Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Electronic Supplementary Information

Propylamino-connected Fluorescent Terpyridine Dimer and Trimer: Syntheses, Photophysical Properties and Formation of Duplex-Type Complexes with Cd(II)

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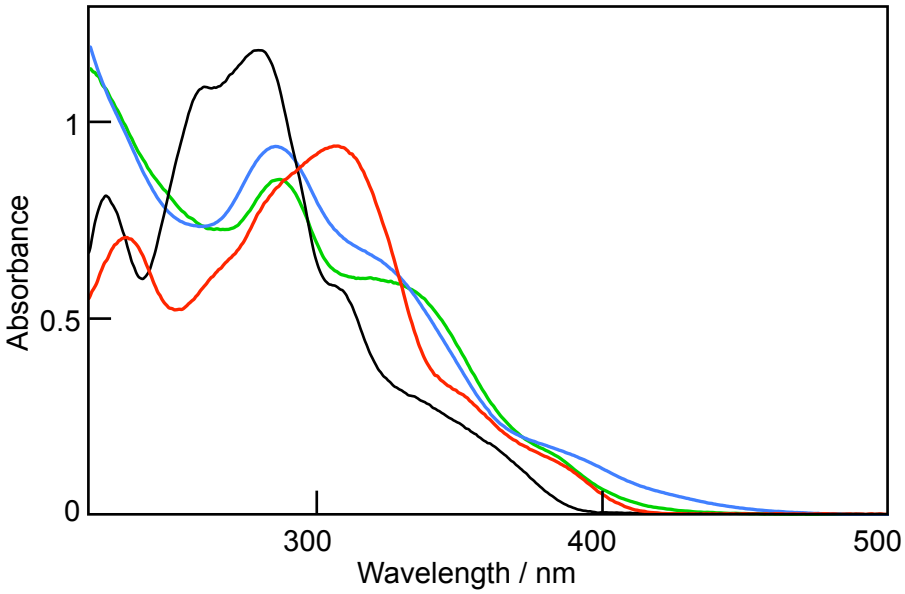


Figure S1. Absorption spectra of **L2** in acetonitrle; in the absence (black) and presence of an equivalent molar of Cd^{2+} (red), Fe^{2+} (blue), and Cu^{2+} (green).

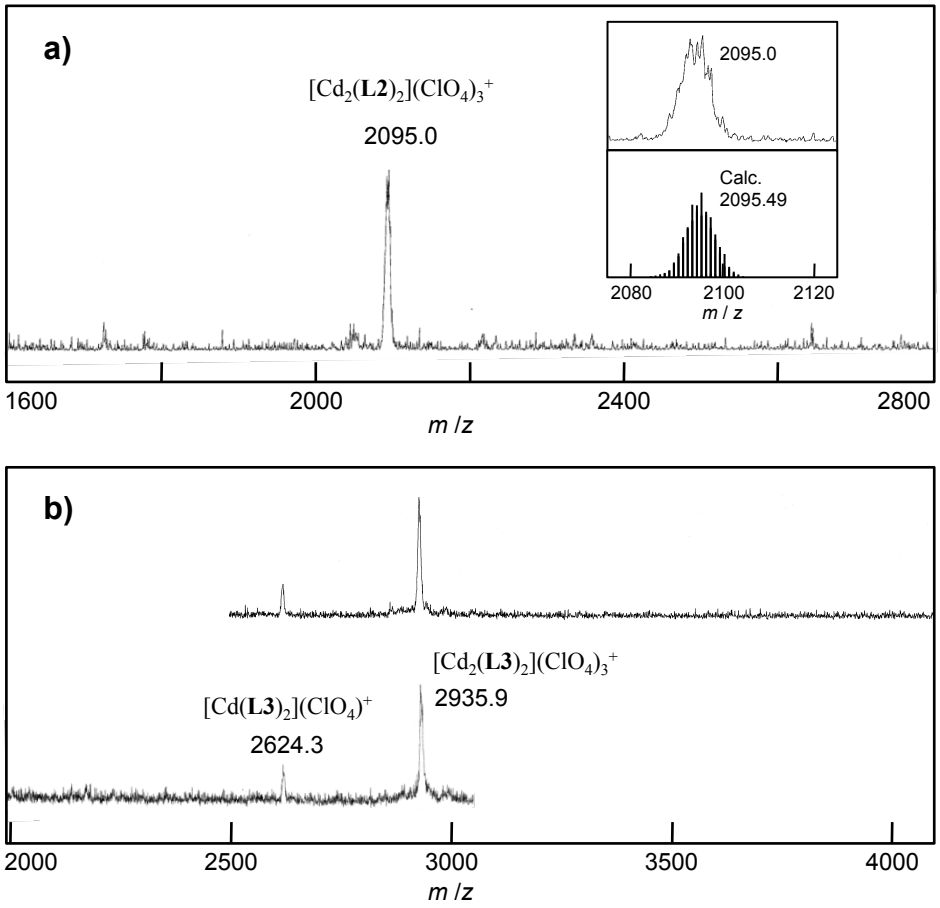
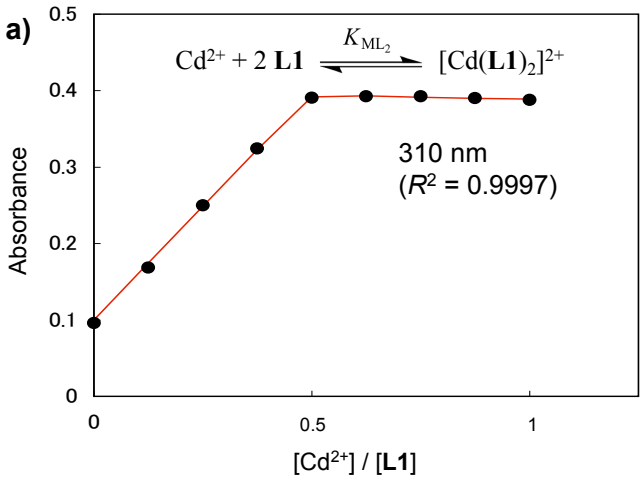
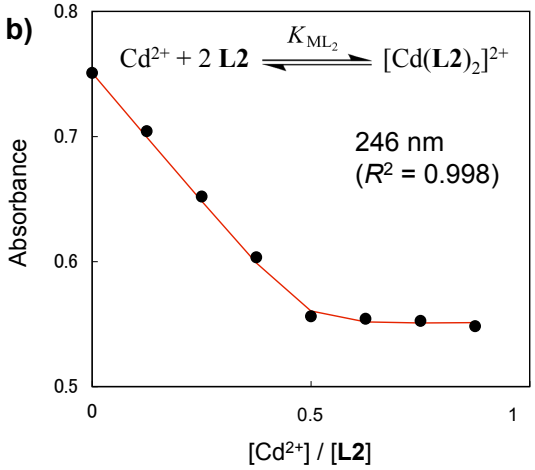


