

Supporting Information

for

Synthesis and characterization of ML and ML₂ metal complexes with amino acid substituted bis(2-picolyl)amine ligands.

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Pevec,^b Iztok Turel^b and Srećko I. Kirin^{*,a}**

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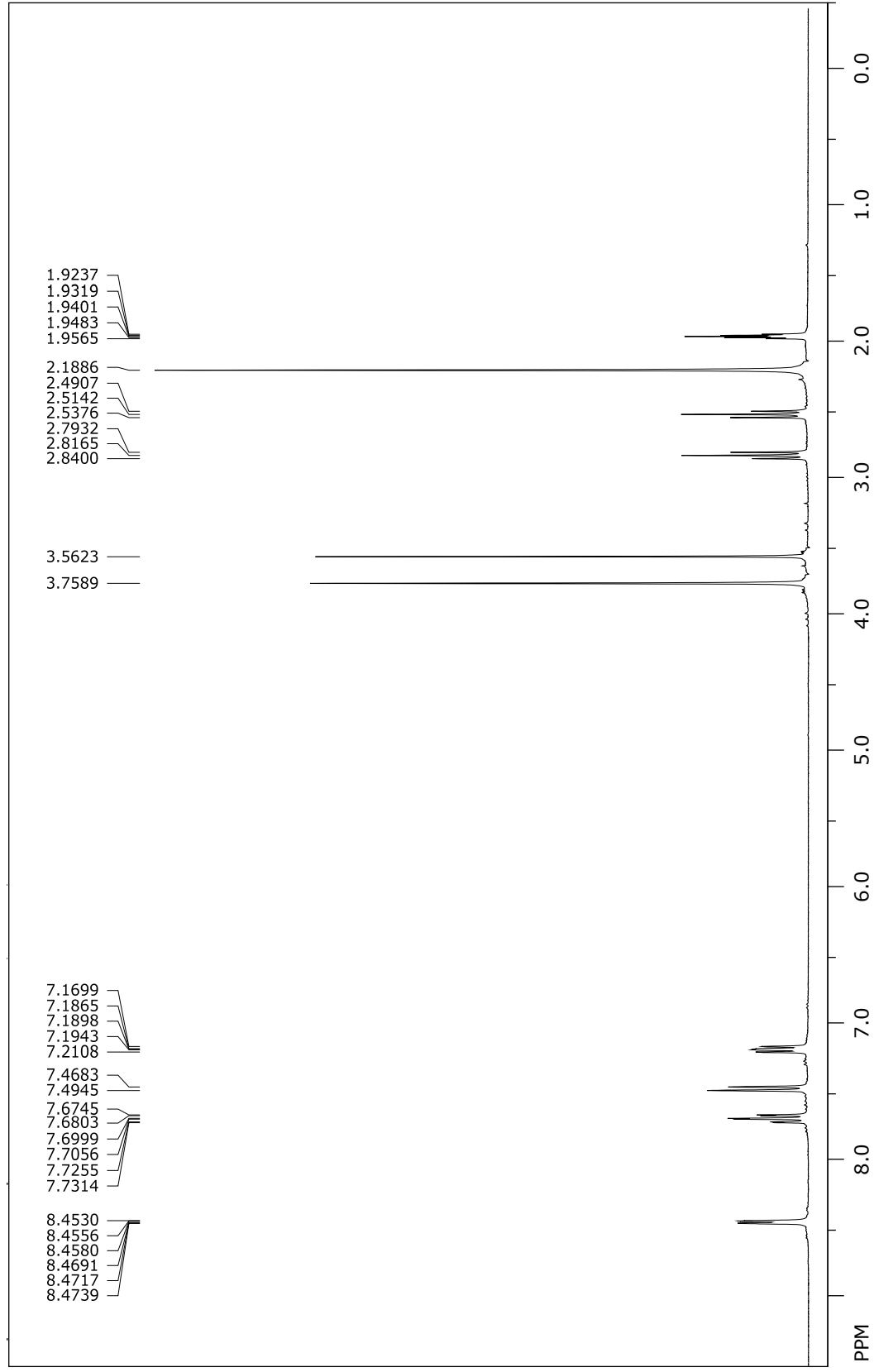
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^b Faculty of Chemistry and Chemical Technology, University of Ljubljana, Vecna pot 113,
1000 Ljubljana, Slovenia.

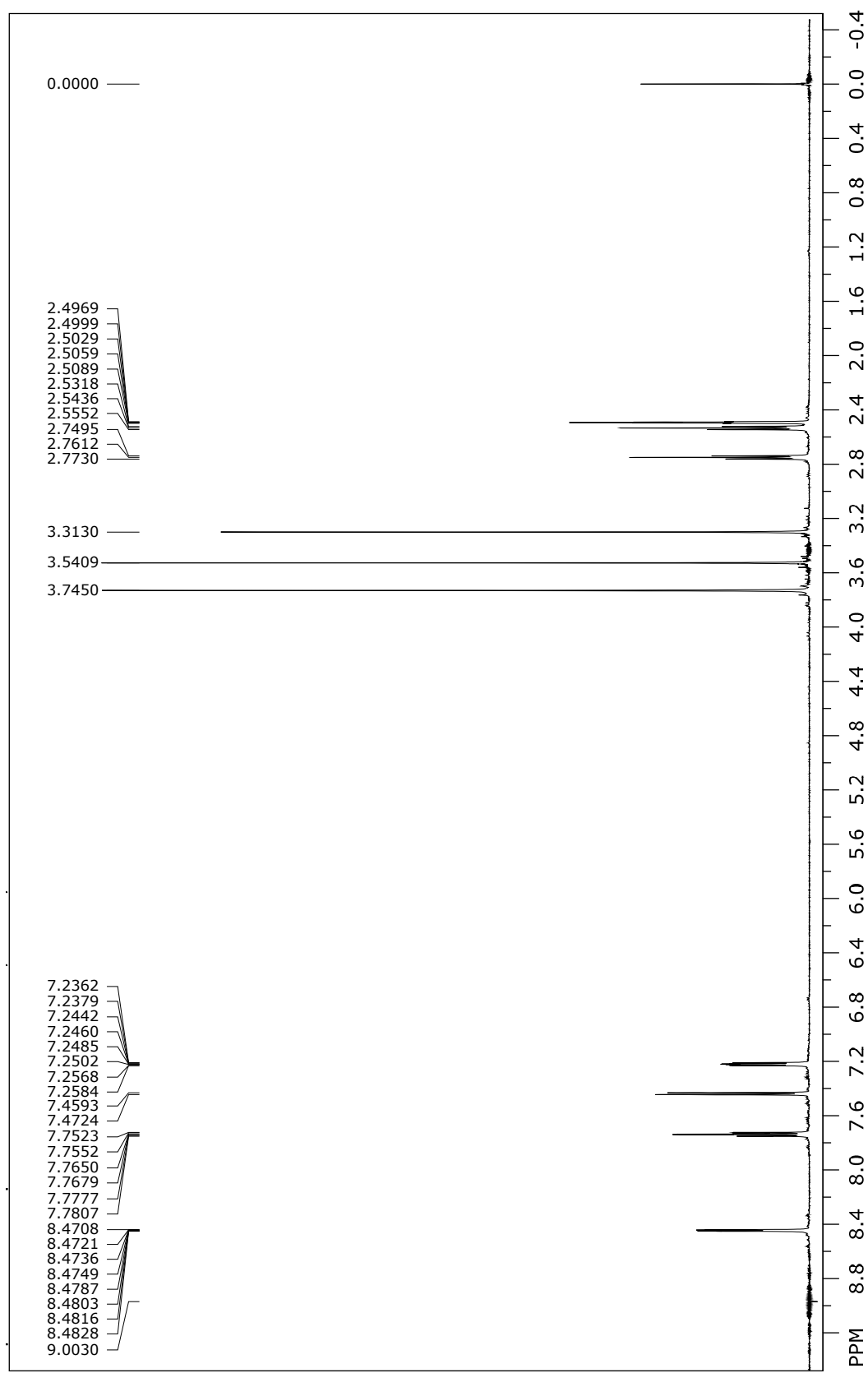
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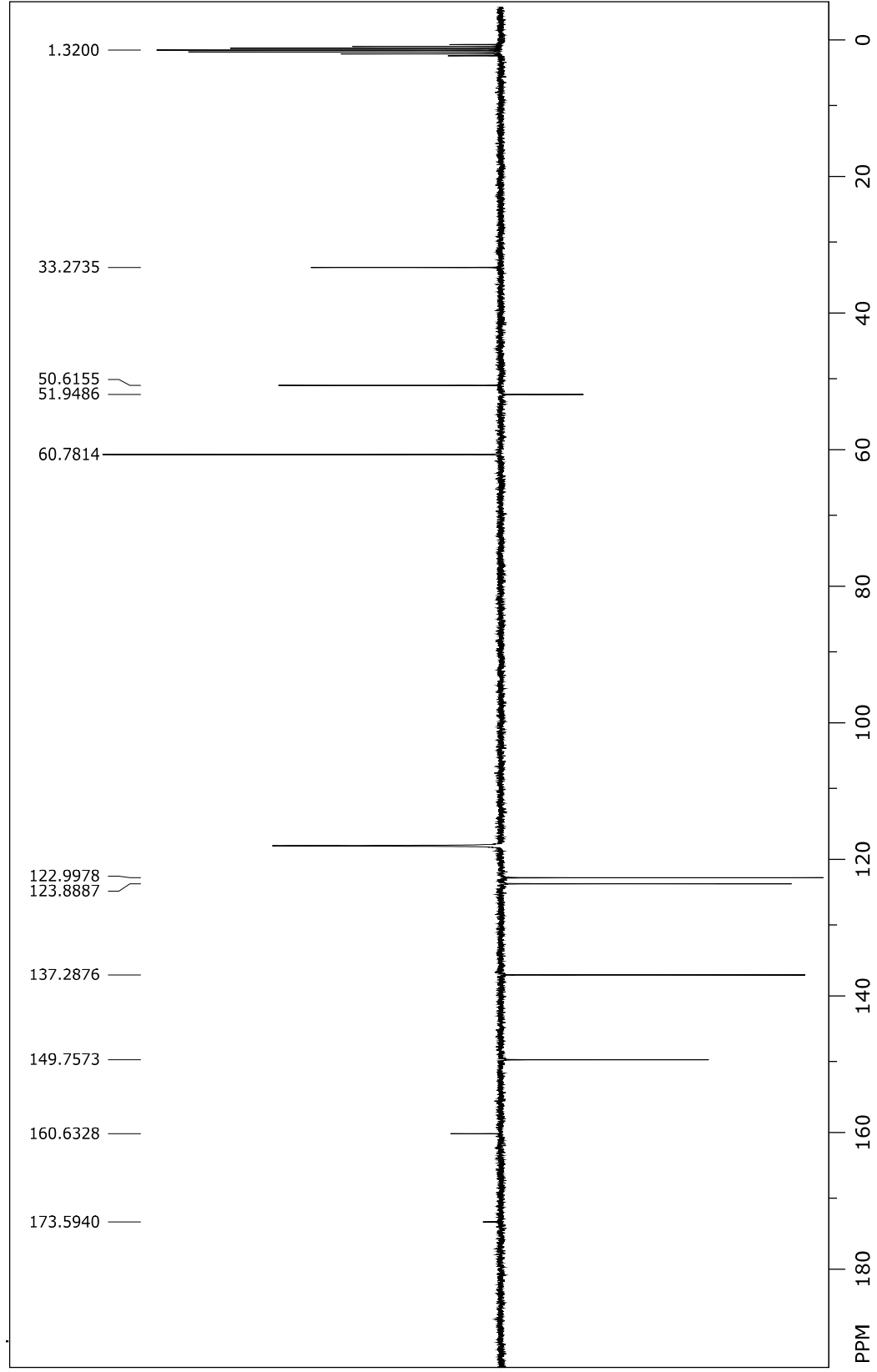
1. NMR spectra of ligands L1-L5.
¹H NMR (300 MHz, CD₃CN) of ligand **L1**. **Bpa-CH₂-CH₂-CO₂Me.**



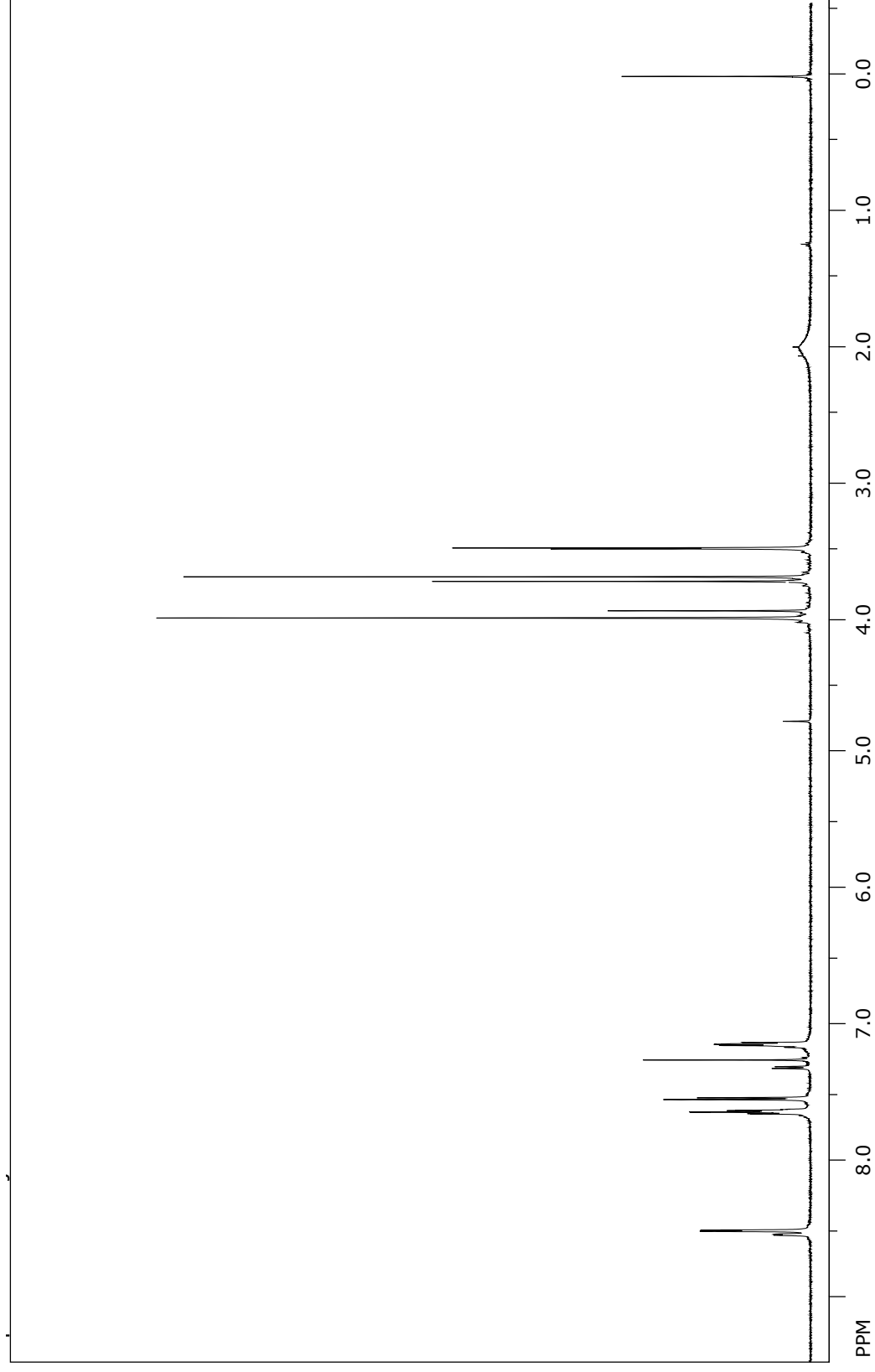
¹H NMR (600 MHz, DMSO-d₆) of ligand L1. Bpa-CH₂-CH₂-CO₂Me.



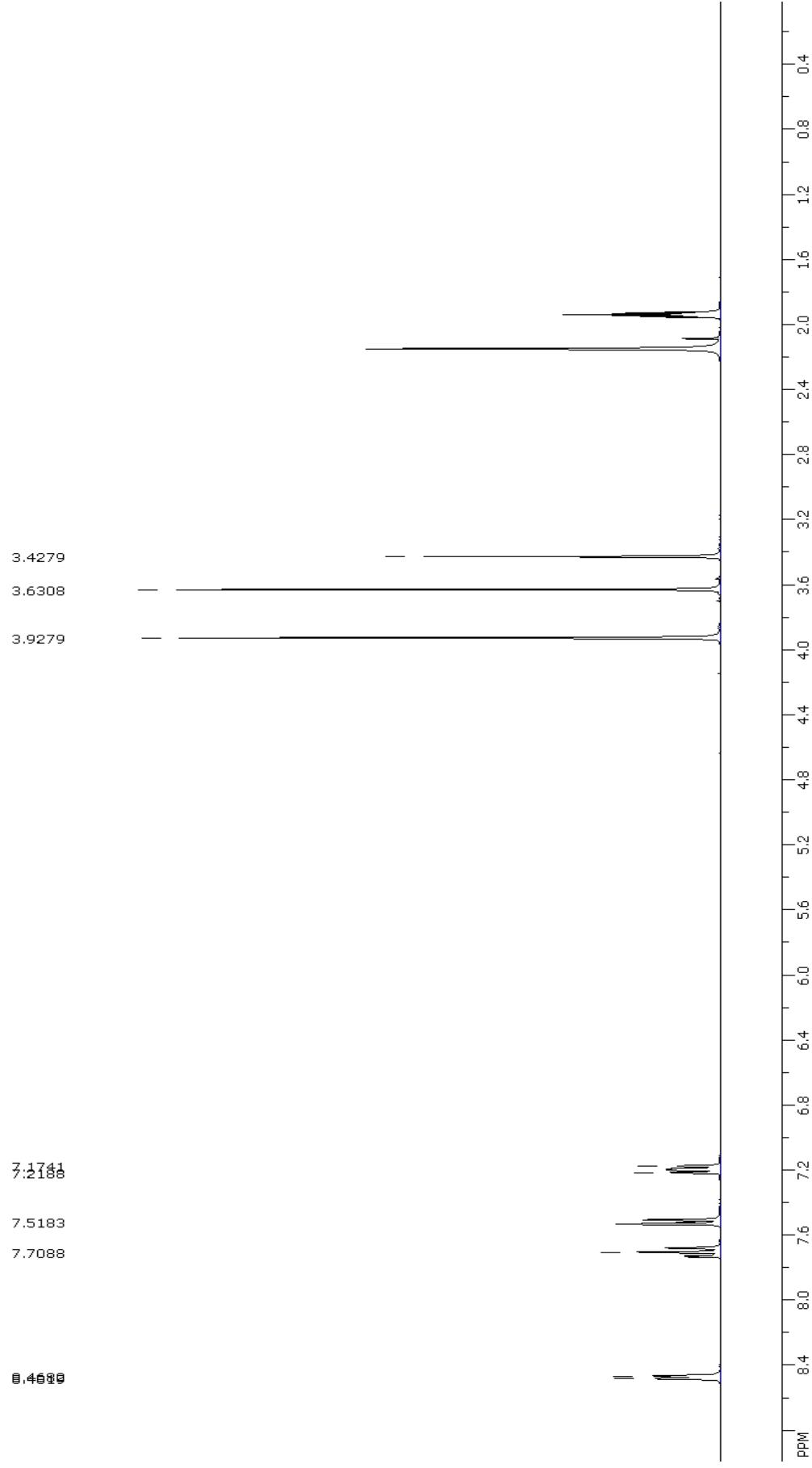
^{13}C NMR (75 MHz, CD_3CN) of ligand **L1**. **Bpa-CH₂-CH₂-CO₂Me**.



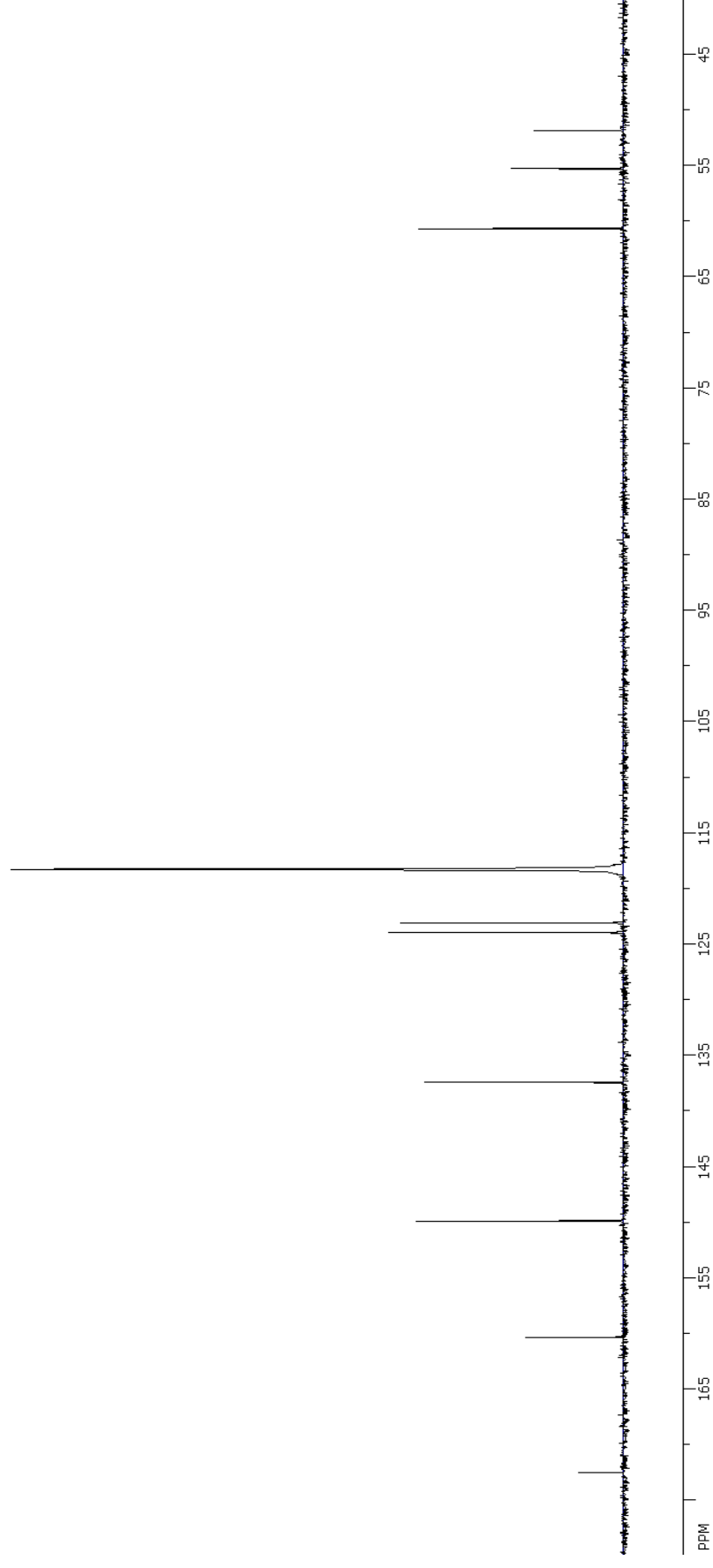
^1H NMR (600 MHz, CDCl_3) of ligand **L2**. **Bpa-CH₂-CO₂Me**.

