

Supporting Information
for
“Stabilizing Unusual Conformations in Small
Peptides and Glucopeptides using a Hydroxylated
Cyclobutane Amino Acid”

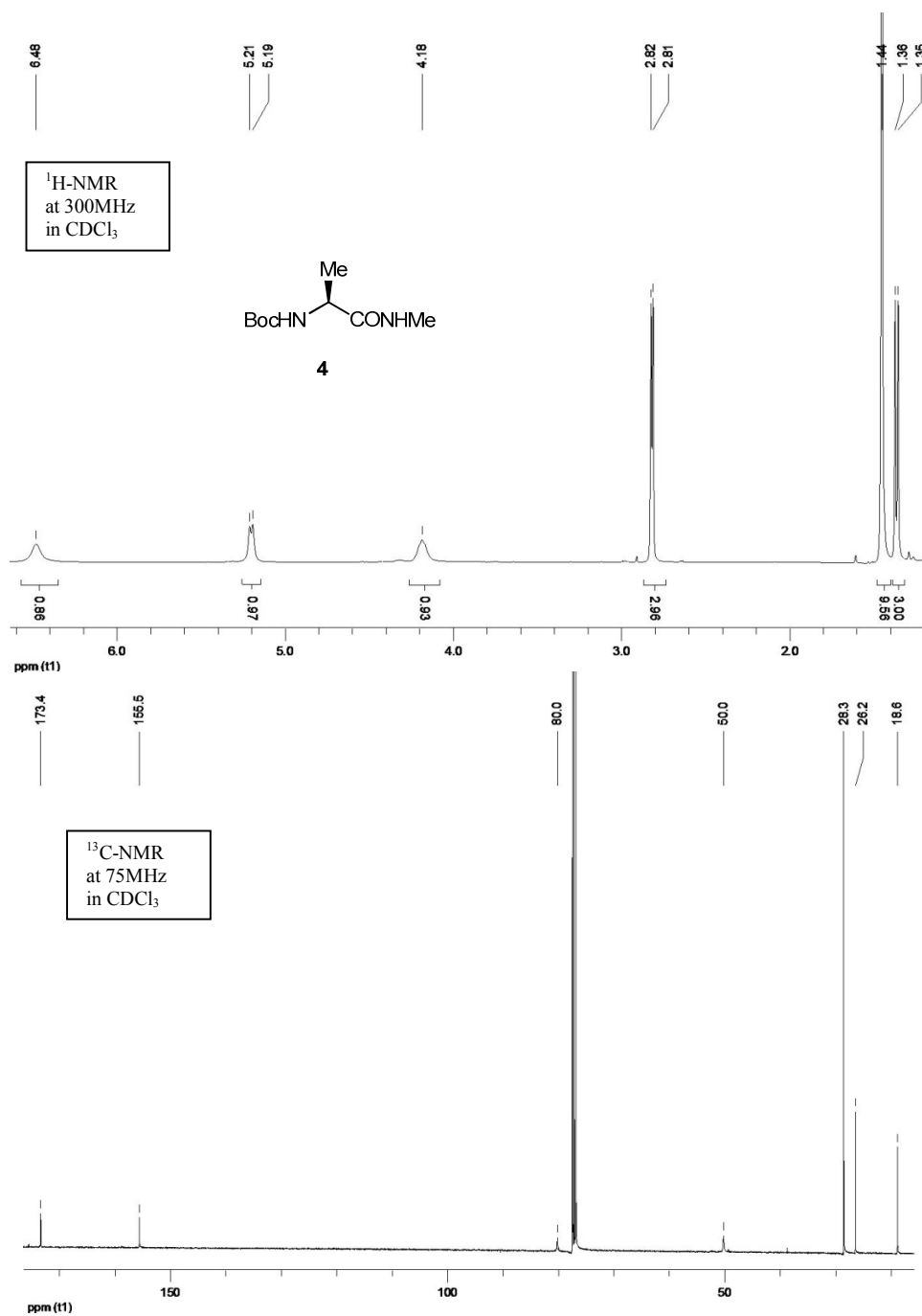
submitted to **Organic & Biomolecular Chemistry** as an ARTICLE by:

