Supplementary Information

Novel Hydroxytyrosol Esters as Potential Anti-Amyloid and Neuroprotective Agents for Alzheimer's Disease

Ioanna Kalpaktsi[1], Anthi Panara[2], Barbara Mavroidi[3], Giorgos Garcia Niforos[4], Amalia D. Kalampaliki[1], Ioanna C. Vlachogianni[5], Eleftheria A. Georgiou,[1] Elizabeth Fragopoulou[5], Anthony Tsarbopoulos[6], Alexios-Leandros Skaltsounis[7], Maria Pelecanou[8], Kontantinos Palikaras[4], Evangelos Gikas[2], Ioannis K. Kostakis[1,*]

[1]Division of Pharmaceutical Chemistry, Department of Pharmacy, National and Kapodistrian University of Athens, Panepistimiopolis Zografou 15771, Athens, Greece
[2]Laboratory of Analytical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis, Zografou, Athens 15771, Greece.
[3]Institute of Biosciences & Applications, National Centre for Scientific Research "Demokritos", 15310 Athens, Greece
[4]Department of Physiology, Medical School, National and Kapodistrian University of Athens, Athens 11527, Athens, Greece
[5]Department of Nutrition & Dietetics, School of Health Sciences and Education, Harokopio University, Athens, Greece
[6]Department of Pharmacology, Medical School, National and Kapodistrian University of Athens, 11527 Athens, Greece
[7]Division of Pharmacognosy and Natural Products Chemistry, Department of Pharmacy, National and Kapodistrian University of Athens, Panepistimiopolis Zografou 15771, Athens, Greece

* Corresponding author.

E-mail address: ikkostakis@pharm.uoa.gr (IKK).

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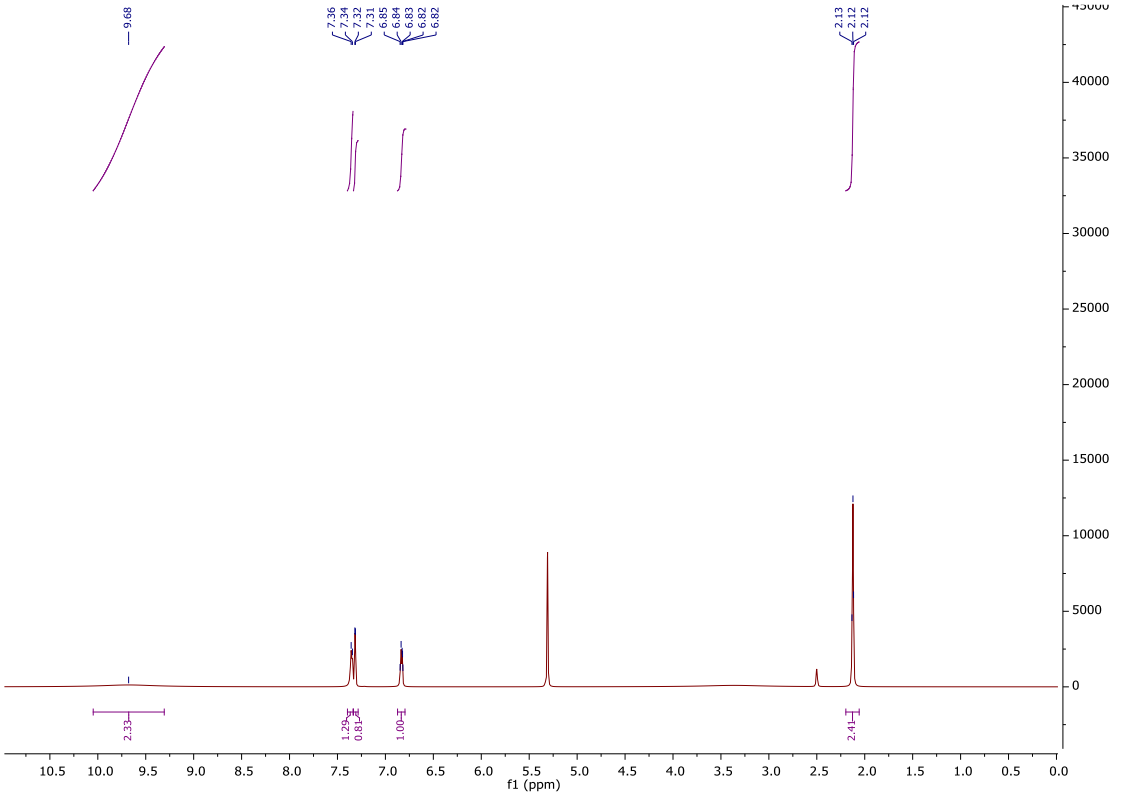
NMR Spectra



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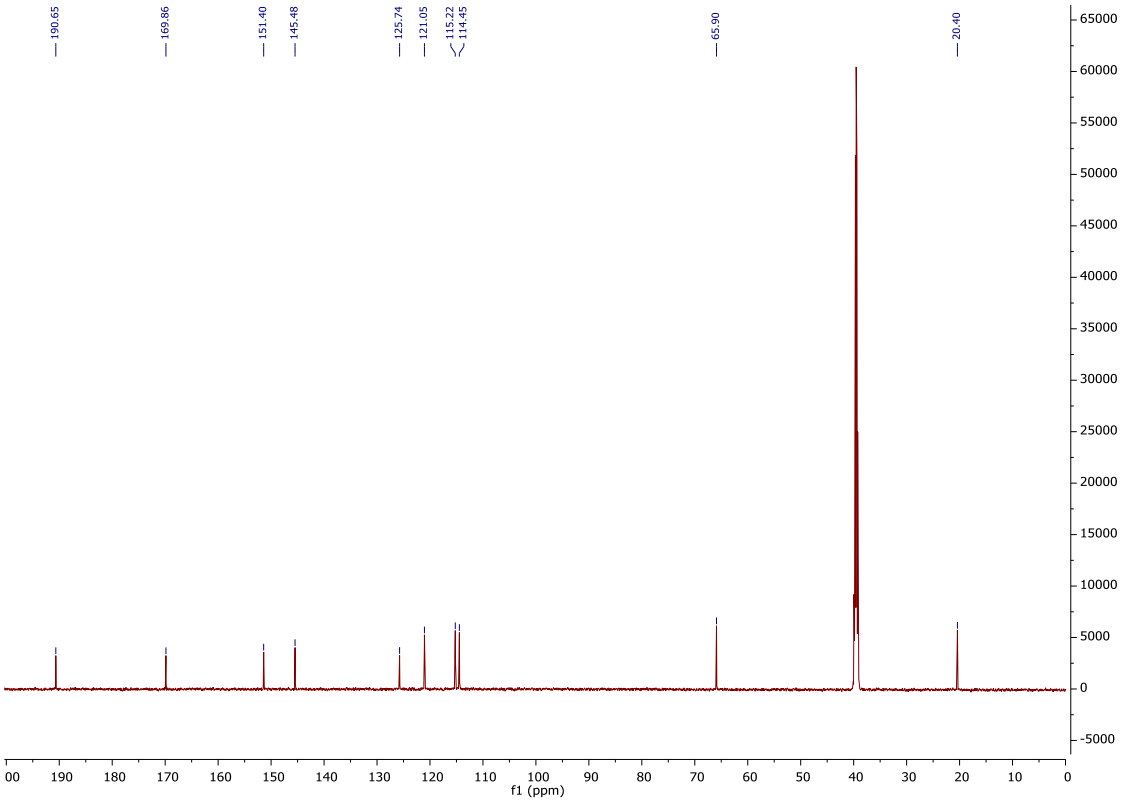

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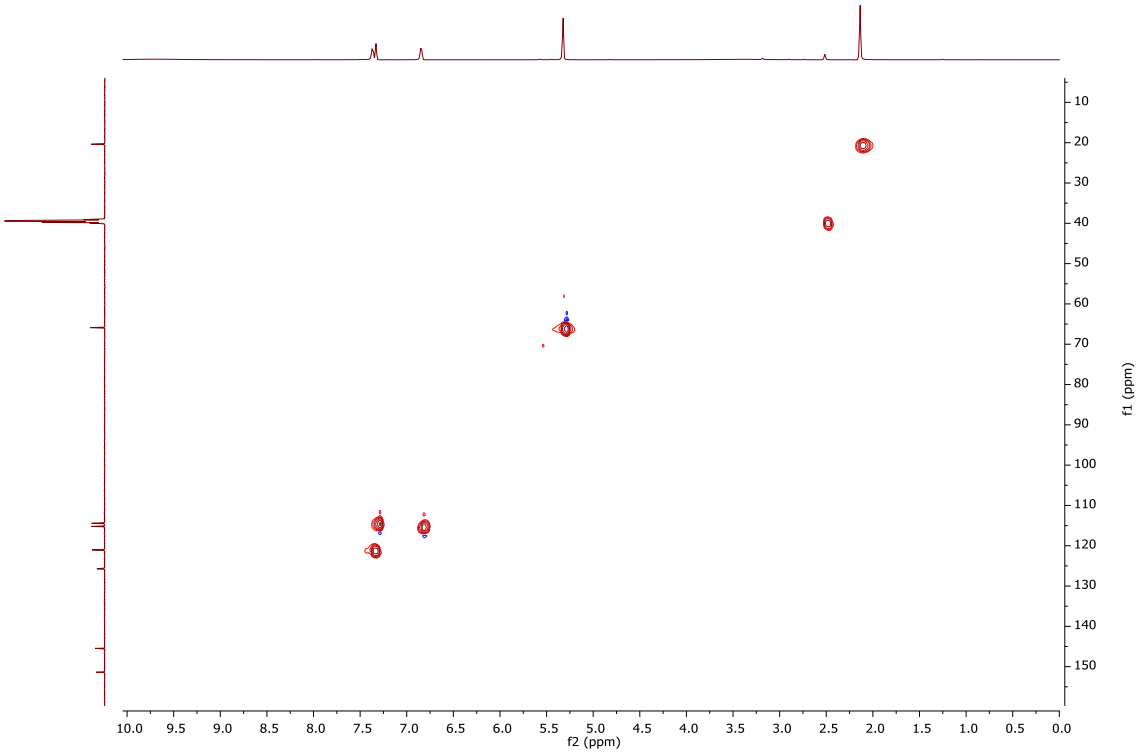

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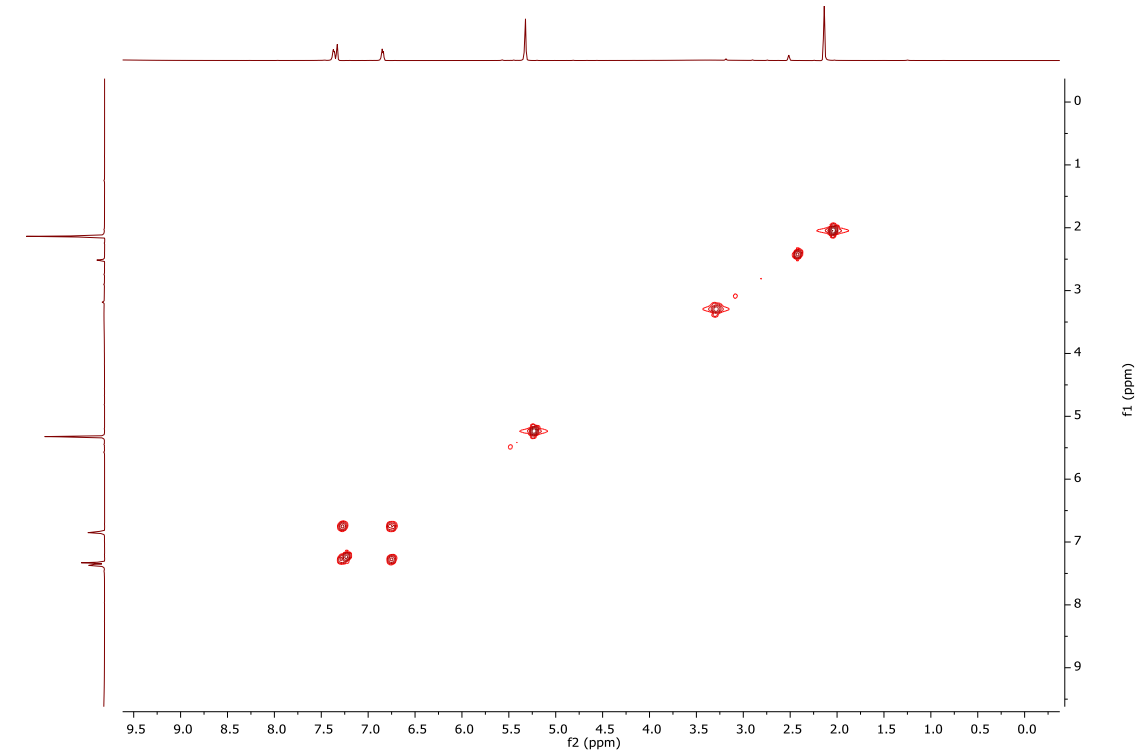

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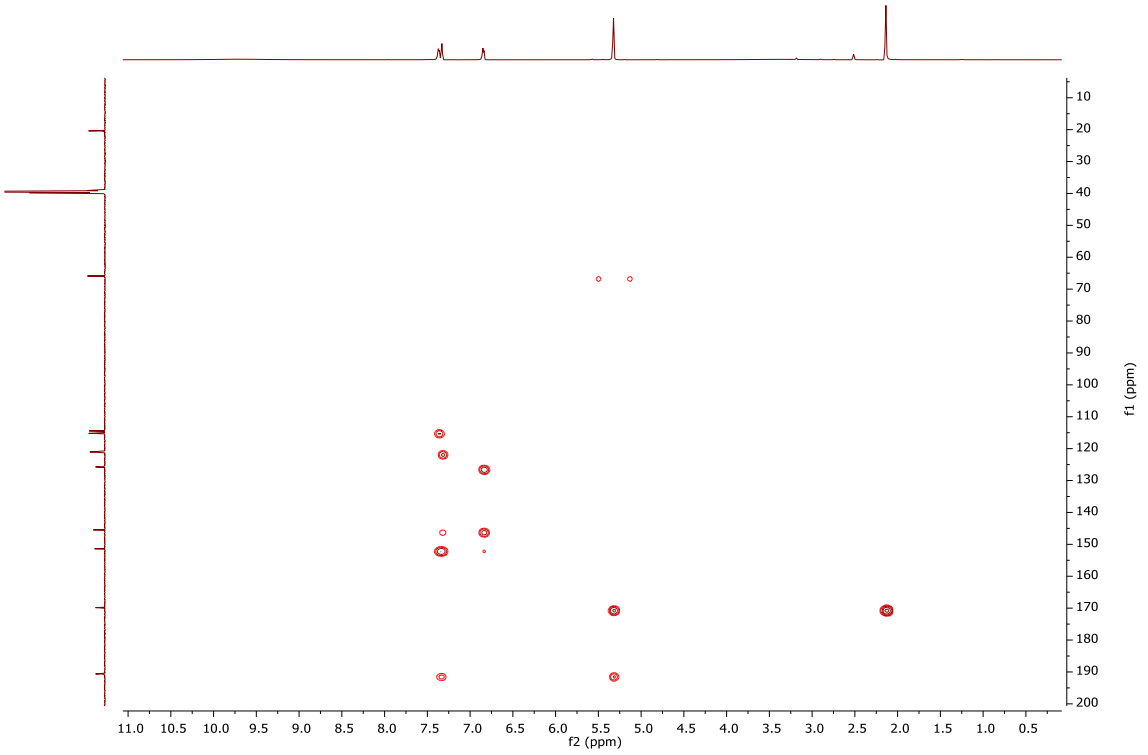

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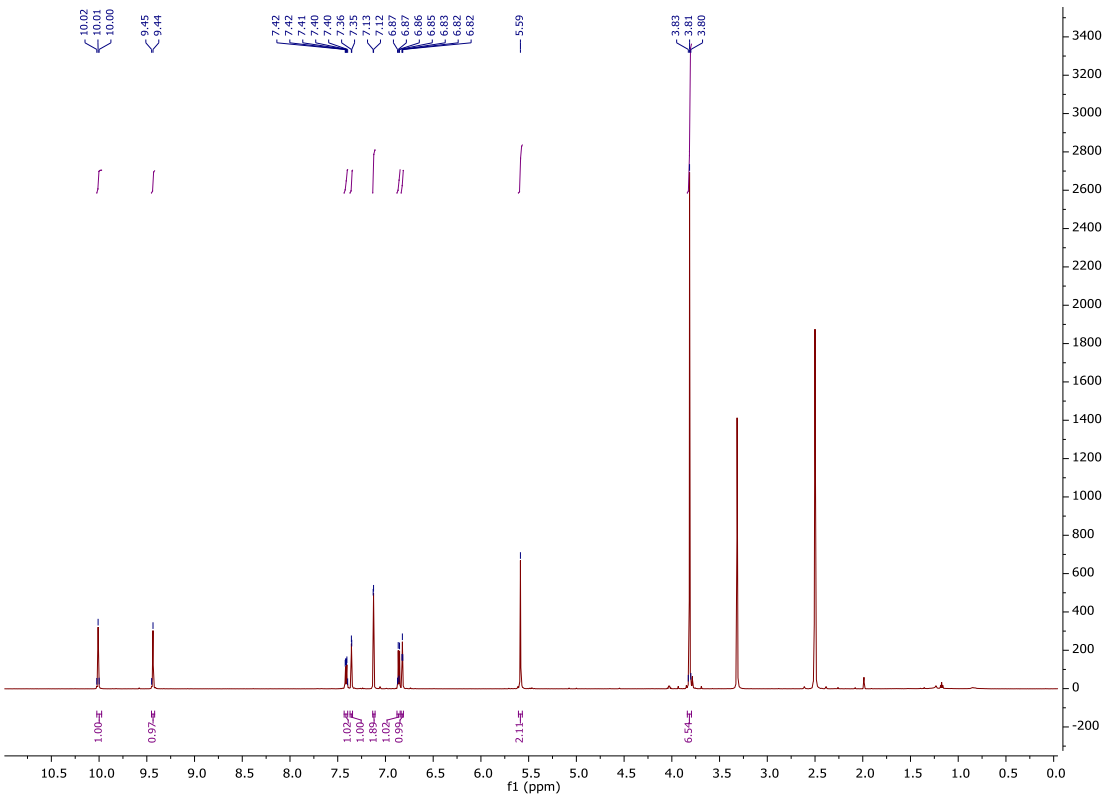

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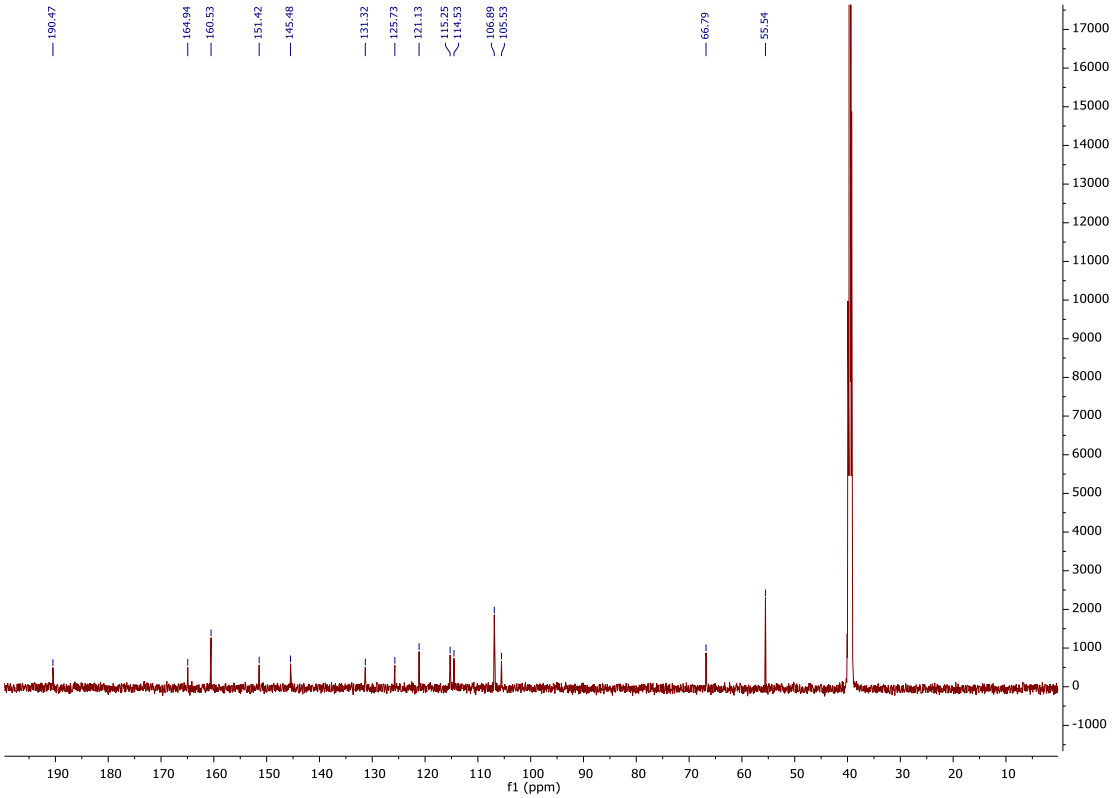

