Supplementary information

Polyunsaturated Fatty Acid-Rich Waste Vegetable Oil-Derived Bio-Based Zwitterionic Surfactants with High Interfacial Activity for Enhanced Oil Recovery

Xue-Mei Zhang[1], Shi-Zhong Yang*[1, 2, 3], Homely Isaya Mtui[1], Bo-Zhong Mu[1, 2, 3]

[1] State Key Laboratory of Bioreactor Engineering, School of Chemistry and Molecular Engineering, East China University of Science and Technology, Shanghai 200237, P. R. China.

[2] Shanghai Collaborative Innovation Center for Biomanufacturing Technology, Shanghai 200237, P.R. China.

[3] MOE Engineering Research Center of Microbial Enhanced Oil Recovery, East China University of Science and Technology, Shanghai 200237, P. R. China.

* Corresponding author: Shi-Zhong Yang, Email: meor@ecust.edu.cn.

Supplementary Material Description

This supplementary material provides additional experimental data and analytical results that support the findings presented in the main manuscript. The content is organized into four main sections:

Section 1: Conversion rate calculation methods for the alkylation, amidation, and quaternization reactions are described. Two approaches are used: the internal standard method (Equation S1.1) and the peak area normalization method (Equation S1.2). The molecular mass information of intermediates and final products at each reaction step in the orthogonal experiment is also provided.

Section 2: GC-MS spectra of intermediate products obtained during the orthogonal experiments are presented, along with selected peak area data used to calculate the conversion rates. Additionally, HPLC-MS and ESI-MS spectra of the final surfactant products are included to confirm the molecular identity.

Section 3: GC-MS, HPLC-MS, and ESI-MS spectra of surfactants synthesized from mixed fatty acids with varying PUFA contents are provided. All syntheses were performed using the optimal reagent combination: phenyl methyl ether, *N,N*-dimethylethylenediamine, and sodium 3-chloro-2-hydroxypropane sulfonate.

Section 4: GC-MS, HPLC-MS, and ESI-MS spectra of surfactants synthesized from different waste vegetable oils (e.g., waste rapeseed oil, gutter oil, soybean oil) are presented. These reactions were also conducted using the optimal reagent combination: phenyl methyl ether, *N,N*-dimethylethylenediamine, and sodium 3-chloro-2-hydroxypropane sulfonate.

1 The calculation formulas for the conversion rates of each step and the molecular weights of the products of each step in the orthogonal experiment

1.1 The calculation formulas for the conversion rates of each step

The Internal Standard Method compares the peak areas of the product and reactant relative to the internal standard, while the Normalization Method calculates the conversion rate based on the relative peak areas of the product and reactant, normalized by the total peak area in the system. The conversion rates for both methods are calculated as follows:

$$\text{Conversion Rate}=\left[1-\frac{\left(\frac{A_{\text{reaction}}}{A_{\text{IS}}}\right)_{\text{after reaction}}}{\left(\frac{A_{\text{reaction}}}{A_{\text{IS}}}\right)_{\text{before reaction}}}\right]\times 100\% \quad \textbf{(S1.1)}$$

and

$$\text{Conversion Rate}=\frac{\sum A_{\text{converted}}}{\sum A_{\text{total}}}\times 100\% \quad \textbf{(S1.2)}$$

where A_{reaction} and A_{IS} represent the peak areas of the reactant and internal standard, respectively. (In the alkylation reaction, methyl palmitate is the internal standard, while in the quaternization reaction, the alkylation product is the internal standard.) In the normalization method, $A_{\text{converted}}$ is the peak area of the converted products, and A_{total} is the total peak area of both the reactants and products. The conversion rates of each step's product and the final product are shown in the text.

1.2 The molecular weights of the products of each step in the orthogonal experiment and the mass-to-charge ratios of the final products

Table S1 The mass-to-charge ratios of the surfactant and the molecular weights of the products at each step of the synthesis process.

Serial number	Main alkylation products	Main amidation products	Main quaternization products	Mass-to-charge ratio of the target products		
	[M]	[M]	[M]	(+)m/z[M-NaCl+H^+]	(+)m/z [M-Cl^-]	(-)m/z[M-NaCl+$HCOO^-$]
1	374*,372*,270*	430,428,326	626.5,624.5,522.5	569,567,465	591,589,487	613,611,509
2	374,372,270	444,442,340	560.5,558.5,456.5	503,501,399	525,523,421	547,545,443
3	374,372,270	472,470,368	643.5,641.5,539.5	609,607,505	631,629,527	653,651,549
4	404,402,270	460,458,326	576.5,574.5,442.5	519,517,385	541,539,407	563,561,429
5	404,402,270	474,472,340	645.5,643.5,511.5	611,609,477	633,631,499	655,653,521
6	404,402,2	502,500,	698.5,696.5,564.5	641,639,507	663,661,529	685,683,551

	70	368				
7	388,386,270	444,442,326	615.5,613.5,497.5	581,579,463	603,601,485	625,623,507
8	388,386,270	458,456,340	654.5,652.5,536.5	597,595,479	619,617,501	641,639,523
9	388,386,270	486,484,368	602.5,600.5,484.5	545,543,427	567,565,449	589,587,471

Notes:

(1) The numbers 374*, 372*, and 270* represent products in the orthogonal experiment synthesized using methyl oleate (C18:1), methyl linoleate (C18:2), and methyl palmitate (C16:0), respectively.

(2) The data in the table are listed in the order of methyl oleate, methyl linoleate, and methyl palmitate as raw materials.

2 GC-MS, HPLC-MS, and ESI-MS spectra of surfactants synthesized from different raw materials in orthogonal experiment (M_1, M_2, and M_3 represent products derived from methyl oleate, methyl linoleate, and methyl palmitate, respectively—note that M_1, M_2, and M_3 refer to different products in each step, with varying structures and molecular weights, although they originate from the same raw materials)

2.1 The GC-MS, HPLC-MS, and ESI-MS spectra of products synthesized from raw materials with a low linoleic/oleic acid ratio

2.1.1 Combination 1: Benzene as the alkylation reagent, N,N-dimethylethylenediamine as the amidation reagent, and sodium 3-chloro-2-hydroxypropane sulfonate as the quaternization reagent

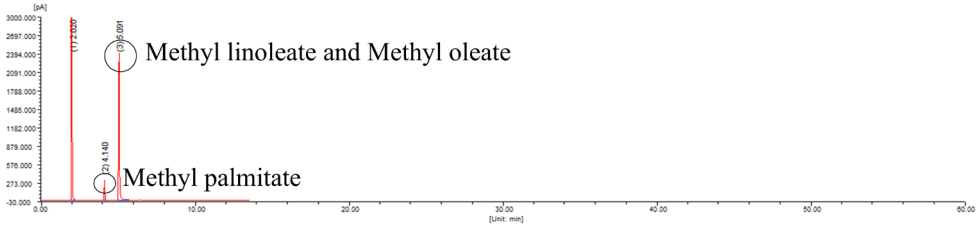

Fig. S1 Gas chromatogram of the mixed fatty acid raw materials.

Table S2 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.140	5.091
Integrated peak area	1078463.3	10316402.9

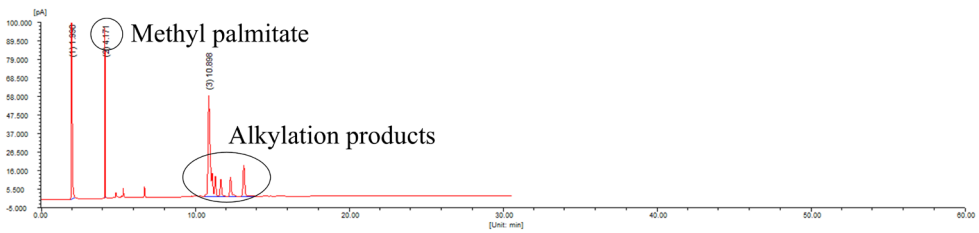

Fig. S2 Gas chromatogram of the product after the alkylation reaction.

Table S3 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.171	5.091

Integrated peak area	175007.1	31952.4

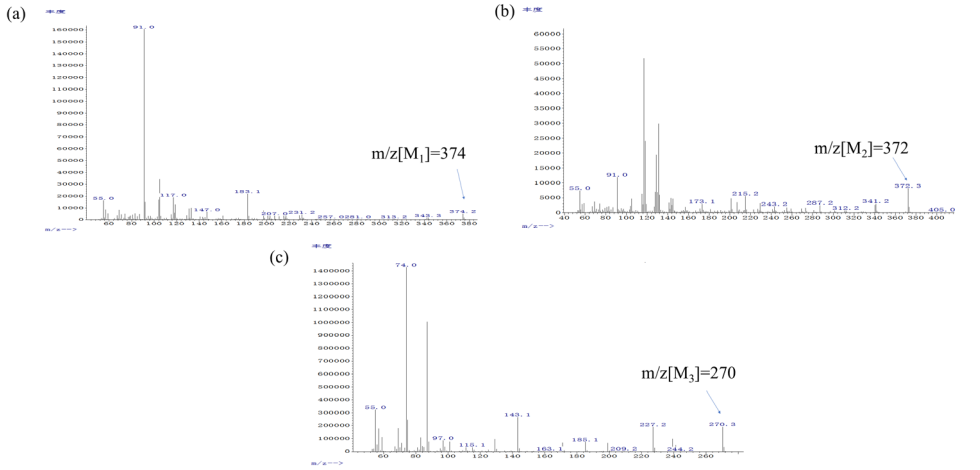

Fig. S3 Mass spectrum of the product after alkylation reaction.

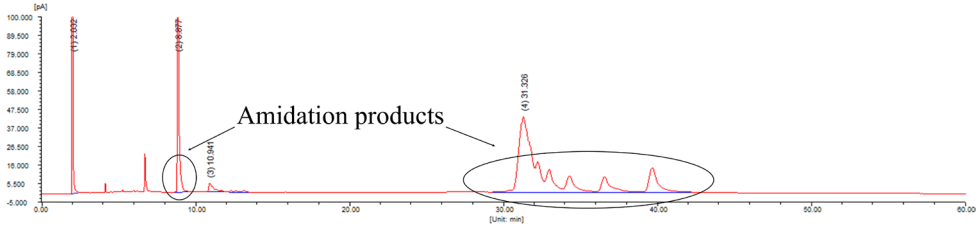

Fig. S4 Gas chromatogram of products after the amidation reaction.

Table S4 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	9.0~15.0	25.0~46.0
Integrated peak area	170983	4788911

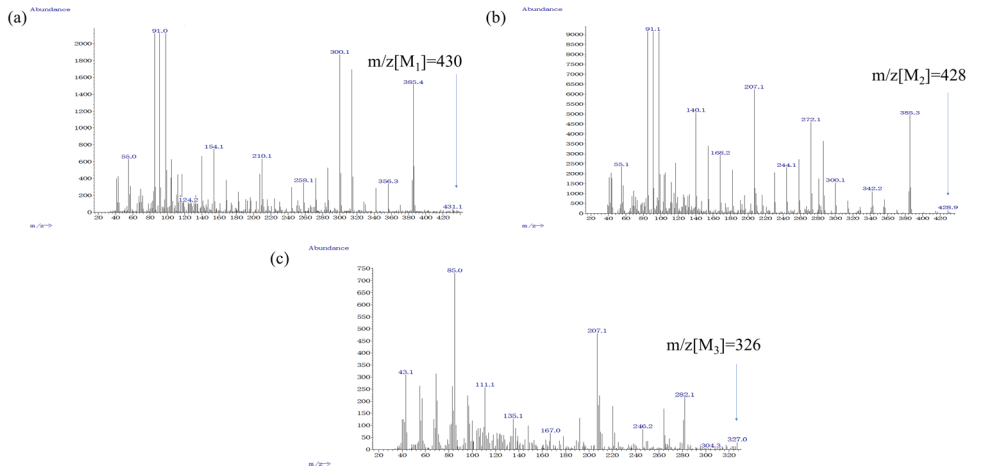

Fig. S5 Mass spectrum of the product after amidation reaction.

