

S1 Supplementary data contents page

Title: Pteridine-, thymidine-, choline- and imidazole-derived Alkaloids from the Australian Ascidian, *Leptoclinides durus*

Authors: Kathryn E. Rudolph,^a Michelle S. Liberio,^b Rohan A. Davis,^b Anthony R. Carroll,^{*a,b}

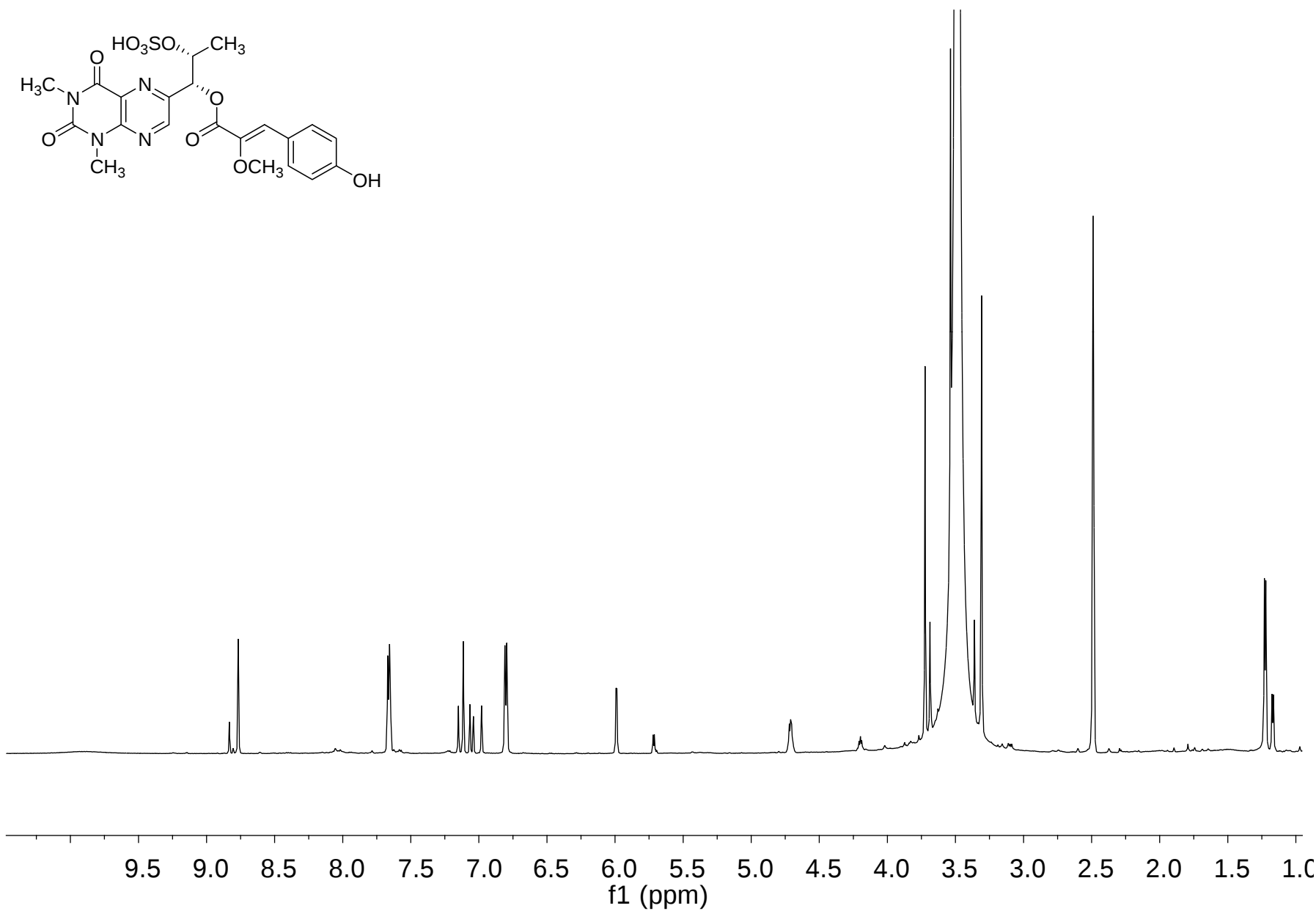
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Corresponding author contact details: Tel.: +61 7 5552 9187; fax: +61 7 5552 9047; e-mail: a.carroll@griffith.edu.au

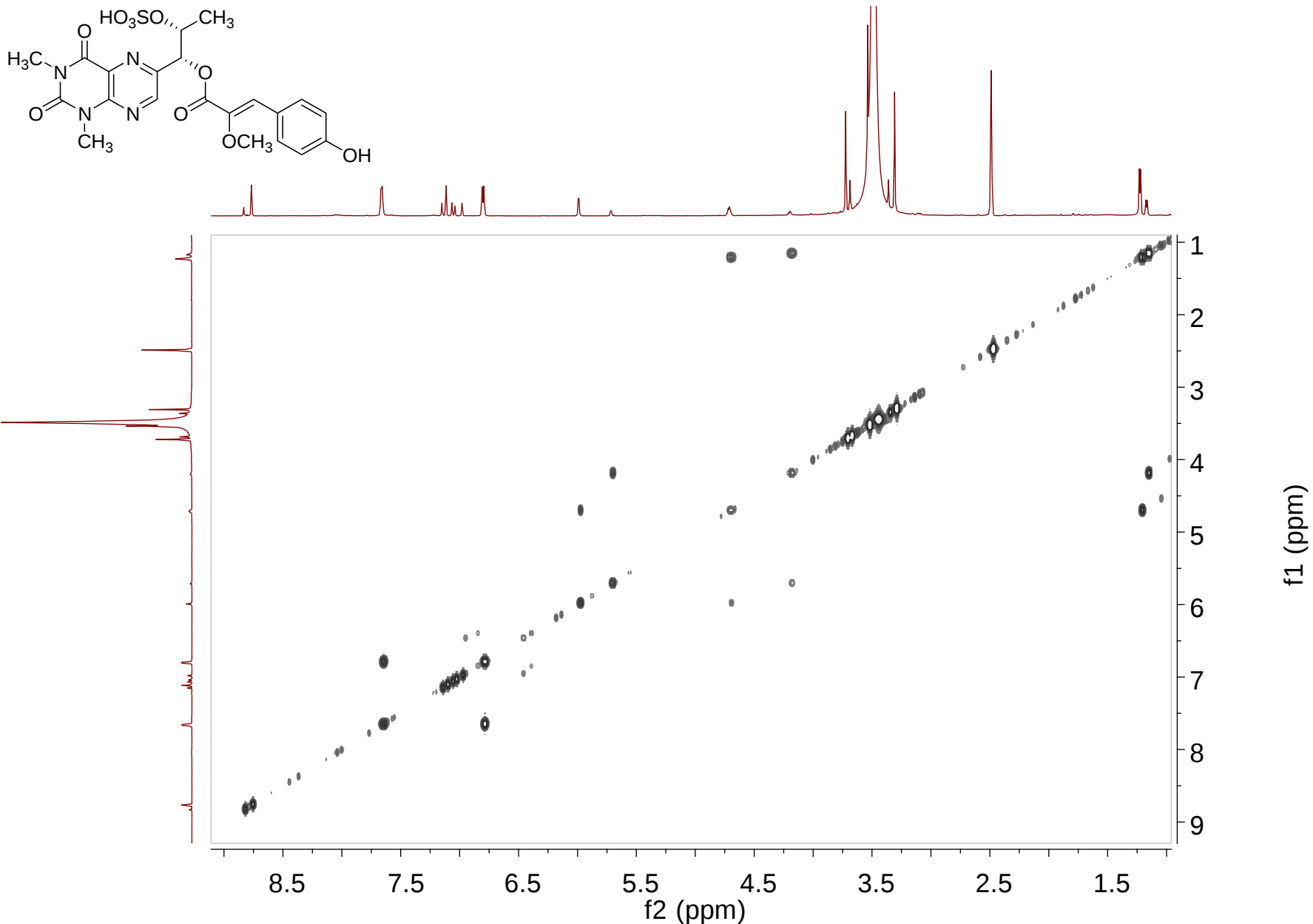
Contents:

S2	¹ H NMR spectrum for duramidine A in DMSO- <i>d</i> ₆	S29	¹³ C NMR spectrum for leptoclinidine B in DMSO- <i>d</i> ₆
S3	gCOSY spectrum for duramidine A in DMSO- <i>d</i> ₆	S30	gCOSY spectrum for leptoclinidine B in DMSO- <i>d</i> ₆
S4	gHSQC spectrum for duramidine A in DMSO- <i>d</i> ₆	S31	gHSQC spectrum for leptoclinidine B in DMSO- <i>d</i> ₆
S5	gHMBC spectrum for duramidine A in DMSO- <i>d</i> ₆	S31	gHMBC spectrum for leptoclinidine B in DMSO- <i>d</i> ₆
S6	¹ H NMR spectrum for duramidine B in DMSO- <i>d</i> ₆	S32	¹ H NMR spectrum for durabetaine A in DMSO- <i>d</i> ₆
S7	gHSQC spectrum for duramidine B in DMSO- <i>d</i> ₆	S33	gCOSY spectrum for durabetaine A in DMSO- <i>d</i> ₆
S8	gHMBC spectrum for duramidine B in DMSO- <i>d</i> ₆	S34	gHSQC spectrum for durabetaine A in DMSO- <i>d</i> ₆
S9	ROESY spectrum for duramidine B in DMSO- <i>d</i> ₆	S35	gHMBC spectrum for durabetaine A in DMSO- <i>d</i> ₆
S10	¹ H NMR spectrum for duramidine C in DMSO- <i>d</i> ₆	S36	ROESY spectrum for durabetaine A in DMSO- <i>d</i> ₆
S11	gCOSY spectrum for duramidine C in DMSO- <i>d</i> ₆	S37	¹ H NMR spectrum for durabetaine B in DMSO- <i>d</i> ₆
S12	gHSQC spectrum for duramidine C in DMSO- <i>d</i> ₆	S38	gCOSY spectrum for durabetaine B in DMSO- <i>d</i> ₆
S13	gHMBC spectrum for duramidine C in DMSO- <i>d</i> ₆	S39	gHSQC spectrum for durabetaine B in DMSO- <i>d</i> ₆
S14	ROESY spectrum for duramidine C in DMSO- <i>d</i> ₆	S40	gHMBC spectrum for durabetaine B in DMSO- <i>d</i> ₆
S15	¹³ C NMR spectrum for duramidine C in DMSO- <i>d</i> ₆	S41	¹ H NMR spectrum for leptoclinidamine D in DMSO- <i>d</i> ₆
S16	¹ H NMR spectrum for duramidine D in DMSO- <i>d</i> ₆	S42	gCOSY spectrum for leptoclinidamine D in DMSO- <i>d</i> ₆
S17	gCOSY spectrum for duramidine D in DMSO- <i>d</i> ₆	S43	gHSQC spectrum for leptoclinidamine D in DMSO- <i>d</i> ₆
S18	gHSQC spectrum for duramidine D in DMSO- <i>d</i> ₆	S44	gHMBC spectrum for leptoclinidamine D in DMSO- <i>d</i> ₆
S19	gHMBC spectrum for duramidine D in DMSO- <i>d</i> ₆	S45	¹ H NMR spectrum for leptoclinidamine E in DMSO- <i>d</i> ₆
S20	ROESY spectrum for duramidine D in DMSO- <i>d</i> ₆	S46	gCOSY spectrum for leptoclinidamine E in DMSO- <i>d</i> ₆
S21	¹³ C NMR spectrum for duramidine C in DMSO- <i>d</i> ₆	S47	gHSQC spectrum for leptoclinidamine E in DMSO- <i>d</i> ₆
S22	¹ H NMR spectrum for leptoclinidine A in DMSO- <i>d</i> ₆	S48	gHMBC spectrum for leptoclinidamine E in DMSO- <i>d</i> ₆
S23	¹³ C NMR spectrum for leptoclinidine A in DMSO- <i>d</i> ₆	S49	¹ H NMR spectrum for leptoclinidamine F in DMSO- <i>d</i> ₆
S24	gCOSY spectrum for leptoclinidine A in DMSO- <i>d</i> ₆	S50	gCOSY spectrum for leptoclinidamine F in DMSO- <i>d</i> ₆
S25	gHSQC spectrum for duramidine A in DMSO- <i>d</i> ₆	S51	gHSQC spectrum for leptoclinidamine F in DMSO- <i>d</i> ₆
S26	gHMBC spectrum for leptoclinidine A in DMSO- <i>d</i> ₆	S52	gHMBC spectrum for leptoclinidamine F in DMSO- <i>d</i> ₆
S27	ROESY spectrum for leptoclinidine A in DMSO- <i>d</i> ₆	S53	Real-time cell analysis
S28	¹ H NMR spectrum for leptoclinidine B in DMSO- <i>d</i> ₆		

