

Electronic Supplementary Information for:

**Chromogenic agents built around a multifunctional double-triazine framework for enzymatically triggered cross-linking under physiological conditions**

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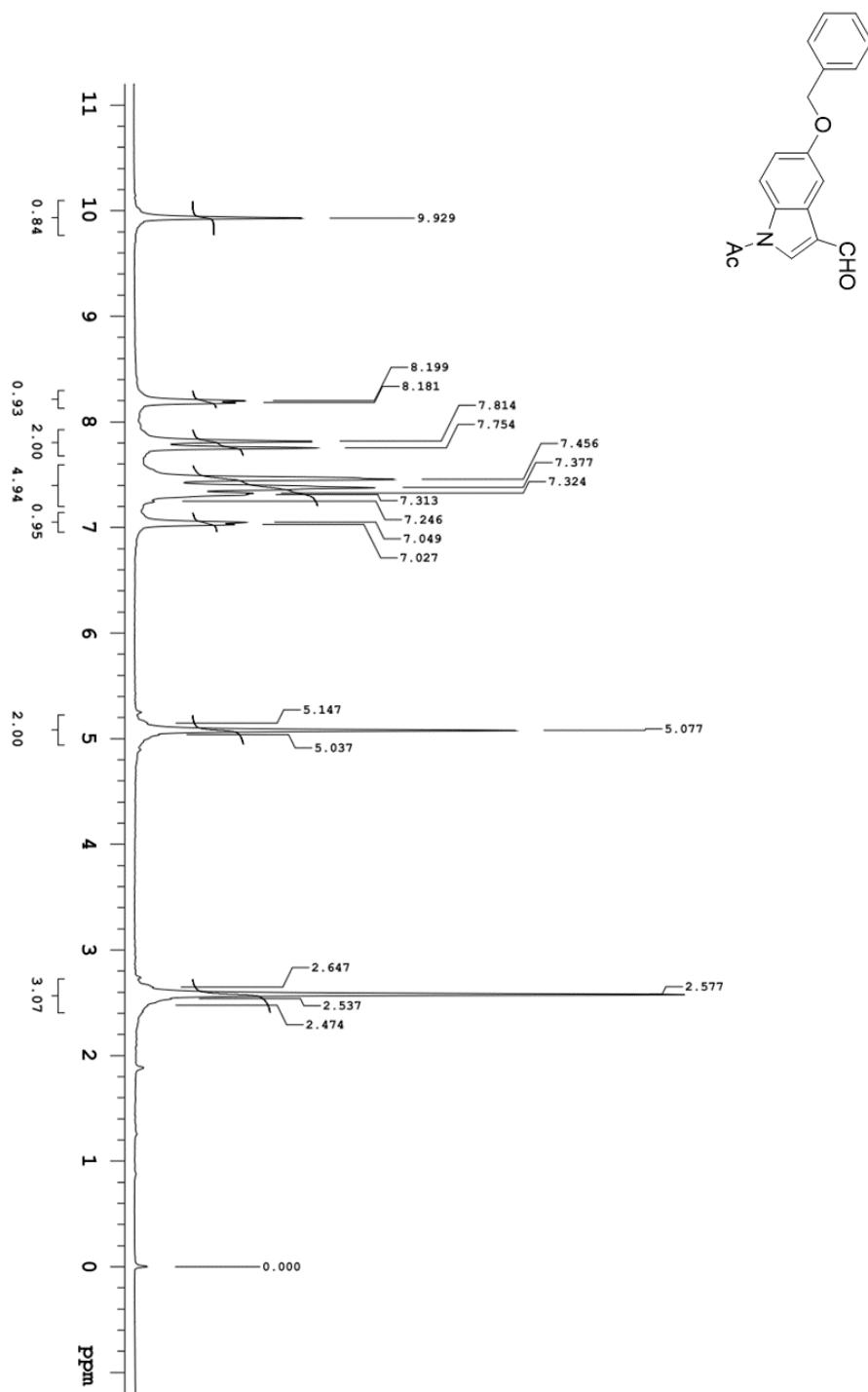
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**1. Single-crystal X-ray data for **6-β**  
(1-acetyl-5-benzyloxy-1*H*-indol-3-yl 2,3,4,6-tetra-*O*-acetyl-β-D-glucopyranoside)**

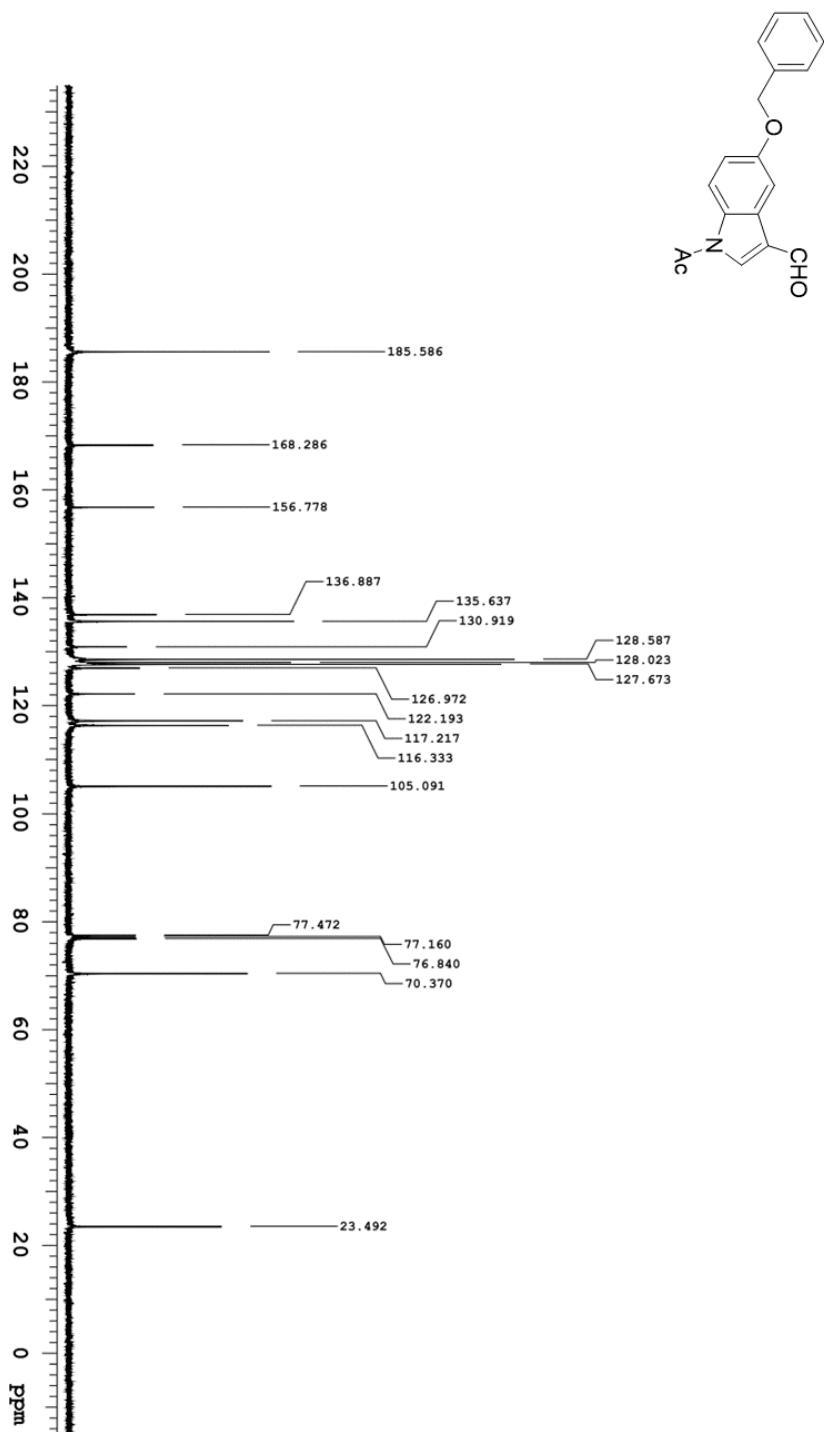
CCDC registry	1902485
Formula	C <sub>31</sub> H <sub>33</sub> NO <sub>12</sub>
Formula Weight (g/mol)	611.58
Crystal Dimensions (mm)	0.142×0.252×0.351
Crystal System	triclinic
Space Group	P 1
Temperature (K)	100
<i>a</i> (Å)	5.6782 (2)
<i>b</i> (Å)	11.7351 (4)
<i>c</i> (Å)	12.7603 (4)
α (°)	115.2260 (9)
β (°)	101.8176 (10)
γ (°)	93.6185 (11)
<i>V</i> (Å <sup>3</sup> )	741.94 (4)
Number of reflections to determine final unit cell	102
Min and Max 2θ for cell determination (°)	3.898, 44.78
<i>Z</i>	1
<i>F</i> (000)	322
ρ (g/cm <sup>3</sup> )	1.369
λ (Å, Mo Kα)	0.71073
μ (mm <sup>-1</sup> )	0.106
Max 2θ for data collection (°)	56.48
Measured fraction of data	0.998
Number of reflections measured	21480
Unique reflections measured	7272
R <sub>merge</sub>	2.05%
Number of parameters in least-squares	402
R <sub>1</sub>	0.0291
wR <sub>2</sub>	0.0691
R <sub>1</sub> (all data)	0.0328
wR <sub>2</sub> (all data)	0.0710

