

Supporting Information

Supplemental tables:

Table S1. The amino acid sequences and chemical formulas of cyclopeptides.

Table S2. Cyclolinopeptide recovery from gum/phosphoric acid residues after acid degumming of flaxseed oil.

Supplemental figures:

Figure S1. The structures of cyclopeptides. Taken from Gui et al. (2012)²⁰ with permission.

Figure S2. Flaxseed fractions after water degumming and manual dissection: (A) whole seed (B) mucilage (C) cotyledon, and (D) seed coat.

Figure S3. Products after cold pressing of flaxseed: (A) whole seed, (B) flaxseed meal, (C) crude oil after settling, and (D) sediment separated from crude oil.

Supplemental file:

File S1. Electrospray ionization mass spectrometry spectra of standard Seg-A and cyclolinopeptides

The standard peptide was prepared in a solution containing 90% methanol, 10% water and 0.1% formic acid in a total volume of 1 mL for mass spectrometry (MS) analysis. MS analysis was performed on a Hybrid Quadrupole-TOF LC/MS/MS system. The solution was introduced into the turbo ion electrospray spectrometer source by loop injection at a rate of 5 μ L per min. Ion scanning experimental data was acquired with the pulsing function turned on, using a dwell time of 50 ms and the step size of one Dalton. All signals were created and analyzed by the Analyst QS 1.1 software.

Table S1. The Amino Acid Sequences and Chemical Formulas of Cyclopeptides

cyclopeptide (code)	amino acid sequence ^a	molecular formula	protonated ion mass (m/z) ^b
Seg-A	<i>cyclo</i> -(Gly-Val-Pro-Val-Trp-Ala)	C ₃₁ H ₄₃ N ₇ O ₆	610.32 ²⁰
Cyclolinopeptide A (1)	<i>cyclo</i> -(Ile-Leu-Val-Pro-Pro-Phe-Phe-Leu-Ile)	C ₅₇ H ₈₅ N ₉ O ₉	1040.65 ¹
Cyclolinopeptide B (2)	<i>cyclo</i> -(Met-Leu-Ile-Pro-Pro-Phe-Phe-Val-Ile)	C ₅₆ H ₈₃ N ₉ O ₉ S	1058.61 ⁶
Cyclolinopeptide C (3)	<i>cyclo</i> -(Mso-Leu-Ile-Pro-Pro-Phe-Phe-Val-Ile)	C ₅₆ H ₈₃ N ₉ O ₁₀ S	1074.56 ⁶
Cyclolinopeptide D (4)	<i>cyclo</i> -(Mso-Leu-Leu-Pro-Phe-Phe-Trp-Ile)	C ₅₇ H ₇₇ N ₉ O ₉ S	1064.54 ⁶
Cyclolinopeptide E (5)	<i>cyclo</i> -(Mso-Leu-Val-Phe-Pro-Leu-Phe-Ile)	C ₅₁ H ₇₆ N ₈ O ₉ S	977.52 ⁶
Cyclolinopeptide F (6)	<i>cyclo</i> -(Mso-Leu-Mso-Pro-Phe-Phe-Trp-Val)	C ₅₅ H ₇₃ N ₉ O ₁₀ S ₂	1084.47 ⁷
Cyclolinopeptide G (7)	<i>cyclo</i> -(Mso-Leu-Mso-Pro-Phe-Phe-Trp-Ile)	C ₅₆ H ₇₅ N ₉ O ₁₀ S ₂	1098.50 ⁷

Taken from Gui et al. (2012)²⁰ with permission.

^a The first and/or third positions of amino acid sequences are displayed in Figure S1. Abbreviations are Met for methionine and Mso for methionine sulfoxide.

^b From reference and ESI-MS data obtained as described in File S1 (Supplemental file).

Table S2. Cyclolinopeptide Recovery from Gum/phosphoric Acid Residues After Acid Degumming of Flaxseed Oil

fraction (n=3) ^a	concentration of cyclolinopeptides (µg/g)							
	1	2	3	4	5	6	7	Total
Gum/phosphoric acid ^b	238.5 ± 3.9	ND ^c	250.2 ± 7.7	ND	233.4 ± 10.9	13.4 ± 1.5	24.0 ± 2.6	759.5 ± 26.6
Crude oil ^d	454.0 ± 16.1	90.5 ± 7.8	358.3 ± 15.5	214.1 ± 4.3	445.5 ± 14.7	82.4 ± 4.5	249.7 ± 3.7	1894.6 ± 66.6

^a Fraction separations after refining treatments were repeated three times.