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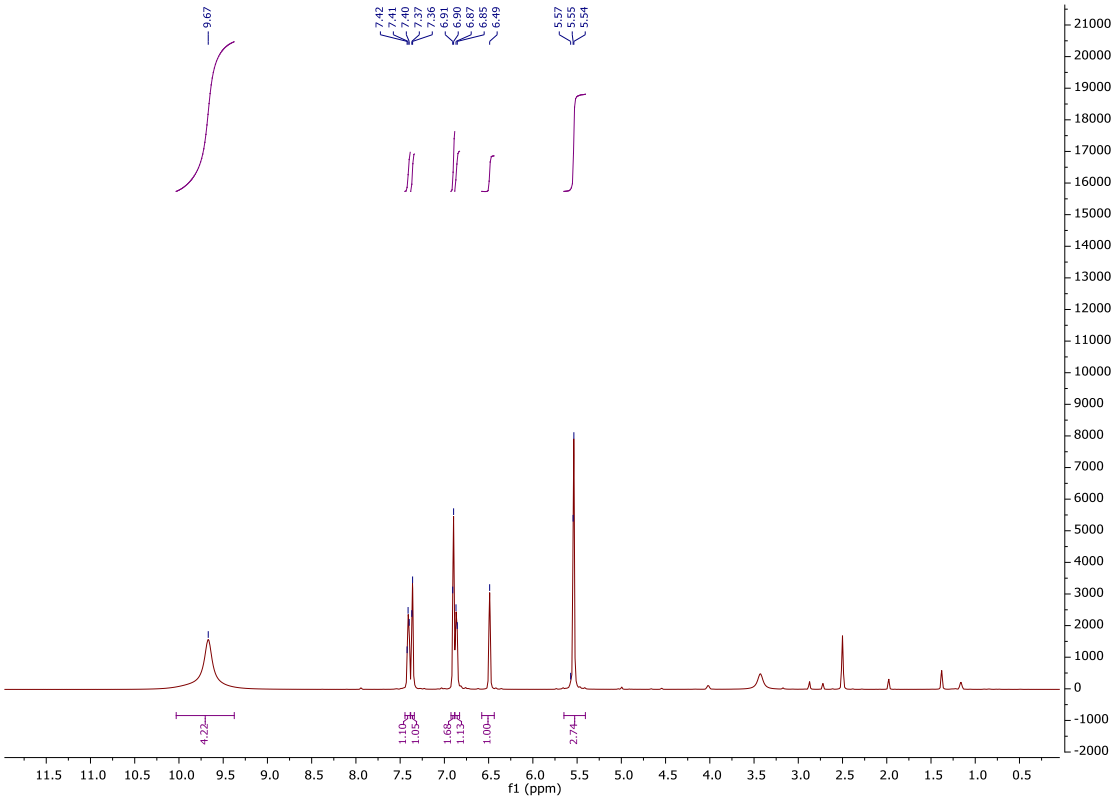

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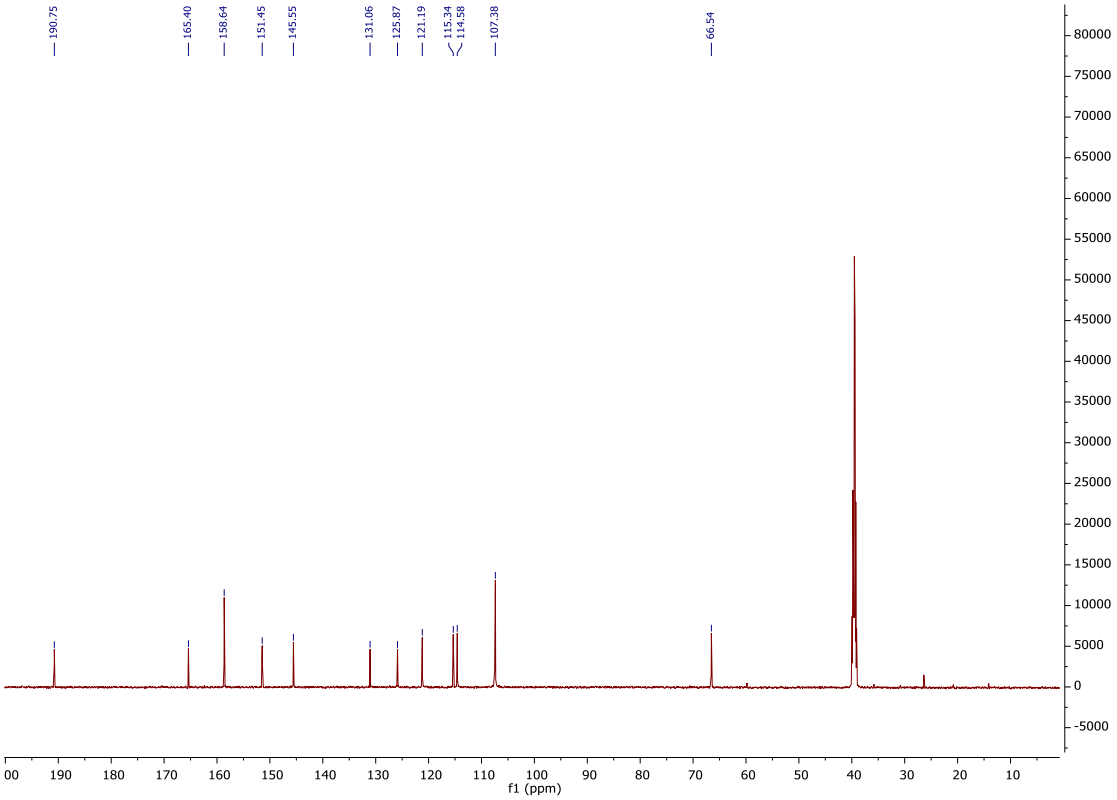

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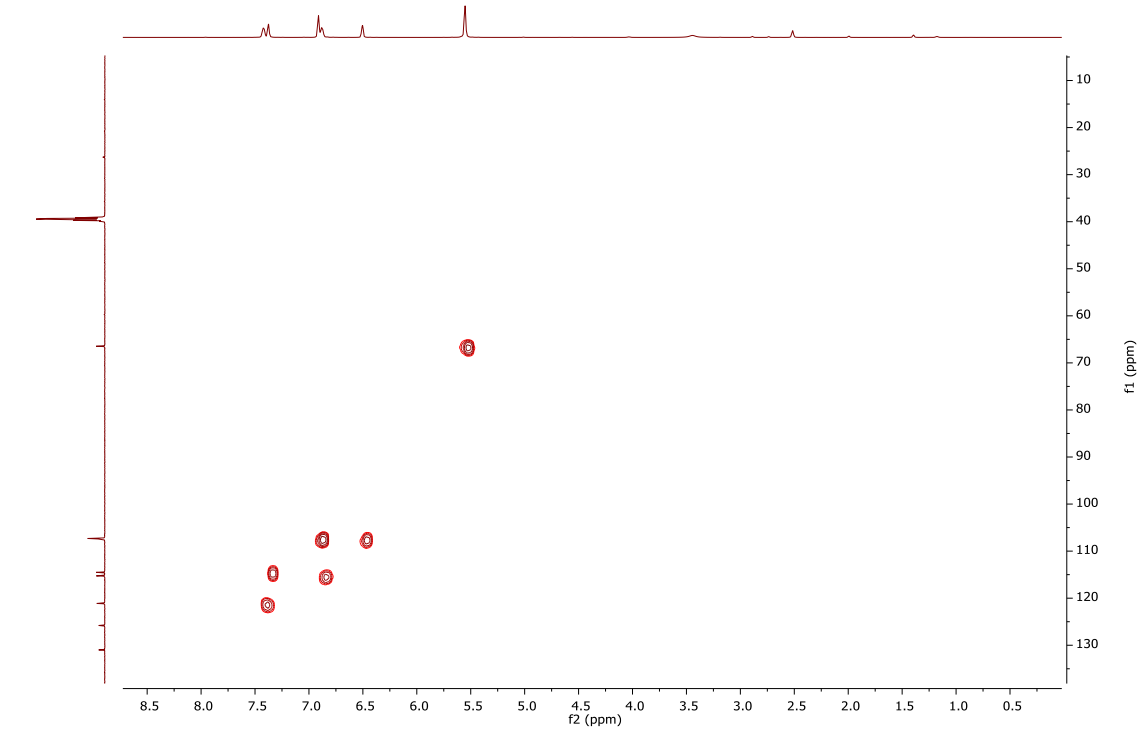

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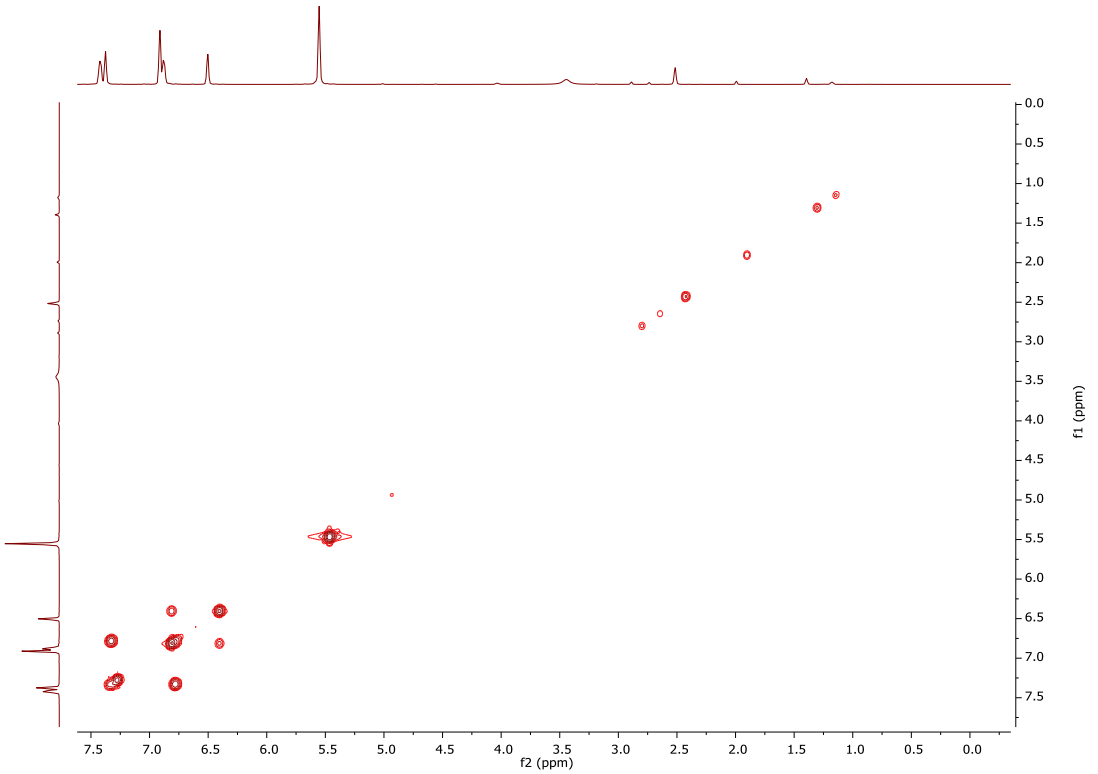

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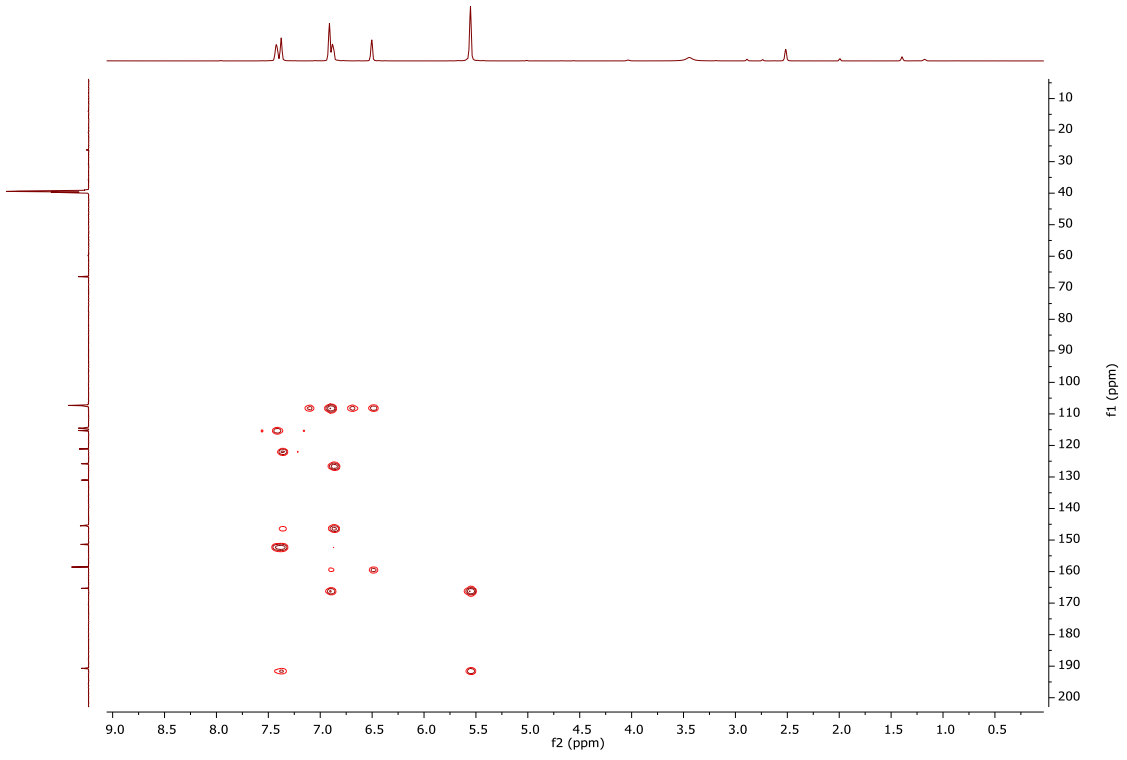

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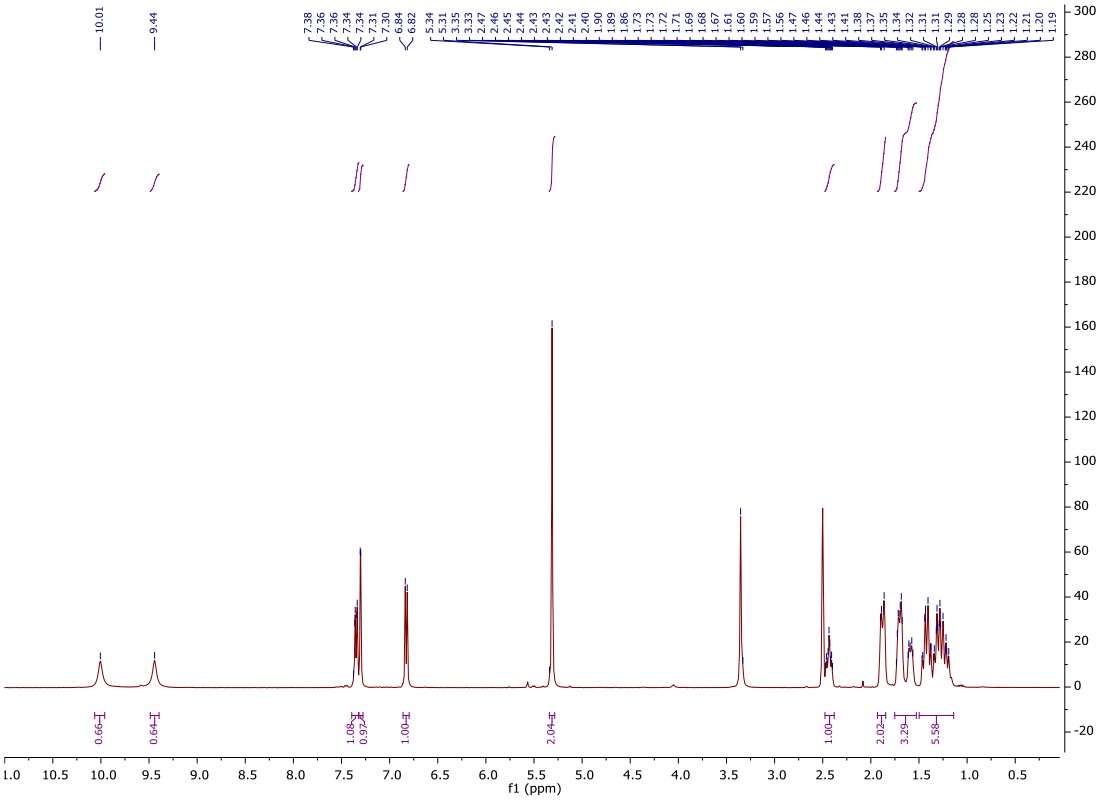

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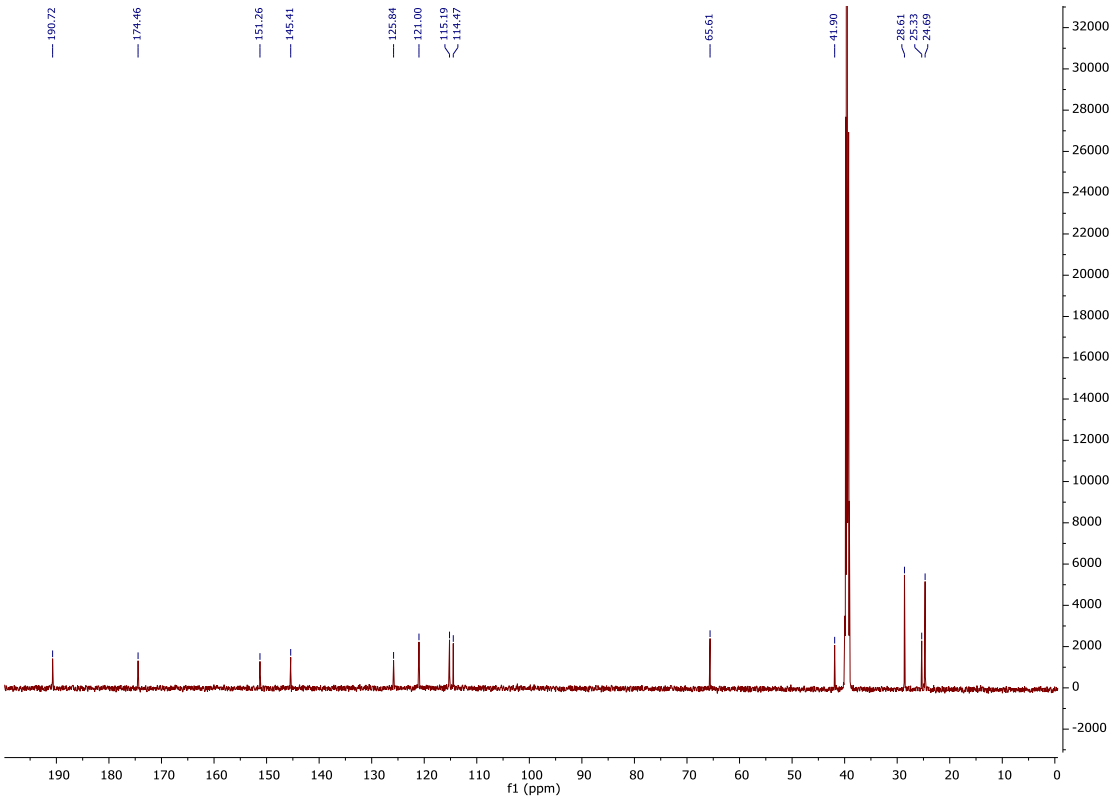

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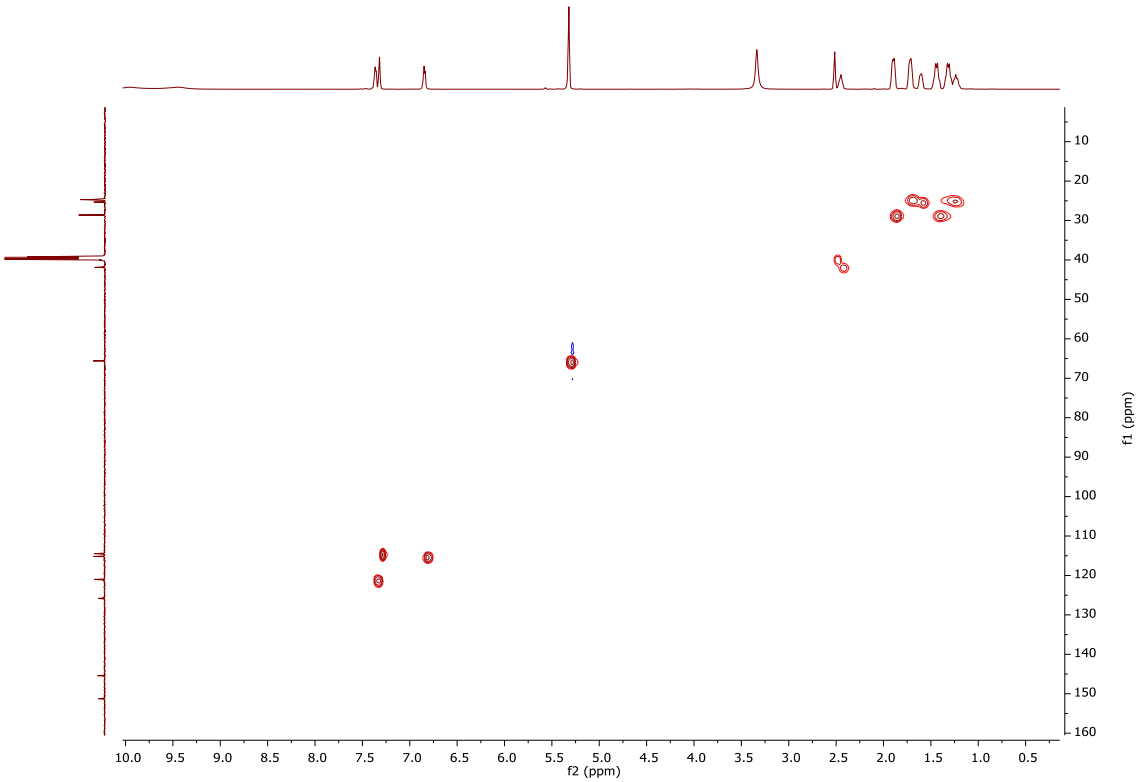

