Electronic Supplementary Material (ESI) for Analyst

Novel Triazole-Based Fluorescent Probe for Pd^{2+} in Aqueous Solutions: Design, Theoretical Calculations and Imaging

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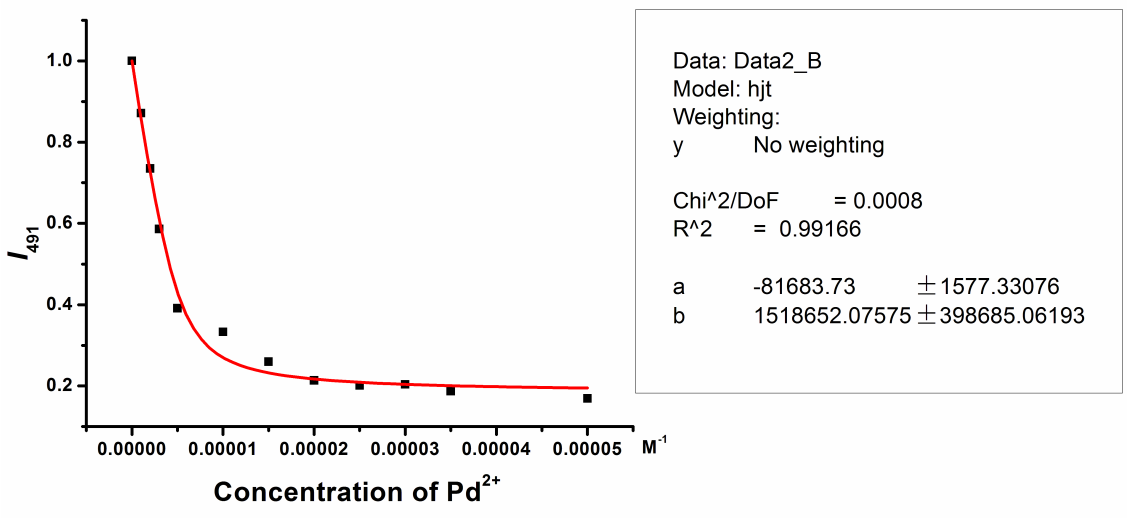


Figure S1 Nonlinear least square analysis of **PS-1** and Pd^{2+}.

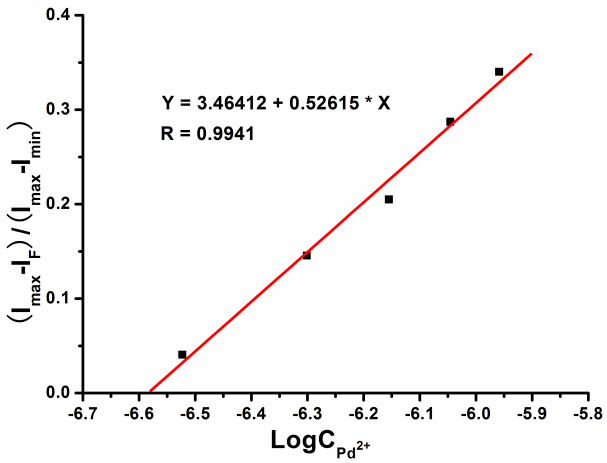


Figure S2 Normalized response of fluorescence signal to changing Pd^{2+} concentrations in the PBS buffer (10 mM, pH = 7.2, containing 0.5% DMF). (λ_{ex} = 410 nm, λ_{em} = 491 nm).

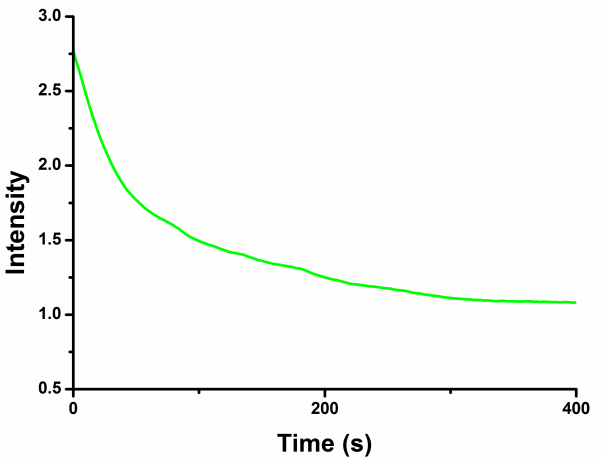


Figure S3 Time-dependent fluorescence intensity changes at 491 nm of **PS-1** (5 μM) with Pd^{2+} (5 μM)

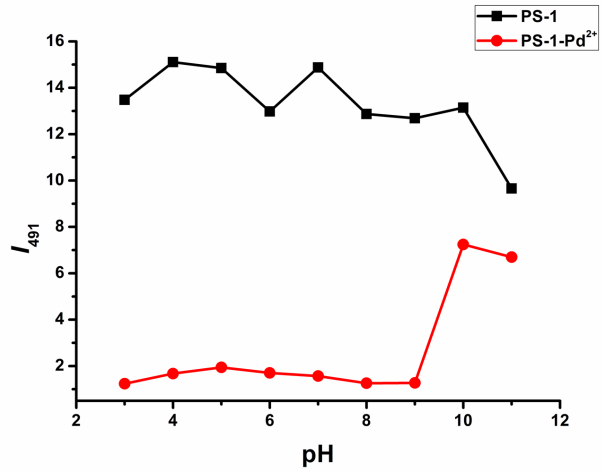


Figure S4 pH titration of **PS-1** (5 μM) with or without Pd^{2+} (50 μM) during pH 3.0-11.0.

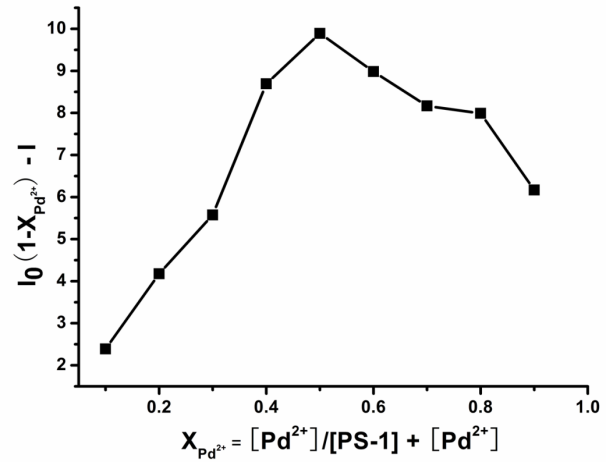


Figure S5 The job plot of a 1:1 complex of **PS-1** with Pd^{2+}.

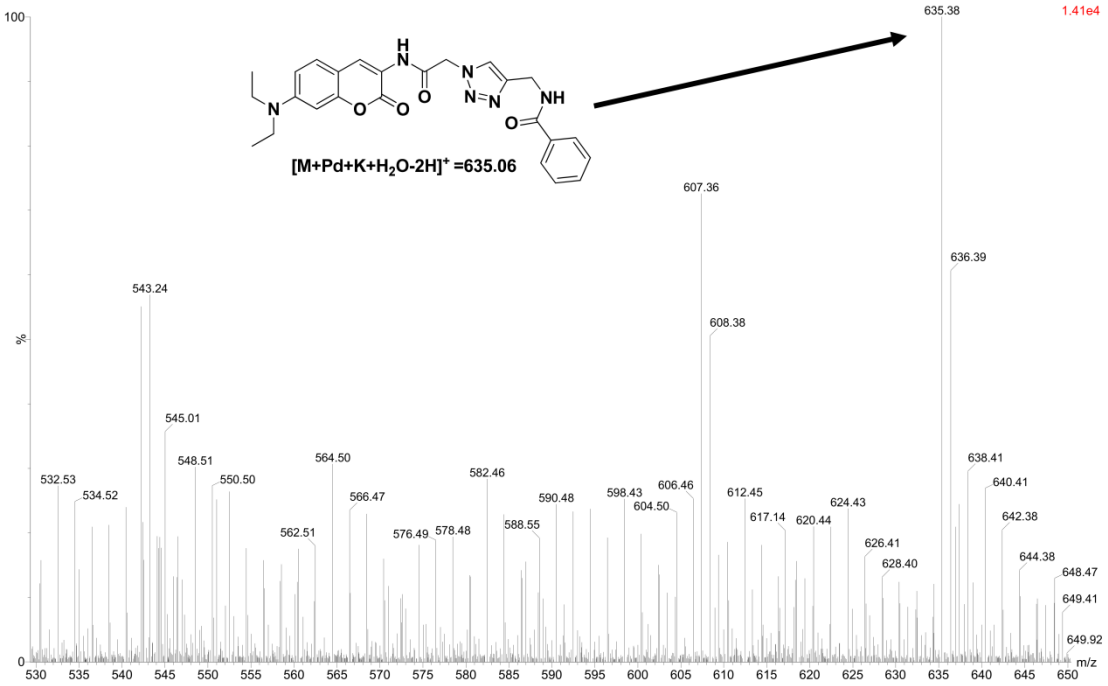


Figure S6 ESI-Mass of complex of **PS-1** with Pd^{2+}.

