ELECTRONIC SUPPLEMENTARY INFORMATION

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

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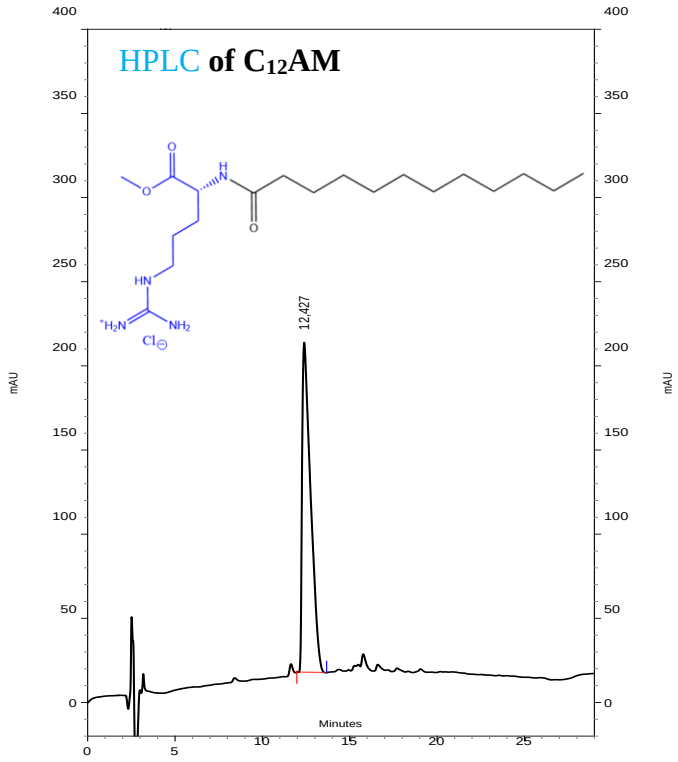
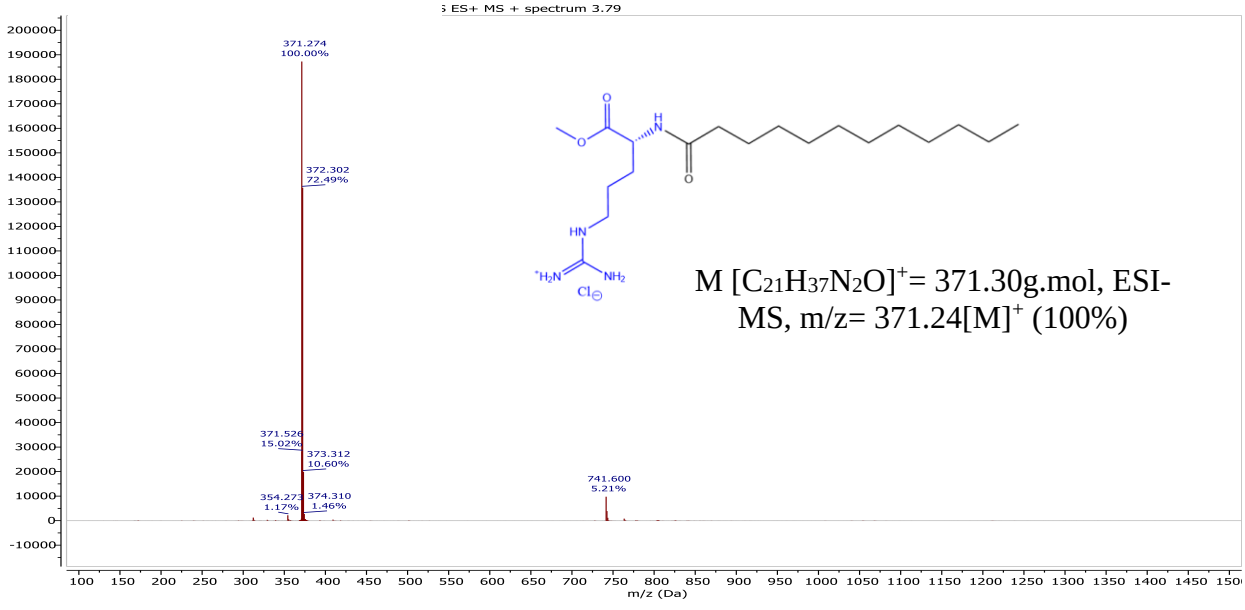
CONTENT

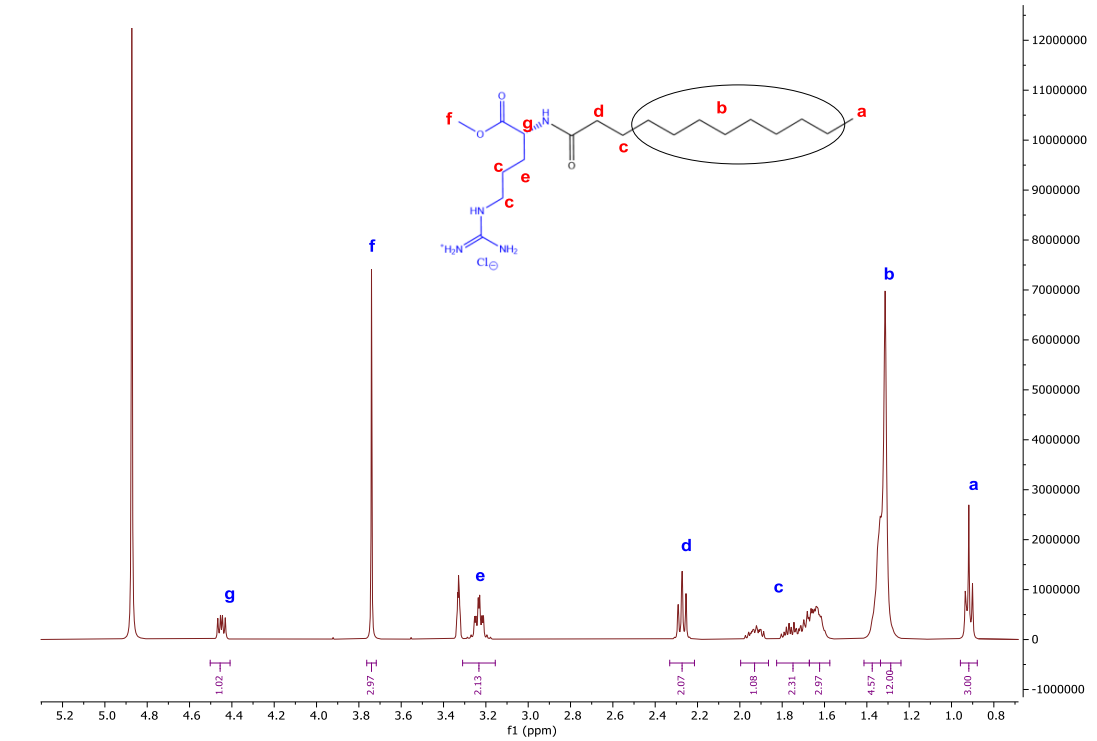


ESI-MS **of C_{12}AM**



M $[C_{21}H_{37}N_2O]^+$= 371.30g.mol, ESI-MS, m/z= 371.24$[M]^+$ (100%)

^{1}H NMR of C_{12}AM



^{13}C NMR of C_{12}AM

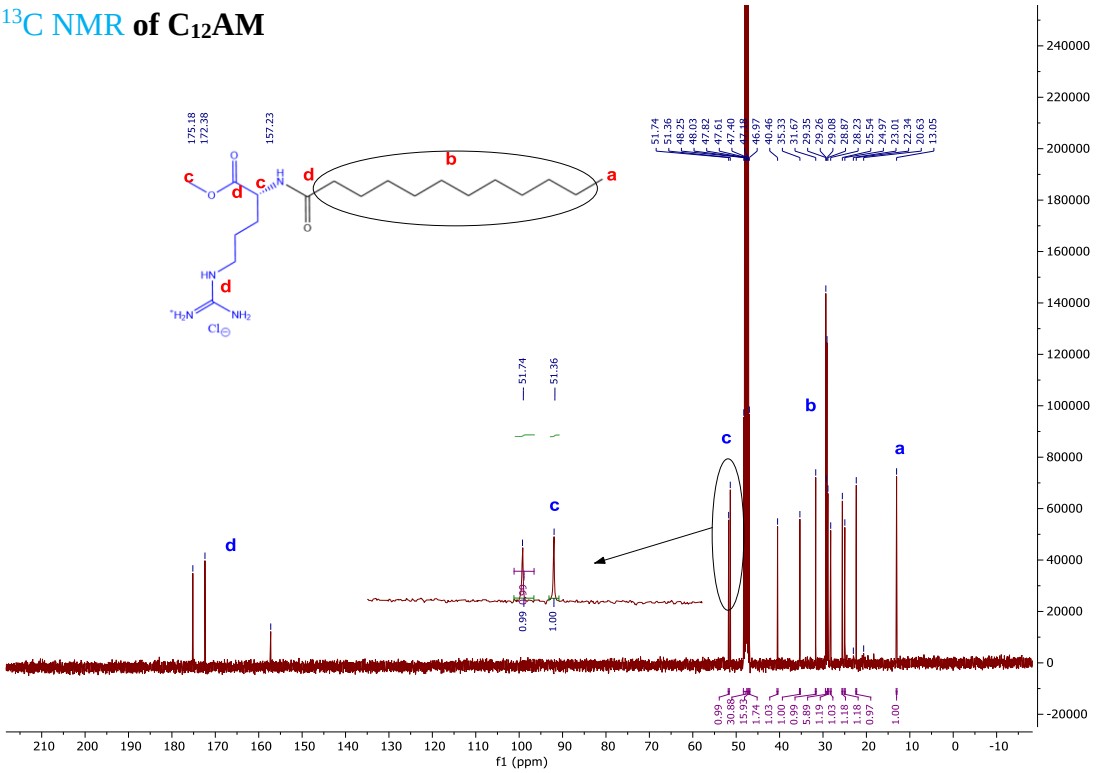
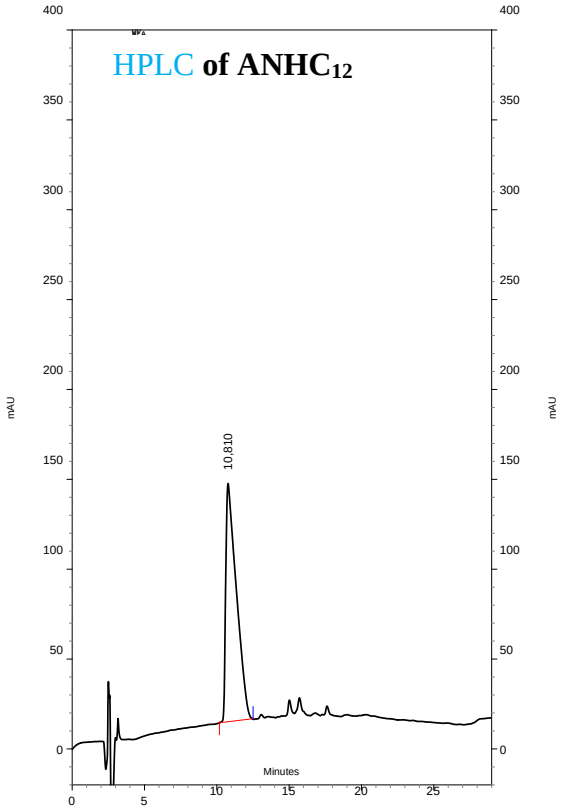
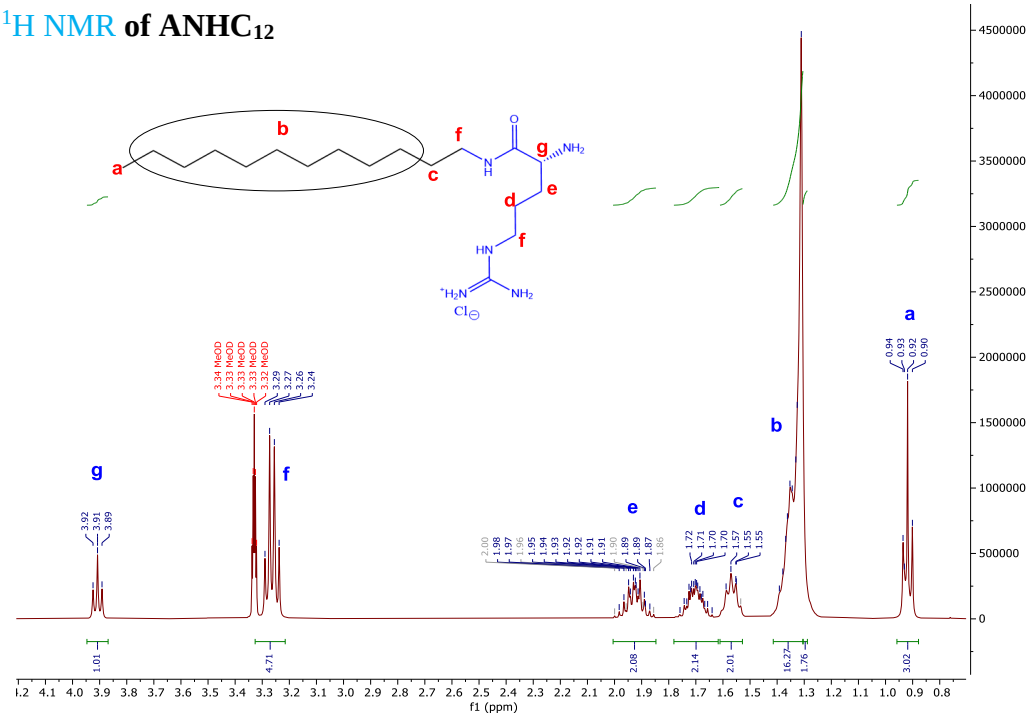


Figure S1. HPLC, ESI-MS, ^{1}H NMR, and ^{13}C NMR of C_{12}AM

HPLC of $ANHC_{12}$



^{1}H NMR of $ANHC_{12}$



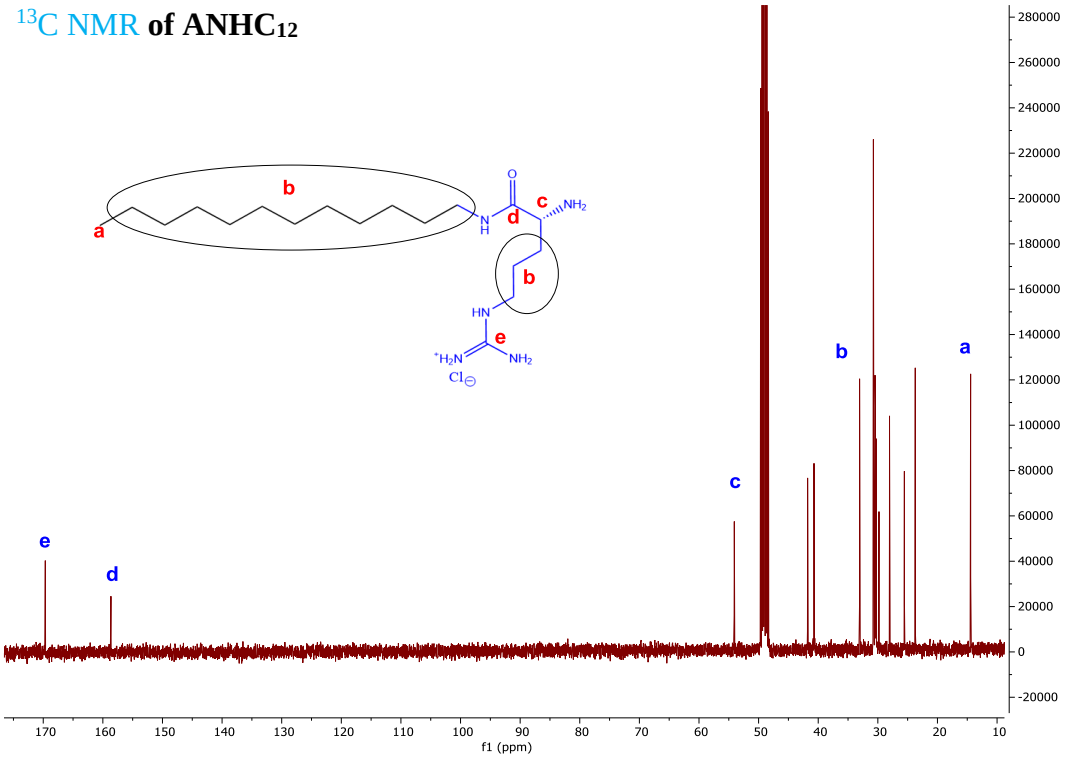
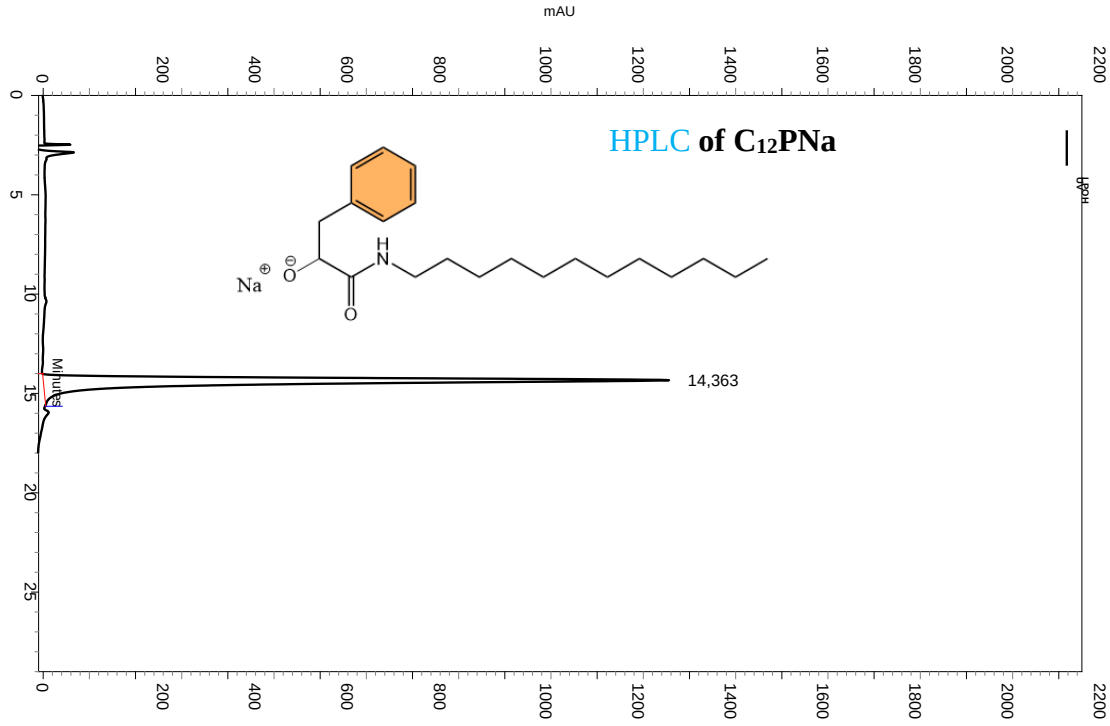
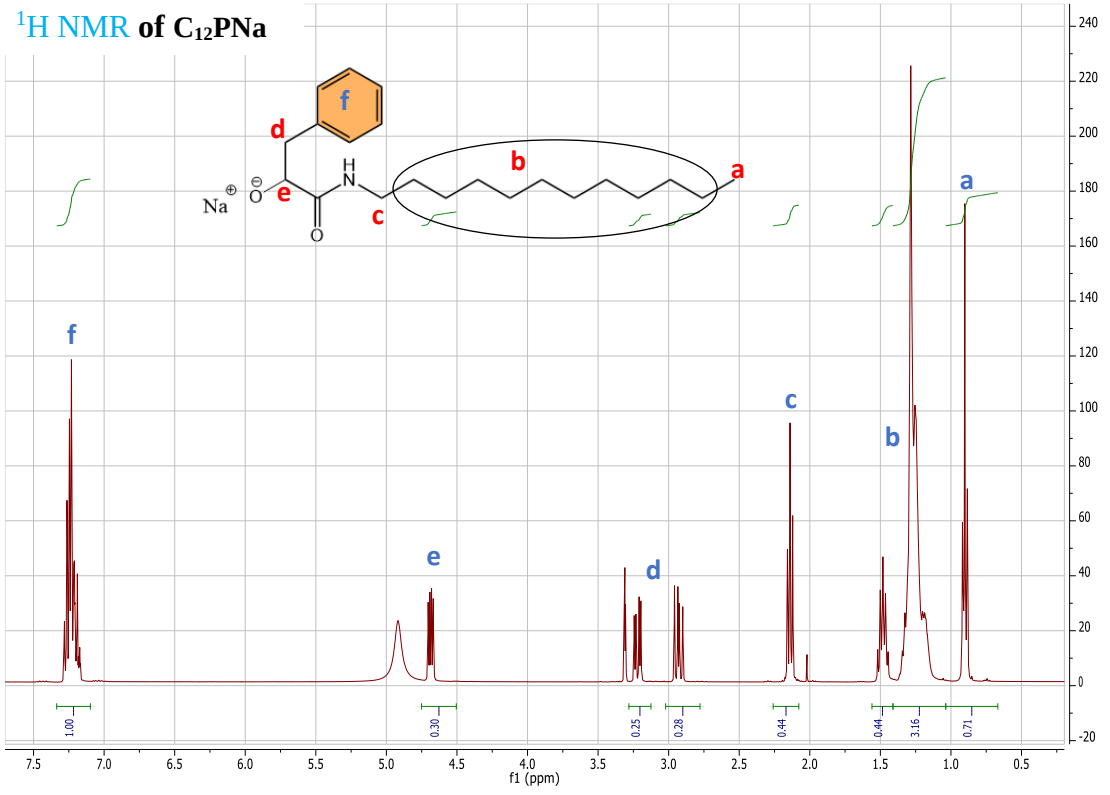


Figure S2. HPLC, ESI-MS, ^{1}H NMR, and ^{13}C NMR of ANHC$_{12}$


mAU
HPLC of C12PNa
14,363
Minutes
mAU


1H NMR of C12PNa
f
d
e
c
b
a
f1 (ppm)

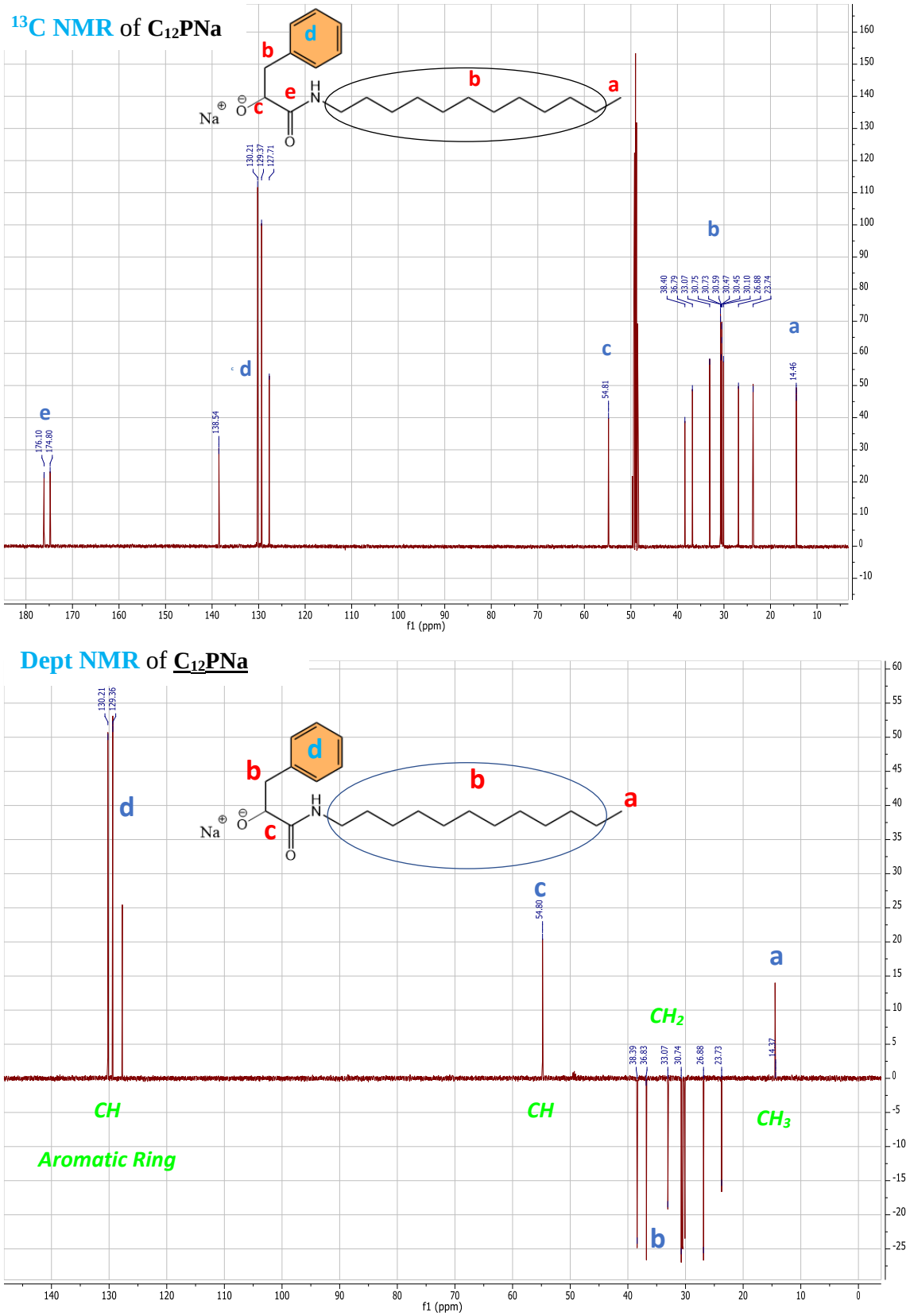
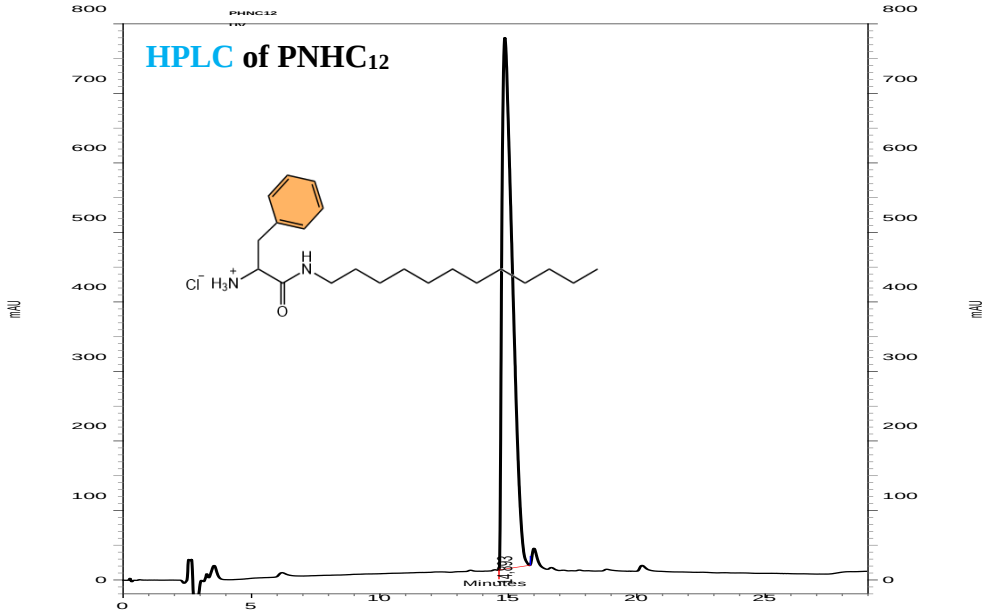
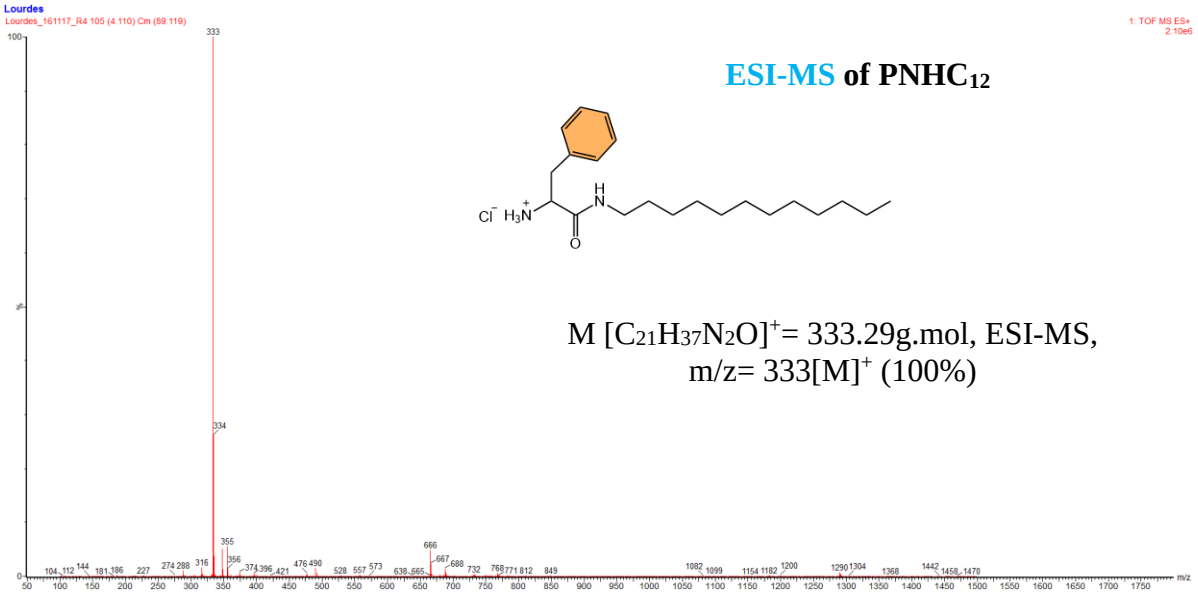


Figure S3. HPLC, ^{1}H NMR, ^{13}C NMR and Dept of C_{12}PNa





ESI-MS of PNHC$_{12}$

M $[C_{21}H_{37}N_2O]^+$= 333.29g.mol, ESI-MS,
m/z= 333$[M]^+$ (100%)

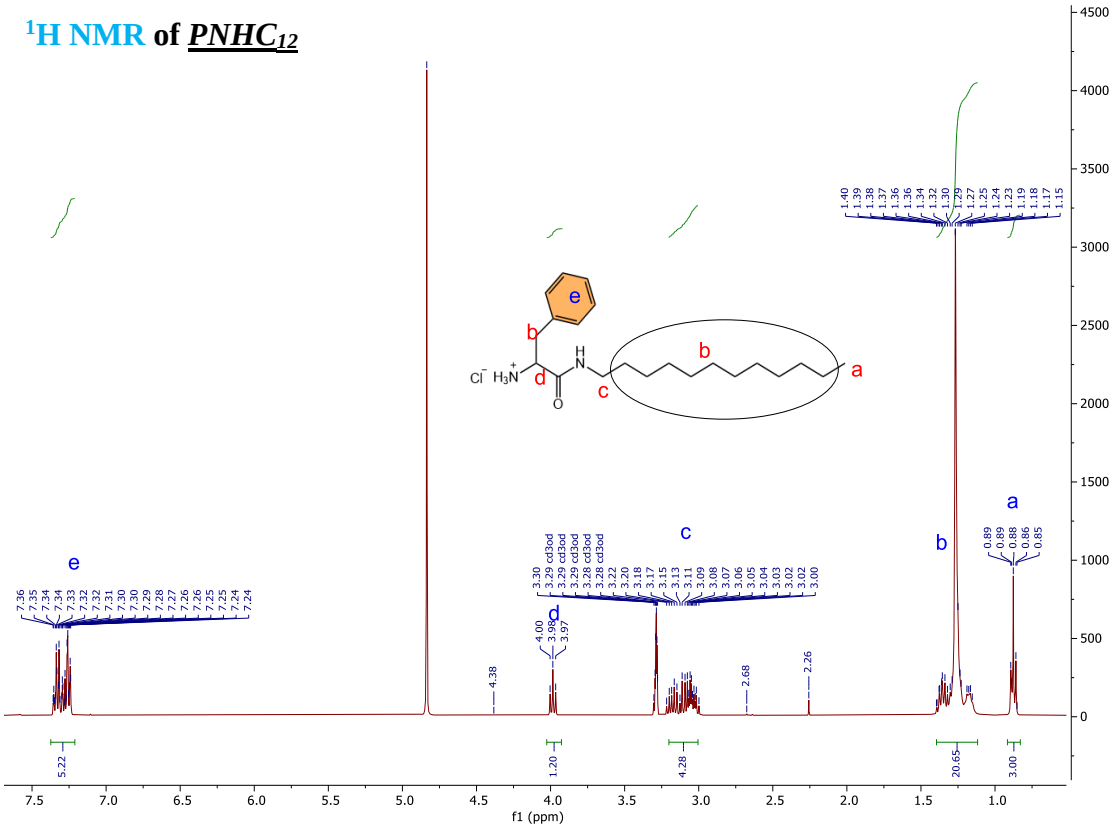
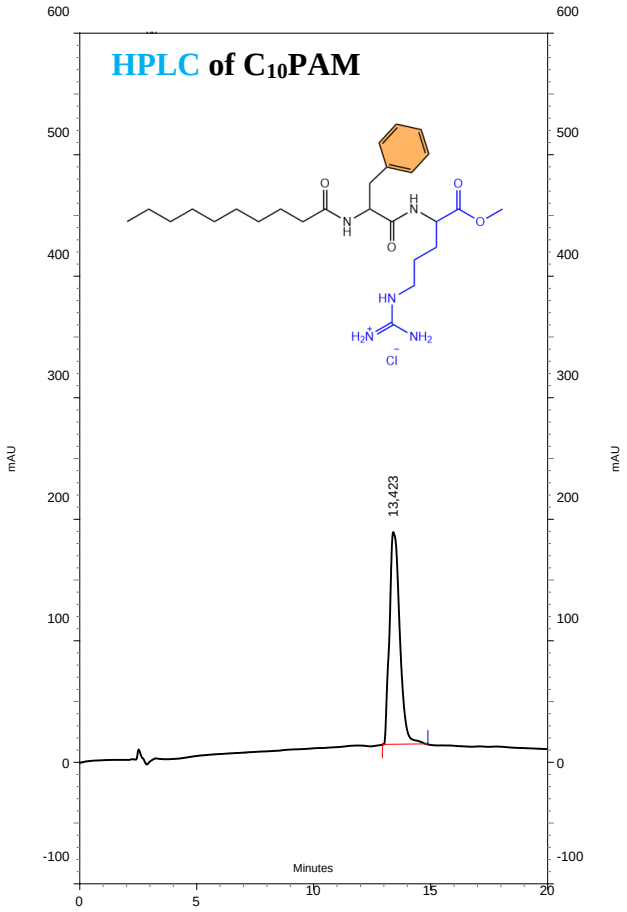
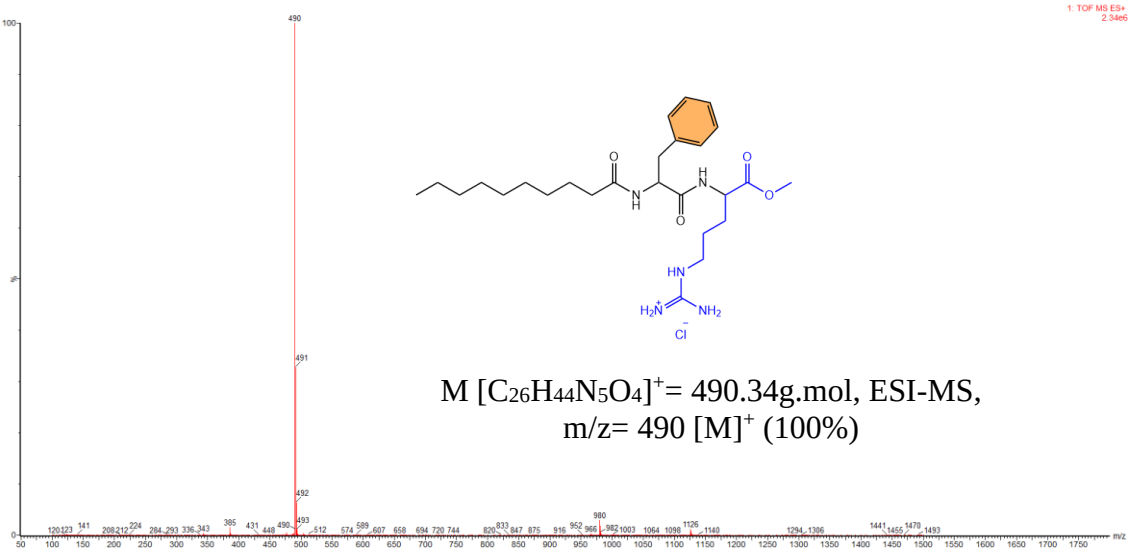


Figure S4. HPLC, ESI-MS and ^{1}H NMR, of PNHC$_{12}$

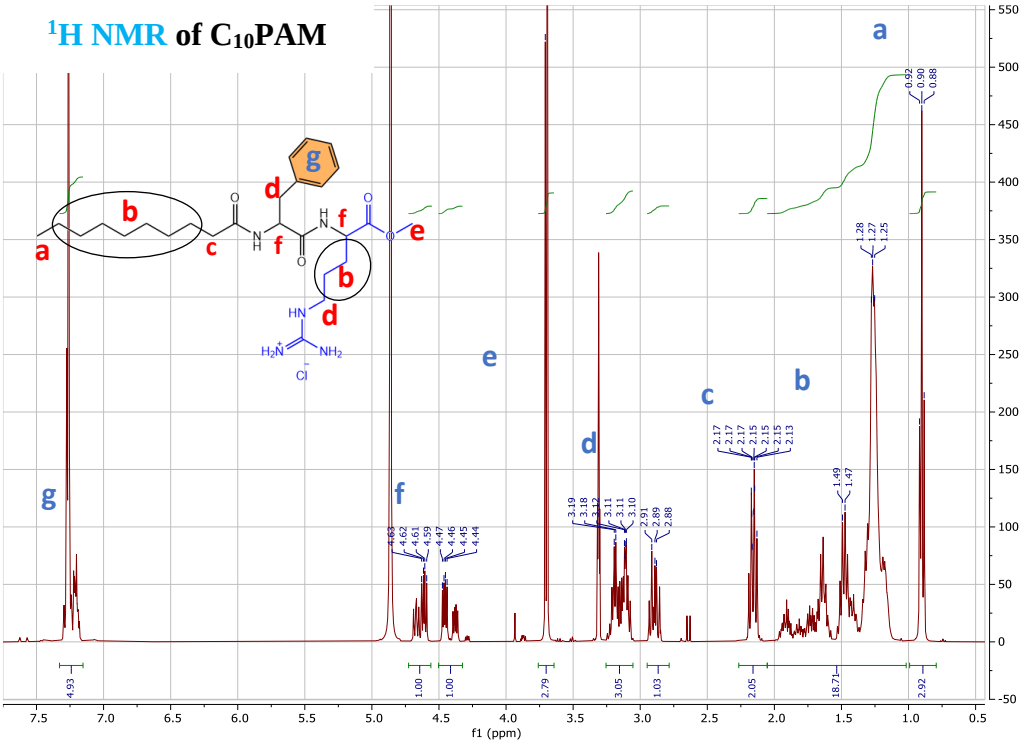


ESI-MS of C_{10}PAM

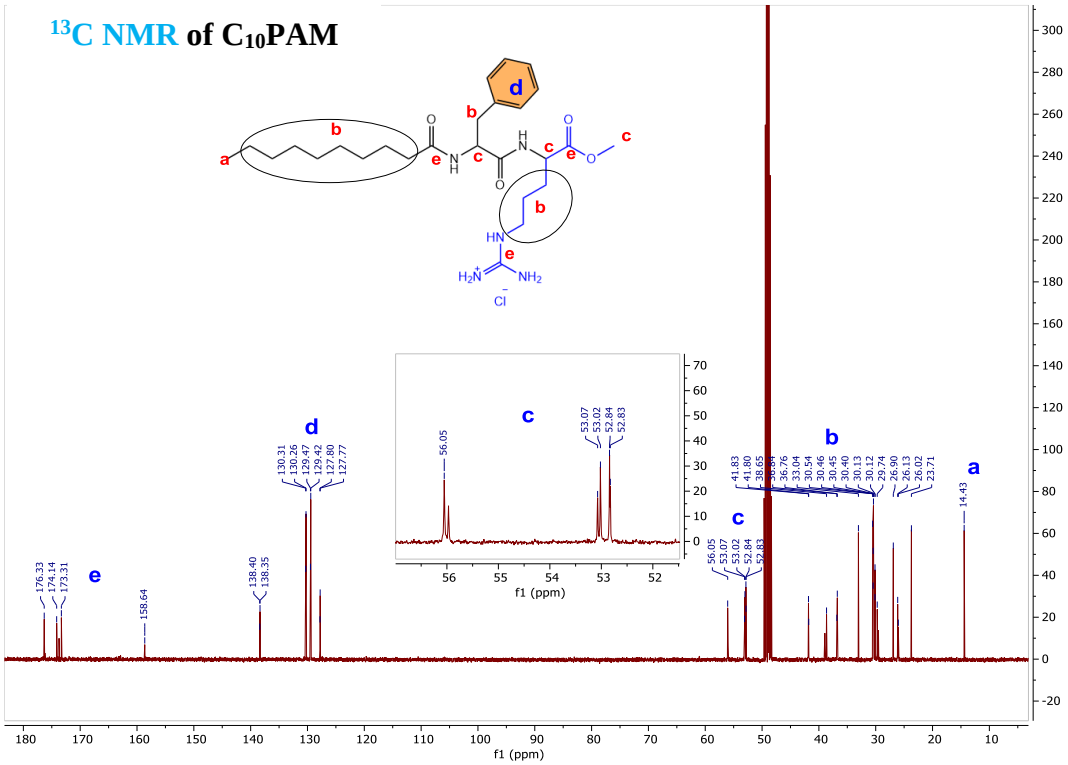


M $[C_{26}H_{44}N_5O_4]^+$= 490.34g.mol, ESI-MS,
m/z= 490 $[M]^+$ (100%)

