



Supplementary Materials

Novel Cyclic Lipopeptide Antibiotics: Effects of Acyl Chain Length and Position

Signe Kastrup Jensen ¹, **Thomas T. Thomsen** ^{2,3}, **Alberto Oddo** ^{1,†}, **Henrik Franzyk** ¹,
Anders Løbner-Olesen ³ and **Paul R. Hansen** ^{1,*}

¹ Department of Drug Design and Pharmacology, Faculty of Health and Medical Sciences, University of Copenhagen, Universitetsparken 2, 2100 Copenhagen, Denmark; signekastrupjensen@outlook.com (S.K.J.); albi.oddo@gmail.com (A.O.); henrik.franzyk@sund.ku.dk (H.F.)

² Department of Clinical Microbiology, Rigshospitalet, Henrik Harpestrengsvej 4A, 2100 Copenhagen, Denmark; thomas.thomsen@bio.ku.dk

³ Department of Biology, Section for functional Genomics, University of Copenhagen, Ole Maaløesvej 5, 2200 Copenhagen, Denmark; lobner@bio.ku.dk

* Correspondence: prh@sund.ku.dk; Tel.: +45-35336625

† Current address: Novo Nordisk A/S, Krogshøjvej 44, 2820 Bagsværd, Denmark

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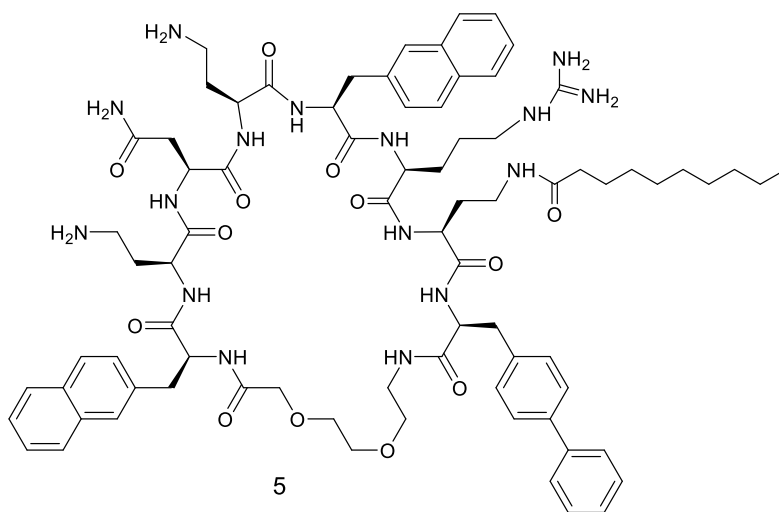
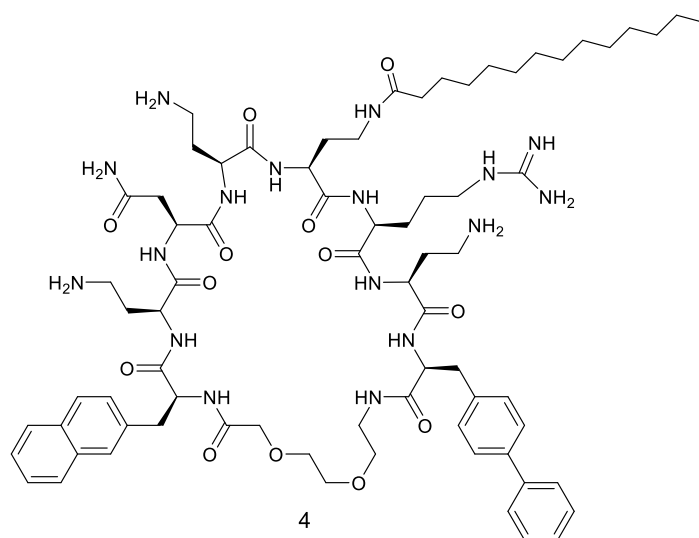
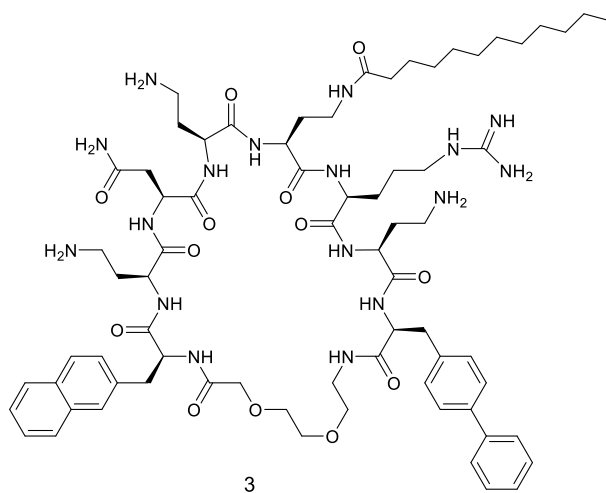
Figure S1: Structure of cyclic peptides

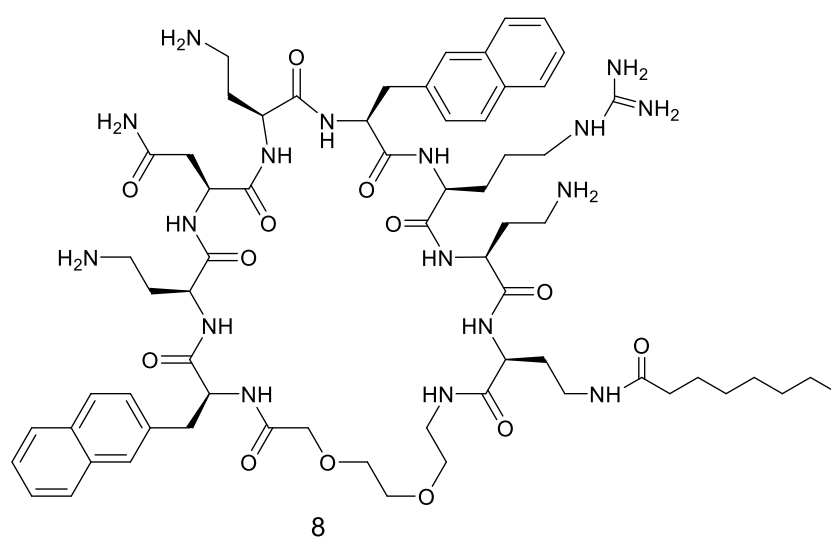
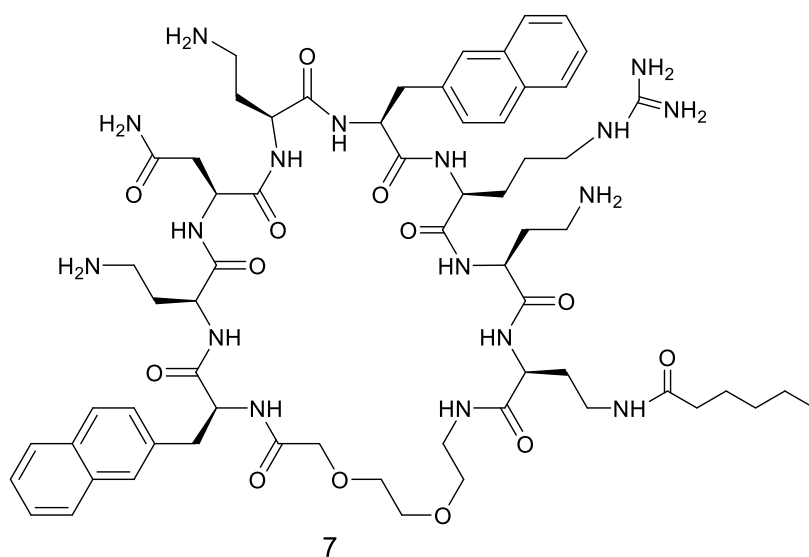
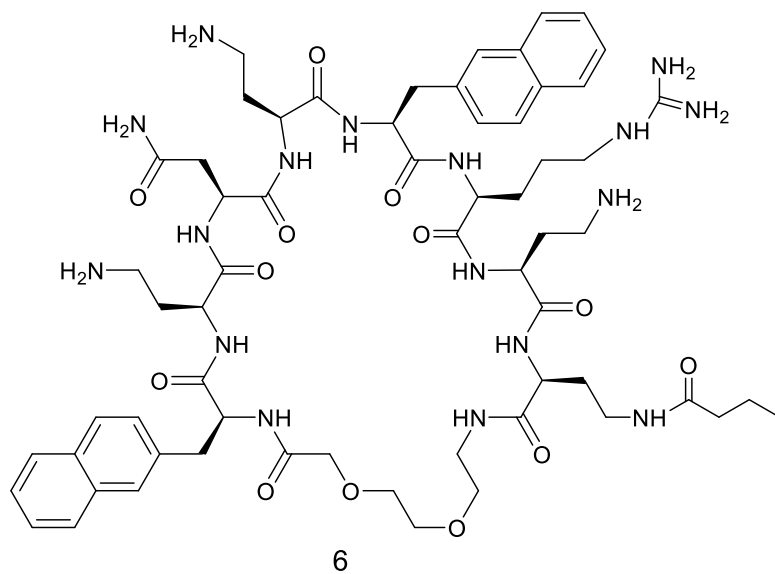
Table S1. Peptide mass, HPLC retention time and purity.

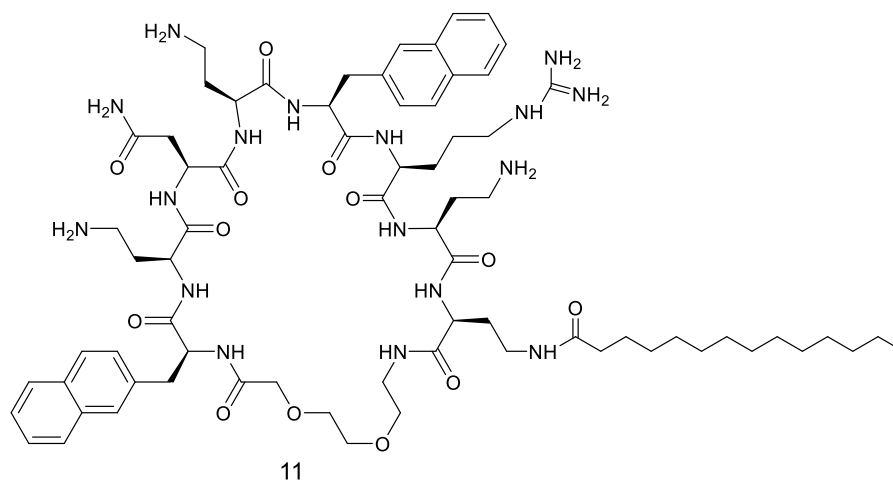
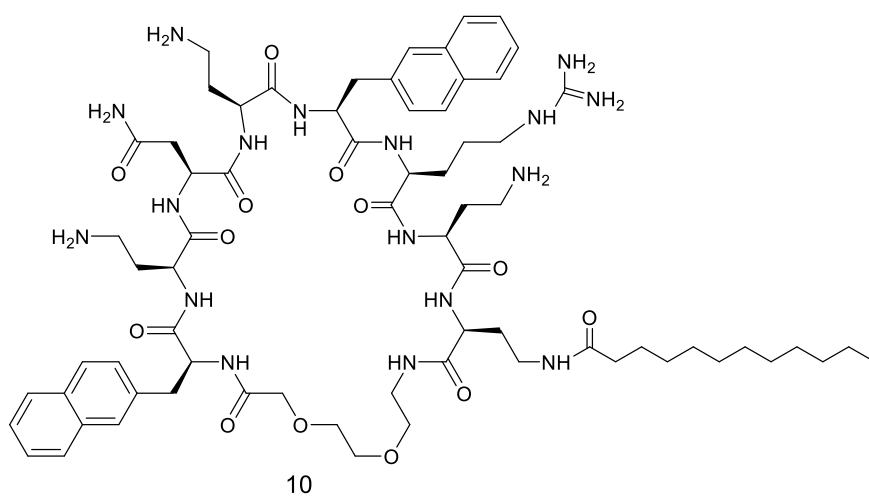
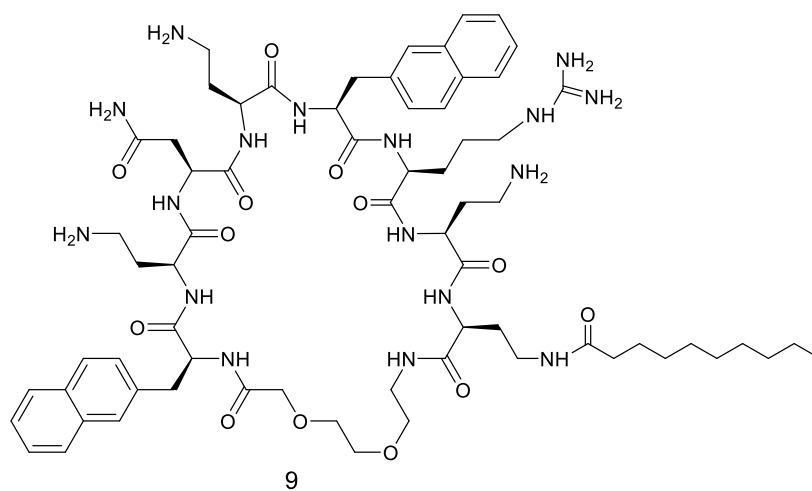
Table S2.: Overview of the analytical data obtained by MALDI-TOF-MS and the peptide purity after purification

