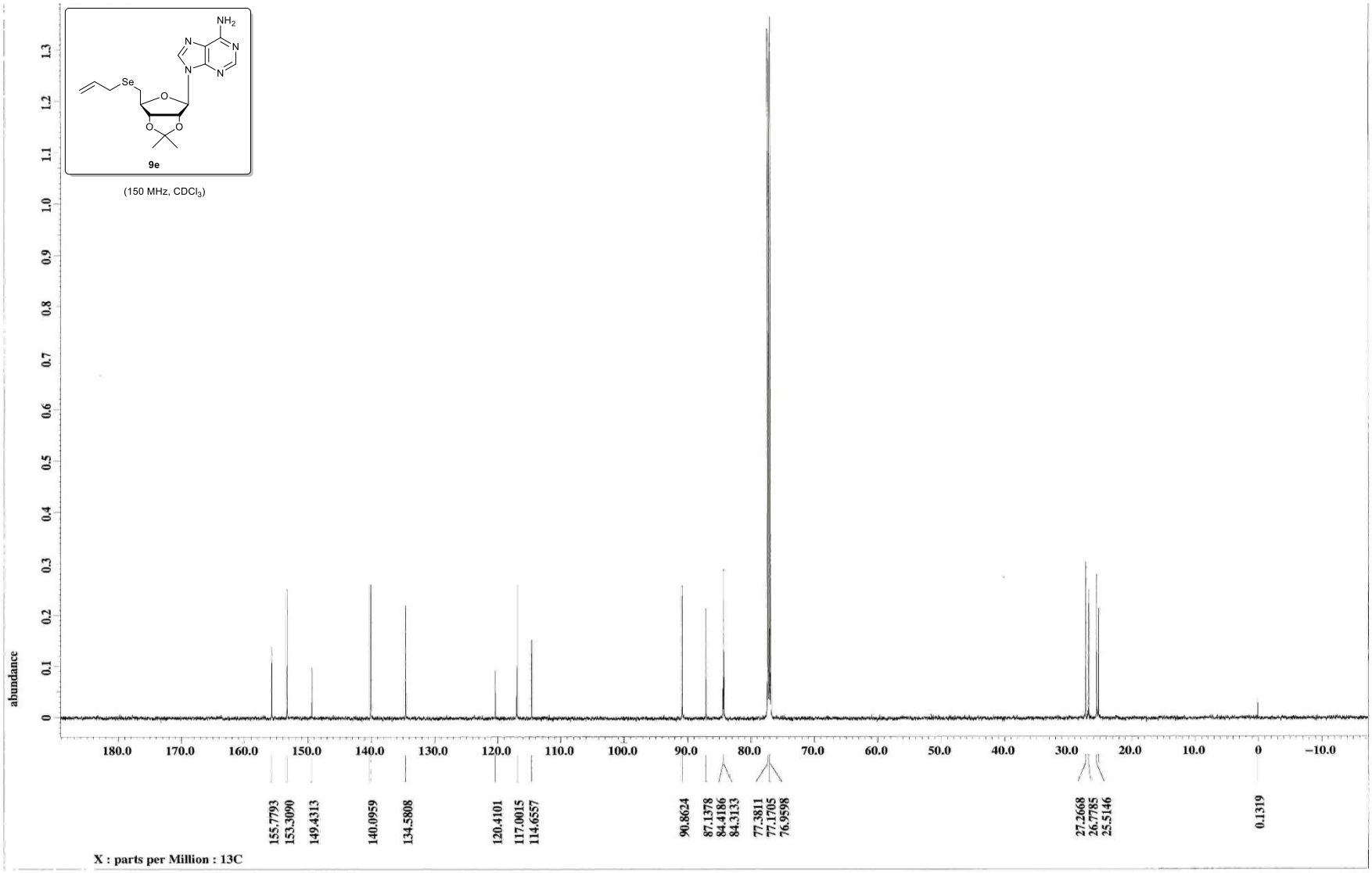

NH2
N
N
N
N
Se
O
O
O
9c
(75 MHz, CDCl3)
50.0
40.0
30.0
20.0
10.0
0
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
−500.0
259.0528

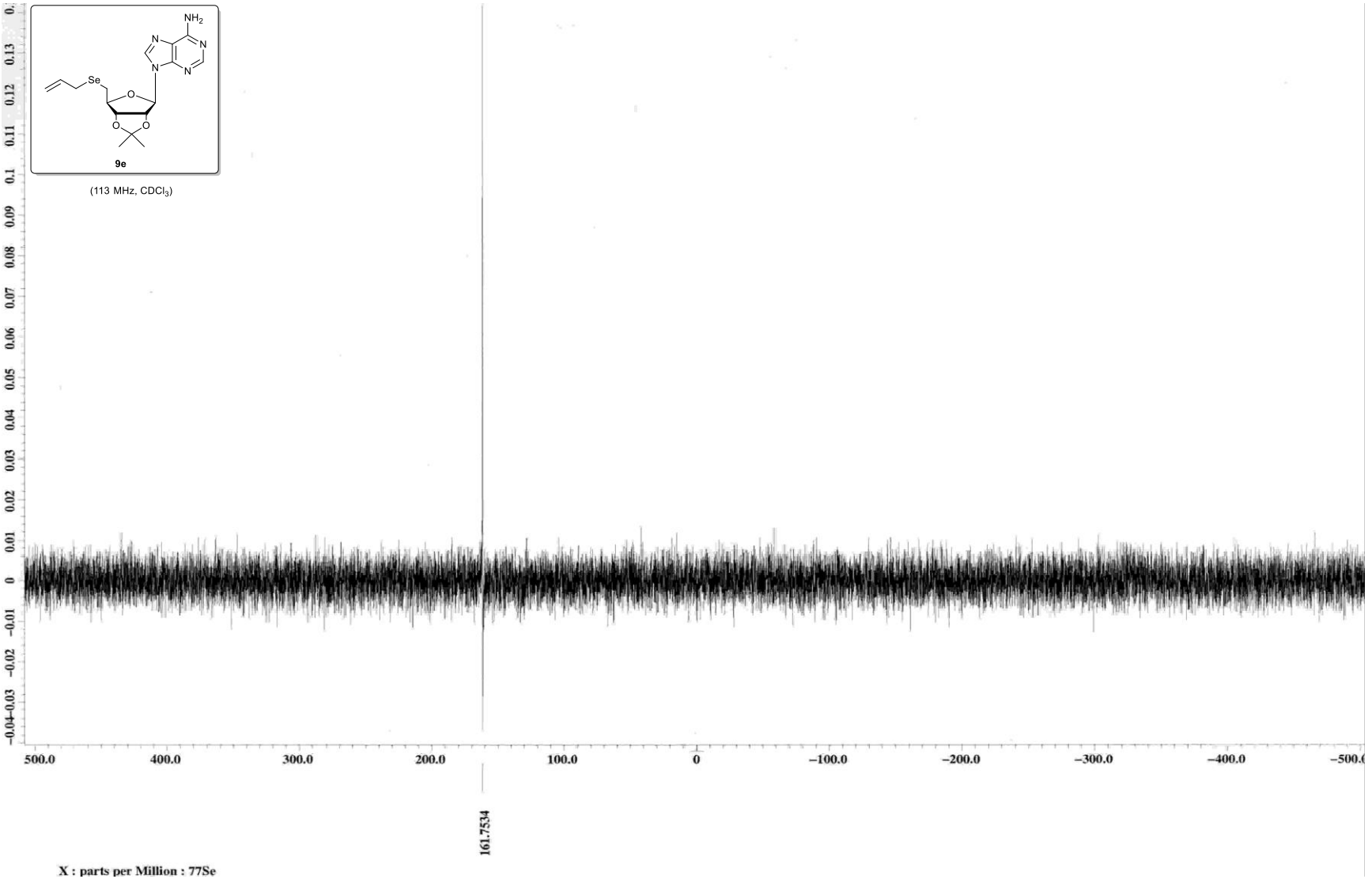

9d
(600 MHz, CDCl3)
abundance
X : parts per Million : 1H
8.3320
7.9106
7.2601
7.2326
7.2040
6.0611
6.0565
5.5869
5.4415
5.4381
4.9124
4.9067
4.3696
4.3673
4.3638
3.7763
3.7649
3.7534
2.8006
2.7880
2.7078
1.6600
1.5970
1.4011
1.3702
1.2545
0.0040
−0.0006

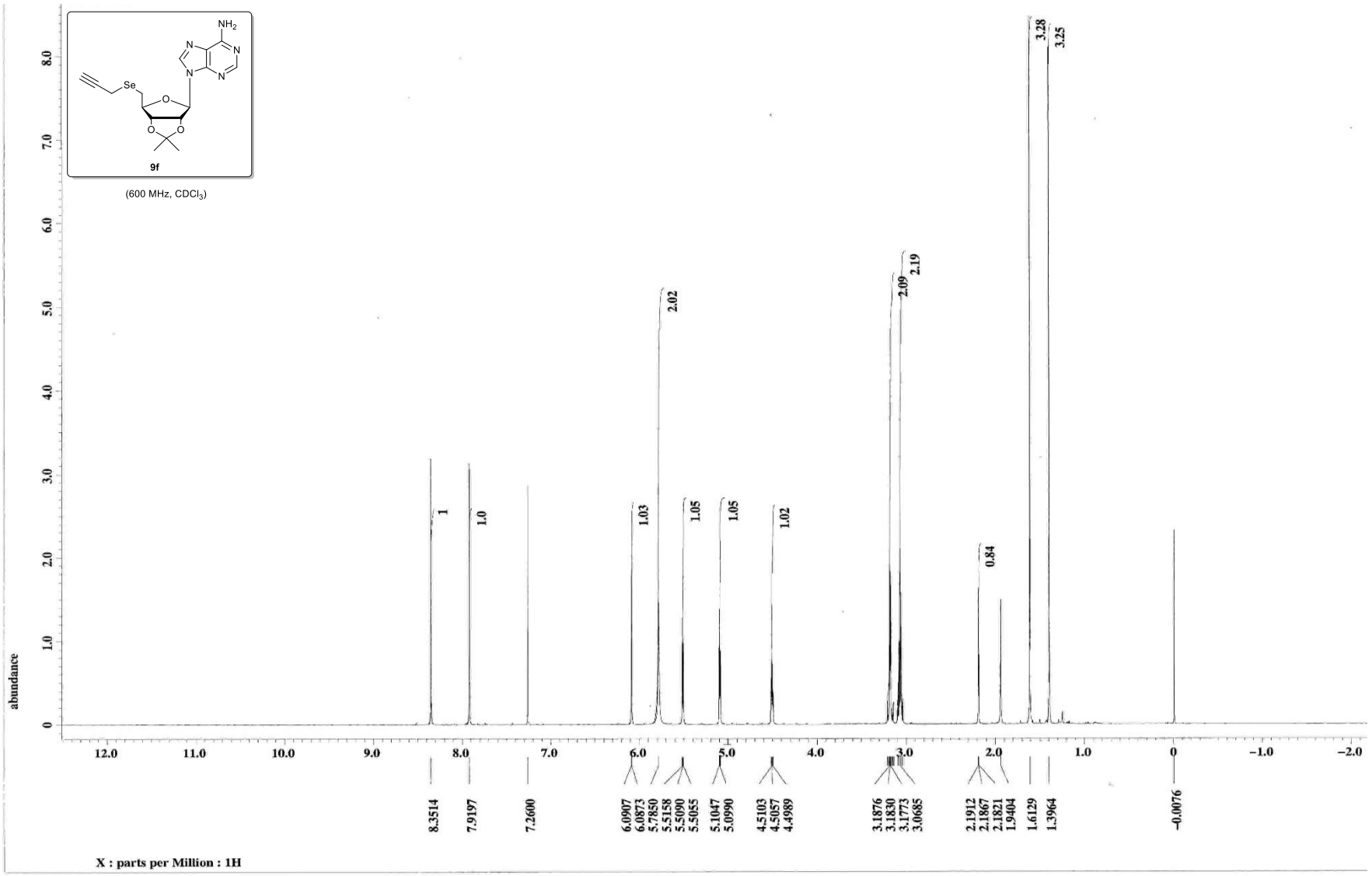

9d
(150 MHz, CDCl3)
abundance
0.3
0.2
0.1
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0
155.5974
153.3569
149.4982
140.1341
138.8894
129.0178
128.7018
127.0645
120.4962
114.6748
90.8240
87.1856
84.3515
84.2653
77.3715
77.1608
76.9502
27.8987
27.2859
25.5241
0.1414
X : parts per Million : 13C