^b Cyclolinopeptides recovery from the gum/phosphoric acid of equivalent to 1 mL oil

^c Not detected by HPLC.

^d Crude oil from the same fresh oil (Table 4, VI) without treatment.

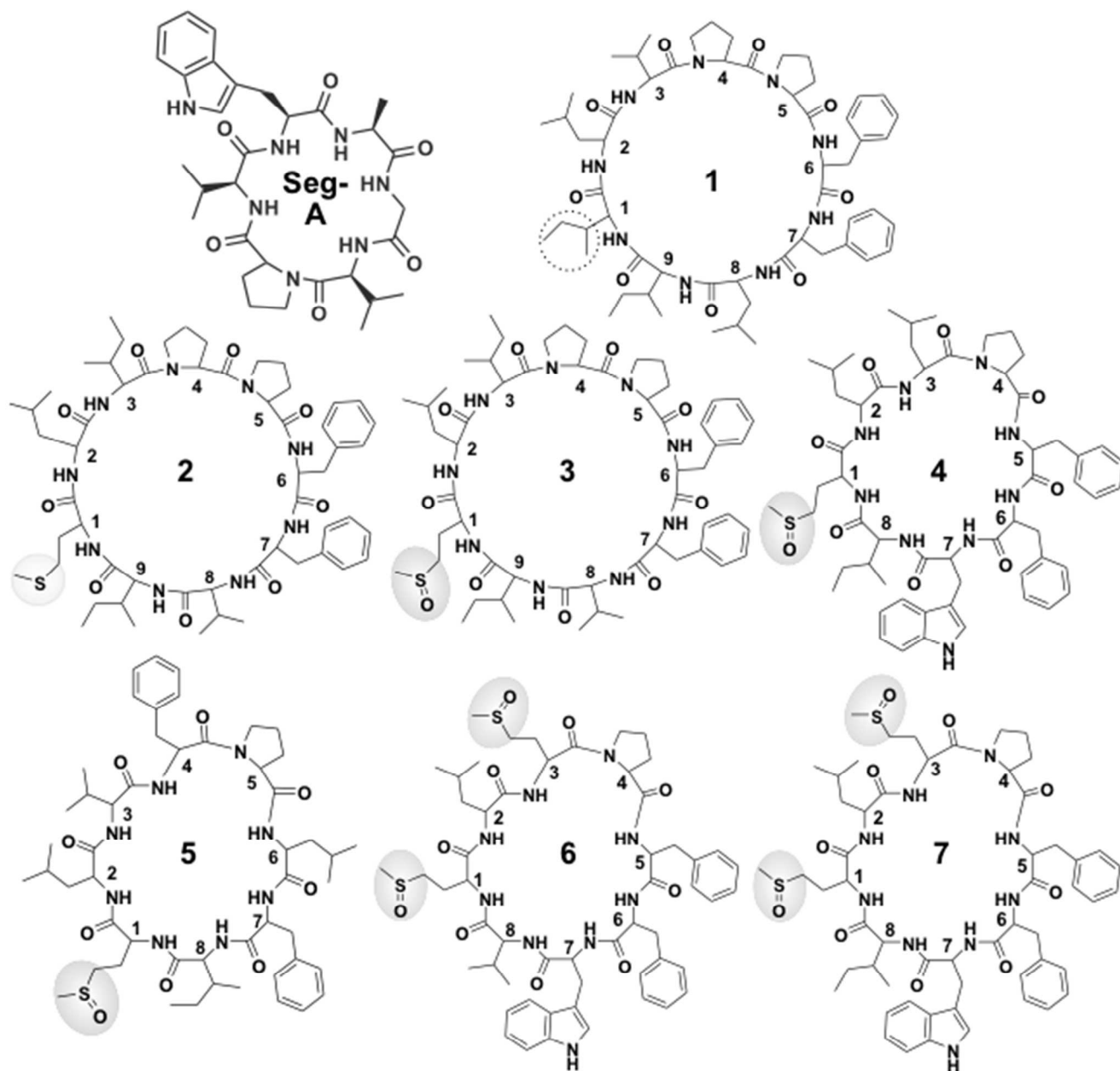


Figure S1.



