

Effect of Steric Constraint at the γ -Backbone Position on the Conformations and Hybridization Properties of PNAs

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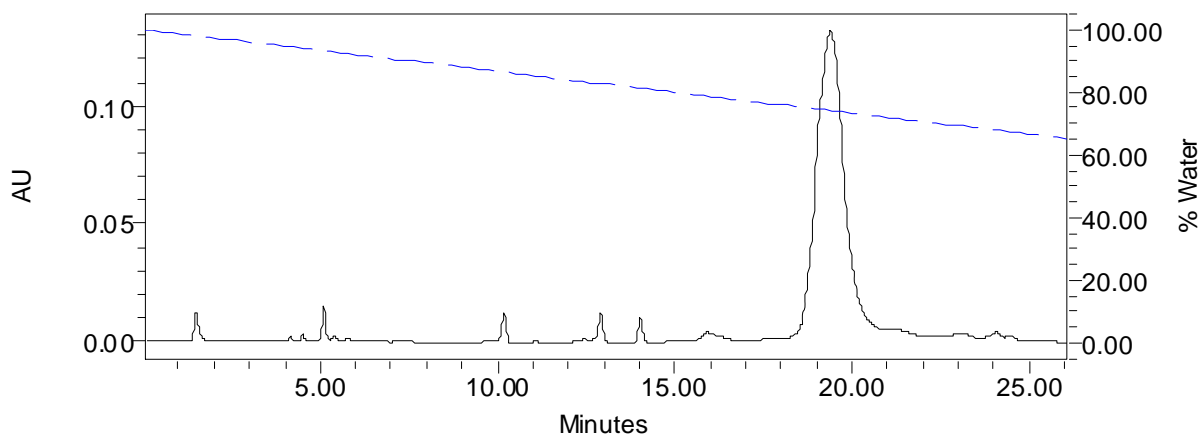


Figure S1. HPLC trace of the crude PNA7 oligomer. Eluent A: 0.1% TFA in water and eluent B: 0.1% TFA in ACN. The gradient was 0-40% of eluent B in 40 minutes at 45°C with a flow rate of 3.0 mL/min.

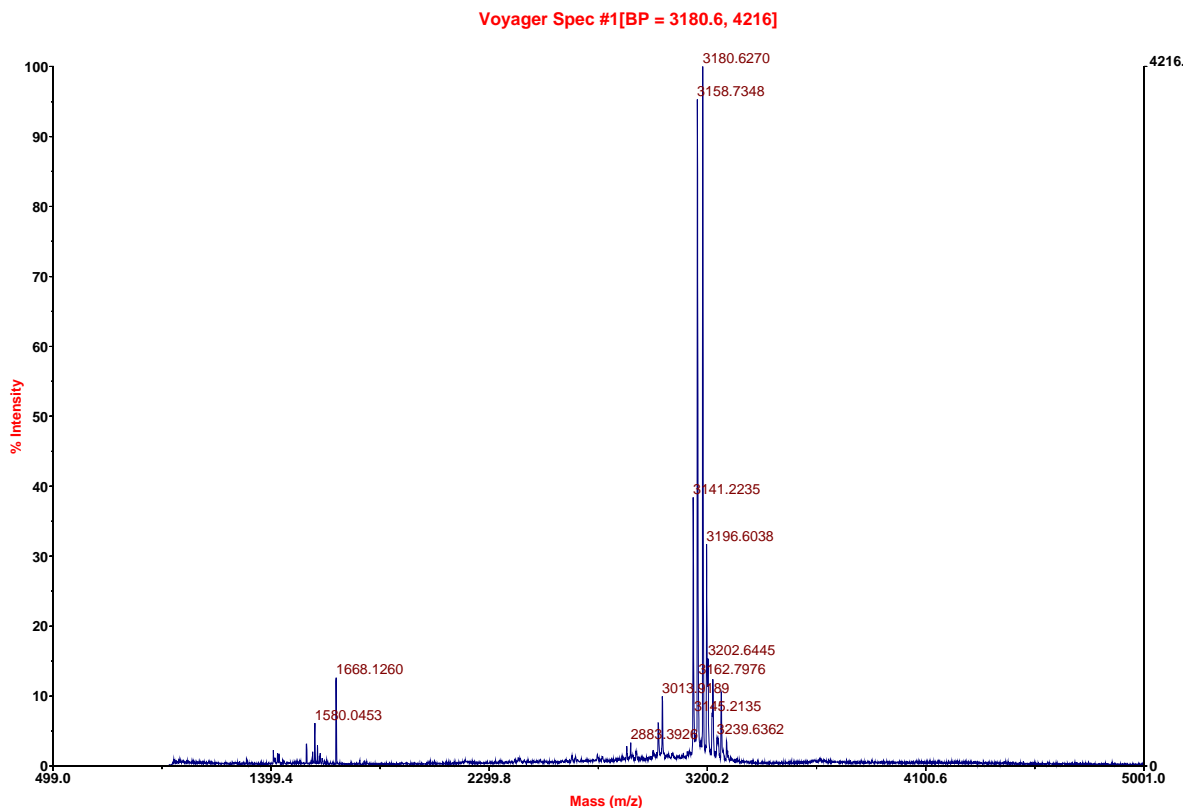


Figure S2. MALDI-TOF profile of PNA7 oligomer. Mass calculated: 3157.0, observed 3158.73, 3180.63 ($3157.0 + \text{Na}^+$), and 1668.13 (1/2 mass).

<i>Oligomer Name</i>	<i>Mass Calculated (m/z)</i>	<i>Experimental Mass (m/z)</i>
PNA1 (Unmodified)	2887	2885
PNA2 (Alanine Mod)	2901	2899
PNA3 (Valine Mod)	2929	2927
PNA4 (Isoleucine Mod)	2943	2942
PNA5 (Phenylalanine Mod)	2977	2976
PNA6 (Phenylalanine 3 Alt Mod)	3157	3158
PNA7 (Phenylalanine 3 Con Mod)	3157	3158
PNA8 (Valine 3 Alt Mod)	3011	3008
PNA9 (Valine 3 Con Mod)	3011	3008

Figure S3. Calculated and observed masses (MALDI-TOF MS) for the PNA and γ -Modified PNA oligomers utilized in the studies.

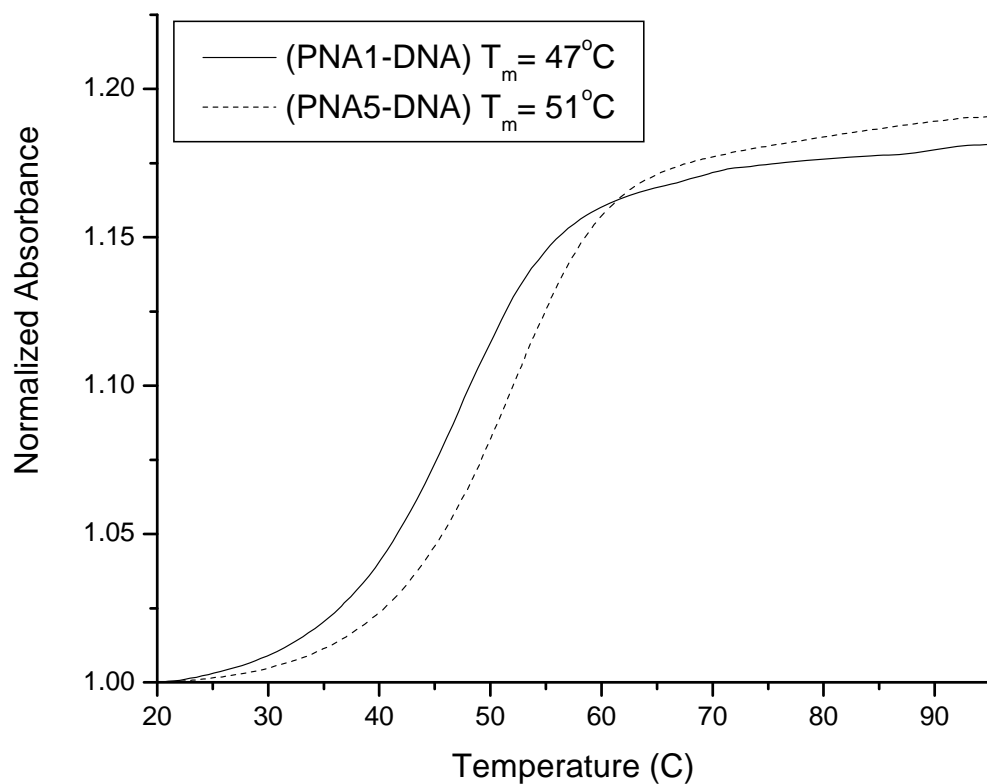


Figure S4. UV-melting curves of PNA1-DNA and PNA5-DNA duplexes containing perfectly matched sequences. The samples were prepared in buffer containing 0.1 mM EDTA, 100 mM NaCl, 10 mM sodium phosphate (pH 7.0) at $5\mu\text{M}$ duplex strand concentration each. The T_m s were determined by taking the first derivatives of the UV-melting curves.

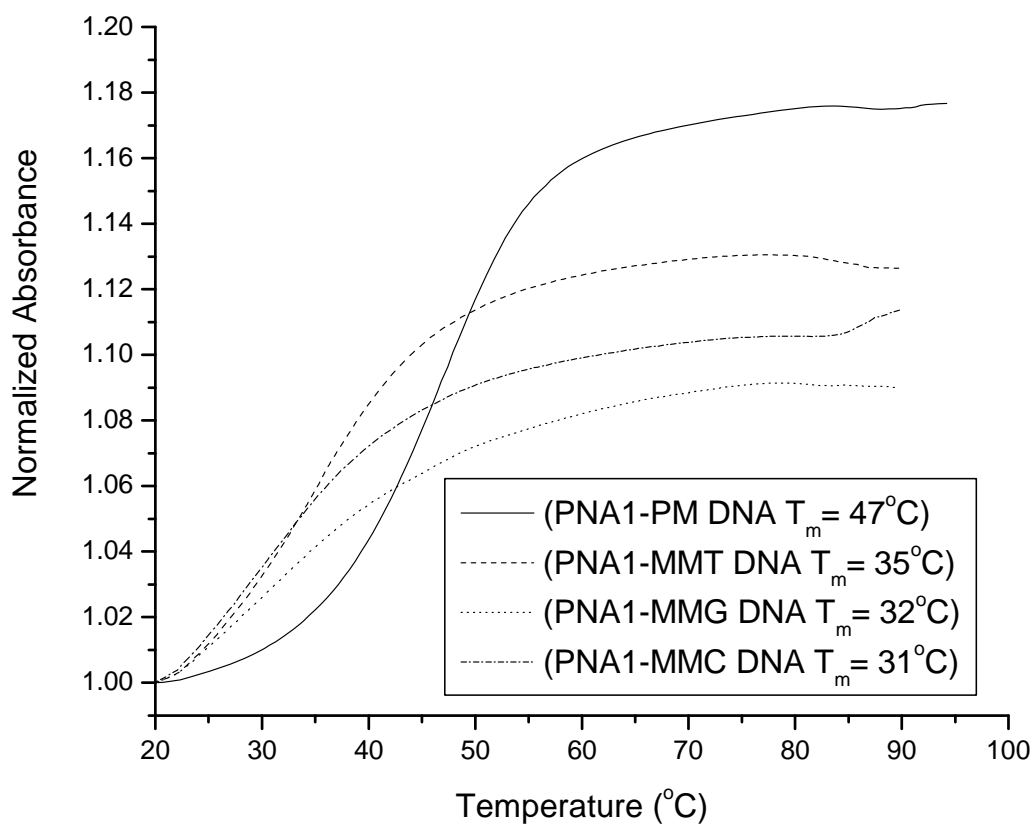


Figure S5. UV-melting curves of PNA1-DNA duplexes containing perfectly matched (PM) and mismatch (MM) sequences. The samples were prepared in buffer containing 0.1 mM EDTA, 100 mM NaCl, 10 mM sodium phosphate (pH 7.0) at 5 μM duplex strand concentration each. The T_m s were determined by taking the first derivatives of the UV-melting curves.

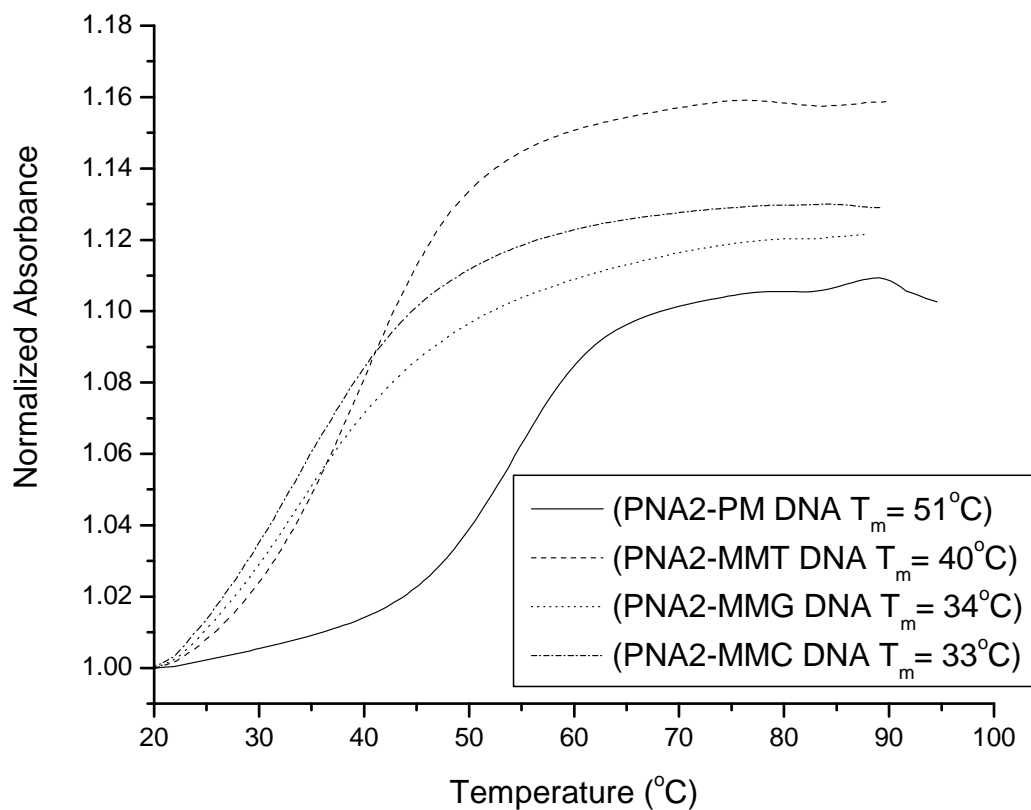


Figure S6. UV-melting curves of PNA2-DNA duplexes containing perfectly matched (PM) and mismatch (MM) sequences. The samples were prepared in buffer containing 0.1 mM EDTA, 100 mM NaCl, 10 mM sodium phosphate (pH 7.0) at 5 μ M duplex strand concentration each. The T_ms were determined by taking the first derivatives of the UV-melting curves.

