

Supplementary Material

On the role of "mental leaps" in small-molecule structure elucidation by NMR spectroscopy

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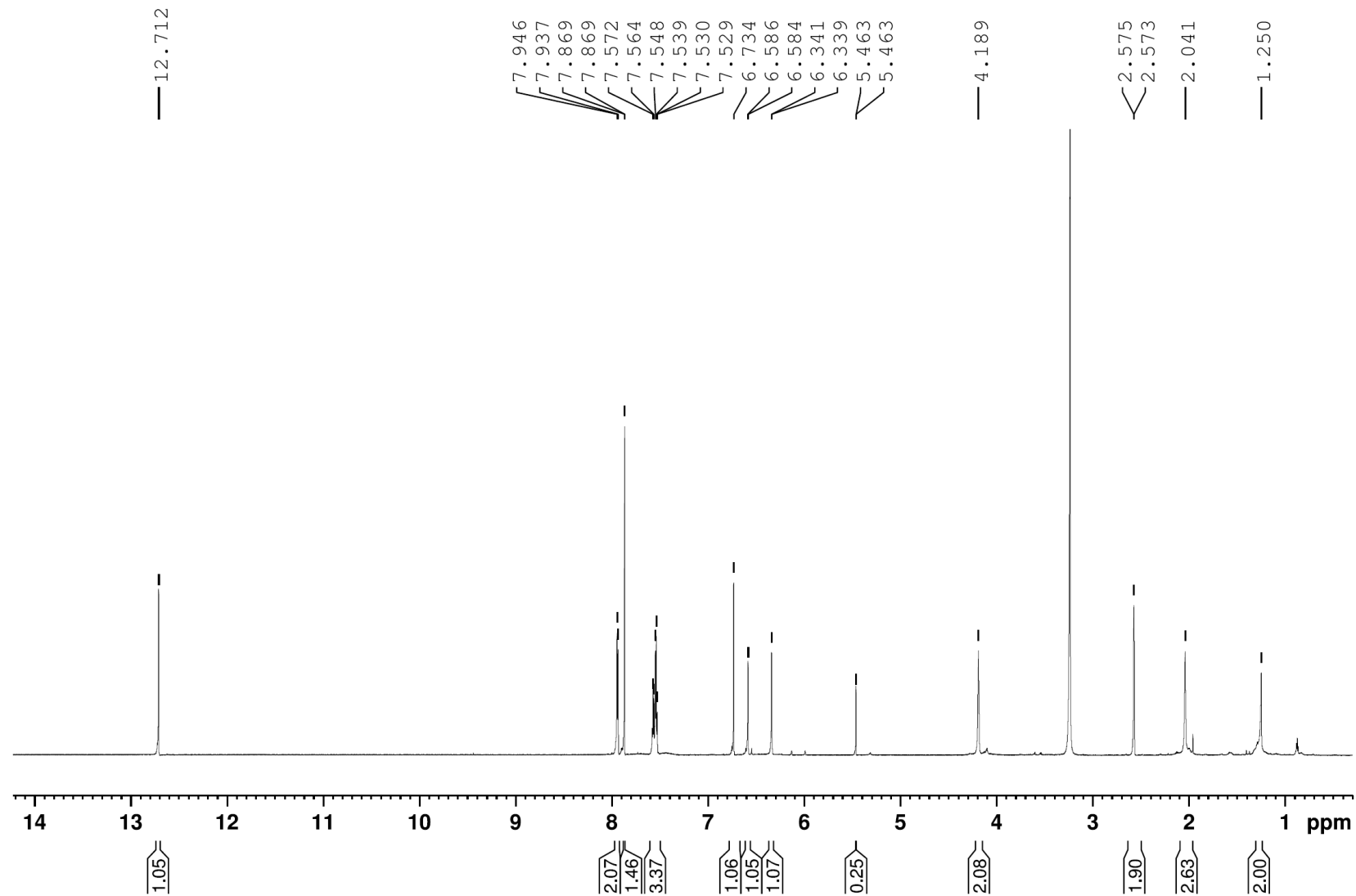
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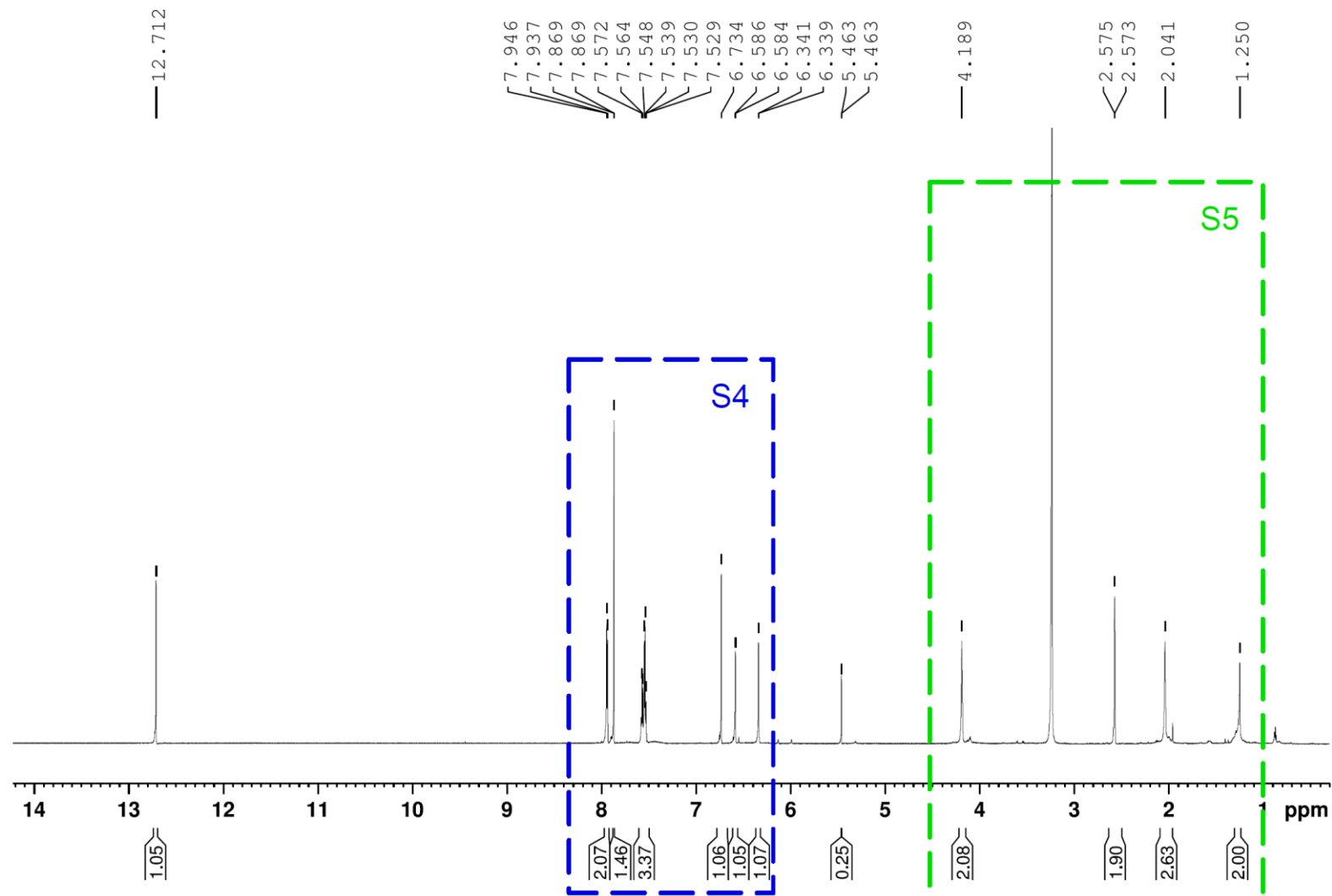
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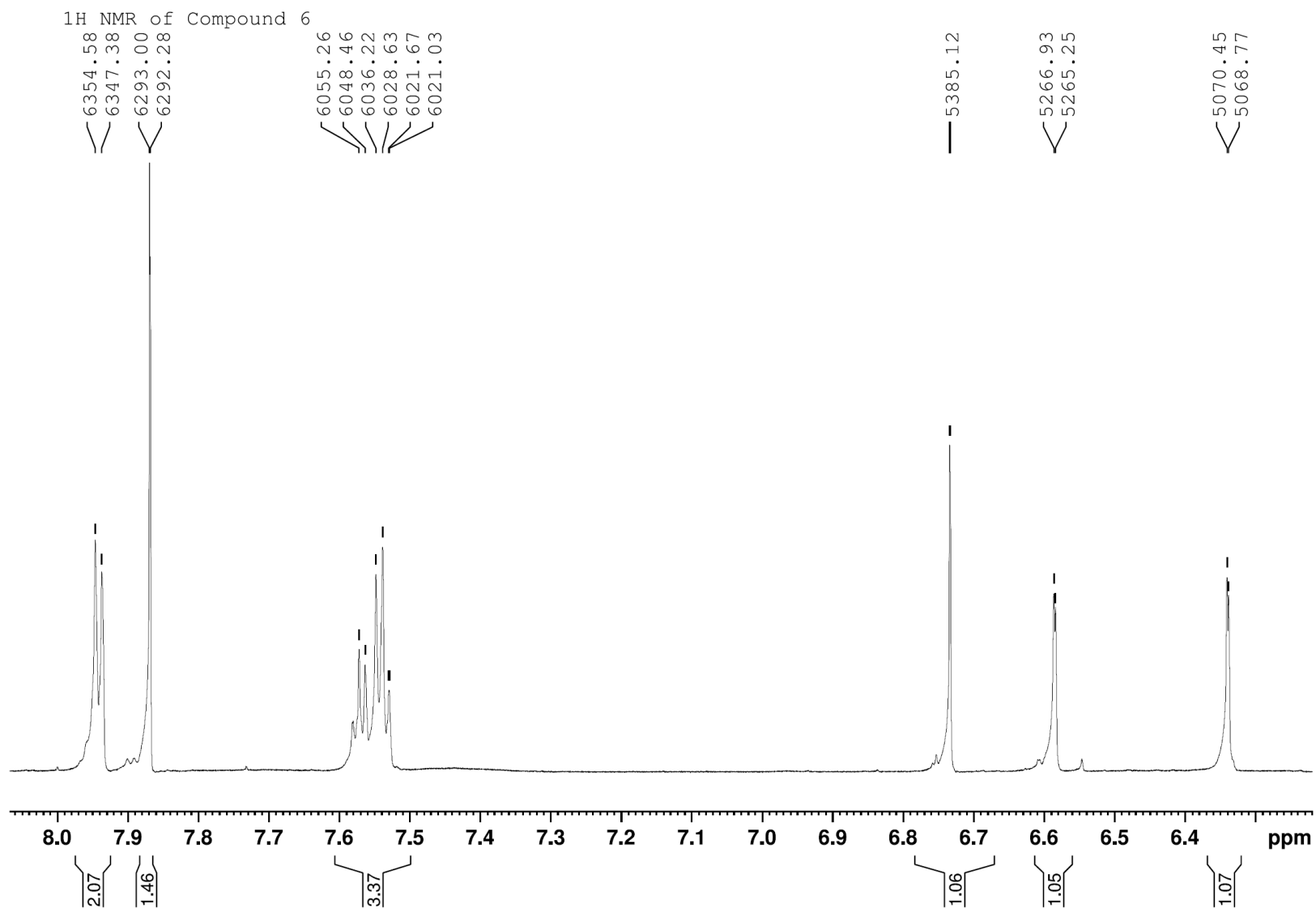
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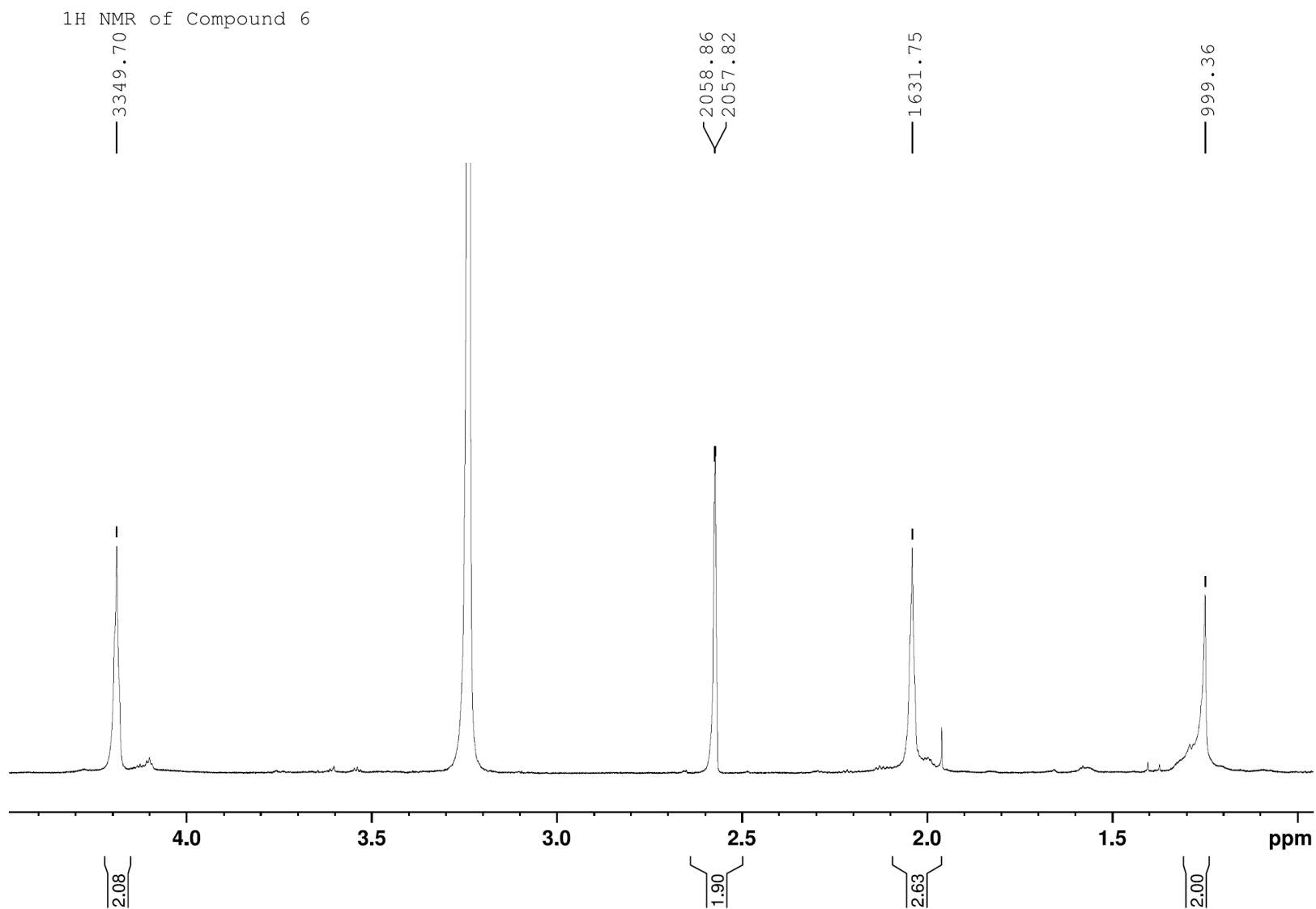
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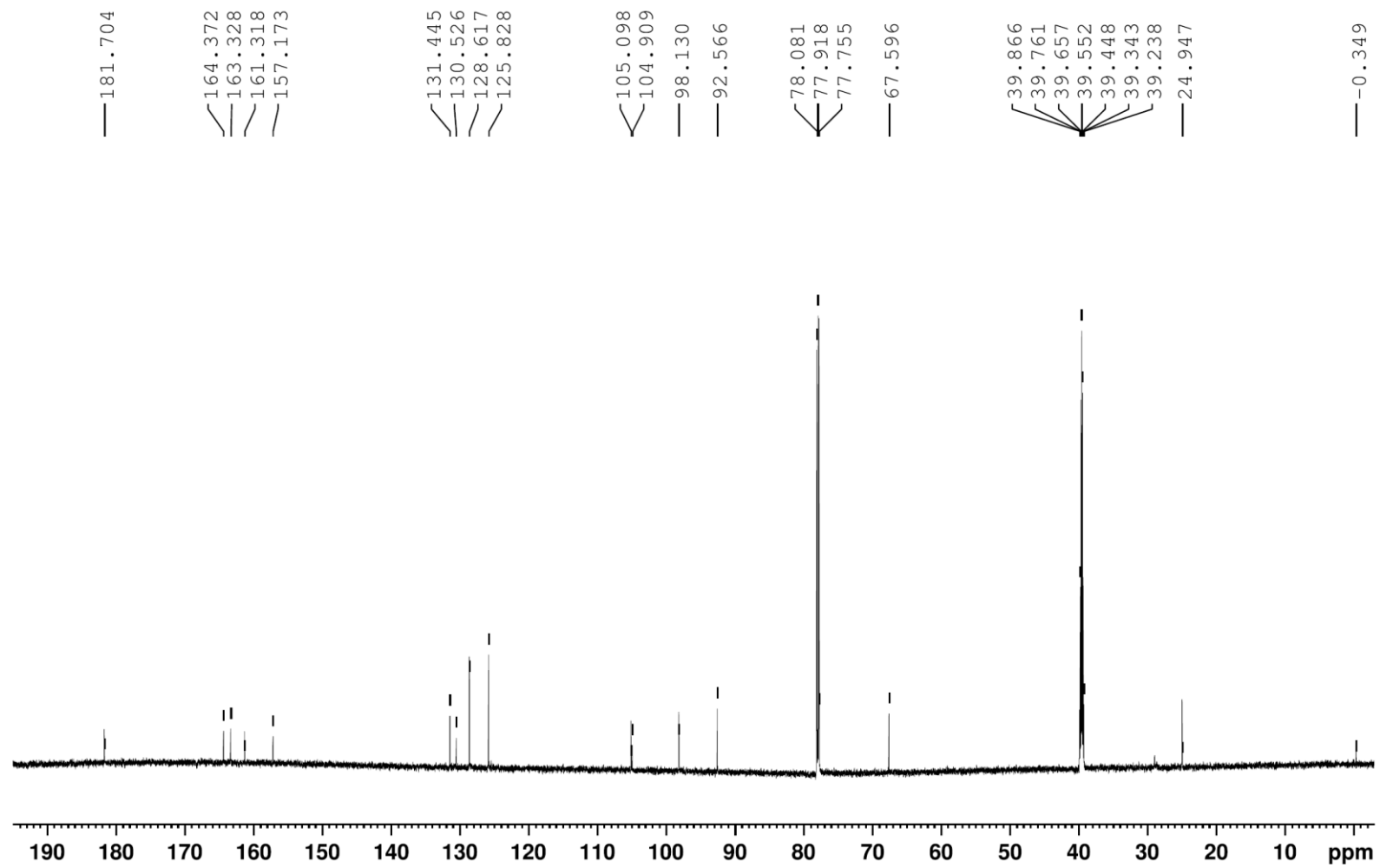
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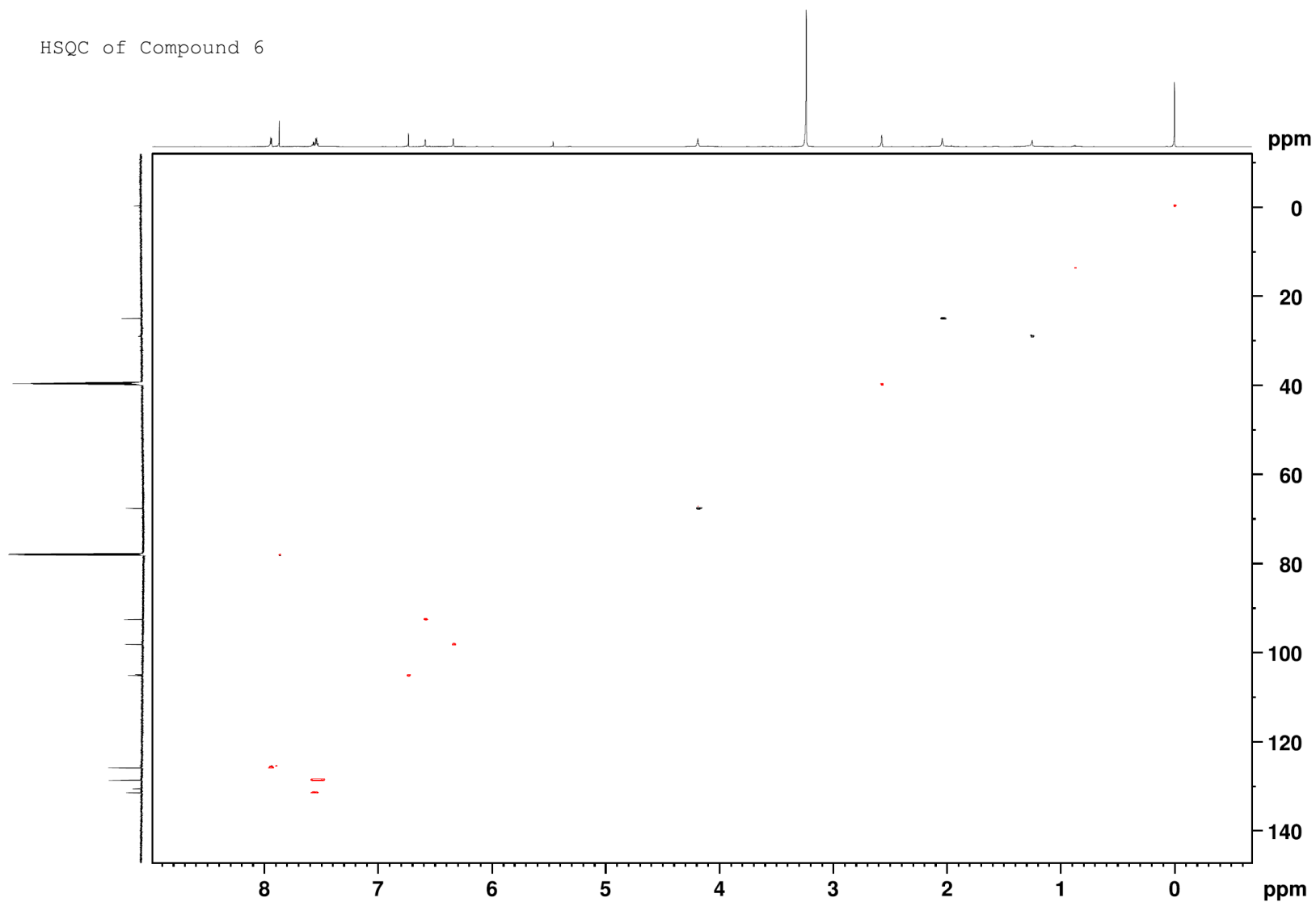




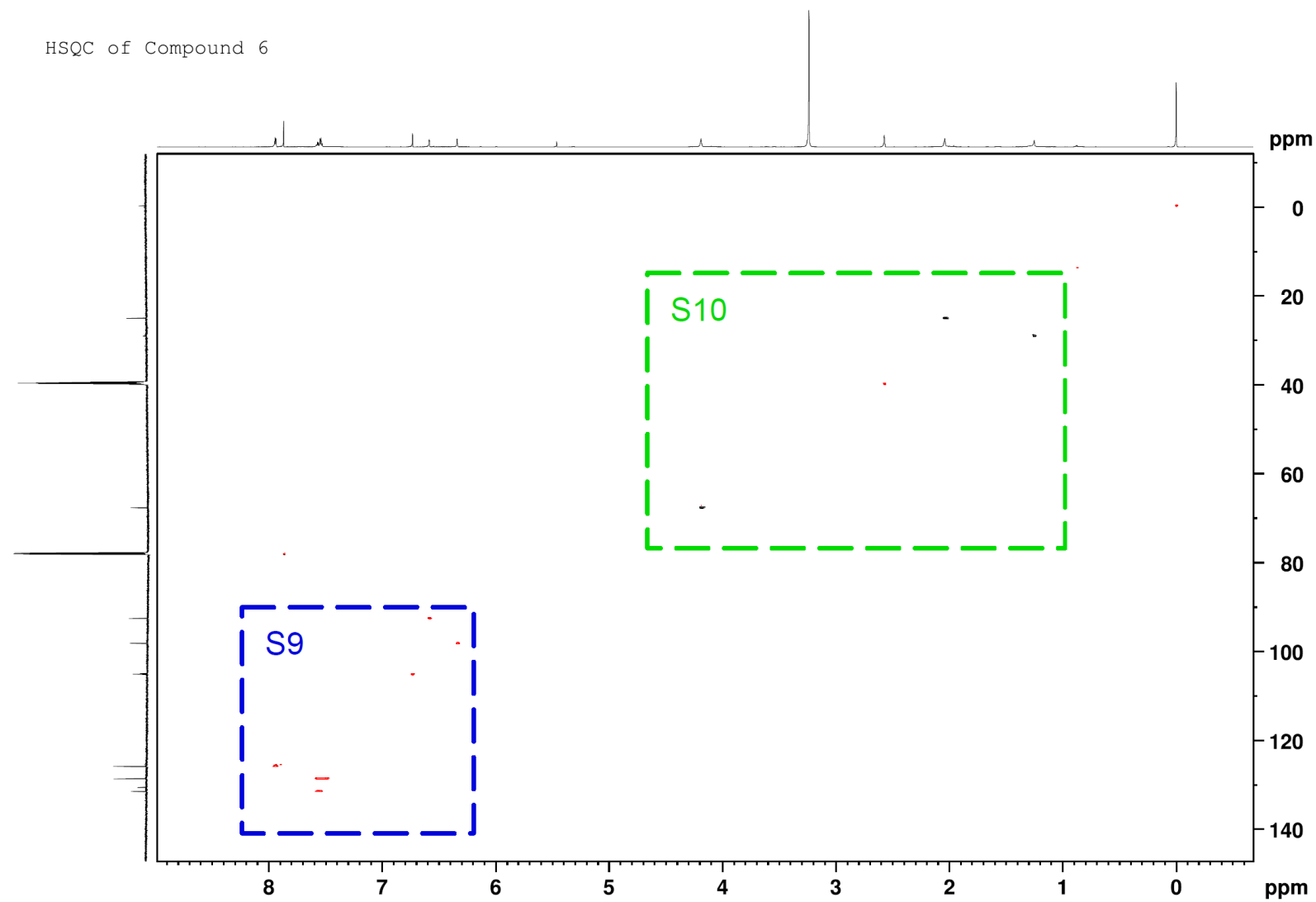
¹³C NMR of Compound 6

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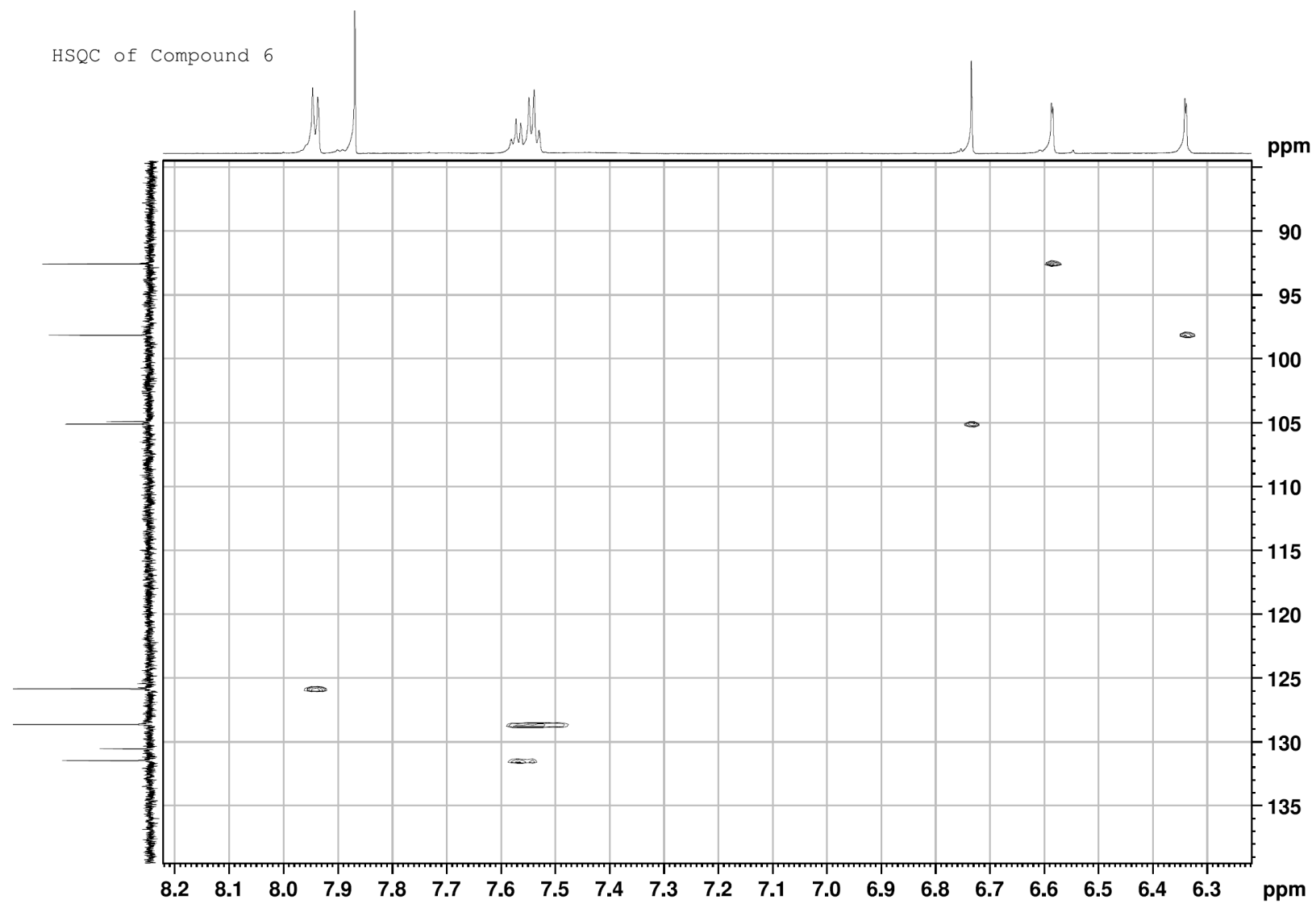
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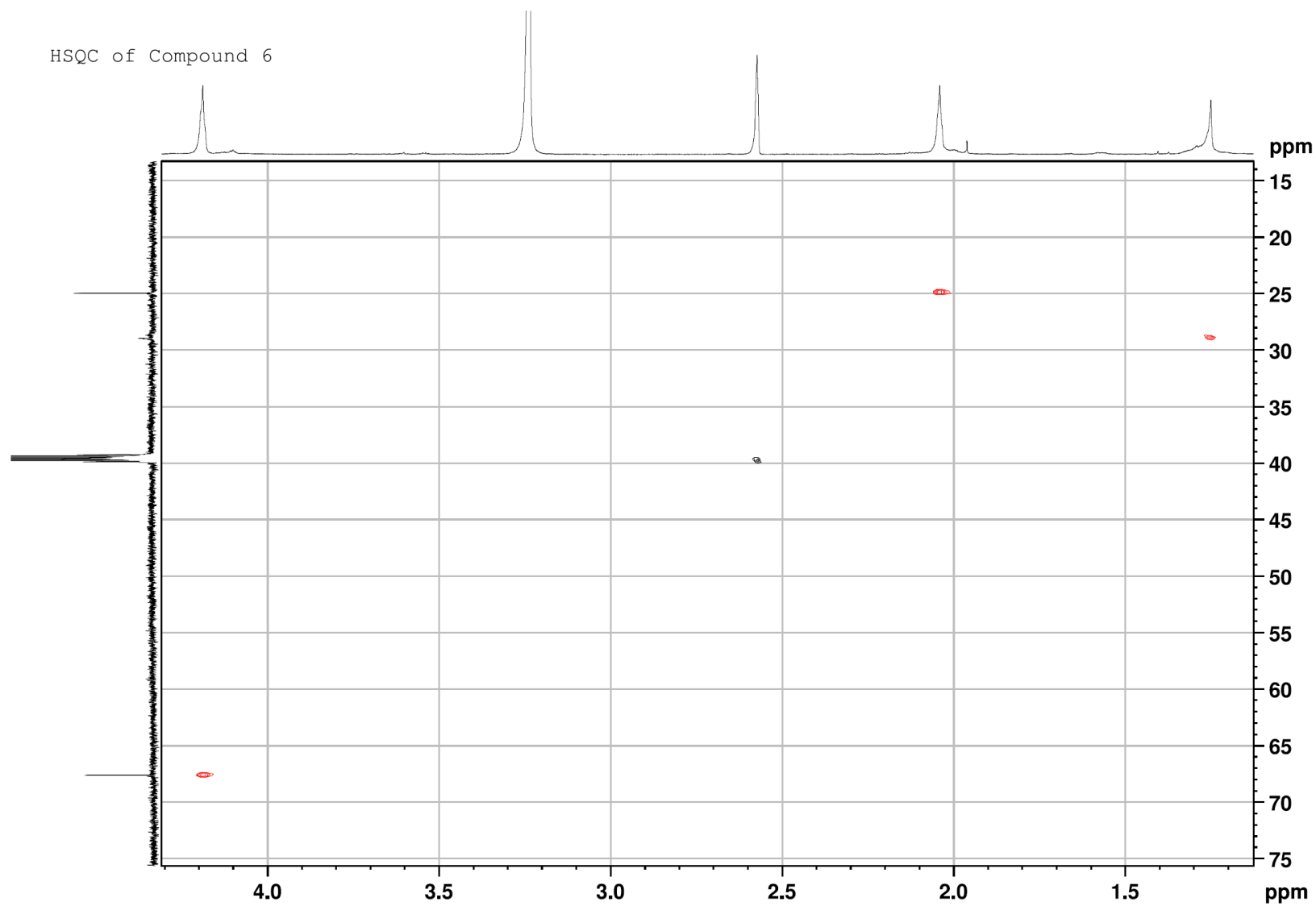


