Supporting Information for

Crystallization-Induced Diasteromer Transformation assists the diastereoselective synthesis of 4-nitroisoxazolidine scaffolds

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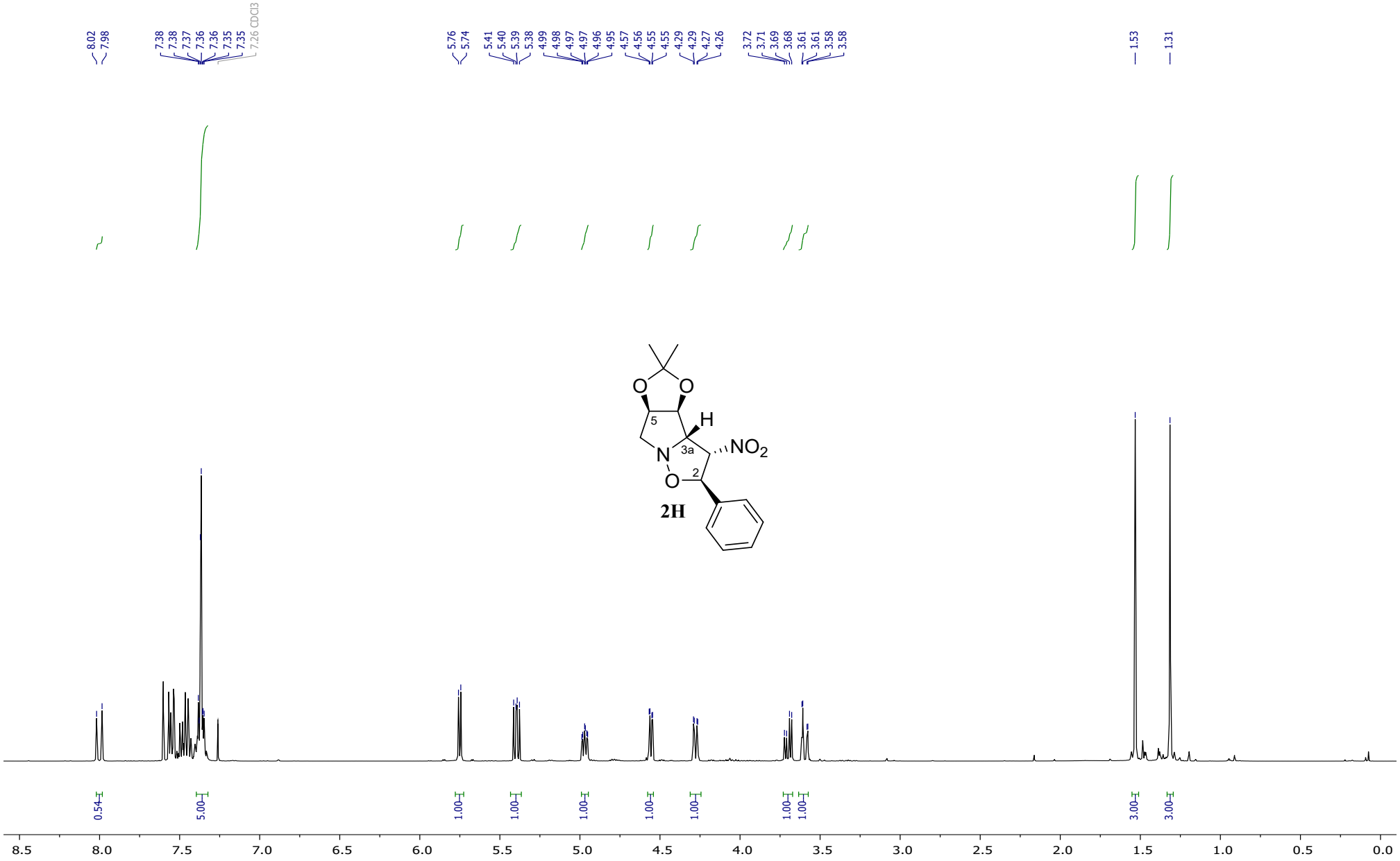

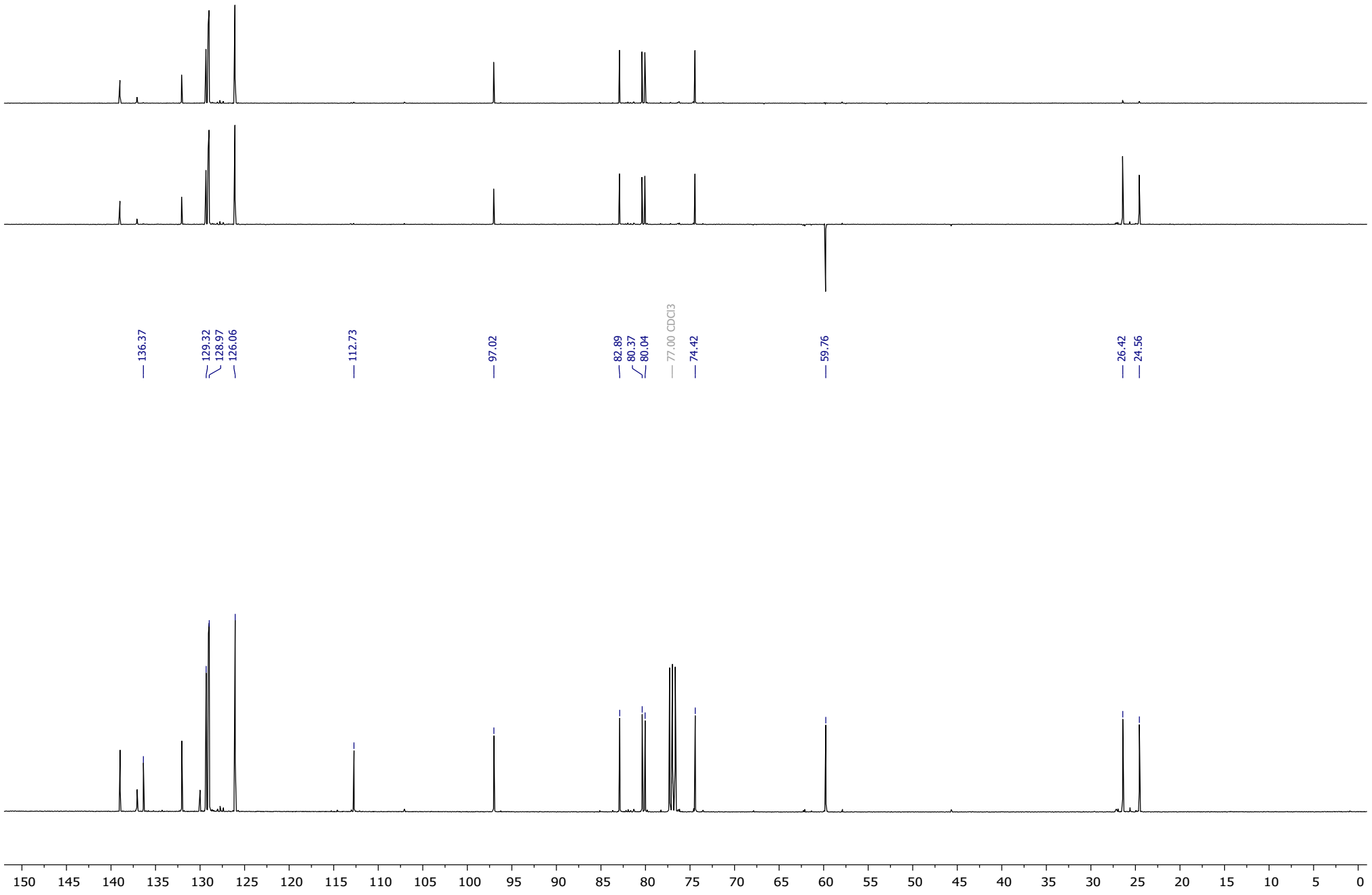
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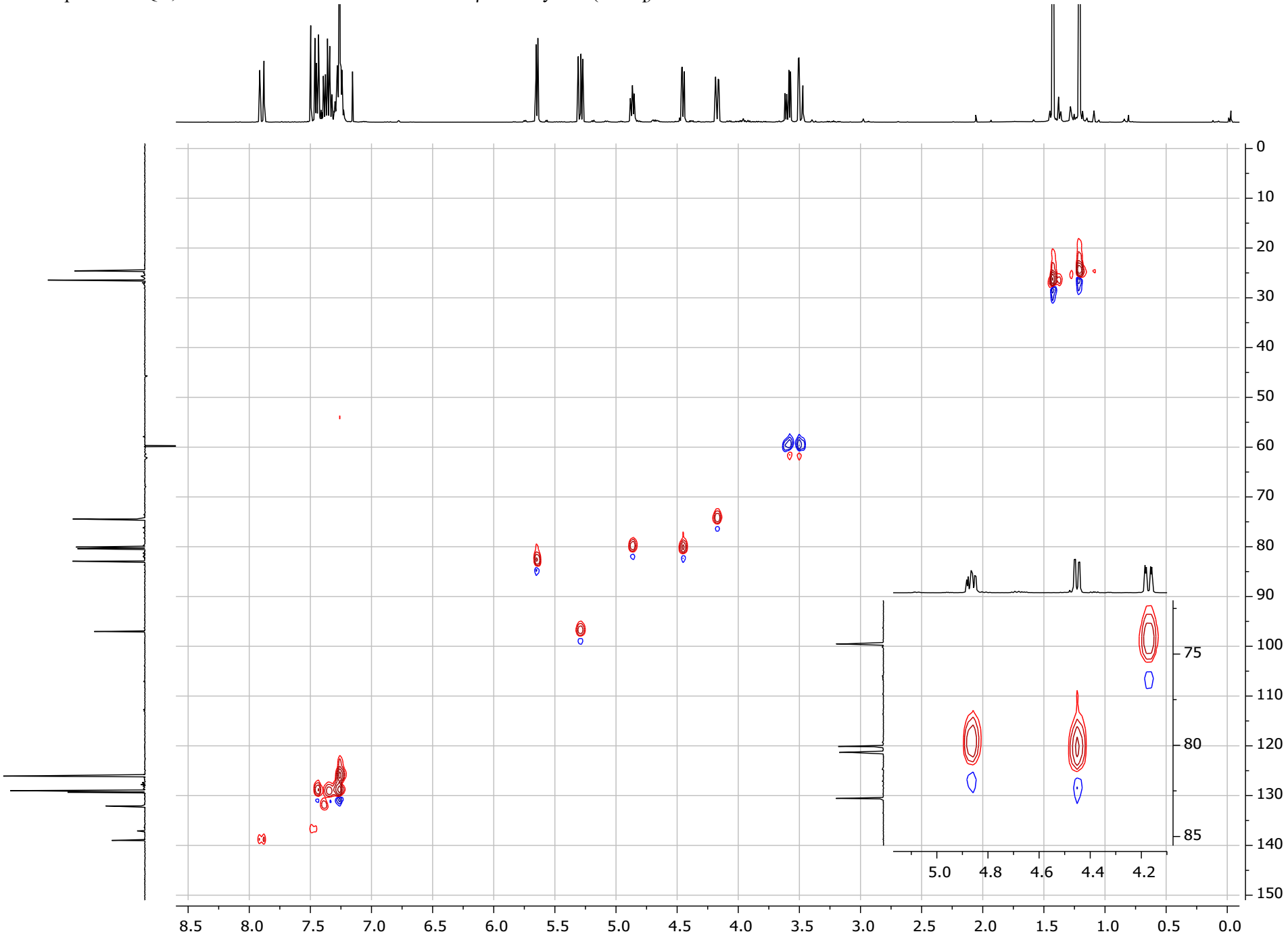
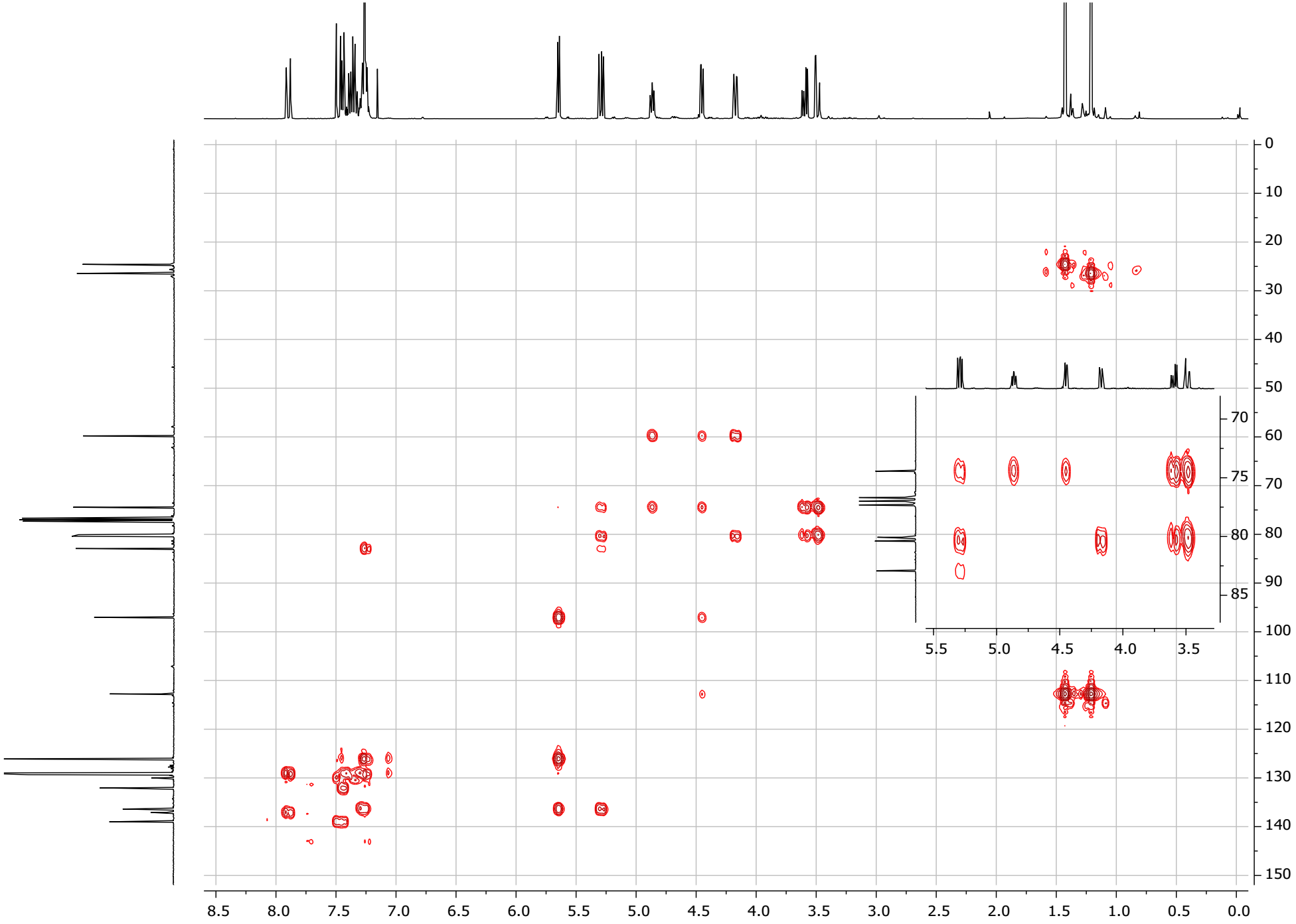
26.42
24.56
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

2D NMR spectra HSQC, HMBC and COSY of **2H** with *trans*-β-nitrostyrene (0.5 eq)

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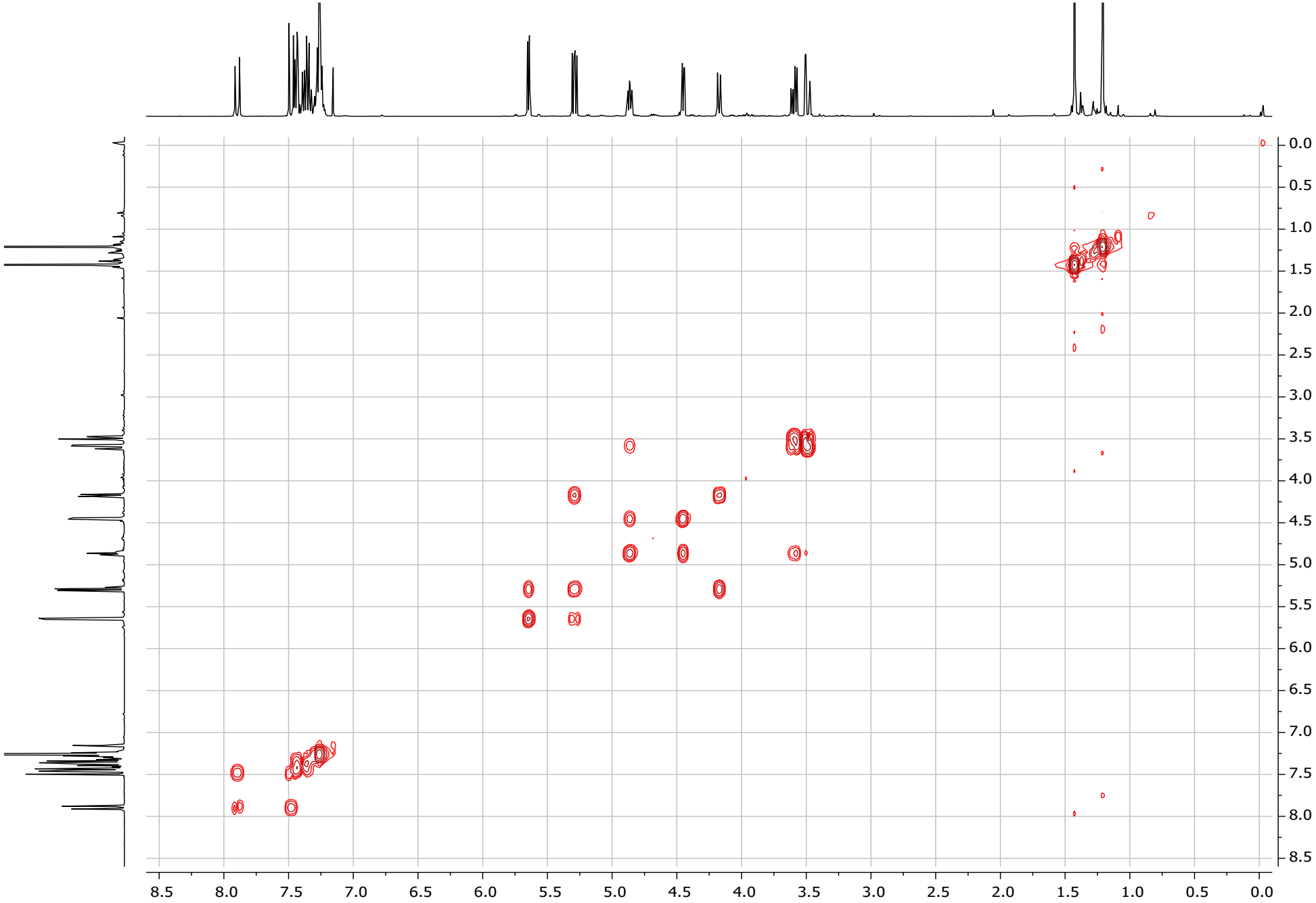
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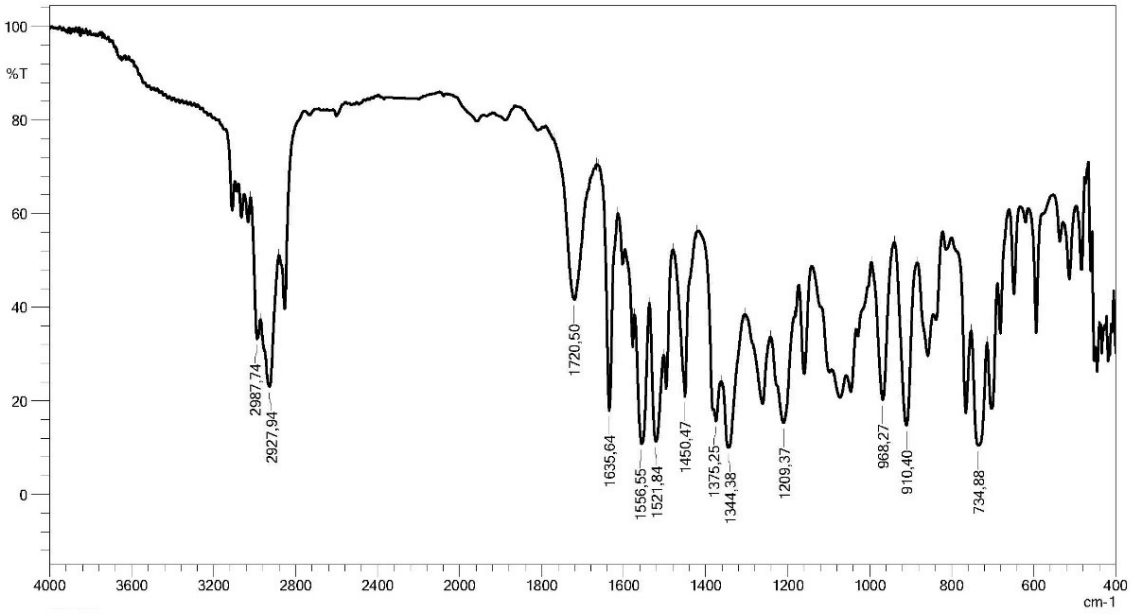
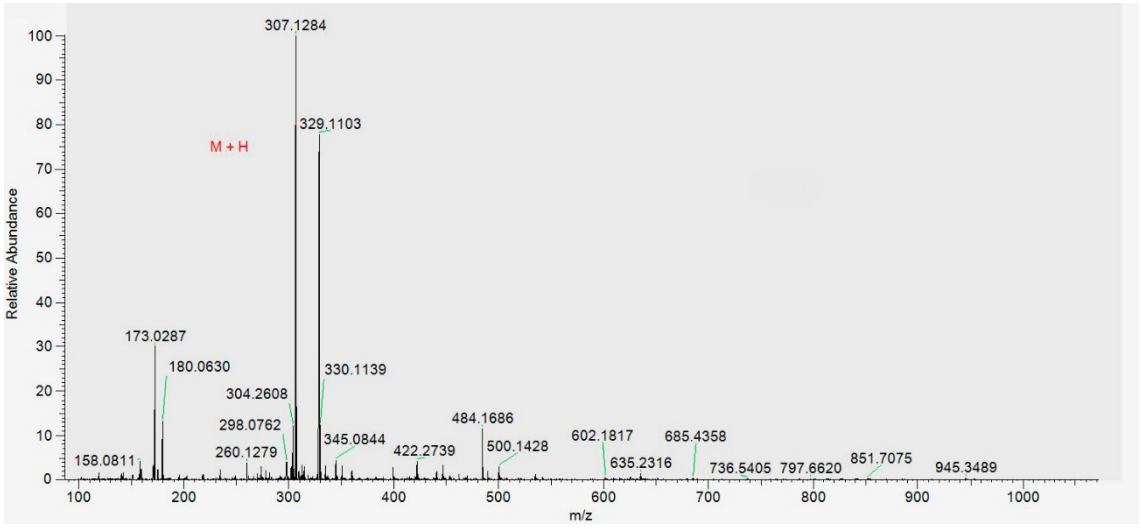
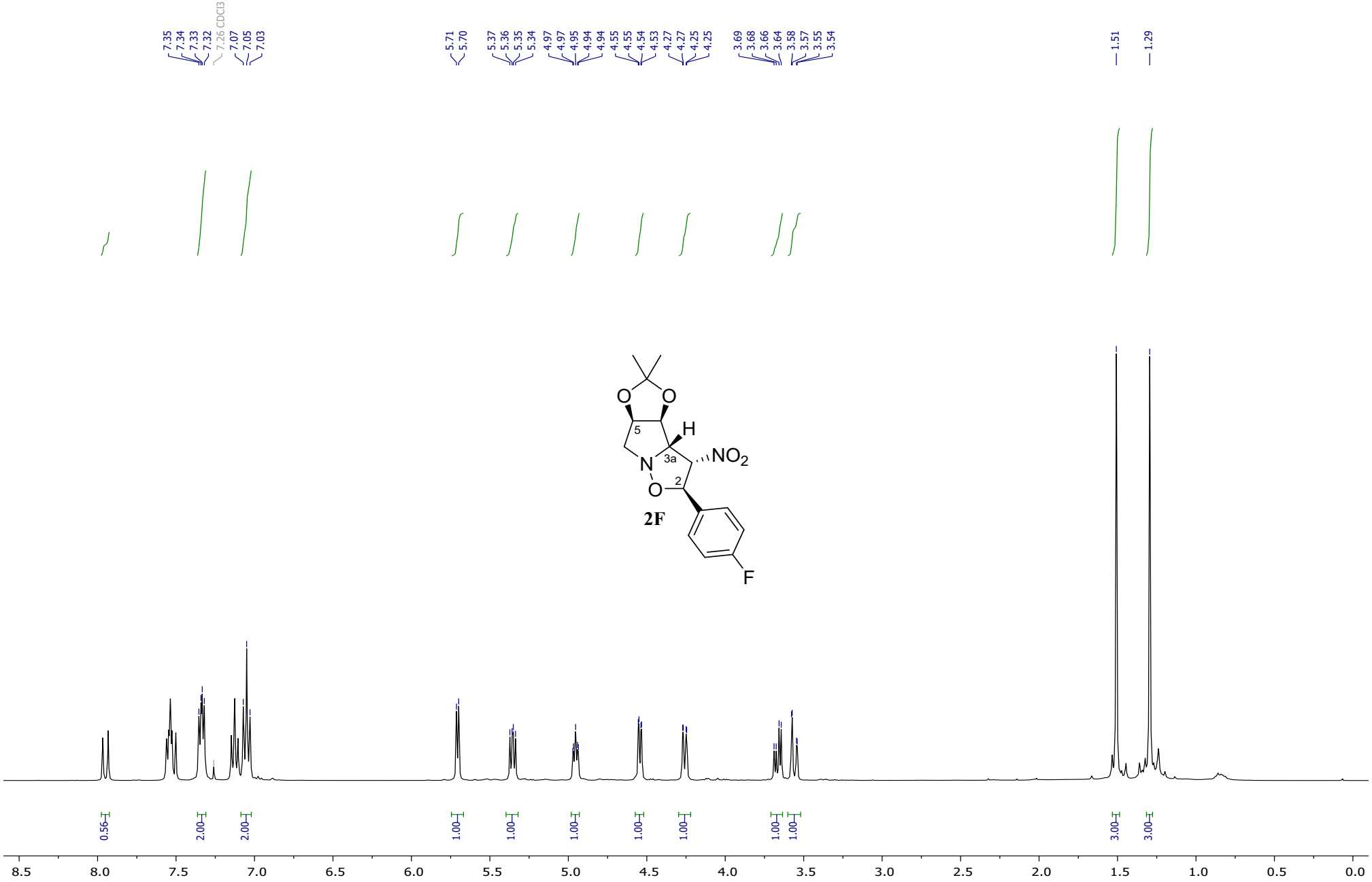
IR spectra of **2H** with *trans*-β-nitrostyrene (0.5 eq)

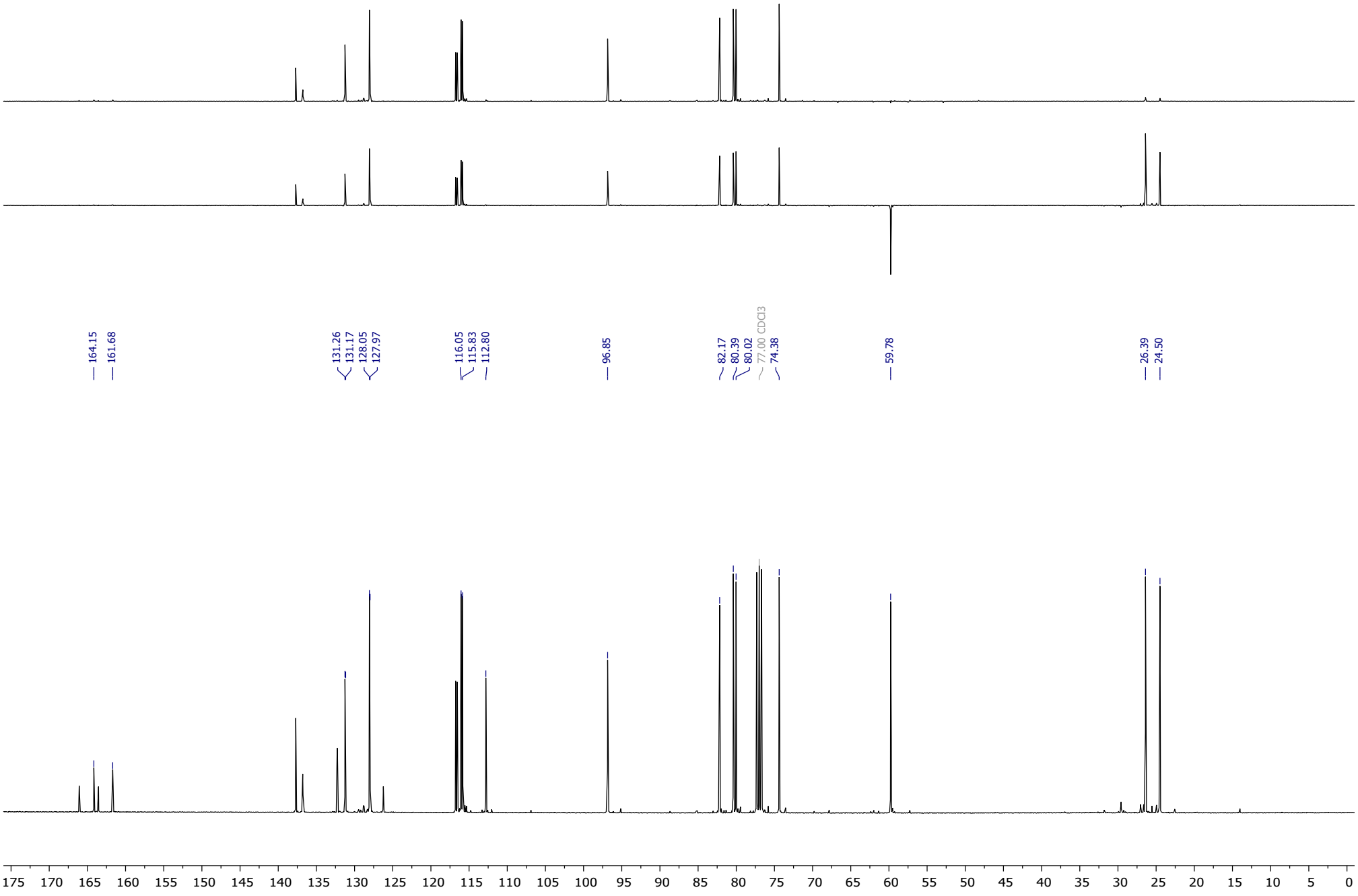


HRMS spectra of **2H** with *trans*-β-nitrostyrene (0.5 eq)



^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **2F** with *trans*-4-fluoro-β-nitrostyrene (0.5 eq)

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74.38
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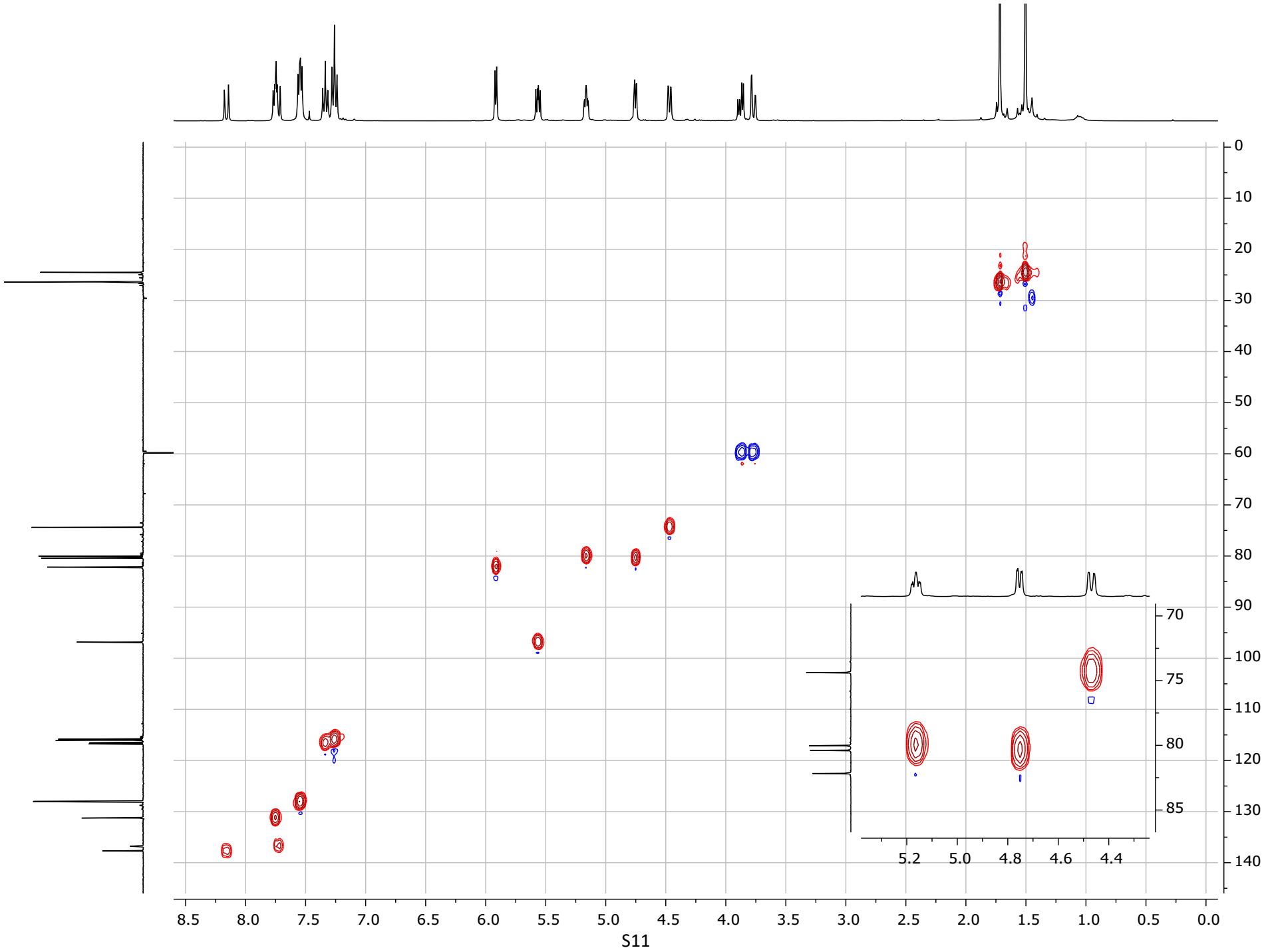
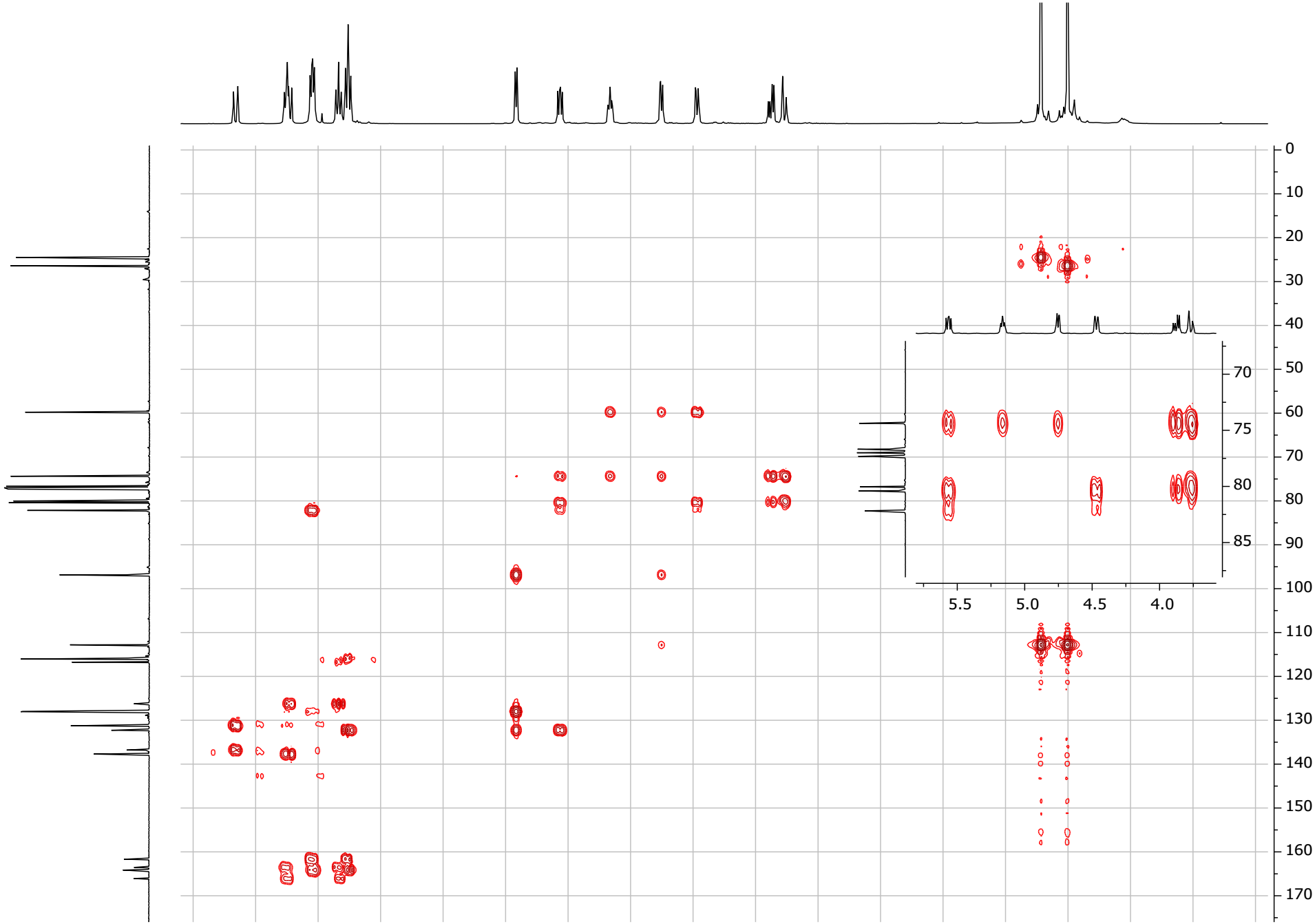
26.39
24.50
175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

2D NMR spectra HSQC, HMBC and COSY of **2F** with *trans*-4-fluoro-β-nitrostyrene (0.5 eq)