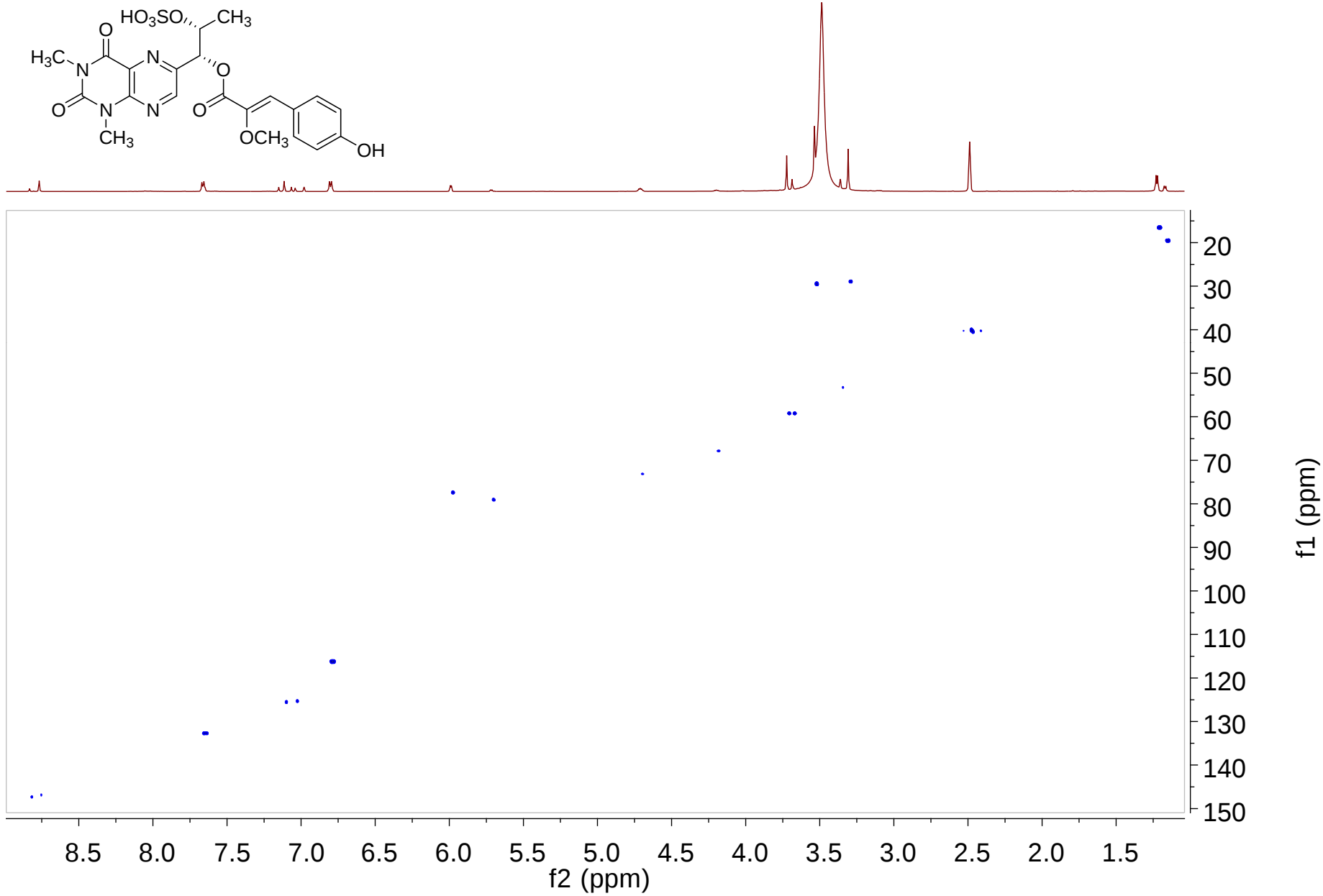
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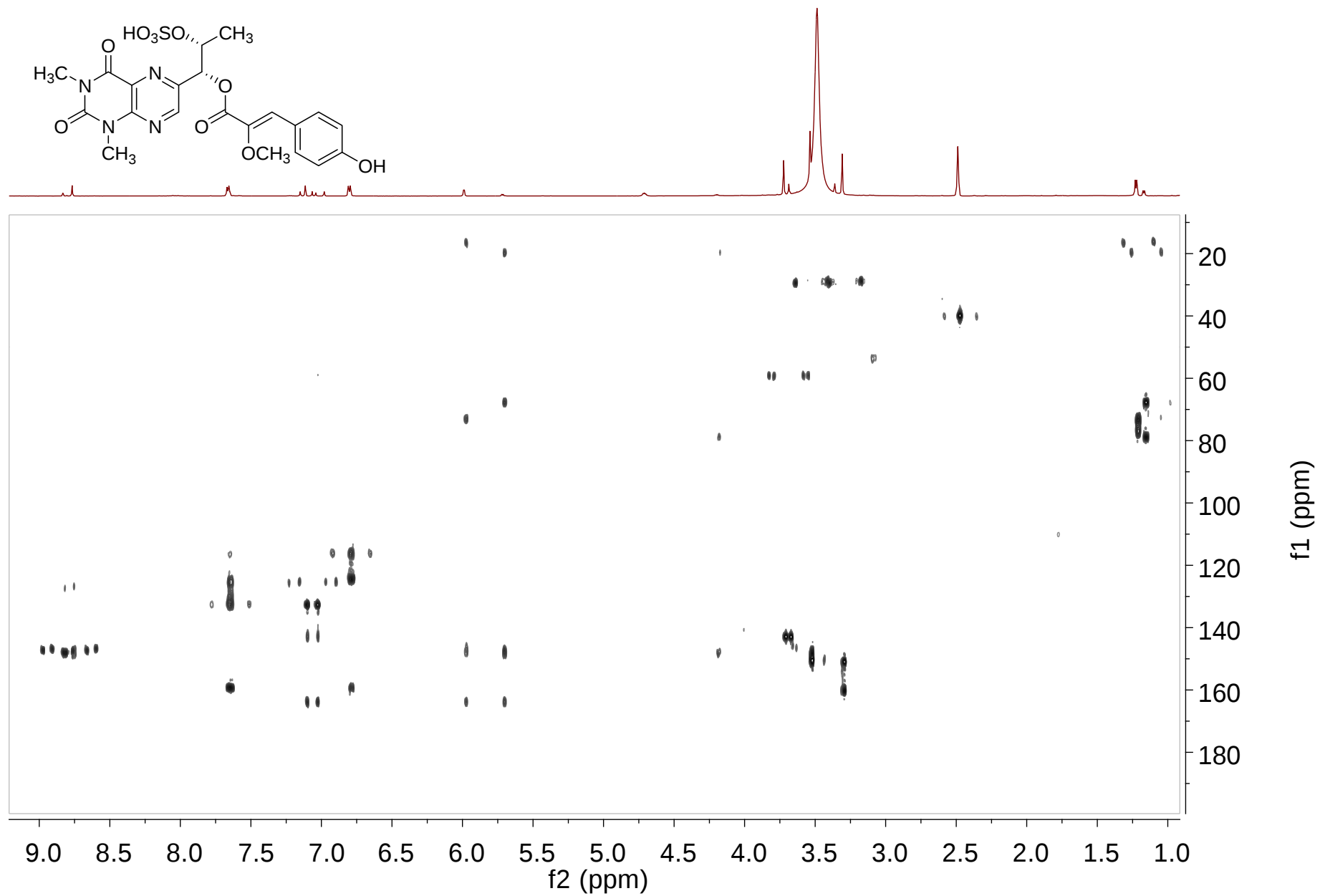
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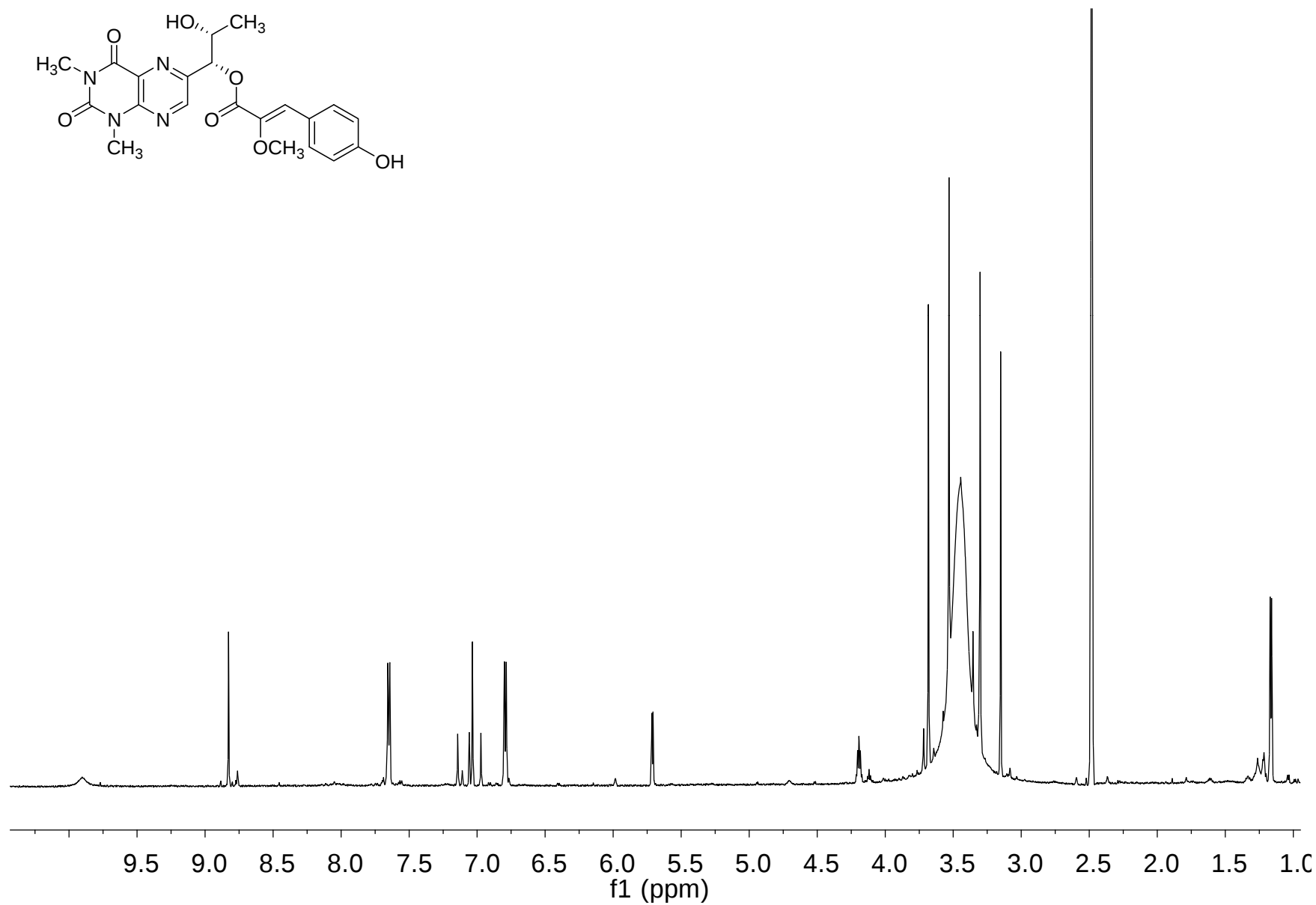
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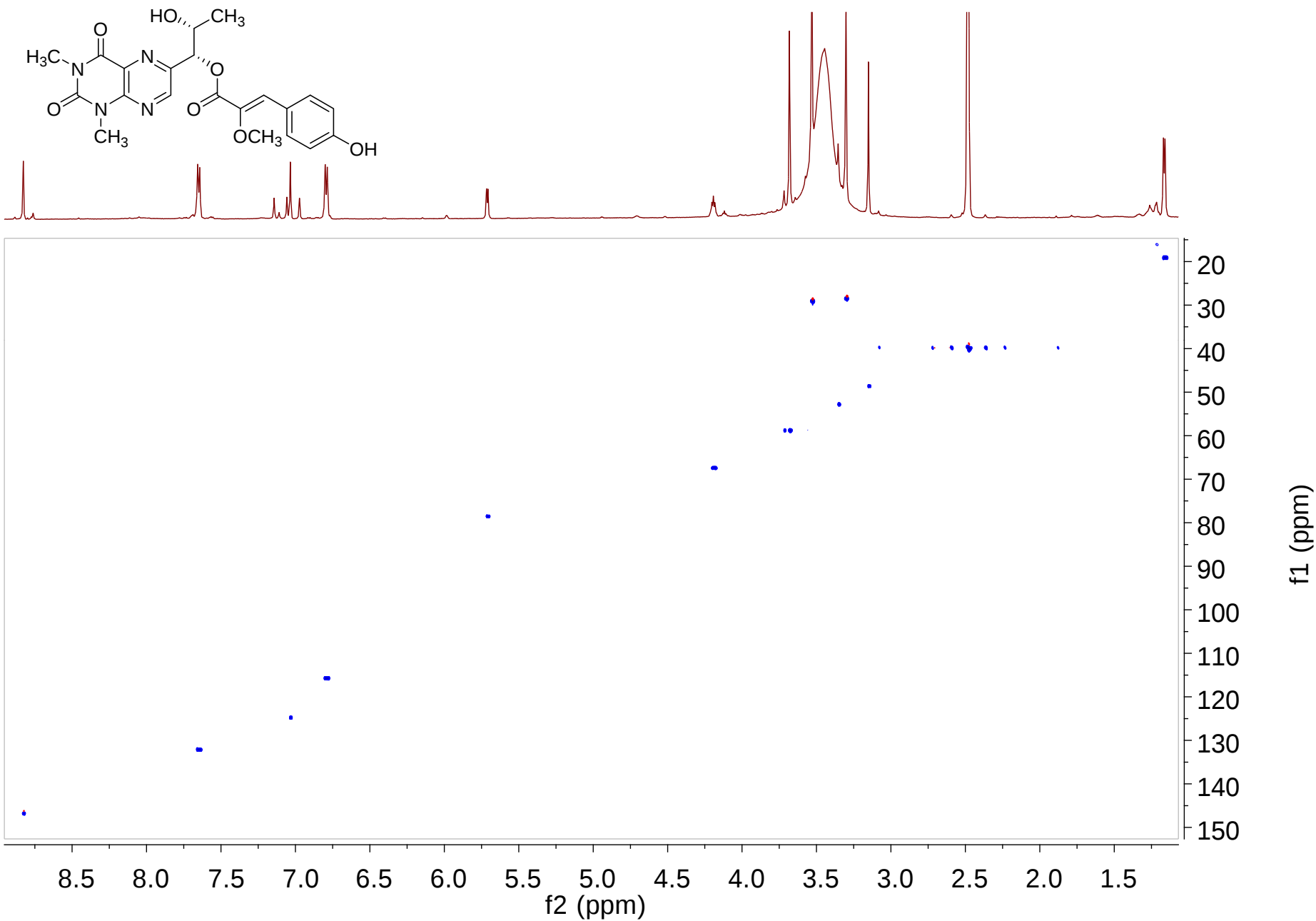
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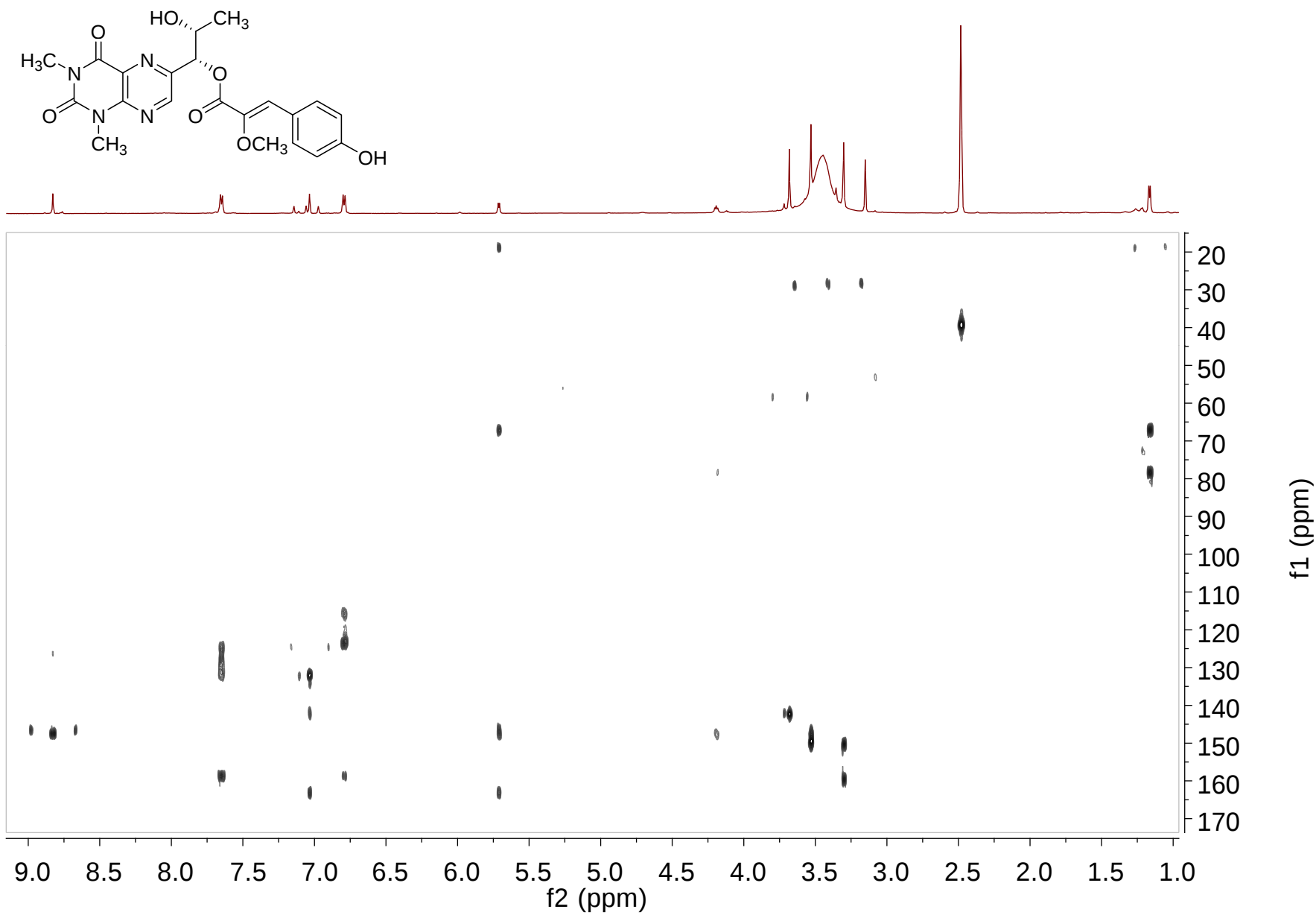
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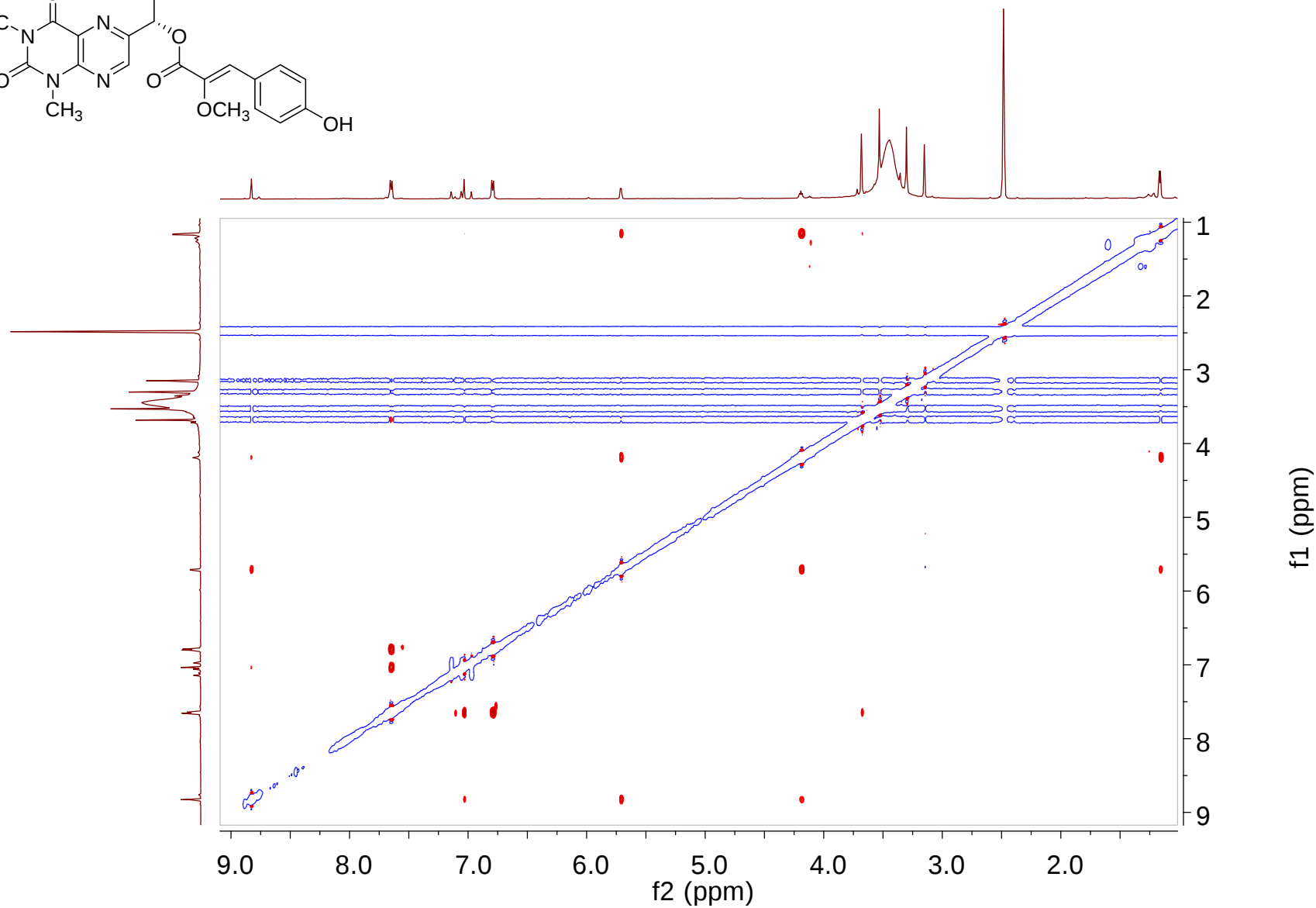
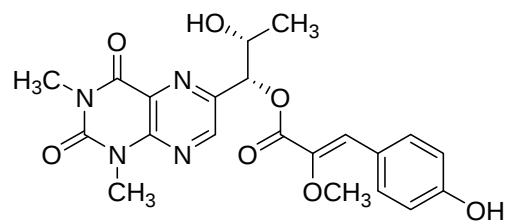
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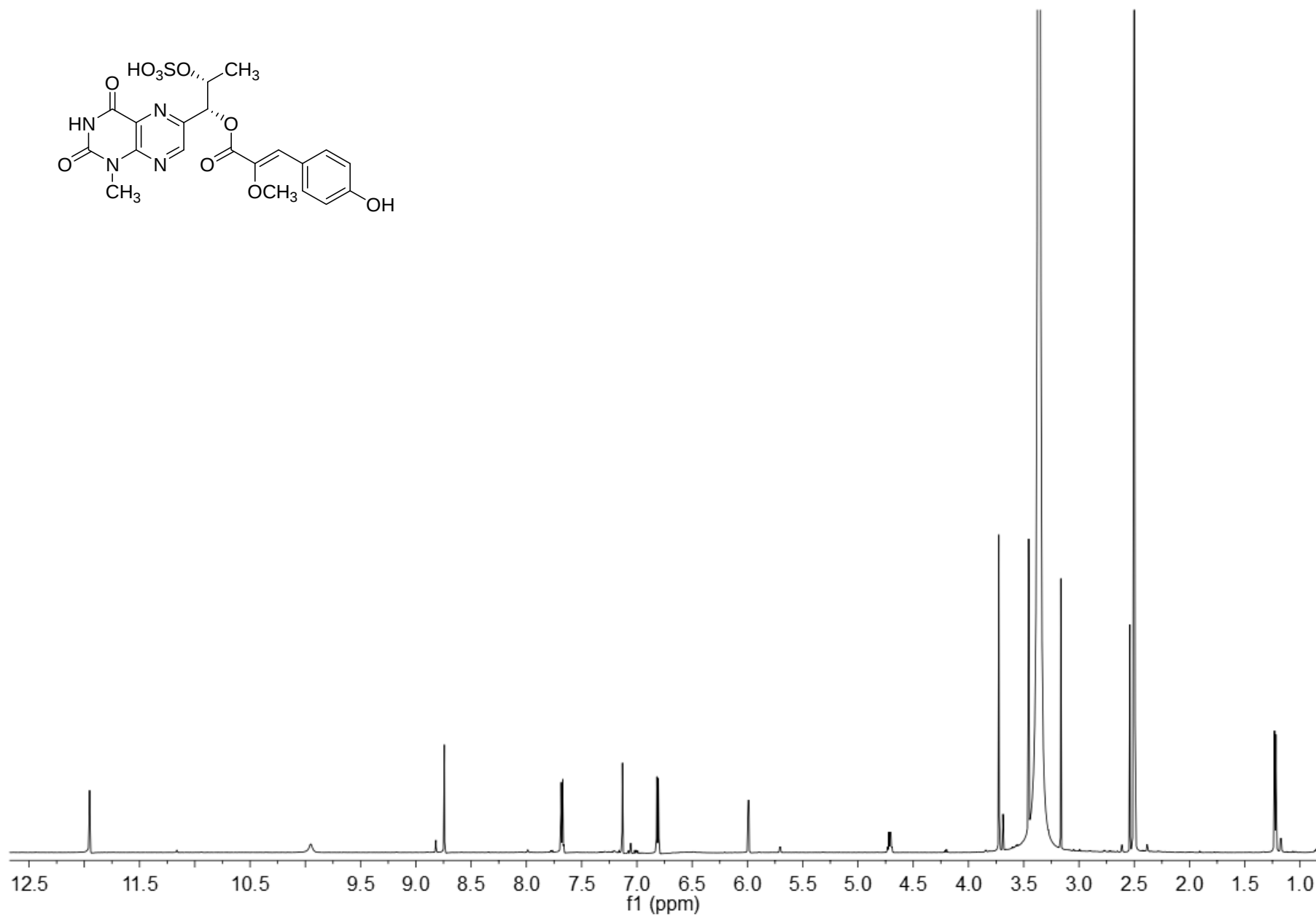
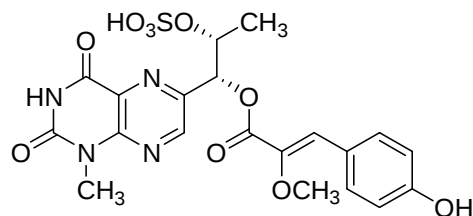
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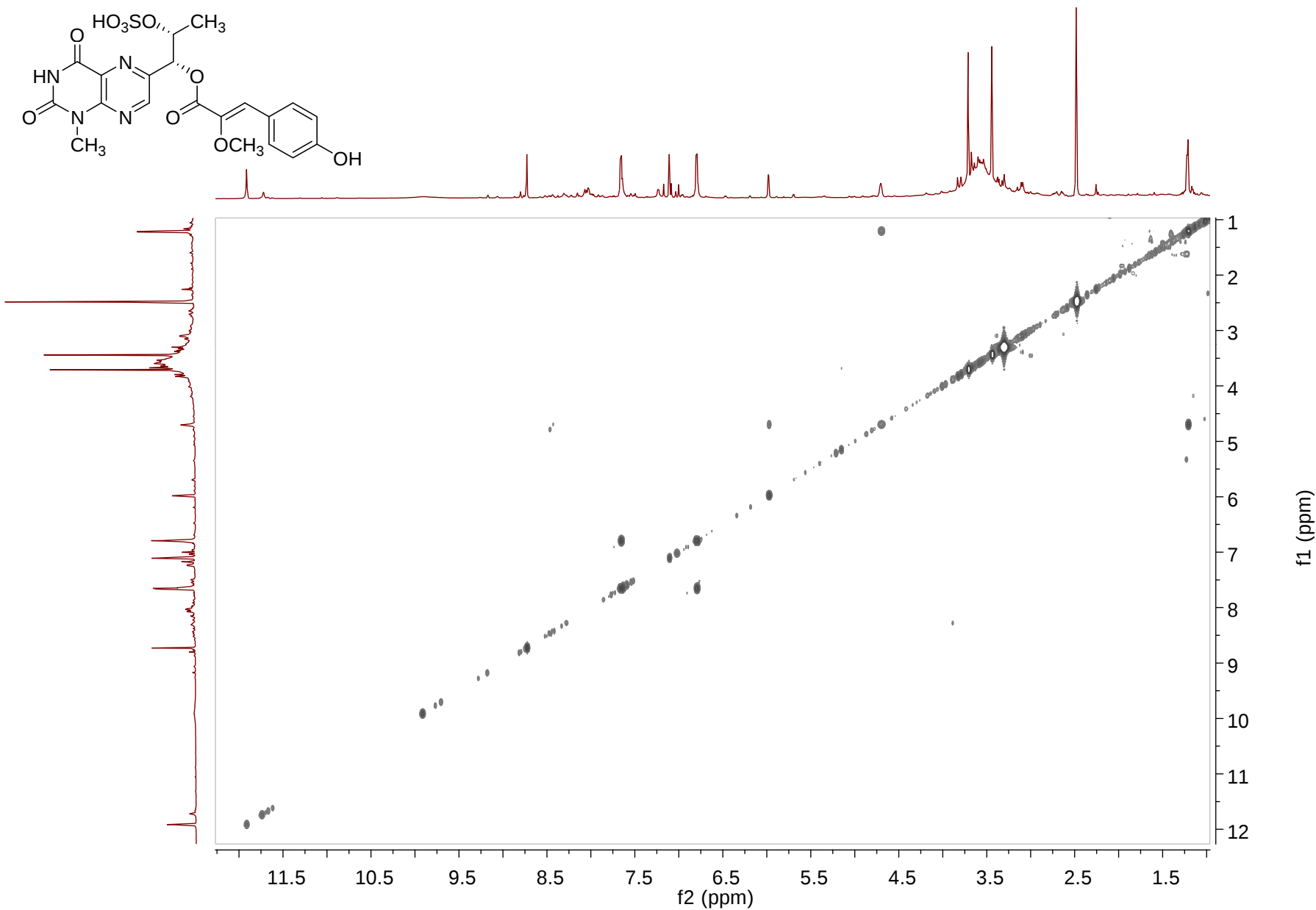
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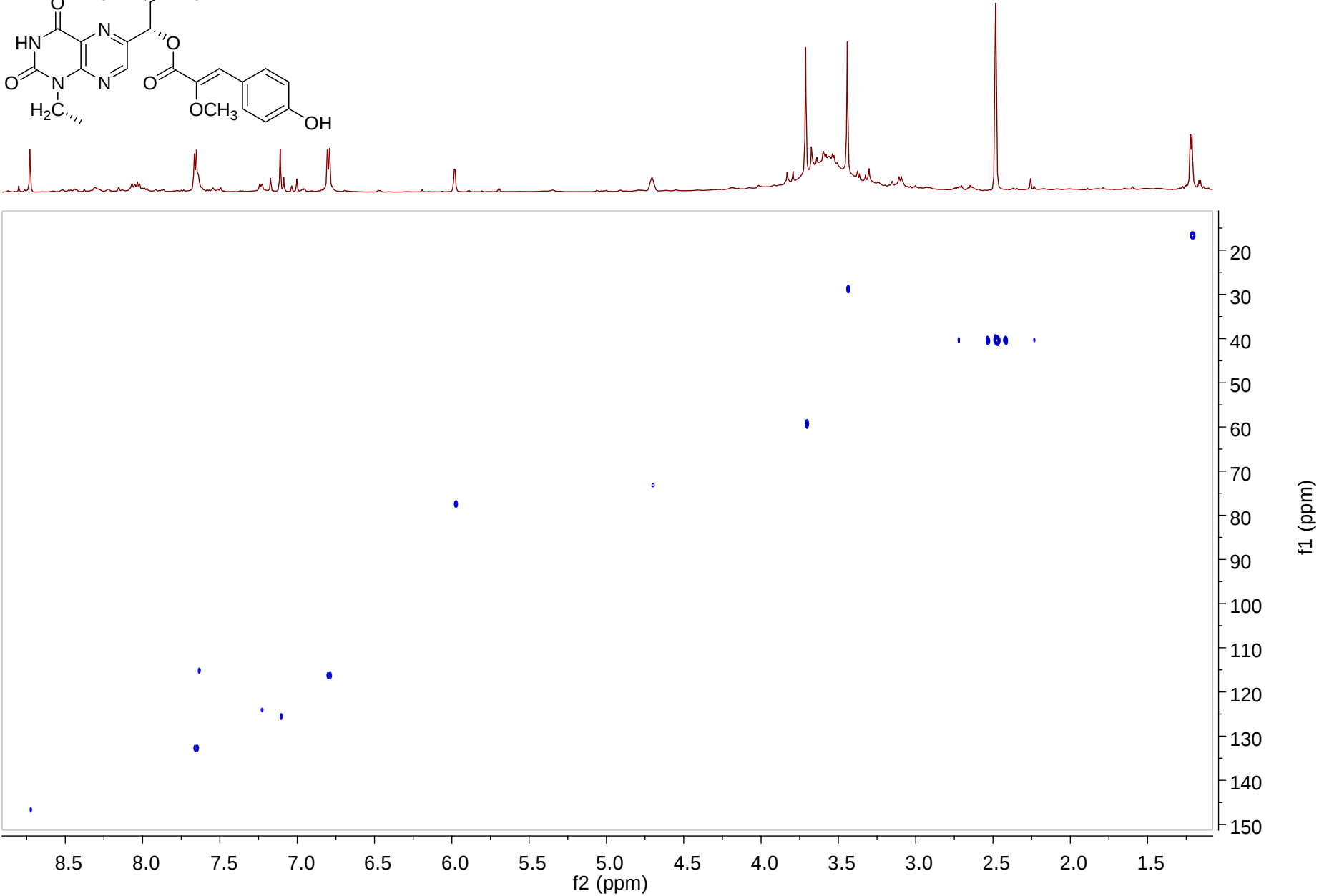
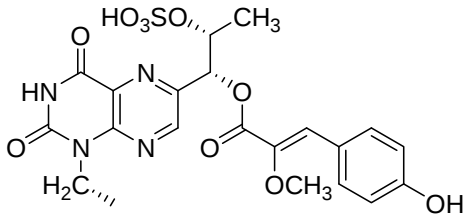
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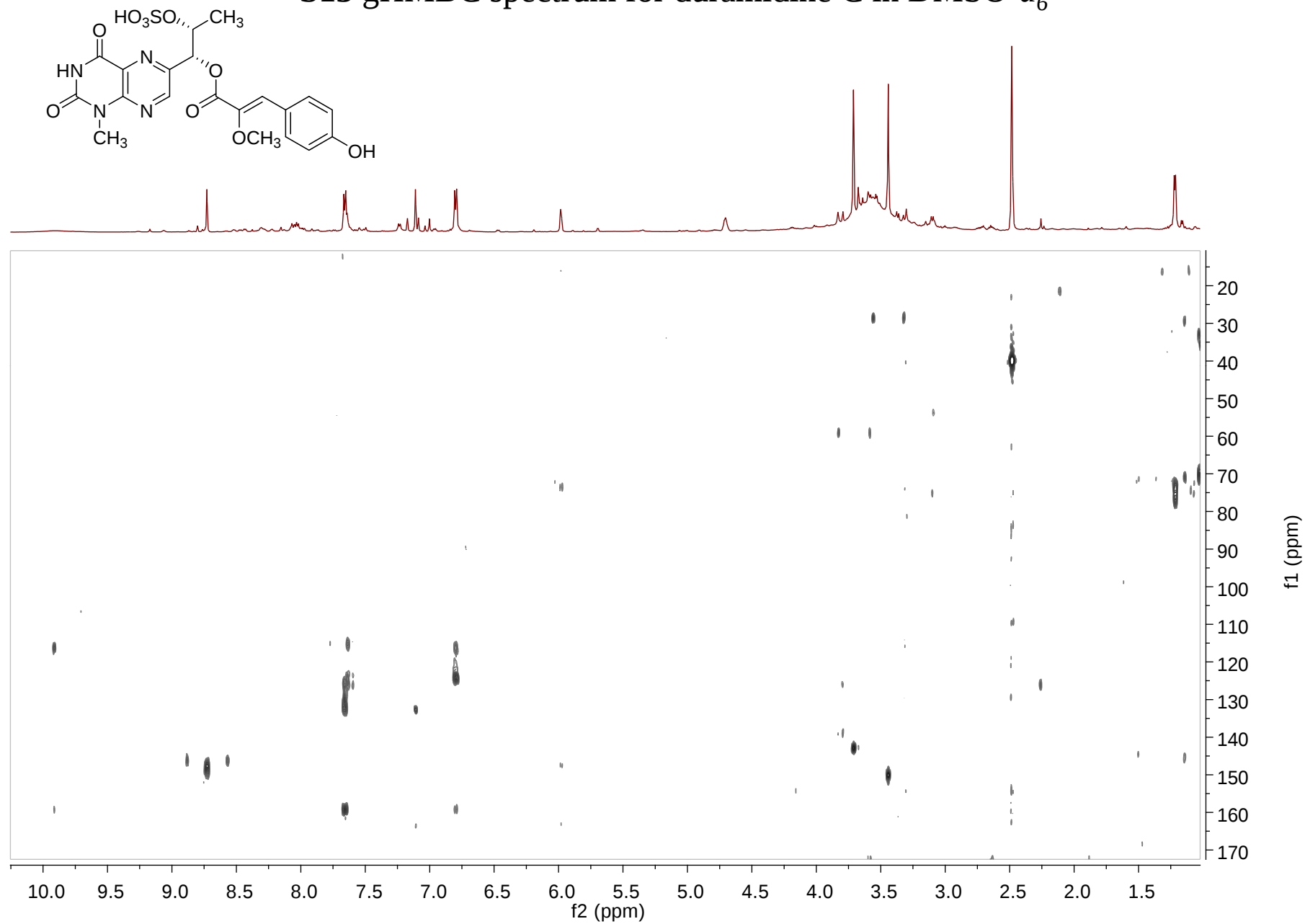
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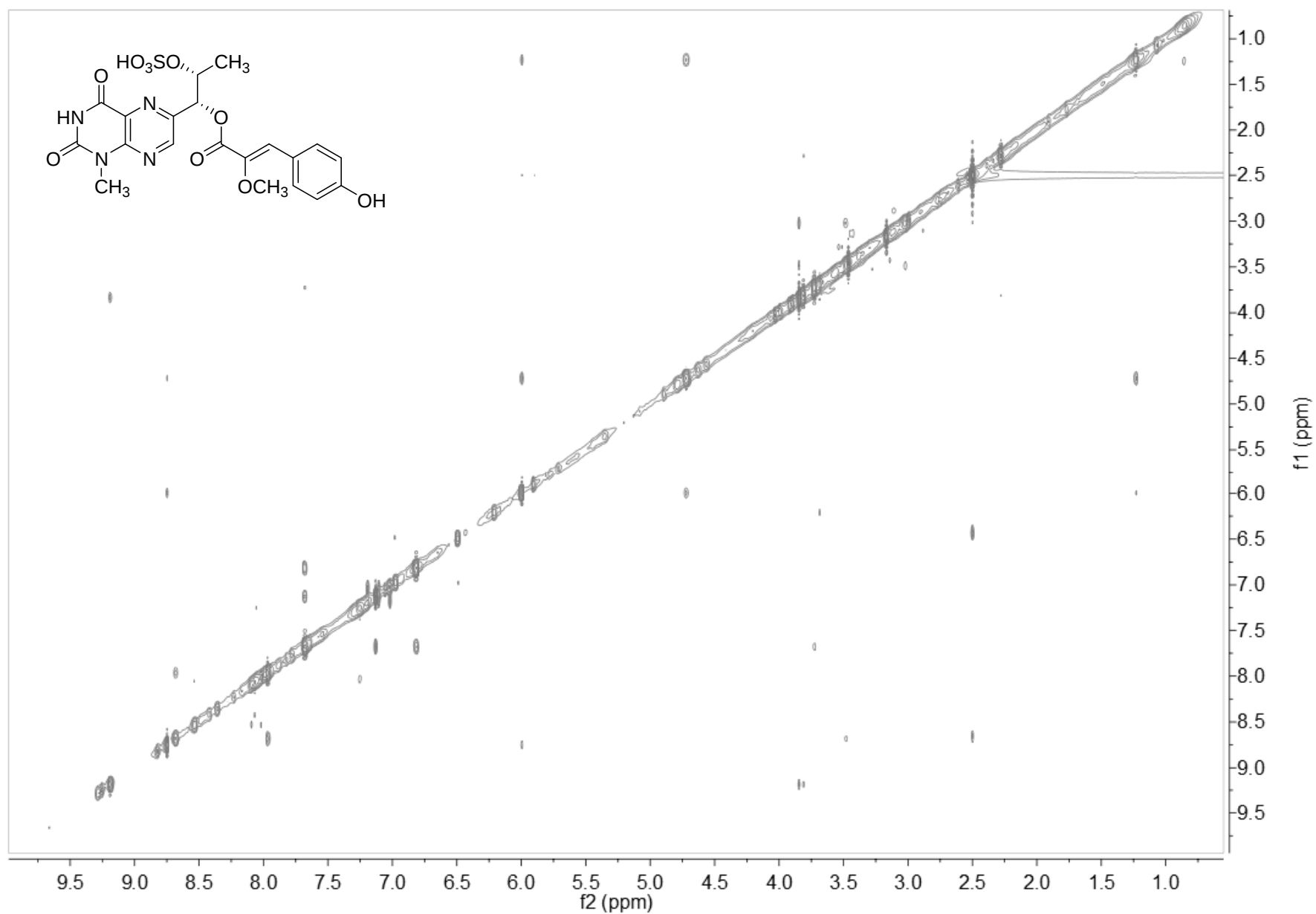
S12 gHSQC spectrum for duramidine C in DMSO-*d*₆