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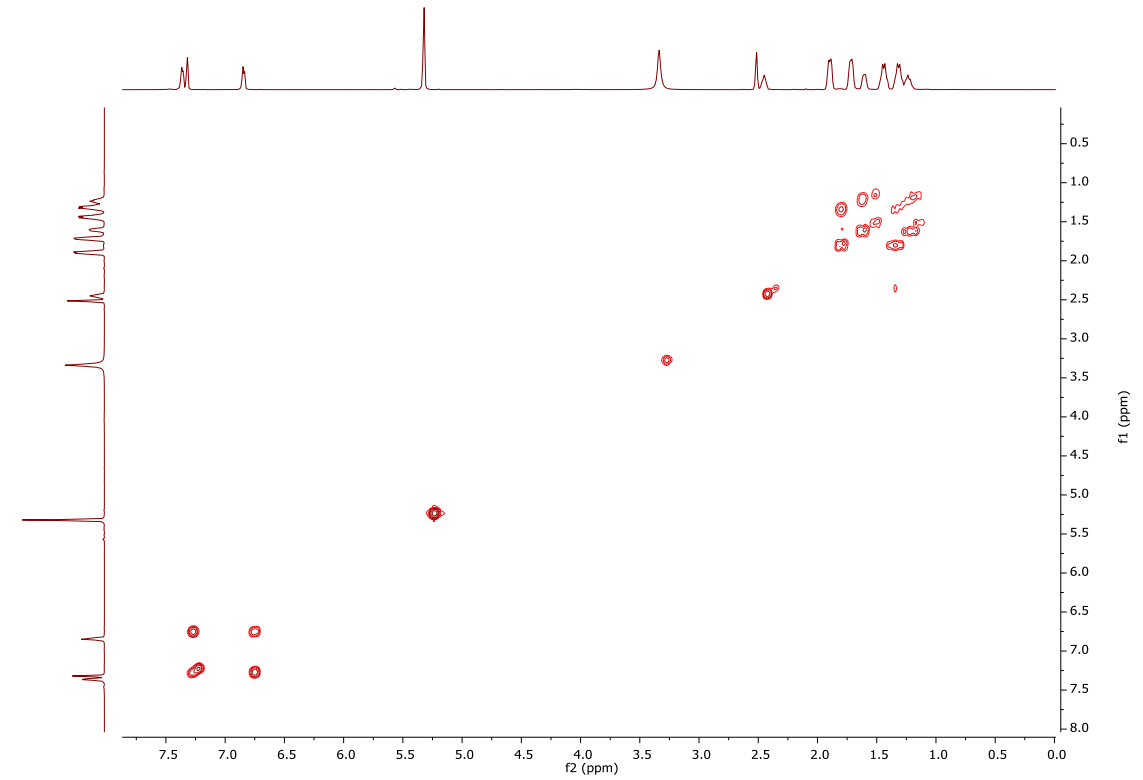

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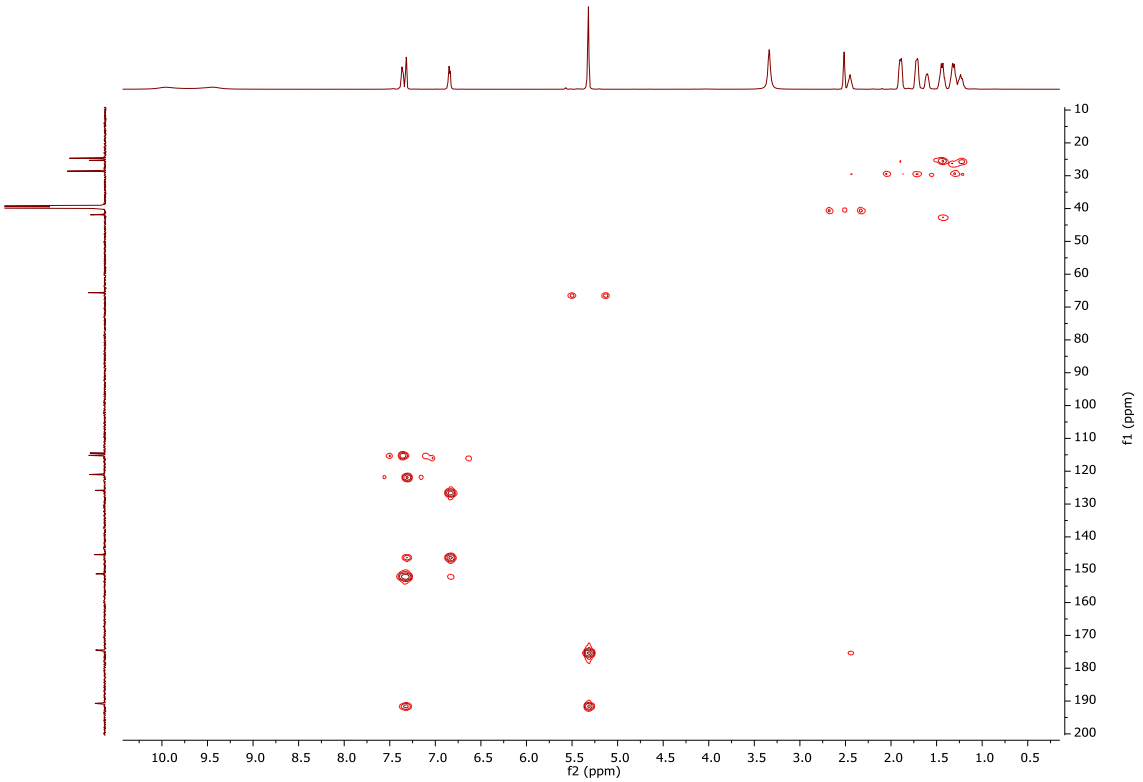

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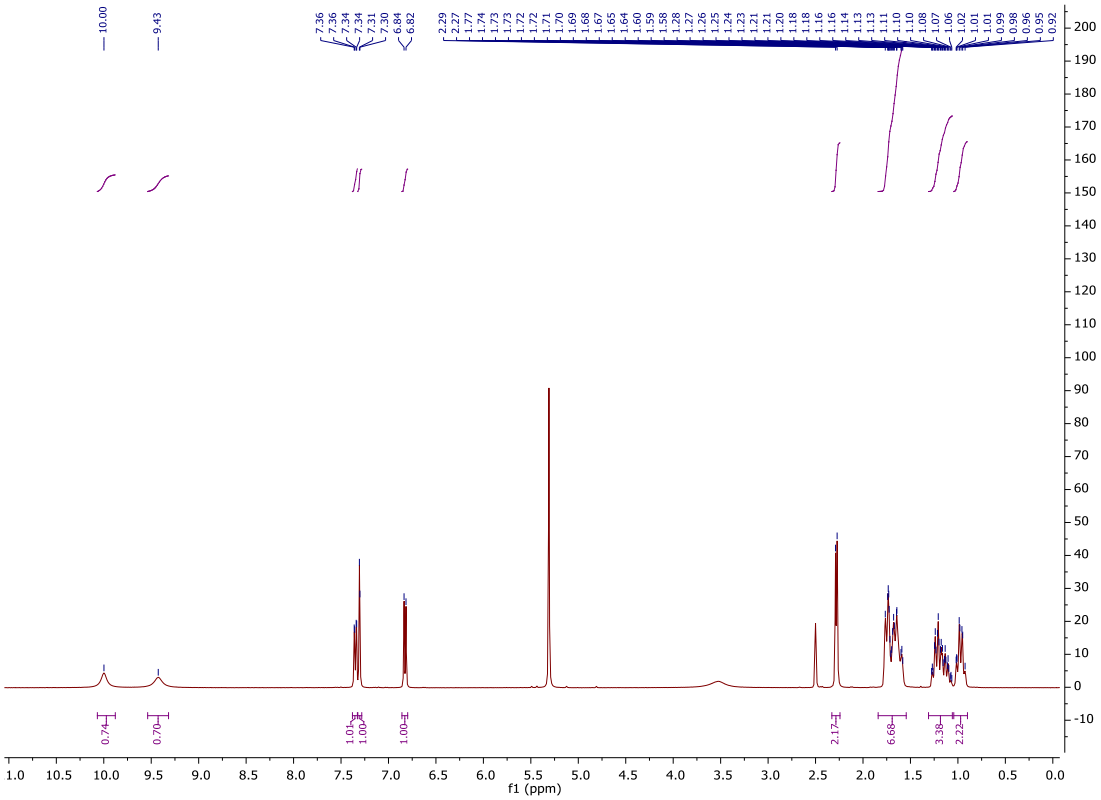

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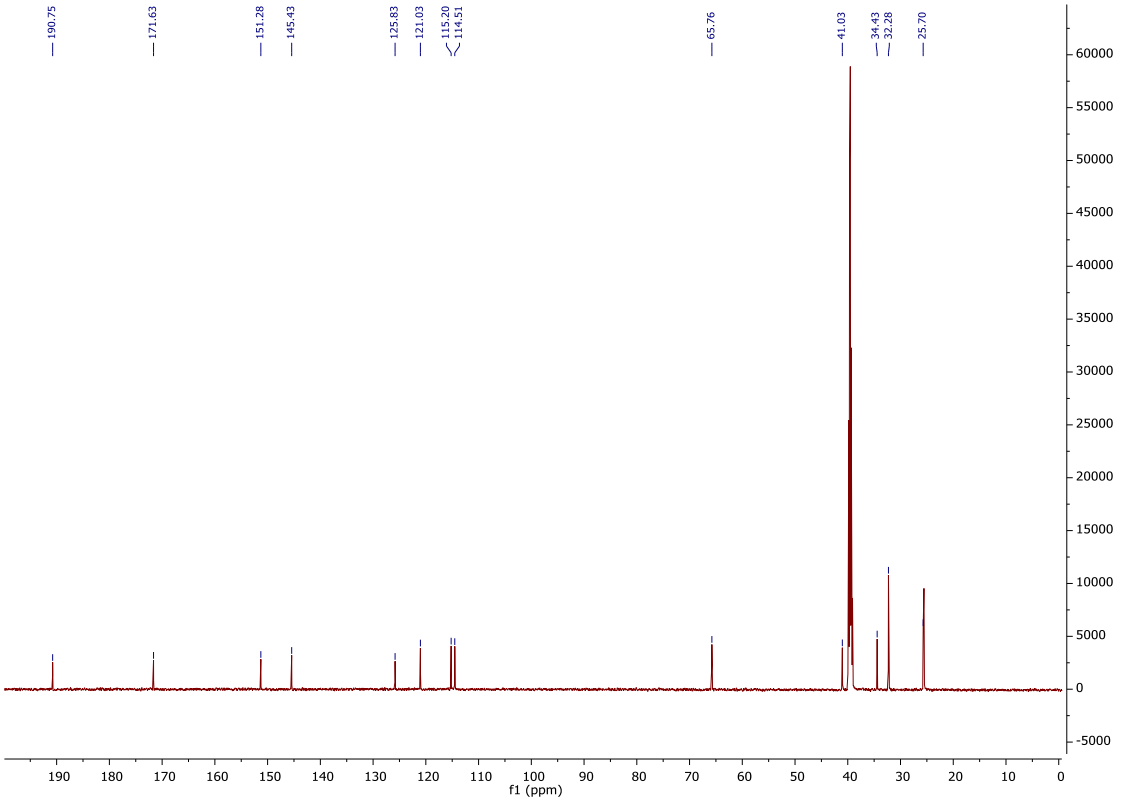

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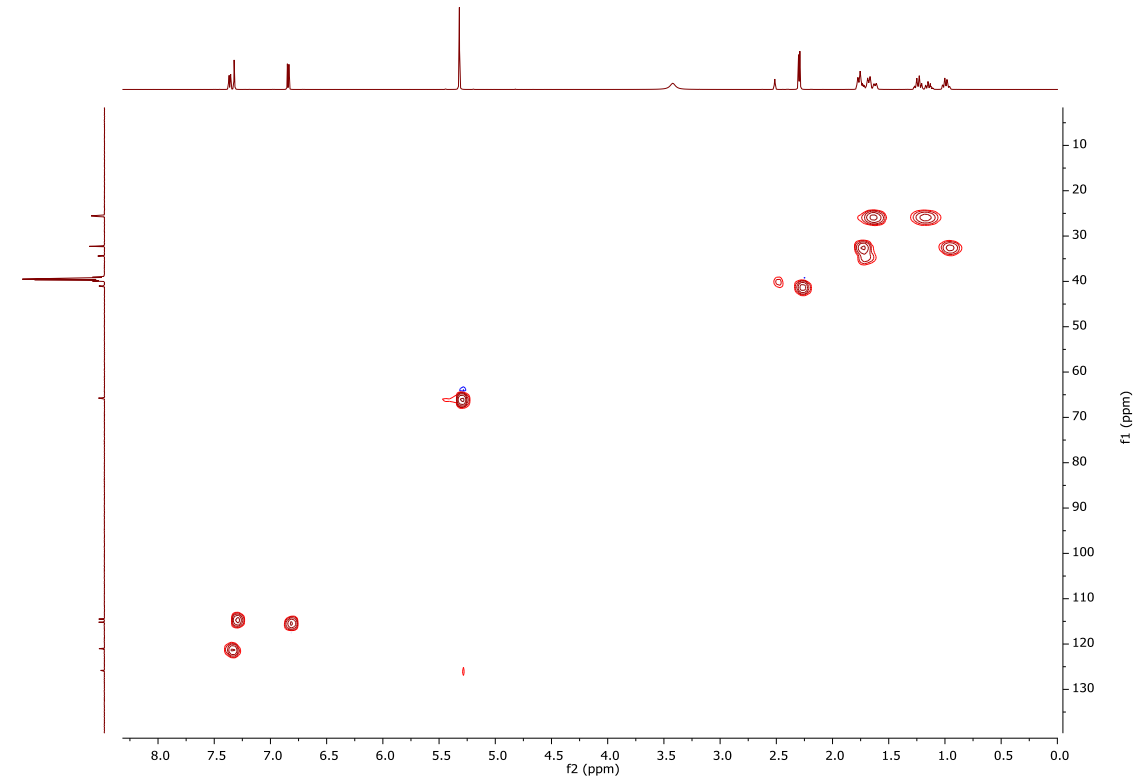

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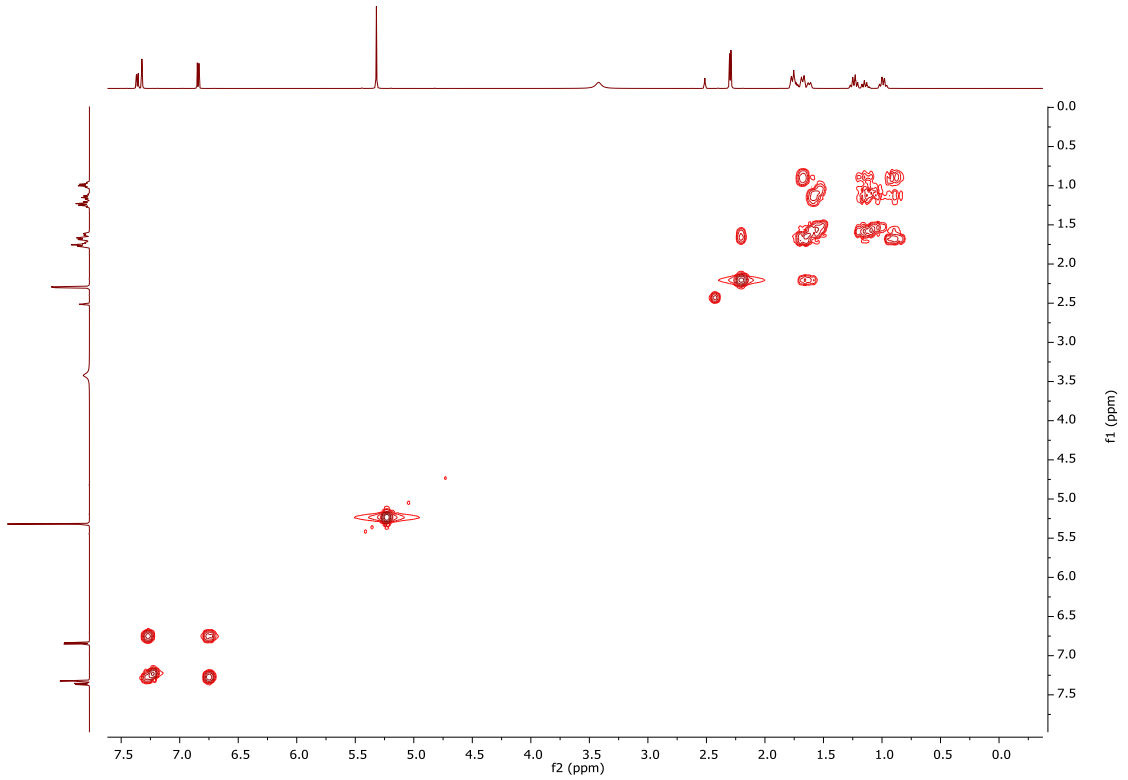

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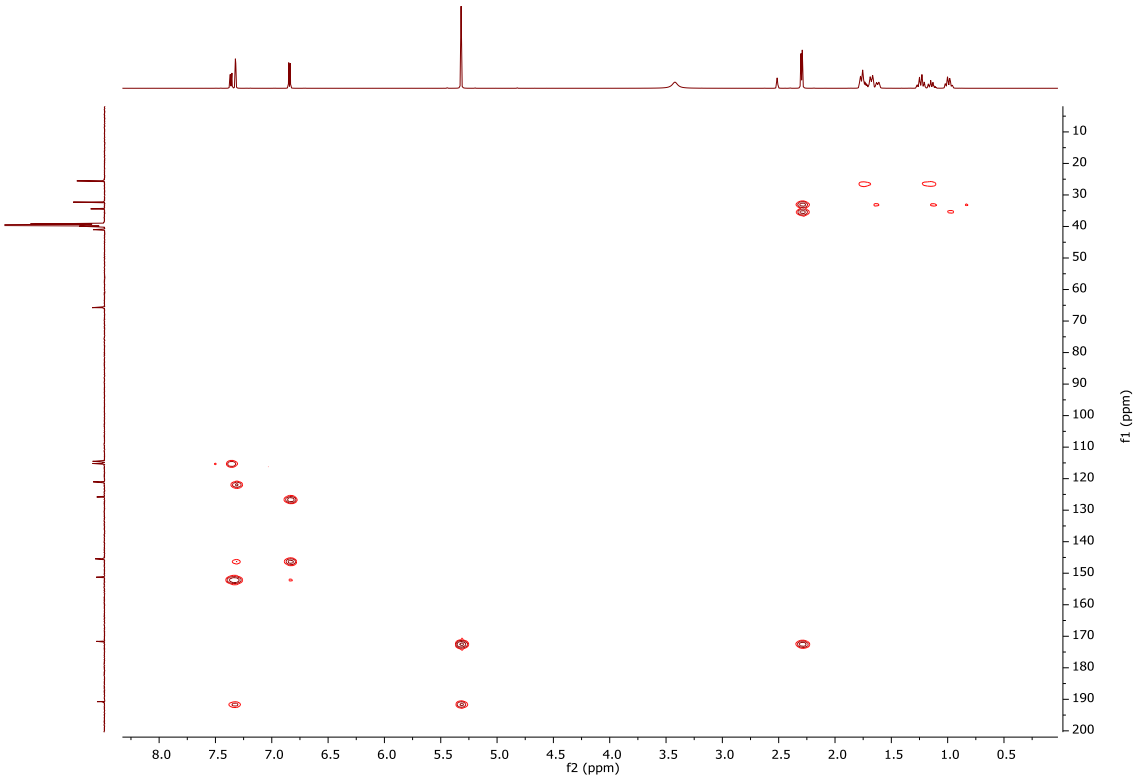

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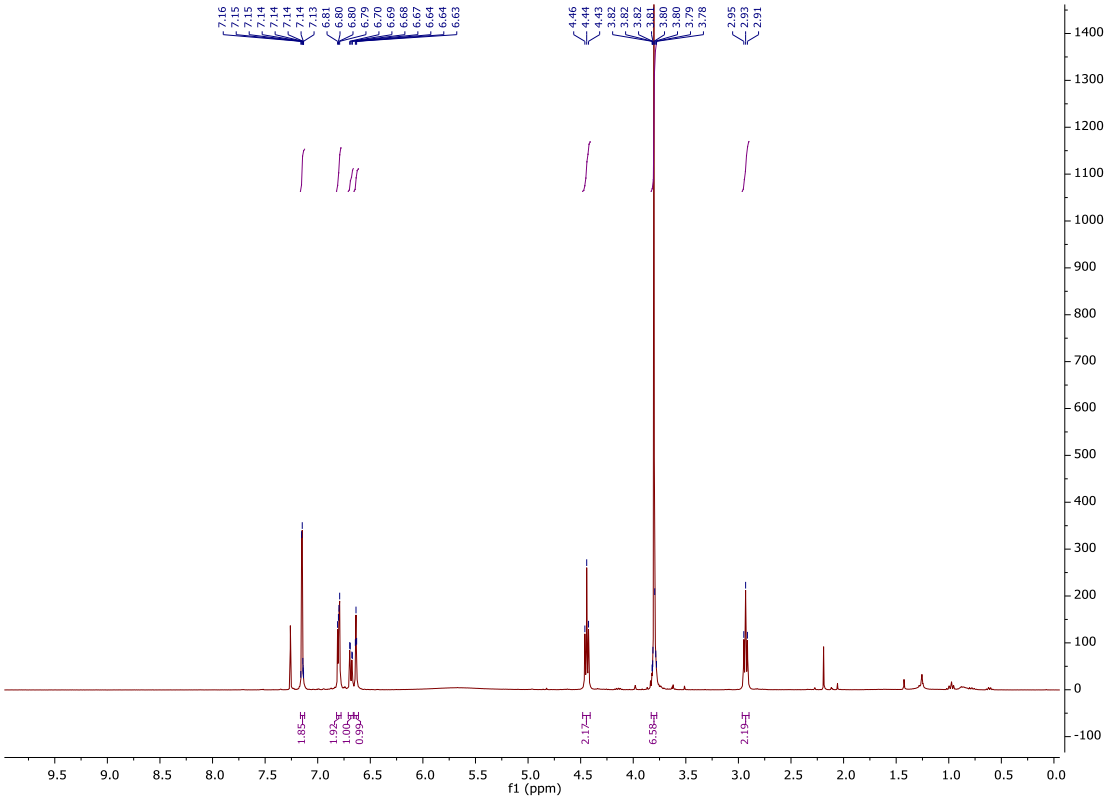

