Electronic Supplementary Information

Luminescent magnetic hollow mesoporous silica nanotheranostics for camptothecin delivery and multimodal imaging

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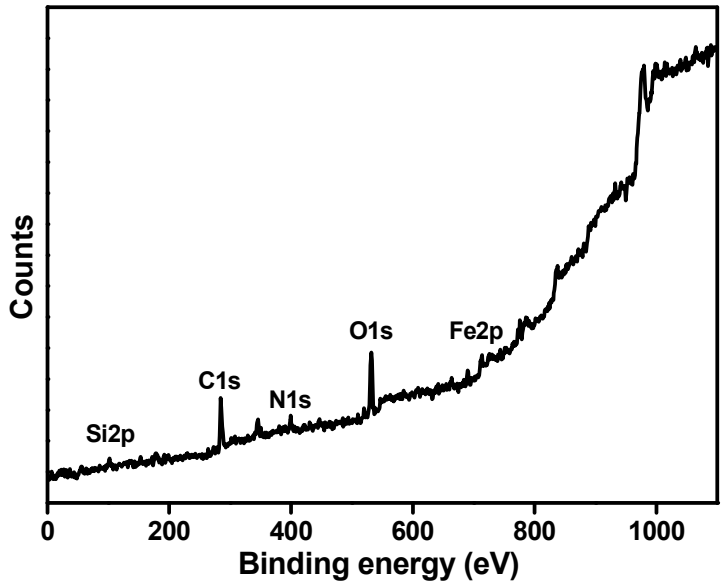


Figure S1 XPS survey spectrum of Fe_3O_4@m-SiO_2-CD-FA-CPT

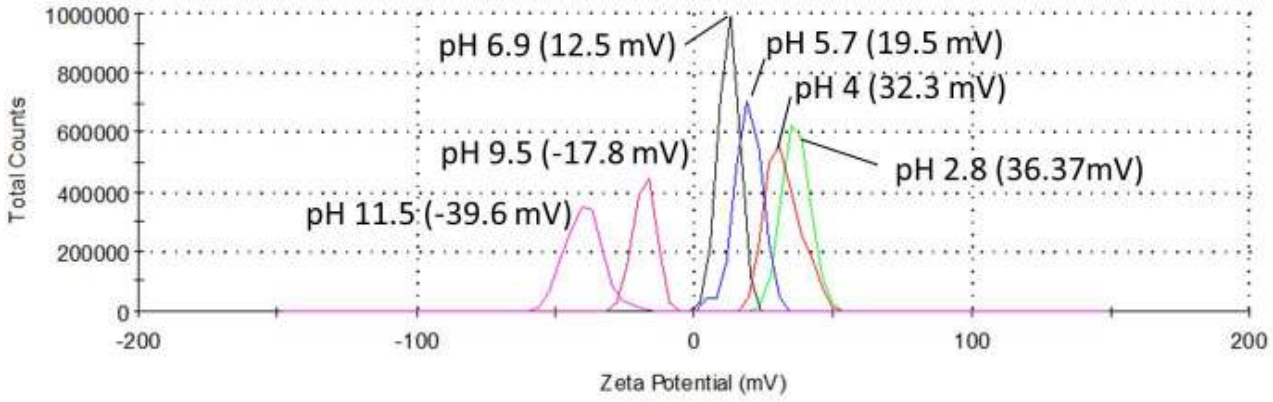


Figure S2 Measurement of zeta potential of the drug loaded nanoparticle against pH.

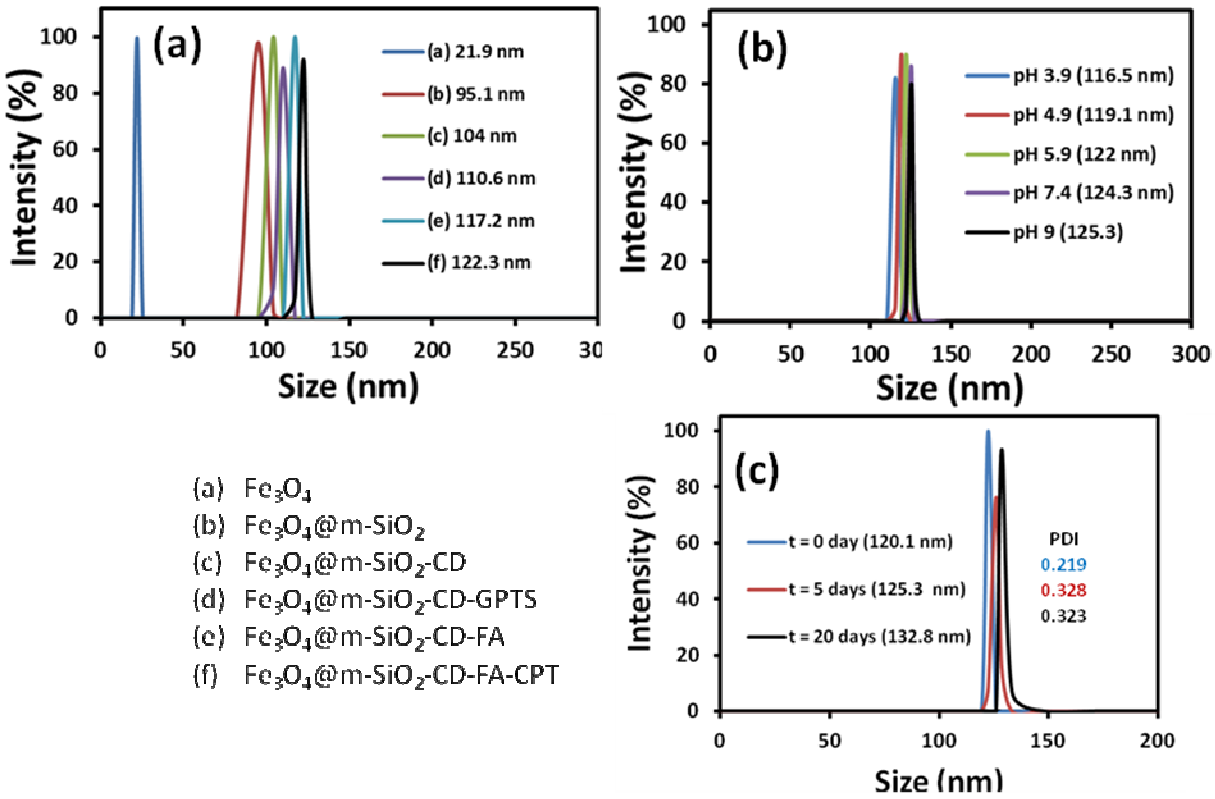


Figure S3 (a) Change in hydrodynamic size of the drug carrier at various stages of synthesis, Variation of the HD size of drug conjugate (b) with pH, (c) with time.

