

A Functional Myoglobin Model Composed of a Strapped Porphyrin/Cyclodextrin Supramolecular Complex with an Overhanging COOH That Increases O₂/CO Binding Selectivity in Aqueous Solution

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²*Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes), UMR 6226, Rennes, F-35000, France*

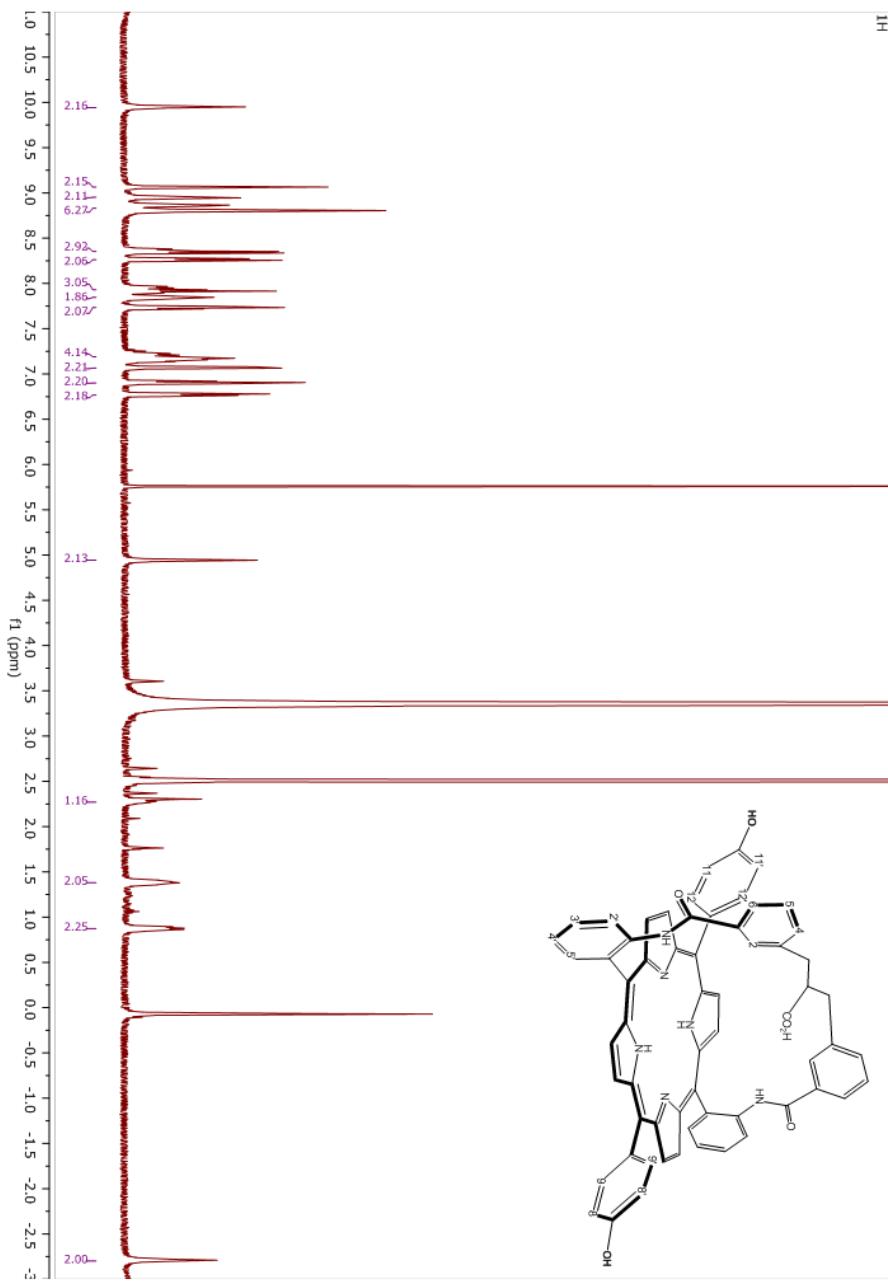
³*Department of Applied Chemistry, Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita 565-0871, Japan*

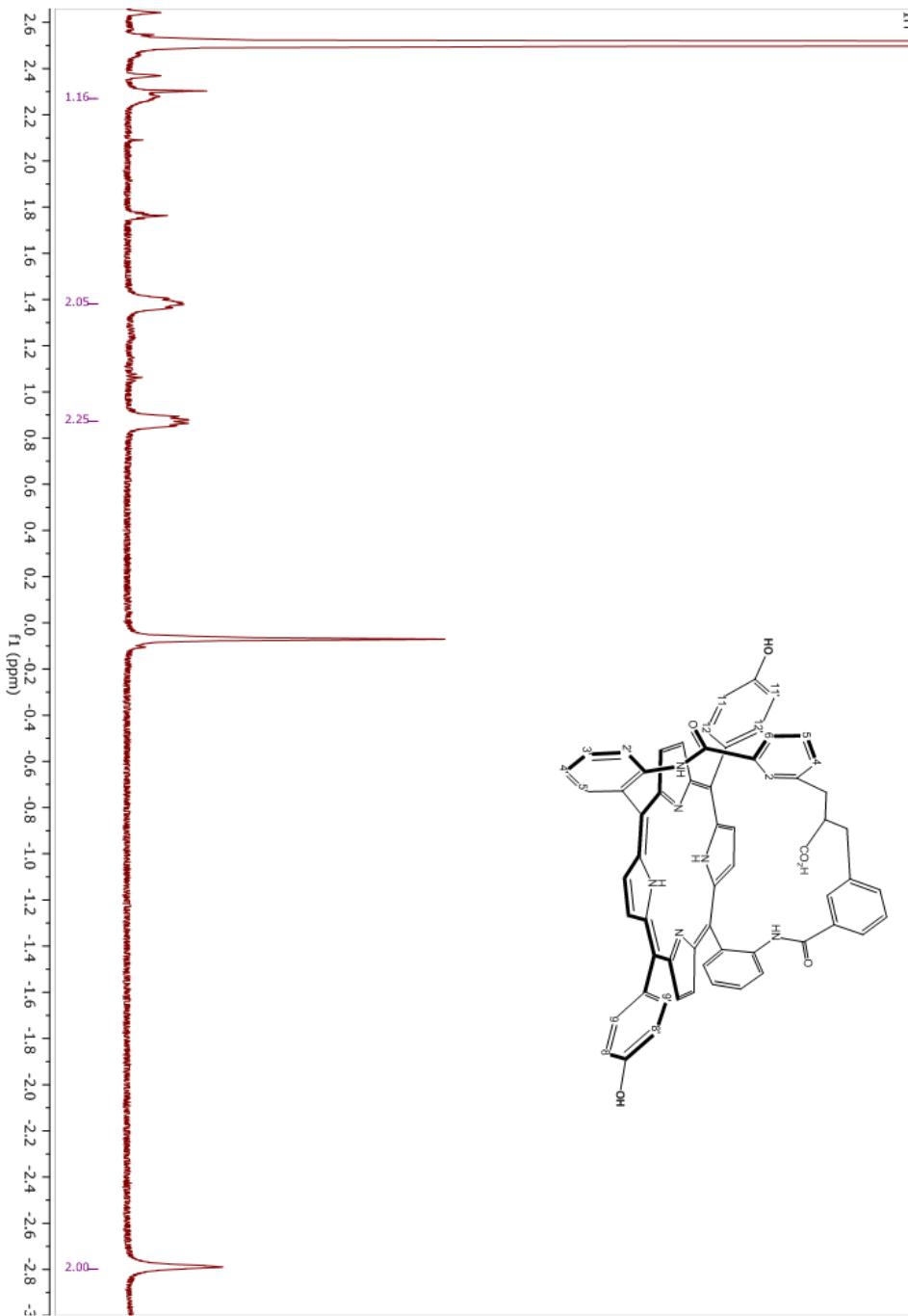
Supplementary Information

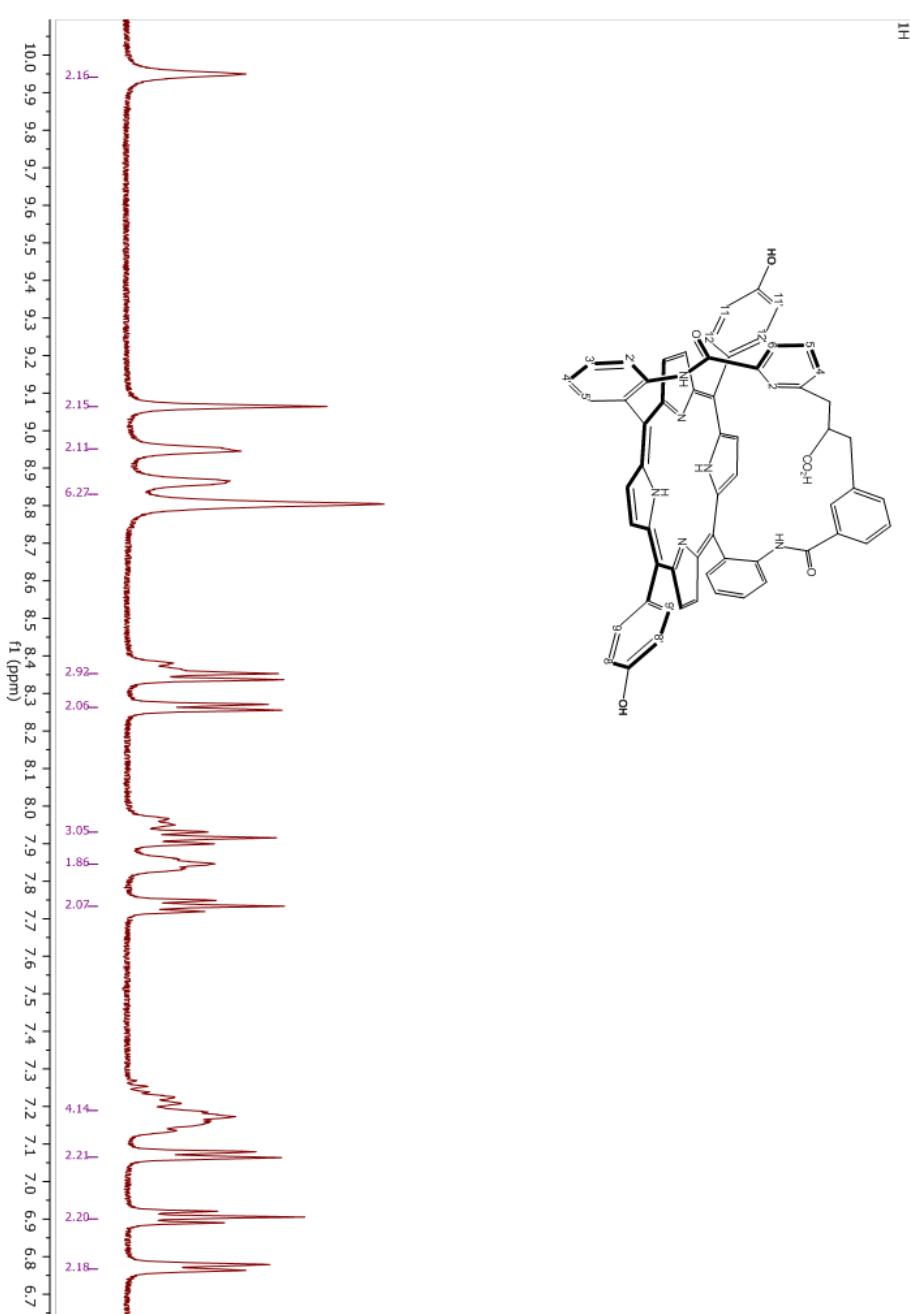
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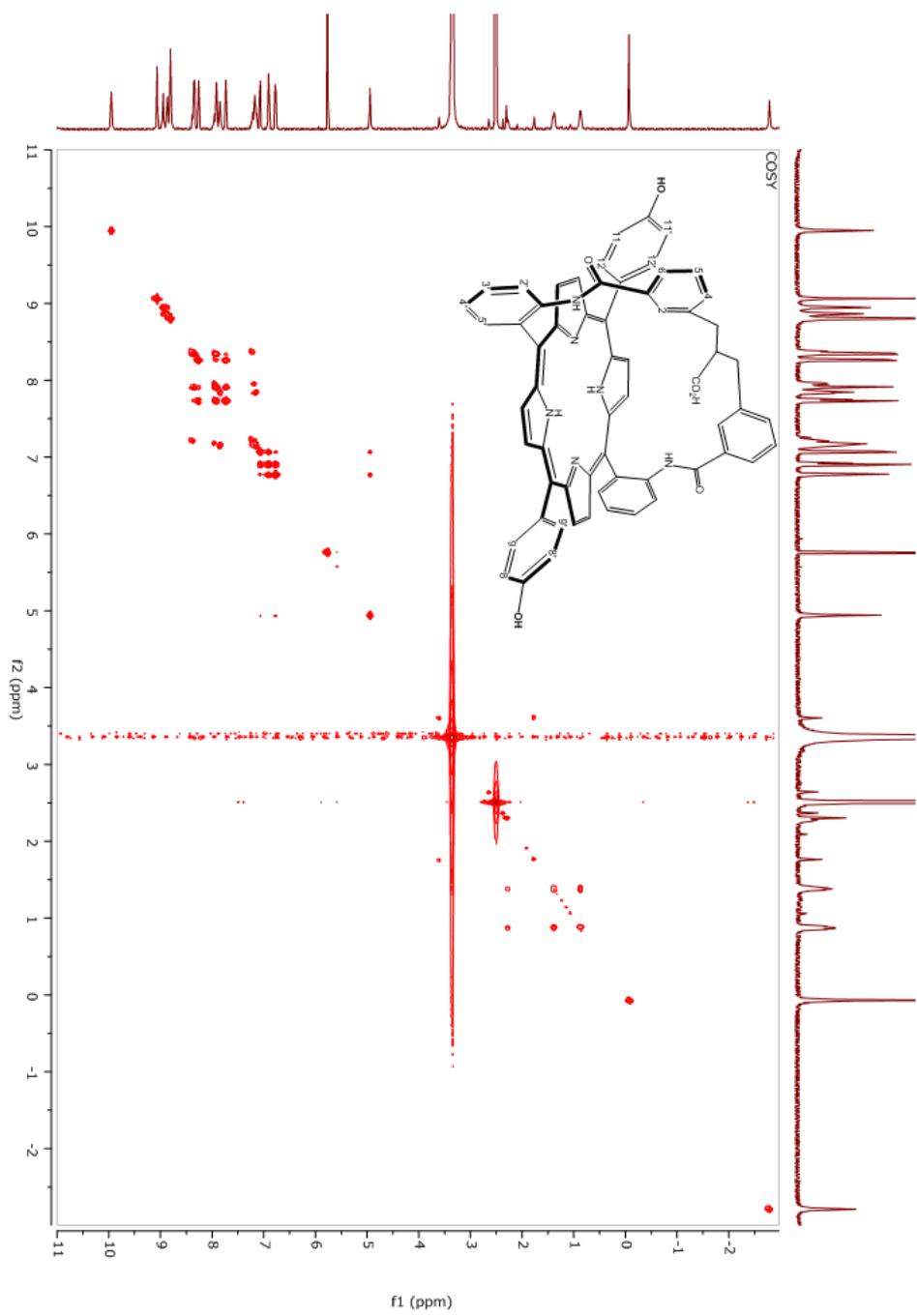
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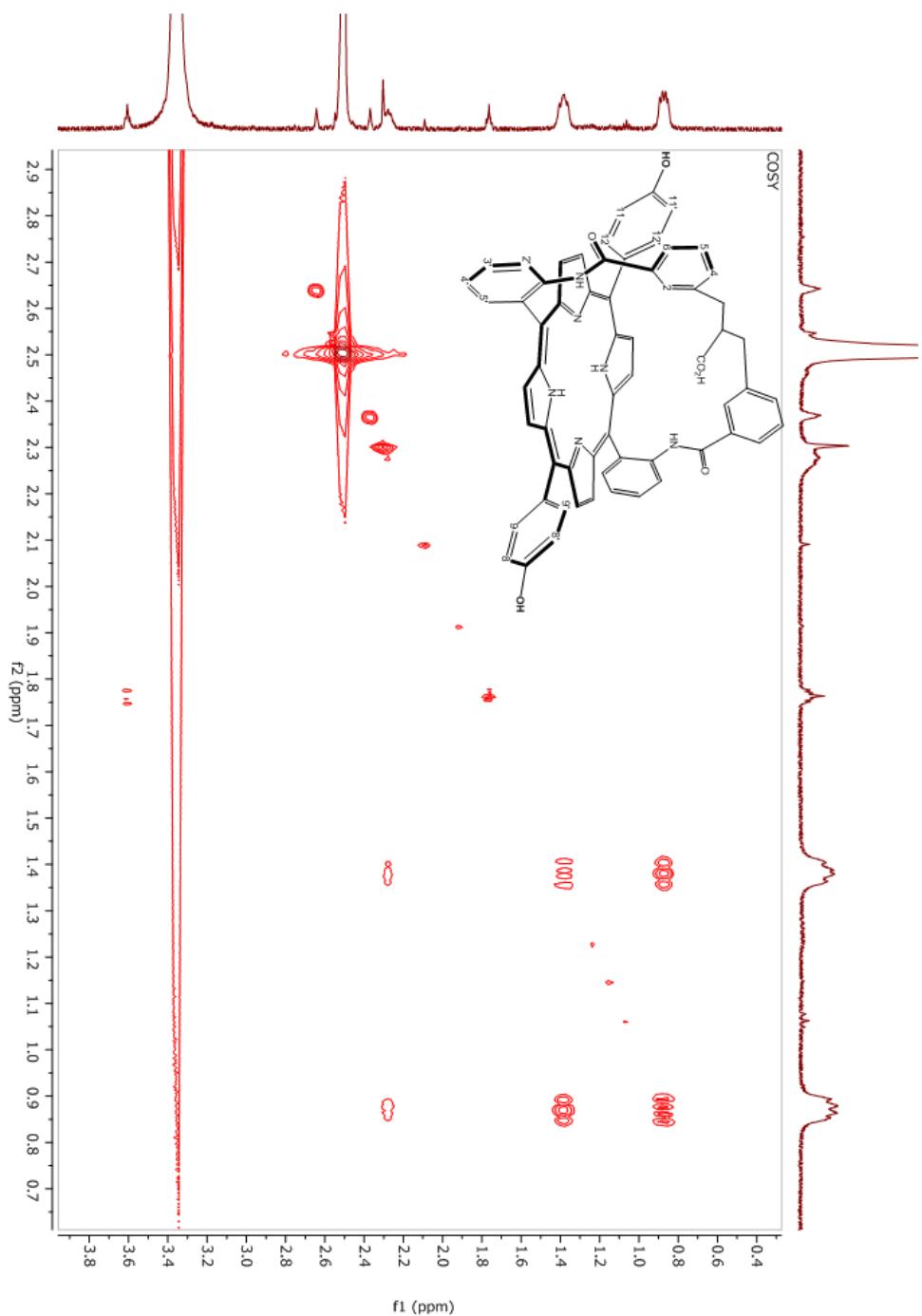
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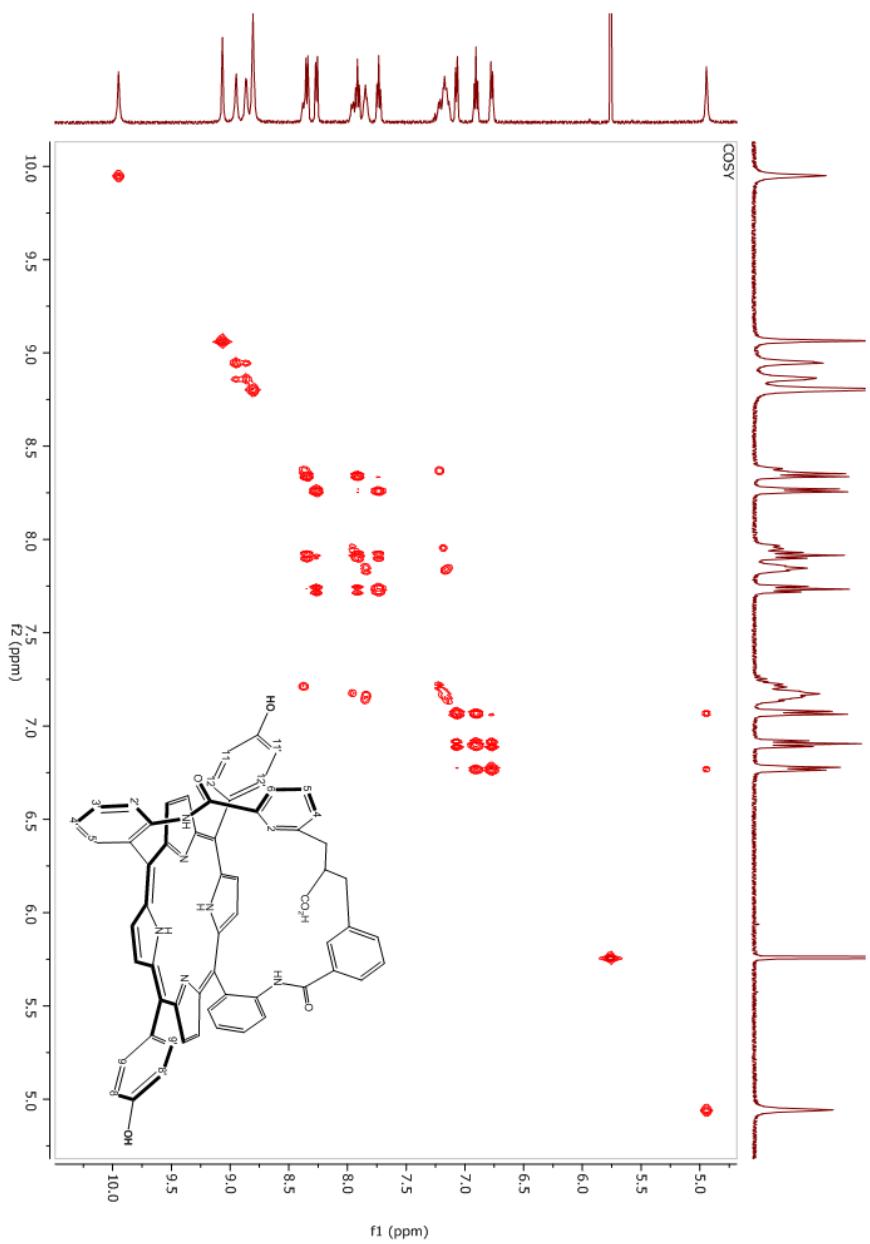


