

# Metal-free $\alpha$ -Amination of Secondary Amines: Computational and Experimental Evidence for Azaquinone Methide and Azomethine Ylide Intermediates

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<sup>‡</sup> *Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, New Jersey 08854, United States*

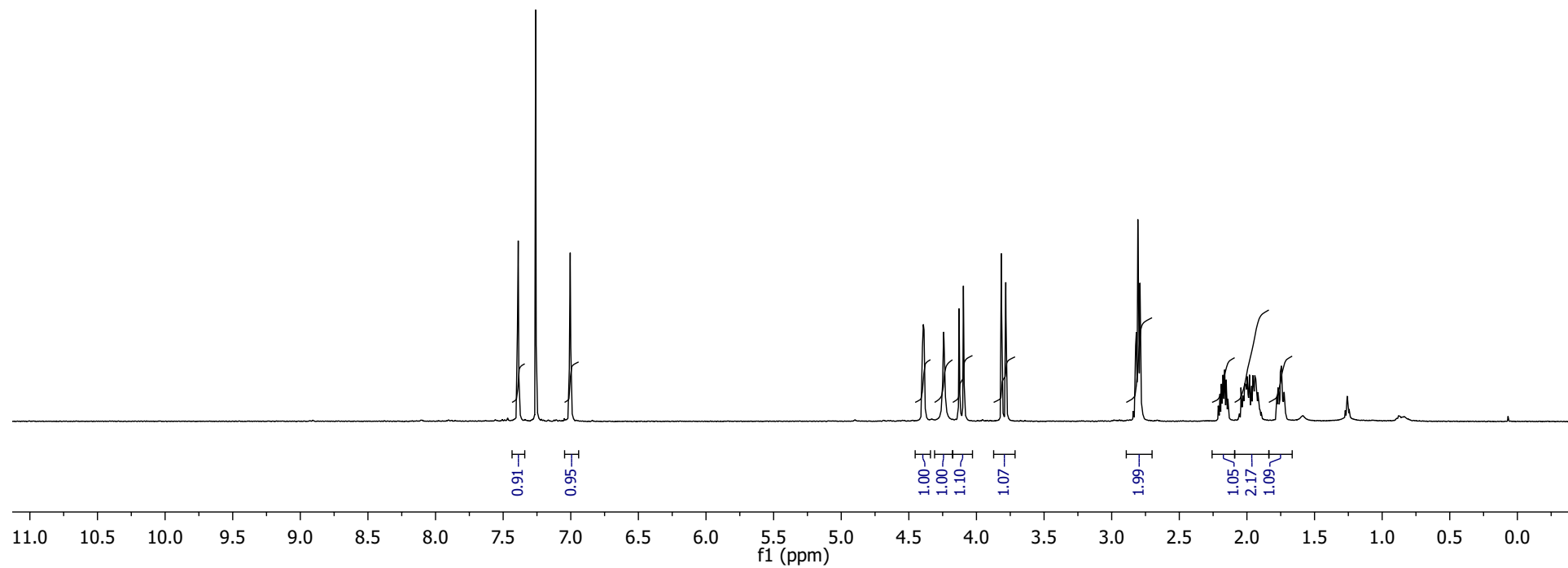
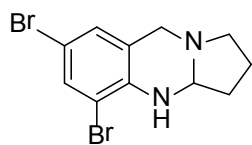
<sup>§</sup> *Department of Organic Synthesis Technology, Ural Federal University, Yekaterinburg, 620002, Russia*

## Supporting Information

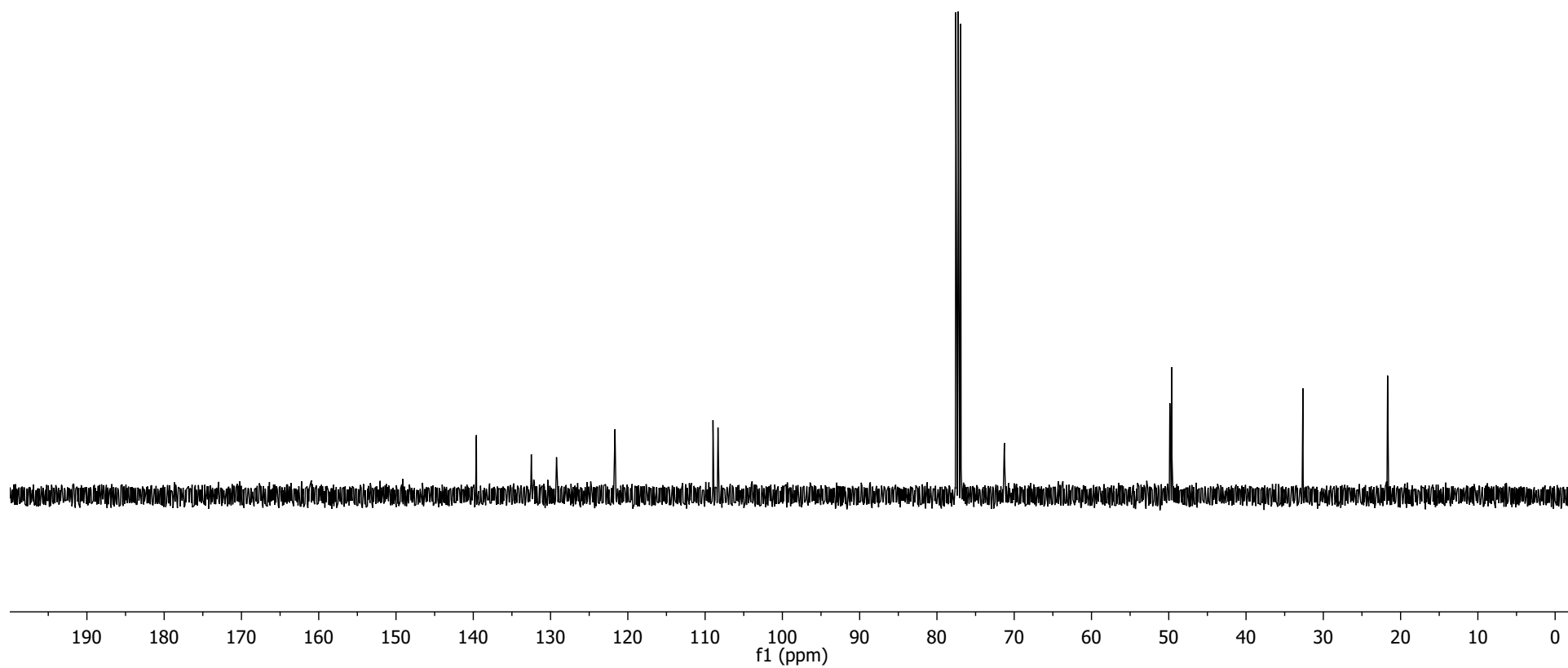
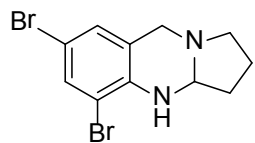
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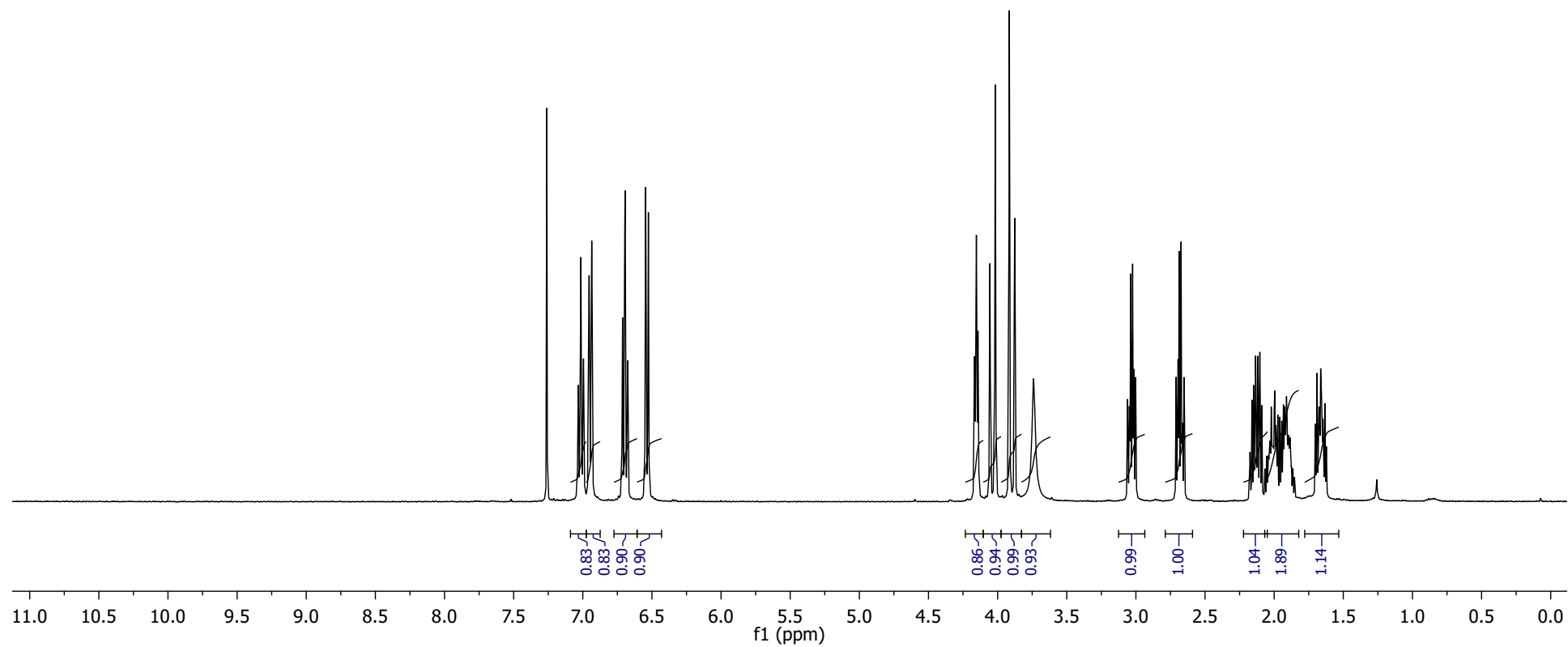
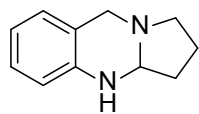
$^1\text{H}$  NMR of **2a** in  $\text{CDCl}_3$



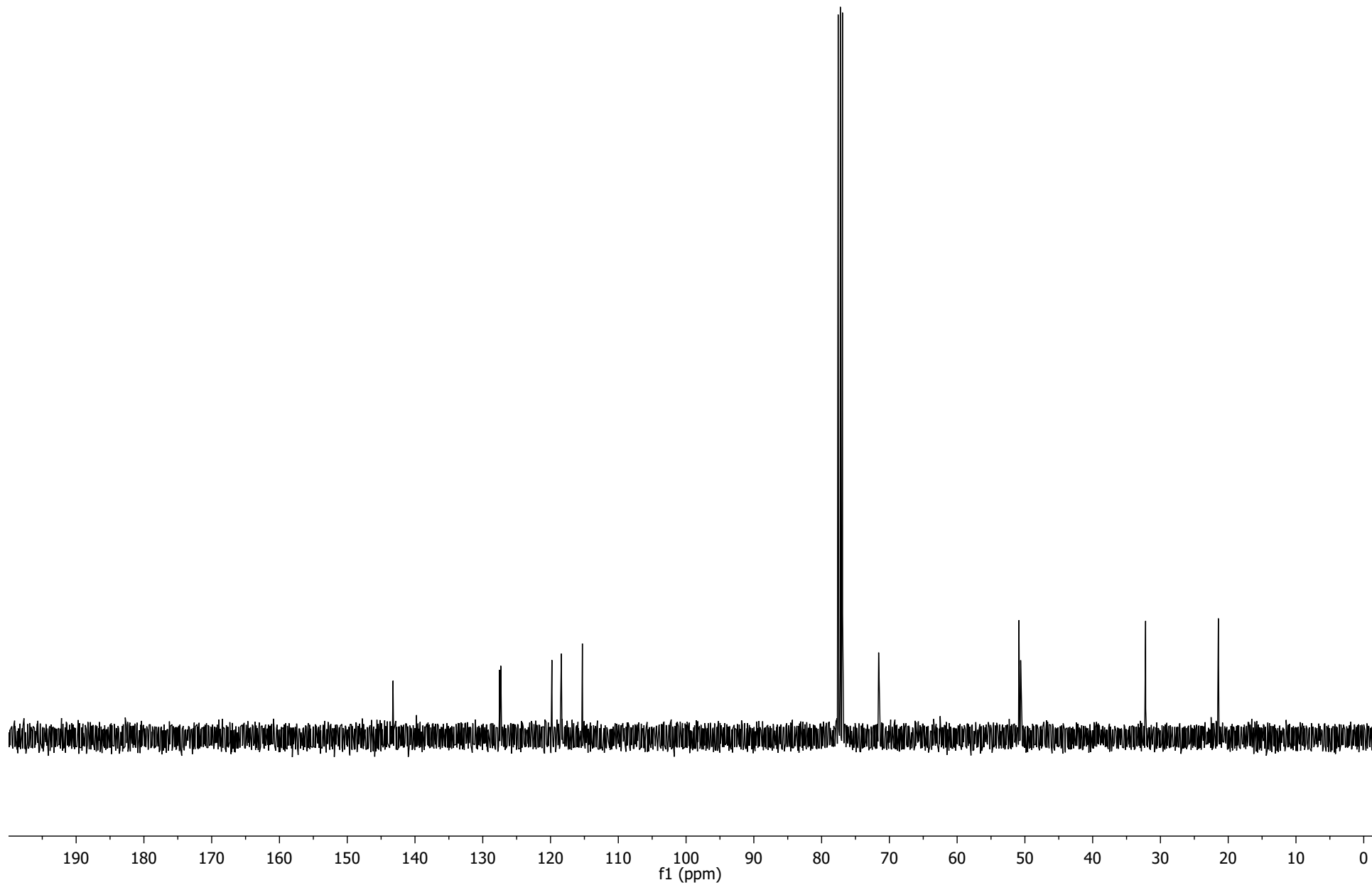
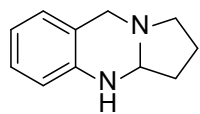
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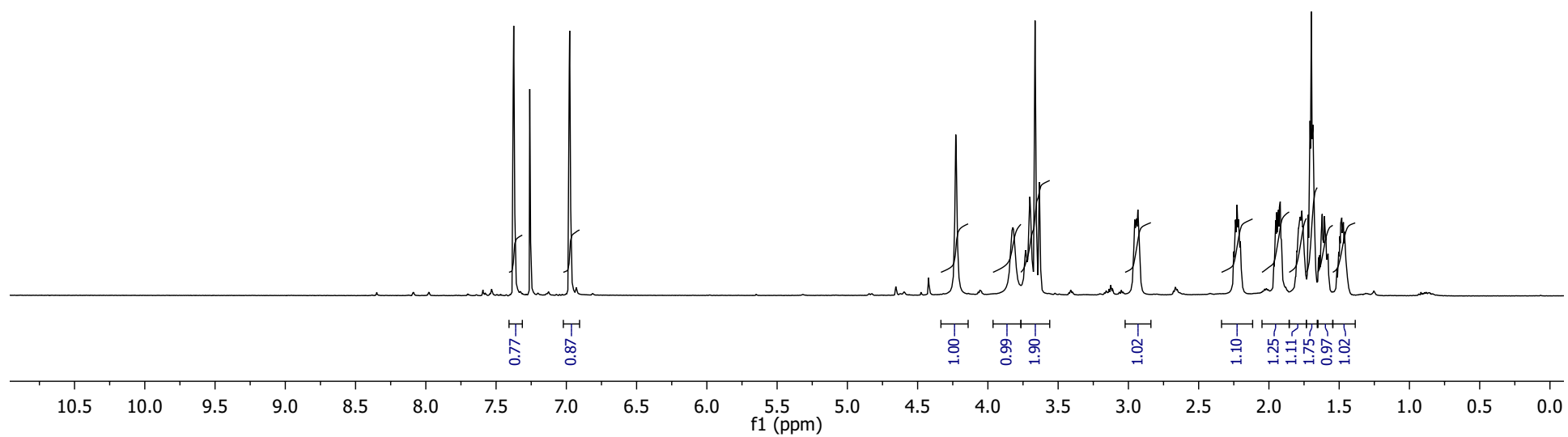
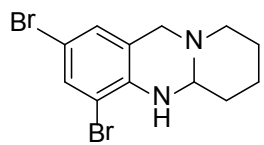
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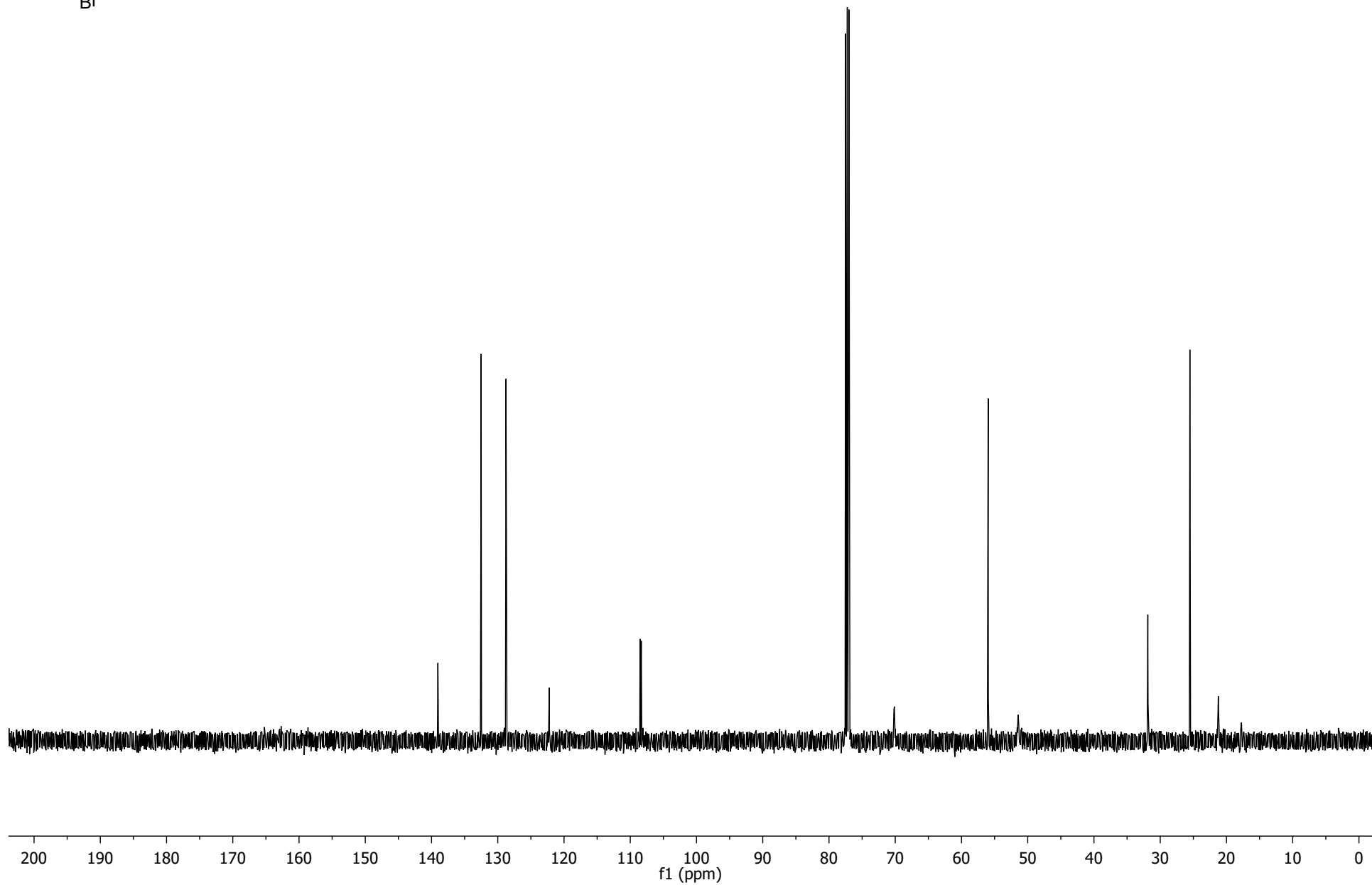
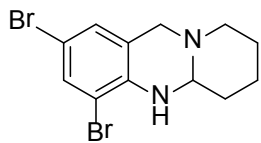
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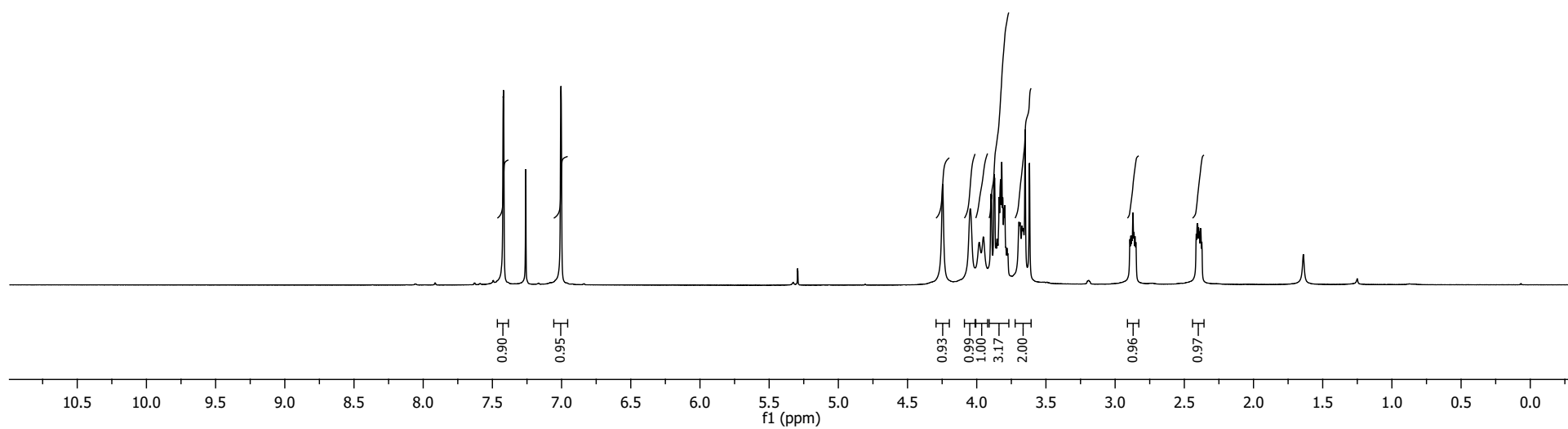
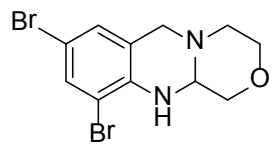
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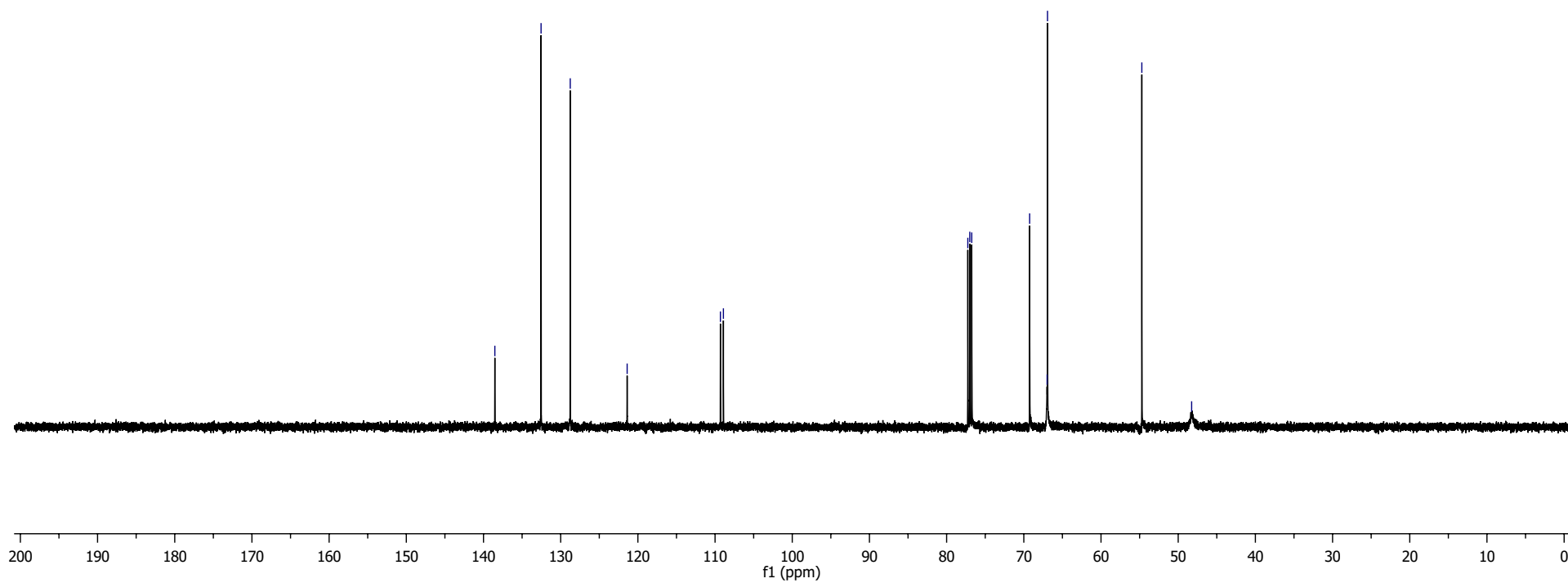
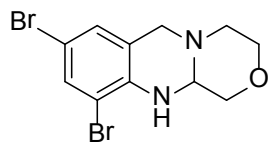