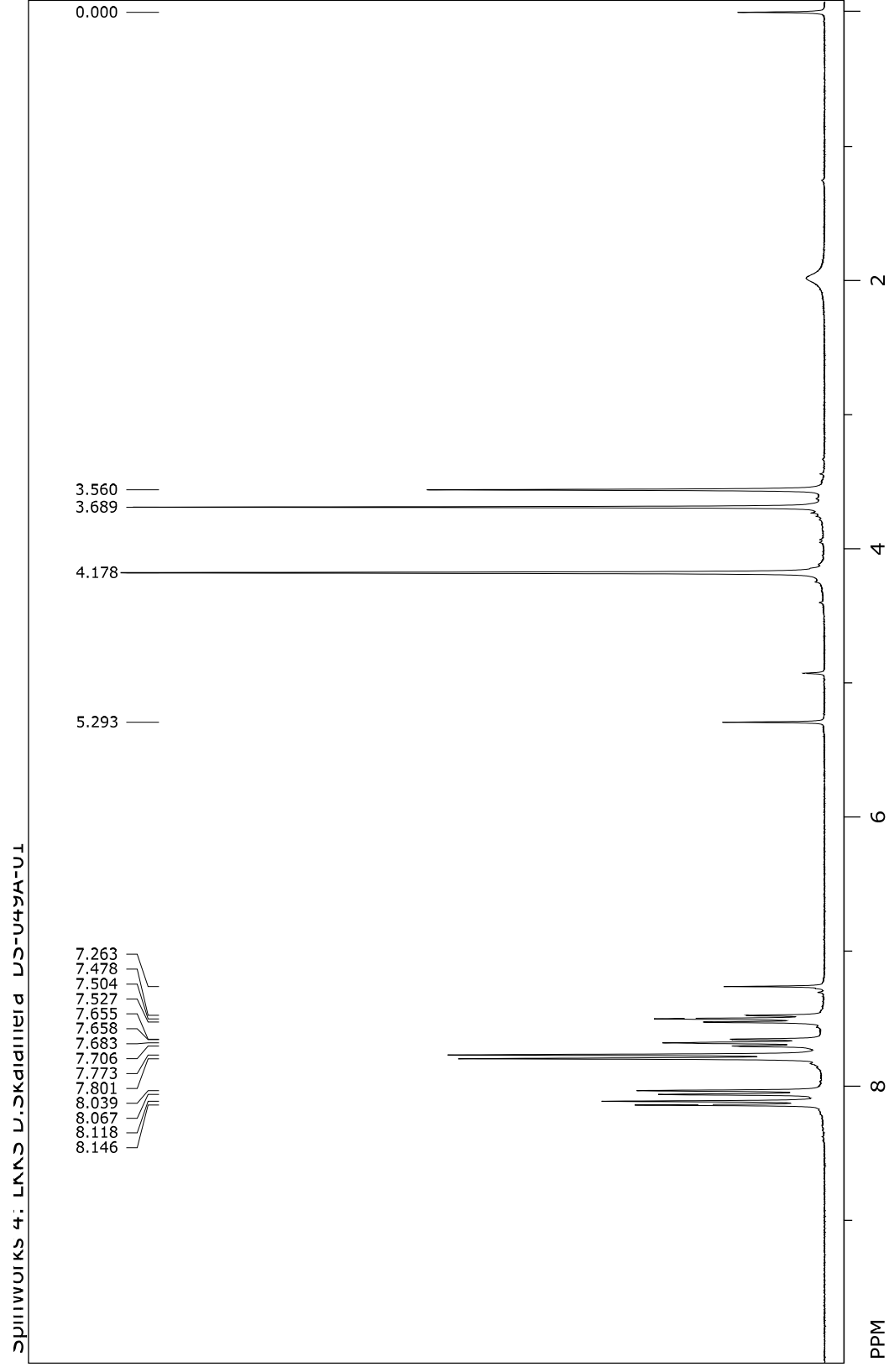


¹H NMR (300 MHz, CD₃CN) of ligand L2: Bpa-CH₂-CO₂Me.

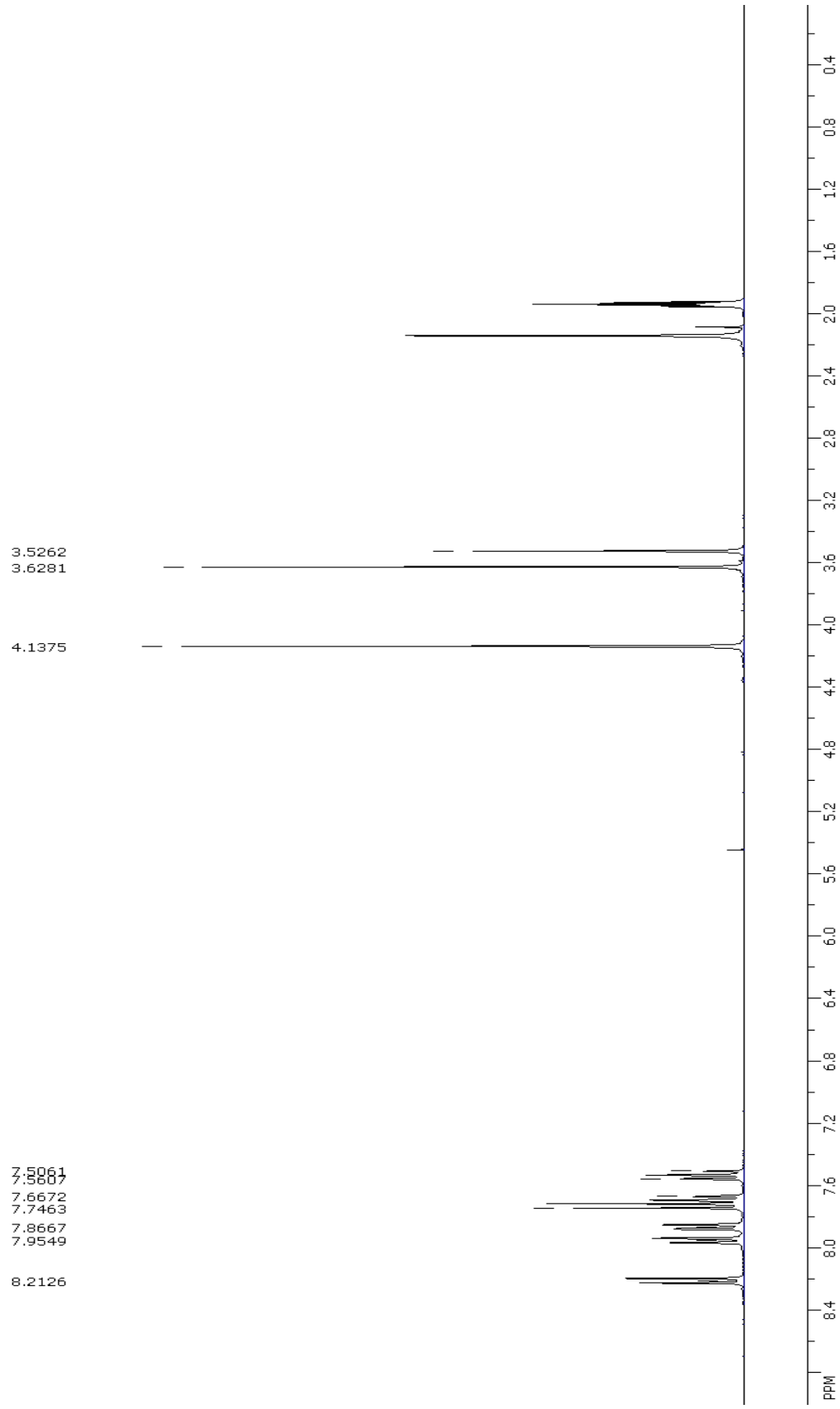


^{13}C NMR (75 MHz, CD_3CN) of ligand **L2**. **Bpa-CH₂-CO₂Me**.

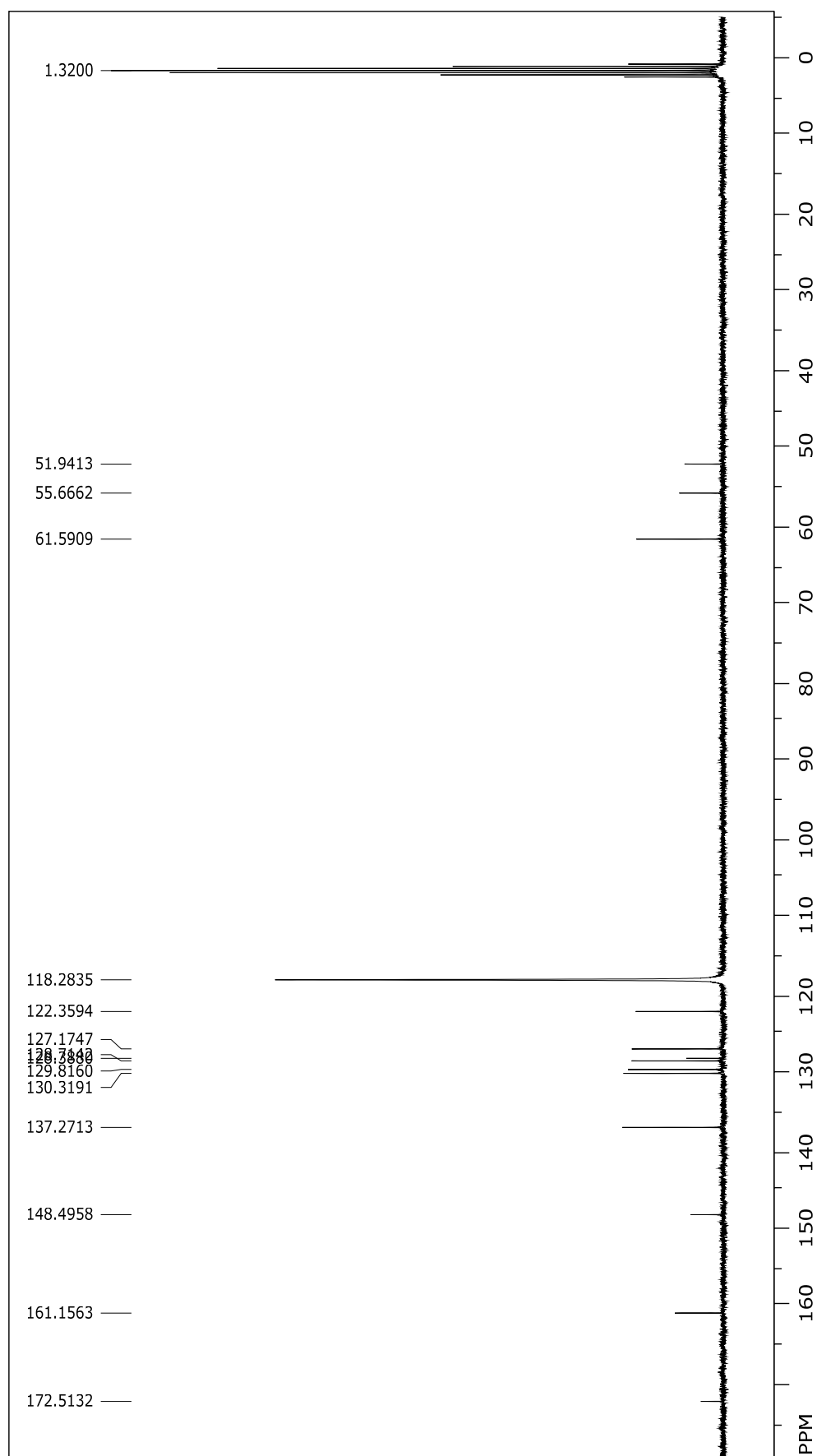


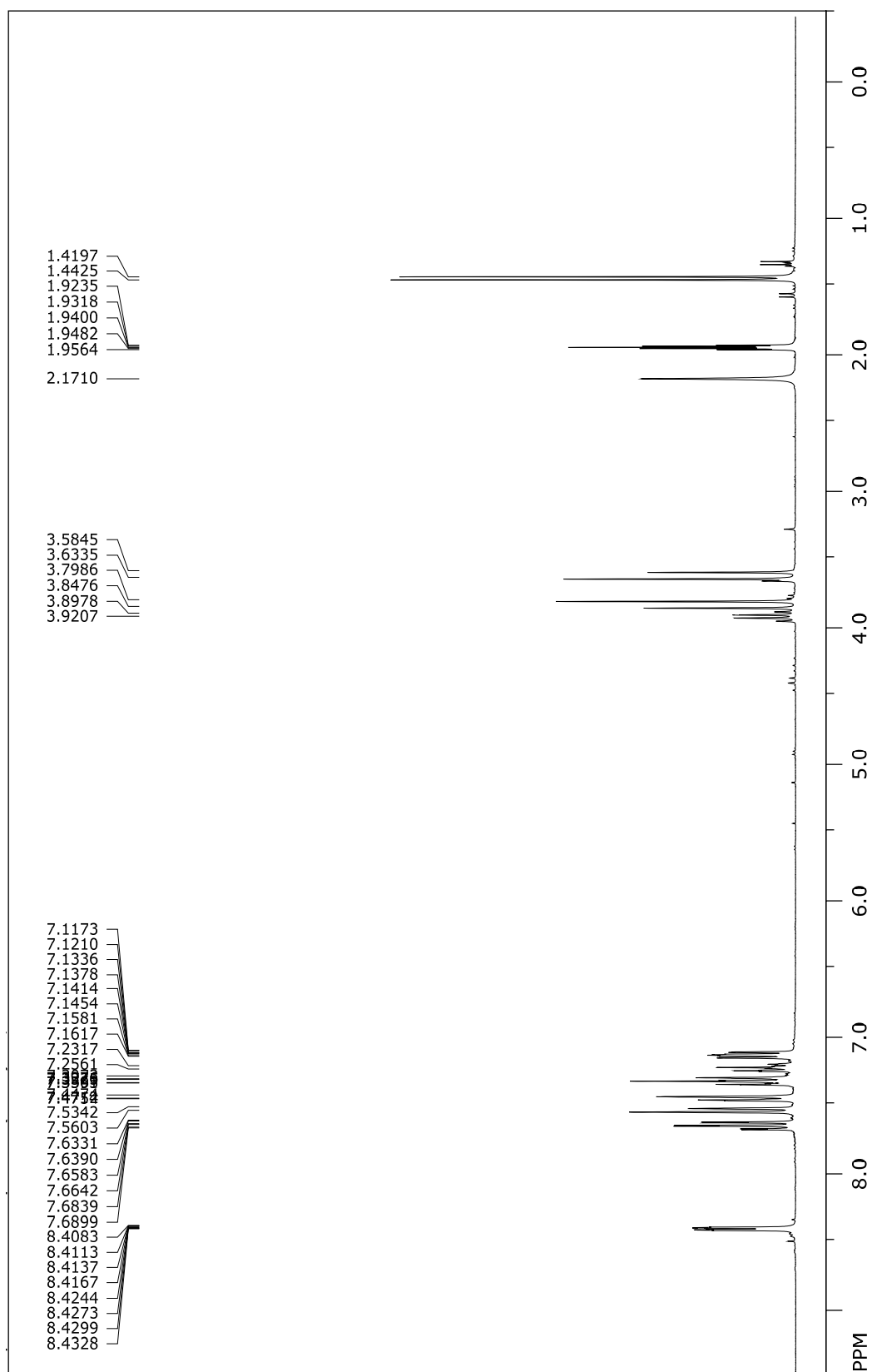
¹H NMR (300 MHz, CDCl₃) of ligand L3. Bqa-CH₂-CO₂Me.

¹H NMR (300 MHz, CD₃CN) of ligand L3. Bqa-CH₂-CO₂Me.

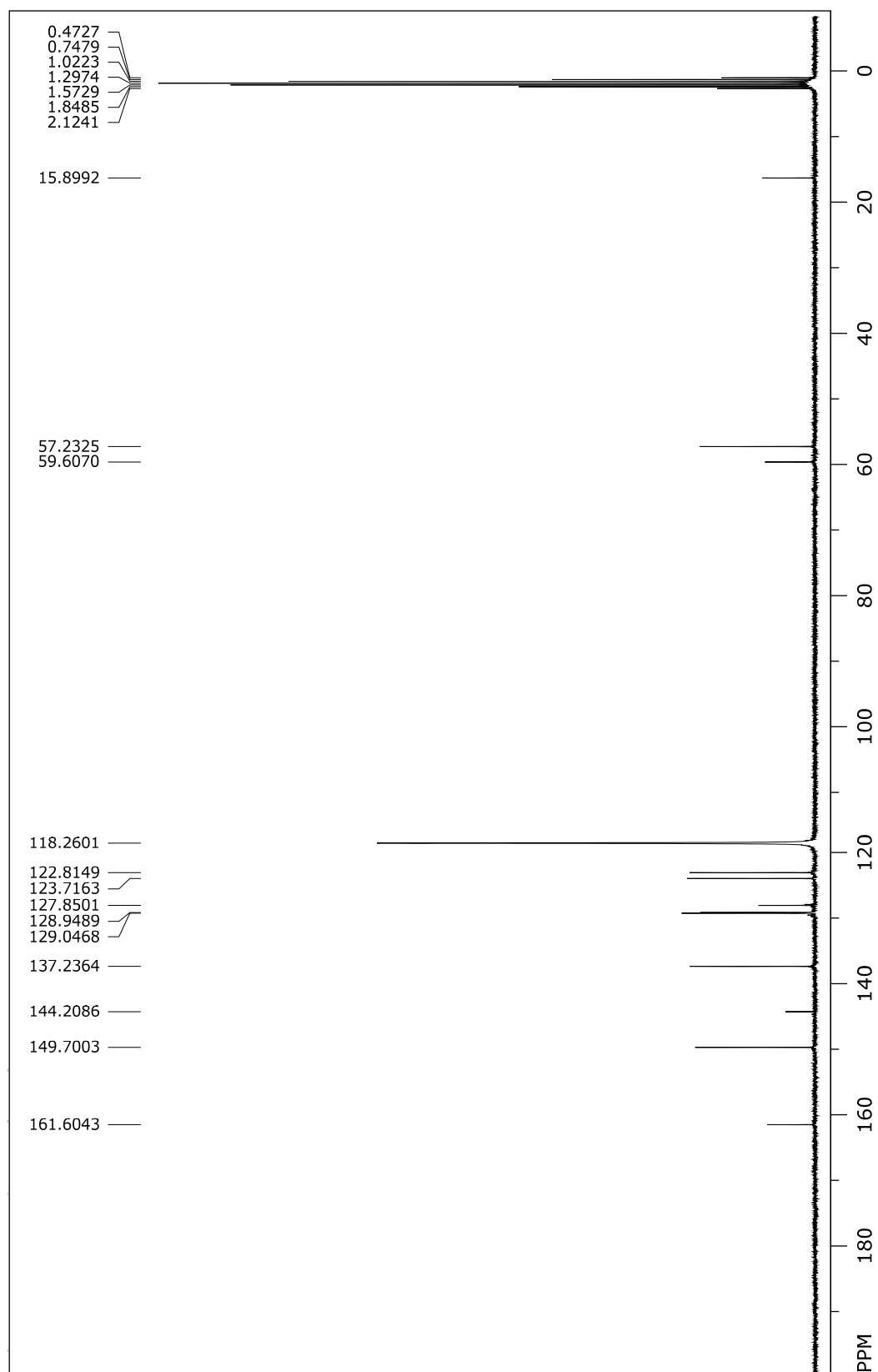


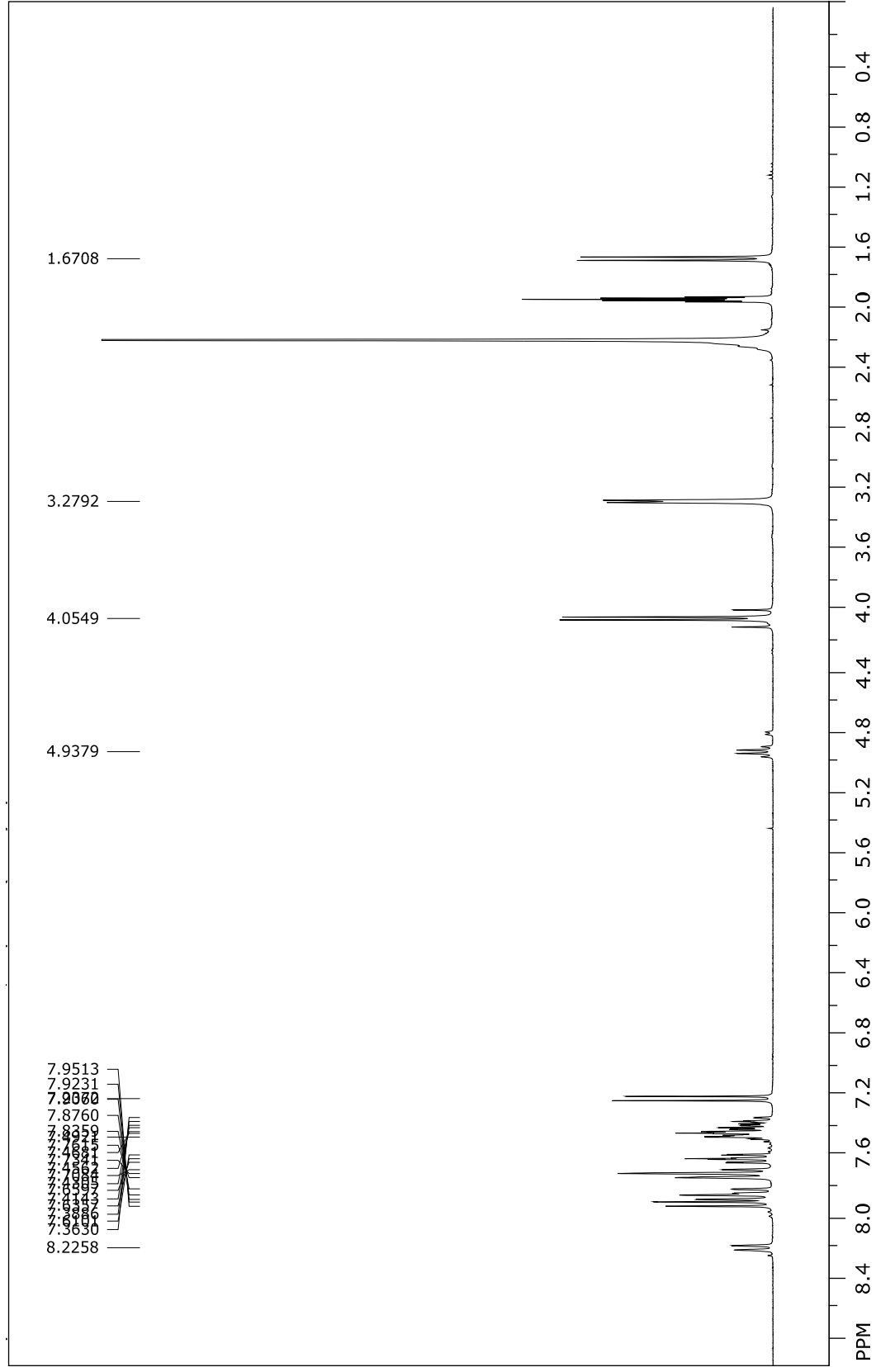
^{13}C NMR (75 MHz, CD_3CN) of ligand **L3**. **Bqa-CH₂-CO₂Me**.