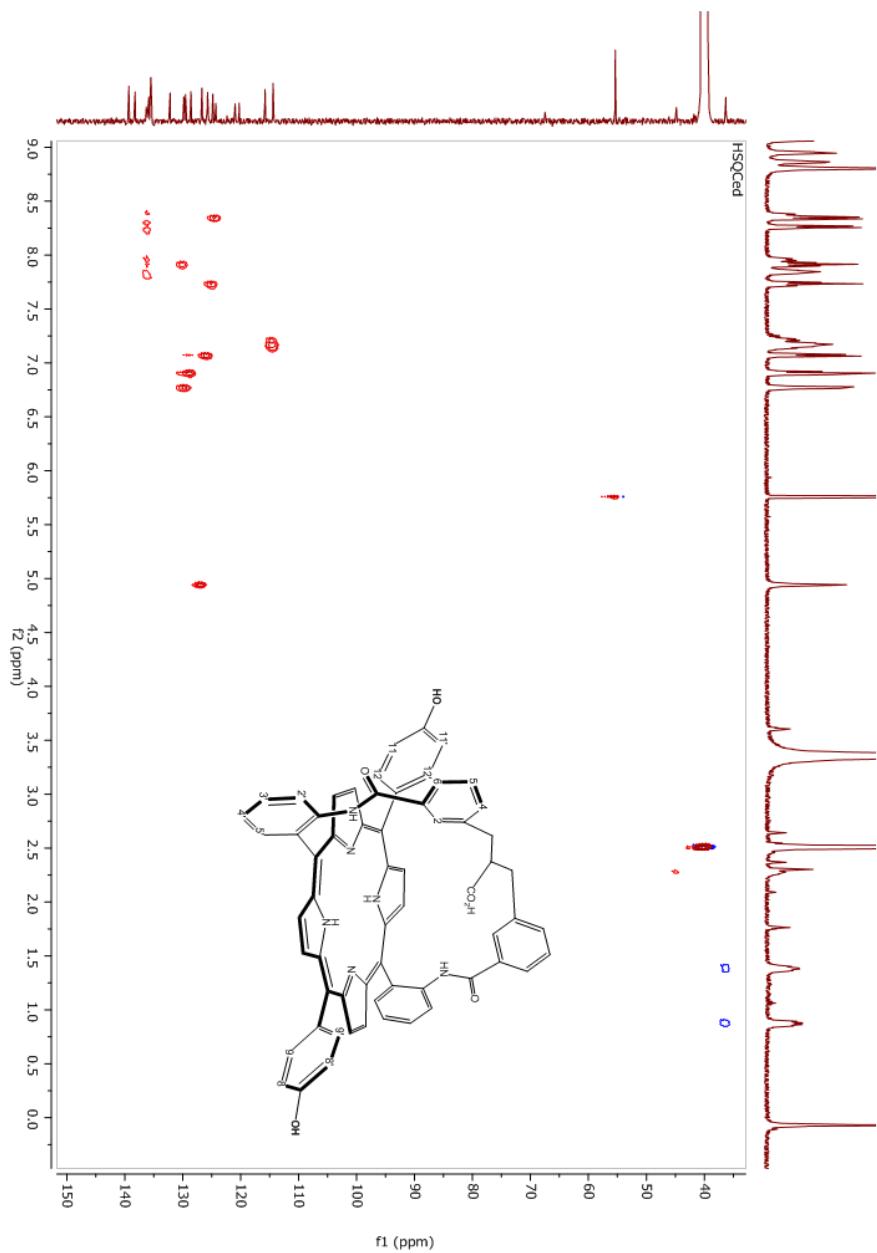


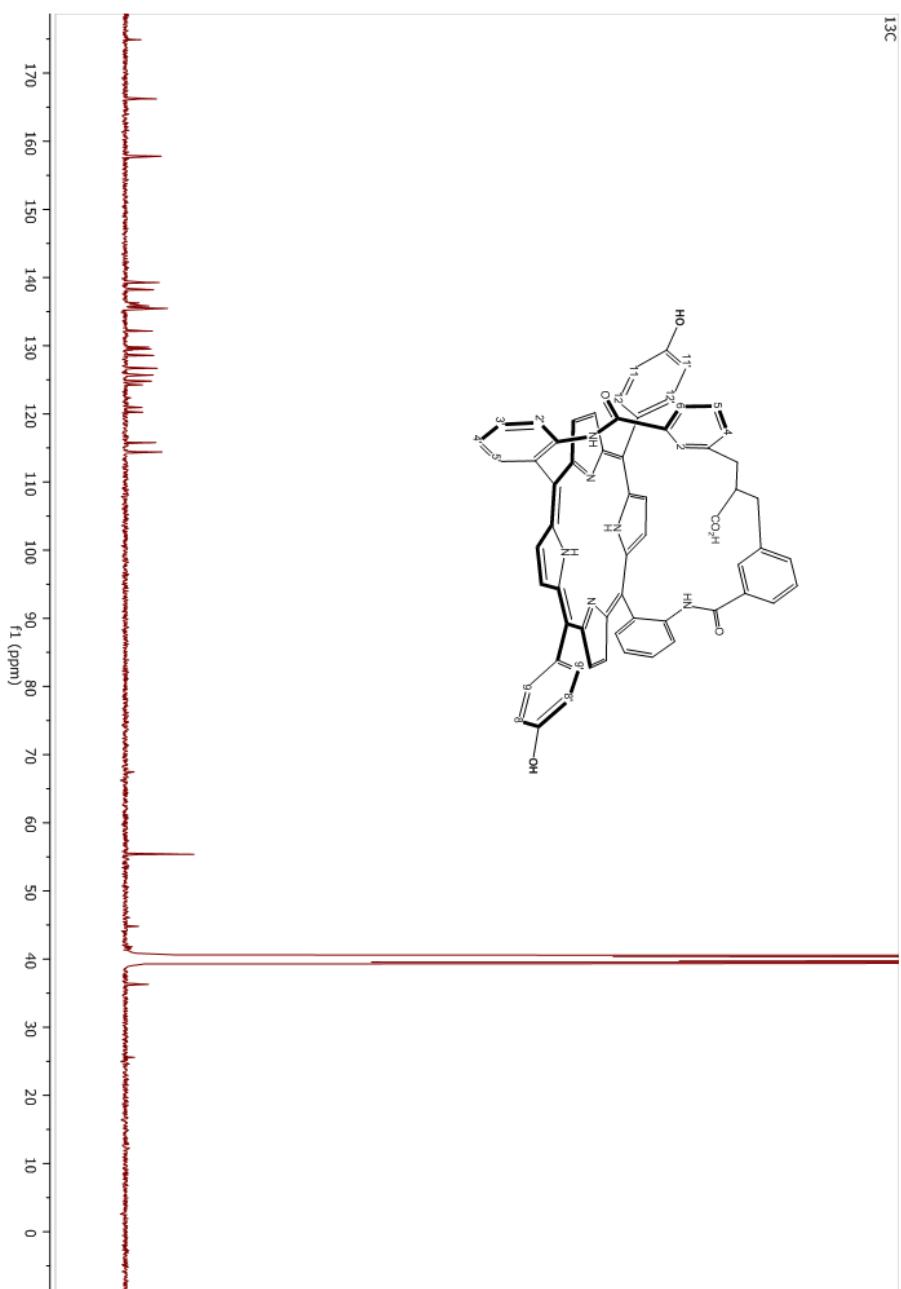




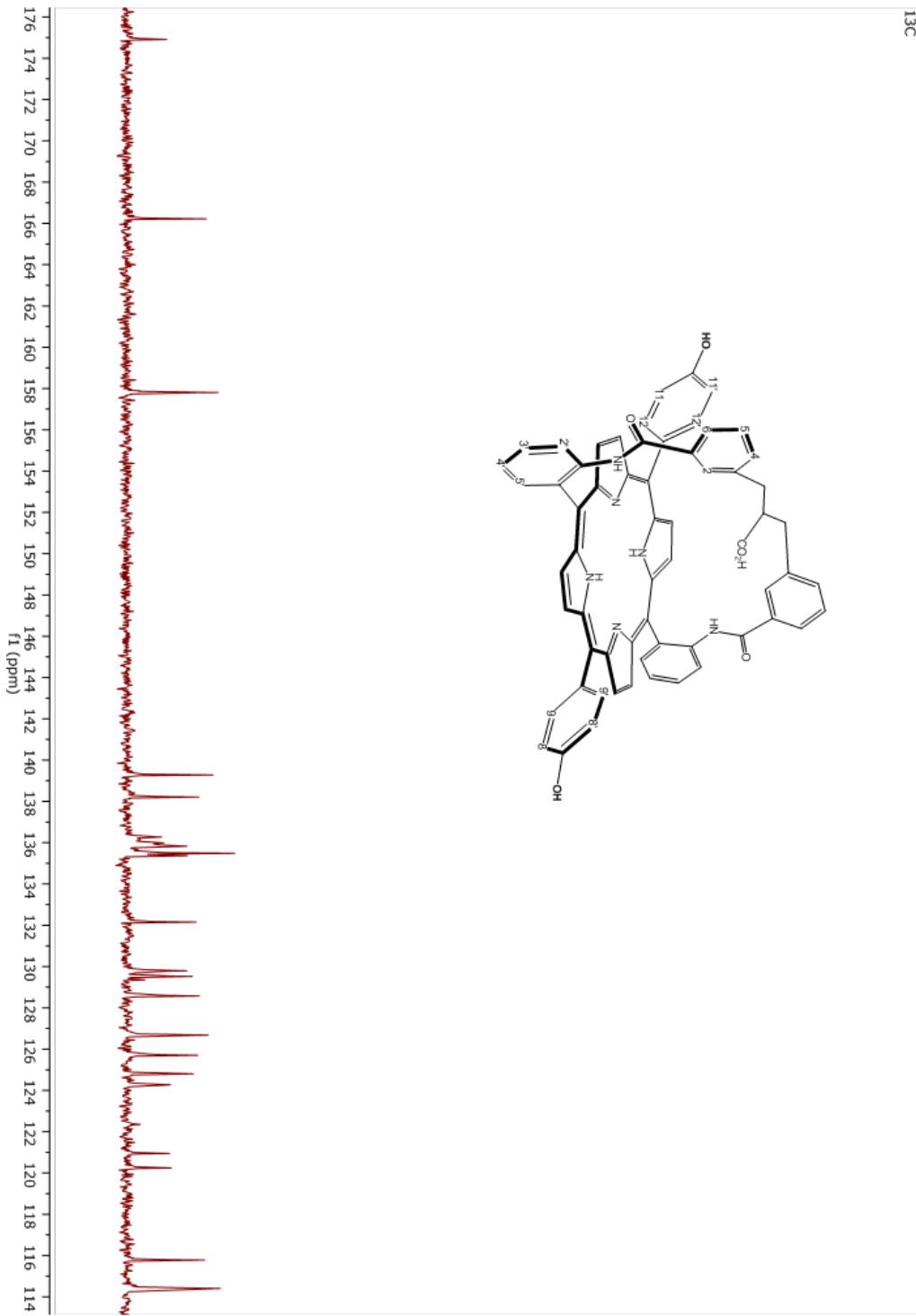








13C



CRMPO

Rapport d'analyse

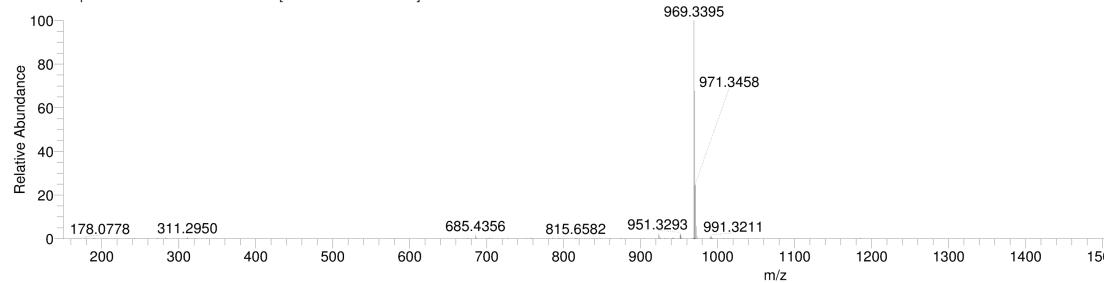
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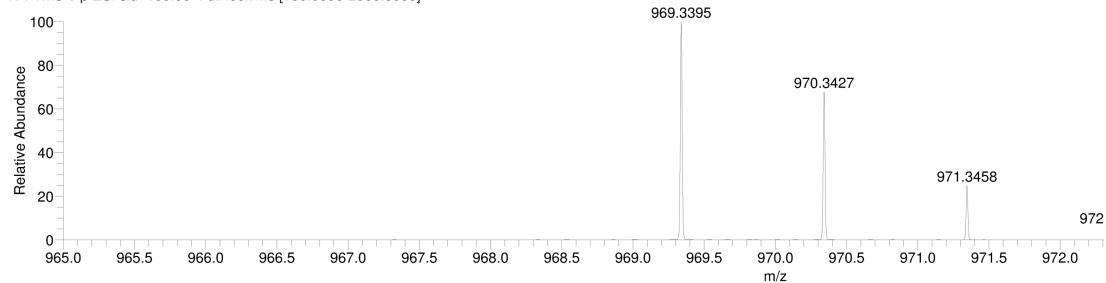
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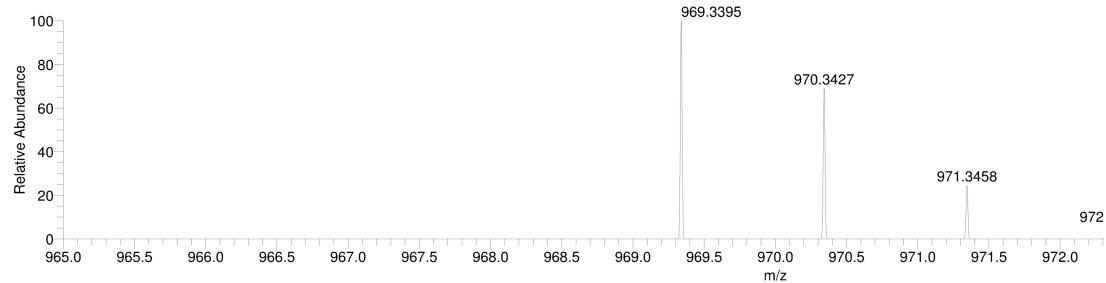
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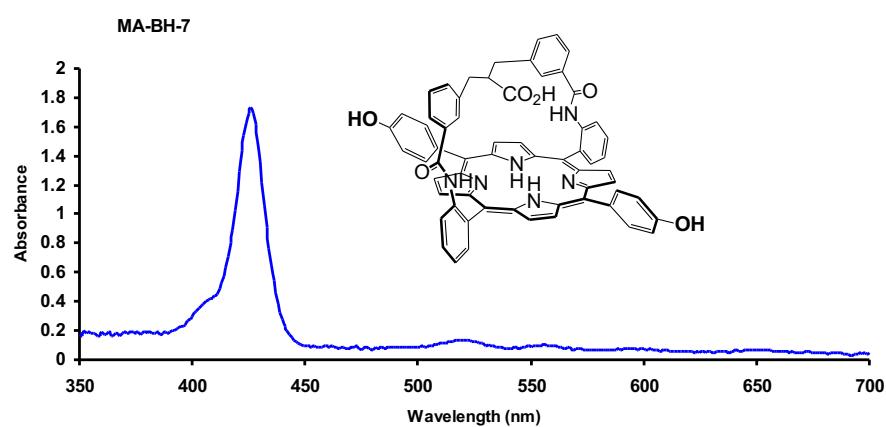


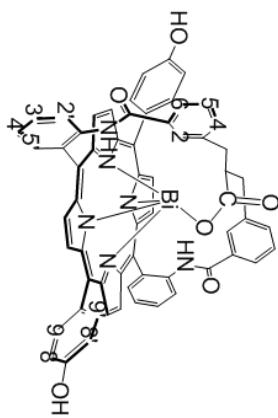
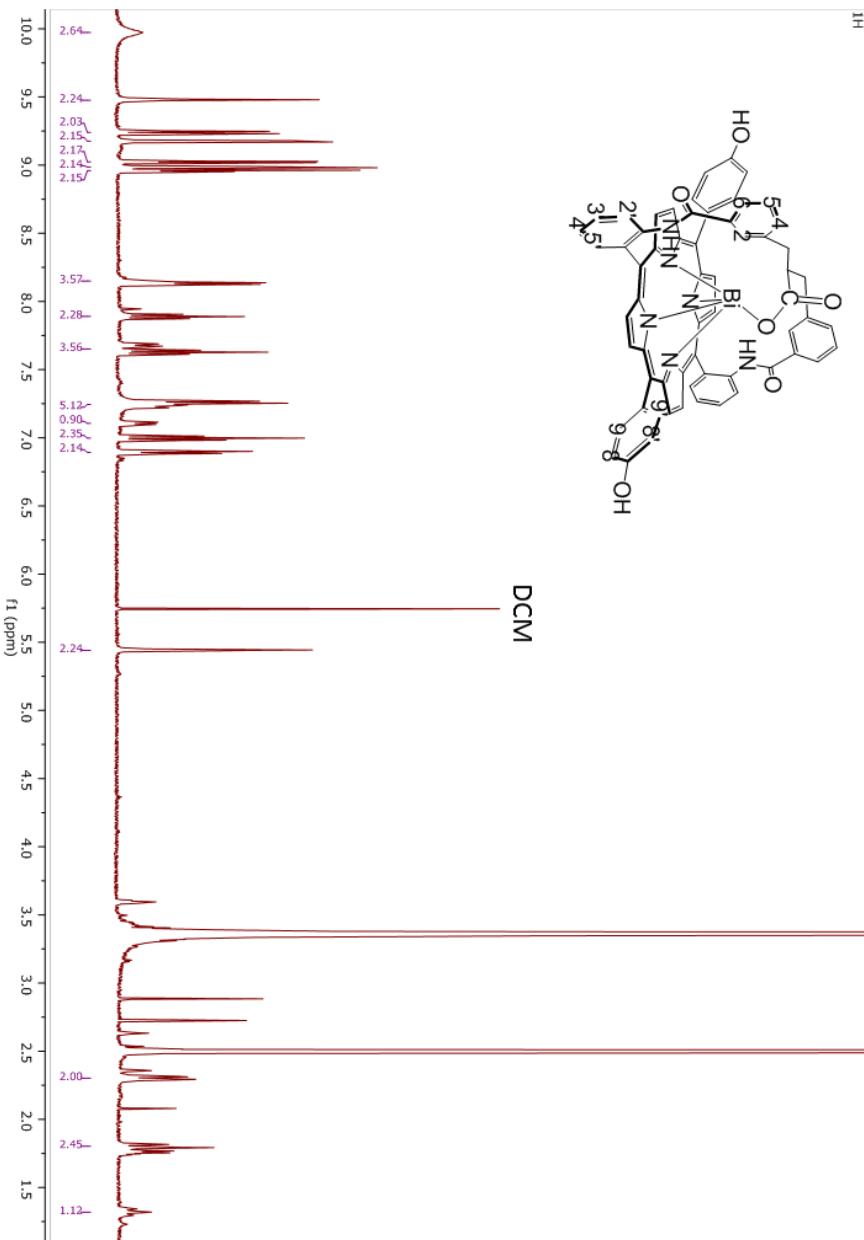
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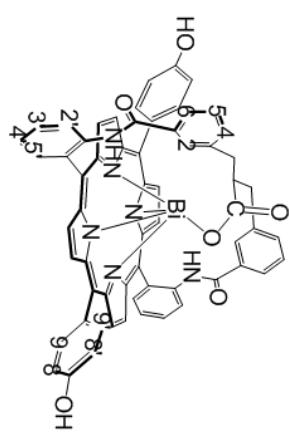
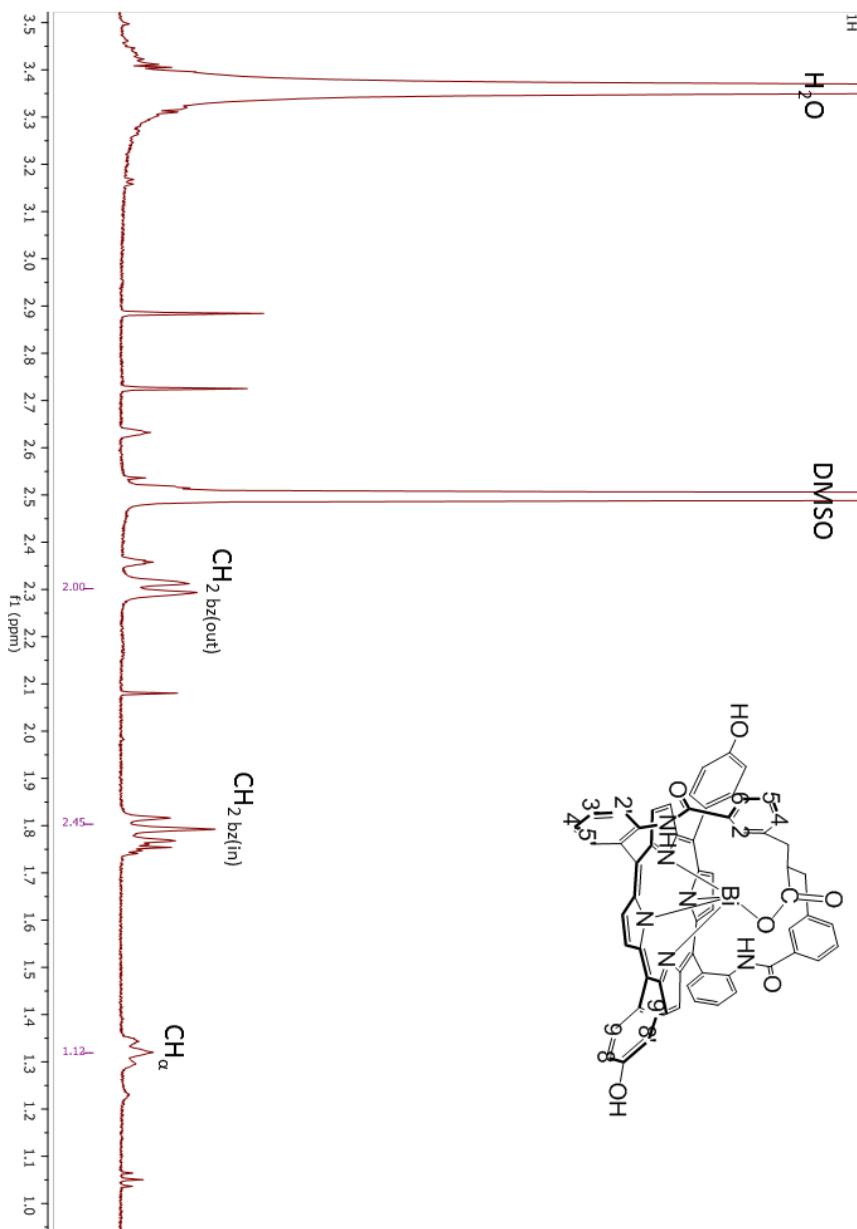


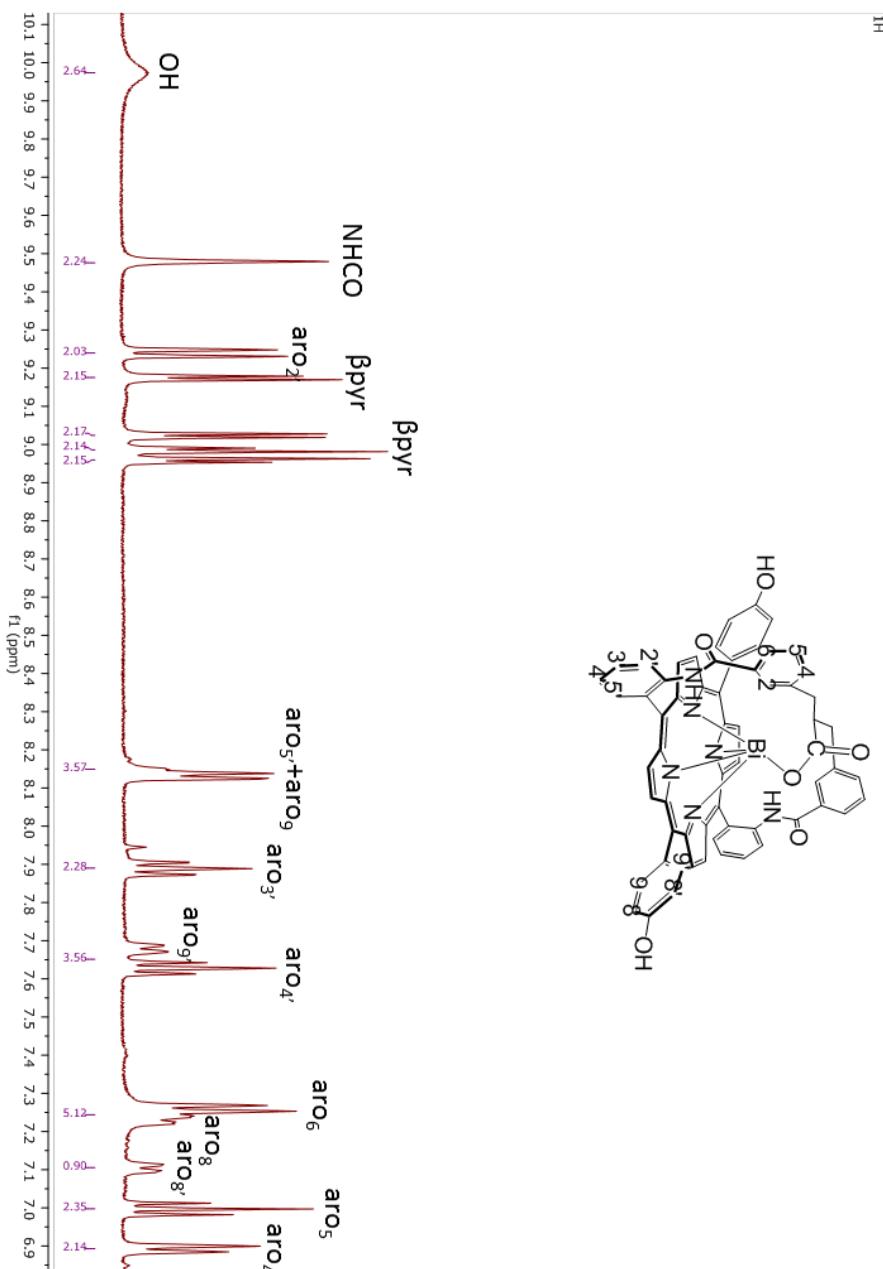
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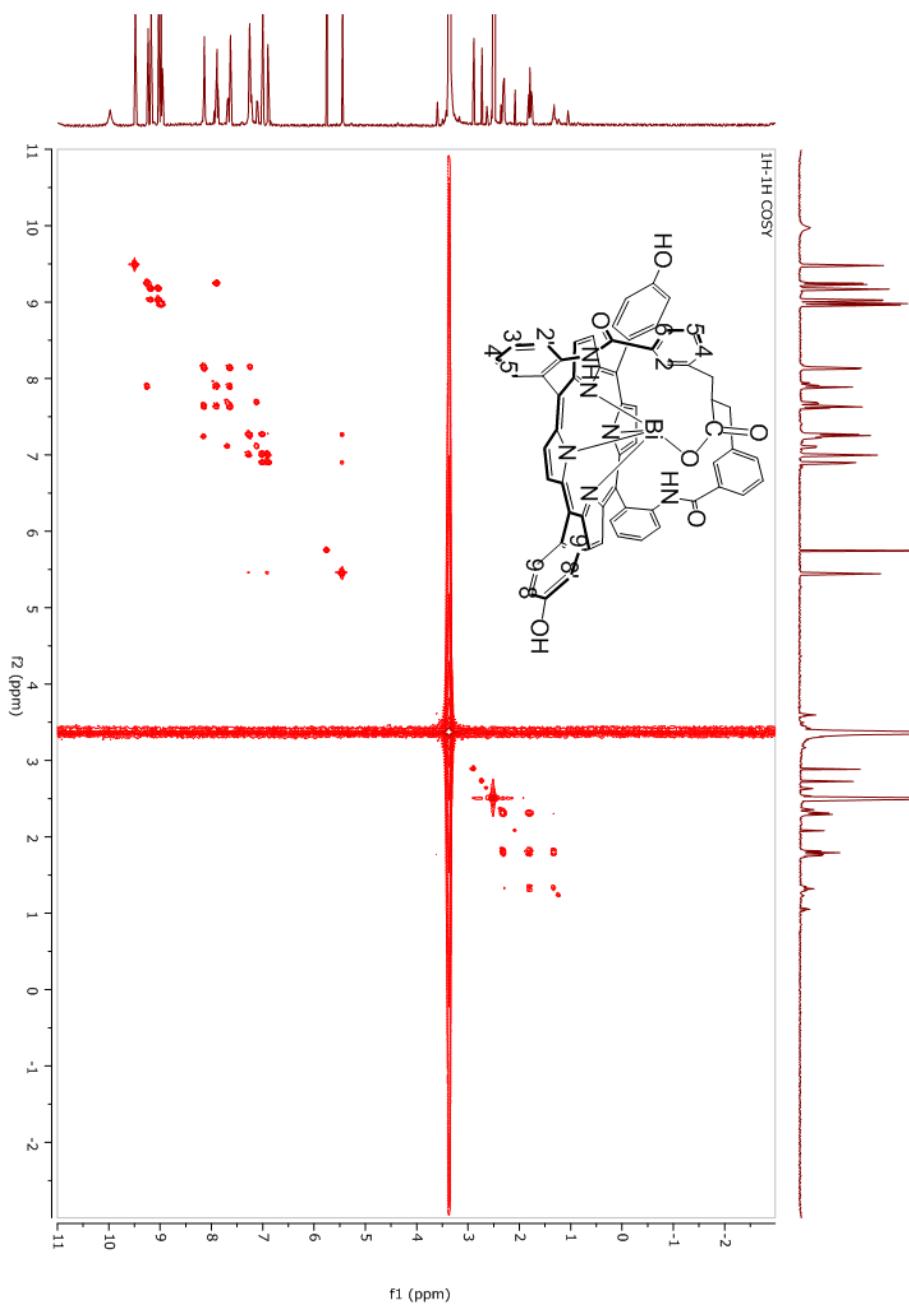