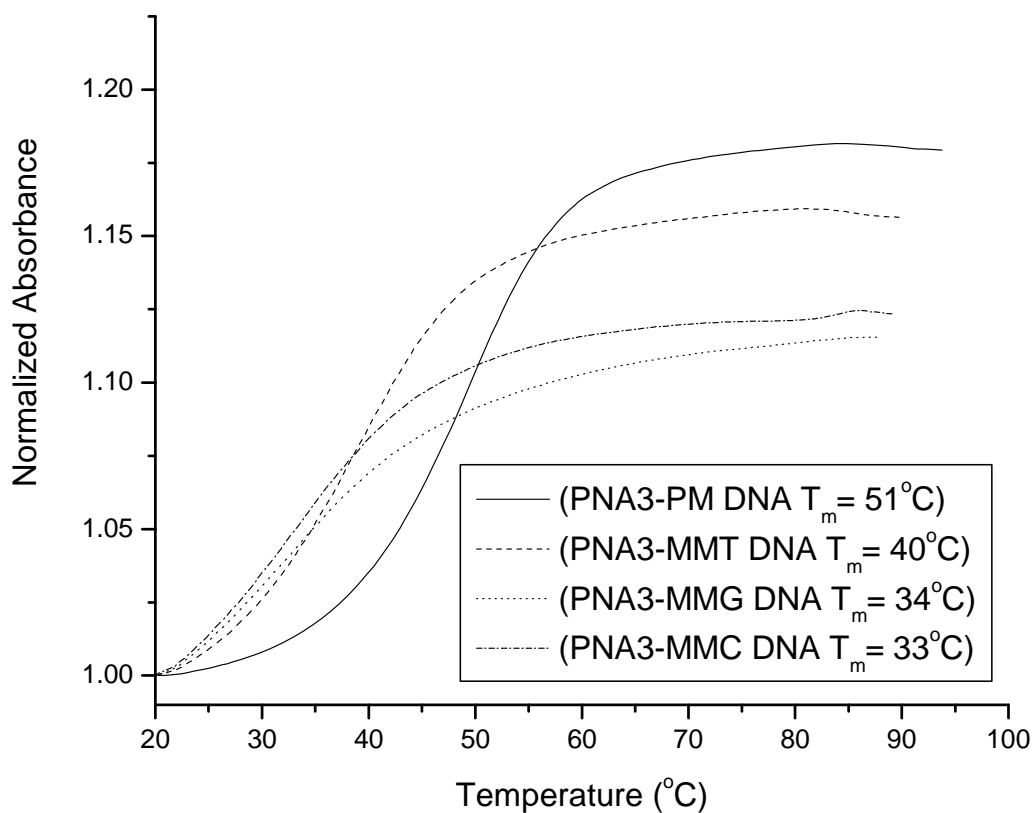


Figure S7. UV-melting curves of PNA3-DNA duplexes containing perfectly matched (PM) and mismatch (MM) sequences. The samples were prepared in buffer containing 0.1 mM EDTA, 100 mM NaCl, 10 mM sodium phosphate (pH 7.0) at 5 μ M duplex strand concentration each. The T_m s were determined by taking the first derivatives of the UV-melting curves.

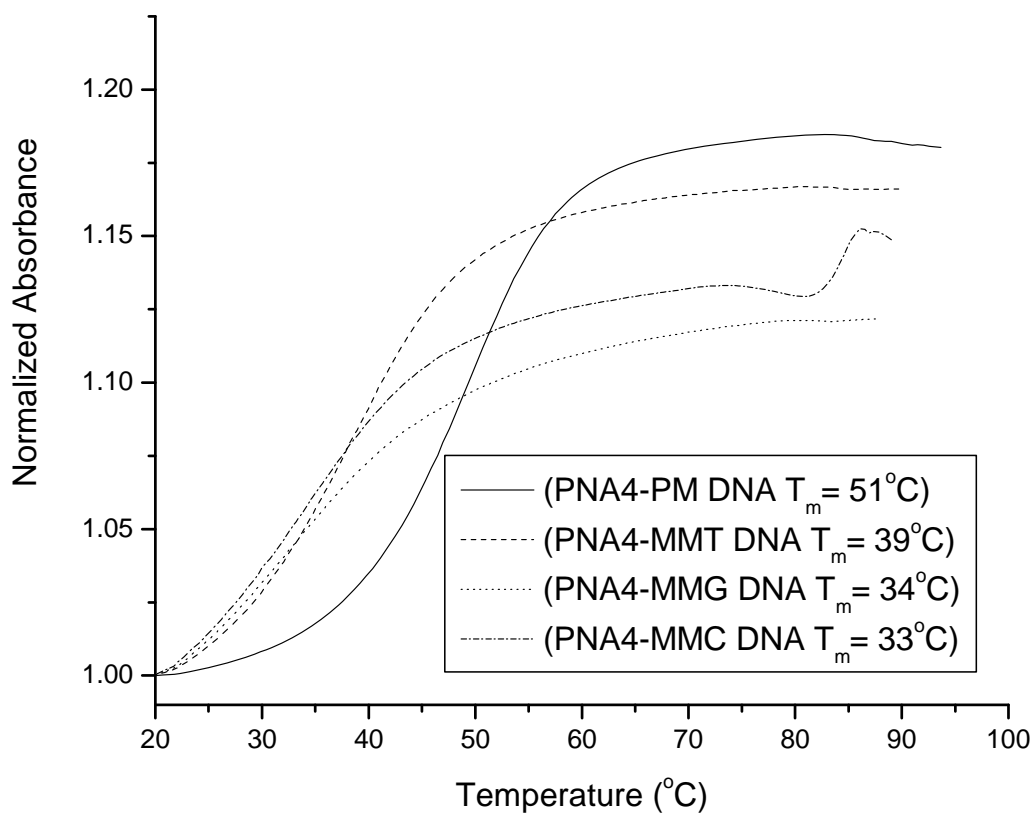


Figure S8. UV-melting curves of PNA4-DNA duplexes containing perfectly matched (PM) and mismatch (MM) sequences. The samples were prepared in buffer containing 0.1 mM EDTA, 100 mM NaCl, 10 mM sodium phosphate (pH 7.0) at 5 μM duplex strand concentration each. The T_m s were determined by taking the first derivatives of the UV-melting curves.

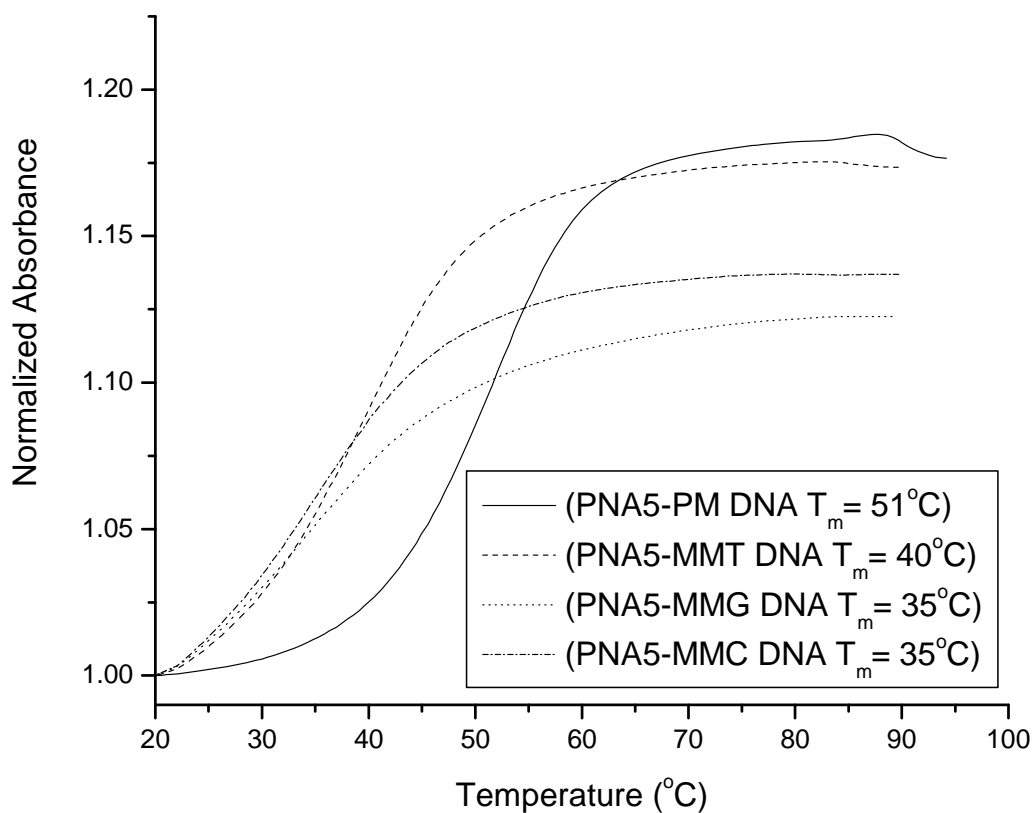


Figure S9. UV-melting curves of PNA5-DNA duplexes containing perfectly matched (PM) and mismatch (MM) sequences. The samples were prepared in buffer containing 0.1 mM EDTA, 100 mM NaCl, 10 mM sodium phosphate (pH 7.0) at $5\mu\text{M}$ duplex strand concentration each. The T_m s were determined by taking the first derivatives of the UV-melting curves.

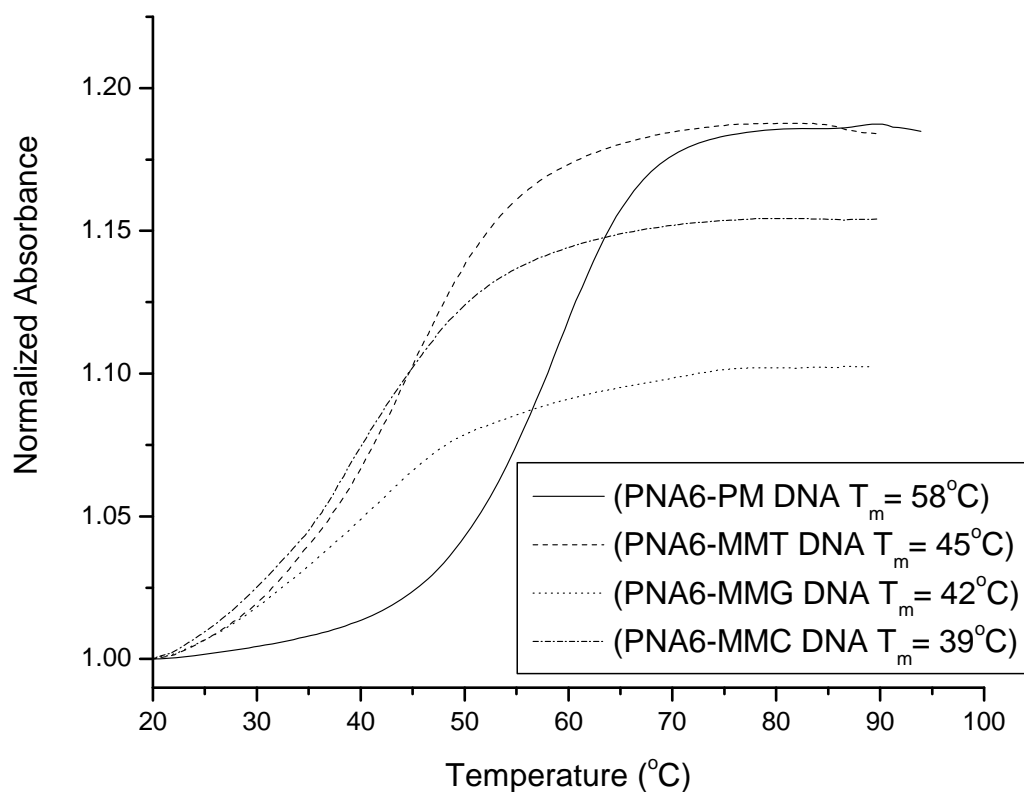


Figure S10. UV-melting curves of PNA6-DNA duplexes containing perfectly matched (PM) and mismatch (MM) sequences. The samples were prepared in buffer containing 0.1 mM EDTA, 100 mM NaCl, 10 mM sodium phosphate (pH 7.0) at $5\mu\text{M}$ duplex strand concentration each. The T_m s were determined by taking the first derivatives of the UV-melting curves.

