

SUPPORTING INFORMATION

Binding ability of first and second generation / carbazolyphenyl dendrimers with Zn(II) tetraphenylporphyrin core towards small heterocyclic substrates

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TABLE OF CONTENTS

1. UV-Vis spectra of the system ZnD3-G1 - L3	2
2. Dependence of the stability constants of ZnTPP, ZnD1-G1, ZnD2-G1, ZnD4-G1, ZnD5-G1, ZnD7-G2, ZnD8-G2 with L2-L5 on the generation type and the nature of bridging fragments	3
3. Molecular modeling of dendrimers ZnD1-G1, ZnD4-G1 and ZnD7-G2	4
4. UV-Vis spectra of the system ZnD3-G1 - L1	5
5. ¹ H NMR and ¹³ C NMR spectra of new compounds	6
6. Mass spectra of new compounds	14

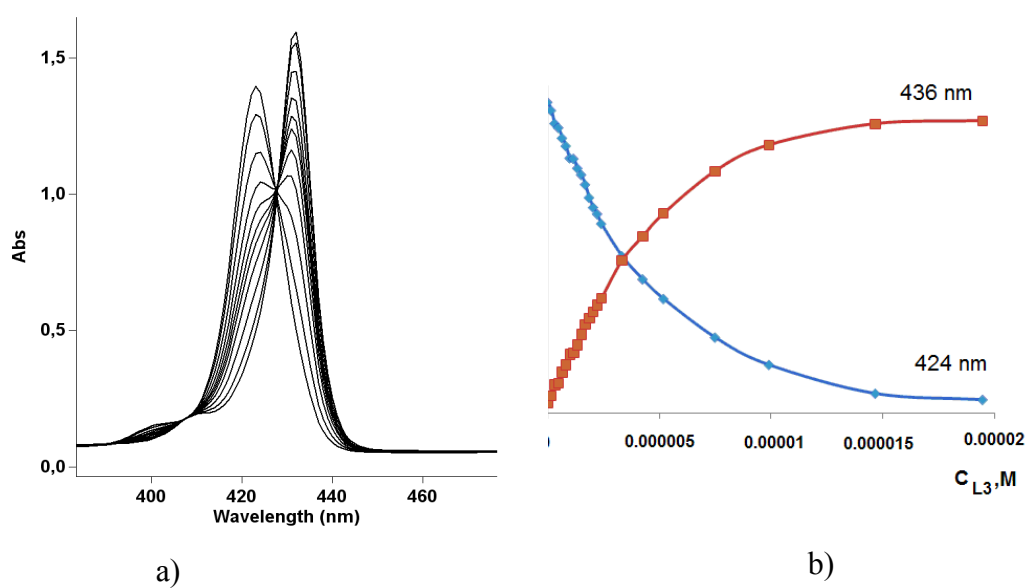
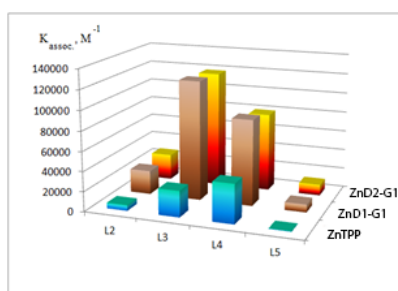
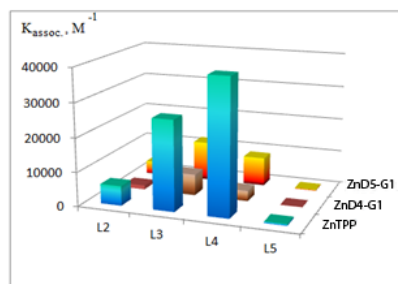
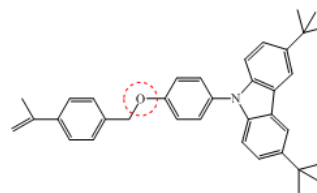


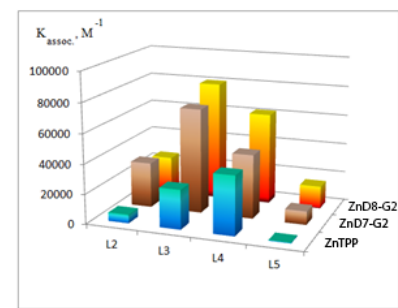
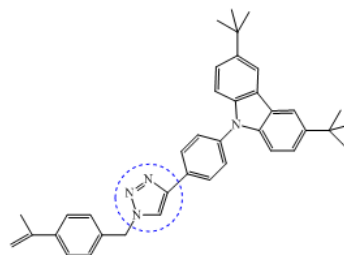
Figure 1S. a) The changes in the UV-Vis spectra of the system **ZnD3-G1 - L3** in toluene at 20°C, $C_{\text{ZnD3-G1}} = 1.0 \times 10^{-5} \text{ M}$; **b)** The binding isotherms of the system **ZnD3-G1 - L3** on the decreasing (424 nm) and the increasing (436 nm) wavelengths in toluene at 20°C, $C_{\text{ZnD3-G1}} = 1.0 \times 10^{-5} \text{ M}$.



a)



b)



c)

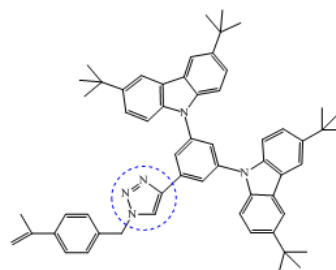
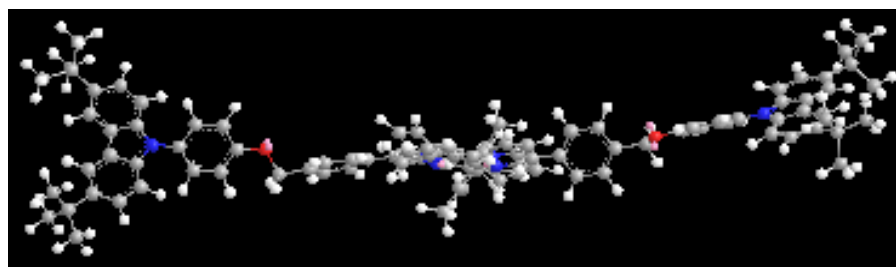
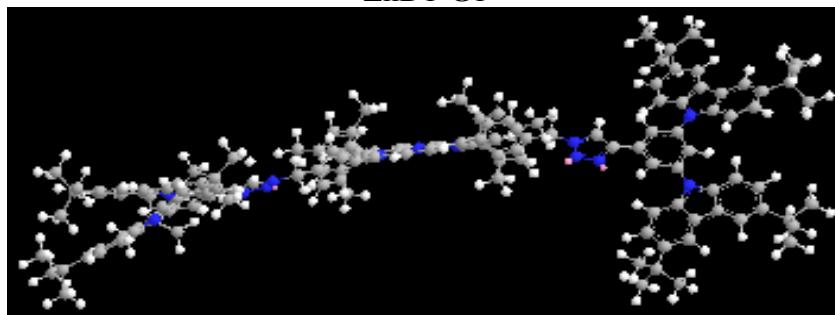


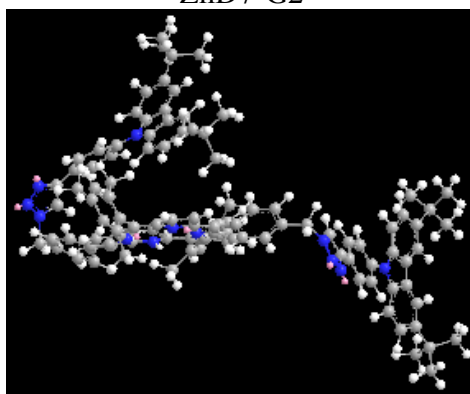
Figure 2S. Dependence of the stability constants of **ZnTPP**, **ZnD1-G1**, **ZnD2-G1**, **ZnD4-G1**, **ZnD5-G1**, **ZnD7-G2**, **ZnD8-G2** with **L2-L5** on the generation type and the nature of bridging fragments between the porphyrin macrocycle and the carbazolyphenyl branches (toluene, 25⁰ C).



ZnD1-G1



ZnD7-G2



ZnD4-G1

Figure 3S. Molecular modeling of dendrimers **ZnD1-G1**, **ZnD4-G1** and **ZnD7-G2**.

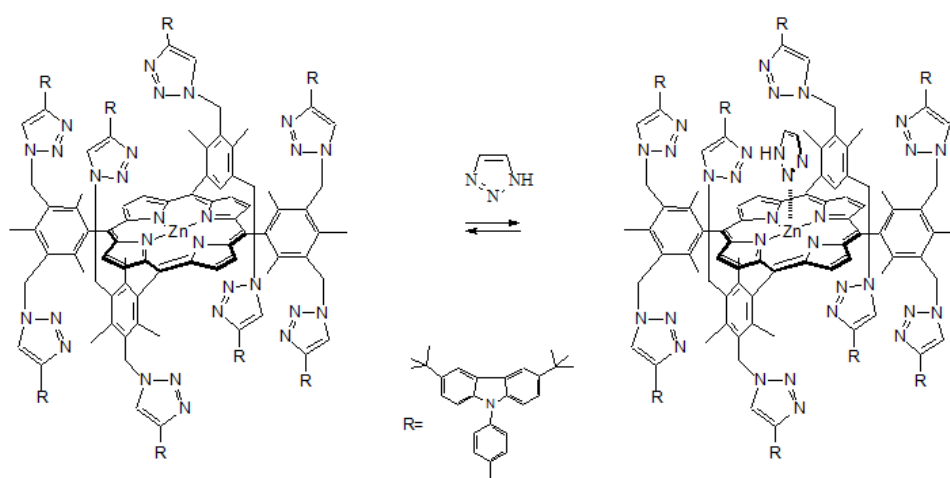


Figure 4S. Possible structure of **ZnD6-G1**

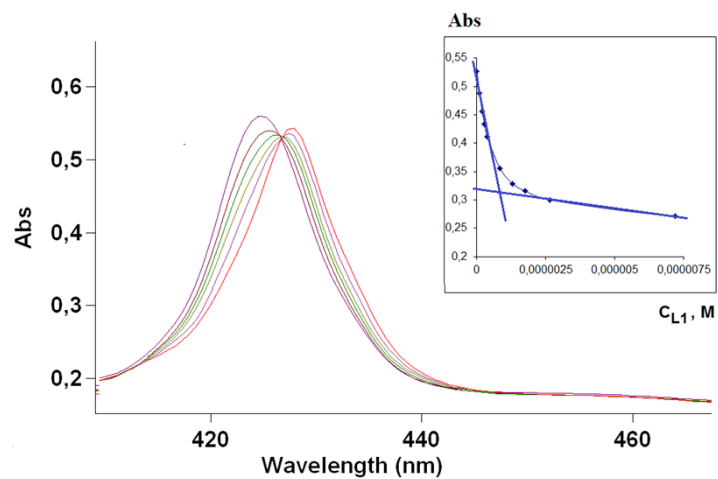


Figure 5S. The changes in the UV-Vis spectra and the binding isotherm of the system **ZnD3-G1 - L1** in toluene at 25°C, $C_{L1} = 1.0 \times 10^{-7}$ to 2.1×10^{-6} M.