## 2. Spectral data for new compounds

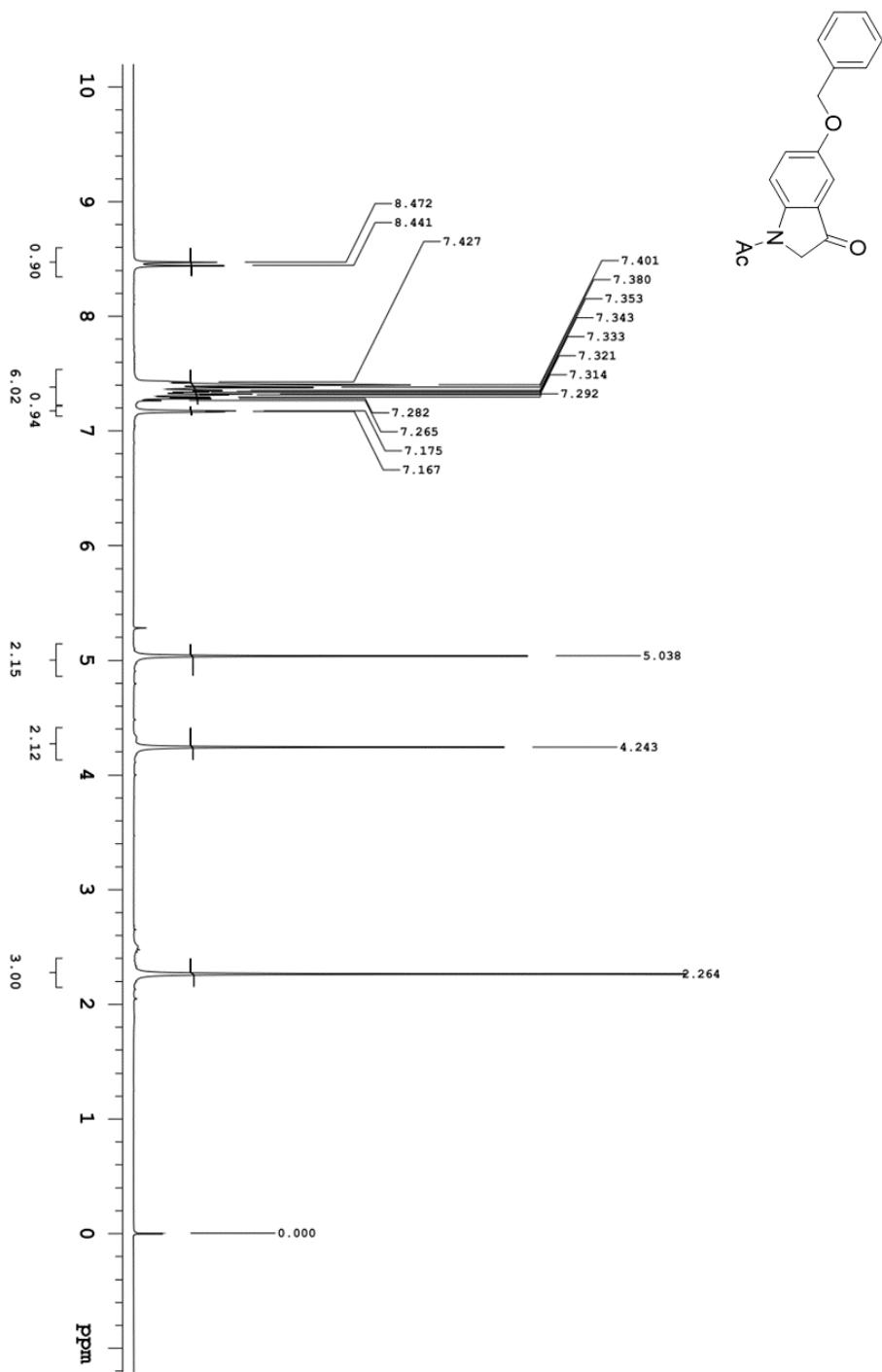
2,  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



