Electronic Supporting Information

Efficient Synthesis of Fused Triazolo[4,5-*d*]quinoline Derivates via Palladium Catalysis Mediated by Tetrabutylammonium Iodide

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General Experimental Procedures

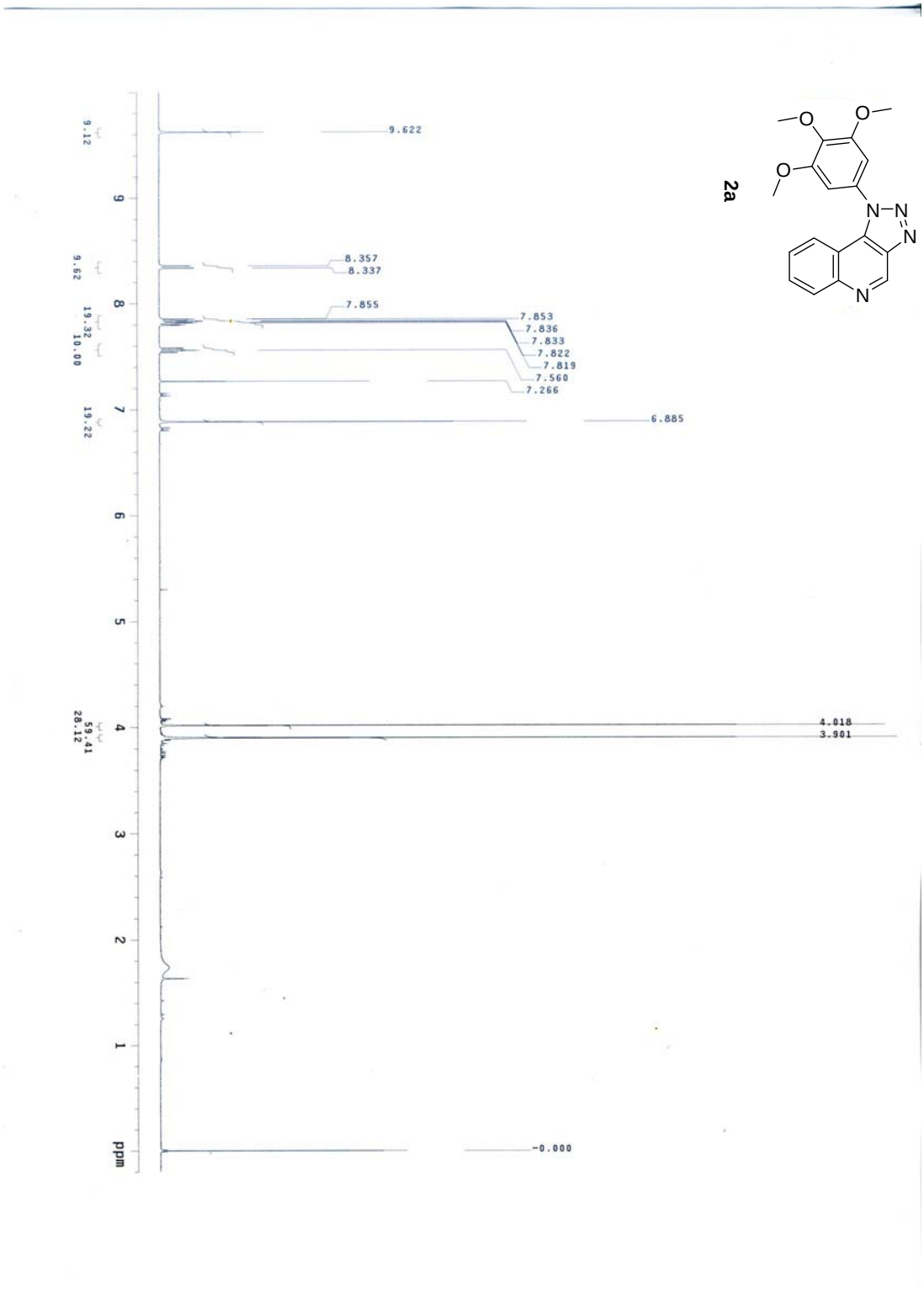
The palladium-catalyzed annulation reactions were performed in mild condition under an atmosphere of nitrogen. All other reactions, unless otherwise indicated, were carried out under ambient atmosphere in single-neck, round bottom flasks fitted with a rubber septum, equipped with a magnetic stir bar. Air- or water- sensitive solvents were transferred via syringe. When required, solvents were degassed by bubbling of nitrogen through a needle. Organic solutions were concentrated by rotary evaporation at 25 – 40 °C under reduced pressure (15 – 30 torr, house vacuum). Analytical Thin Layer Chromatography (TLC) was performed using pre-coated UV 254 plates (0.2 mm) from EM Separations. Visualization was accomplished with a 254 nm UV light source, generally followed by immersion in potassium permanganate ($KMnO_4$) or anisaldehyde solutions, with subsequent heating with a heat gun.

Instrumentation

^{1}H NMR and ^{13}C NMR spectra were recorded at 400 and 100 MHz, respectively, using $CDCl_3$ as a solvent. ^{1}H NMR chemical shifts are referenced to TMS or $CDCl_3$ (0; 7.26 ppm). ^{13}C NMR was referenced to $CDCl_3$ (77.0 ppm). Mass spectra and high-resolution mass spectra (HRMS) were measured using the electron-impact (EI, 70 eV) technique by Taichung Regional Instrument Center of NSC at NCHU. Elemental analyses were performed by Tainan Regional Instrument Center of NSC at NCKU. Flash chromatography was carried out on silica gel 60 (E. Merck, 230-400 mesh). Spectral data are represented in the following order: chemical shift; multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, td = triplet of doublets, m = multiplet); coupling constant (*J*, Hz); number of protons.

Materials

Unless otherwise noted, all reagents, and catalysts were purchased from commercial sources (Sigma-Aldrich, Alfa Aesar, TCI) and used as received. Tetrahydrofuran and *N*,*N*-dimethyl foramide were purified by distillation under nitrogen immediately prior to use. All other solvents were used as supplied without further purification.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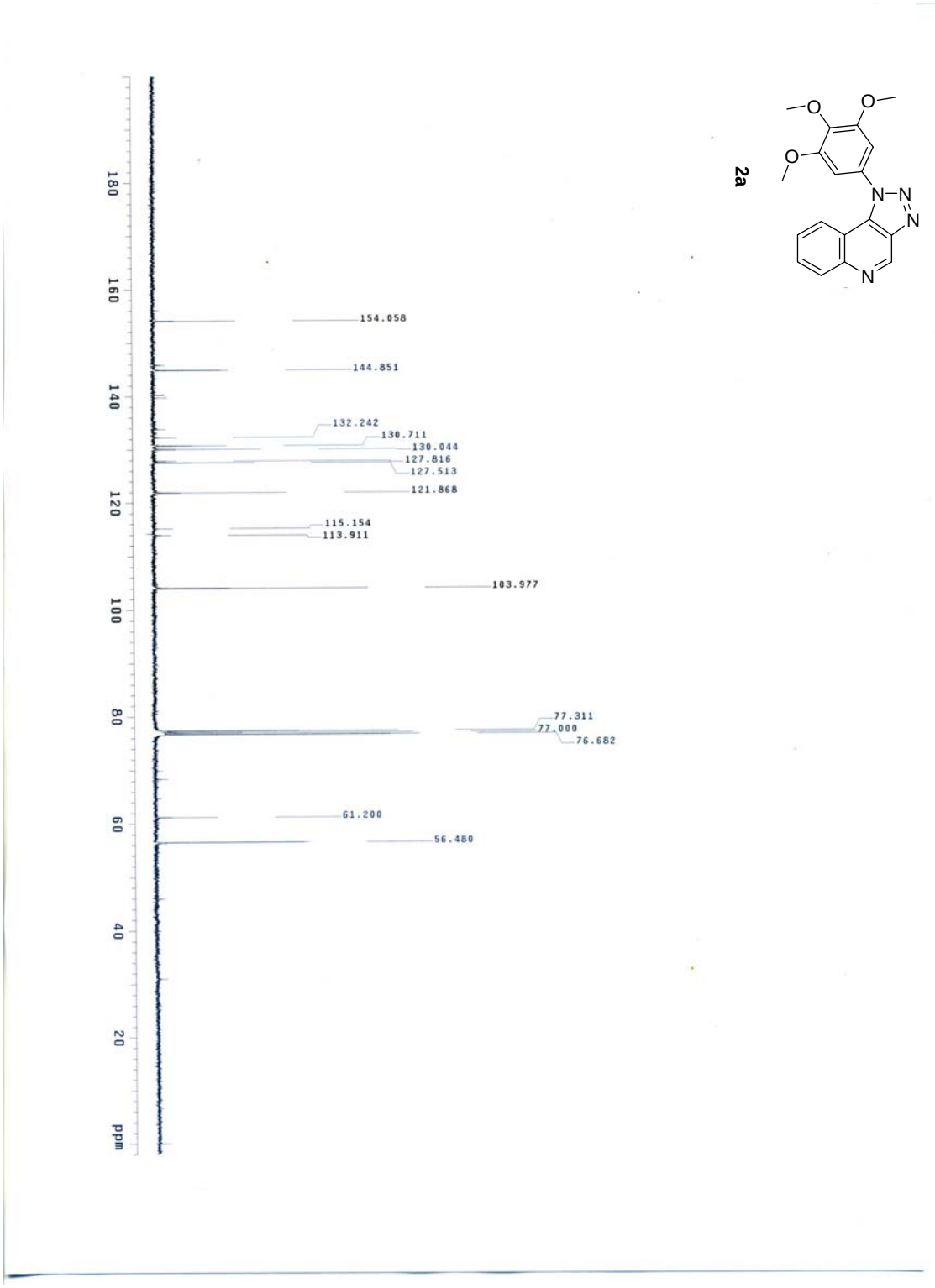
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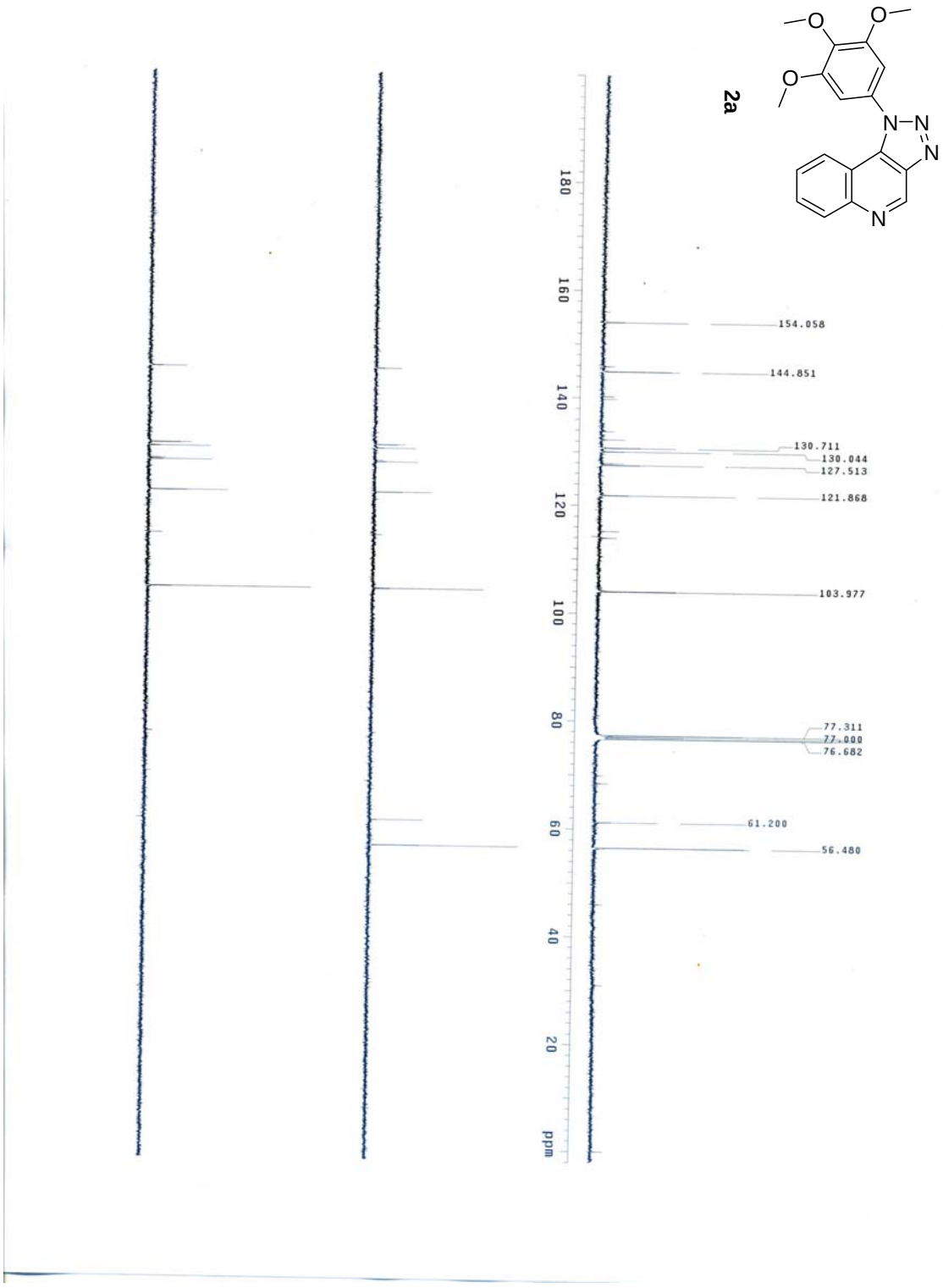
20
ppm

2a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20
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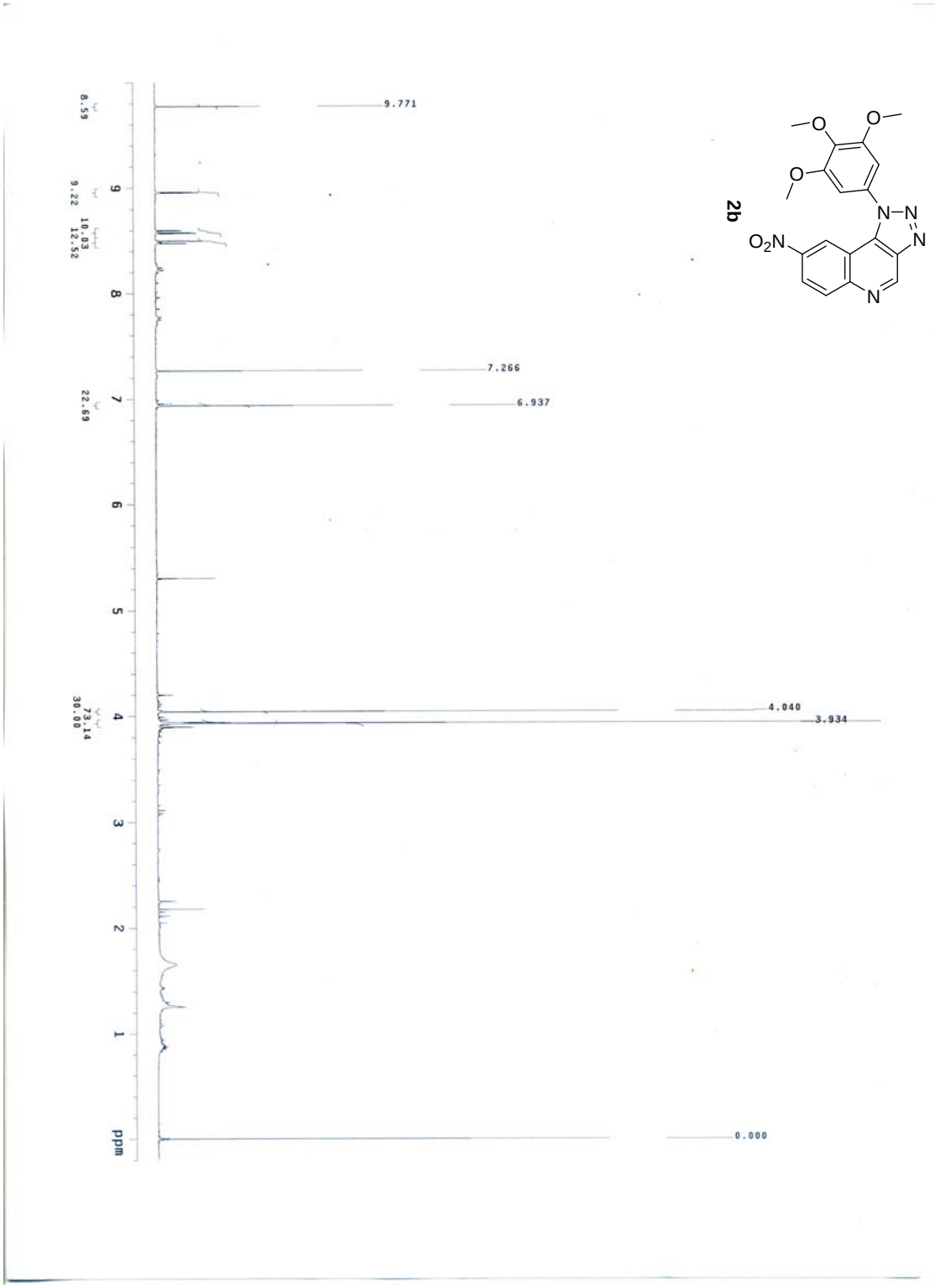

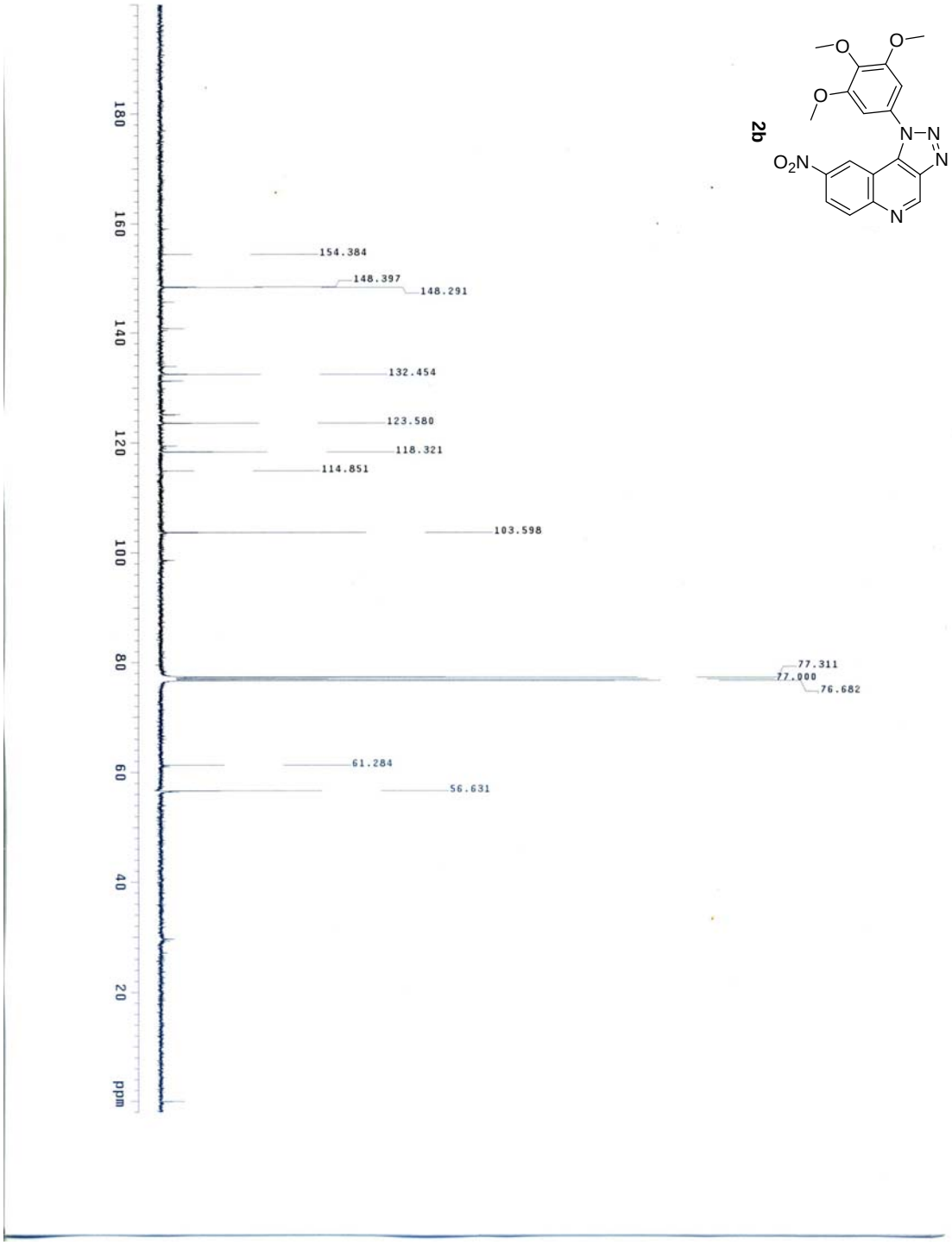

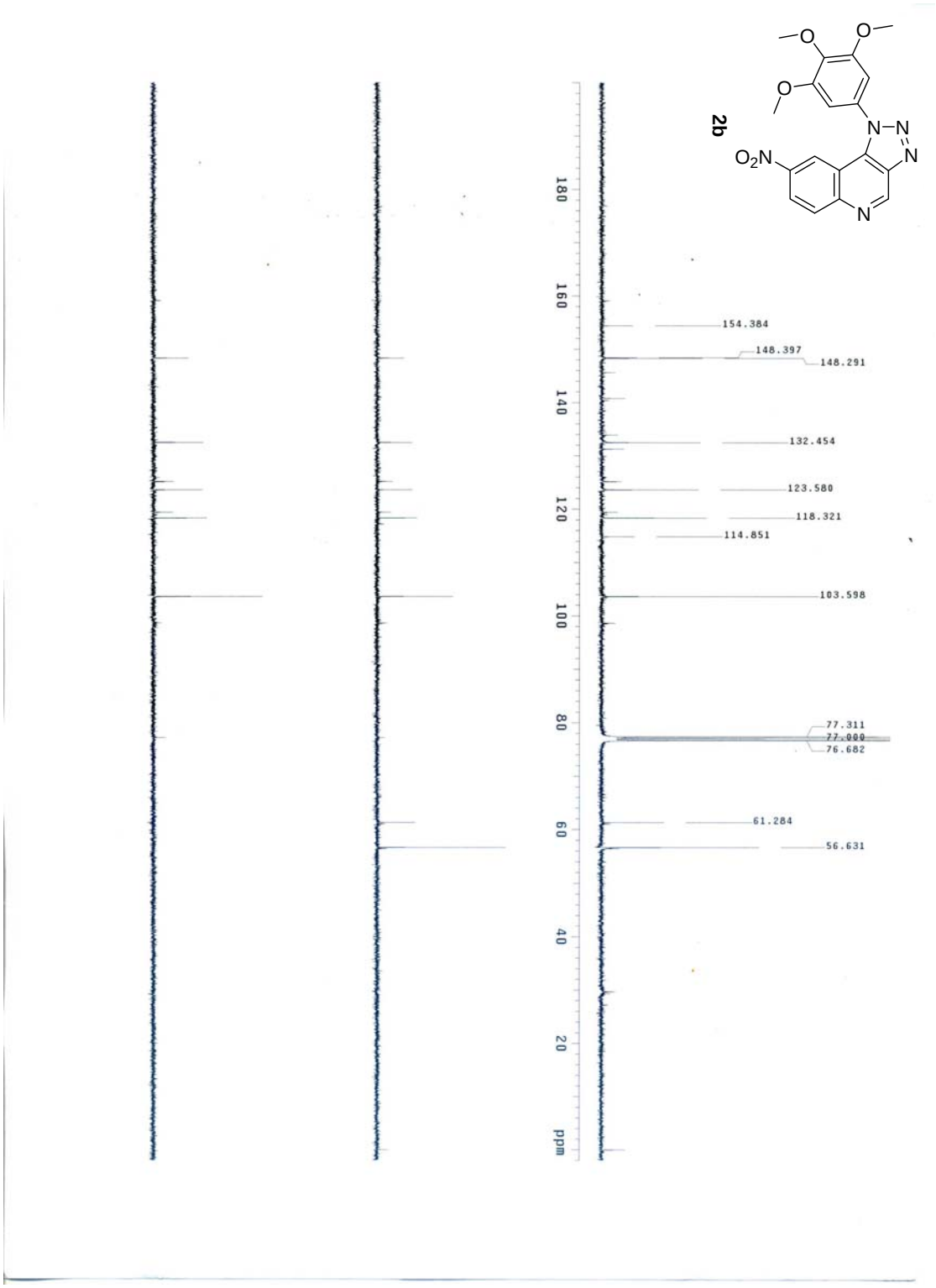
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O
O
N
N
N
O_2N
N
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160
140
120
100
80
60
40
20
ppm
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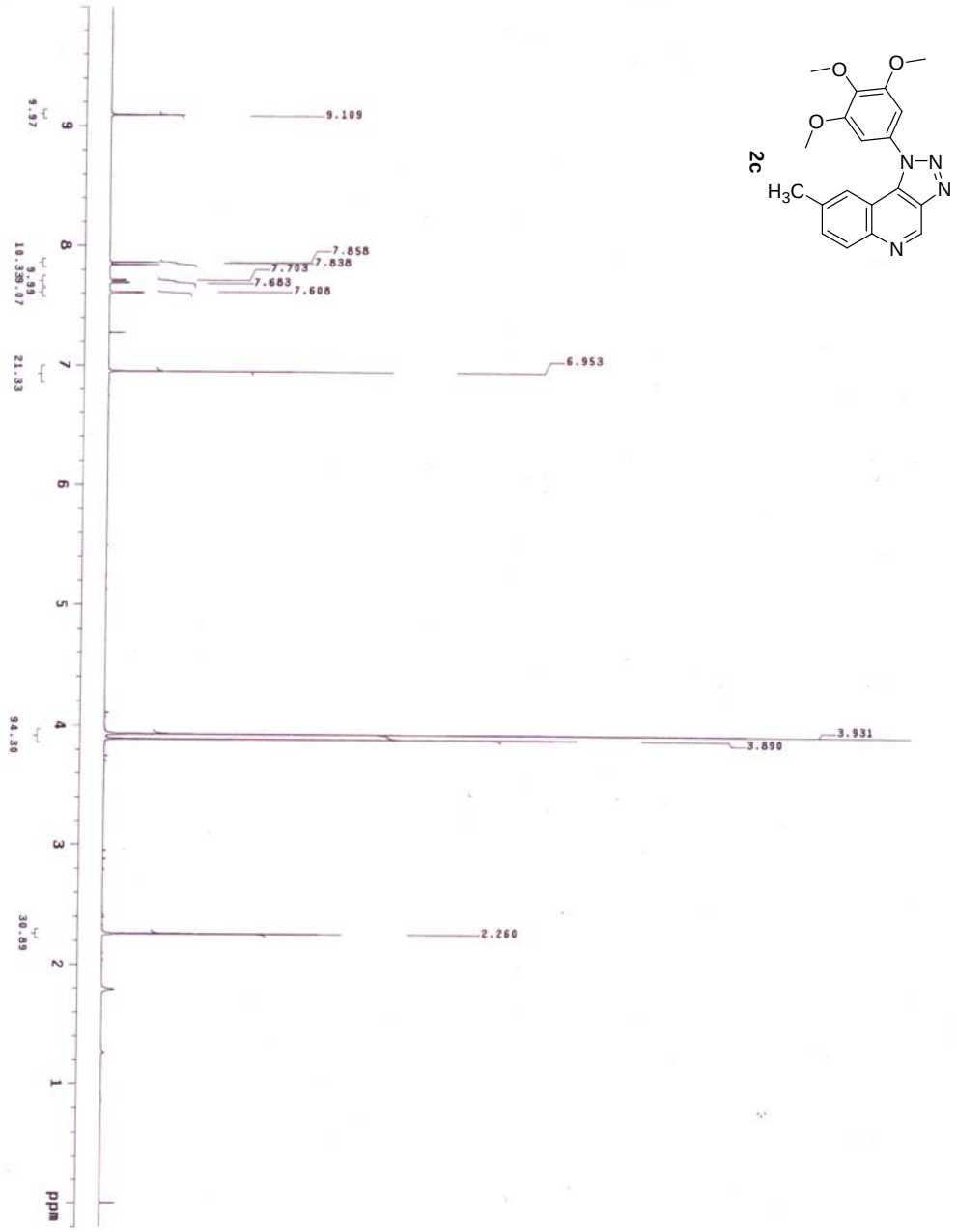

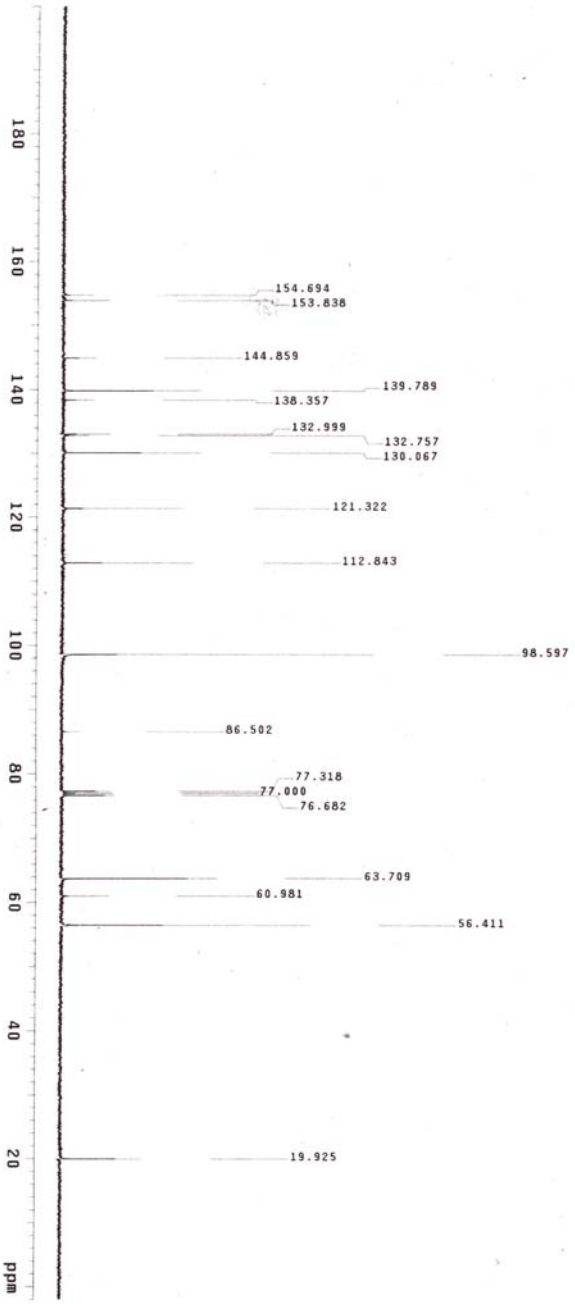

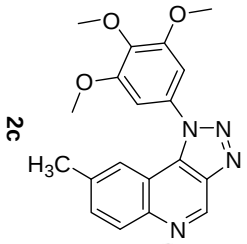

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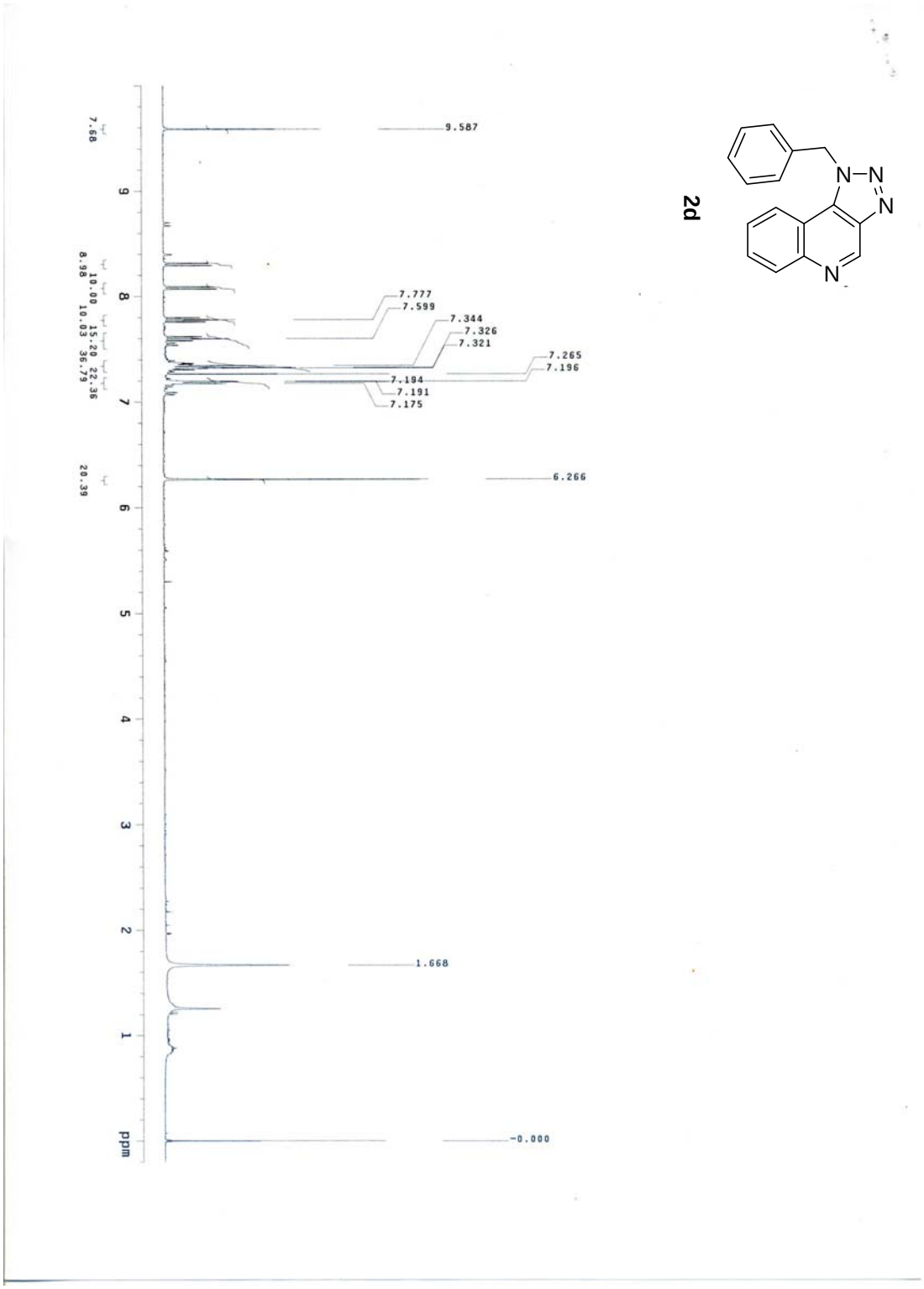