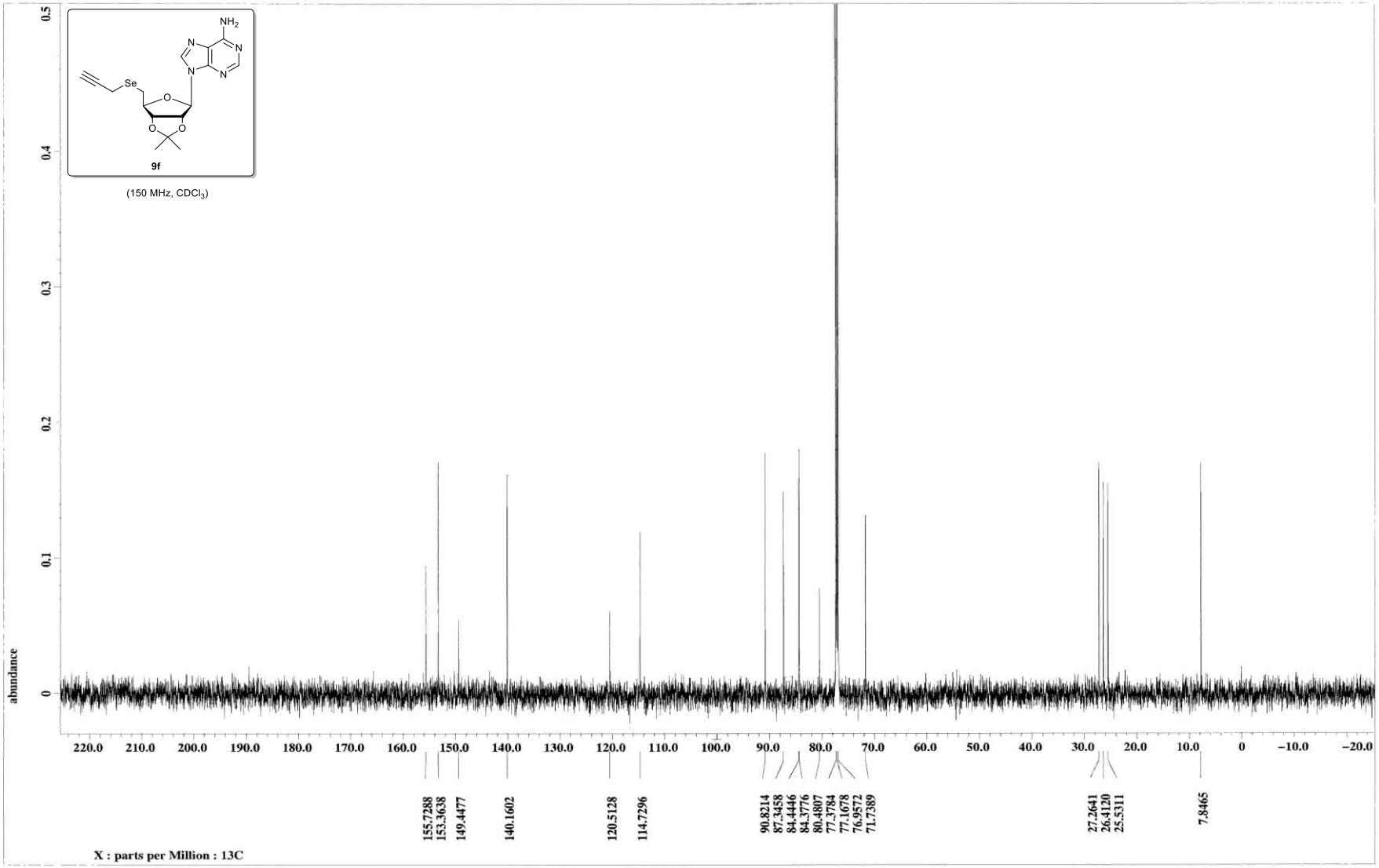

9d
(113 MHz, CDCl3)
40.0
30.0
20.0
10.0
0
-10.0
-20.0
500.0
400.0
300.0
200.0
100.0
0
-100.0
-200.0
-300.0
-400.0
-500.0
227.0516

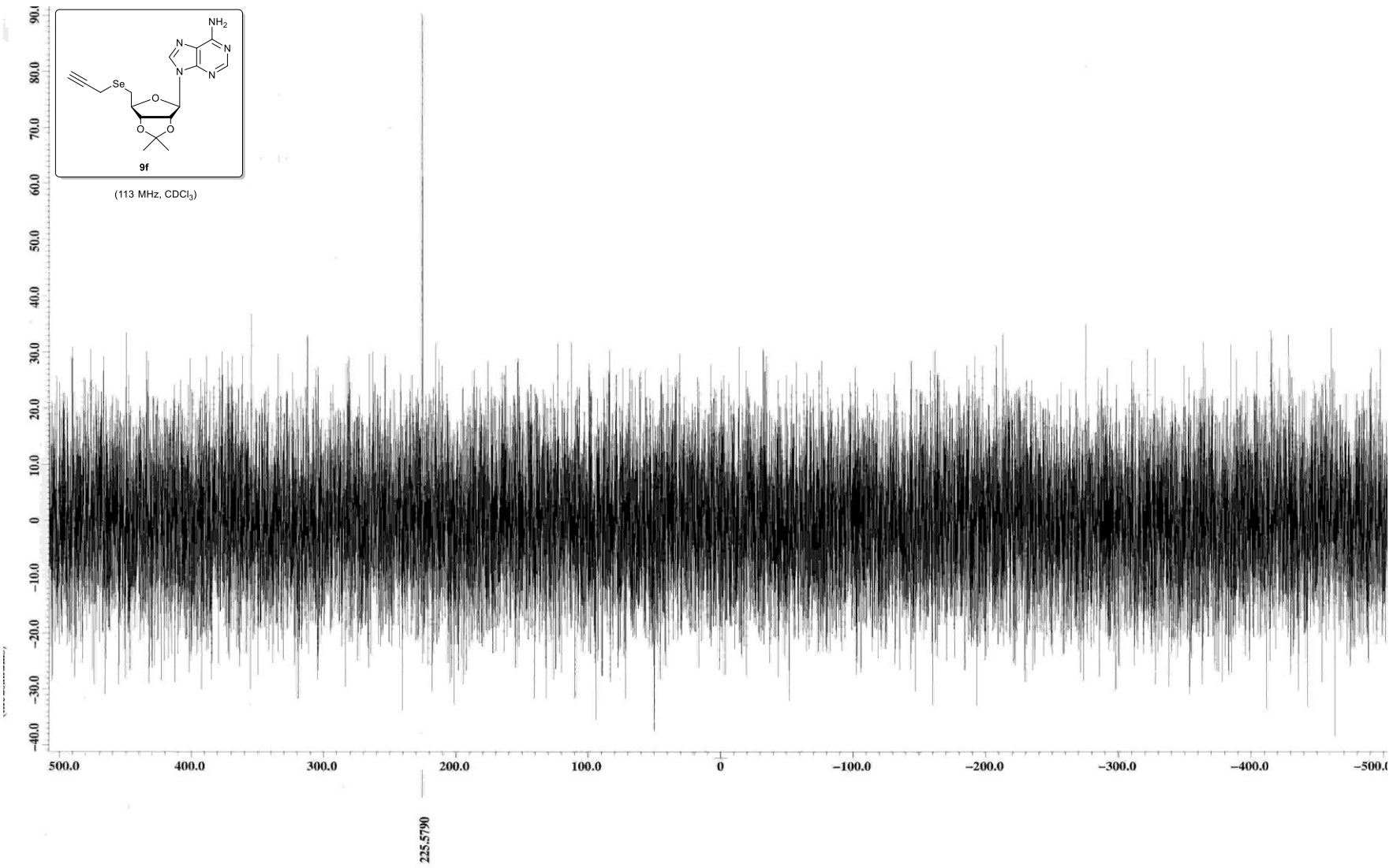

9e
(600 MHz, CDCl3)
abundance
X : parts per Million : 1H
8.3378
7.9255
7.2601
6.0794
6.0748
5.9362
5.5079
5.5045
5.4976
4.9616
4.9456
4.9181
4.4085
4.4062
4.3993
3.6332
3.1705
3.1568
2.8201
2.8075
2.7365
2.1043
1.6084
1.3908
1.2442
0.0601
-0.0121

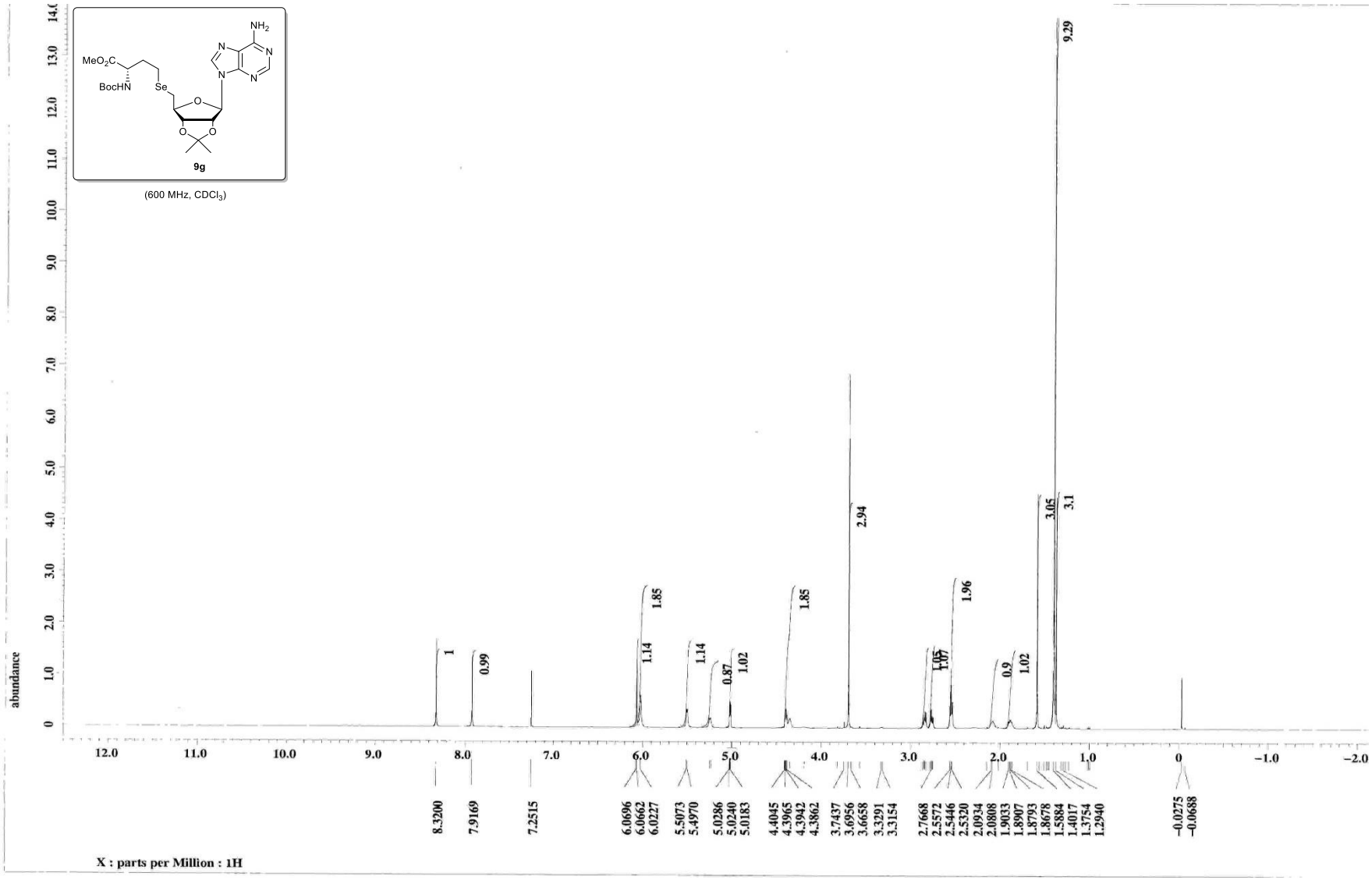

9e
(150 MHz, CDCl3)
abundance
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
155.7793
153.3090
149.4313
140.0959
134.5808
120.4101
117.0015
114.6557
90.8624
87.1378
84.4186
84.3133
77.3811
77.1705
76.9598
27.2668
26.7785
25.5146
0.1319
X : parts per Million : 13C

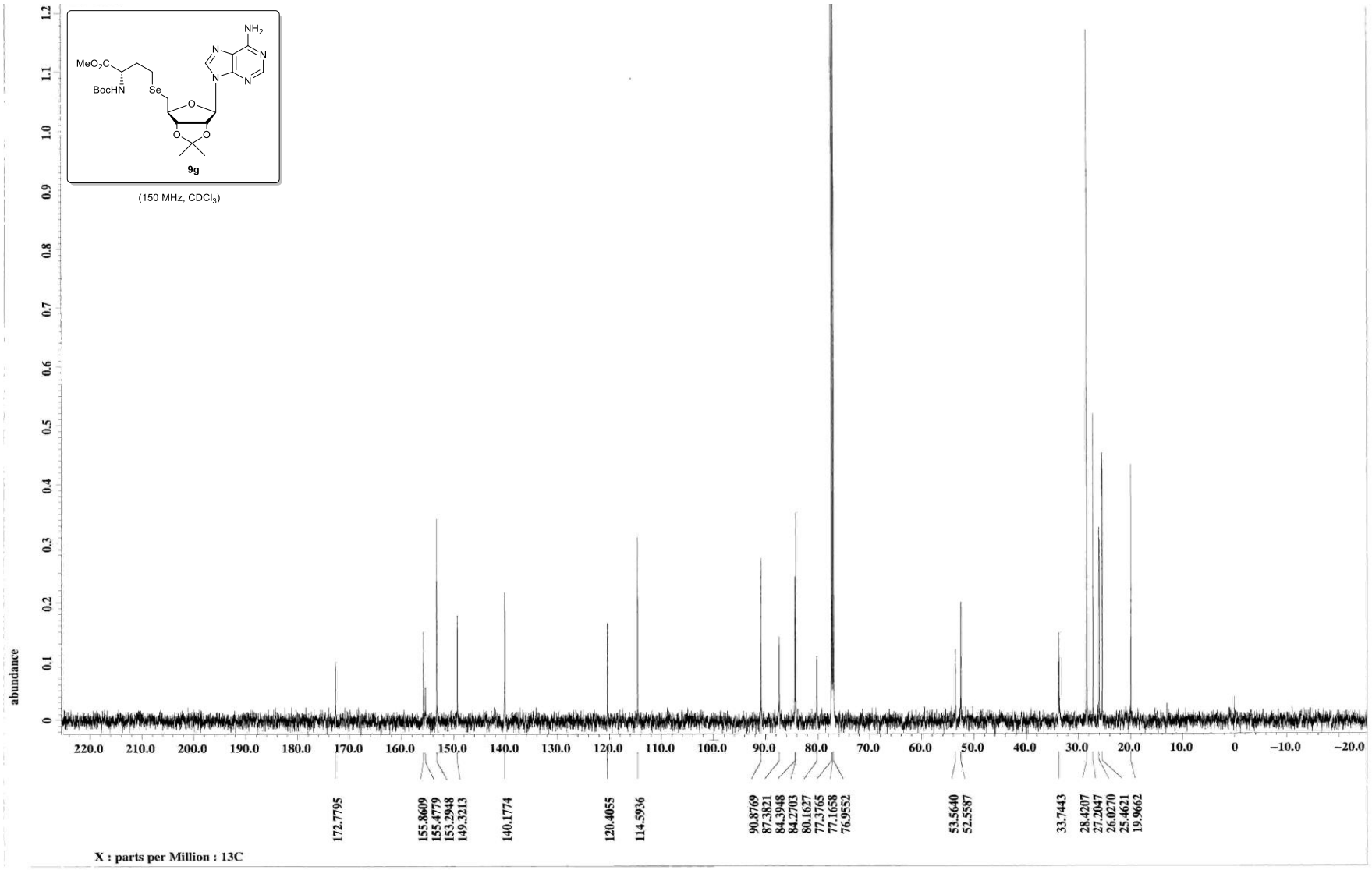

NH2
N
N
N
N
Se
O
O
O
9e
(113 MHz, CDCl3)
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
−0.01
−0.02
−0.03
−0.04
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
161.7534
X : parts per Million : 77Se

