

Supporting Information

Tetrathienylethene-based red aggregation-enhanced emission probes: super red-shifted mechanochromic behavior and highly photostable cell membrane imaging

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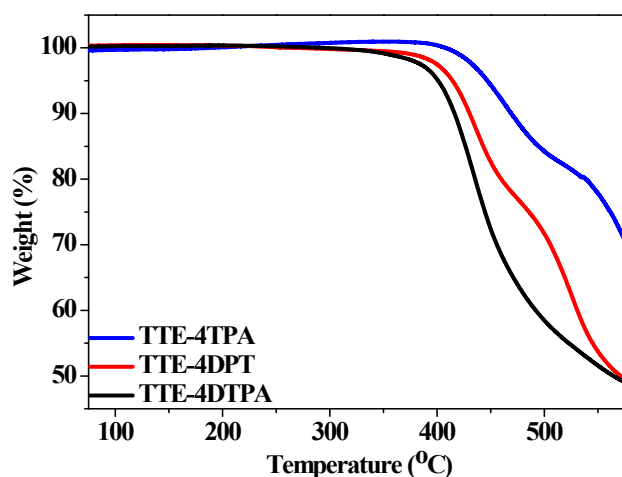


Figure S1. Thermogravimetric analysis (TGA) of TTE-4TPA, TTE-4DPT and TTE-4DTPA with a heating rate at 10 °C/min under N₂ atmosphere.

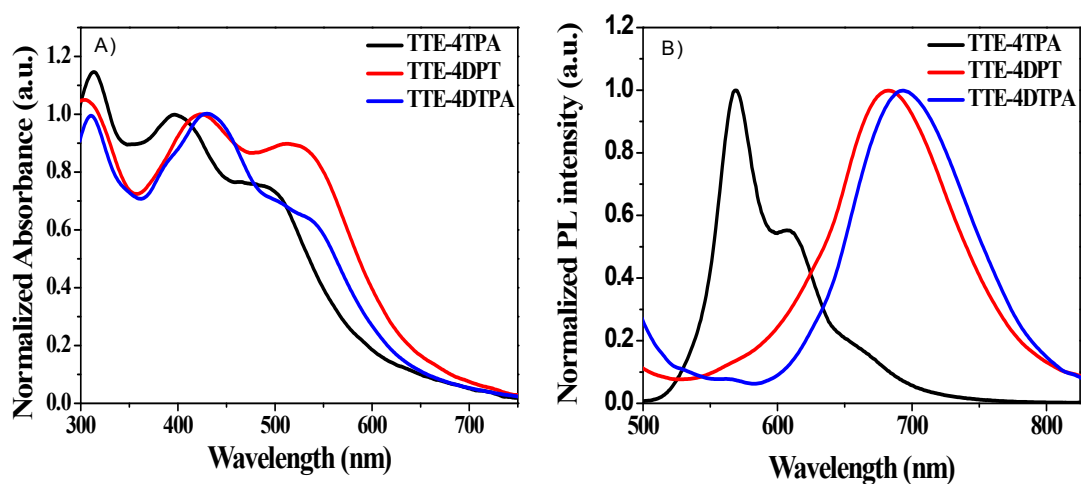


Figure S2. A) The absorption spectra of **TTE-4TPA**, **TTE-4DPT** and **TTE-4DTPA** in films; (B) the emission spectra of **TTE-4TPA**, **TTE-4DPT** and **TTE-4DTPA** in solid states.

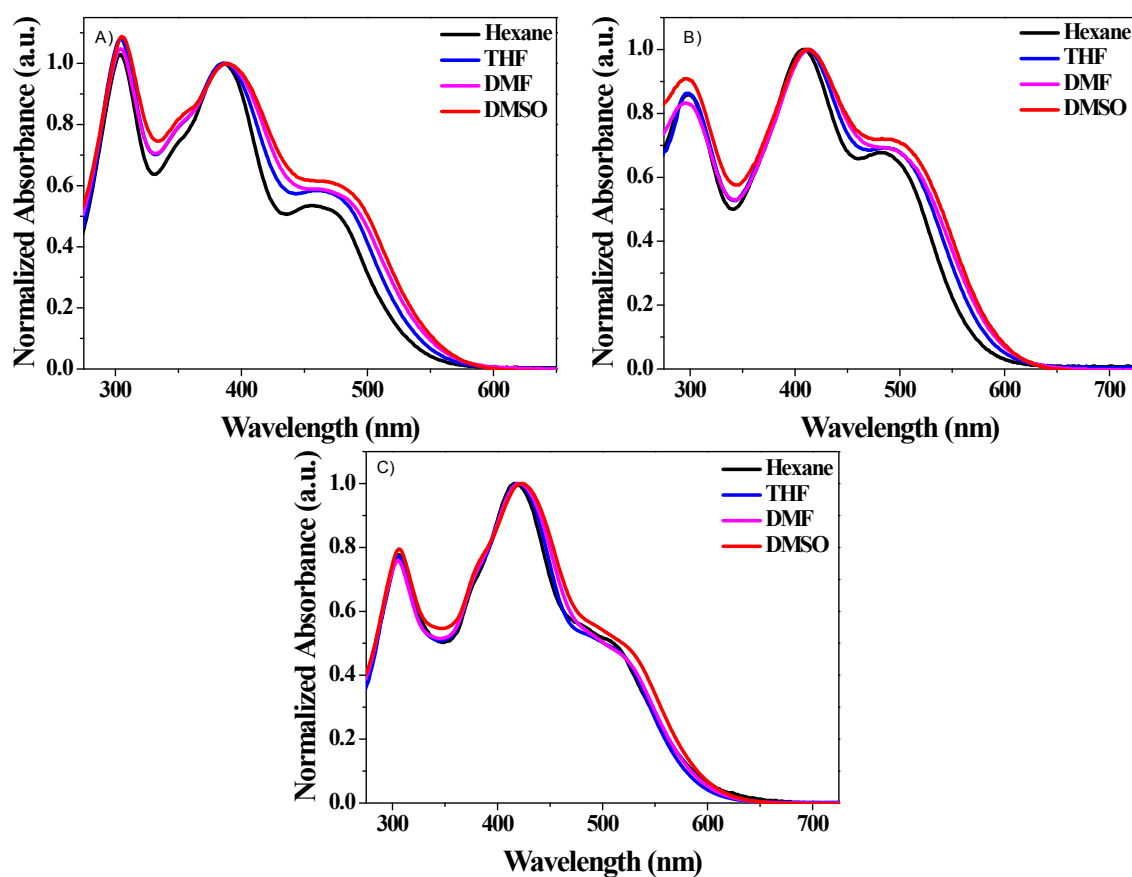


Figure S3. A) The absorption spectra of **TTE-4TPA** in solvents with different polarity; B) The absorption spectra of **TTE-4DPT** in solvents with different polarity; C) The absorption spectra of **TTE-4DTPA** in solvents with different polarity.

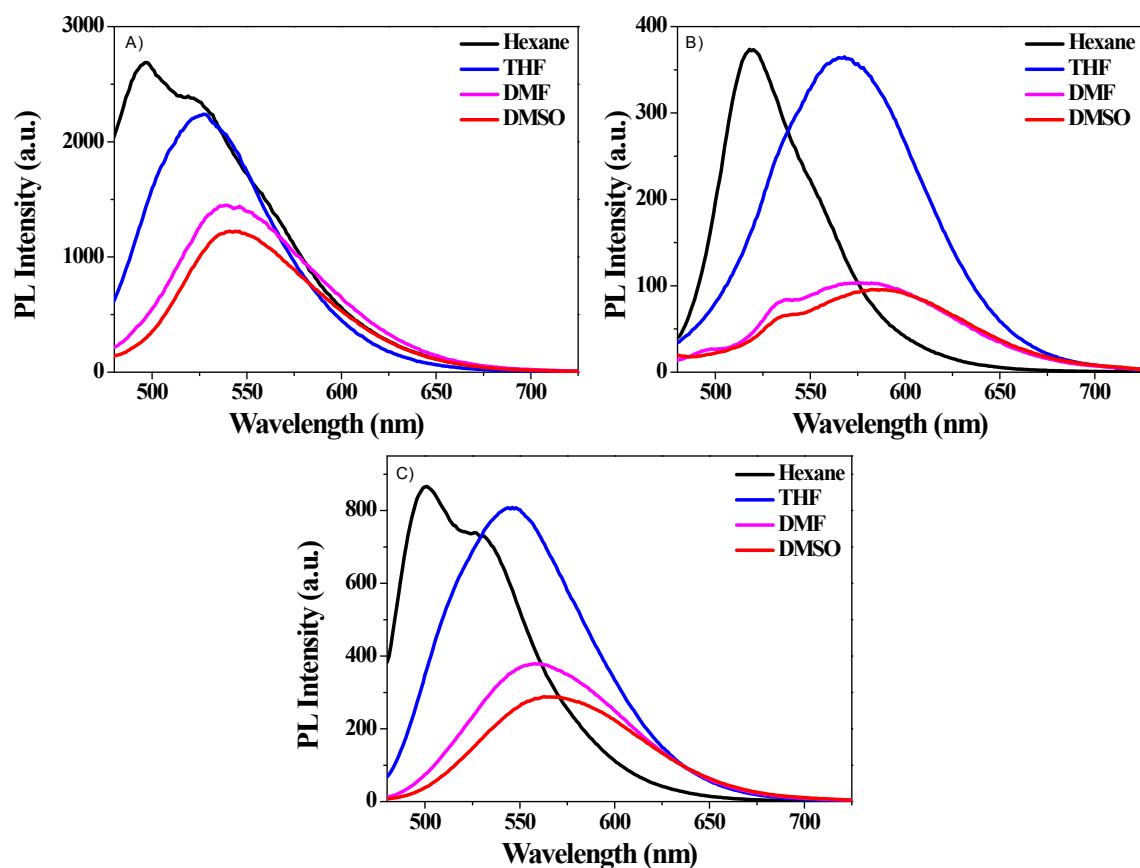


Figure S4. A) Emission spectra of **TTE-4TPA** in solvents with different polarity; B) Emission spectra of **TTE-4DPT** in solvents with different polarity; C) Emission spectra of **TTE-4DTPA** in solvents with different polarity.

Table 1. fluorescence lifetime of **TTE-4TPA**, **TTE-4DPT** and **TTE-4DTPA** in different polar solvents.^a

Compd	Hexane	THF	DMF	DMSO
TTE-4TPA	3.0 ns	2.6 ns	3.3 ns	2.6 ns
TTE-4DPT	3.9 ns	3.4 ns	4.1 ns	4.0 ns
TTE-4DTPA	2.9 ns	4.0 ns	3.7 ns	2.7 ns

^aexcited at 365 nm and emission decay curve was monitored at the wavelength of maximum emission peak.

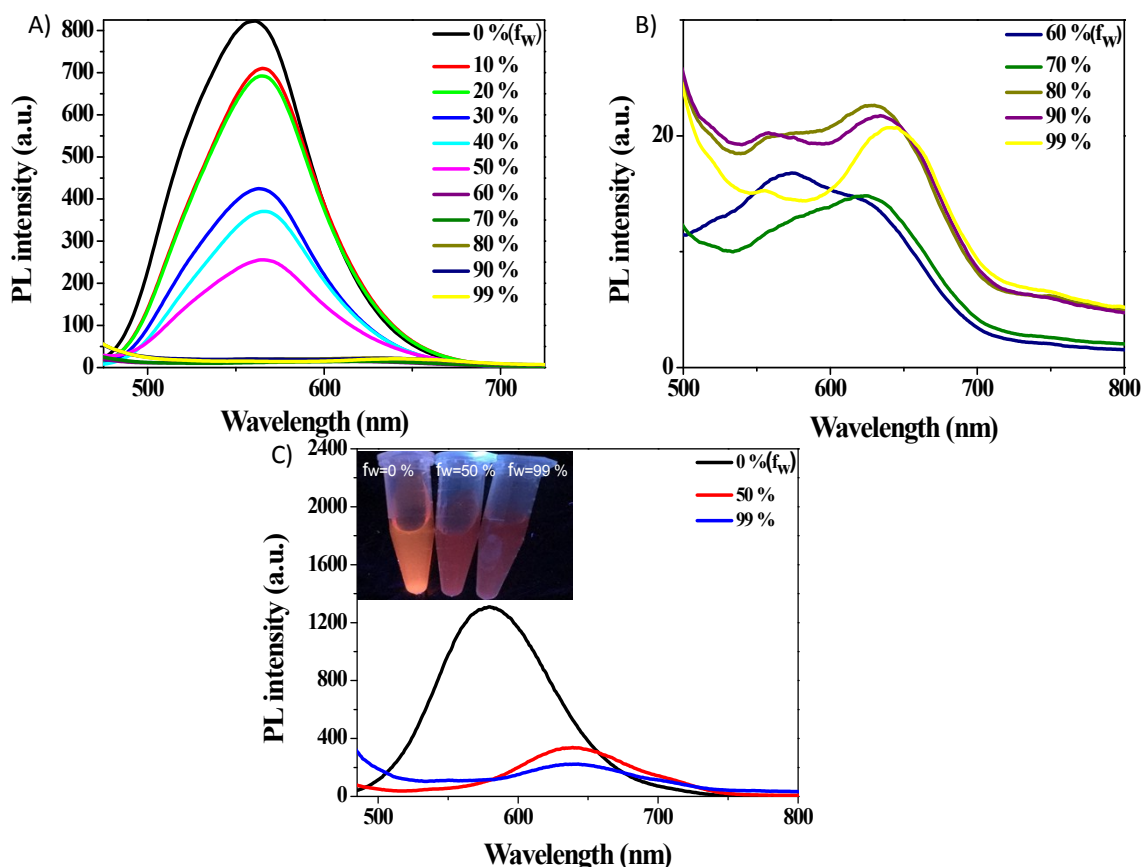


Figure S5. A) Emission spectra of **TTE-4DTPA** in THF-water mixtures with different water fractions (f_w); B) Enlarged emission spectra of **TTE-4DTPA** when f_w was over 60 %; C) Emission spectra of **TTE-4DTPA** in DMSO-water mixtures with different water fractions (f_w); Inset: photos of **TTE-4DTPA** with different water fractions under UV lamp illumination.

