

Solvatochromism in diketopyrrolopyrrole derivatives, experimental and computational studies

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(1) Computational data

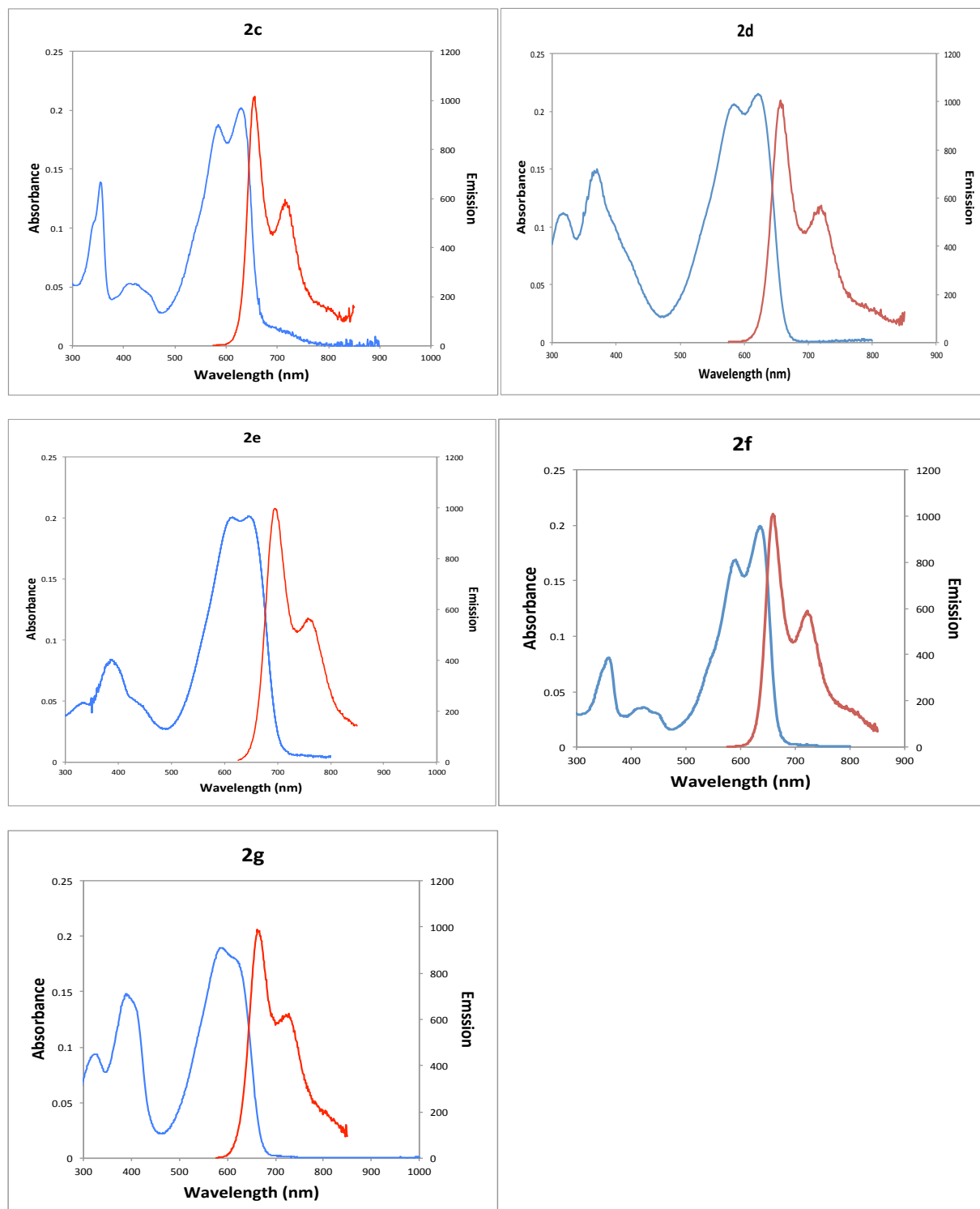
B3LYP/6-31G(d,p) calculated partial atomic charges of **2a-NMe** as a function of solvent.^a

	S ₀ ground state				S ₁ excited state			
	thio	DPP	S	O	thio	DPP	S	O
Mulliken charges								
toluene	0.046	-0.092	0.270	-0.546	0.041	-0.083	0.263	-0.487
chloroform	0.050	-0.099	0.273	-0.553	0.046	-0.091	0.266	-0.494
THF	0.051	-0.102	0.275	-0.556	0.047	-0.095	0.268	-0.497
acetone	0.053	-0.106	0.277	-0.559	0.050	-0.100	0.270	-0.501
acetonitrile	0.054	-0.107	0.277	-0.560	0.051	-0.101	0.271	-0.502
water	0.054	-0.108	0.278	-0.561	0.051	-0.102	0.271	-0.503
NBO charges								
toluene	0.084	-0.167	0.457	-0.628	0.038	-0.075	0.429	-0.615
chloroform	0.087	-0.175	0.459	-0.635	0.044	-0.089	0.432	-0.622
THF	0.089	-0.178	0.461	-0.638	0.047	-0.095	0.433	-0.626
acetone	0.091	-0.182	0.463	-0.641	0.051	-0.102	0.435	-0.630
acetonitrile	0.091	-0.183	0.463	-0.642	0.052	-0.104	0.436	-0.631
water	0.092	-0.183	0.464	-0.643	0.053	-0.106	0.436	-0.632