Figure S2. ESI-MS spectra of a mixture of (a) Cd^{2+} and **L2** (1:1) and (b) Cd^{2+} and **L3** (3:2) in acetonitrile.



Estimated K_{ML_2} / mol^{-2} dm^6 and sum of squared residuals (SSR)

Estimated K_{ML2} / mol^{-2} dm^6	SSR
4×10^{14}	6.99 E-05
1×10^{15}	6.02 E-05
1×10^{16}	5.68 E-05
1×10^{17}	6.52 E-05
1×10^{18}	7.22 E-05



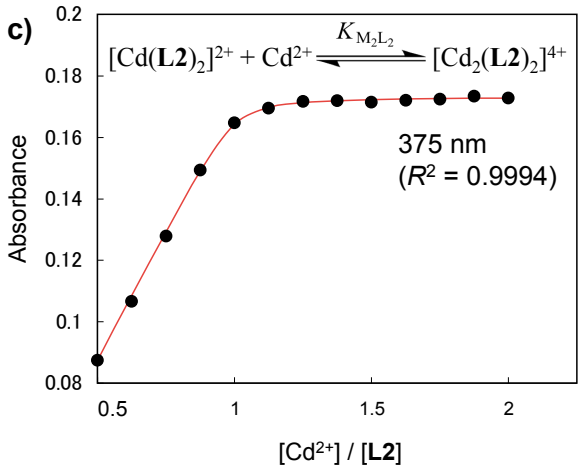


Figure S3. Evaluation of the association constants (K_{MiLj}) by non-linear curve fitting (red line) of the absorptional titration data (filled circle).

In the case of $[Cd(\mathbf{L1})_2]^{2+}$ (Fig. S3a), the least-square curve fitting resulted in similar SSR for a wide range of the estimated association constants (see Table), because of a very large value of K_{ML2} = [$[Cd(\mathbf{L1})_2]^{2+}$] / ($[Cd^{2+}]$ • $[\mathbf{L1}]^2$).

Similar discussion is also applied to the association constant of $[Cd(\mathbf{L2})_2]^{2+}$ (Fig. S3b).