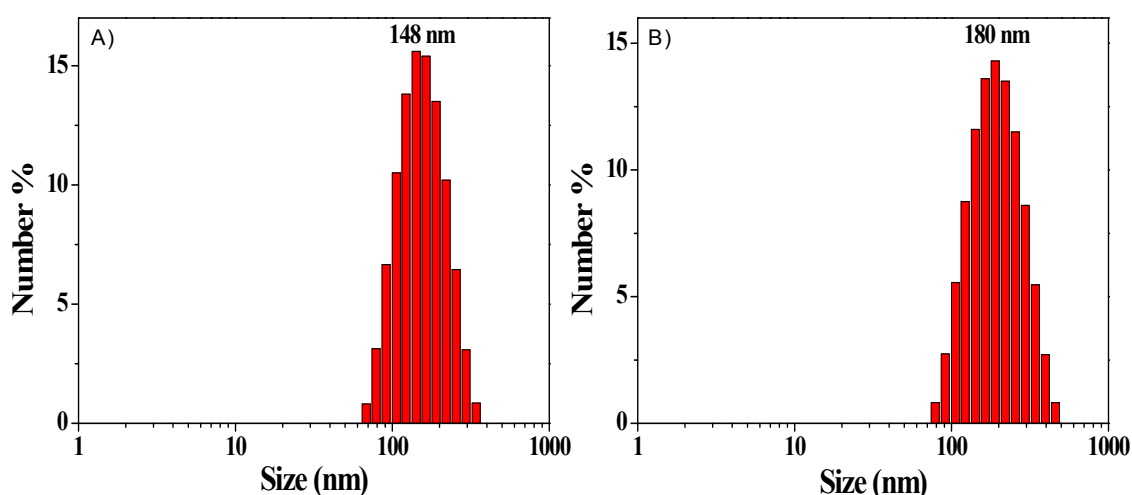


Figure S6. A) DLS plot of compound **TTE-4DPT** (10^{-5} M) in 99 % water/THF mixture; B) DLS plot of compound **TTE-4DTPA** (10^{-5} M) in 99 % water/THF mixture.

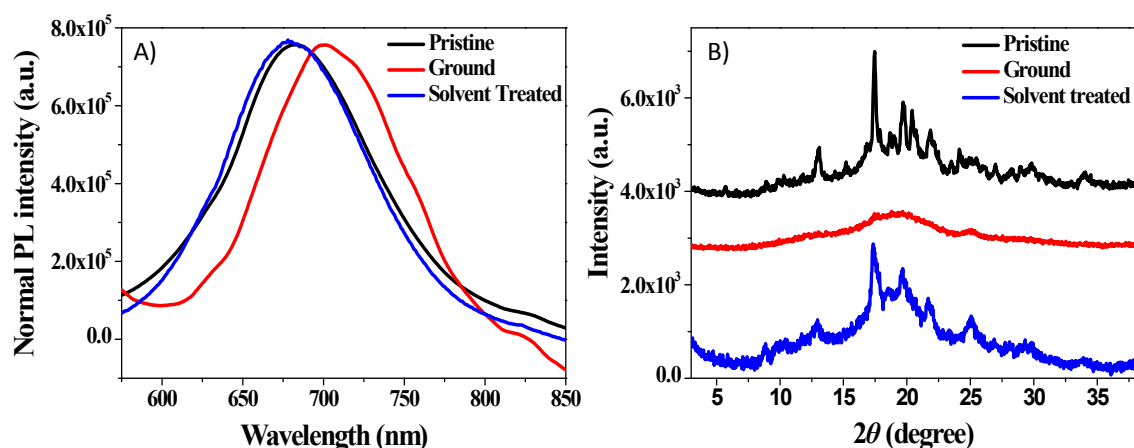


Figure S7. A) Emission spectra of TTE-4DPT as-pristine, ground, and solvent treated; (B) XRD of TTE-4DPT as-pristine, ground, and solvent treated.

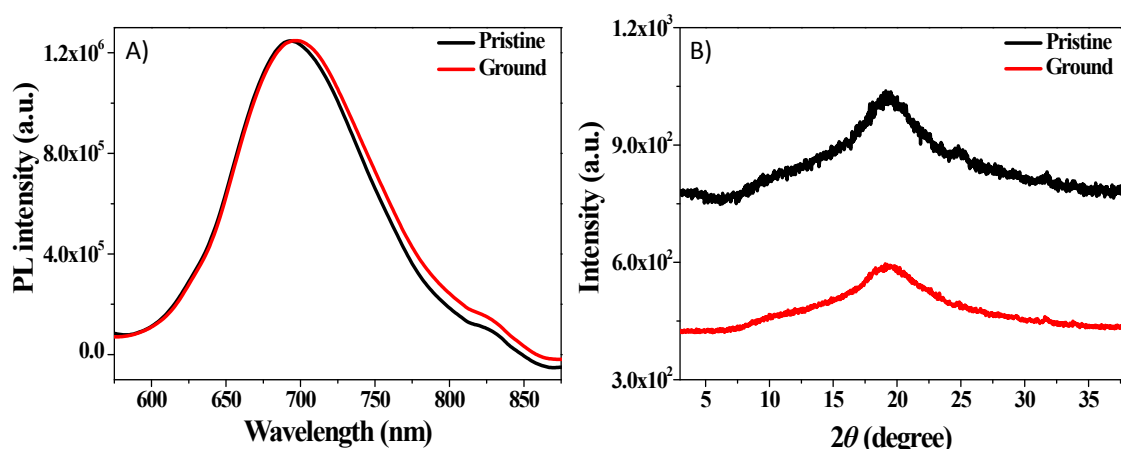


Figure S8. A) Emission spectra of TTE-4DTPA as-pristine and ground, (B) XRD of TTE-4DTPA as-pristine and ground.

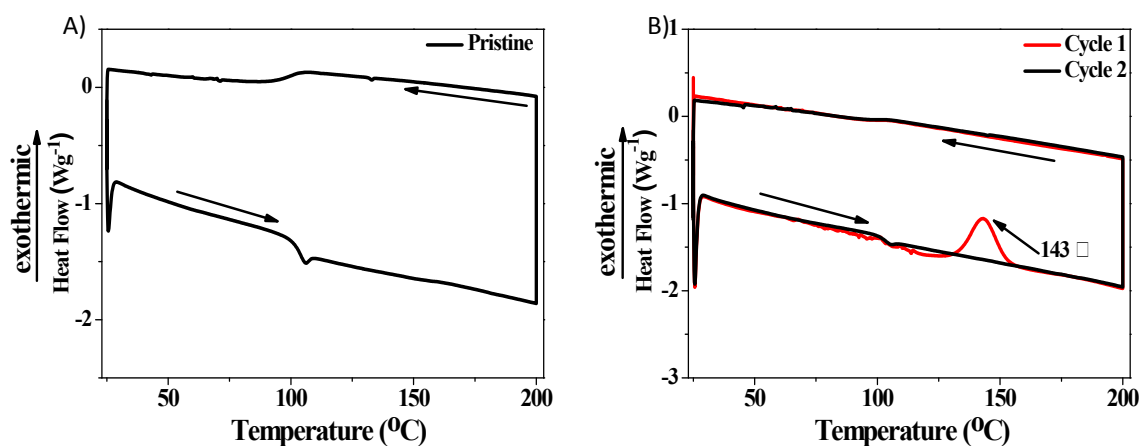


Figure S9. A) DSC thermograms of pristine TTE-4DPT recorded under N_2 atmosphere at a heating rate of $10^{\circ}\text{Cmin}^{-1}$. (B) DSC thermograms of ground TTE-4DPT recorded under N_2 at a heating rate of $10^{\circ}\text{C min}^{-1}$.

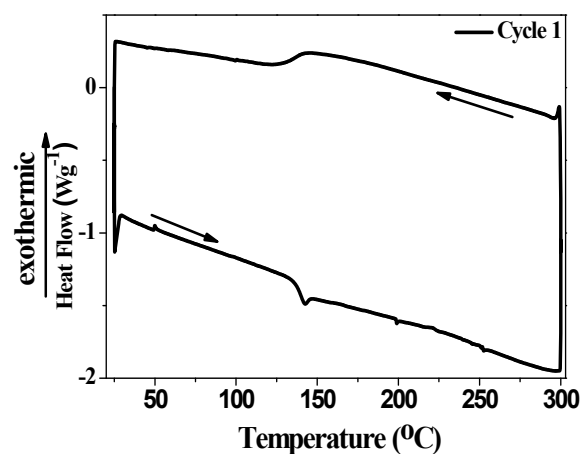


Figure S10. DSC thermograms of ground **TTE-4DTPA** recorded under N_2 atmosphere at a heating rate of $10\text{ }^{\circ}\text{C min}^{-1}$.

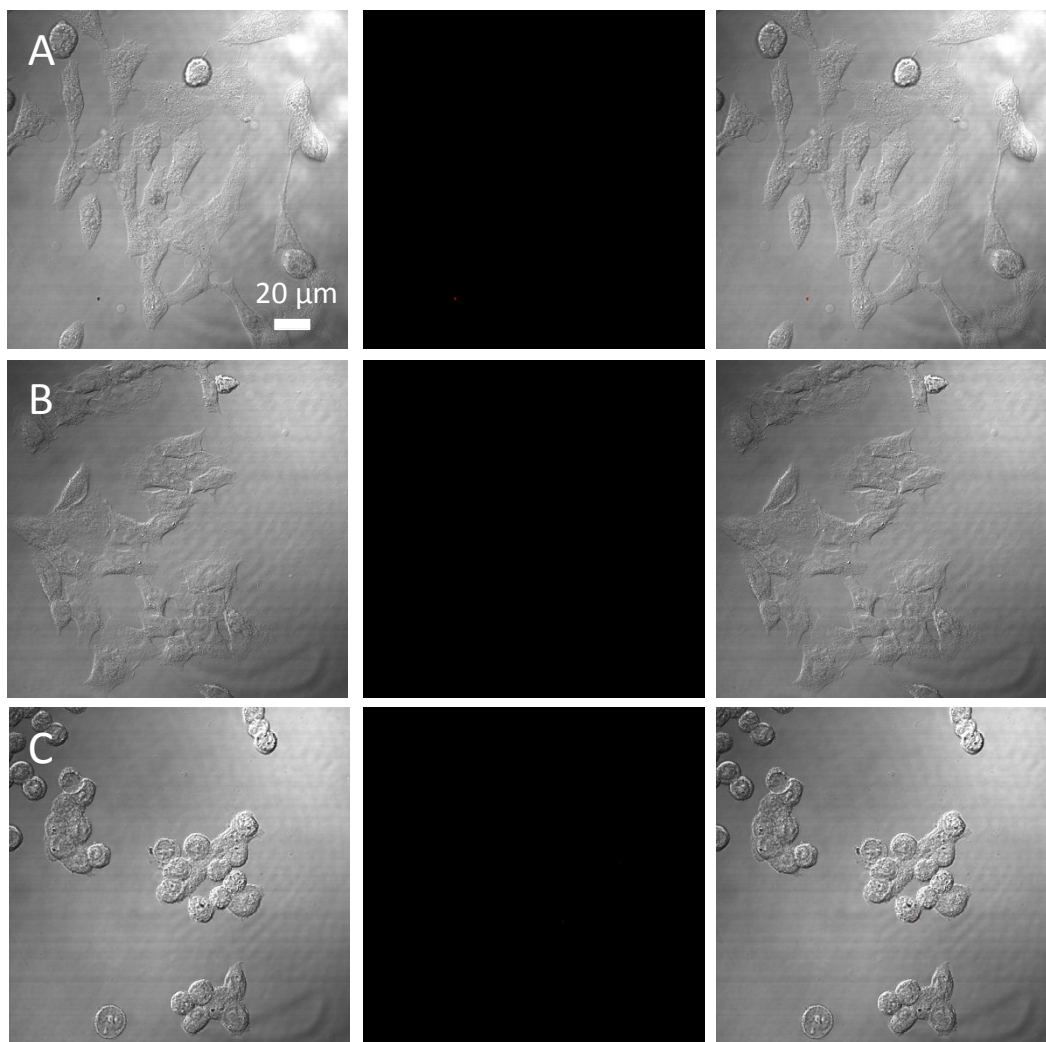


Figure S11. Confocal fluorescent images of HeLa cells incubated with different concentrations of **TTE-4TPA** (A, $10\text{ }\mu\text{M}$), (B, $20\text{ }\mu\text{M}$), (C, $50\text{ }\mu\text{M}$) for 4 h. From left

to right are bright field images, fluorescent images, and the merged images. Excitation wavelength: 405 nm; emission collected: 540-600 nm. The scale bar is 20 μ m.