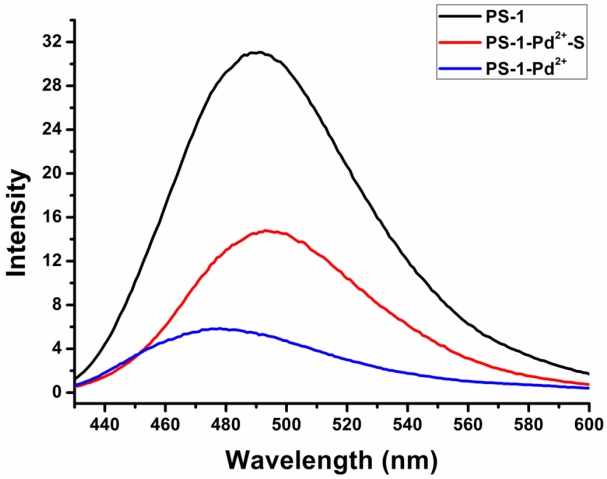


Figure S7 Fluorescence spectral changes of **PS-1**-Pd^{2+} solution upon addition of an excess amount of S^{2-} ion.

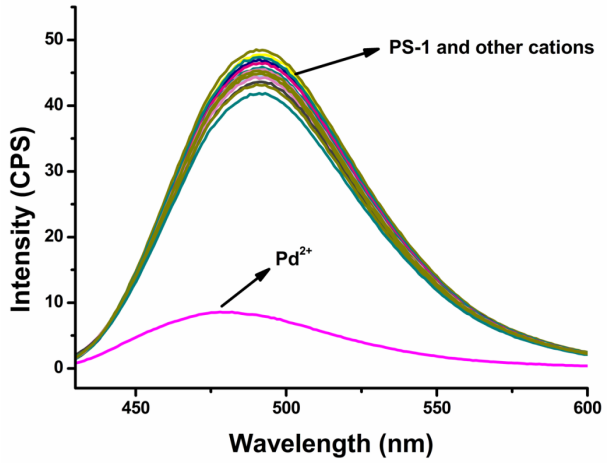


Figure S8 Fluorescent spectra of compound **PS-1** (5 μM) upon addition of 10 equiv metal ions in PBS buffer (10 mM, pH = 7.2, containing 0.5% DMF). (λ_{ex} =410 nm, slit = 3.0 nm/3.0 nm)

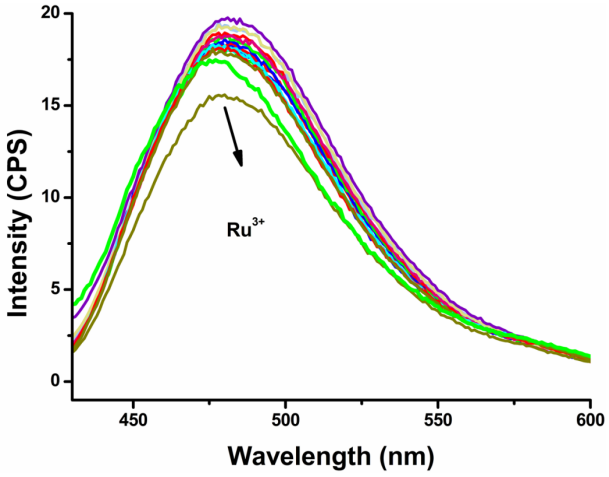


Figure S9 Fluorescence response of **PS-1** (50 μM) to various metal ions (10 equiv) in the presence of Pd^{2+} (10 equiv) PBS buffer (10 mM, pH = 7.2, containing 0.5% DMF). (λ_{ex} =410 nm, slit = 3.0 nm/3.0 nm).

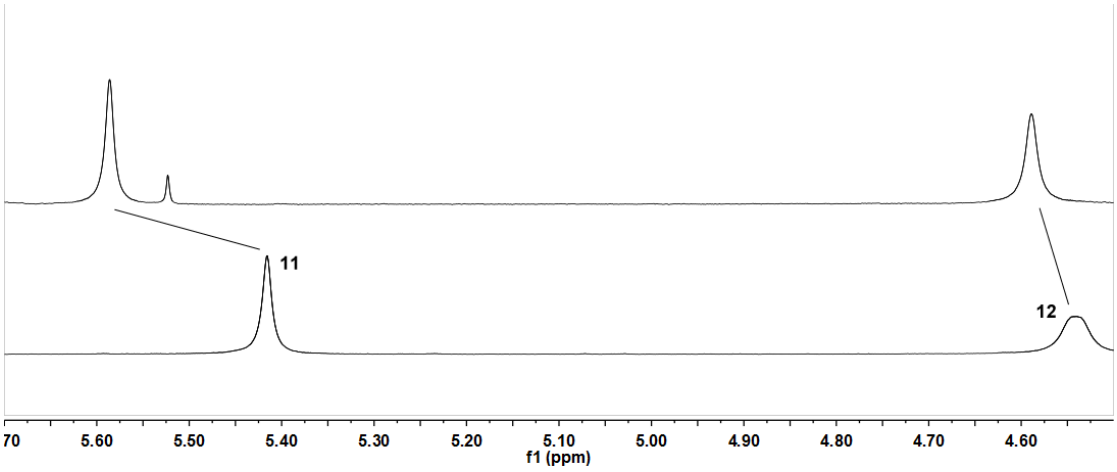


Figure S10 Partial ^{1}H NMR spectra of **PS-1** in the absence or presence of 3 equiv Pd^{2+} in DMSO-d_6 **(**Alkyl area). (top : PS-1 with Pd^{2+}; bottom: PS-1)

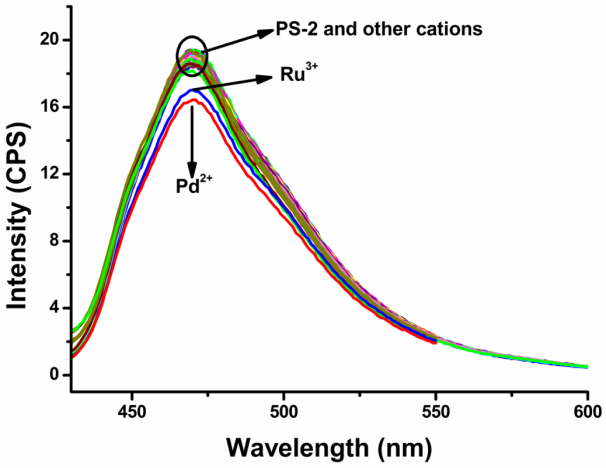


Figure S11 Fluorescent spectra of compound **PS-2** (5 μM) upon addition of 10 equiv metal ions in PBS buffer (10 mM, pH = 7.2, containing 0.5% DMF). (λ_{ex} =410 nm, slit = 3.0 nm/3.0 nm)

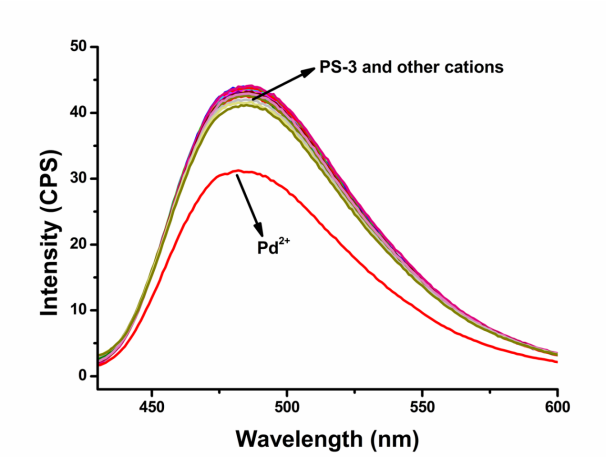


Figure S12 Fluorescent spectra of compound **PS-3** (5 μM) upon addition of 10 equiv metal ions in PBS buffer (10 mM, pH = 7.2, containing 0.5% DMF). (λ_{ex} =410 nm, slit = 3.0 nm/3.0 nm)

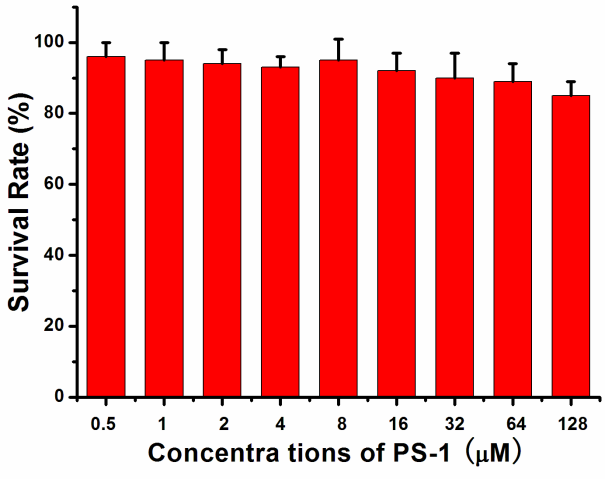


Figure S13 Effects of **PS-1** at varied concentrations on the viability of Hela cells. The results are the mean standard deviation of three separate measurements.