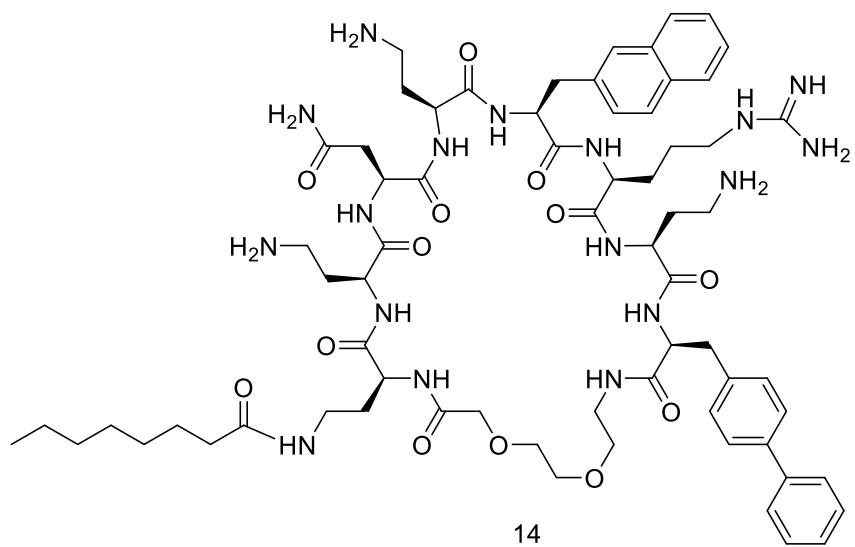
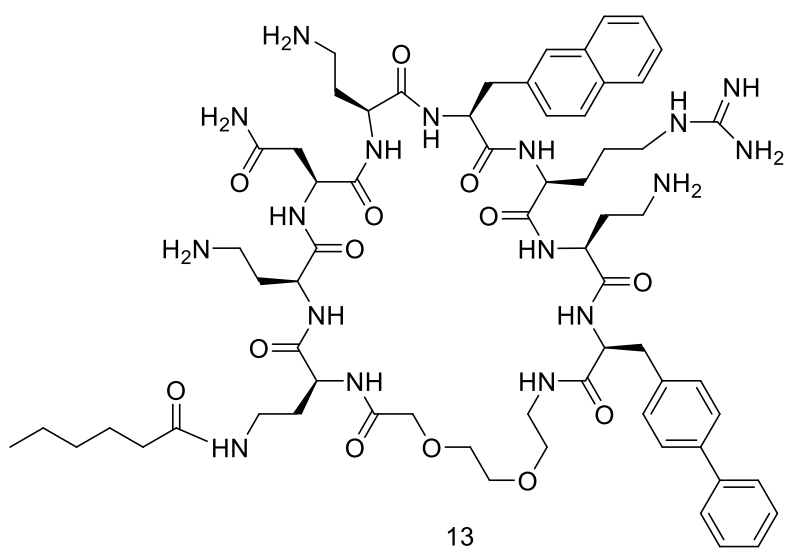
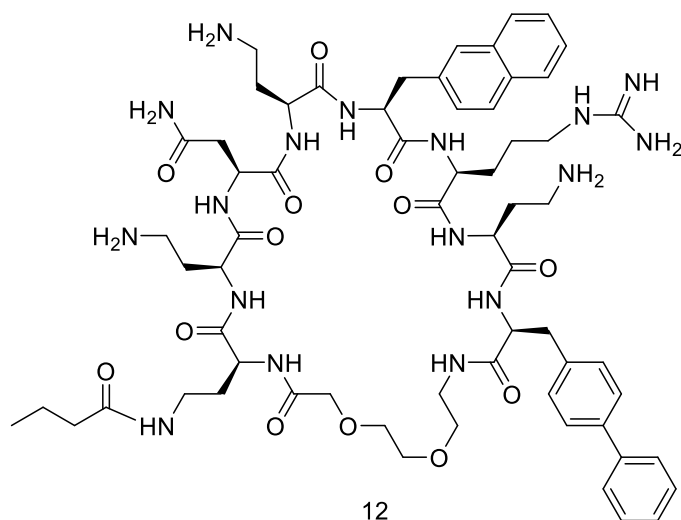
Table S3.: Analytical chromatograms before and after purification III: MALDI-TOF-MS spectra of all purified peptides

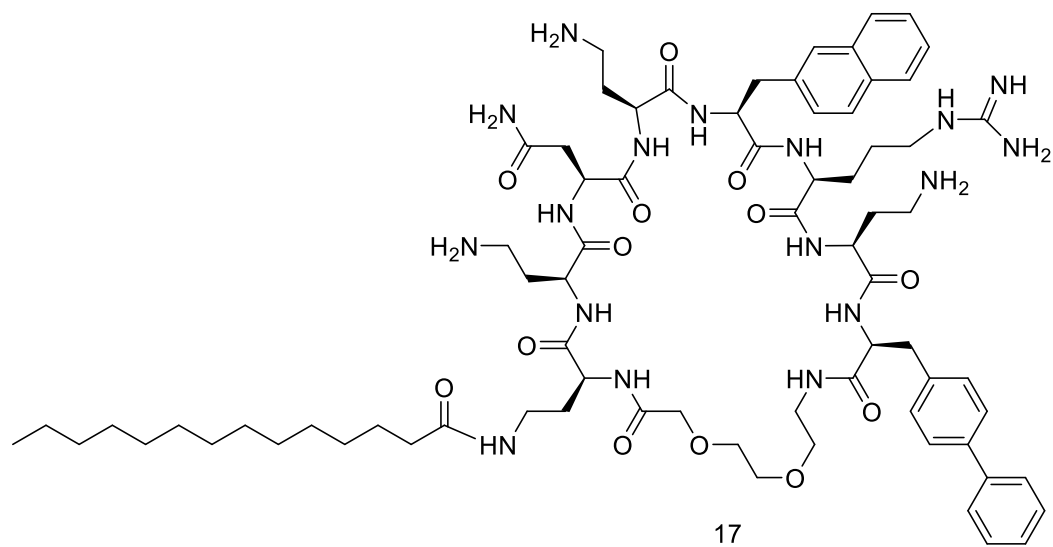
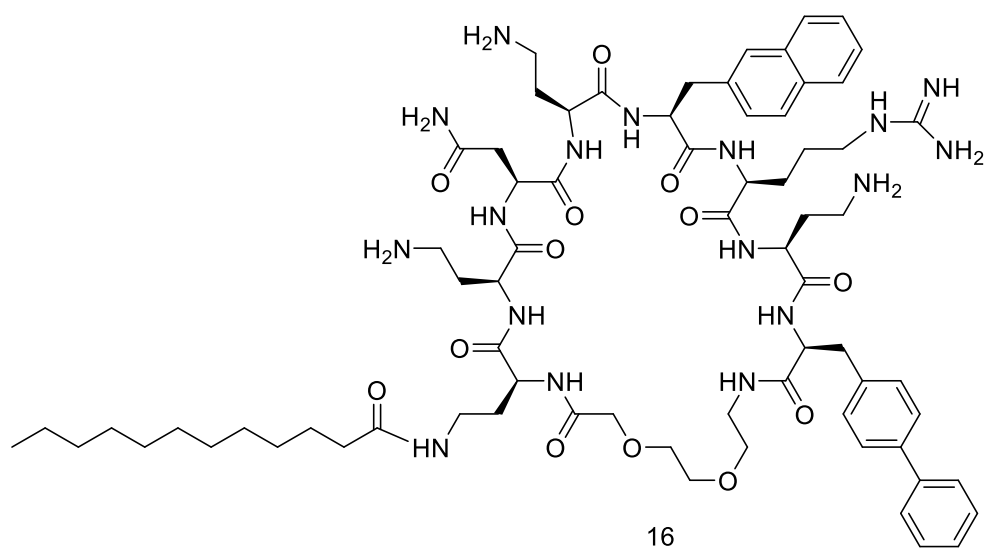
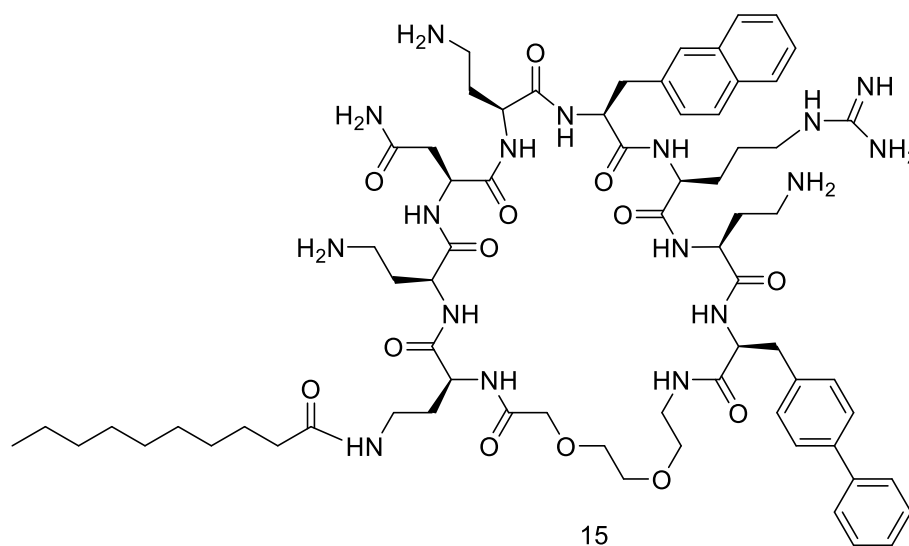
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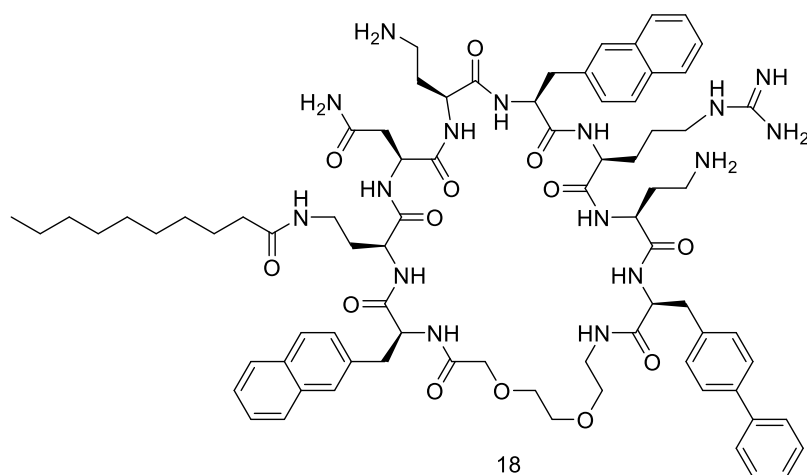