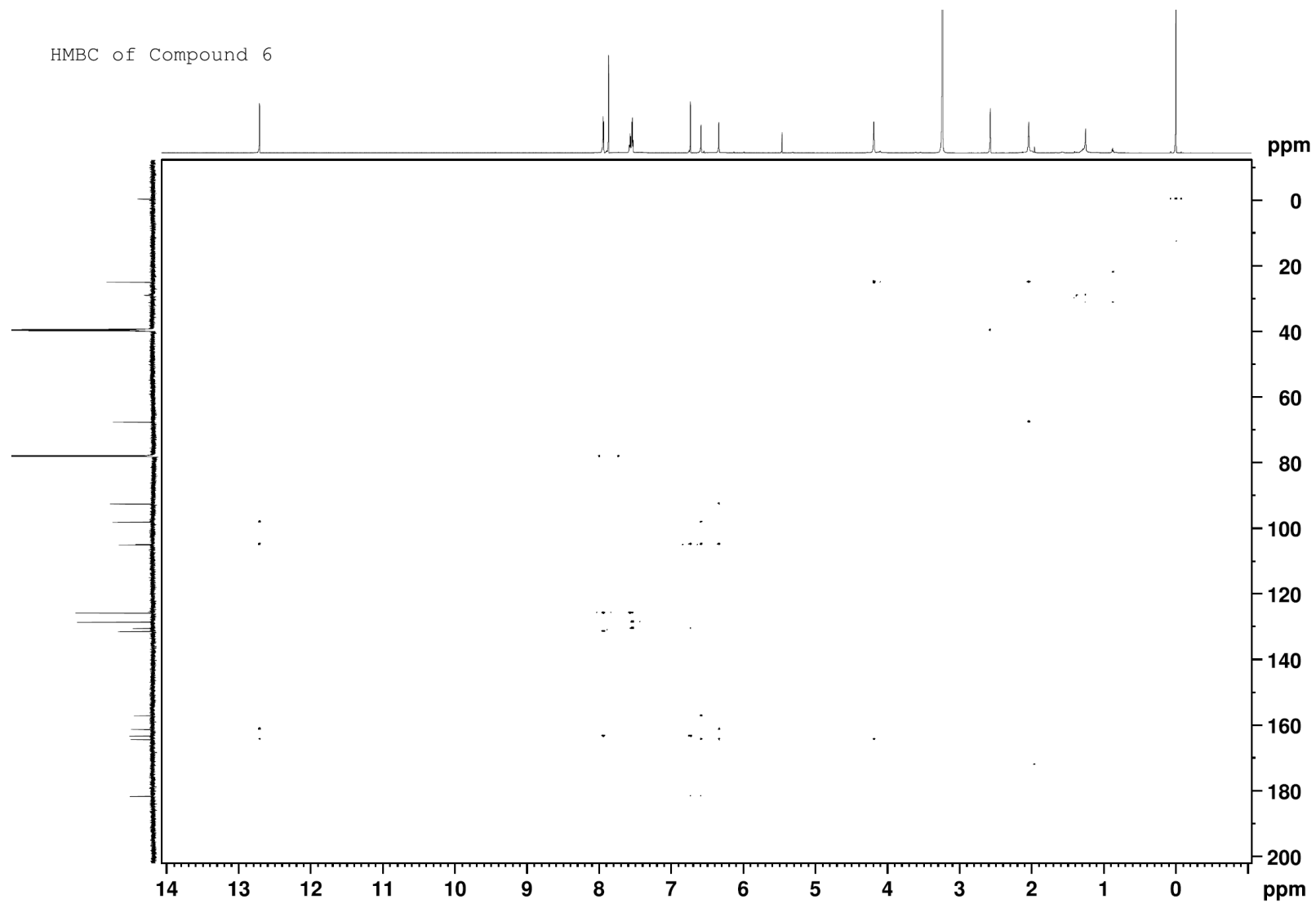
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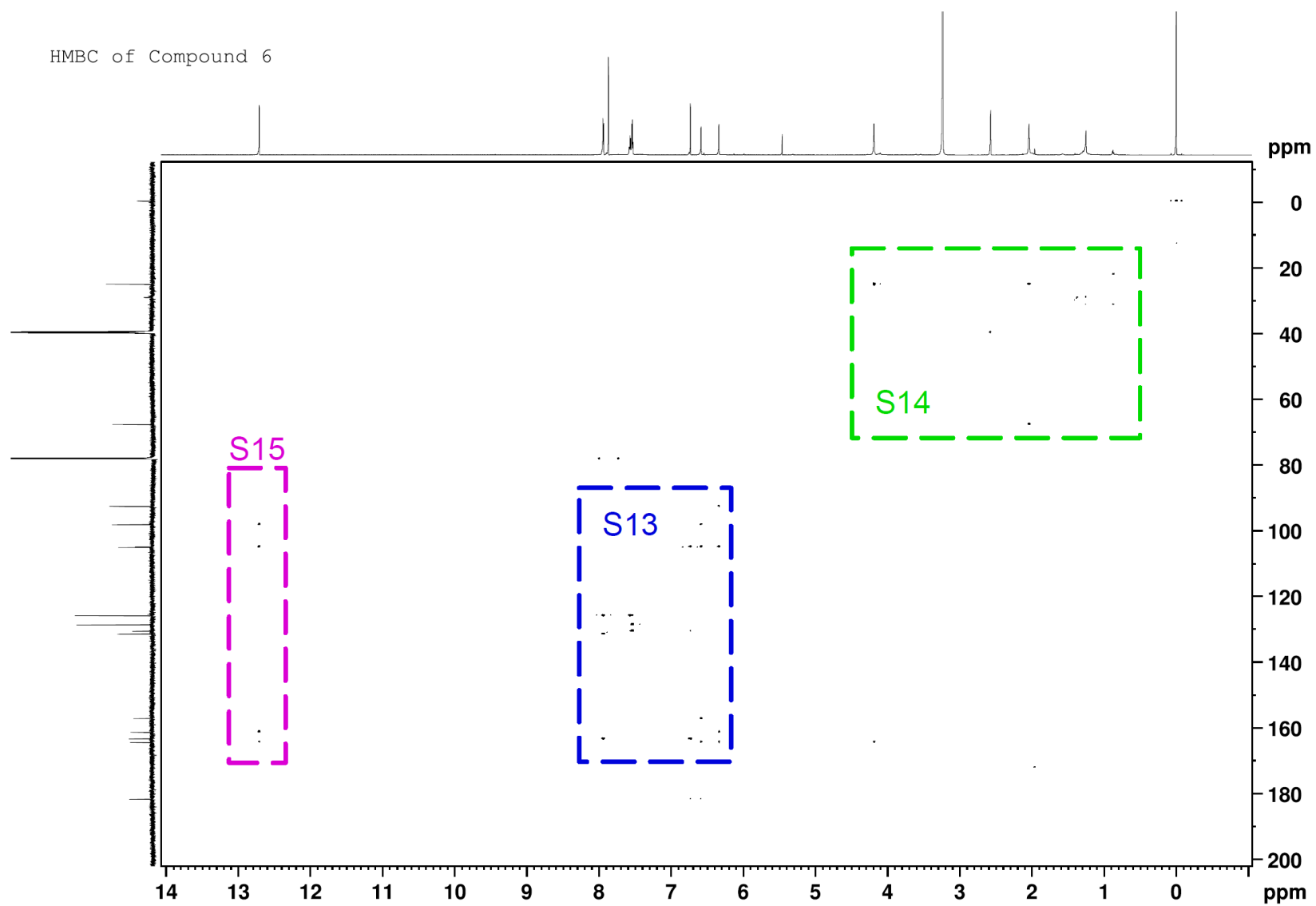




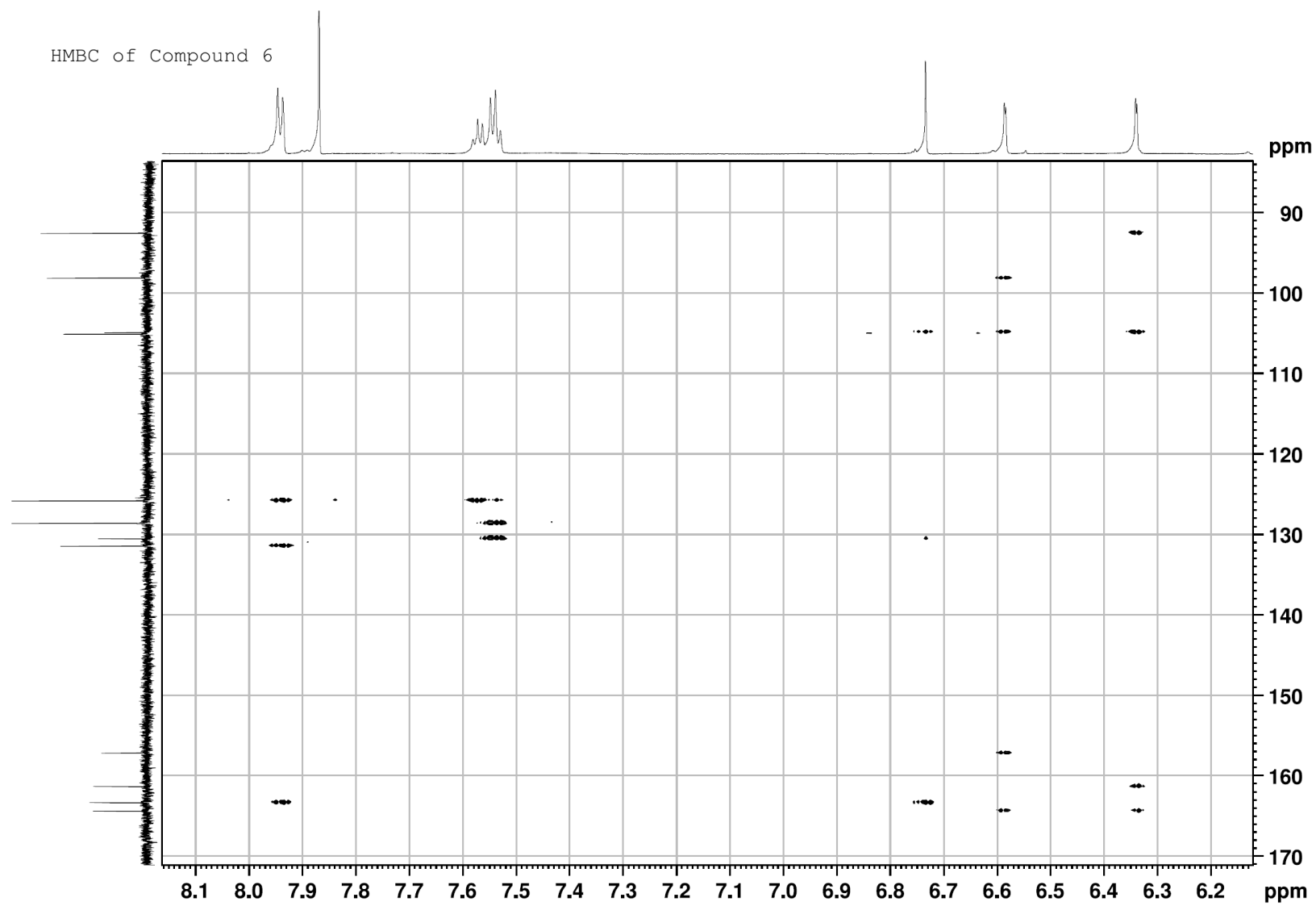


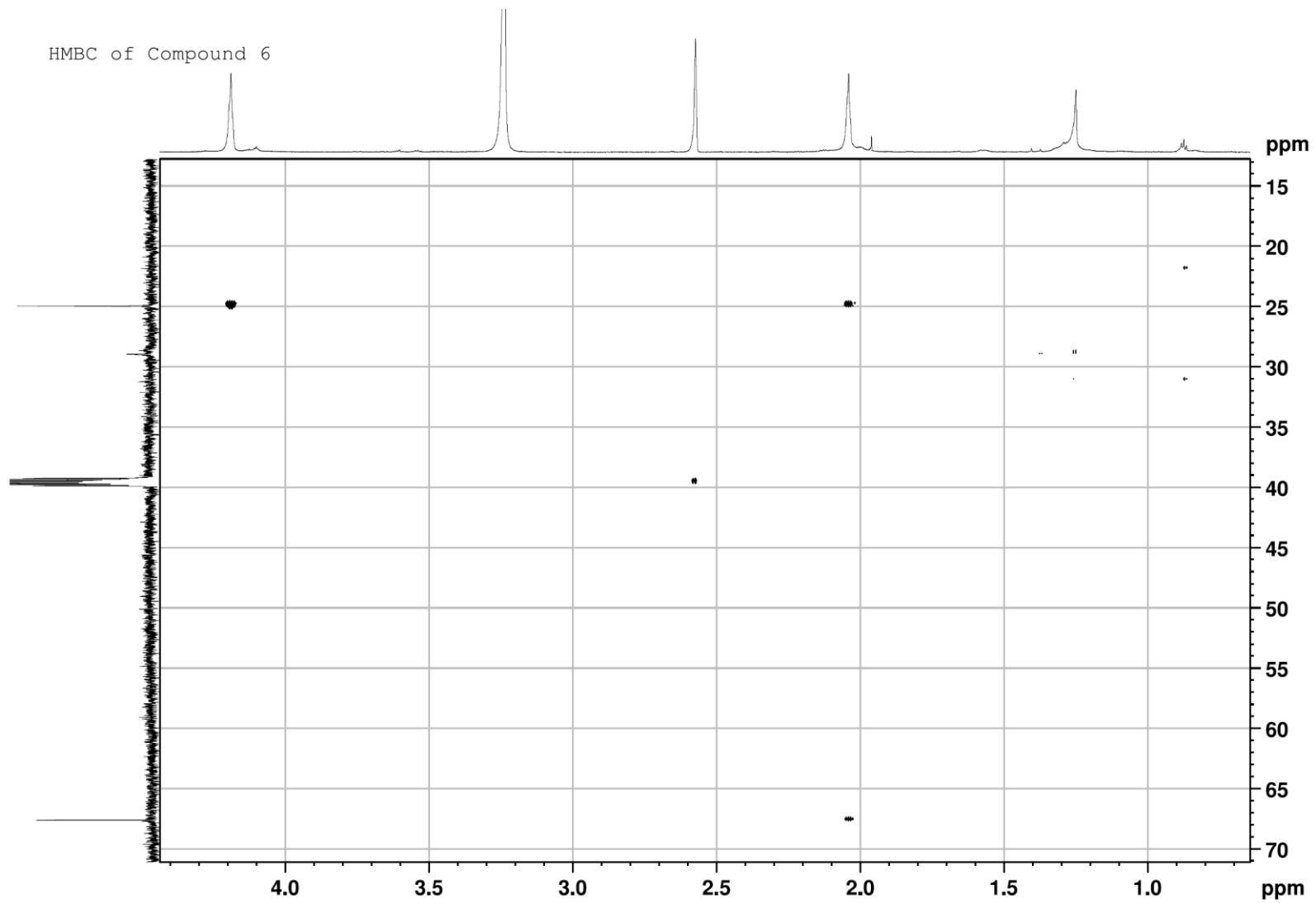
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HMBC of Compound 6



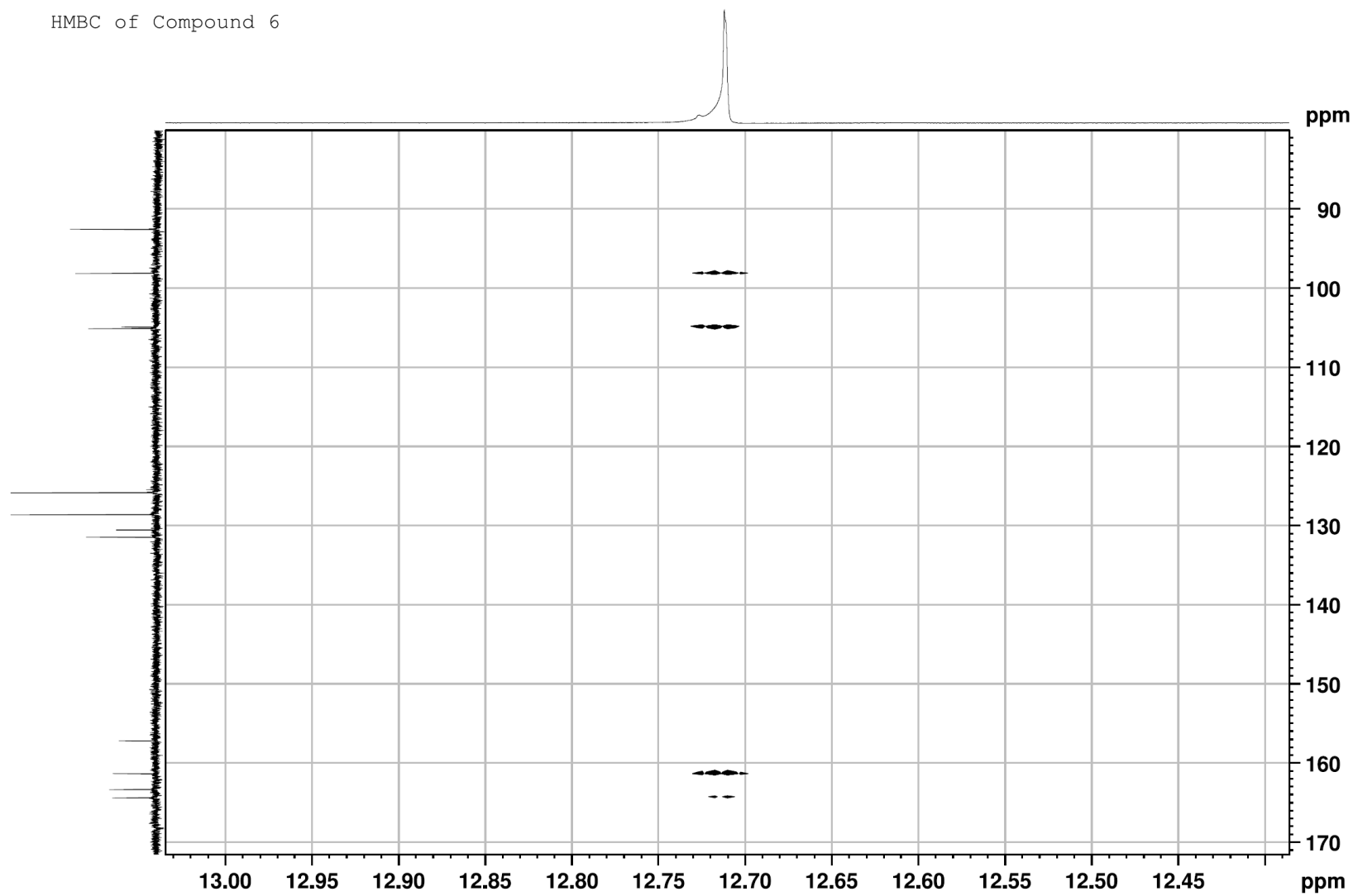
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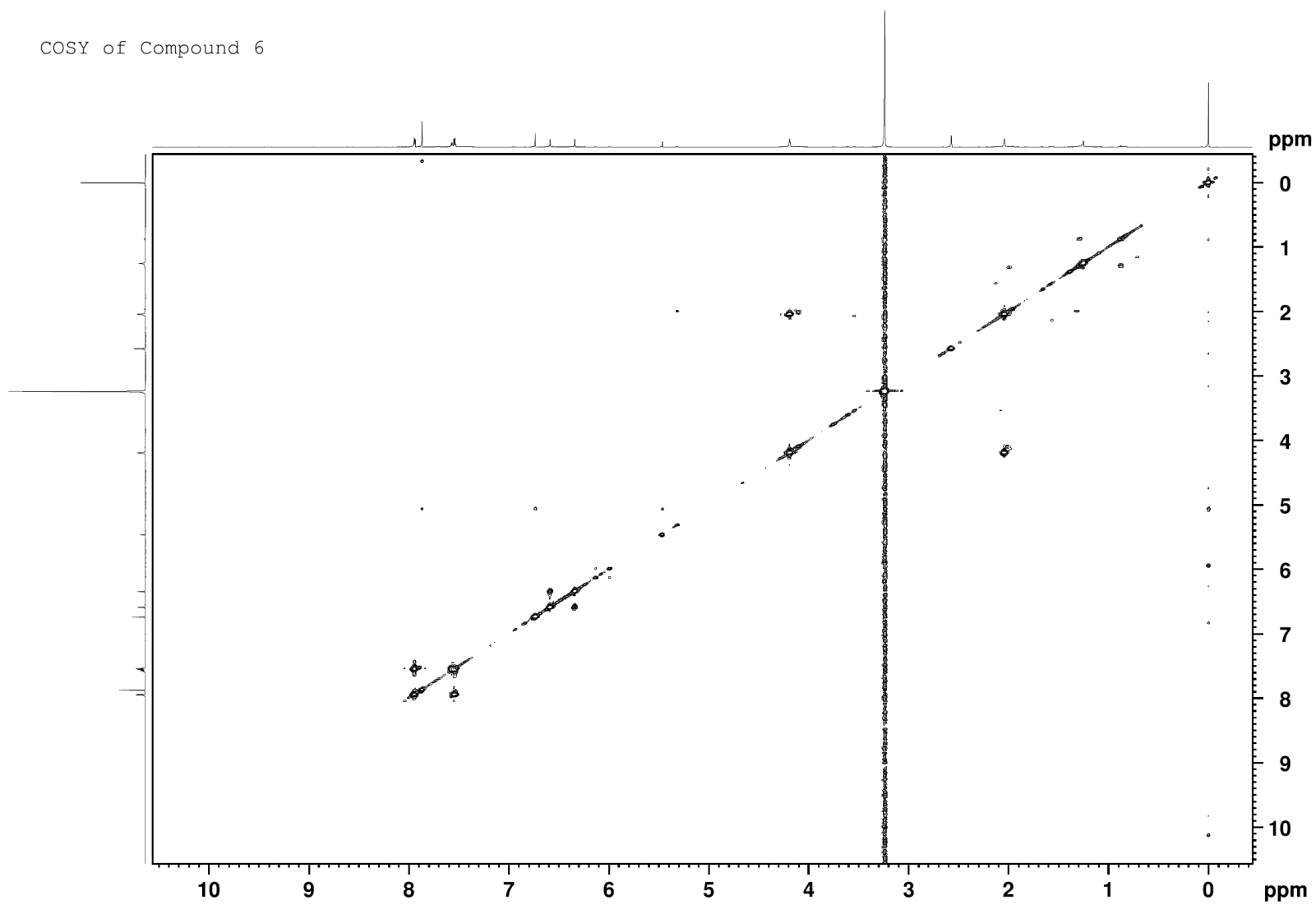


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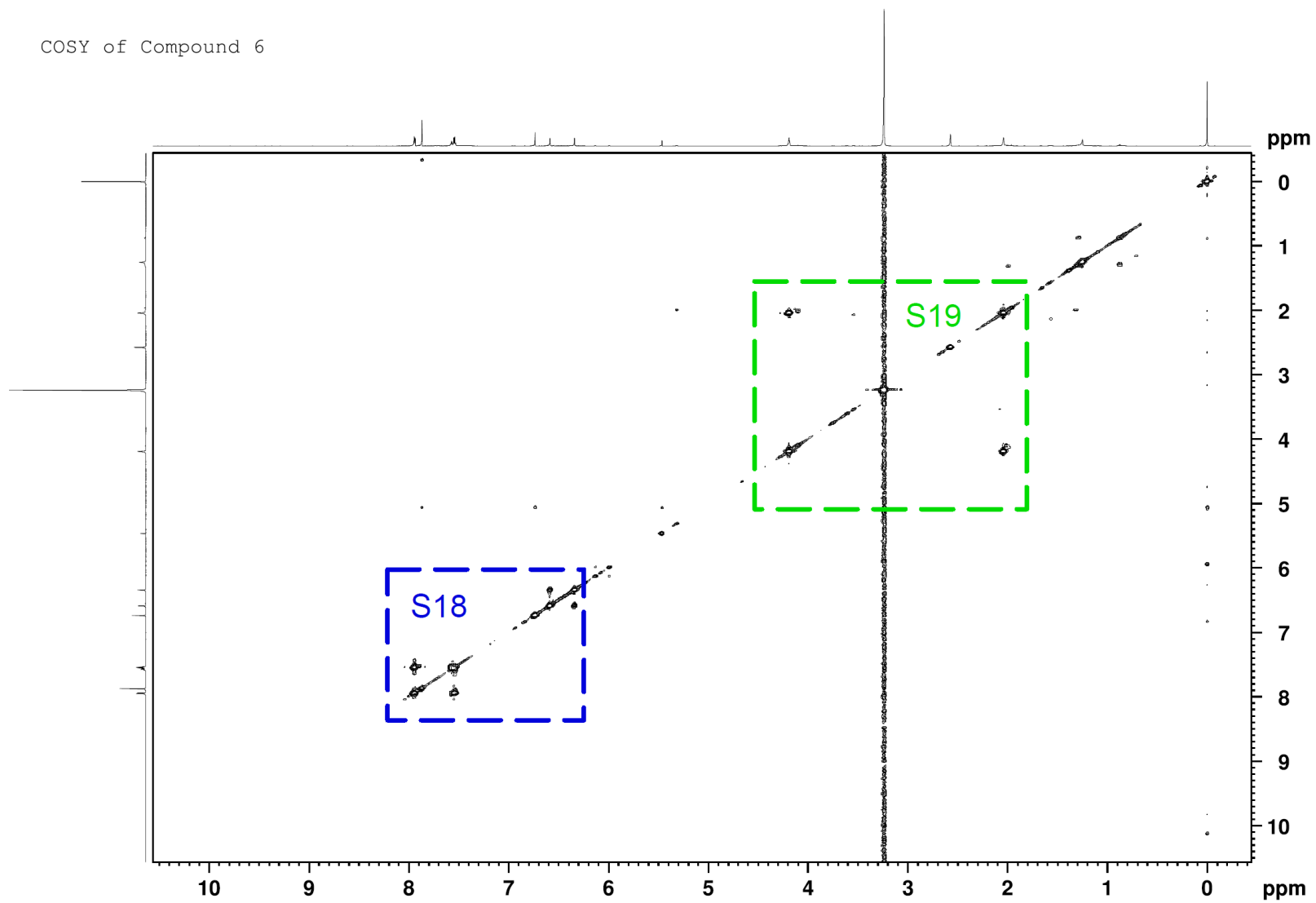


COSY of Compound 6



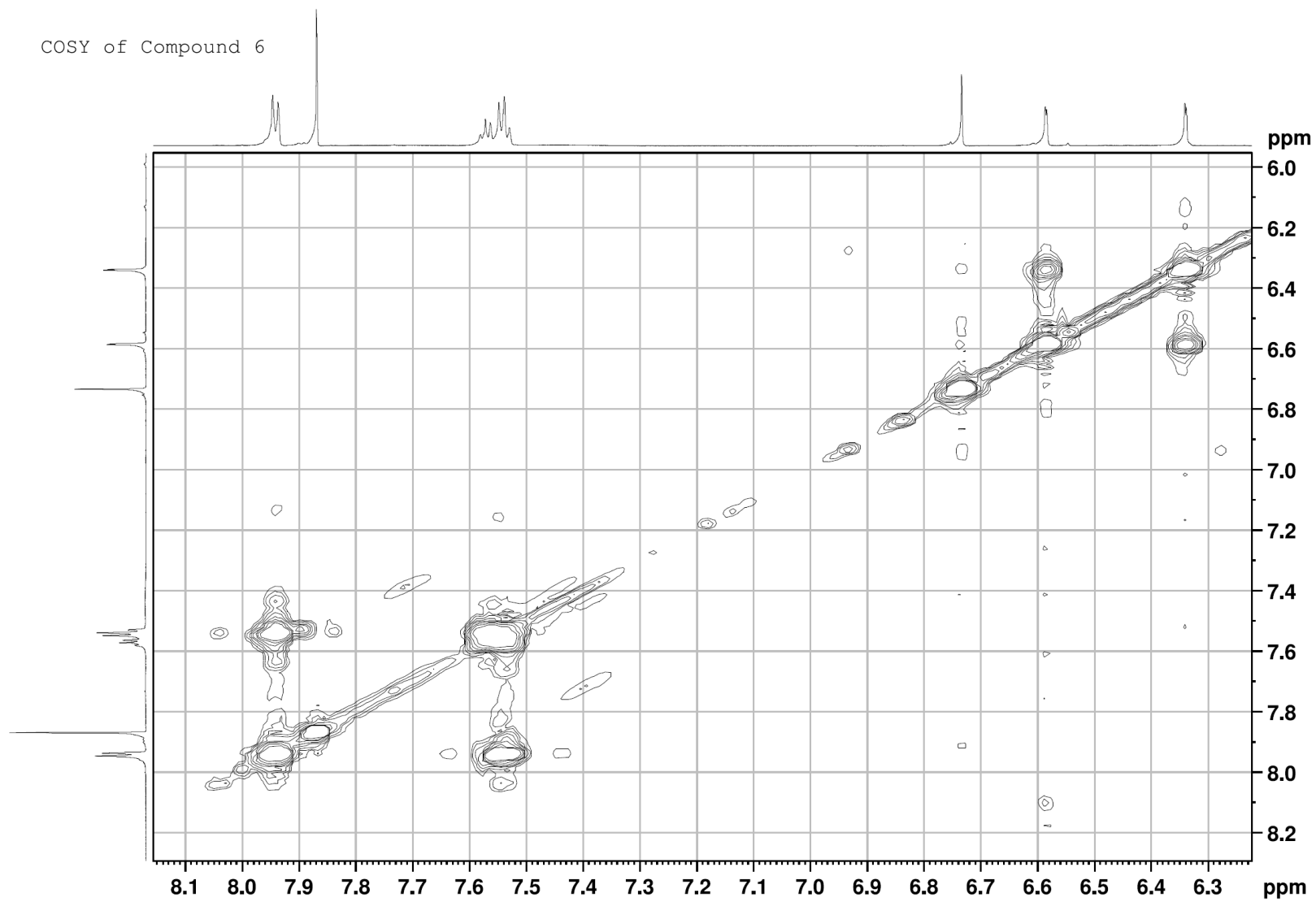
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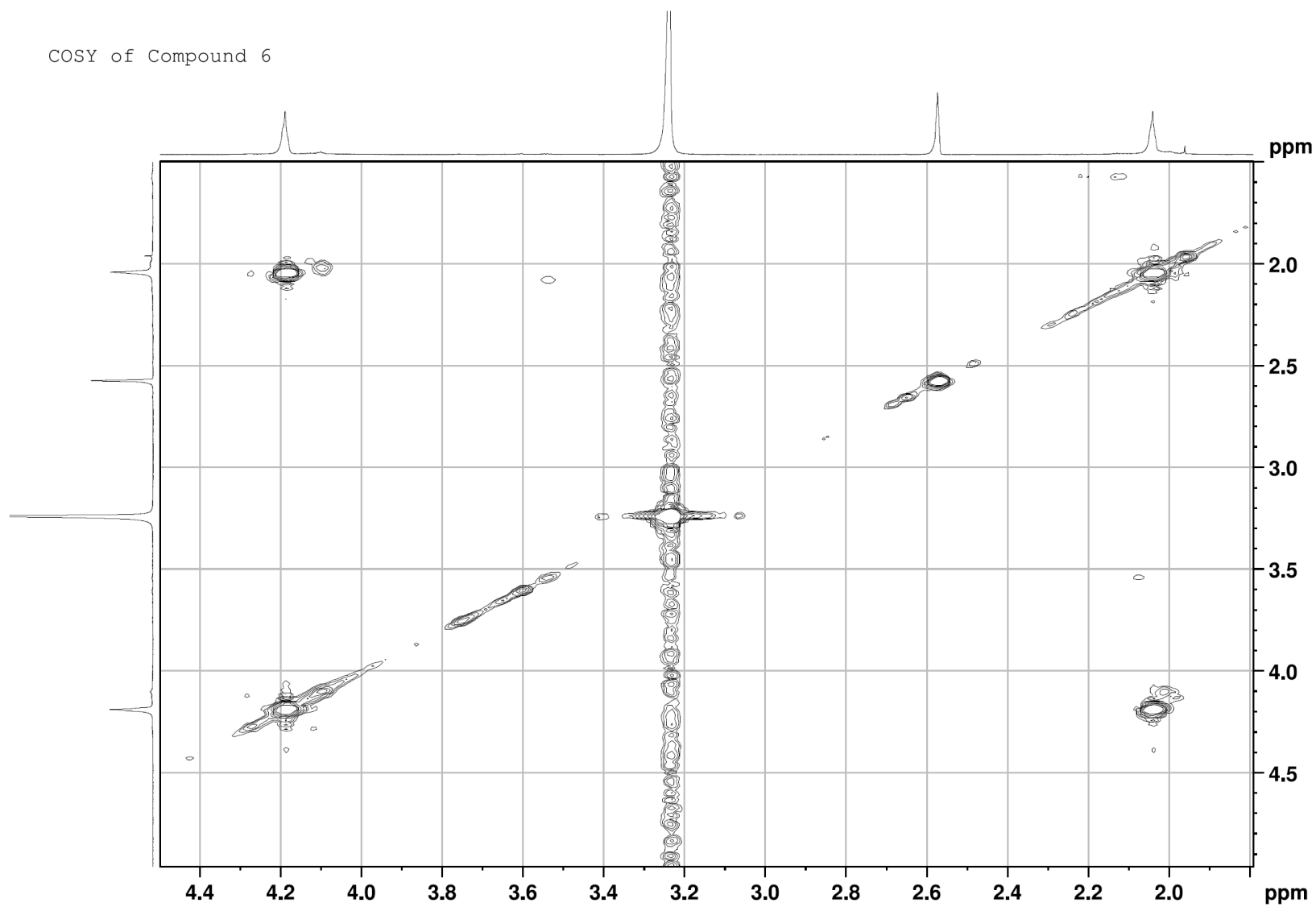