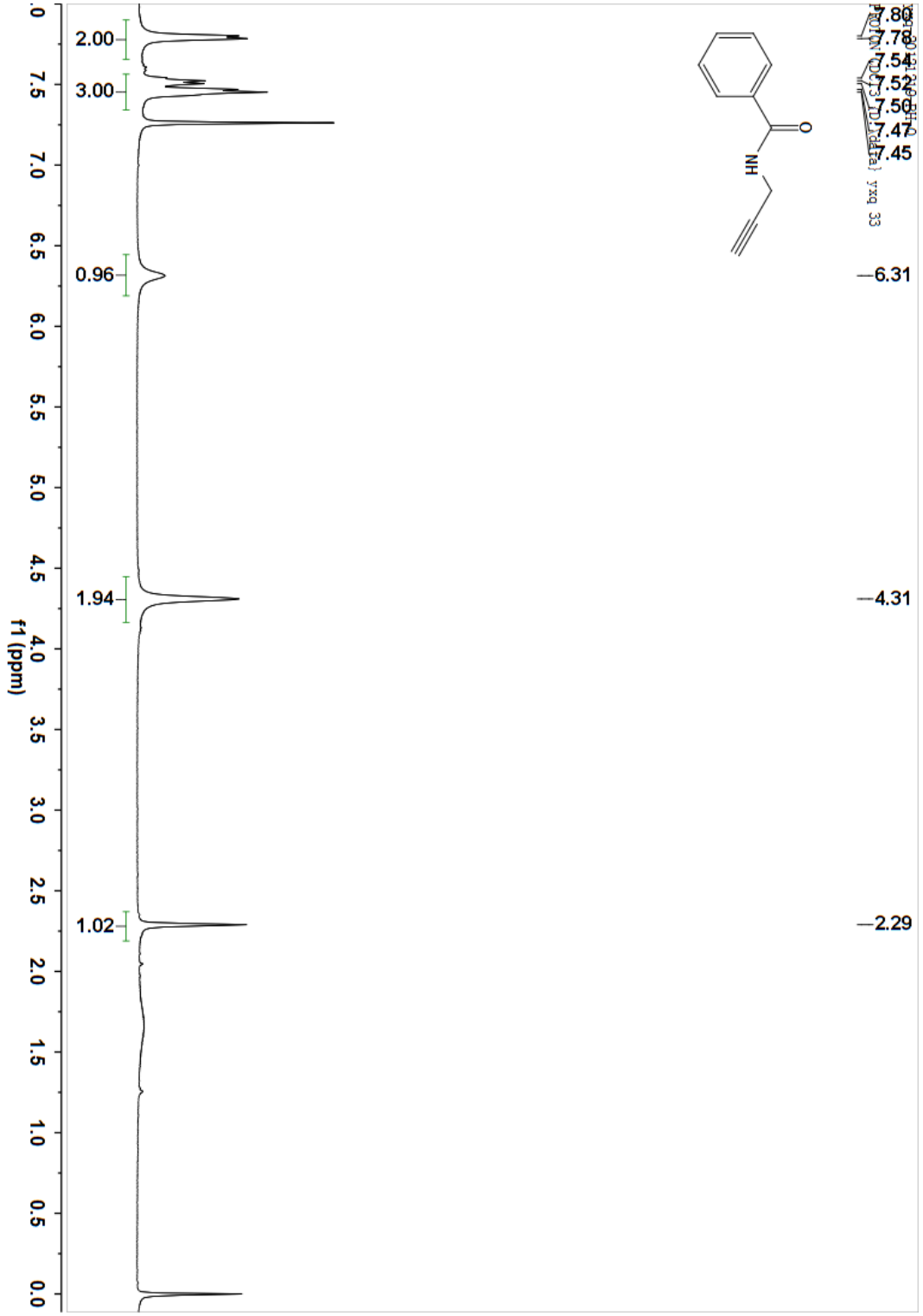
Table S1 Quantum yields of **PS-1/2/3** with or without Pd^{2+}.

Species	Φ_F
PS-1	0.077
PS-1-Pd^{2+}	0.015
PS-2	0.045
PS-2-Pd^{2+}	0.039
PS-3	0.021
PS-3-Pd^{2+}	0.017

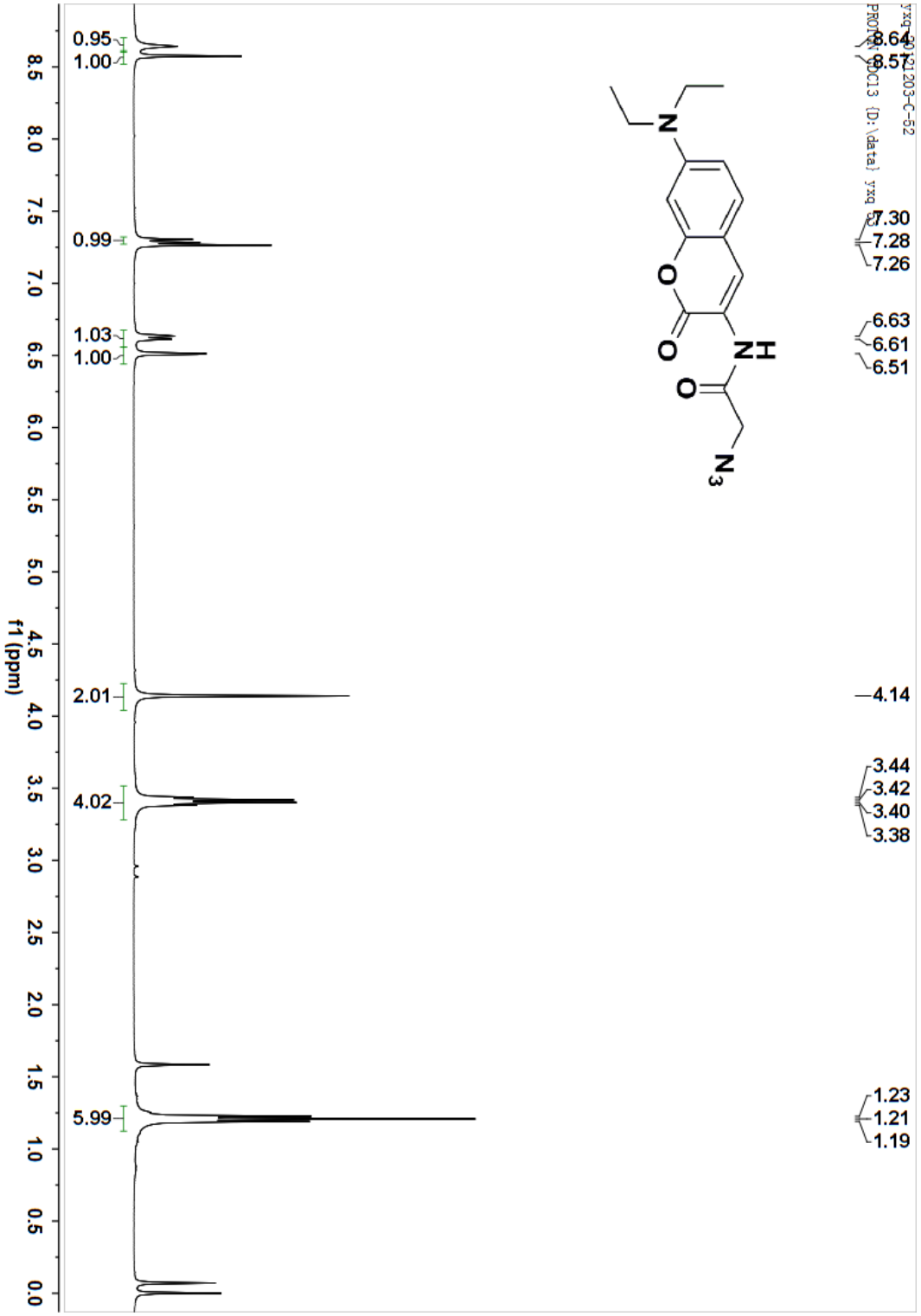
Table S2 B3LYP optimized bond distances (Å) of **PS-1/2/3** with Pd^{2+}.