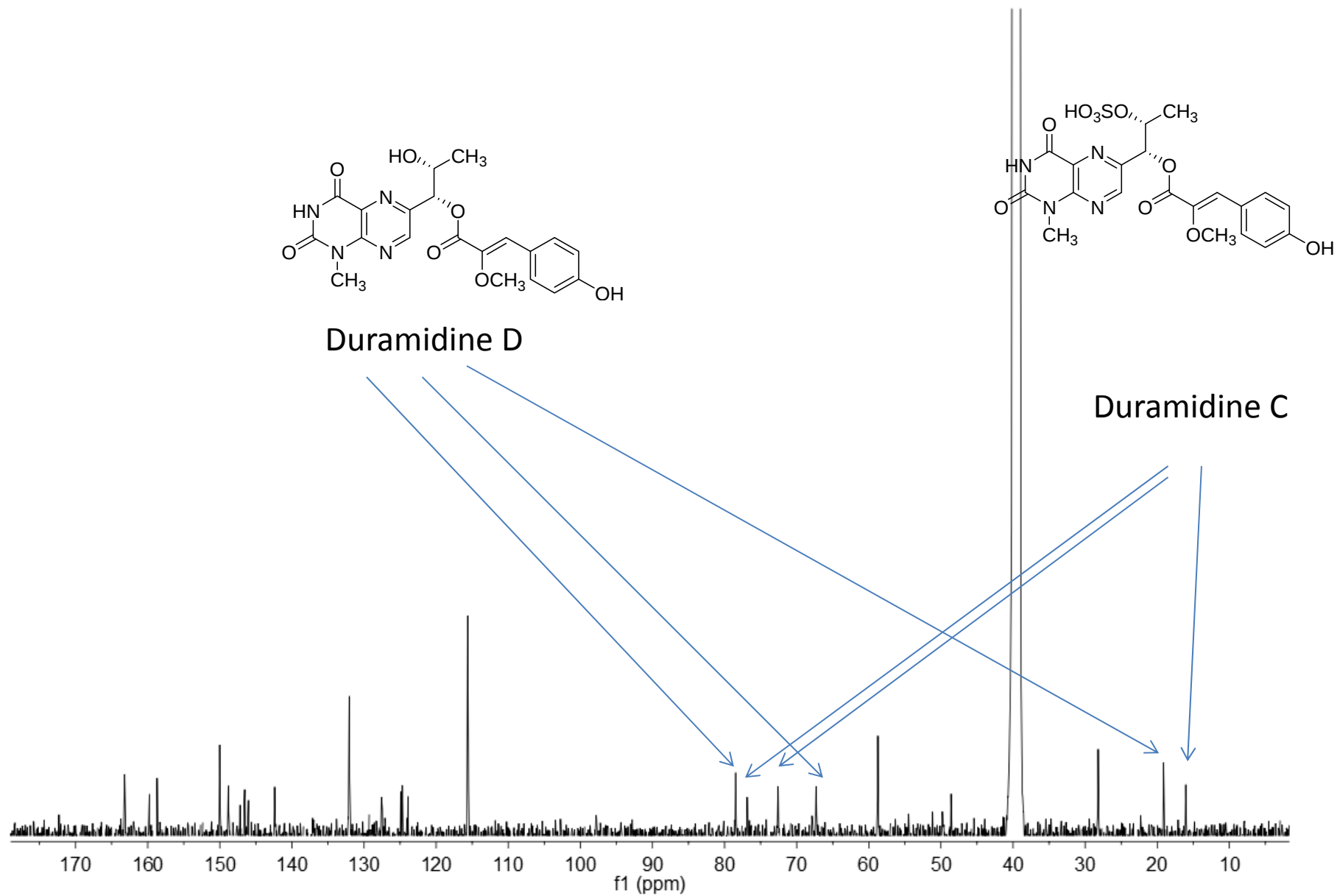
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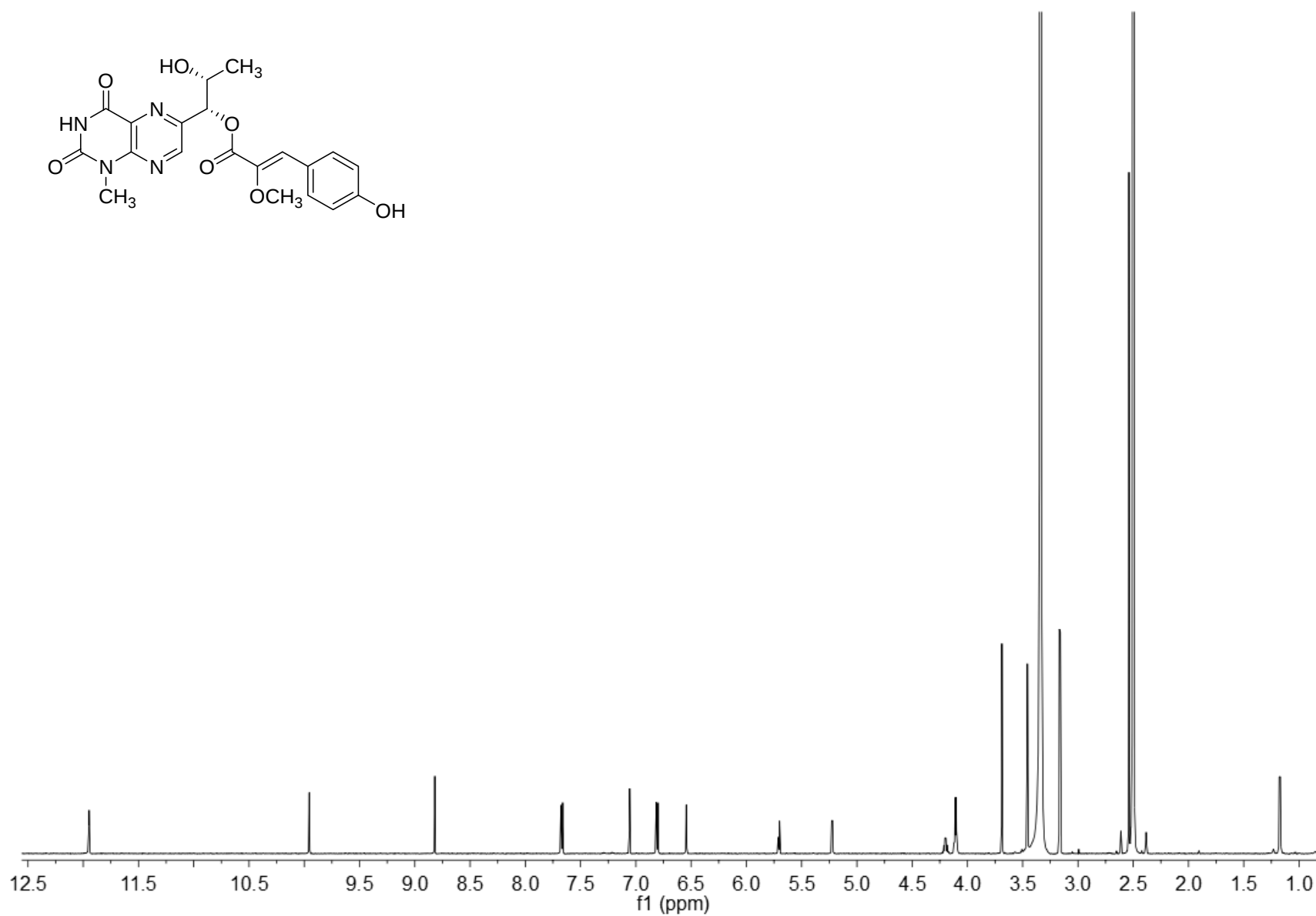
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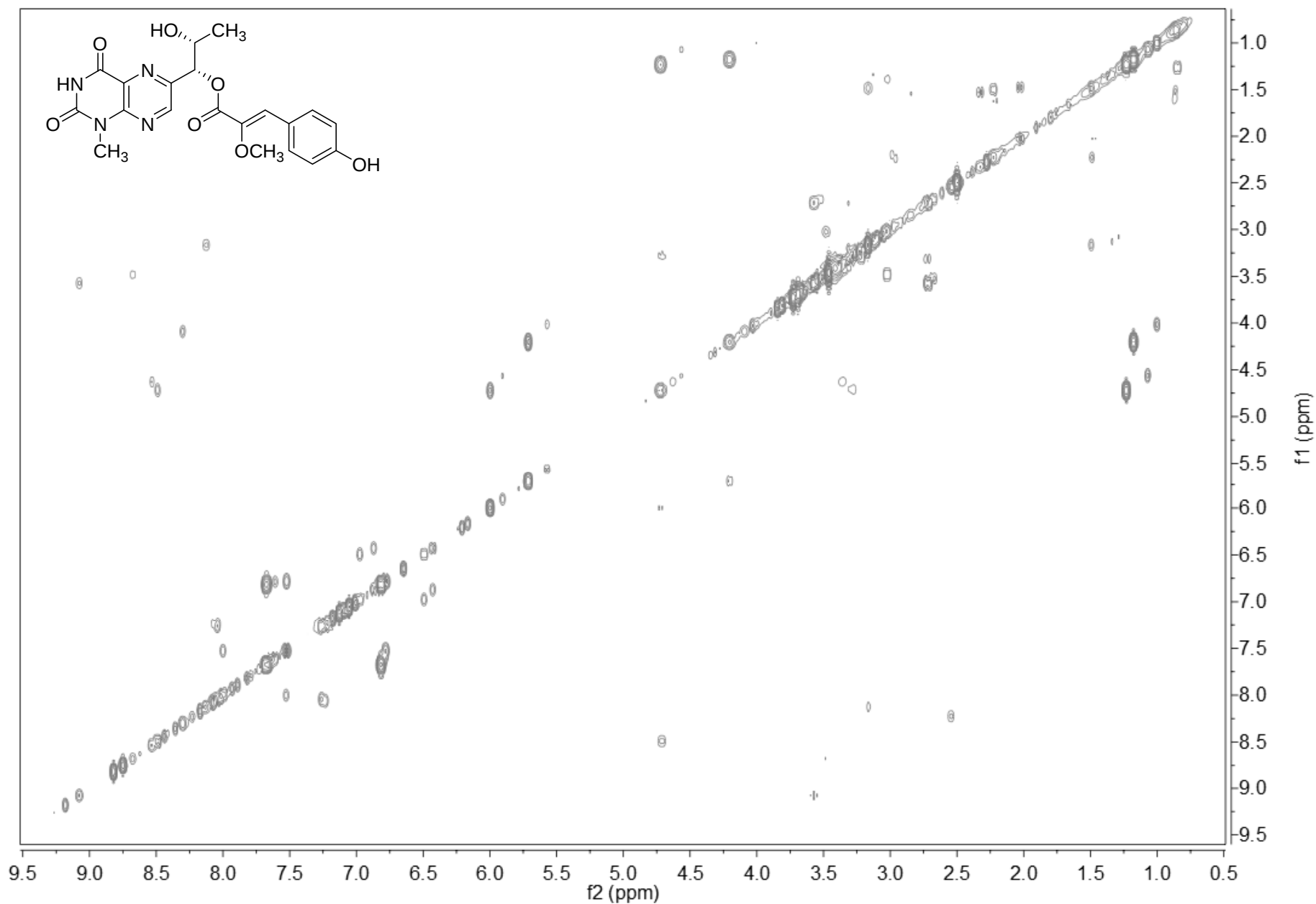
S15 ^{13}C NMR spectrum for mixture of duramidine C and D in $\text{DMSO-}d_6$



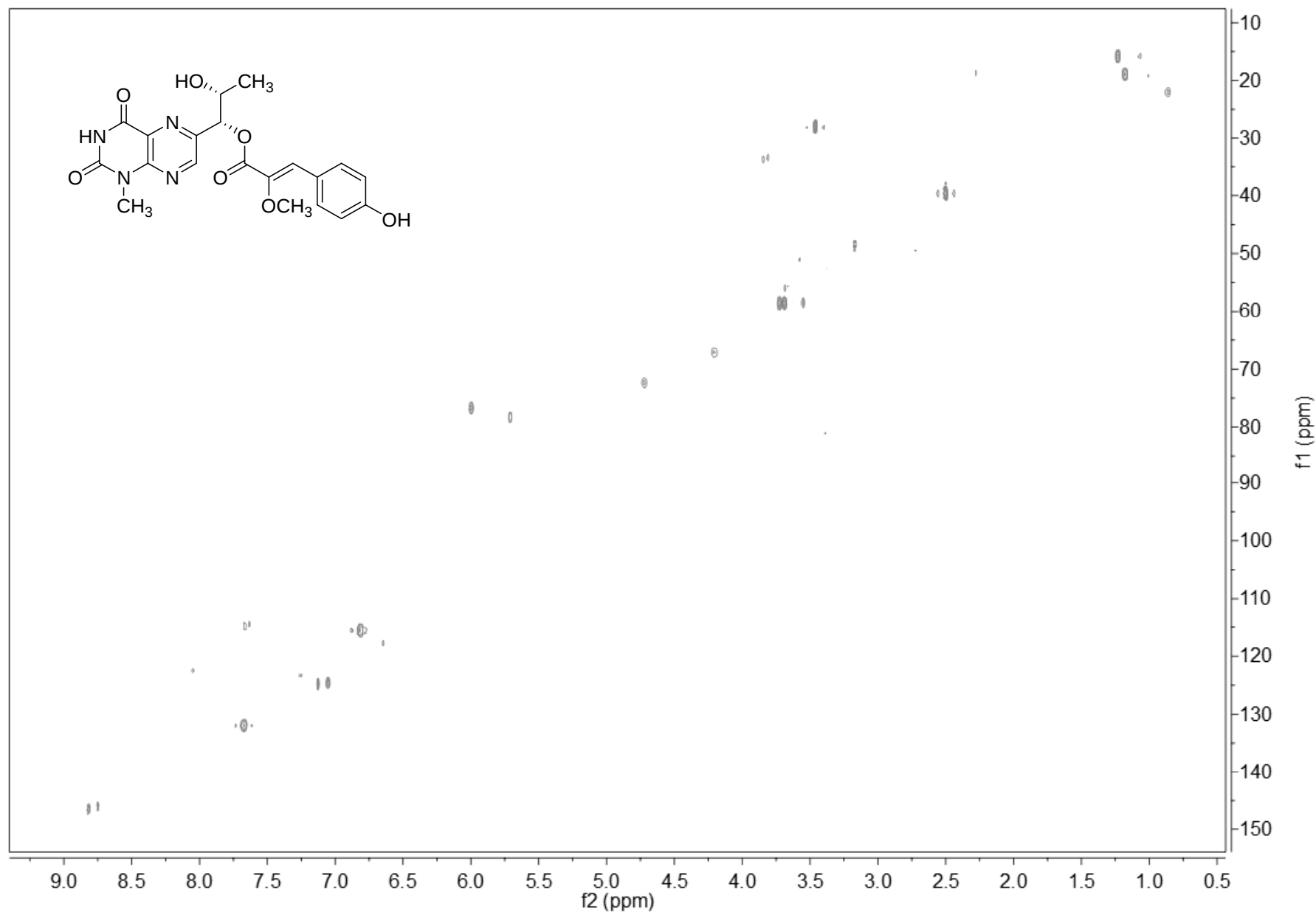
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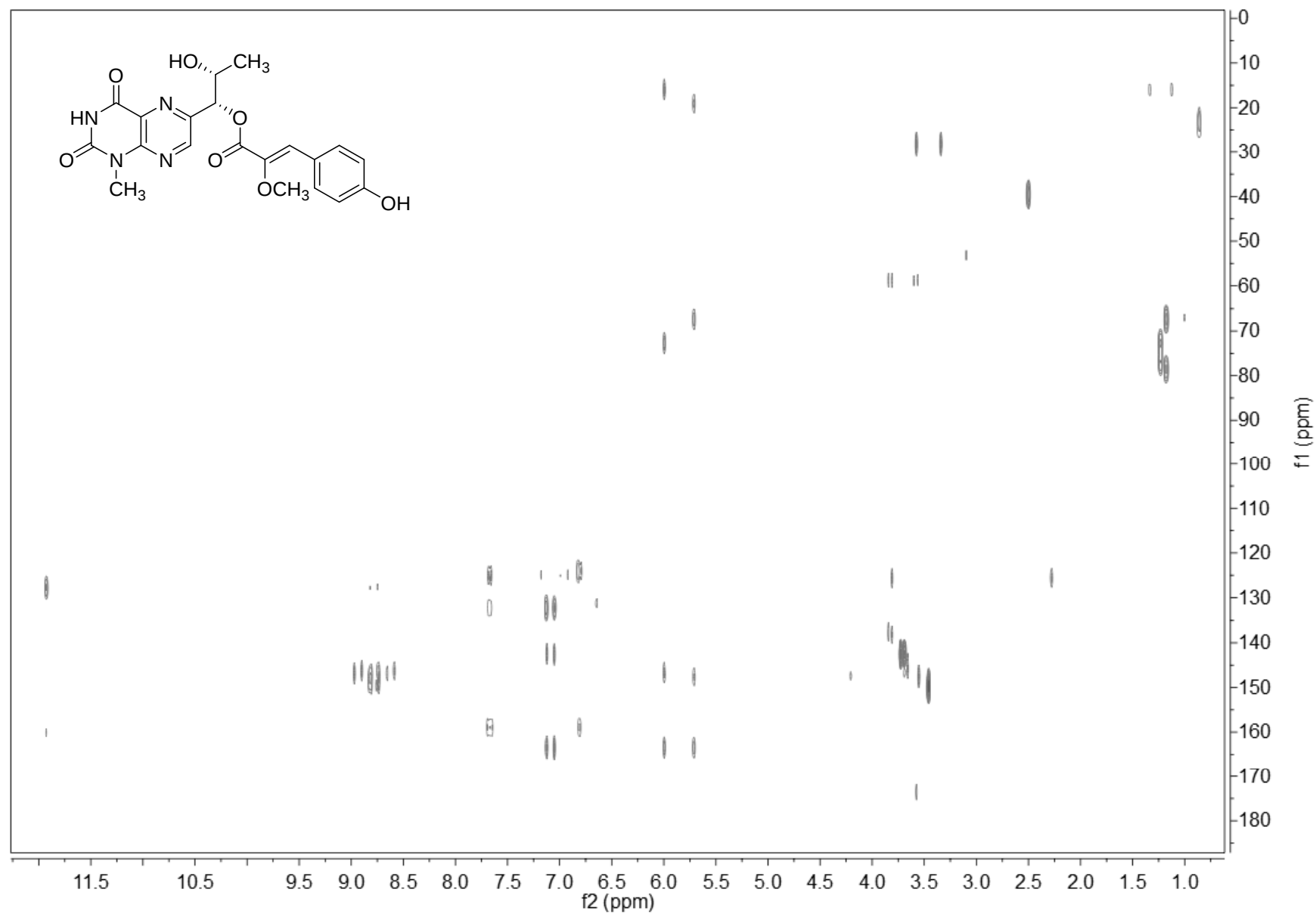
S17 gCOSY spectrum for duramidine D in DMSO-*d*₆