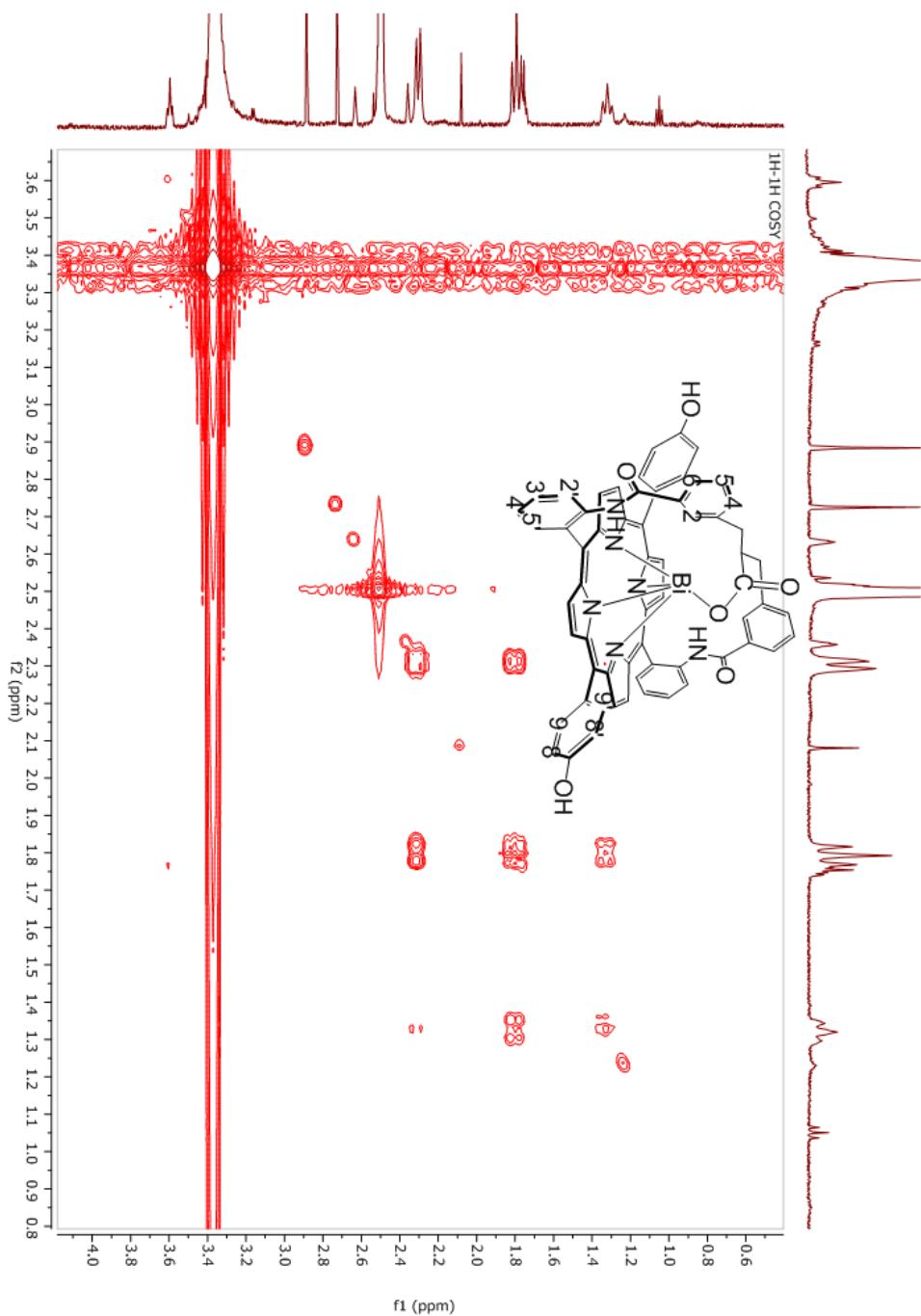


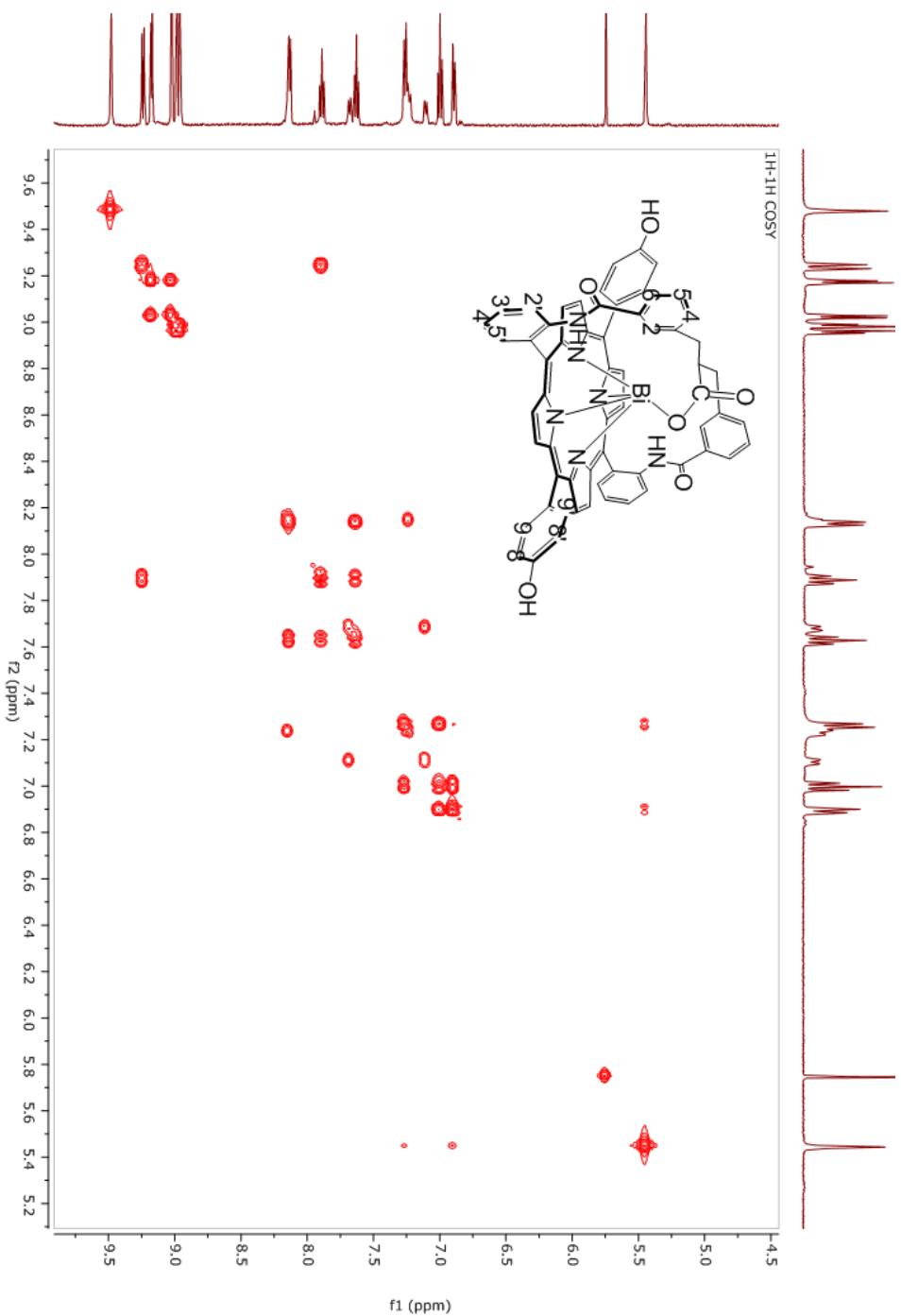


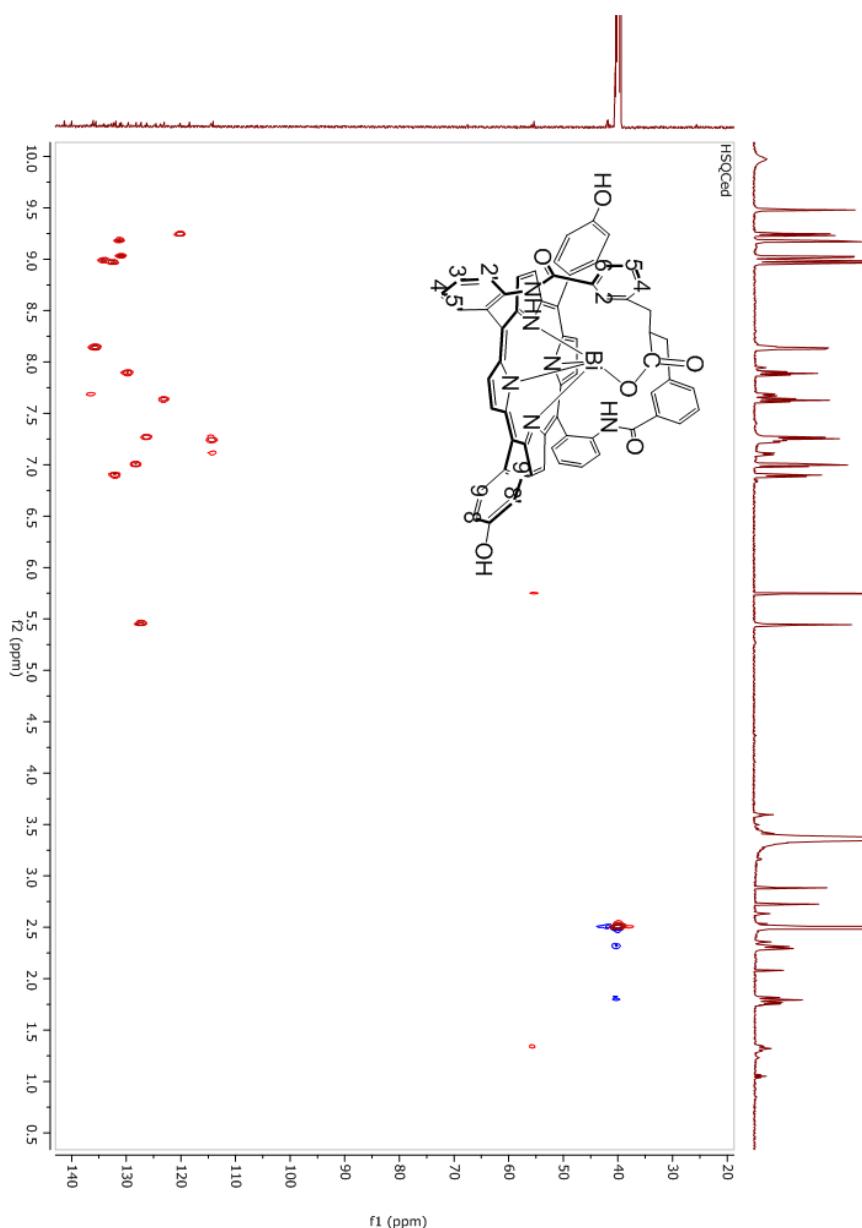


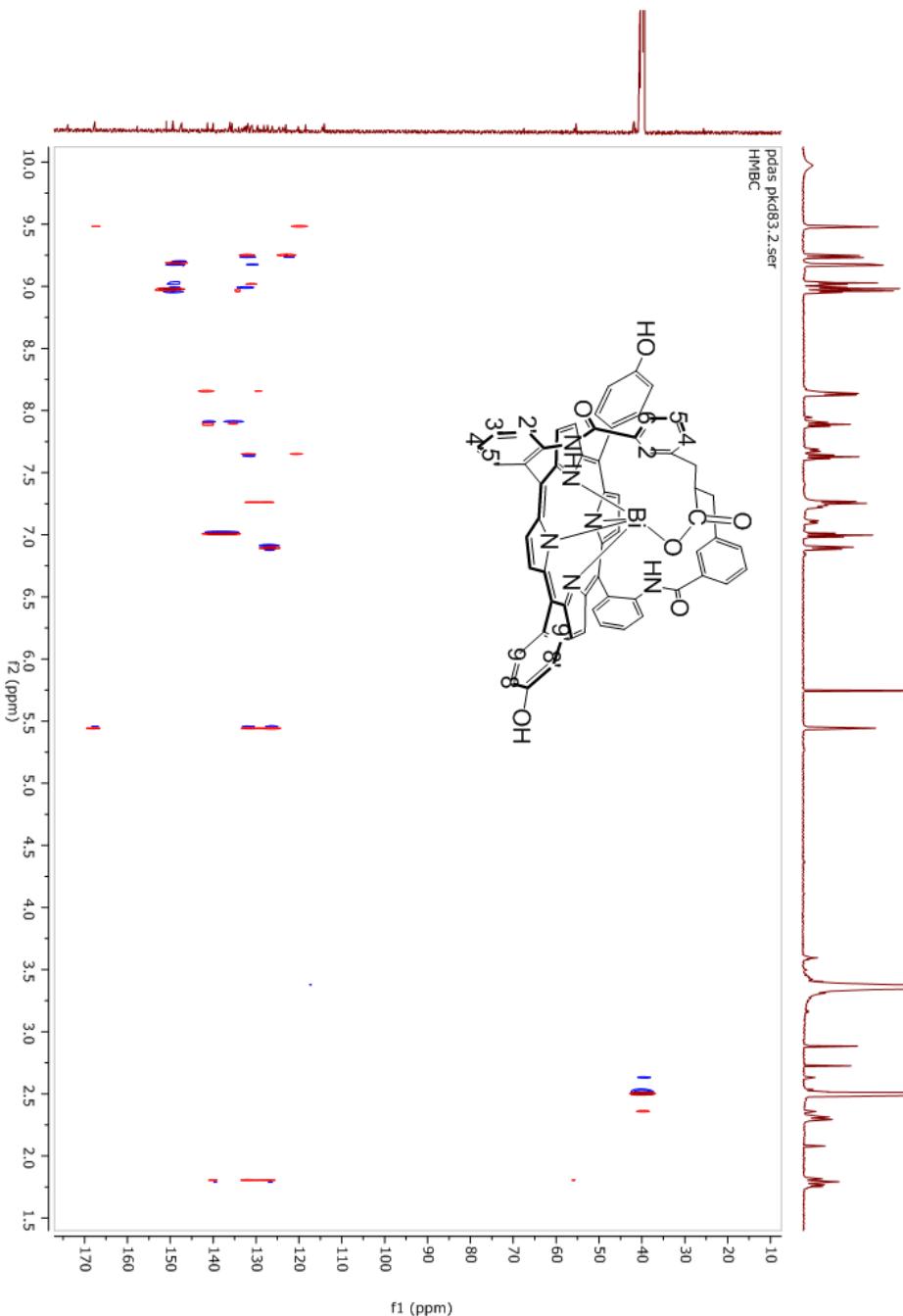


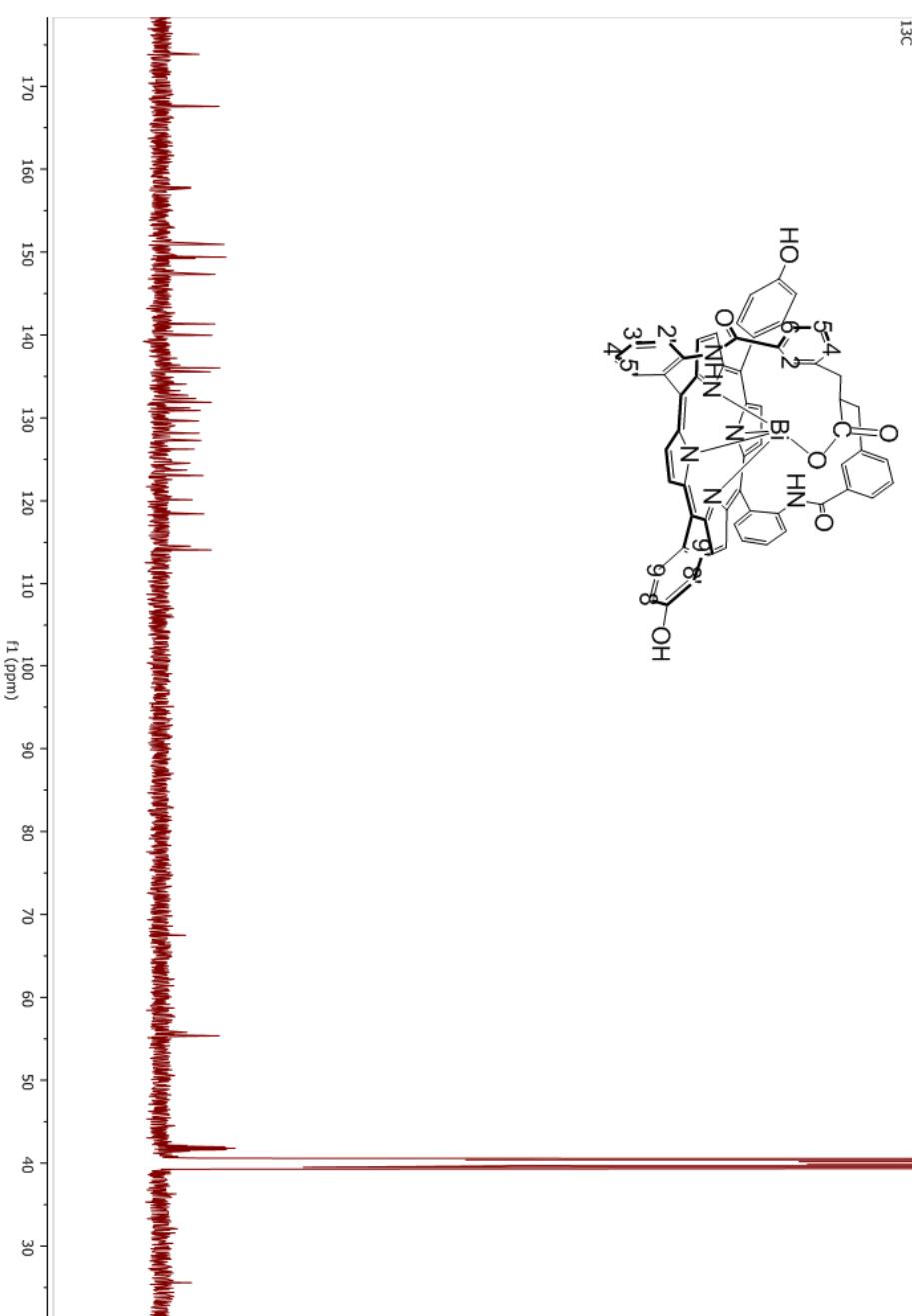




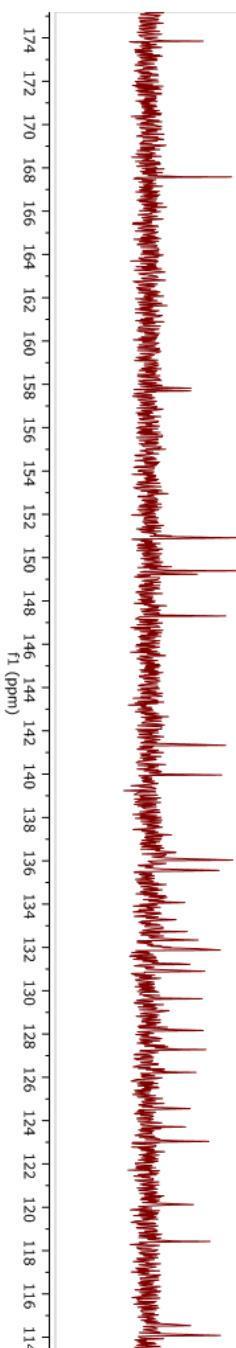
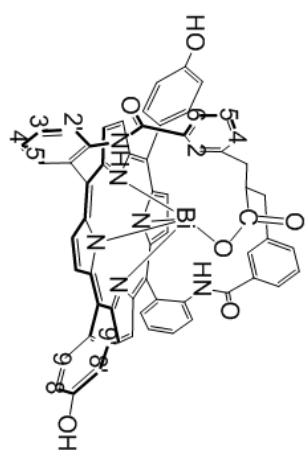








¹³C



CRMPO

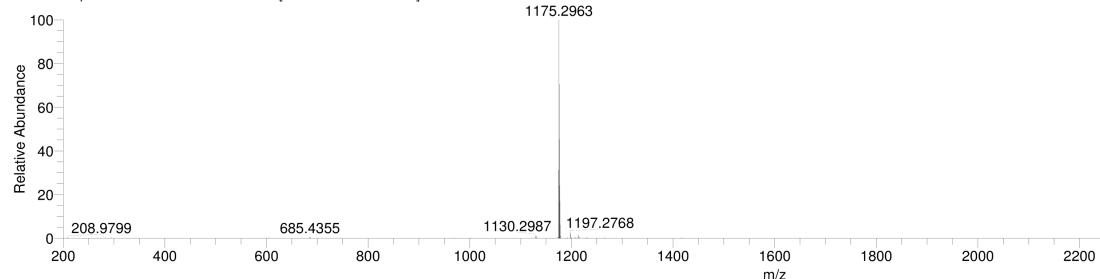
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Rapport d'analyse

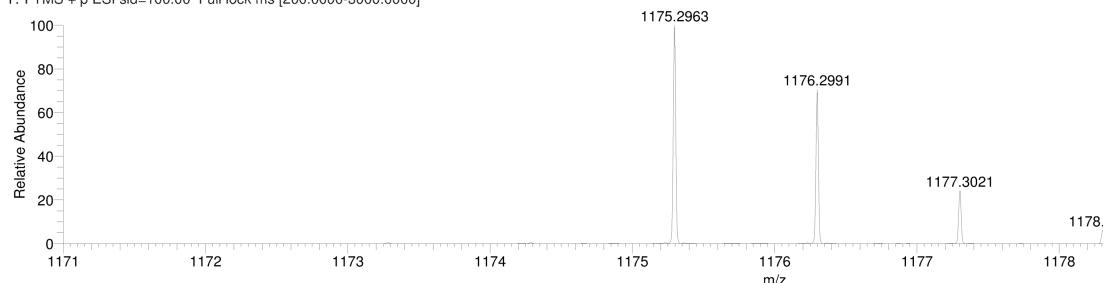
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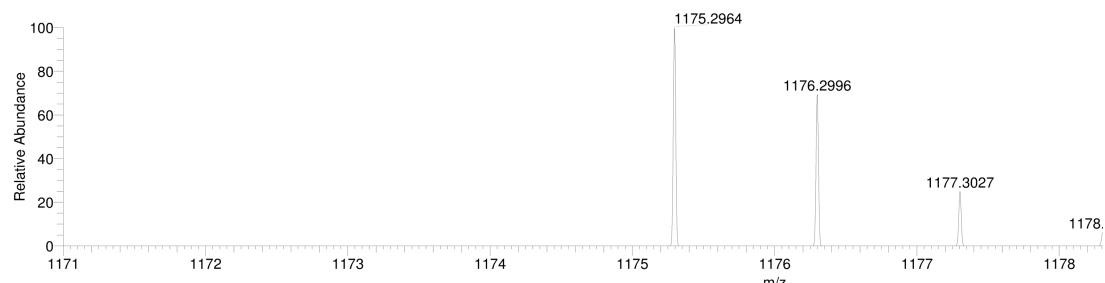
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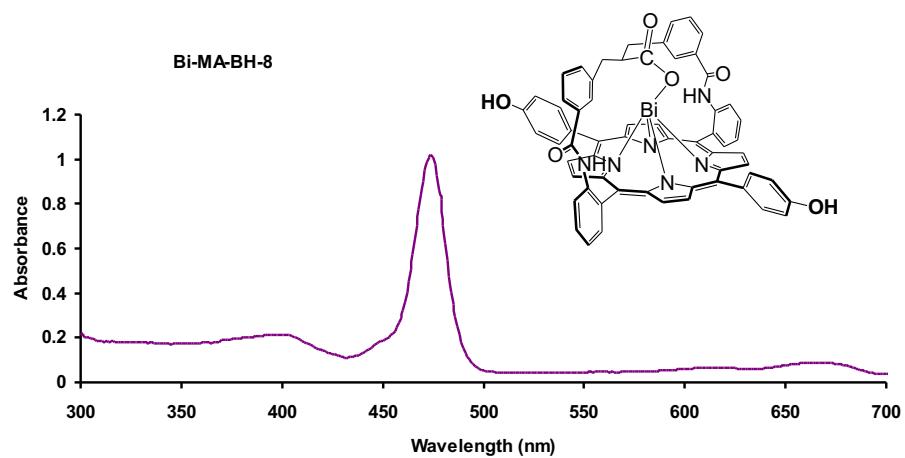


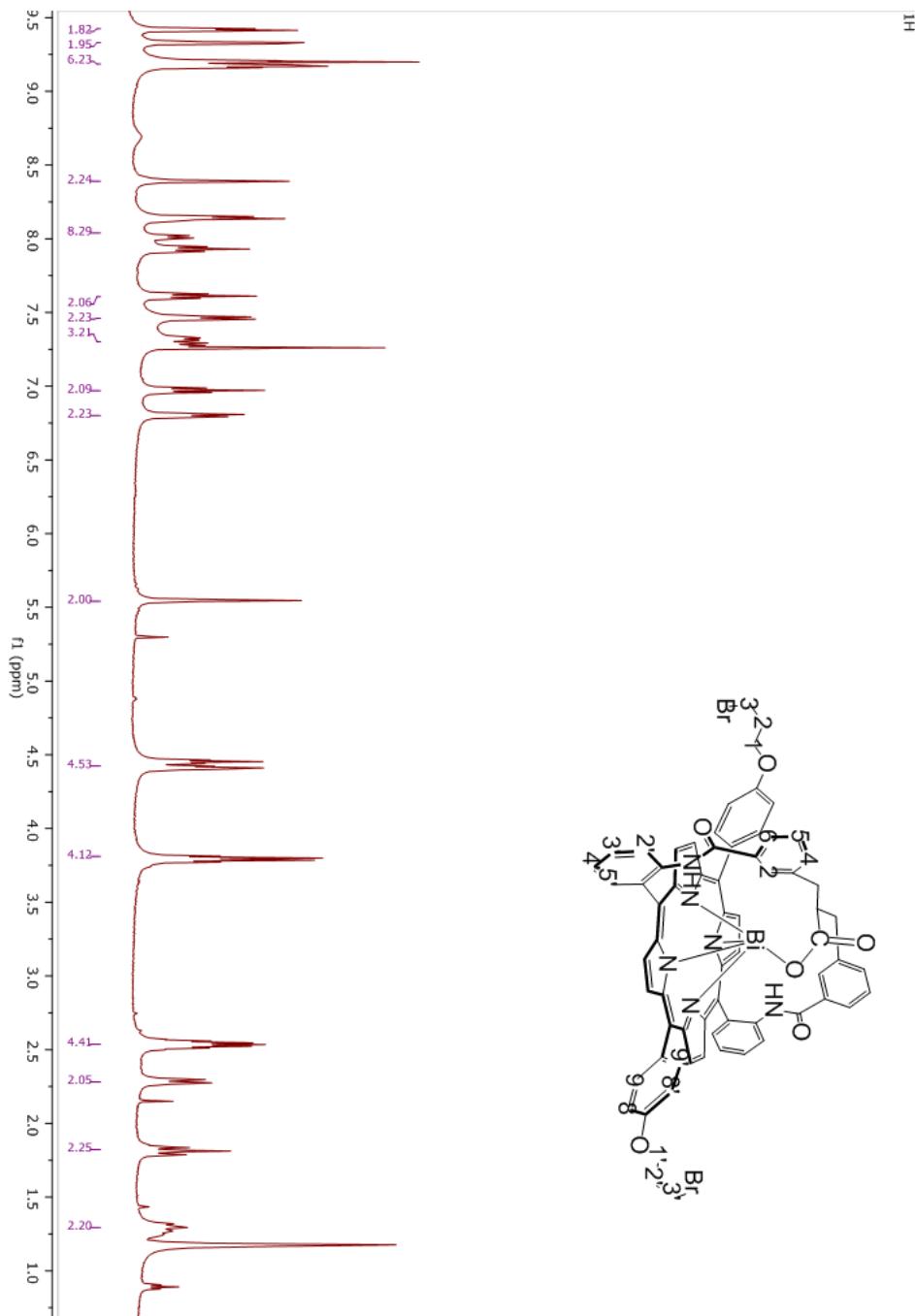
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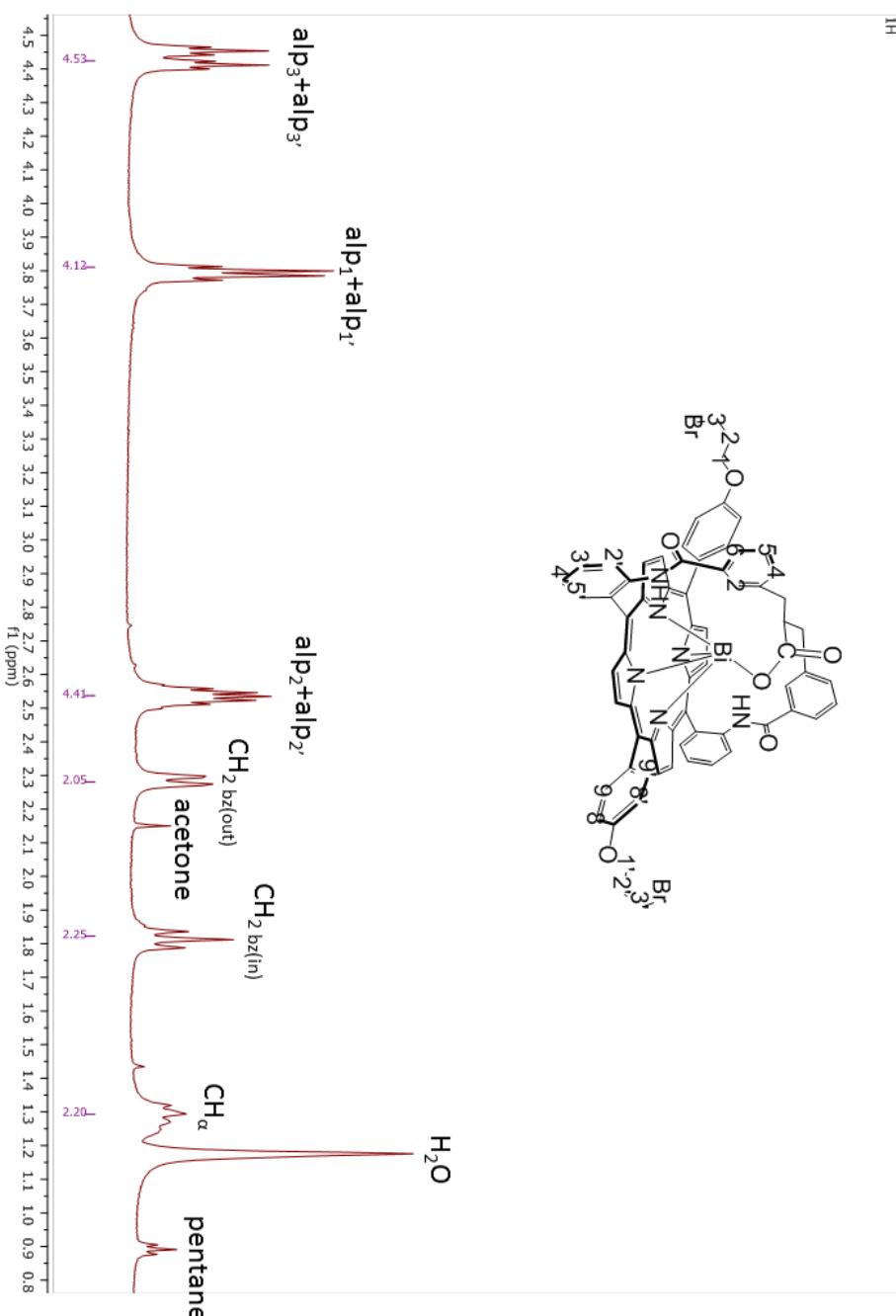
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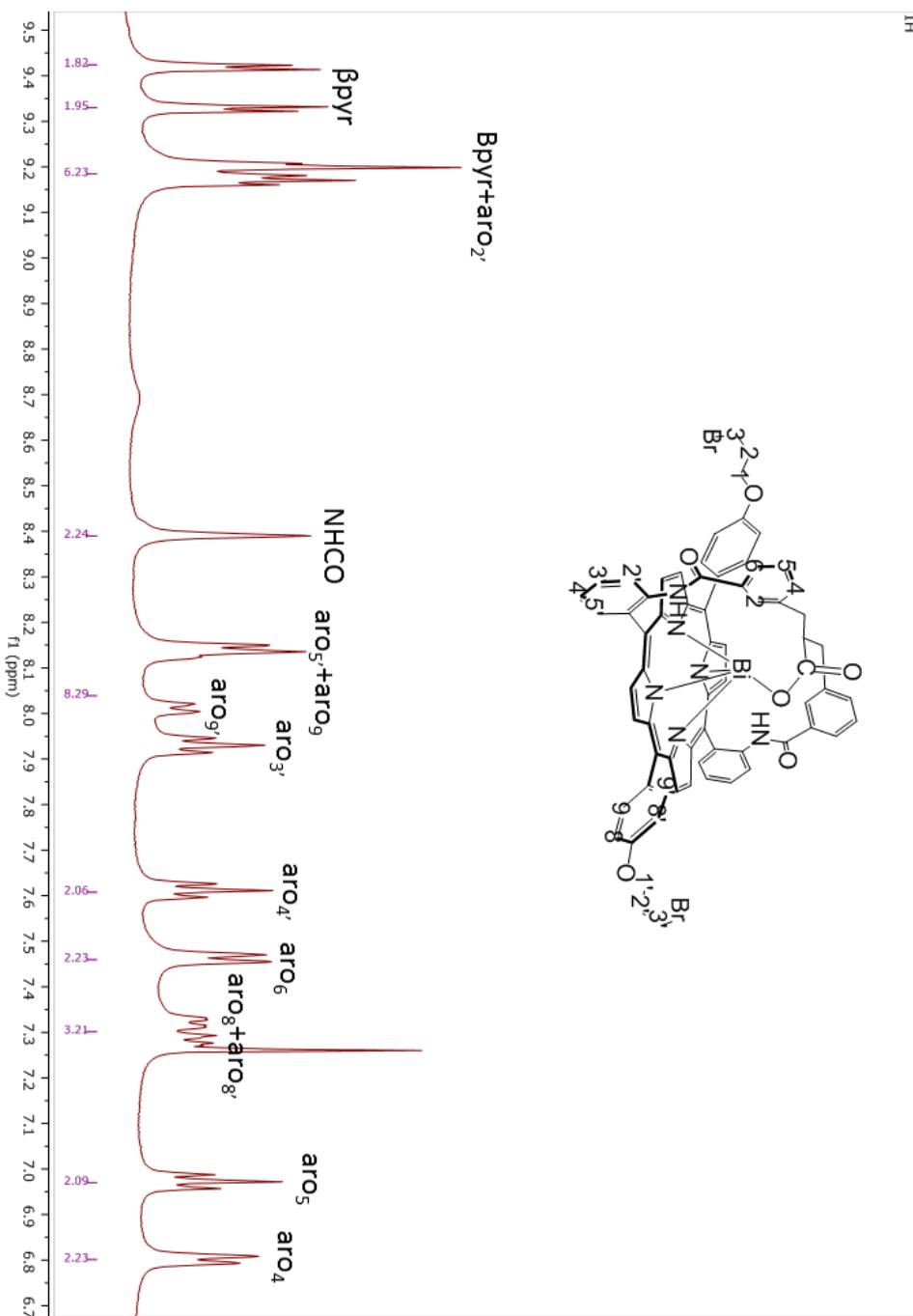


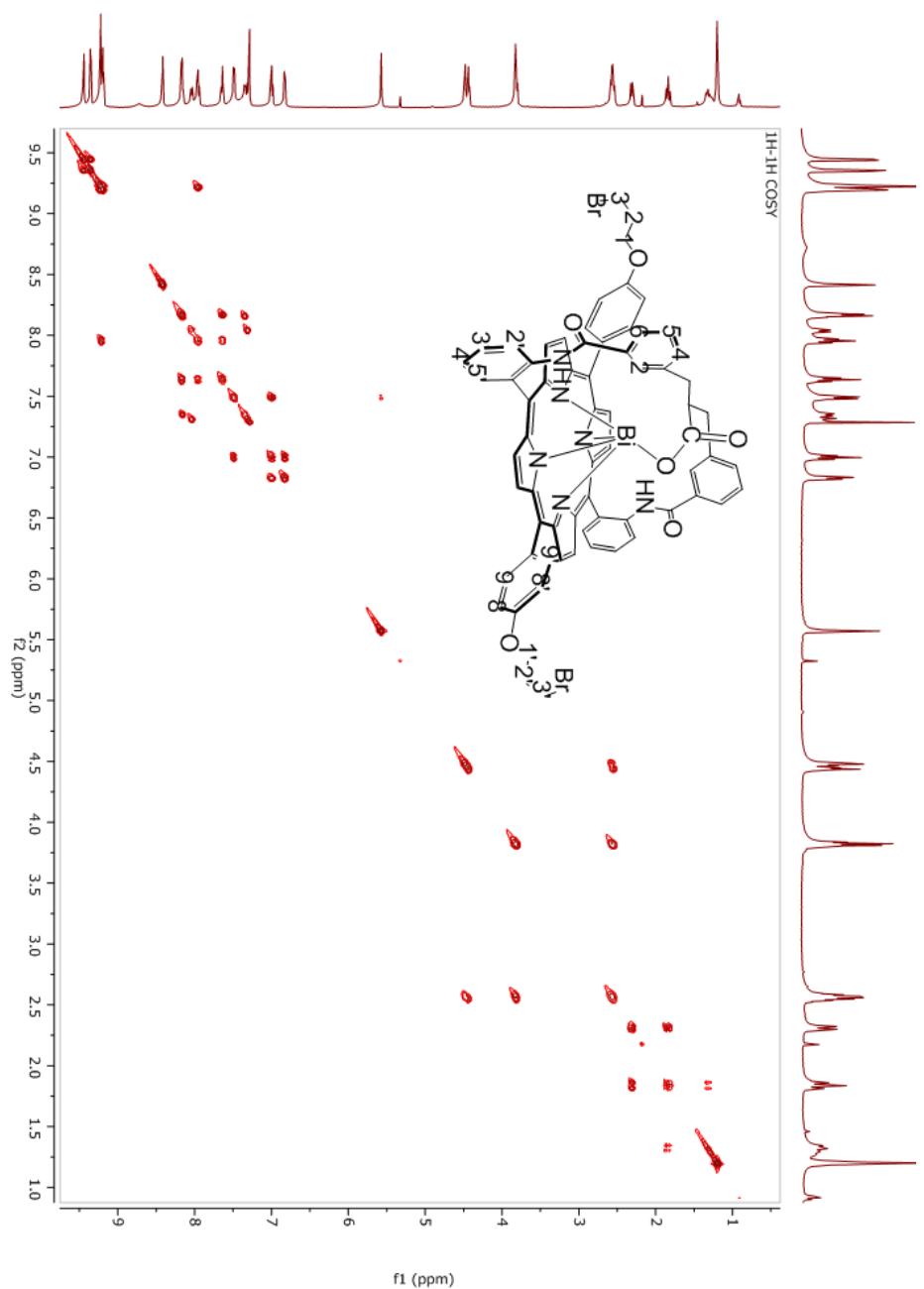


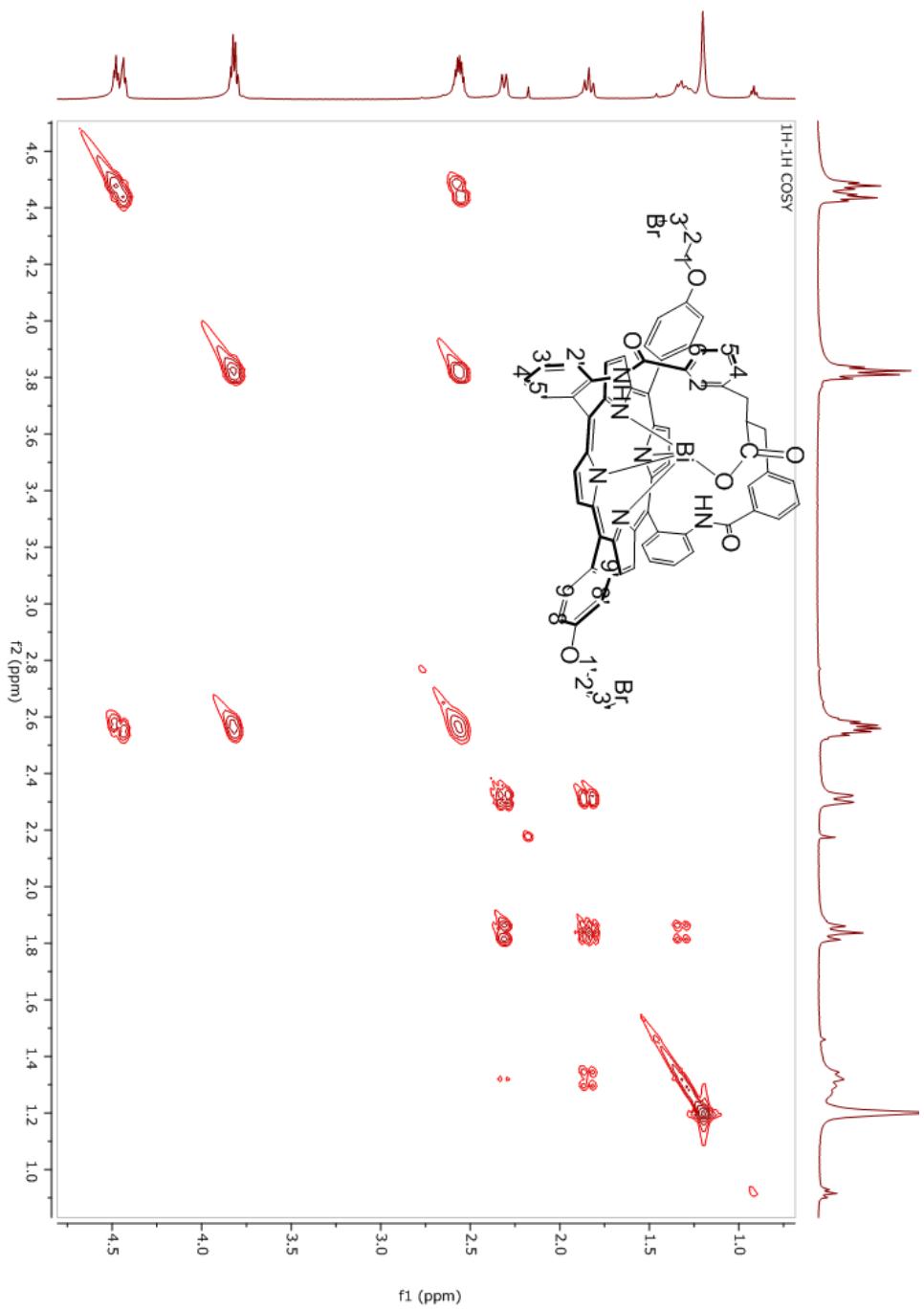
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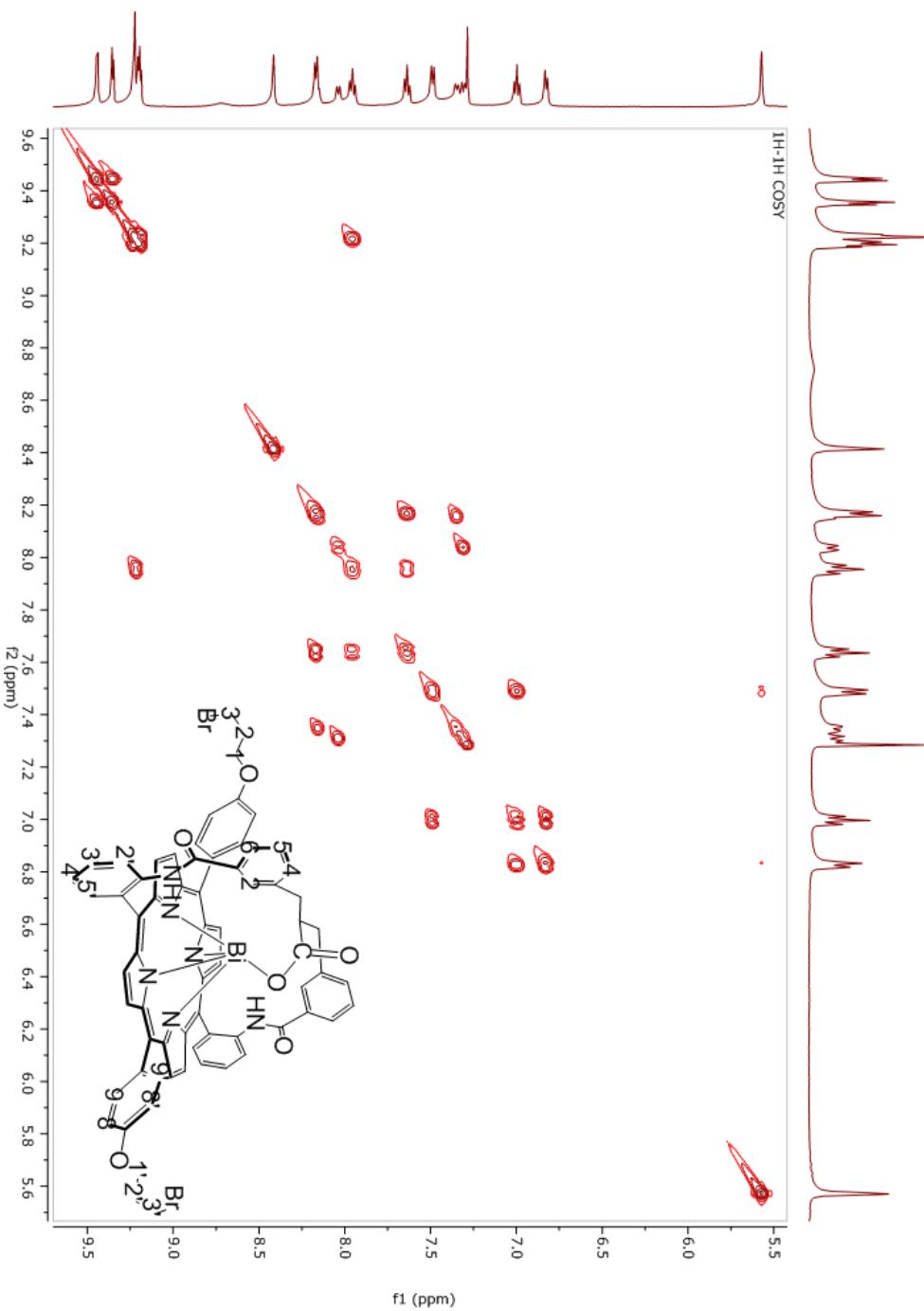