^{1}H NMR of C_{10}PAM



^{13}C NMR of C_{10}PAM



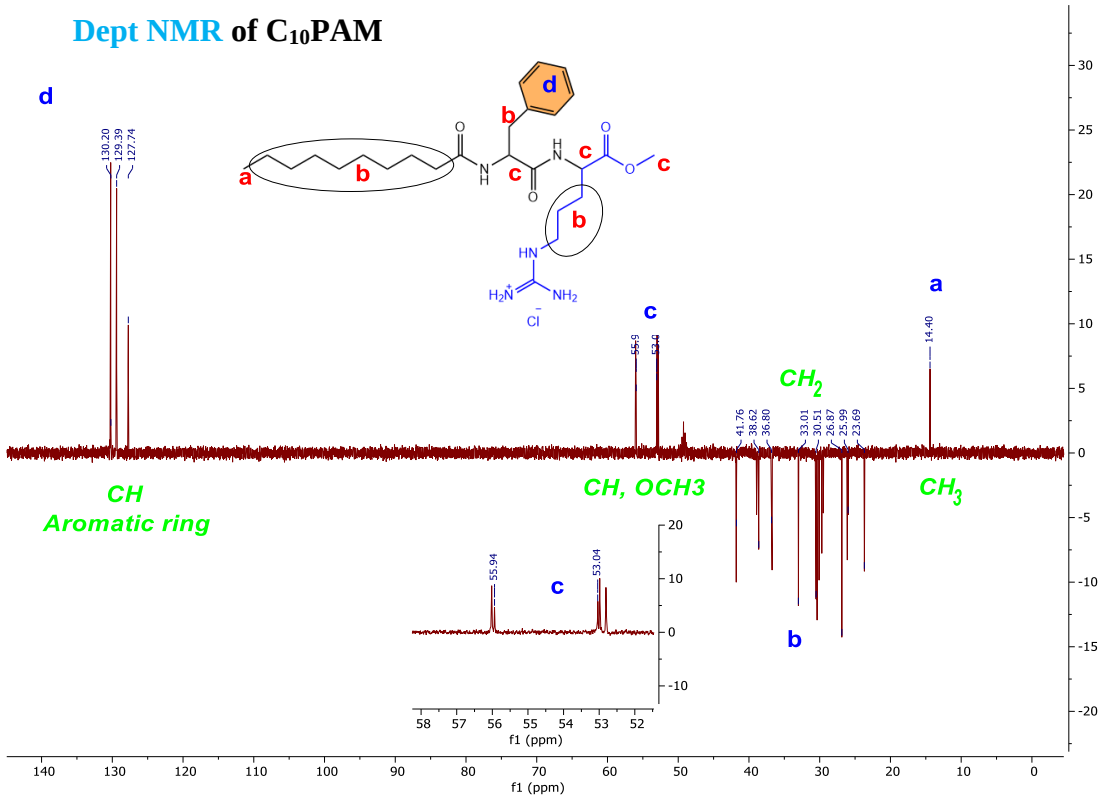
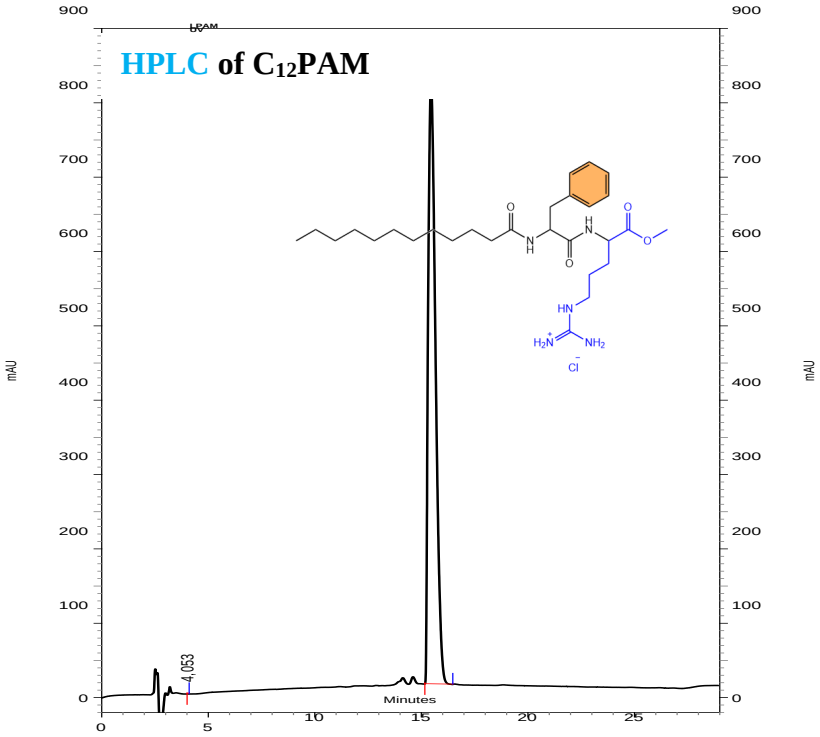
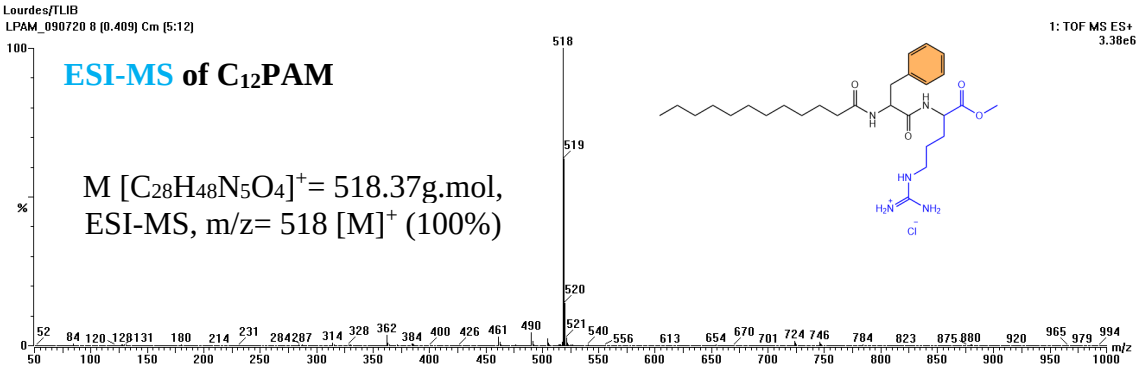
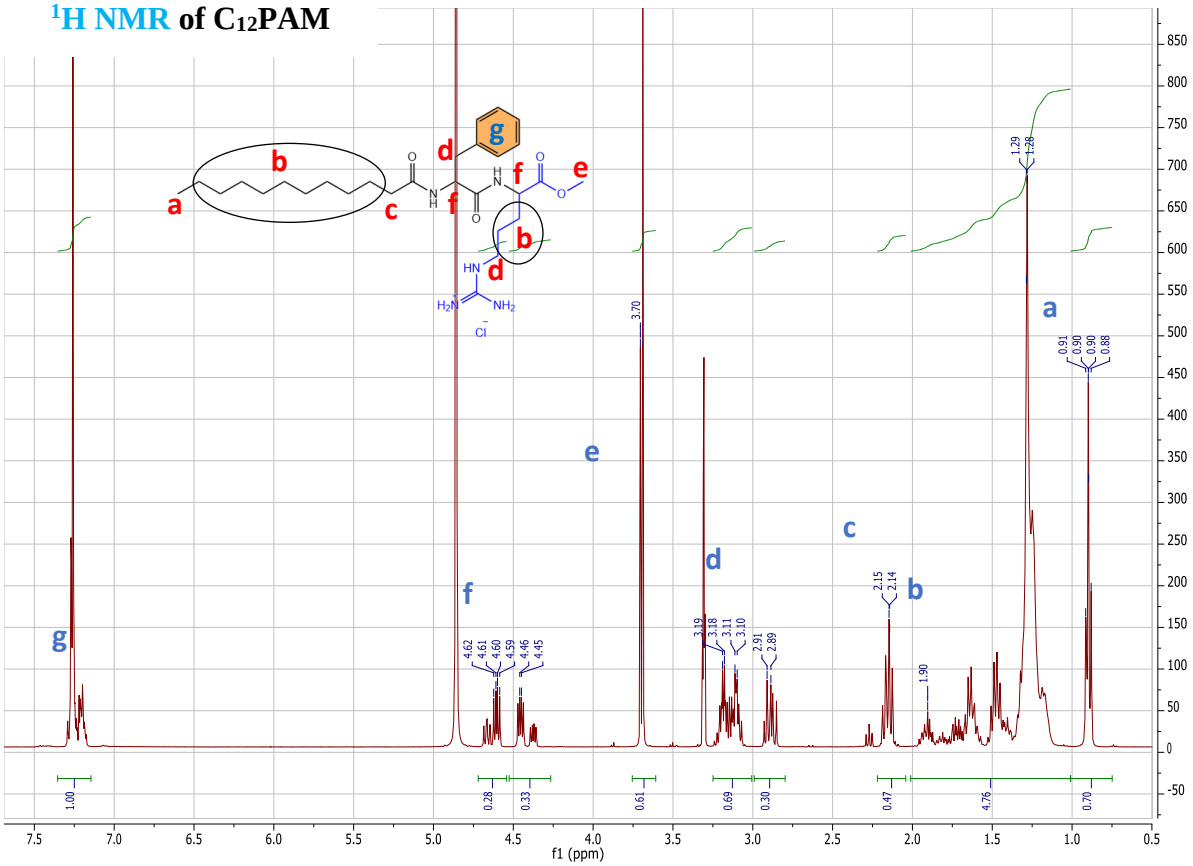


Figure S5. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of C_{10}PAM

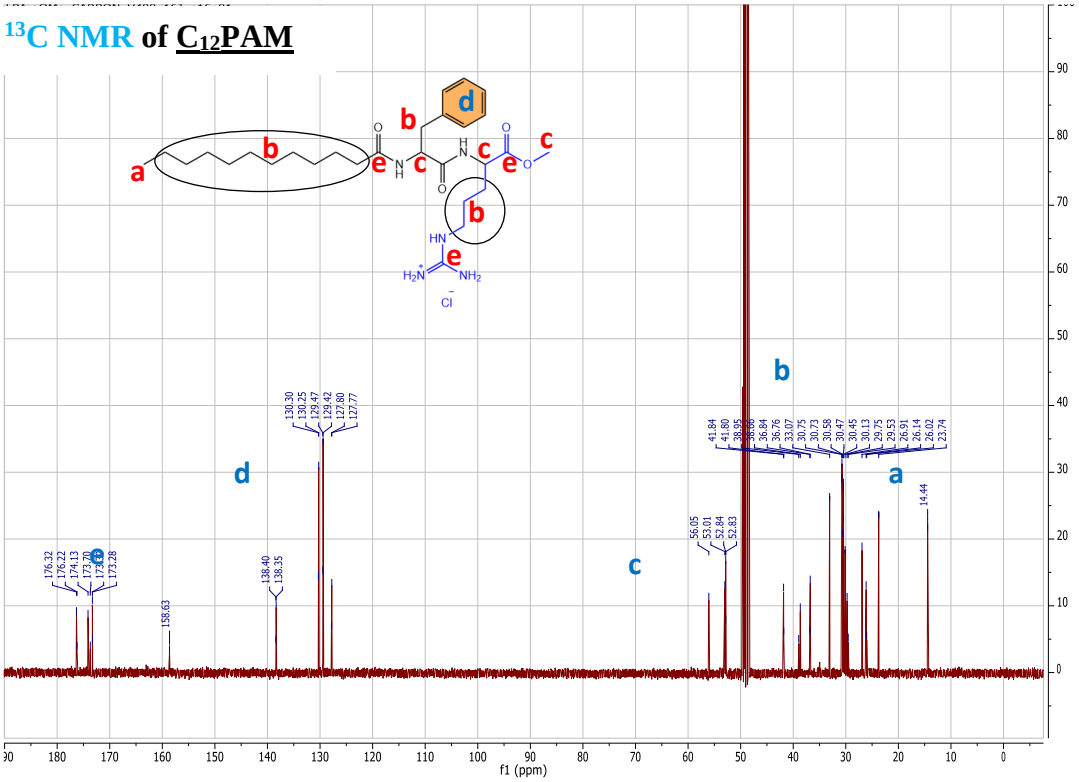

HPLC of C12PAM
mAU
Minutes
4.053


Lourdes/TLIB
LPAM_090720 8 (0.409) Cm (5:12)
1: TOF MS ES+
3.38e6
ESI-MS of C12PAM
M [C28H48N5O4]+= 518.37g.mol,
ESI-MS, m/z= 518 [M]+ (100%)
m/z

^{1}H NMR of C_{12}PAM



^{13}C NMR of C_{12}PAM



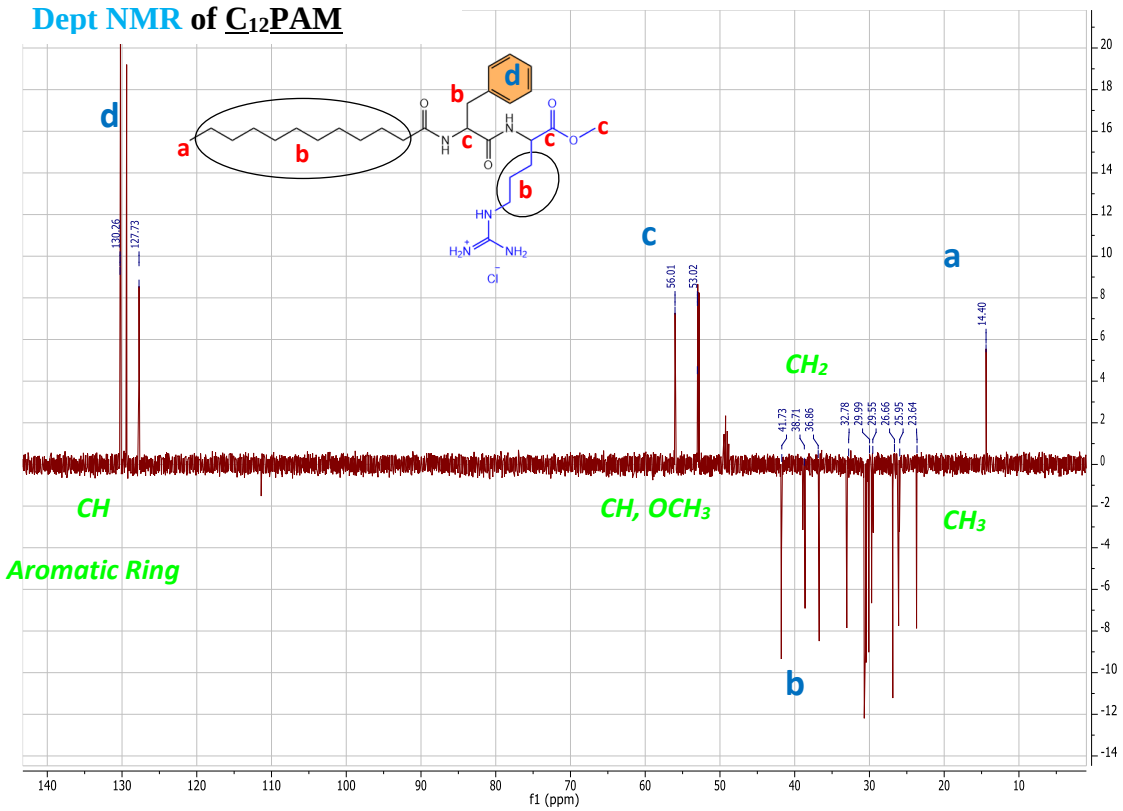
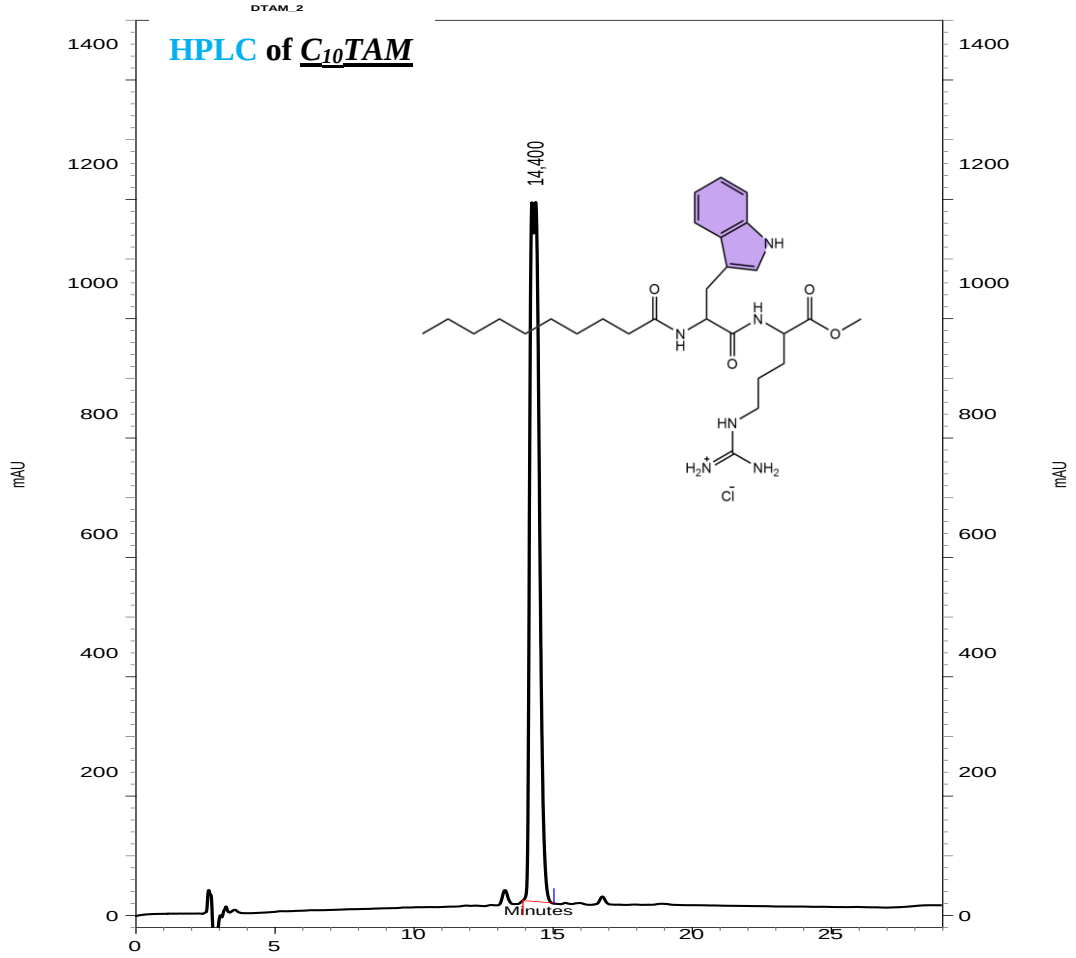
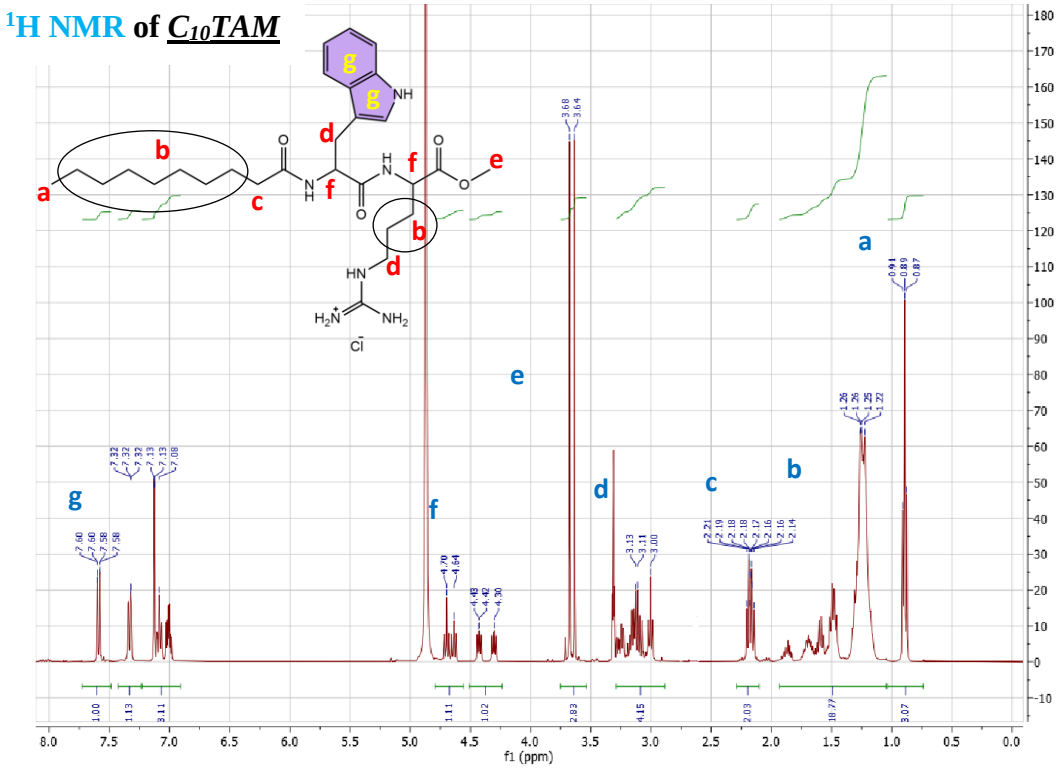


Figure S6. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of C_{12}PAM

HPLC of *C10TAM*



^{1}H NMR of *C10TAM*



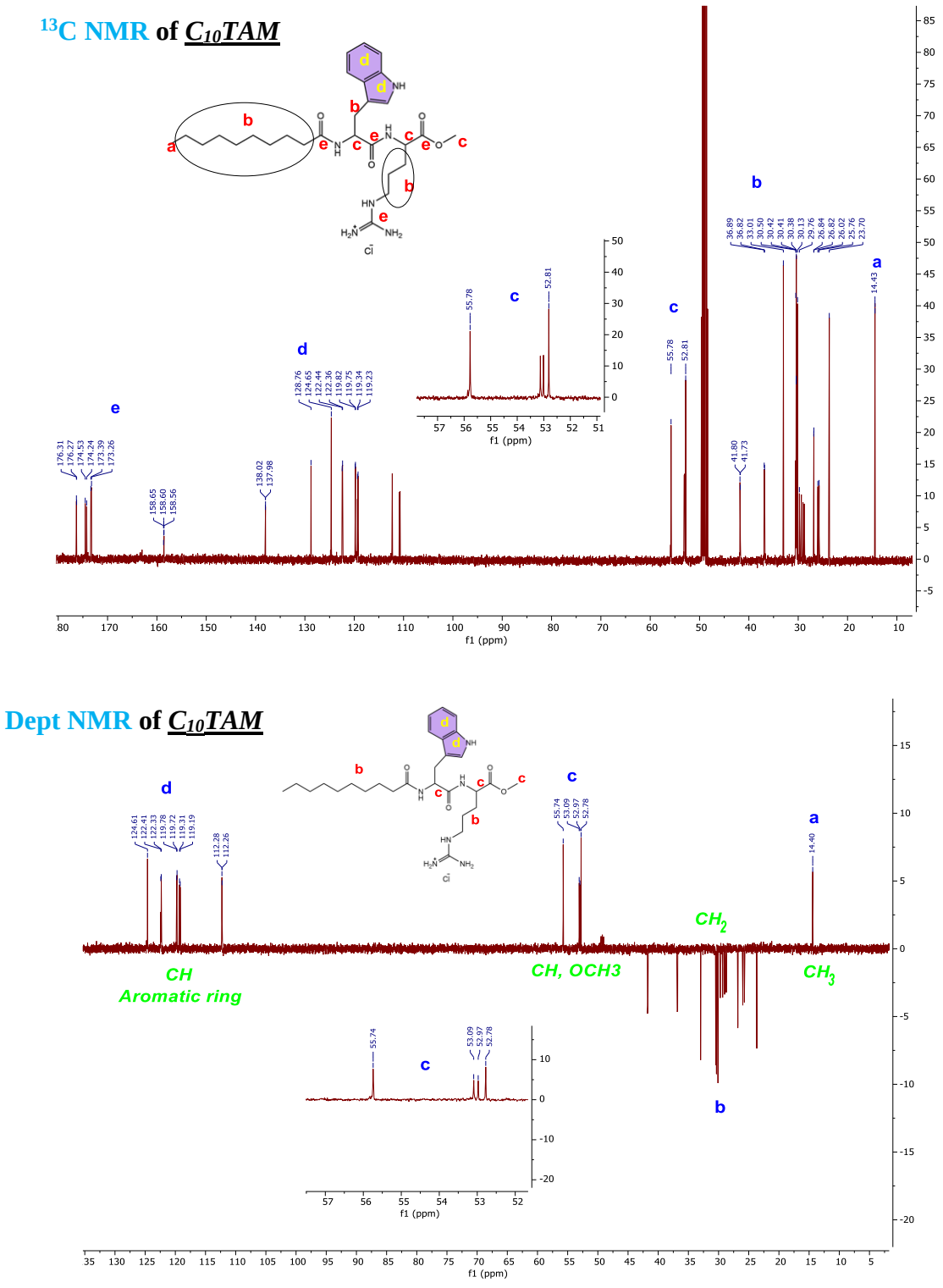
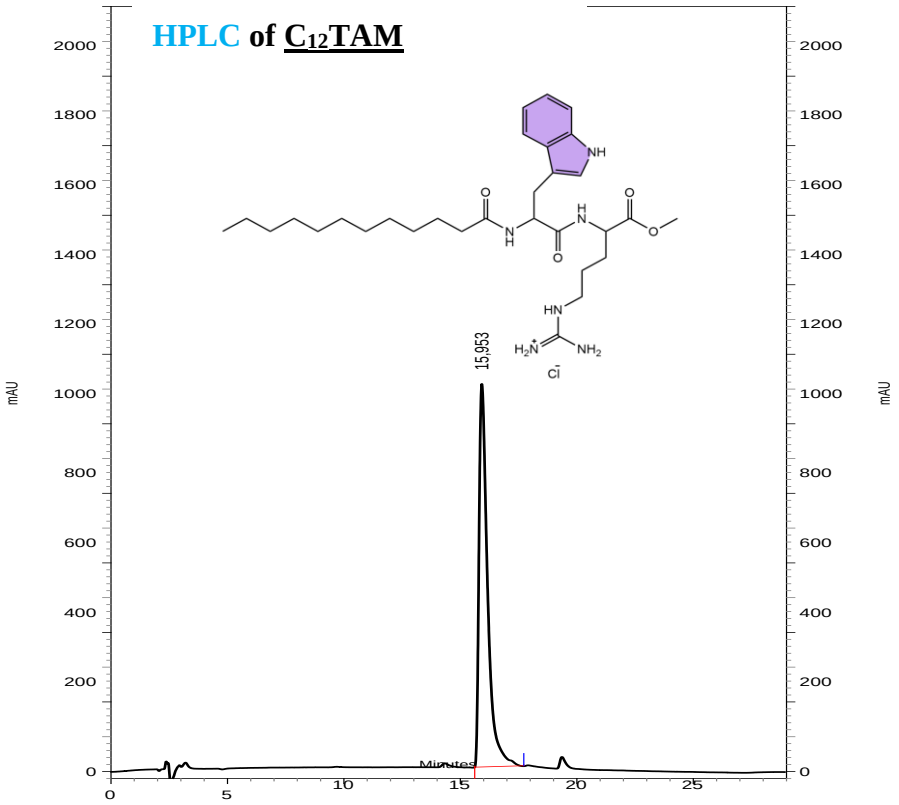


Figure S7. HPLC,^{1}H NMR,^{13}C NMR and Dept of C_{10}TAM

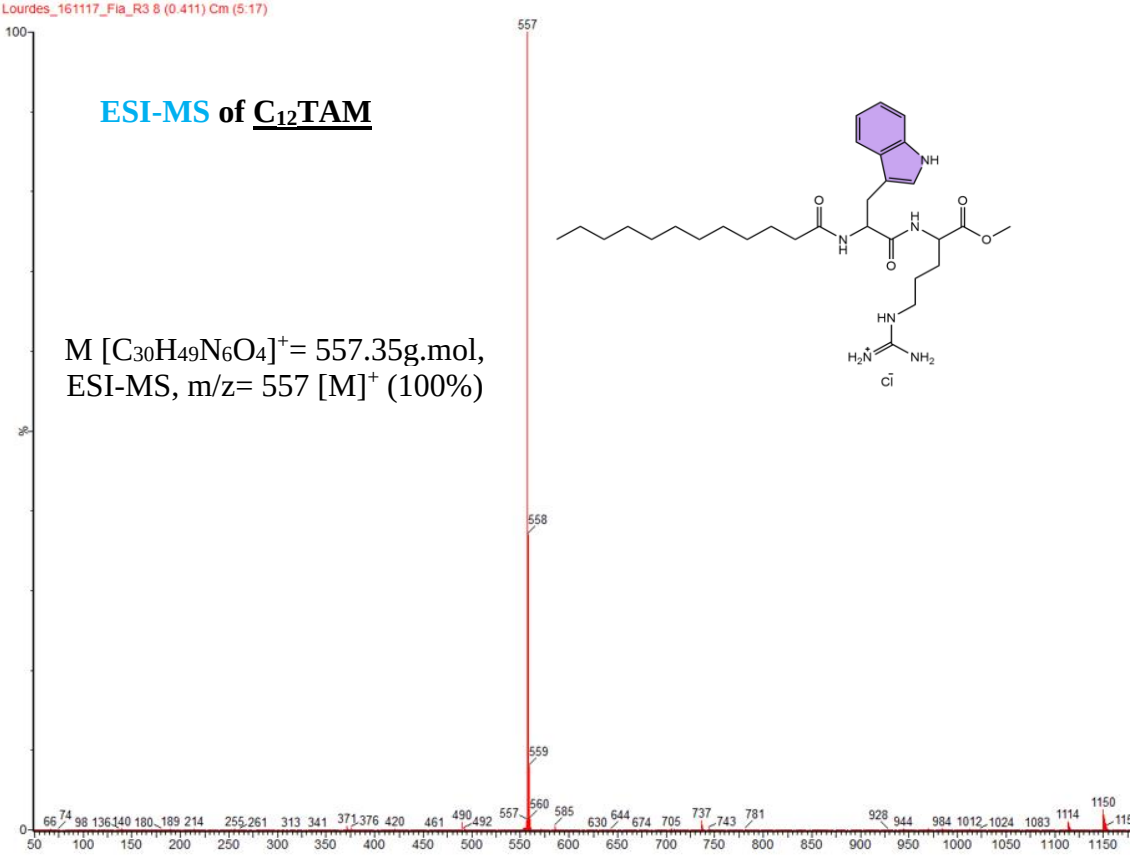
HPLC of C_{12}TAM



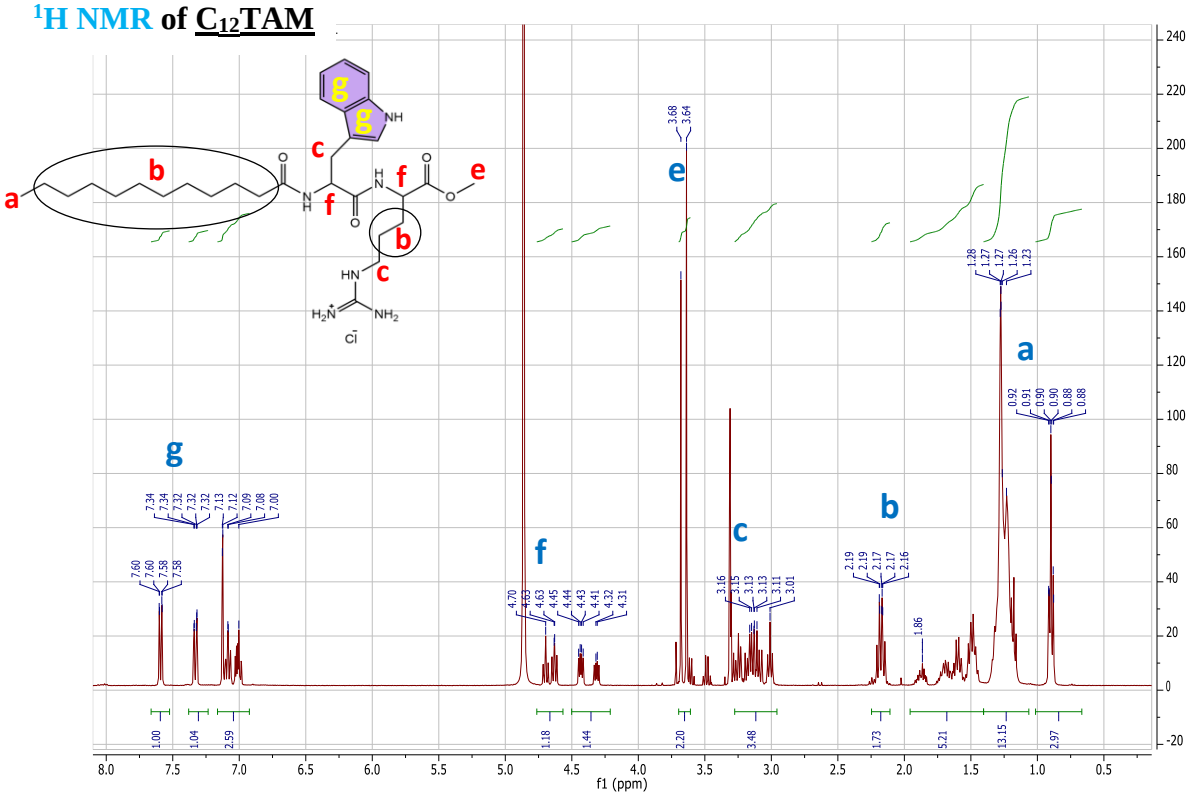
Lourdes
Lourdes_161117_Fia_R3 8 (0.411) Cm (5:17)

ESI-MS of C_{12}TAM

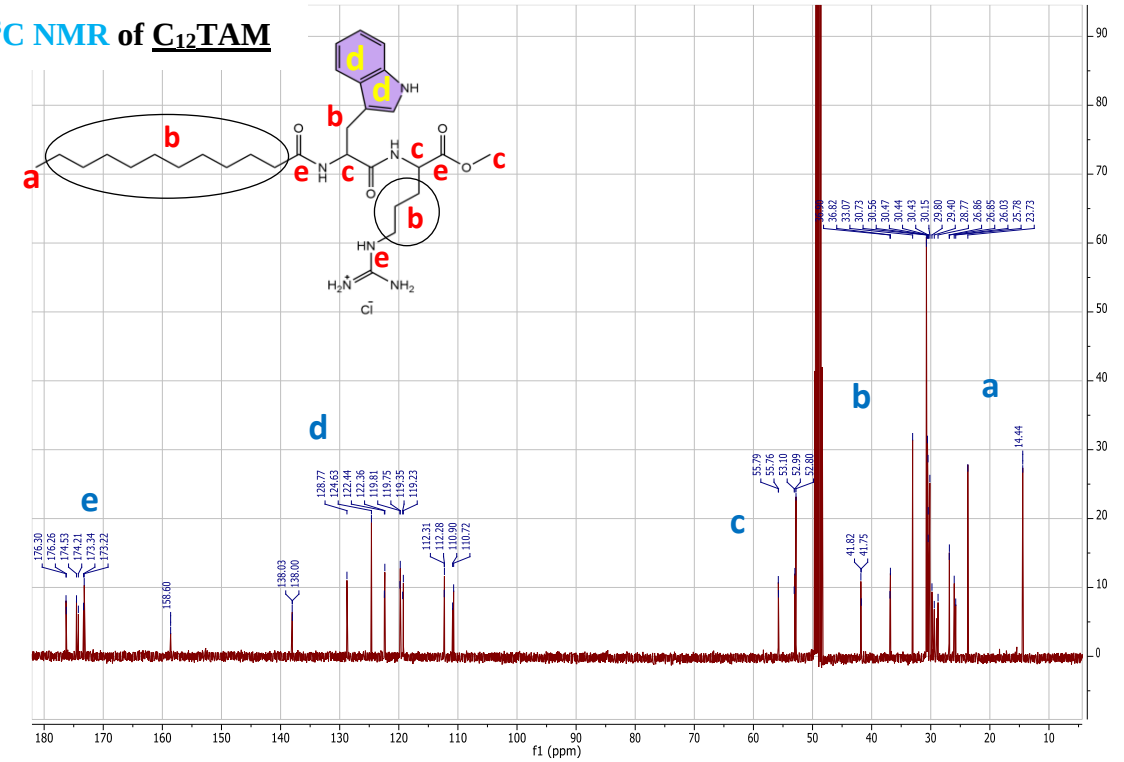
M $[C_{30}H_{49}N_6O_4]^+$= 557.35g.mol,
ESI-MS, m/z= 557 $[M]^+$ (100%)