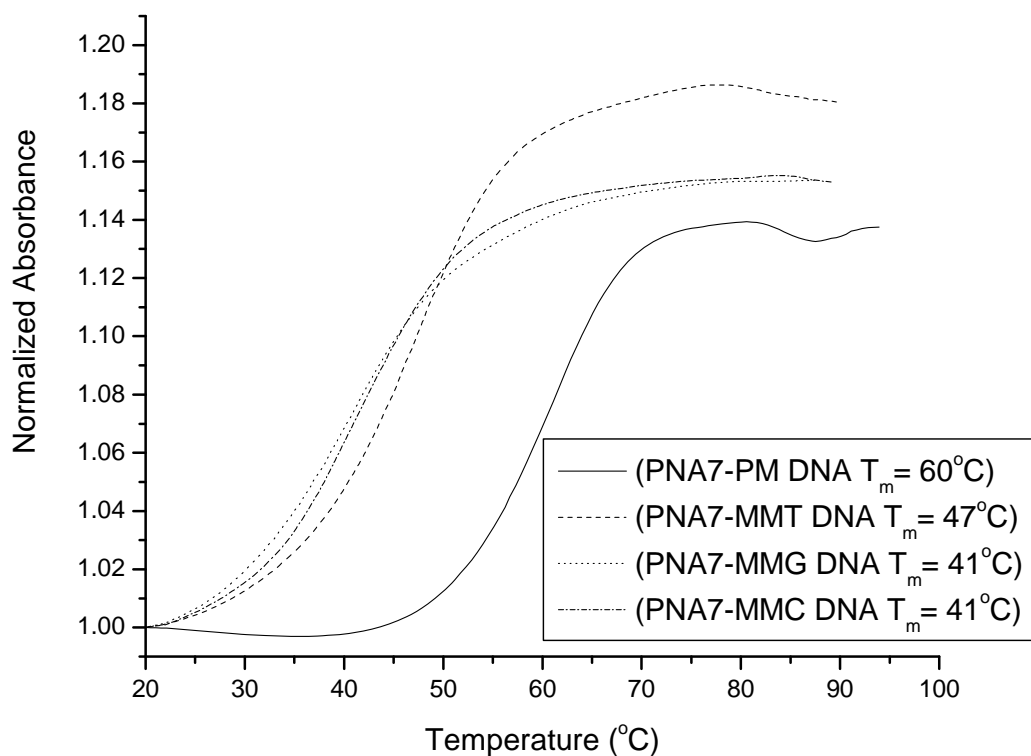


Figure S11. UV-melting curves of PNA7-DNA duplexes containing perfectly matched (PM) and mismatch (MM) sequences. The samples were prepared in buffer containing 0.1 mM EDTA, 100 mM NaCl, 10 mM sodium phosphate (pH 7.0) at $5\mu\text{M}$ duplex strand concentration each. The T_m s were determined by taking the first derivatives of the UV-melting curves.

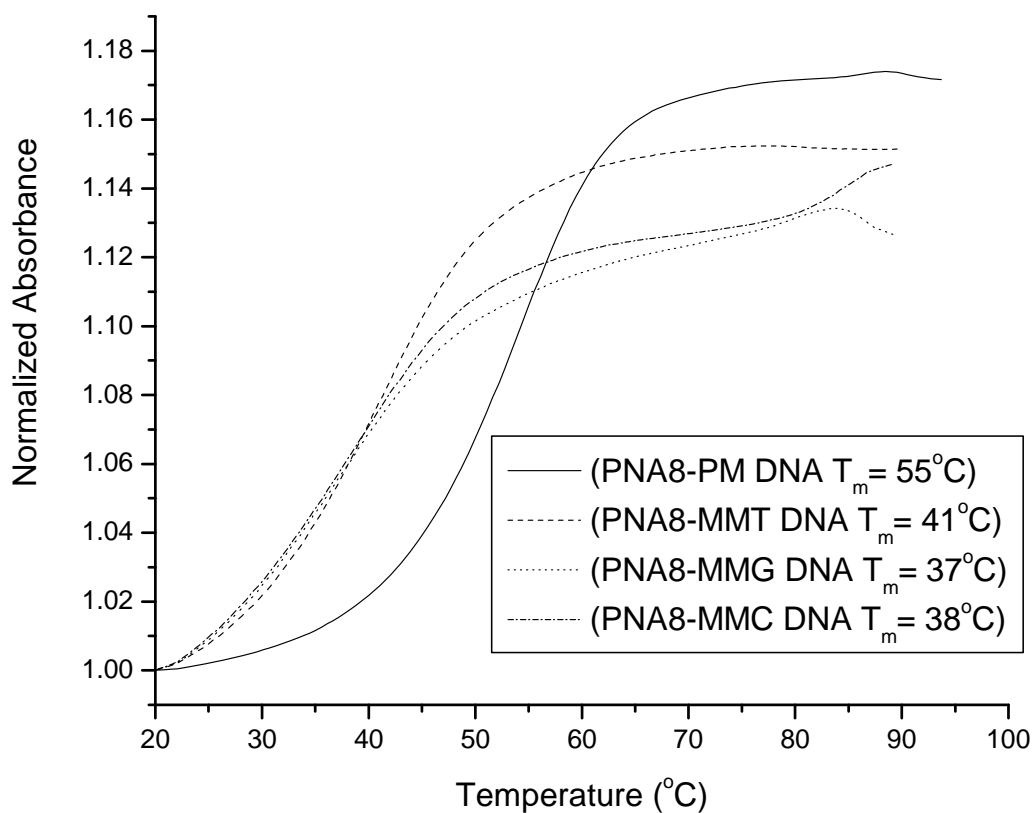


Figure S12. UV-melting curves of PNA8-DNA duplexes containing perfectly matched (PM) and mismatch (MM) sequences. The samples were prepared in buffer containing 0.1 mM EDTA, 100 mM NaCl, 10 mM sodium phosphate (pH 7.0) at 5 μM duplex strand concentration each. The T_m s were determined by taking the first derivatives of the UV-melting curves.