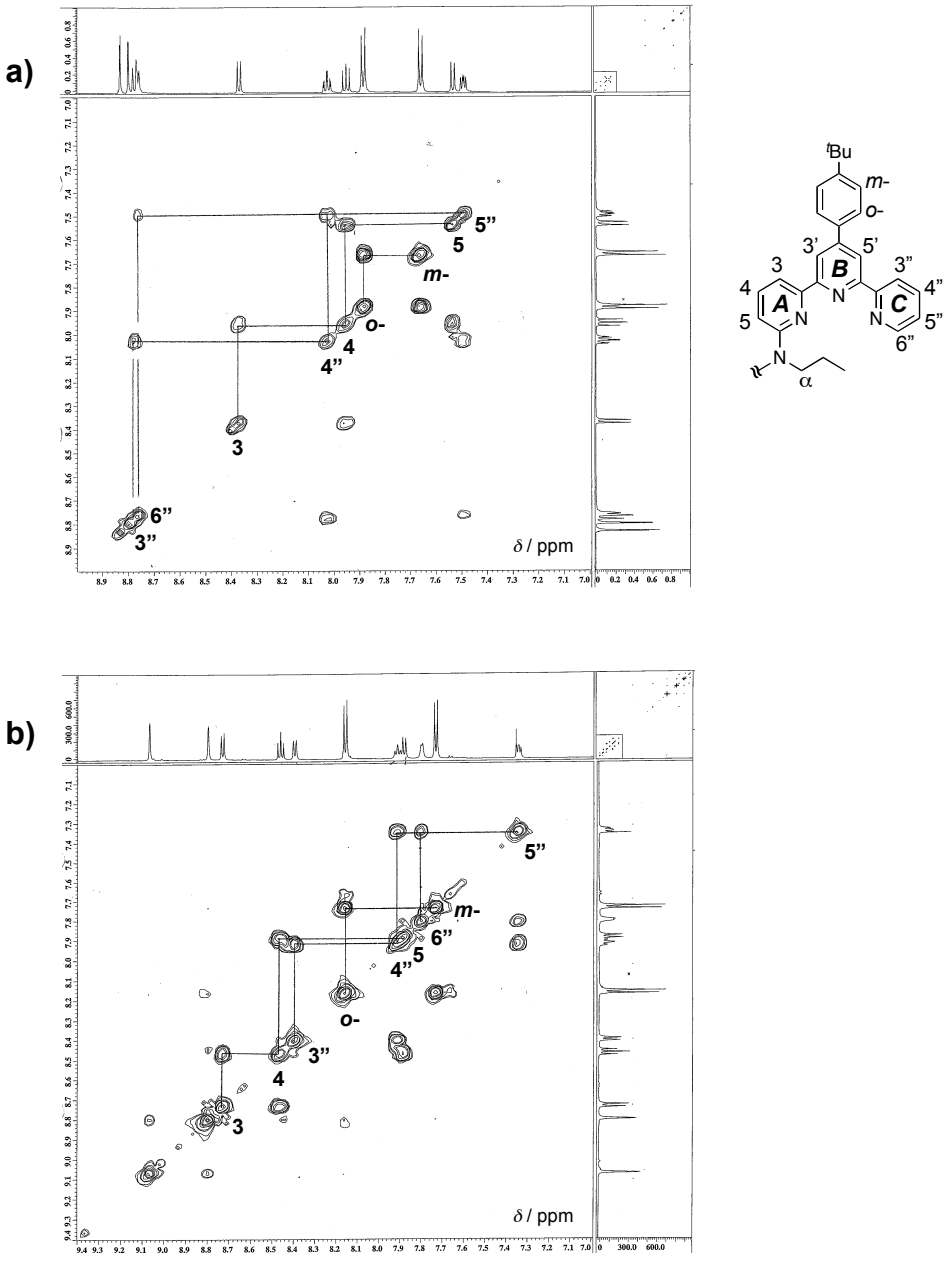


Figure S4. ^{1}H-^{1}H COSY of **L2** (a) and $[Cd_2(\mathbf{L2})_2]^{2+}$ (b) in acetone-d_6.

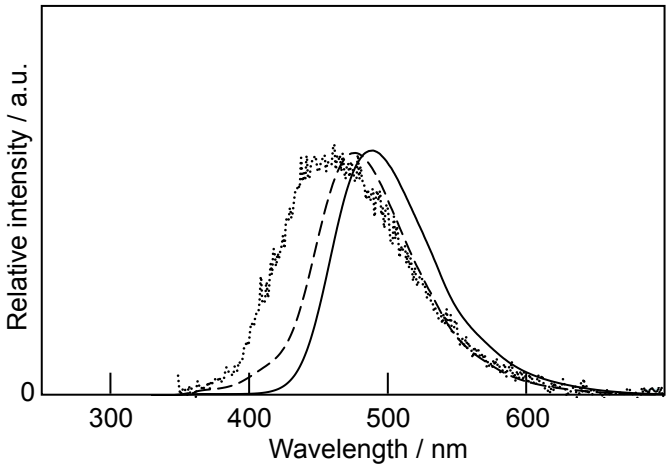


Figure S5. Normalized emission spectra of $[Cd_2(\mathbf{L2})_2](ClO_4)_4$ in acetonitrle solution (dotted line), PMMA film (broken line) and powdery solid (solid line).