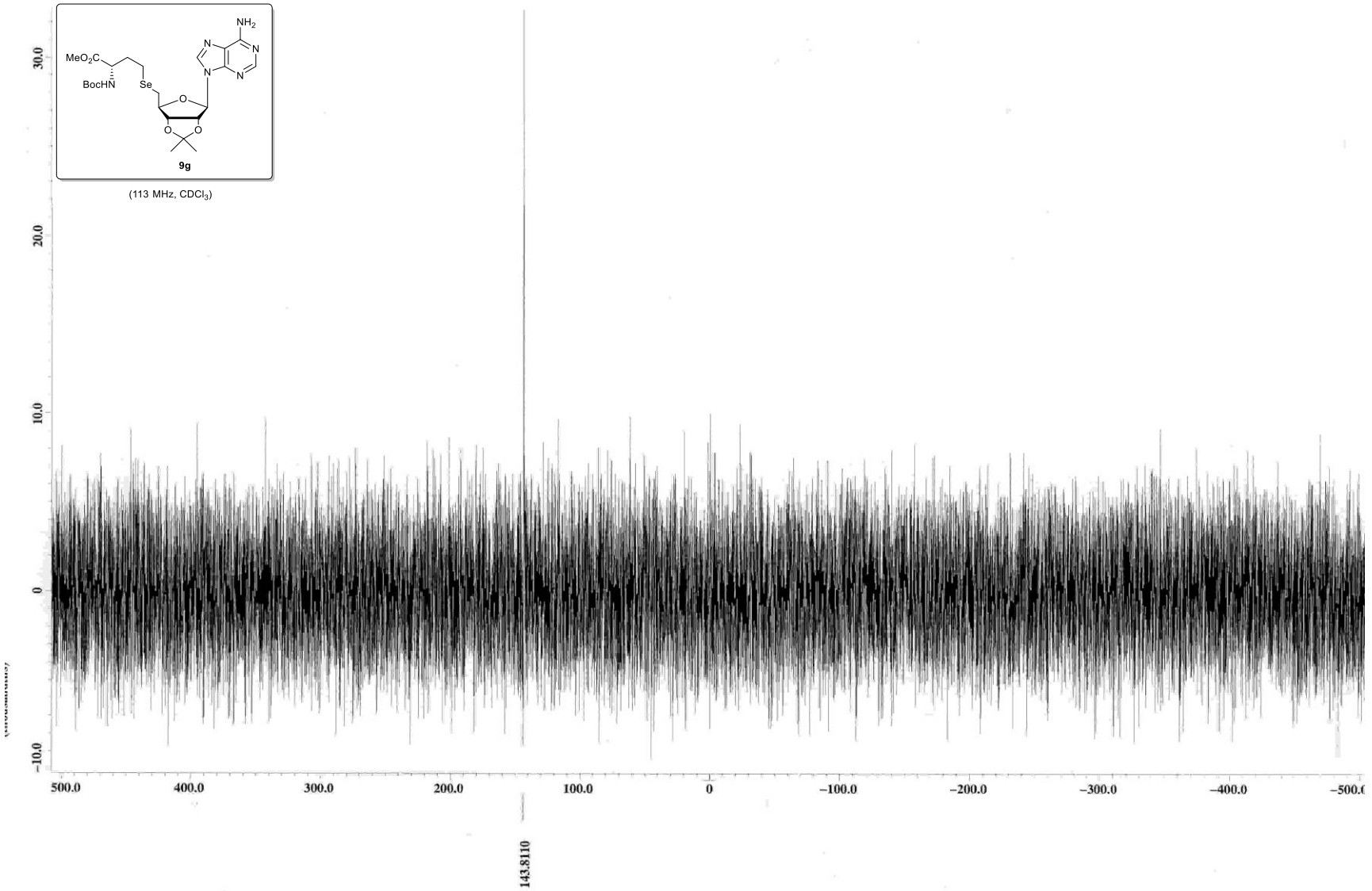

9f
(600 MHz, CDCl3)
abundance
X : parts per Million : 1H
8.3514
7.9197
7.2600
6.0907
6.0873
5.7850
5.5158
5.5090
5.5055
5.1047
5.0990
4.5103
4.5057
4.4989
3.1876
3.1830
3.1773
3.0685
2.1912
2.1867
2.1821
1.9404
1.6129
1.3964
-0.0076
1
1.0
1.03
2.02
1.05
1.05
1.02
0.84
2.09
2.19
3.28
3.25

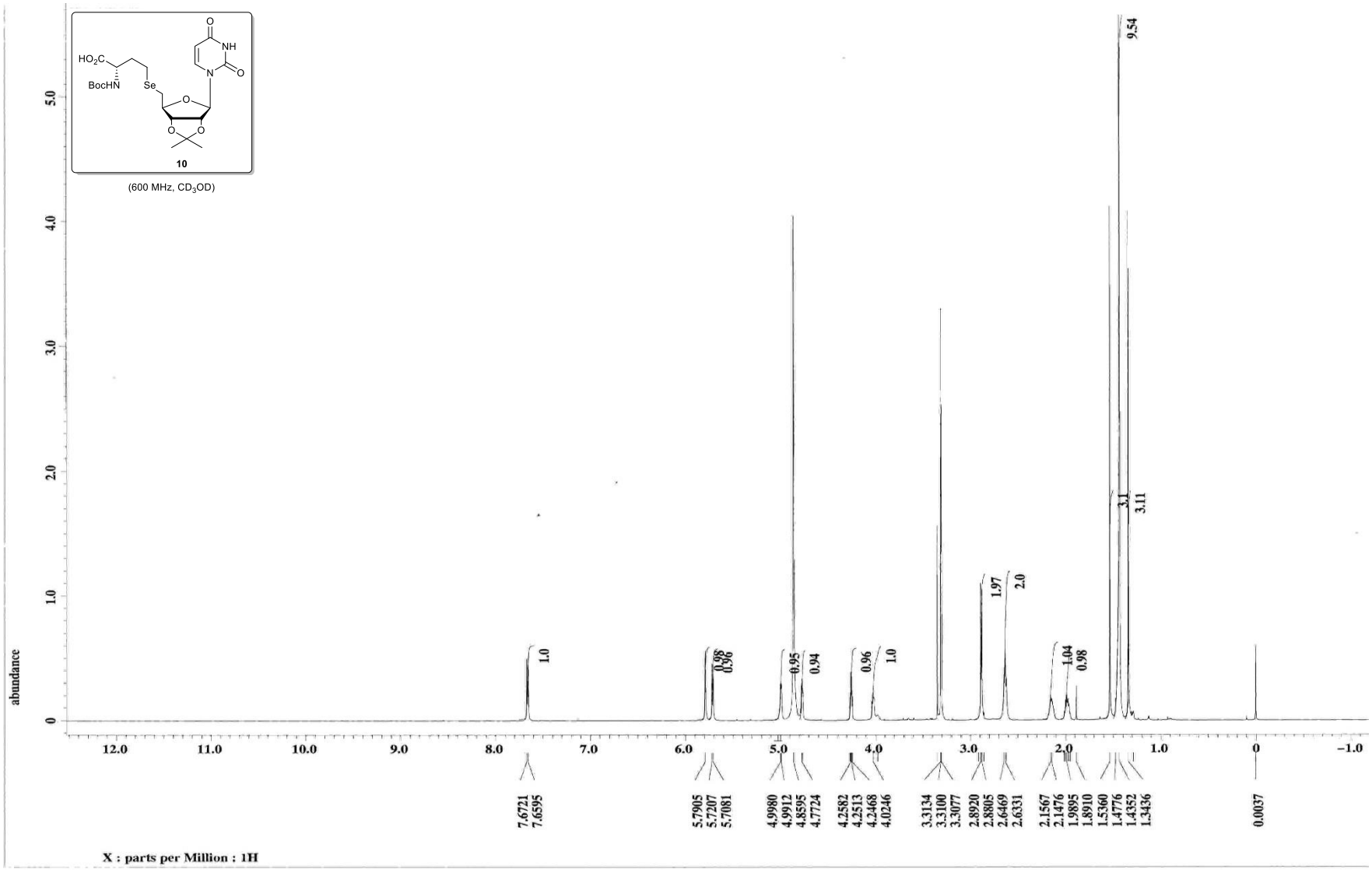

9f
(150 MHz, CDCl3)
abundance
X : parts per Million : 13C
155.7288
153.3638
149.4477
140.1602
120.5128
114.7296
90.8214
87.3458
84.4446
84.3776
80.4807
77.3784
77.1678
76.9572
71.7389
27.2641
26.4120
25.5311
7.8465

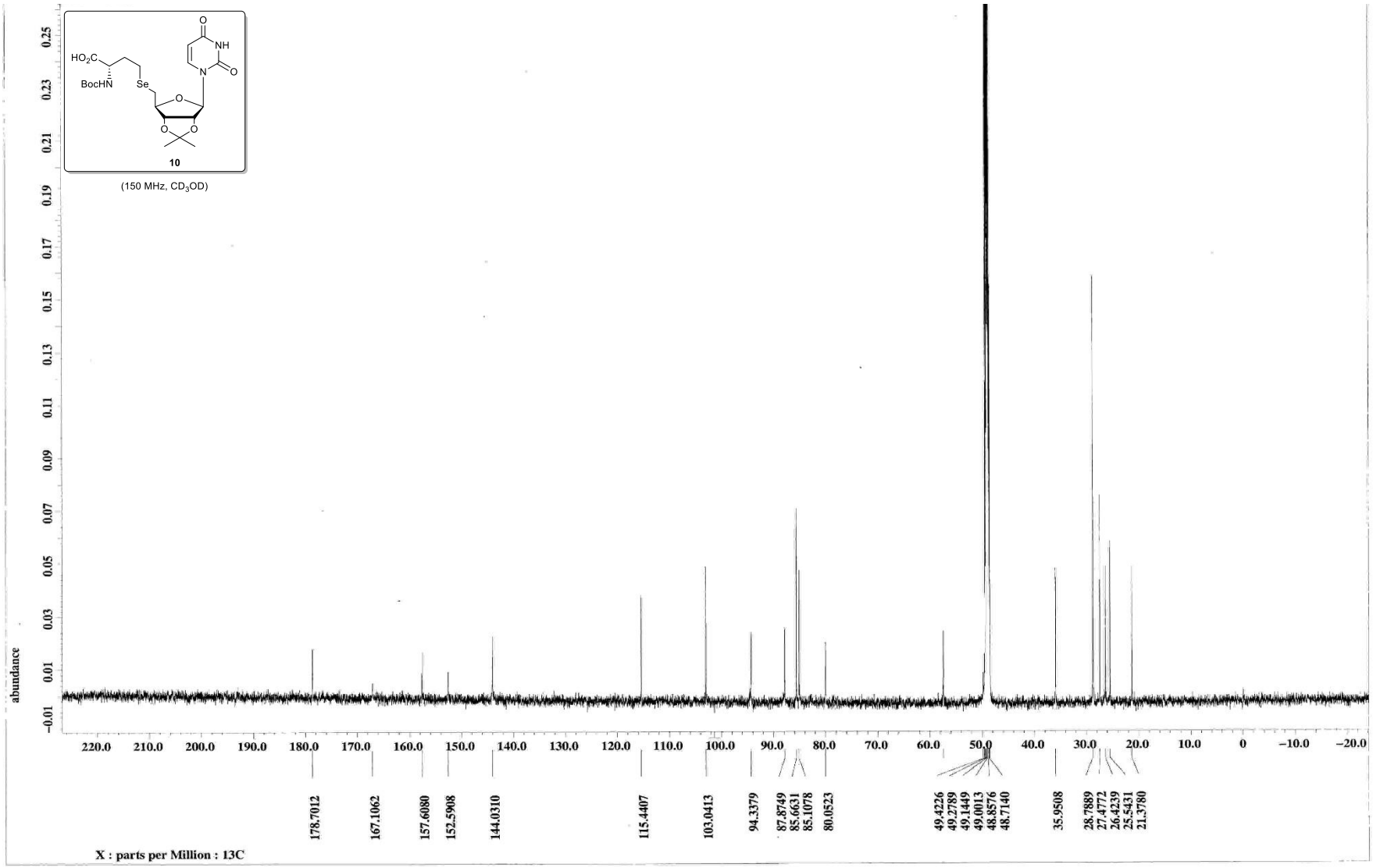

NH2
N
N
N
N
Se
O
O
O
9f
(113 MHz, CDCl3)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
-30.0
-40.0
500.0
400.0
300.0
200.0
100.0
0
-100.0
-200.0
-300.0
-400.0
225.5790
X : parts per Million : 77Se