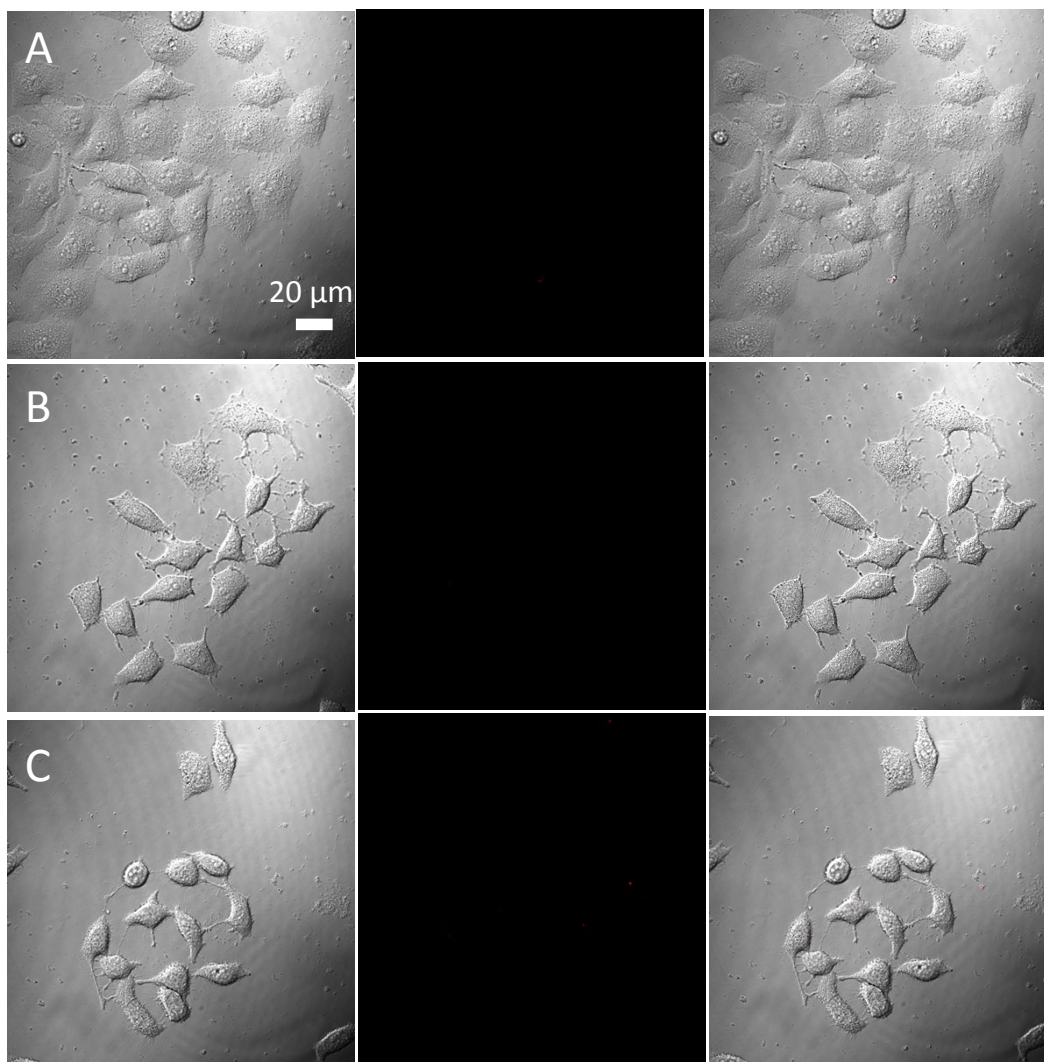


Figure S12. Confocal fluorescent images of HeLa cells incubated with different concentrations of **TTE-4DPT** (A, 10 μ M), (B, 20 μ M), (C, 50 μ M) for 4 h. From left to right are bright field images, fluorescent images, and the merged images. Excitation wavelength: 405 nm; emission collected: 540-600 nm. The scale bar is 20 μ m.

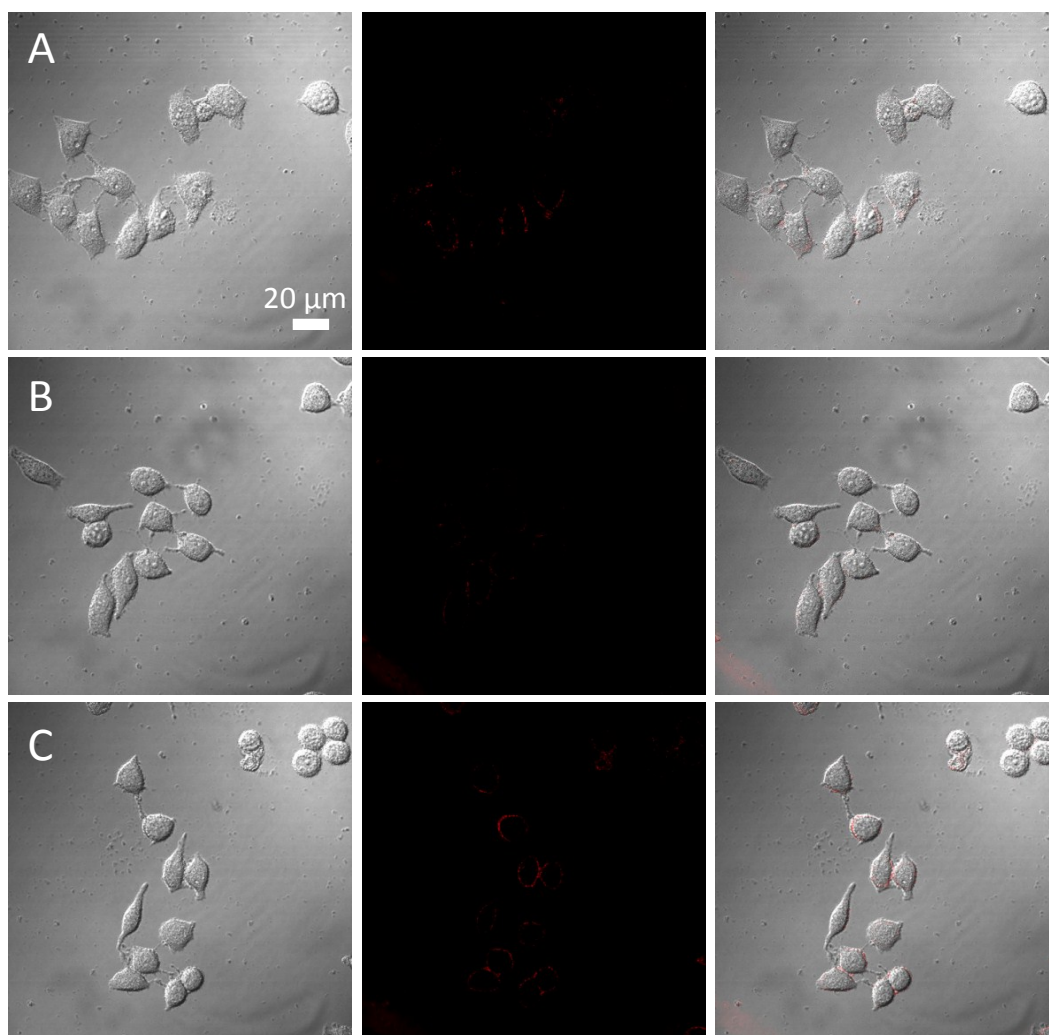


Figure S13. Confocal fluorescent images of HeLa cells incubated with **TTE-4DTPA** at different concentrations (A, 10 μ M), (B, 20 μ M), (C, 50 μ M) for 4 h. From left to right are bright field images, fluorescent images, and the merged images. Excitation wavelength: 405 nm; emission collected: 540-600 nm. The scale bar is 20 μ m.