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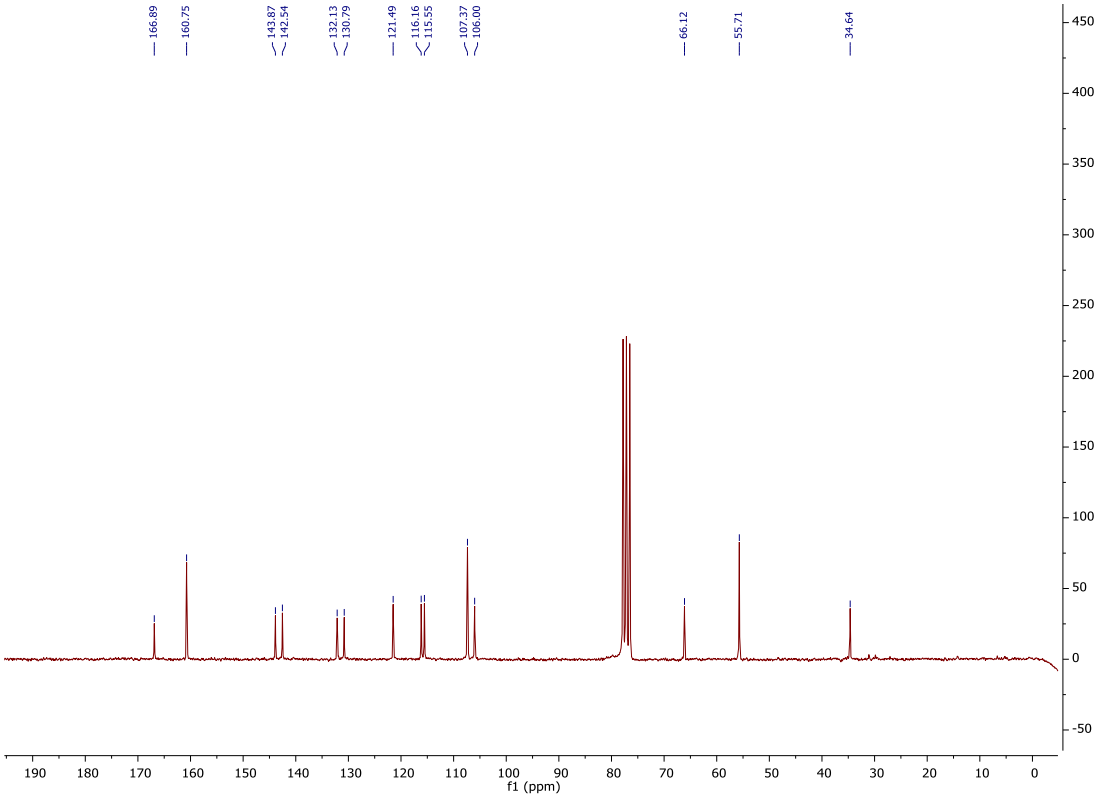

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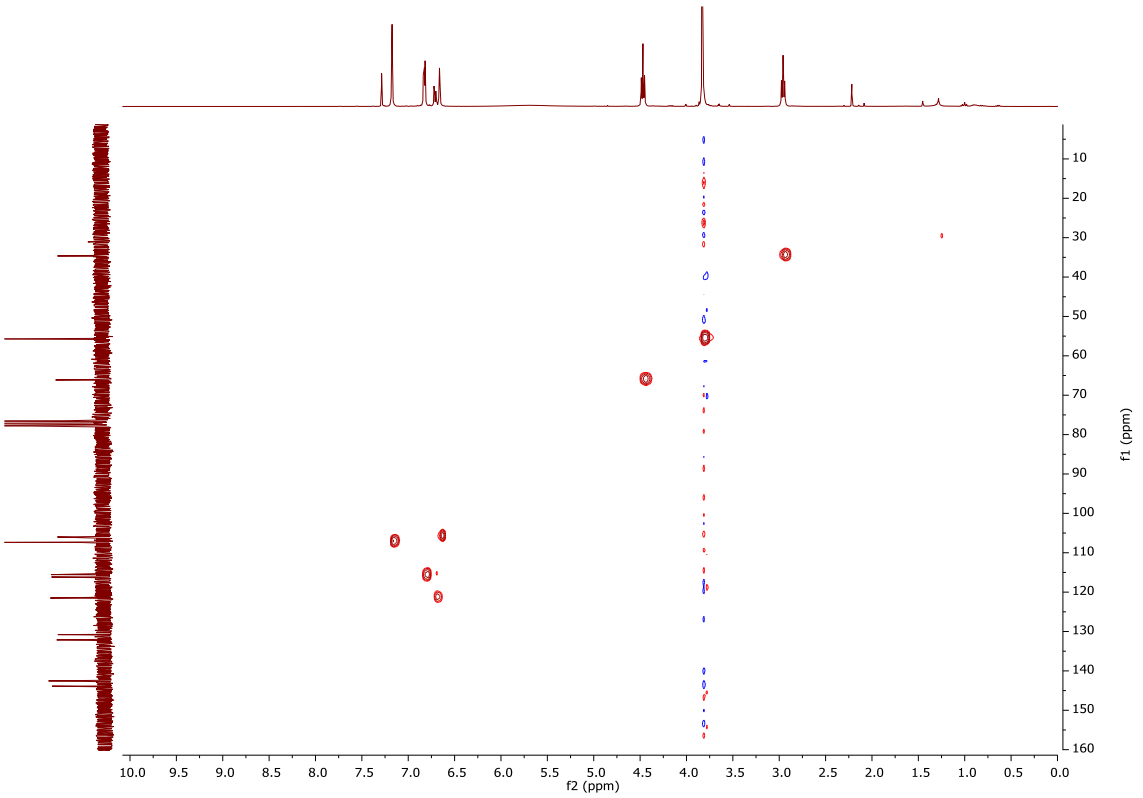

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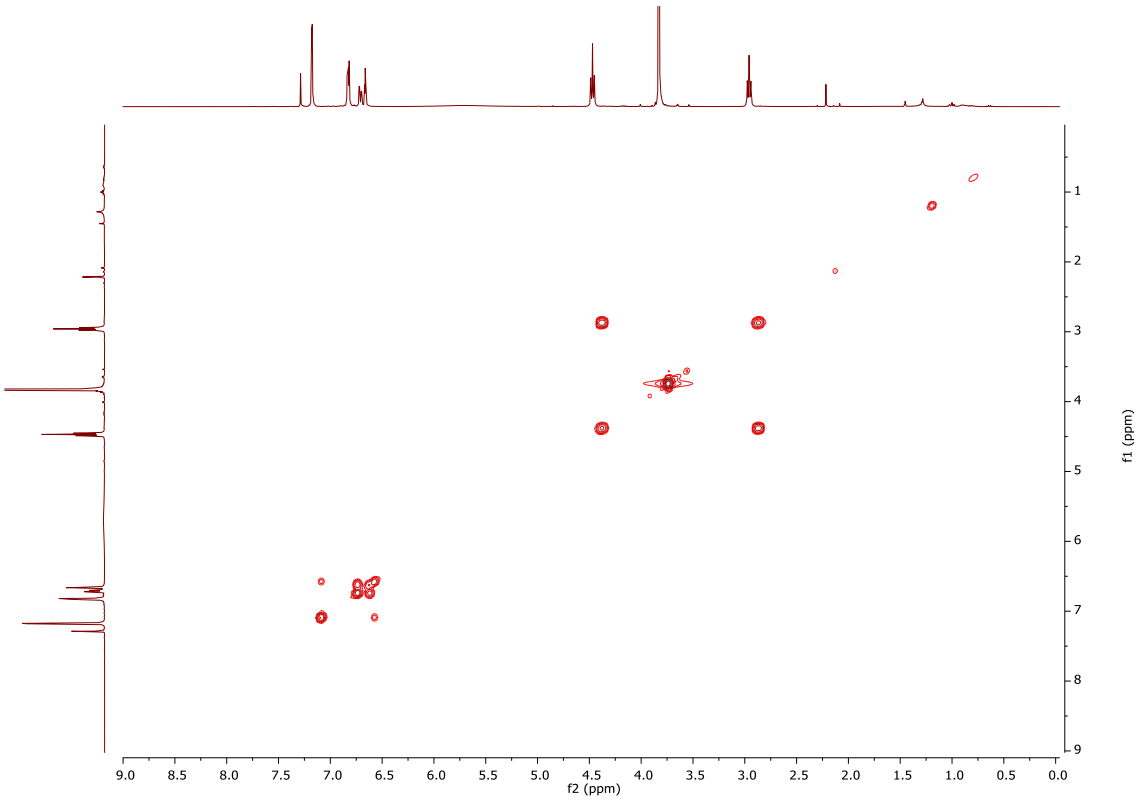

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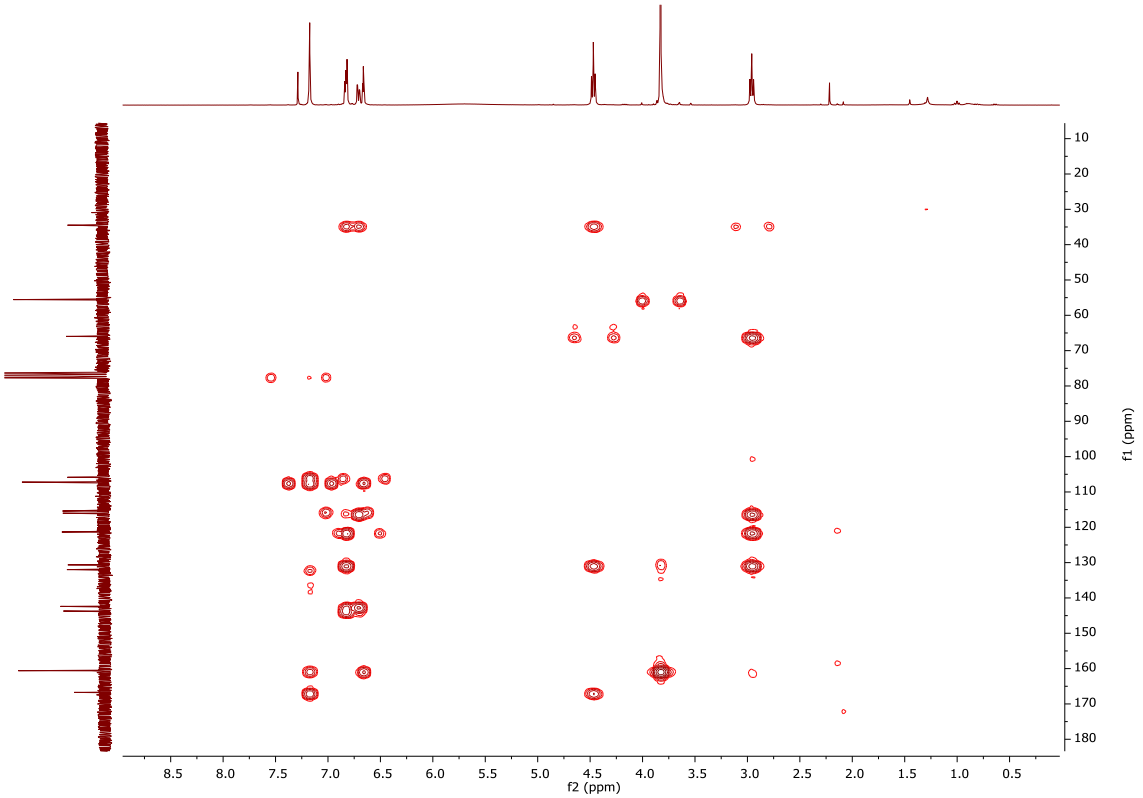

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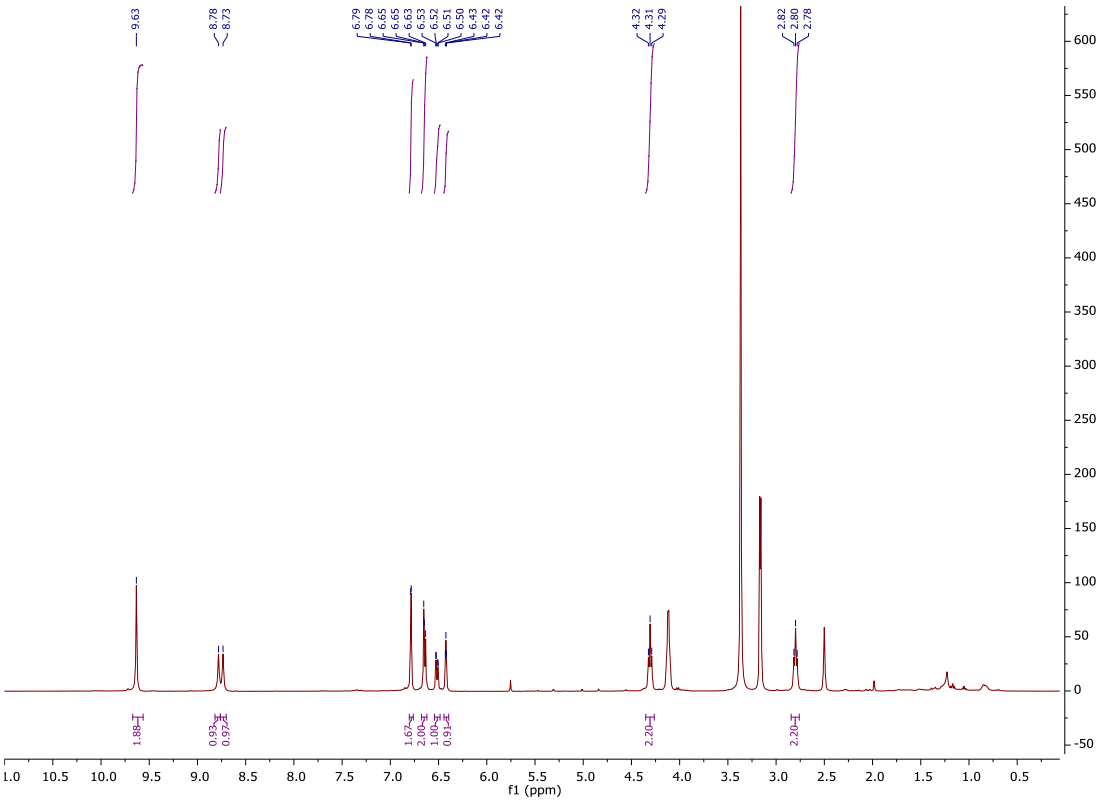

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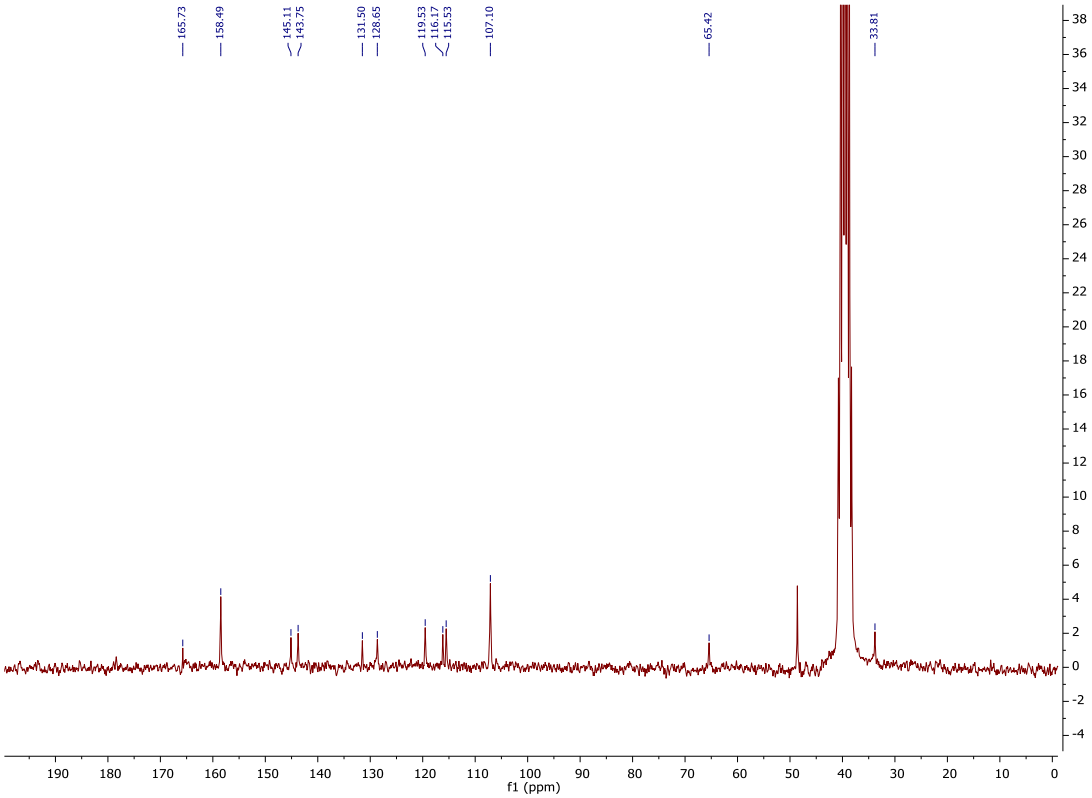

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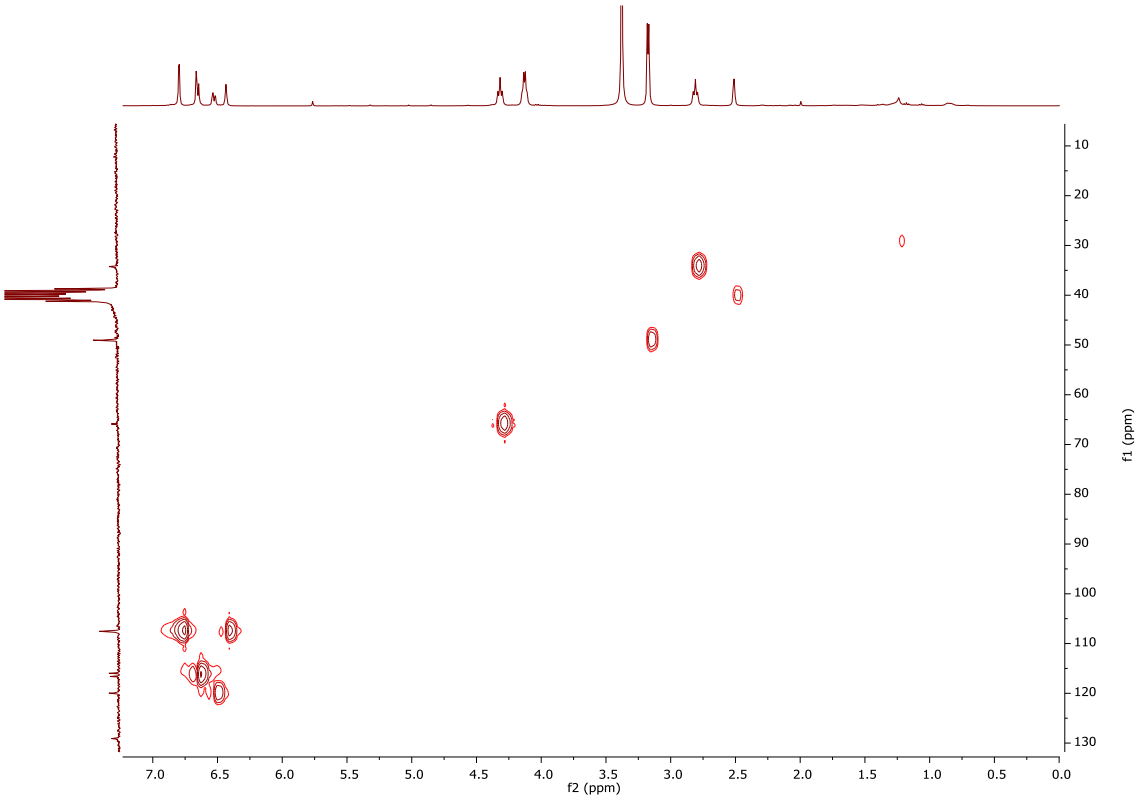

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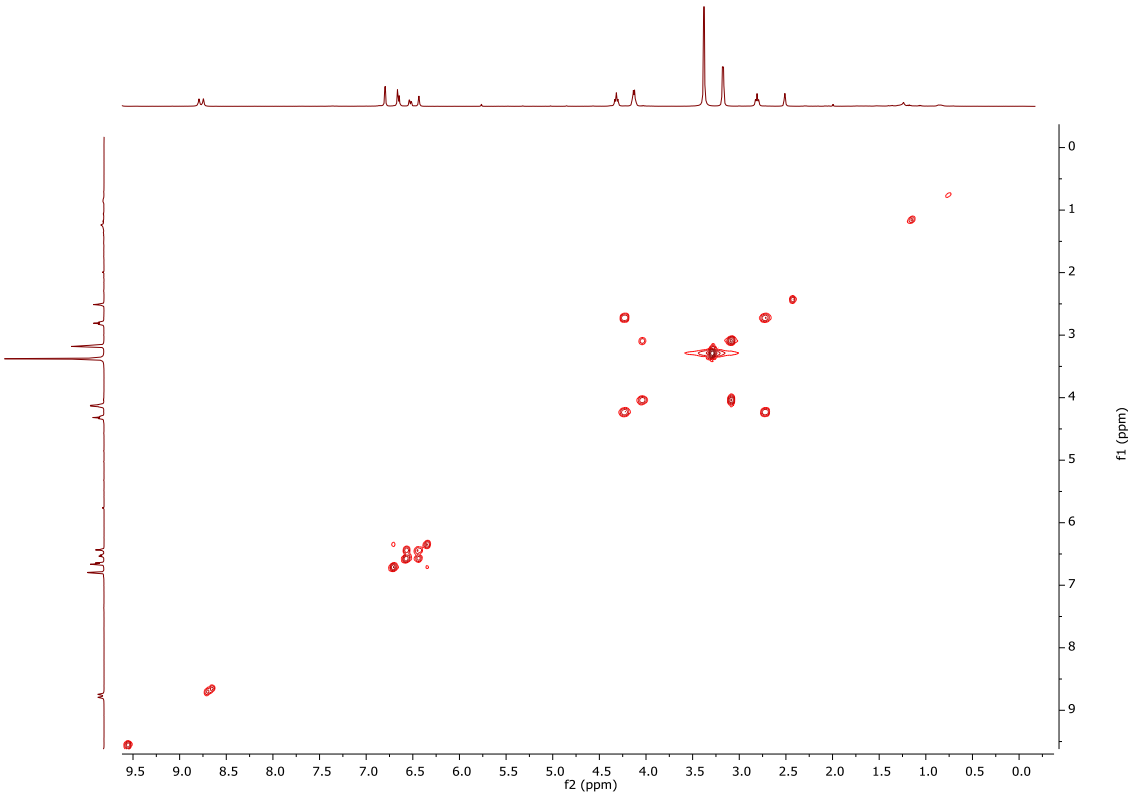

