

## ELECTRONIC SUPPLEMENTARY INFORMATION

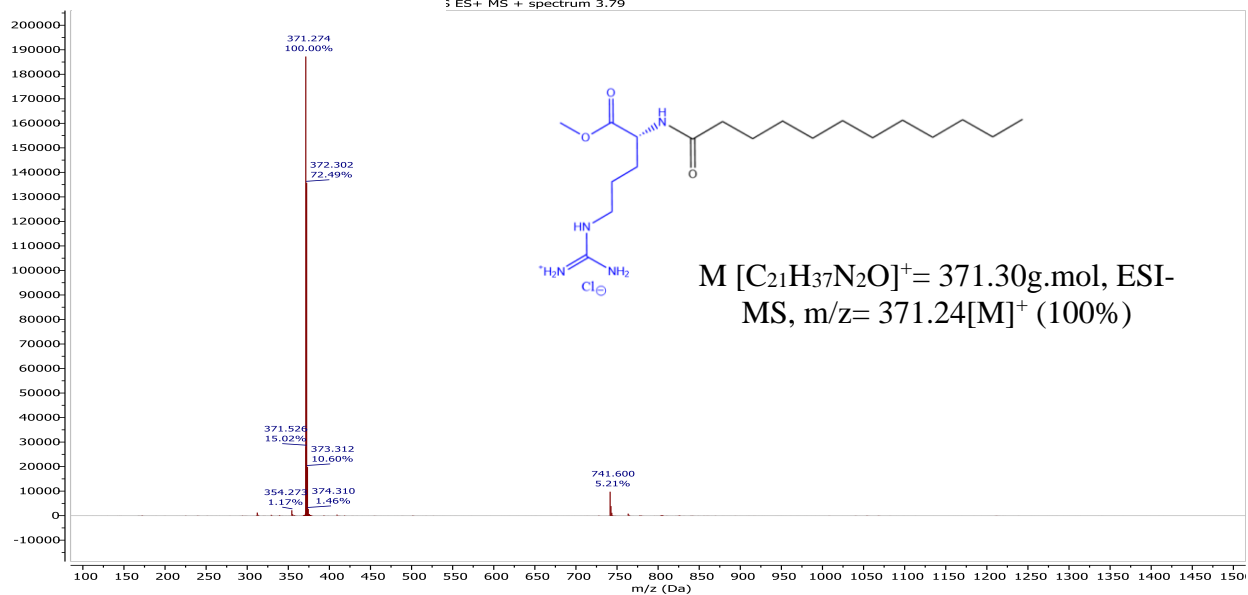
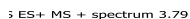
### Cationic Surfactants Based on Arginine-Phenylalanine and Arginine-Tryptophan: Synthesis, Aggregation Behavior, Antimicrobial Activity, and Biodegradation

L.Pérez, M.T. Garcia, A. Pinazo, E. Pérez, Z. Hafidi, E. Bautista

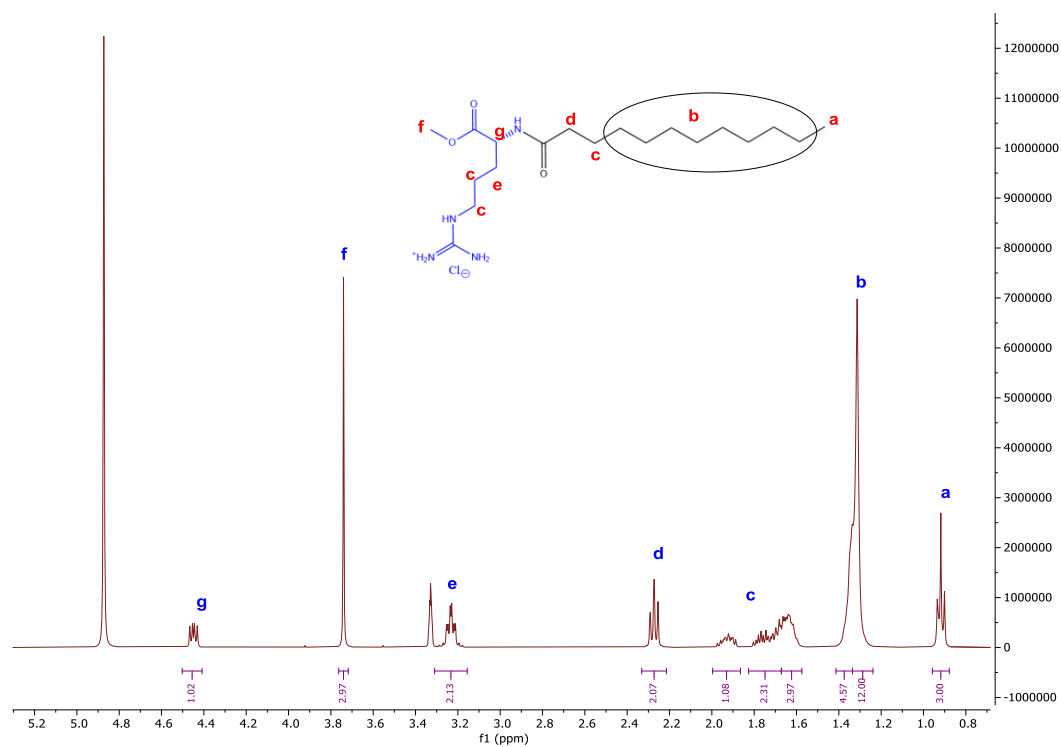
Department of Surfactants and Nanobiotechnology, IQAC-CSIC, c/Jordi Girona, 18-26,  
08034 Barcelona, Spain

#### CONTENT

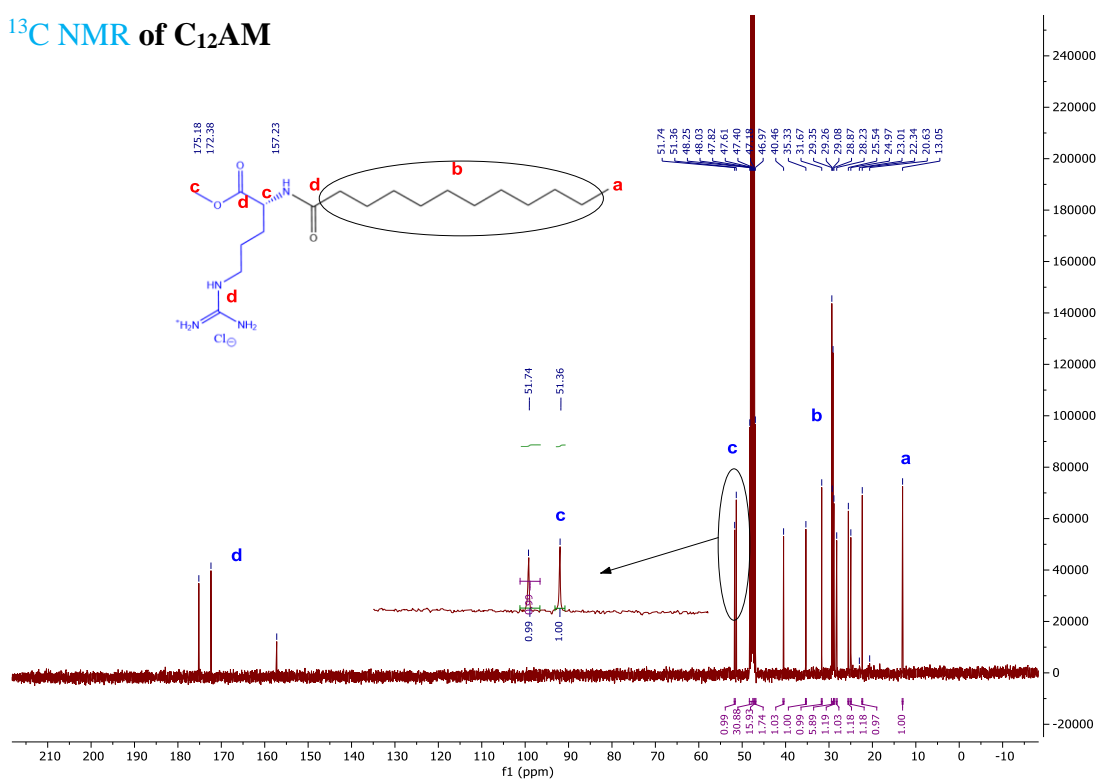
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**Figure S26.** Specific conductivity-concentration curves for the amino acid-based surfactants



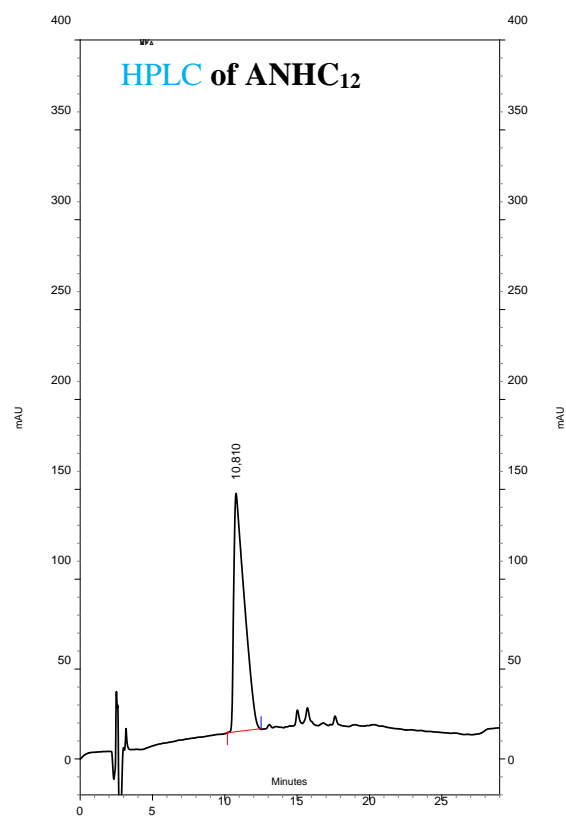
# <sup>1</sup>H NMR of C<sub>12</sub>AM



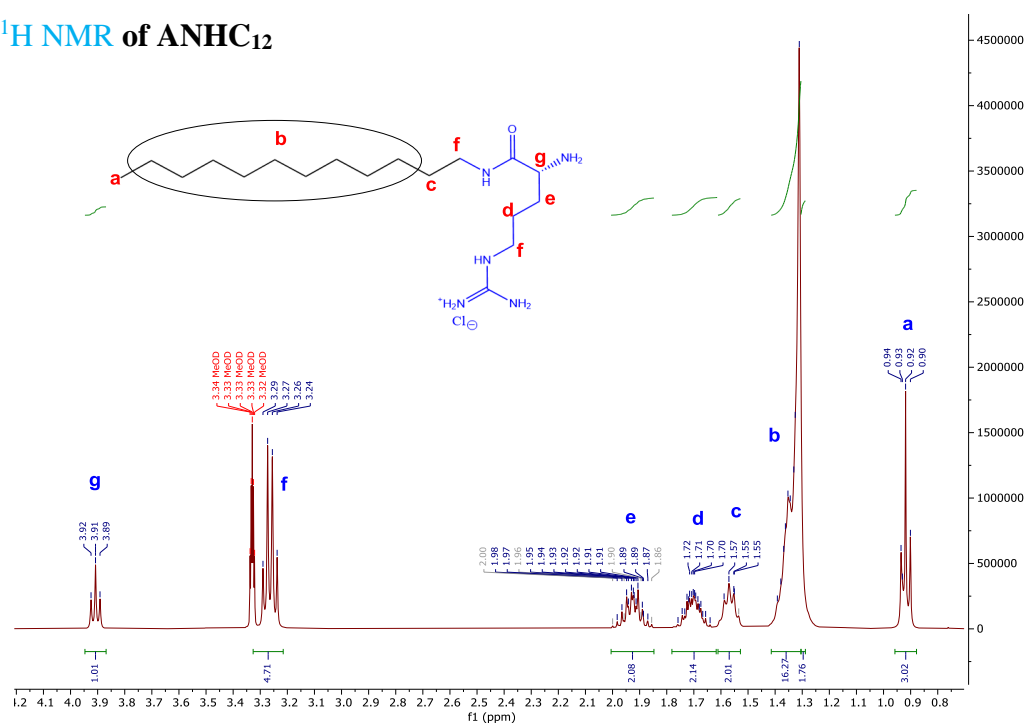
# <sup>13</sup>C NMR of C<sub>12</sub>AM



**Figure S1.** HPLC, ESI-MS, <sup>1</sup>H NMR, and <sup>13</sup>C NMR of C<sub>12</sub>AM

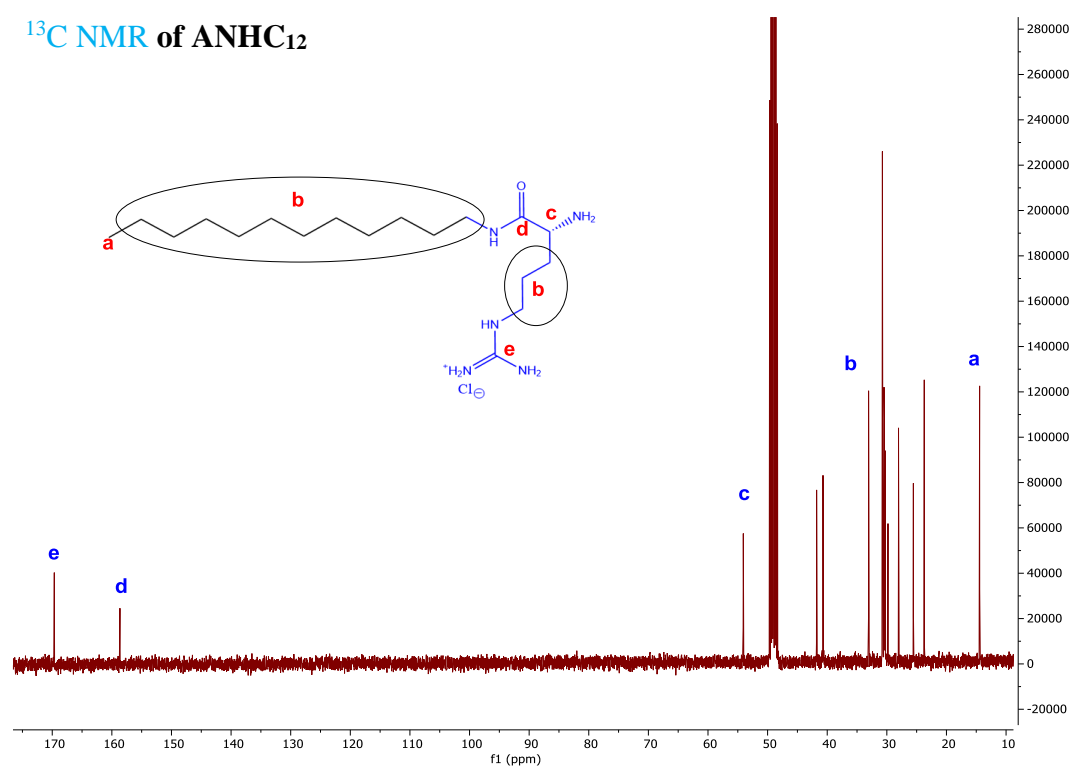


### <sup>1</sup>H NMR of ANHC<sub>12</sub>

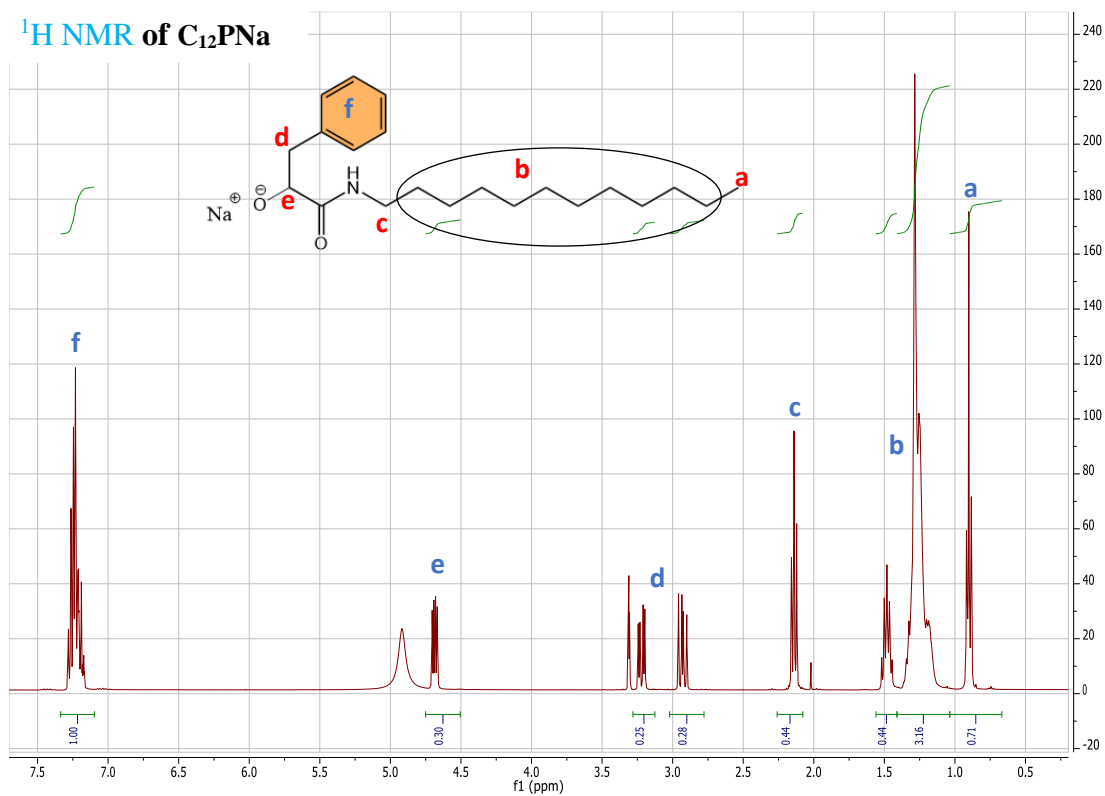
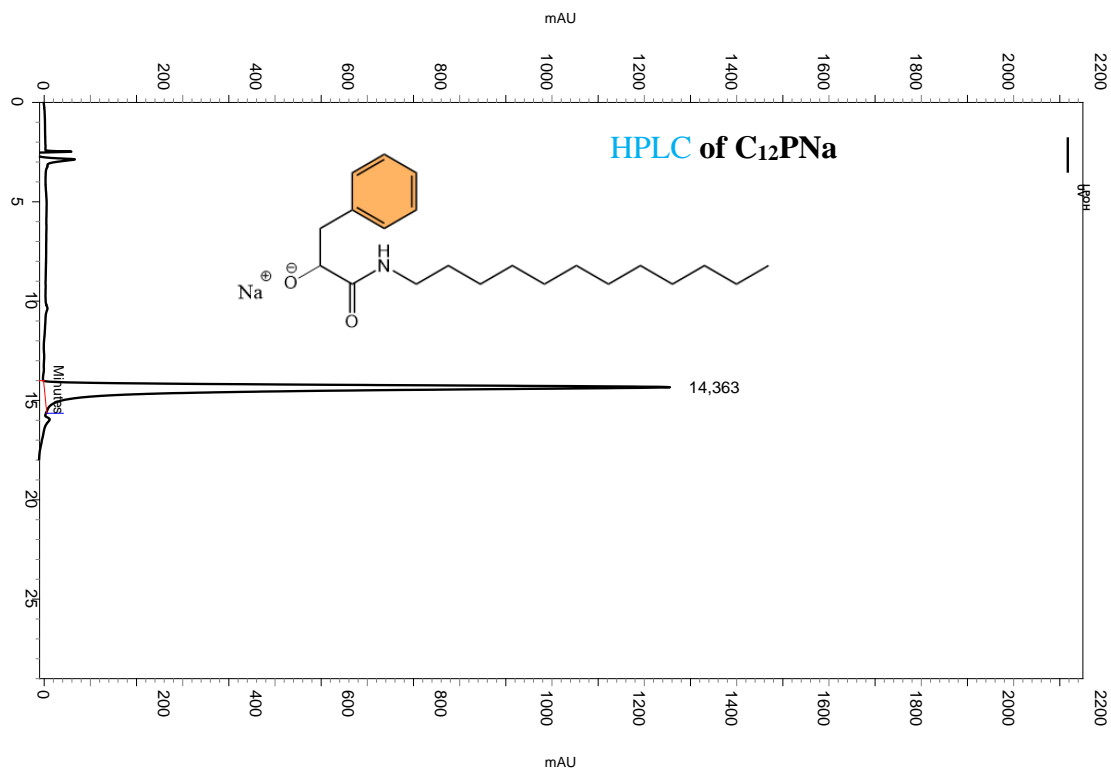


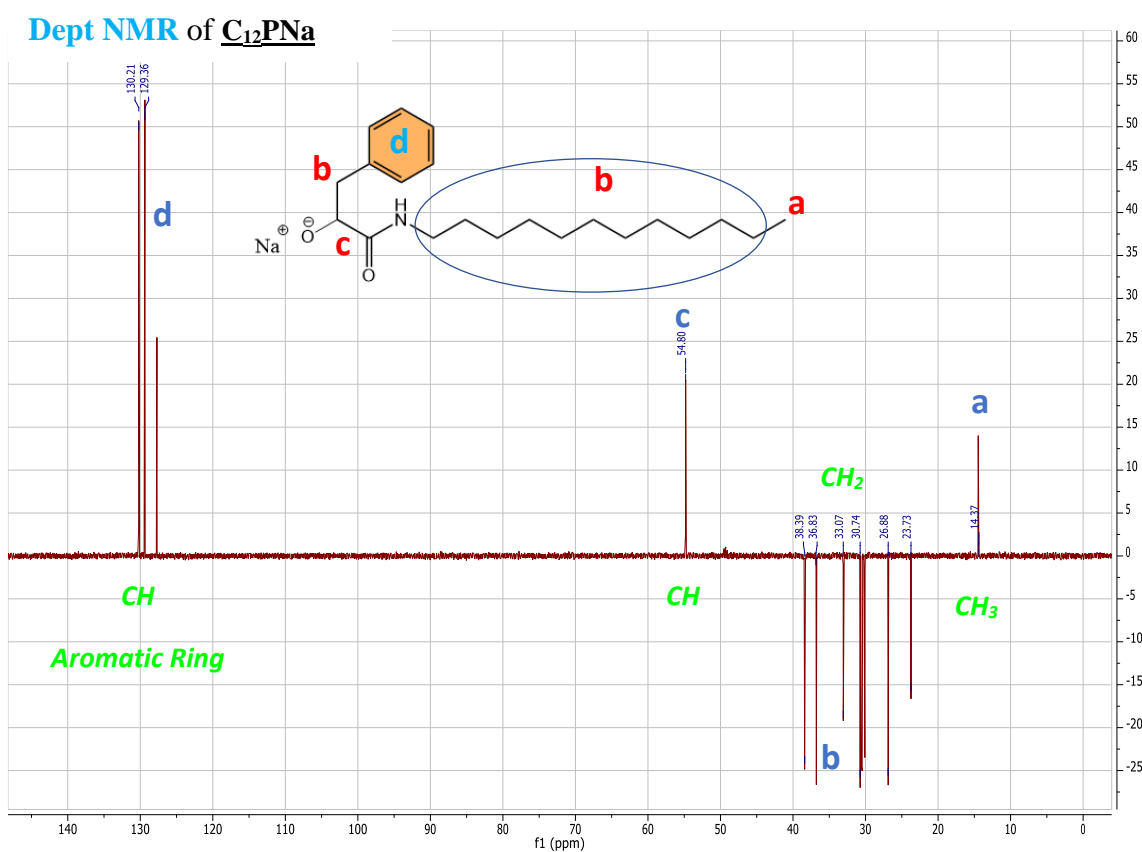
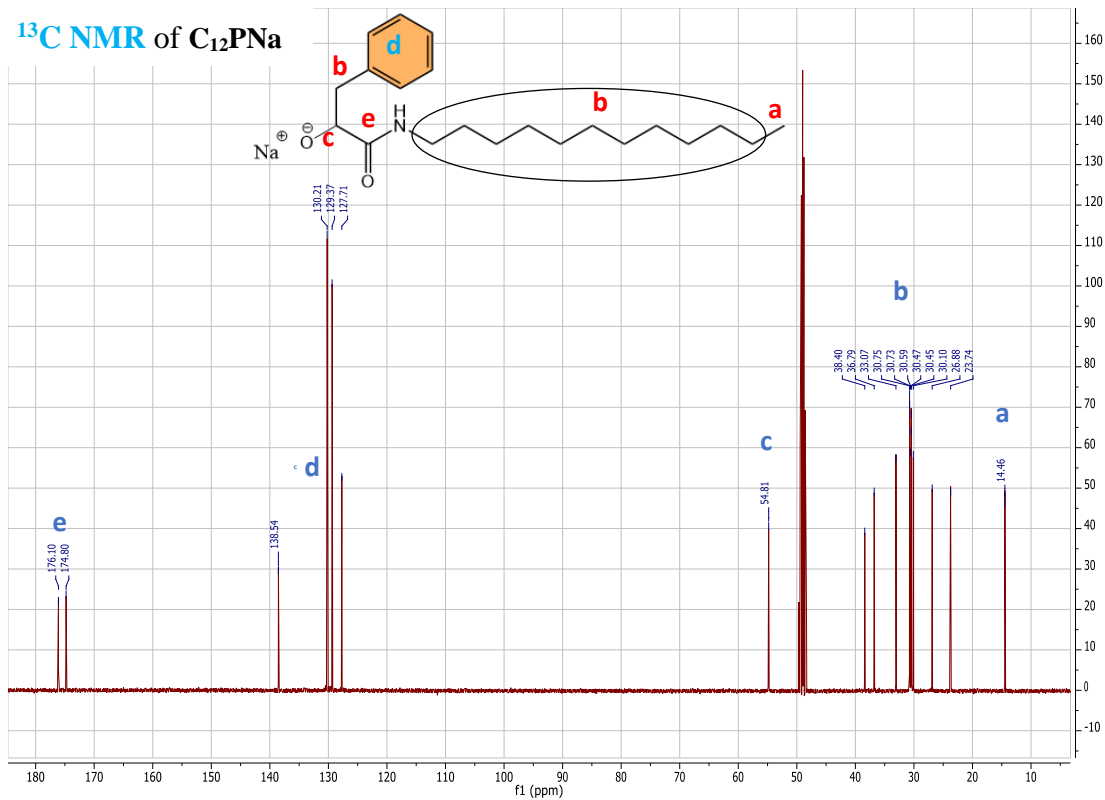


<sup>13</sup>C NMR of ANHC<sub>12</sub>

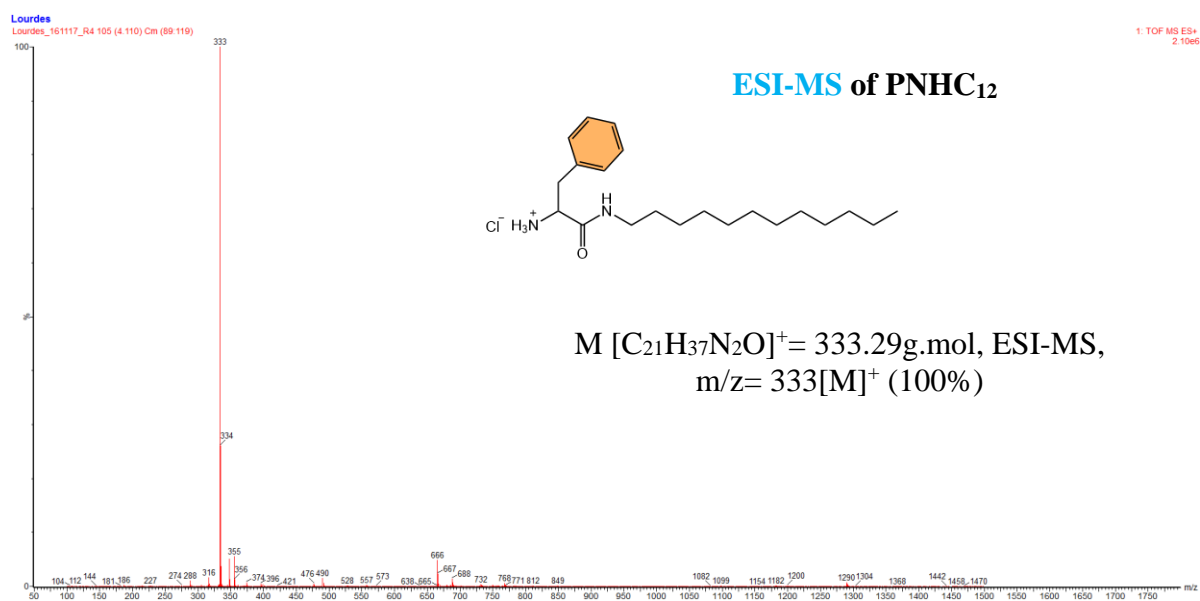
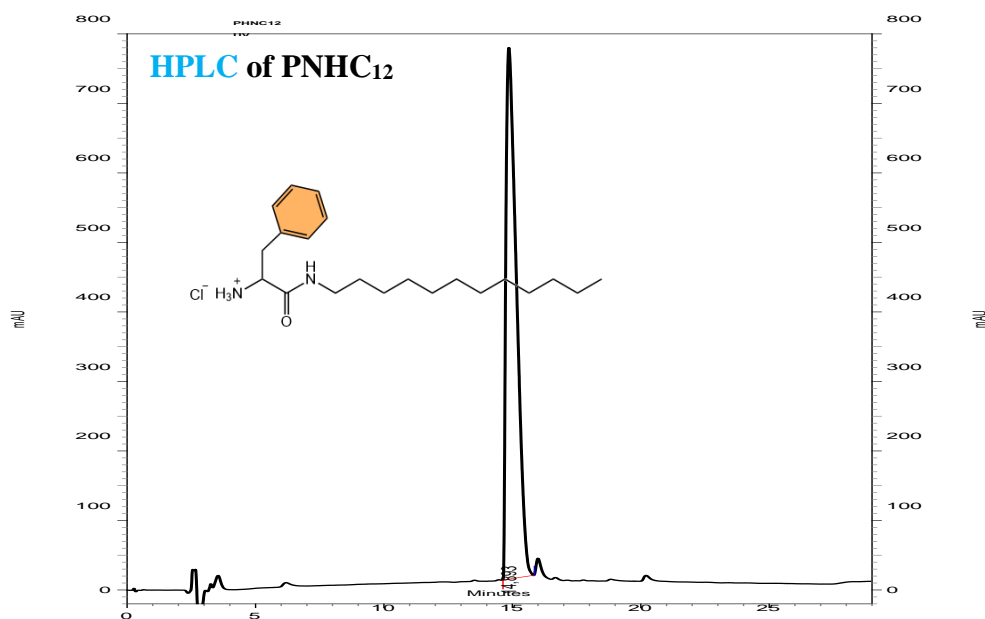


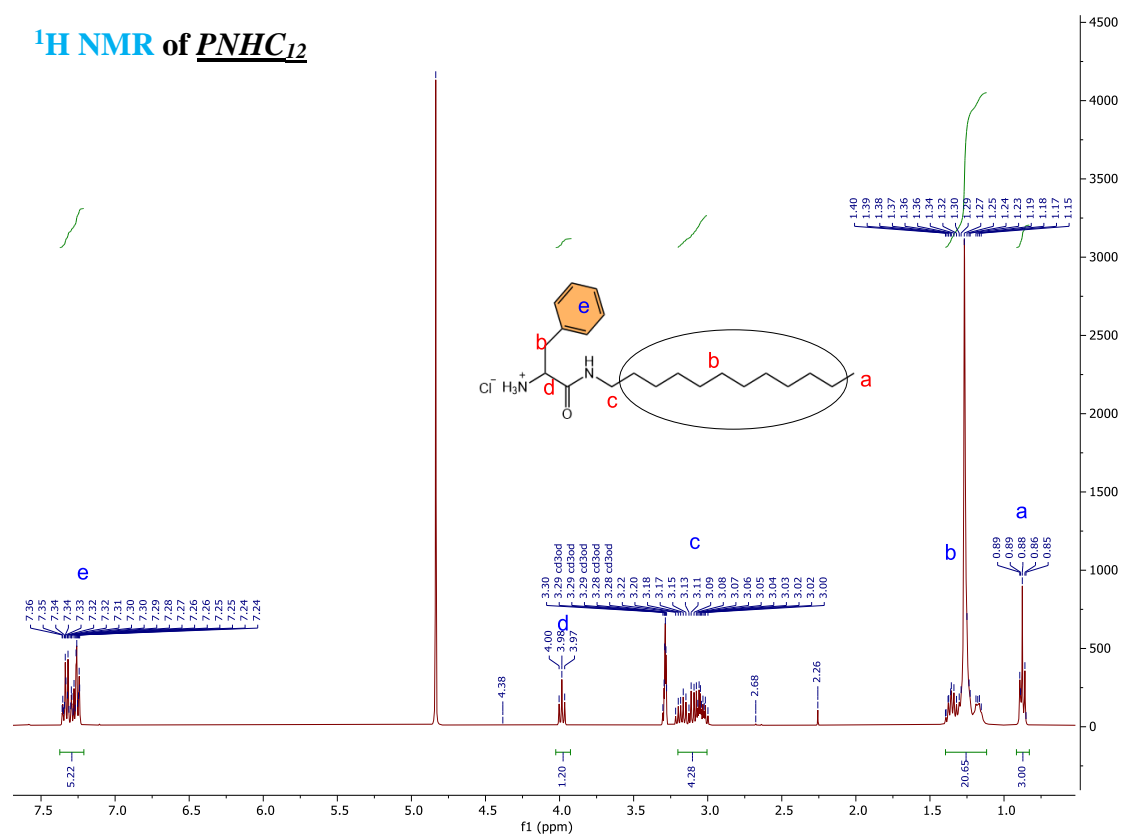
**Figure S2.** HPLC, ESI-MS, <sup>1</sup>H NMR, and <sup>13</sup>C NMR of ANHC<sub>12</sub>



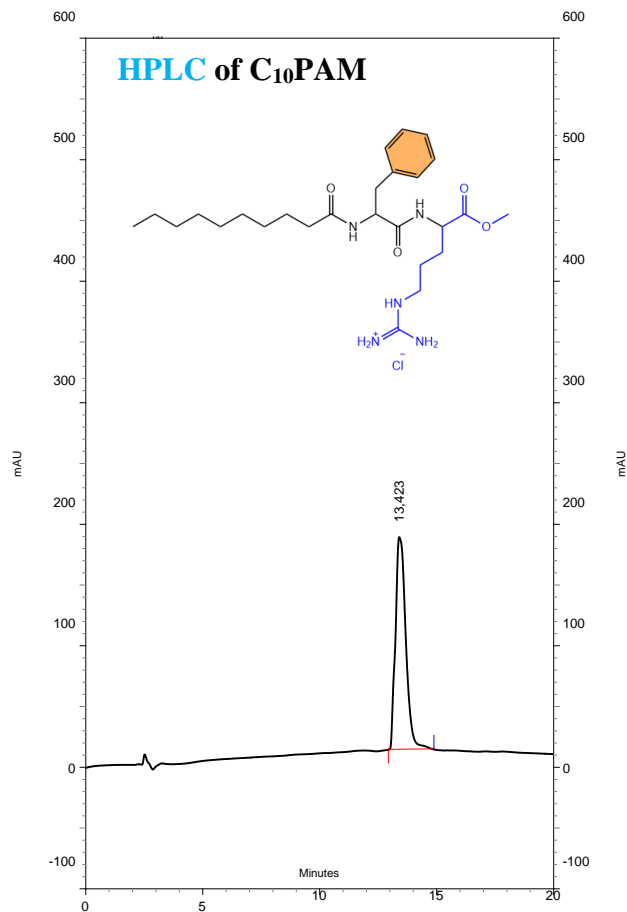


**Figure S3.** HPLC,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and Dept of  $\text{C}_{12}\text{PNa}$

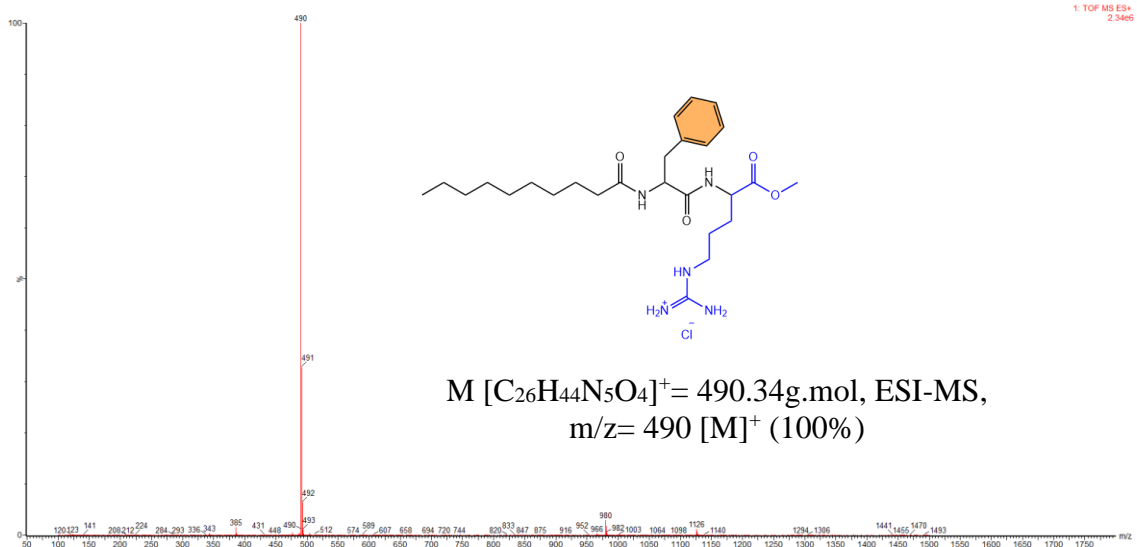




**Figure S4.** HPLC, ESI-MS and  $^1\text{H}$  NMR, of  $\text{PNHC}_{12}$



## ESI-MS of C<sub>10</sub>PAM



**$^1\text{H}$  NMR of  $\text{C}_{10}\text{PAM}$**

The chemical structure of  $\text{C}_{10}\text{PAM}$  is shown with protons labeled a through g. The  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{D}_2\text{O}$ ) displays the following peaks and integrations:

- g**: Aromatic protons (7.3-7.5 ppm), integration 4.93.
- f**: Amide protons (4.4-4.7 ppm), integration 1.00.
- e**: Methyl protons of the amide group (~3.3 ppm), integration 2.79.
- d**: Protons of the guanidinium group (2.8-3.2 ppm), integration 3.05.
- c**: Methylene protons adjacent to the amide group (2.1-2.3 ppm), integration 2.05.
- b**: Methylene protons of the  $\text{C}_{10}$  chain (1.2-1.5 ppm), integration 18.71.
- a**: Methyl protons of the  $\text{C}_{10}$  chain (~0.9 ppm), integration 2.92.