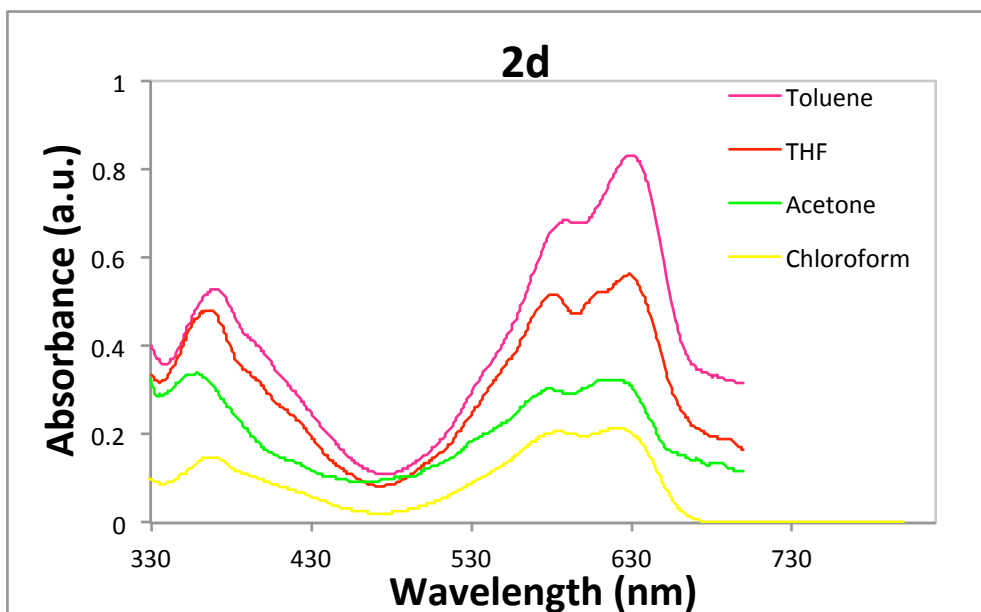
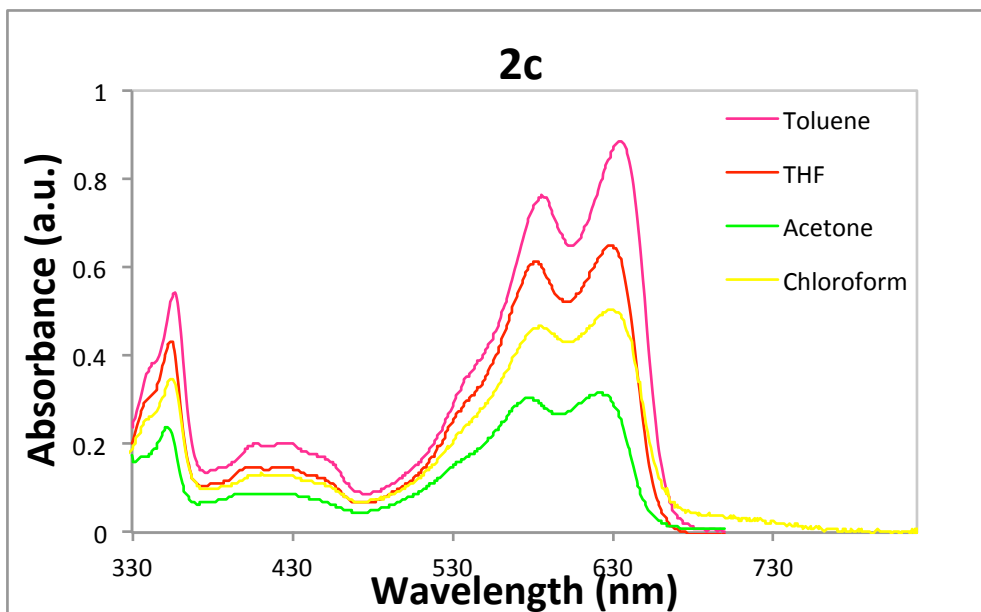
^a Atomic partial charges on S and O atoms, and sum of charges on the thiophene and DPP core groups.

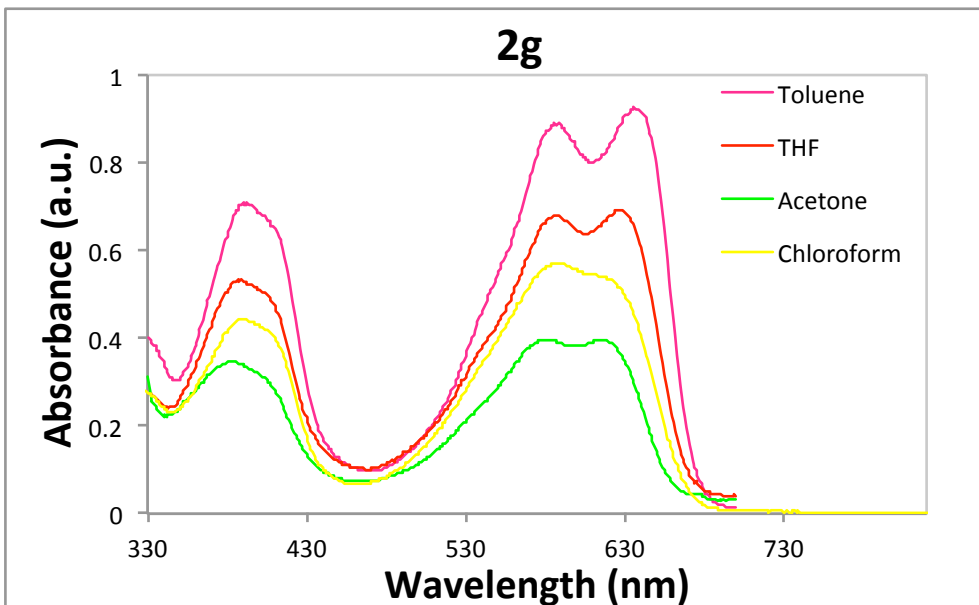
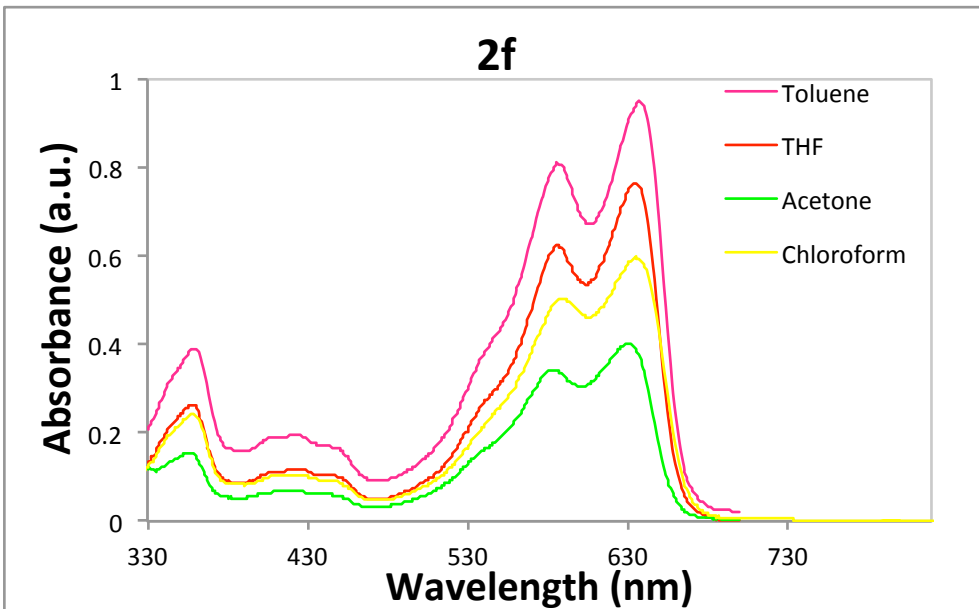
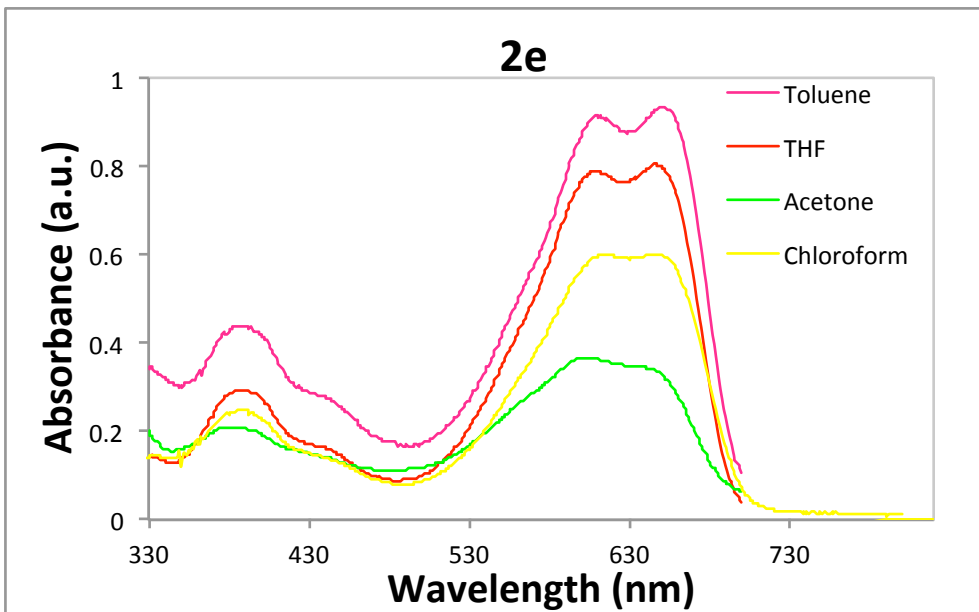
(2) Photophysical data