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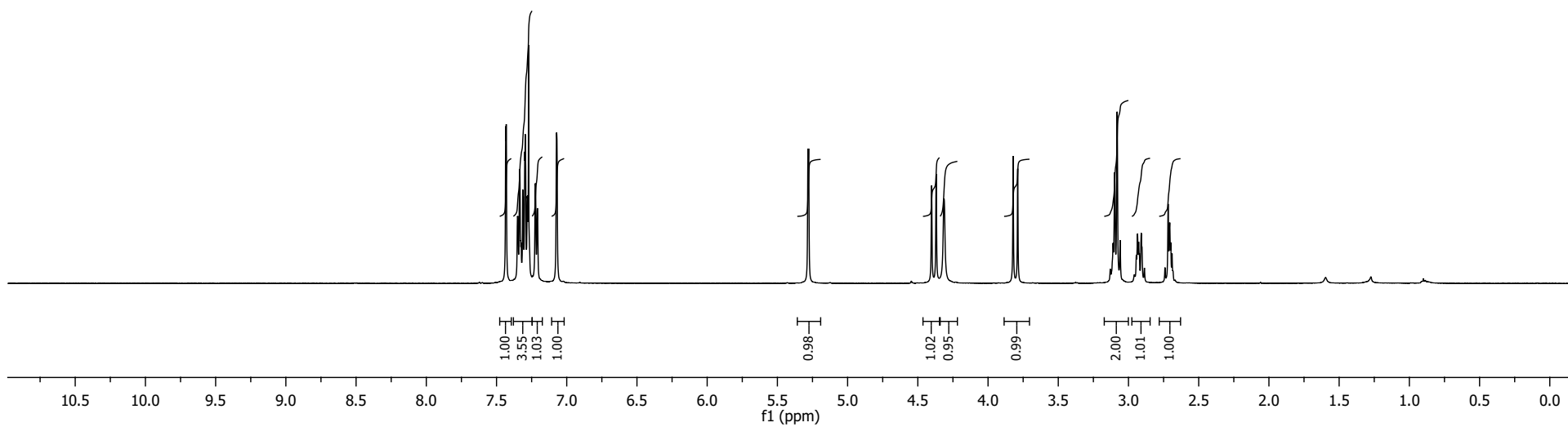
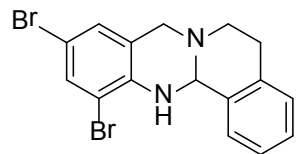




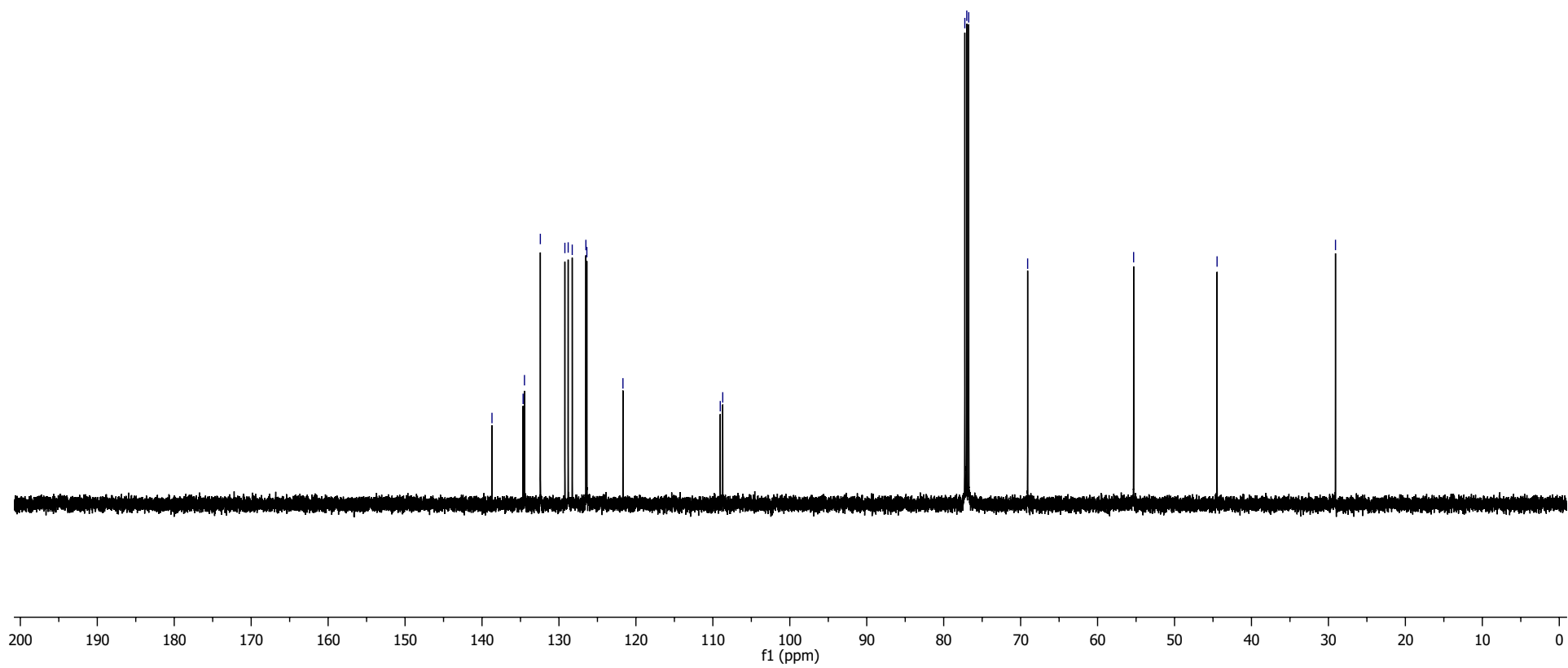
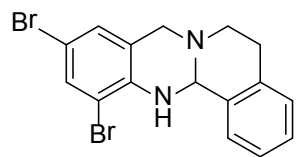
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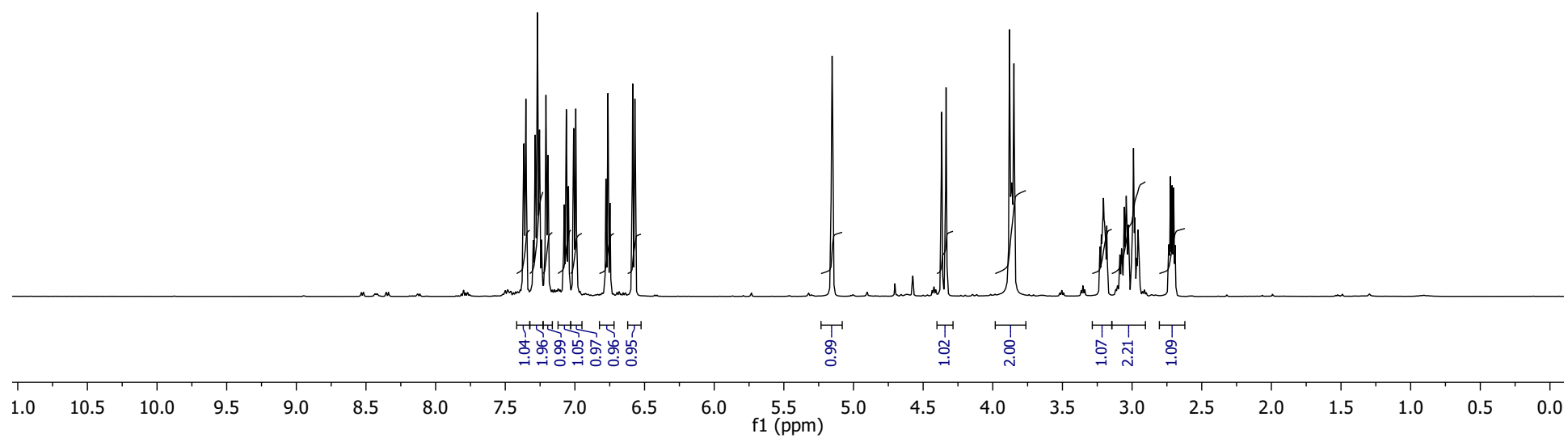
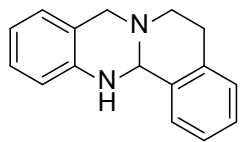
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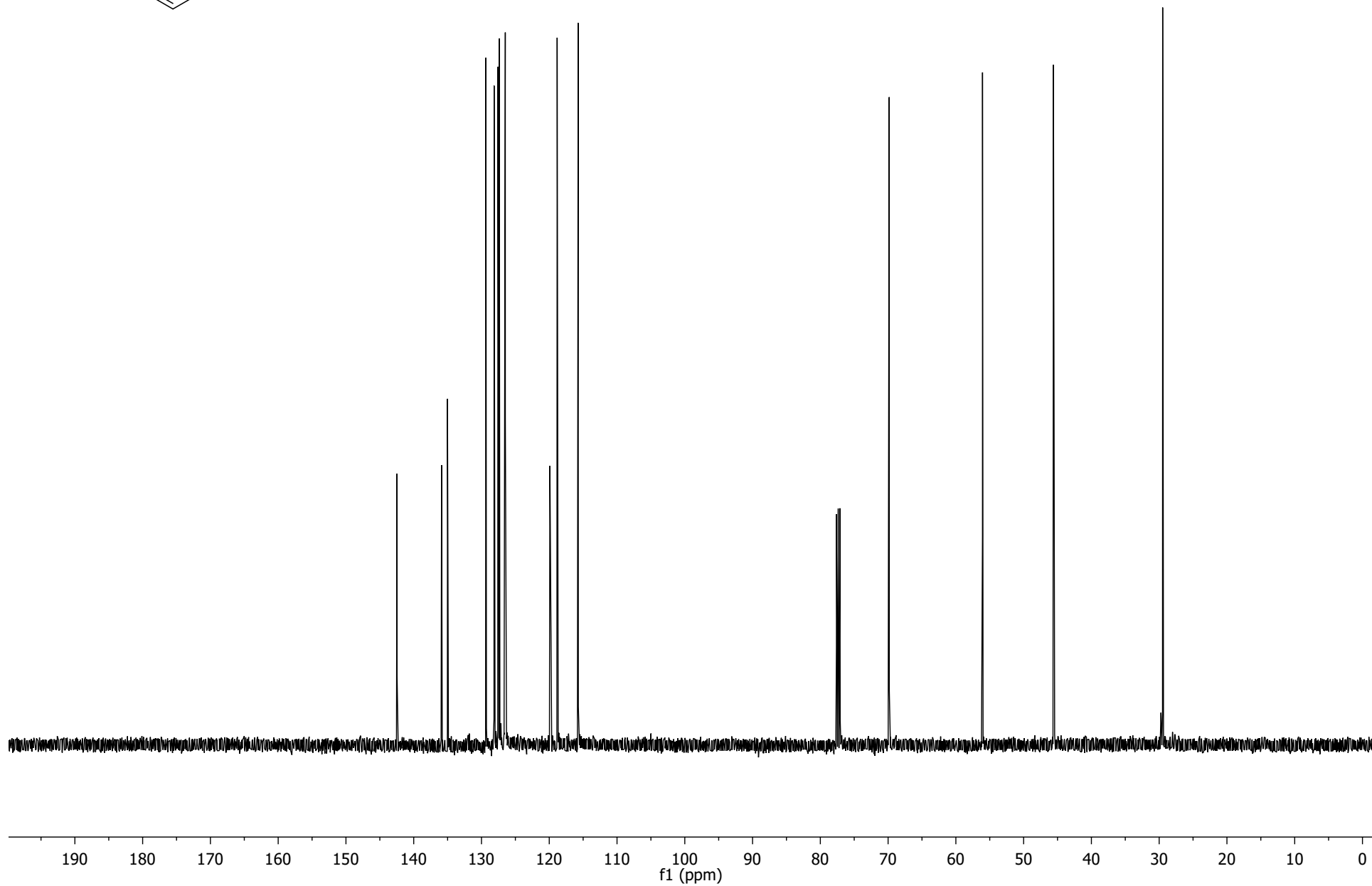
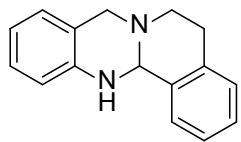
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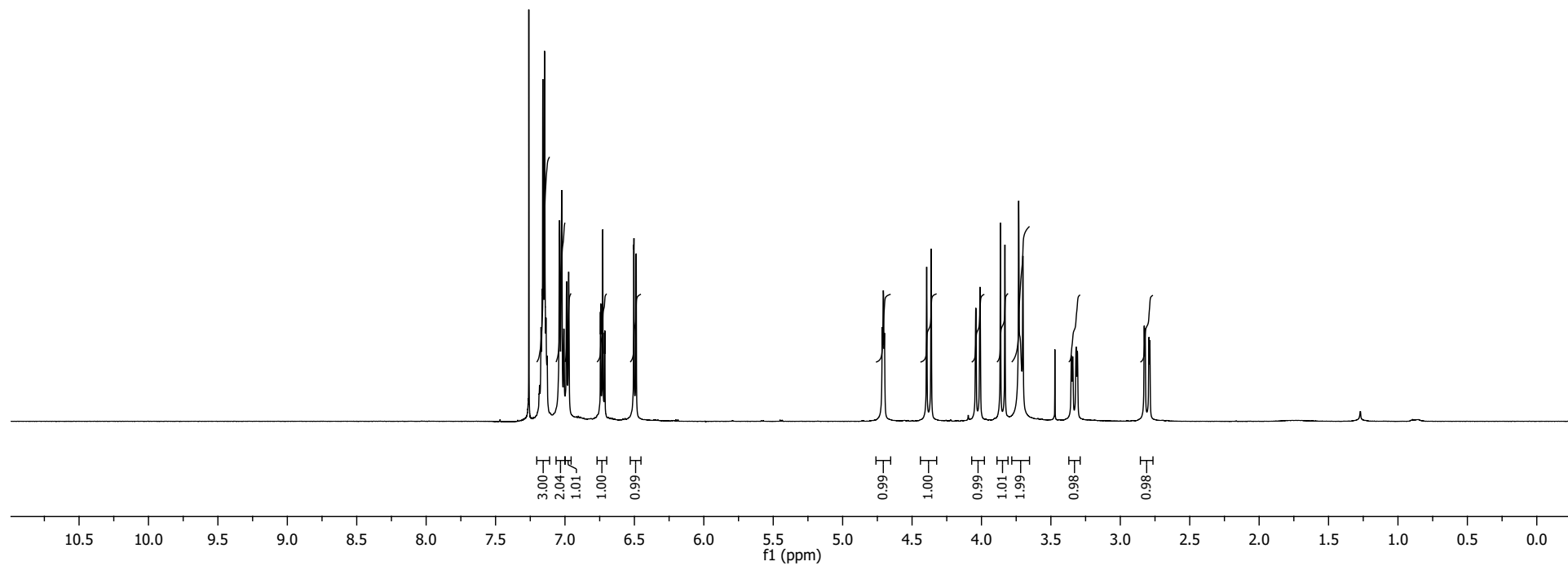
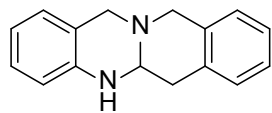
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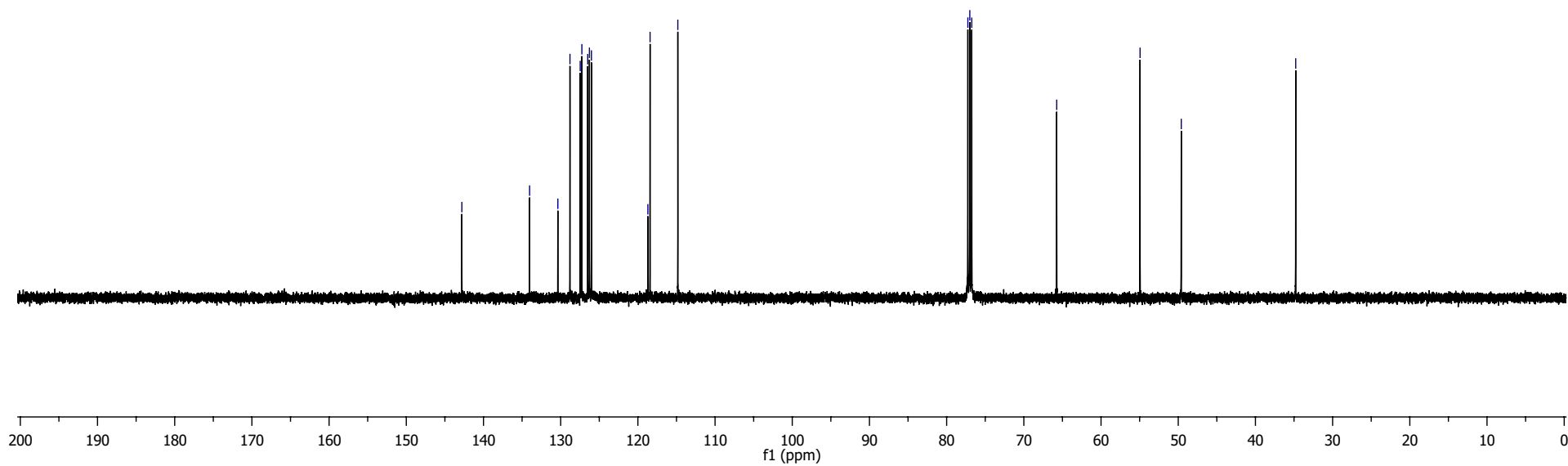
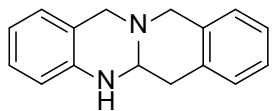
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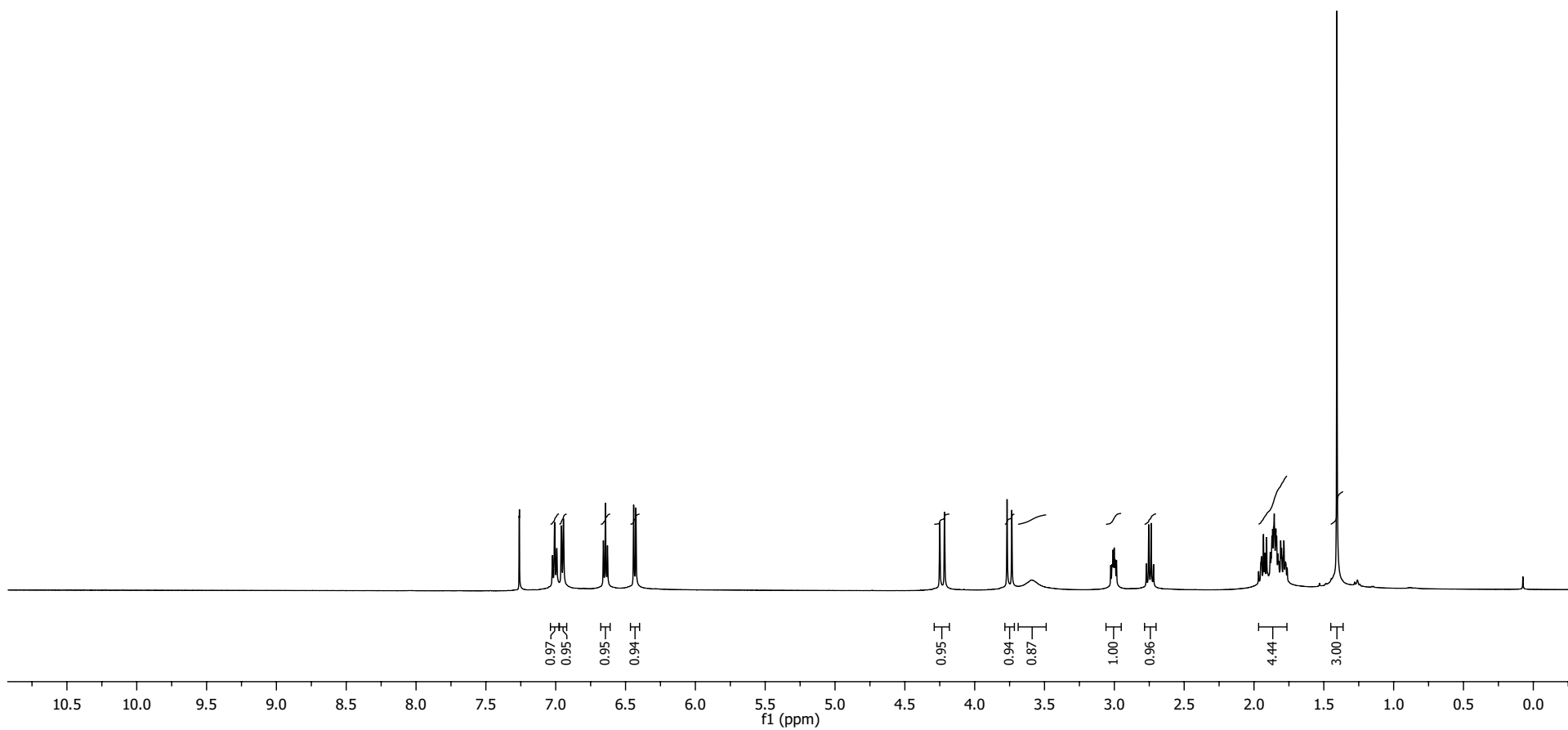
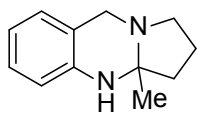
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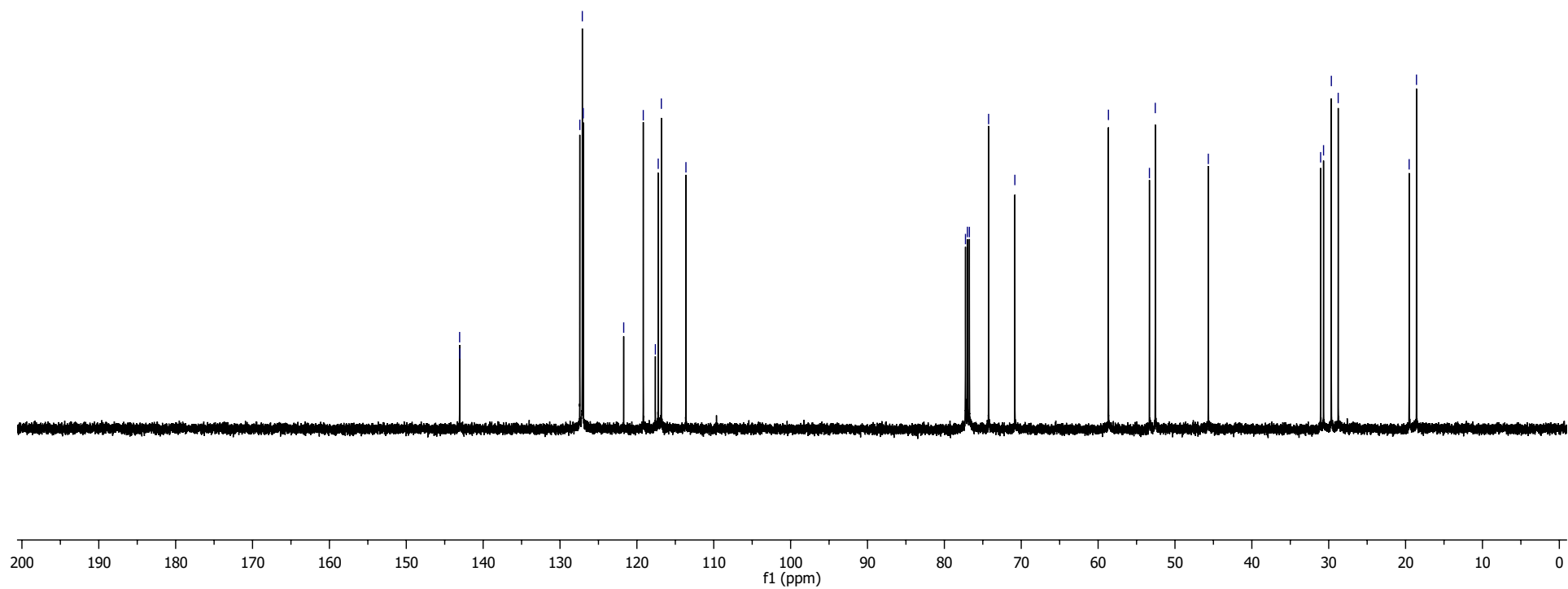
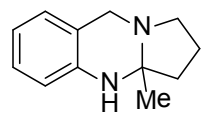