**$^{13}\text{C}$  NMR of C<sub>10</sub>PAM**

The figure displays the  $^{13}\text{C}$  NMR spectrum of C<sub>10</sub>PAM, showing the chemical structure and the corresponding spectrum with peak assignments.

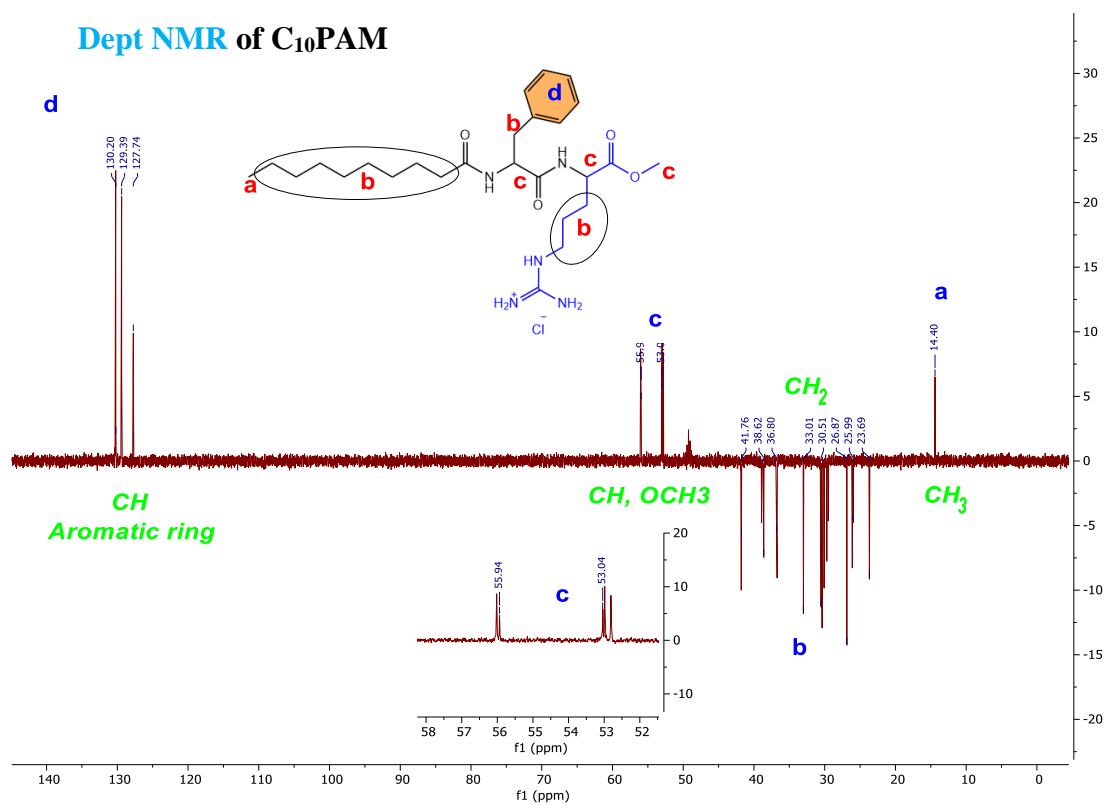
**Chemical Structure:** The structure shows a C<sub>10</sub>PAM molecule with a long alkyl chain (labeled 'a'), a benzene ring (labeled 'd'), and a quaternary carbon (labeled 'b'). The amide group is labeled 'c', and the carbonyl carbon is labeled 'e'. The structure also includes a guanidinium cation (labeled 'e') and a chloride anion (Cl<sup>-</sup>).

**$^{13}\text{C}$  NMR Spectrum:** The spectrum shows peaks corresponding to the labeled carbons. The x-axis represents the chemical shift in ppm (f1), ranging from 180 to 10. The y-axis represents the intensity in arbitrary units (f2), ranging from -20 to 300.

**Peak Assignments (ppm):**

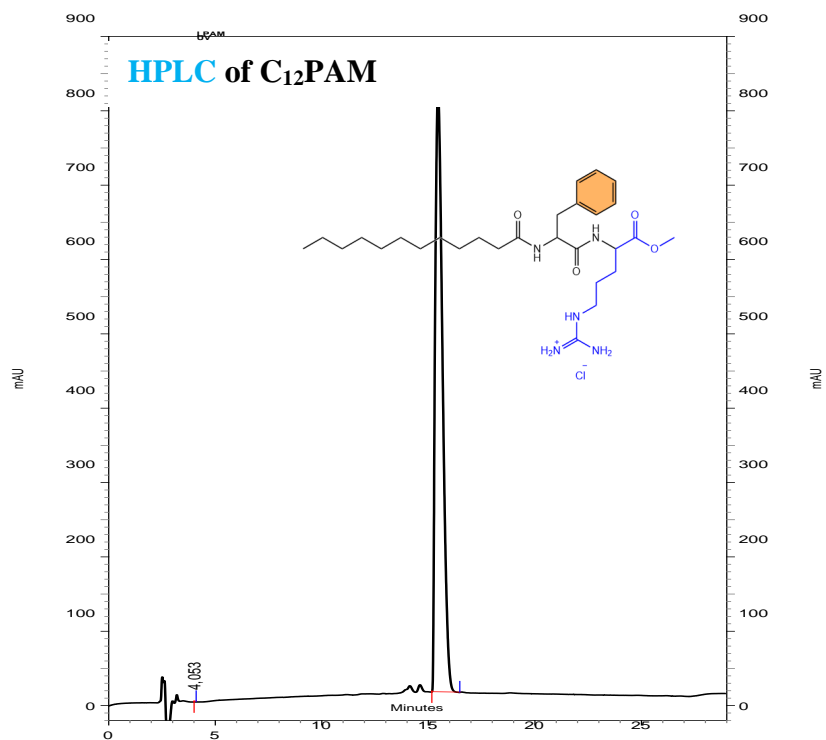
- a:** 14.43
- b:** 36.76, 33.04, 30.94, 30.54, 30.45, 30.40, 30.13, 29.74, 26.90, 26.13, 23.71
- c:** 52.83, 52.84, 53.02, 53.07
- d:** 130.31, 130.26, 129.76, 129.42, 127.80, 127.77
- e:** 176.33, 174.14, 173.31, 158.64

An inset spectrum shows the region from 52 to 56 ppm, highlighting the peaks for the amide group (labeled 'c').

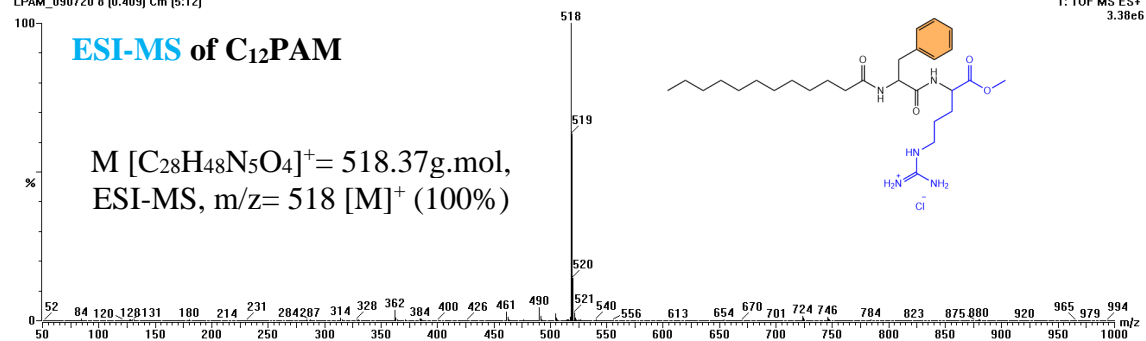


**Figure S5.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of C<sub>10</sub>PAM

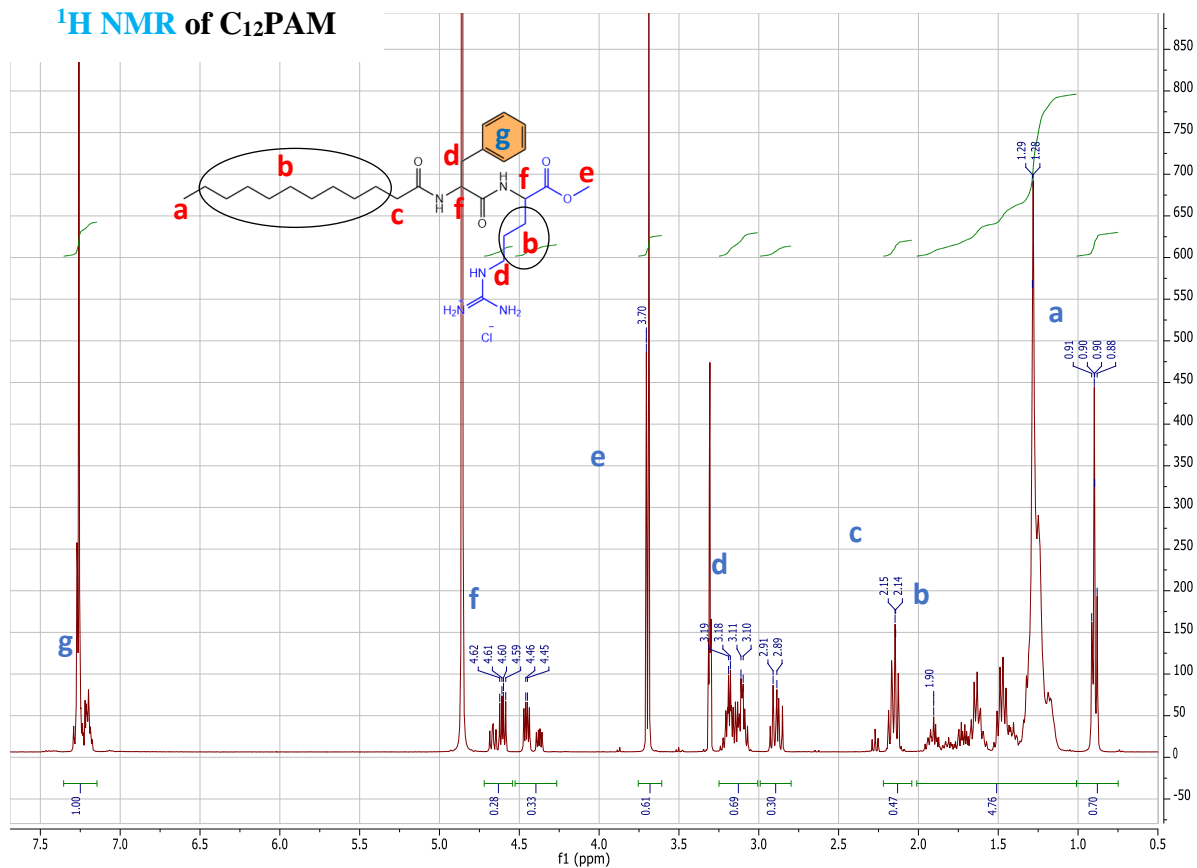




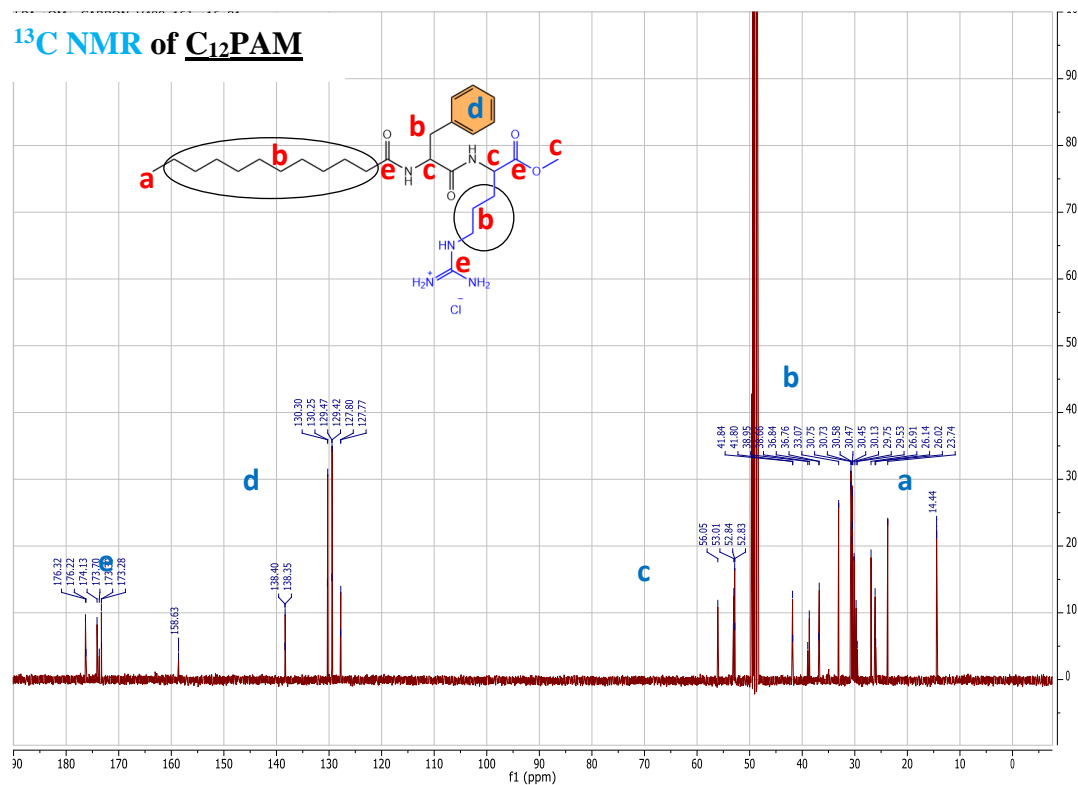
Lourdes/TLIB  
LPAM\_090720 8 [0.409] Cm [5:12]

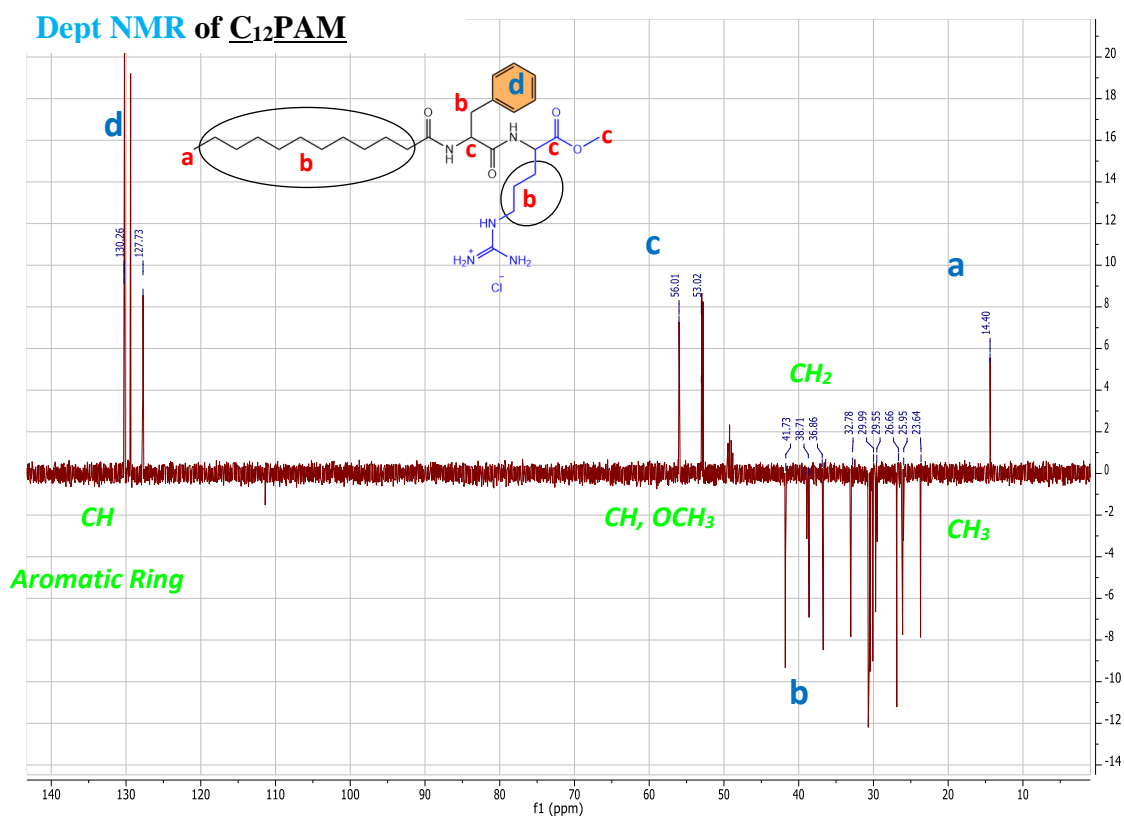


# <sup>1</sup>H NMR of C<sub>12</sub>PAM

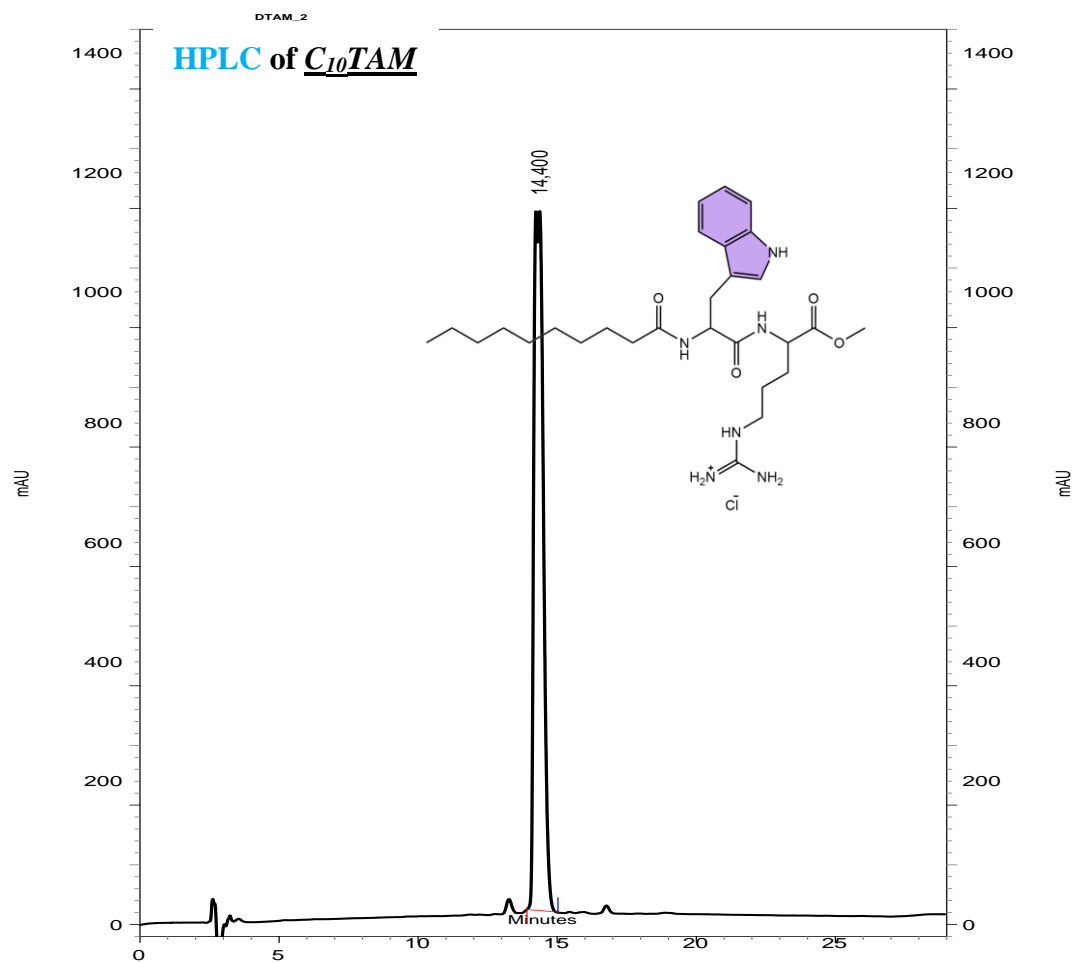


# <sup>13</sup>C NMR of C<sub>12</sub>PAM

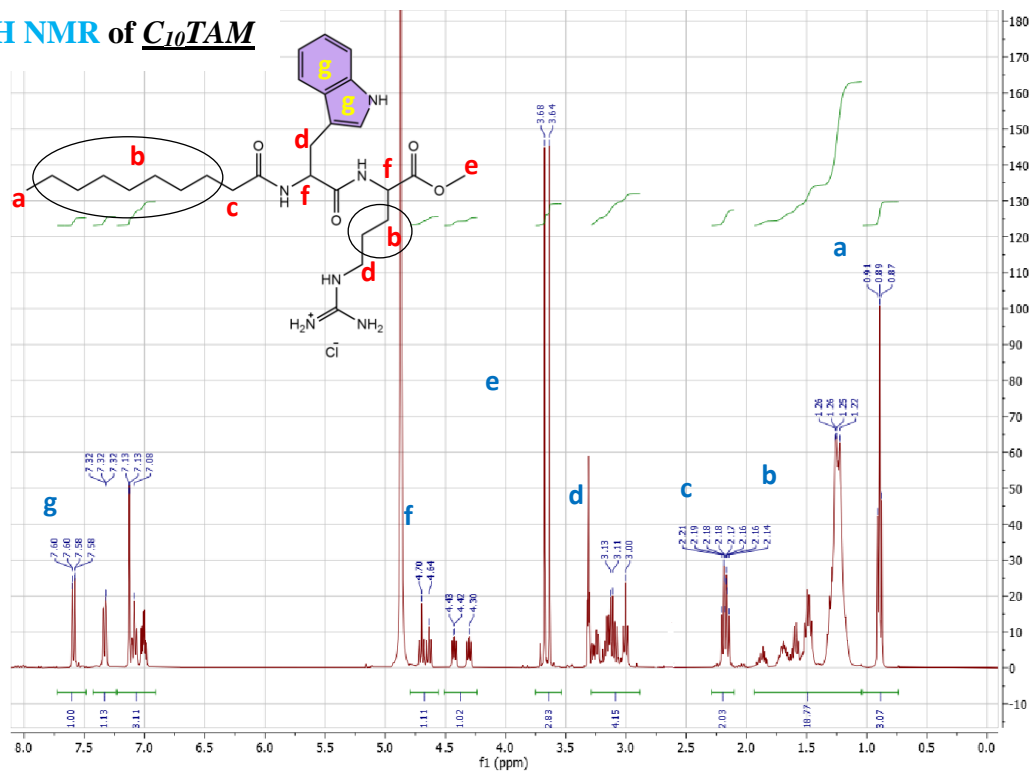




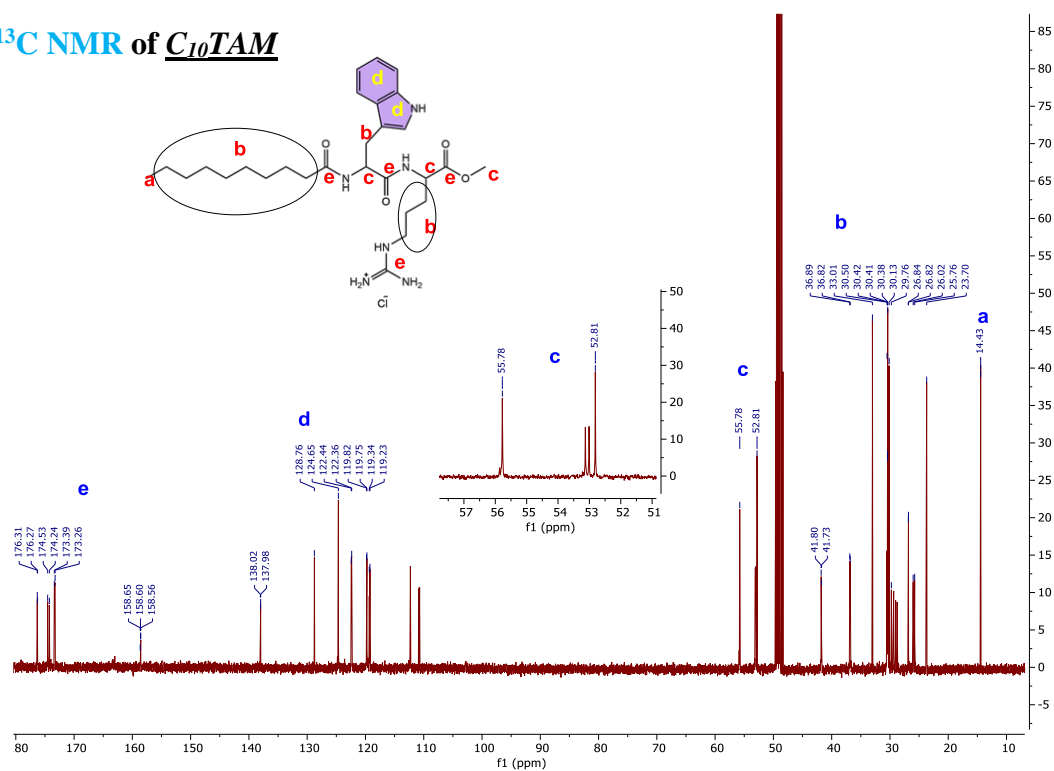
**Figure S6.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of C<sub>12</sub>PAM



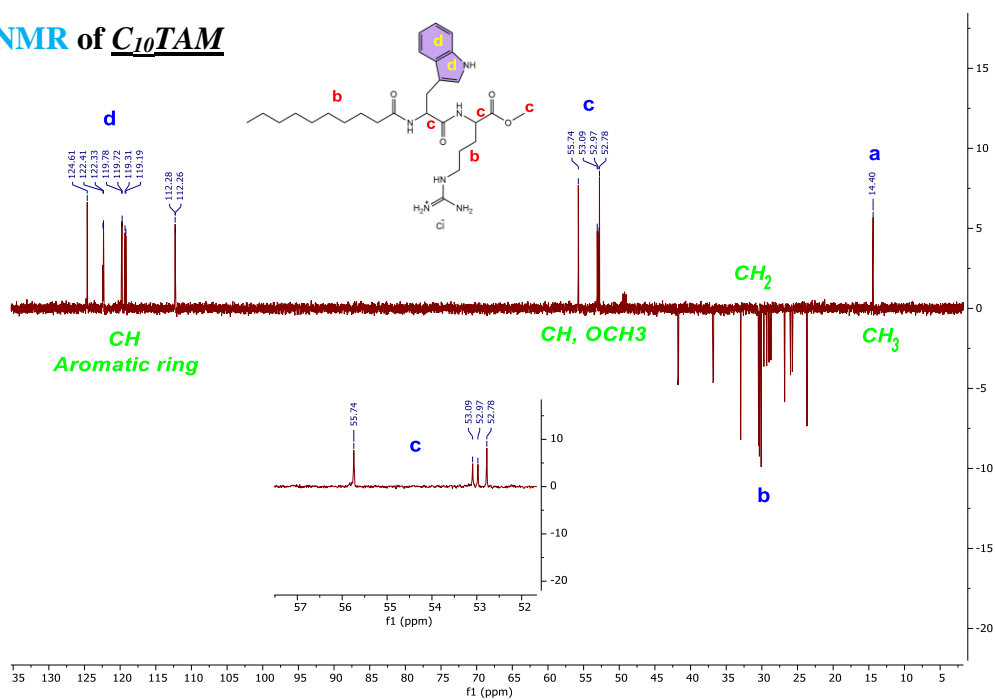
### $^1\text{H}$ NMR of $C_{10}$ TAM



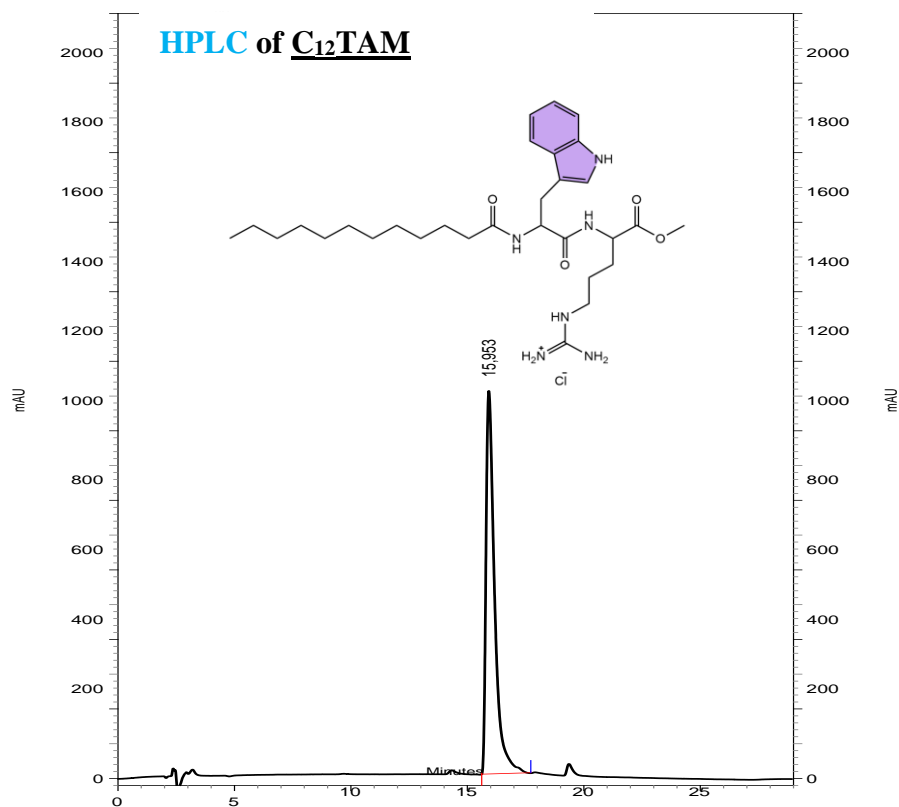
### $^{13}\text{C}$ NMR of $C_{10}\text{TAM}$



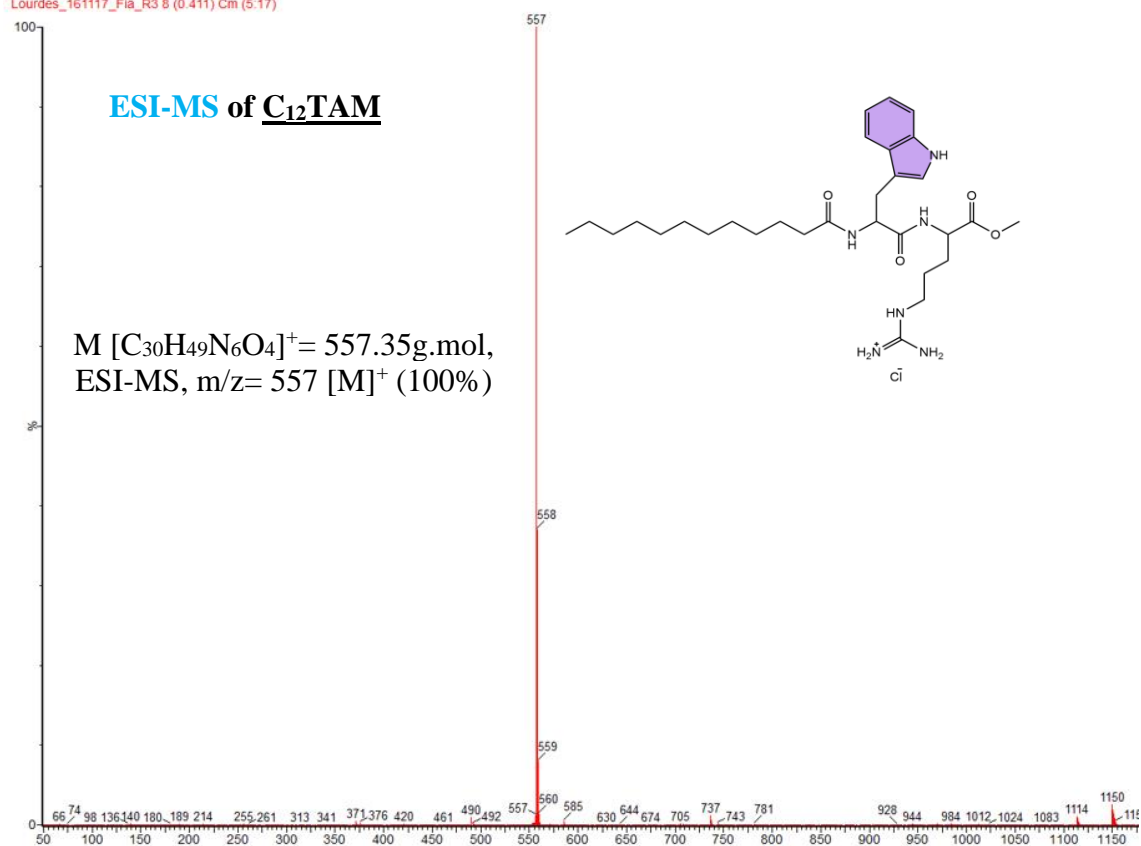
### Dept NMR of $C_{10}\text{TAM}$



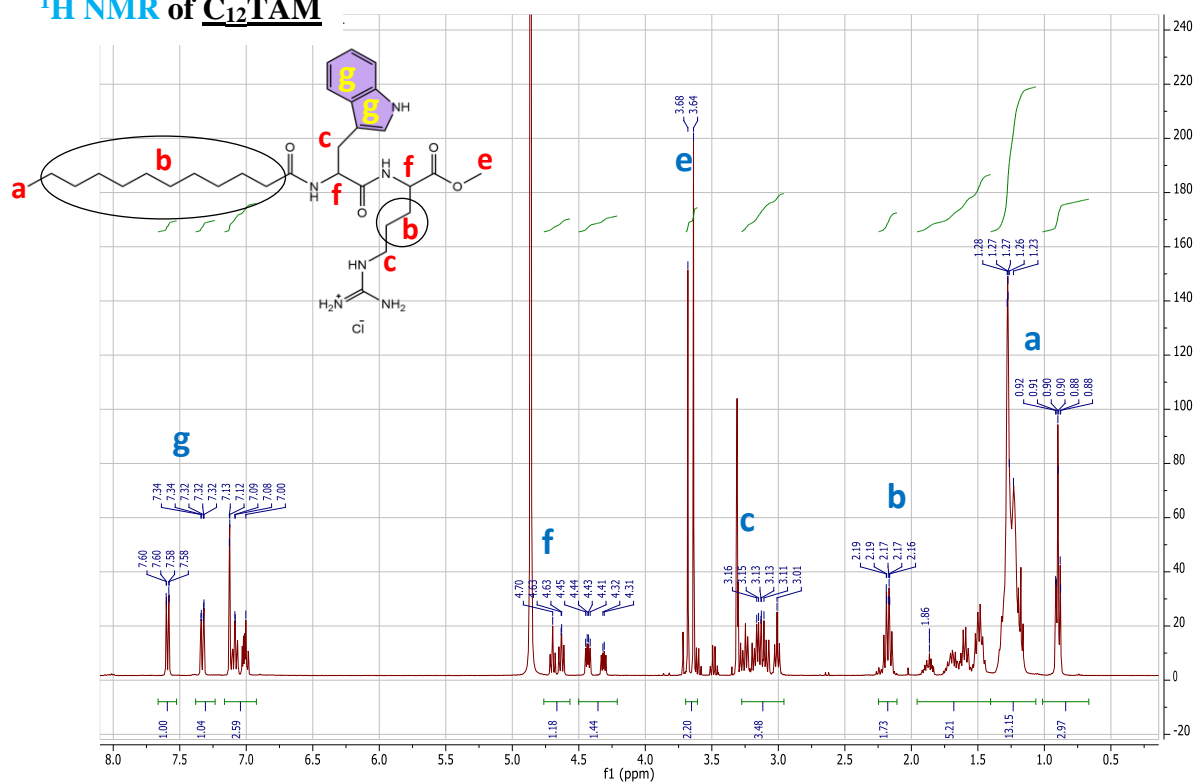
**Figure S7.** HPLC,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and Dept of  $C_{10}\text{TAM}$



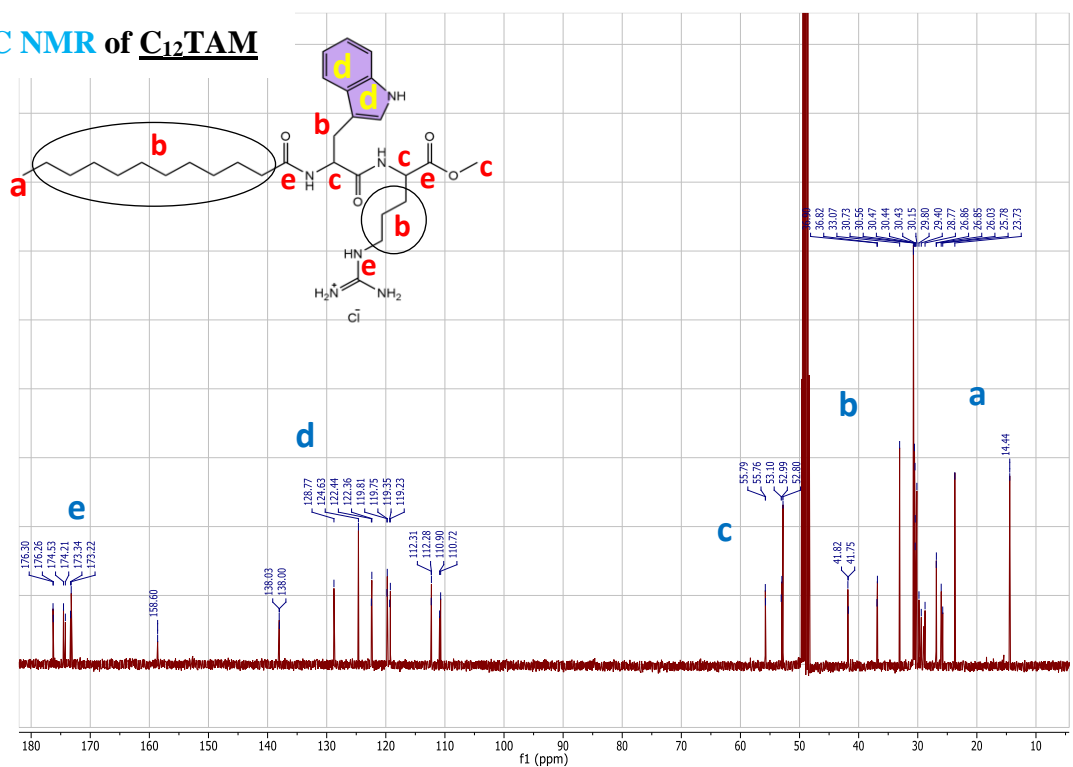
Lourdes  
 Lourdes\_161117\_Fla\_R3 8 (0.411) Cm (5.17)