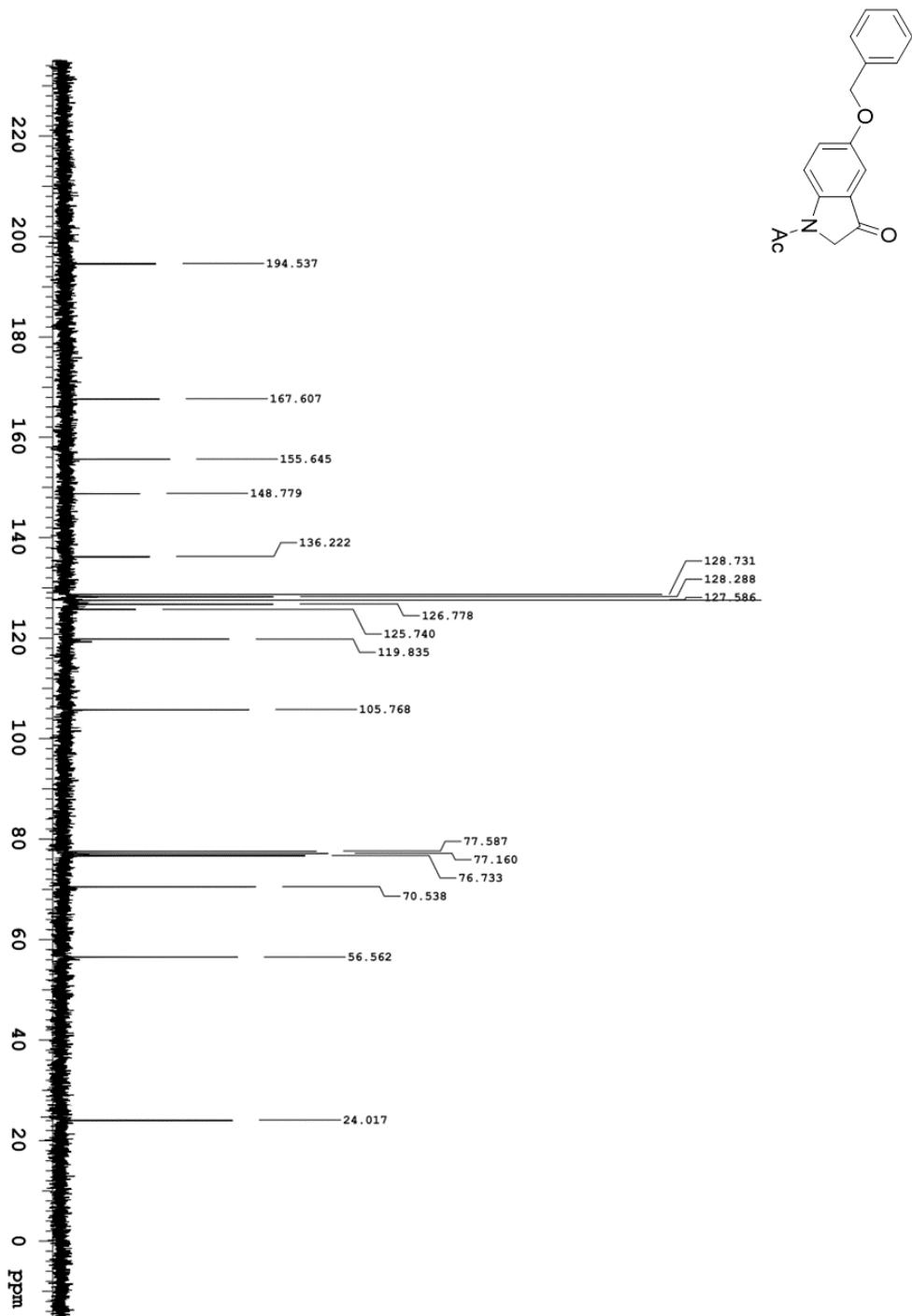
**2,  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )**



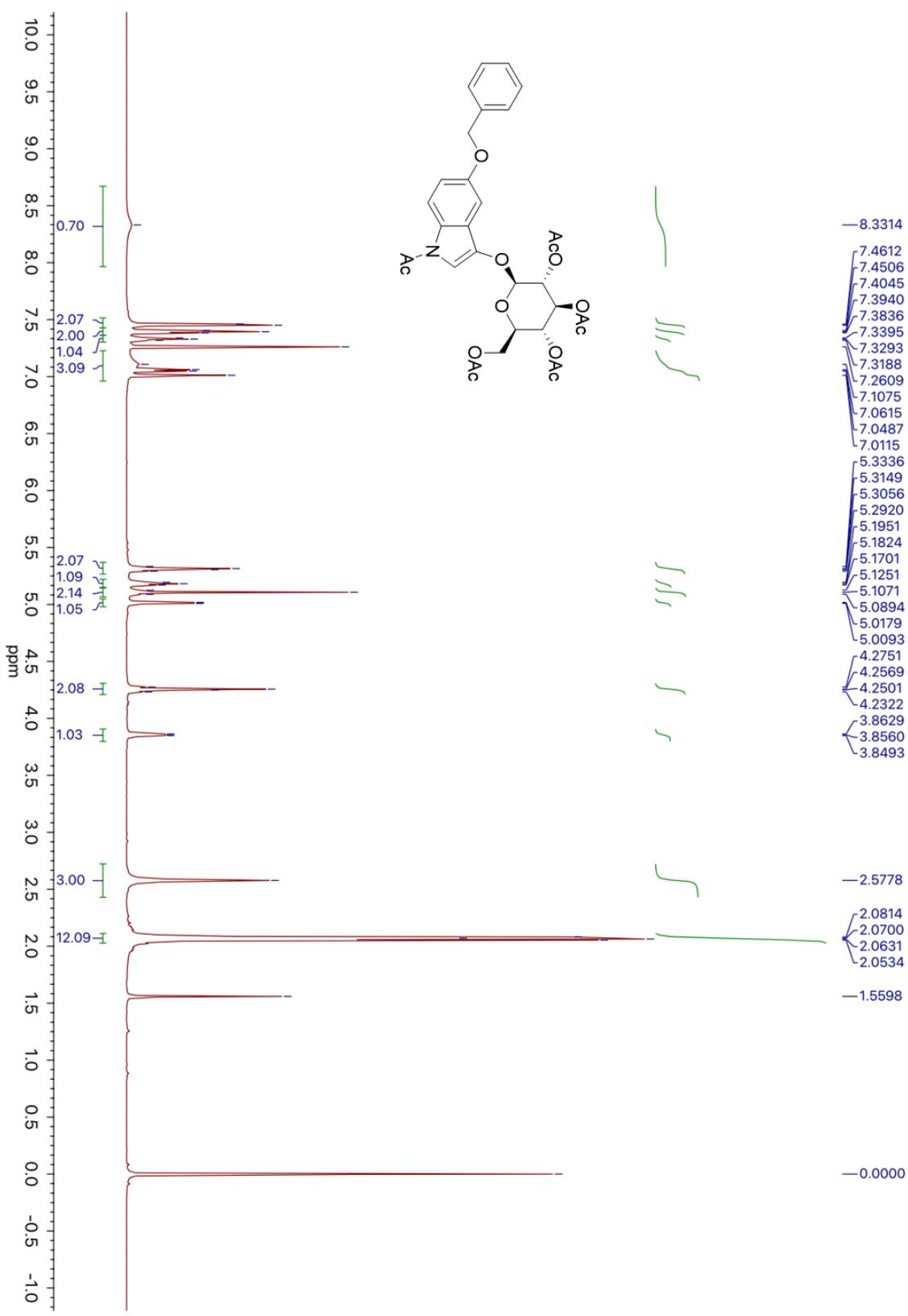
**3**,  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