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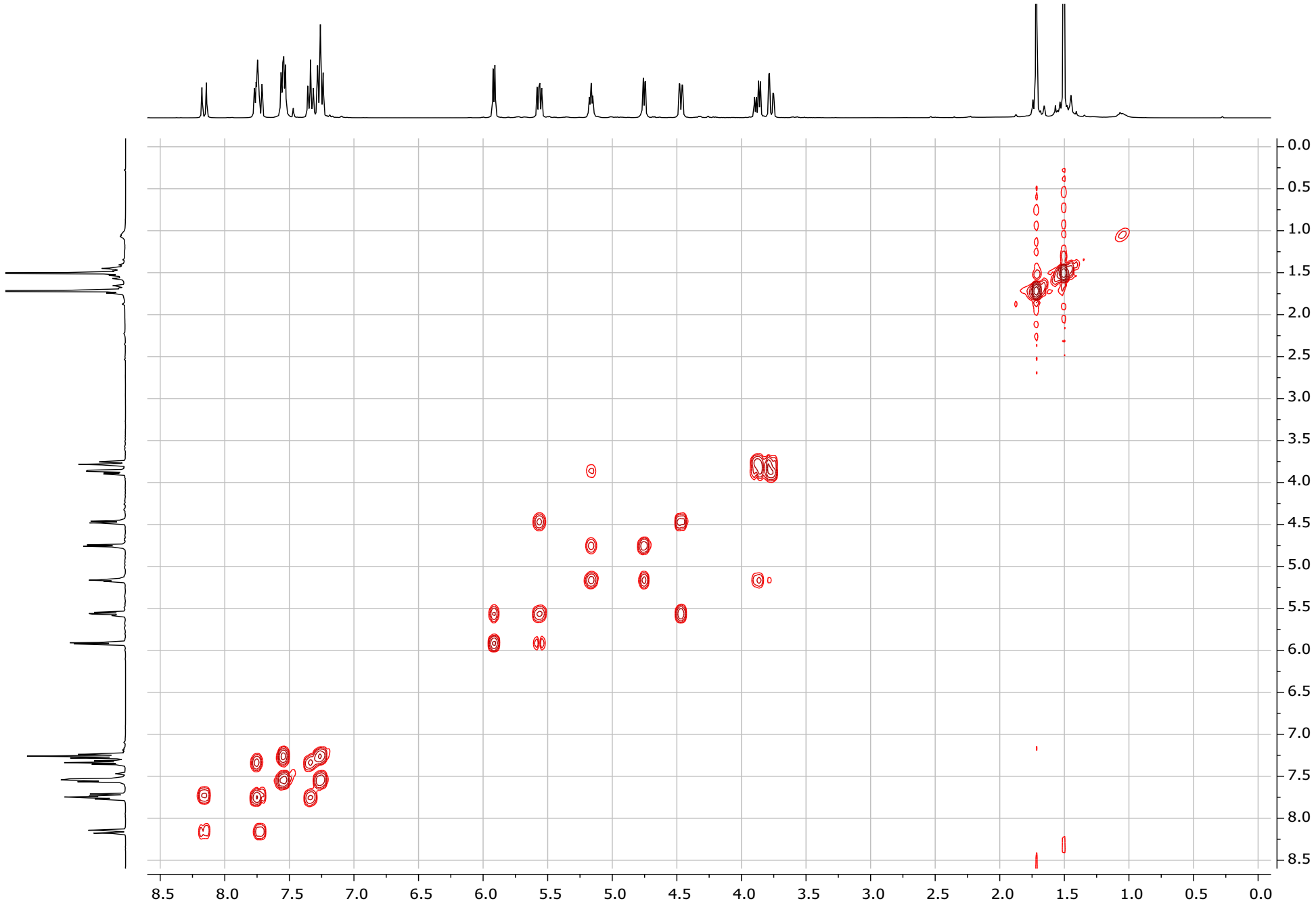
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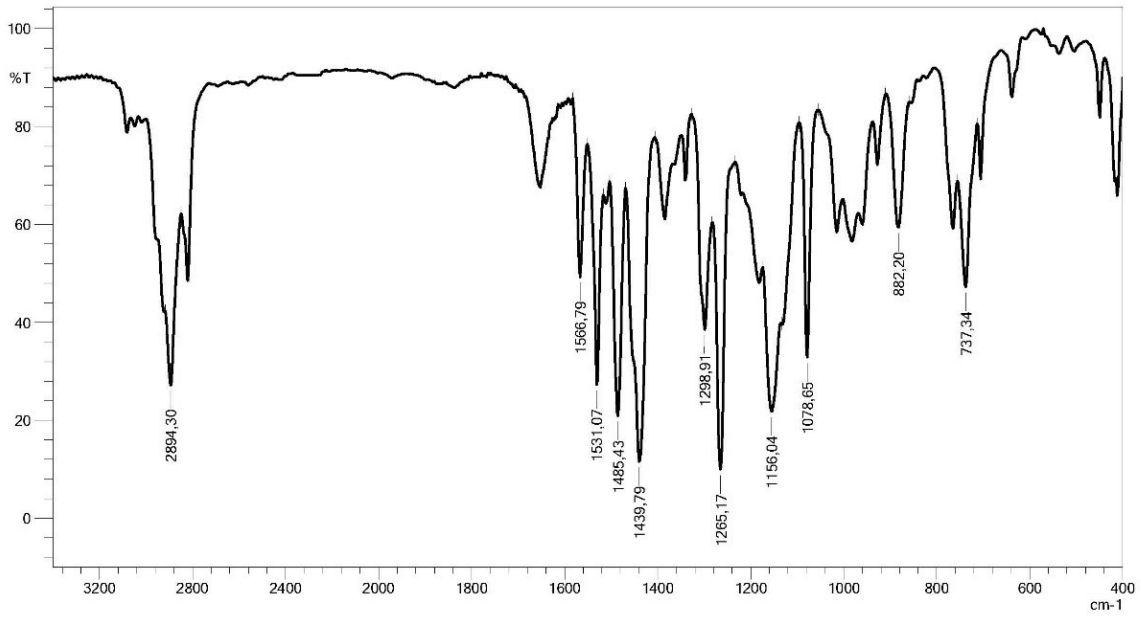
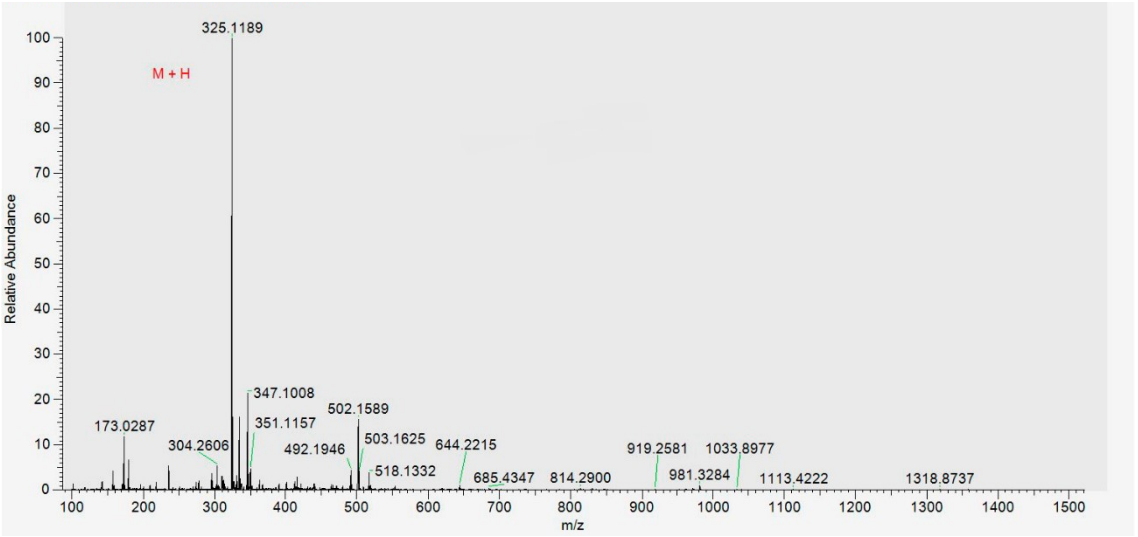
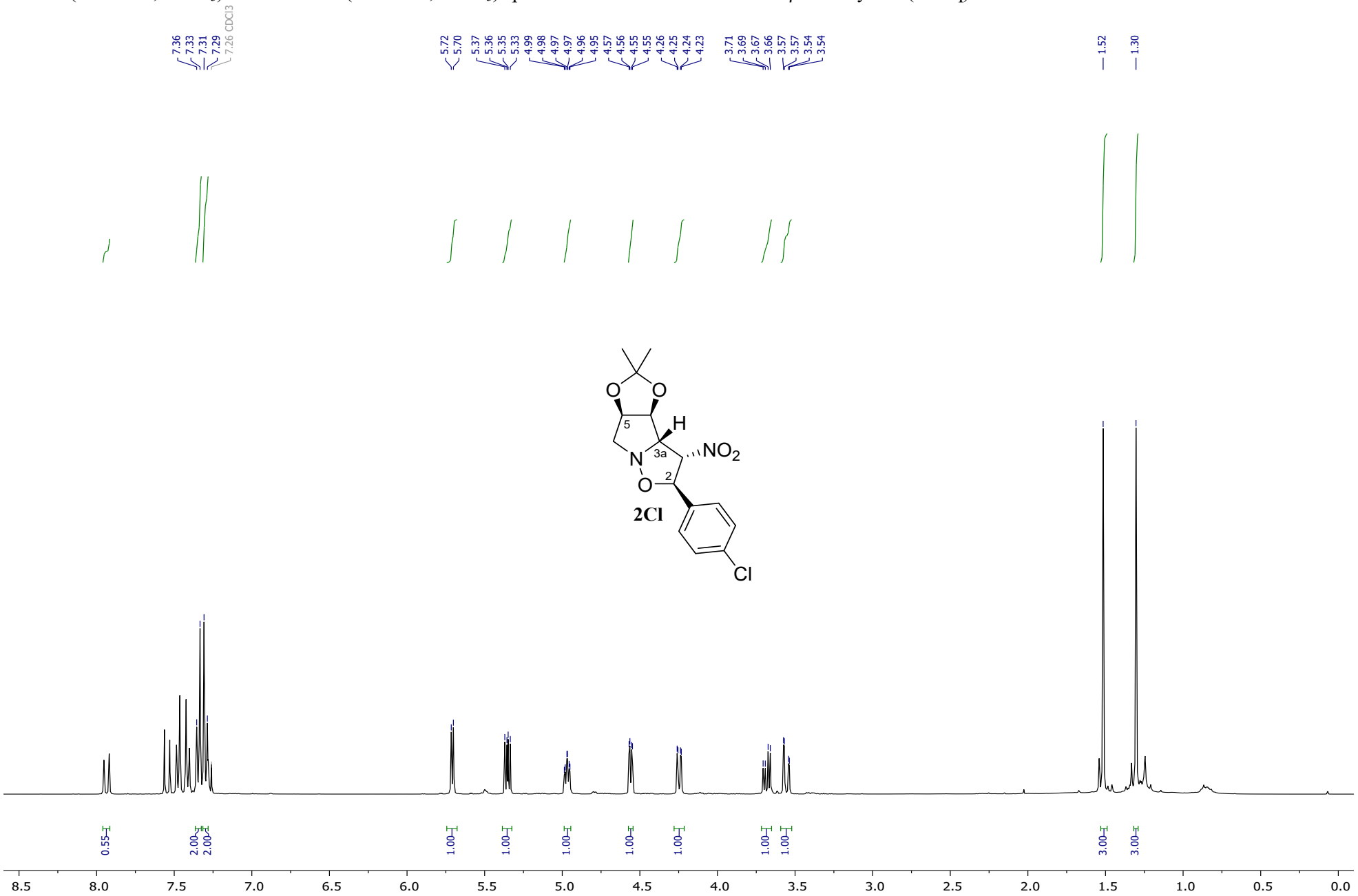
IR spectra of **2F** with *trans*-4-fluoro-β-nitrostyrene (0.5 eq)

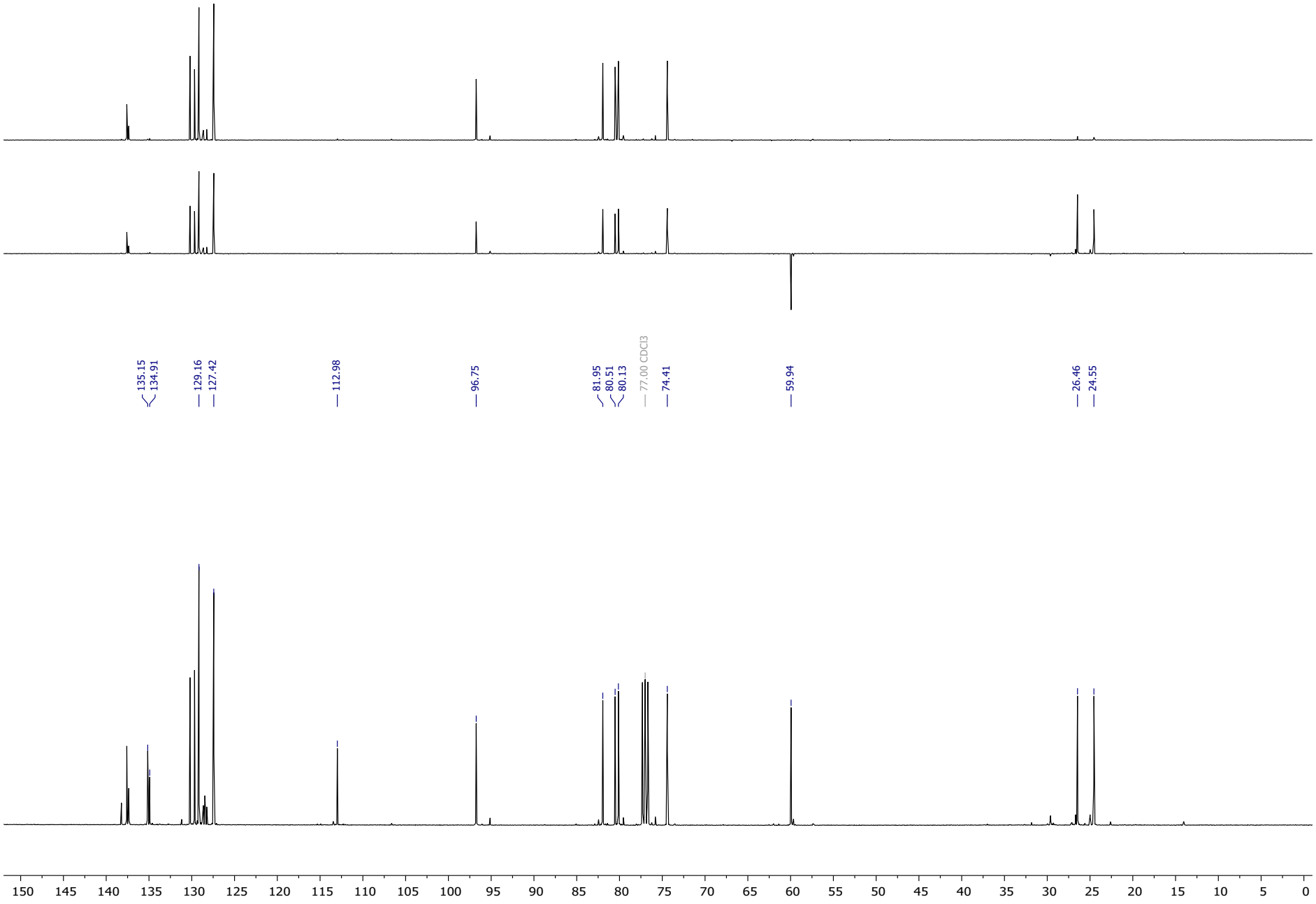


HRMS spectra of **2F** with *trans*-4-fluoro-β-nitrostyrene (0.5 eq)



^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **2Cl** with *trans*-4-chloro-β-nitrostyrene (0.5 eq)

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77.00 CDCl3
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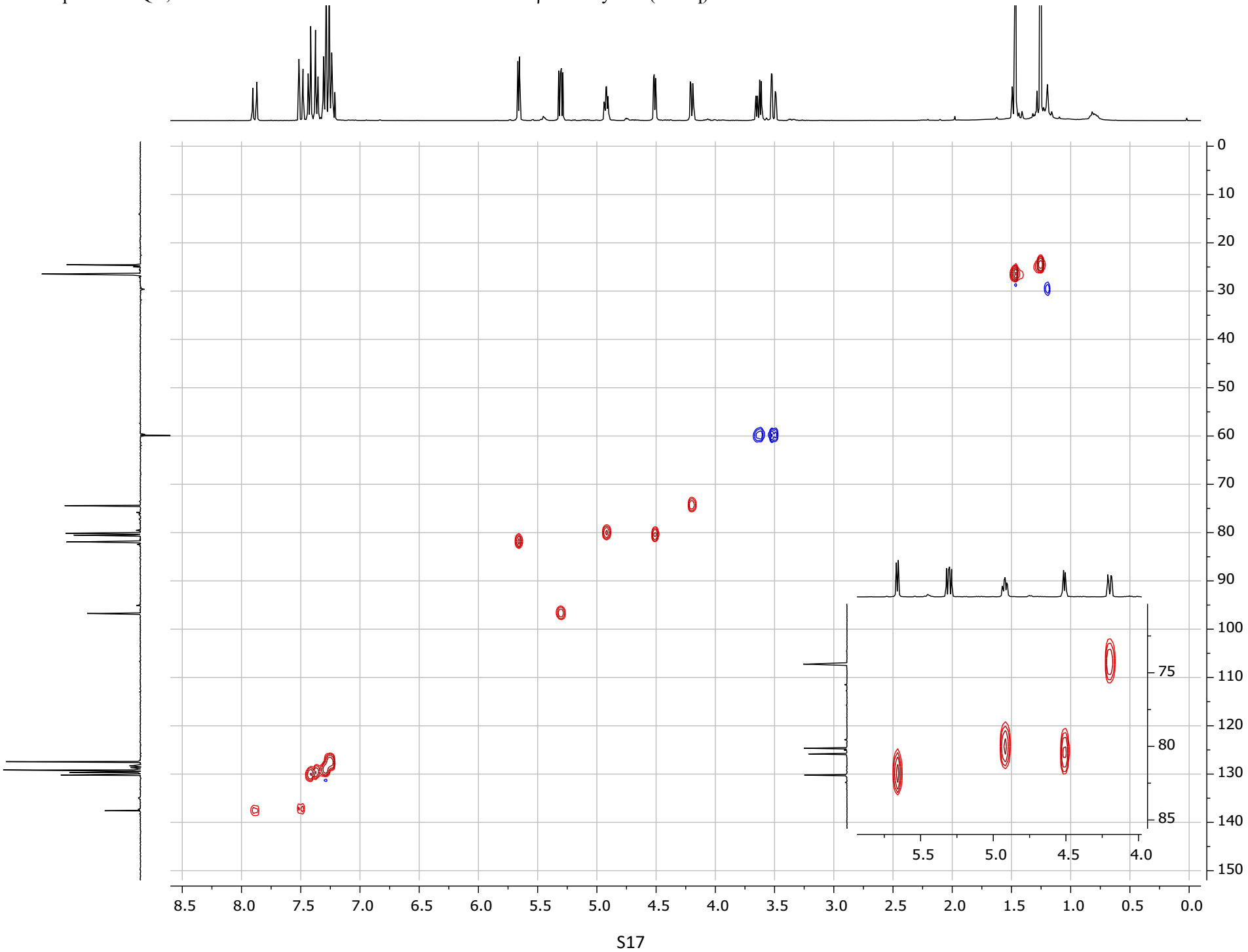
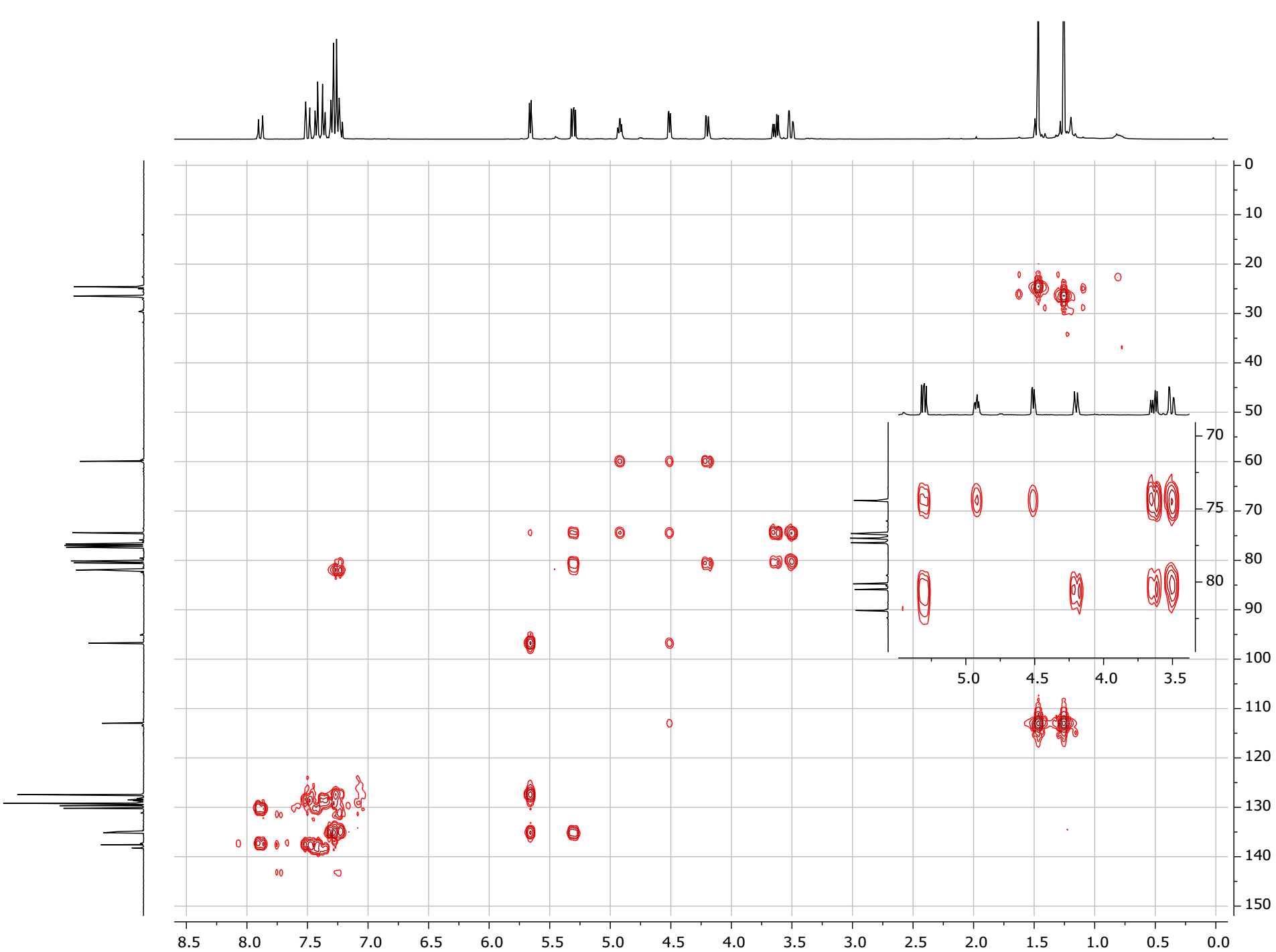
59.94
26.46
24.55
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

2D NMR spectra HSQC, HMBC and COSY of **2Cl** with *trans*-4-chloro-β-nitrostyrene (0.5 eq)

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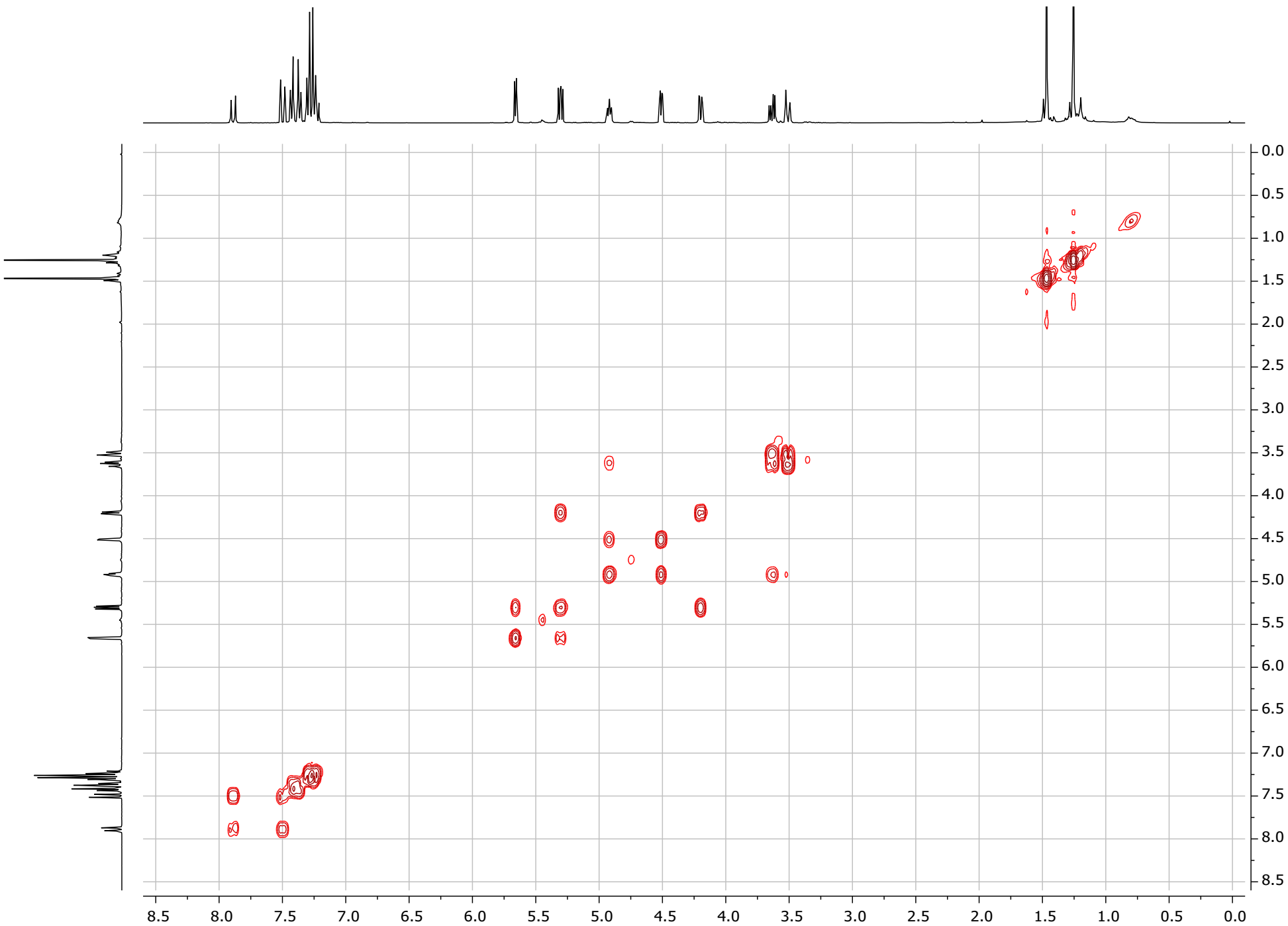
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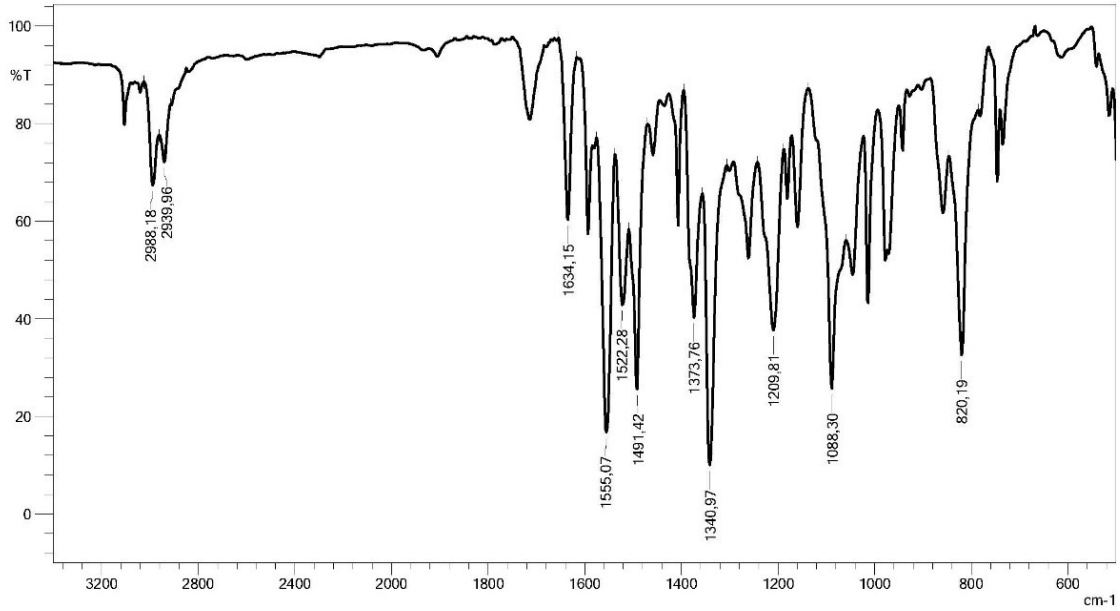
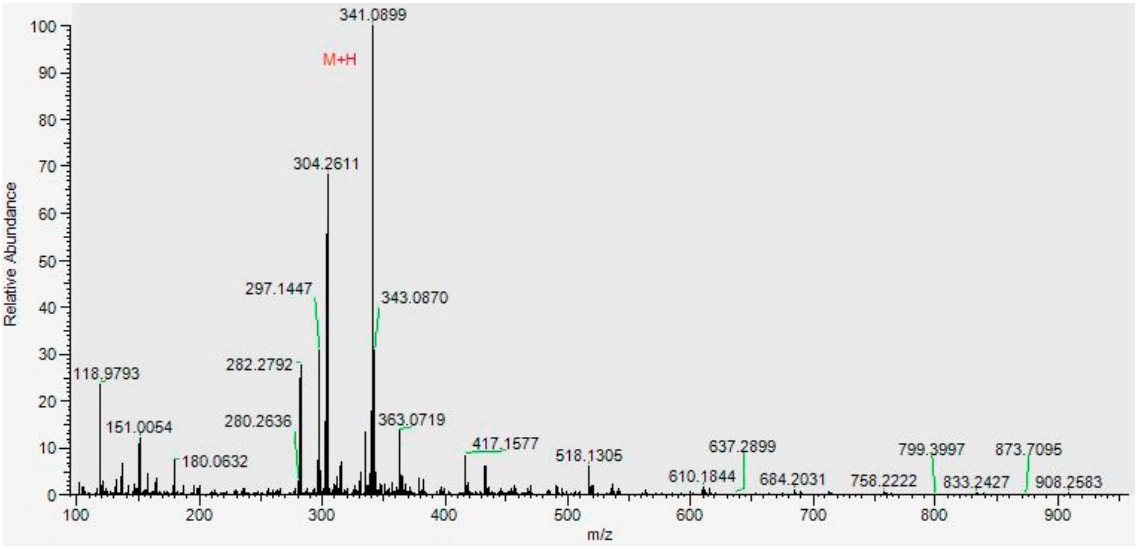
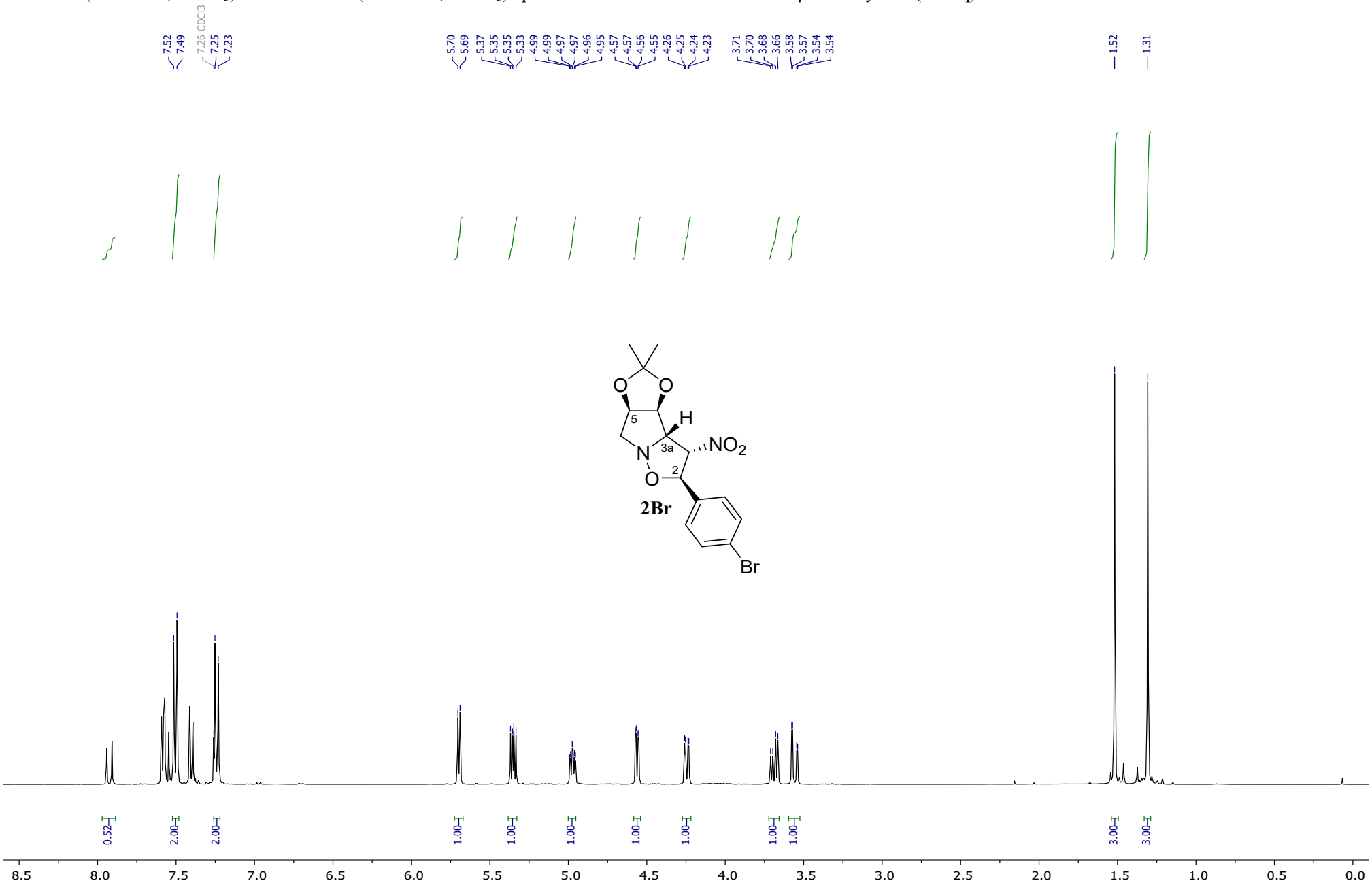
IR spectra of **2Cl** with *trans*-4-chloro-β-nitrostyrene (0.5 eq)

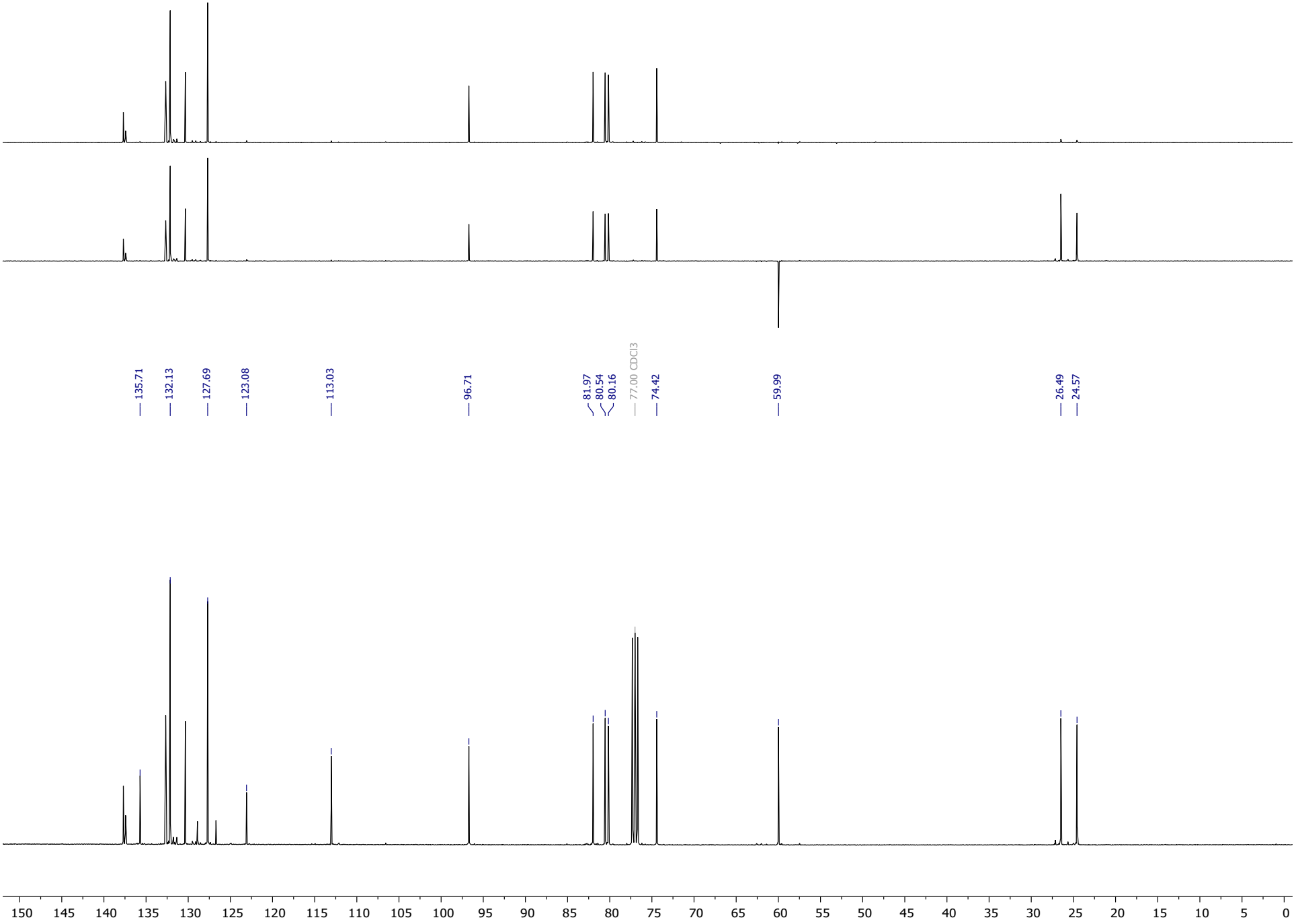


HRMS spectra of **2Cl** with *trans*-4-chloro-β-nitrostyrene (0.5 eq)



^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **2Br** with *trans*-4-bromo-β-nitrostyrene (0.5 eq)