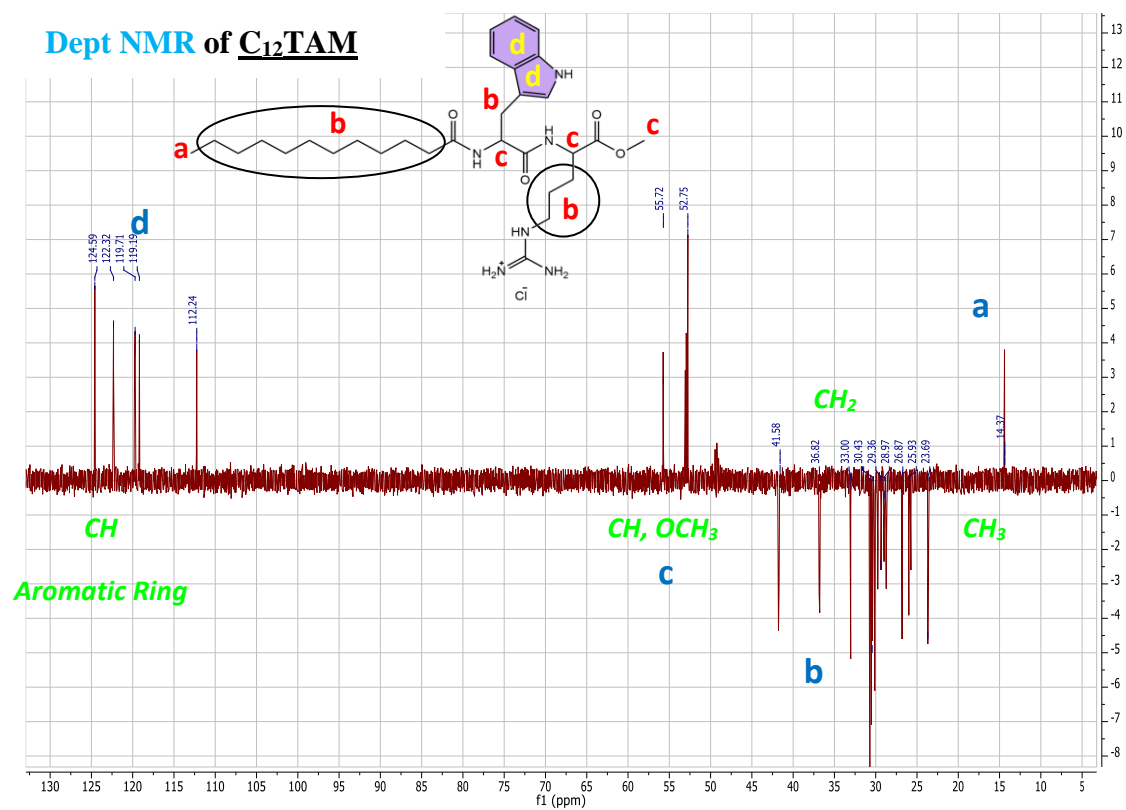


# <sup>1</sup>H NMR of C<sub>12</sub>TAM



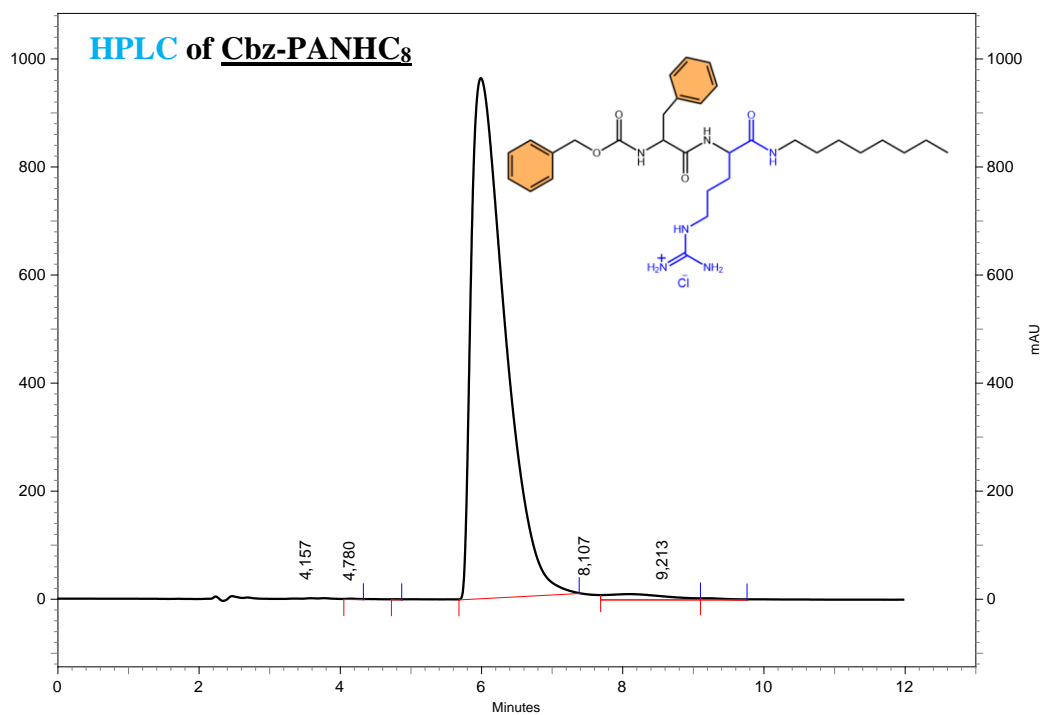
# <sup>13</sup>C NMR of C<sub>12</sub>TAM



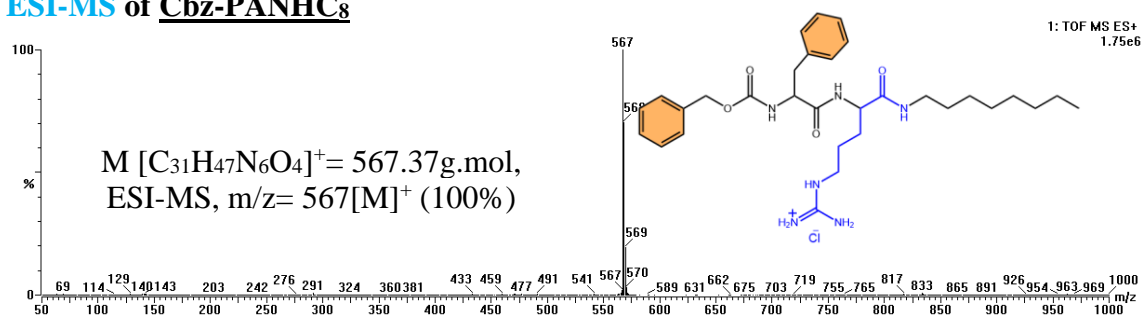


**Figure S8.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of C<sub>10</sub>TAM





**ESI-MS of Cbz-PANHC<sub>8</sub>**



<sup>1</sup>H NMR of Cbz-PANHC<sub>8</sub>

The figure displays the <sup>1</sup>H NMR spectrum of Cbz-PANHC<sub>8</sub> in CDCl<sub>3</sub>. The chemical structure is shown with protons labeled a through f. The spectrum features several distinct signals: aromatic protons (f) at ~7.3 ppm, the Cbz benzyloxy protons (e) at ~5.1 ppm, the PANHC<sub>8</sub> backbone protons (d) at ~4.3 ppm, the PANHC<sub>8</sub> backbone protons (c) at ~3.3 ppm, the PANHC<sub>8</sub> backbone protons (b) at ~1.3 ppm, and the PANHC<sub>8</sub> backbone protons (a) at ~1.0 ppm. Integration values are provided for each major peak group.

Chemical structure of Cbz-PANHC<sub>8</sub> is shown with labels a through f indicating the corresponding protons in the spectrum.

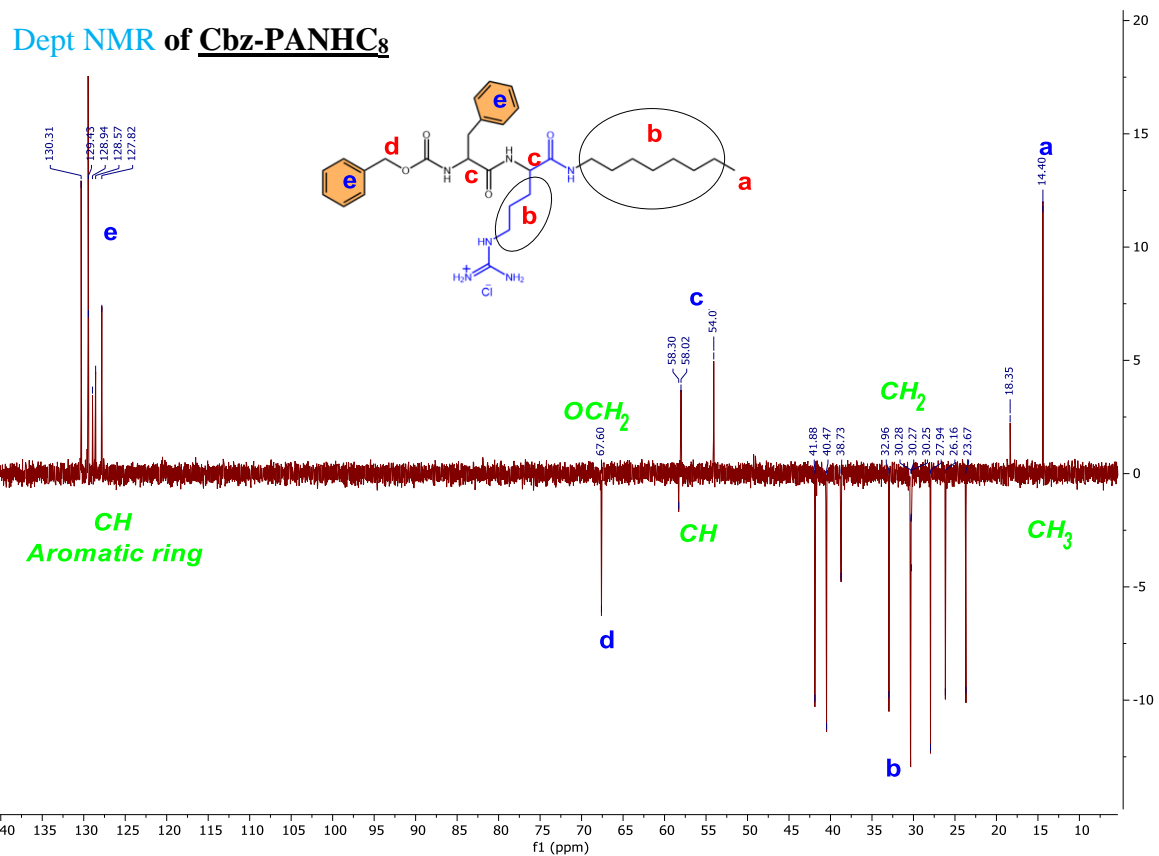
<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) showing chemical shifts (f1, ppm) on the x-axis (0.5 to 8.0) and intensity on the y-axis (0 to 1100). The spectrum displays several peaks corresponding to the structure:

- Peak f:** Aromatic protons, multiplet at ~7.3 ppm (integration: 8.57).
- Peak e:** Cbz benzyloxy protons, doublet at ~5.1 ppm (integration: 1.97).
- Peak d:** PANHC<sub>8</sub> backbone protons, multiplet at ~4.3 ppm (integration: 1.90).
- Peak c:** PANHC<sub>8</sub> backbone protons, multiplet at ~3.3 ppm (integration: 0.98).
- Peak b:** PANHC<sub>8</sub> backbone protons, multiplet at ~1.3 ppm (integration: 8.75).
- Peak a:** PANHC<sub>8</sub> backbone protons, multiplet at ~1.0 ppm (integration: 3.00).

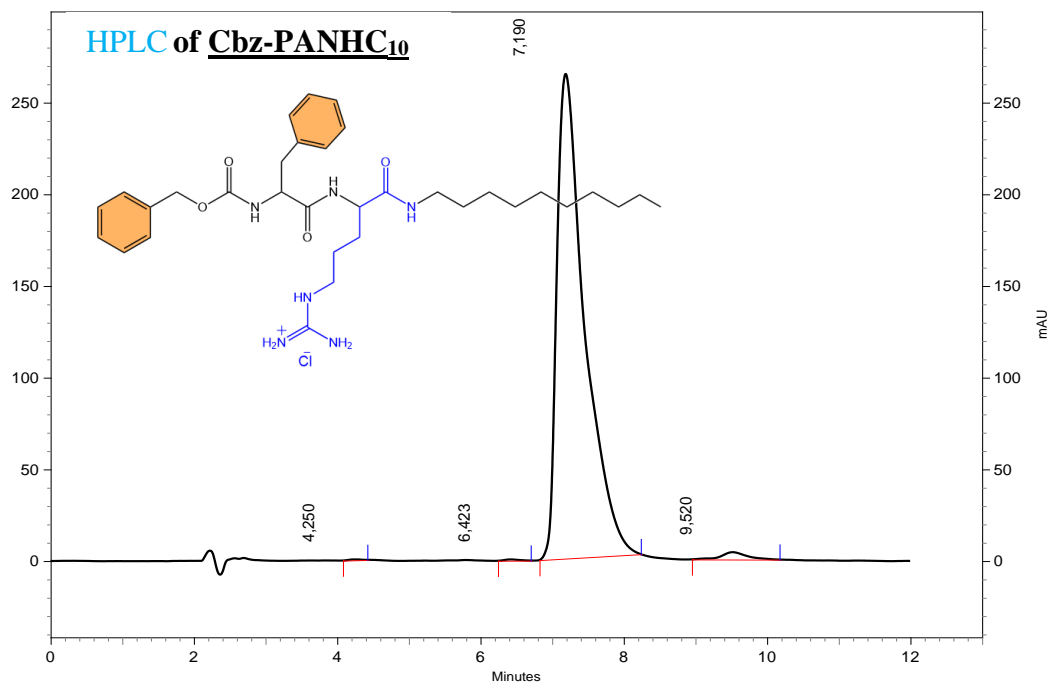
Integration values are provided for each major peak group.

The figure displays the chemical structure of Cbz-PANC8 and its corresponding <sup>1</sup>H and <sup>13</sup>C NMR spectra. The chemical structure is a benzyl carbamate derivative of a poly(amic acid) chain, with protons and carbons labeled a through e. The <sup>13</sup>C NMR spectrum (top) shows peaks from 127.84 to 174.25 ppm, with an inset showing the region from 54.09 to 67.62 ppm. The <sup>1</sup>H NMR spectrum (bottom) shows peaks from 1.44 to 7.25 ppm, with an inset showing the region from 5.41 to 5.84 ppm. The assignments are as follows:

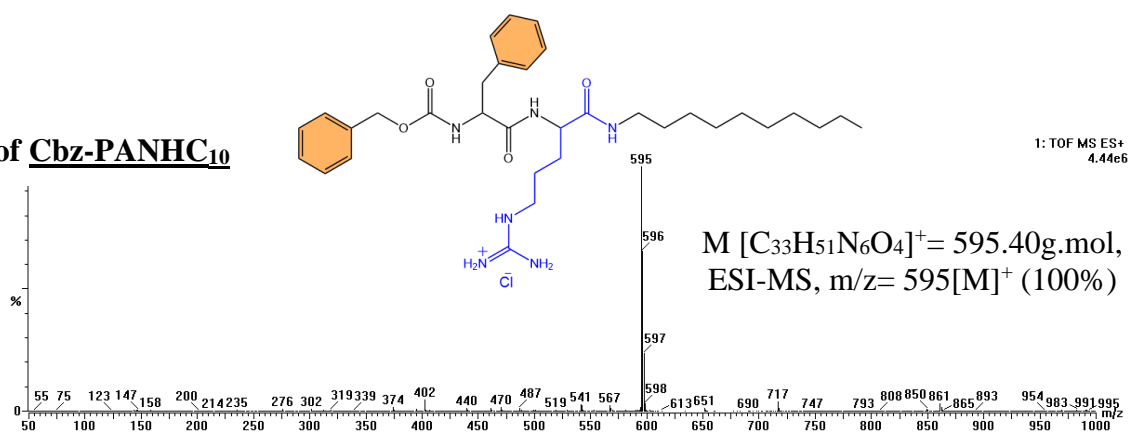
- <sup>13</sup>C NMR (ppm):** 174.25 (e), 173.17 (e), 158.57 (e), 156.36 (e), 138.28 (d), 130.33 (d), 129.69 (d), 129.47 (d), 128.45 (d), 128.96 (d), 127.84 (d), 67.62 (c), 58.32 (c), 58.04 (c), 54.09 (c).
- <sup>1</sup>H NMR (ppm):** 7.25 (d), 7.19 (d), 7.15 (d), 7.11 (d), 7.07 (d), 7.03 (d), 6.99 (d), 6.95 (d), 6.91 (d), 6.87 (d), 6.83 (d), 6.79 (d), 6.75 (d), 6.71 (d), 6.67 (d), 6.63 (d), 6.59 (d), 6.55 (d), 6.51 (d), 6.47 (d), 6.43 (d), 6.39 (d), 6.35 (d), 6.31 (d), 6.27 (d), 6.23 (d), 6.19 (d), 6.15 (d), 6.11 (d), 6.07 (d), 6.03 (d), 6.00 (d), 5.96 (d), 5.92 (d), 5.88 (d), 5.84 (d), 5.80 (d), 5.76 (d), 5.72 (d), 5.68 (d), 5.64 (d), 5.60 (d), 5.56 (d), 5.52 (d), 5.48 (d), 5.44 (d), 5.40 (d), 5.36 (d), 5.32 (d), 5.28 (d), 5.24 (d), 5.20 (d), 5.16 (d), 5.12 (d), 5.08 (d), 5.04 (d), 5.00 (d), 4.96 (d), 4.92 (d), 4.88 (d), 4.84 (d), 4.80 (d), 4.76 (d), 4.72 (d), 4.68 (d), 4.64 (d), 4.60 (d), 4.56 (d), 4.52 (d), 4.48 (d), 4.44 (d), 4.40 (d), 4.36 (d), 4.32 (d), 4.28 (d), 4.24 (d), 4.20 (d), 4.16 (d), 4.12 (d), 4.08 (d), 4.04 (d), 4.00 (d), 3.96 (d), 3.92 (d), 3.88 (d), 3.84 (d), 3.80 (d), 3.76 (d), 3.72 (d), 3.68 (d), 3.64 (d), 3.60 (d), 3.56 (d), 3.52 (d), 3.48 (d), 3.44 (d), 3.40 (d), 3.36 (d), 3.32 (d), 3.28 (d), 3.24 (d), 3.20 (d), 3.16 (d), 3.12 (d), 3.08 (d), 3.04 (d), 3.00 (d), 2.96 (d), 2.92 (d), 2.88 (d), 2.84 (d), 2.80 (d), 2.76 (d), 2.72 (d), 2.68 (d), 2.64 (d), 2.60 (d), 2.56 (d), 2.52 (d), 2.48 (d), 2.44 (d), 2.40 (d), 2.36 (d), 2.32 (d), 2.28 (d), 2.24 (d), 2.20 (d), 2.16 (d), 2.12 (d), 2.08 (d), 2.04 (d), 2.00 (d), 1.96 (d), 1.92 (d), 1.88 (d), 1.84 (d), 1.80 (d), 1.76 (d), 1.72 (d), 1.68 (d), 1.64 (d), 1.60 (d), 1.56 (d), 1.52 (d), 1.48 (d), 1.44 (d), 1.40 (d), 1.36 (d), 1.32 (d), 1.28 (d), 1.24 (d), 1.20 (d), 1.16 (d), 1.12 (d), 1.08 (d), 1.04 (d), 1.00 (d), 0.96 (d), 0.92 (d), 0.88 (d), 0.84 (d), 0.80 (d), 0.76 (d), 0.72 (d), 0.68 (d), 0.64 (d), 0.60 (d), 0.56 (d), 0.52 (d), 0.48 (d), 0.44 (d), 0.40 (d), 0.36 (d), 0.32 (d), 0.28 (d), 0.24 (d), 0.20 (d), 0.16 (d), 0.12 (d), 0.08 (d), 0.04 (d), 0.00 (d).



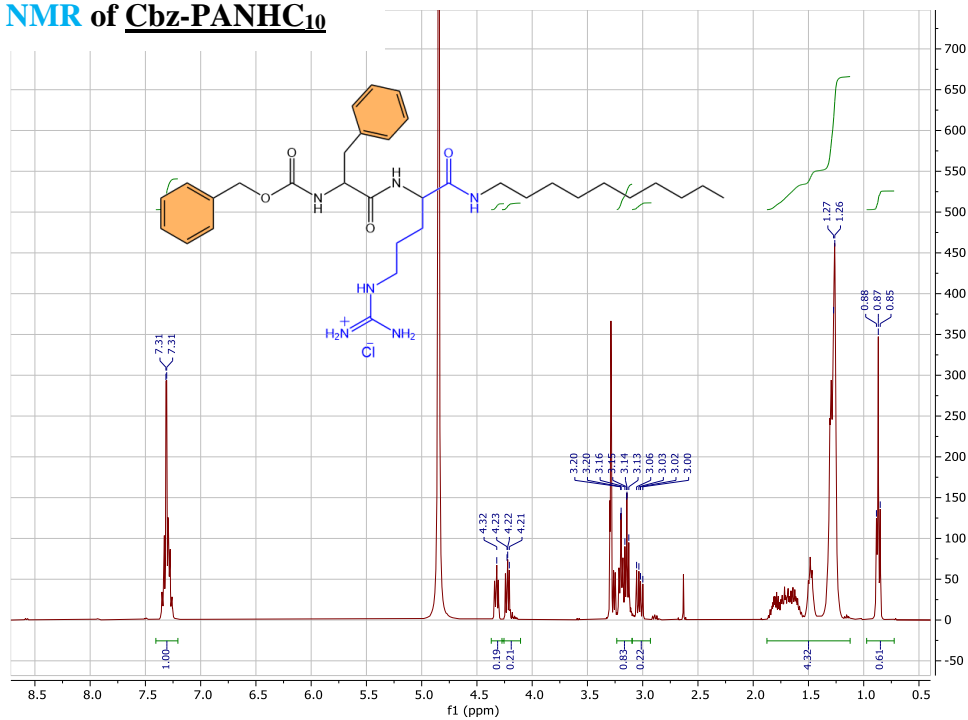
**Figure S9.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of Cbz-PANHC<sub>8</sub>



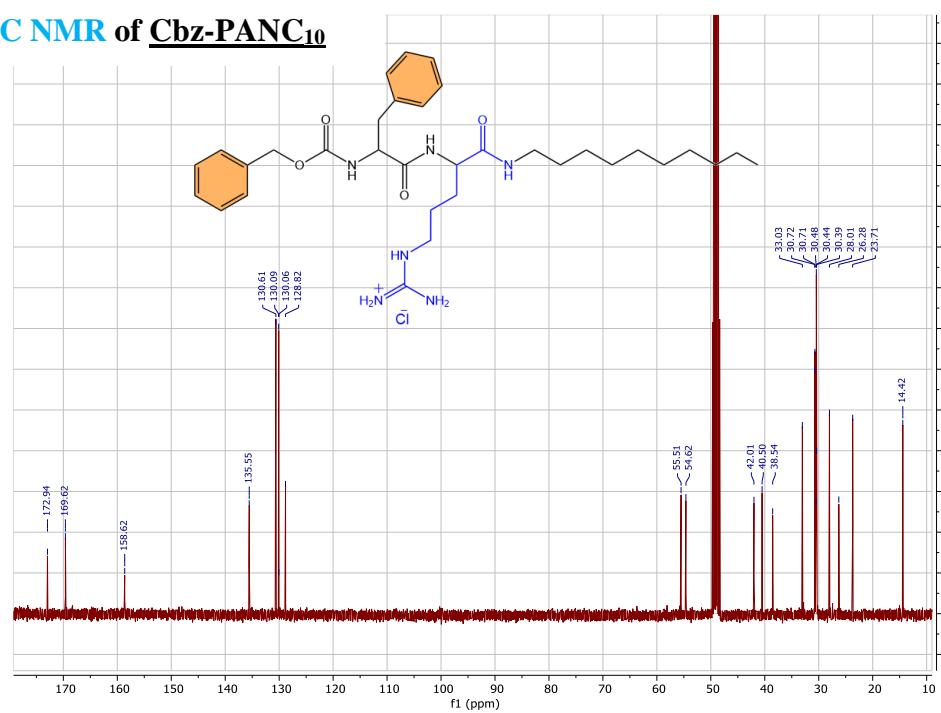
**ESI-MS of Cbz-PANHC<sub>10</sub>**



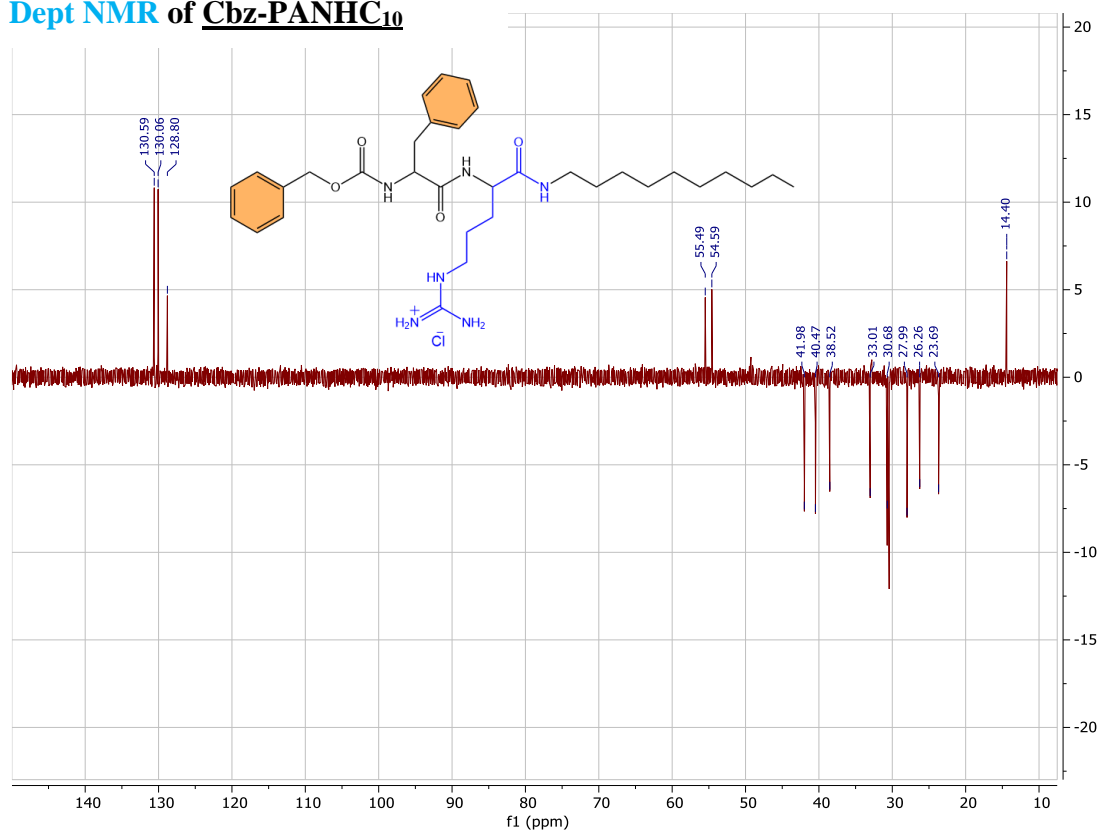
### <sup>1</sup>H NMR of Cbz-PANHC<sub>10</sub>



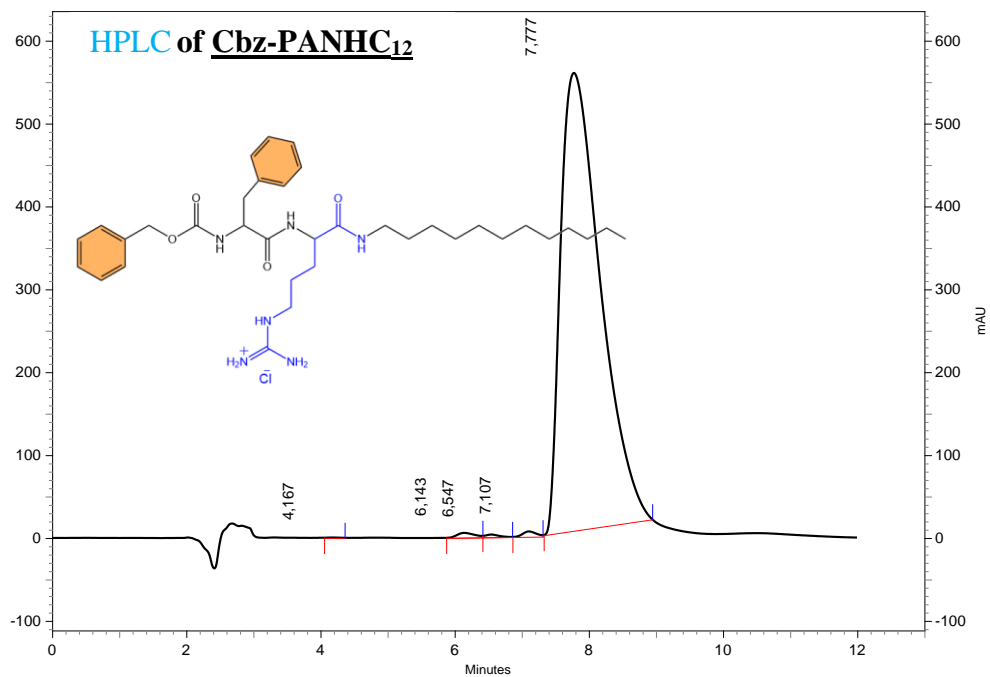
### <sup>13</sup>C NMR of Cbz-PANHC<sub>10</sub>



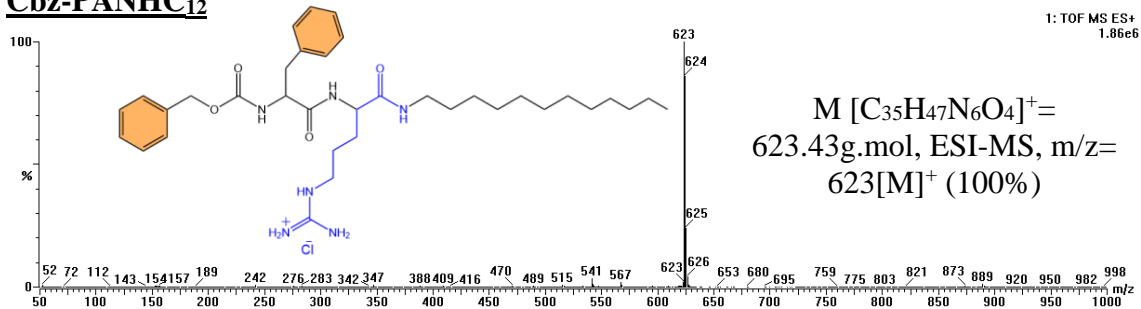
Dept NMR of **Cbz-PANHC<sub>10</sub>**



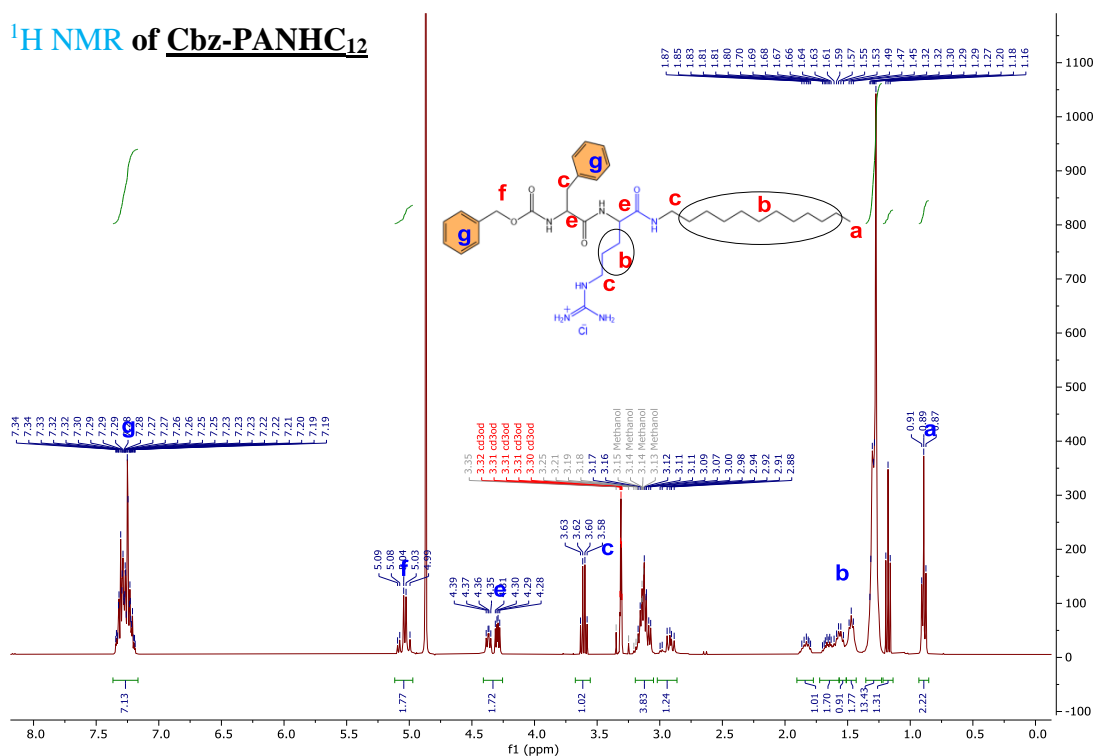
**Figure S10.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of Cbz-PANHC<sub>10</sub>