Bond	**Bond lengths (Å)**		
	PS-1-Pd	**PS-2**-Pd	**PS-3**-Pd
Pd-N1	**2.016**	**2.011**	4.267
Pd-N2	2.871	2.946	2.918
Pd-N3	3.442	**2.064**	3.525
Pd-N4	3.287	2.965	3.433
Pd-C1	2.534	4.059	2.702
Pd-C2	**2.181**	4.053	**2.23**
Pd-O1	4.207	4.066	**2.095**
Pd-N5	**2.095**		3.515
Pd-O2	3.166		**2.069**

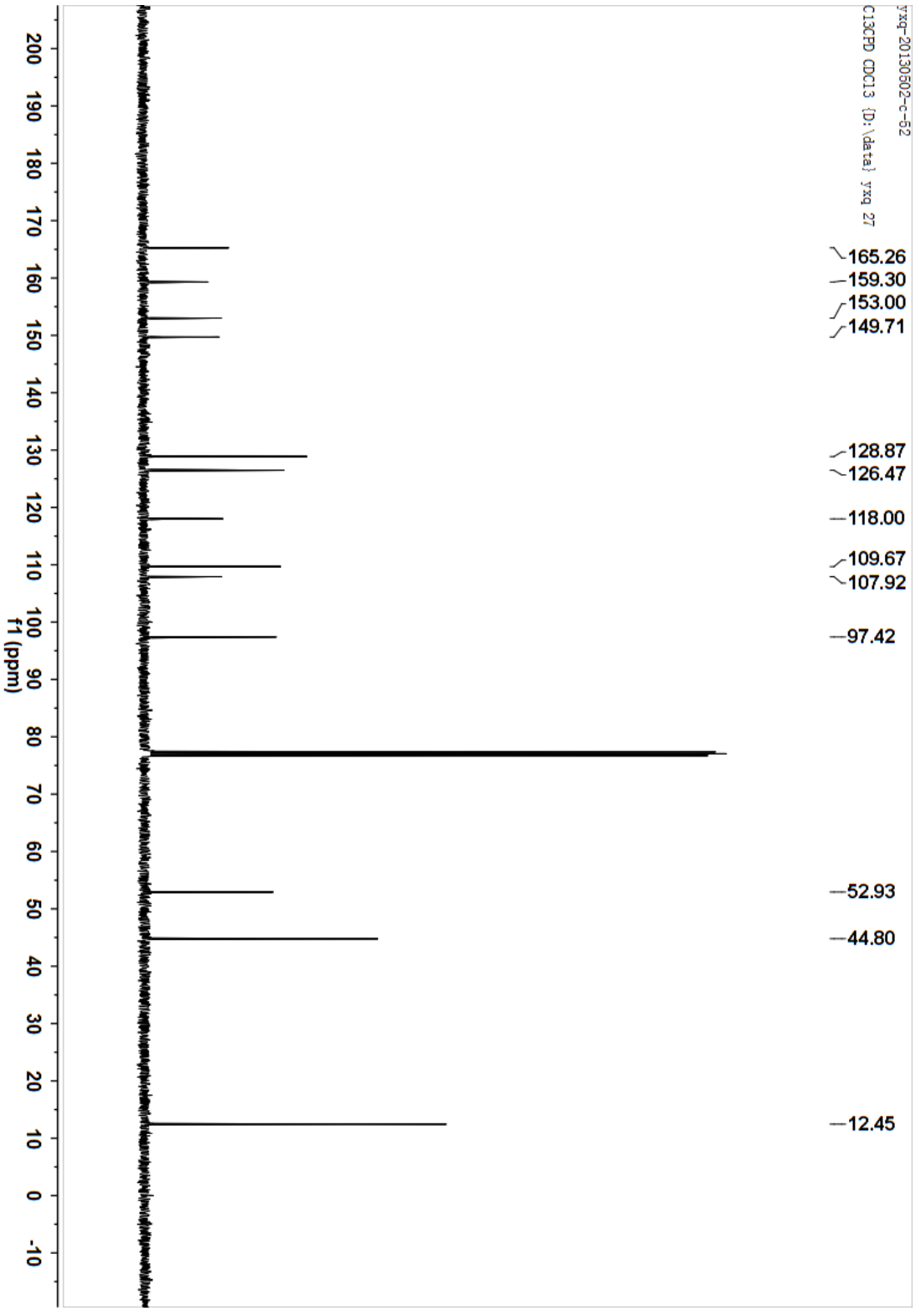
^{1}H-NMR Spectrum of **A-1** in $CDCl_3$ (400 MHz):



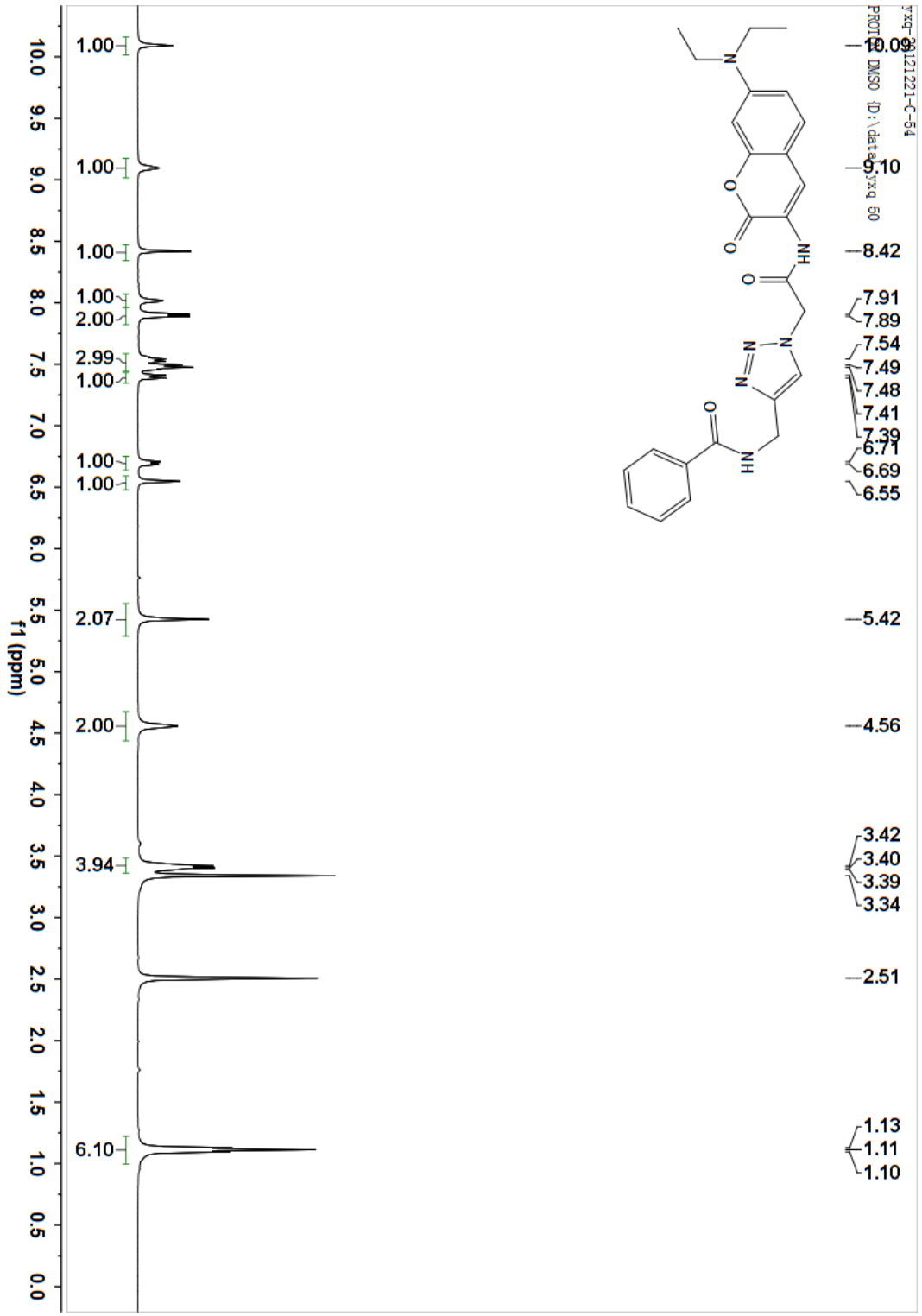
^{1}H-NMR Spectrum of **C-2** in $CDCl_3$ (400 MHz):