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Jesús M. Peregrina**

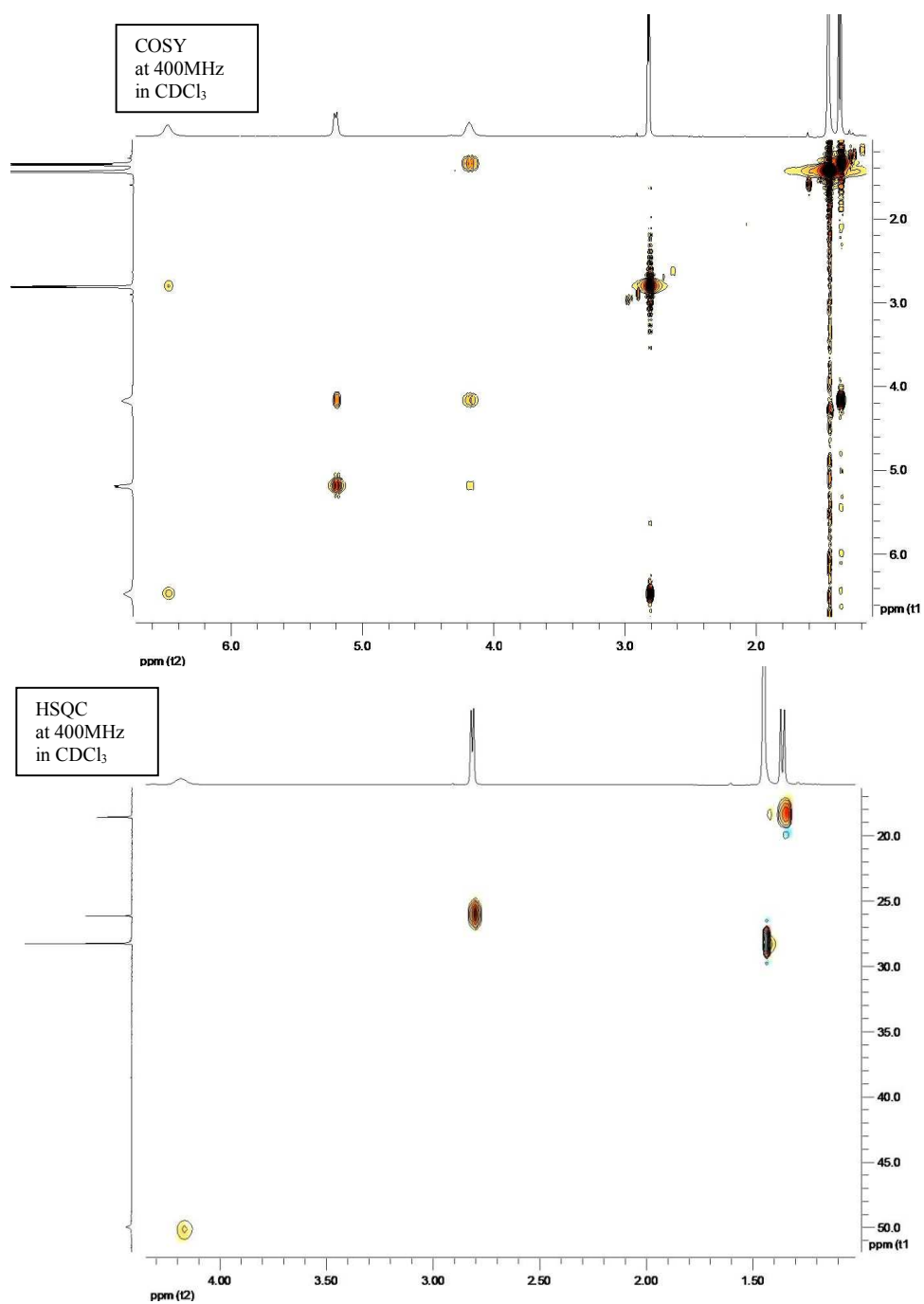
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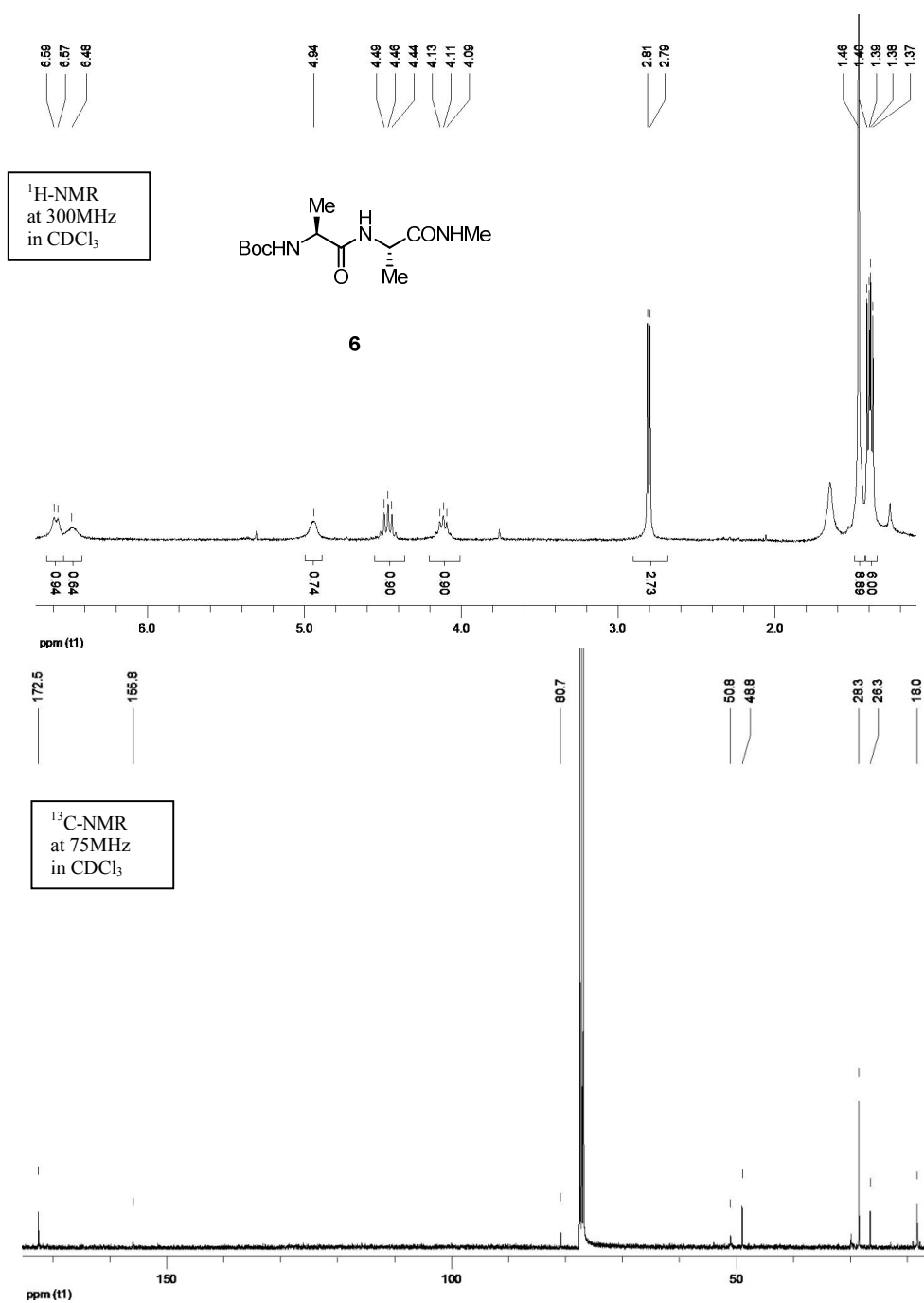
