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Supporting Information  
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## Supporting Information

### **Decarbonylative-dibromination of 5-phenylthiophene-2-carbaldehyde with bromine**

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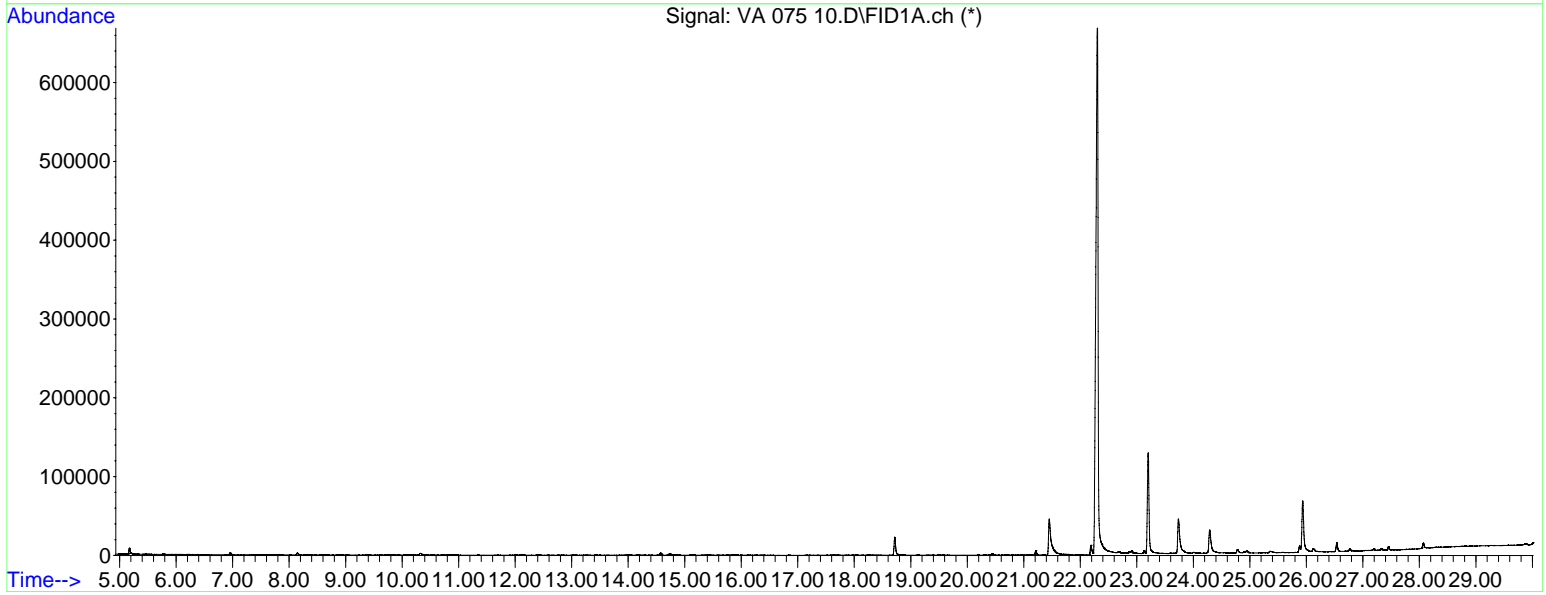
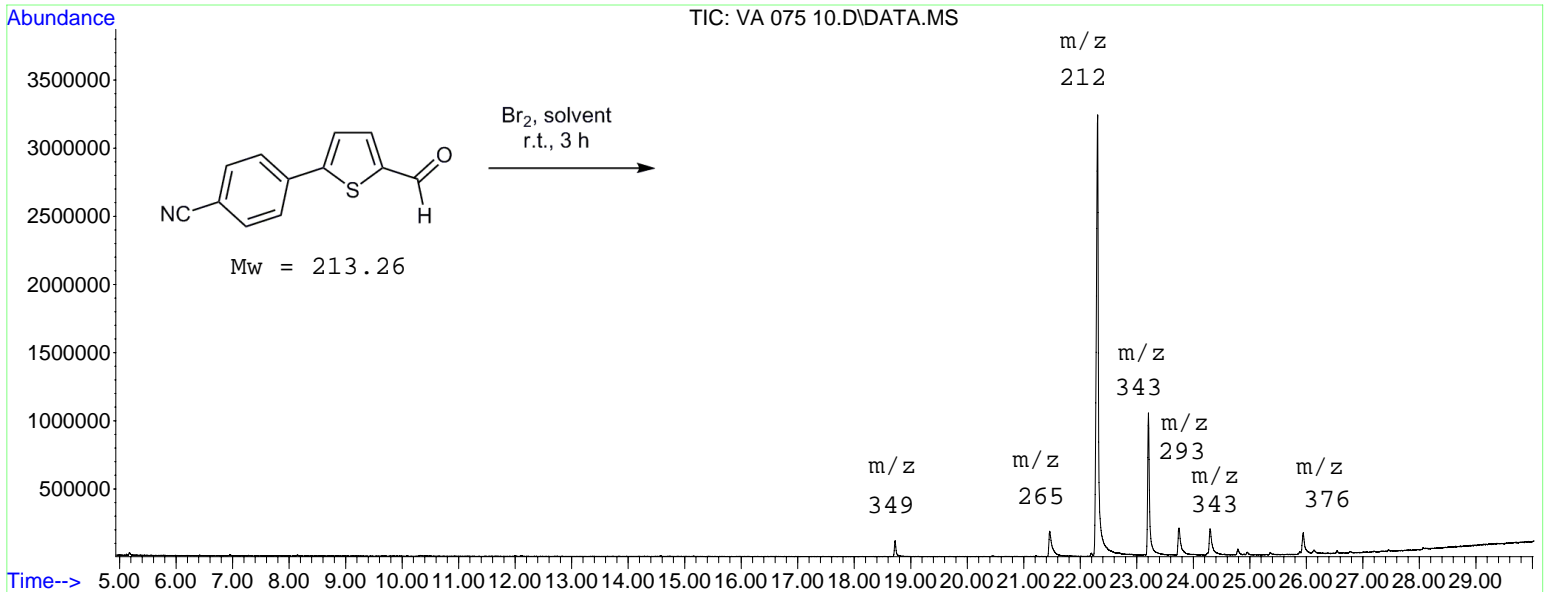
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\* Corresponding author.

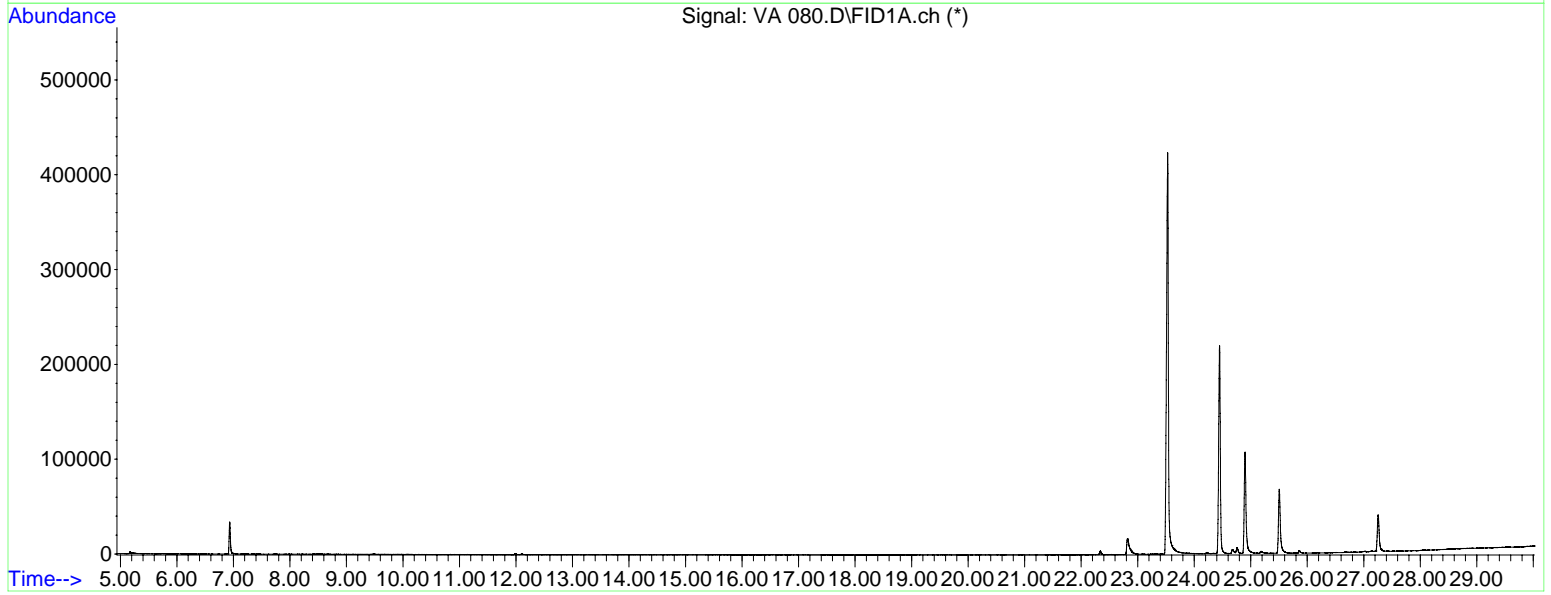
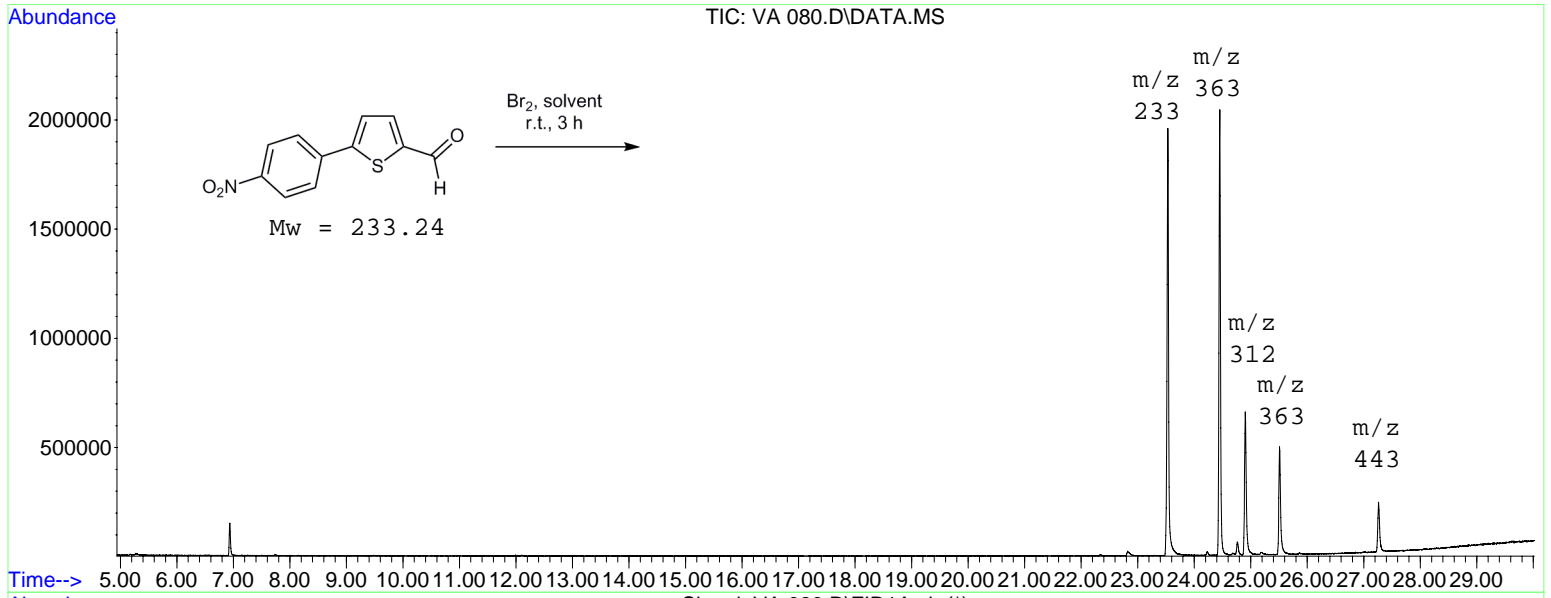
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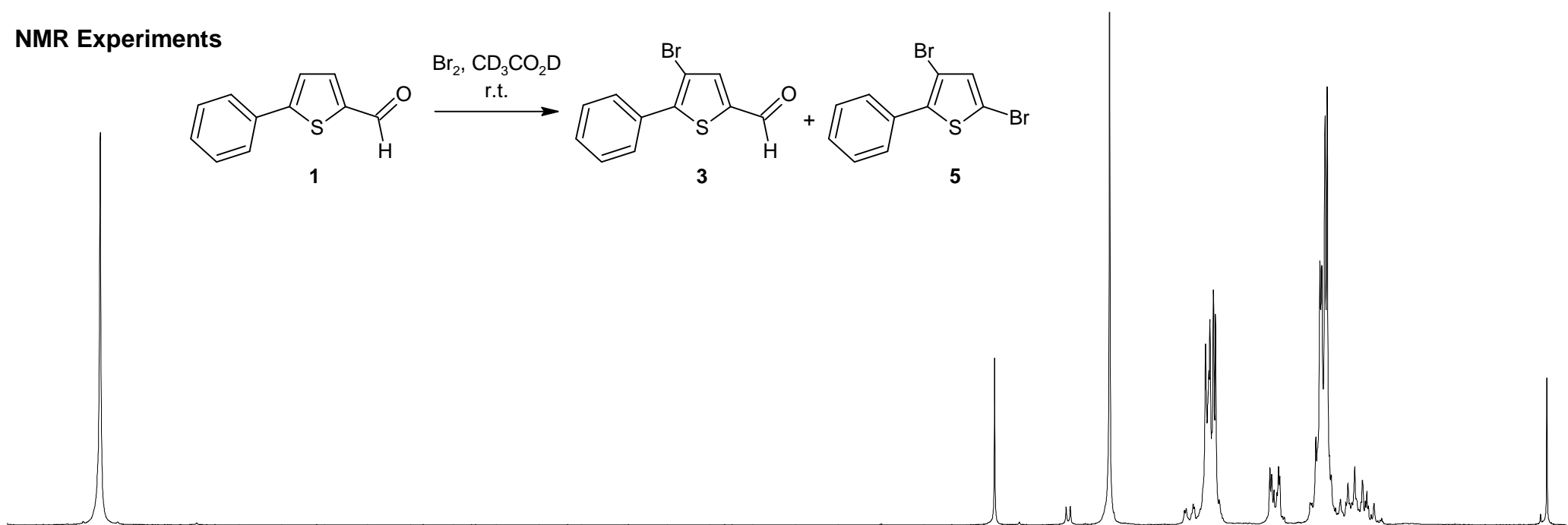
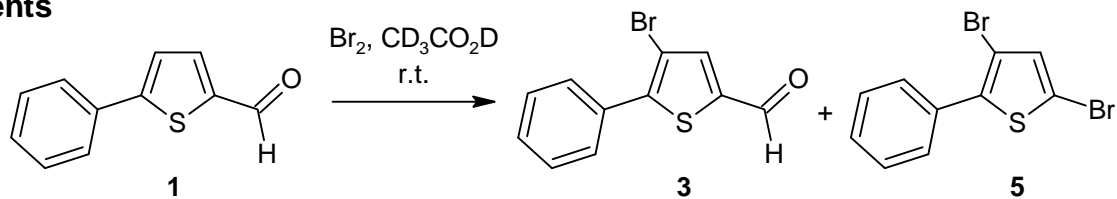
# GC-MS Analysis