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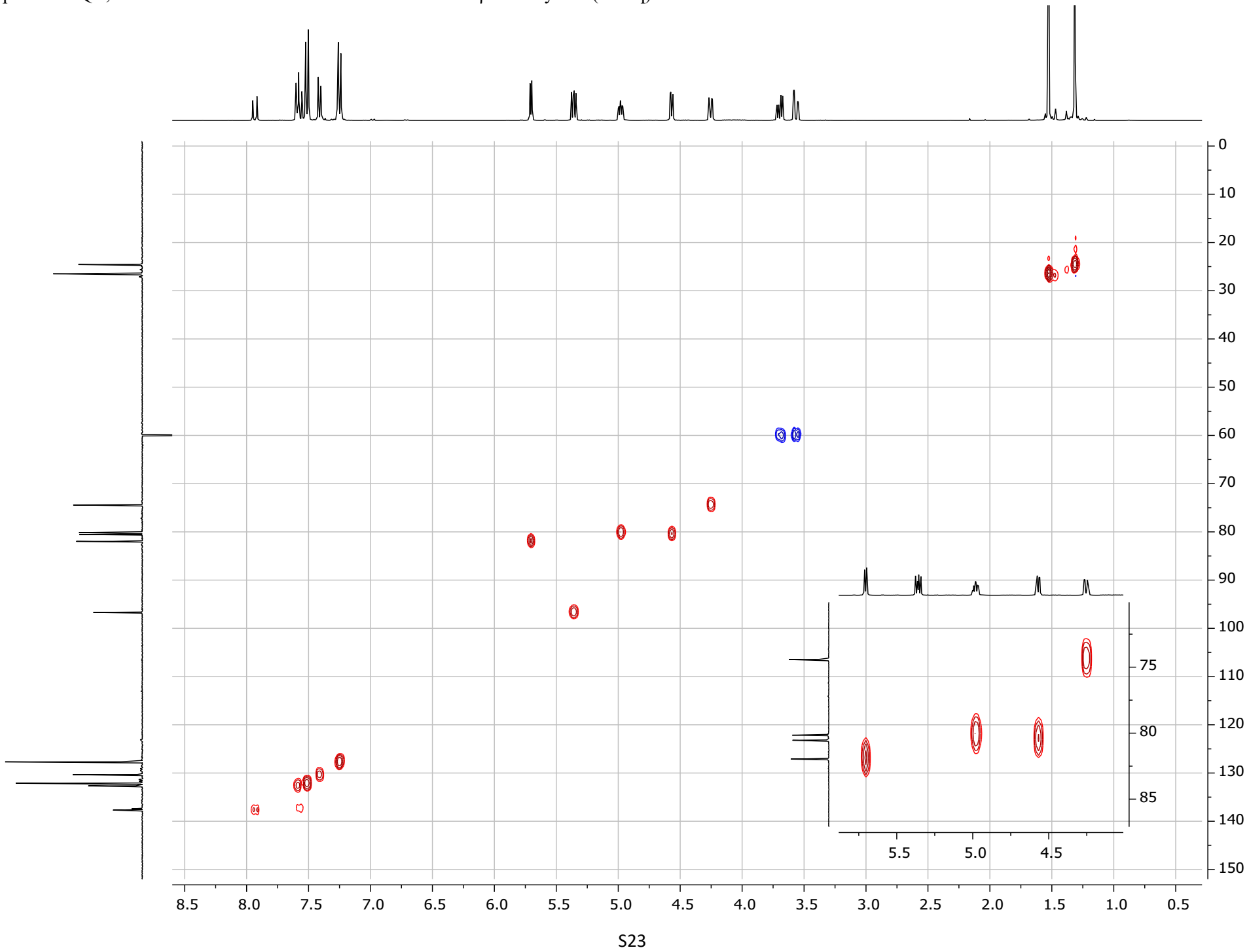
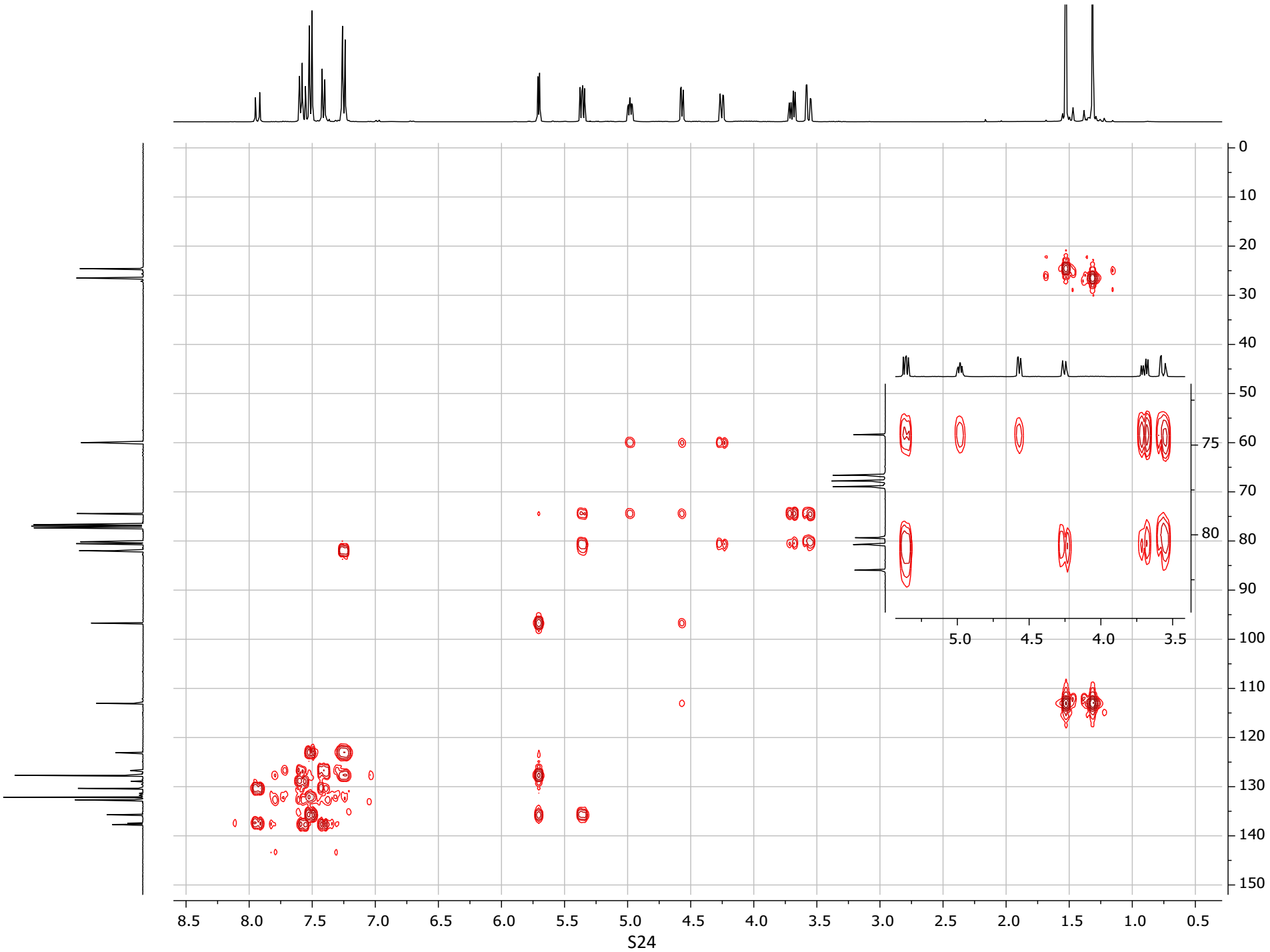
77.00 CDCl3
74.42
59.99
26.49
24.57
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

2D NMR spectra HSQC, HMBC and COSY of **2Br** with *trans*-4-bromo-β-nitrostyrene (0.5 eq)

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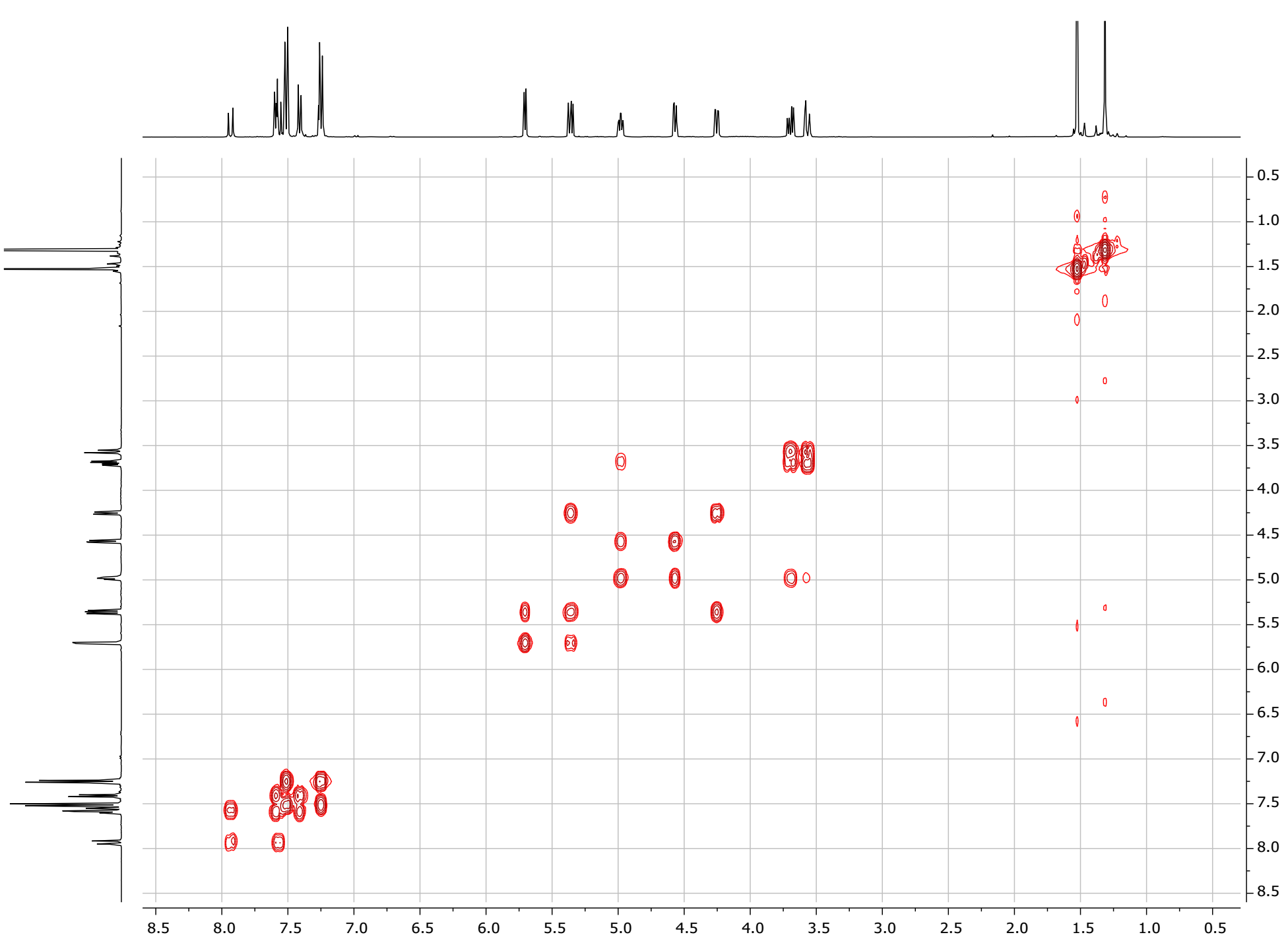
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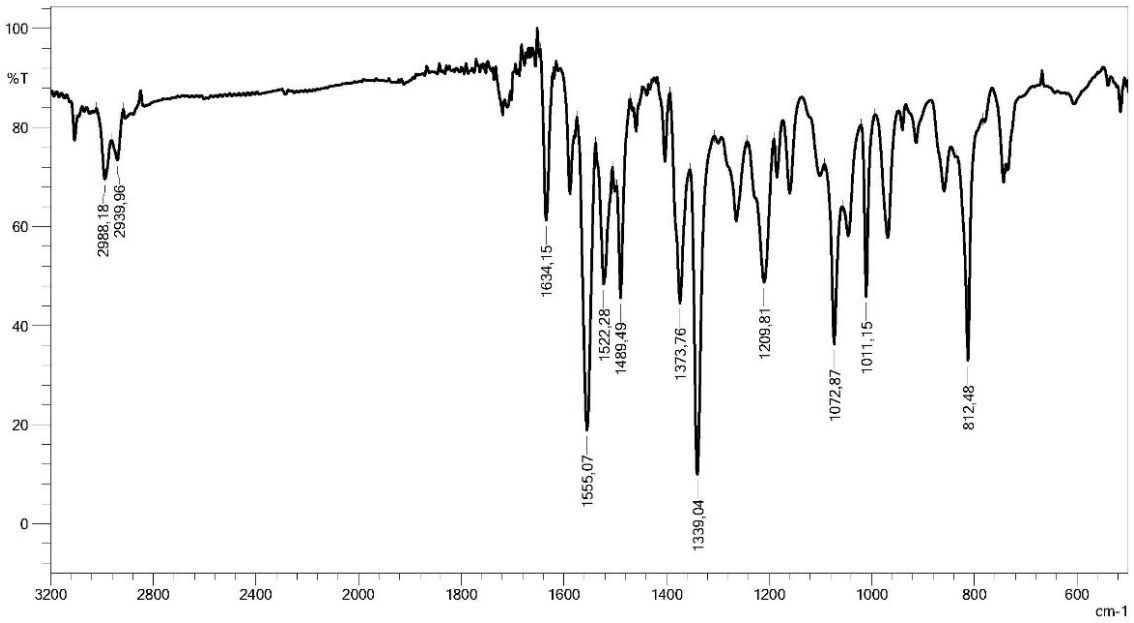
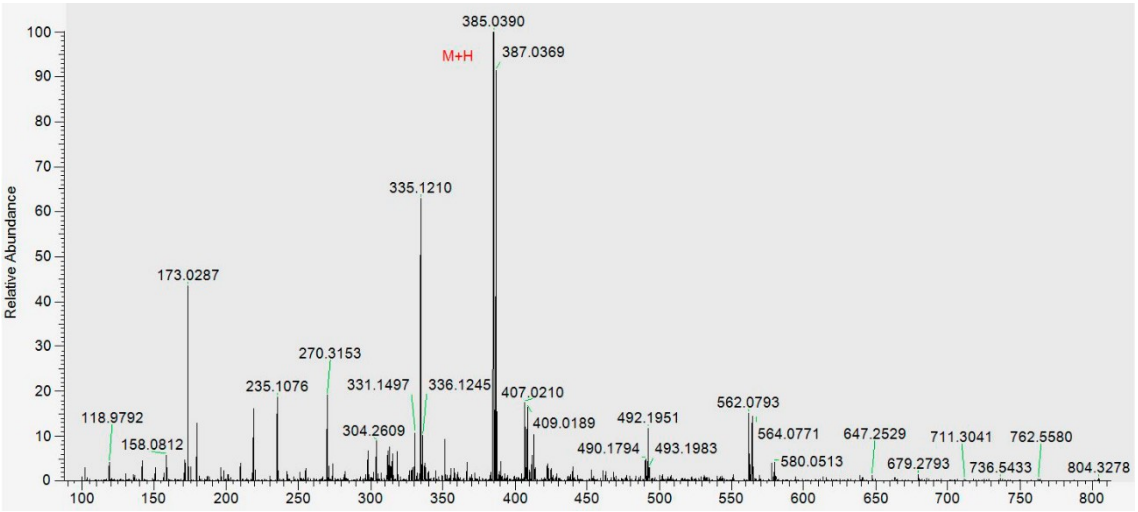
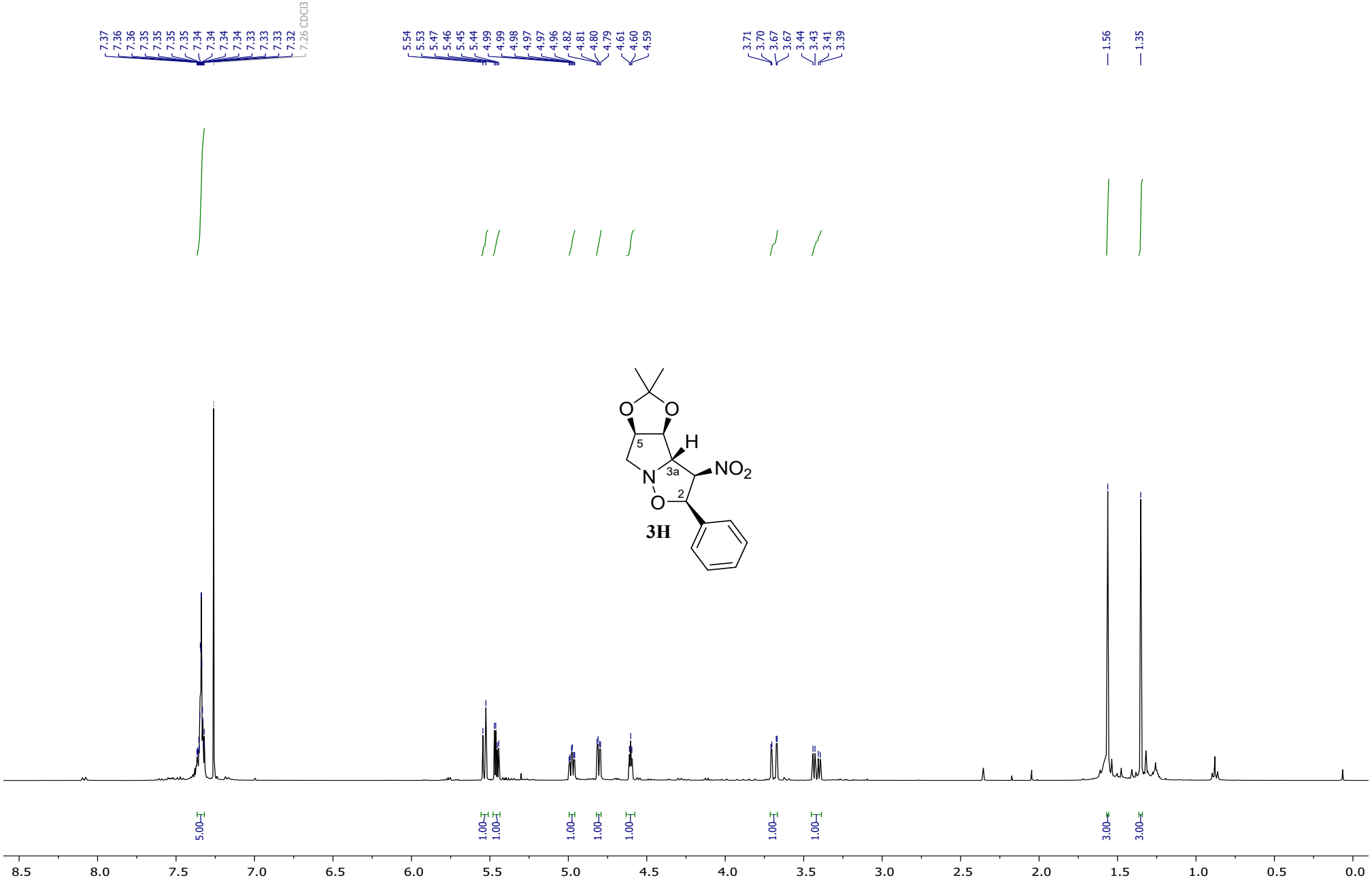
IR spectra of **2Br** with *trans*-4-bromo-β-nitrostyrene (0.5 eq)

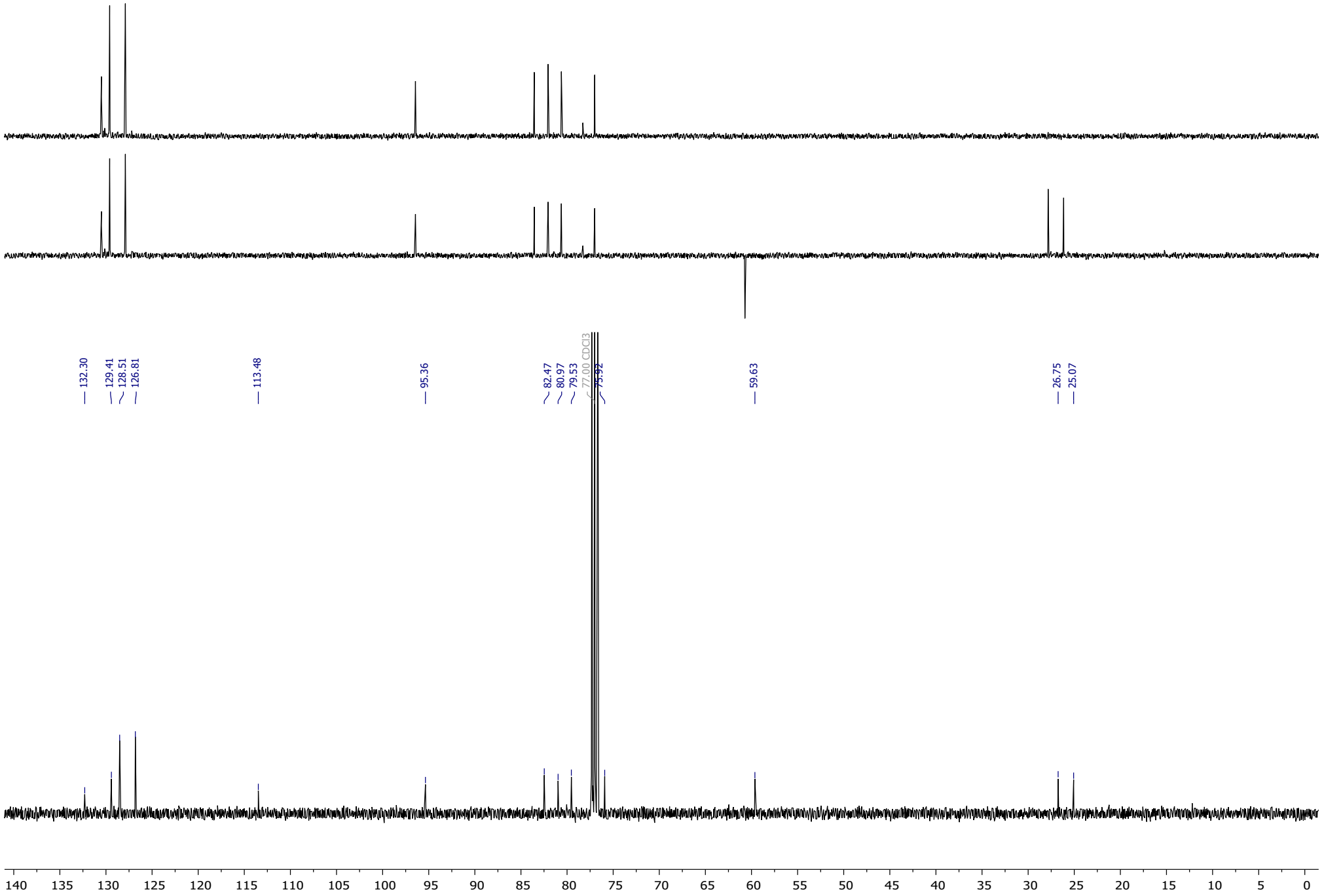


HRMS spectra of **2Br** with *trans*-4-bromo-β-nitrostyrene $_3$(0.5 eq)



^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3H**

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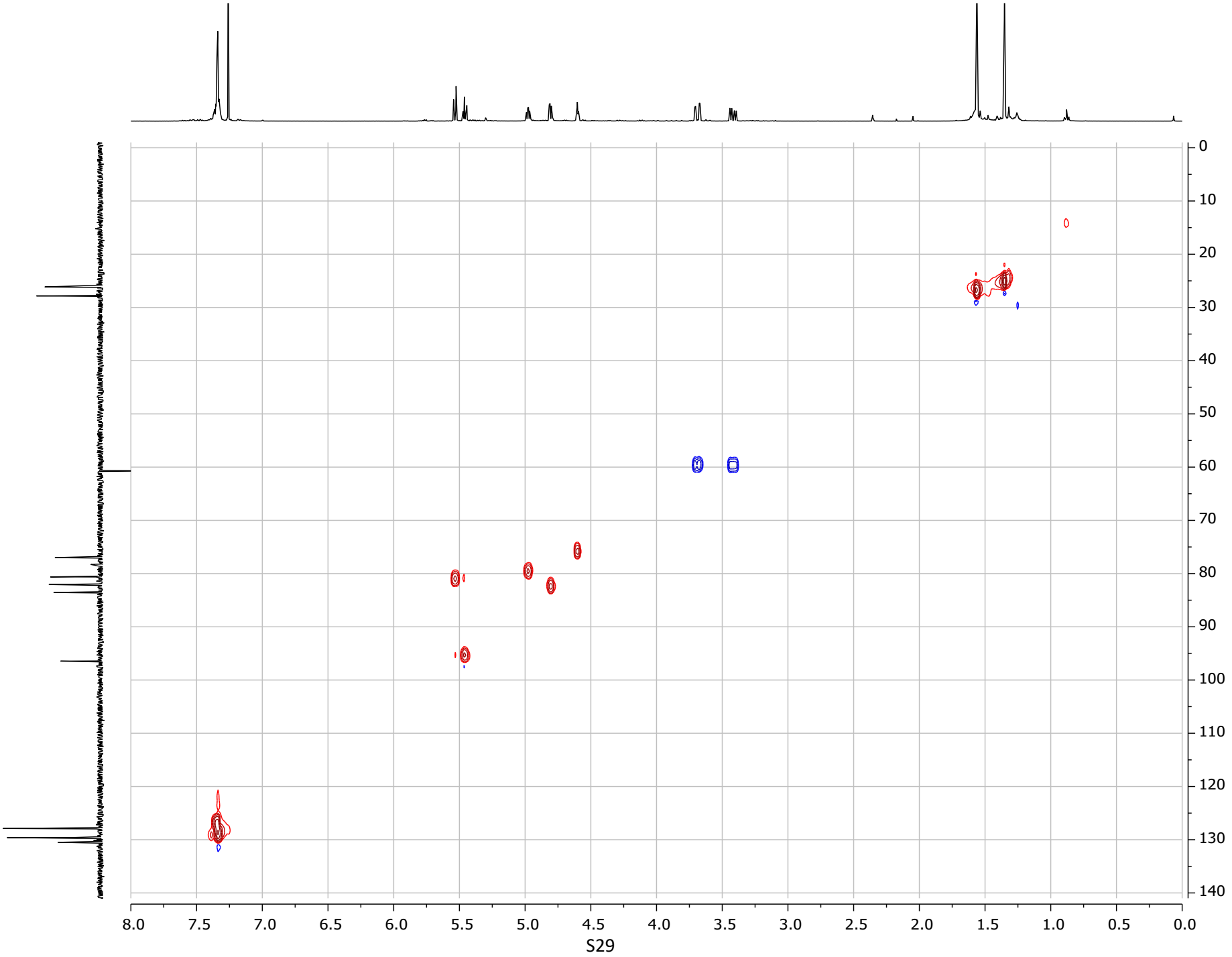
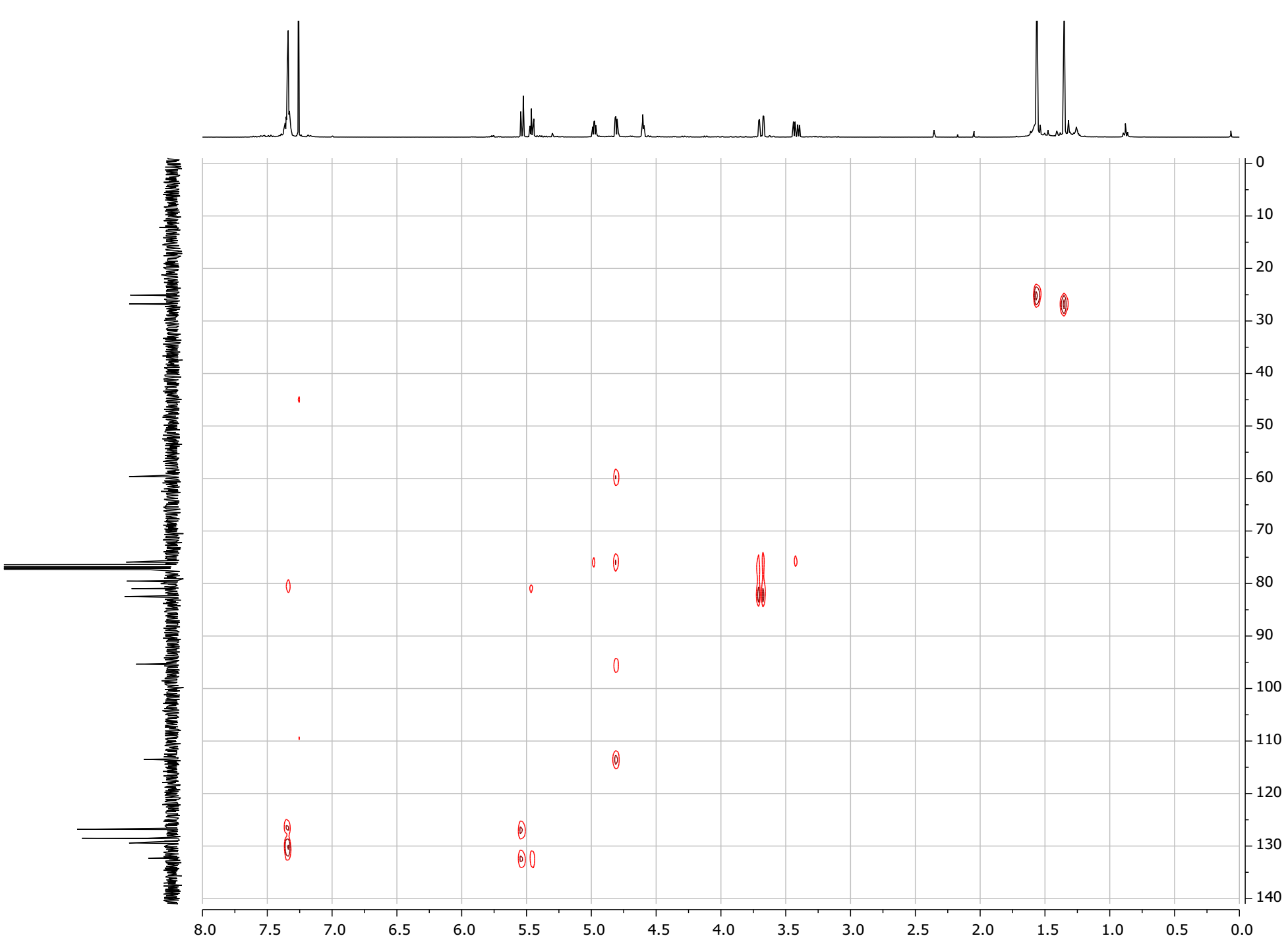
2D NMR spectra HSQC, HMBC and COSY of **3H**

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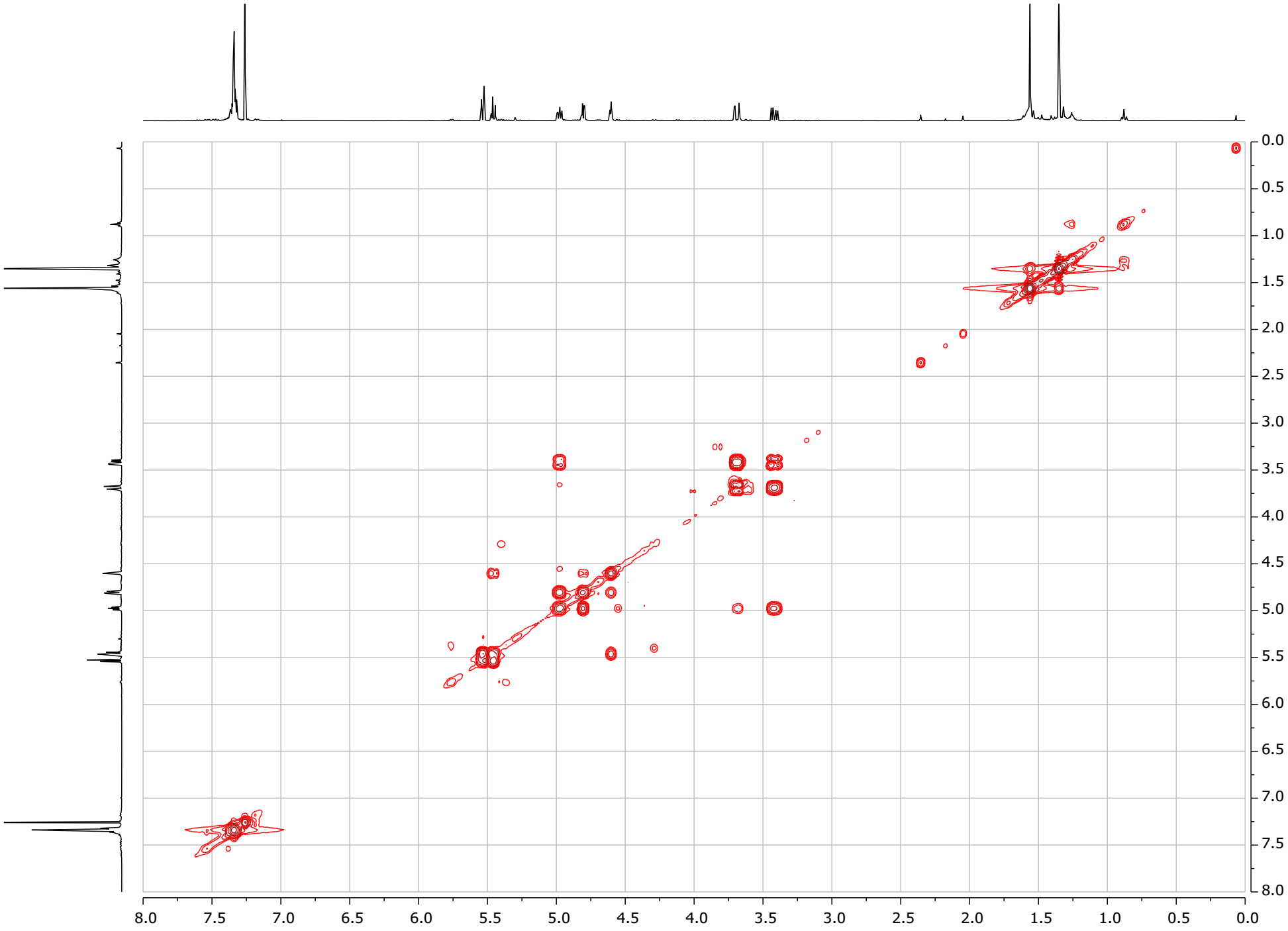
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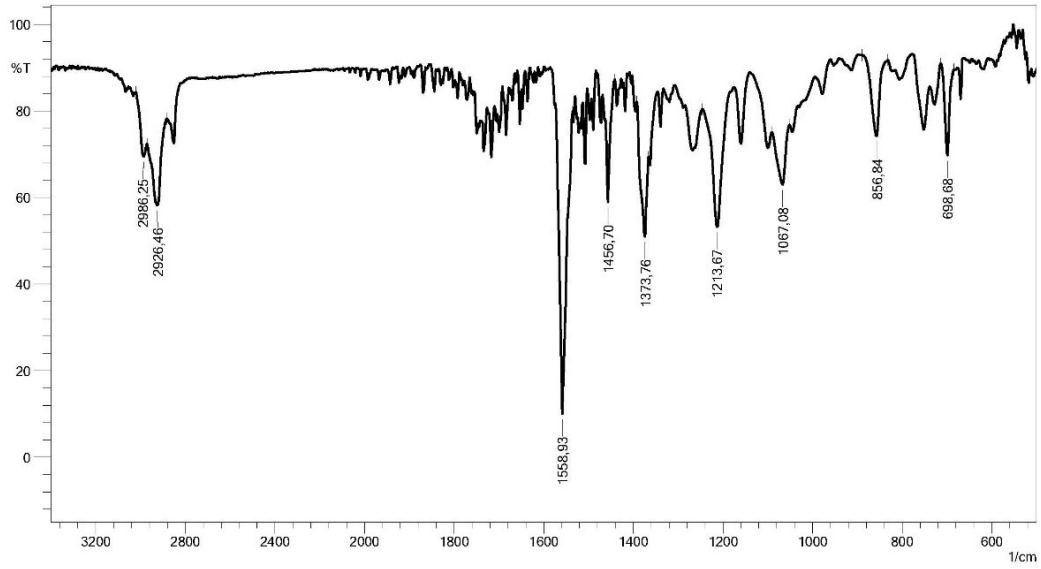
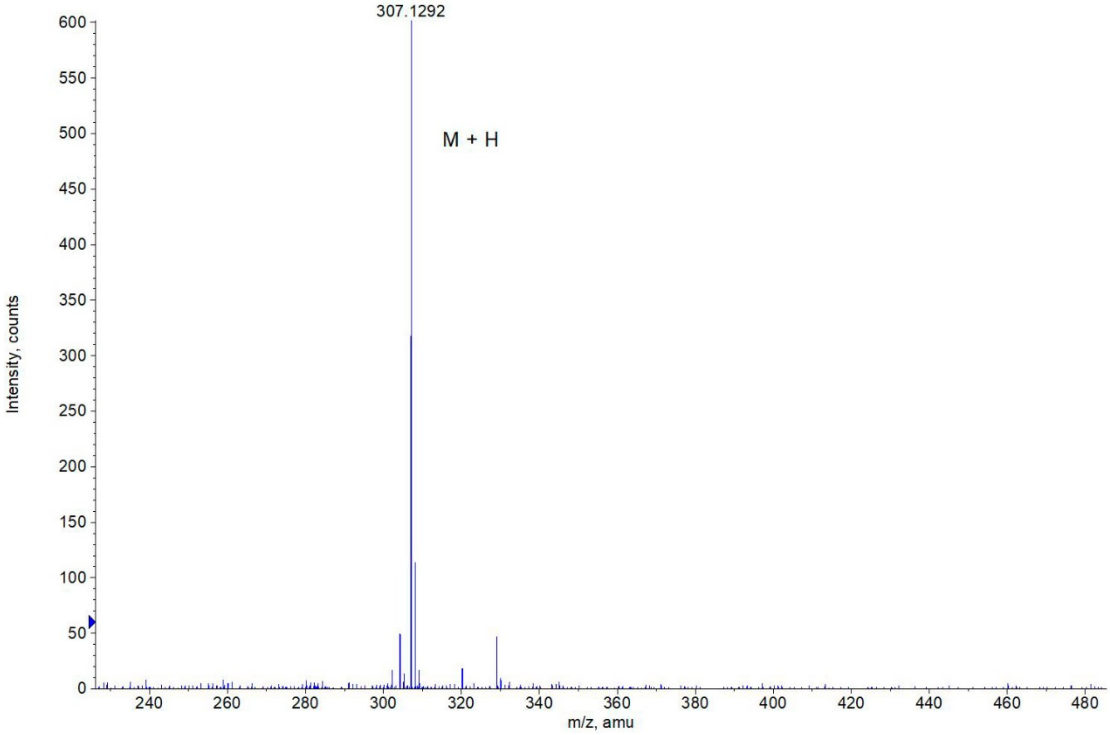
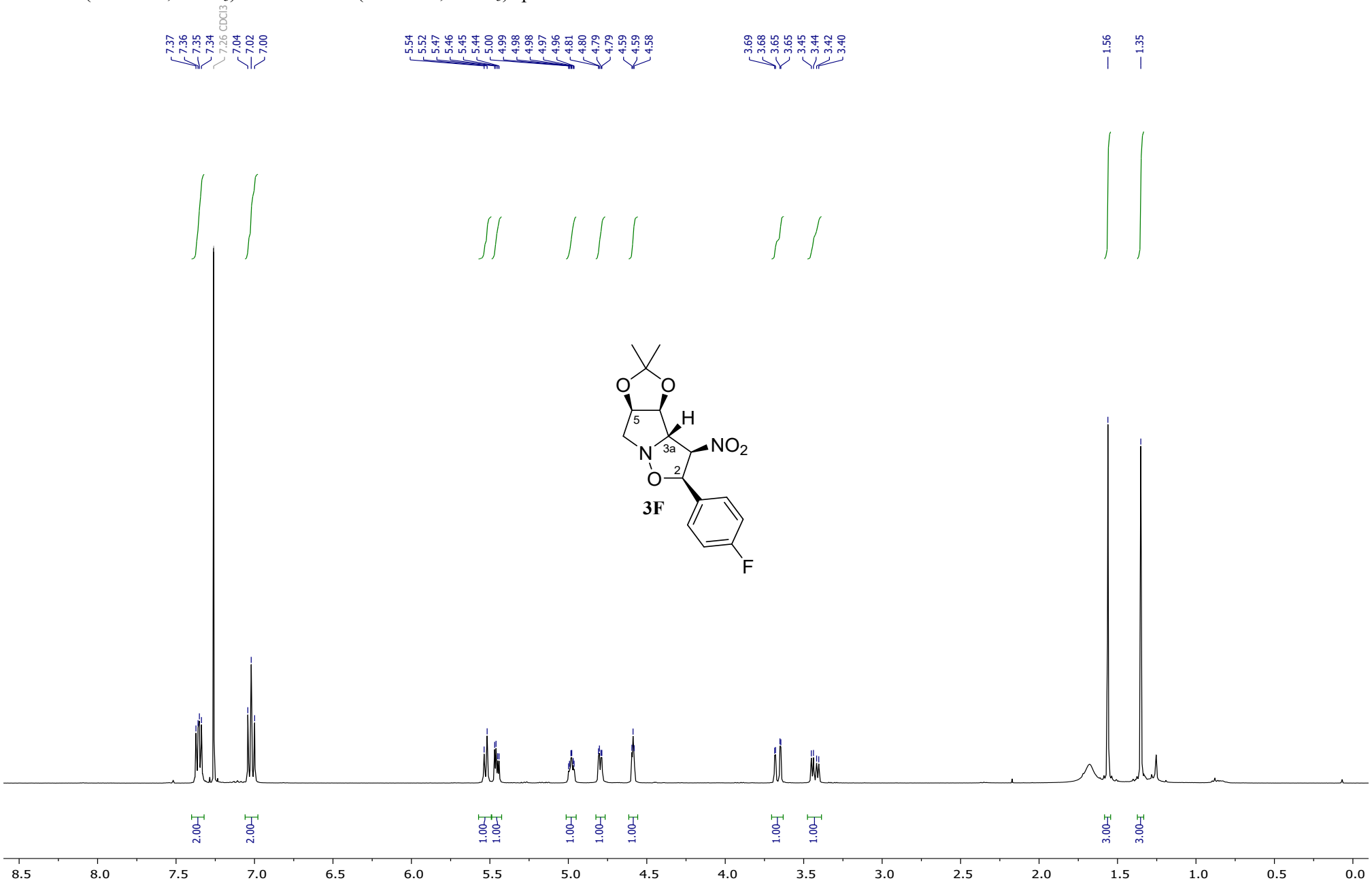
IR spectra of **3H**