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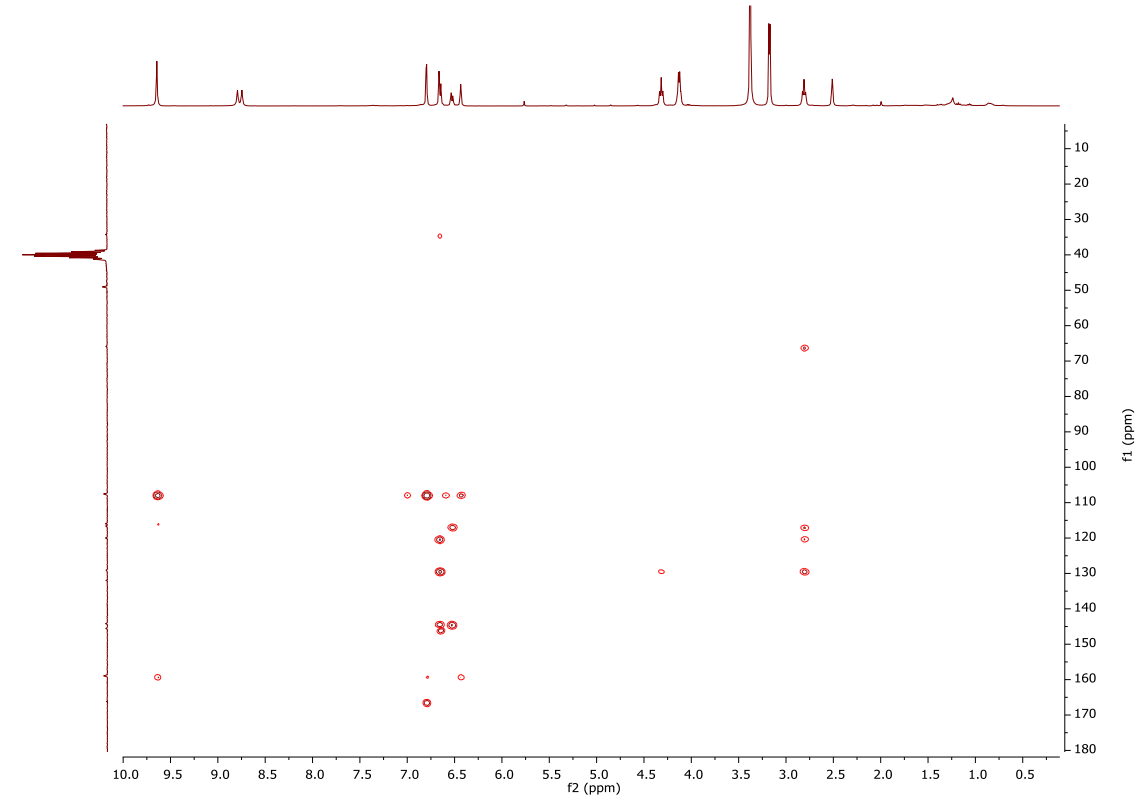

HMBC spectrum of **4c**

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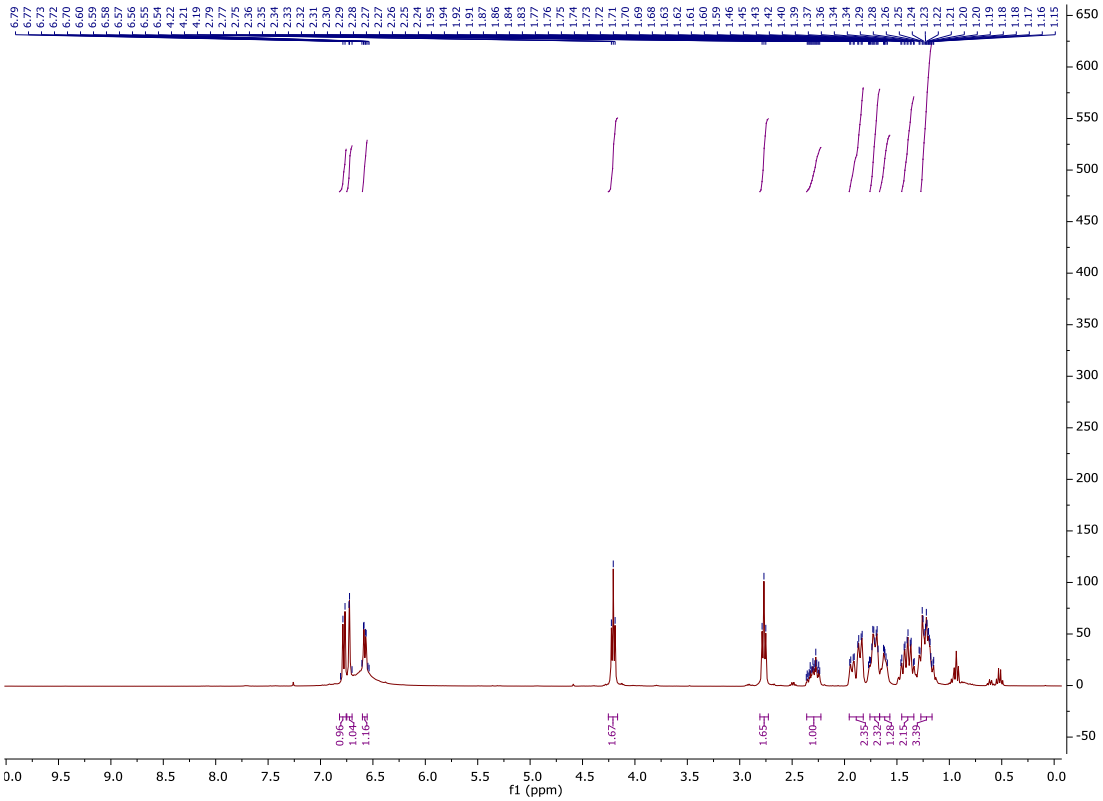

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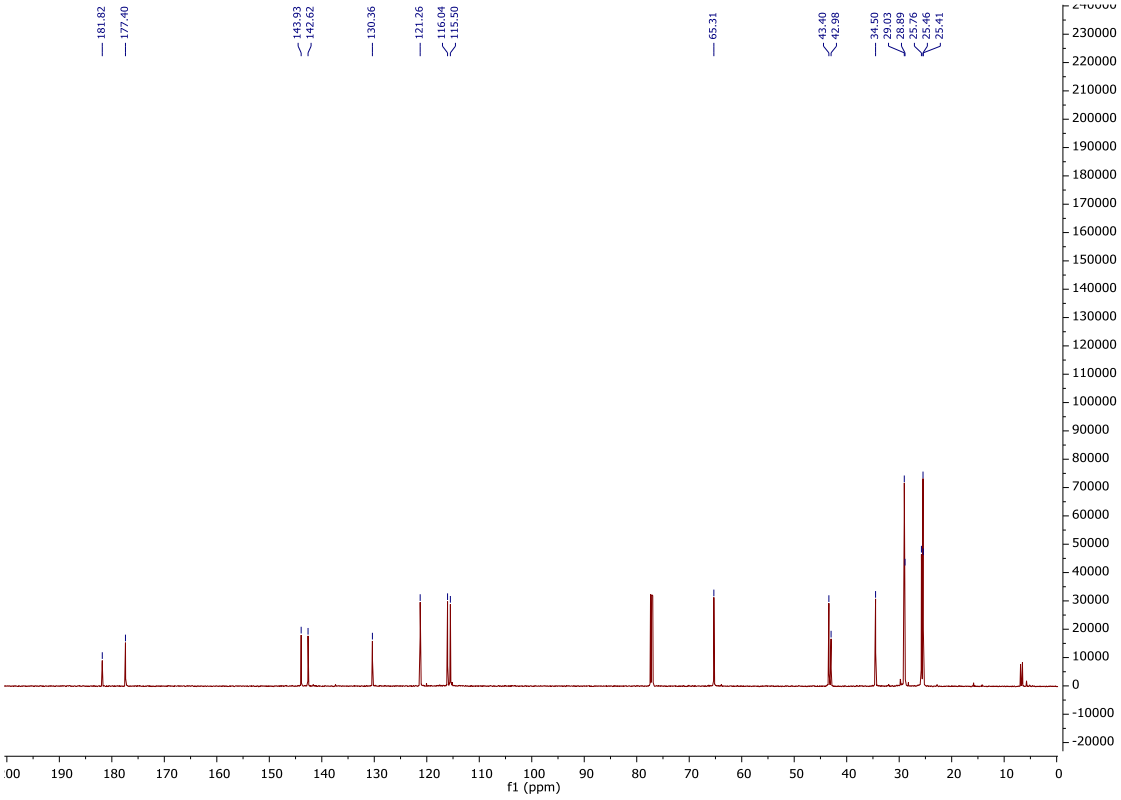

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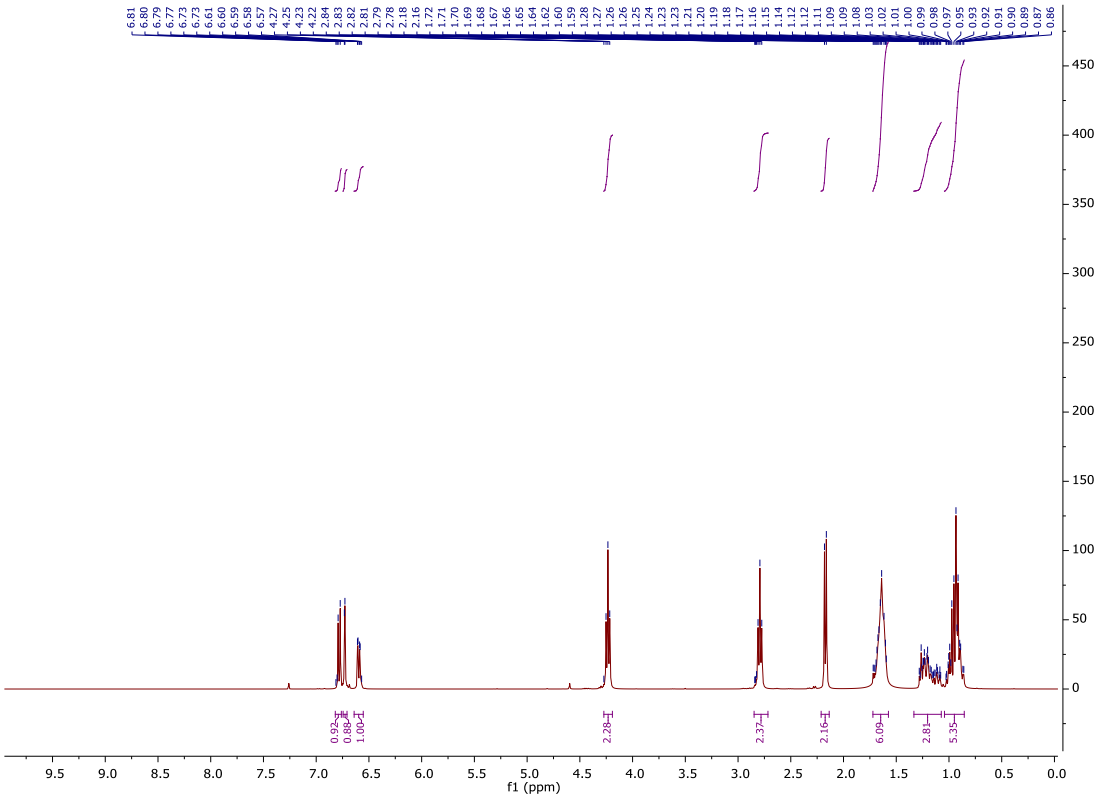

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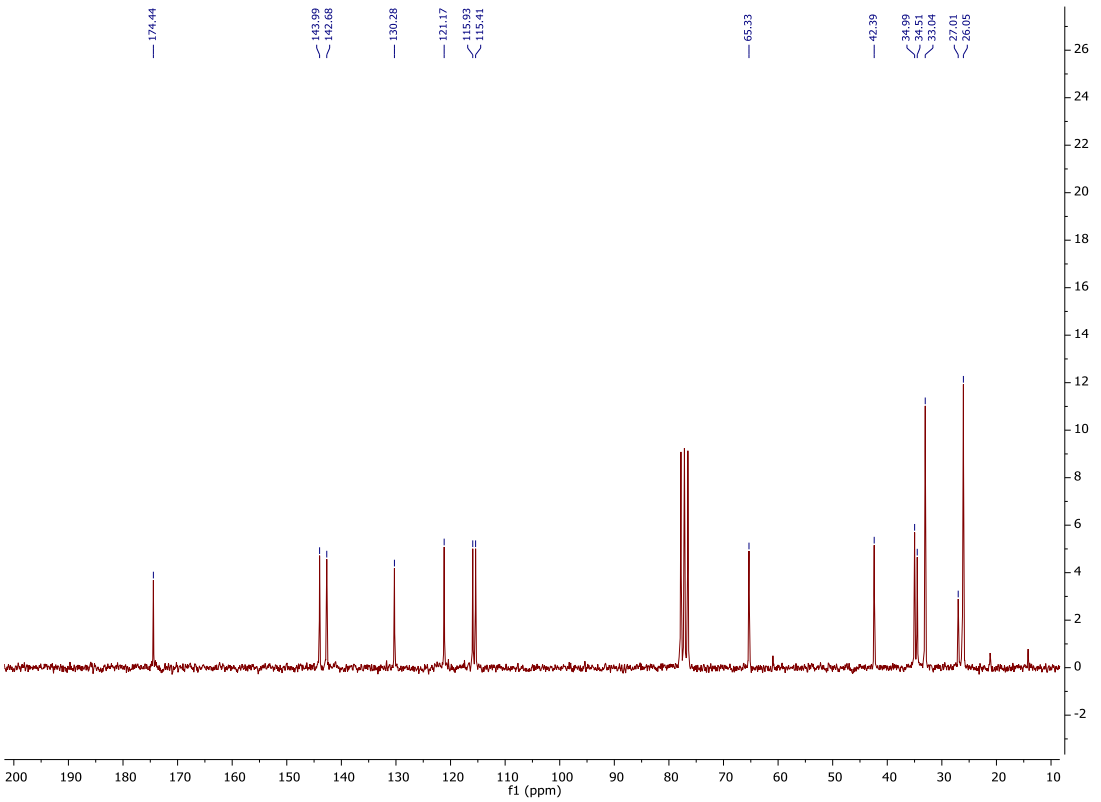

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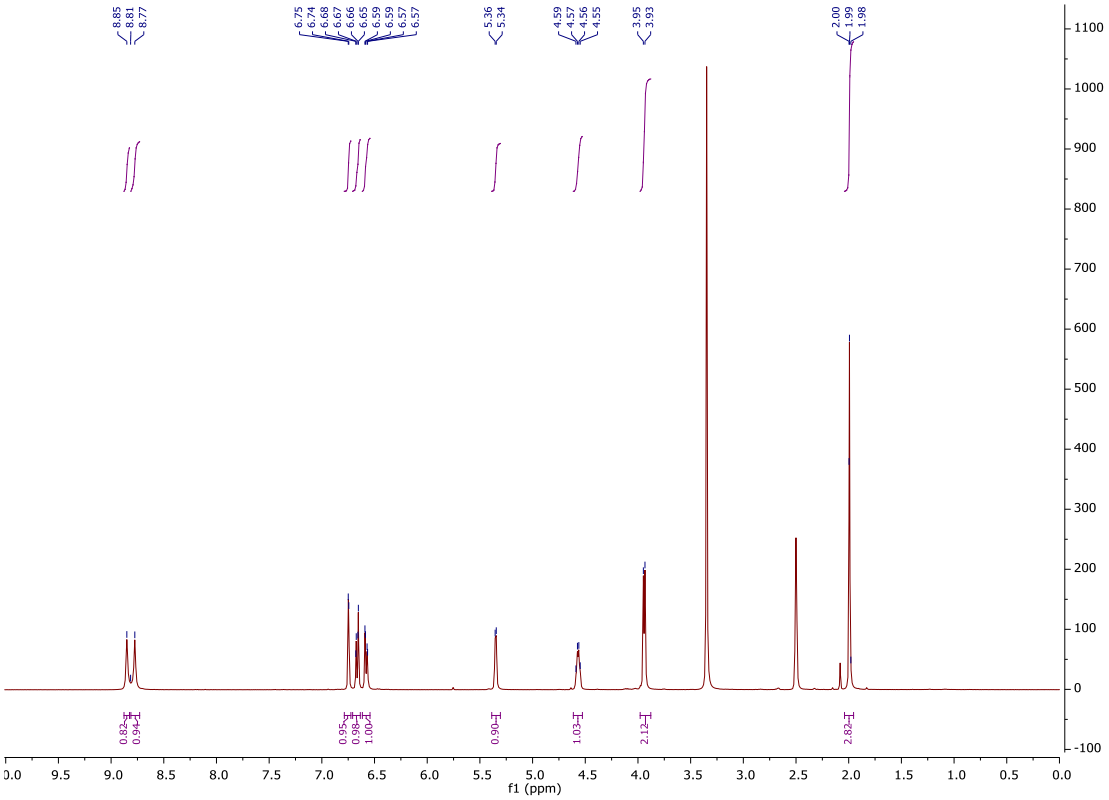

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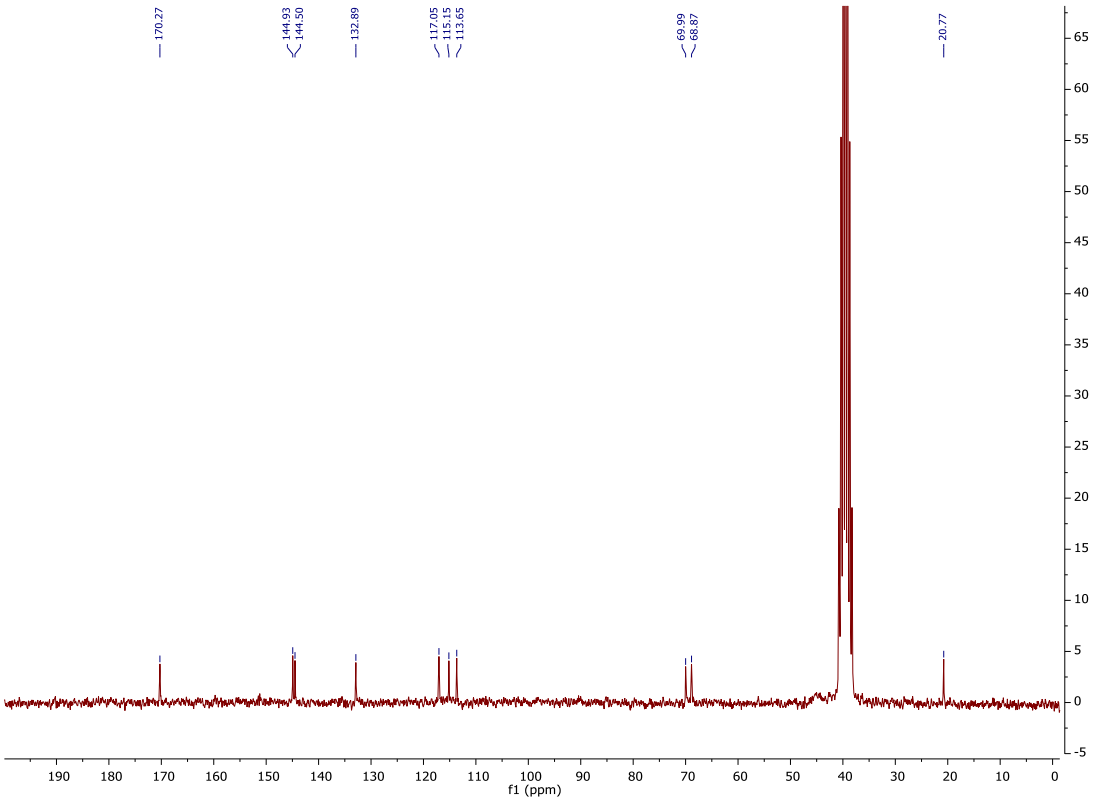