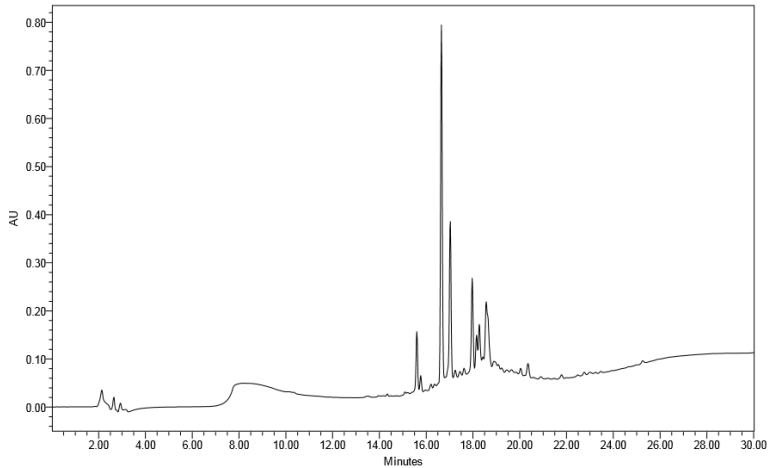
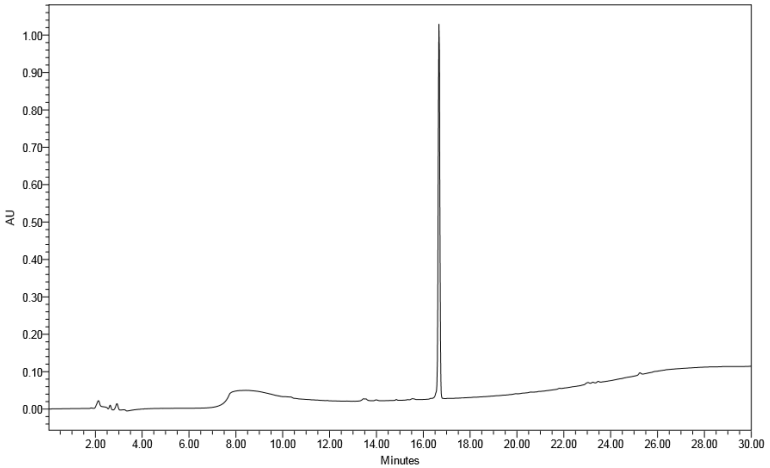
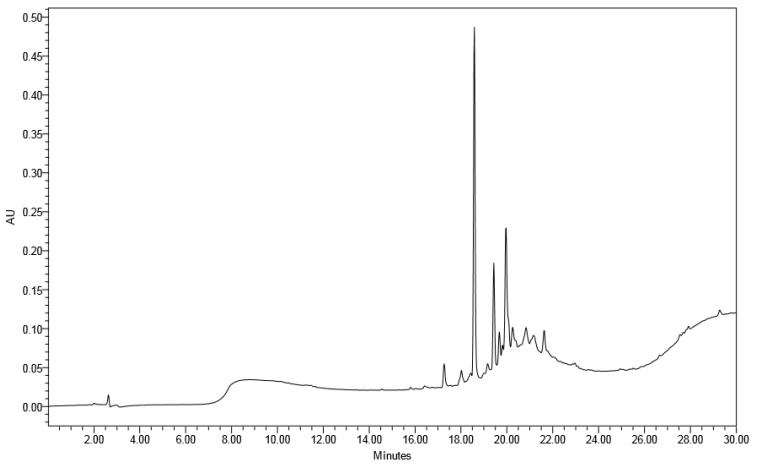
Figure S1. Structure of cyclic peptides. (S3(B)) and (1–18) are cyclic lipopeptides

Table S1. Peptide mass, HPLC retention time and purity.

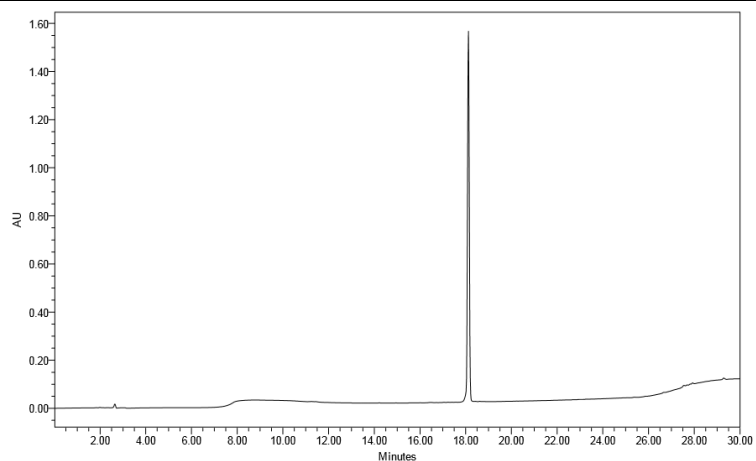
Peptide		Mw ^a	[MH ⁺] ^b	t _R (min) ^c	Purity
S3(B)	S3(B)	1333.68	1334.37	14.1	99.5%
1	(C ₁₀) ¹	1487.82	1488.98	16.7	98.2%
2	(C ₁₀) ²	1390.70	1391.53	15.1	98.6%
3	(C ₁₂) ²	1418.75	1419.48	15.8	98.6%
4	(C ₁₄) ²	1446.81	1447.61	16.7	97.6%
5	(C ₁₀) ⁴	1487.82	1489.07	17.0	98.9%
6	(C ₄) ⁵	1280.50	1281.63	12.3	95.1%
7	(C ₆) ⁵	1308.55	1309.66	13.0	98.1%
8	(C ₈) ⁵	1336.61	1337.77	13.8	100%
9	(C ₁₀) ⁵	1364.66	1365.58	14.8	97.4%
10	(C ₁₂) ⁵	1392.72	1393.79	15.6	98.0%
11	(C ₁₄) ⁵	1420.77	1421.53	16.6	98.8%
12	(C ₄) ⁷	1306.54	1307.75	12.7	95.1%
13	(C ₆) ⁷	1334.59	1335.28	13.7	99.1%
14	(C ₈) ⁷	1362.65	1363.68	14.1	96.0%
15	(C ₁₀) ⁷	1390.70	1391.43	14.8	98.8%
16	(C ₁₂) ⁷	1418.75	1419.60	15.8	97.3%
17	(C ₁₄) ⁷	1446.81	1447.74	16.8	98.4%
18	(C ₁₀) ⁸	1487.82	1488.89	16.8	99.5%

^a Molecular weight of the peptides, g/mol; ^b Mass-to-charge value; ^c Retention time obtained by RP-HPLC.

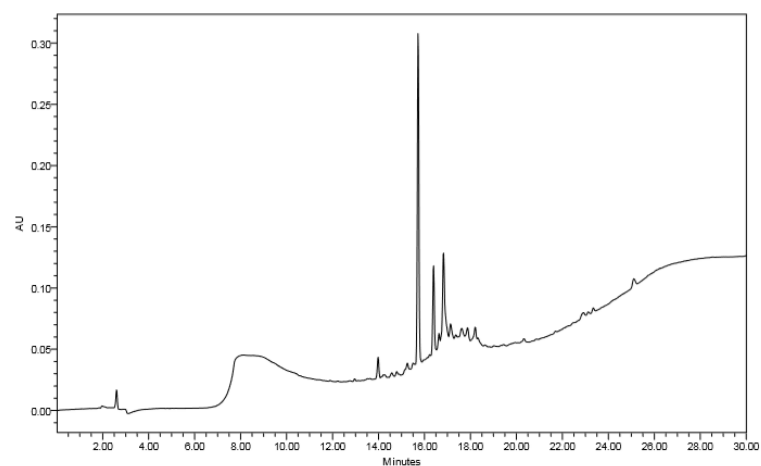
Table S2. Overview of the analytical data obtained by MALDI-TOF-MS and the peptide purity after purification.

Analytical HPLC chromatograms	Cyclic Lipopeptide	Analytical HPLC chromatograms
(C ₁₀) ¹	Crude tr: 16.7 min	
(C ₁₀) ¹	<u>Purified</u> tr: 16.7 min Purity: 98.2%	
(C ₁₀) ²	<u>Crude</u> tr: 18.6 min (method <i>Pep1</i>)	

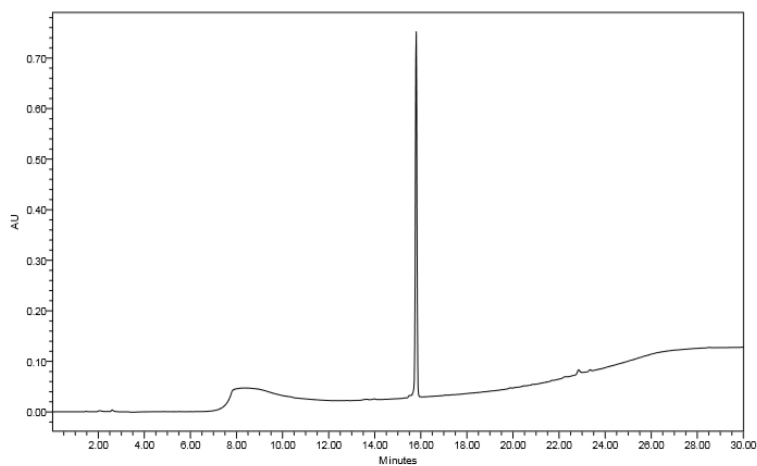
(C₁₀)² Purified
tr: 18.1 min
Purity: 98.6%