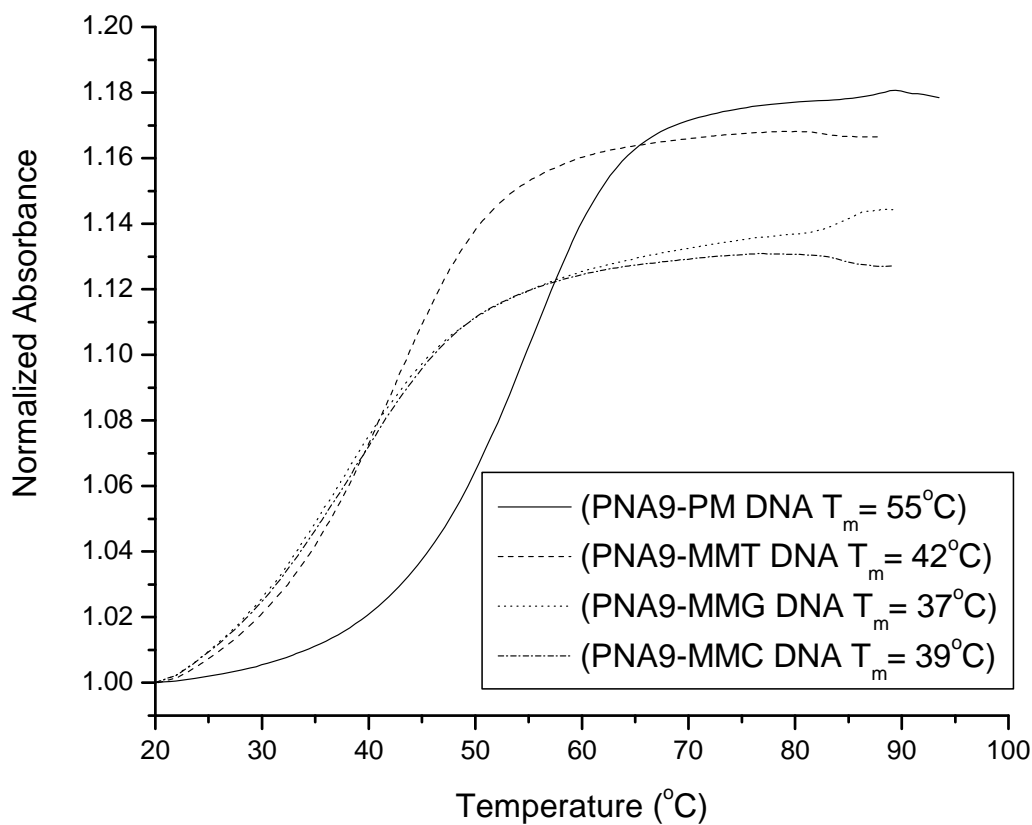
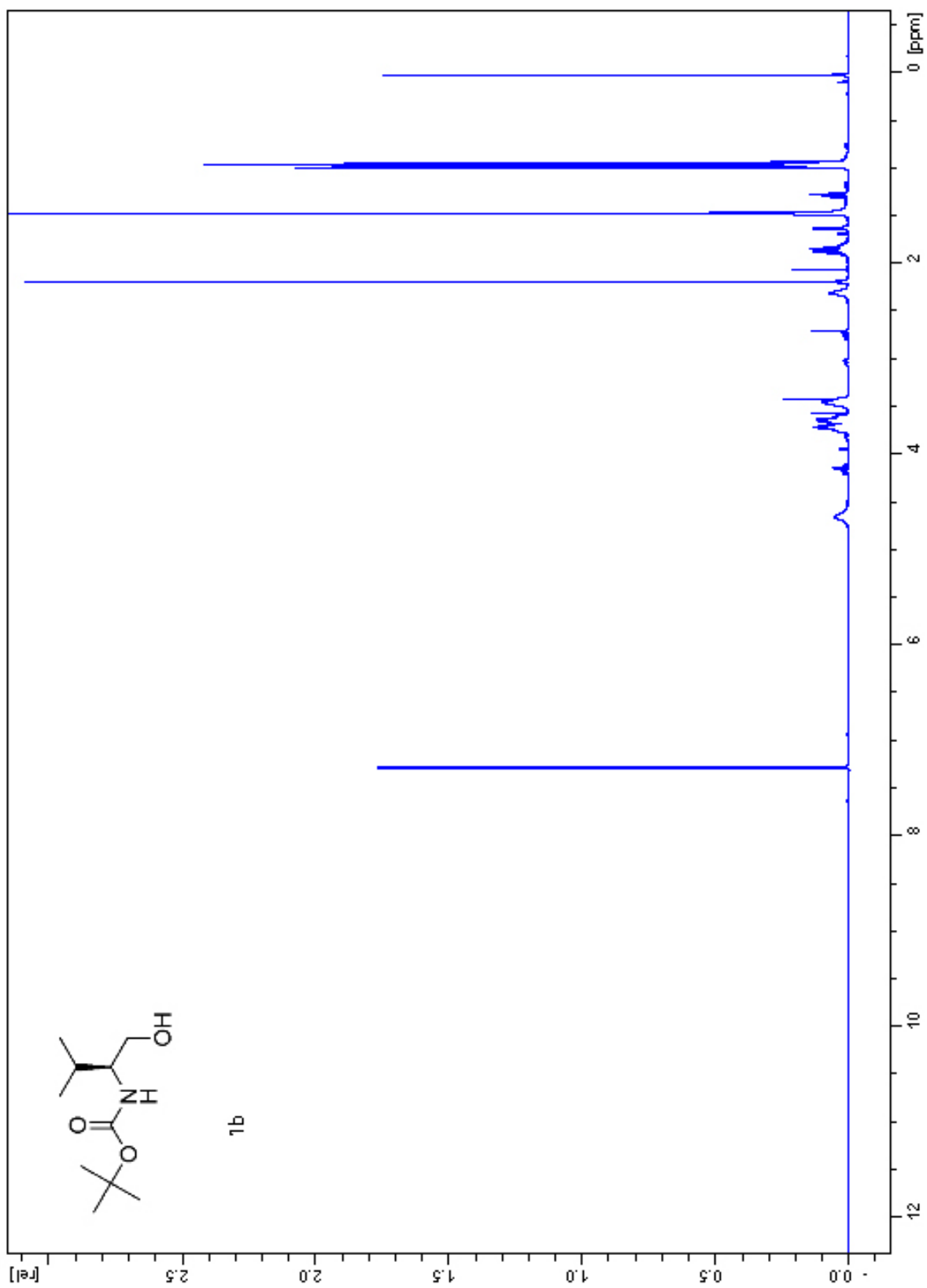
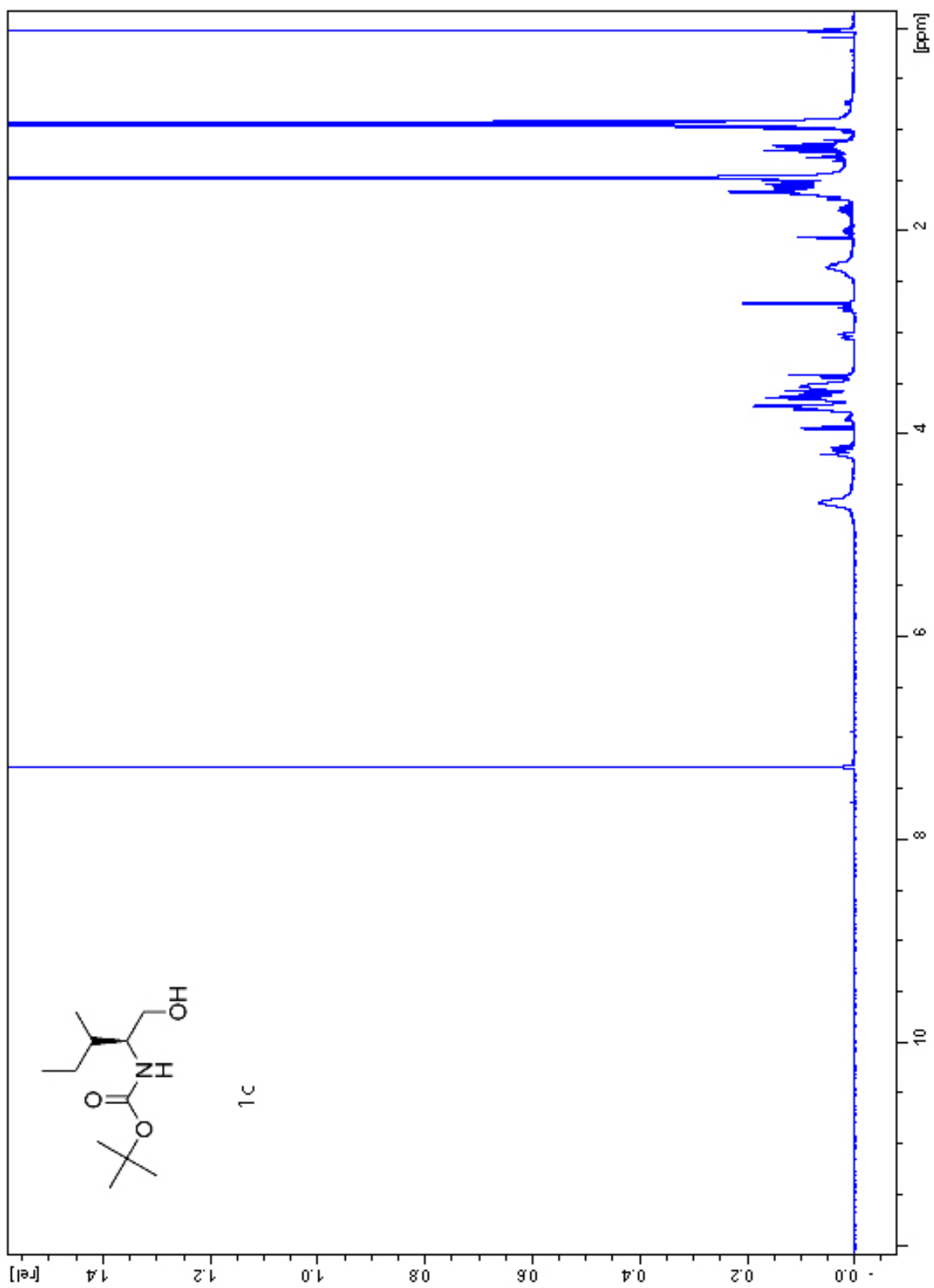
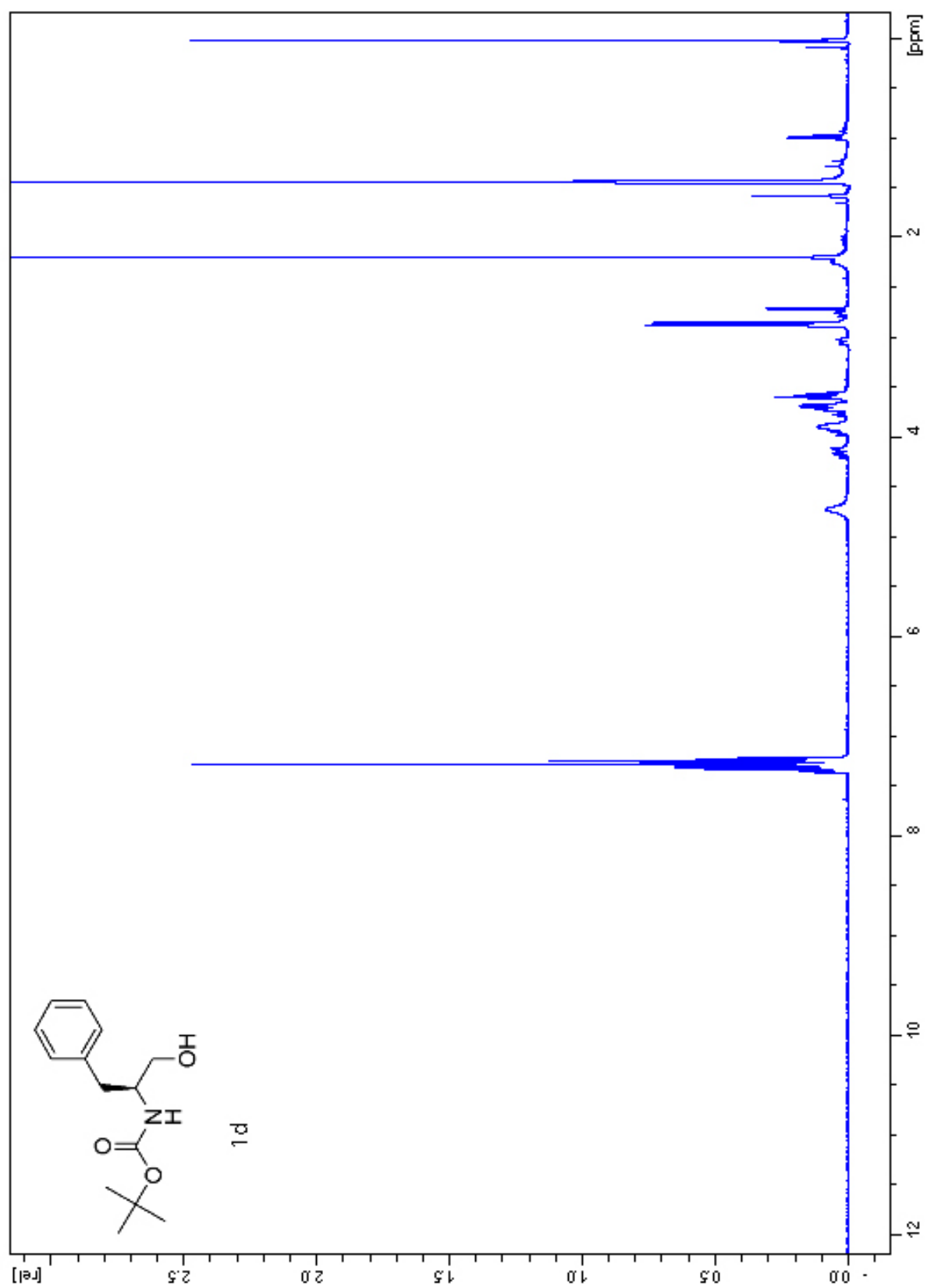
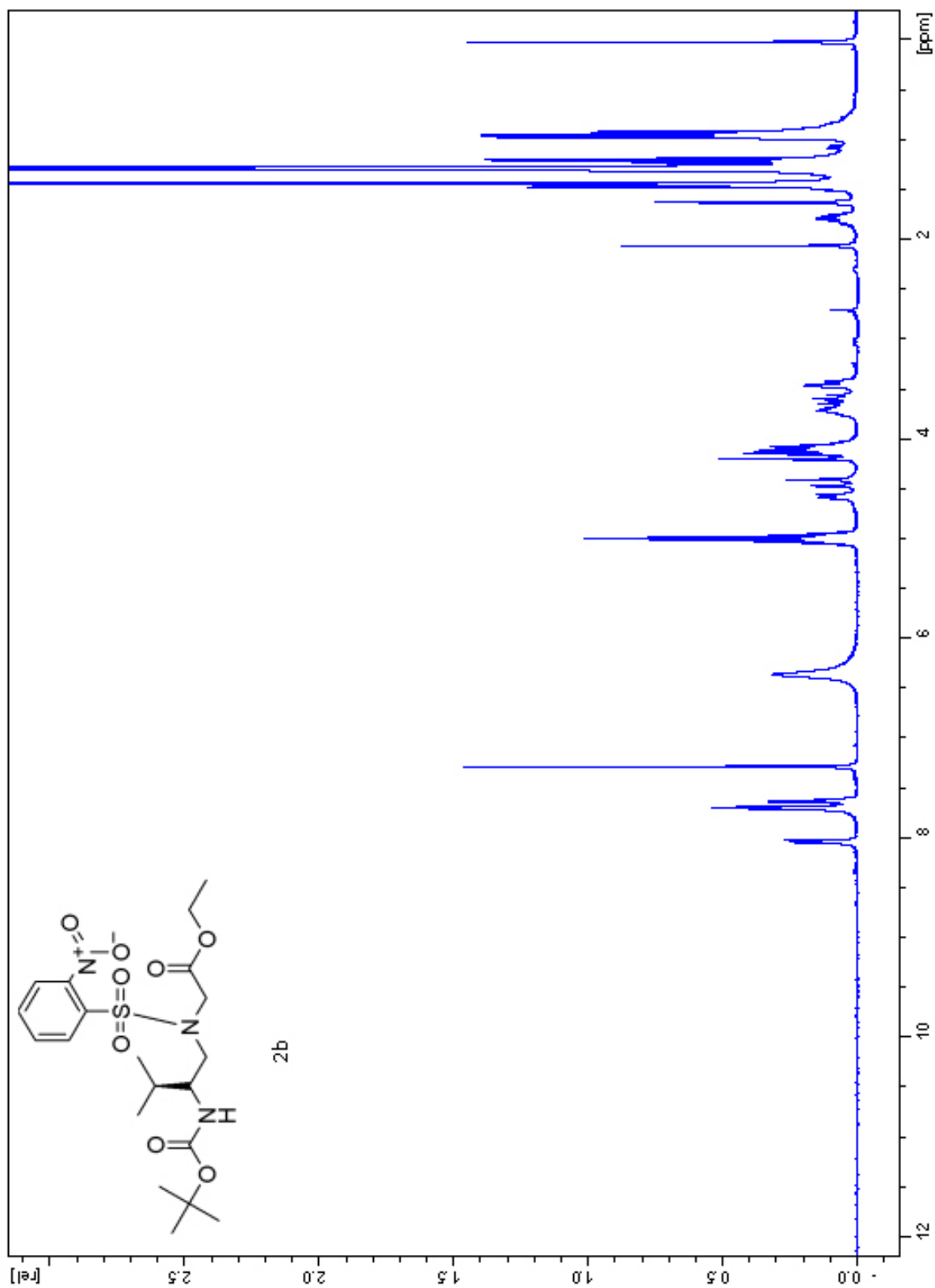


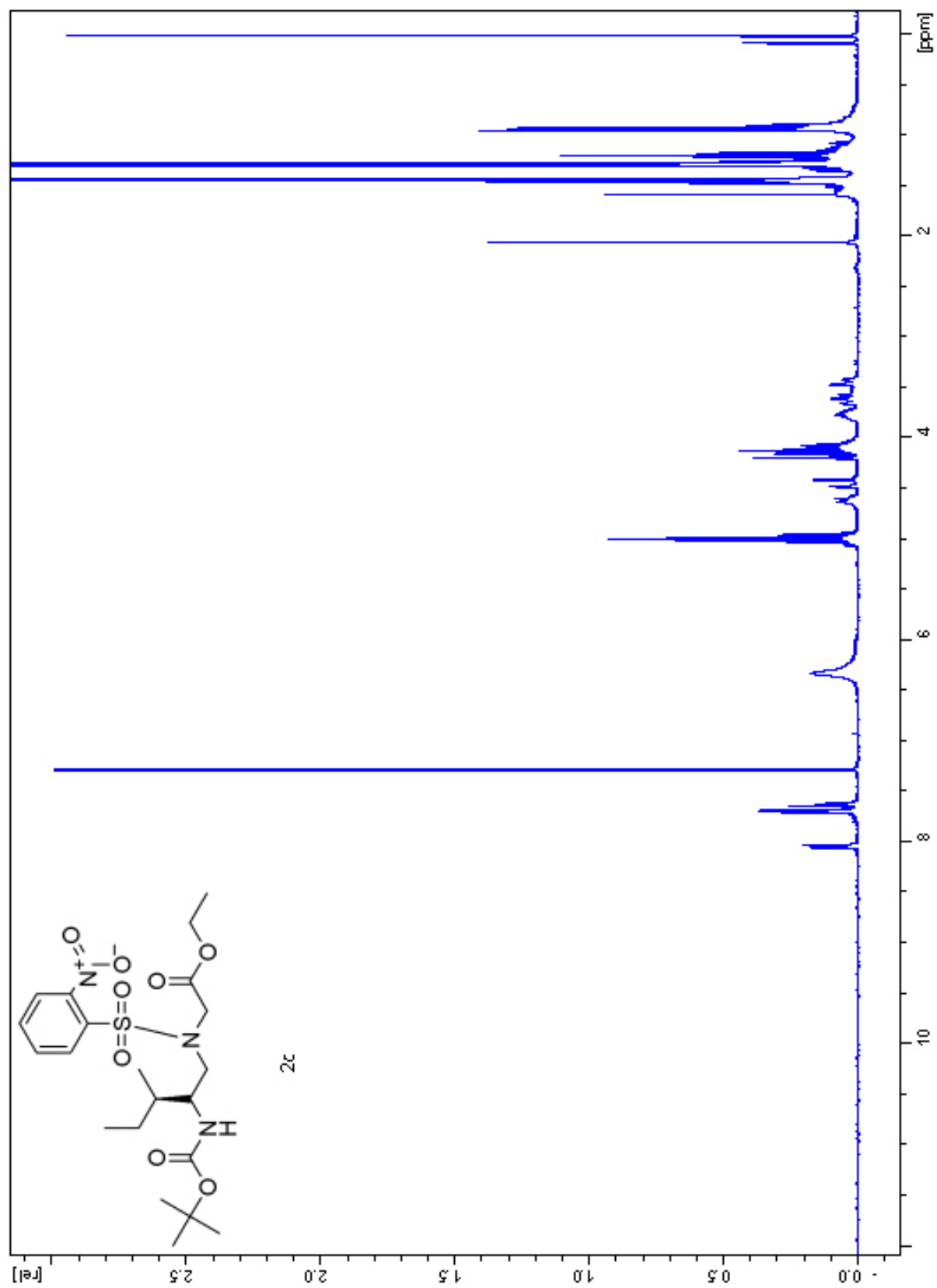
Figure S13. UV-melting curves of PNA9-DNA duplexes containing perfectly matched (PM) and mismatch (MM) sequences. The samples were prepared in buffer containing 0.1 mM EDTA, 100 mM NaCl, 10 mM sodium phosphate (pH 7.0) at 5 μM duplex strand concentration each. The T_m s were determined by taking the first derivatives of the UV-melting curves.