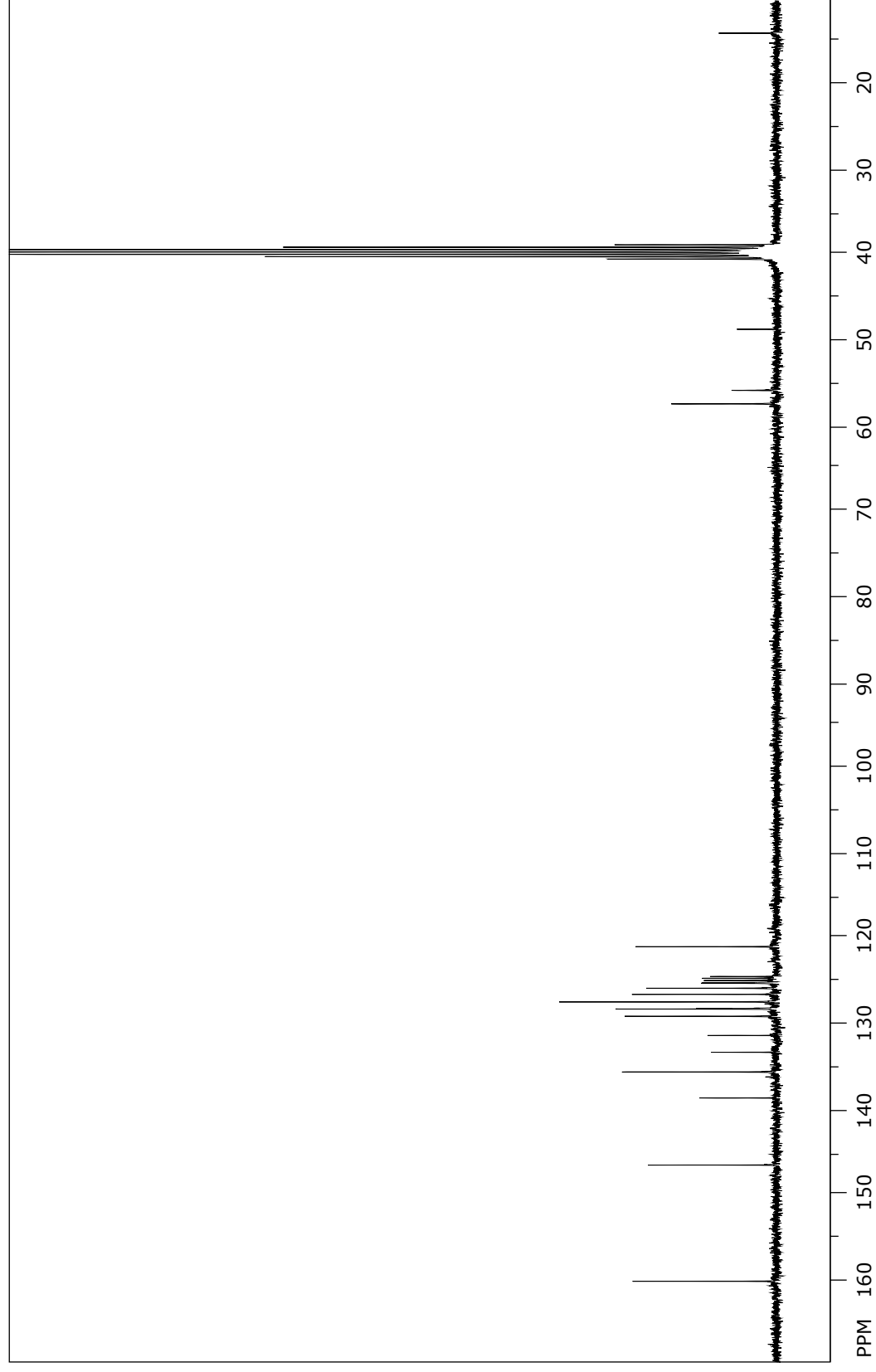
¹H NMR (300 MHz, CD₃CN) of ligand L4. Bpa-CH(CH₃)Ph.

¹³C NMR (75 MHz, CD₃CN) of ligand L4. Bpa-CH(CH₃)Ph.



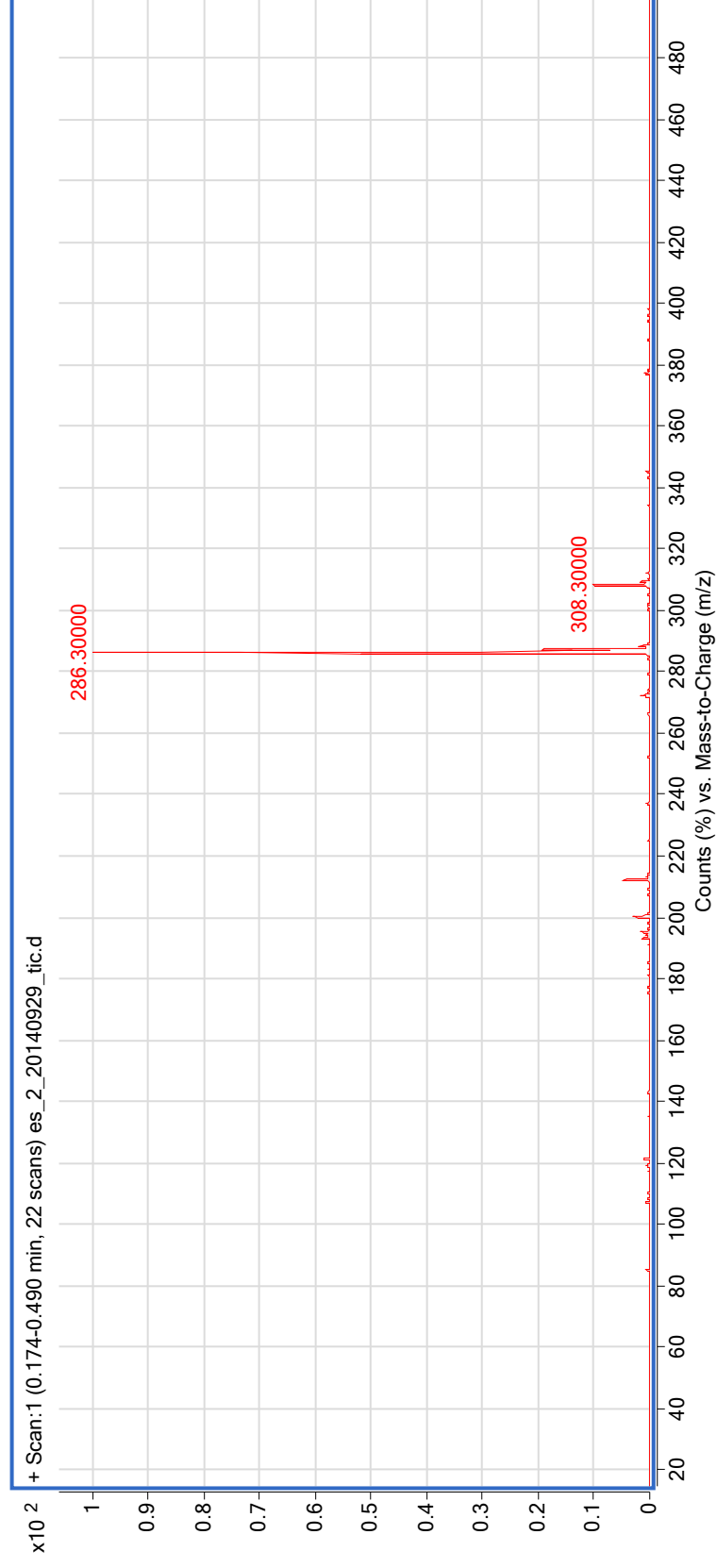
¹H NMR (300 MHz, DMSO-d₆) of ligand L5: **Bqa-CH(CH₃)Nph.**

^{13}C NMR (75 MHz, DMSO-d_6) of ligand **L5**. **Bqa-CH(CH₃)Nph.**

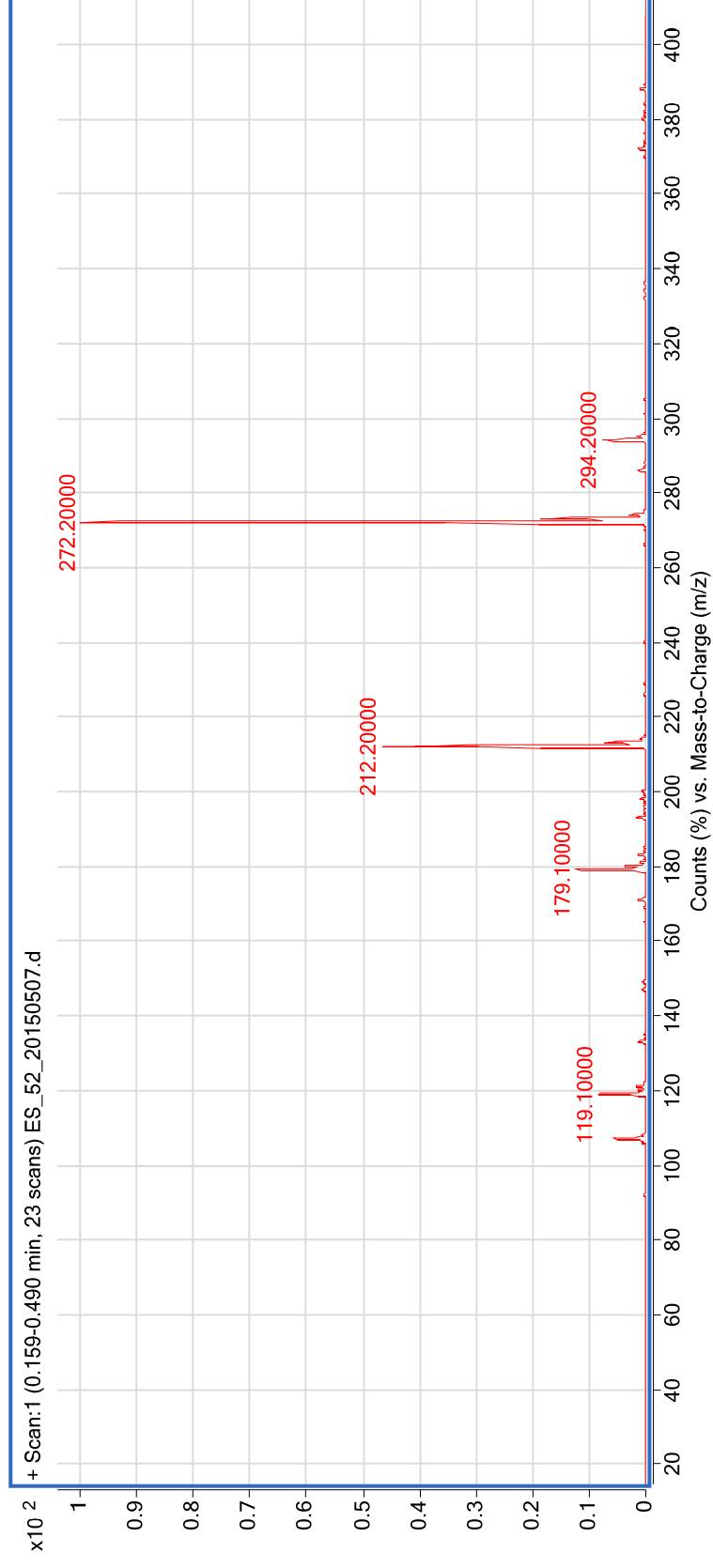


2. MS spectra of ligands L1 - L5.

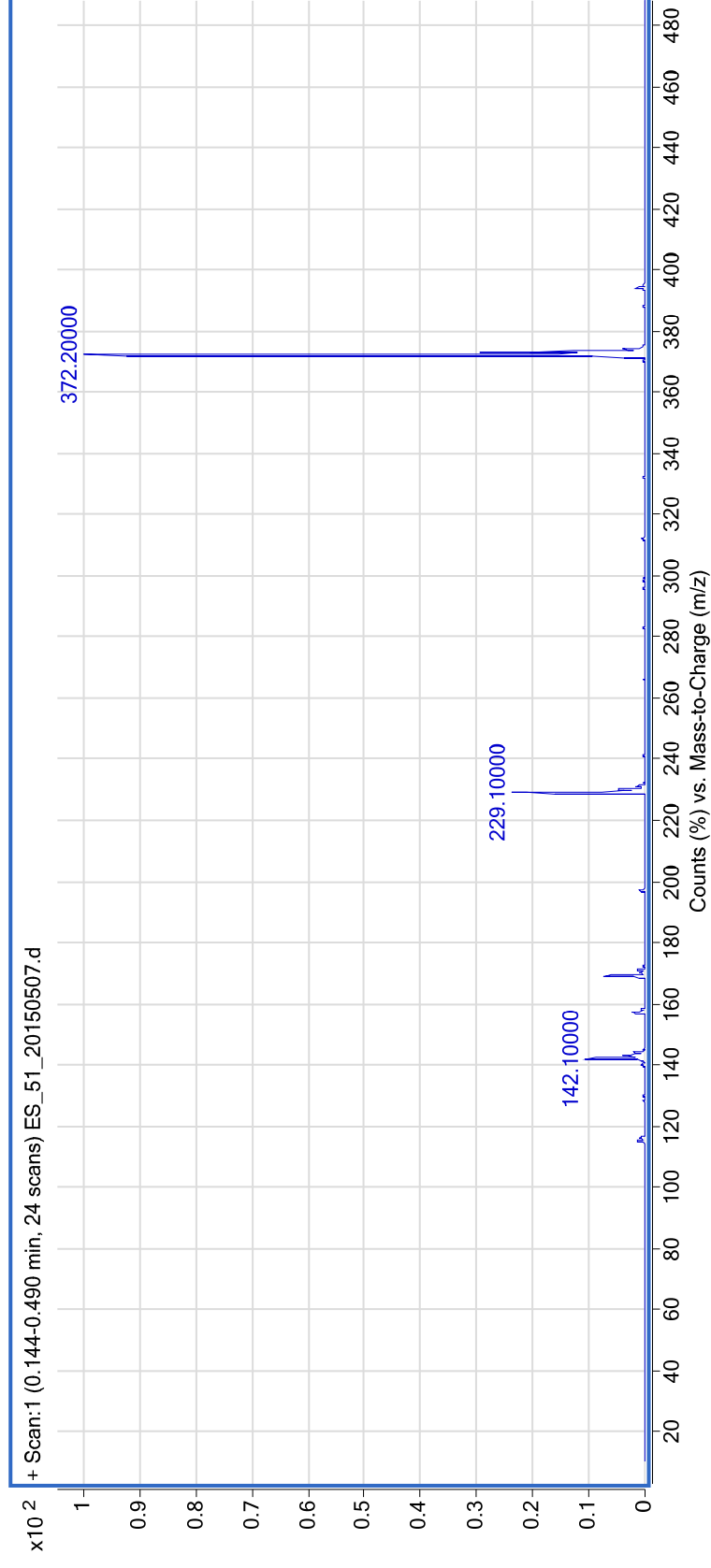
MS of ligand L1. **Bpa-CH₂-CH₂-CO₂Me.**



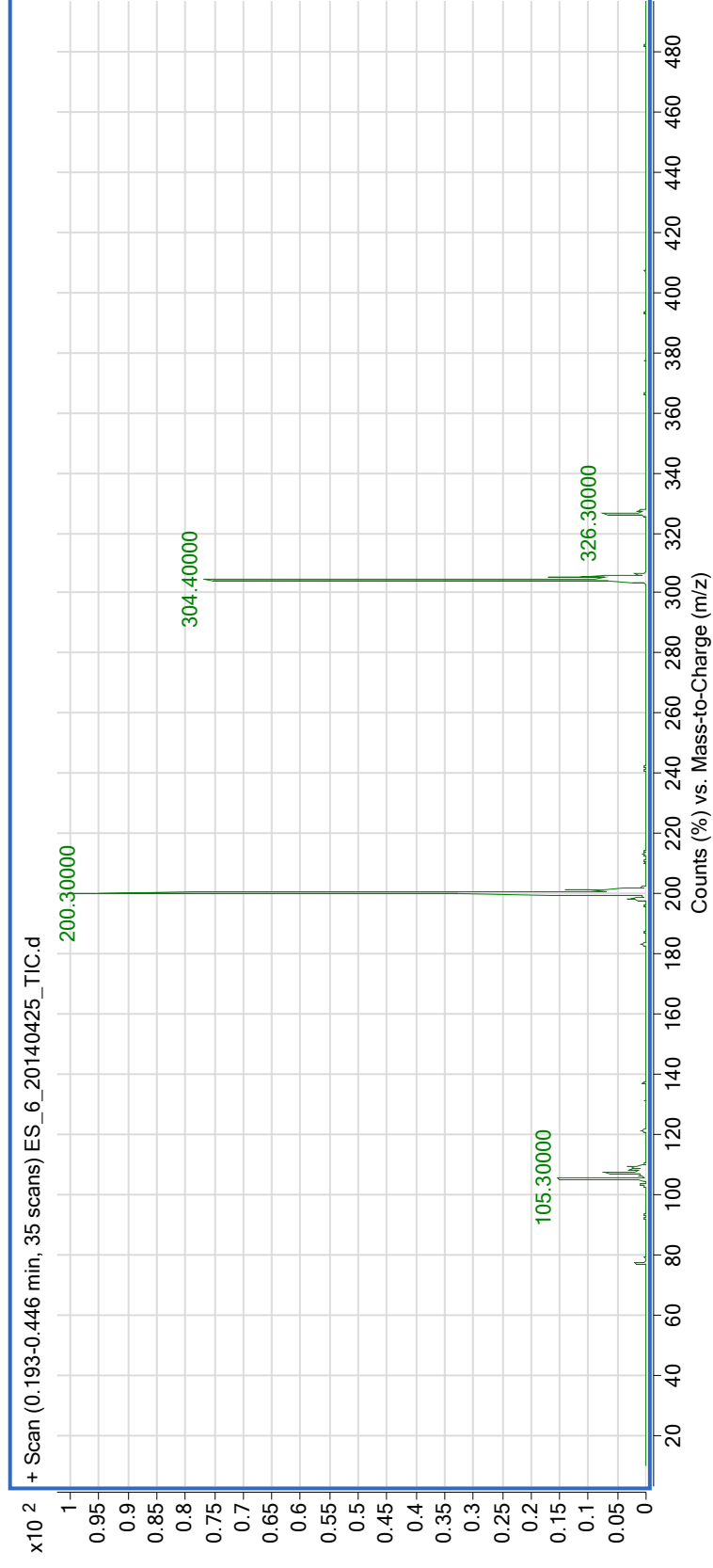
MS of L2. Bpa-CH₂-CO₂Me



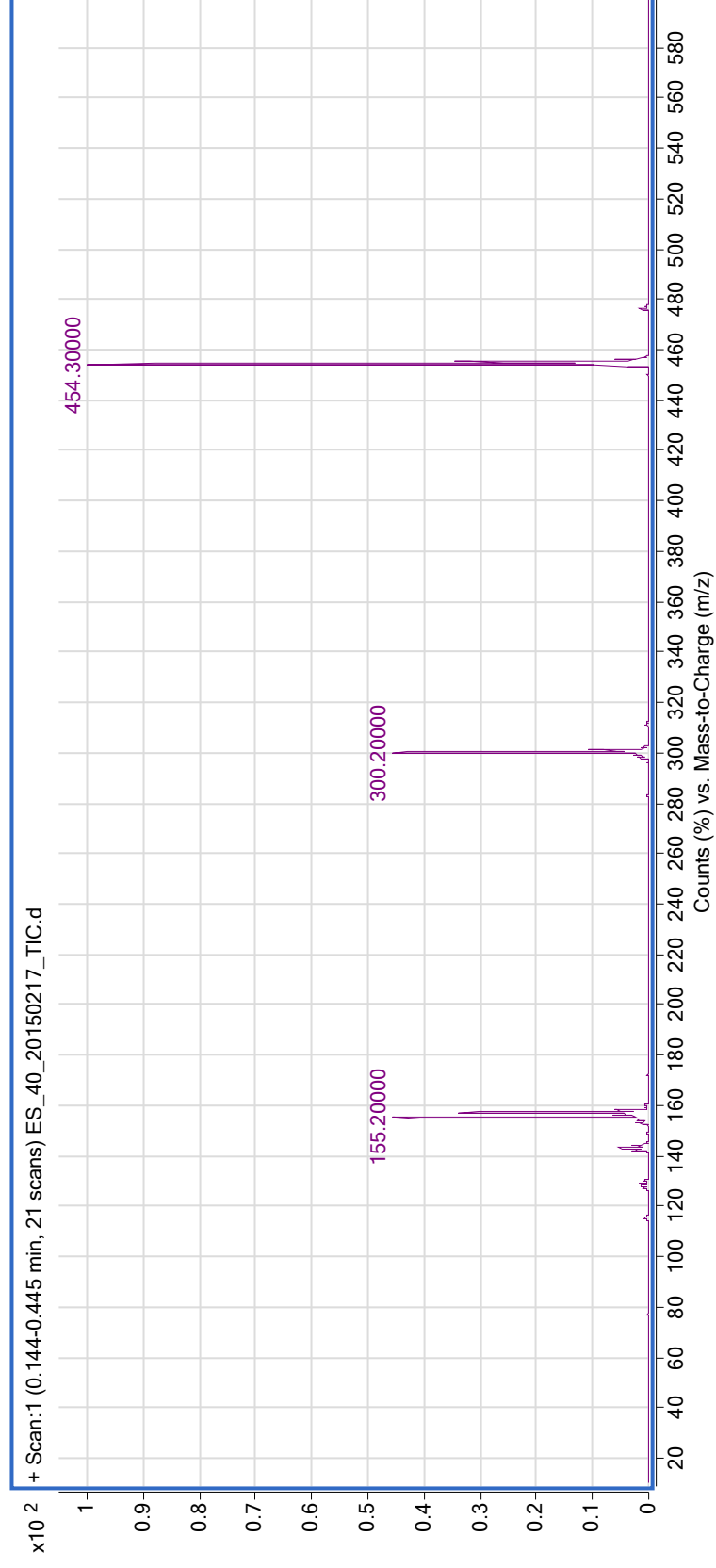
MS of ligand **L3. Bqa-CH₂-CO₂Me.**



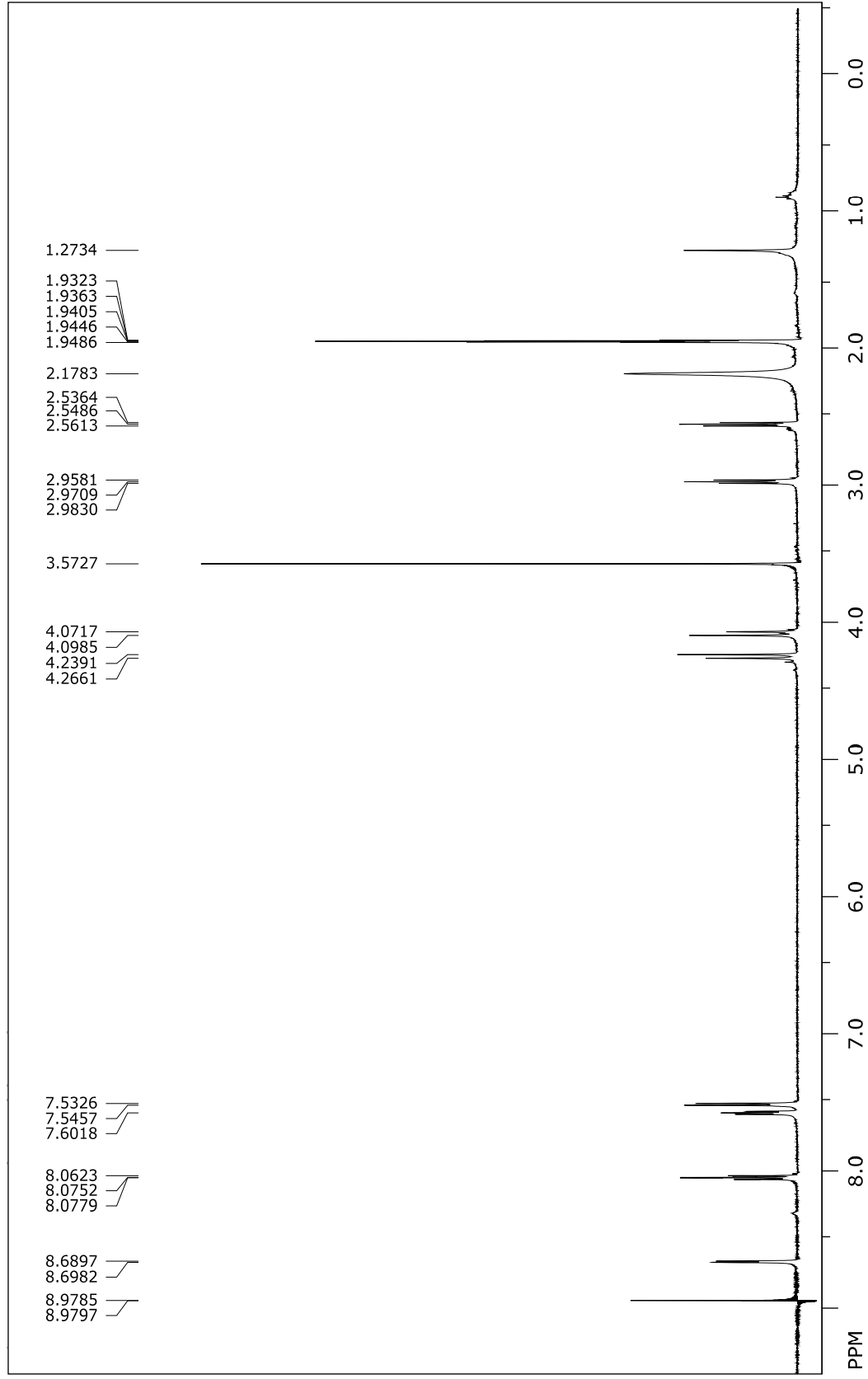
MS of ligand L4. Bpa-CH(CH₃)Ph.