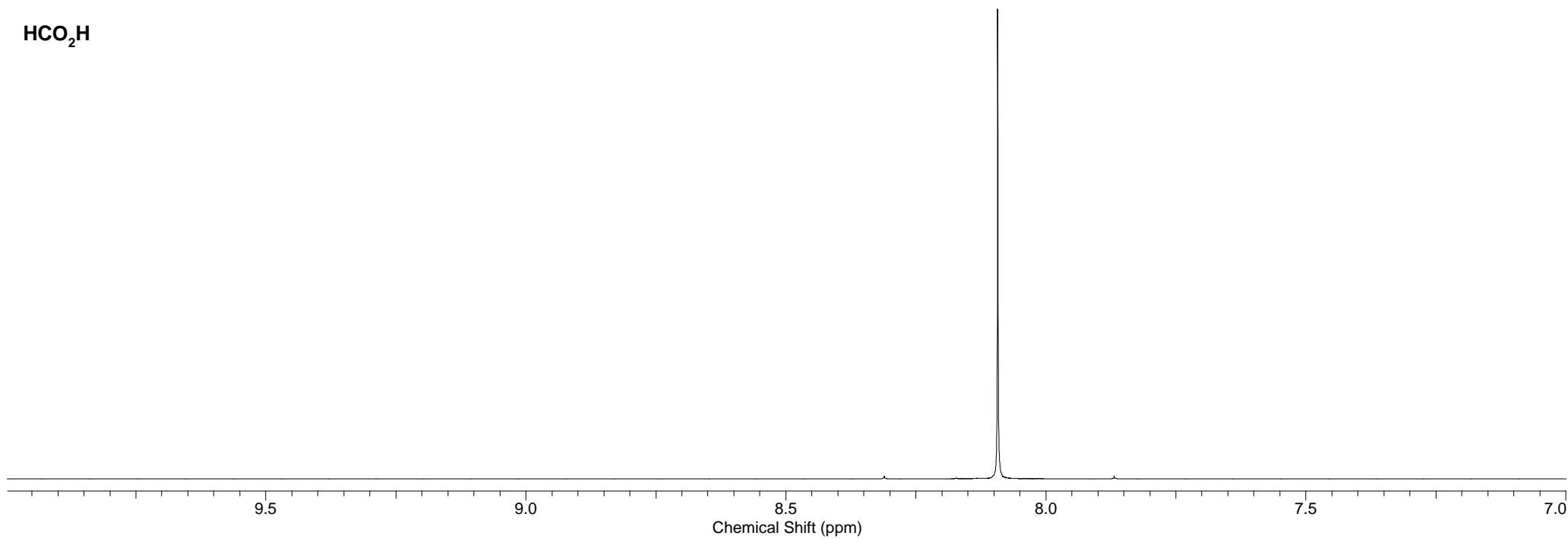
# GC-MS Analysis



# NMR Experiments

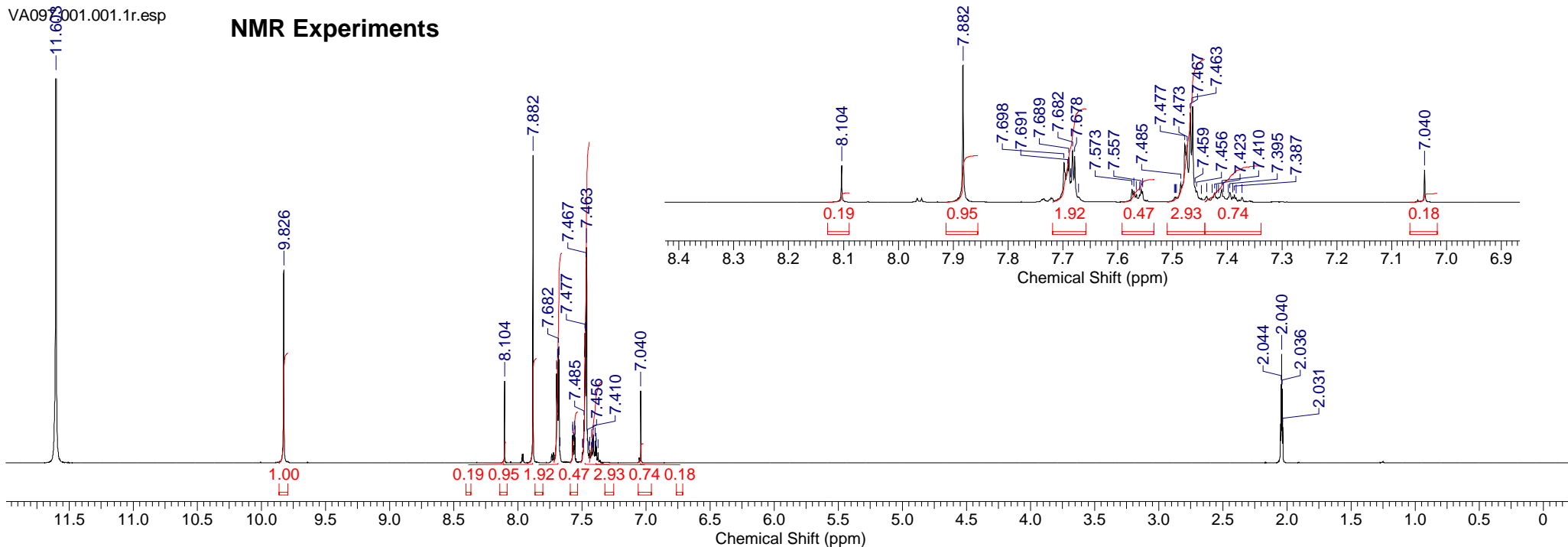


HCO<sub>2</sub>H

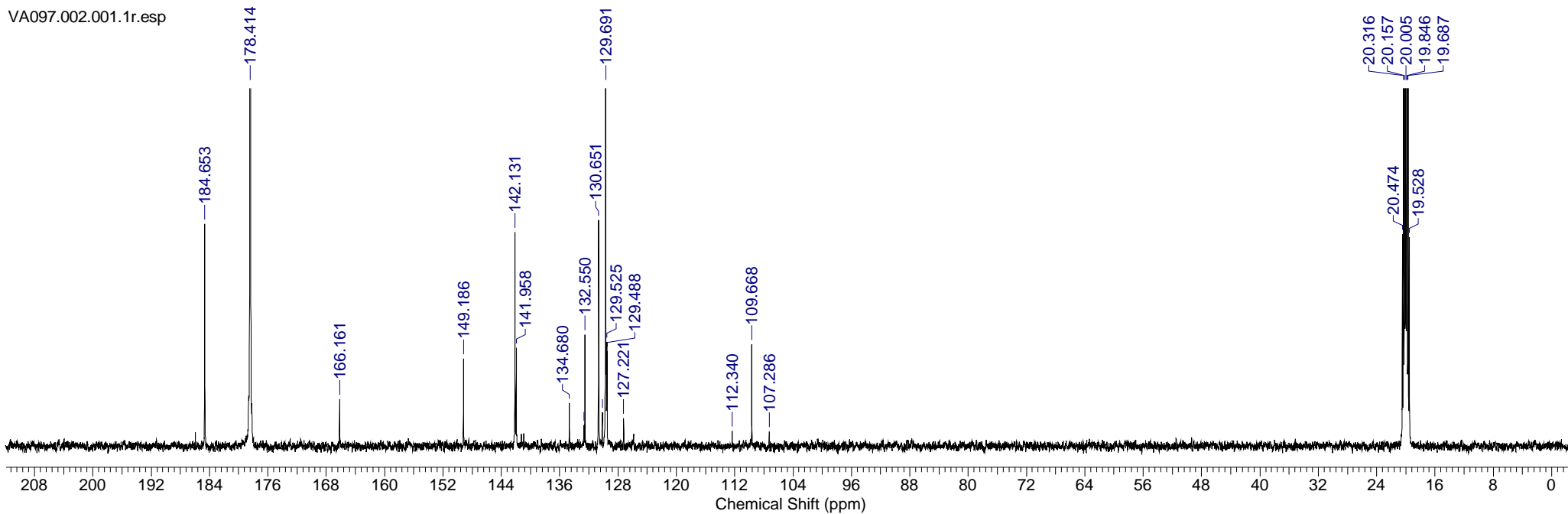


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### NMR Experiments

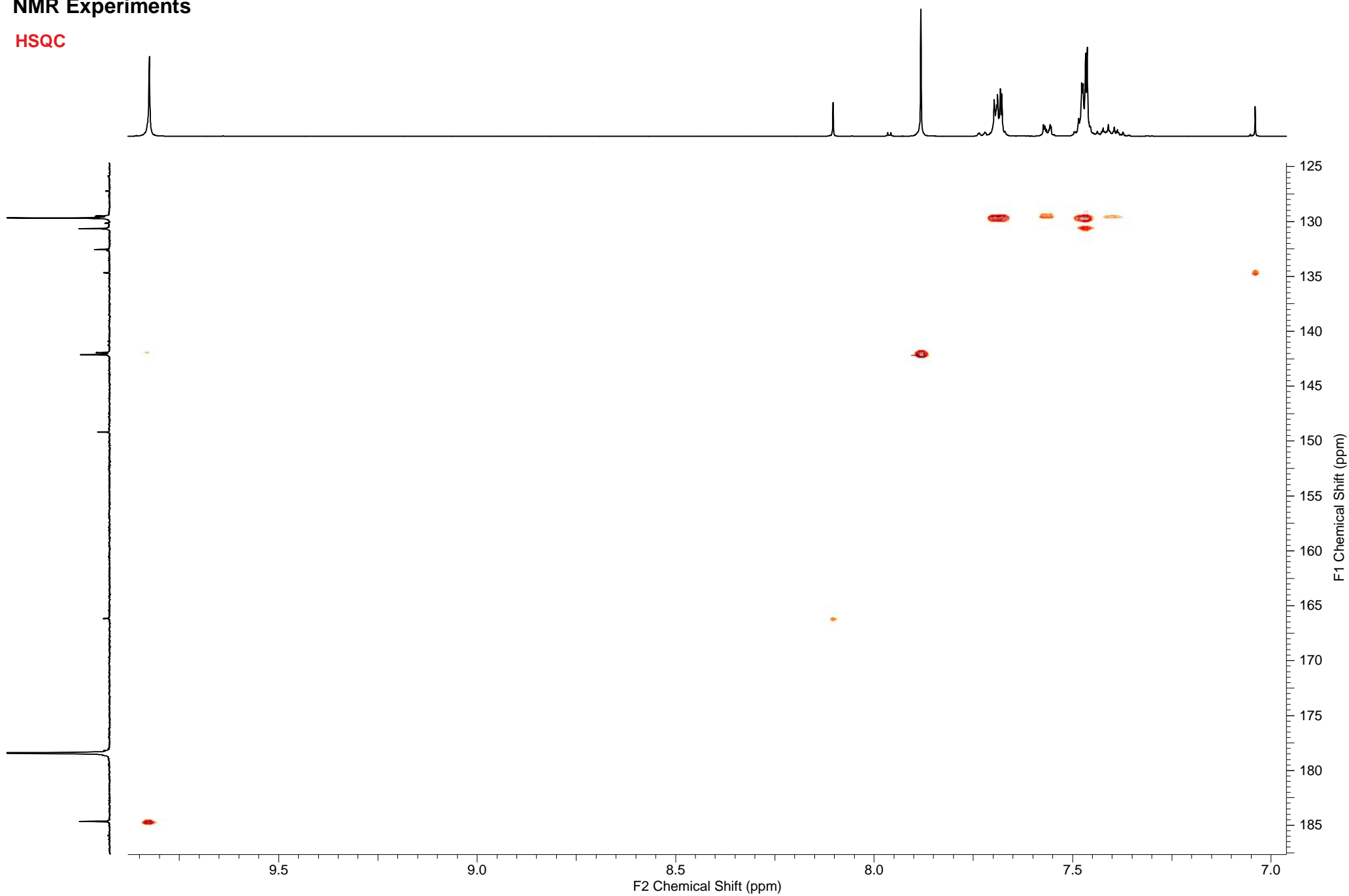


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# NMR Experiments

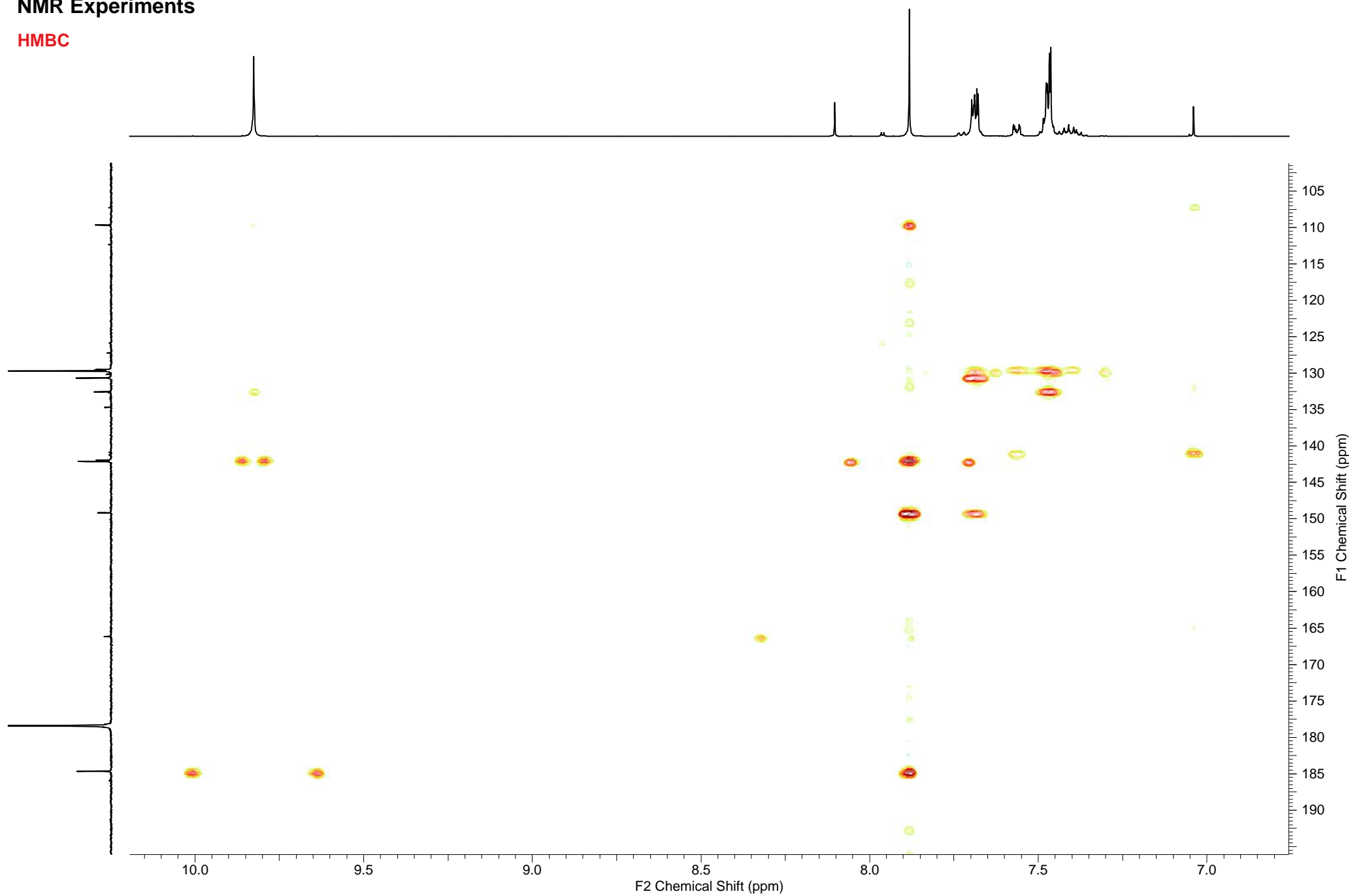
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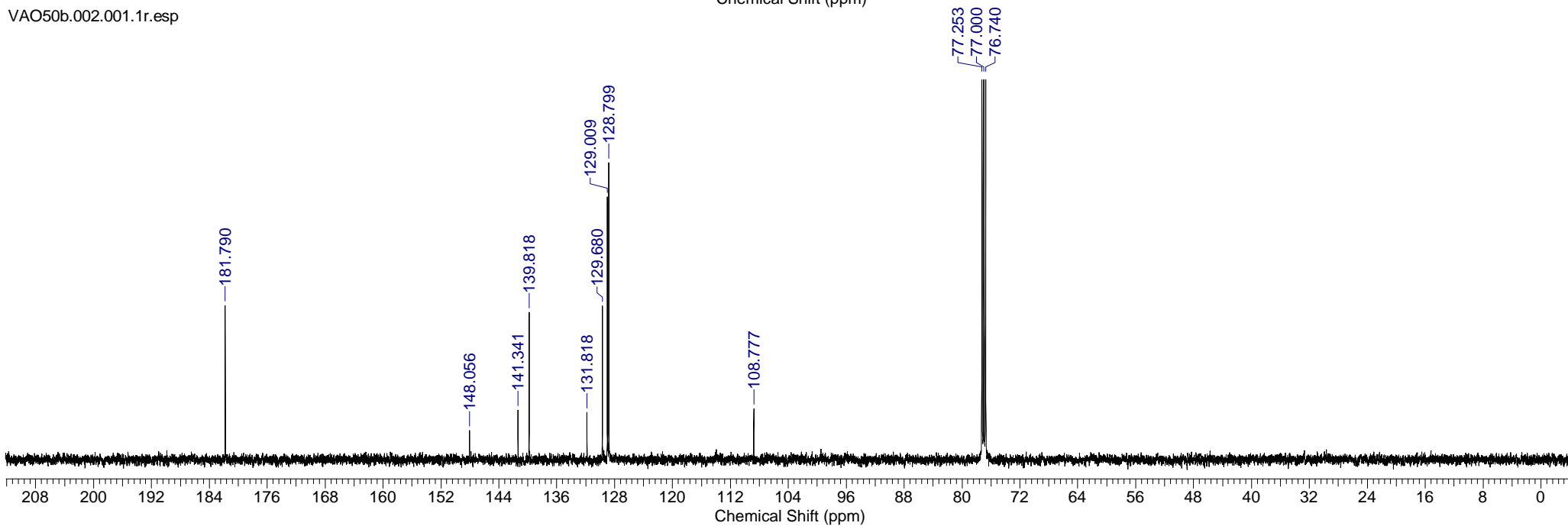
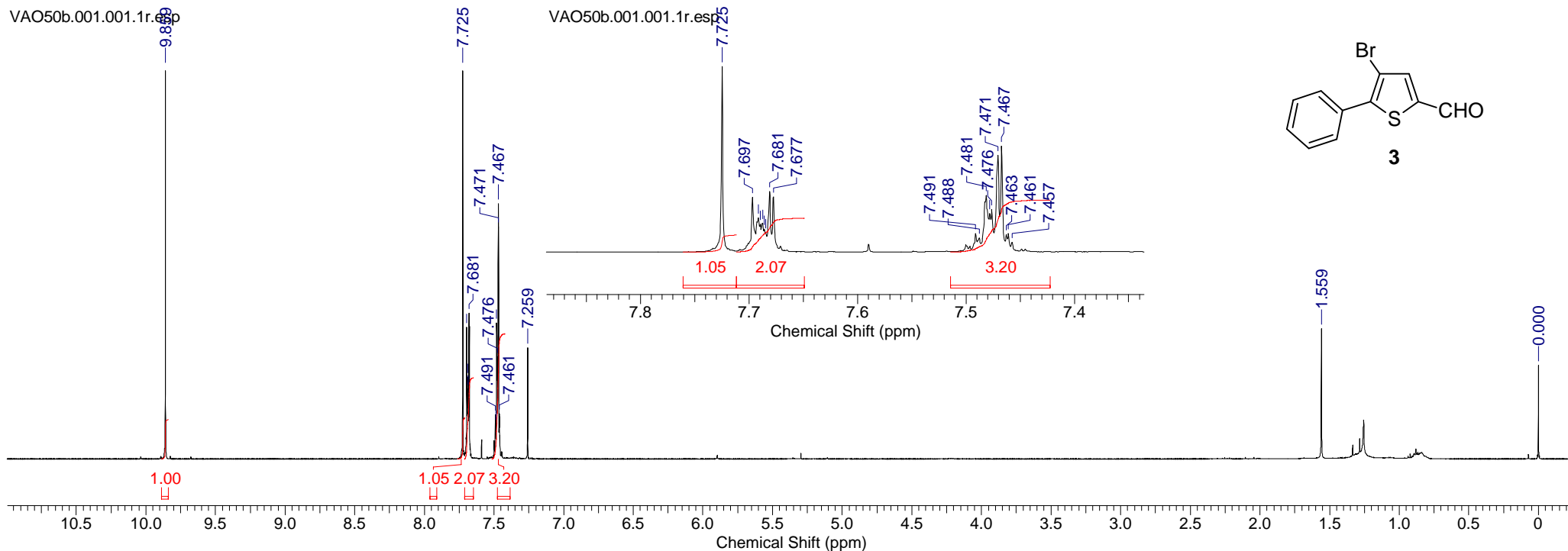




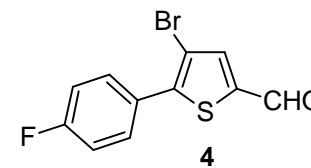
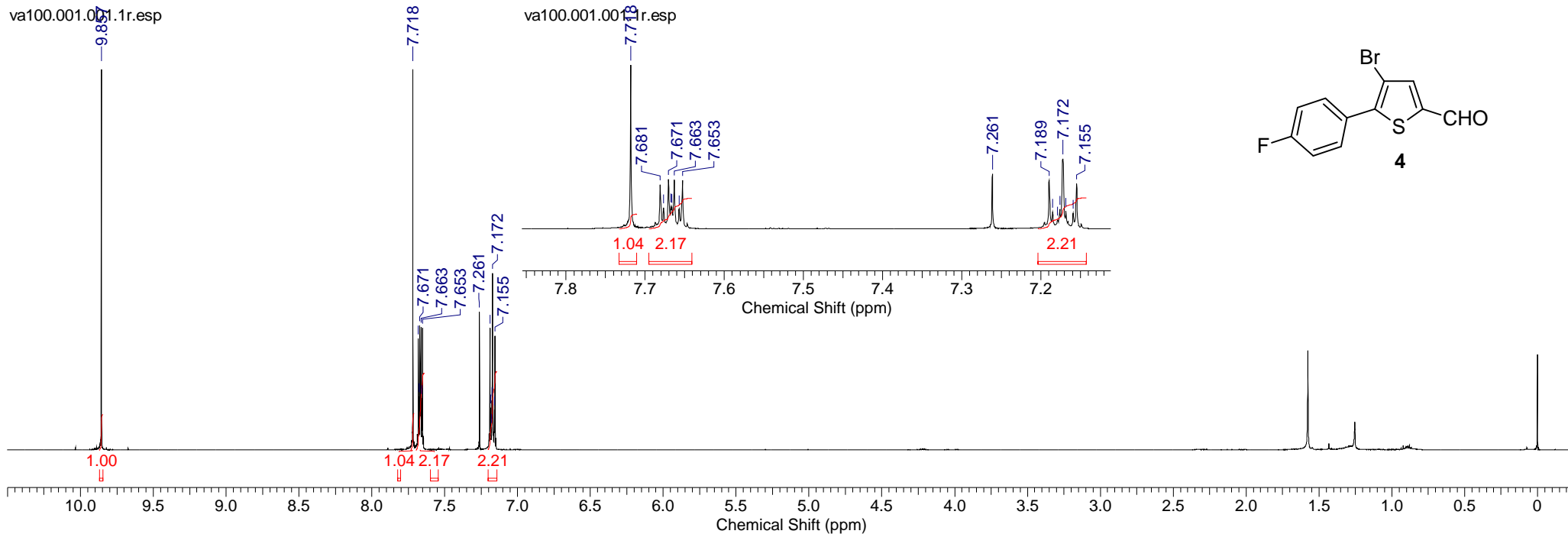
# NMR Experiments