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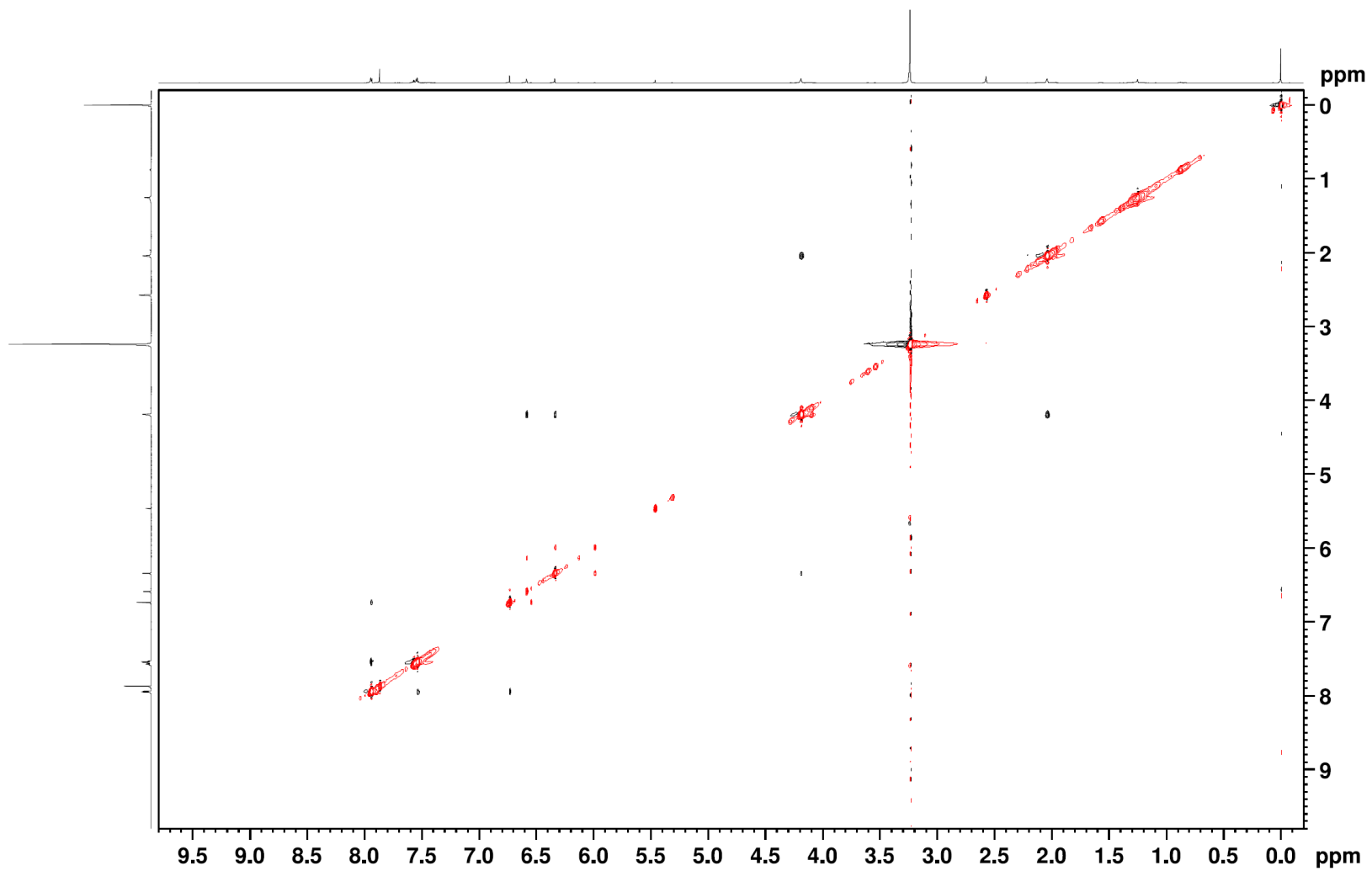
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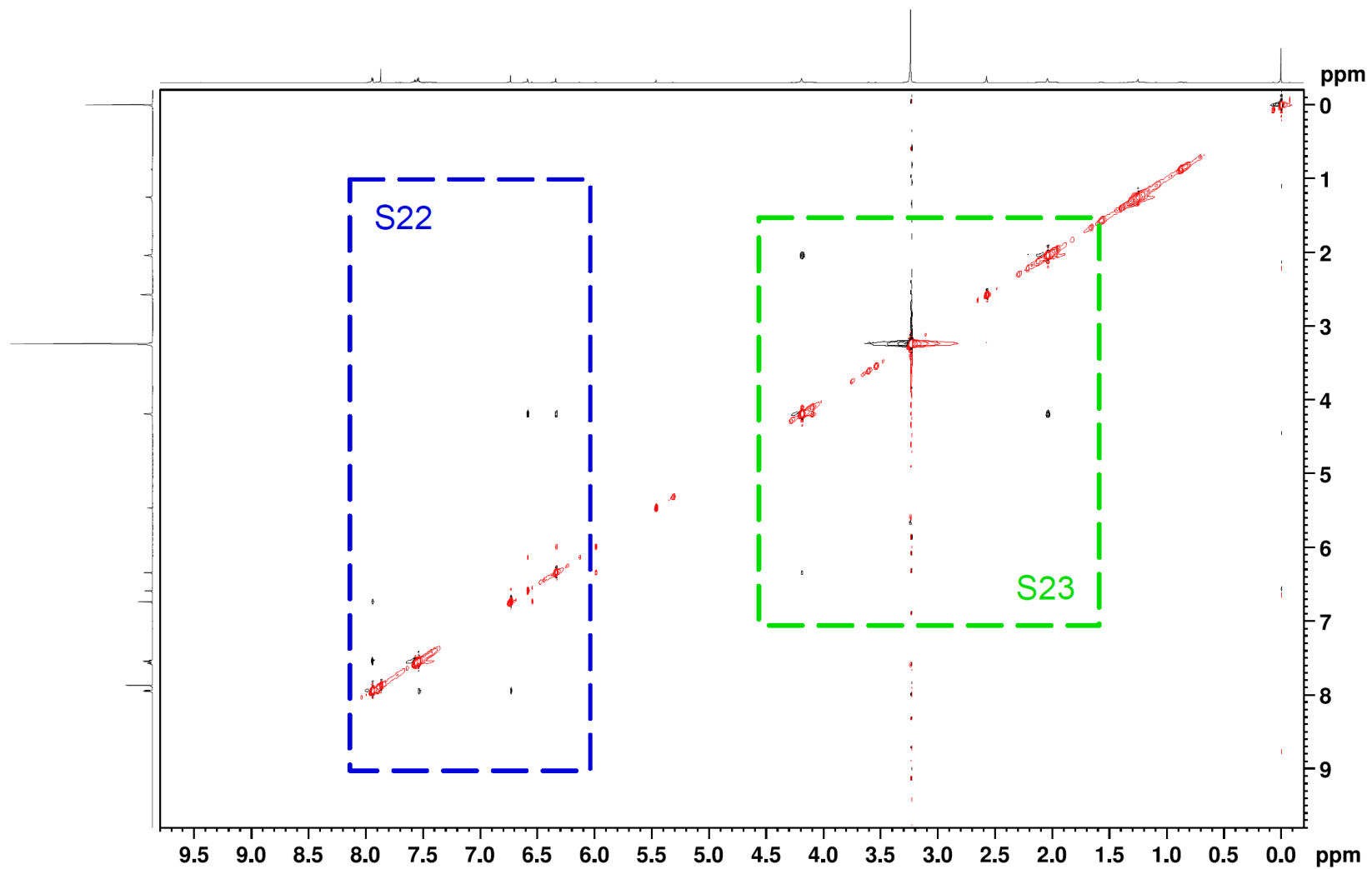


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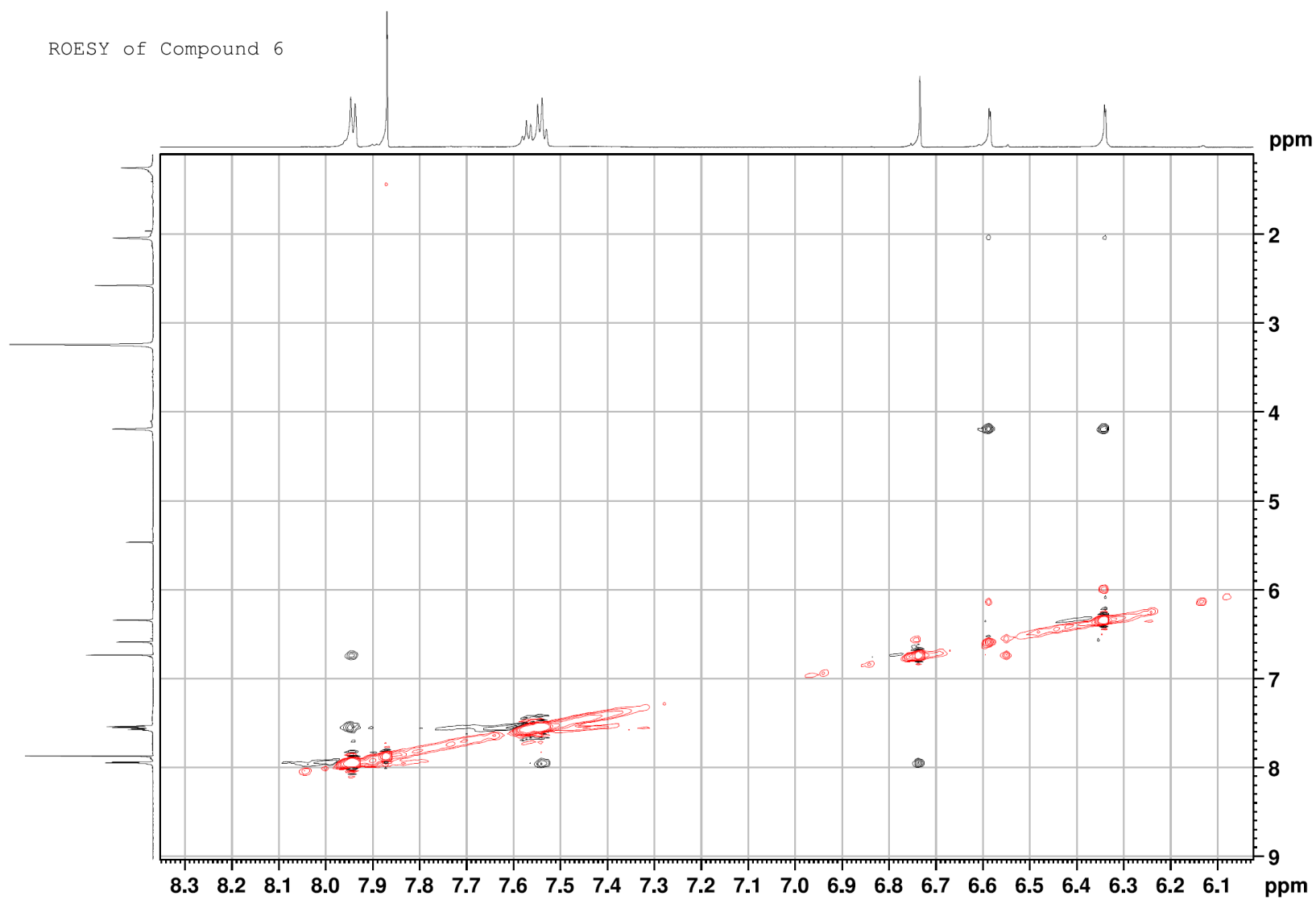


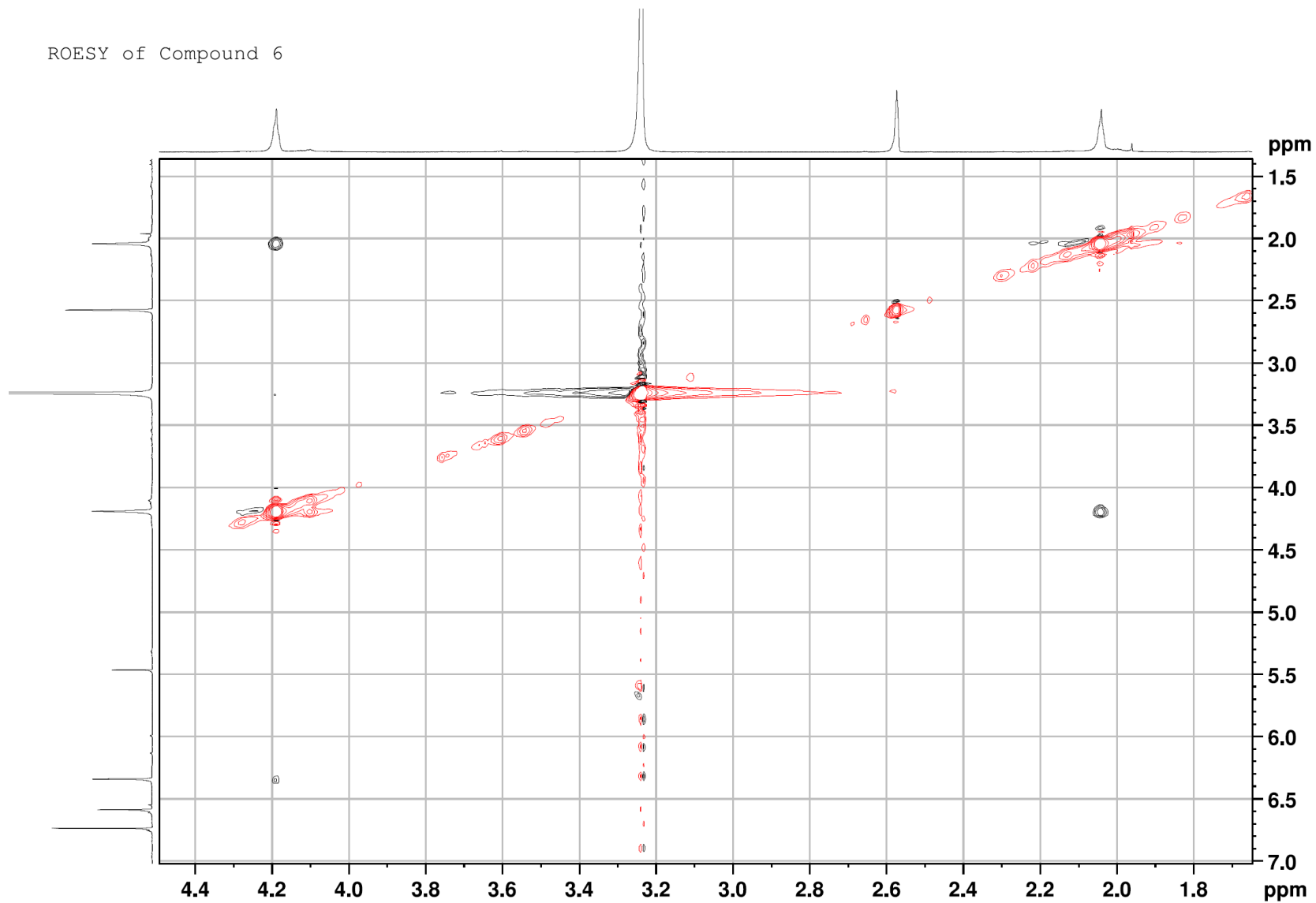
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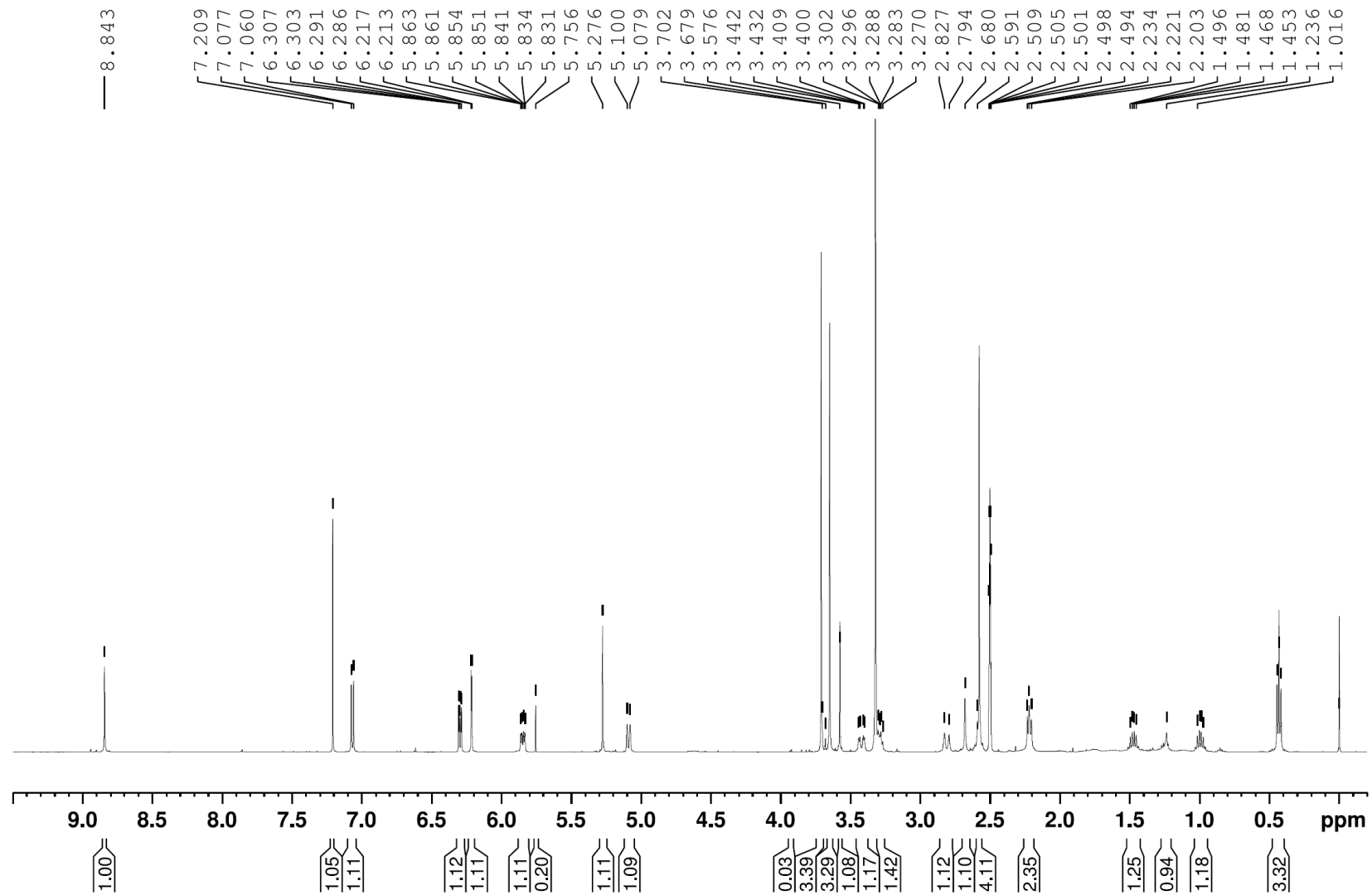
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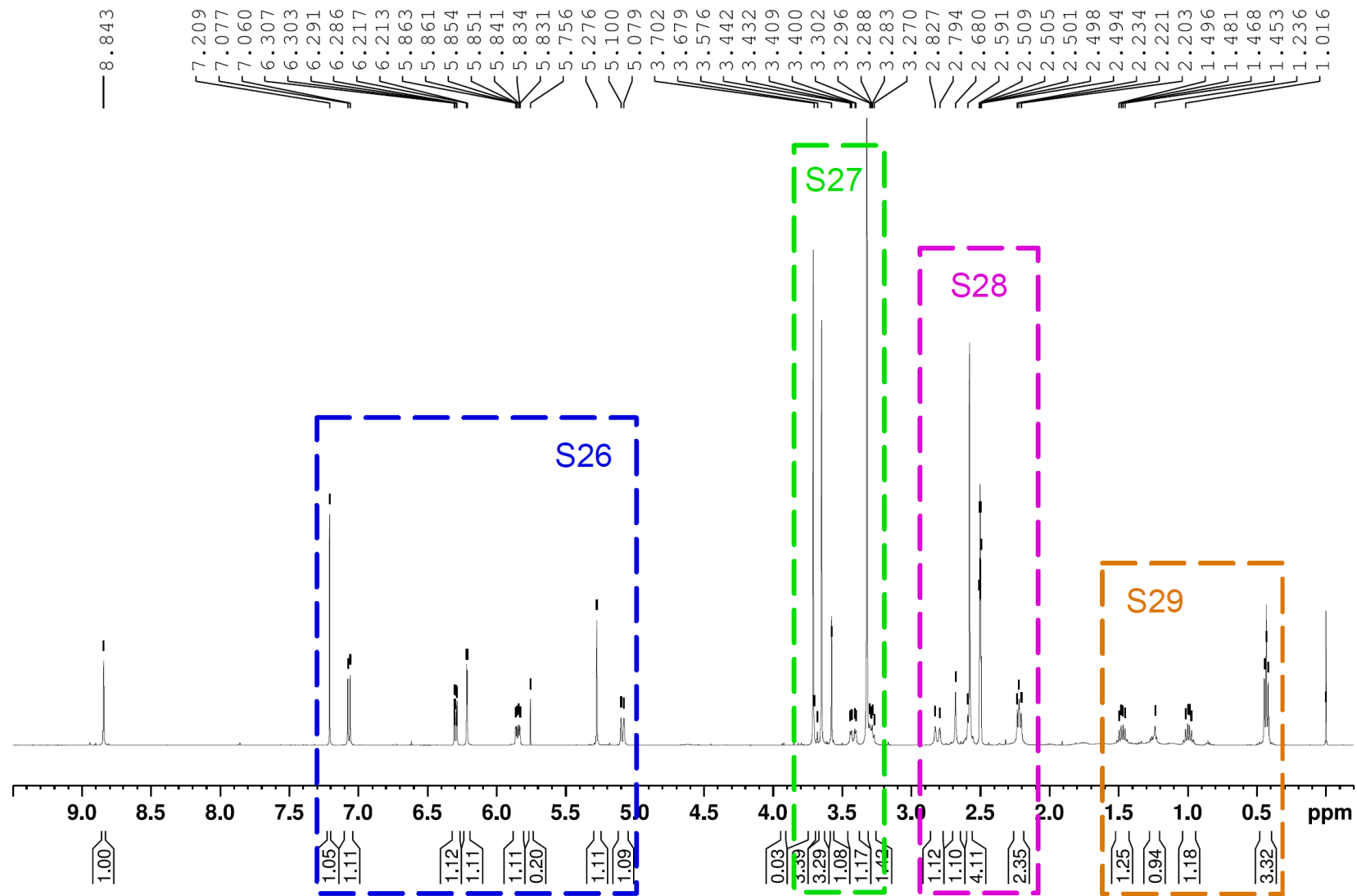
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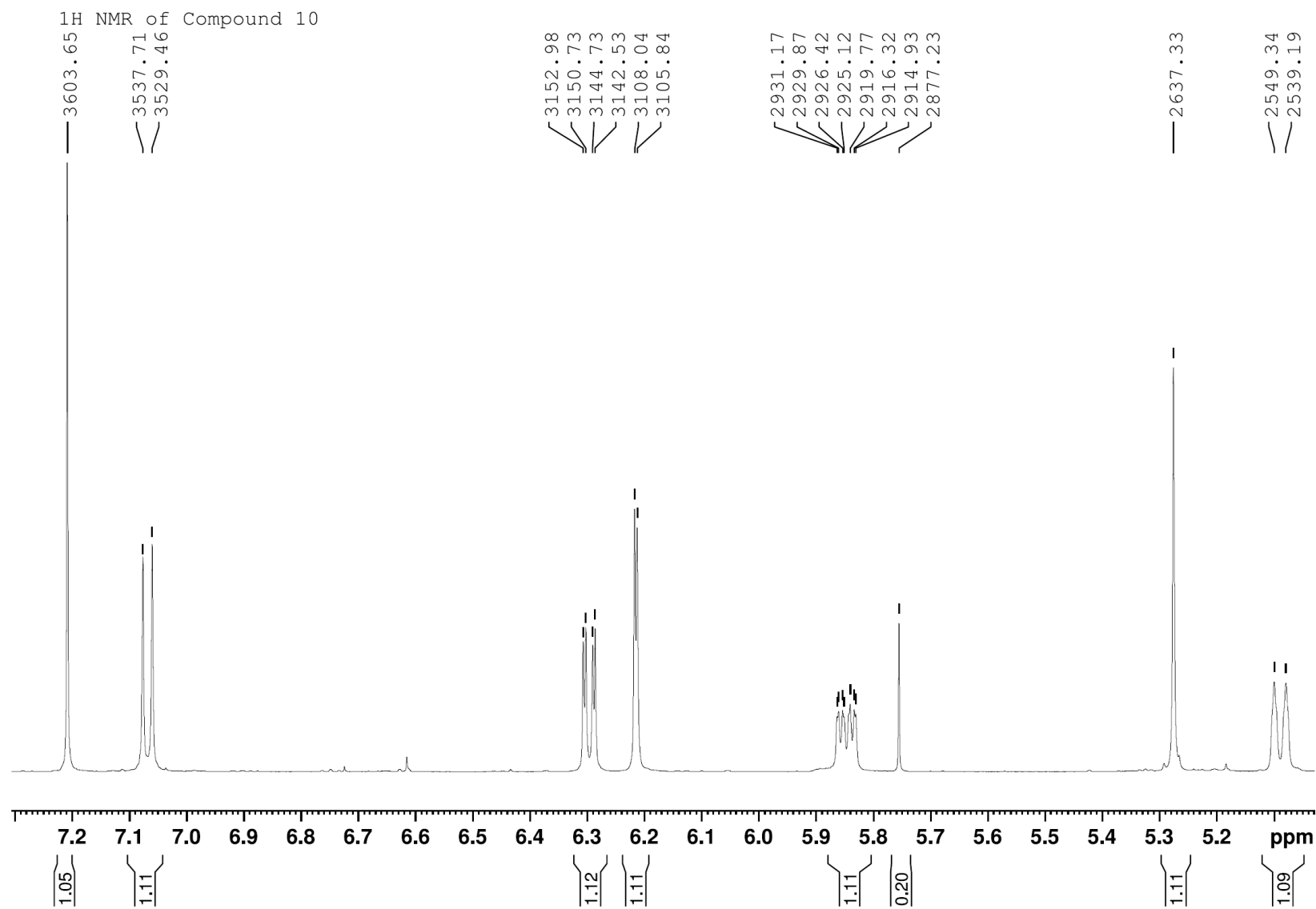


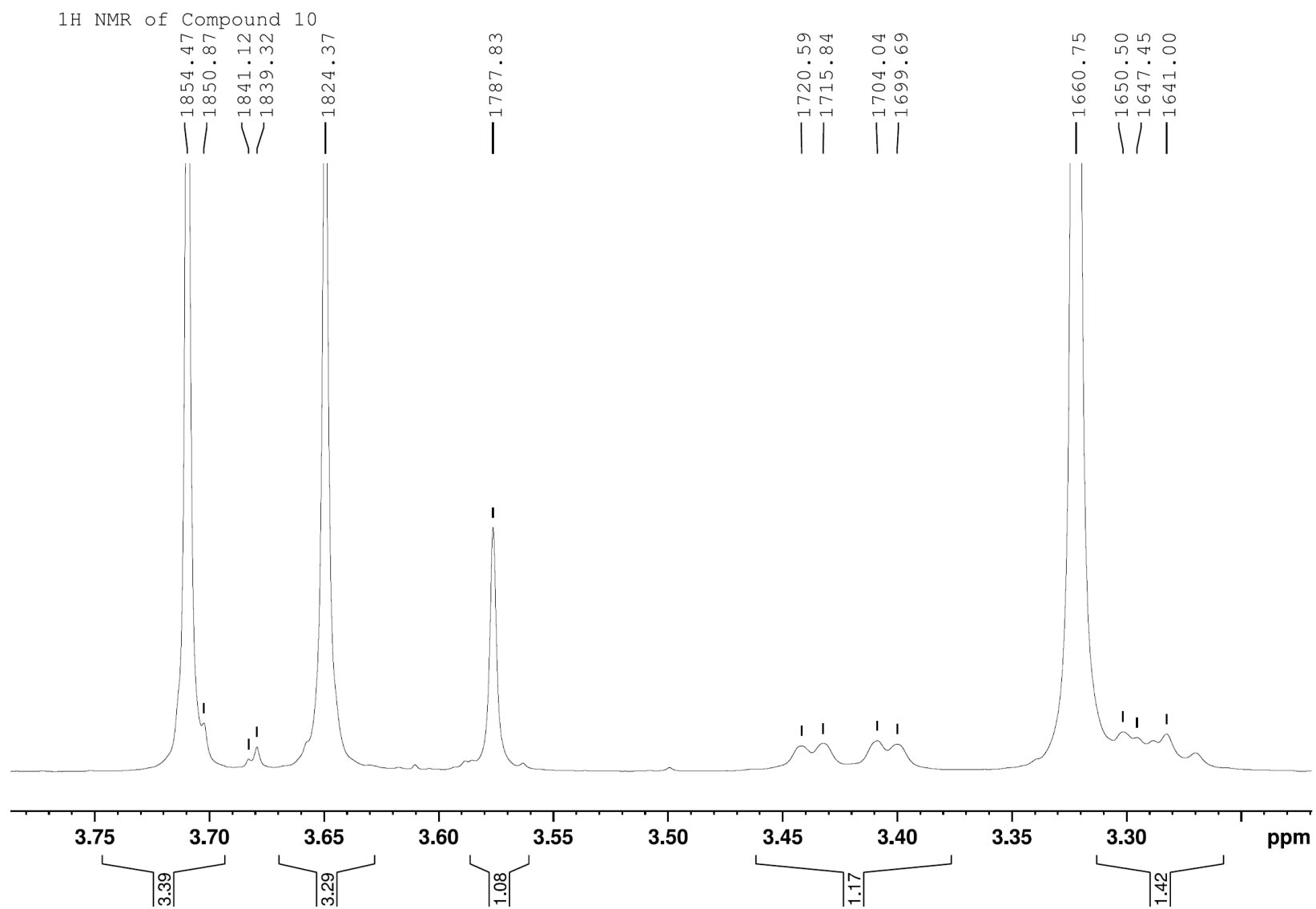
¹H NMR of Compound 10

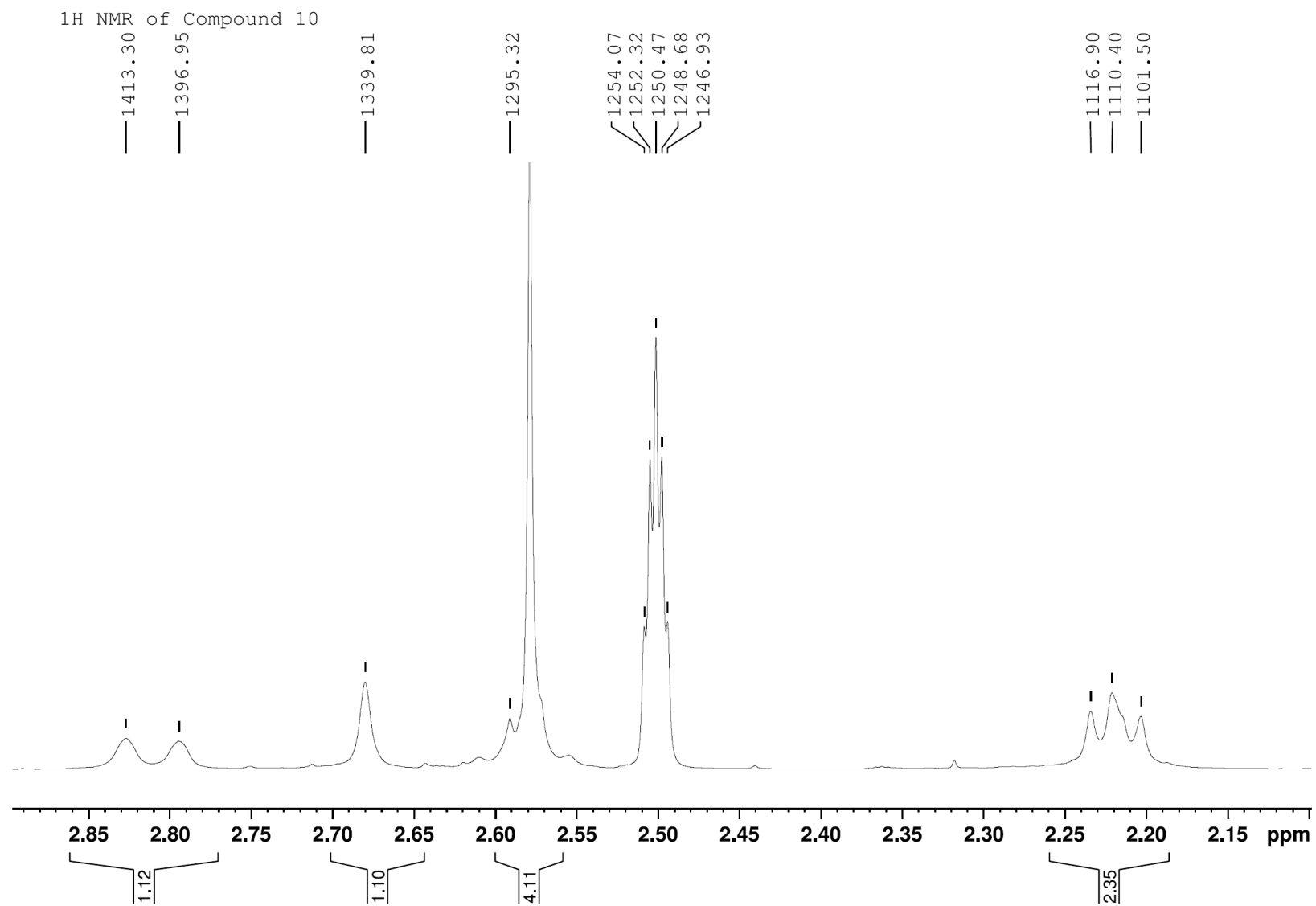
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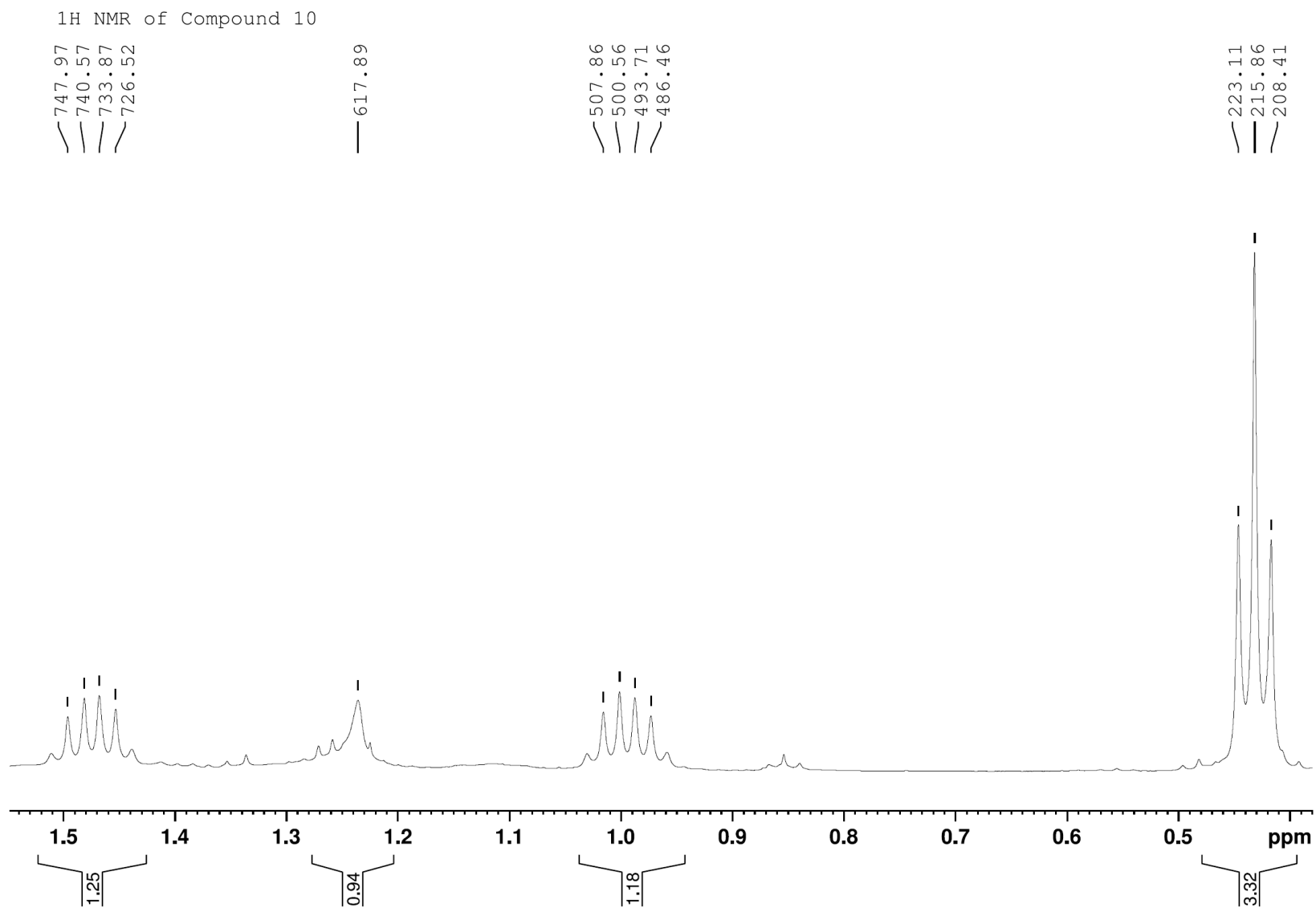
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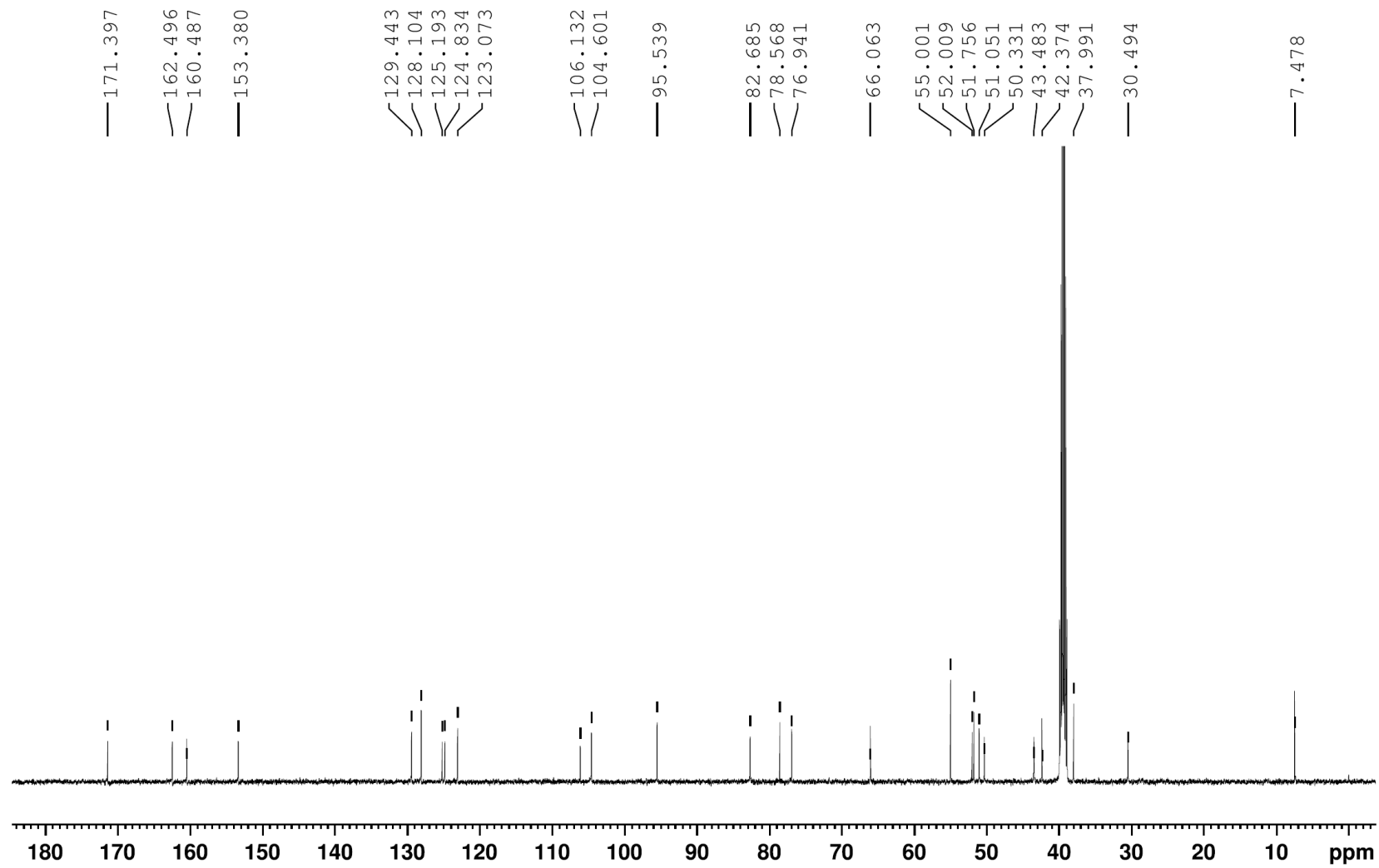