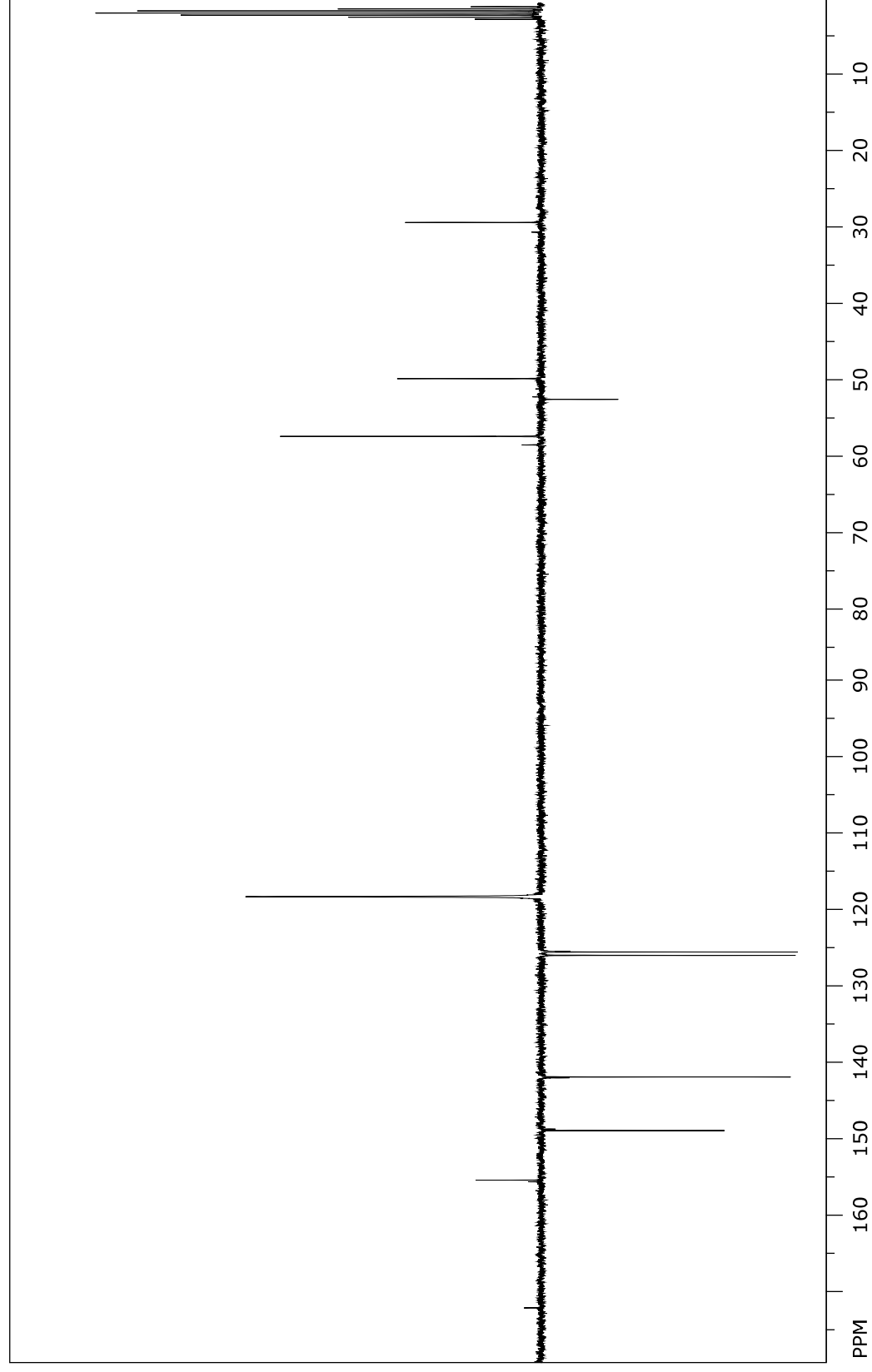
MS of ligand L5. **Bqa-CH(CH₃)Nph.**



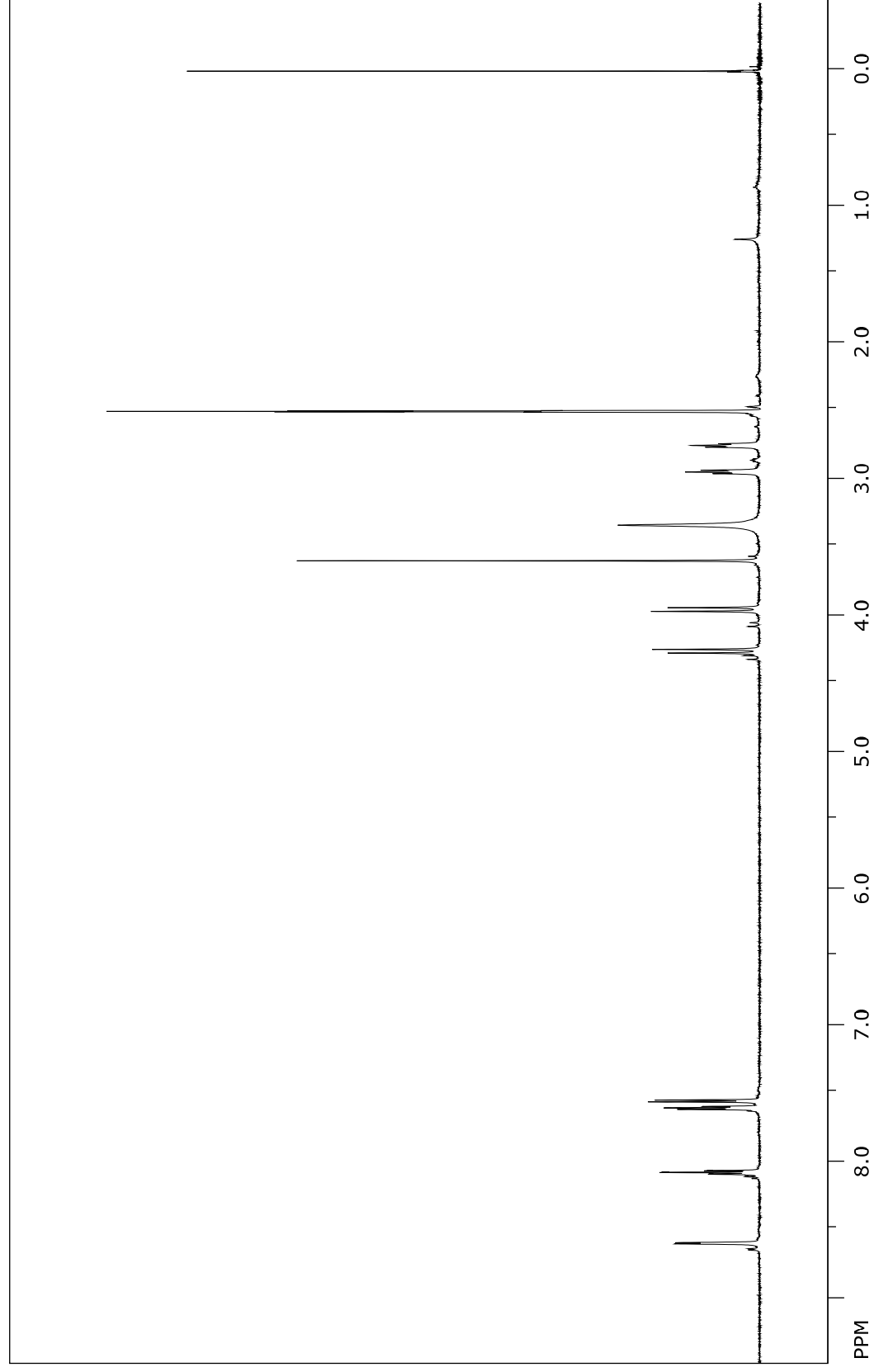
3. NMR spectra of ML complexes.
¹H NMR (600 MHz, CD₃CN) of complex **1n**. [Zn(L1)(NO₃)₂].



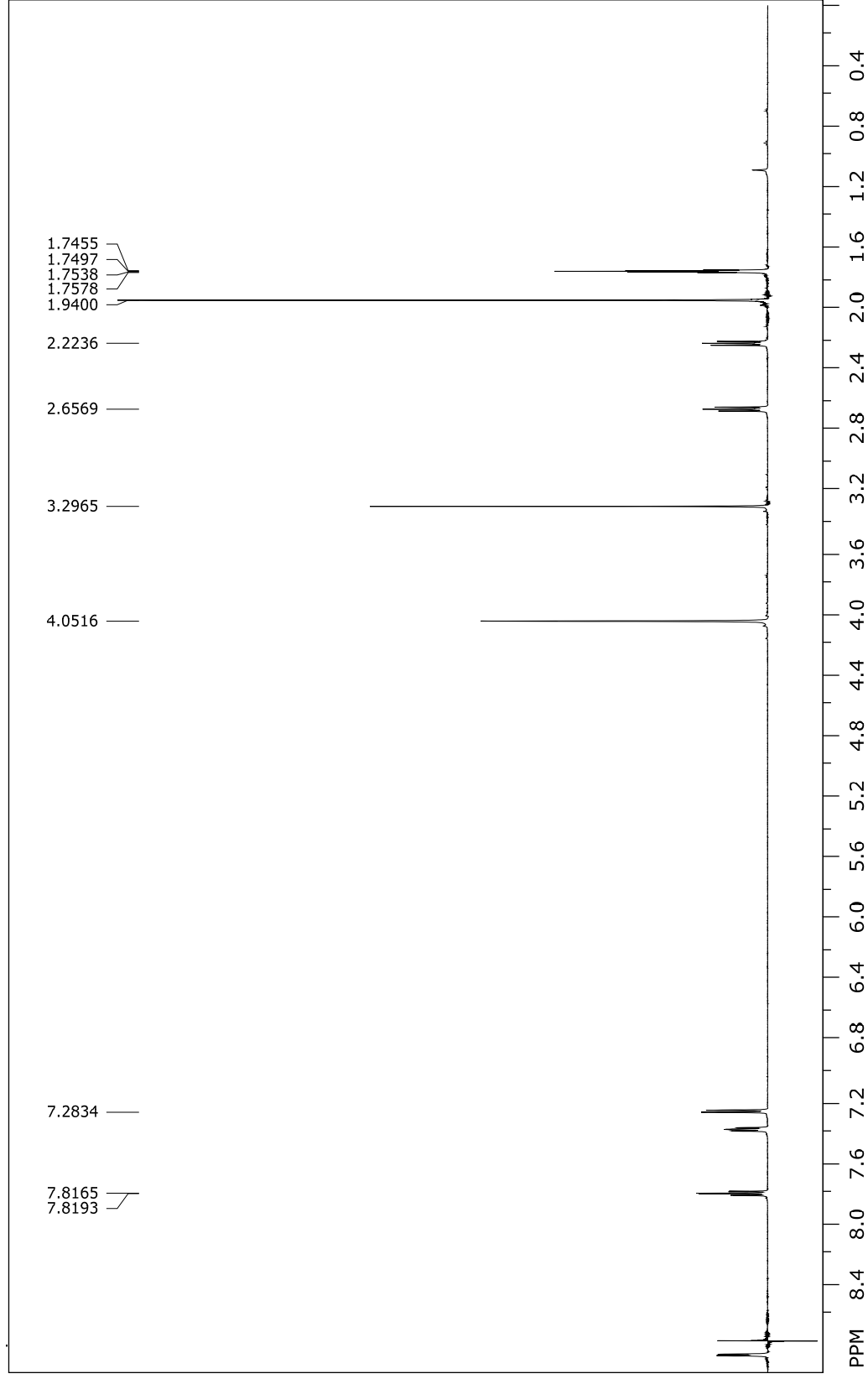
^{13}C NMR (75 MHz, CD_3CN) of complex **1n**. $[\text{Zn}(\text{L1})(\text{NO}_3)_2]$.



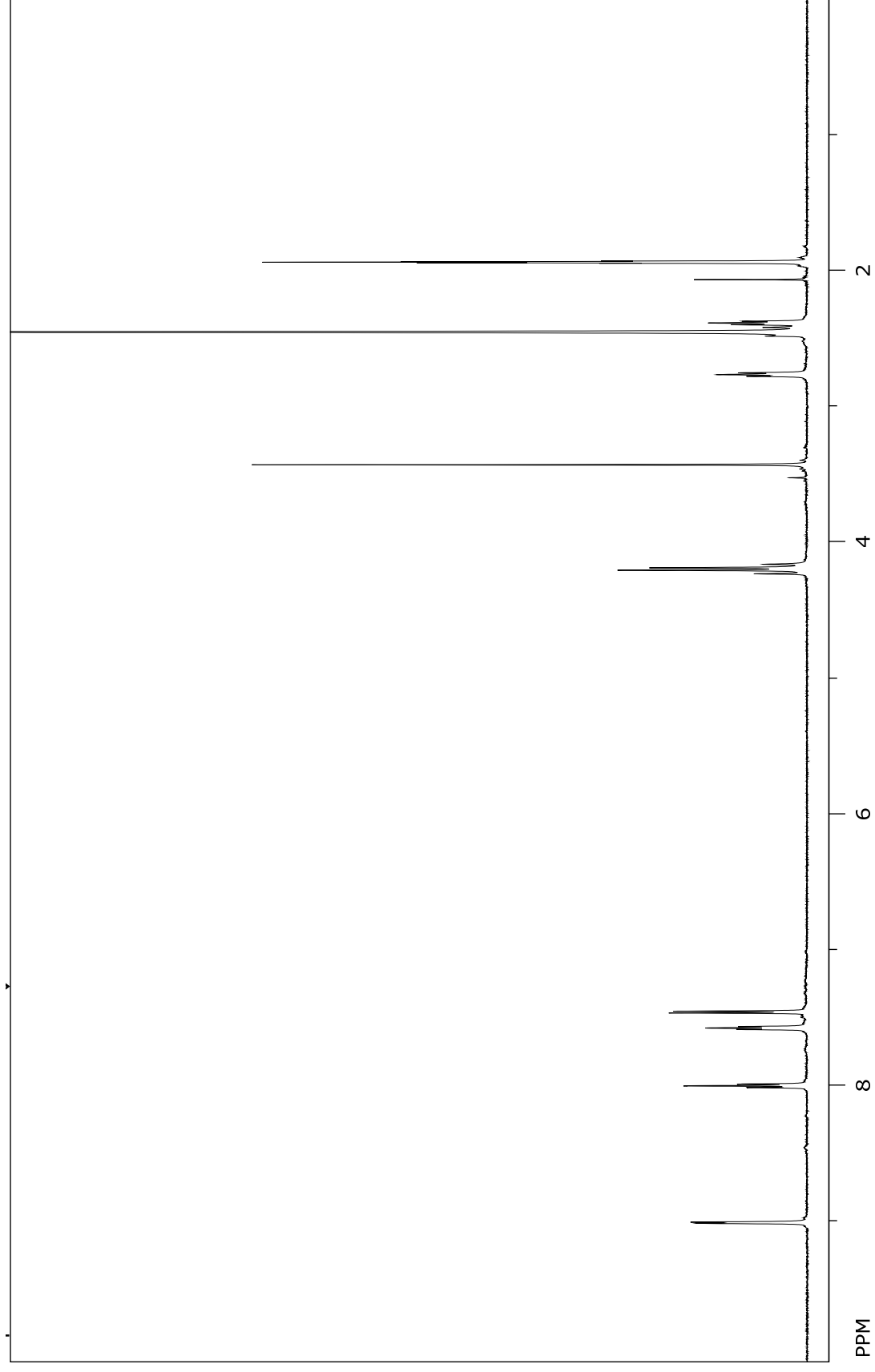
^1H NMR (600 MHz, DMSO- d_6) of complex **1n**. $[\text{Zn}(\text{L1})(\text{NO}_3)_2]$.



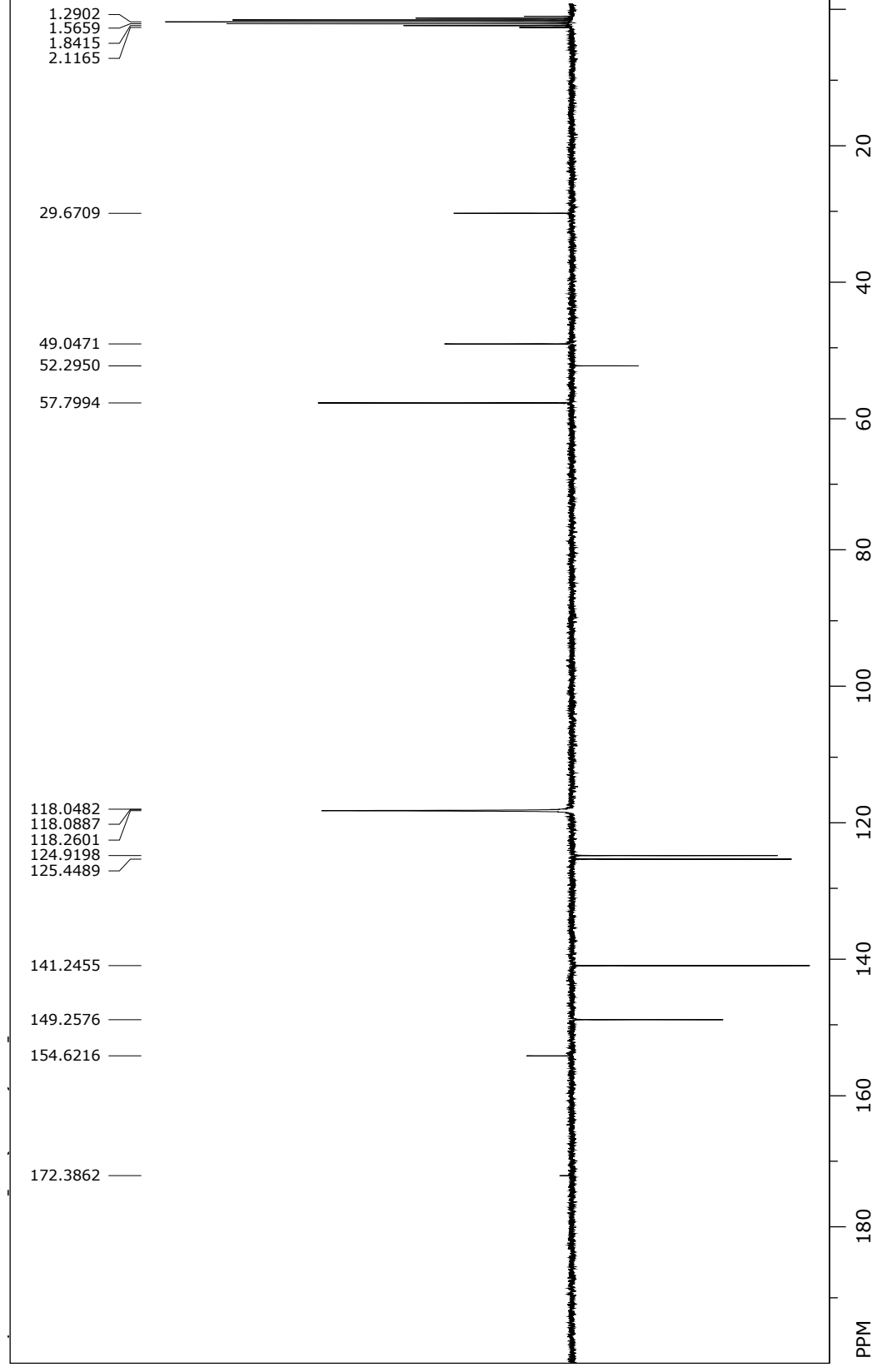
^1H NMR (600 MHz, CD_3CN) of complex **1b**. $[\text{Zn}(\text{L1})\text{Br}_2]$.