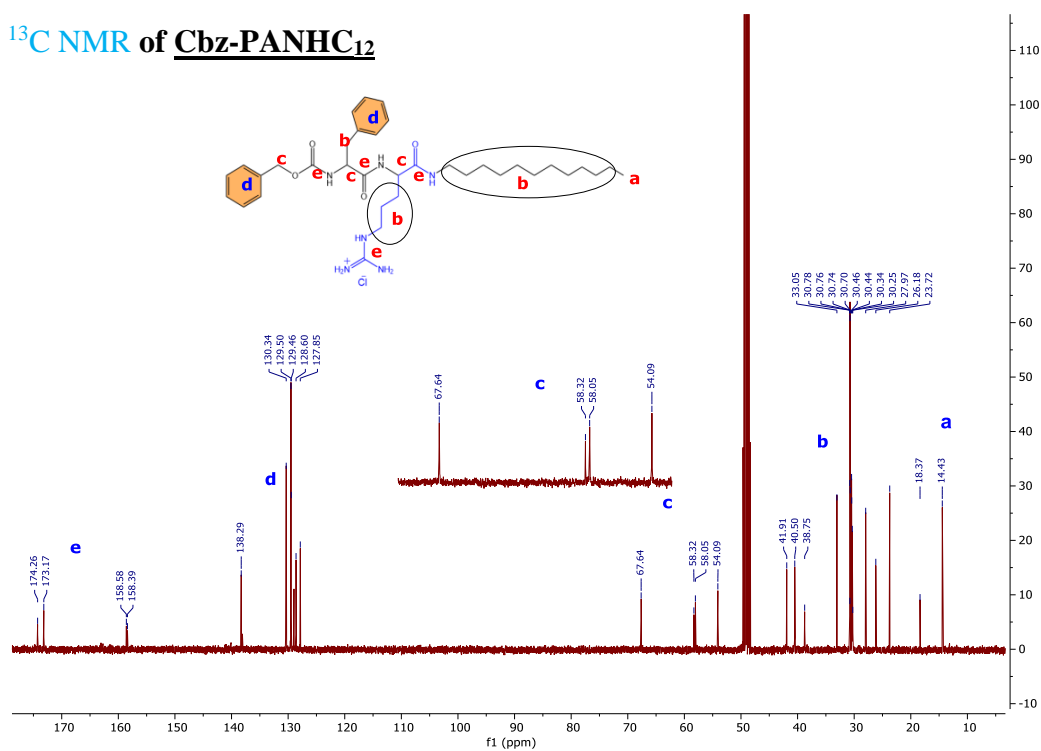
**ESI-MS of Cbz-PANHC<sub>12</sub>**



# <sup>1</sup>H NMR of Cbz-PANHC<sub>12</sub>

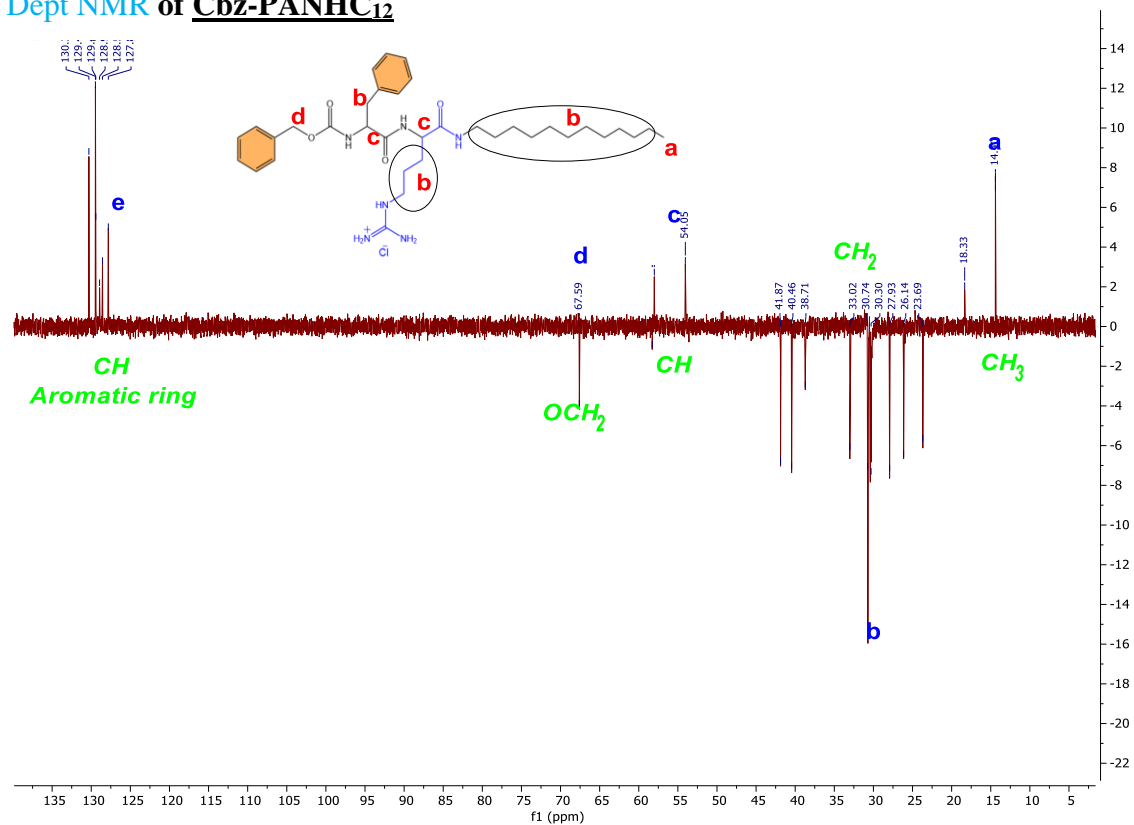


# <sup>13</sup>C NMR of Cbz-PANHC<sub>12</sub>

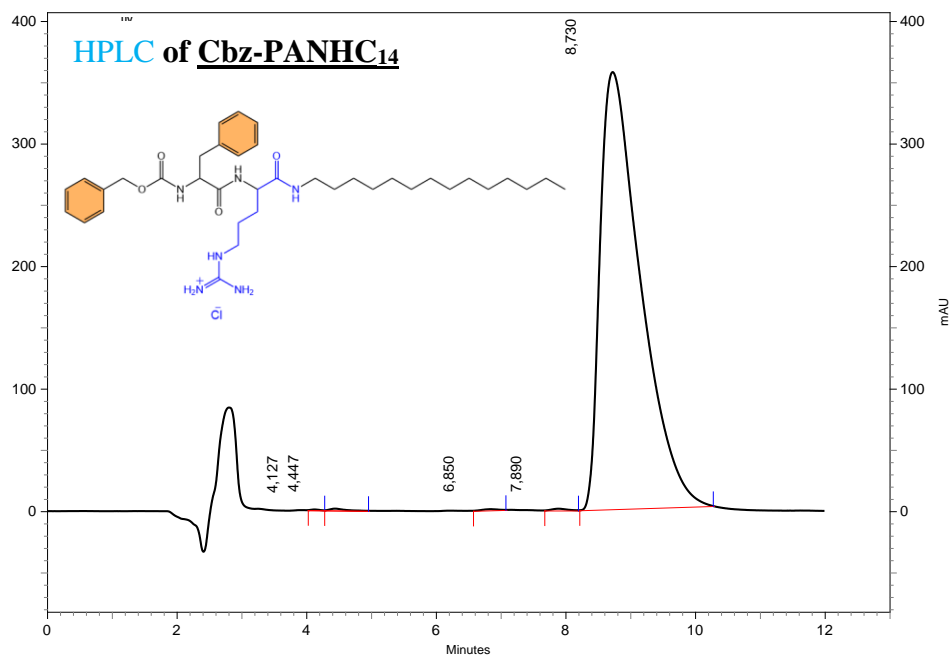




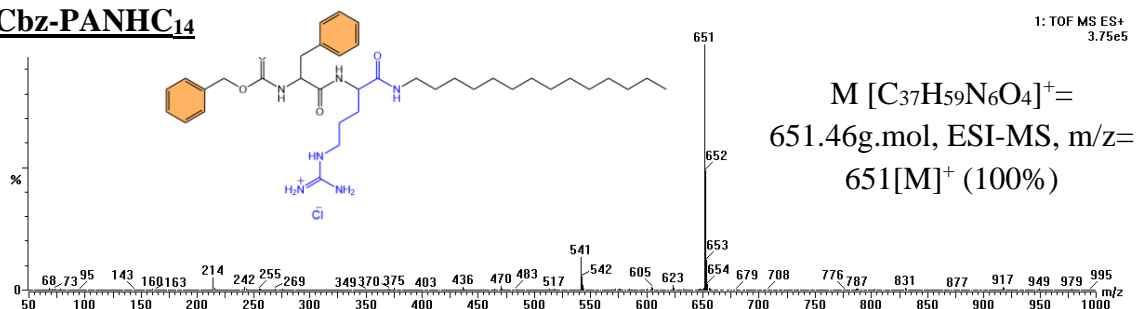
# Dept NMR of Cbz-PANHC<sub>12</sub>



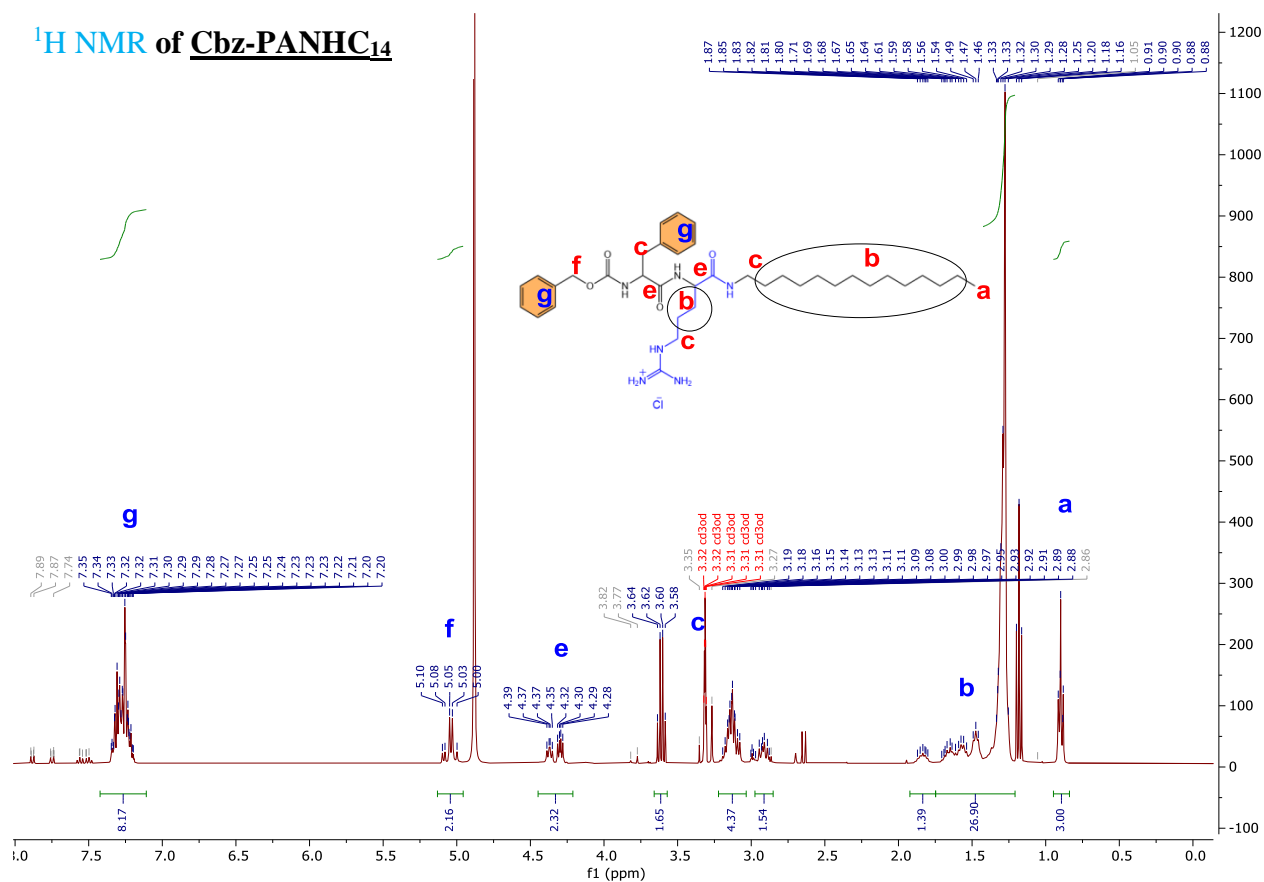
**Figure S11.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of Cbz-PANHC<sub>12</sub>



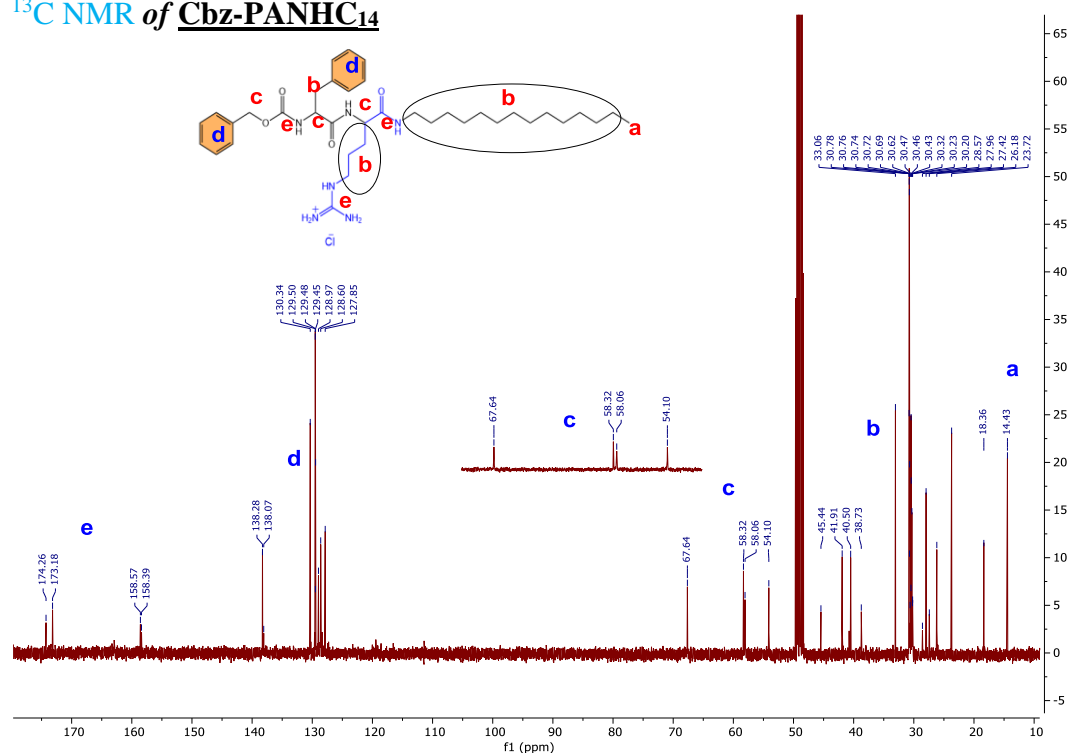
**ESI-MS of Cbz-PANHC<sub>14</sub>**



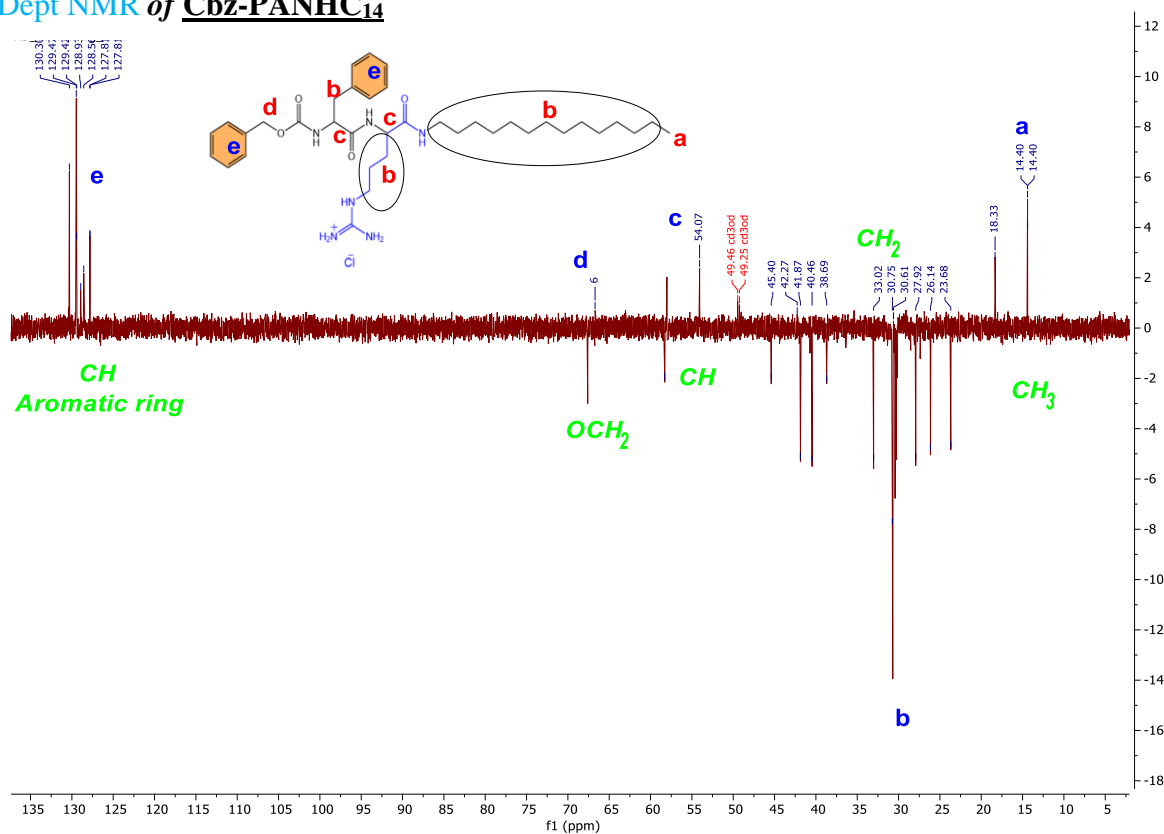
# <sup>1</sup>H NMR of Cbz-PANHC<sub>14</sub>



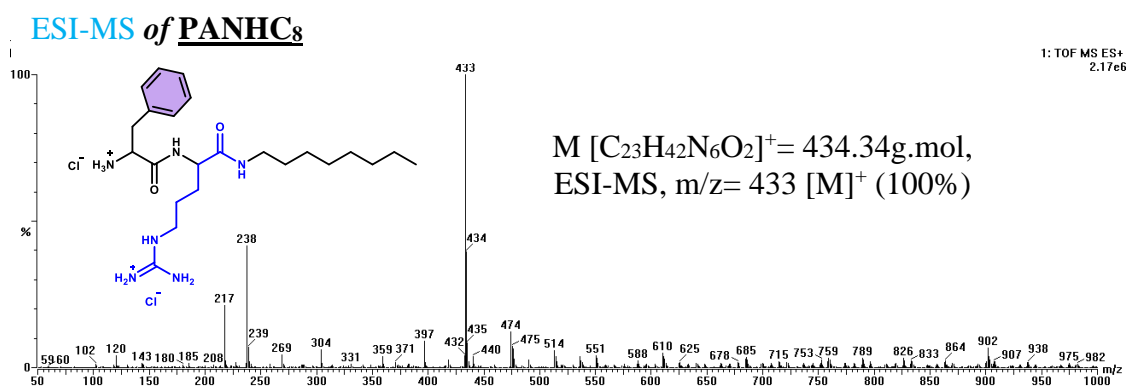
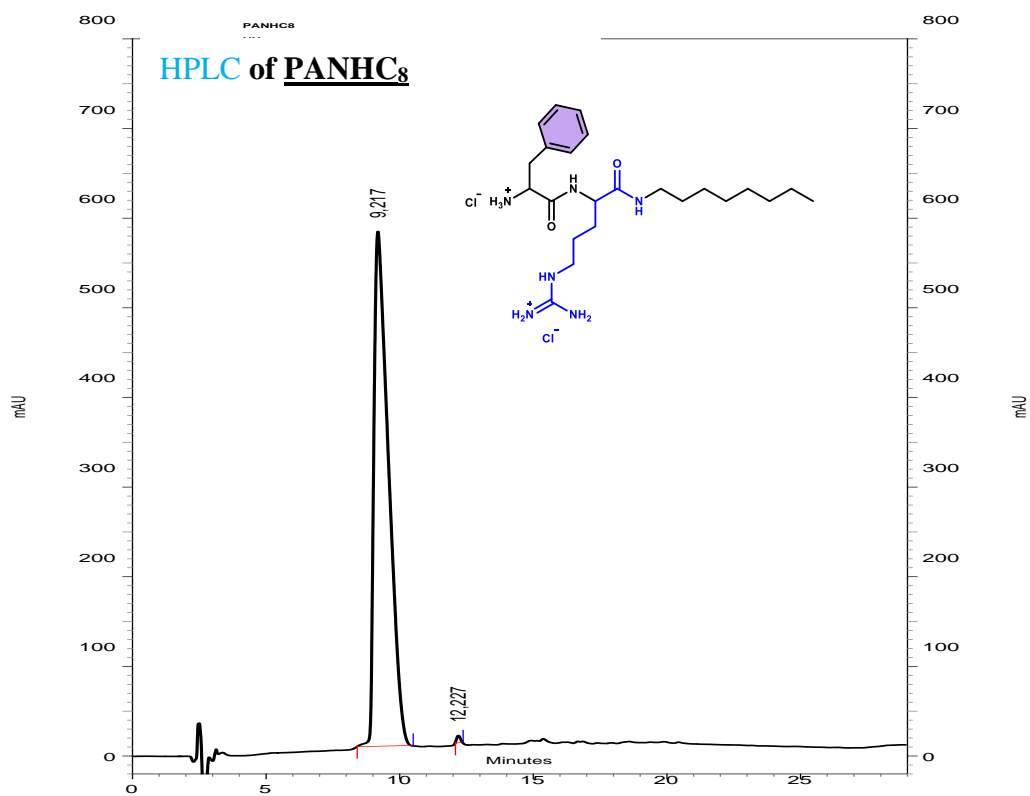
# <sup>13</sup>C NMR of Cbz-PANHC<sub>14</sub>



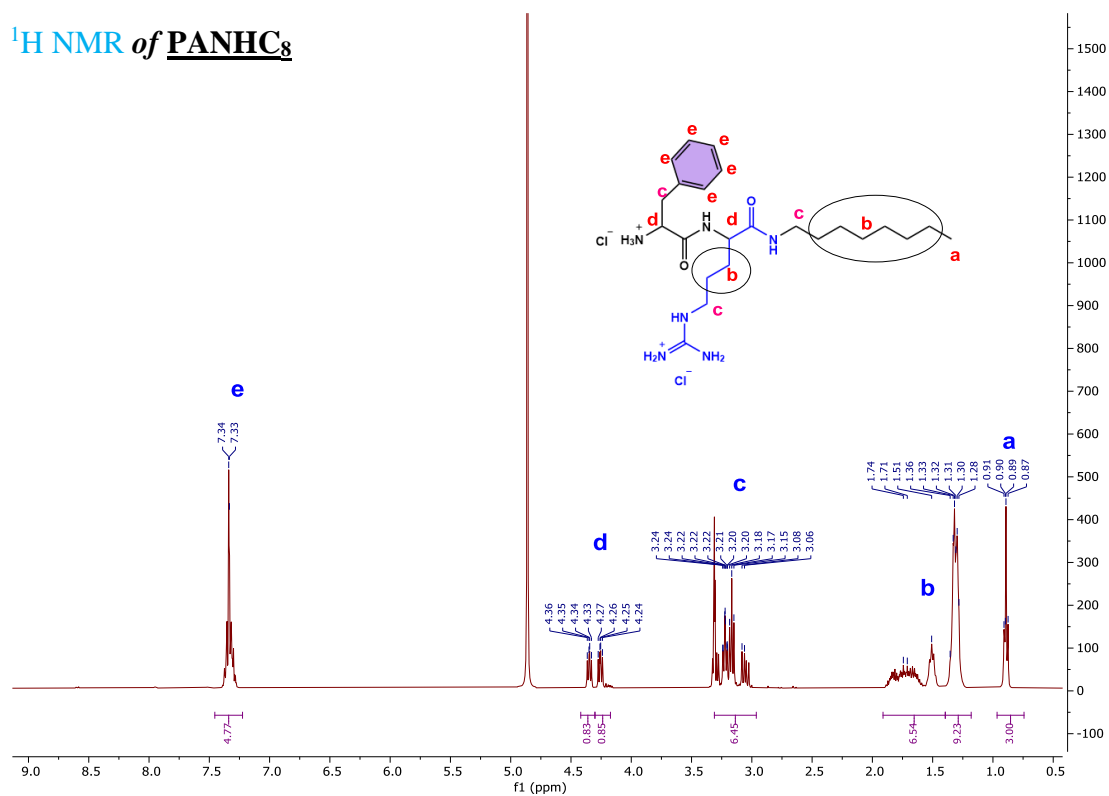
# Dept NMR of Cbz-PANHC<sub>14</sub>



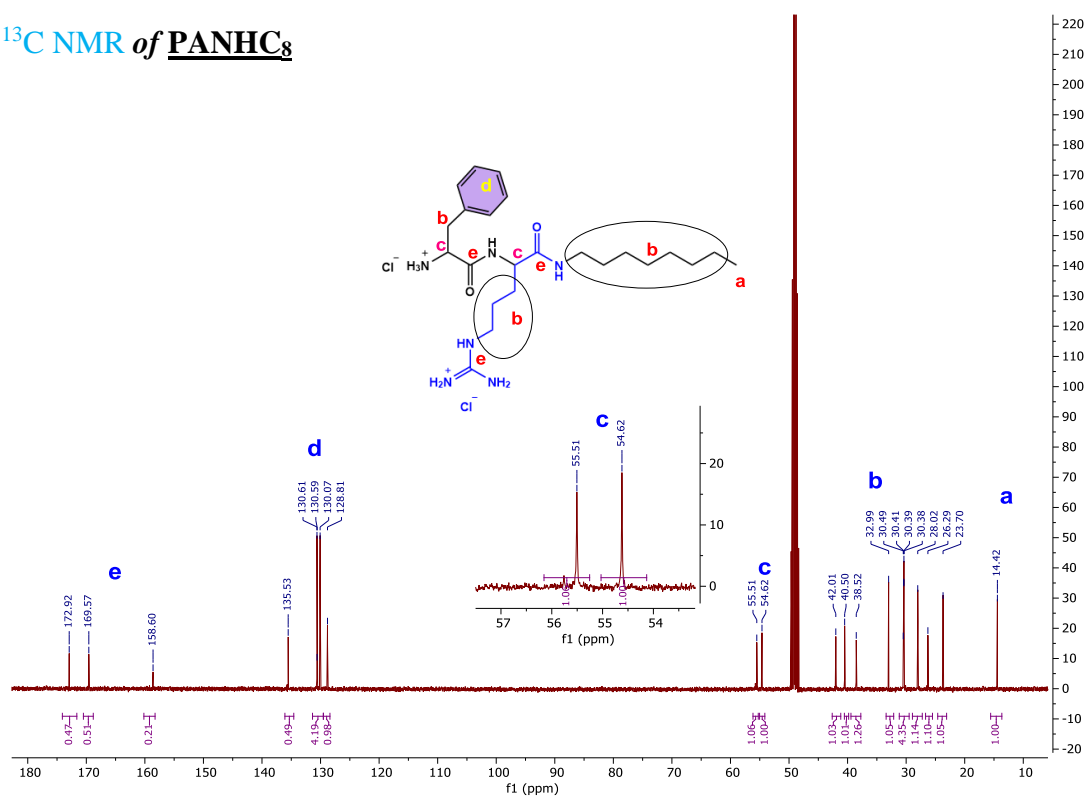
**Figure S12.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of Cbz-PANHC<sub>14</sub>



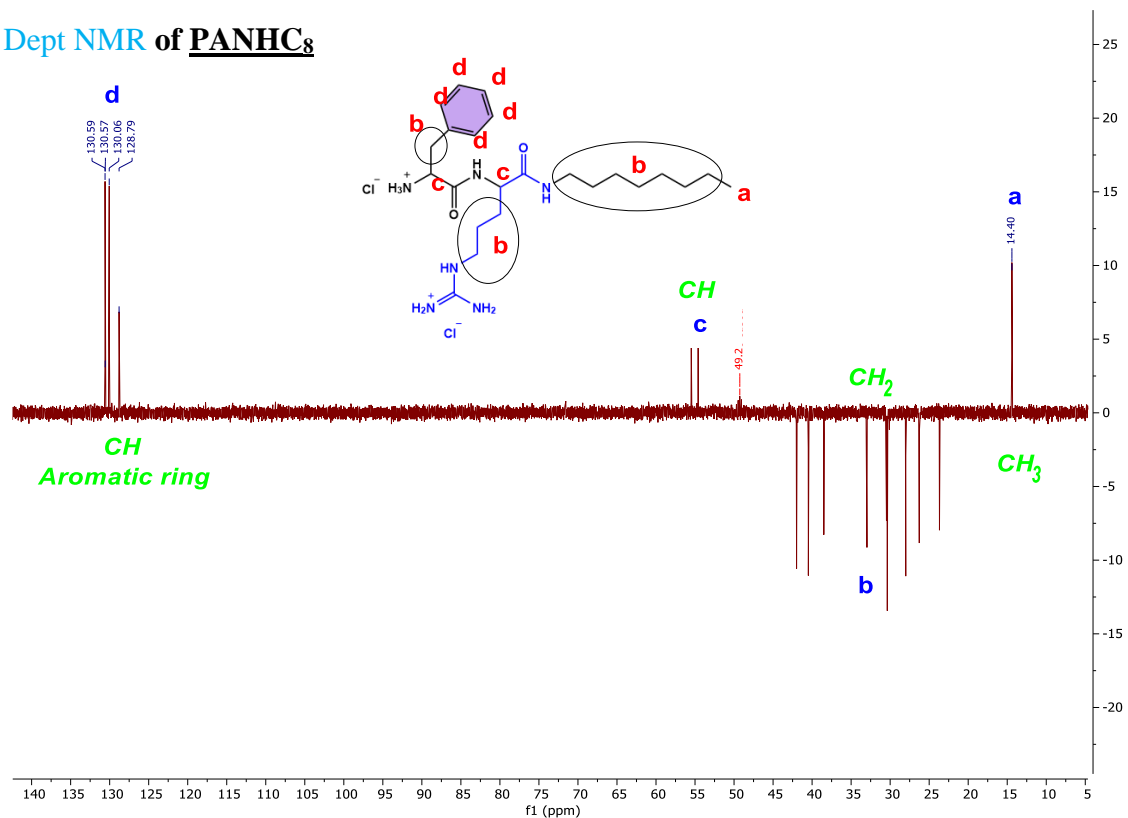
# <sup>1</sup>H NMR of PANHC<sub>8</sub>



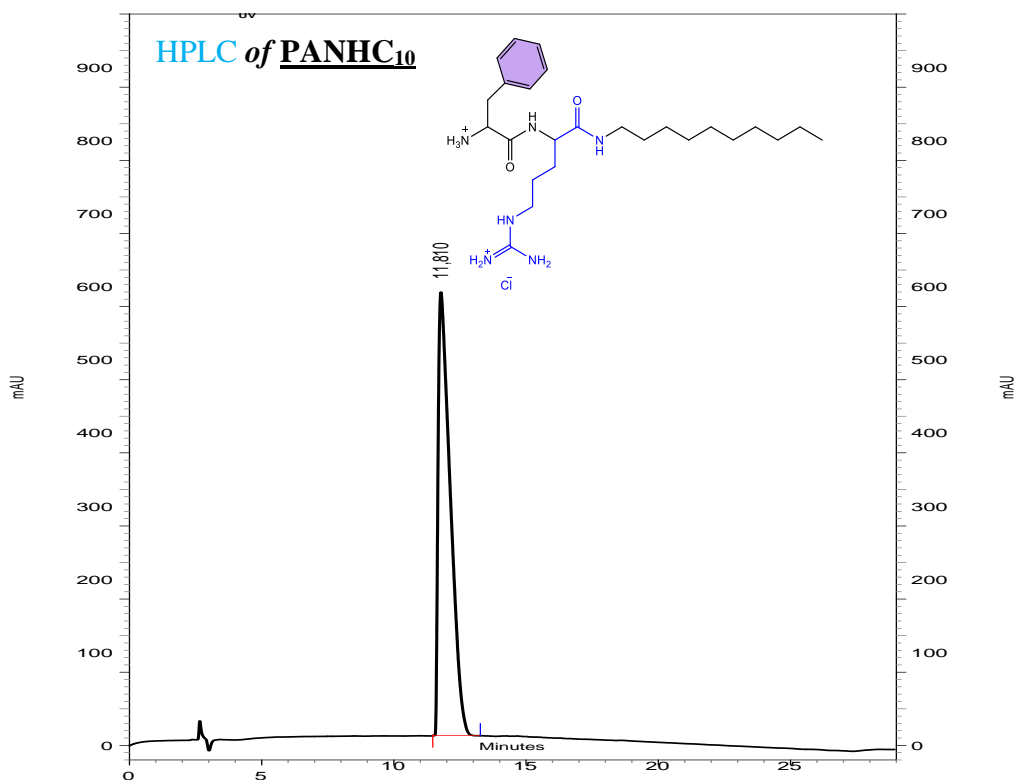
# <sup>13</sup>C NMR of PANHC<sub>8</sub>



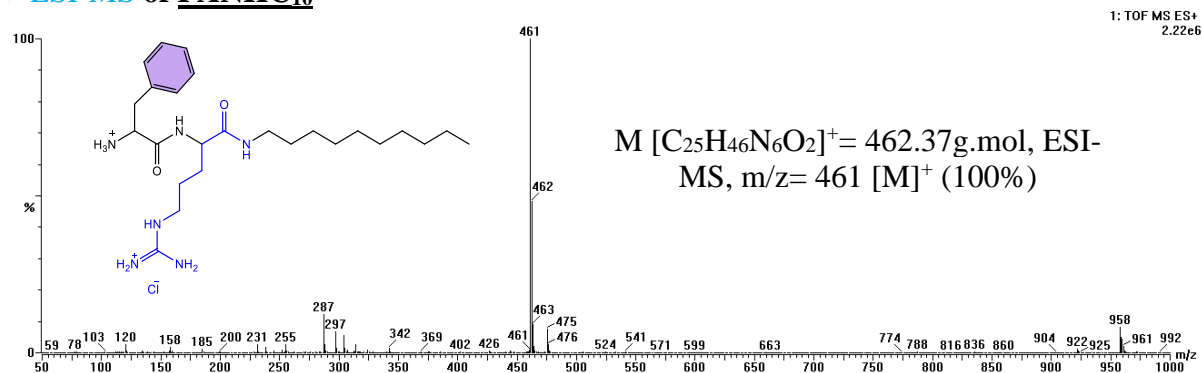
# Dept NMR of PANHC<sub>8</sub>



. **Figure S13.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of PANHC<sub>8</sub>

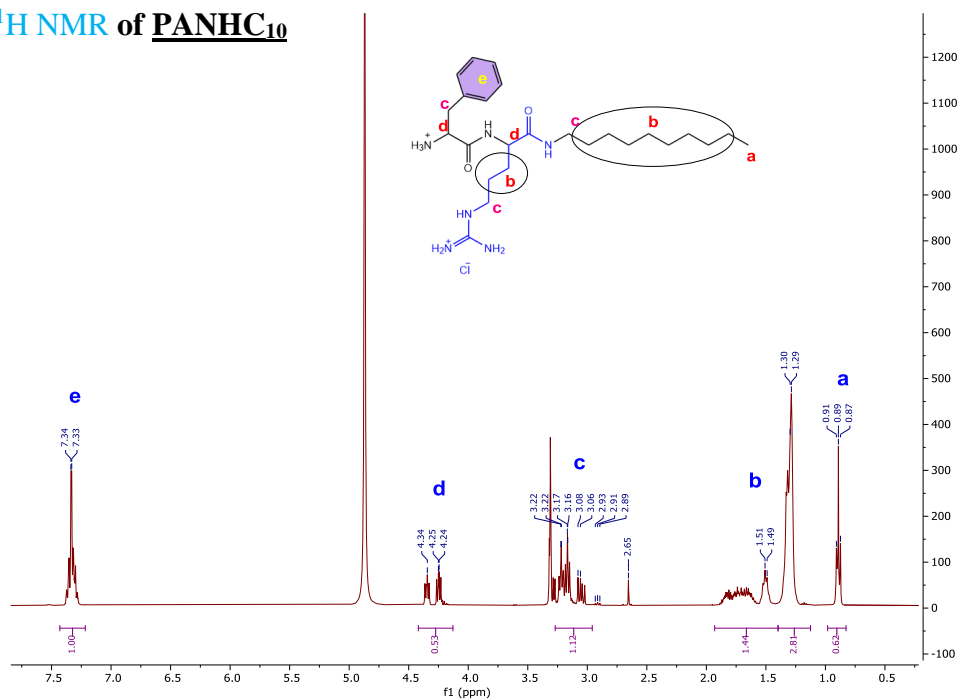


### ESI-MS of PANHC<sub>10</sub>

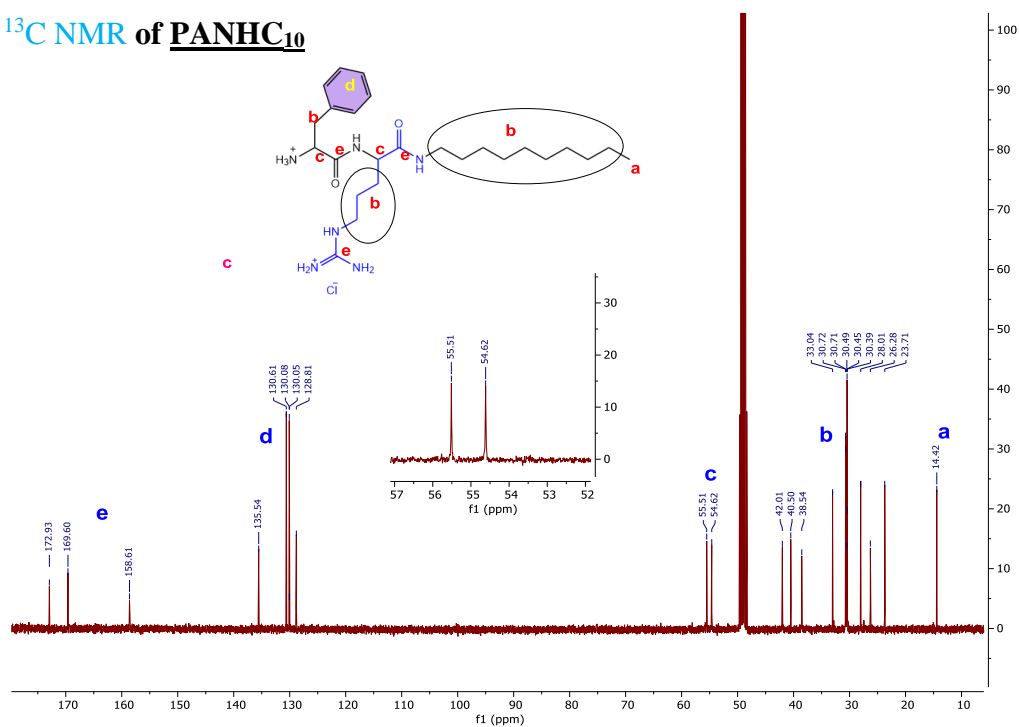




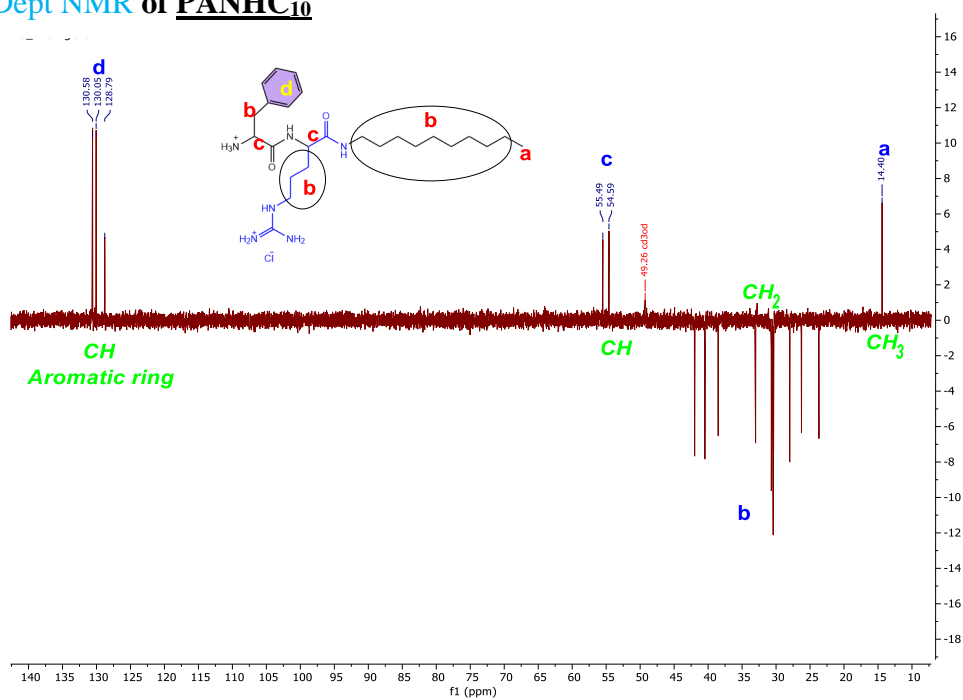
# <sup>1</sup>H NMR of PANHC<sub>10</sub>