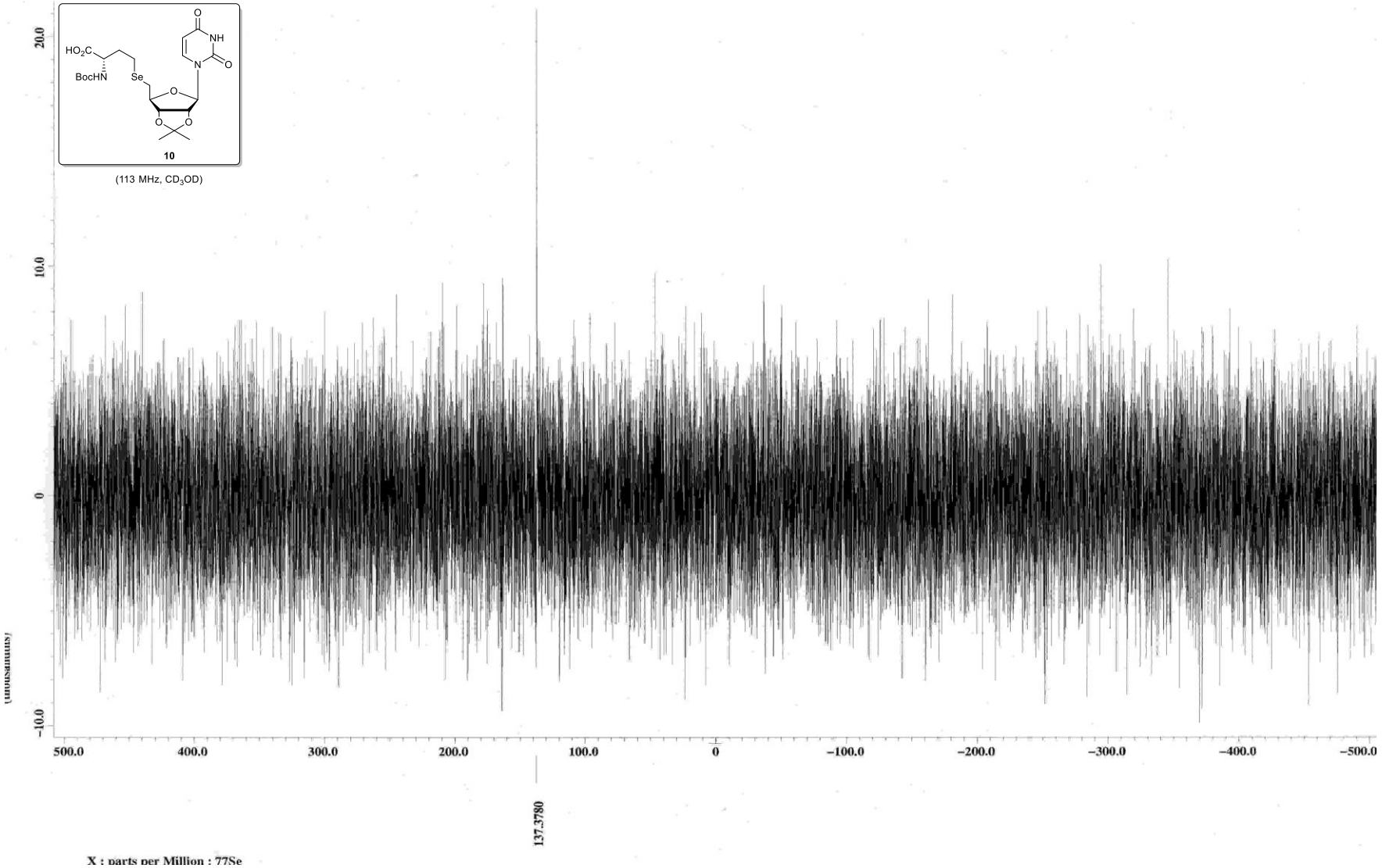

MeO2C
BocHN
Se
NH2
N
N
N
N
O
O
O
9g
(600 MHz, CDCl3)
abundance
9.29
3.1
3.05
2.94
1.96
1.85
1.85
1.14
1.14
1.02
1
0.99
0.87
1.02
0.9
1.05
1.07
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
−2.0
8.3200
7.9169
7.2515
6.0696
6.0662
6.0227
5.5073
5.4970
5.0286
5.0240
5.0183
4.4045
4.3965
4.3942
4.3862
3.7437
3.6956
3.6658
3.3291
3.3154
2.7668
2.5572
2.5446
2.5320
2.0934
2.0808
1.9033
1.8907
1.8793
1.8678
1.5884
1.4017
1.3754
1.2940
−0.0275
−0.0688
X : parts per Million : 1H

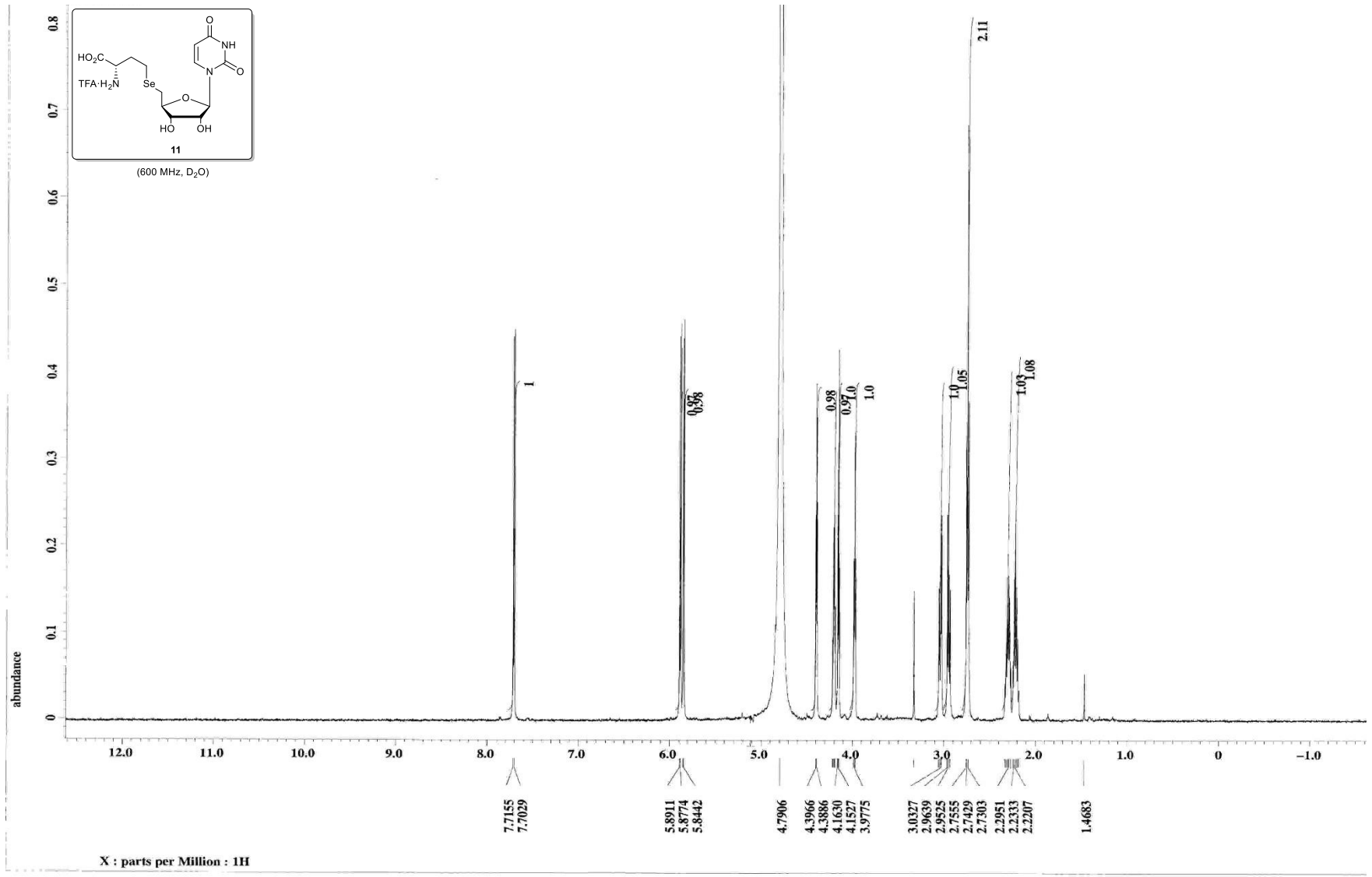

9g
(150 MHz, CDCl3)
abundance
X : parts per Million : 13C
172.7795
155.8609
155.4779
153.2948
149.3213
140.1774
120.4055
114.5936
90.8769
87.3821
84.3948
84.2703
80.1627
77.3765
77.1658
76.9552
53.5640
52.5587
33.7443
28.4207
27.2047
26.0270
25.4621
19.9662

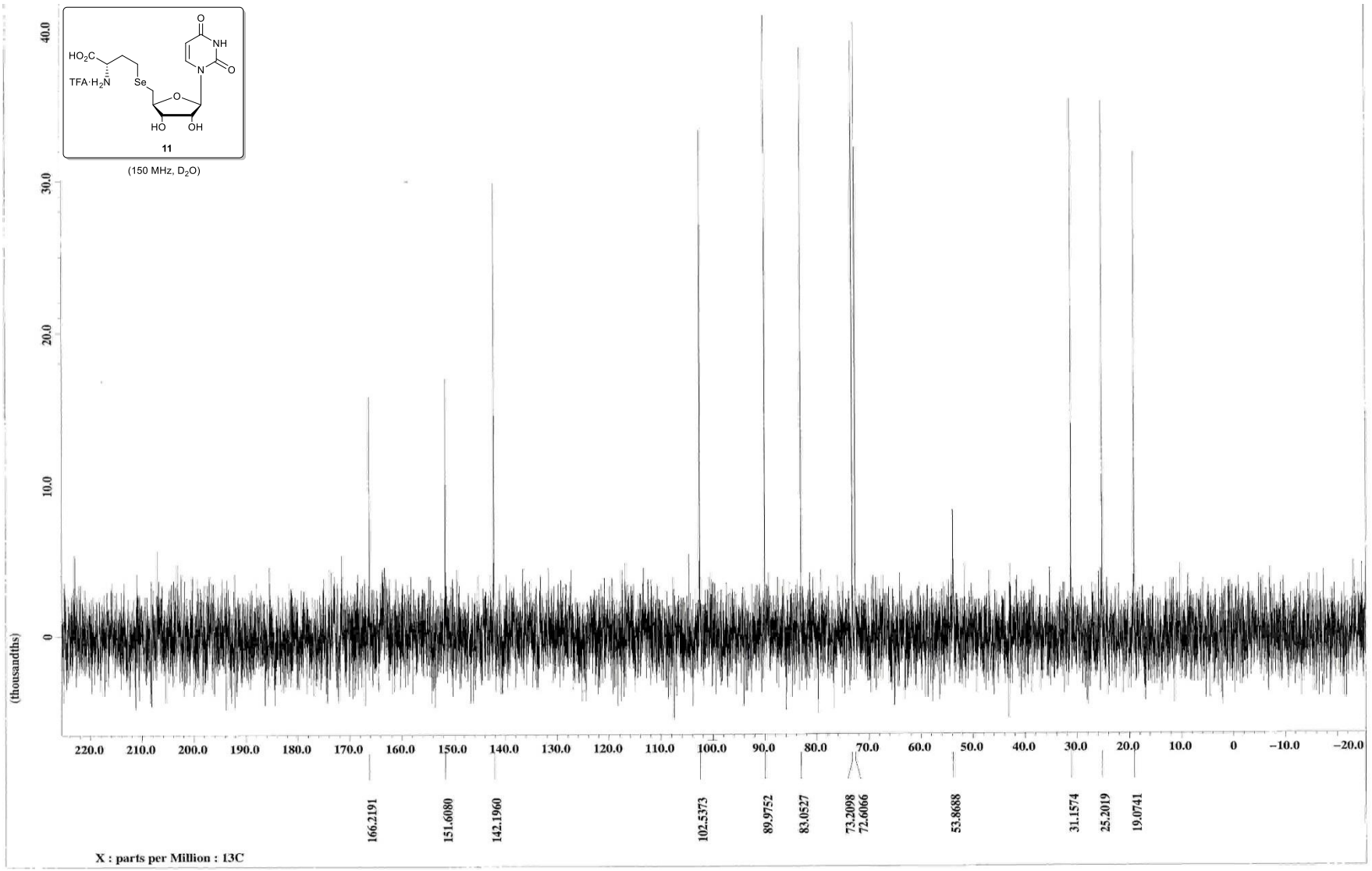

MeO2C
BocHN
Se
NH2
N
N
N
N
O
O
O
9g
(113 MHz, CDCl3)
30.0
20.0
10.0
0
−10.0
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
−500.0
143.8110