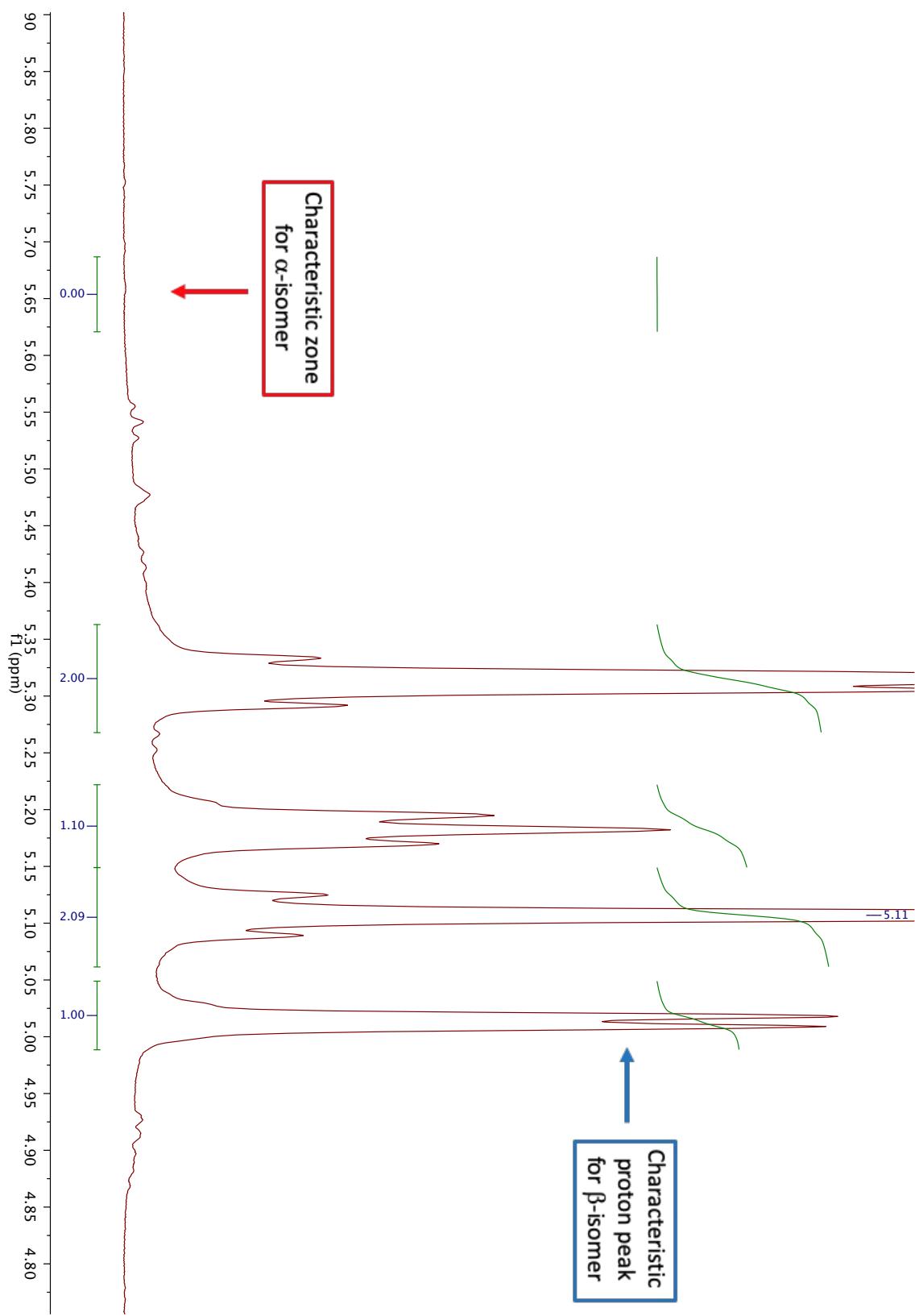
**3,  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )**



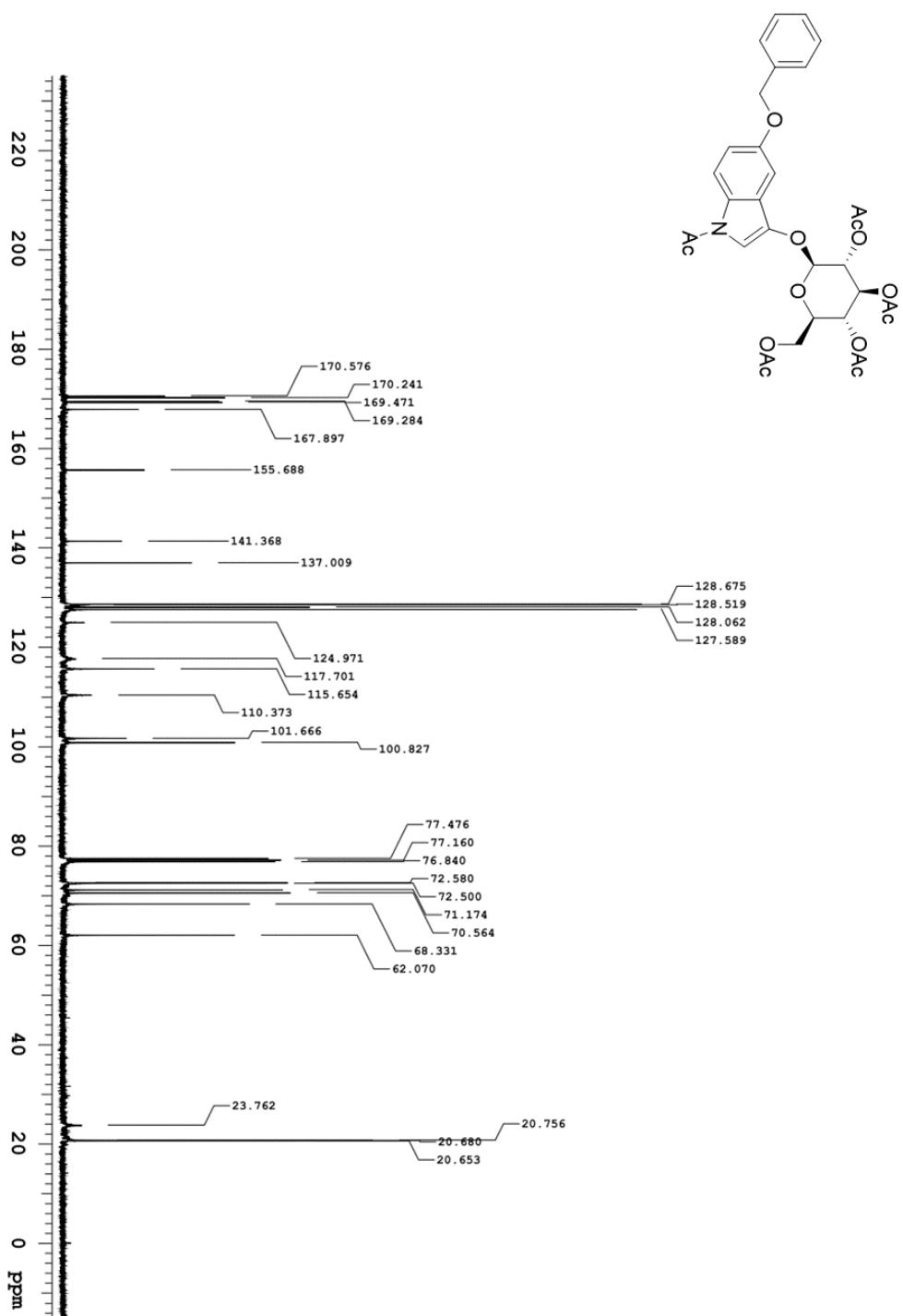
**6- $\beta$ ,  $^1\text{H}$  NMR (700 MHz,  $\text{CDCl}_3$ )**