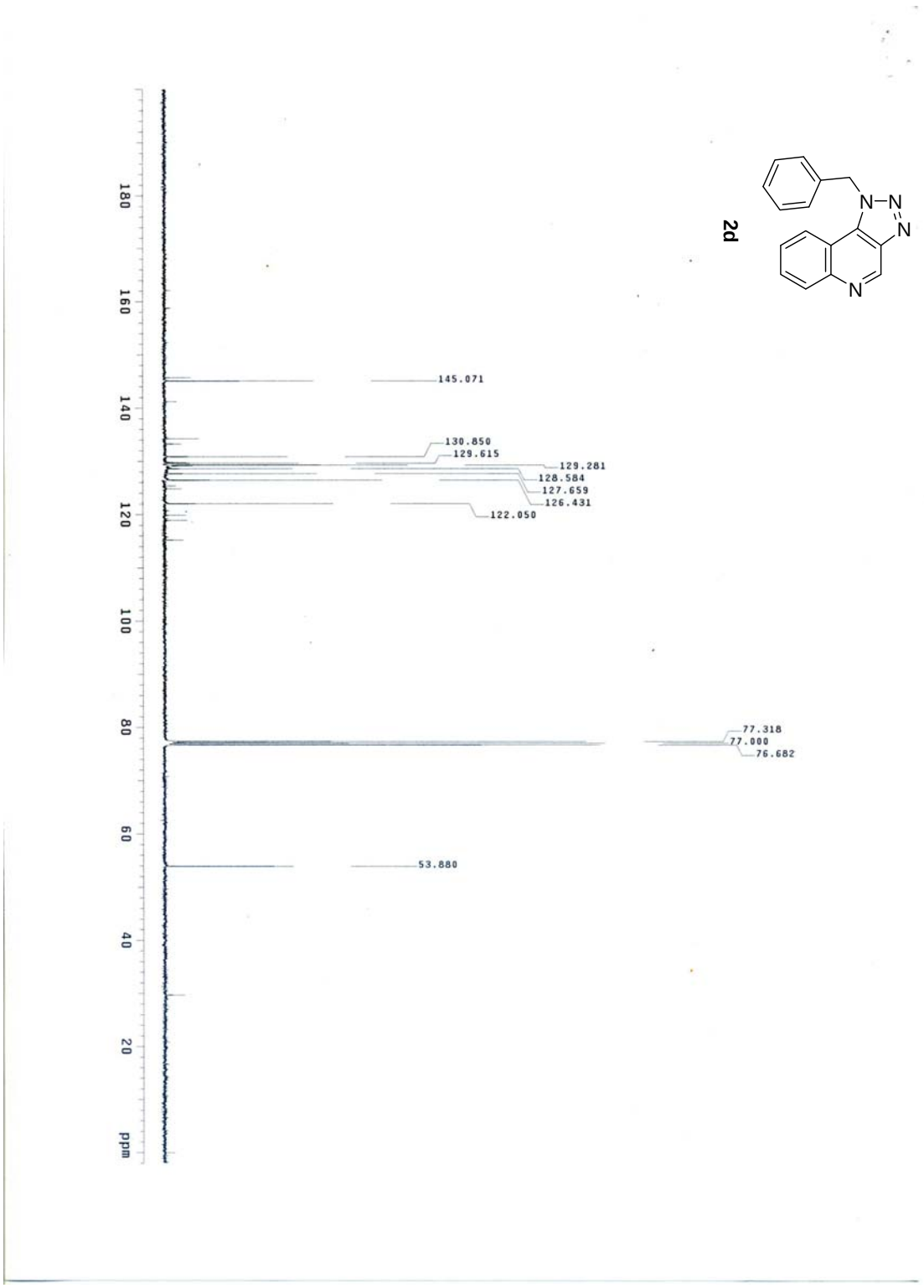

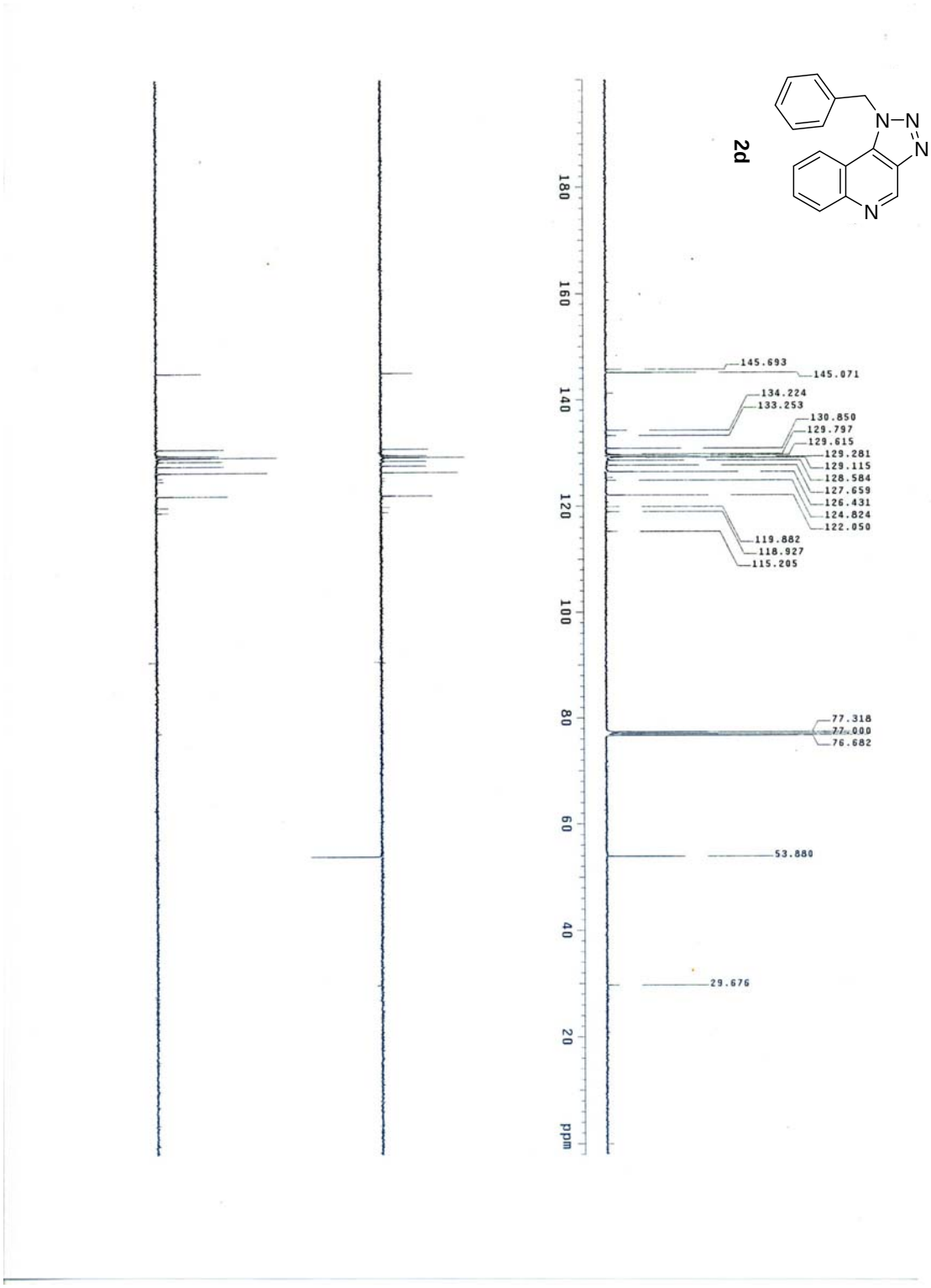
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N
N
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160
140
120
100
80
60
40
20
ppm
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129.797
129.615
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129.115
128.584
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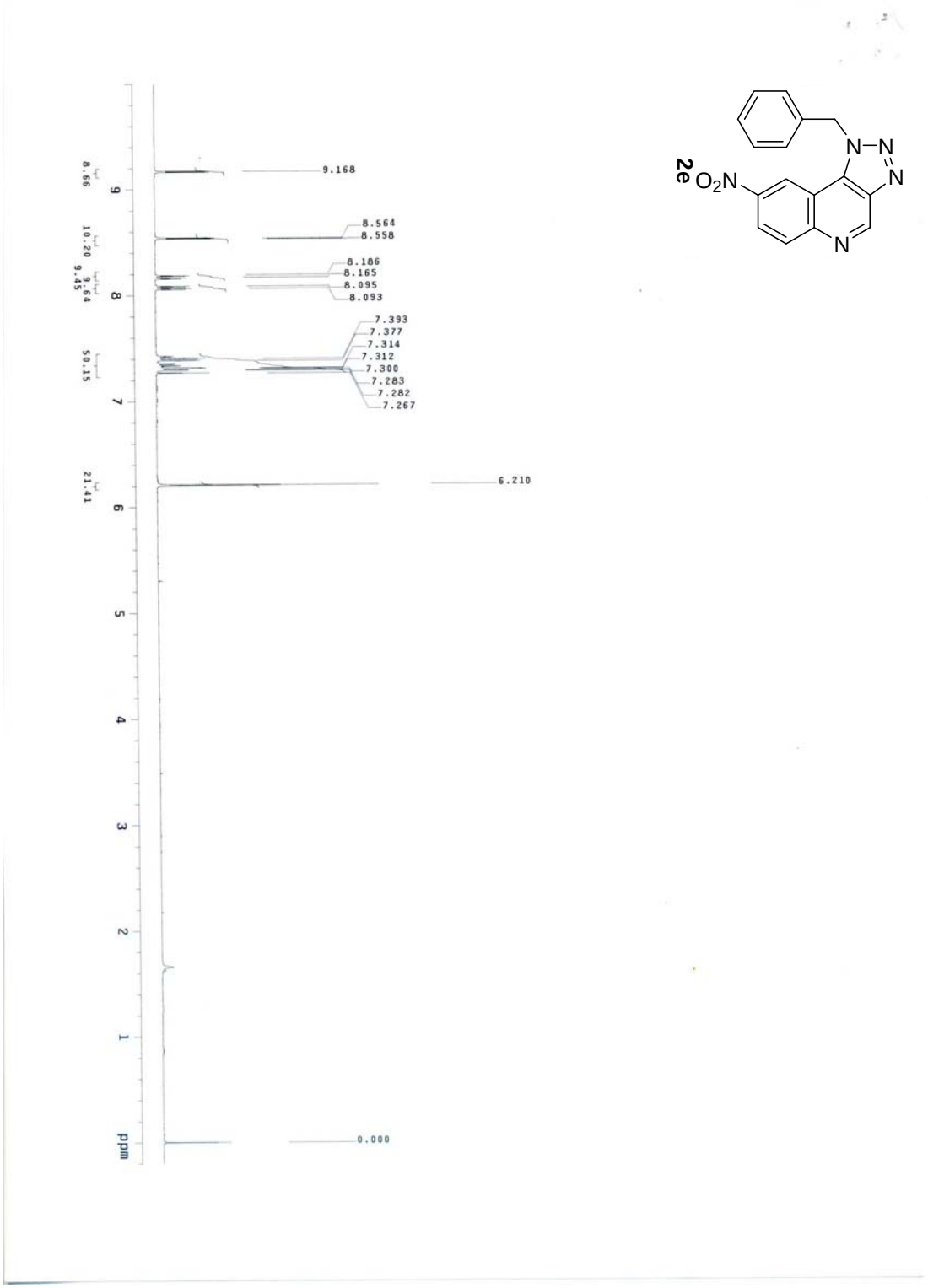

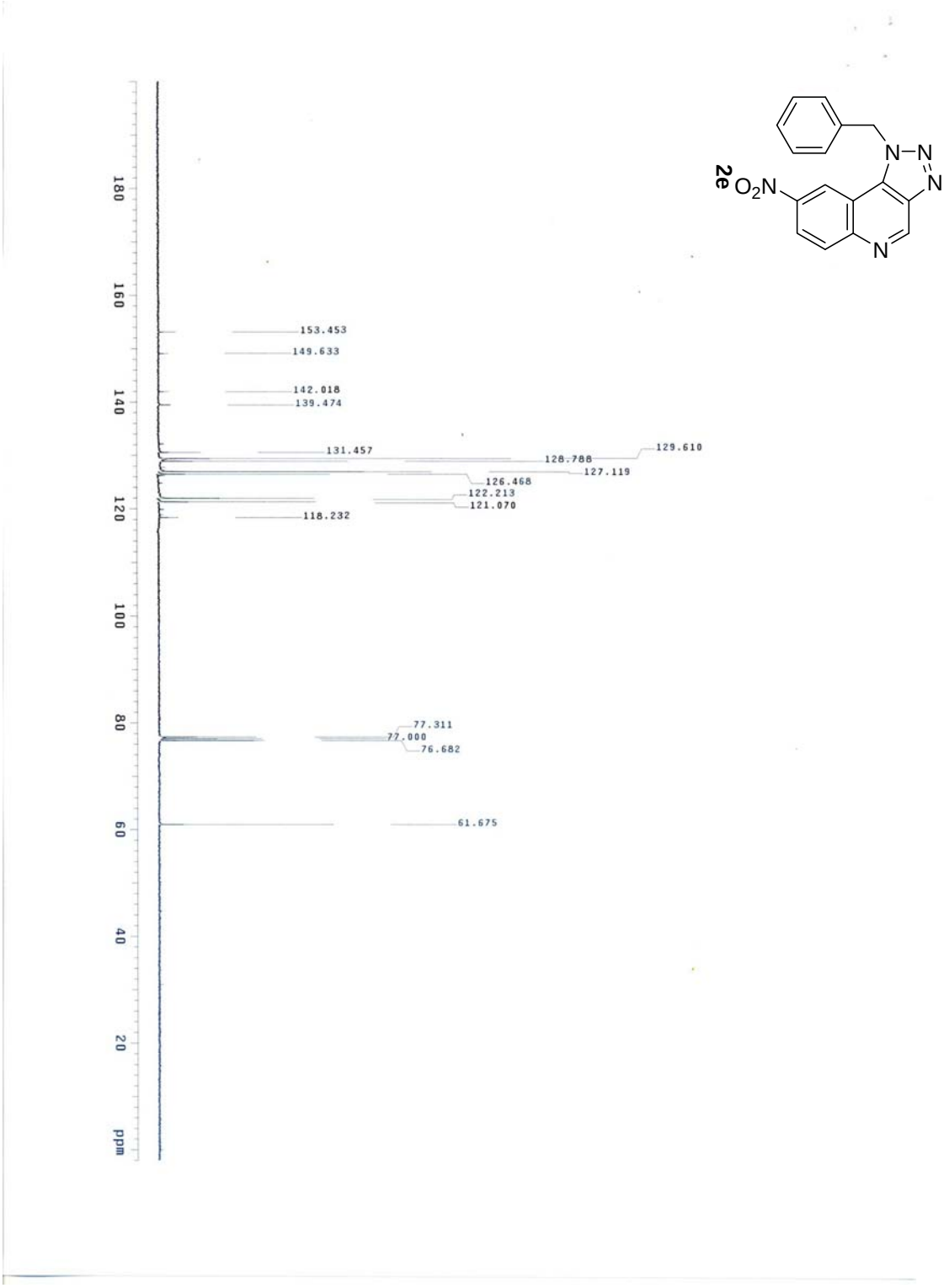

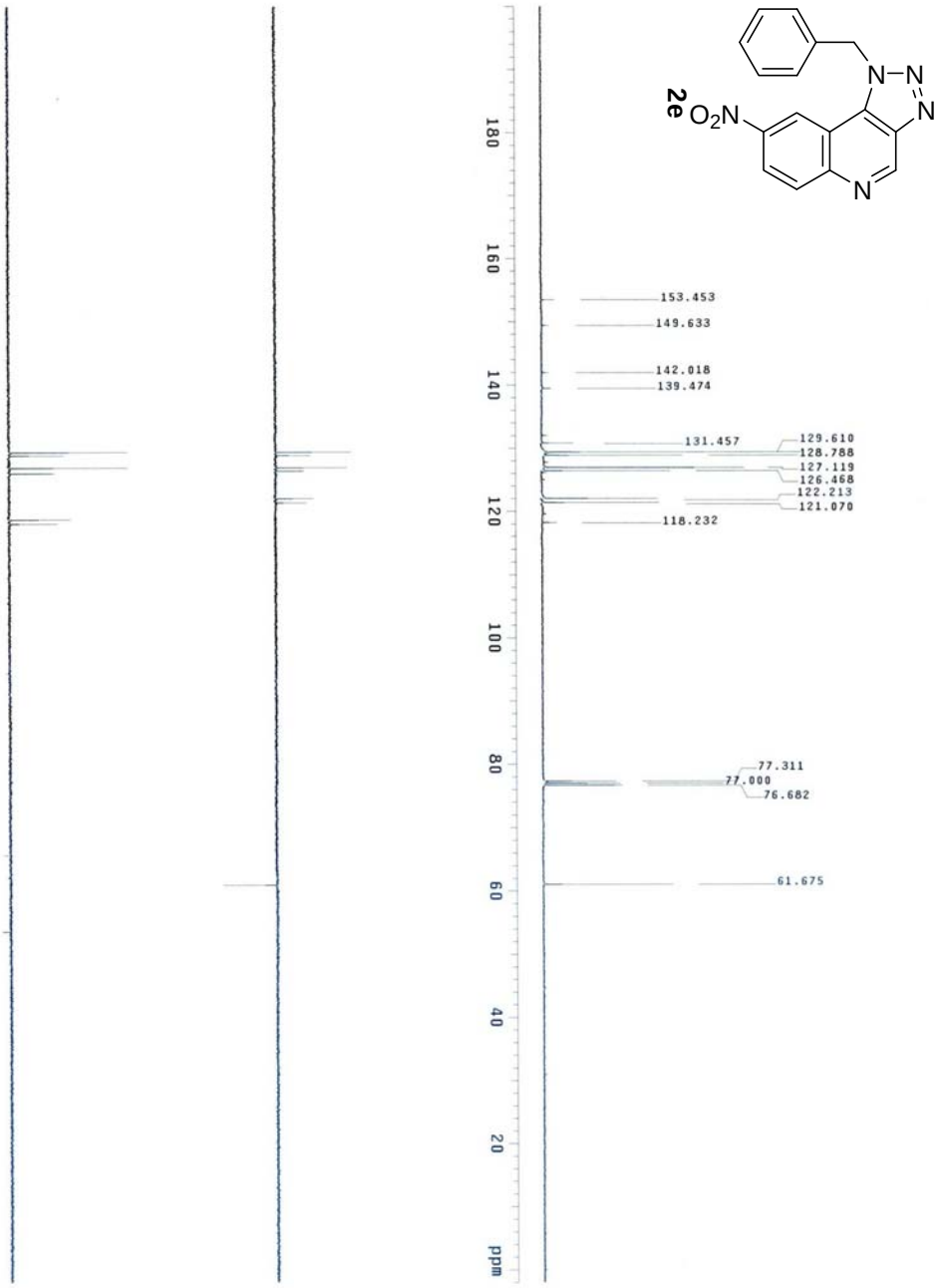

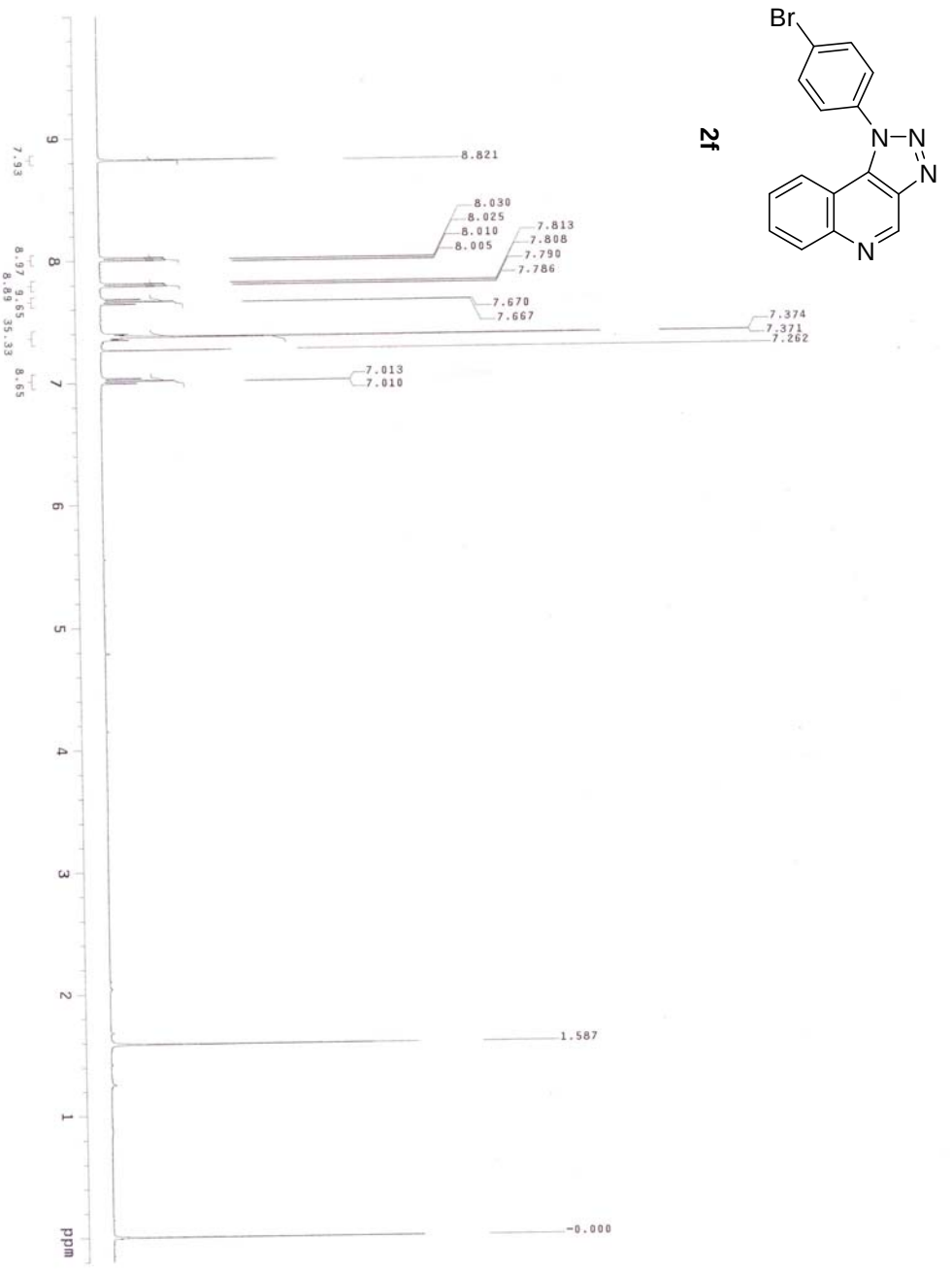
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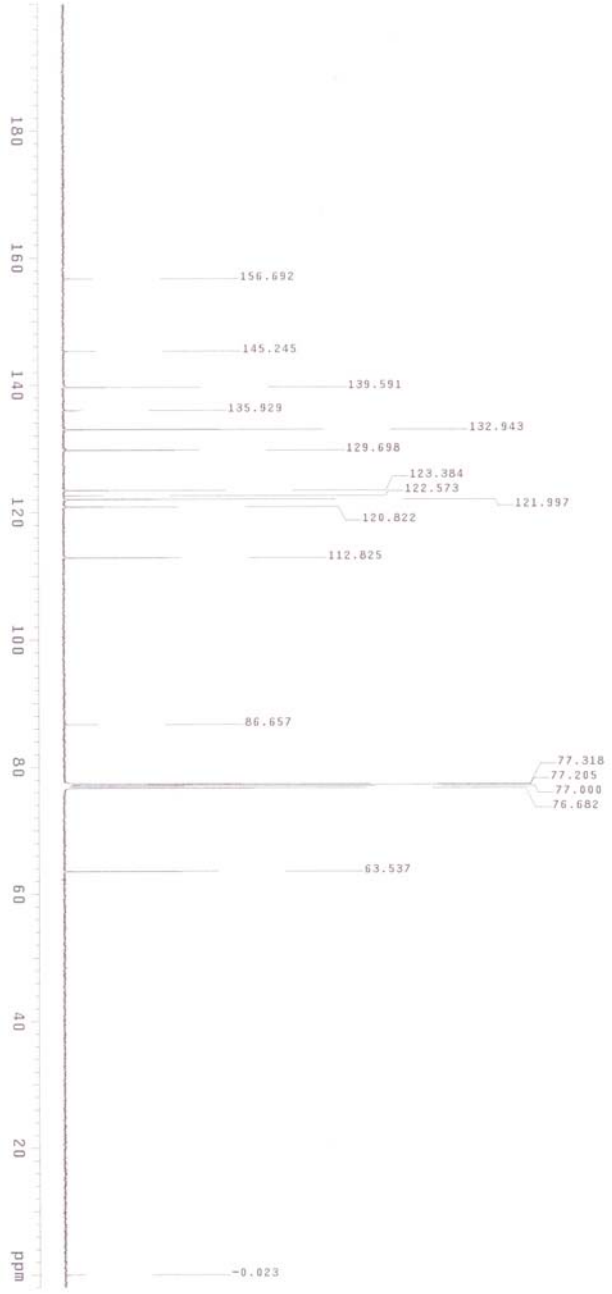
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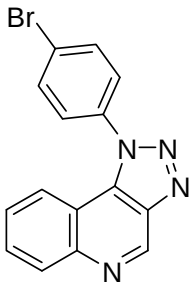
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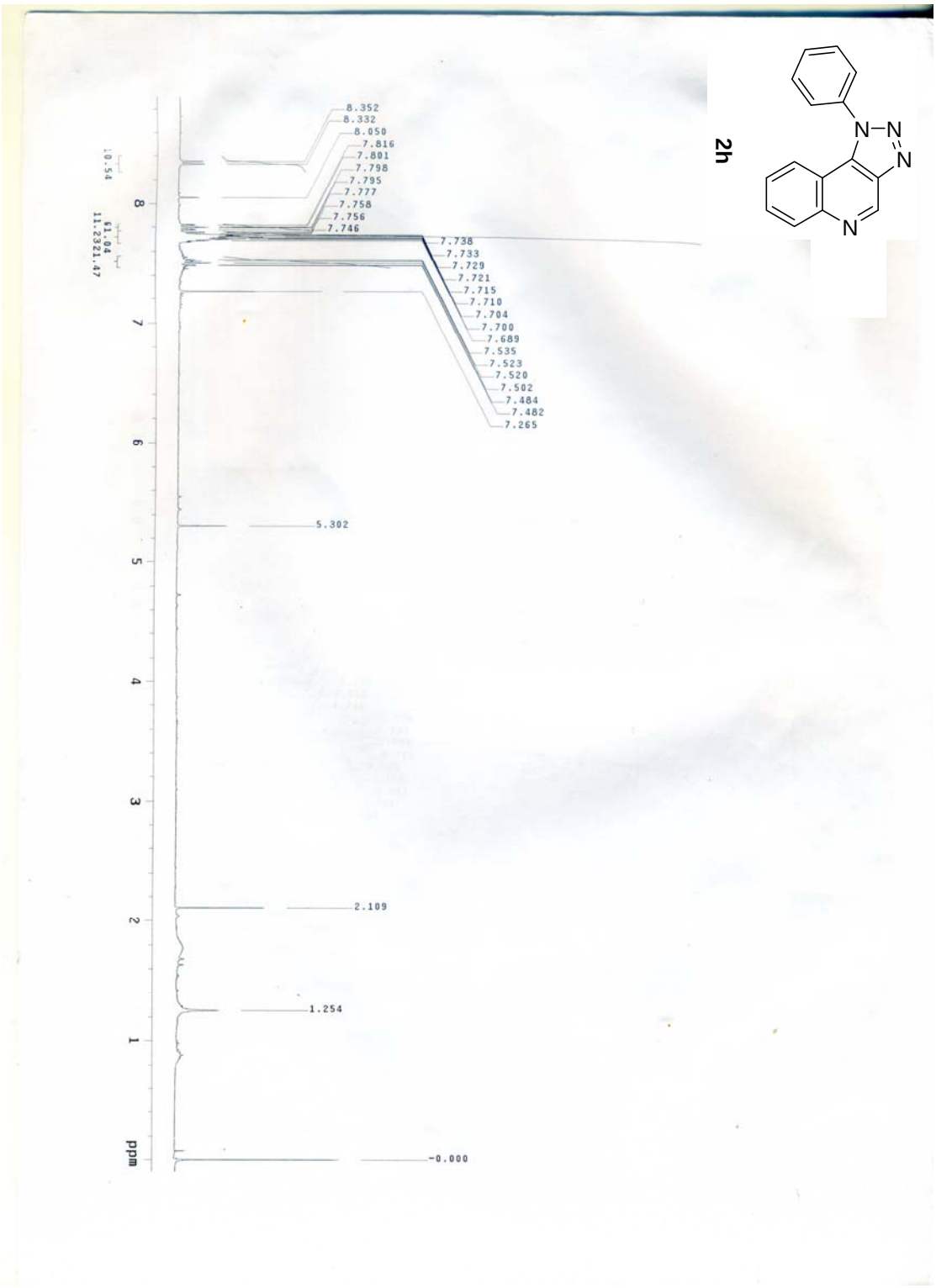
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7.715
7.710
7.704
7.700
7.689
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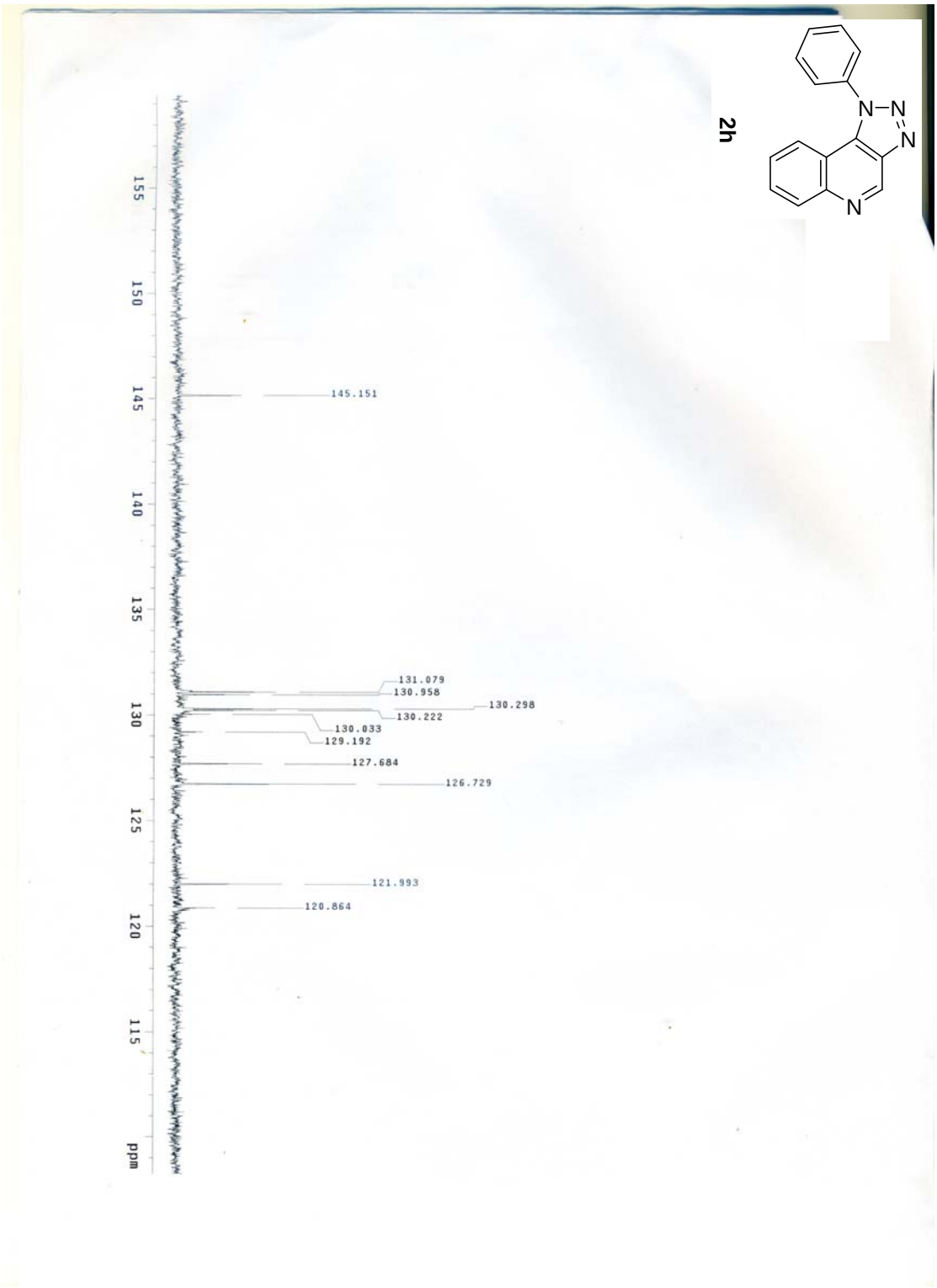

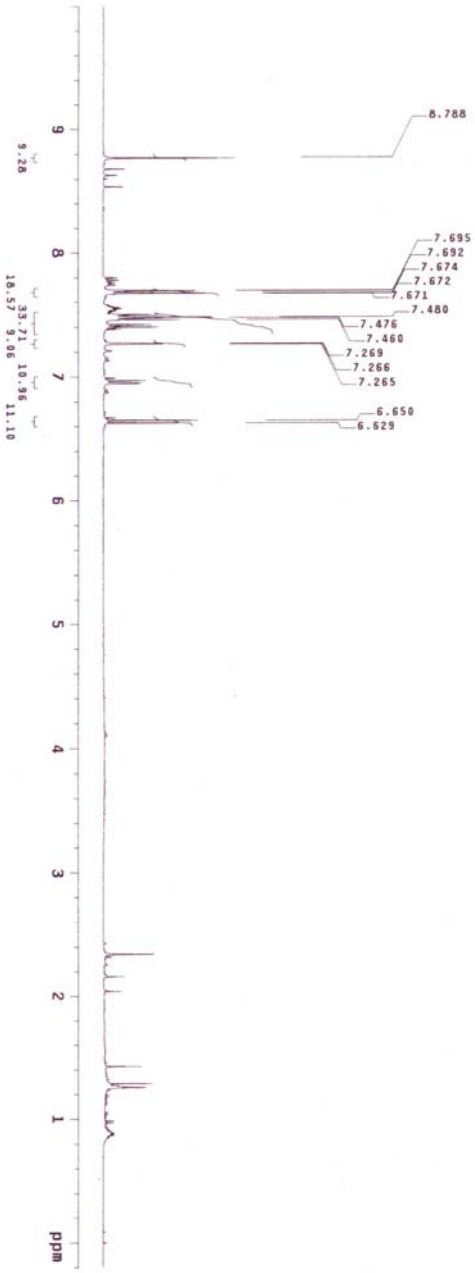
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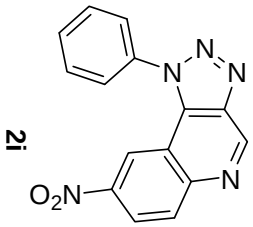
2i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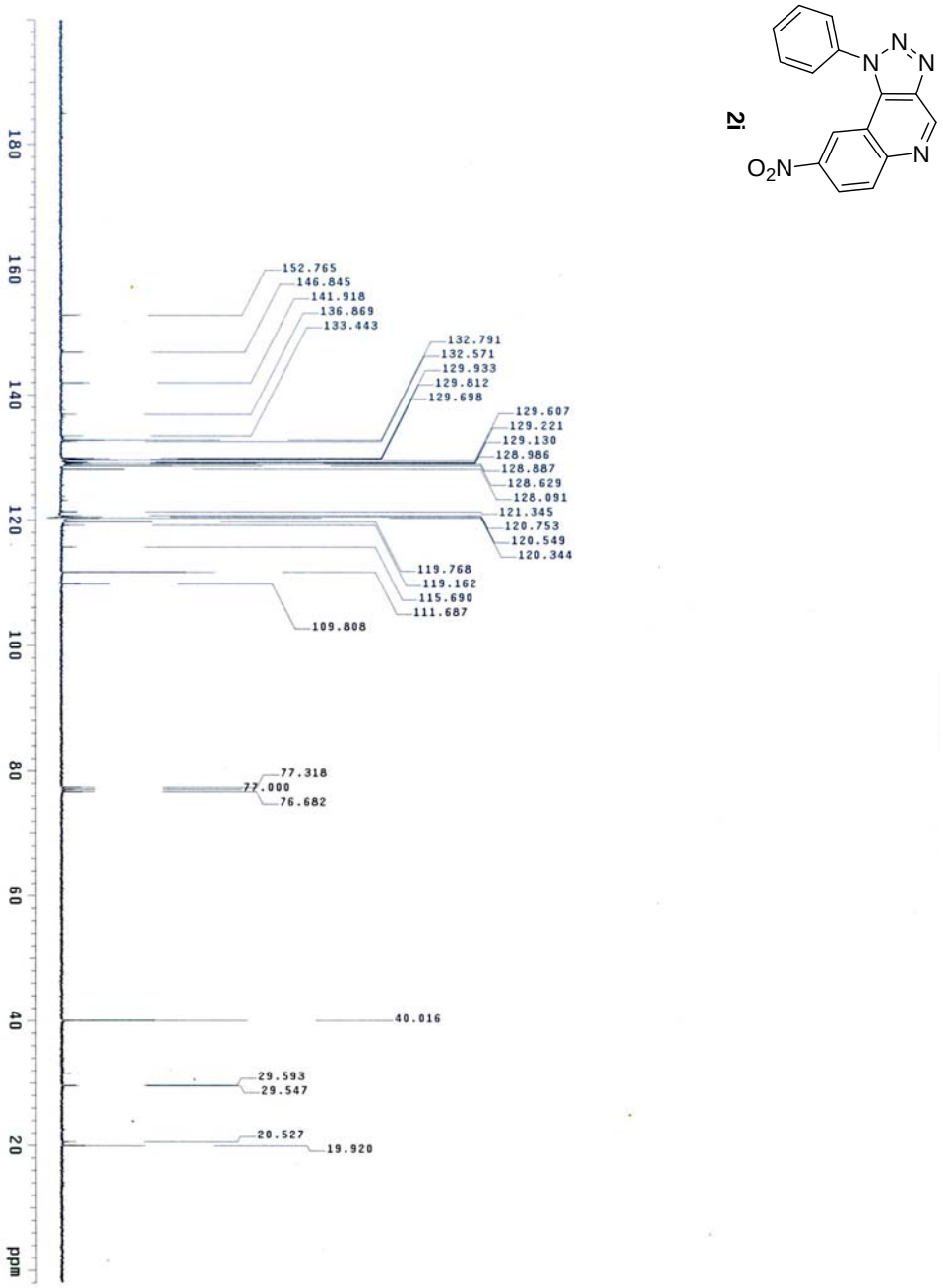