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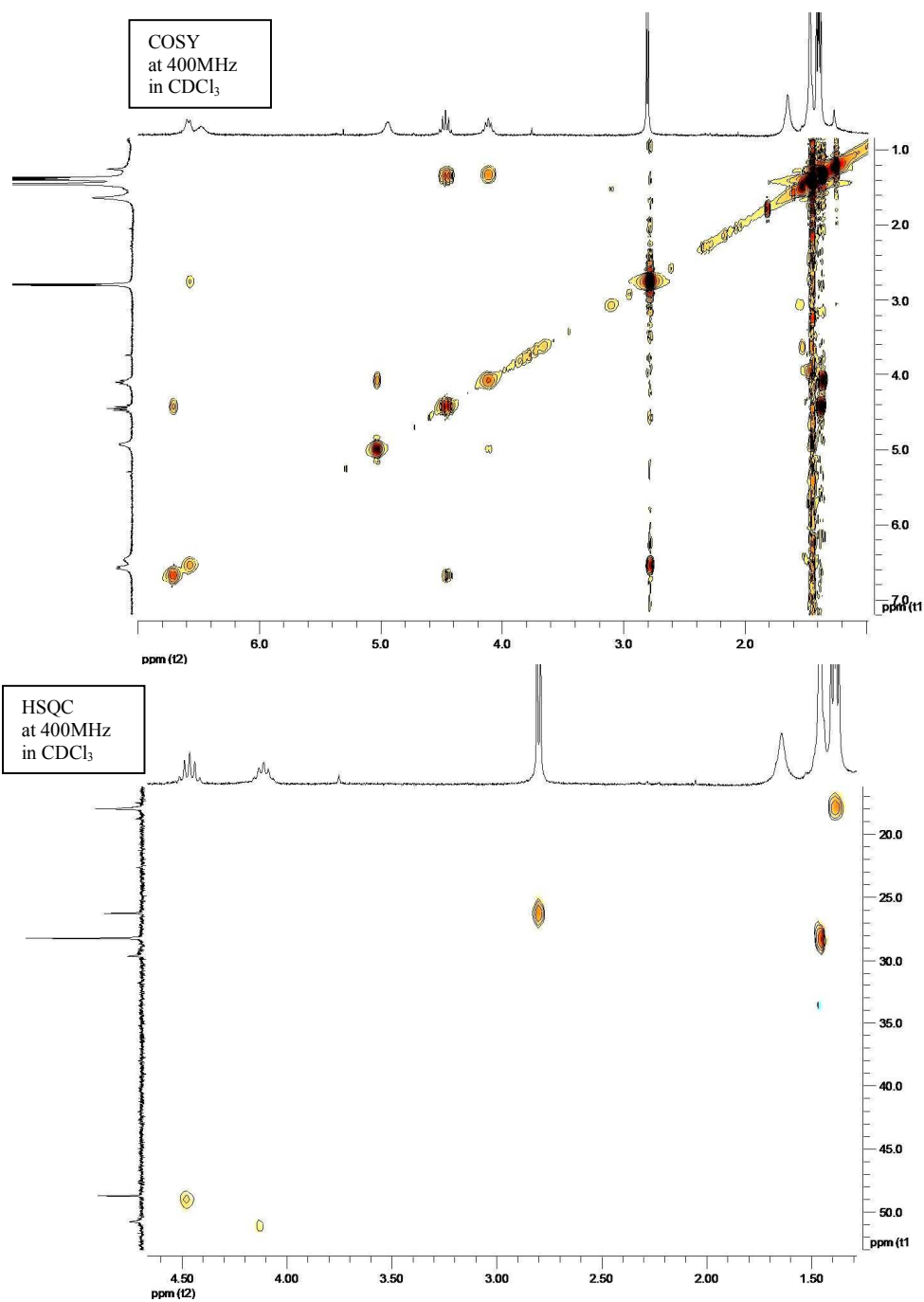
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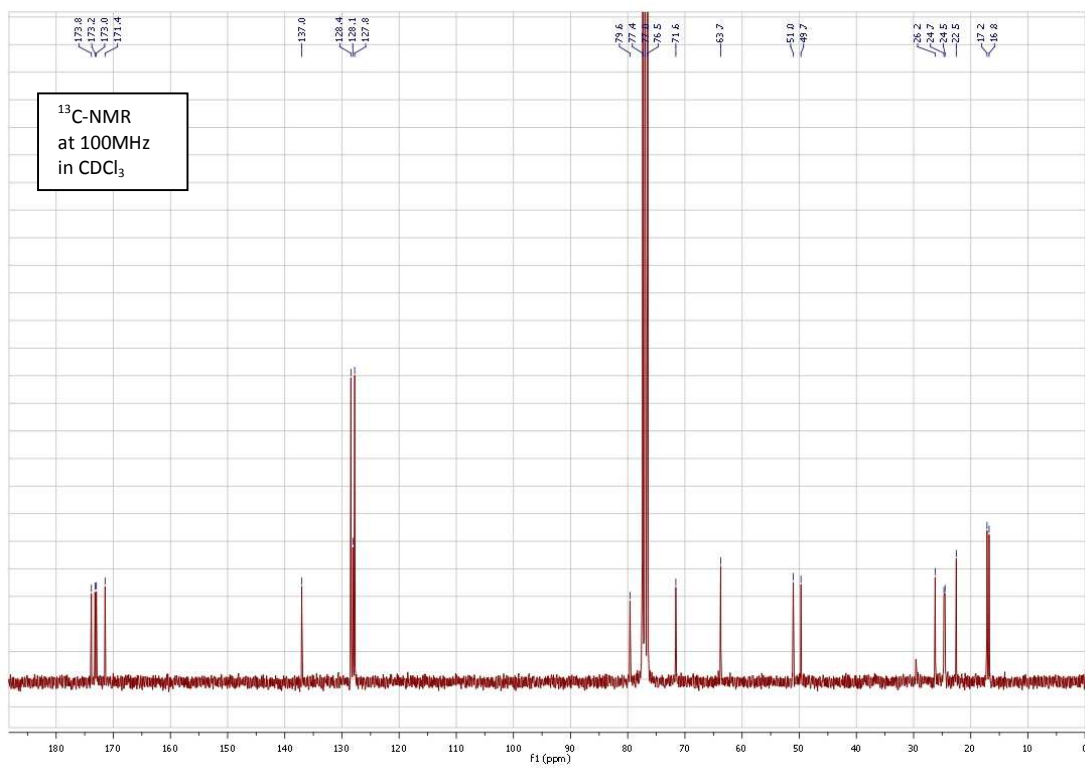
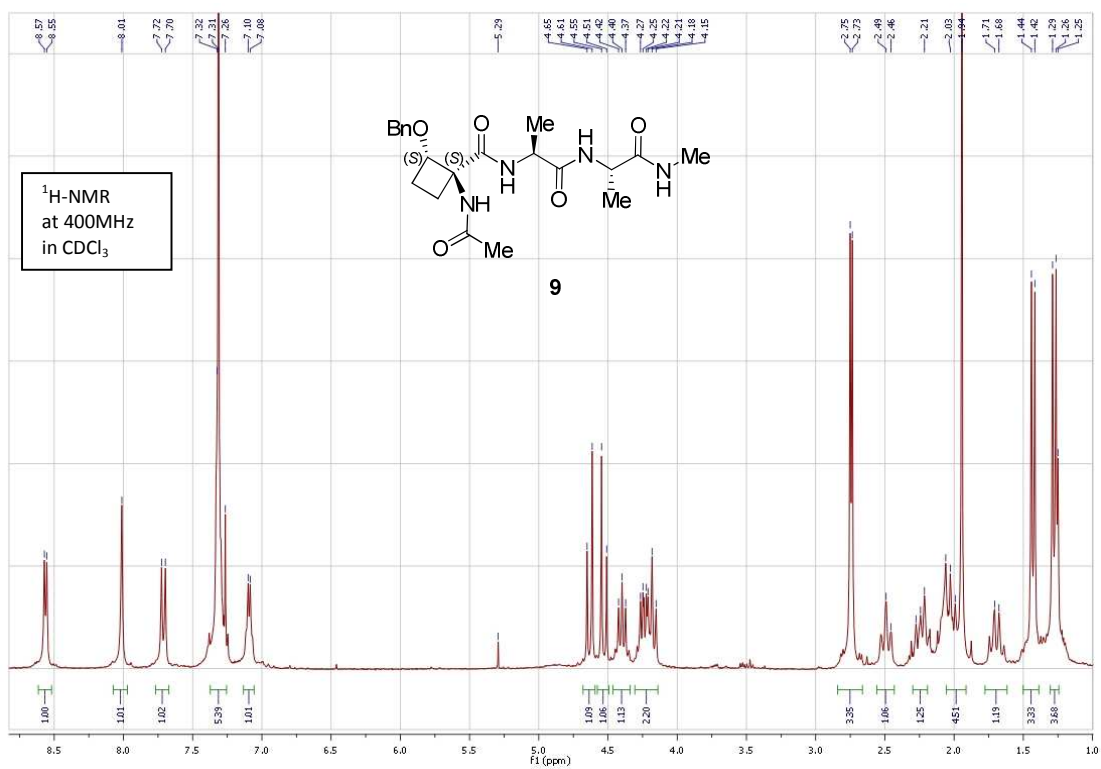