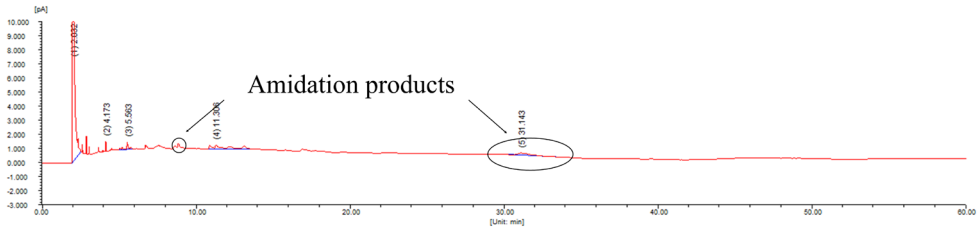

Fig. S6 Gas chromatogram of the product after the quaternization reaction.

Table S5 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	9.0~15.0	25.0~46.0
Integrated peak area	20139.8	17865.1

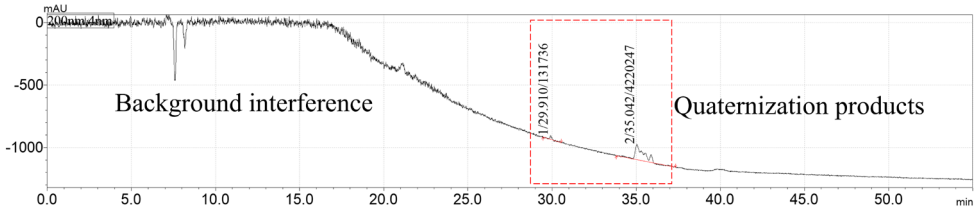

Fig. S7 Liquid chromatogram in liquid chromatography–mass spectrometry test of the first combination product derived from low-linoleic-acid-content raw materials.

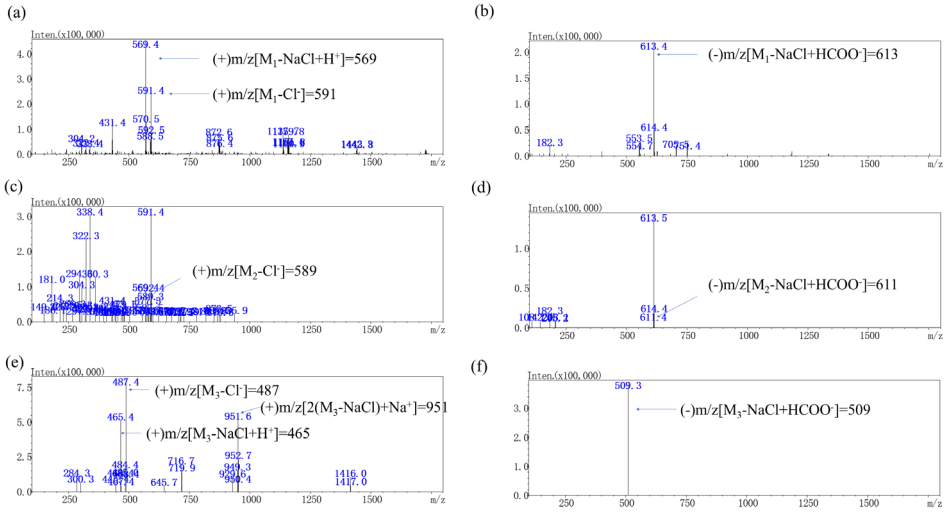

Fig. S8 Mass spectrum of the first combination product derived from low-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

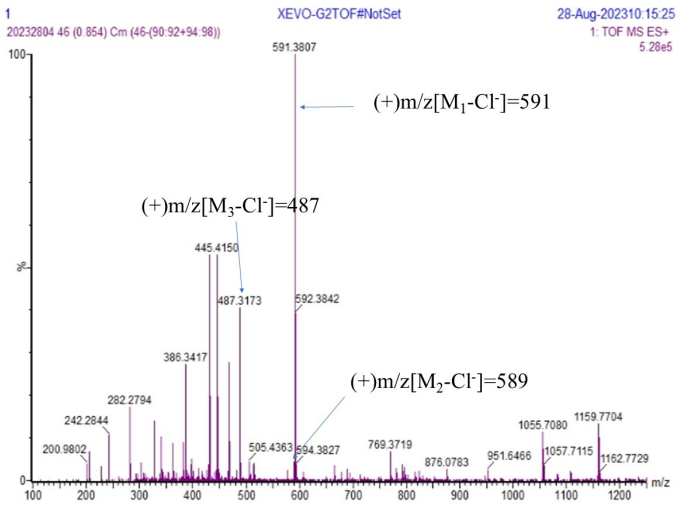

Fig. S9 Electrospray mass spectrum of the product prepared from the first combination of raw materials with a low linoleic acid content.

2.1.2 Combination 2: Benzene was used as the alkylation reagent, N,N-dimethyl-1,3-propanediamine as the amidation reagent, and sodium chloroacetate as the quaternization reagent

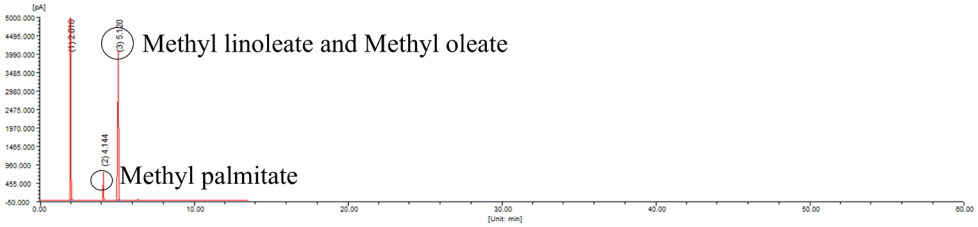

Fig. S10 Gas chromatogram of the mixed fatty acid raw materials.

Table S6 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.144	5.120
Integrated peak area	1813963.3	16863411.3

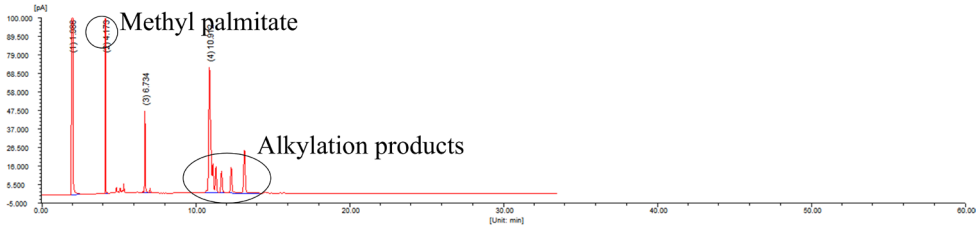

Fig. S11 Gas chromatogram of the product after the alkylation reaction.

Table S7 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.173	5.120
Integrated peak area	239058.8	45659.0

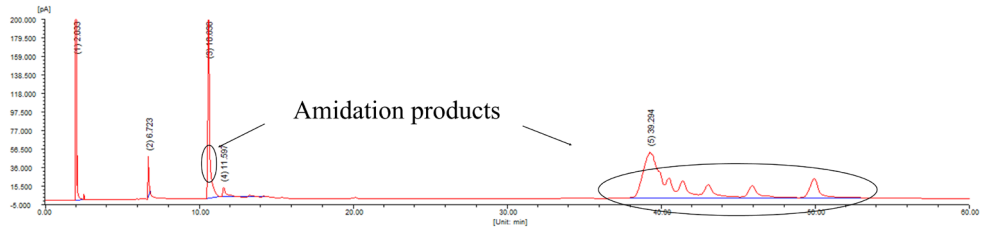

Fig. S12 Gas chromatogram of products after the amidation reaction.

Table S8 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	9.0~15.0	36.0~58.0
Integrated peak area	877757.7	7956969.0

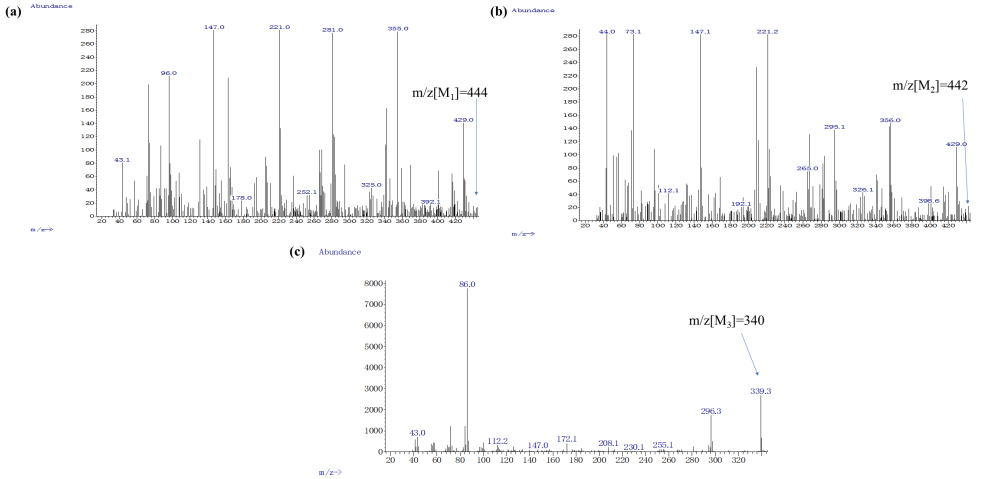

Fig. S13 Mass spectrum of the product after amidation reaction.

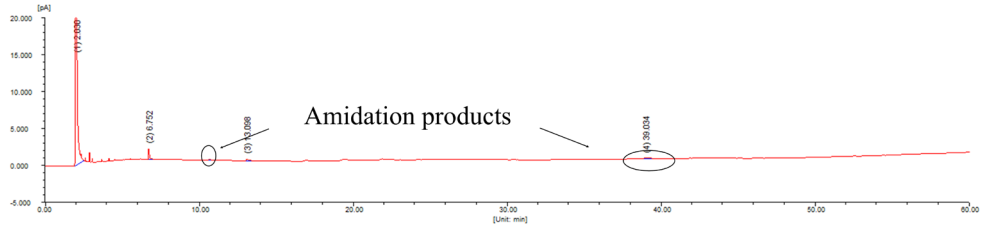

Fig. S14 Gas chromatogram of the product after the quaternization reaction.

Table S9 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	9.0~15.0	36.0~58.0
Integrated peak area	9870.3	7869.7

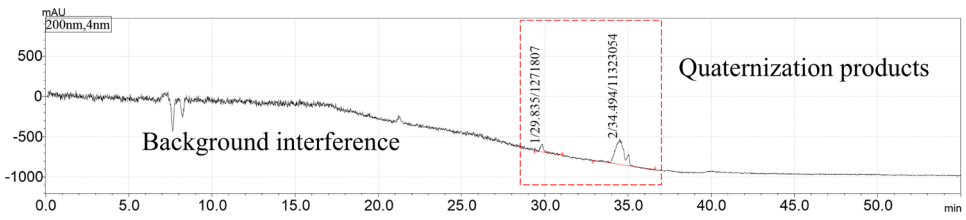

Fig. S15 Liquid chromatogram in liquid chromatography–mass spectrometry test of the second

combination product derived from low-linoleic-acid-content raw materials.