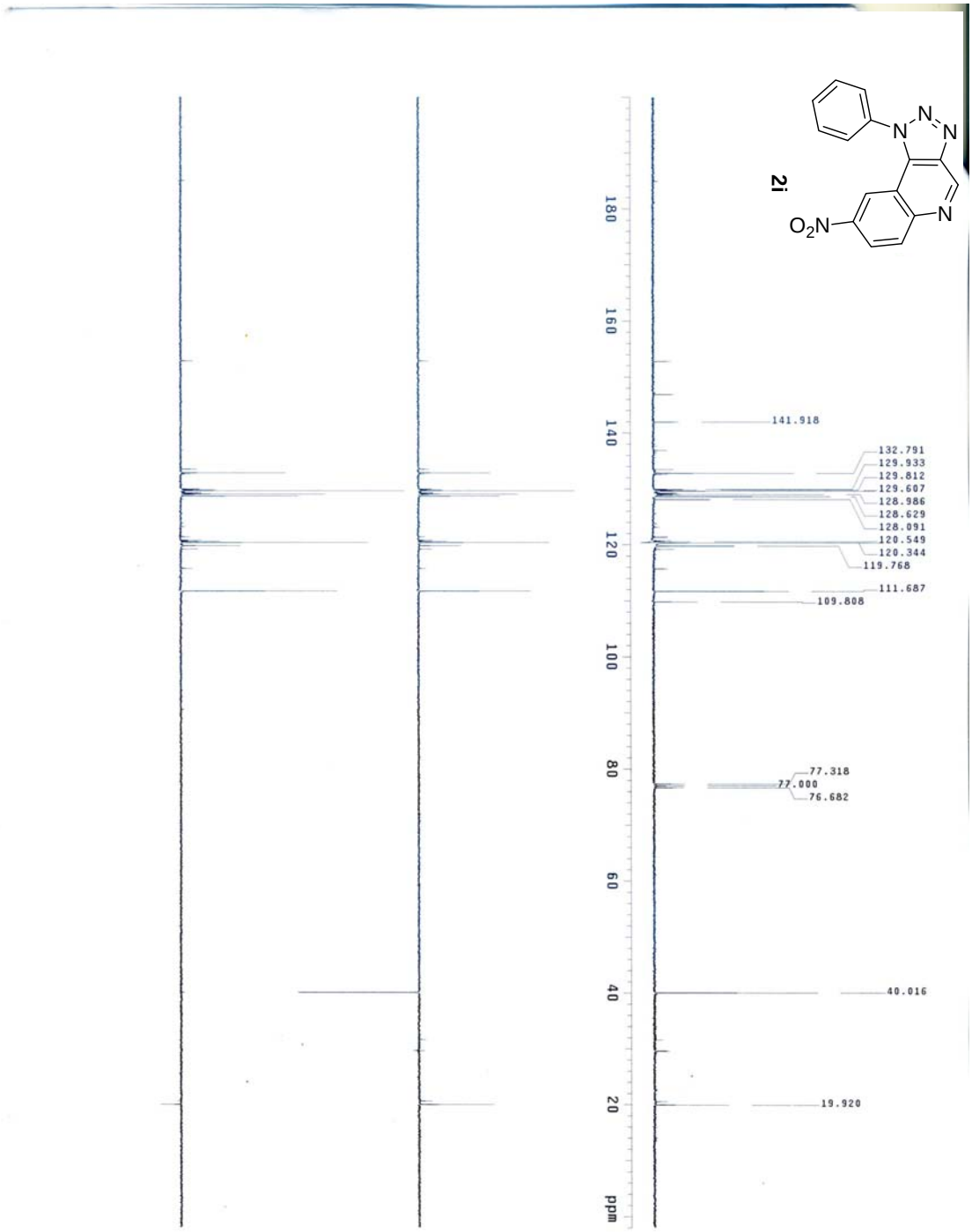
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60
40
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128.986
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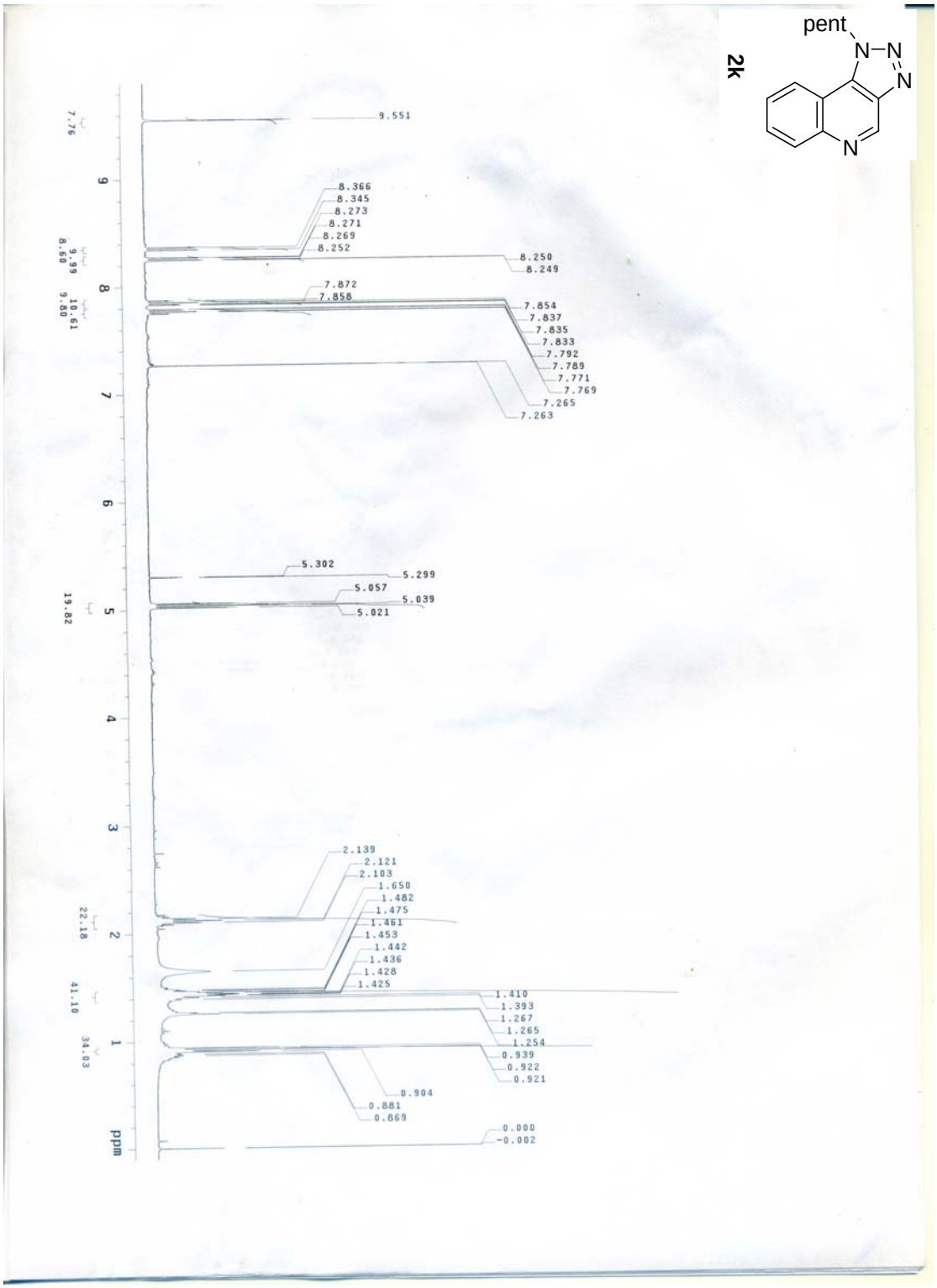
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7.835
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7.792
7.789
7.771
7.769
7.265
7.263
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5.299
5.057
5.039
5.021
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2.121
2.103
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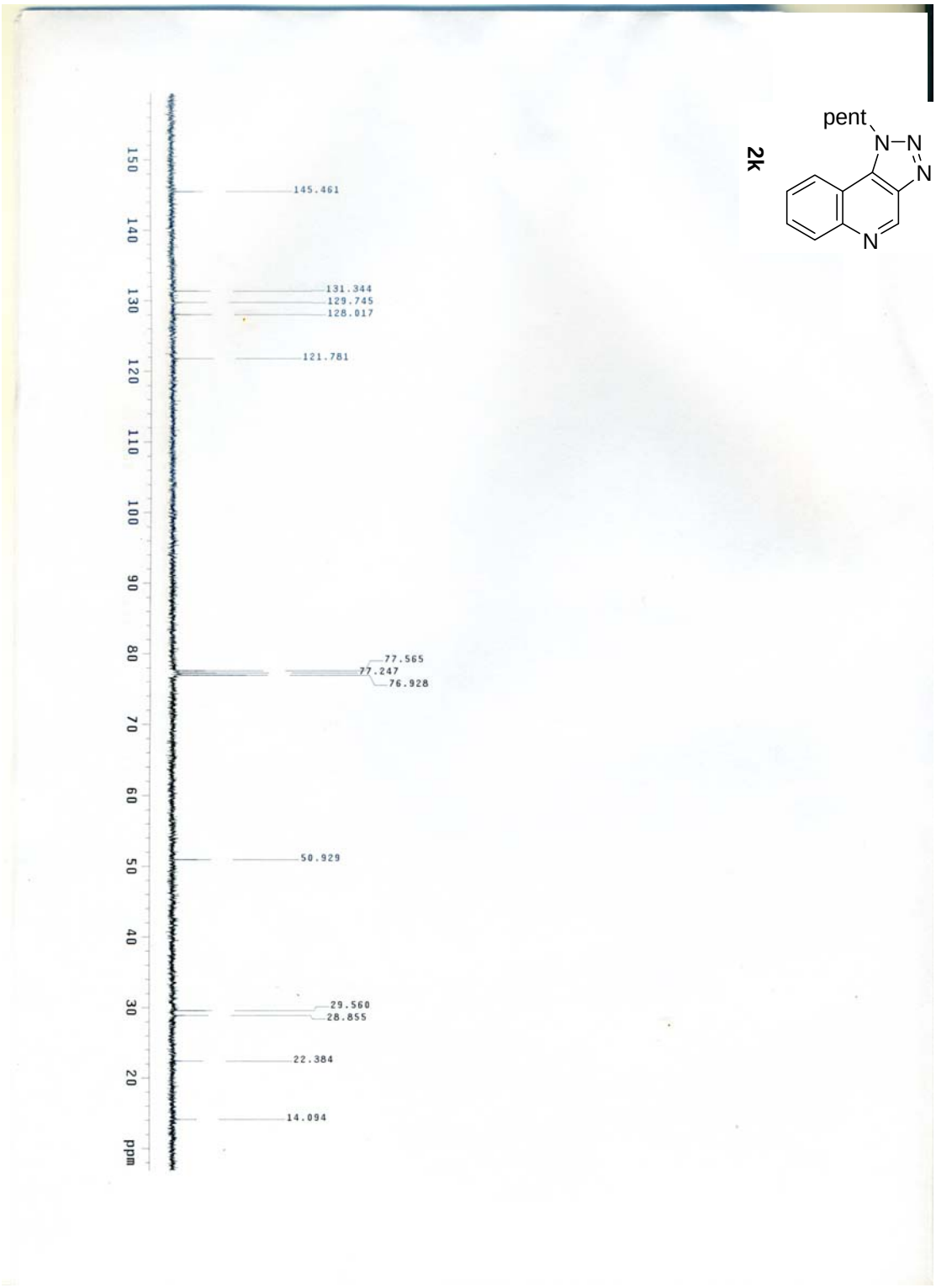
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14.094
ppm

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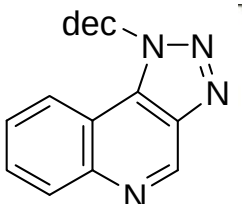
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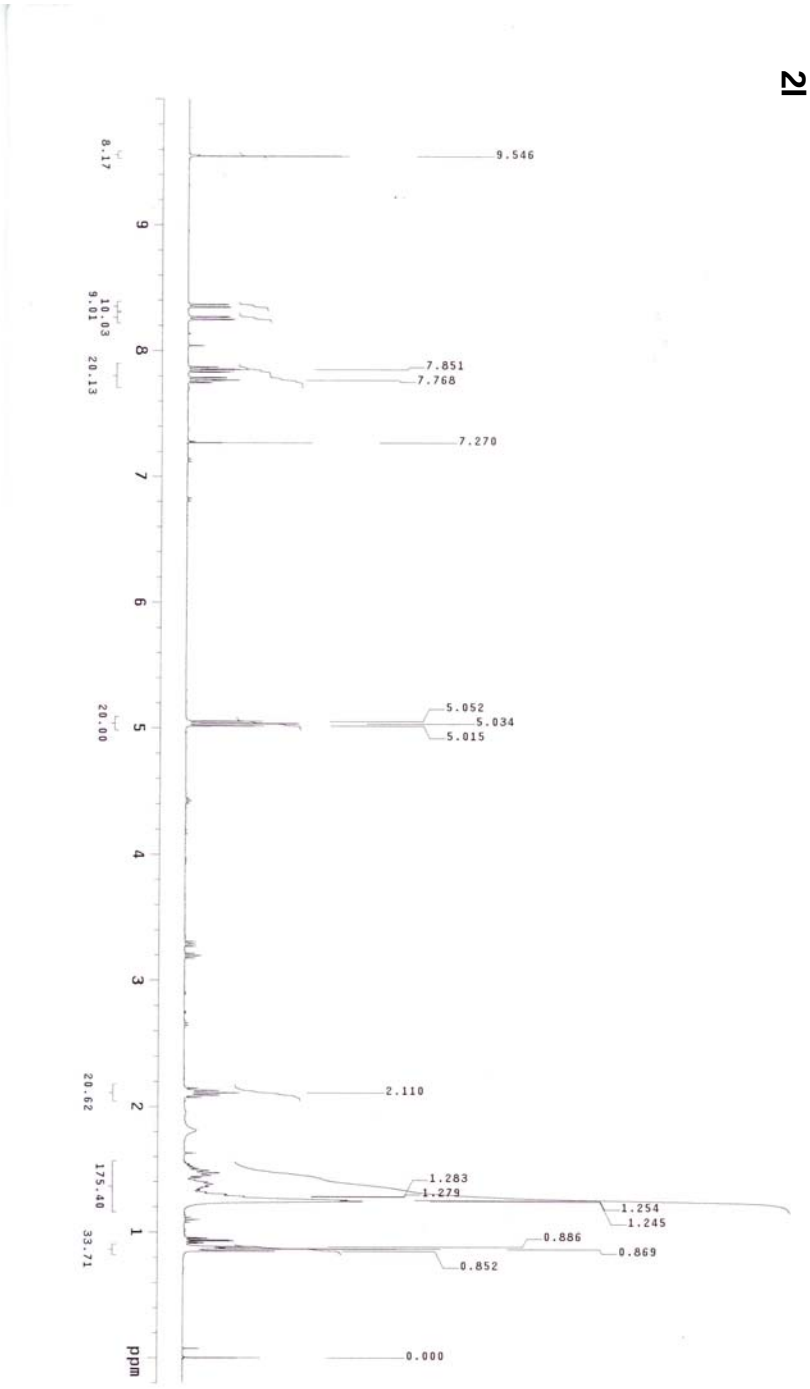
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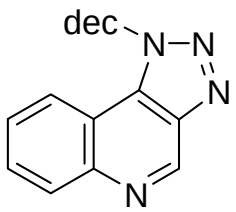
21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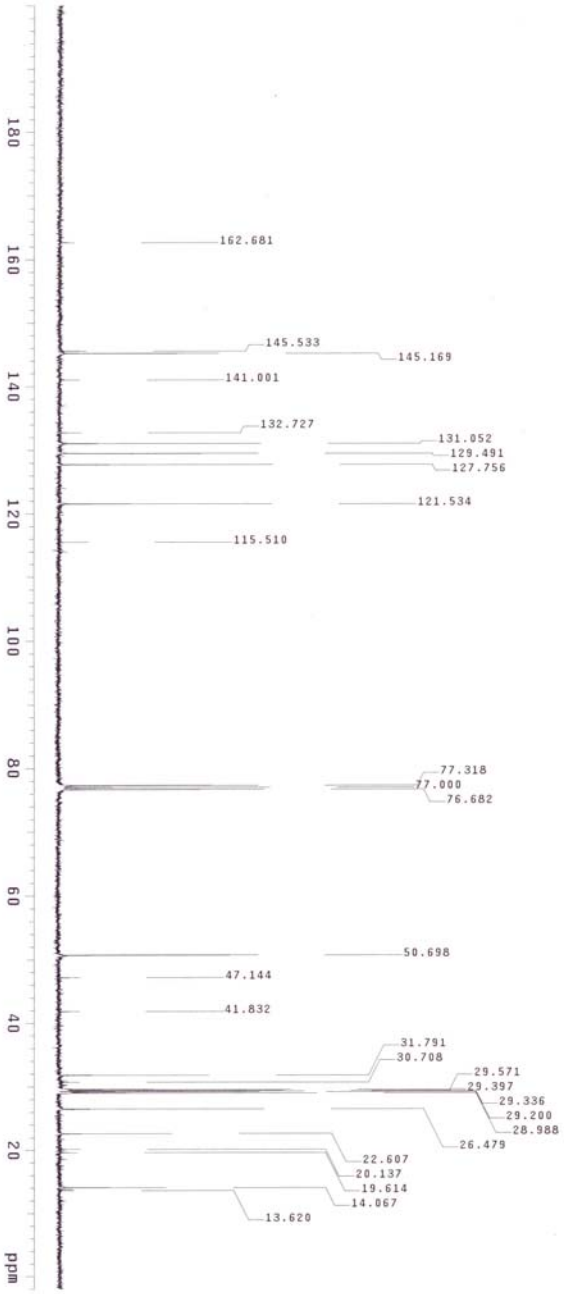
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120
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80
60
40
20
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129.491
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121.534
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77.318
77.000
76.682
50.698
47.144
41.832
31.791
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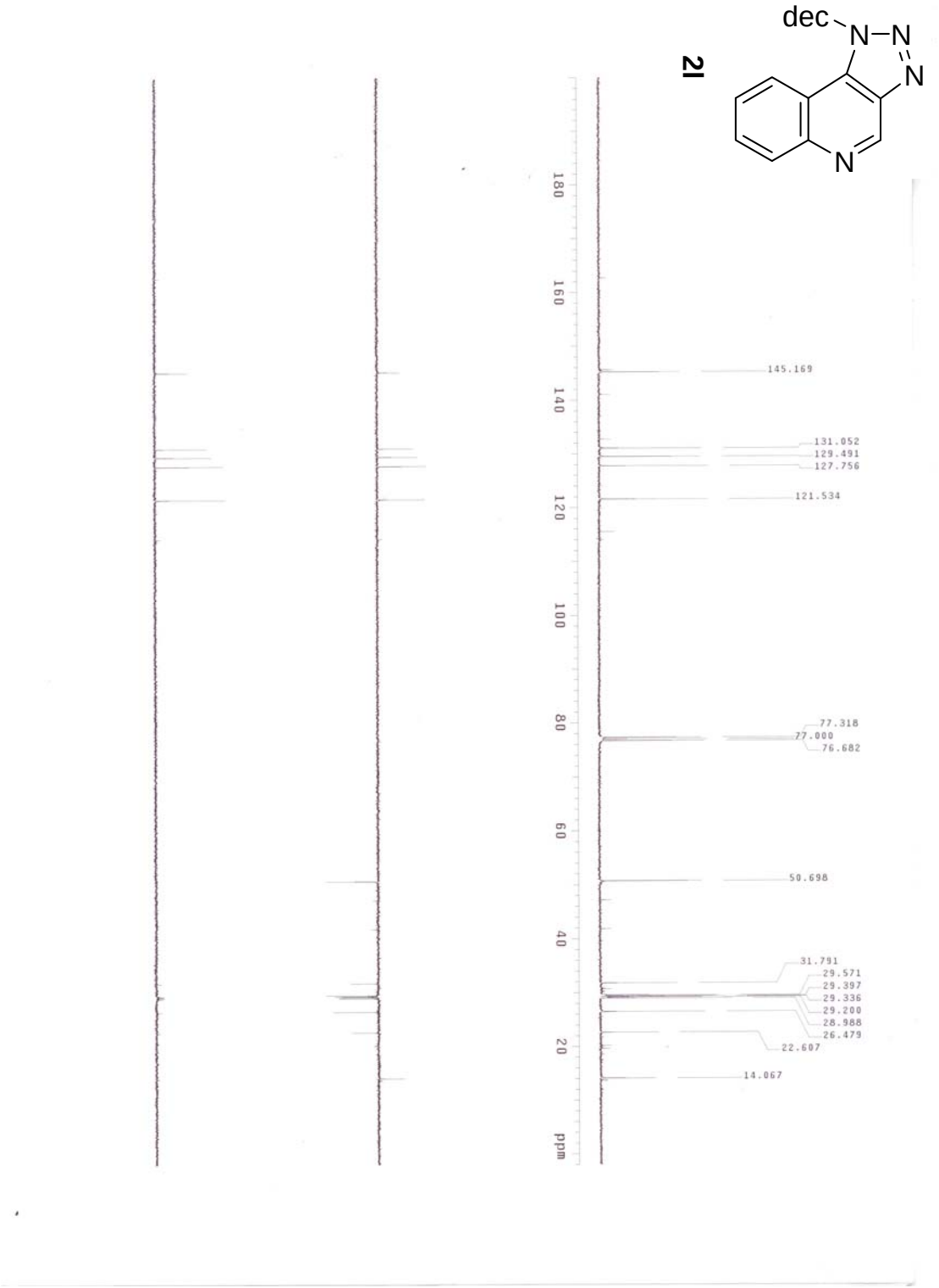
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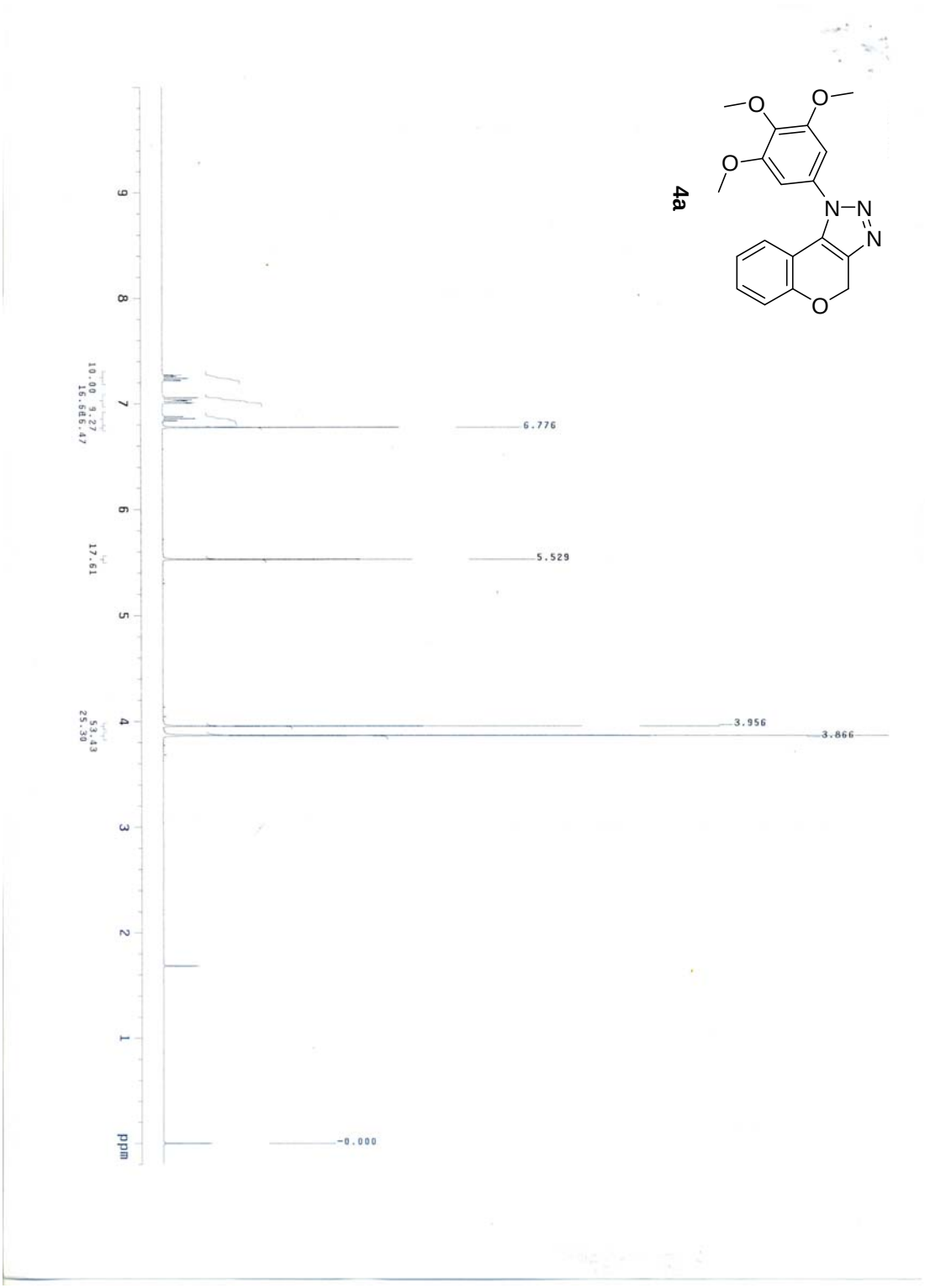
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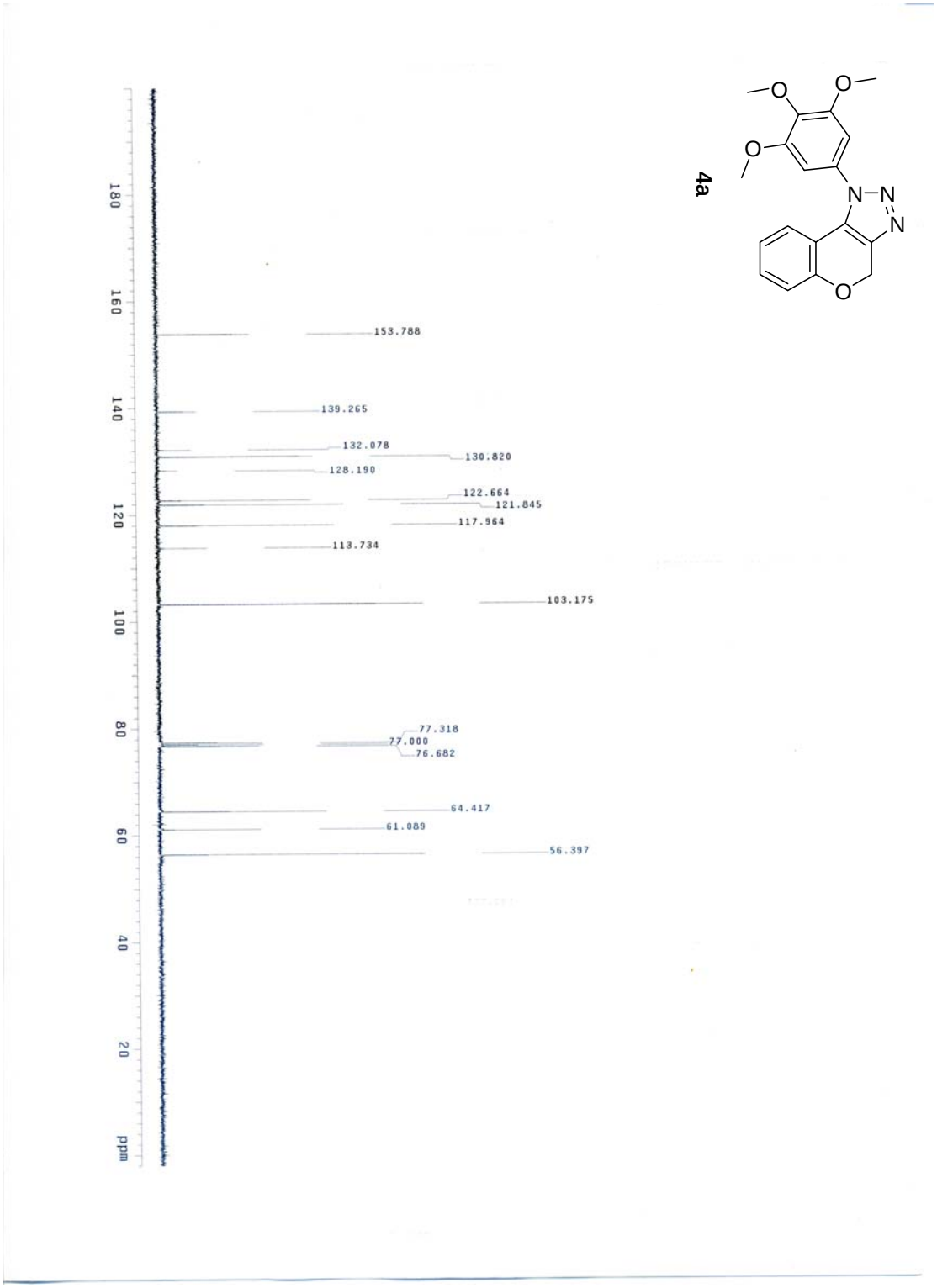
4a
O
O
O
N–N
N
O
180
160
140
120
100
80
60
40
20
ppm
153.788
139.265
132.078
130.820
128.190
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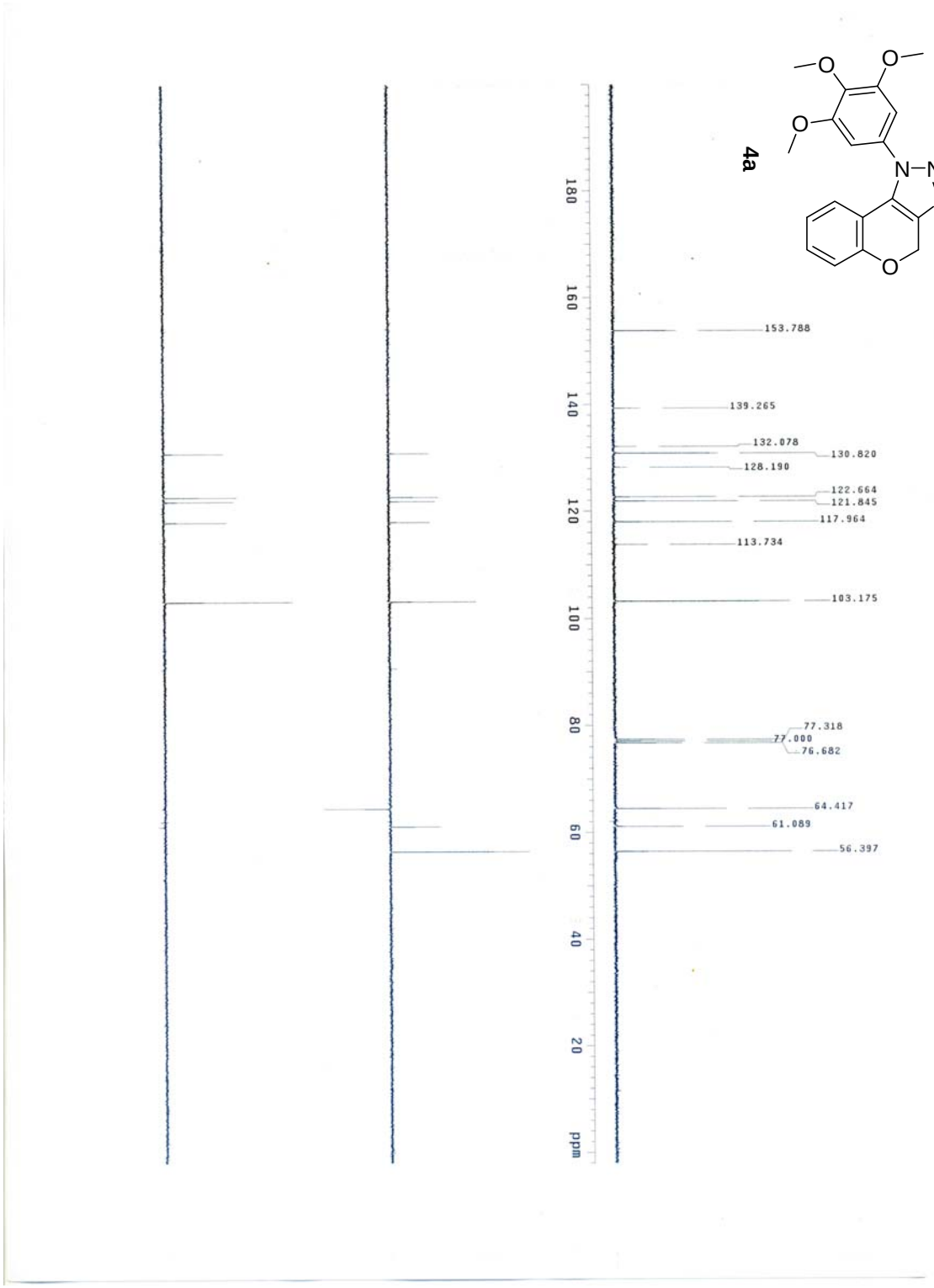
4a
O
O
O
N–N
N
O
180
160
140
120
100
80
60
40
20
ppm
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139.265
132.078
130.820
128.190
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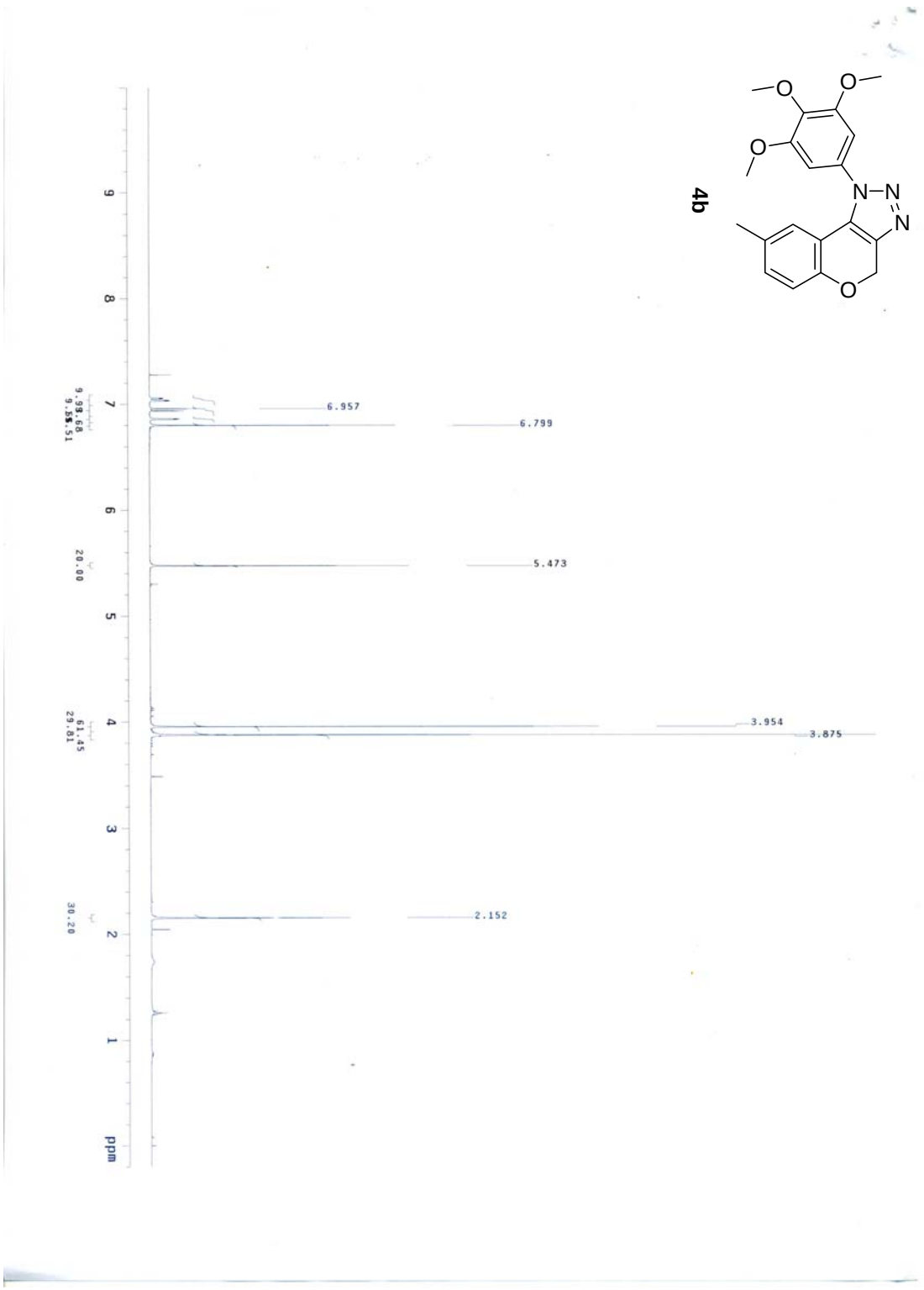