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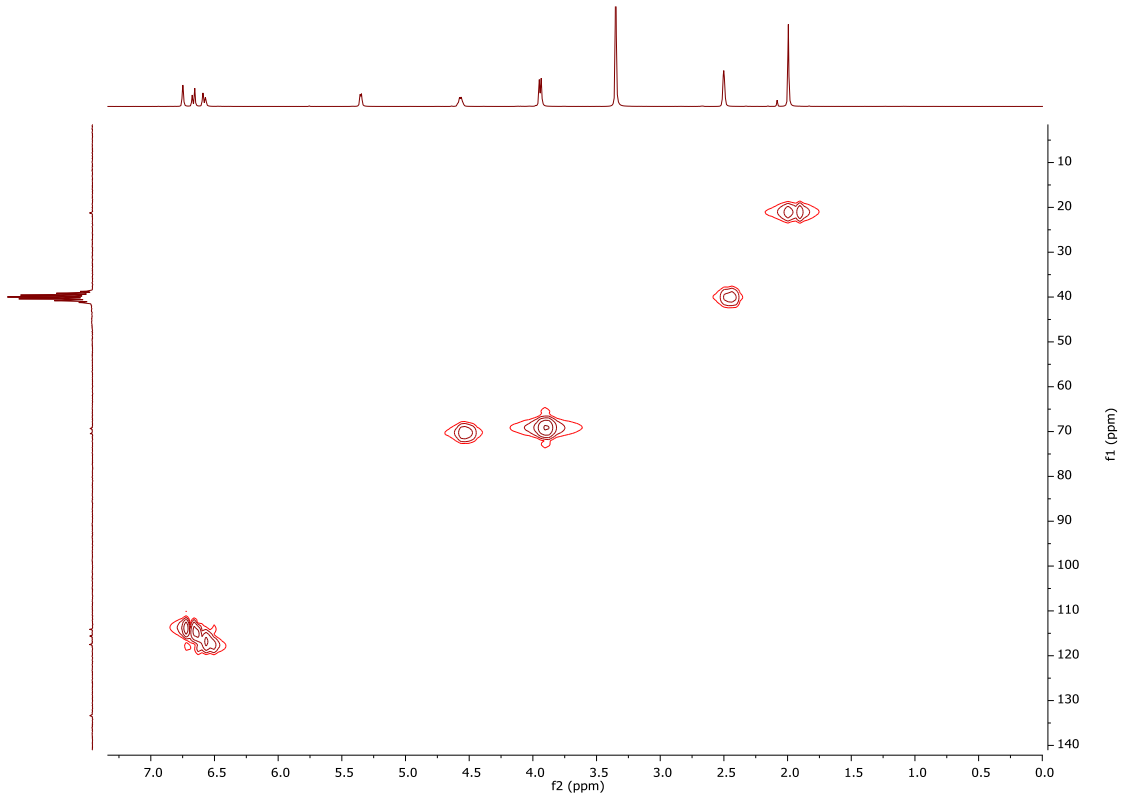

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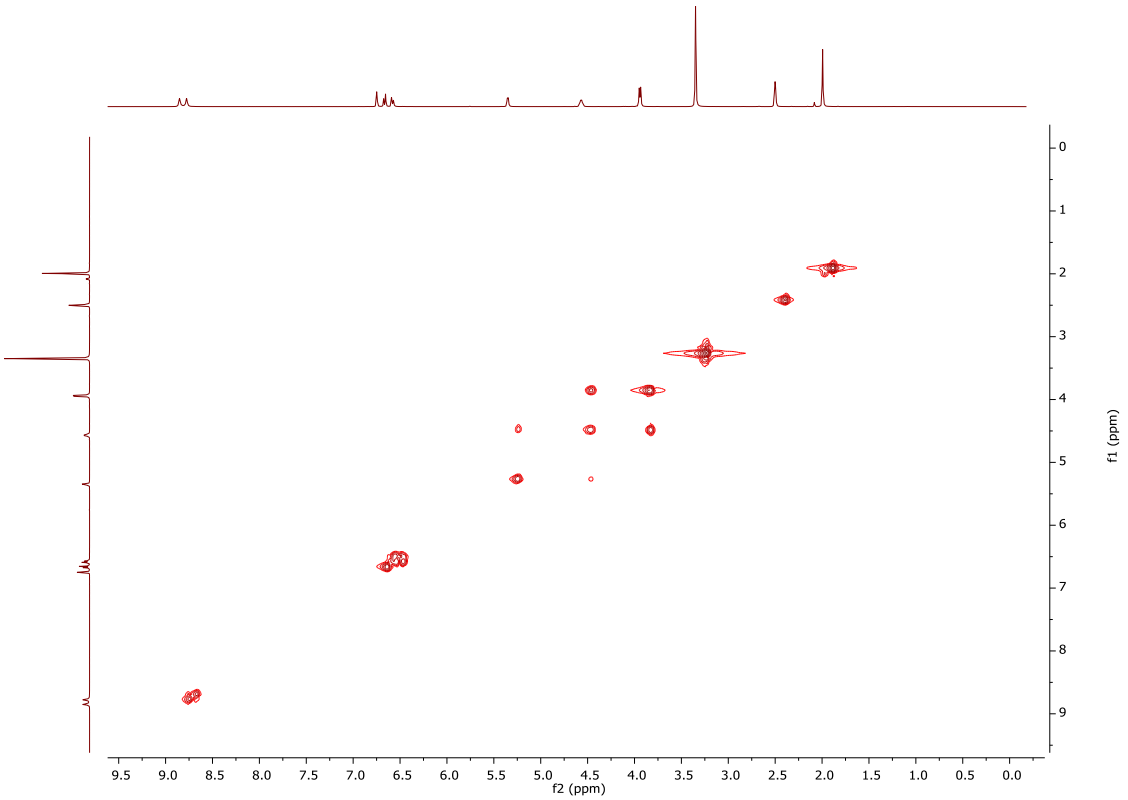

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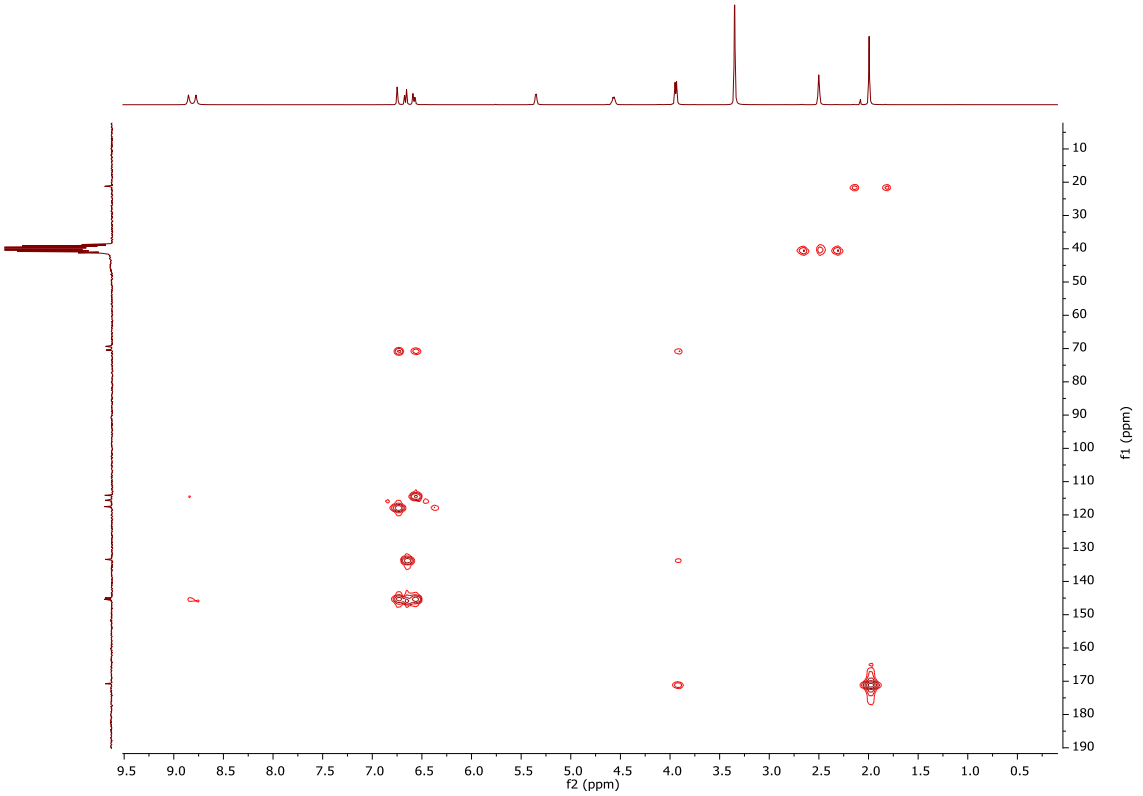

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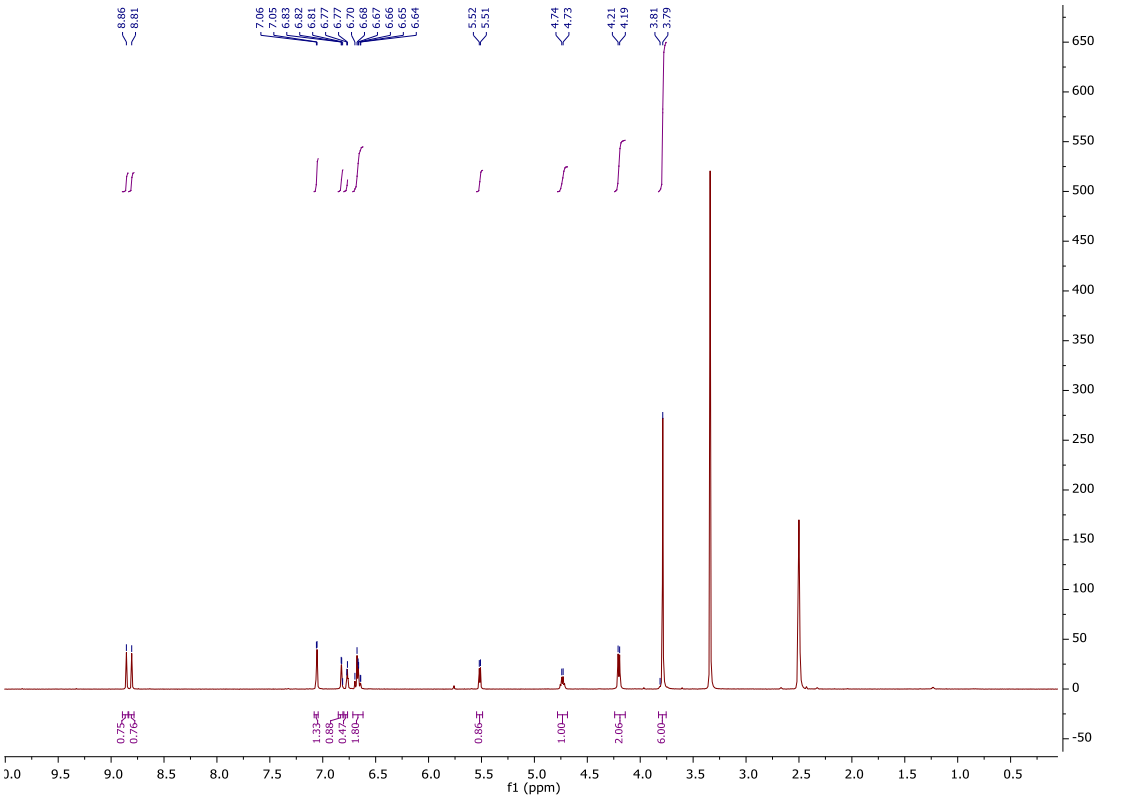

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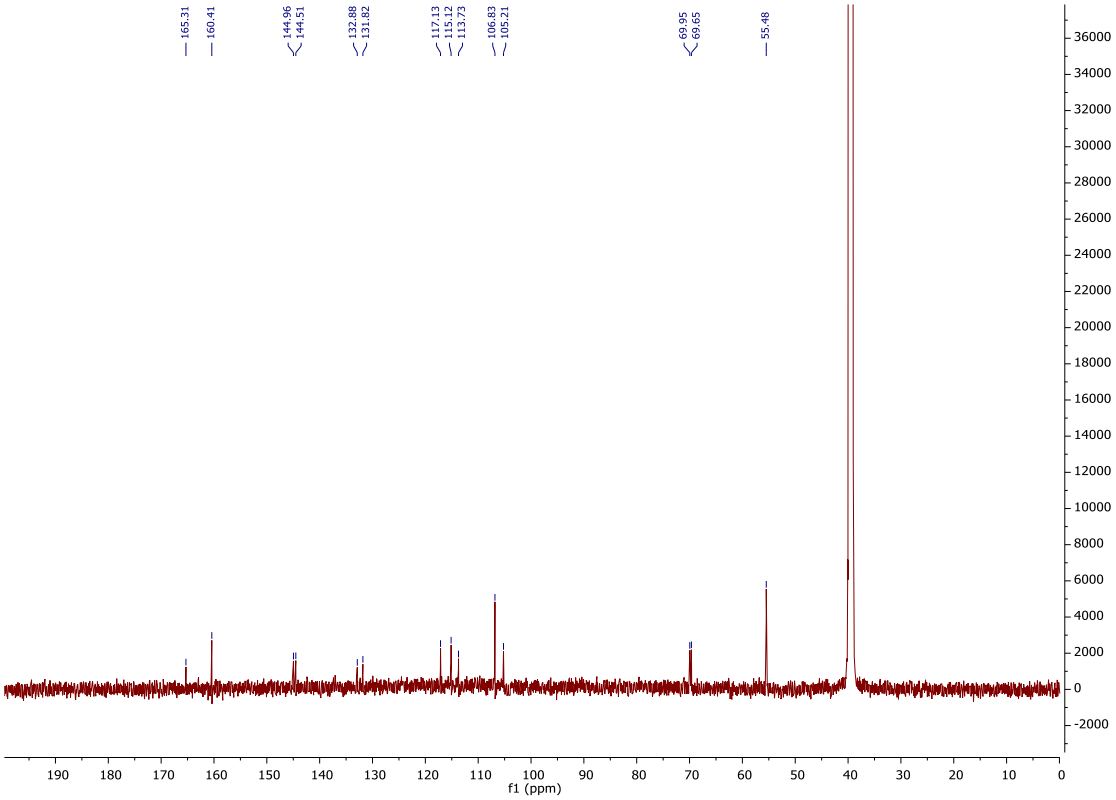

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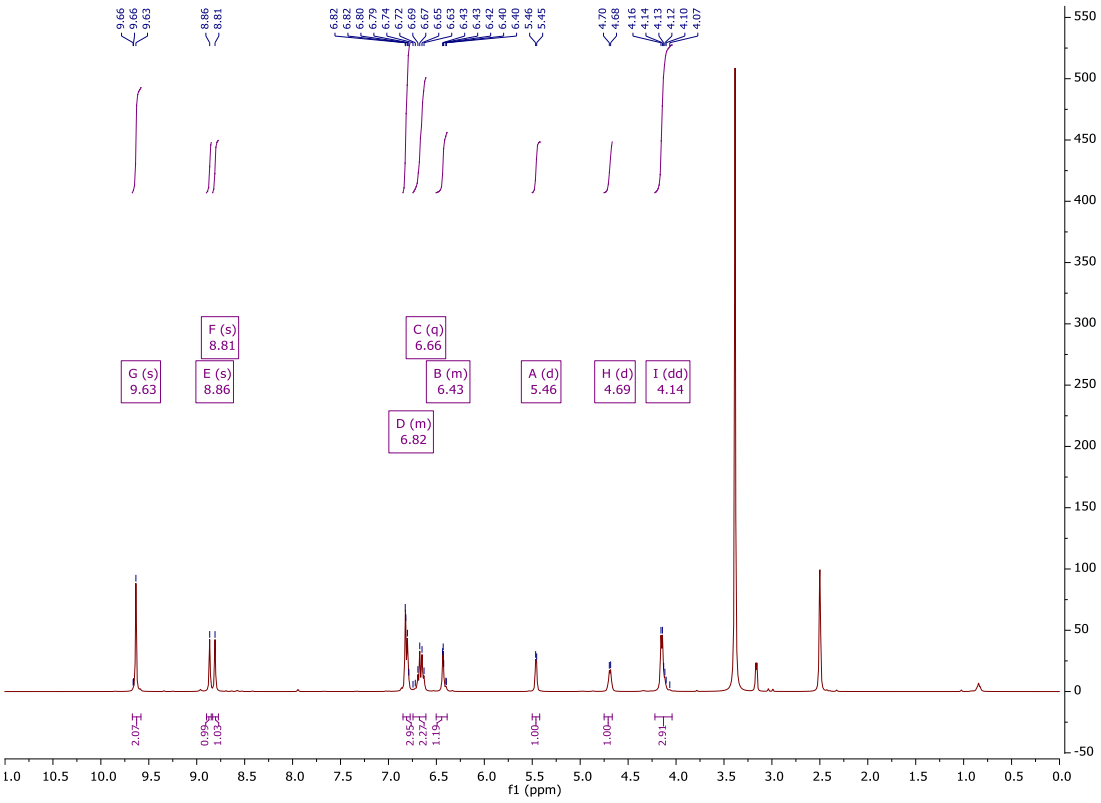

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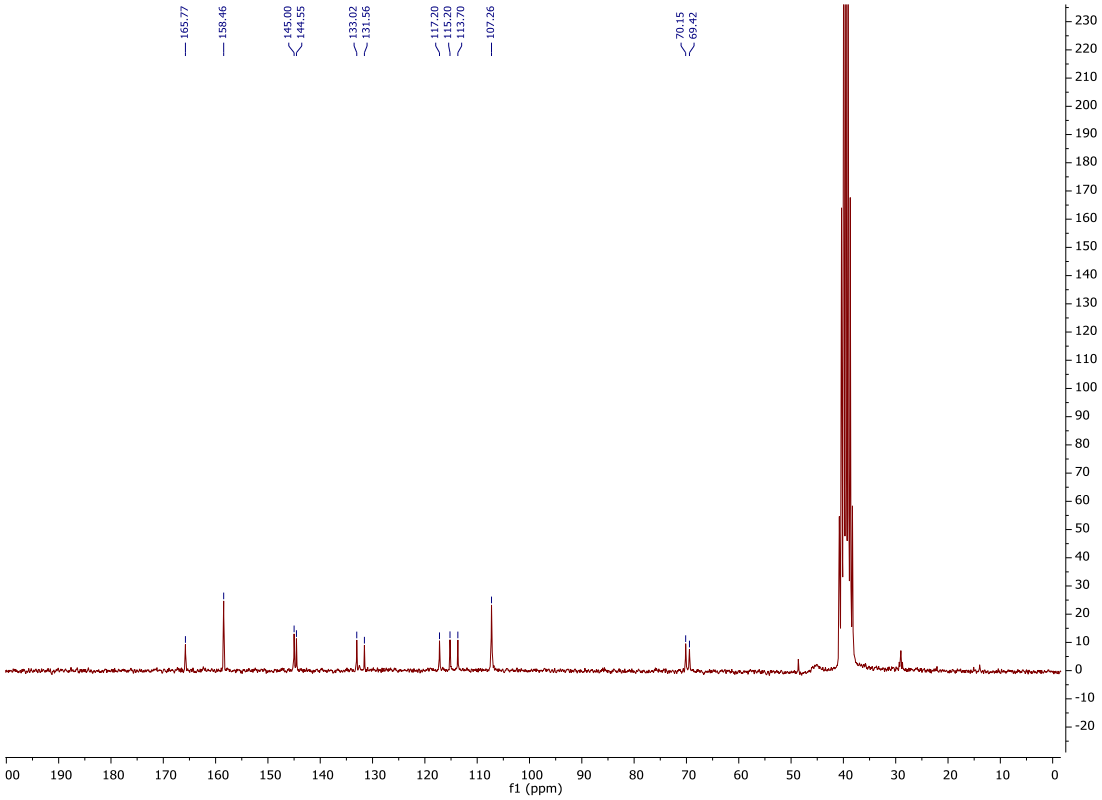

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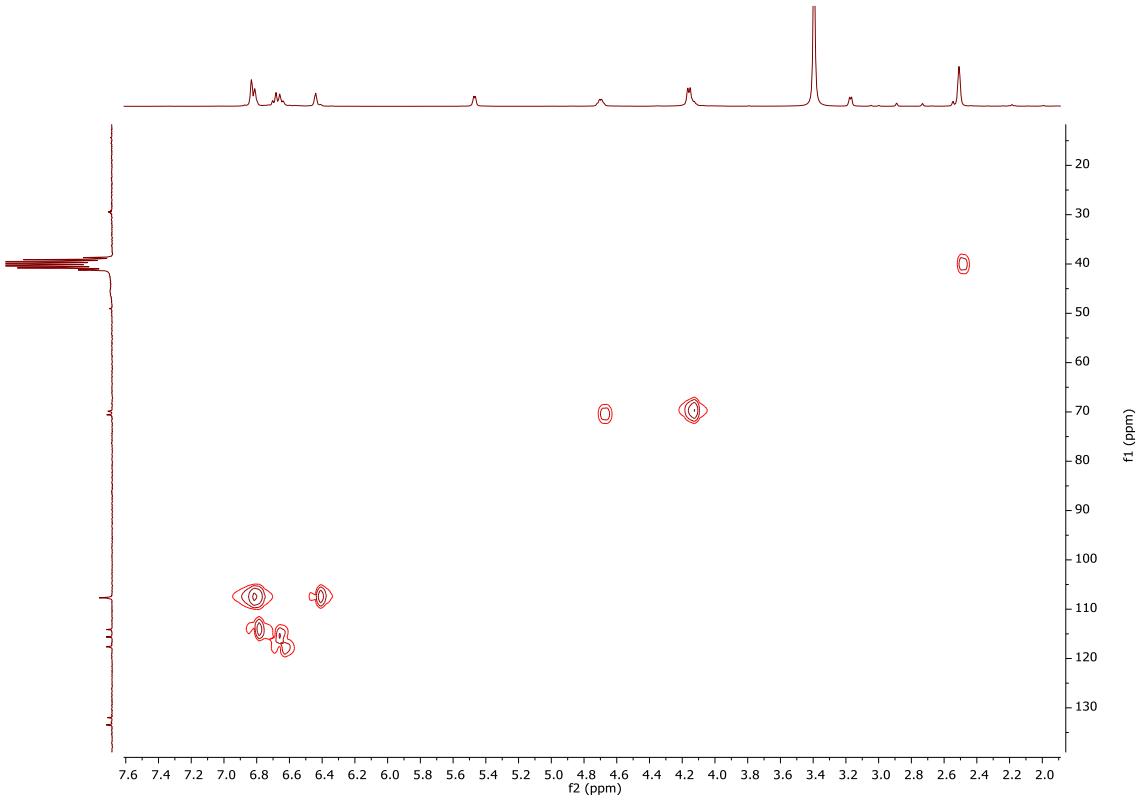