^{1}H NMR of C_{12}TAM



^{13}C NMR of C_{12}TAM



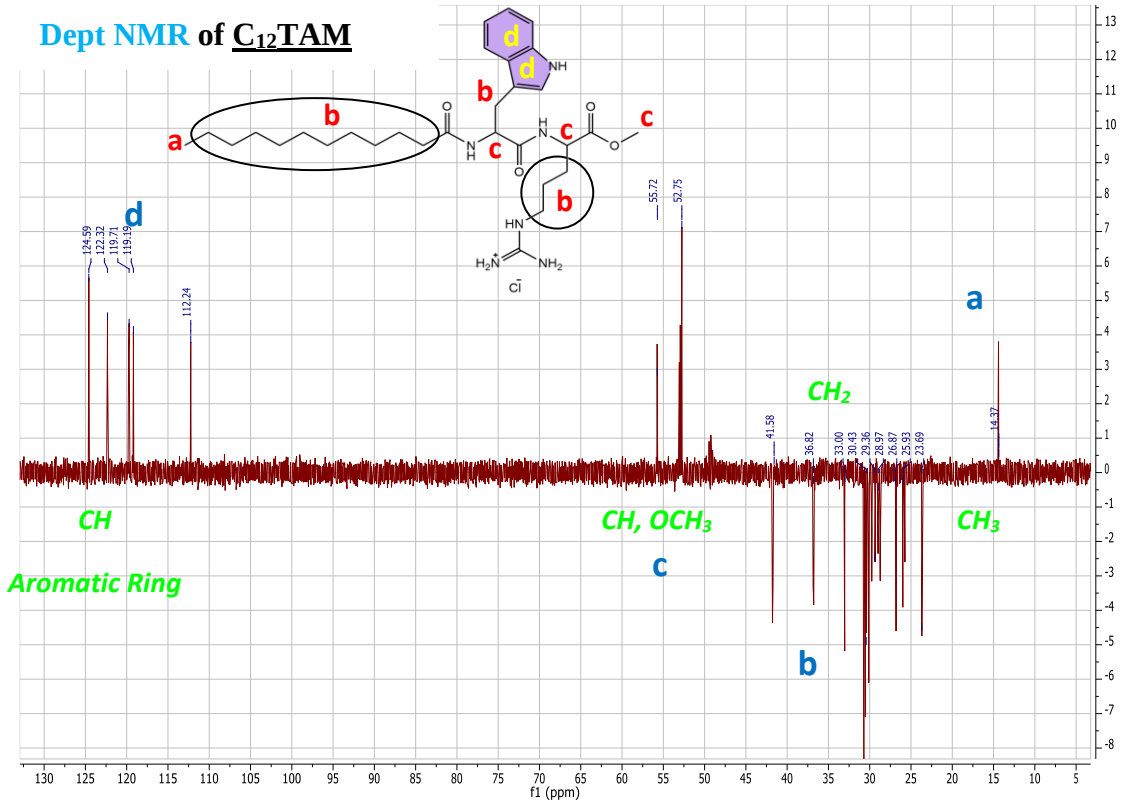
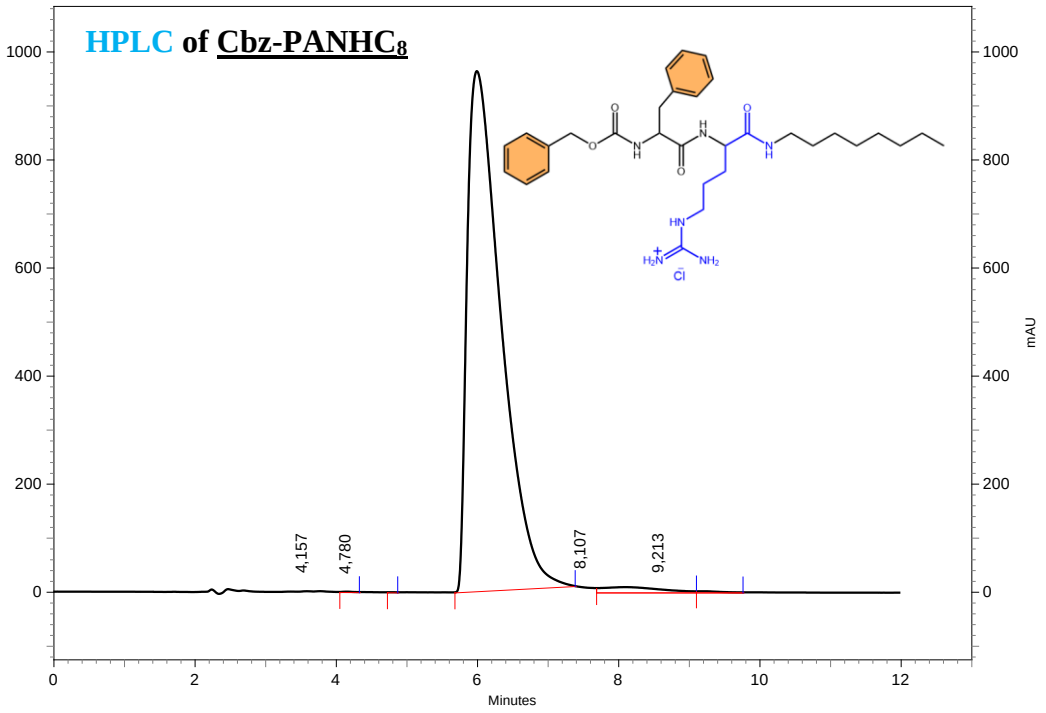
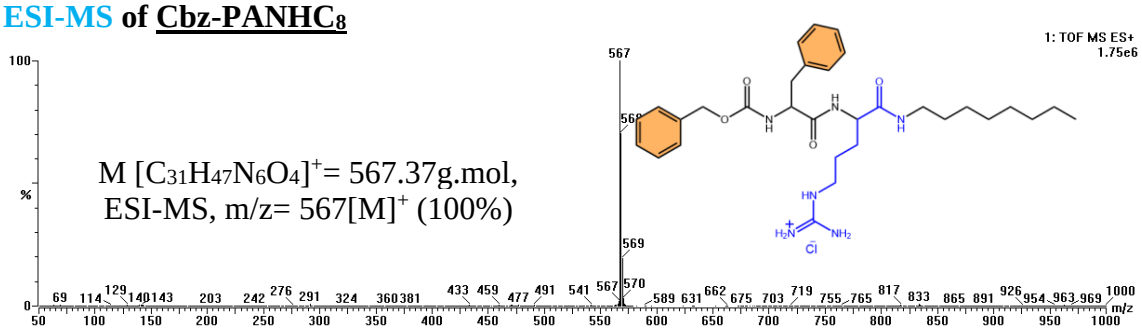


Figure S8. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of C_{10}TAM

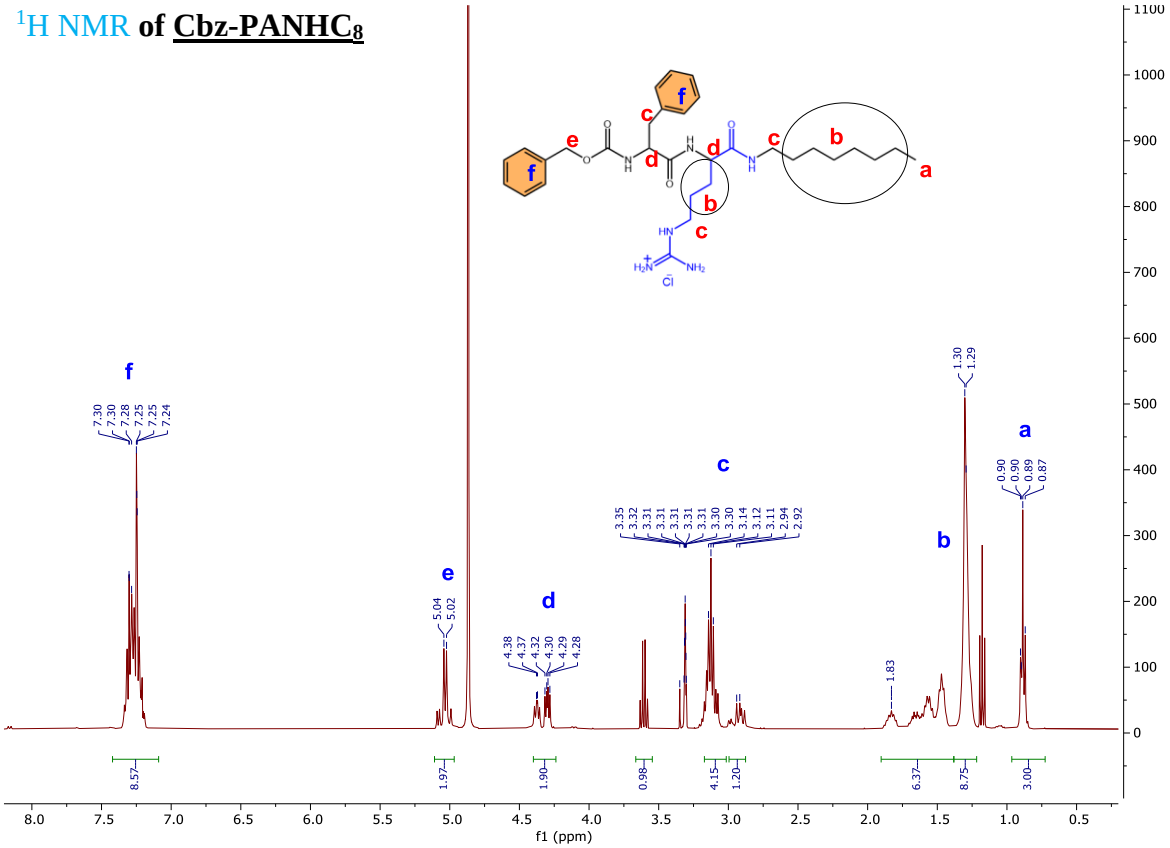
HPLC of Cbz-PANHC$_8$



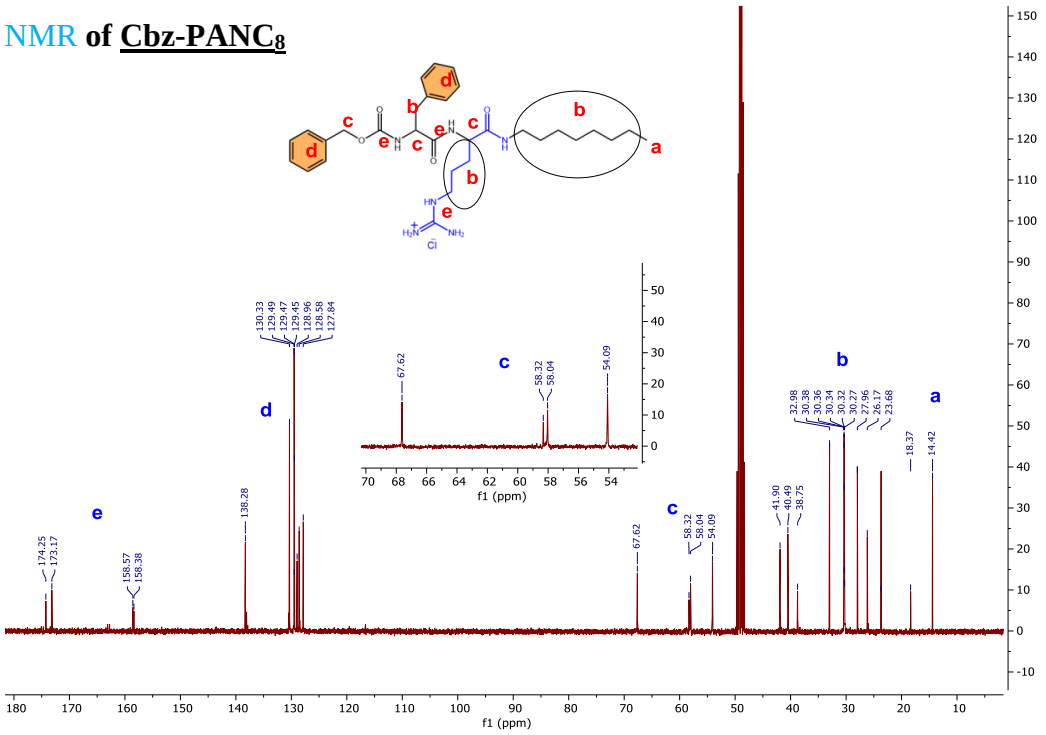
ESI-MS of Cbz-PANHC$_8$



^{1}H NMR of **Cbz-PANHC$_8$**



^{13}C NMR of **Cbz-PANC$_8$**



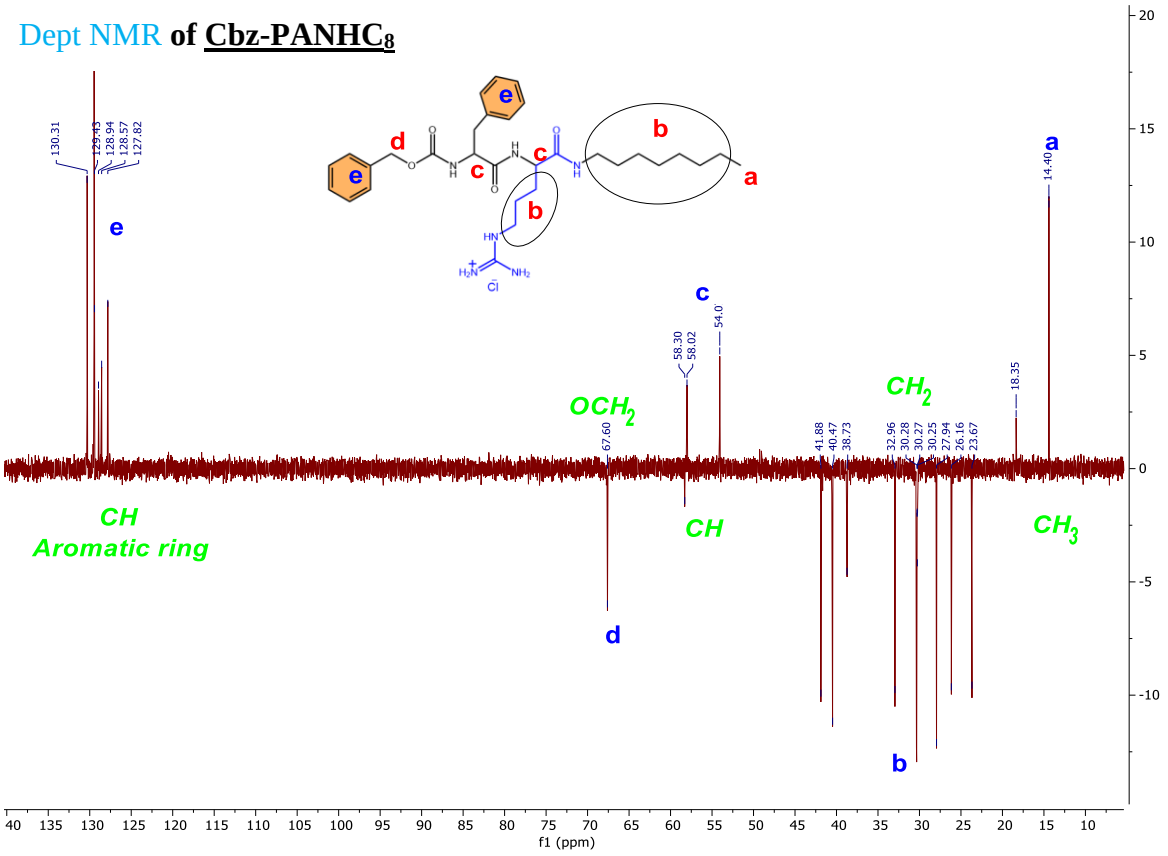
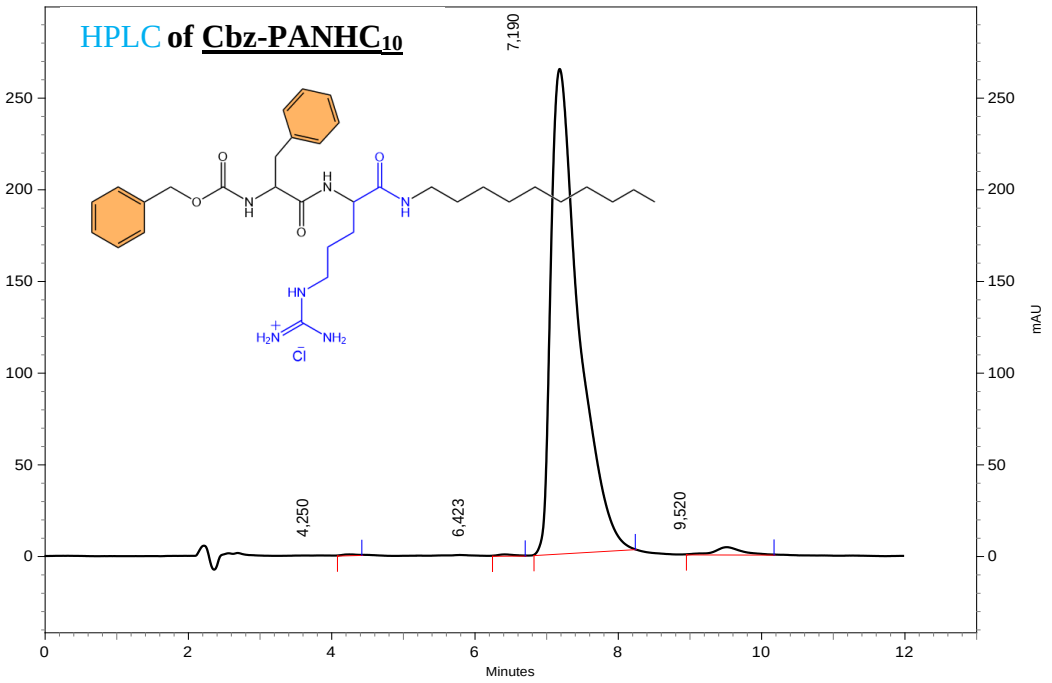
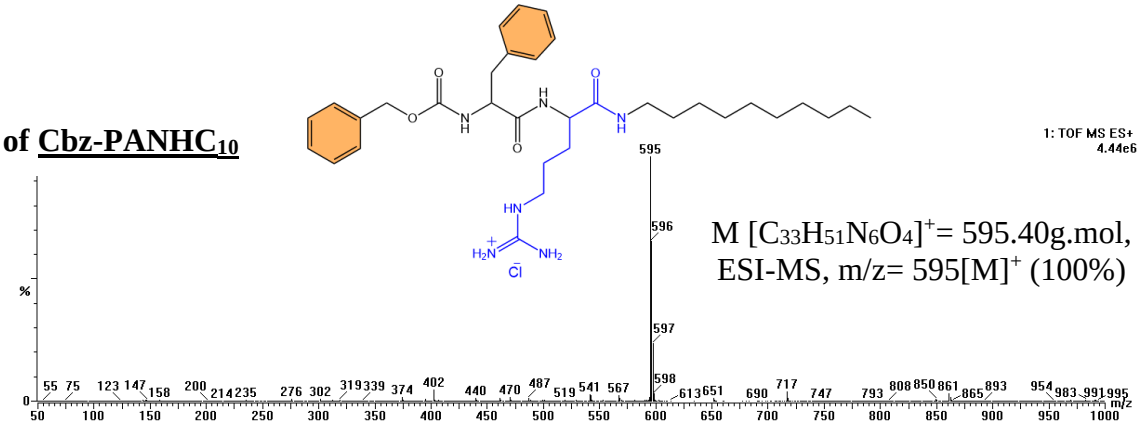


Figure S9. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of Cbz-PANHC$_8$

HPLC of Cbz-PANHC$_{10}$

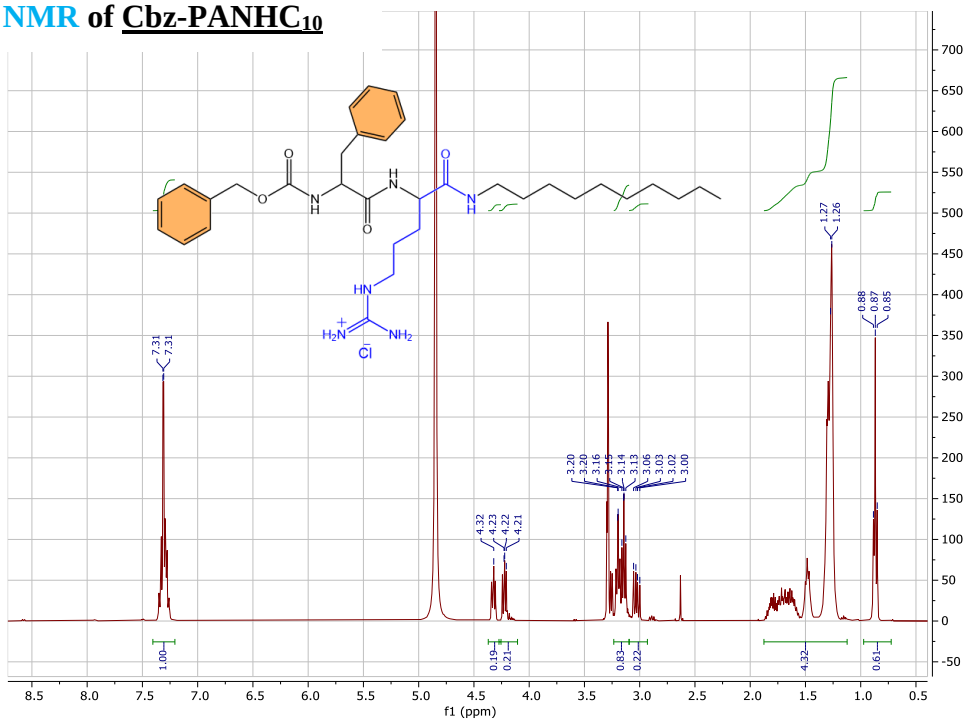


ESI-MS of Cbz-PANHC$_{10}$

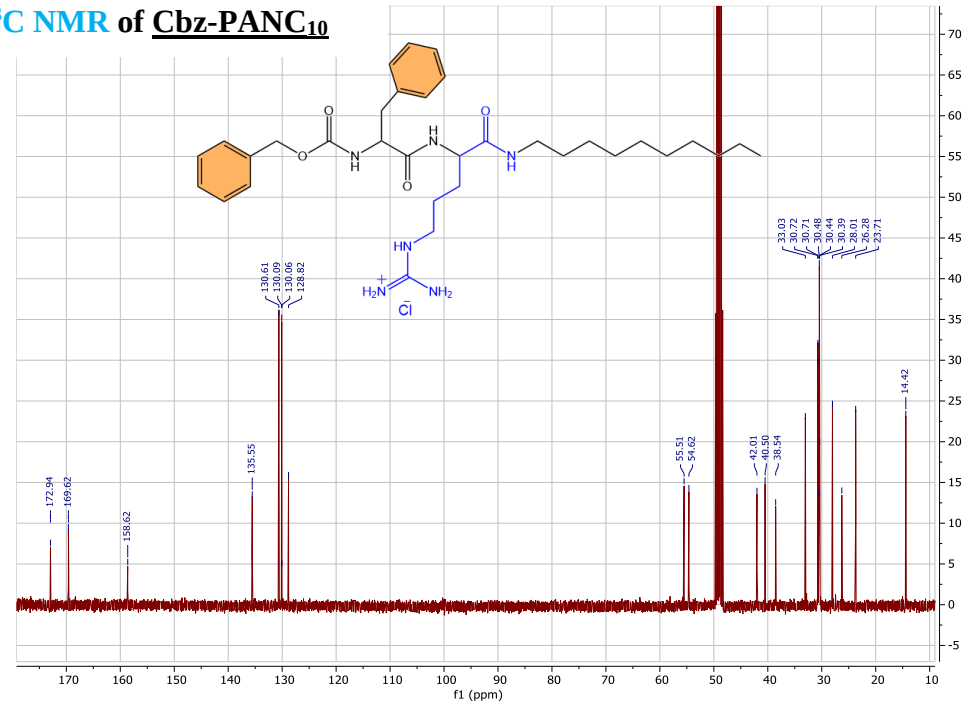


M $[C_{33}H_{51}N_6O_4]^+$= 595.40g.mol,
ESI-MS, m/z= 595$[M]^+$ (100%)

^{1}H NMR of Cbz-PANHC$_{10}$



^{13}C NMR of Cbz-PANC$_{10}$



Dept NMR of Cbz-PANHC$_{10}$

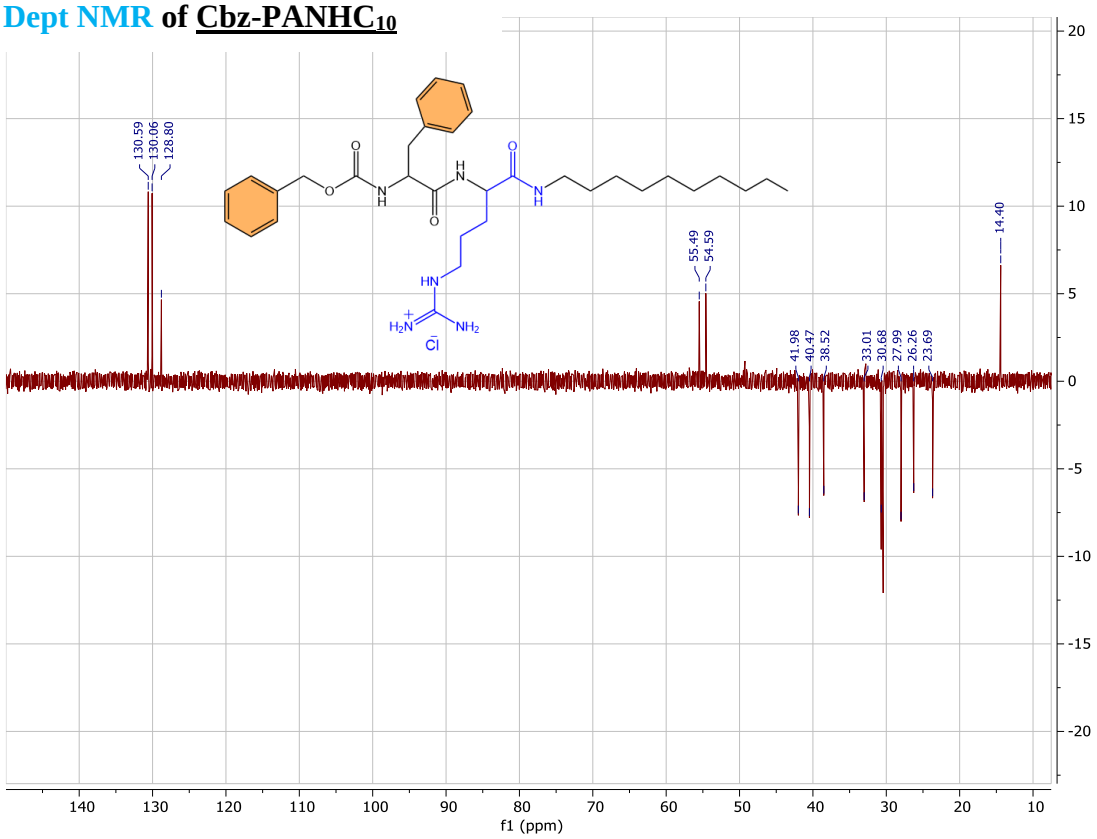
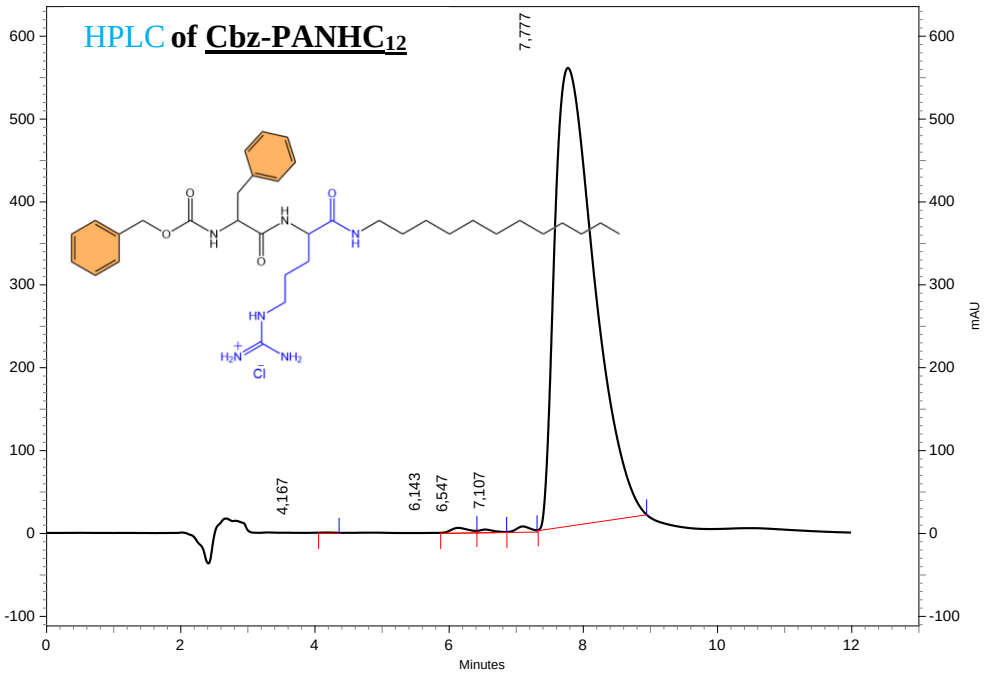
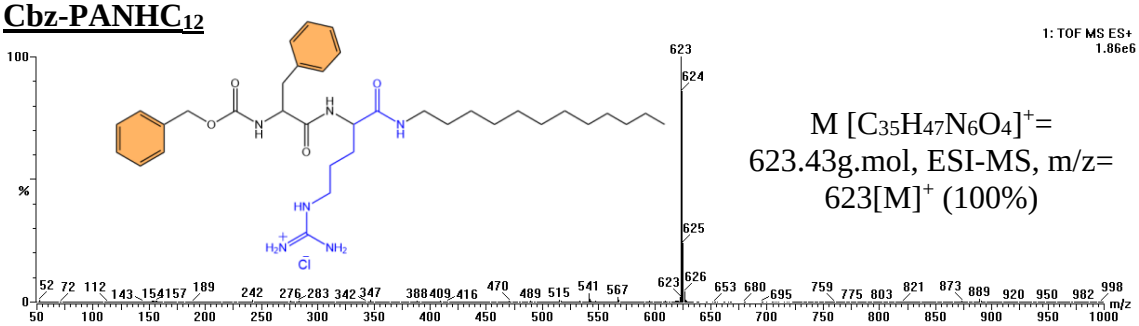


Figure S10. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of Cbz-PANHC$_{10}$

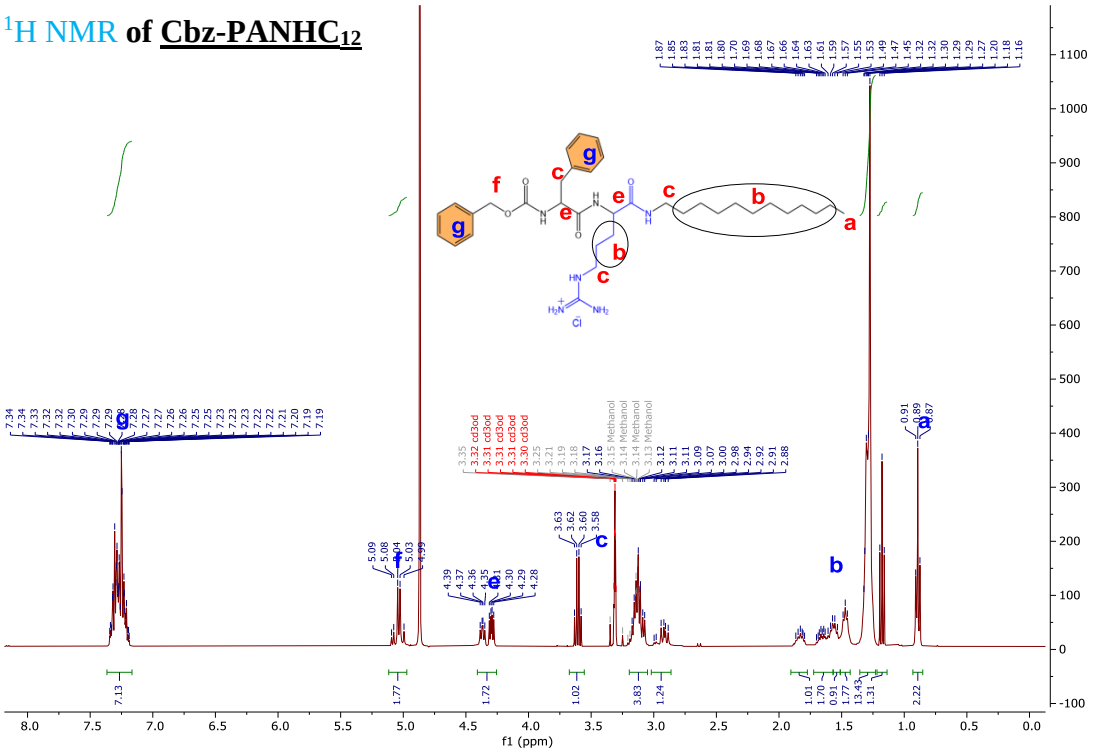


ESI-MS *of* **Cbz-PANHC$_{12}$**

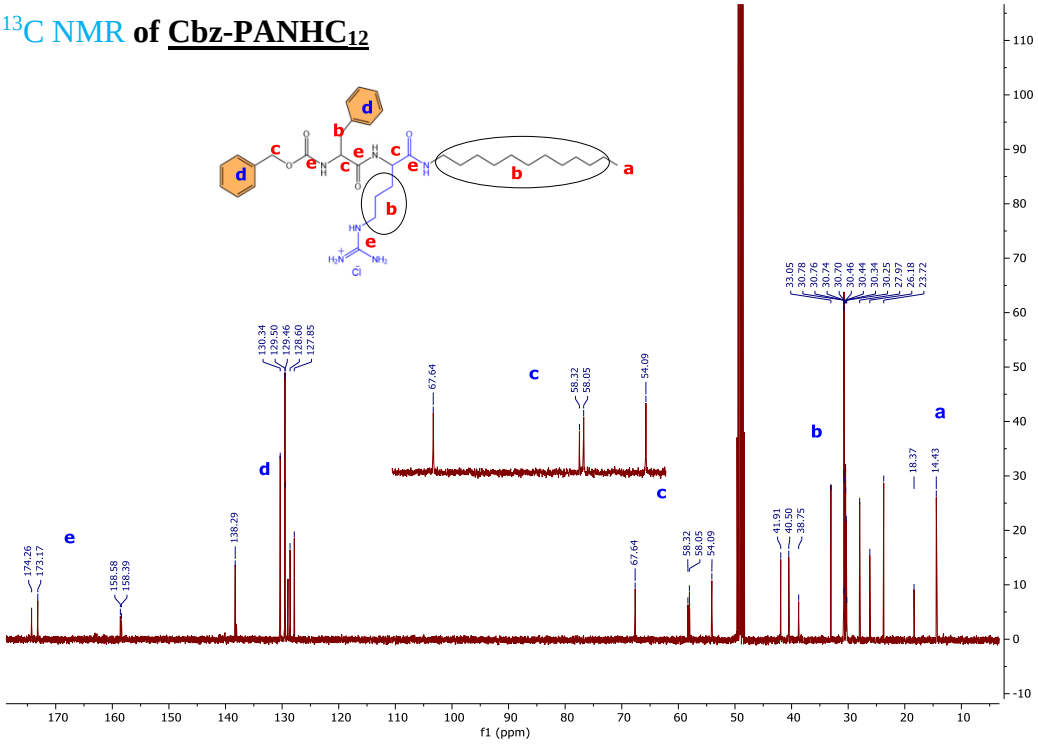


M $[C_{35}H_{47}N_6O_4]^+$= 623.43g.mol, ESI-MS, m/z= 623$[M]^+$ (100%)

^{1}H NMR of **Cbz-PANHC$_{12}$**



^{13}C NMR of **Cbz-PANHC$_{12}$**



Dept NMR **of <u>Cbz-PANHC$_{12}$</u>**

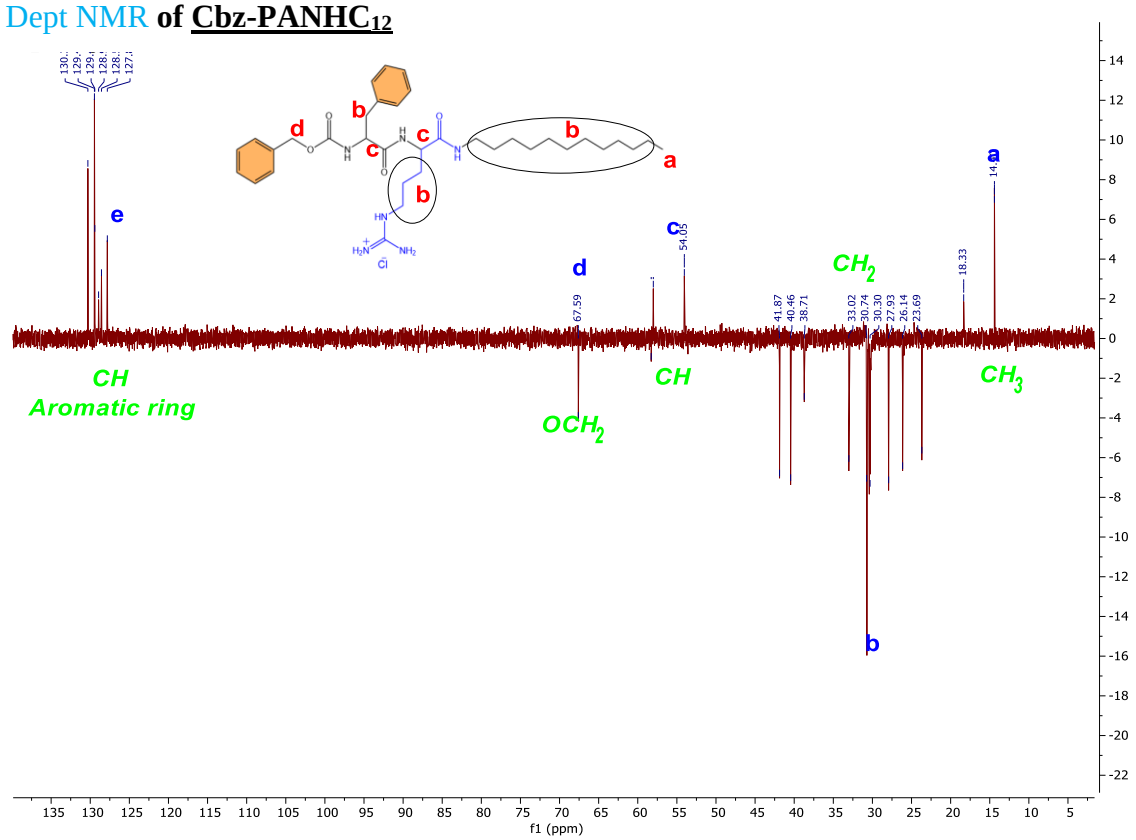
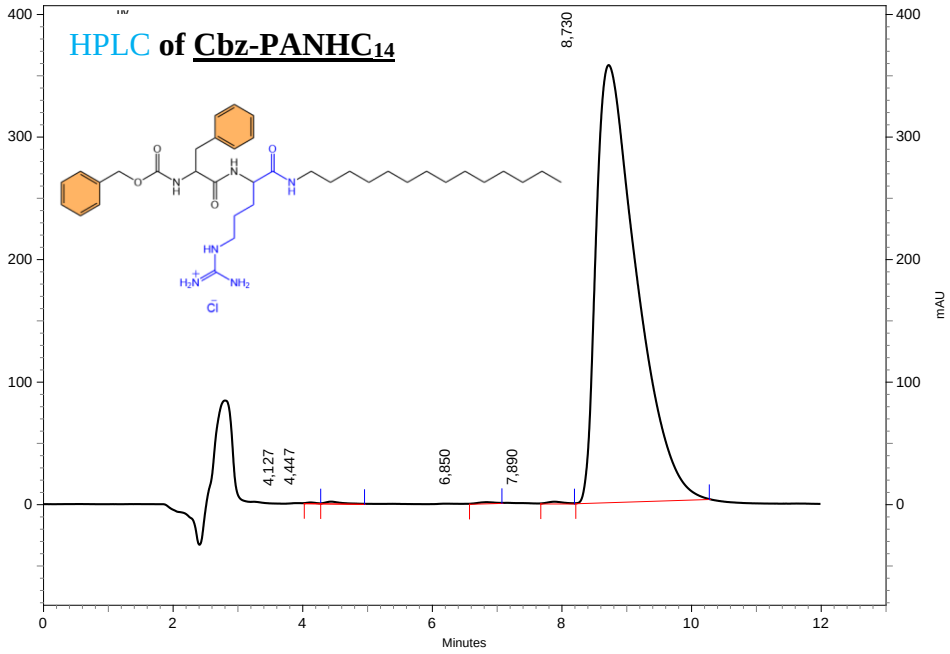
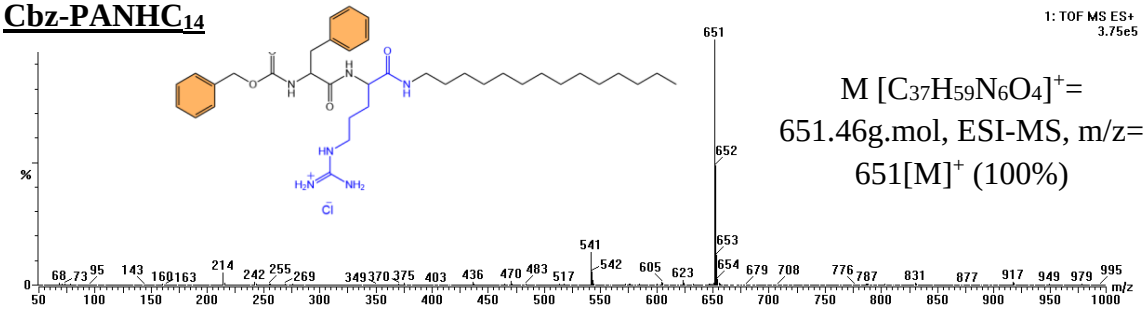


Figure S11. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of Cbz-PANHC$_{12}$