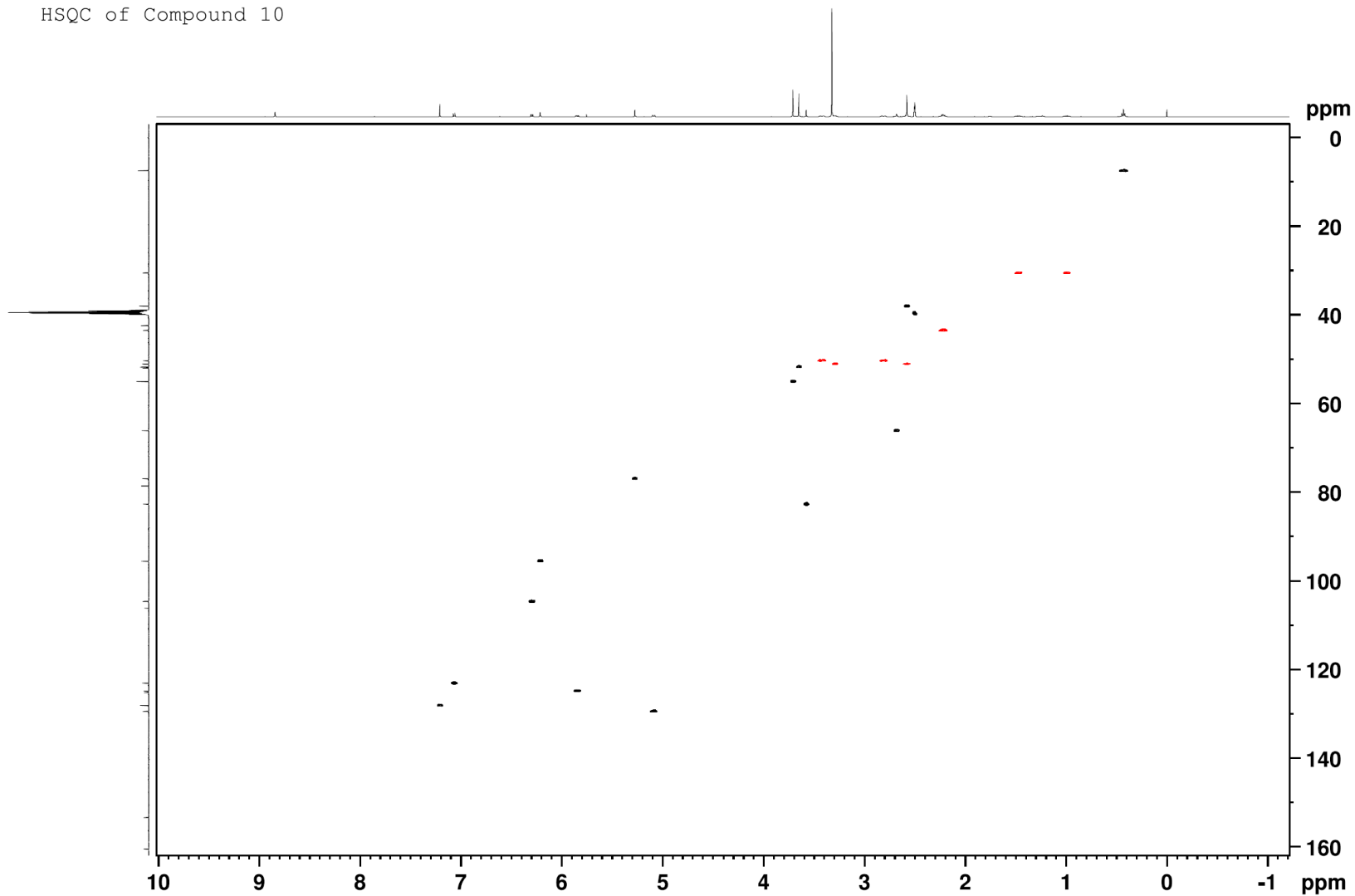
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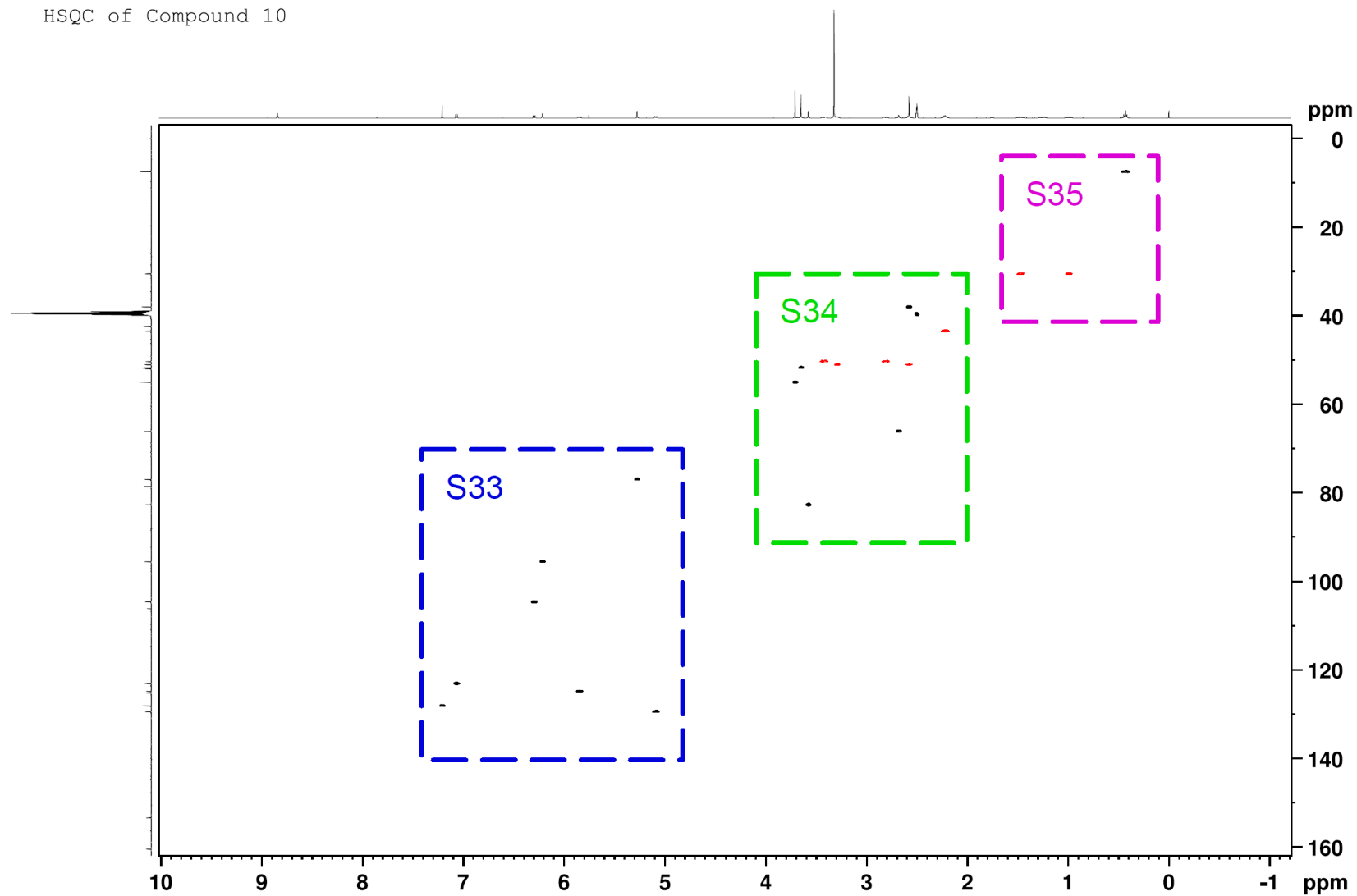
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^{13}C NMR of Compound 10

HSQC of Compound 10

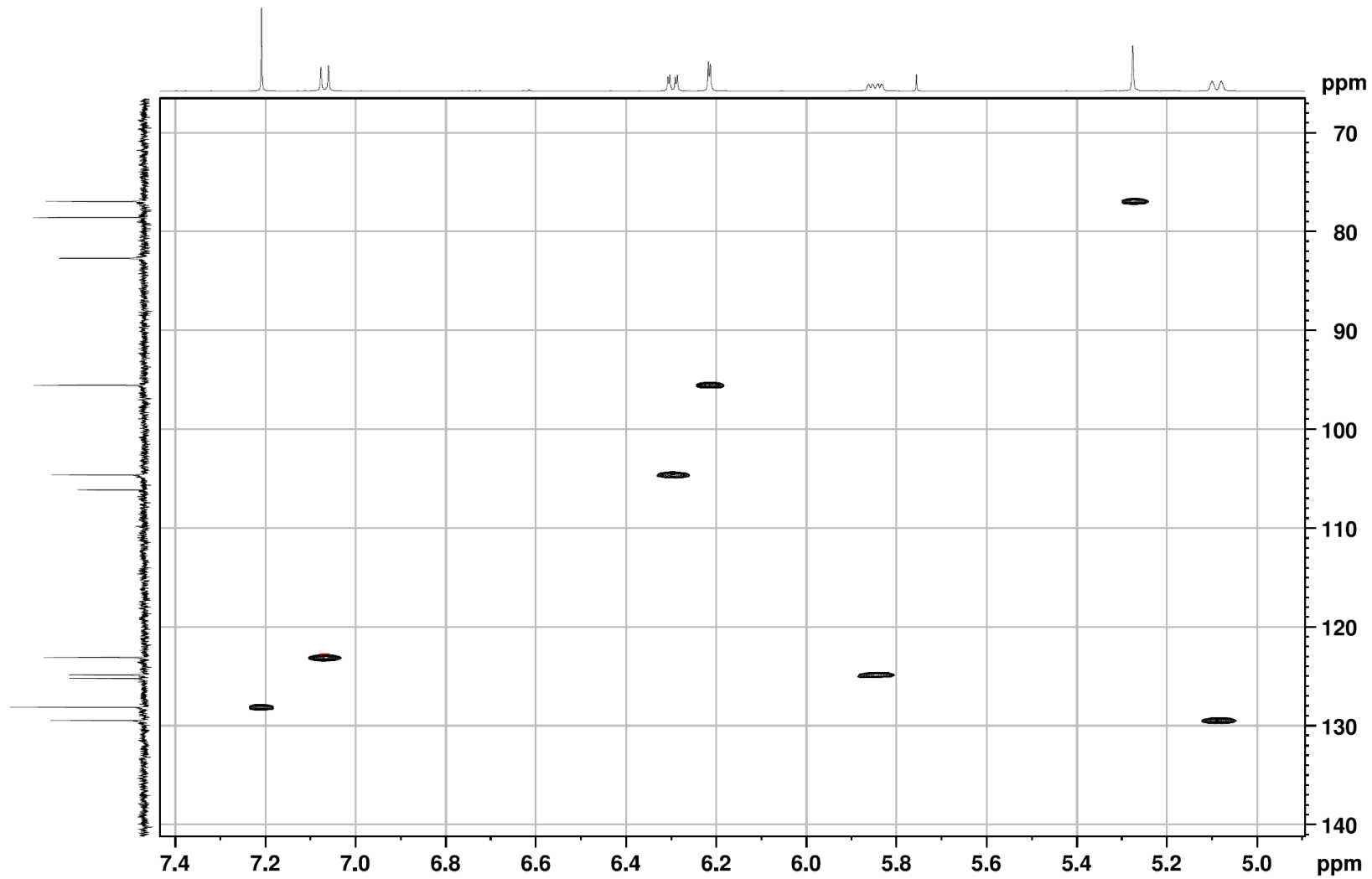


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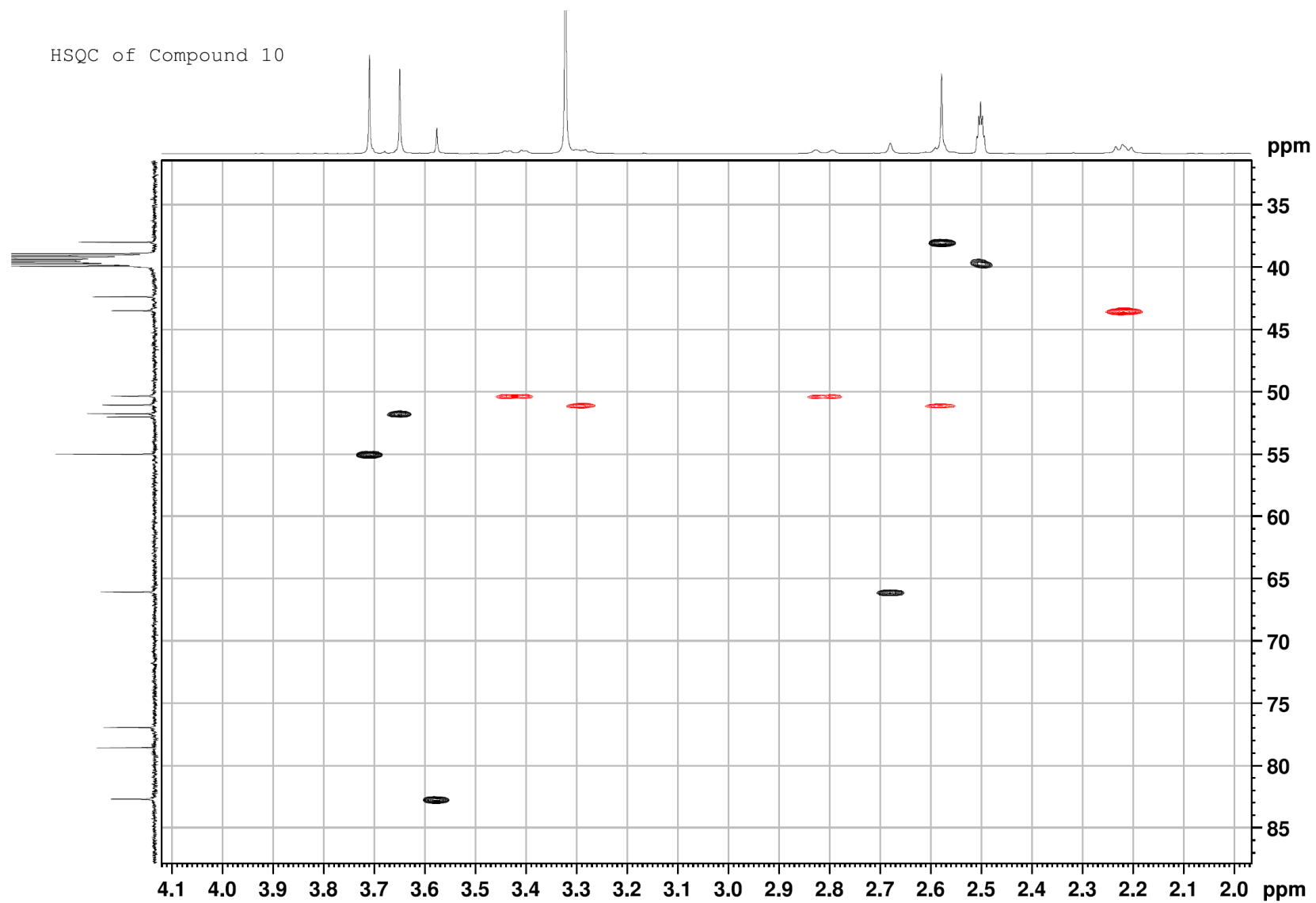


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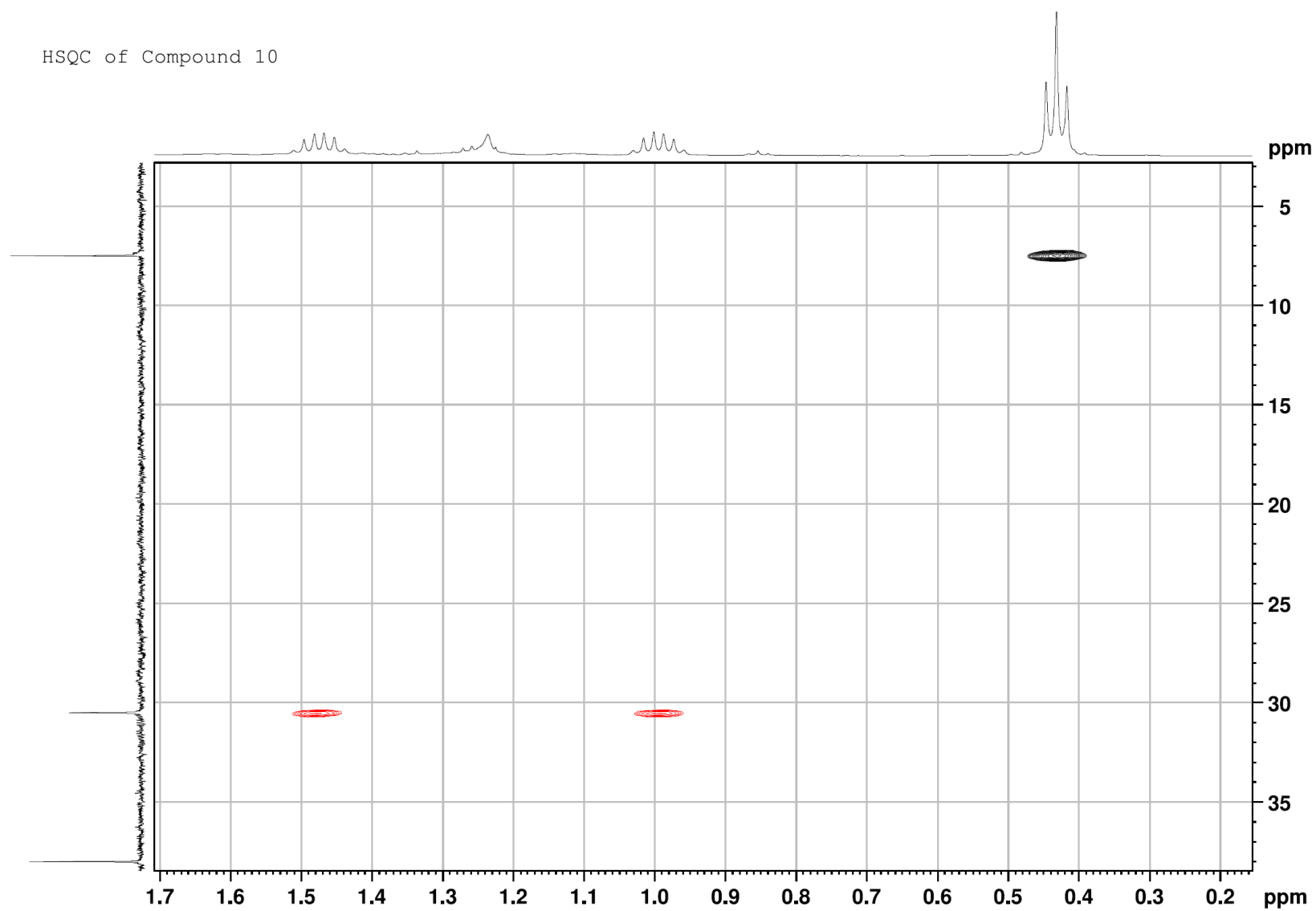
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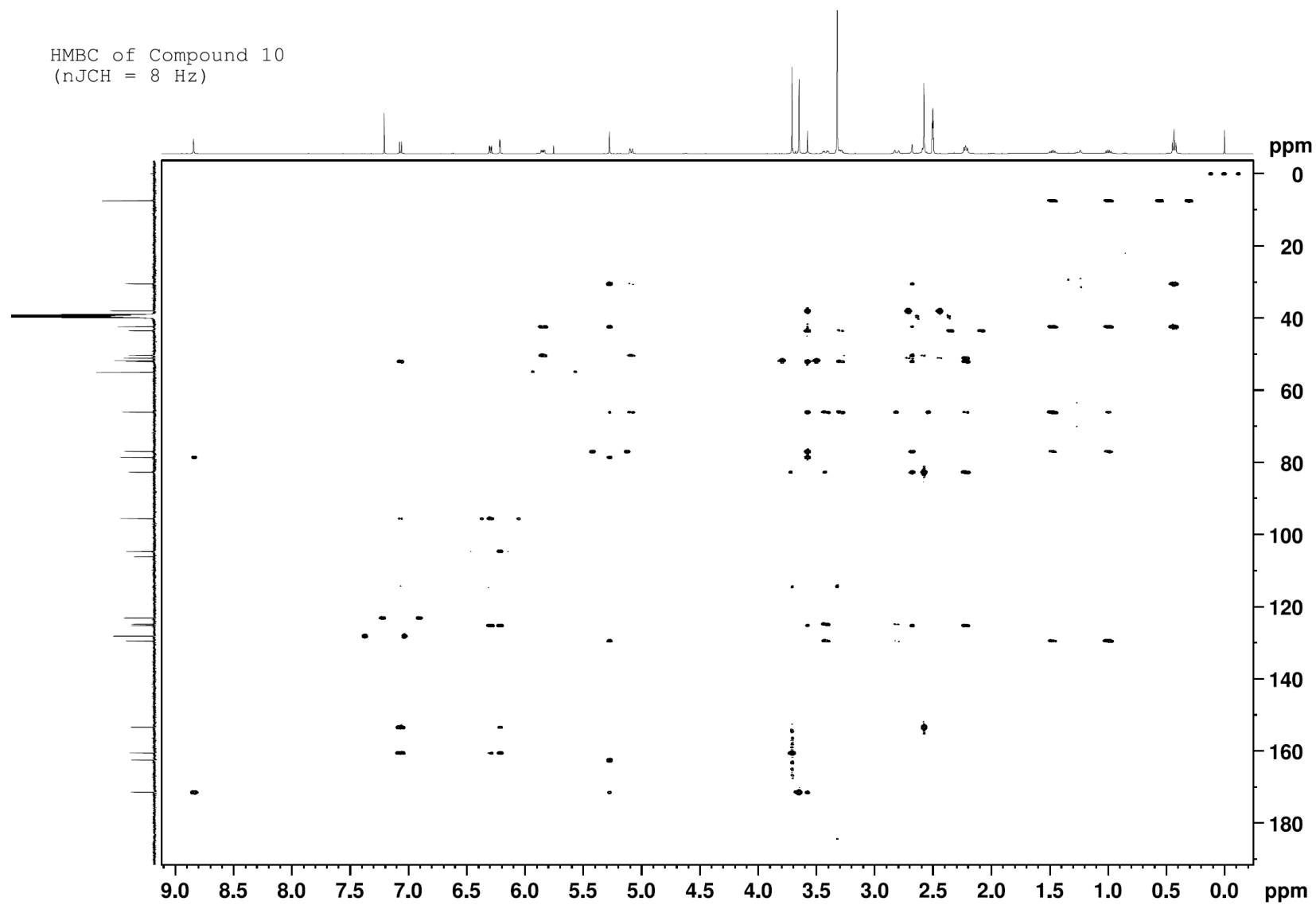
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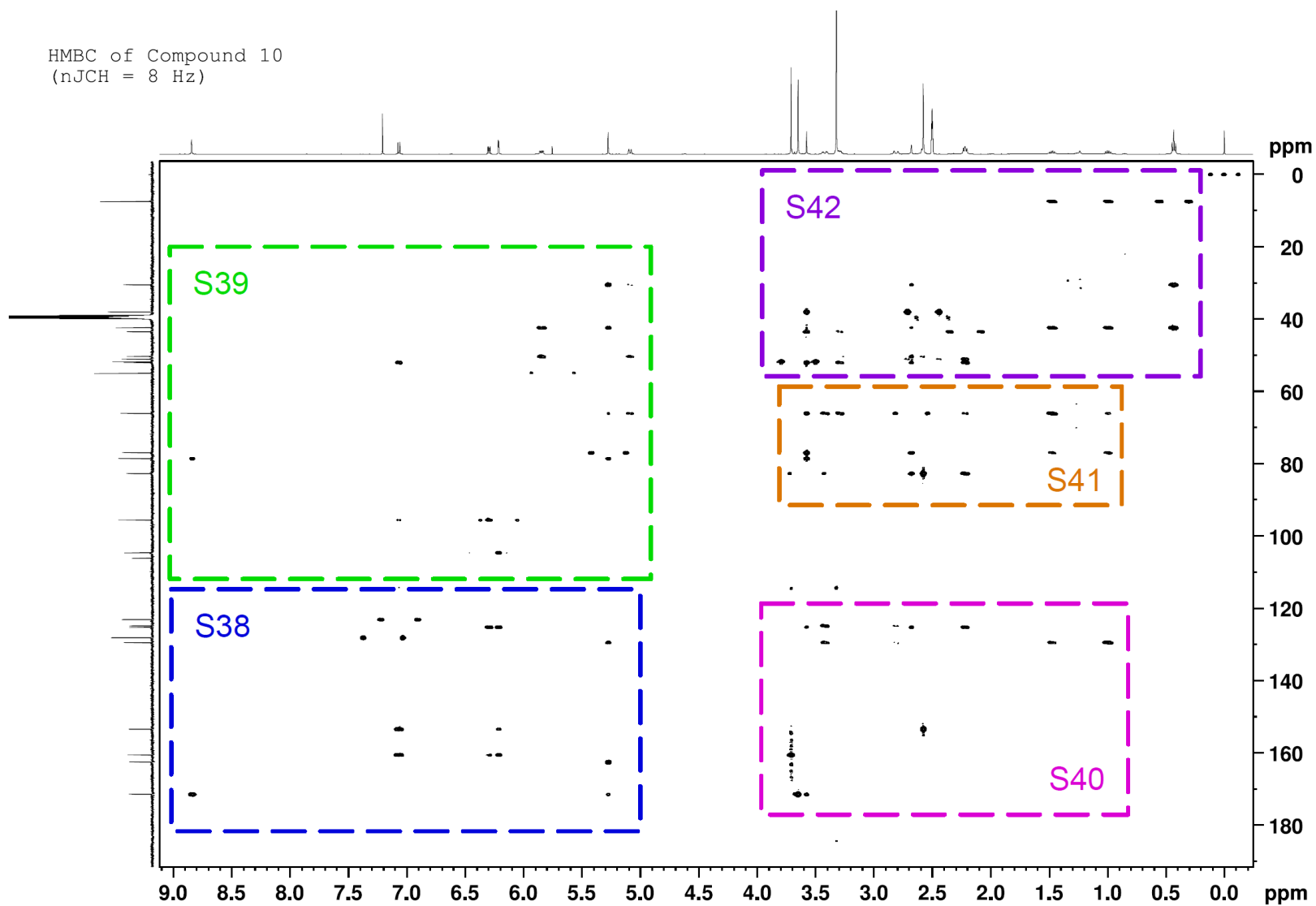


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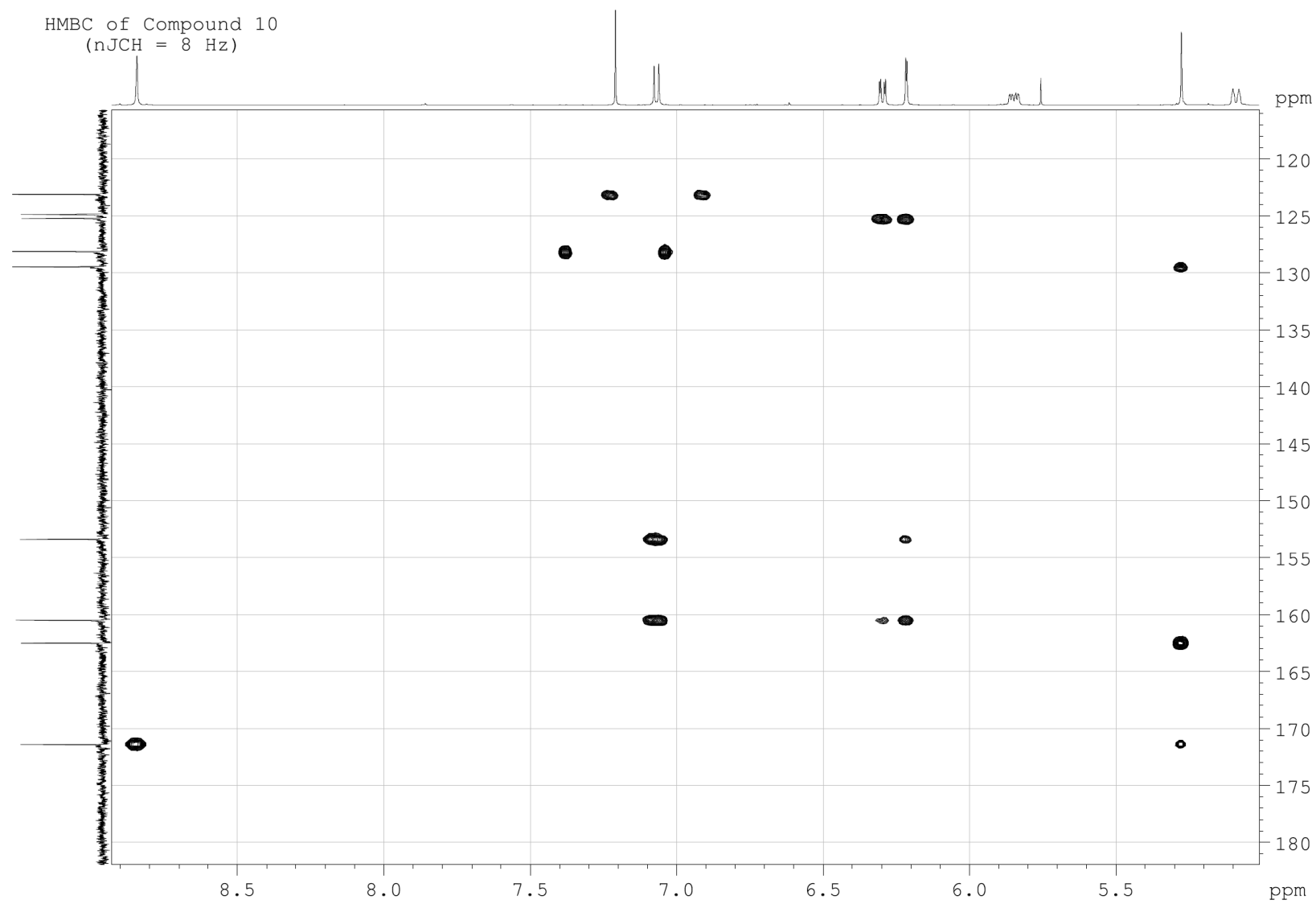


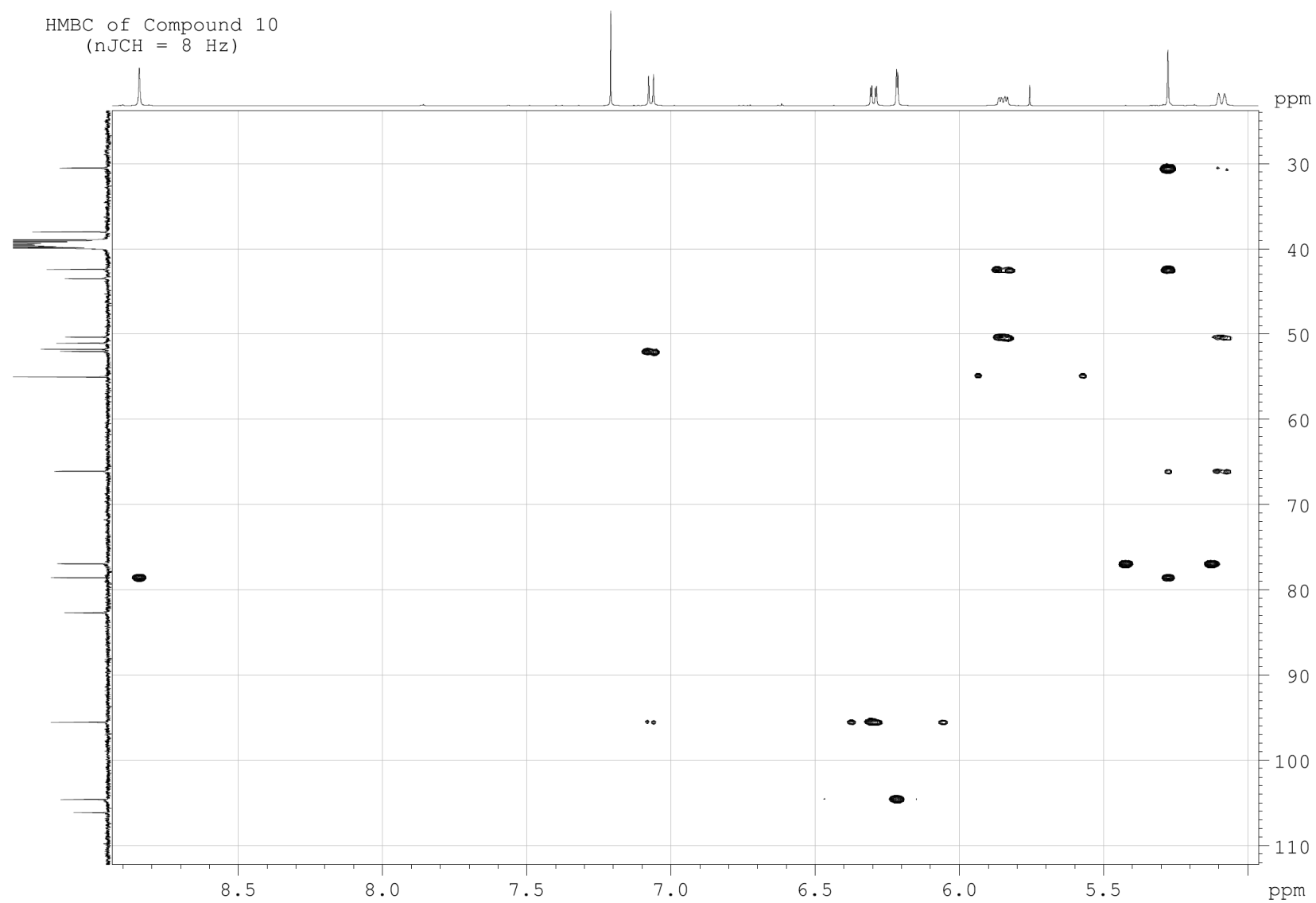
HMBC of Compound 10
($nJ_{CH} = 8$ Hz)