HMBC

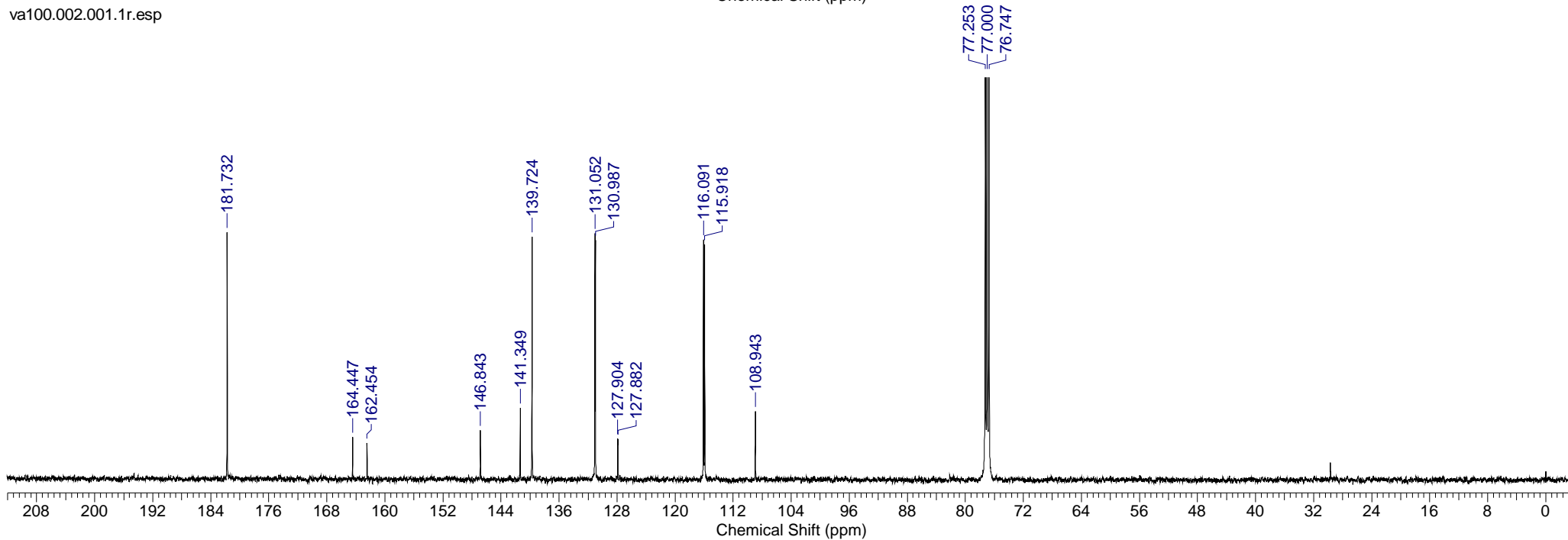




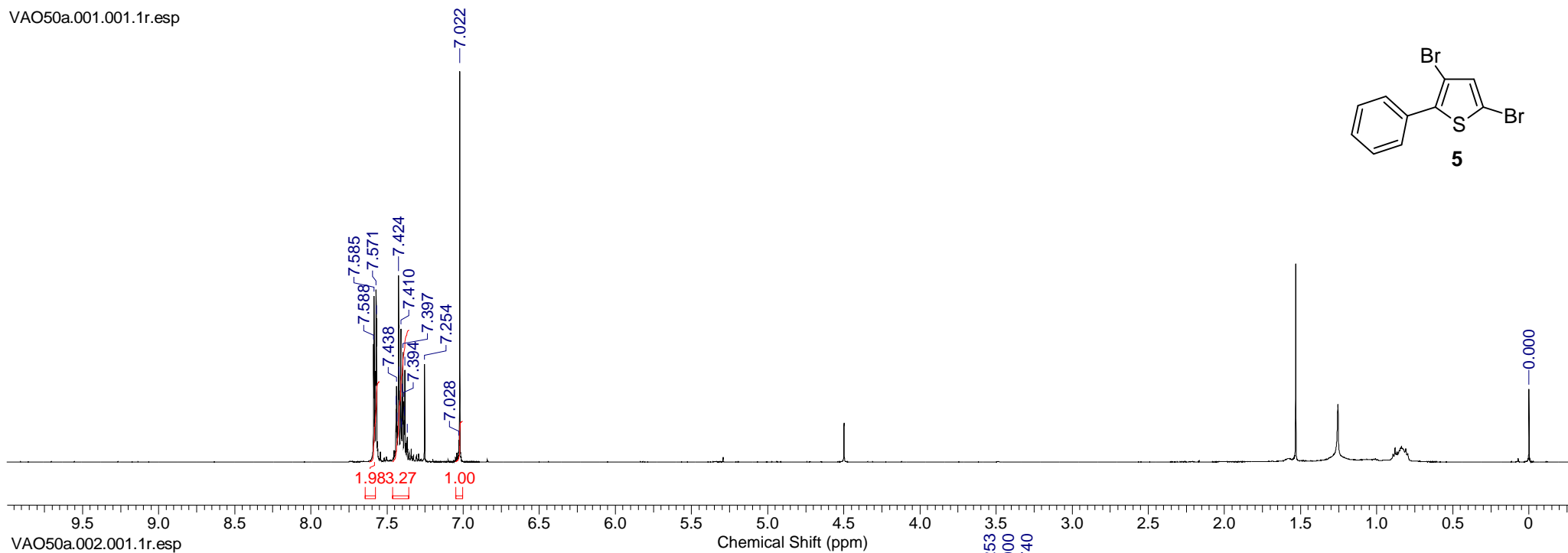
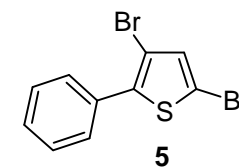
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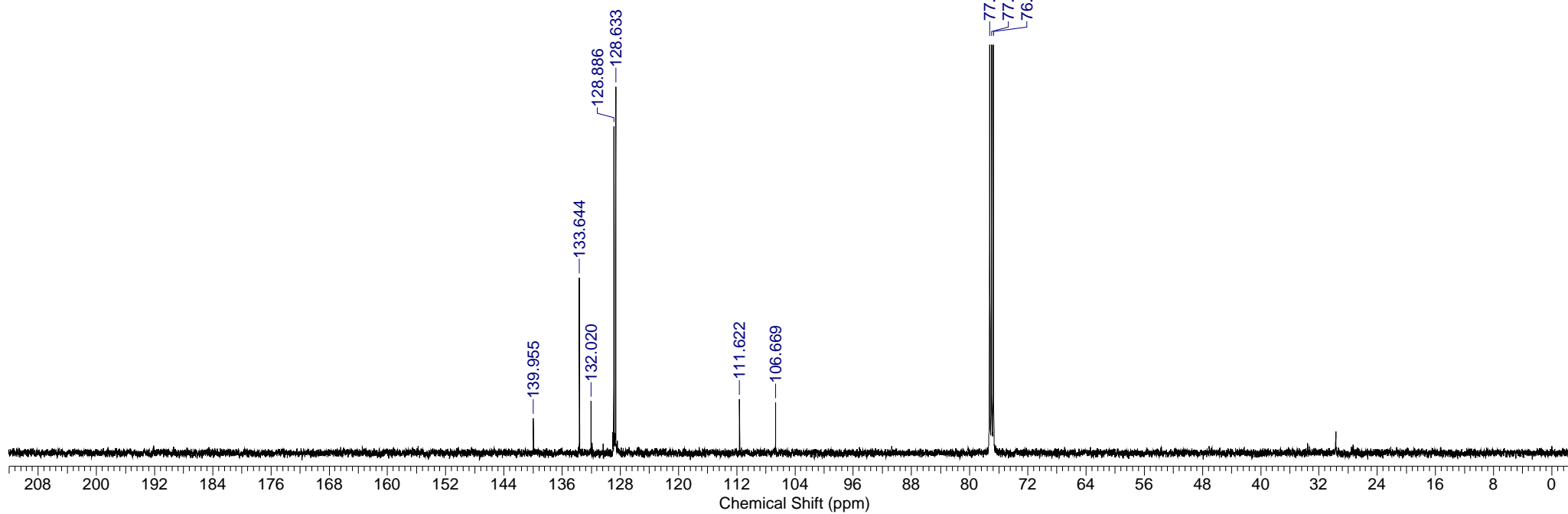
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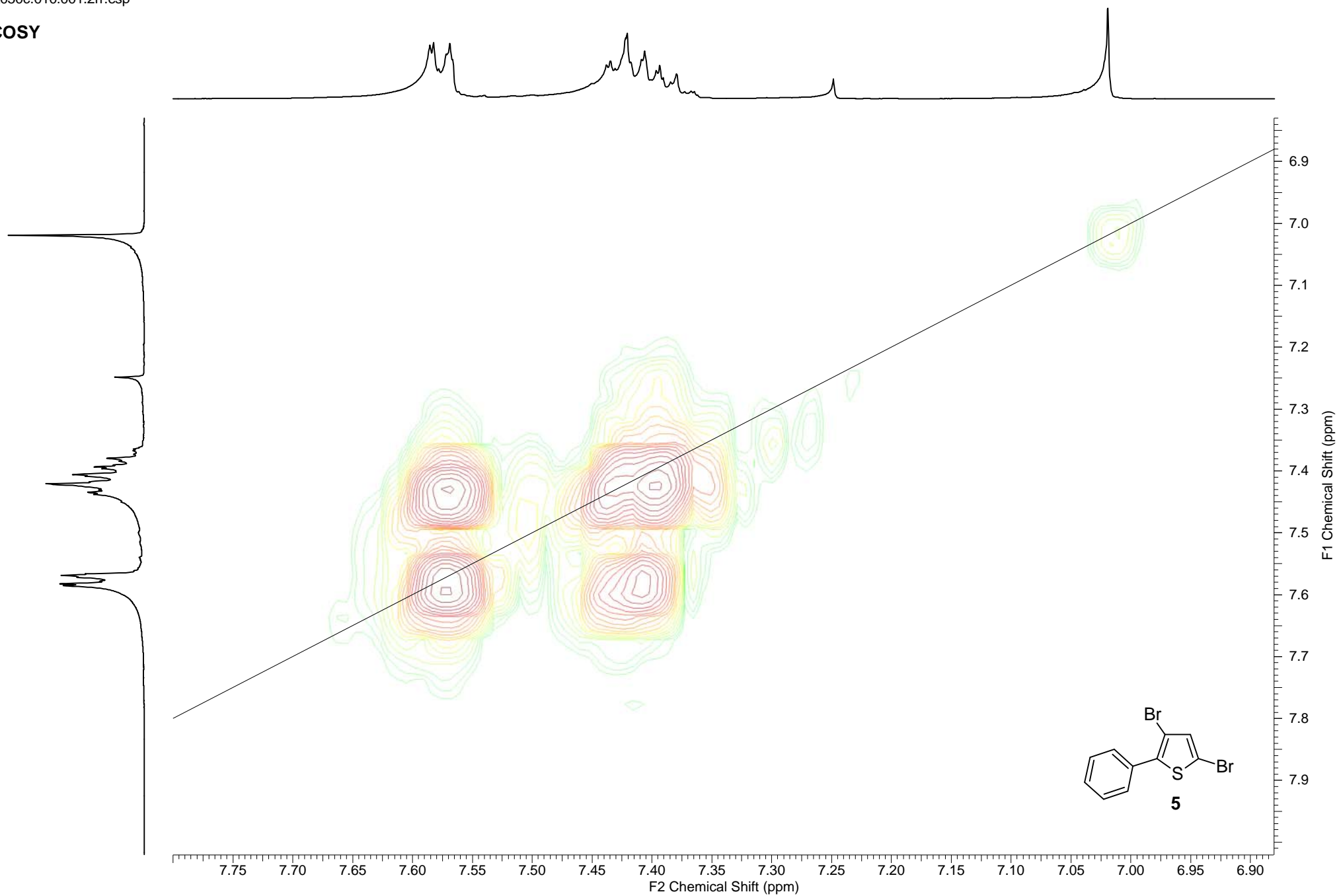
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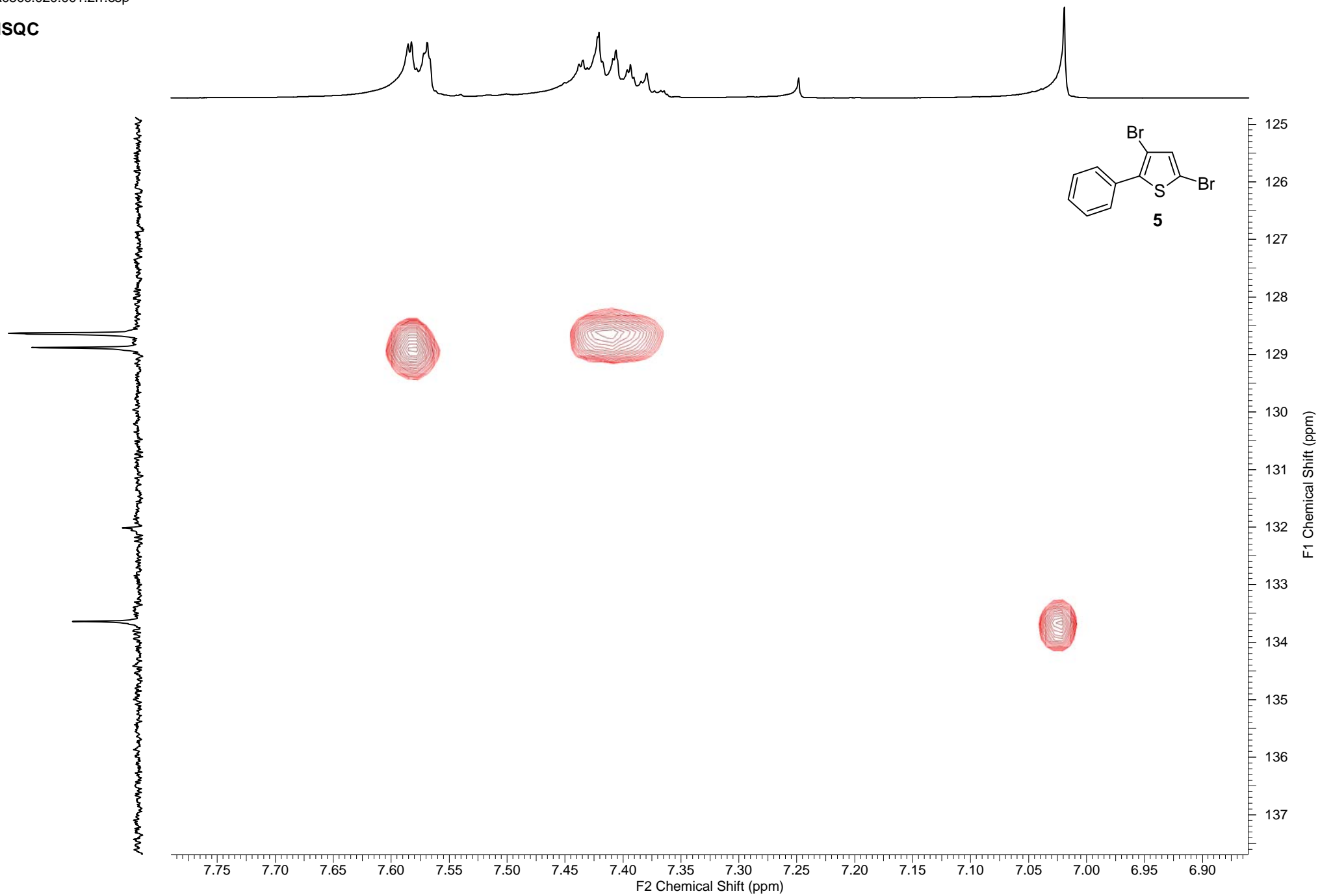
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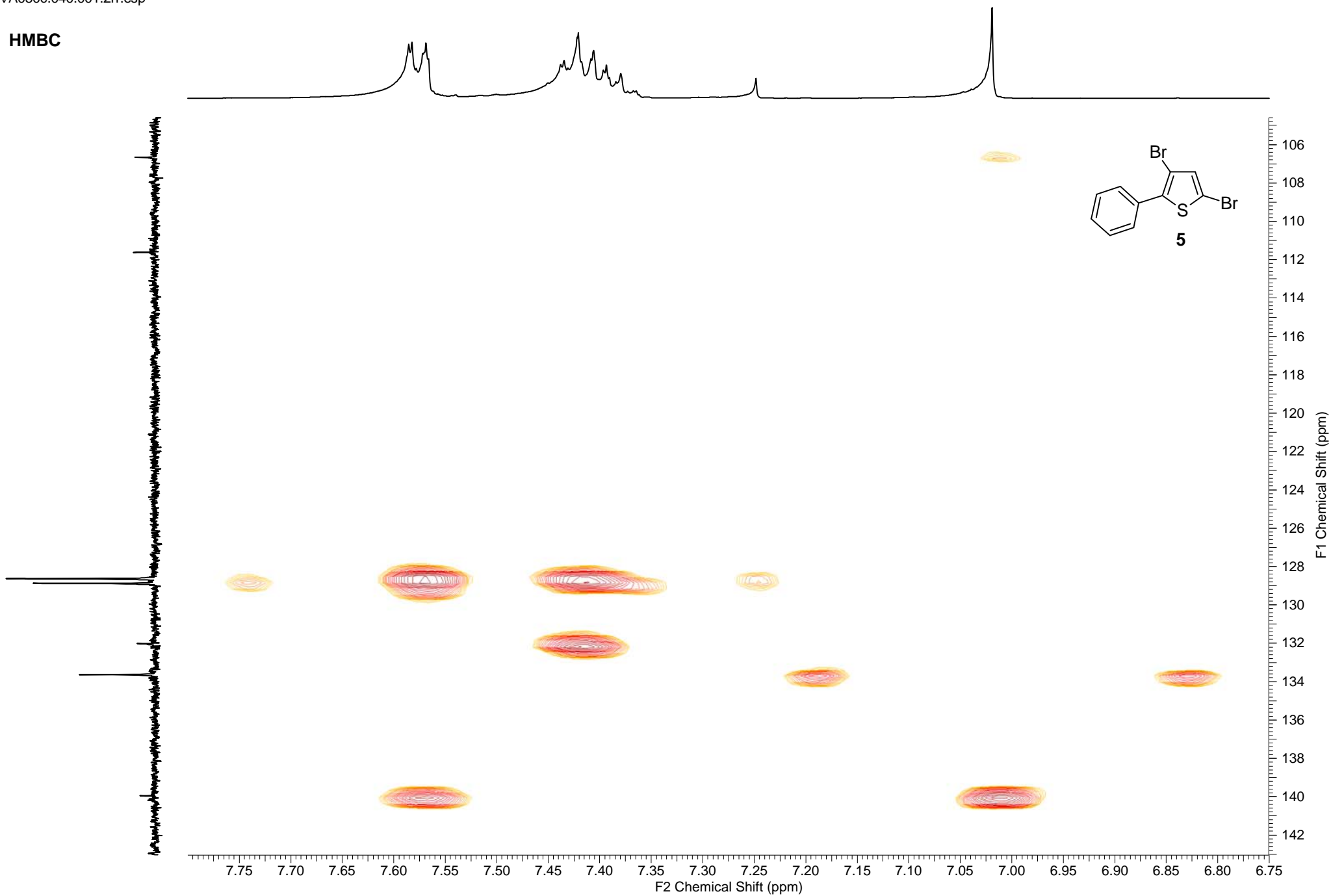
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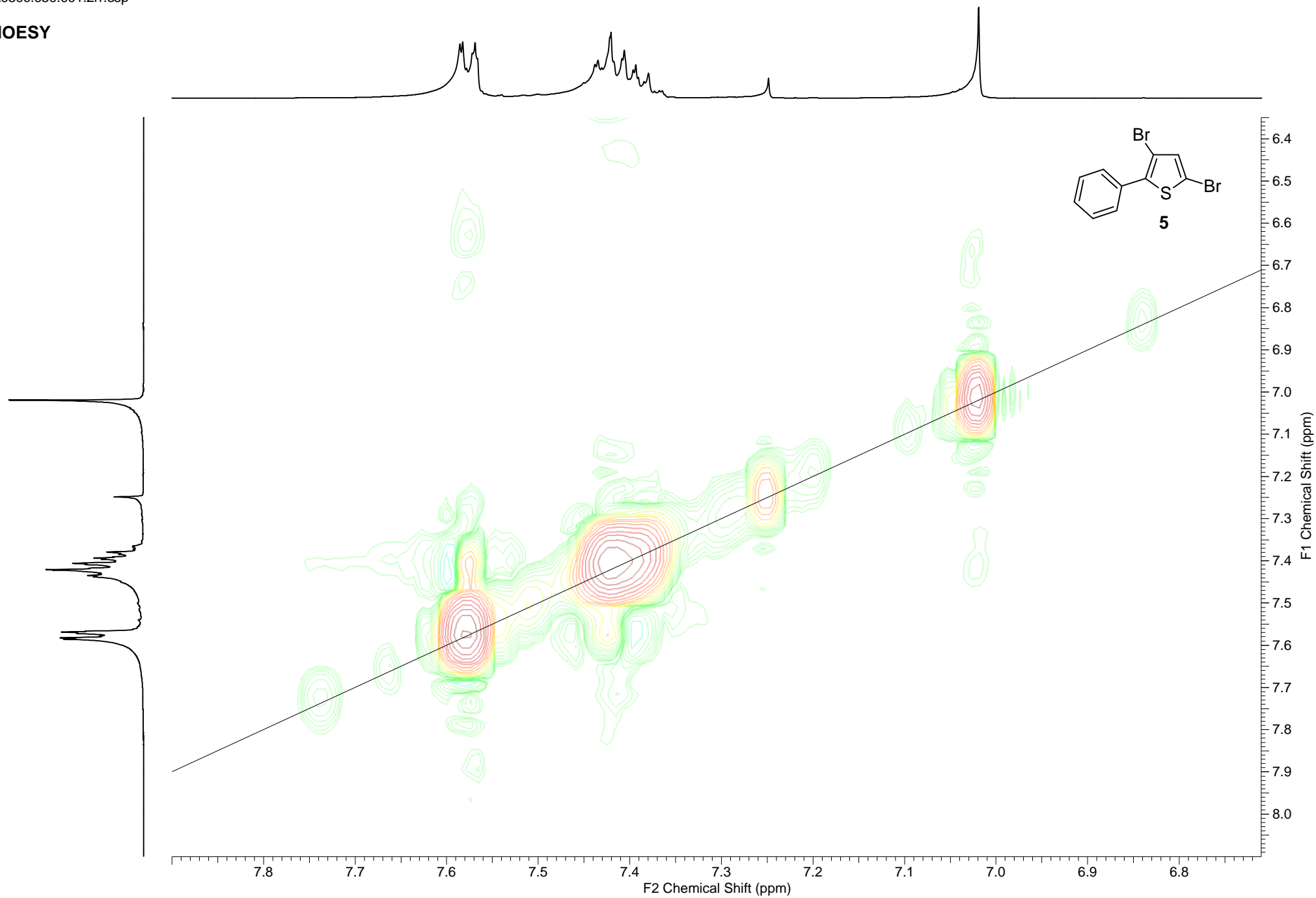
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## HMBC