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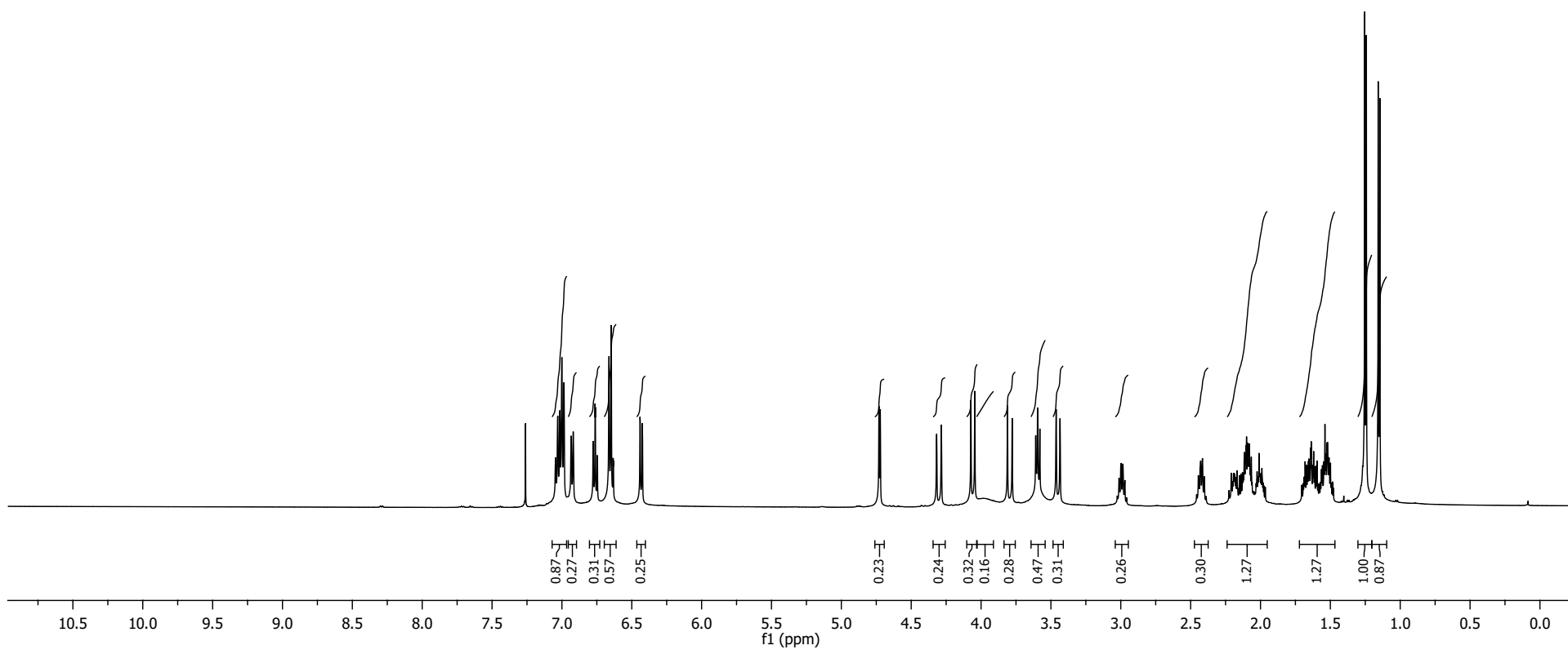
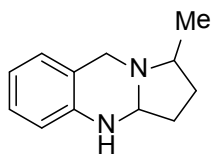