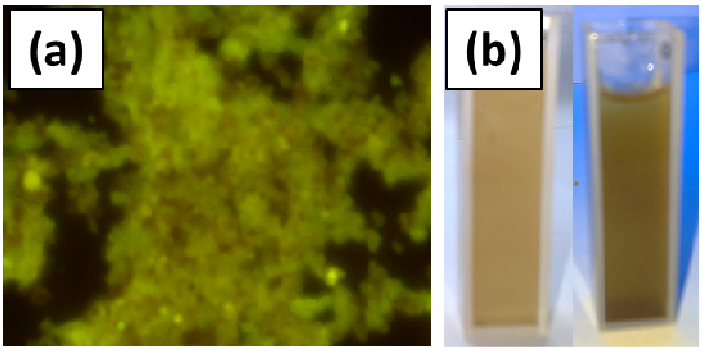


Figure S4. (a) Typical Fluorescence microscopy image and (b) digital photograph under daylight (left) and UV lamp (right) of Fe_3O_4@m-SiO_2-CD

Drug-loading content (%) = $\frac{\text{Weight of the drug in nanoparticles}}{\text{weight of the nanoparticles}}$ x 100…….(**1**)

$$= \frac{17.5}{100} \times 100$$

$$= 17.5\ \%$$

Encapsulation efficiency (%) = $\frac{\text{Weight of the drug in nanoparticles}}{\text{Weight of the feeding drug}}$ x 100……. (**2**)

$$= \frac{17.5}{20} \times 100 = 87.5\%$$

Quantum Yield Calculations

The quantum yield (Φ) of the Fe_3O_4@m-SiO_2-CD was calculated using quinine sulfate as reference.[12] For calculation of quantum yield, five concentrations of each compound were made, all of which had absorbance less than 0.1 nm at 340 nm. Quinine sulfate (literature Φ = 0.54) was dissolved in 0.1 M H_2SO_4 (refractive index (η) of 1.33) while the nanoparticle was taken in water (η = 1.33). Their fluorescence spectra were recorded at same excitation of 340 nm. Then by comparing the integrated photoluminescence intensities (excited at 340 nm) and the absorbency values (at 340 nm) of the sample with the references quinine sulfate quantum yield was determined. The data was plotted (Figure S5) and the slopes of the sample and the standards were determined. The data showed good linearity with intercepts of approximately zero.

The quantum yield was calculated using the below equation

$$\Phi_x = \Phi_{ST} \ (m_x / m_{ST}) \ (\eta^2_x / \eta^2_{ST})$$

Where Φ is the quantum yield, m is slope, η is the refractive index of the solvent, ST is the standard and X is the sample. The quantum yield for Fe3O4@m-SiO2-CD is found to be 12.4 %.

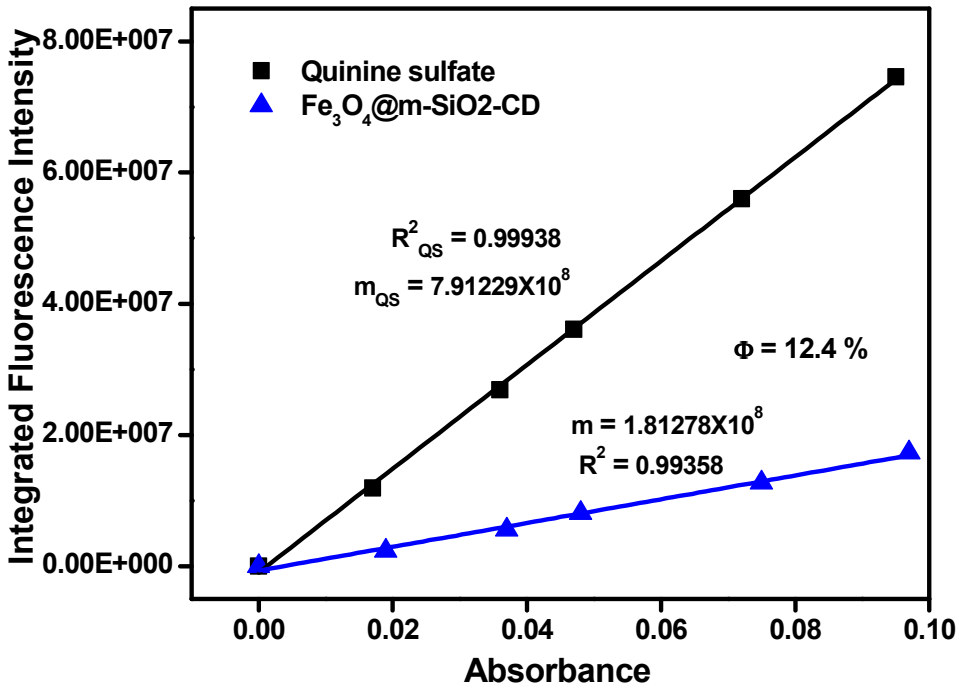


Figure S5 Fluorescence and Absorbance of the Fe_3O_4@m-SiO_2-CD and Quinine Sulfate

Calculation of number of Camptothecin, Folic acid and Fe_3O_4 per hollow sphere

From TGA analysis the weight loss for surface organic modification is 4%

Weightloss of 1 g sample is 0.04 g

During the synthesis, the ratio of camptothecin (CPT) and folic acid (FA) conjugates has been maintained as 5:1,

So, total organic content in 1g of drug and folic acid conjugated hybrid nanoparticle is
$5 \times mol\ wt\ of\ camptothecin\ conjugate \times x + 1 \times mol\ wt\ of\ folic\ acid\ conjugate$

Using the above equation, we calculated that, 1 g sample contains 4.5×10^{-5} mole of CPT and 9.25×10^{-6} mole of FA

BET surface area of the Fe_3O_4@m-SiO_2-CD hollow sphere is found to be 135 m^2/g

From TEM, the surface area of single hollow sphere is calculated as $9.36 \times 10^{-16} m^2$

Total number of hollow sphere present in 1 g sample is $\frac{135}{9.36 \times 10^{-16}} = 1.4 \times 10^{17}$

Thus 9.36×10^{-16} hollow spheres are conjugated with 4.5×10^{-5} and 9.25×10^{-6} mole of CPT and FA respectively.