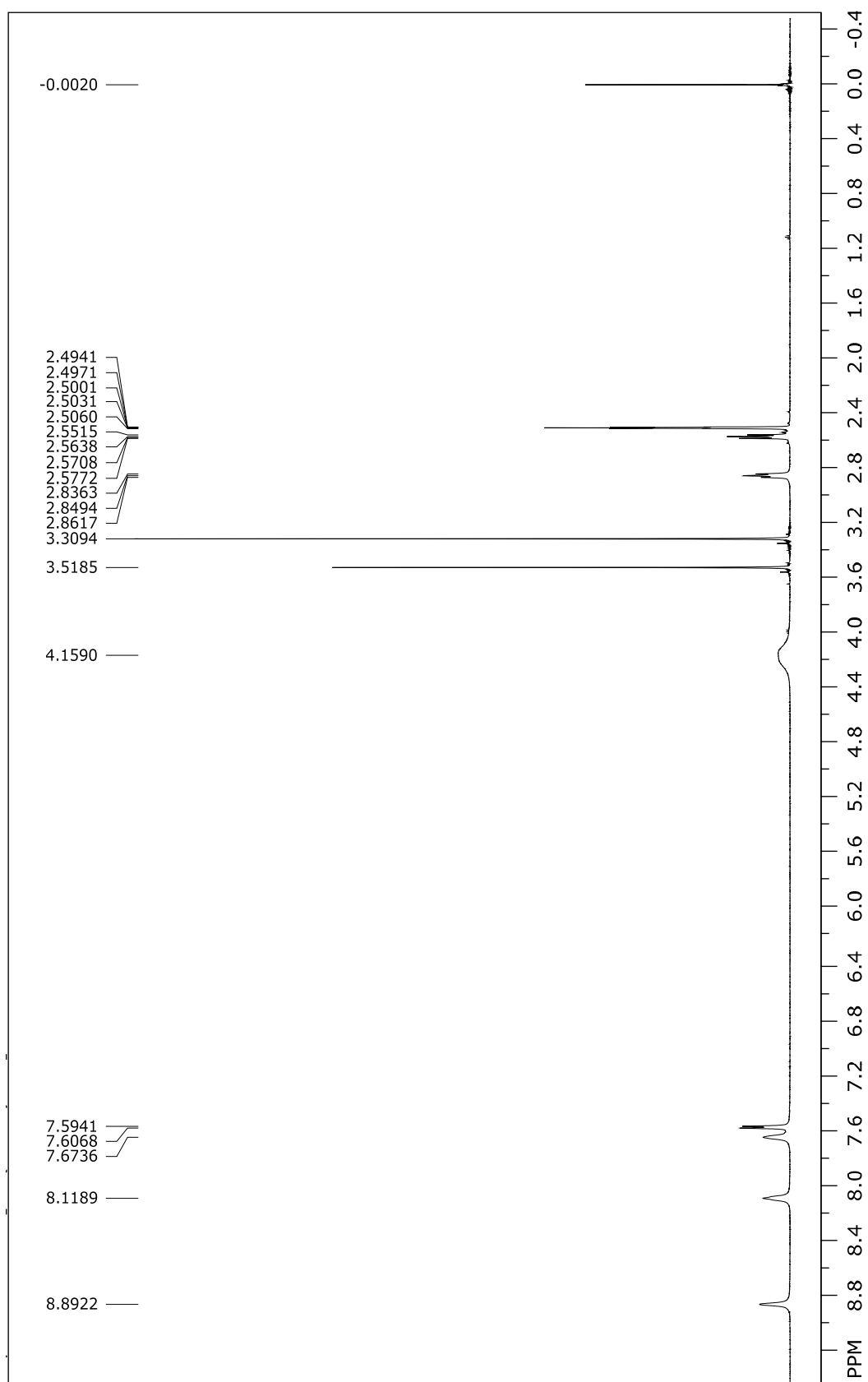
^1H NMR (600 MHz, CD_3CN) at -40°C of complex **1b**. $[\text{Zn}(\text{L1})\text{Br}_2]$.



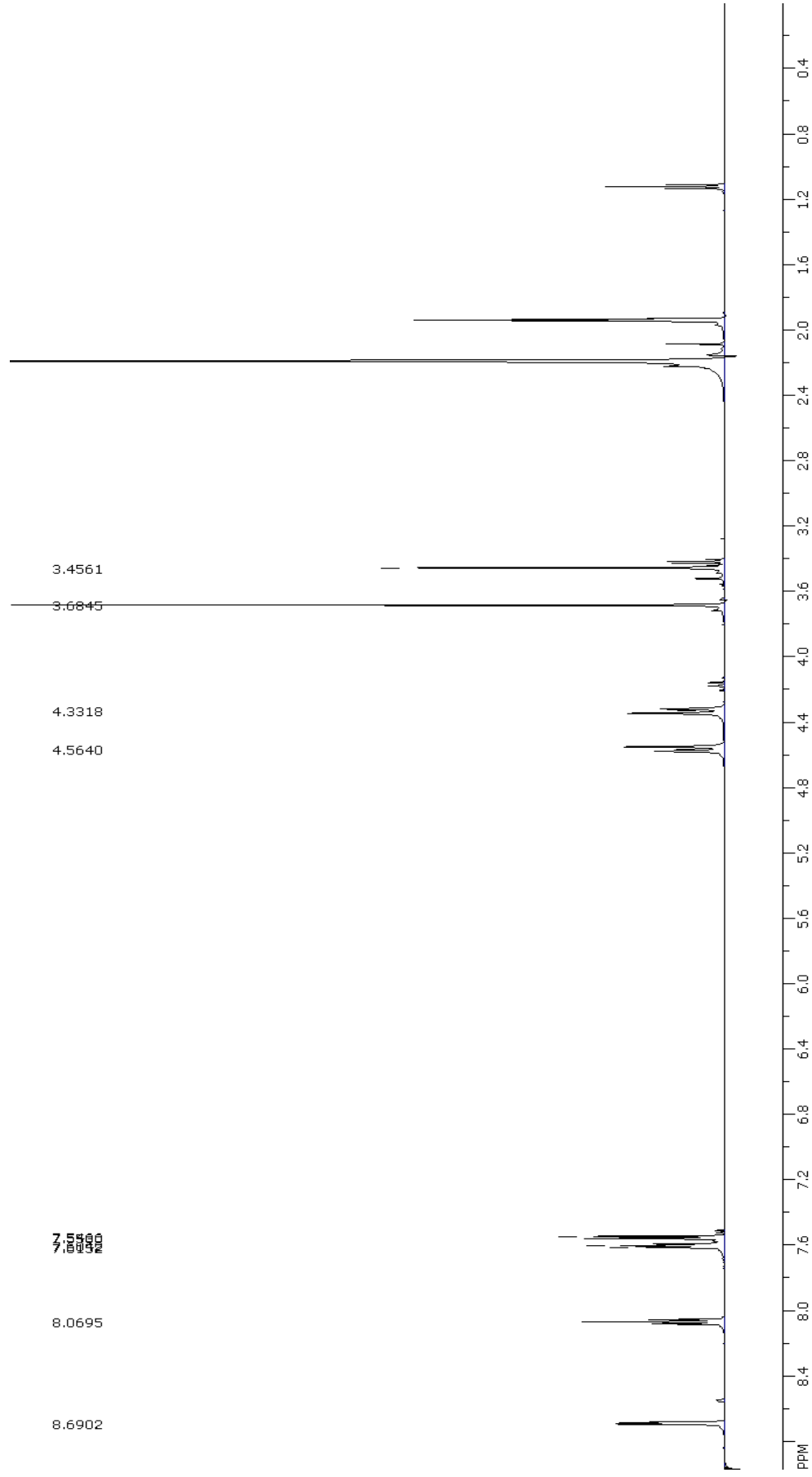
^{13}C NMR (75 MHz, CD_3CN) of complex **1b**. $[\text{Zn}(\text{L1})\text{Br}_2]$.



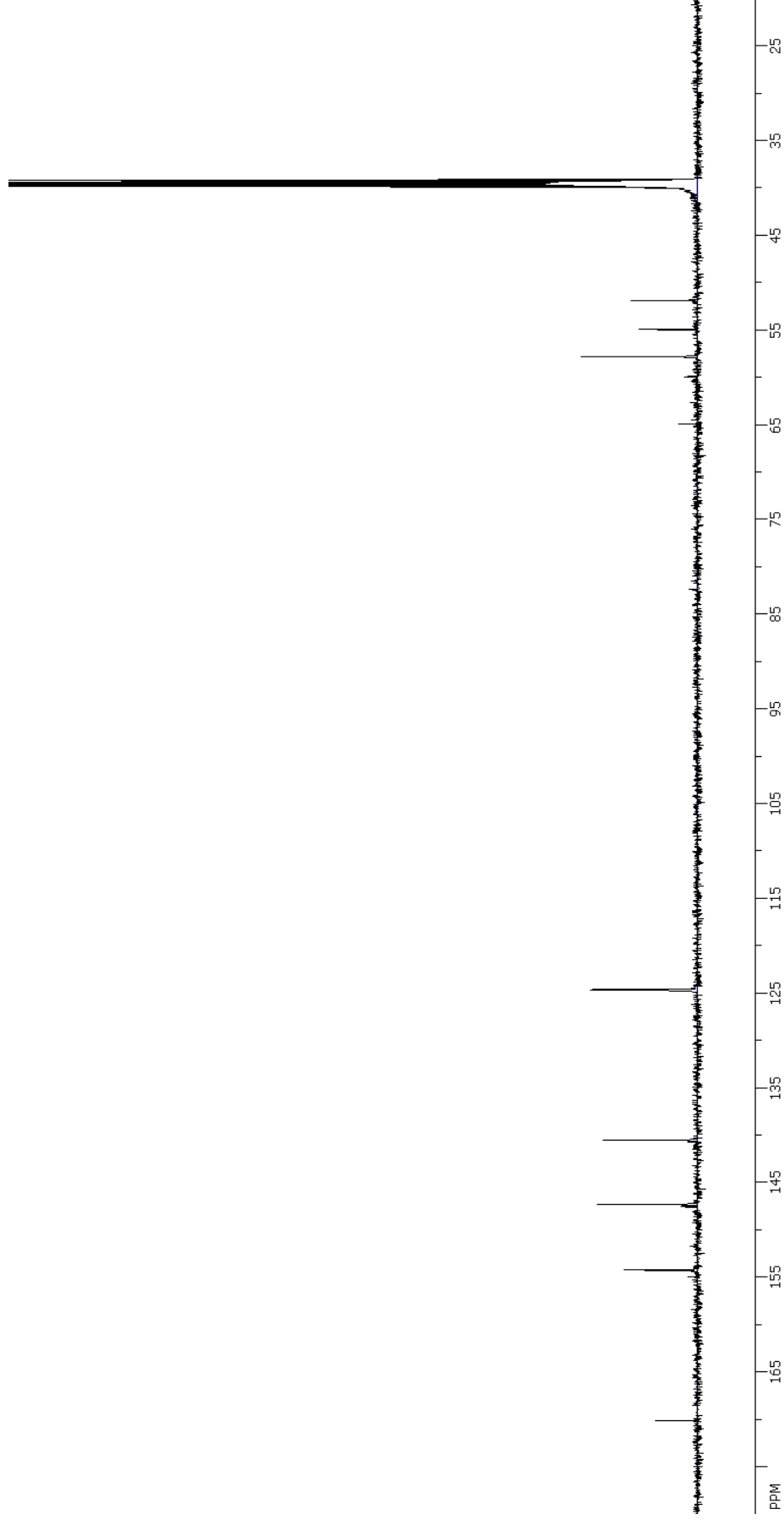
¹H NMR (600 MHz, DMSO-d₆) of complex **1b**. [Zn(L1)Br₂].



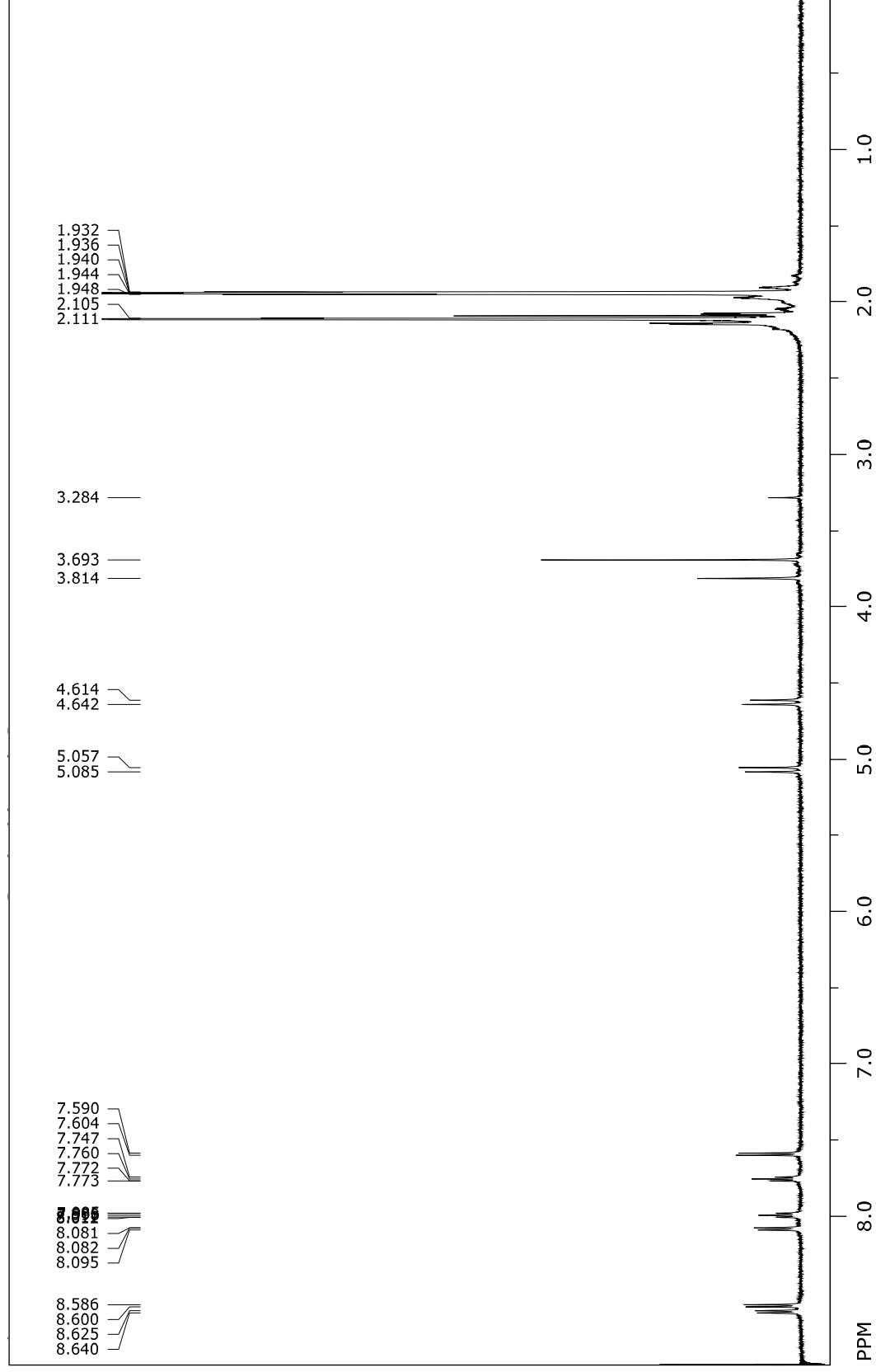
^1H NMR (600 MHz, CD_3CN) of complex **2n**. $[\text{Zn}(\text{L2})(\text{NO}_3)_2]$.



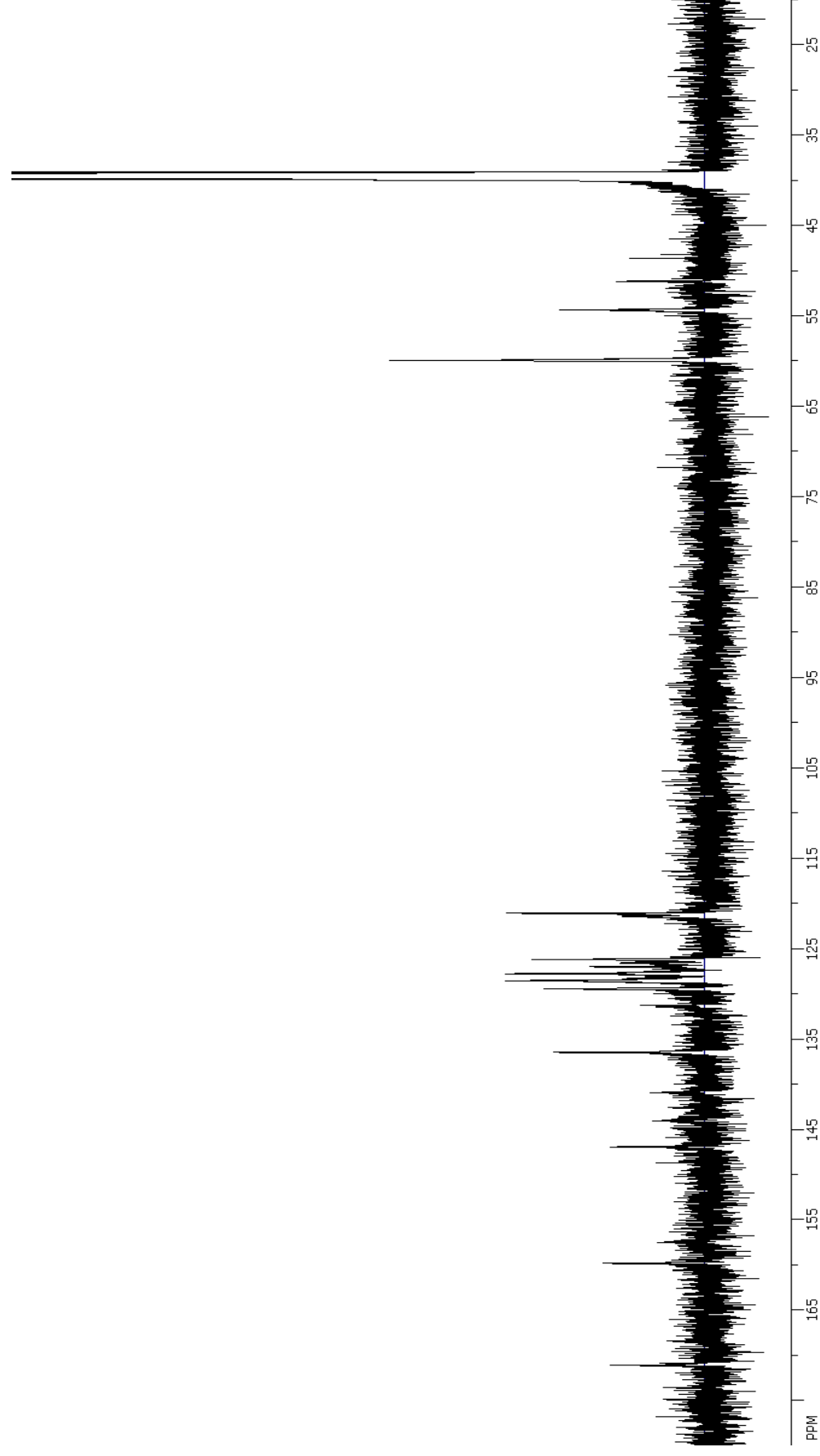
^{13}C NMR (150 MHz, DMSO- d_6) of complex **2n**. $[\text{Zn}(\text{L2})(\text{NO}_3)_2]$.



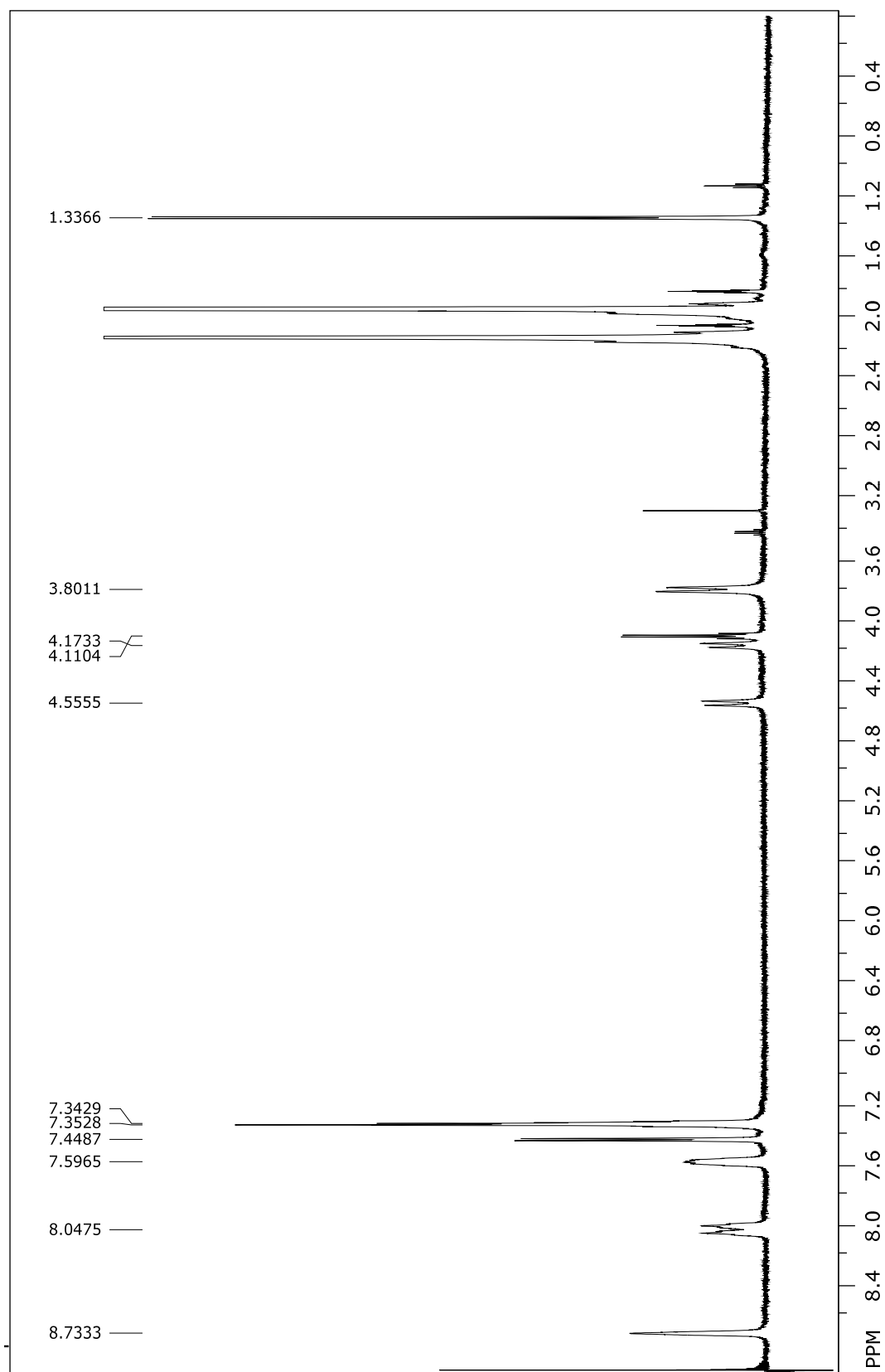
^1H NMR (600 MHz, CD_3CN) of complex **3n**. $[\text{Zn}(\text{L3})(\text{NO}_3)_2]$.