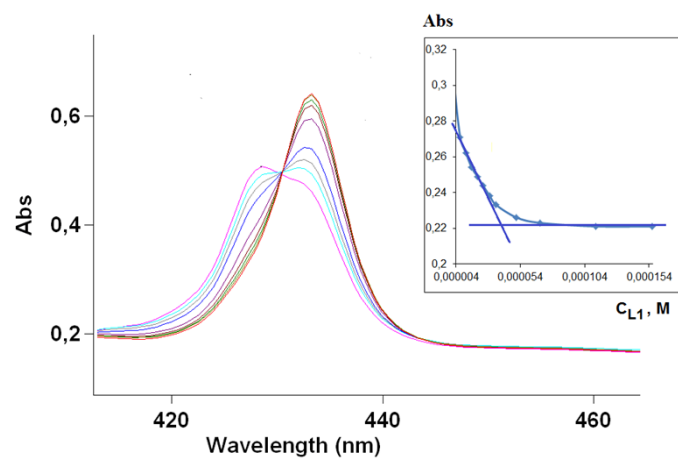
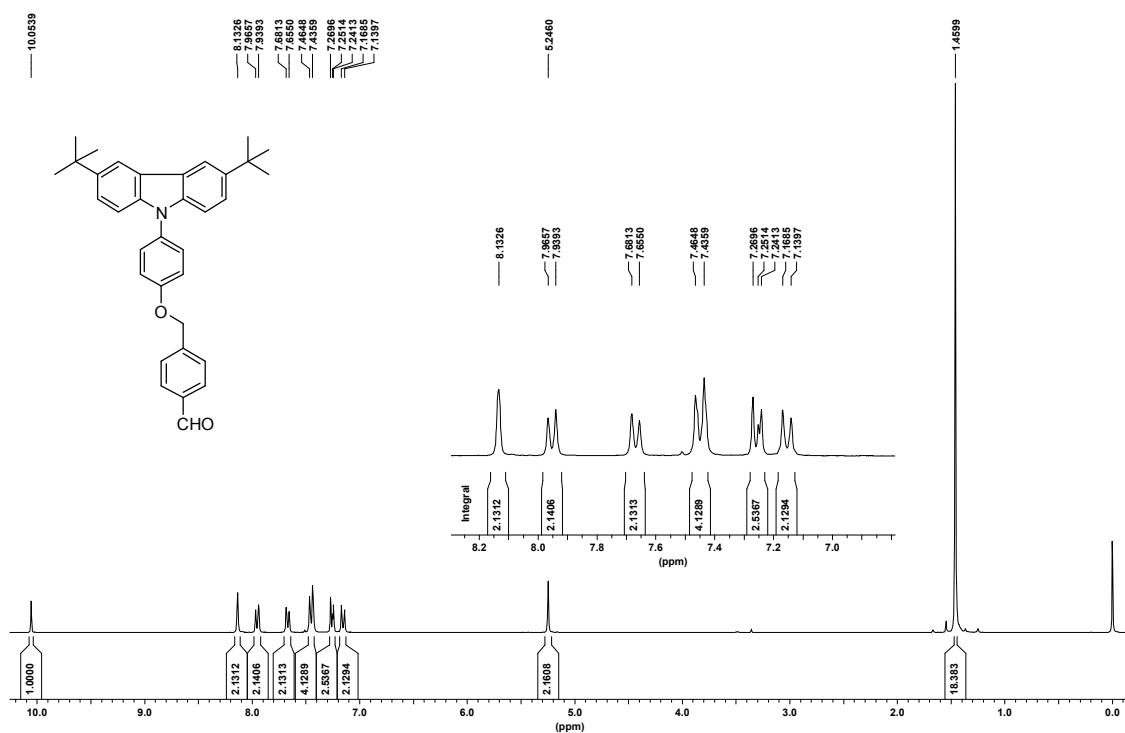
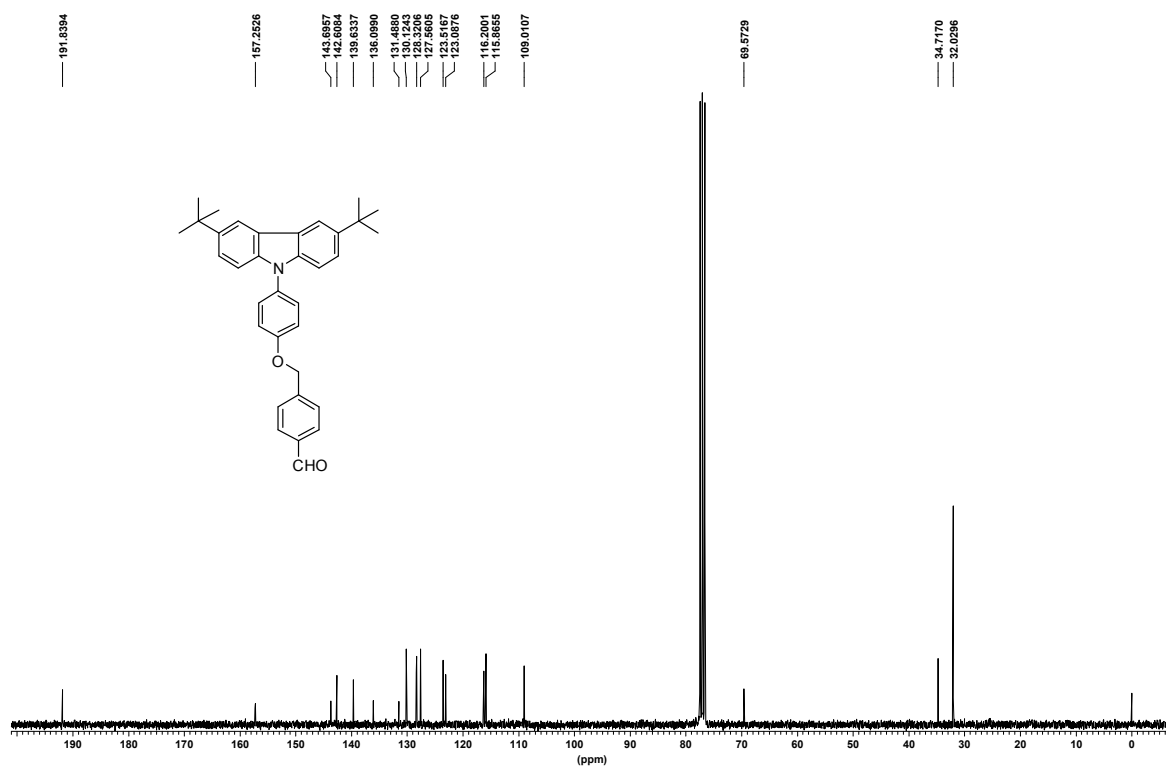


Figure 6S. The changes in the UV-Vis spectra and the binding isotherm of the system **ZnD3-G1 - L1** in toluene at 25°C, $C_{L1} = 2.1 \times 10^{-6}$ to 1.0×10^{-4} M.