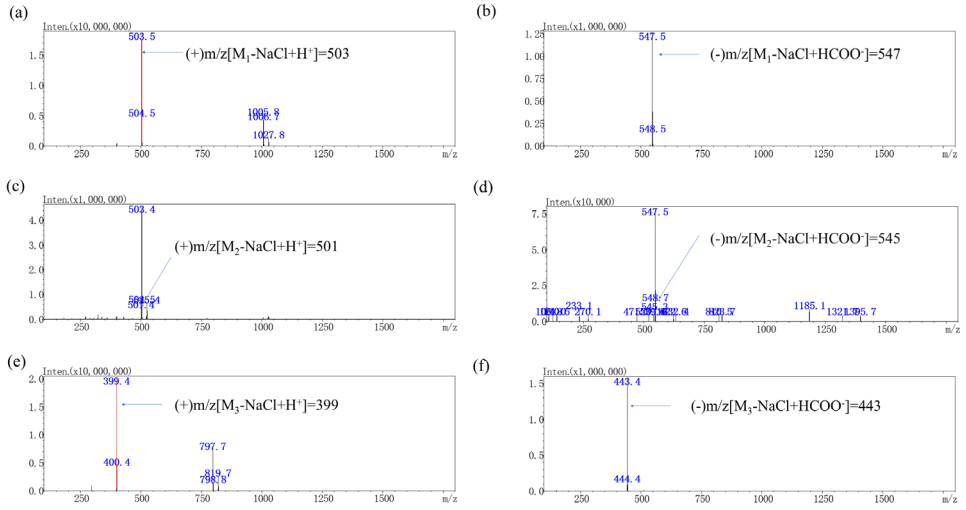

Fig. S16 Mass spectrum of the second combination product derived from low-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

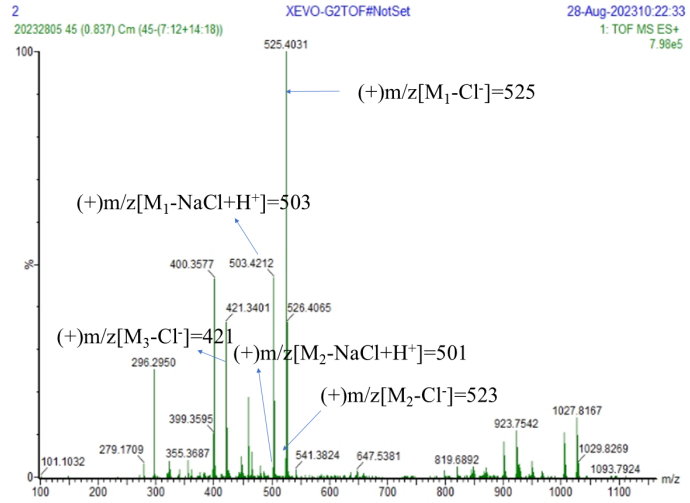

Fig. S17 Electrospray mass spectrum of the product prepared from the second combination of raw materials with a low linoleic acid content.

2.1.3 Combination 3: Benzene was used as the alkylation reagent, N,N-diethyl-1,3-propanediamine as the amidation reagent, and butanesultone as the quaternization reagent

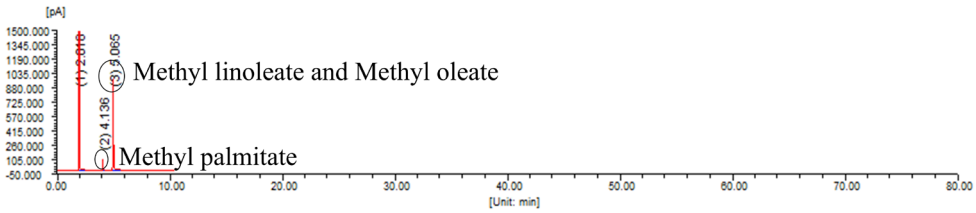

Fig. S18 Gas chromatogram of the mixed fatty acid raw materials.

Table S10 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.136	5.065

Integrated peak area	367221.3	3586844.3

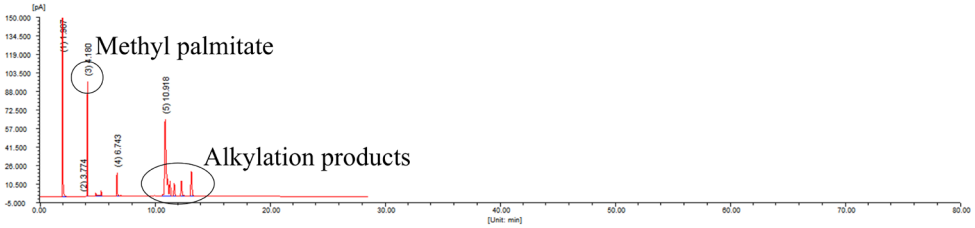

Fig. S19 Gas chromatogram of the product after the alkylation reaction.

Table S11 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.180	5.065
Integrated peak area	181789.8	36869.1

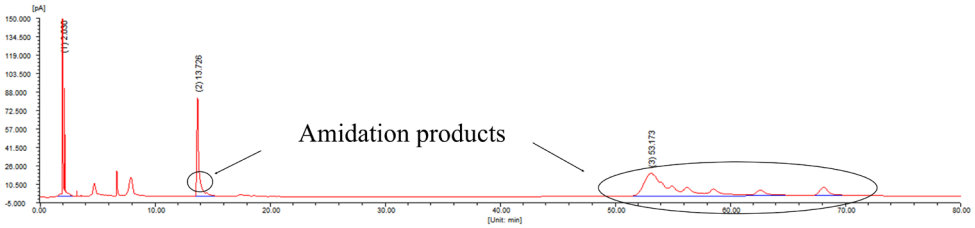

Fig. S20 Gas chromatogram of products after the amidation reaction.

Table S12 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	9.0~15.0	50.0~72.0
Integrated peak area	84707.3	4419045.4

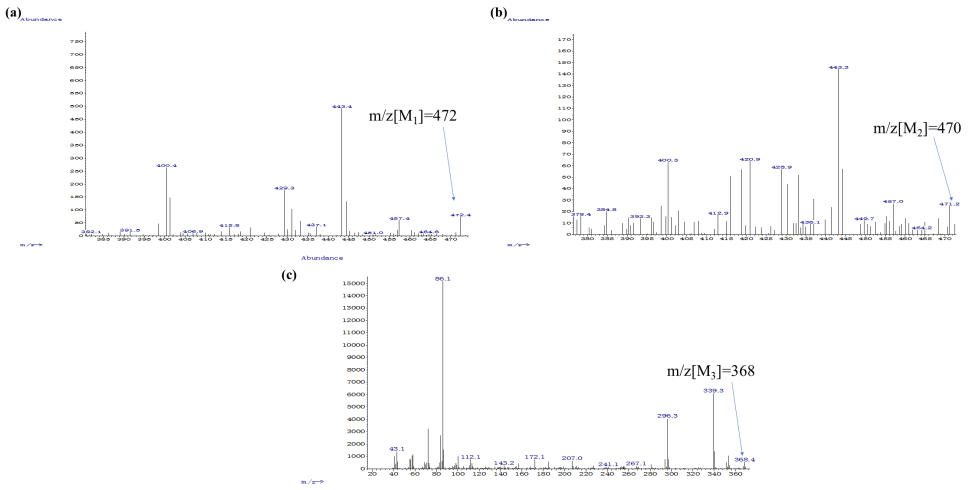

Fig. S21 Mass spectrum of the product after amidation reaction.

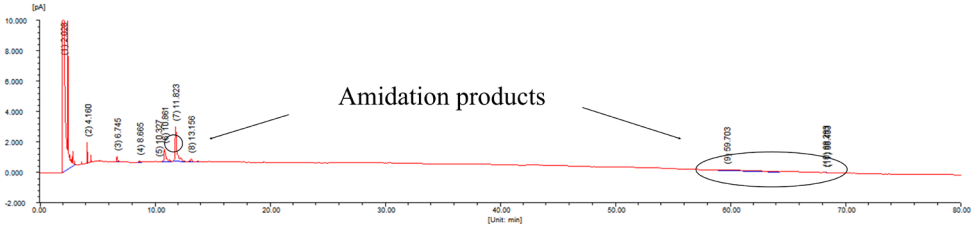

Fig. S22 Gas chromatogram of the product after the quaternization reaction.

Table S13 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	9.0~15.0	50.0~72.0
Integrated peak area	43987.9	9285.3

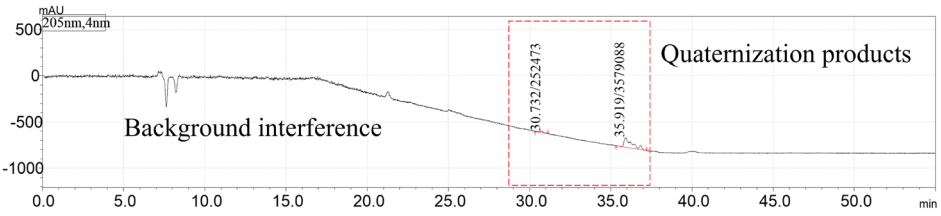

Fig. S23 Liquid chromatogram in liquid chromatography–mass spectrometry test of the third combination product derived from low-linoleic-acid-content raw materials.

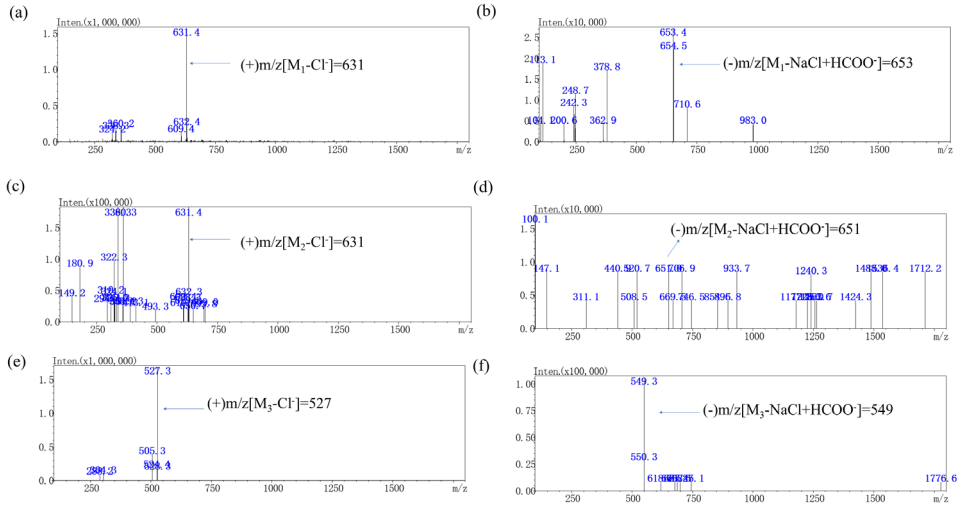

Fig. S24 Mass spectrum of the third combination product derived from low-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

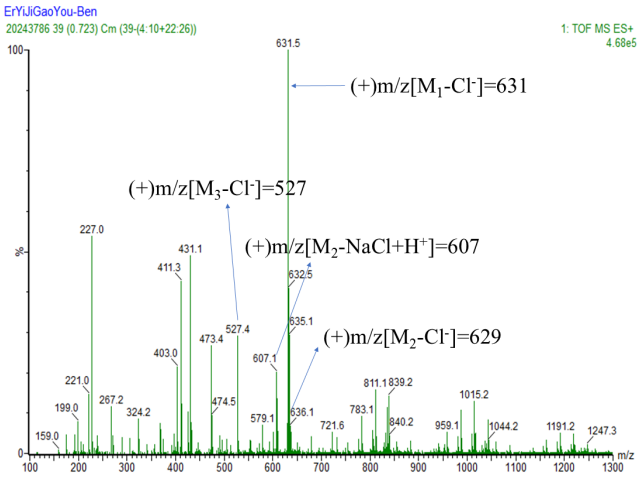

Fig. S25 Electrospray mass spectrum of the product prepared from the third combination of raw materials with a low linoleic acid content.

2.1.4 Combination 4: Anisole was used as the alkylation reagent, N,N-dimethylethylenediamine as the amidation reagent, and sodium chloroacetate as the quaternization reagent

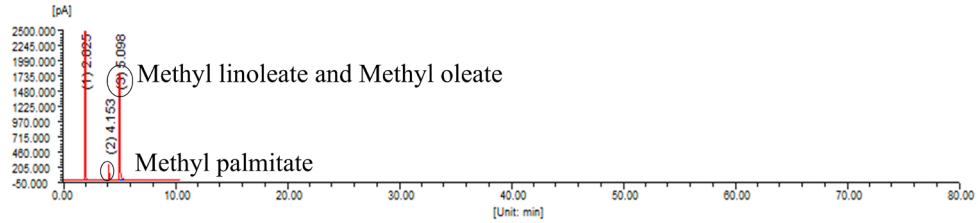

Fig. S26 Gas chromatogram of the mixed fatty acid raw materials.