Each hollow sphere is conjugated with 199 (3.3×10^{-22}mole) and 40 (6.6×10^{-23}mole) numbers of CPT and FA respectively.

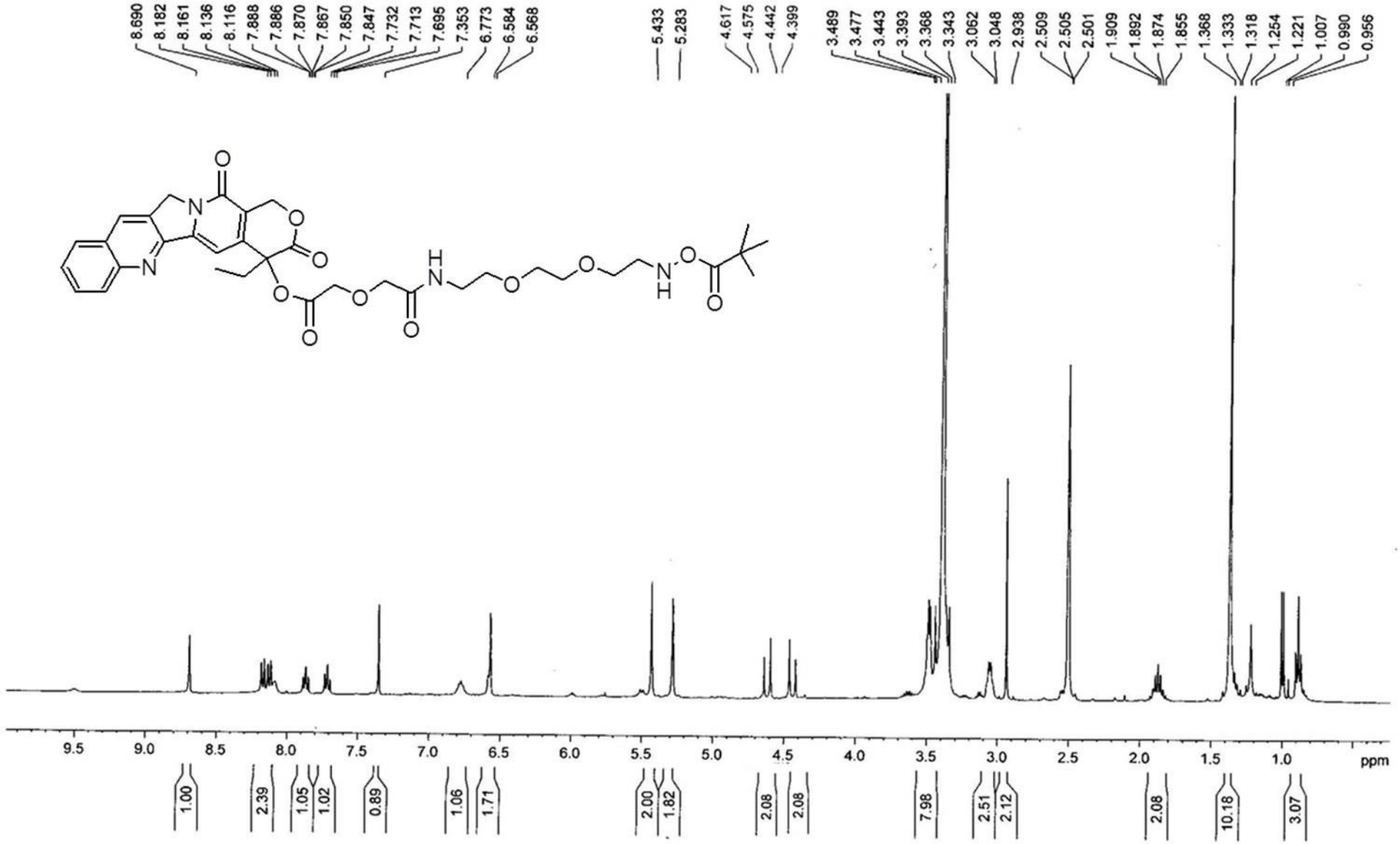
From TEM, volume of single Fe_3O_4 nanoparticle is calculated to 4.188×10^{-19} m^3

Mass of single Fe_3O_4 nanoparticle = volume×density = 2.165×10^{-15}mg (density of the magnetite nanoparticle is 5.17 g/cm^3)

From AAS analysis 1 g CPT and FA conjugated nanoparticle contains 348 mg iron

Then number of Fe_3O_4 nanoparticle present in 1 g composite is $\frac{348}{2.165 \times 10^{-15}} = 16 \times 10^{16}$