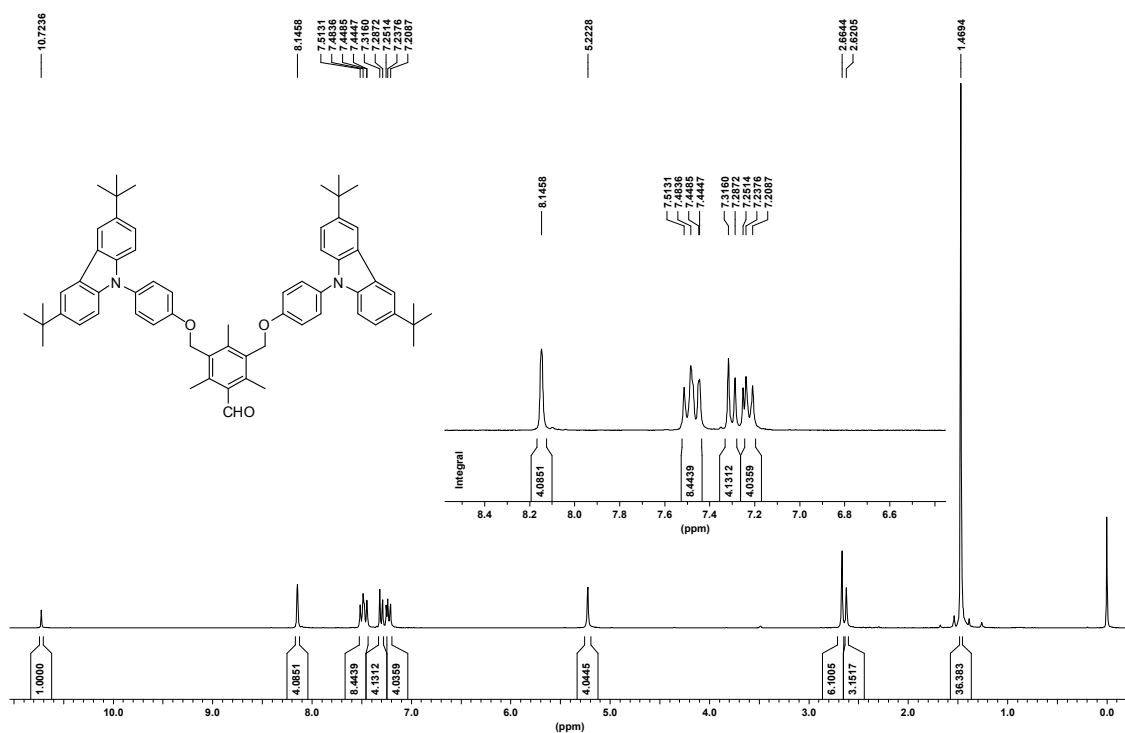
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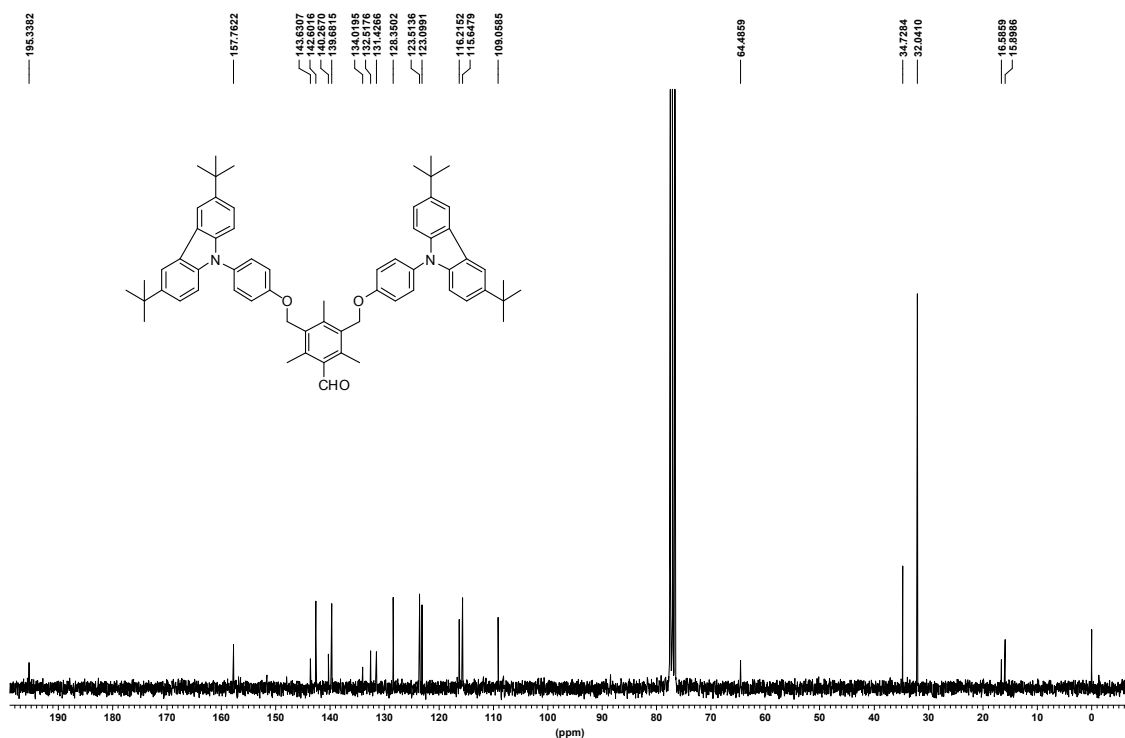
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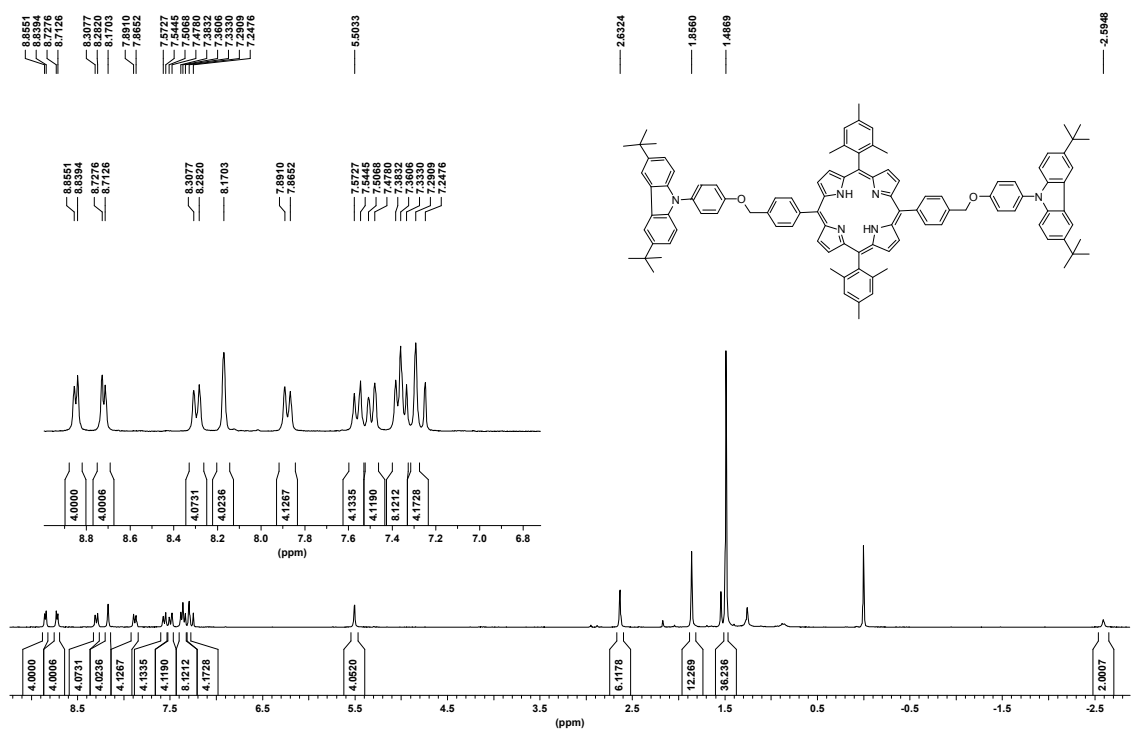
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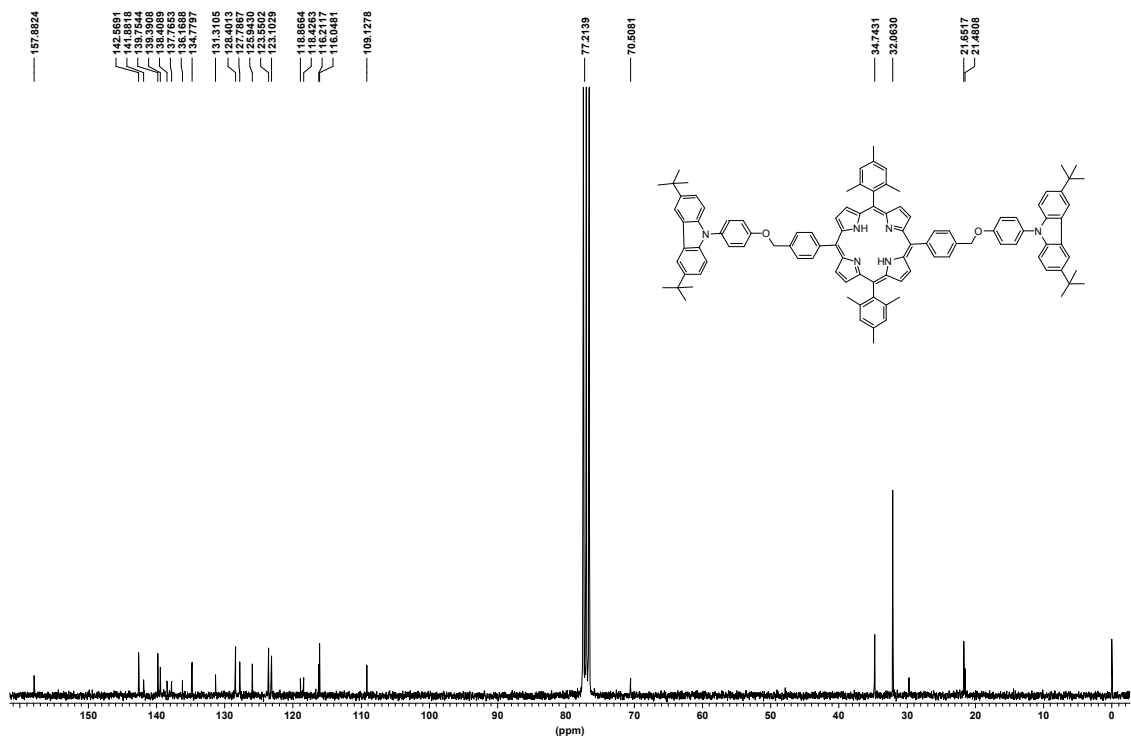
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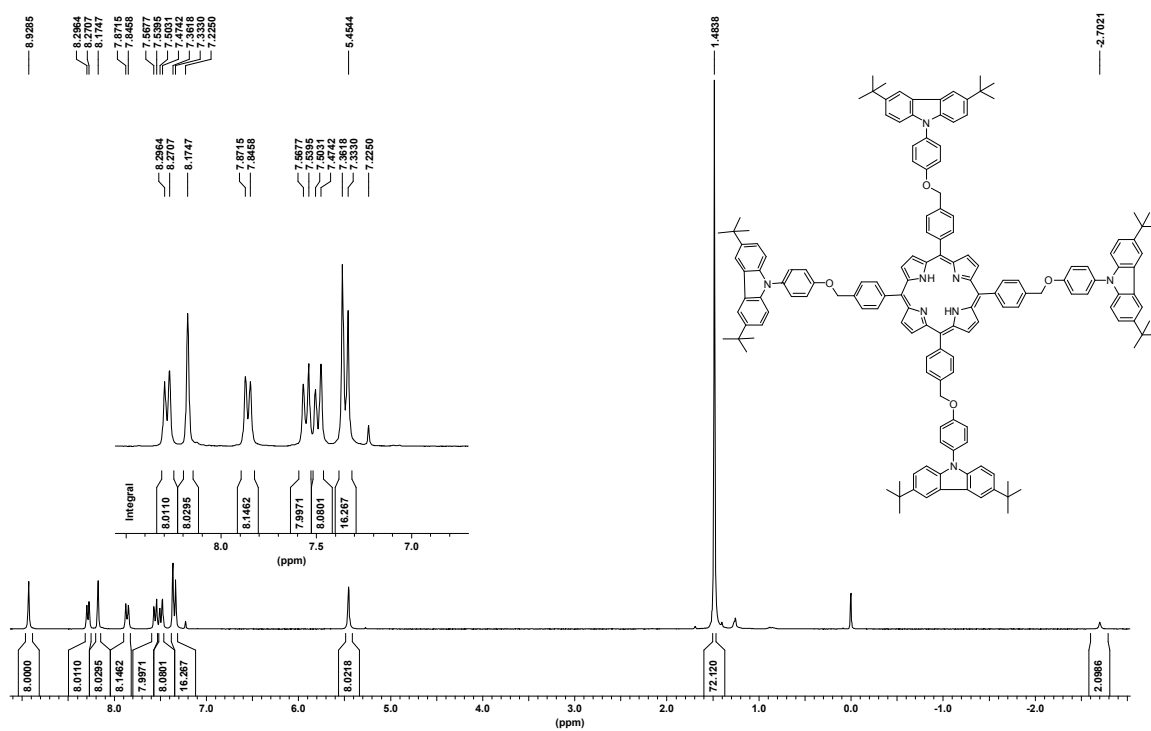
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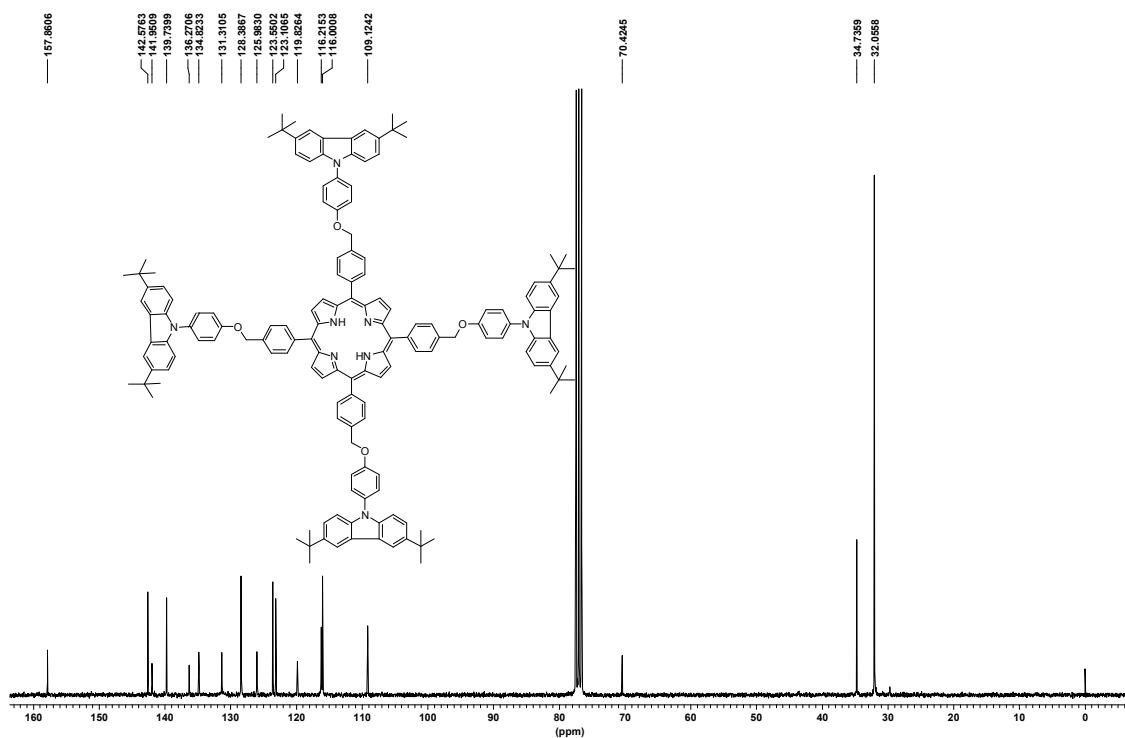
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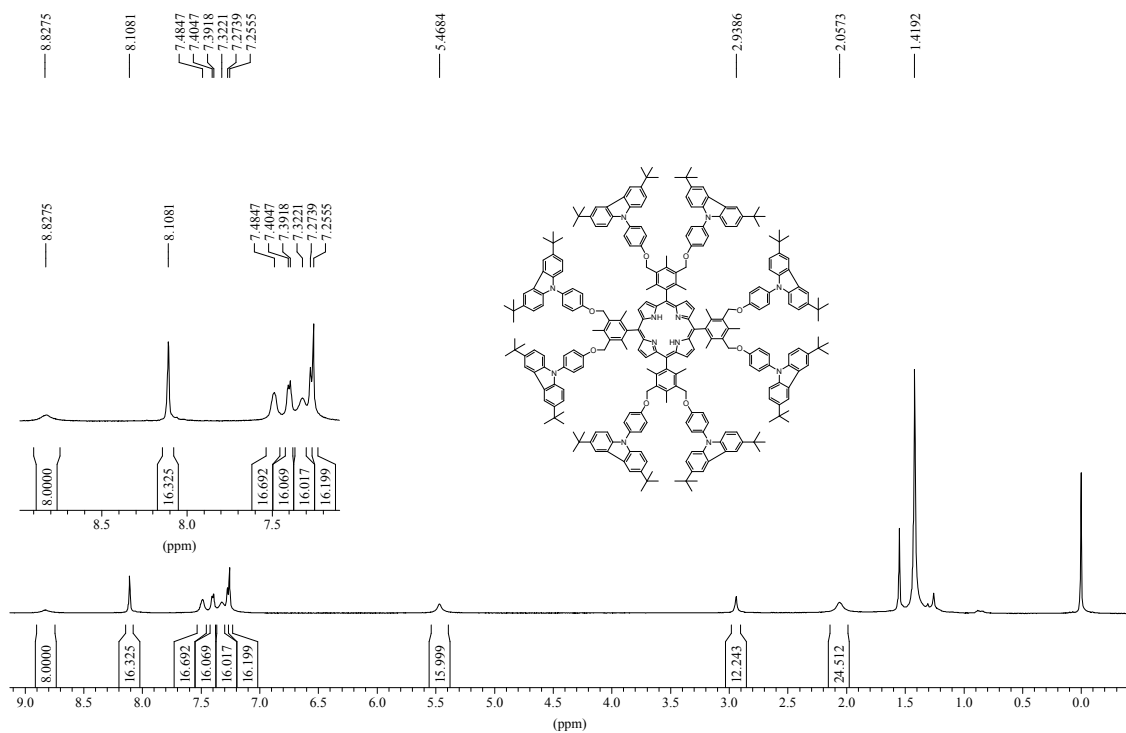
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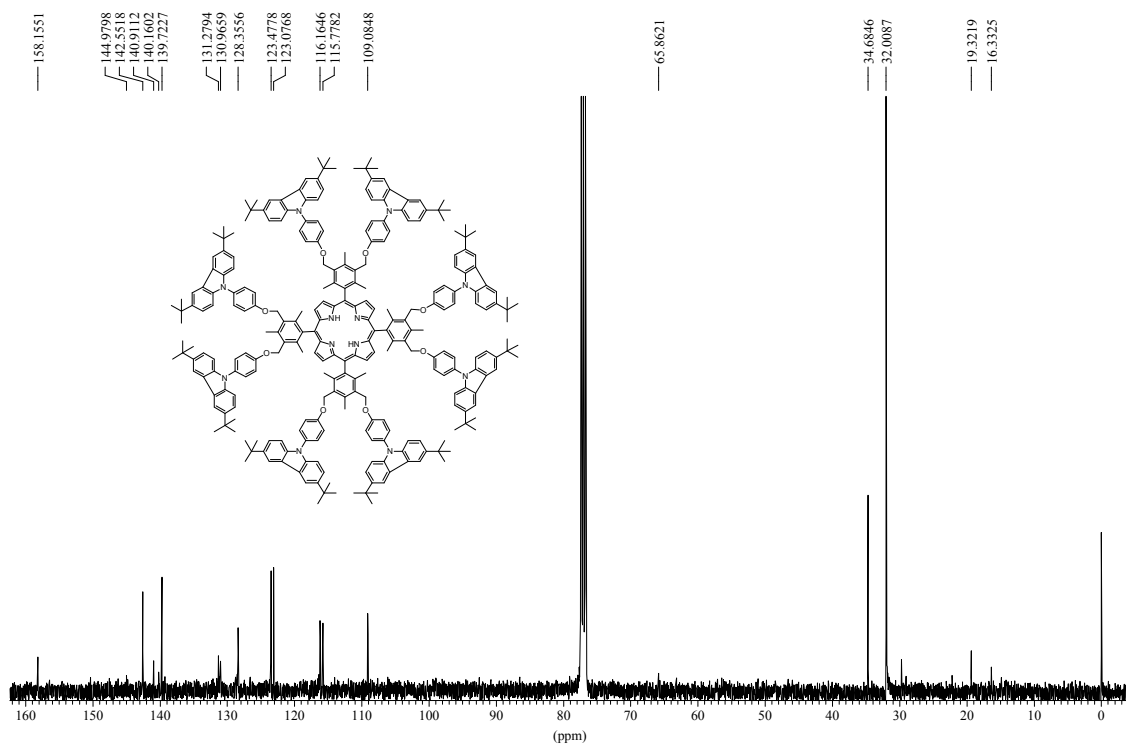
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DENDRIMER I 600MHz