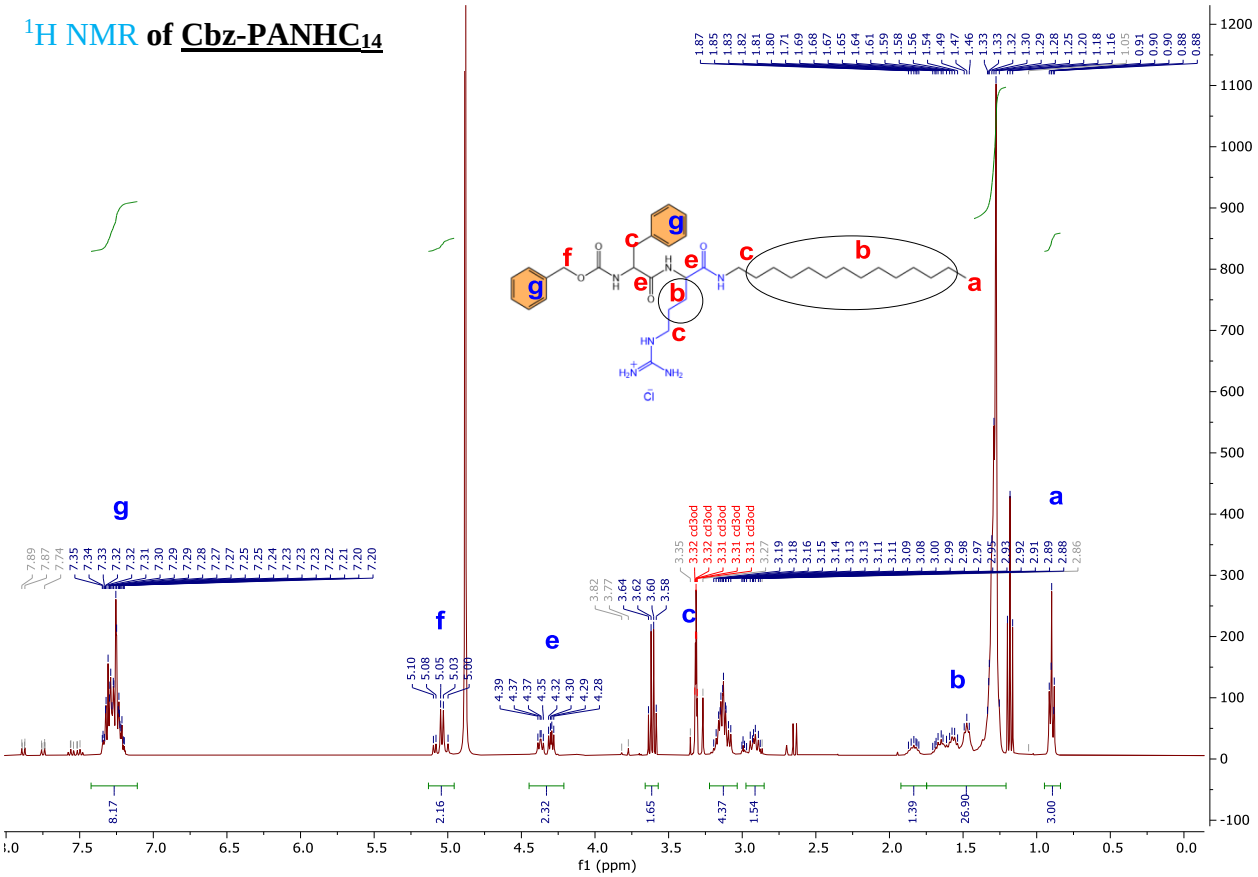


ESI-MS **of** **Cbz-PANHC$_{14}$**

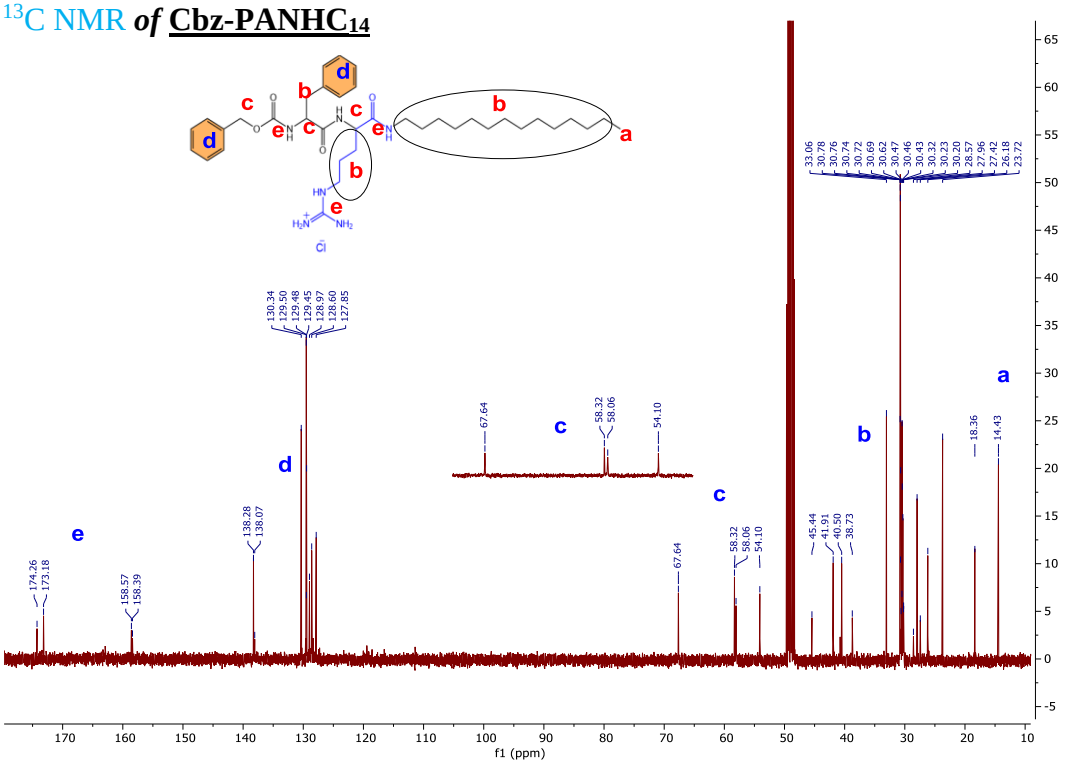


M $[C_{37}H_{59}N_6O_4]^+$= 651.46g.mol, ESI-MS, m/z= 651$[M]^+$ (100%)

^{1}H NMR **of Cbz-PANHC$_{14}$**



^{13}C NMR *of* **Cbz-PANHC$_{14}$**



Dept NMR *of* **Cbz-PANHC$_{14}$**

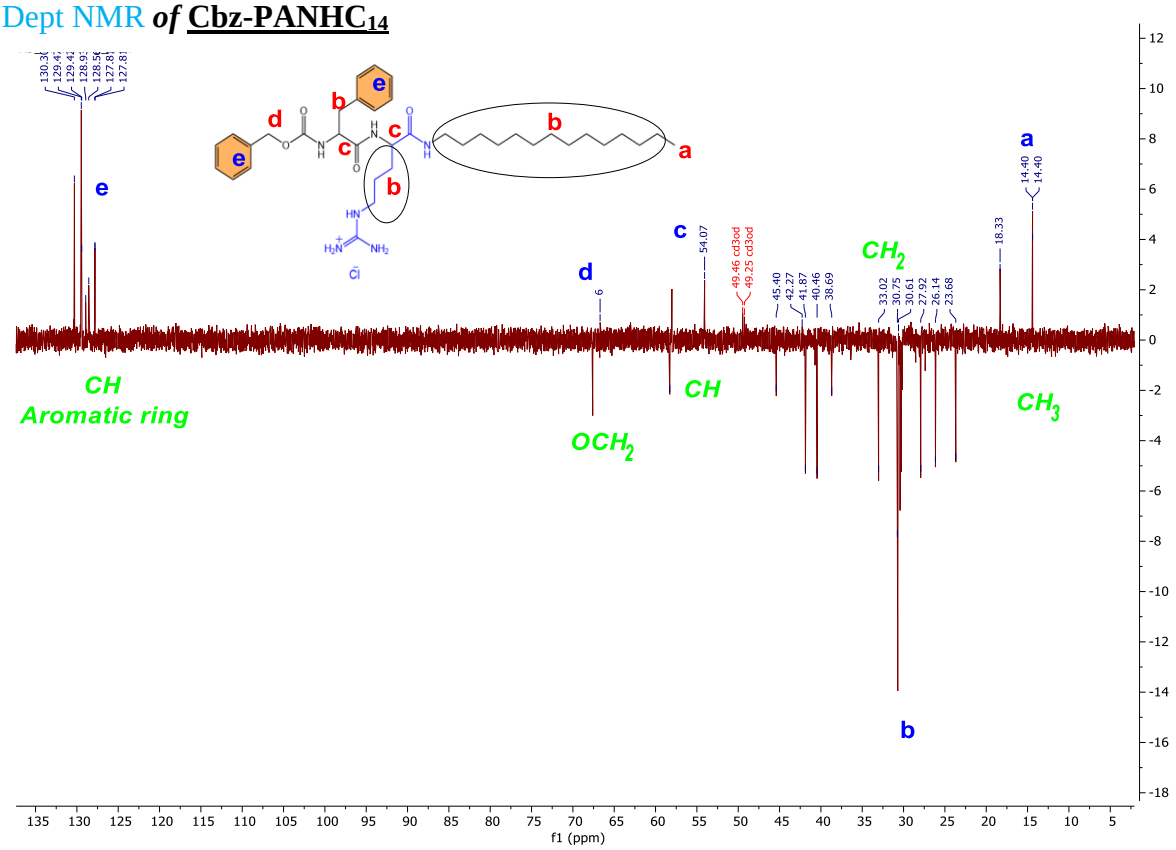
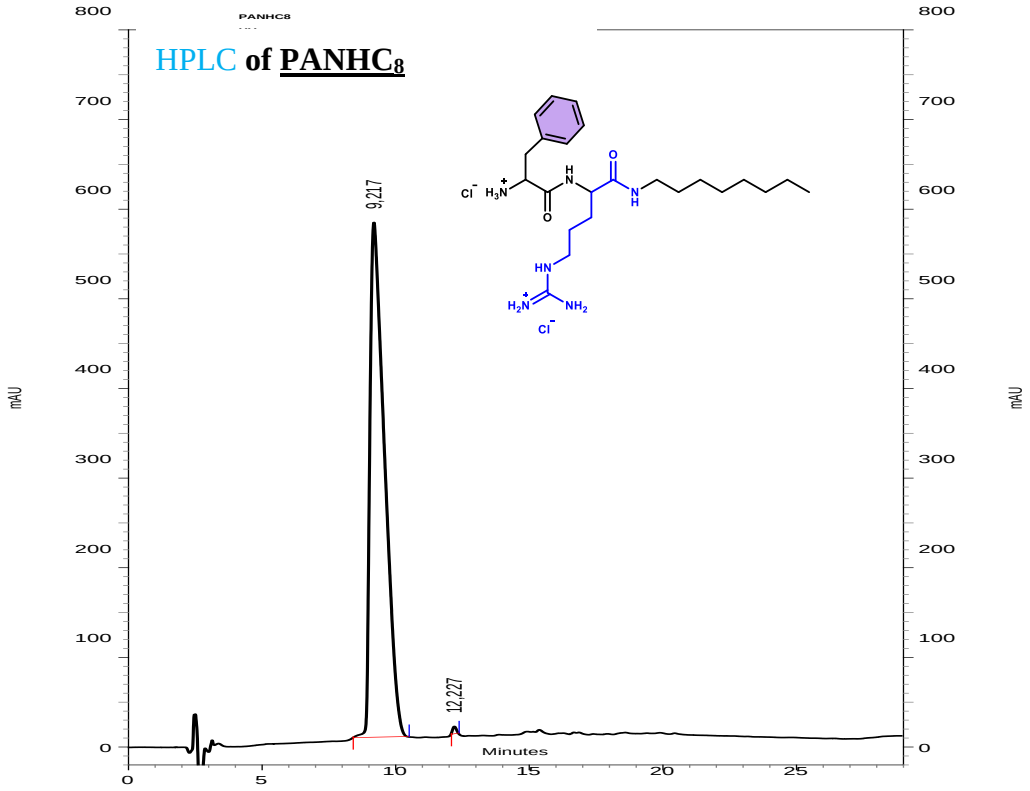
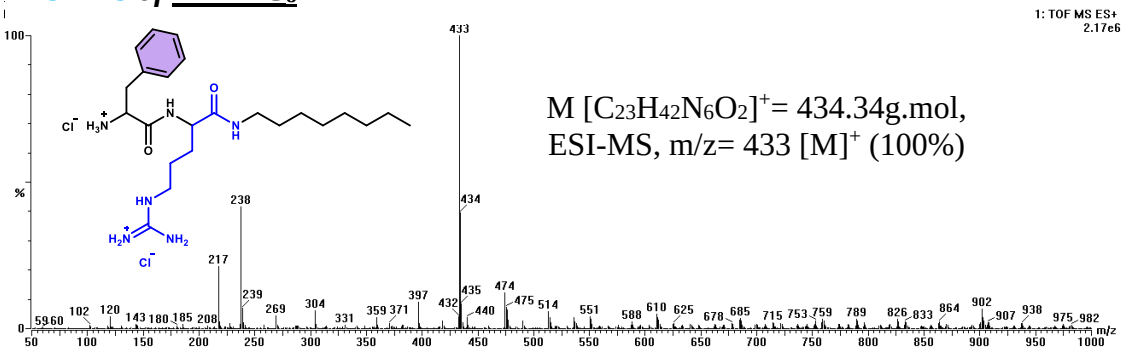


Figure S12. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of Cbz-PANHC$_{14}$

HPLC of **PANHC$_8$**

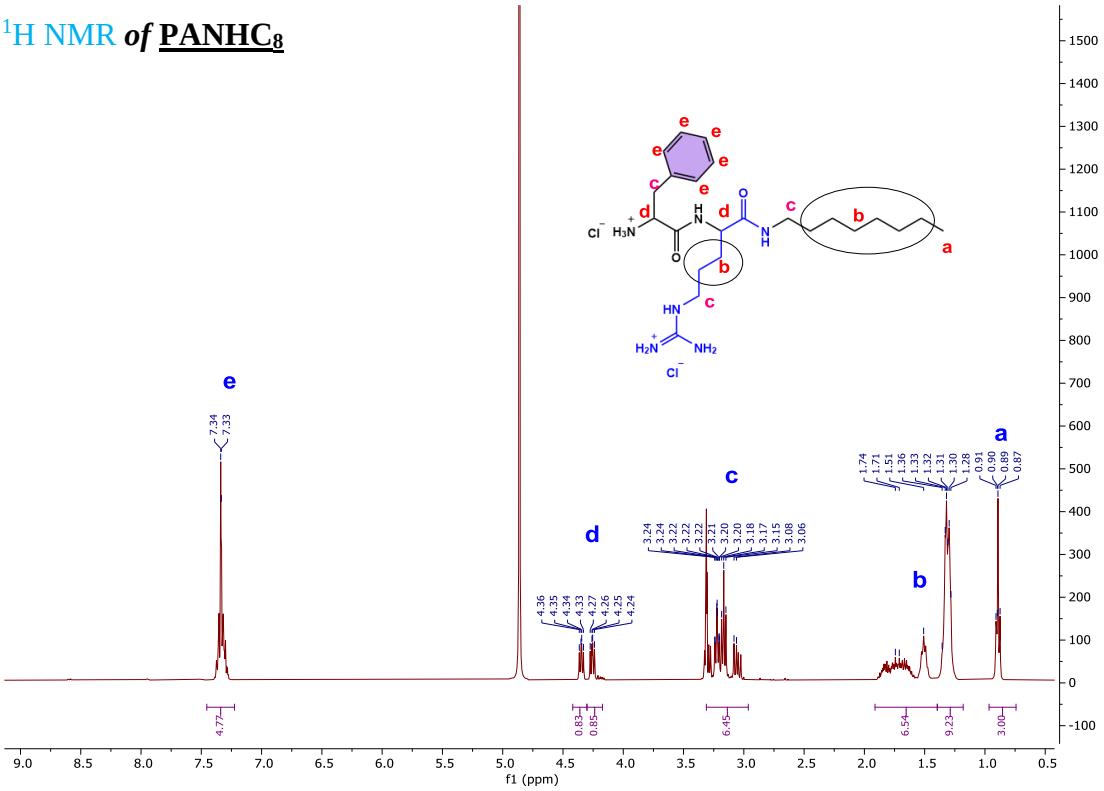


ESI-MS *of* **PANHC$_8$**

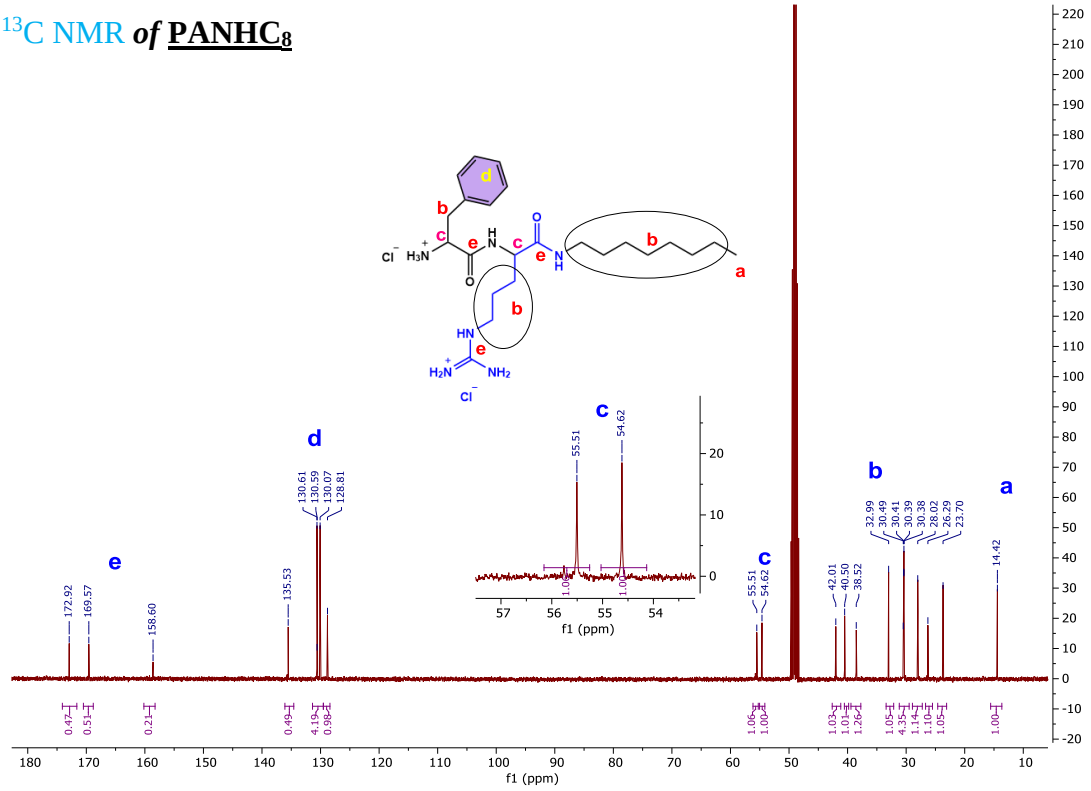


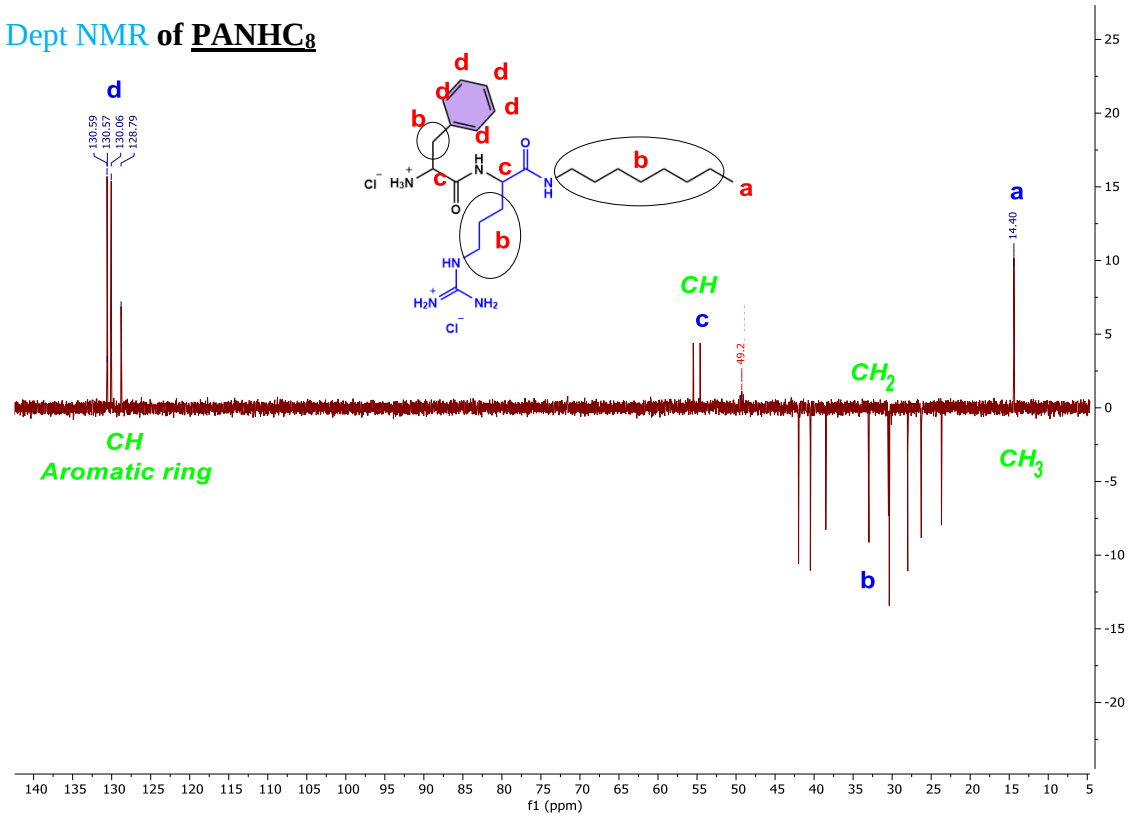
M $[C_{23}H_{42}N_6O_2]^+$= 434.34g.mol,
ESI-MS, m/z= 433 $[M]^+$ (100%)

^{1}H NMR *of* **PANHC$_8$**

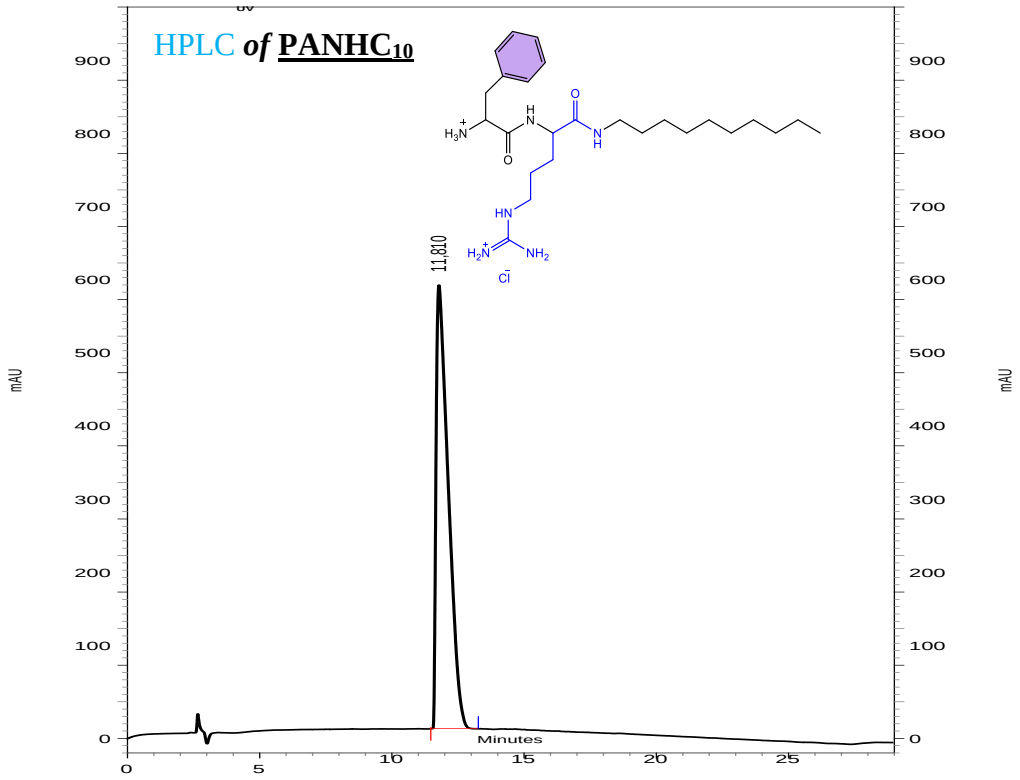


^{13}C NMR *of* **PANHC$_8$**

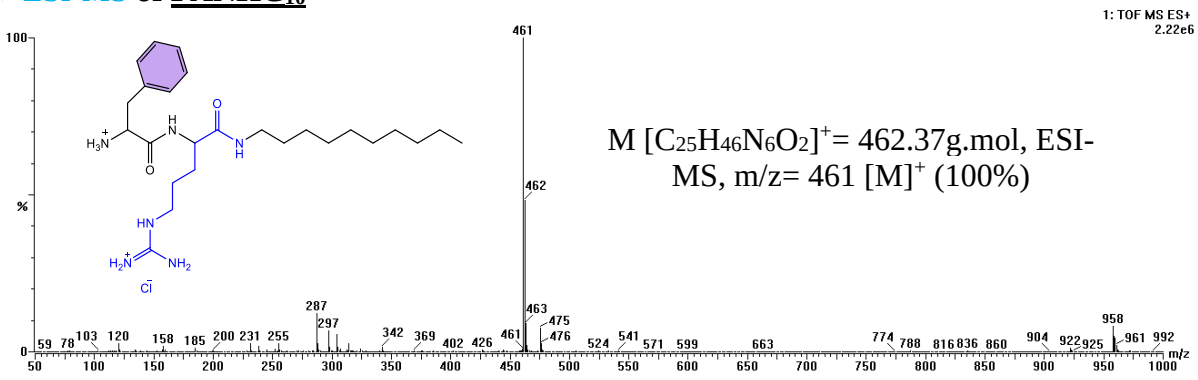




. **Figure S13.** HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of PANHC$_8$

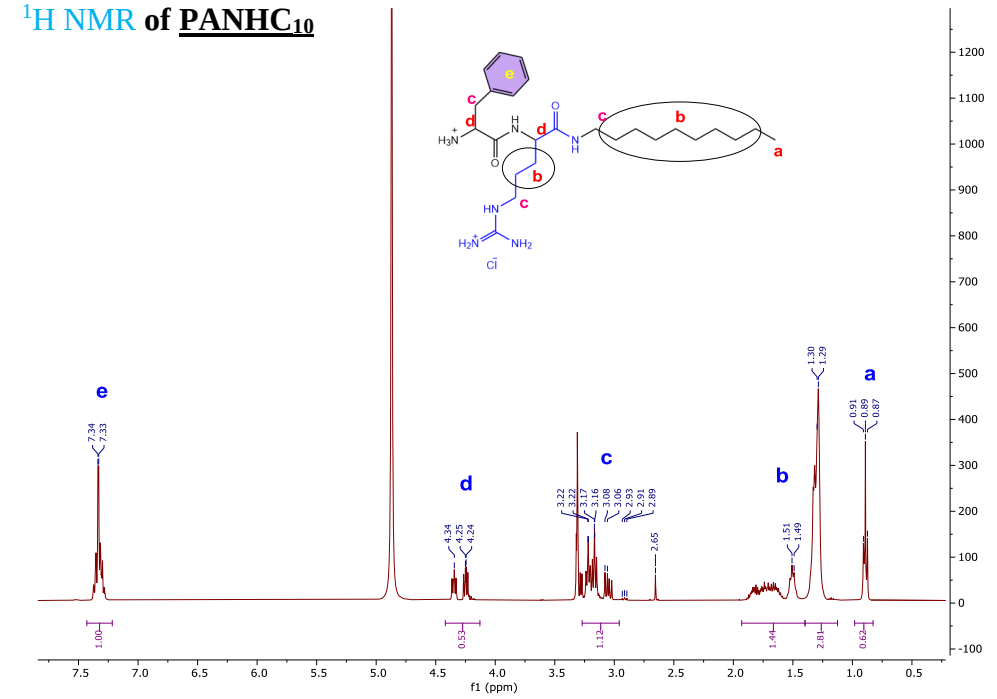


ESI-MS **of** **PANHC$_{10}$**

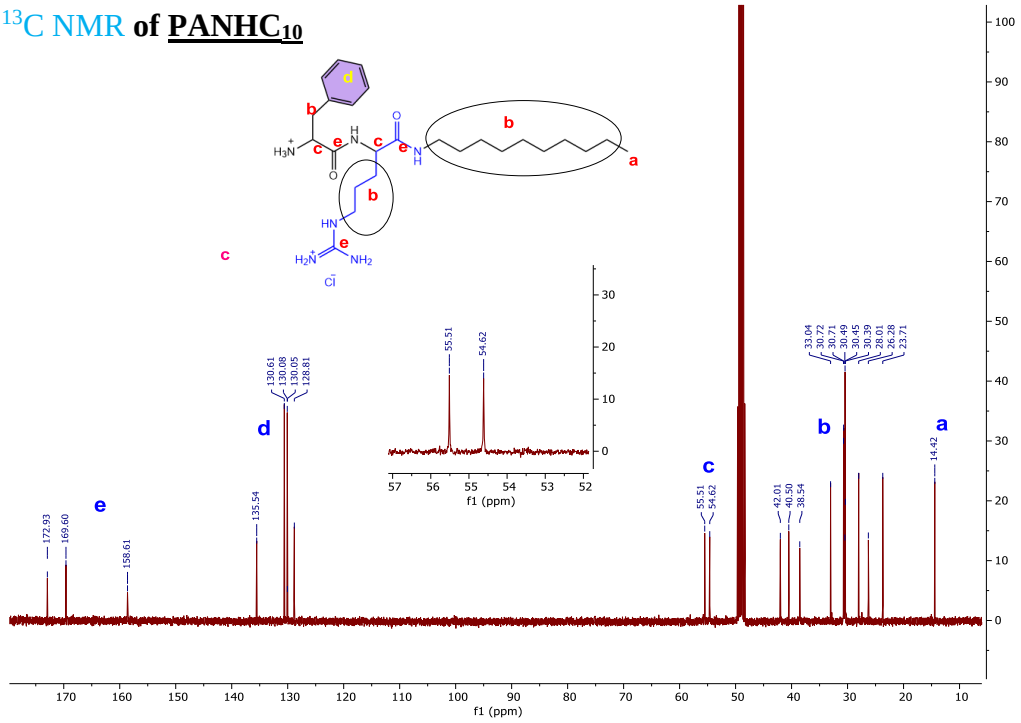


M $[C_{25}H_{46}N_6O_2]^+$= 462.37g.mol, ESI-MS, m/z= 461 $[M]^+$ (100%)

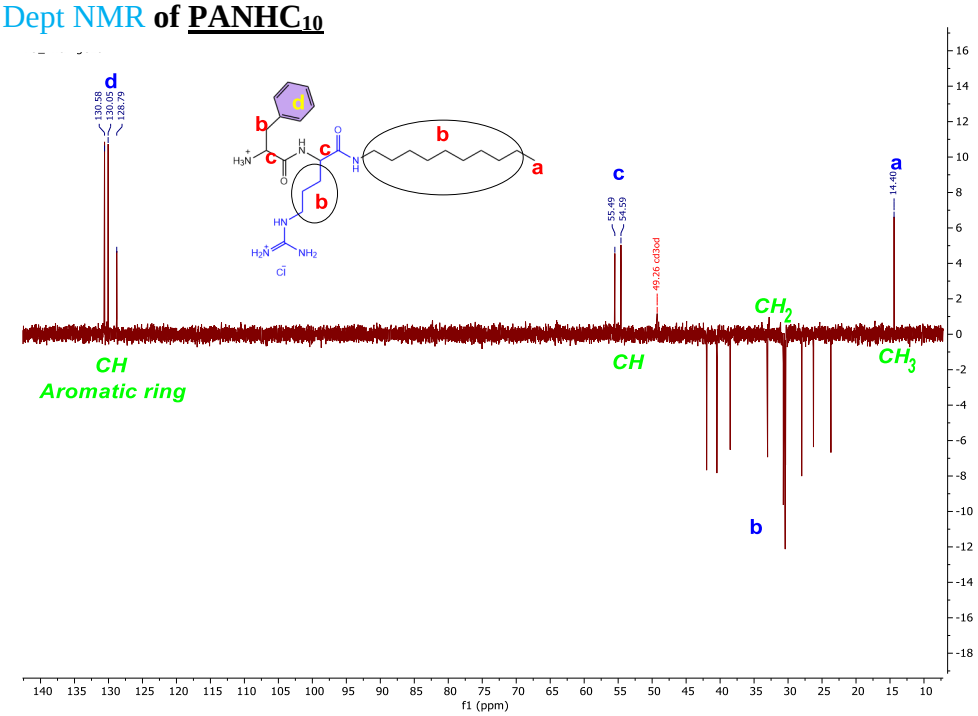
^{1}H NMR of **PANHC$_{10}$**



^{13}C NMR of **PANHC$_{10}$**

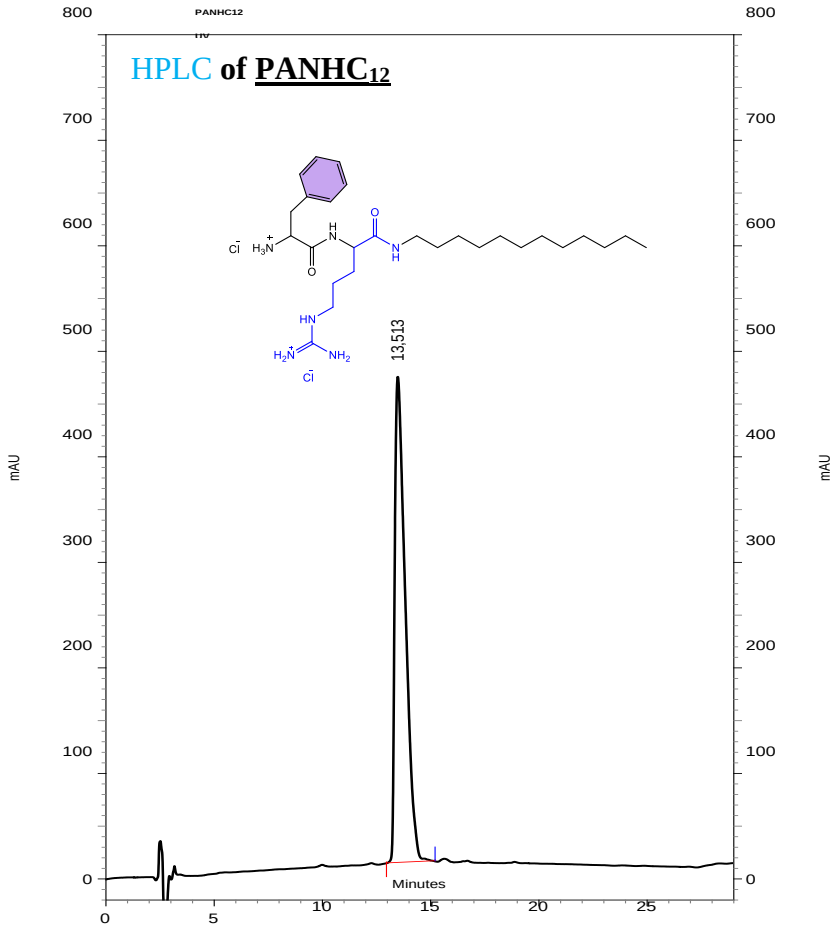


Dept NMR **of <u>PANHC$_{10}$</u>**



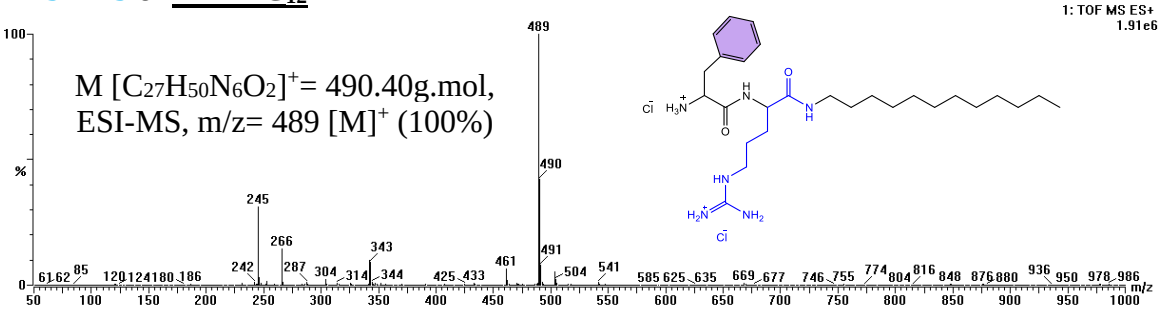
. **Figure S14.** HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of PANHC$_{10}$

HPLC **of PANHC$_{12}$**

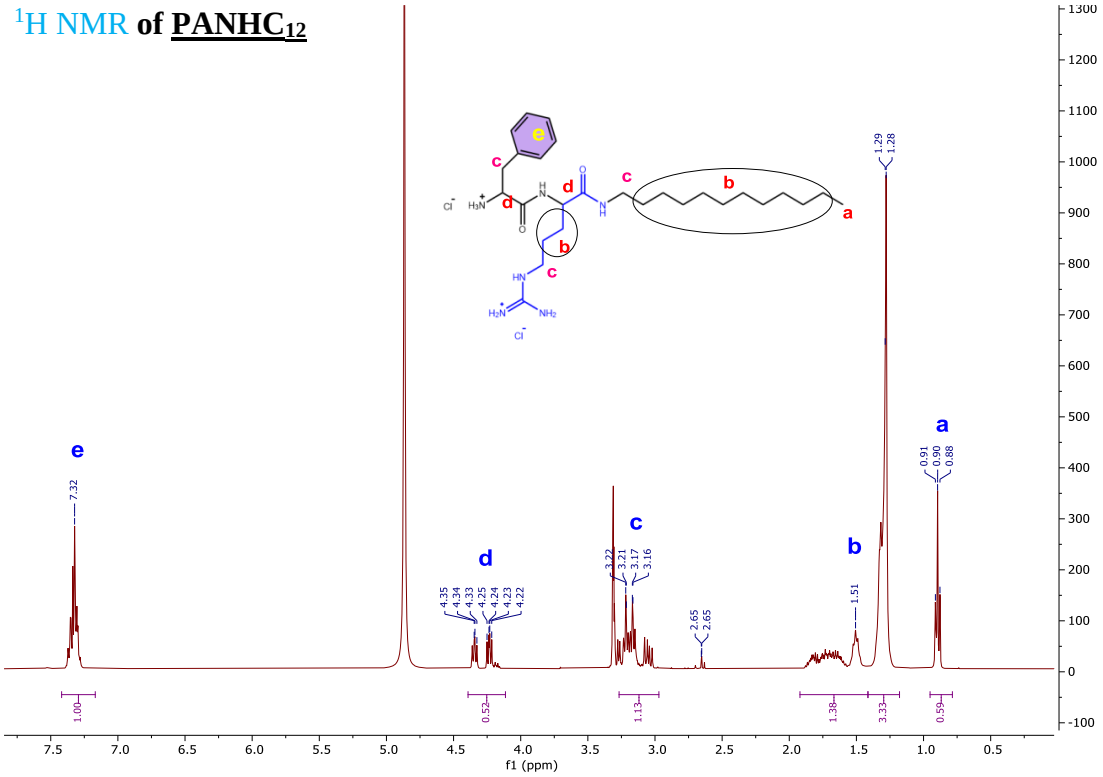


ESI-MS **of PANHC$_{12}$**

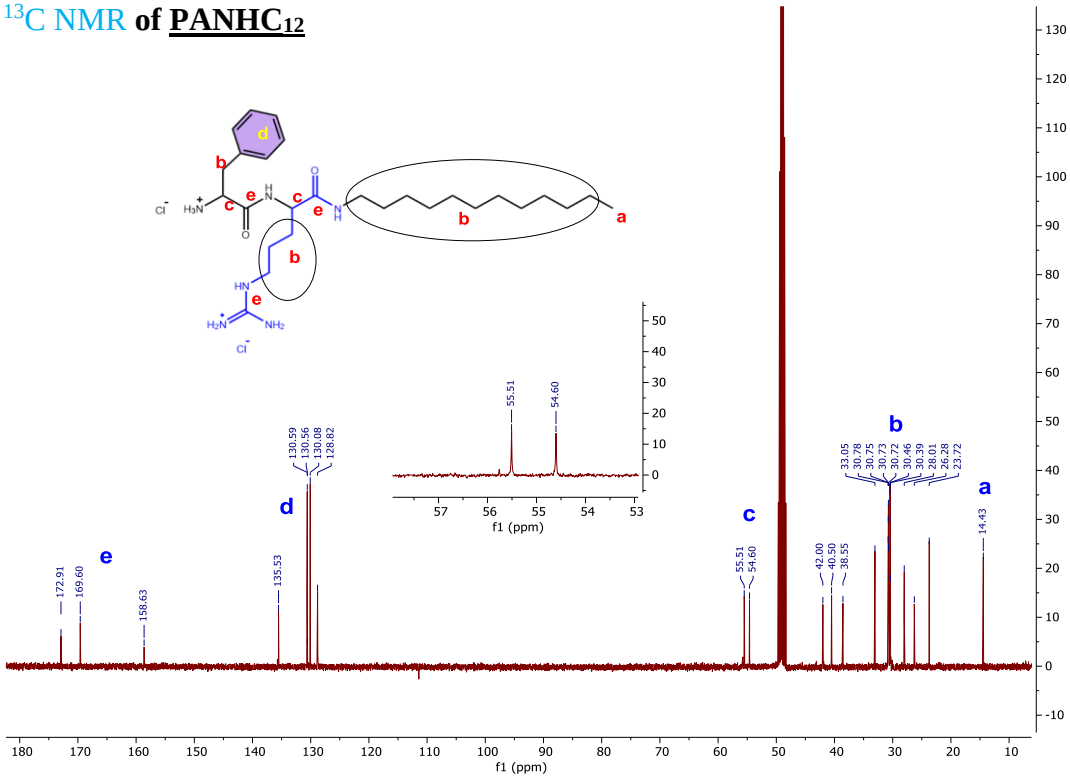
M $[C_{27}H_{50}N_6O_2]^+$= 490.40g.mol,
ESI-MS, m/z= 489 $[M]^+$ (100%)