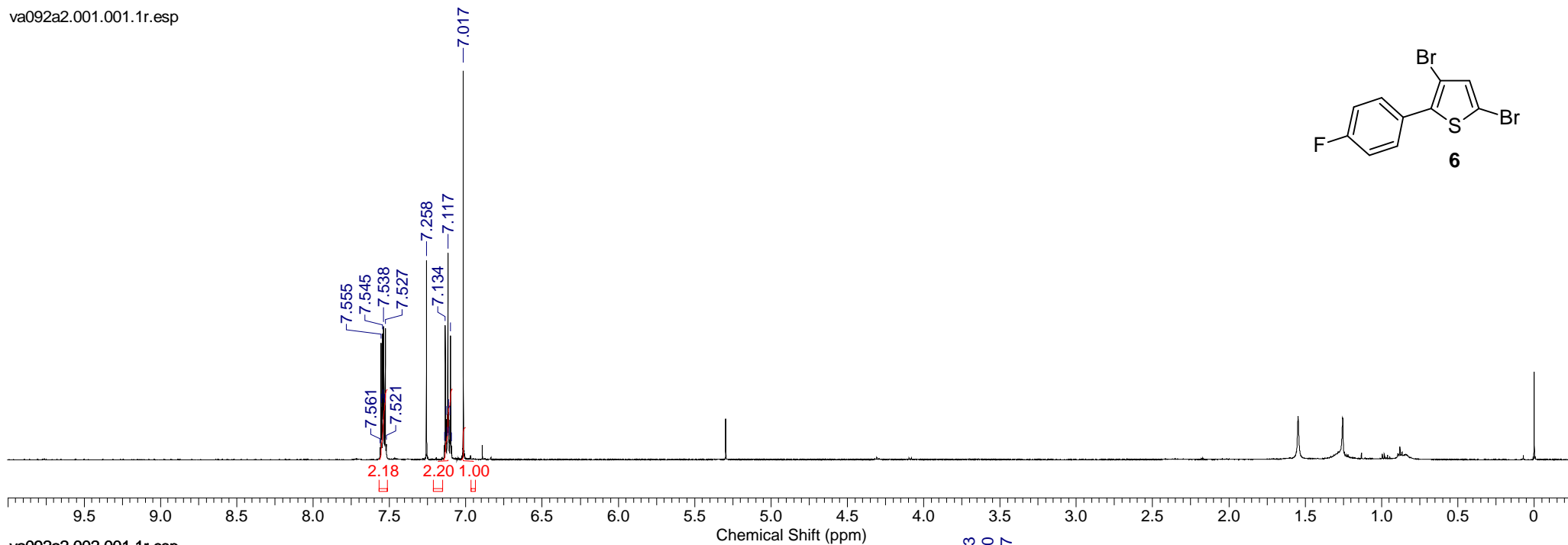
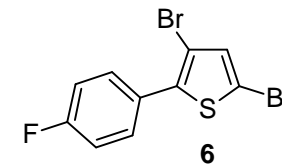


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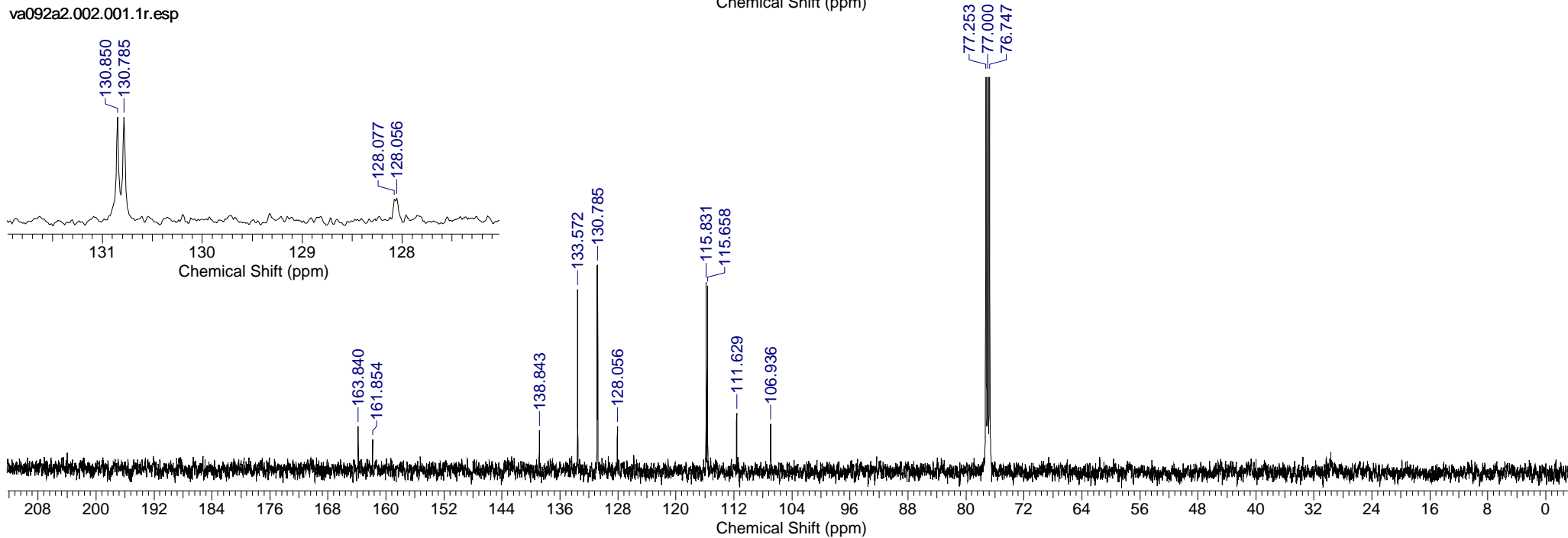




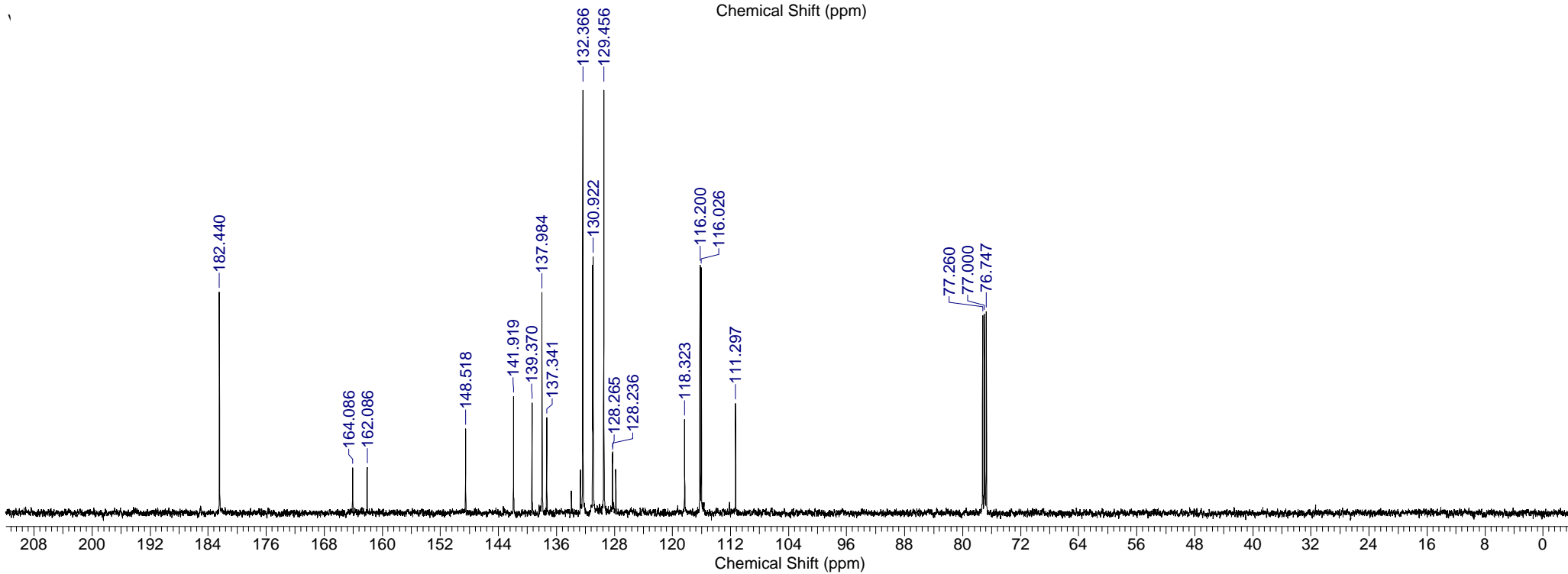
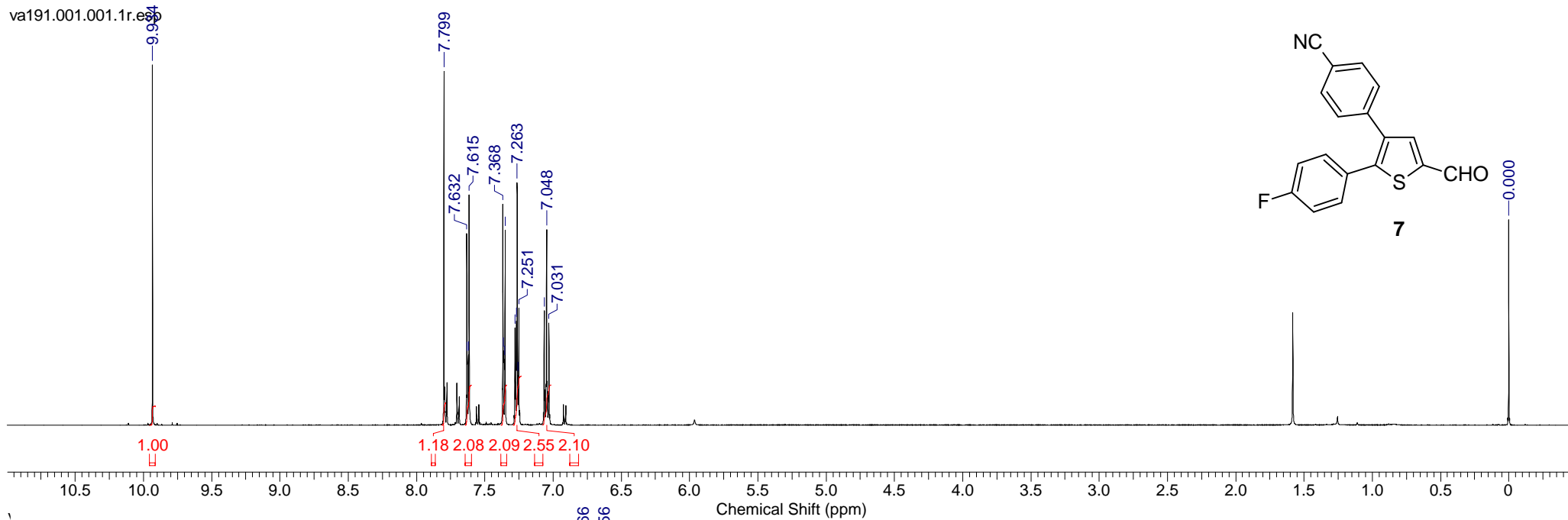
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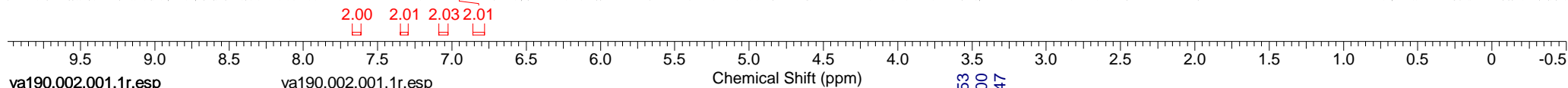
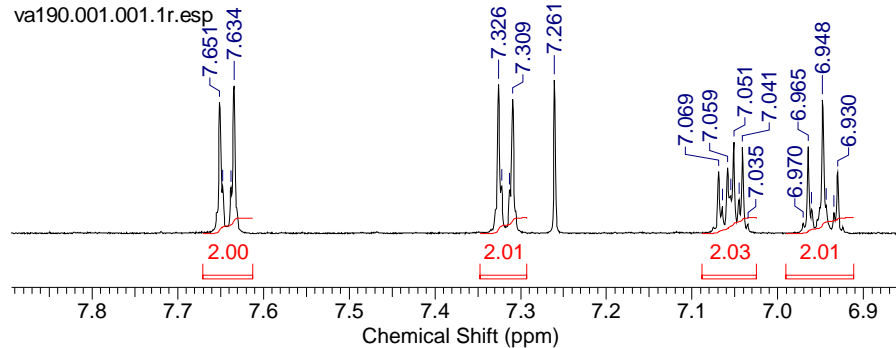
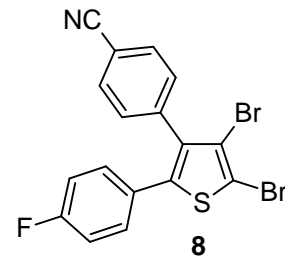