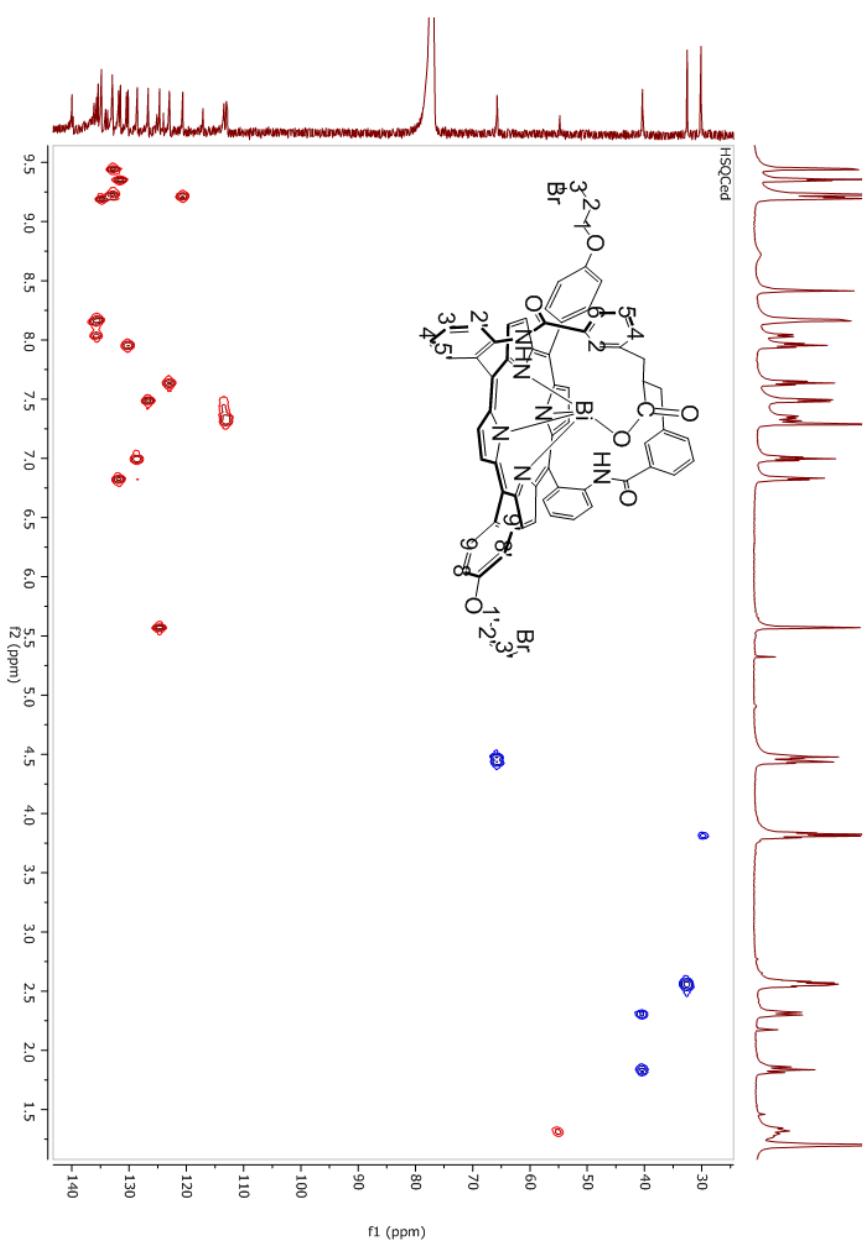
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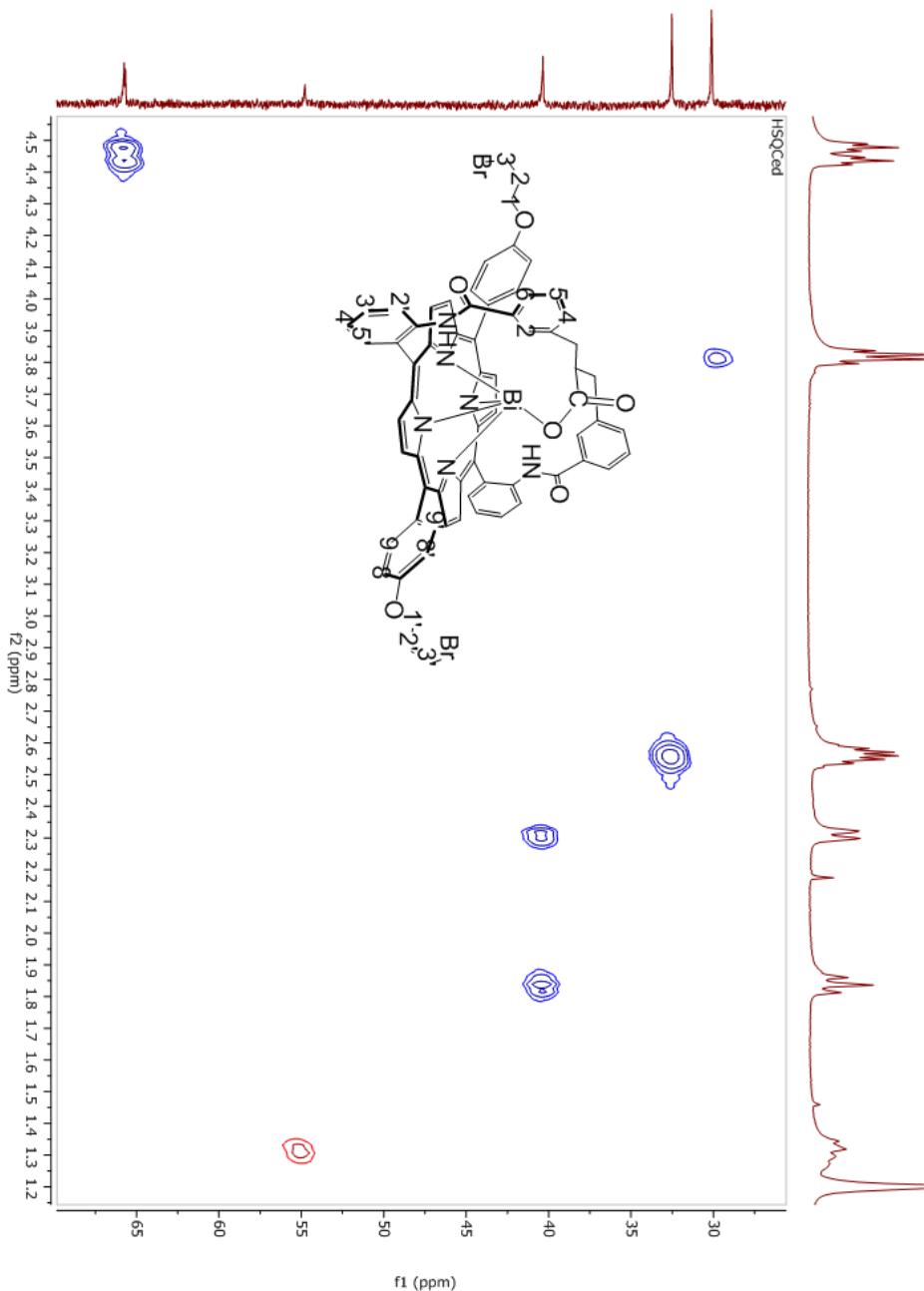


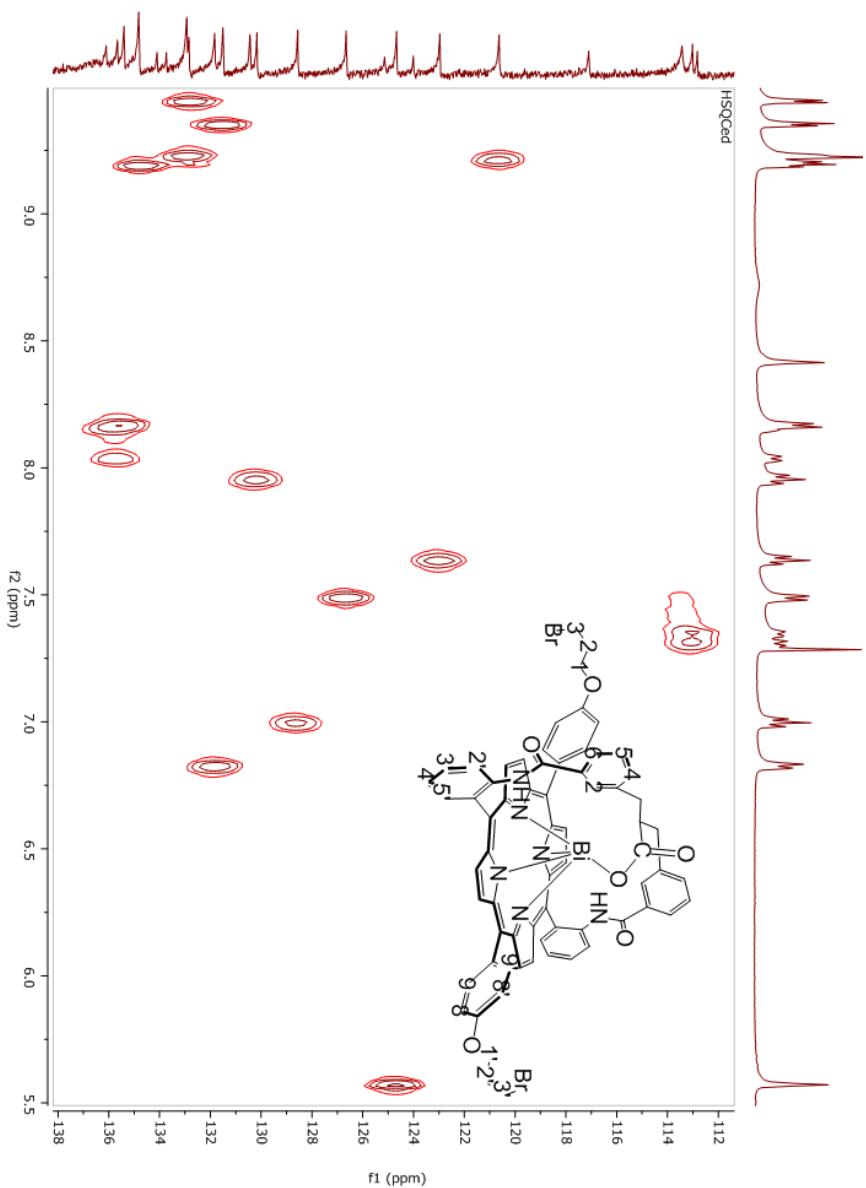


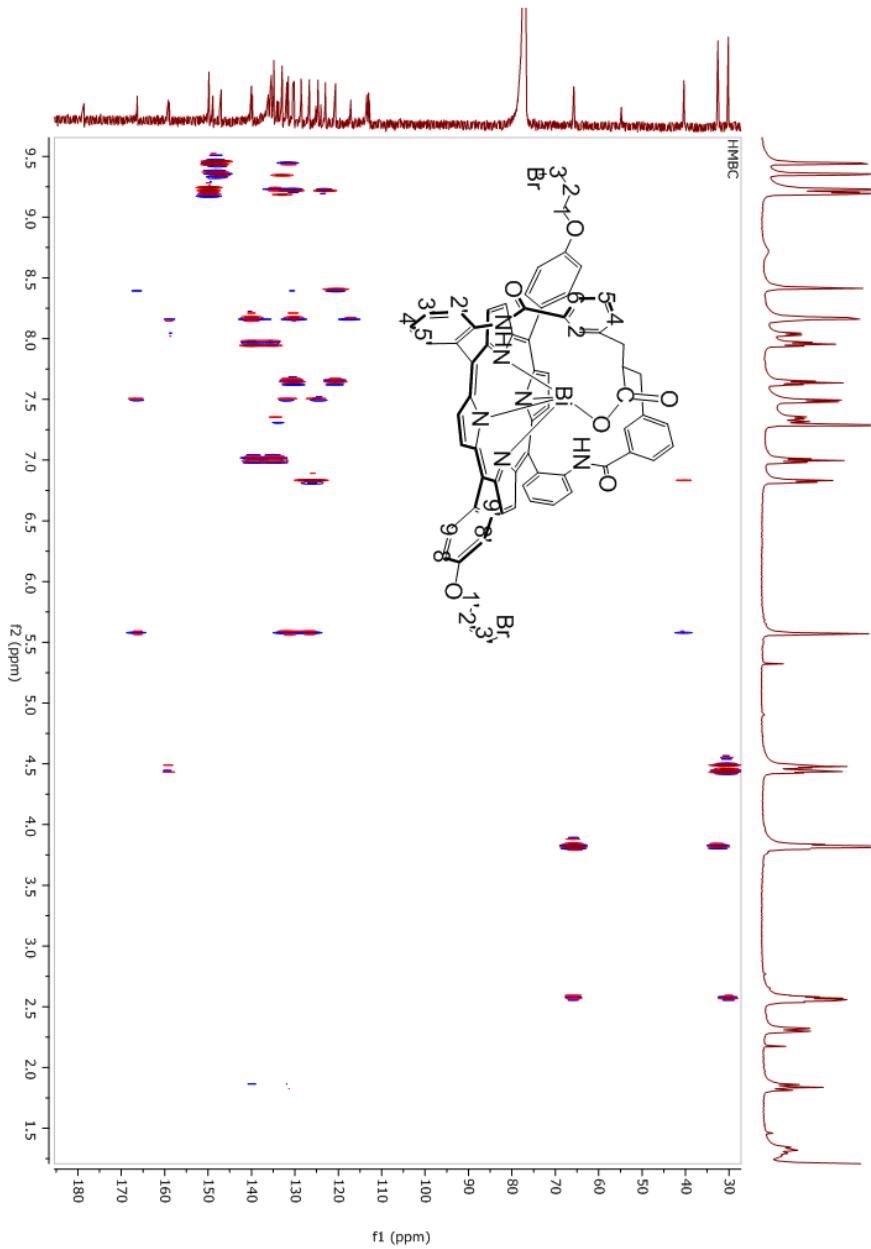




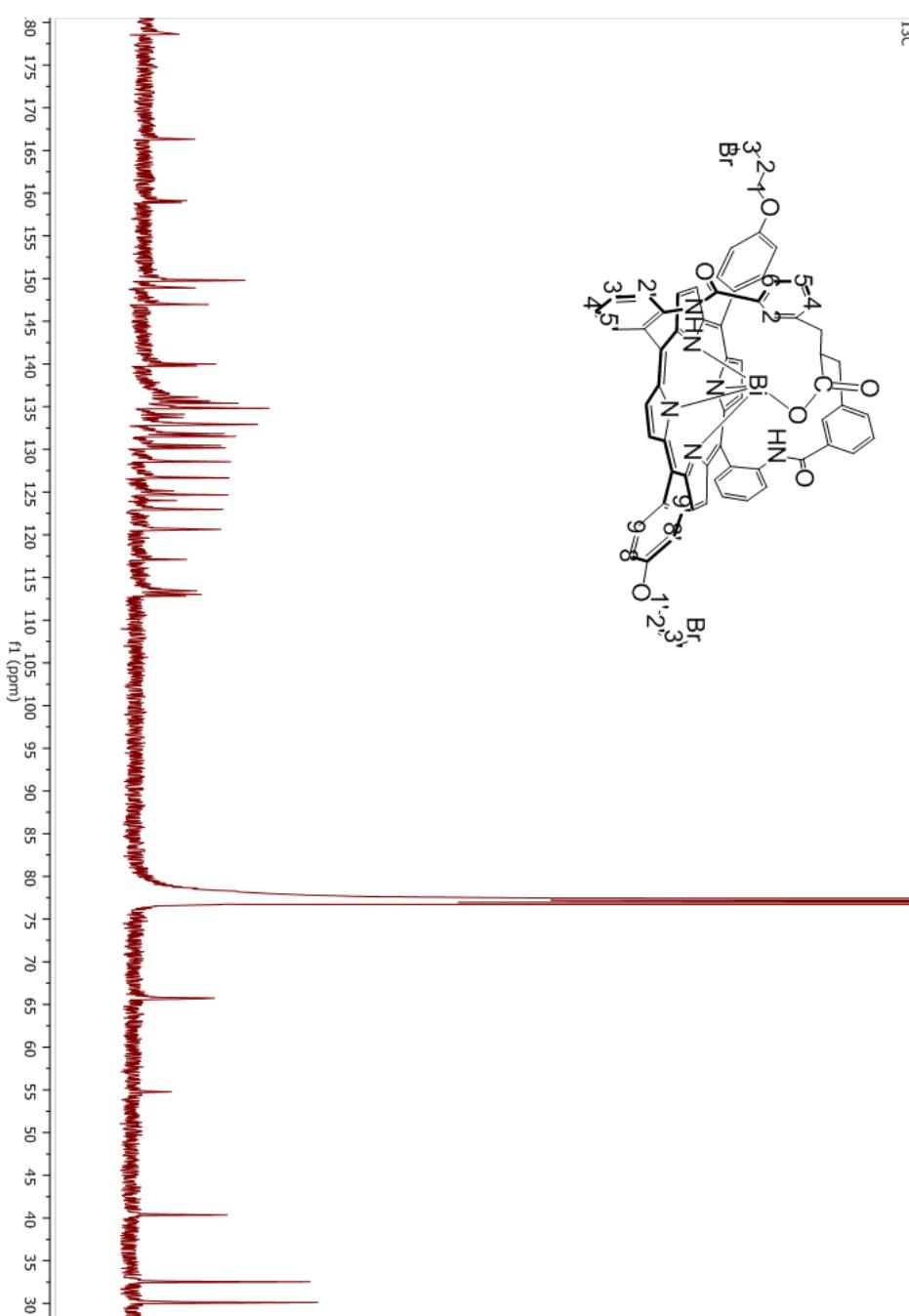
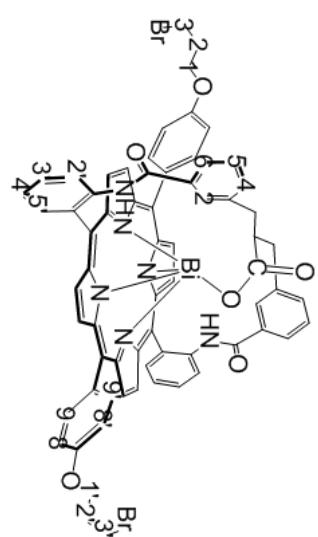




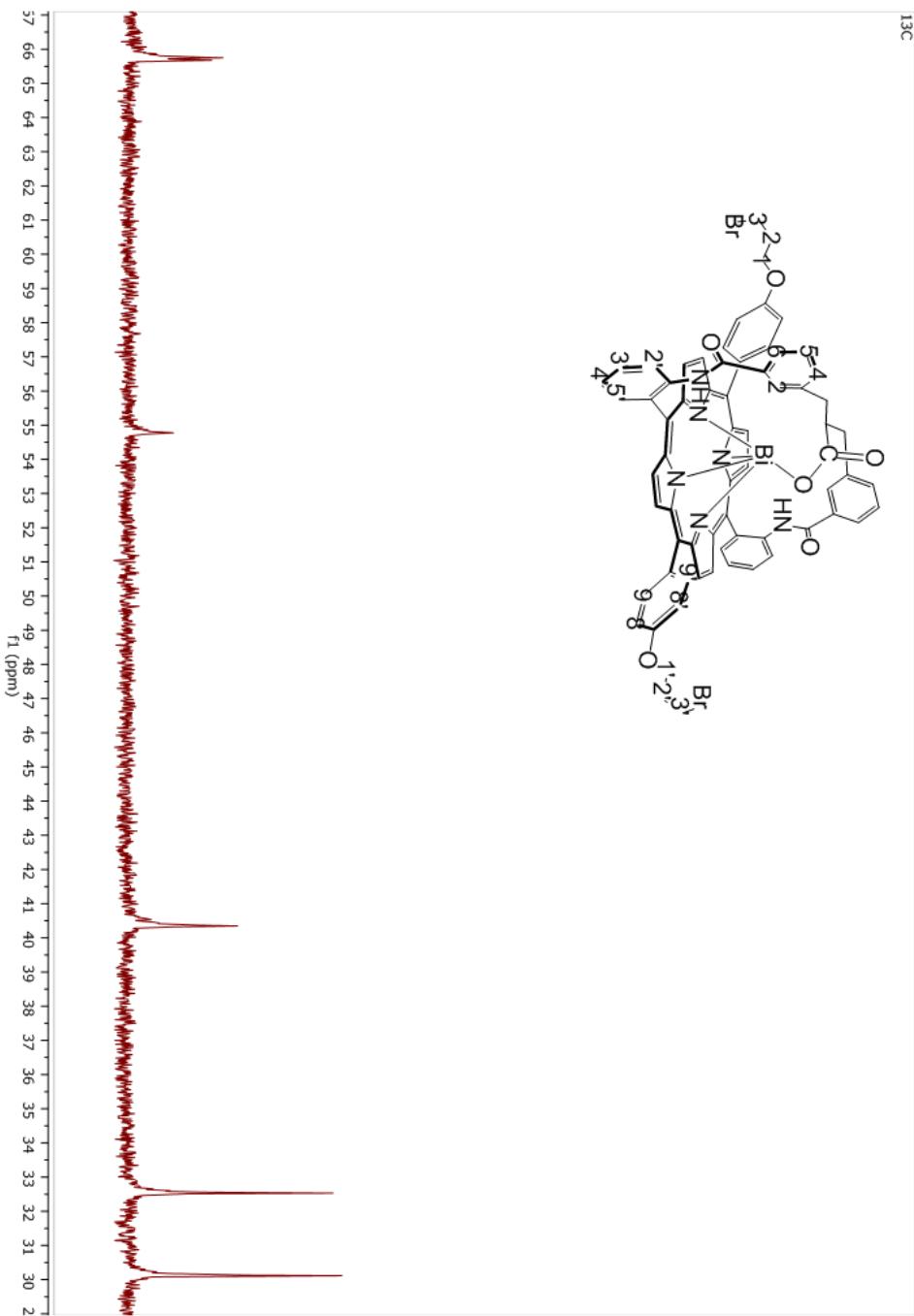
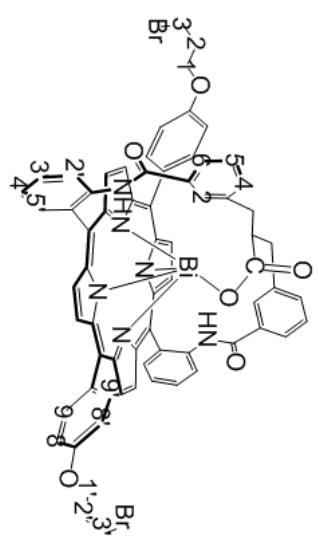




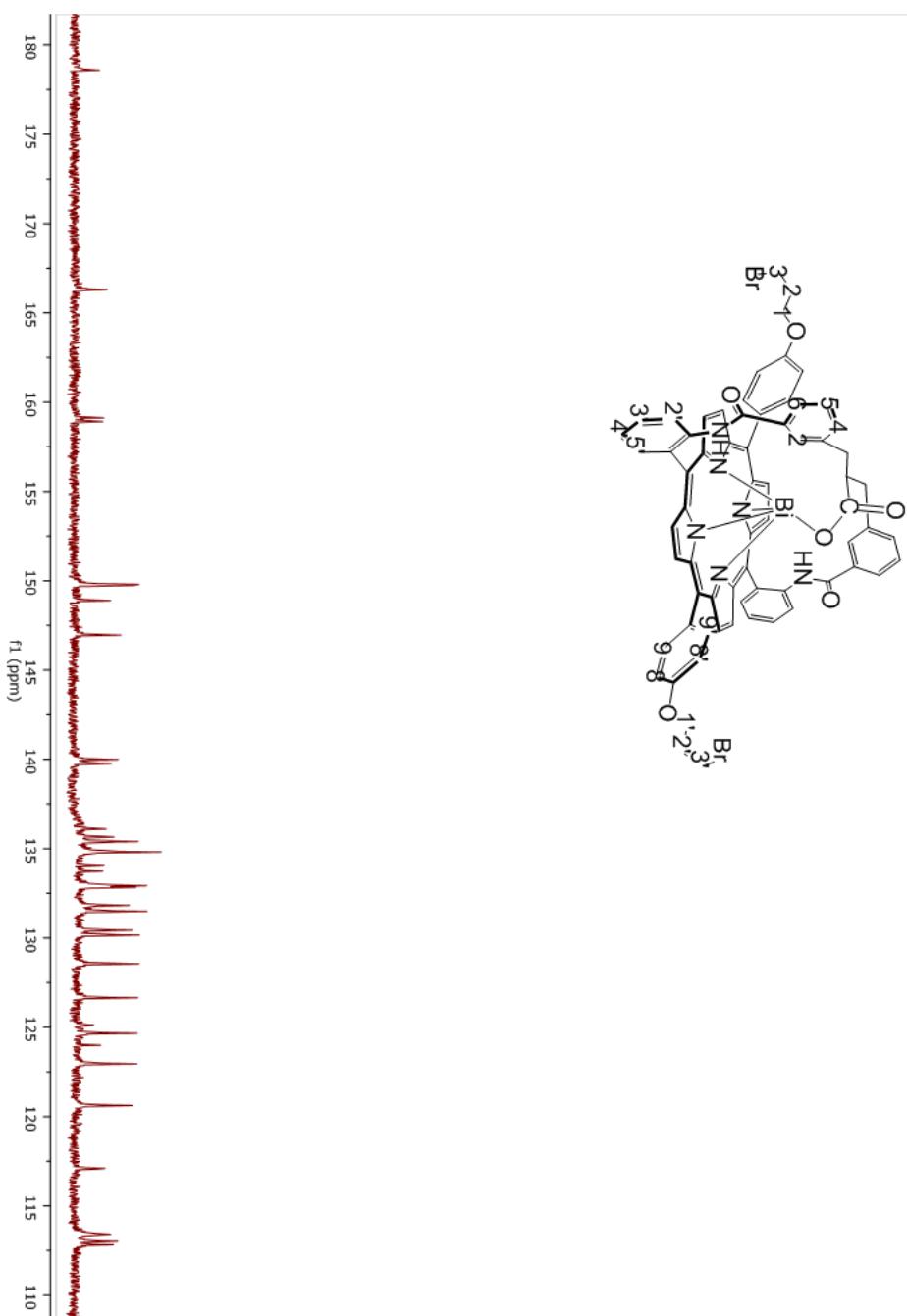
¹³C



13C



¹³C



CRMPO

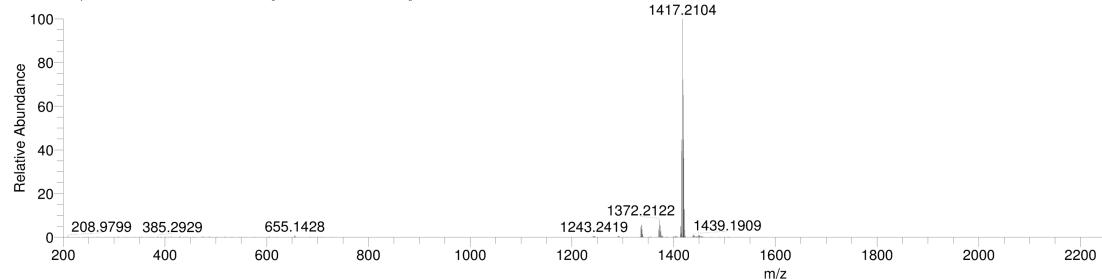
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Rapport d'analyse