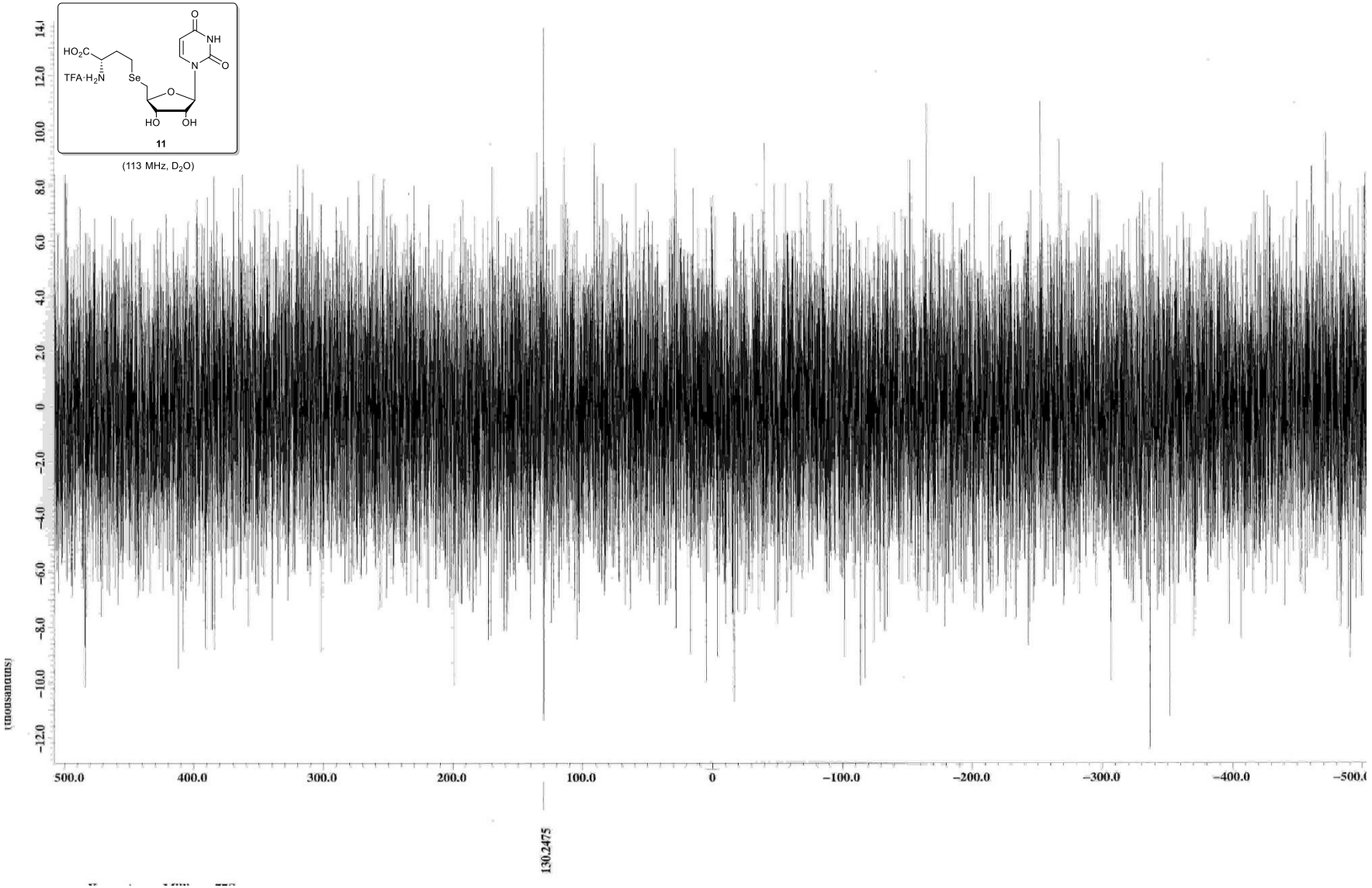

HO2C
BocHN
Se
NH
O
O
O
O
O
10
(600 MHz, CD3OD)
abundance
X : parts per Million : 1H
9.54
3.1
3.11
1.97
2.0
1.04
0.98
1.0
0.95
0.94
0.96
1.0
0.98
0.96
7.6721
7.6595
5.7905
5.7207
5.7081
4.9980
4.9912
4.8595
4.7724
4.2582
4.2513
4.2468
4.0246
3.3134
3.3100
3.3077
2.8920
2.8805
2.6469
2.6331
2.1567
2.1476
1.9895
1.8910
1.5360
1.4776
1.4352
1.3436
0.0037

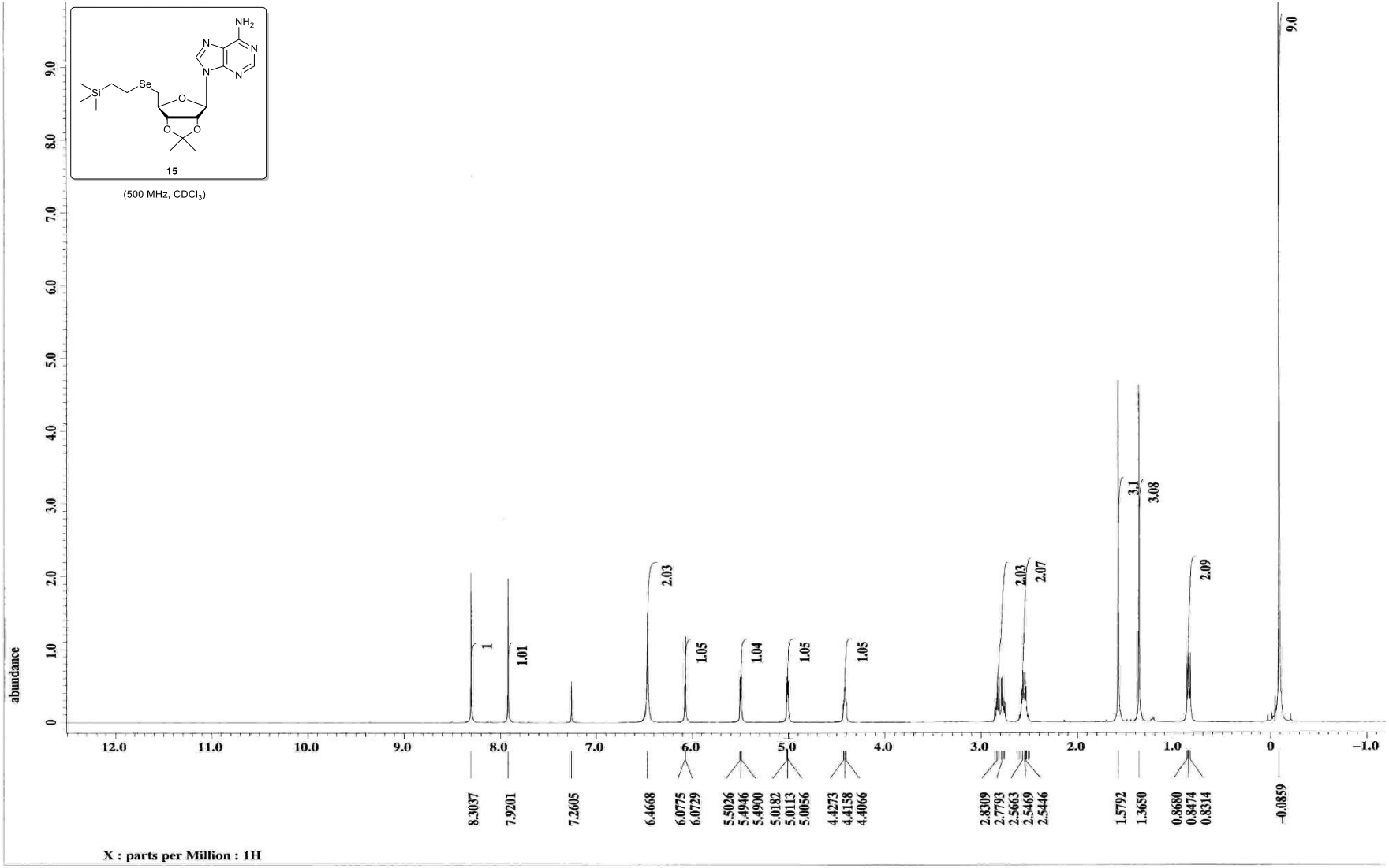

HO2C
BocHN
Se
O
NH
N
O
O
O
O
10
(150 MHz, CD3OD)
abundance
0.25
0.23
0.21
0.19
0.17
0.15
0.13
0.11
0.09
0.07
0.05
0.03
0.01
−0.01
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
−20.0
178.7012
167.1062
157.6080
152.5908
144.0310
115.4407
103.0413
94.3379
87.8749
85.6631
85.1078
80.0523
49.4226
49.2789
49.1449
49.0013
48.8576
48.7140
35.9508
28.7889
27.4772
26.4239
25.5431
21.3780
X : parts per Million : 13C

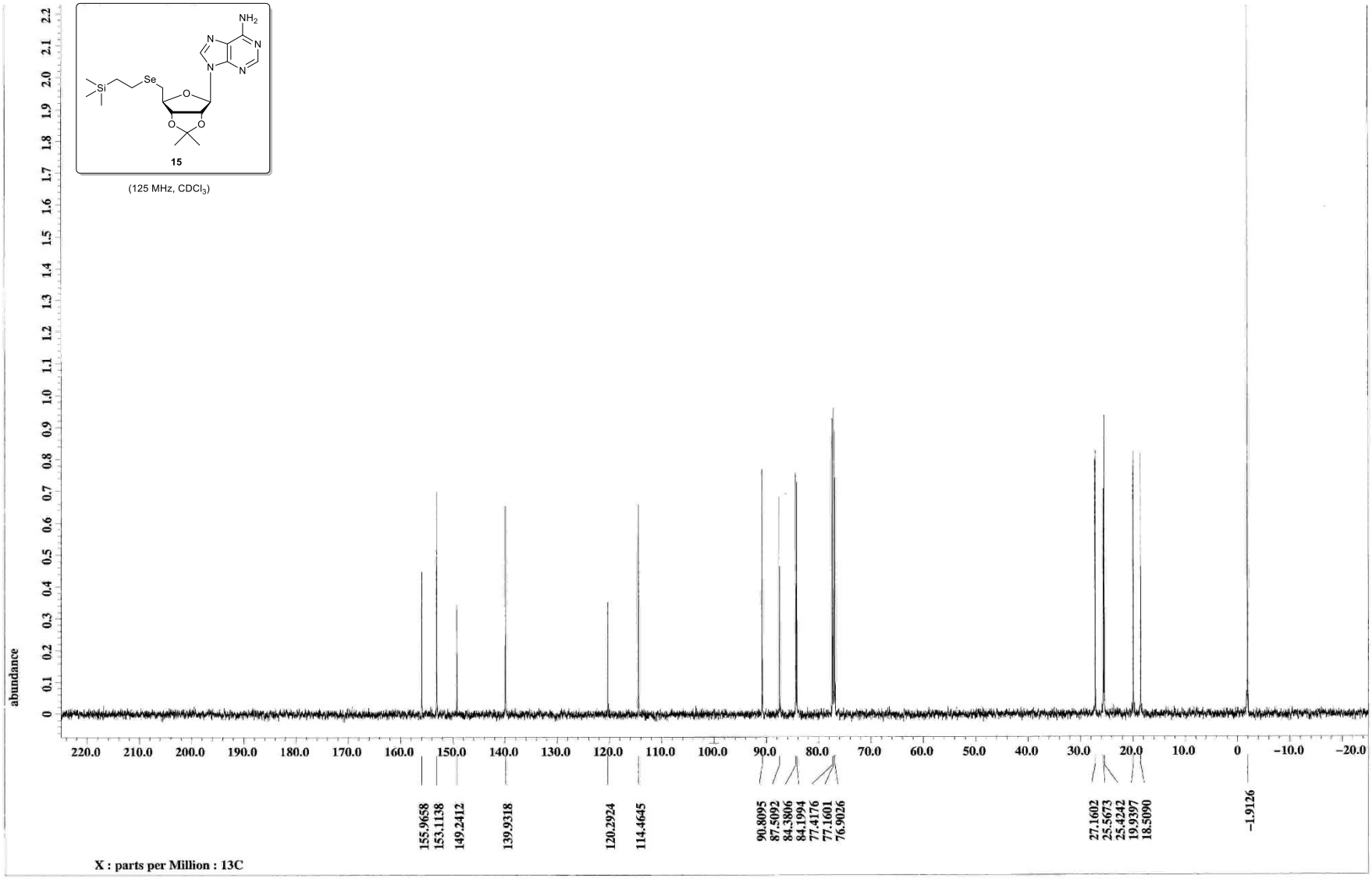

HO2C
BocHN
Se
NH
O
N
O
O
O
O
10
(113 MHz, CD3OD)
20.0
10.0
0
−10.0
(unnormalized)
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
−500.0
137.3780
X : parts per Million : 77Se