(C₁₂)² Crude
tr: 15.7 min

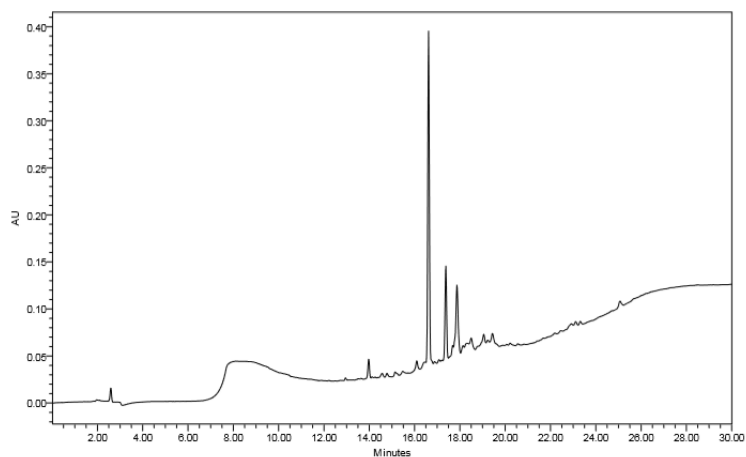


(C₁₂)² Purified
tr: 15.8 min
Purity: 98.6%

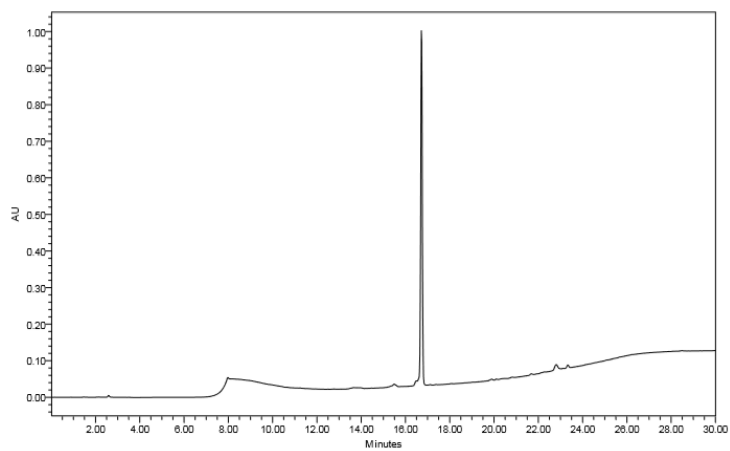


$(C_{14})^2$

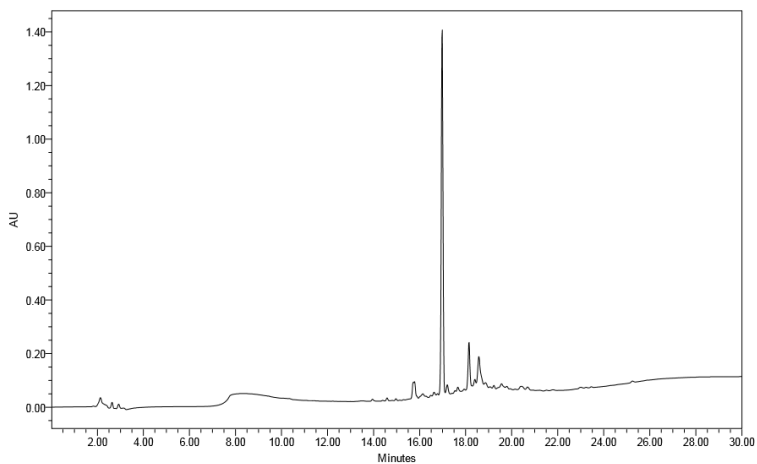
Crude
tr: 16.6 min

 $(C_{14})^2$

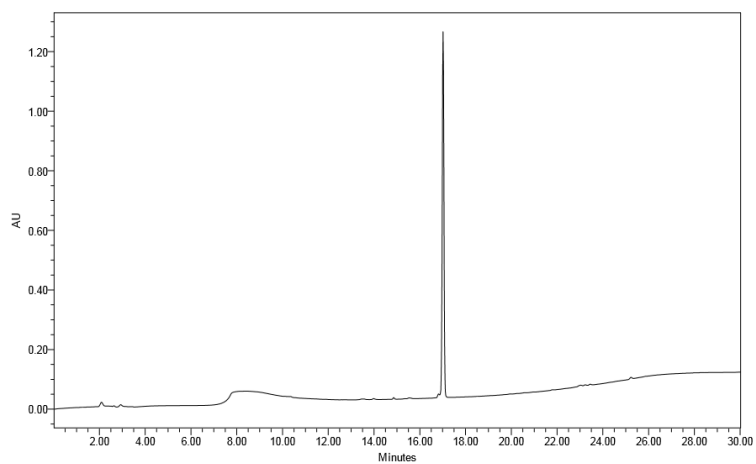
Purified
tr: 16.7 min
Purity: 97.6%

 $(C_{10})^4$

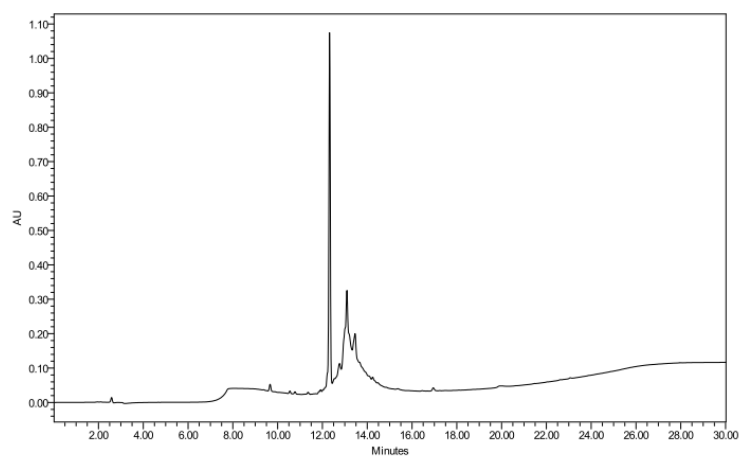
Crude
tr: 17.0 min



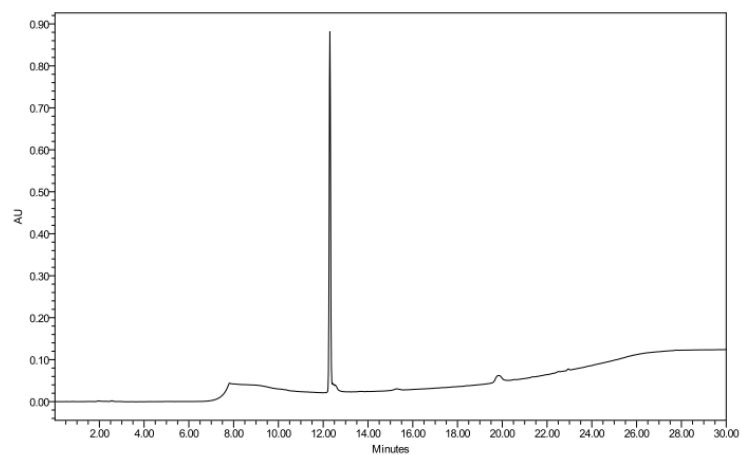
(C₁₀)⁴ Purified
tr: 17.0 min
Purity: 98.9%



(C₄)⁵ Crude
tr: 12.3 min

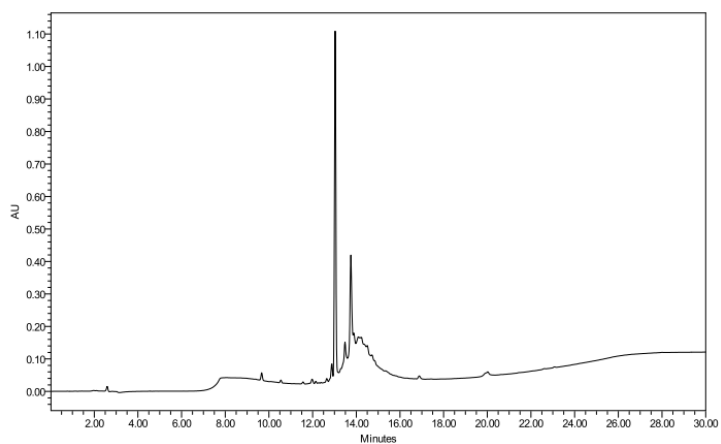


(C₄)⁵ Purified
tr: 12.3 min
Purity: 95.1%

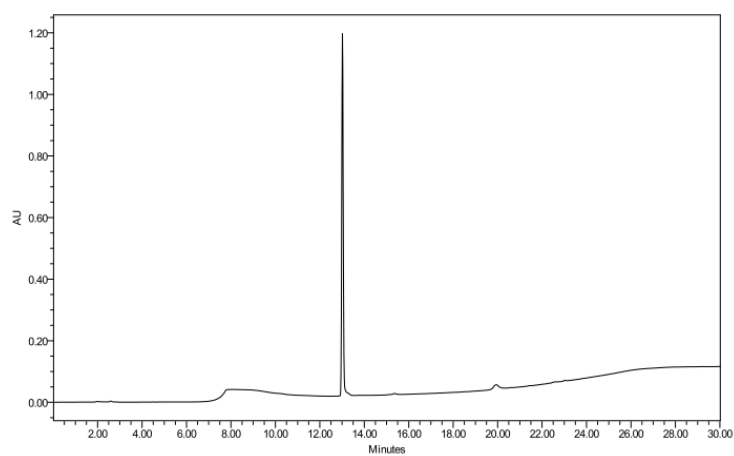


$(C_6)^5$

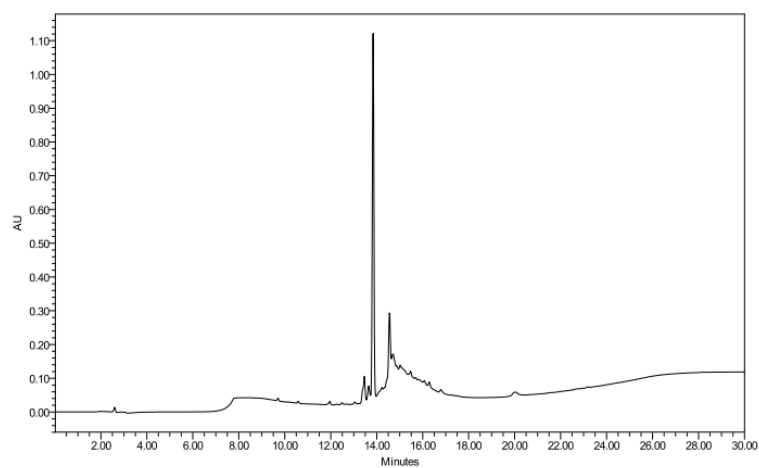
Crude
tr: 13.0 min

 $(C_6)^5$

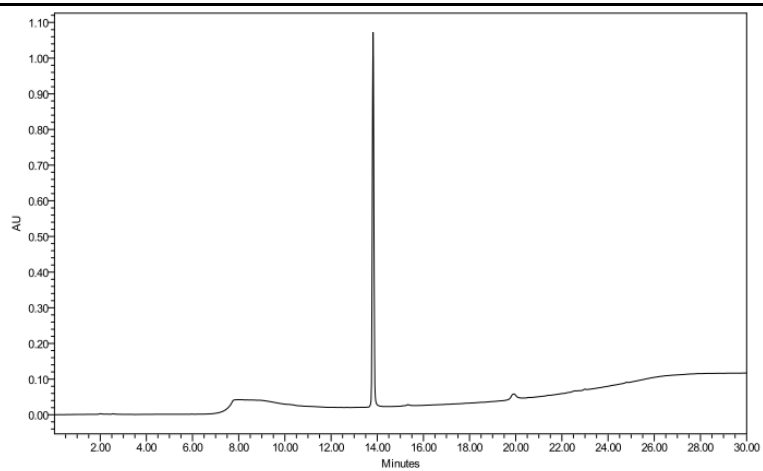
Purified
tr: 13.0 min
Purity: 98.1%

 $(C_8)^5$

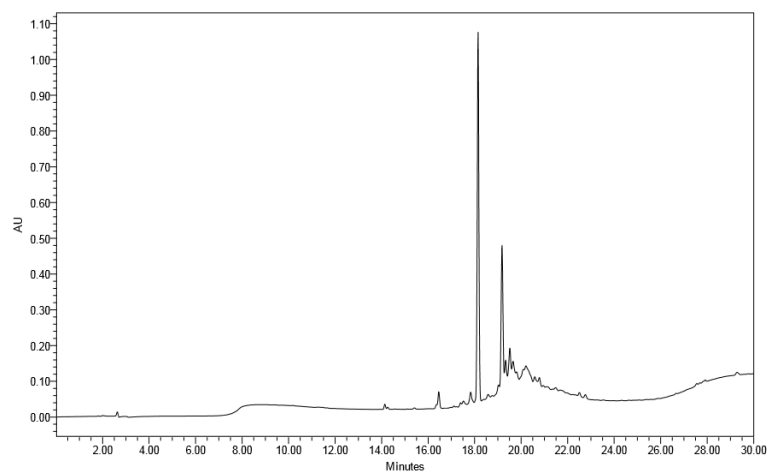
Crude
tr: 13.8 min



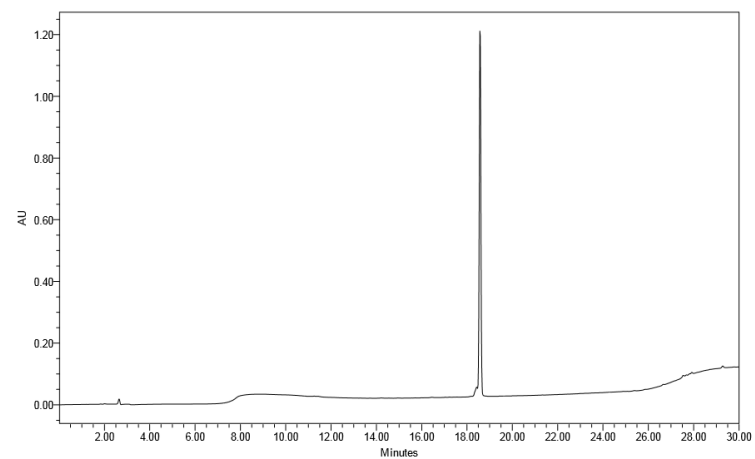
(C₈)⁵
Purified
tr: 13.8 min
Purity: 100%



(C₁₀)⁵
Crude
tr: 18.2 min
(method
Pep1)

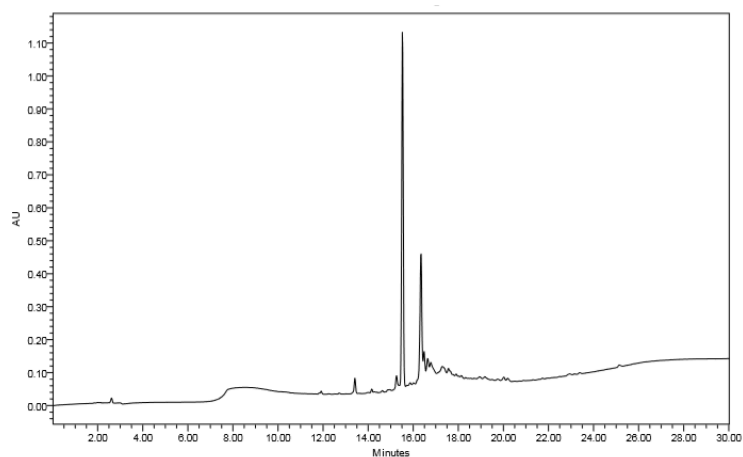


(C₁₀)⁵
Purified
tr: 18.6 min
(method
Pep1(shown
) / 14.8 min
(method
O_100 %B)
Purity: 97.4%