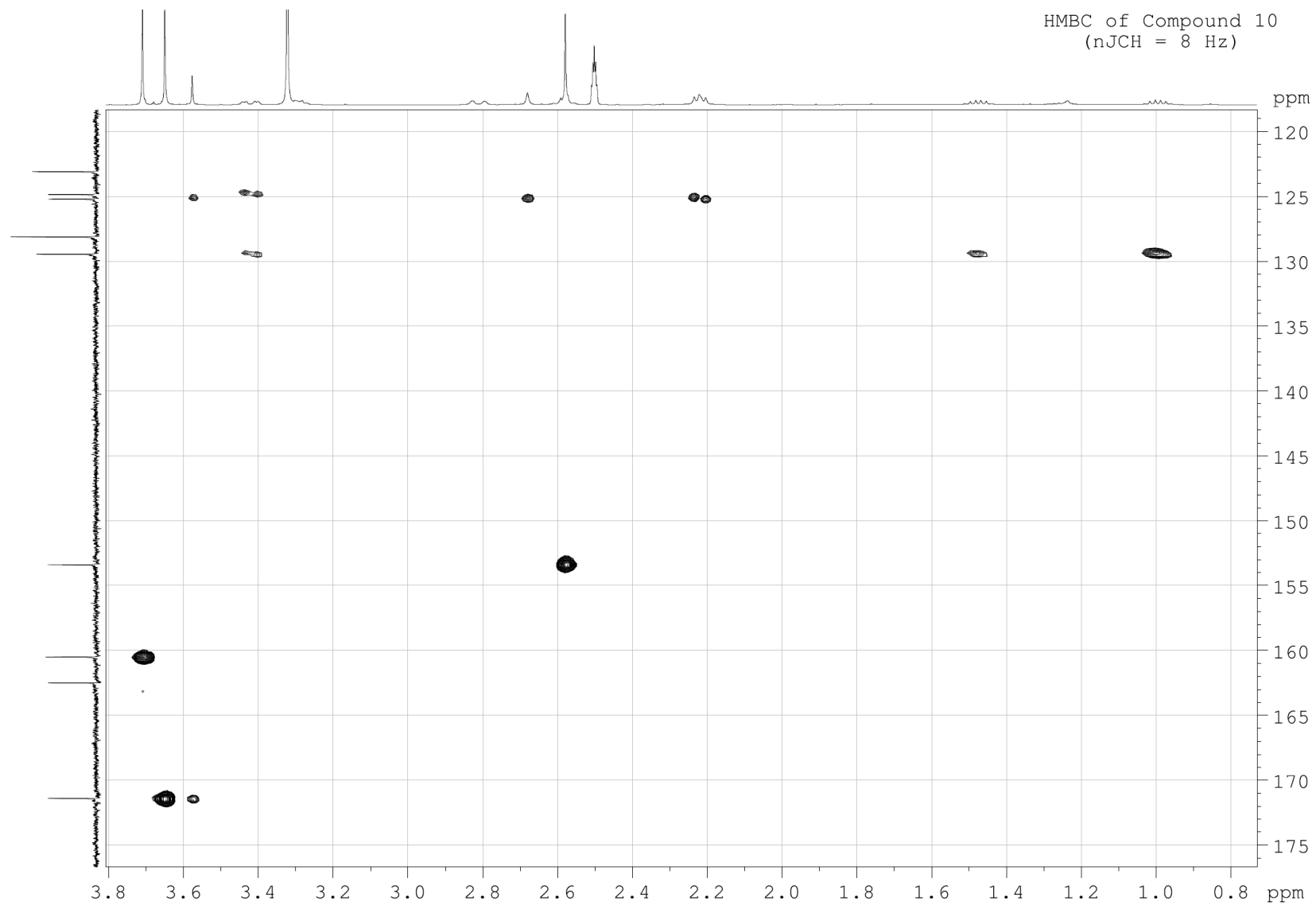


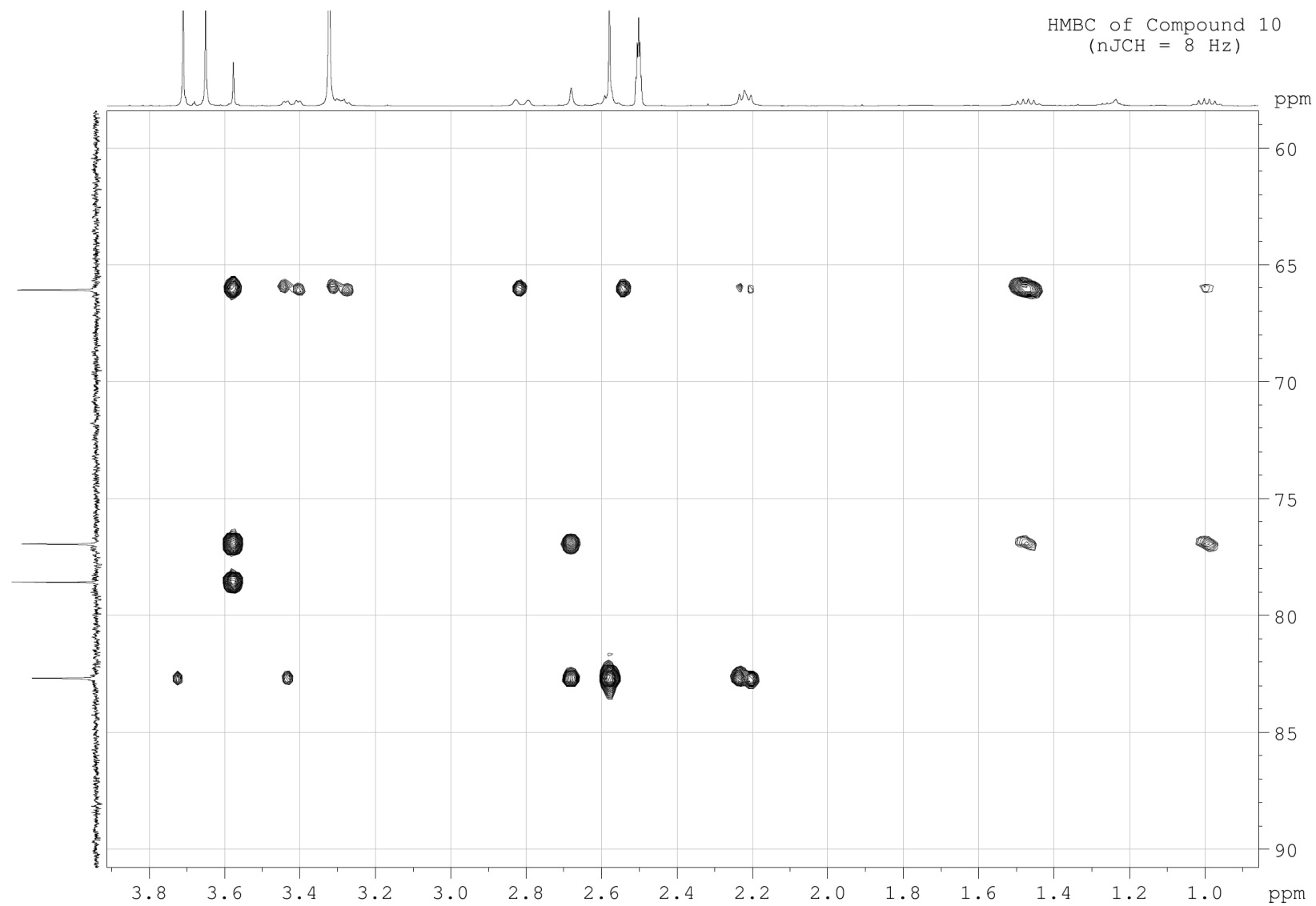
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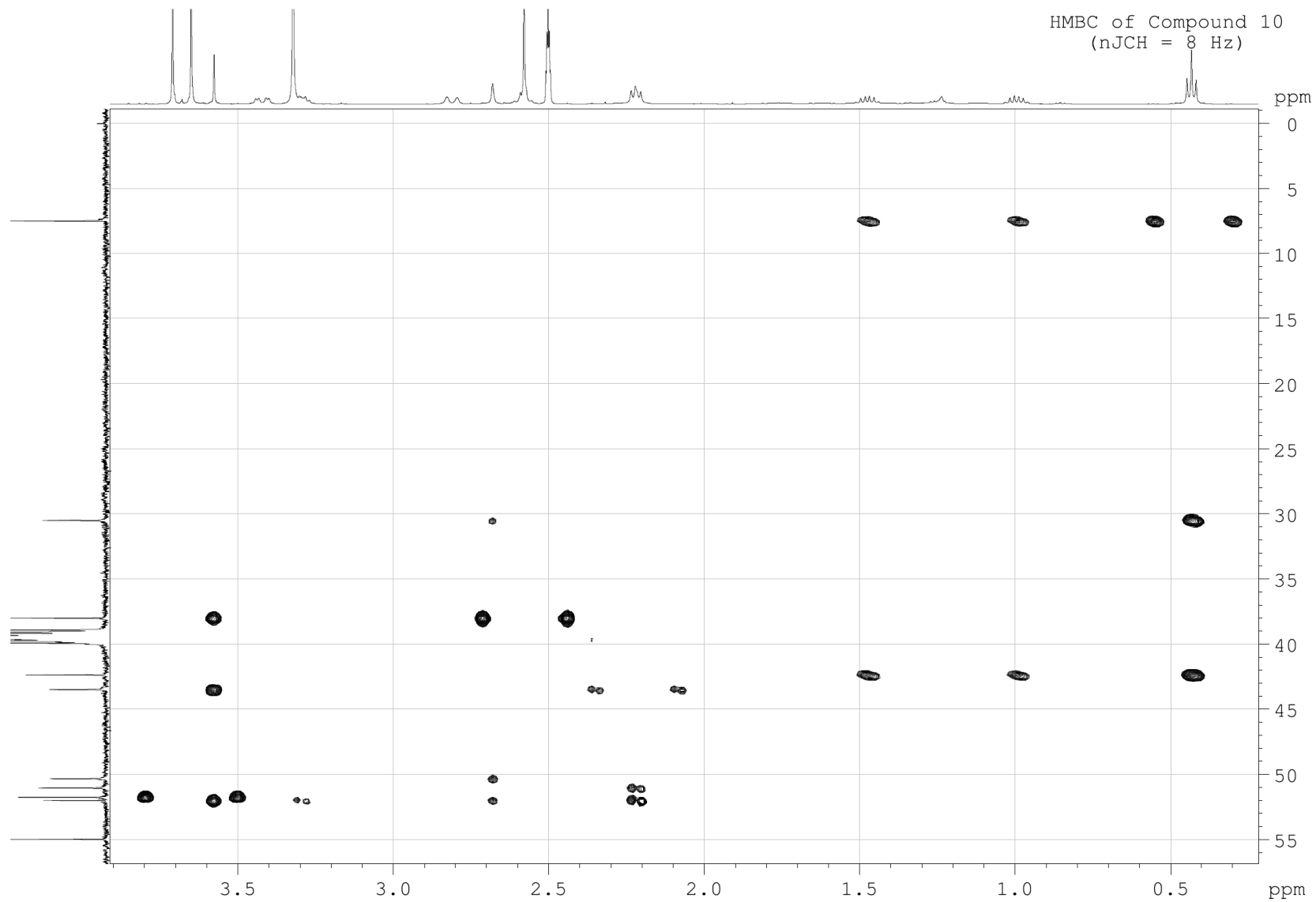




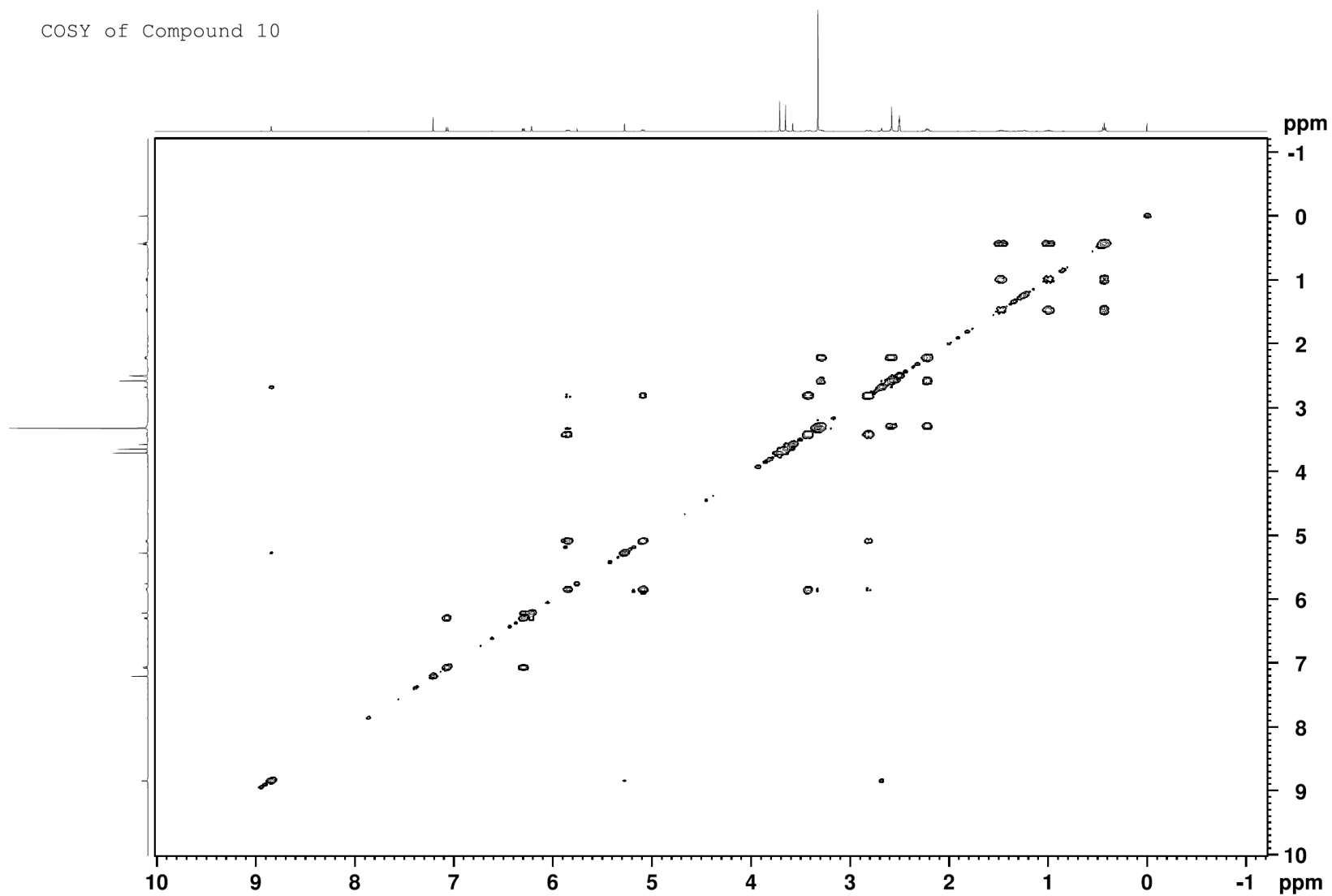
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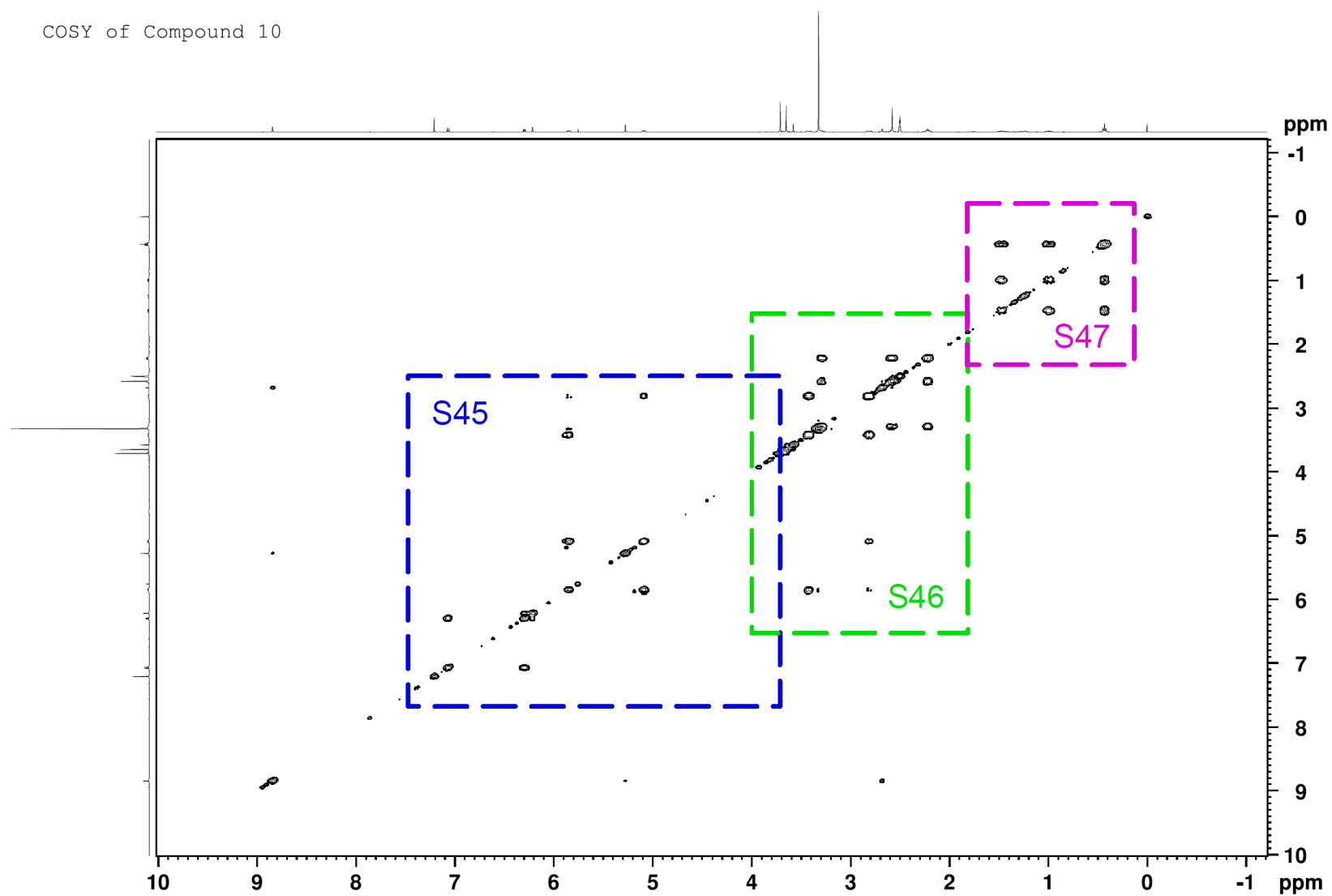




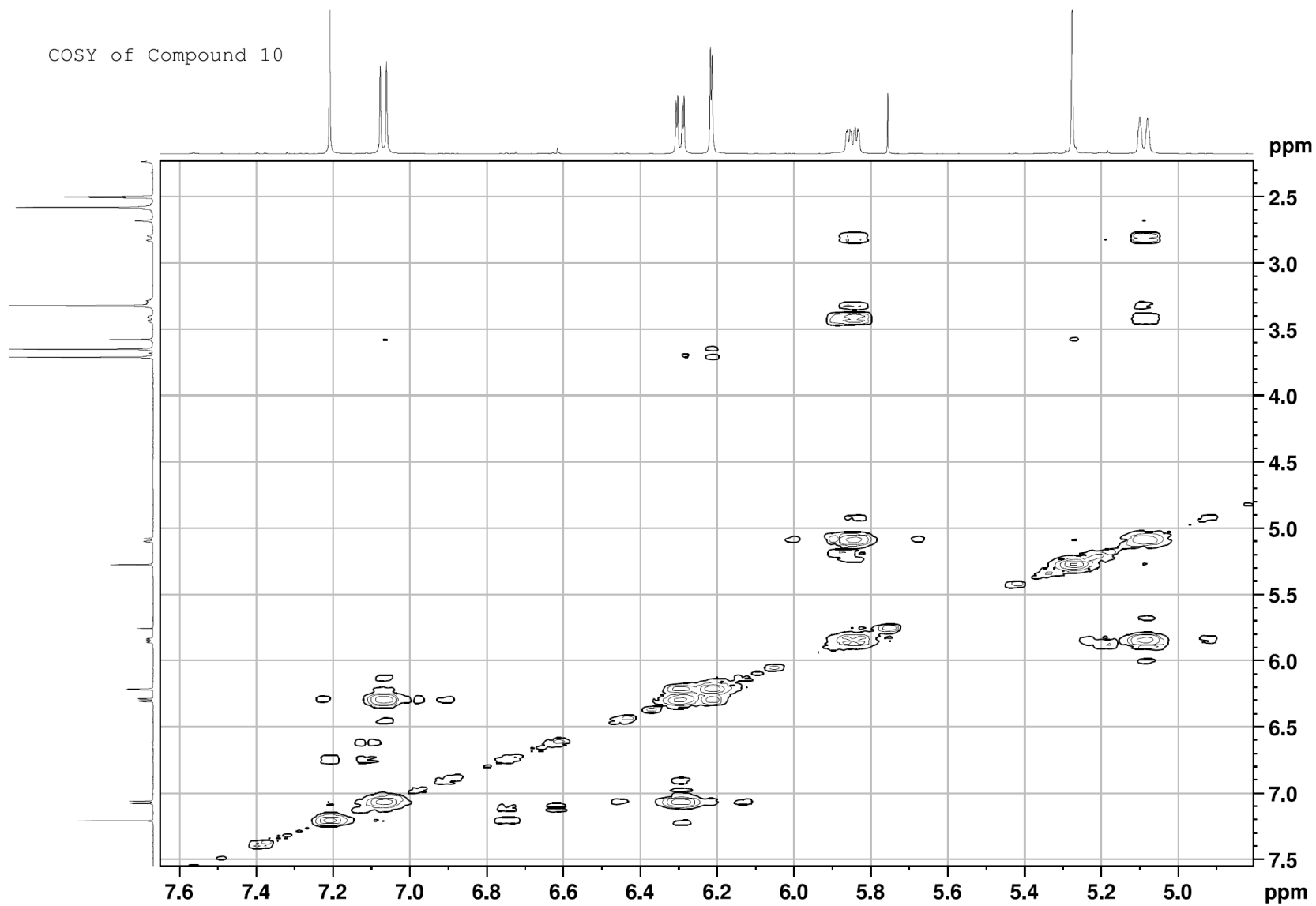
COSY of Compound 10

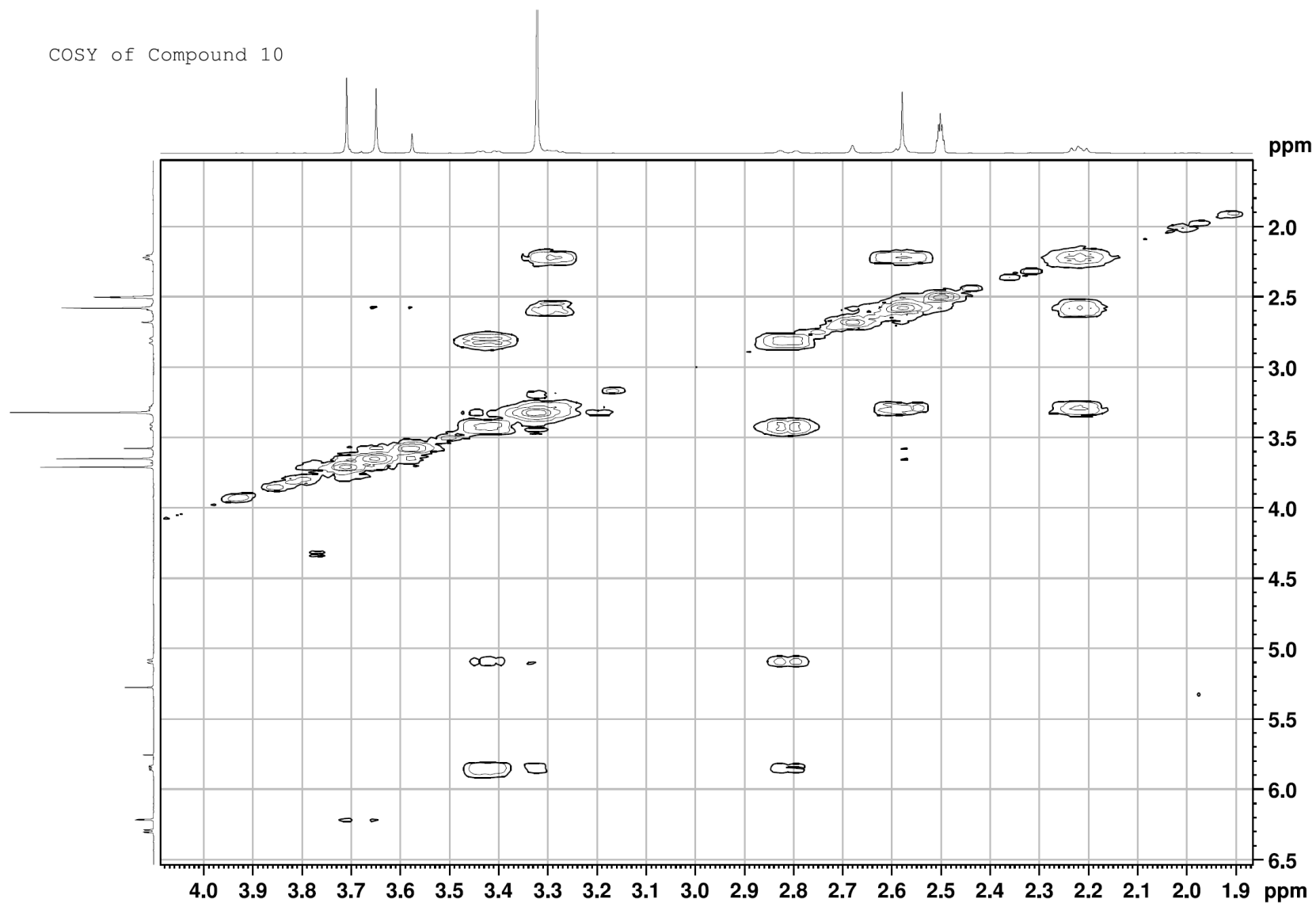


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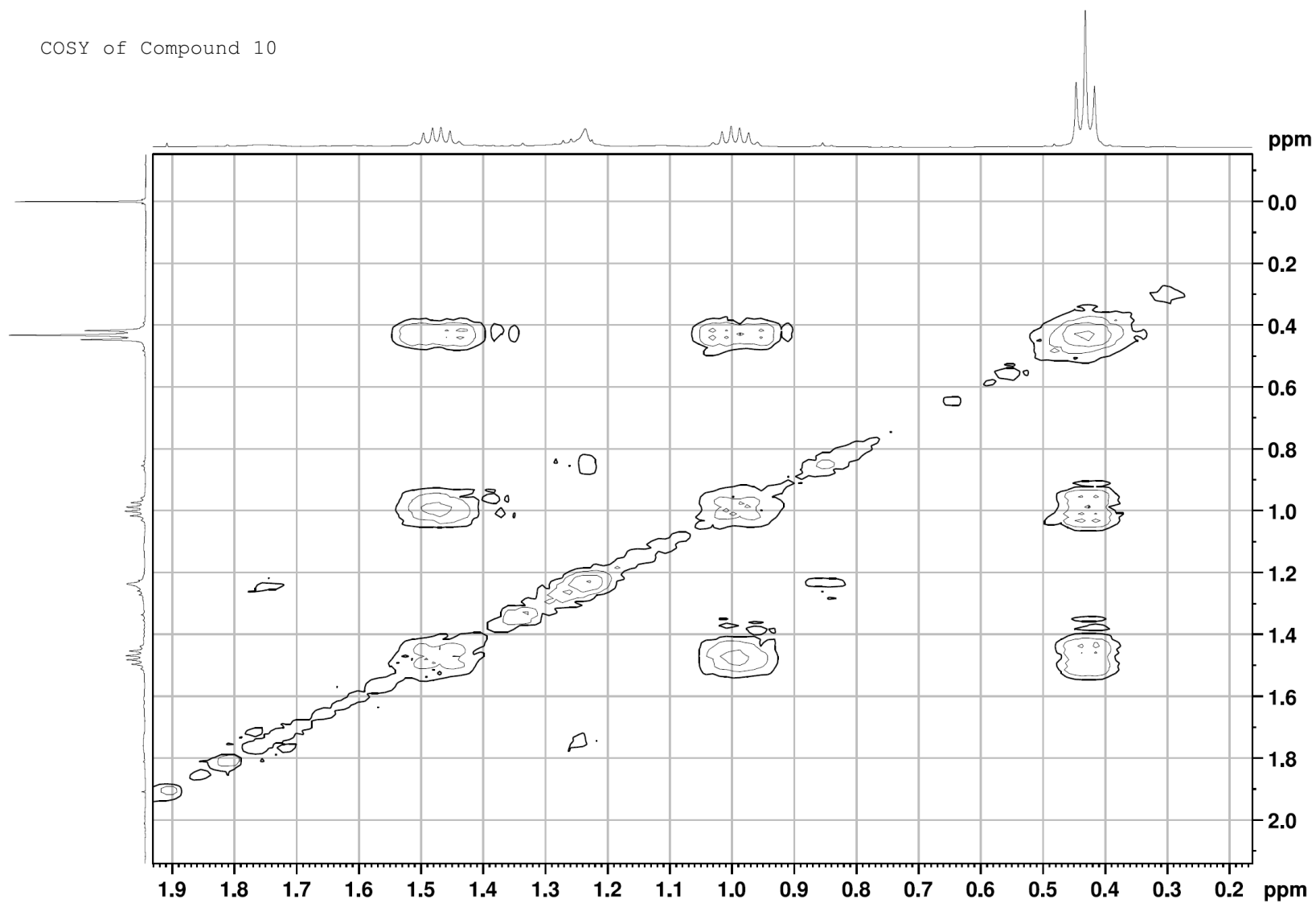


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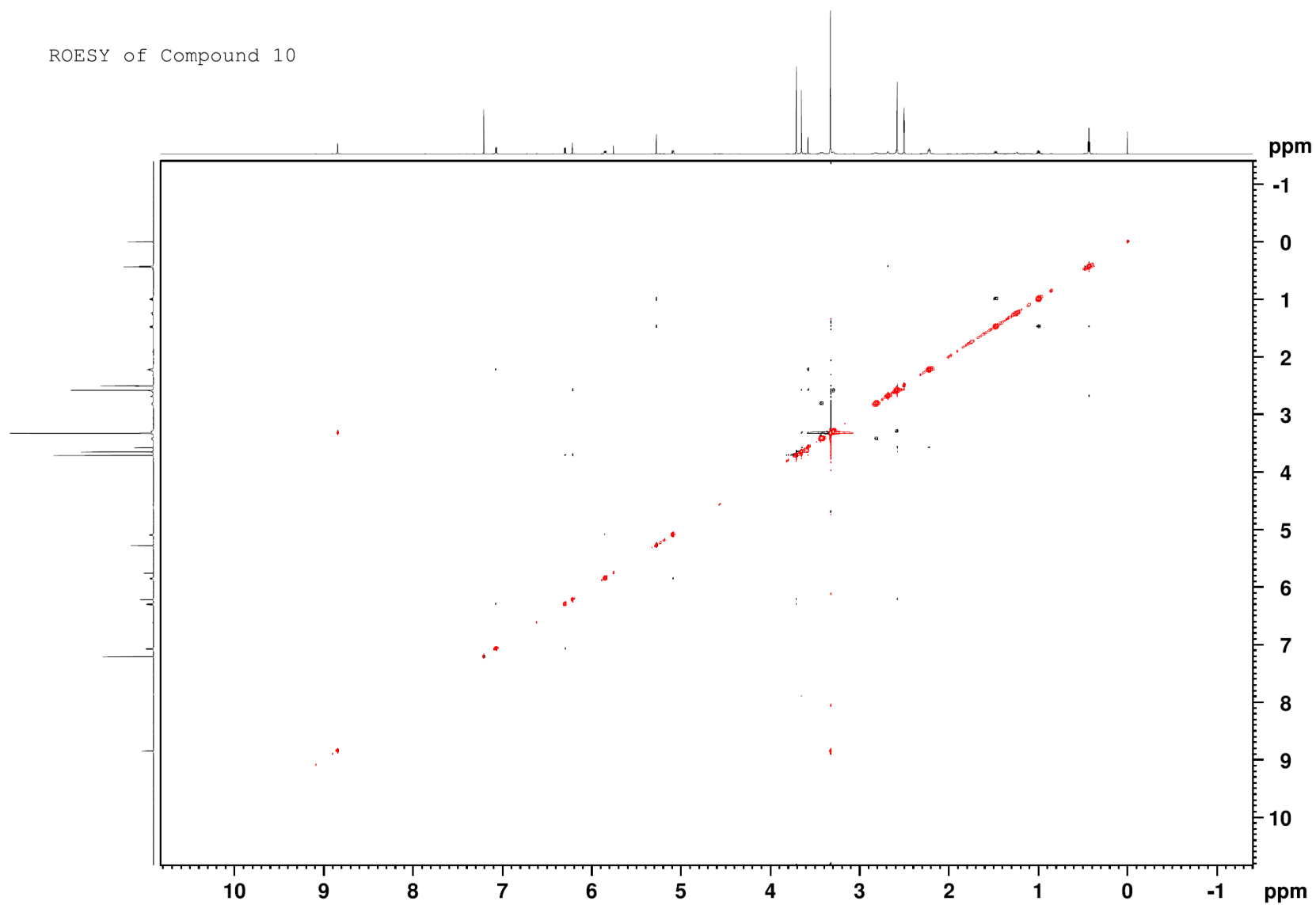