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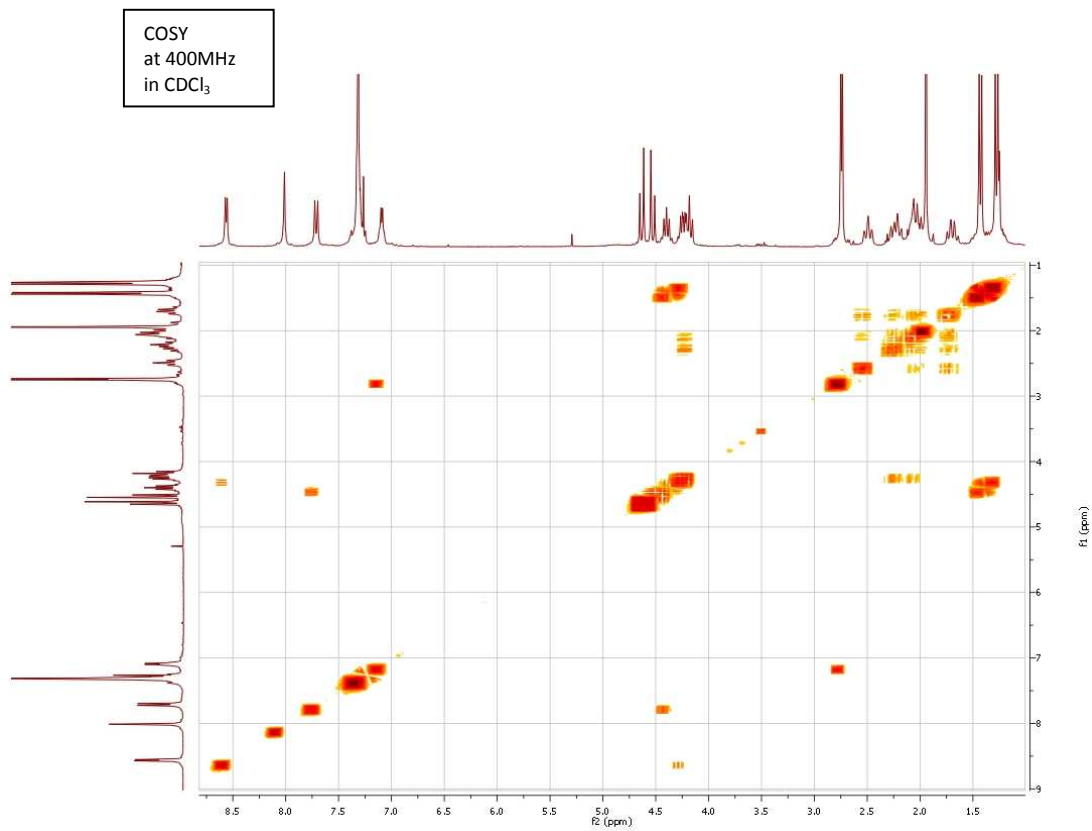
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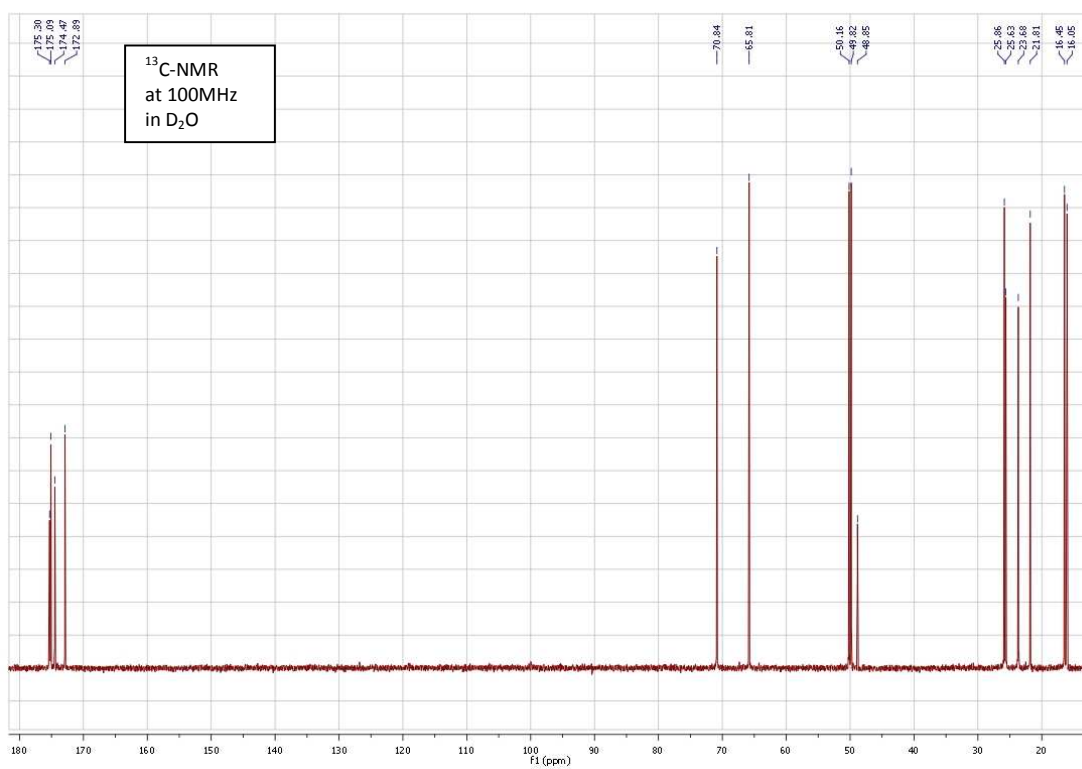
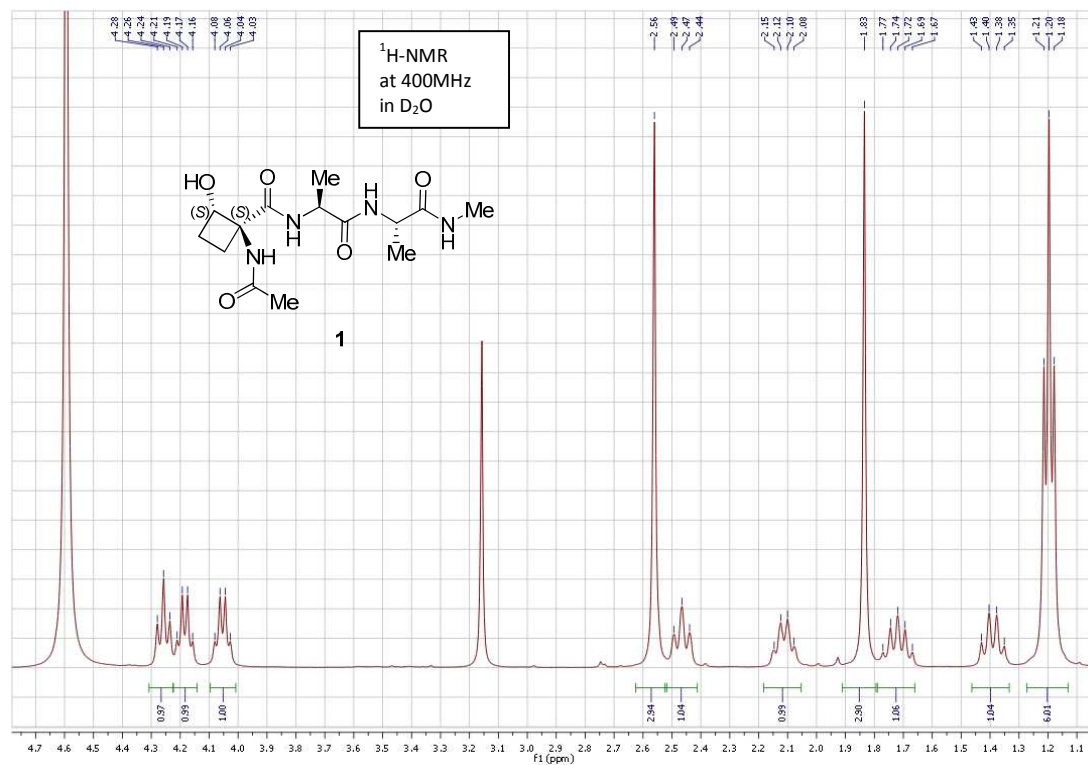