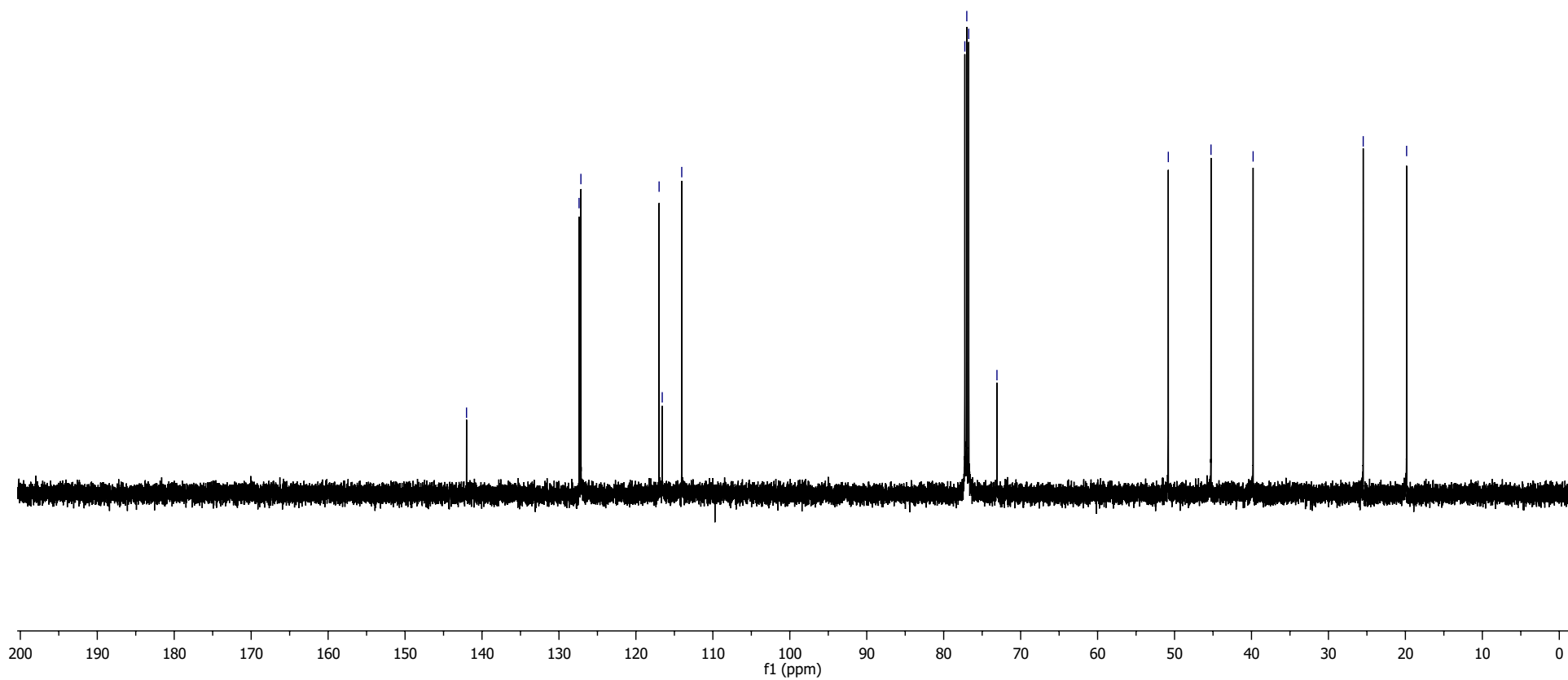
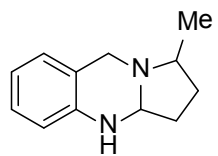
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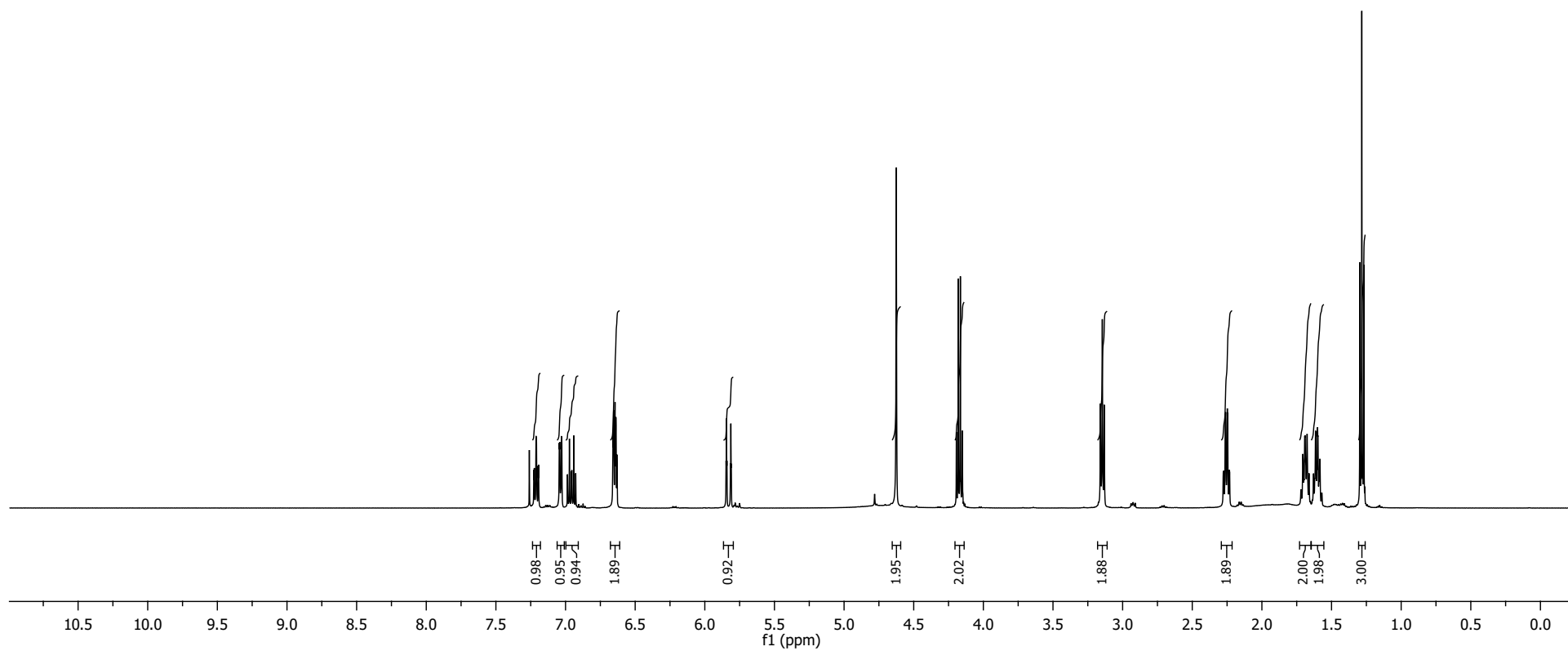
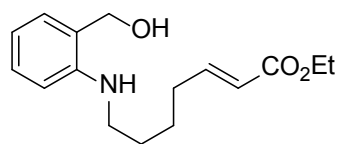
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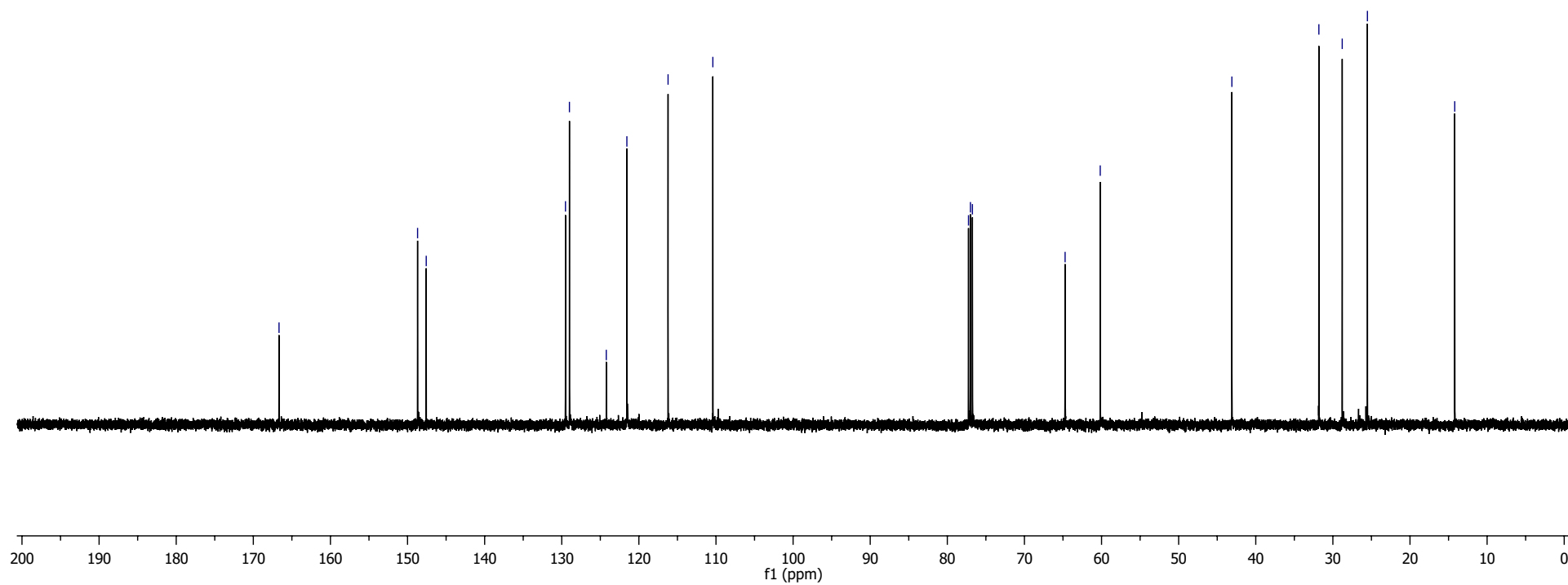
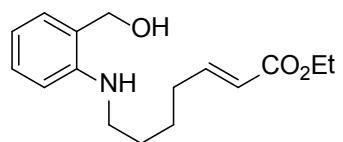
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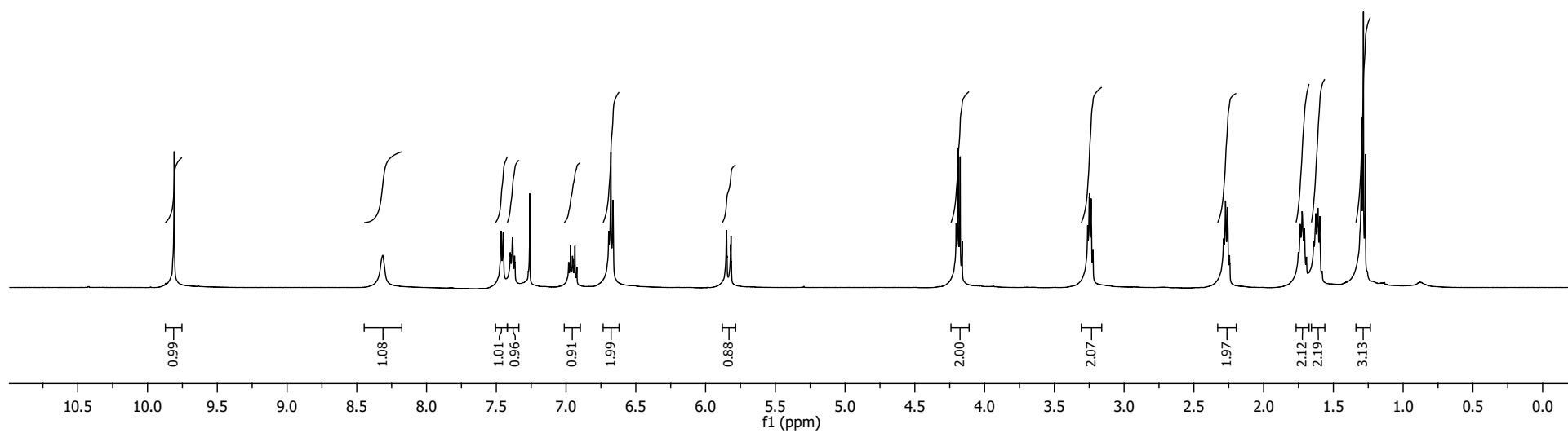
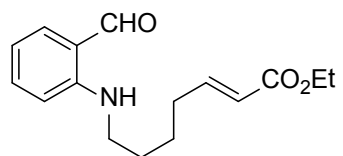
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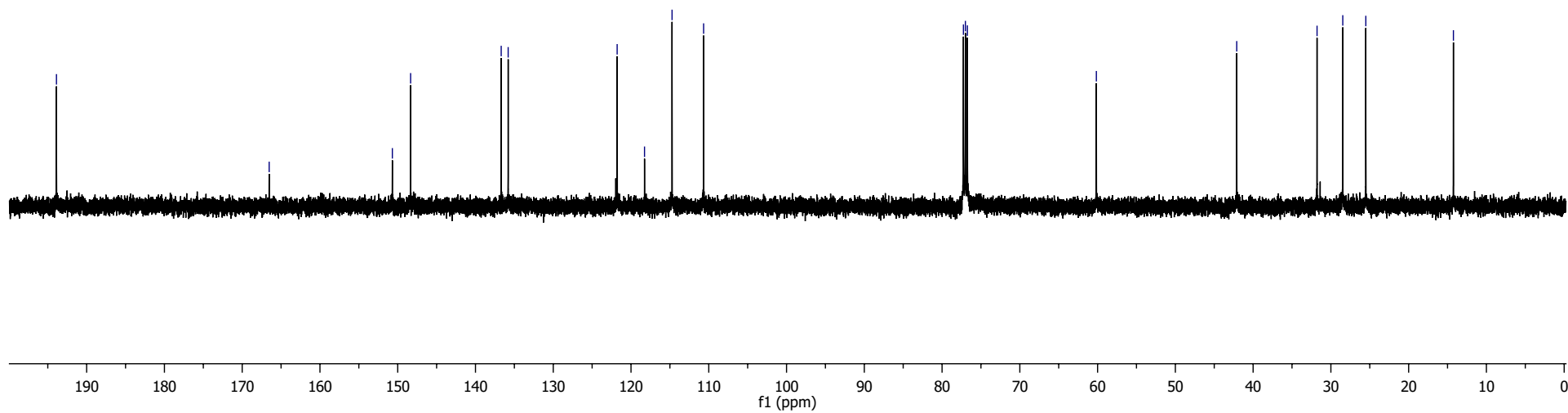
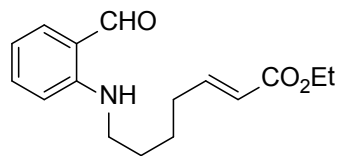
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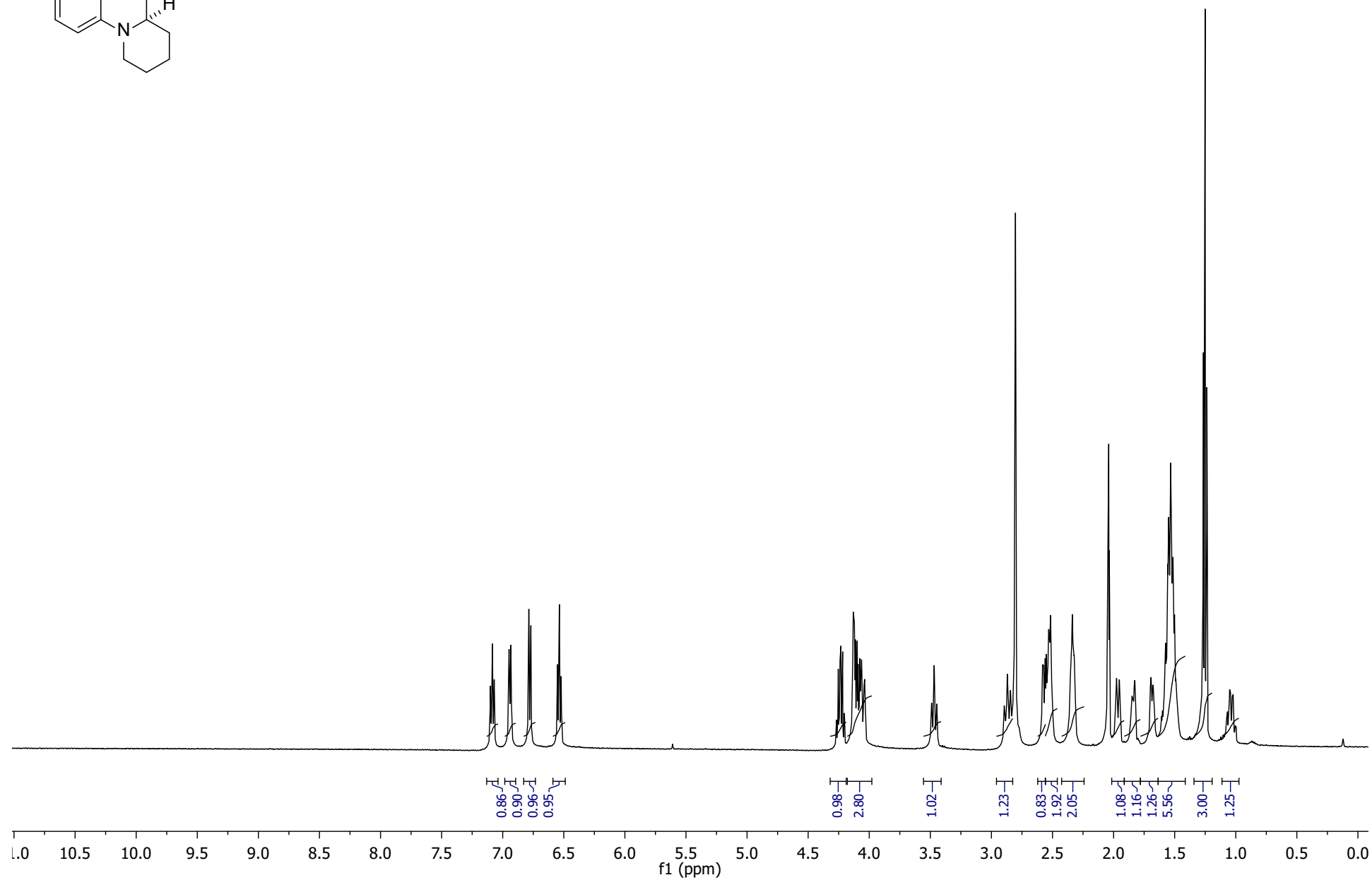
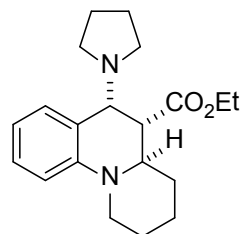
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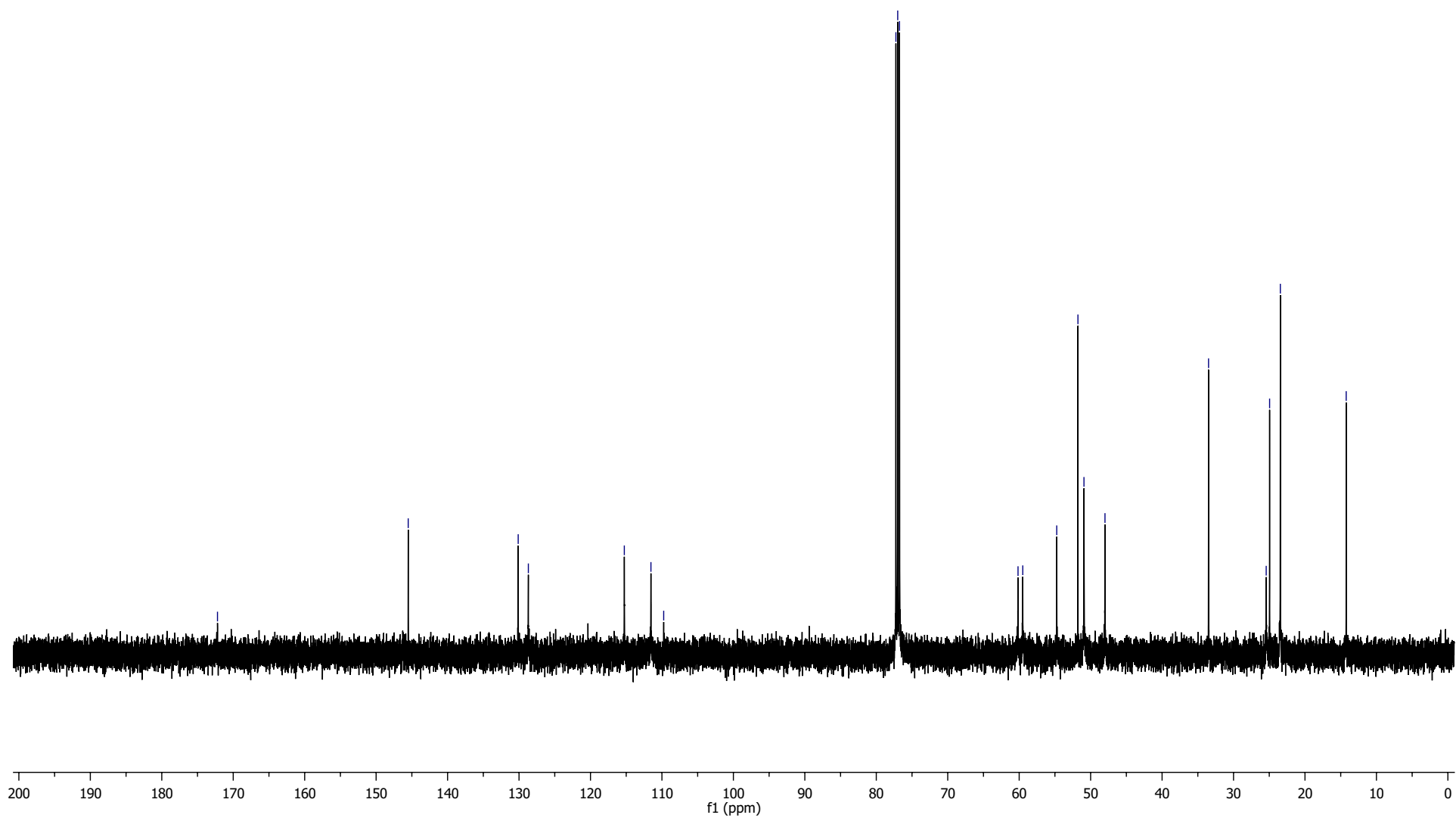
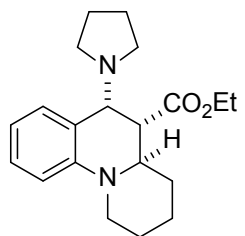


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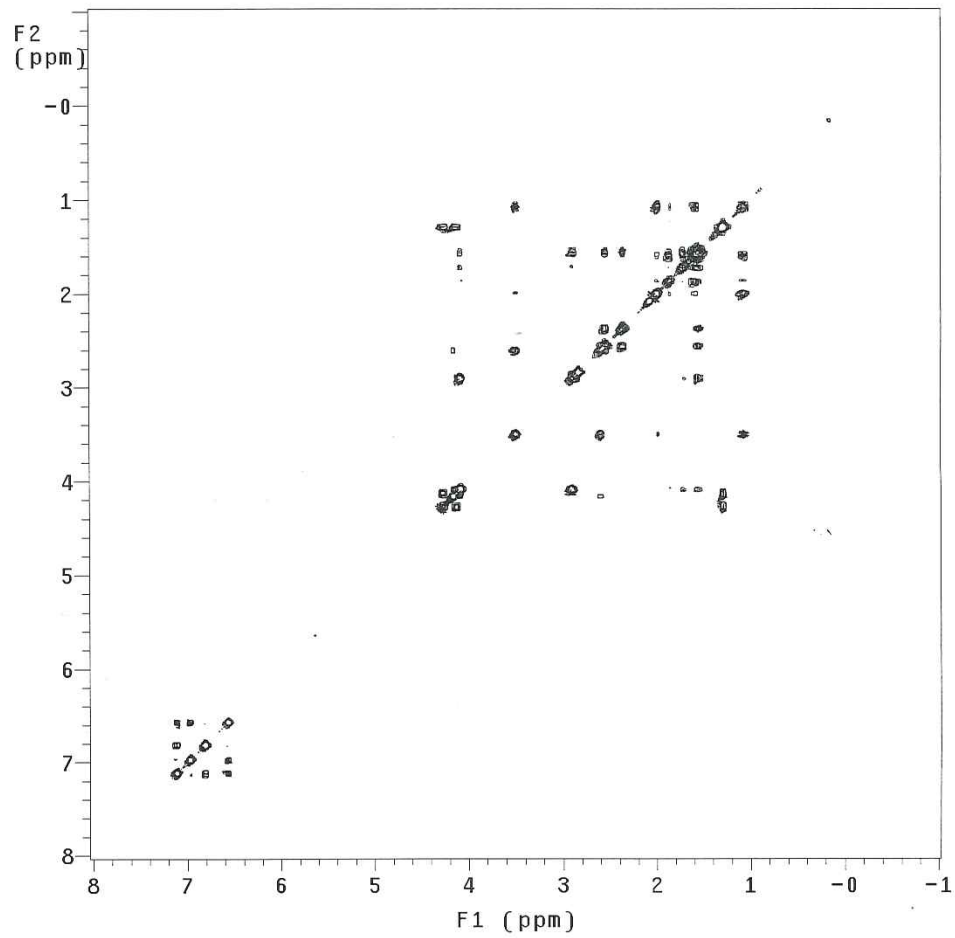
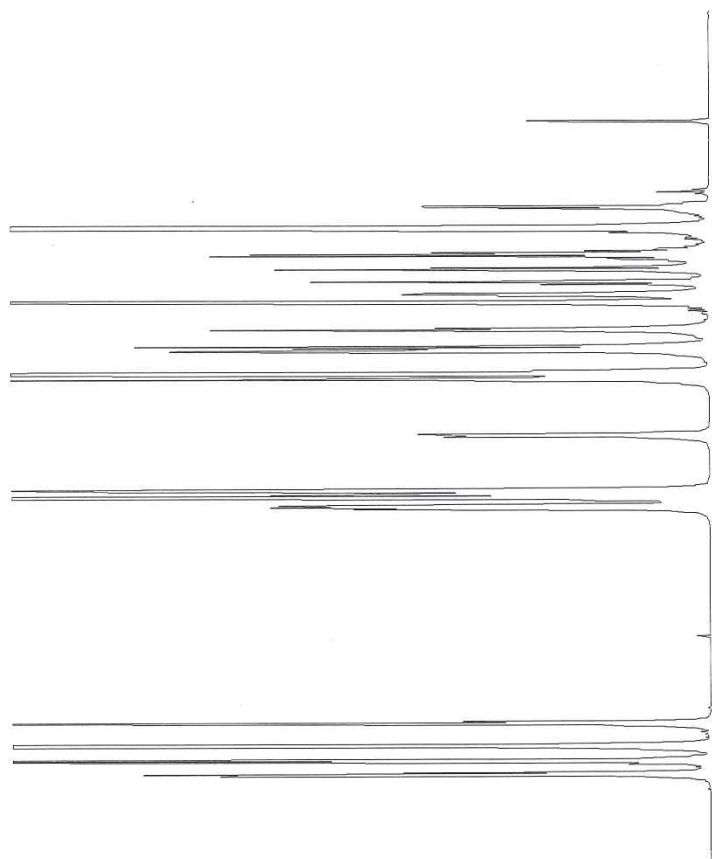
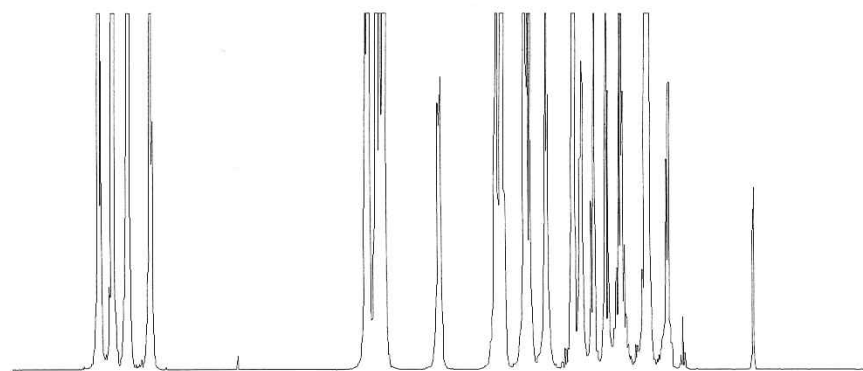
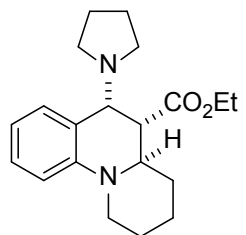