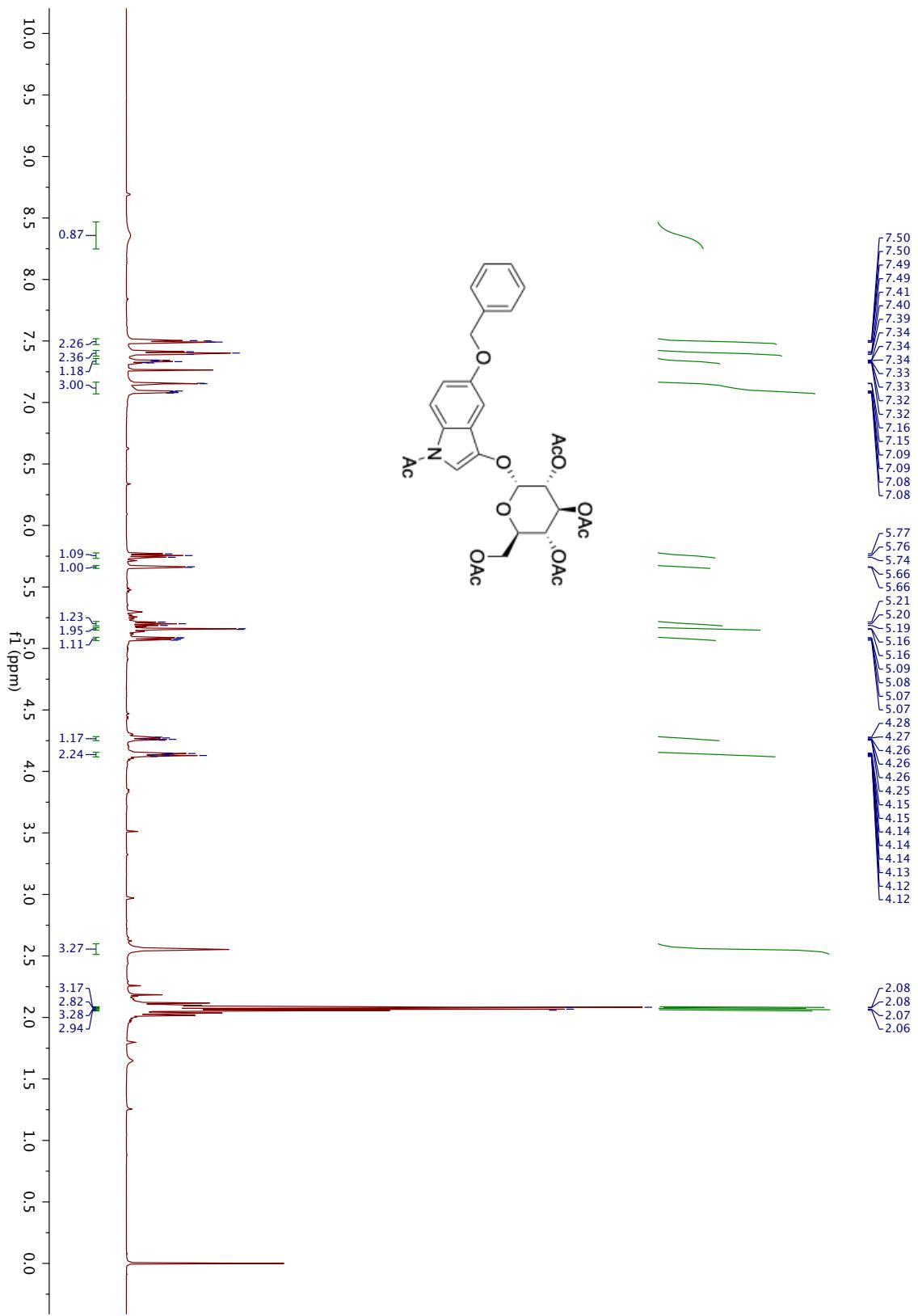
**6- $\beta$ ,  $^1\text{H}$  NMR (700 MHz,  $\text{CDCl}_3$ ), zoomed-in version**



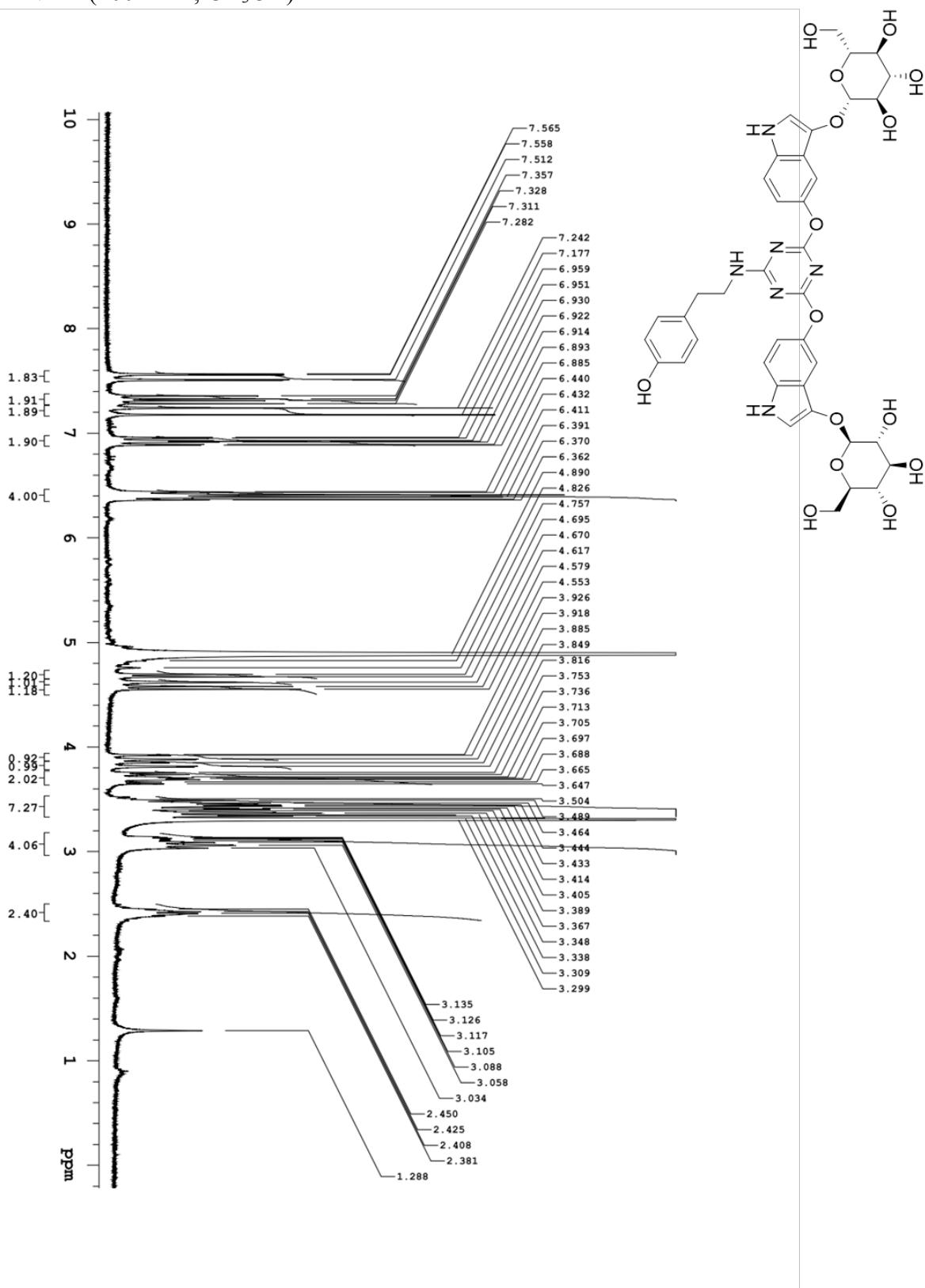
**6- $\beta$ ,  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )**