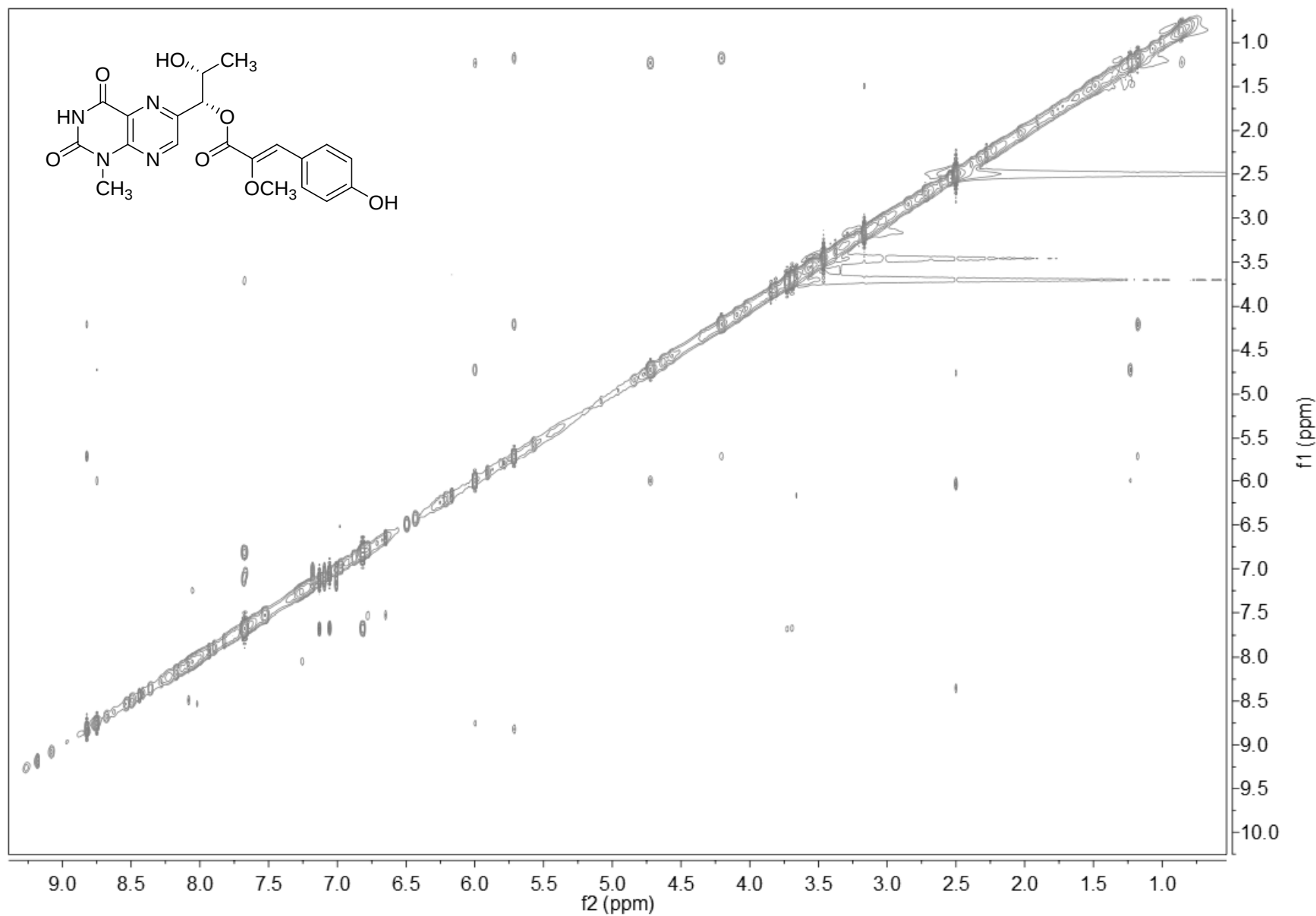
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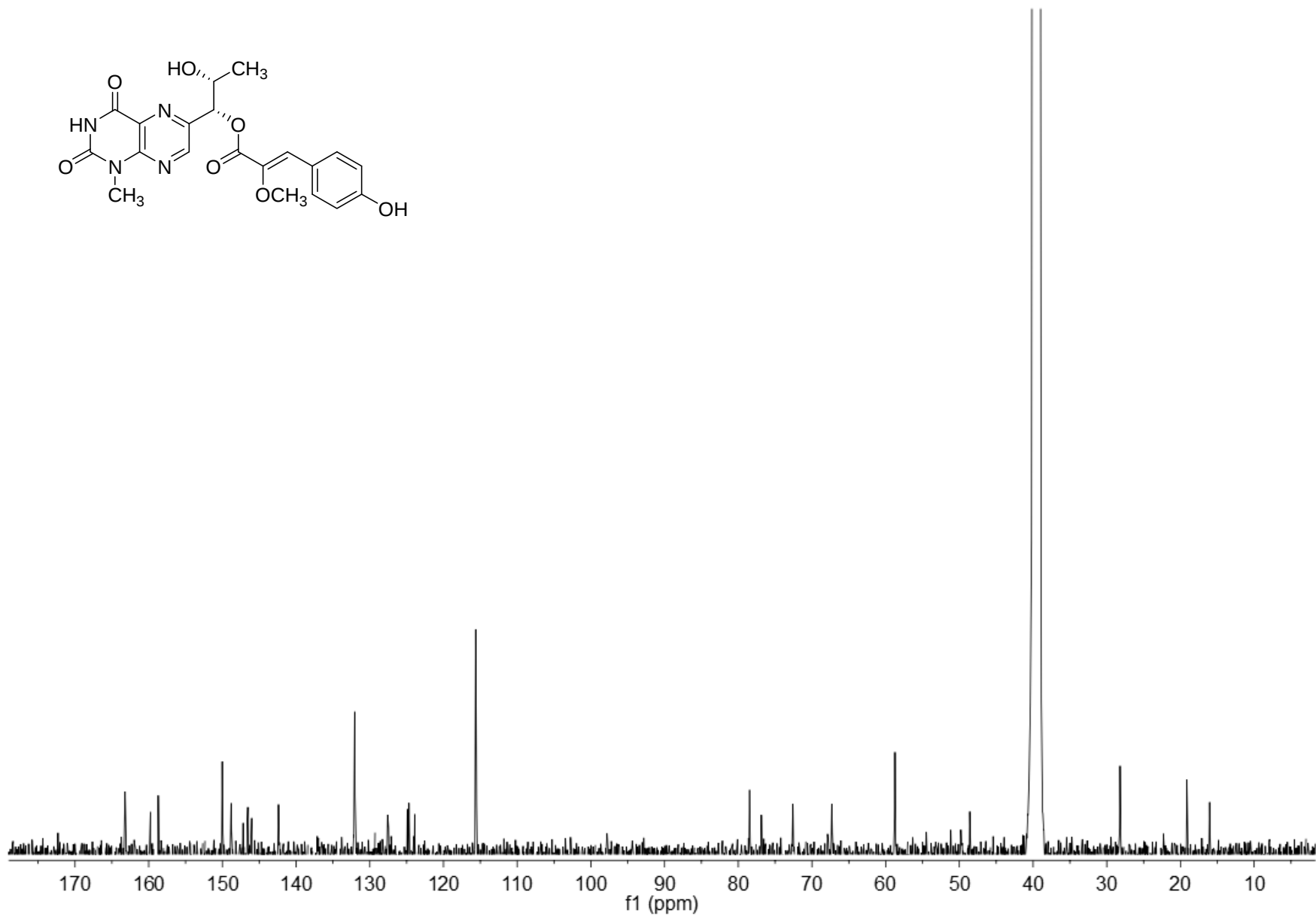
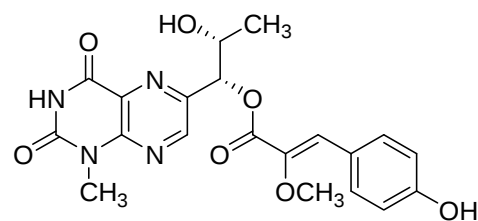
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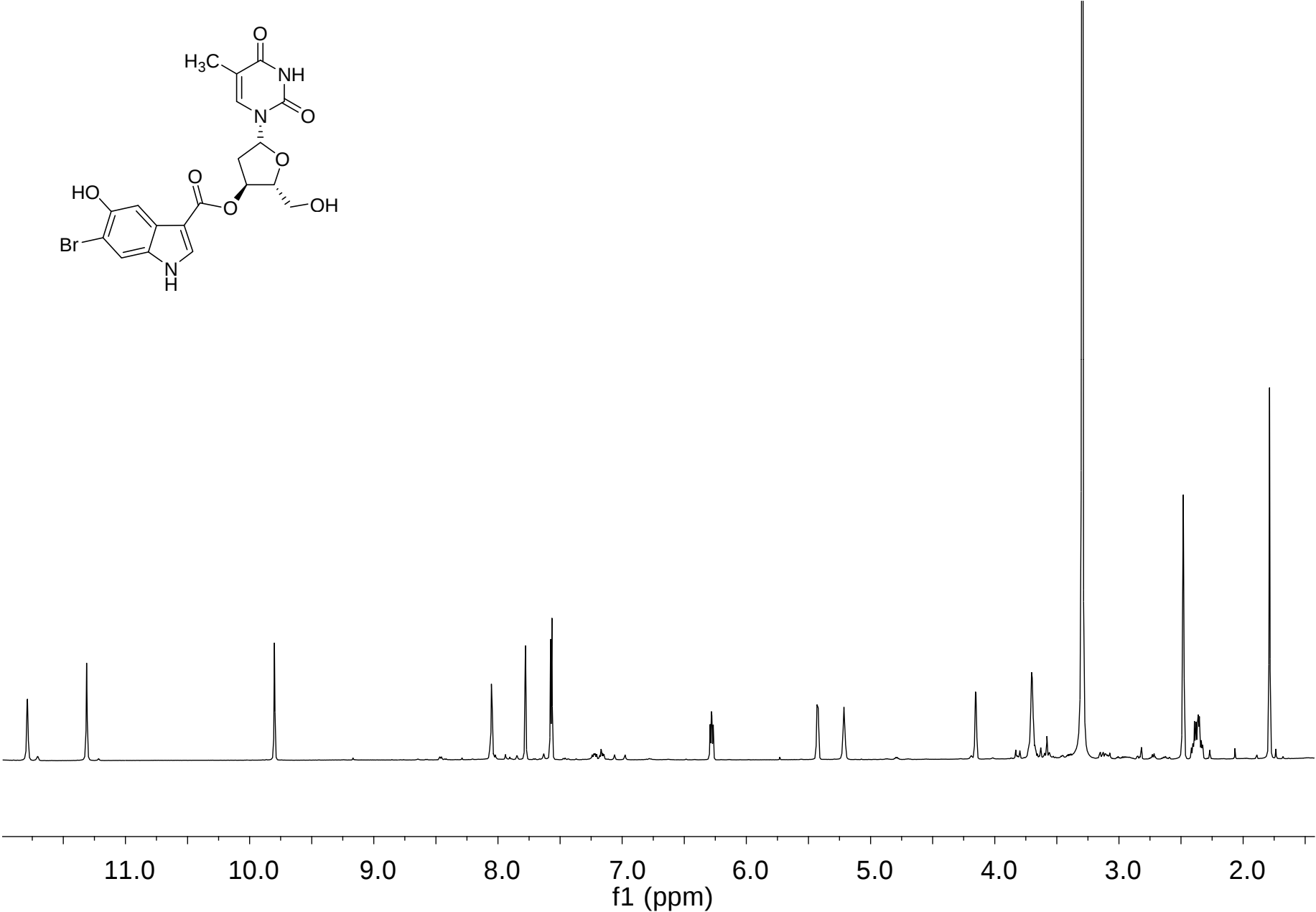
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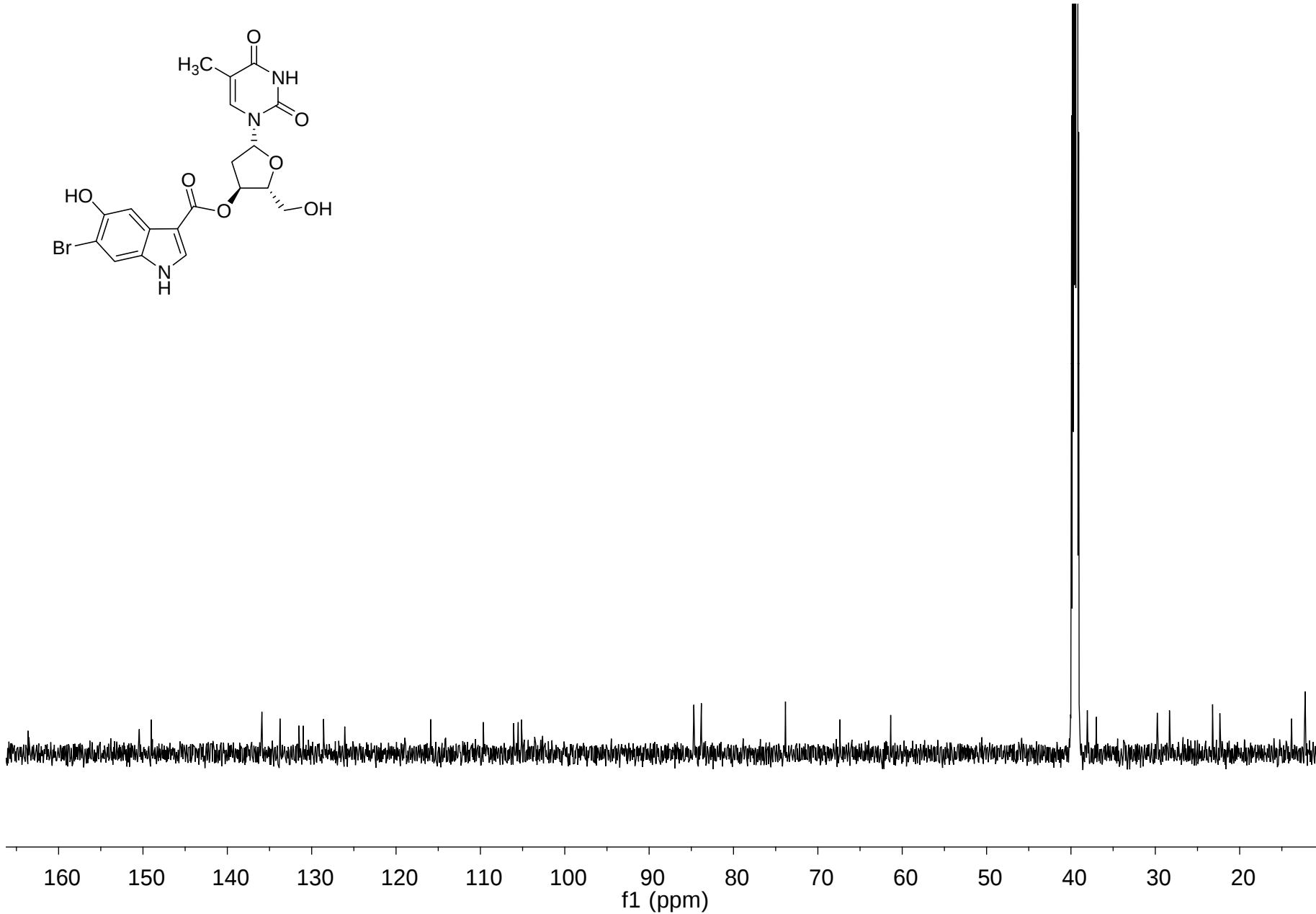
S21 ^{13}C NMR spectrum for duramidine D in $\text{DMSO-}d_6$



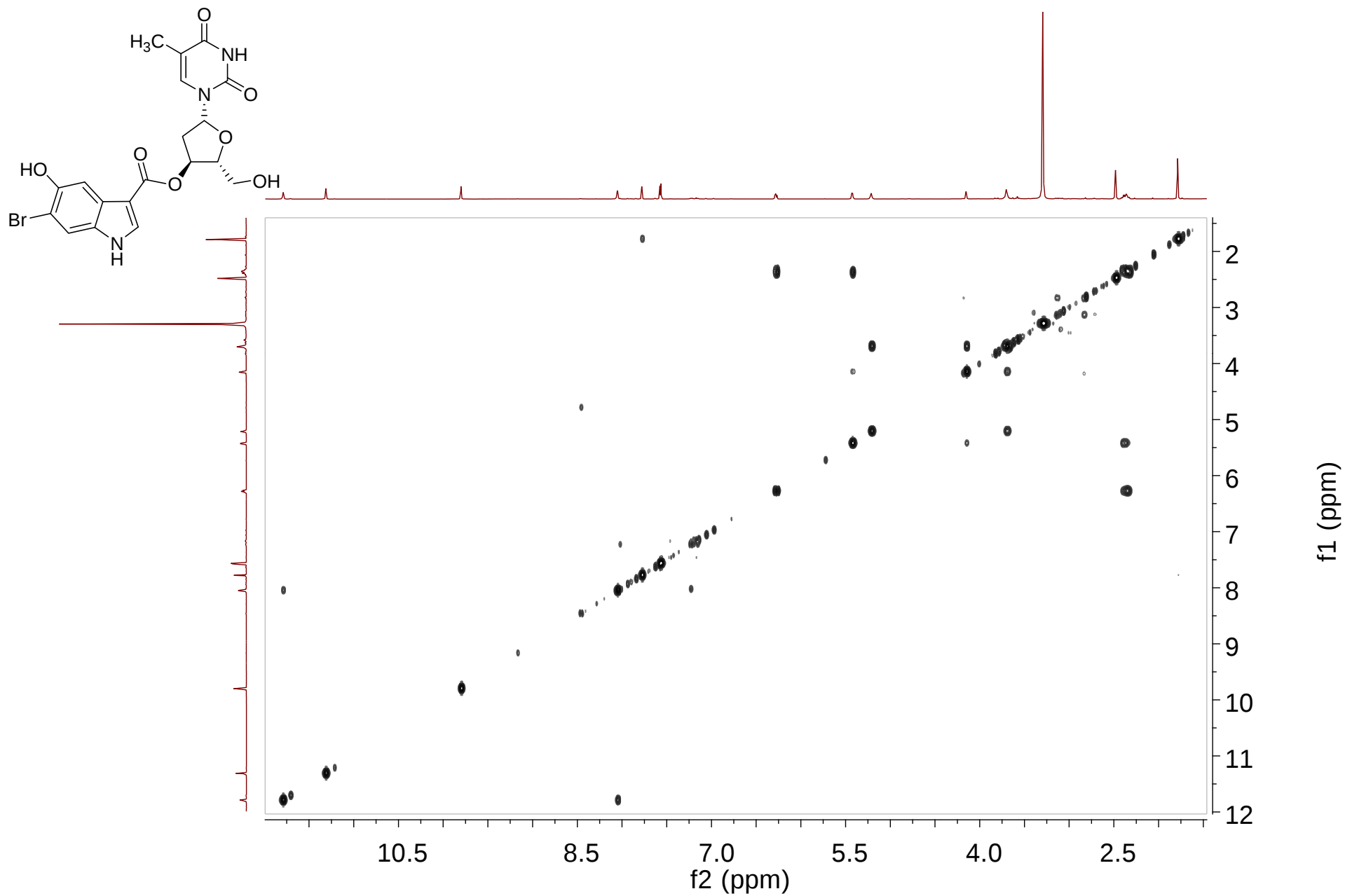
S22 ¹H NMR spectrum for leptoclinidine A in DMSO-*d*₆



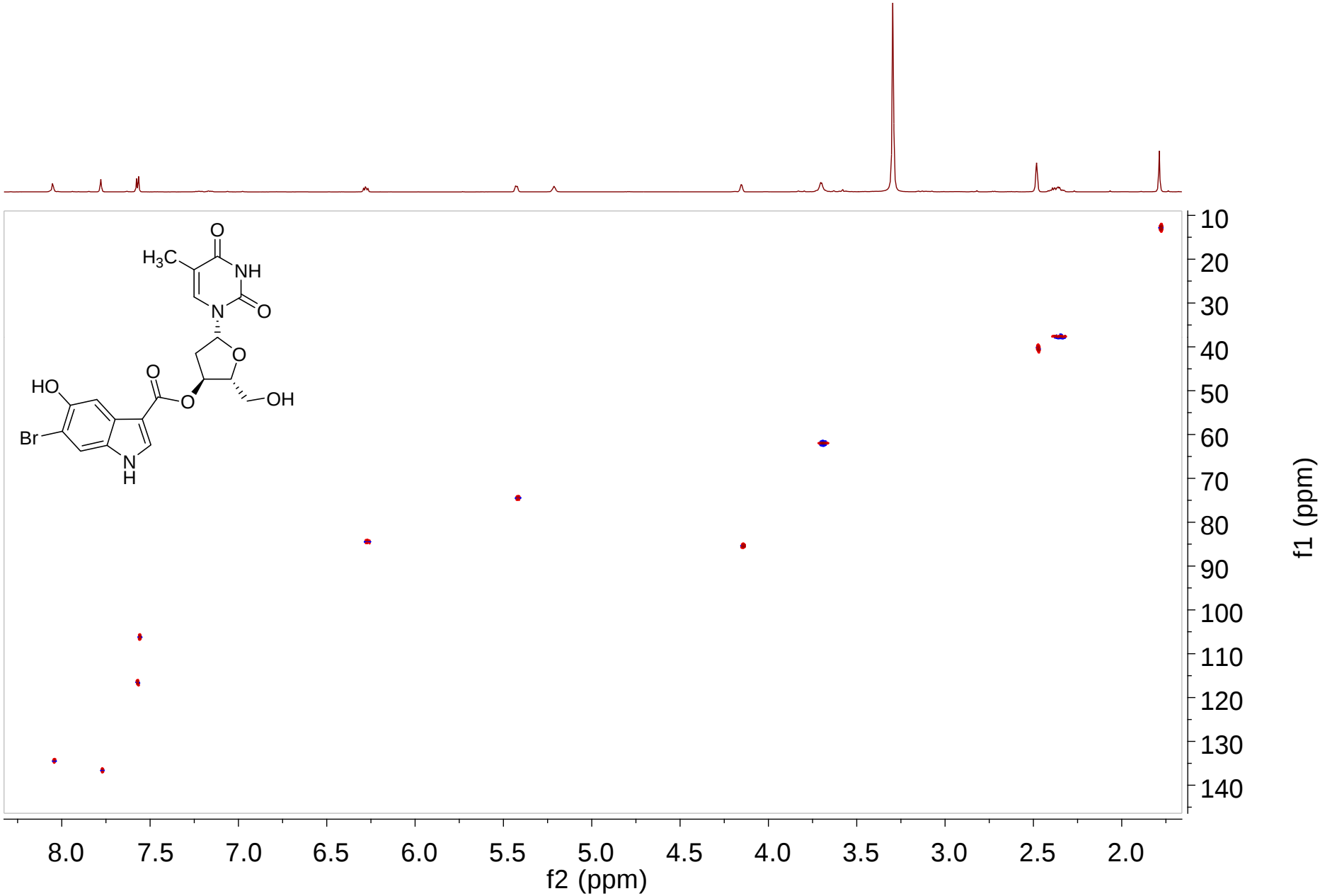
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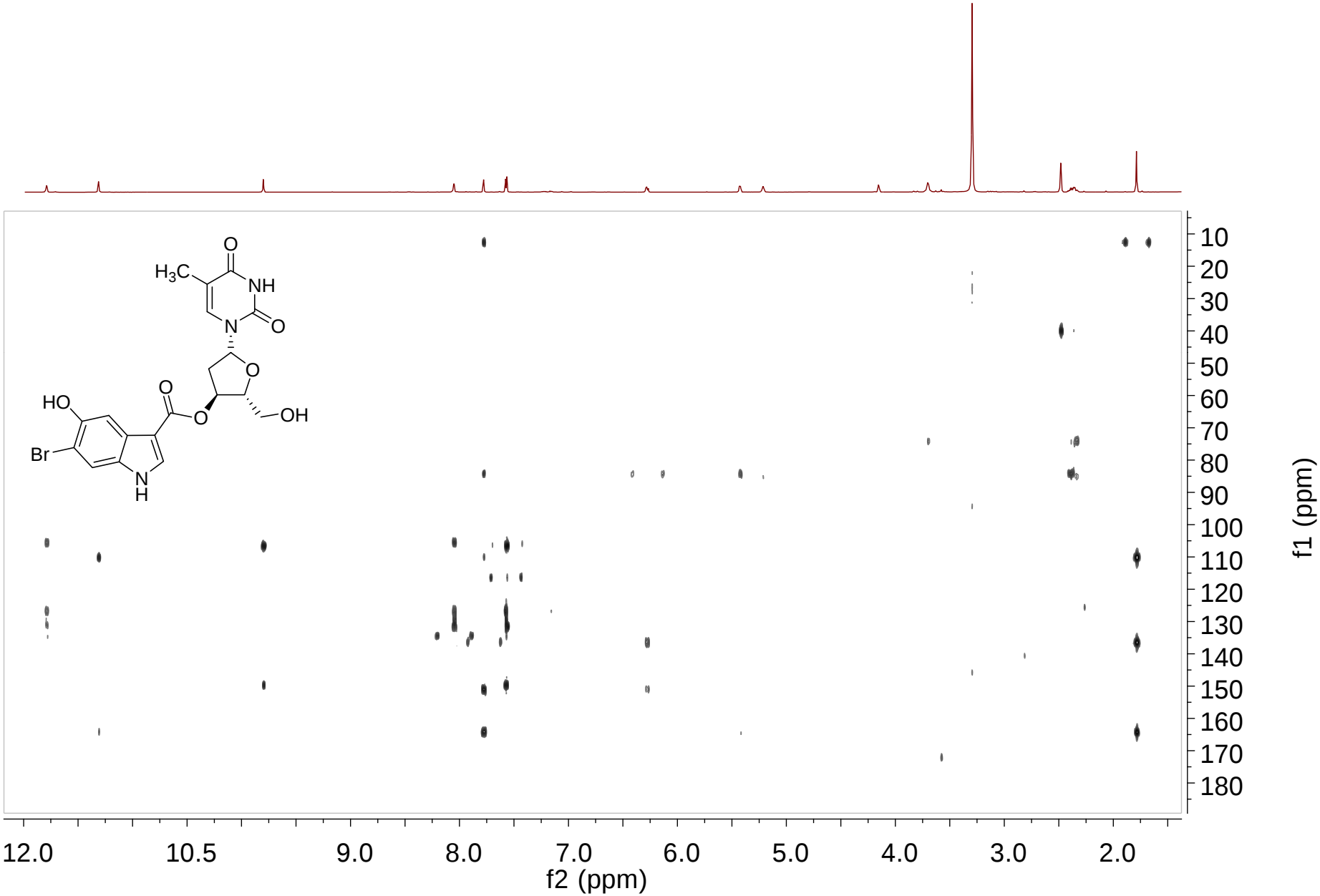
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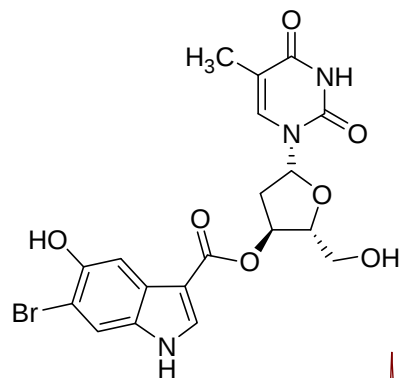