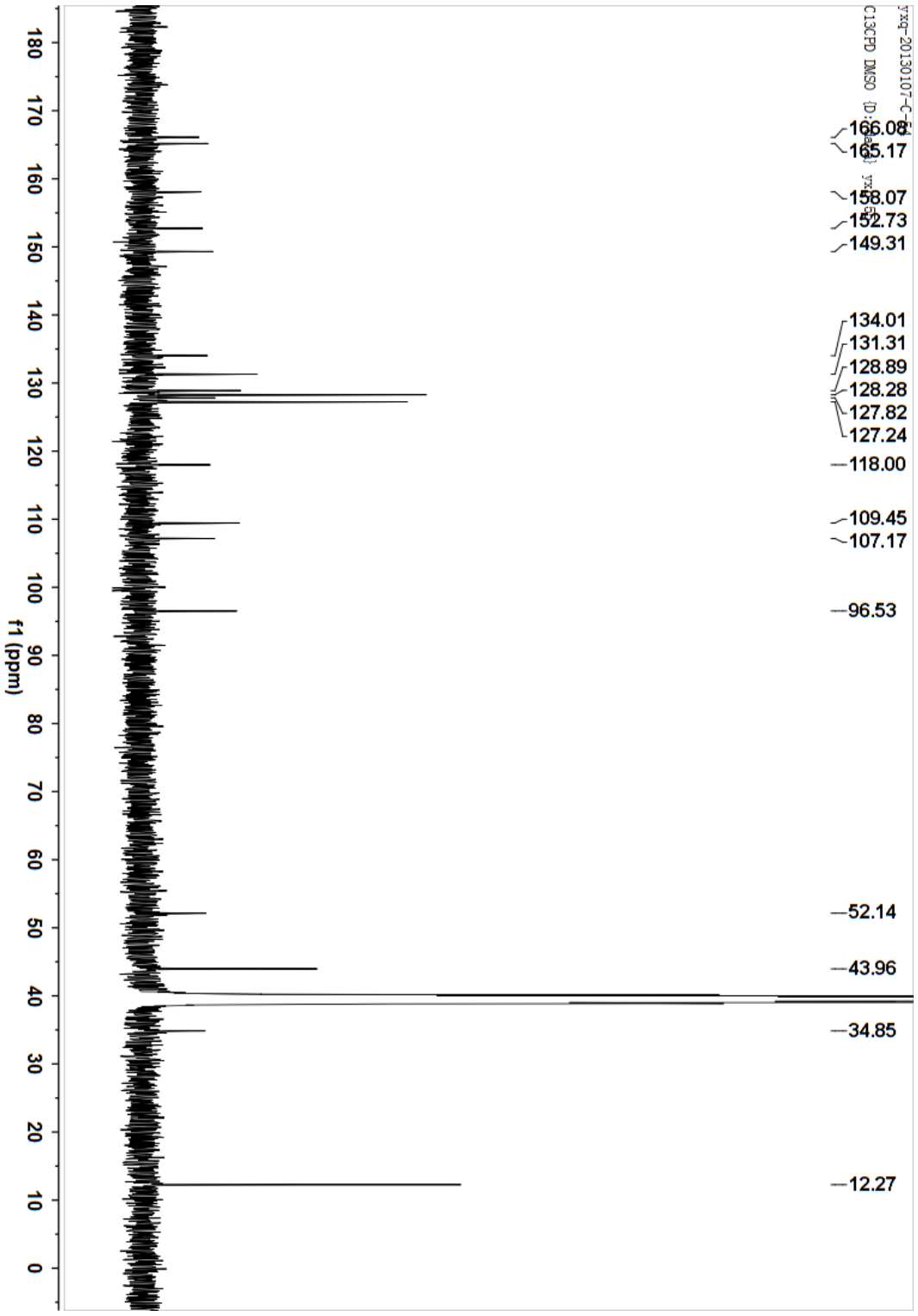
^{13}C-NMR Spectrum of **C-2** in $CDCl_3$ (100 MHz):



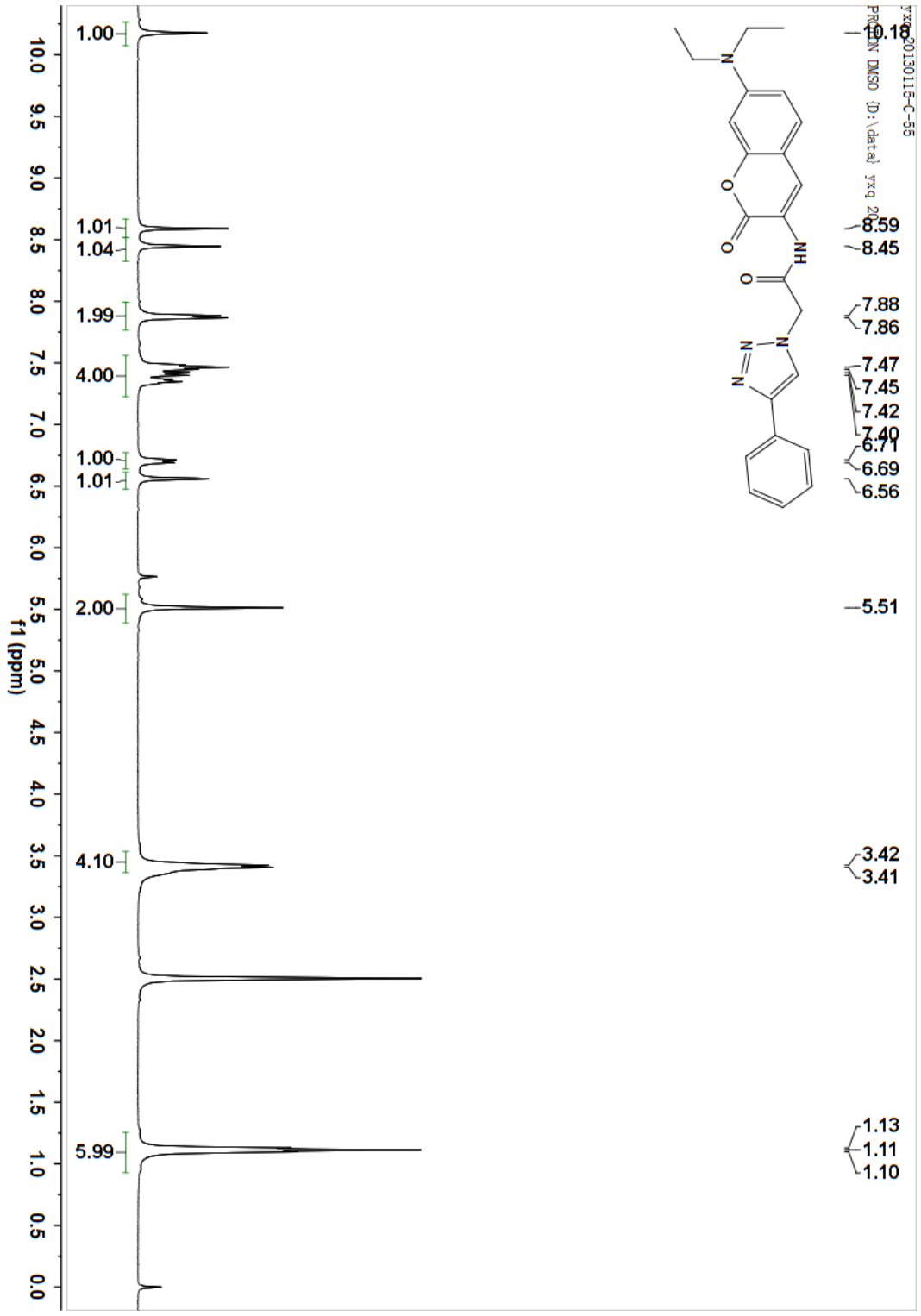
^{1}H-NMR Spectrum of **PS-1** in DMSO-d_6 (400 MHz):