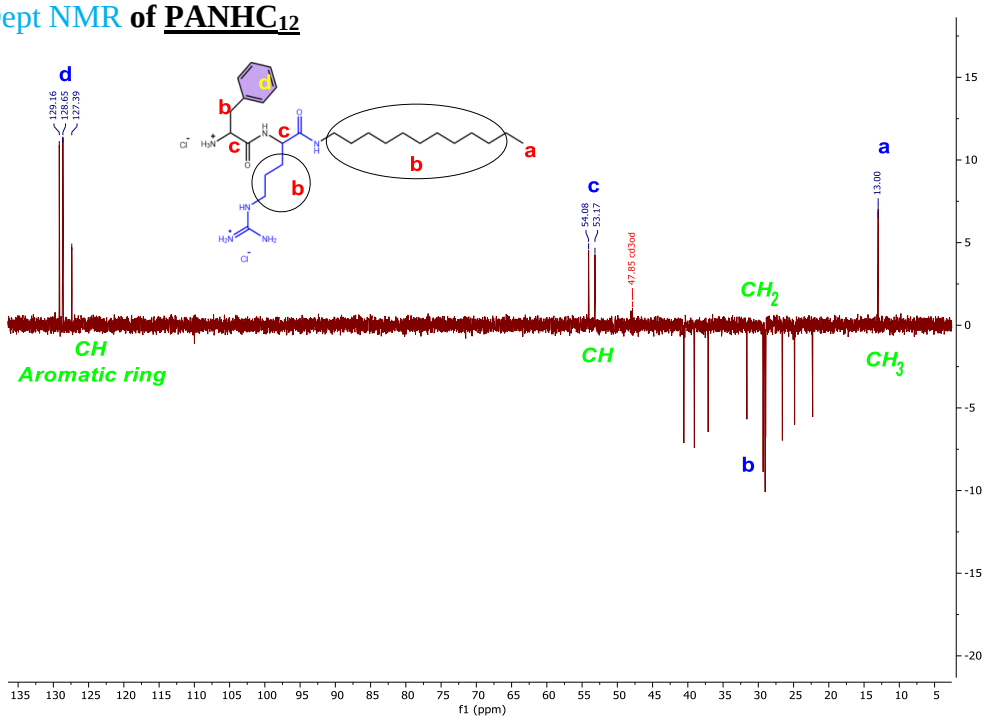
^{1}H NMR of **PANHC$_{12}$**



^{13}C NMR of **PANHC$_{12}$**

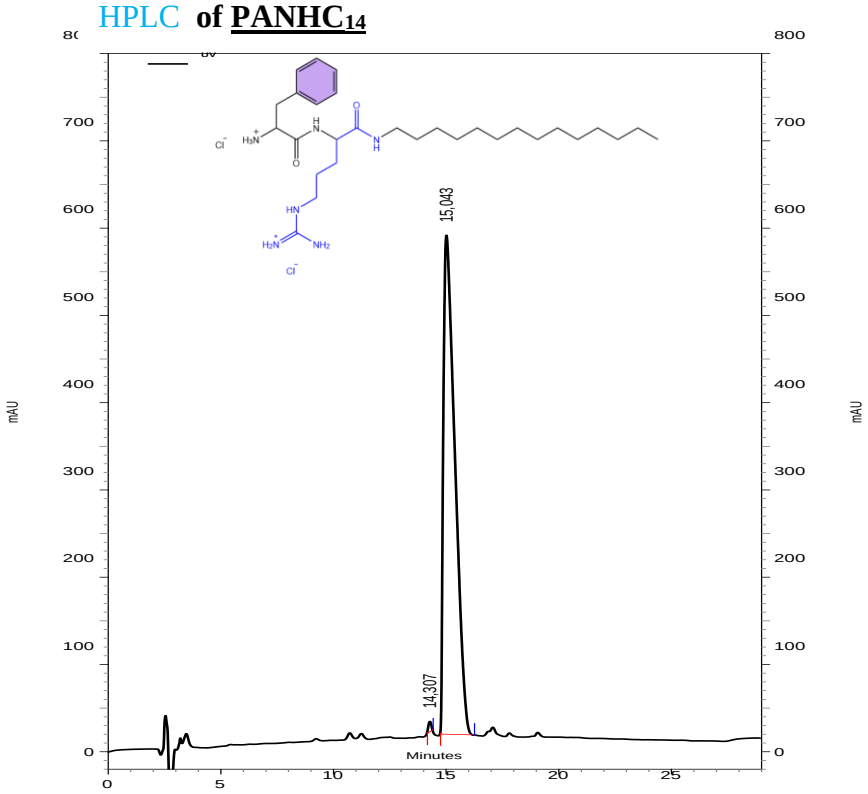


Dept NMR **of <u>PANHC$_{12}$</u>**

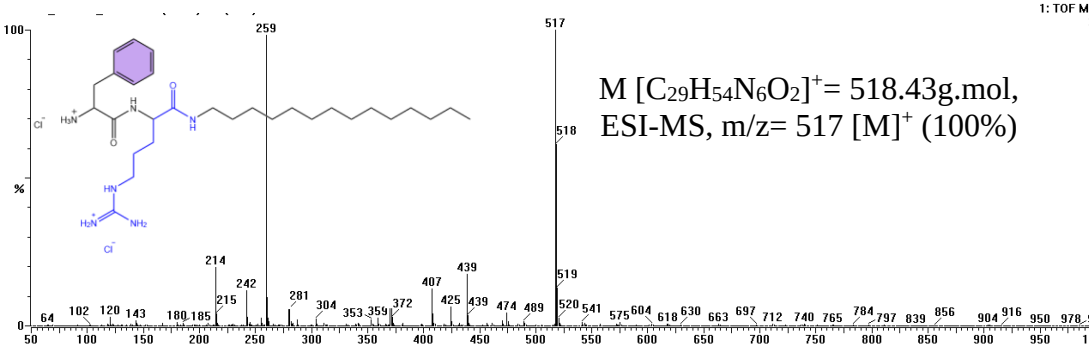


. **Figure S15.** HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of PANHC$_{12}$

HPLC of **PANHC$_{14}$**

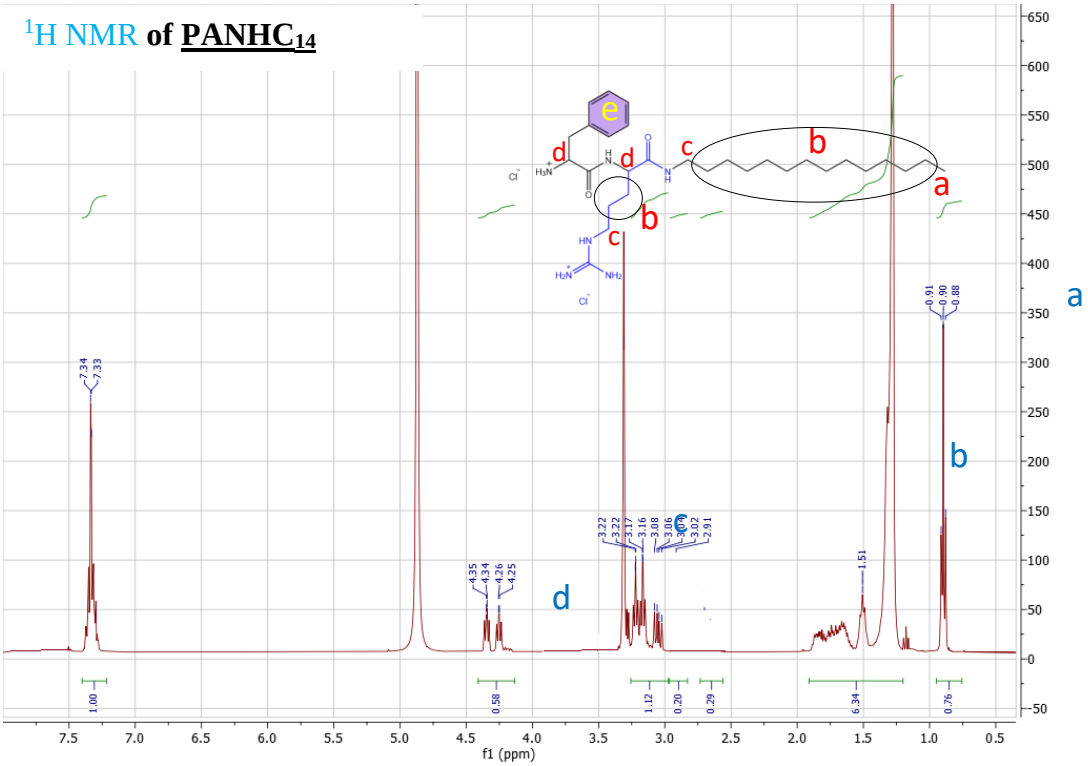


ESI-MS of **PANHC$_{14}$**

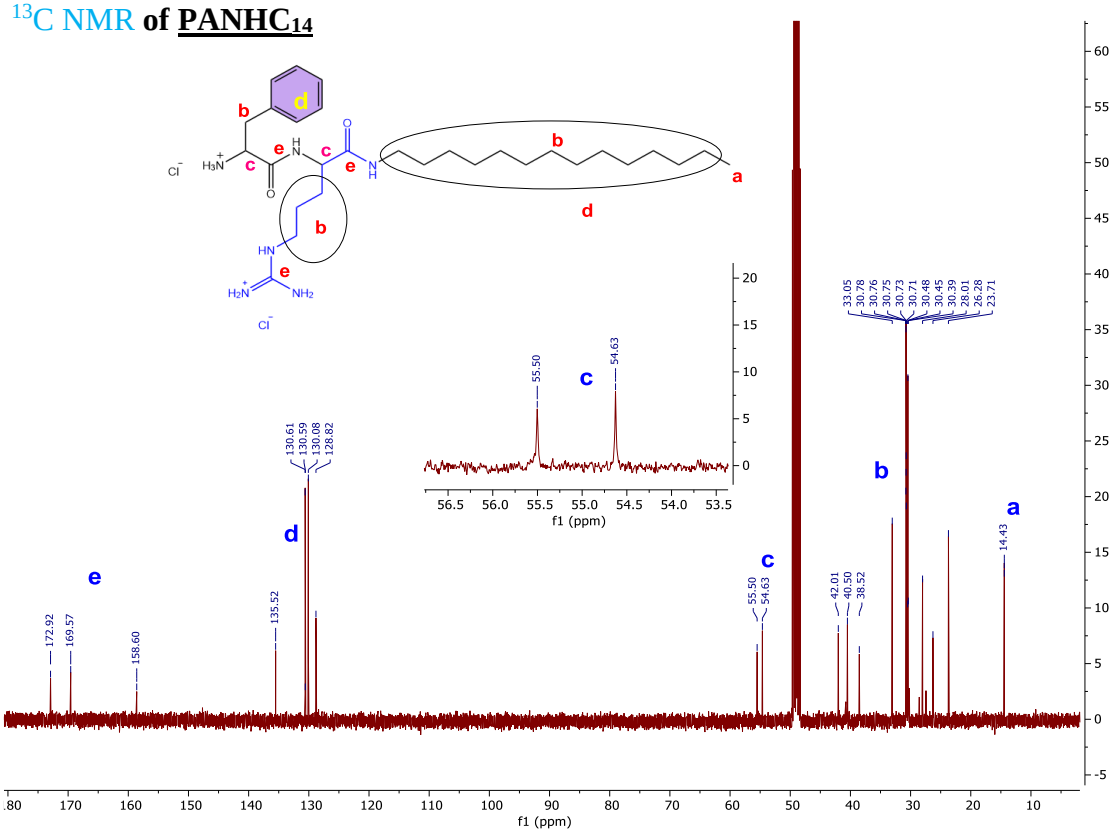


M $[C_{29}H_{54}N_6O_2]^+$= 518.43g.mol,
ESI-MS, m/z= 517 $[M]^+$ (100%)

^{1}H NMR of **PANHC$_{14}$**



^{13}C NMR of **PANHC$_{14}$**



Dept NMR **of PANHC$_{14}$**

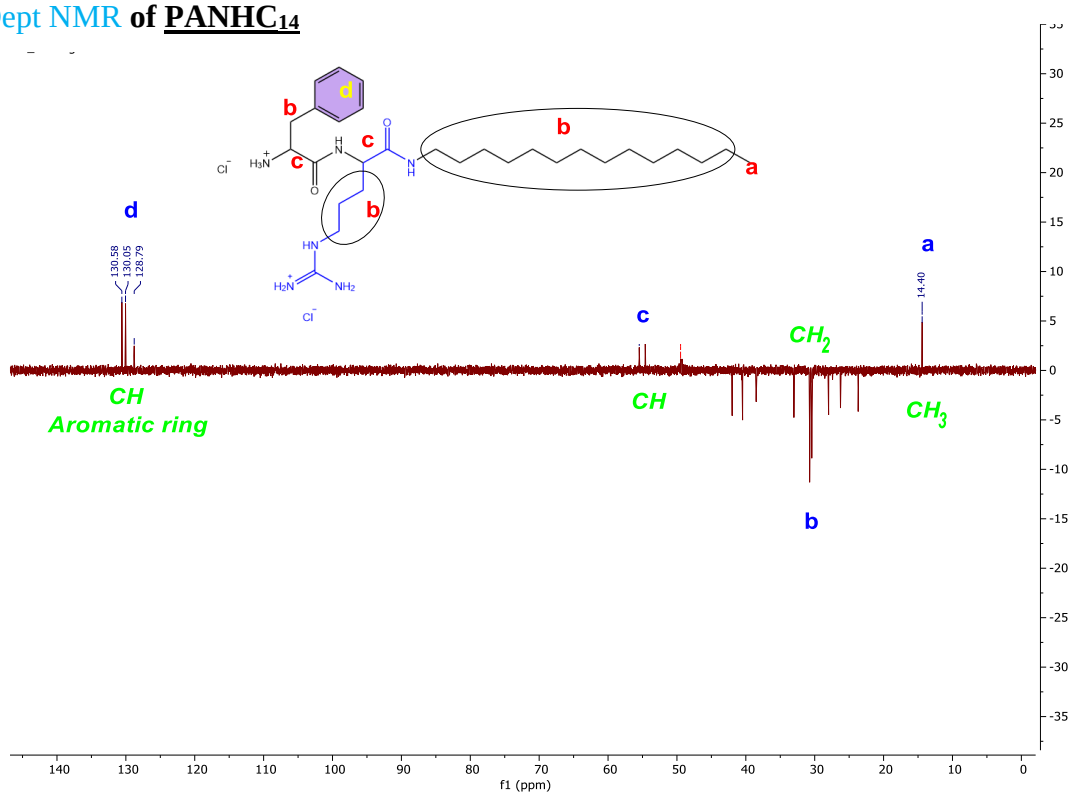
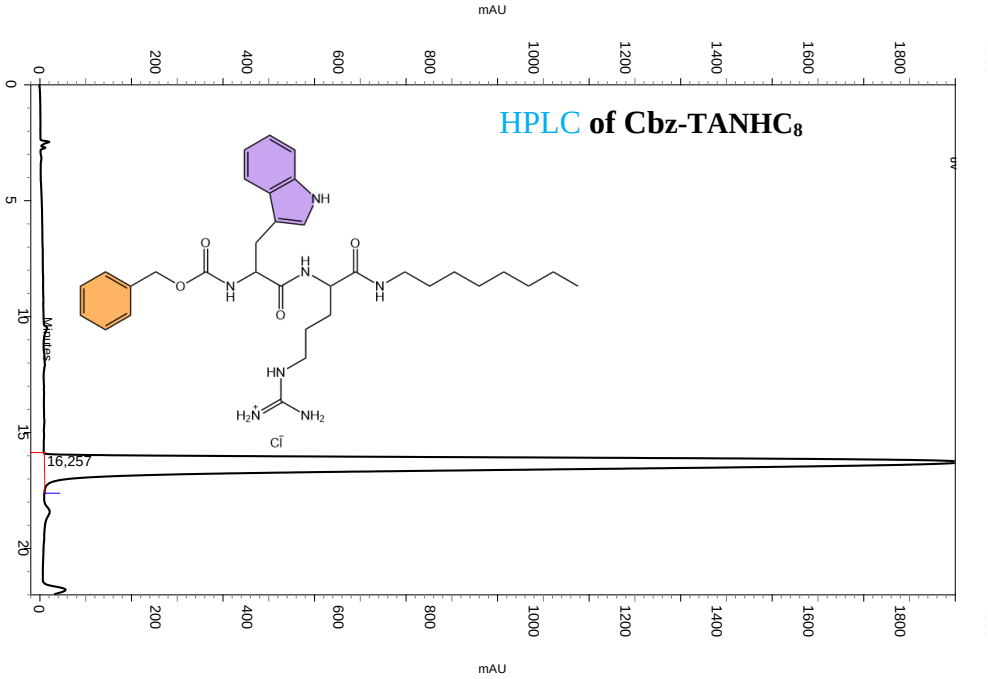
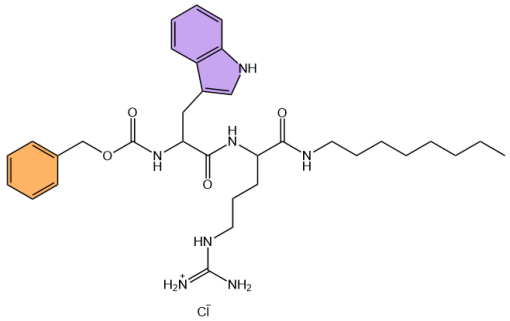


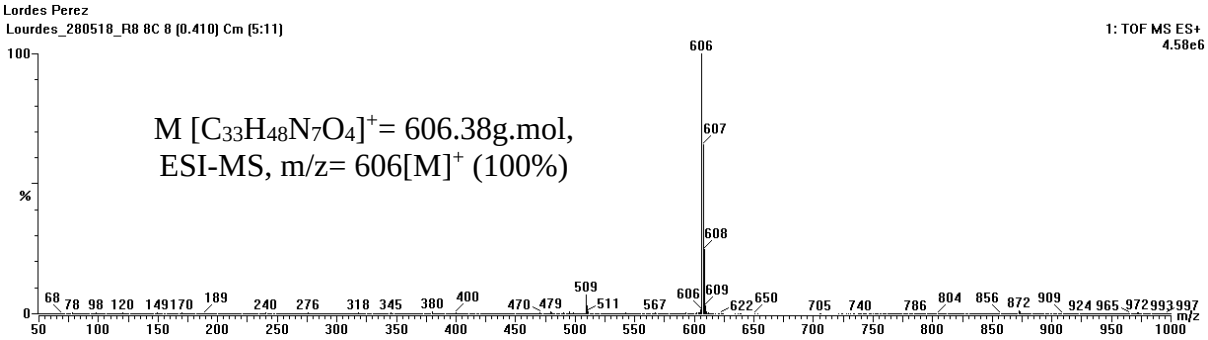
Figure S16. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of PANHC$_{14}$



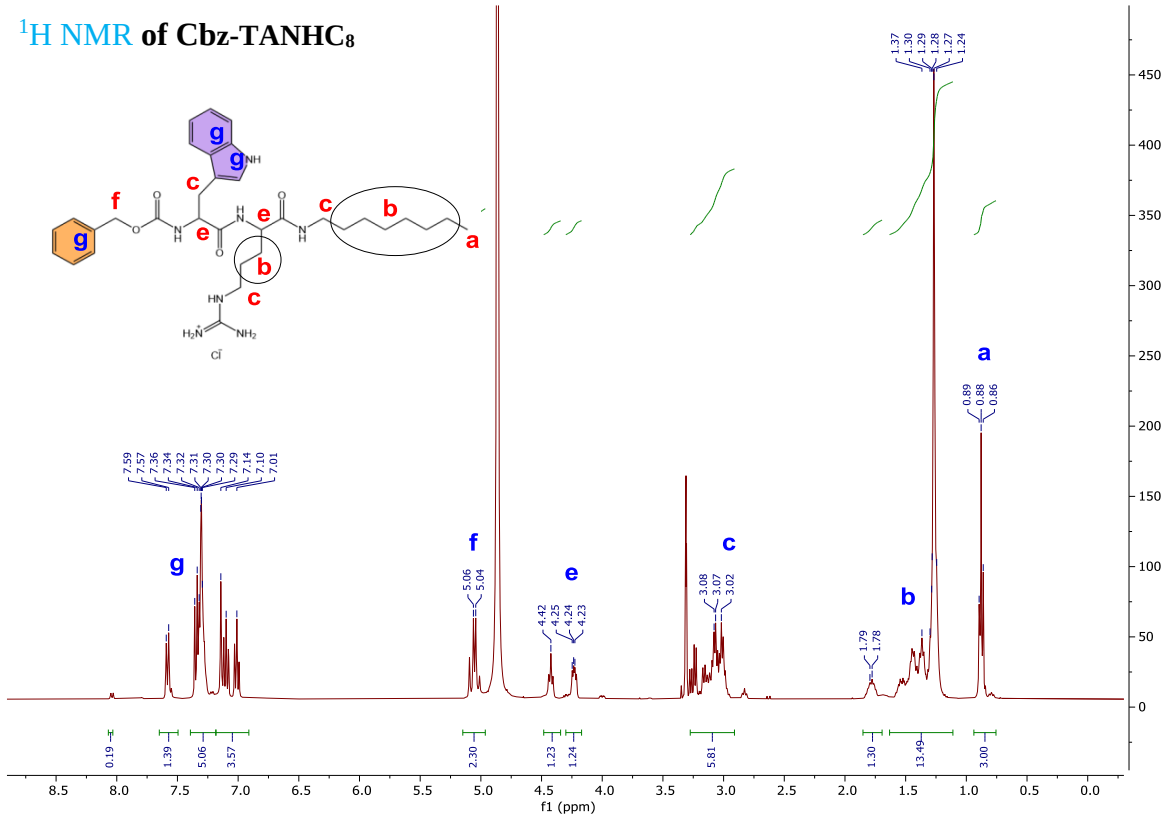
HPLC of Cbz-TANHC$_8$



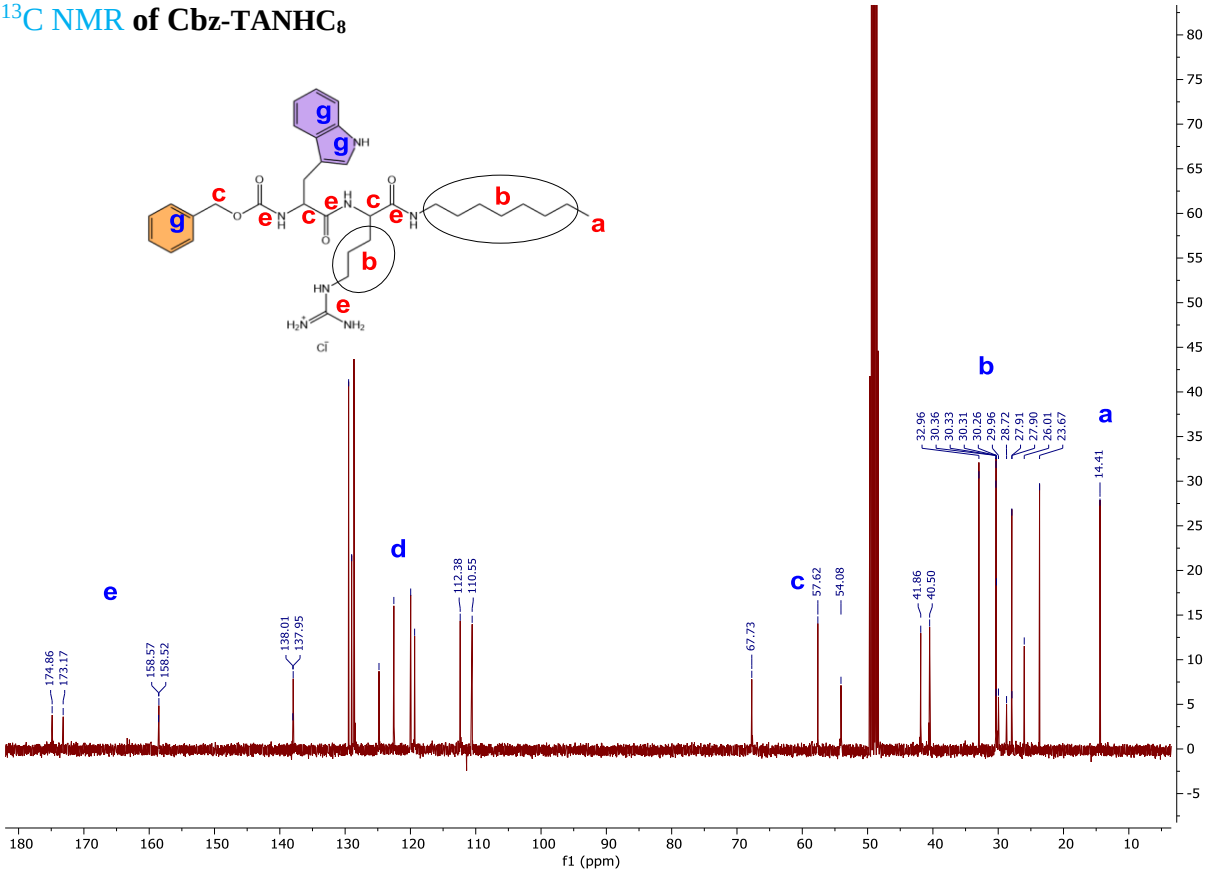
ESI-MS of Cbz-TANHC$_8$



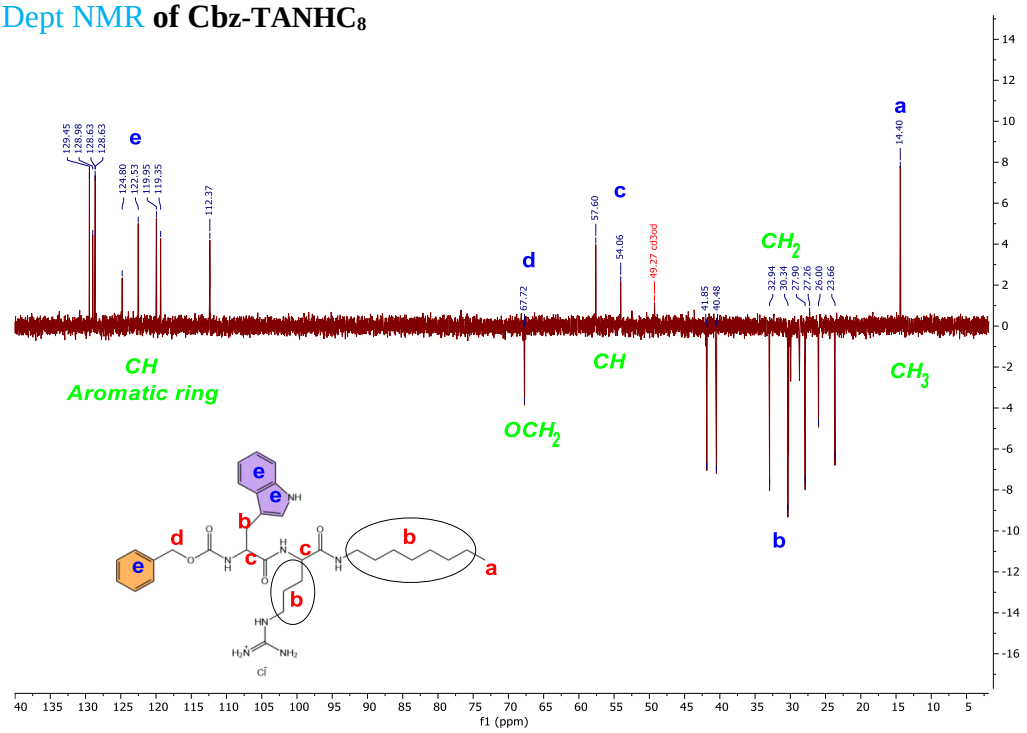
^{1}H NMR of Cbz-TANHC$_8$



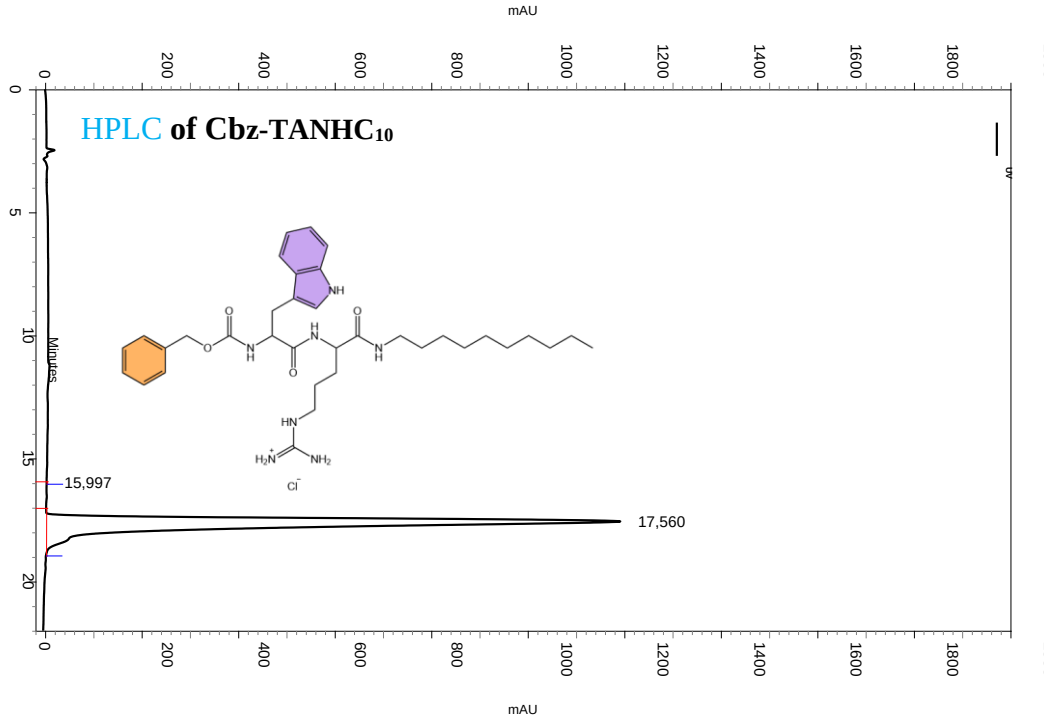
^{13}C NMR of Cbz-TANHC$_8$

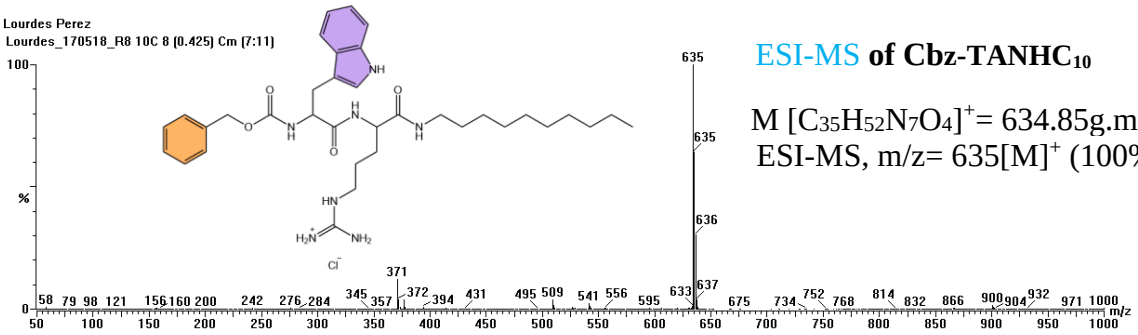


Dept NMR **of Cbz-TANHC$_8$**



. **Figure S17.** HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of Cbz-TANHC$_8$

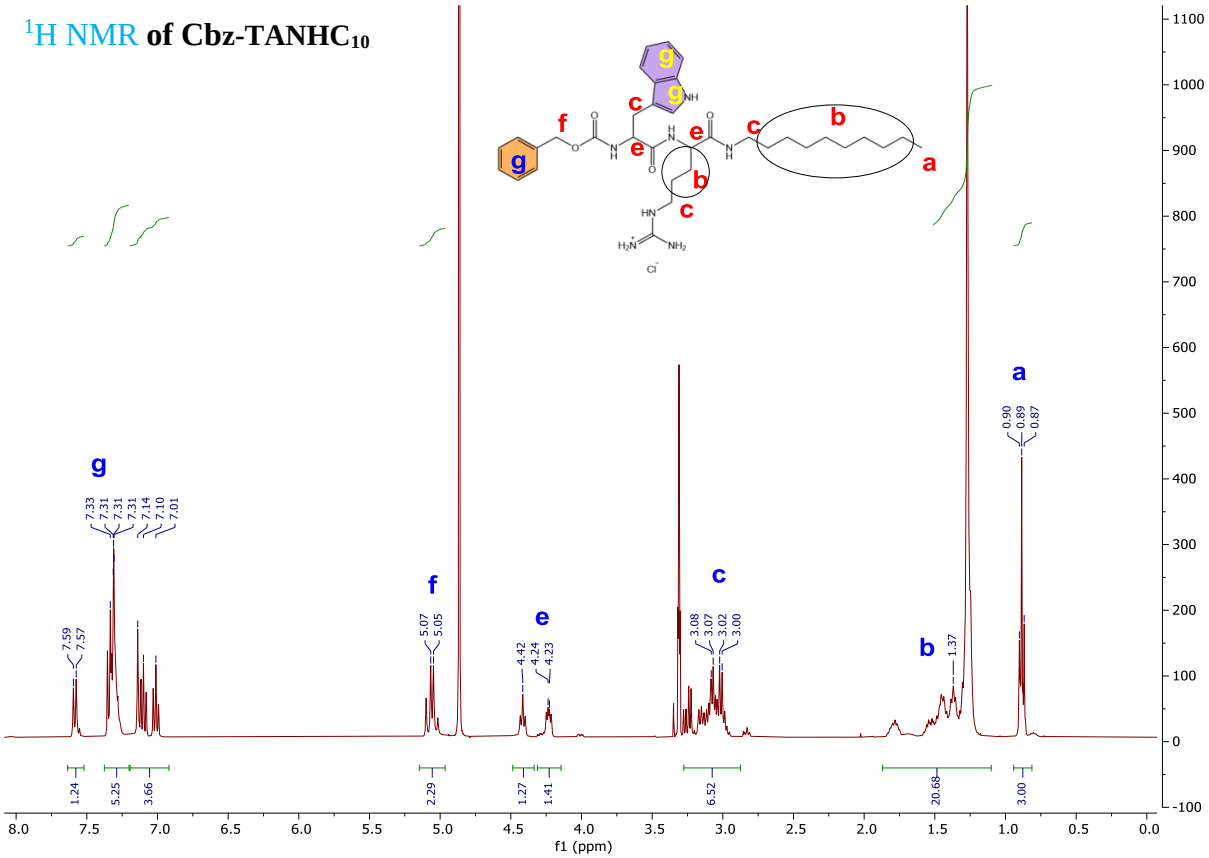




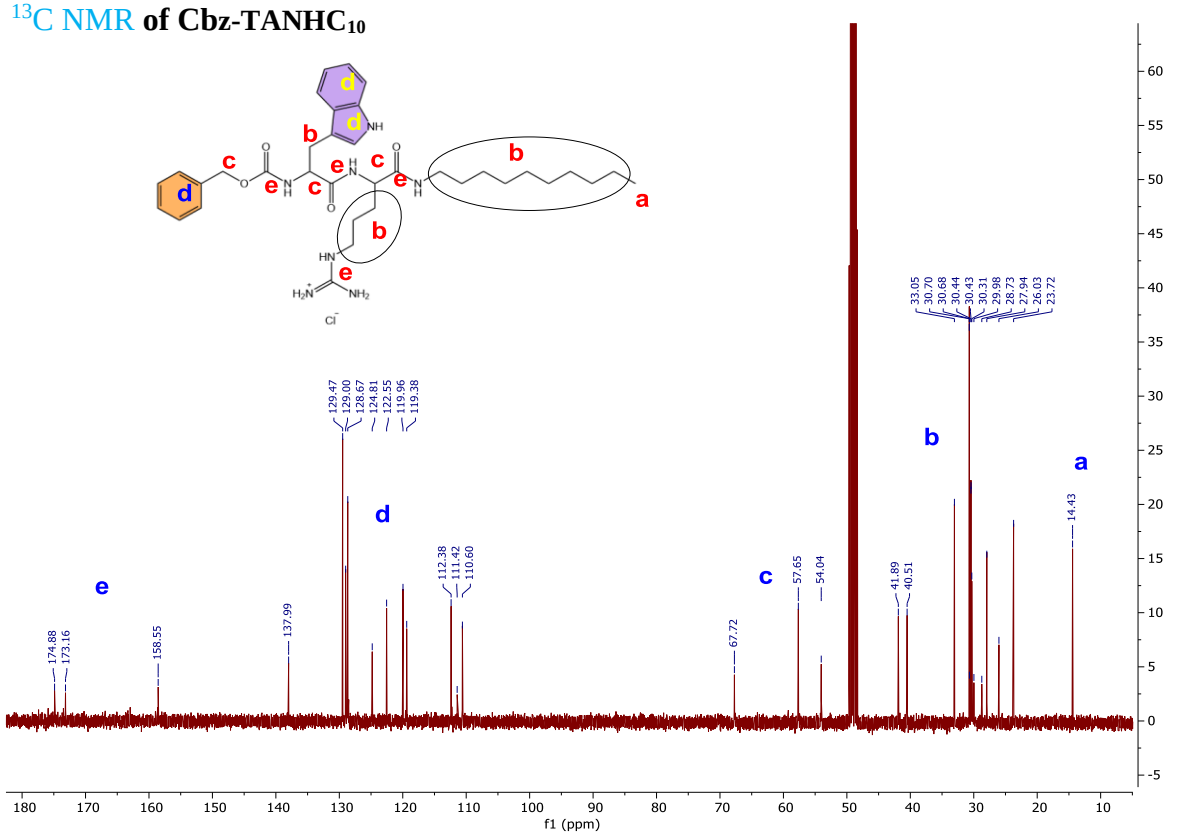
ESI-MS **of Cbz-TANHC$_{10}$**

M $[C_{35}H_{52}N_7O_4]^+$= 634.85g.mol,
ESI-MS, m/z= 635$[M]^+$ (100%)