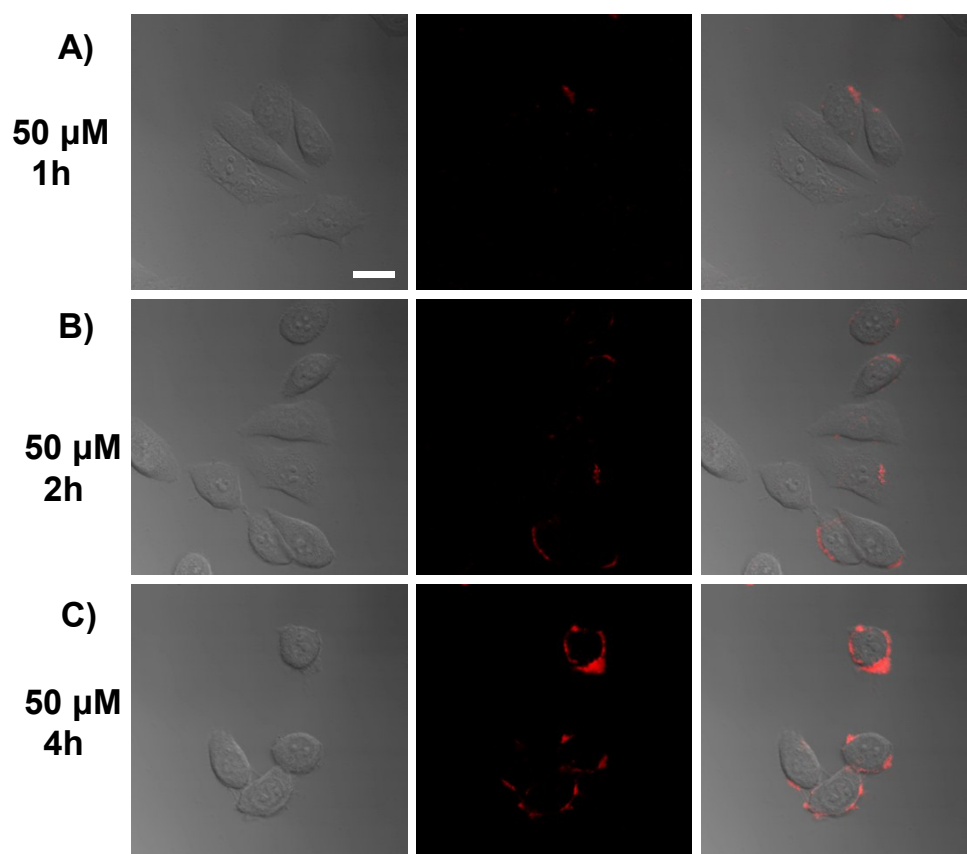
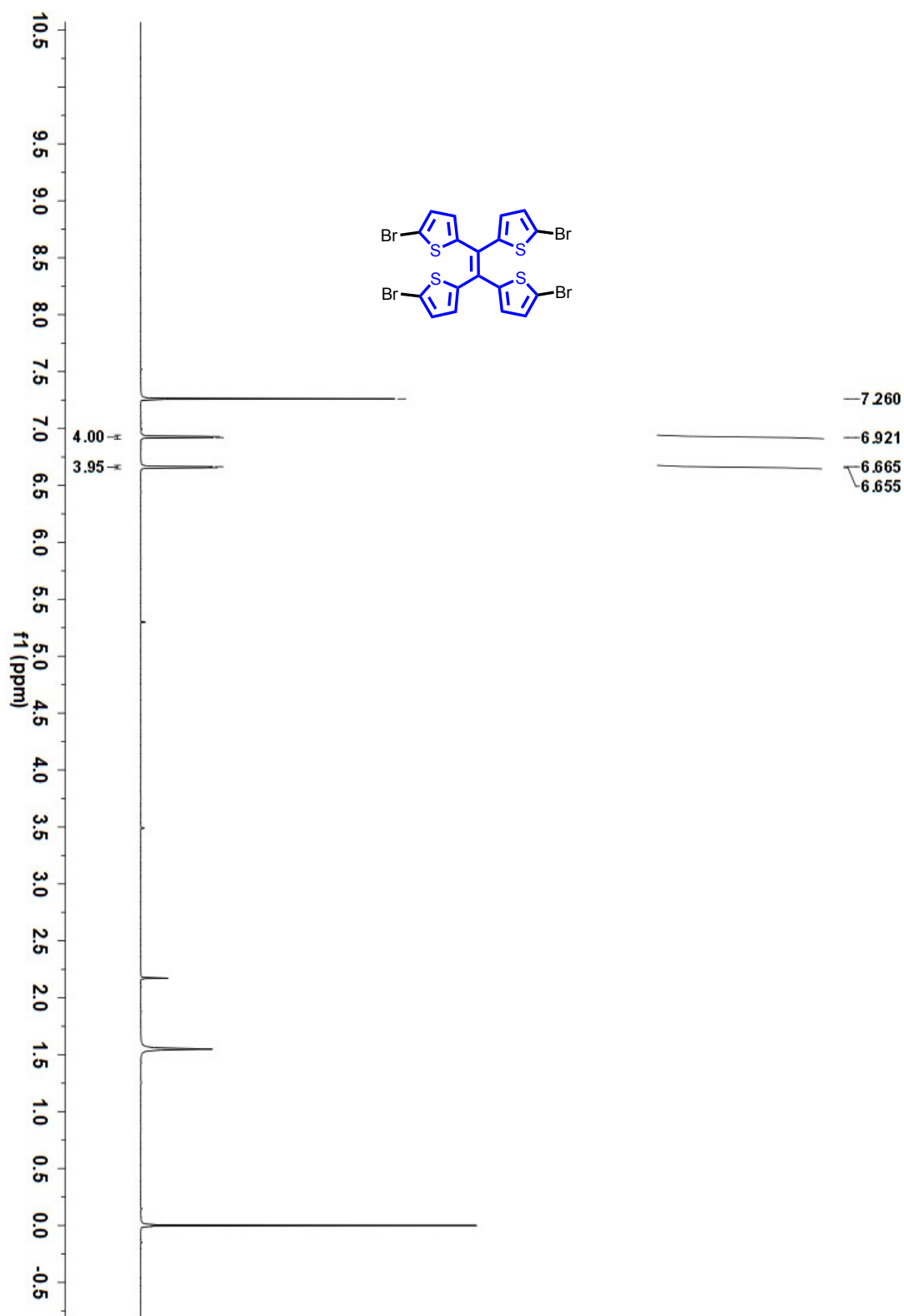
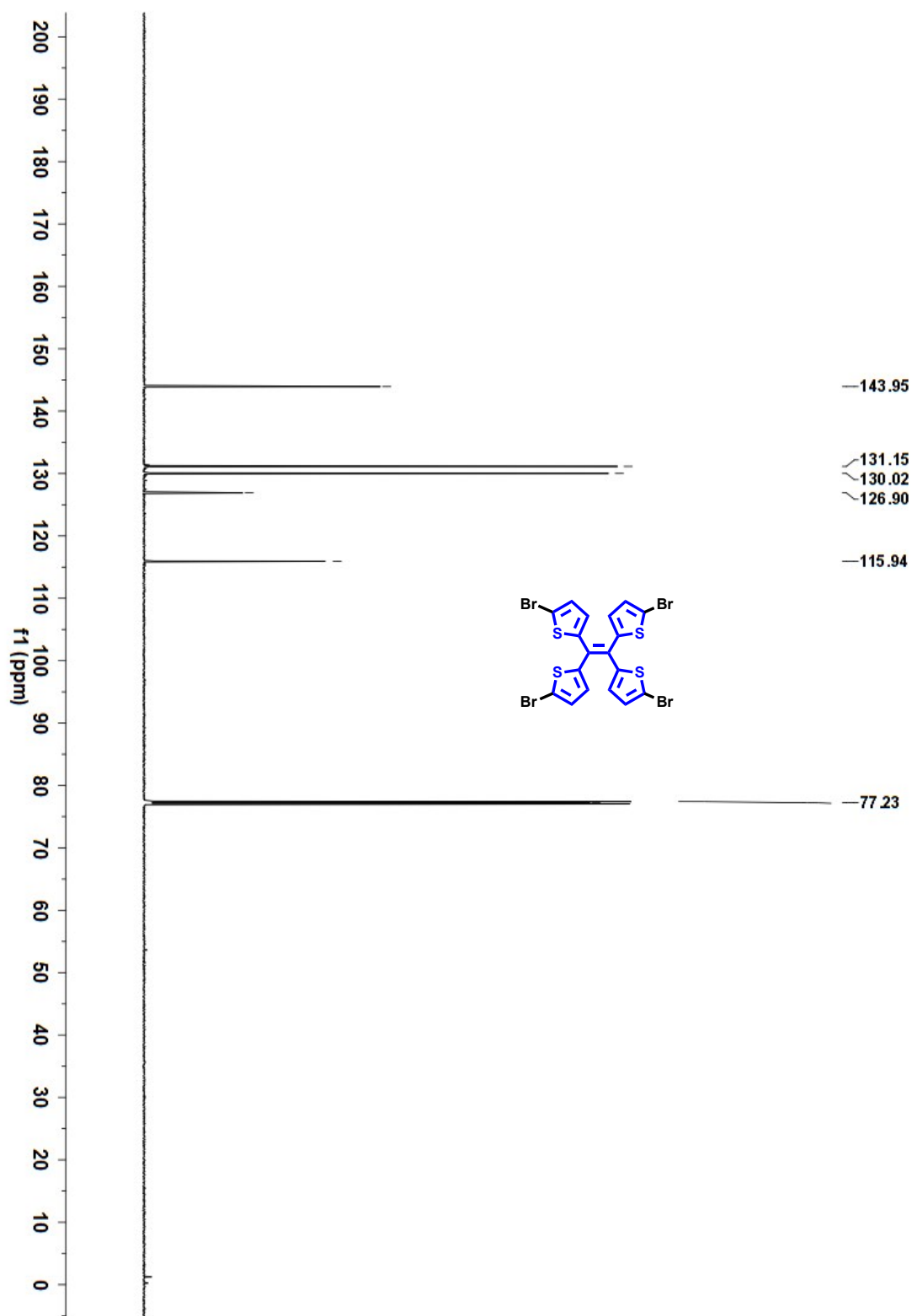


Figure S14. Confocal fluorescent images of HeLa cells incubated with 50 μ M **TTE-4DTPA** for different incubation time (A, 1 h), (B, 2 h), (C, 4 h), from left to right are bright field images, fluorescent images, and the merge images. Excitation wavelength: 405 nm; emission collected: 540-600 nm. The scale bar is 20 μ m.

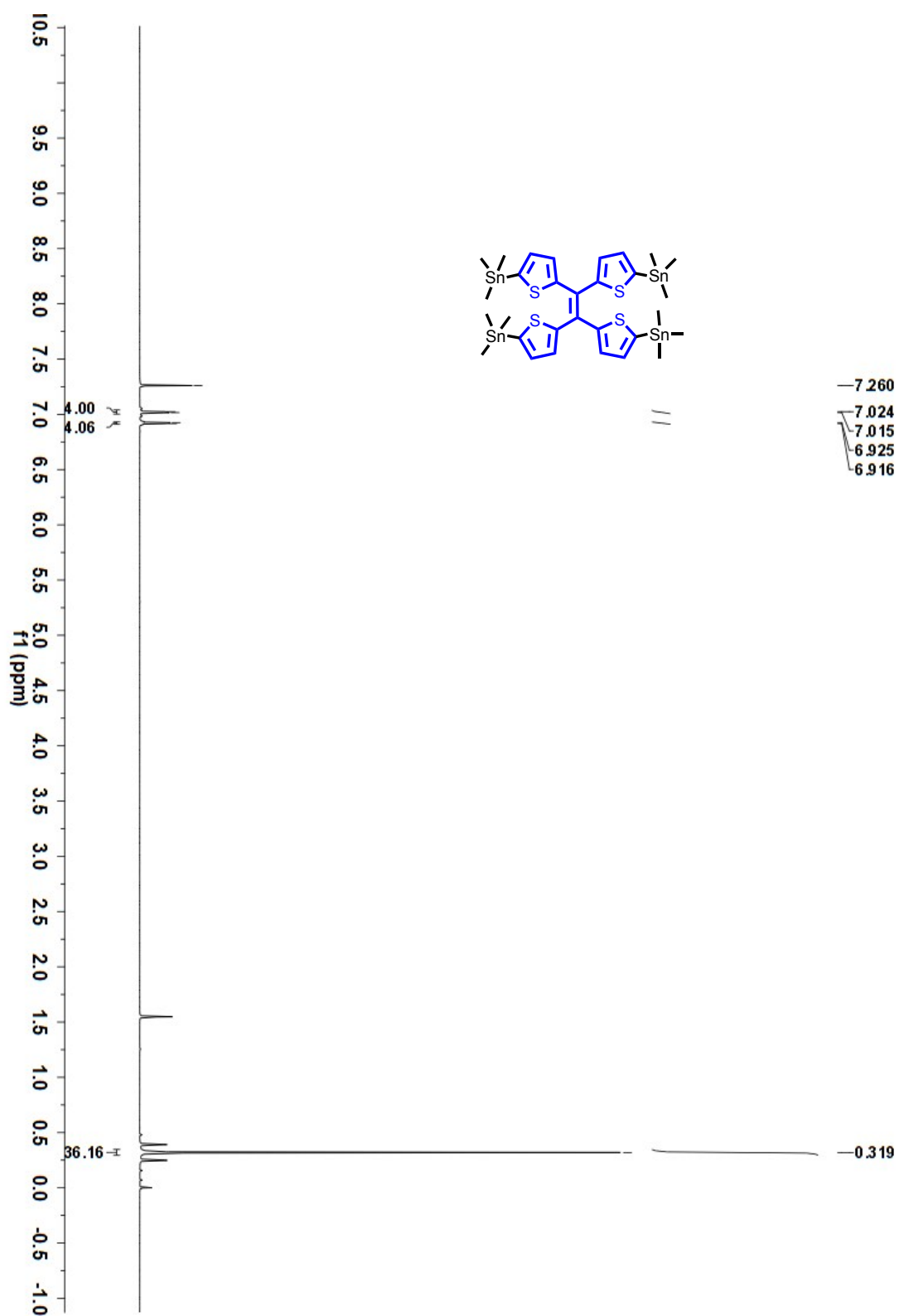
Copies of ^1H , ^{13}C NMR Spectra and MS Spectra