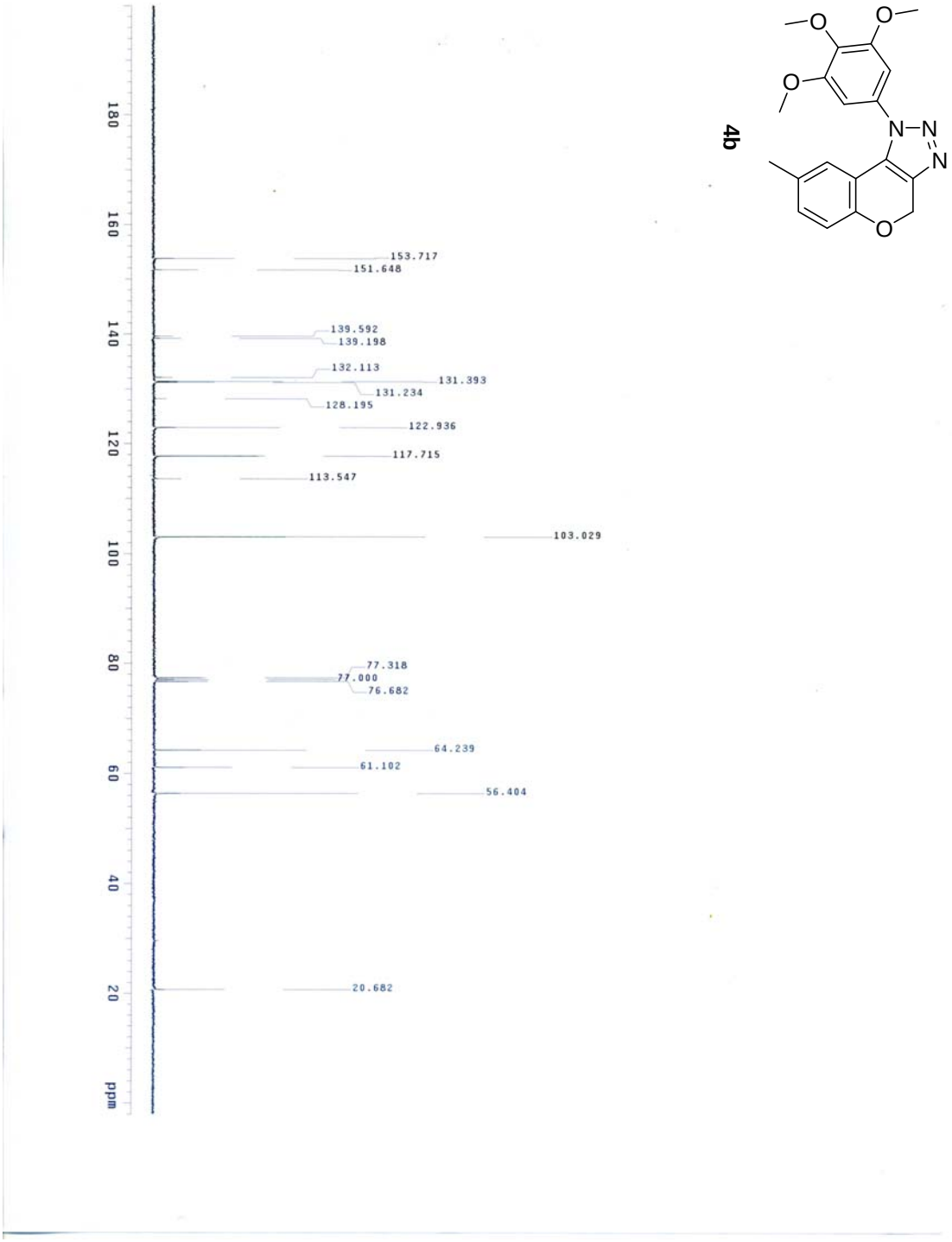
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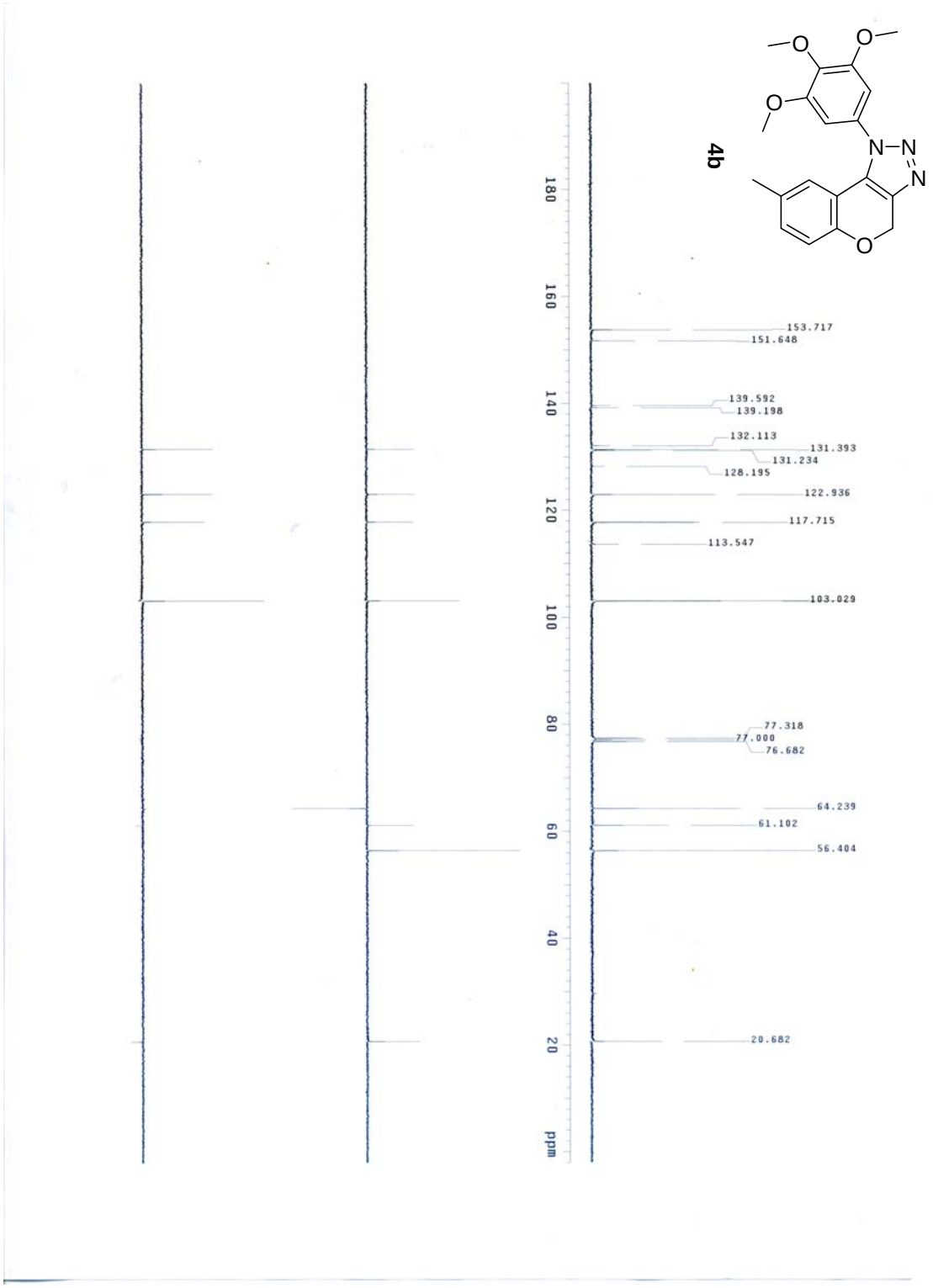
ppm
4b


4b
O
O
O
N–N
N
O
180
160
140
120
100
80
60
40
20
ppm
153.717
151.648
139.592
139.198
132.113
131.393
131.234
128.195
122.936
117.715
113.547
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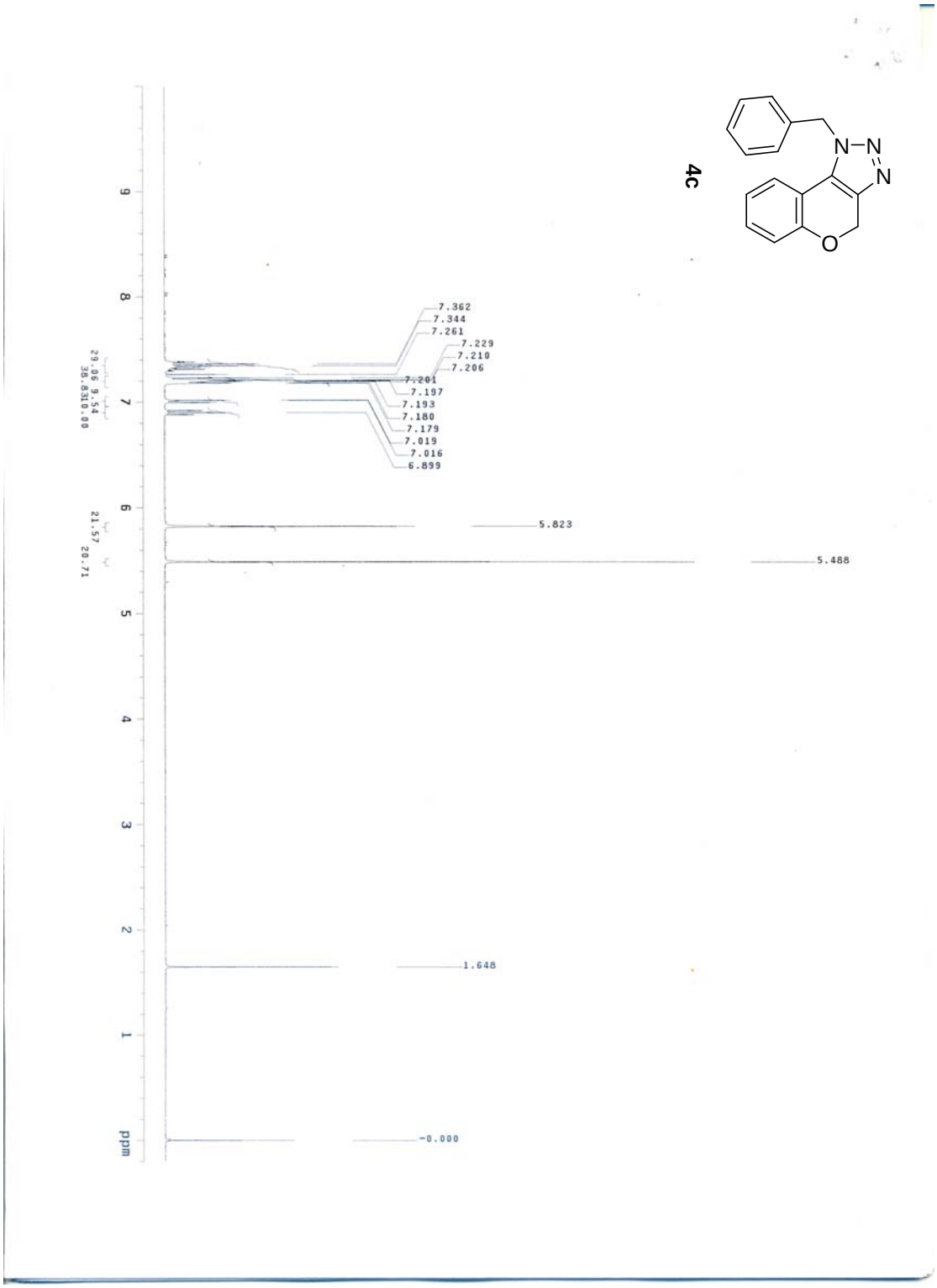
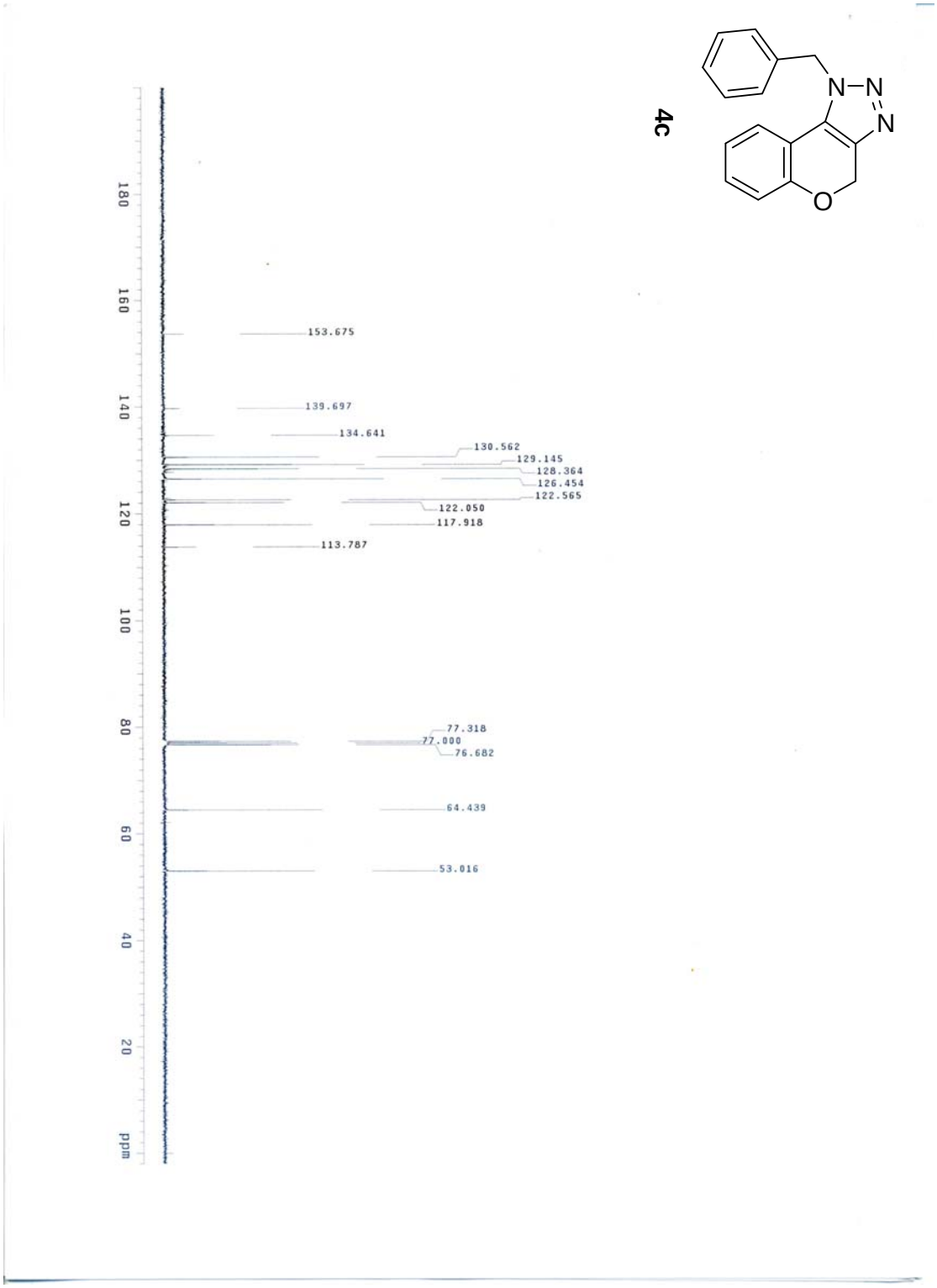
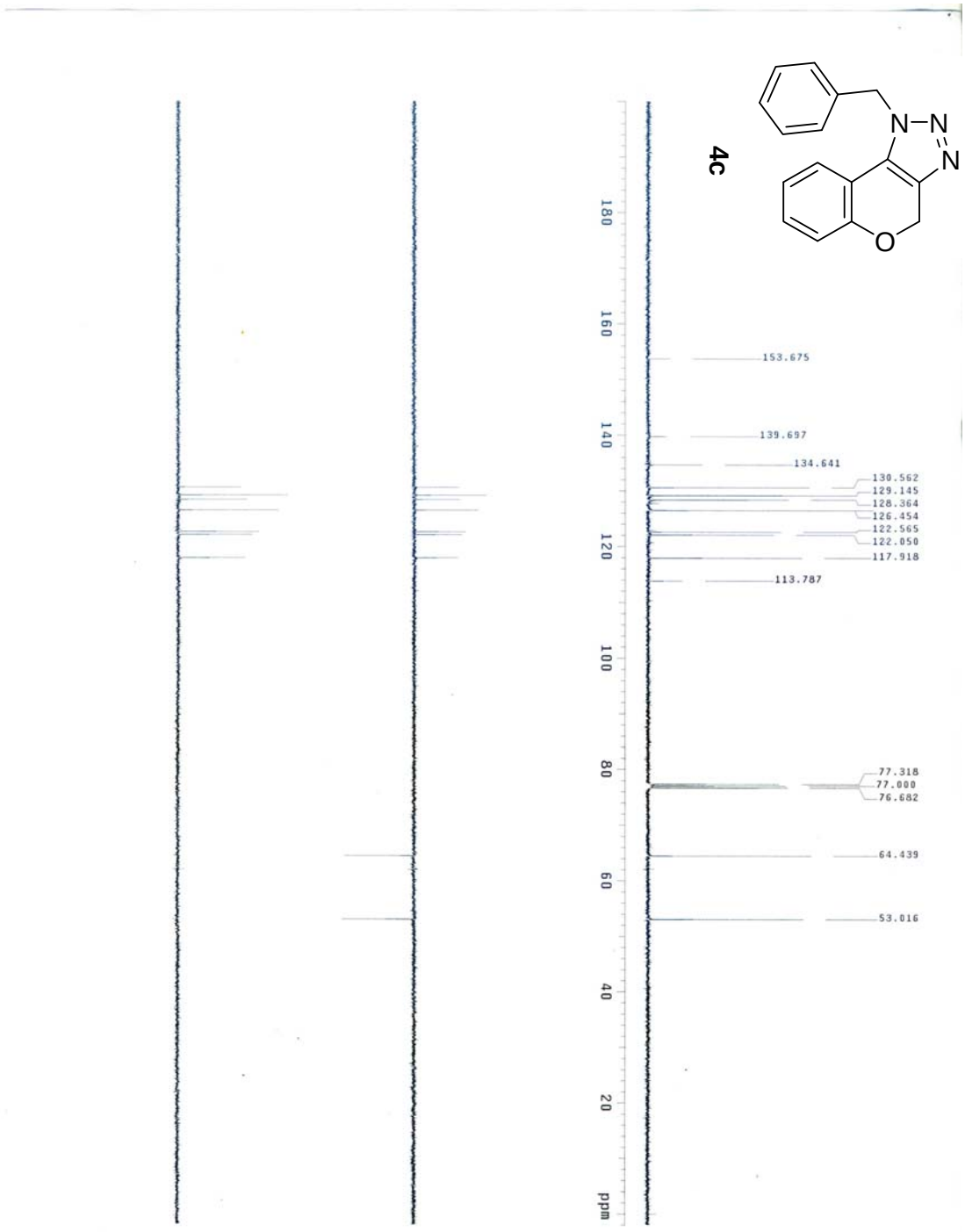
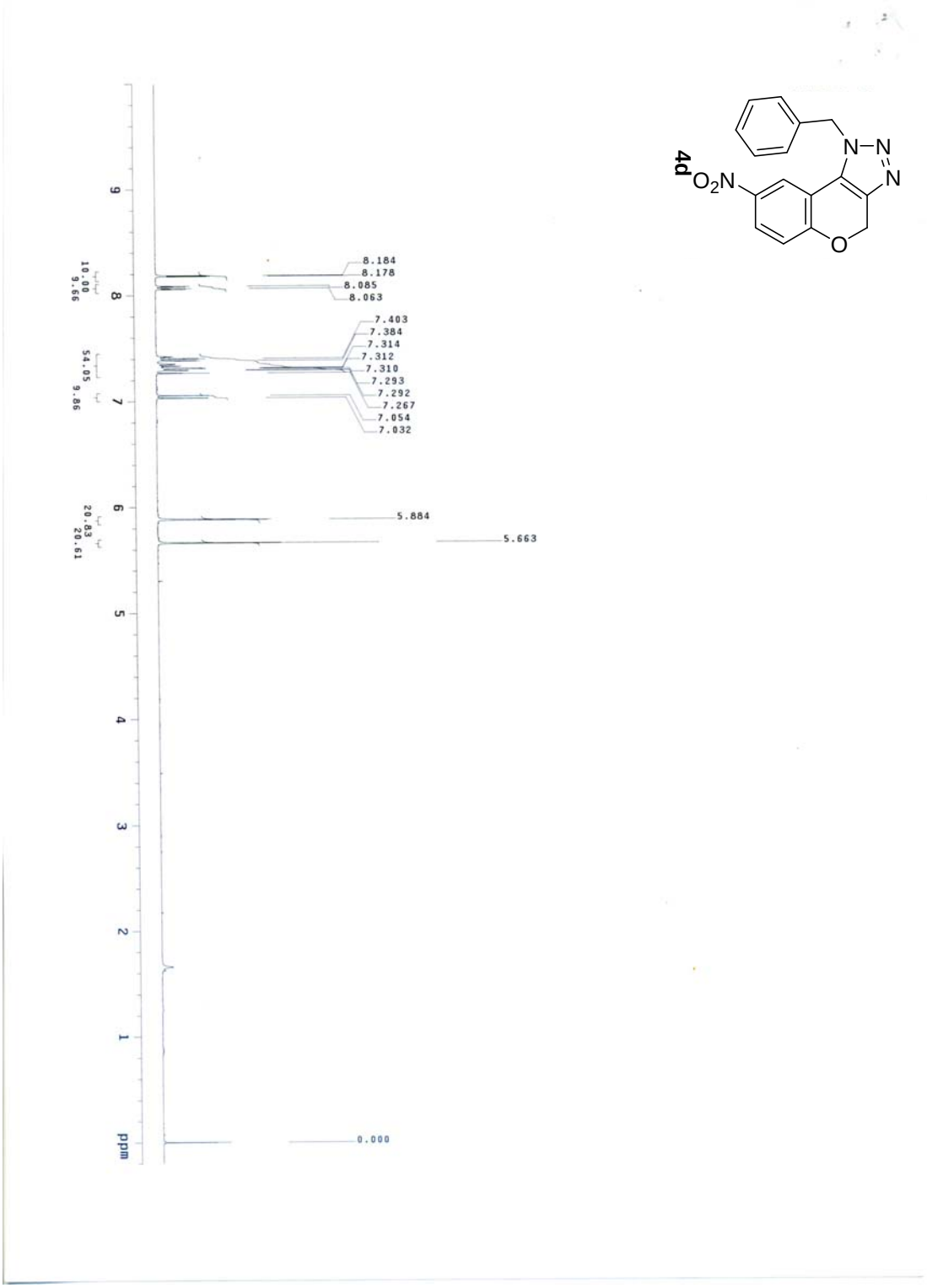
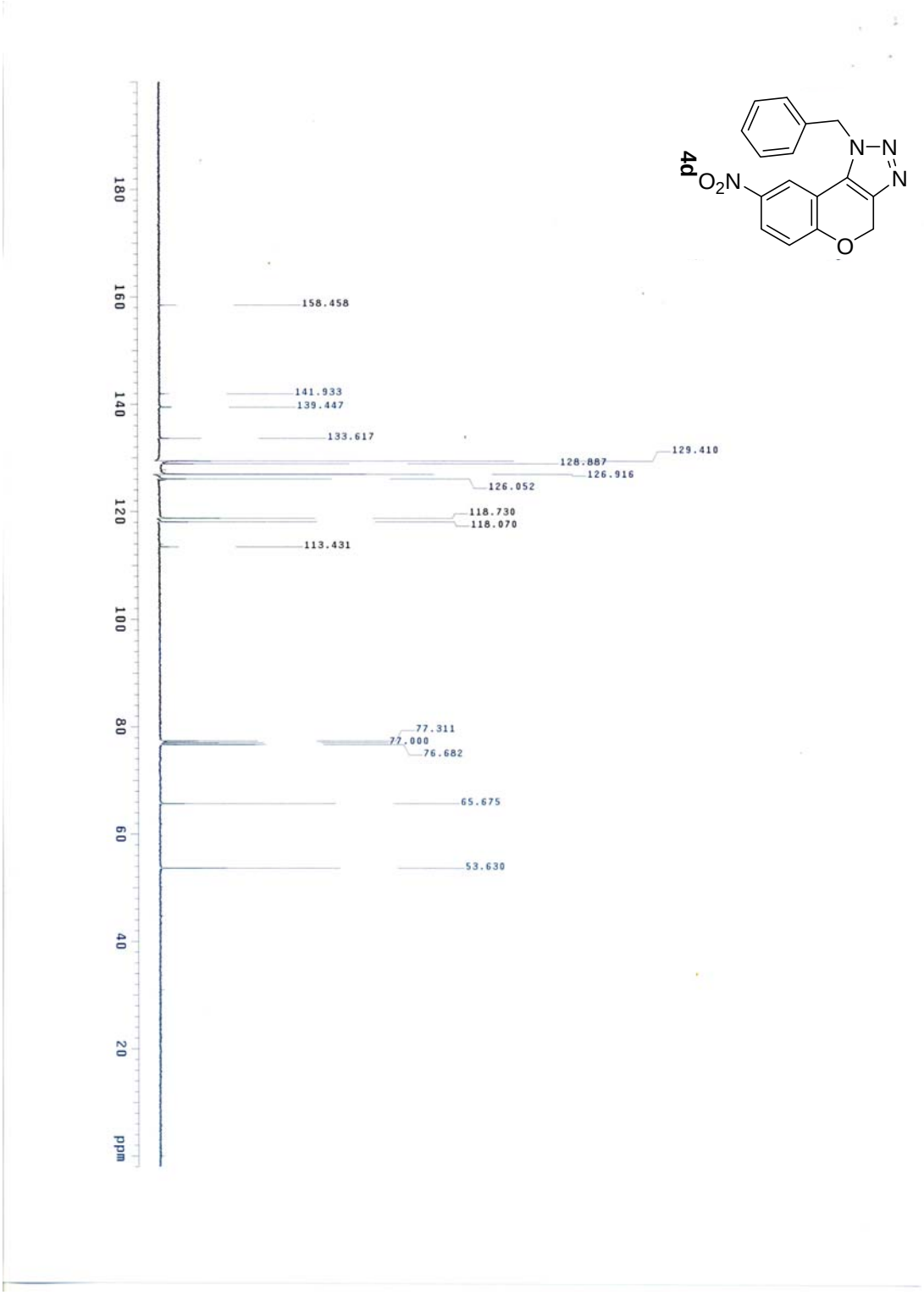
77.318
77.000
76.682
64.239
61.102
56.404
20.682

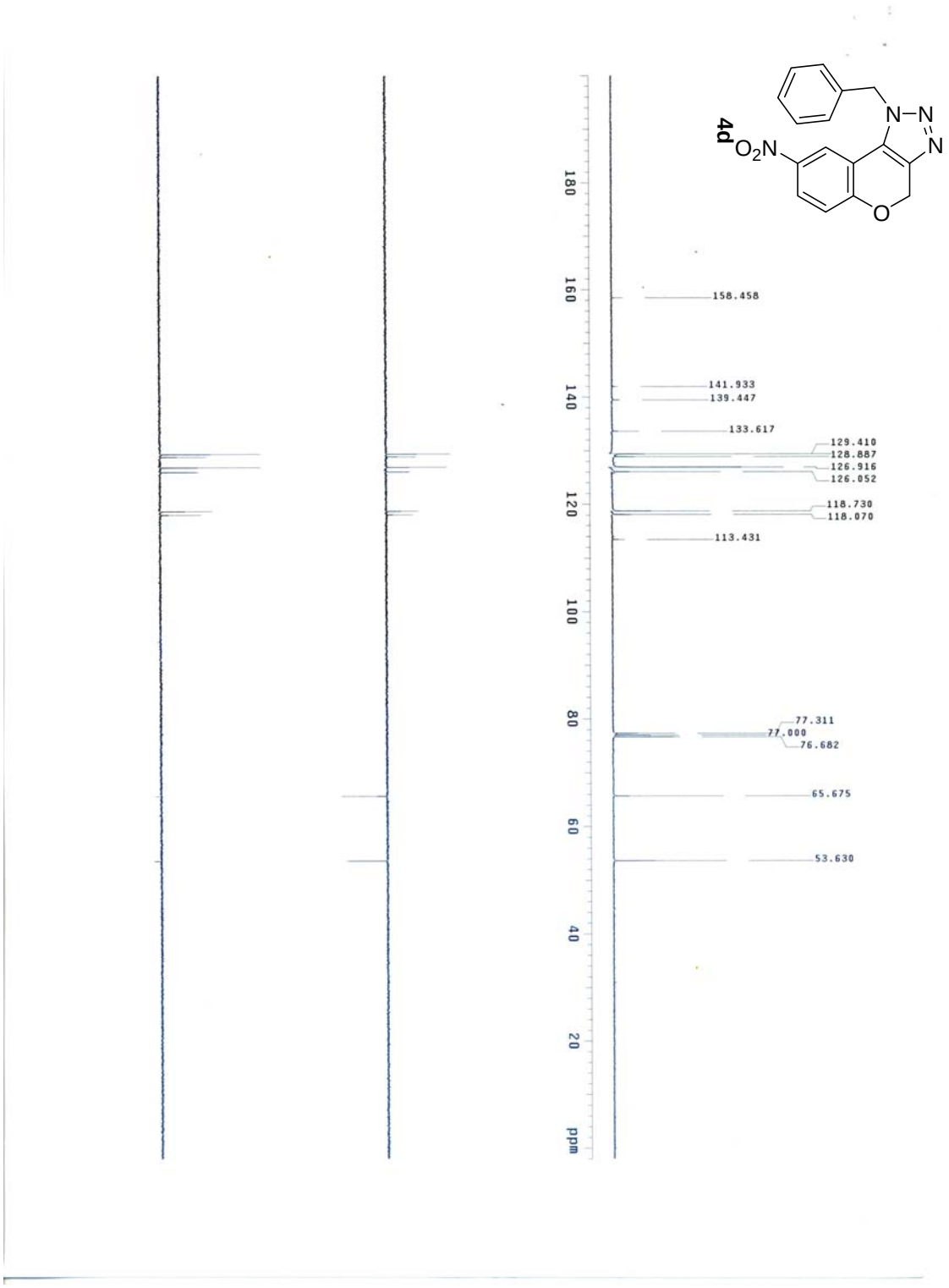

4c
N
N
N
O
7.362
7.344
7.261
7.229
7.210
7.206
7.201
7.197
7.193
7.180
7.179
7.019
7.016
6.899
5.823
5.488
1.648
-0.000
ppm

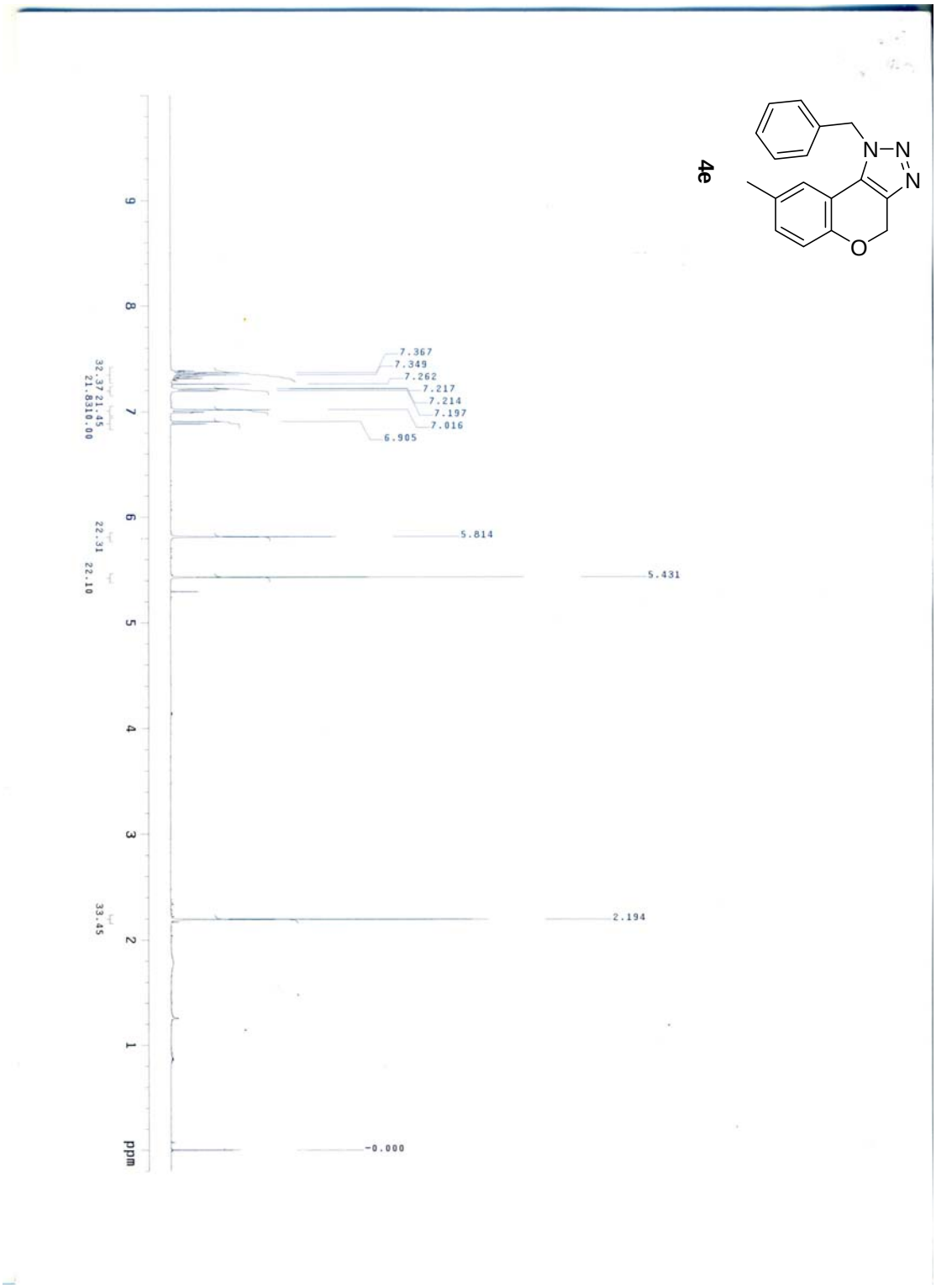

4c
N–N
N
O
153.675
139.697
134.641
130.562
129.145
128.364
126.454
122.565
122.050
117.918
113.787
77.318
77.000
76.682
64.439
53.016
180
160
140
120
100
80
60
40
20
ppm

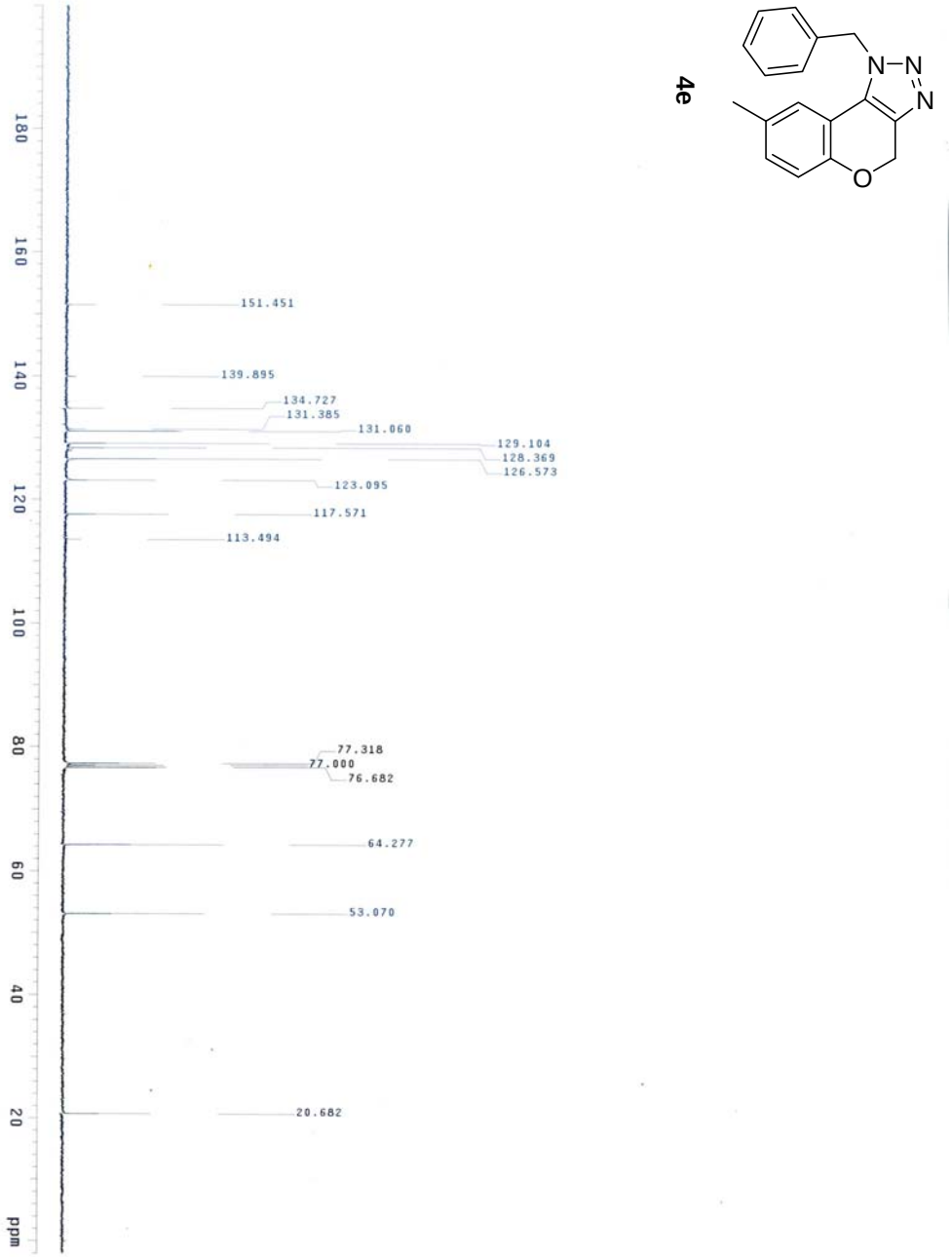


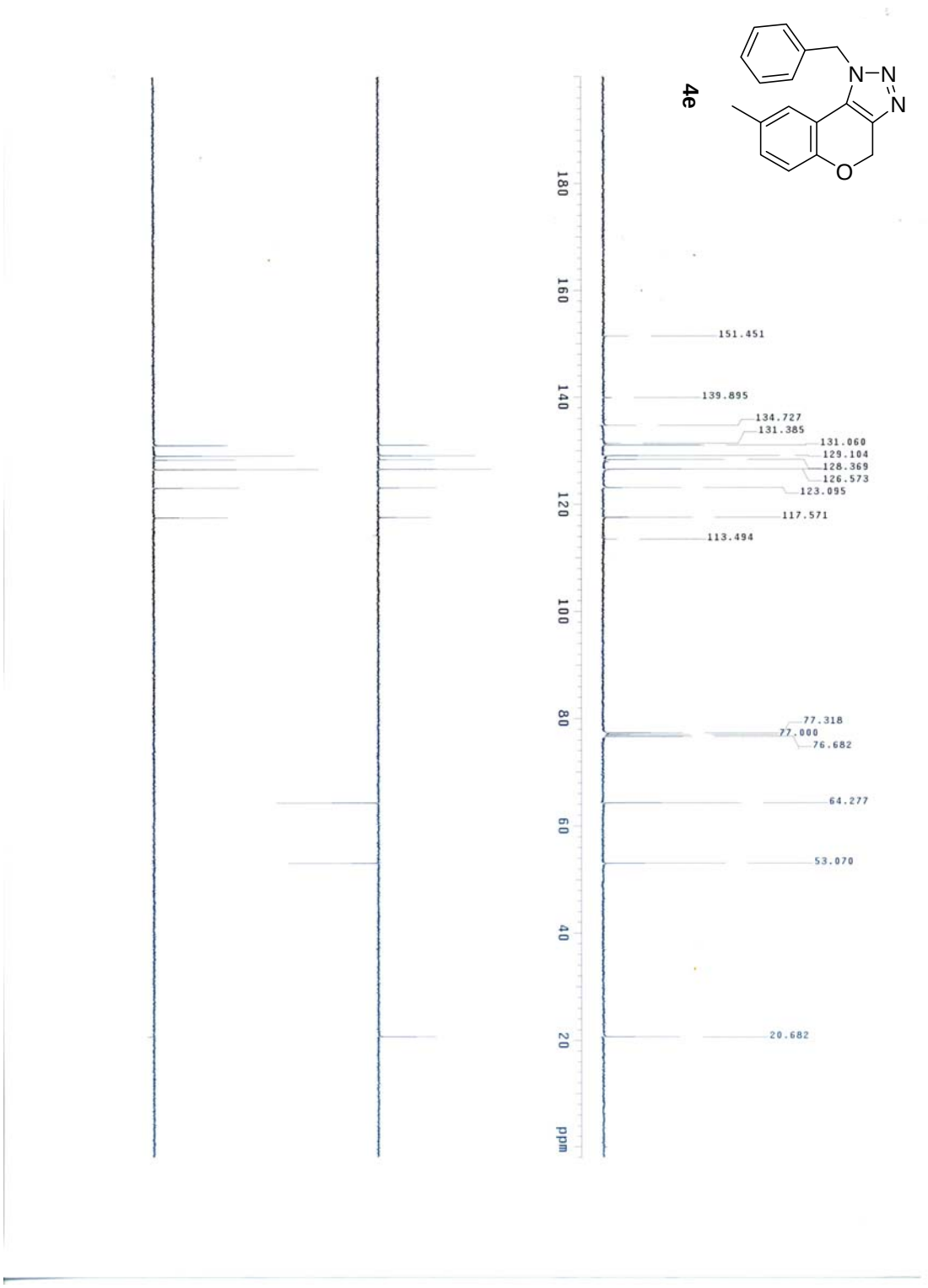

4d
O2N
N–N
N
O
8.184
8.178
8.085
8.063
7.403
7.384
7.314
7.312
7.310
7.293
7.292
7.267
7.054
7.032
5.884
5.663
0.000
ppm