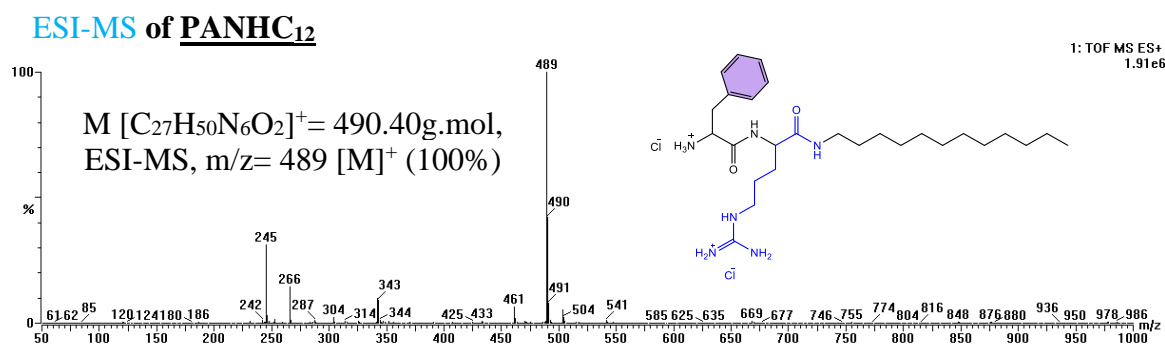
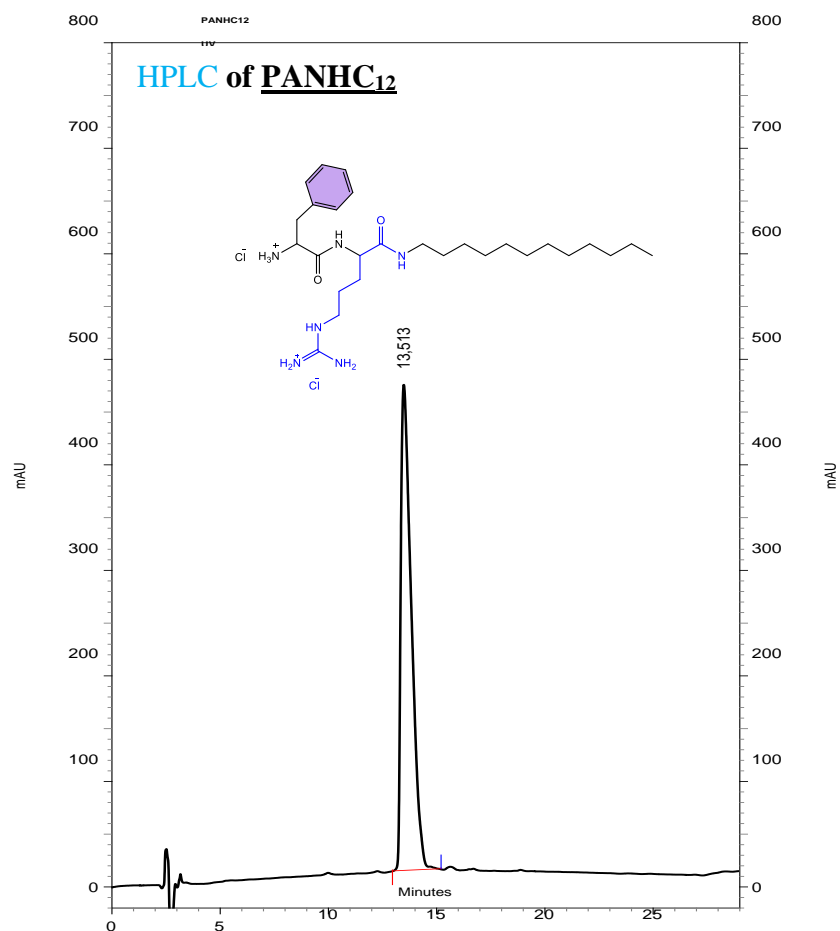
# <sup>13</sup>C NMR of PANHC<sub>10</sub>



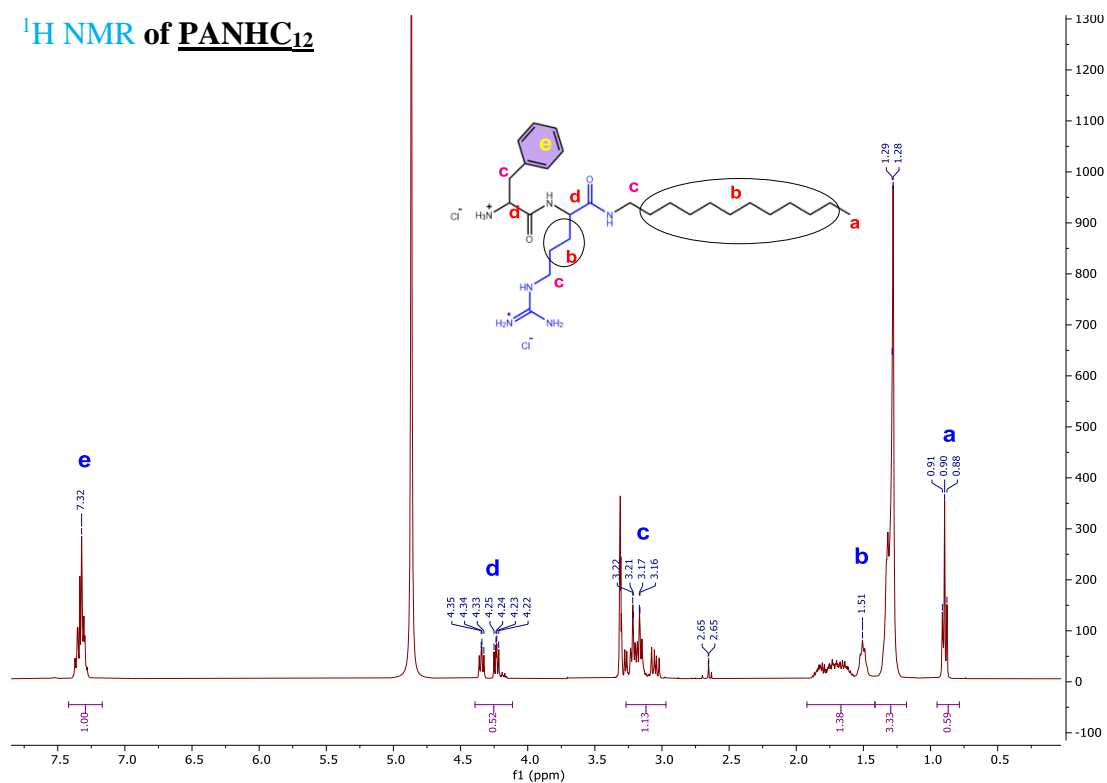
# Dept NMR of PANHC<sub>10</sub>



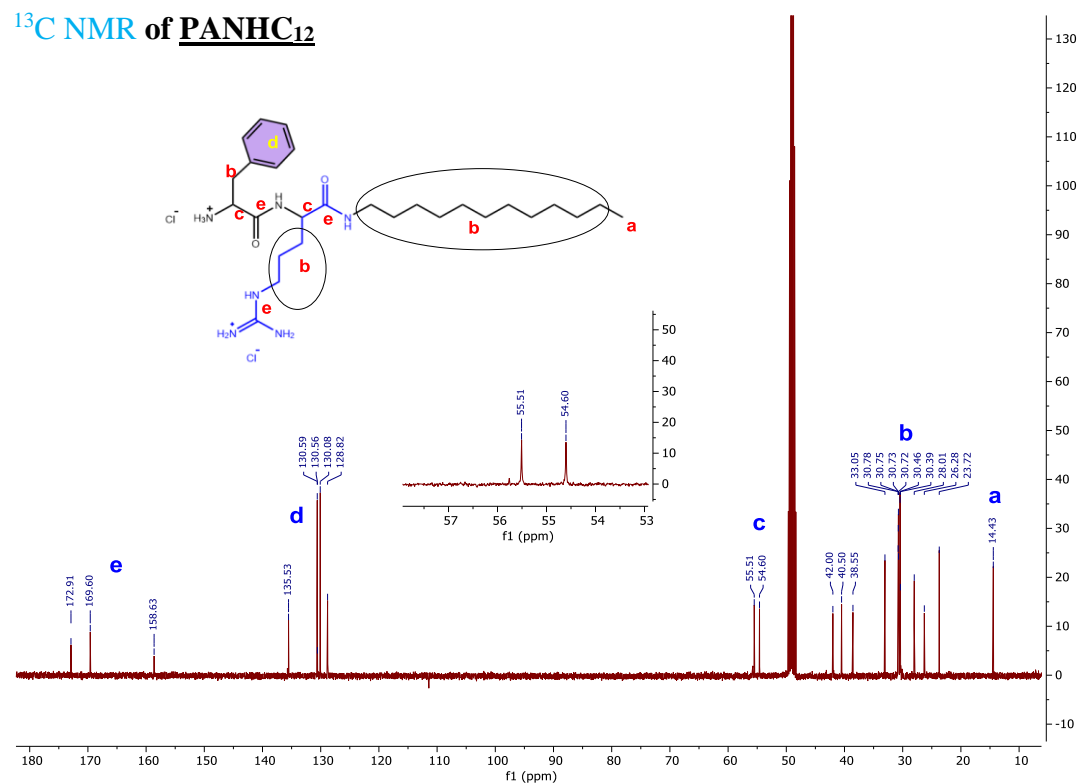
. **Figure S14.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of PANHC<sub>10</sub>



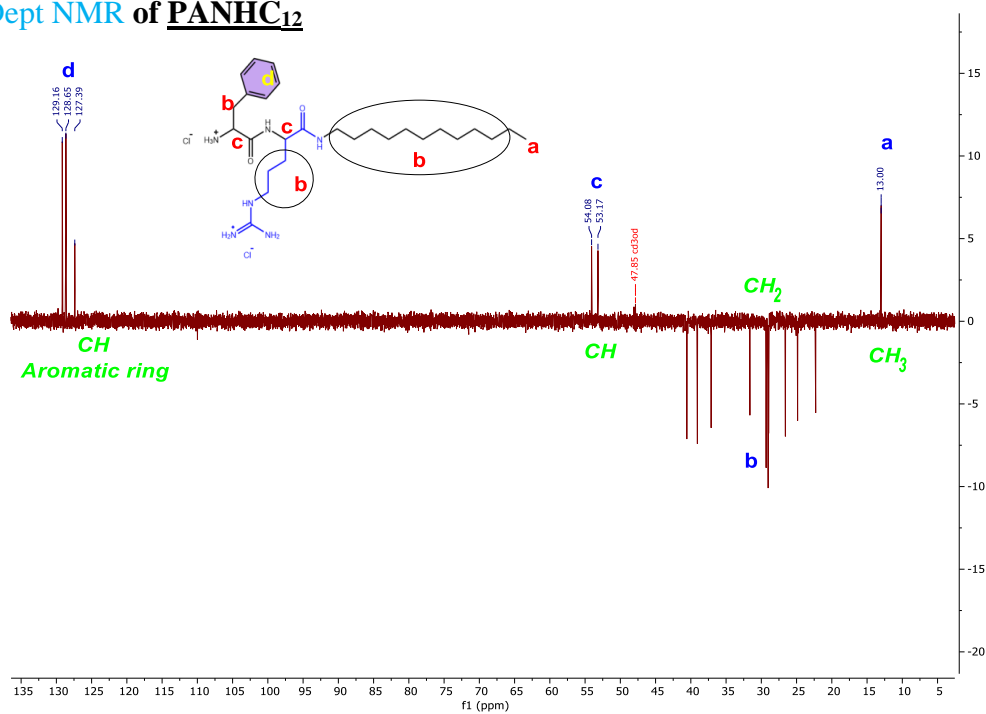
# $^1\text{H}$ NMR of PANHC<sub>12</sub>



# $^{13}\text{C}$ NMR of PANHC<sub>12</sub>

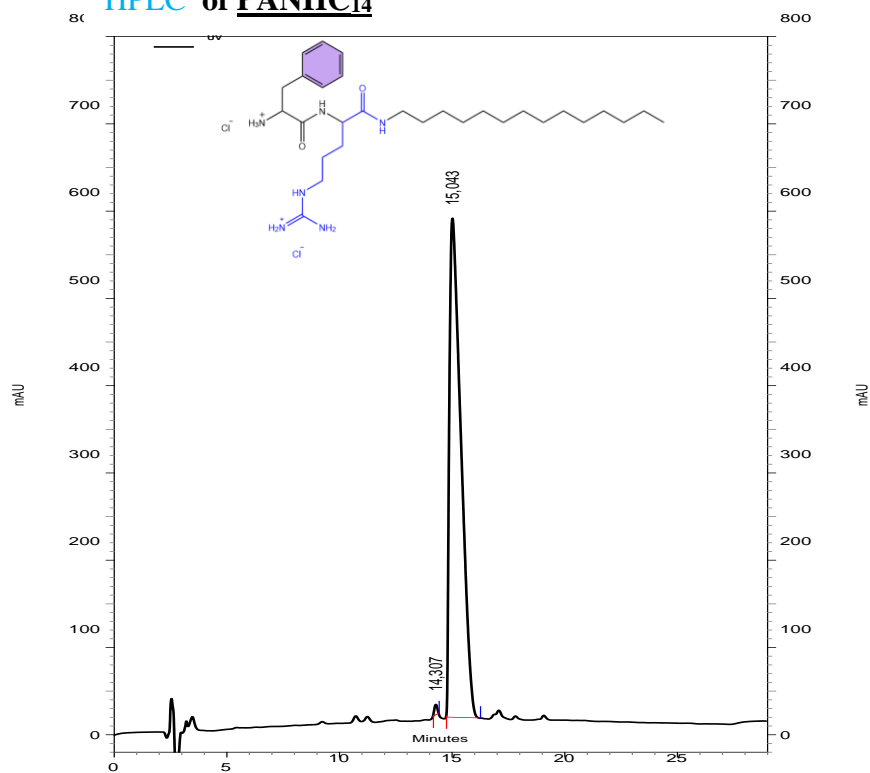


# Dept NMR of **PANHC<sub>12</sub>**

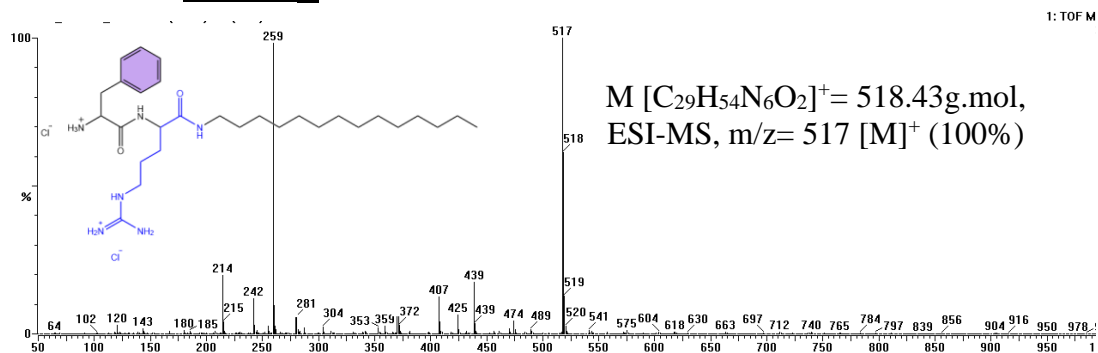


. **Figure S15.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of PANHC<sub>12</sub>

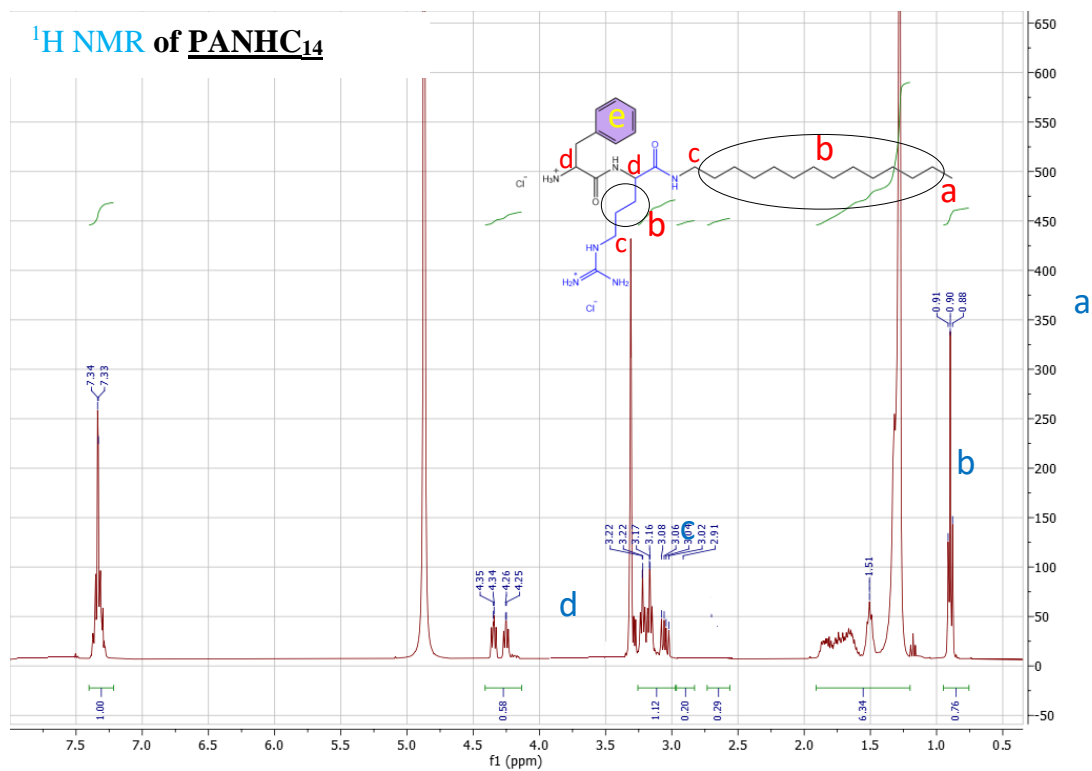
## HPLC of PANHC<sub>14</sub>



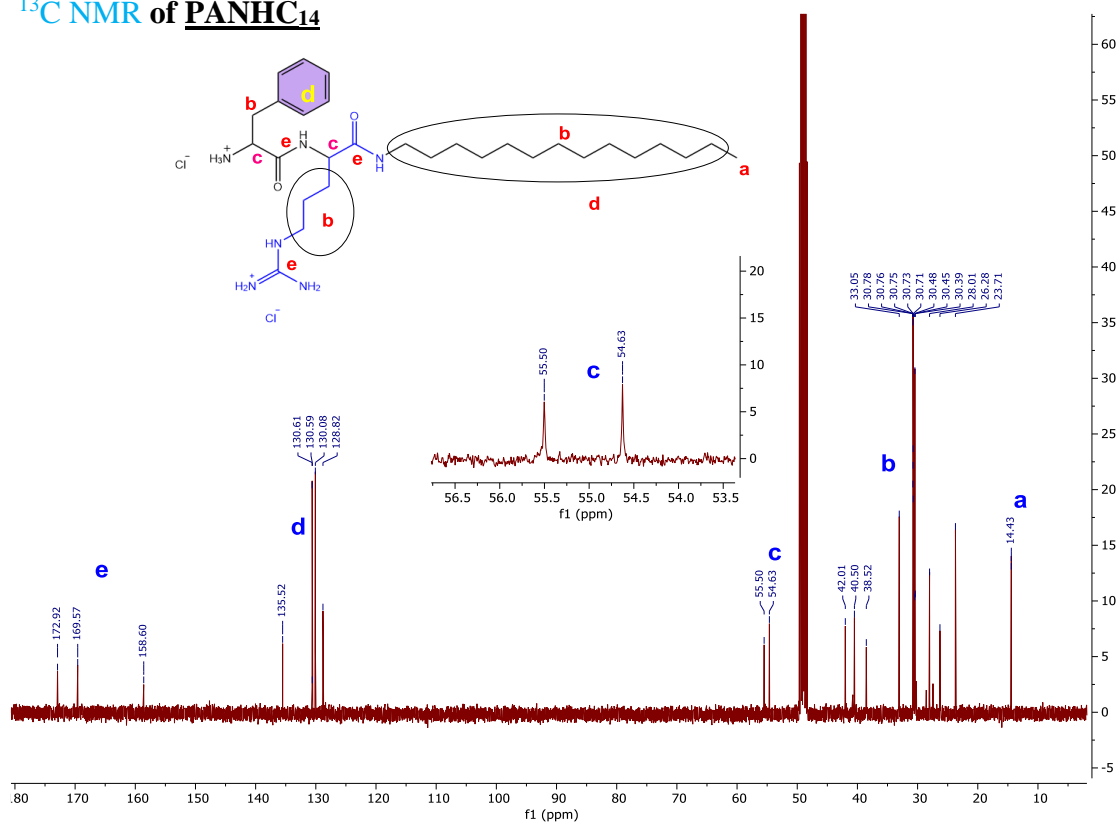
## ESI-MS of PANHC<sub>14</sub>



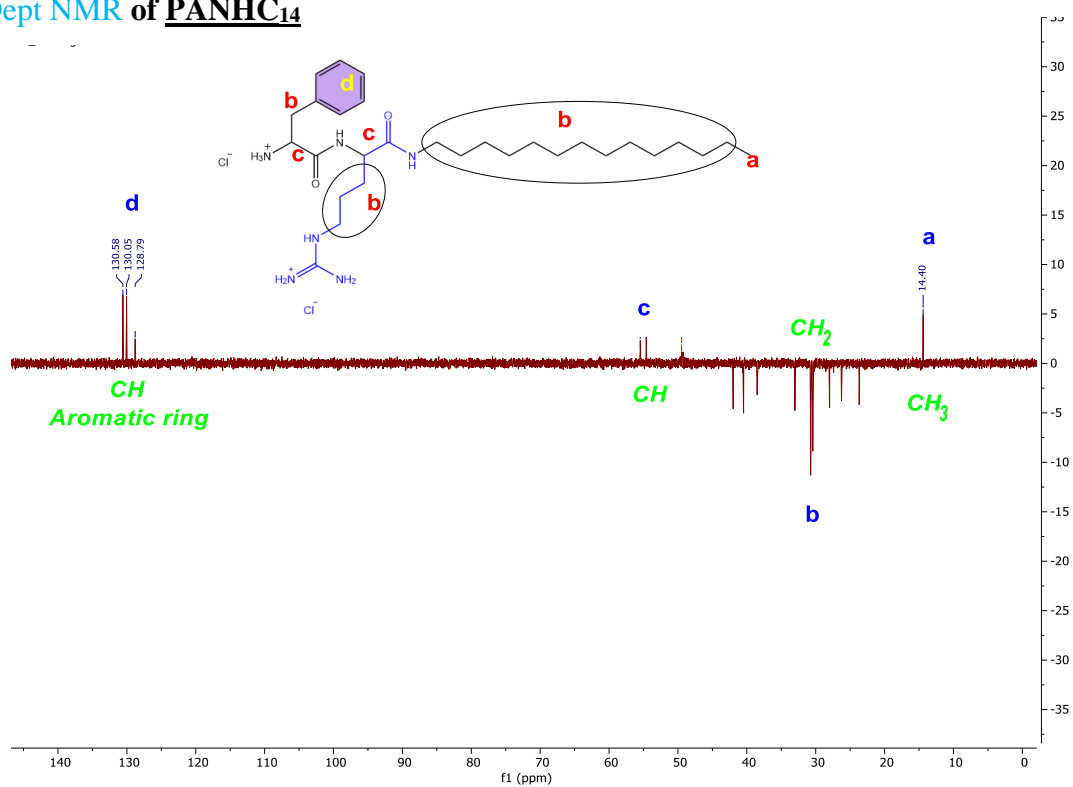
# <sup>1</sup>H NMR of PANHC<sub>14</sub>



# <sup>13</sup>C NMR of PANHC<sub>14</sub>

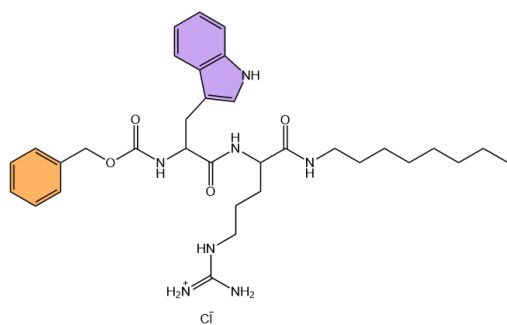
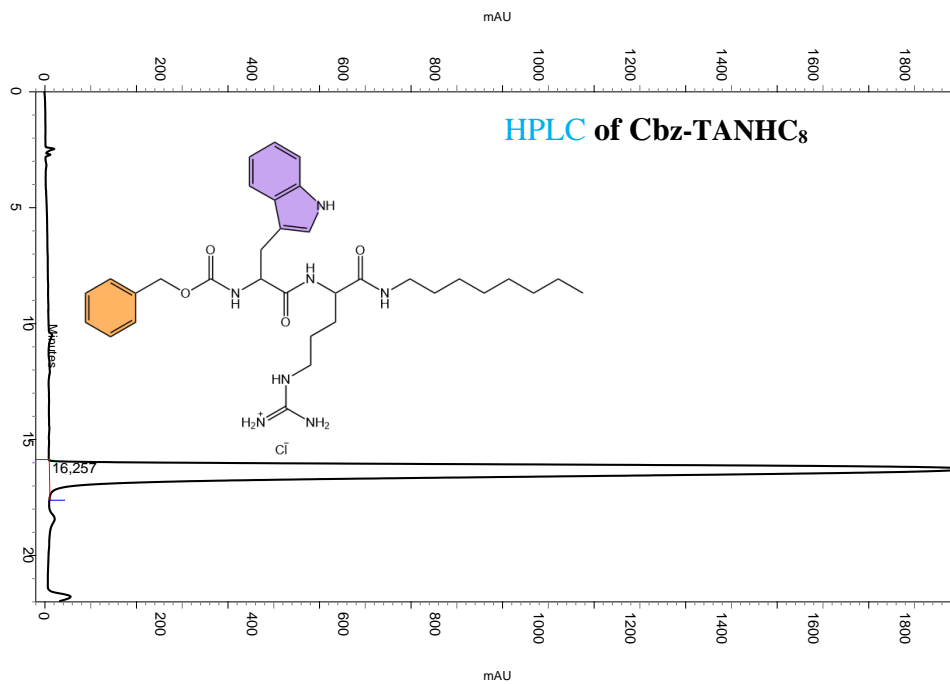


# Dept NMR of PANHC<sub>14</sub>



**Figure S16.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of PANHC<sub>14</sub>

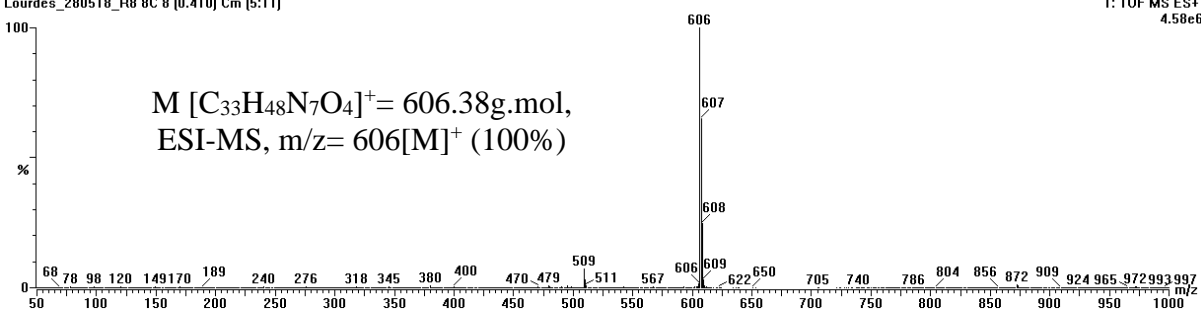




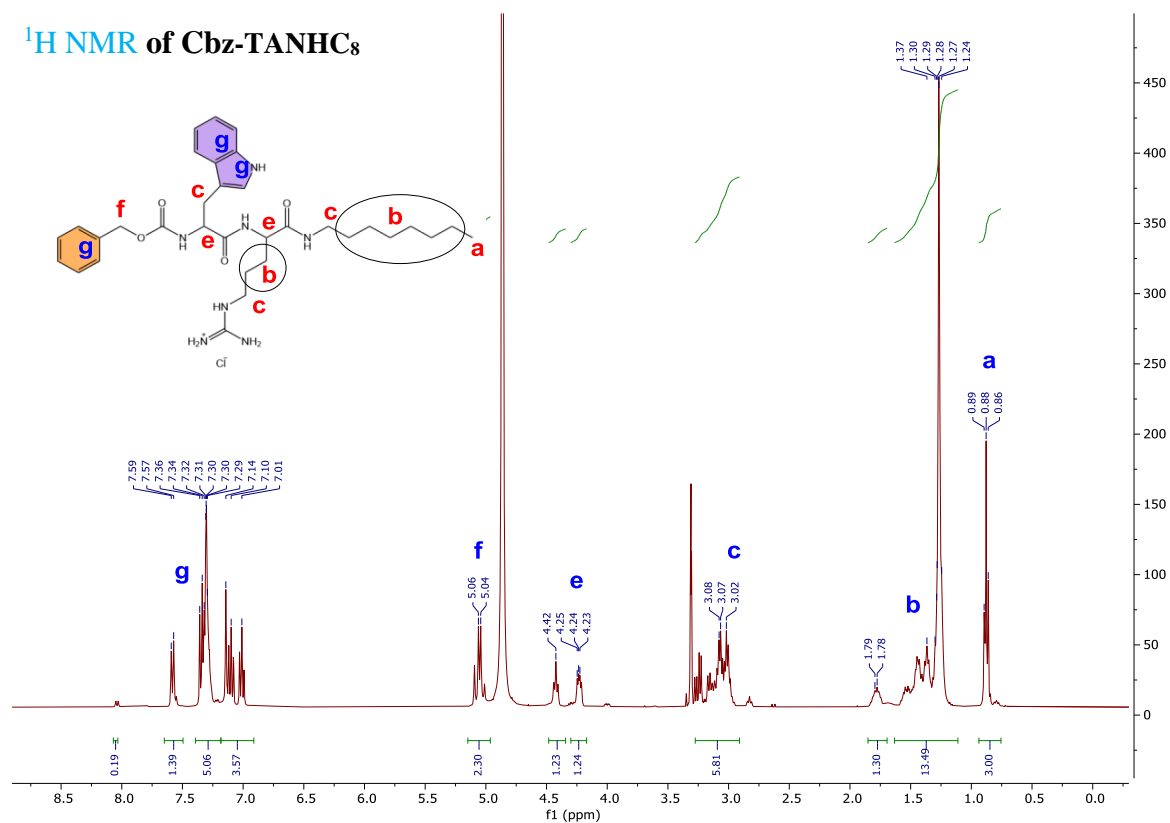
### ESI-MS of Cbz-TANHC<sub>8</sub>

Lordes Perez  
 Lourdes\_280518\_R8 8C 8 [0.410] Cm [5:11]

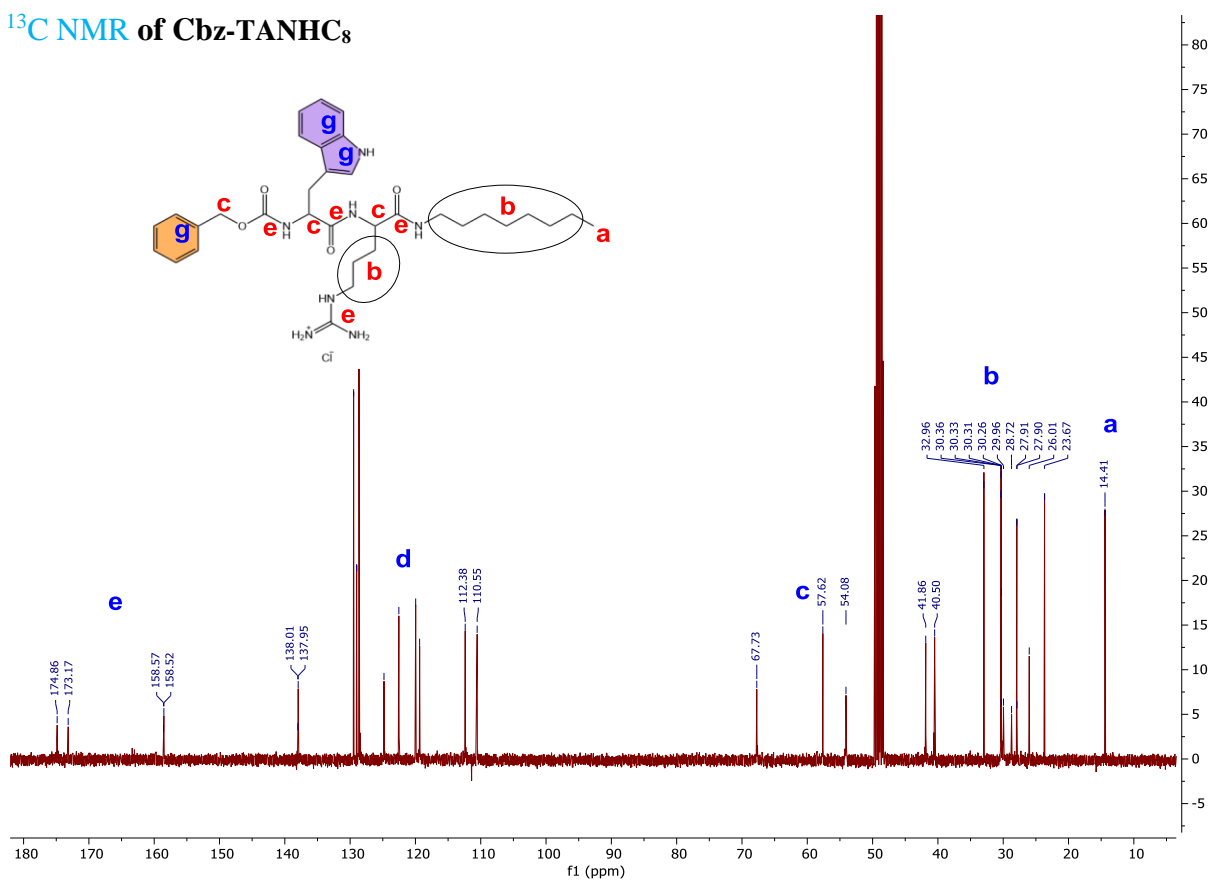
1: TOF MS ES+  
 4.58e6



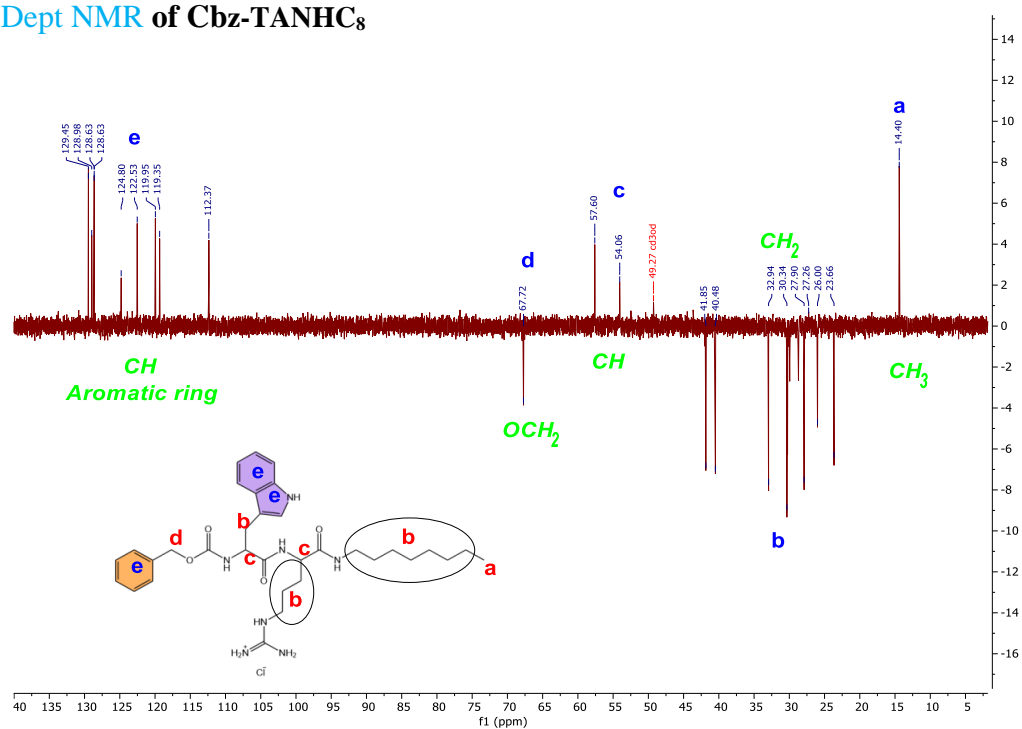
# <sup>1</sup>H NMR of Cbz-TANHC<sub>8</sub>



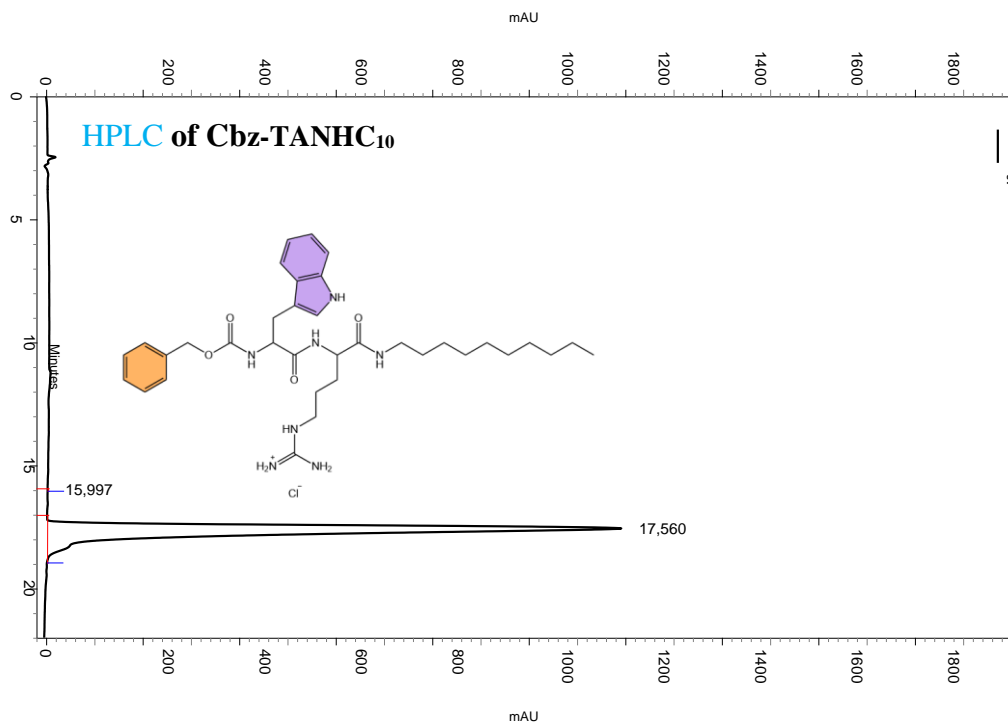
# <sup>13</sup>C NMR of Cbz-TANHC<sub>8</sub>