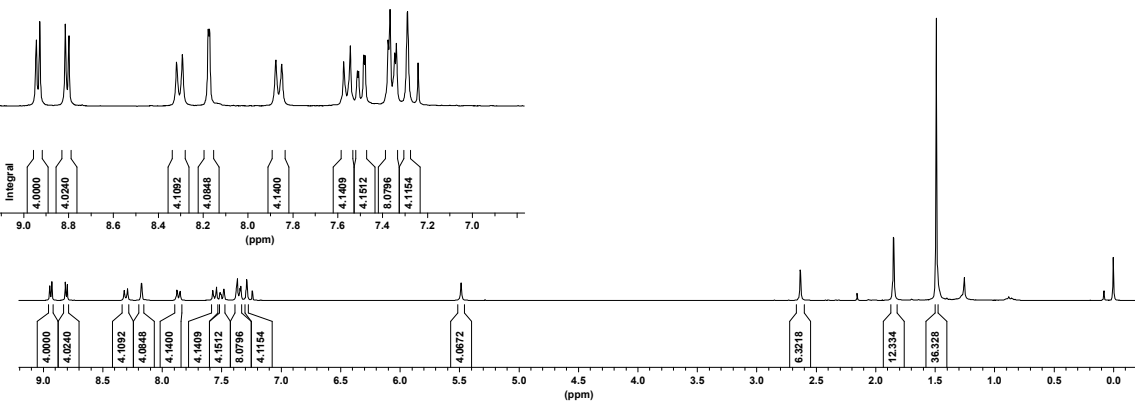
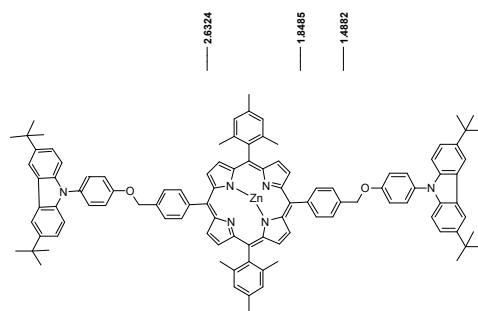


DENDRIMER I 100MHz



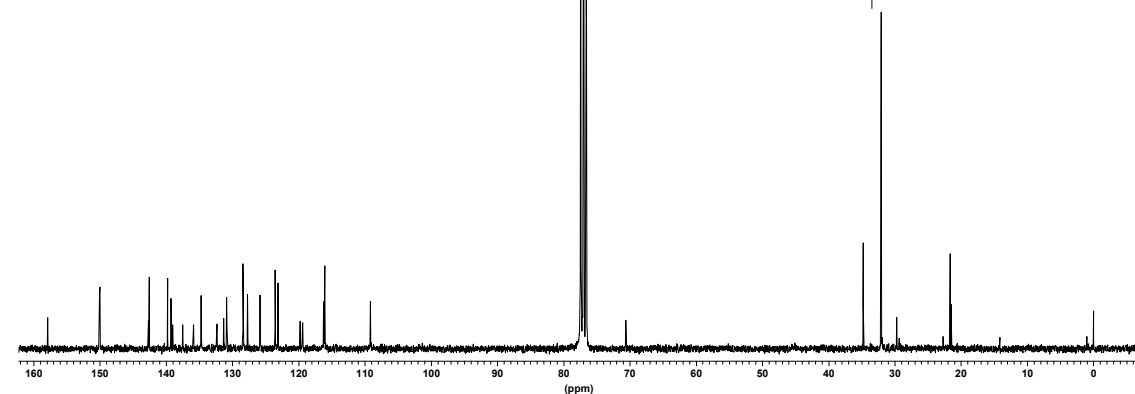
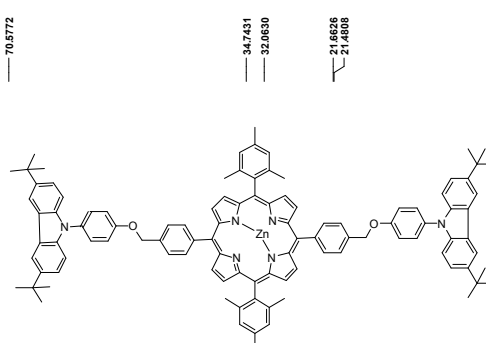
¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm, ranging from 7.0 to 9.0. The y-axis represents the integral of the peaks. The spectrum shows several multiplets and doublets, with integration values provided below the peaks. The chemical shift values are listed on the right side of the spectrum.