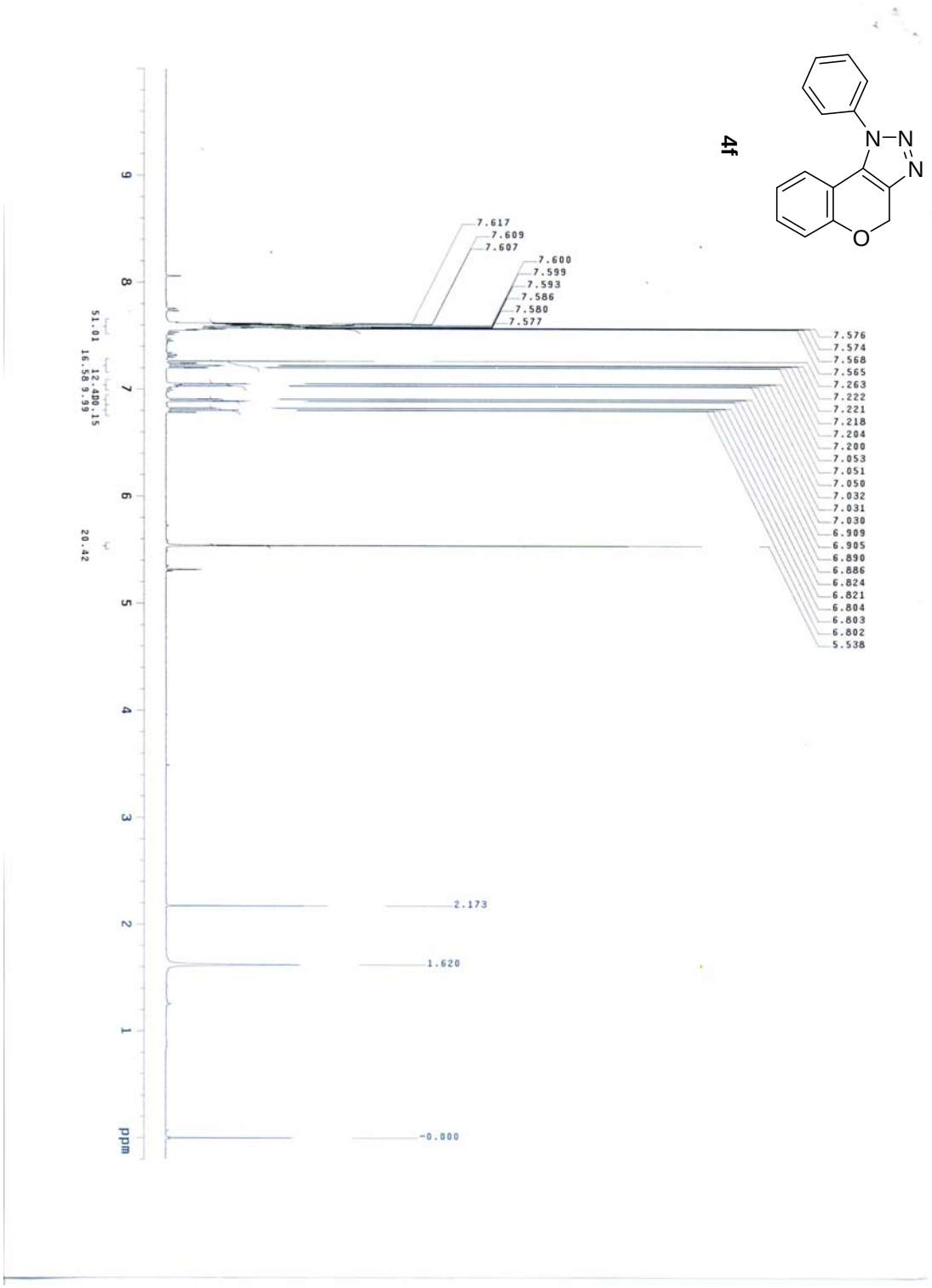

4d
O2N
N–N
N
O
158.458
141.933
139.447
133.617
129.410
128.887
126.916
126.052
118.730
118.070
113.431
77.311
77.000
76.682
65.675
53.630
ppm

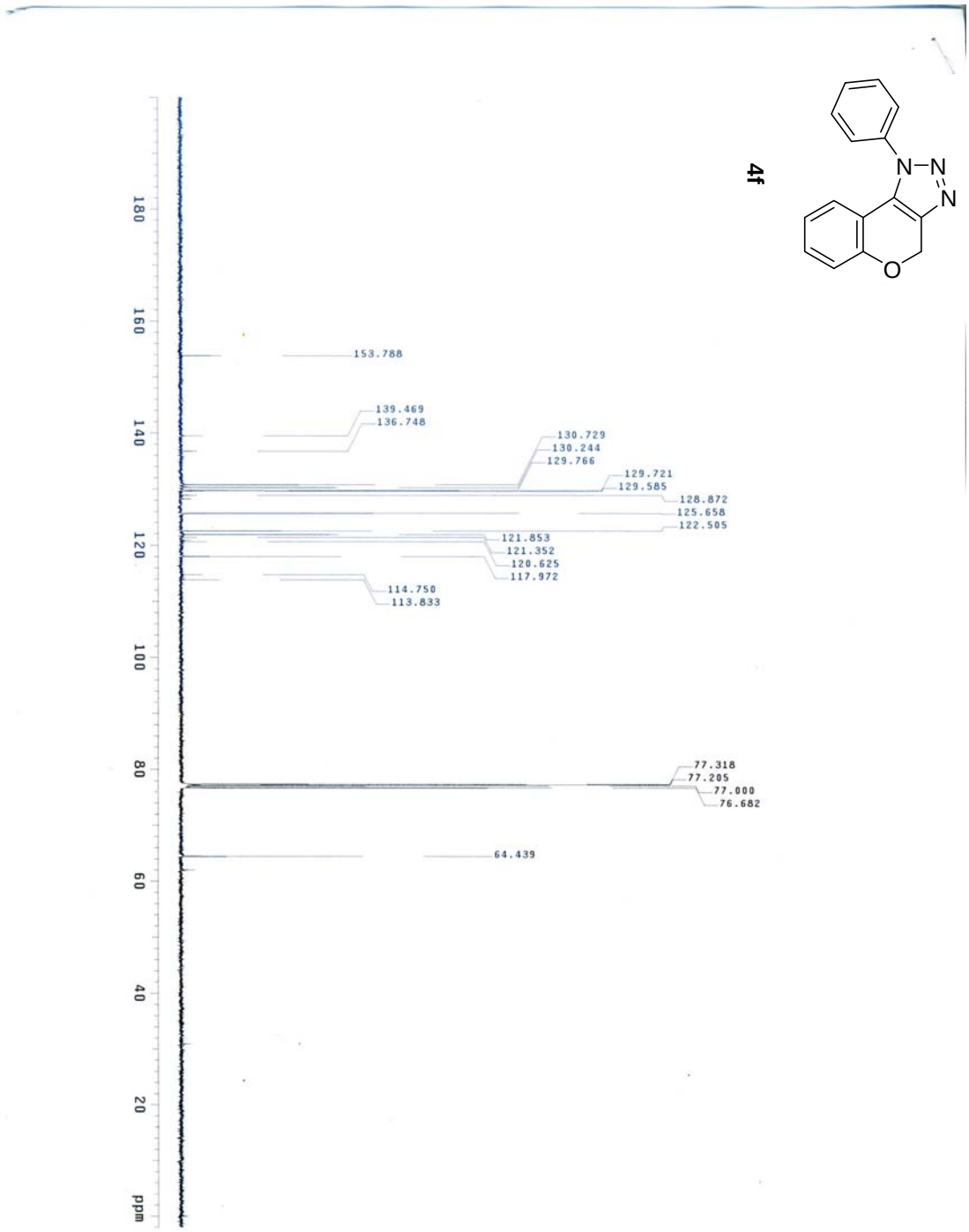


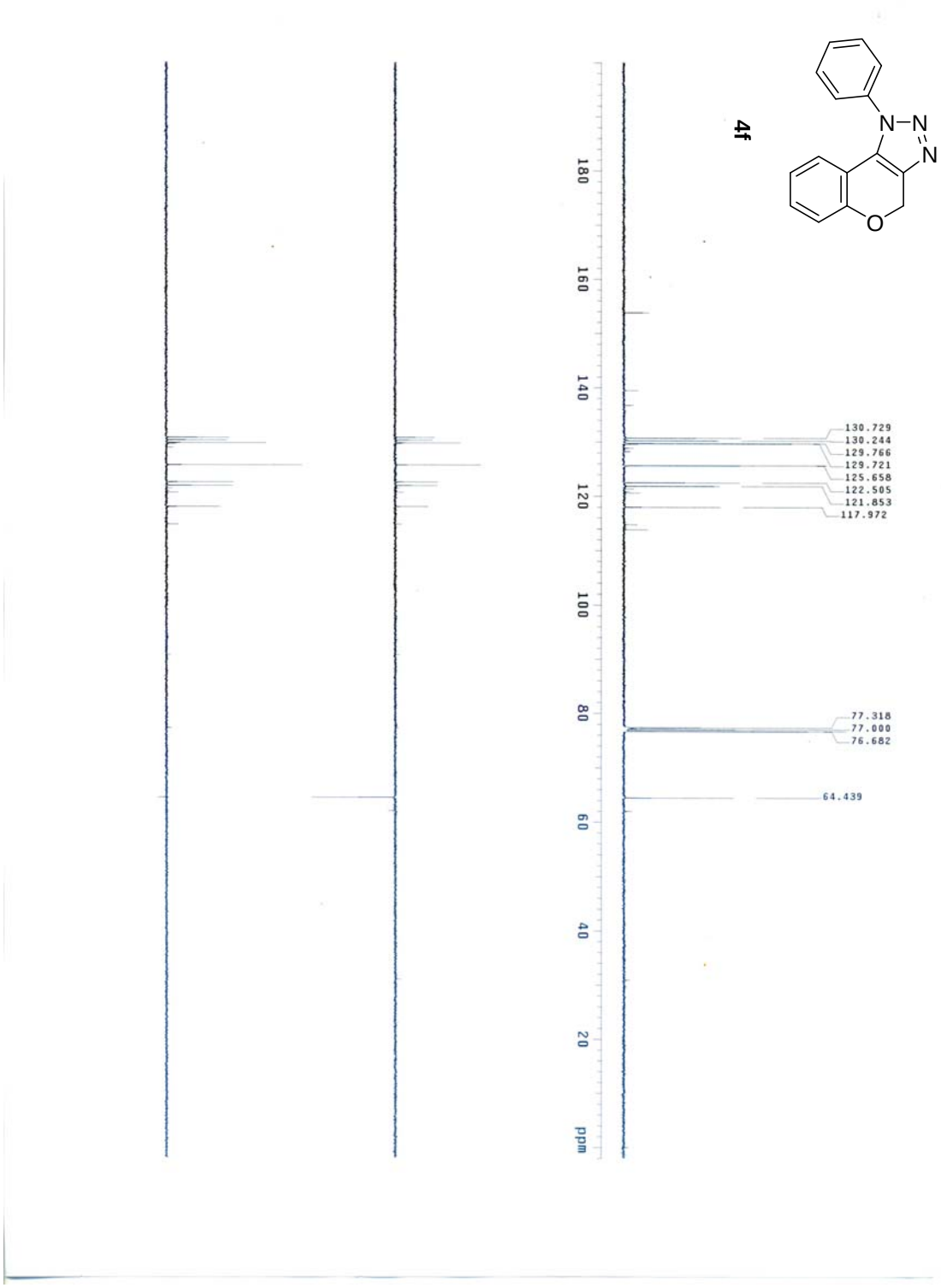

4e
N–N
N
O
7.367
7.349
7.262
7.217
7.214
7.197
7.016
6.905
5.814
5.431
2.194
-0.000
ppm

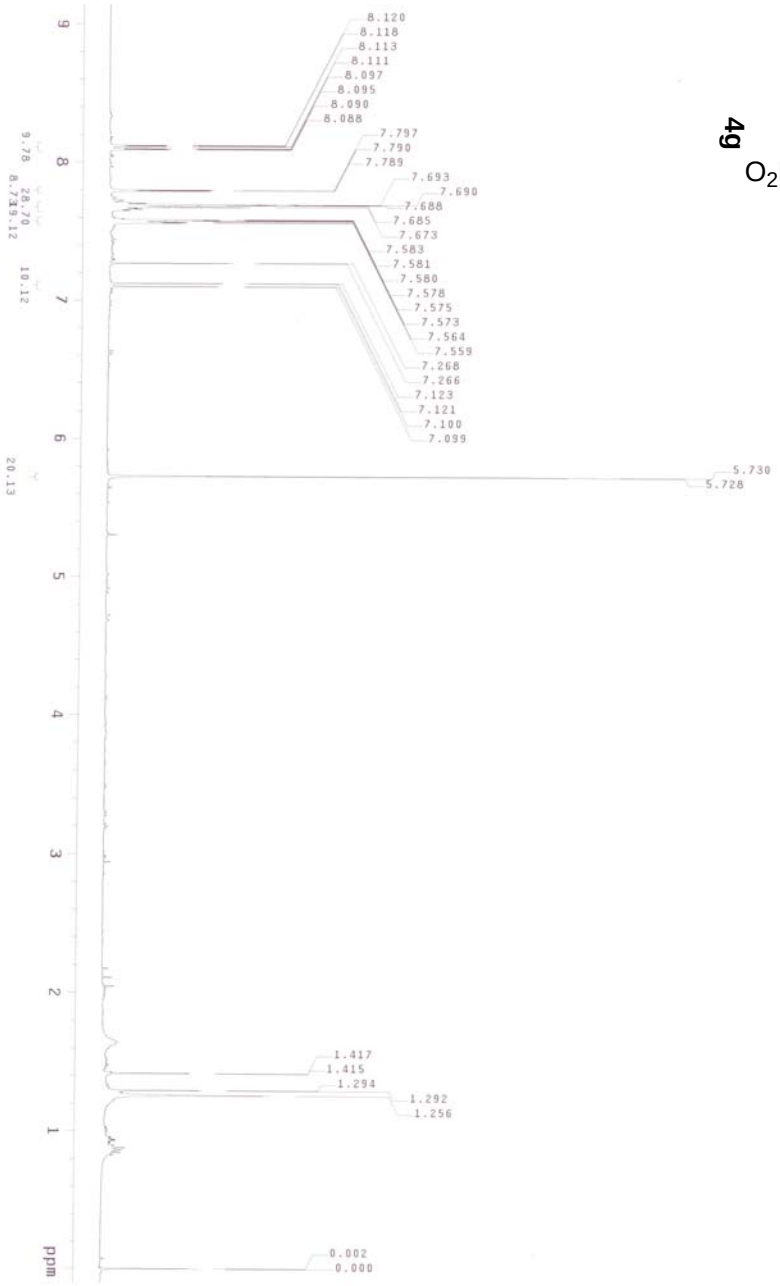


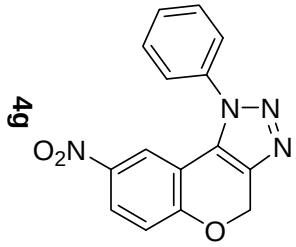

4e
N–N
N
O
180
160
140
120
100
80
60
40
20
ppm
151.451
139.895
134.727
131.385
131.060
129.104
128.369
126.573
123.095
117.571
113.494
77.318
77.000
76.682
64.277
53.070
20.682

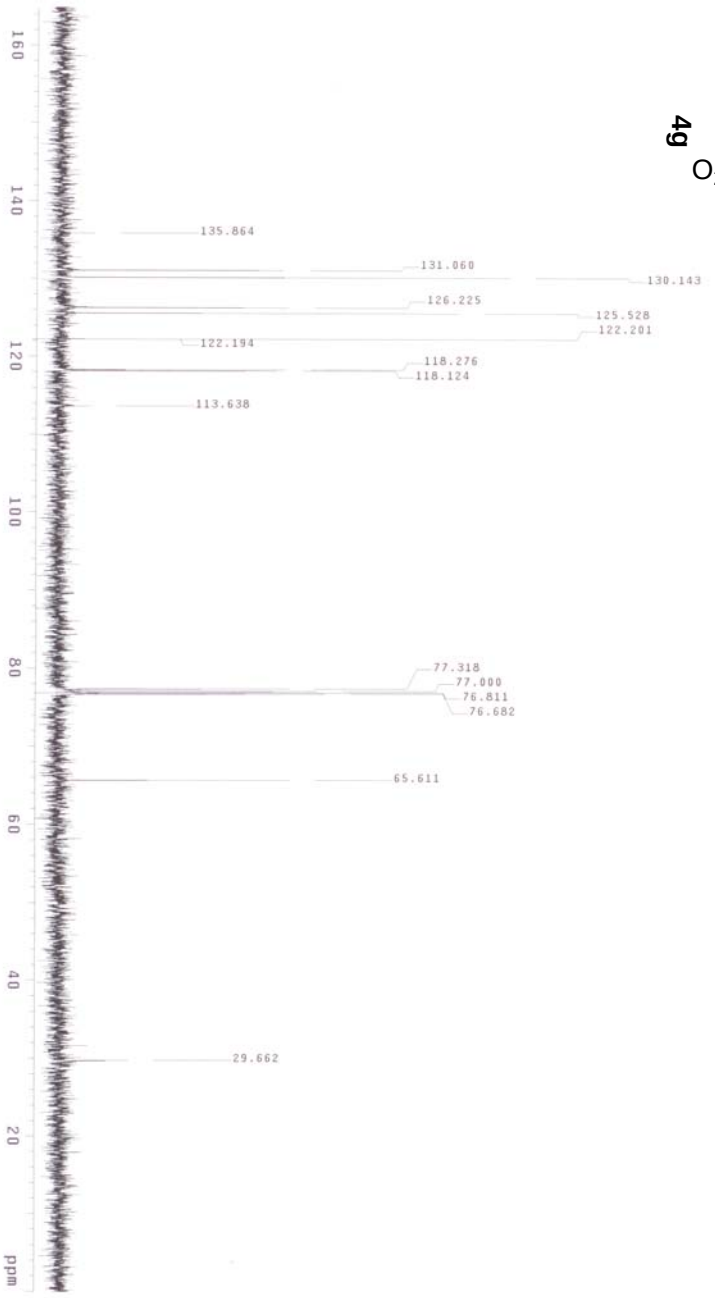


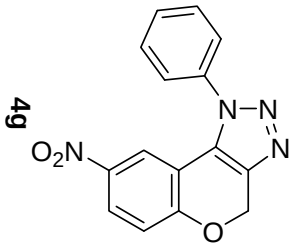

4f
N
N
N
O
153.788
139.469
136.748
130.729
130.244
129.766
129.721
129.585
128.872
125.658
122.505
121.853
121.352
120.625
117.972
114.750
113.833
77.318
77.205
77.000
76.682
64.439
180
160
140
120
100
80
60
40
20
ppm

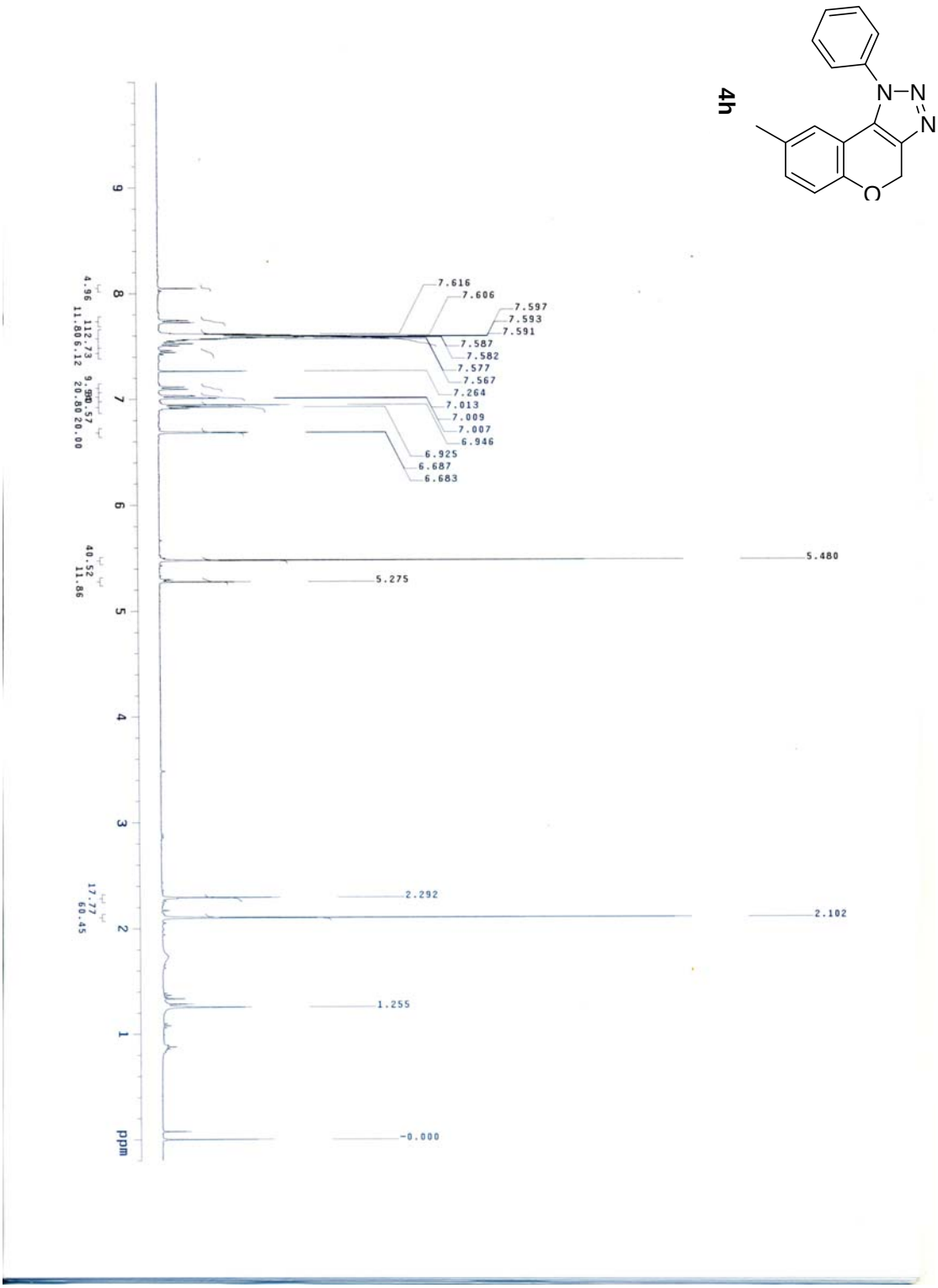


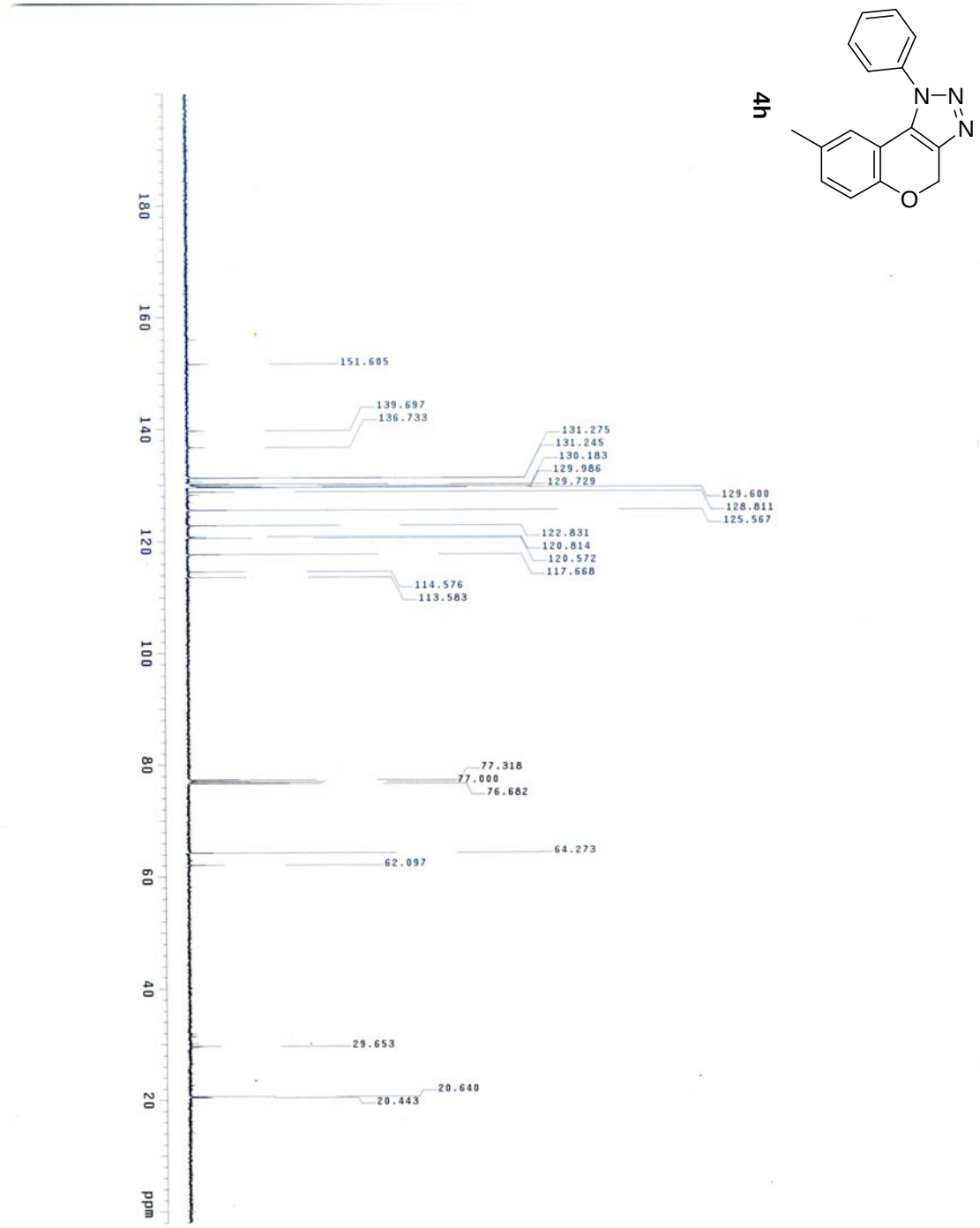

8.120
8.118
8.113
8.111
8.097
8.095
8.090
8.088
7.797
7.790
7.789
7.693
7.690
7.688
7.685
7.673
7.583
7.581
7.580
7.578
7.575
7.573
7.564
7.559
7.268
7.266
7.123
7.121
7.100
7.099
5.730
5.728
1.417
1.415
1.294
1.292
1.256
0.002
0.000
ppm

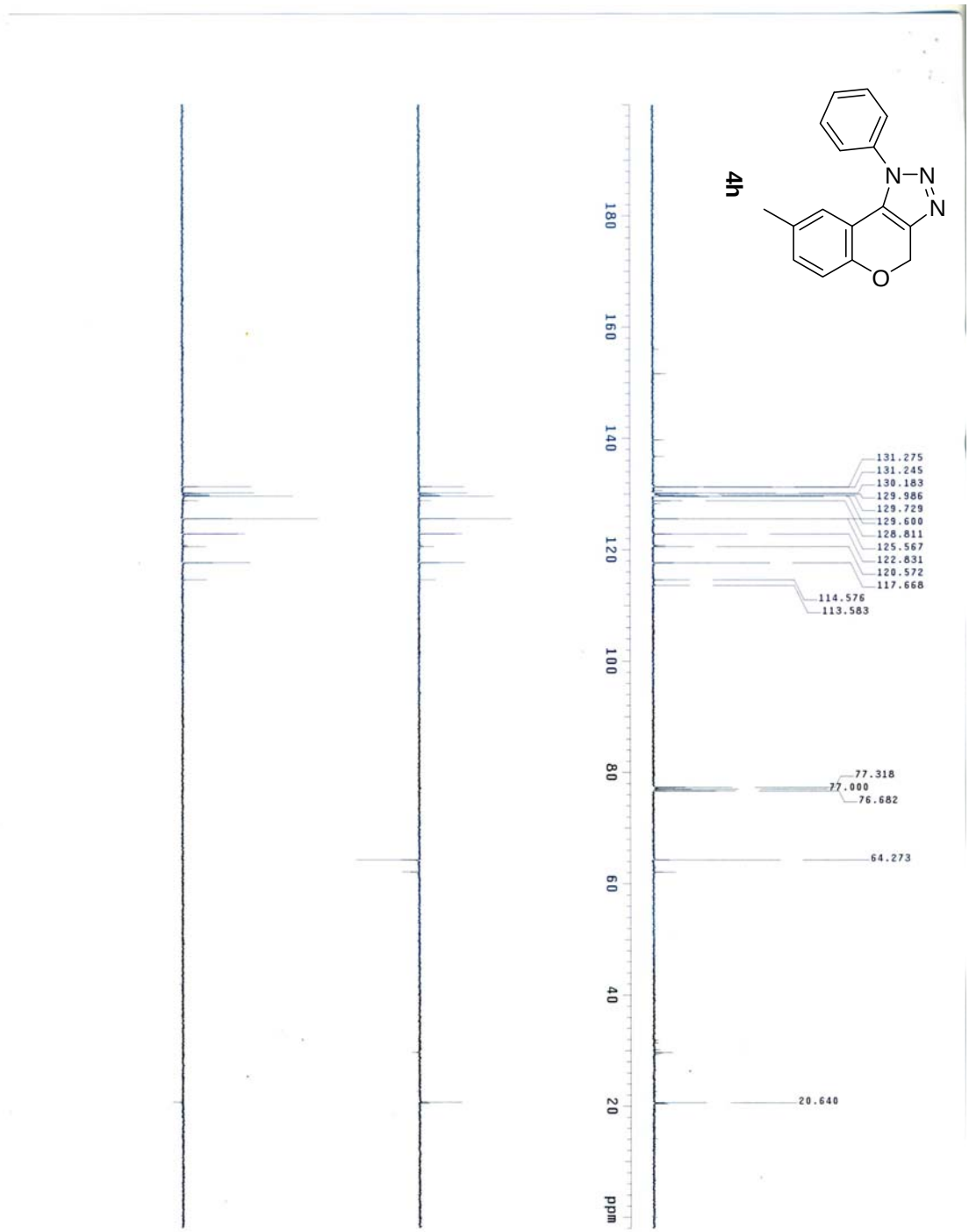

4g
O2N
N
N
N
O

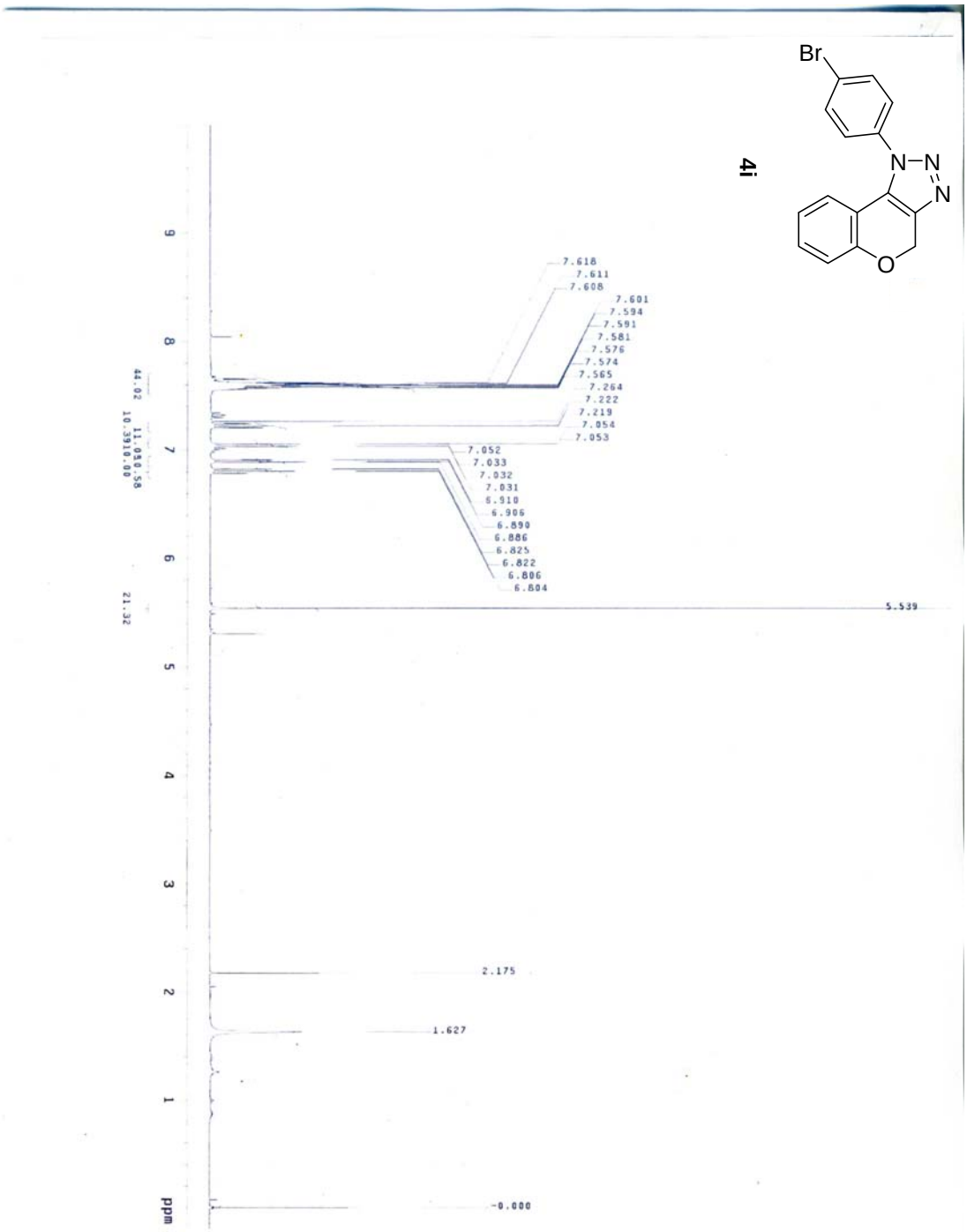

160
140
120
100
80
60
40
20
ppm
135.864
131.060
130.143
126.225
125.528
122.201
122.194
118.276
118.124
113.638
77.318
77.000
76.811
76.682
65.611
29.662