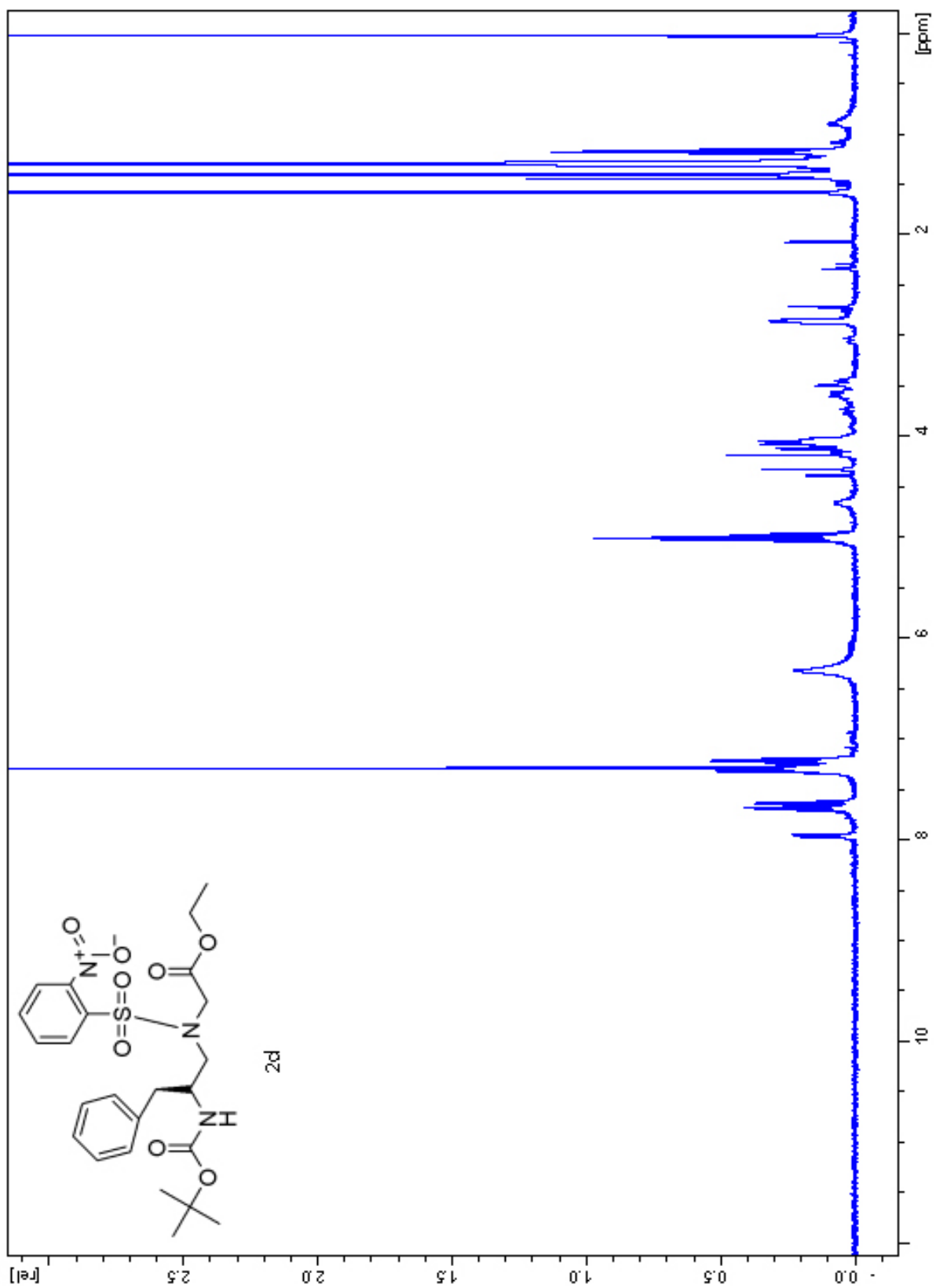
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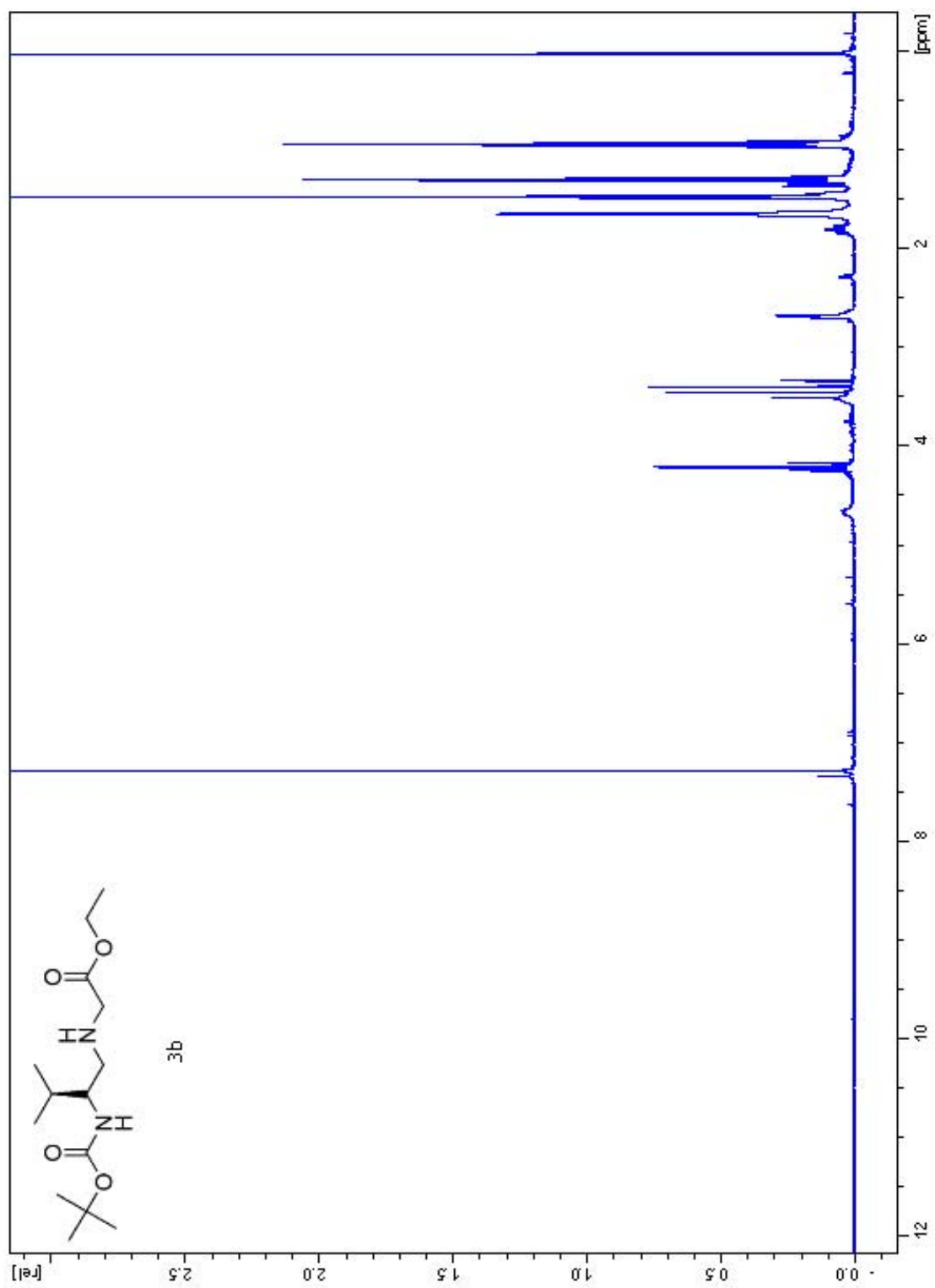
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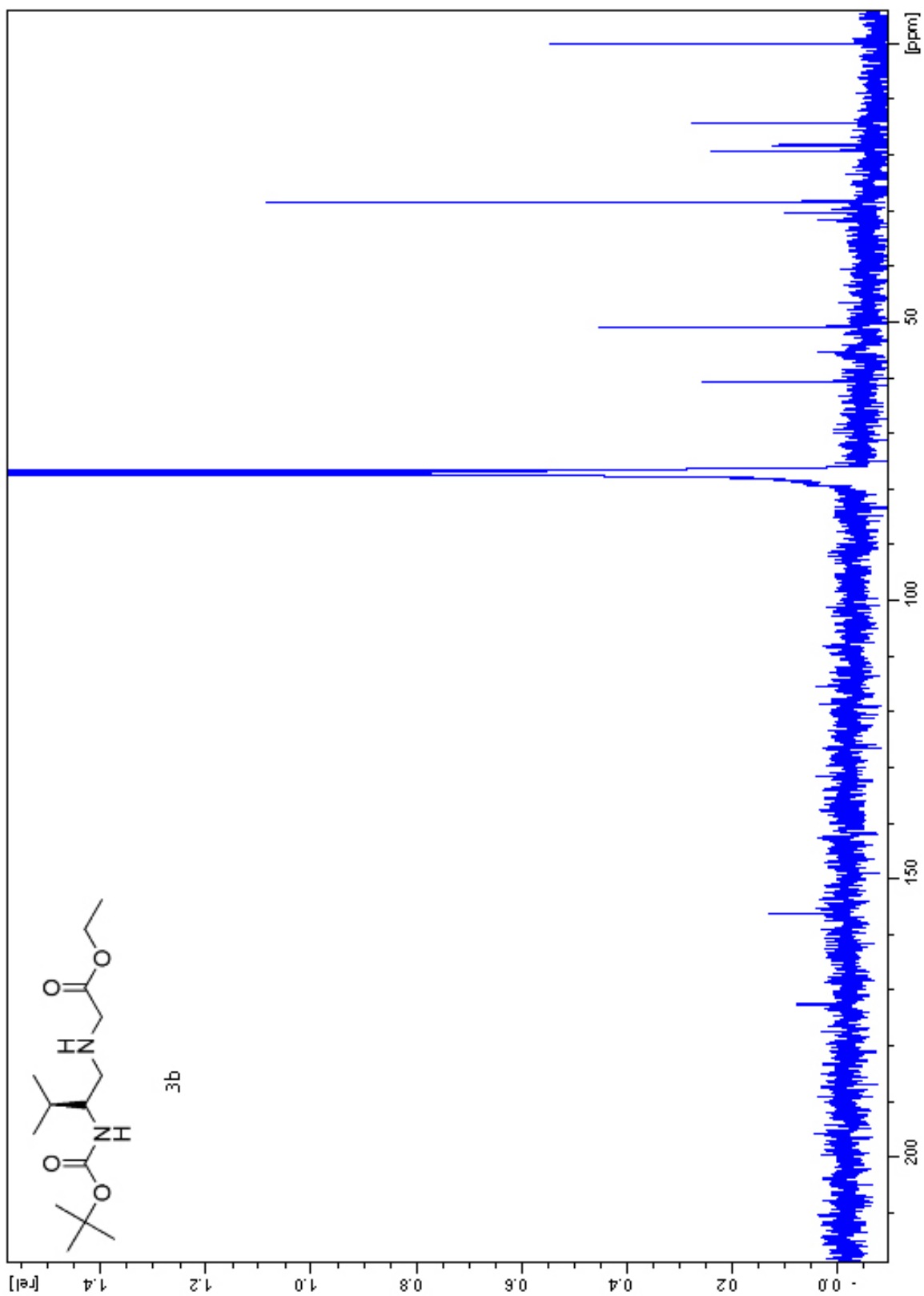
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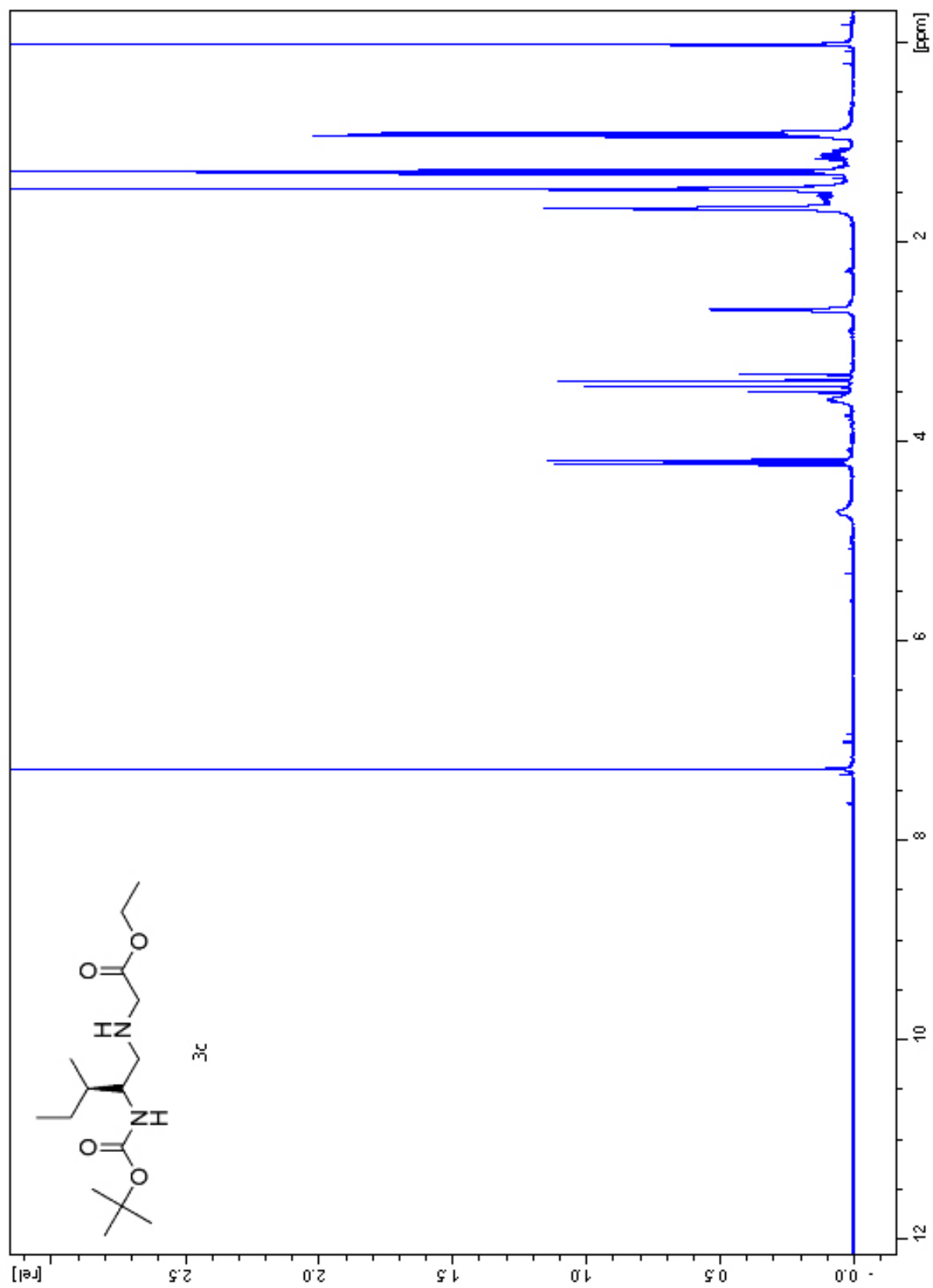