SUPP Figure 1. Absorption (blue) and emission (red) spectra of DPP derivatives **2c-2g** in spectroscopic grade chloroform



SUPP Figure 2. Absorption spectra of compounds **2c-2g** in solvents of varying polarity.



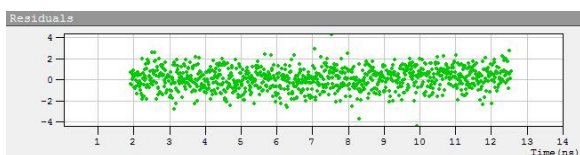


SUPP Figure 3. Fluorescence Decay Data and Results of Single Exponential Fitting for Compounds **2f** and **2g**.

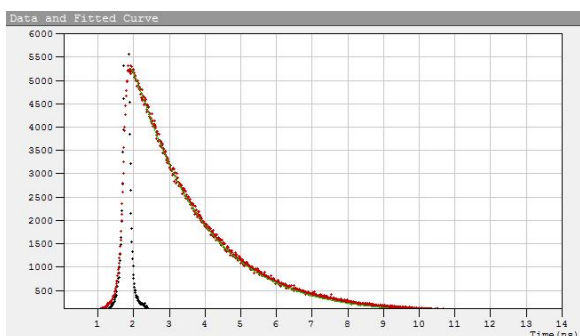
Fitted lifetime τ_f ; Reduced chi-square fitting parameter χ^2 ; Weighted residuals, fluorescence decay data, instrument response function and fitted curve. Solvent: chloroform; excitation wavelength: 400nm, emission wavelength: 650 nm.