Thus number of Fe_3O_4 nanoparticle per each hollow sphere is found to be $\frac{16 \times 10^{16}}{1.4 \times 10^{17}} = 1.14 \approx 1$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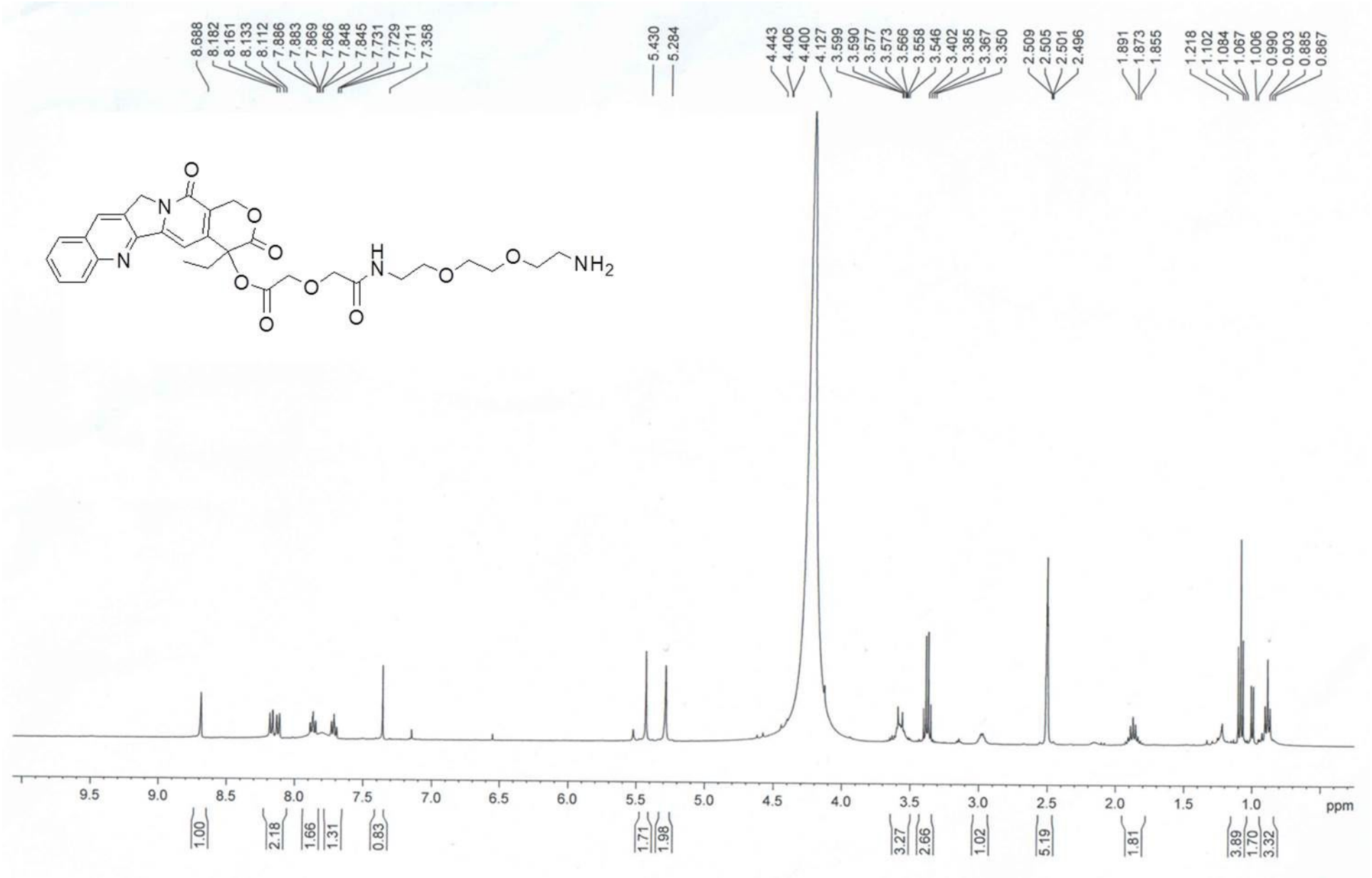
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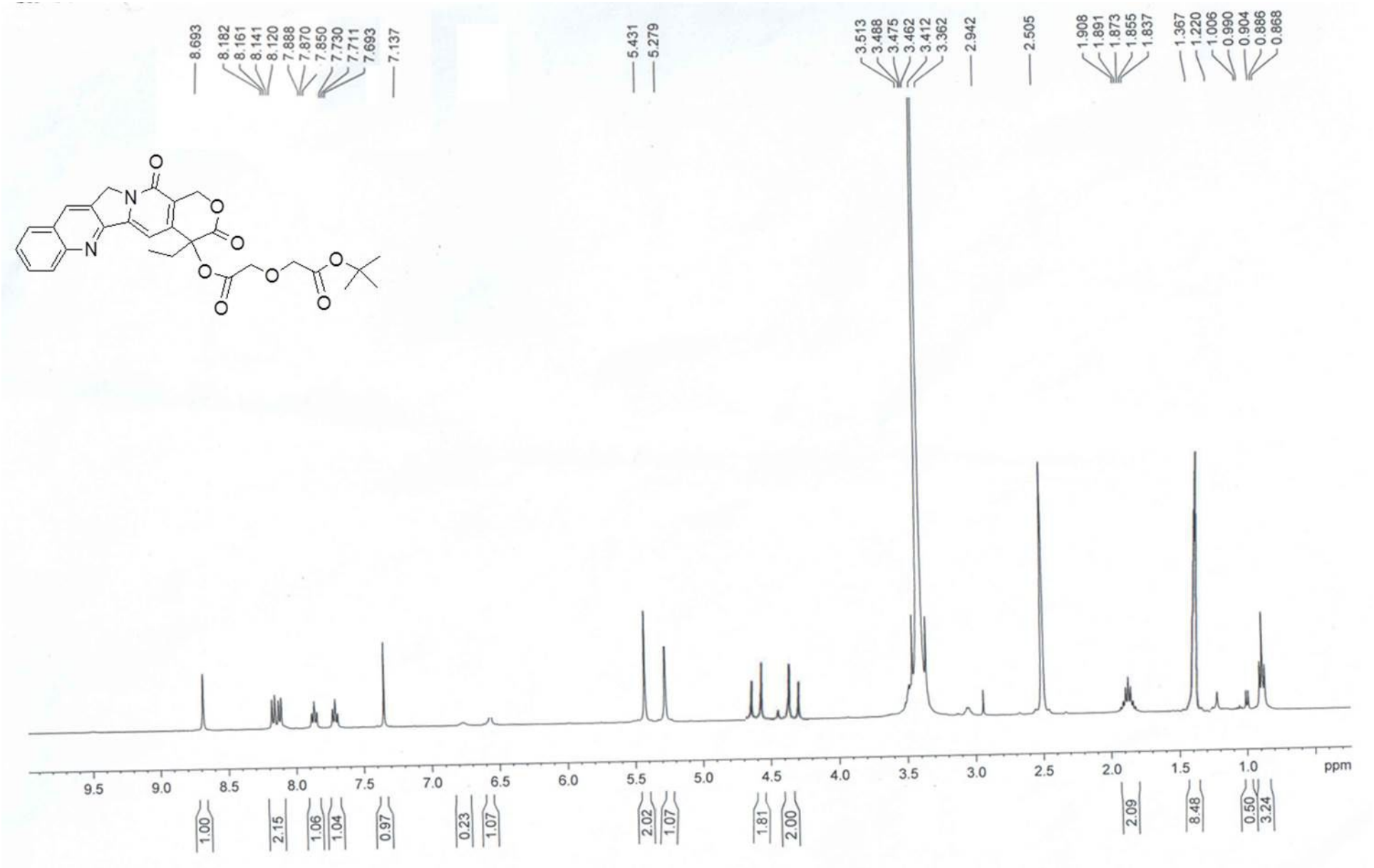