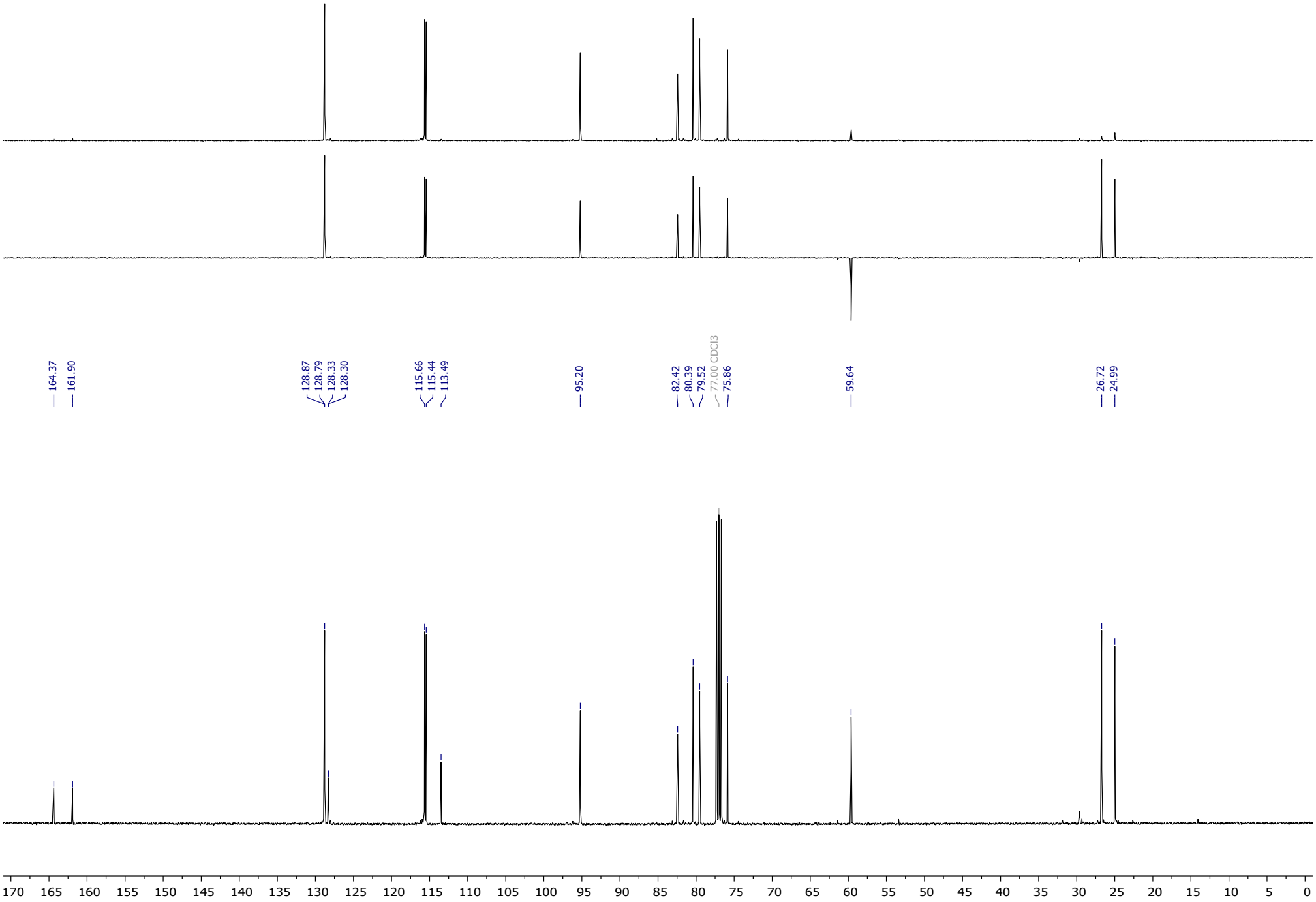


HRMS spectra of **3H**



^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3F**

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77.00 CDCl3
75.86
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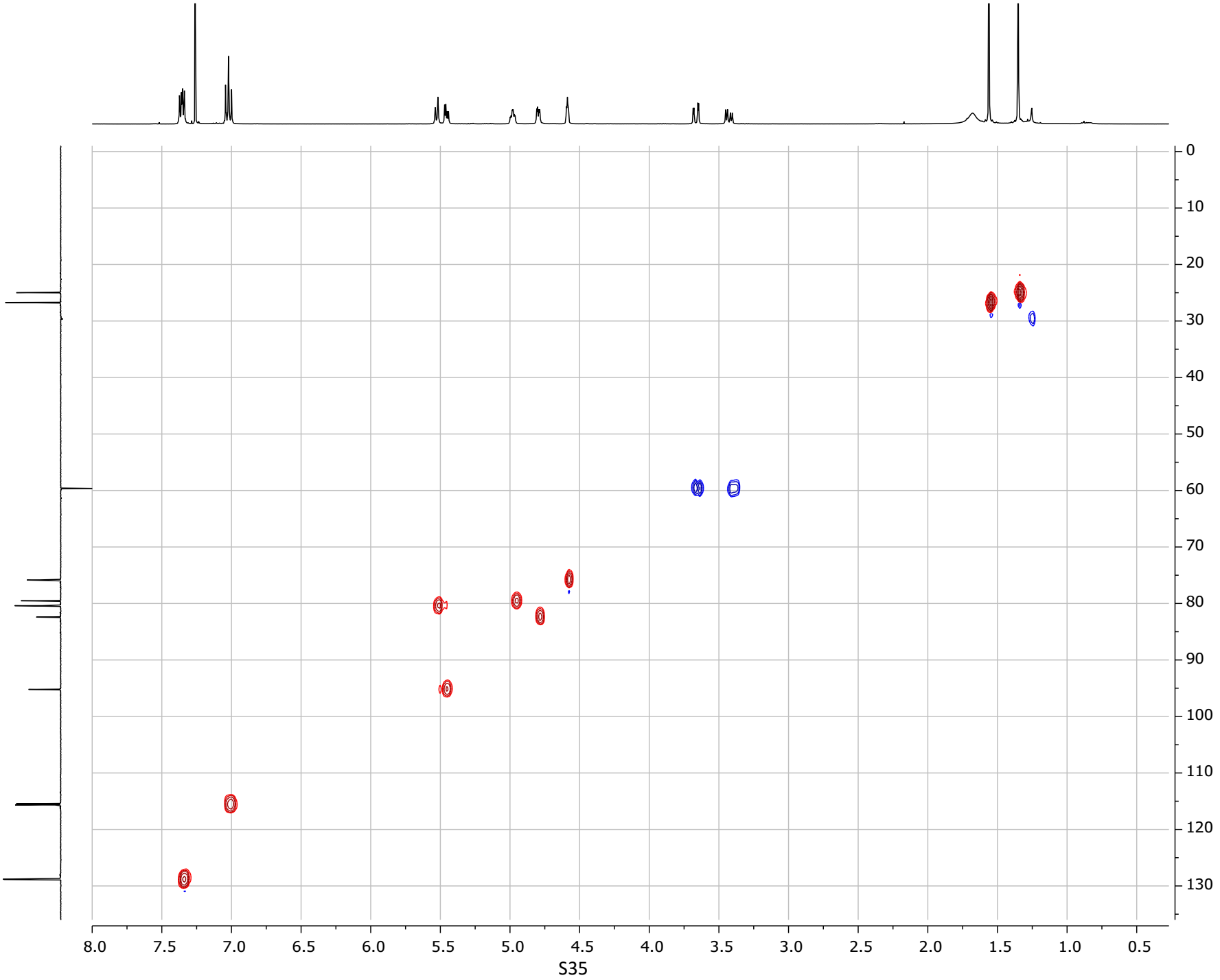
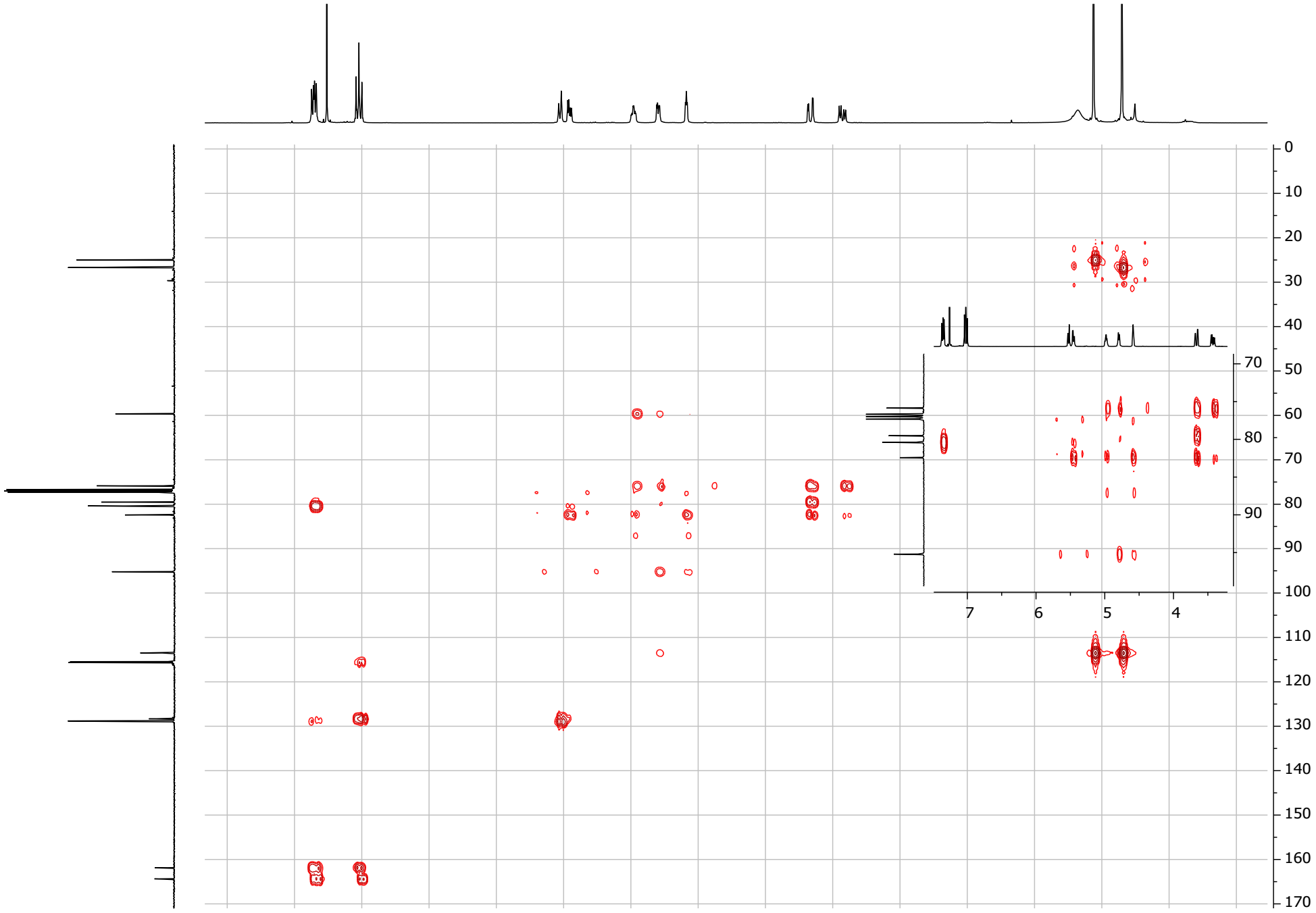
26.72
24.99
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

2D NMR spectra HSQC, HMBC and COSY of **3F**

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6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
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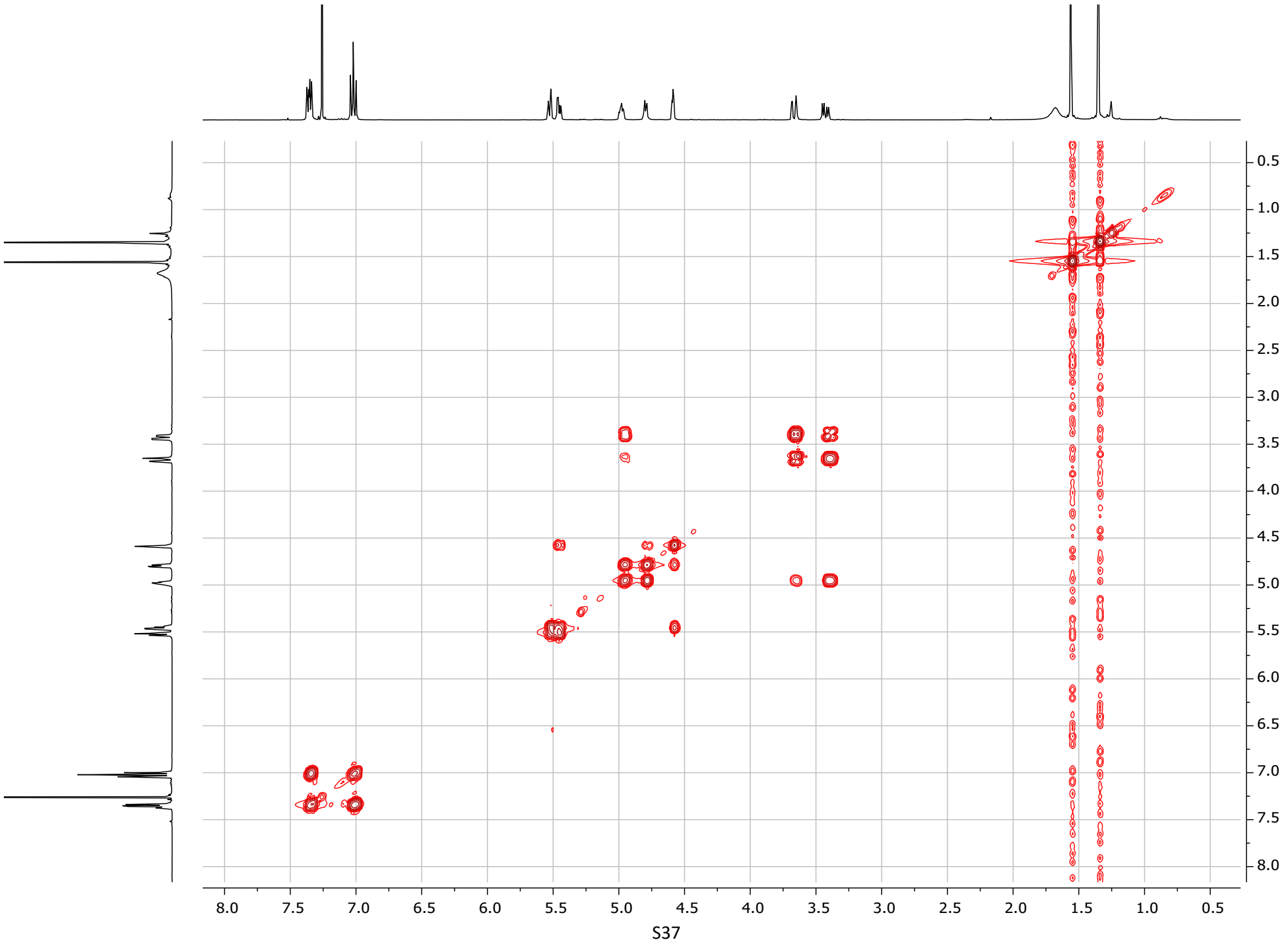
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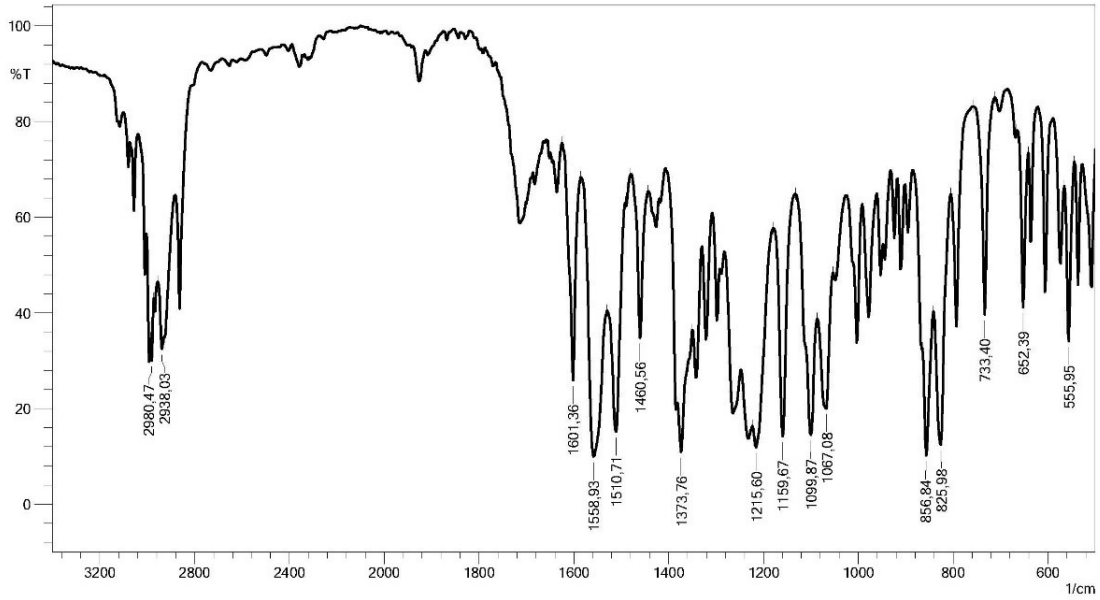
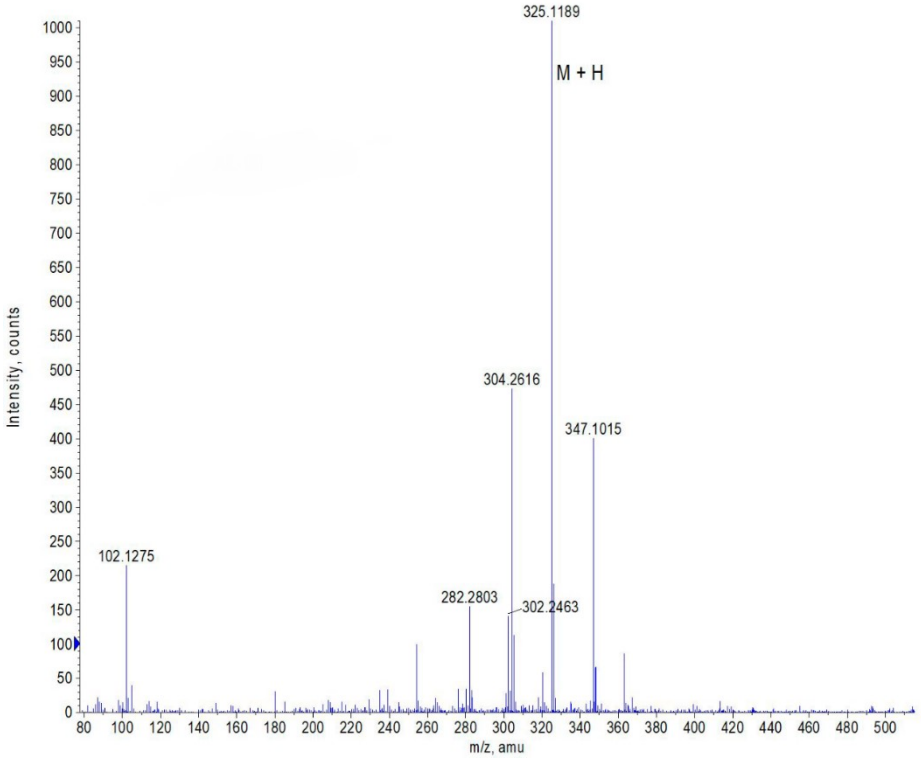
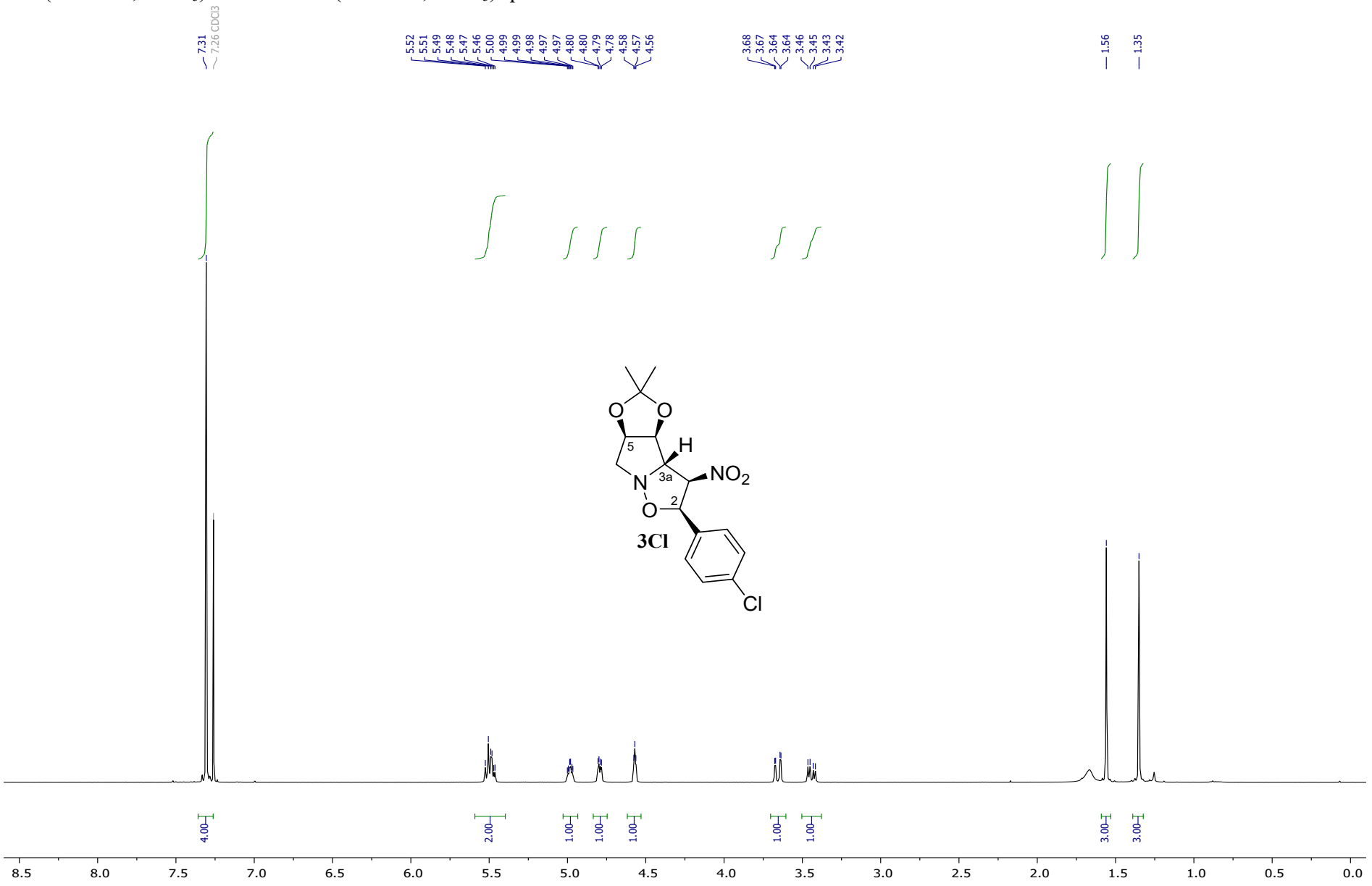
IR spectra of **3F**

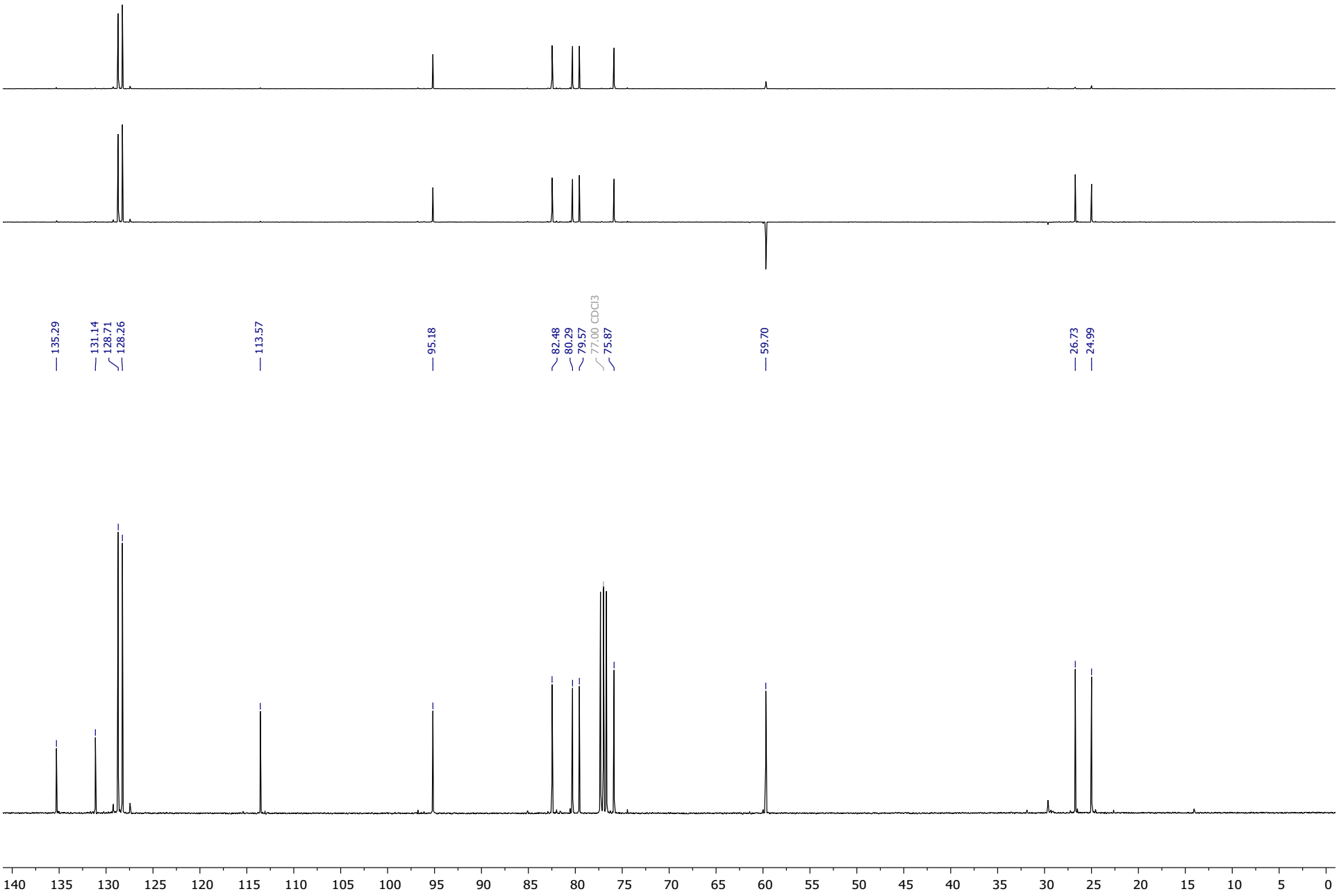


HRMS spectra of **3F**

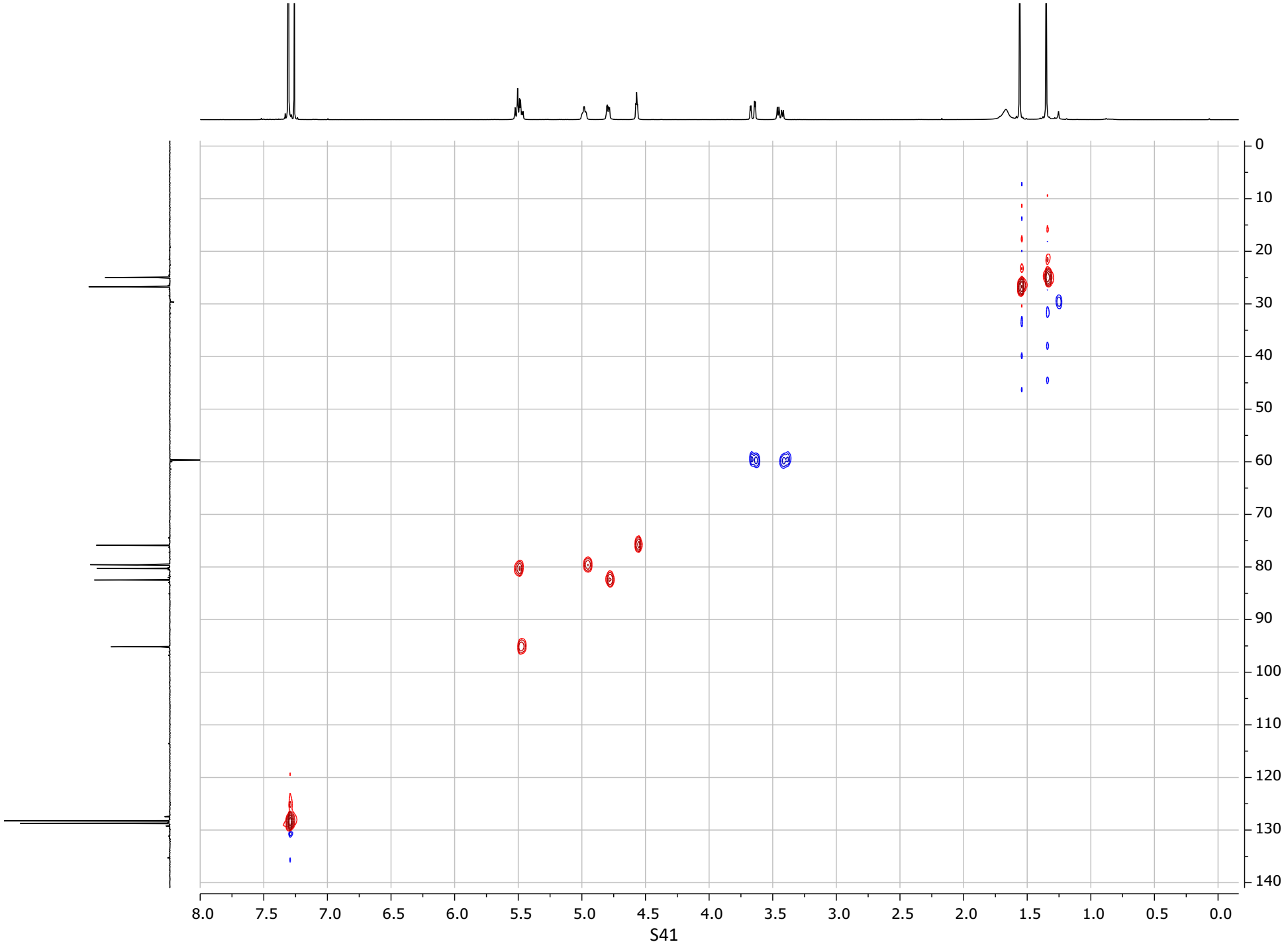


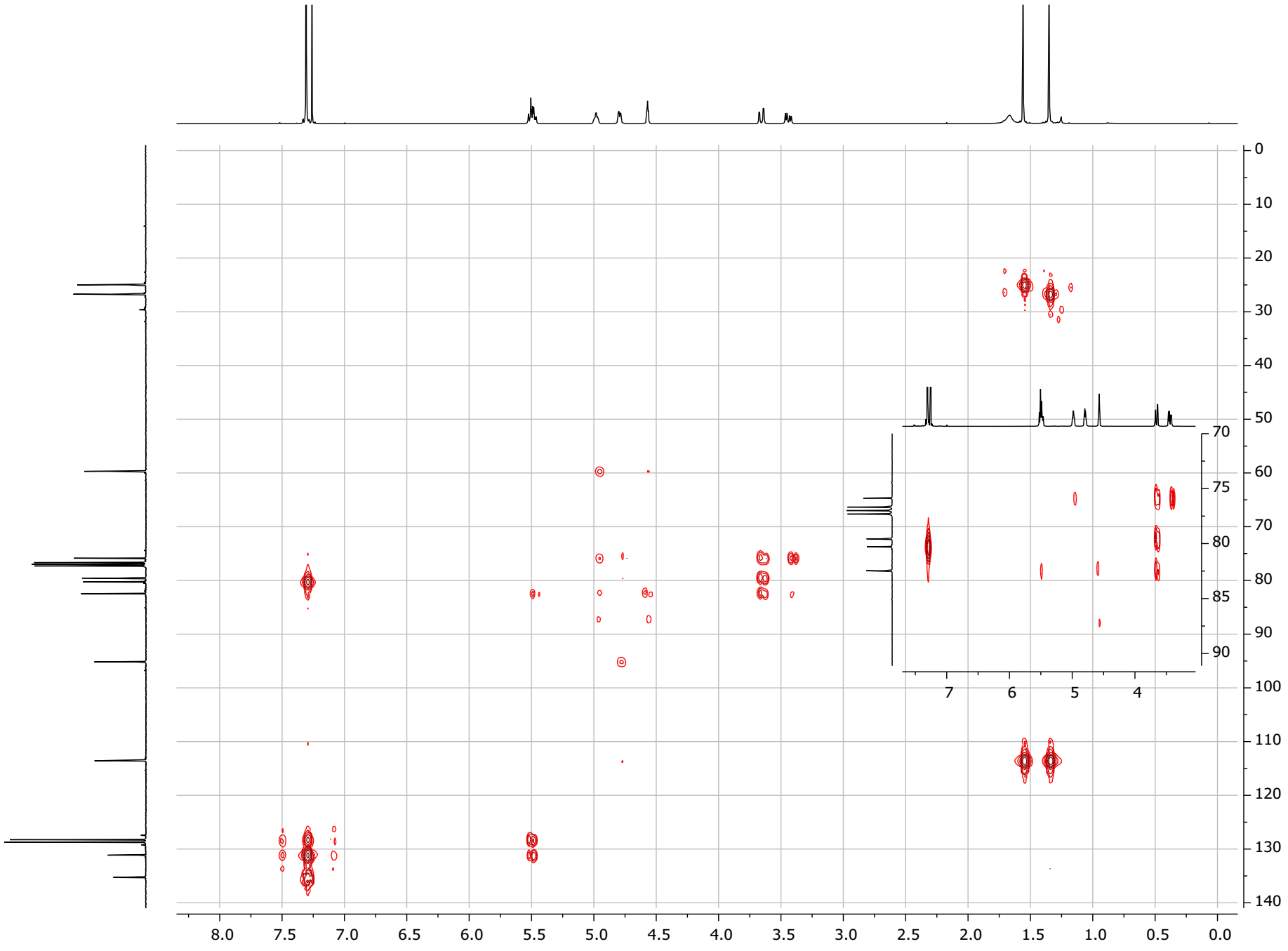
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3Cl**




135.29
131.14
128.71
128.26
113.57
95.18
82.48
80.29
79.57
77.00 CDCl3
75.87
59.70
26.73
24.99
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

2D NMR spectra HSQC, HMBC and COSY of **3Cl**

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3.0
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2.0
1.5
1.0
0.5
0.0
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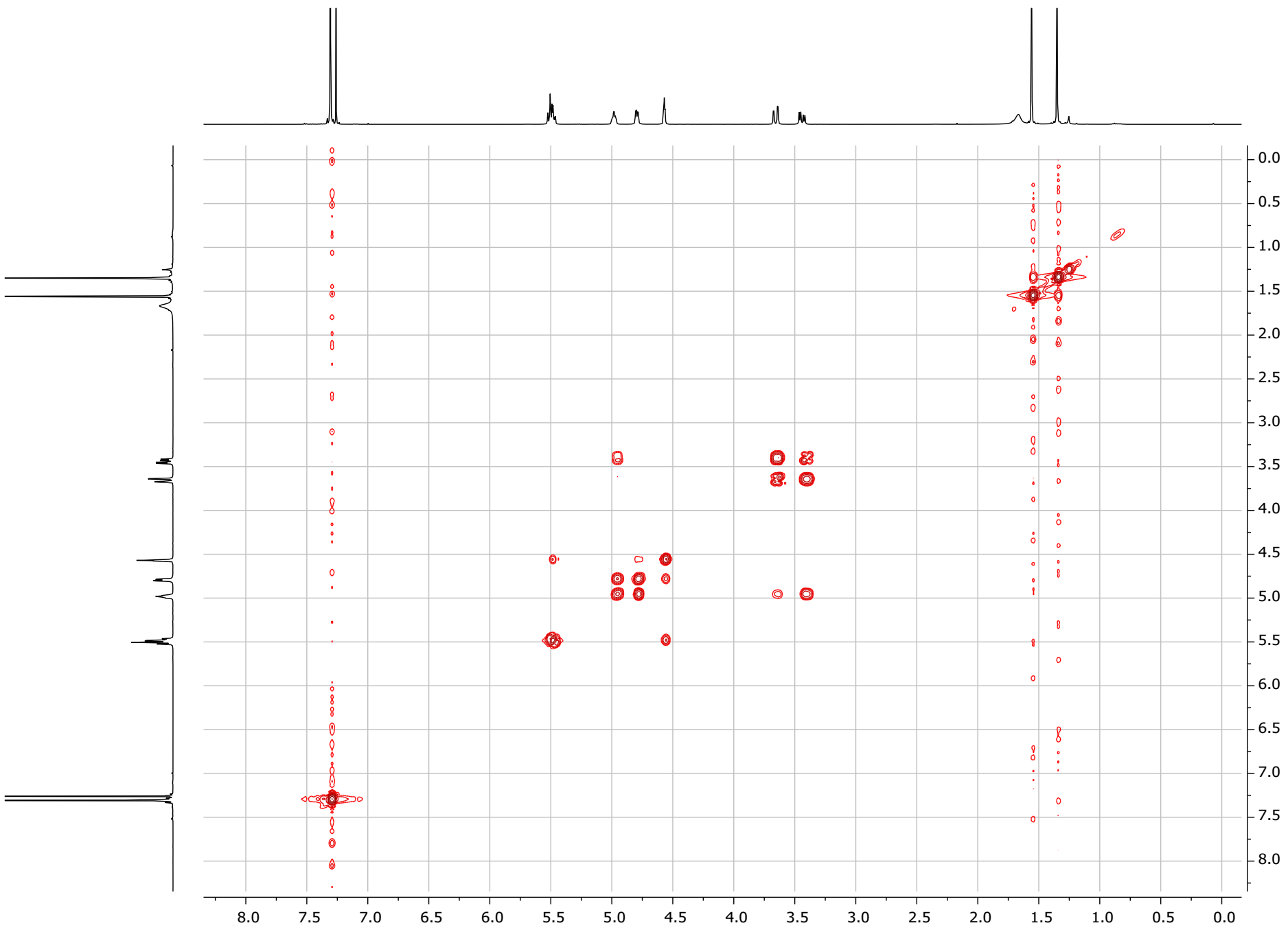
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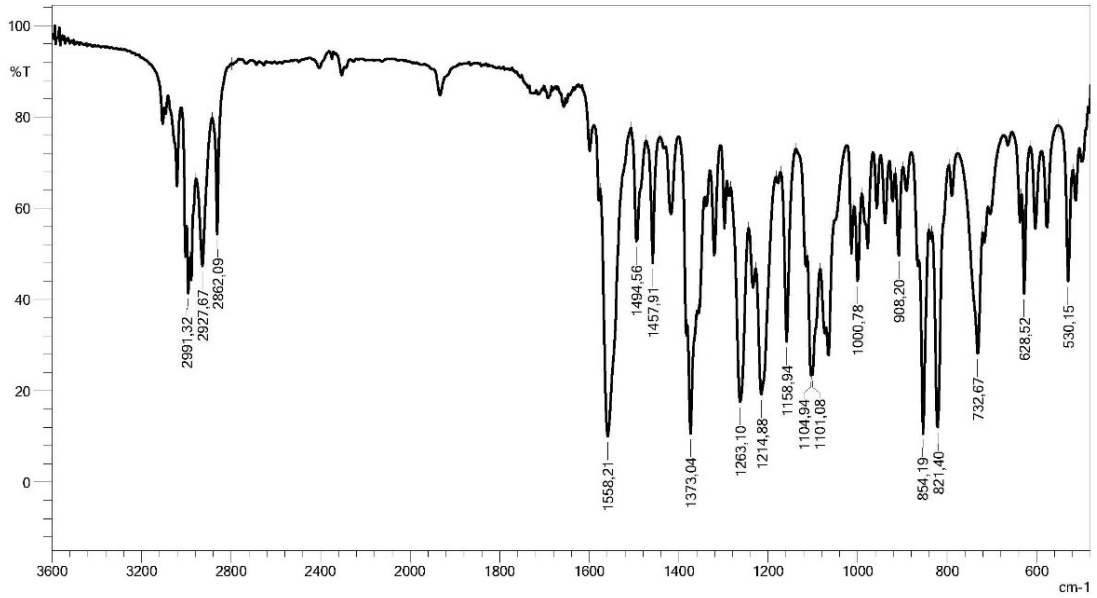
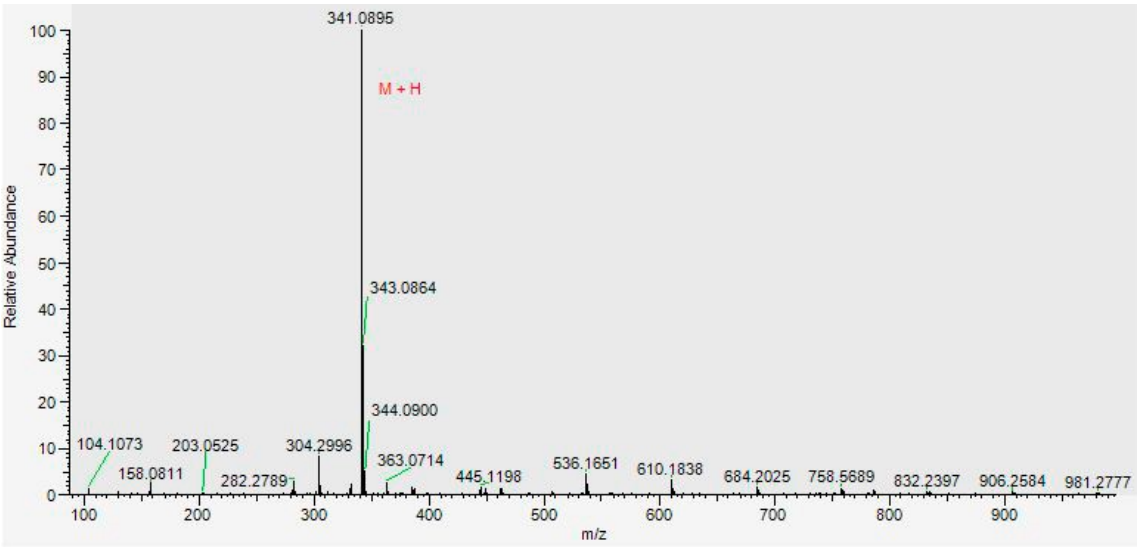
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