^{1}H NMR of Cbz-TANHC$_{10}$



^{13}C NMR of Cbz-TANHC$_{10}$



Dept NMR **of Cbz-TANHC$_{10}$**

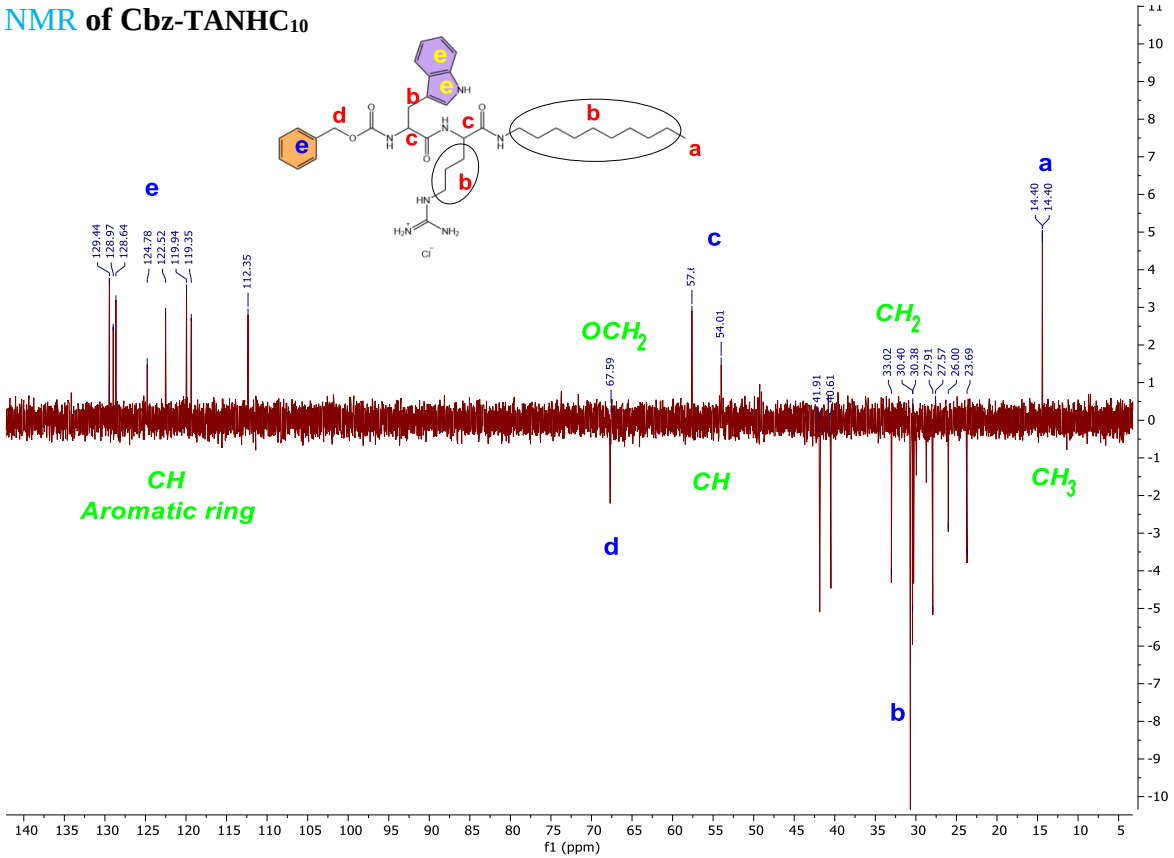
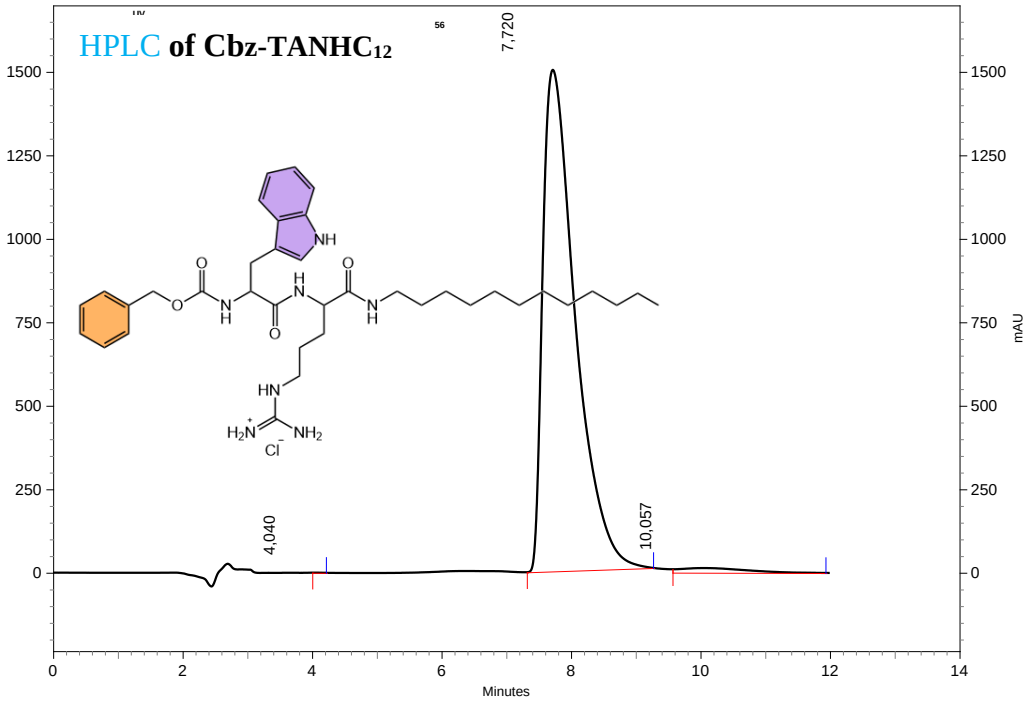
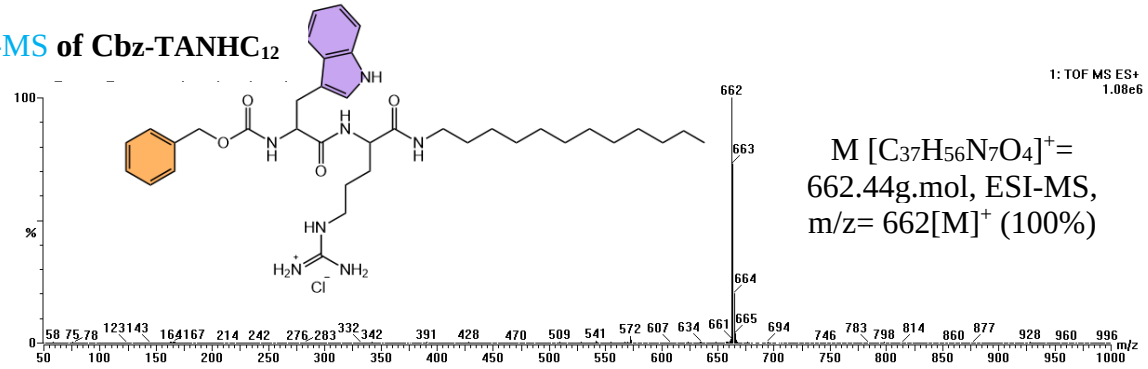


Figure S18. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of Cbz-TANHC$_{10}$

HPLC **of Cbz-TANHC$_{12}$**

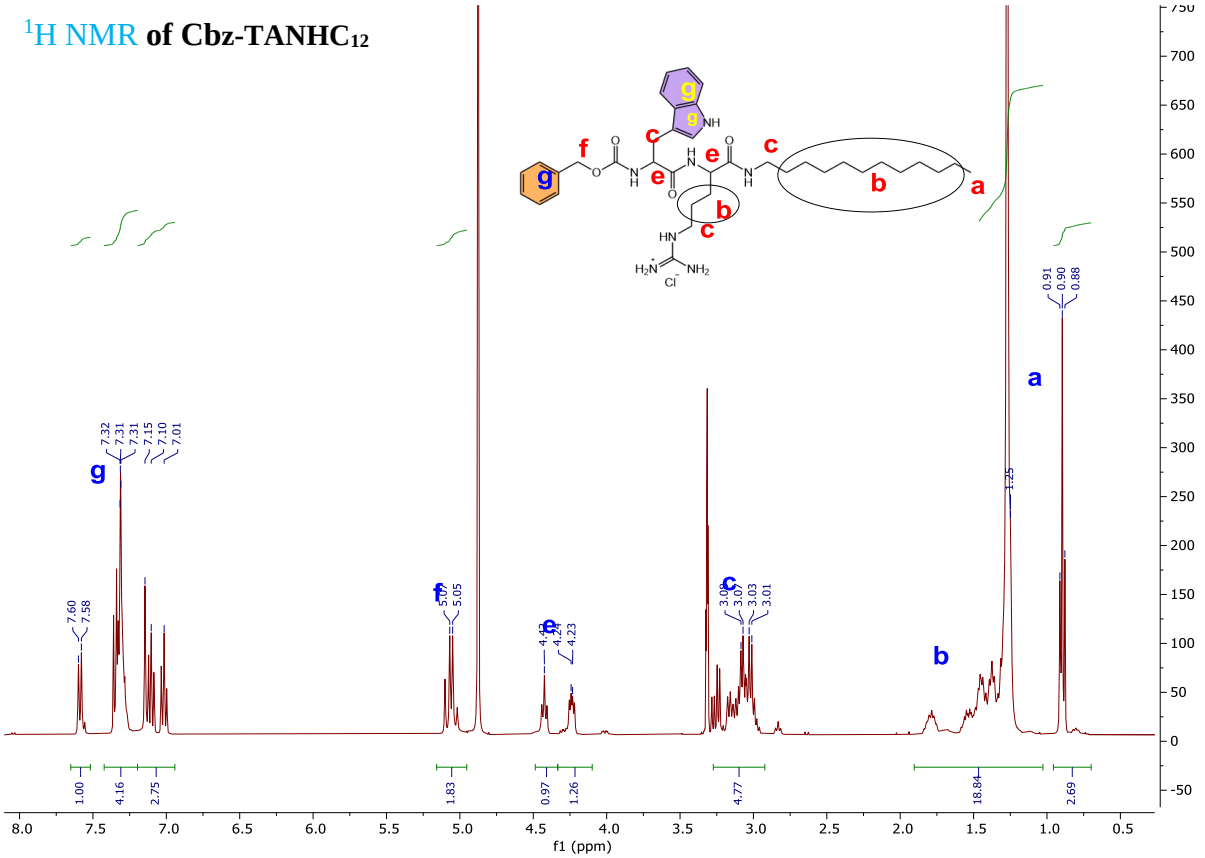


ESI-MS **of Cbz-TANHC$_{12}$**

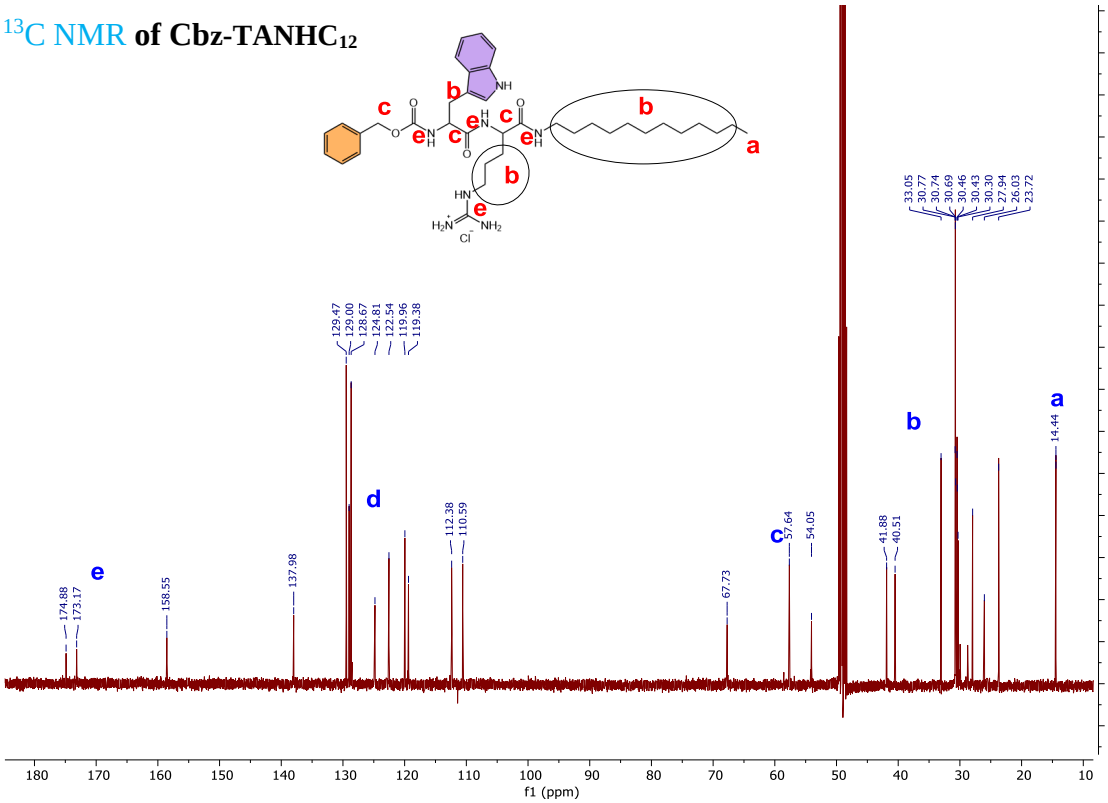


M $[C_{37}H_{56}N_7O_4]^+$= 662.44g.mol, ESI-MS, m/z= 662$[M]^+$ (100%)

^{1}H NMR of Cbz-TANHC$_{12}$



^{13}C NMR of Cbz-TANHC$_{12}$



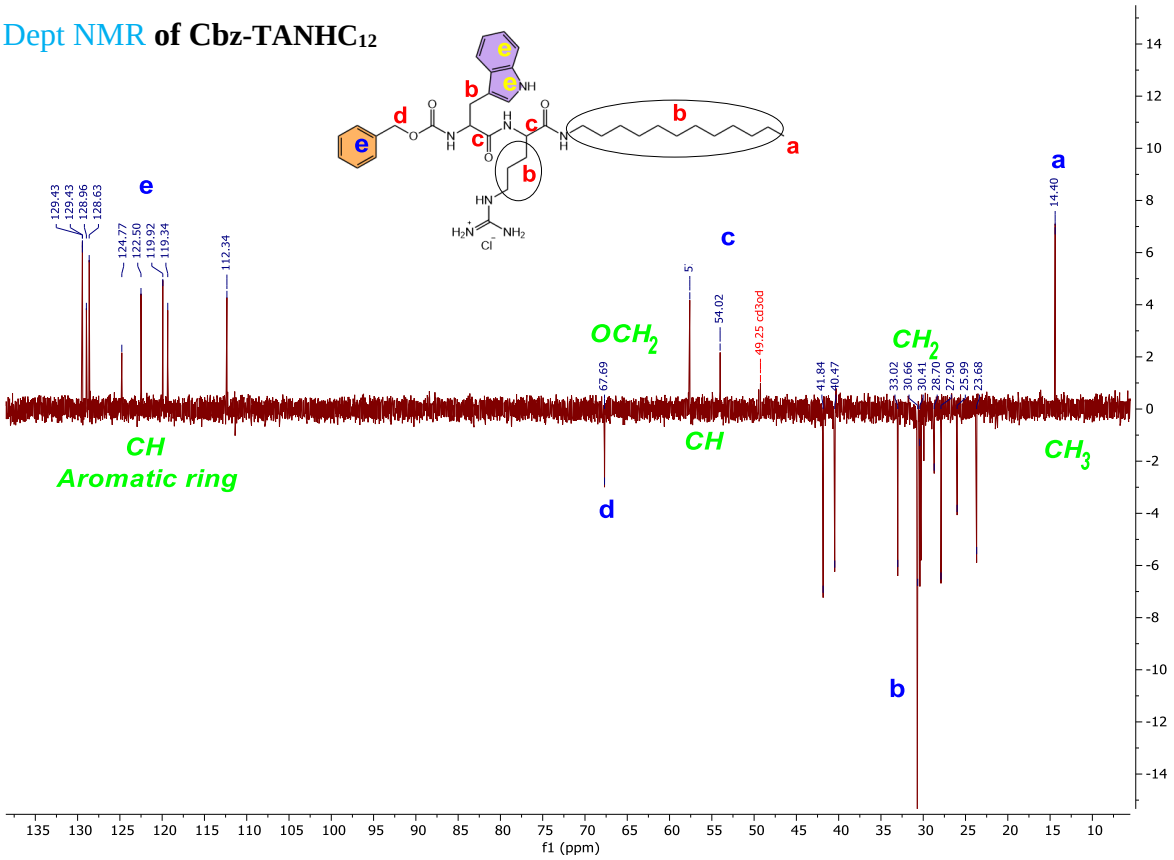
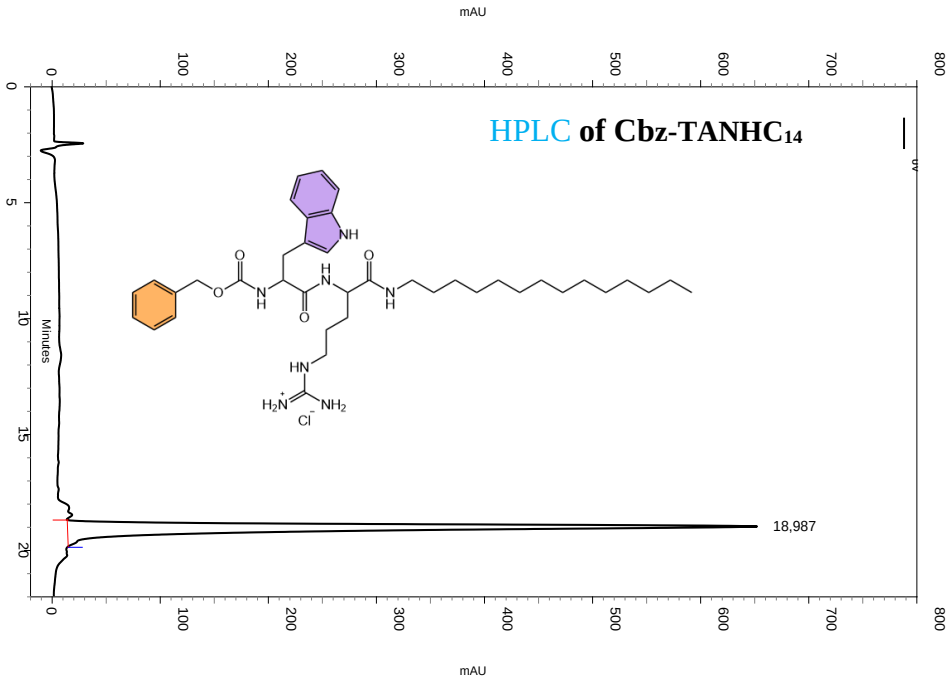
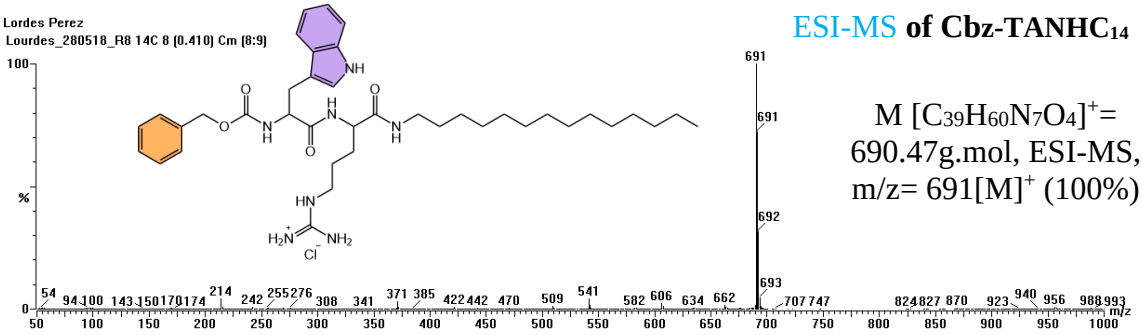


Figure S19. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of Cbz-TANHC$_{12}$

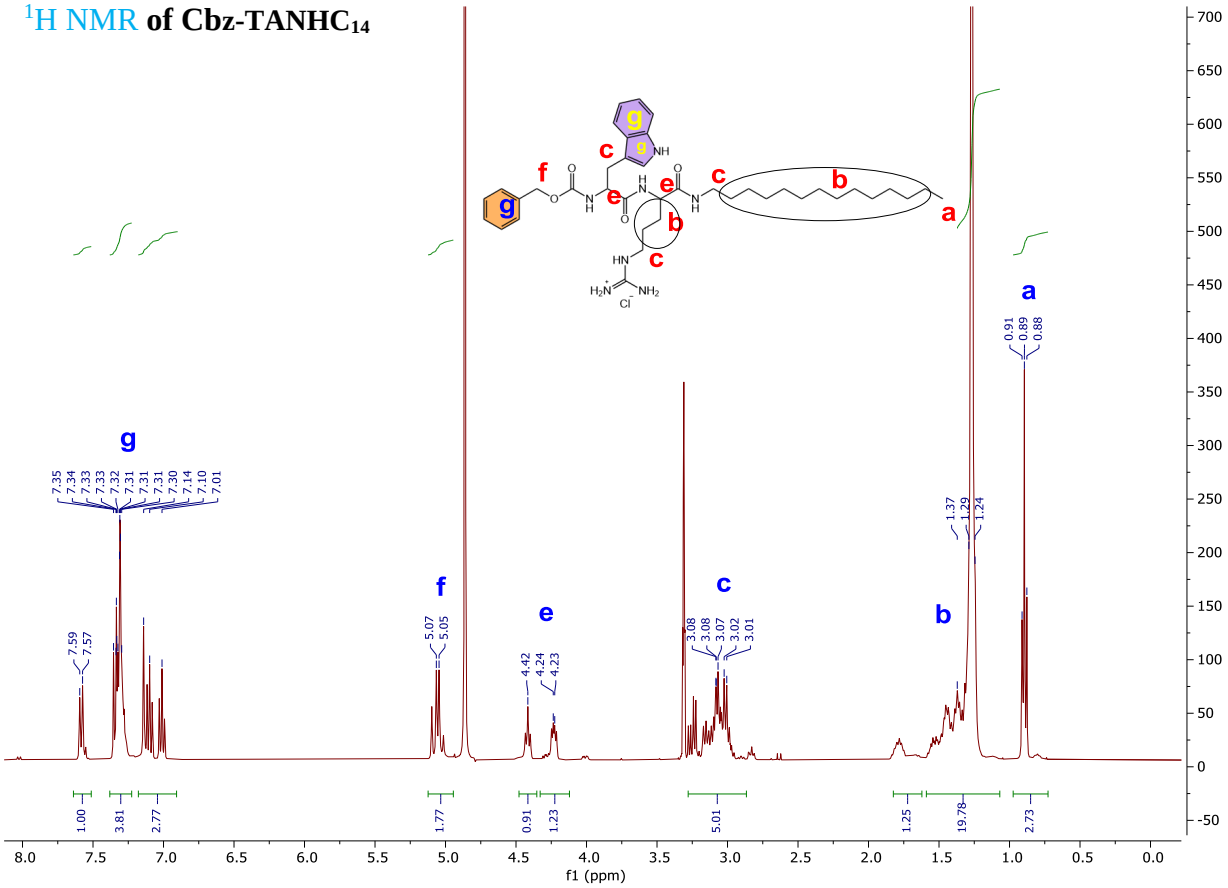




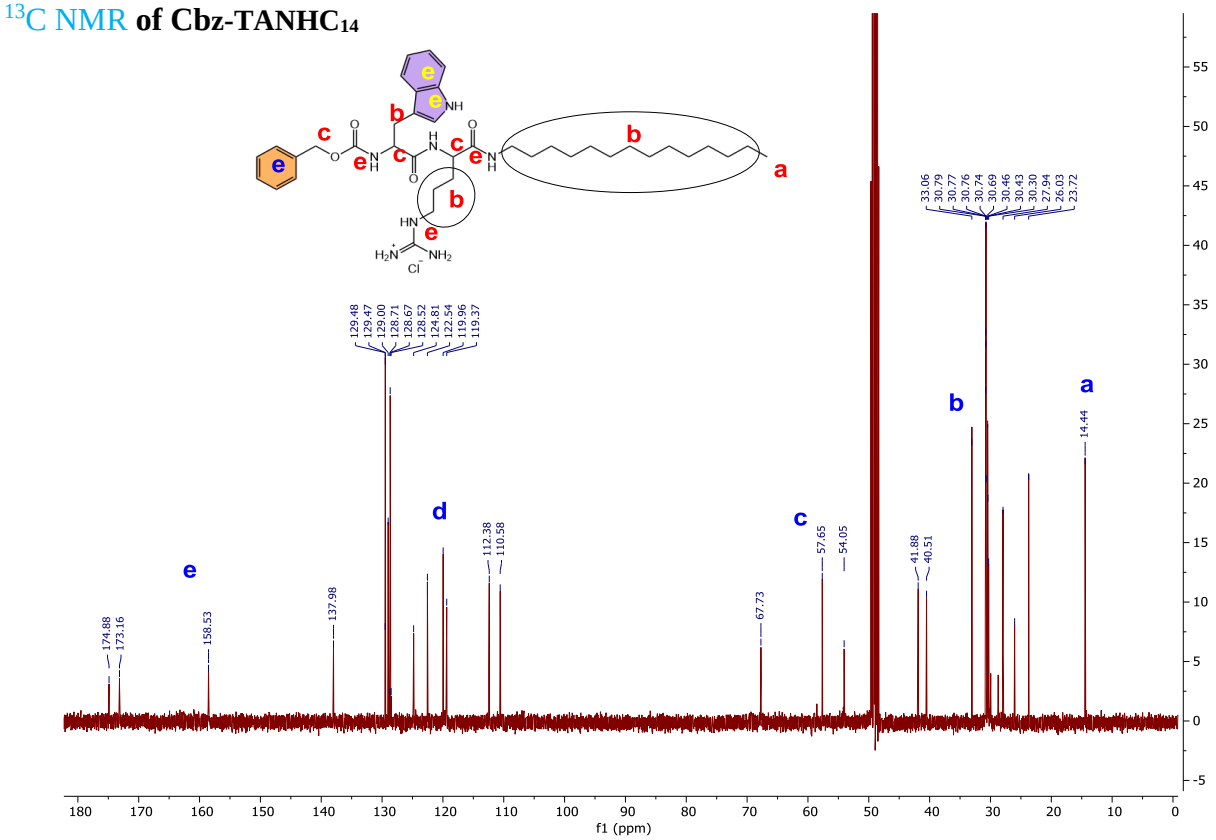
ESI-MS **of Cbz-TANHC$_{14}$**

M $[C_{39}H_{60}N_7O_4]^+$= 690.47g.mol, ESI-MS, m/z= 691$[M]^+$ (100%)

^{1}H NMR **of Cbz-TANHC$_{14}$**



^{13}C NMR **of Cbz-TANHC$_{14}$**



Dept NMR **of Cbz-TANHC$_{14}$**

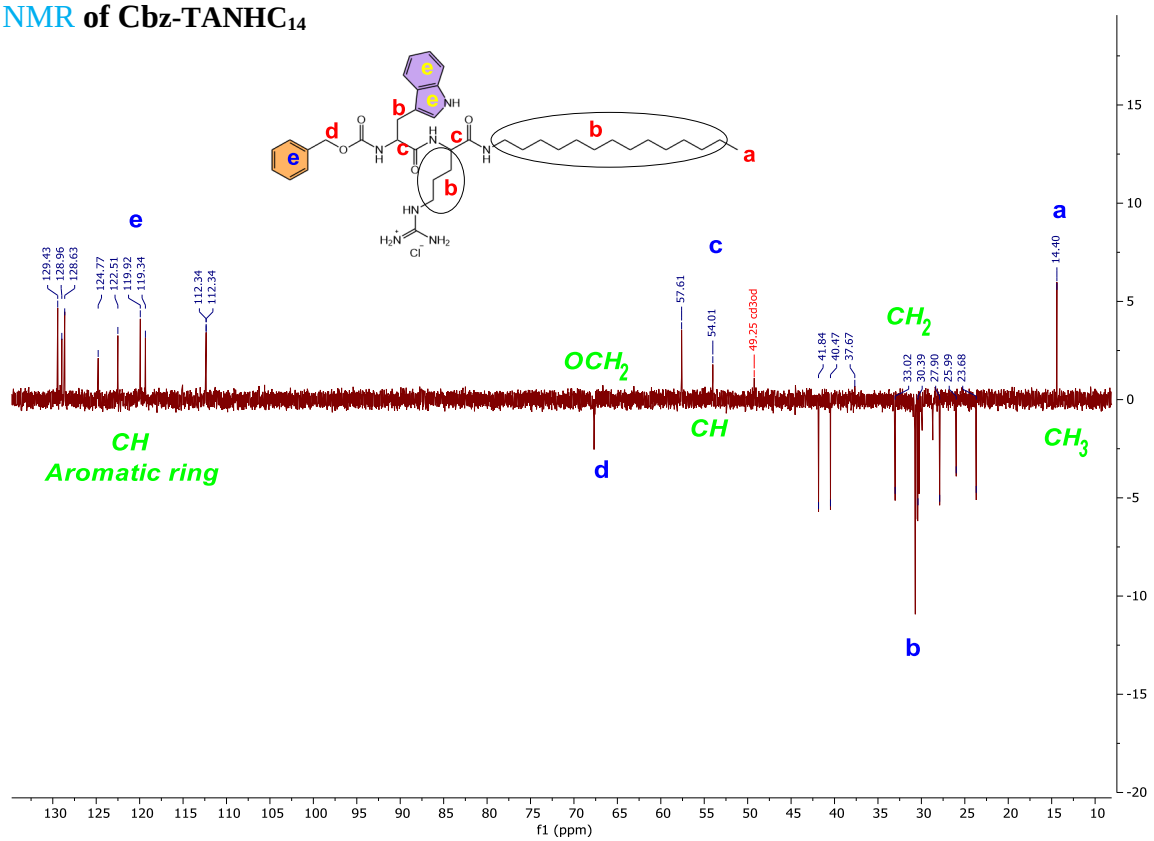
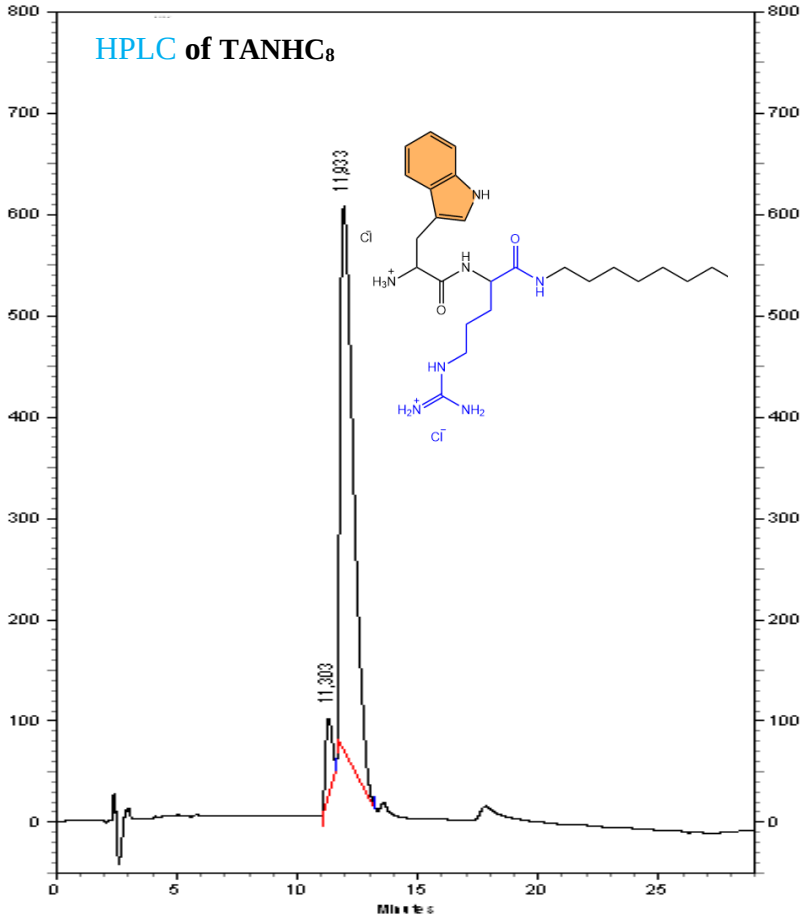


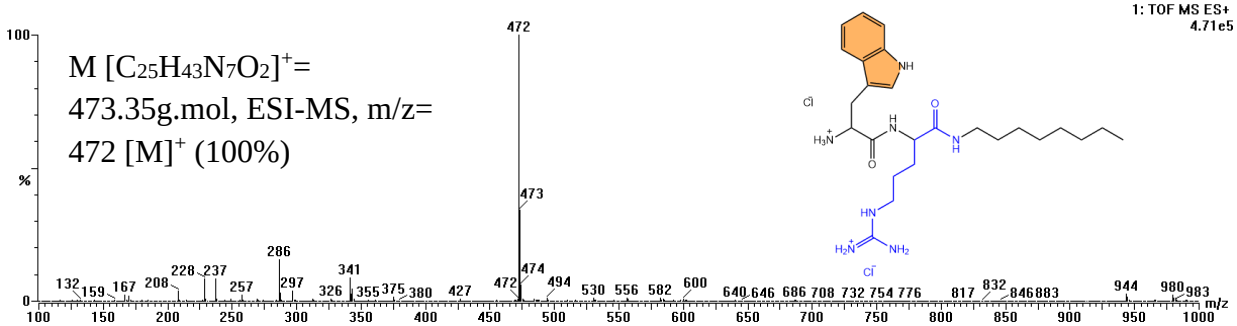
Figure S20. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of Cbz-TANHC$_{14}$

HPLC **of TANHC$_8$**

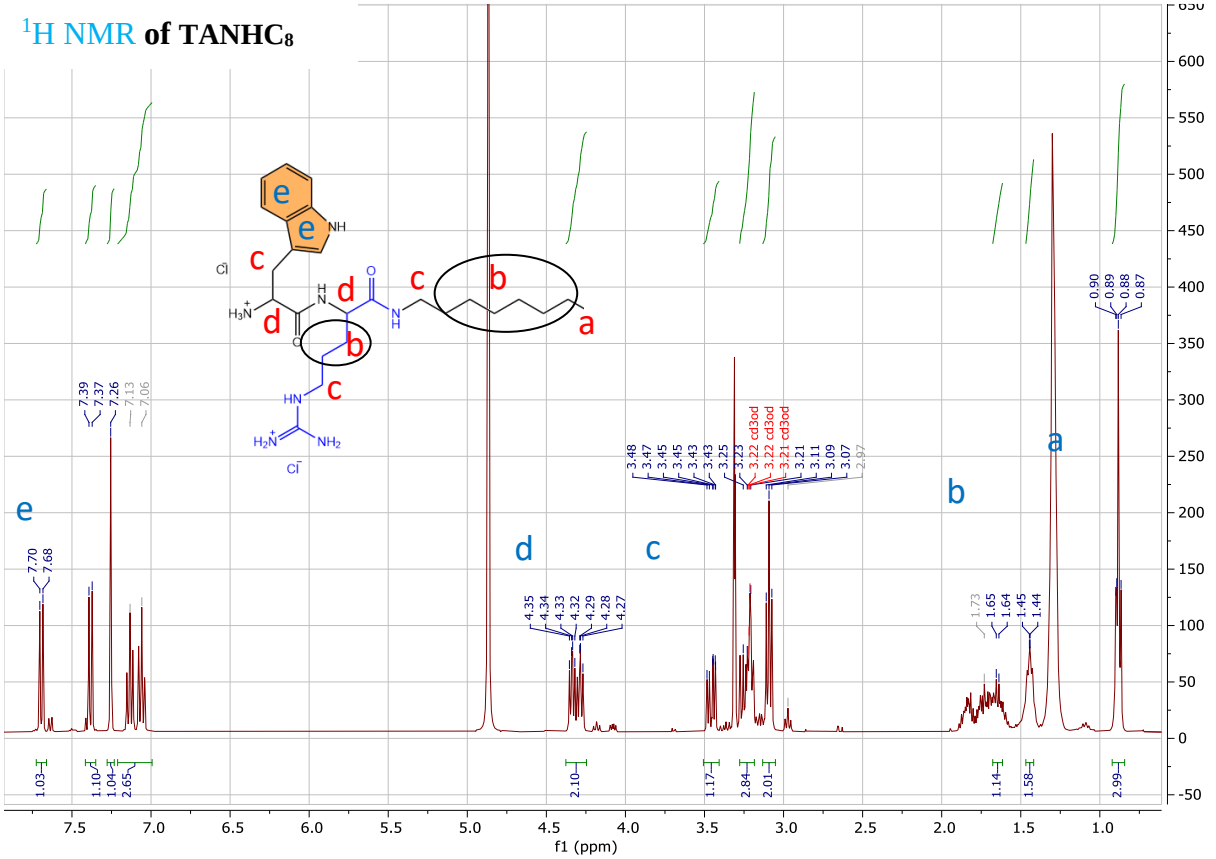


ESI-MS **of TANHC$_8$**

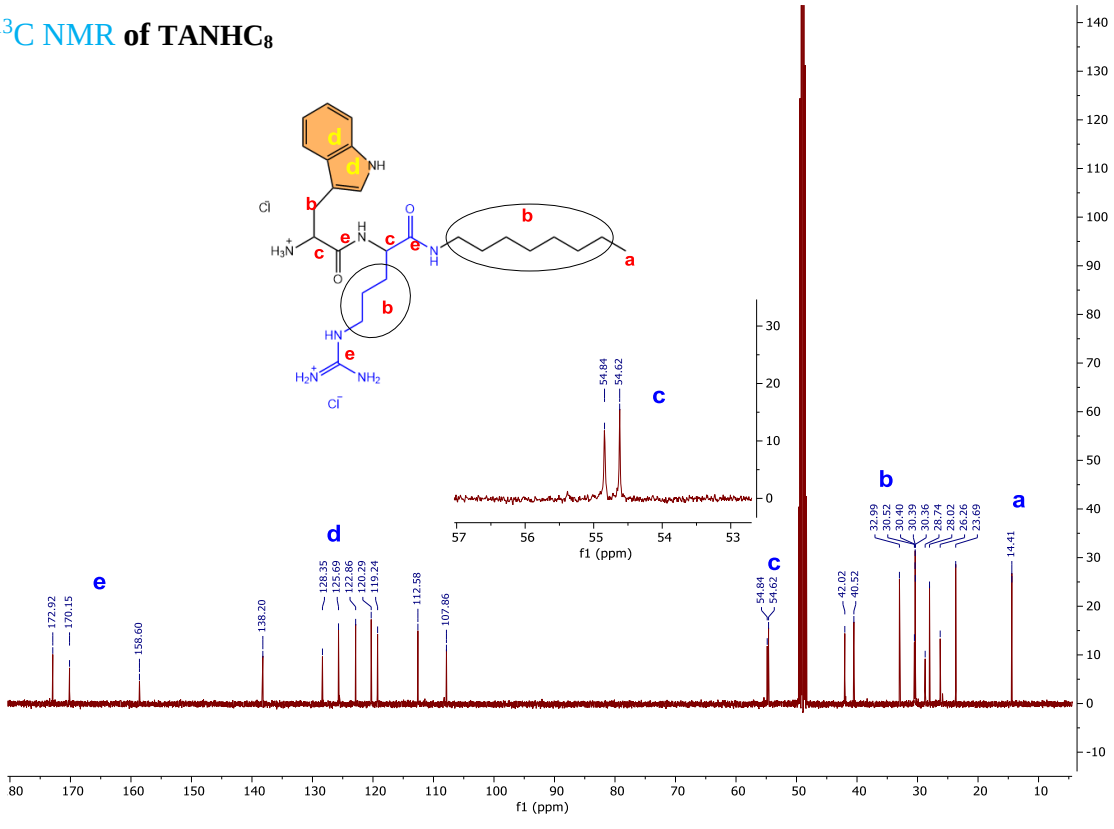
M $[C_{25}H_{43}N_7O_2]^+$= 473.35g.mol, ESI-MS, m/z= 472 $[M]^+$ (100%)