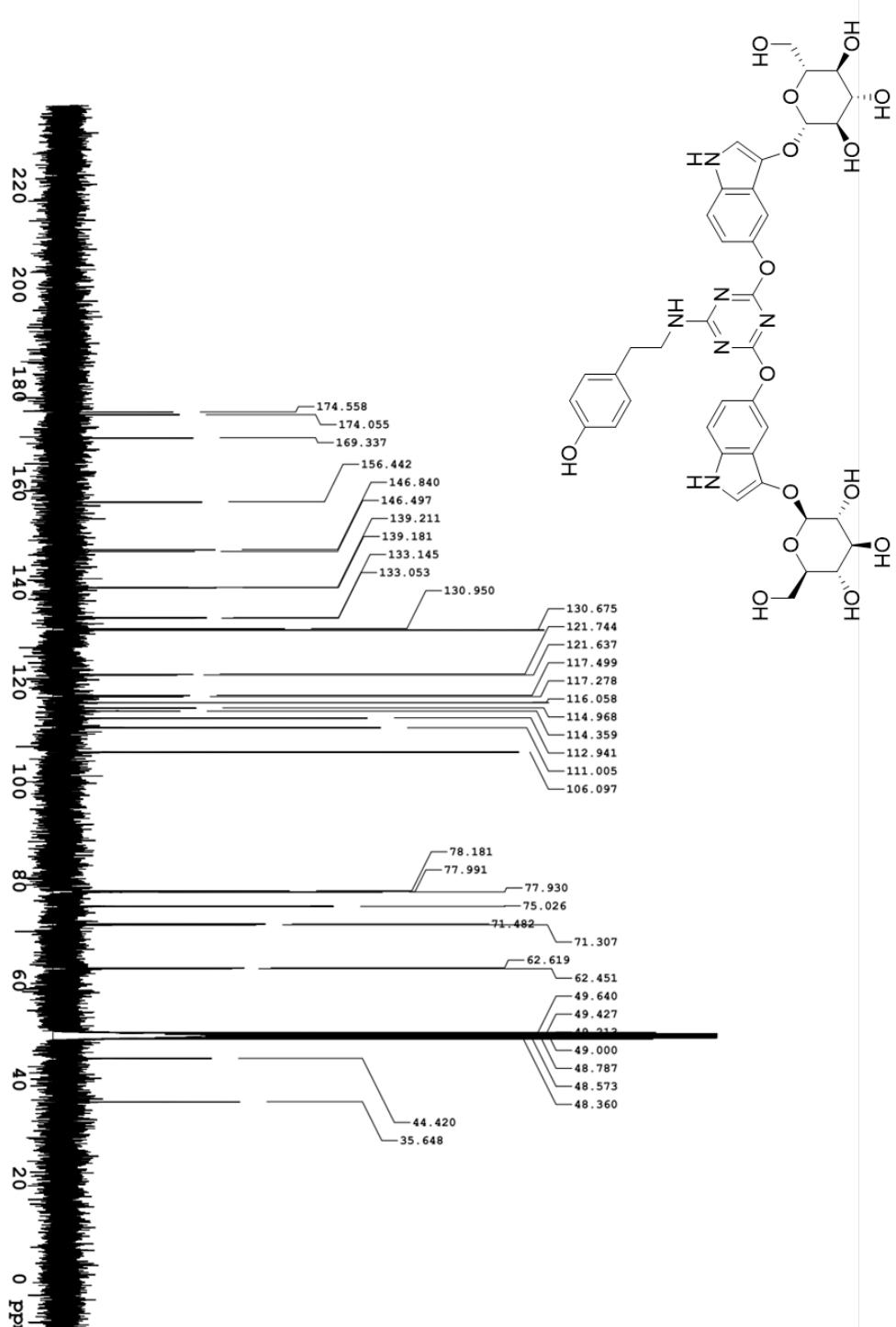
**6- $\alpha$ ,  $^1\text{H}$  NMR (700 MHz,  $\text{CDCl}_3$ )**



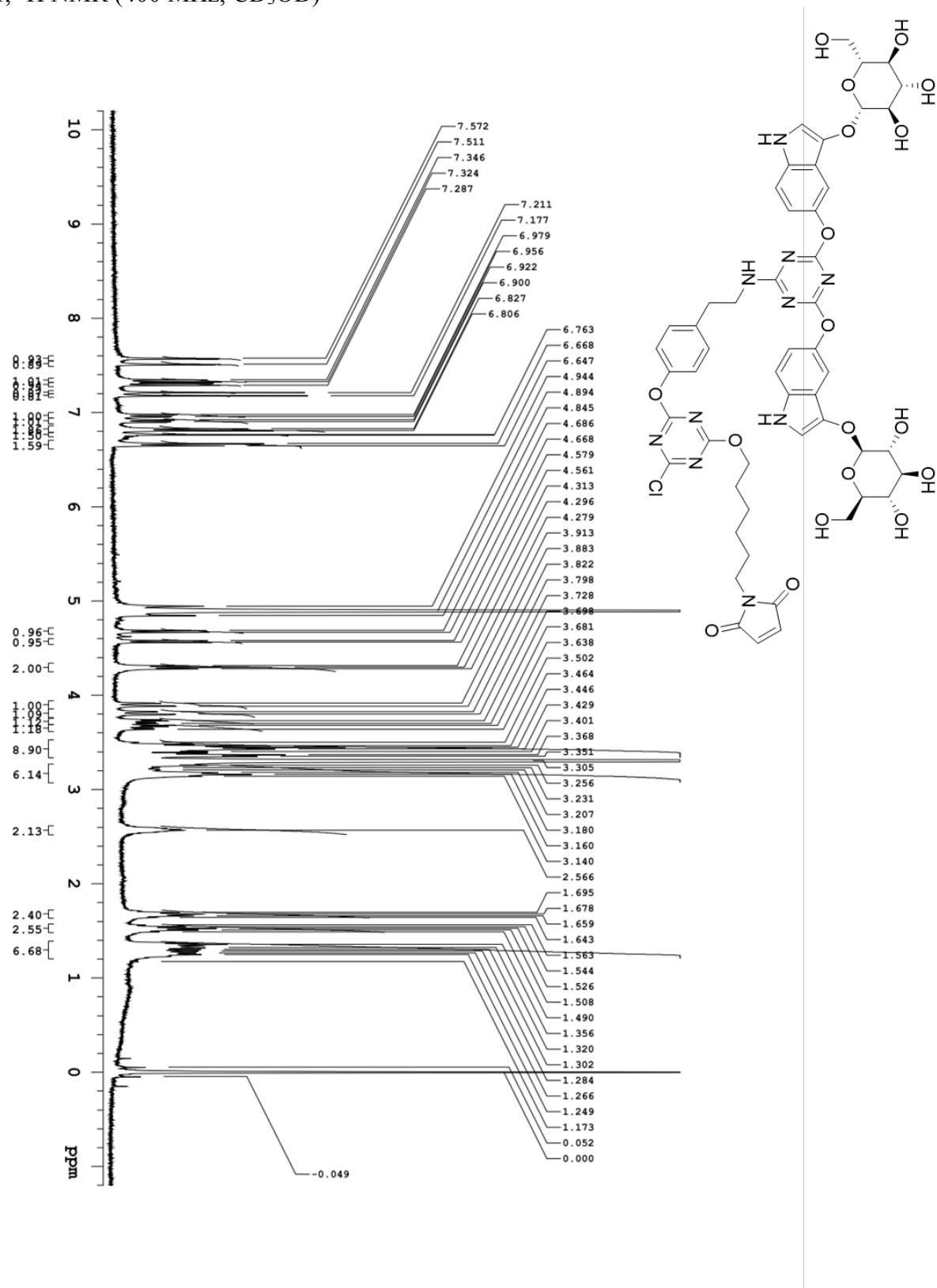
**9,  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ )**