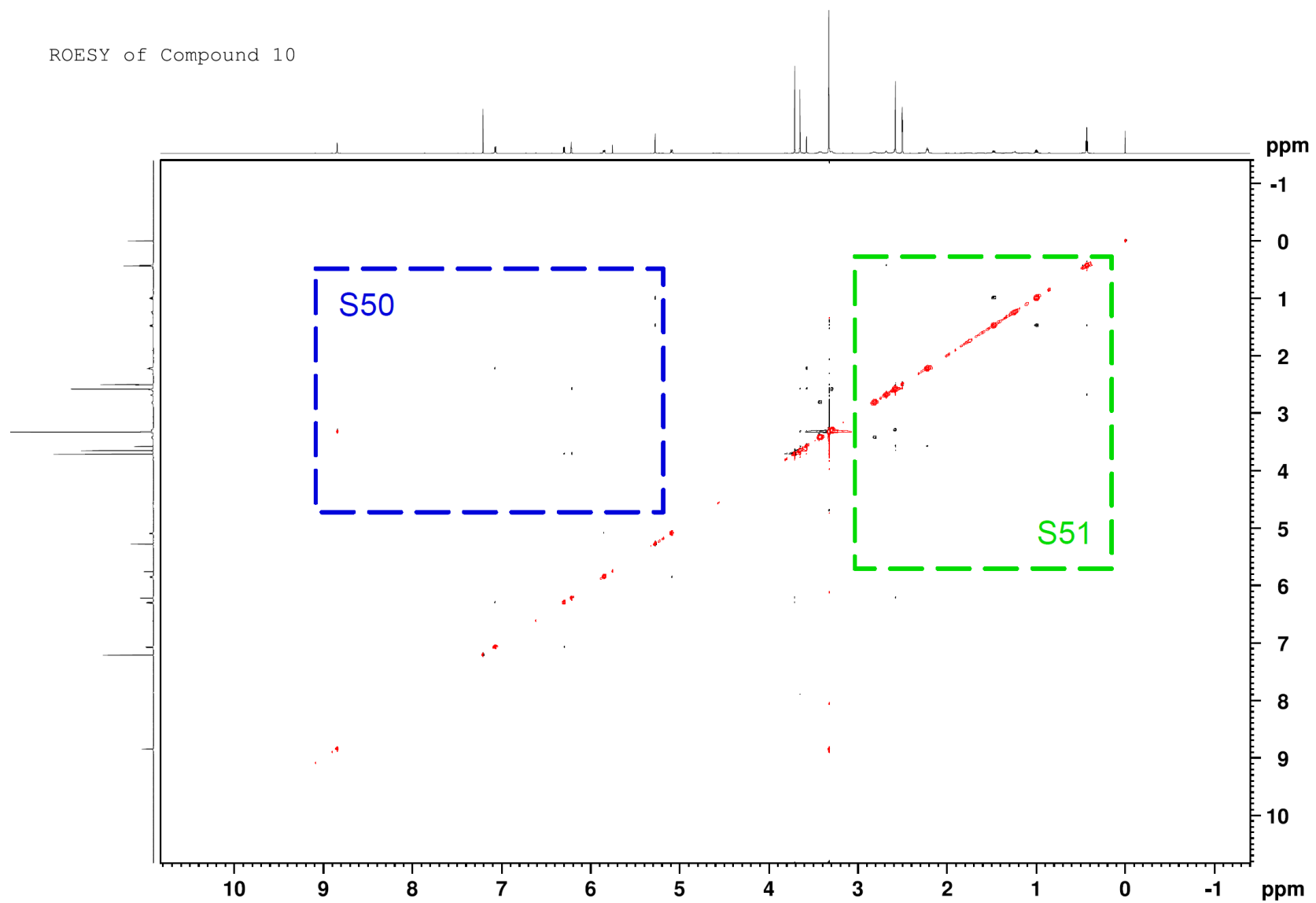
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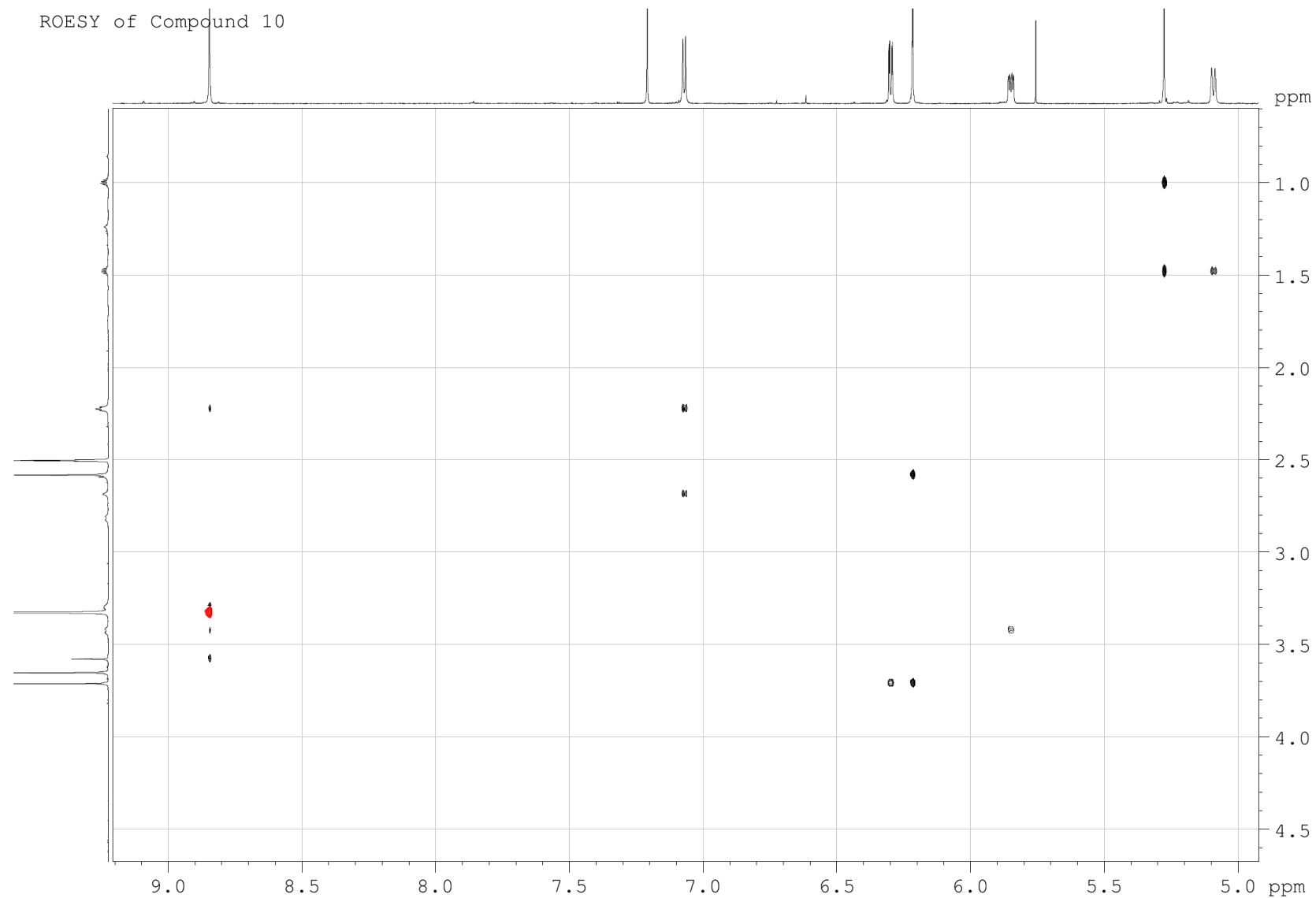
ROESY of Compound 10

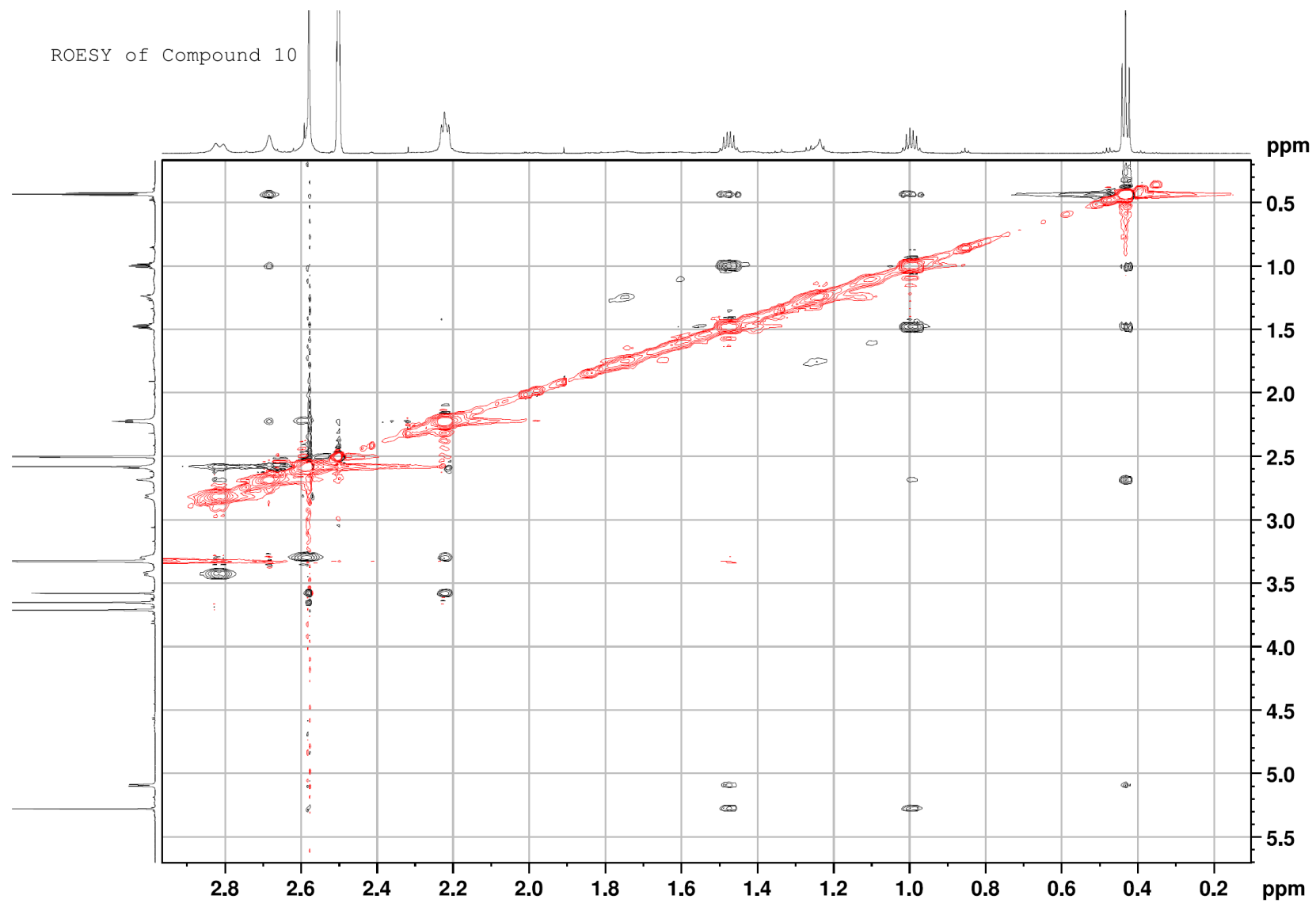


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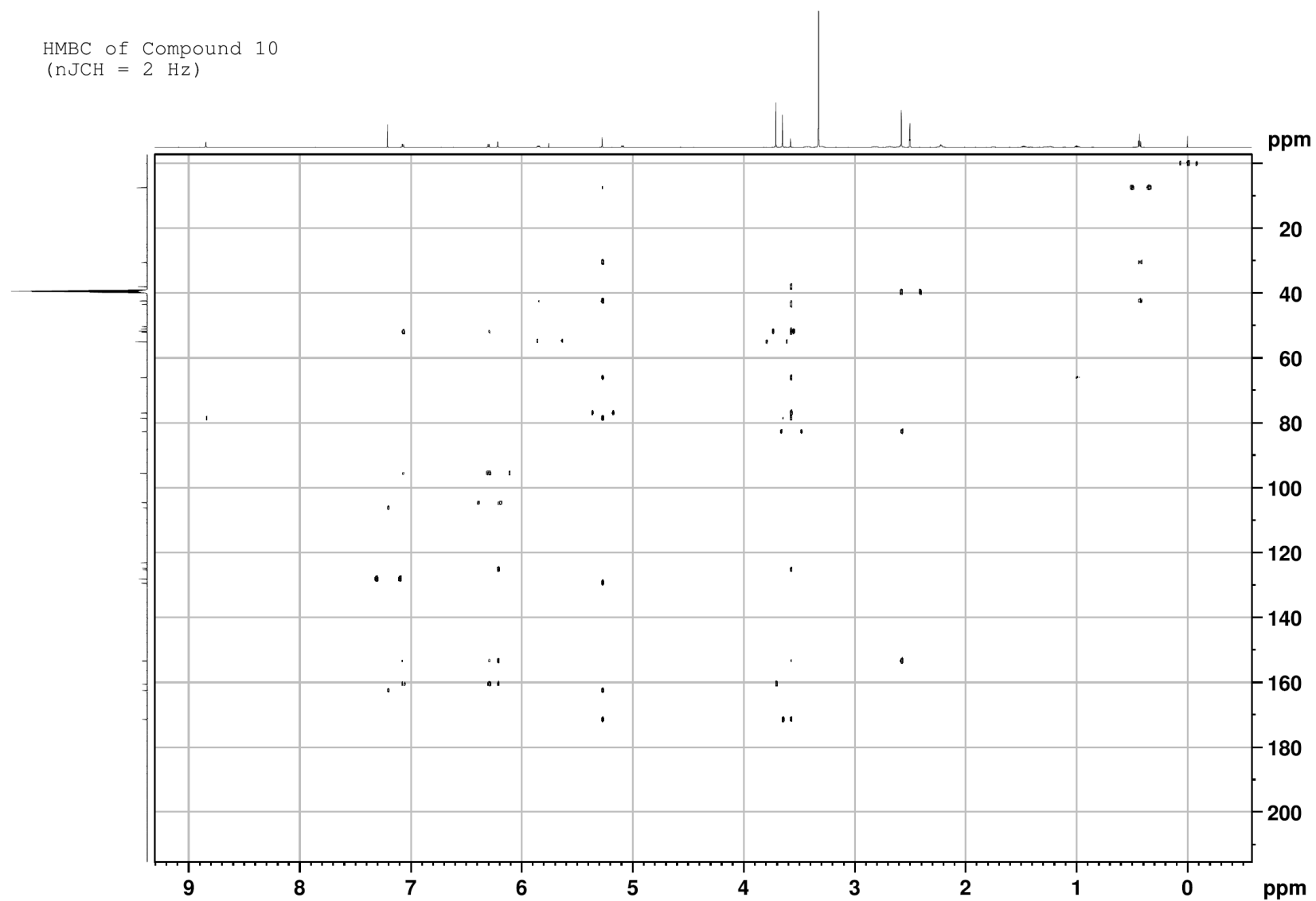


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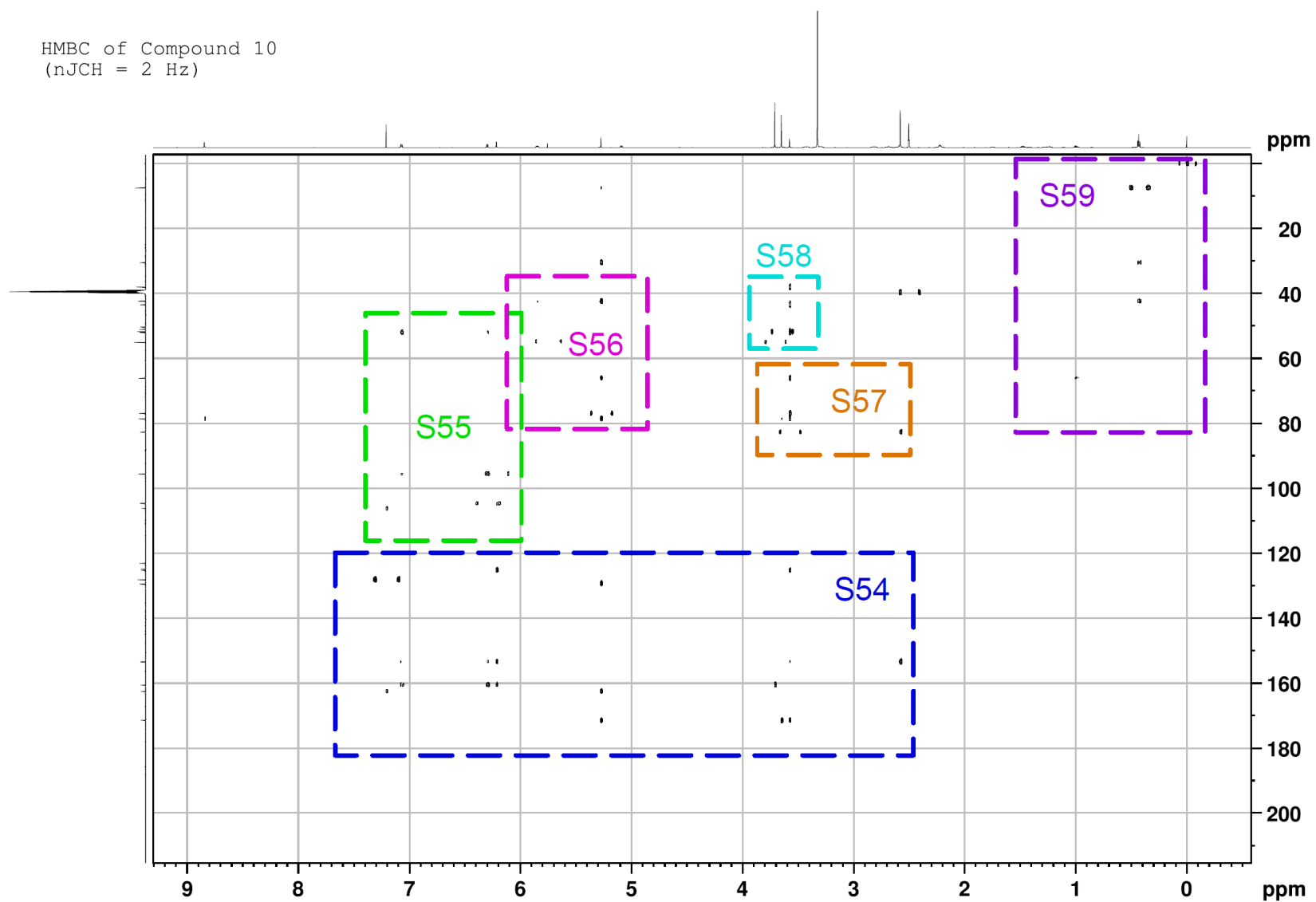


HMBC of Compound 10
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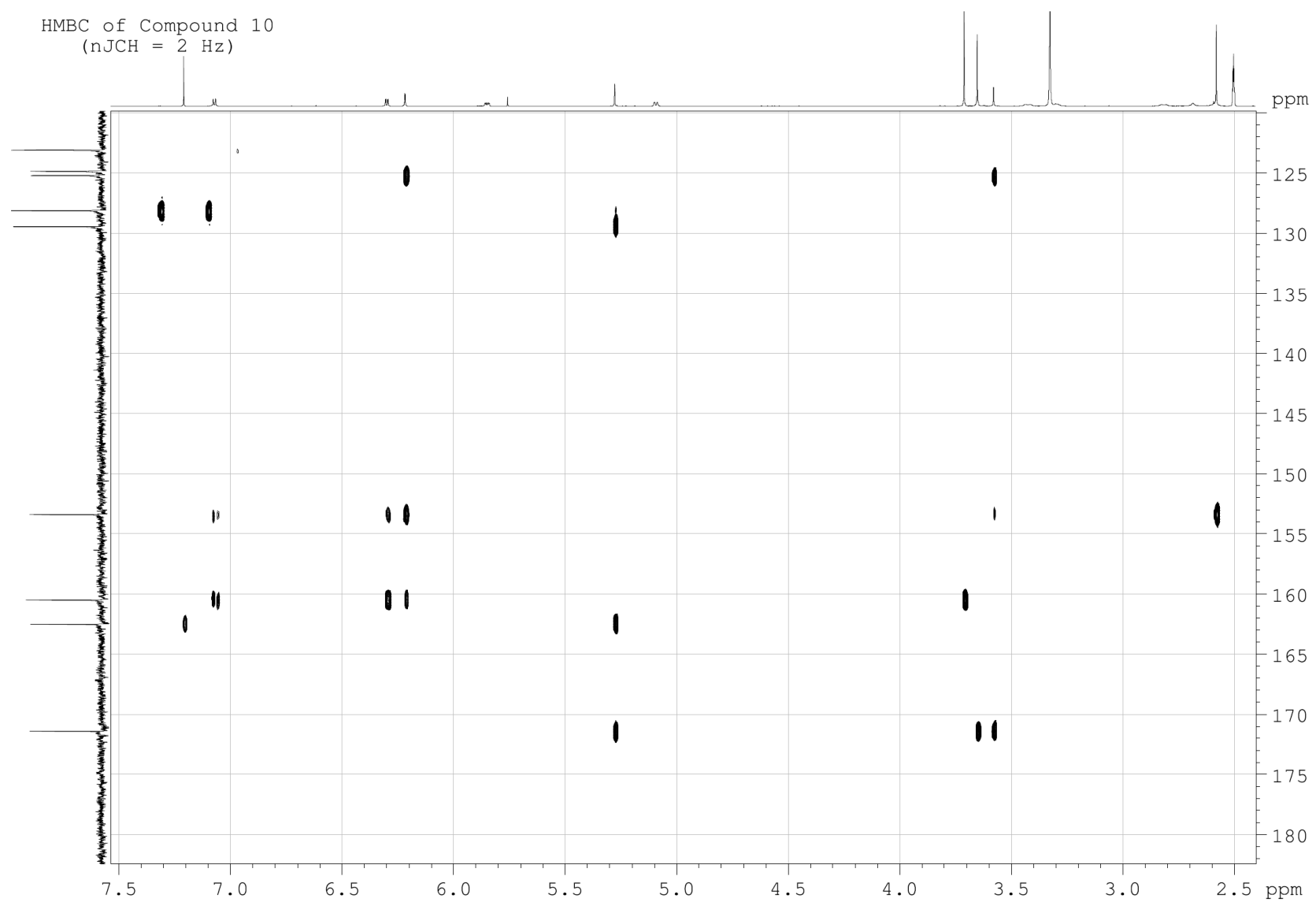


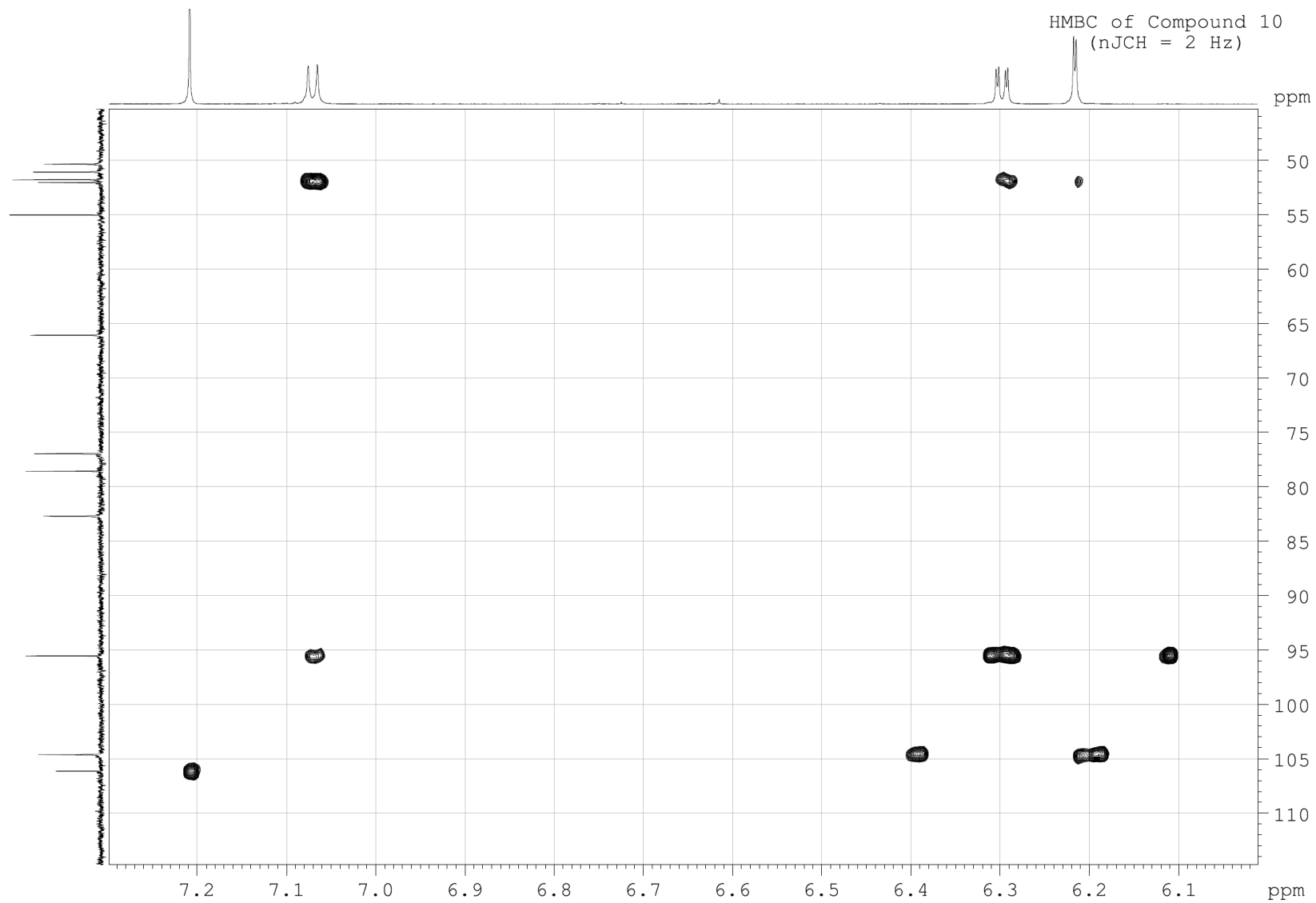
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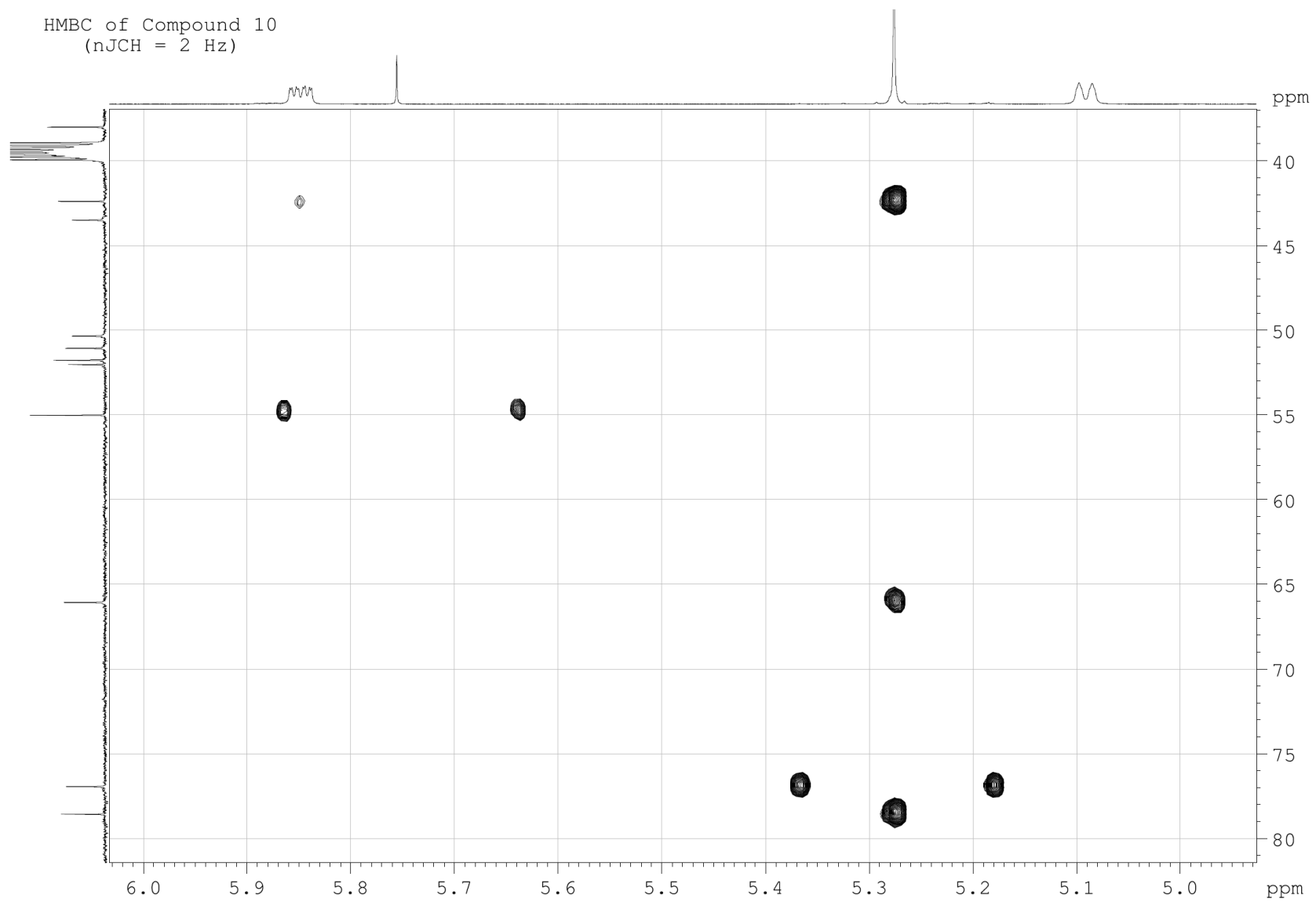
HMBC of Compound 10
($nJ_{CH} = 2$ Hz)