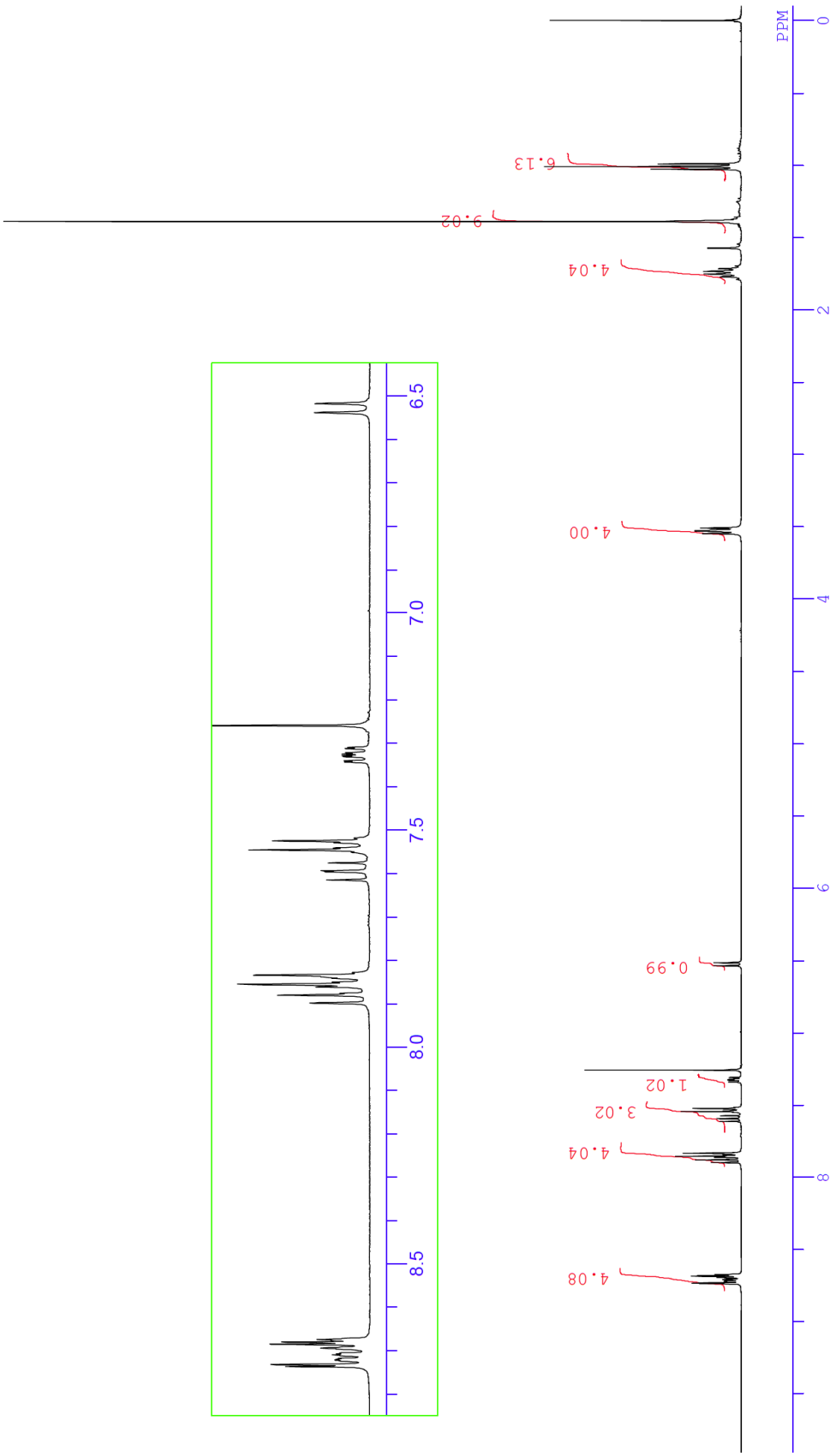


Figure S6. ^{1}H NMR spectrum of **L1** in chloroform-*d*.