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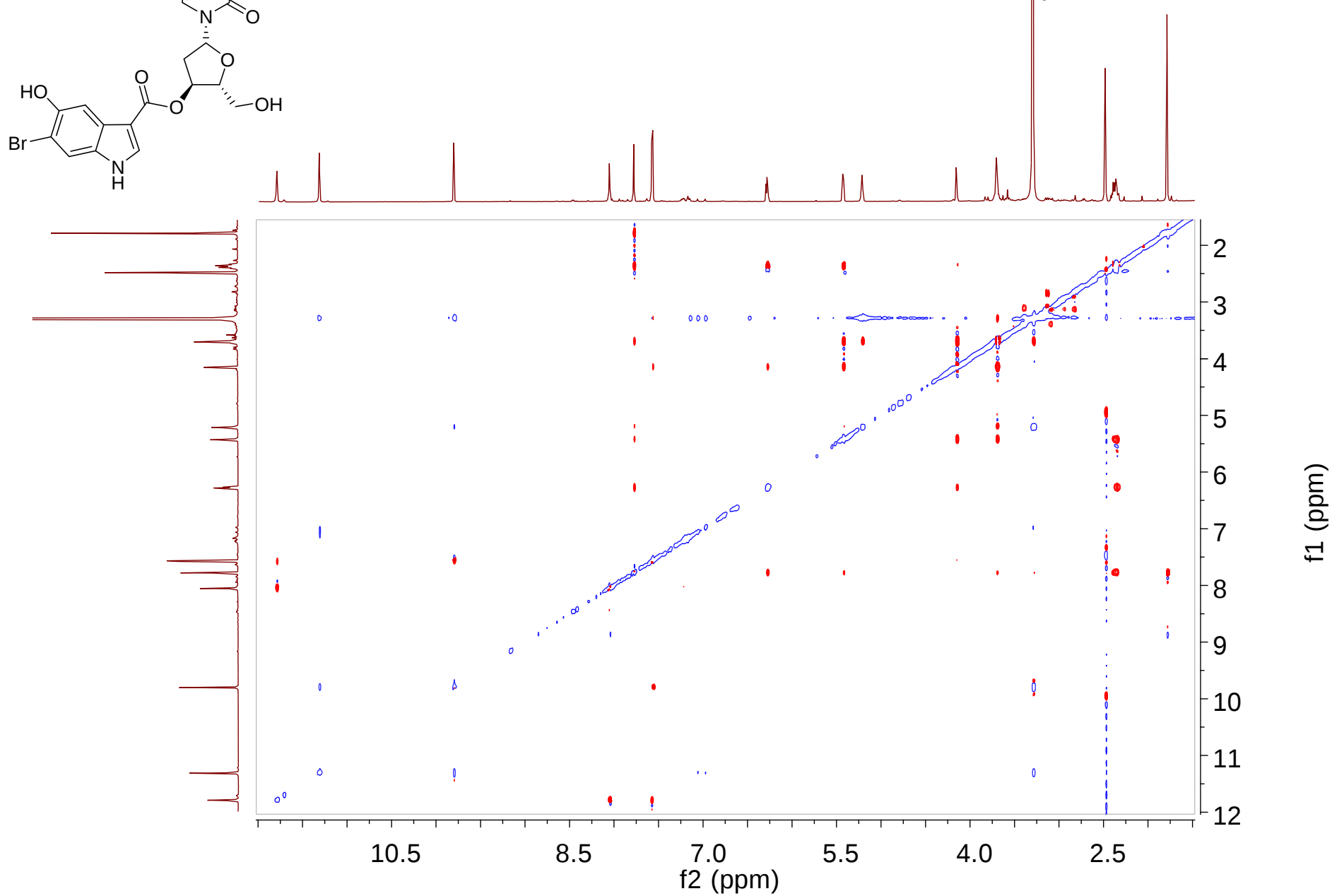


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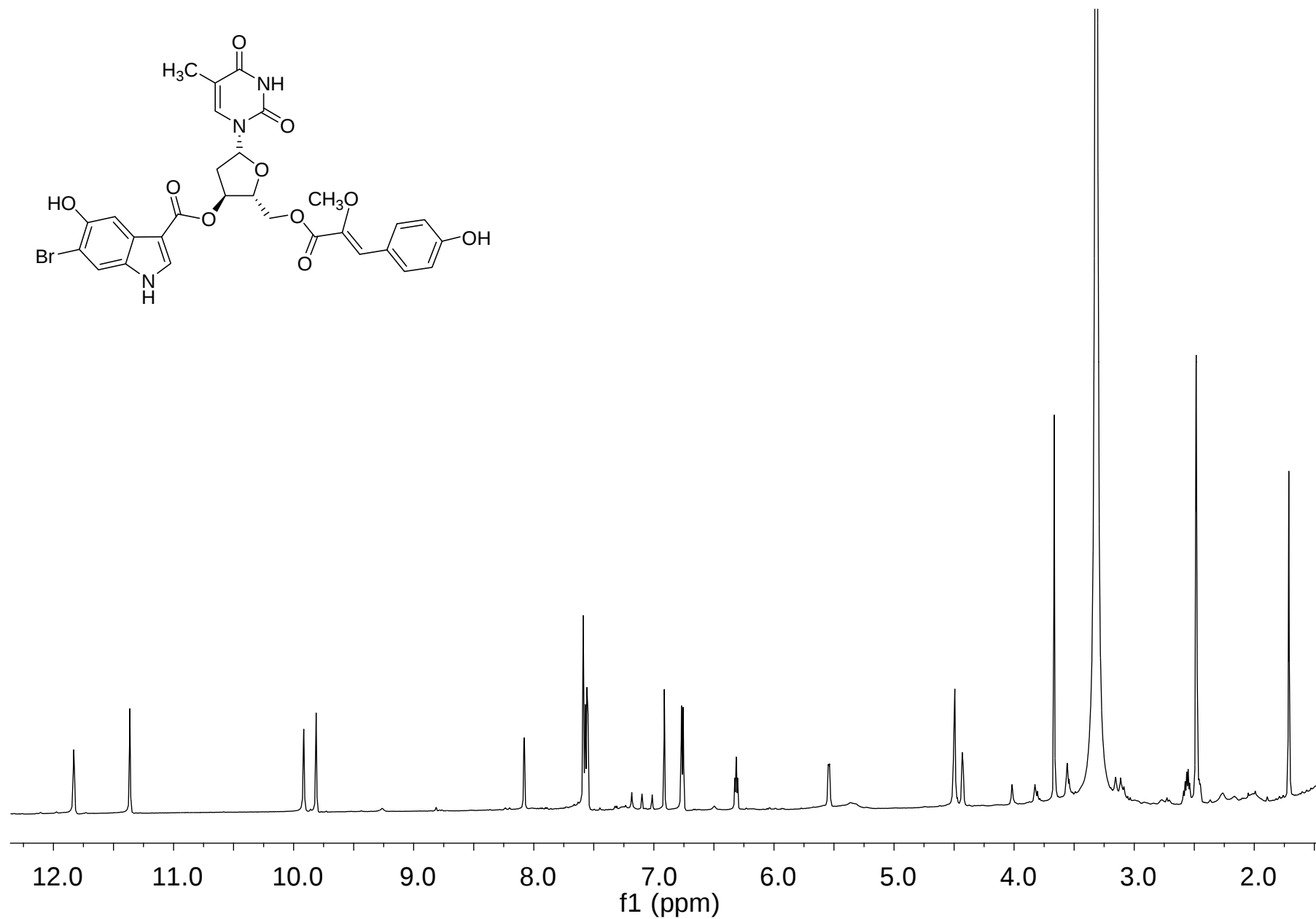




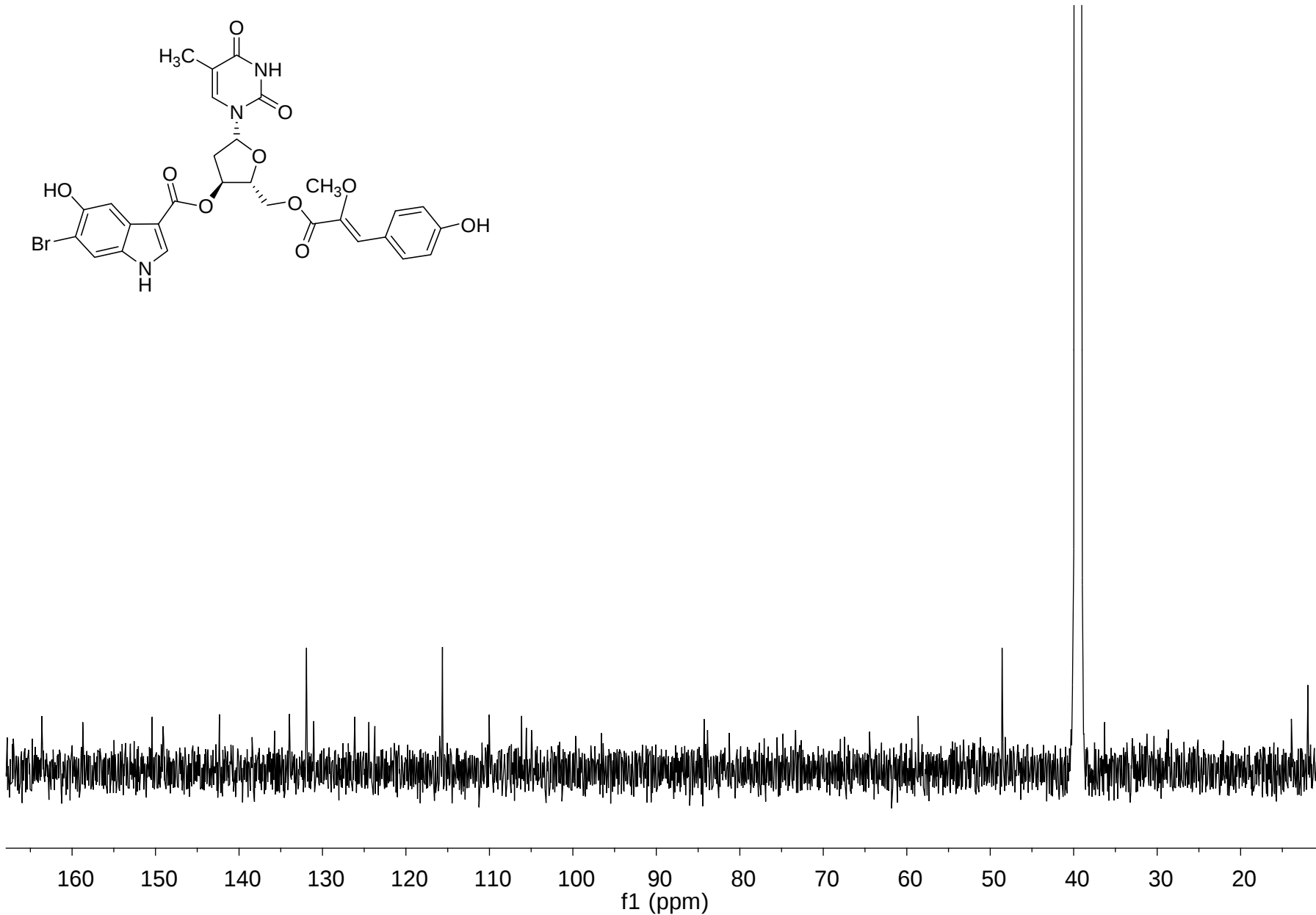
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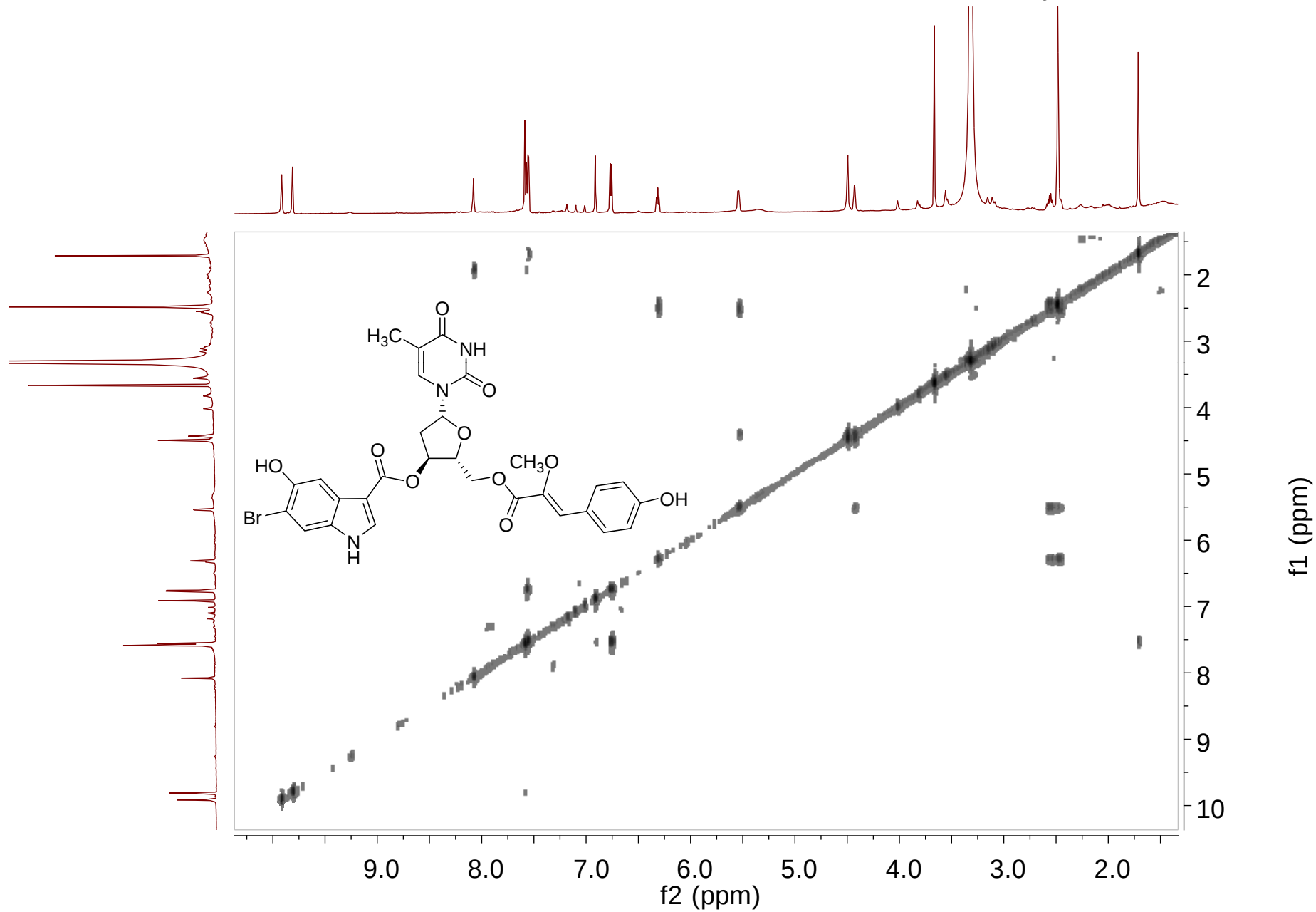
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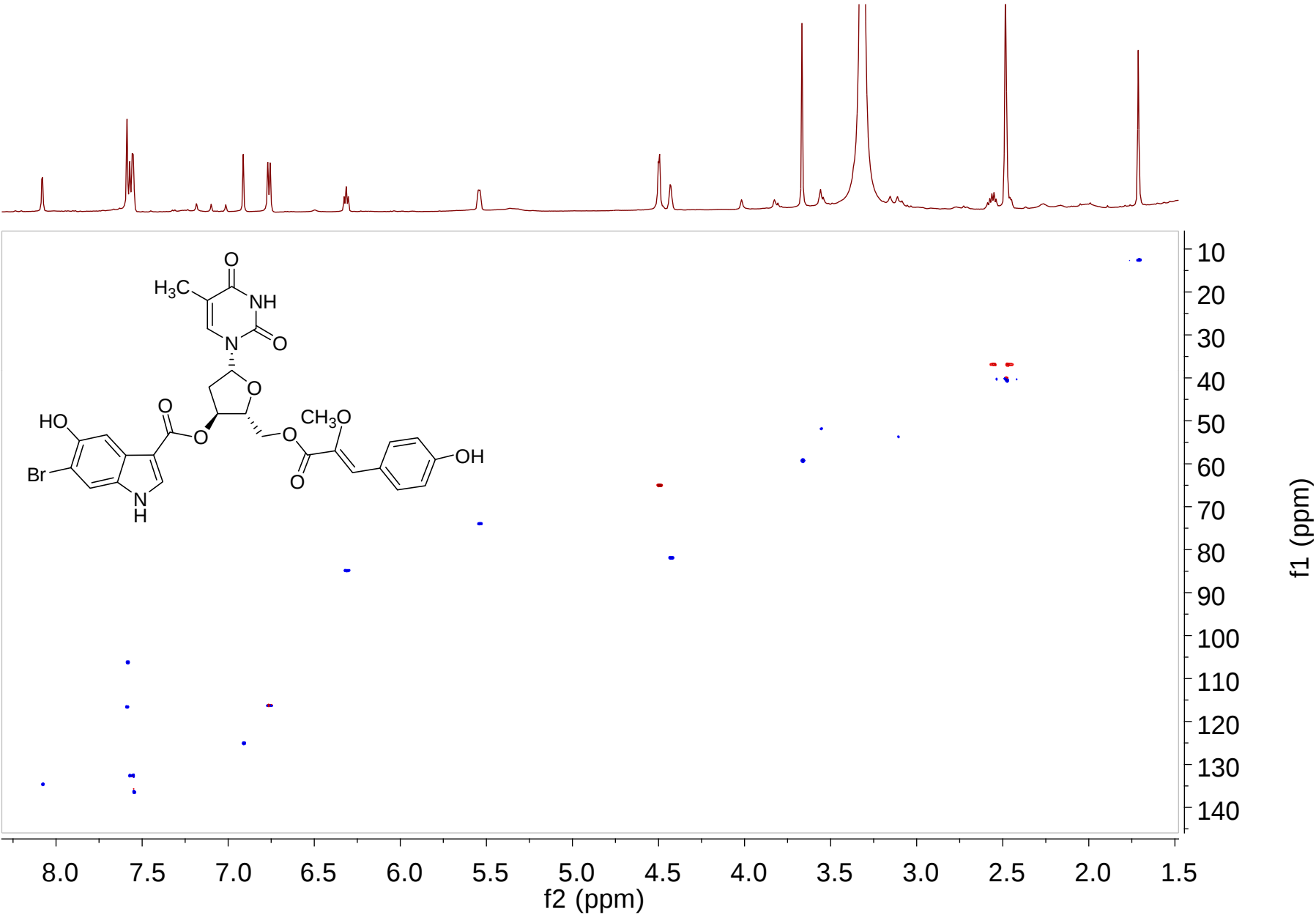
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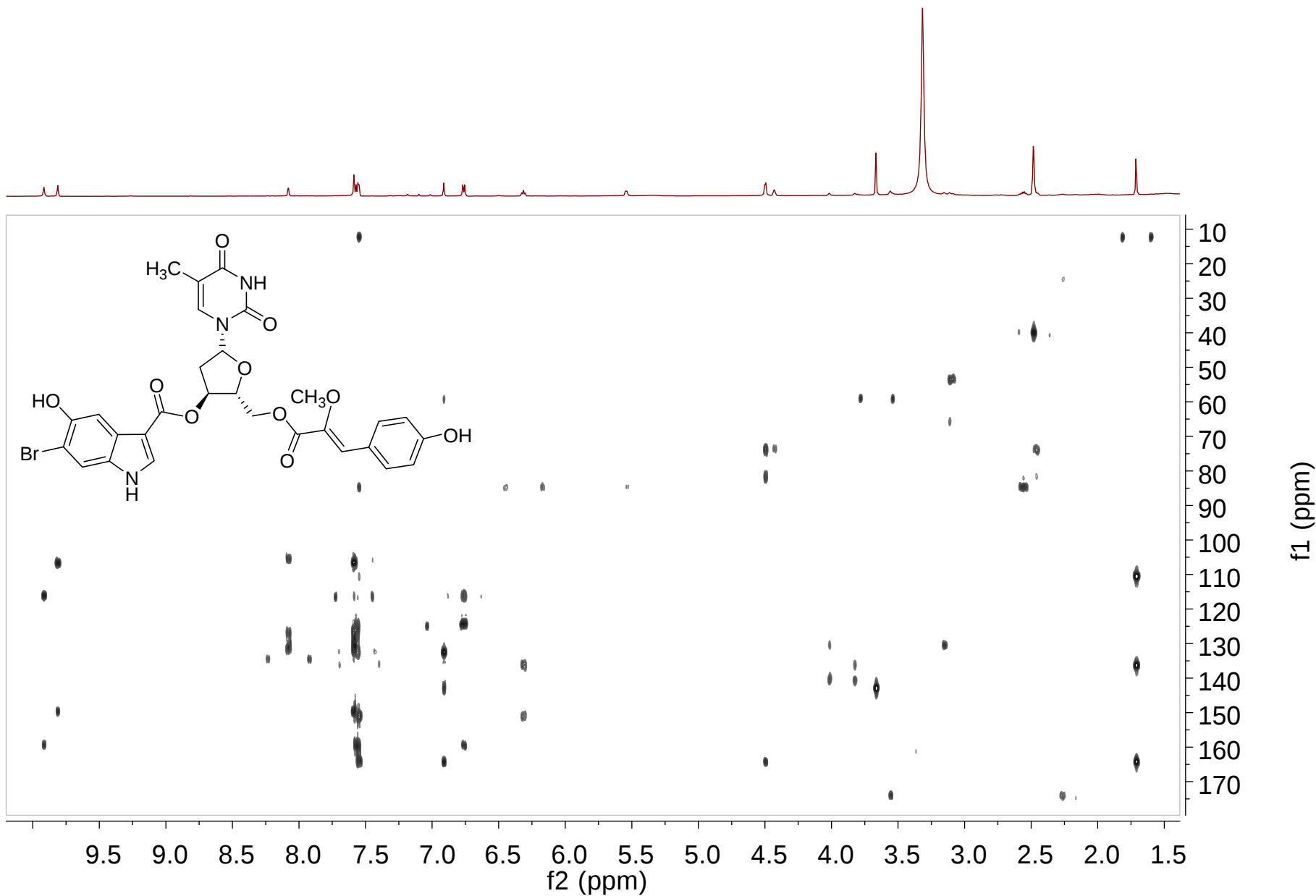
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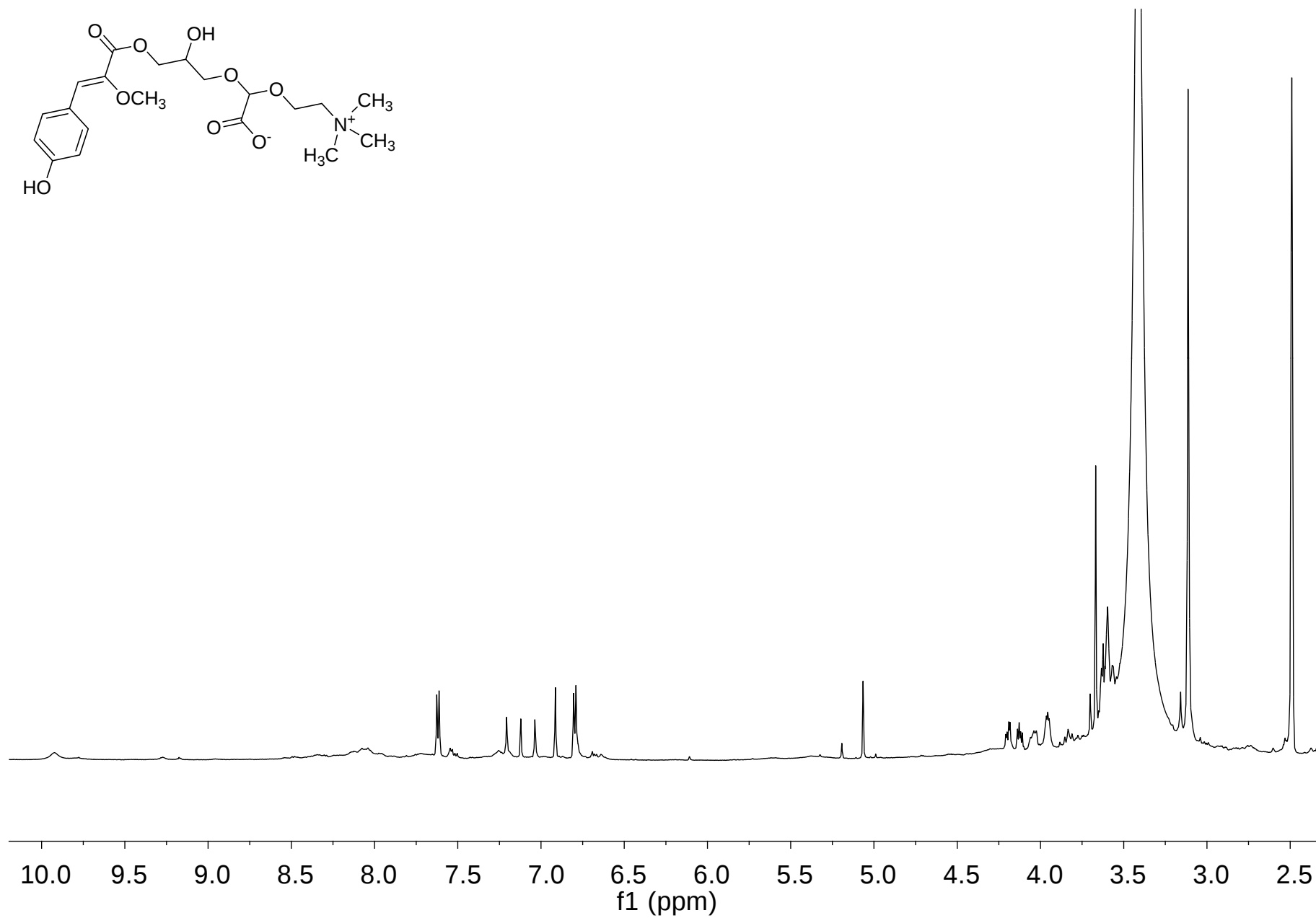
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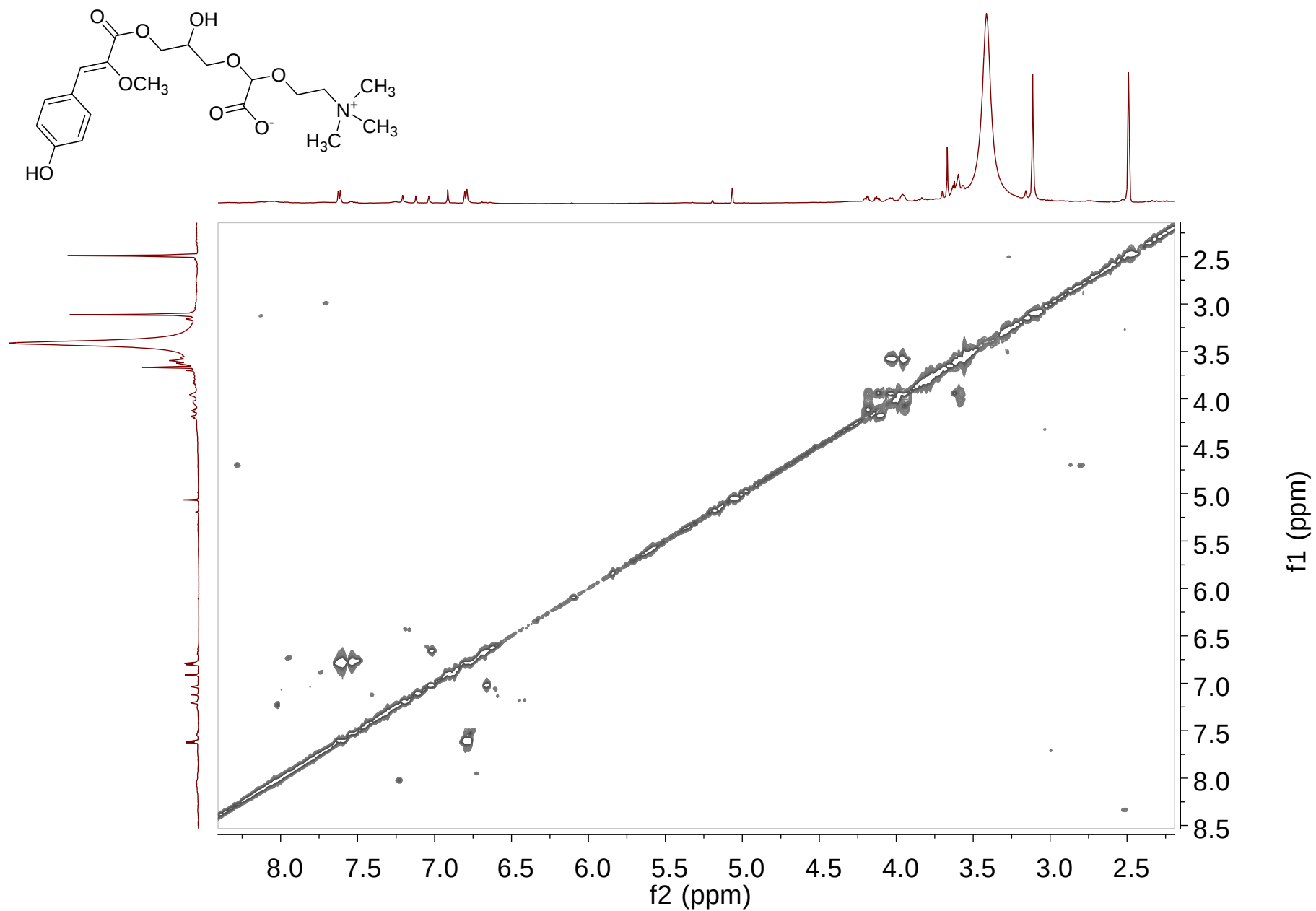
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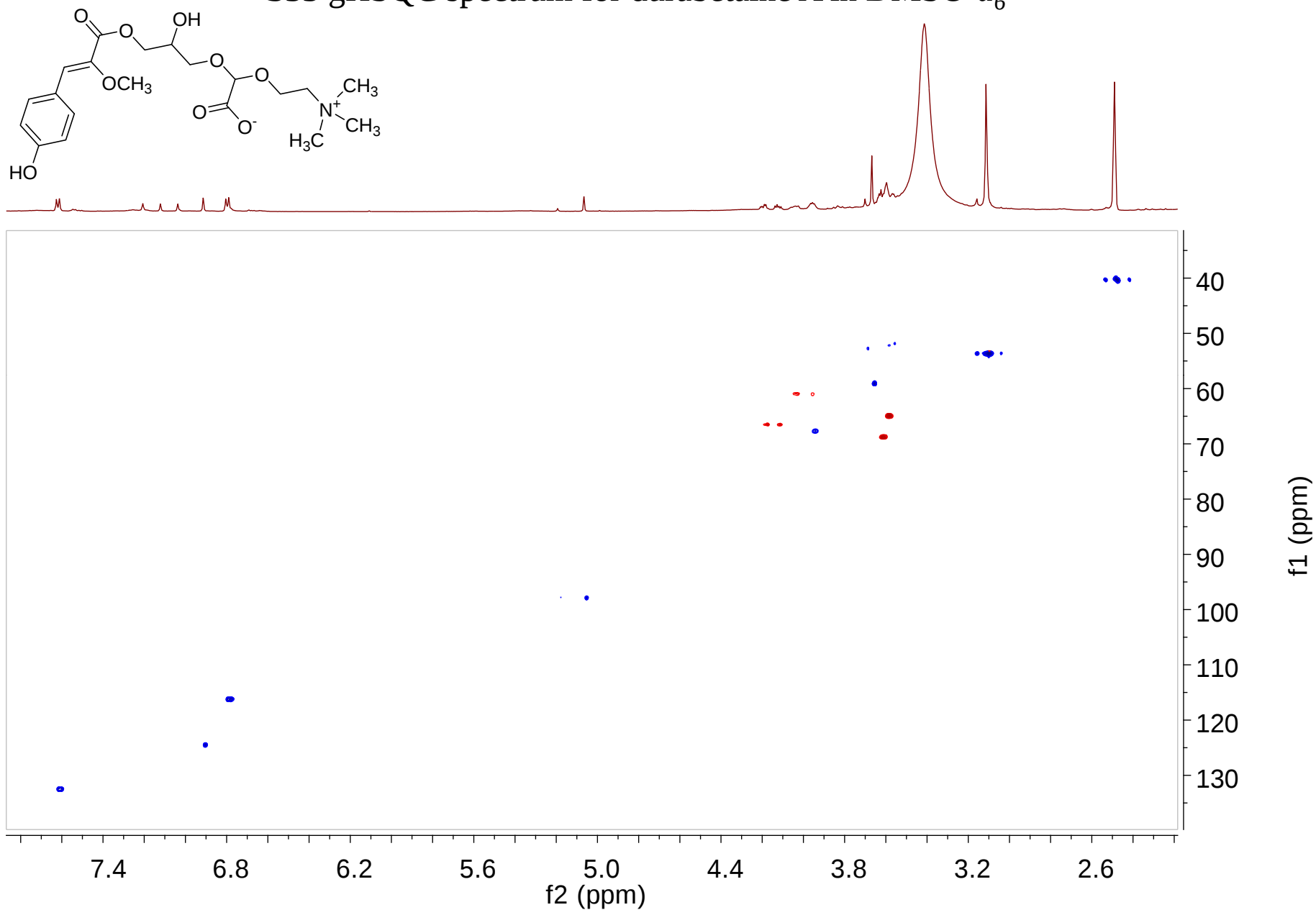
S33 ^1H NMR spectrum for durabetaine A in $\text{DMSO-}d_6$