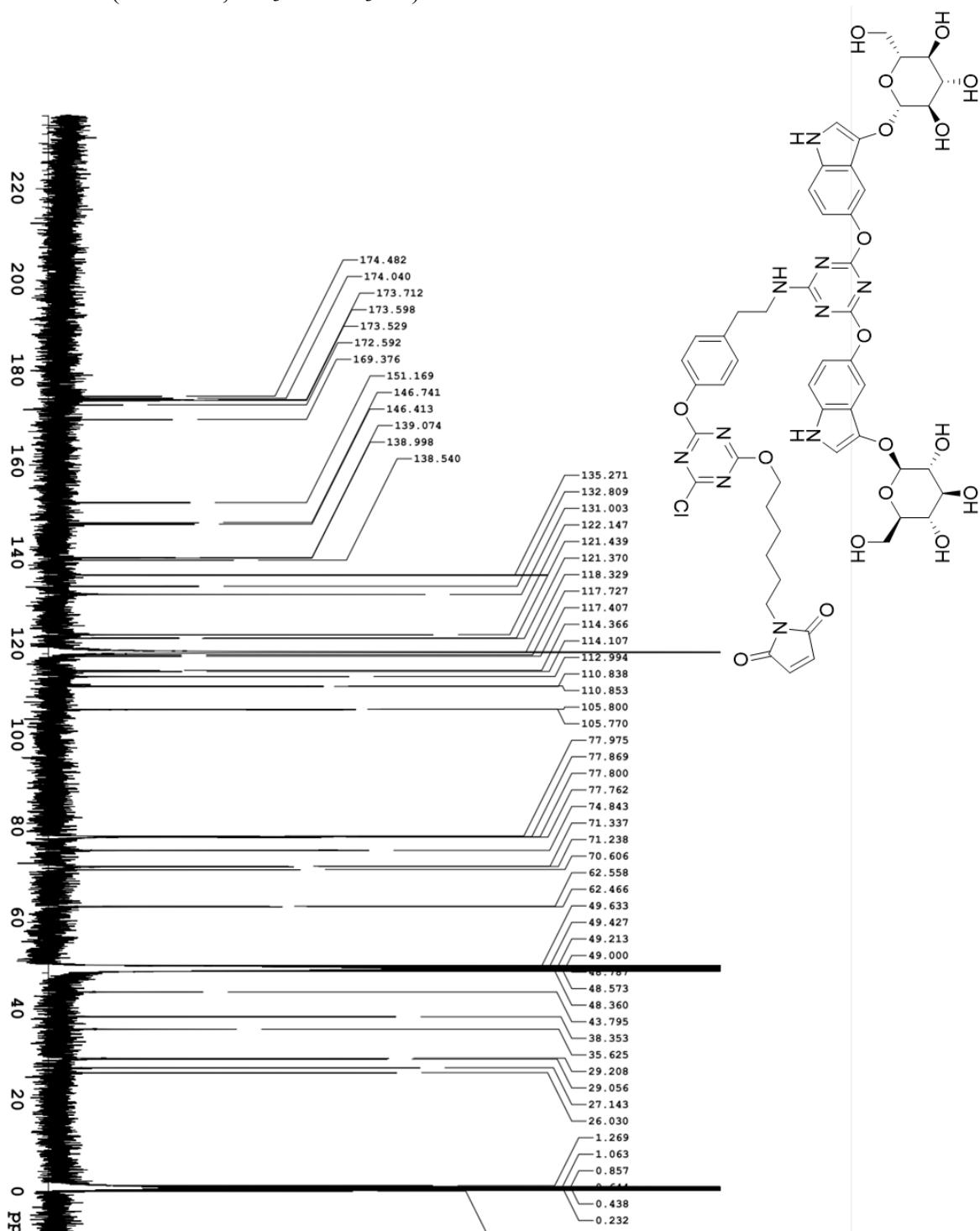
**9,  $^{13}\text{C}$  NMR (100 MHz,  $\text{CD}_3\text{OD}$ )**



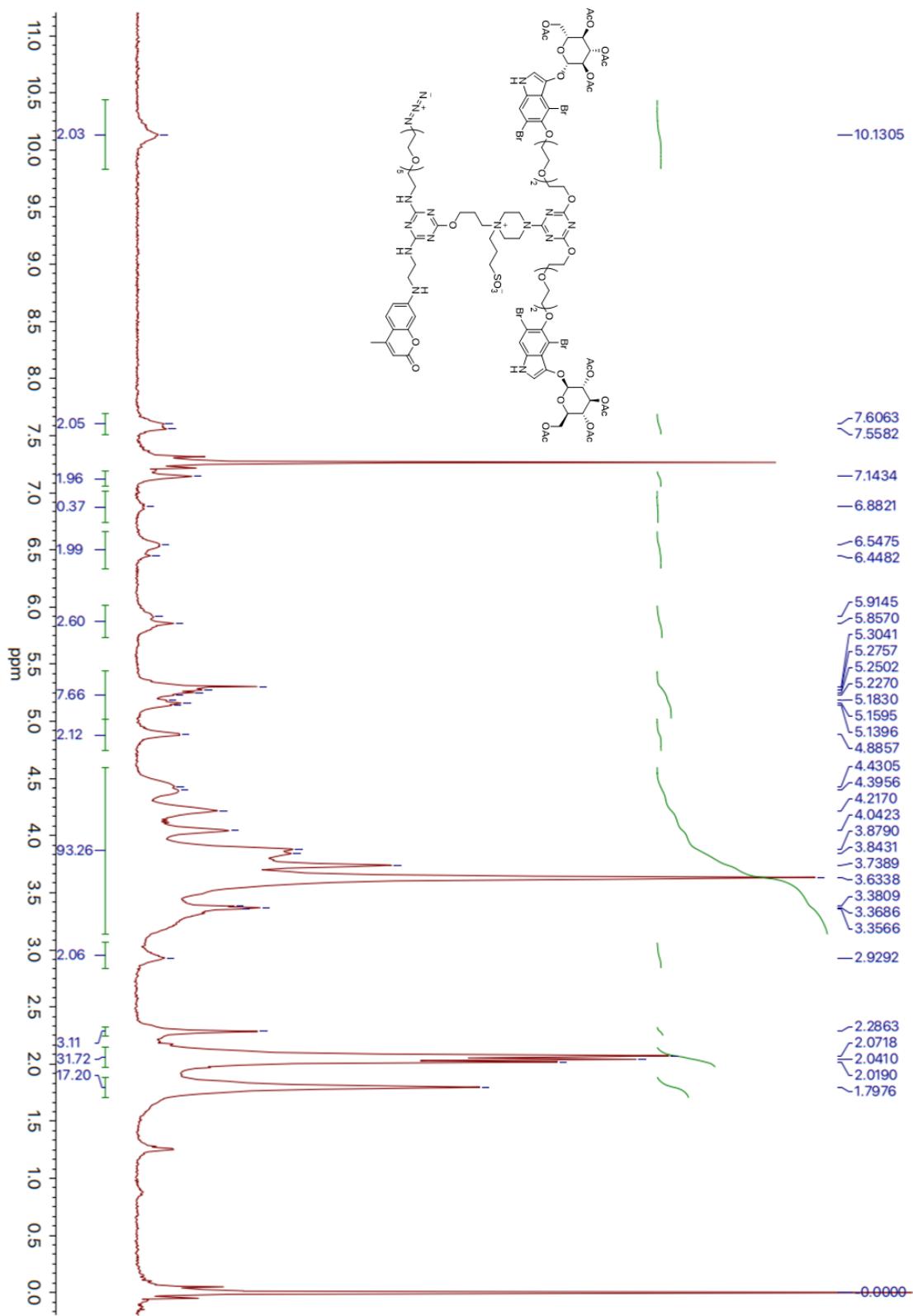
**11,  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ )**