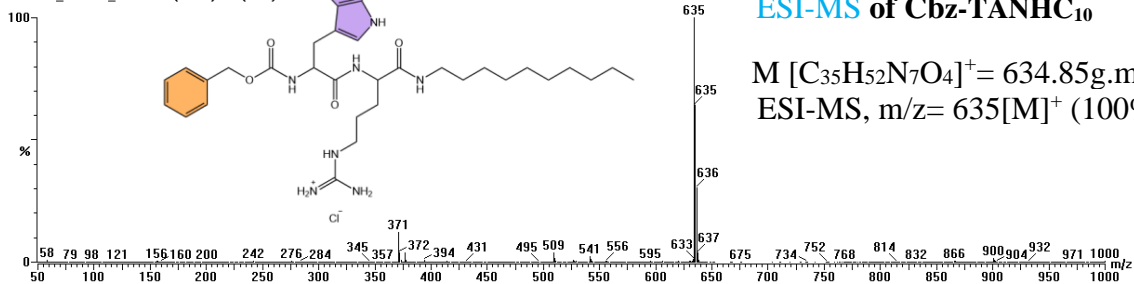
# Dept NMR of Cbz-TANHC<sub>8</sub>



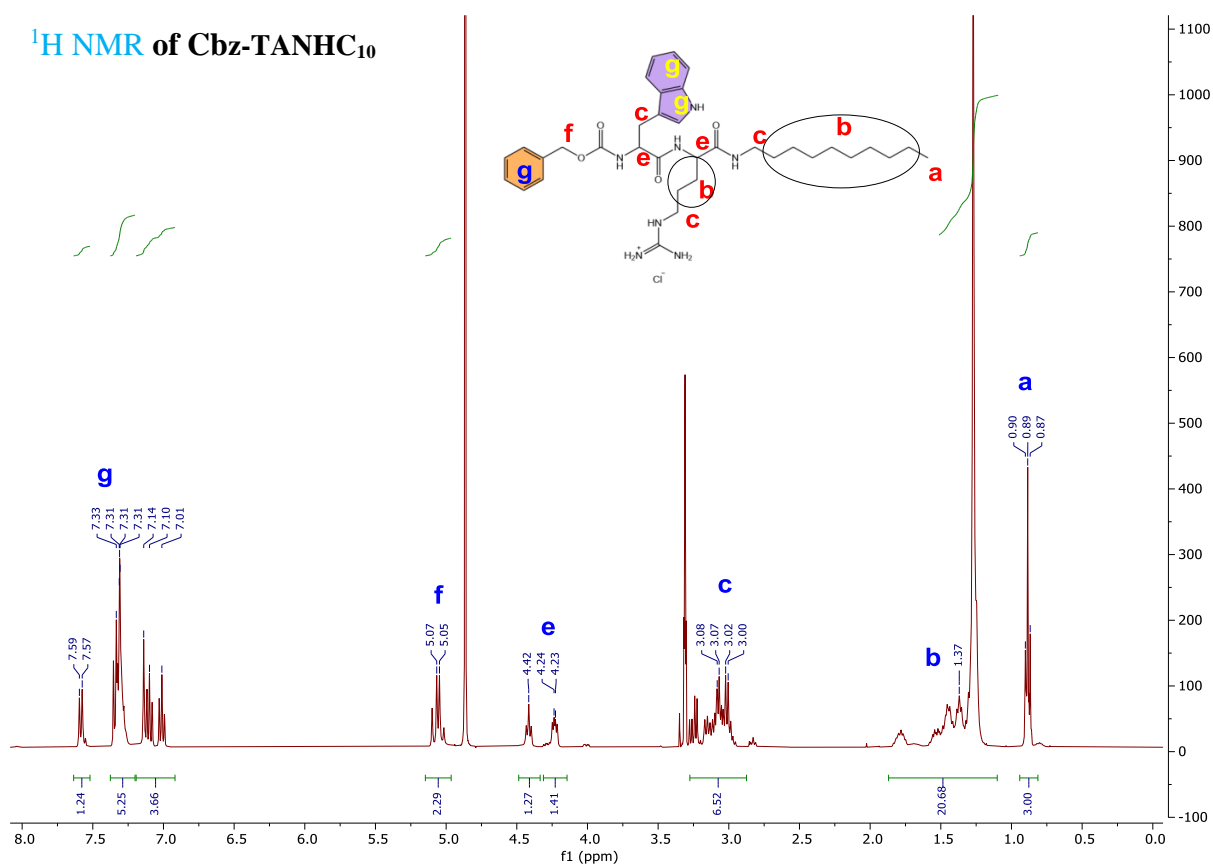
. **Figure S17.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of Cbz-TANHC<sub>8</sub>



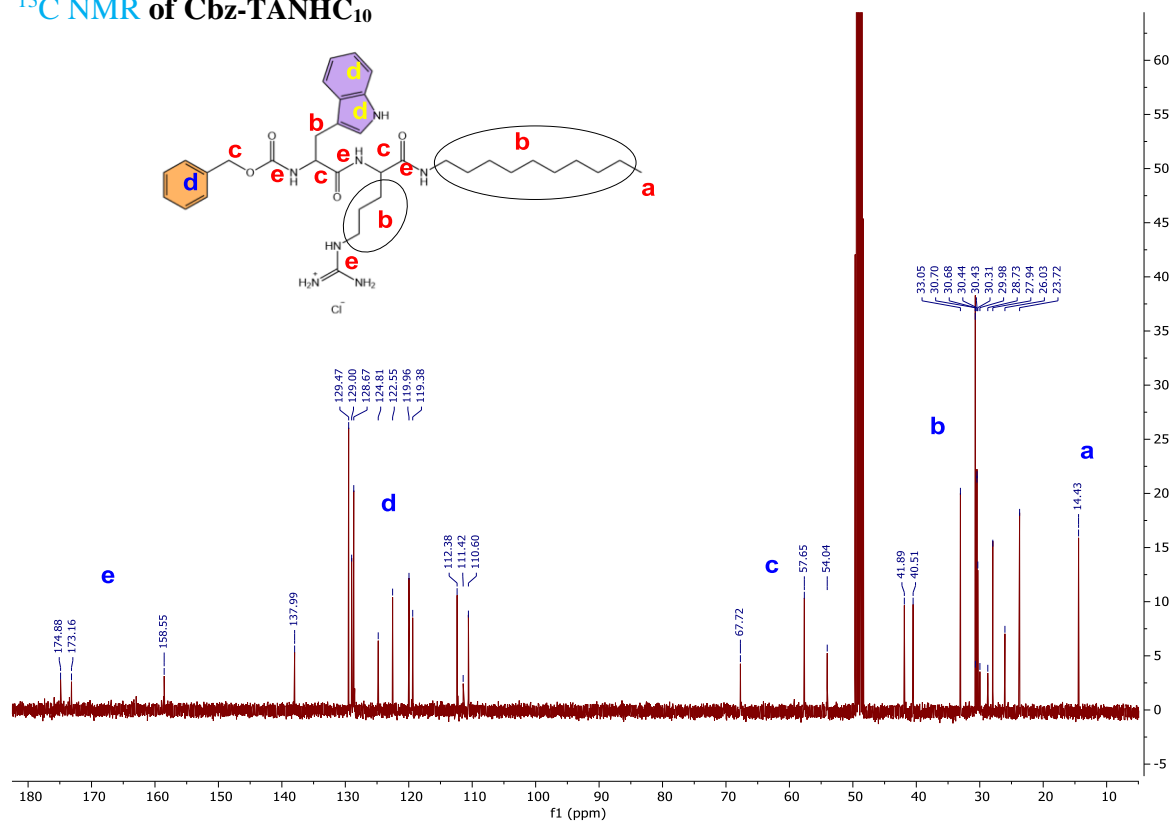
Lourdes Perez  
 Lourdes\_170518\_R8 10C 8 (0.425) Cm (7:11)



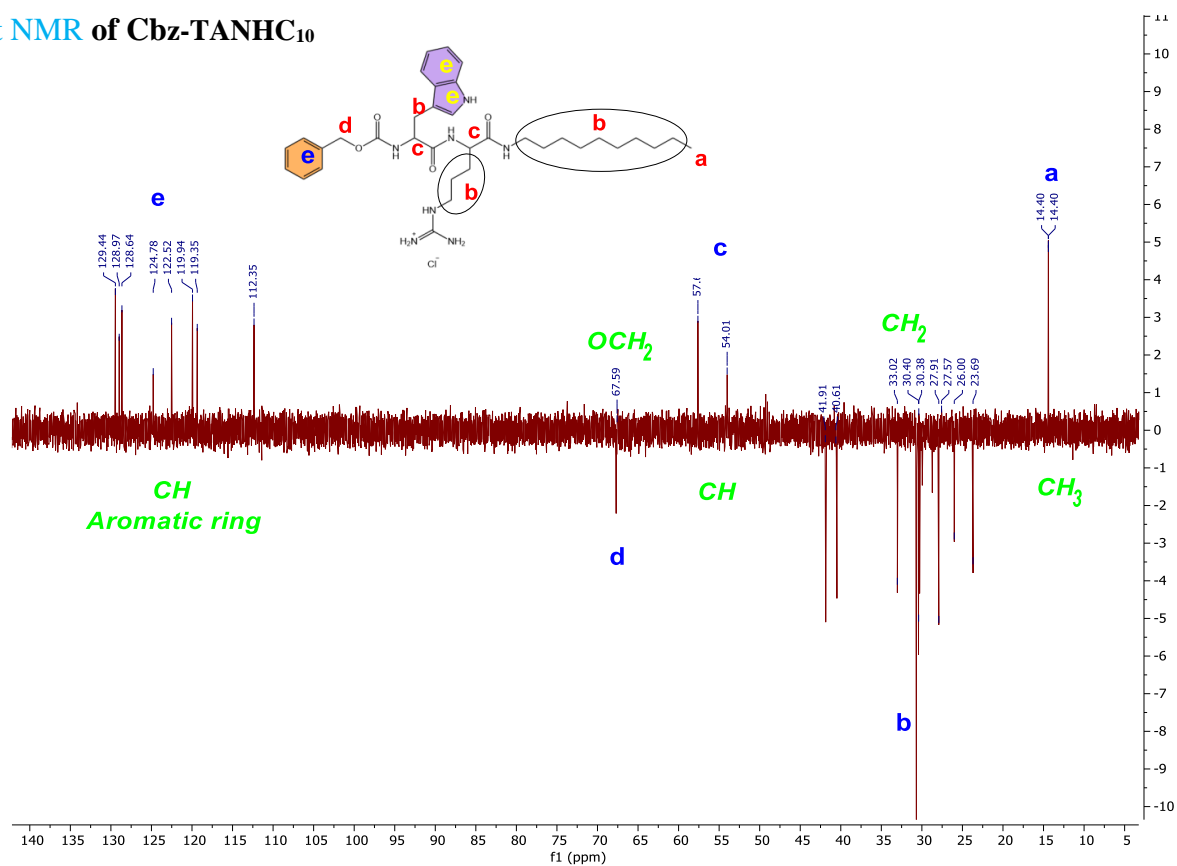
# <sup>1</sup>H NMR of Cbz-TANHC<sub>10</sub>



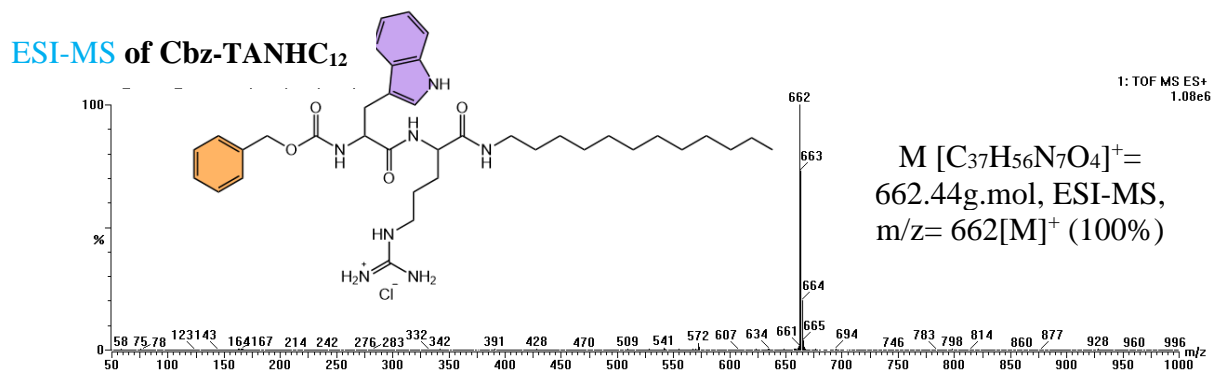
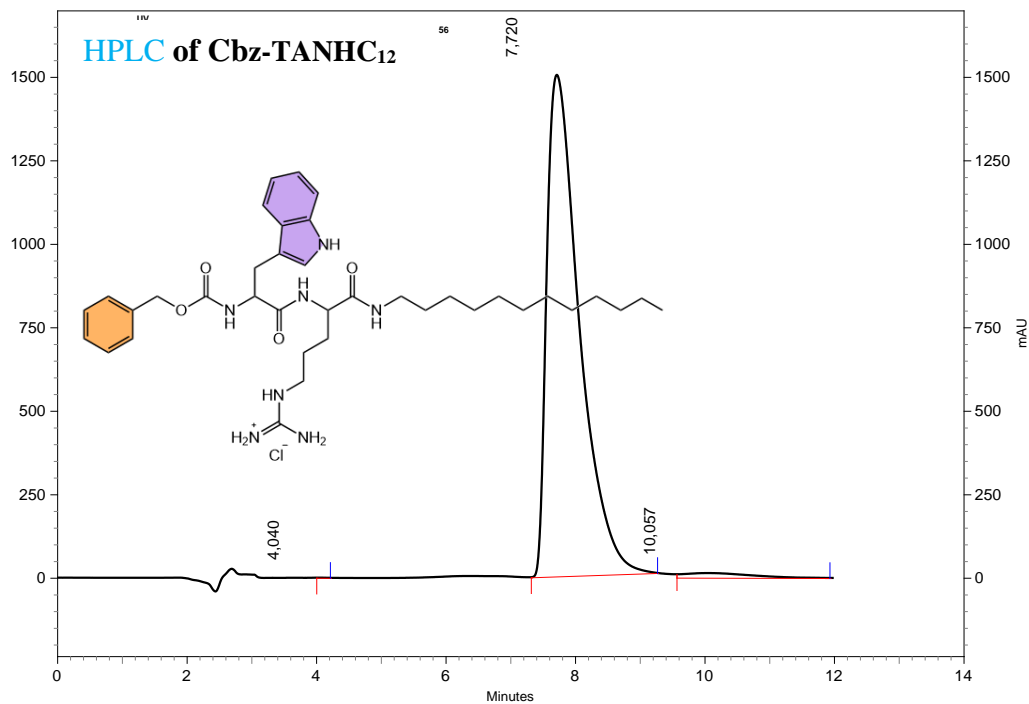
# <sup>13</sup>C NMR of Cbz-TANHC<sub>10</sub>



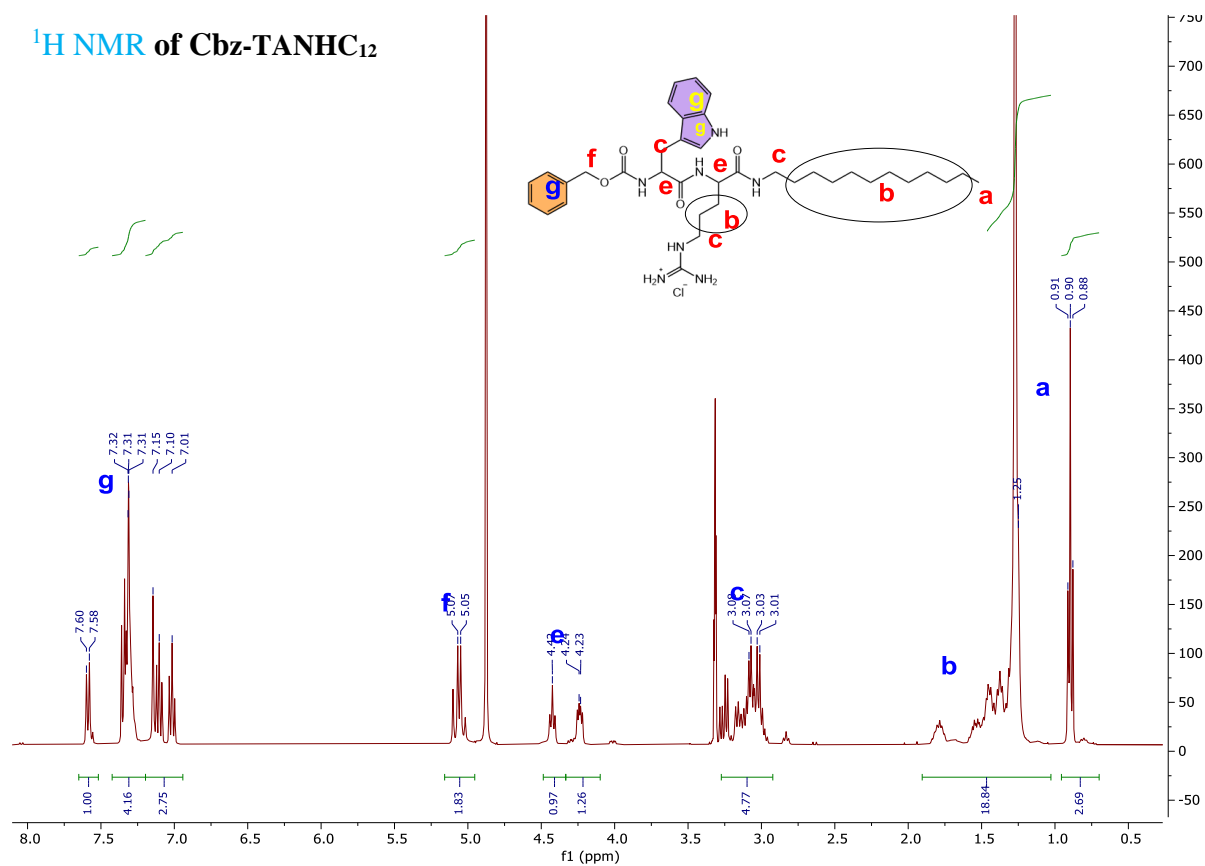
# Dept NMR of Cbz-TANHC<sub>10</sub>



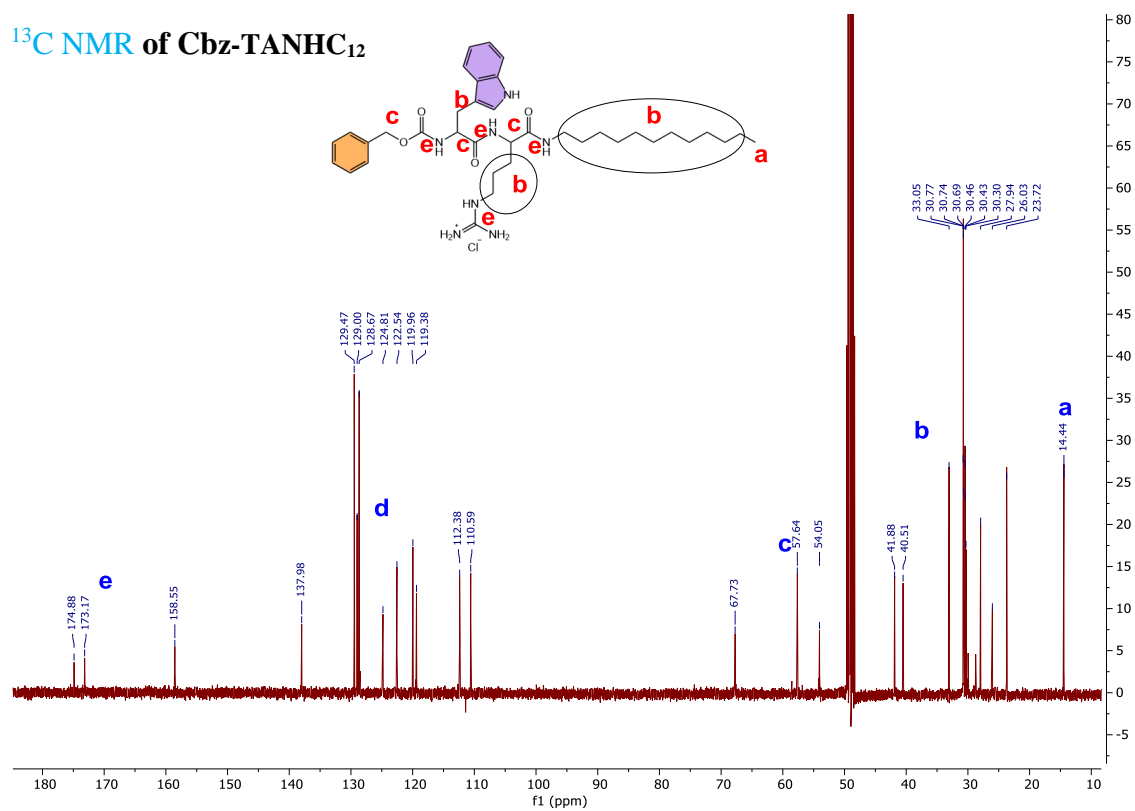
**Figure S18.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of Cbz-TANHC<sub>10</sub>



# <sup>1</sup>H NMR of Cbz-TANHC<sub>12</sub>

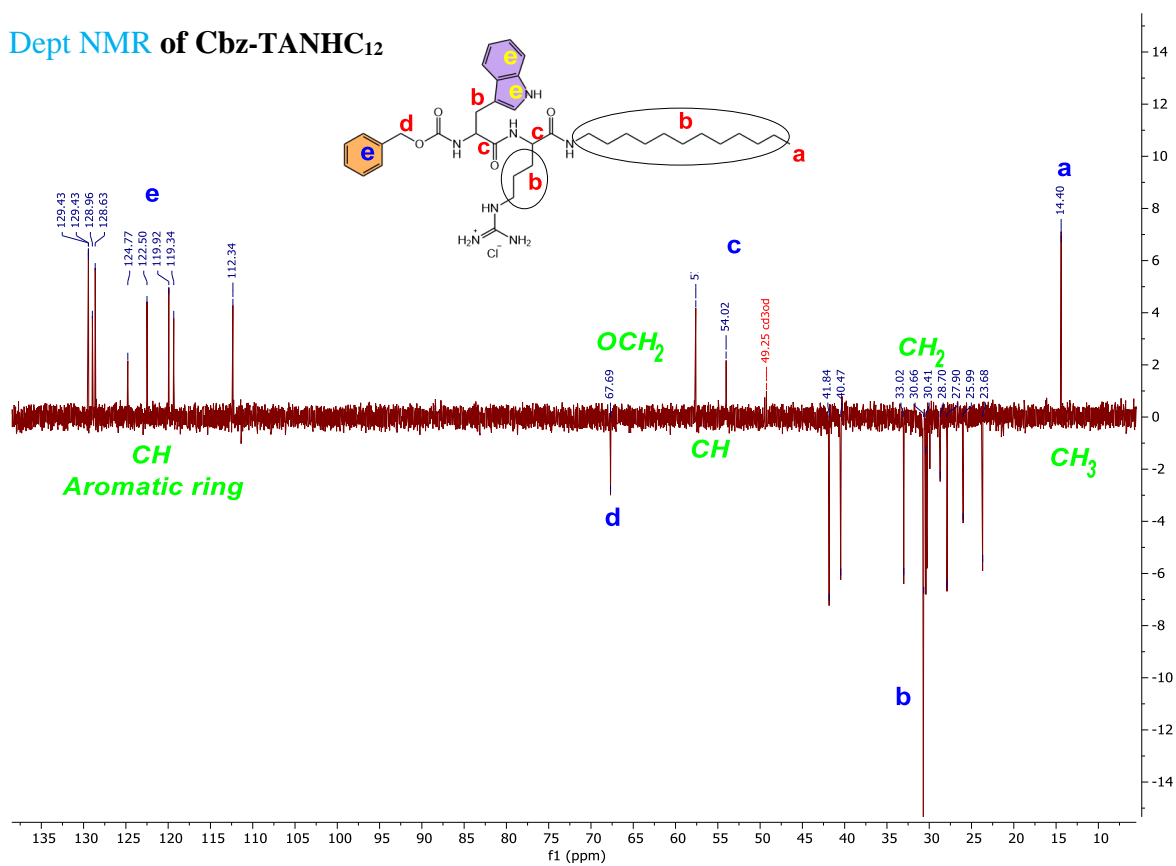


# <sup>13</sup>C NMR of Cbz-TANHC<sub>12</sub>





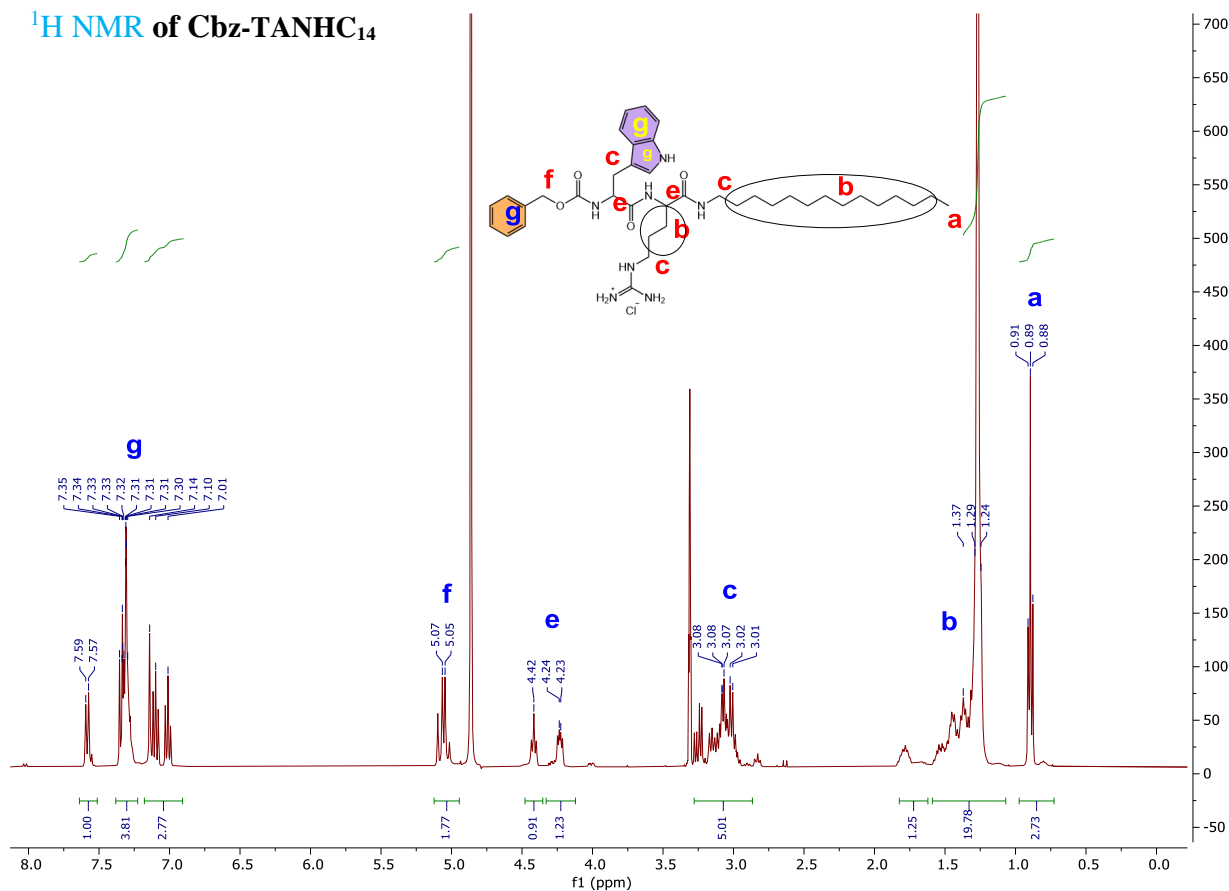
# Dept NMR of Cbz-TANHC<sub>12</sub>



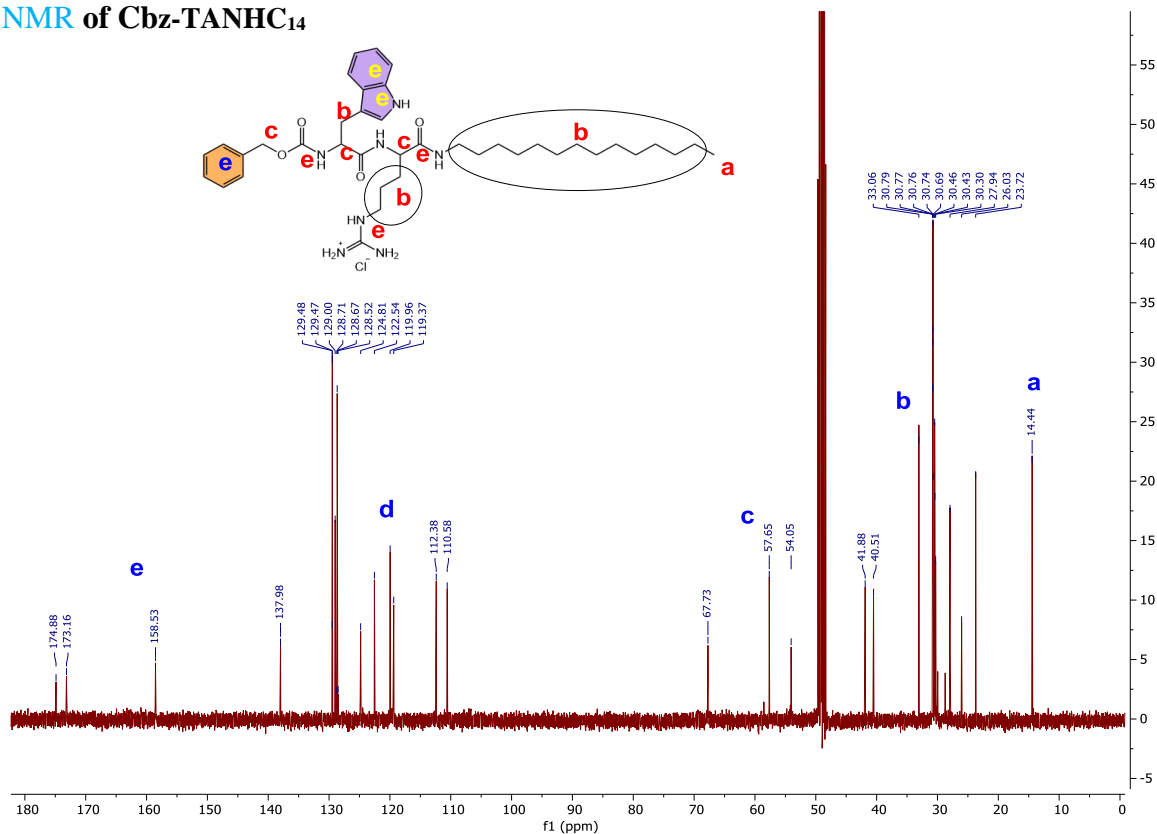
**Figure S19.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of Cbz-TANHC<sub>12</sub>



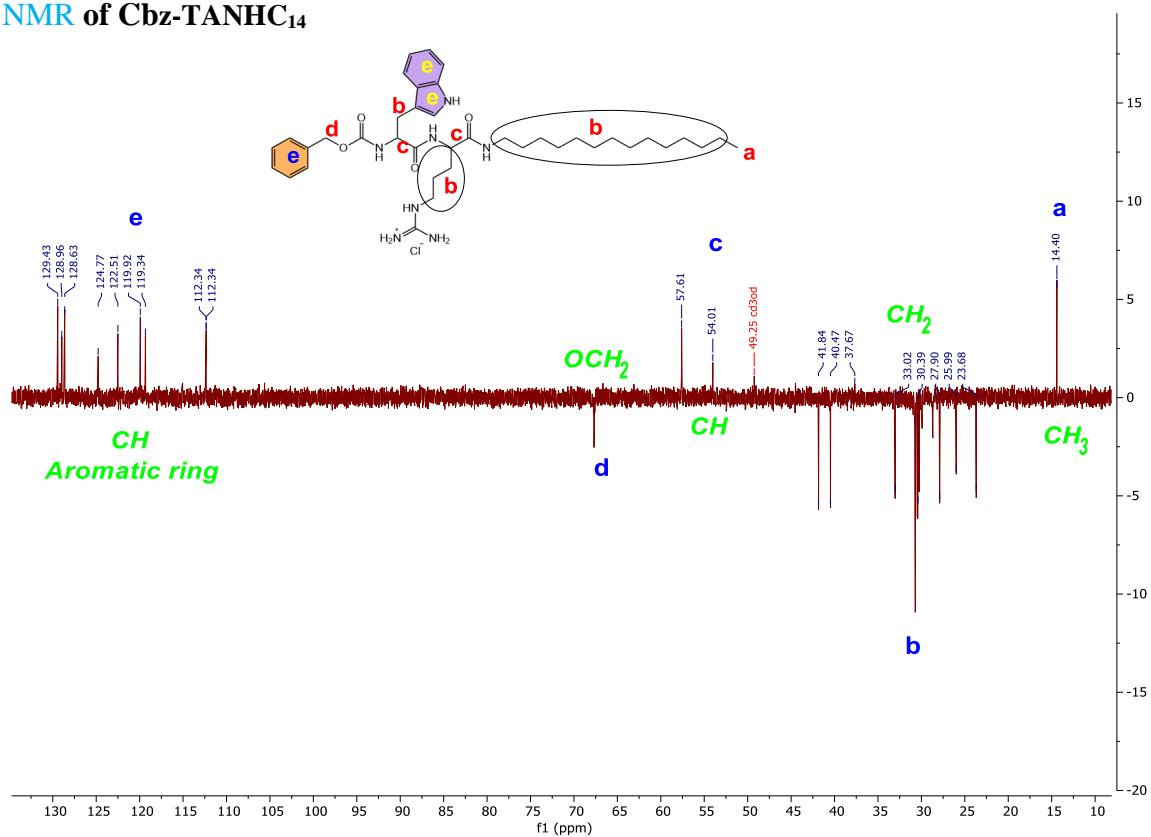
# <sup>1</sup>H NMR of Cbz-TANHC<sub>14</sub>



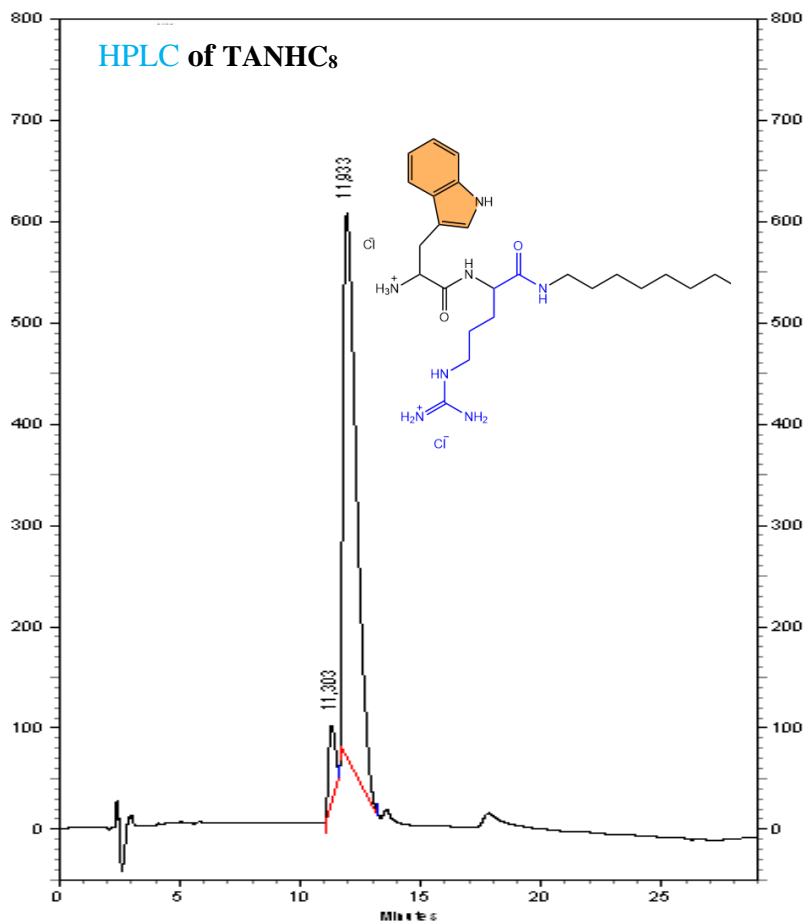
# <sup>13</sup>C NMR of Cbz-TANHC<sub>14</sub>



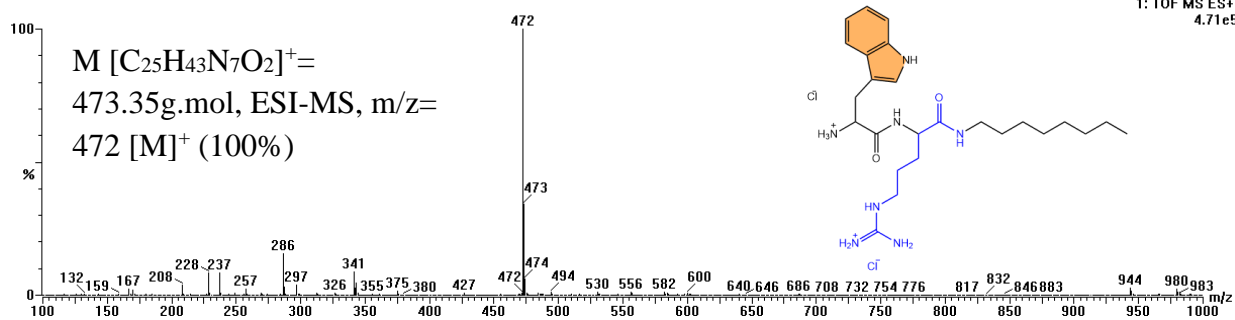
# Dept NMR of Cbz-TANHC<sub>14</sub>



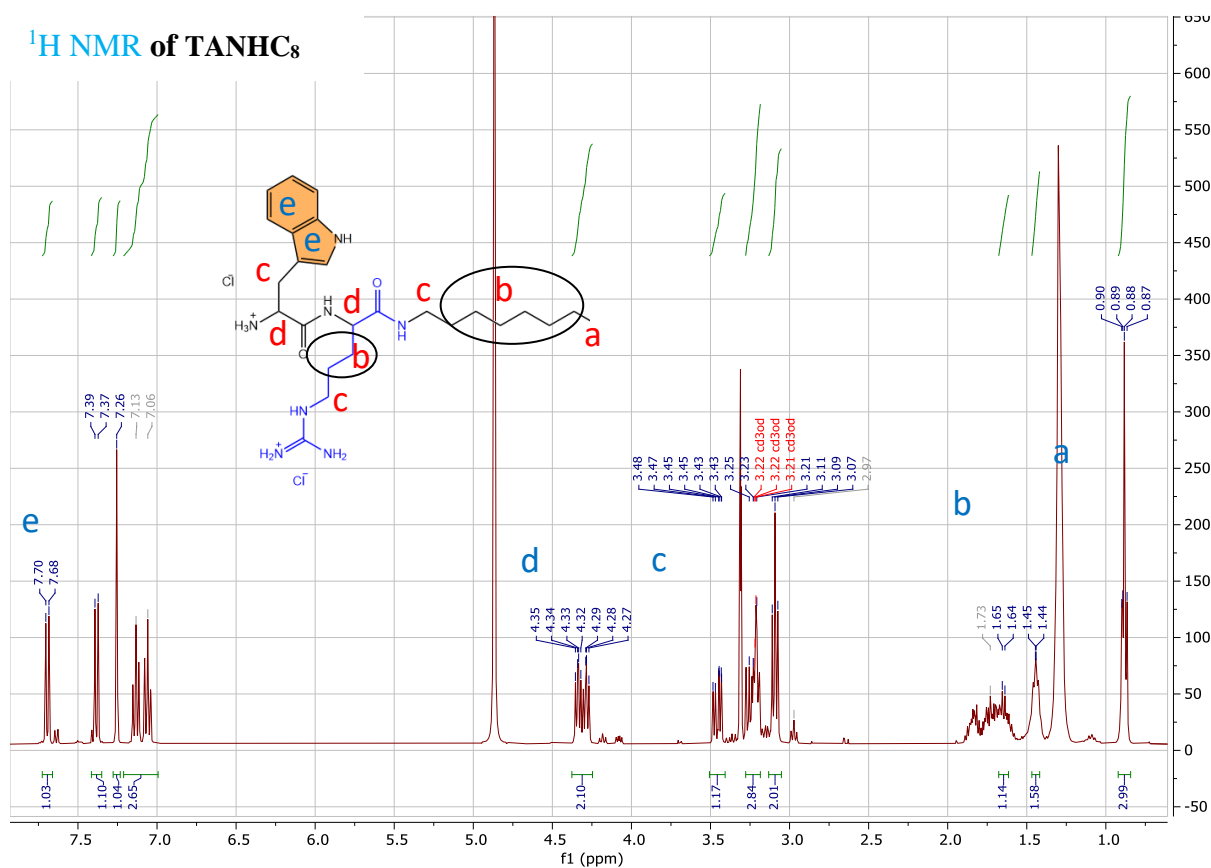
**Figure S20.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of Cbz-TANHC<sub>14</sub>