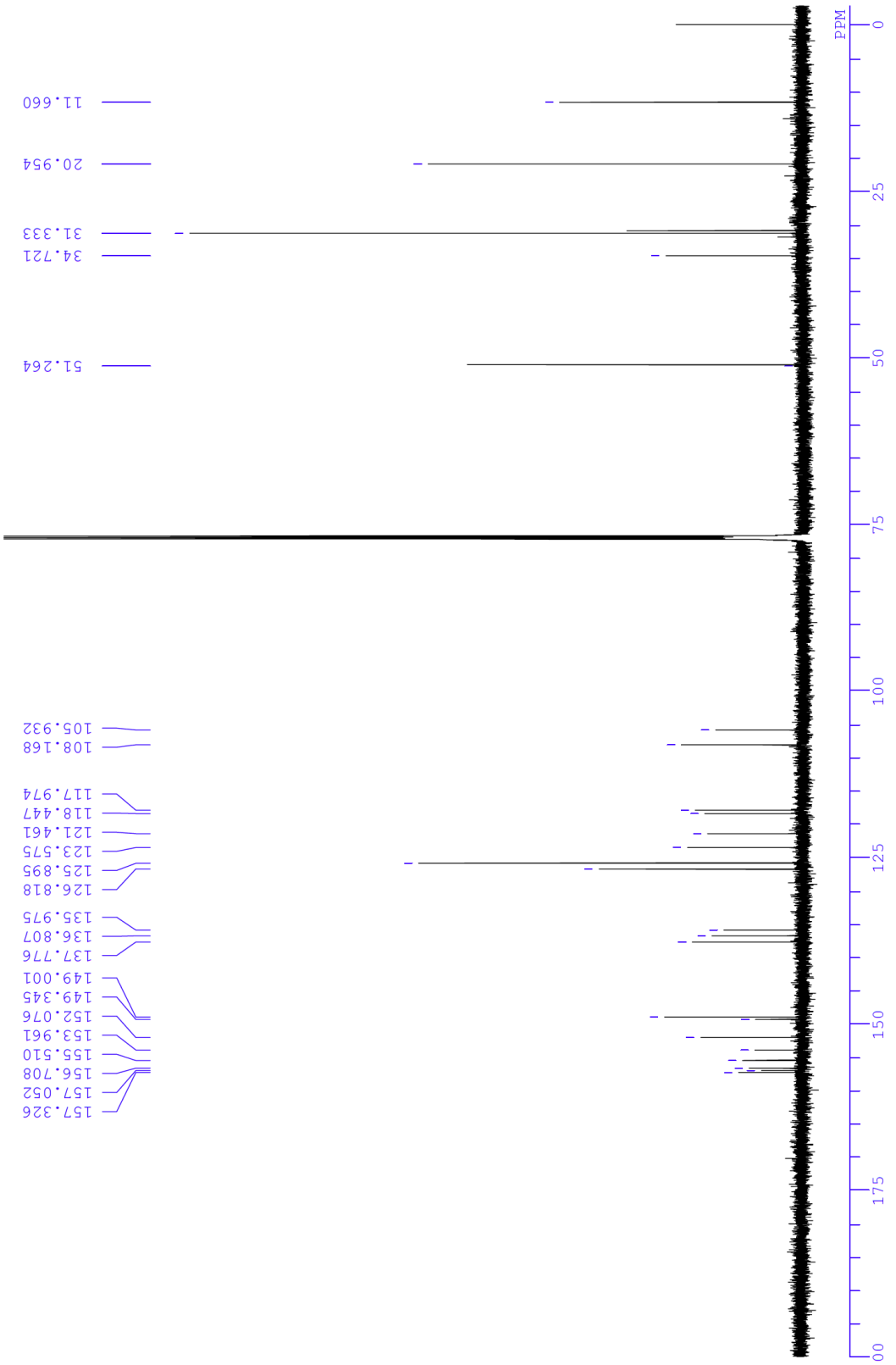


Figure S7. ^{13}C NMR spectrum of **L1** in chloroform-*d*.