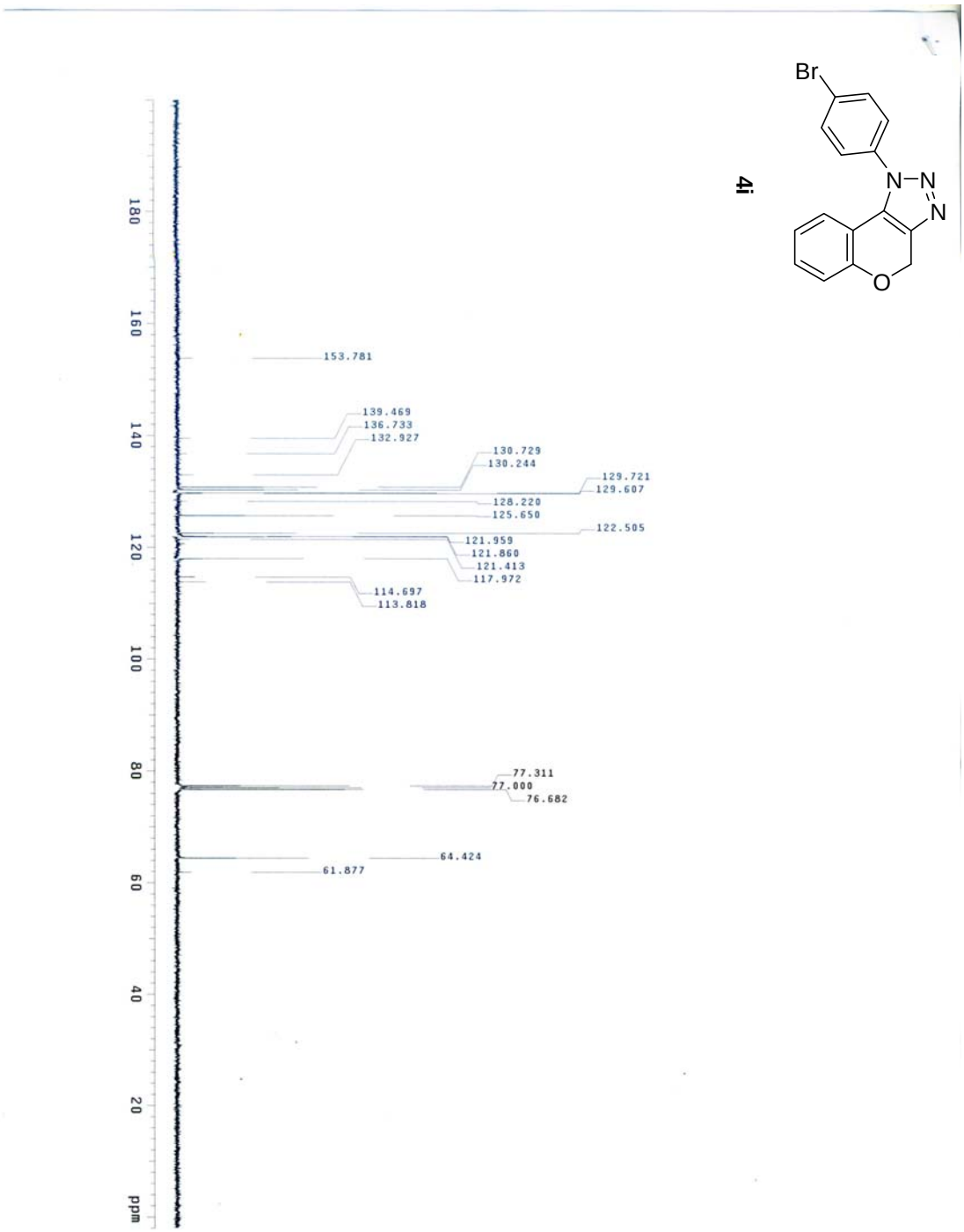

49
N–N
N
O_2N
O

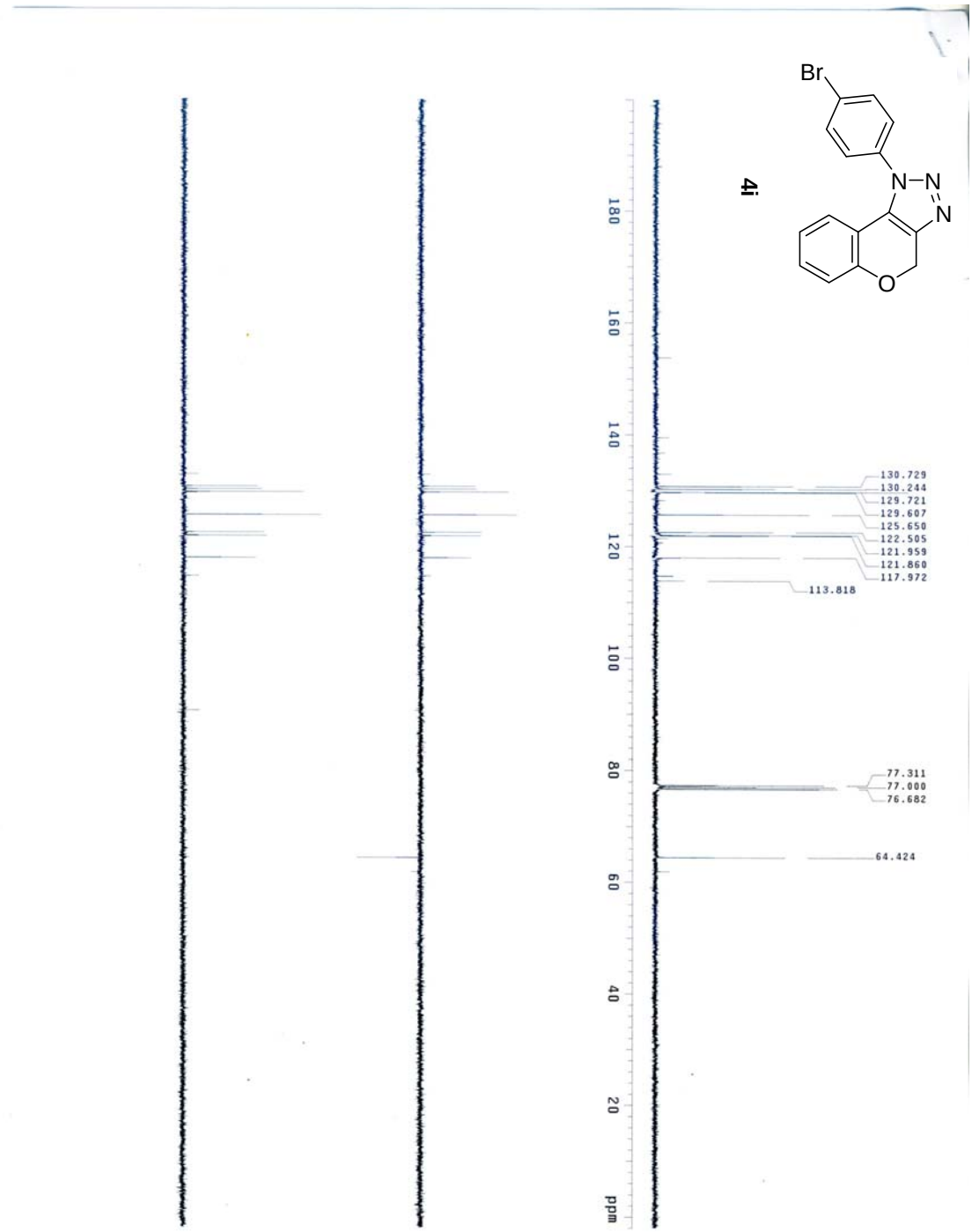

4h
N–N
N
O
7.616
7.606
7.597
7.593
7.591
7.587
7.582
7.577
7.567
7.264
7.013
7.009
7.007
6.946
6.925
6.687
6.683
5.480
5.275
2.292
2.102
1.255
-0.000
ppm

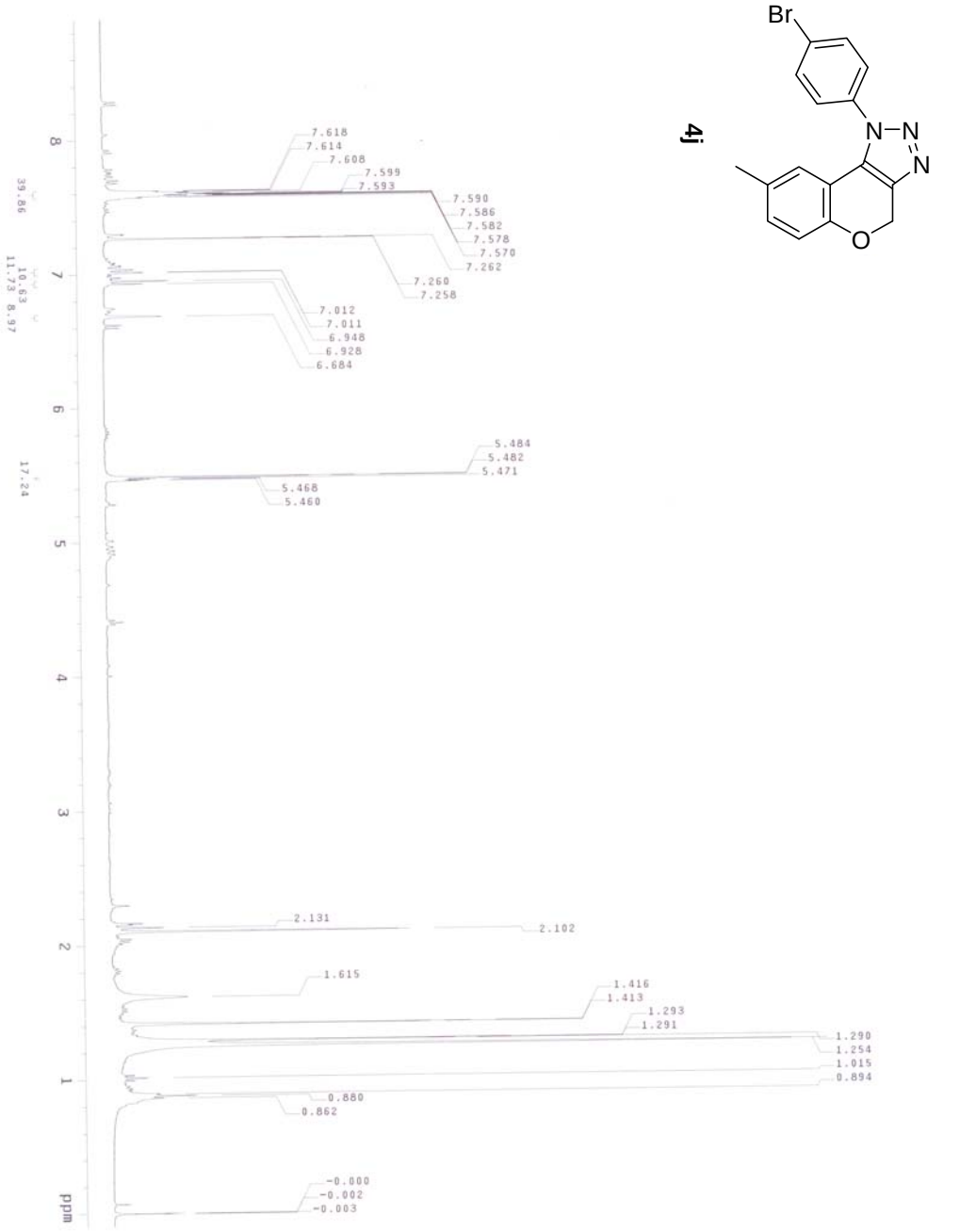

4h
N–N
N
O
180
160
140
120
100
80
60
40
20
ppm
151.605
139.697
136.733
131.275
131.245
130.183
129.986
129.729
129.600
128.811
125.567
122.831
120.814
120.572
117.668
114.576
113.583
77.318
77.000
76.682
64.273
62.097
29.653
20.640
20.443

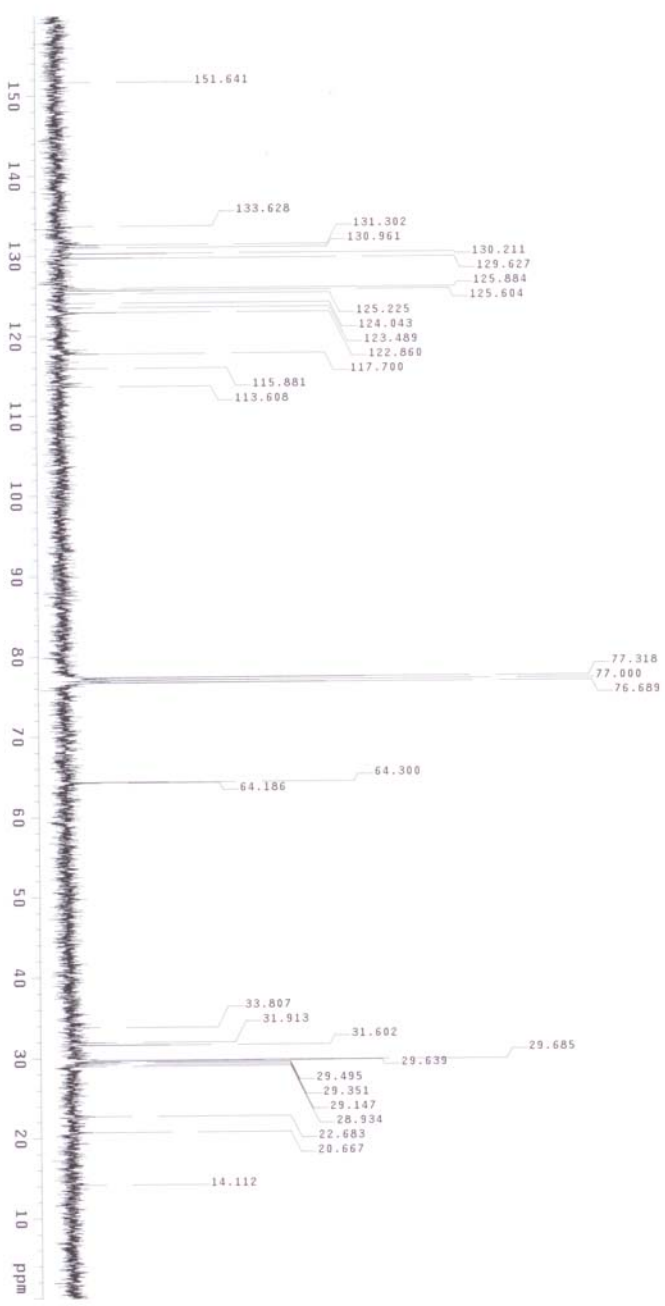



4i
Br
N
N
N
O
7.618
7.611
7.608
7.601
7.594
7.591
7.581
7.576
7.574
7.565
7.264
7.222
7.219
7.054
7.053
7.052
7.033
7.032
7.031
6.910
6.906
6.890
6.886
6.825
6.822
6.806
6.804
5.539
2.175
1.627
0.000
ppm

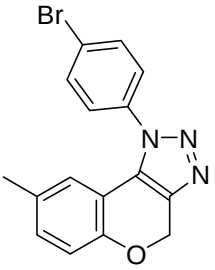

4i
Br
N
N
N
O
153.781
139.469
136.733
132.927
130.729
130.244
129.721
129.607
128.220
125.650
122.505
121.959
121.860
121.413
117.972
114.697
113.818
77.311
77.000
76.682
64.424
61.877
180
160
140
120
100
80
60
40
20
ppm

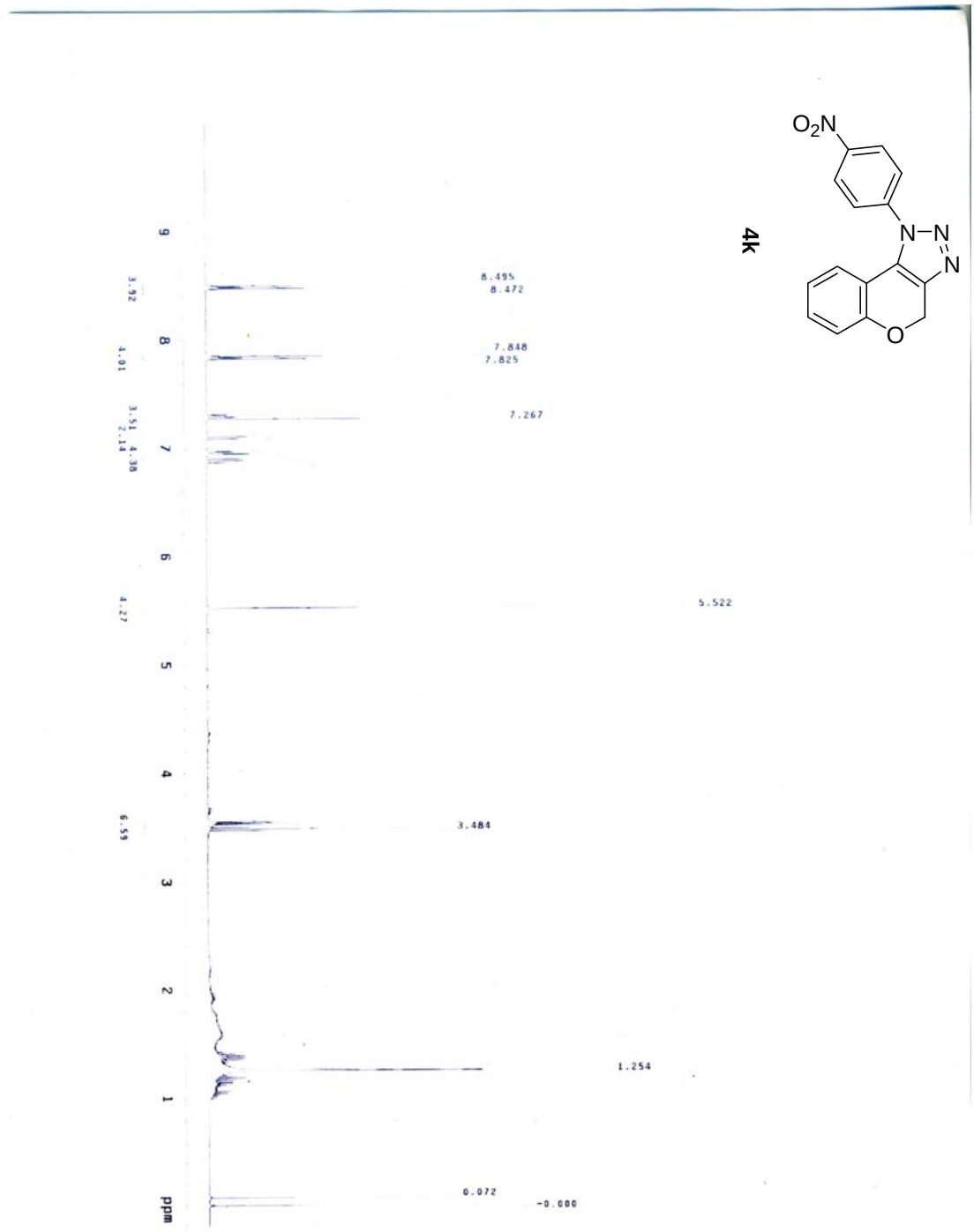


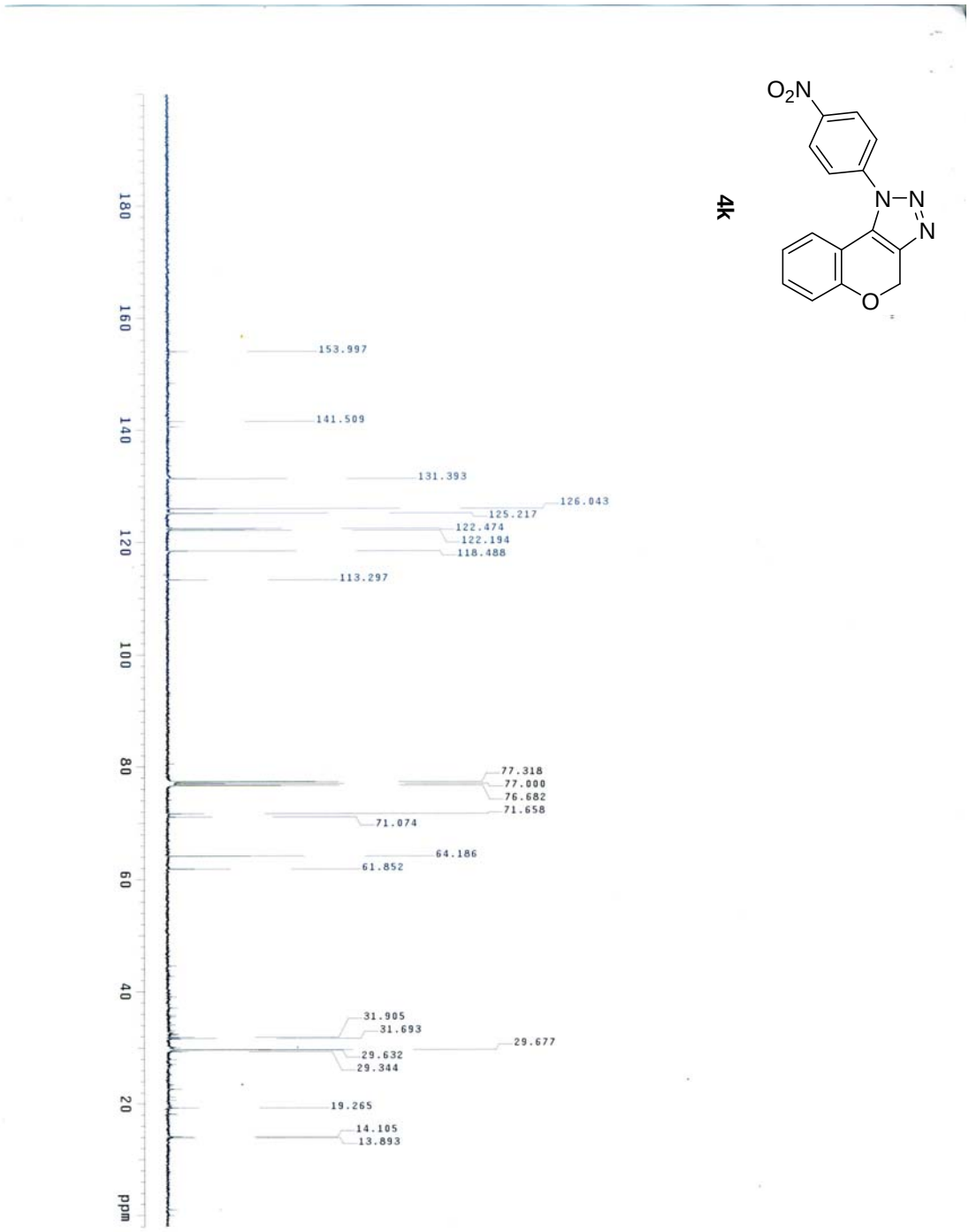

4j
Br
N
N
N
O
7.618
7.614
7.608
7.599
7.593
7.590
7.586
7.582
7.578
7.570
7.262
7.260
7.258
7.012
7.011
6.948
6.928
6.684
5.484
5.482
5.471
5.468
5.460
2.131
2.102
1.615
1.416
1.413
1.293
1.291
1.290
1.254
1.015
0.894
0.880
0.862
-0.000
-0.002
-0.003
ppm

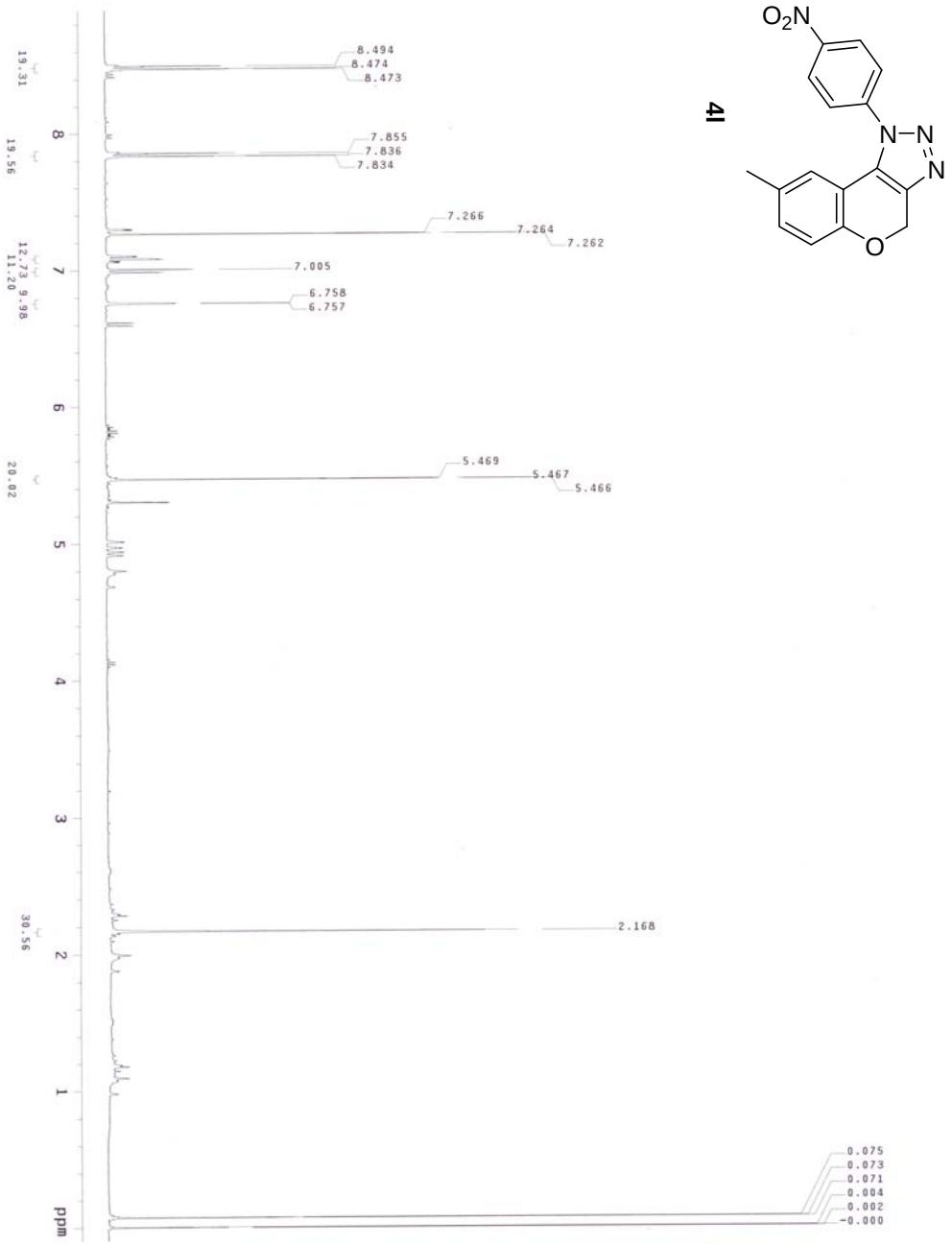

151.641
133.628
131.302
130.961
130.211
129.627
125.884
125.604
125.225
124.043
123.489
122.860
117.700
115.881
113.608
77.318
77.000
76.689
64.300
64.186
33.807
31.913
31.602
29.685
29.639
29.495
29.351
29.147
28.934
22.683
20.667
14.112
ppm

4i


Br
N
N
N
O

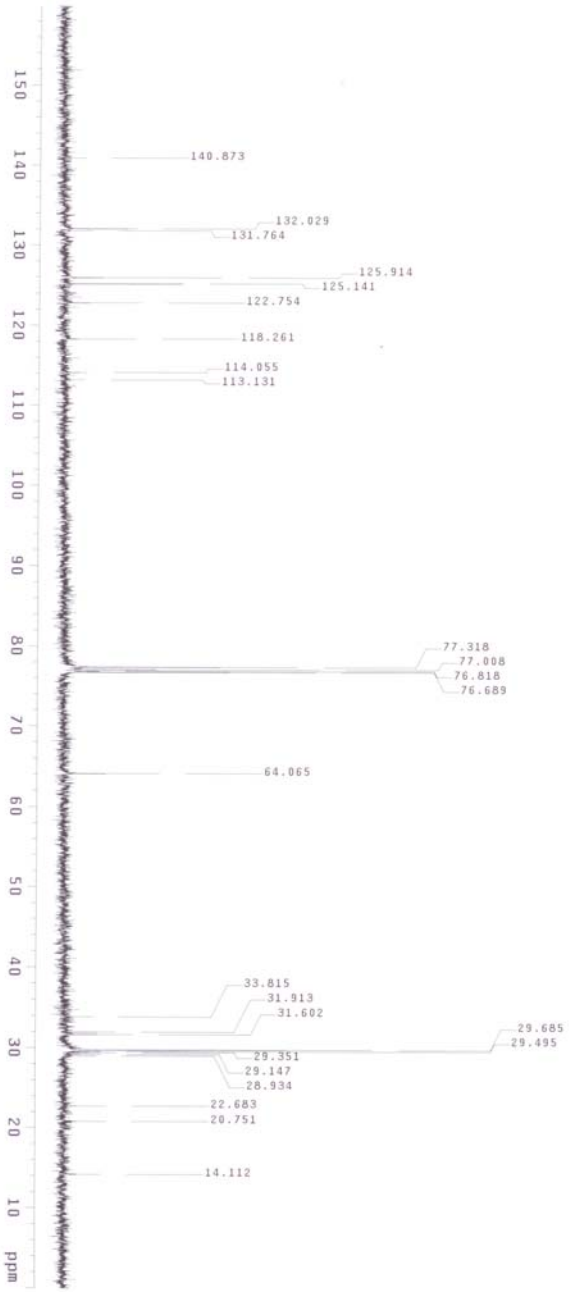

4k
O2N
N–N
N
O
8.495
8.472
7.848
7.825
7.267
5.522
3.484
1.254
0.072
-0.000
3.92
4.01
3.51
2.14
4.39
4.27
6.59
ppm


153.997
141.509
131.393
126.043
125.217
122.474
122.194
118.488
113.297
77.318
77.000
76.682
71.658
71.074
64.186
61.852
31.905
31.693
29.677
29.632
29.344
19.265
14.105
13.893
ppm
4k
O2N
N–N
N
O

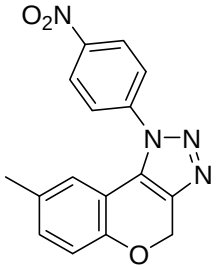

8.494
8.474
8.473
7.855
7.836
7.834
7.266
7.264
7.262
7.005
6.758
6.757
5.469
5.467
5.466
2.168
0.075
0.073
0.071
0.004
0.002
-0.000
ppm

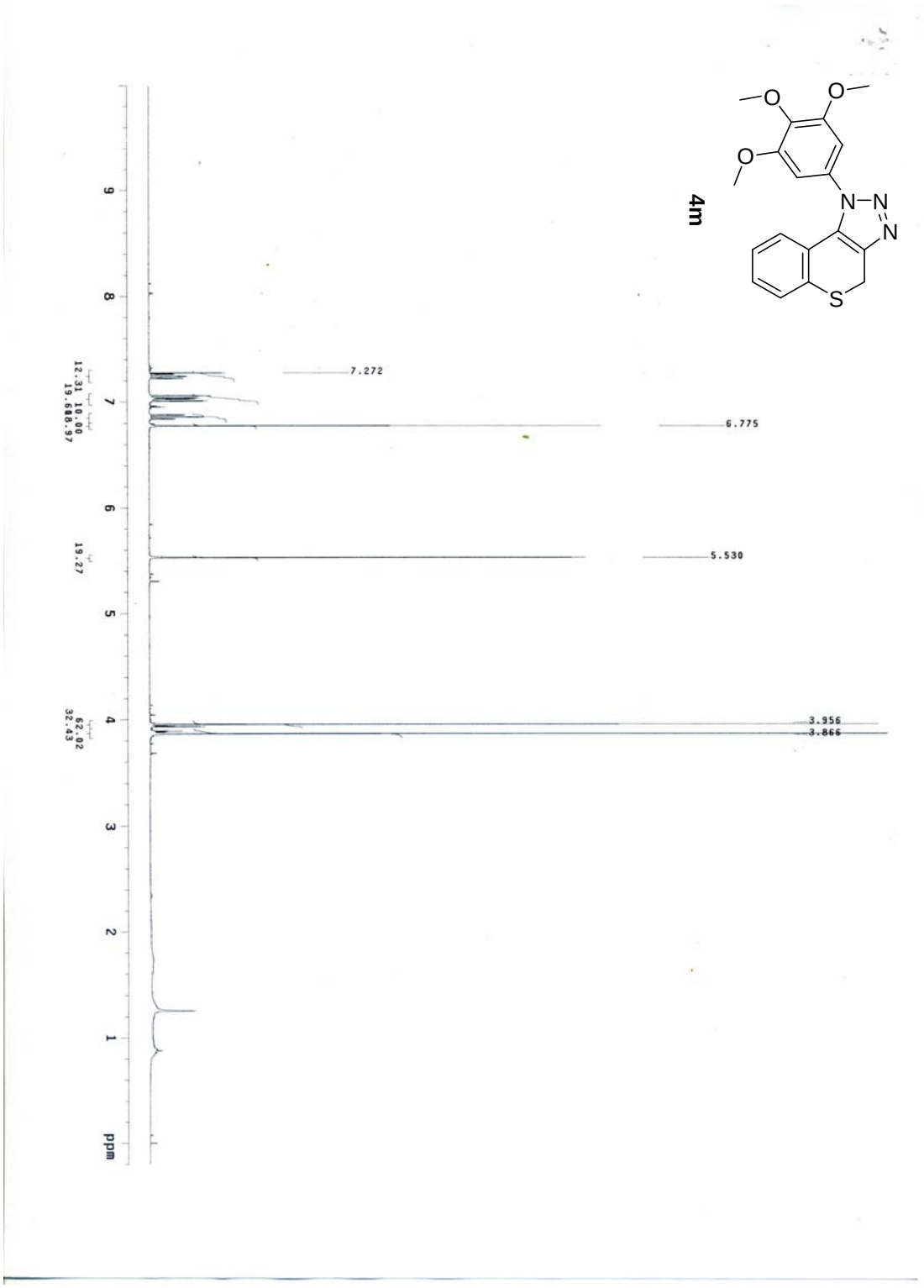
O2N
N–N
N
O

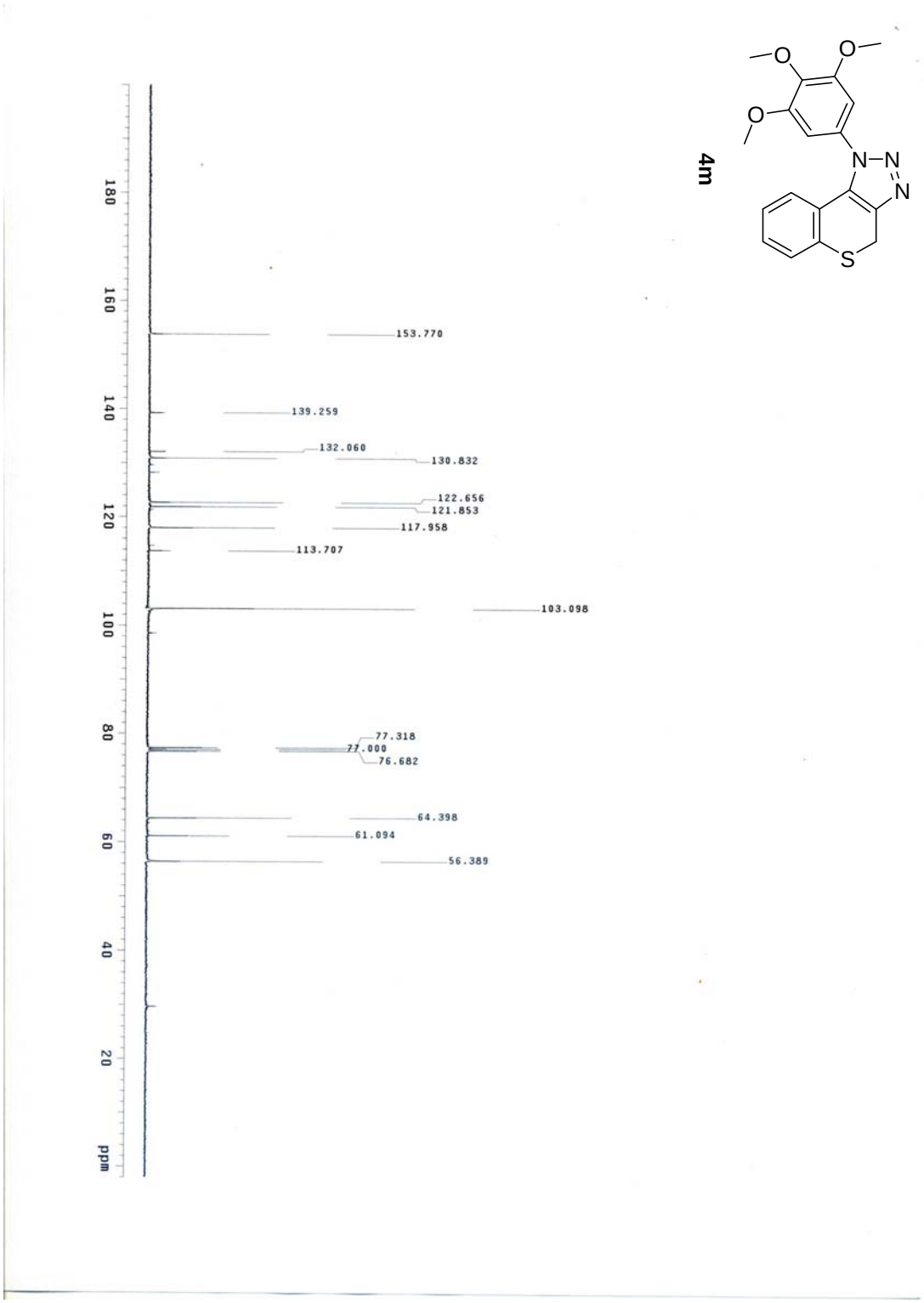
4l

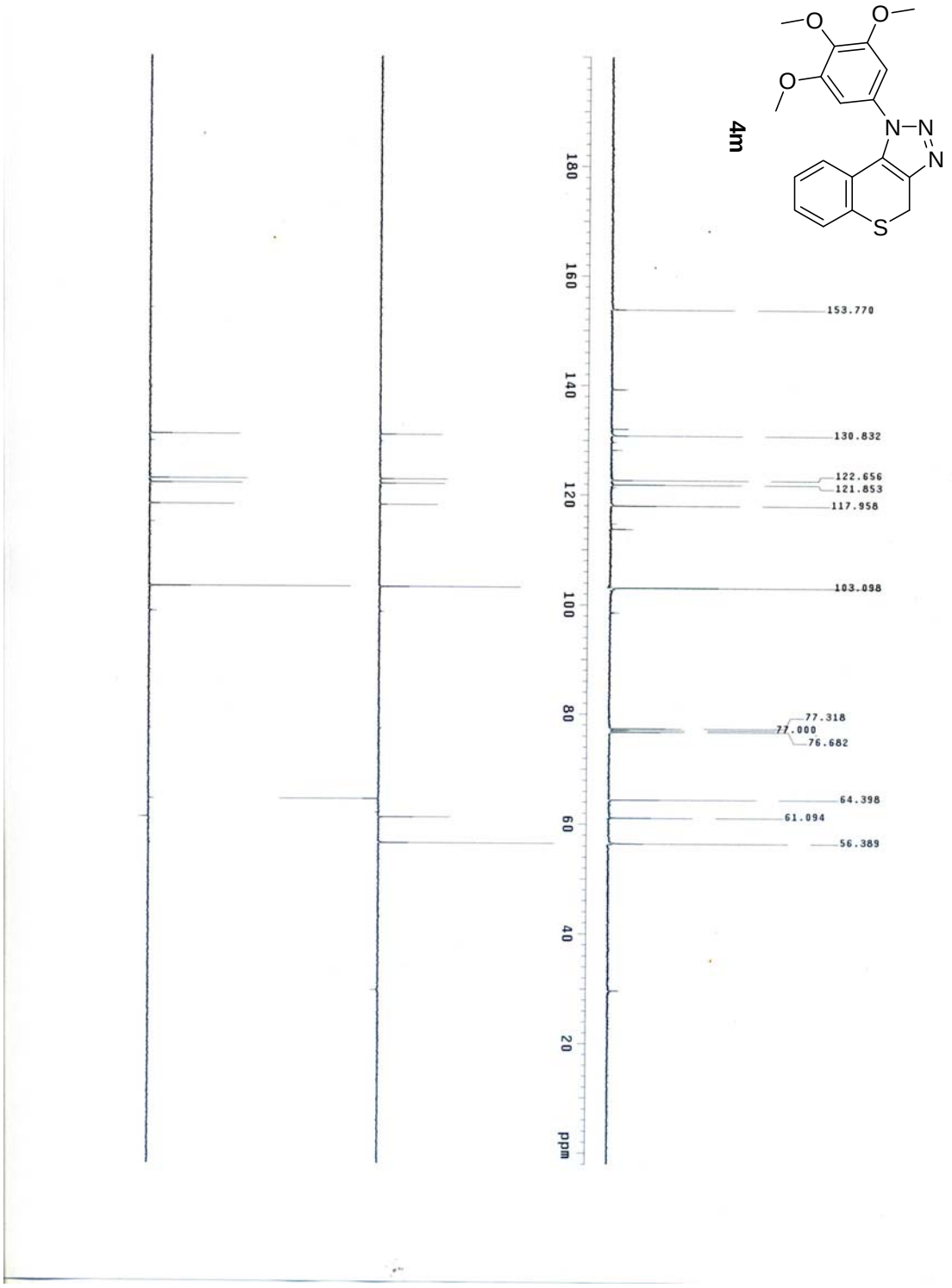

140.873
132.029
131.764
125.914
125.141
122.754
118.261
114.055
113.131
77.318
77.008
76.818
76.689
64.065
33.815
31.913
31.602
29.685
29.495
29.351
29.147
28.934
22.683
20.751
14.112
ppm