Compound 2f

$\tau_f = 1.92$ ns; $\chi^2 = 1.05$



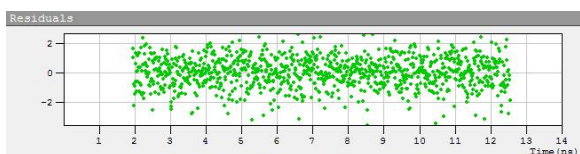
Residuals



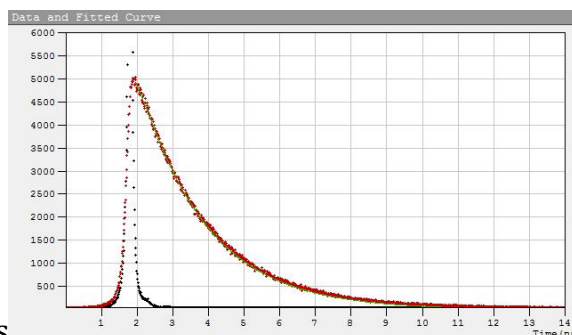
Fluorescence decay and fitted curve

Compound 2g

$\tau_f = 1.91$ ns; $\chi^2 = 1.08$

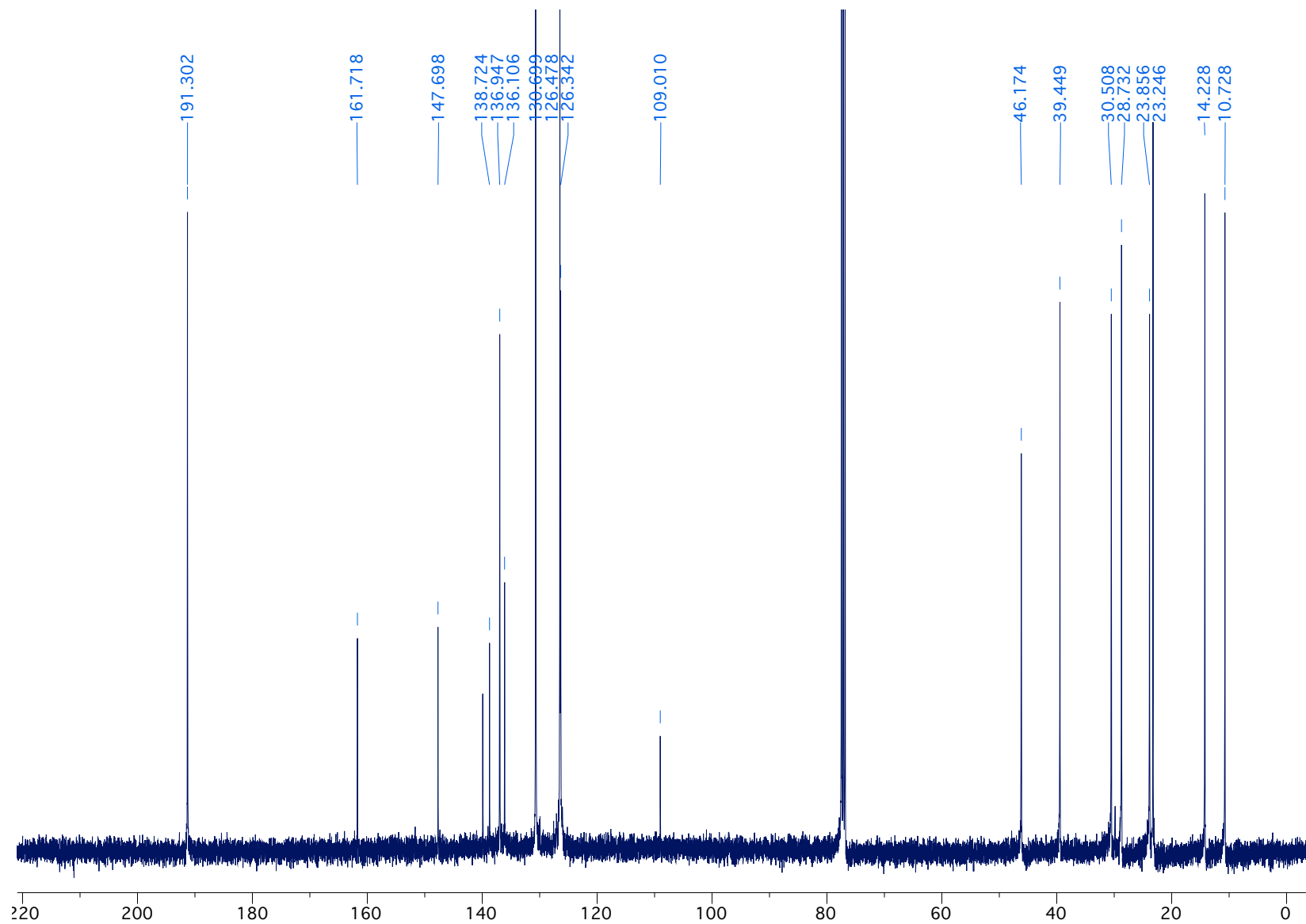


Residuals

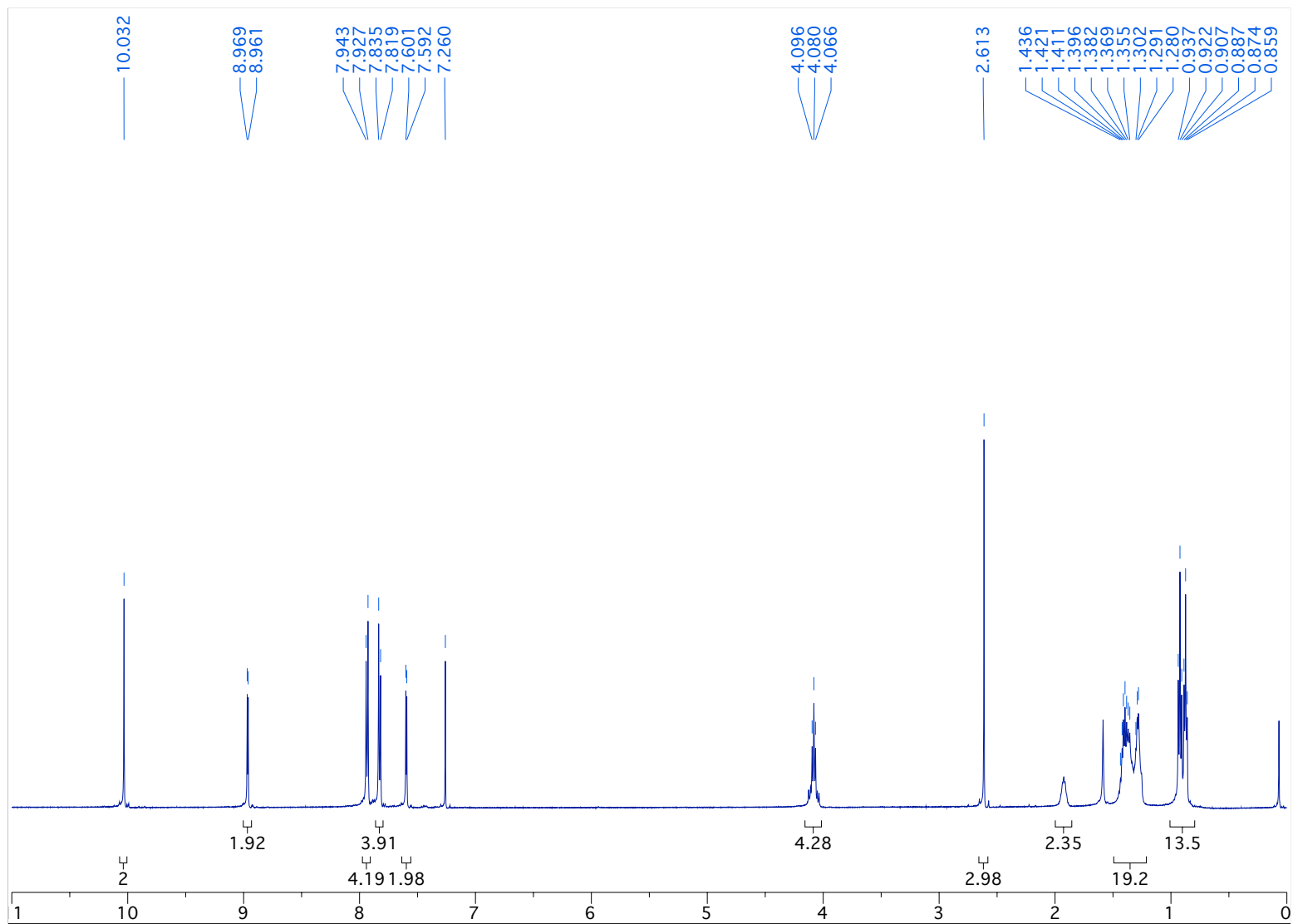