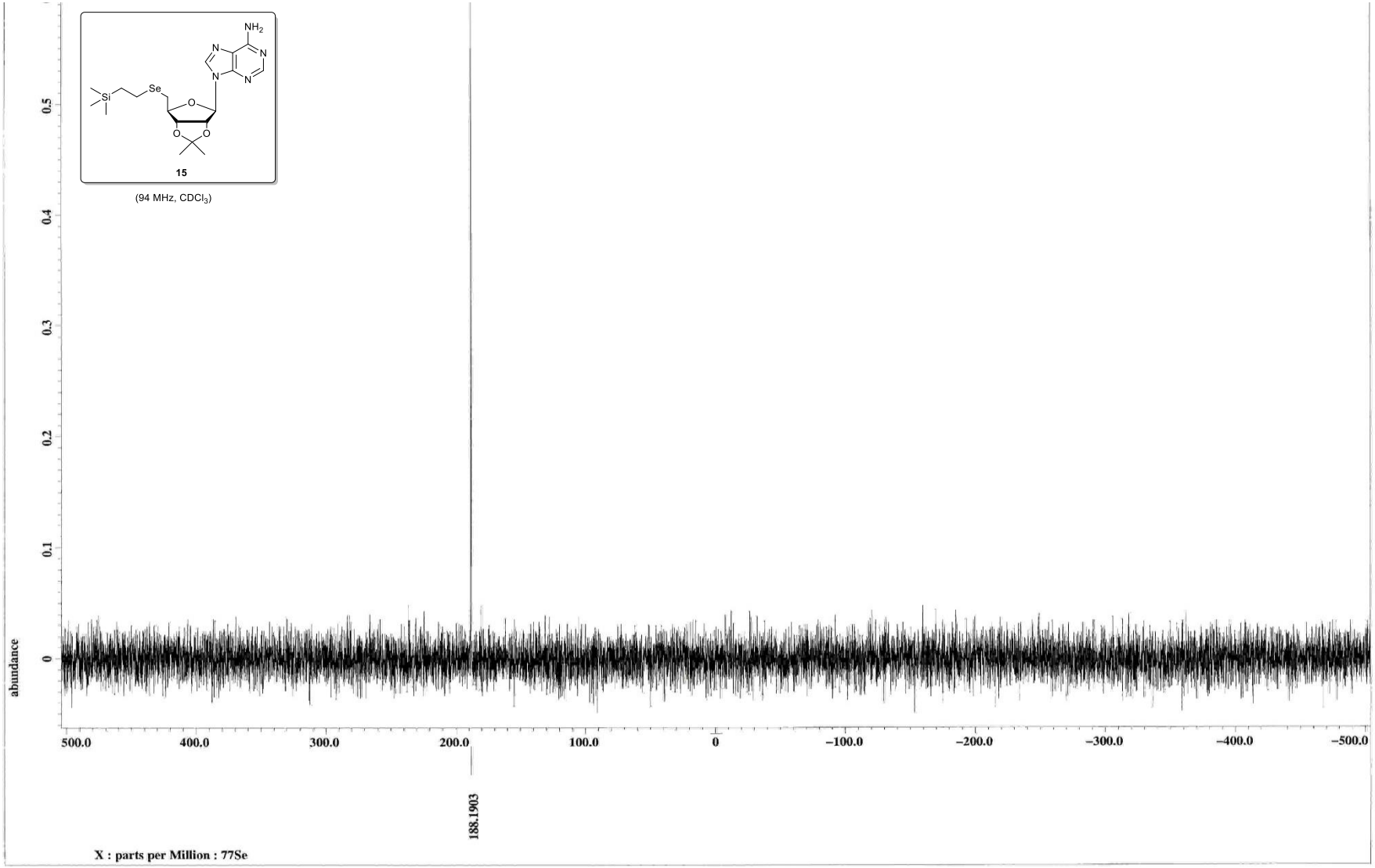

HO2C
TFA·H2N
Se
O
NH
N
O
HO
OH
11
(600 MHz, D2O)
abundance
X : parts per Million : 1H
7.7155
7.7029
5.8911
5.8774
5.8442
4.7906
4.3966
4.3886
4.1630
4.1527
3.9775
3.0327
2.9639
2.9525
2.7555
2.7429
2.7303
2.2951
2.2333
2.2207
1.4683

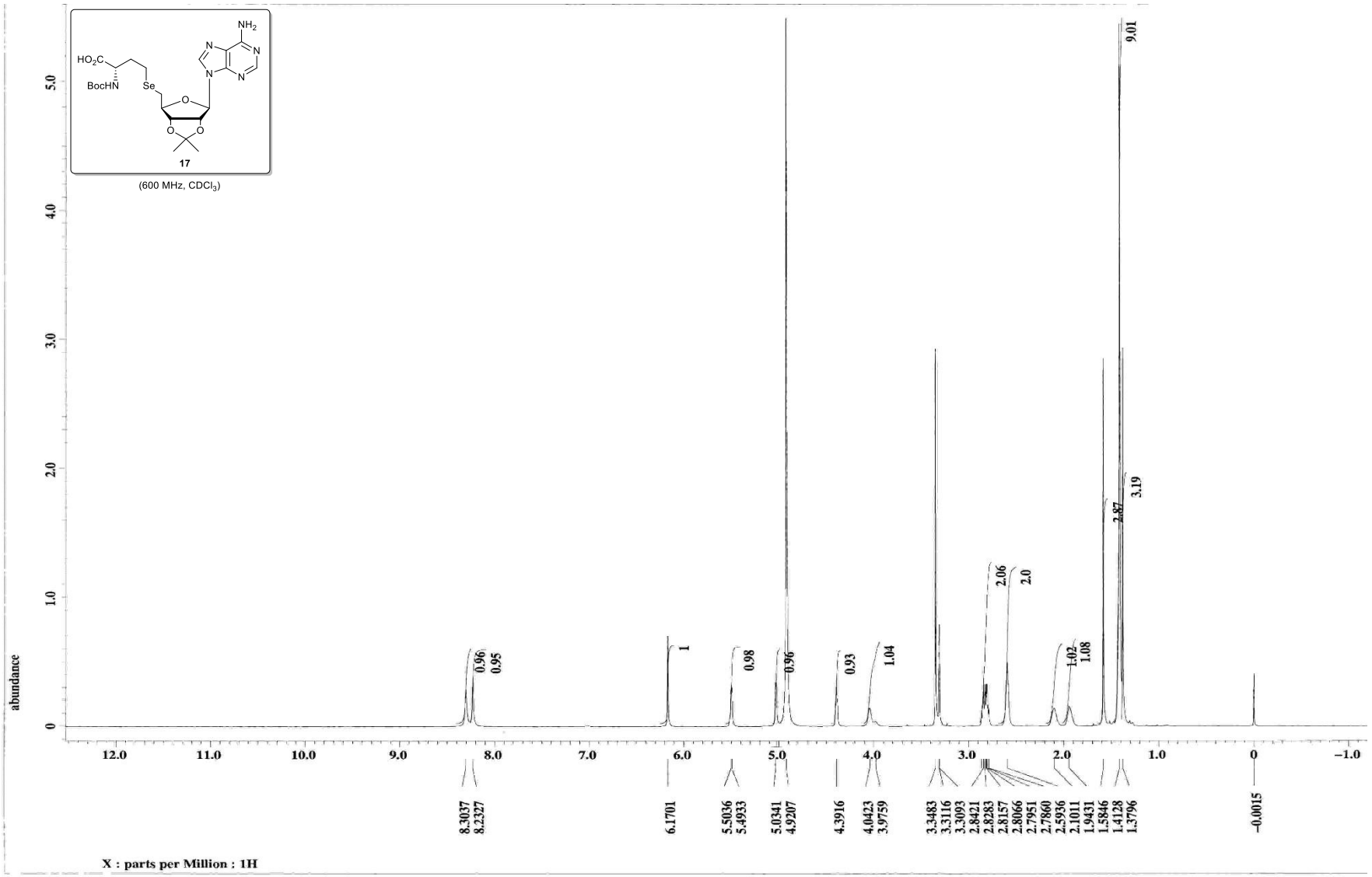

11
(150 MHz, D_2O)
(thousandths)
40.0
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0 −20.0
166.2191
151.6080
142.1960
102.5373
89.9752
83.0527
73.2098
72.6066
53.8688
31.1574
25.2019
19.0741
X : parts per Million : 13C

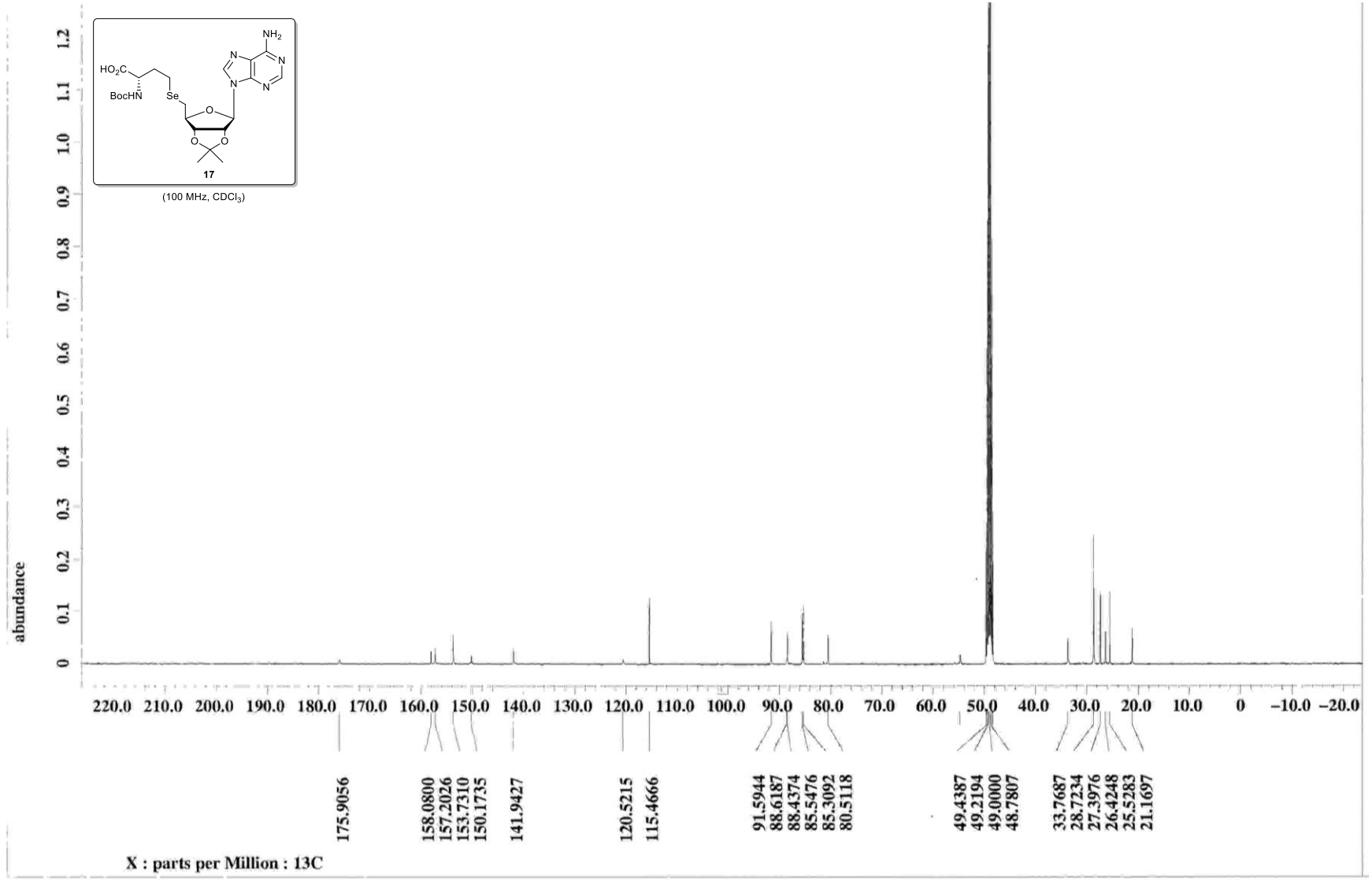

HO2C
TFA·H2N
Se
O
NH
N
O
HO
OH
11
(113 MHz, D2O)
14.
12.0
10.0
8.0
6.0
4.0
2.0
0
−2.0
−4.0
−6.0
−8.0
−10.0
−12.0
(thousands)
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
−500.
130.2475

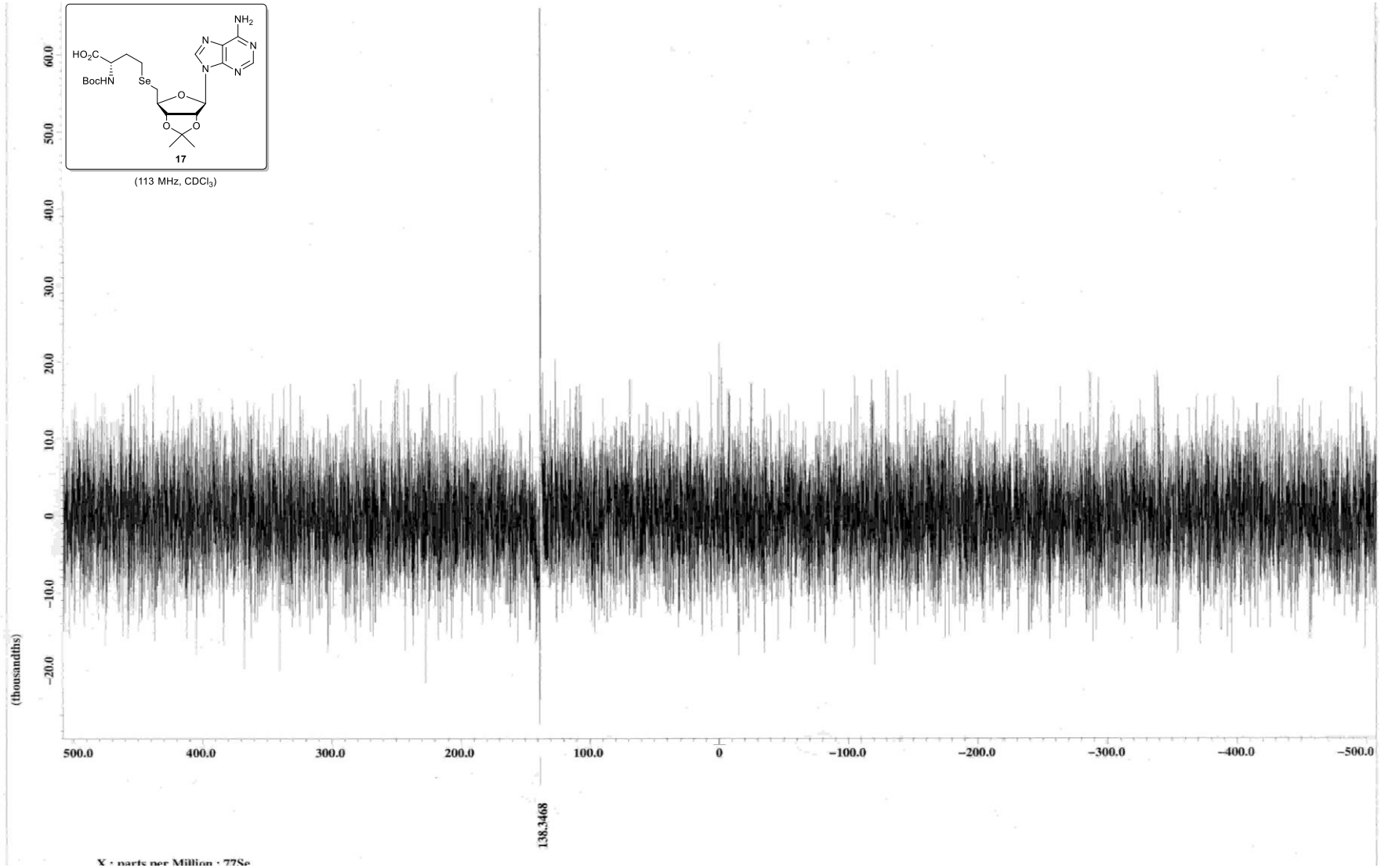

15
(500 MHz, CDCl3)
abundance
X : parts per Million : 1H
8.3037
7.9201
7.2605
6.4668
6.0775
6.0729
5.5026
5.4946
5.4900
5.0182
5.0113
5.0056
4.4273
4.4158
4.4066
2.8309
2.7793
2.5663
2.5469
2.5446
1.5792
1.3650
0.8680
0.8474
0.8314
-0.0859