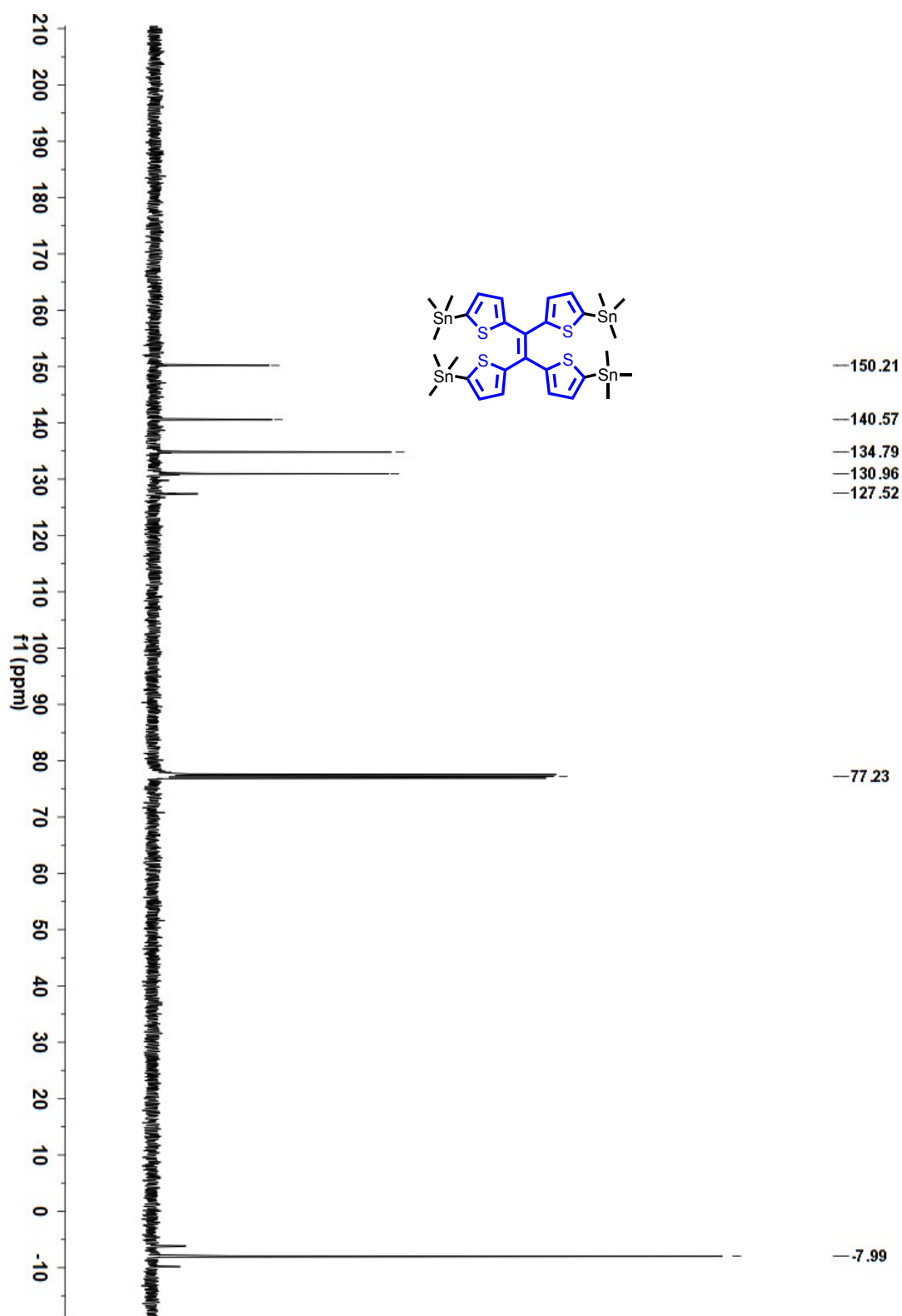
^1H NMR spectrum of compound **2** in CDCl_3 .



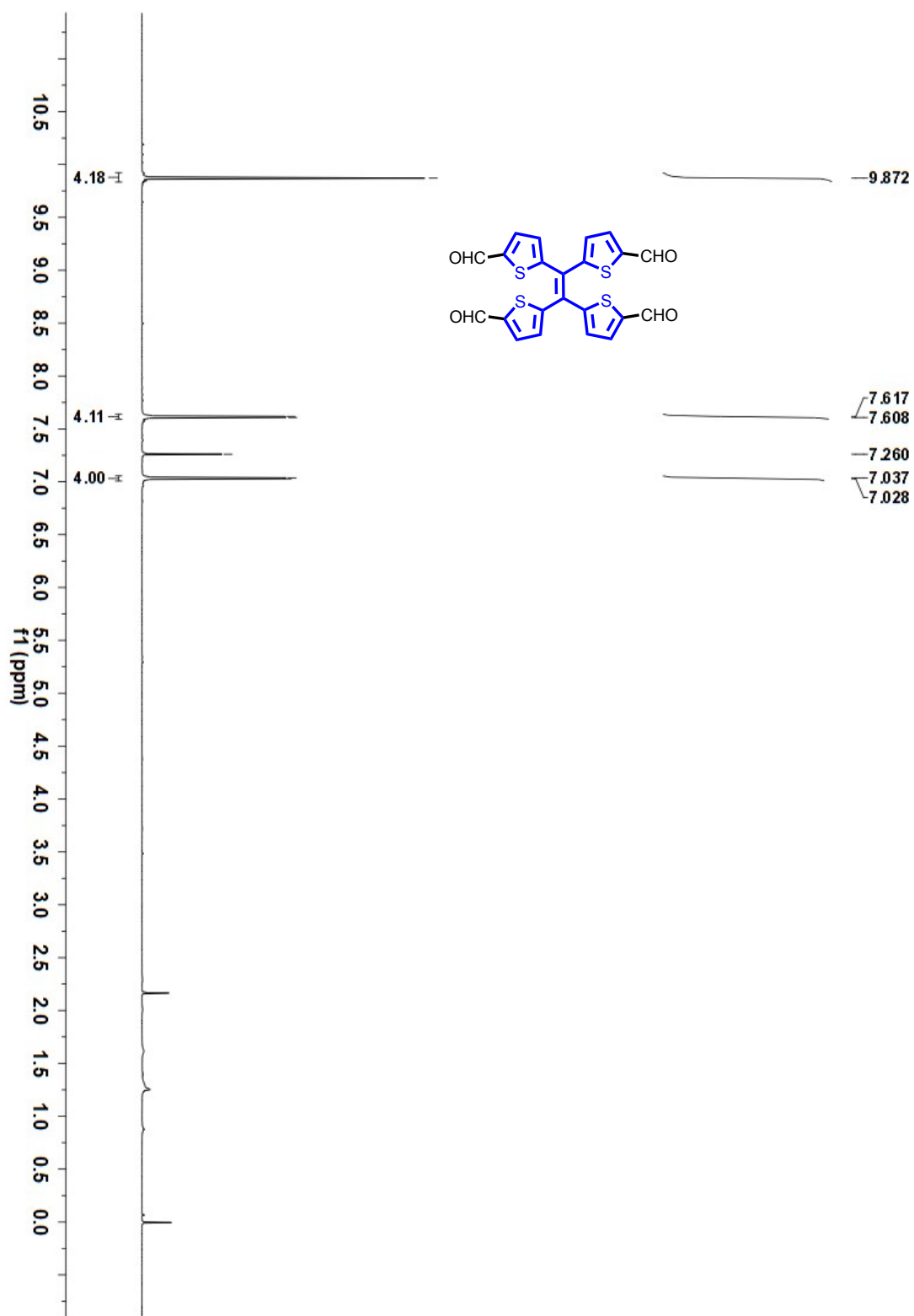
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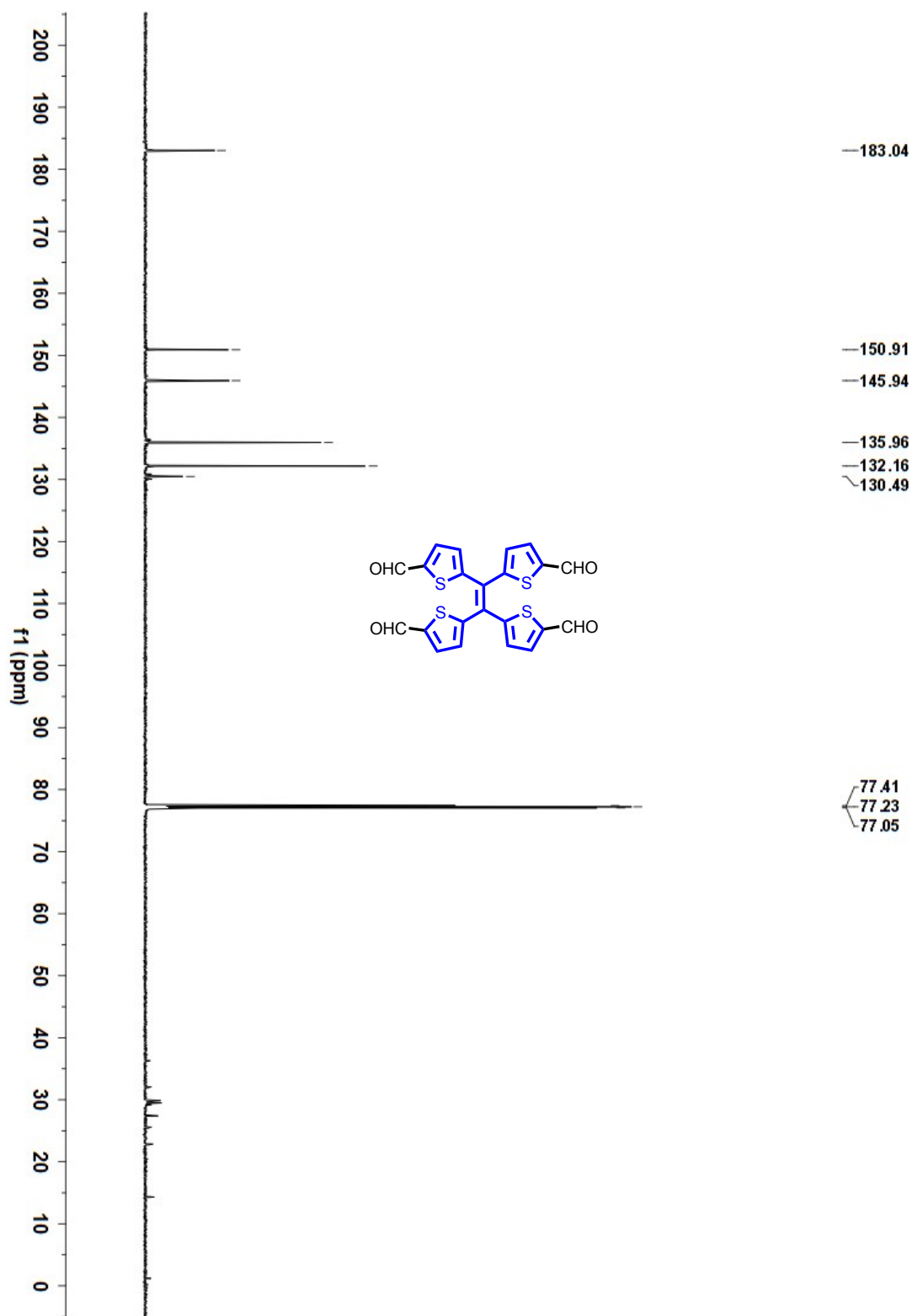
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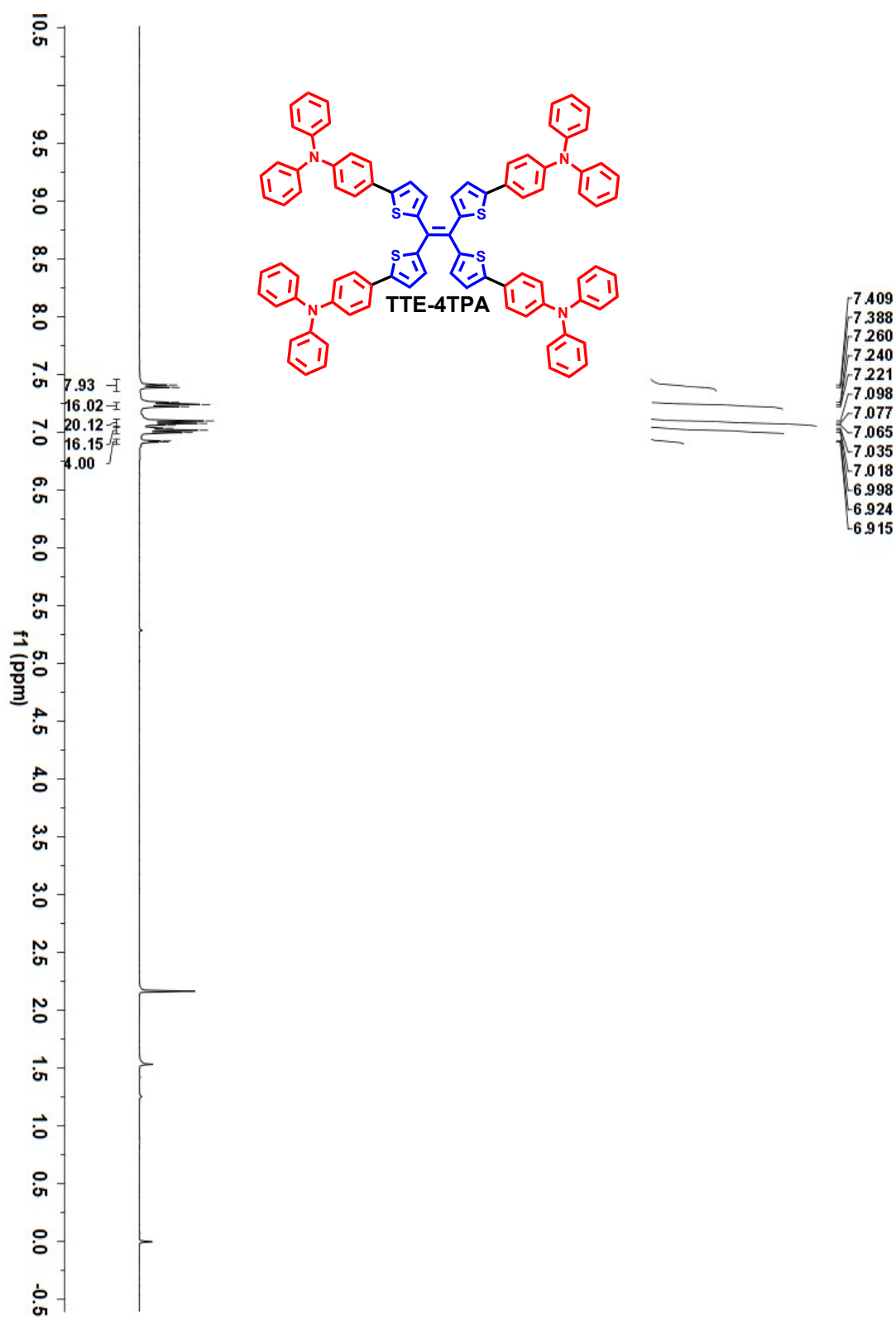
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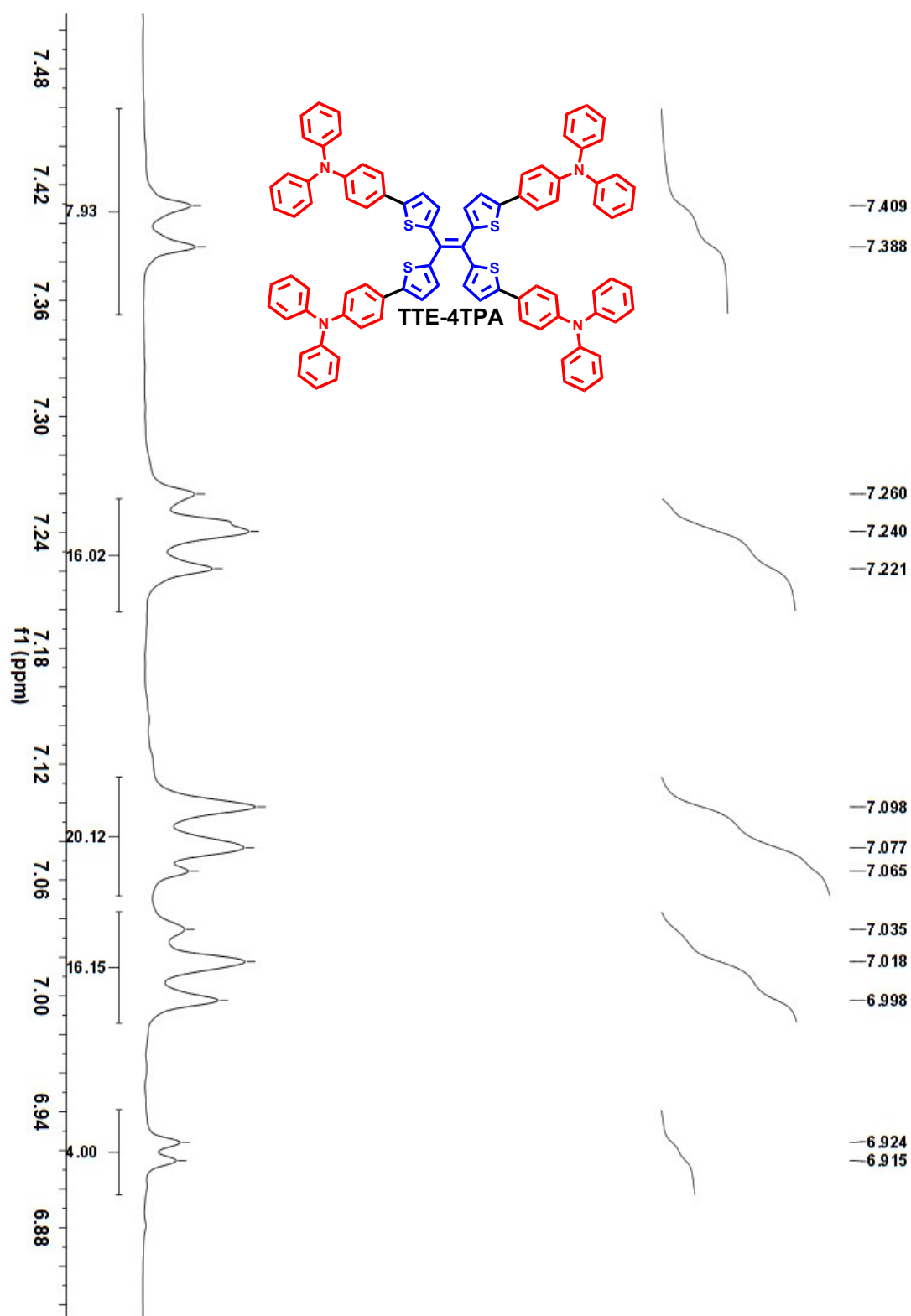
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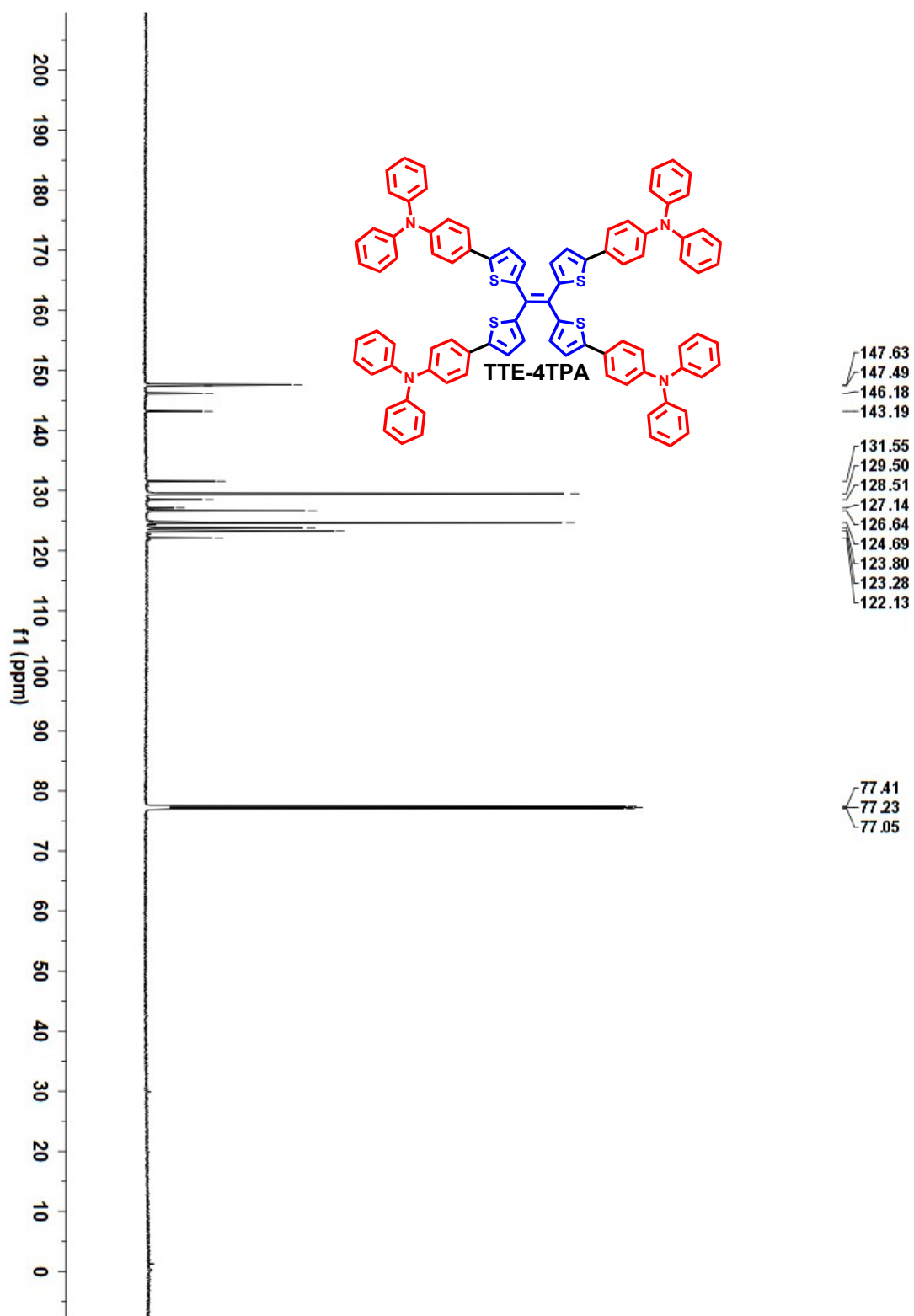
¹³C NMR spectrum of compound **6** in CDCl₃.