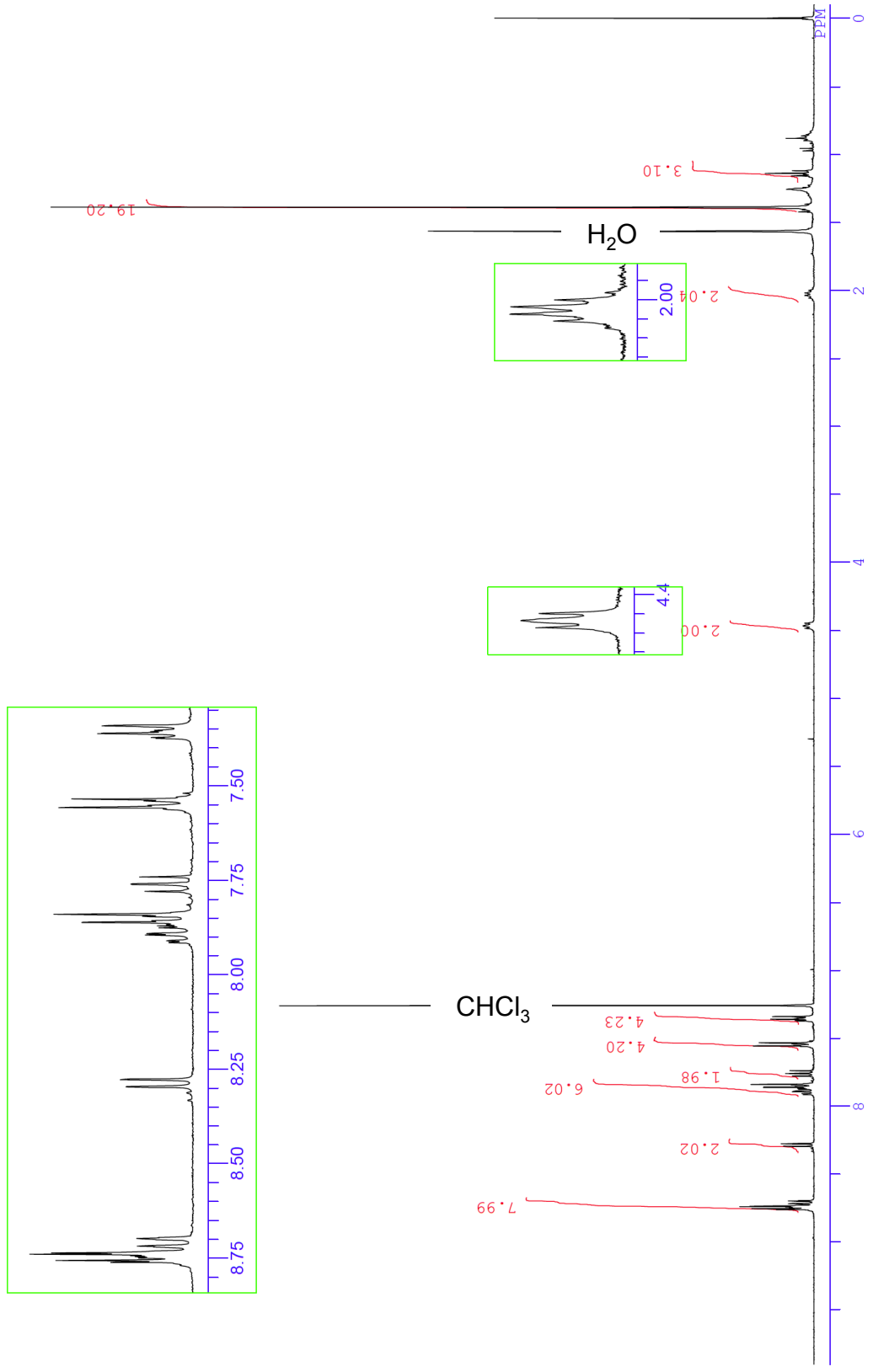


Figure S8. ^{1}H NMR spectrum of **L2** in chloroform-*d*.