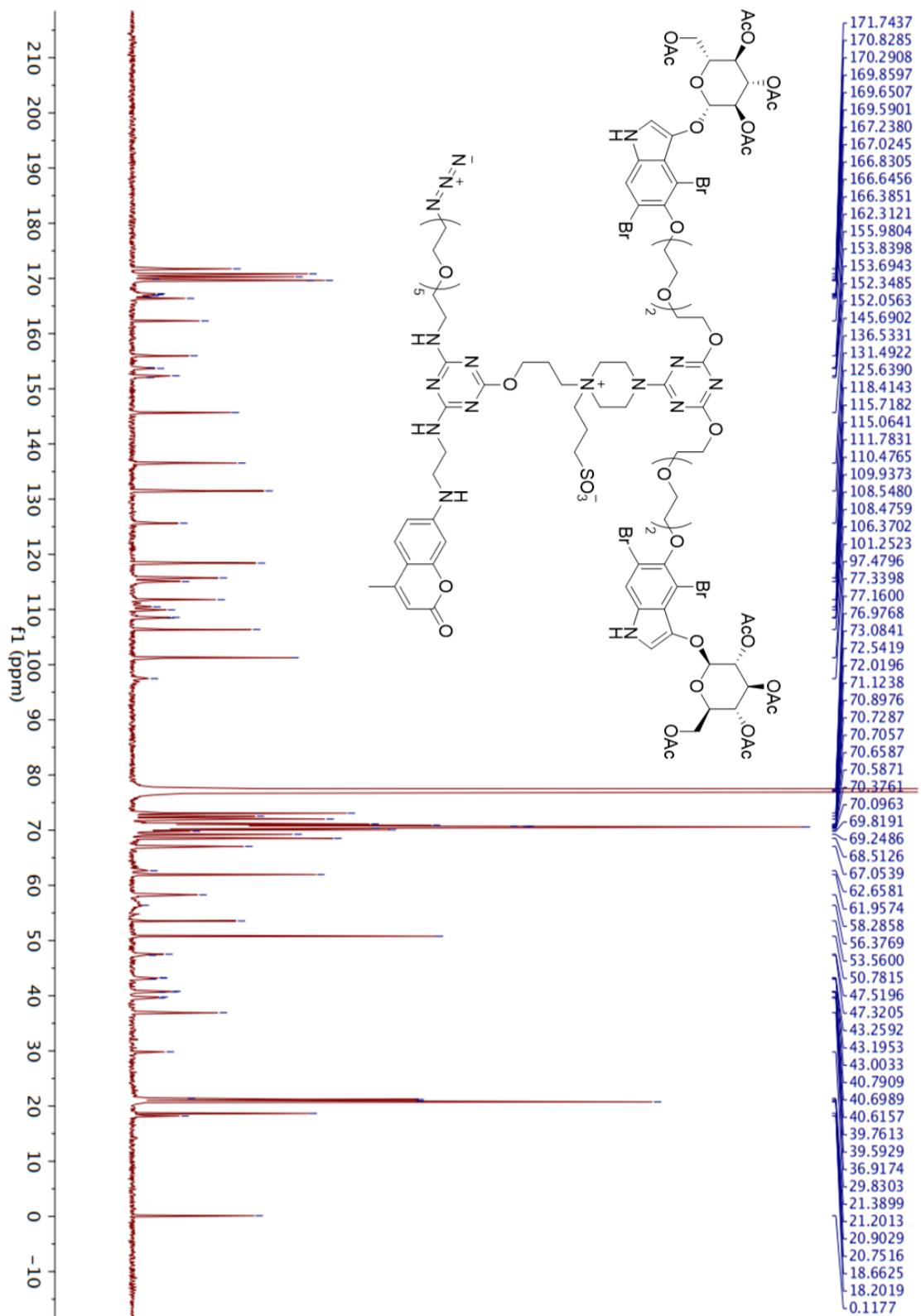
11,  $^1\text{H}$  NMR (100 MHz,  $\text{CD}_3\text{OD}/\text{CD}_3\text{CN}$ )



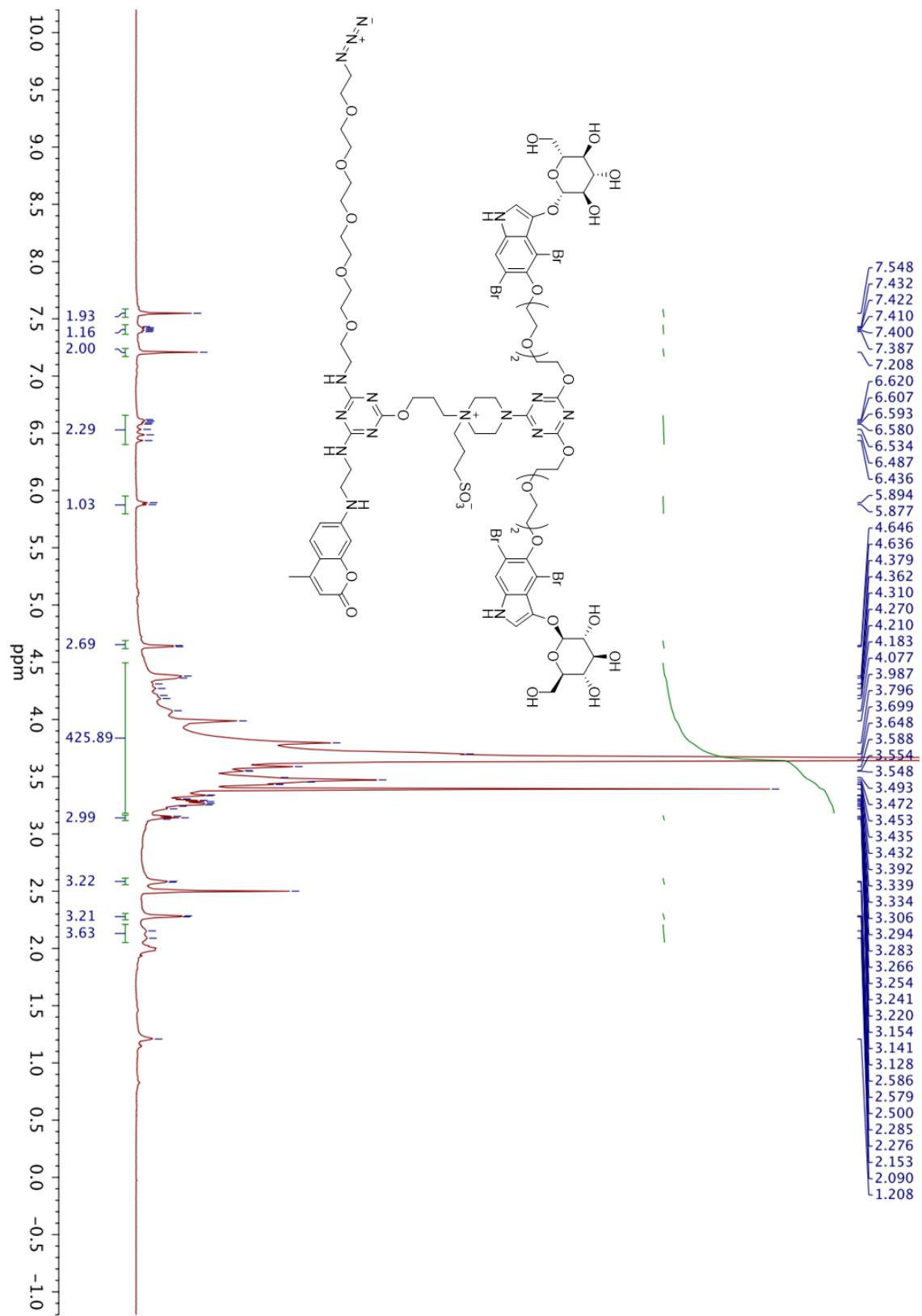
**18,  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )**



**18,  $^{13}\text{C}$  NMR (175 MHz,  $\text{CDCl}_3$ )**



**1**,  $^1\text{H}$  NMR [700 MHz,  $(\text{CD}_3)_2\text{SO}$ ]



**1,  $^{13}\text{C}$  NMR [175 MHz,  $(\text{CD}_3)_2\text{SO}$ ]**