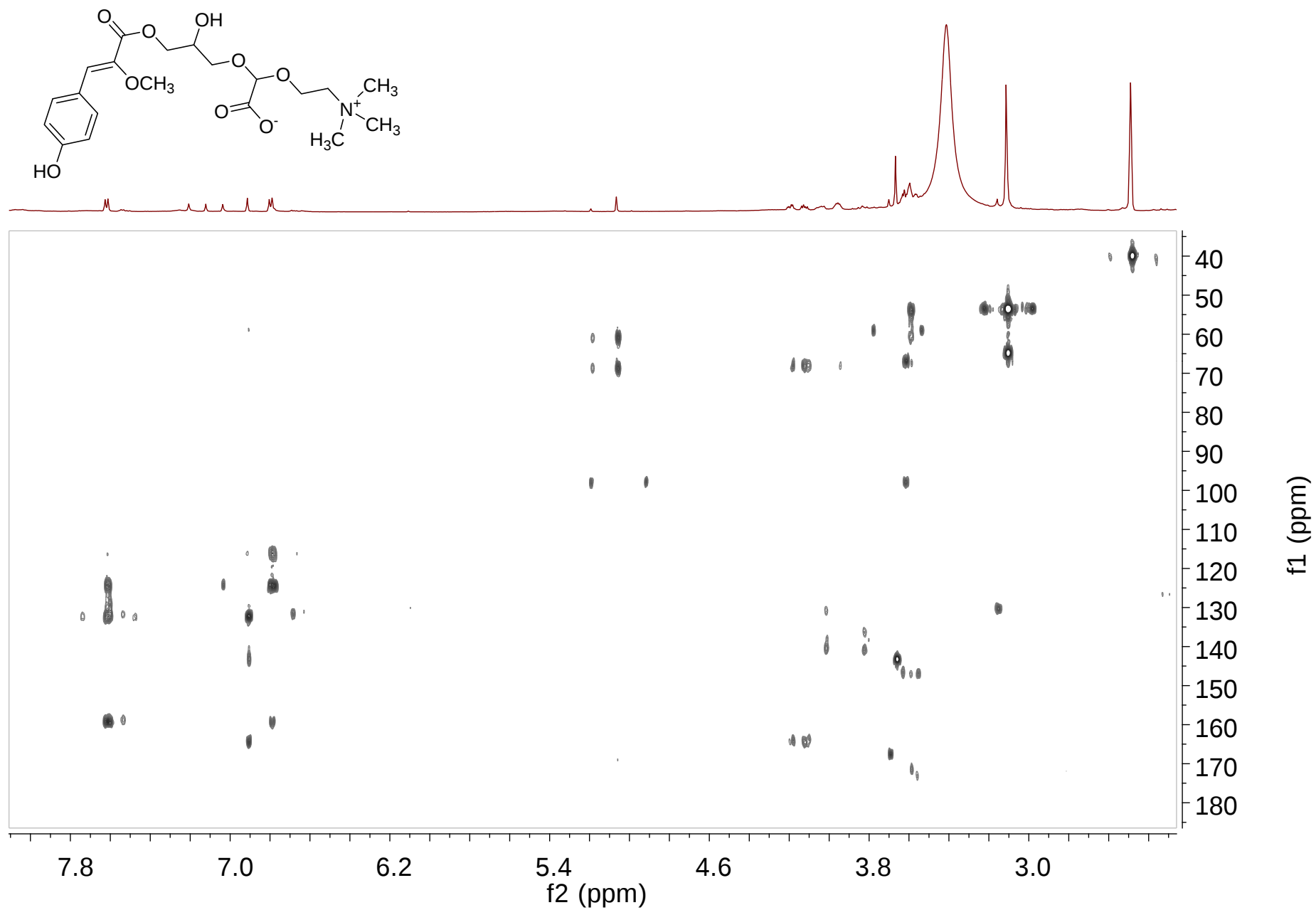
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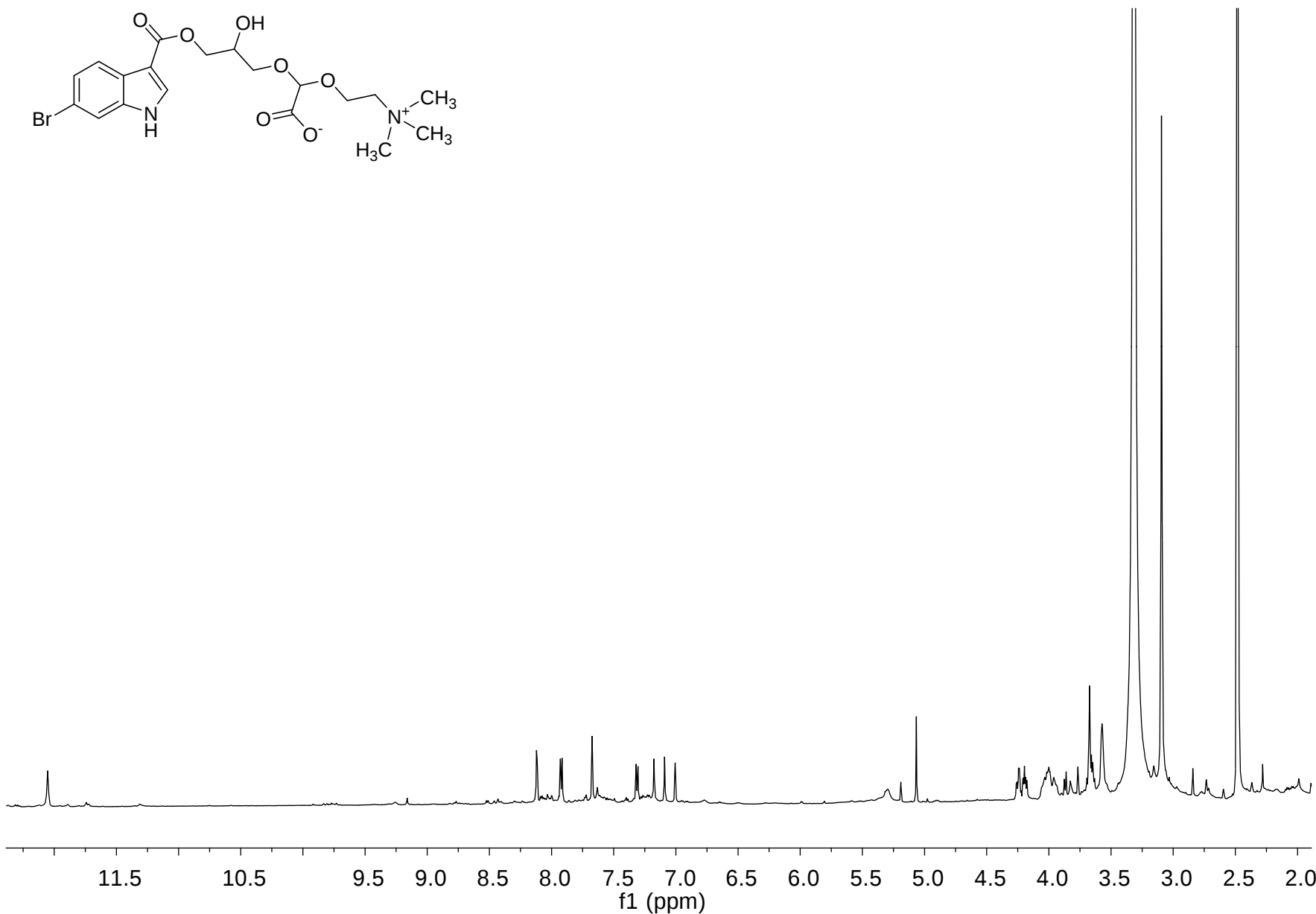
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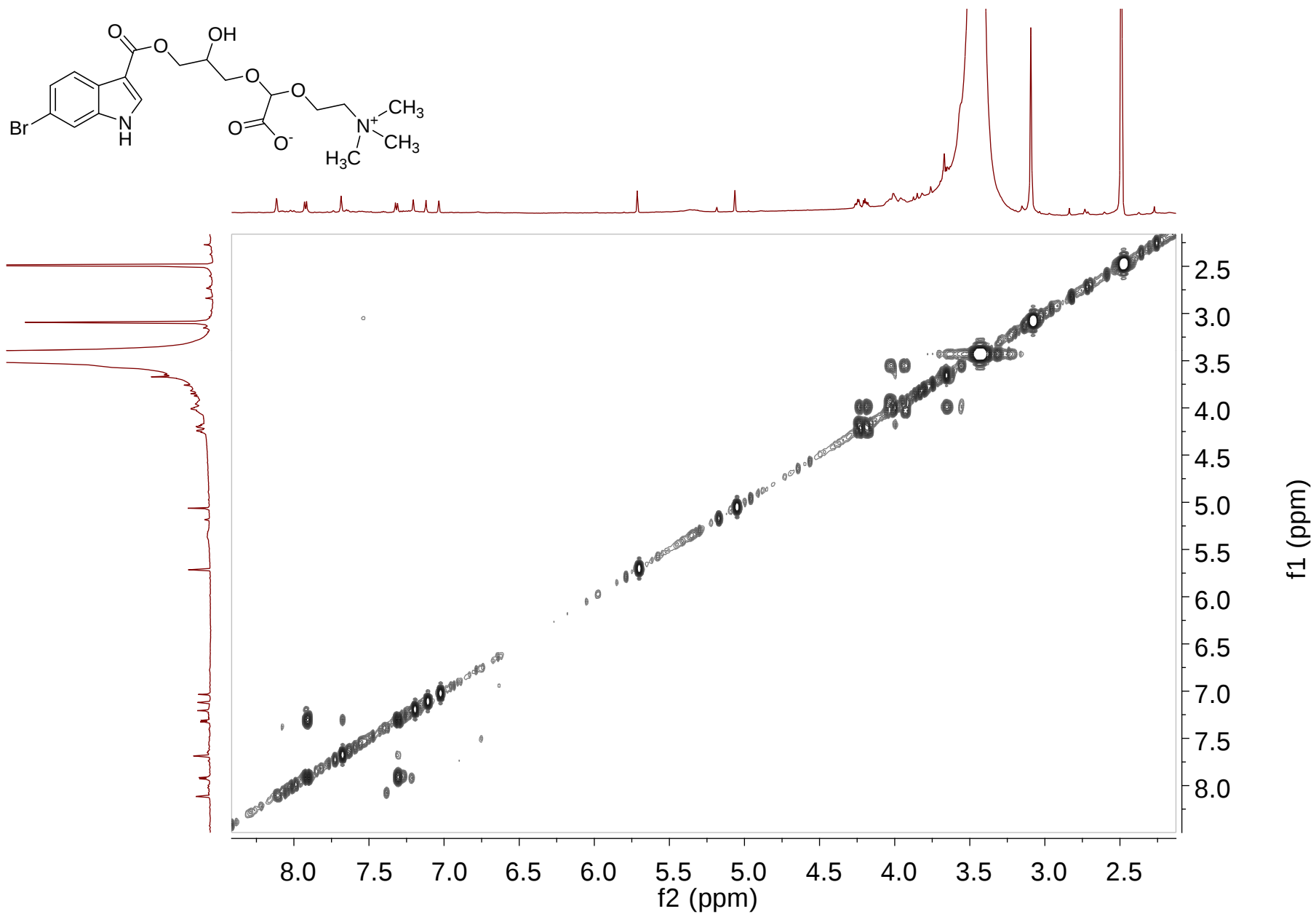
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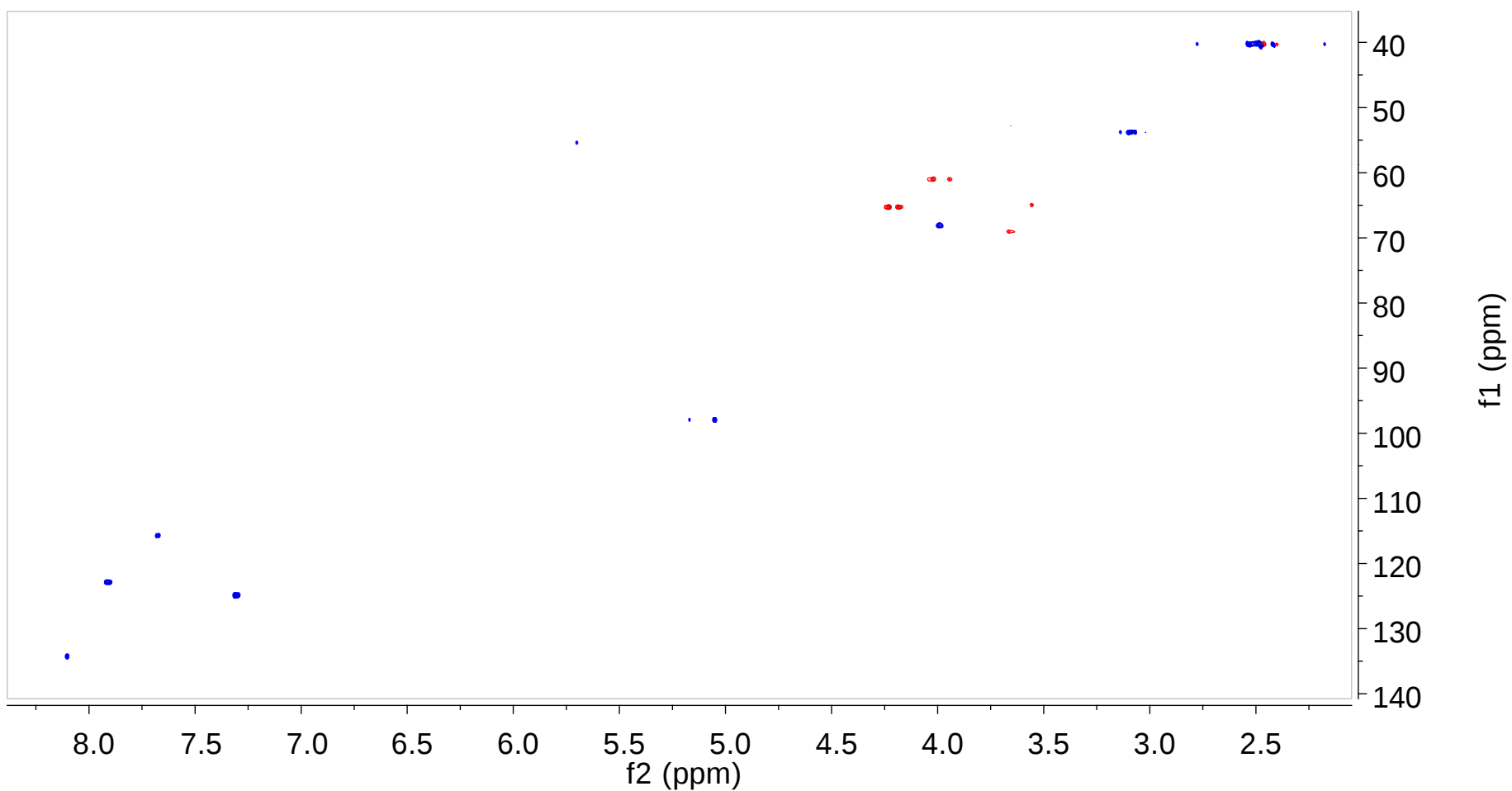
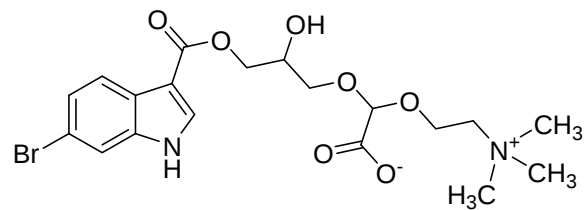
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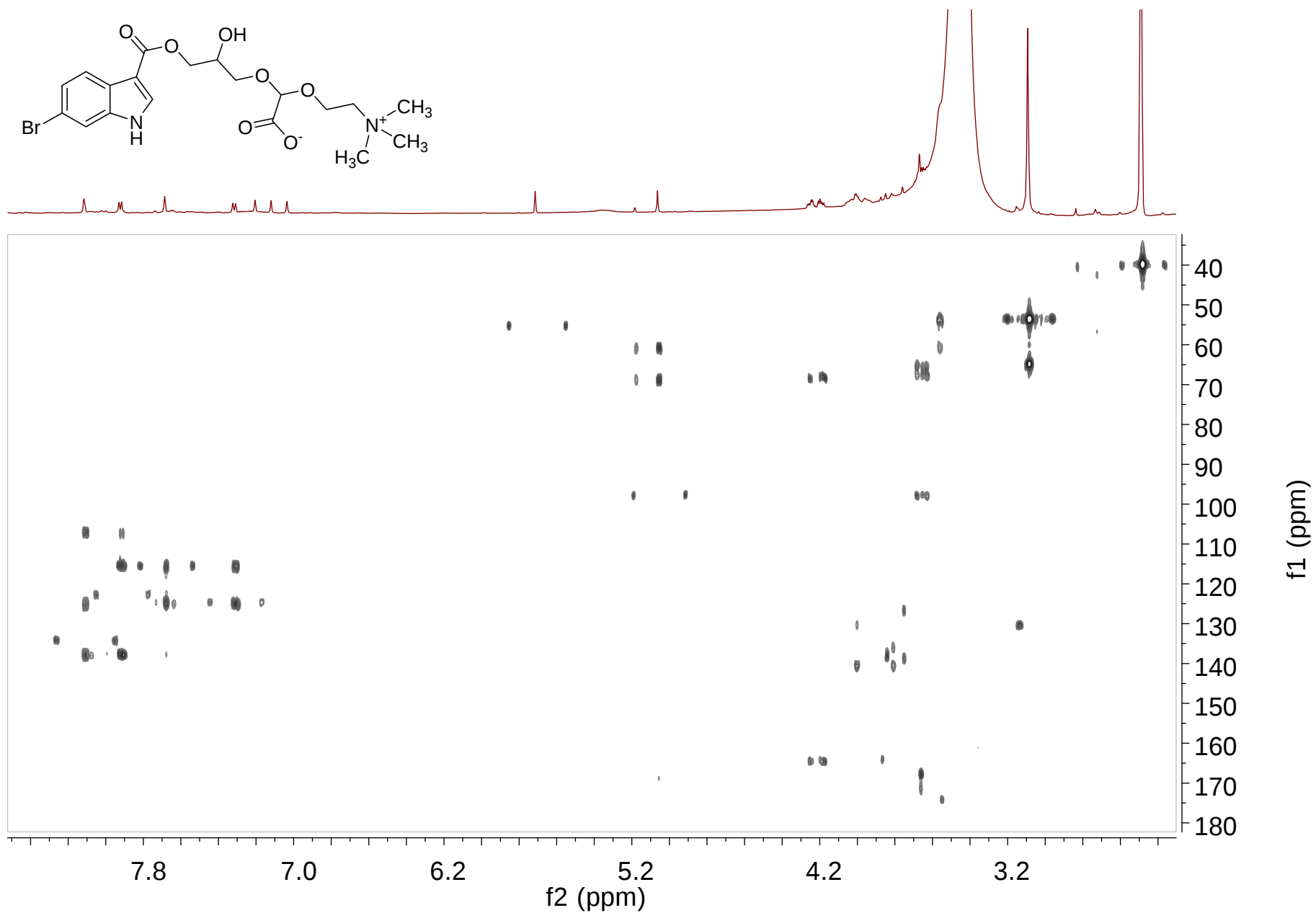
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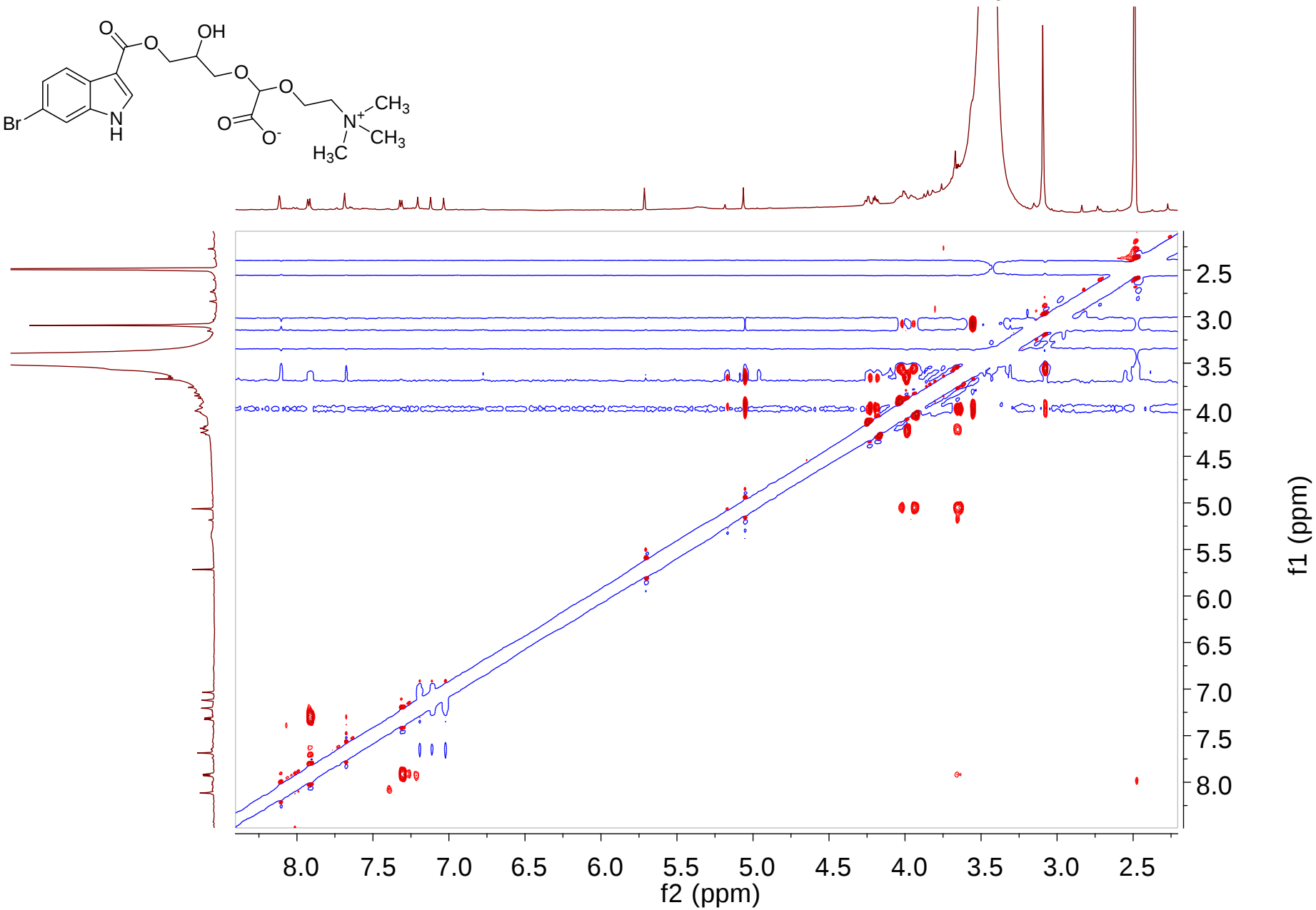
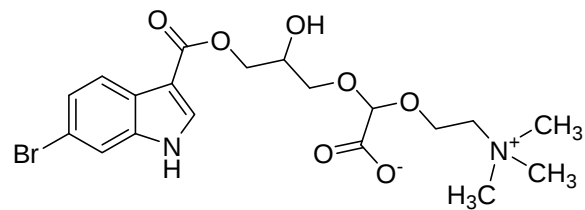
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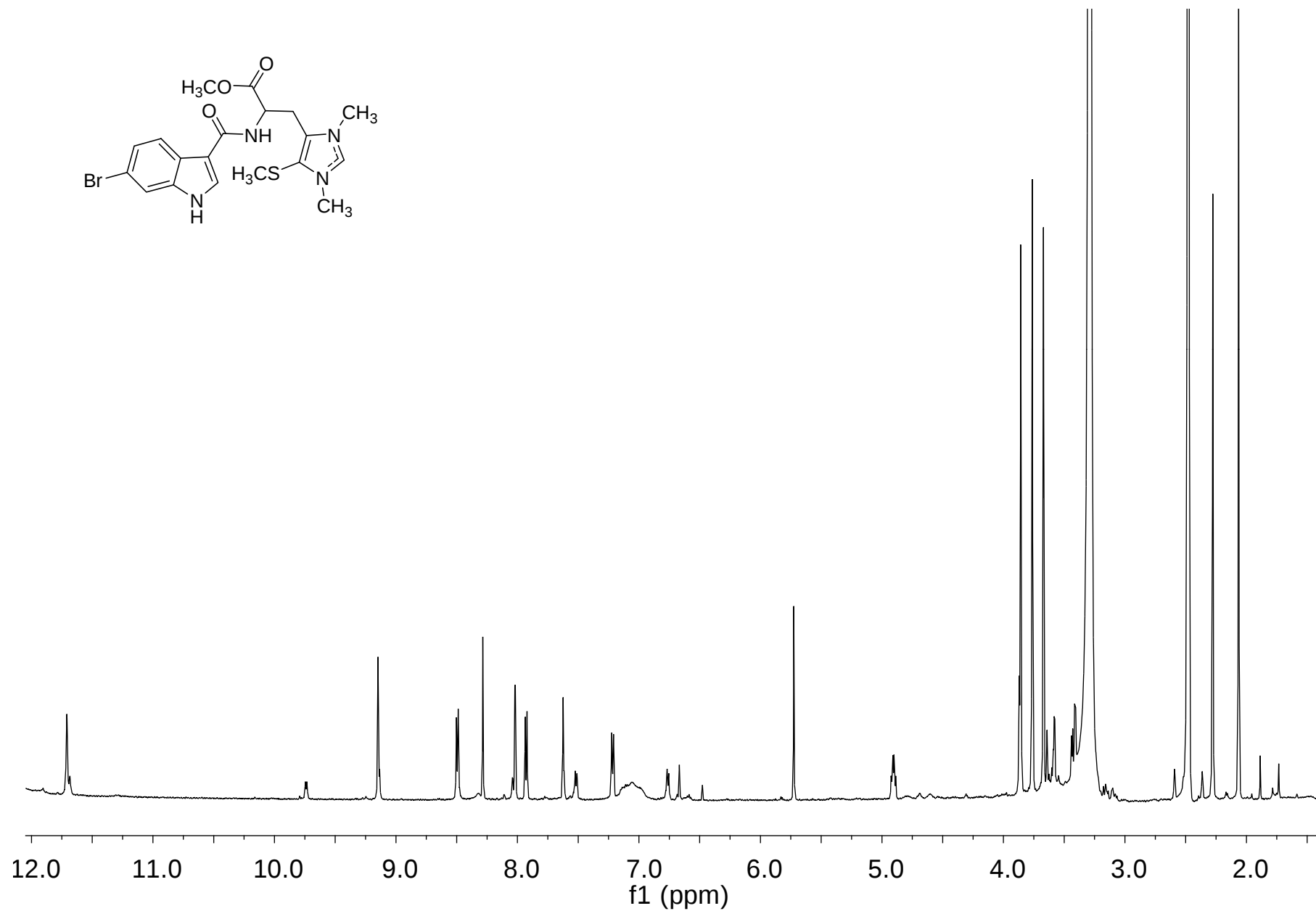
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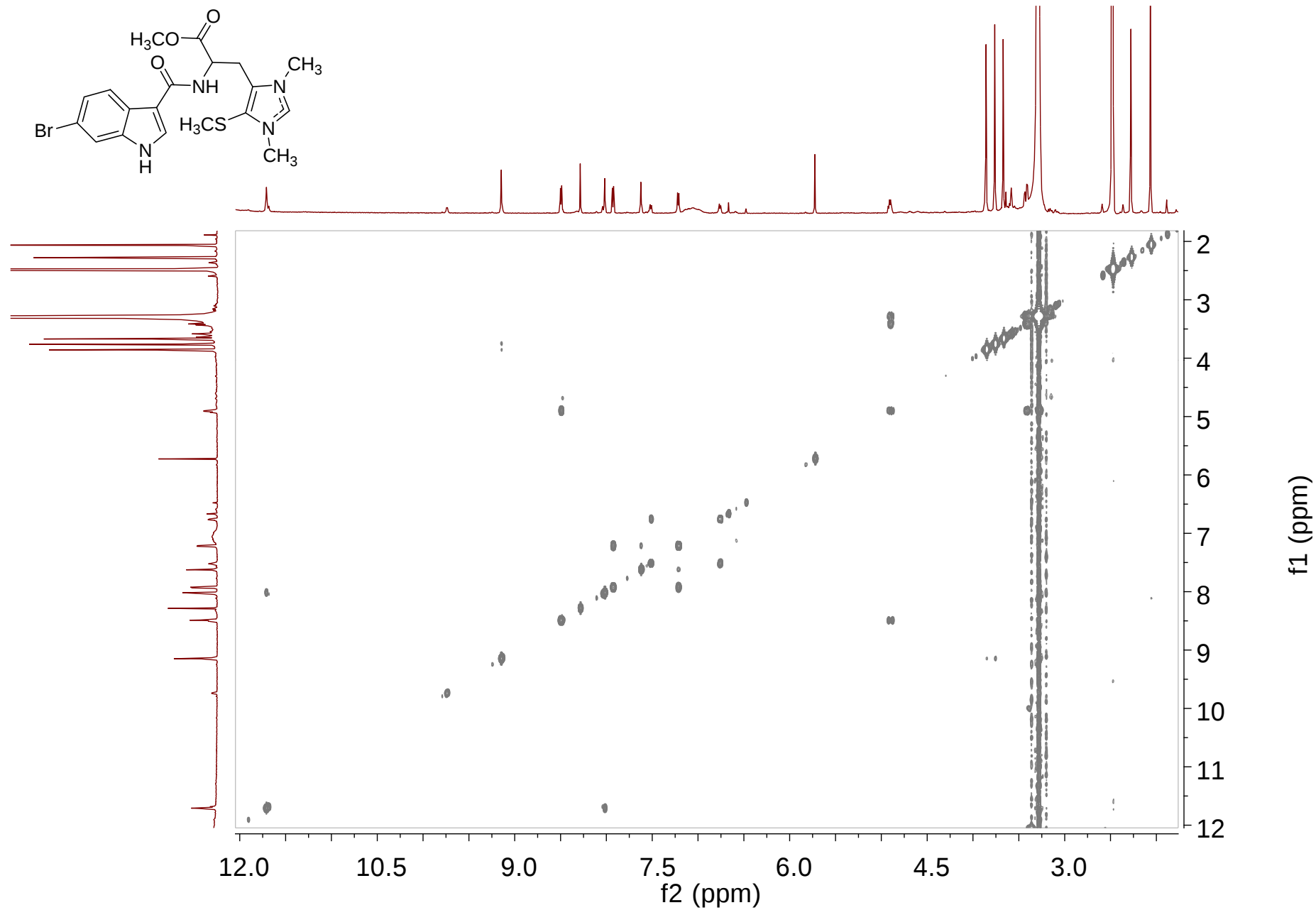
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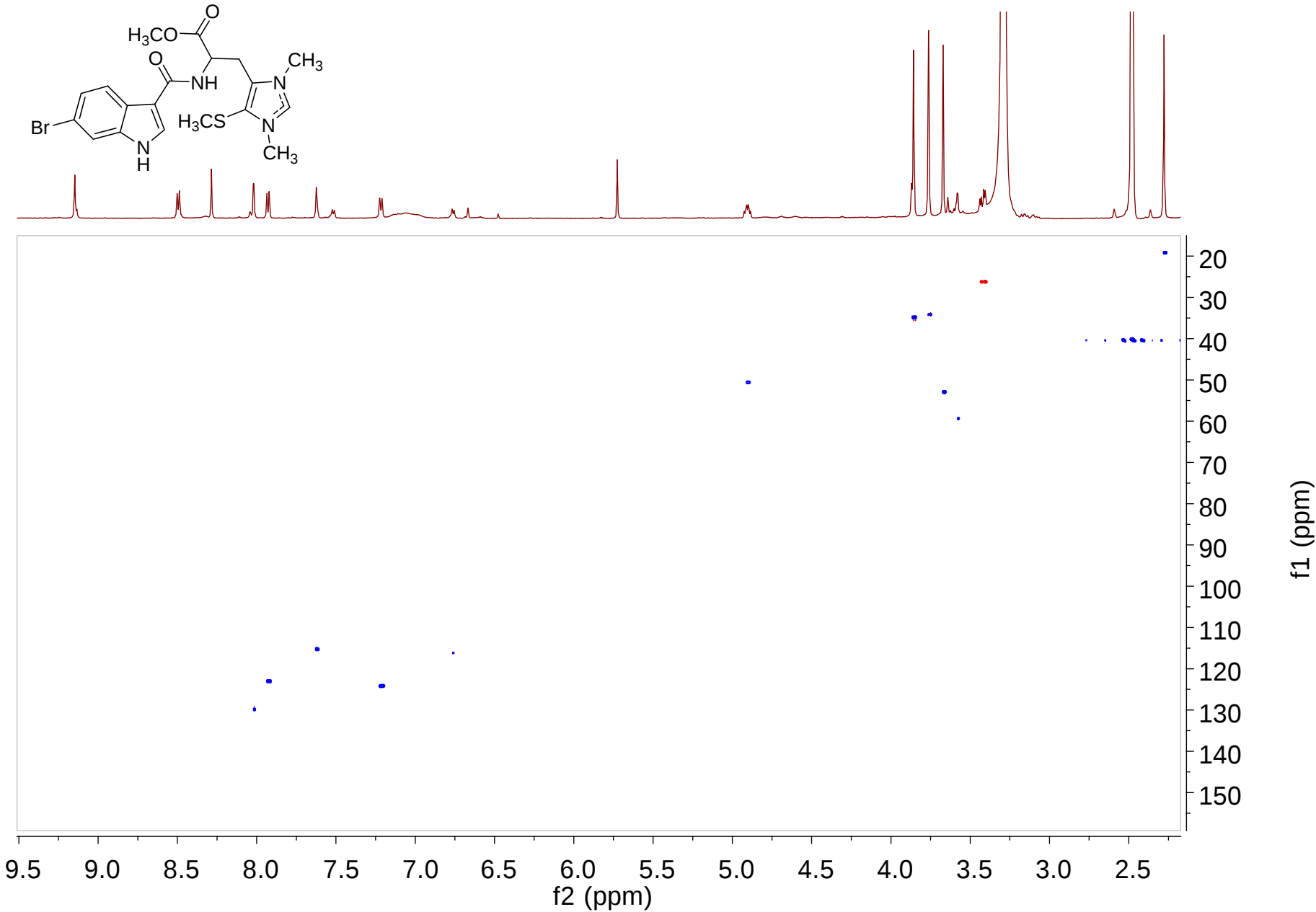
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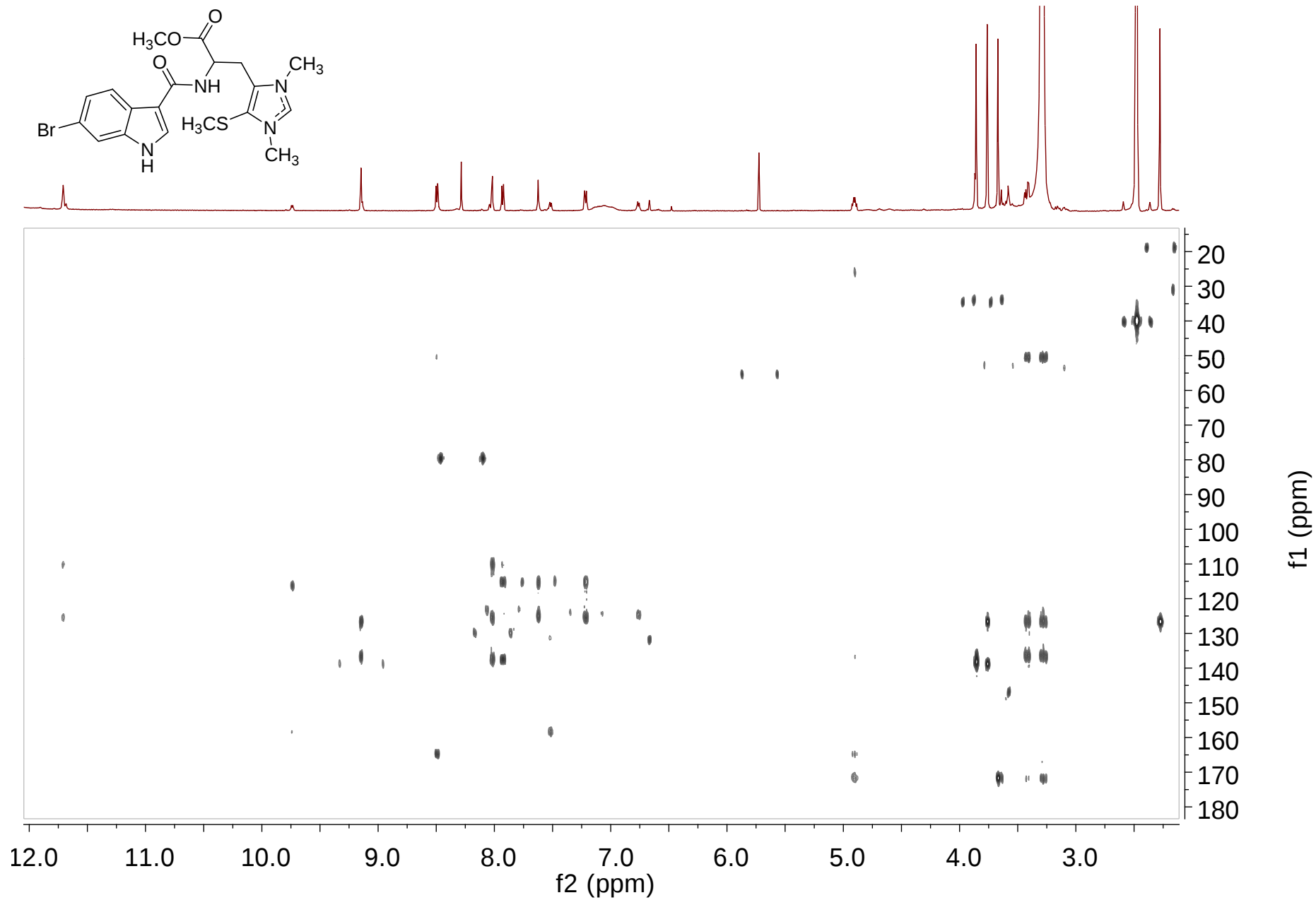
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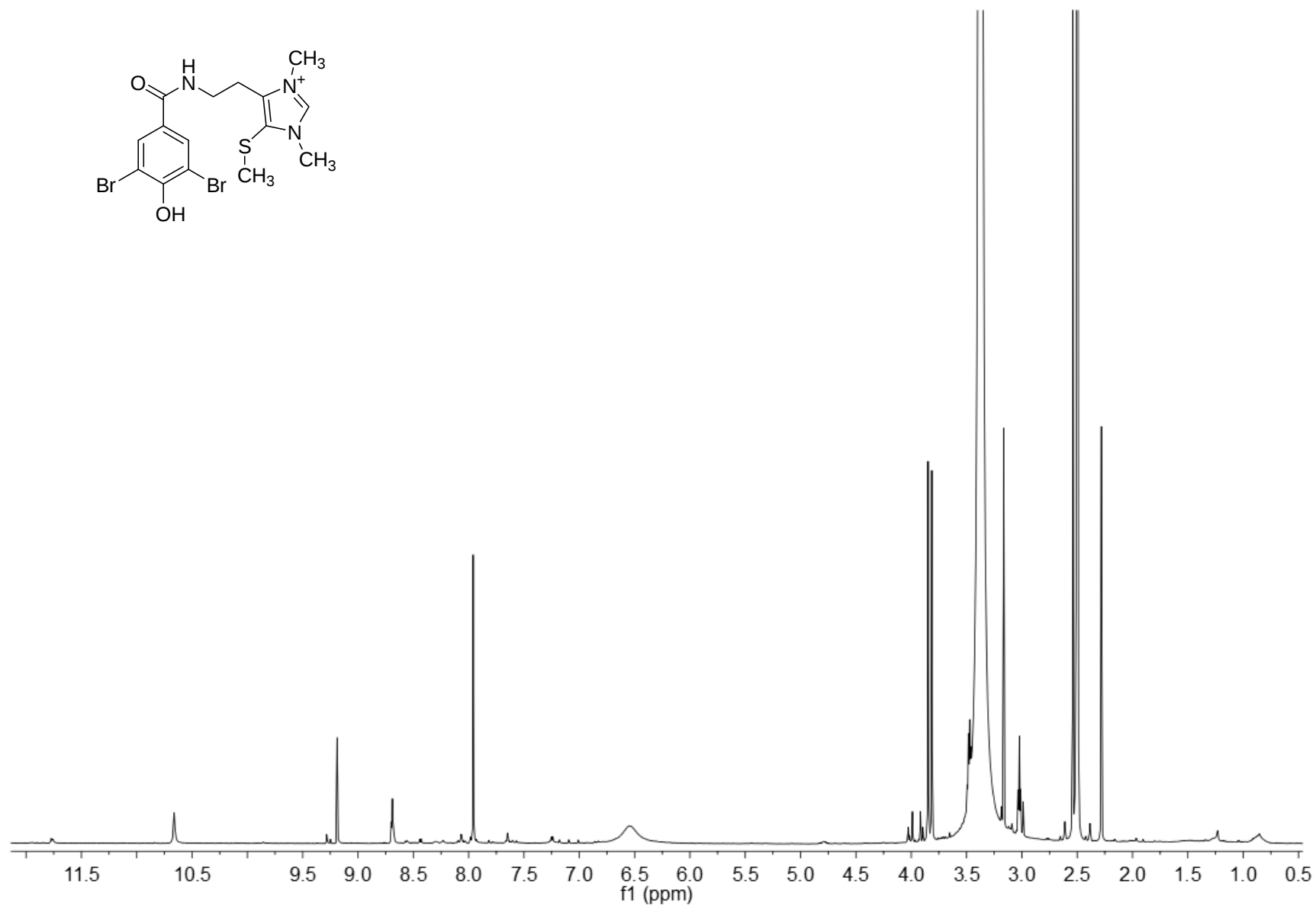
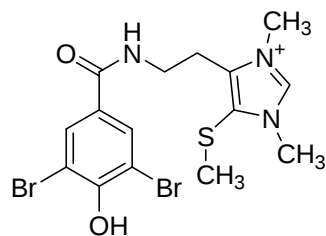
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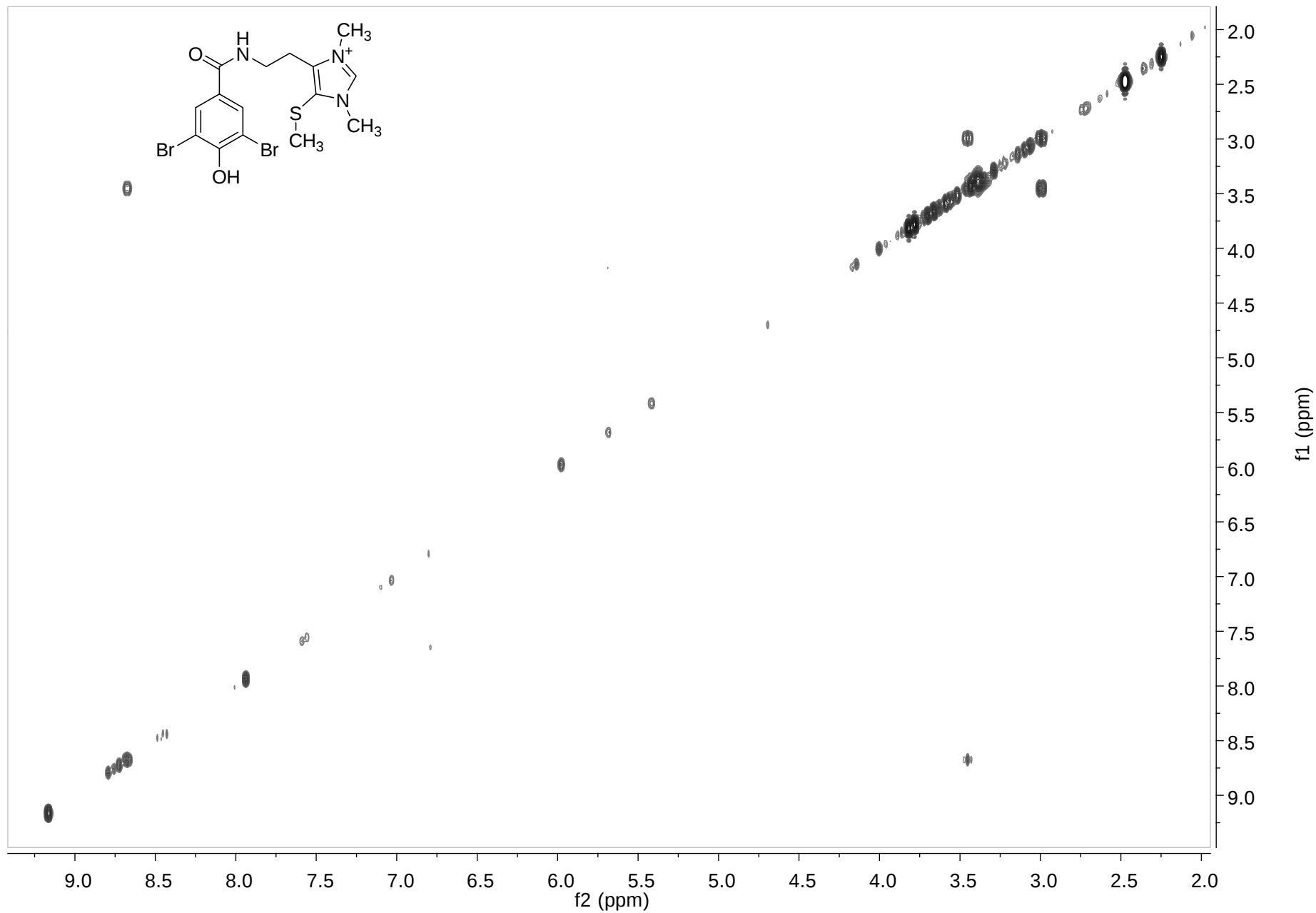
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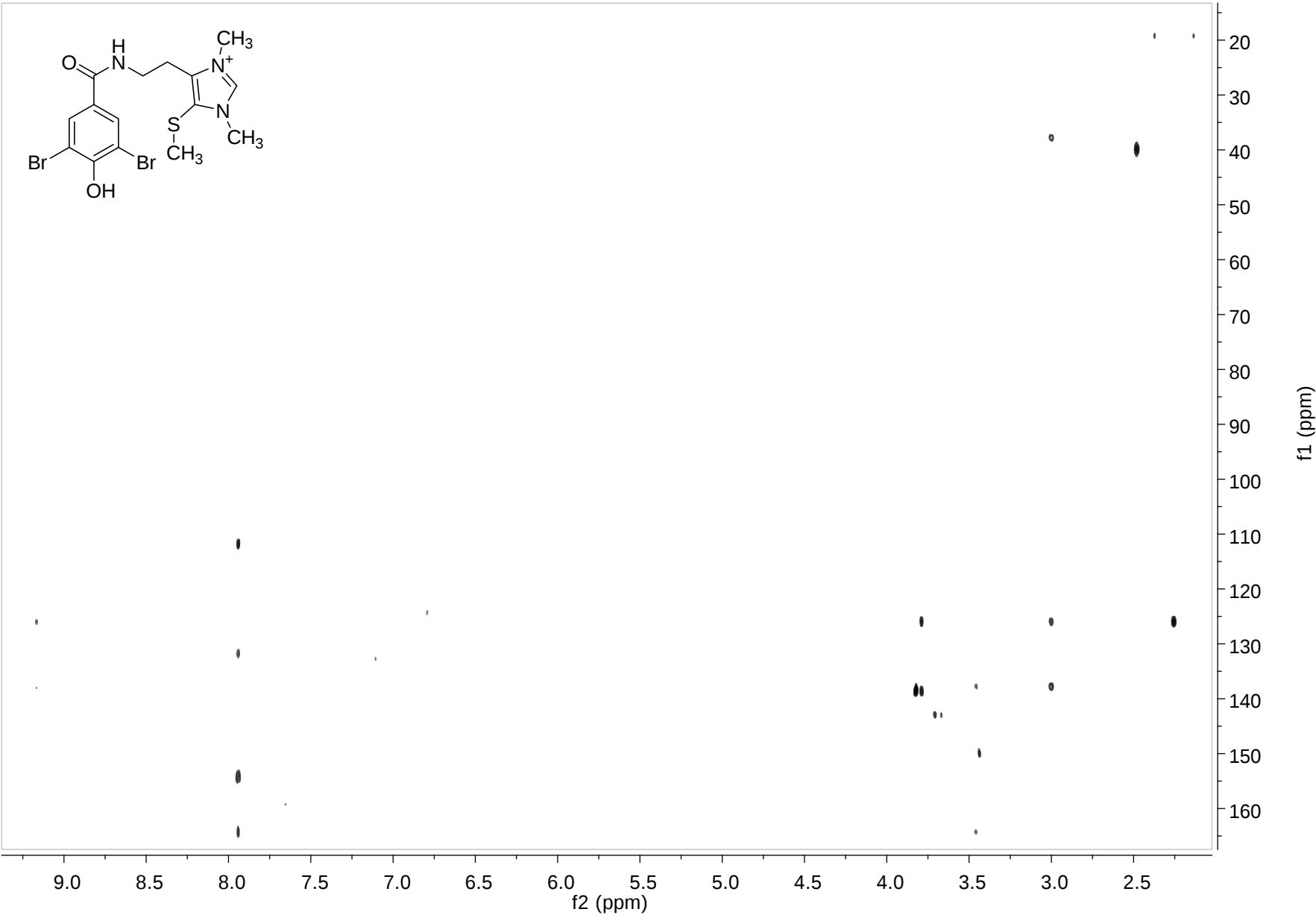
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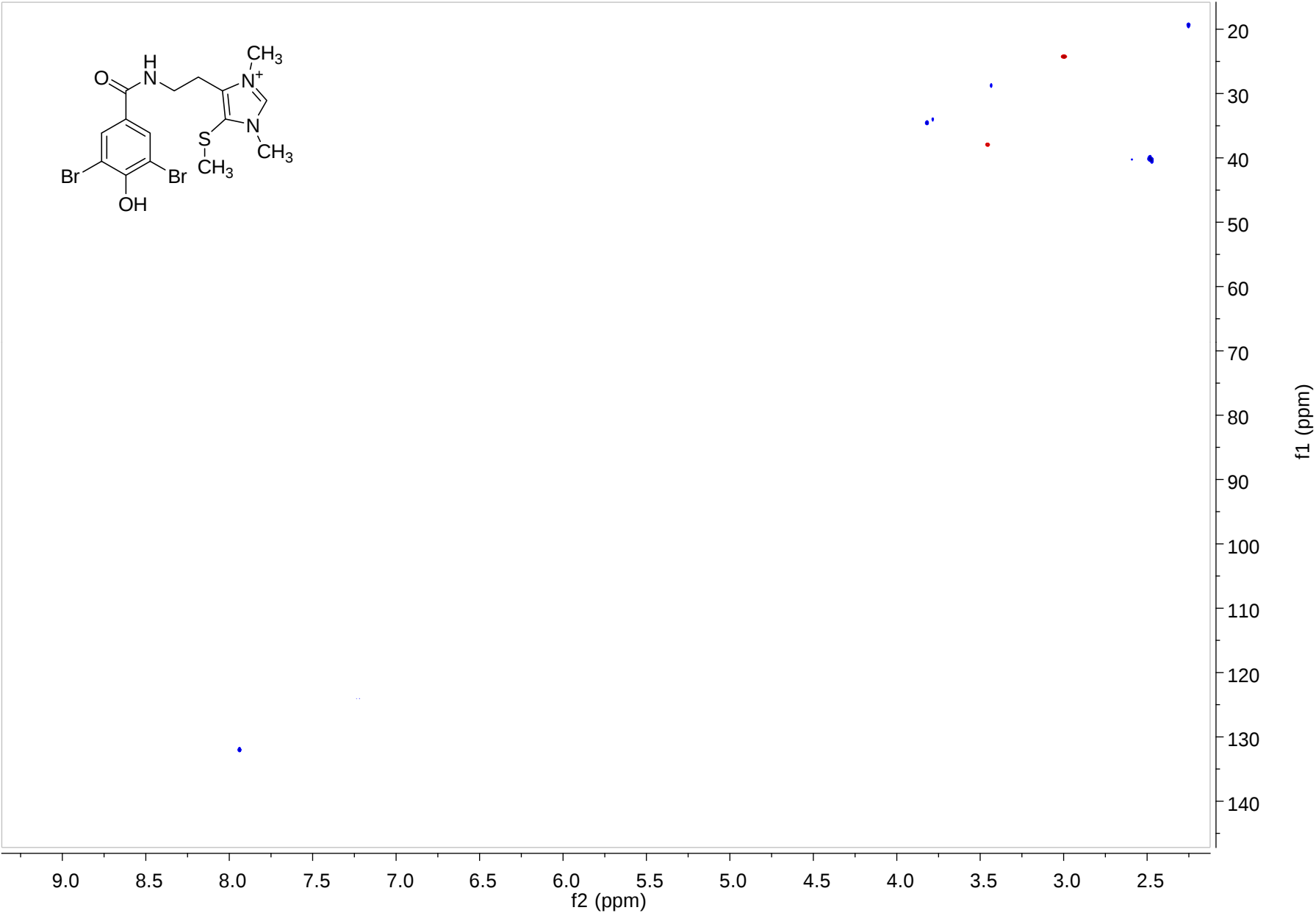
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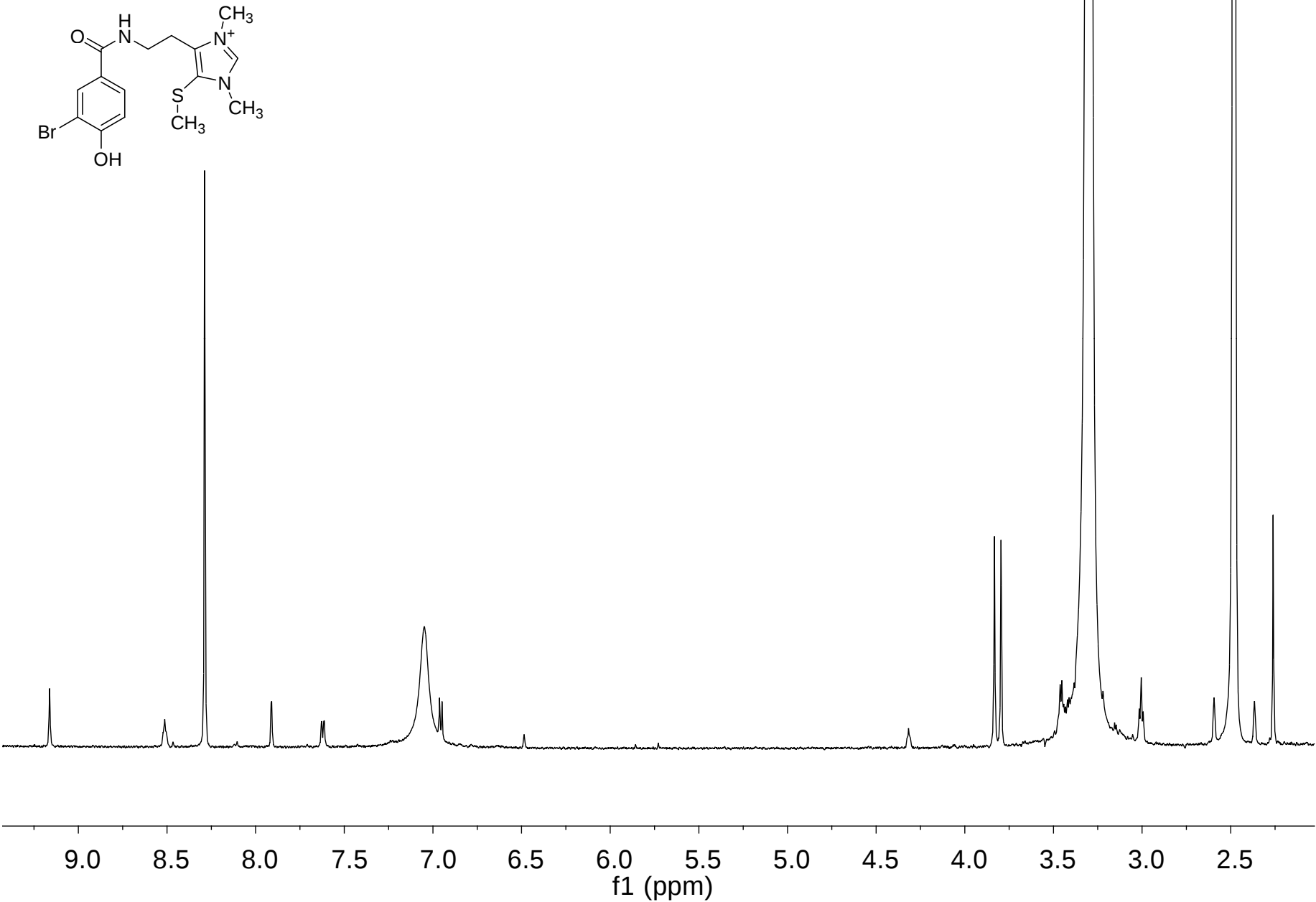
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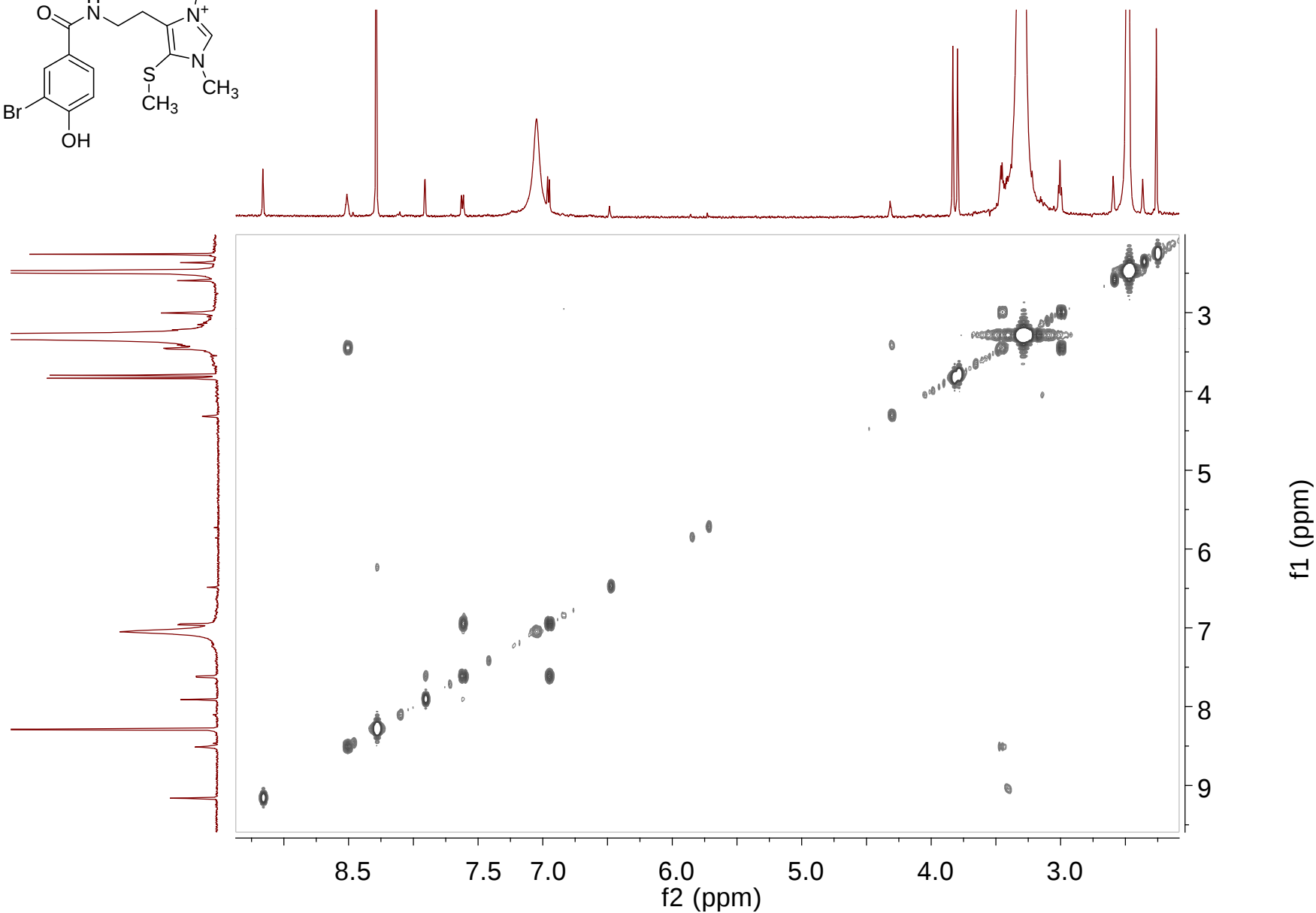
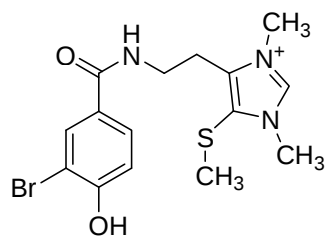
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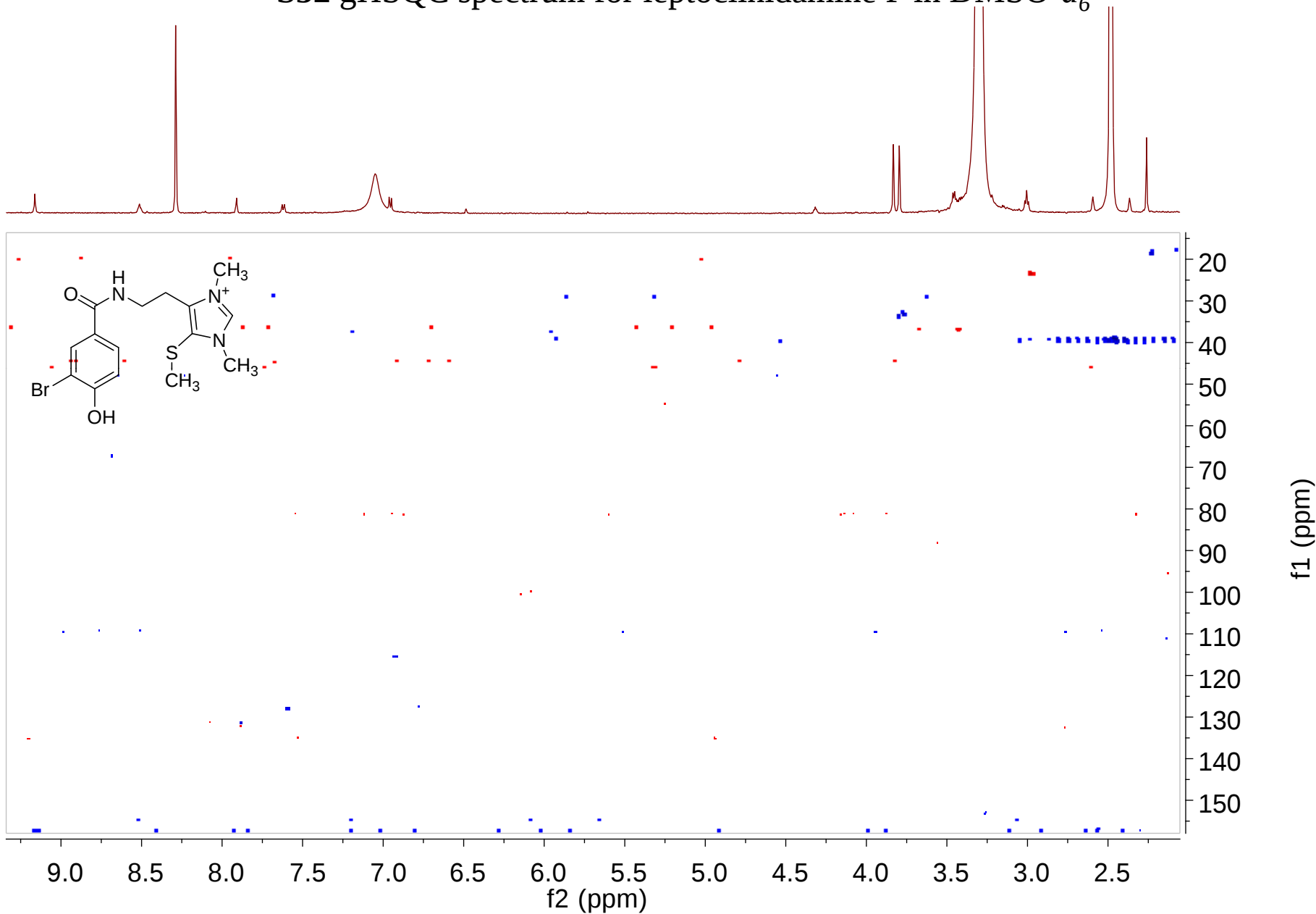
S50 ¹H NMR spectrum for leptoclinidamine F in DMSO-*d*₆