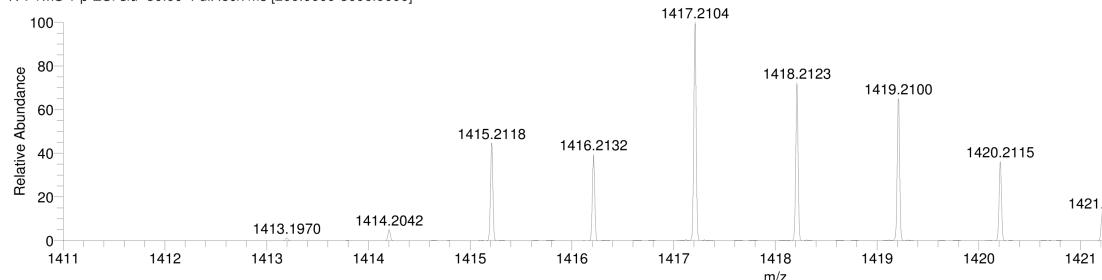
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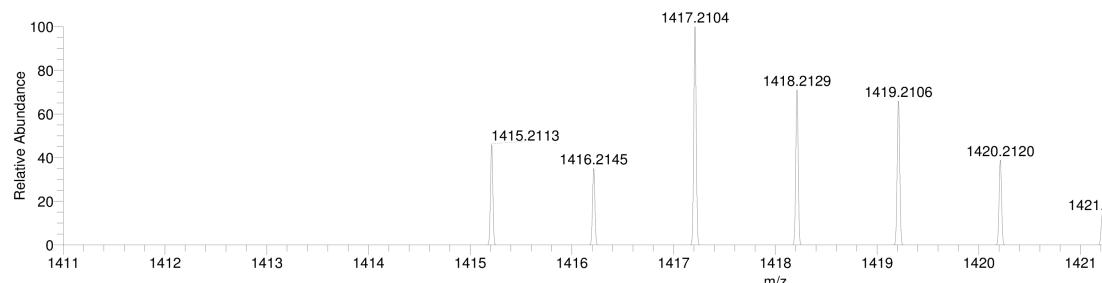
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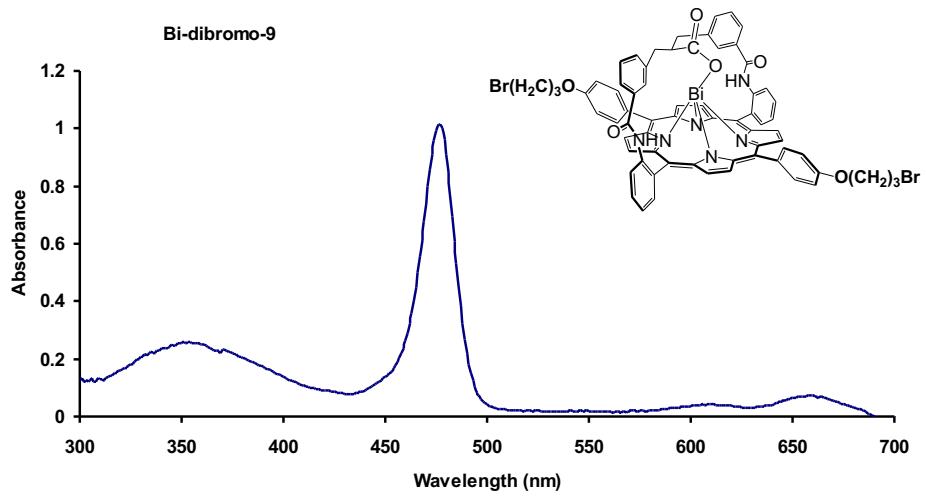


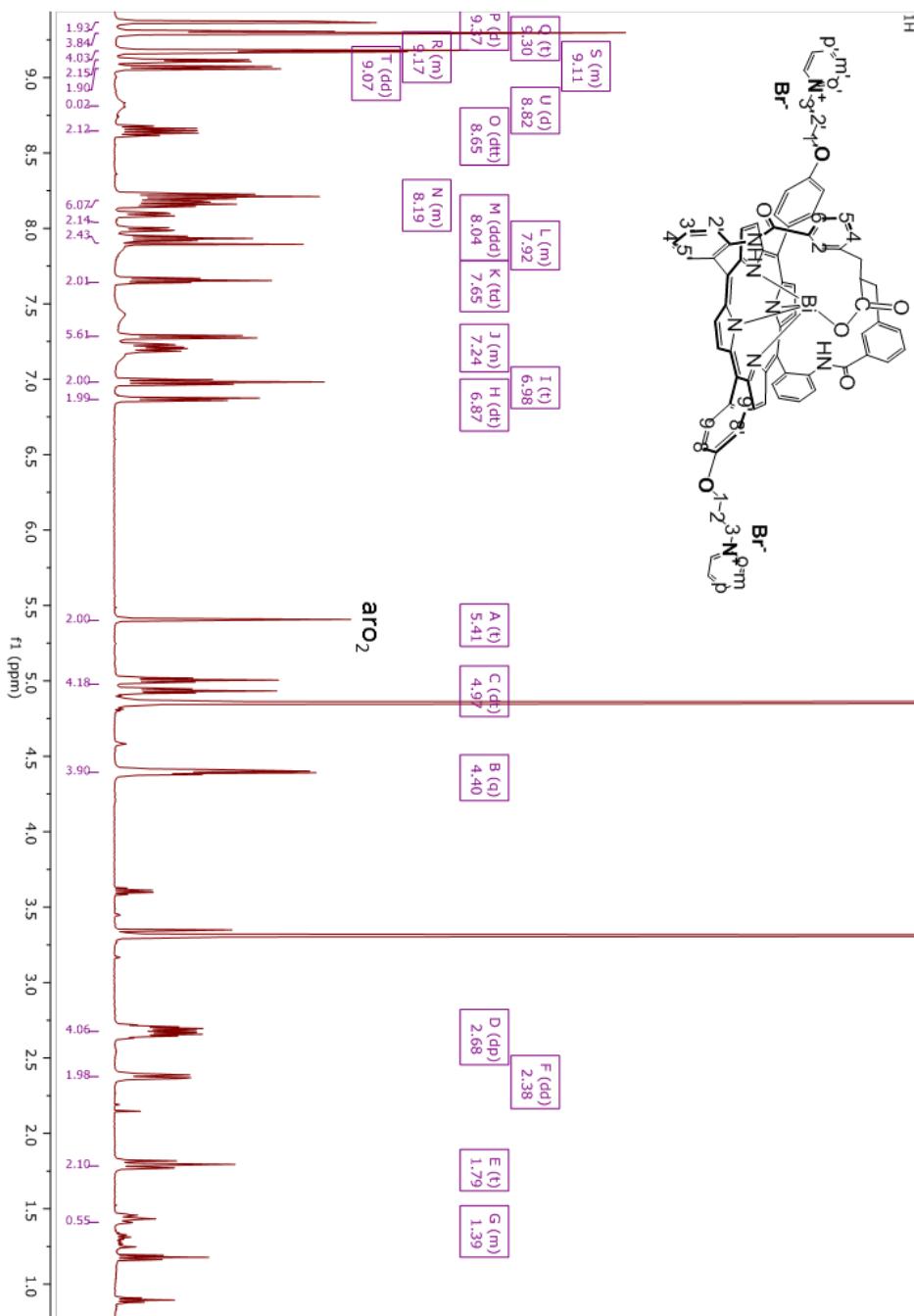
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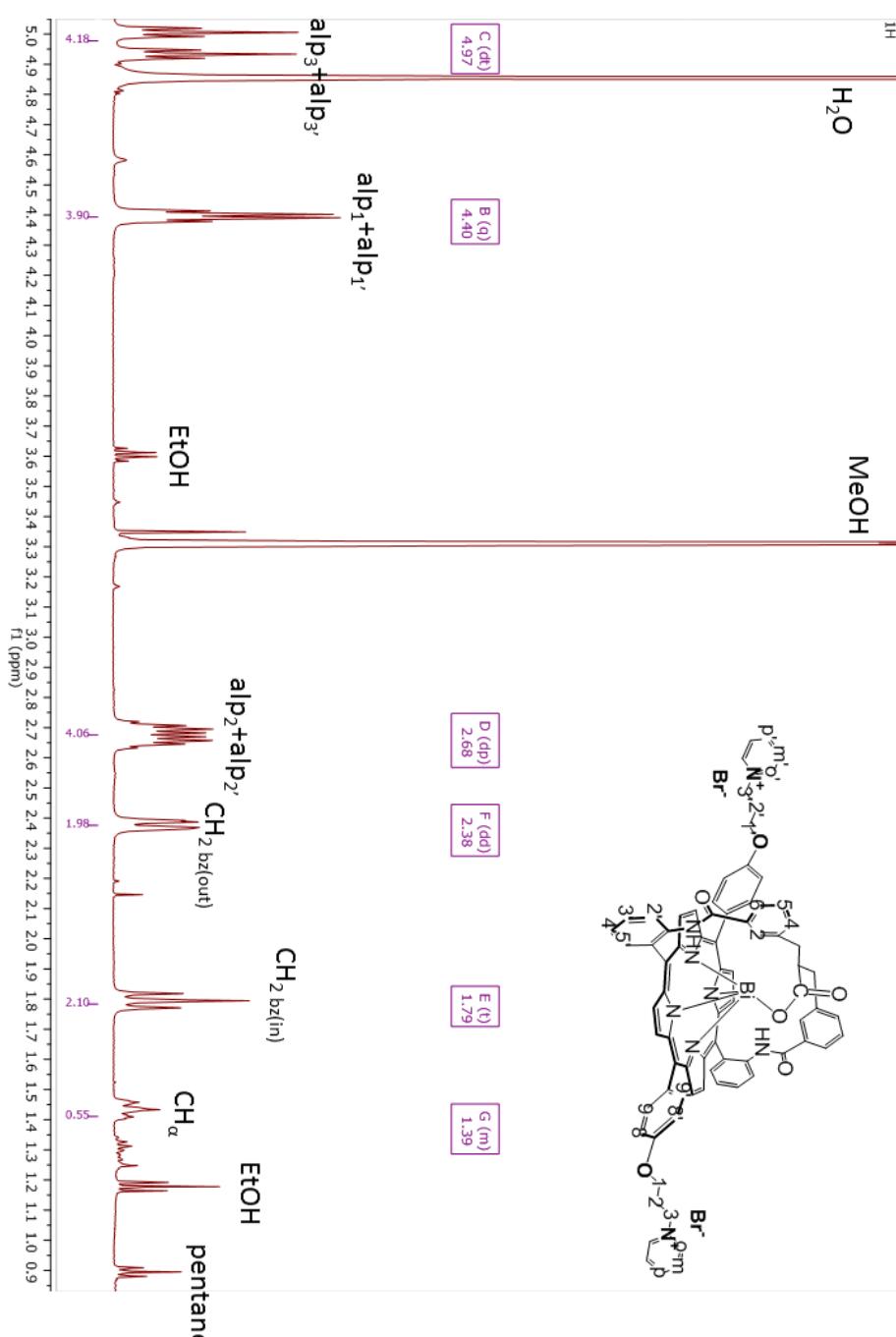


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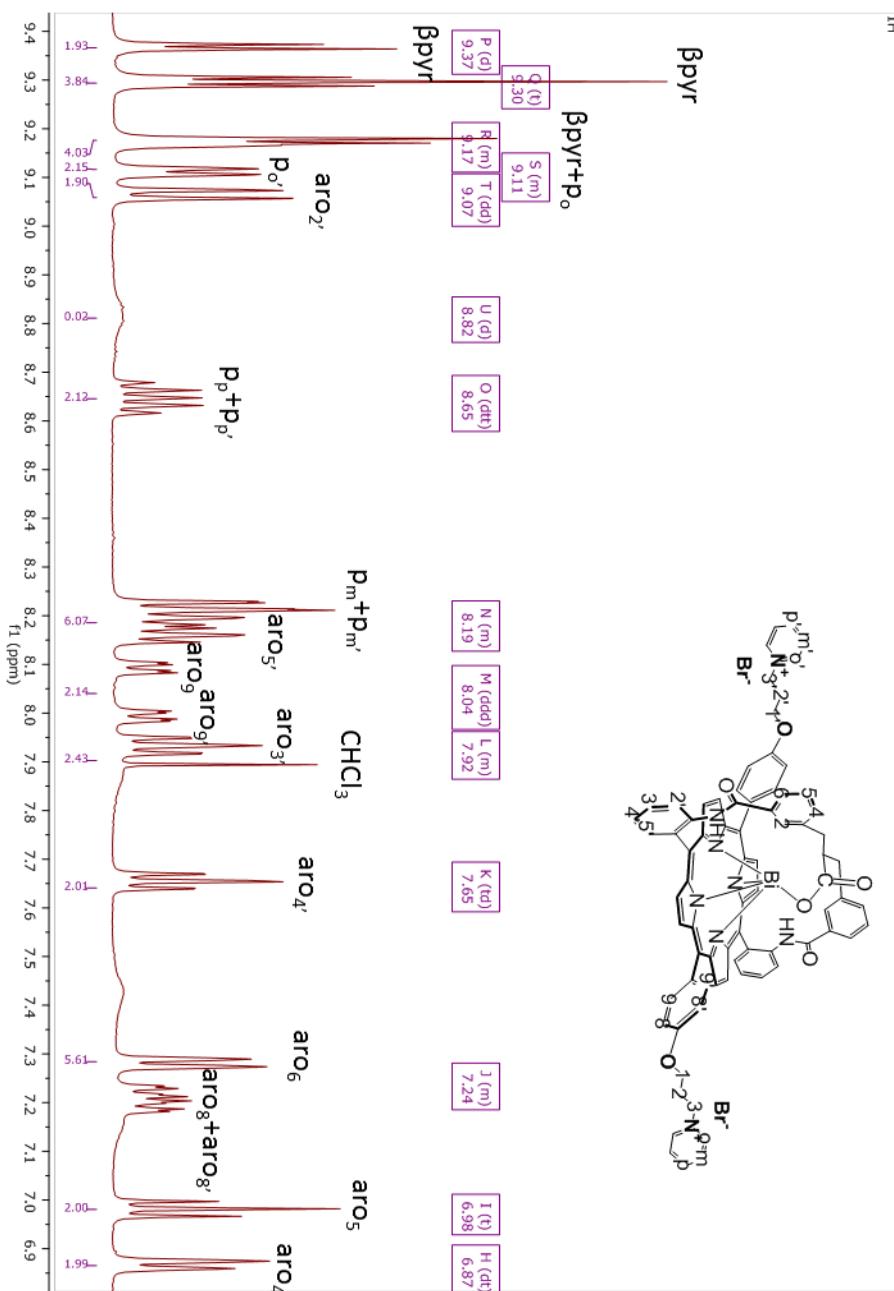