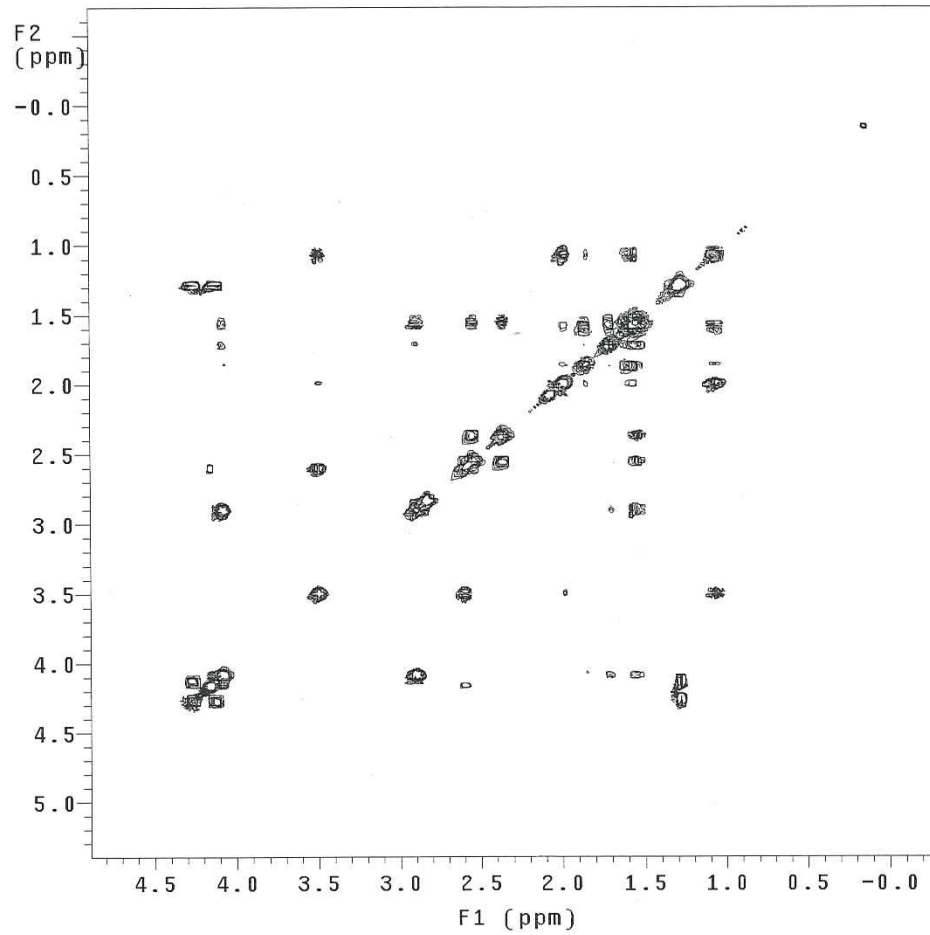
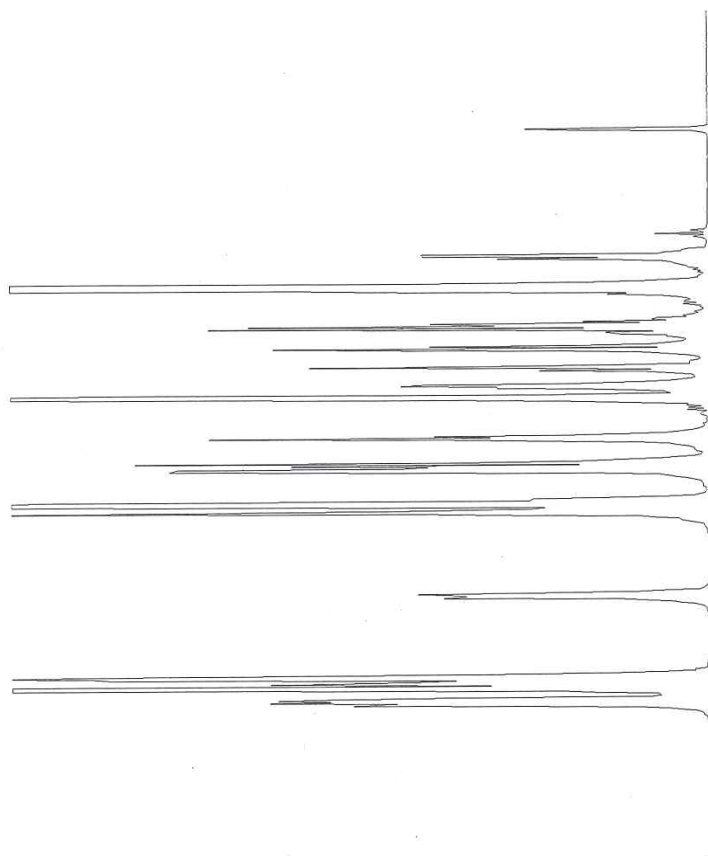
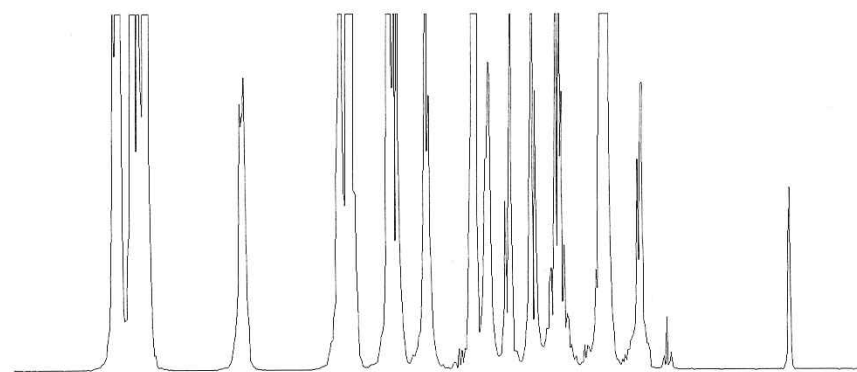
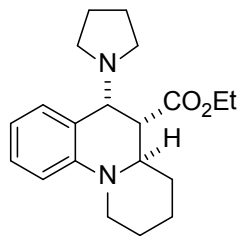
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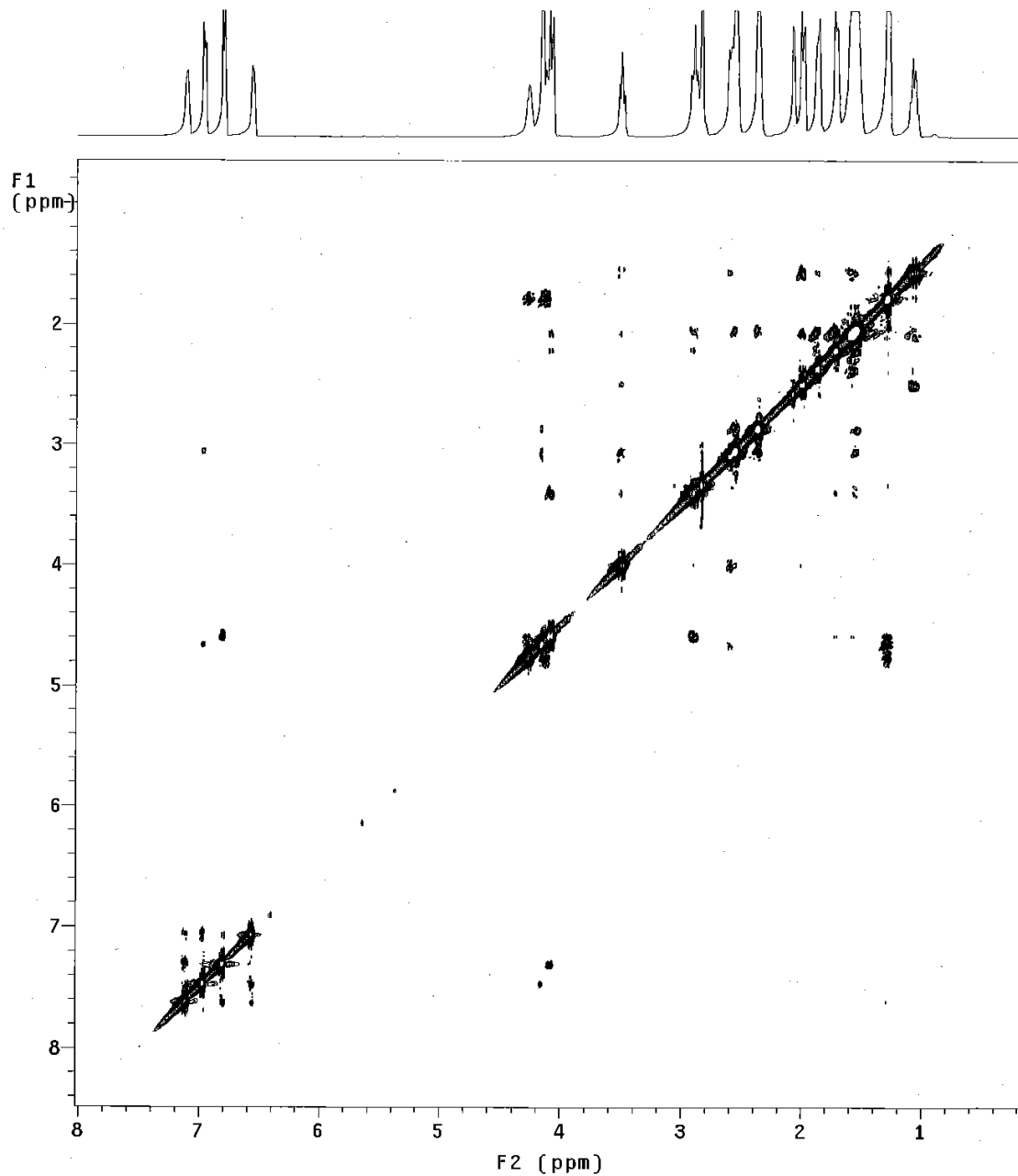
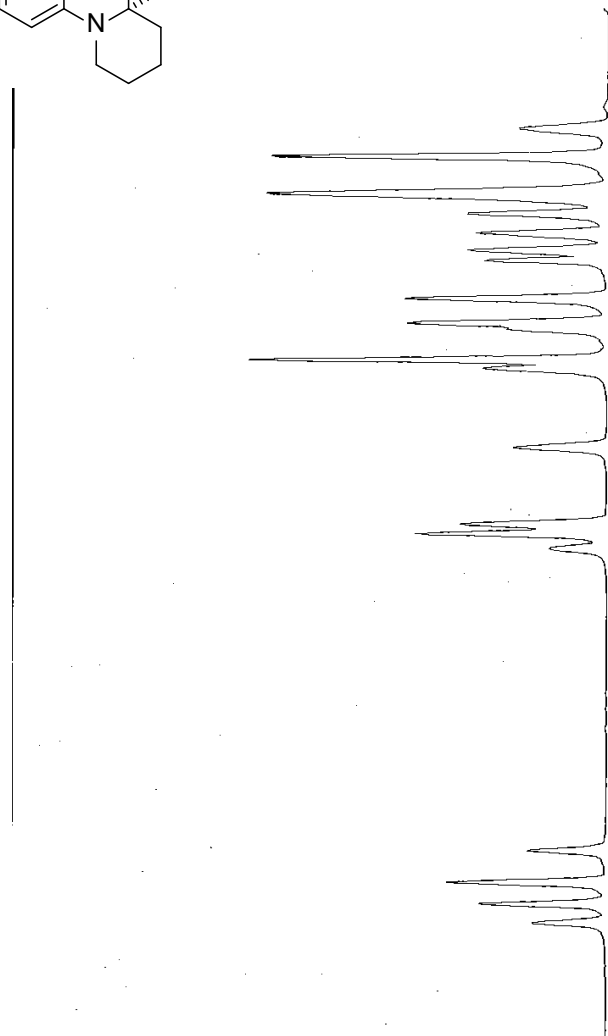
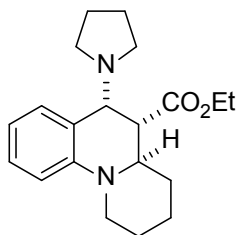
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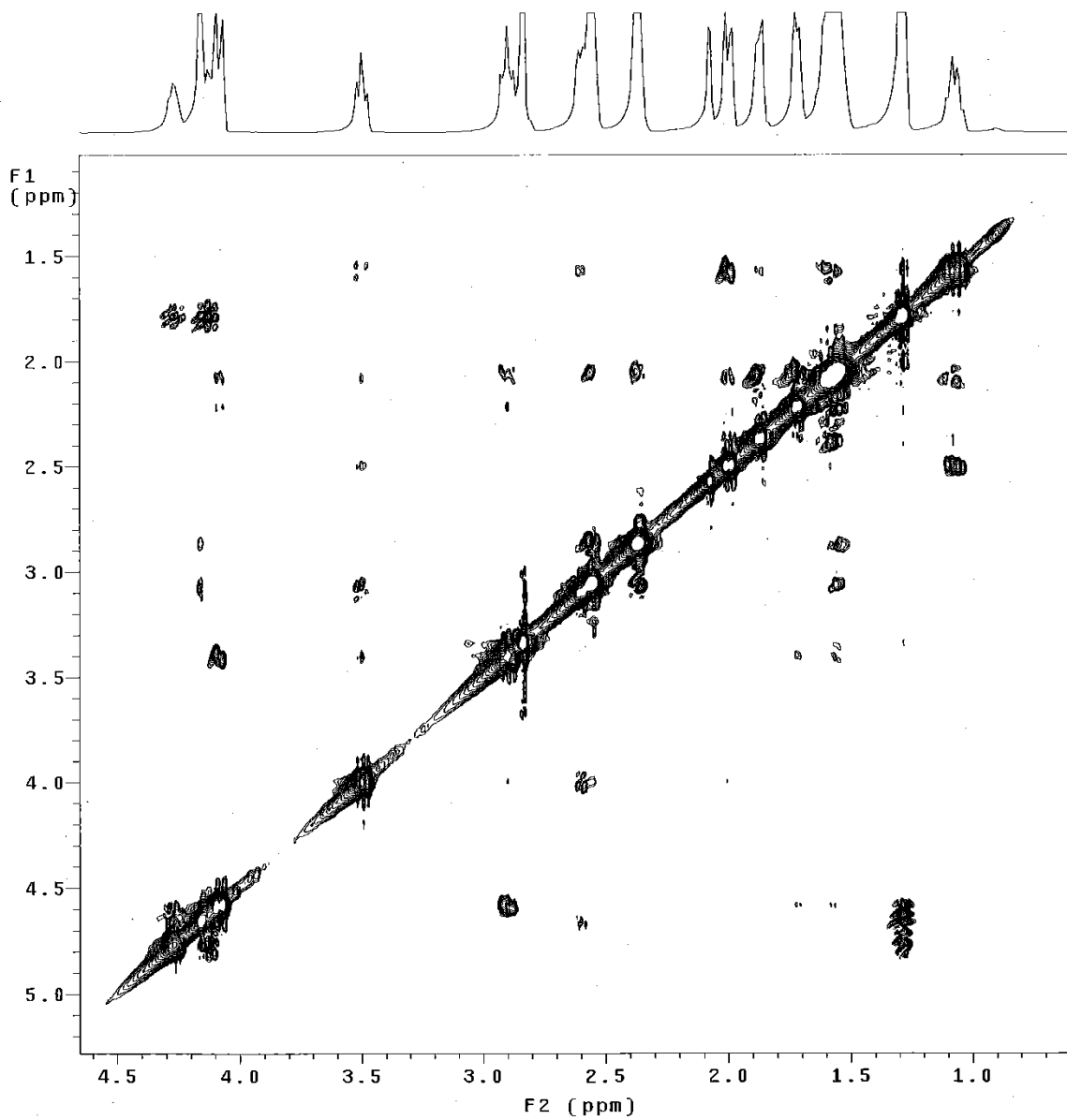
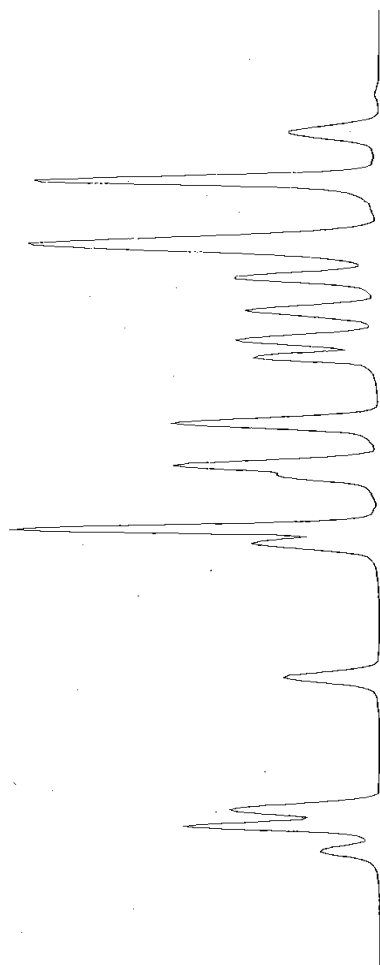
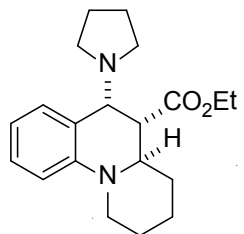
GCOSY of **12** in  $(\text{CD}_3)_2\text{CO}$  (zoomed)