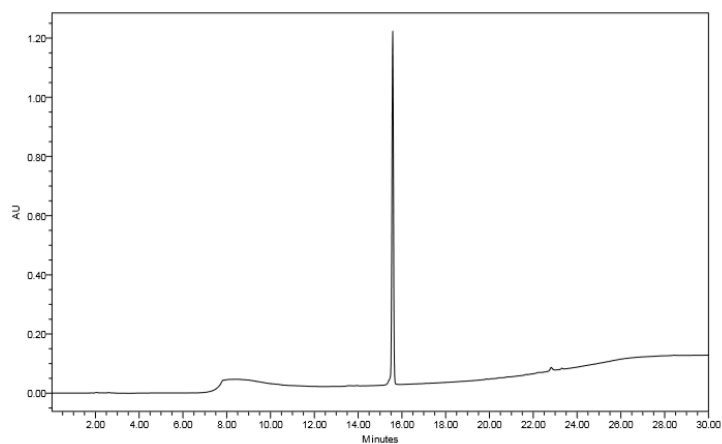


$(C_{12})^5$

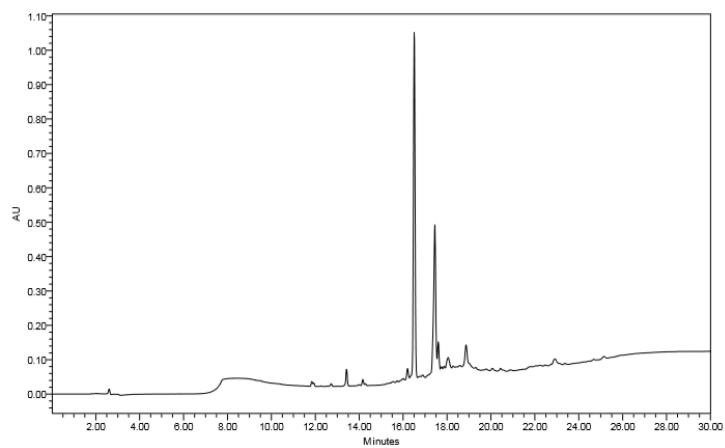
Crude
tr: 15.5 min

 $(C_{12})^5$

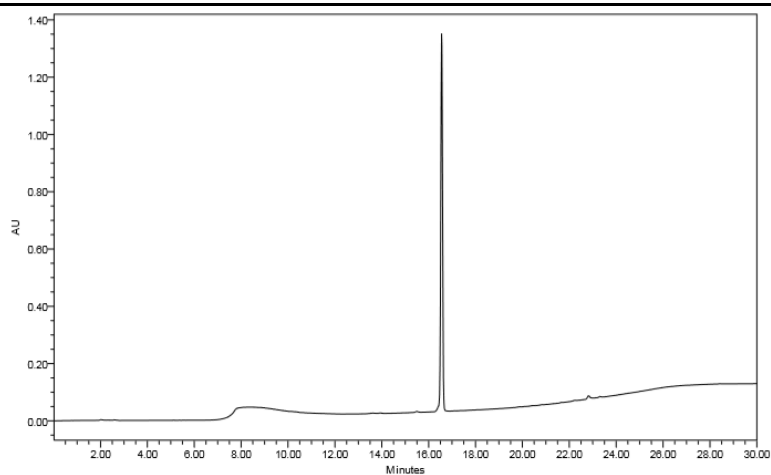
Purified
tr: 15.6 min
Purity: 98.0%

 $(C_{14})^5$

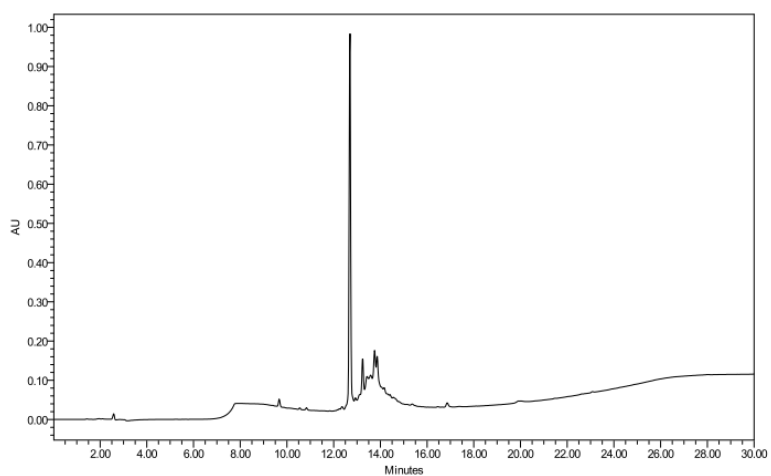
Crude
tr: 16.5 min



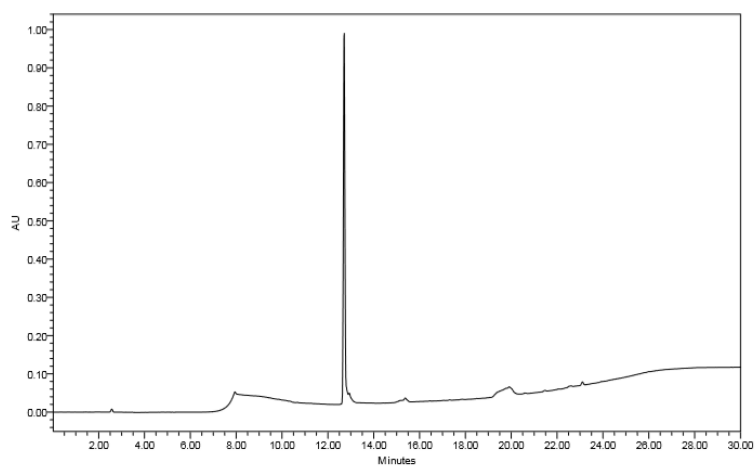
(C₁₄)⁵ Purified
tr: 16.6 min
Purity: 98.8%