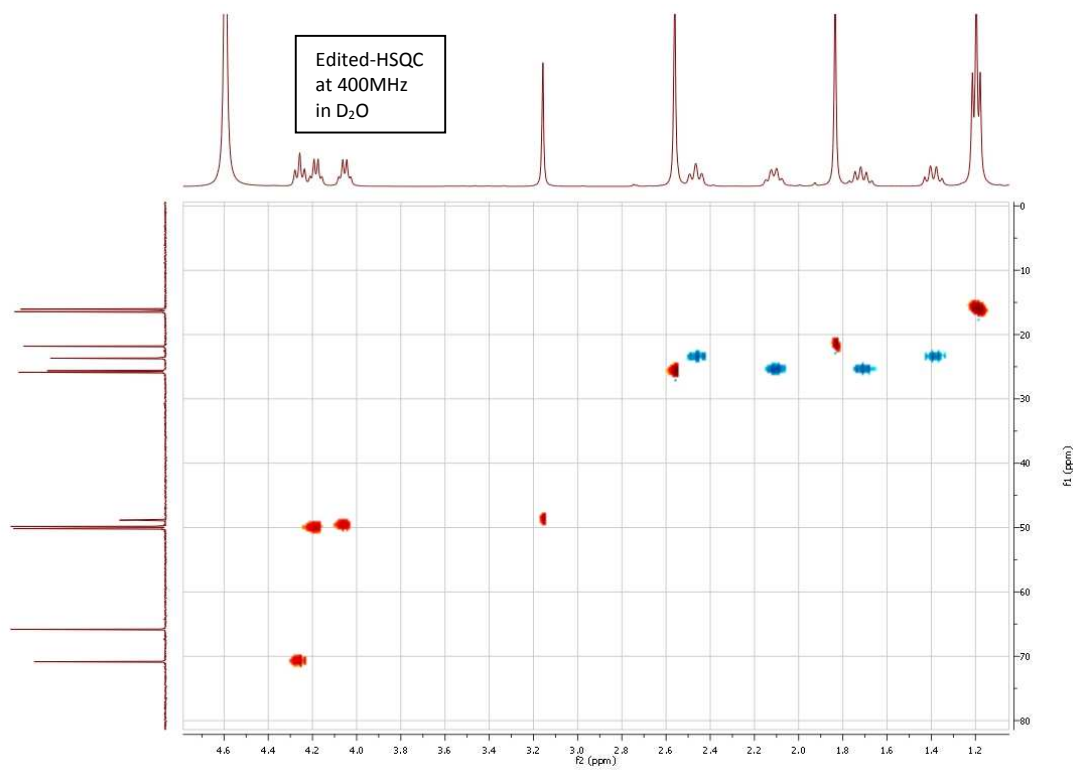
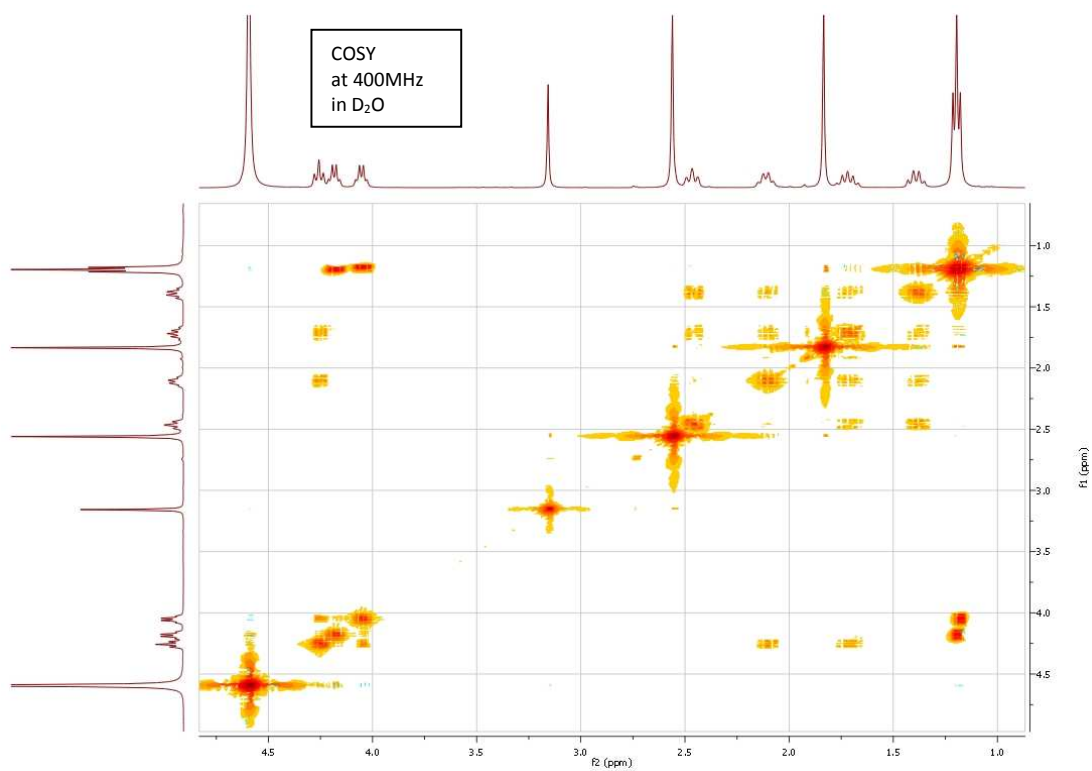
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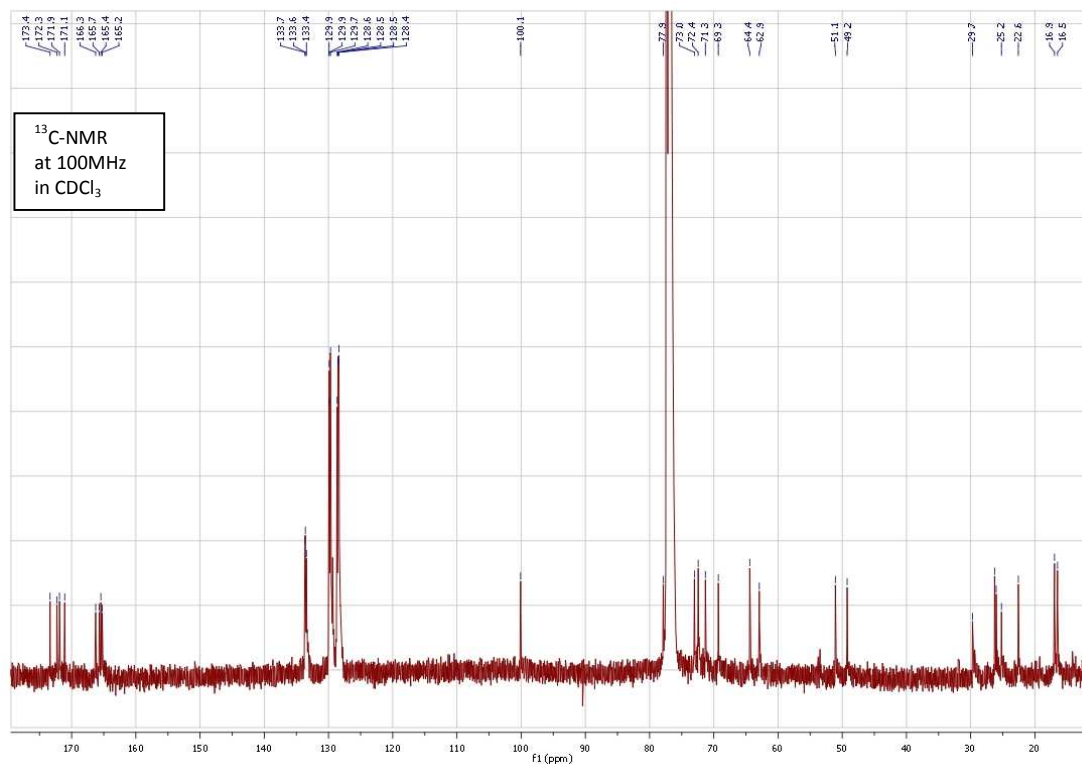