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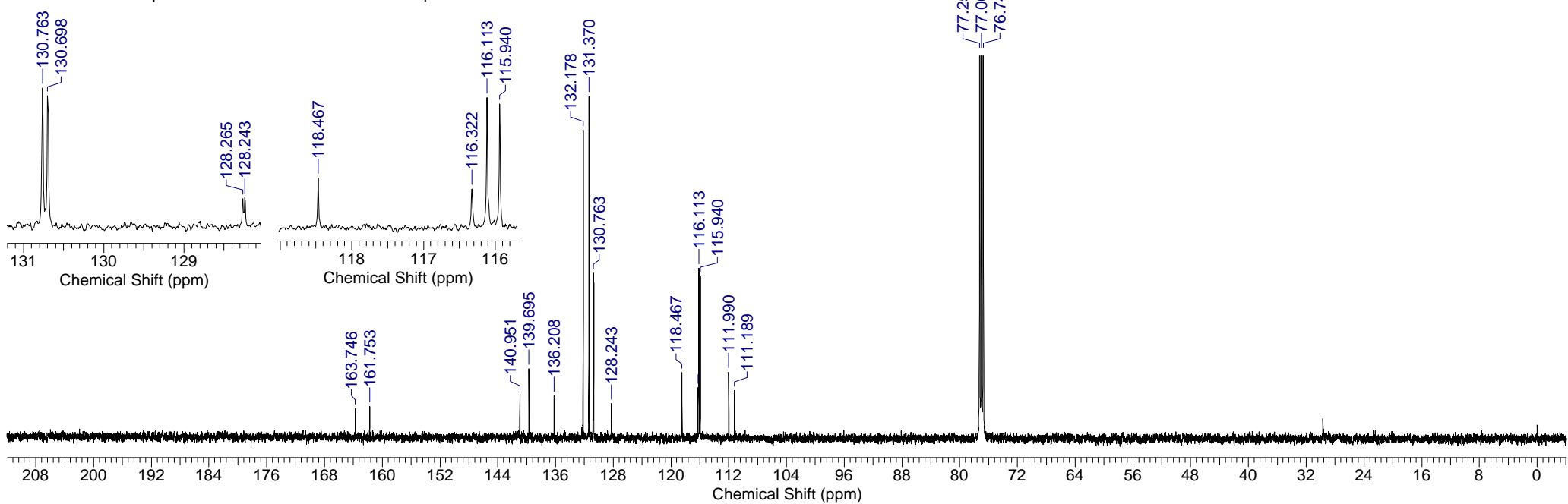
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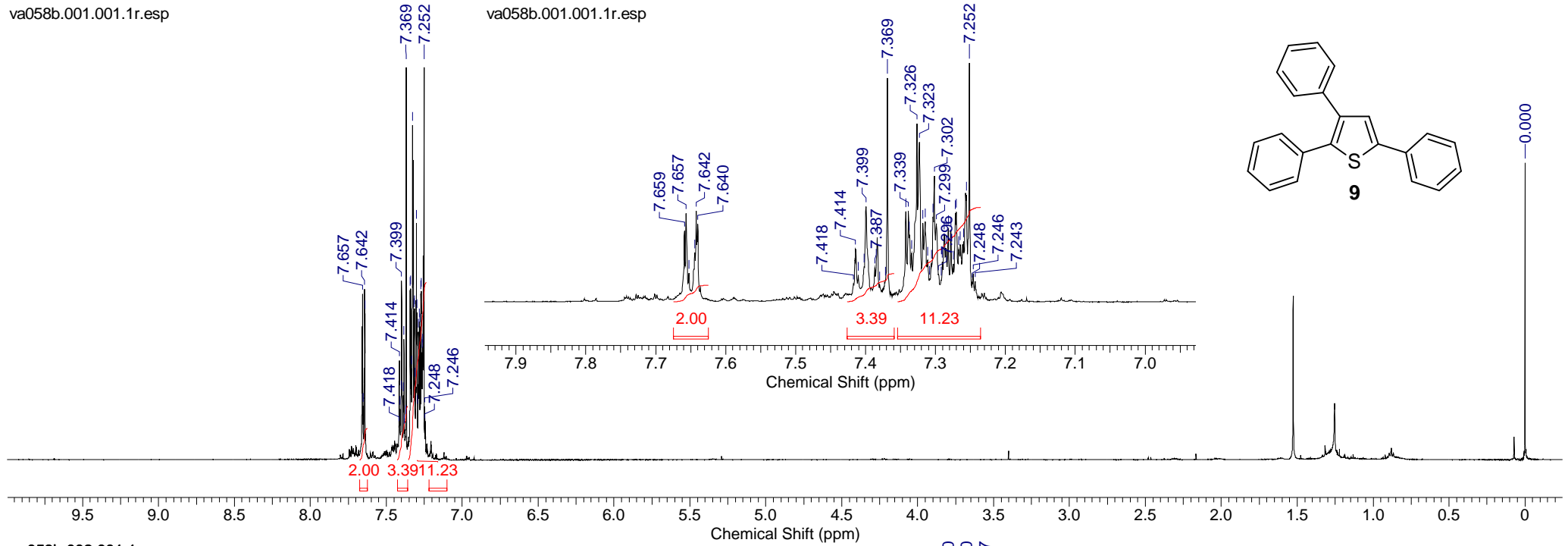
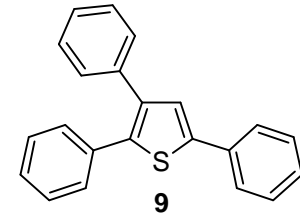
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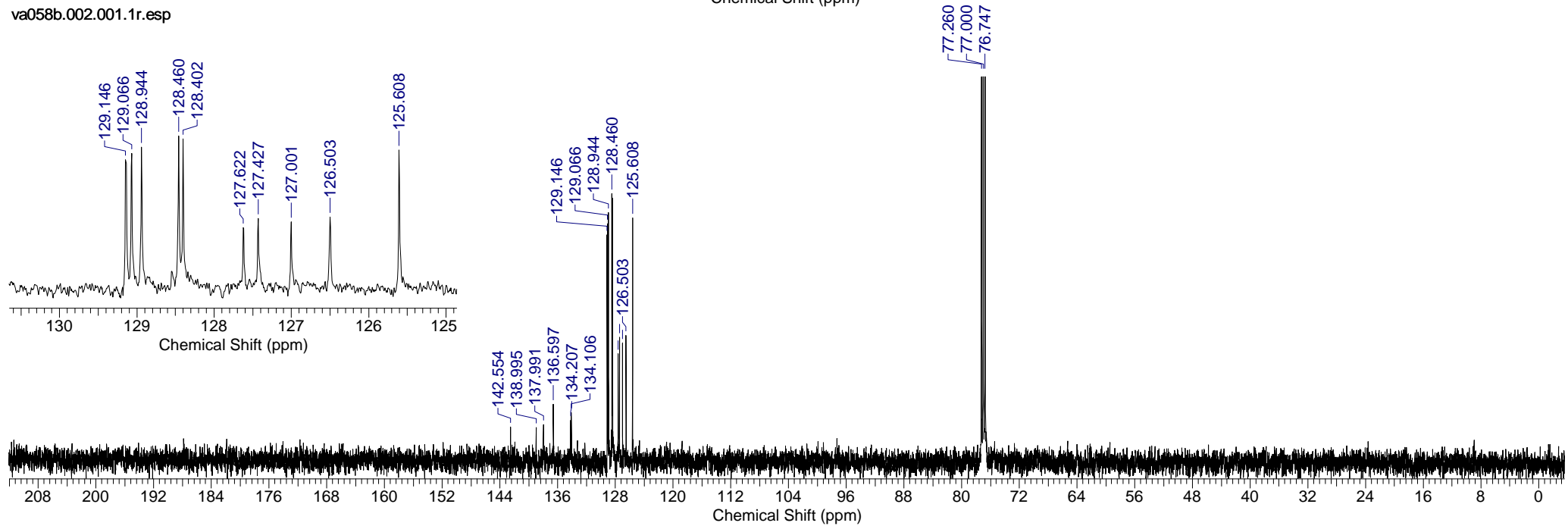