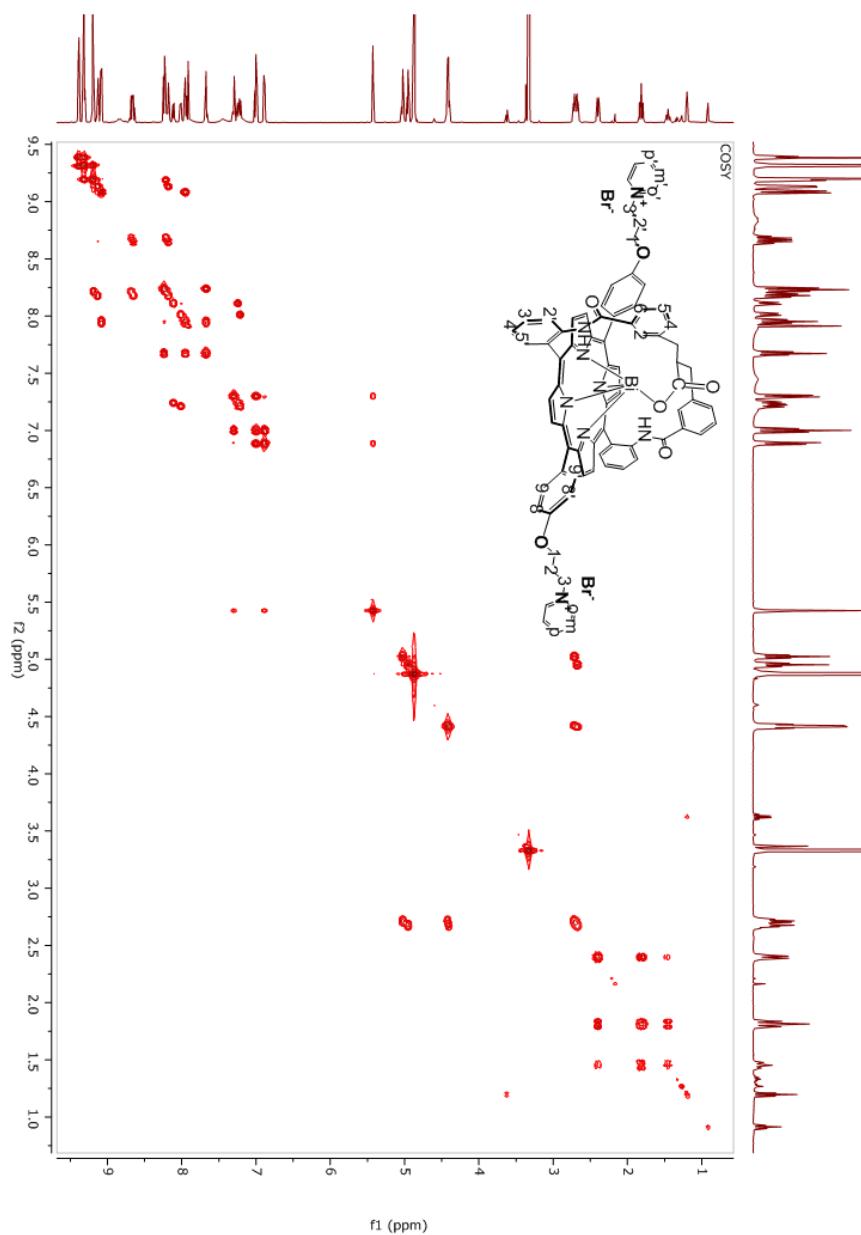


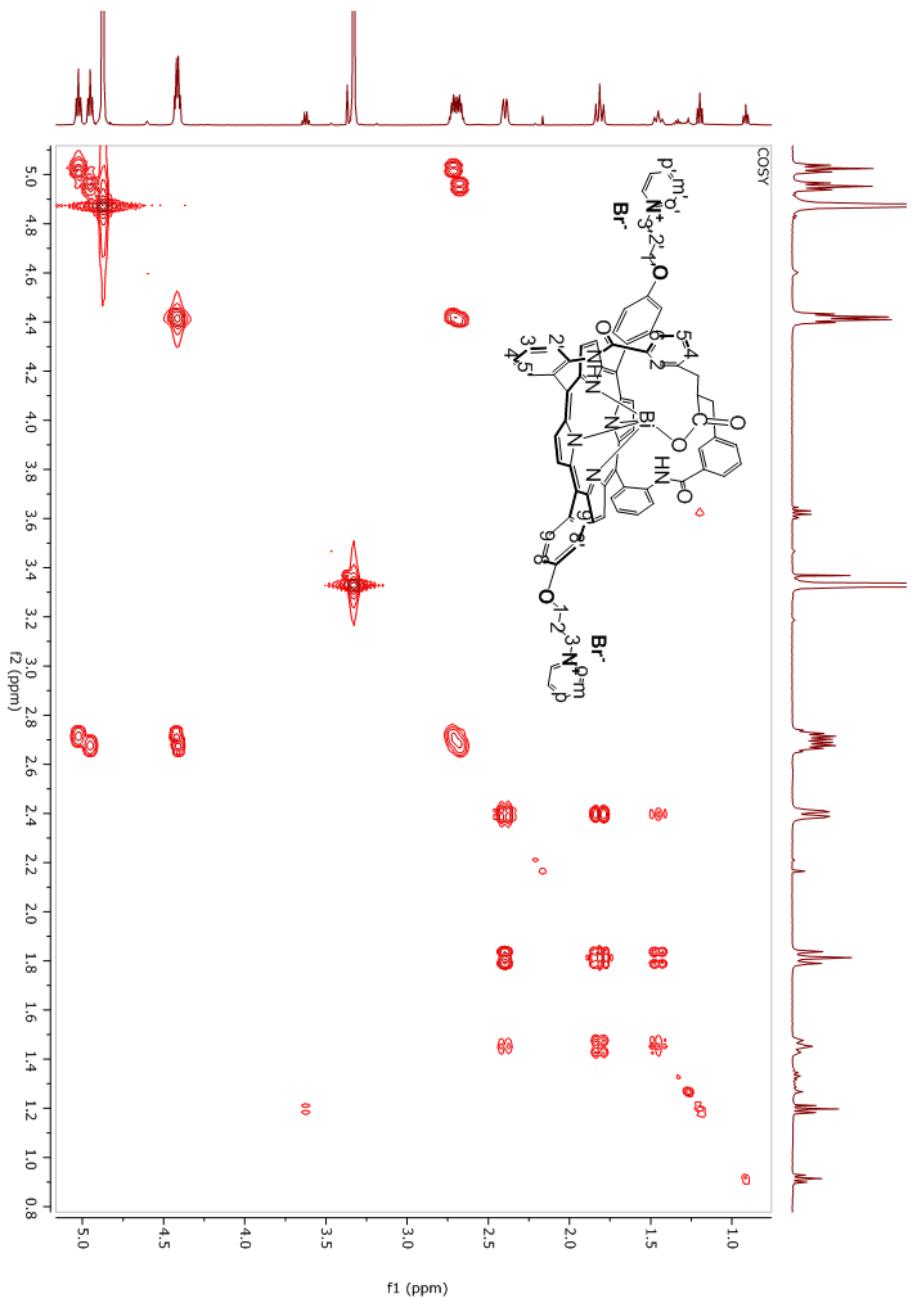


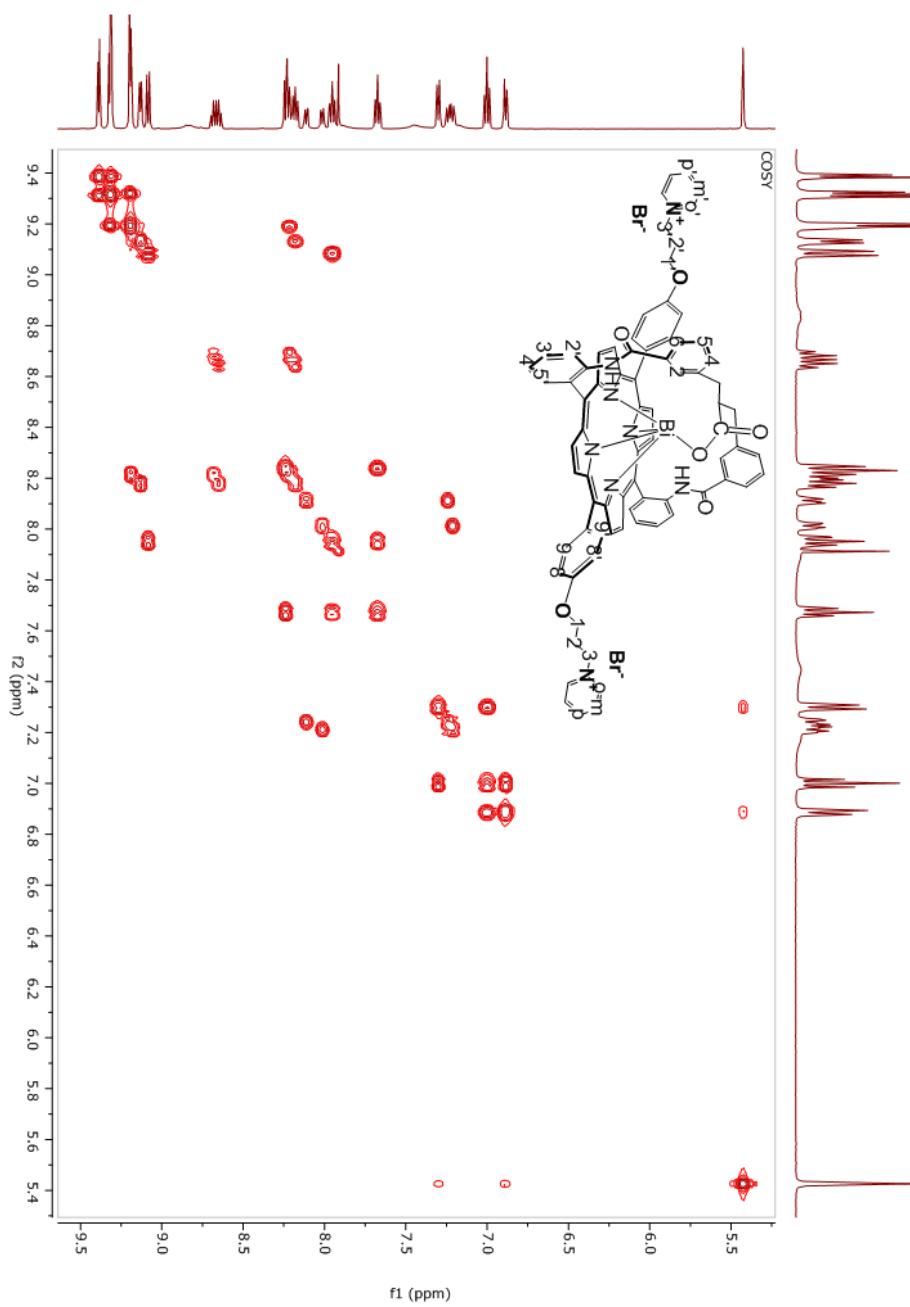


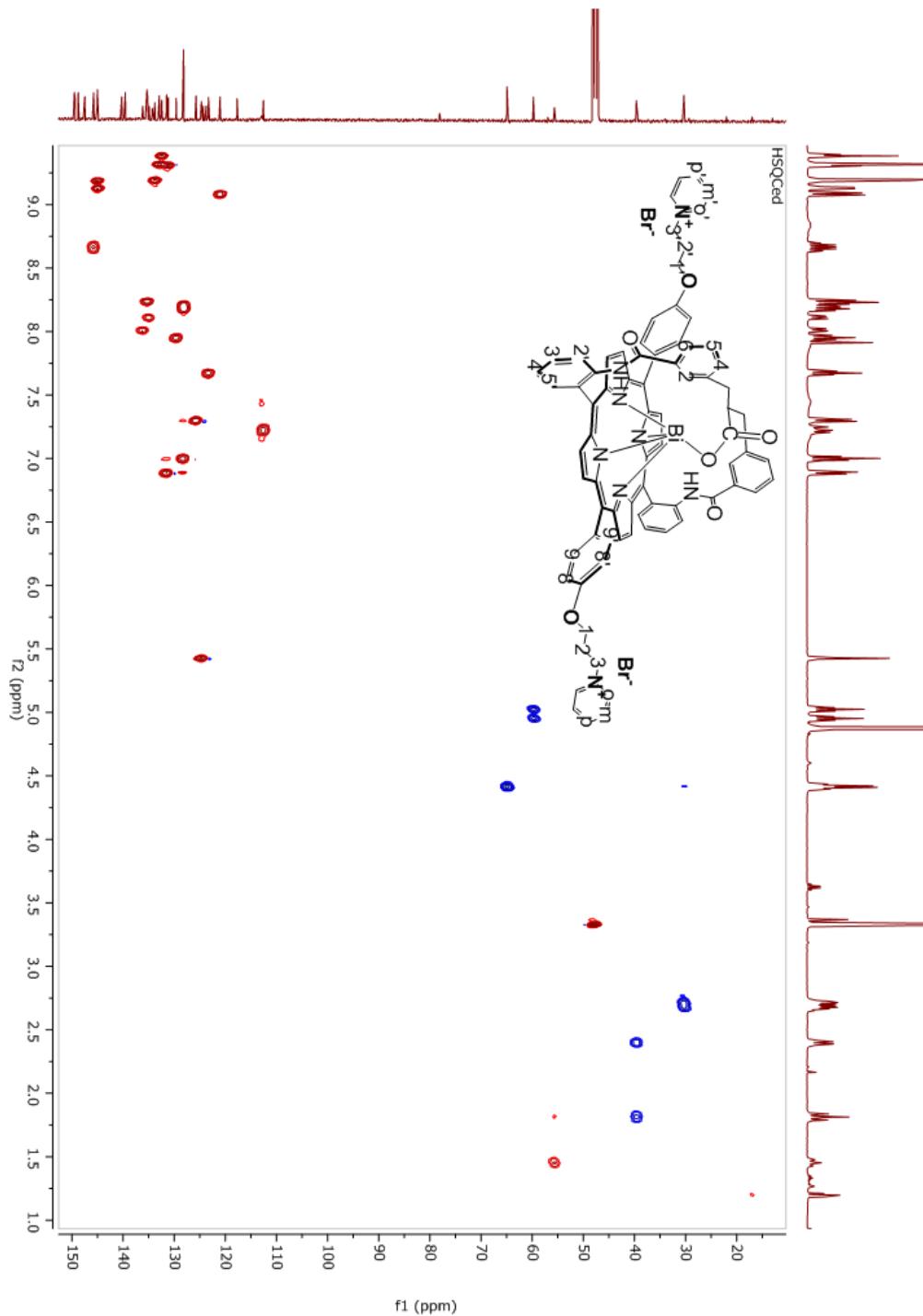
1H

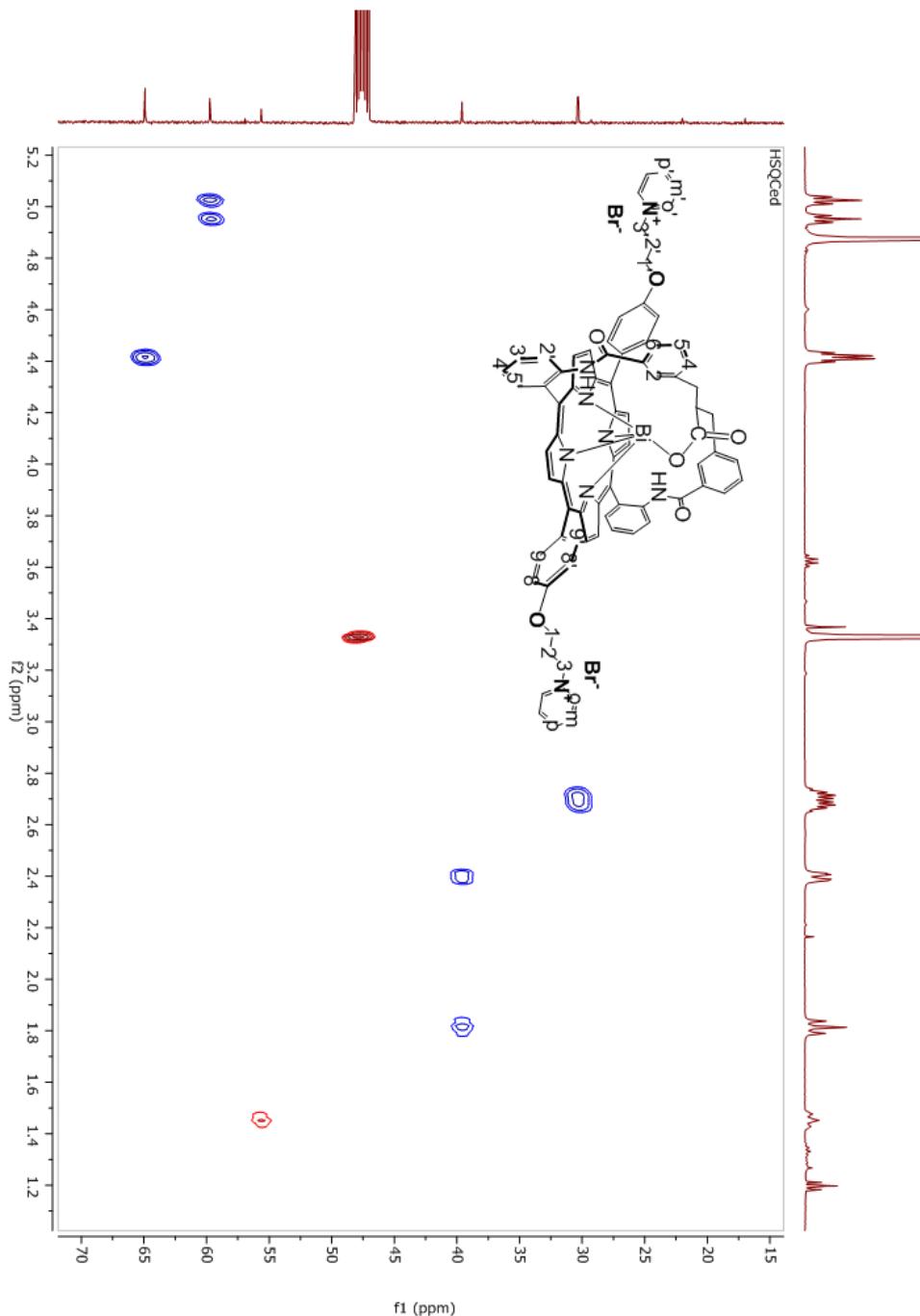


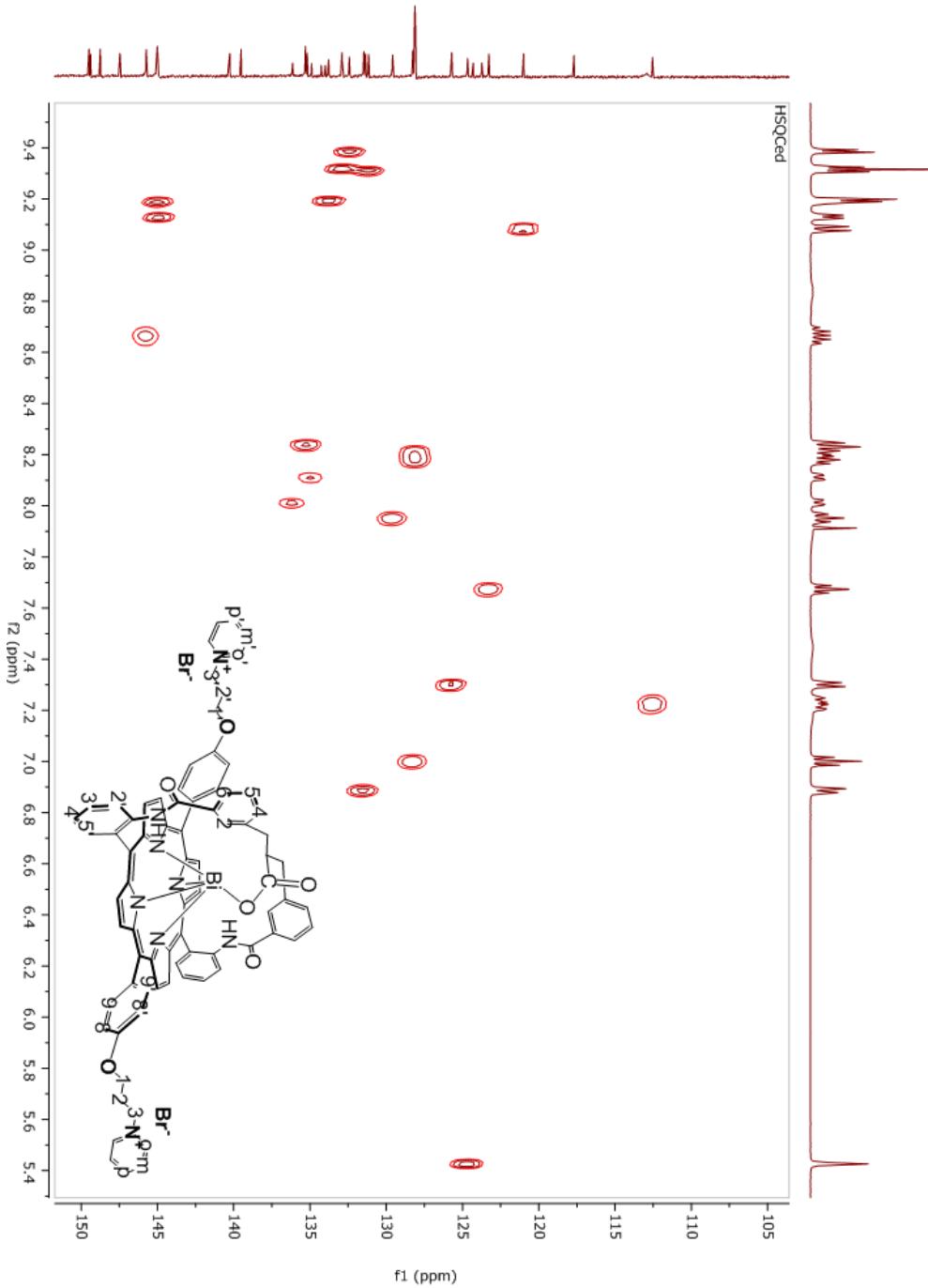


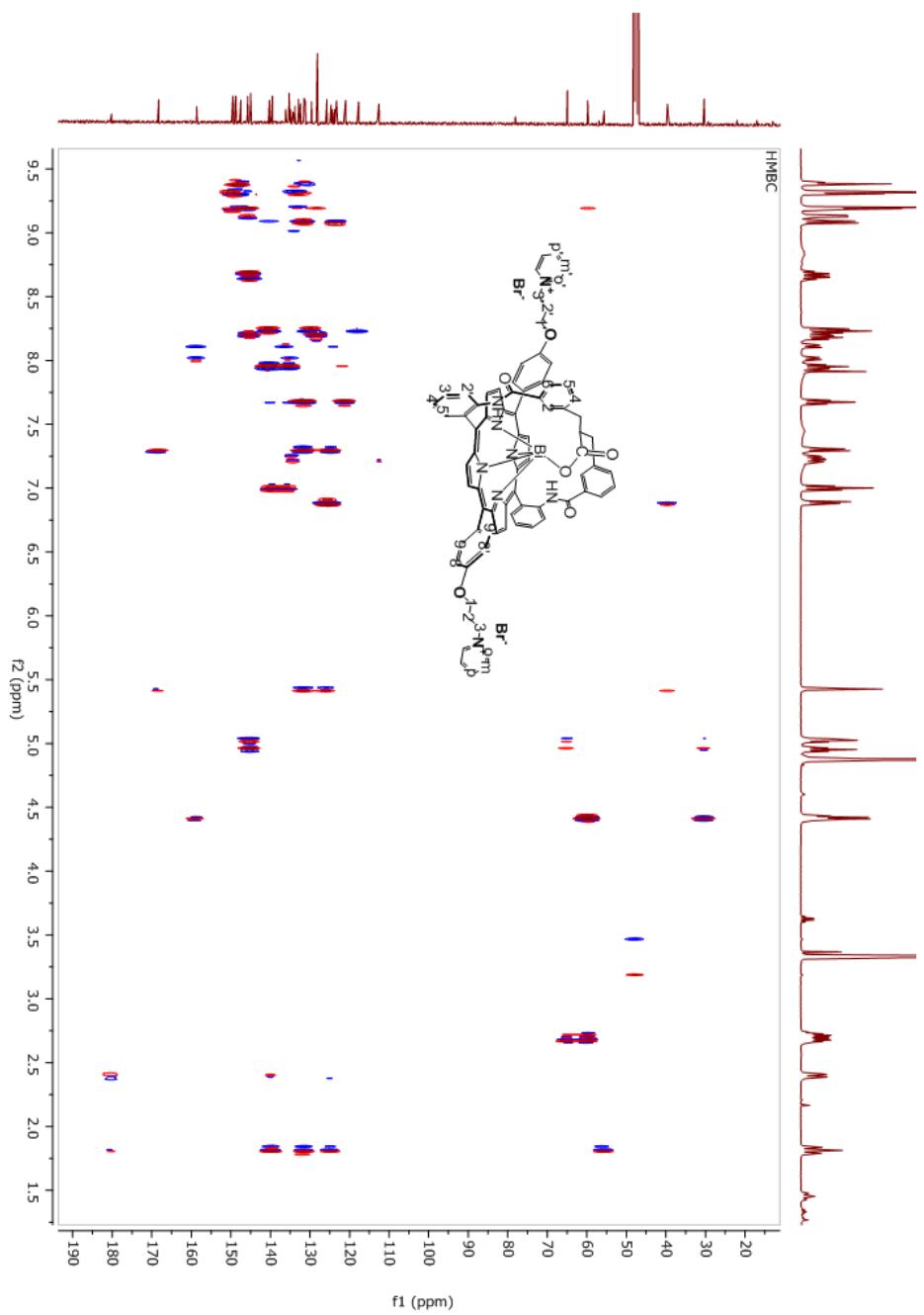


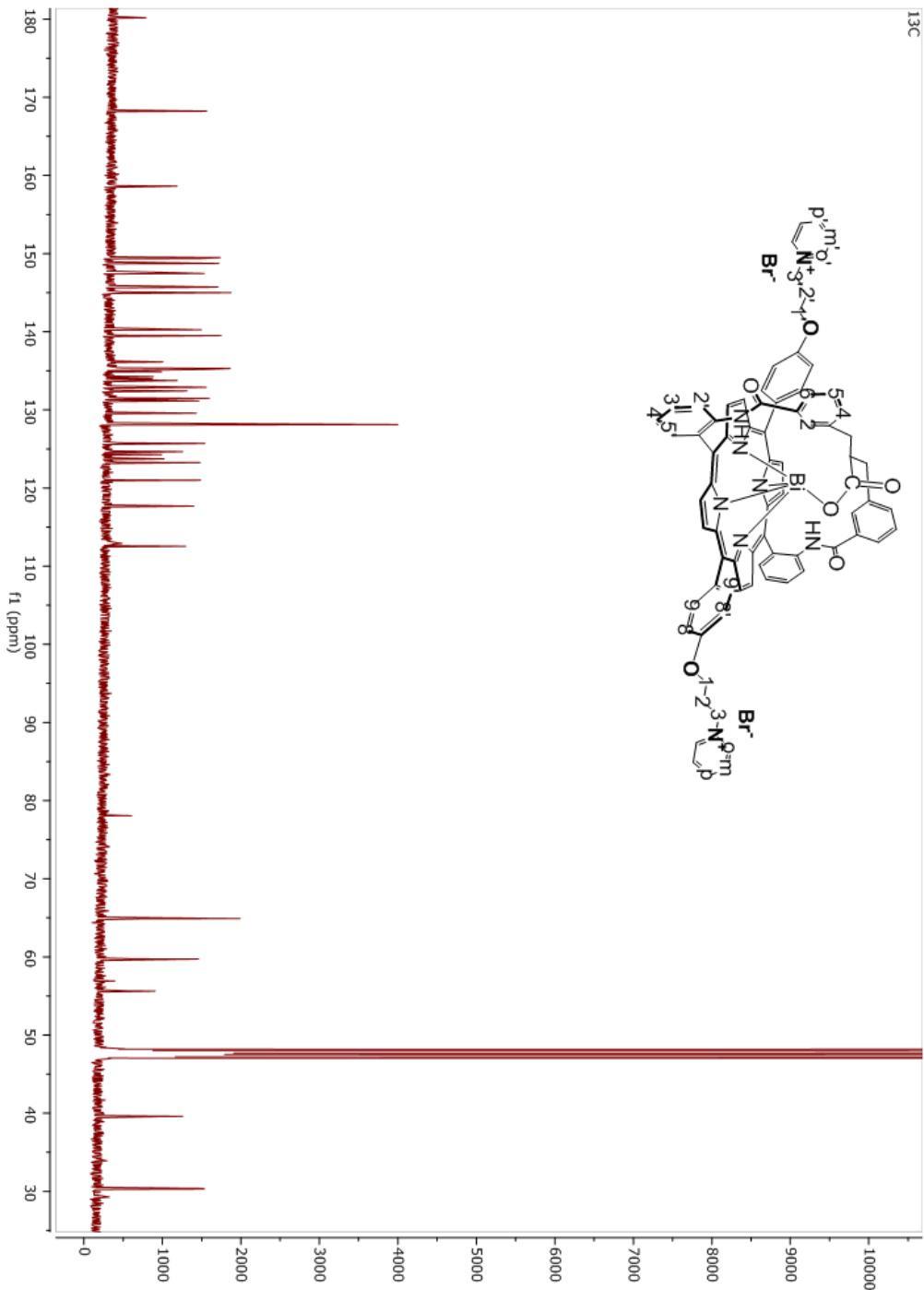




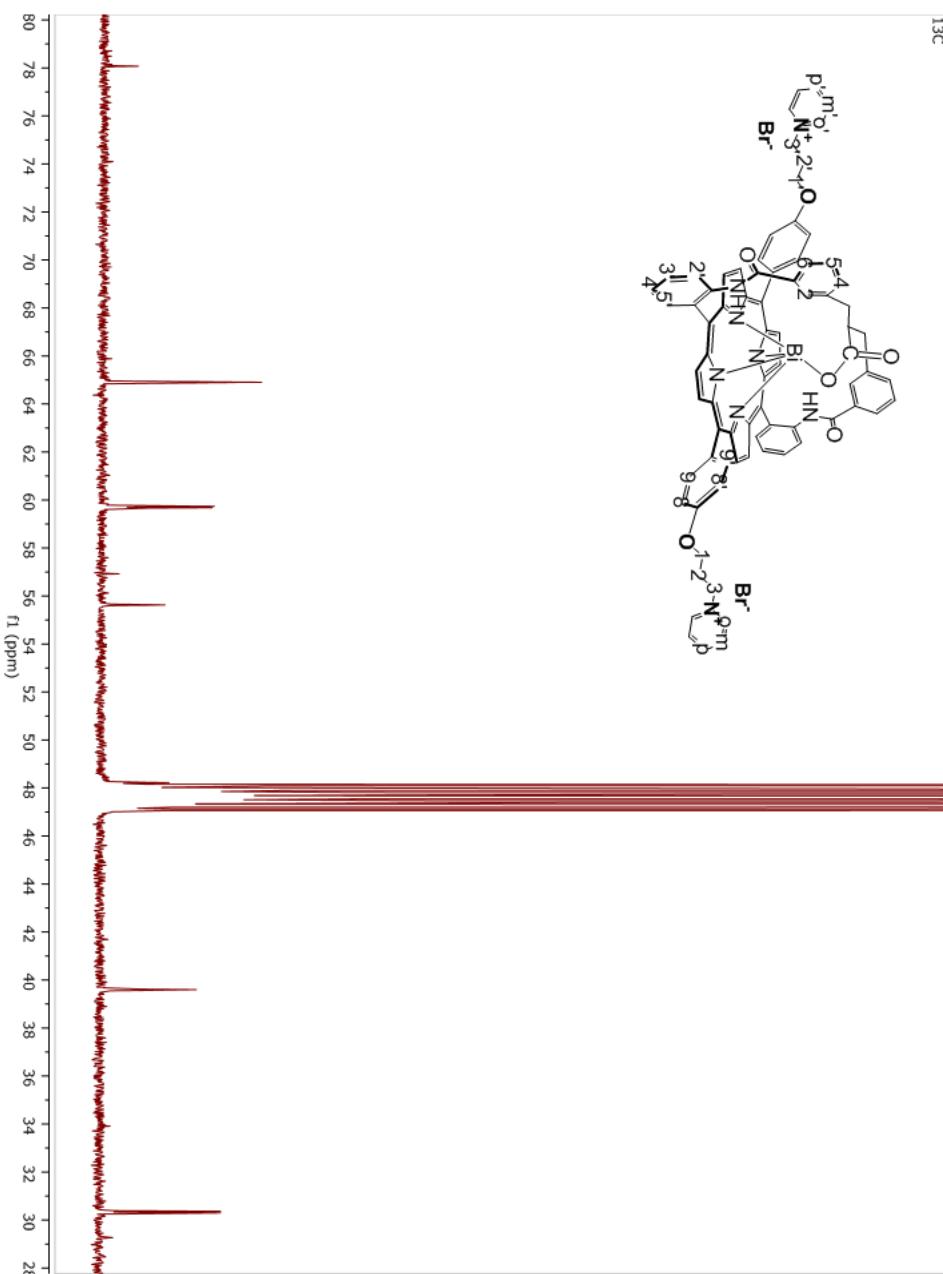
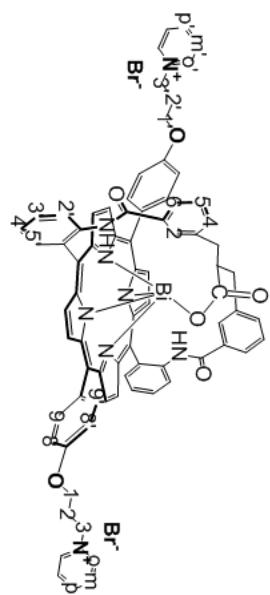




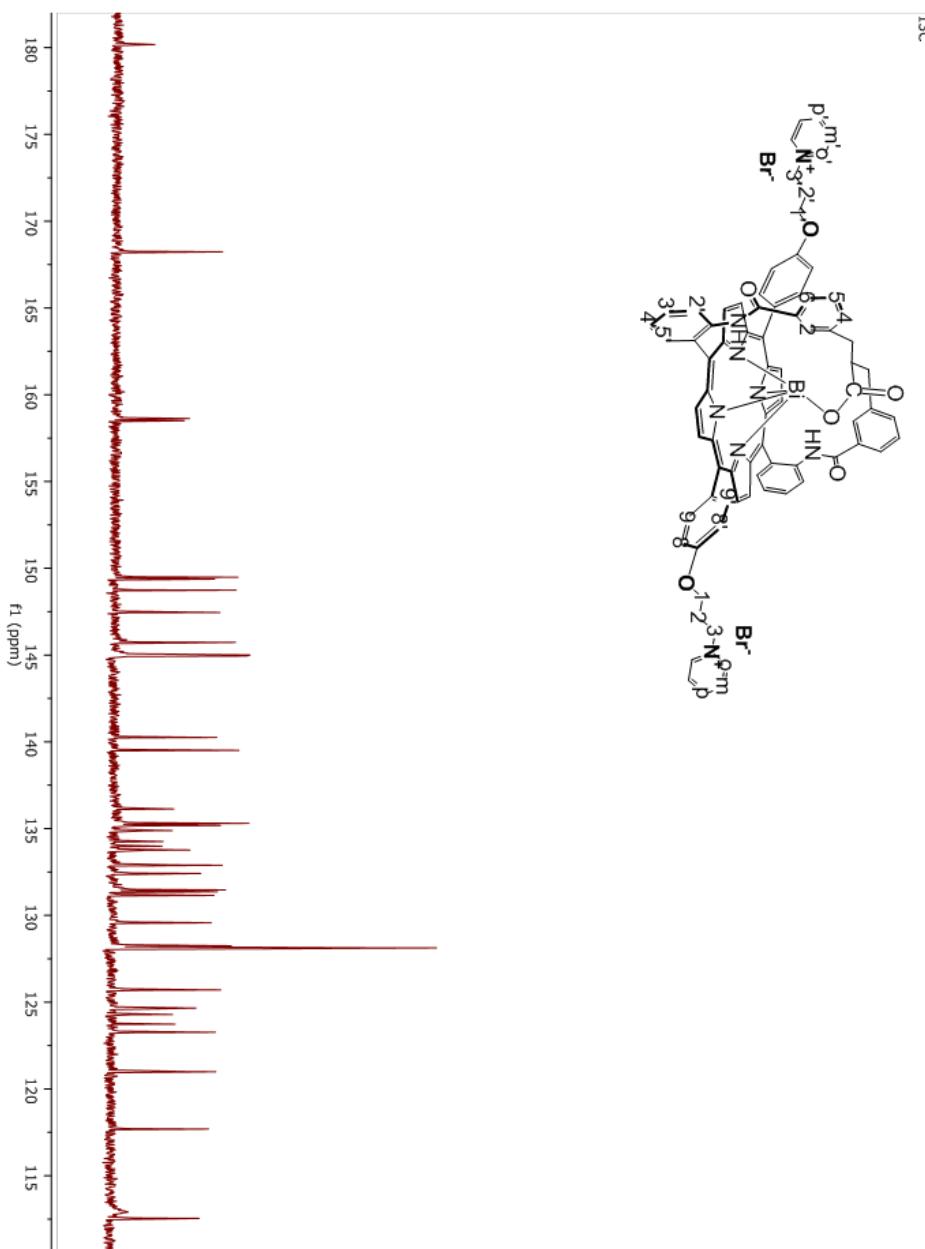
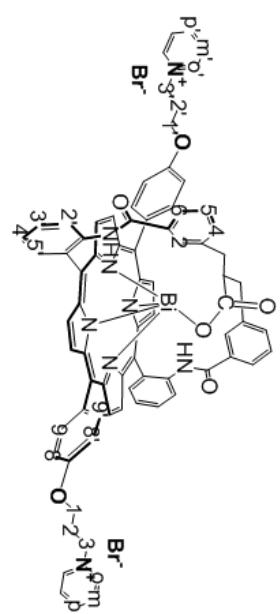




¹³C



¹³C



CRMPO

P. DAS 27 PJ Solvant : CH3CN

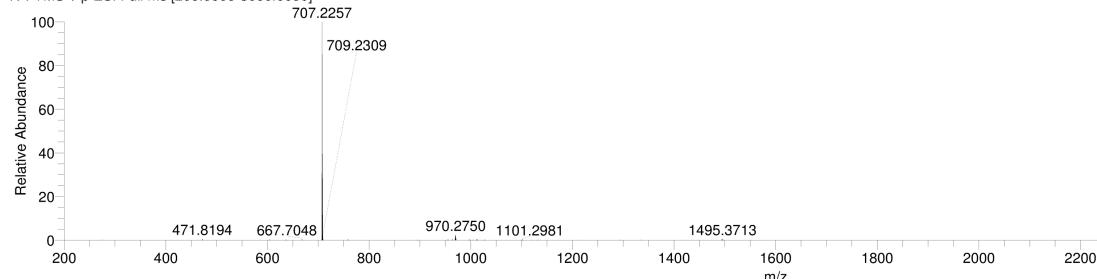
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Rapport d'analyse

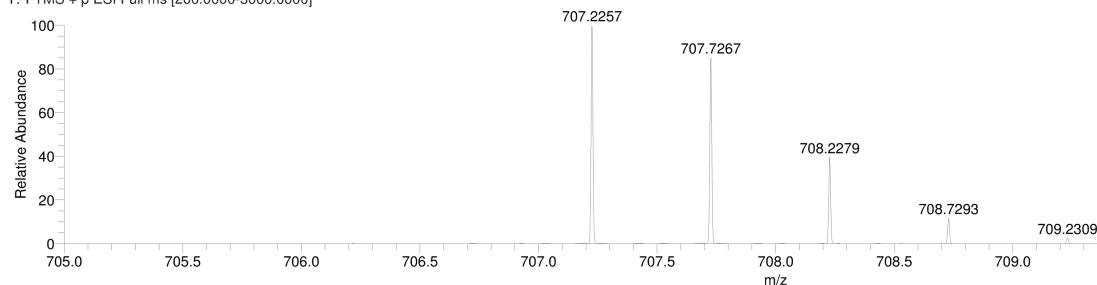
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Thermo Fisrh

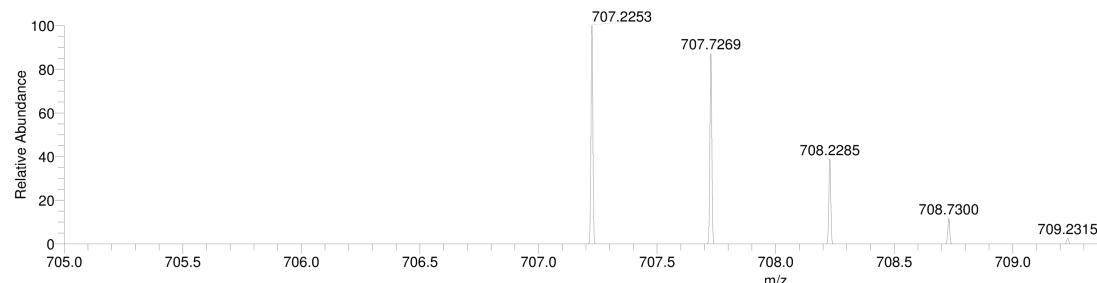
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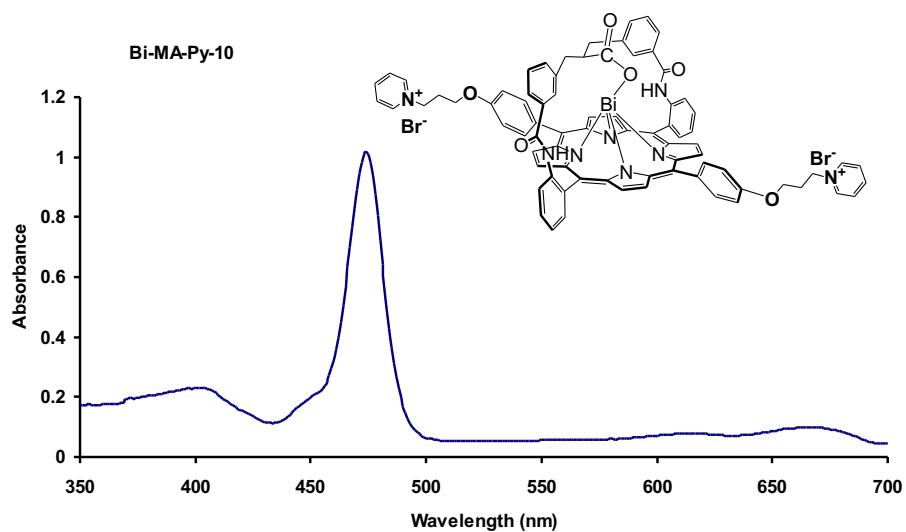


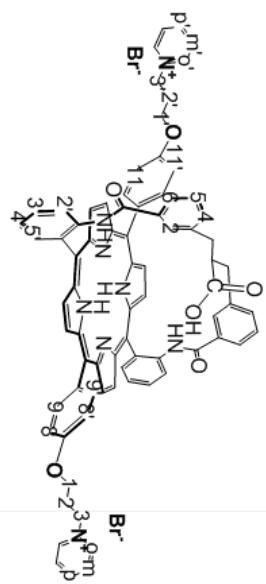
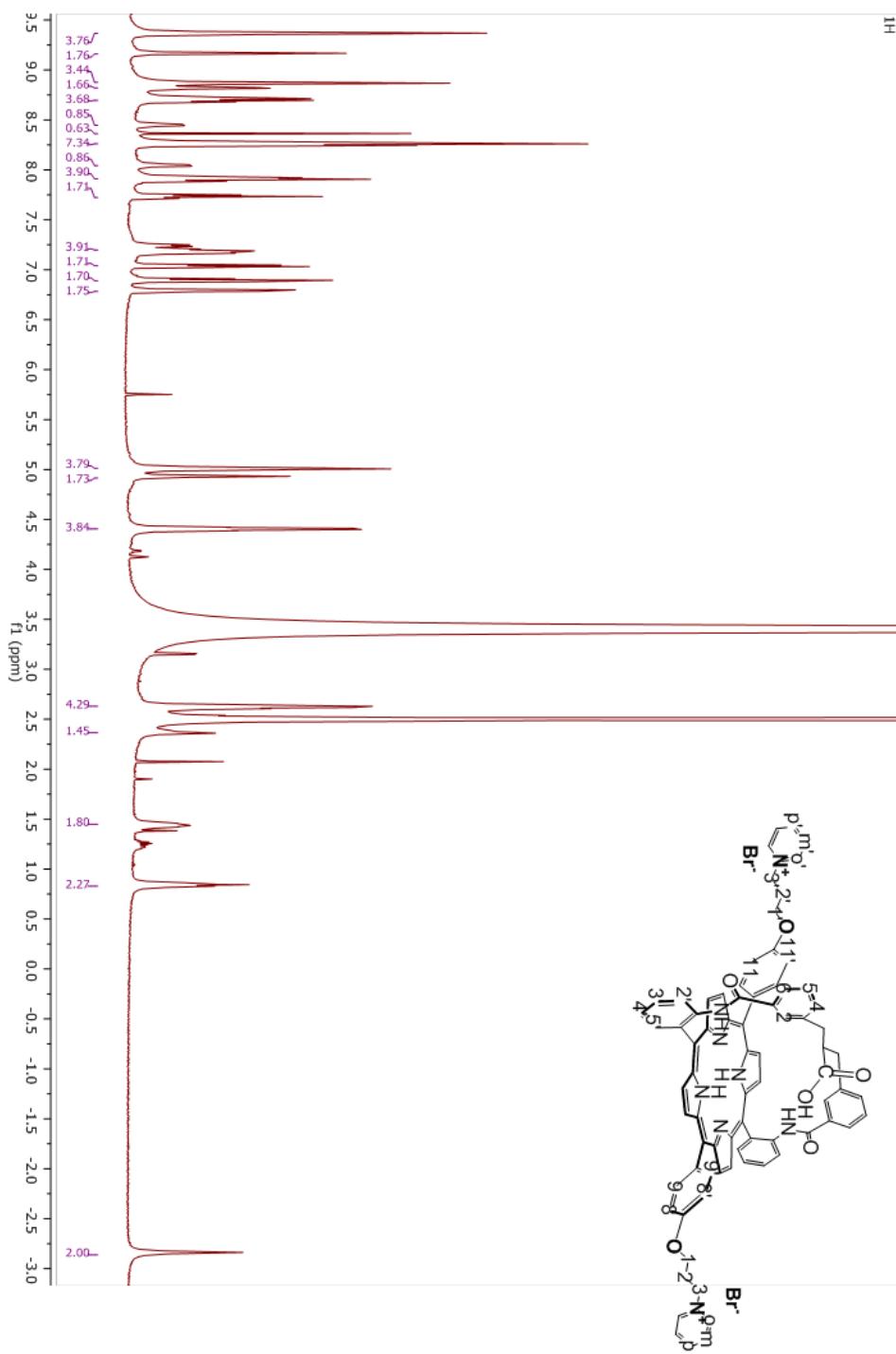
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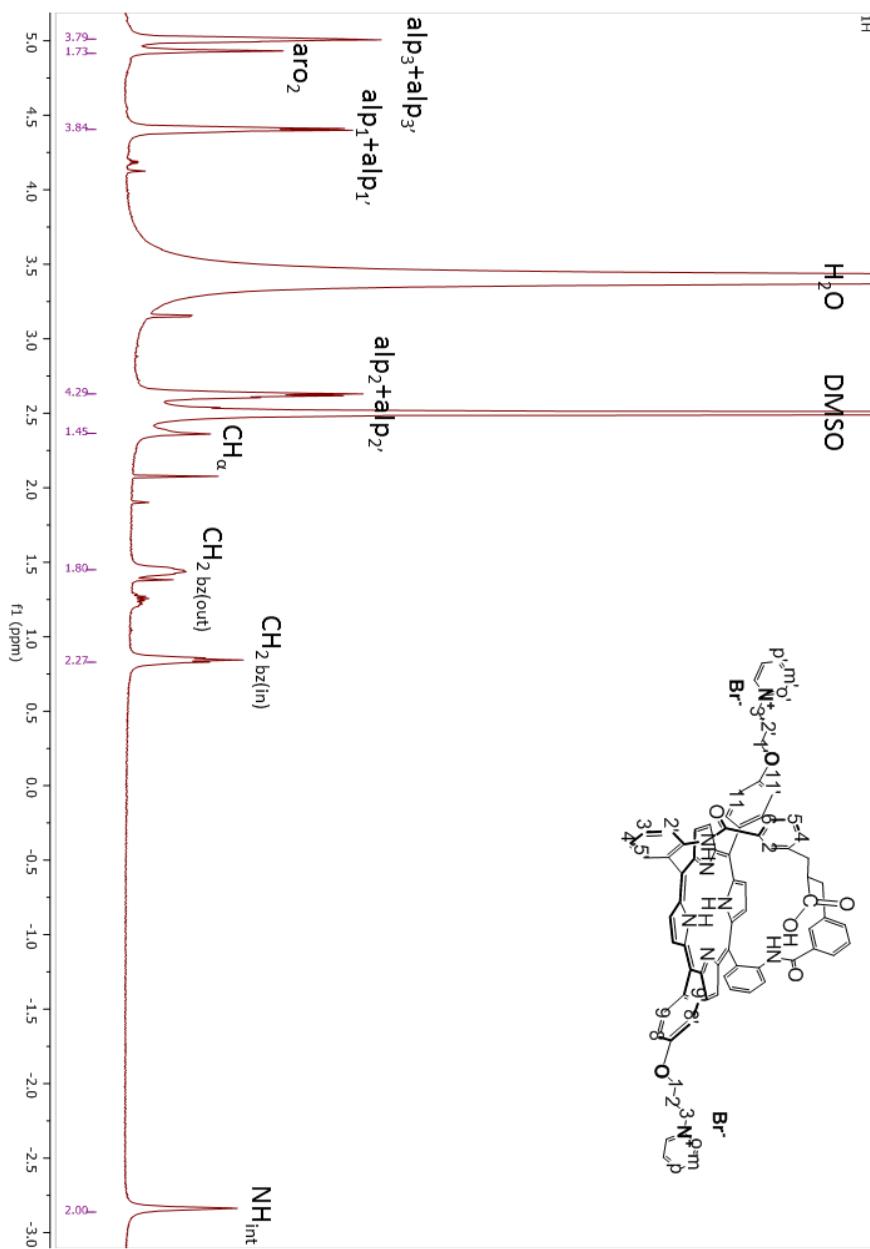


C78H61N8O6Bi: C78 H61 N8 O6 Bi1 p(gss, s/p:40) Chrg ...