Chemical Shift (ppm)	Integration
8.9436	4.0000
8.9279	4.0240
8.8136	4.1092
8.7979	4.0848
8.3178	4.1400
8.3114	4.1409
8.1759	4.1512
8.1709	8.0796
7.8583	4.1154
7.8489	4.1400
7.8277	4.1409
7.8116	4.1512
7.7662	8.0796
7.7490	4.1154
7.7344	4.1400
7.7337	4.1409
7.6862	4.1512
7.6774	8.0796
7.6374	4.1154
7.5884	4.1400
7.5432	4.1409
7.5119	4.1512
7.5062	8.0796
7.4773	4.1154
7.3744	4.1400
7.3682	4.1409
7.3449	4.1512
7.3374	8.0796
7.3181	4.1154
7.2413	4.1400

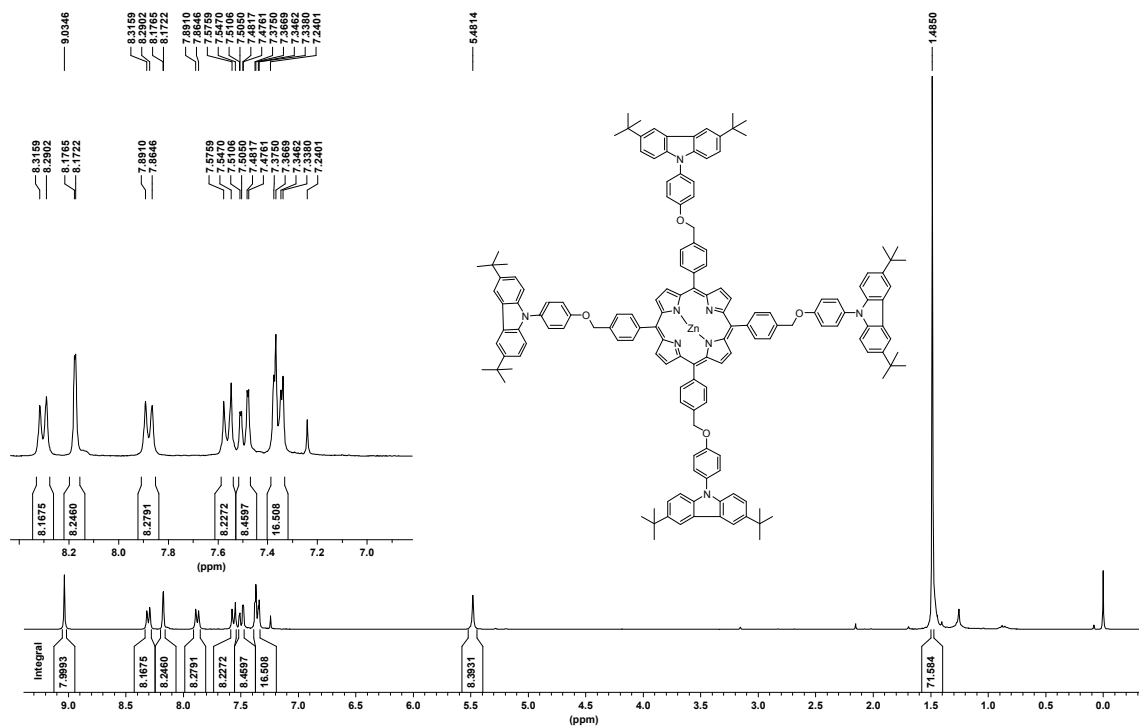


Mass spectrum of compound 10. The x-axis represents the mass-to-charge ratio (m/z) from 90 to 160. The y-axis represents the relative intensity from 0 to 100. The base peak is at m/z 130. Other significant peaks are labeled with their m/z values.

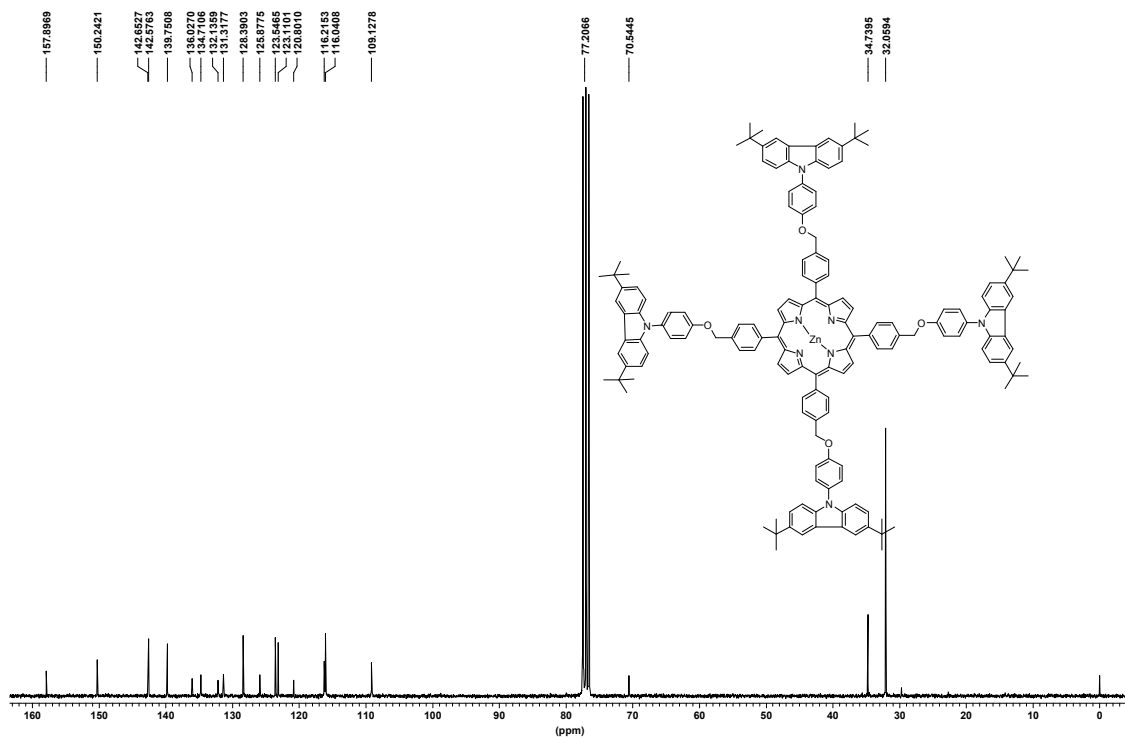
m/z	Relative Intensity (%)
157.5933	~5
150.0457	~10
149.9803	~10
142.6854	~15
142.6518	~15
138.9818	~15
139.2453	~15
138.9908	~15
137.2622	~15
136.7743	~15
134.6888	~15
132.3396	~15
132.3396	~15
130.5223	~15
130.5623	~15
128.8331	~15
128.8463	~15
126.8084	~15
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119.3973	~15
118.6861	~15
116.0699	~15
109.1387	~15



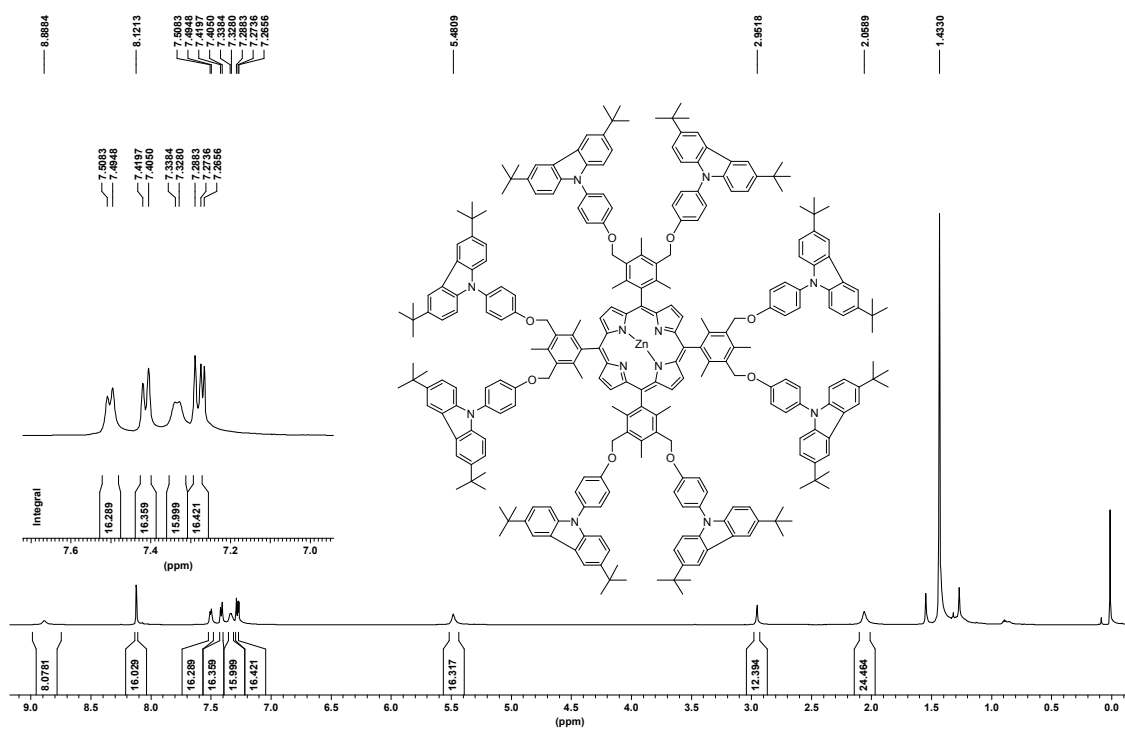
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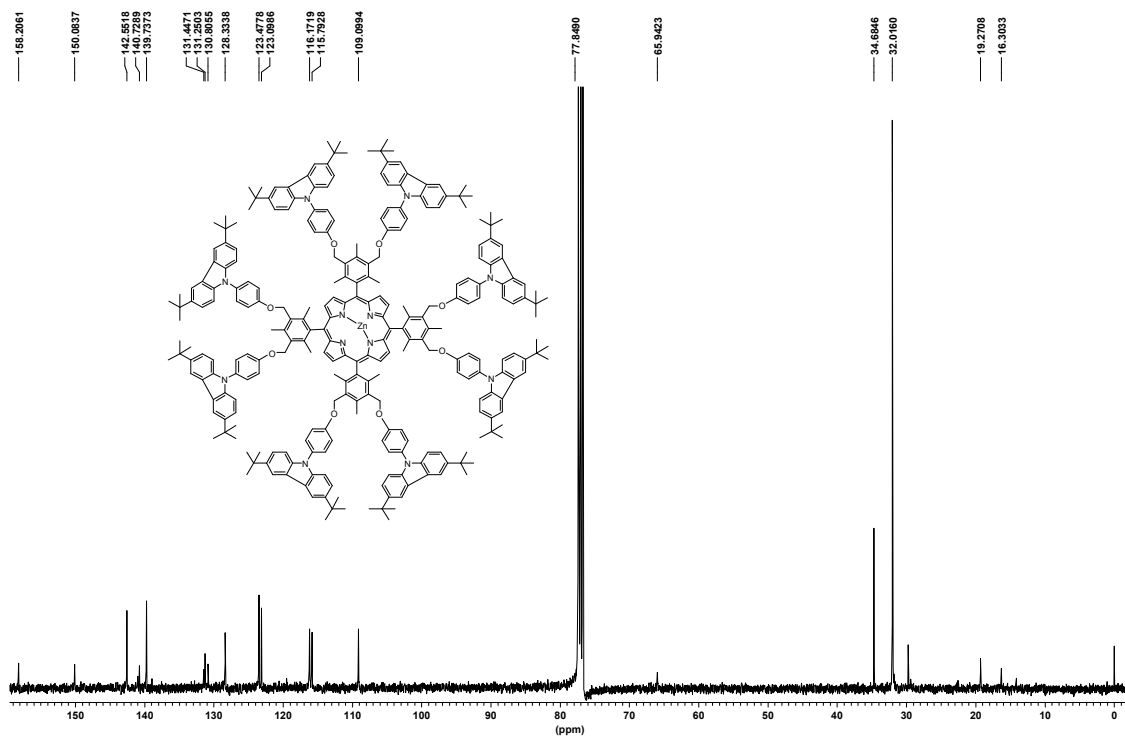
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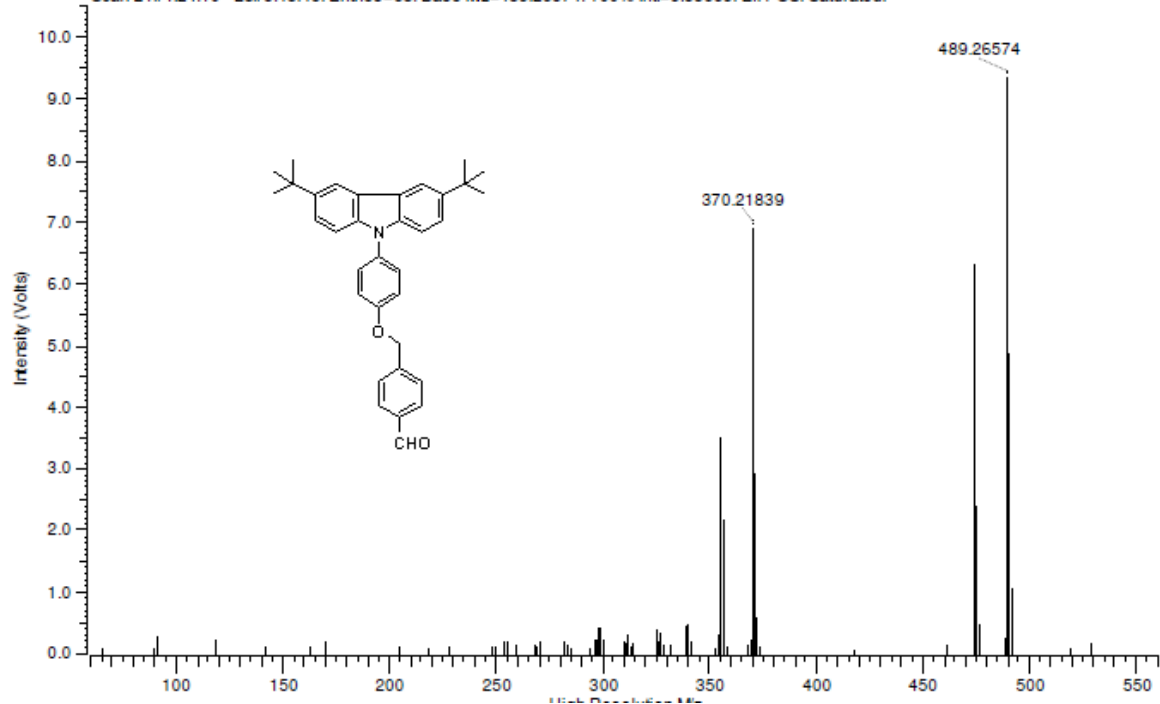
Zn-I 600MHz