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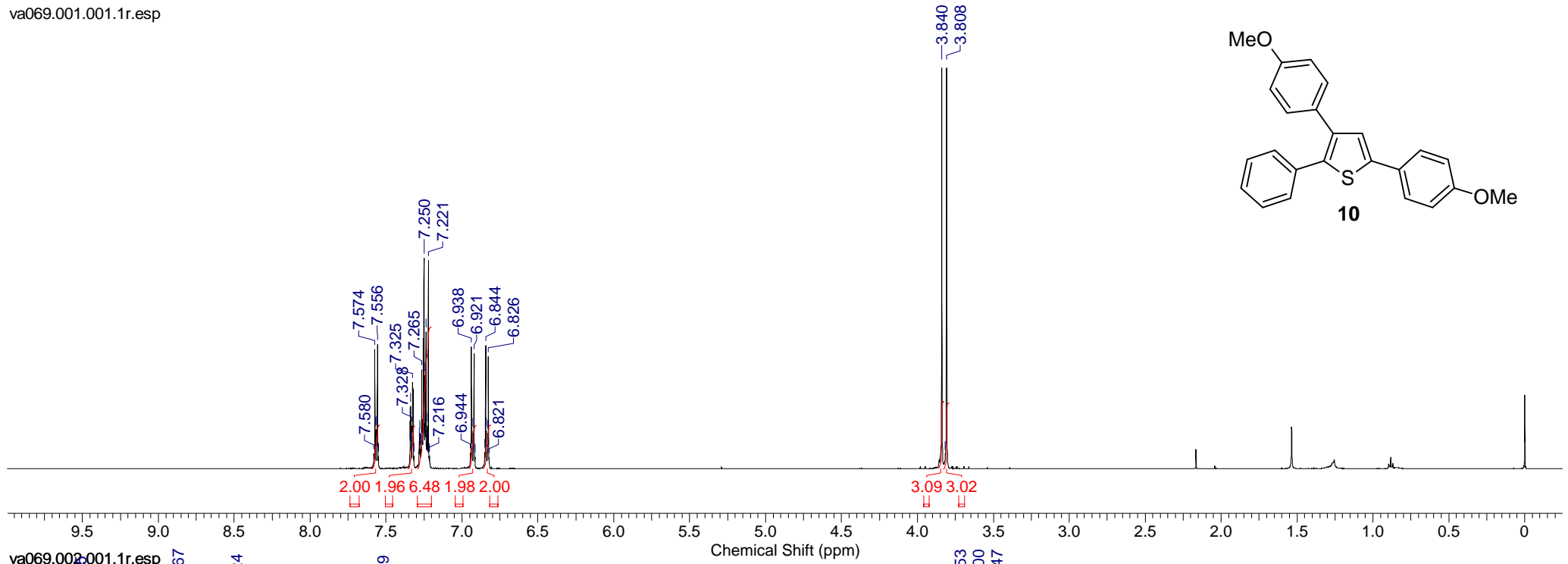
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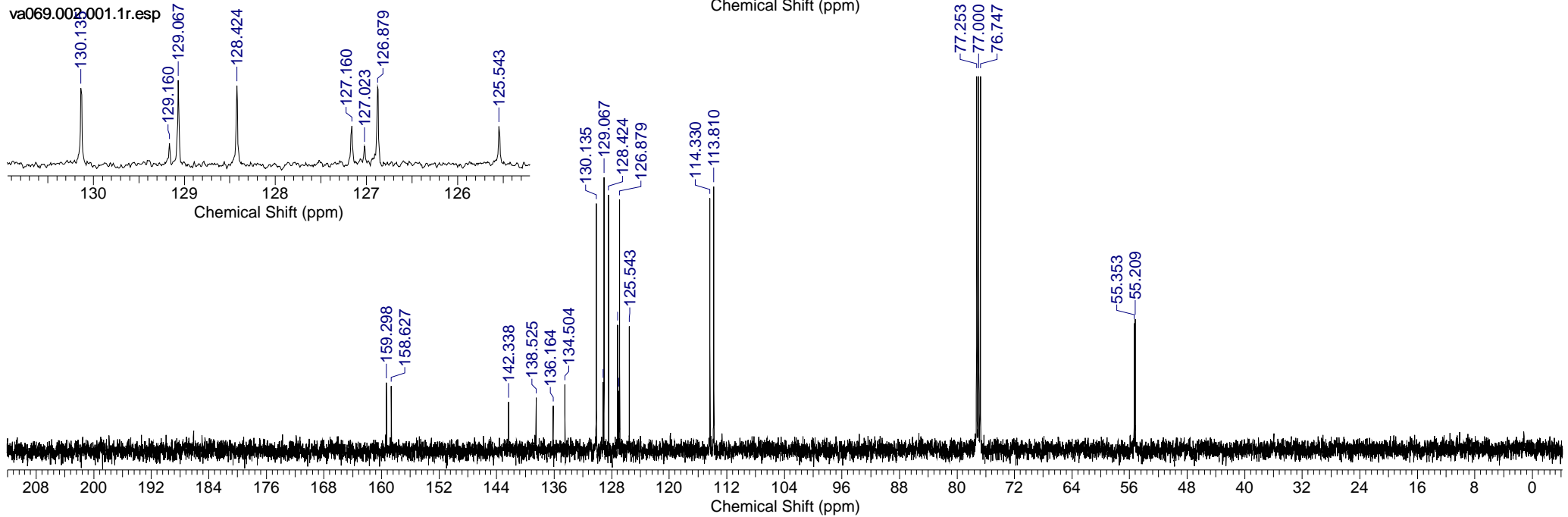
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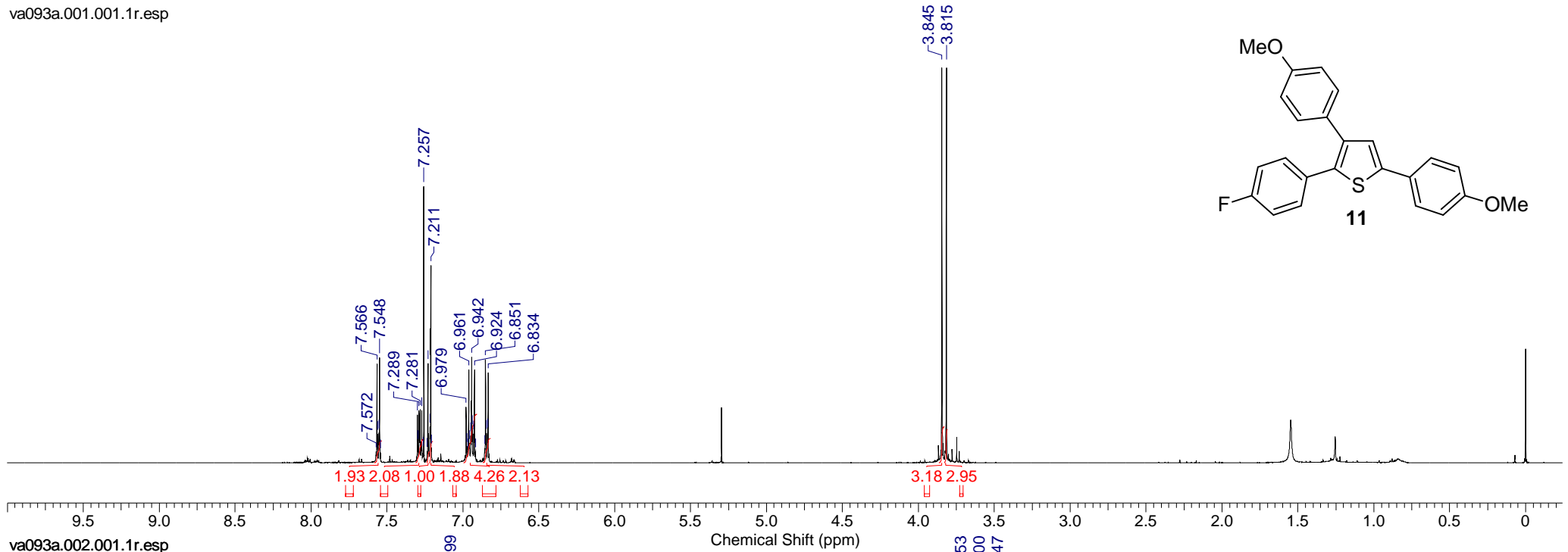
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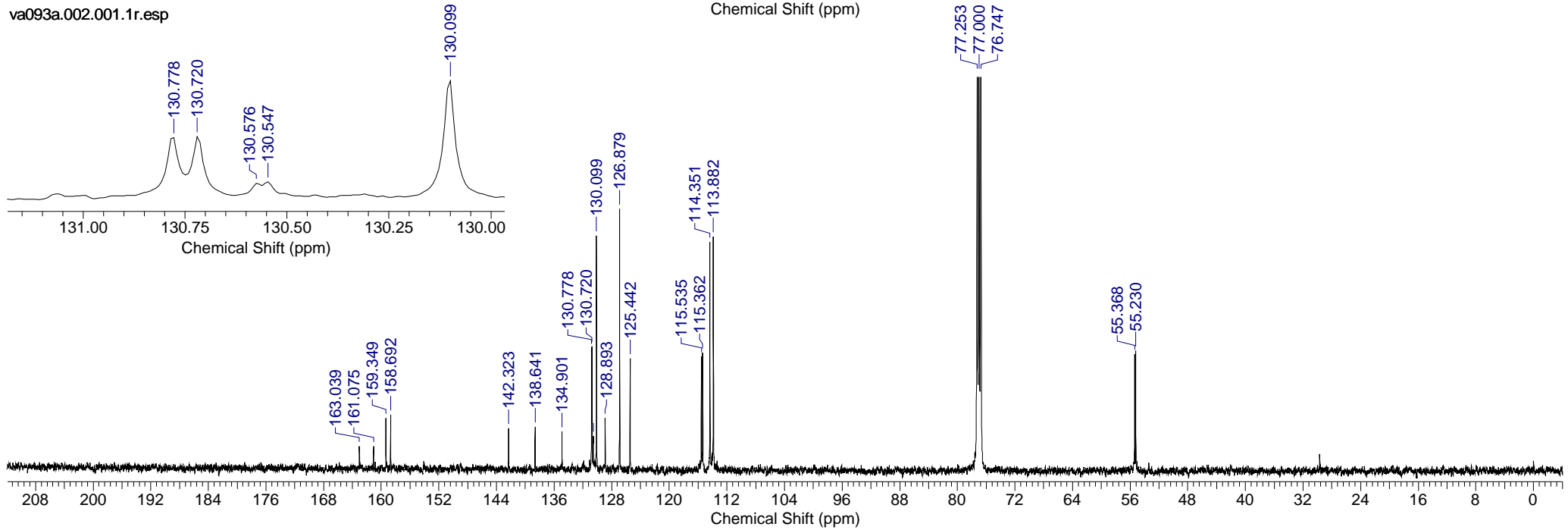
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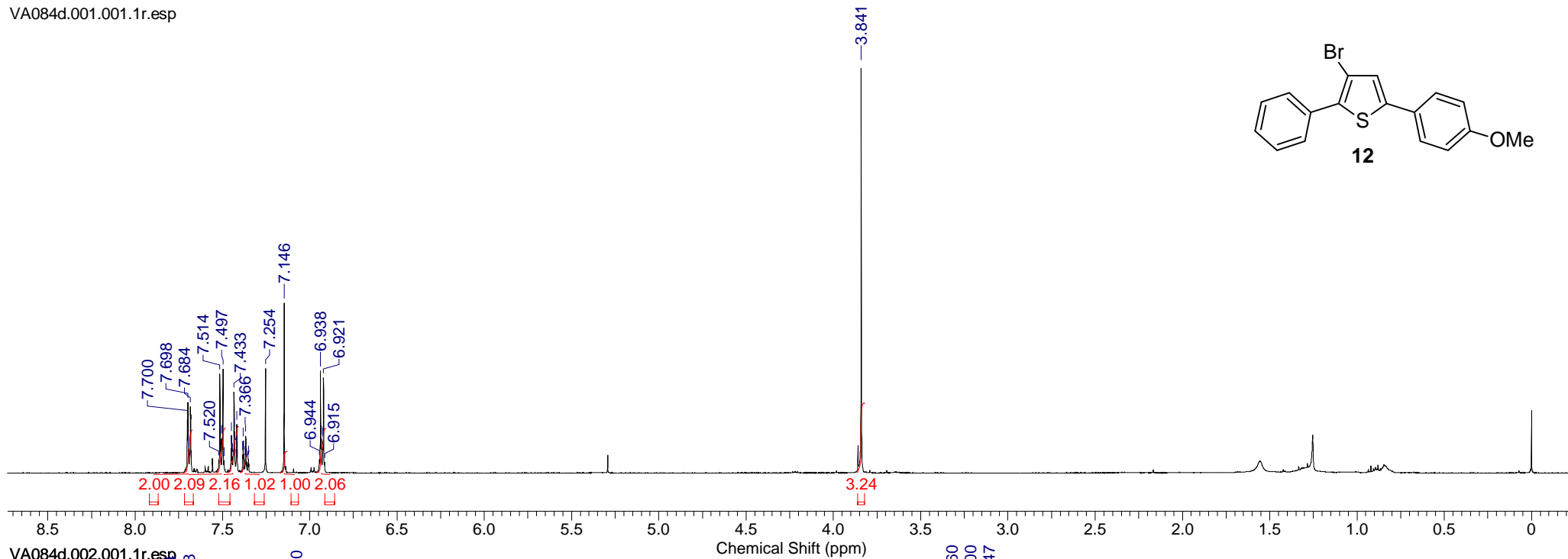