Table S14 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.153	5.098
Integrated peak area	952159.4	9177456.7

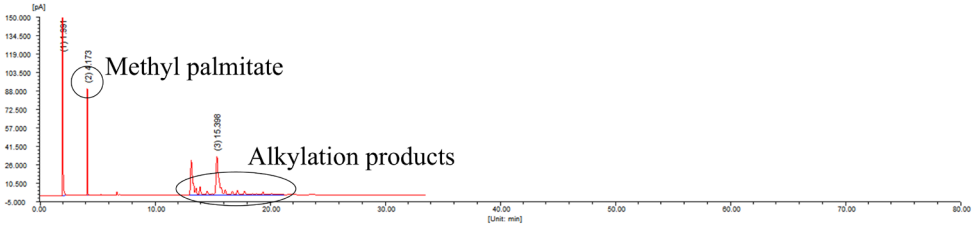

Fig. S27 Gas chromatogram of the product after the alkylation reaction.

Table S15 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.173	5.098
Integrated peak area	178839.3	6948.3

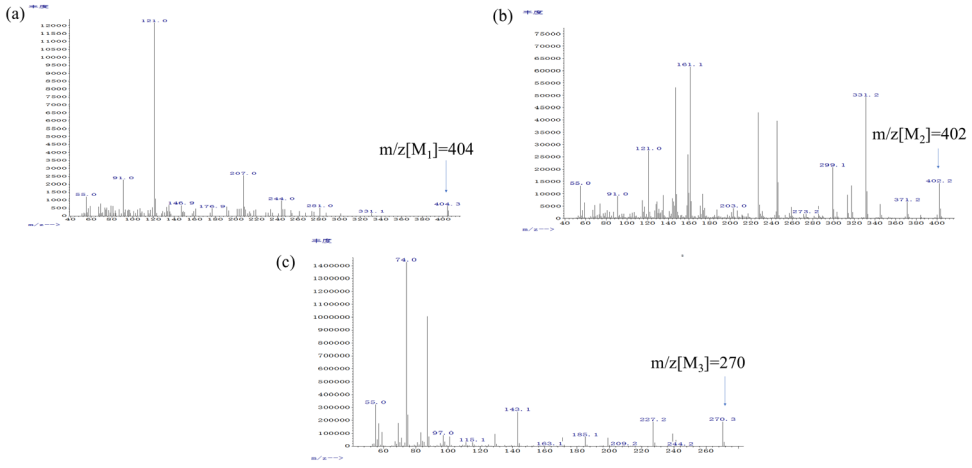

Fig. S28 Mass spectrum of the product after alkylation reaction.

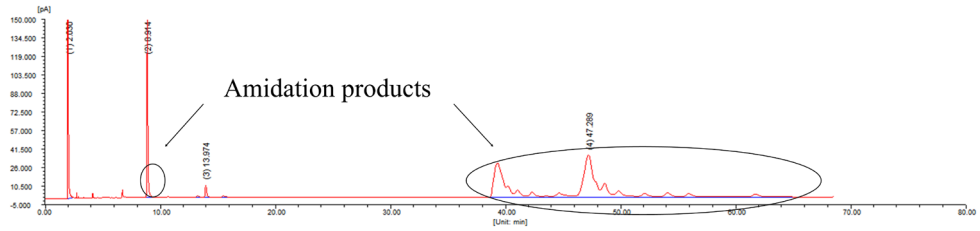

Fig. S29 Gas chromatogram of products after the amidation reaction.

Table S16 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	12.0~25.0	38.0~68.0
Integrated peak area	220599.1	6345955.8

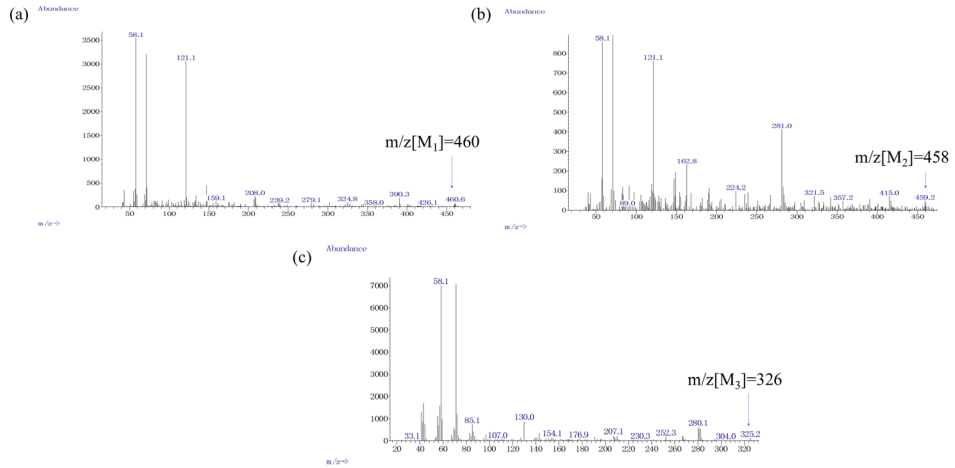

Fig. S30 Mass spectrum of the product after amidation reaction.

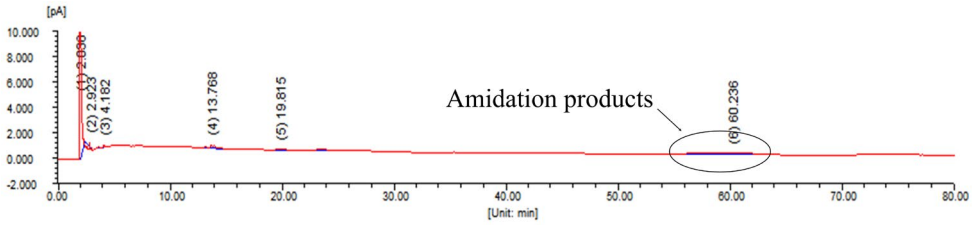

Fig. S31 Gas chromatogram of the product after the quaternization reaction.

Table S17 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	12.0~25.0	38.0~68.0
Integrated peak area	22607.8	55924

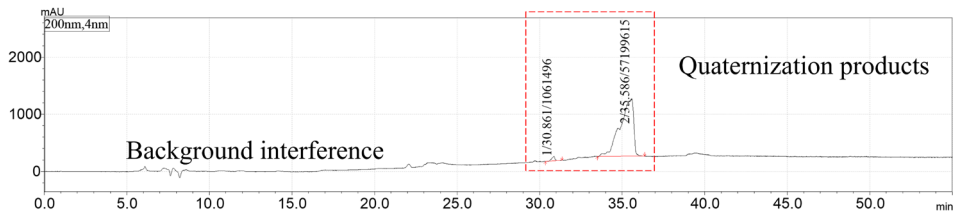

Fig. S32 Liquid chromatogram in liquid chromatography–mass spectrometry test of the fourth

combination product derived from low-linoleic-acid-content raw materials.

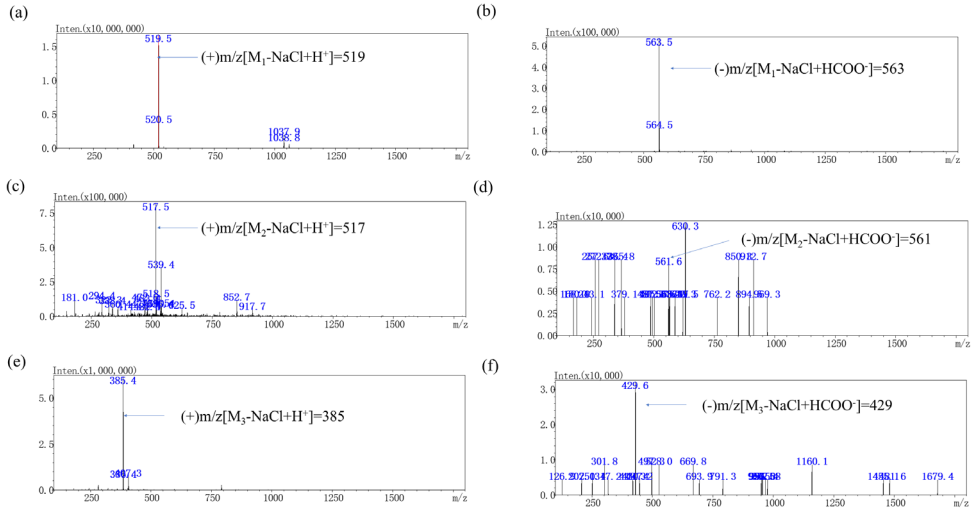

Fig. S33 Mass spectrum of the fourth combination product derived from low-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

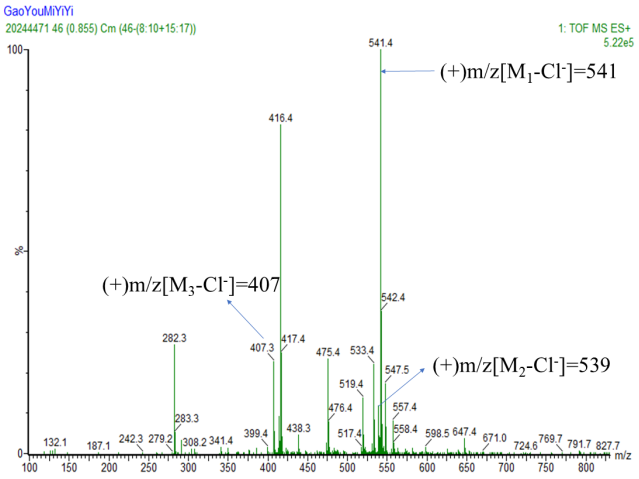

Fig. S34 Electrospray mass spectrum of the product prepared from the fourth combination of raw materials with a low linoleic acid content.

2.1.5 Combination 5: Anisole was used as the alkylation reagent, N,N-dimethyl-1,3-propanediamine as the amidation reagent, and butanesultone as the quaternization reagent

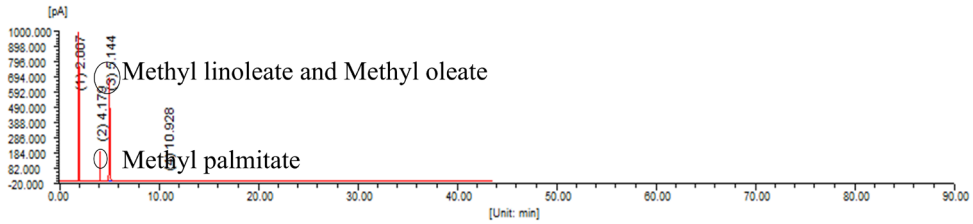

Fig. S35 Gas chromatogram of the mixed fatty acid raw materials.

Table S18 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.179	5.144

Integrated peak area	585710.8	5719842.2

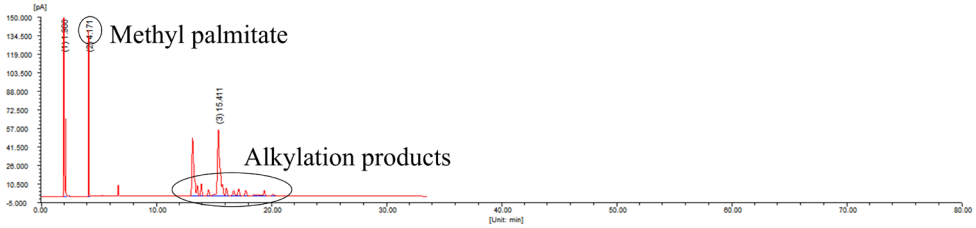

Fig. S36 Gas chromatogram of the product after the alkylation reaction.

Table S19 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.179	5.144
Integrated peak area	266361.0	6418.4

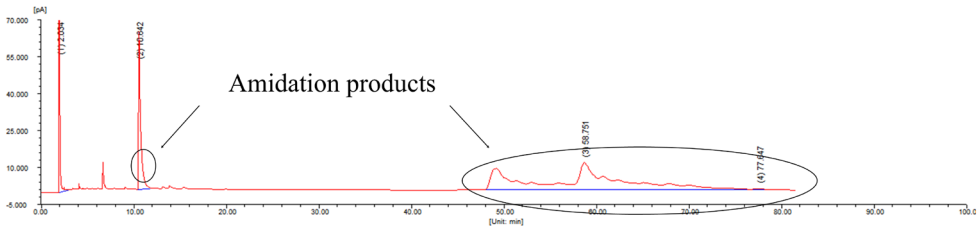

Fig. S37 Gas chromatogram of products after the amidation reaction.