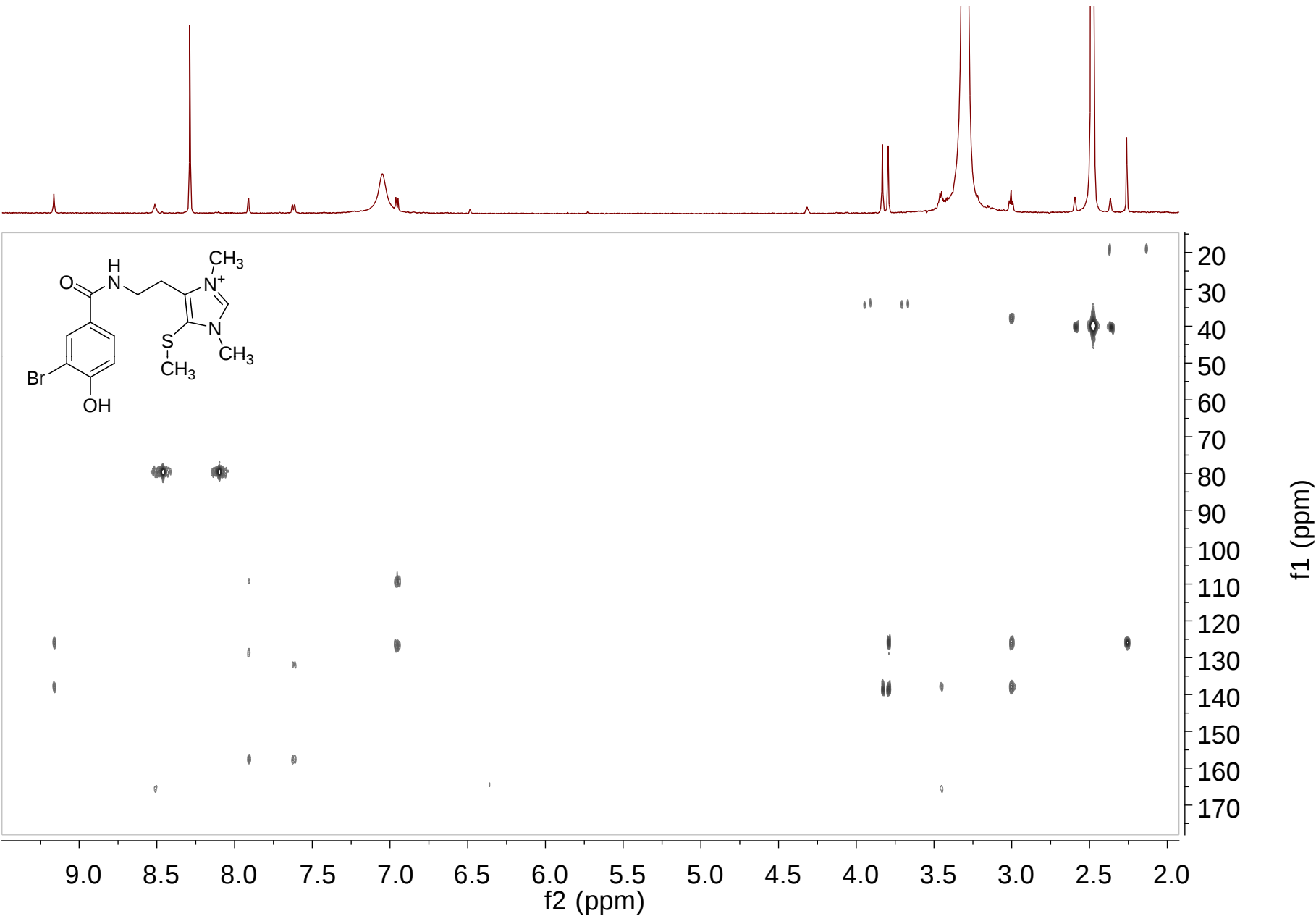
S51 gCOSY spectrum for leptoclinidamine F in DMSO- d_6