(C₄)⁷ Crude
tr: 12.7 min

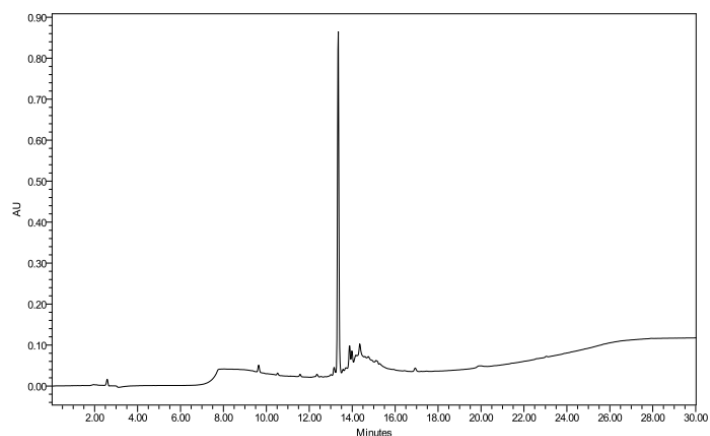


(C₄)⁷ Purified
tr: 12.7 min
Purity: 95.1%

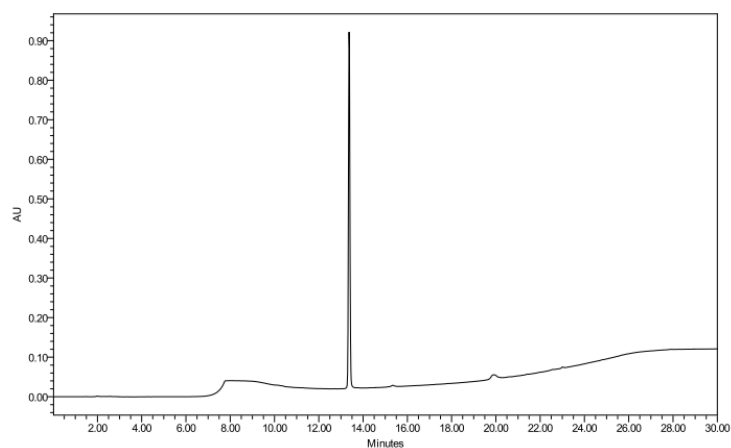


$(C_6)^7$

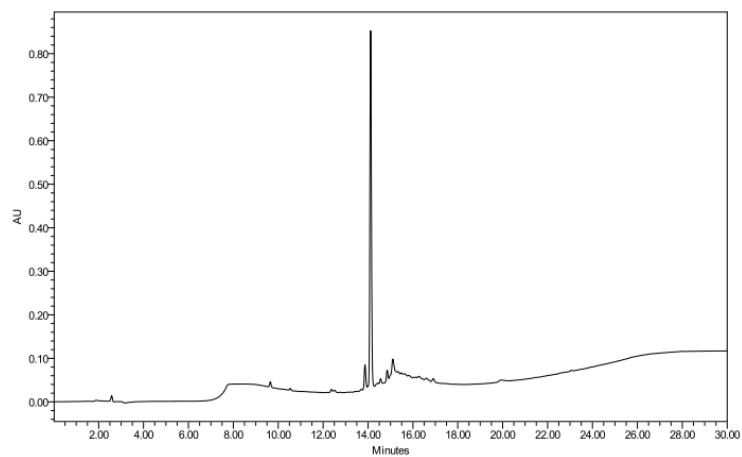
Crude
tr: 13.4 min

 $(C_6)^7$

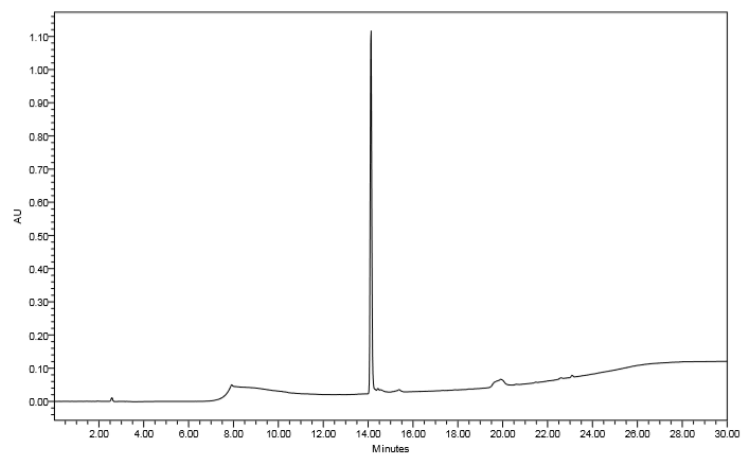
Purified
tr: 13.7 min
Purity: 99.1%

 $(C_8)^7$

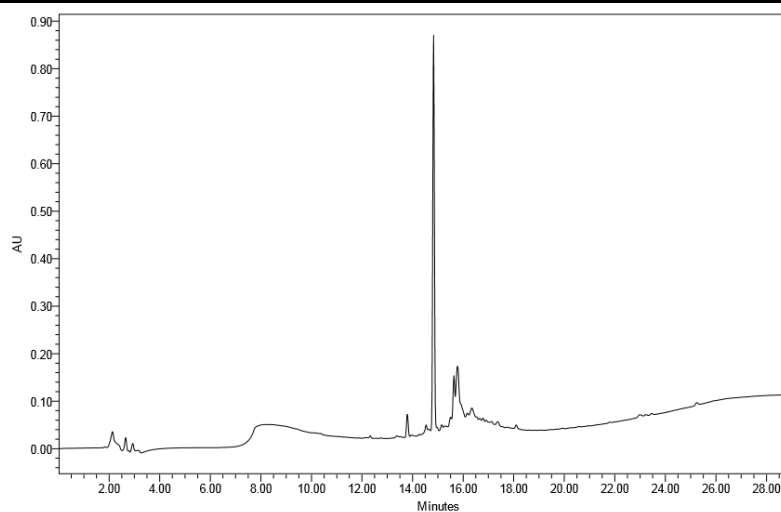
Crude
tr: 14.1 min

 $(C_8)^7$

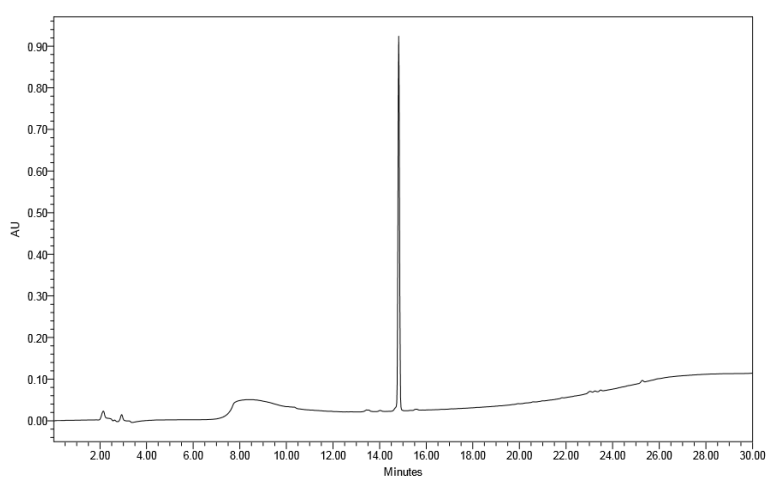
Purified
tr: 14.1 min
Purity: 96.0%



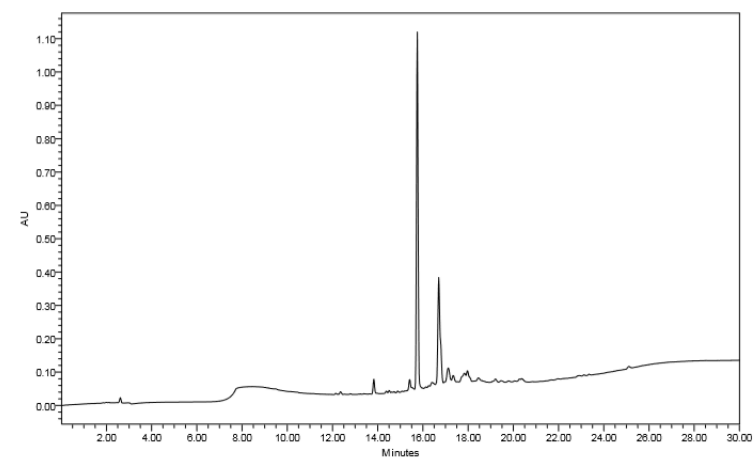
(C₁₀)⁷ Crude
tr: 14.8 min



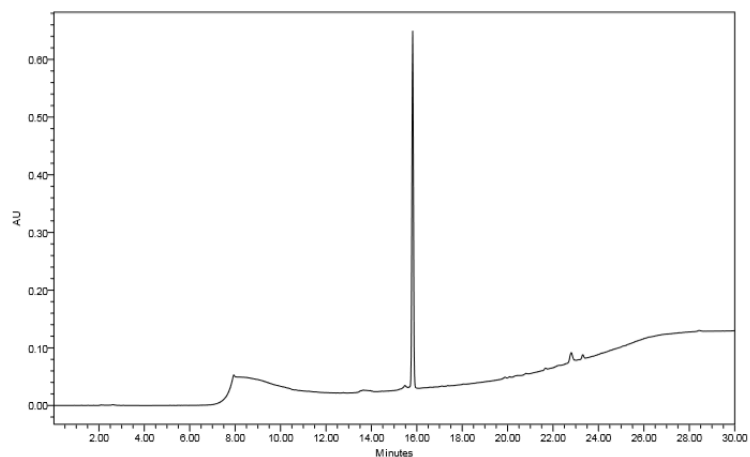
(C₁₀)⁷ Purified
tr: 14.8 min
Purity: 98.8%



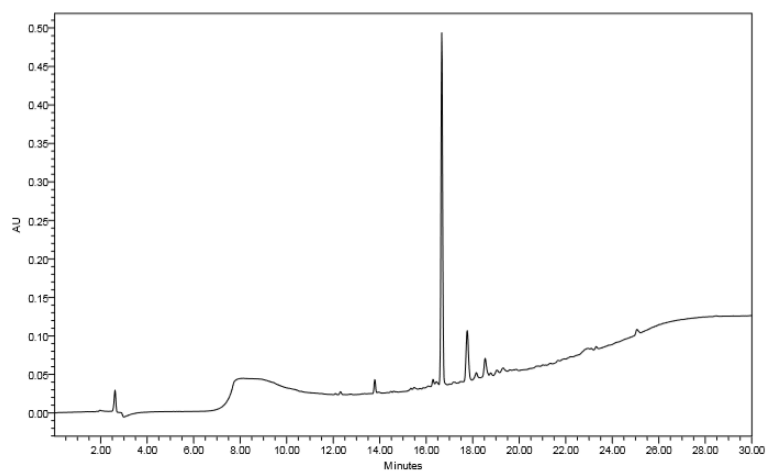
(C₁₂)⁷ Crude
tr: 15.8 min



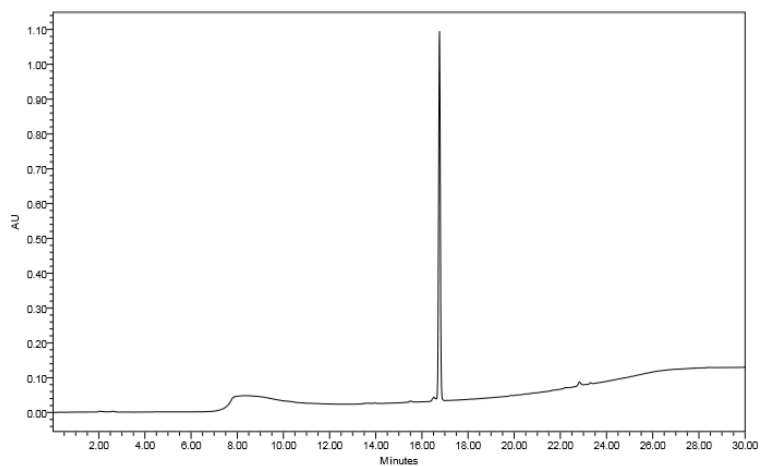
(C₁₂)⁷ Purified
tr: 15.8 min
Purity: 97.3%

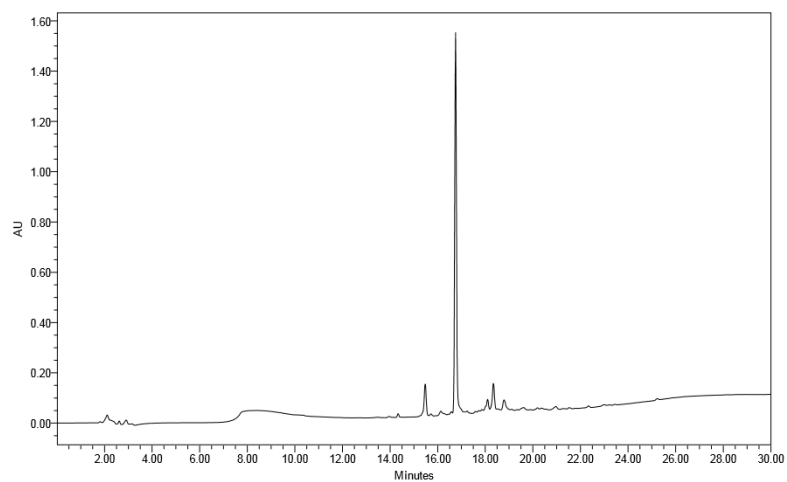
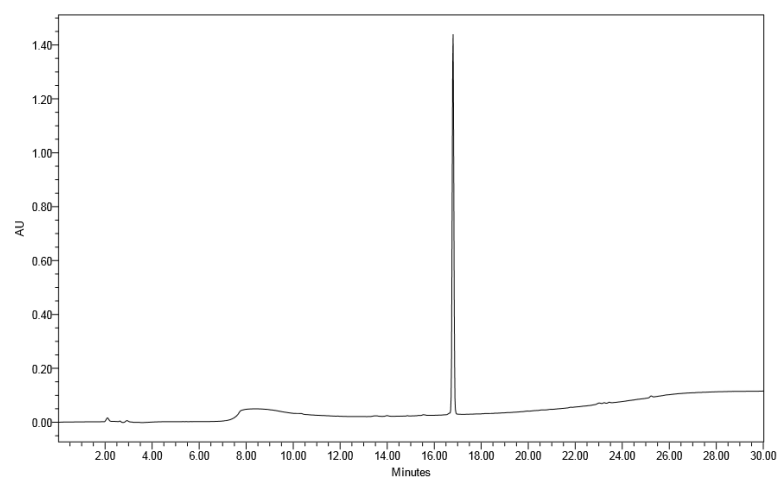