Table S20 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	12.0~25.0	44.0~80.0
Integrated peak area	80186.5	5579051.5

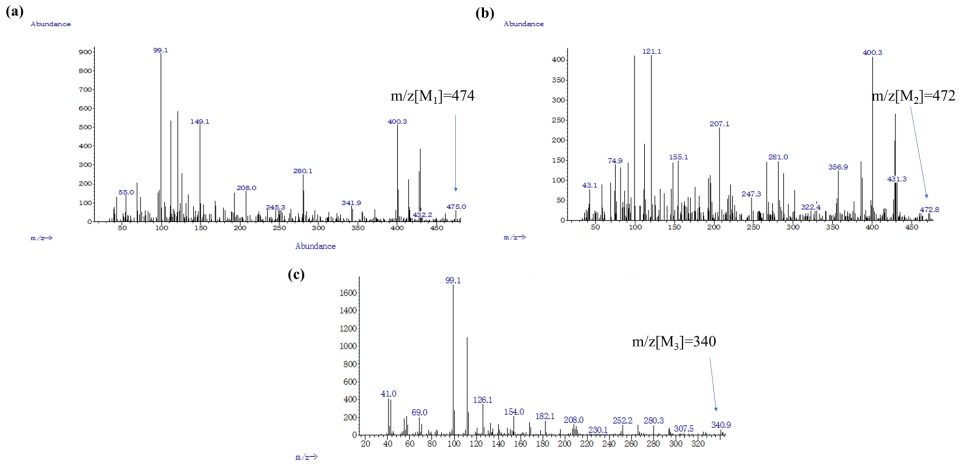

Fig. S38 Mass spectrum of the product after amidation reaction.

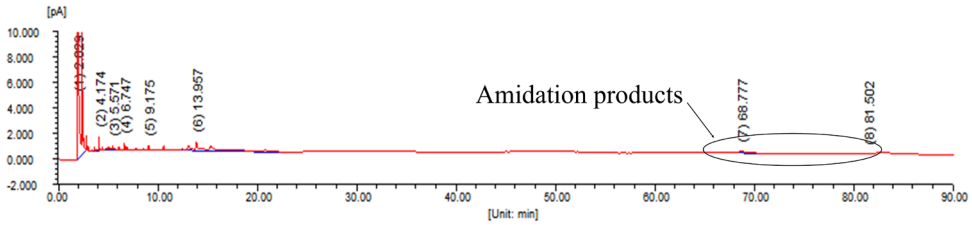

Fig. S39 Gas chromatogram of the product after the quaternization reaction.

Table S21 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	12.0~25.0	44.0~80.0
Integrated peak area	88189.1	25758.8

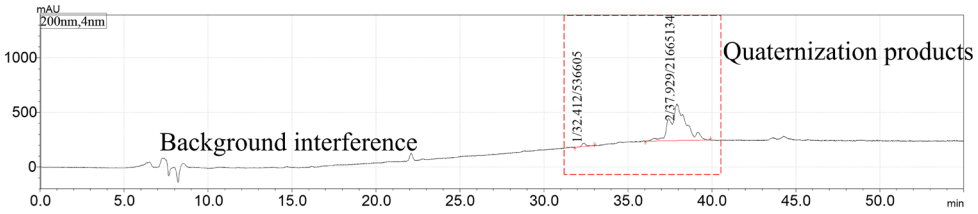

Fig. S40 Liquid chromatogram in liquid chromatography–mass spectrometry test of the fifth combination product derived from low-linoleic-acid-content raw materials.

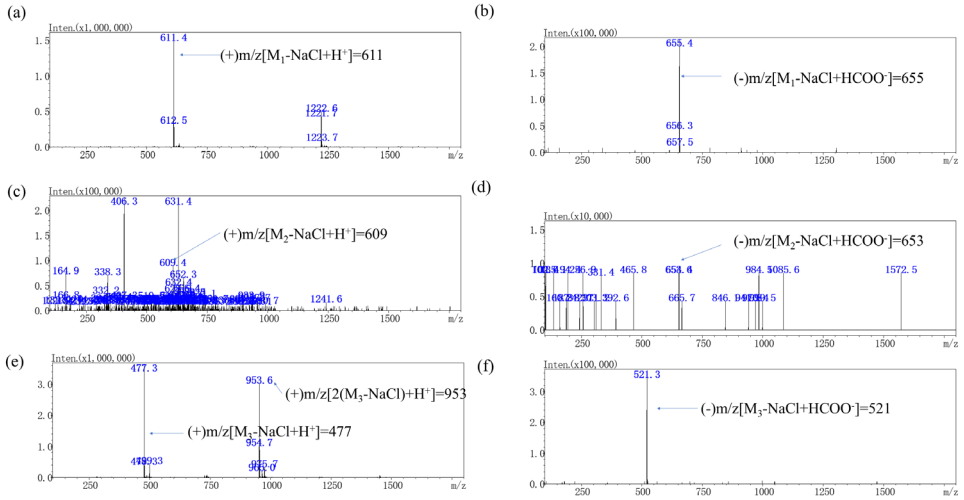

Fig. S41 Mass spectrum of the fifth combination product derived from low-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

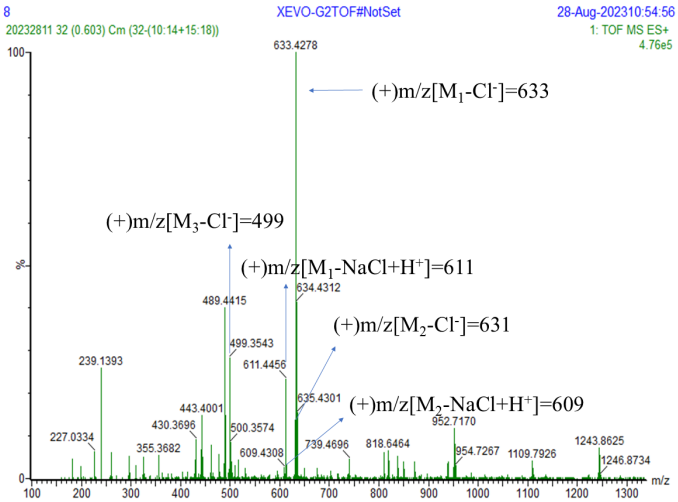

Fig. S42 Electrospray mass spectrum of the product prepared from the fifth combination of raw materials with a low linoleic acid content.

2.1.6 Combination 6: Anisole was used as the alkylation reagent, N,N-diethyl-1,3-propanediamine as the amidation reagent, and sodium 3-chloro-2-hydroxypropane sulfonate as the quaternization reagent

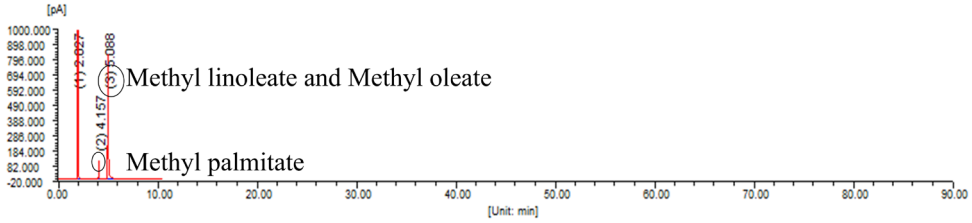

Fig. S43 Gas chromatogram of the mixed fatty acid raw materials.

Table S22 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.157	5.088
Integrated peak area	438269.4	4300048.4

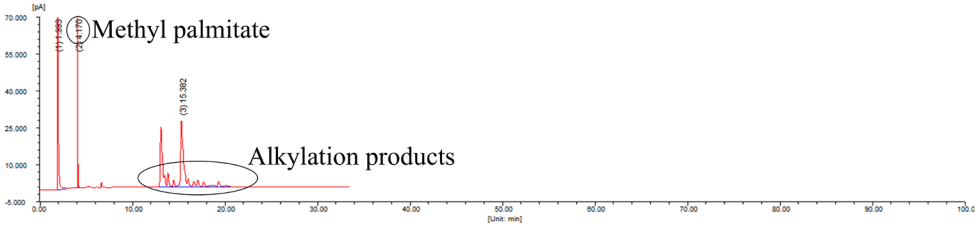

Fig. S44 Gas chromatogram of the product after the alkylation reaction.

Table S23 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.157	5.088
Integrated peak area	180483.8	4028.5

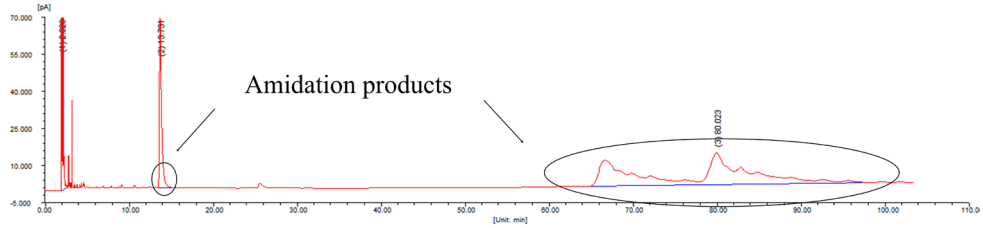

Fig. S45 Gas chromatogram of products after the amidation reaction.

Table S24 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	12.0~25.0	65.0~100.0
Integrated peak area	12810.1	7283430.2

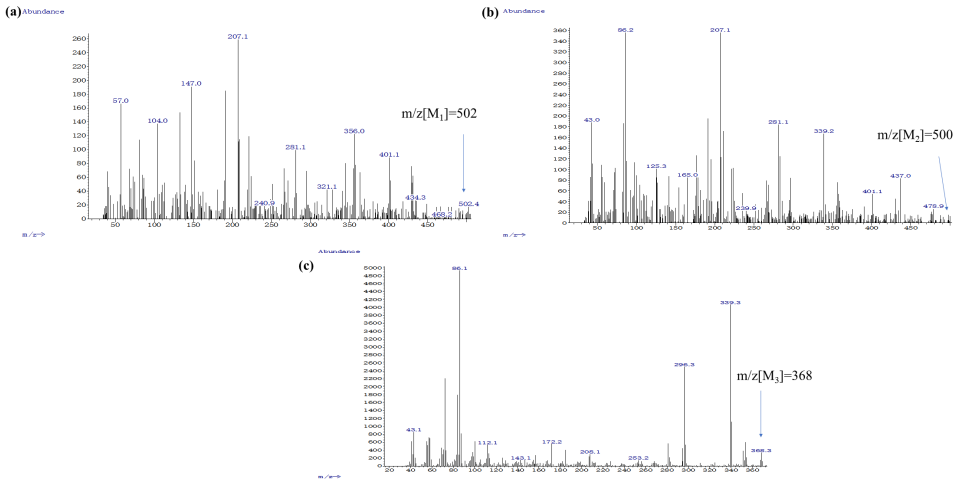

Fig. S46 Mass spectrum of the product after amidation reaction.

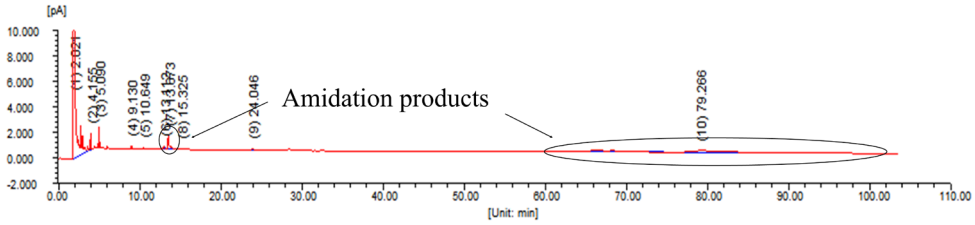

Fig. S47 Gas chromatogram of the product after the quaternization reaction.