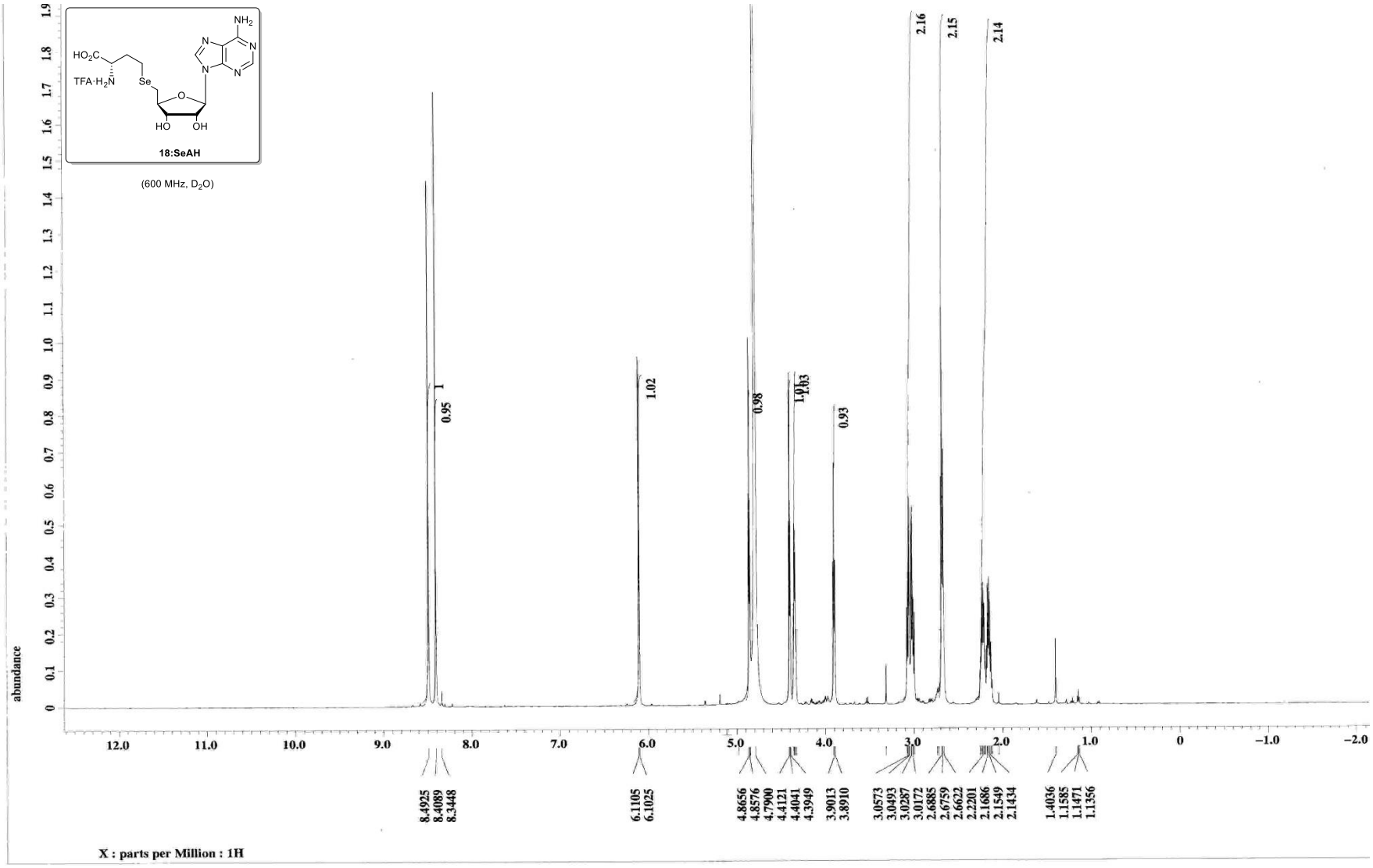

15
(125 MHz, CDCl3)
abundance
155.9658
153.1138
149.2412
139.9318
120.2924
114.4645
90.8095
87.5092
84.3806
84.1994
77.4176
77.1601
76.9026
27.1602
25.5673
25.4242
19.9397
18.5090
-1.9126
X : parts per Million : 13C

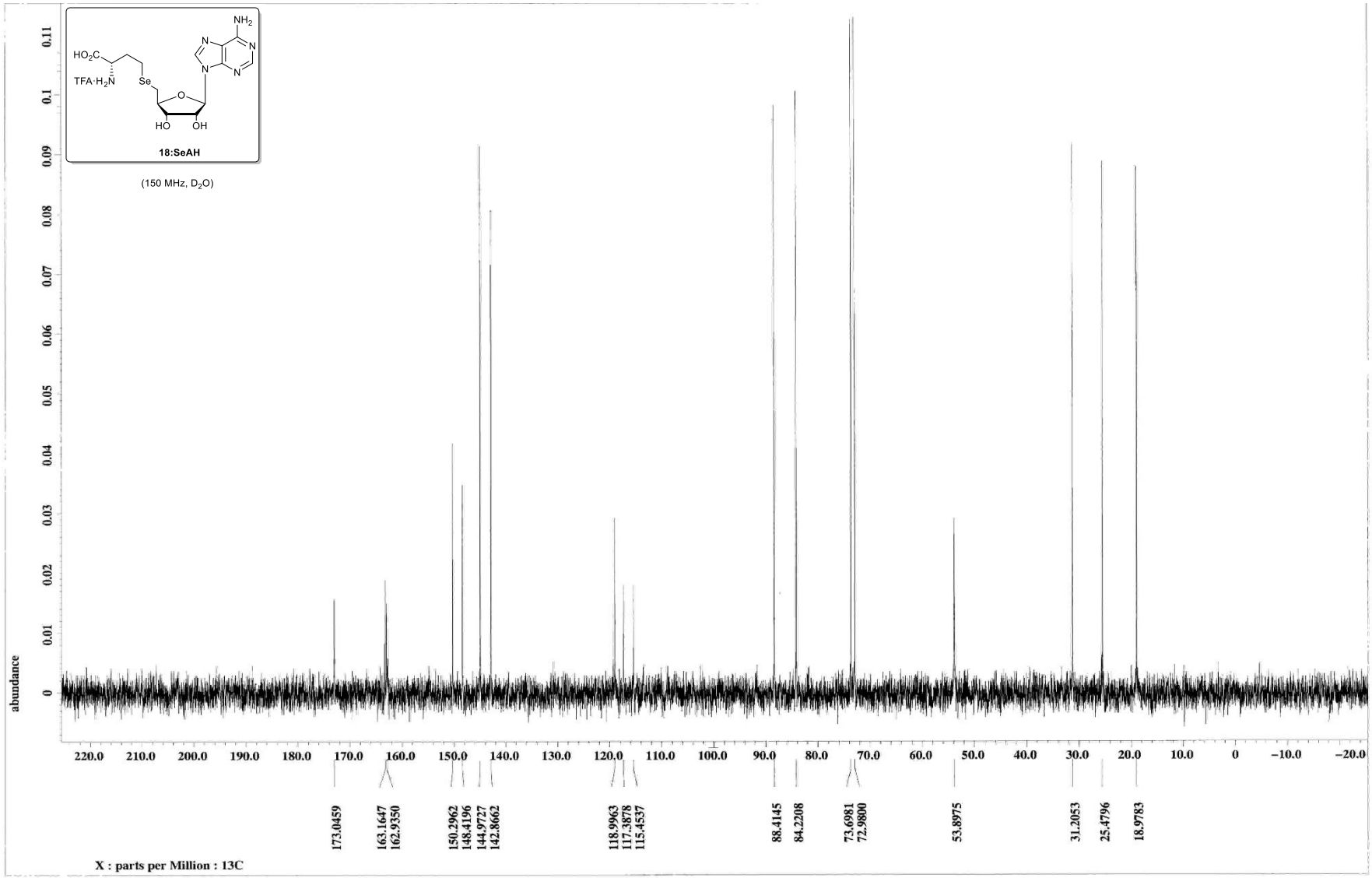

15
(94 MHz, CDCl3)
abundance
0.5
0.4
0.3
0.2
0.1
0
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
−500.0
188.1903
X : parts per Million : 77Se

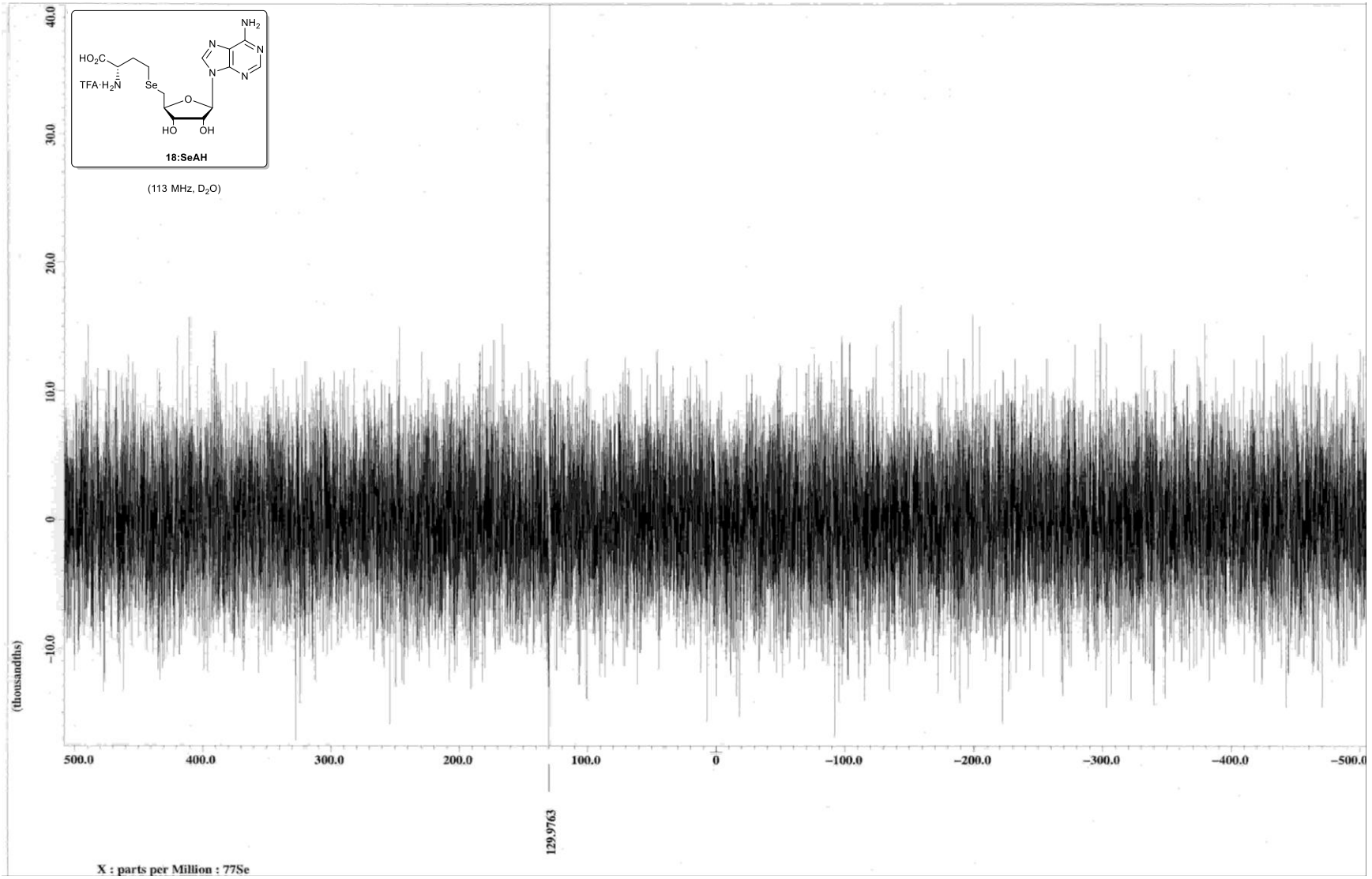

17
(600 MHz, CDCl3)
abundance
X : parts per Million : 1H
9.01
3.19
2.87
2.06
2.0
1.08
1.04
1
0.98
0.96
0.95
0.93
1.02
8.3037
8.2327
6.1701
5.5036
5.4933
5.0341
4.9207
4.3916
4.0423
3.9759
3.3483
3.3116
3.3093
2.8421
2.8283
2.8157
2.8066
2.7951
2.7860
2.5936
2.1011
1.9431
1.5846
1.4128
1.3796
−0.0015