Fluorescence decay and fitted curve

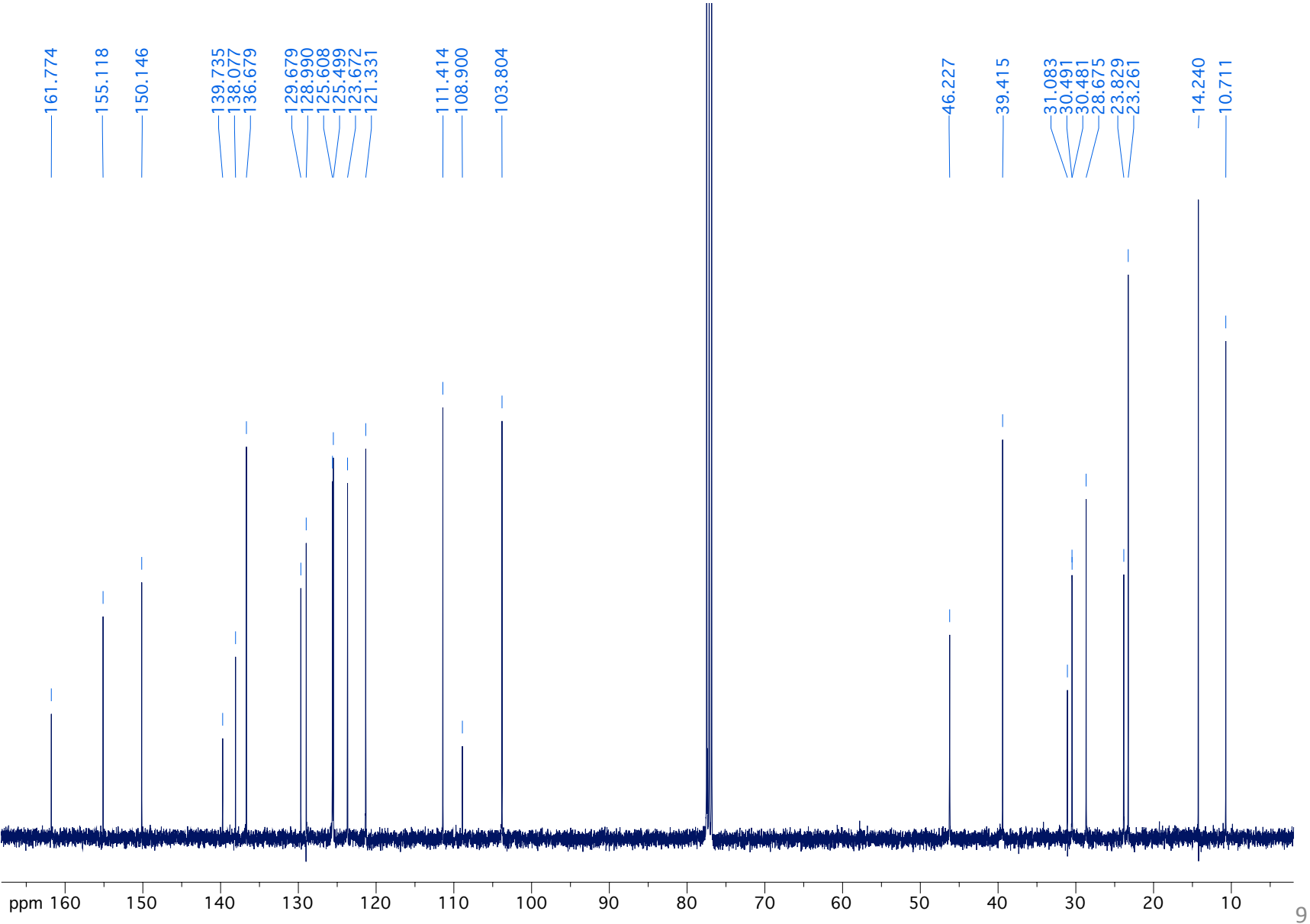
13C-Compound 2b



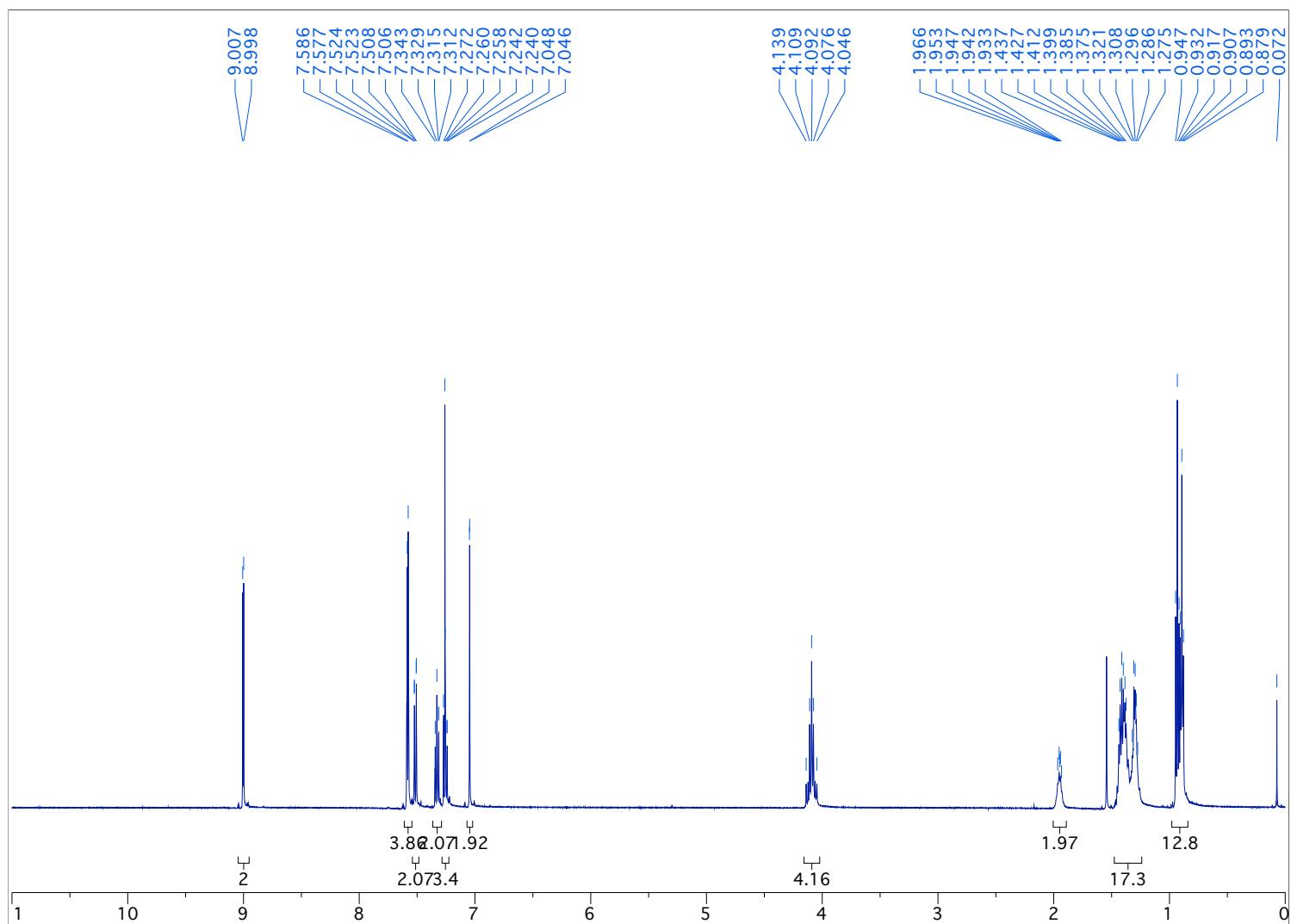
1H - Compound 2b



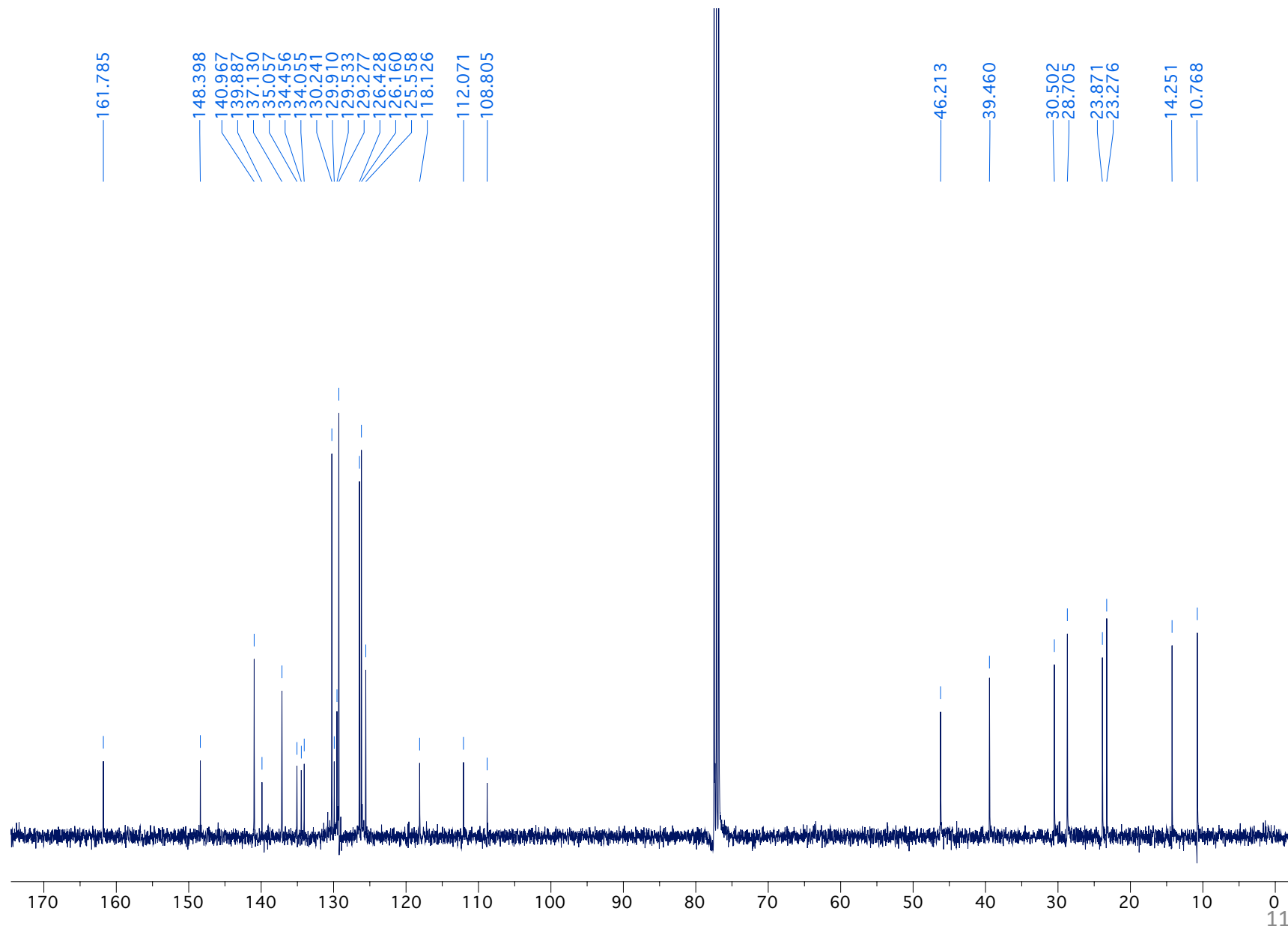