Table S25 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	12.0~26.0	65.0~100.0
Integrated peak area	9373.5	34843.1

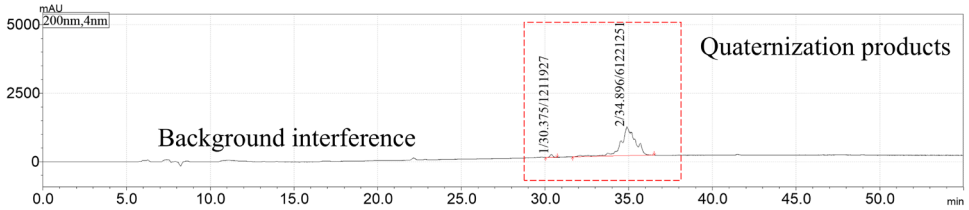

Fig. S48 Liquid chromatogram in liquid chromatography–mass spectrometry test of the sixth combination product derived from low-linoleic-acid-content raw materials.

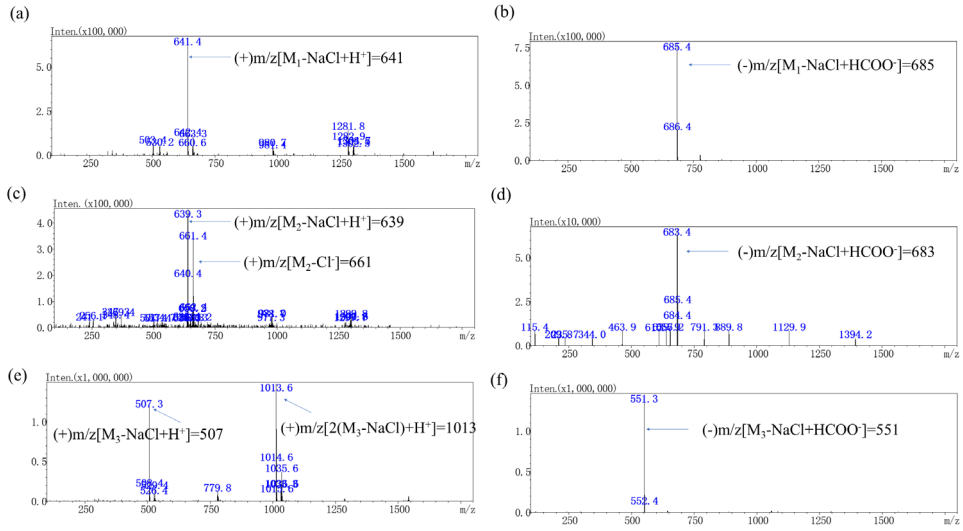

Fig. S49 Mass spectrum of the sixth combination product derived from low-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

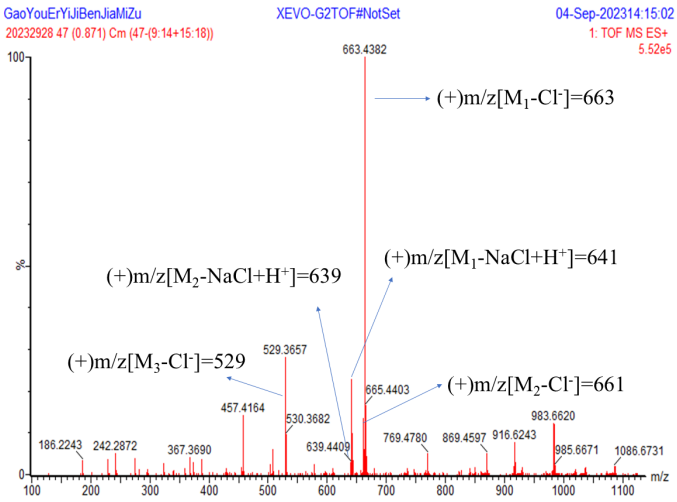

Fig. S50 Electrospray mass spectrum of the product prepared from the sixth combination of raw materials with a low linoleic acid content.

2.1.7 Combination 7: Toluene was used as the alkylation reagent, N,N-dimethylethylenediamine as the amidation reagent, and butanesultone as the quaternization reagent

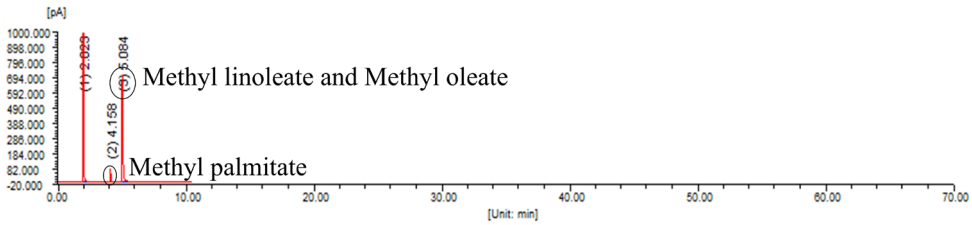

Fig. S51 Gas chromatogram of the mixed fatty acid raw materials.

Table S26 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.158	5.084

Integrated peak area	410467.8	4092262.6

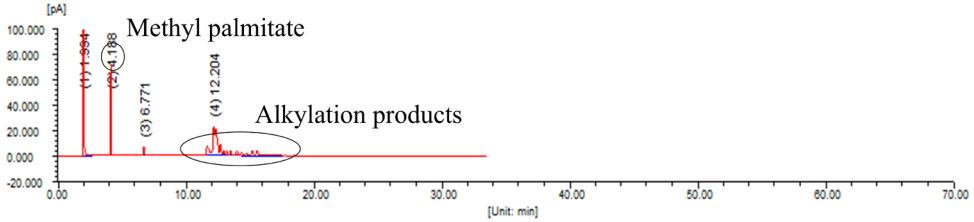

Fig. S52 Gas chromatogram of the product after the alkylation reaction.

Table S27 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.158	5.084
Integrated peak area	140283.2	8914.7

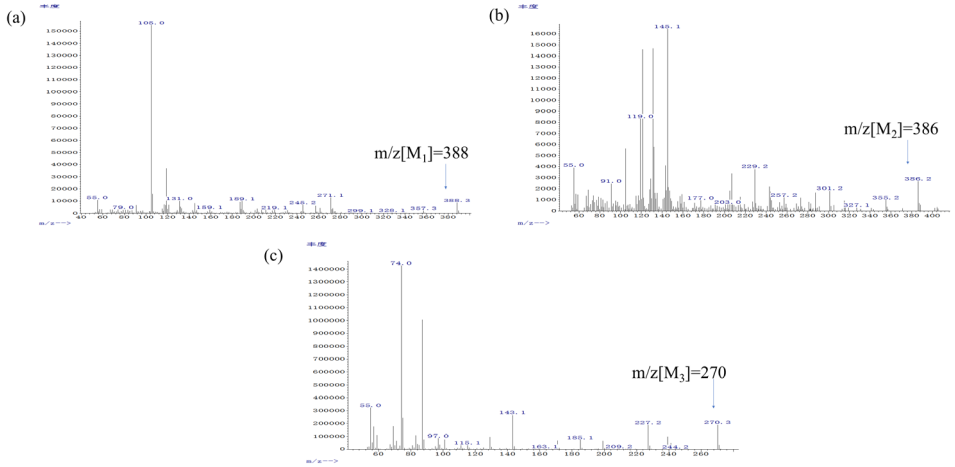

Fig. S53 Mass spectrum of the product after alkylation reaction.

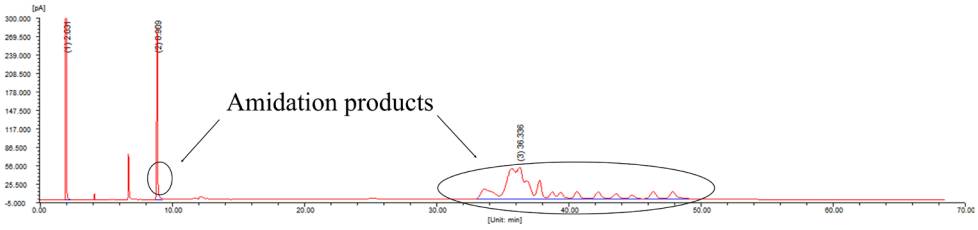

Fig. S54 Gas chromatogram of products after the amidation reaction.

Table S28 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~20.0	32.0~60.0
Integrated peak area	276947.5	10358031.0

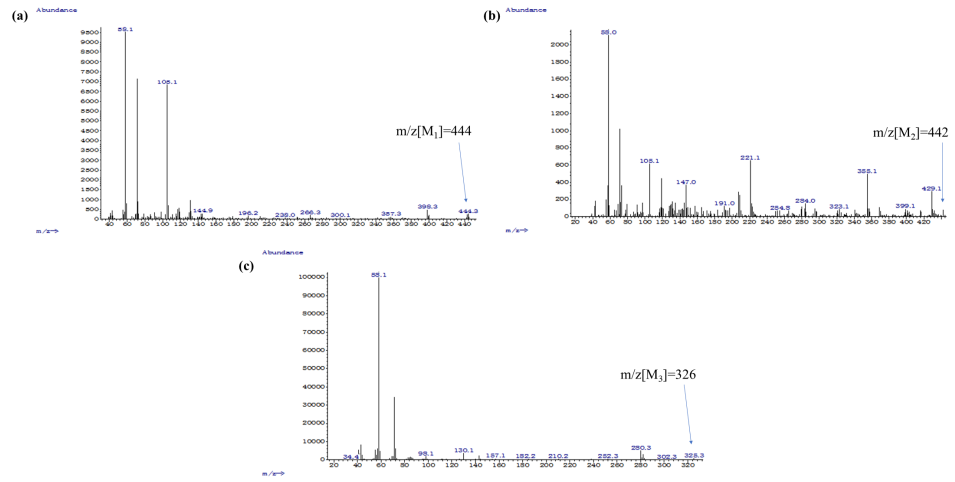

Fig. S55 Mass spectrum of the product after amidation reaction.

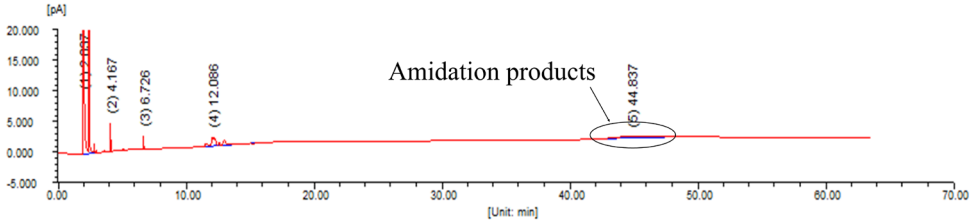

Fig. S56 Gas chromatogram of the product after the quaternization reaction.

Table S29 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~20.0	32.0~60.0
Integrated peak area	76708.4	74210.8

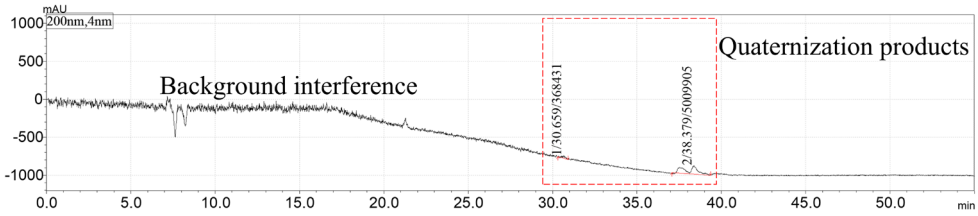

Fig. S57 Liquid chromatogram in liquid chromatography–mass spectrometry test of the seventh combination product derived from low-linoleic-acid-content raw materials.