S52 gHSQC spectrum for leptoclinidamine F in DMSO-*d*₆



S53 gHMBC spectrum for leptoclinidamine F in DMSO-*d*₆



S54 Real-time cell analysis

The breast cancer cell line MDA-MB-231 and the prostate cancer cell line LNCaP were routinely maintained in culture flasks at 37° C in 5% CO₂. LNCaP was grown in RPMI medium without phenol red (Invitrogen) supplemented with 5% (v/v) fetal bovine serum (FBS; Invitrogen). The MDA-MB-231 cell line was maintained in DEMEM medium (Invitrogen) with 10% (v/v) FBS. Each cell line was seeded on 96-well E-plates at a density of 5×10^3 cells (MDA-MB-231) or 10×10^3 cells (LNCaP) in their respective medium supplemented with FBS. The wells for the experiment with the prostate cancer cell line were coated with poly-l-ornithine overnight at 37 °C and washed with PBS before cell seeding. The adhesion and spreading of the cells were monitored for 24 h at 37 °C in 5% CO₂ then the cells were treated with 200 µL duramidines A-C diluted in medium at a final concentration of 10 µM (final concentration of 0.1% DMSO). The plates were monitored for more 72 h using a real-time cell analyser (xCELLigence, ROCHE), which detects any change in cell number, morphology or adhesion. The cell status was monitored using changes in the electrical impedance measured by the microelectrodes localized on the bottom of the E-plate, which is translated as the quantitative measure called *cell index*. Compounds **1-14** were analysed in triplicates in two independent experiments. The controls used were 10 µM doxorubicin and 0.1 % DMSO. For the analysis of the data the cell index was normalized to the last time point before compound addition (24 h).