13C - Compound 2c



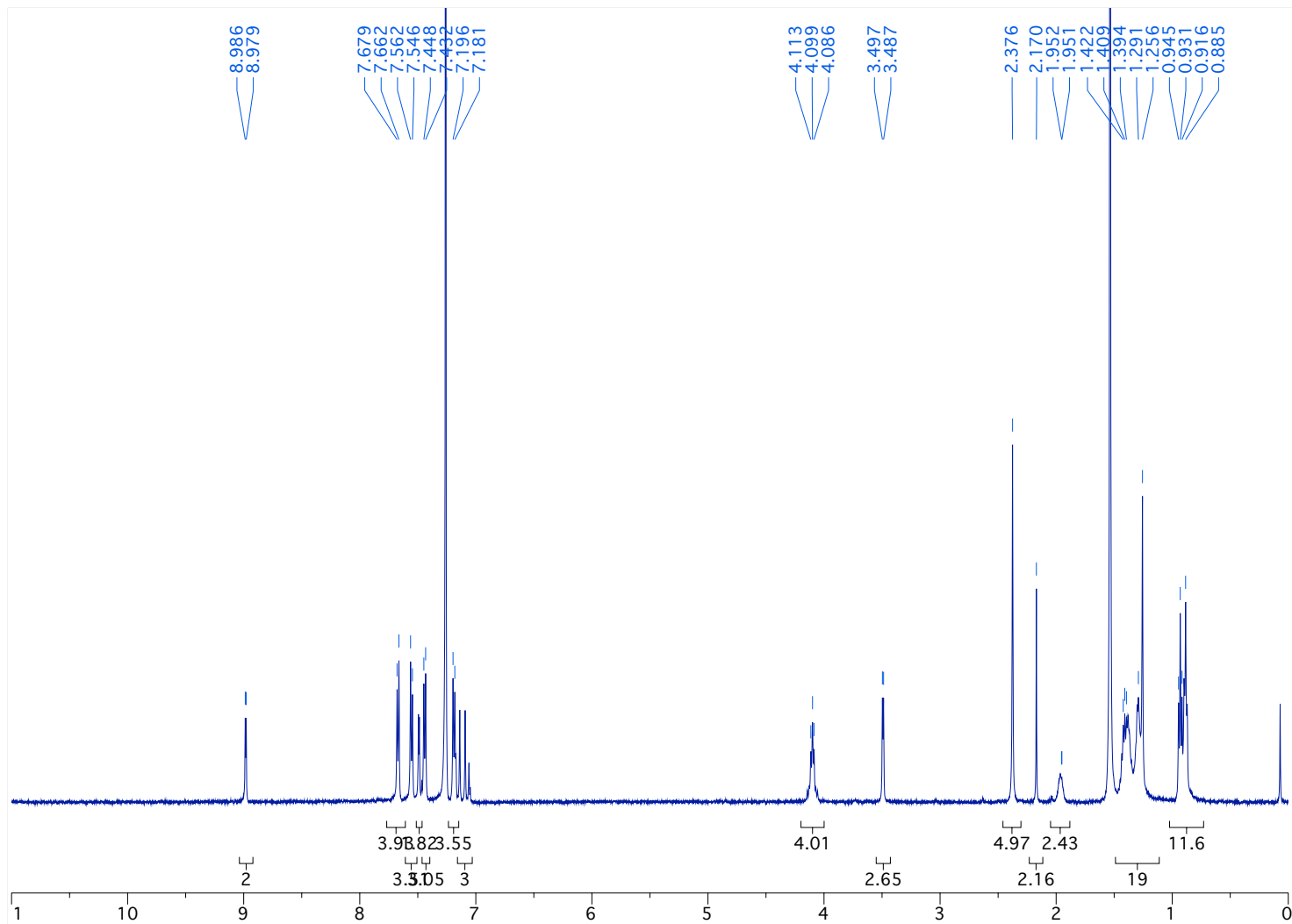
1H – Compound 2c



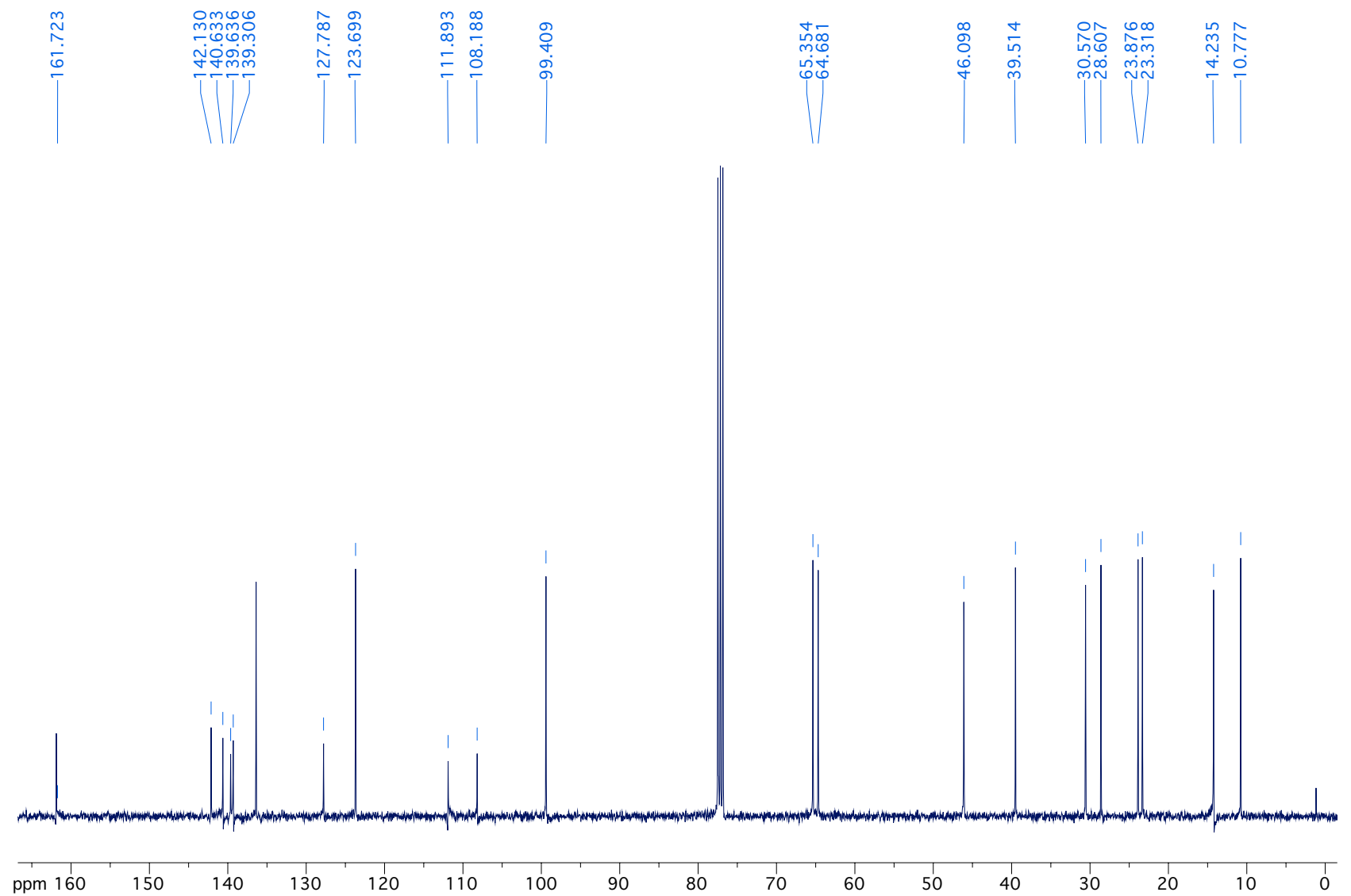
13C - Compound 2d