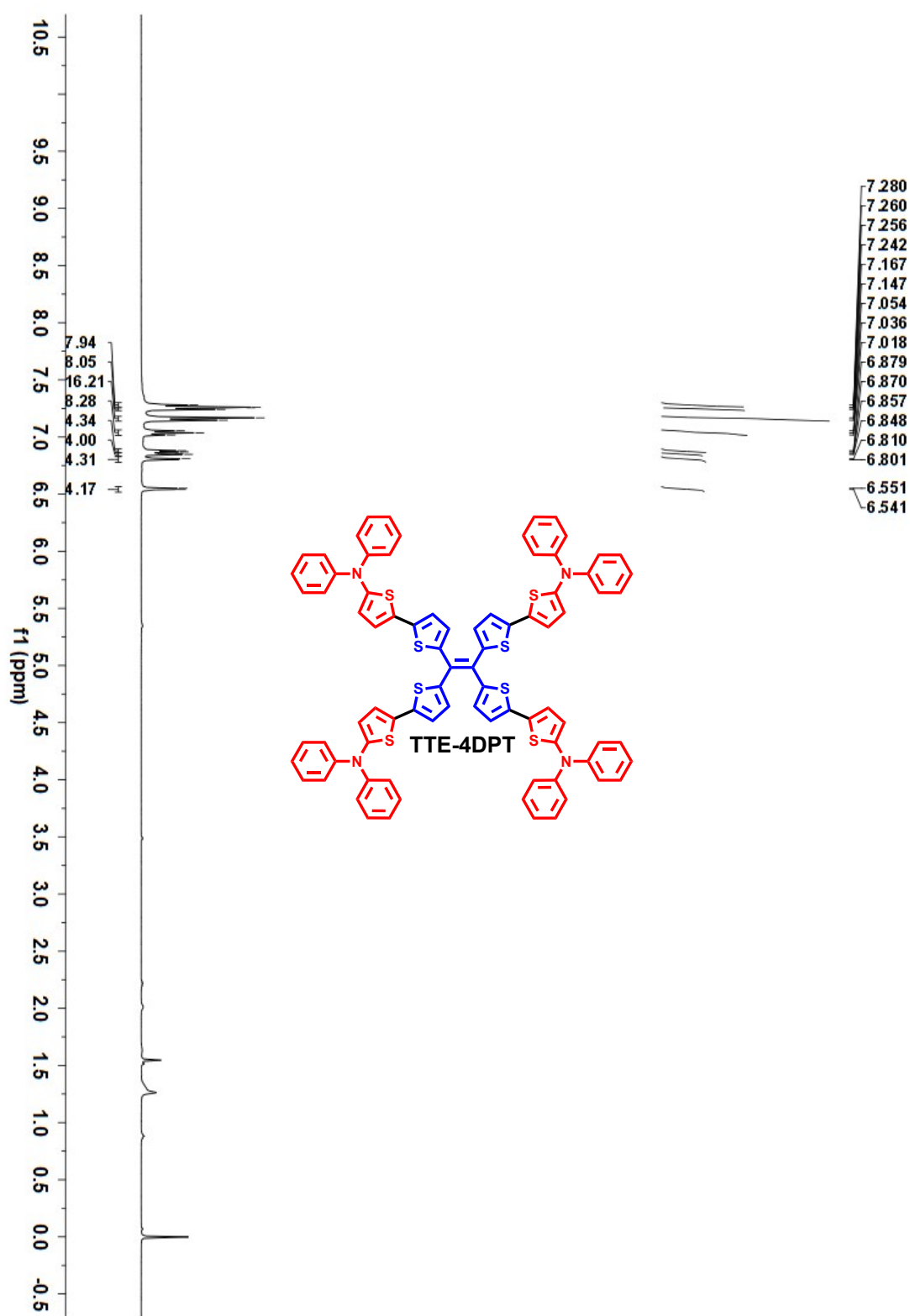
^1H NMR spectrum of **TTE-4TPA** in CDCl_3 .