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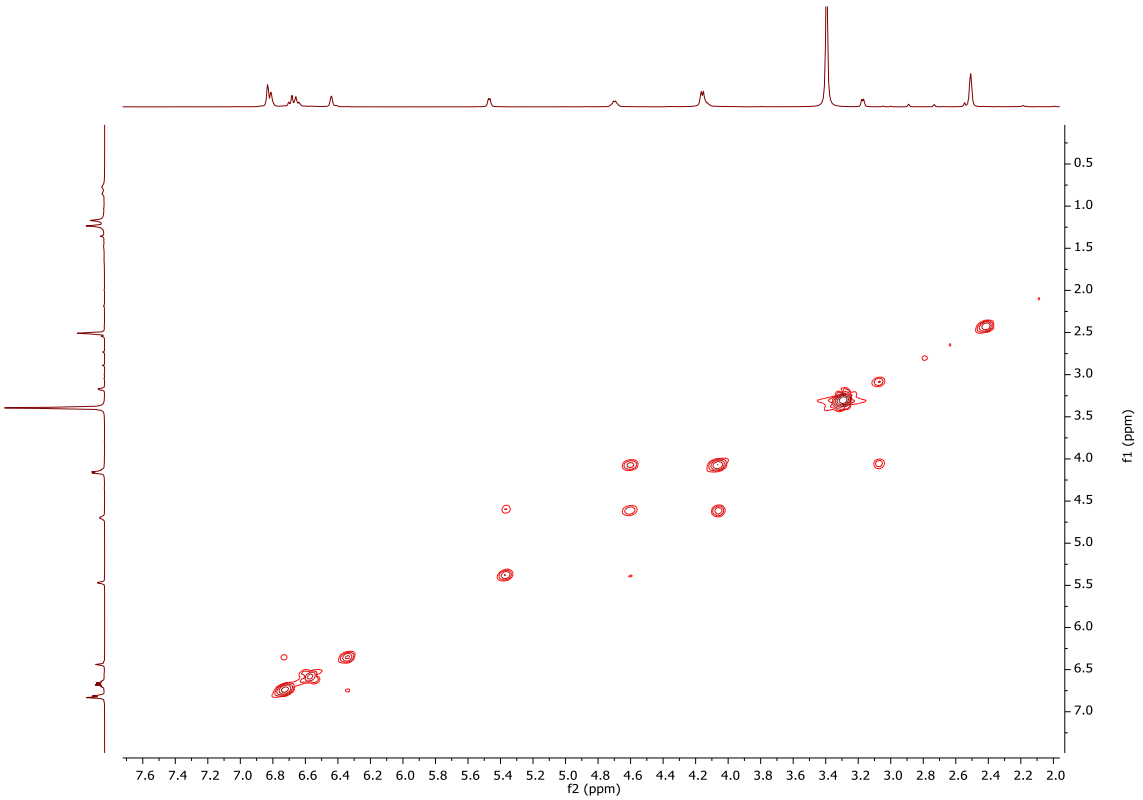

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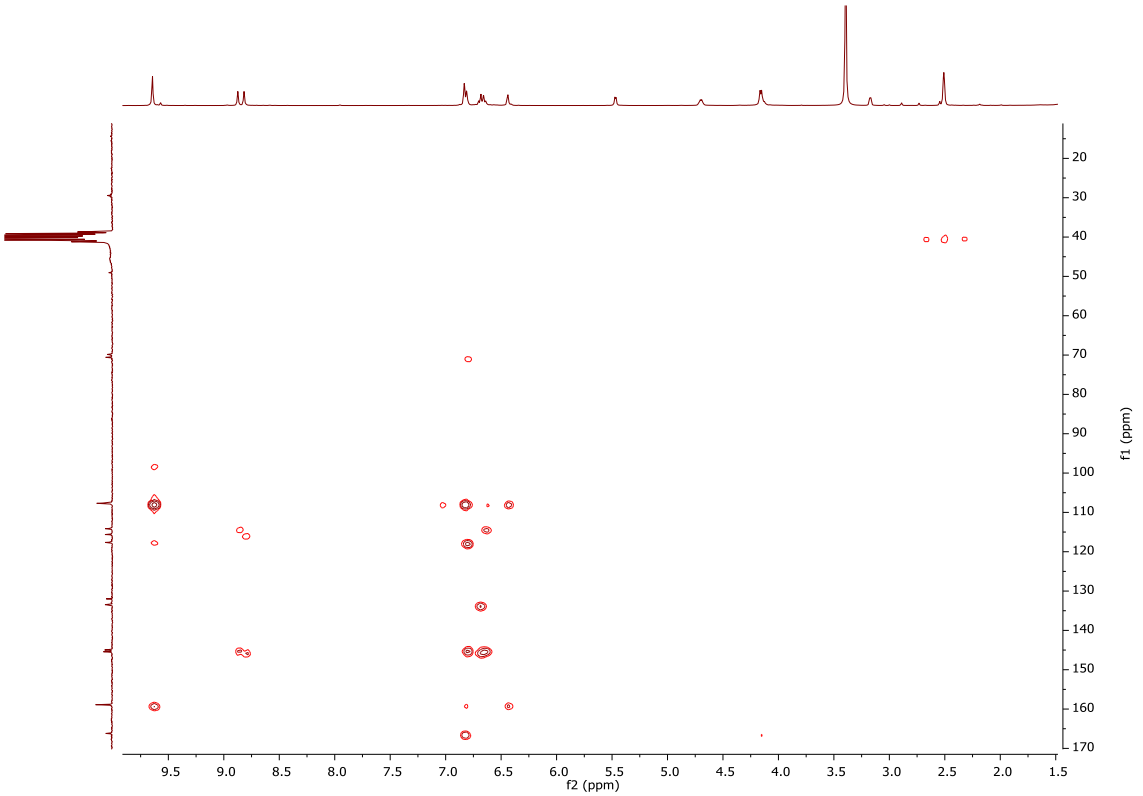

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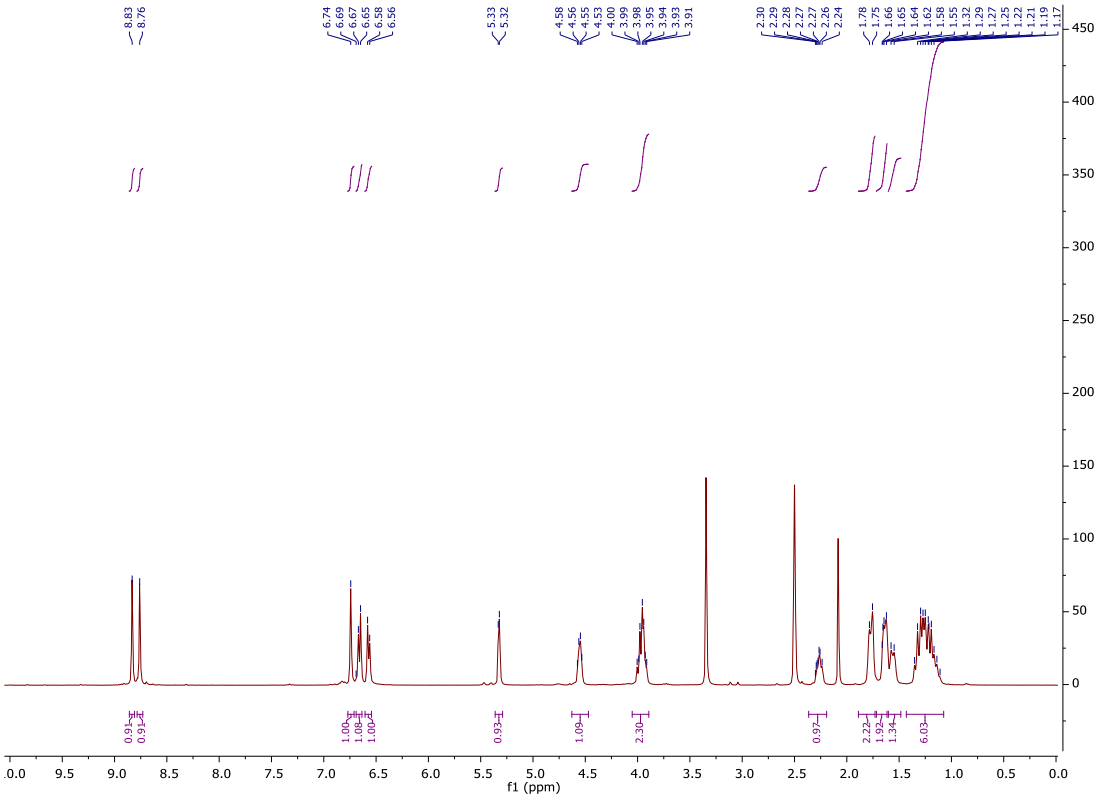

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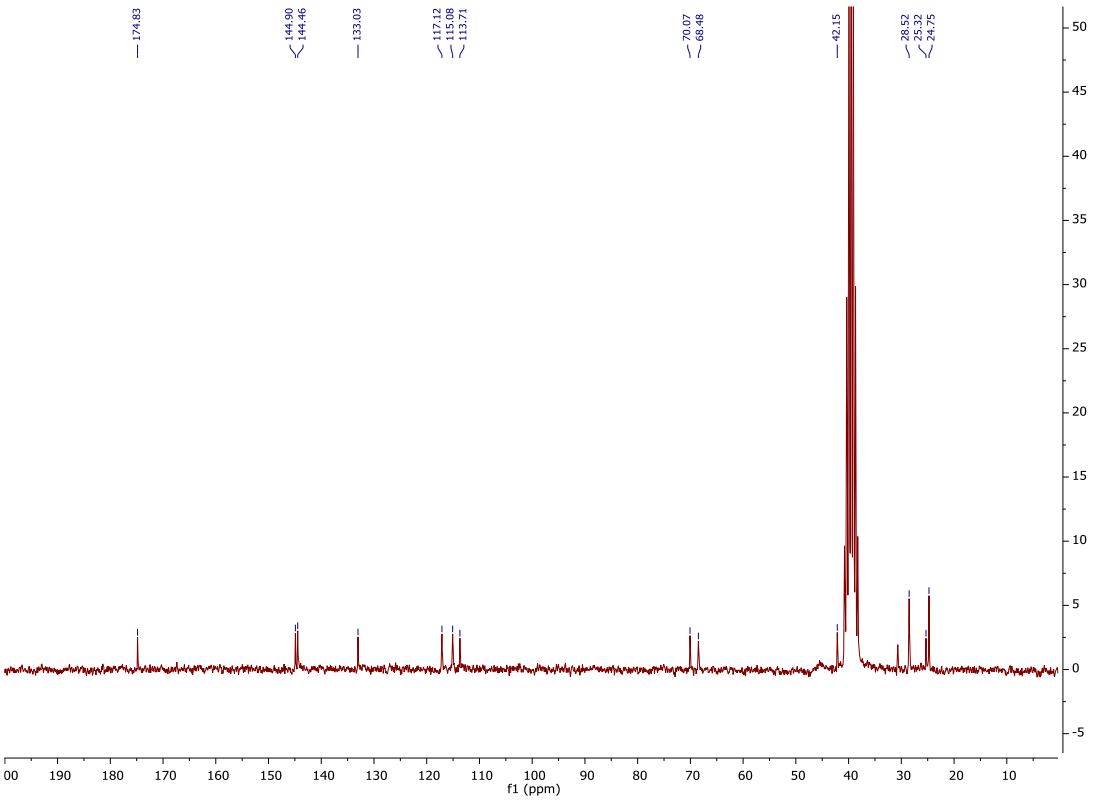

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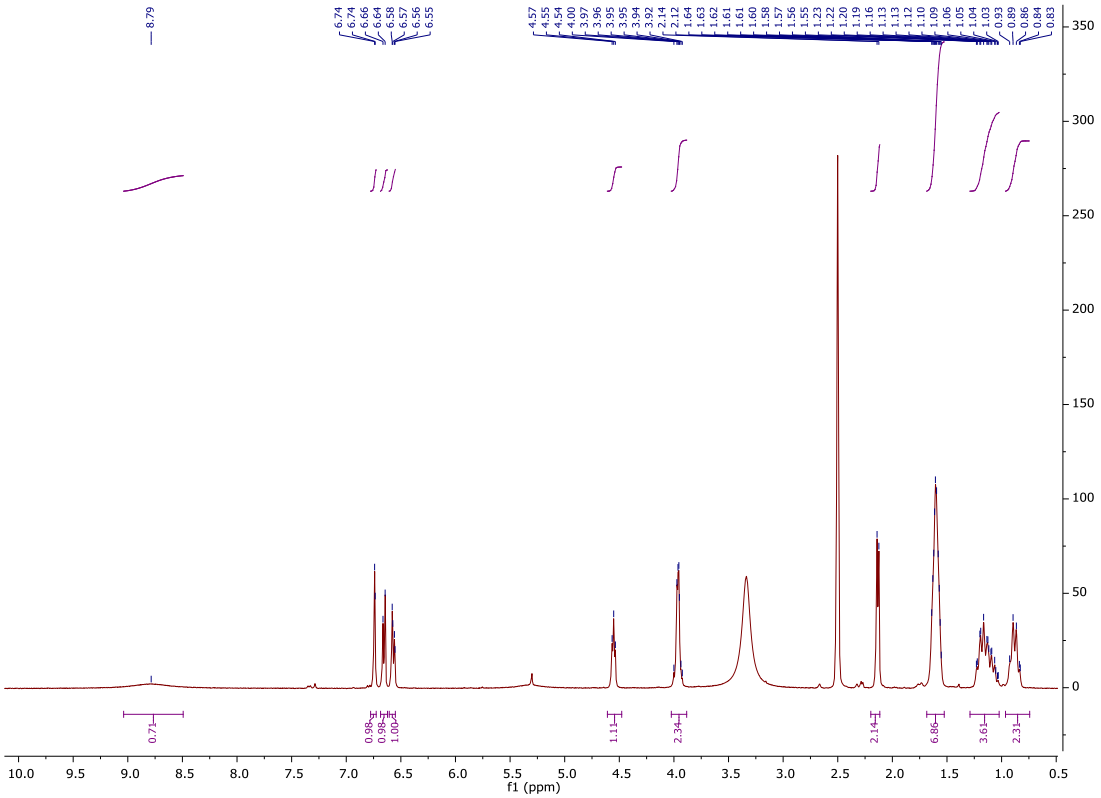

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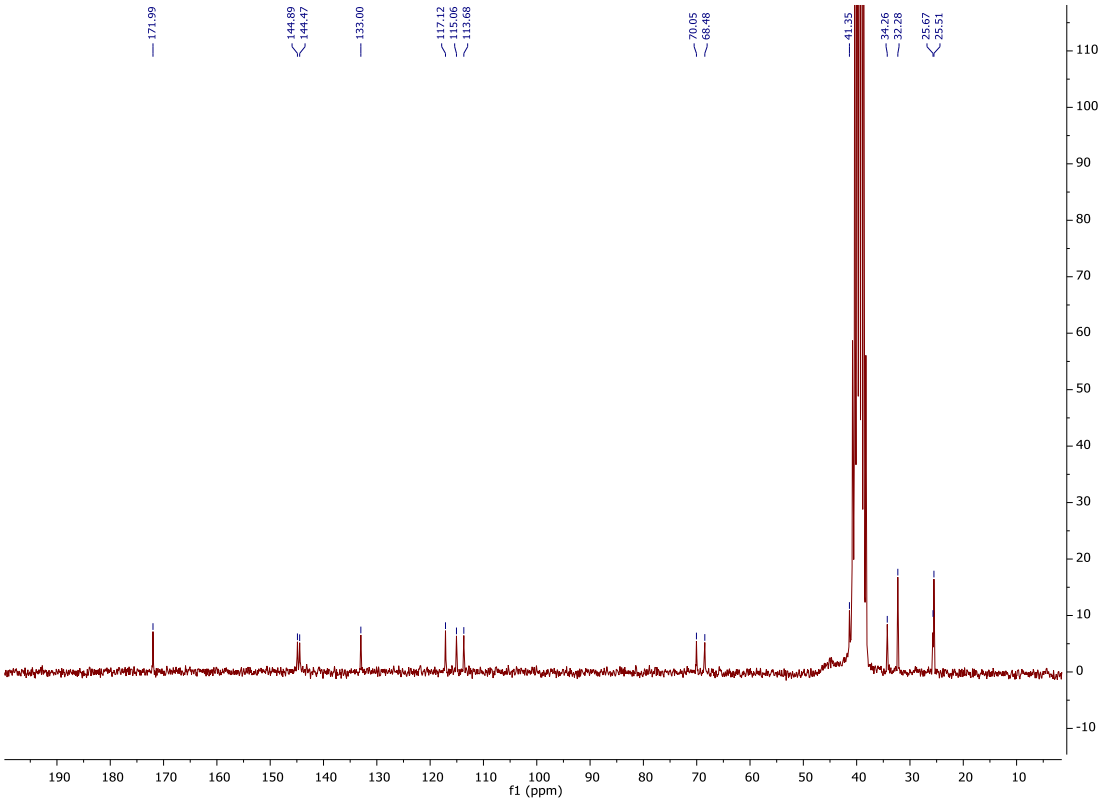

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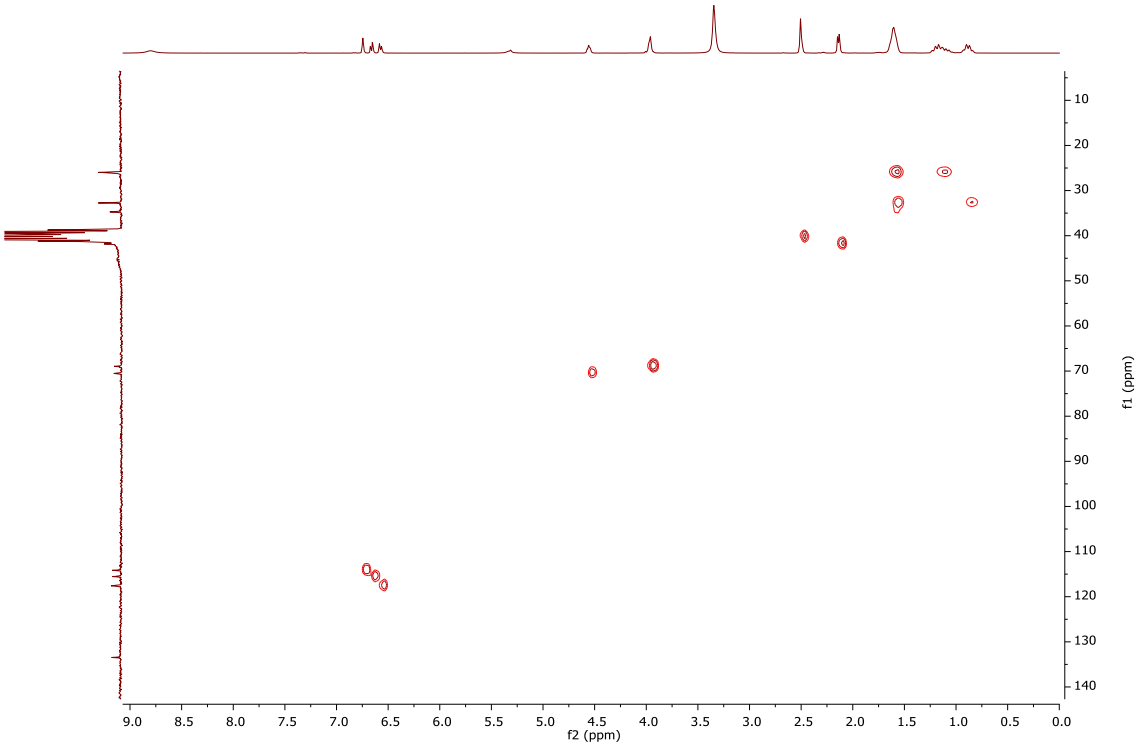