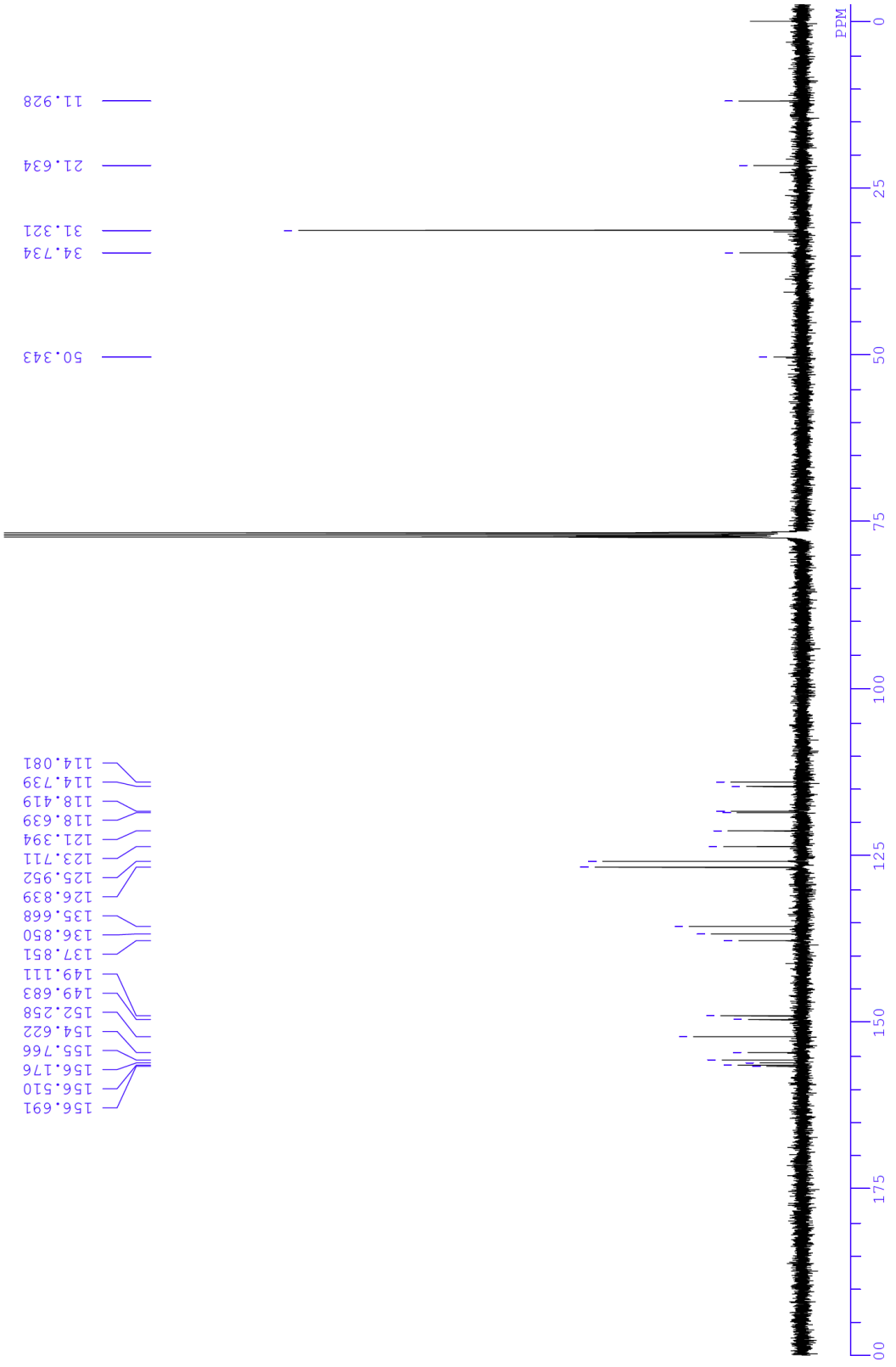


Figure S9. ^{13}C NMR spectrum of **L2** in chloroform-*d*.