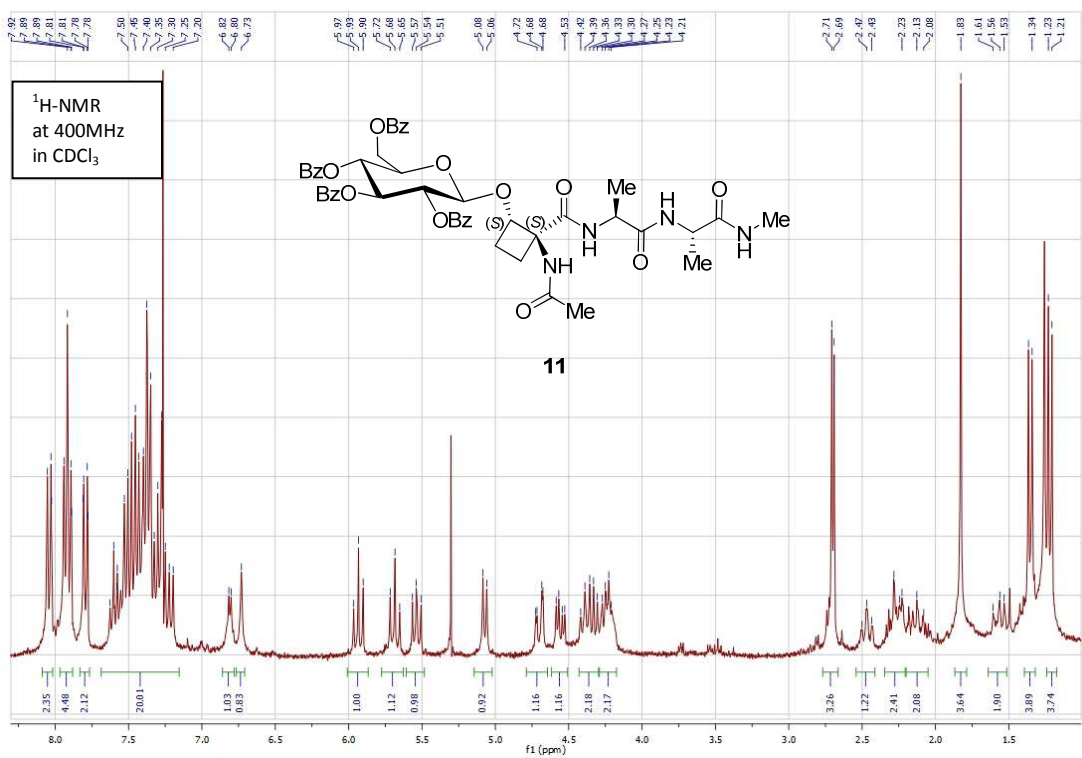
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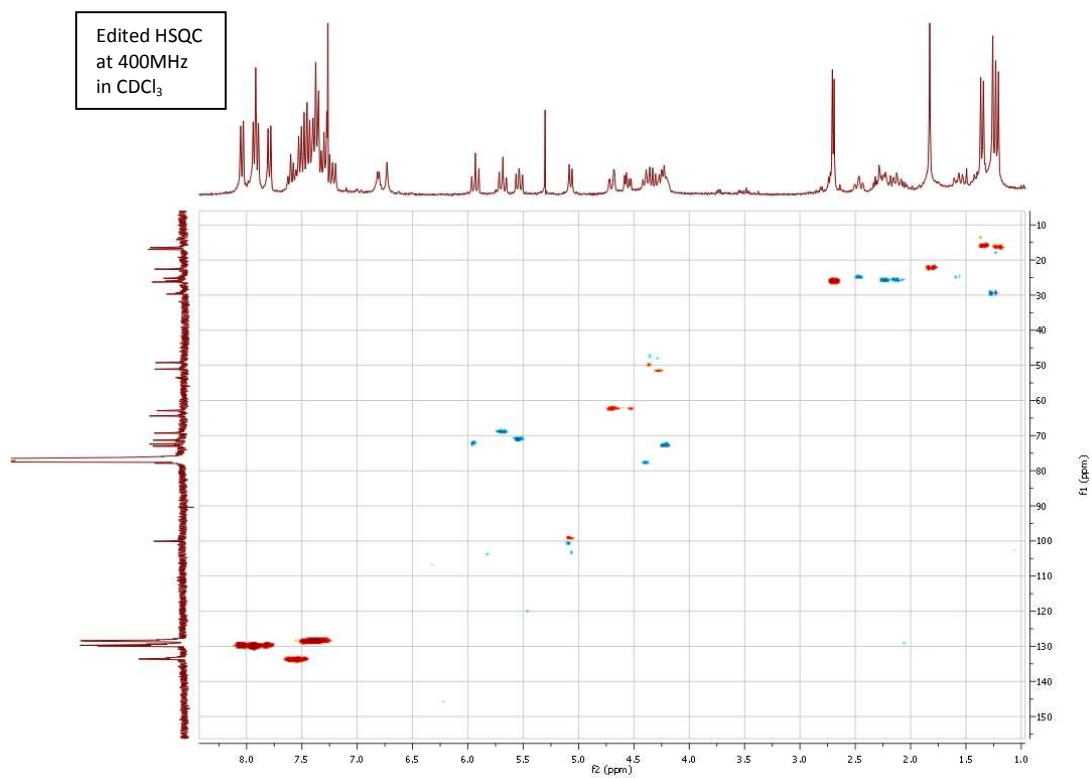
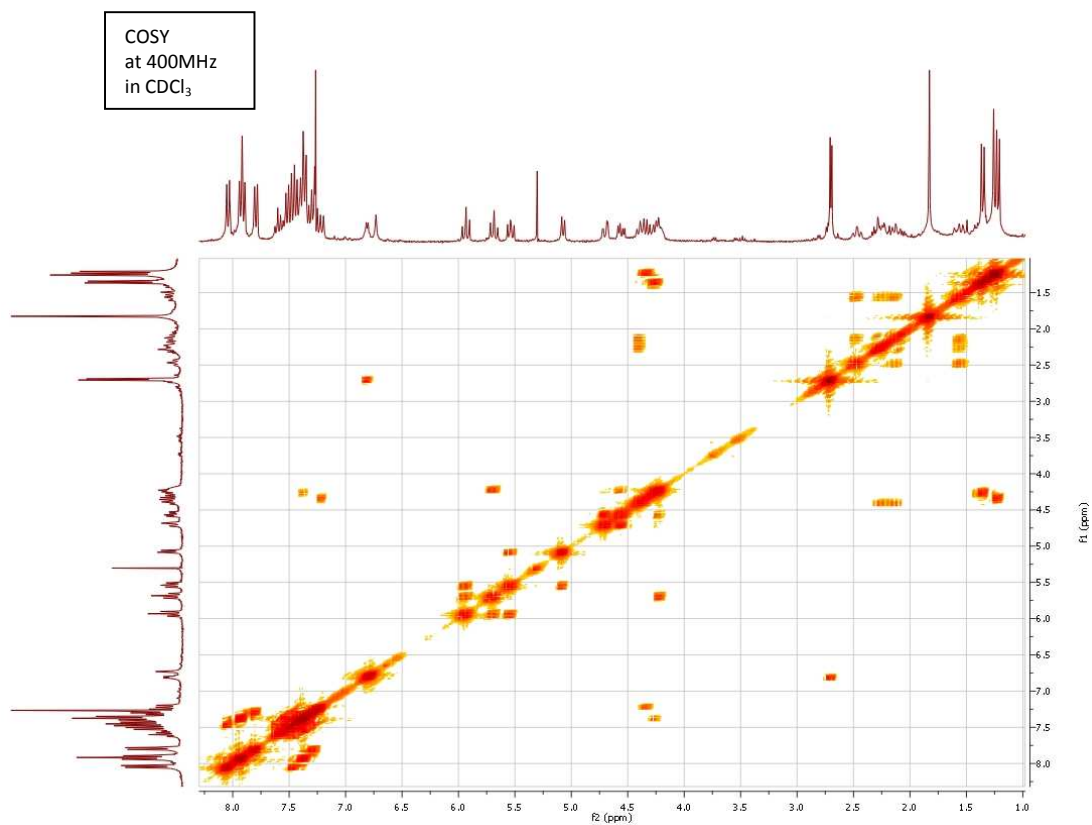