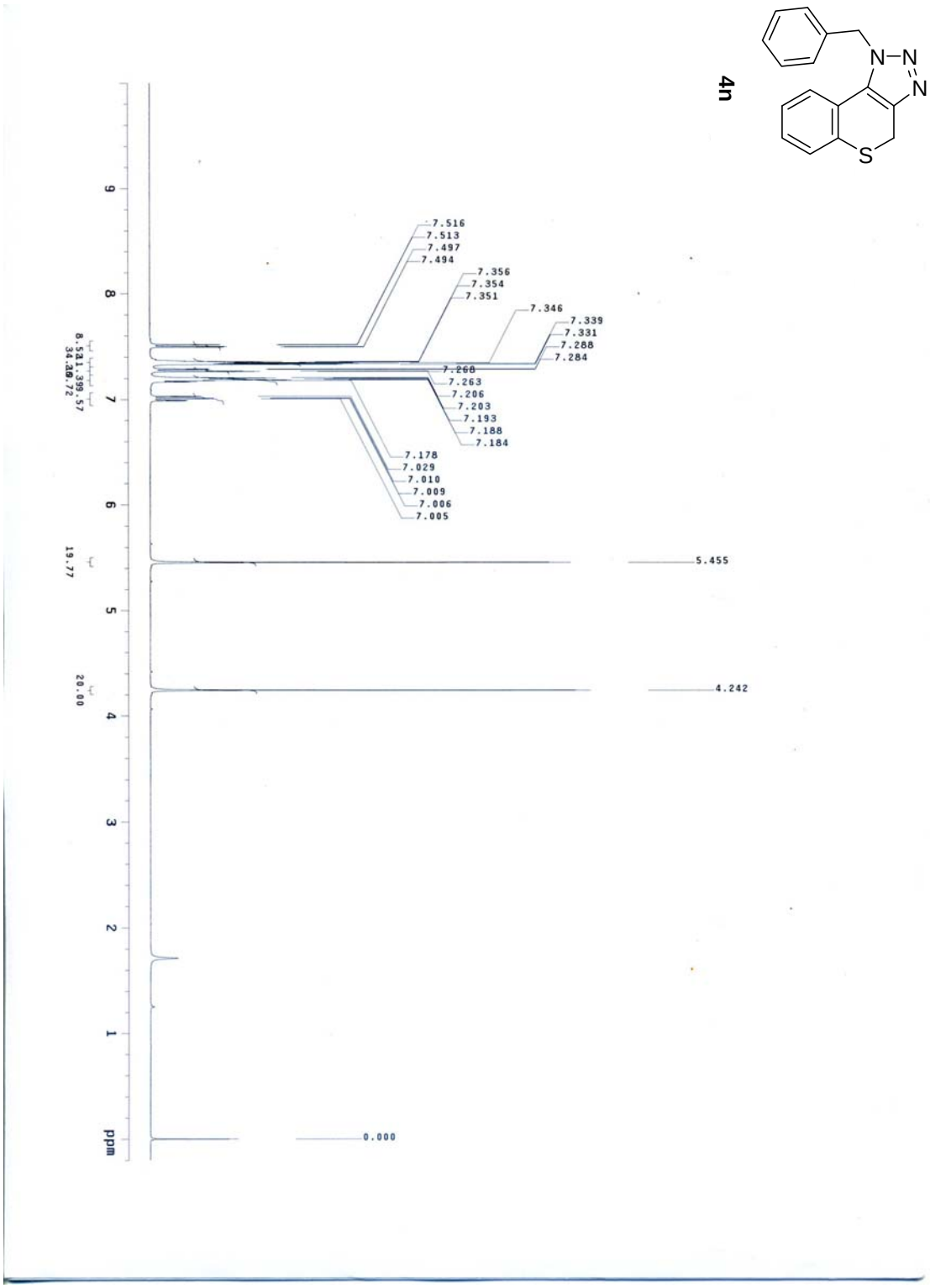
4l

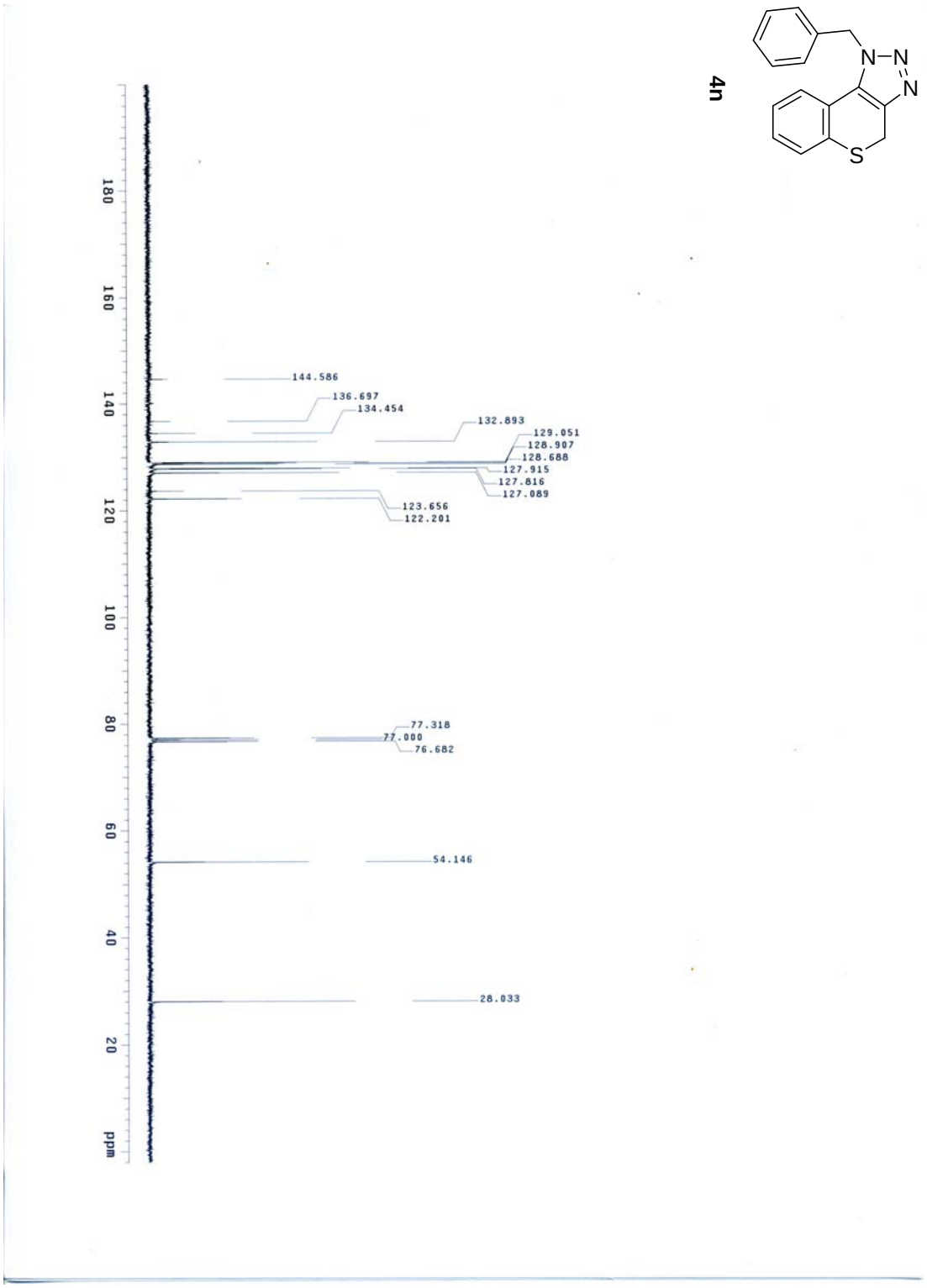

O2N
N–N
N
O

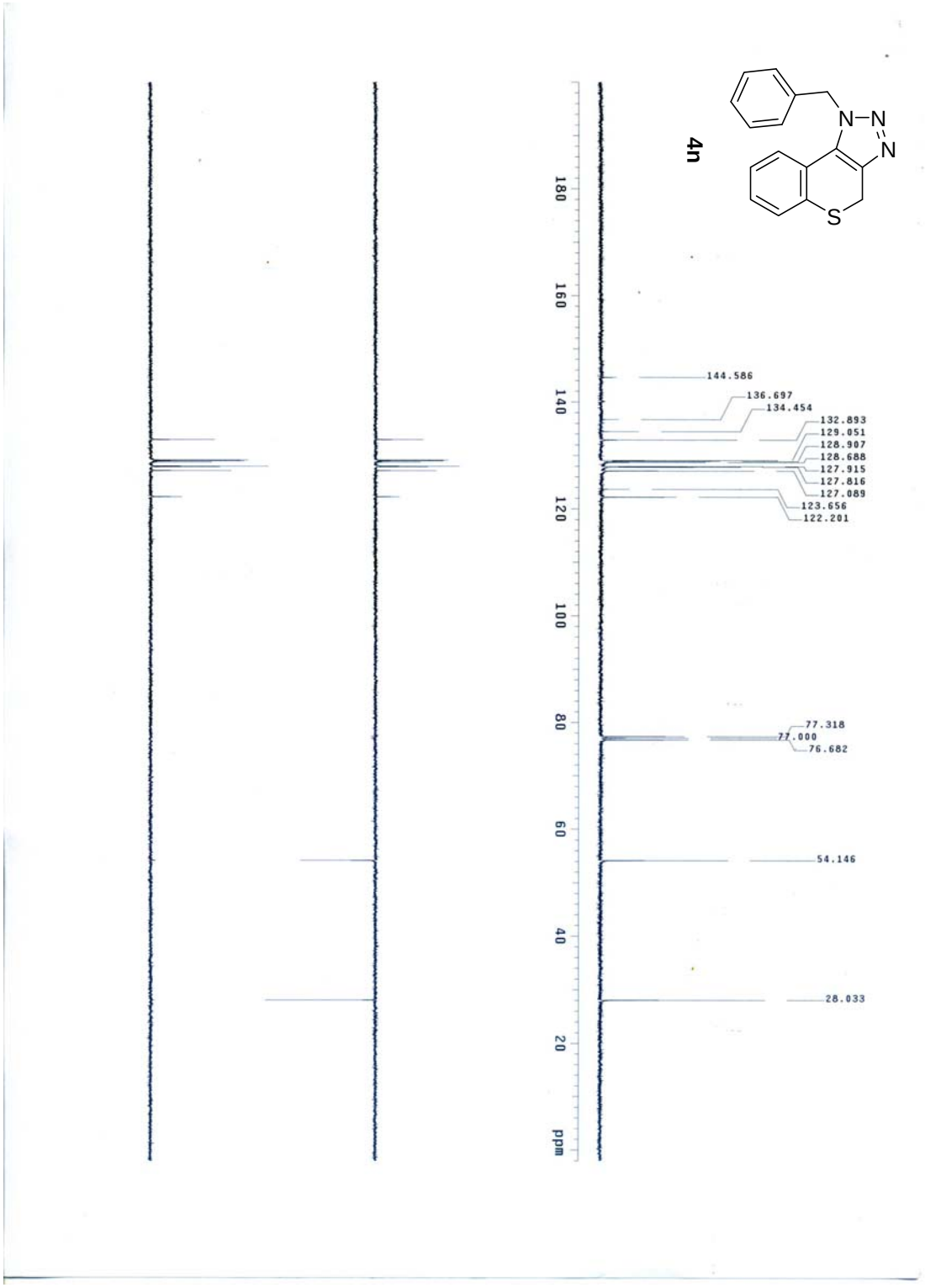

4m
O
O
O
N
N
N
S
7.272
6.775
5.530
3.956
3.866
12.31
10.00
19.68
8.97
19.27
62.02
32.43
9
8
7
6
5
4
3
2
1
ppm

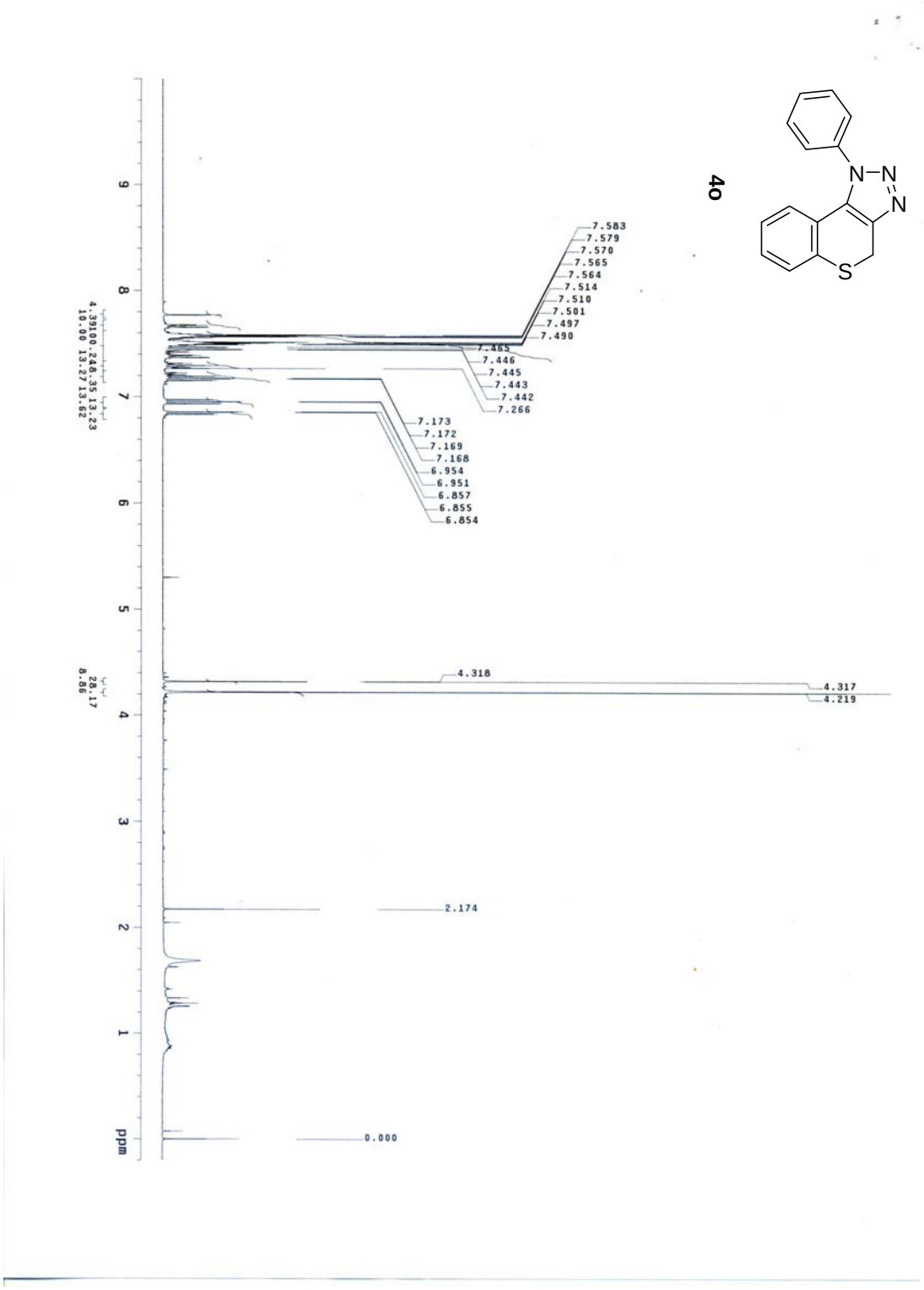

4m
O
O
O
N–N
N
S
180
160
140
120
100
80
60
40
20
ppm
153.770
139.259
132.060
130.832
122.656
121.853
117.958
113.707
103.098
77.318
77.000
76.682
64.398
61.094
56.389

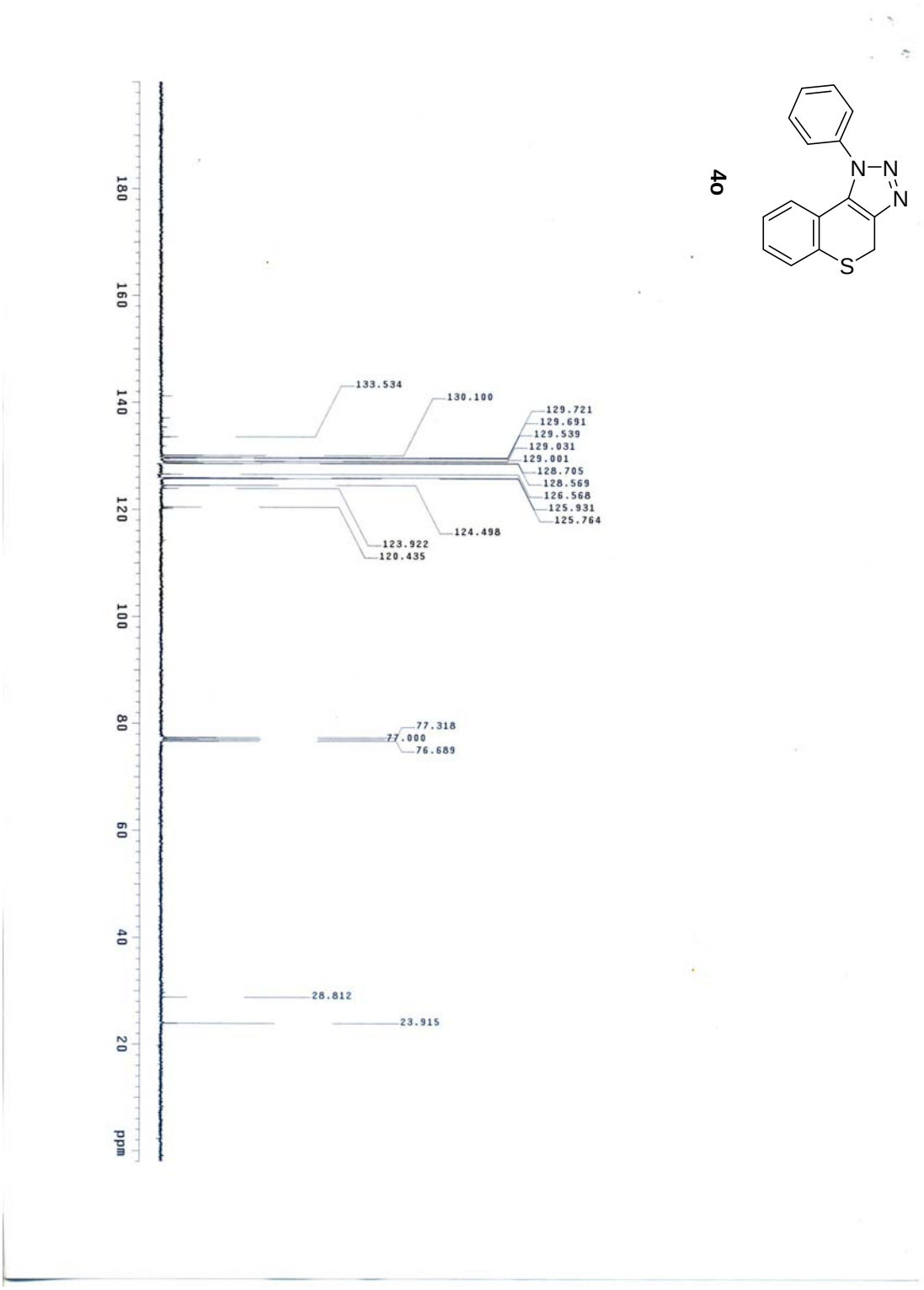

4m
O
O
O
N
N
N
S
153.770
130.832
122.656
121.853
117.958
103.098
77.318
77.000
76.682
64.398
61.094
56.389
180
160
140
120
100
80
60
40
20
ppm

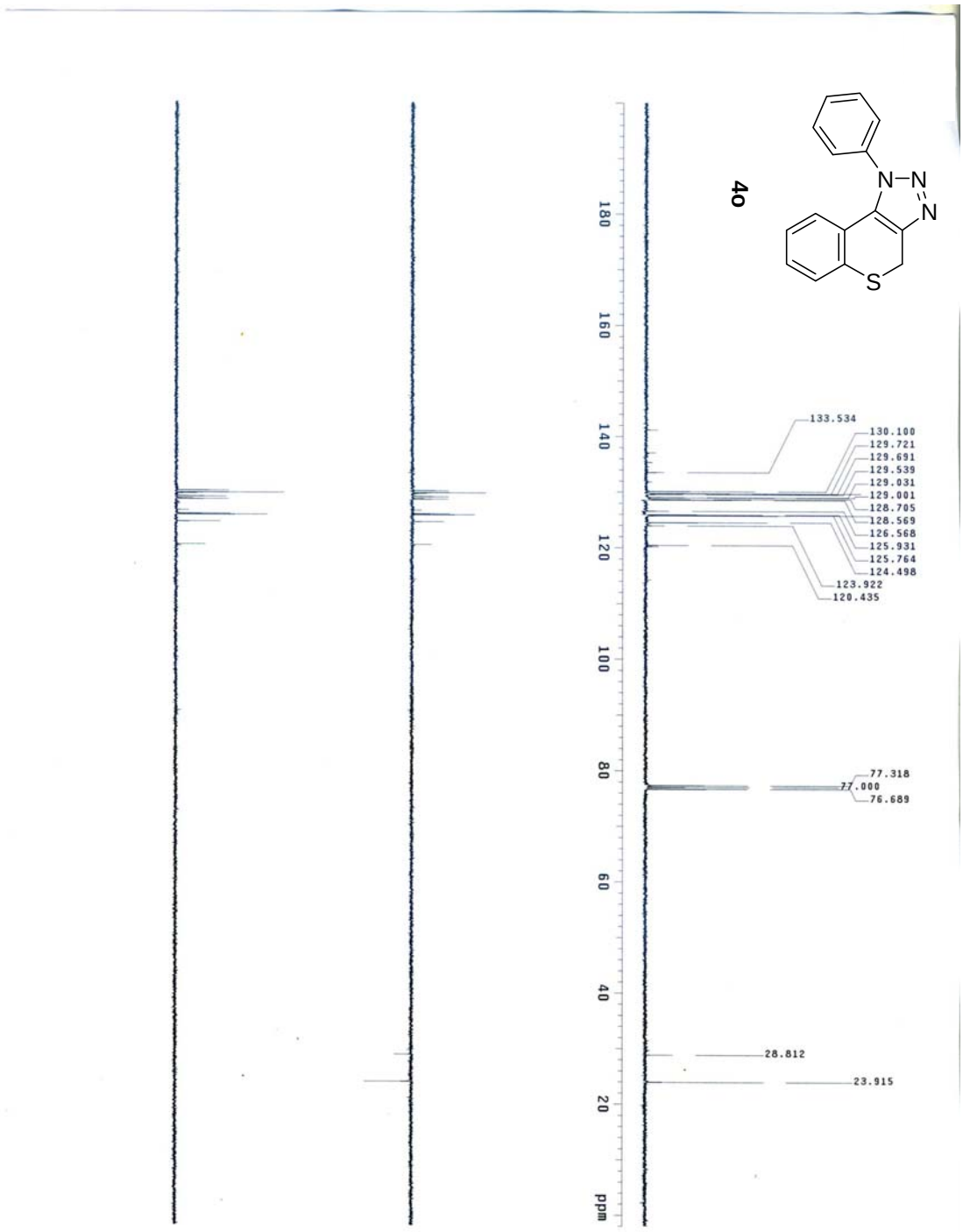

4n
N–N
N
S
7.516
7.513
7.497
7.494
7.356
7.354
7.351
7.346
7.339
7.331
7.288
7.284
7.268
7.263
7.206
7.203
7.193
7.188
7.184
7.178
7.029
7.010
7.009
7.006
7.005
5.455
4.242
0.000
ppm

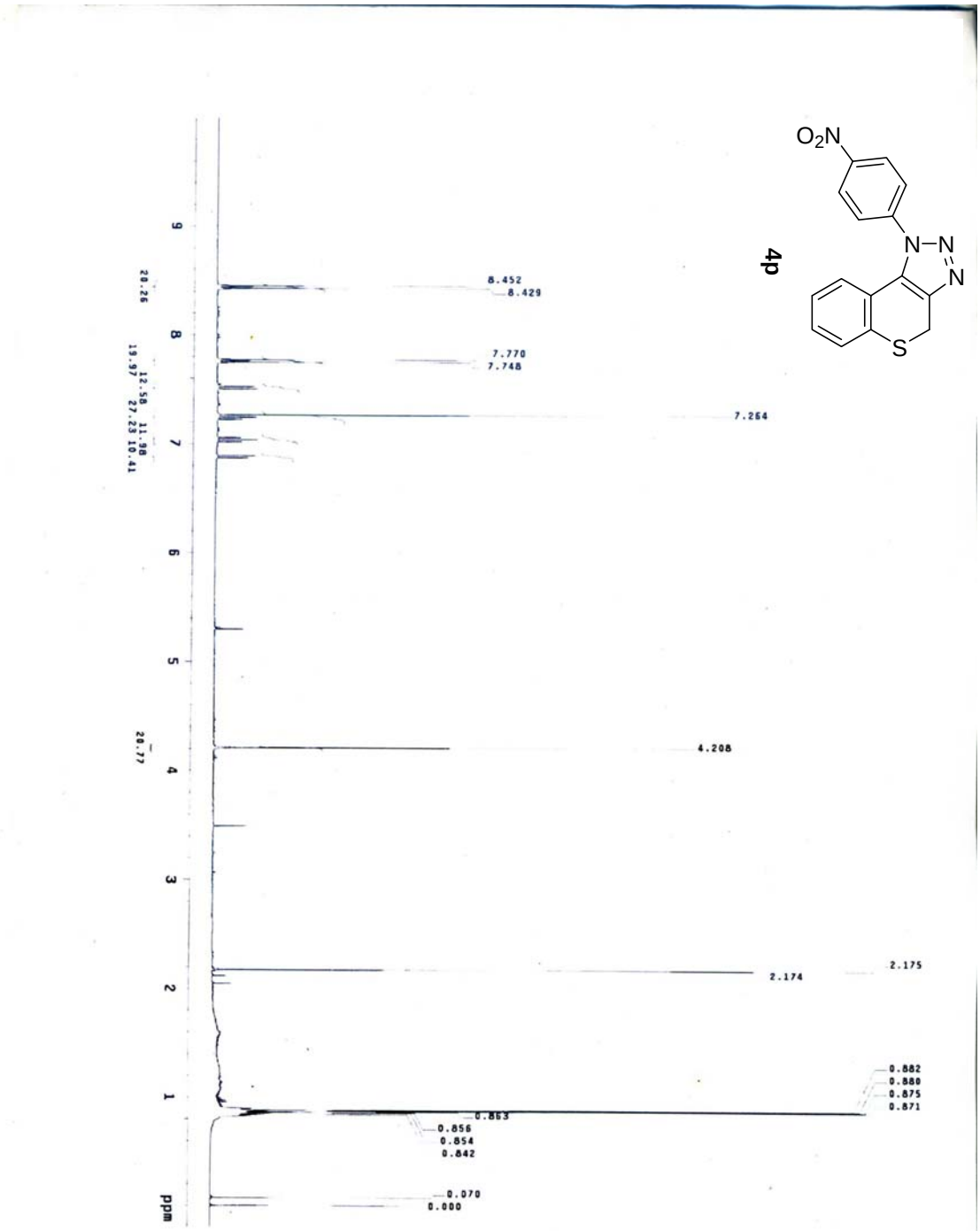

4n
N
N
N
S
144.586
136.697
134.454
132.893
129.051
128.907
128.688
127.915
127.816
127.089
123.656
122.201
77.318
77.000
76.682
54.146
28.033
180
160
140
120
100
80
60
40
20
ppm

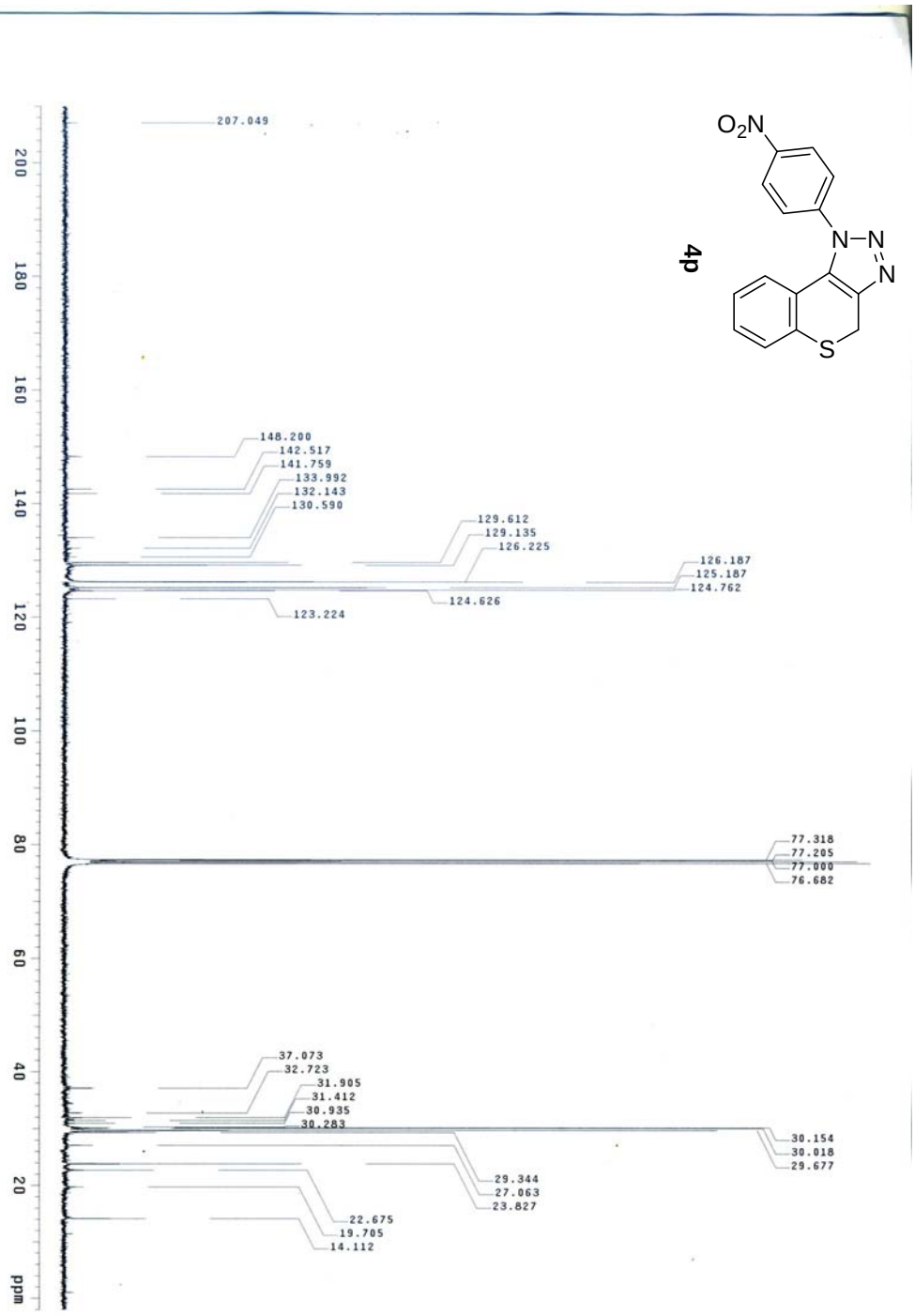

4n
N
N
N
S
144.586
136.697
134.454
132.893
129.051
128.907
128.688
127.915
127.816
127.089
123.656
122.201
77.318
77.000
76.682
54.146
28.033
180
160
140
120
100
80
60
40
20
ppm


4o
N–N
N
S
7.583
7.579
7.570
7.565
7.564
7.514
7.510
7.501
7.497
7.490
7.465
7.446
7.445
7.443
7.442
7.266
7.173
7.172
7.169
7.168
6.954
6.951
6.857
6.855
6.854
4.318
4.317
4.219
2.174
0.000
ppm


4o
N
N
N
S
133.534
130.100
129.721
129.691
129.539
129.031
129.001
128.705
128.569
126.568
125.931
125.764
124.498
123.922
120.435
77.318
77.000
76.689
28.812
23.915
180
160
140
120
100
80
60
40
20
ppm

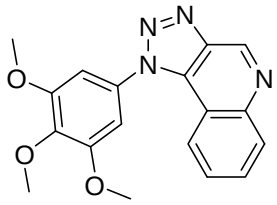

4o
N
N
N
S
133.534
130.100
129.721
129.691
129.539
129.031
129.001
128.705
128.569
126.568
125.931
125.764
124.498
123.922
120.435
77.318
77.000
76.689
28.812
23.915
180
160
140
120
100
80
60
40
20
ppm


4p
O2N
N
N
N
S
8.452
8.429
7.770
7.748
7.264
4.208
2.175
2.174
0.882
0.880
0.875
0.871
0.863
0.856
0.854
0.842
0.070
0.000
ppm

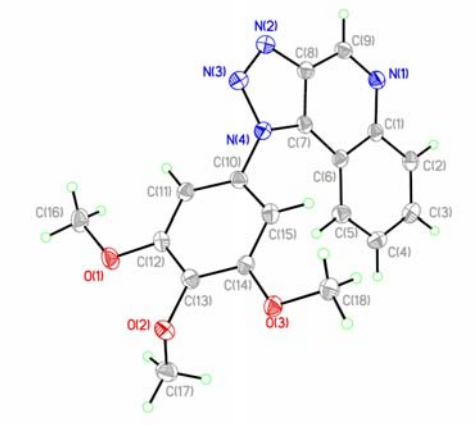


4. ORTEP Diagram for 2a、4a and 4n

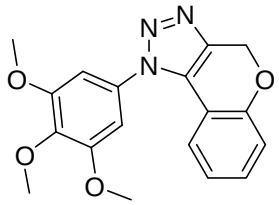
1-(3,4,5-trimethoxyphenyl)-1H-[1,2,3]triazolo[4,5-c]quinoline (2a)



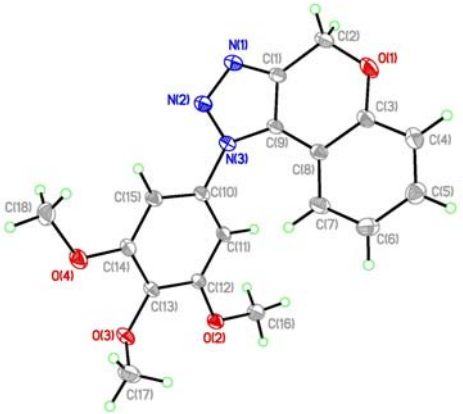
2a



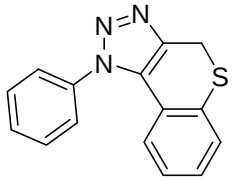
1-(3,4,5-trimethoxyphenyl)-1,4-dihydrochromeno[4,3-d][1,2,3]triazole(4a)