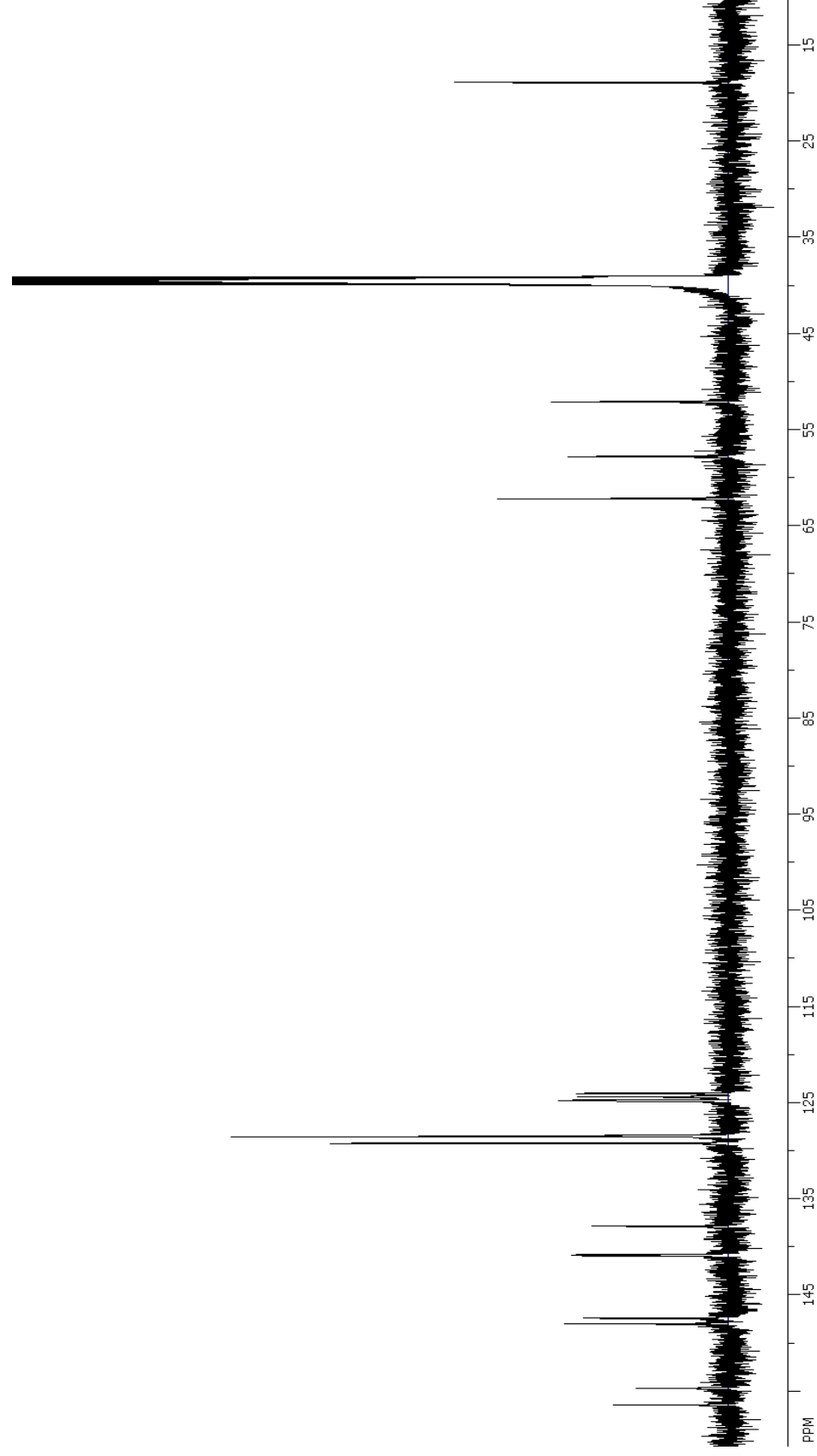
^{13}C NMR (150 MHz, DMSO- d_6) of complex **3n**. $[\text{Zn}(\text{L3})(\text{NO}_3)_2]$.



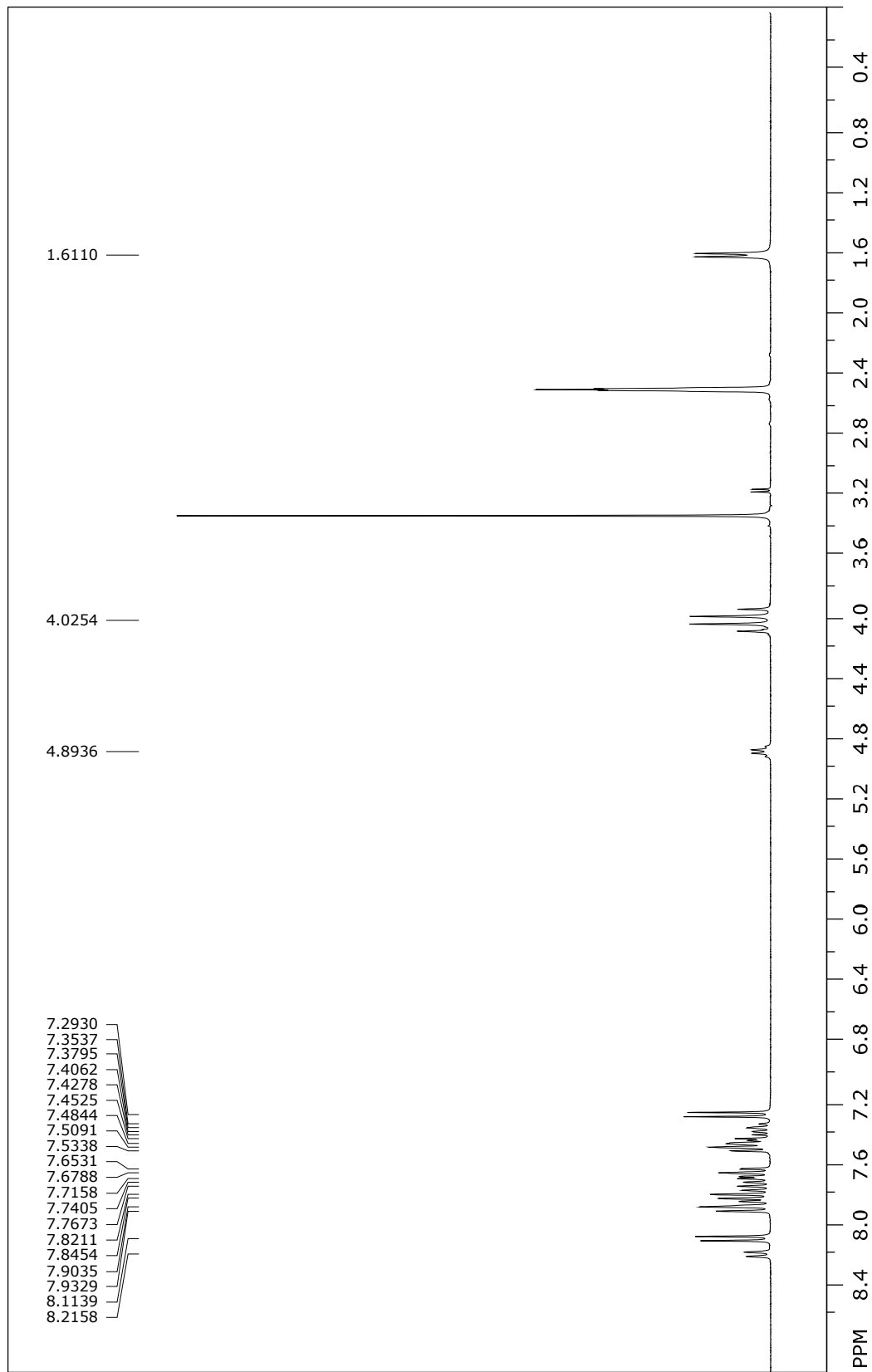
¹H NMR (600 MHz, CD₃CN) of complex **4n**. [Zn(L4)(NO₃)₂].



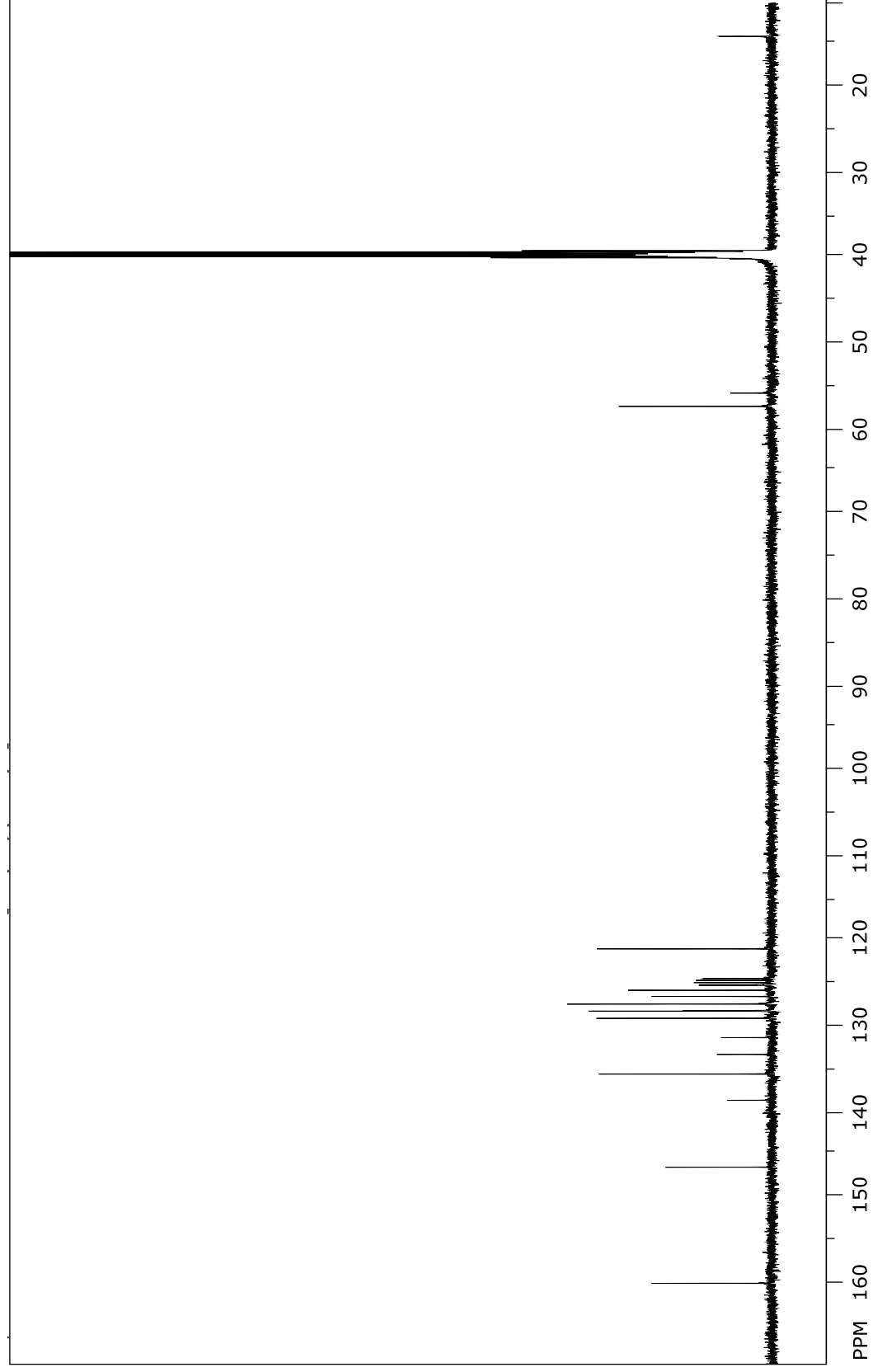
^{13}C NMR (150 MHz, DMSO- d_6) of complex **4n**. $[\text{Zn}(\text{L4})(\text{NO}_3)_2]$.



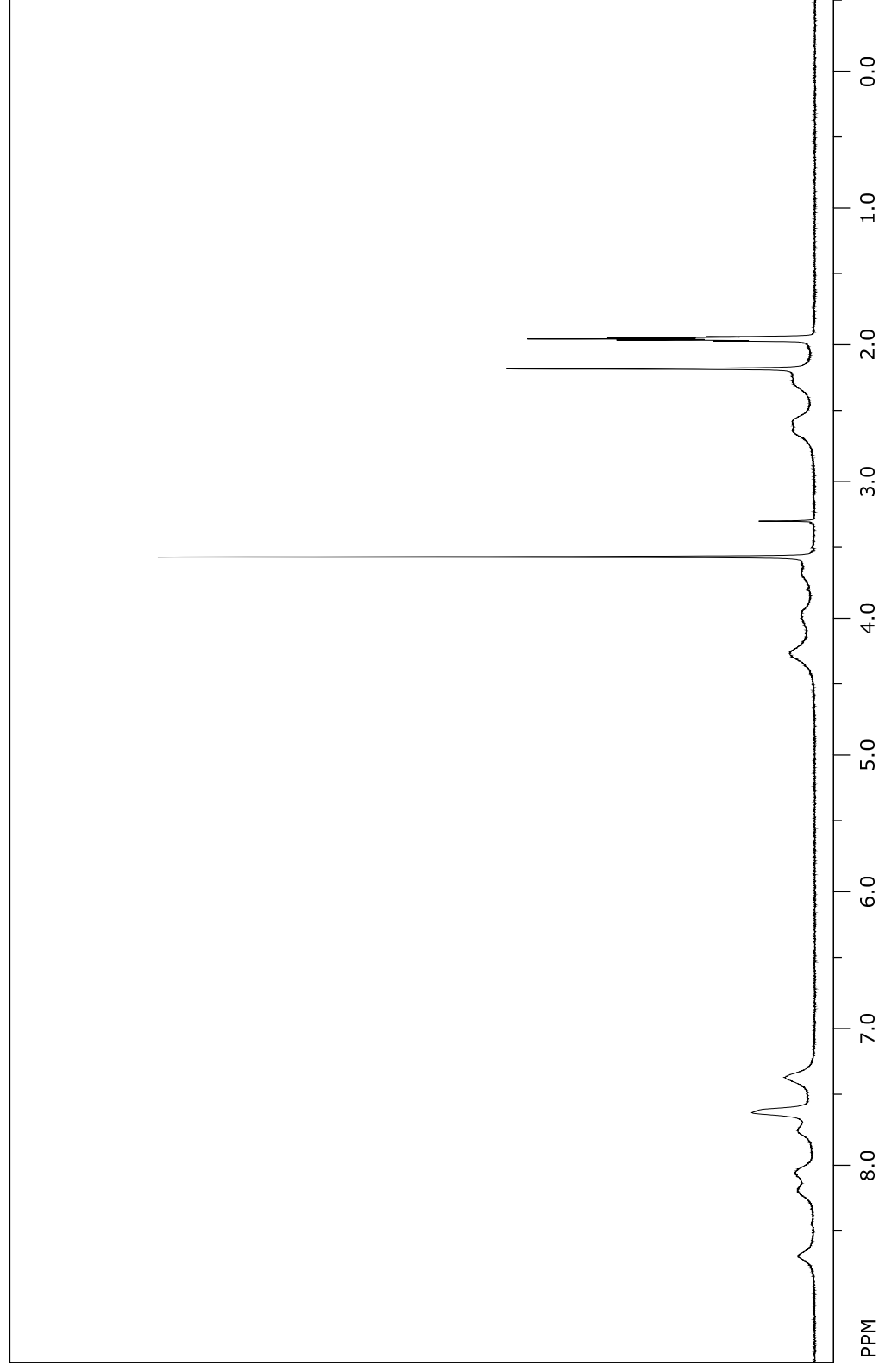
^1H NMR (300 MHz, DMSO-d_6) of complex **5n**. $[\text{Zn}(\text{L5})(\text{NO}_3)_2]$.



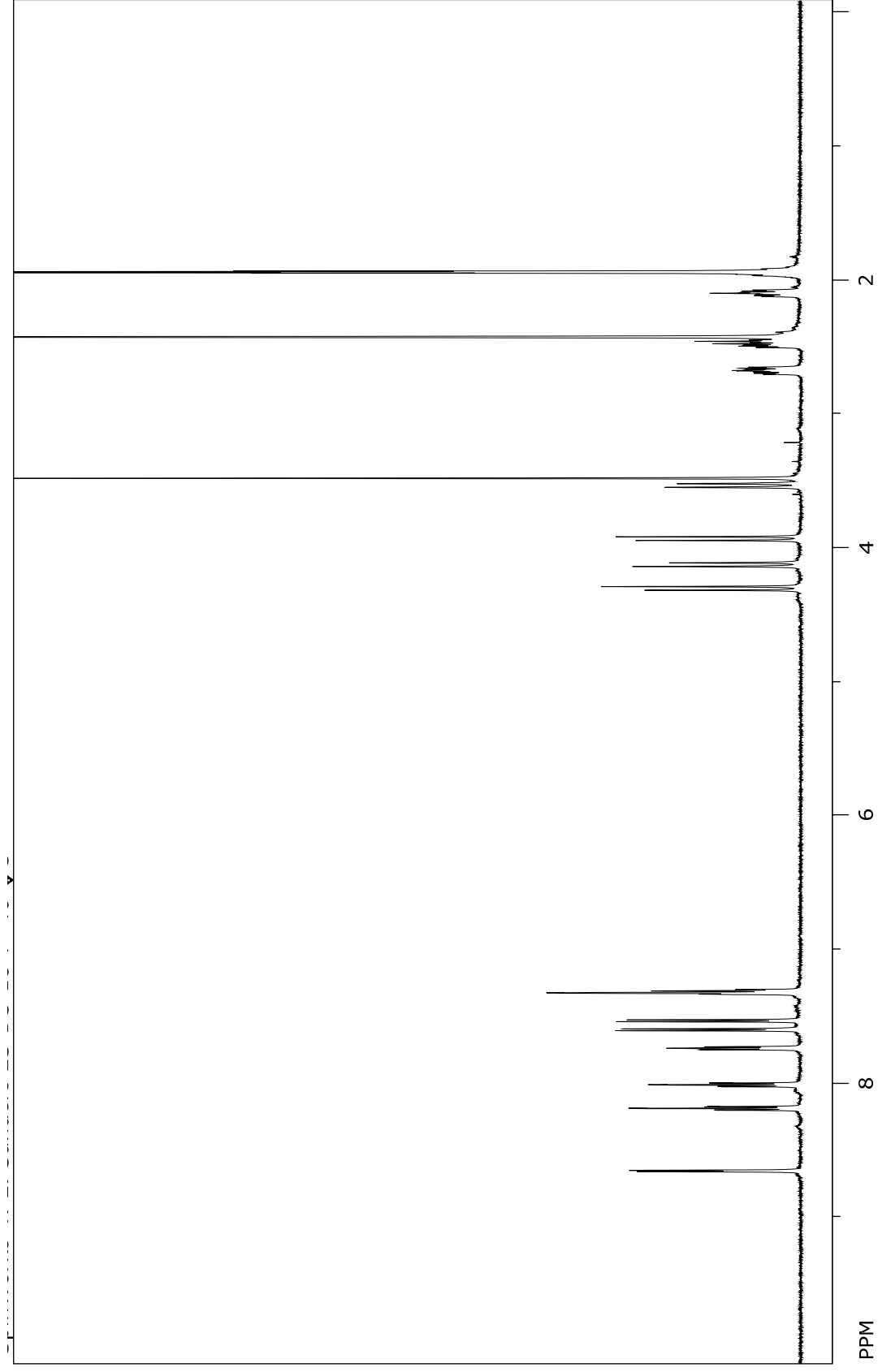
^{13}C NMR (150 MHz, DMSO- d_6) of complex **5n**. $[\text{Zn}(\text{L5})(\text{NO}_3)_2]$.



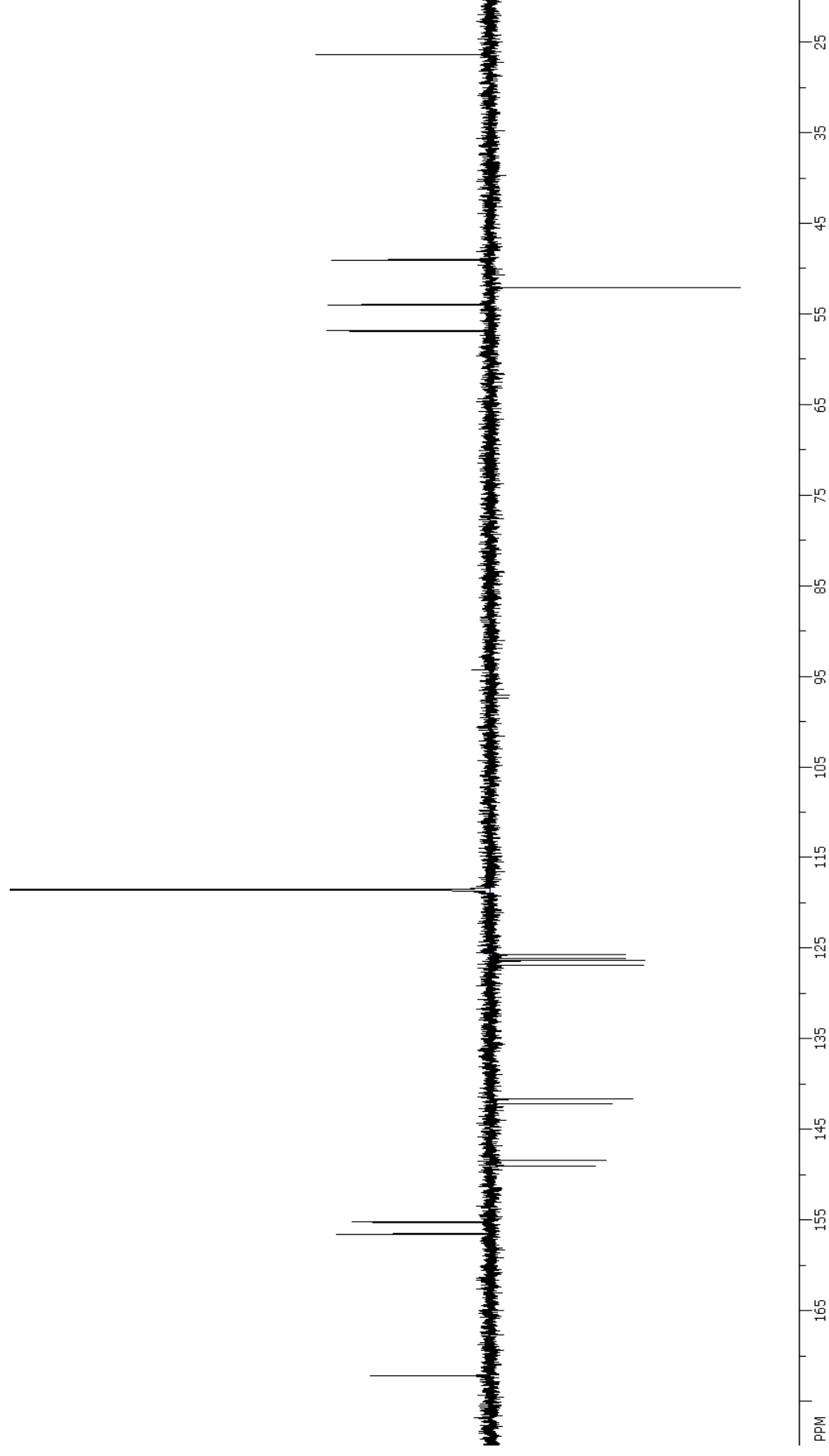
4. NMR spectra of complex **1₂Zn**. ¹H NMR spectra of complex **1₂Zn**.