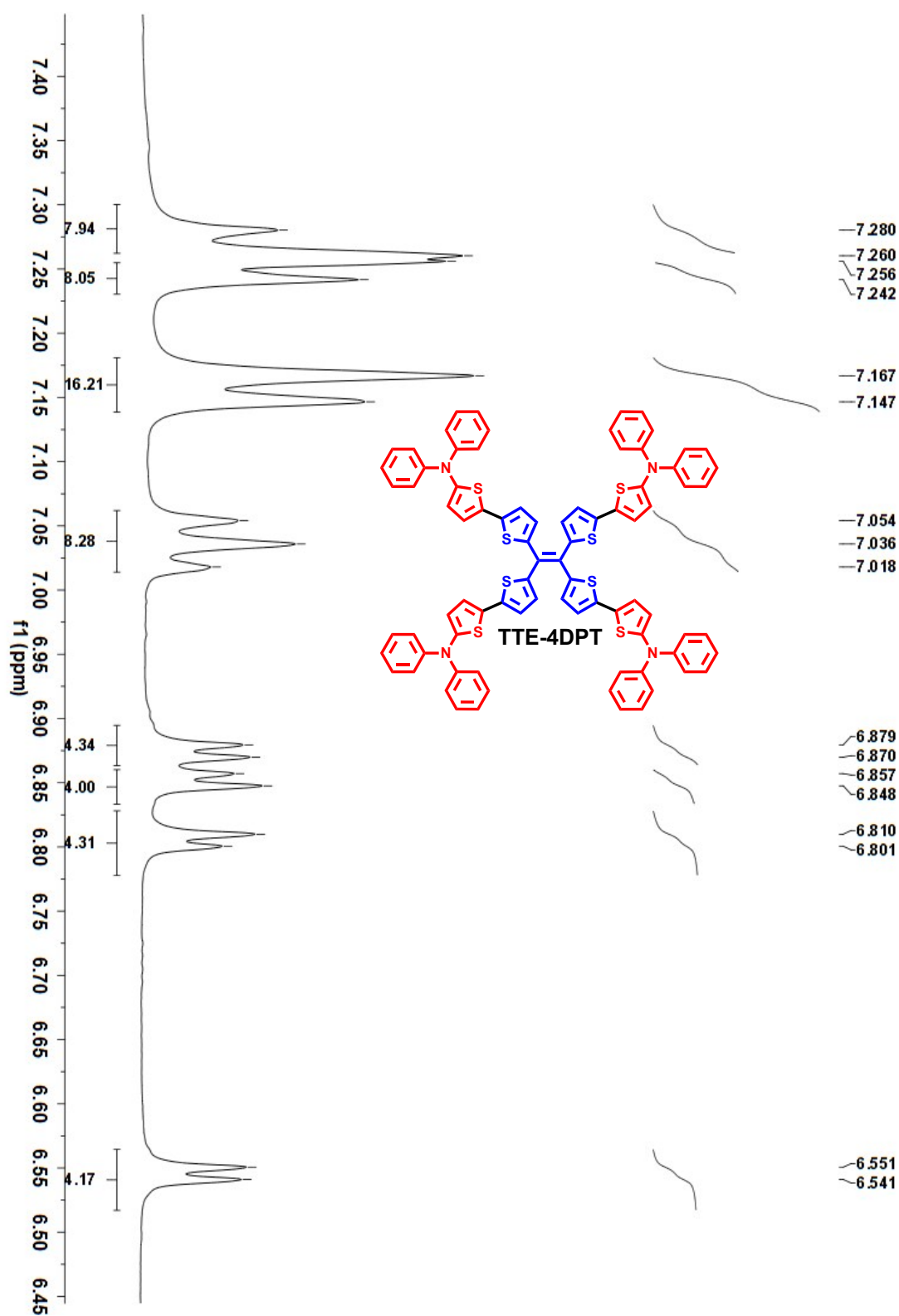
The expanded ¹H NMR spectrum of **TTE-4TPA** in CDCl₃.



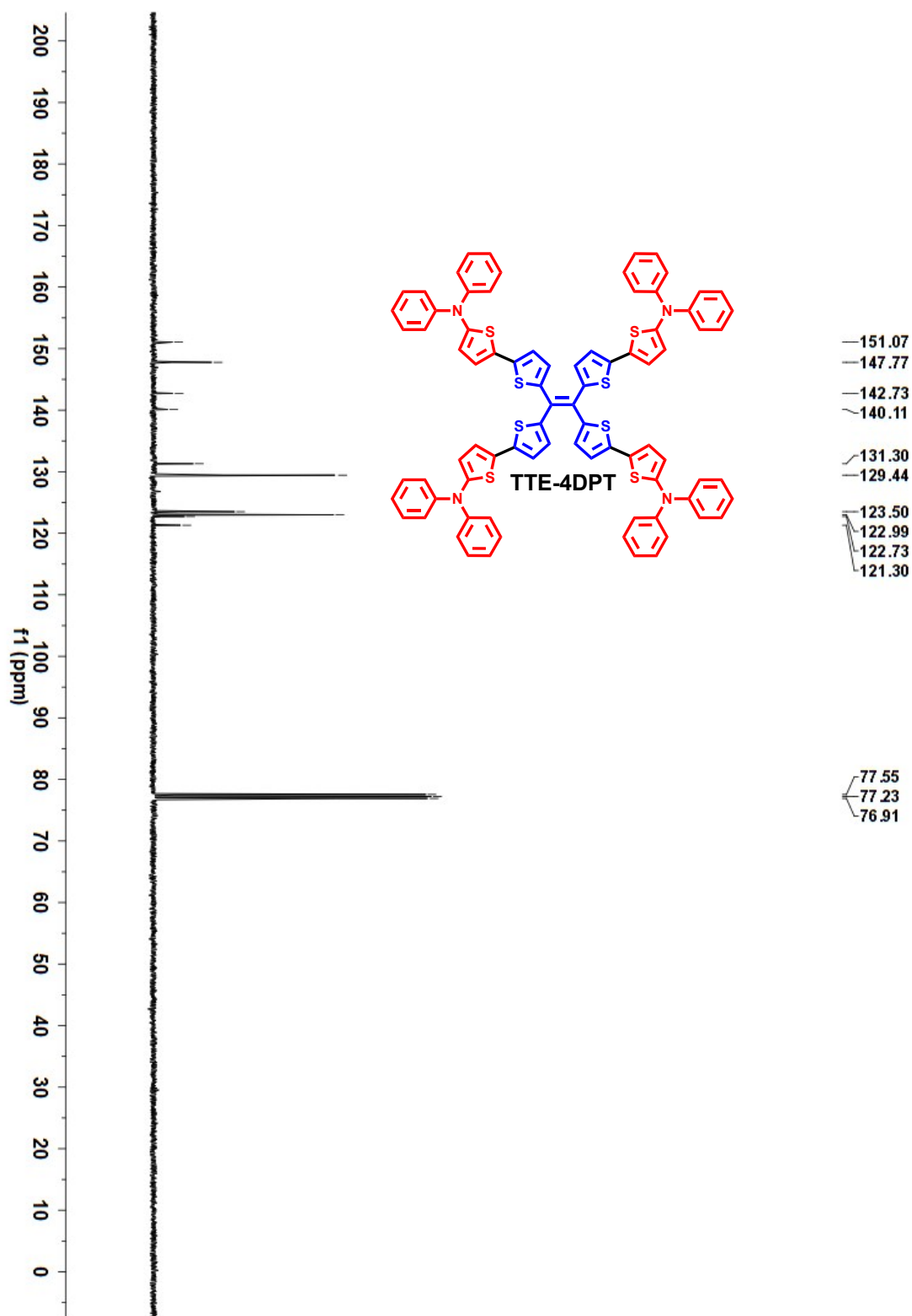
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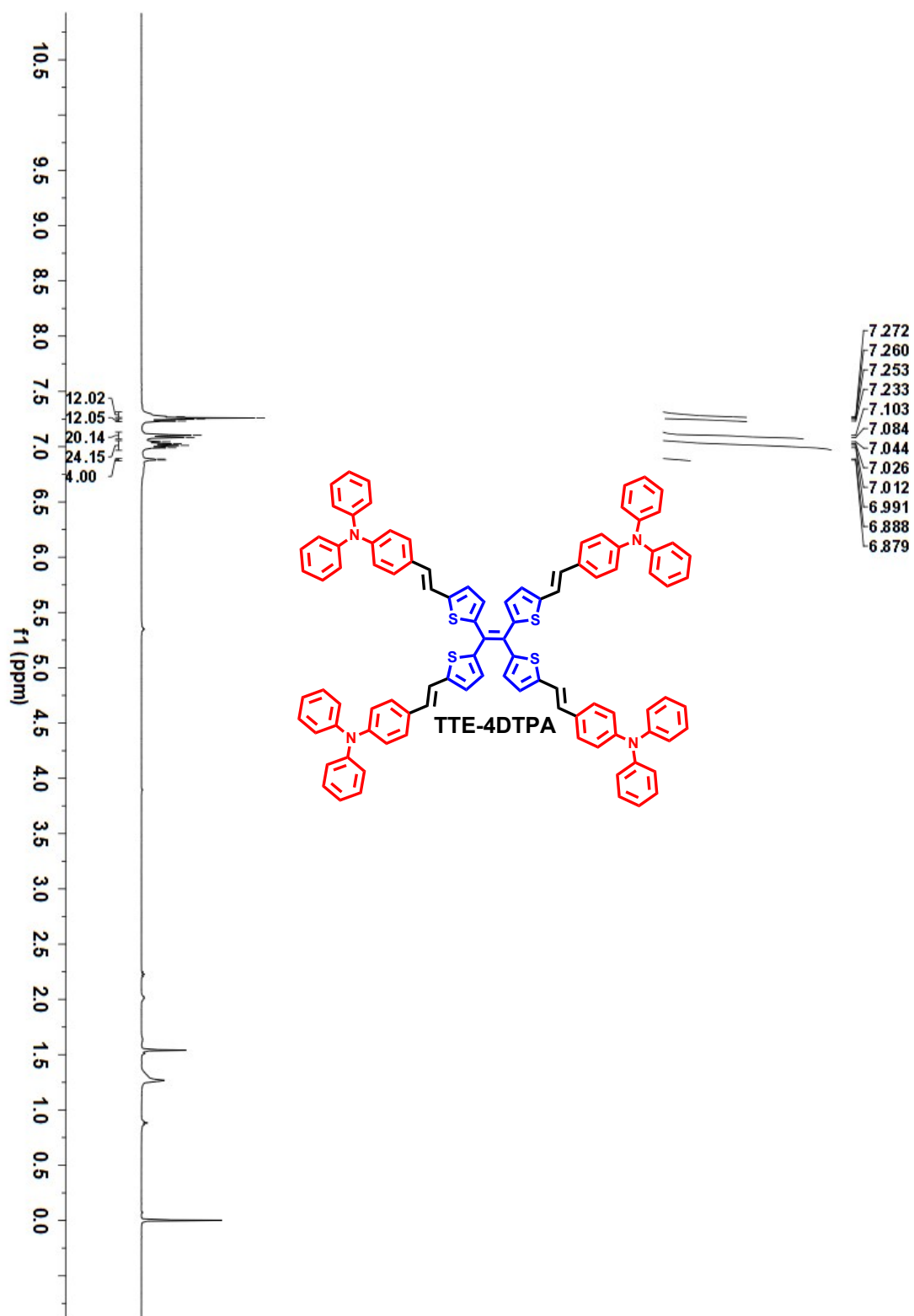