(C₁₄)⁷ Crude
tr: 16.7 min

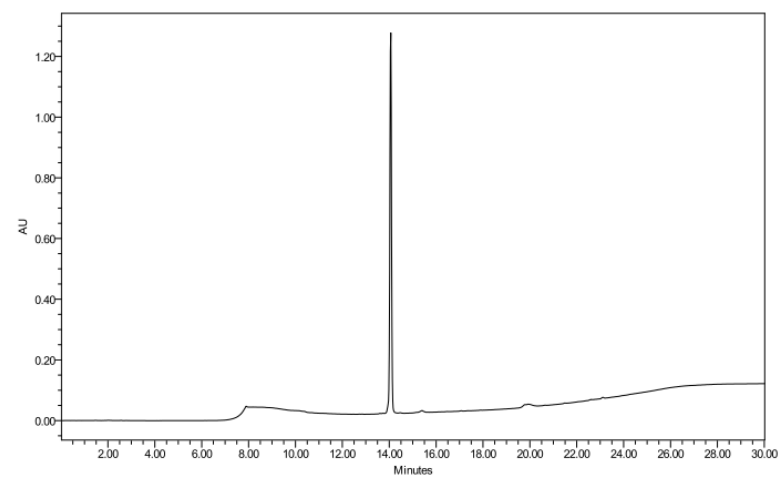


(C₁₄)⁷ Purified
tr: 16.8 min
Purity: 98.4%

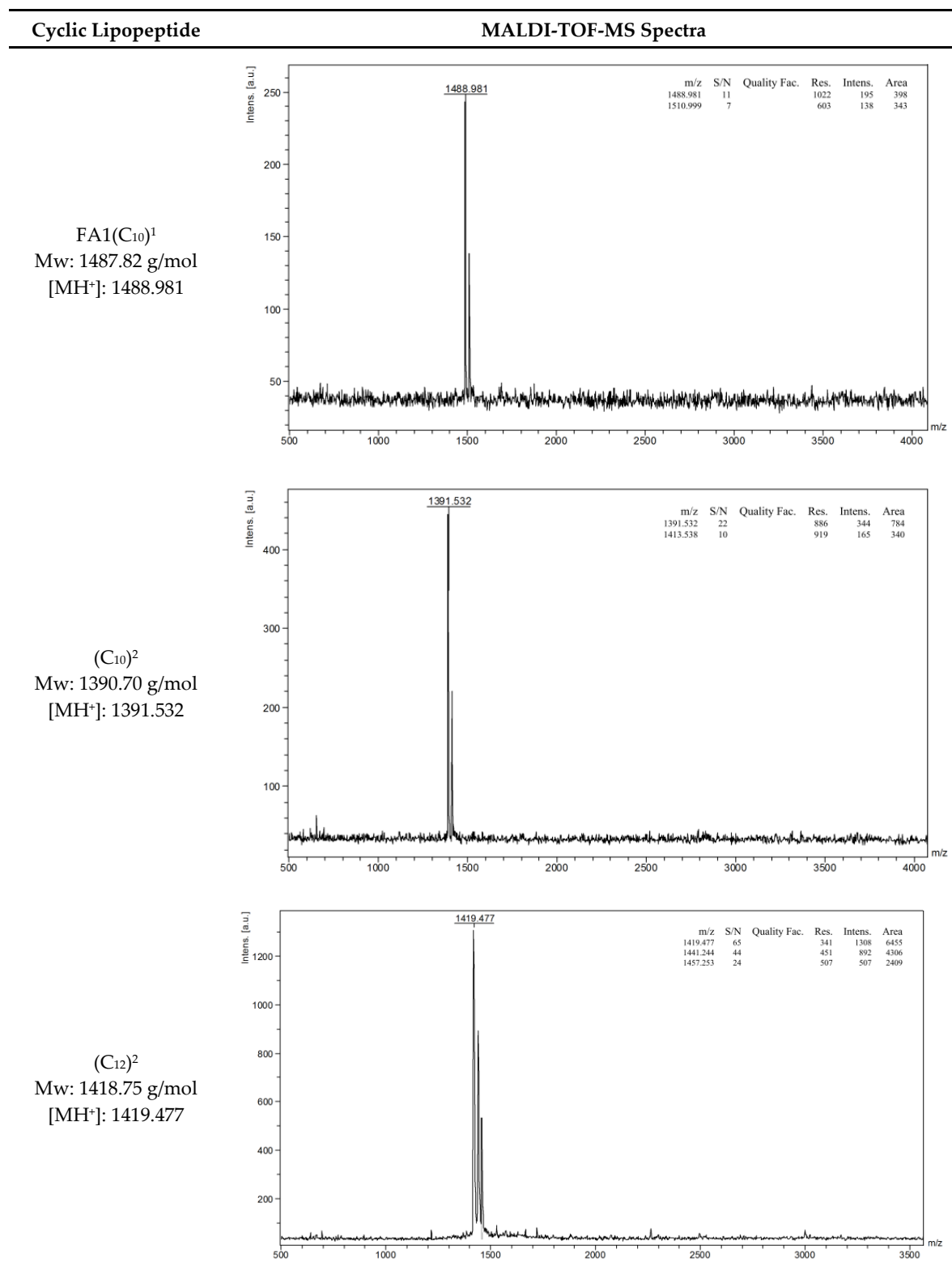


$(C_{10})^8$ Crude
tr: 16.8 min $(C_{10})^8$ Purified
tr: 16.8 min
Purity: 99.5%

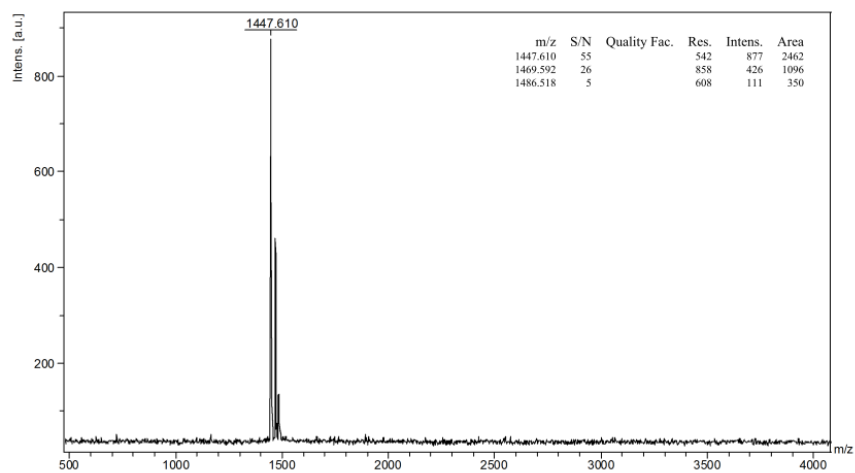
S3(B)

Purified
tr: 14.1 min
Purity: 99.5%

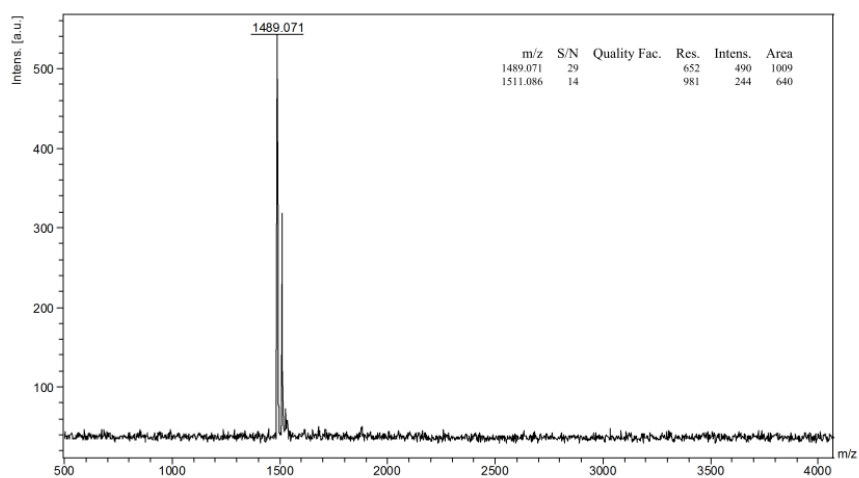
tr: retention time.

Table S3. Analytical chromatograms before and after purification III: MALDI-TOF-MS spectra of all purified peptides.

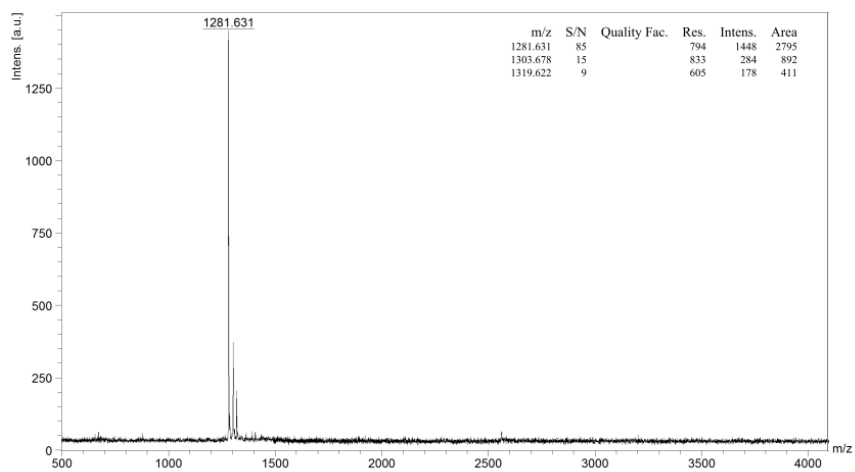
$(C_{14})^2$
Mw: 1446.81 g/mol
[MH⁺]: 1447.610



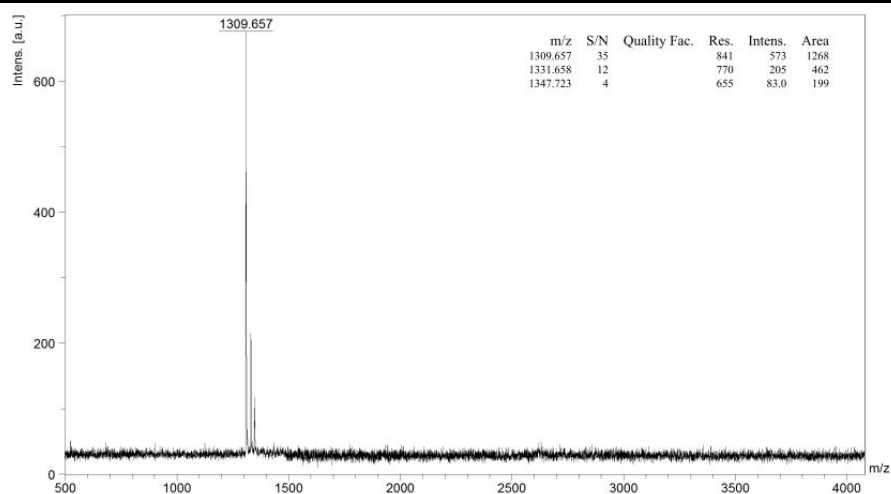
$(C_{10})^4$
Mw: 1487.82 g/mol
[MH⁺]: 1489.071



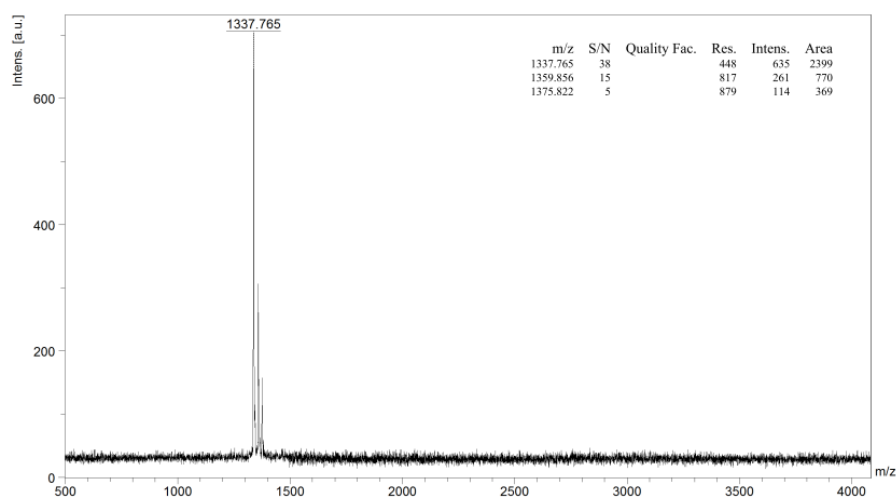
$(C_4)^5$
Mw: 1280.50 g/mol
[MH⁺]: 1281.631



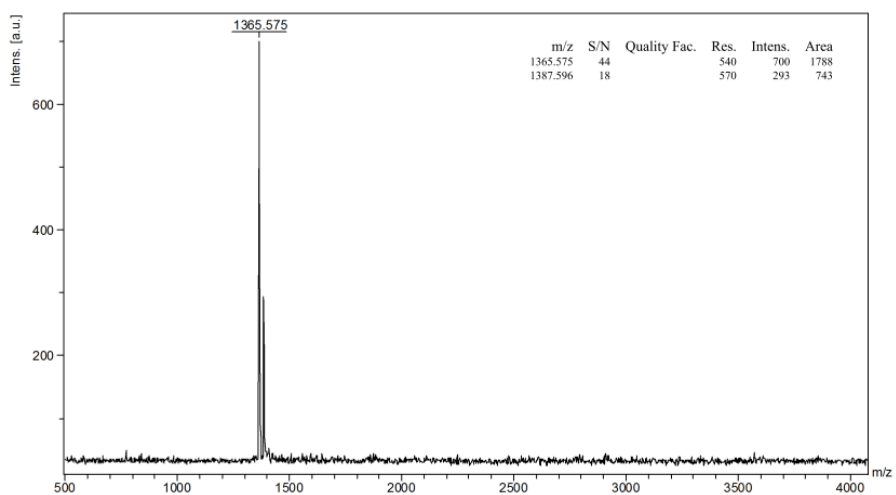
$(C_6)^5$
Mw: 1308.55 g/mol
[MH⁺]: 1309.657



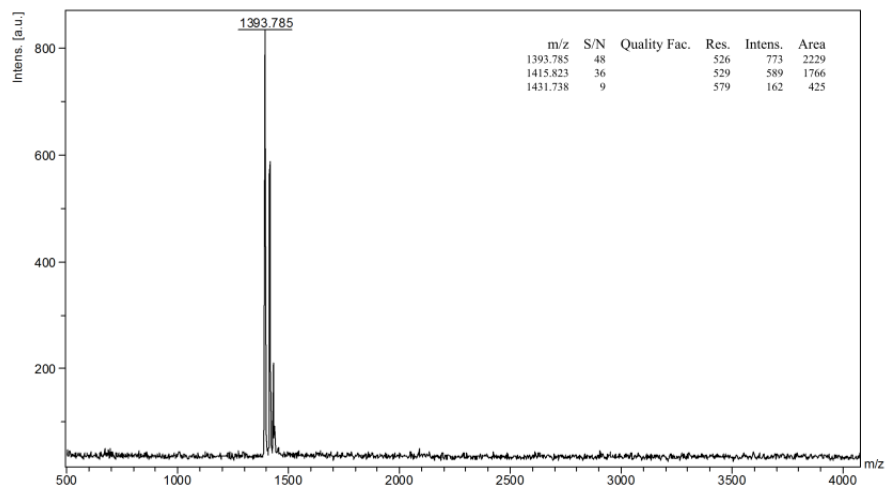
$(C_8)^5$
Mw: 1336.61 g/mol
[MH⁺]: 1337.765



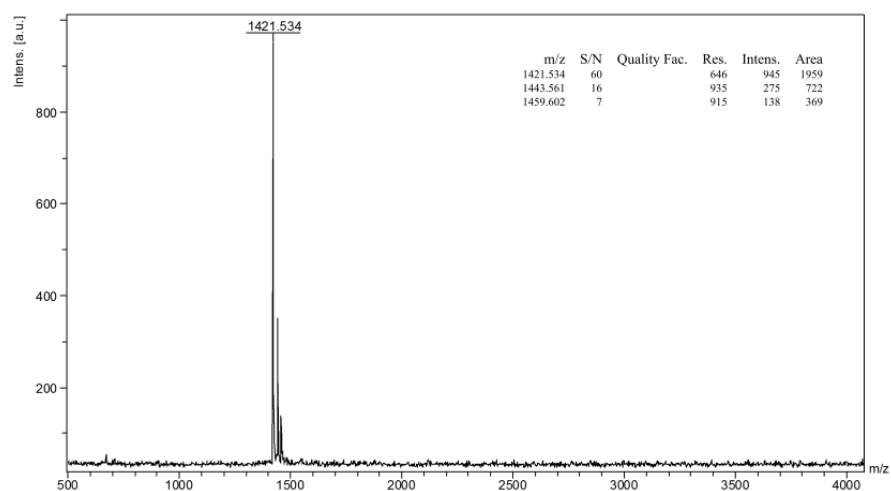
$(C_{10})^5$
Mw: 1364.66 g/mol
[MH⁺]: 1365.575