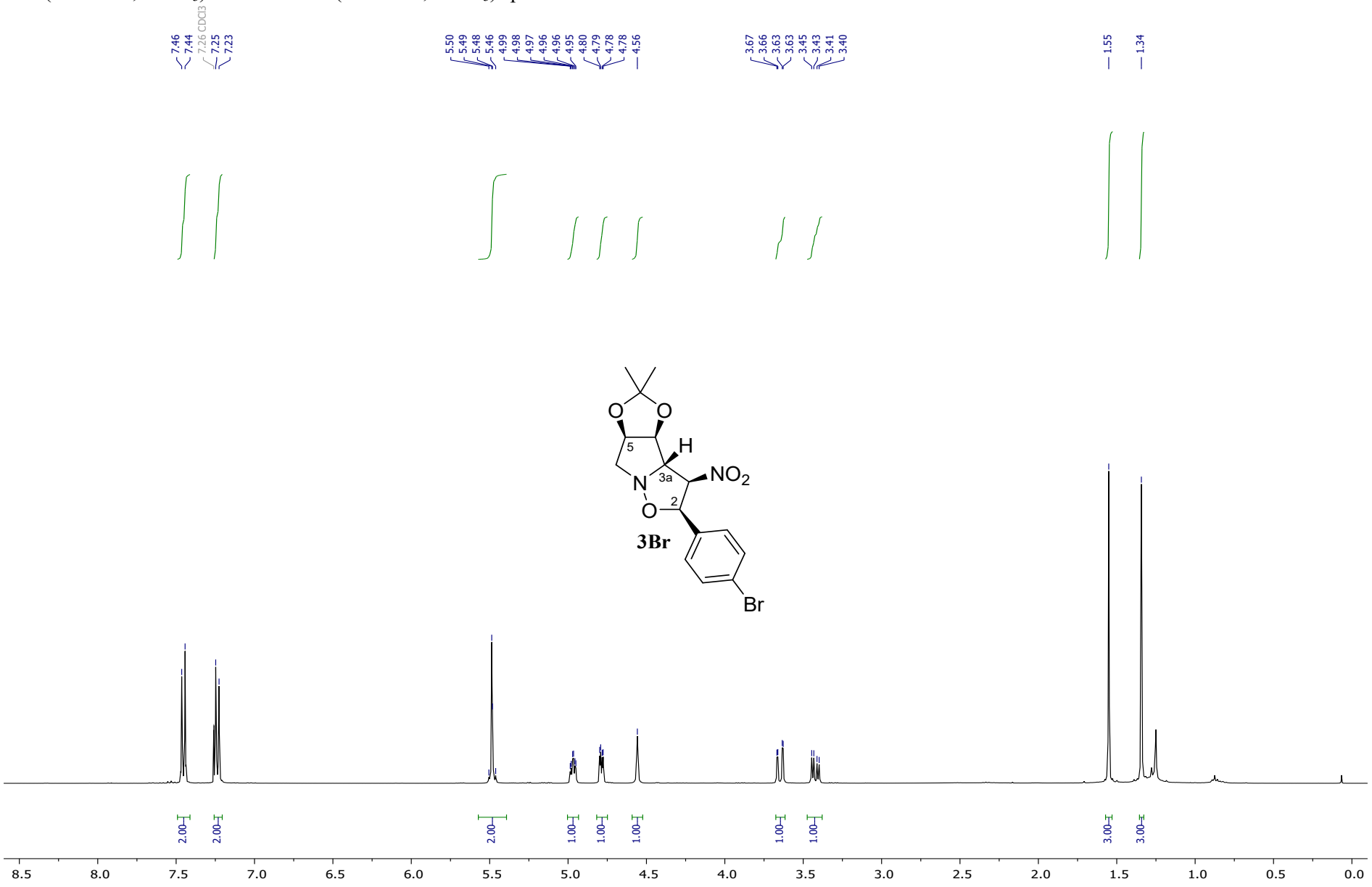
IR spectra of **3Cl**

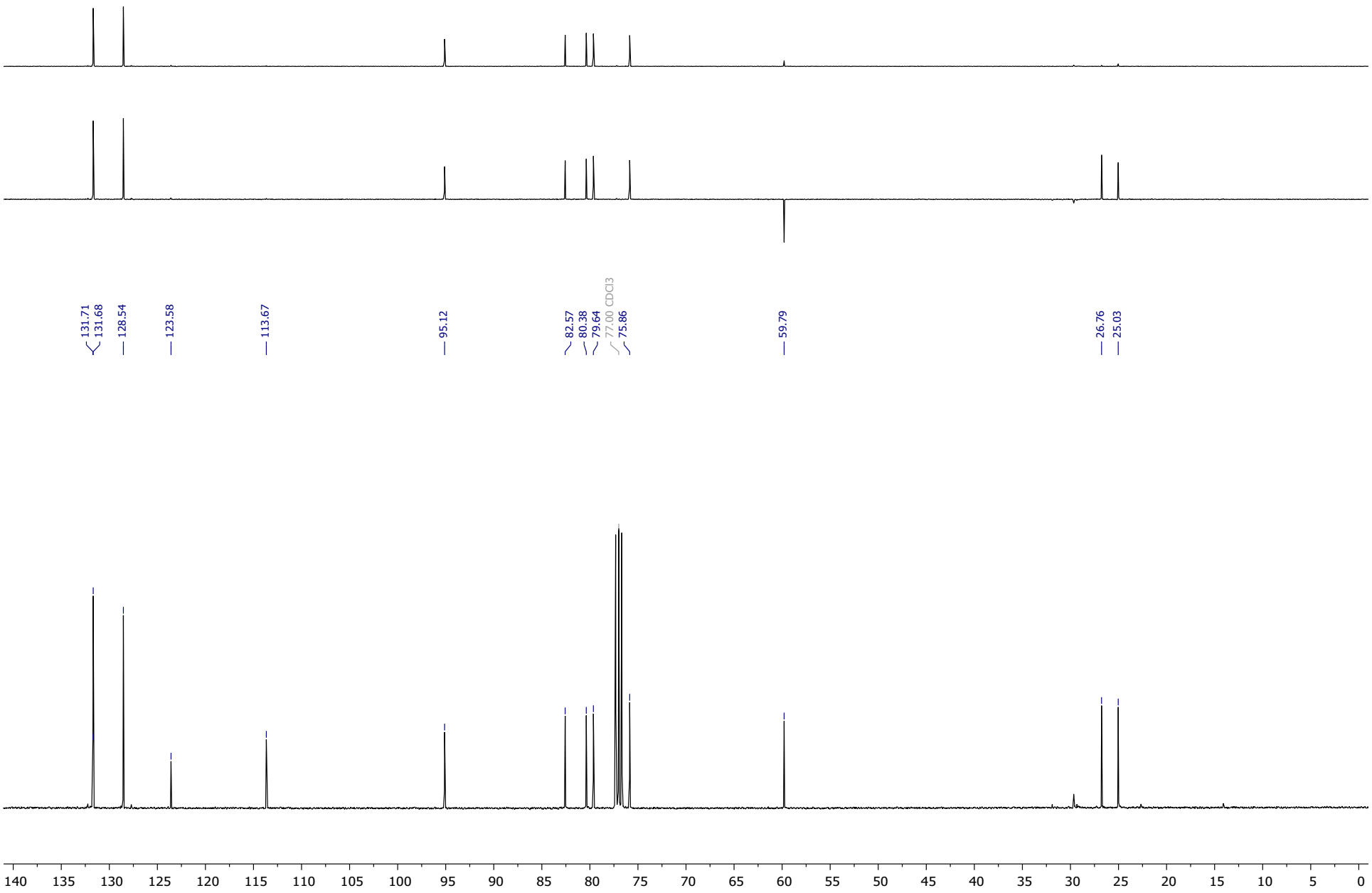


HRMS spectra of **3Cl**



^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3Br**




131.71
131.68
128.54
123.58
113.67
95.12
82.57
80.38
79.64
77.00 CDCl3
75.86
59.79
26.76
25.03
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
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45
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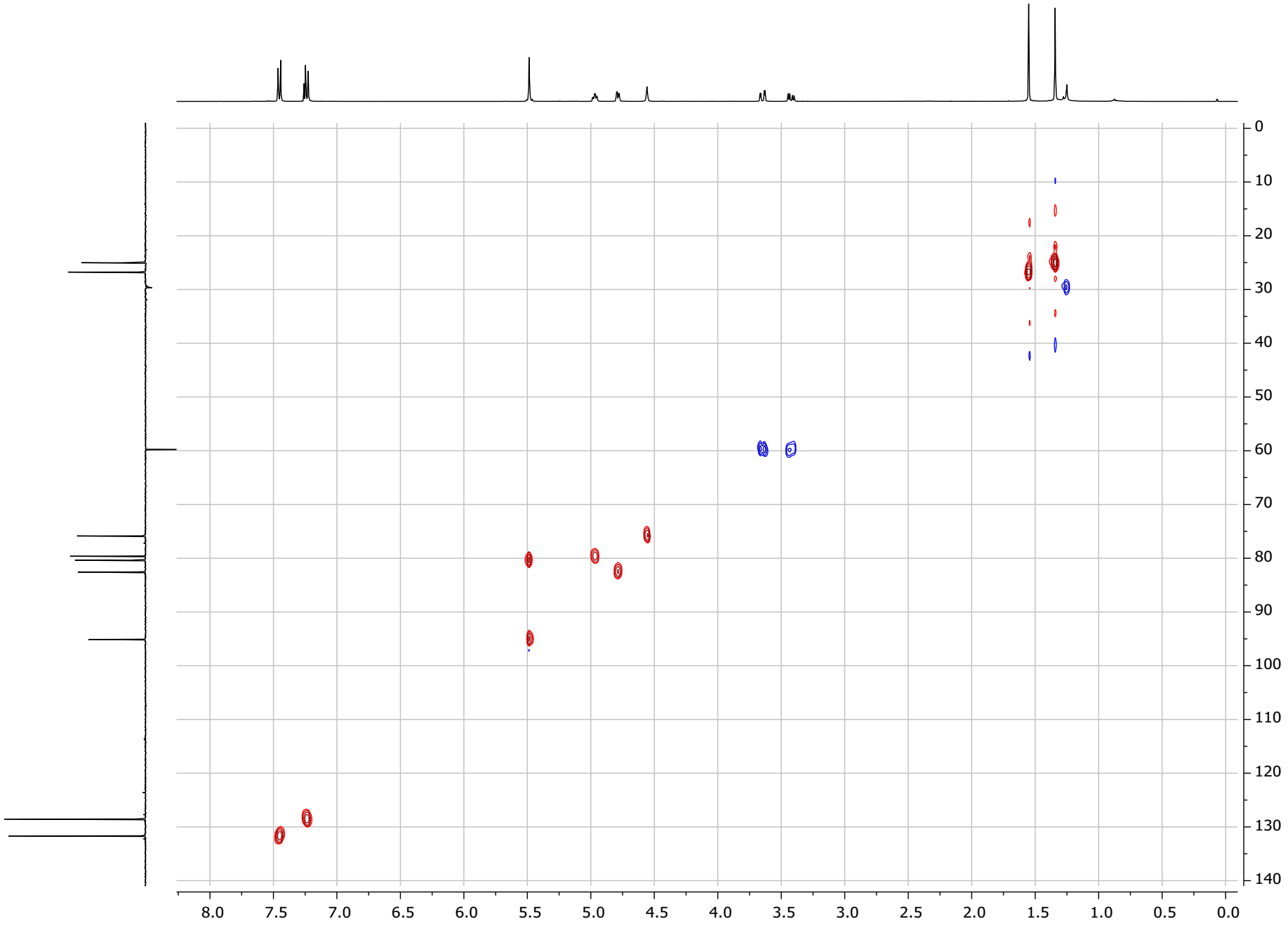
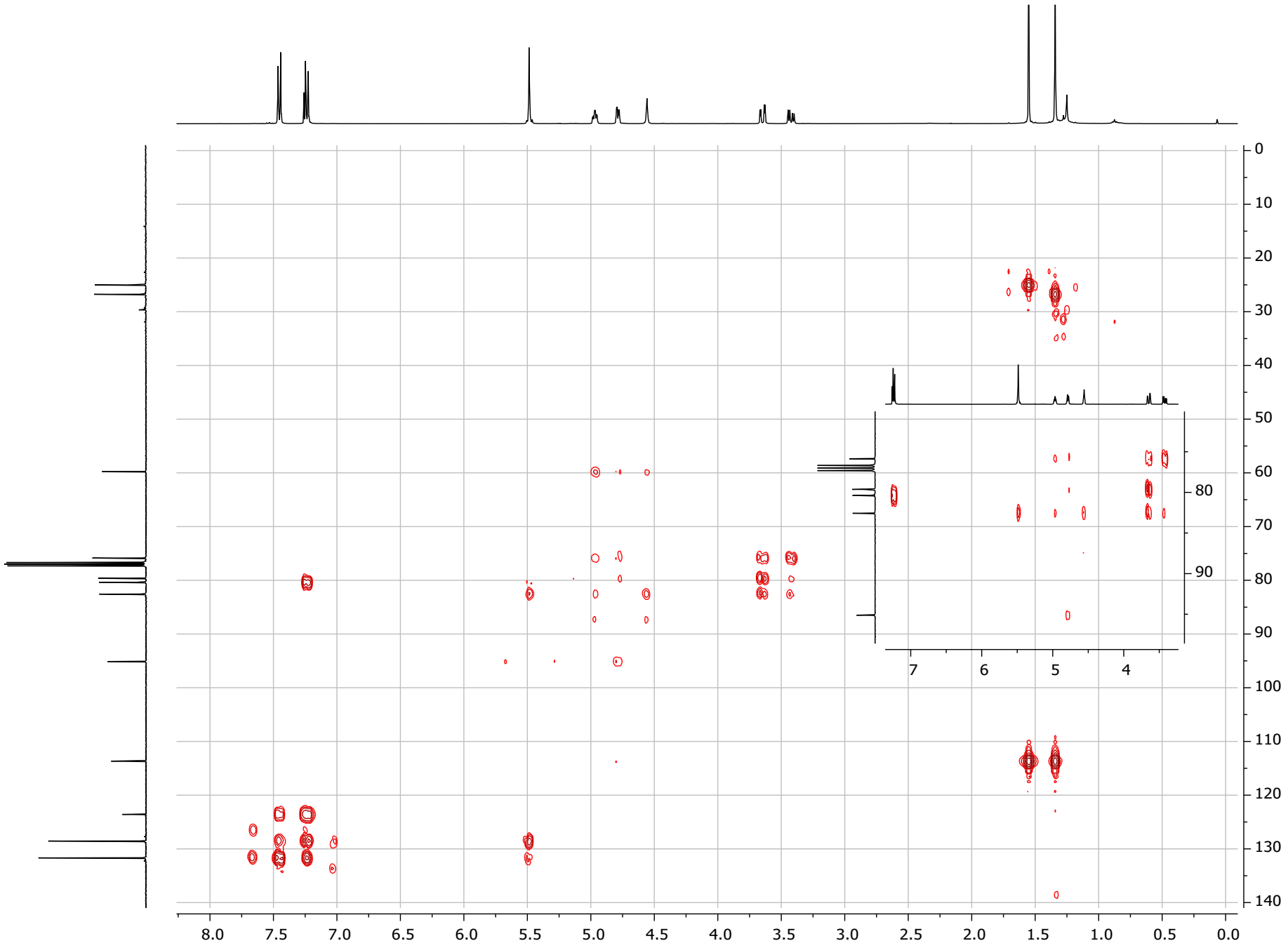
25
20
15
10
5
0

2D NMR spectra HSQC, HMBC and COSY of **3Br**




0
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20
30
40
50
60
70
80
90
100
110
120
130
140
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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2.5
2.0
1.5
1.0
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0.0
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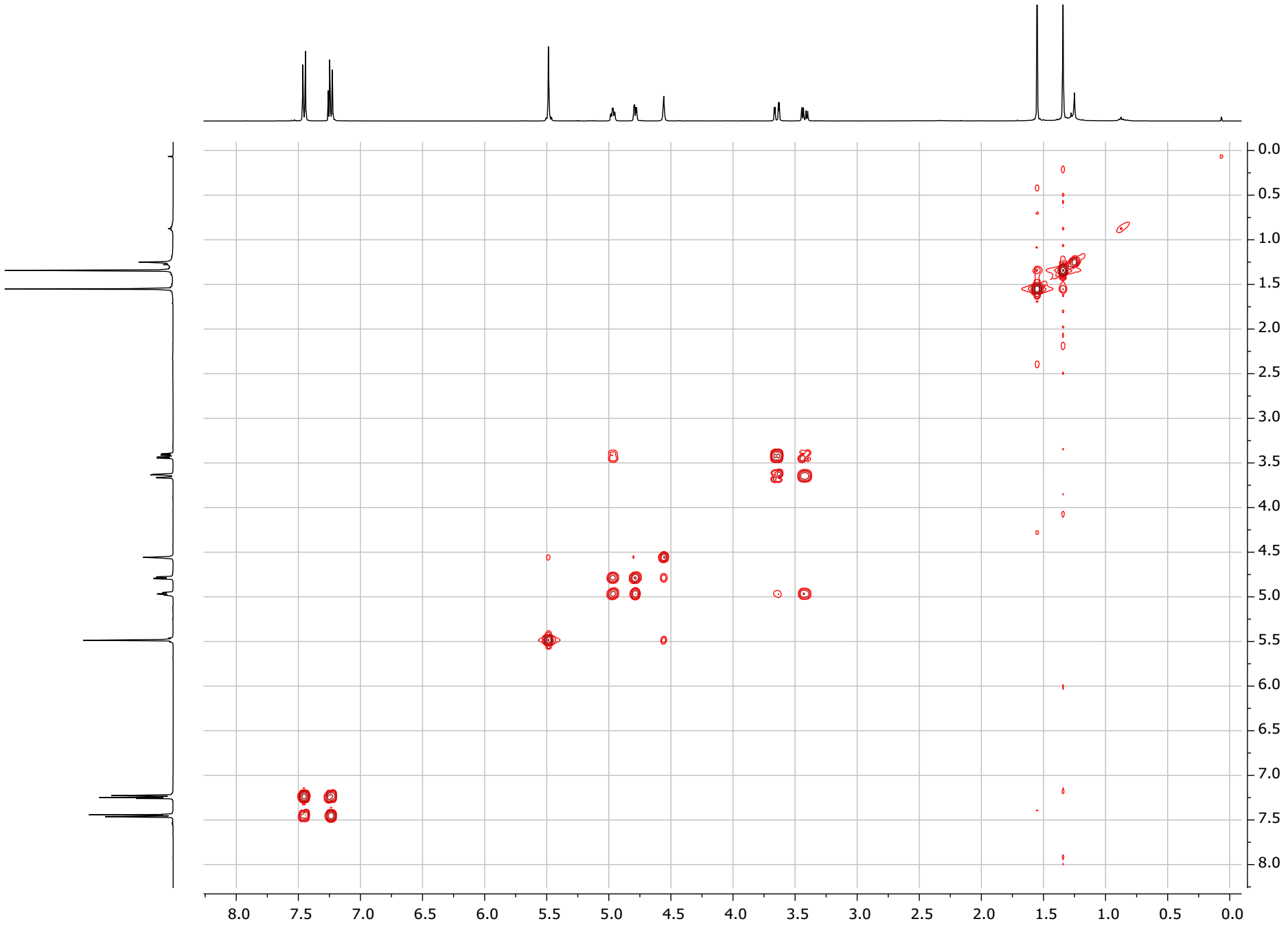
90
7
6
5
4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7.0
6.5
6.0
5.5
5.0
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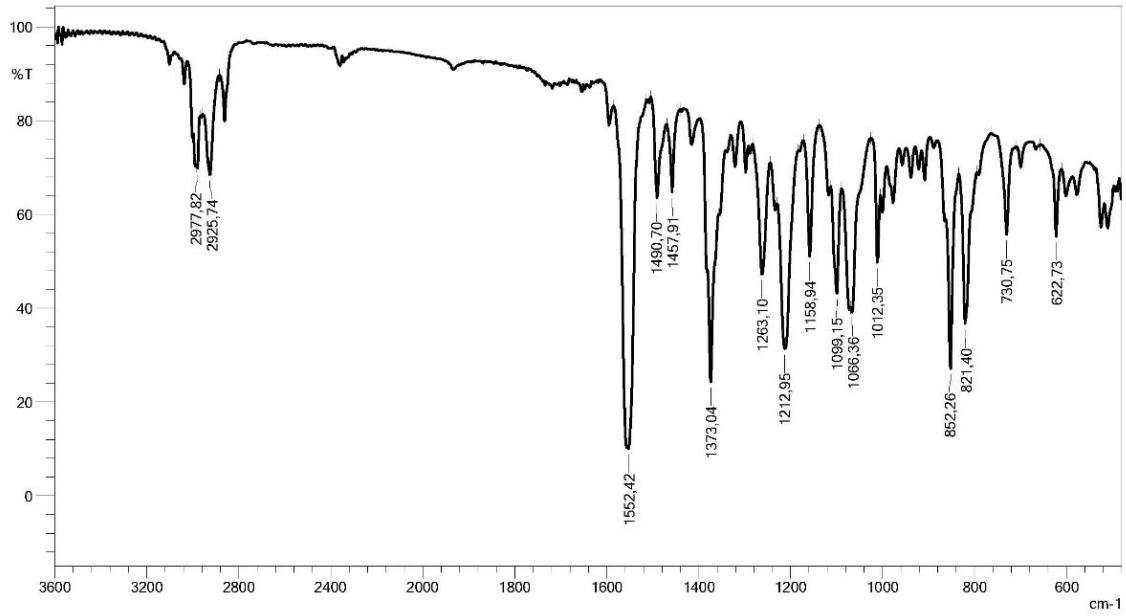
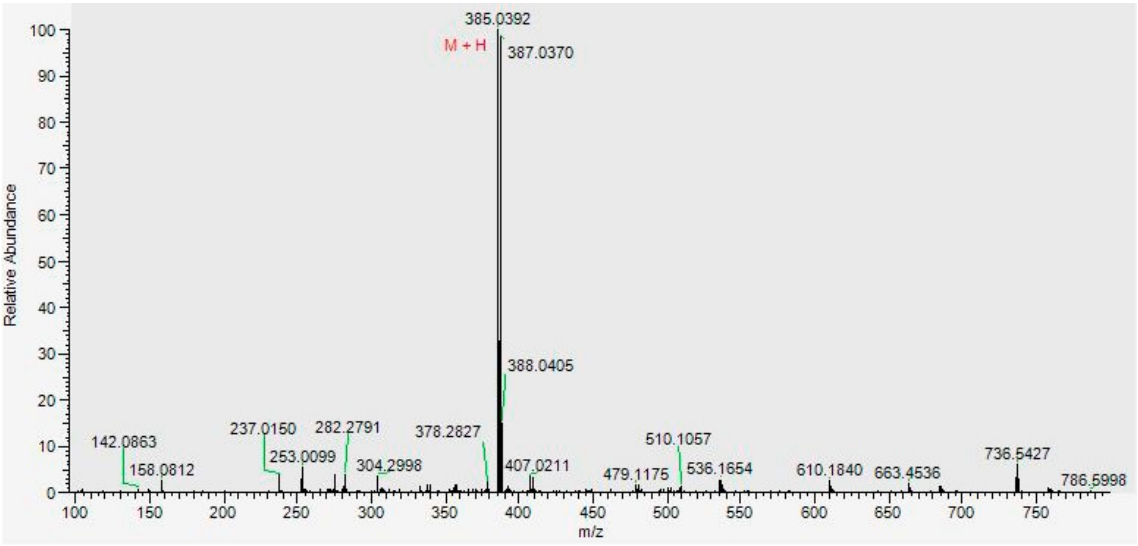
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

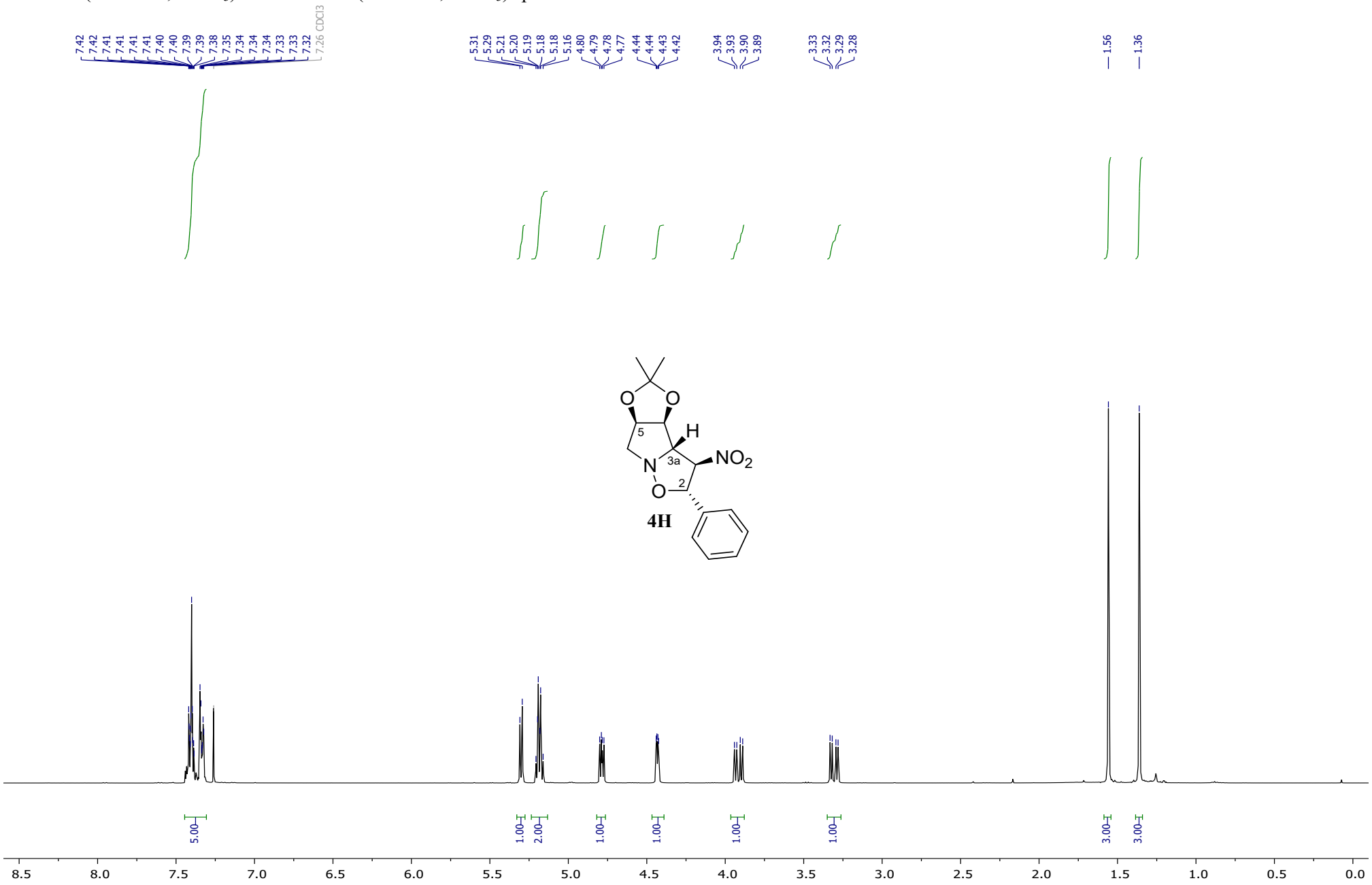
IR spectra of **3Br**

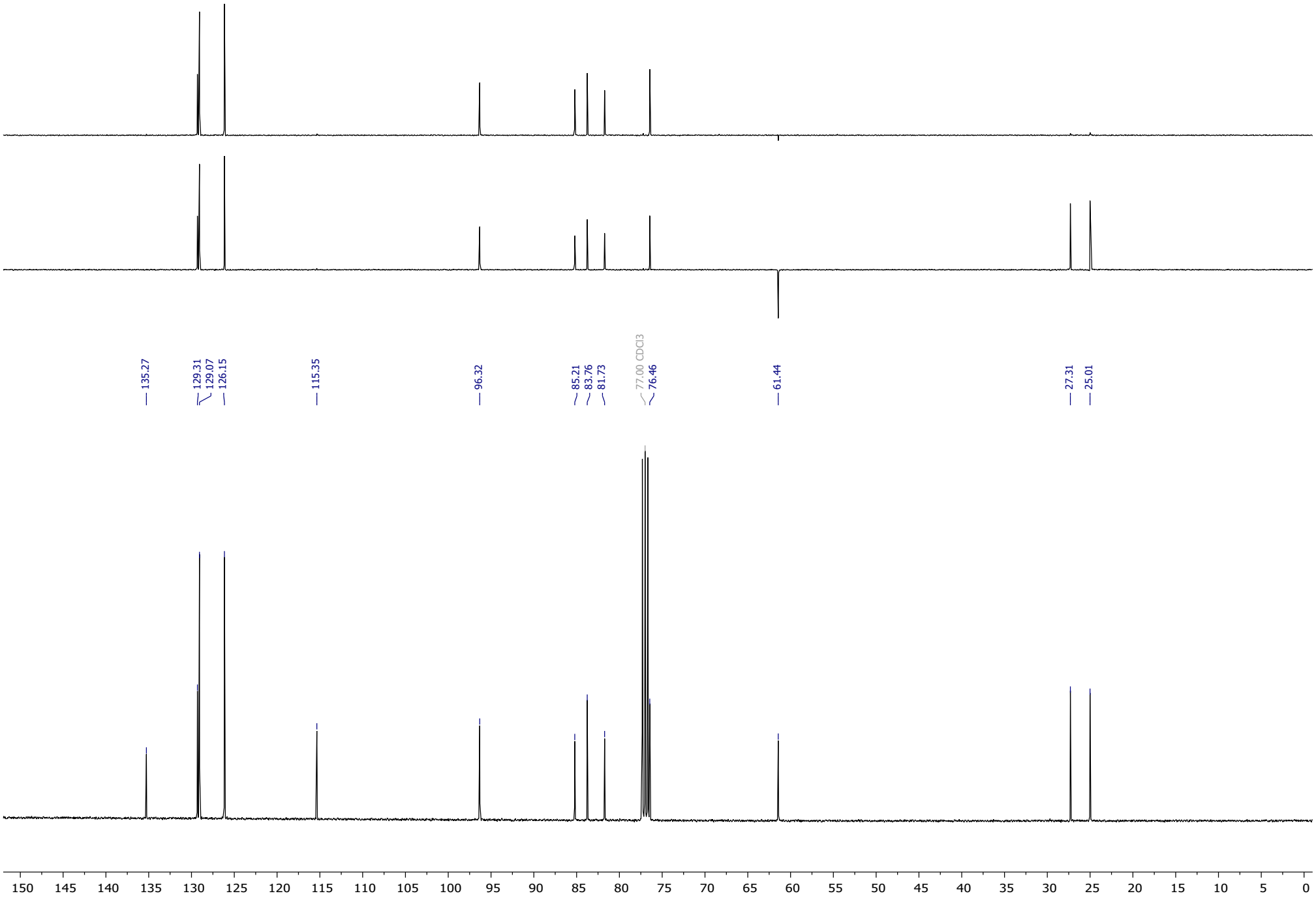


HRMS spectra of **3Br**

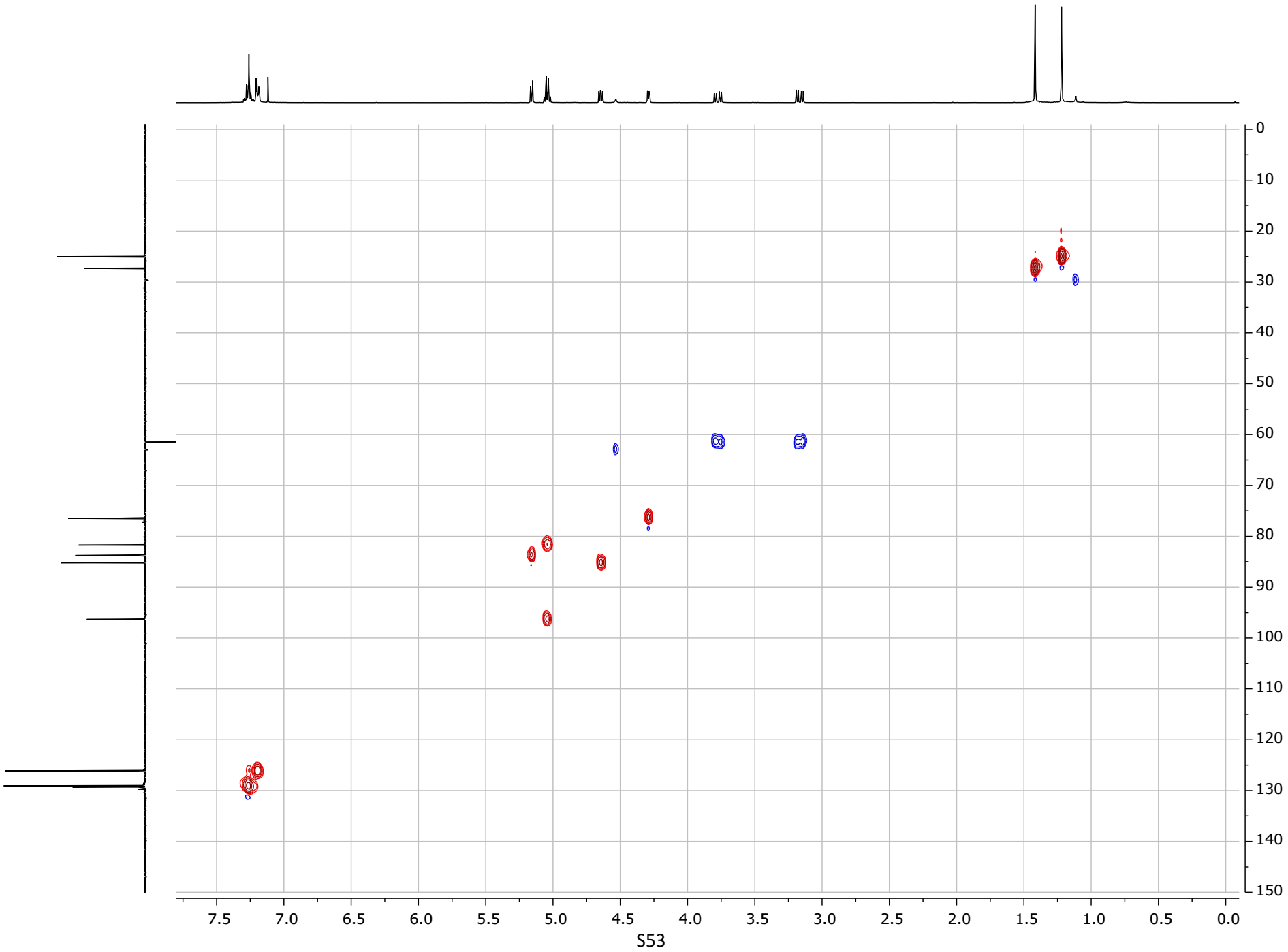


^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **4H**




135.27
129.31
129.07
126.15
115.35
96.32
85.21
83.76
81.73
77.00 CDCl3
76.46
61.44
27.31
25.01
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

2D NMR spectra HSQC, HMBC and COSY of **4H**




0
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20
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40
50
60
70
80
90
100
110
120
130
140
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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2.0
1.5
1.0
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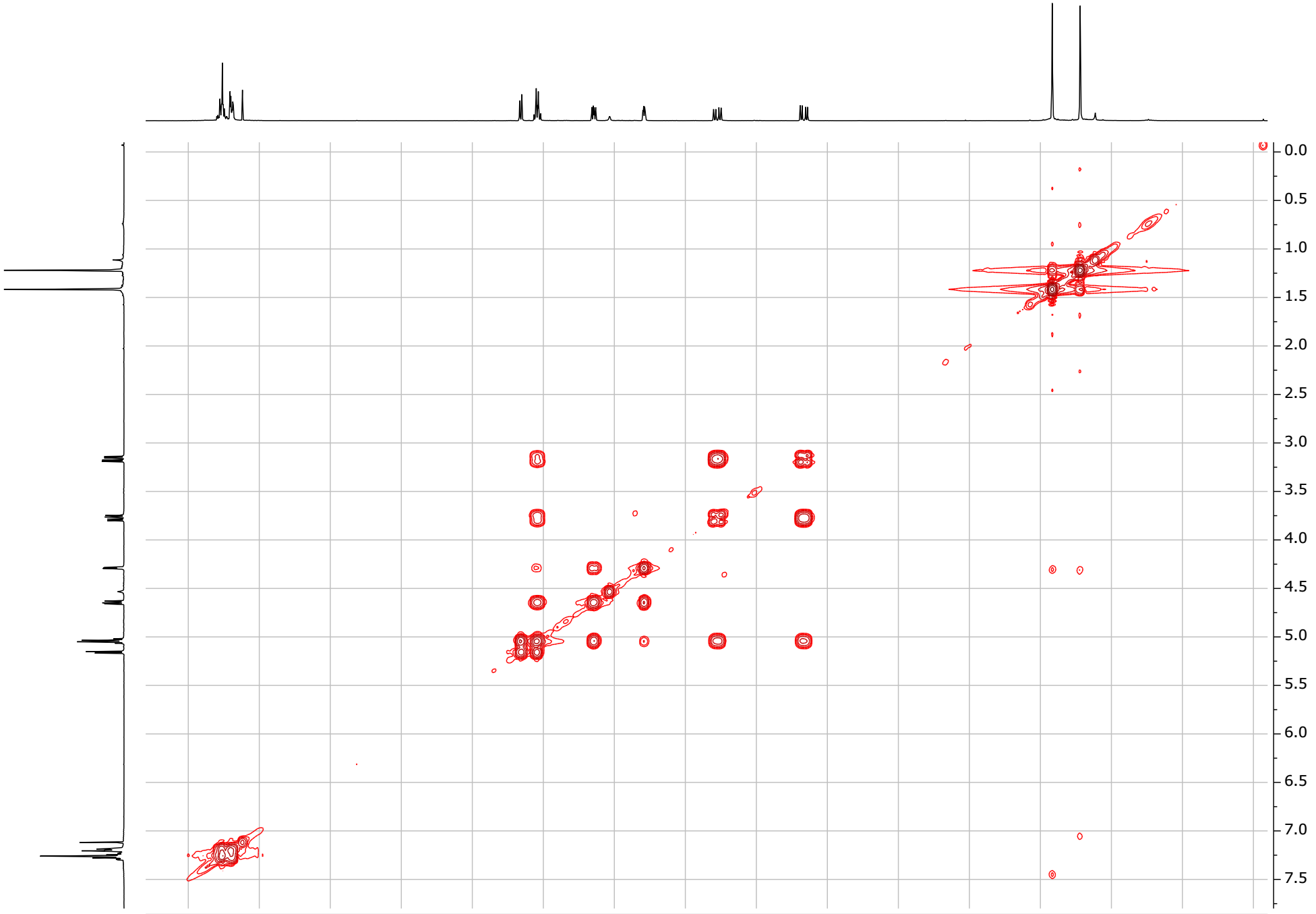
0.0