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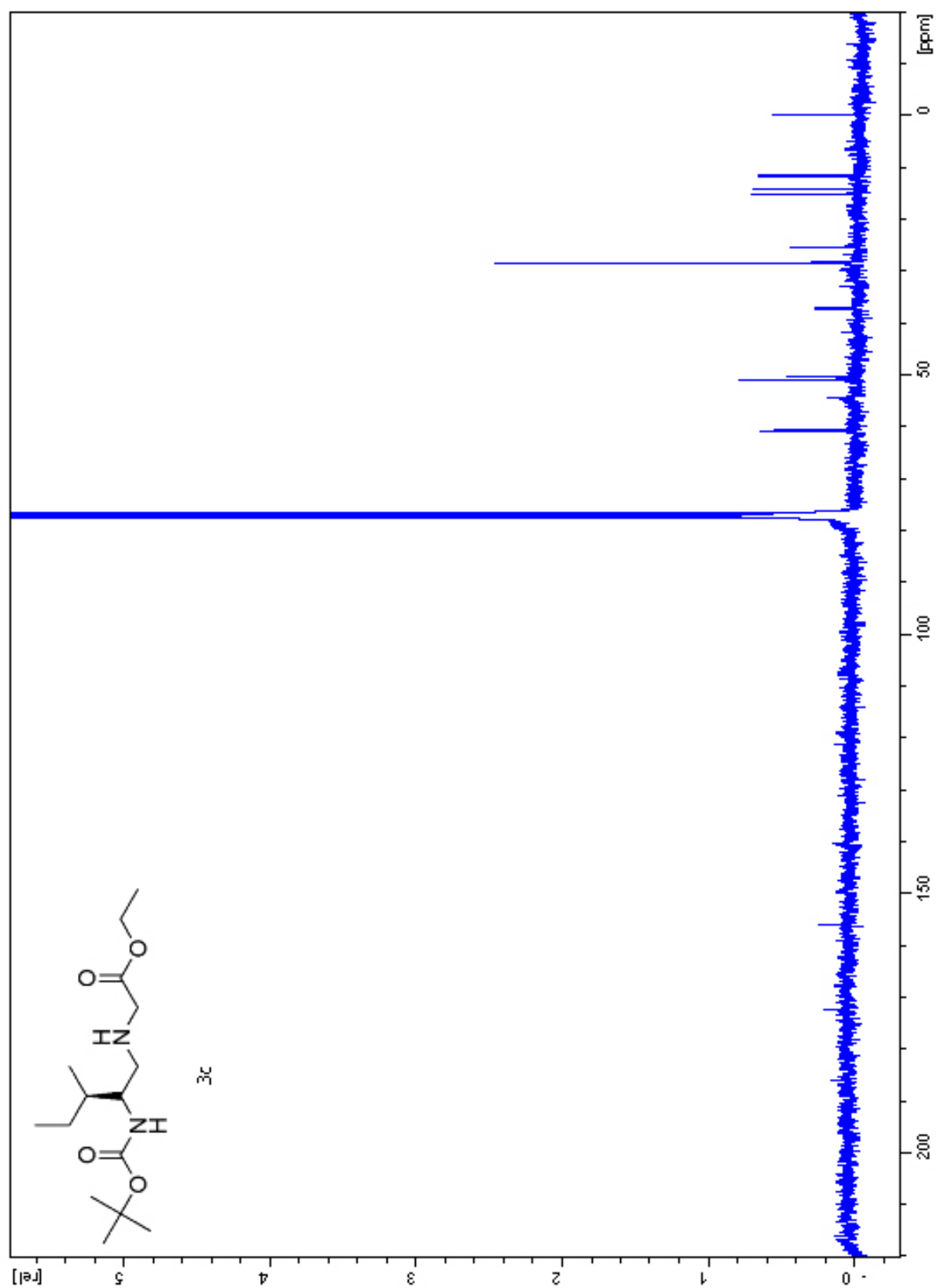
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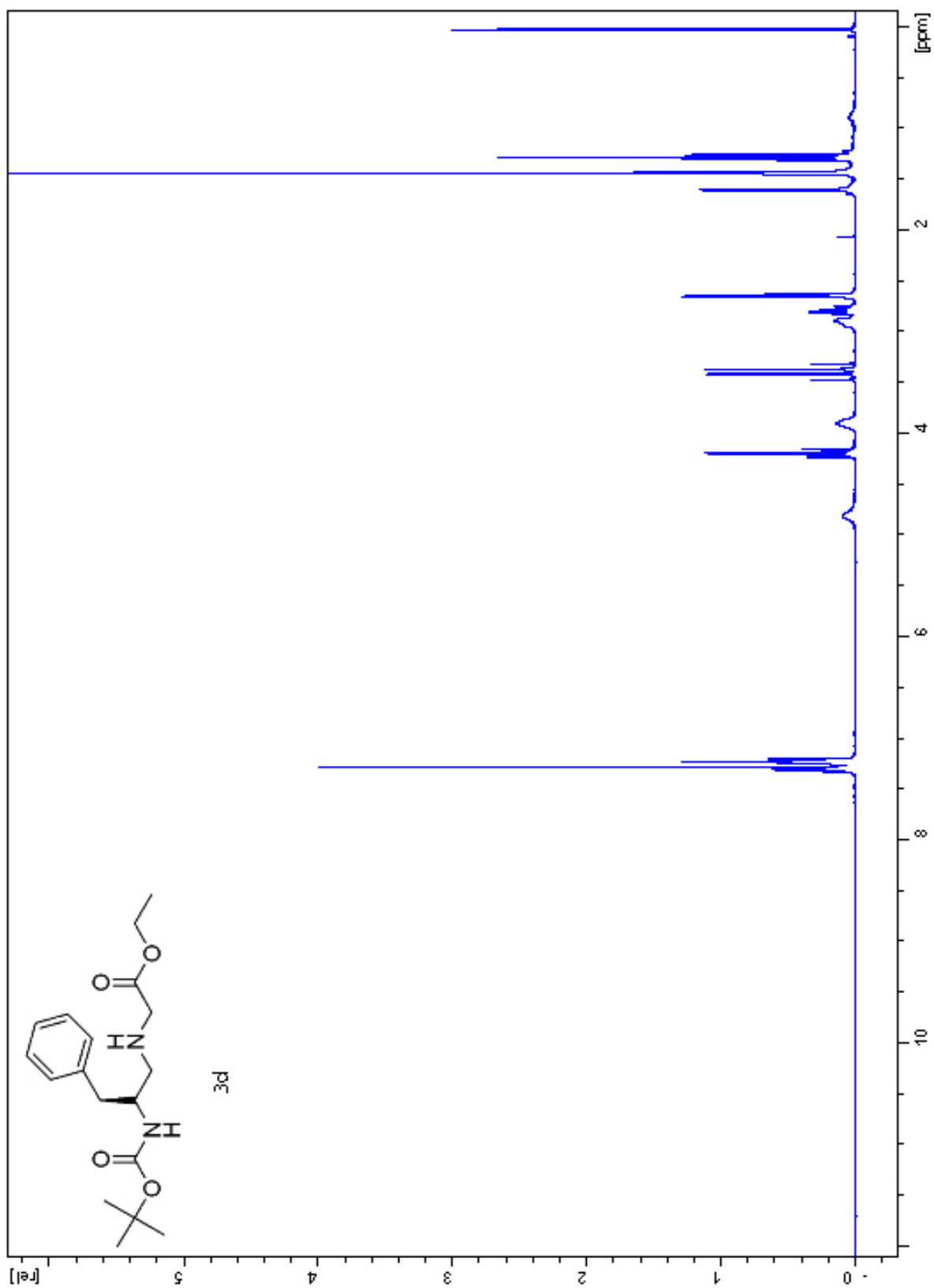
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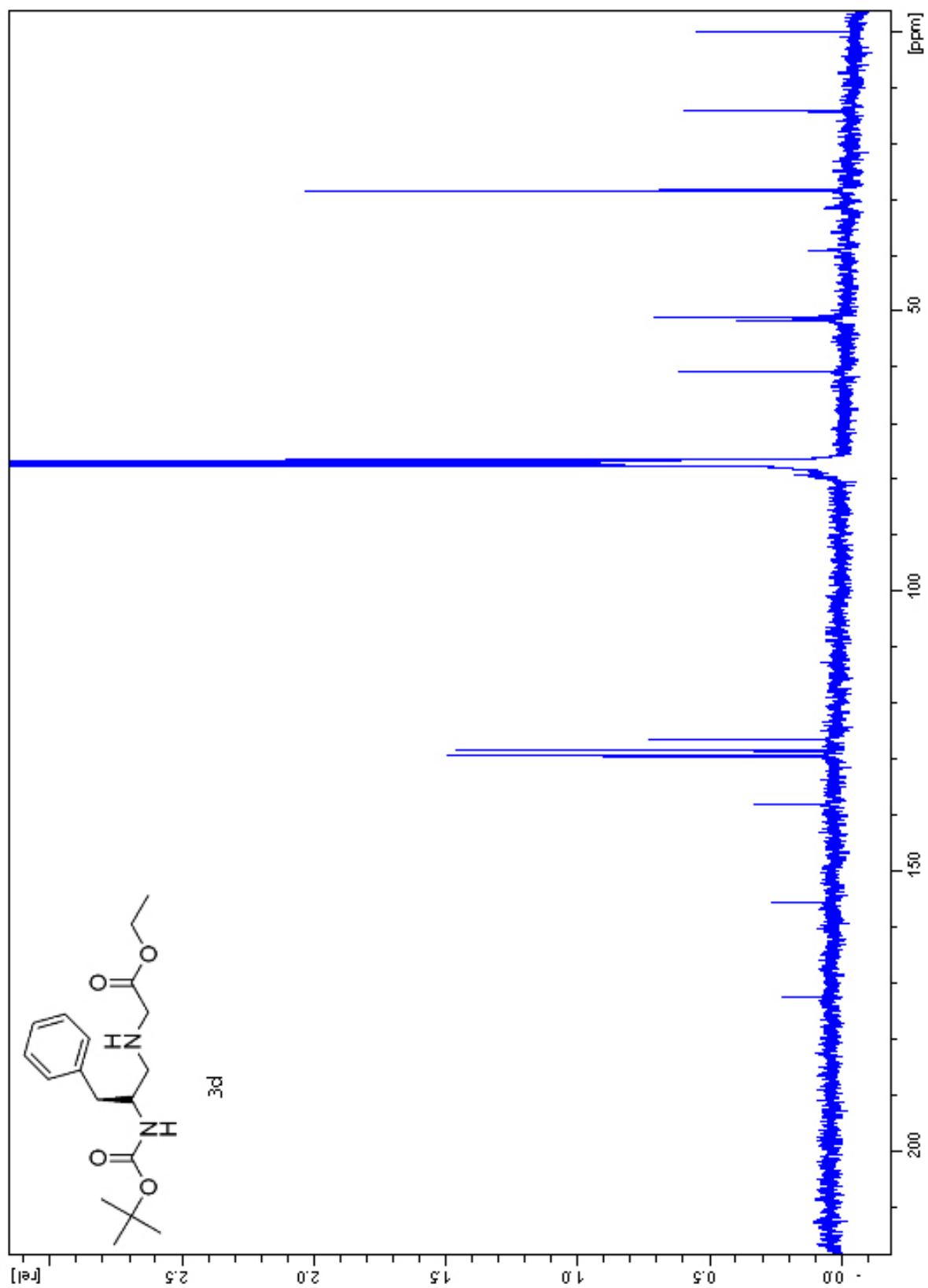
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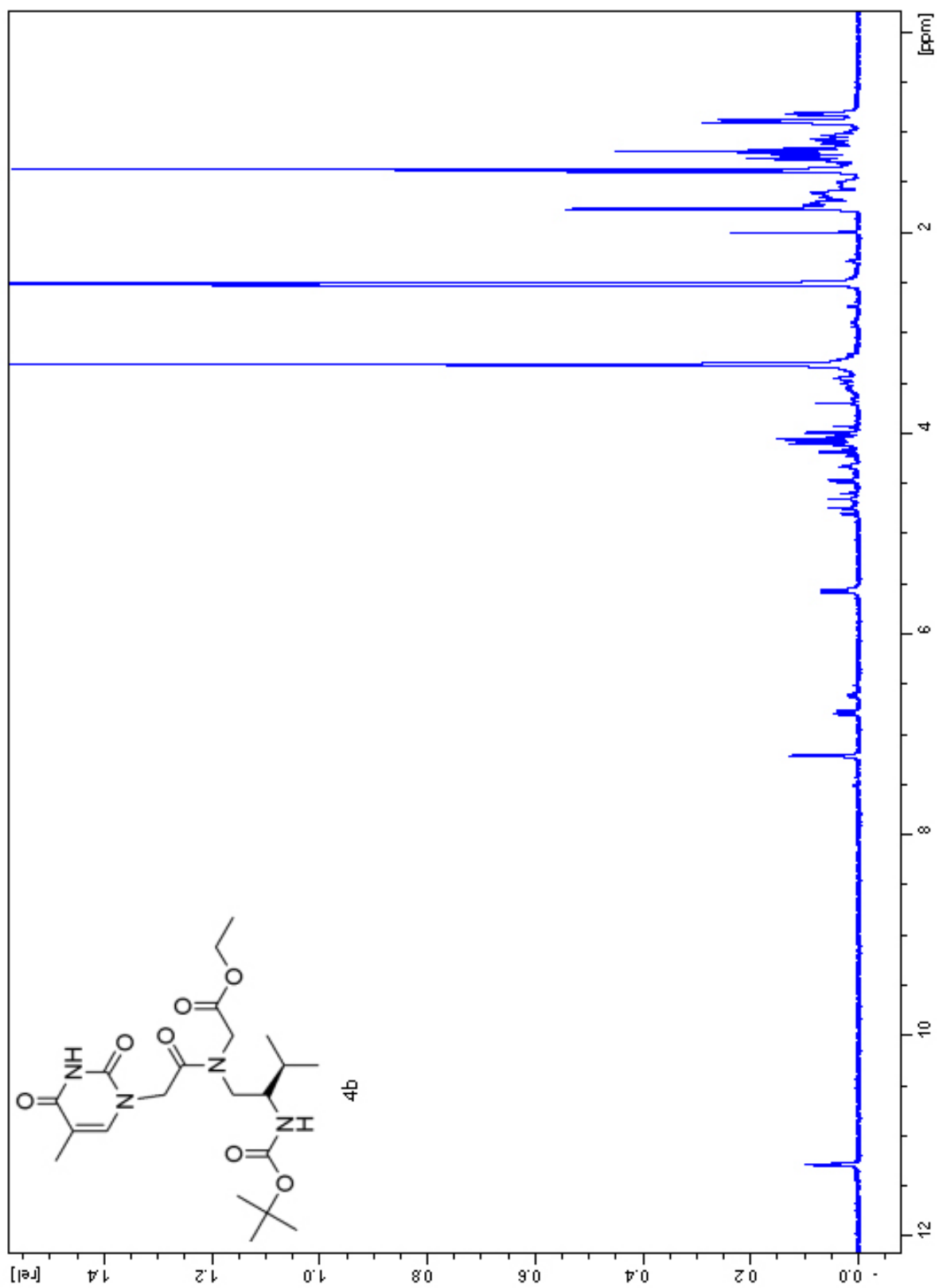