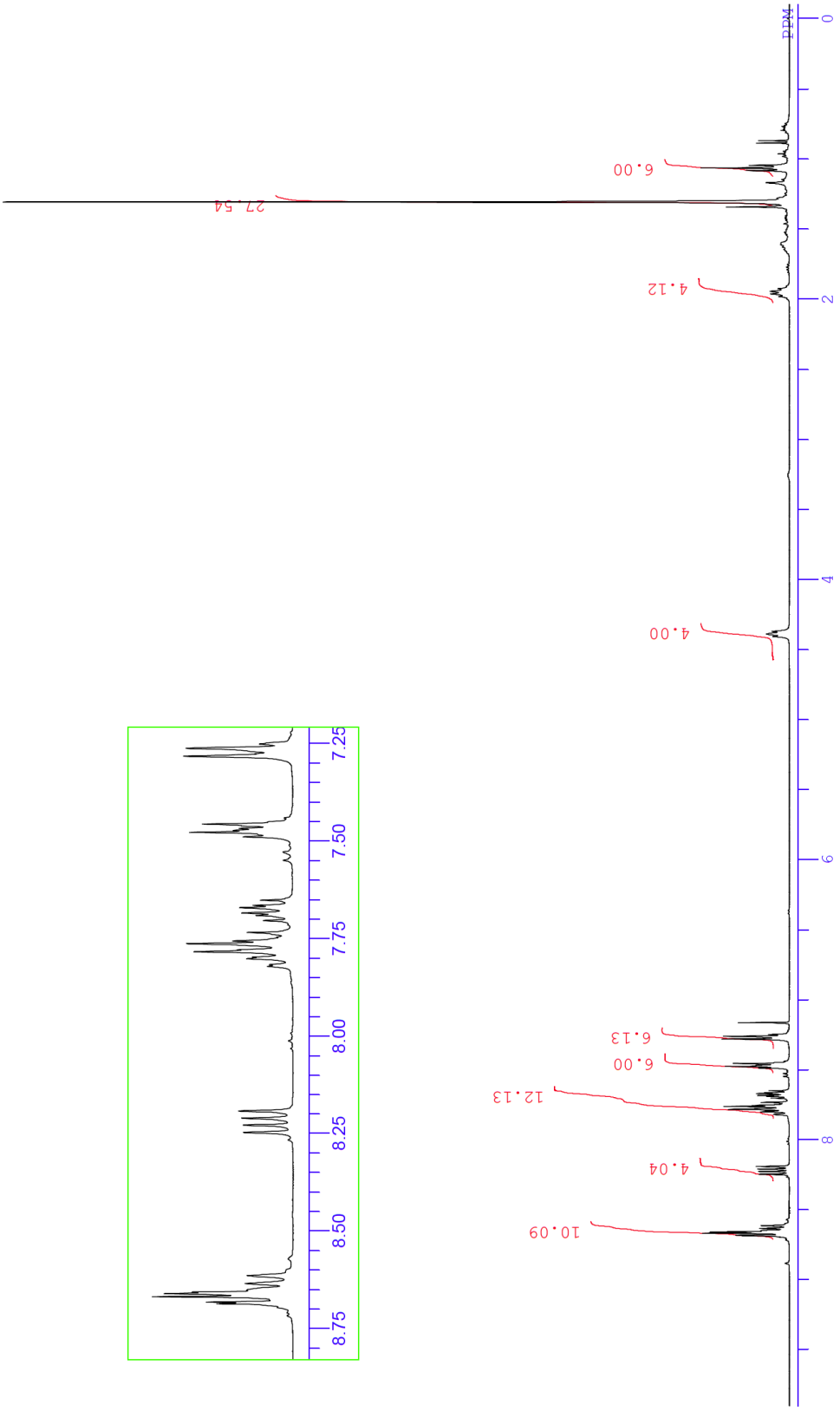


Figure S10. ^{1}H NMR spectrum of **L3** in chloroform-*d*.

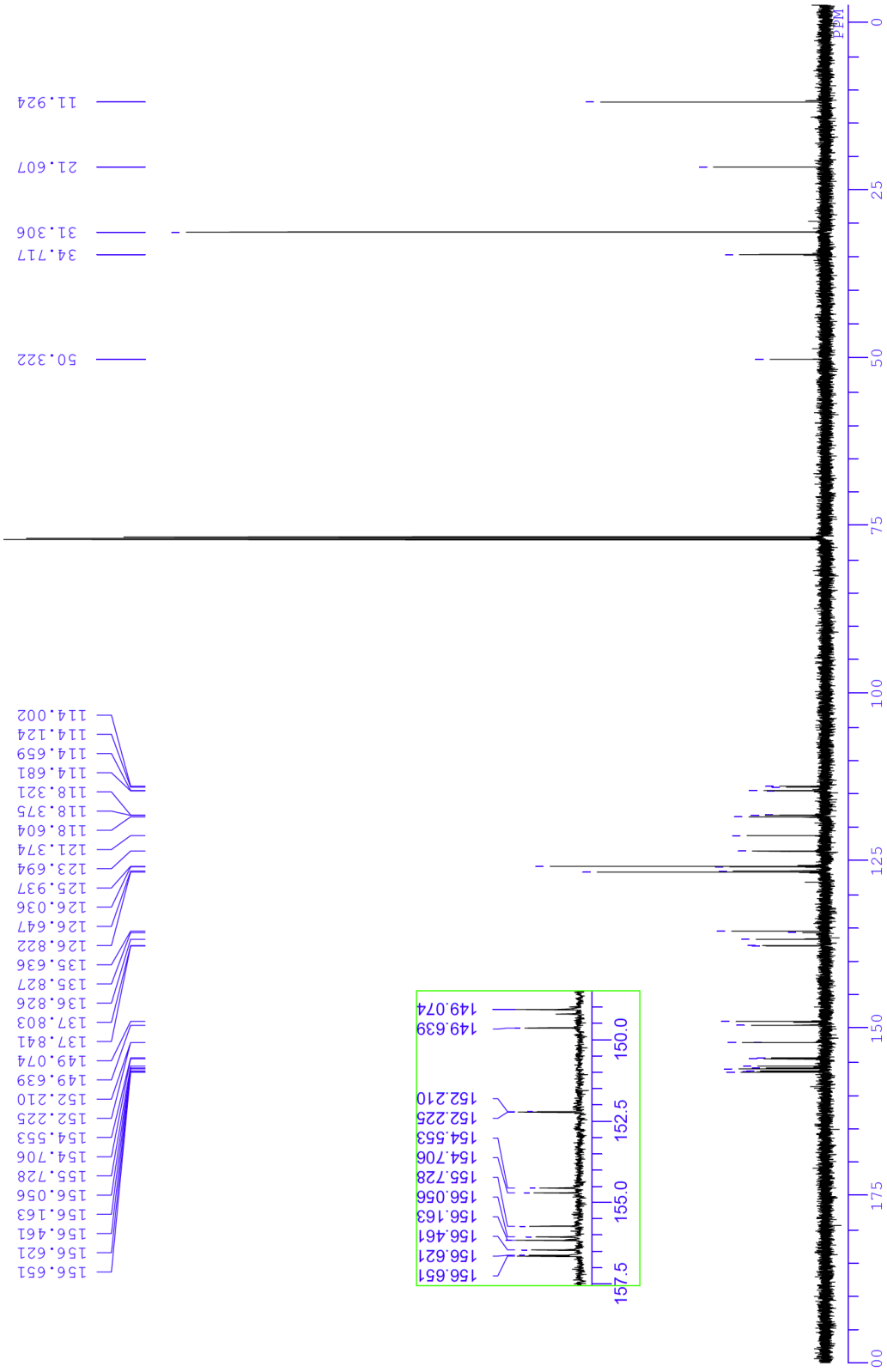


Figure S11. ^{13}C NMR spectrum of **L3** in chloroform-*d*.