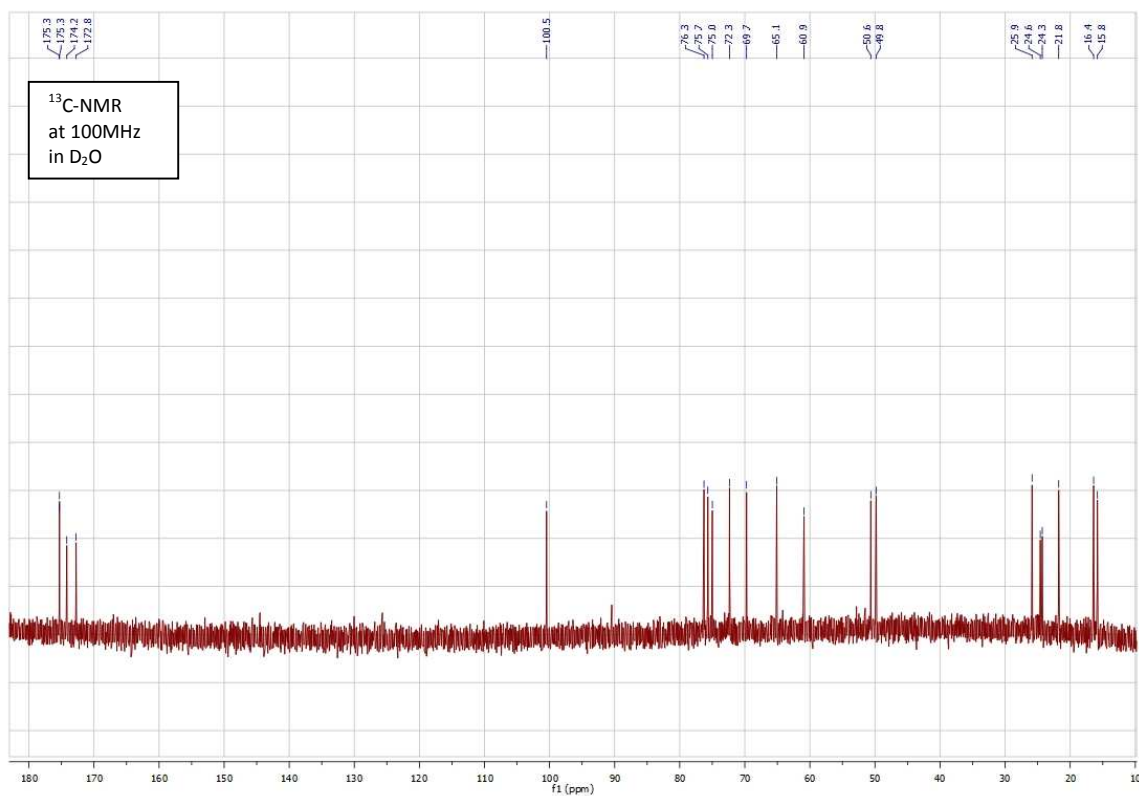
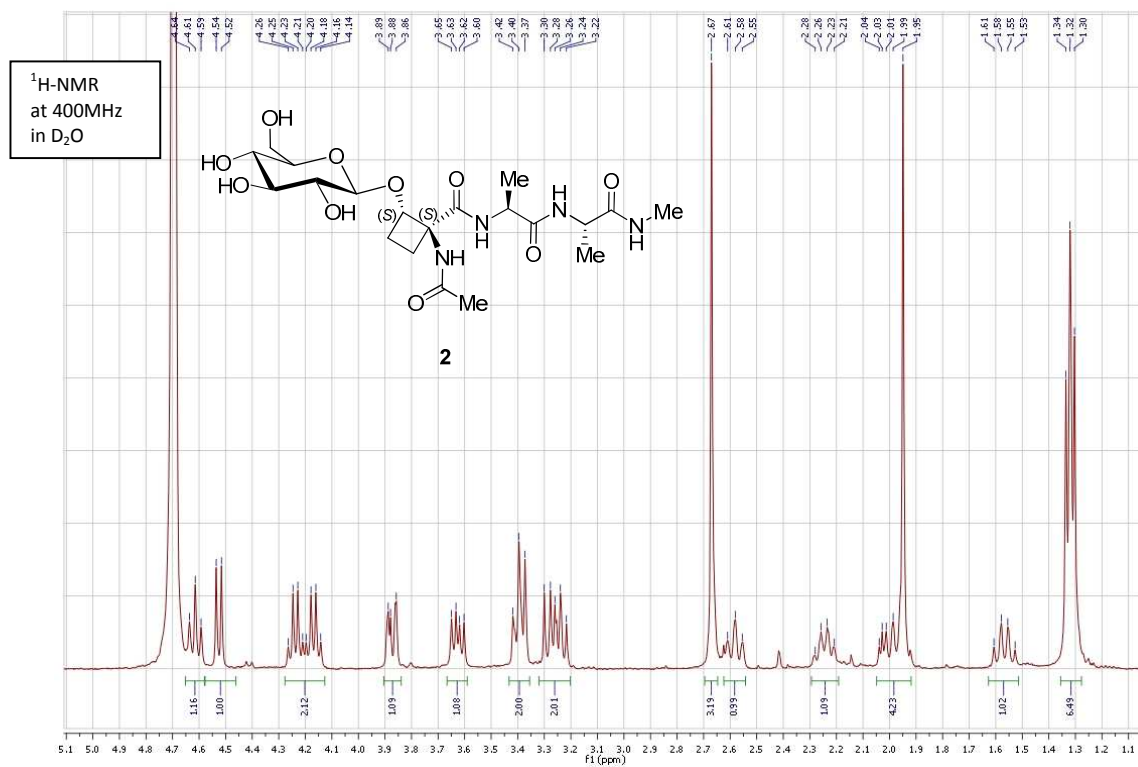