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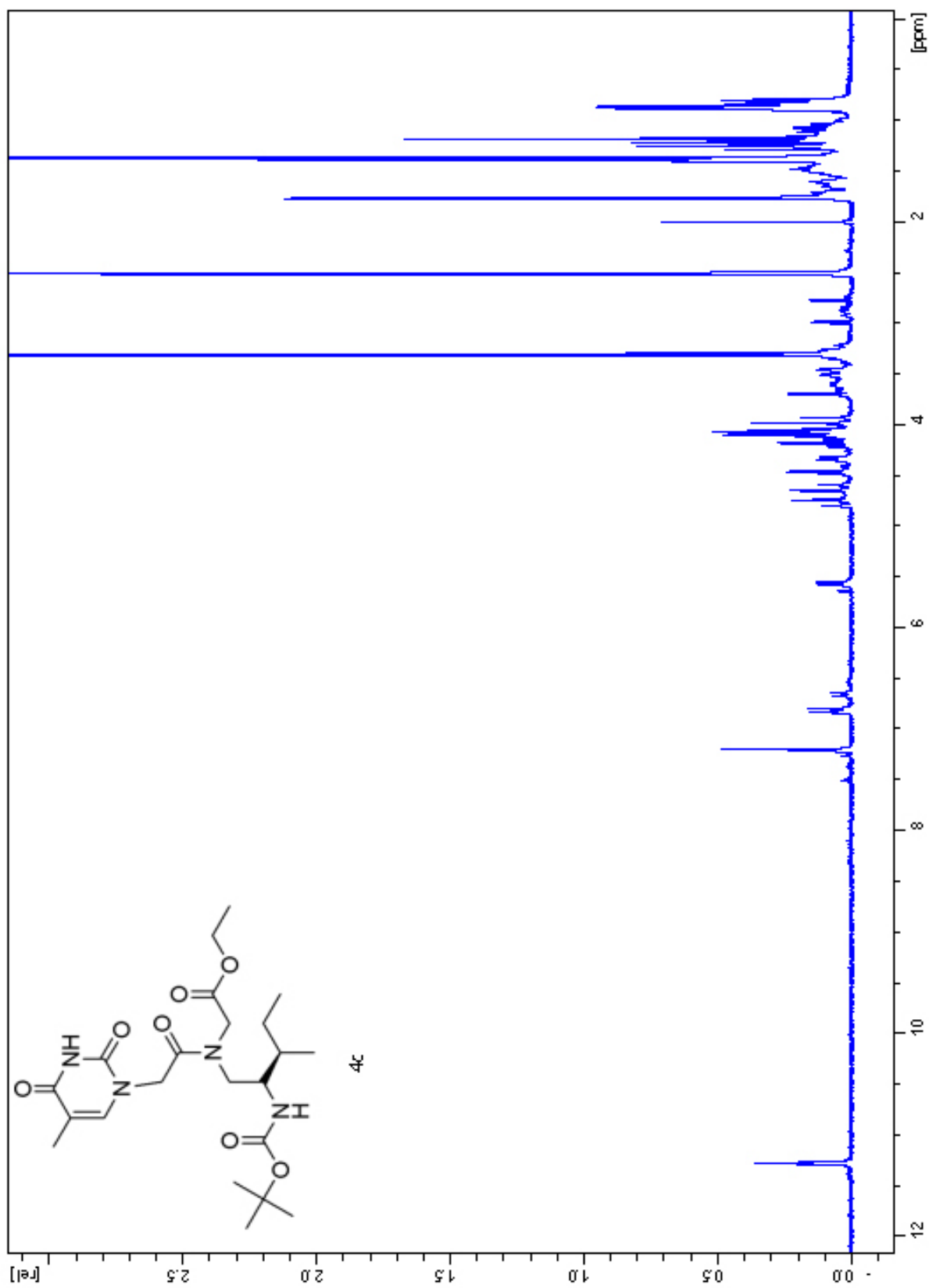
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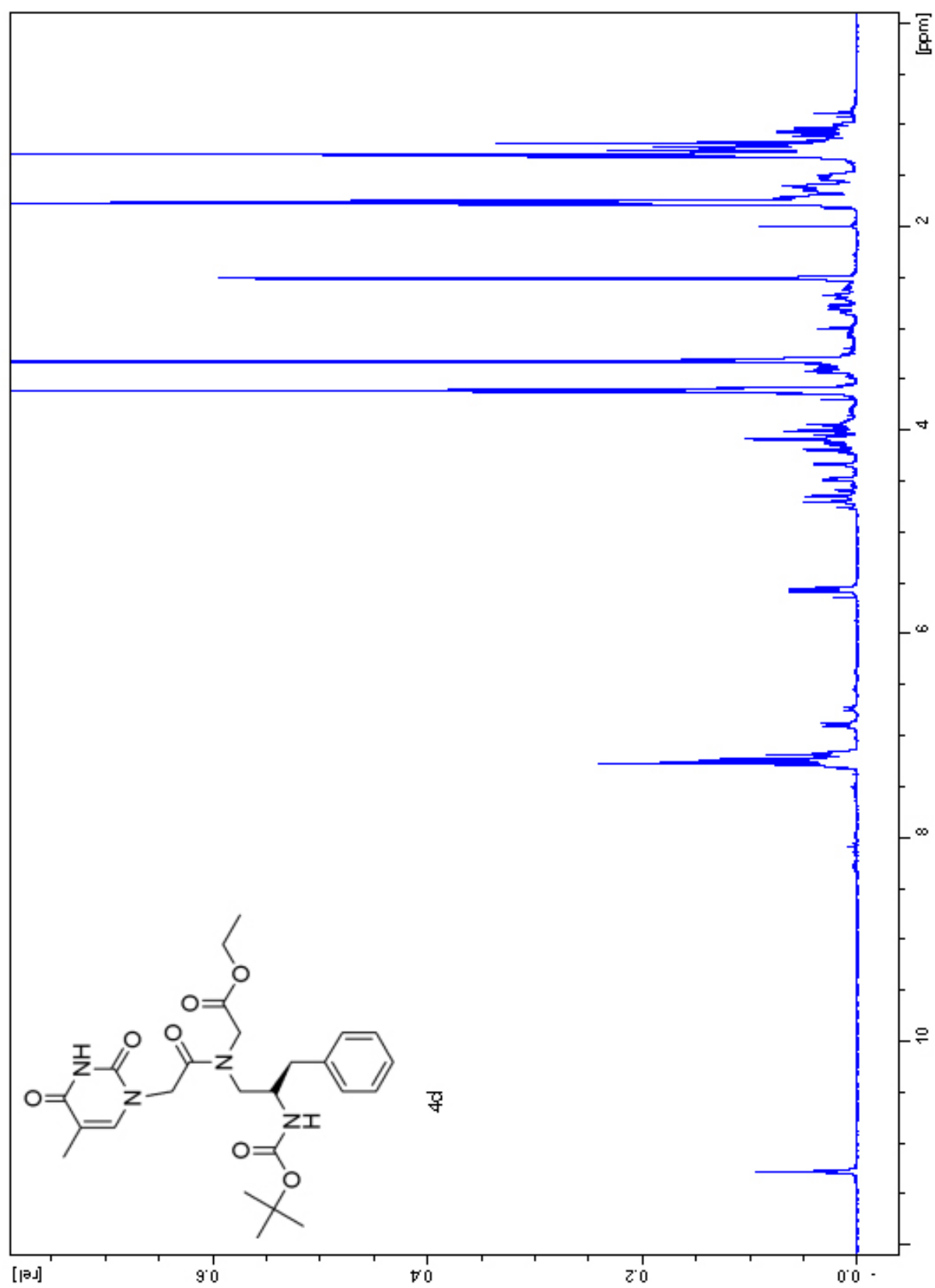
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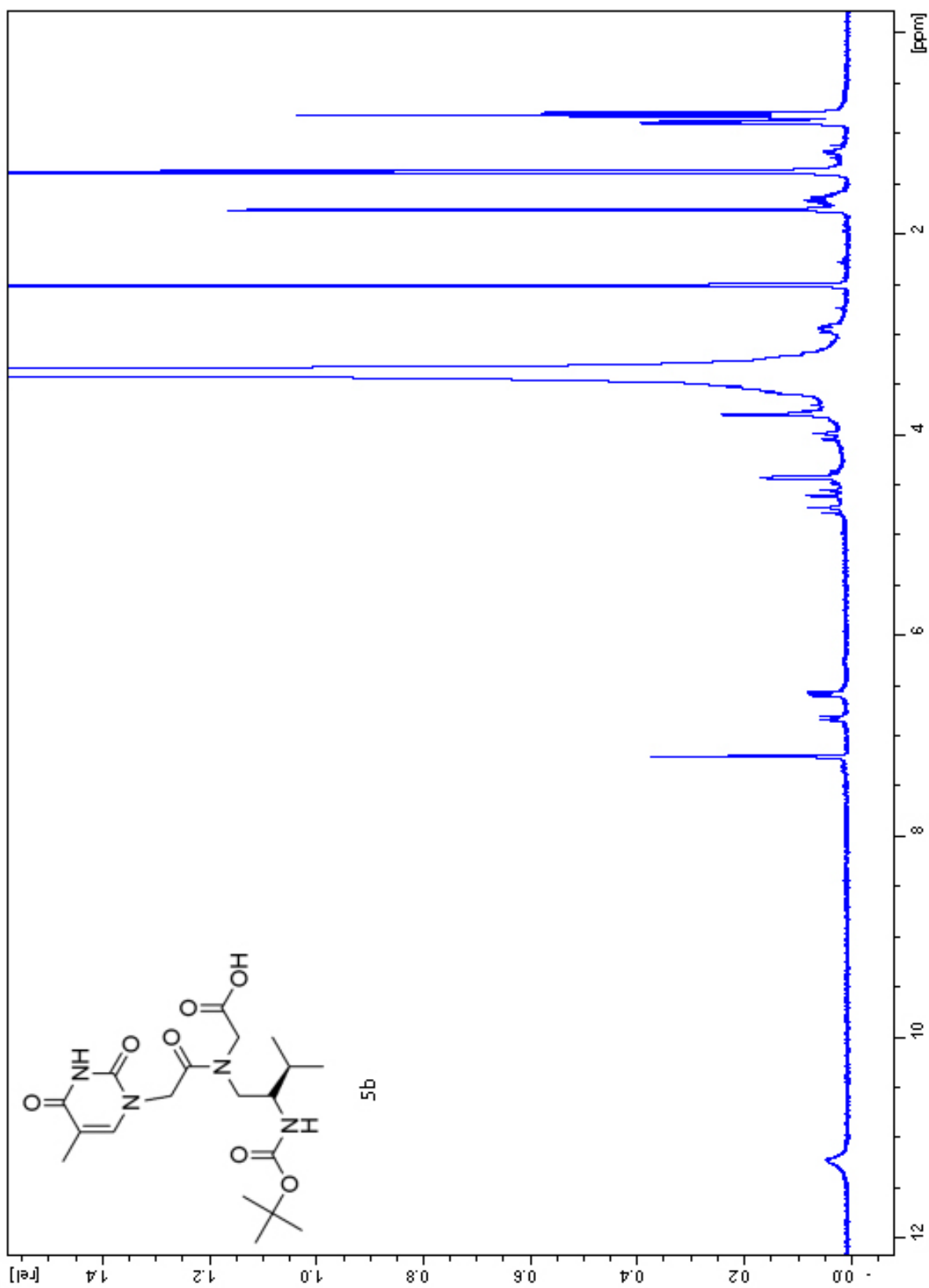
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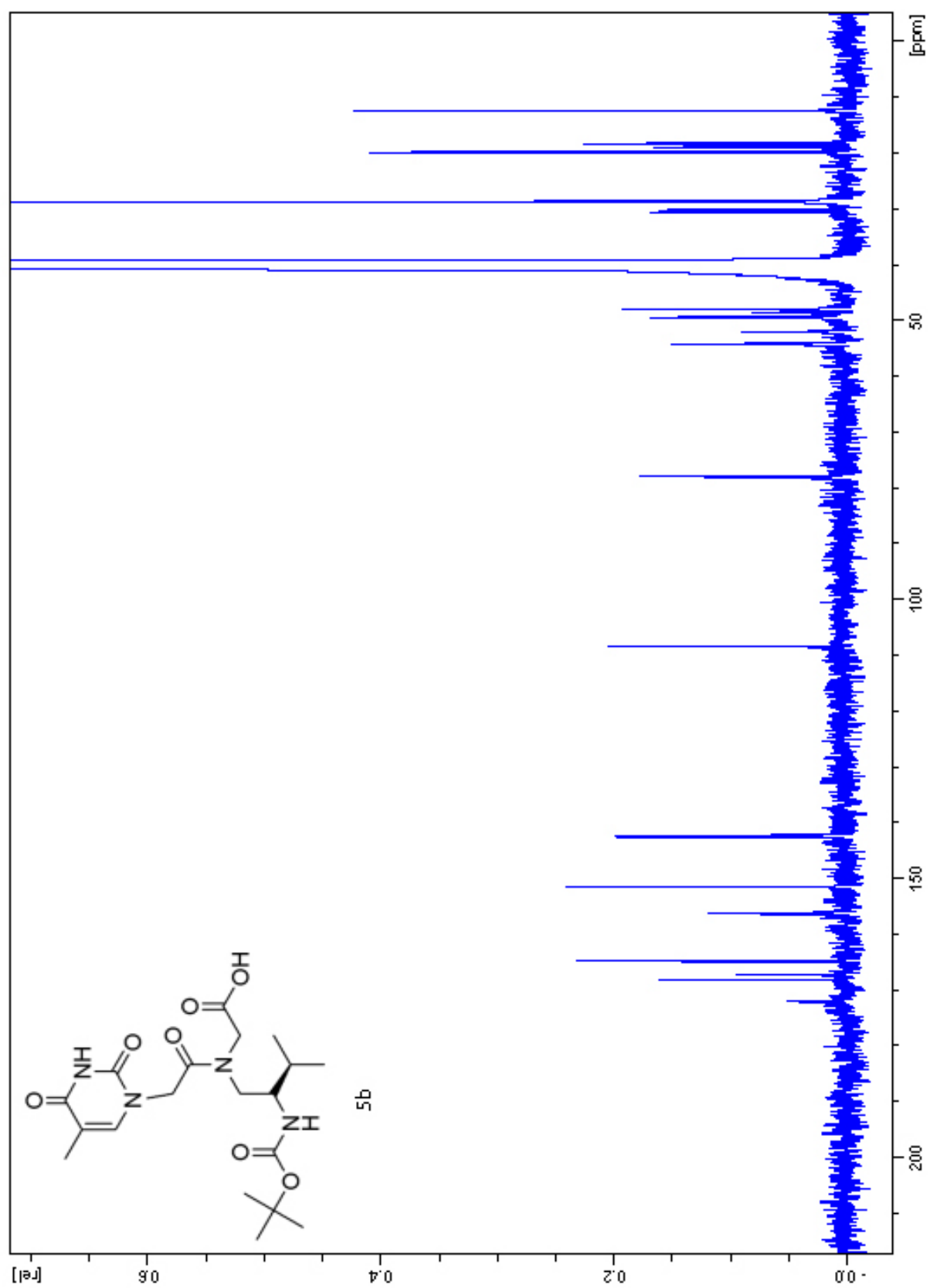