¹H NMR (300 MHz, CD₃CN) of complex **1**₂Zn. [Zn(L1)₂](BF₄)₂.

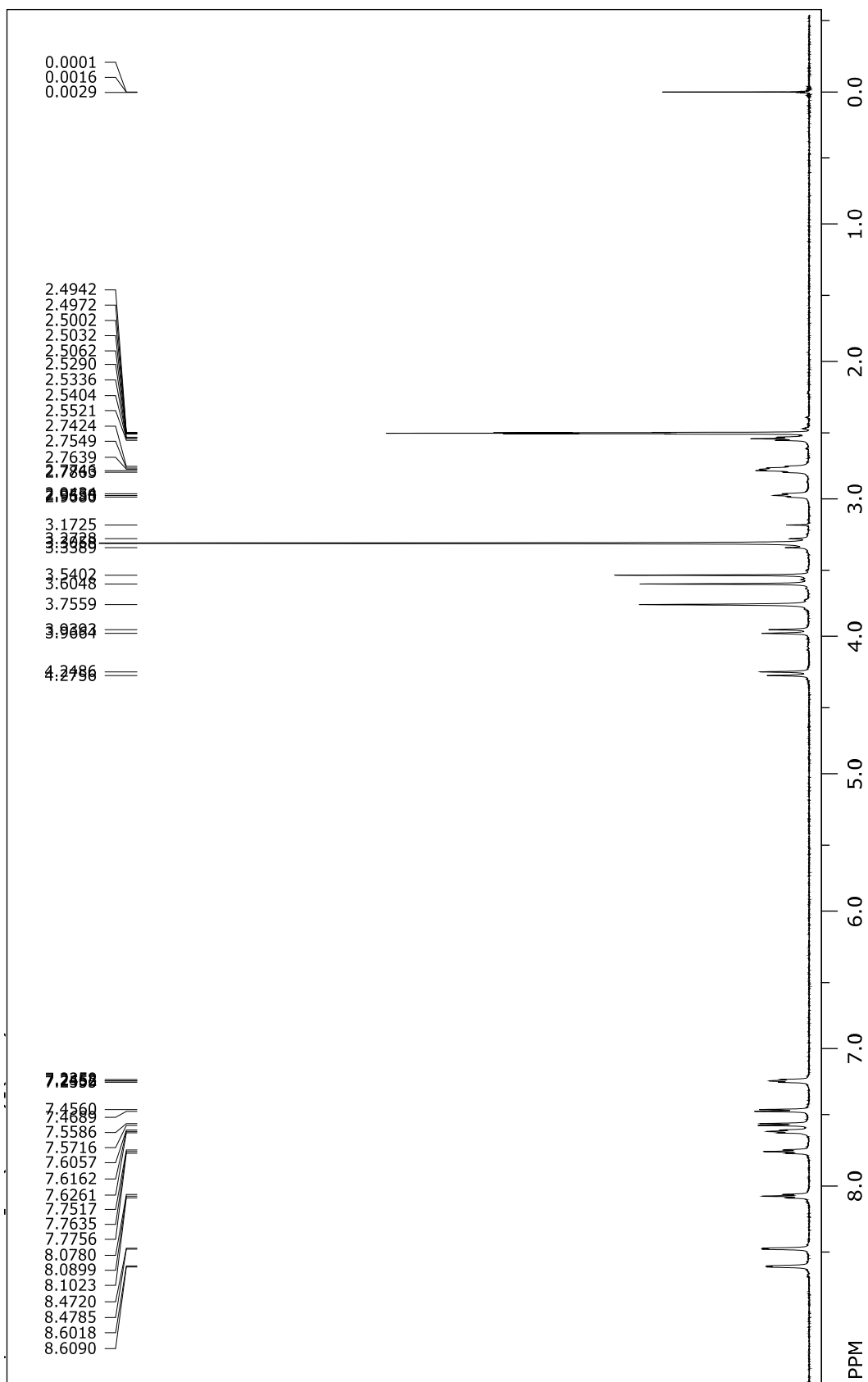
^1H NMR (600 MHz, CD_3CN) at -40°C of complex $\mathbf{1}_2\text{Zn}$. $[\text{Zn}(\text{L1})_2](\text{BF}_4)_2$.



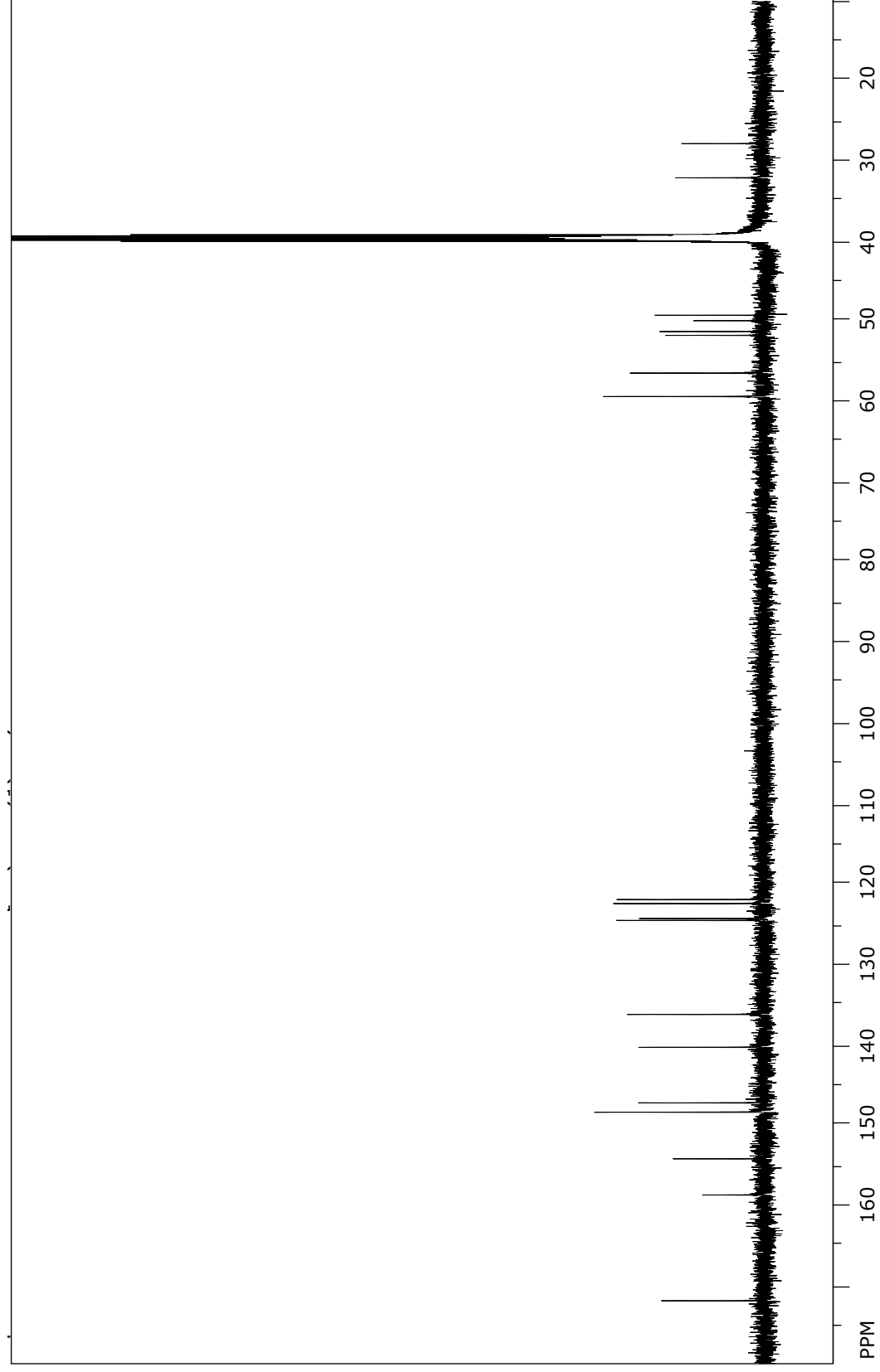
^{13}C NMR (150 MHz, CD_3CN) at -40°C of complex 1_2Zn . $[\text{Zn}(\text{L1})_2](\text{BF}_4)_2$.



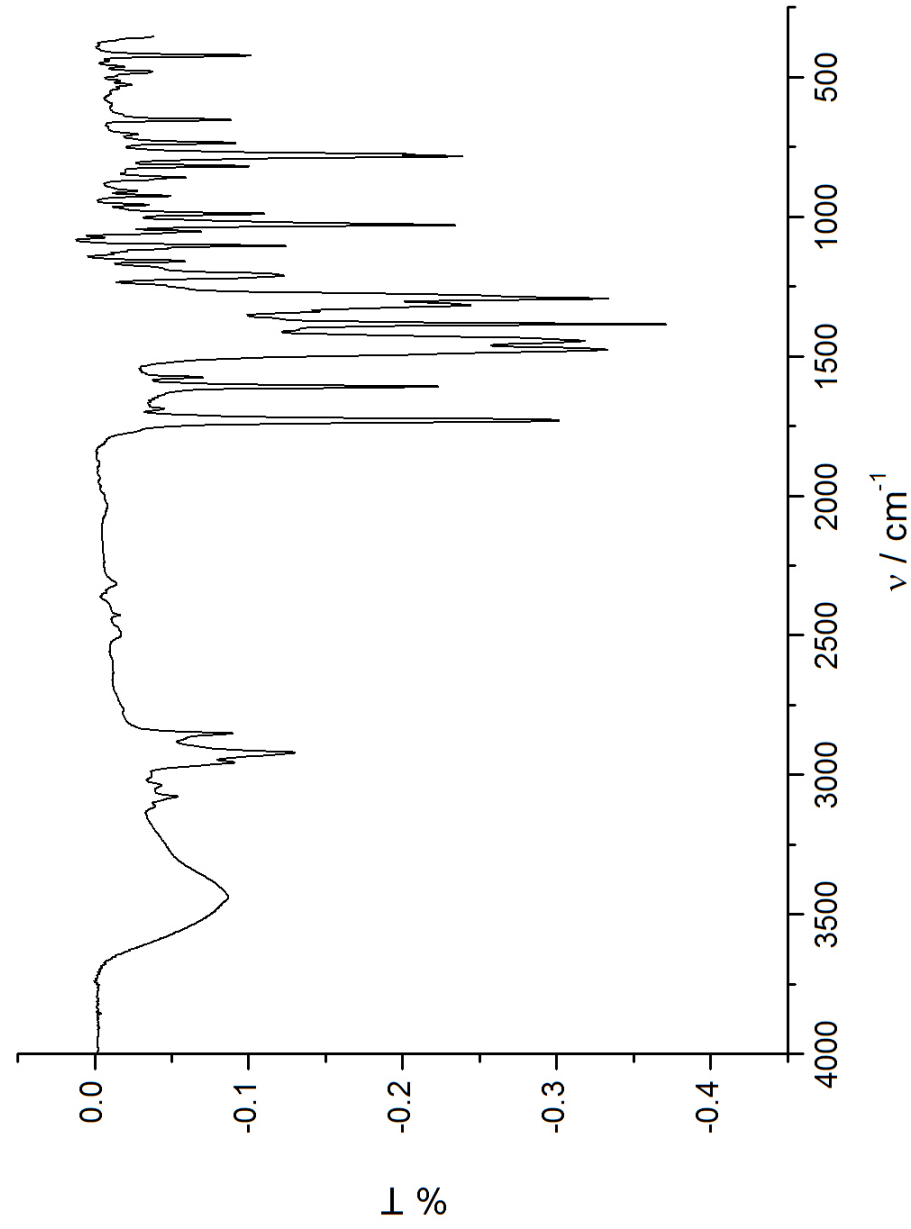
^1H NMR (600 MHz, DMSO- d_6) of complex $1_2\text{Zn} \cdot [\text{Zn}(\text{L}1)_2](\text{BF}_4)_2$.



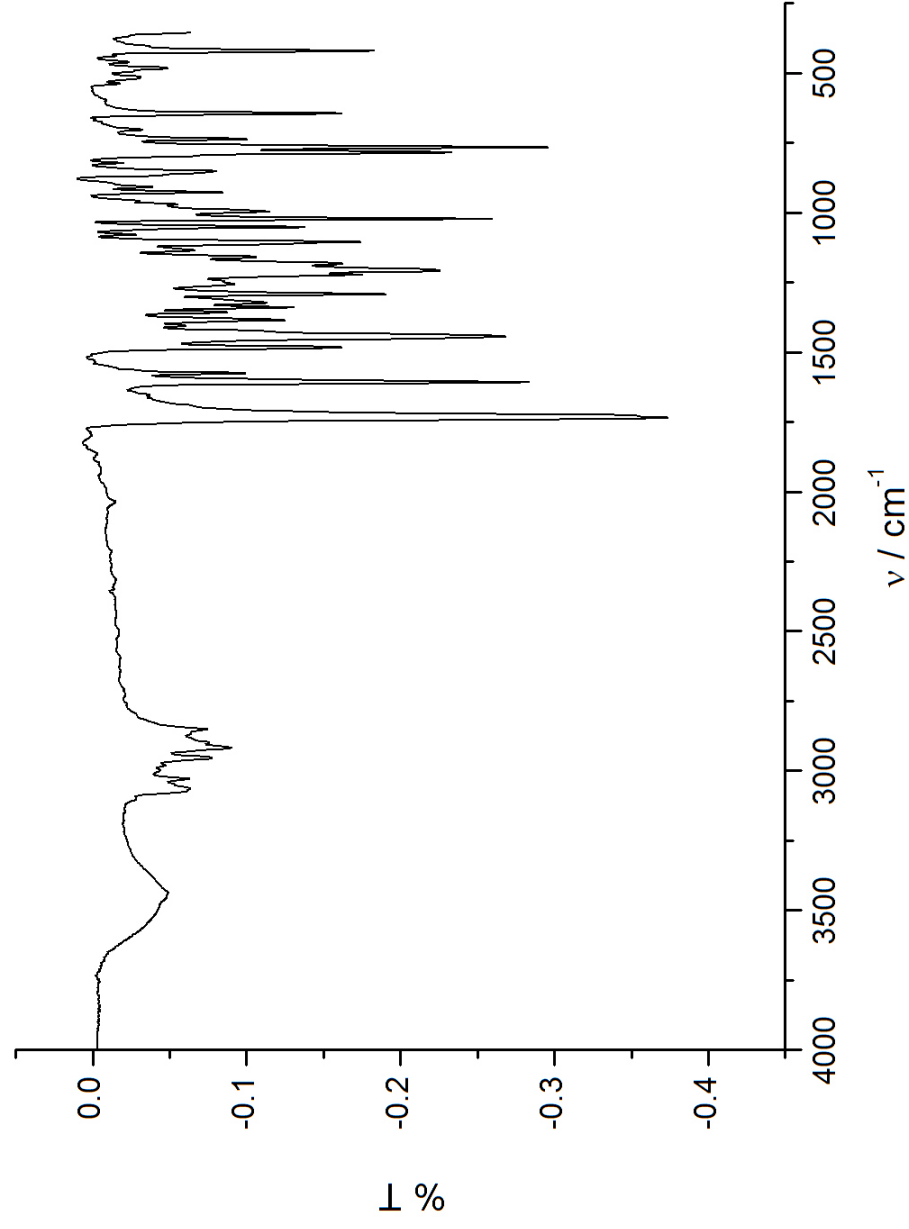
^{13}C NMR (75 MHz, DMSO- d_6) of complex 1_2Zn . $[\text{Zn}(\text{L1})_2](\text{BF}_4)_2$.



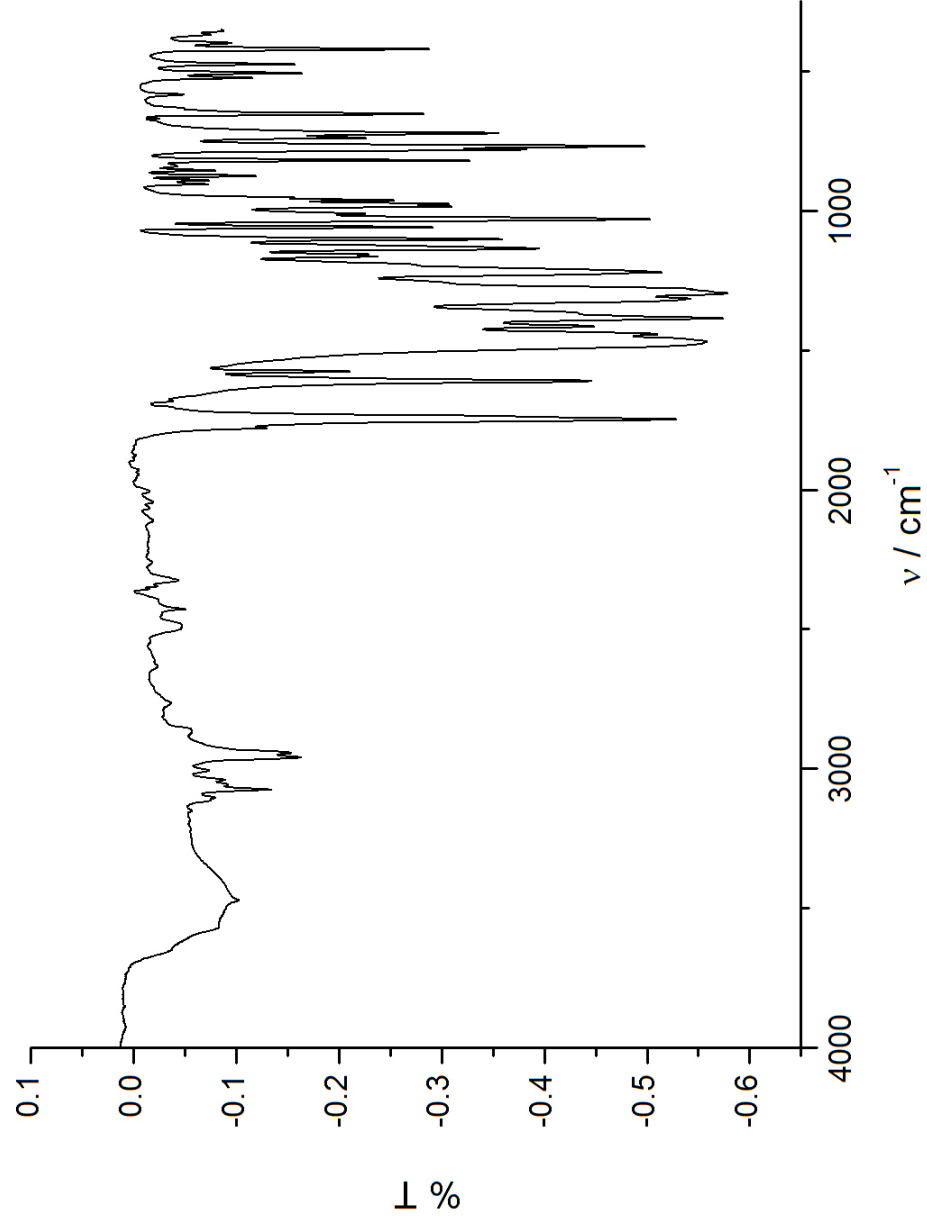
5. IR spectra of metal complexes.
IR (KBr) of complex **1n**. $[\text{Zn}(\text{L1})(\text{NO}_3)_2]$.



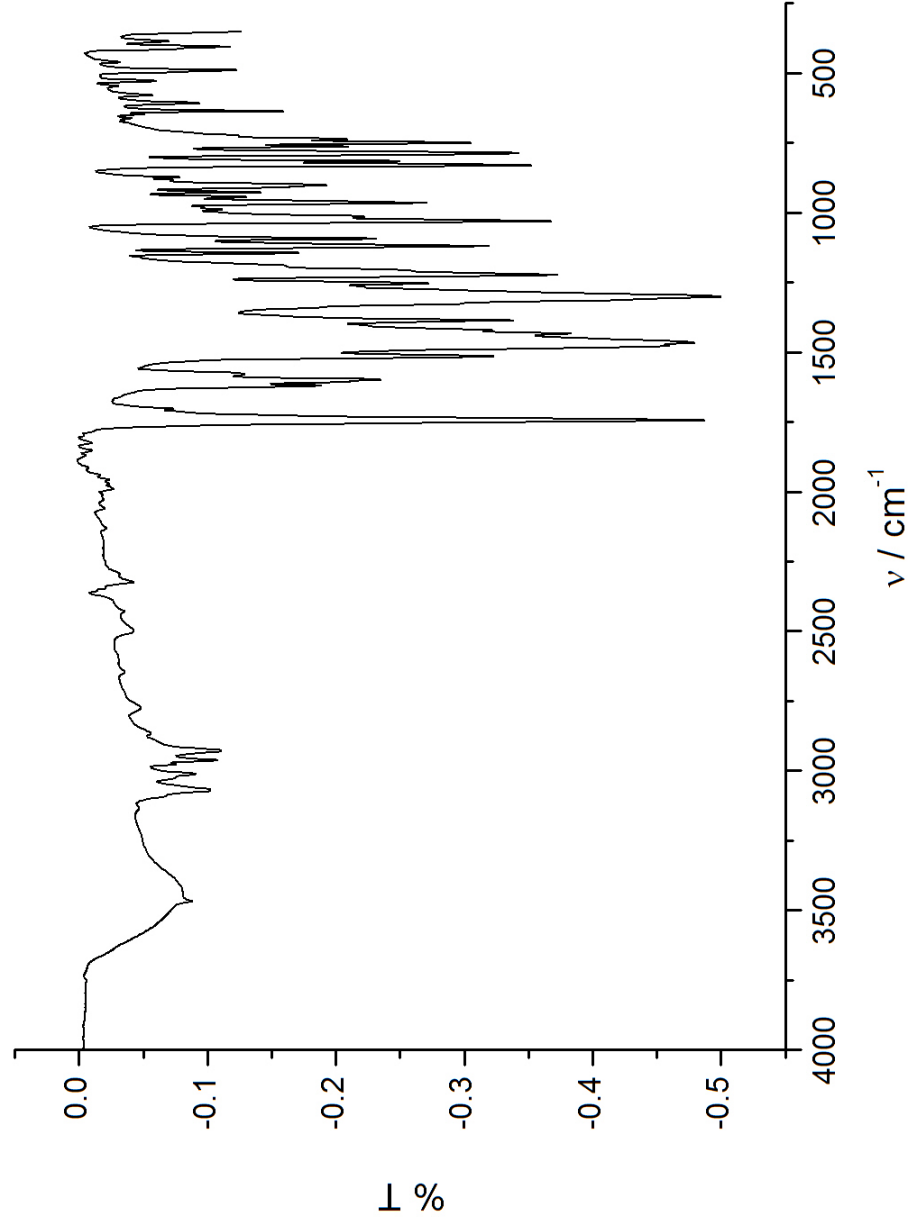
IR (KBr) of complex **1b**. [Zn(L1)Br₂].