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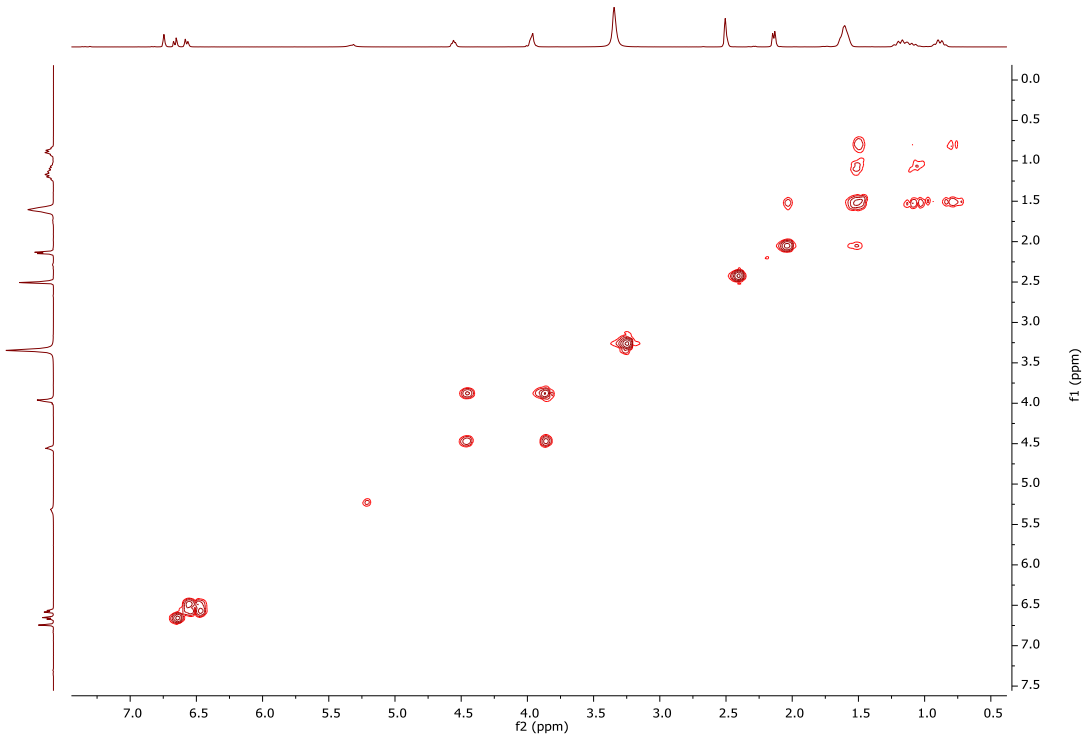
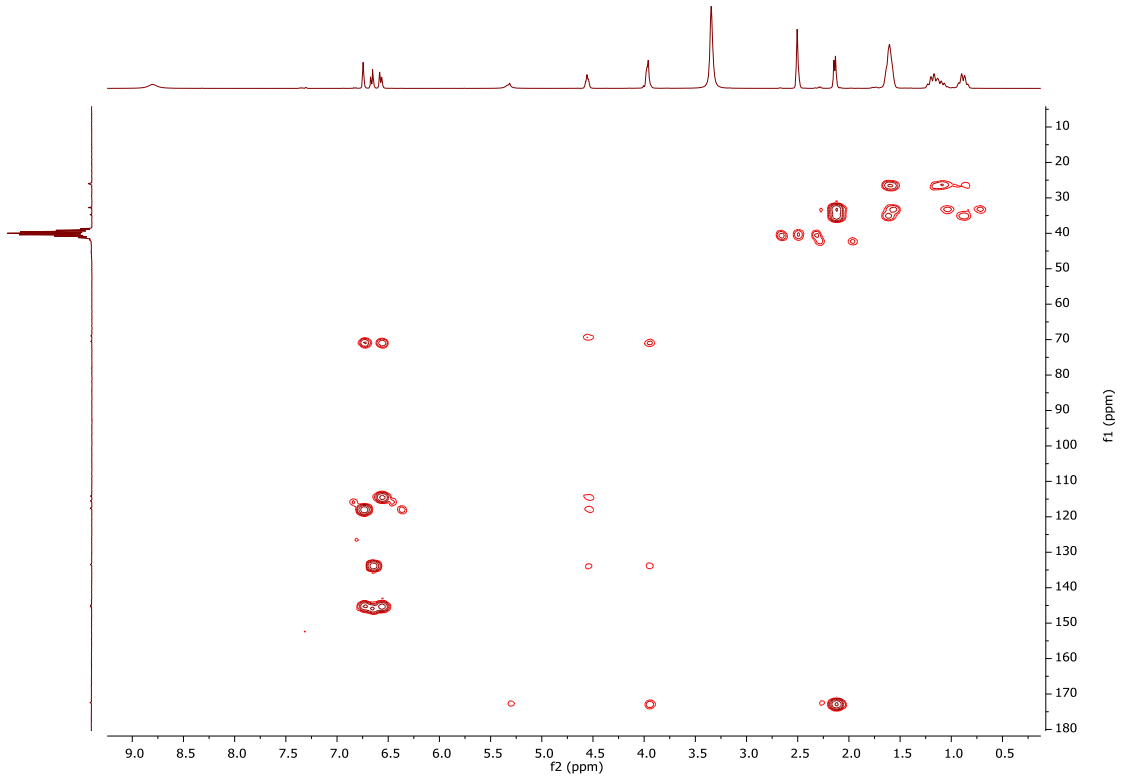


COSY spectrum of **5e**



HMBC spectrum of **5e**

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Figures

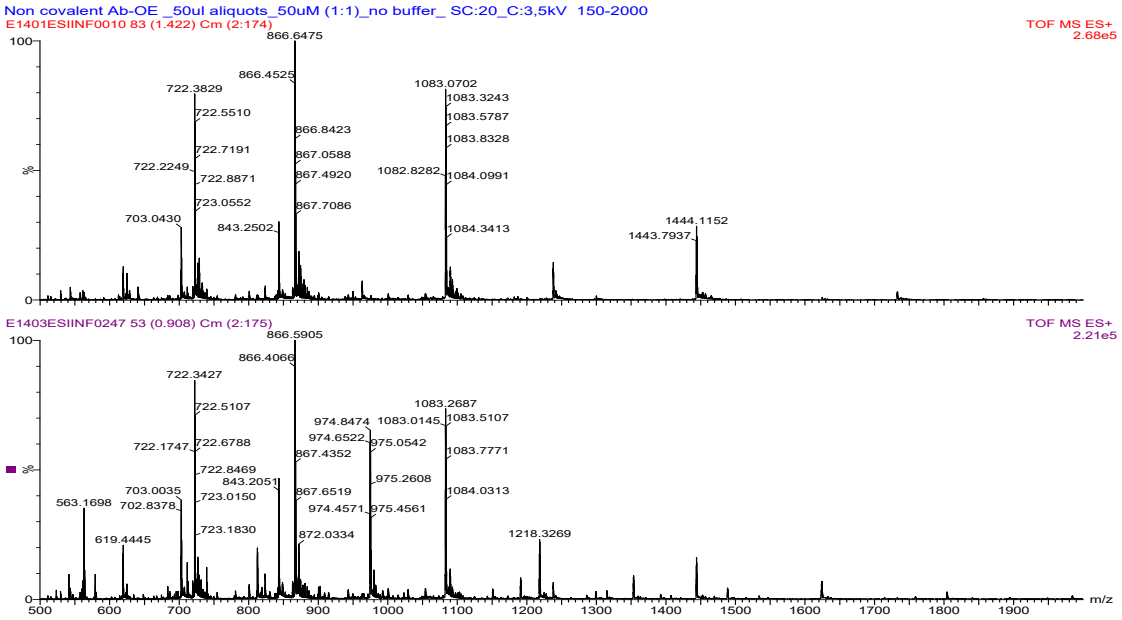

Figure S1: Positive Ionisation ESI Mass Spectrum of Aβ(1-40) along with the complex Aβ(1-40) and Oleuropein

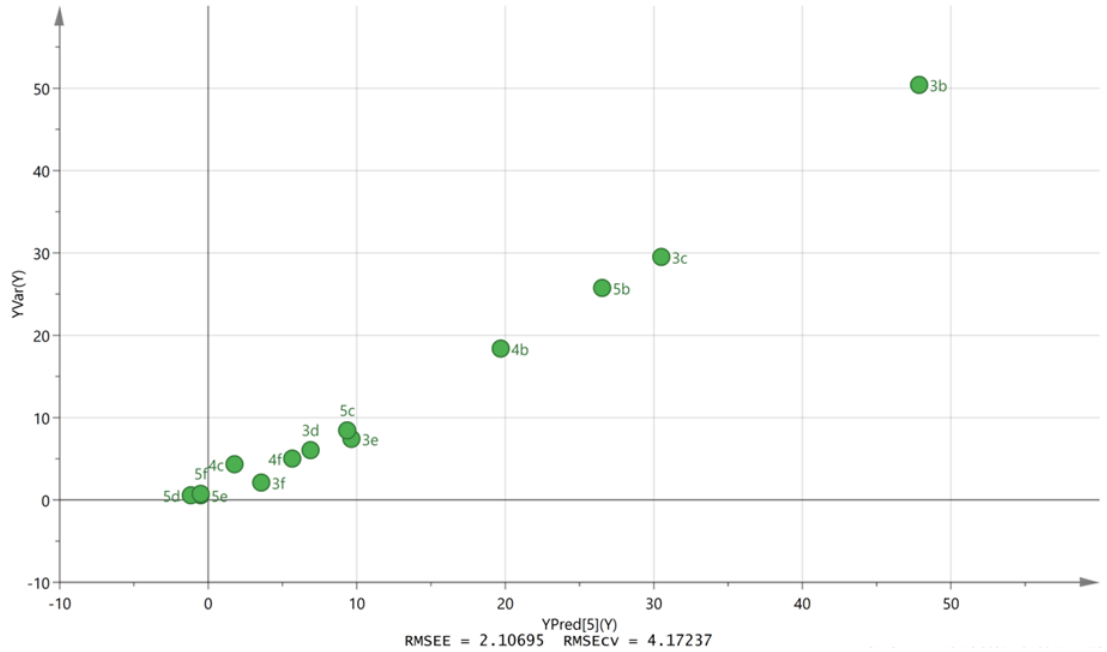

Figure S2: experimental vs calculated values (from the QSAR model) of the analogues complexing activity, based on the reduced model.

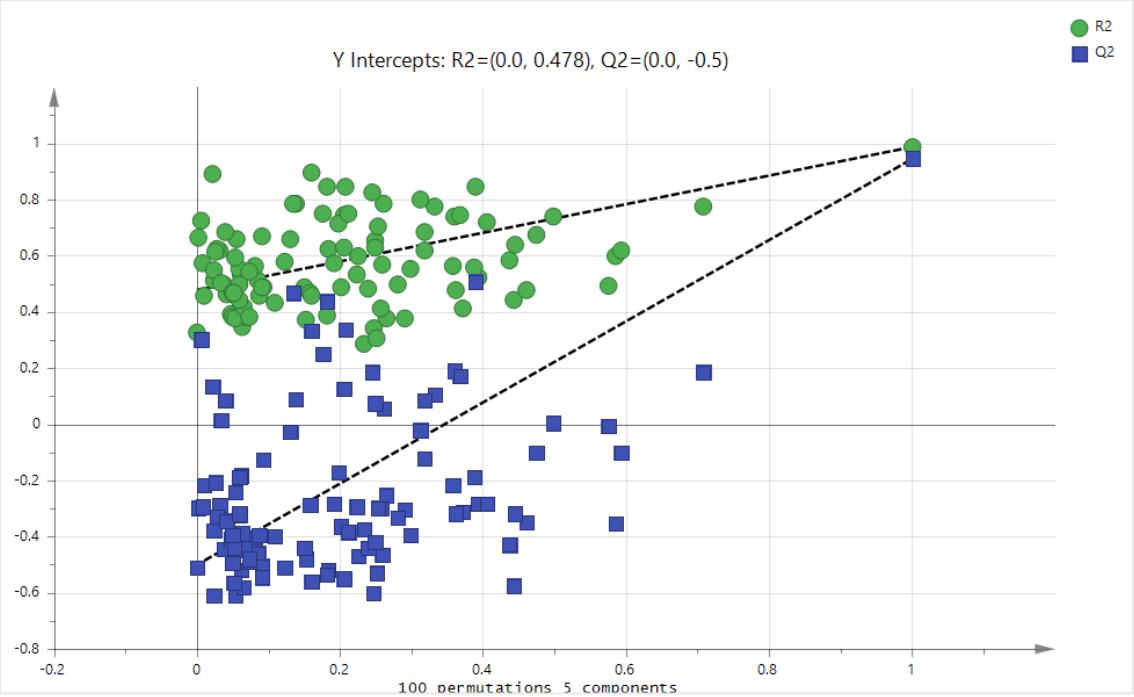

Figure S3: Permutation testing on the generated QSAR reduced model (n=100 permutations)

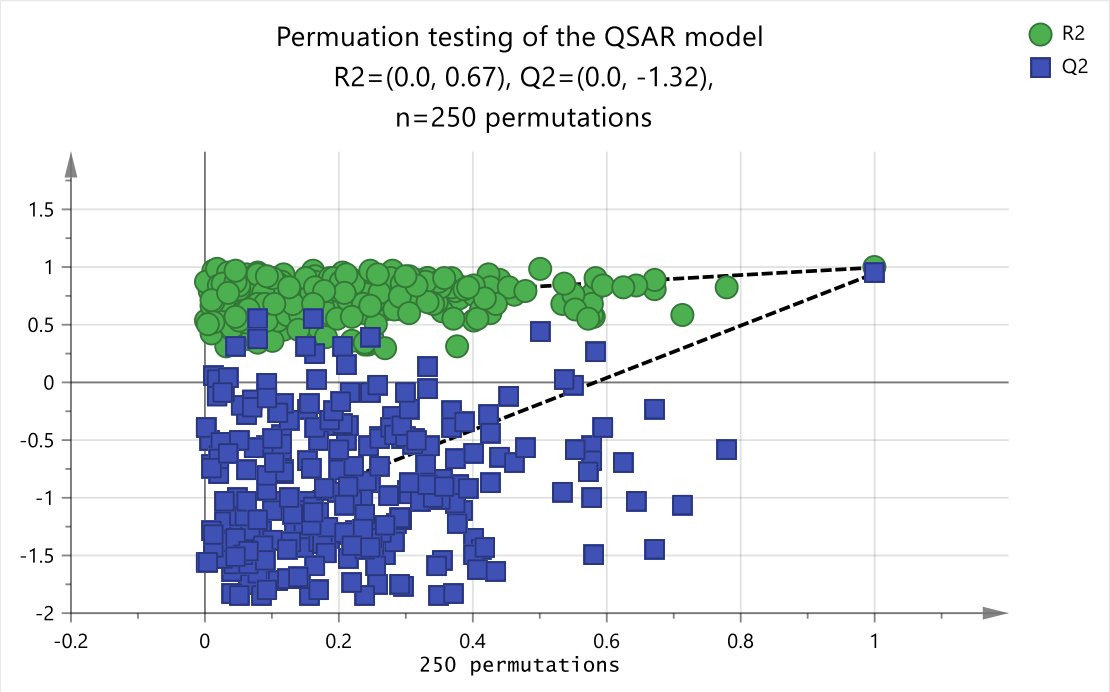

Figure S4: Permutation testing on the generated QSAR reduced model (n=250 permutations)

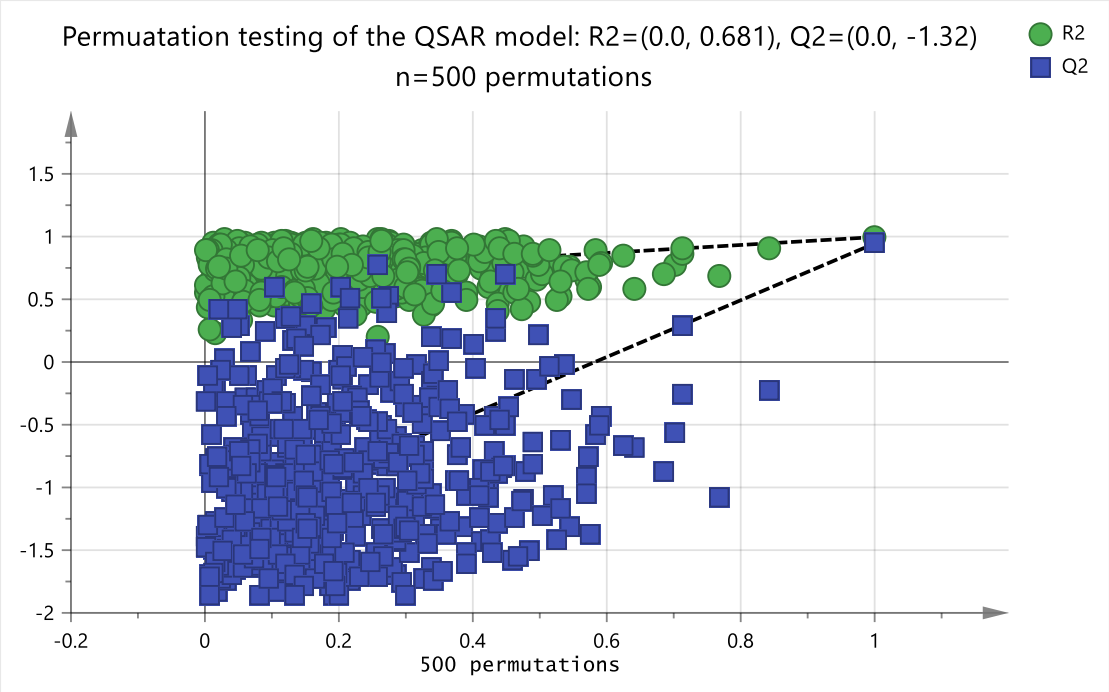

Figure S5: Permutation testing on the generated QSAR reduced model (n=500 permutations)

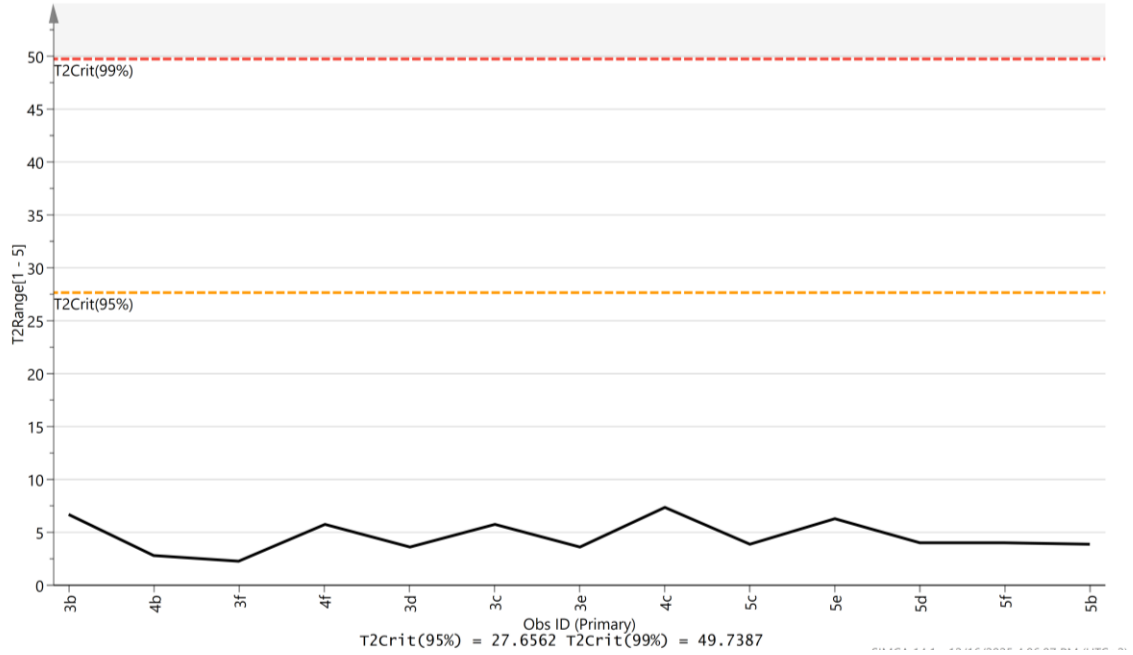

Figure S6: Validation of the QSAR model, T2 Hotteling testing for severe outliers of the reduced model

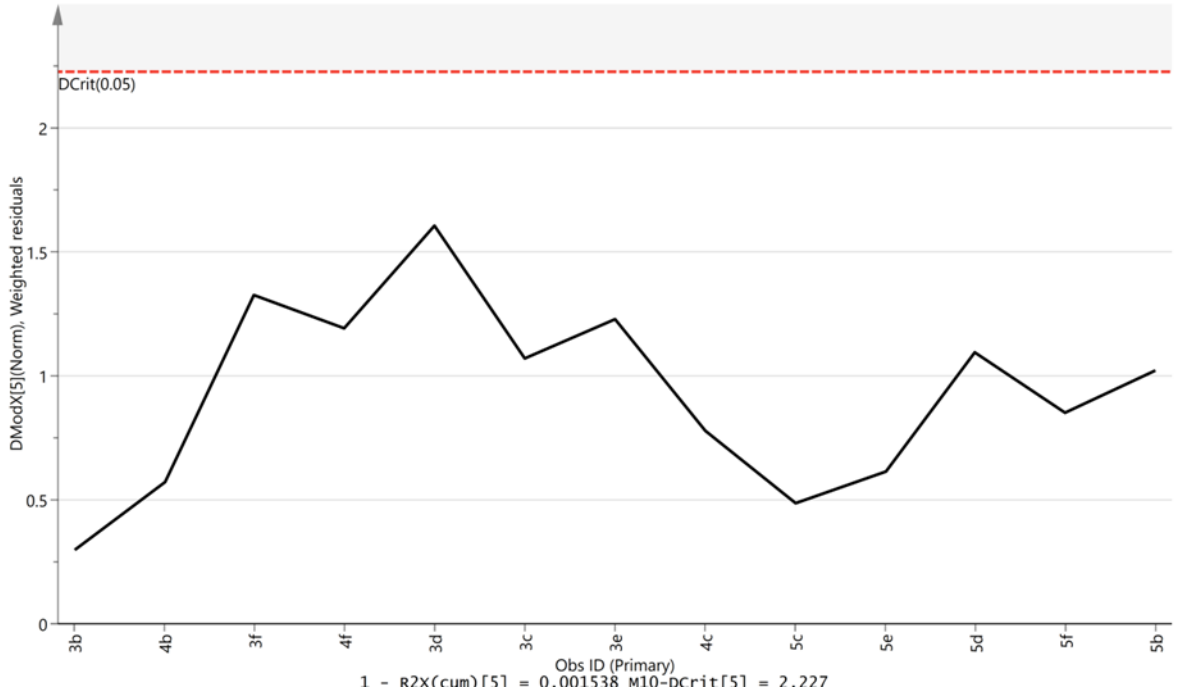

Figure S7: Validation of the QSAR reduced model DModX testing for mild outliers

Tables

Table S1: Parameters used for the exploration of the non-covalent complexes between the Aβ and the examined molecules

Capillary (kV)	3.5
Source (^{O}C)	120
L.M.	4.7
H.M.	15.0
Collision Energy (V)	5.0
Sampling Cone (V)	2.0
Desolvation (^{O}C)	220
Cell Entrance (V)	2.0
Extraction Cone (V)	2.0
Cone	Off
Ion Energy (V)	0.5
Cell Exit (V)	-10
Ion Guide: (V)	3.0
Desolvation (L/hr)	400
Pre Filter (V)	2.0
Scan range (m/z)	150-2000
Detector (V)	1900

Table S2: Cross validation testing

Number of groups (k)	**R^2**	**Q^2**
2	0.987	0.934
5	0.987	0.925
7	0.987	0.944
10	0.987	0.922
16 (Leave one out)	0.996	0.935