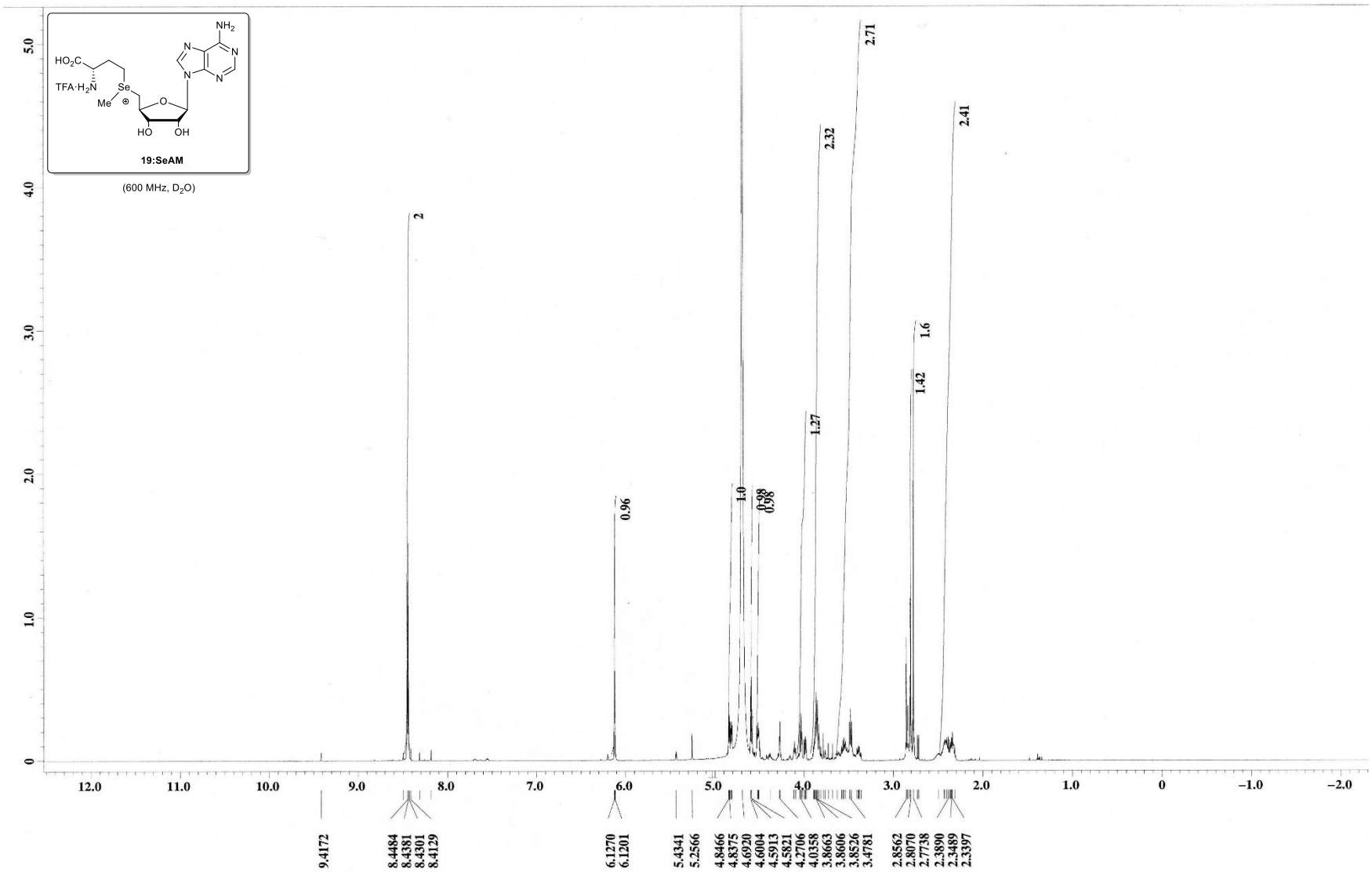

17
(100 MHz, CDCl3)
abundance
X : parts per Million : 13C
175.9056
158.0800
157.2026
153.7310
150.1735
141.9427
120.5215
115.4666
91.5944
88.6187
88.4374
85.5476
85.3092
80.5118
49.4387
49.2194
49.0000
48.7807
33.7687
28.7234
27.3976
26.4248
25.5283
21.1697

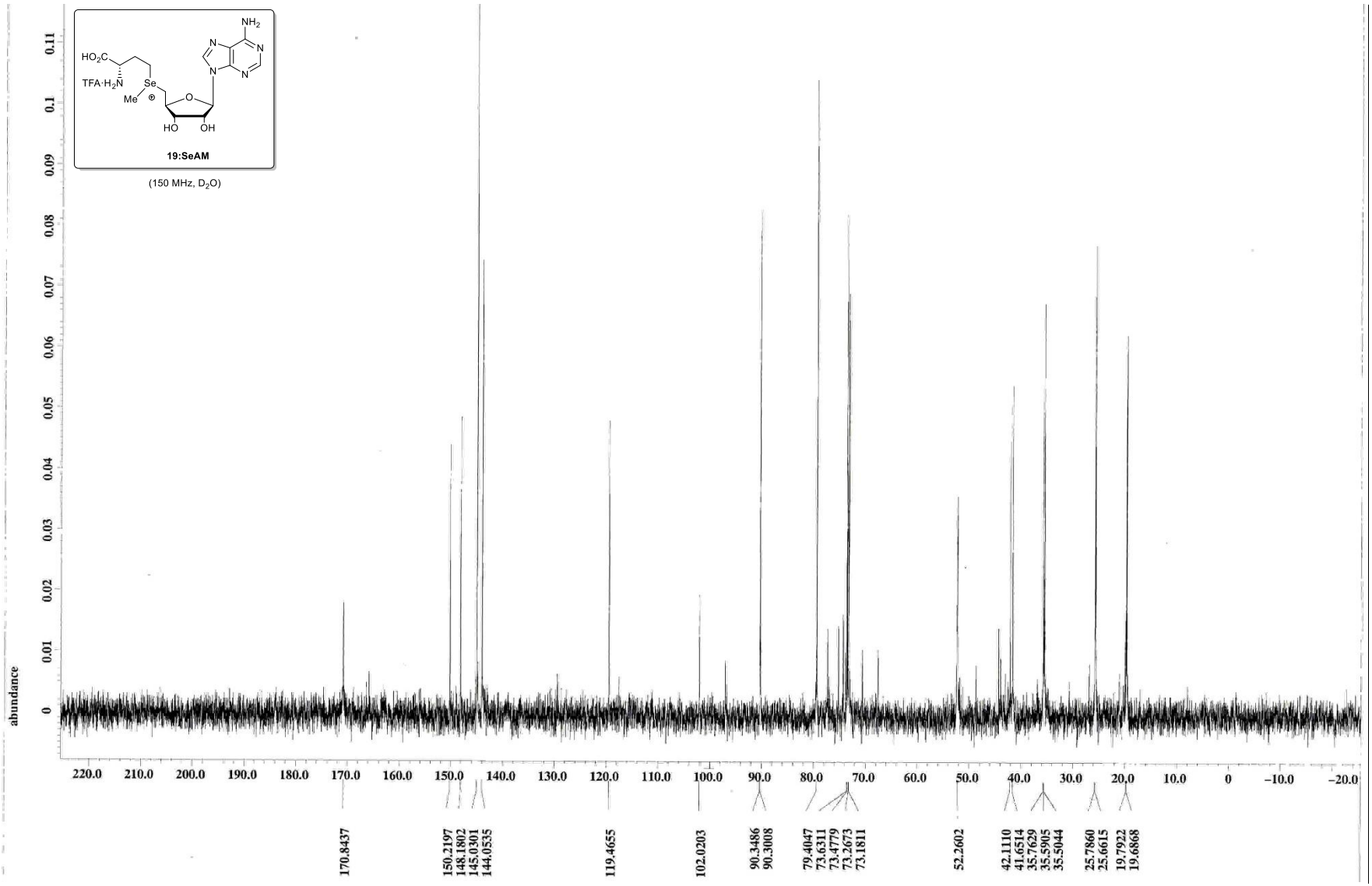

17
(113 MHz, CDCl3)
(thousandths)
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
−20.0
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
−500.0
138.3468

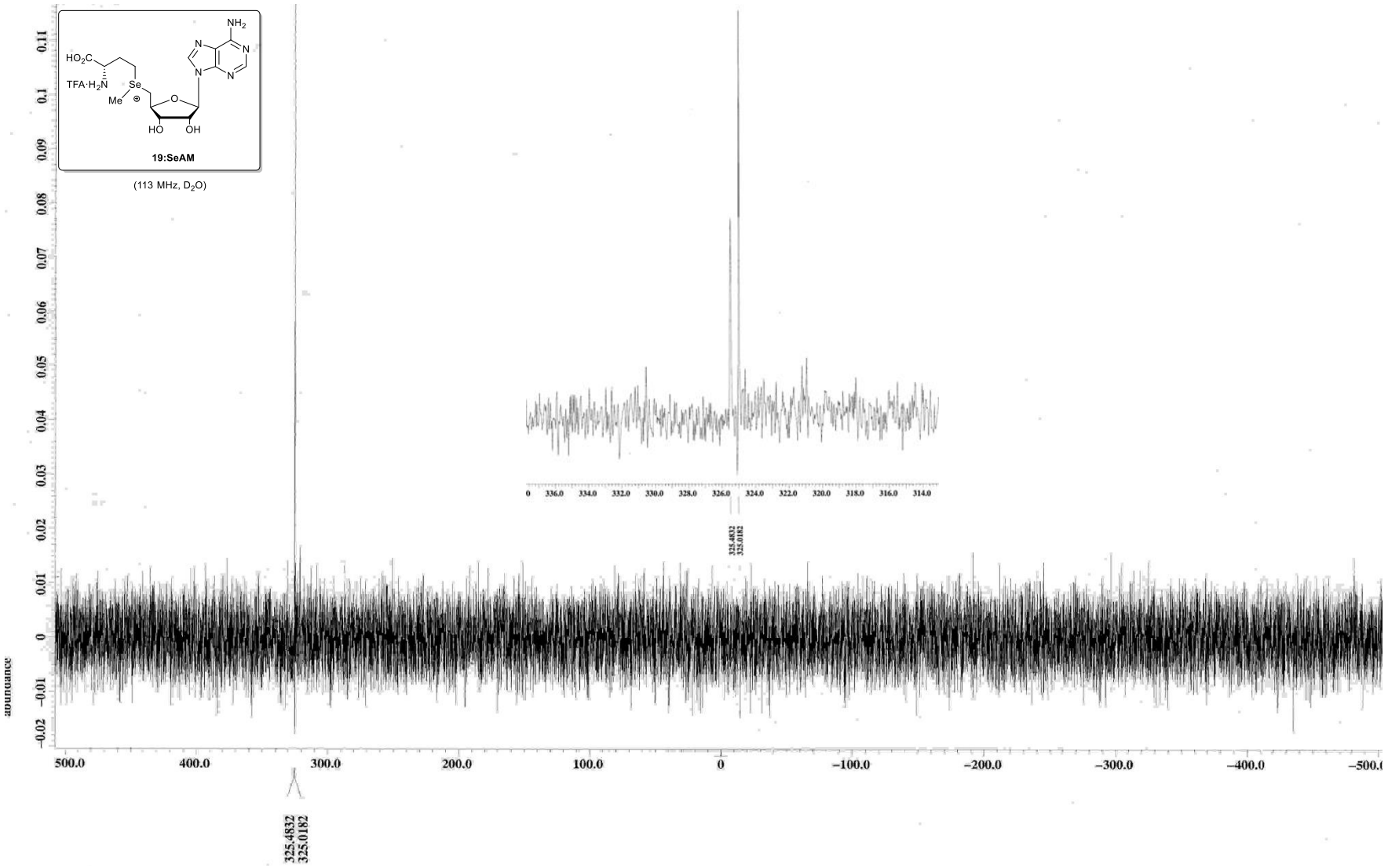

18:SeAH
(600 MHz, D2O)
abundance
X : parts per Million : 1H
0.95
1
1.02
0.98
1.01
1.03
0.93
2.16
2.15
2.14
8.4925
8.4089
8.3448
6.1105
6.1025
4.8656
4.8576
4.7900
4.4121
4.4041
4.3949
3.9013
3.8910
3.0573
3.0493
3.0287
3.0172
2.6885
2.6759
2.6622
2.2201
2.1686
2.1549
2.1434
1.4036
1.1585
1.1471
1.1356


18:SeAH
(150 MHz, D2O)
abundance
X : parts per Million : 13C
173.0459
163.1647
162.9350
150.2962
148.4196
144.9727
142.8662
118.9963
117.3878
115.4537
88.4145
84.2208
73.6981
72.9800
53.8975
31.2053
25.4796
18.9783


18:SeAH
(113 MHz, D2O)
(thousandths)
40.0
30.0
20.0
10.0
0
−10.0
500.0
400.0
300.0
200.0
100.0
0
−100.0
−200.0
−300.0
−400.0
−500.0
129.9763
X : parts per Million : 77Se


19:SeAM
(600 MHz, D2O)
2
0.96
1.0
0.98
0.98
1.27
2.32
2.71
2.41
1.6
1.42
9.4172
8.4484
8.4381
8.4301
8.4129
6.1270
6.1201
5.4341
5.2566
4.8466
4.8375
4.6920
4.6004
4.5913
4.5821
4.2706
4.0358
3.8663
3.8606
3.8526
3.4781
2.8562
2.8070
2.7738
2.3890
2.3489
2.3397


19:SeAM
(150 MHz, D2O)
abundance
170.8437
150.2197
148.1802
145.0301
144.0535
119.4655
102.0203
90.3486
90.3008
79.4047
73.6311
73.4779
73.2673
73.1811
52.2602
42.1110
41.6514
35.7629
35.5905
35.5044
25.7860
25.6615
19.7922
19.6868


19:SeAM
(113 MHz, D2O)
325.4832
325.0182