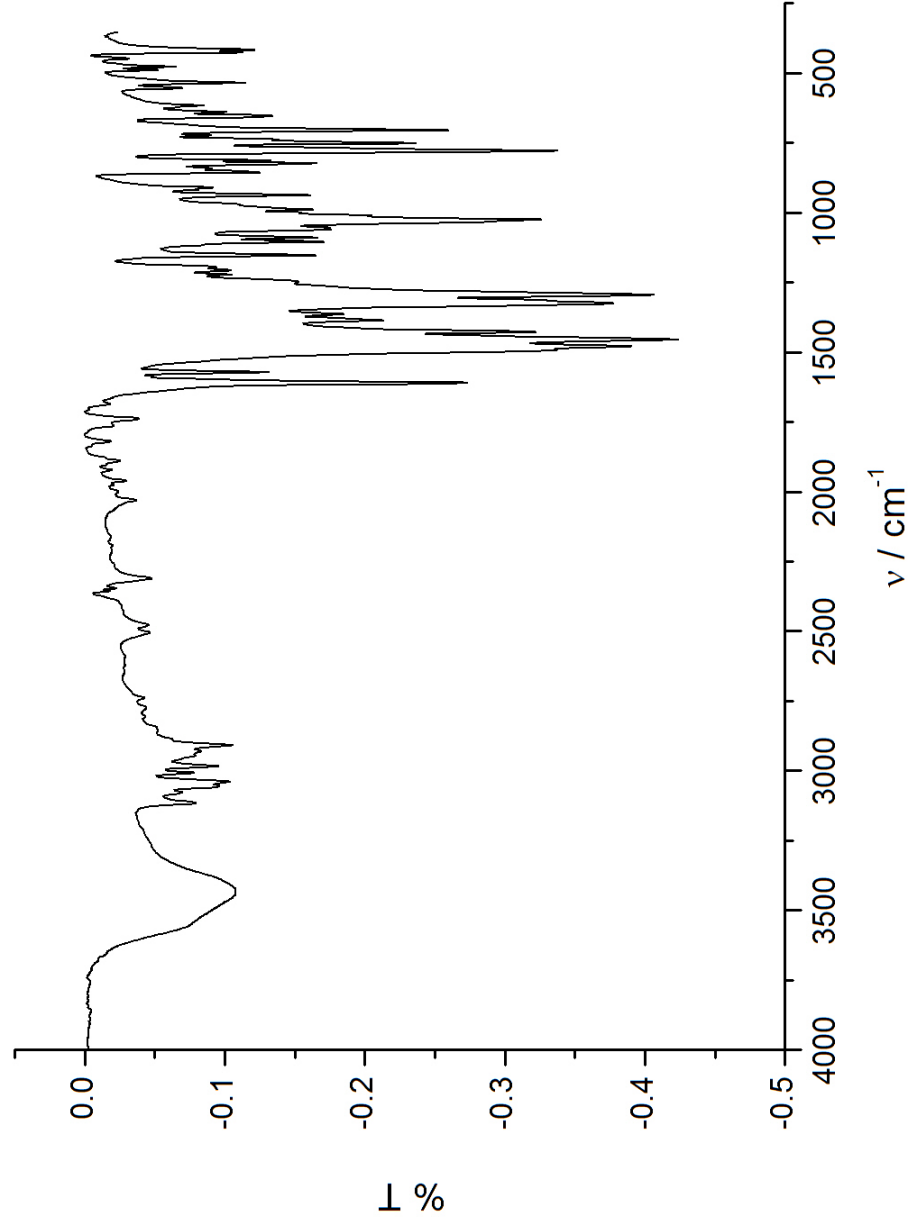
IR (KBr) of complex **2n**. $[\text{Zn}(\text{L2})(\text{NO}_3)_2]$.



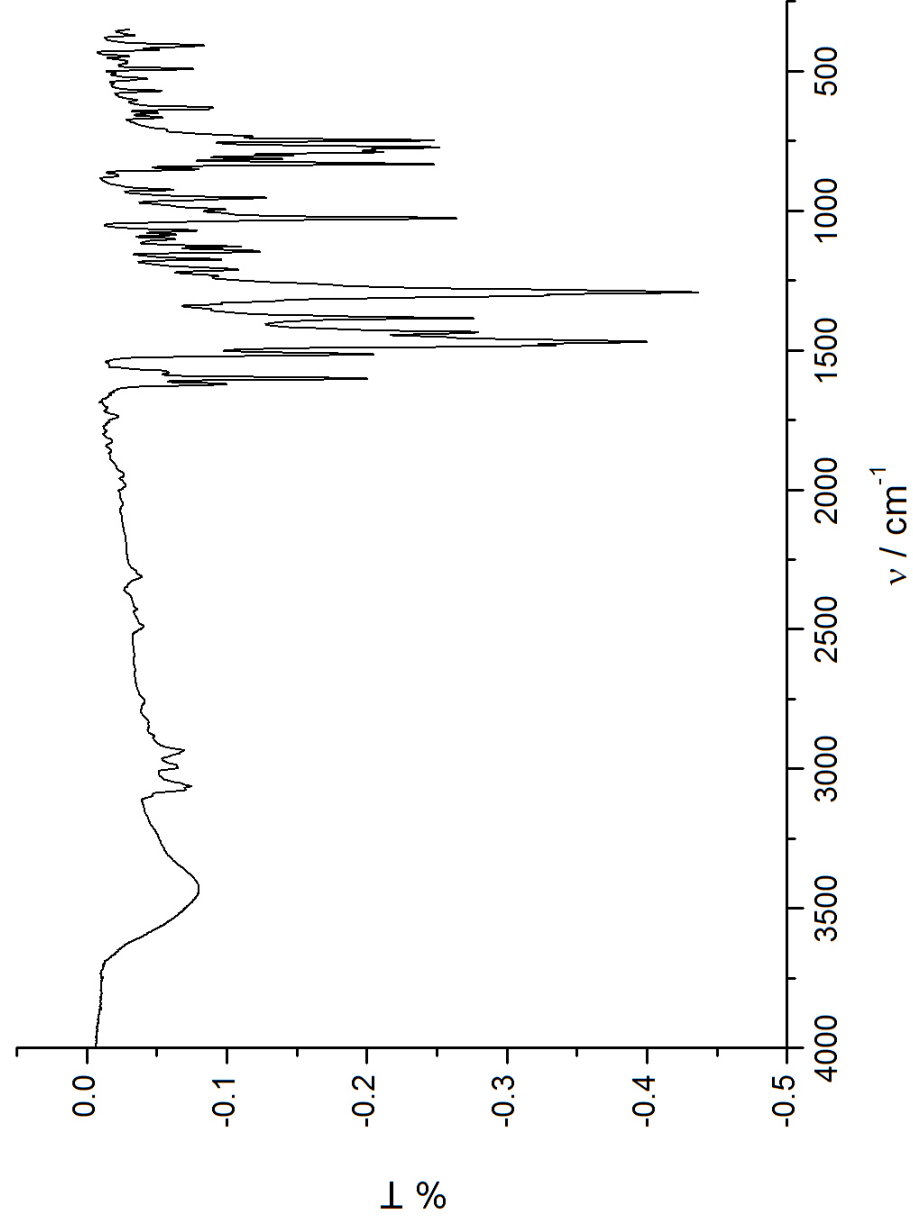
IR (KBr) of complex **3n**. $[\text{Zn}(\text{L3})(\text{NO}_3)_2]$.



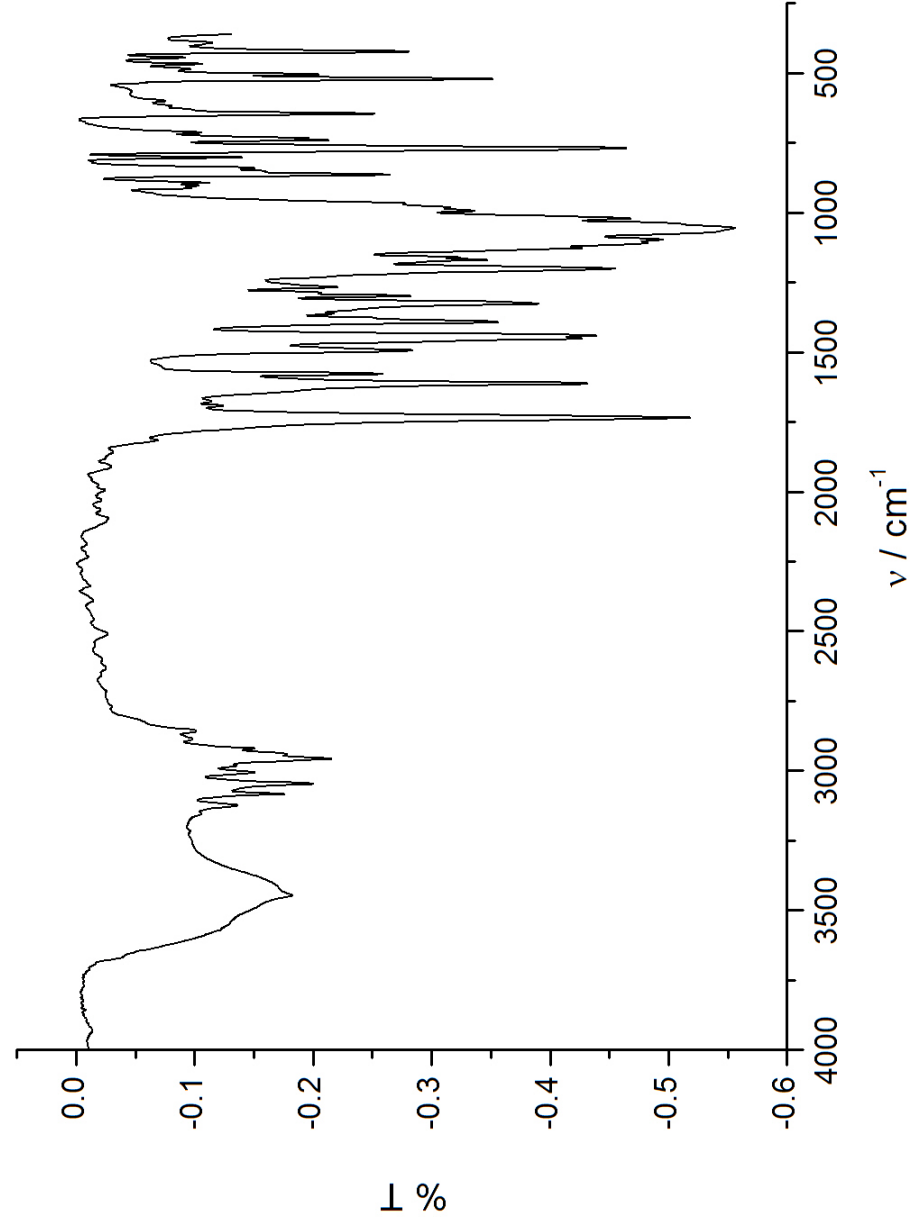
IR (KBr) of complex **4n**. $[\text{Zn}(\text{L4})(\text{NO}_3)_2]$.



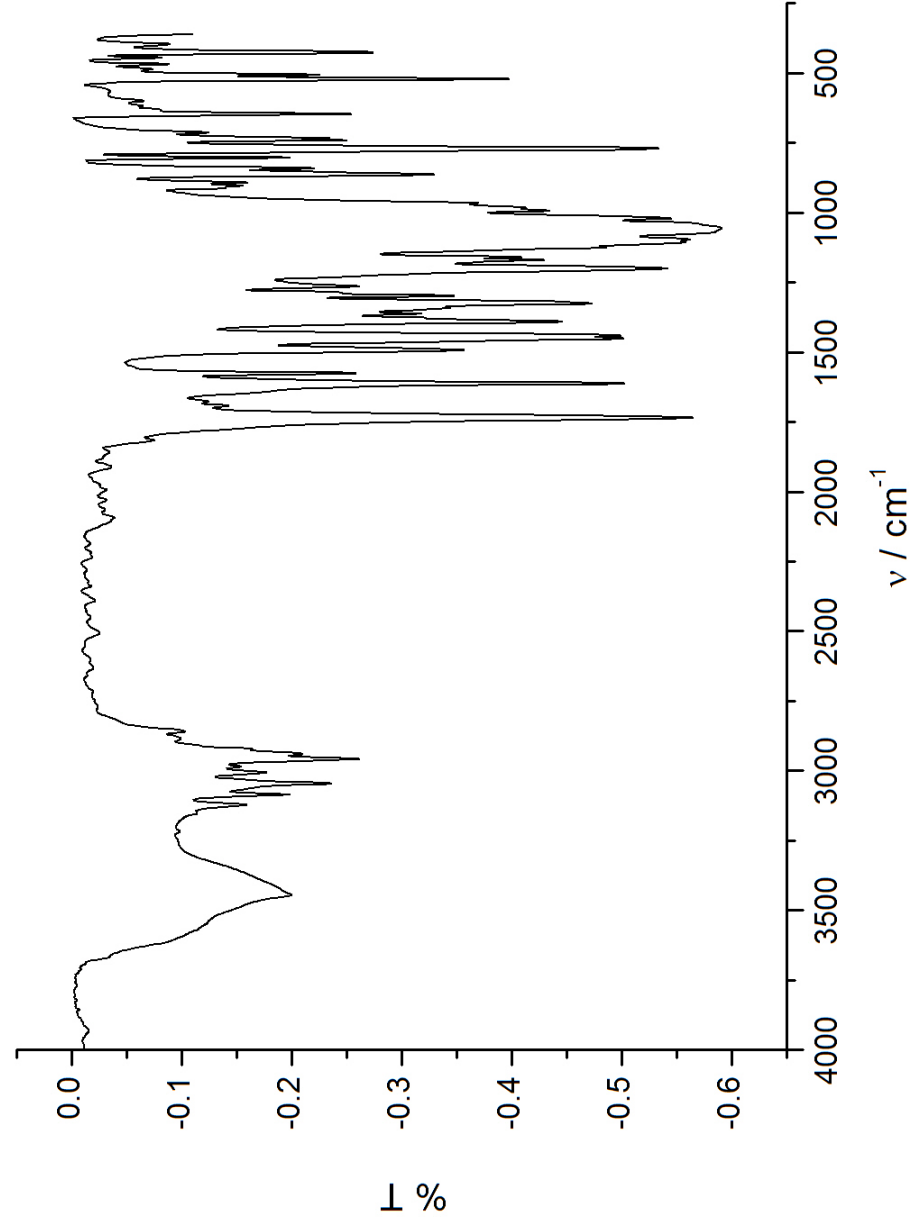
IR (KBr) of complex **5n**. $[\text{Zn}(\text{L5})(\text{NO}_3)_2]$.



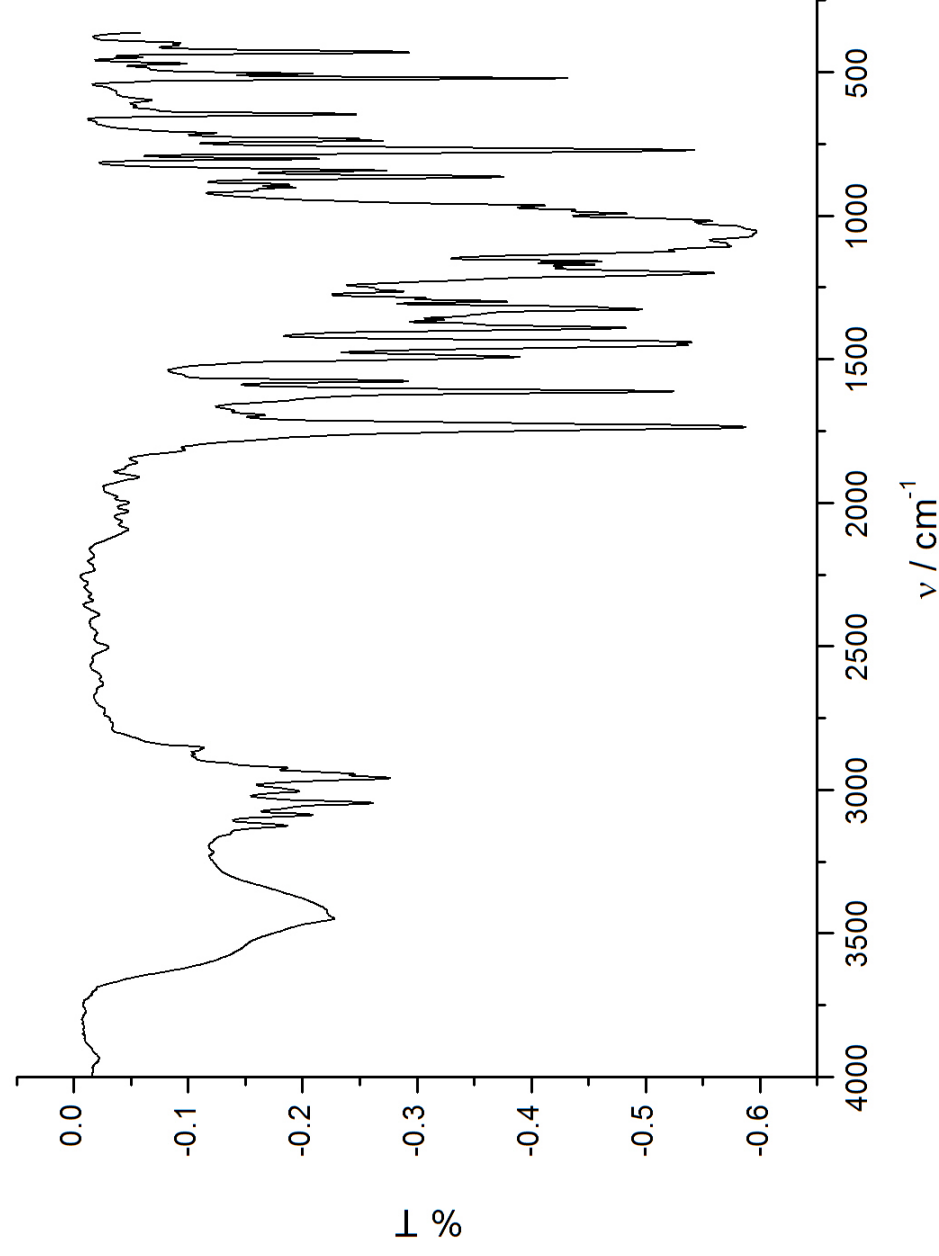
IR (KBr) of complex $1_2\text{Zn} \cdot [\text{Zn}(\text{L1})_2](\text{BF}_4)_2$.



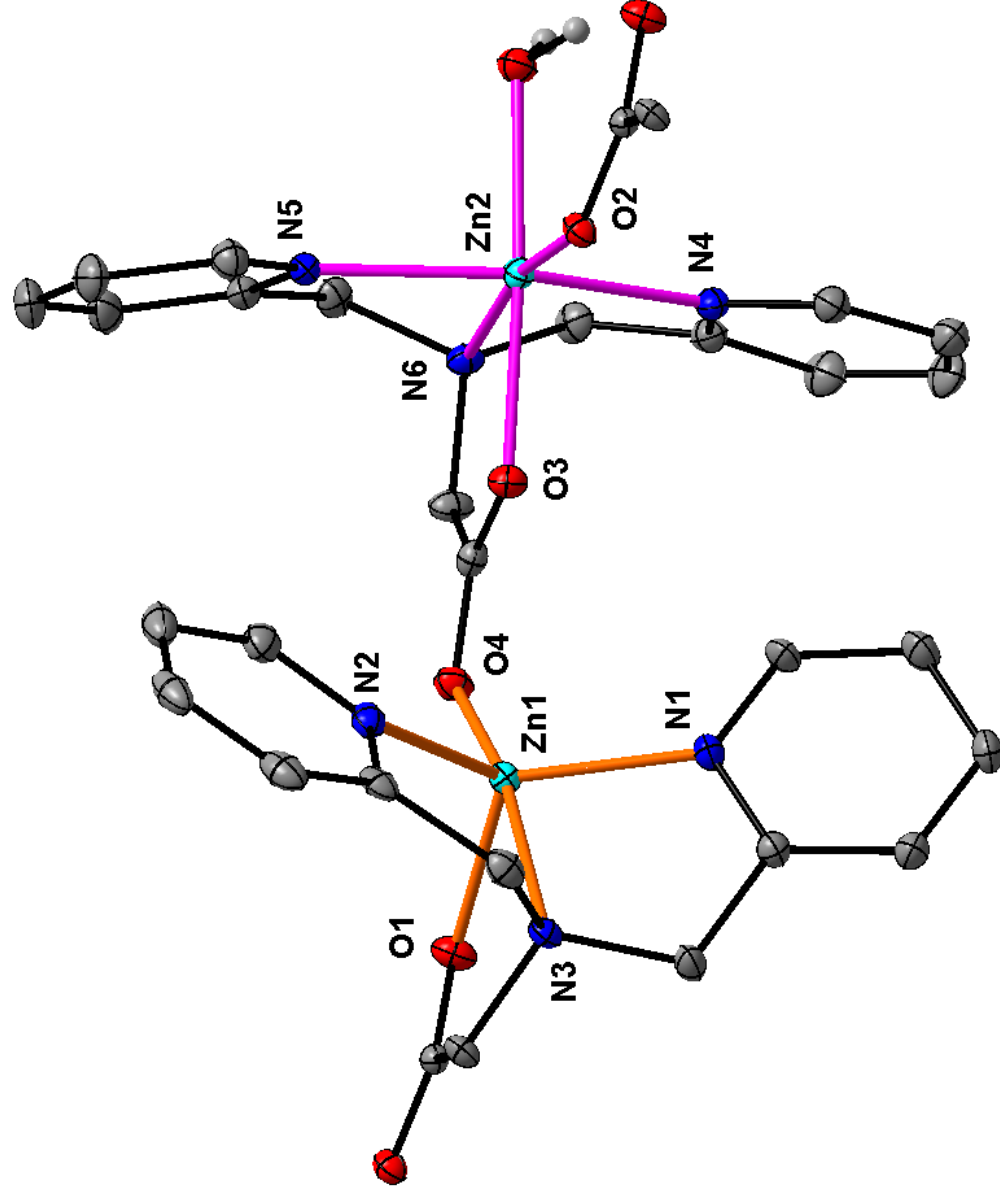
IR (KBr) of complex **1**₂Co. [Co(L1)₂](BF₄)₂.



IR (KBr) of complex **1**₂Ni. [Ni(L1)₂](BF₄)₂.



6. X-ray single crystal structure of coordination polymer **2p** (two monomer units).



7. Crystallographic numbering scheme, exemplified on complexes **1₂M** and **3n**, **M** = Zn, Co or Ni.