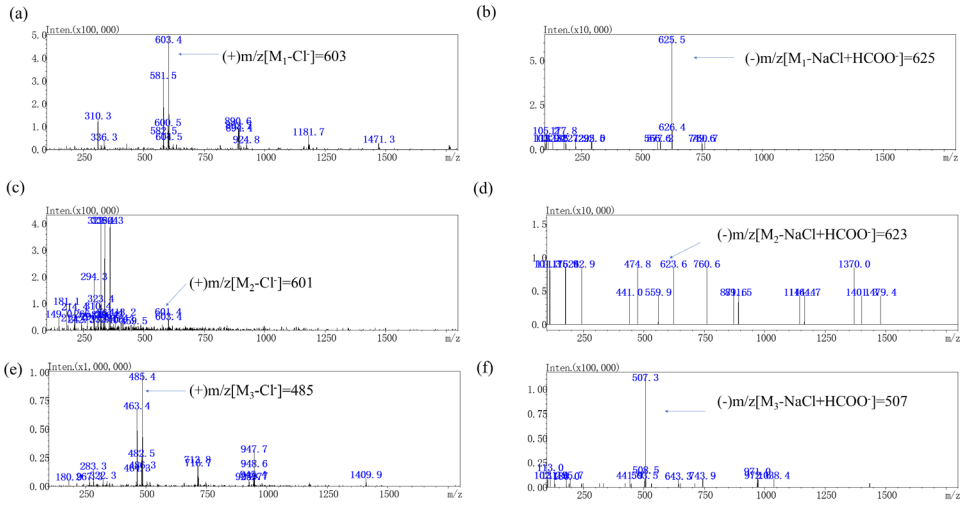

Fig. S58 Mass spectrum of the seventh combination product derived from low-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

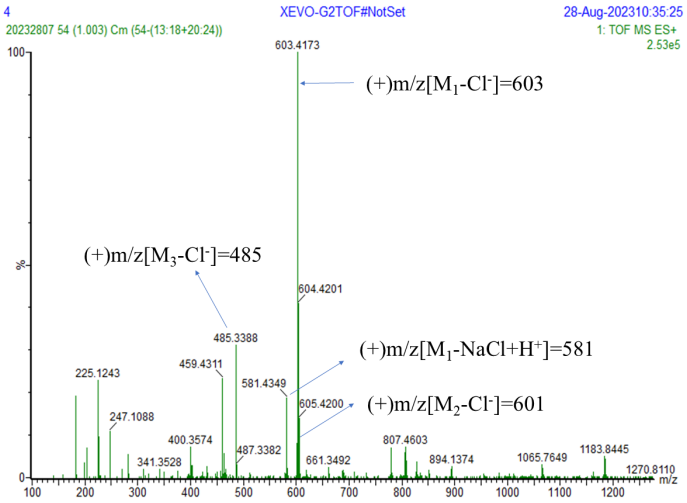

Fig. S59 Electrospray mass spectrum of the product prepared from the seventh combination of raw materials with a low linoleic acid content.

2.1.8 Combination 8: Toluene was used as the alkylation reagent, N,N-dimethyl-1,3-propanediamine as the amidation reagent, and sodium 3-chloro-2-hydroxypropane sulfonate as the quaternization reagent

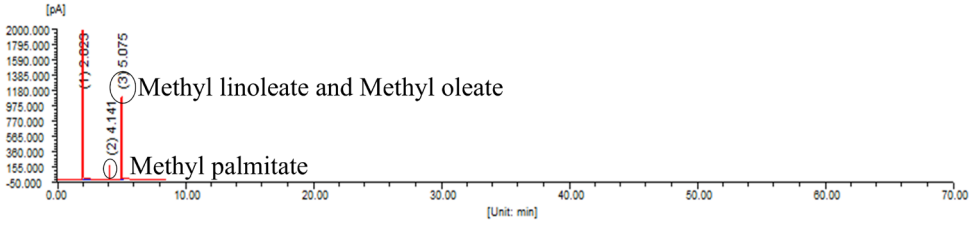

Fig. S60 Gas chromatogram of the mixed fatty acid raw materials.

Table S30 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.141	5.075
Integrated peak area	401382.5	3669817.7

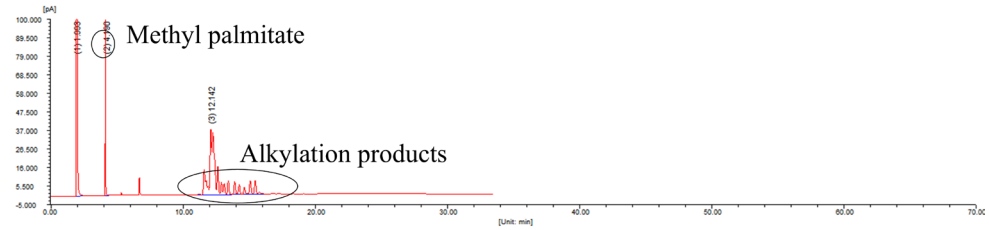

Fig. S61 Gas chromatogram of the product after the alkylation reaction.

Table S31 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.190	5.075
Integrated peak area	224694.2	14033.7

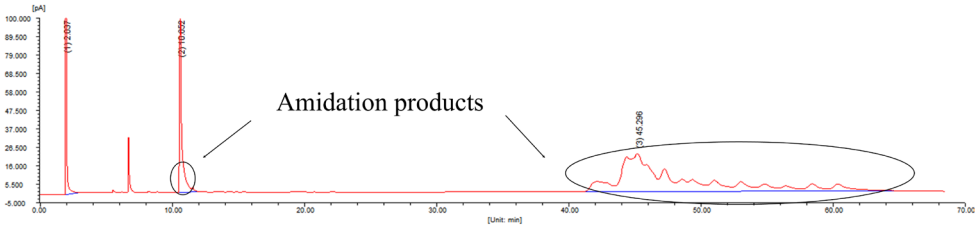

Fig. S62 Gas chromatogram of products after the amidation reaction.

Table S32 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~20.0	40.0~65.0
Integrated peak area	36755.2	7039493.4

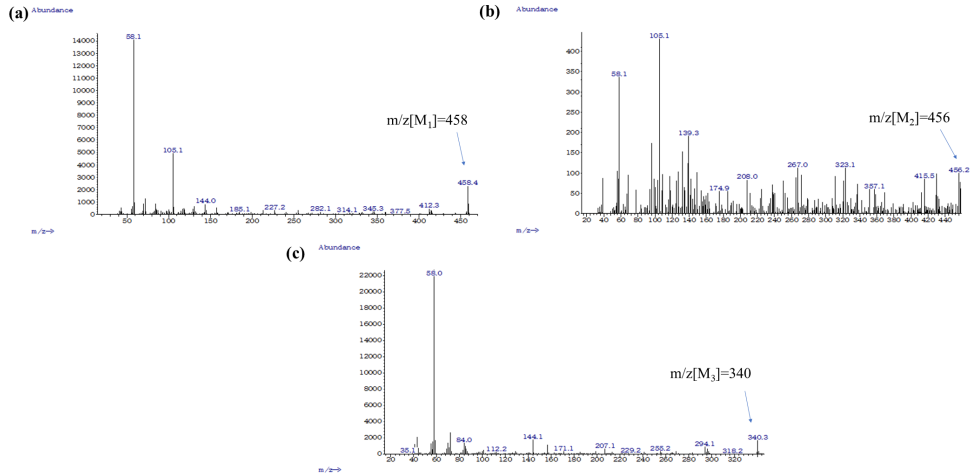

Fig. S63 Mass spectrum of the product after amidation reaction.

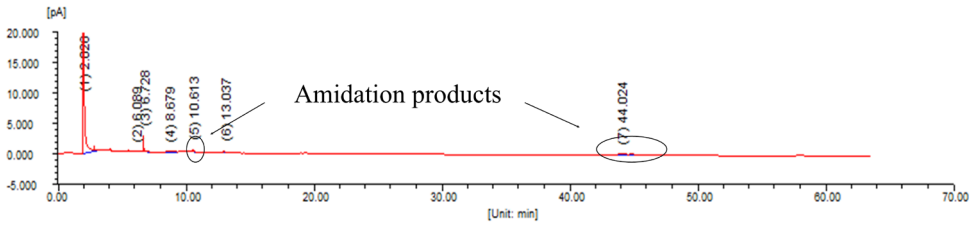

Fig. S64 Gas chromatogram of the product after the quaternization reaction.

Table S33 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~20.0	40.0~65.0
Integrated peak area	19119.4	22272.0

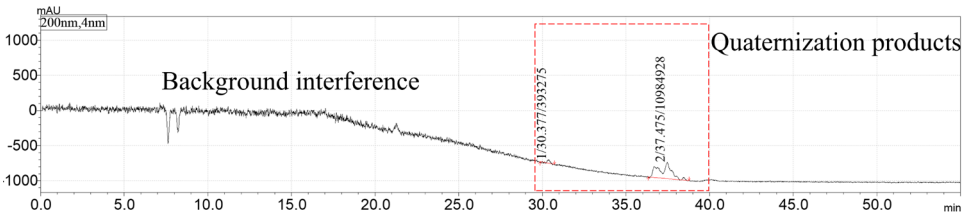

Fig. S65 Liquid chromatogram in liquid chromatography–mass spectrometry test of the eighth combination product derived from low-linoleic-acid-content raw materials.

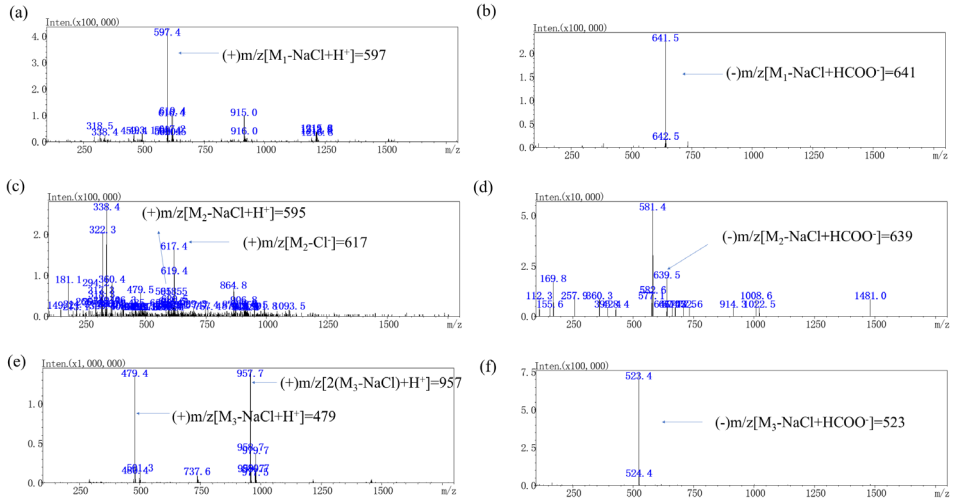

Fig. S66 Mass spectrum of the eighth combination product derived from low-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

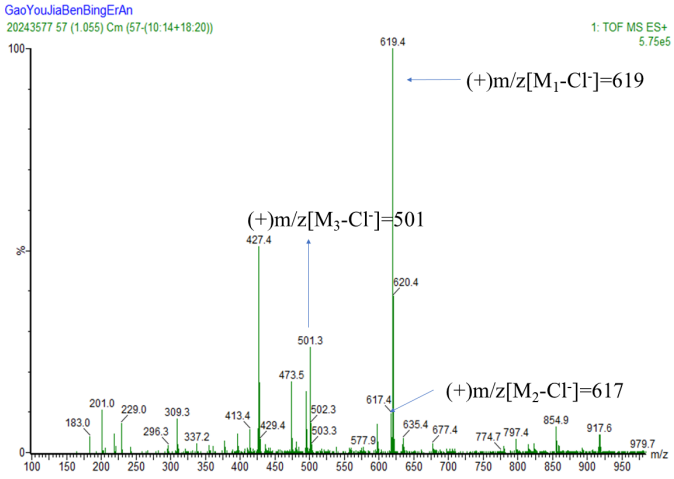

Fig. S67 Electrospray mass spectrum of the product prepared from the eighth combination of raw materials with a low linoleic acid content.

2.1.9 Combination 9: Toluene was used as the alkylation reagent, N,N-diethyl-1,3-propanediamine as the amidation reagent, and sodium chloroacetate as the quaternization reagent

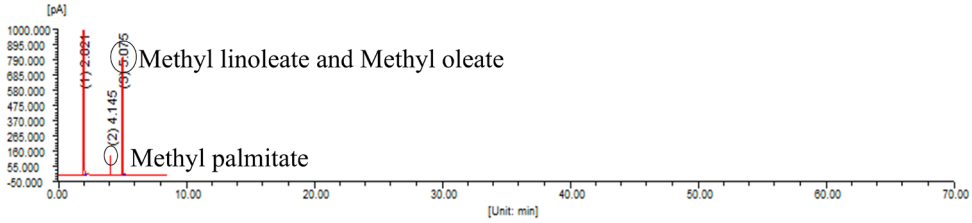

Fig. S68 Gas chromatogram of the mixed fatty acid raw materials.