(A)



(B)



(C)



(D)

Figure S2.



(A)



(B)

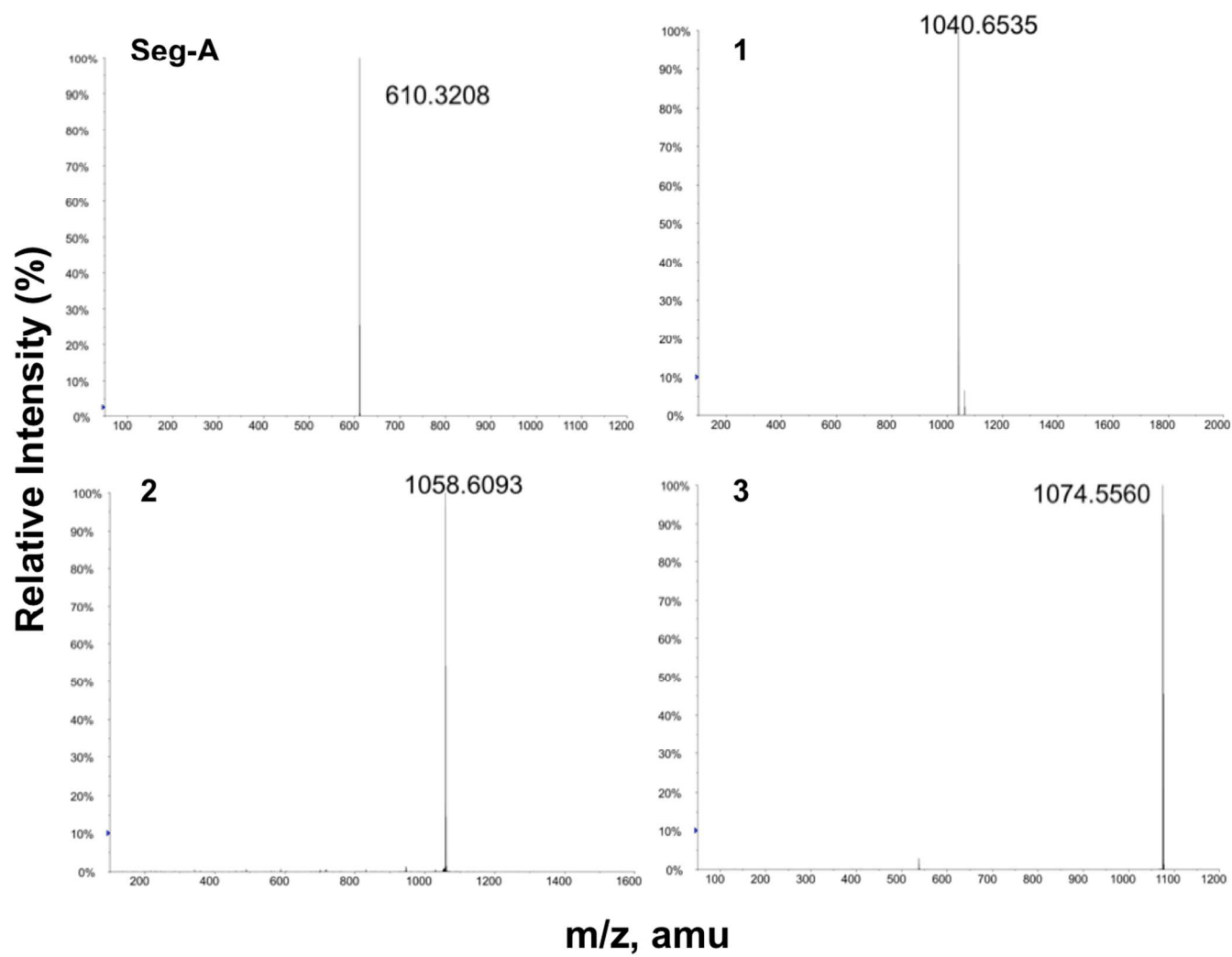


(C)



(D)

Figure S3.



File S1.