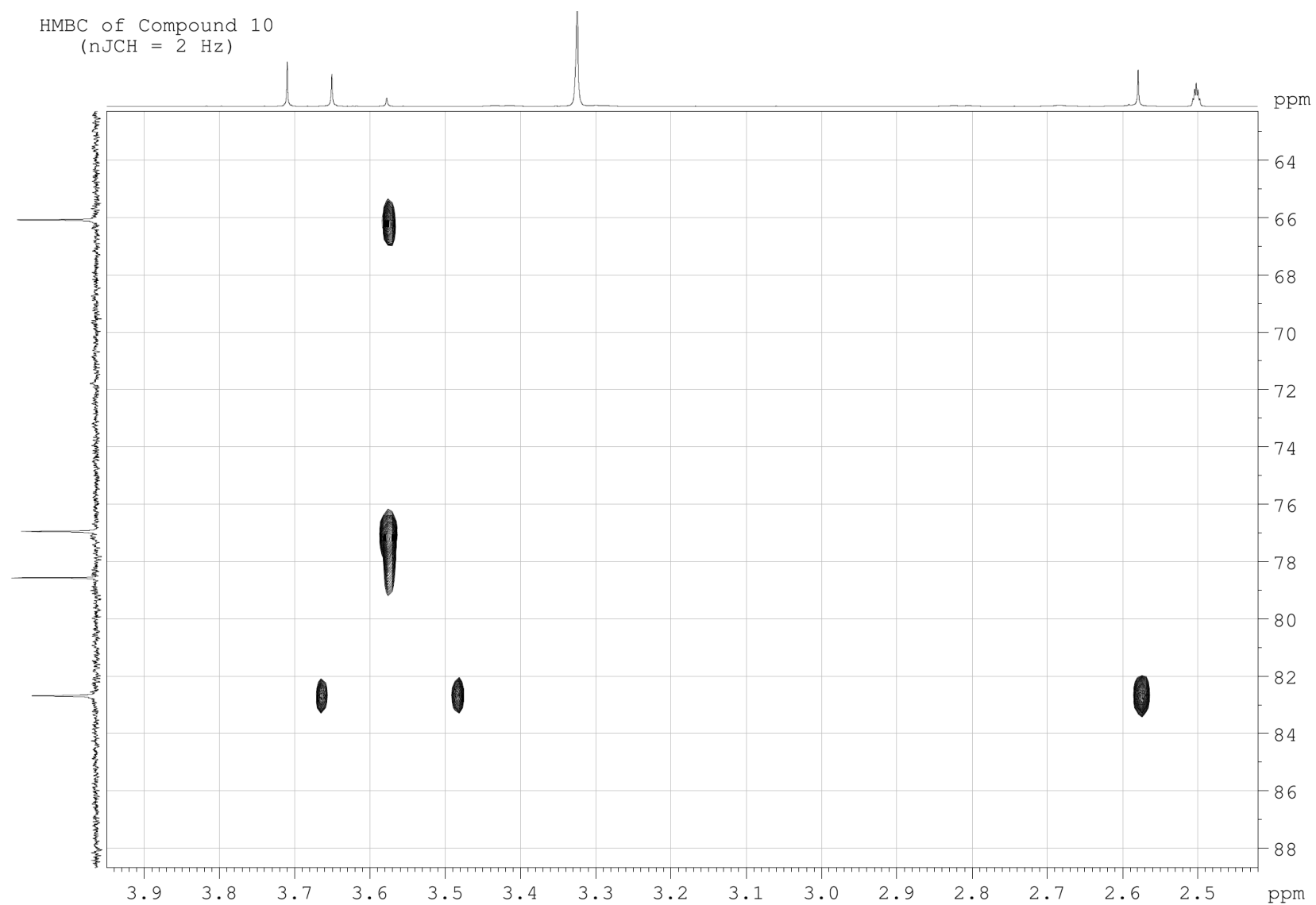


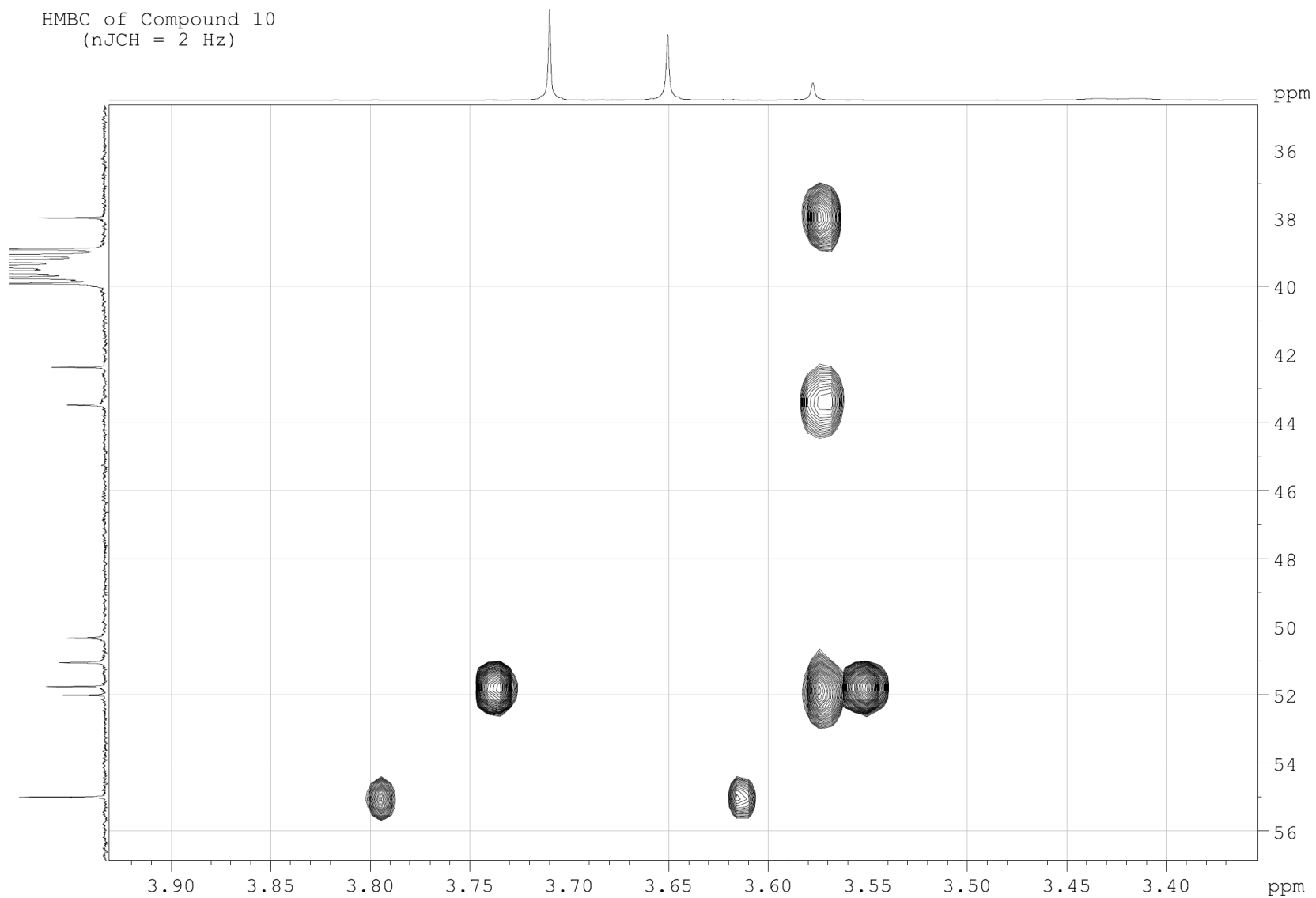
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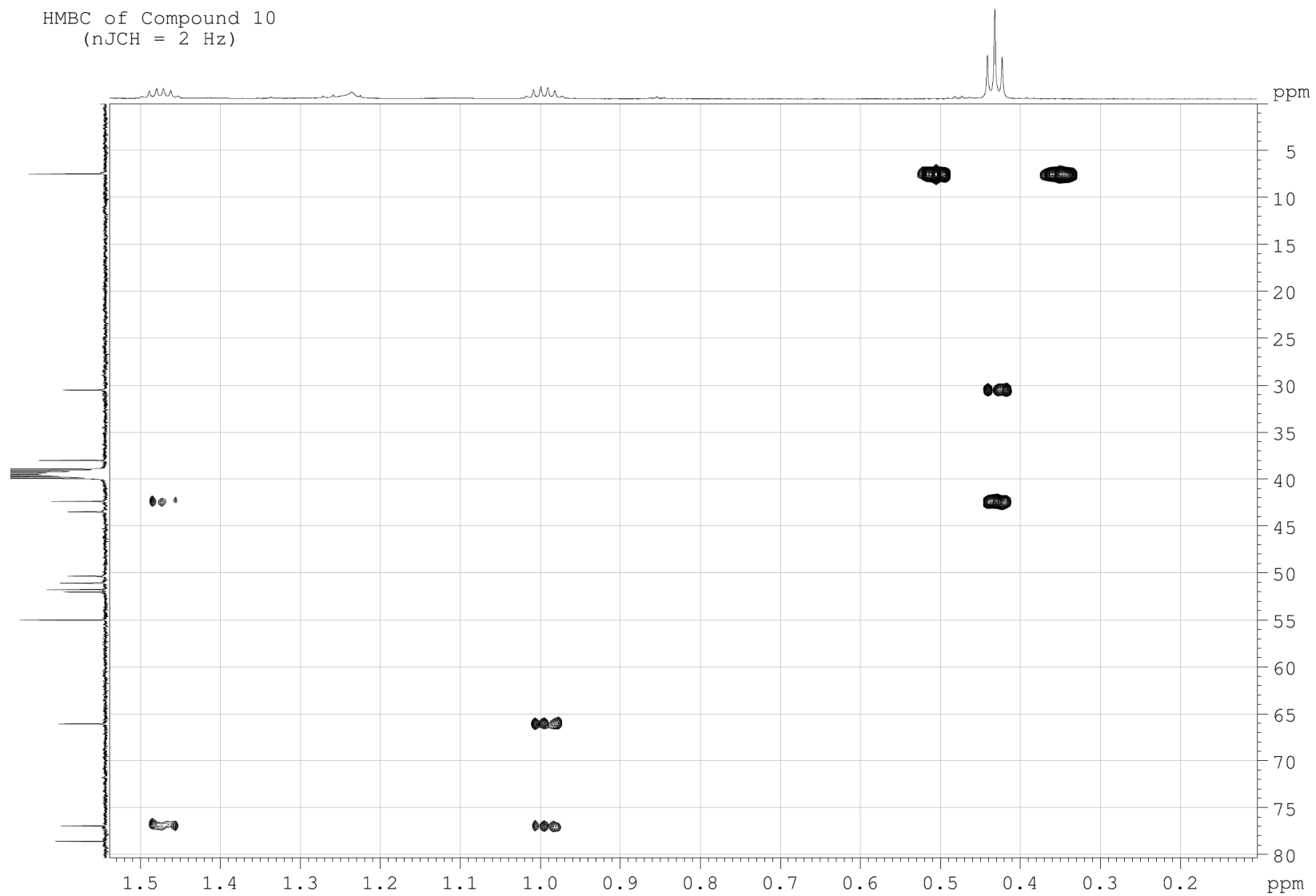




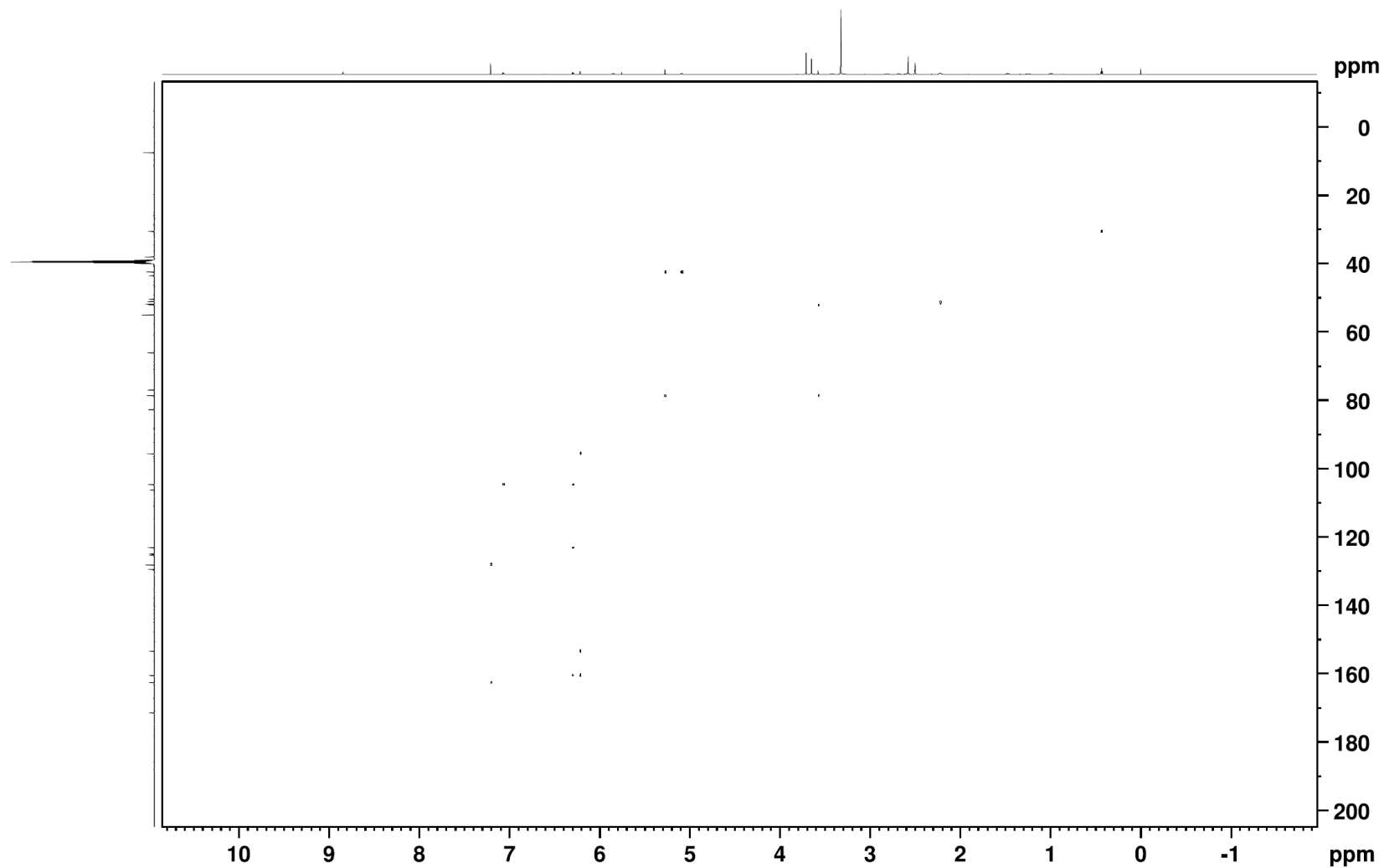






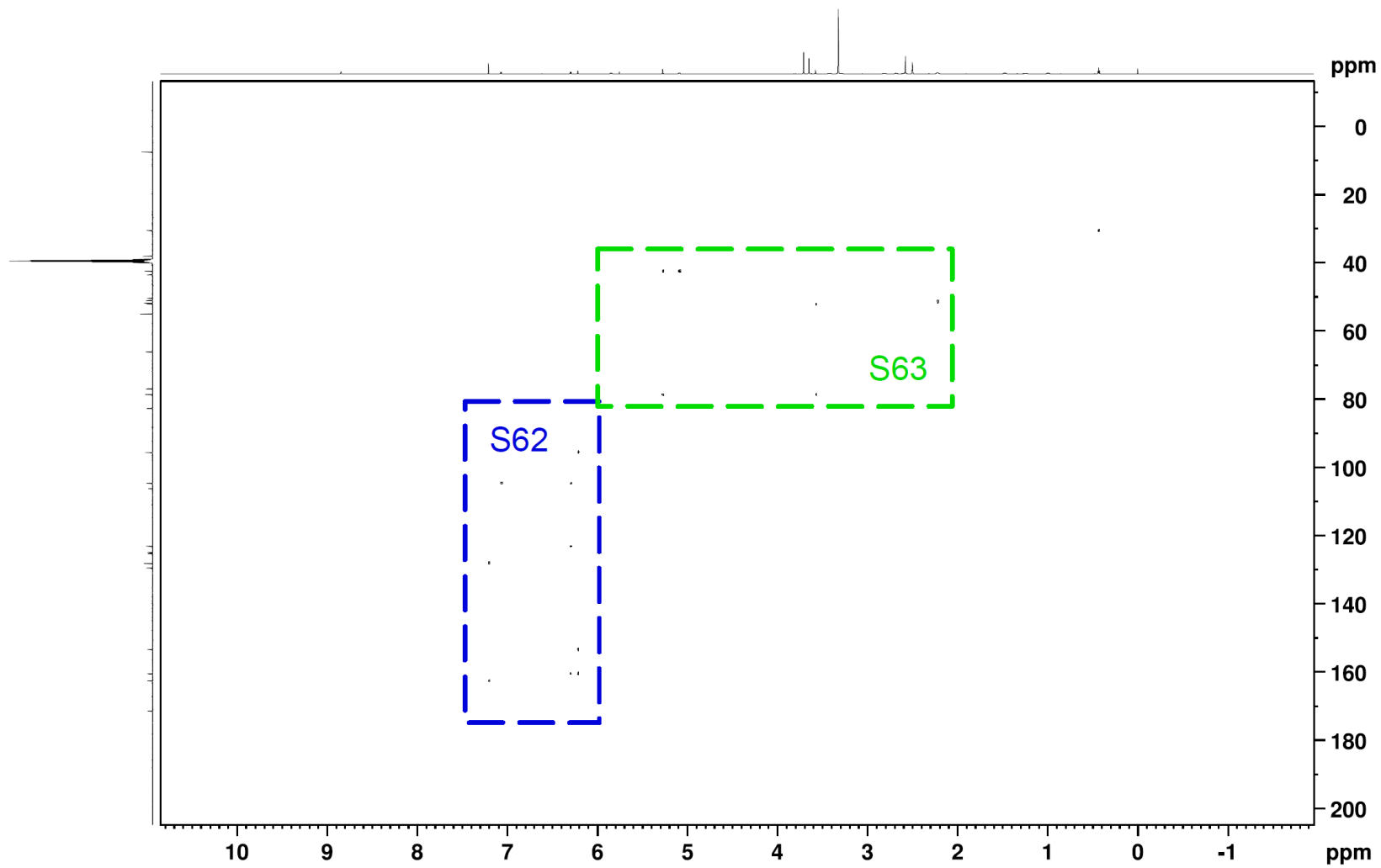


1,1-ADEQUATE of Compound 10

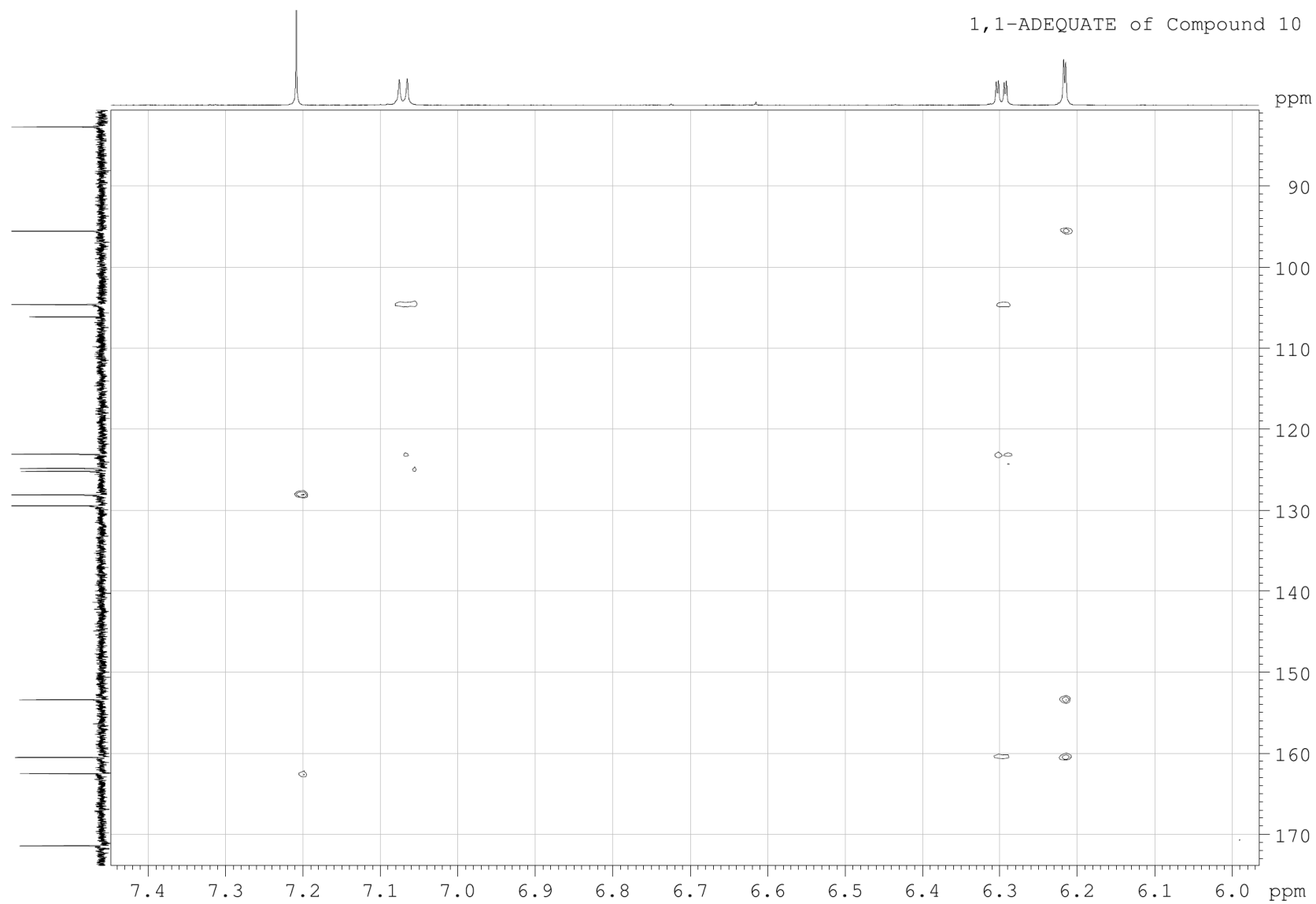


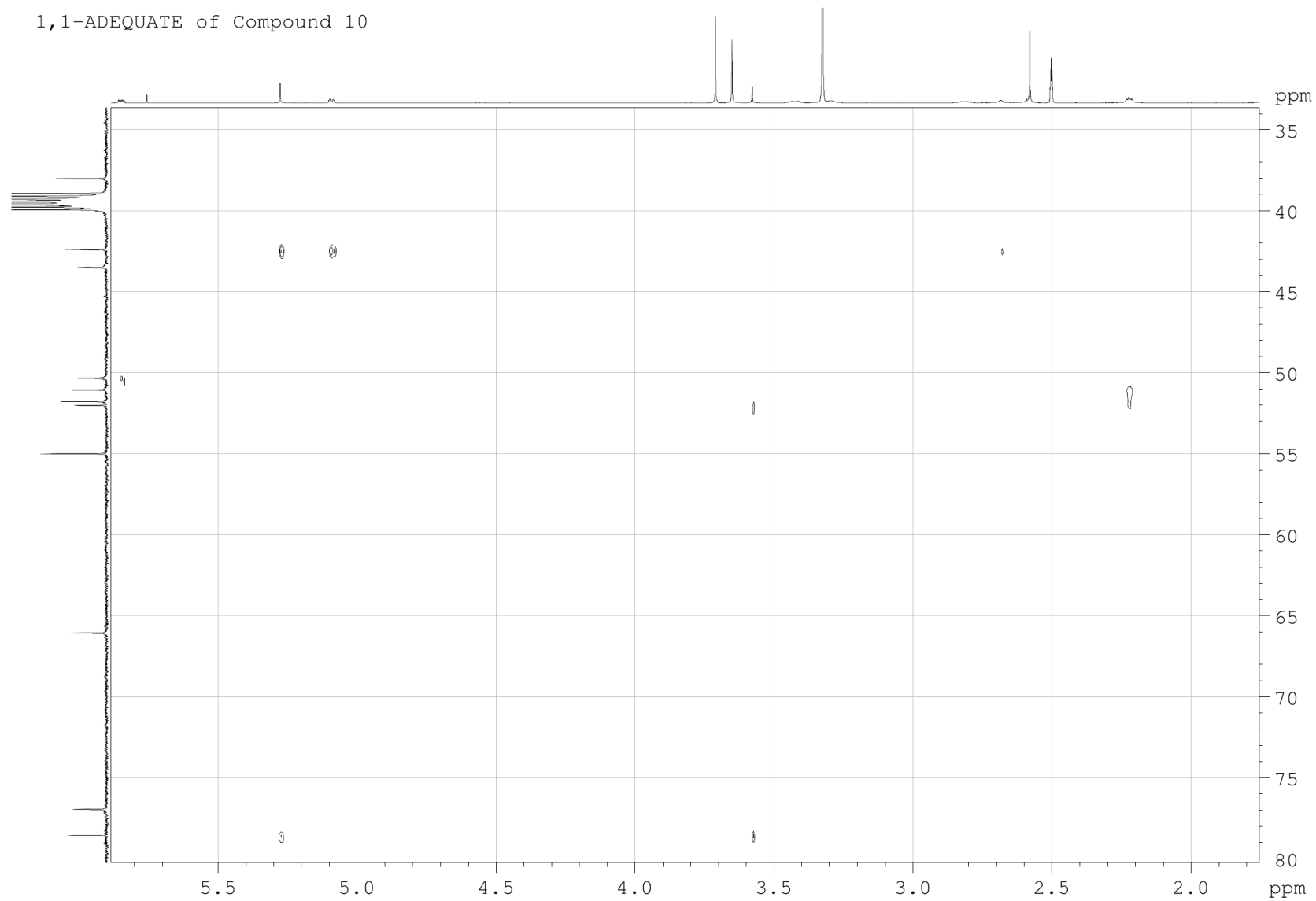
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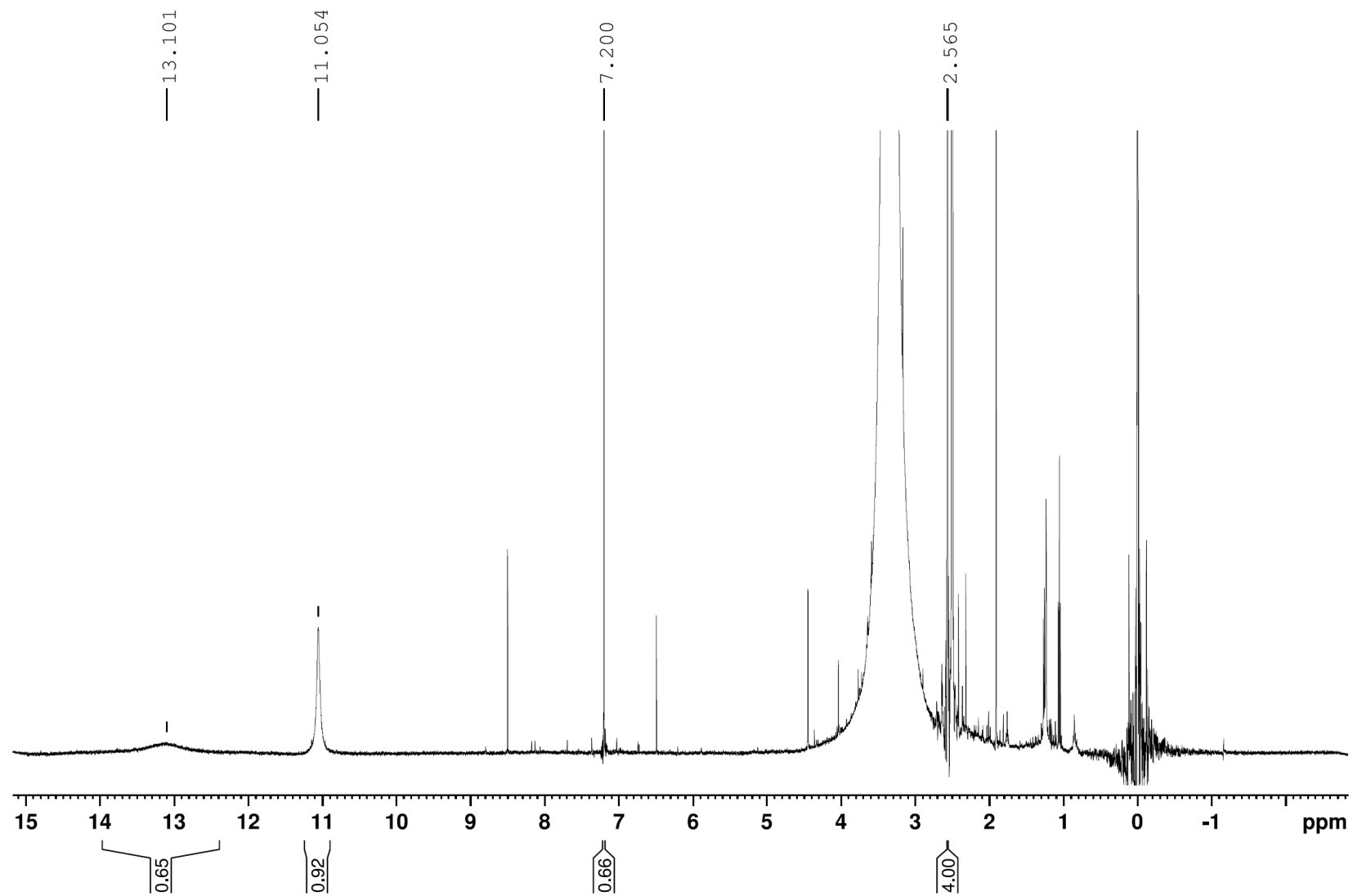


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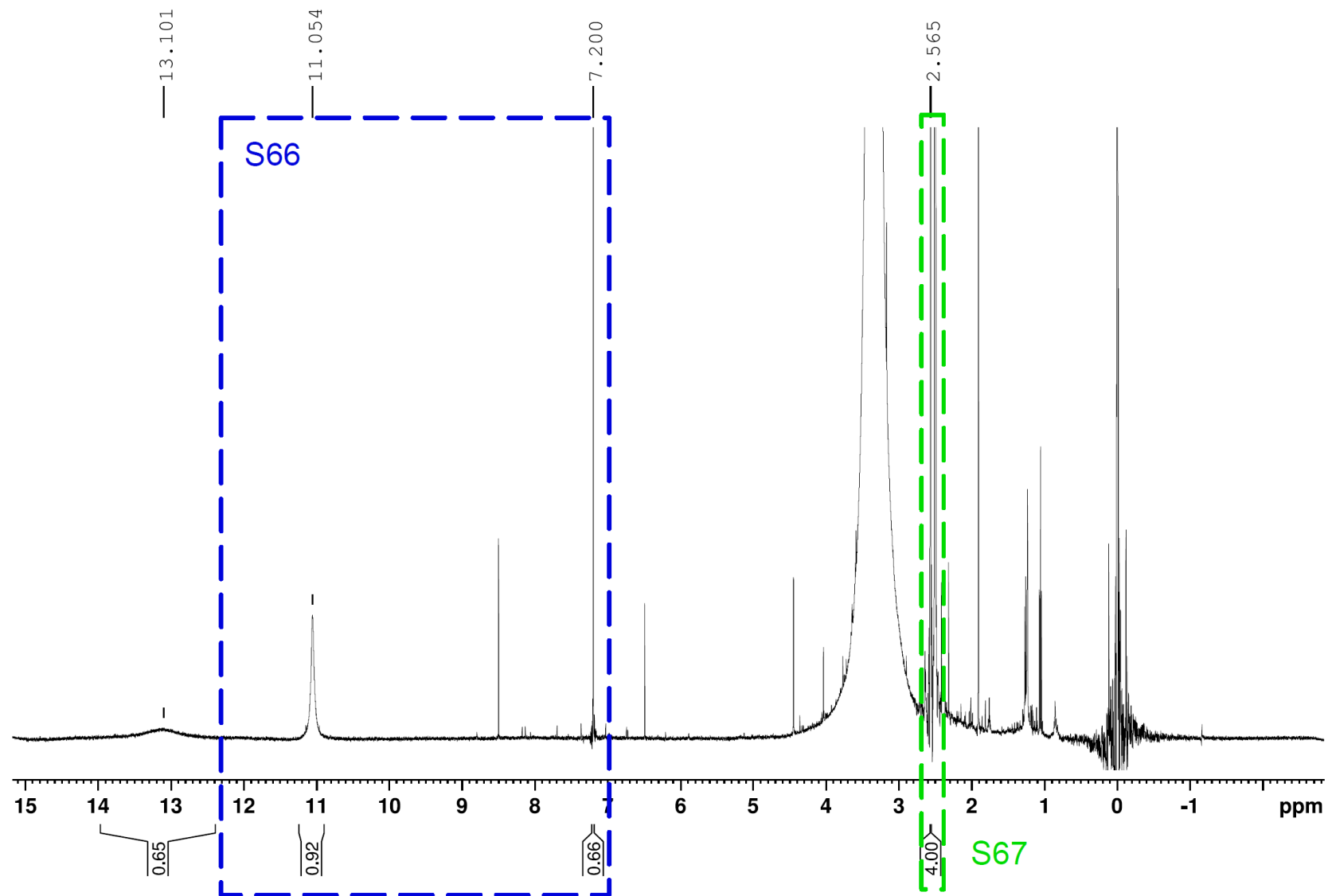


¹H NMR of Compounds 7, 14 and 15

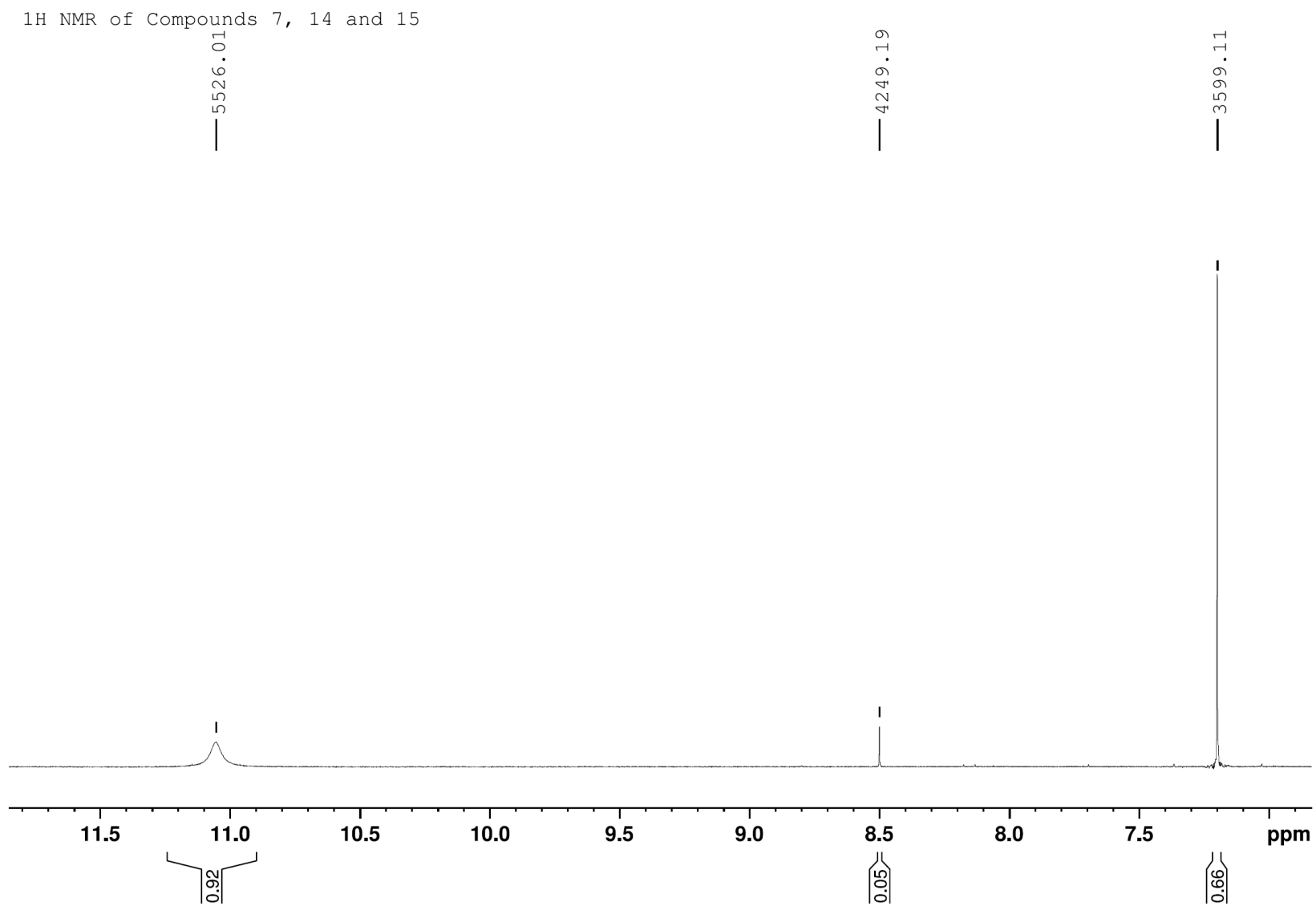


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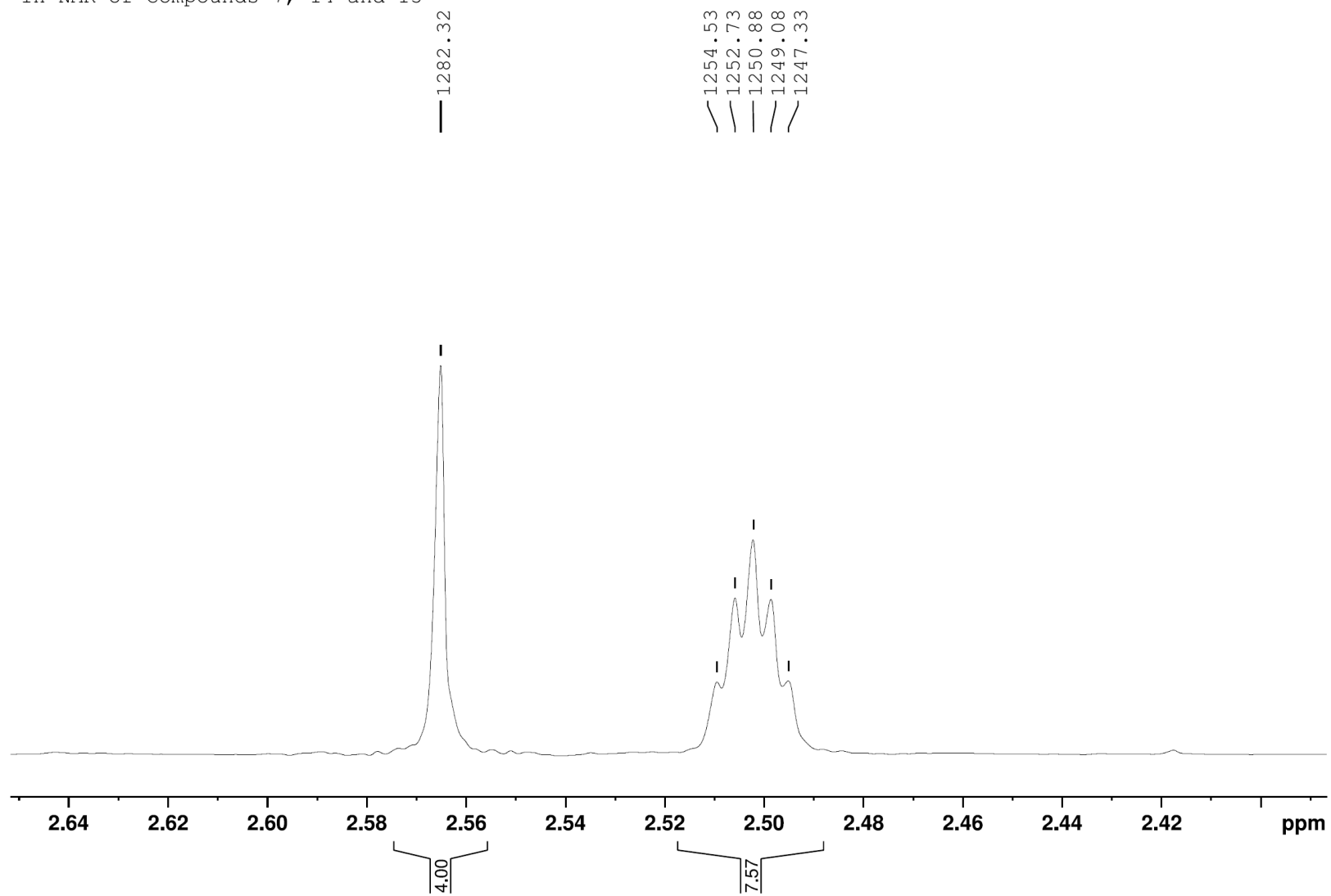
^1H NMR of Compounds 7, 14 and 15