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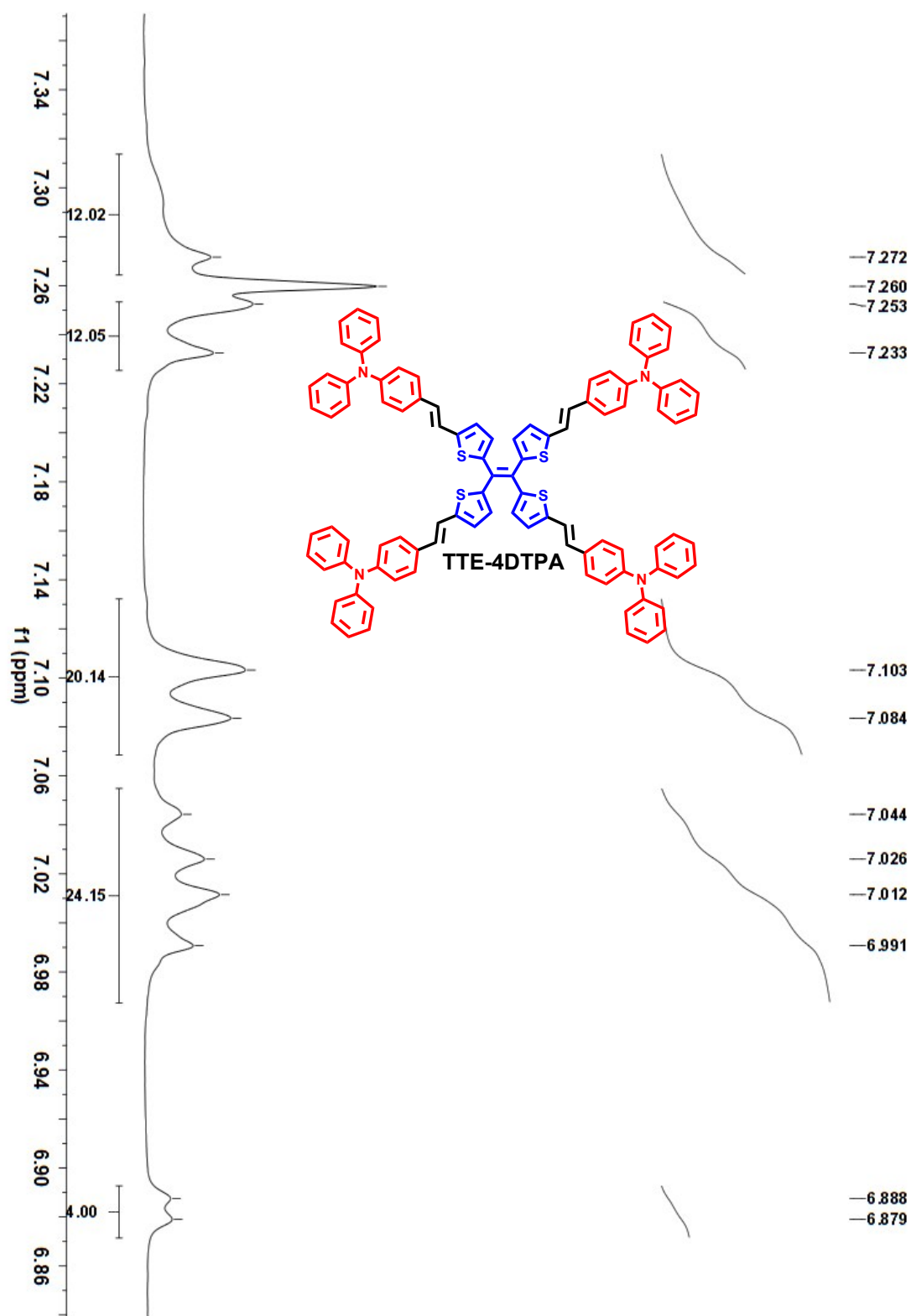


The expanded ^1H NMR spectrum of TTE-4DPT in CDCl_3 .

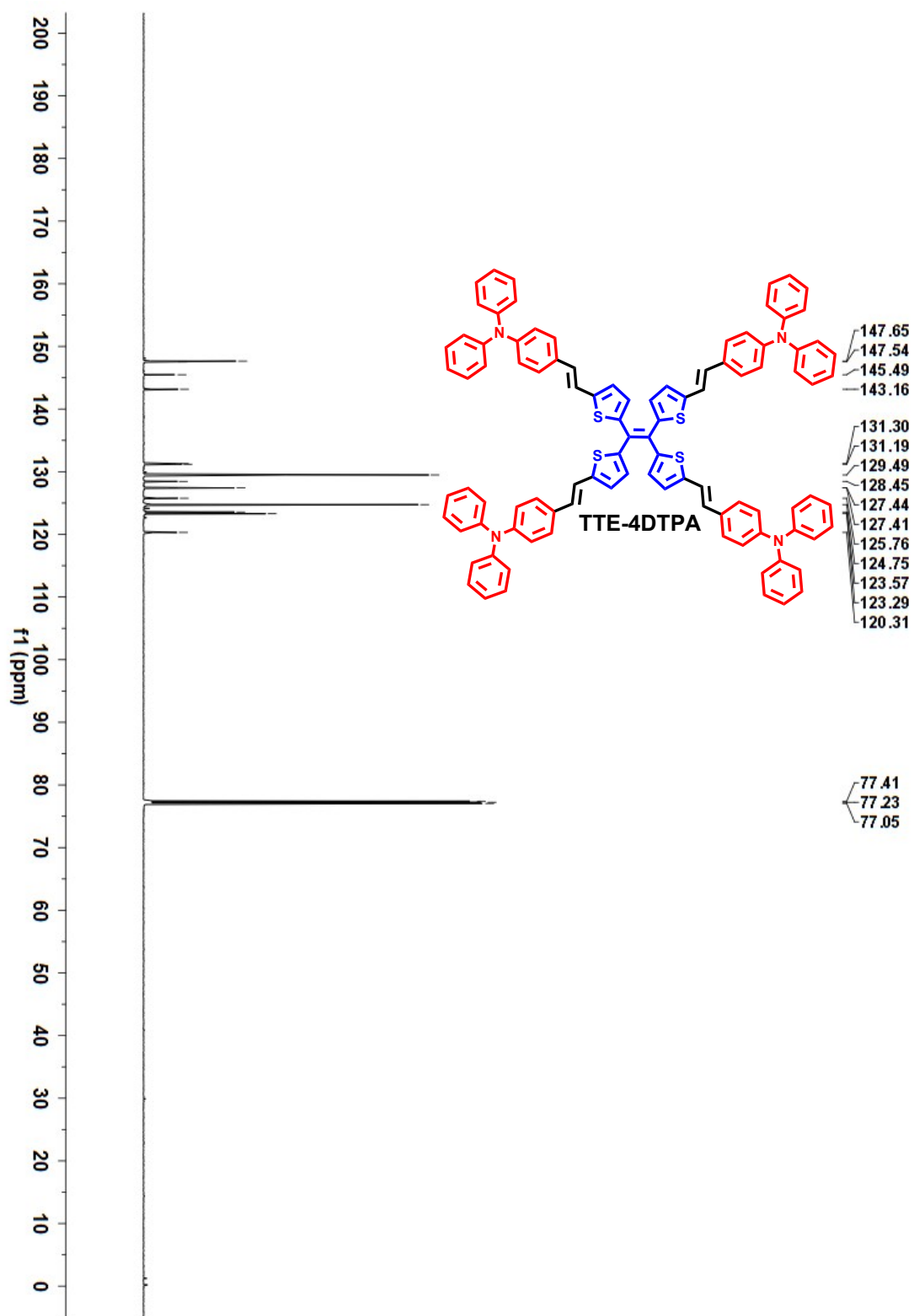




¹H NMR spectrum of **TTE-4DTPA** in CDCl₃.



The expanded ^1H NMR spectrum of **TTE-4DTPA** in CDCl_3 .



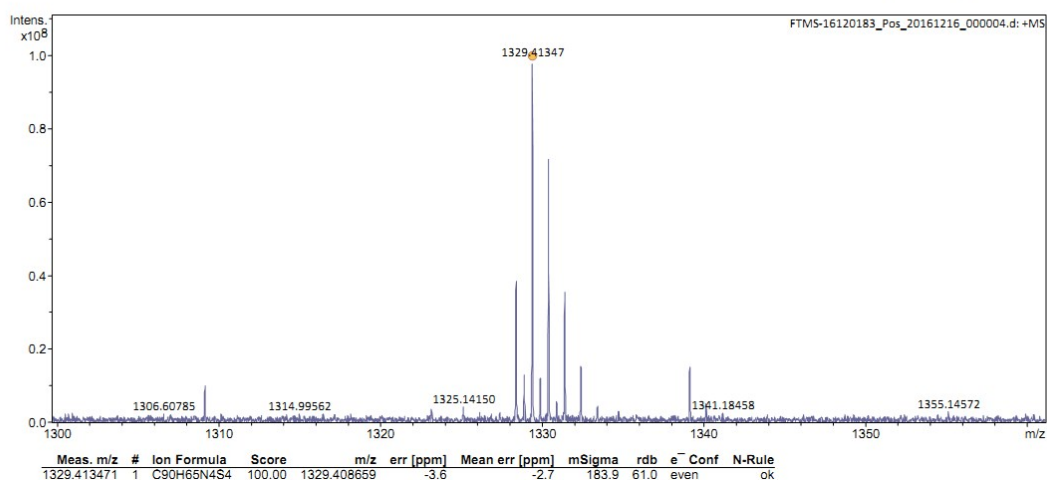
¹³C NMR spectrum of TTE-4DTPA in CDCl₃.

Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

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 Comment

Acquisition Date 12/16/2016 4:29:09 PM
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 Operator Peking University

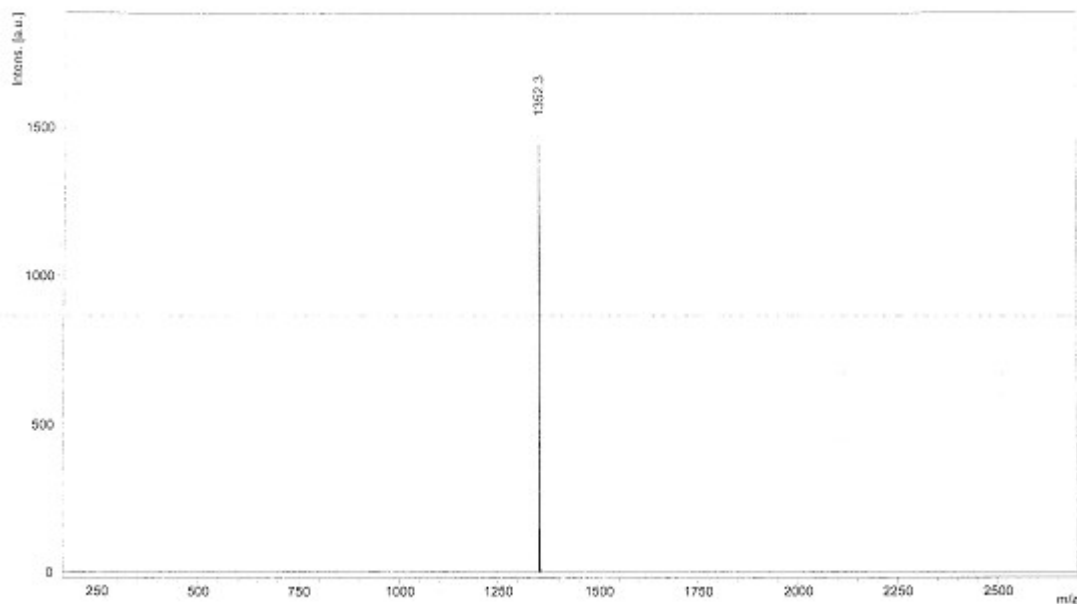


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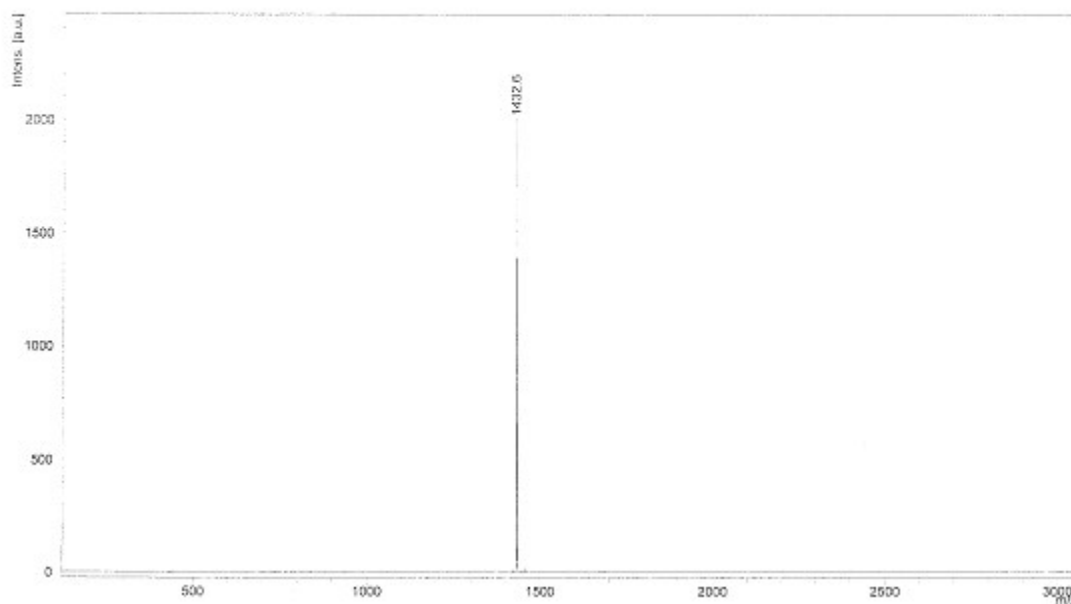
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MALDI-TOF MS Spectra for TTE-4DPT

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MALDI-TOF MS Spectra for **TTE-4DTPA**