7.5
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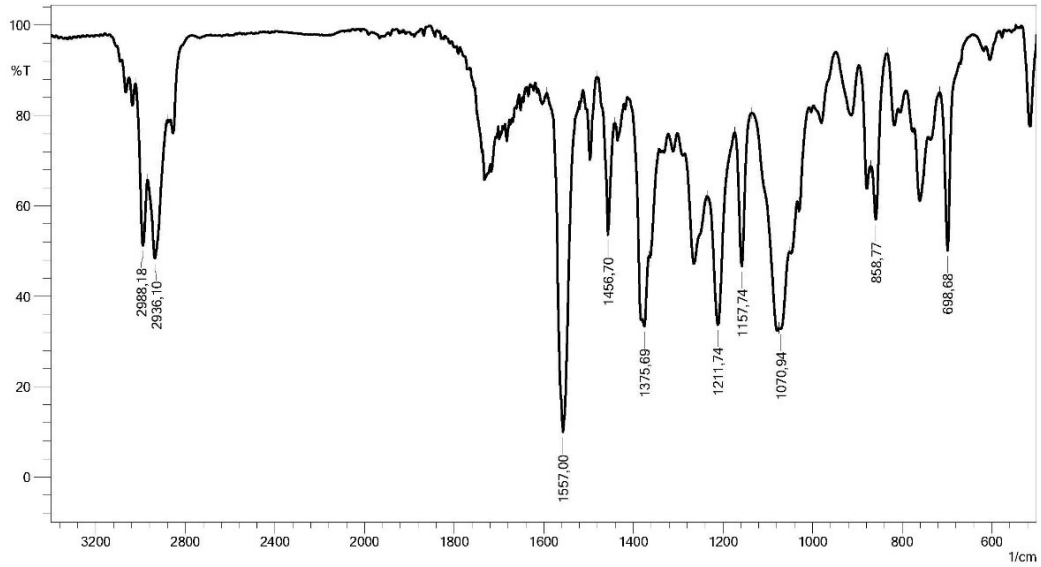
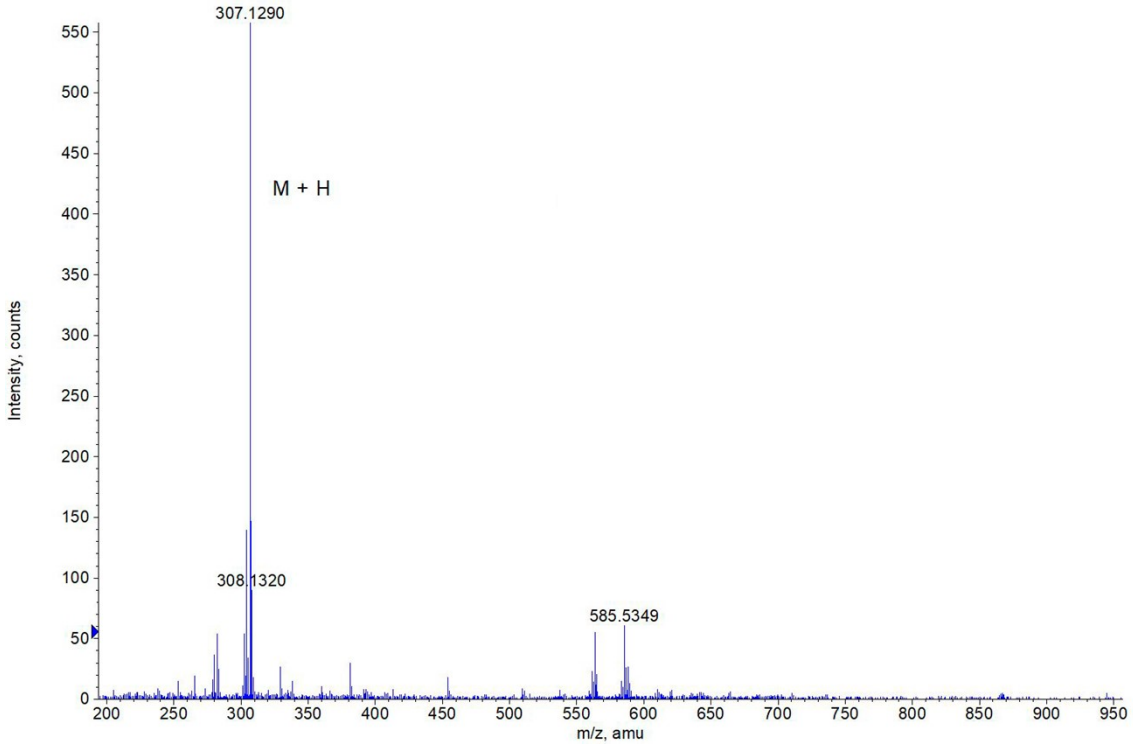
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

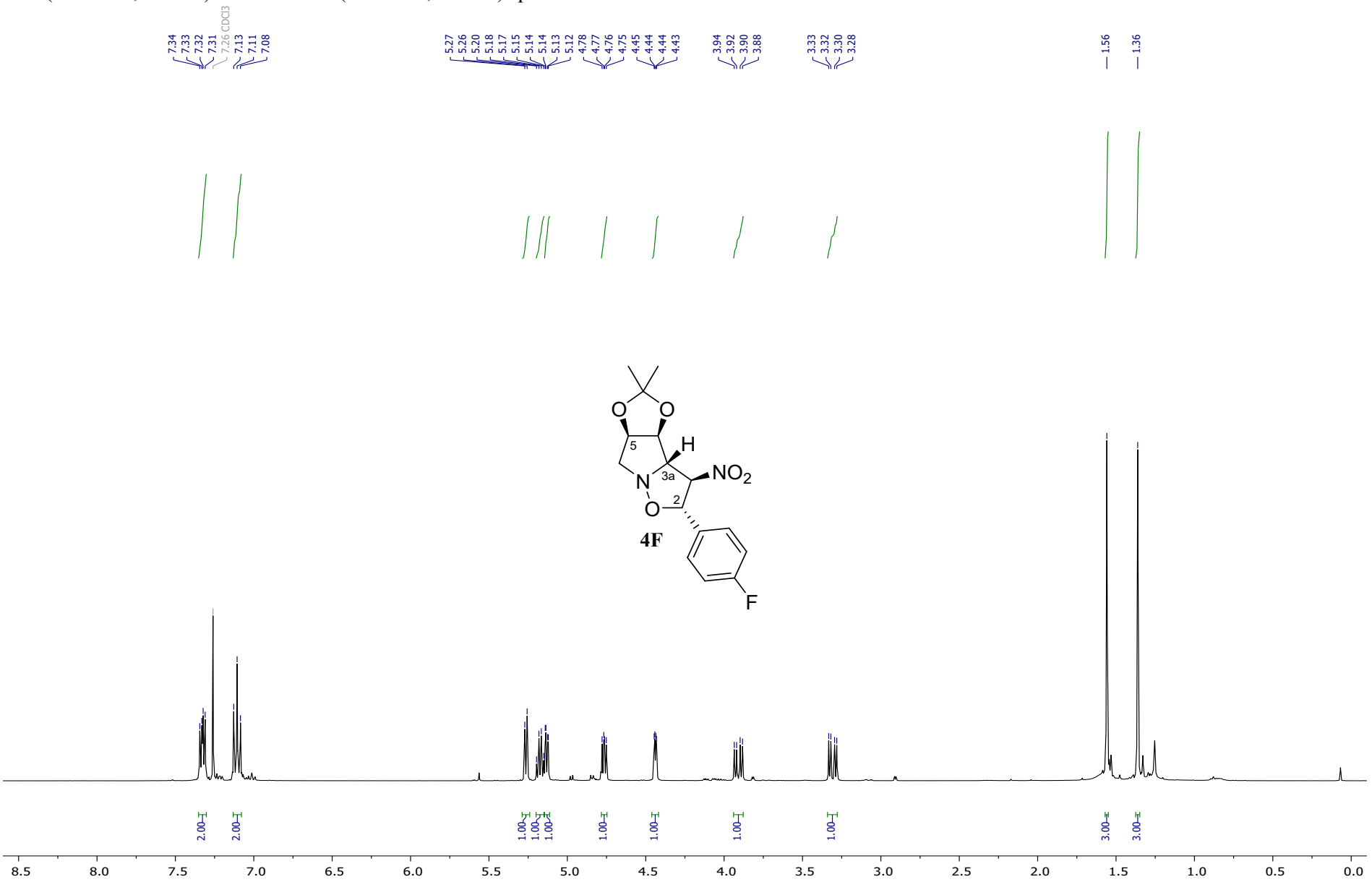
IR spectra of **4H**

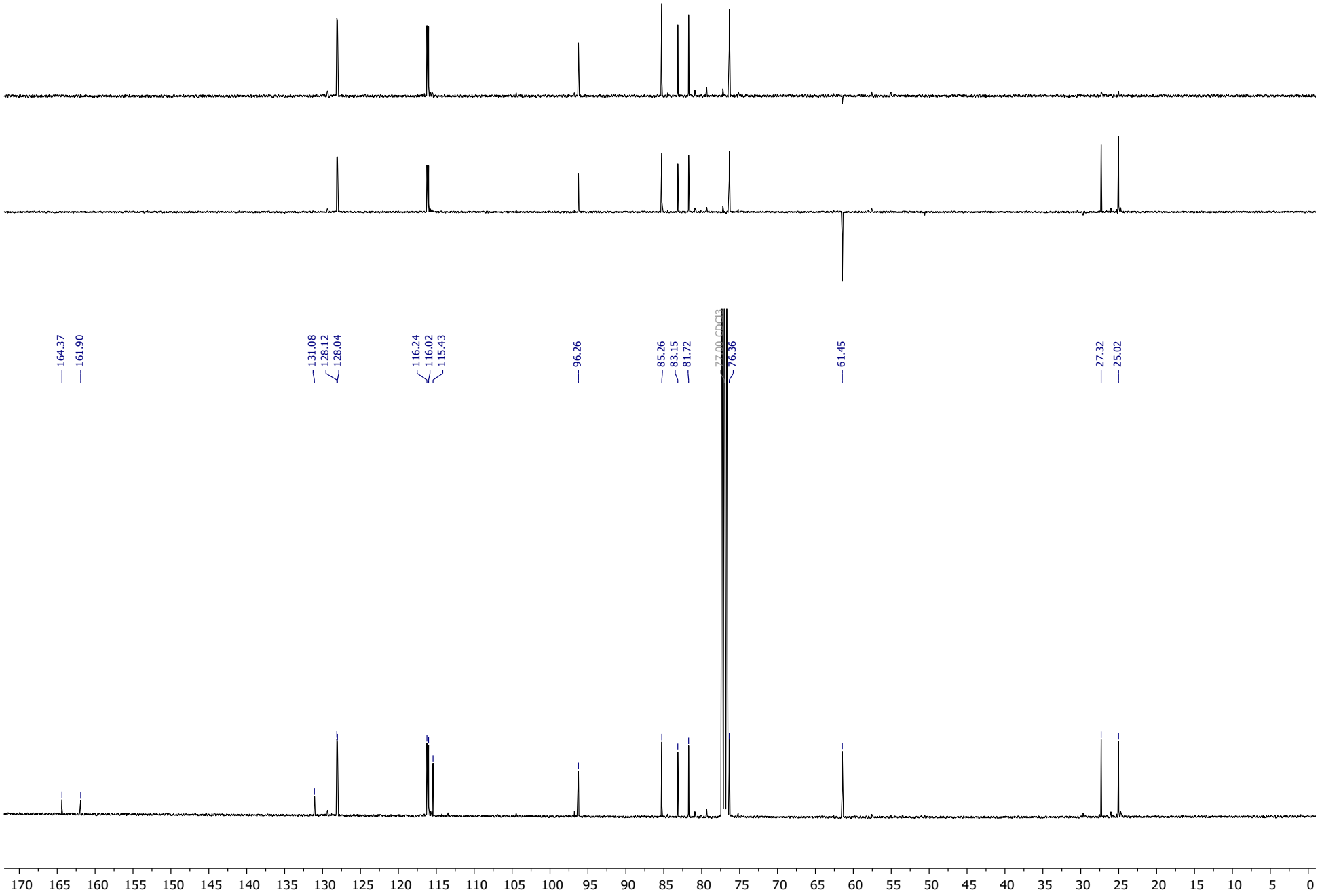


HRMS spectra of **4H**

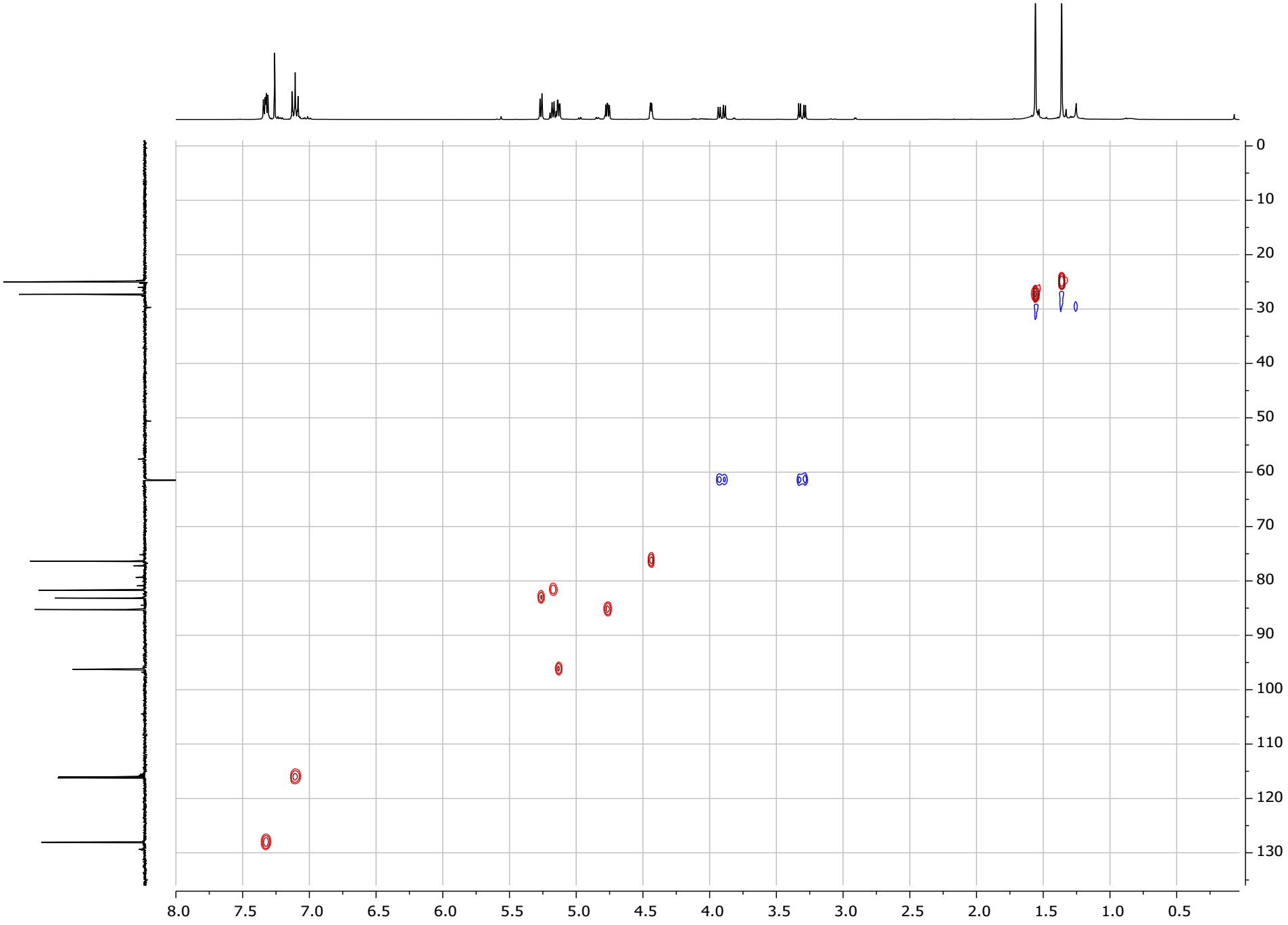


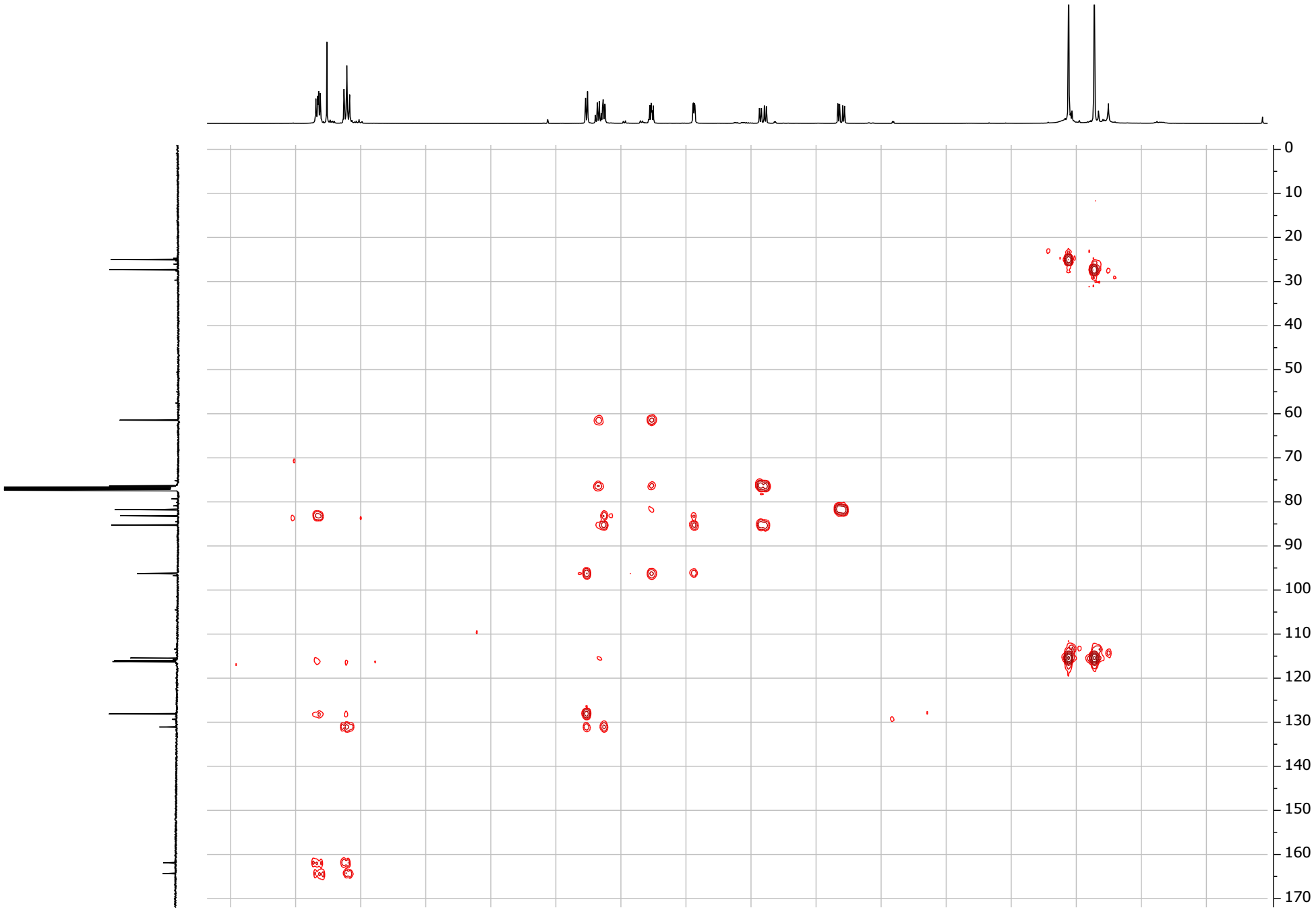
^{1}H NMR (400 MHz, CDCl3) and ^{13}C NMR (100 MHz, CDCl3) spectra of **4F**




164.37
161.90
131.08
128.12
128.04
116.24
116.02
115.43
96.26
85.26
83.15
81.72
77.00 CDCl3
76.36
61.45
27.32
25.02
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

2D NMR spectra HSQC, HMBC and COSY of **4F**




0
10
20
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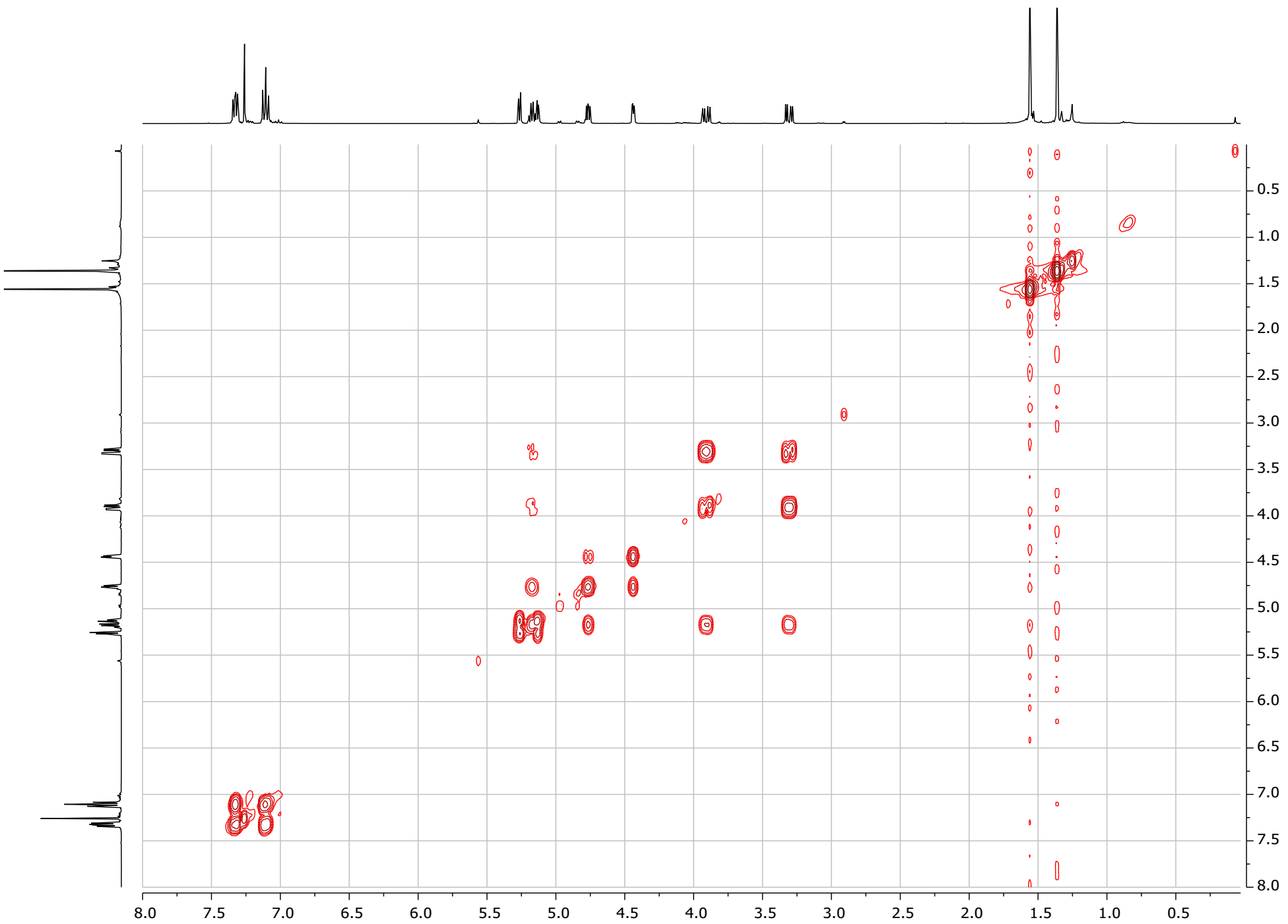
40
50
60
70
80
90
100
110
120
130
140
150
160
170
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5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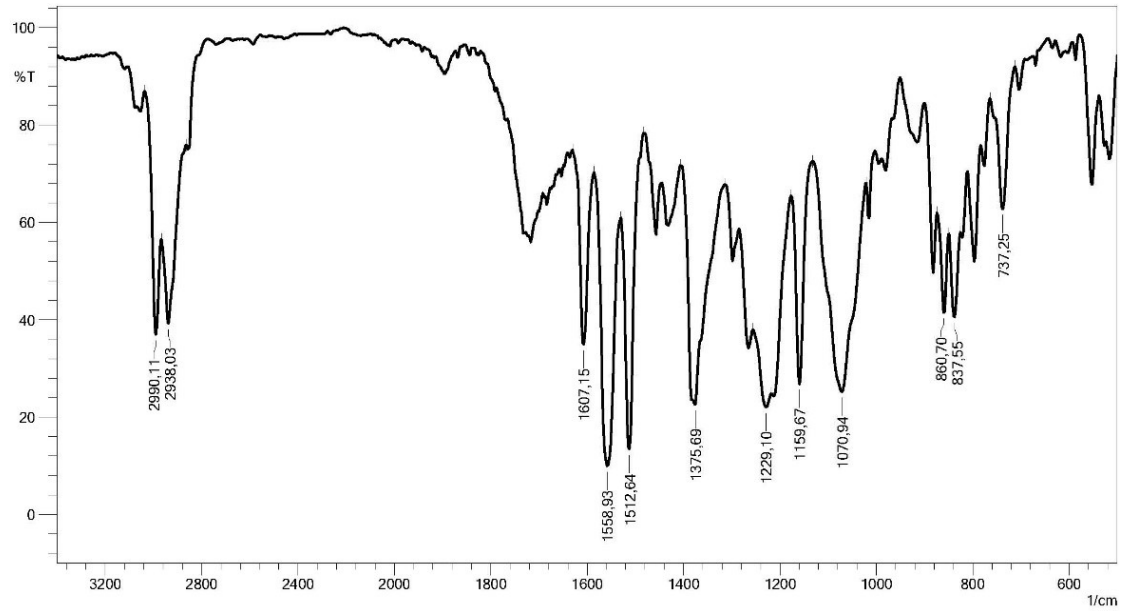
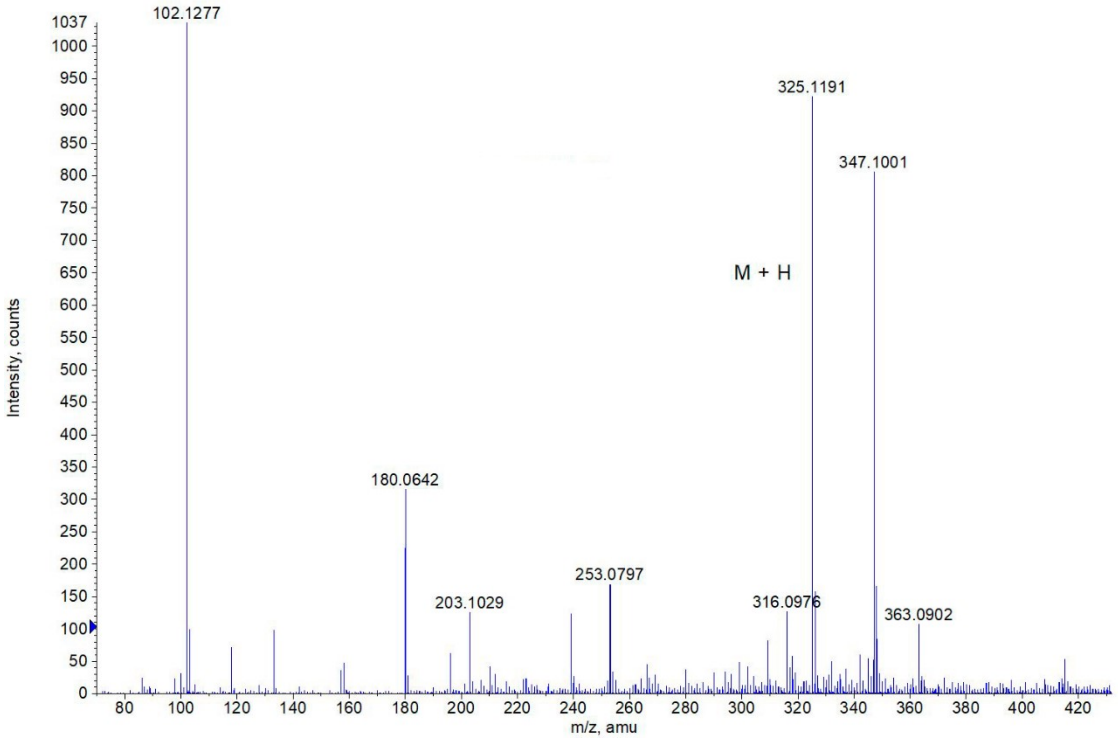
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5

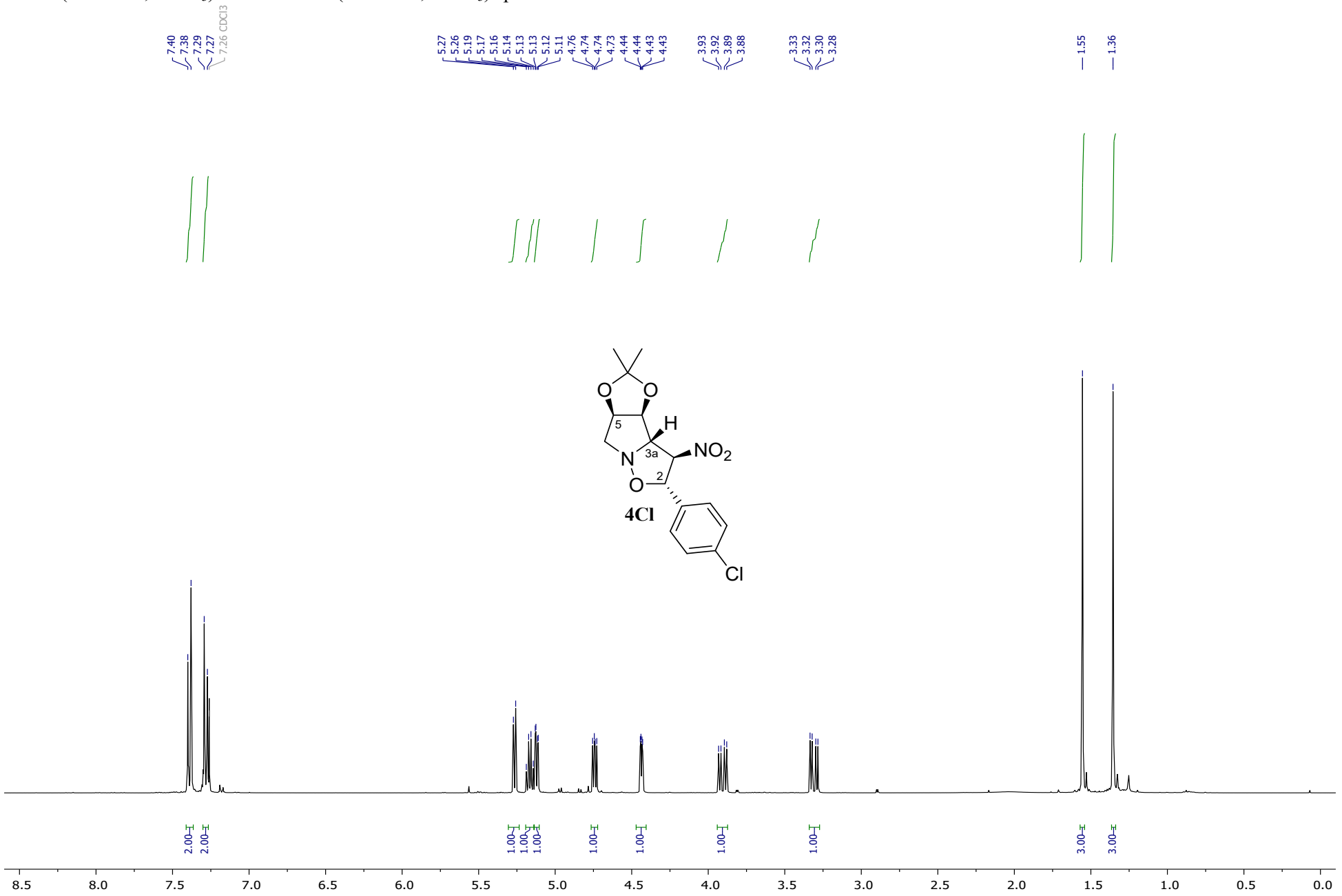
IR spectra of **4F**

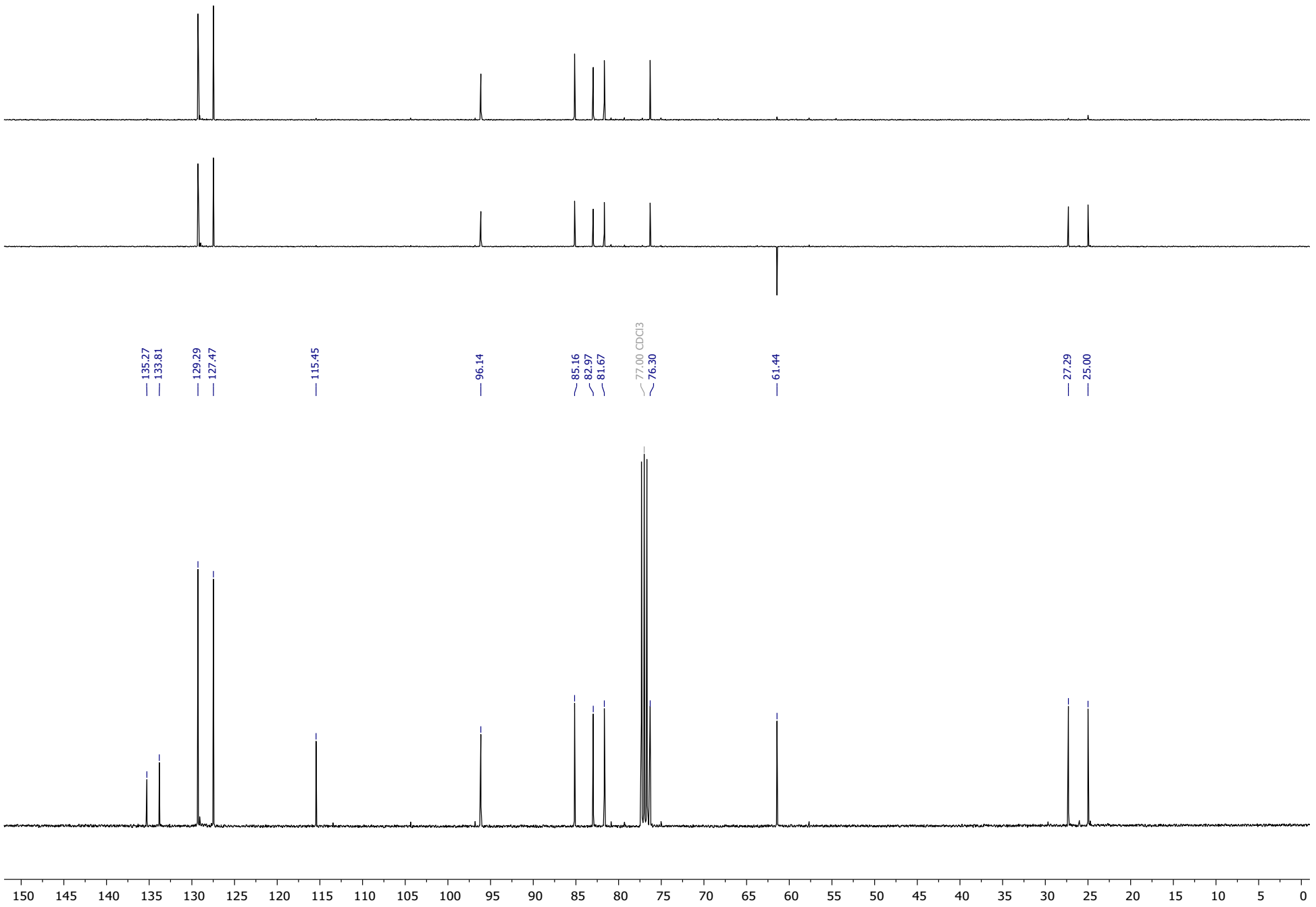


HRMS spectra of **4F**

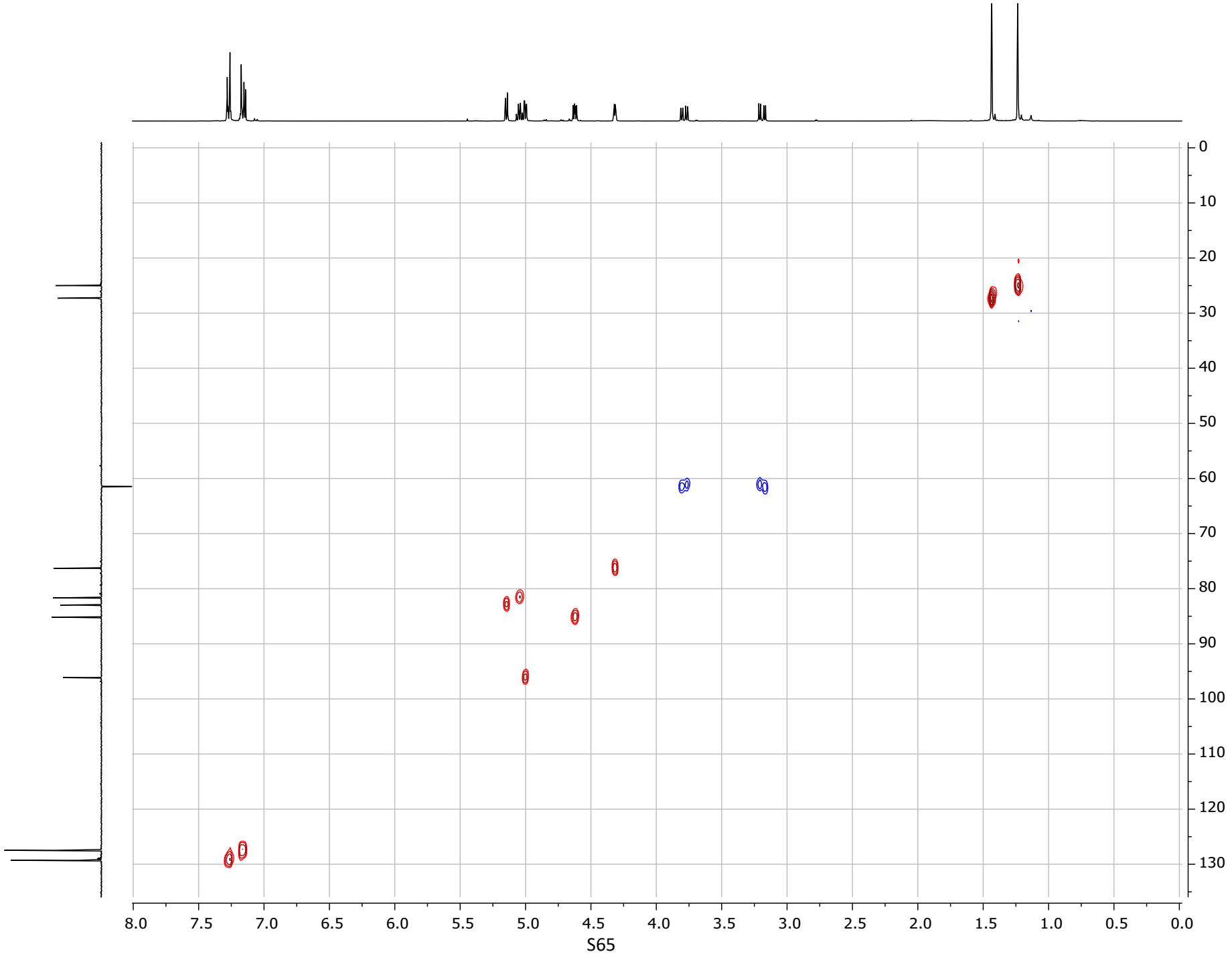


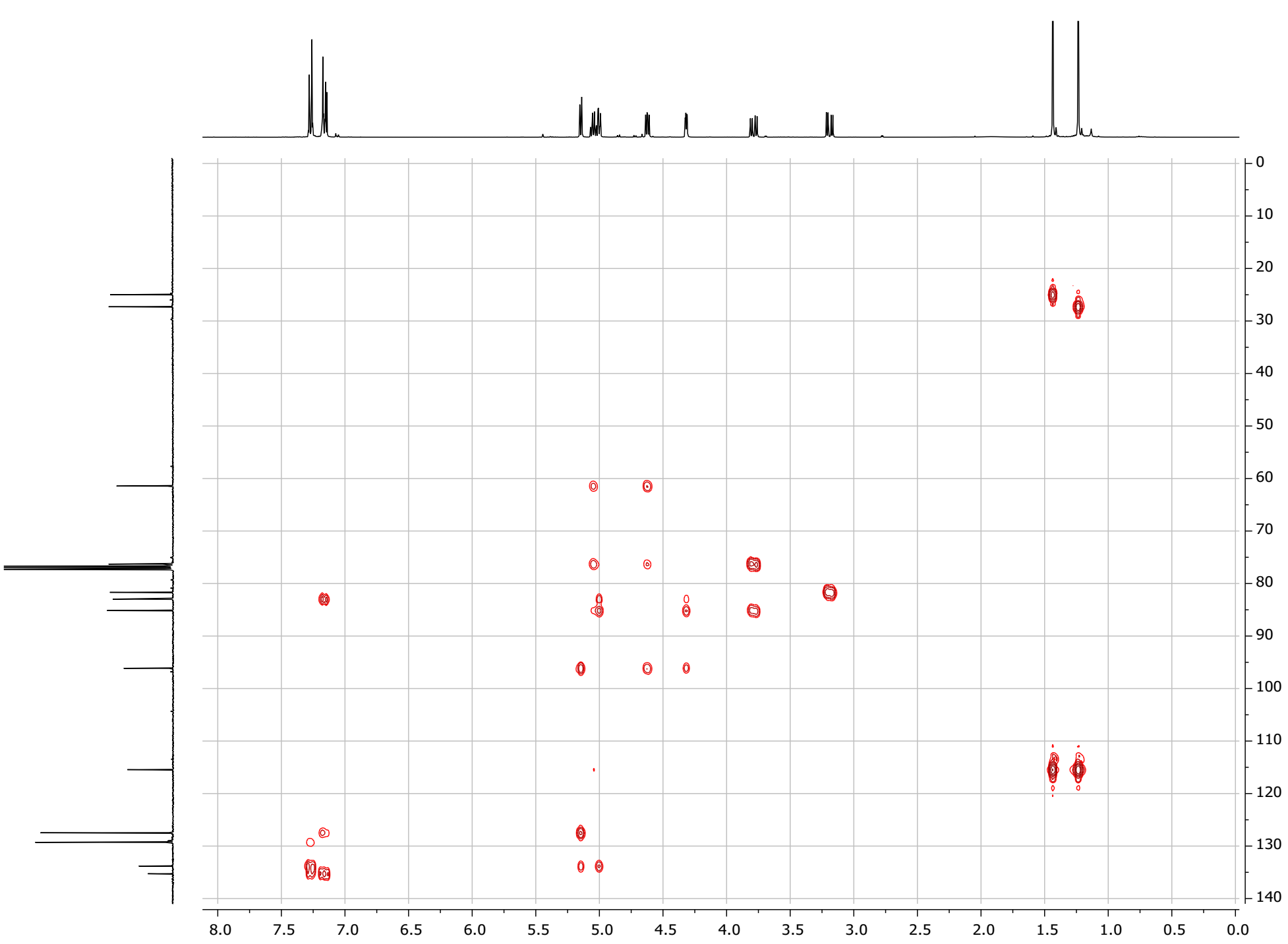
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **4Cl**