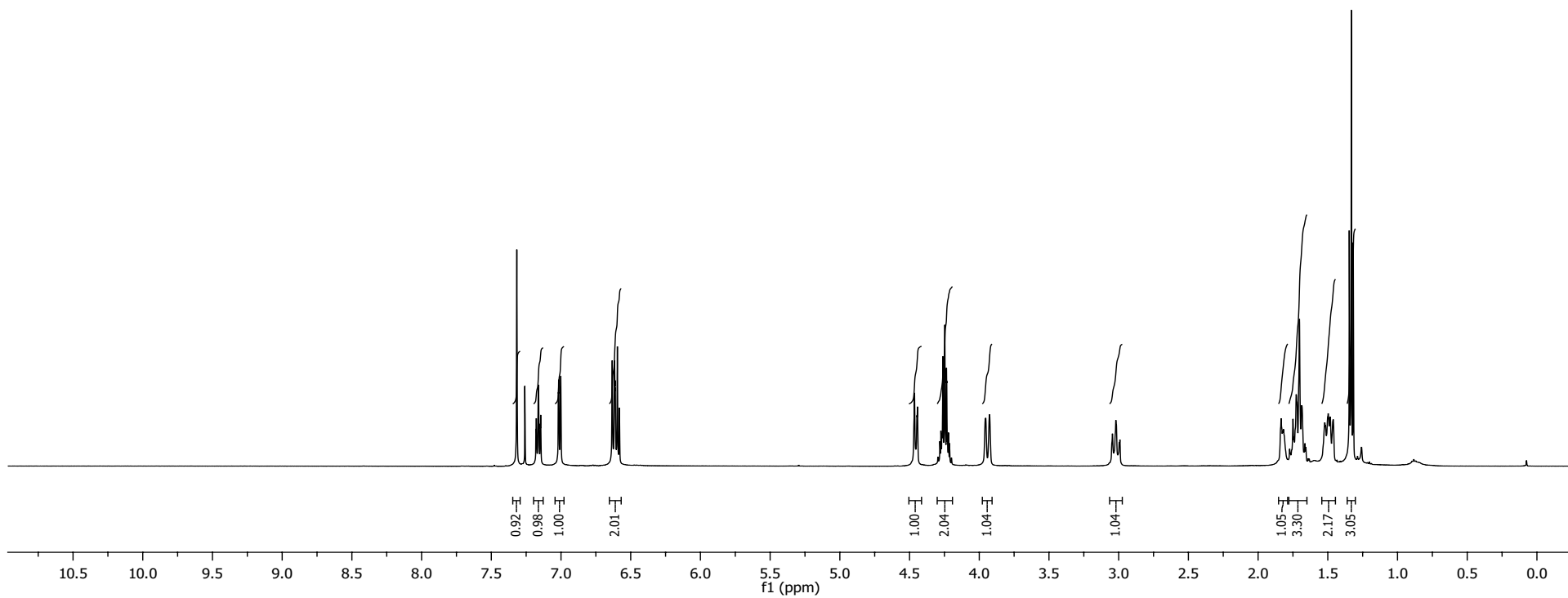
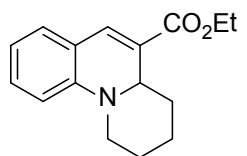
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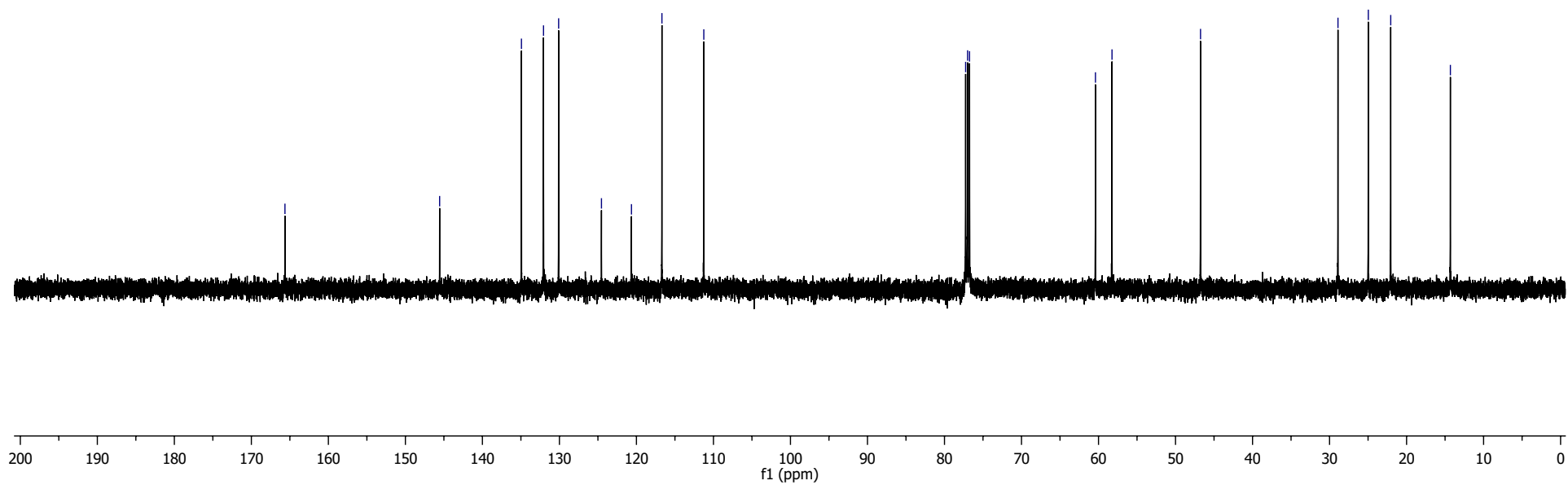
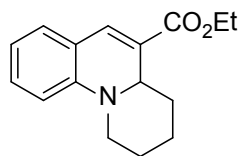
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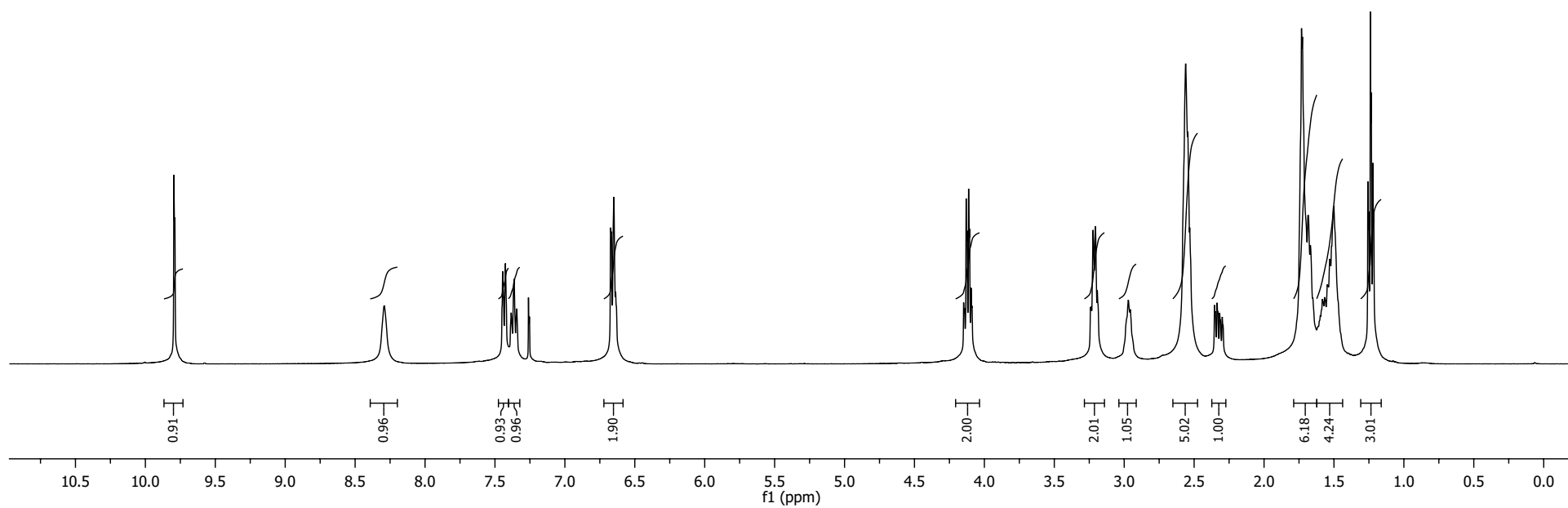
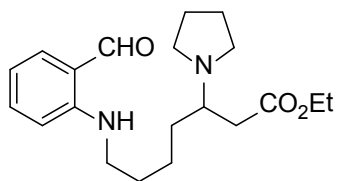
$^1\text{H}$  NMR of **13** in  $\text{CDCl}_3$



$^{13}\text{C}$  NMR of **13** in  $\text{CDCl}_3$

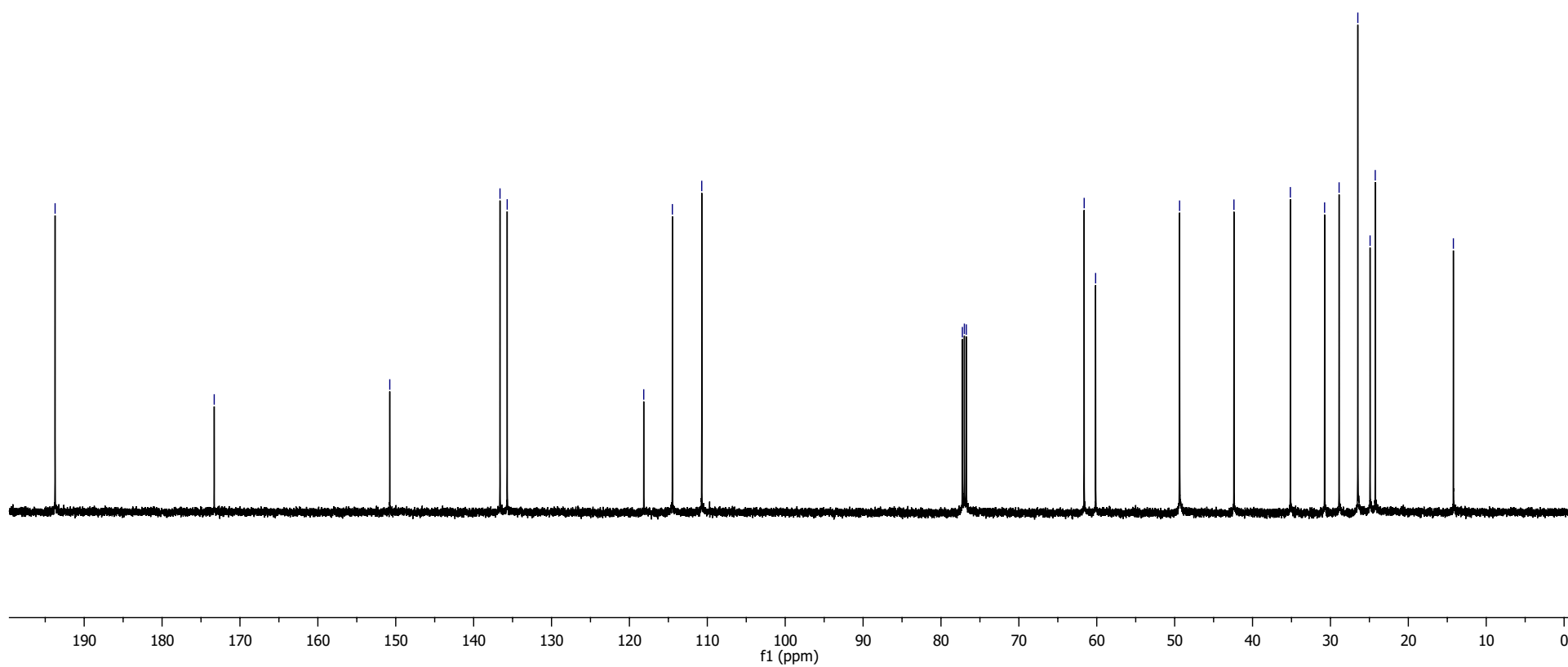
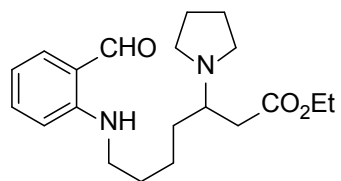


<sup>1</sup>H NMR of **14** in CDCl<sub>3</sub>

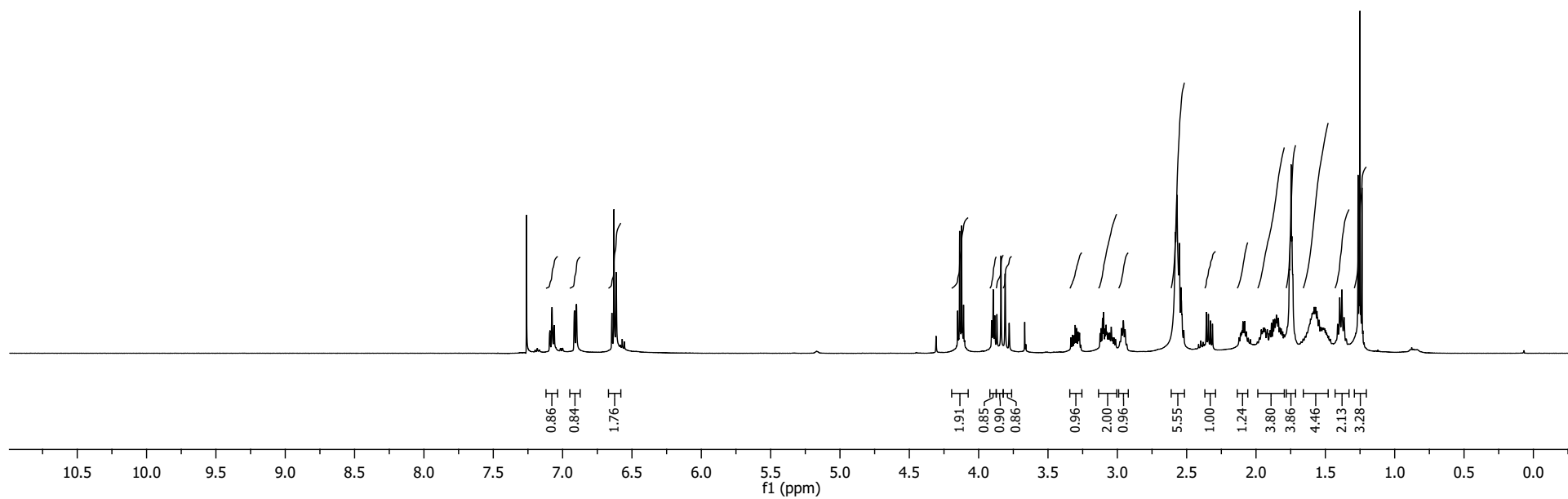
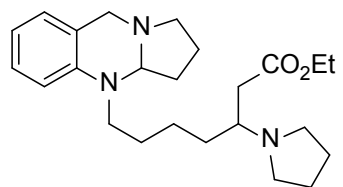




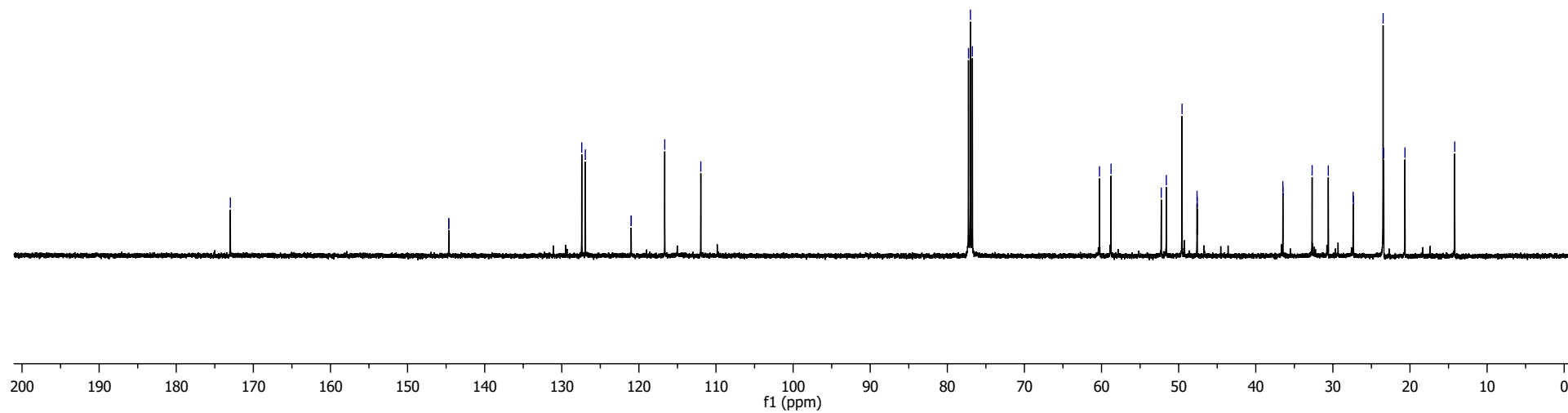
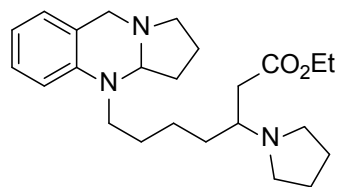
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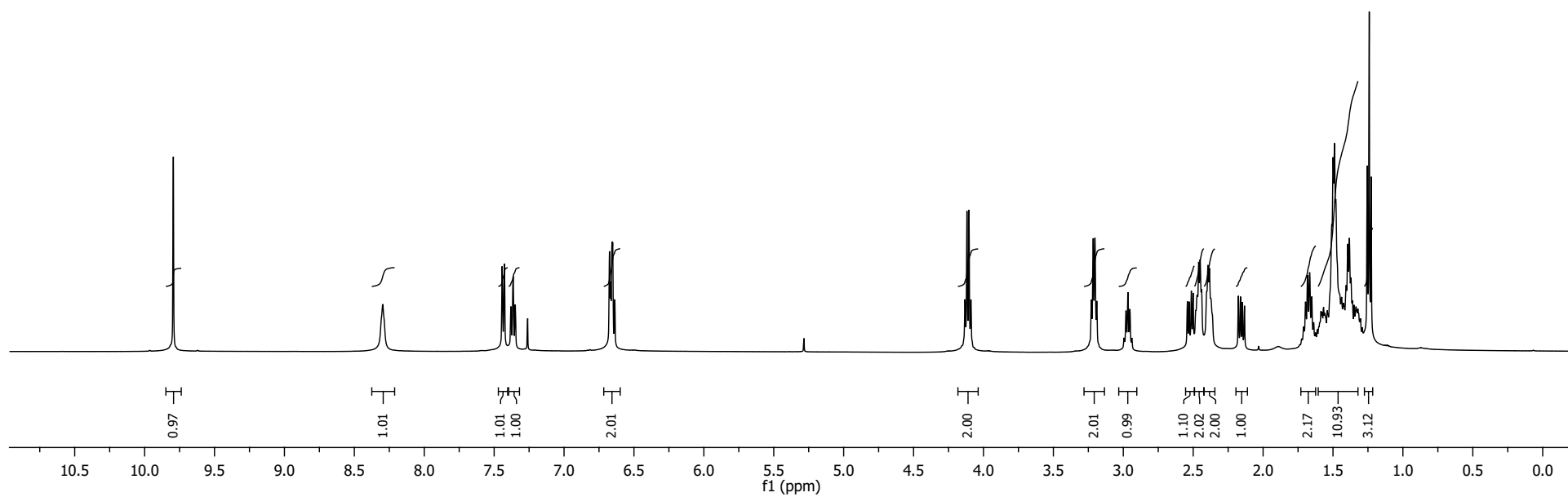
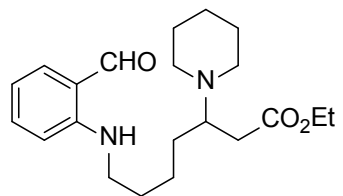
<sup>1</sup>H NMR of **15** in CDCl<sub>3</sub>