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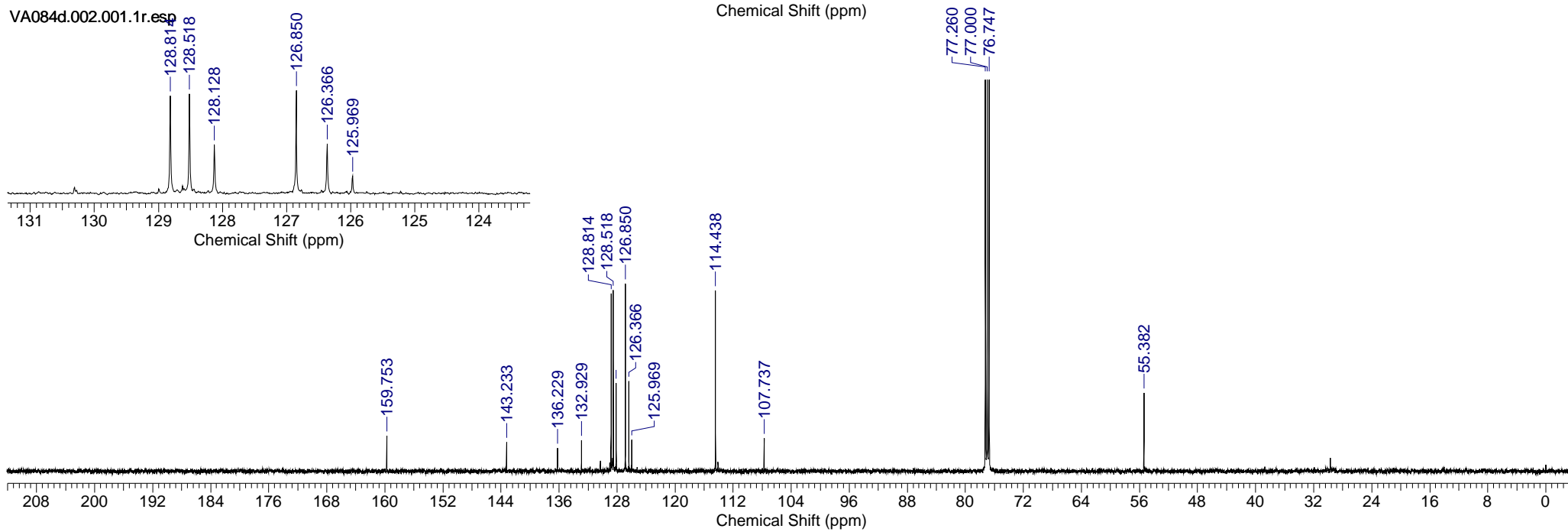
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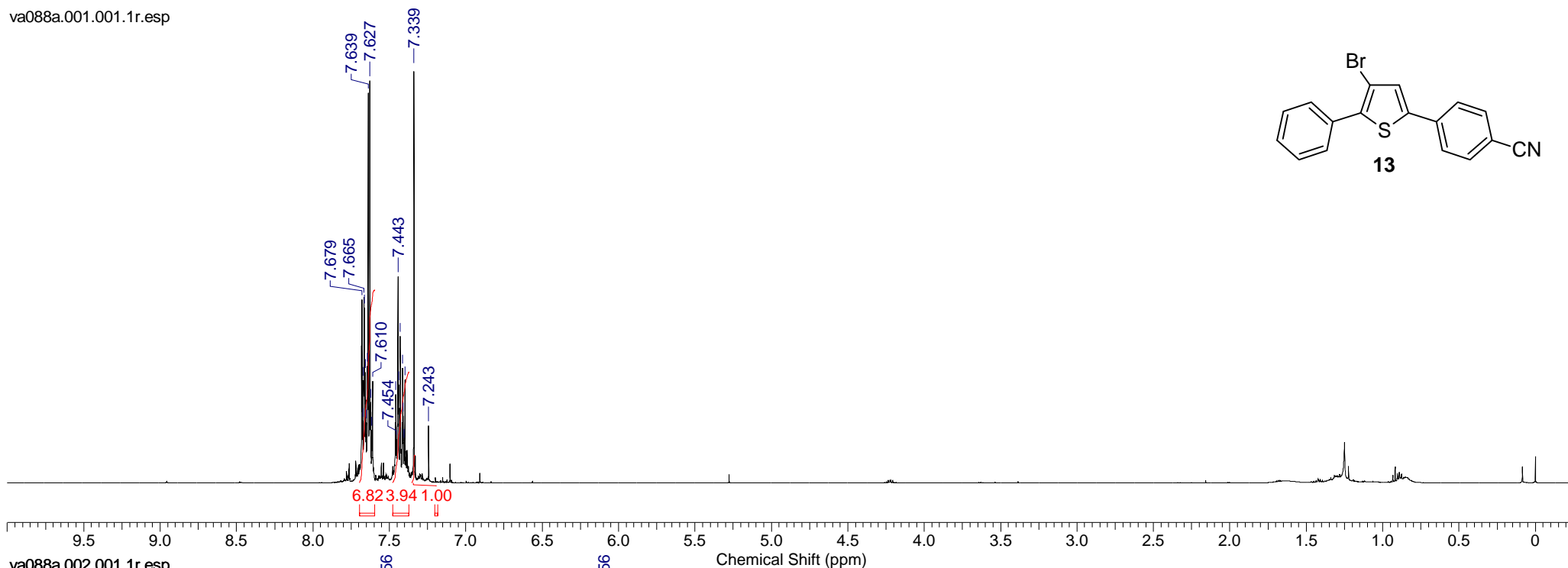
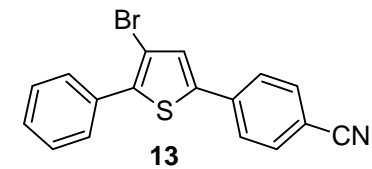
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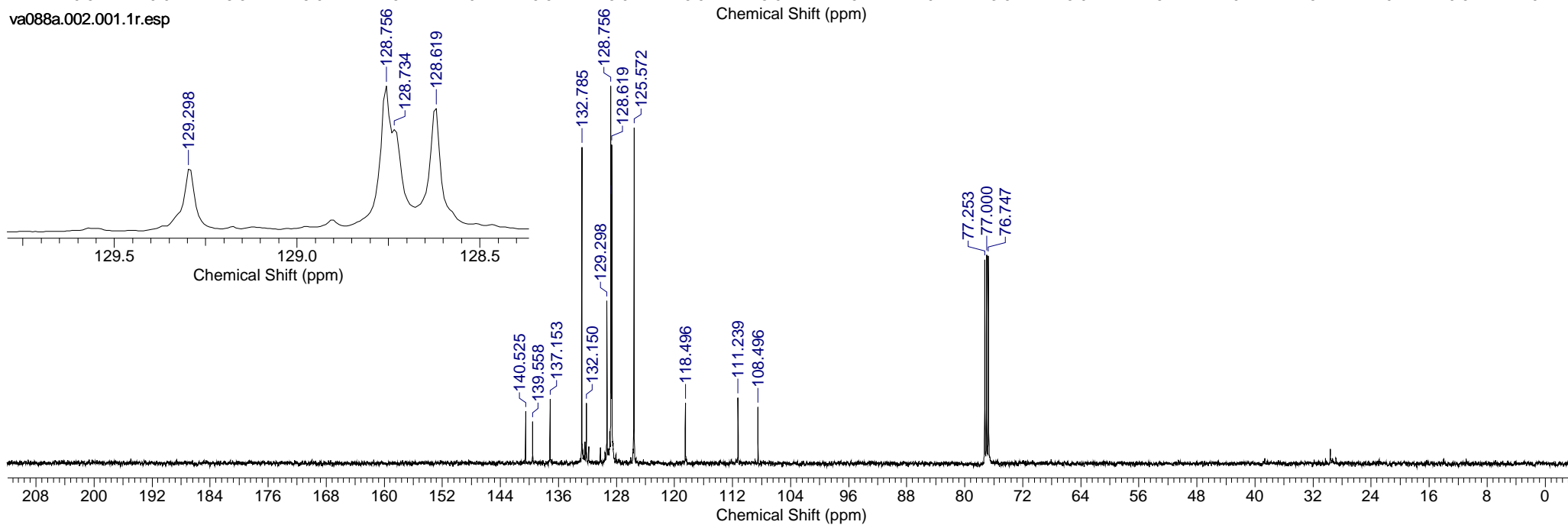
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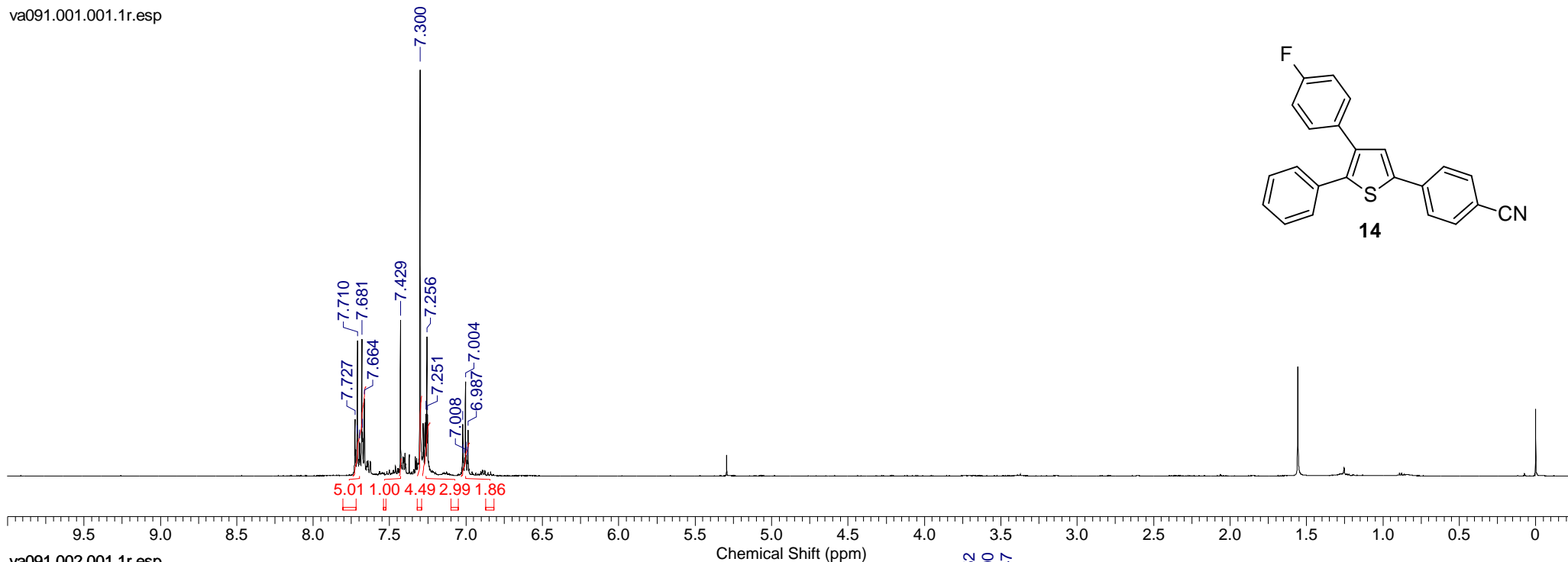