135.27
133.81
129.29
127.47
115.45
96.14
85.16
82.97
81.67
77.00 CDCl3
76.30
61.44
27.29
25.00
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

2D NMR spectra HSQC, HMBC and COSY of **4Cl**




0
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110
120
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8.0
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7.0
6.5
6.0
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3.0
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2.0
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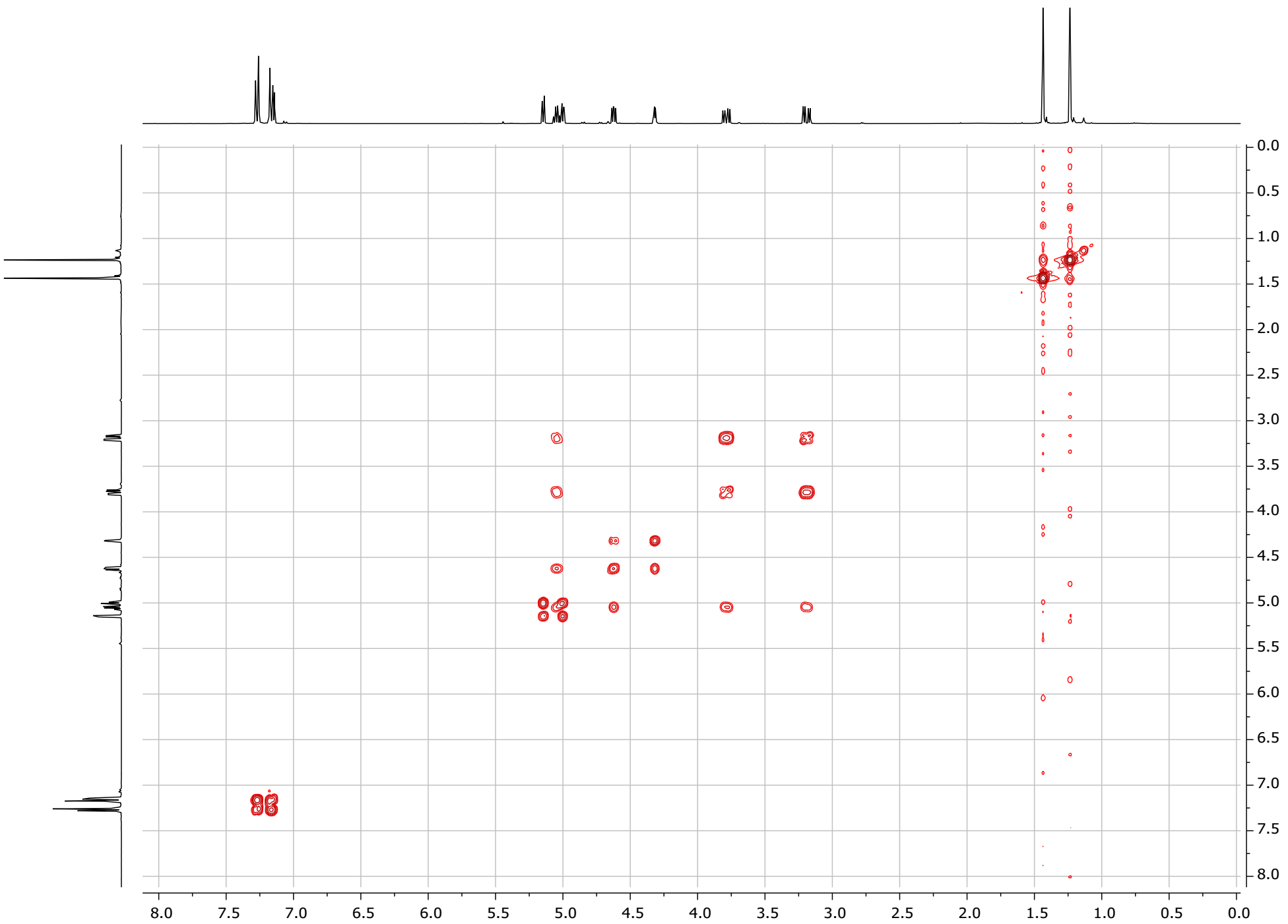
1.0
0.5
0.0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4.5
5.0
5.5
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6.5
6.0
5.5
5.0
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4.0
3.5
3.0
2.5
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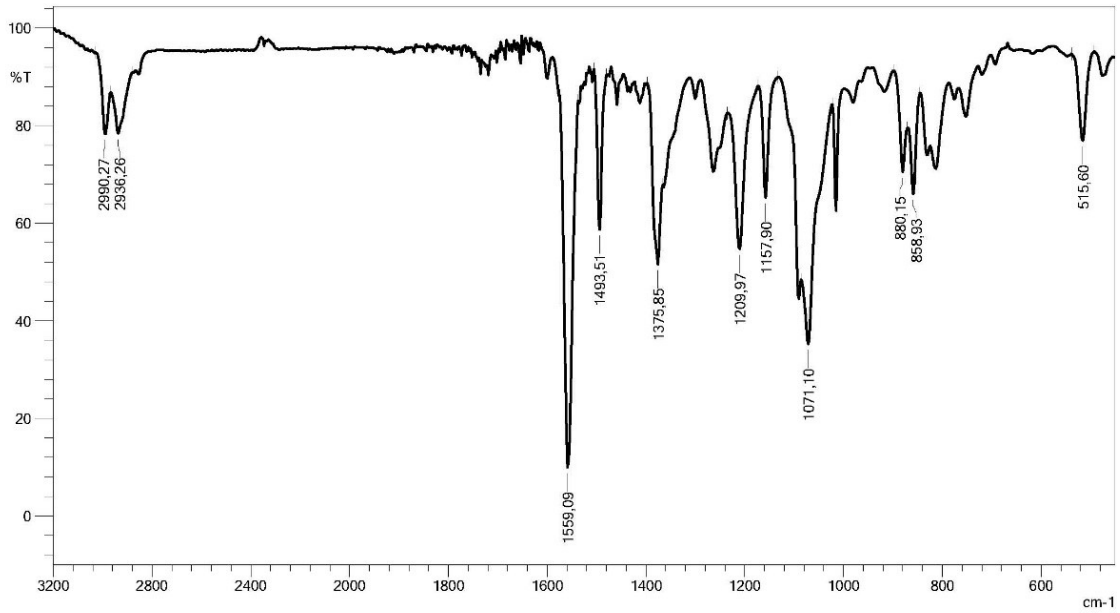
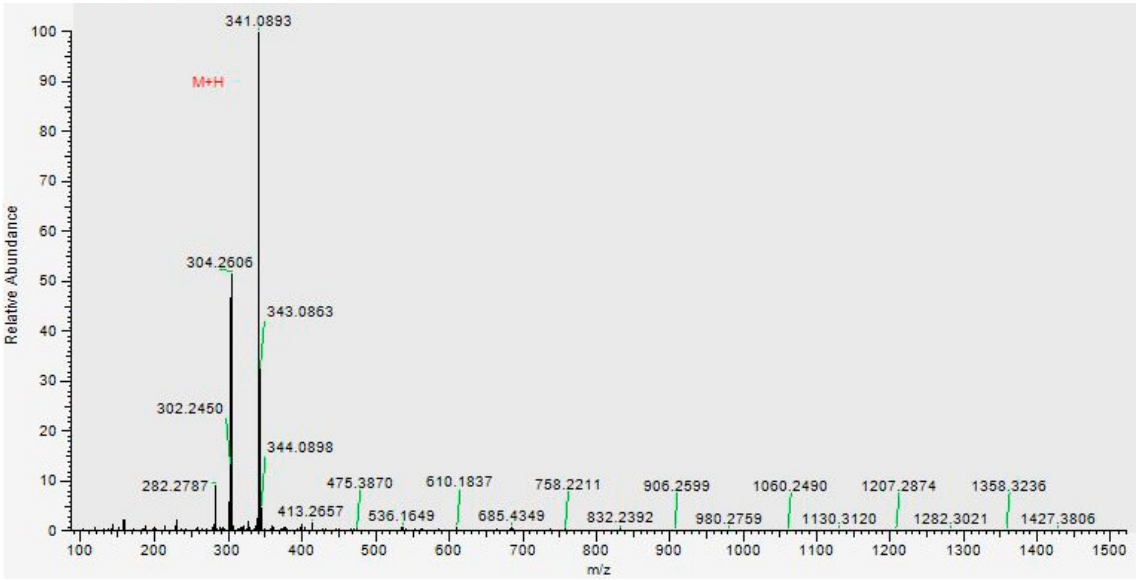
1.5
1.0
0.5
0.0

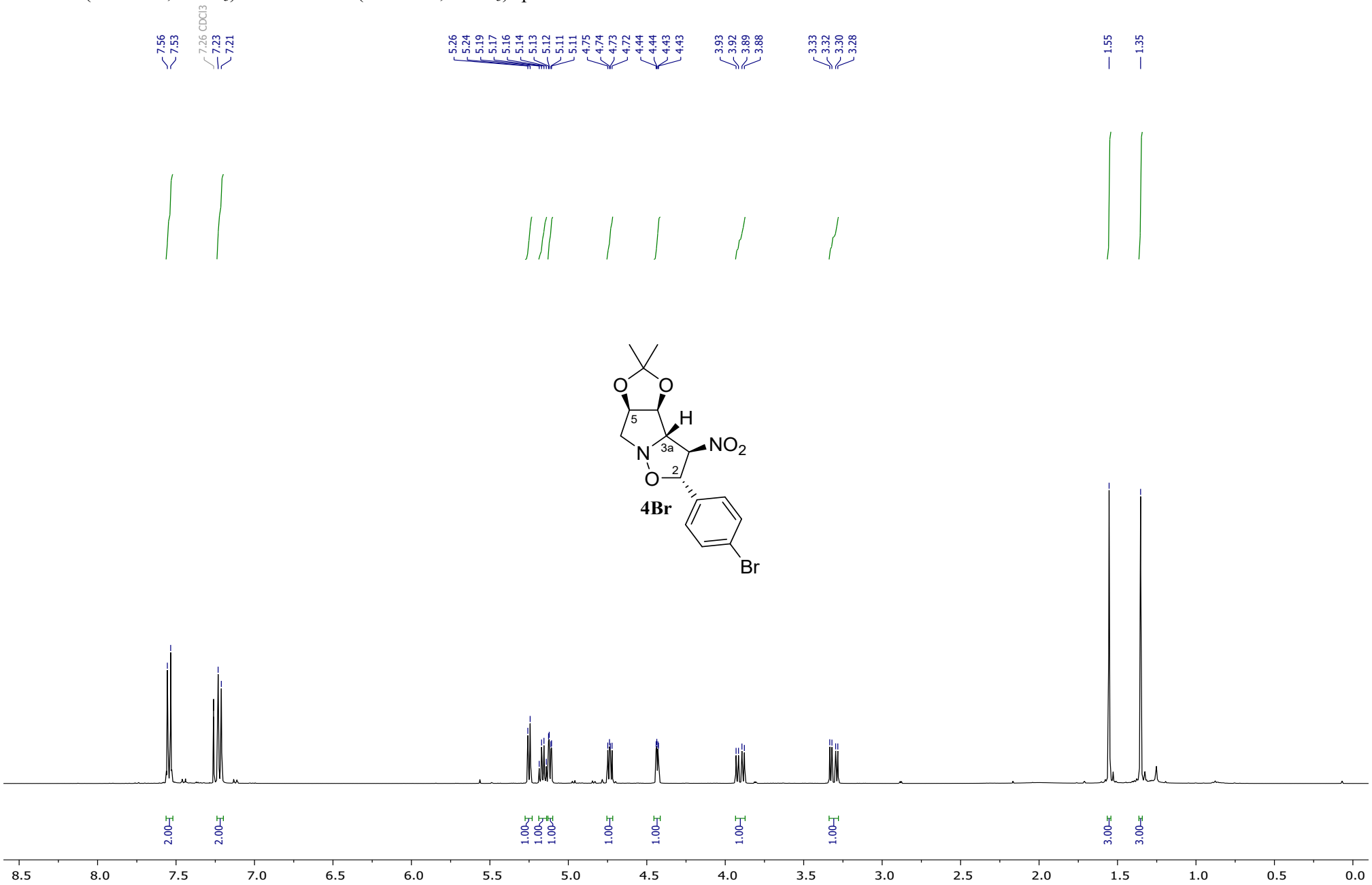
IR spectra of **4Cl**

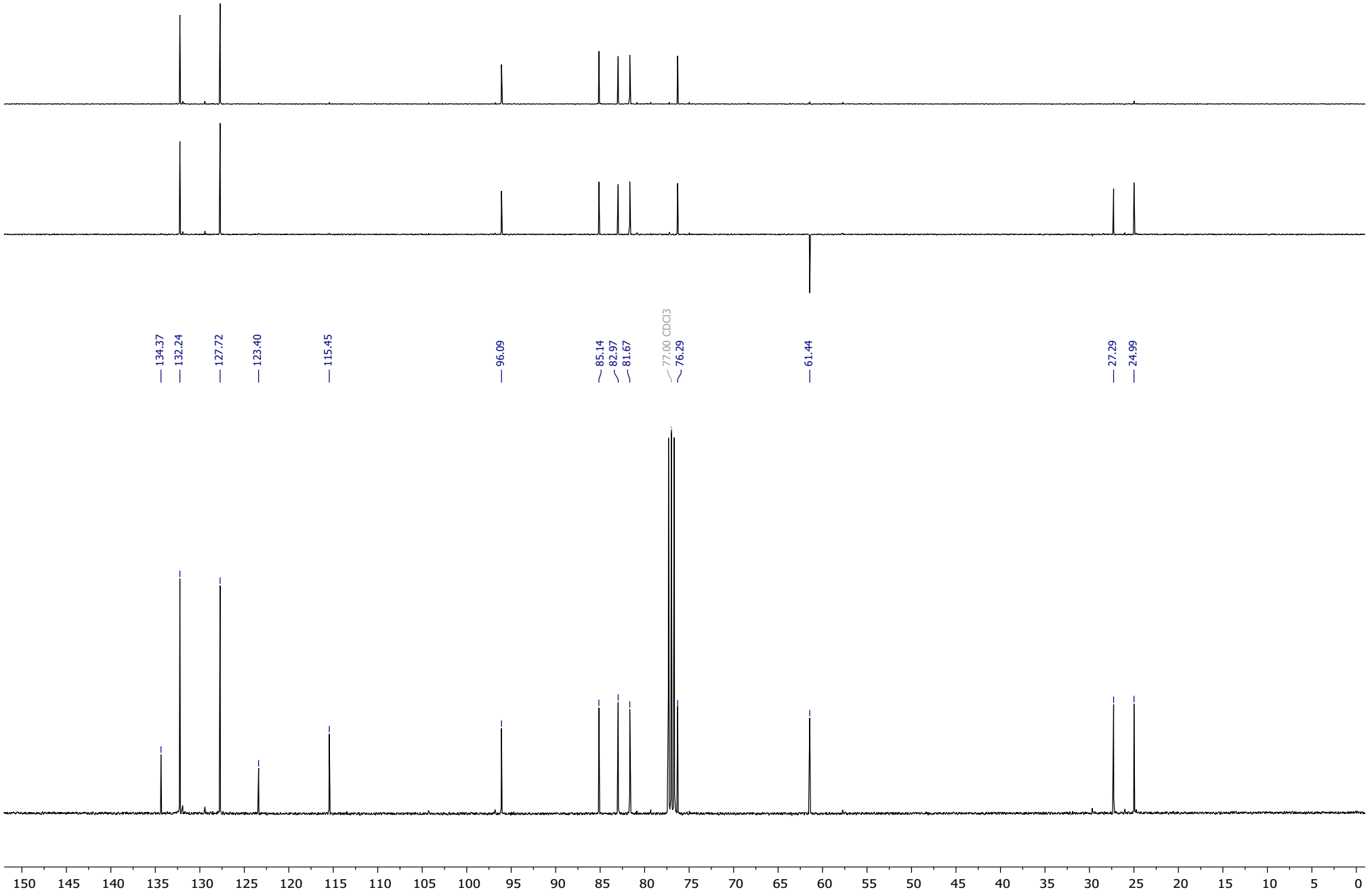


HRMS spectra of **4Cl**

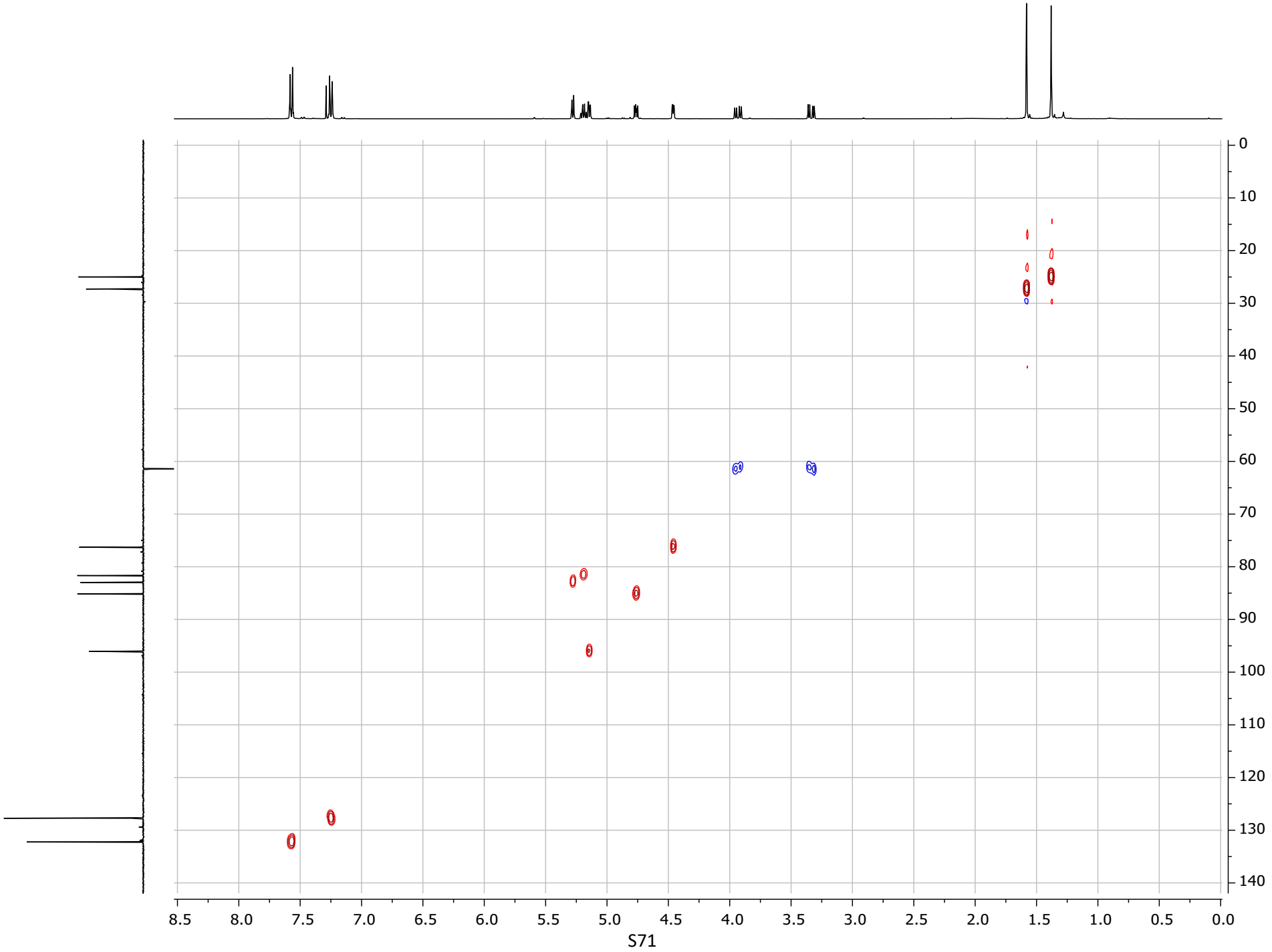


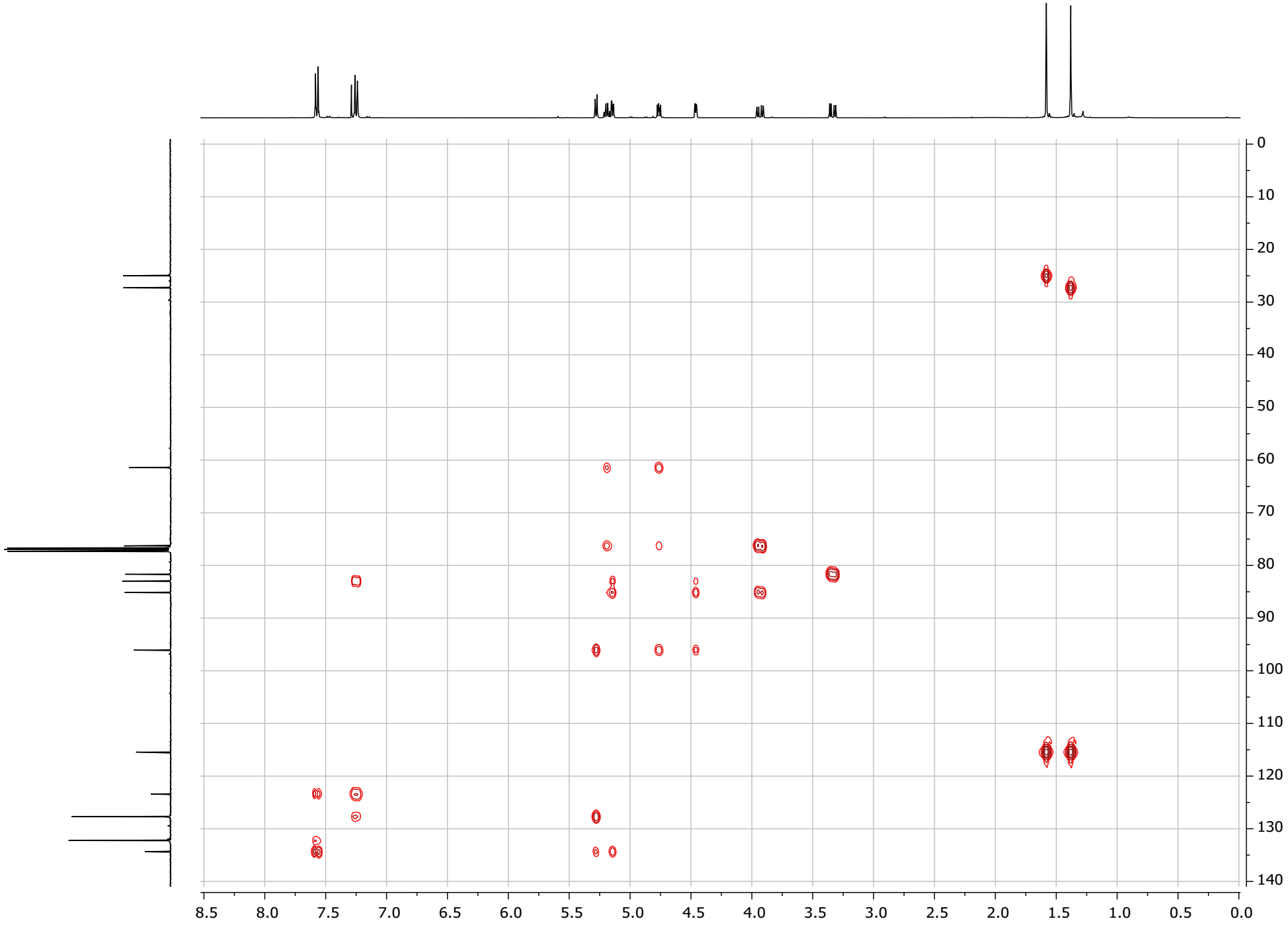
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **4Br**




134.37
132.24
127.72
123.40
115.45
96.09
85.14
82.97
81.67
77.00 CDCl3
76.29
61.44
27.29
24.99
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

2D NMR spectra HSQC, HMBC and COSY of **4Br**




0
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100
110
120
130
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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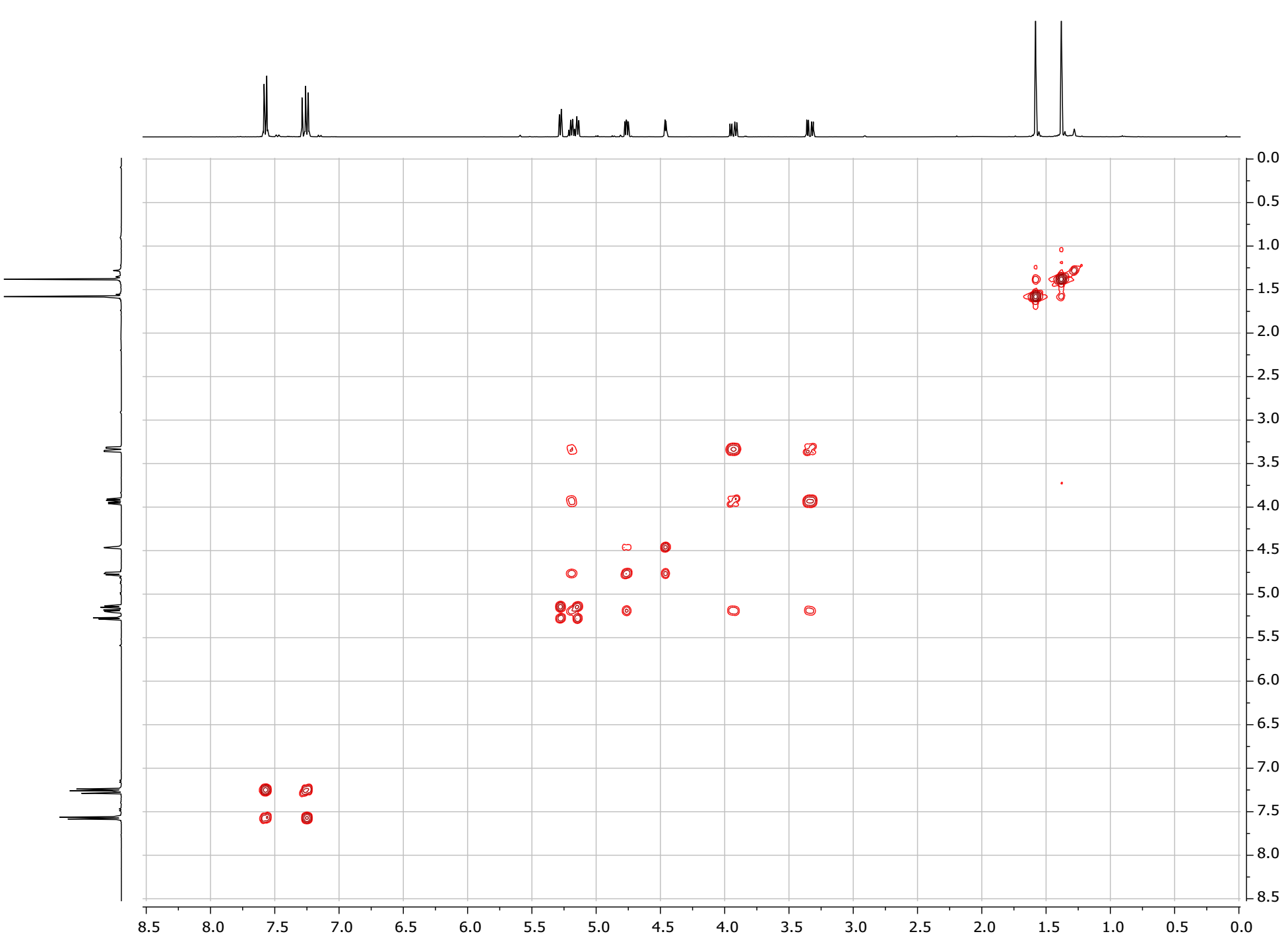
0.0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2.0
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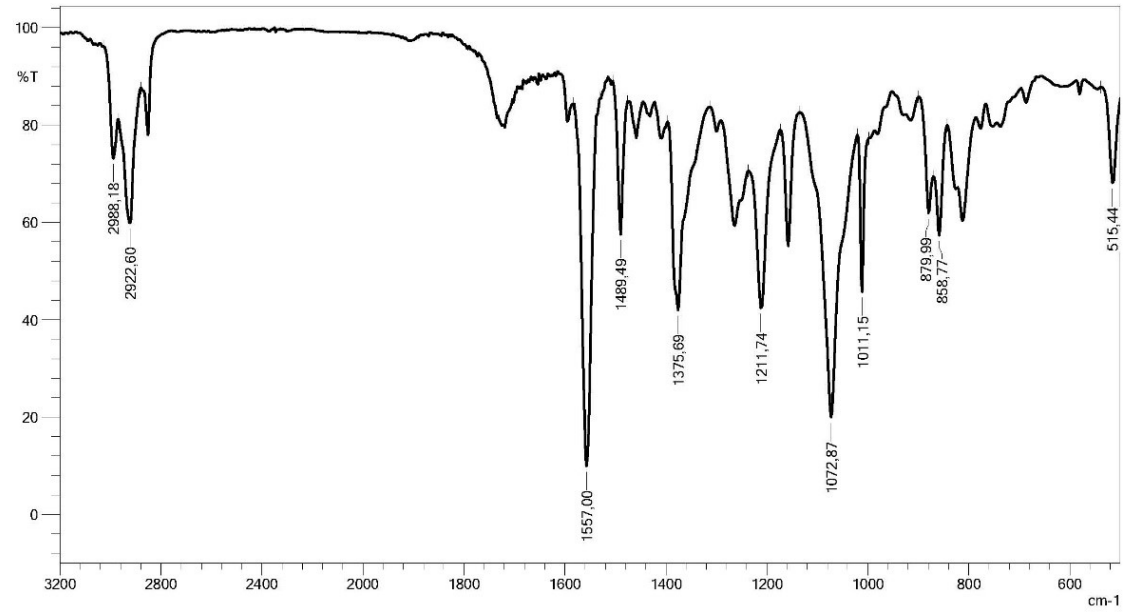
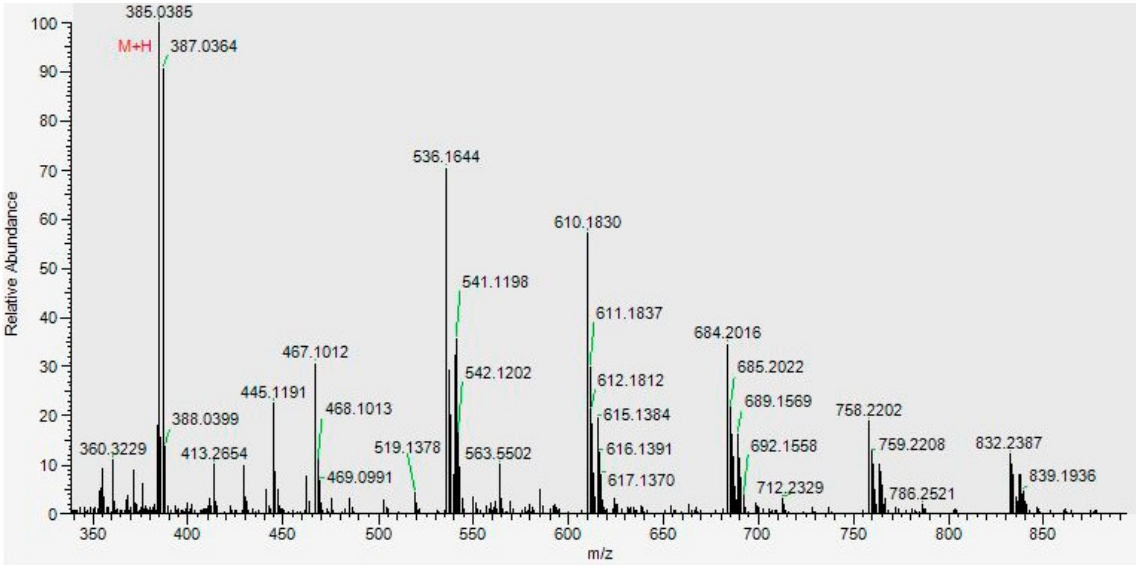
1.0
0.5
0.0

IR spectra of **4Br**



HRMS spectra of **4Br**



3D representation of the obtained transition states

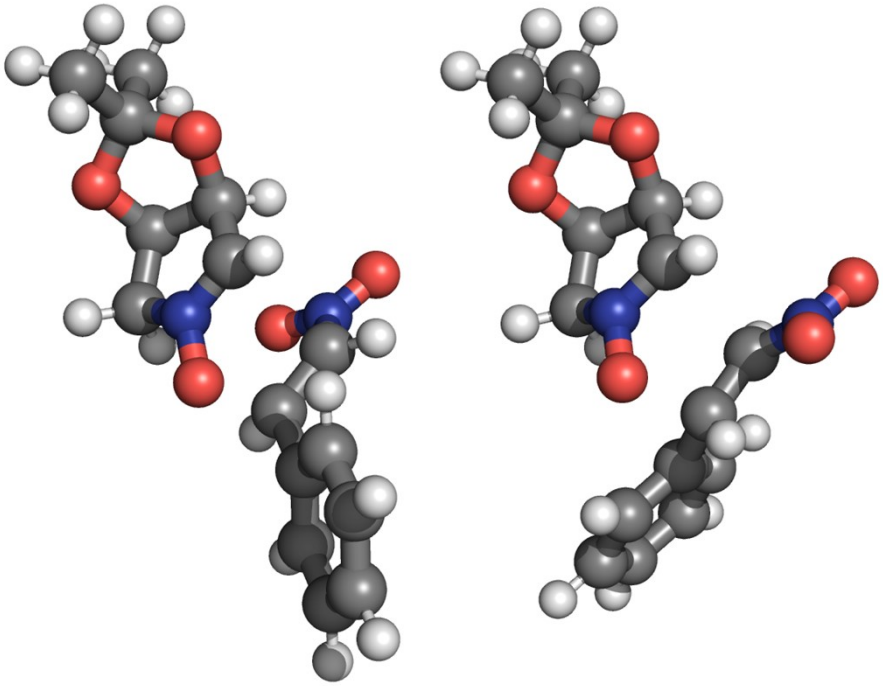


Figure S1. *Calculated structures of TS2 (23.28 kcal/mol) and TS4 (26.48 kcal/mol).*

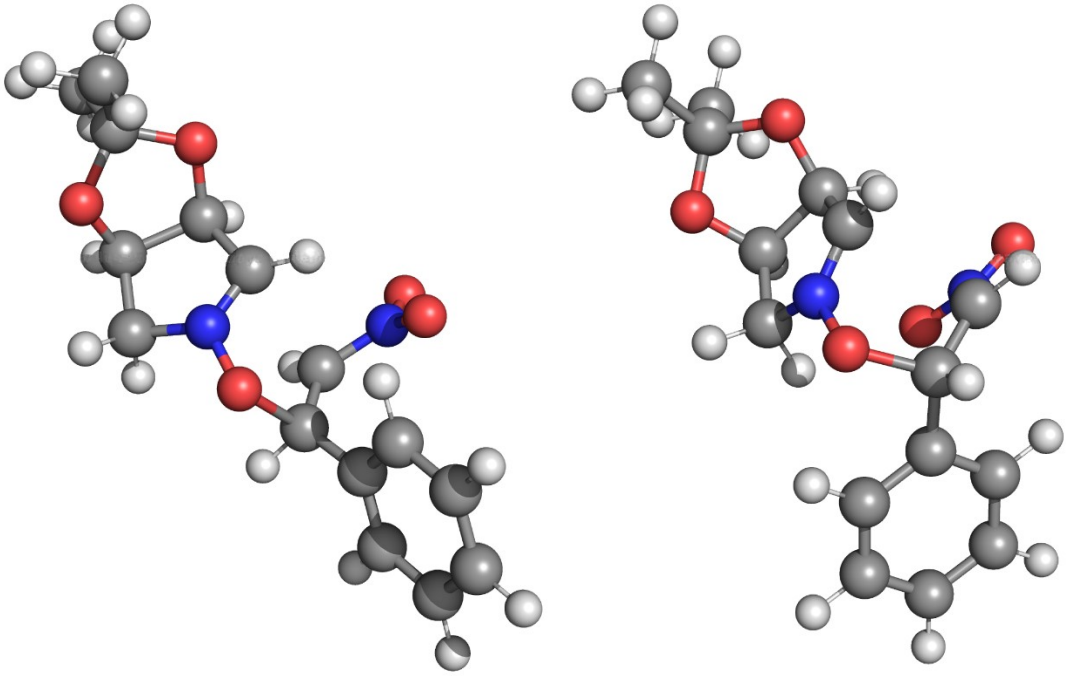


Figure S2. *Calculated structures of TS3 (30.59 kcal/mol) and TS5 (30.31 kcal/mol)*

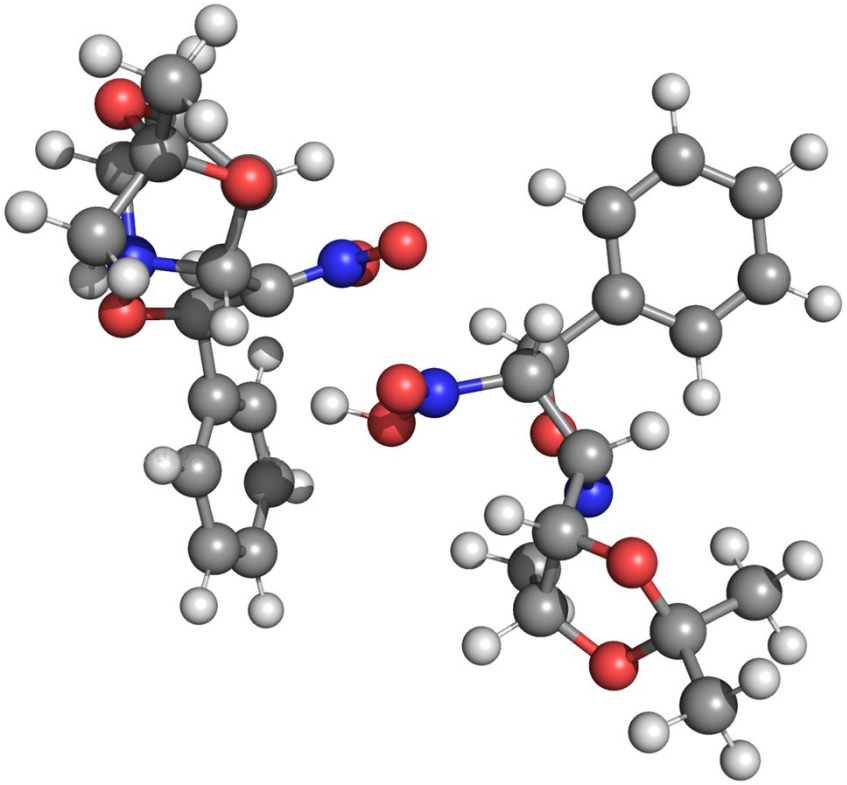


Figure S3. *Calculated structures of TS_CIDT (50.31 kcal/mol).*

Cartesian coordinates for the optimized geometries

Table S1. M06-2X/maug-cc-pVDZ optimized geometries (Cartesian coordinates in Å) for the structures shown in Figures 4,6 and 7.