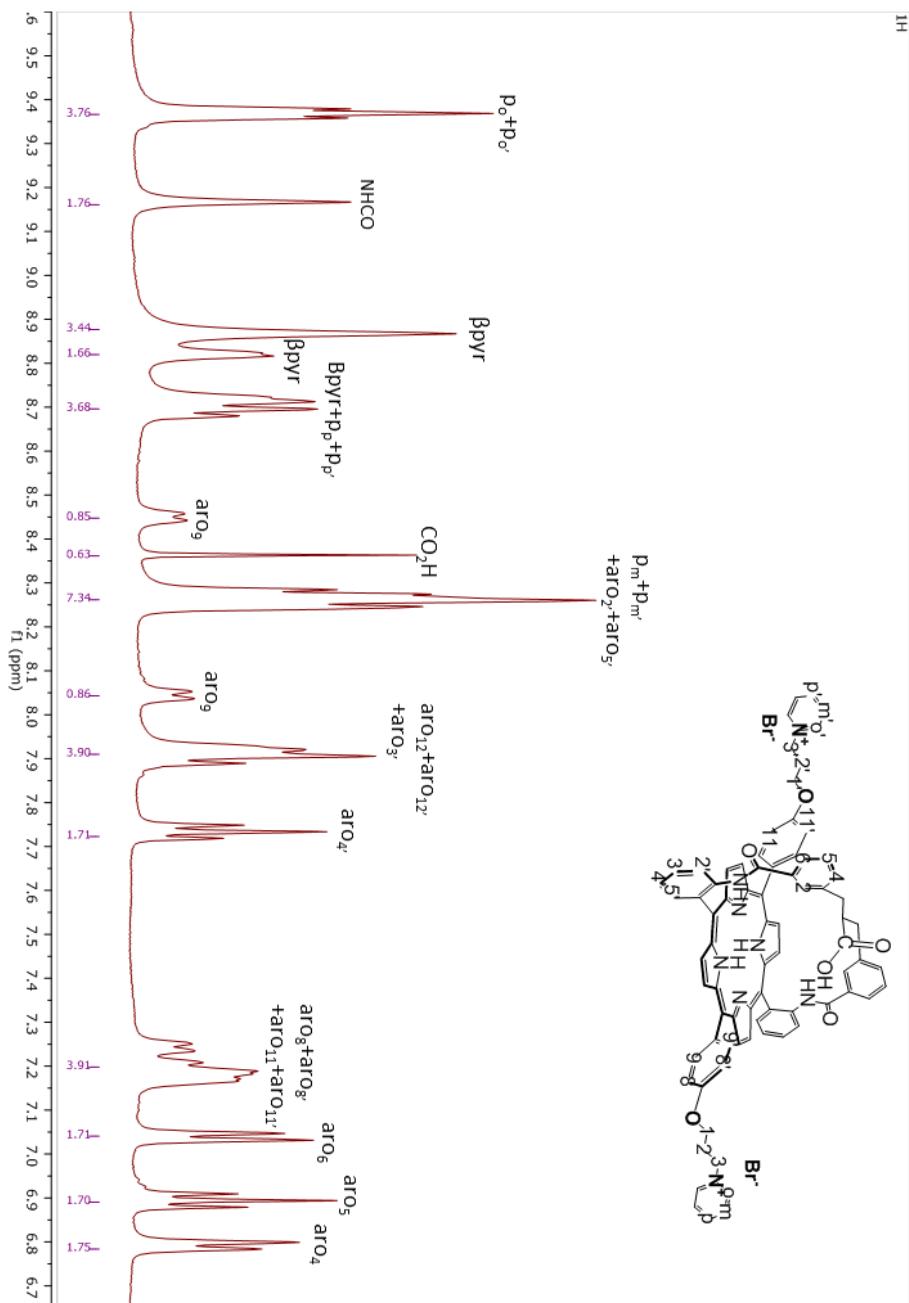


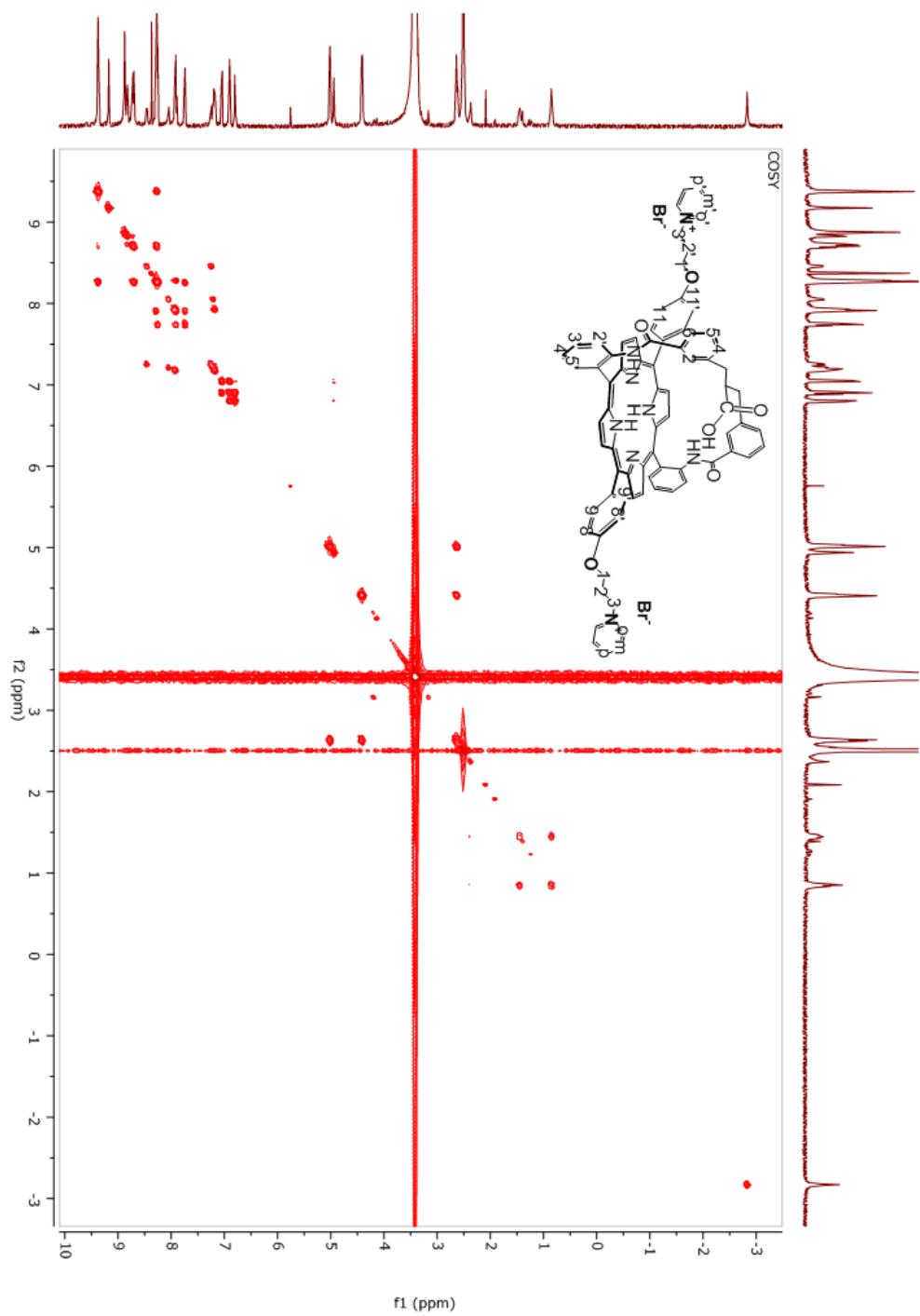


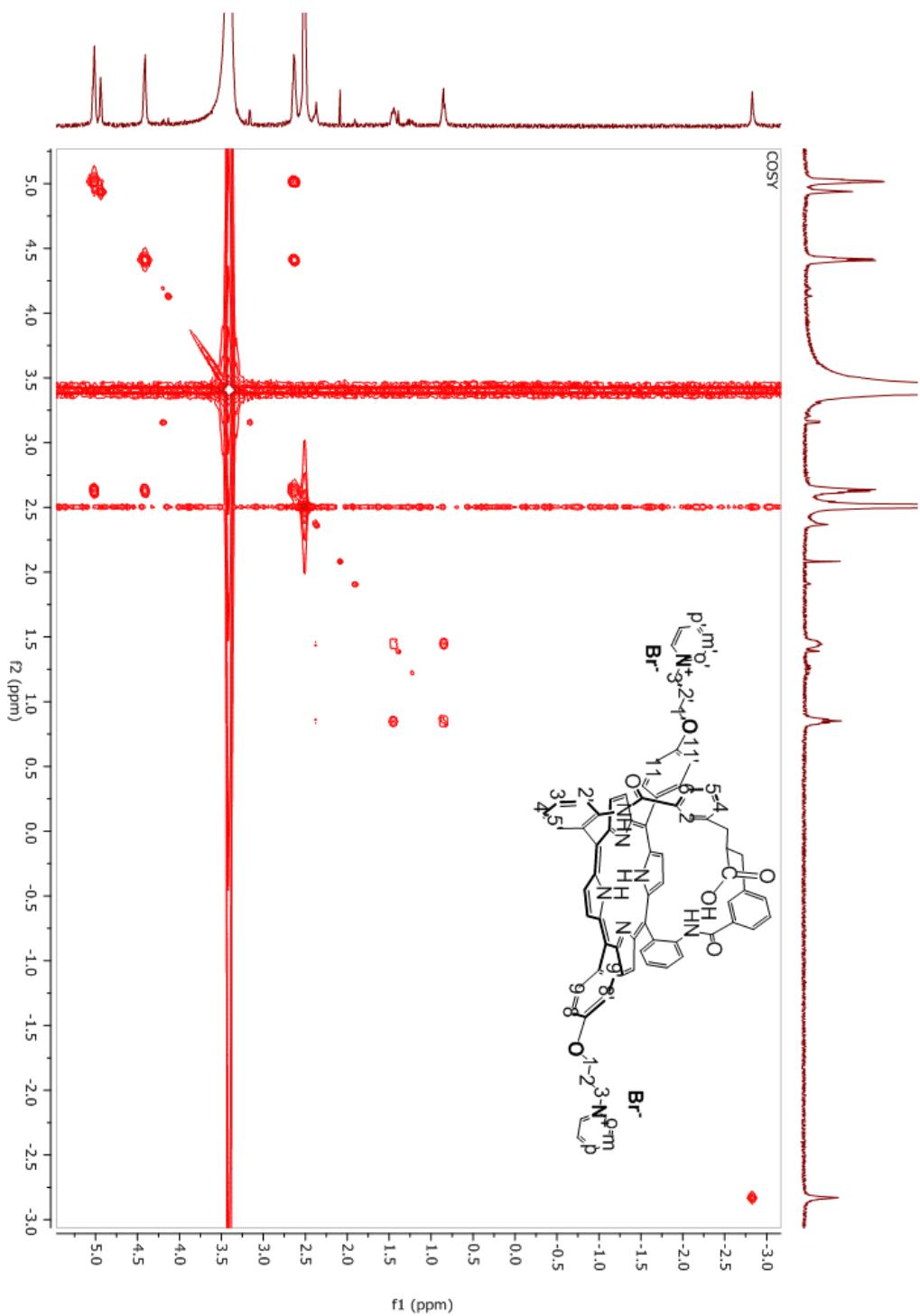


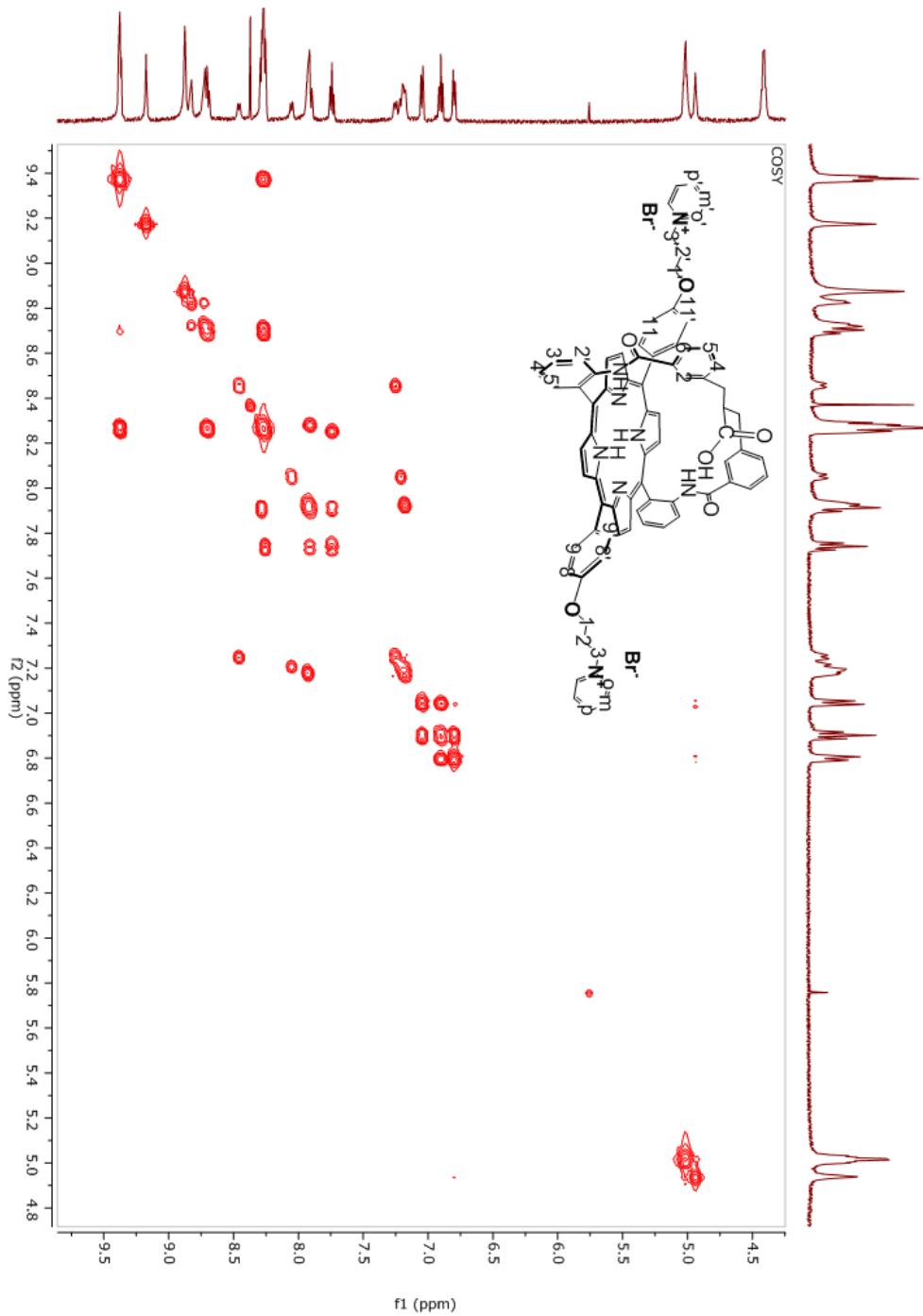


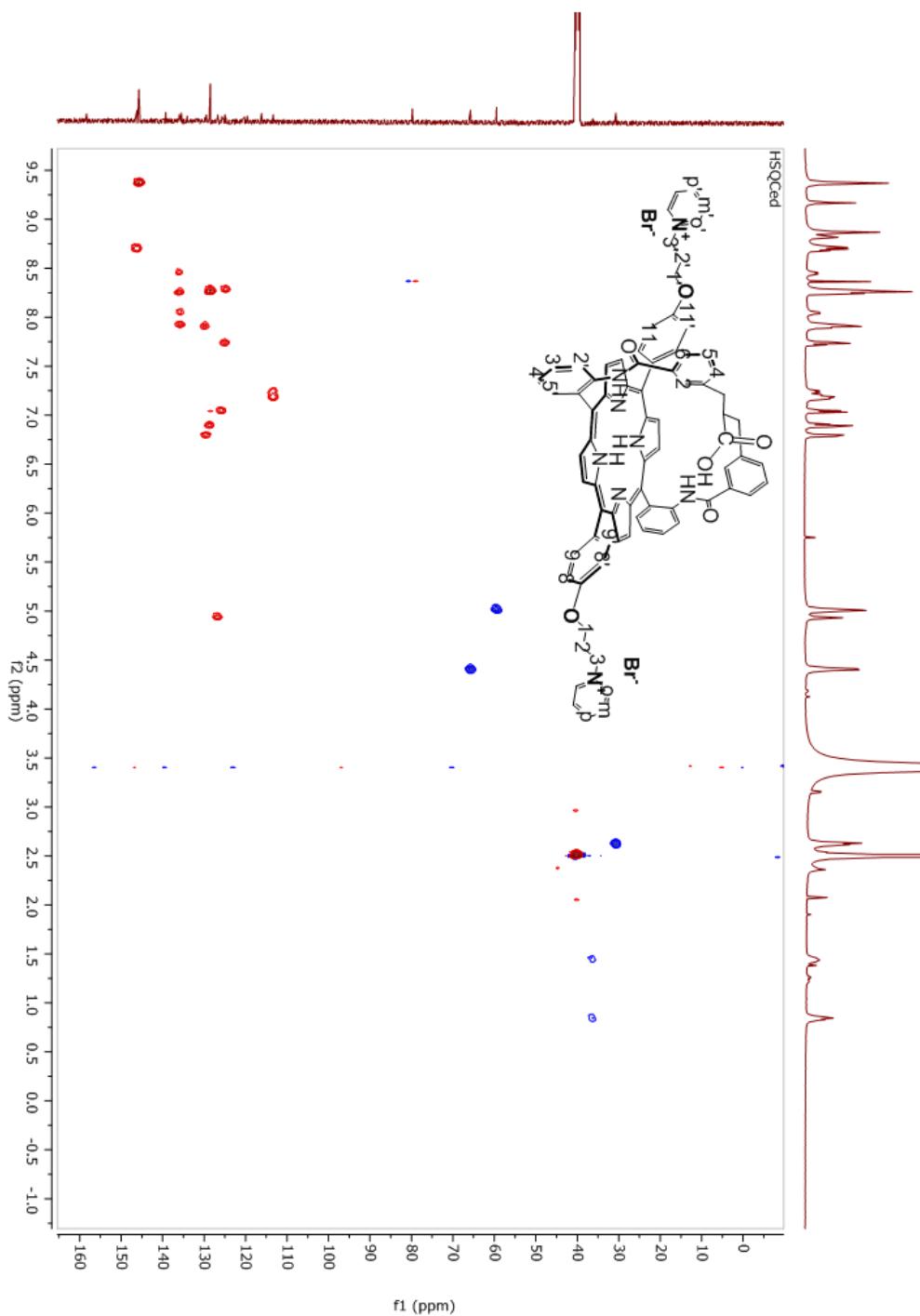
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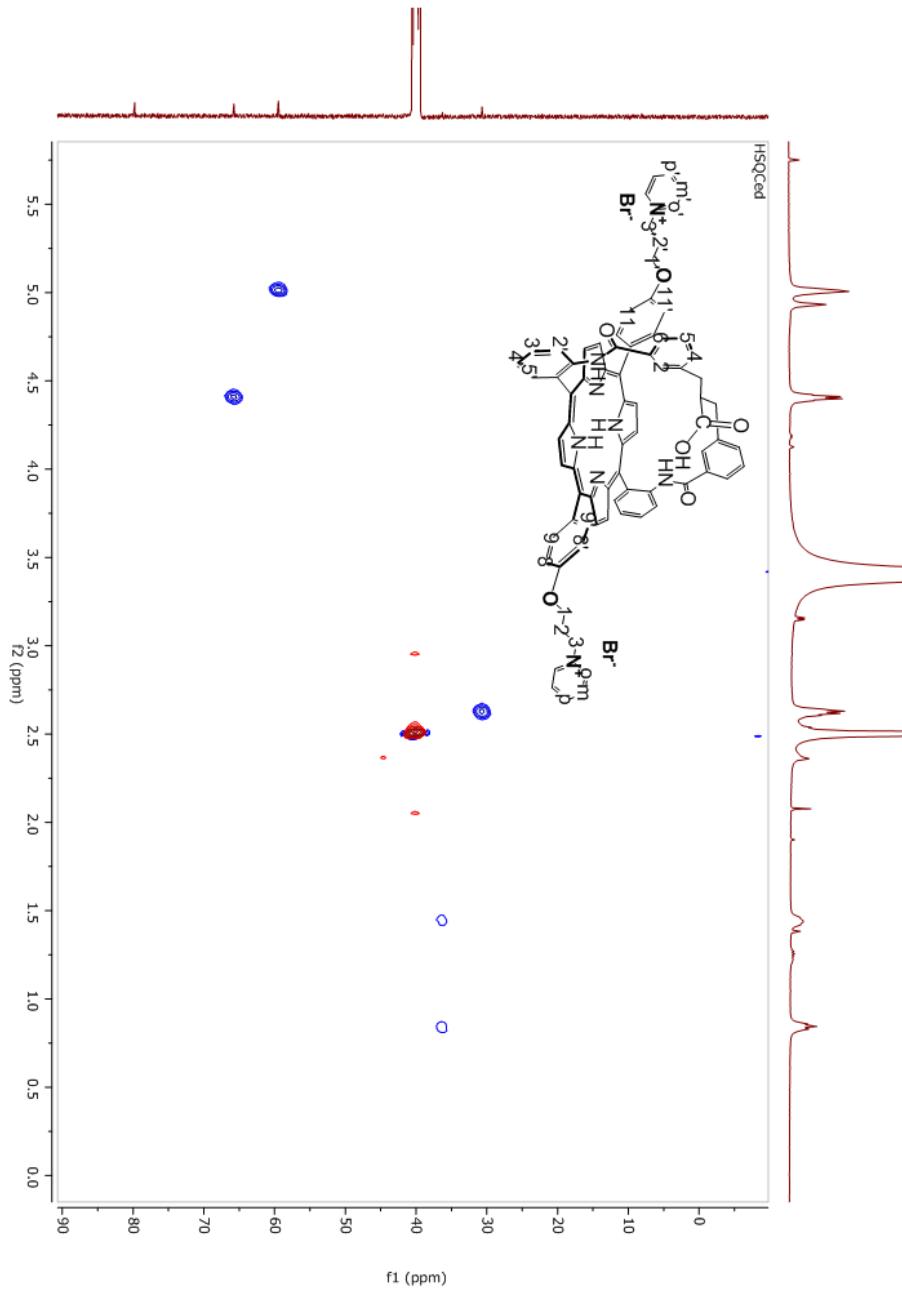