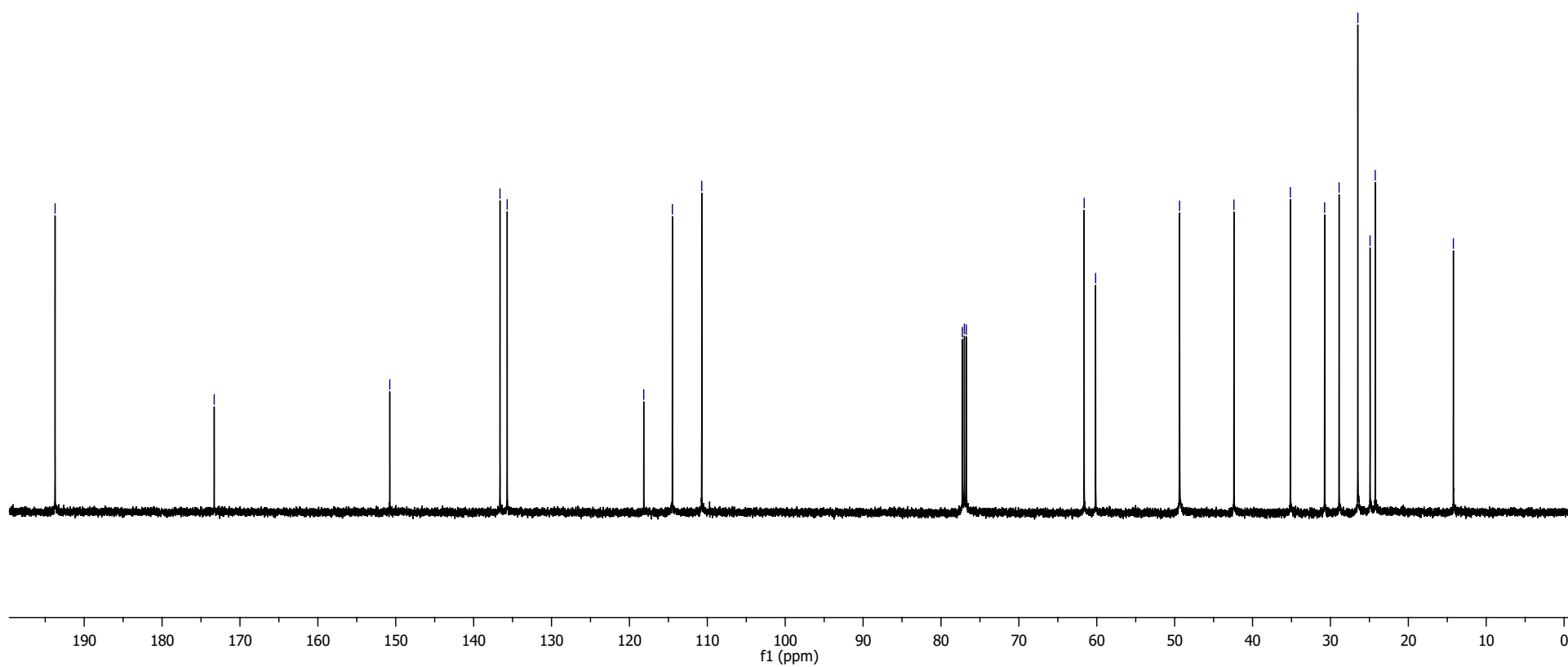
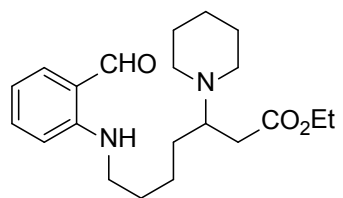
$^{13}\text{C}$  NMR of **15** in  $\text{CDCl}_3$



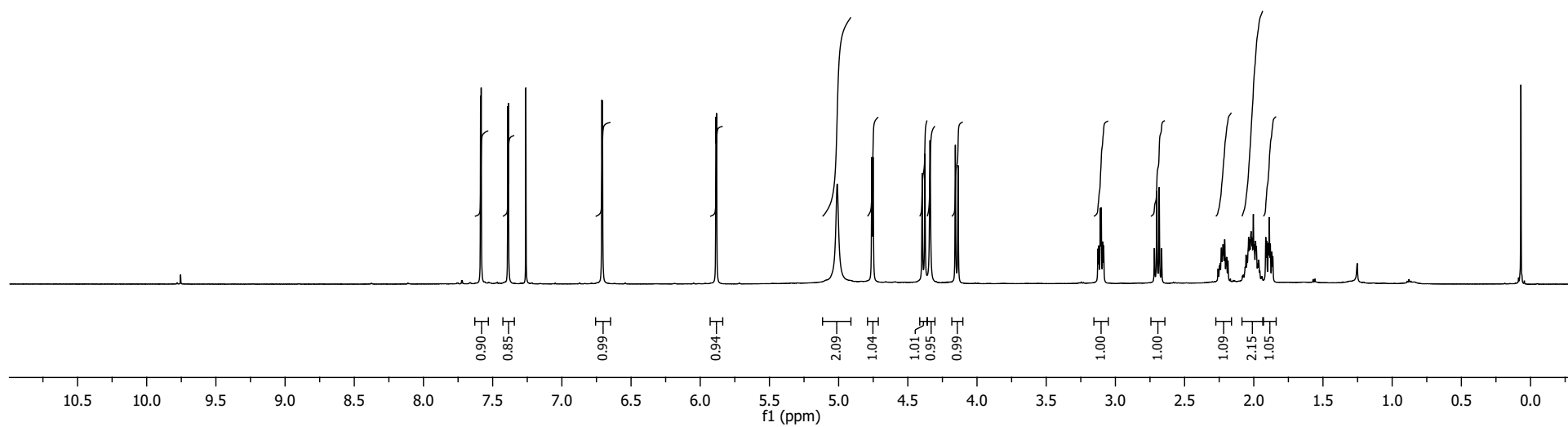
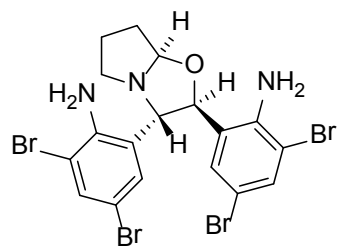
$^1\text{H}$  NMR of **18** in  $\text{CDCl}_3$



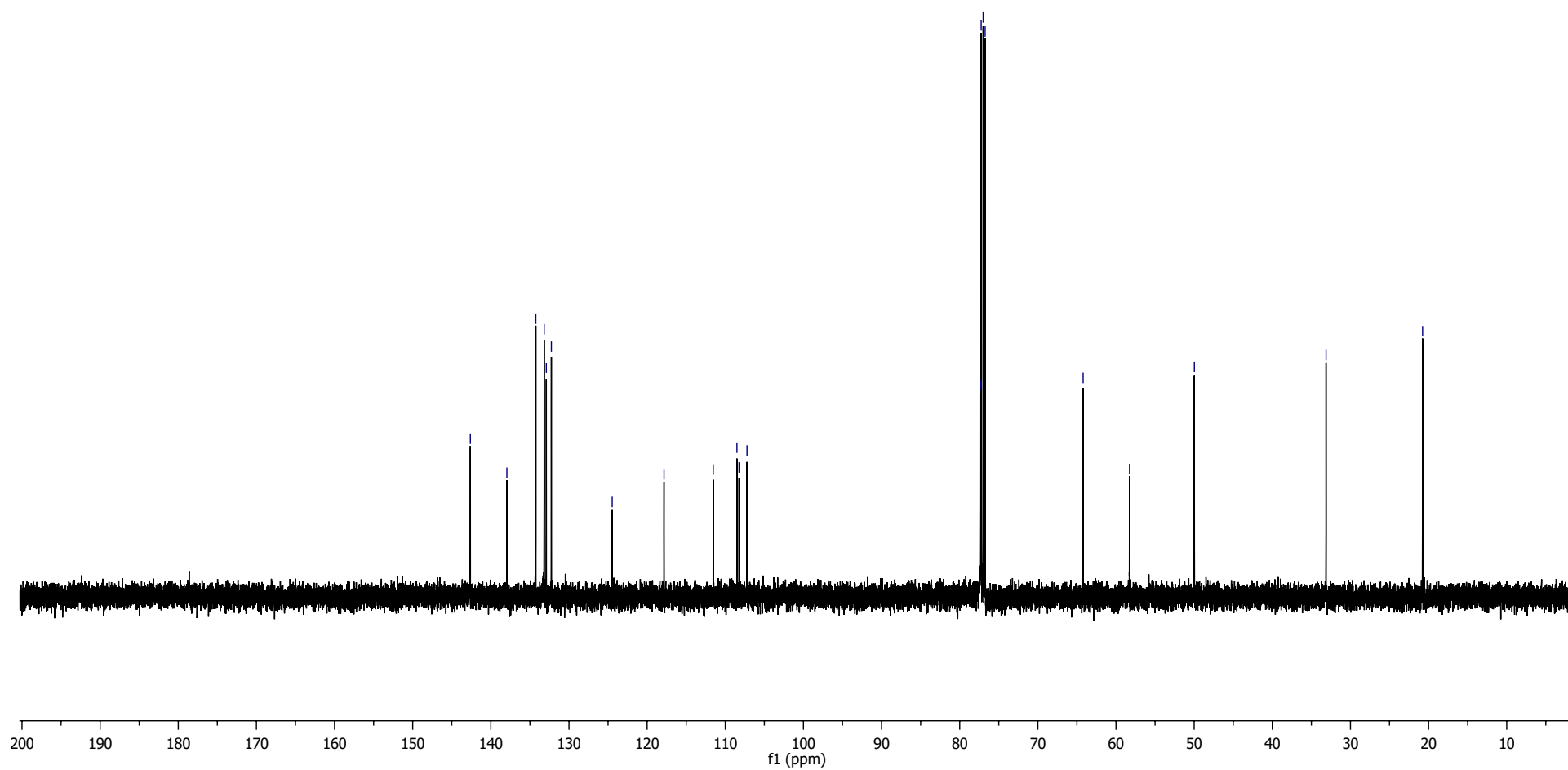
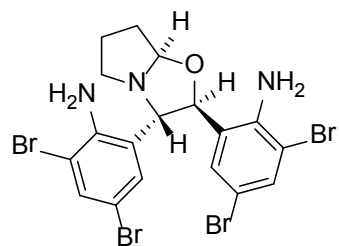
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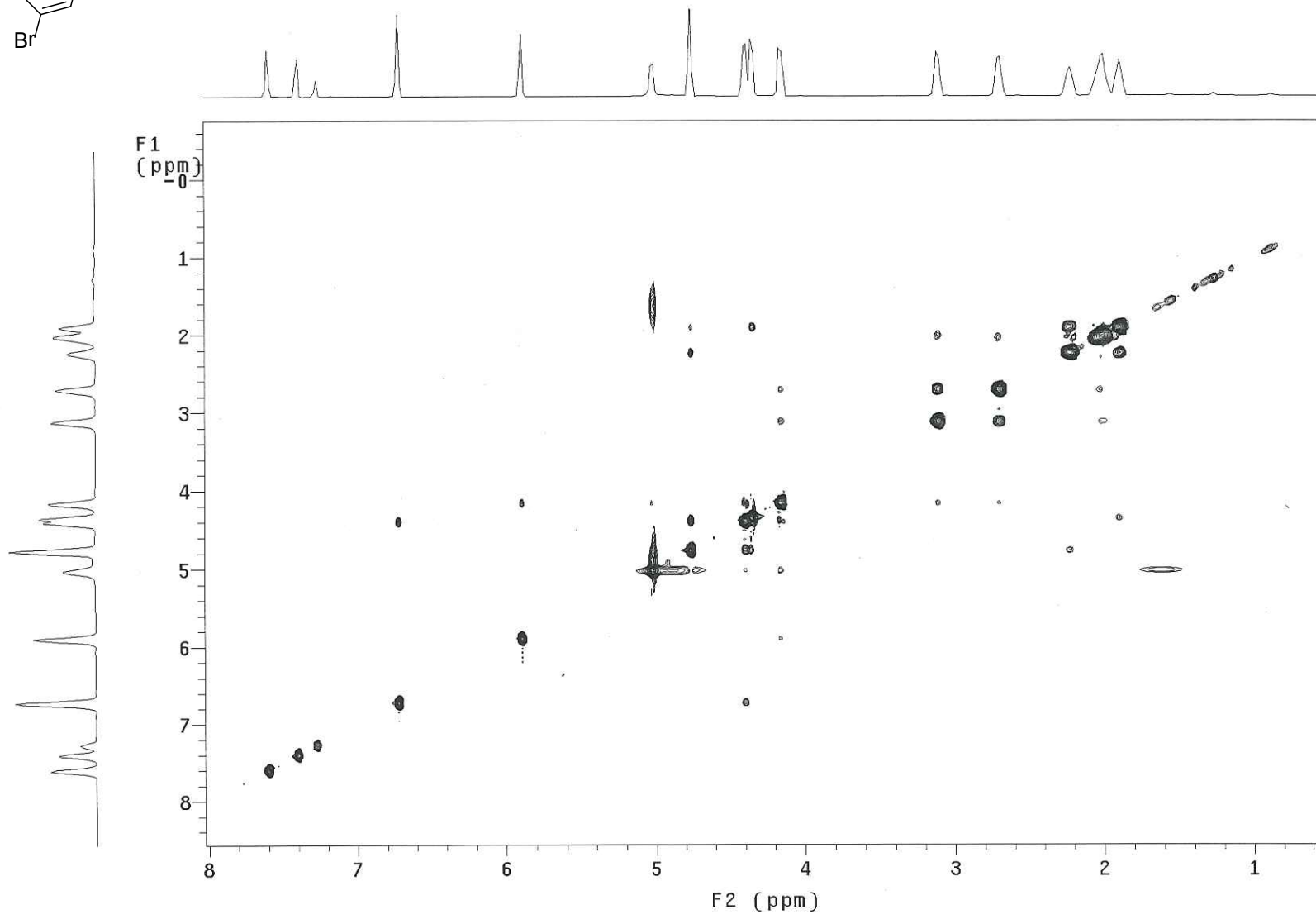
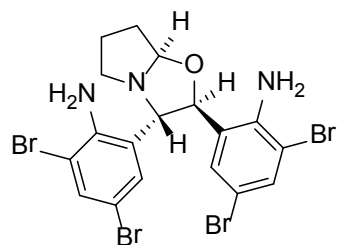
$^1\text{H}$  NMR of **20** in  $\text{CDCl}_3$



$^{13}\text{C}$  NMR of **20** in  $\text{CDCl}_3$

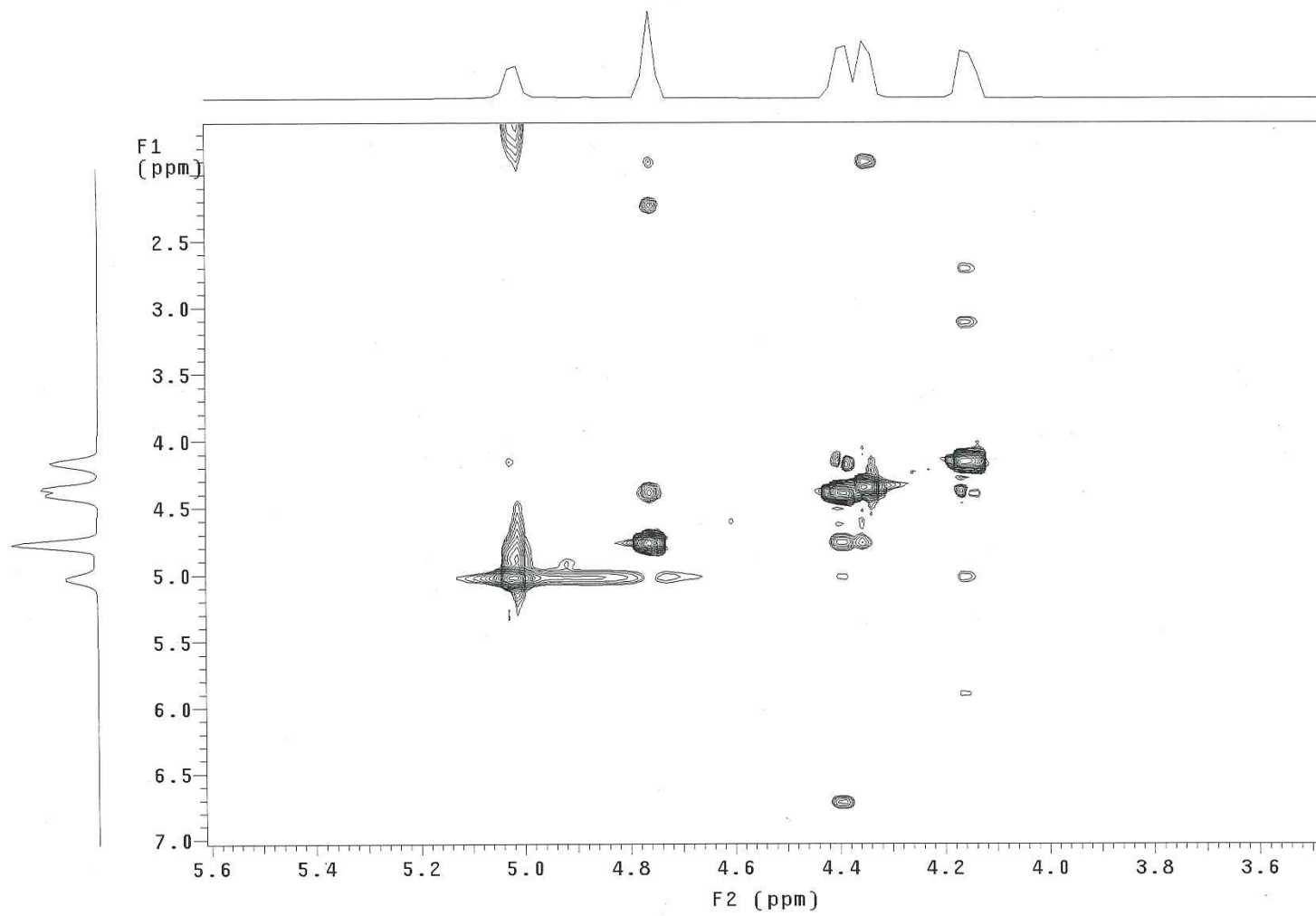
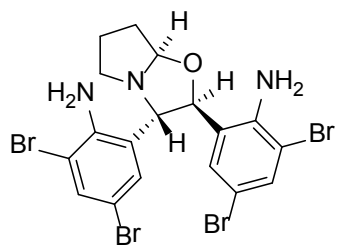


NOESY of **20** in CDCl<sub>3</sub>

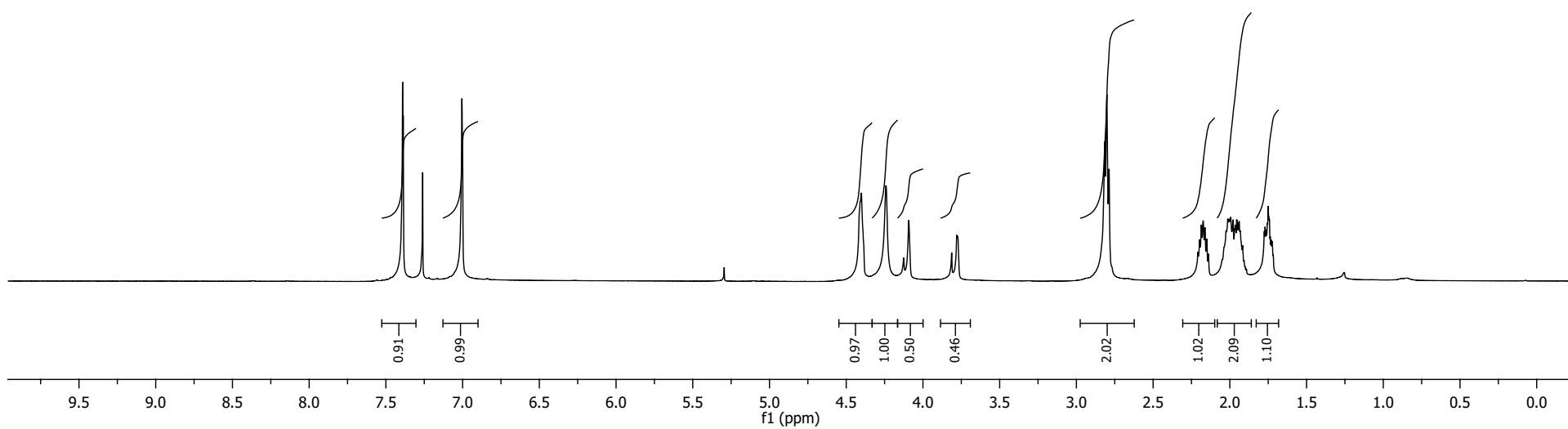
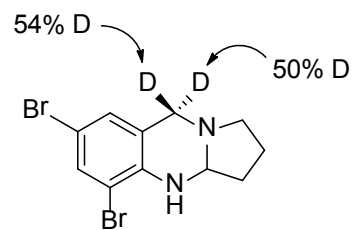