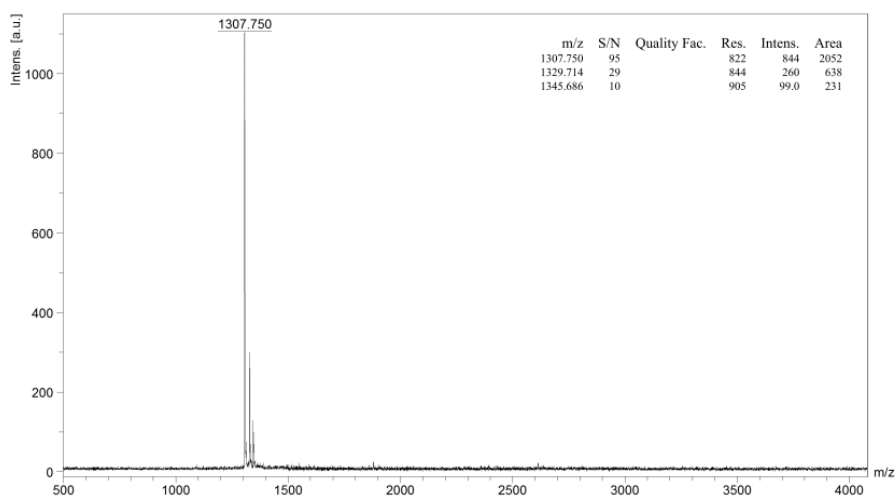
$(C_{12})^5$
Mw: 1392.72 g/mol
[MH⁺]: 1393.785



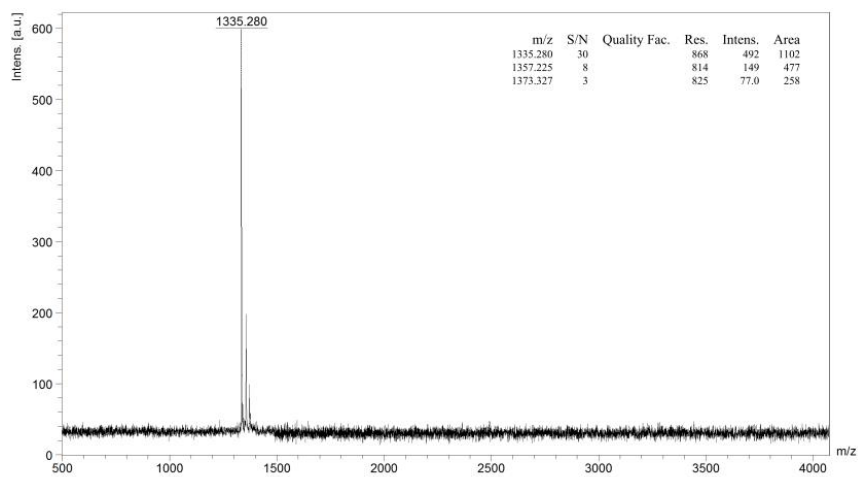
$(C_{14})^5$
Mw: 1420.77 g/mol
[MH⁺]: 1421.534



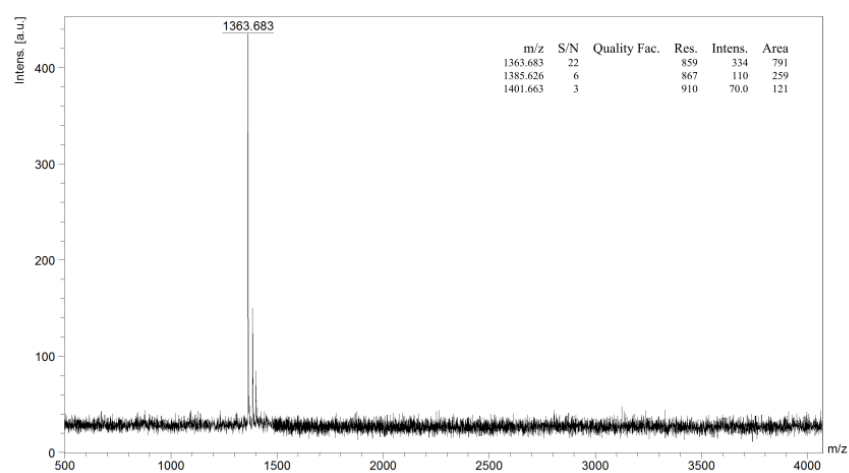
$(C_4)^7$
Mw: 1306.54 g/mol
[MH⁺]: 1307.750



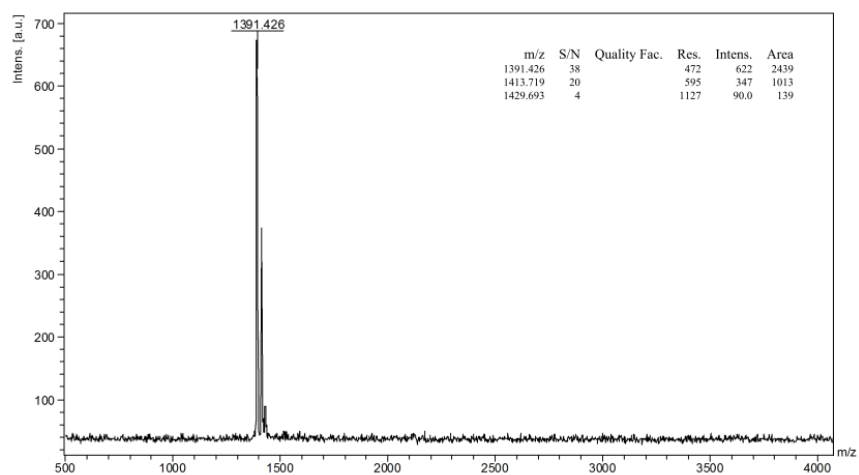
$(C_6)^6$
Mw: 1334.59 g/mol
[MH⁺]: 1335.280



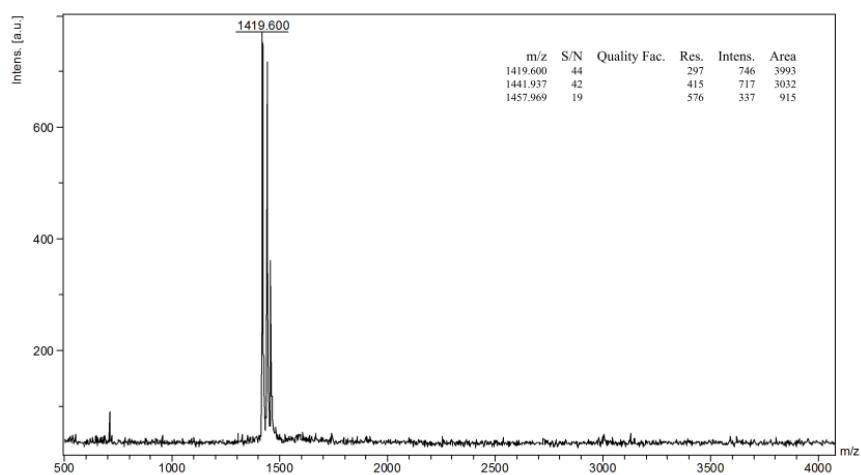
$(C_8)^7$
Mw: 1362.65 g/mol
[MH⁺]: 1363.683



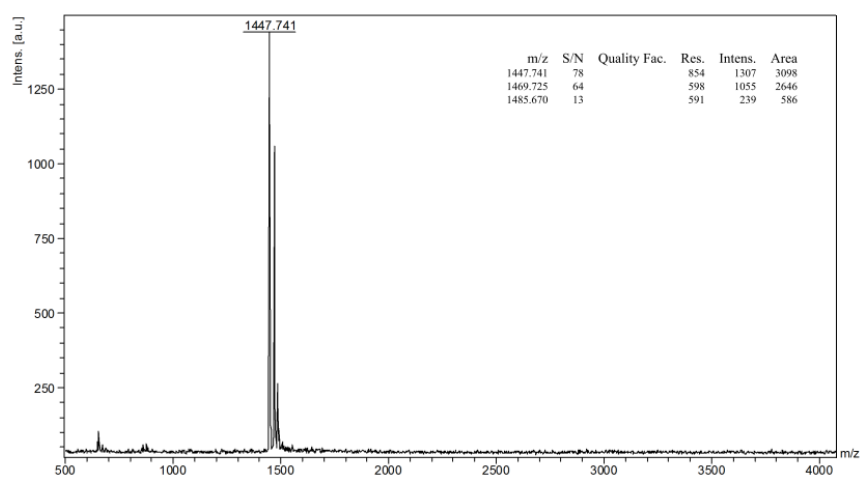
$(C_{10})^7$
Mw: 1390.70 g/mol
[MH⁺]: 1391.426



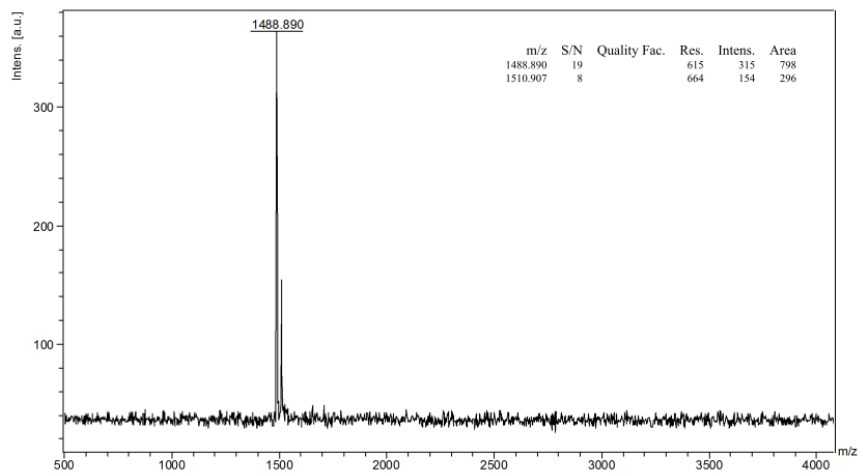
$(C_{12})^7$
Mw: 1418.75 g/mol
[MH⁺]: 1419.600



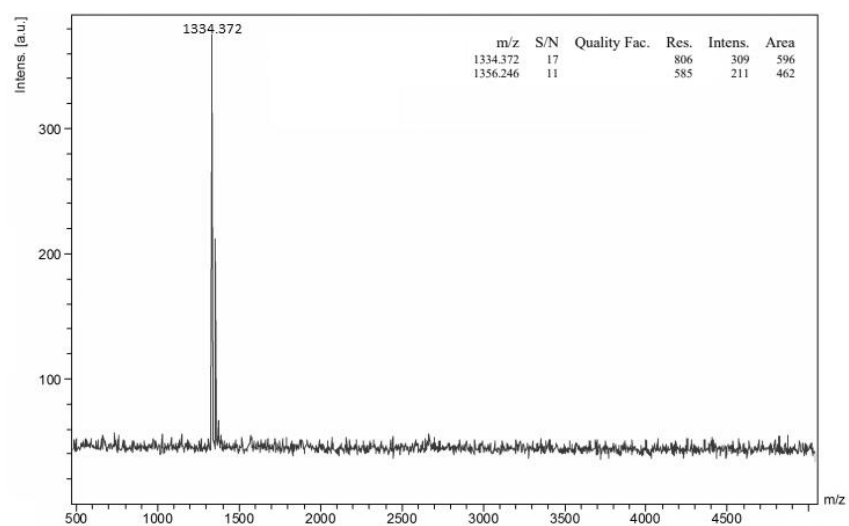
$(C_{14})^7$
Mw: 1446.81 g/mol
[MH⁺]: 1447.741



$(C_{10})^8$
Mw: 1487.82
[MH⁺]: 1488.890



S3(B)
Mw: 1333.68
[MH⁺]: 1332.910



m/z: mass/charge ratio; S/N: Signal/Noise ratio; Mw: Molecular weight.