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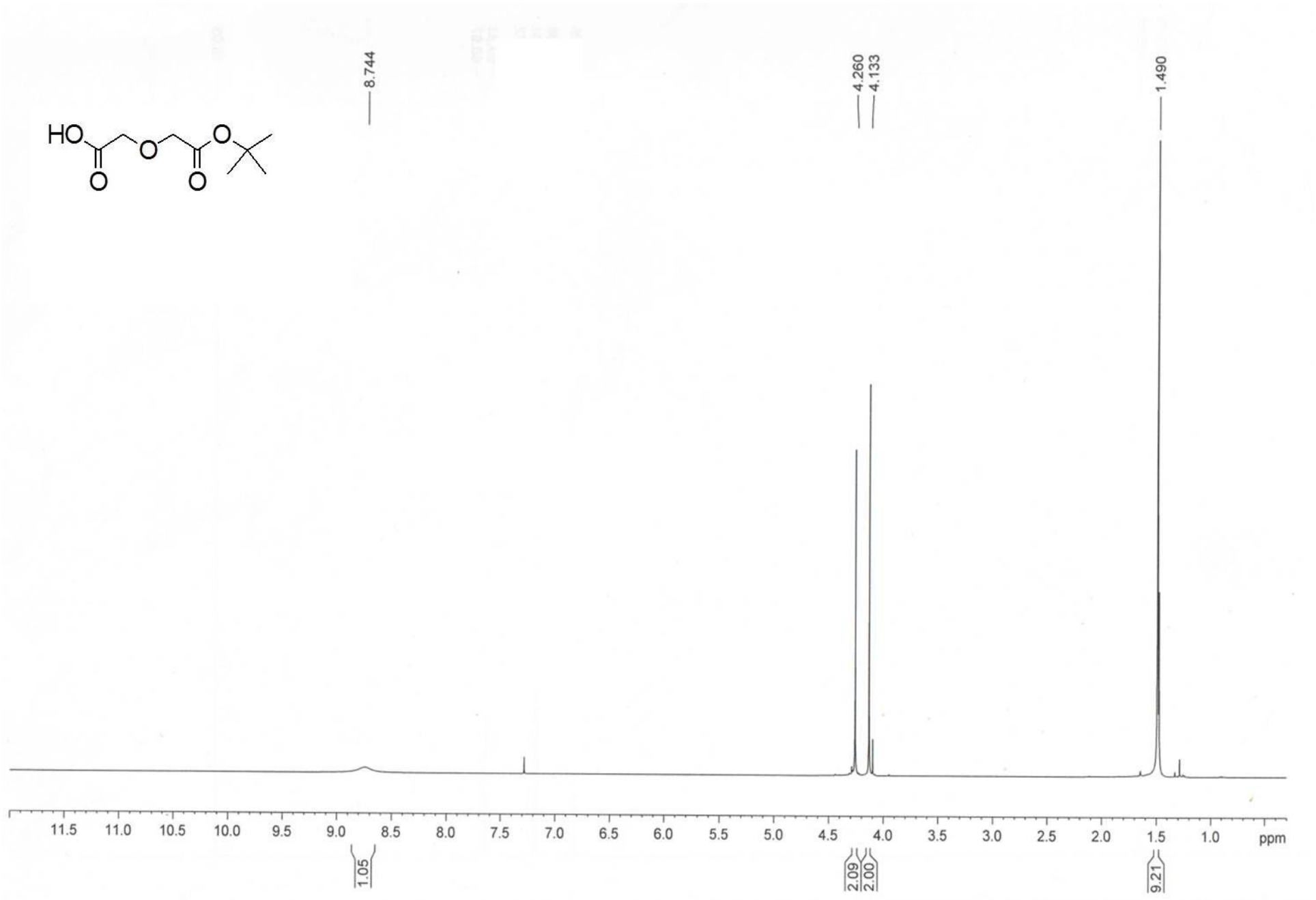
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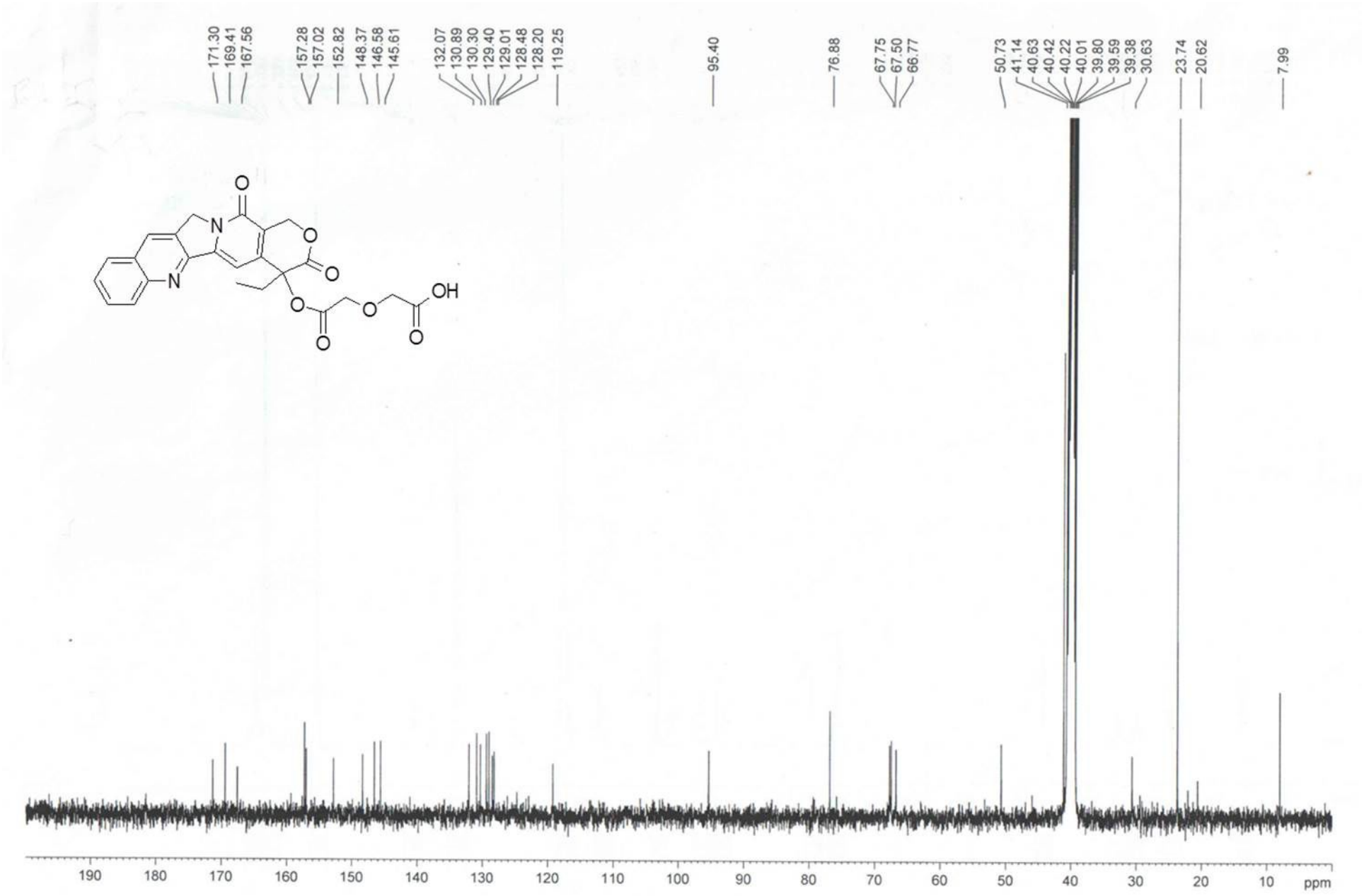
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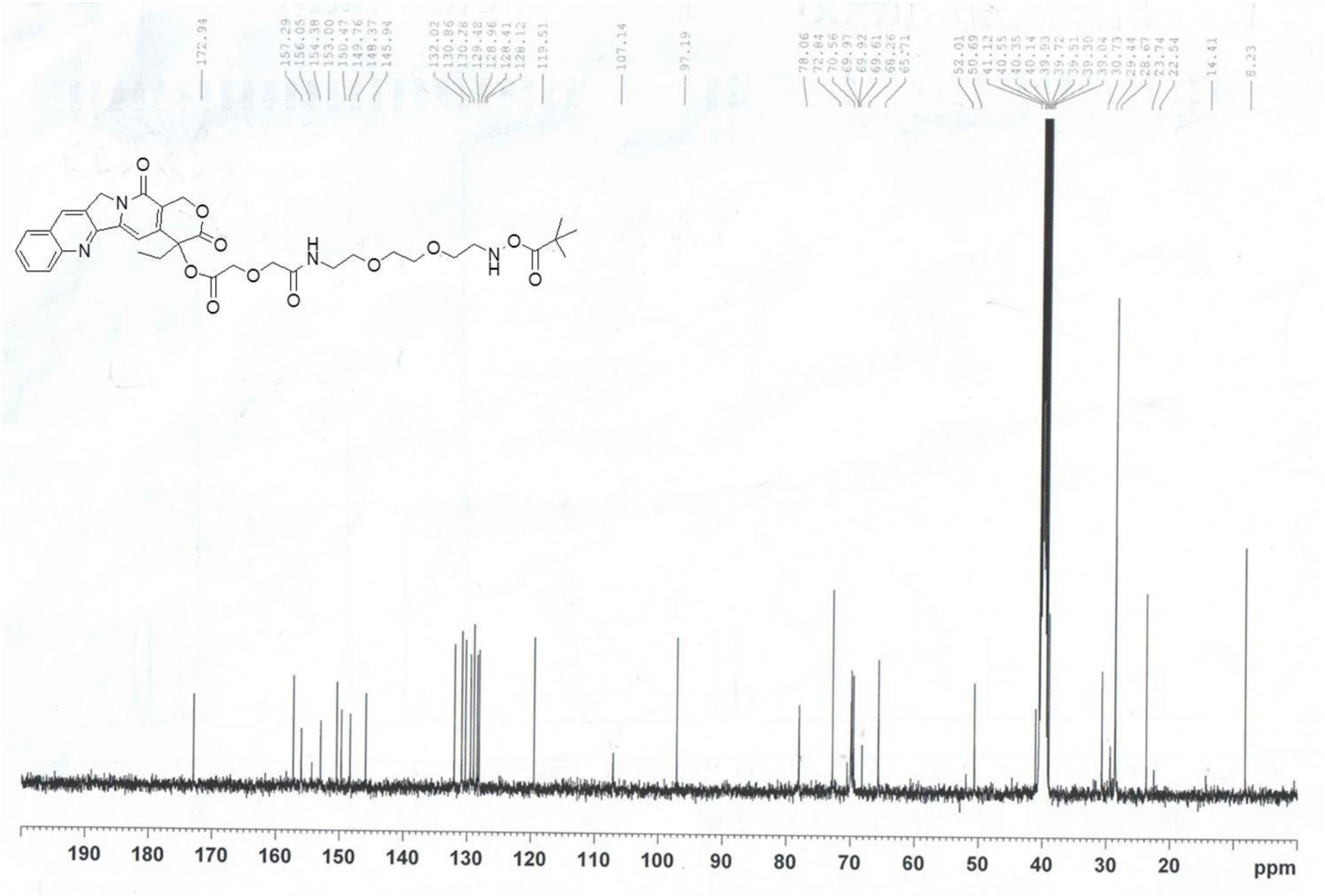
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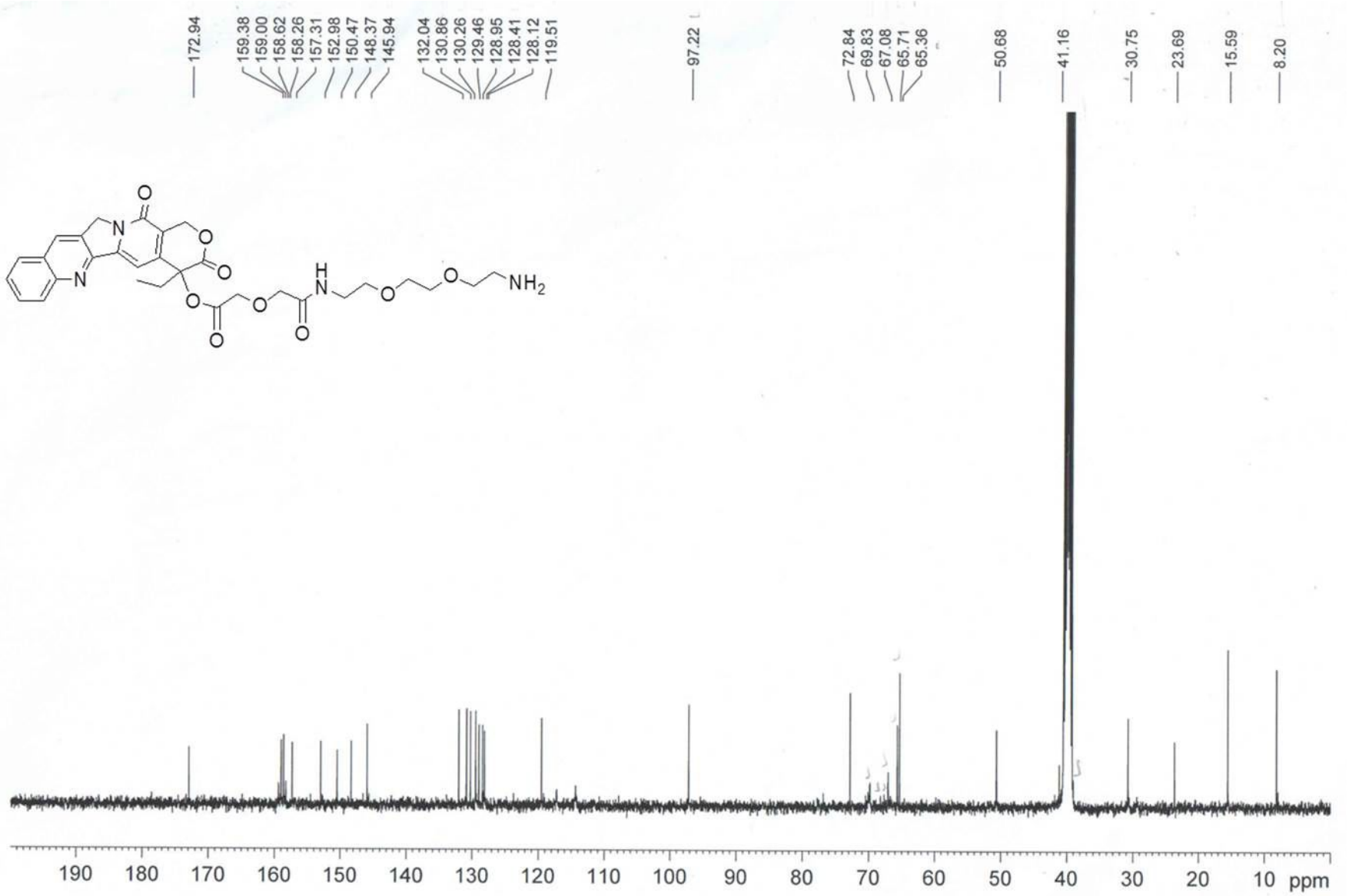