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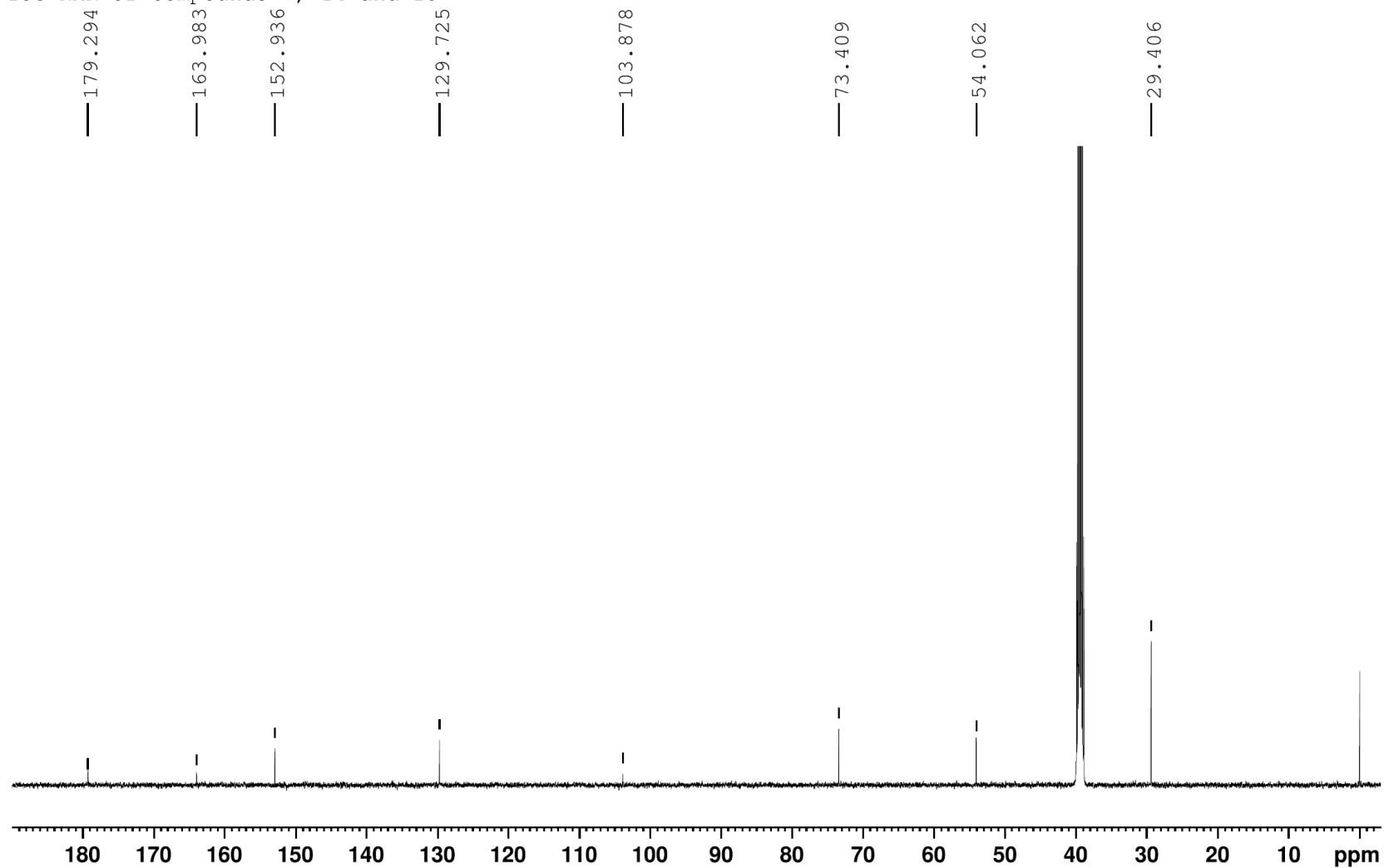


¹H NMR of Compounds 7, 14 and 15

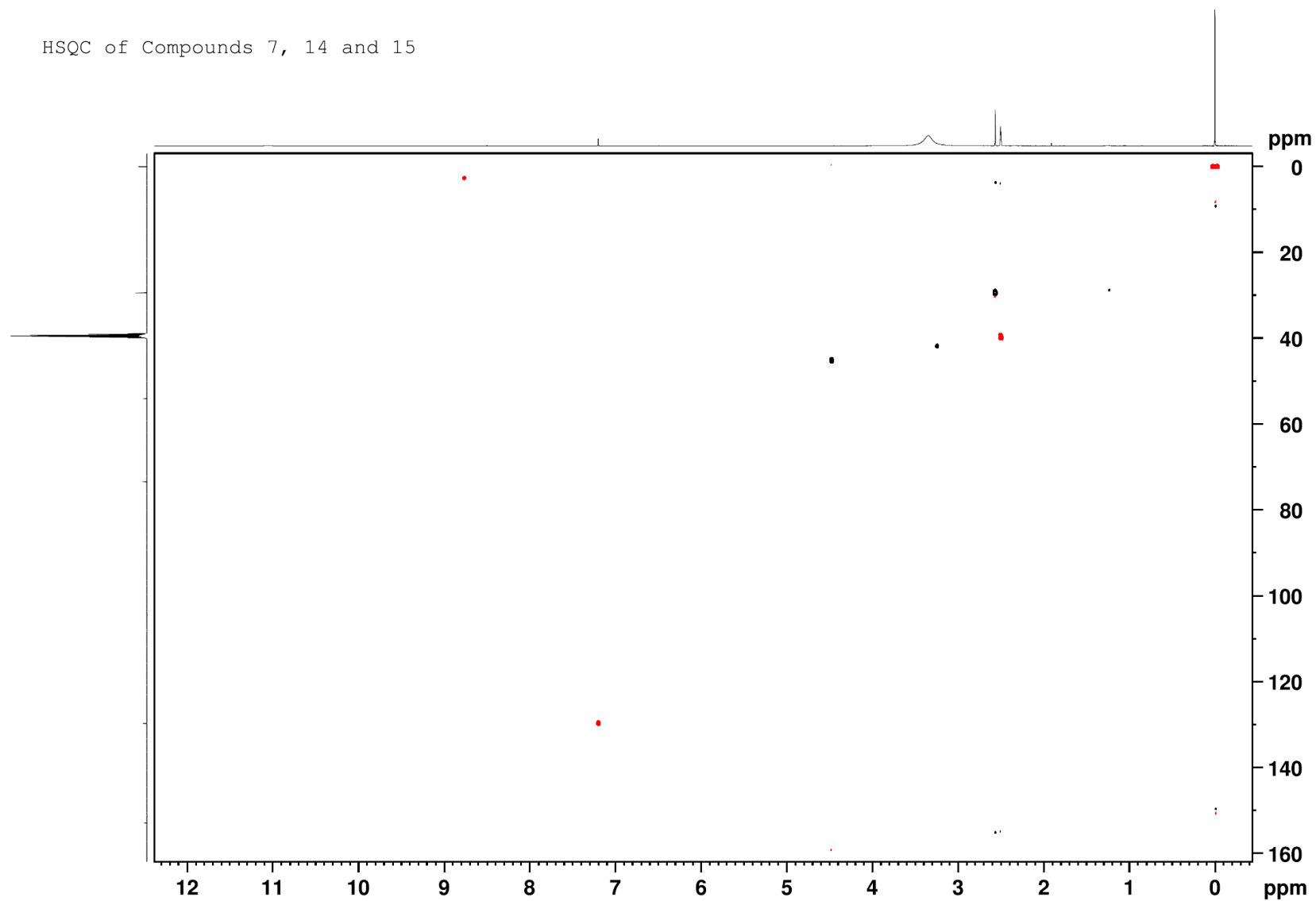


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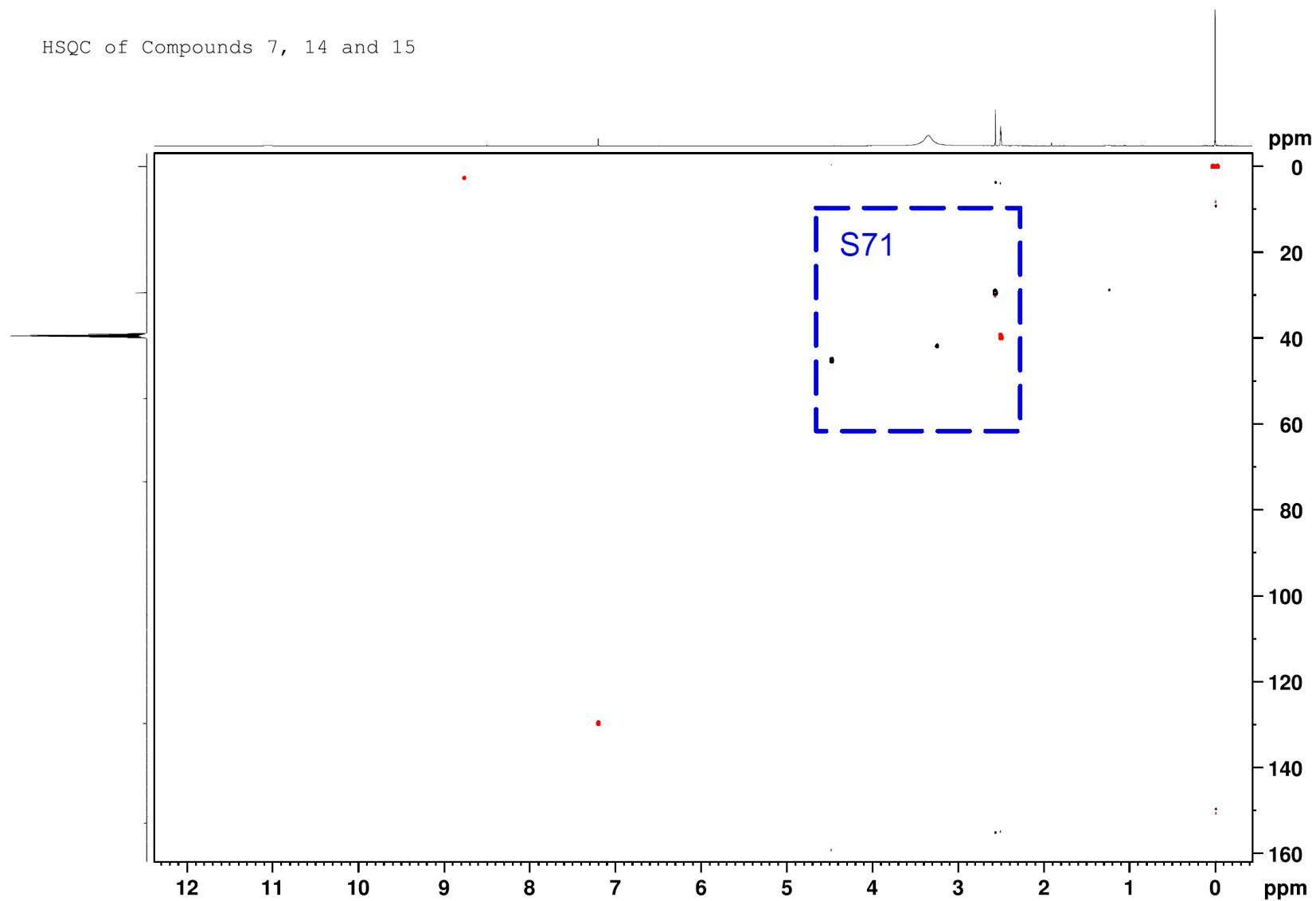
¹³C NMR of Compounds 7, 14 and 15



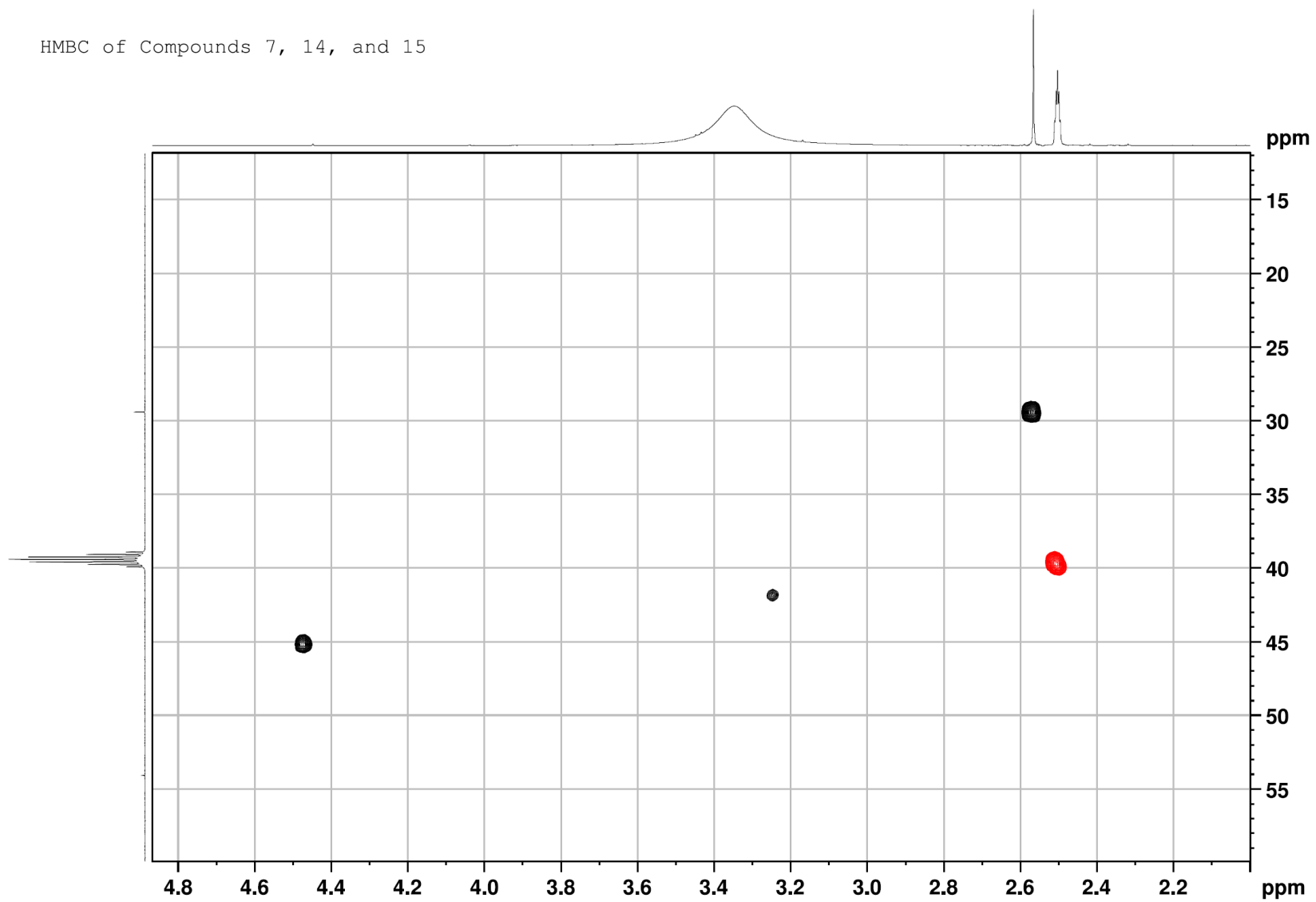
HSQC of Compounds 7, 14 and 15



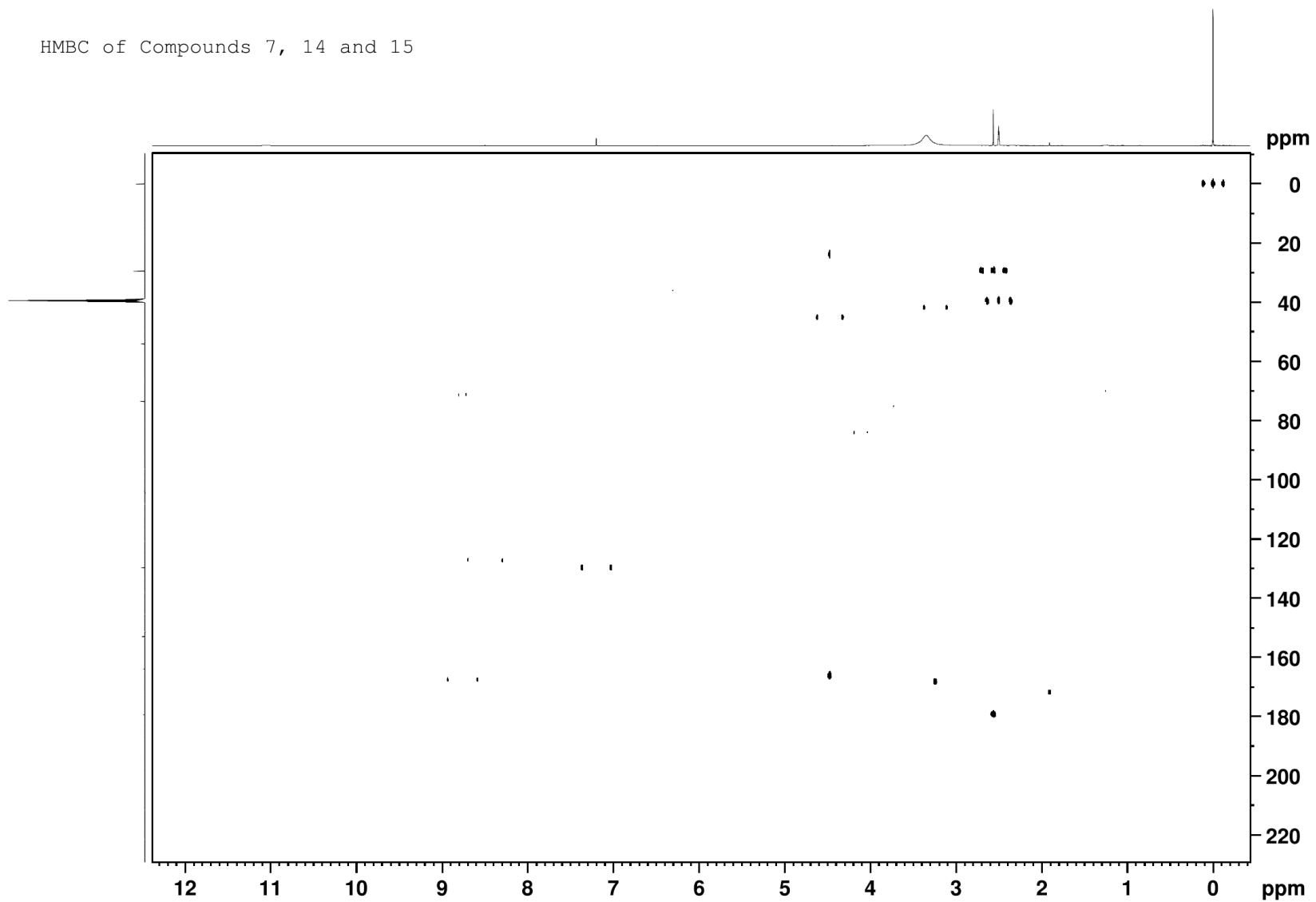
HSQC of Compounds 7, 14 and 15



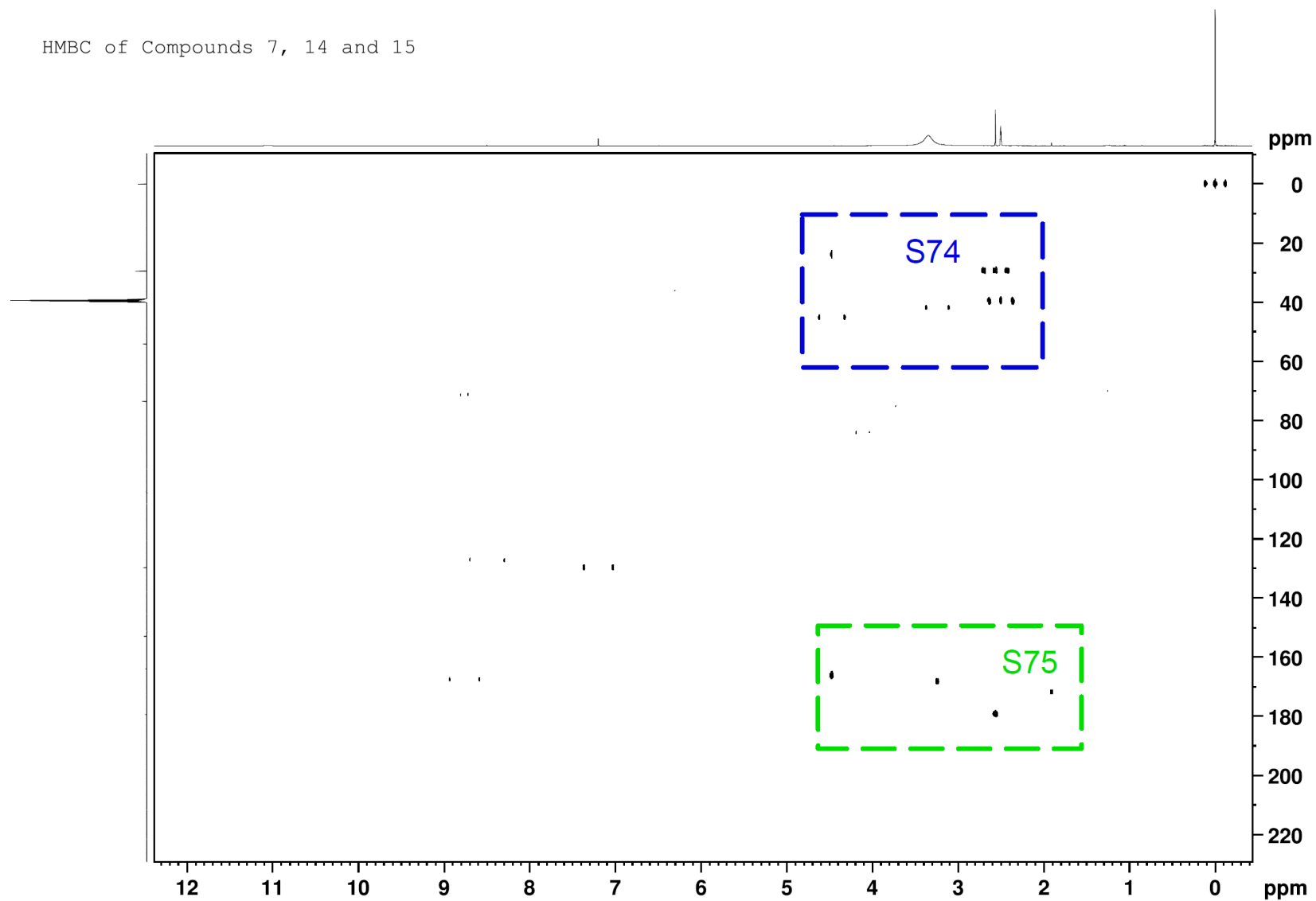
HMBC of Compounds 7, 14, and 15



HMBC of Compounds 7, 14 and 15

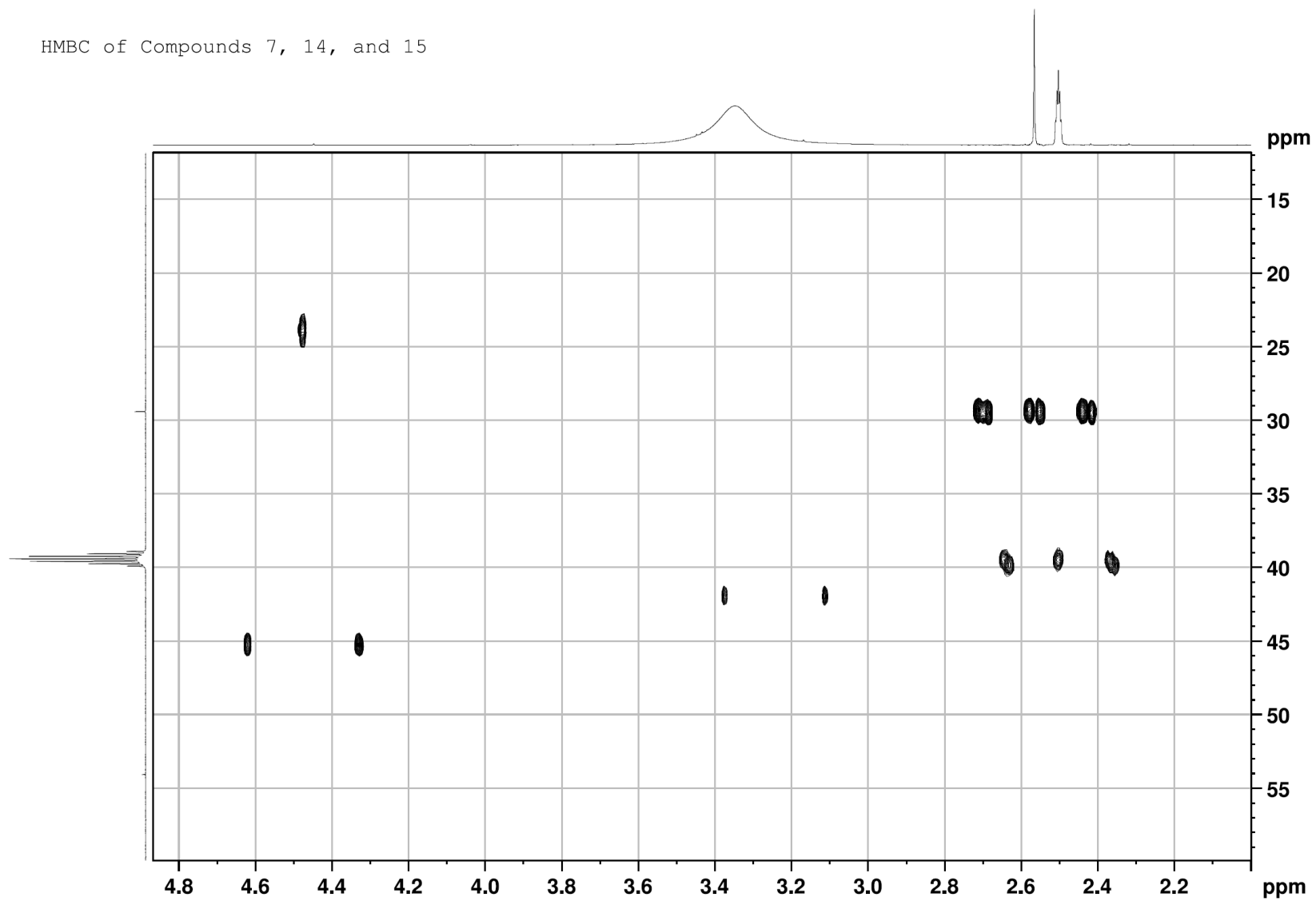


HMBC of Compounds 7, 14 and 15



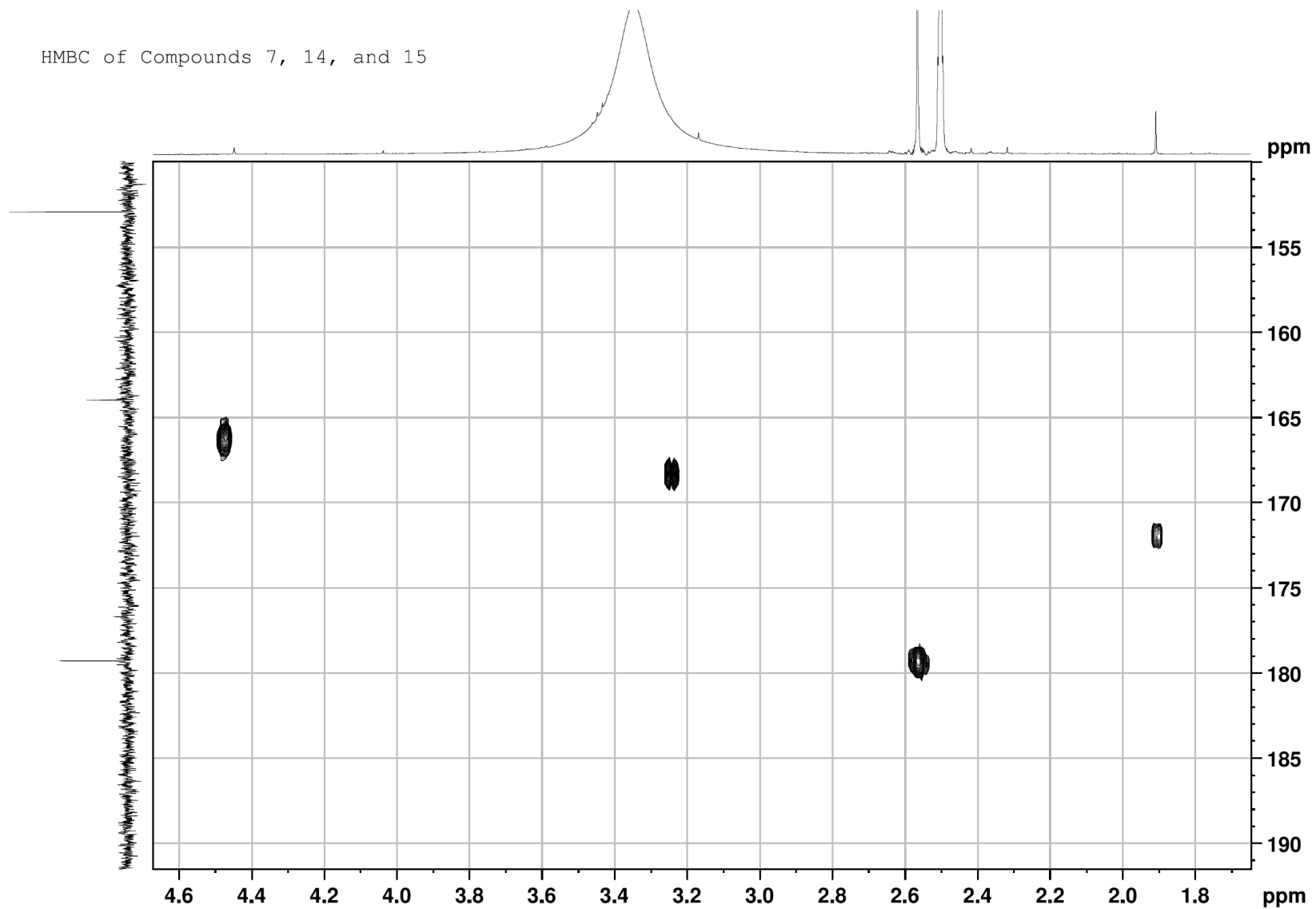
S73

HMBC of Compounds 7, 14, and 15

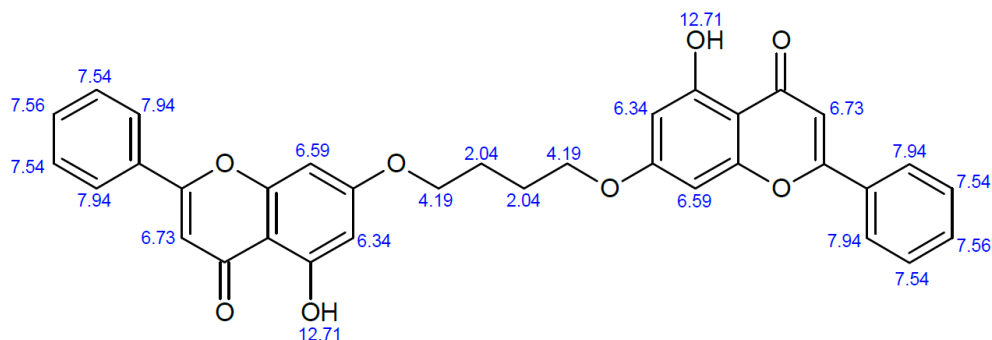
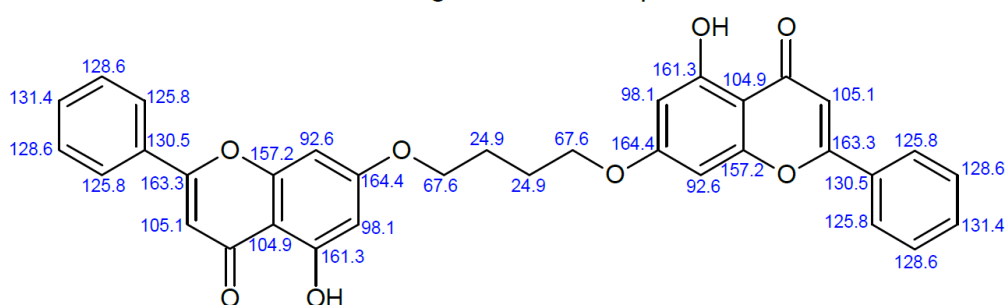
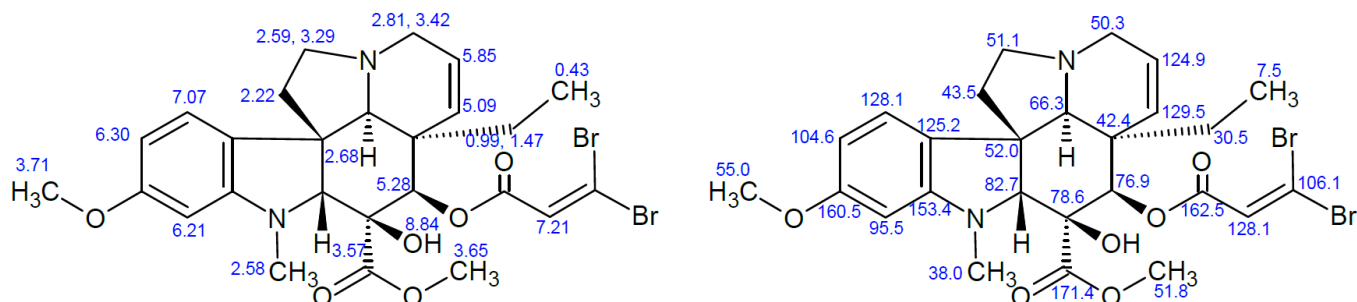
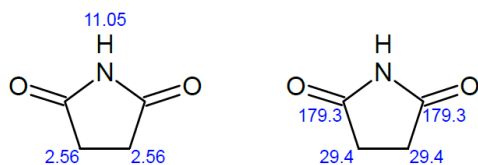
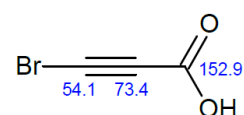


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HMBC of Compounds 7, 14, and 15



Detailed NMR assignments of Compounds 6, 7, 10, 14 and 15

¹H NMR assignments of Compound 6¹³C NMR assignments of Compound 6¹H NMR and ¹³C NMR assignments of Compound 10¹H NMR and ¹³C NMR assignments of Compound 14¹³C NMR assignments of Compound 7¹H NMR and ¹³C NMR assignments of Compound 15