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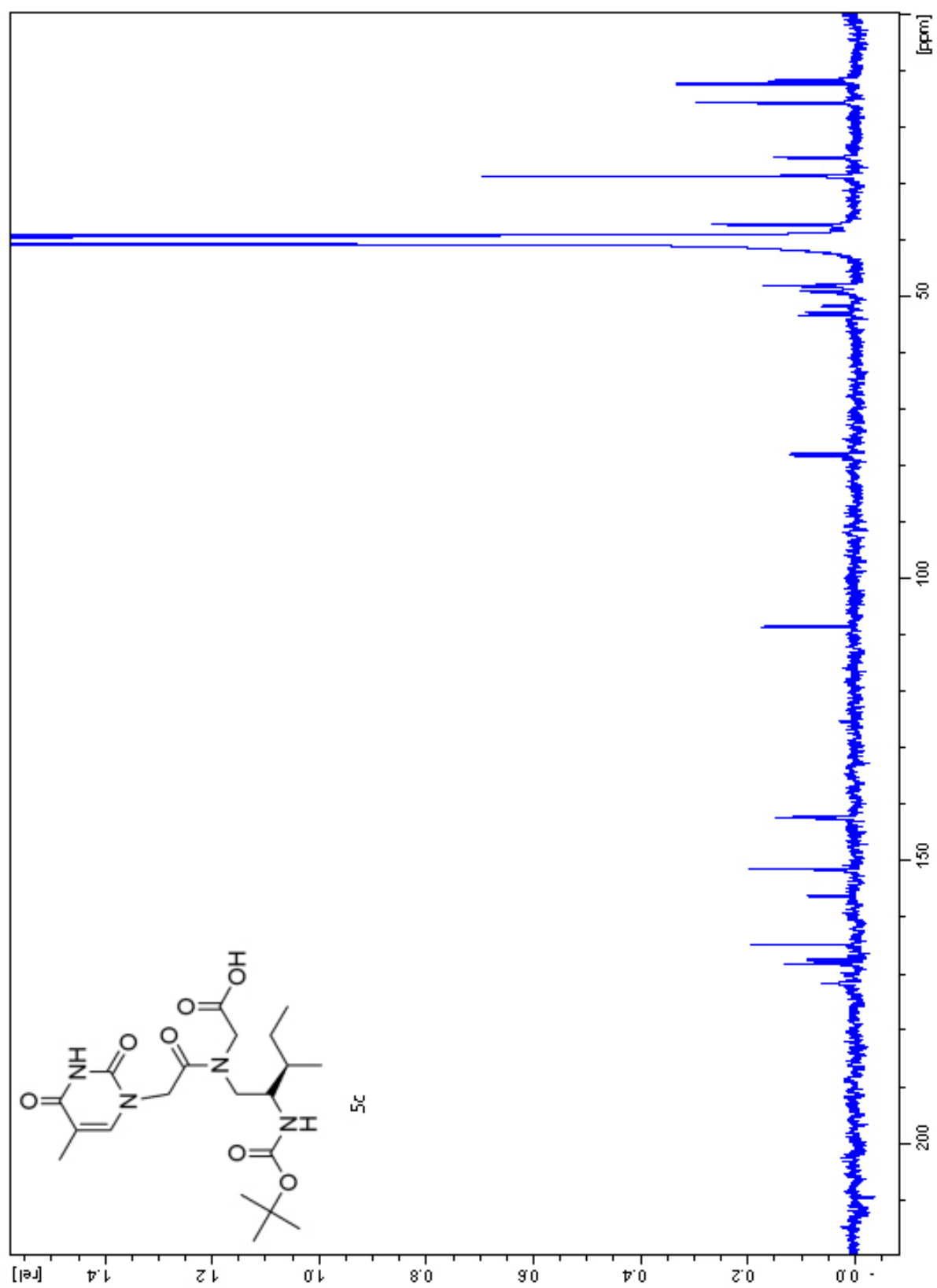
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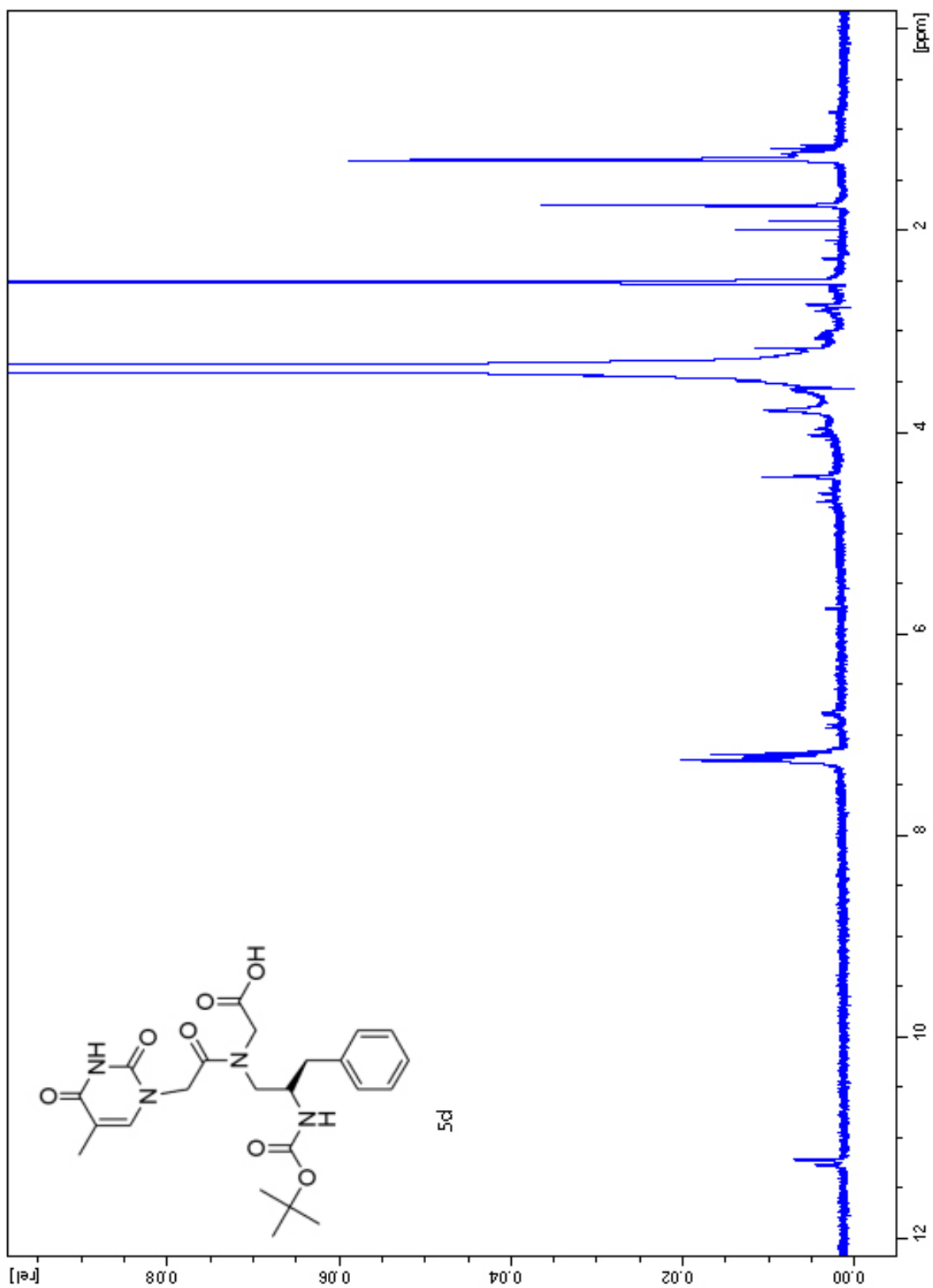
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^1H NMR

^1H NMR

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