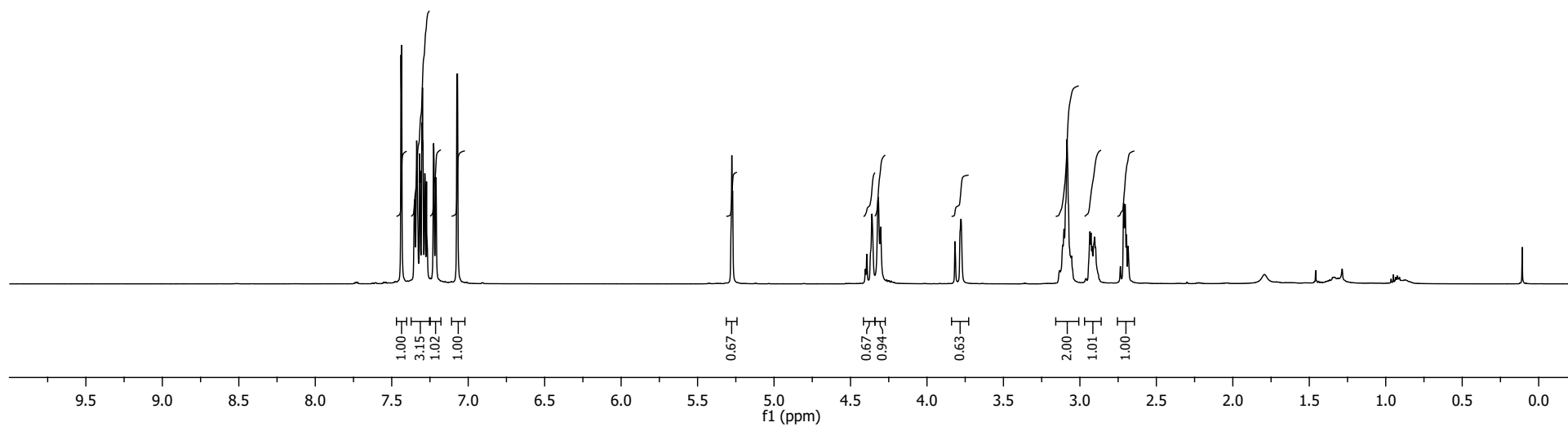
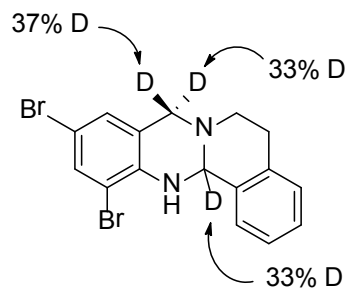
NOESY of **20** in CDCl<sub>3</sub> (zoomed)



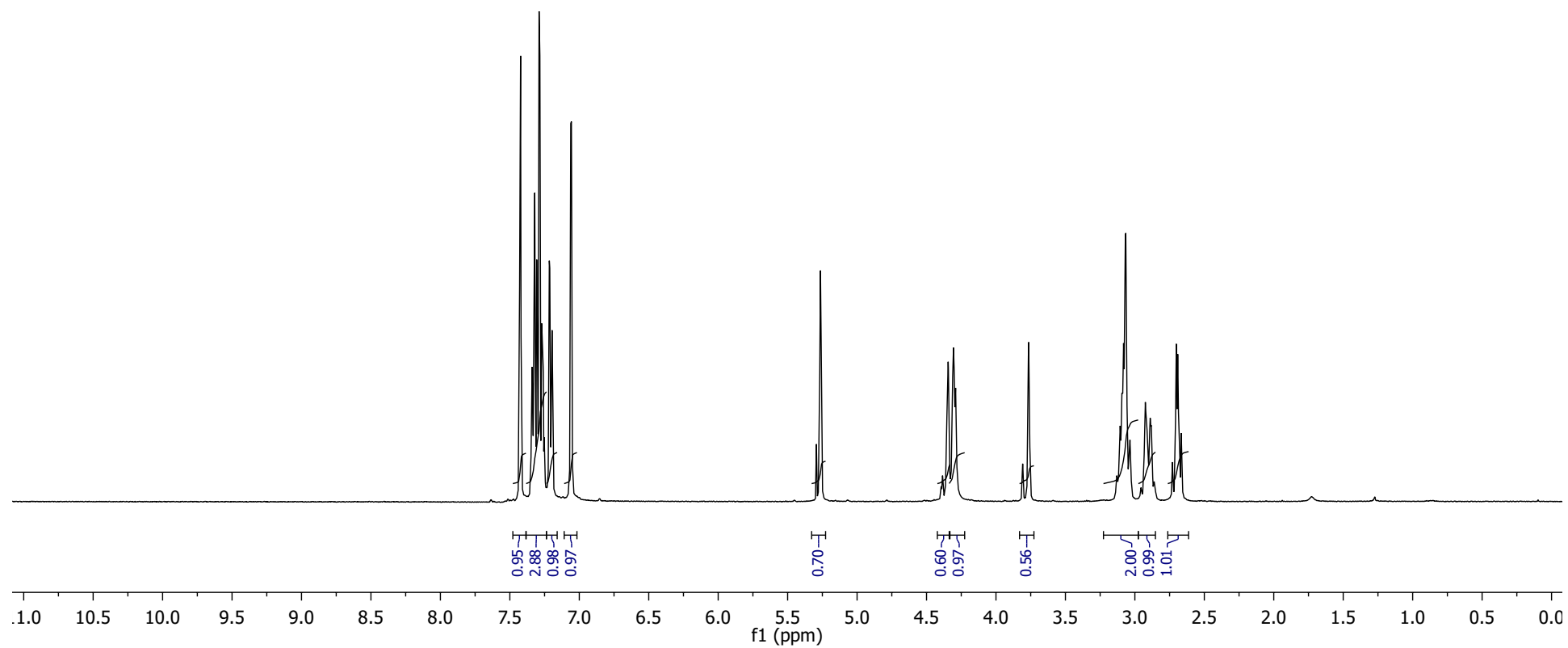
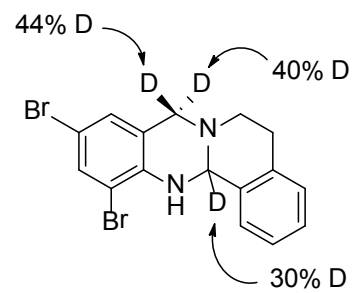
$^1\text{H}$  NMR of **2a-6** in  $\text{CDCl}_3$



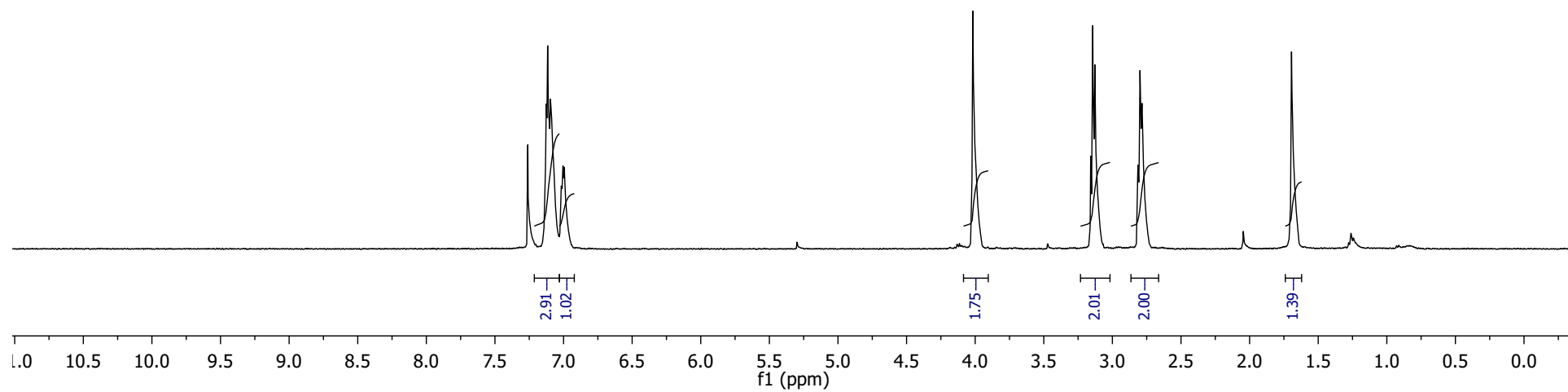
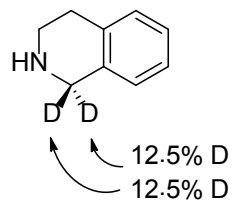
$^1\text{H}$  NMR of **2e-7** in  $\text{CDCl}_3$



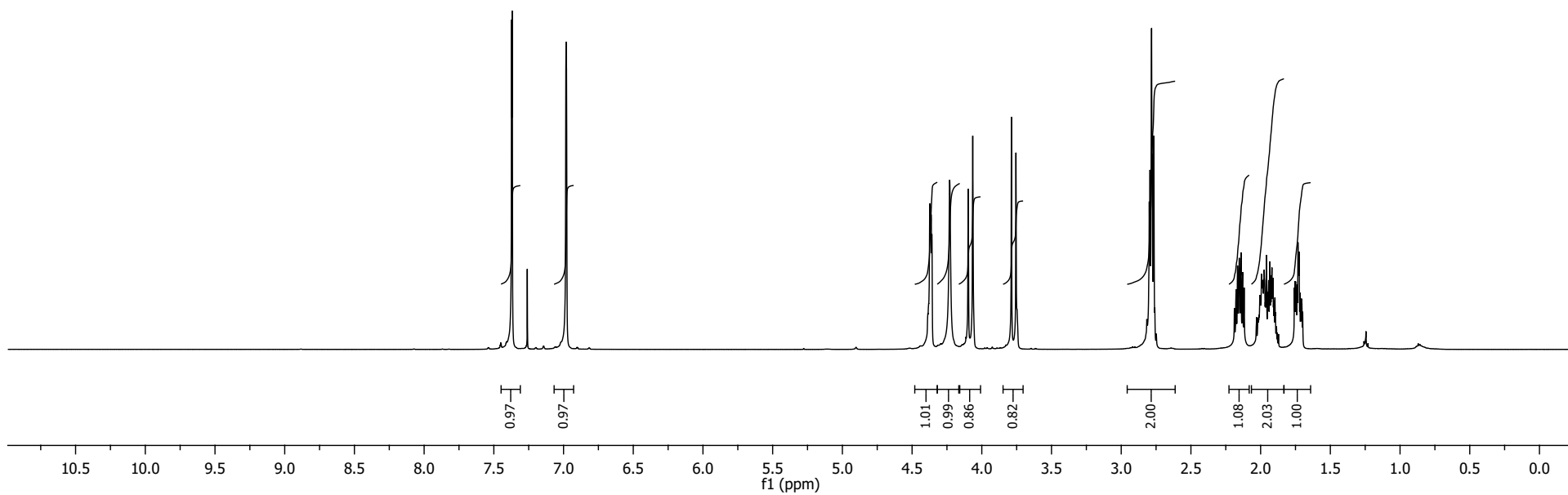
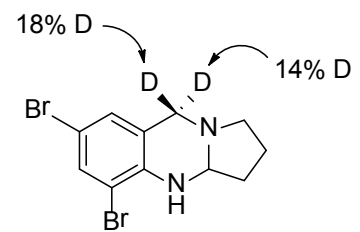
$^1\text{H}$  NMR of **2e-8** in  $\text{CDCl}_3$



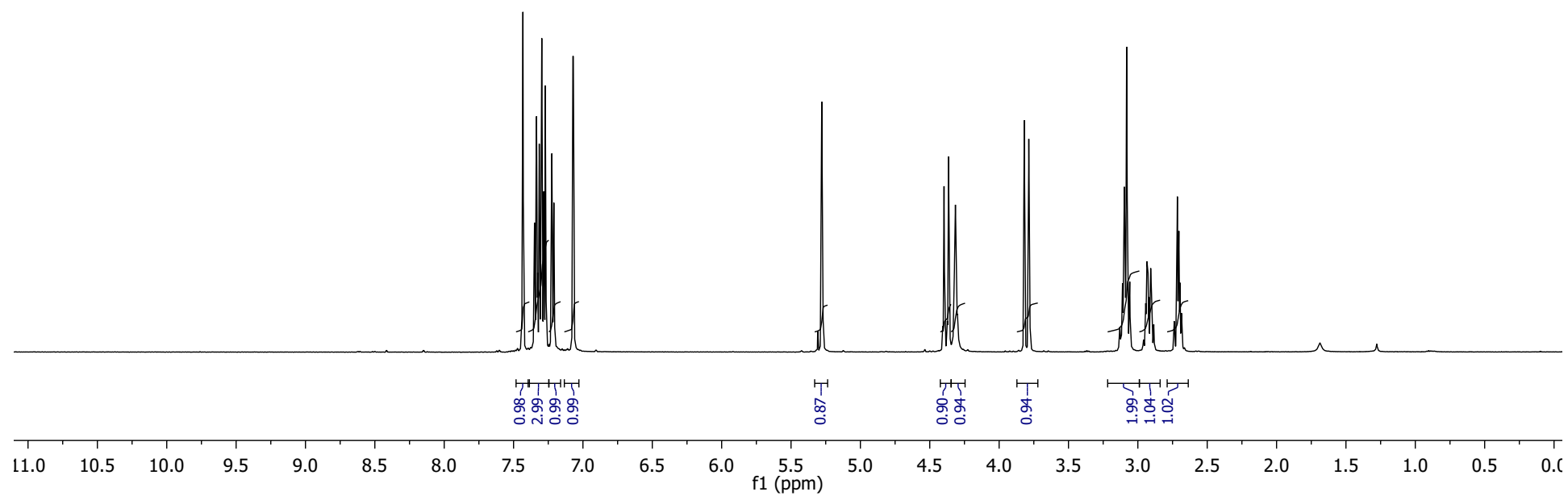
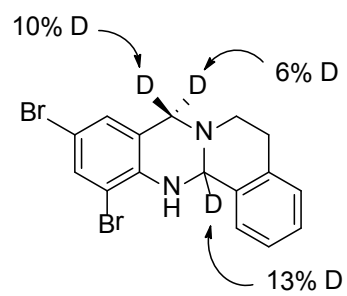
$^1\text{H}$  NMR of **THIQ-d** in  $\text{CDCl}_3$



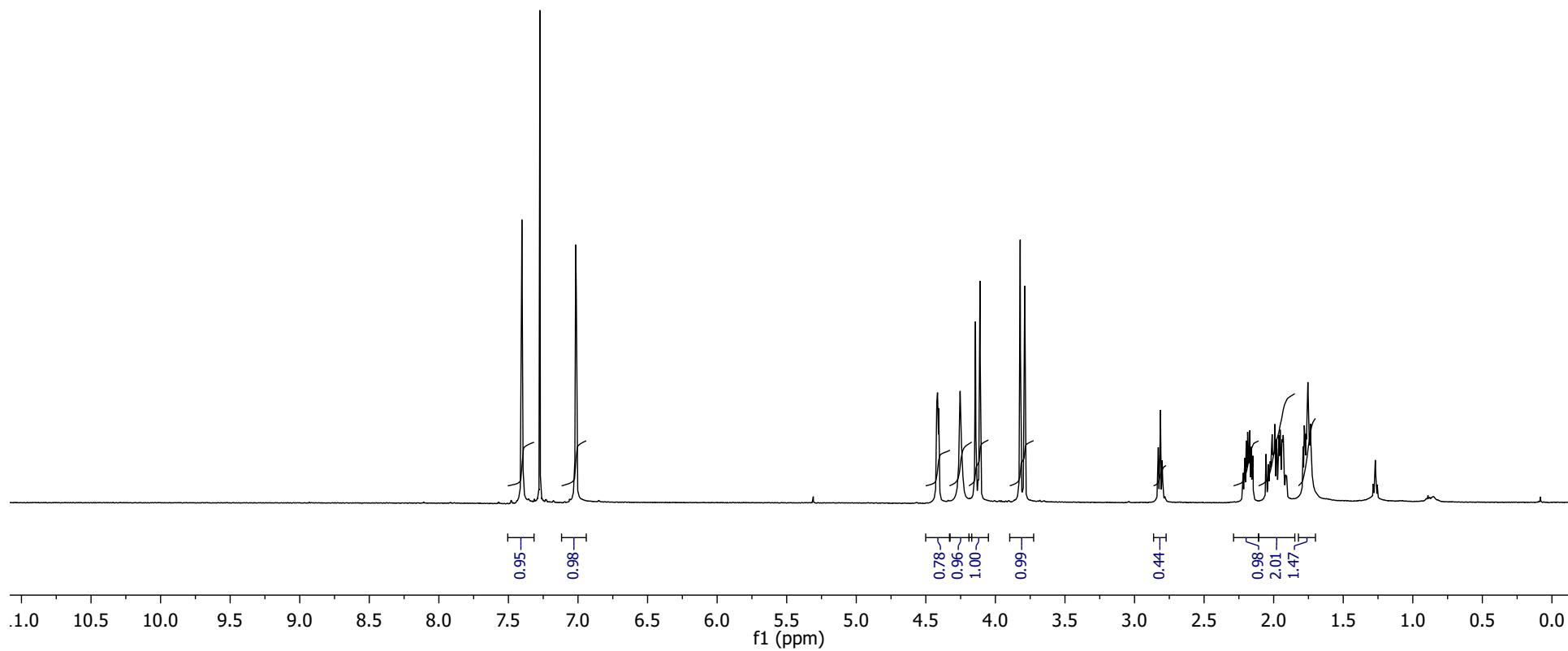
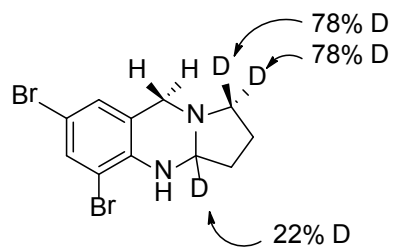
$^1\text{H}$  NMR of **2a-9** in  $\text{CDCl}_3$



$^1\text{H}$  NMR of **2e-10** in  $\text{CDCl}_3$

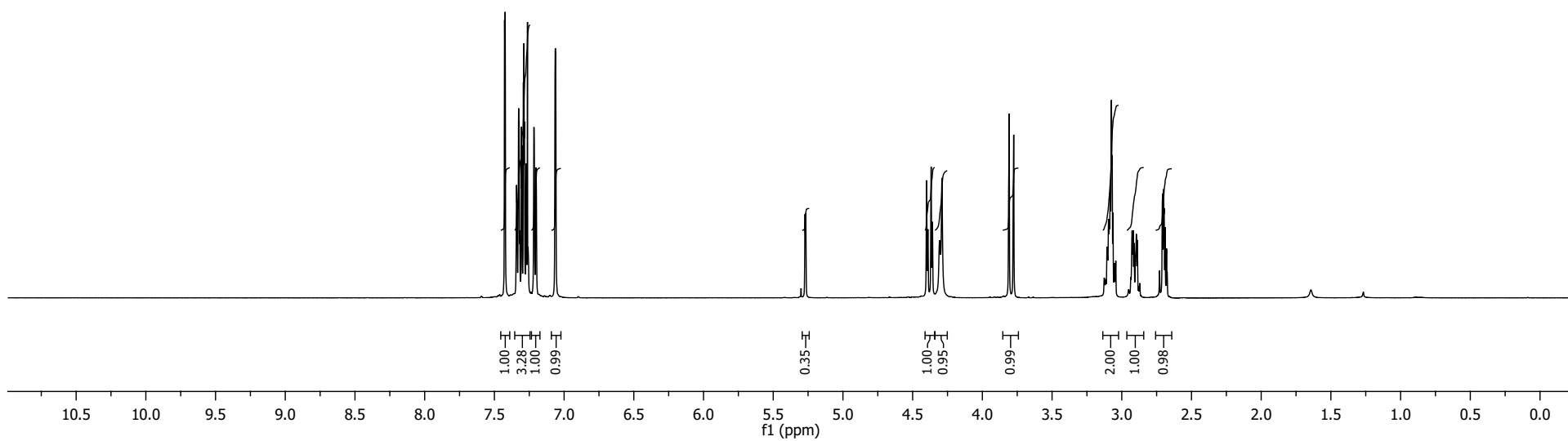
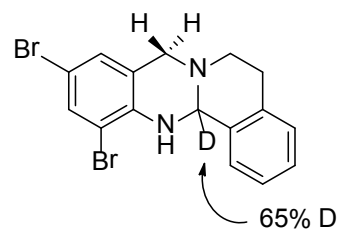


$^1\text{H}$  NMR of **2a-11** in  $\text{CDCl}_3$





$^1\text{H}$  NMR of **2e-12** in  $\text{CDCl}_3$



$^1\text{H}$  NMR of **2e-13** in  $\text{CDCl}_3$