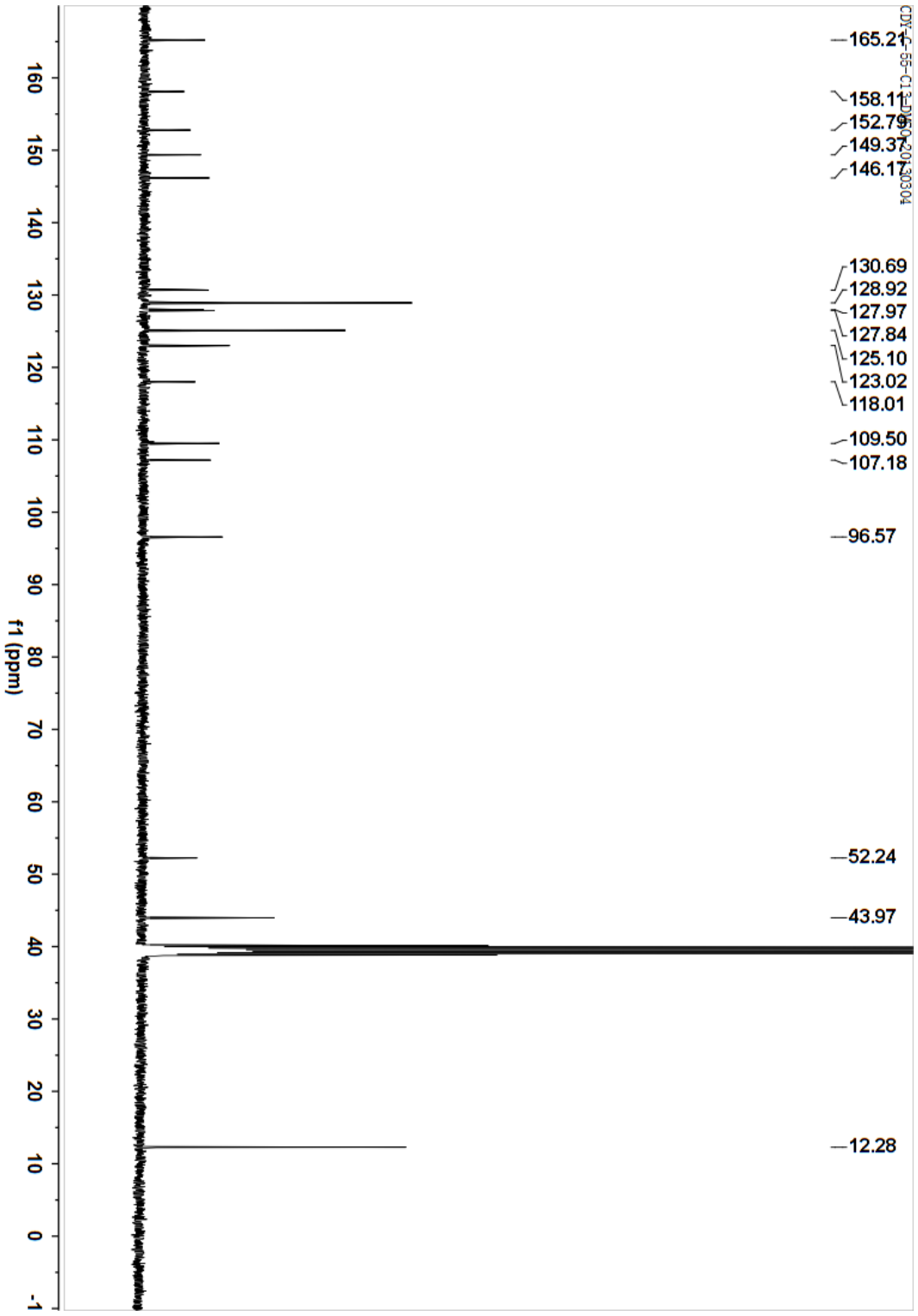
^{13}C-NMR Spectrum of **PS-1** in DMSO-d_6 (100 MHz):



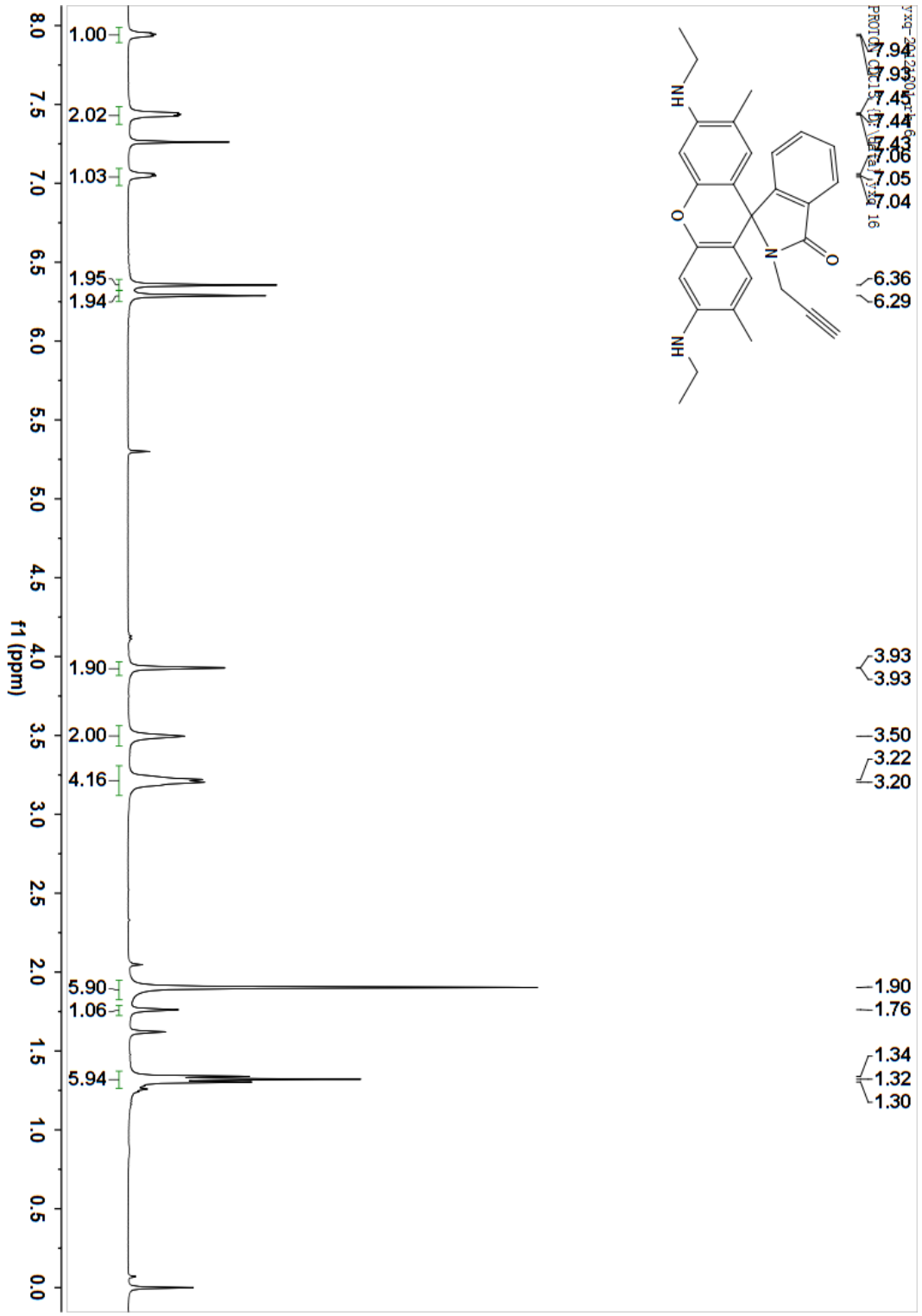
^{1}H-NMR Spectrum of **PS-2** in DMSO-d_6 (400 MHz):



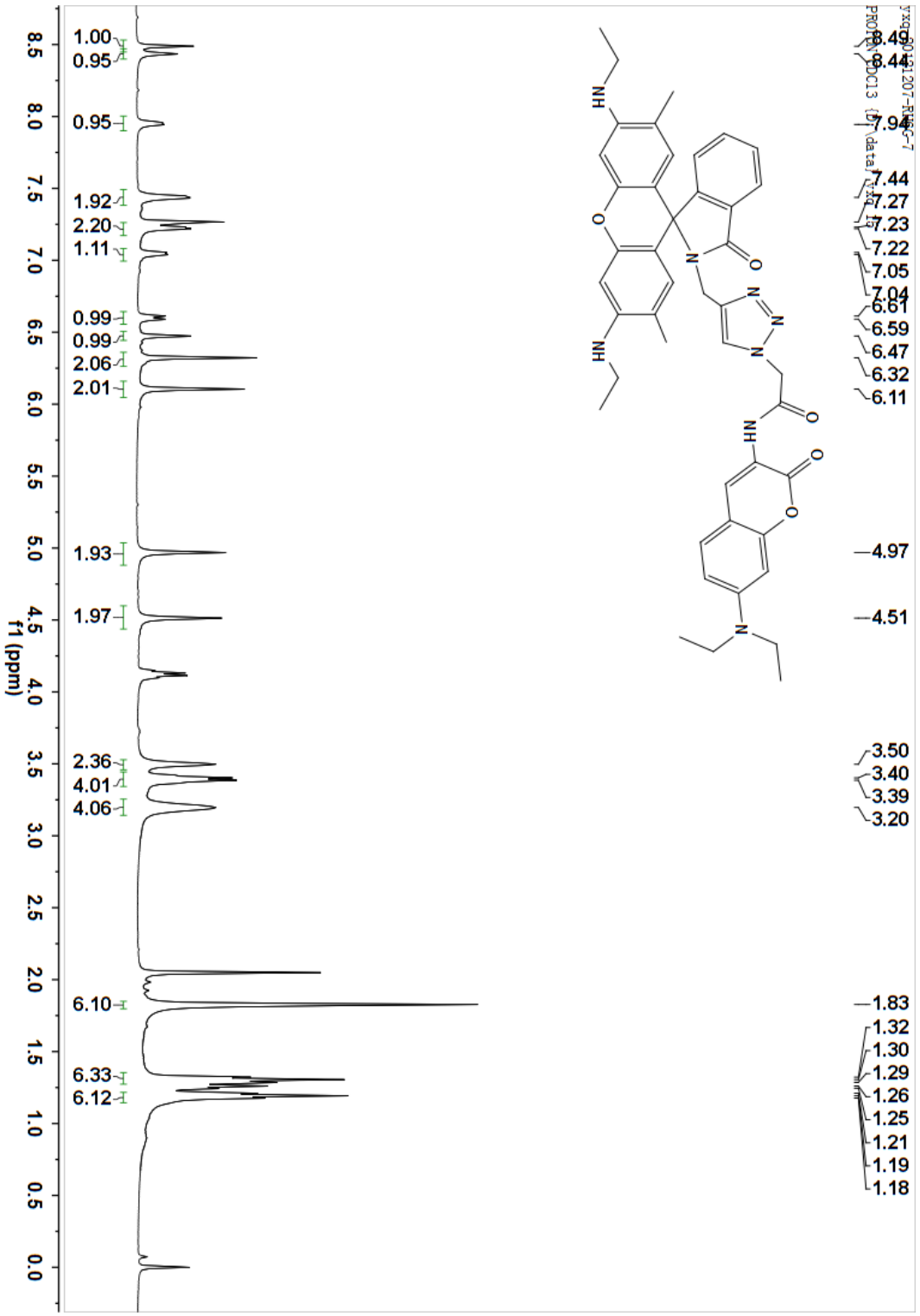
13C-NMR Spectrum of **PS-2** in DMSO-d6 (100 MHz):