^{1}H NMR **of TANHC$_8$**



^{13}C NMR **of TANHC$_8$**



Dept NMR **of TANHC$_8$**

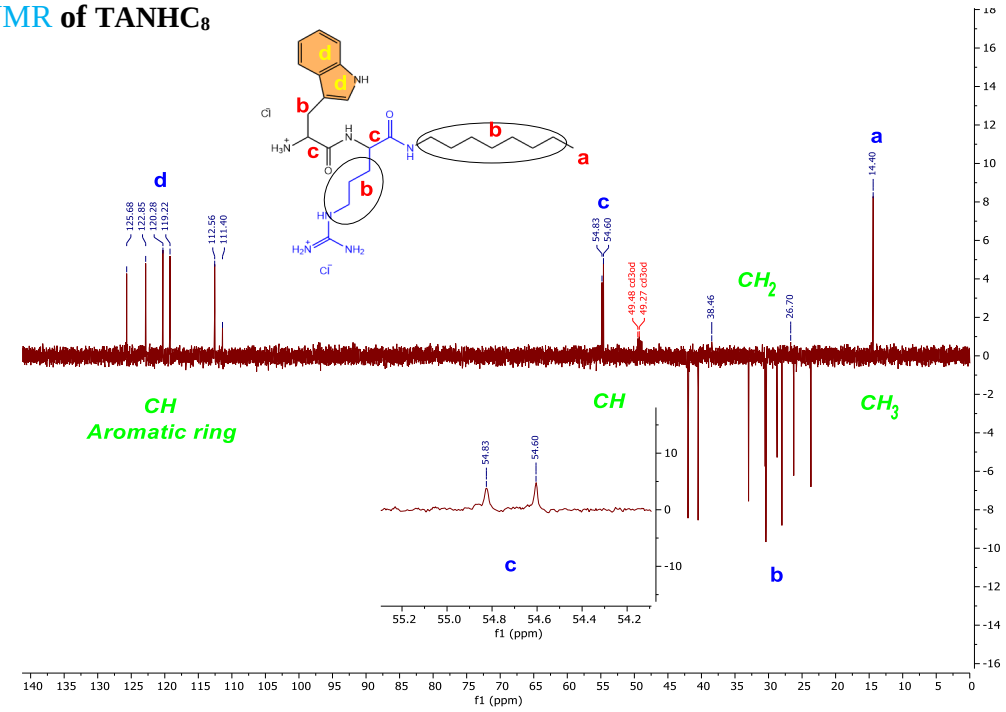
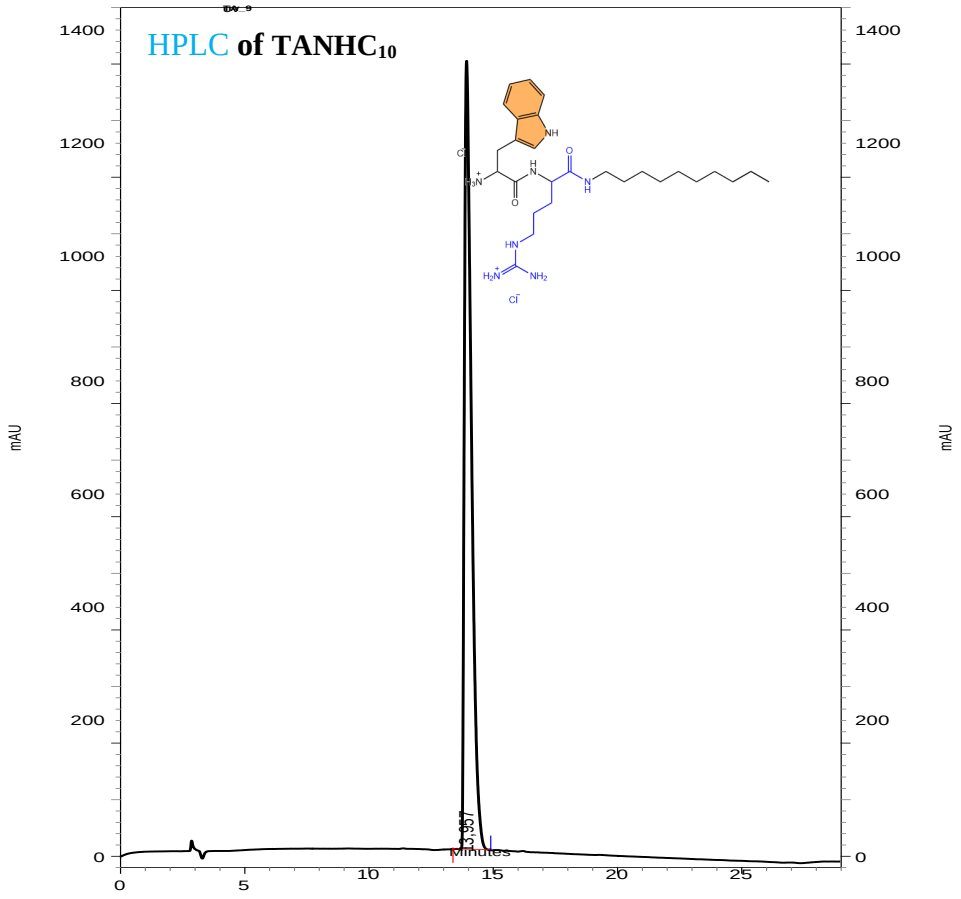
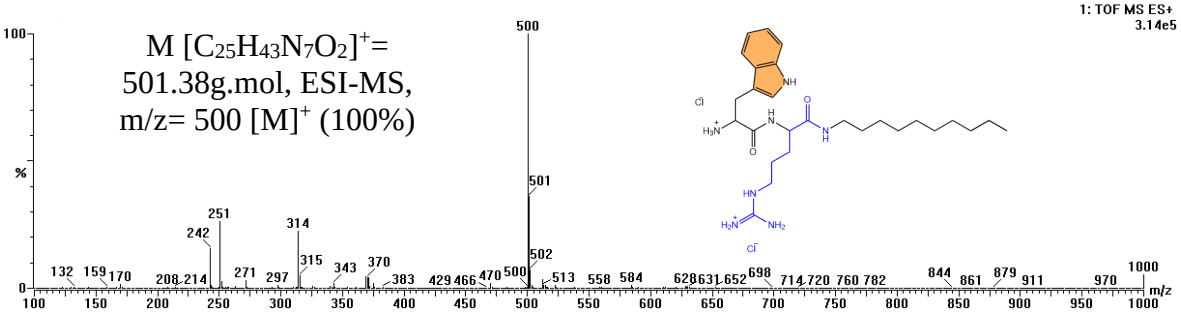


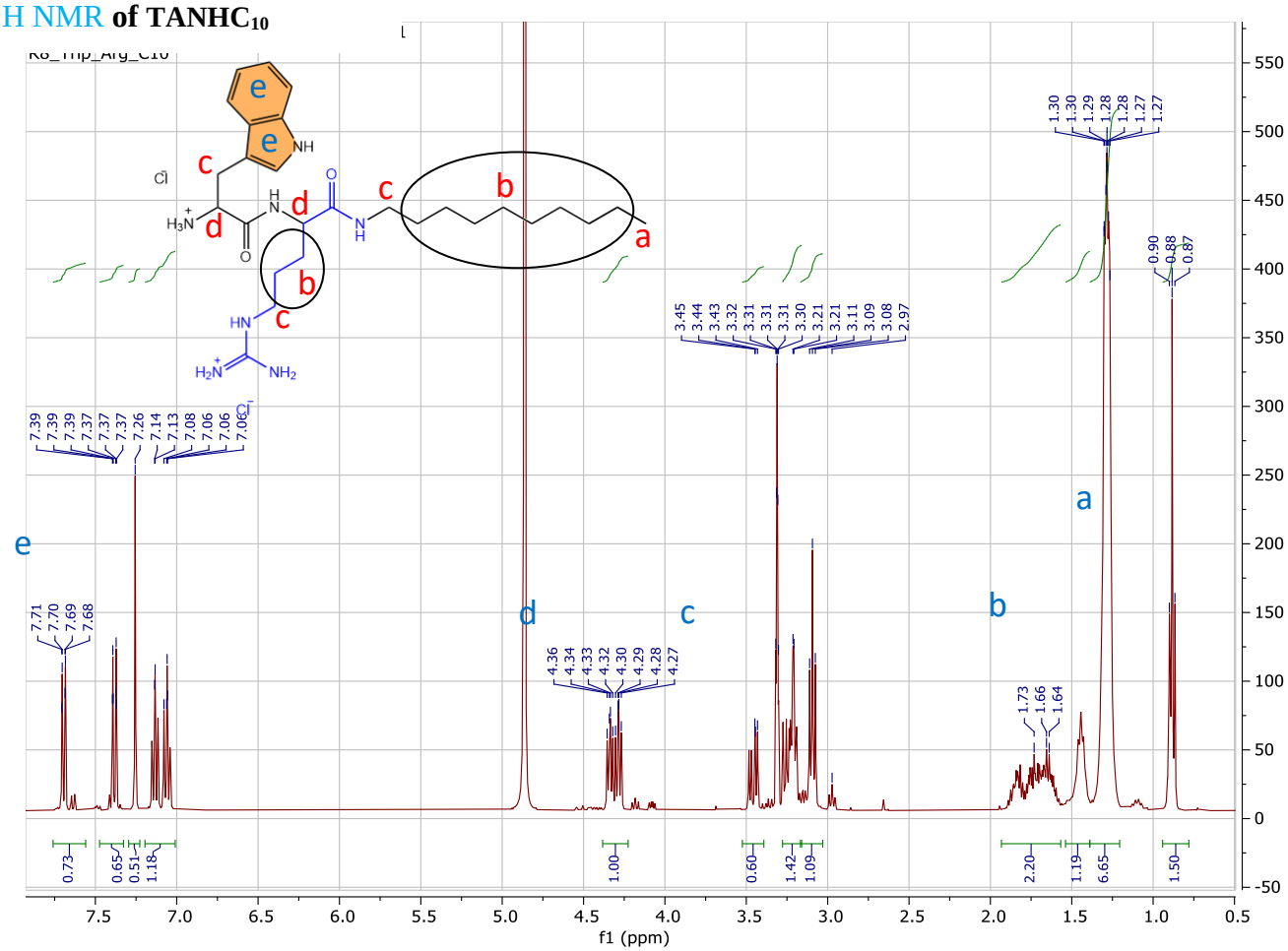
Figure S21. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of TANHC$_8$



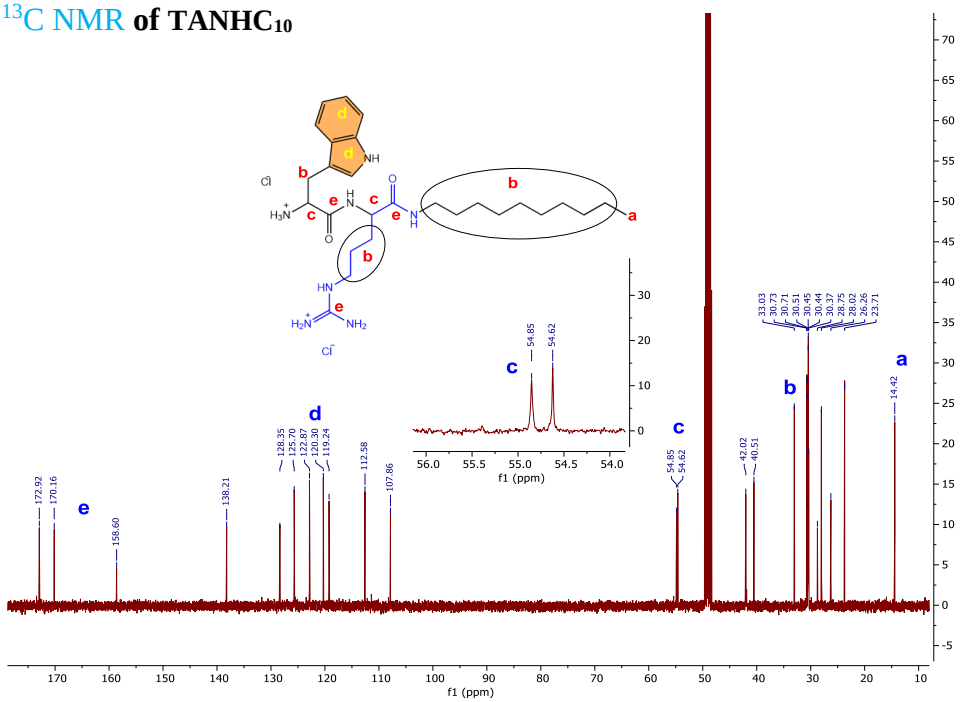
ESI-MS **of TANHC$_{10}$**



^{1}H NMR **of TANHC$_{10}$**



^{13}C NMR **of TANHC$_{10}$**



Dept NMR **of TANHC$_{10}$**

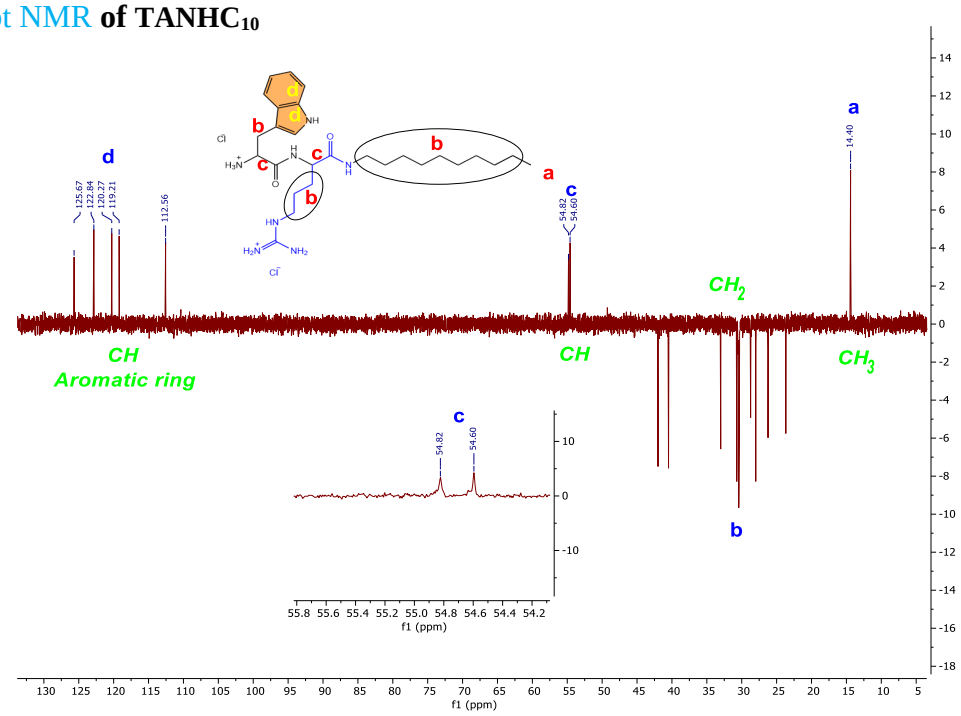
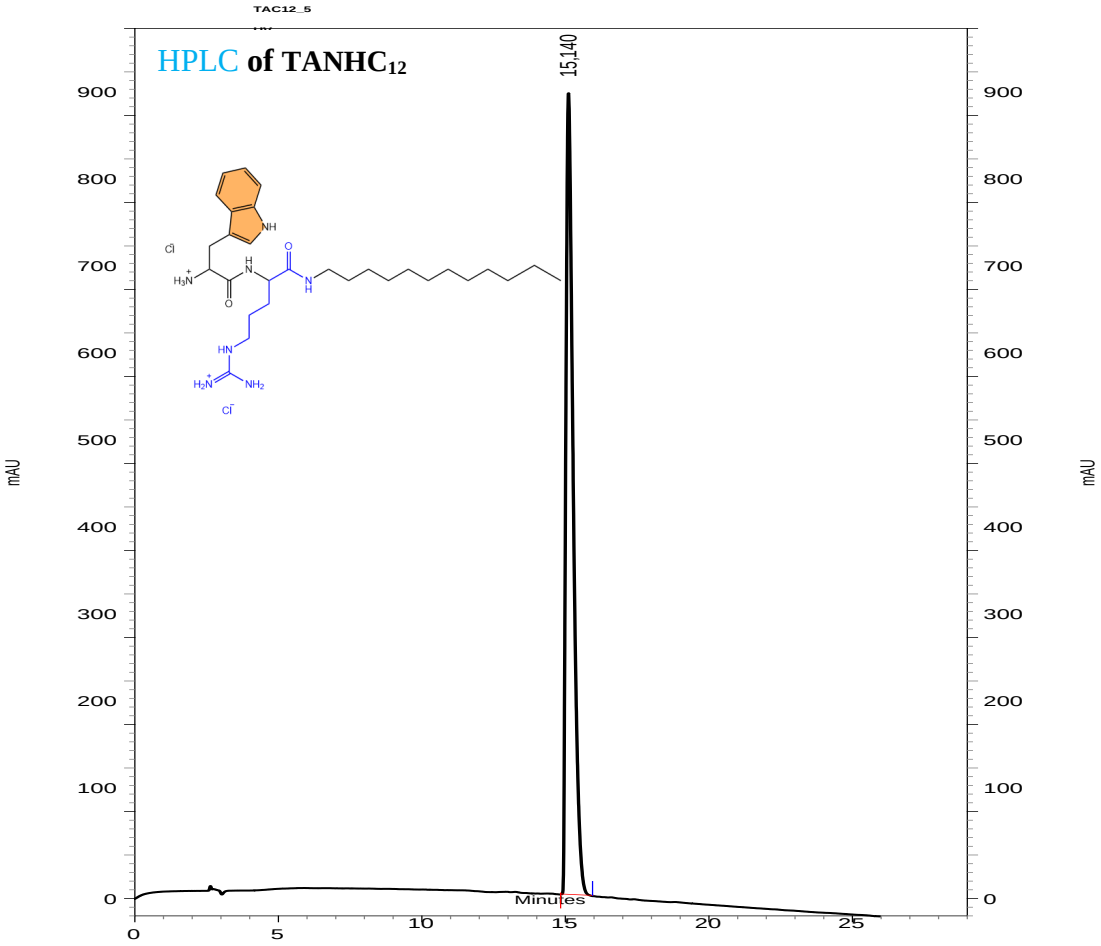
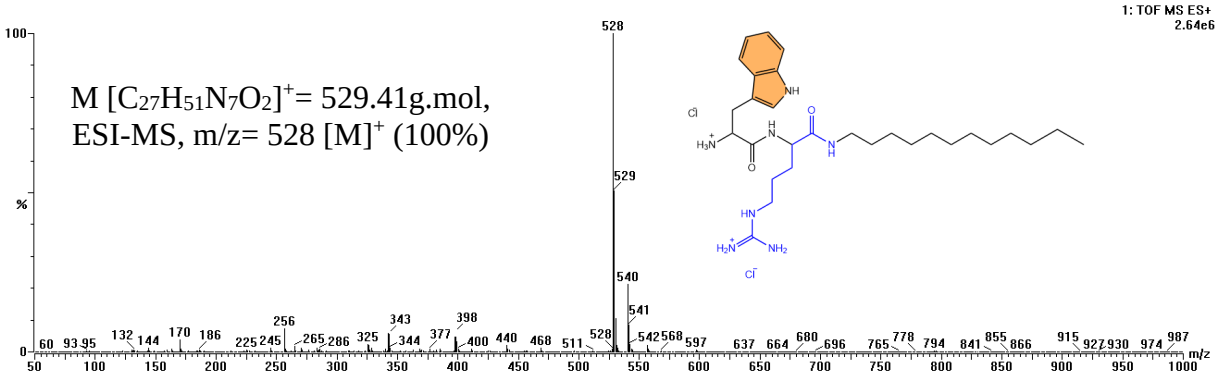


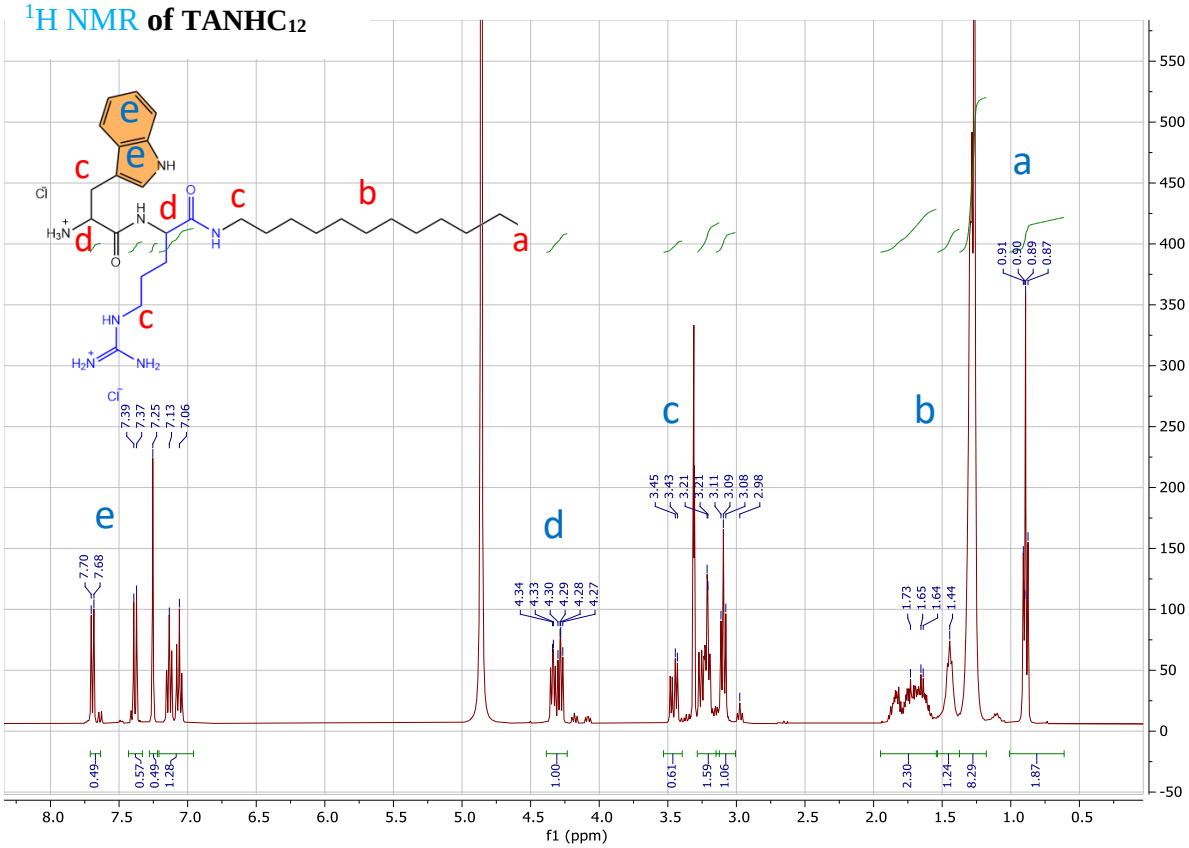
Figure S22. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of TANHC$_{10}$



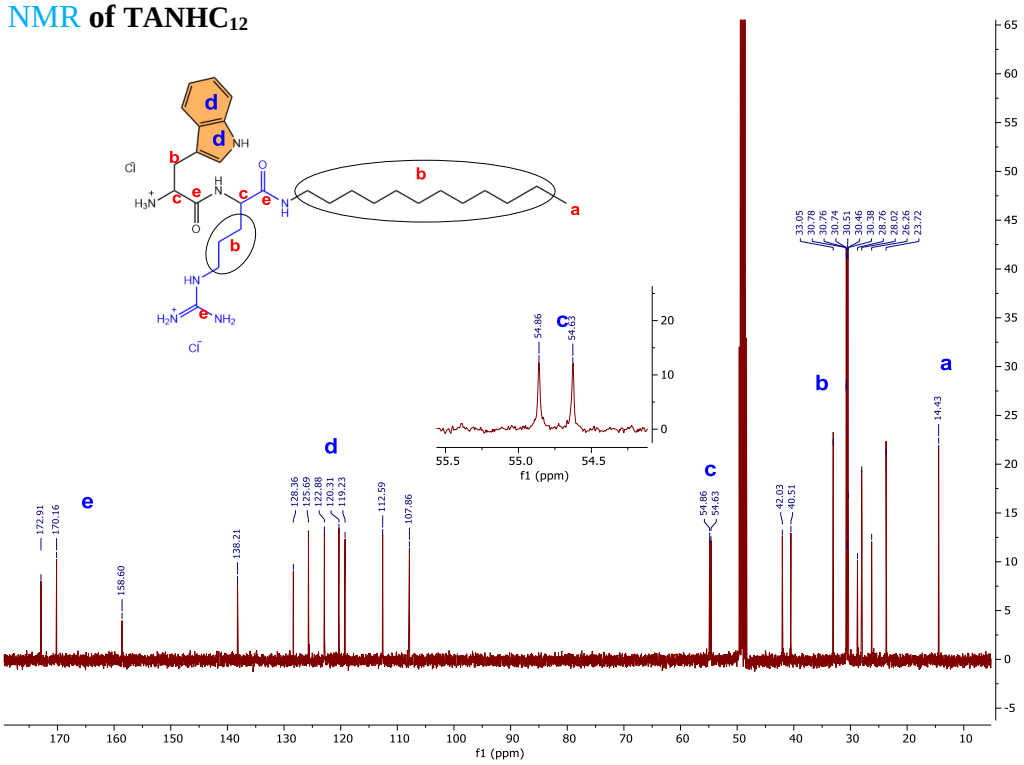
ESI-MS of TANHC$_{12}$



^{1}H NMR **of TANHC$_{12}$**



^{13}C NMR **of TANHC$_{12}$**



Dept NMR **of TANHC$_{12}$**

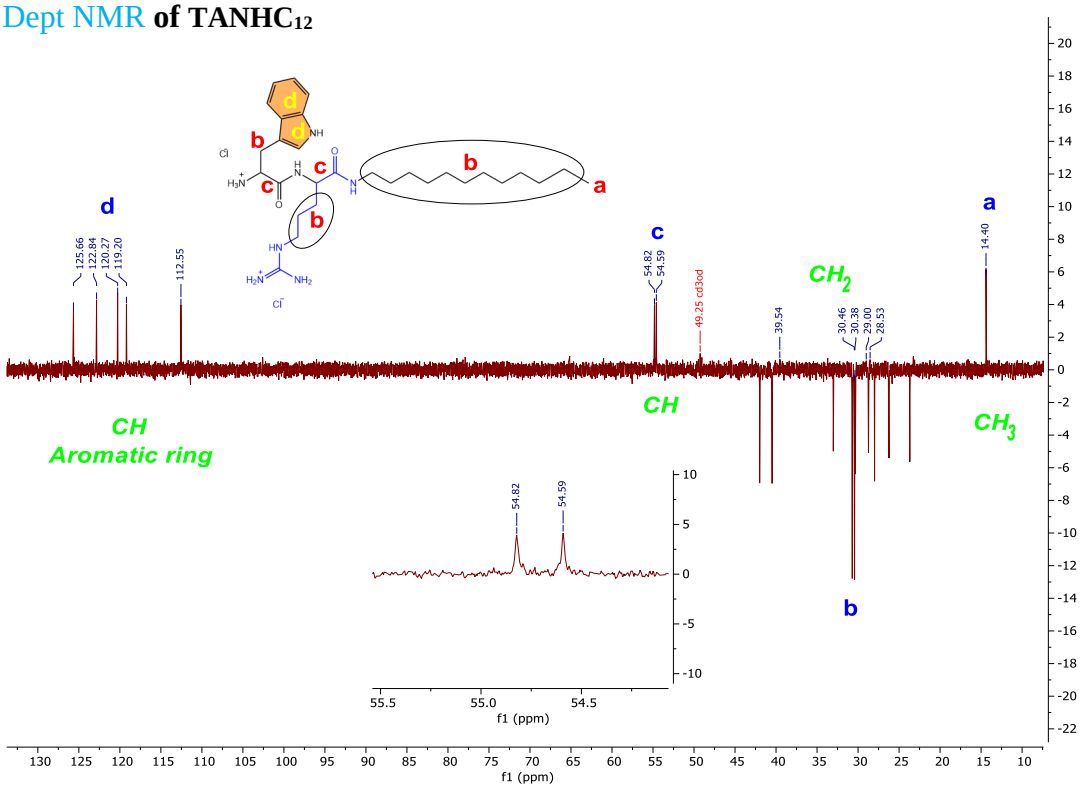
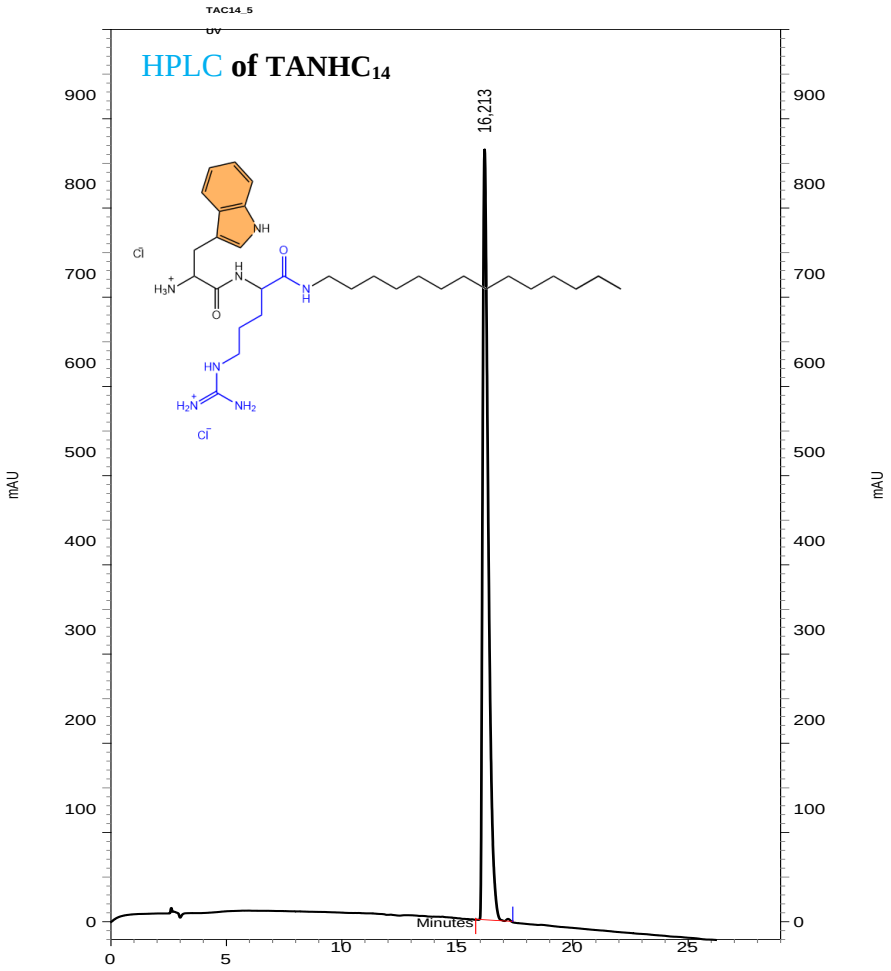
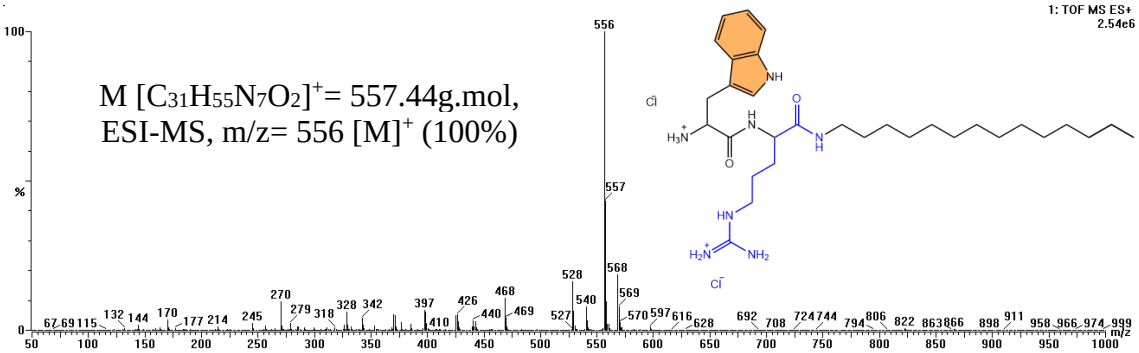


Figure S23. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of TANHC$_{12}$

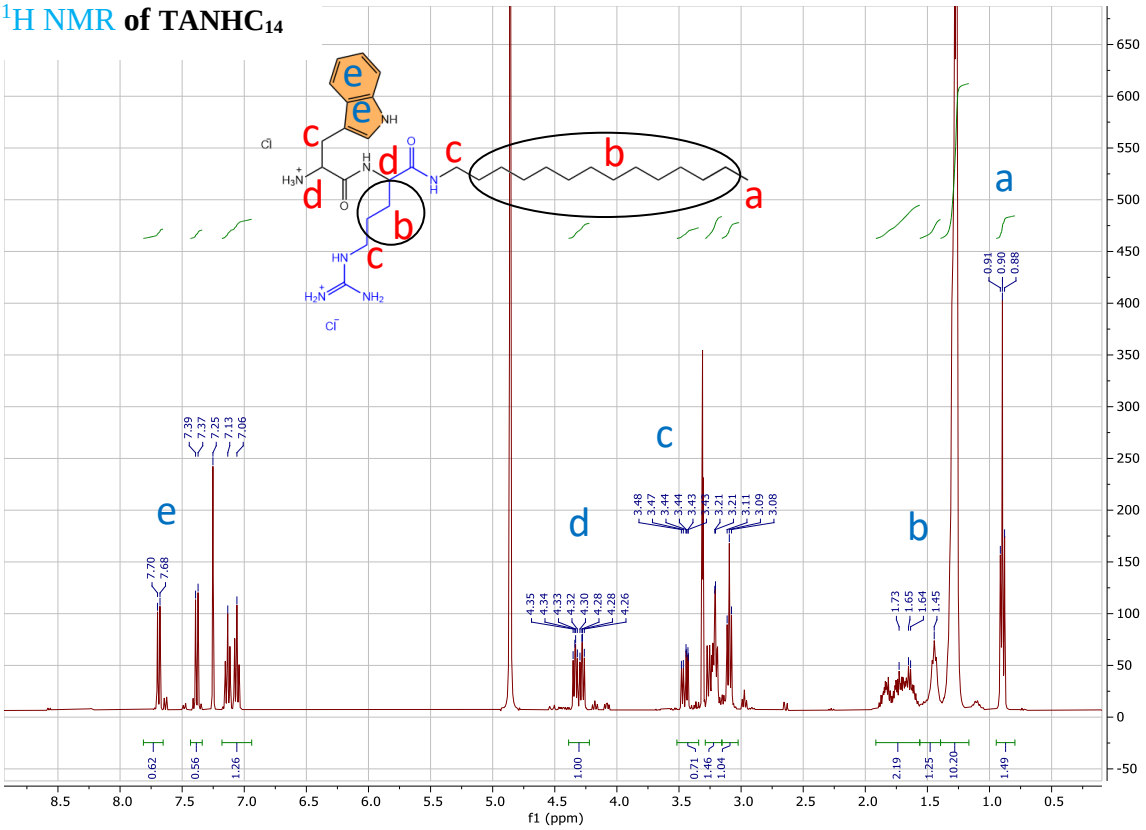


ESI-MS of **TANHC$_{14}$**

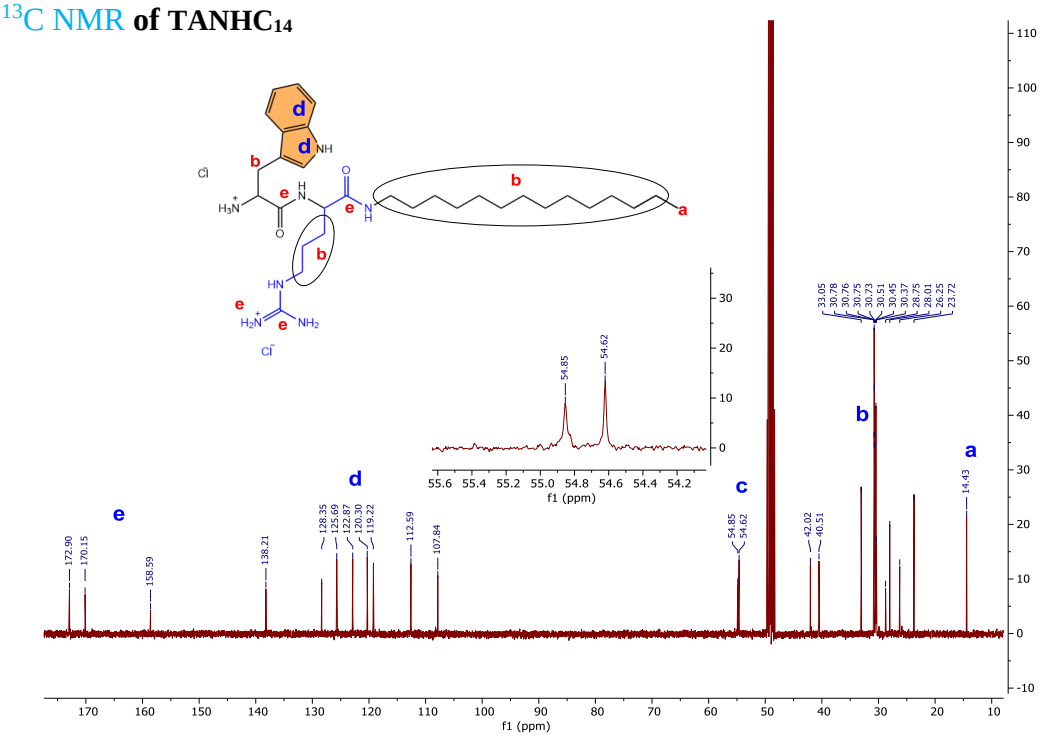
M $[C_{31}H_{55}N_7O_2]^+$= 557.44g.mol,
ESI-MS, m/z= 556 $[M]^+$ (100%)