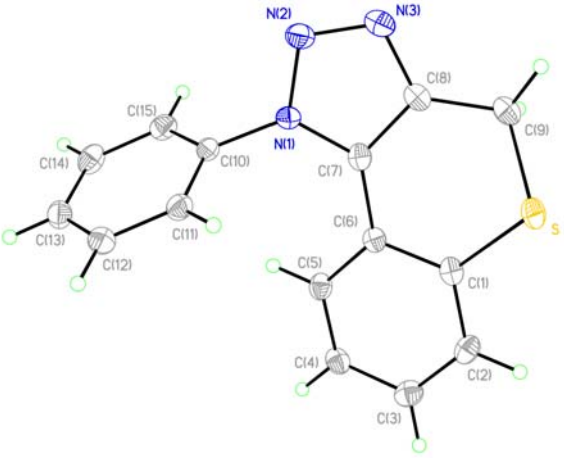
4a



1-phenyl-1,4-dihydrothiochromeno[4,3-d][1,2,3]triazole (4o)



4o



5. Biological results of compounds 2a、2d、2f、4a、4c、4i、4m and 4n:

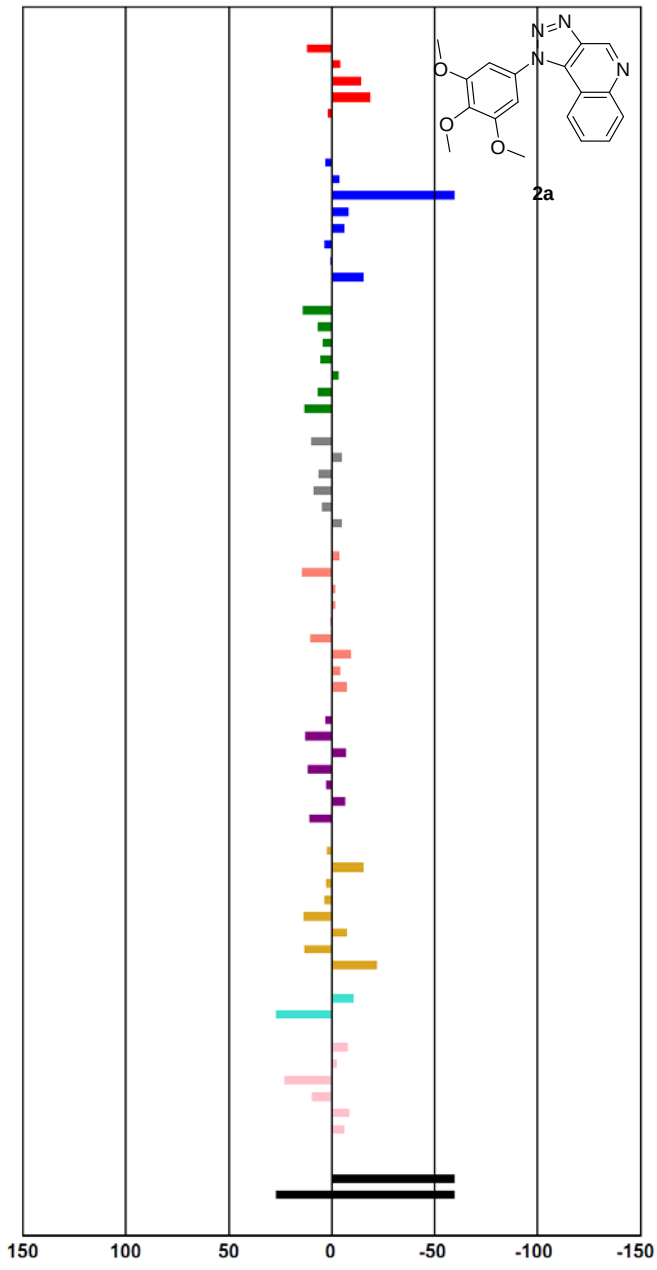
1-(3,4,5-trimethoxyphenyl)-1H-[1,2,3]triazolo[4,5-c]quinoline (2a)

Developmental Therapeutics Program
One Dose Mean Graph

NSC: D-754640 / 1 | Conc: 1.00E-5 Molar | Test Date: Oct 18, 2010
Experiment ID: 1010OS37 | Report Date: Nov 25, 2010

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	101.92
HL-60(TB)	113.60
K-562	98.26
MOLT-4	88.16
RPMI-8226	83.70
SR	103.44
Non-Small Cell Lung Cancer	
A549/ATCC	101.72
EKVX	104.62
HOP-62	98.75
HOP-92	42.61
NCI-H226	94.24
NCI-H23	96.33
NCI-H322M	105.32
NCI-H460	102.28
NCI-H522	86.95
Colon Cancer	
COLO 205	115.50
HCC-2998	108.54
HCT-116	105.95
HCT-15	107.32
HT29	98.91
KM12	108.39
SW-620	114.88
CNS Cancer	
SF-268	111.60
SF-295	97.36
SF-539	108.08
SNB-19	110.41
SNB-75	106.42
U251	97.58
Melanoma	
LOX IMVI	98.67
MALME-3M	116.26
M14	100.54
MDA-MB-435	100.58
SK-MEL-2	102.21
SK-MEL-28	112.19
SK-MEL-5	92.85
UACC-257	98.44
UACC-62	95.01
Ovarian Cancer	
IGROV1	104.94
OVCAR-3	114.33
OVCAR-4	95.45
OVCAR-5	113.06
OVCAR-8	104.51
NCI/ADR-RES	95.82
SK-OV-3	112.52
Renal Cancer	
786-0	103.93
A498	87.01
ACHN	104.20
CAKI-1	105.13
RXF 393	115.36
SN12C	95.03
TK-10	114.90
UO-31	80.23
Prostate Cancer	
PC-3	91.58
DU-145	128.81
Breast Cancer	
MCF7	94.60
MDA-MB-231/ATCC	99.81
HS 578T	124.74
BT-549	111.11
T-47D	93.76
MDA-MB-468	96.21
Mean	101.94
Delta	59.33
Range	86.20

Mean Growth Percent - Growth Percent



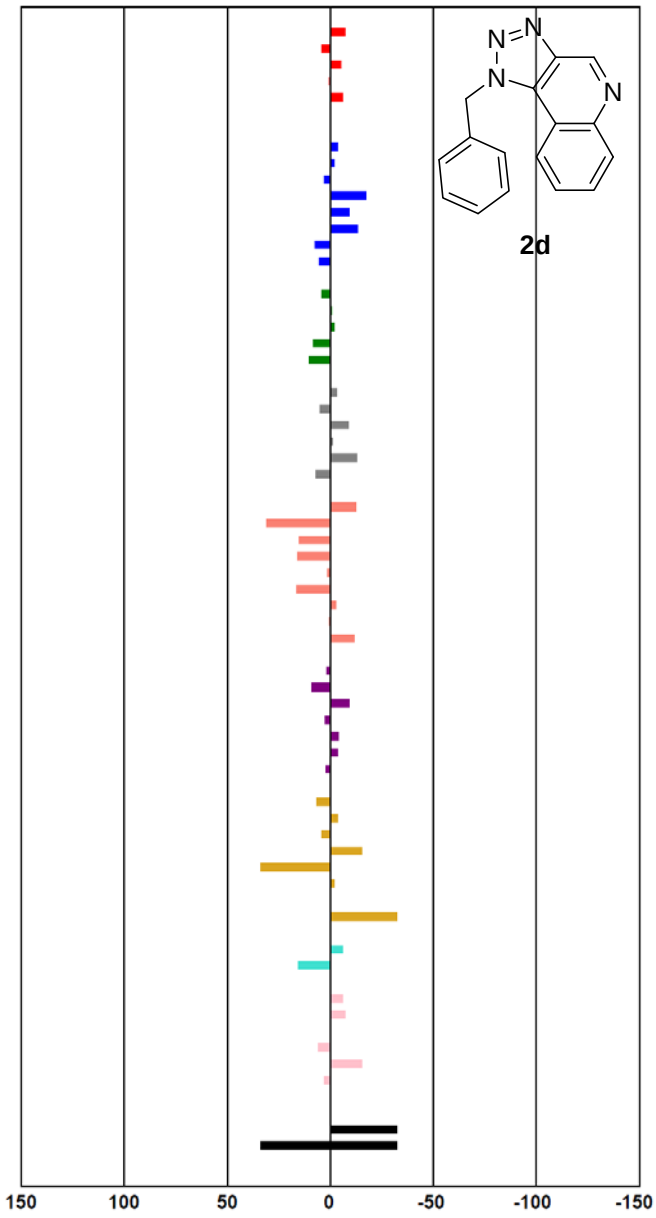
1- benzyl-1H-[1,2,3]triazolo[4,5-c]quinoline (2d)

Developmental Therapeutics Program
One Dose Mean Graph

NSC: D-752754 / 1 | **Conc:** 1.00E-5 Molar | **Test Date:** Apr 26, 2010
Experiment ID: 1004OS47 | **Report Date:** Nov 25, 2010

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	90.66
HL-60(TB)	101.55
K-562	92.73
MOLT-4	97.83
RPMI-8226	91.73
SR	97.40
Non-Small Cell Lung Cancer	
A549/ATCC	94.05
EKVX	95.67
HOP-62	100.14
HOP-92	80.30
NCI-H226	88.60
NCI-H23	84.39
NCI-H322M	104.58
NCI-H460	102.73
Colon Cancer	
COLO 205	101.68
HCT-116	97.09
HT29	95.88
KM12	105.72
SW-620	107.65
CNS Cancer	
SF-268	94.73
SF-295	102.30
SF-539	88.76
SNB-19	96.64
SNB-75	85.03
U251	104.37
Melanoma	
LOX IMVI	85.46
MALME-3M	128.21
M14	112.27
MDA-MB-435	113.08
SK-MEL-2	98.68
SK-MEL-28	113.73
SK-MEL-5	95.06
UACC-257	97.89
UACC-62	86.06
Ovarian Cancer	
IGROV1	99.13
OVCAR-3	106.48
OVCAR-4	88.32
OVCAR-5	99.83
OVCAR-8	93.83
NCI/ADR-RES	94.19
SK-OV-3	99.61
Renal Cancer	
786-0	103.99
A498	94.11
ACHN	101.31
CAKI-1	82.35
RXF 393	131.18
SN12C	95.98
TK-10	97.61
UO-31	65.54
Prostate Cancer	
PC-3	91.76
DU-145	112.79
Breast Cancer	
MCF7	91.76
MDA-MB-231/ATCC	90.60
HS 578T	97.38
BT-549	103.14
T-47D	82.59
MDA-MB-468	100.20
Mean	97.48
Delta	31.94
Range	65.64

Mean Growth Percent - Growth Percent



2d

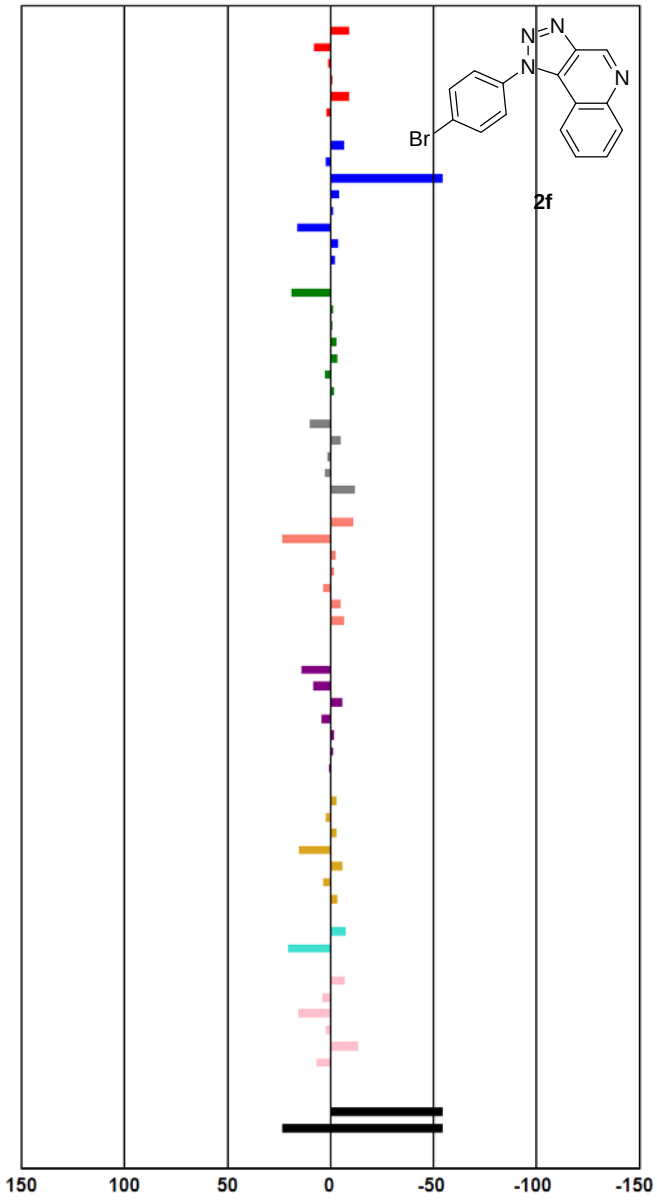
1-(4-bromophenyl)-1H-[1,2,3]triazolo[4,5-c]quinoline (2f)

Developmental Therapeutics Program
One Dose Mean Graph

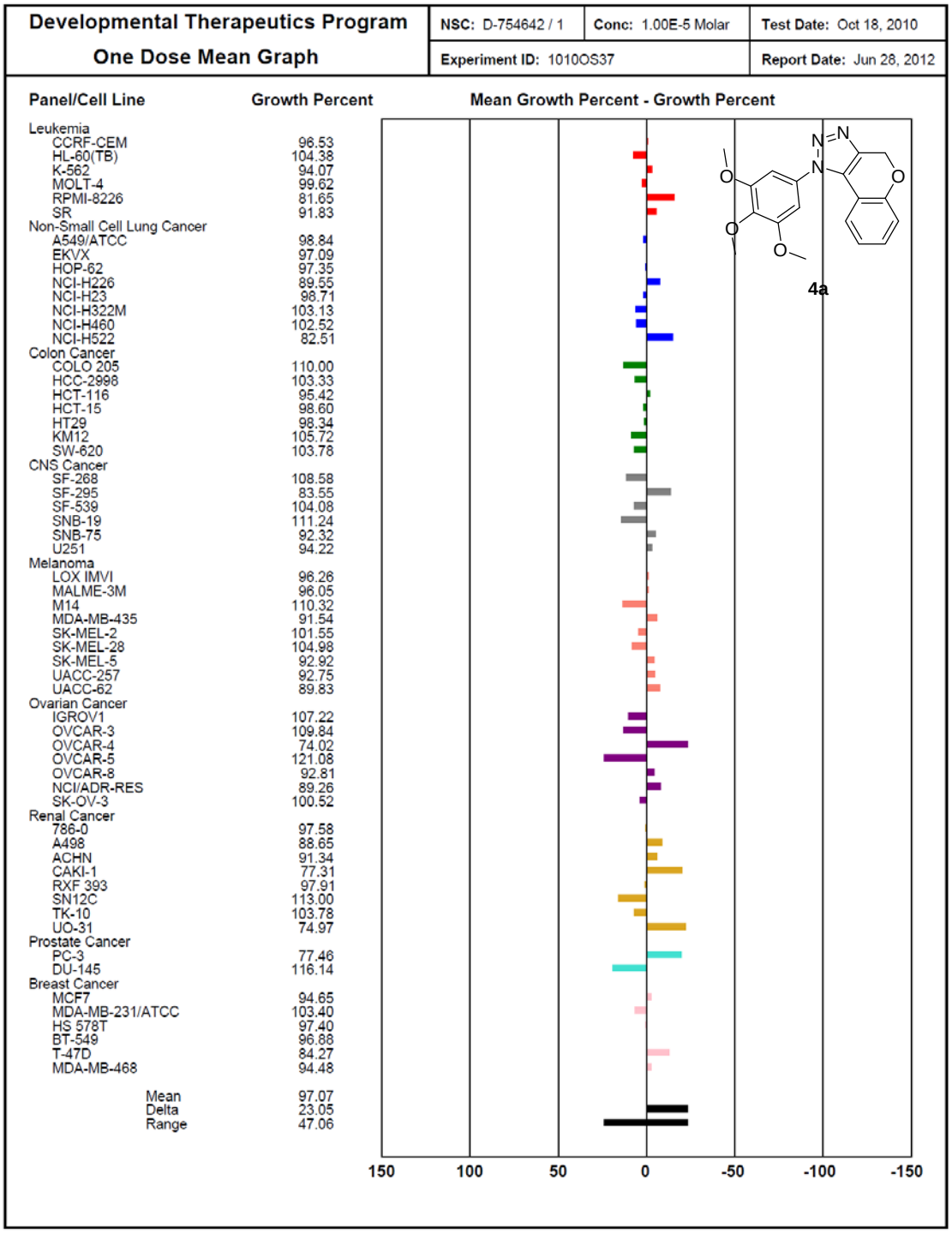
NSC: D-754641 / 1	Conc: 1.00E-5 Molar	Test Date: Oct 18, 2010
Experiment ID: 1010OS37		Report Date: Nov 25, 2010

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	99.45
HL-60(TB)	115.70
K-562	108.93
MOLT-4	107.56
RPMI-8226	99.35
SR	109.68
Non-Small Cell Lung Cancer	
A549/ATCC	101.75
HOP-62	109.87
HOP-92	54.21
NCI-H226	104.25
NCI-H23	107.13
NCI-H322M	123.69
NCI-H460	104.81
NCI-H522	106.22
Colon Cancer	
COLO 205	126.41
HCC-2998	107.11
HCT-116	107.34
HCT-15	105.38
HT29	105.08
KM12	110.39
SW-620	106.65
CNS Cancer	
SF-268	117.49
SF-539	103.65
SNB-19	109.04
SNB-75	110.31
U251	96.63
Melanoma	
LOX IMVI	97.59
MALME-3M	131.00
M14	105.97
SK-MEL-2	106.78
SK-MEL-28	111.22
SK-MEL-5	103.34
UACC-257	101.99
UACC-62	108.14
Ovarian Cancer	
IGROV1	121.93
OVCAR-3	115.92
OVCAR-4	102.56
OVCAR-5	112.05
OVCAR-8	106.80
NCI/ADR-RES	107.29
SK-OV-3	108.20
Renal Cancer	
786-0	105.50
A498	110.14
ACHN	105.64
RXF 393	122.91
SN12C	102.85
TK-10	111.13
UO-31	105.29
Prostate Cancer	
PC-3	100.90
DU-145	128.11
Breast Cancer	
MCF7	101.49
MDA-MB-231/ATCC	111.74
HS 578T	123.36
BT-549	110.06
T-47D	95.15
MDA-MB-468	114.34
Mean	107.99
Delta	53.78
Range	76.79

Mean Growth Percent - Growth Percent



1-(3,4,5-trimethoxyphenyl)-1,4-dihydrochromeno[4,3-d][1,2,3]triazole(4a)

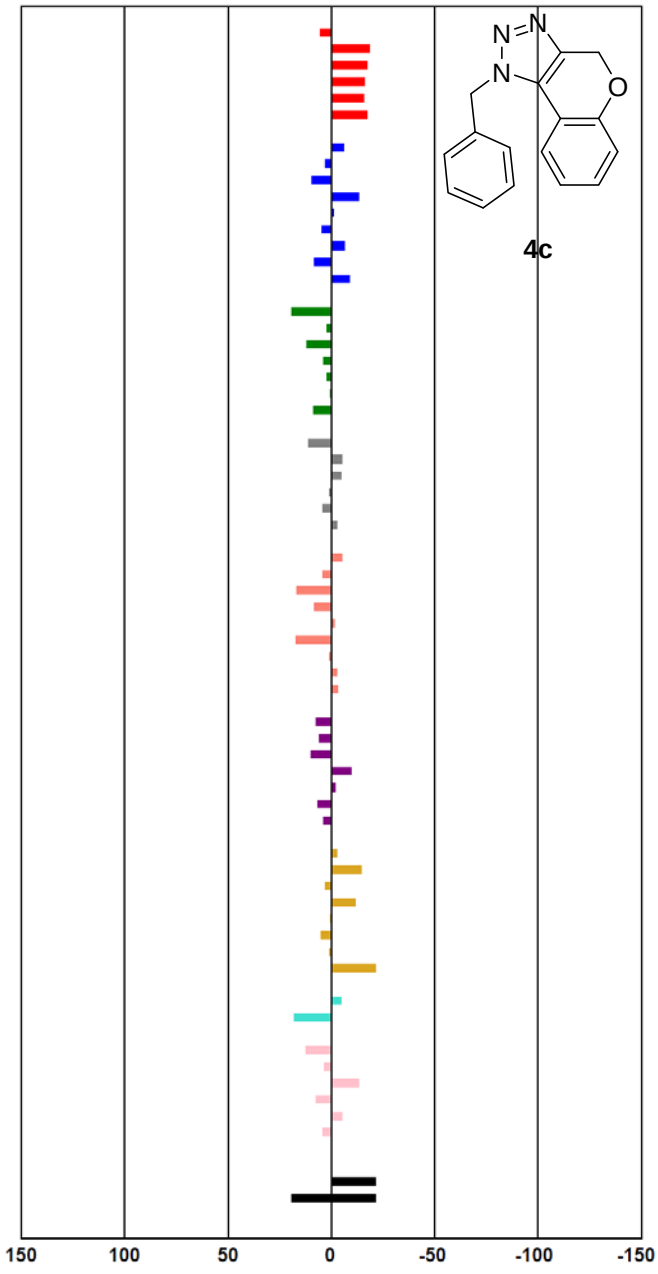


1- benzyl-1,4-dihydrochromeno[4,3-d][1,2,3]triazole(4c)

Developmental Therapeutics Program
One Dose Mean Graph

NSC: D-760025 / 1	Conc: 1.00E-5 Molar	Test Date: Jun 27, 2011
Experiment ID: 1106OS73		Report Date: Jun 28, 2012

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	104.71
HL-60(TB)	81.23
K-562	82.30
MOLT-4	83.63
RPMI-8226	83.87
SR	82.34
Non-Small Cell Lung Cancer	
A549/ATCC	93.70
EKVX	102.04
HOP-62	108.50
HOP-92	86.31
NCI-H226	98.48
NCI-H23	103.67
NCI-H322M	93.09
NCI-H460	107.49
NCI-H522	91.01
Colon Cancer	
COLO 205	118.21
HCC-2998	101.22
HCT-116	111.15
HCT-15	103.08
HT29	101.34
KM12	99.80
SW-620	107.74
CNS Cancer	
SF-268	110.09
SF-295	94.35
SF-539	94.76
SNB-19	100.08
SNB-75	103.49
U251	96.85
Melanoma	
LOX IMVI	94.46
MALME-3M	103.35
M14	115.83
MDA-MB-435	107.33
SK-MEL-2	98.25
SK-MEL-28	116.52
SK-MEL-5	100.04
UACC-257	97.10
UACC-62	96.38
Ovarian Cancer	
IGROV1	106.68
OVCAR-3	104.87
OVCAR-4	109.27
OVCAR-5	90.19
OVCAR-8	97.70
NCI/ADR-RES	105.88
SK-OV-3	103.03
Renal Cancer	
786-0	97.06
A498	85.31
ACHN	102.33
CAKI-1	87.79
RXF 393	99.92
SN12C	104.04
TK-10	99.97
UO-31	78.13
Prostate Cancer	
PC-3	94.84
DU-145	117.34
Breast Cancer	
MCF7	111.33
MDA-MB-231/ATCC	102.55
HS 578T	86.31
BT-549	106.80
T-47D	94.46
MDA-MB-468	103.40
Mean	99.38
Delta	21.25
Range	40.08



1-(4-bromophenyl)-1,4-dihydrochromeno[4,3-d][1,2,3] triazole(4i)

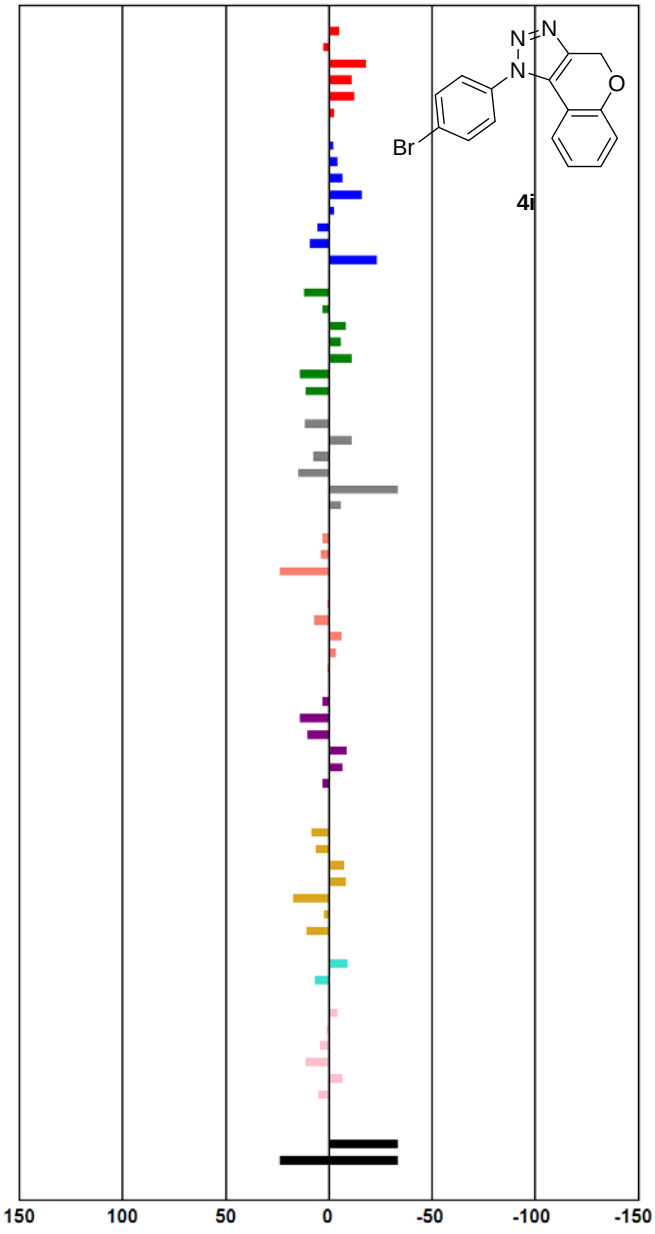
Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-754644 / 1	Conc: 1.00E-5 Molar	Test Date: Oct 18, 2010
Experiment ID: 1010OS37		Report Date: Jun 28, 2012

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	88.06
HL-60(TB)	94.79
K-562	75.21
MOLT-4	82.05
RPMI-8226	80.81
SR	90.46
Non-Small Cell Lung Cancer	
A549/ATCC	90.83
EKVX	88.74
HOP-62	86.39
NCI-H226	77.11
NCI-H23	90.56
NCI-H322M	97.61
NCI-H460	101.32
NCI-H522	69.94
Colon Cancer	
COLO 205	104.33
HCC-2998	95.44
HCT-116	84.77
HCT-15	87.15
HT29	81.86
KM12	106.22
SW-620	103.27
CNS Cancer	
SF-268	103.78
SF-295	81.81
SF-539	99.86
SNB-19	106.91
SNB-75	59.46
U251	87.08
Melanoma	
LOX IMVI	95.17
MALME-3M	95.93
M14	115.88
MDA-MB-435	92.56
SK-MEL-2	92.84
SK-MEL-28	99.55
SK-MEL-5	86.74
UACC-257	89.53
UACC-62	92.99
Ovarian Cancer	
IGROV1	95.25
OVCAR-3	106.26
OVCAR-5	102.61
OVCAR-8	84.22
NCI/ADR-RES	86.38
SK-OV-3	95.30
Renal Cancer	
786-0	92.35
A498	100.73
ACHN	98.43
CAKI-1	85.56
RXF 393	84.83
SN12C	109.60
TK-10	94.61
UO-31	102.92
Prostate Cancer	
PC-3	84.00
DU-145	98.79
Breast Cancer	
MCF7	88.98
MDA-MB-231/ATCC	93.27
HS 578T	96.70
BT-549	103.56
T-47D	86.58
MDA-MB-468	97.52
Mean	92.51
Delta	33.05
Range	56.42

Mean Growth Percent - Growth Percent



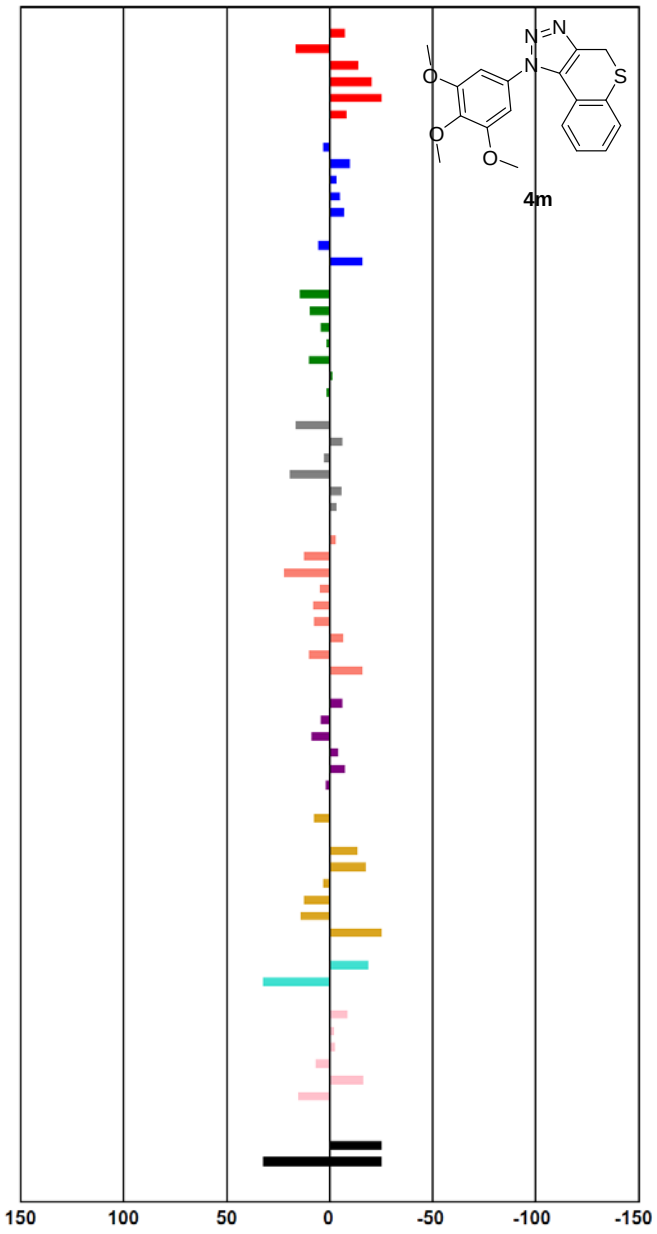
4i

1-(3,4,5-trimethoxyphenyl)-1,4-dihydrothiochromeno [4,3-d][1,2,3]triazole(4m)

Developmental Therapeutics Program One Dose Mean Graph	NSC: D-754643 / 1	Conc: 1.00E-5 Molar	Test Date: Oct 18, 2010
	Experiment ID: 1010OS37		Report Date: Jun 28, 2012

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	85.57
HL-60(TB)	108.67
K-562	79.03
MOLT-4	72.78
RPMI-8226	67.81
SR	84.89
Non-Small Cell Lung Cancer	
A549/ATCC	95.39
EKVX	83.28
HOP-62	89.79
NCI-H226	87.93
NCI-H23	85.88
NCI-H322M	92.46
NCI-H460	97.66
NCI-H522	77.12
Colon Cancer	
COLO 205	106.76
HCC-2998	101.74
HCT-116	96.48
HCT-15	93.92
HT29	102.40
KM12	91.76
SW-620	93.90
CNS Cancer	
SF-268	108.85
SF-295	87.05
SF-539	94.99
SNB-19	111.72
SNB-75	87.17
U251	89.88
Melanoma	
LOX IMVI	90.26
MALME-3M	104.88
M14	114.32
MDA-MB-435	97.14
SK-MEL-2	100.18
SK-MEL-28	99.82
SK-MEL-5	86.47
UACC-257	102.34
UACC-62	77.23
Ovarian Cancer	
IGROV1	86.98
OVCAR-3	96.42
OVCAR-5	100.96
OVCAR-8	88.93
NCI/ADR-RES	85.62
SK-OV-3	94.33
Renal Cancer	
786-0	99.71
A498	92.53
ACHN	79.40
CAKI-1	75.32
RXF 393	95.29
SN12C	104.77
TK-10	106.23
UO-31	67.78
Prostate Cancer	
PC-3	74.42
DU-145	124.69
Breast Cancer	
MCF7	84.46
MDA-MB-231/ATCC	90.92
HS 578T	90.64
BT-549	98.92
T-47D	76.69
MDA-MB-468	107.40
Mean	92.59
Delta	24.81
Range	56.91

Mean Growth Percent - Growth Percent



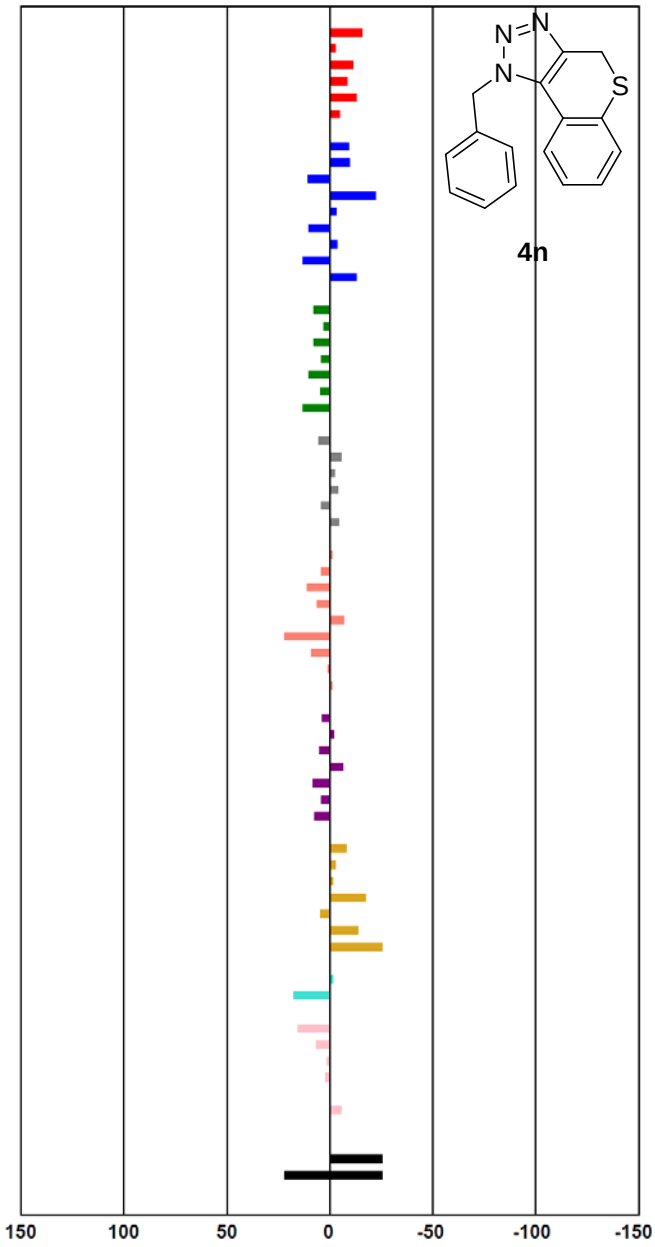
4m

1-benzyl-1,4-dihydrothiochromeno[4,3-d][1,2,3]triazole(4n)

Developmental Therapeutics Program One Dose Mean Graph	NSC: D-760026 / 1	Conc: 1.00E-5 Molar	Test Date: Jun 27, 2011
	Experiment ID: 1106OS73		Report Date: Jun 28, 2012

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	79.73
HL-60(TB)	92.49
K-562	84.25
MOLT-4	86.84
RPMI-8226	82.41
SR	90.71
Non-Small Cell Lung Cancer	
A549/ATCC	85.96
EKVX	85.56
HOP-62	105.48
HOP-92	73.15
NCI-H226	92.15
NCI-H23	105.00
NCI-H322M	91.79
NCI-H460	107.83
NCI-H522	82.31
Colon Cancer	
COLO 205	102.81
HCC-2998	97.70
HCT-116	102.78
HCT-15	99.03
HT29	104.99
KM12	99.60
SW-620	108.08
CNS Cancer	
SF-268	100.46
SF-295	89.68
SF-539	92.86
SNB-19	91.31
SNB-75	99.10
U251	90.99
Melanoma	
LOX IMVI	94.31
MALME-3M	98.94
M14	106.02
MDA-MB-435	100.96
SK-MEL-2	88.44
SK-MEL-28	116.79
SK-MEL-5	103.89
UACC-257	96.01
UACC-62	94.42
Ovarian Cancer	
IGROV1	98.56
OVCAR-3	93.54
OVCAR-4	99.91
OVCAR-5	89.15
OVCAR-8	103.09
NCI/ADR-RES	99.28
SK-OV-3	102.35
Renal Cancer	
786-0	87.41
A498	92.57
ACHN	93.92
CAKI-1	78.00
SN12C	99.55
TK-10	81.60
UO-31	69.73
Prostate Cancer	
PC-3	93.97
DU-145	112.39
Breast Cancer	
MCF7	110.44
MDA-MB-231/ATCC	101.42
HS 578T	96.45
BT-549	97.24
T-47D	95.00
MDA-MB-468	89.67
Mean	95.09
Delta	25.36
Range	47.06

Mean Growth Percent - Growth Percent



6. CCDC No of **2a**、**4a** and **4o**.

(a) CCDC No of **2a**: CCDC 890286

(b) CCDC No of **4a**: CCDC 890287

(a) CCDC No of **4o**: CCDC 890285