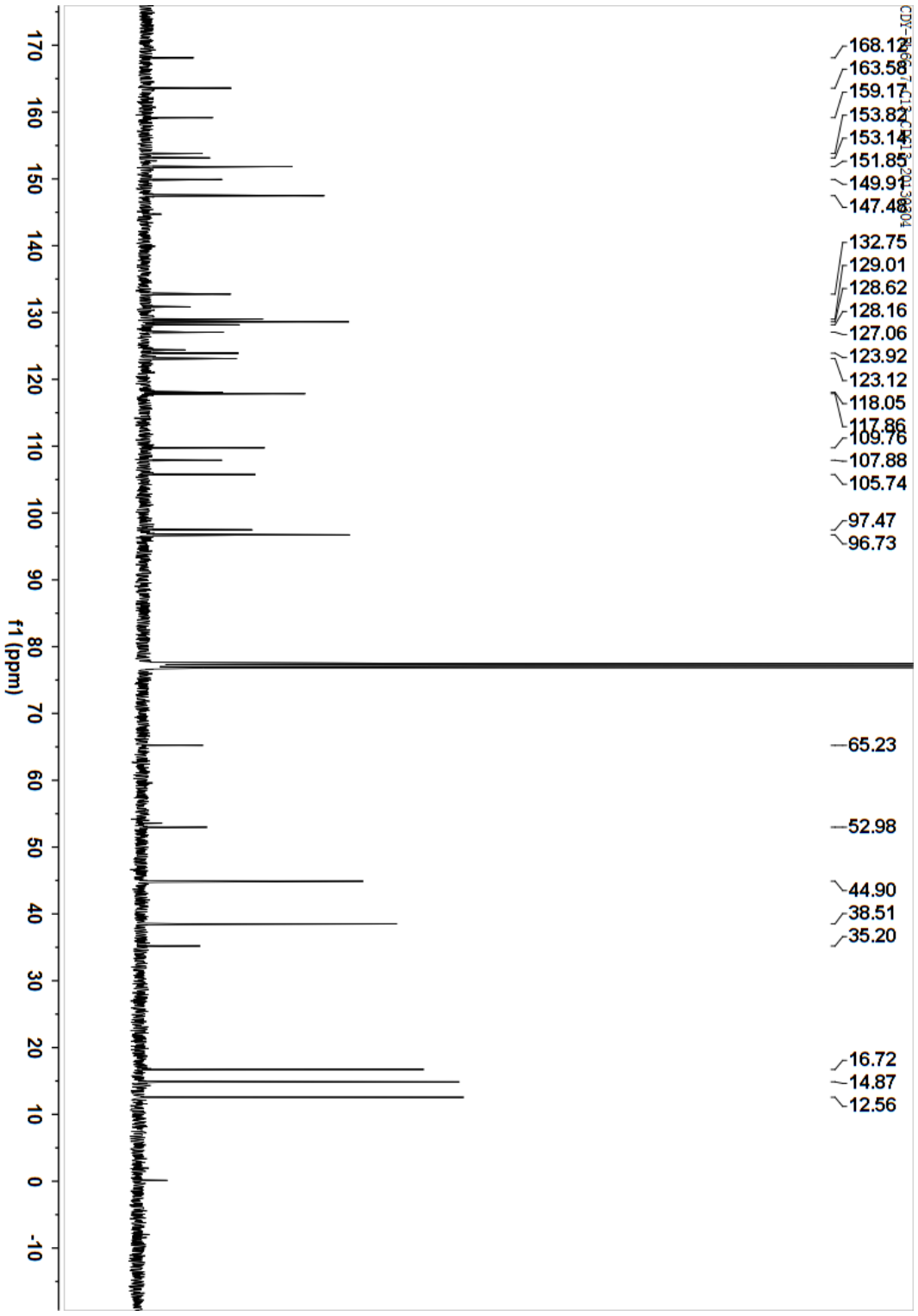
^{1}H-NMR Spectrum of **A-2** in $CDCl_3$ (400 MHz):



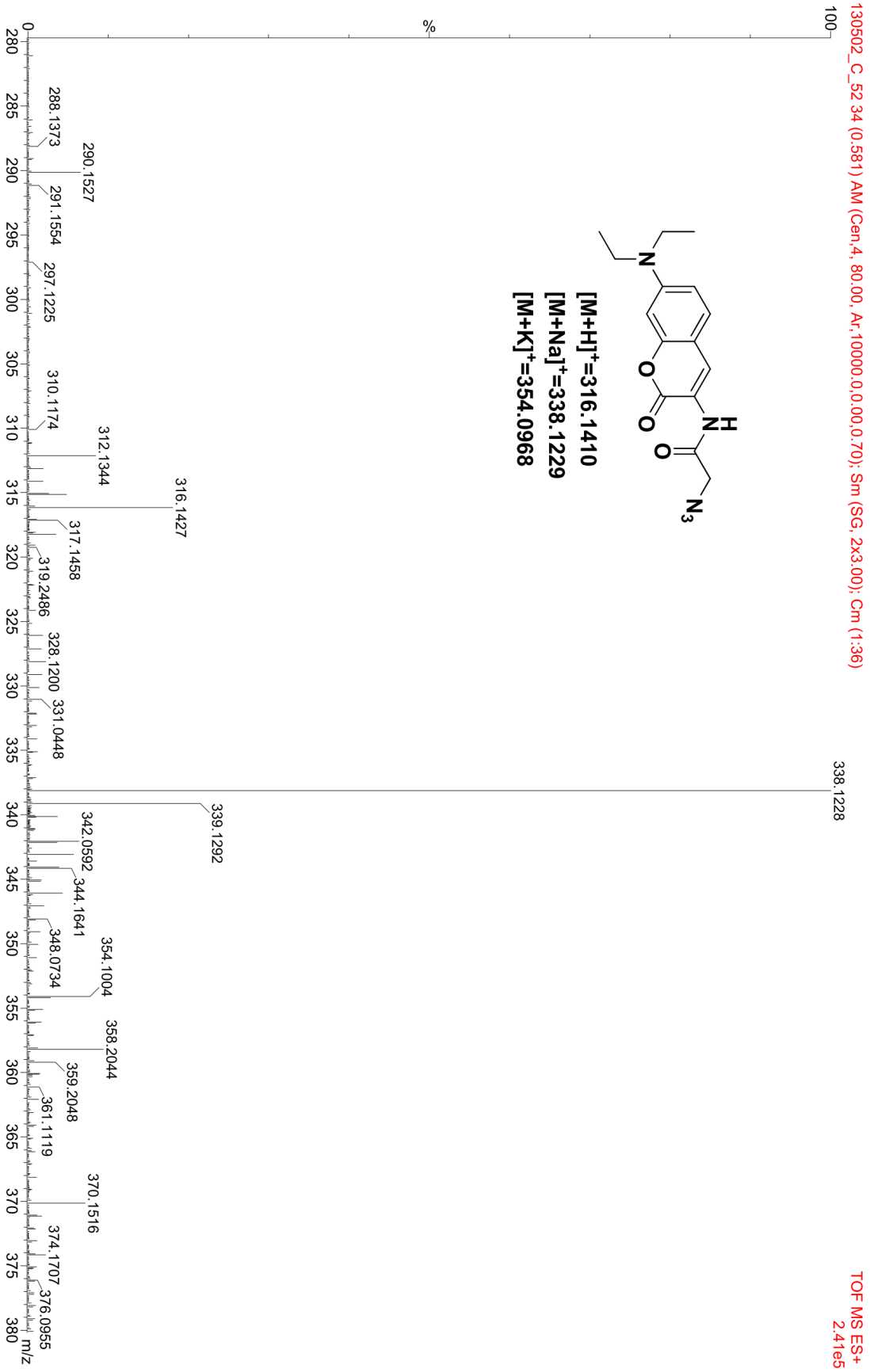
^{1}H-NMR Spectrum of **PS-3** in $CDCl_3$ (400 MHz):