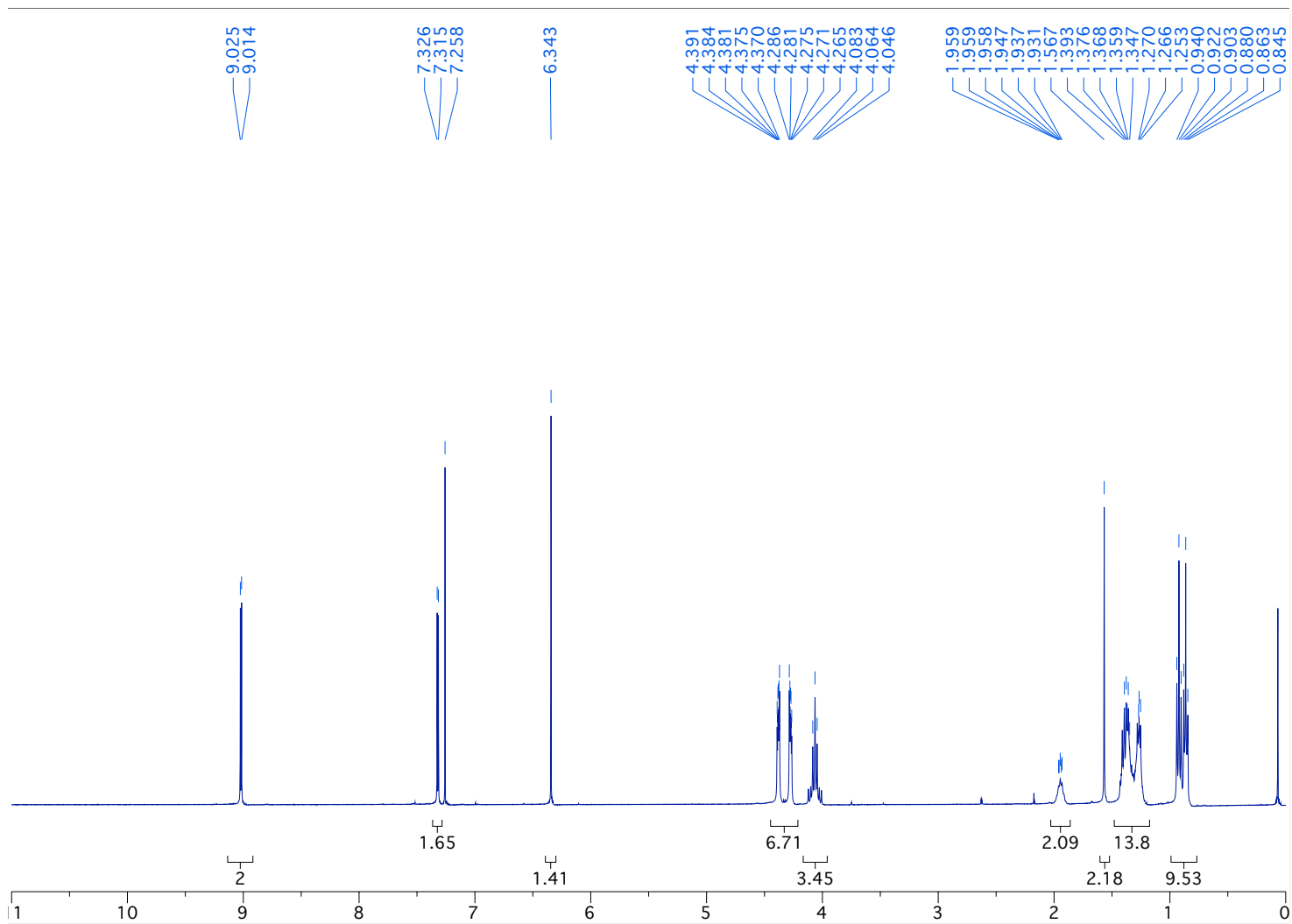
1H – Compound 2d



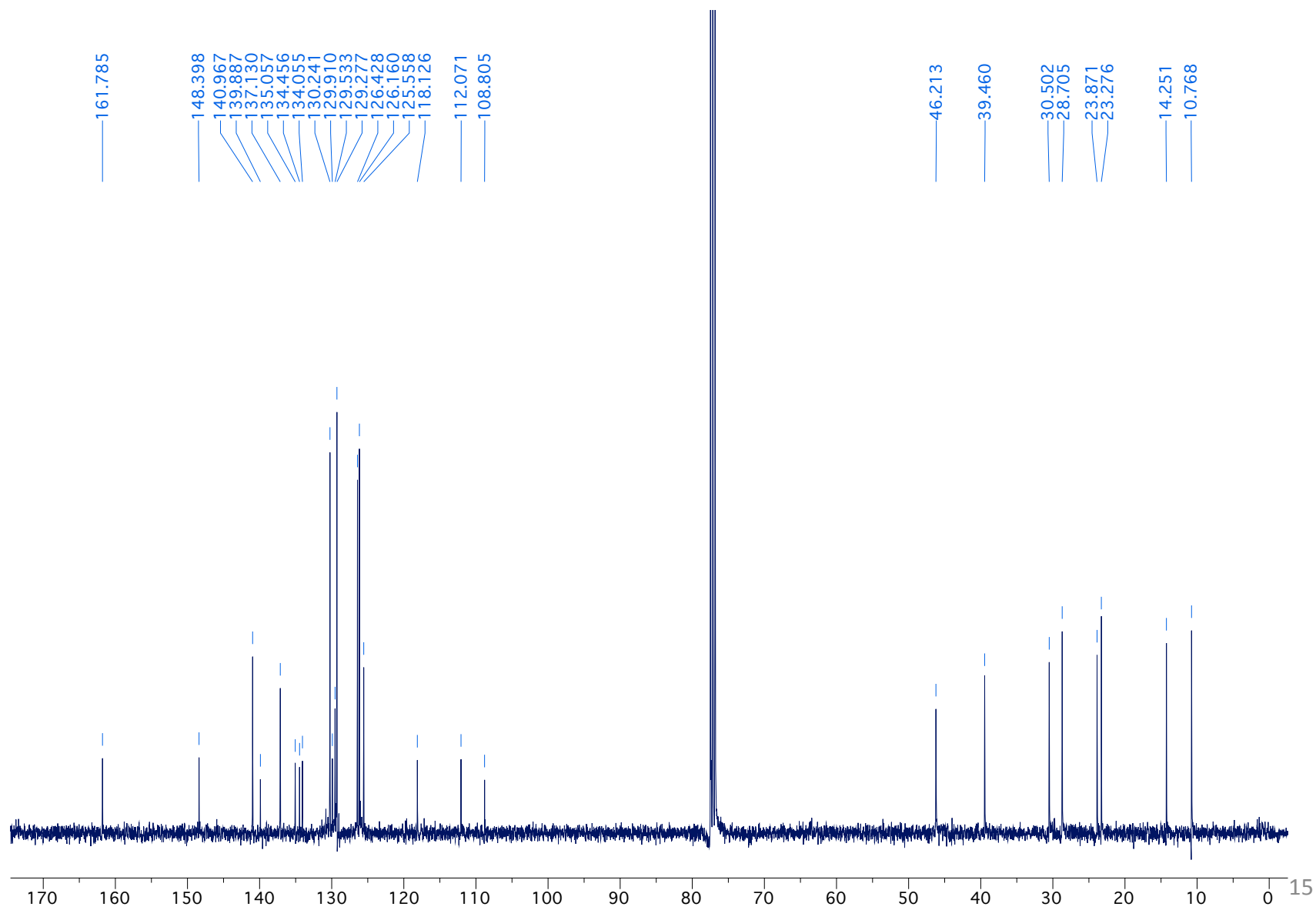
13C - Compound 2f



1H – Compound 2f



13C - Compound 2g



1H – Compound 2g