^{1}H NMR of TANHC$_{14}$



^{13}C NMR of TANHC$_{14}$



Dept NMR **of TANHC$_{14}$**

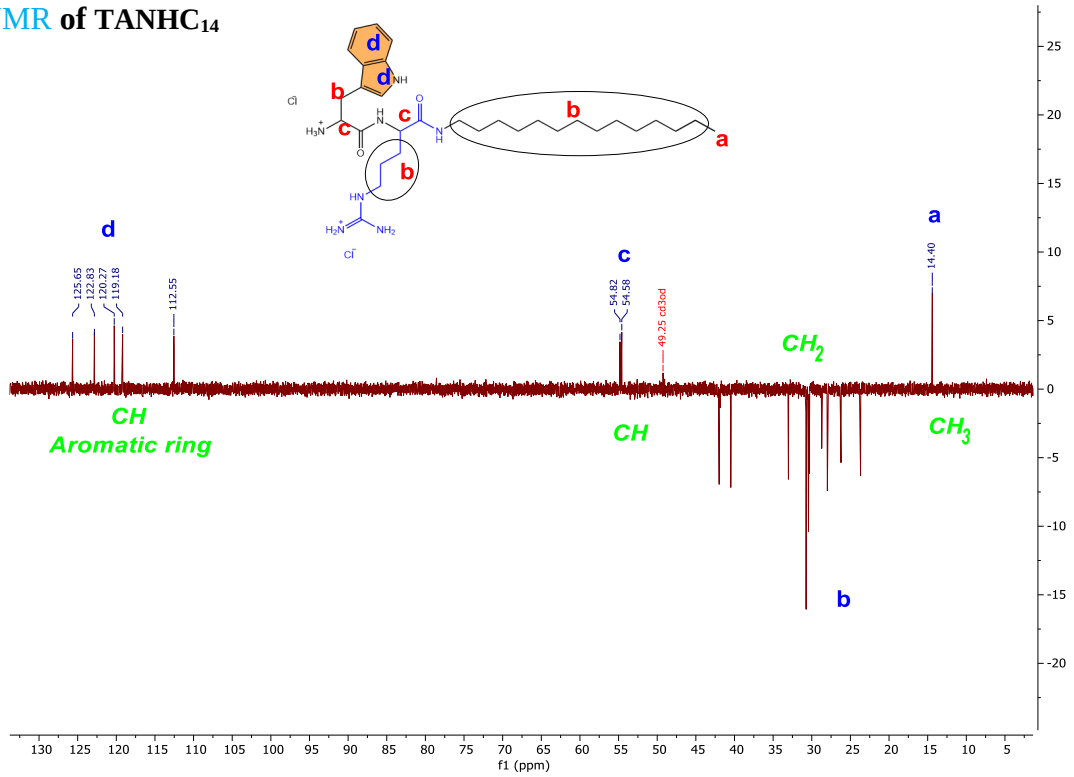
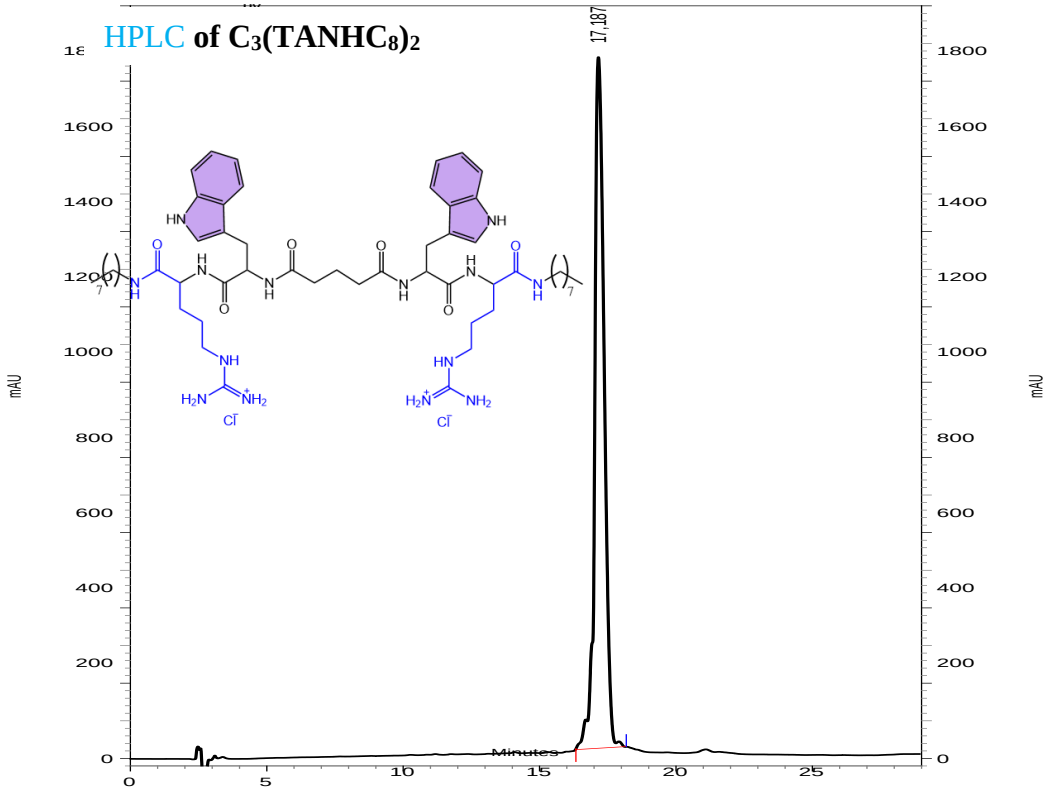
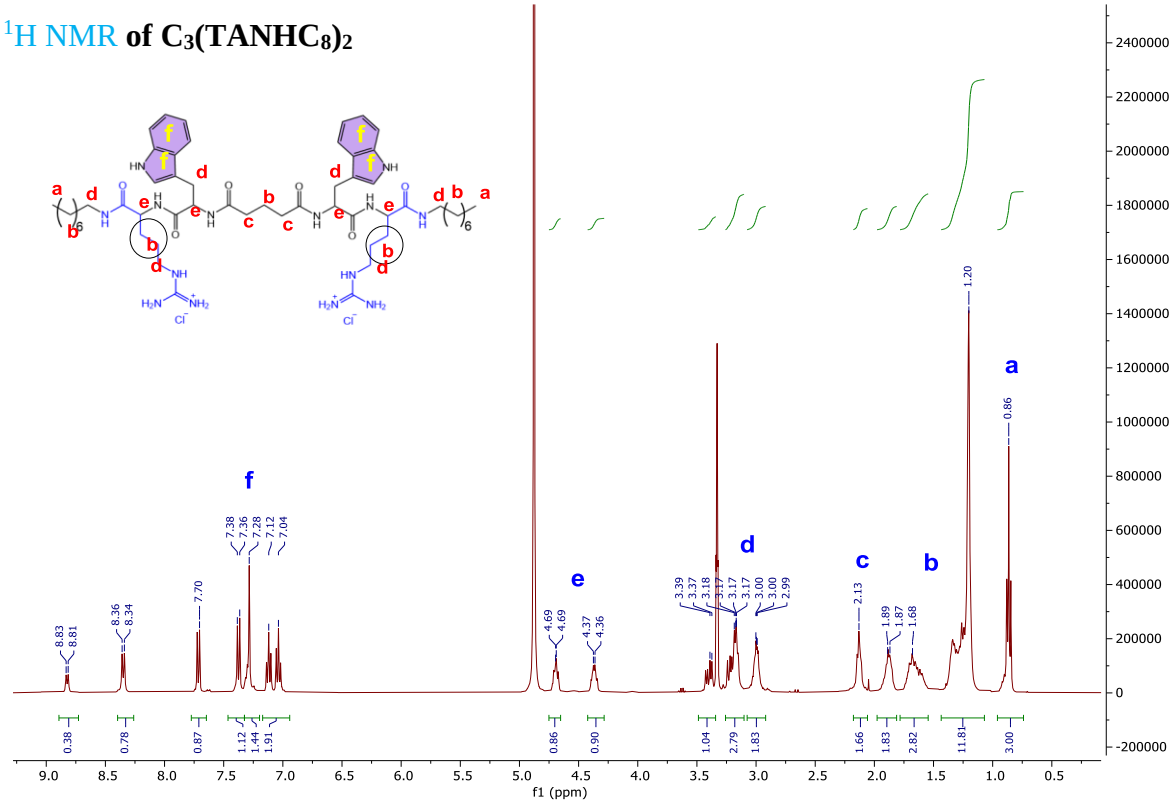


Figure S24. HPLC, ESI-MS, ^{1}H NMR,^{13}C NMR and Dept of TANHC$_{14}$

HPLC of $C_3(TANHC_8)_2$



^{1}H NMR of $C_3(TANHC_8)_2$



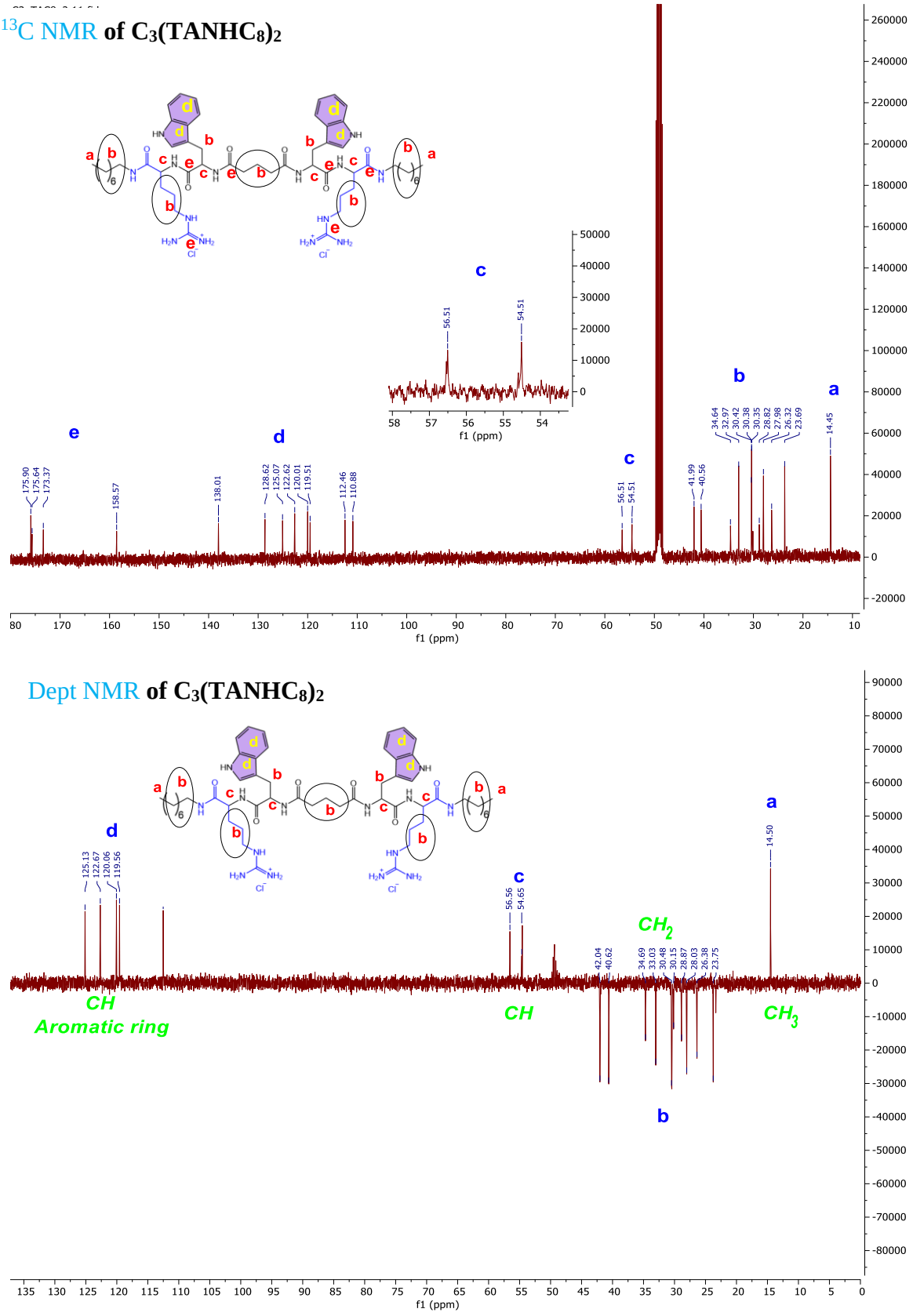
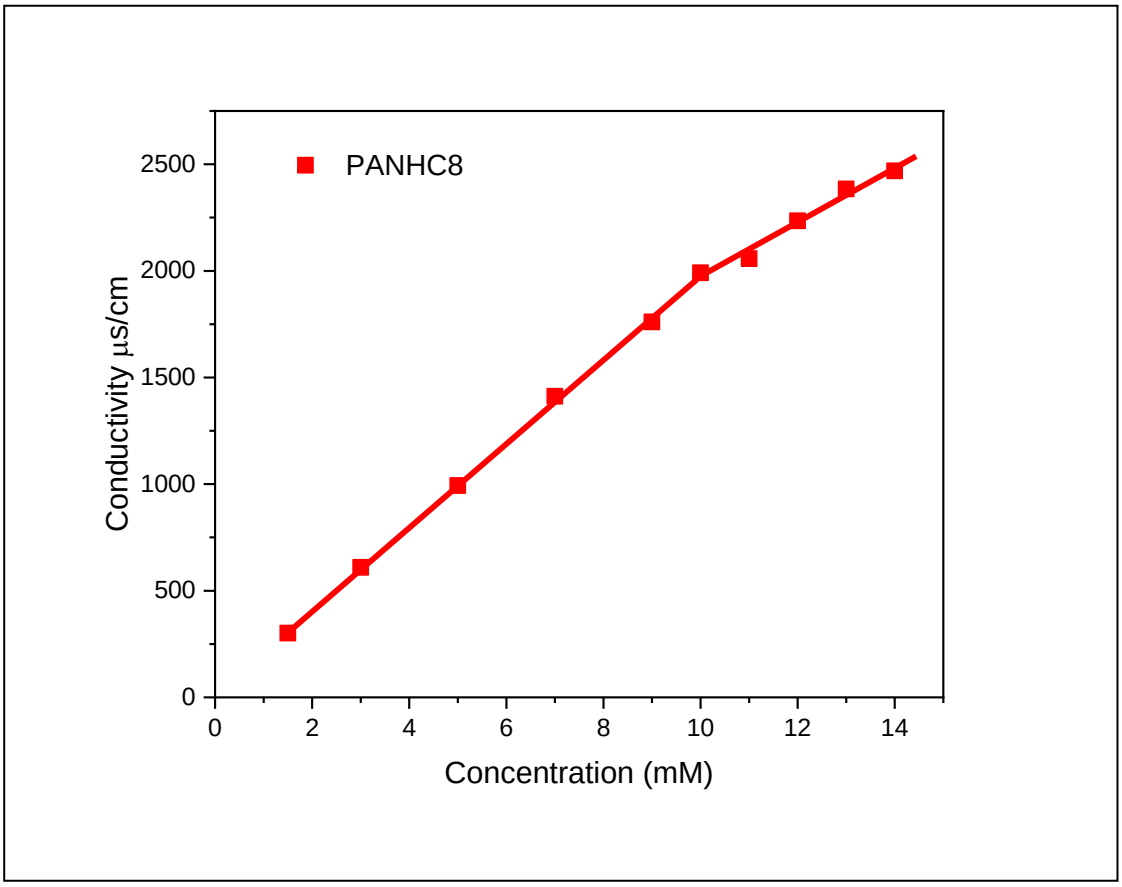
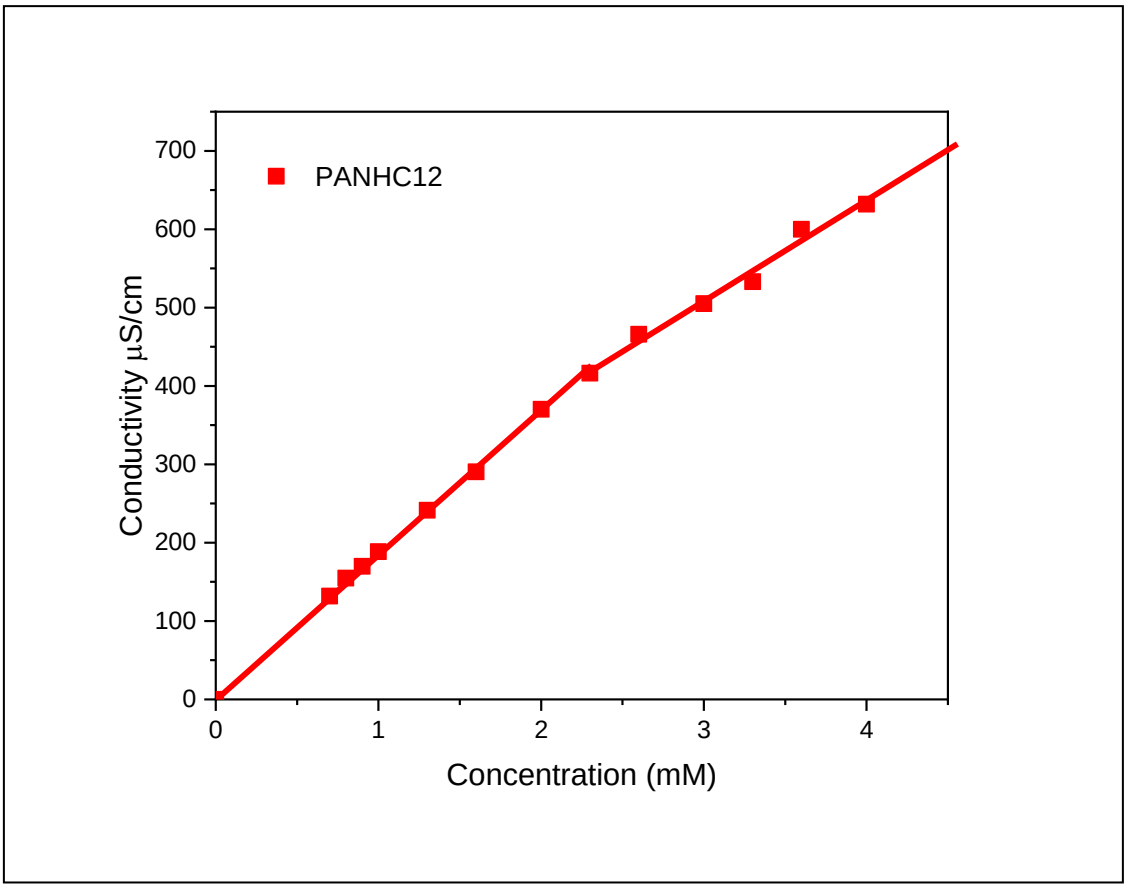
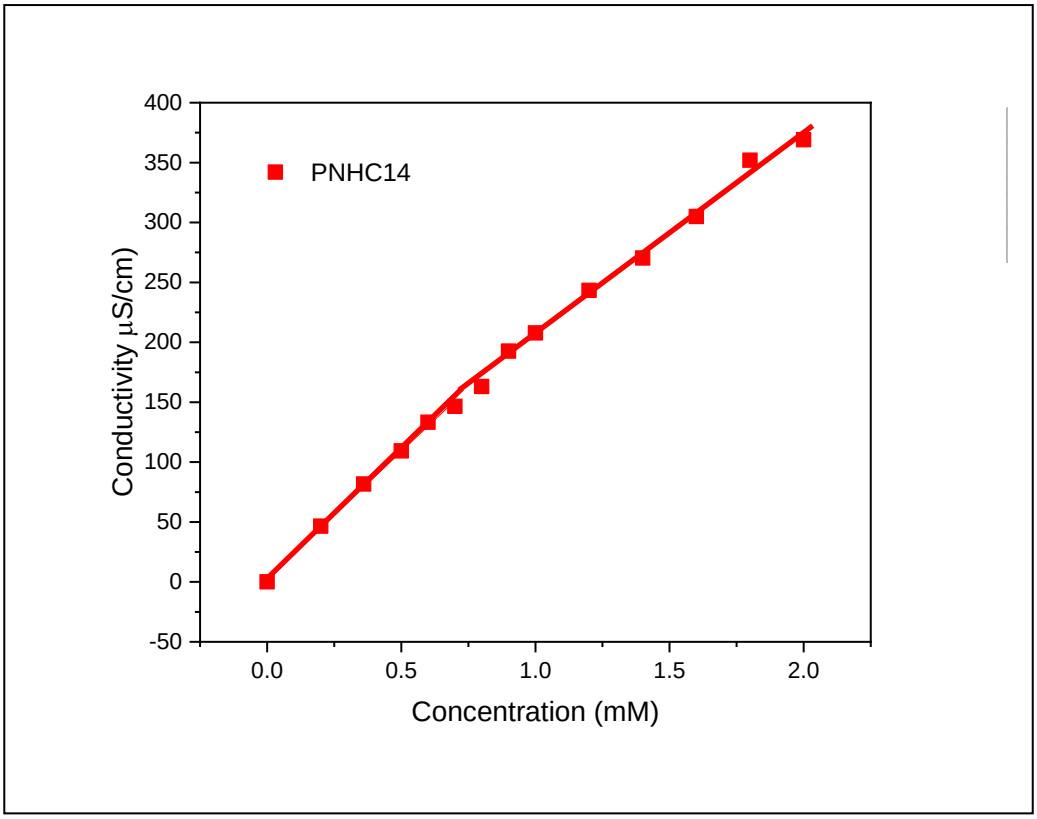
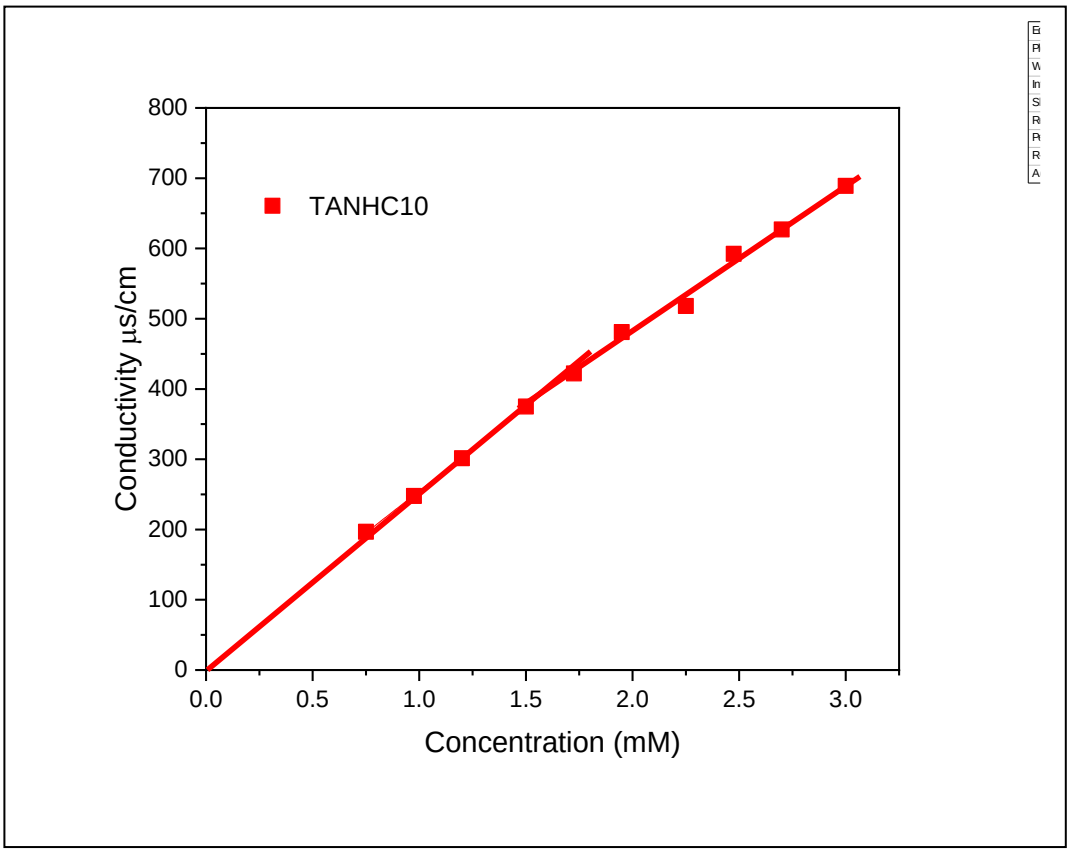


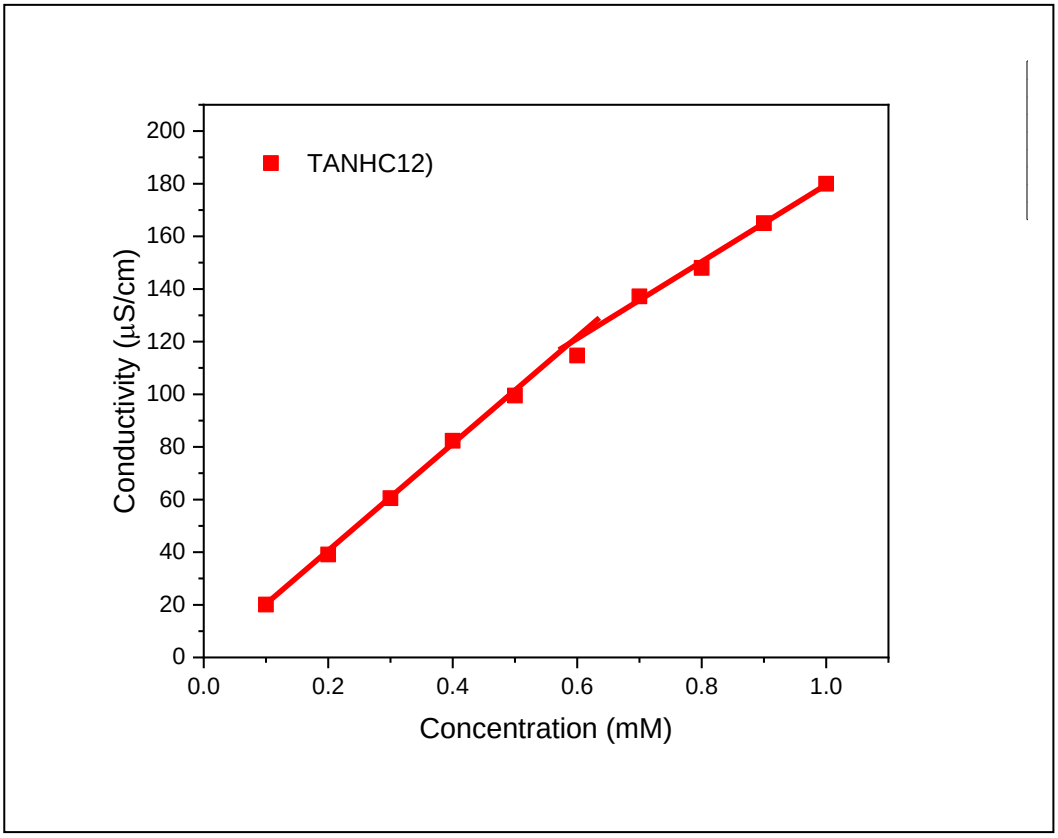
Figure S25. HPLC, ^{1}H NMR,^{13}C NMR and Dept of $C_3(TANHC_8)_2$

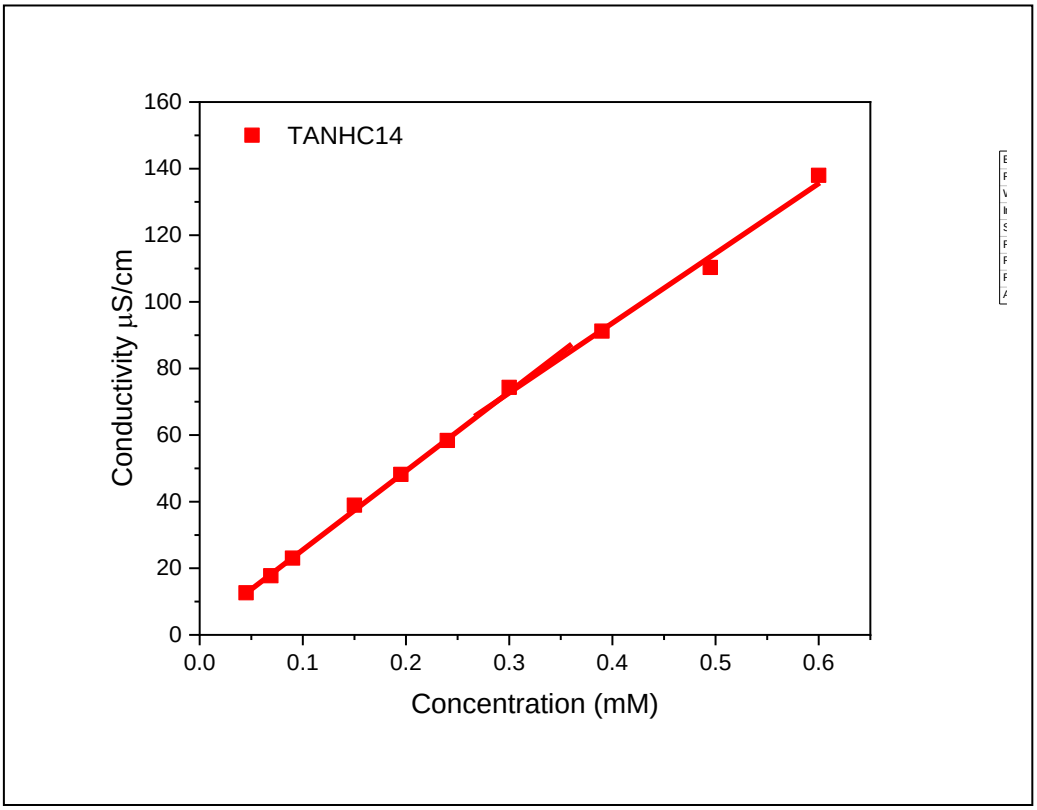

PANHC8
Conductivity µs/cm
Concentration (mM)
0
500
1000
1500
2000
2500
0
2
4
6
8
10
12
14

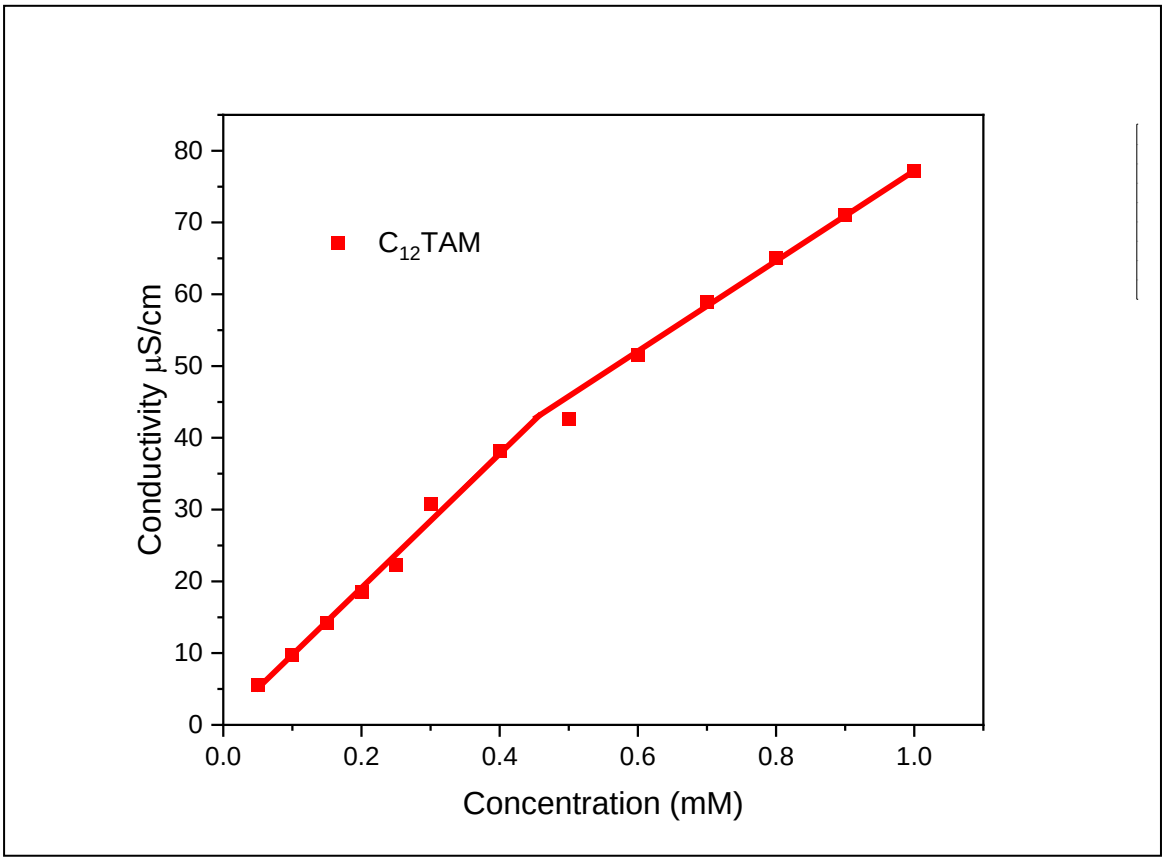

PANHC12
Conductivity µS/cm
Concentration (mM)
0
100
200
300
400
500
600
700
0
1
2
3
4

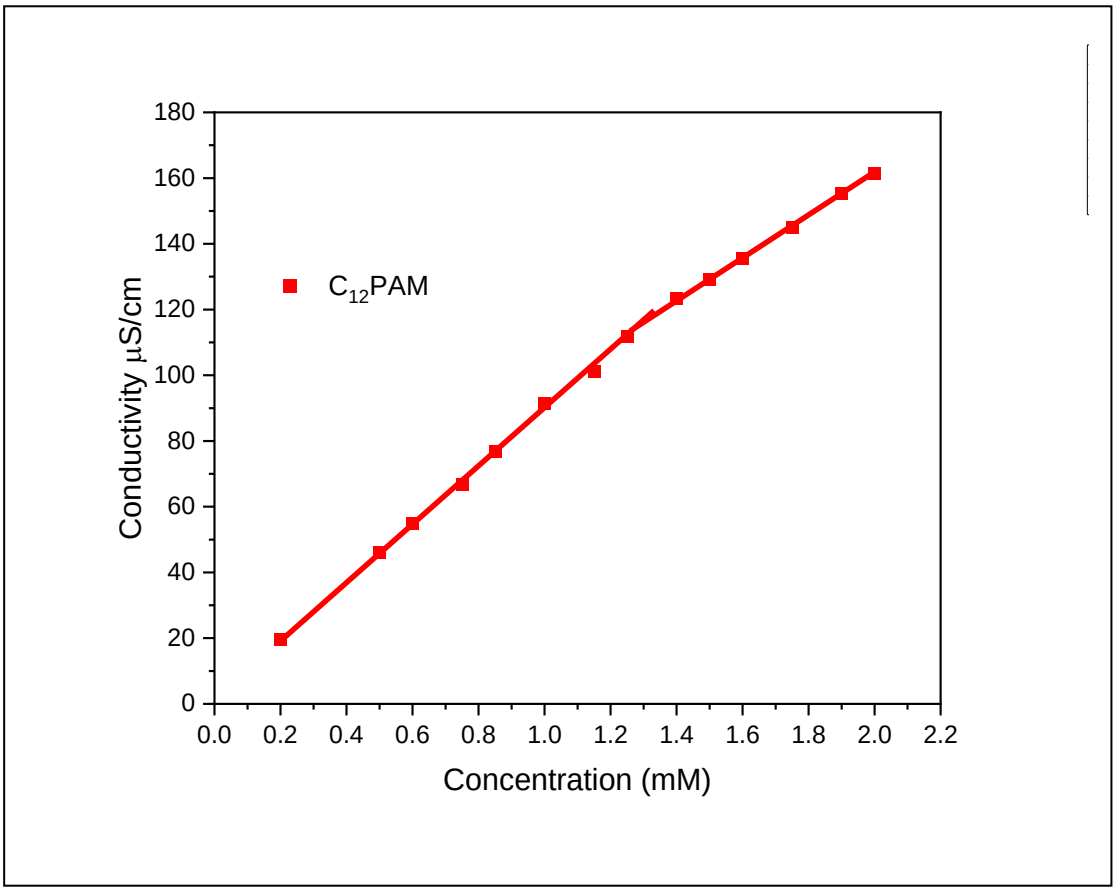

PNHC14
Conductivity µS/cm)
Concentration (mM)
400
350
300
250
200
150
100
50
0
-50
0.0
0.5
1.0
1.5
2.0

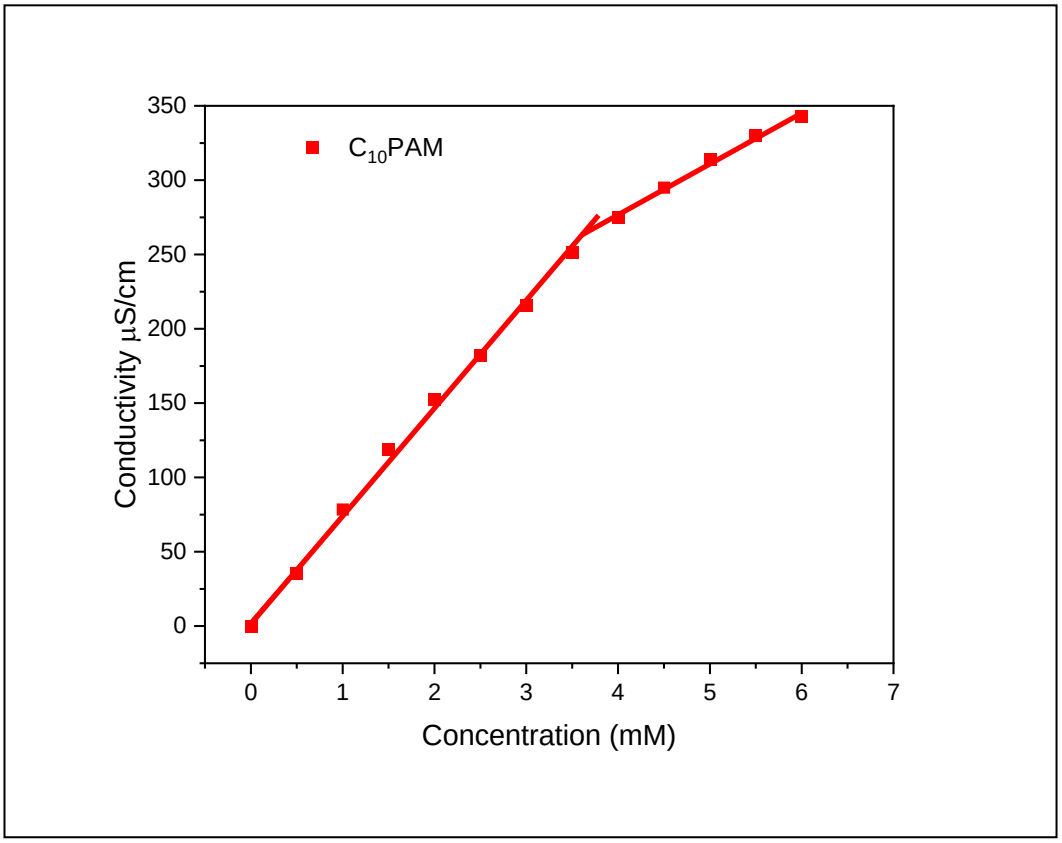

TANHC10
Conductivity µs/cm
Concentration (mM)
800
700
600
500
400
300
200
100
0
0.0
0.5
1.0
1.5
2.0
2.5
3.0


TANHC12)
Conductivity (µS/cm)
Concentration (mM)
0
20
40
60
80
100
120
140
160
180
200
0.0
0.2
0.4
0.6
0.8
1.0


TANHC14
Conductivity µS/cm
Concentration (mM)
0
20
40
60
80
100
120
140
160
0.0
0.1
0.2
0.3
0.4
0.5
0.6


Conductivity µS/cm
Concentration (mM)
C12TAM
0
10
20
30
40
50
60
70
80
0.0
0.2
0.4
0.6
0.8
1.0


Conductivity µS/cm
Concentration (mM)
C12PAM
0
20
40
60
80
100
120
140
160
180
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2



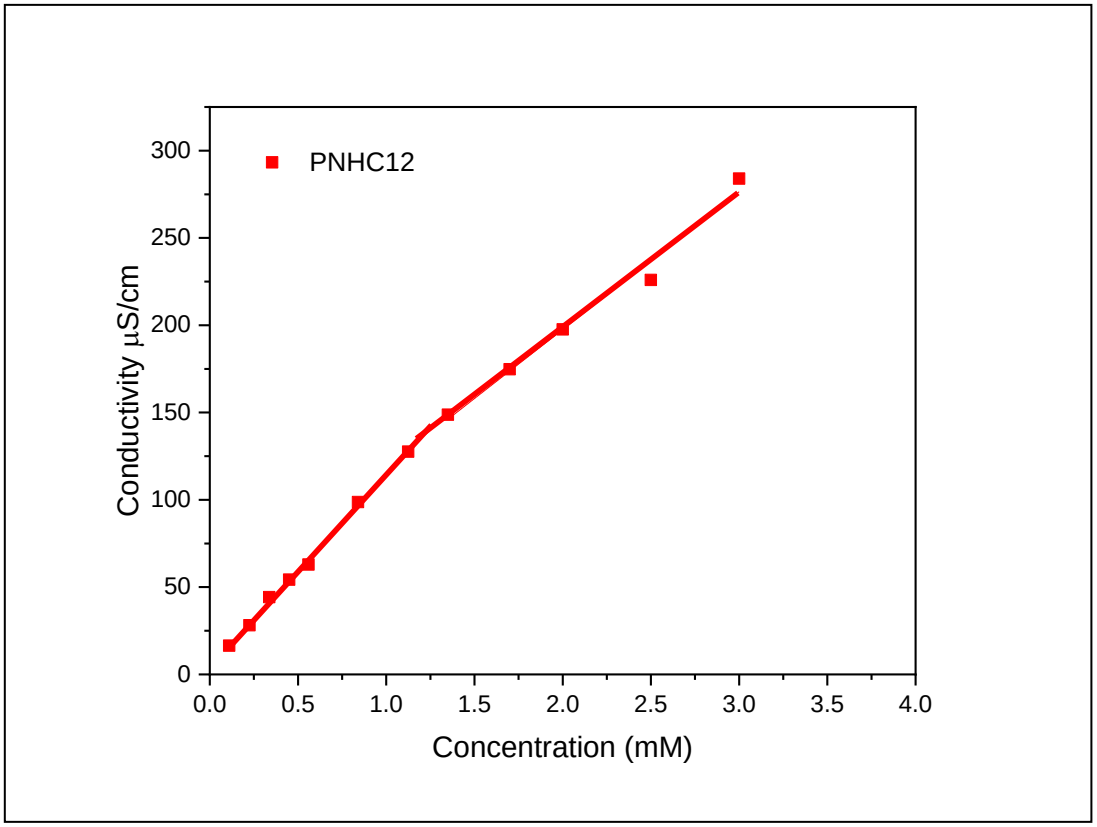


Figure S26. Specific conductivity-concentration curves for the amino acid-based surfactants.