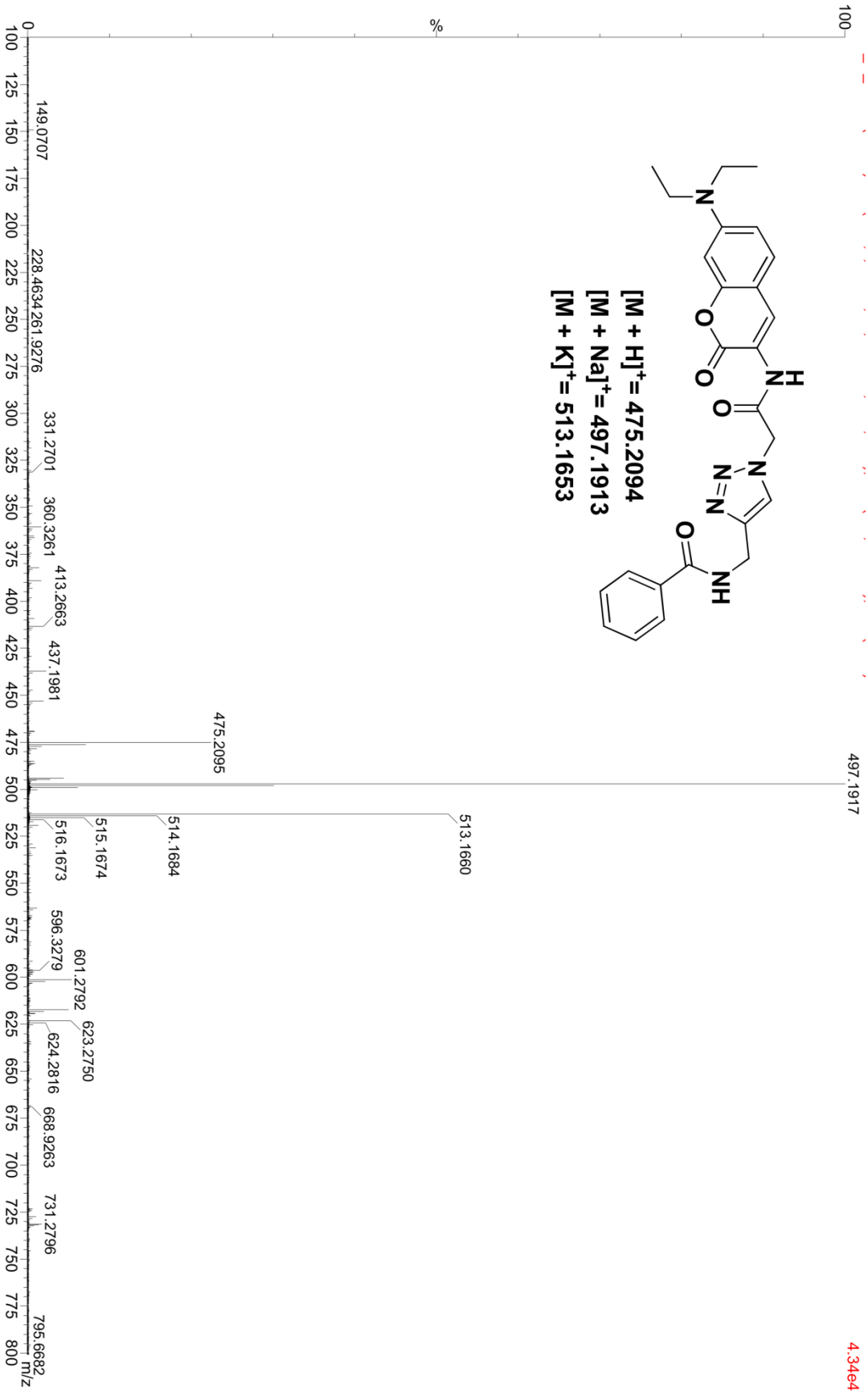
^{13}C-NMR Spectrum of **PS-3** in $CDCl_3$ (100 MHz):



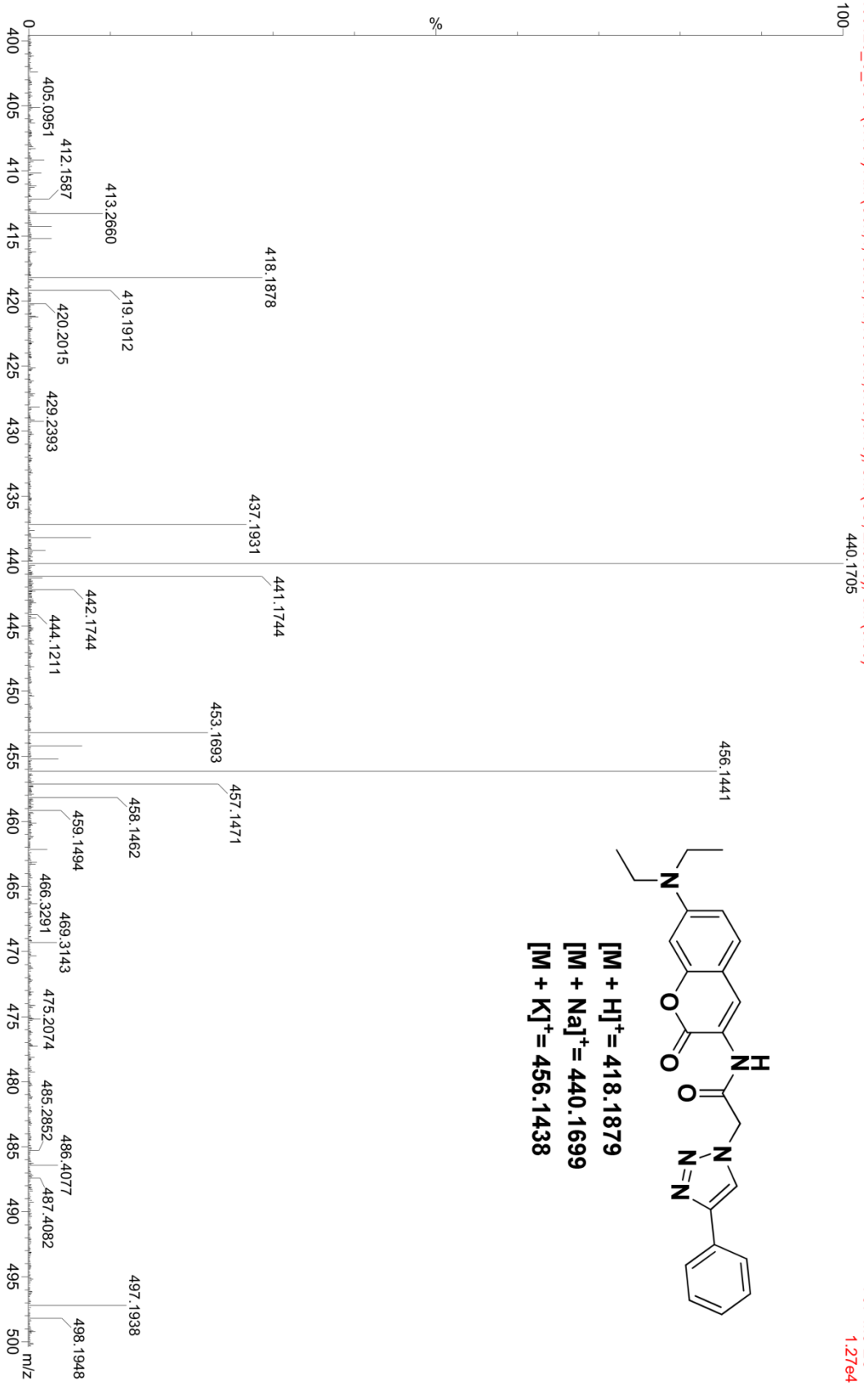
HRMS spectra of **C-2**



HRMS spectra of **PS-1**



HRMS spectra of **PS-2**



HRMS spectra of **PS-3**