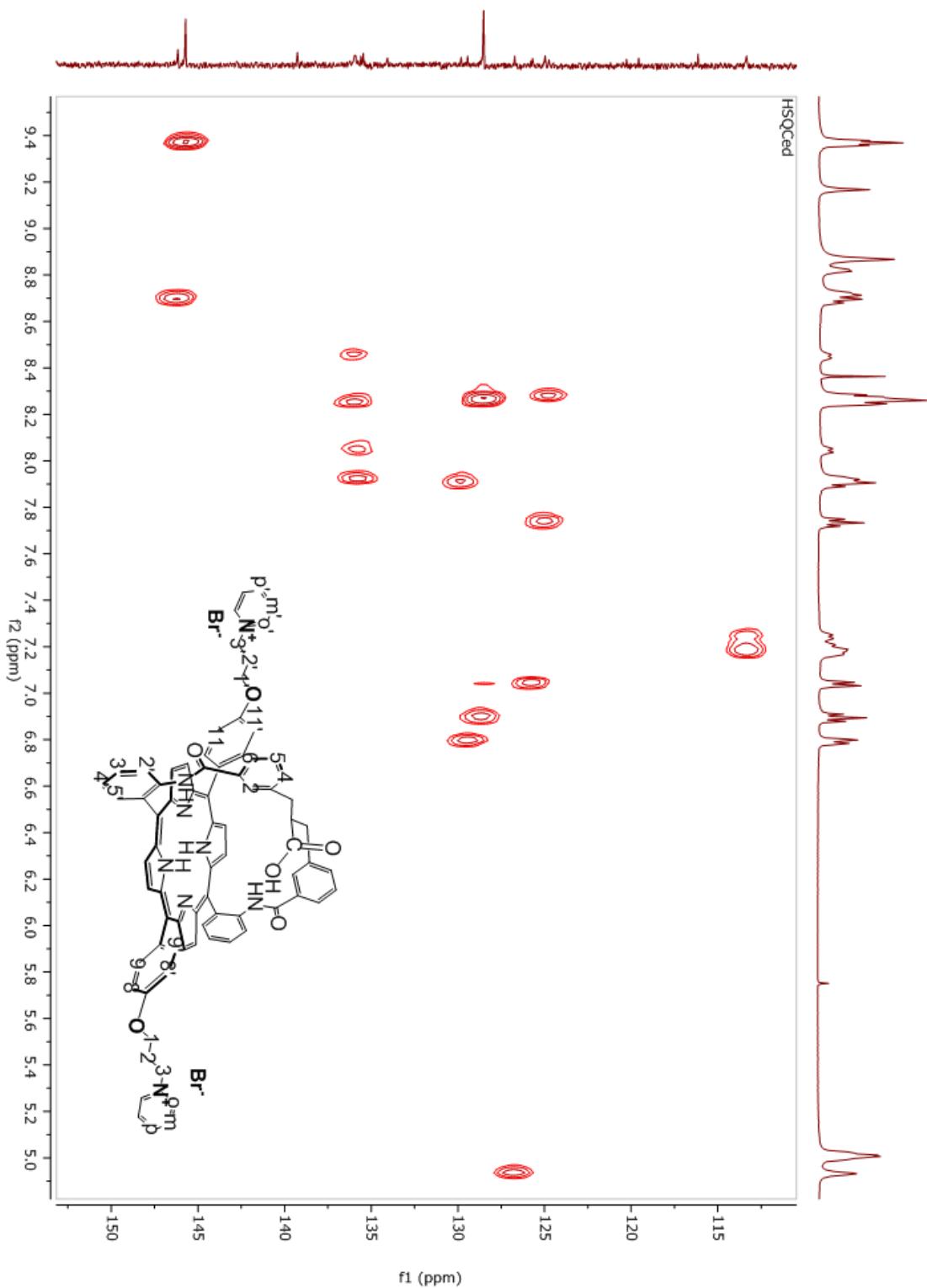


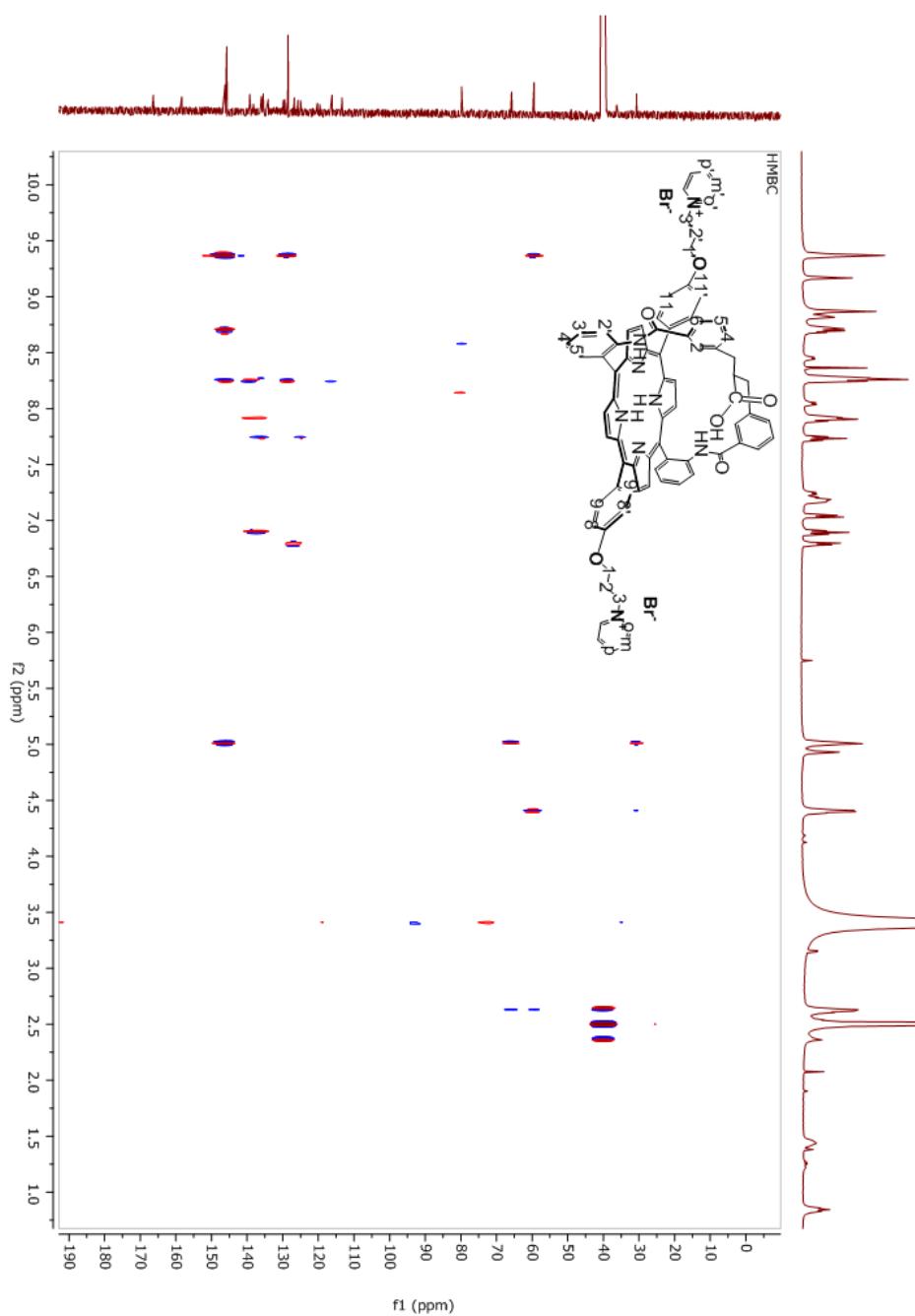


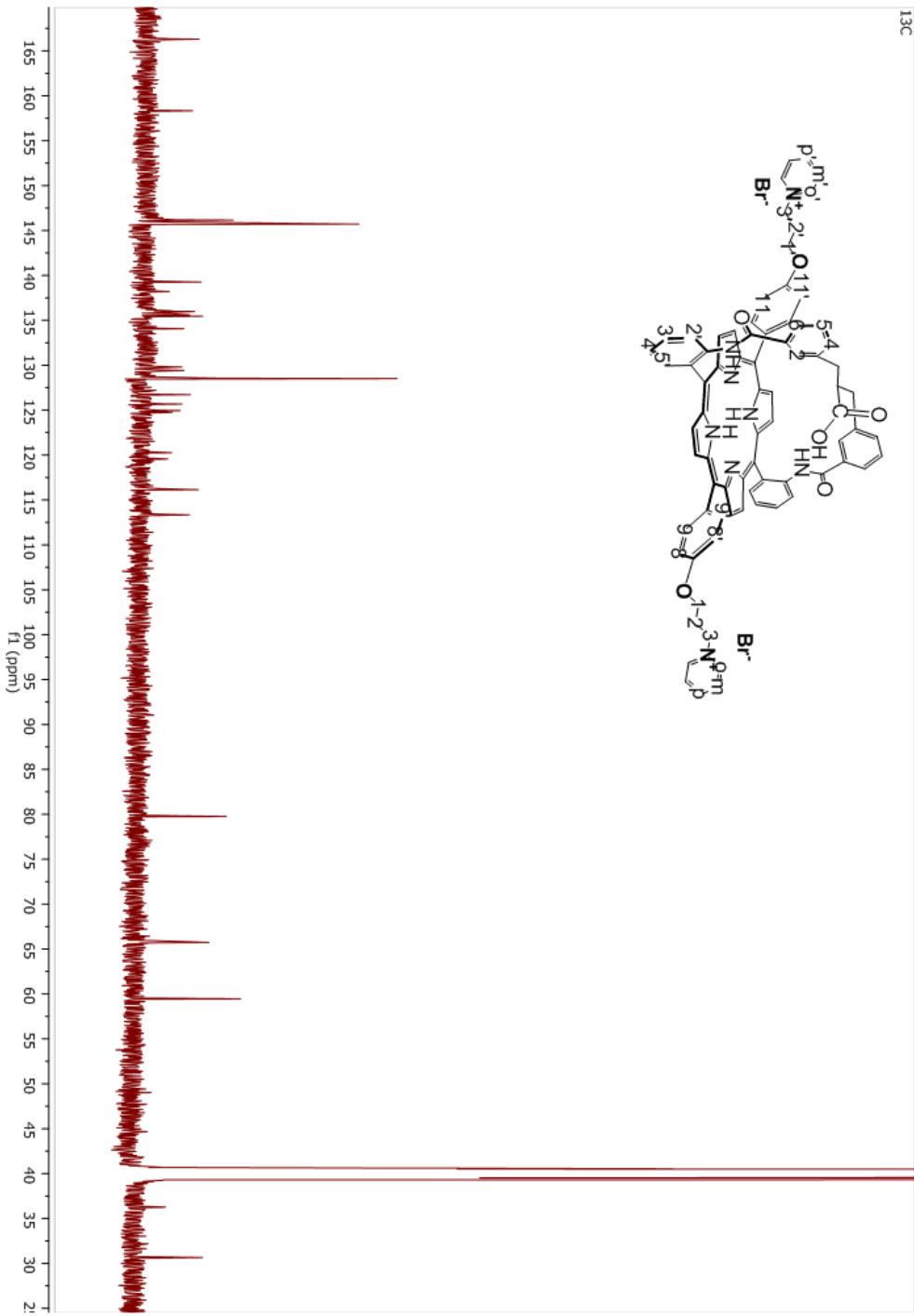




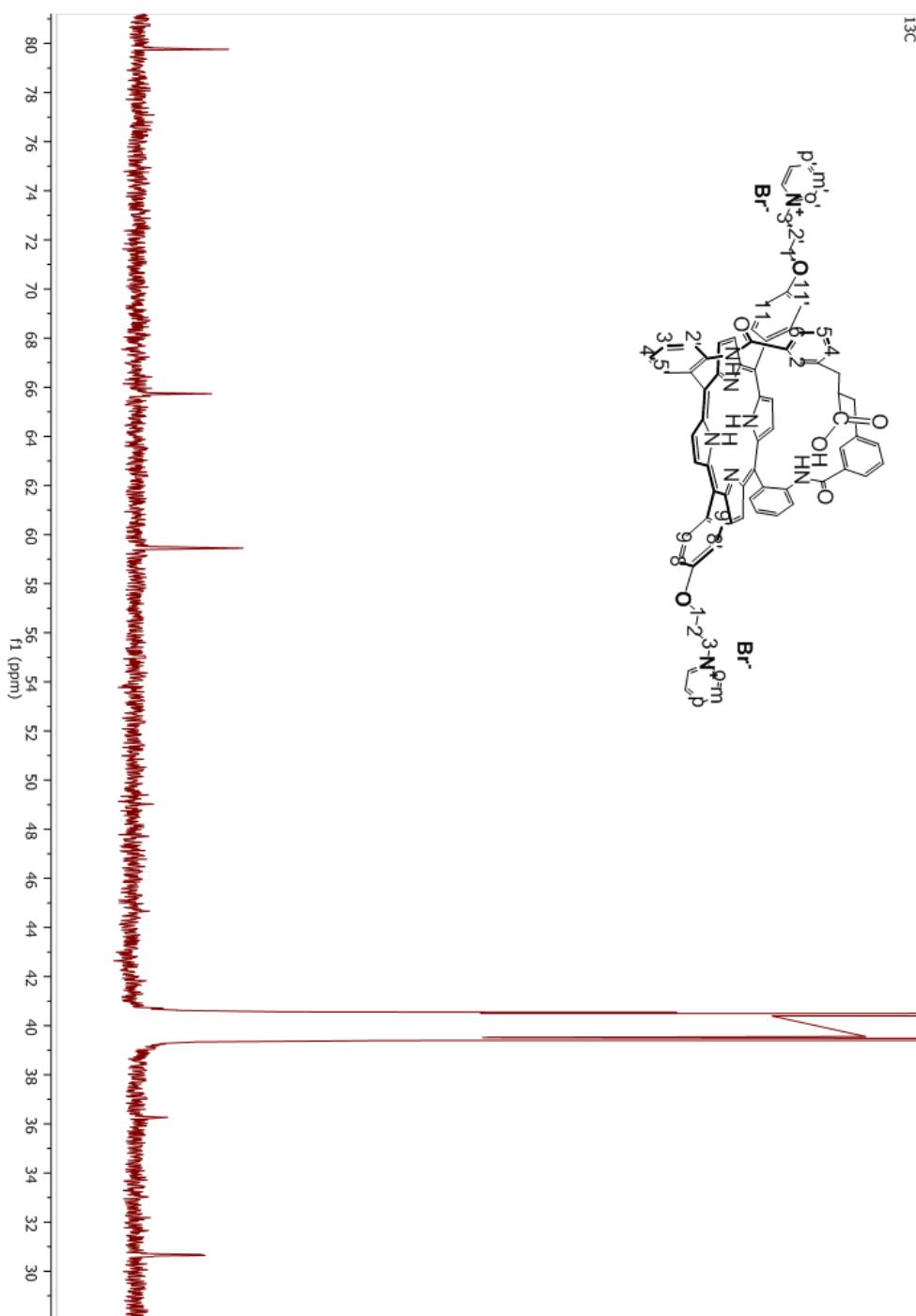
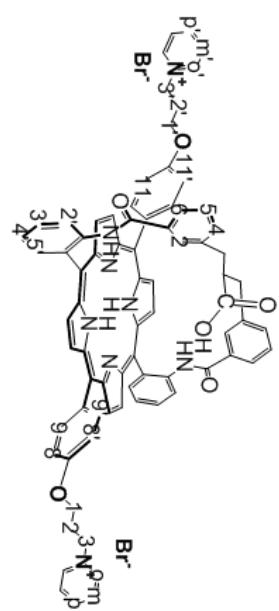




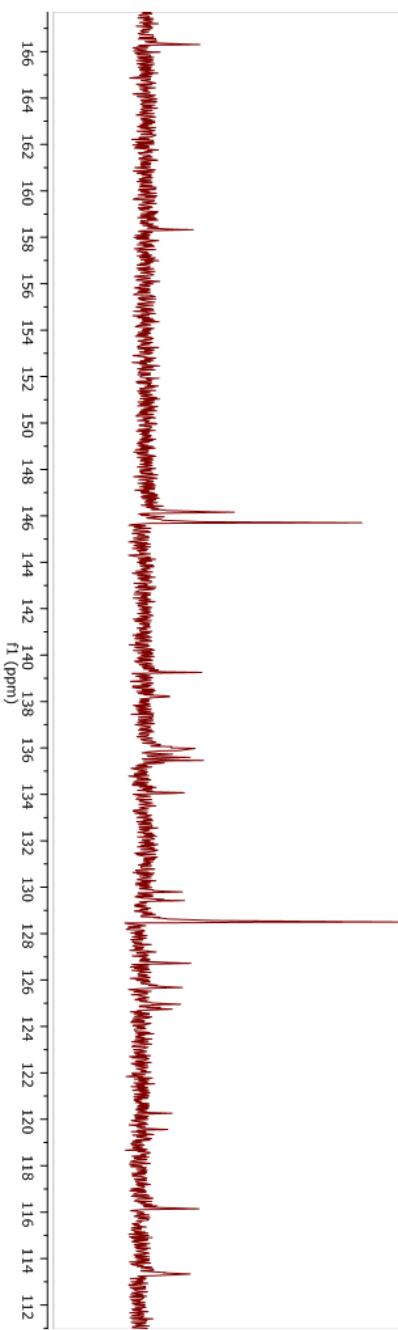
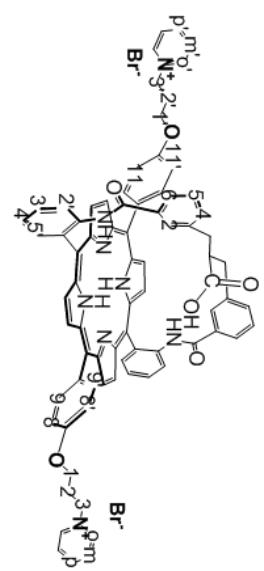




13C



13C

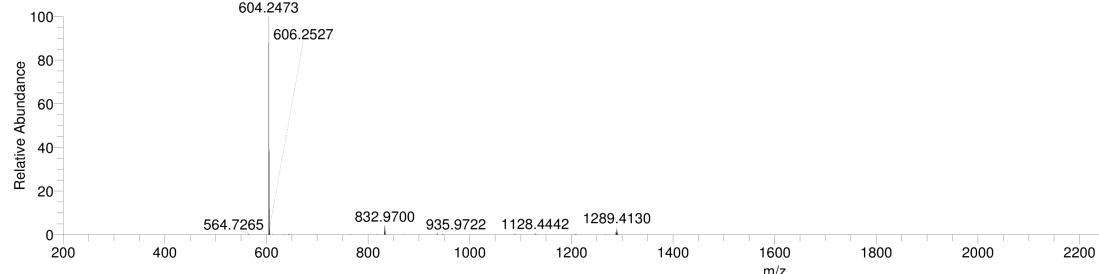


CRMPO
P. DAS 28 PJ Solvant : CH₂Cl₂
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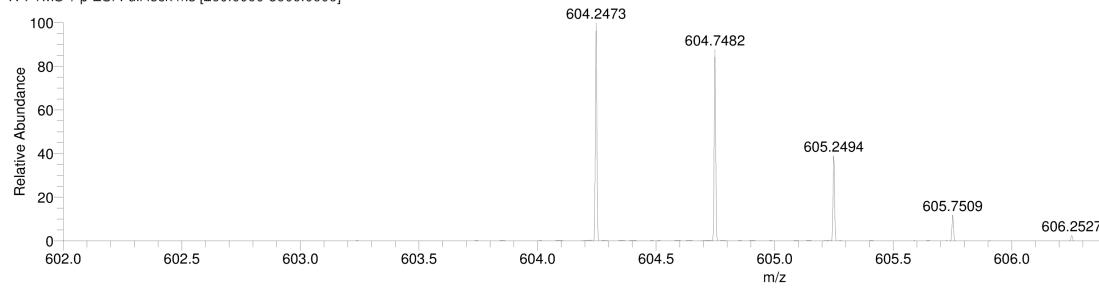
Rapport d'analyse
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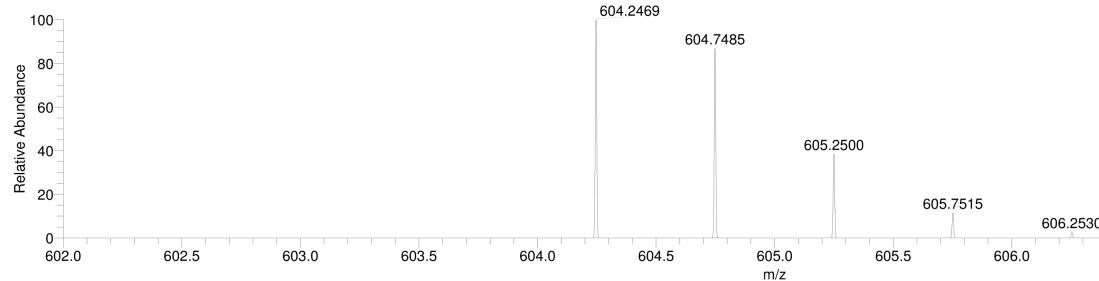
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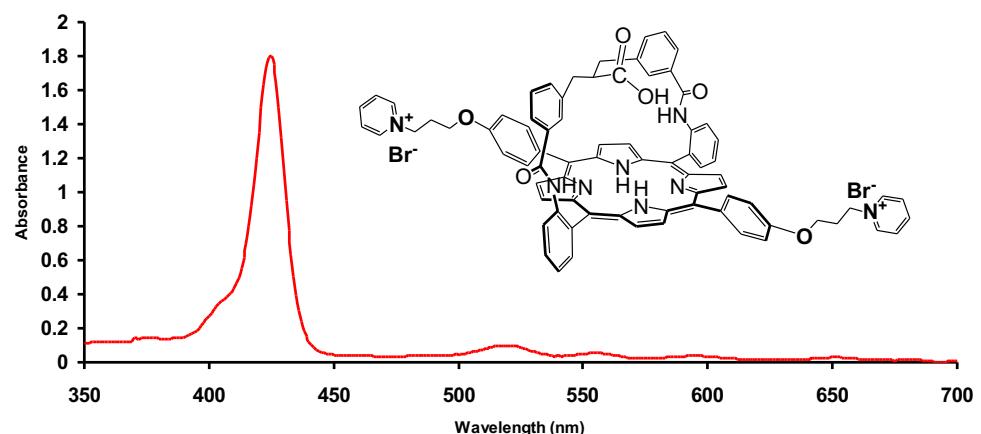
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C78H64N8O6: C78 H64 N8 O6 p(gss, s/p:40) Chrg 2R: ...



dPy-11



CRMPO

Rapport d'analyse

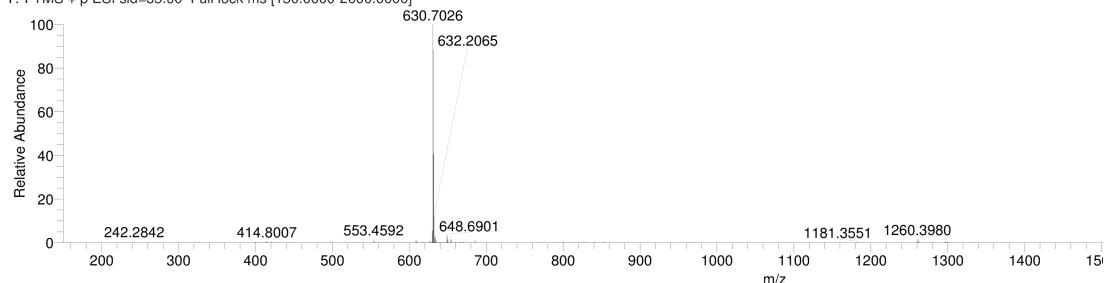
Thermo Fish

P. DAS 29 PJ Solvant : CH₂Cl₂ (+ 0.1% acide formique)

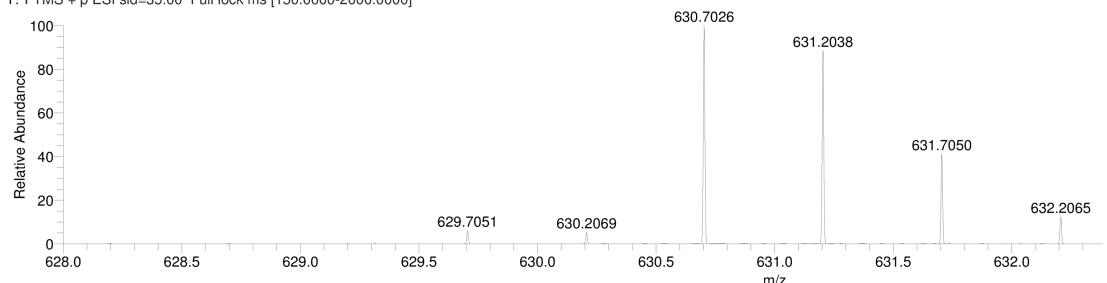
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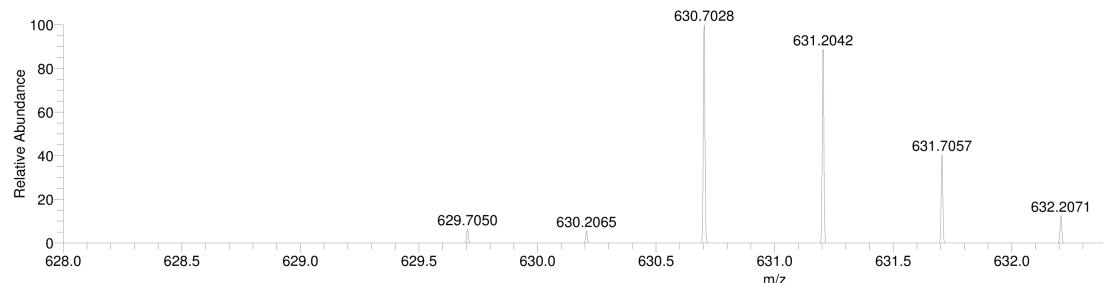
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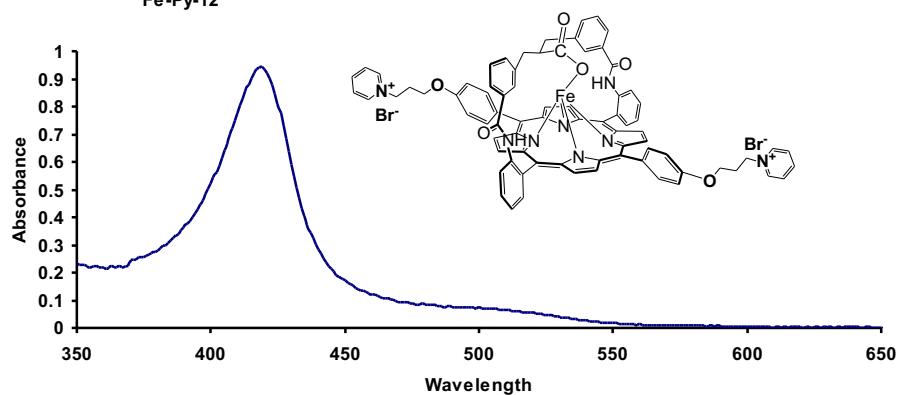
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T: FTMS + p ESI sid=35.00 Full lock ms [150.0000-2000.0000]



C78H61N8O6Fe: C78 H61 N8 O6 Fe1 p(gss, s/p:40) Chrg ...



Fe-Py-12



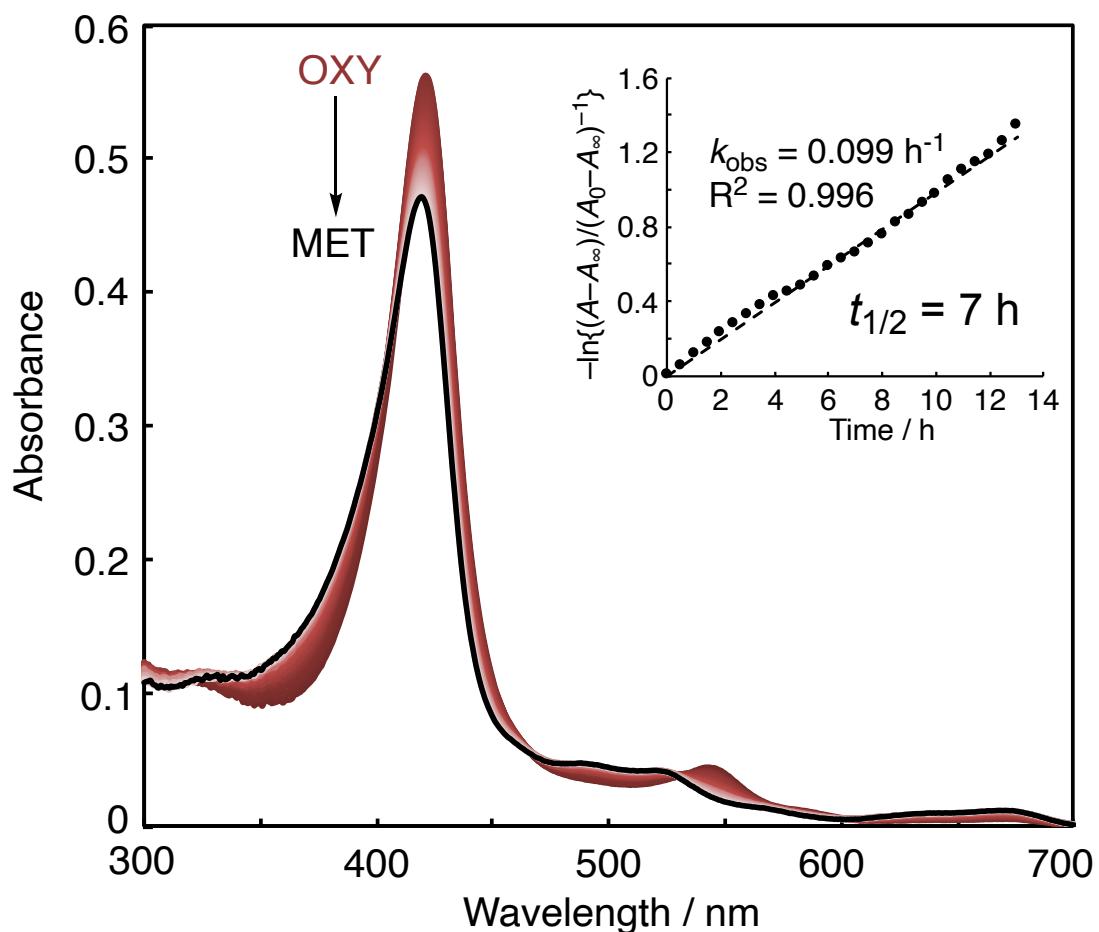


Figure S1. UV-vis spectral changes in autoxidation of the **O₂-Fe^{II}-PorCD-1** complex in 0.05 M phosphate buffer at pH 7.0 and 25°C. Scans were made at 30 min intervals. The first-order plot for the absorbance changes at 422 nm.

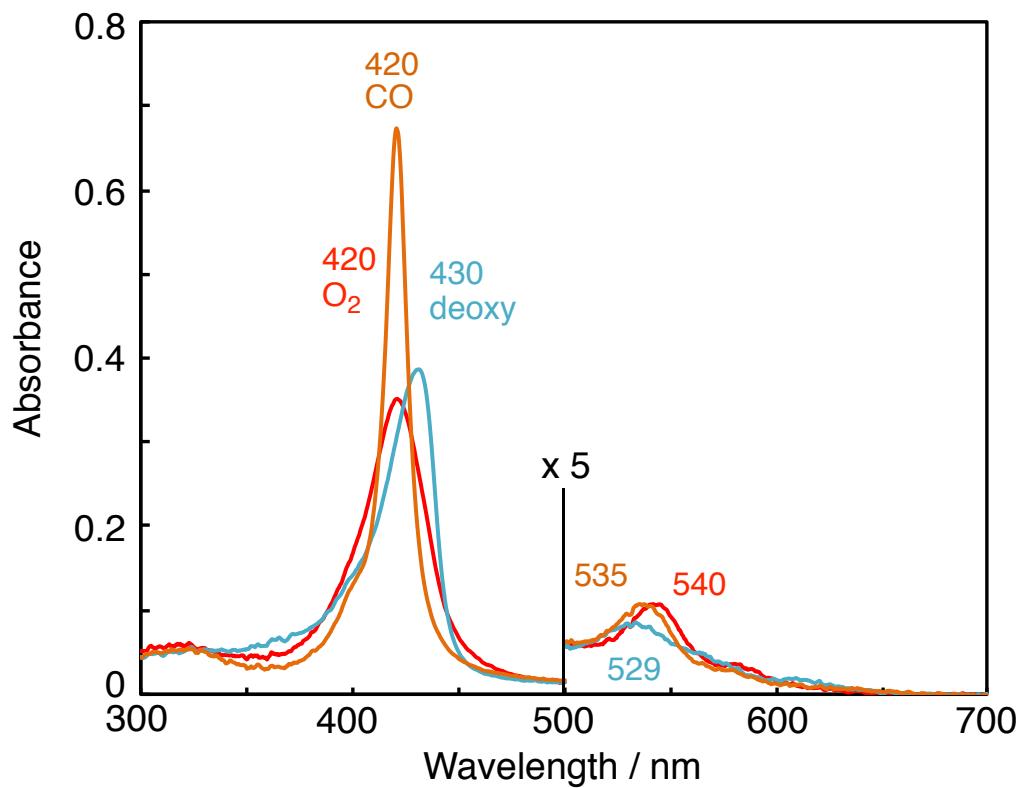


Figure S2. UV-vis spectra of the **Fe^{II}PorCD-2** complex in the deoxy (blue), oxy (red) and CO (orange) forms in 0.05 M phosphate buffer at pH 7.0 and 25°C.

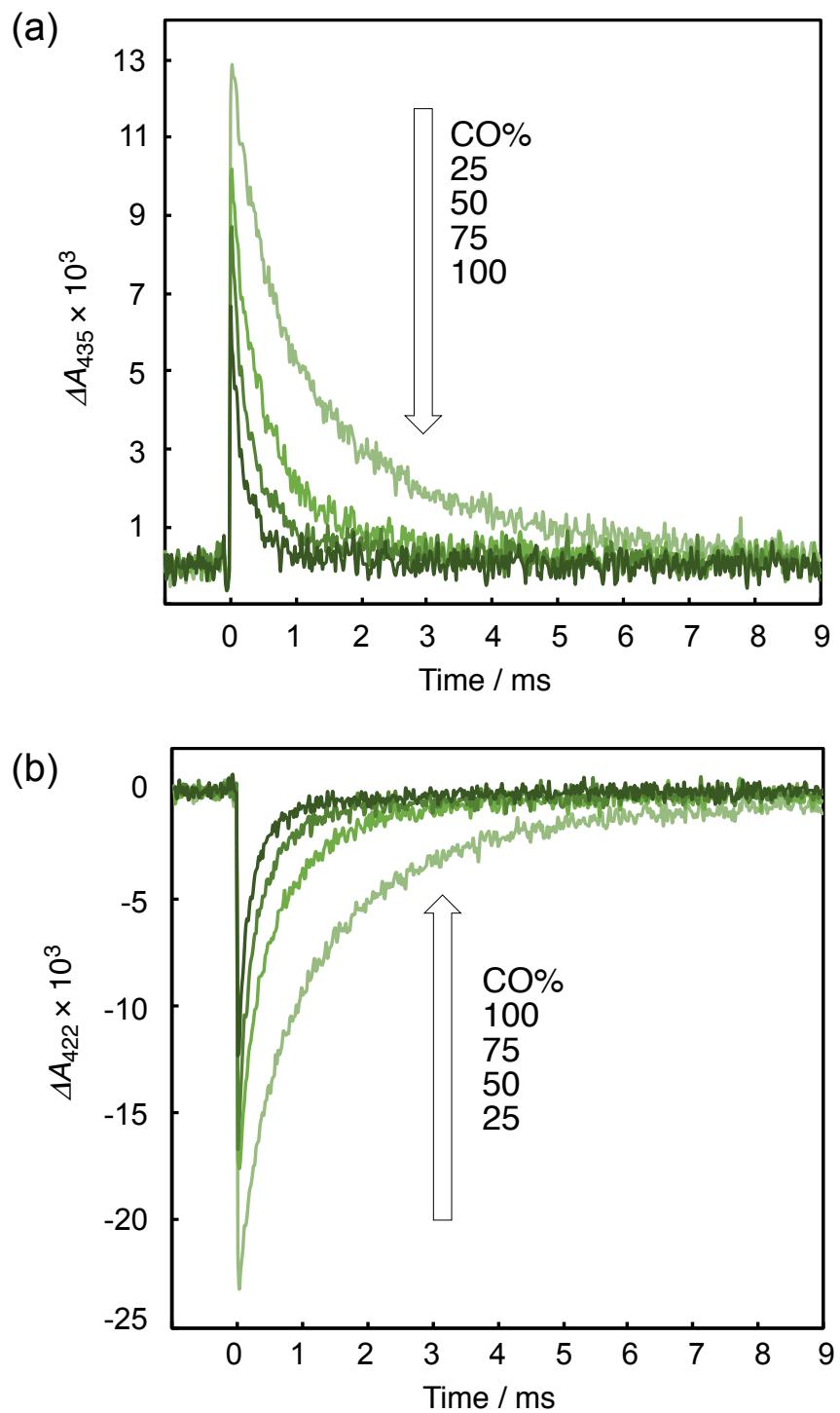


Figure S3. The time course absorption changes of **CO-Fe^{II}PorCD-1** after flash photolysis under the various partial pressures of CO in 0.05 M phosphate buffer at pH 7.0 and 25 °C (a) at 435 nm. (b) at 422 nm. The reactions were carried out by using a laser flash photolysis system with Nd: YAG laser (532 nm).

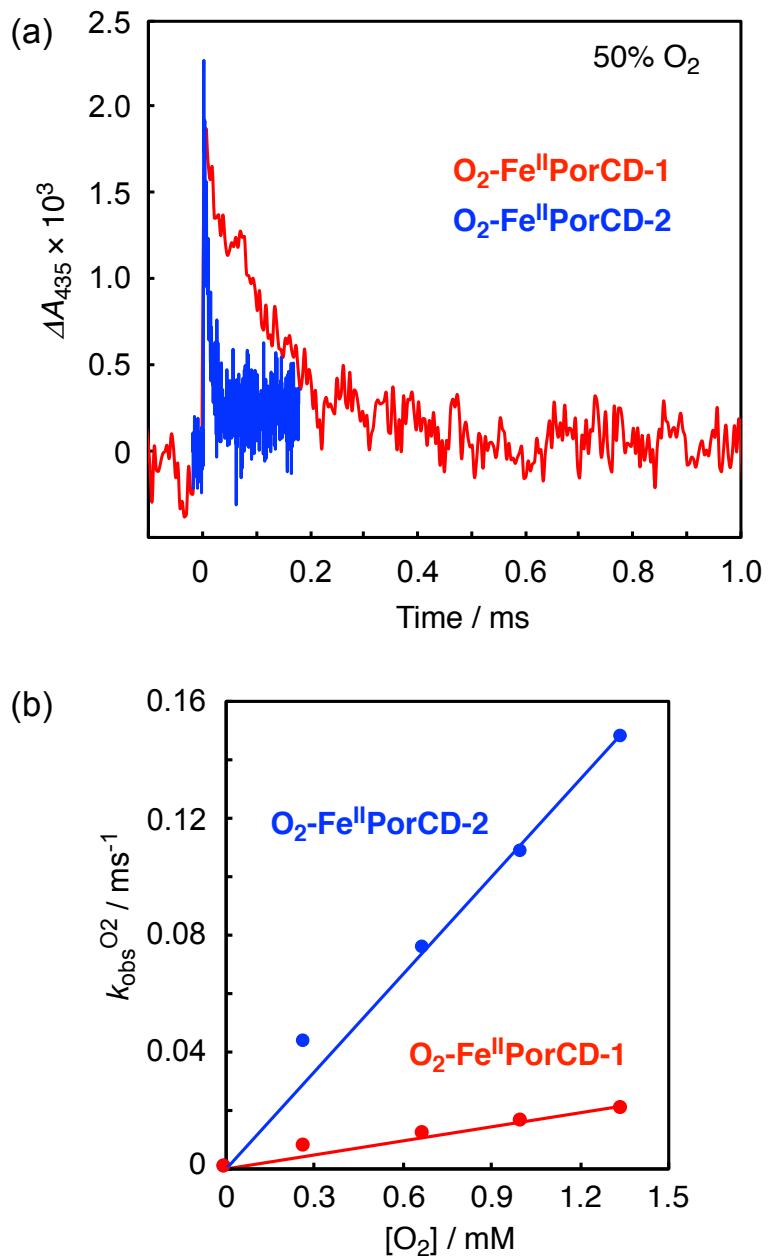


Figure S4. Laser flash photolysis for the kinetic study. (a) The time course for O_2 association with $\text{Fe}^{II}\text{PorCD-1}$ (red) and $\text{Fe}^{II}\text{PorCD-2}$ (blue) generated by laser flash irradiation (532 nm) to $O_2\text{-Fe}^{II}\text{PorCD-1}$ and $O_2\text{-Fe}^{II}\text{PorCD-2}$, respectively, in 0.05 M phosphate buffer at pH 7.0 and 25°C. (b) Plots for the observed rate constants, $k_{\text{obs}} O_2$, for O_2 association with $\text{Fe}^{II}\text{PorCD-1}$ (red) and $\text{Fe}^{II}\text{PorCD-2}$ (blue) versus $[O_2]$. The second order rate constants ($k_{\text{on}} O_2$) were determined from the slope of the linear regression lines.