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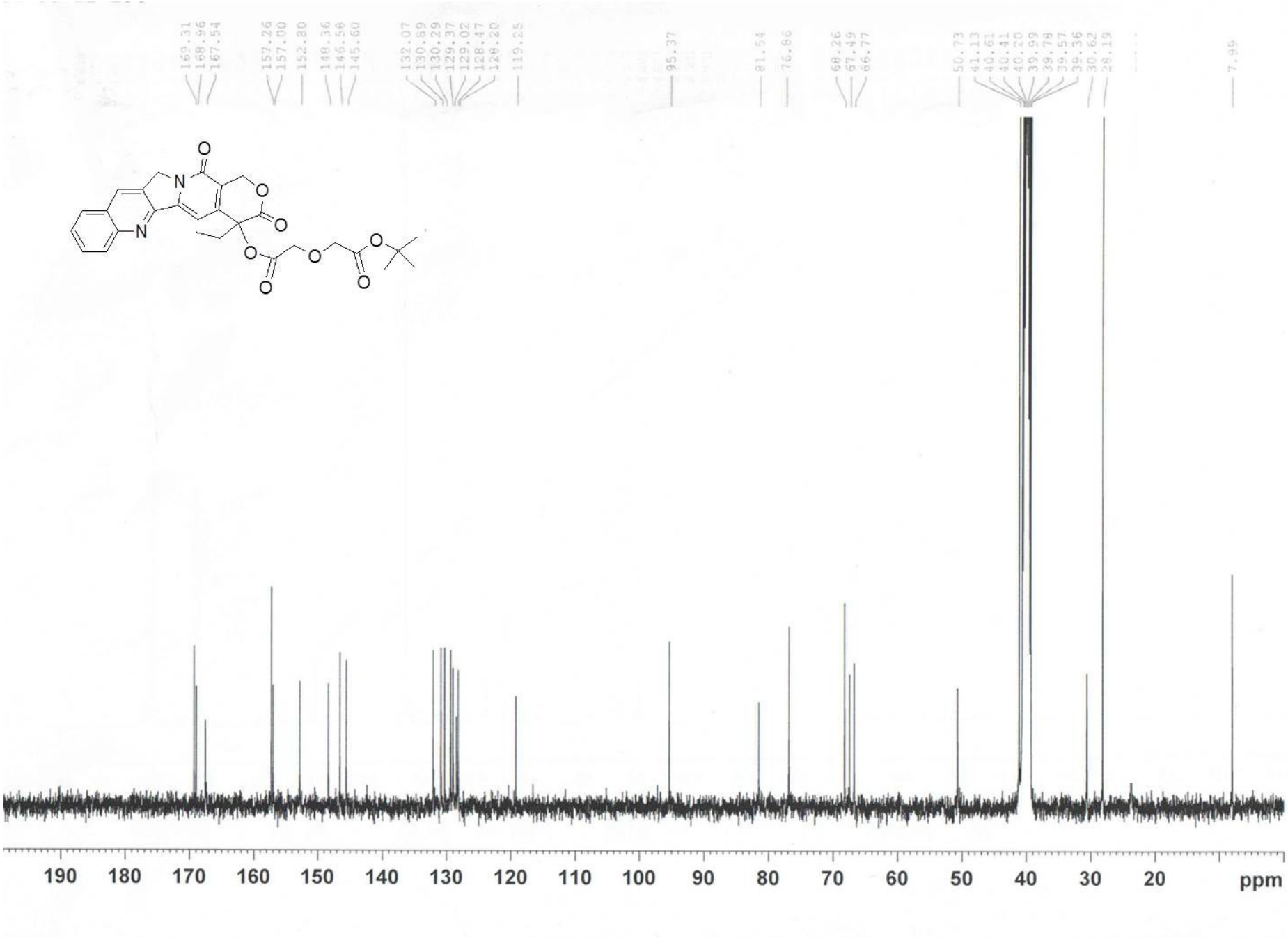
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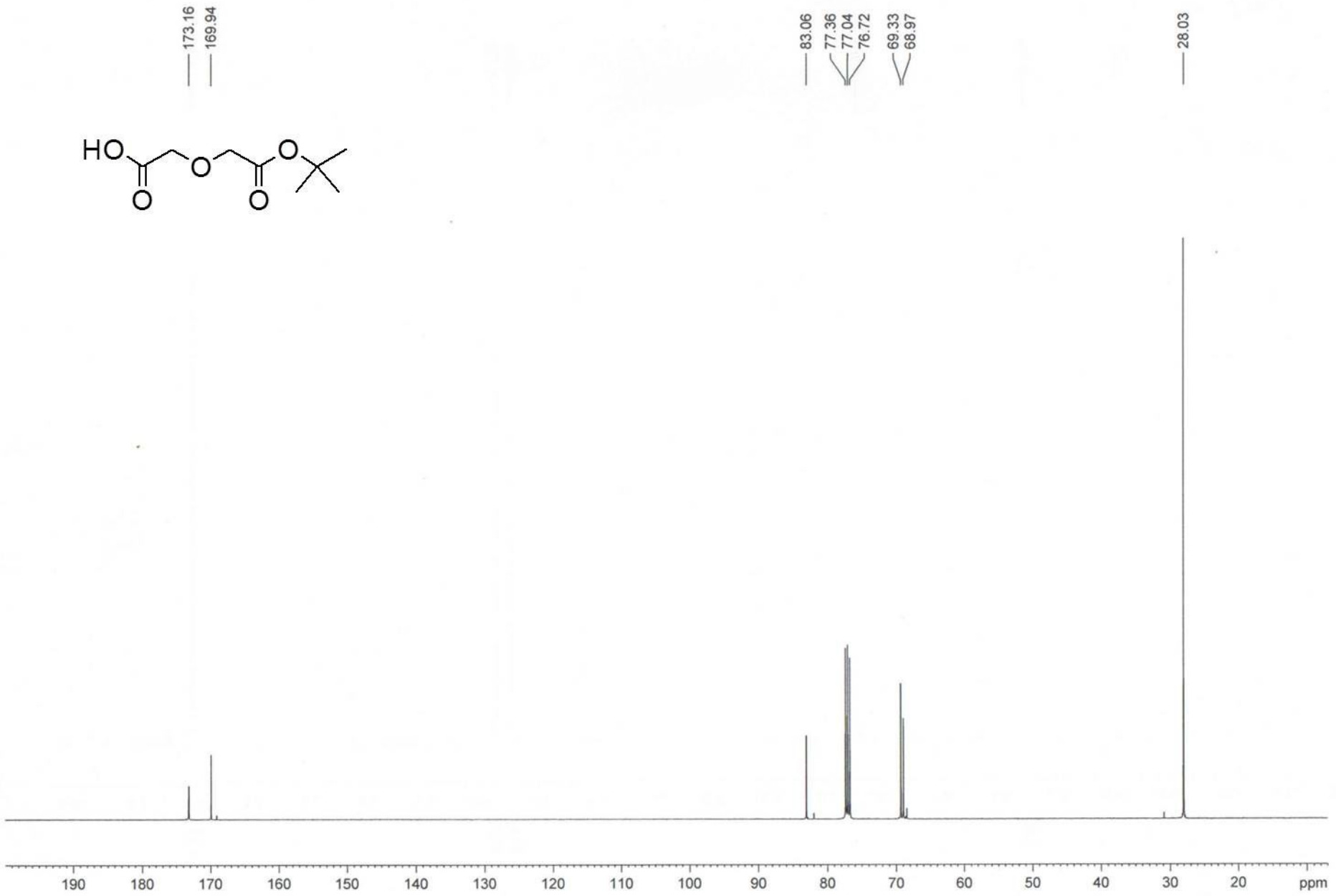
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190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

Size Distribution Report by Intensity

v2.1

Malvern

Sample Details

Sample Name: np-drug 1

SOP Name: mansettings.nano

General Notes:

File Name:	smss-20.9.13	**Dispersant Name:**	Water
Record Number:	3	**Dispersant RI:**	1.330
Material RI:	1.59	**Viscosity (cP):**	0.8872
Material Absorbtion:	0.01	**Measurement Date and Time:**	Friday, September 20, 2013...

System

Temperature (°C):	25.0	**Duration Used (s):**	60
Count Rate (kcps):	166.4	**Measurement Position (mm):**	4.65
Cell Description:	Disposable sizing cuvette	**Attenuator:**	11

Results

			Size (r.nm):	% Intensity	Width (r.nm):
Z-Average (r.nm):	108.7	**Peak 1:**	120.1	100.0	0.000
PdI:	0.219	**Peak 2:**	0.000	0.0	0.000
Intercept:	1.33	**Peak 3:**	0.000	0.0	0.000

Result quality : Good