S10



S11





S13

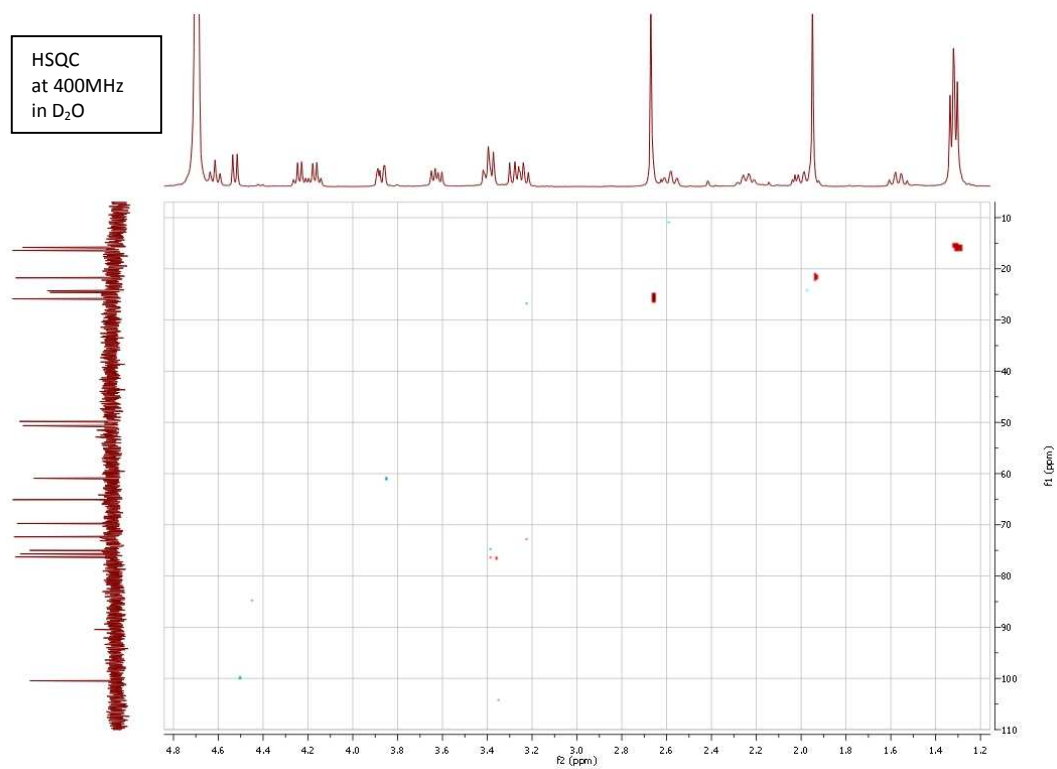
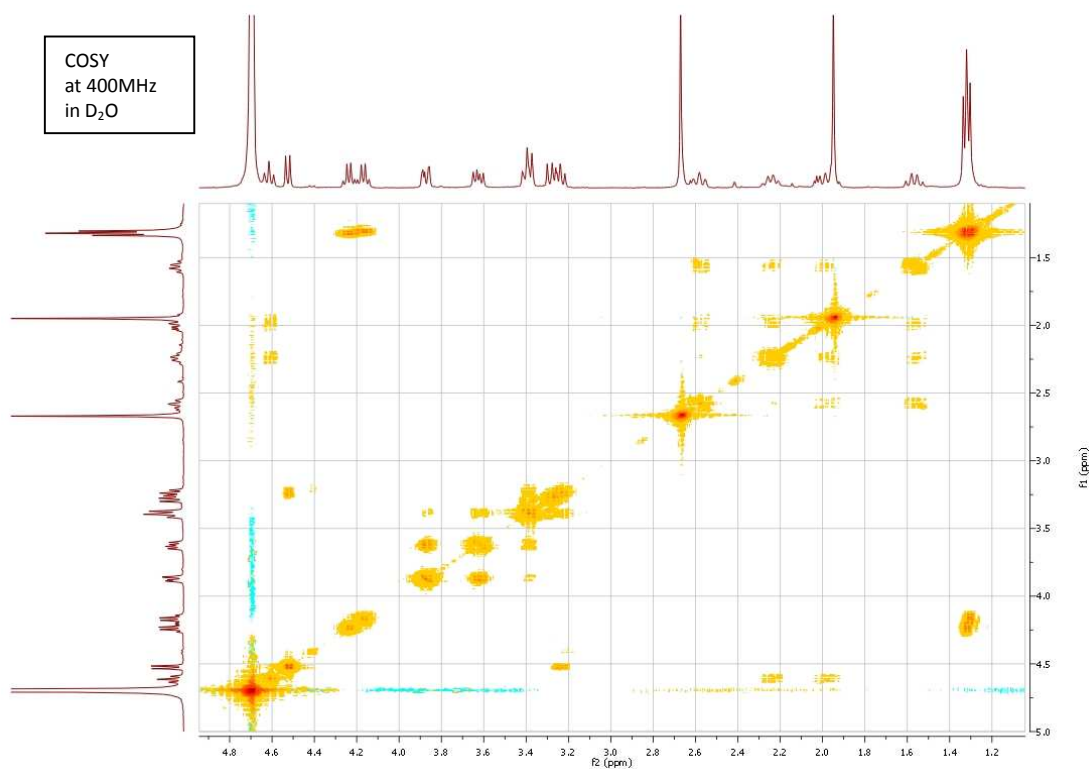
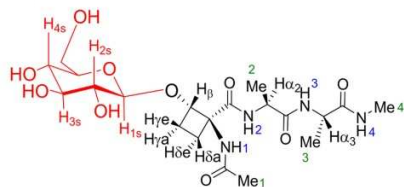


Table S1. Full assignment of protons and $^nJ_{\text{H,H}}$ couplings for **2^a**



δ (in ppm)	proton	splitting ^b (# protons)	$^nJ_{\text{H,H}}$ (in Hz)
1.28-1.35	Me2, Me3	m (6H)	--
1.57	H δ a	m (1H)	--
1.95	Me1	s (3H)	--
1.95-2.06	H γ a	m (1H)	--
2.25	H γ e	m (1H)	--
2.54-2.63	H δ e	m (1H)	--
2.67	Me4	s (3H)	--
3.20-3.32	H2s ^c , H4s ^c	m (2H)	--
3.35-3.44	H3s ^c , H5s ^c	m (2H)	--
3.59-3.67	H6s ^c	m (1H)	--
3.84-3.90	H6s ^c	m (1H)	--
4.17	H α 3	q (1H)	$^3J_{\text{H}\alpha 3, \text{Me}3}=7.3$
4.24	H α 2	q (1H)	$^3J_{\text{H}\alpha 2, \text{Me}2}=7.2$
4.53	H1s	d (1H)	$^3J_{\text{H}1\text{s}, \text{H}2\text{s}}=7.9$
4.61	H β	't' (1H)	$^3J_{\text{H}\beta, \text{H}\gamma}=8.8$
7.52-7.59 ^d	NH4 ^d	m (1H) ^d	--
7.72 ^d	NH3 ^d	d (1H) ^d	$^3J_{\text{H}3, \text{H}\alpha 3}=6.7^{\text{d}}$
8.37 ^d	NH2 ^d	d (1H) ^d	$^3J_{\text{H}2, \text{H}\alpha 2}=5.6^{\text{d}}$
8.87 ^d	NH1 ^d	s (1H) ^d	--

^a Data extracted from 1D ^1H NMR experiment carried out in D_2O (20 °C, pH = 5.2) at 400 MHz.

^b s = singlet, d = doublet, q = quartet, m = multiplet.

^c Letter 's' makes reference to sugar moiety.

^d Data extracted from 1D ^1H NMR experiment carried out in $\text{H}_2\text{O}/\text{D}_2\text{O}$ (9/1) (20 °C, pH = 5.2) at 400 MHz.

Figure S1. Sections of the 800 ms 2D NOESY spectra (400 MHz) in H₂O/D₂O (9:1) at 25 °C and pH = 4.90 of compound **2**.