Zn-I

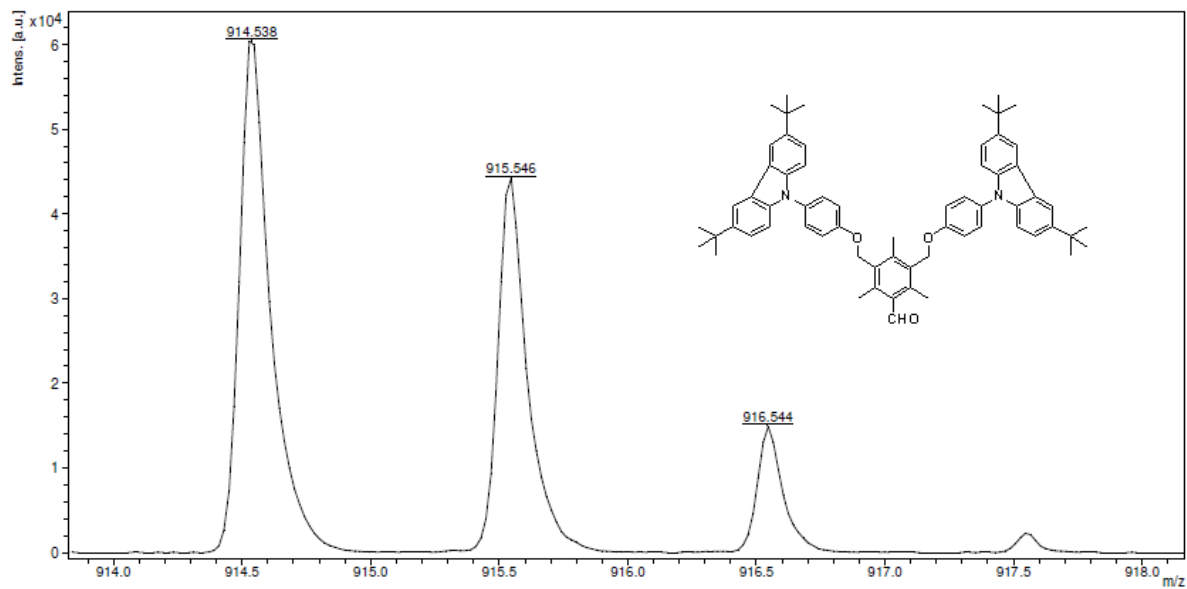


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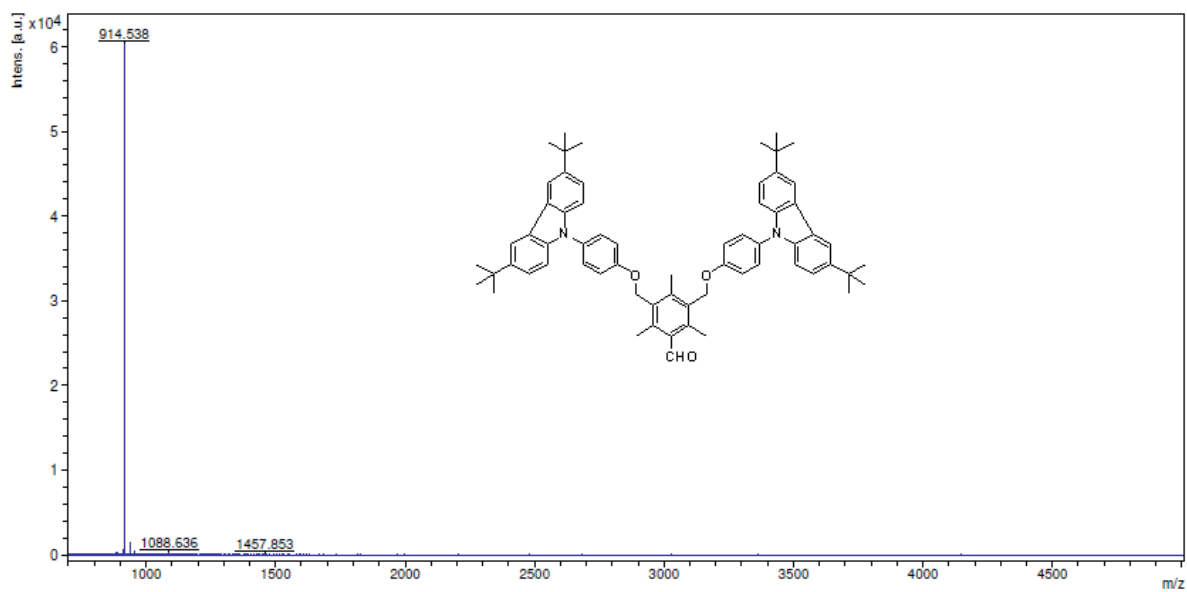