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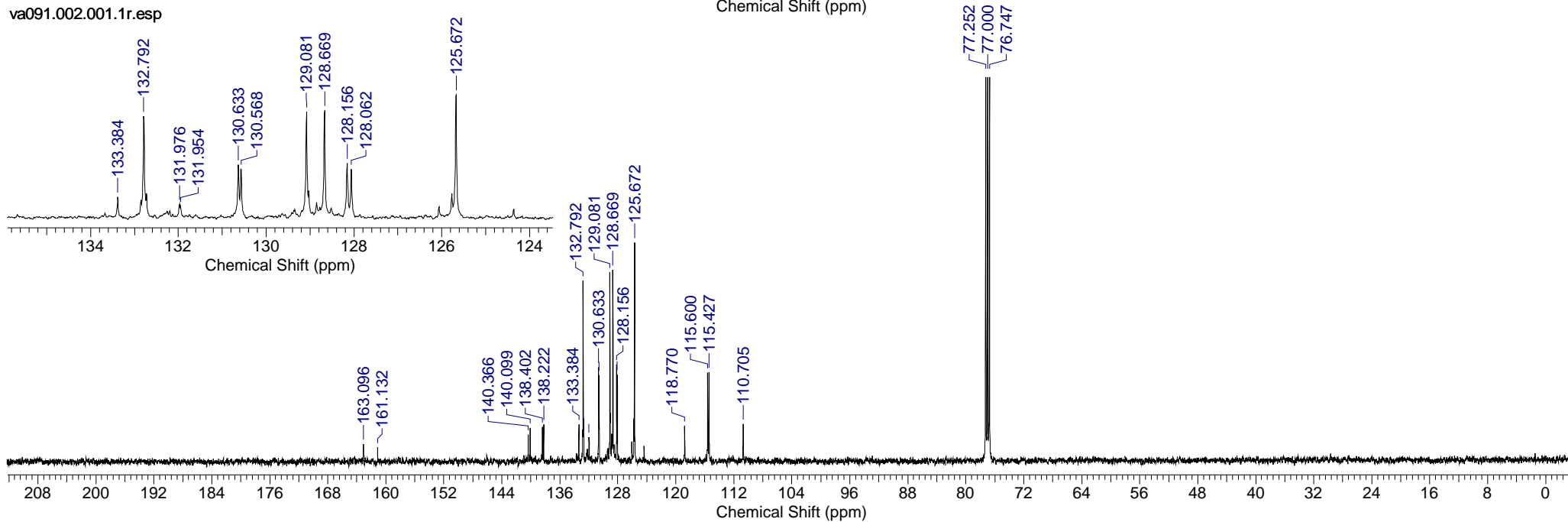




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## Coordinates of optimized structures

### *TS1*

Electronic energy = -3457.18

Gibbs free energy = -3383.37

C	-3.374733	-1.809847	0.907028
C	-2.019286	-1.642450	0.741845
C	-1.517687	-0.750324	-0.236739
C	-2.439429	-0.038594	-1.044175
C	-3.794338	-0.219215	-0.877739
C	-4.266244	-1.099722	0.098325
H	-3.747536	-2.484653	1.663017
H	-1.338590	-2.187534	1.380305
H	-2.092457	0.660803	-1.788387
H	-4.491711	0.326660	-1.496048
H	-5.330937	-1.229926	0.232447
C	-0.118537	-0.543620	-0.377866
S	1.069417	-1.463795	0.464776
C	1.956210	0.196254	-1.357145
C	2.379434	-0.724917	-0.465749
H	2.606410	0.754766	-2.011428
C	3.773660	-1.120900	-0.164625
H	4.545102	-0.629393	-0.780606
O	4.034850	-1.917158	0.703971
C	0.535267	0.364014	-1.337141
H	-0.011220	0.929475	-2.072470
Br	0.248399	2.102868	0.258287

### *$\sigma$ -complex-1*

Electronic energy = -3467.65

Gibbs free energy = -3394.74

C	-3.421316	1.759028	-0.866730
C	-2.061514	1.596061	-0.729229
C	-1.542247	0.675993	0.212422
C	-2.443878	-0.072935	1.006206
C	-3.803310	0.121701	0.882374
C	-4.294724	1.030468	-0.055175
H	-3.810608	2.442275	-1.606775
H	-1.390591	2.139032	-1.380254
H	-2.077000	-0.772301	1.741668
H	-4.486509	-0.429079	1.512087
H	-5.361785	1.169399	-0.158325
C	-0.140633	0.508930	0.370259
S	1.004073	1.656774	-0.110750
C	1.967041	-0.461379	1.078662
C	2.364513	0.687462	0.528345
H	2.627435	-1.182833	1.535294
C	3.727789	1.243523	0.395825
H	4.531908	0.619721	0.821130
O	3.931987	2.305466	-0.140177
C	0.510163	-0.699060	0.984655
H	0.049418	-1.023097	1.913003
Br	0.211649	-2.204223	-0.315102

## TS2

Electronic energy = -3455.40

Gibbs free energy = -3382.54

C	-4.360000	-0.878000	1.078600
C	-3.018000	-0.569400	1.033000
C	-2.477500	0.111300	-0.085300
C	-3.343400	0.463300	-1.151800
C	-4.687200	0.170100	-1.085500
C	-5.198100	-0.504400	0.025300
H	-4.765400	-1.411500	1.925400
H	-2.372800	-0.881700	1.843100
H	-2.963500	1.004500	-2.003200
H	-5.343000	0.460400	-1.892200
H	-6.251900	-0.745100	0.068400
C	-1.101100	0.463400	-0.156600
C	-0.394200	0.899300	-1.298100
S	-0.057100	0.419400	1.264500
H	-0.843100	0.960500	-2.274600
C	1.306300	0.942000	0.316300
C	0.923700	1.159900	-1.065200
H	1.631200	1.565500	-1.769900
C	2.581200	1.493000	0.919300
H	2.897700	1.049800	1.874200
O	3.152400	2.396100	0.372700
Br	2.451900	-1.010700	-0.575000

## $\sigma$ -complex-2

Electronic energy = -3468.64

Gibbs free energy = -3396.09

C	-4.338700	-0.622100	1.148700
C	-2.970500	-0.485600	1.070500
C	-2.371300	0.066700	-0.086200
C	-3.204100	0.485600	-1.151800
C	-4.574600	0.363600	-1.054600
C	-5.143500	-0.195600	0.088900
H	-4.788900	-1.065800	2.024400
H	-2.353900	-0.843800	1.883400
H	-2.777500	0.943600	-2.030500
H	-5.204600	0.702700	-1.863800
H	-6.217200	-0.302800	0.155100
C	-0.956900	0.217500	-0.193200
C	-0.235000	0.421300	-1.421000
S	0.090000	0.164000	1.166300
H	-0.731600	0.454300	-2.376300
C	1.583200	0.436000	0.119400
C	1.093800	0.519500	-1.271700
H	1.802100	0.678400	-2.070300
C	2.325800	1.718900	0.595600
H	2.716500	1.662700	1.624300
O	2.454800	2.664000	-0.123600
Br	2.881500	-1.069100	0.279000