***E*-β-nitrostyrene**			
C	-0.616931	0.462295	0.000064
H	-0.917294	1.513447	0.000159
C	-1.591536	-0.453633	-0.000013
H	-1.494735	-1.535986	-0.000117
N	-2.983221	-0.034177	0.000034
O	-3.256064	1.152307	0.000159
O	-3.811543	-0.929142	-0.000093
C	0.820262	0.182845	0.000021
C	1.341635	-1.122345	0.000143
C	1.707198	1.269683	-0.000144
C	2.715798	-1.328331	0.000098
H	0.669782	-1.981986	0.000283
C	3.084987	1.061458	-0.000199
H	1.307135	2.285803	-0.000230
C	3.591034	-0.237468	-0.000075
H	3.110707	-2.345166	0.000205
H	3.763843	1.915293	-0.000330
H	4.669283	-0.404508	-0.000107

***Z*-β-nitrostyrene**

C	0.626266	1.379449	-0.373856
C	1.914334	1.044918	-0.241392
H	2.740089	1.707095	-0.490875
N	2.399549	-0.251868	0.223768
O	1.743632	-0.884236	1.026188
O	3.481762	-0.601535	-0.213702
C	-0.608451	0.594001	-0.211990
C	-1.751287	1.254037	0.261446
C	-0.702433	-0.756502	-0.577655
C	-2.953561	0.566606	0.414815
H	-1.691177	2.312897	0.522002
C	-1.909223	-1.435586	-0.444175
H	0.165881	-1.275549	-0.985630
C	-3.034016	-0.780183	0.062382
H	-3.831208	1.087306	0.800153
H	-1.972900	-2.483907	-0.738660
H	-3.976757	-1.318568	0.171338
H	0.476300	2.419530	-0.682037

1

O	-3.079552	0.881668	-0.218289
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O	1.060345	-0.110542	1.219313
N	-2.046364	0.209071	0.043064
C	-1.378490	0.148133	1.157253
C	-0.191347	-0.757470	1.069778
C	-0.203234	-1.248390	-0.406037
C	-1.470658	-0.656184	-1.019095
H	-1.275659	-0.025760	-1.896146
H	-2.235687	-1.401754	-1.268954
C	1.549152	0.240844	-0.072541
C	3.054156	0.084339	-0.068556
H	3.453235	0.283283	-1.072730
H	3.317665	-0.938802	0.230166
H	3.502289	0.795781	0.638703
C	1.113681	1.643946	-0.477037
H	0.020102	1.745512	-0.495836
H	1.502236	1.874652	-1.479135
H	1.514486	2.376545	0.237752
H	-1.705314	0.733366	2.014603
H	-0.228852	-1.564693	1.813042
H	-0.179217	-2.340429	-0.496778

2H

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O	2.919233	-0.301795	-1.176250
N	0.493245	-1.145210	0.590963
C	-1.540659	-0.054479	0.573457
C	-0.711572	0.576000	-0.571729
C	0.588500	-0.277358	-0.590017
C	1.942442	0.422396	-0.454867
C	2.347278	0.244598	1.040117
C	1.175580	-0.459935	1.707233
H	1.514120	-1.197965	2.443926
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H	5.360938	0.831735	-1.414716
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H	3.999507	-2.607233	-0.599841
H	5.561789	-1.971408	0.004970
H	5.106244	-1.733113	-1.706670
C	-2.982126	-0.315001	0.225905
C	-3.330398	-1.383576	-0.607671
H	-2.554862	-2.062428	-0.967202
C	-4.663152	-1.587816	-0.958734
H	-4.930706	-2.426320	-1.603425
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C	-5.310056	0.339431	0.345554
H	-6.080815	1.012648	0.723355
C	-3.976371	0.540857	0.704294
H	-3.707195	1.368610	1.364607
H	-6.697596	-0.887593	-0.762137
H	-1.479890	0.599430	1.457300
H	0.570111	-0.886547	-1.501600
H	1.925272	1.473225	-0.780132
H	2.591134	1.197422	1.531616
N	-0.432614	2.025975	-0.302801
O	-0.689292	2.816959	-1.183884
O	0.064565	2.321742	0.768205
H	-1.229702	0.564438	-1.533511

3H

O	0.641544	-1.499778	0.419493
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O	-3.062027	0.932955	0.494163
O	1.850916	2.480237	-0.876488
O	1.352399	1.892181	1.131915
N	-0.722730	-1.158686	0.386401
N	1.288964	1.766641	-0.070862
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C	-2.571789	-0.795961	-1.023470
C	-1.412773	-1.746907	-0.777772
H	-1.750245	-2.763864	-0.545886
H	-0.763331	-1.777513	-1.670712
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C	-5.155560	0.734005	-0.703169
H	-6.011169	0.068546	-0.884134
H	-4.646172	0.917210	-1.661341
H	-5.522244	1.695644	-0.318249
C	-4.841870	-0.165352	1.647428
H	-4.102449	-0.624596	2.316576
H	-5.697374	-0.844181	1.529083
H	-5.194315	0.777966	2.086310
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C	4.537700	-0.463162	1.482497
H	4.847287	-0.482476	2.528265
C	5.487038	-0.288832	0.475105
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H	5.824637	-0.133101	-1.653466
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H	6.541117	-0.171918	0.731521
H	1.264669	-1.184084	-1.547053
H	0.309025	0.896932	-1.670570
H	-0.681148	0.803630	1.169818
H	-2.017866	1.361013	-1.249315
H	-2.865450	-0.764025	-2.083356

4H

H	5.022222	-3.173713	-0.952985
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O	-2.516397	-0.001913	-1.132069
O	2.283196	2.793313	-0.977591
O	0.324348	3.536954	-0.495676
N	-0.499369	1.003222	1.574255
N	1.123793	2.642450	-0.646929
C	1.570021	0.612766	0.741620
C	0.701440	1.210766	-0.415729
C	-0.711574	1.071051	0.112477
C	-1.413272	-0.245843	-0.282252
C	-2.039538	-0.773723	1.034220
C	-1.640106	0.255344	2.104512
H	-2.461435	0.972500	2.239923
H	-1.370028	-0.173811	3.075423
C	-3.618549	-0.756905	-0.626851
C	-3.580180	-2.180019	-1.167553
H	-2.633341	-2.675626	-0.906539
H	-3.674697	-2.167199	-2.262315
H	-4.407004	-2.765033	-0.741500
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H	-4.863023	0.988137	-0.545084
C	2.535097	-0.462017	0.306455
C	3.804426	-0.094826	-0.150954
H	4.093237	0.957939	-0.152975
C	4.693610	-1.066959	-0.606396
H	5.682044	-0.771508	-0.961348
C	4.323942	-2.412848	-0.601049
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H	2.771043	-3.833273	-0.120242
C	2.166853	-1.810286	0.314462
H	1.185051	-2.099755	0.691368
H	2.110420	1.438650	1.234667
H	-1.351076	1.926587	-0.133995
H	0.874518	0.717699	-1.379702
H	-0.720114	-0.969958	-0.739163
H	-1.707337	-1.792628	1.281624

5H

C	-1.807759	-1.078506	1.869006
C	-0.818835	0.779903	0.831256
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C	-1.958290	-1.341206	0.358985
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H	-2.725639	-0.631434	2.274103
H	-1.569219	1.561415	1.006609
H	-0.446499	-0.434950	-0.979967
H	-1.512287	-2.299609	0.066176
O	-3.290674	-1.323929	-0.116097
O	-2.279630	0.438066	-1.140846
C	-3.555165	-0.079000	-0.761131
C	-4.276871	0.877653	0.181537
C	-4.354394	-0.346834	-2.019150
N	-0.734904	-0.093134	2.023578
O	0.478365	-0.829038	1.707289
C	1.447663	0.160995	1.418532
C	0.592350	1.360615	0.864240
H	0.639179	2.200164	1.561436
H	1.921178	0.504745	2.351590
C	2.494611	-0.389028	0.482320
C	3.725345	0.268805	0.387406
C	2.247661	-1.509845	-0.314868
C	4.695012	-0.180686	-0.507257
H	3.926965	1.139923	1.015335
C	3.224182	-1.964438	-1.200846
H	1.293849	-2.031628	-0.231645
C	4.445792	-1.299067	-1.303269
H	5.649656	0.342248	-0.578596
H	3.026591	-2.843011	-1.816712
H	5.205524	-1.654098	-2.001109
N	1.145013	1.923108	-0.410576
O	1.893631	2.872291	-0.283534
O	0.869474	1.399258	-1.465933
H	-5.320835	-0.801372	-1.760801
H	-3.794448	-1.031440	-2.669774
H	-4.535538	0.594612	-2.556207
H	-3.711873	1.041685	1.109068
H	-5.258517	0.462188	0.449939
H	-4.424023	1.847715	-0.314429

TS2

O	-0.946993	-0.882049	0.953896
O	3.430631	-0.746681	1.042773
O	3.006925	-0.538716	-1.164942
N	0.306162	-0.635592	0.705819
C	-1.851237	0.541416	0.405382
C	-1.123739	1.121270	-0.668812
C	0.688217	-0.367238	-0.524237
C	2.046185	0.272306	-0.518731
C	2.447181	0.271092	0.986890
C	1.206156	-0.146202	1.765381
H	1.413557	-0.967040	2.462394
H	0.718208	0.688810	2.280312
C	4.063744	-0.791981	-0.229691
C	5.128753	0.288093	-0.349044
H	5.914385	0.124996	0.401836
H	4.696033	1.287459	-0.194594
H	5.576682	0.259467	-1.351776
C	4.592958	-2.187394	-0.459017
H	3.777059	-2.913963	-0.349584
H	5.381374	-2.413113	0.271896
H	5.014330	-2.264060	-1.470473
C	-3.169702	-0.080229	0.113888
C	-3.340395	-0.930792	-0.985957
H	-2.490806	-1.160744	-1.632618
C	-4.584510	-1.495934	-1.251586
H	-4.707402	-2.158585	-2.109507
C	-5.672005	-1.220487	-0.418593
C	-5.506249	-0.383618	0.683766
H	-6.350040	-0.169263	1.341272
C	-4.258043	0.179311	0.952076
H	-4.126496	0.831729	1.817714
H	-6.646747	-1.663831	-0.627970
H	-1.811052	1.103069	1.342111
H	0.229196	-0.867152	-1.373426
H	2.011677	1.281005	-0.963071
H	2.840298	1.239856	1.323268
N	-0.270980	2.215248	-0.419440
O	0.096450	2.898882	-1.373316
O	0.132256	2.420667	0.731940
H	-1.444574	1.069264	-1.705538

TS3

O	0.643140	-1.389642	-0.189709
O	-3.624976	-1.217341	-0.392196
O	-3.193611	0.636388	0.826845
O	0.823386	3.282944	-0.266086
O	1.622876	1.843218	1.129521
N	-0.569961	-0.950900	-0.266743
N	1.164809	2.141079	0.031008
C	1.696848	-0.079284	-0.978382
C	0.955416	1.119737	-0.935638
C	-0.894654	0.211396	0.249557
C	-2.251274	0.646029	-0.226931
C	-2.683251	-0.511460	-1.173730
C	-1.436285	-1.355004	-1.384902
H	-1.628891	-2.432836	-1.337957
H	-0.913093	-1.108607	-2.321948
C	-4.242212	-0.276981	0.480878
C	-5.362249	0.469760	-0.227749
H	-6.146379	-0.234778	-0.538165
H	-4.985472	0.993560	-1.118858
H	-5.796790	1.216899	0.450358
C	-4.693673	-0.998900	1.727625
H	-3.840510	-1.521266	2.180061
H	-5.475696	-1.728219	1.475833
H	-5.099855	-0.276521	2.448370
C	2.995512	-0.363569	-0.295642
C	3.116408	-0.612903	1.075623
H	2.228214	-0.594840	1.703824
C	4.364847	-0.888712	1.629241
H	4.446476	-1.082978	2.699724
C	5.506134	-0.913256	0.825793
C	5.392261	-0.671798	-0.542512
H	6.276299	-0.694636	-1.181553
C	4.141169	-0.410109	-1.099842
H	4.052709	-0.233068	-2.174333
H	6.481917	-1.125254	1.265937
H	1.674936	-0.507195	-1.985802
H	0.477605	1.511639	-1.830262
H	-0.381475	0.582314	1.137988
H	-2.210840	1.633392	-0.710271
H	-3.119588	-0.163077	-2.120142

TS4

O	-0.760349	0.001248	-1.679599
O	2.816236	-1.723375	-0.119950
O	3.278242	0.477188	0.124460
N	0.308095	-0.224583	-0.983026
C	-1.871097	0.947998	-0.555511
C	-1.032064	1.558774	0.397951
C	0.963756	0.792877	-0.461101
C	1.947069	0.314807	0.570887
C	1.708624	-1.222966	0.601101
C	0.425341	-1.453481	-0.180235
H	0.468704	-2.328471	-0.838831
H	-0.458048	-1.519918	0.473807
C	3.895672	-0.815099	0.068250
C	4.619726	-1.094979	1.376409
H	5.054161	-2.104215	1.357528
H	3.929692	-1.022904	2.230075
H	5.422501	-0.359150	1.521611
C	4.794667	-0.875496	-1.143466
H	4.207438	-0.669140	-2.048002
H	5.248779	-1.872621	-1.223468
H	5.593415	-0.127148	-1.051555
H	1.039993	1.729463	-1.015853
H	1.792854	0.815482	1.537787
H	1.662036	-1.639502	1.616987
C	-2.841955	-0.109978	-0.136153
C	-3.428539	-0.924519	-1.116241
C	-3.210147	-0.295964	1.201940
C	-4.343424	-1.912602	-0.764338
H	-3.147715	-0.784835	-2.161241
C	-4.124240	-1.290679	1.554941
H	-2.803029	0.352106	1.979104
C	-4.690318	-2.104149	0.575331
H	-4.788928	-2.537630	-1.539808
H	-4.401798	-1.419546	2.602296
H	-5.407286	-2.878772	0.851535
H	-2.207292	1.597440	-1.366368
N	-0.648908	2.920331	0.221544
H	-0.958765	1.248334	1.436466
O	-0.173318	3.504633	1.190490
O	-0.753241	3.435747	-0.886687

TS5

O	0.733345	-0.737259	1.806760
O	-2.911720	-1.380443	-0.546552
O	-3.347162	0.622051	0.406164
N	-0.342895	-0.572101	1.068249
C	1.812636	0.463322	1.429785
C	1.114204	1.674093	1.085554
C	-1.080331	0.492161	1.214513
C	-1.986781	0.663696	0.032704
C	-1.740516	-0.626170	-0.802583
C	-0.523373	-1.312869	-0.194634
H	-0.715475	-2.367516	0.038985
H	0.383634	-1.198022	-0.797310
C	-3.966101	-0.455118	-0.313790
C	-4.538356	0.065609	-1.623425
H	-4.965434	-0.765144	-2.202293
H	-3.760431	0.554218	-2.228262
H	-5.325470	0.803745	-1.417213
C	-4.996049	-1.107315	0.576912
H	-4.515359	-1.465884	1.496724
H	-5.459210	-1.955369	0.054434
H	-5.777784	-0.380469	0.835752
H	-1.136607	1.016694	2.164351
H	-1.737106	1.592315	-0.508034
H	-1.605467	-0.421294	-1.872586
N	0.765300	2.003886	-0.219113
O	0.404478	3.161816	-0.465220
O	0.755998	1.122625	-1.097232
H	1.035301	2.507828	1.775581
C	2.819037	-0.163178	0.487115
C	3.629059	0.668486	-0.296190
C	3.037395	-1.544338	0.453459
C	4.623590	0.129364	-1.108839
H	3.474916	1.749192	-0.275752
C	4.031442	-2.083670	-0.365338
H	2.424760	-2.203943	1.067457
C	4.826864	-1.250633	-1.150074
H	5.238544	0.793204	-1.718400
H	4.184533	-3.163984	-0.383839
H	5.602976	-1.673336	-1.789945
H	2.241022	0.564293	2.434023

2_CIDT

O	4.7275870000	-0.3162780000	-0.8252410000
O	4.1372280000	3.4123960000	1.7633530000
O	2.2975770000	3.1944610000	0.4557980000
N	4.3678880000	0.9366920000	-0.2942570000
C	3.8745030000	-1.3205230000	-0.2507930000
C	2.5283790000	-0.5825910000	-0.0438660000
C	2.9033930000	0.9193360000	-0.2043350000
C	2.5575500000	1.8916820000	0.9314270000
C	3.8596290000	2.0254800000	1.7702920000
C	4.9070030000	1.1555070000	1.0642690000
H	5.8724740000	1.6619720000	1.0041660000
H	5.0293290000	0.2079820000	1.6004190000
C	3.4110910000	4.0519680000	0.7196350000
C	2.8843050000	5.3732070000	1.2419350000
H	3.7193940000	6.0286680000	1.5002100000
H	2.2732120000	5.1973050000	2.1294740000
H	2.2779990000	5.8603010000	0.4746740000
C	4.2713560000	4.2145290000	-0.5262480000
H	4.6322520000	3.2437110000	-0.8736020000
H	5.1260510000	4.8567120000	-0.2981380000
H	3.6811670000	4.6802600000	-1.3198830000
C	3.8027610000	-2.4951530000	-1.1875390000
C	3.5355410000	-2.2936330000	-2.5454940000
H	3.4140740000	-1.2823640000	-2.9245660000
C	3.4396380000	-3.3829220000	-3.4059580000
H	3.2357680000	-3.2222240000	-4.4597100000
C	3.6048970000	-4.6800990000	-2.9148190000
C	3.8713280000	-4.8833520000	-1.5626960000
H	4.0050830000	-5.8890970000	-1.1776930000
C	3.9738720000	-3.7907850000	-0.7006640000
H	4.1906030000	-3.9473780000	0.3528220000
H	3.5284500000	-5.5286230000	-3.5872140000
H	4.2616030000	-1.6365680000	0.7247680000
H	2.4601940000	1.2612310000	-1.1417130000
H	1.6889460000	1.5687470000	1.5094550000
H	3.7317320000	1.7168800000	2.8087970000
N	1.9690300000	-0.8875200000	1.3119560000
O	2.6796660000	-0.6950380000	2.2822590000
O	0.8181880000	-1.2896430000	1.3738590000
H	1.7562570000	-0.8929530000	-0.7461130000
O	-3.0986730000	-2.0592920000	-0.4910180000
O	-4.9626720000	1.3559910000	-2.7244660000
O	-4.1641670000	2.4333390000	-0.8962970000
N	-3.8303620000	-0.8829080000	-0.8755050000
C	-2.2182990000	-1.7408000000	0.5768940000
C	-1.9010010000	-0.2531790000	0.4079410000
C	-3.2320030000	0.2670170000	-0.1699710000
C	-3.2094490000	1.4376360000	-1.1743410000
C	-3.6615160000	0.8263470000	-2.5251680000
C	-3.6376330000	-0.6839080000	-2.3269640000
H	-4.4383630000	-1.1729360000	-2.8848890000
H	-2.6718040000	-1.0975540000	-2.6344370000
C	-5.3700010000	2.1319310000	-1.5997980000
C	-5.9672750000	3.4350740000	-2.0891180000

H	-6.8585550000	3.2307900000	-2.6867150000
H	-5.2344990000	3.9650150000	-2.7008190000
H	-6.2488390000	4.0590020000	-1.2374830000
C	-6.3321670000	1.3350440000	-0.7272630000
H	-5.8945950000	0.3750740000	-0.4409620000
H	-7.2508020000	1.1402050000	-1.2865500000
H	-6.5787520000	1.9083410000	0.1701180000
C	-2.8544830000	-1.9784530000	1.9355510000
C	-4.2387050000	-2.1008090000	2.0616800000
H	-4.8616270000	-2.0509840000	1.1728220000
C	-4.8084680000	-2.2940790000	3.3208380000
H	-5.8855780000	-2.3907760000	3.4145460000
C	-3.9993680000	-2.3669120000	4.4534840000
C	-2.6145410000	-2.2461540000	4.3265290000
H	-1.9794030000	-2.3081410000	5.2045540000
C	-2.0426330000	-2.0522520000	3.0711870000
H	-0.9637730000	-1.9605820000	2.9693800000
H	-4.4442700000	-2.5207690000	5.4314940000
H	-1.3235060000	-2.3565080000	0.4505250000
H	-3.8484160000	0.5408770000	0.6925950000
H	-2.2317430000	1.9230720000	-1.2158080000
H	-3.0346700000	1.1298520000	-3.3668830000
N	-0.7595180000	-0.0119010000	-0.5345110000
O	-0.0778340000	0.9795290000	-0.3260240000
O	-0.5791720000	-0.7838110000	-1.4582420000
H	-1.6126880000	0.2527610000	1.3269730000

TS_CIDT

O	-4.1811140000	-1.8681940000	-0.6121800000
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O	-3.7281820000	1.9379970000	1.8665380000
N	-4.5193840000	-0.7089450000	0.1309070000
C	-3.0778010000	-1.5678130000	-1.4843800000
C	-2.4227420000	-0.3931640000	-0.8031770000
C	-3.2425990000	-0.0088550000	0.4135970000
C	-3.6269950000	1.4814100000	0.5361430000
C	-5.0713960000	1.5663700000	-0.0156270000
C	-5.3137890000	0.2252550000	-0.6883530000
H	-6.3646760000	-0.0674780000	-0.6860550000
H	-4.9493710000	0.2645590000	-1.7253910000
C	-5.0741170000	1.8083370000	2.3190860000
C	-5.4321550000	3.0581620000	3.0998410000
H	-6.4753210000	3.0082940000	3.4208210000
H	-5.2902440000	3.9367010000	2.4668820000
H	-4.7945170000	3.1418230000	3.9834100000
C	-5.2551290000	0.5351150000	3.1338720000
H	-5.0125560000	-0.3392160000	2.5259620000
H	-6.2950640000	0.4556570000	3.4615440000
H	-4.6080970000	0.5657800000	4.0145380000
C	-2.1531420000	-2.7665560000	-1.5386020000
C	-1.9226290000	-3.5197710000	-0.3804350000
H	-2.4891430000	-3.2969270000	0.5198480000
C	-0.9909610000	-4.5571250000	-0.3934410000
H	-0.8239030000	-5.1437490000	0.5046440000
C	-0.2826910000	-4.8459690000	-1.5609340000
C	-0.5133830000	-4.0983710000	-2.7154500000
H	0.0350580000	-4.3201120000	-3.6253990000
C	-1.4469650000	-3.0619890000	-2.7061490000
H	-1.6177520000	-2.4653240000	-3.5969330000
H	0.4425520000	-5.6535150000	-1.5715910000
H	-3.4196620000	-1.3081700000	-2.4958330000
H	-2.8249390000	-0.3767200000	1.3566250000
H	-2.9101520000	2.1141420000	0.0159360000
H	-5.2300670000	2.4059080000	-0.6970530000
N	-1.5646170000	0.3743100000	-1.4827070000
O	-1.2340400000	0.0782660000	-2.6658800000
O	-0.9703180000	1.3436800000	-0.8866310000
H	-0.6808470000	-1.3242600000	-0.2017360000
O	2.8276480000	-0.3816970000	-1.5779720000
O	4.8703430000	-1.8194300000	2.1079270000
O	3.9786600000	0.1200490000	2.8816370000
N	3.5863720000	-0.5166550000	-0.3664320000
C	1.9429880000	0.7255780000	-1.4680710000
C	1.6417330000	0.8369370000	0.0309320000
C	2.9881570000	0.3741660000	0.6402670000
C	3.0267800000	-0.3869000000	1.9827120000
C	3.5380410000	-1.8055880000	1.6256190000
C	3.4385450000	-1.9066850000	0.1099650000
H	4.2261420000	-2.5359180000	-0.3075970000
H	2.4626150000	-2.3085890000	-0.1869790000
C	5.2211880000	-0.5586540000	2.6769960000
C	5.8593530000	-0.7839270000	4.0317220000

H	6.7821450000	-1.3562290000	3.9137060000
H	5.1698340000	-1.3361600000	4.6732340000
H	6.0967570000	0.1765020000	4.4953300000
C	6.1210090000	0.2160460000	1.7230560000
H	5.6608850000	0.3017860000	0.7352750000
H	7.0704490000	-0.3137520000	1.6121770000
H	6.3167750000	1.2127470000	2.1265460000
C	2.5572510000	2.0253390000	-1.9497710000
C	3.9381790000	2.1602400000	-2.0923660000
H	4.5839960000	1.3124200000	-1.8794380000
C	4.4741580000	3.3755770000	-2.5202210000
H	5.5484900000	3.4795310000	-2.6350650000
C	3.6337310000	4.4510680000	-2.8039270000
C	2.2515620000	4.3120560000	-2.6631200000
H	1.5943960000	5.1449120000	-2.8923670000
C	1.7116770000	3.1011480000	-2.2363790000
H	0.6362130000	2.9747800000	-2.1298200000
H	4.0530570000	5.3941740000	-3.1398870000
H	1.0429190000	0.4868170000	-2.0434090000
H	3.5732010000	1.2959610000	0.7303960000
H	2.0599590000	-0.3844070000	2.4918700000
H	2.9787410000	-2.6031790000	2.1205850000
N	0.4995330000	-0.0216080000	0.4462150000
O	-0.1161170000	0.1551860000	1.4454910000
O	0.3017640000	-1.0920090000	-0.2784620000
H	1.3425510000	1.8263410000	0.3727540000

Int_CIDT

O	-4.0967270000	-2.0947300000	-0.3493250000
O	-5.9514570000	1.5739620000	1.1415720000
O	-3.7747380000	2.0367930000	1.6110470000
N	-4.4772390000	-0.8923020000	0.3063180000
C	-3.0903930000	-1.8044870000	-1.3371360000
C	-2.5206510000	-0.5035180000	-0.8519160000
C	-3.2521990000	-0.0576880000	0.3852130000
C	-3.7531950000	1.4013630000	0.3518770000
C	-5.2420980000	1.3022160000	-0.0576430000
C	-5.4248040000	-0.1304490000	-0.5306430000
H	-6.4414640000	-0.4984520000	-0.3845080000
H	-5.1628470000	-0.1994190000	-1.5963840000
C	-5.0537770000	1.8608460000	2.2139650000
C	-5.4562120000	3.1725030000	2.8601490000
H	-6.4564110000	3.0823660000	3.2904870000
H	-5.4561680000	3.9642340000	2.1079340000
H	-4.7515090000	3.4288080000	3.6551370000
C	-5.0375780000	0.7010140000	3.2002710000
H	-4.7694370000	-0.2259540000	2.6885560000
H	-6.0309760000	0.5818340000	3.6409600000
H	-4.3185040000	0.9050330000	3.9980320000
C	-2.0417910000	-2.8985930000	-1.3031210000
C	-1.6312330000	-3.4306940000	-0.0709810000
H	-2.1462420000	-3.1257670000	0.8356630000
C	-0.5801170000	-4.3502010000	-0.0169120000
H	-0.2749530000	-4.7639390000	0.9390470000
C	0.0718350000	-4.7359550000	-1.1906550000
C	-0.3364330000	-4.2076370000	-2.4157920000
H	0.1710610000	-4.5001290000	-3.3292150000
C	-1.3902250000	-3.2942710000	-2.4734520000
H	-1.6924890000	-2.8600390000	-3.4208950000
H	0.8915990000	-5.4458350000	-1.1494100000
H	-3.5234390000	-1.7308090000	-2.3444580000
H	-2.7187140000	-0.2620190000	1.3200590000
H	-3.1383110000	2.0021140000	-0.3176710000
H	-5.5373640000	2.0295850000	-0.8181320000
N	-1.6071320000	0.1517640000	-1.5303410000
O	-1.2318160000	-0.2426460000	-2.6863350000
O	-1.0105570000	1.1684720000	-0.9901750000
H	-0.1446380000	-1.9536480000	-0.5278940000
O	2.9363880000	-0.0000910000	-1.7868800000
O	5.1121380000	-1.7583810000	1.7061150000
O	3.9059880000	-0.1402350000	2.7426790000
N	3.6938390000	-0.2199010000	-0.5867180000
C	1.8978600000	0.9343030000	-1.5276200000
C	1.5522510000	0.7304610000	-0.0469460000
C	2.9401130000	0.3650640000	0.5338860000
C	3.0713350000	-0.6153260000	1.7183600000
C	3.8155140000	-1.8479550000	1.1432290000
C	3.7889830000	-1.6774780000	-0.3703460000
H	4.6939290000	-2.0712470000	-0.8359820000
H	2.9158570000	-2.1817510000	-0.8004340000
C	5.2457990000	-0.5735830000	2.4898970000
C	5.8820210000	-0.9263480000	3.8178020000

H	6.8866540000	-1.3213090000	3.6513460000
H	5.2758080000	-1.6795400000	4.3248410000
H	5.9530300000	-0.0344210000	4.4447790000
C	6.0311090000	0.4815160000	1.7216440000
H	5.5859270000	0.6645610000	0.7400990000
H	7.0549840000	0.1300680000	1.5715310000
H	6.0567690000	1.4125910000	2.2933840000
C	2.3281910000	2.3737380000	-1.7371470000
C	3.6779690000	2.7131040000	-1.8308990000
H	4.4314880000	1.9322350000	-1.7759440000
C	4.0457500000	4.0480060000	-2.0054830000
H	5.0960740000	4.3112100000	-2.0817850000
C	3.0690800000	5.0393720000	-2.0851820000
C	1.7187860000	4.6961840000	-1.9924310000
H	0.9558270000	5.4651240000	-2.0617120000
C	1.3458590000	3.3656460000	-1.8175340000
H	0.2982420000	3.0802920000	-1.7488680000
H	3.3576550000	6.0765590000	-2.2236890000
H	1.0495250000	0.6756520000	-2.1688610000
H	3.3701230000	1.3318160000	0.8182170000
H	2.1055370000	-0.8561140000	2.1697670000
H	3.3709390000	-2.7990890000	1.4468230000
N	0.5543430000	-0.3551380000	0.1548280000
O	-0.1345490000	-0.4484530000	1.1136030000
O	0.5924000000	-1.3104040000	-0.7335900000
H	1.0887020000	1.5832380000	0.4441630000

X-ray data

Procedure for the single crystal preparation

Single crystals suitable for X-ray diffraction measurements were obtained by slowly evaporating saturated solutions of the compounds **3F** and **4F** in DCM. 10 mg of the products **3F** and **4F** were dissolved in 1 mL of DCM in a clean and dry 10 mL glass vial. The mouth of the glass vial was covered with a cap having a small hole and kept it for slow evaporation at room temperature. At the end of the process, prismatic single crystals of **3F** and **4F** were obtained after around 7 days.

X-Ray Crystallography

Suitable single crystals of compounds **3F** and **4F** were mounted on glass fibre for data collection on a Bruker Kappa APEX II diffractometer. Data were collected at 298(2) K using Cu K_α radiation (λ = 1.54178 Å) and ω scan technique and were corrected for Lorentz and polarization effects. The detector was placed at a distance of approximately 37.5 mm from the crystal.

A series of narrow frames of data were collected with a scan width of 0.5º in ω and an exposure time of 10 s per frame. The data were integrated with SAINT[1] to a resolution of 0.78 Å using a narrow-frame algorithm. Data were corrected for absorption effects using the multi-scan method using SADABS. [2]

Subsequent structure solution and refinement were carried out with SHELXT and SHELXL, respectively.[3,4] The structures were solved by direct methods combined with difference Fourier synthesis and refined by full-matrix least-squares procedures, with anisotropic thermal parameters in the last cycles of refinement for all non-hydrogen atoms. The refinement was based on F^2 for all reflections, weighted R factors (*wR*) and goodness-of-fit (GoF) values are based on F^2, while conventional R factors (R) are based on F. The $Fo^2 > 2\sigma(Fo^2)$ criterion was used only for calculating R factors and it is not relevant to the choice of reflections for the refinement. The R factors based on F^2 are about twice as large as those based on F. Scattering factors were taken from the International Tables for Crystallography.[5] There is one independent molecule in the asymmetric unit of compound **4F**. The asymmetric unit of the compound **3F** contains two crystallographically independent molecules with similar geometries. H atoms of SP^3 hybridized carbons were located directly in a difference Fourier map and freely refined. The rest of the hydrogen atoms were positioned geometrically. Mercury 4.2.0 program was used for analysis and molecular and crystal structure drawings preparation.[6]

a. Crystal Data

Table S2. Crystal data and structure refinement for compound **3F**. **CCDC 2194507**.

Empirical formula	$C_{15}H_{17}FN_2O_5$
Formula weight	324.31
Temperature (K)	298(2)
Wavelength (Å)	1.54178
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions:	
a (Å)	6.3774(3)
b (Å)	8.9628(5)
c (Å)	13.9221(7)
α [º], β[º], γ[º]	90.00, 99.748(4), 90.00
Volume, Z	784.29(7), 2
Density (calculated) (Mg/m^3)	1.373
Absorption coefficient (mm^{-1})	0.950
F(000)	340
Crystal size (mm)	0.15 x 0.12 x 0.10
2Θ range for data collection (°)	3.22 to 65.79
Limiting indices	$-7 \leq h \leq 7$, $-8 \leq k \leq 10$, $-16 \leq l \leq 15$
Reflections collected/Independent	6847 / 2238 (R_{int} = 0.0350)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2238 / 1 / 231
Goodness-of-fit on F^2	1.045
Final R indices [I>2σ(I)]	R1 = 0.0316, wR2 = 0.0701
R indices (all data)	R1 = 0.0365, wR2 = 0.0728
peak and hole ($eÅ^{-3}$)	0.113 and -0.114

Table S3. Crystal data and structure refinement for compound **4F**. **CCDC 2194506**.

Empirical formula	$C_{15}H_{17}FN_2O_5$
Formula weight	324.31
Temperature (K)	298(2)
Wavelength (Å)	1.54178
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions:	
a (Å)	10.4371(6)
b (Å)	9.9381(4)
c (Å)	15.5195(8)
α [º], β[º], γ[º]	90, 104.104(4), 90
Volume, Z	1561.23(14), 4
Density (calculated) (Mg/m^3)	1.380
Absorption coefficient (mm^{-1})	0.954
F(000)	680
Crystal size (mm)	0.20 x 0.16 x 0.12
2Θ range for data collection (°)	2.94 to 67.55
Limiting indices	$-12 \leq h \leq 11$, $-8 \leq k \leq 11$, $-18 \leq l \leq 17$
Reflections collected/Independent	7012 /3463 (R_{int} = 0.0429)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3463 / 1 / 459
Goodness-of-fit on F^2	1.046
Final R indices [I>2σ(I)]	R1 = 0.0397, wR2 = 0.0915
R indices (all data)	R1 = 0.0539, wR2 = 0.1010
Largest diff. peak and hole ($eÅ^{-3}$)	0.134 and -0.153

b. Molecular structures of the title compounds

$C_{15}H_{17}FN_2O_5$

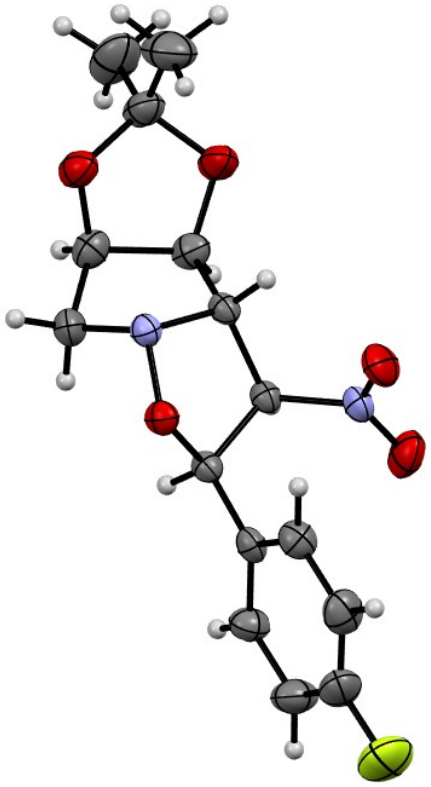

Figure S4. Molecular structure of compound **3F**. Displacement ellipsoids are drawn at 50 % probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

$C_{15}H_{17}FN_2O_5$

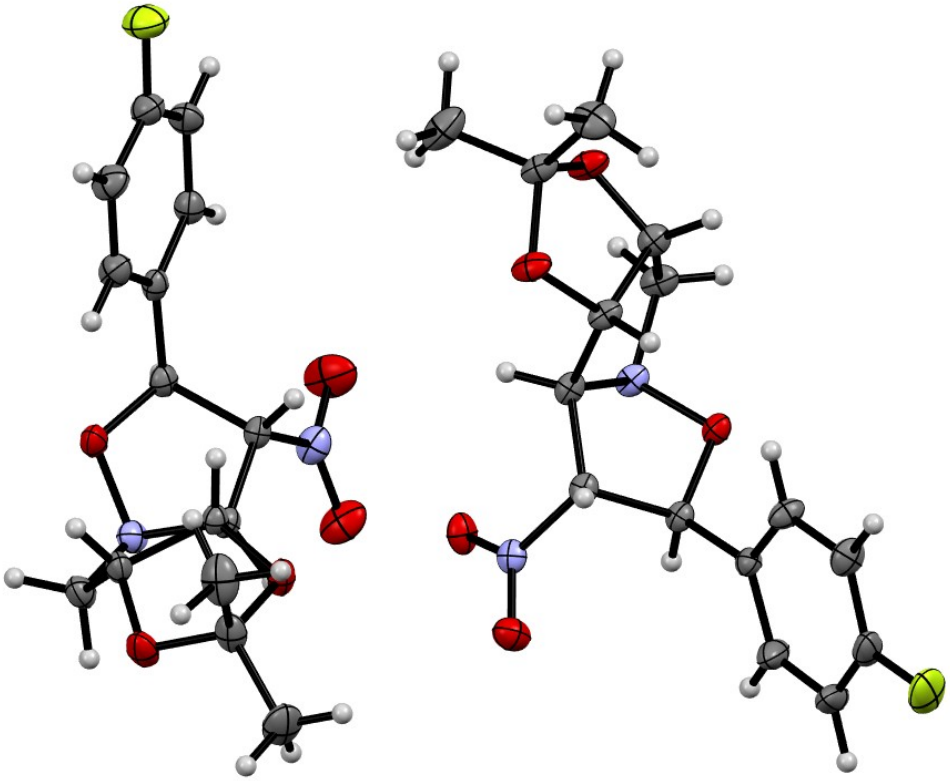

Figure S5. Molecular structure of compound **4F**. Displacement ellipsoids are drawn at 50 % probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

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