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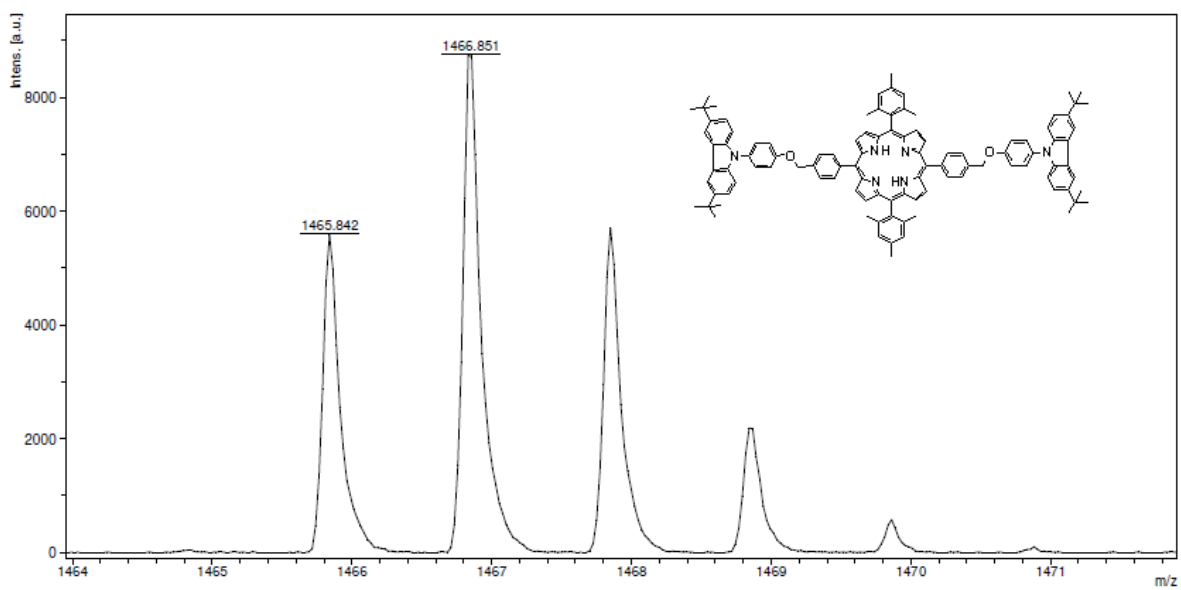
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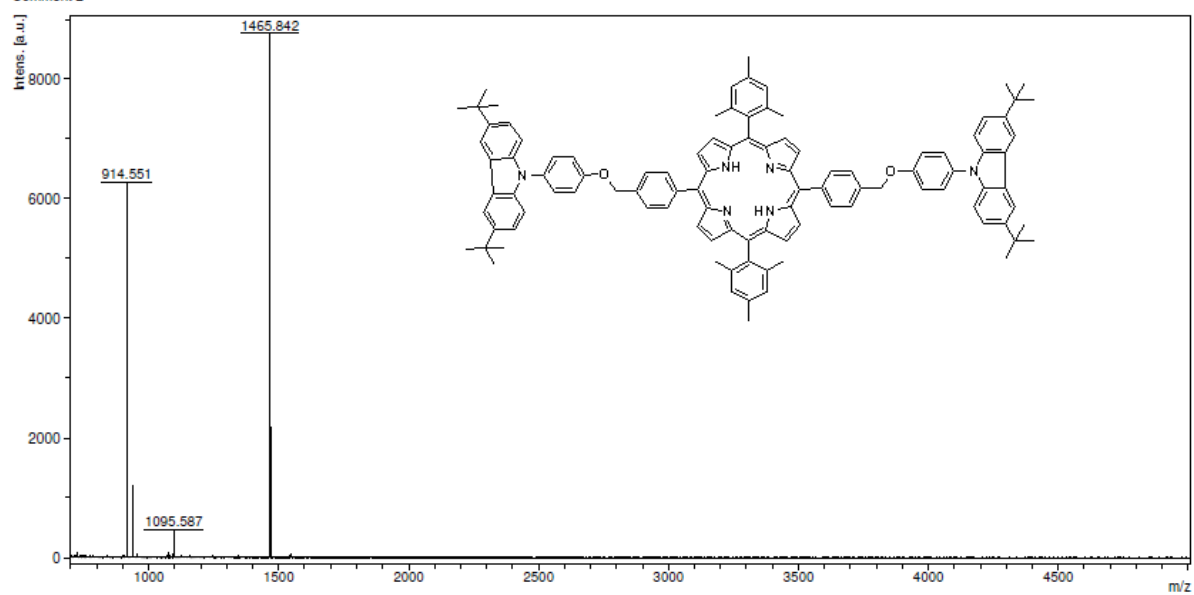
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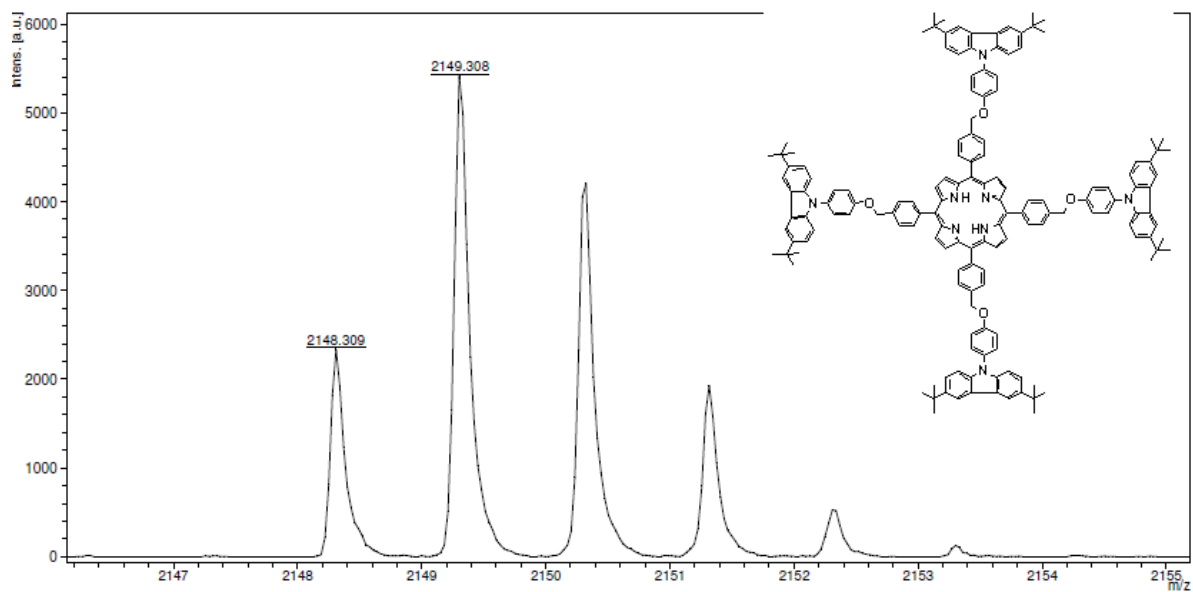


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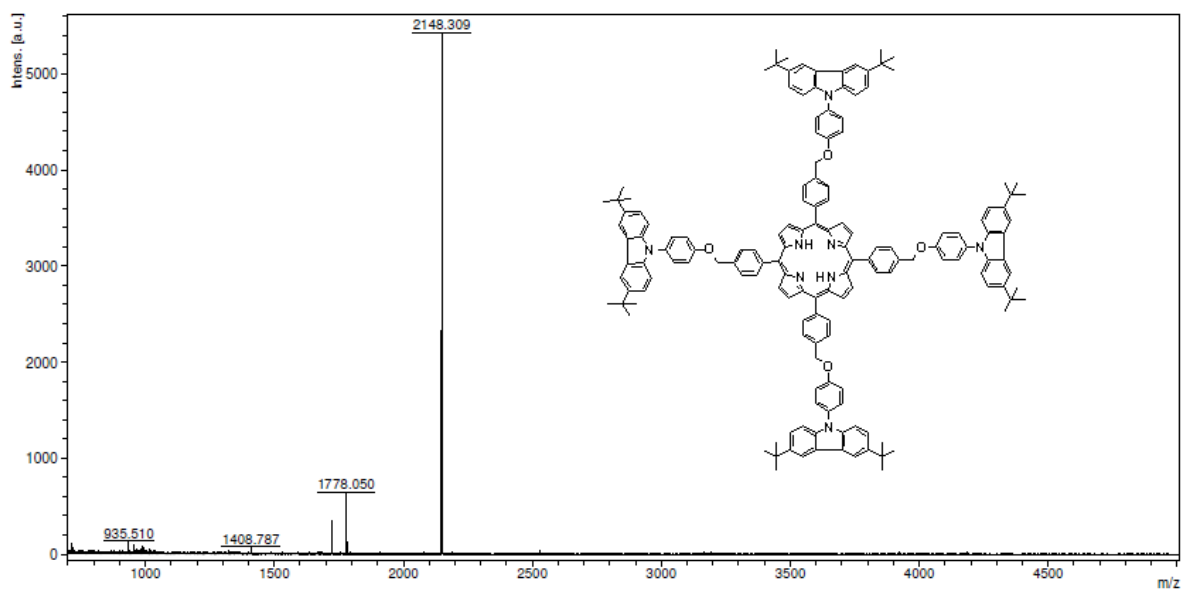