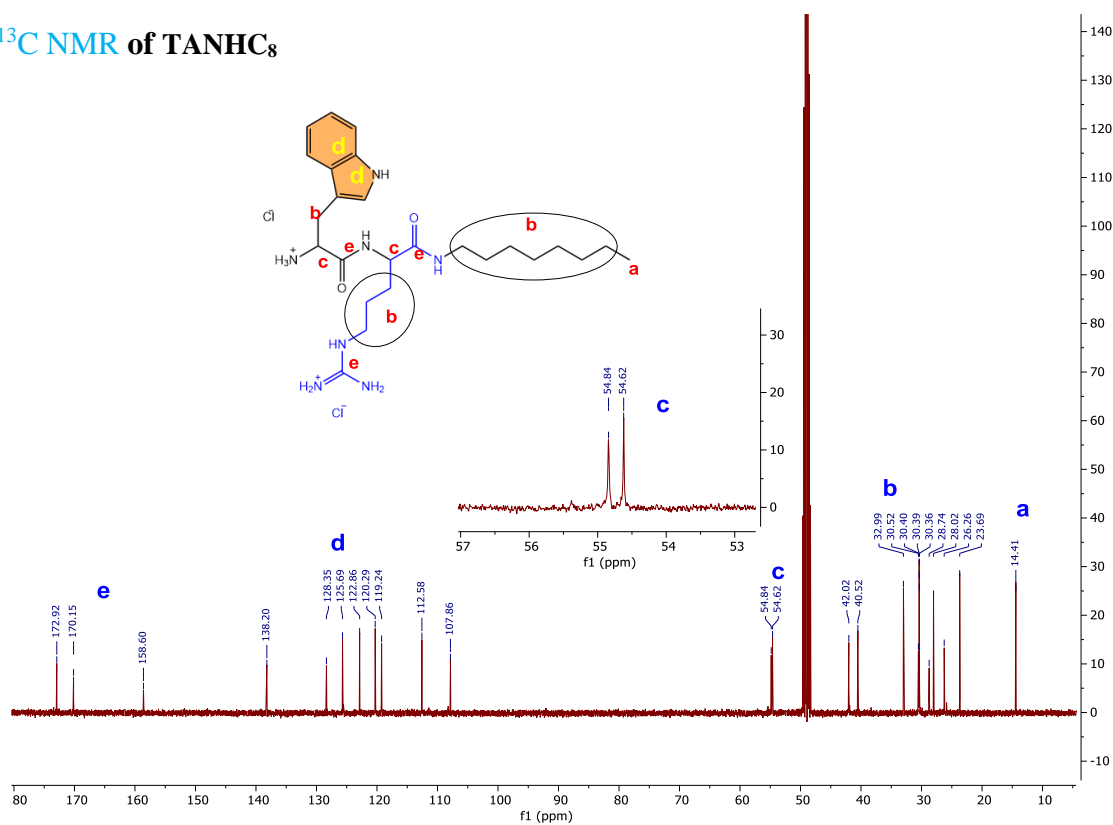
### ESI-MS of TANHC<sub>8</sub>



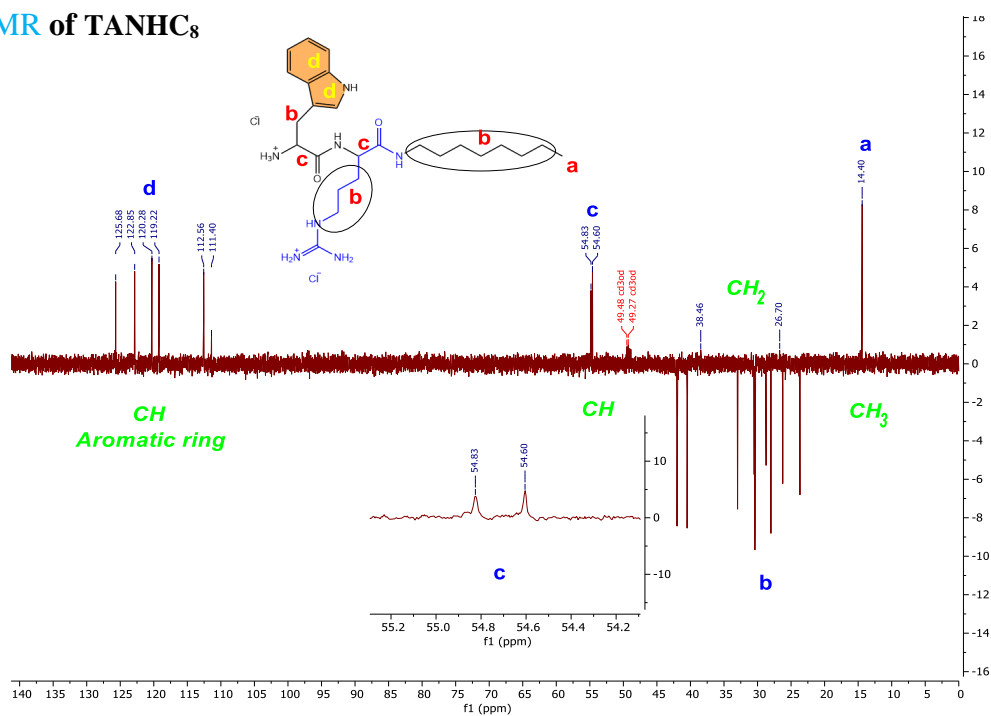
# <sup>1</sup>H NMR of TANHC<sub>8</sub>



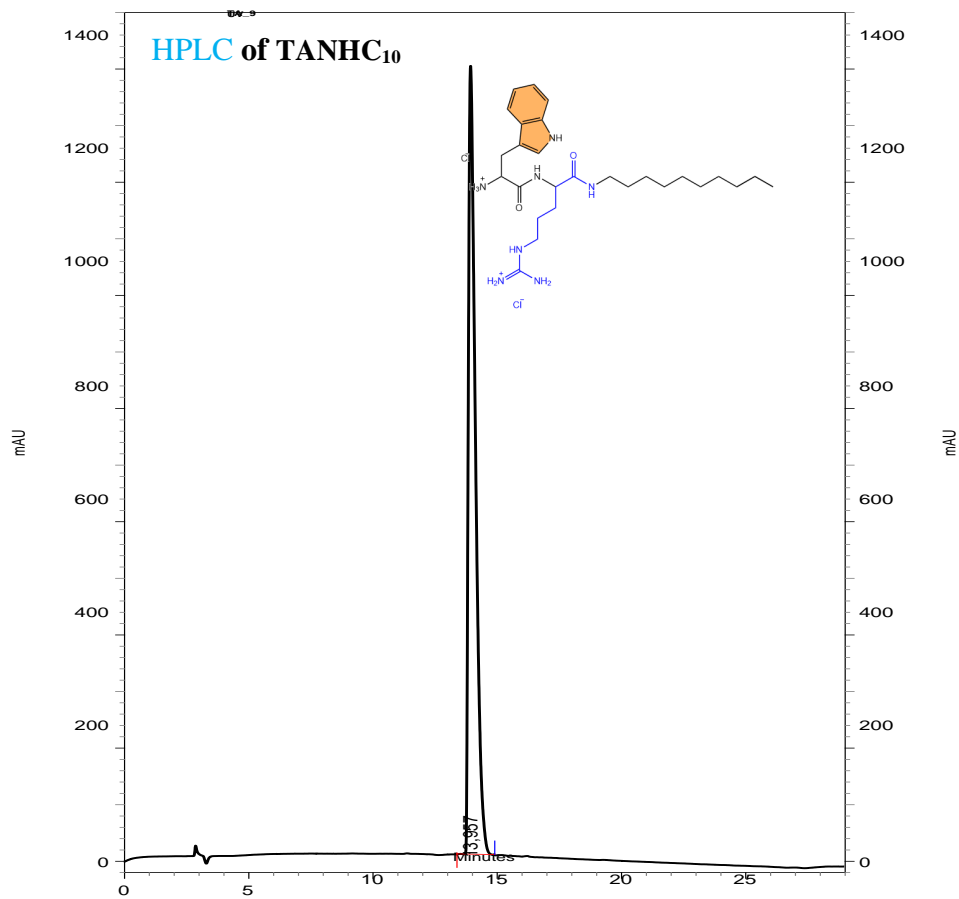
# <sup>13</sup>C NMR of TANHC<sub>8</sub>



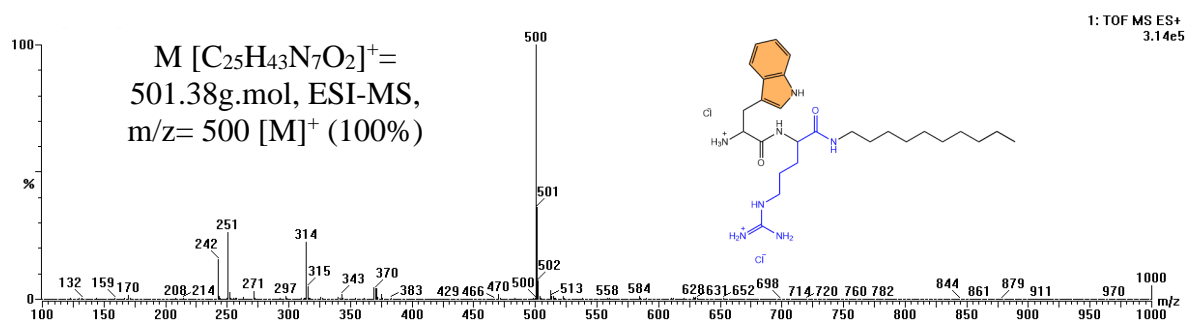
# Dept NMR of TANHC<sub>8</sub>



**Figure S21.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of TANHC<sub>8</sub>

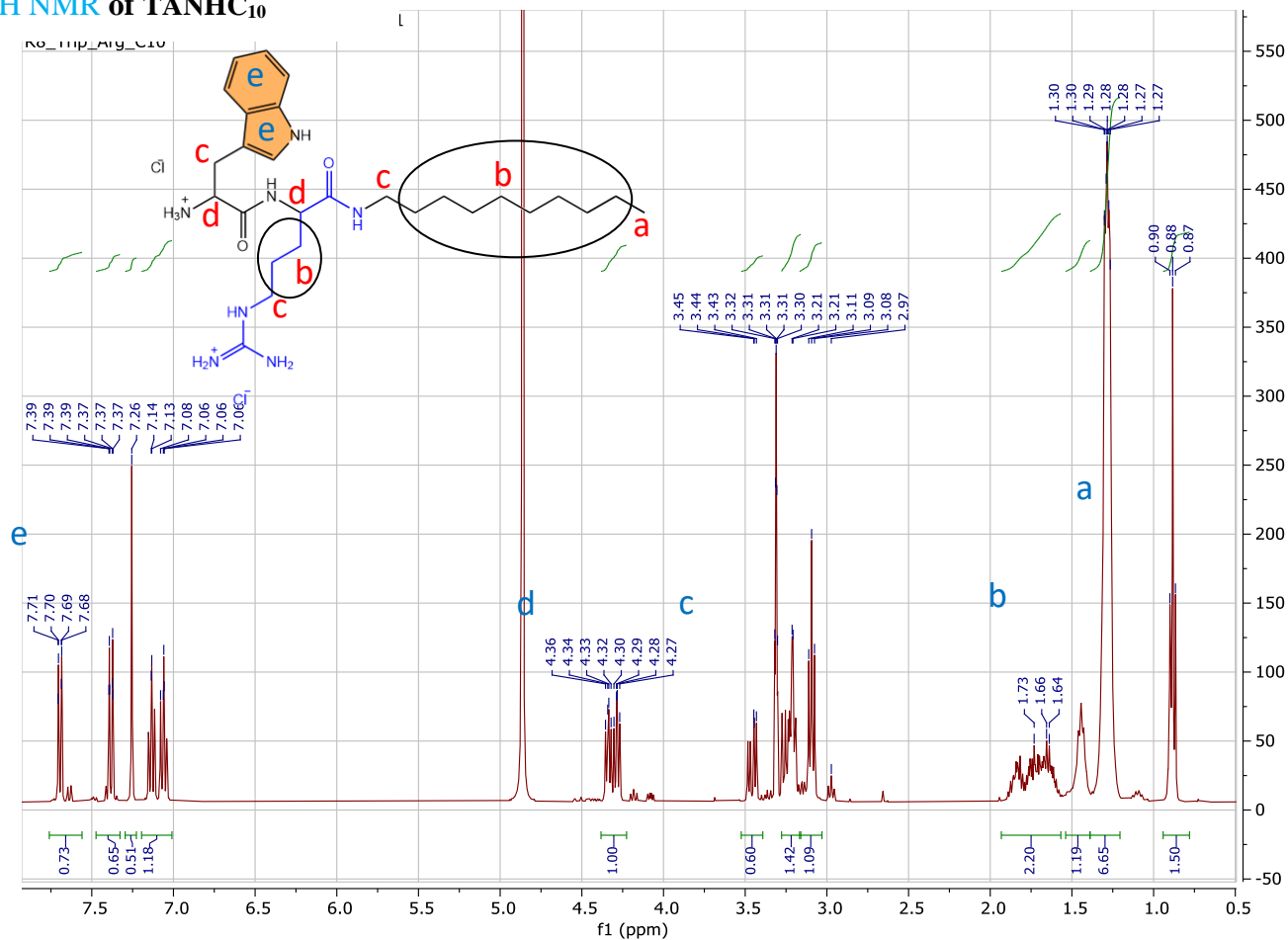


**ESI-MS of TANHC<sub>10</sub>**

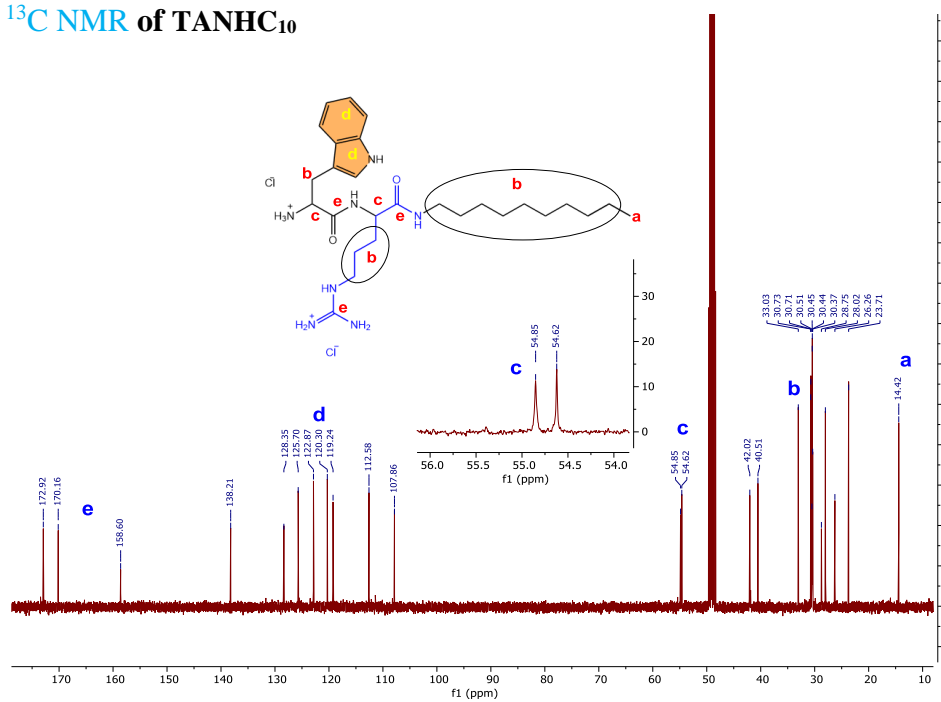




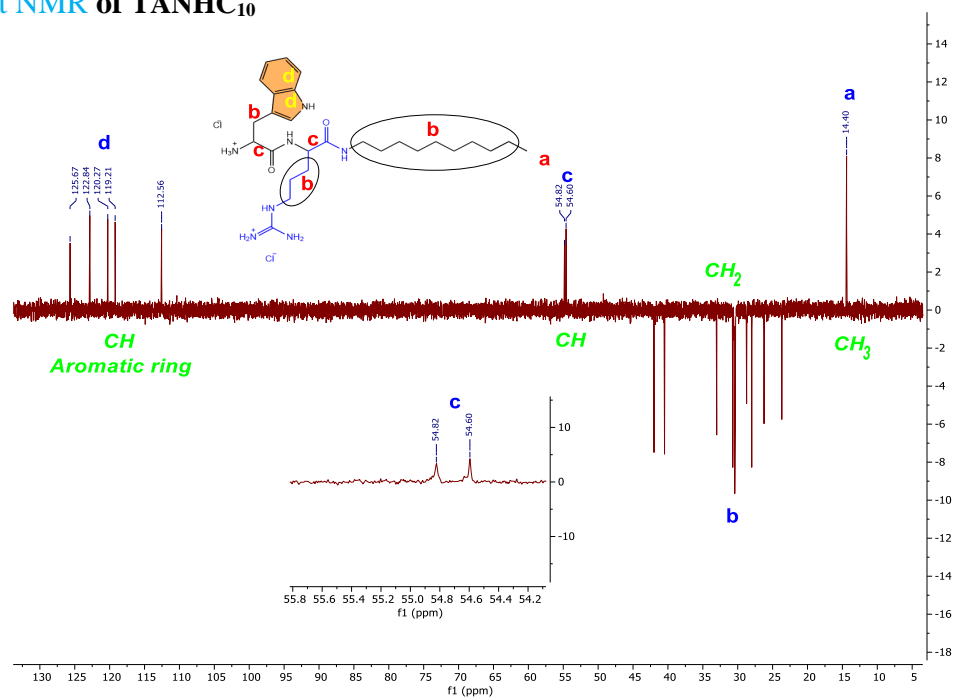
# <sup>1</sup>H NMR of TANHC<sub>10</sub>



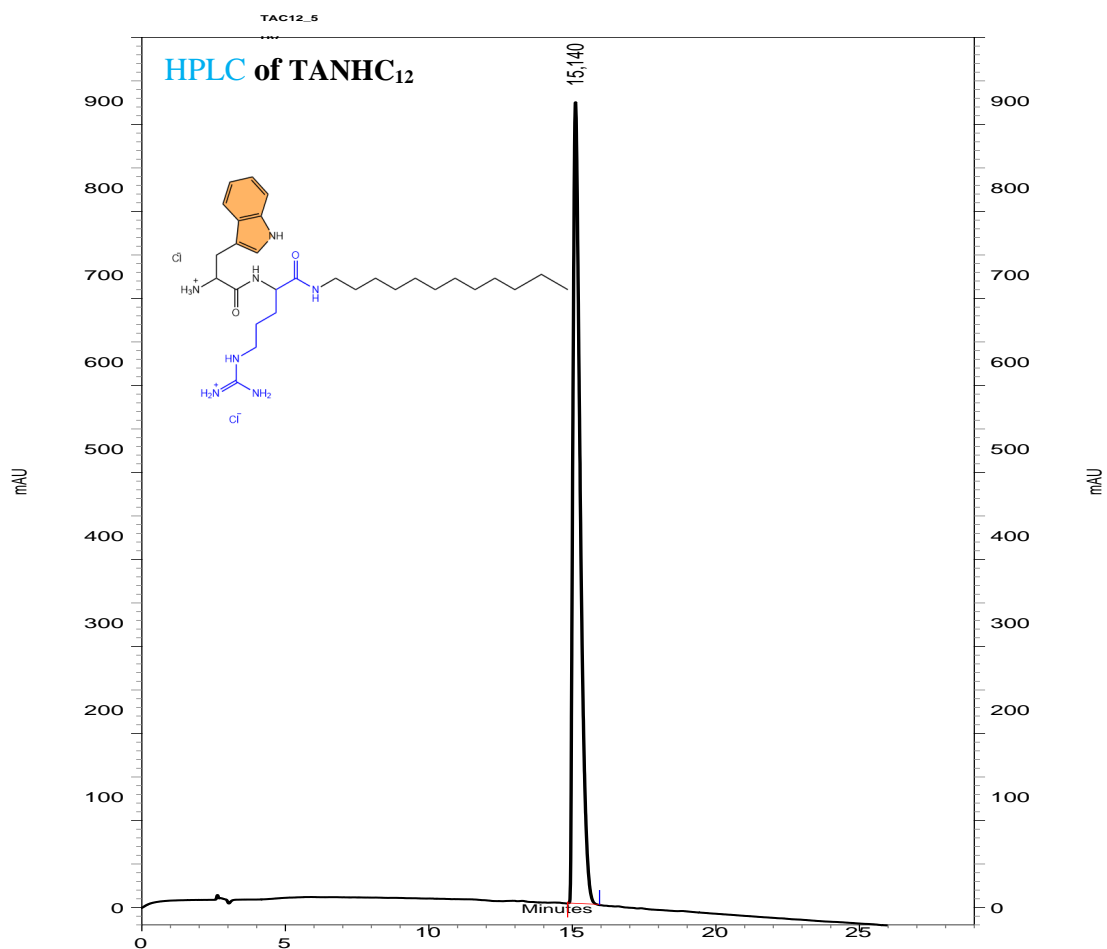
# <sup>13</sup>C NMR of TANHC<sub>10</sub>



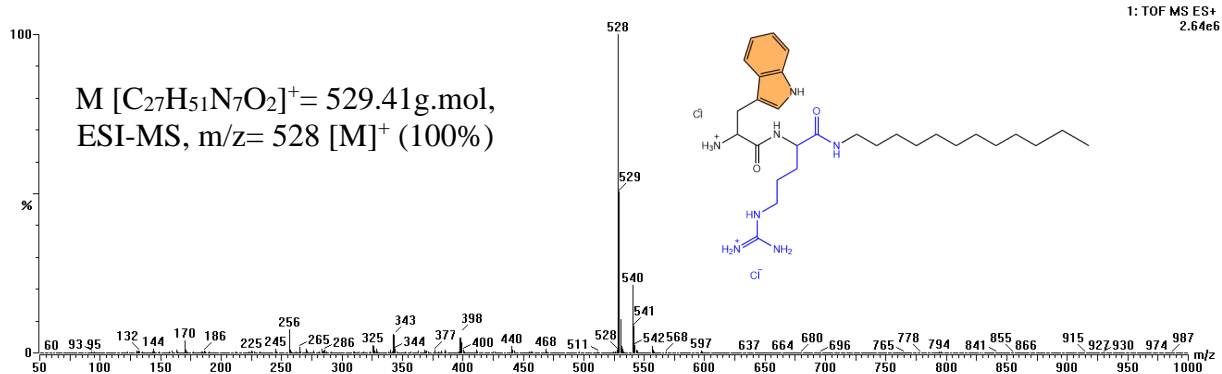
# Dept NMR of TANHC<sub>10</sub>



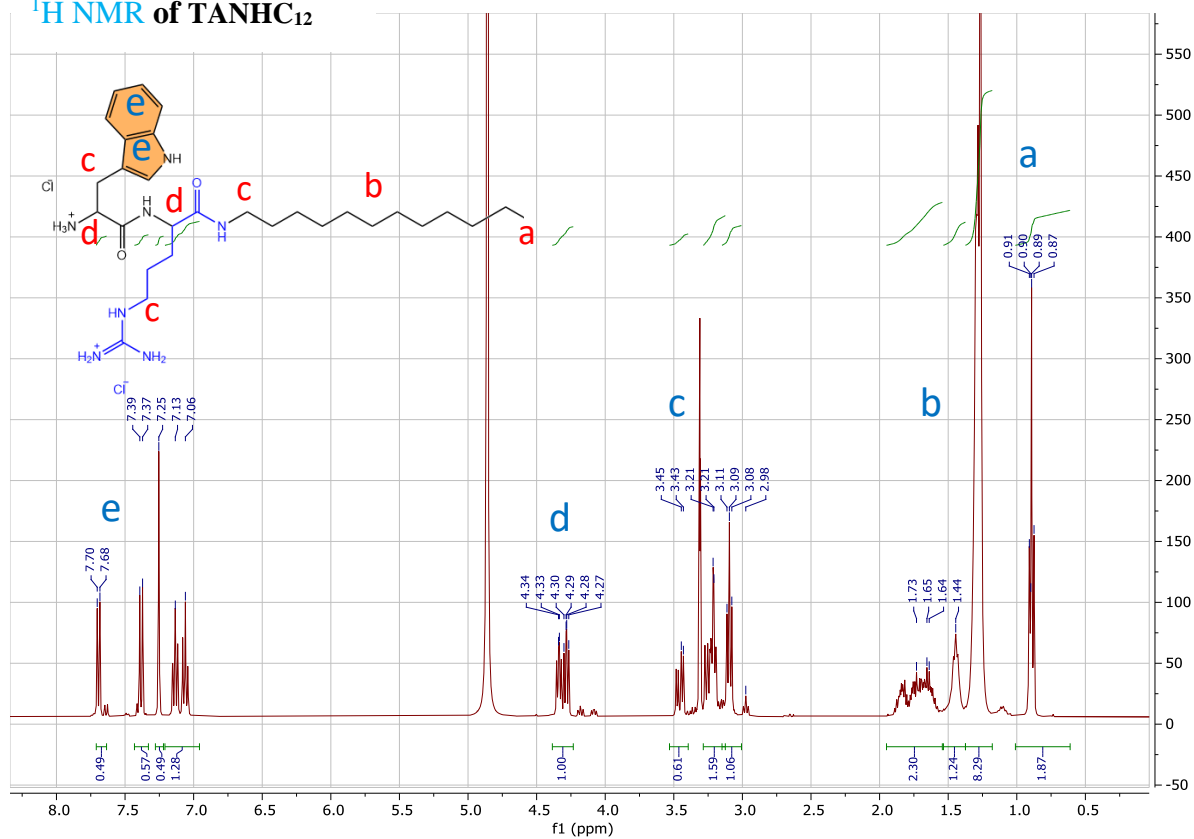
**Figure S22.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of TANHC<sub>10</sub>



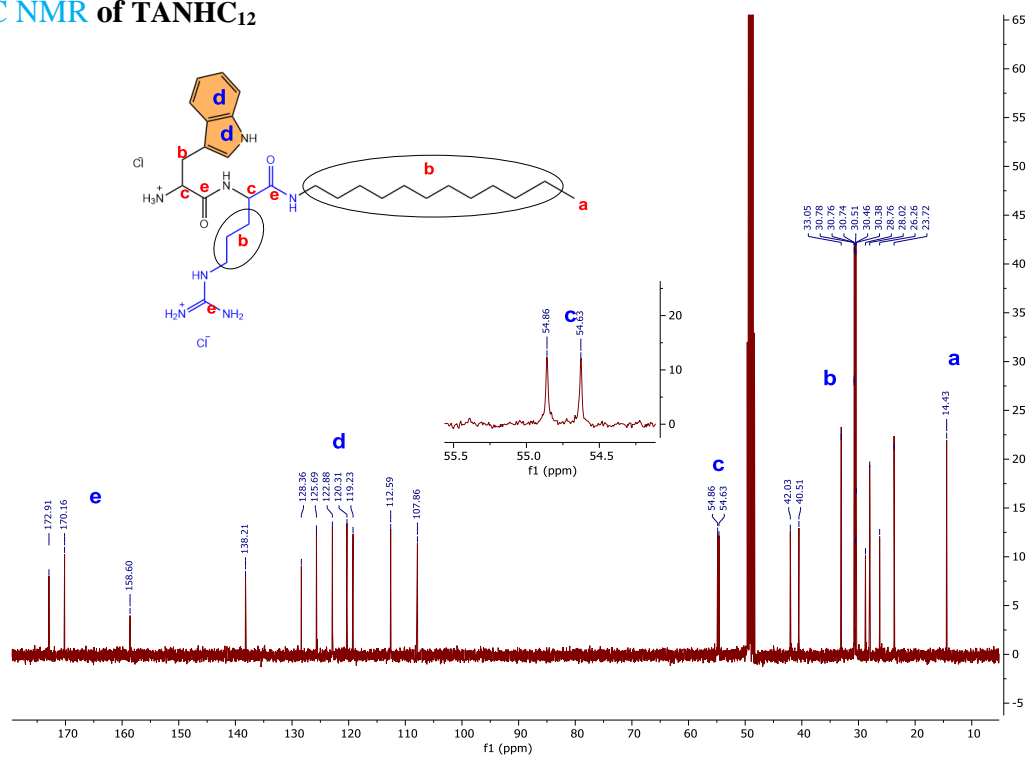
### ESI-MS of TANHC<sub>12</sub>



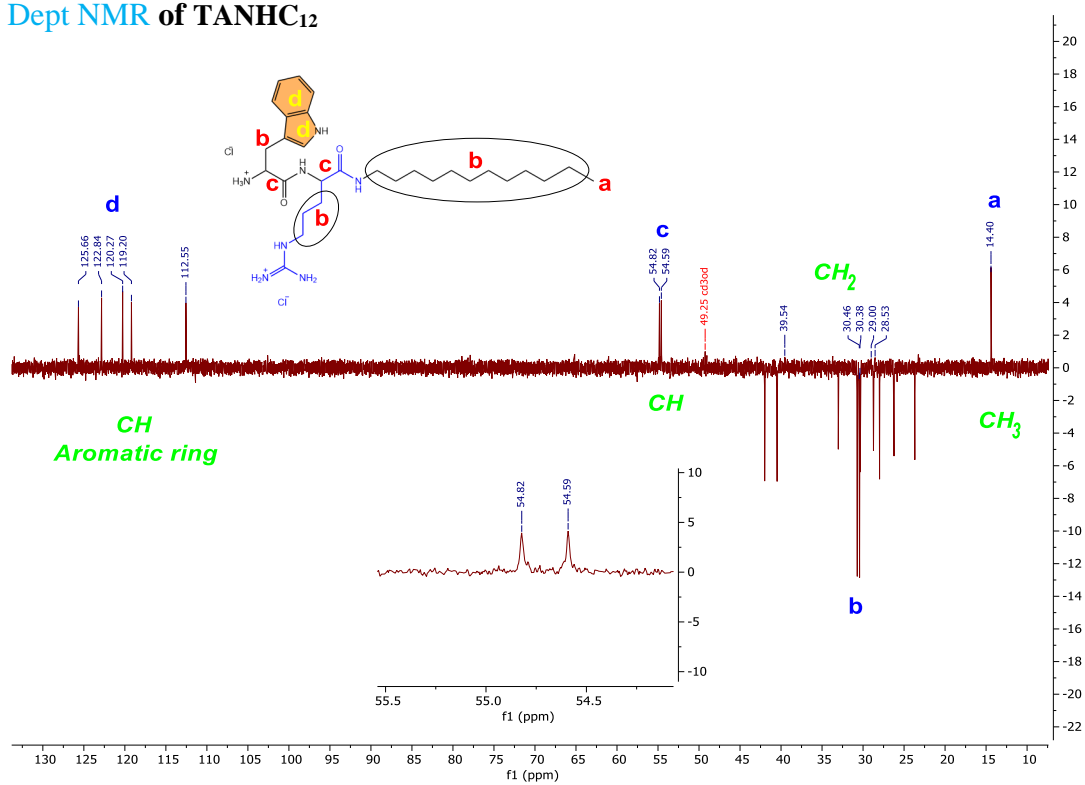
# <sup>1</sup>H NMR of TANHC<sub>12</sub>



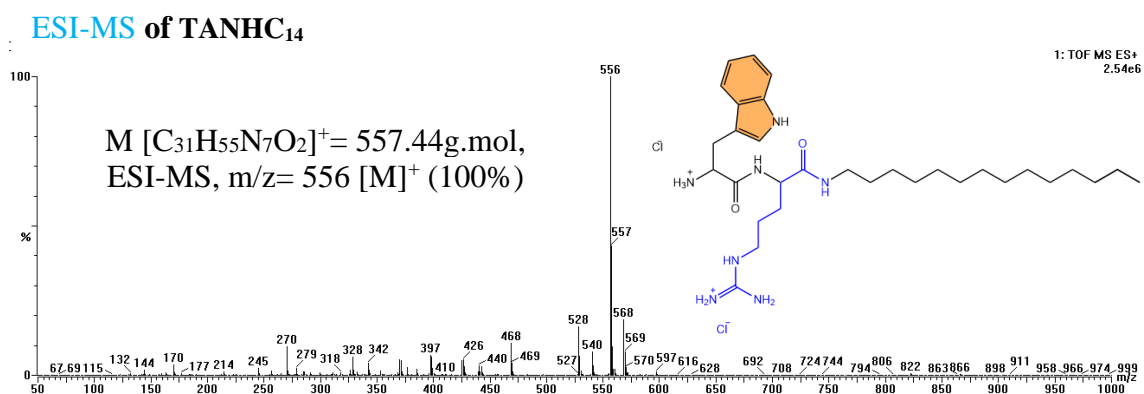
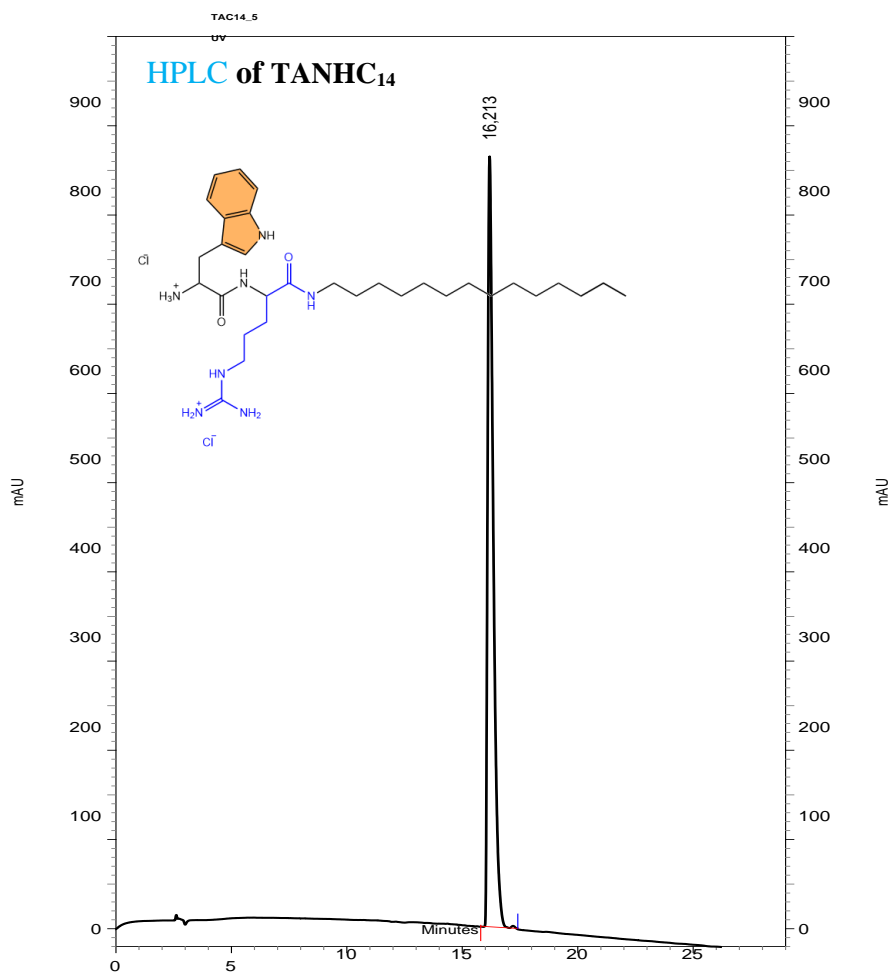
# <sup>13</sup>C NMR of TANHC<sub>12</sub>