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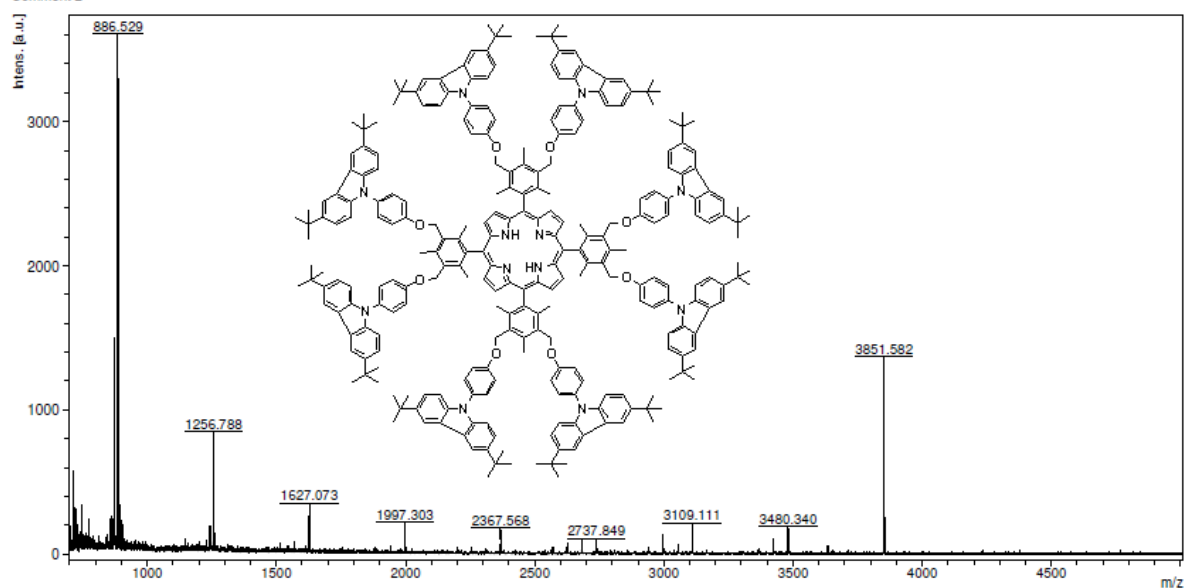
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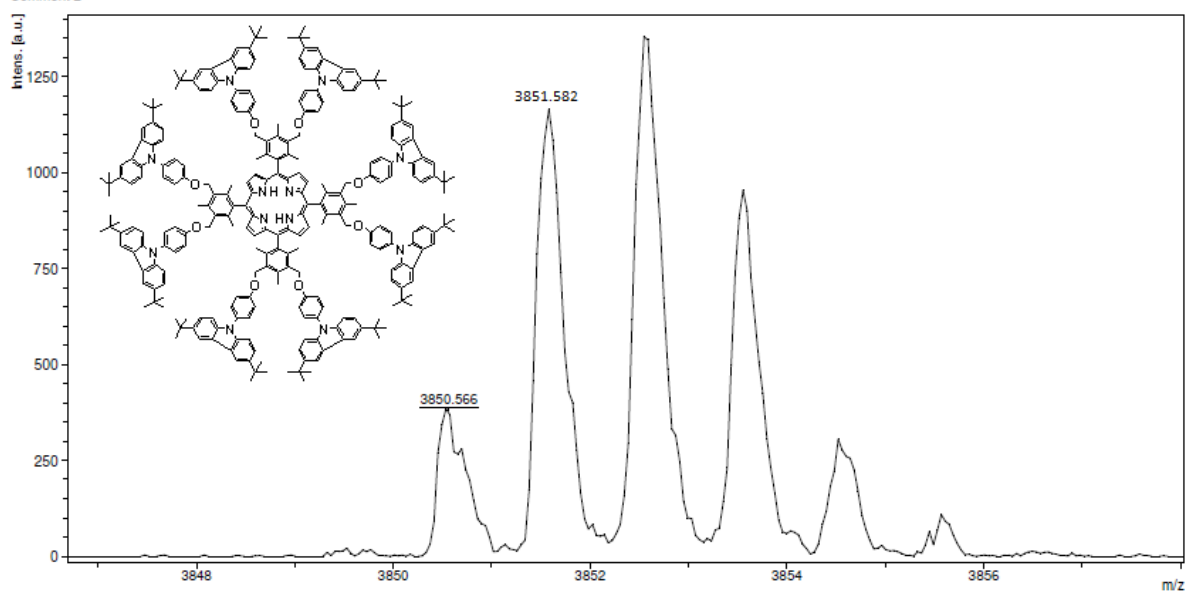
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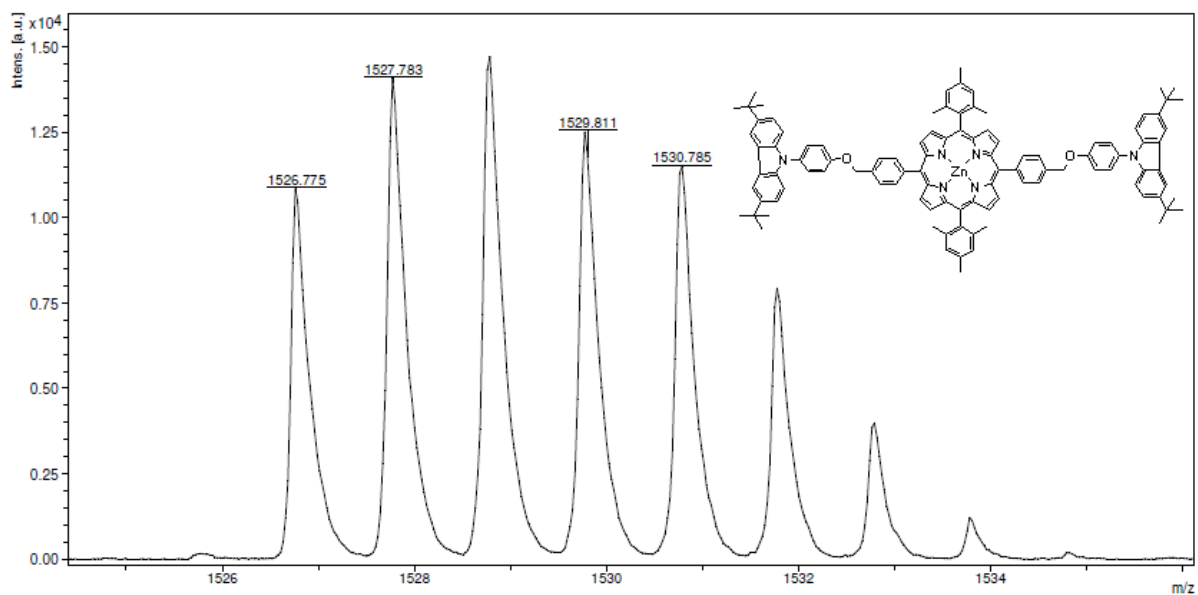
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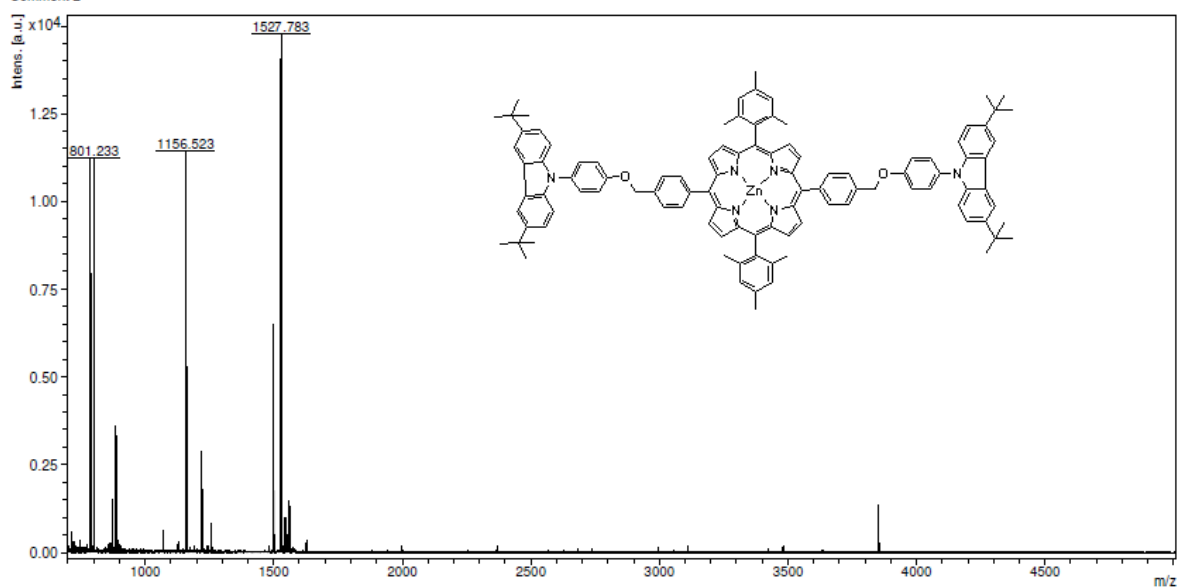
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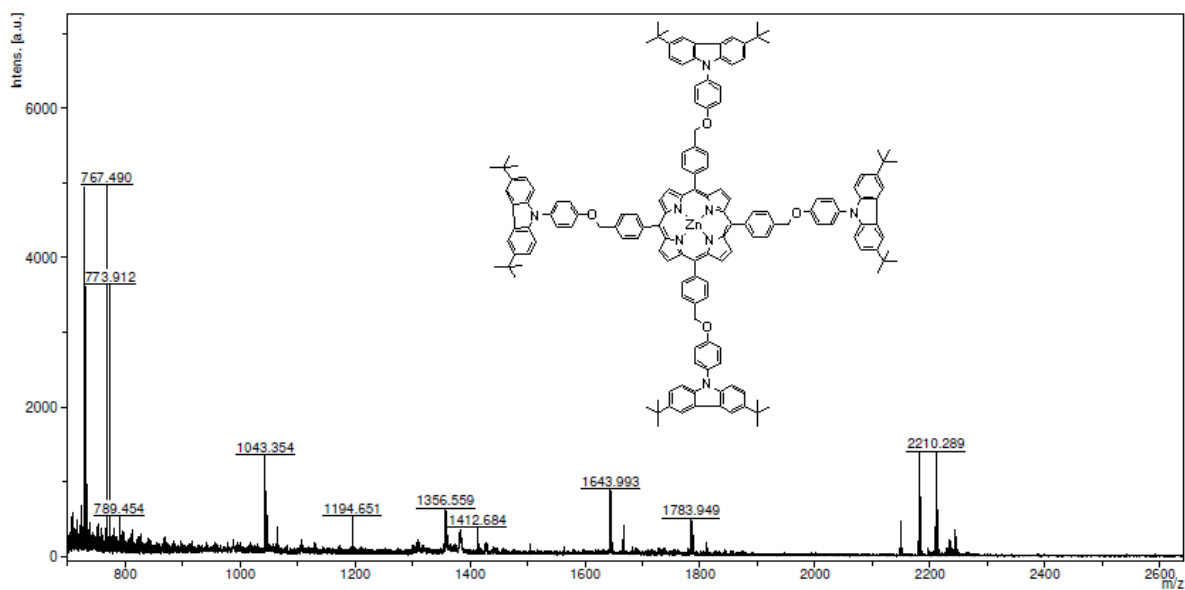
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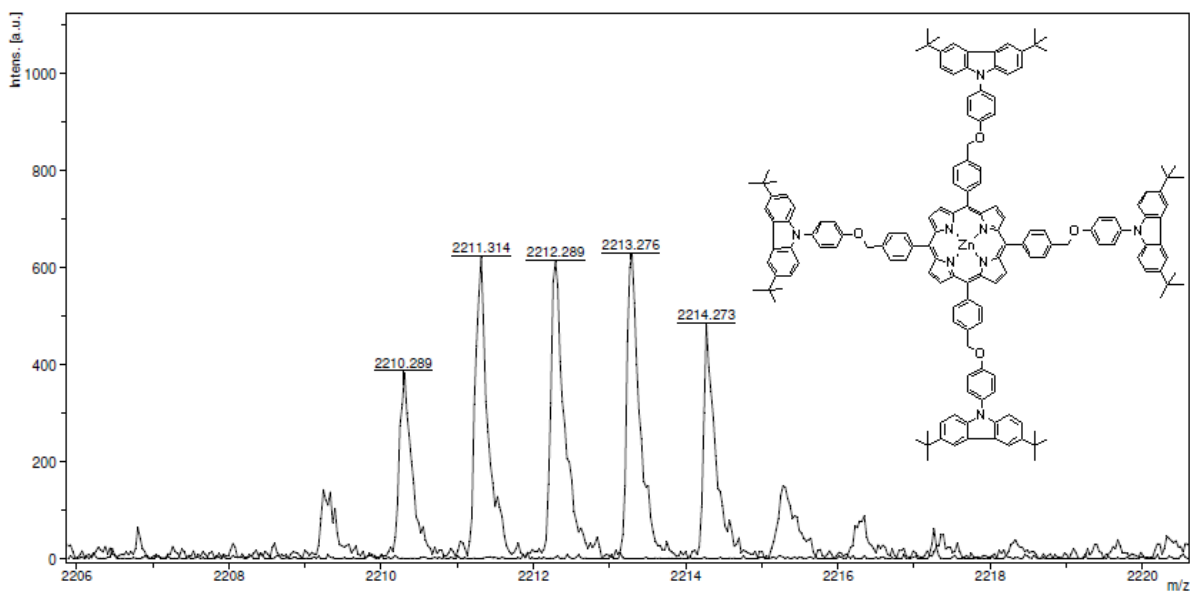
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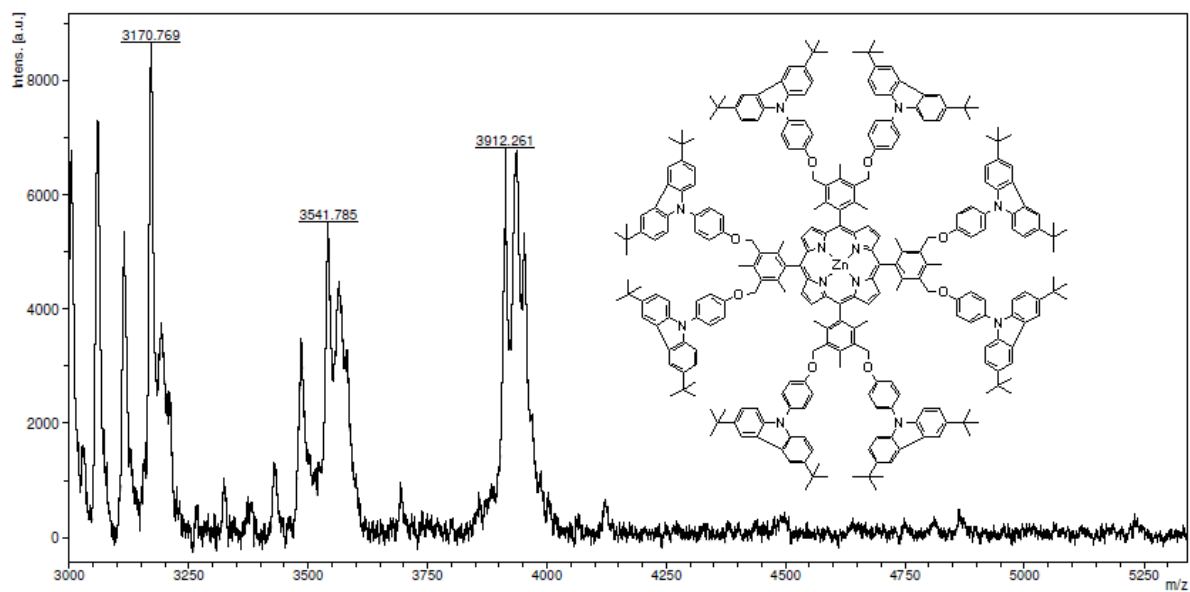
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