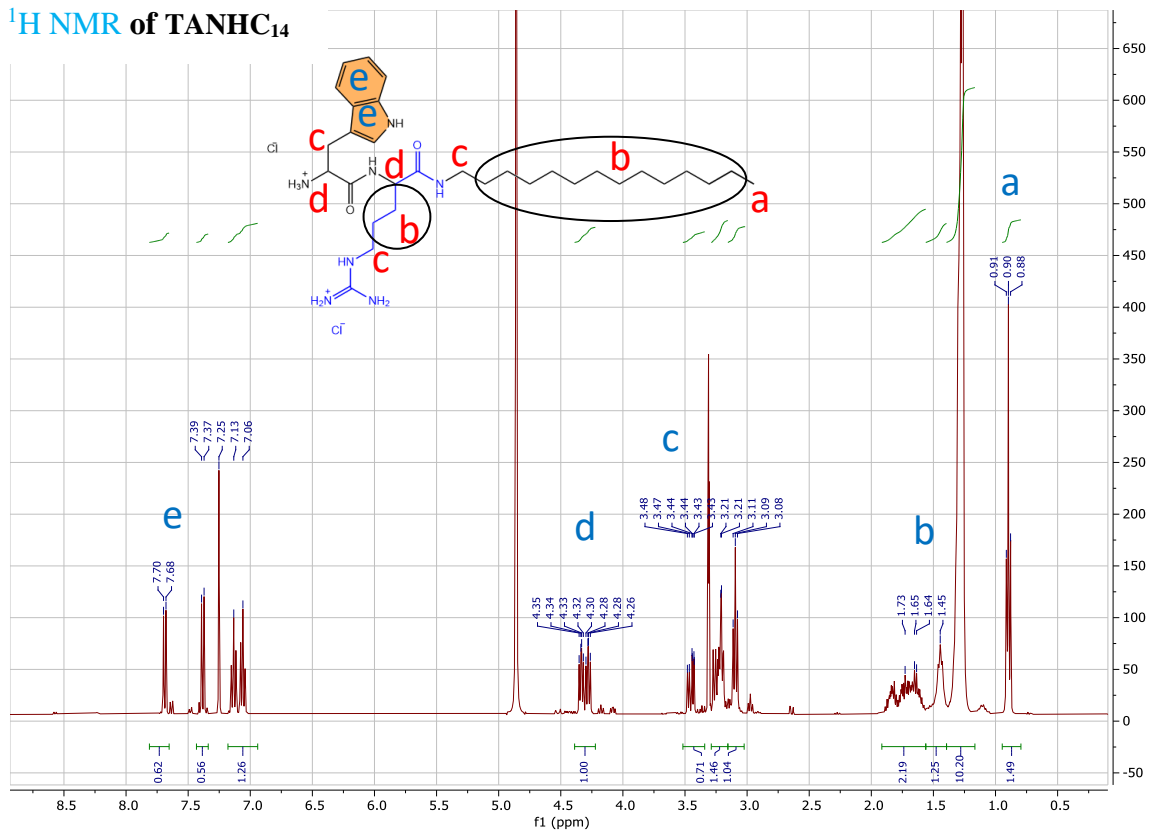
# Dept NMR of TANHC<sub>12</sub>



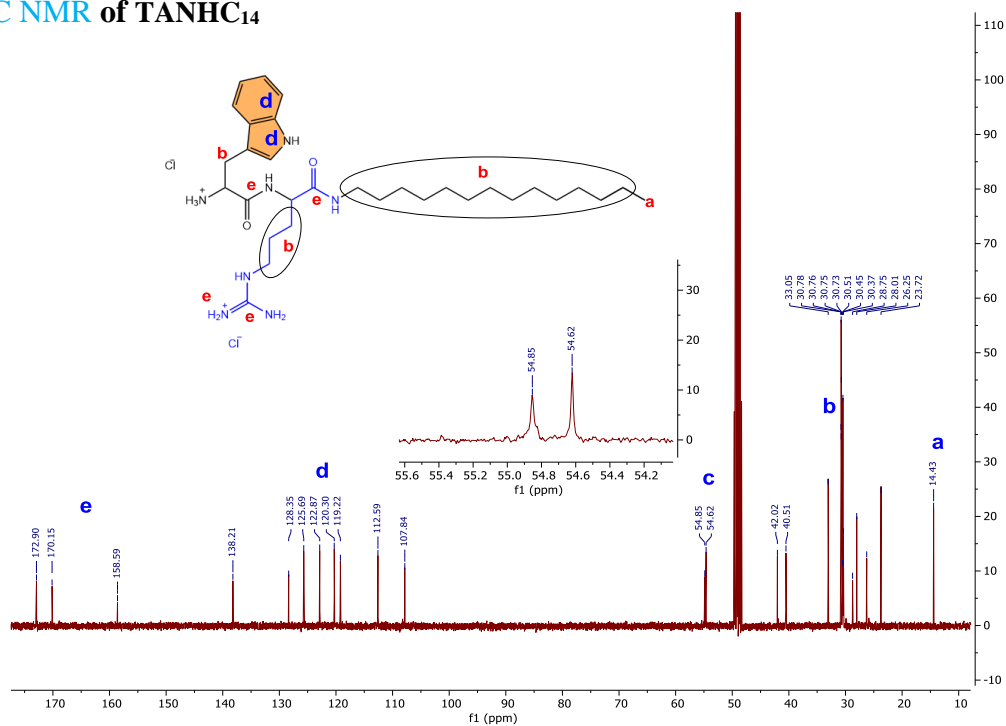
**Figure S23.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of TANHC<sub>12</sub>



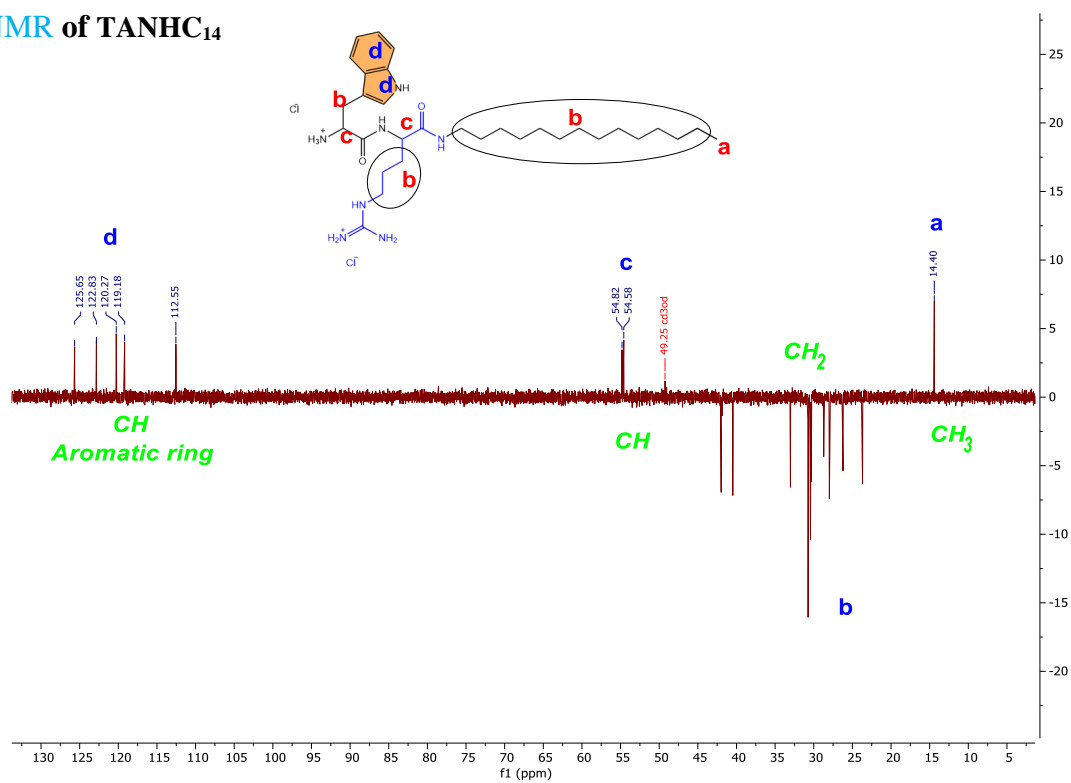
# <sup>1</sup>H NMR of TANHC<sub>14</sub>



# <sup>13</sup>C NMR of TANHC<sub>14</sub>

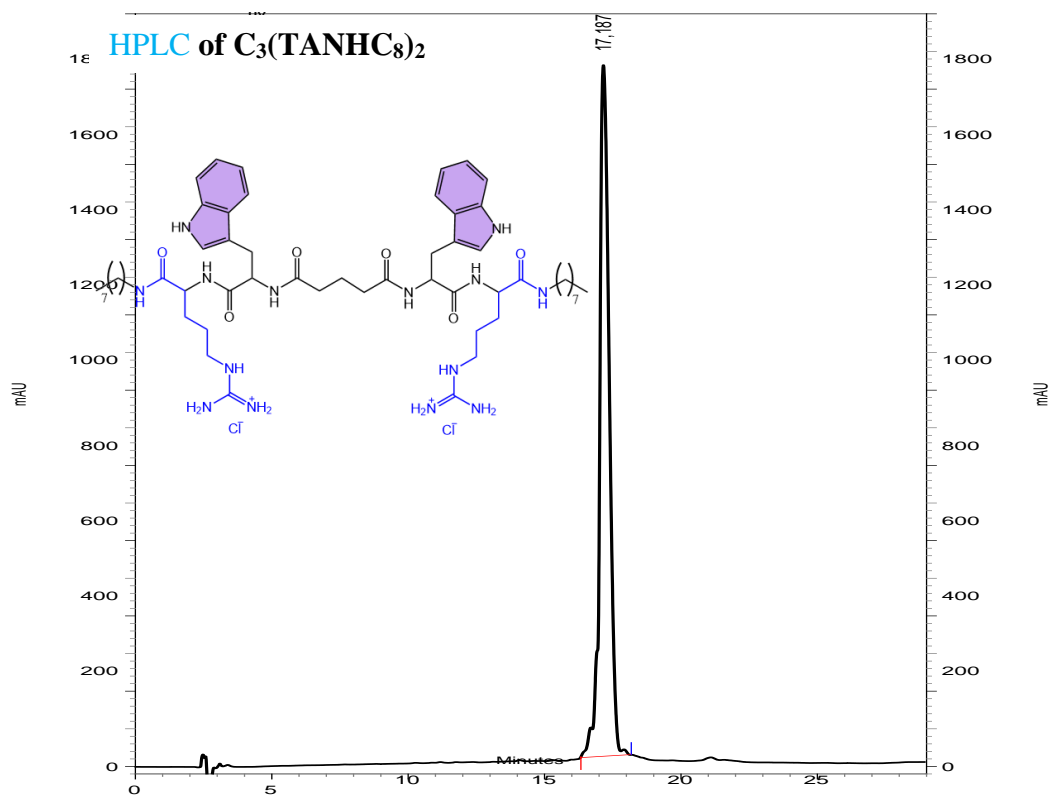


# Dept NMR of TANHC<sub>14</sub>

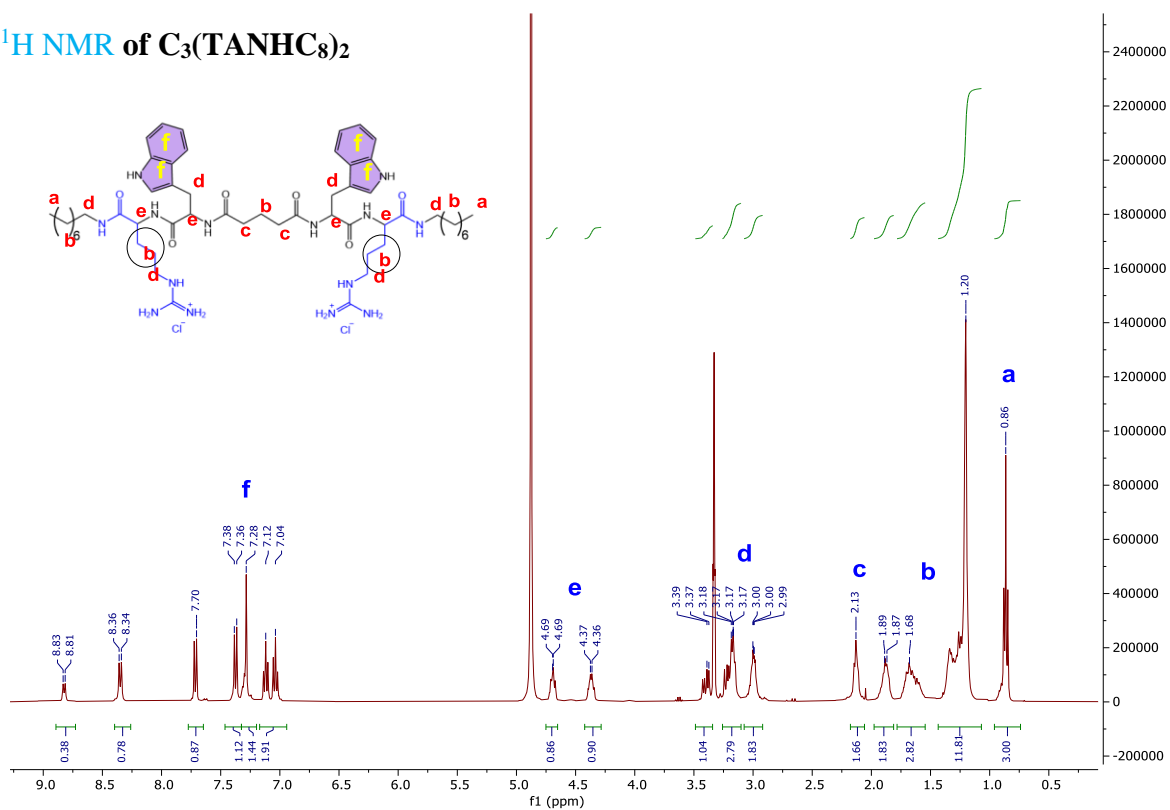


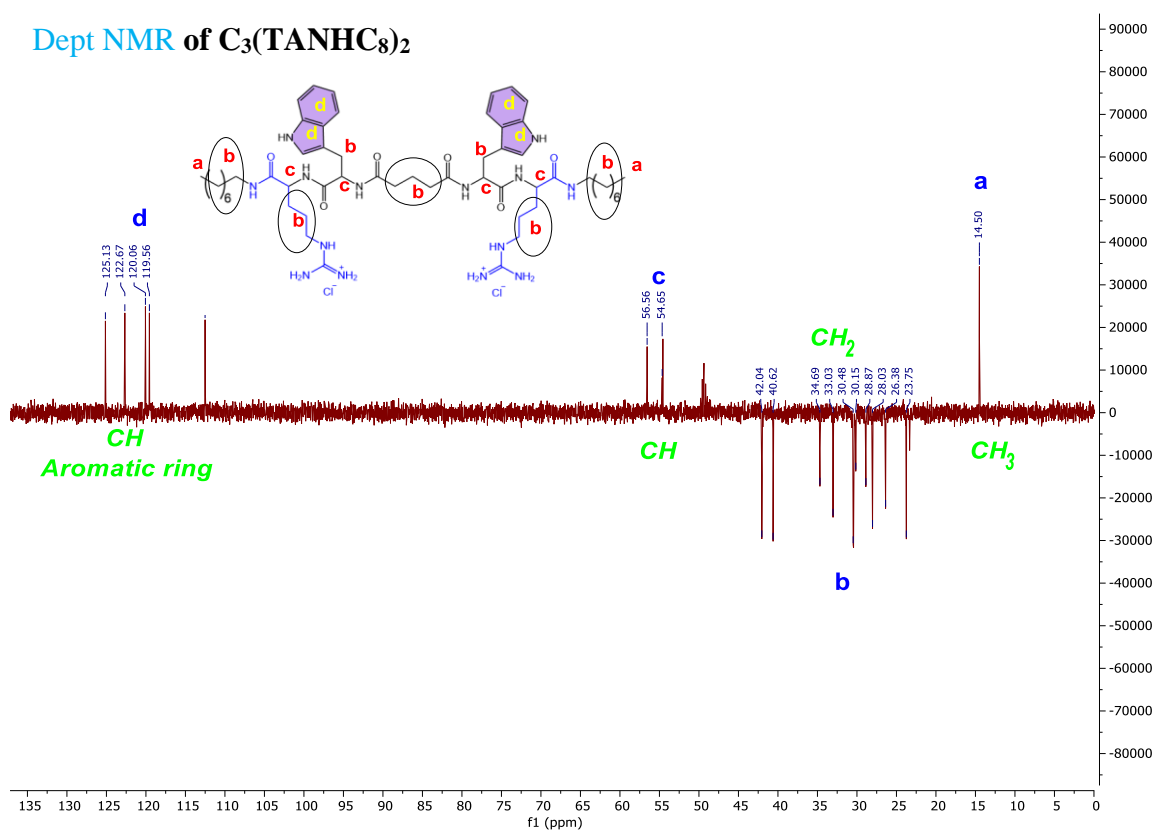
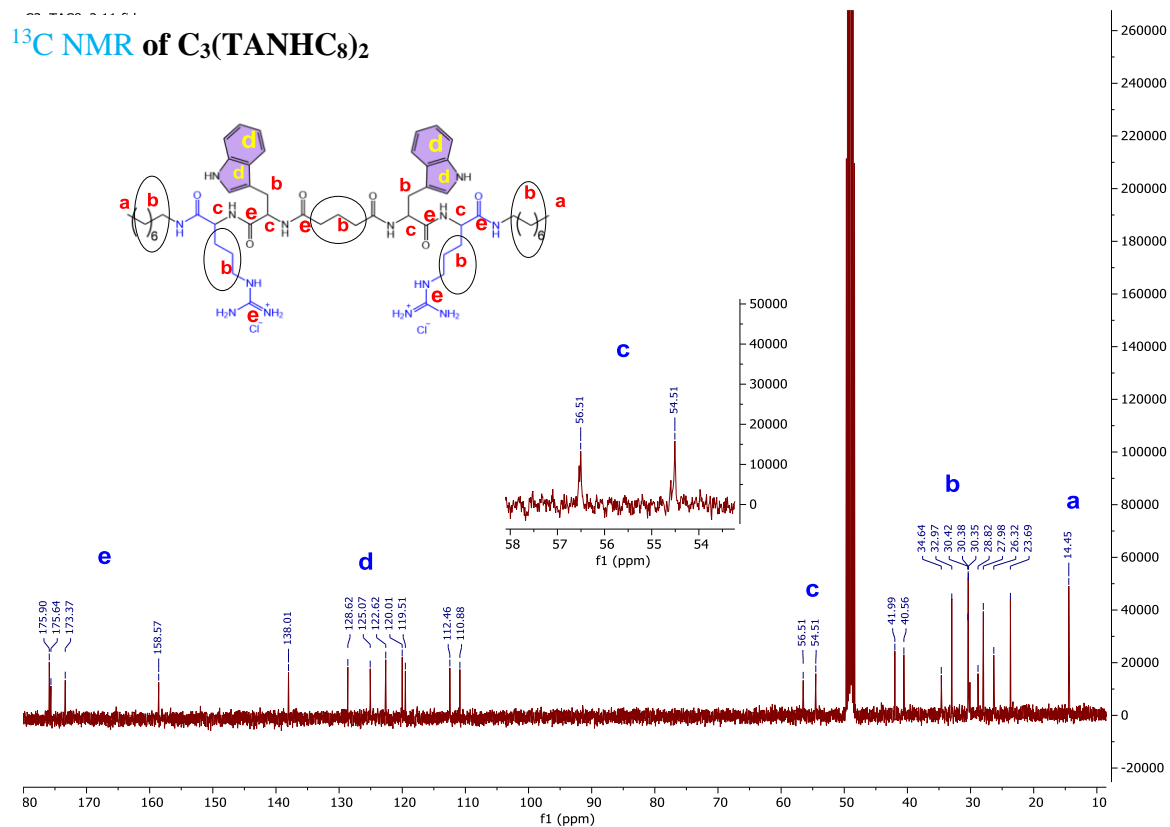
**Figure S24.** HPLC, ESI-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Dept of TANHC<sub>14</sub>



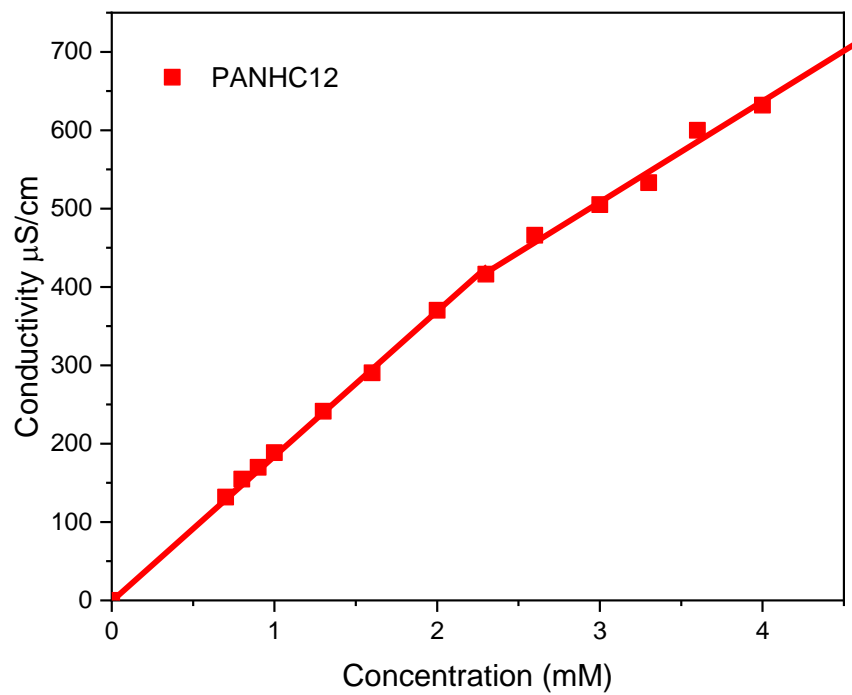
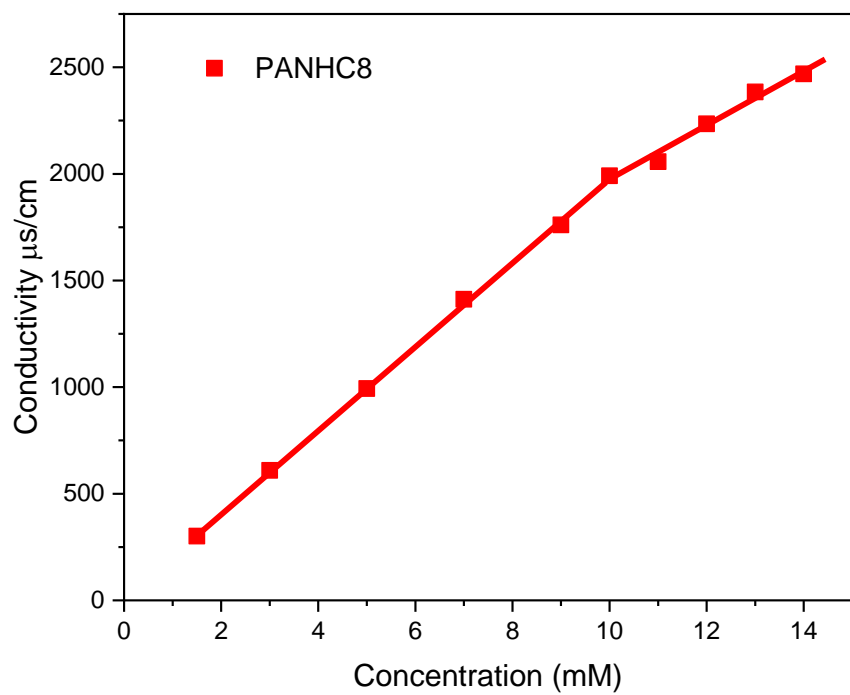


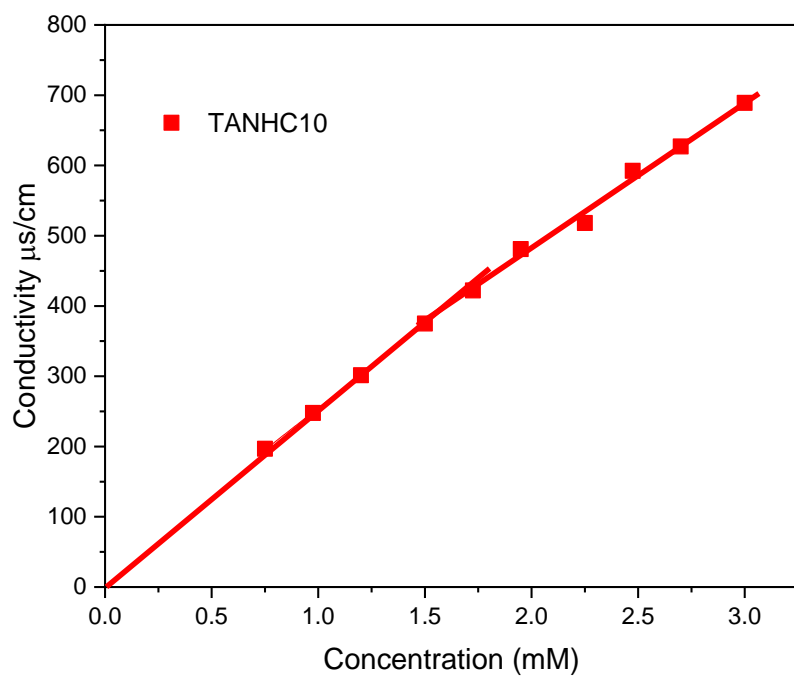
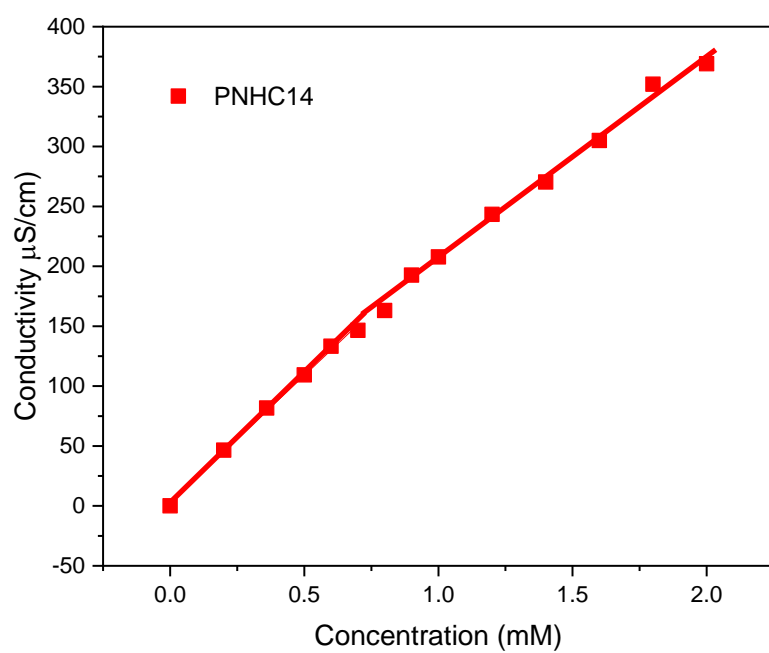
### $^1\text{H}$ NMR of $C_3(\text{TANHC}_8)_2$

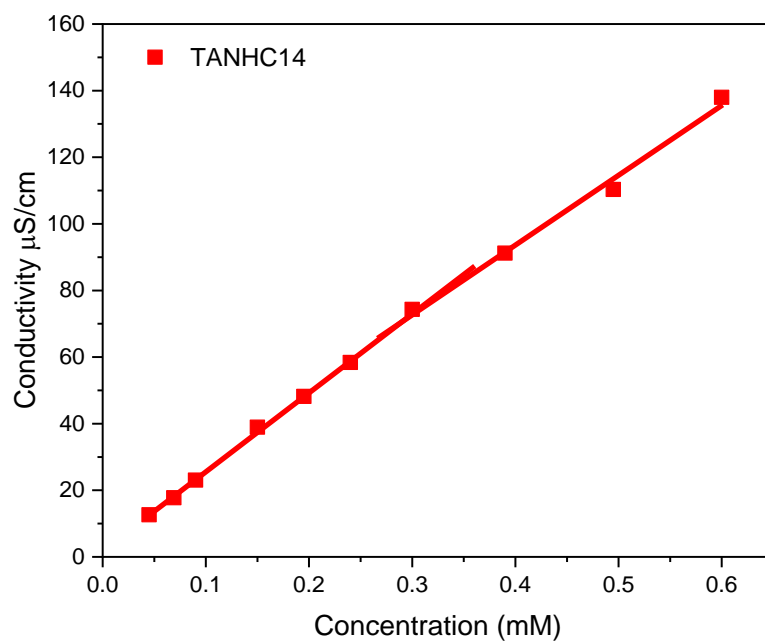
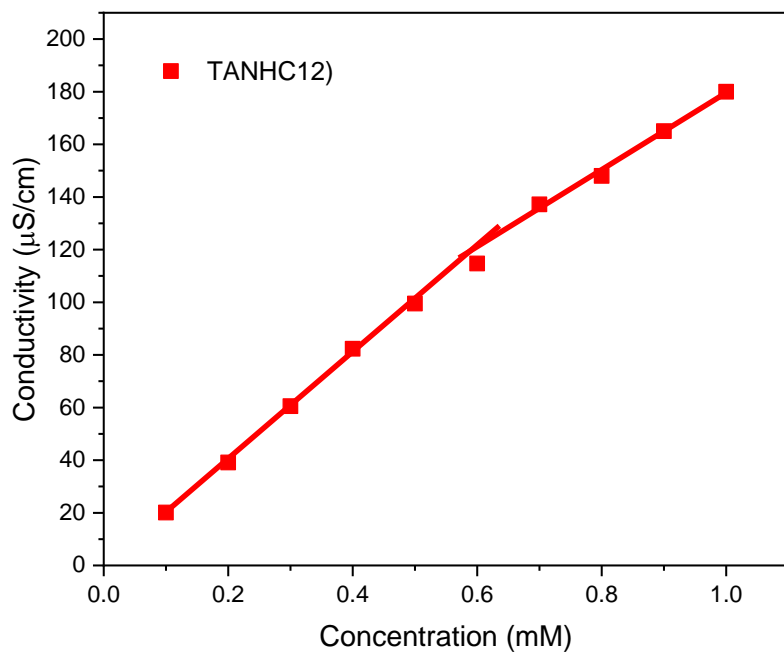


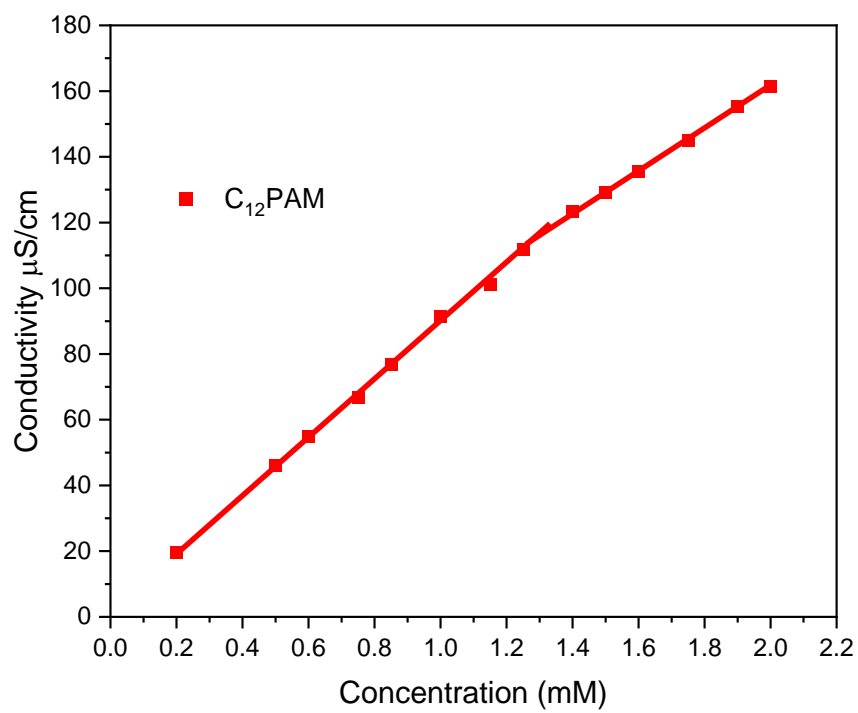
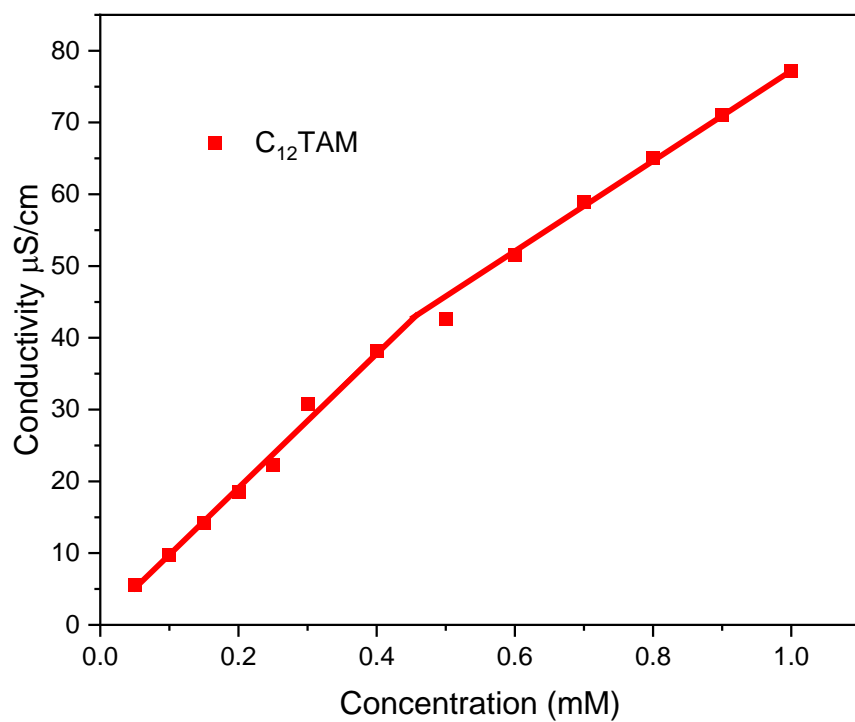


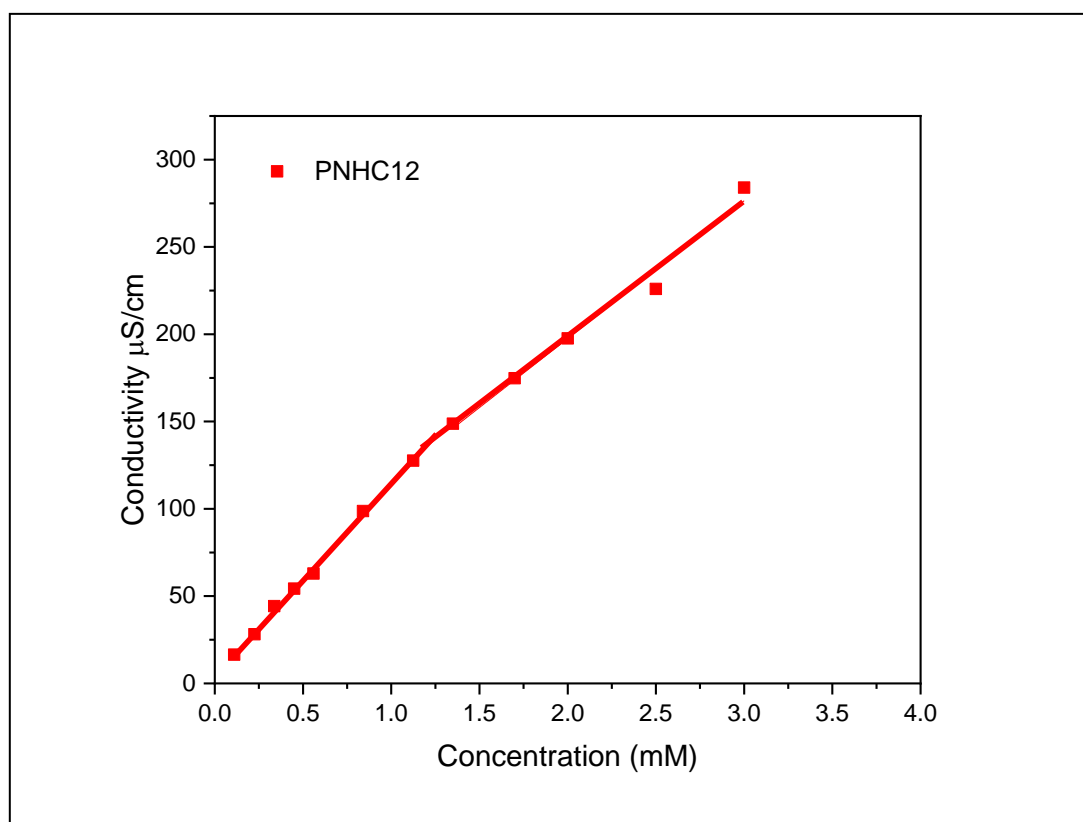
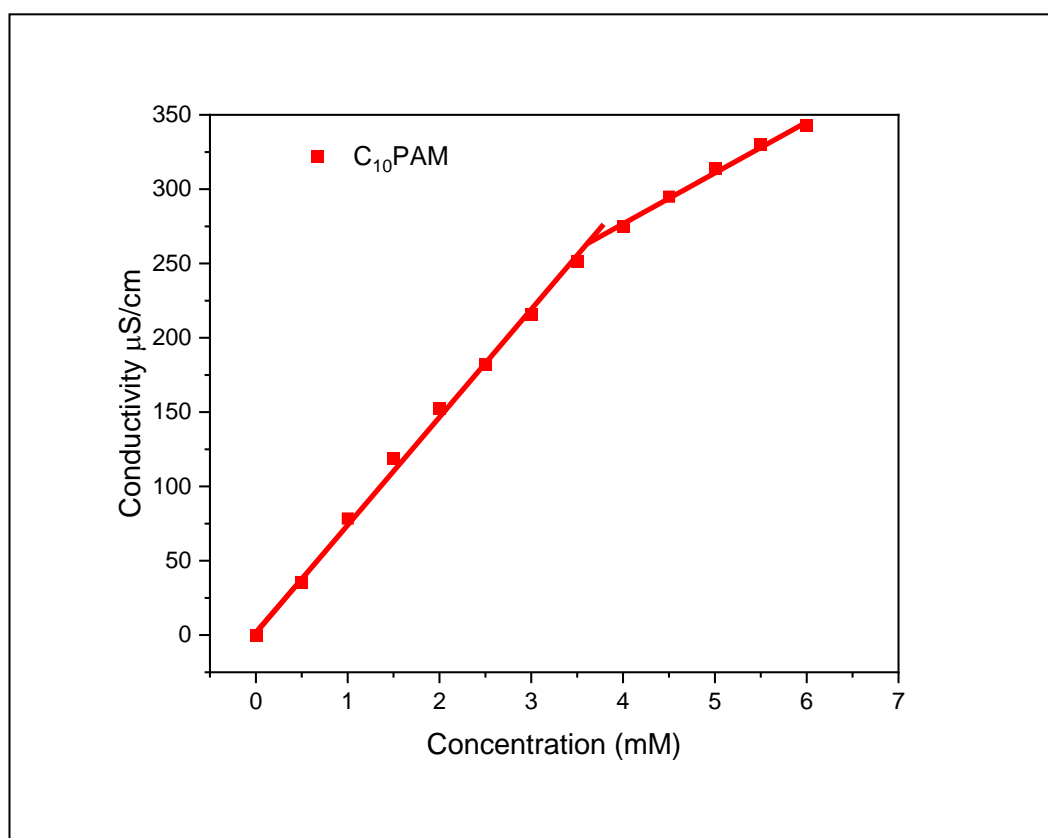
**Figure S25.** HPLC,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and Dept of  $\text{C}_3(\text{TANHC}_8)_2$











**Figure S26.** Specific conductivity-concentration curves for the amino acid-based surfactants.