Table S34 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.145	5.075
Integrated peak area	268968.0	2580133.0

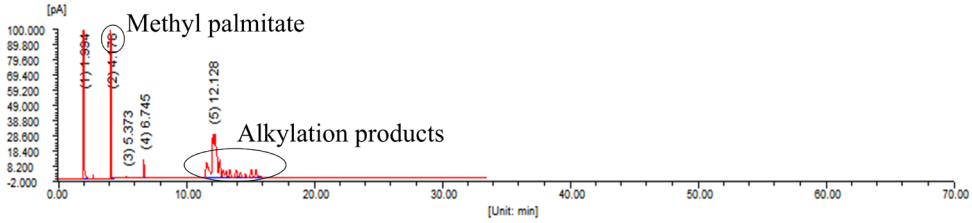

Fig. S69 Gas chromatogram of the product after the alkylation reaction.

Table S35 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.178	5.075
Integrated peak area	198377.5	1666.9

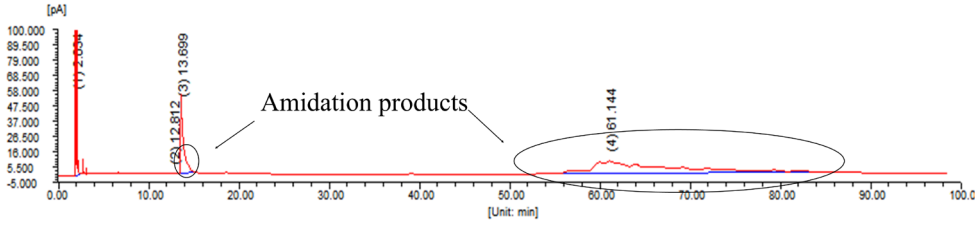

Fig. S70 Gas chromatogram of products after the amidation reaction.

Table S36 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~20.0	54.0~90.0
Integrated peak area	65114.6	5742678.2

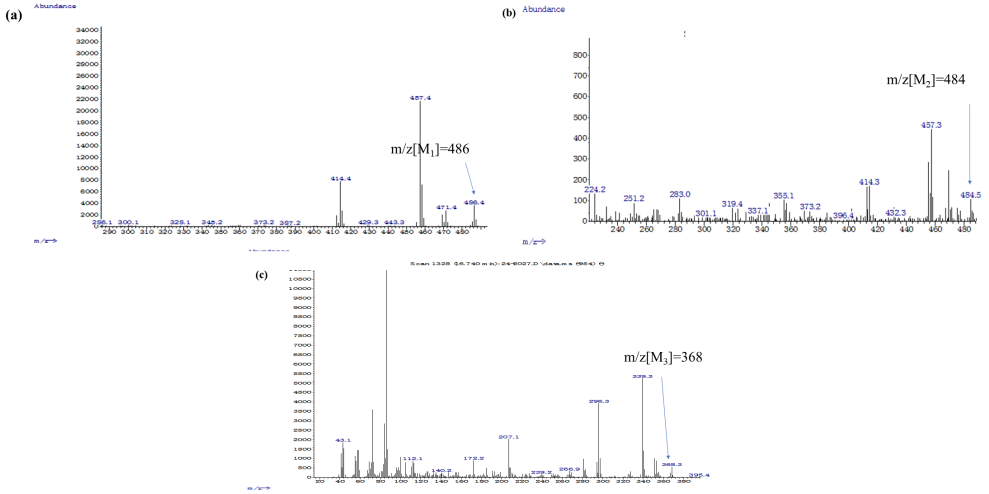

Fig. S71 Mass spectrum of the product after amidation reaction.

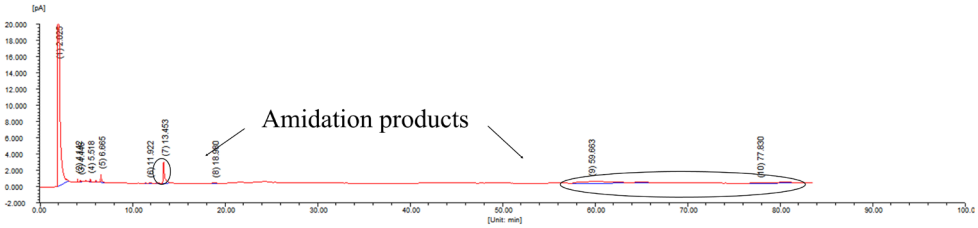

Fig. S72 Gas chromatogram of the product after the quaternization reaction.

Table S37 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~20.0	54.0~90.0
Integrated peak area	8516.1	73605.6

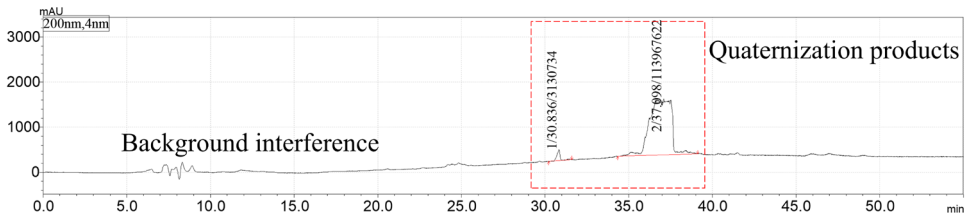

Fig. S73 Liquid chromatogram in liquid chromatography–mass spectrometry test of the ninth combination product derived from low-linoleic-acid-content raw materials.

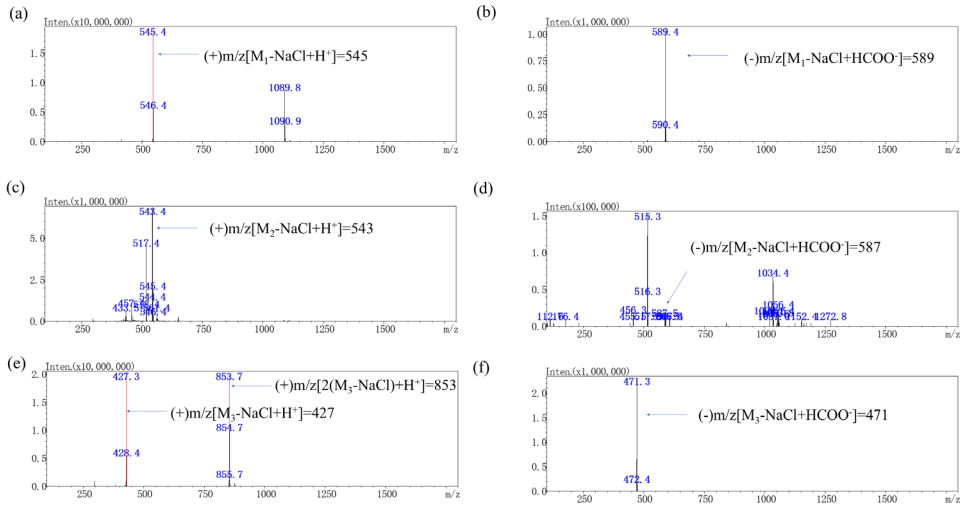

Fig. S74 Mass spectrum of the ninth combination product derived from low-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

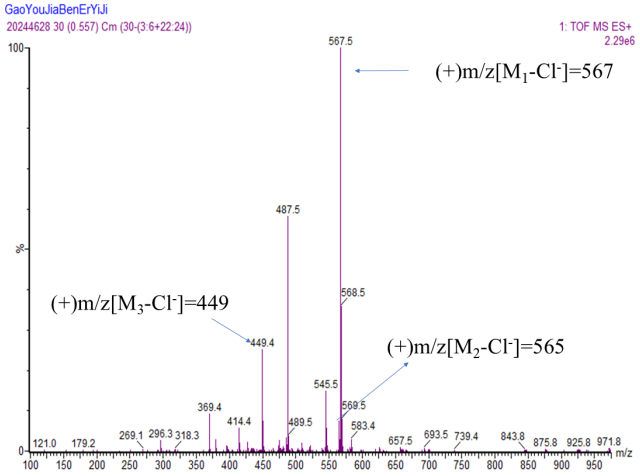

Fig. S75 Electrospray mass spectrum of the product prepared from the ninth combination of raw materials with a low linoleic acid content.

2.2 The GC-MS, HPLC-MS, and ESI-MS spectra of products synthesized from raw materials with a moderate linoleic/oleic acid ratio

2.2.1 Combination 1: Benzene as the alkylation reagent, N,N-dimethylethylenediamine as the amidation reagent, and sodium 3-chloro-2-hydroxypropane sulfonate as the quaternization reagent

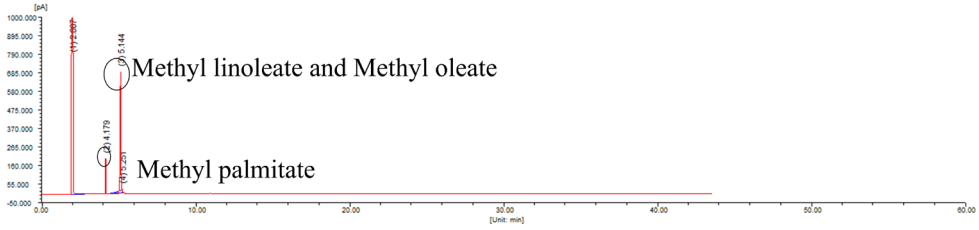

Fig. S76 Gas chromatogram of the mixed fatty acid raw materials.

Table S38 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)

Retention time/min	4.179	5.144
Integrated peak area	439406.7	2724157.1

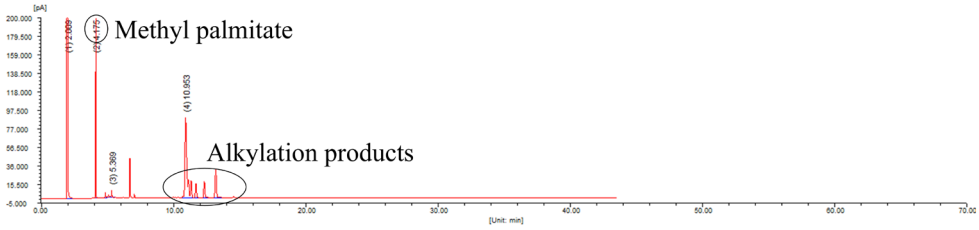

Fig. S77 Gas chromatogram of the product after the alkylation reaction.

Table S39 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.175	5.144
Integrated peak area	367130.9	86031.3

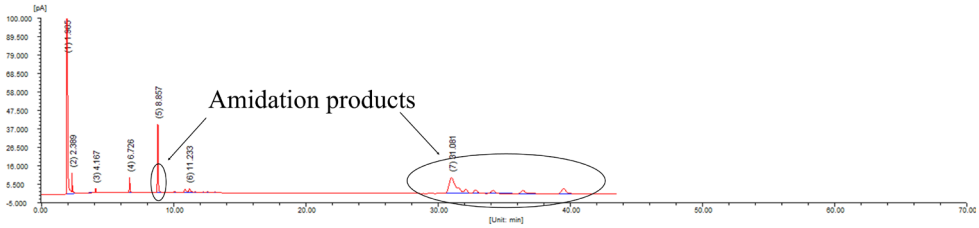

Fig. S78 Gas chromatogram of products after the amidation reaction.

Table S40 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~15.0	25.0~46.0
Integrated peak area	70327.6	638217.8

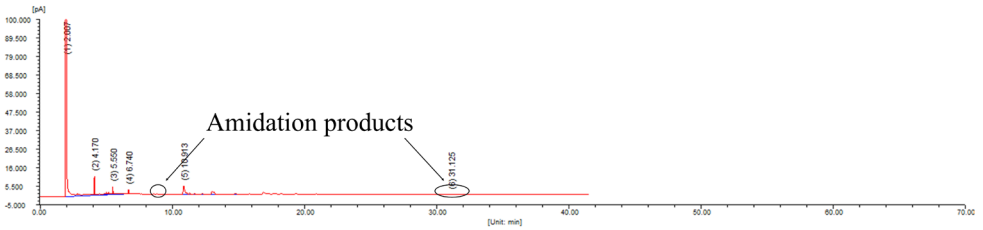

Fig. S79 Gas chromatogram of the product after the quaternization reaction.

Table S41 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~15.0	25.0~46.0
Integrated peak area	94162.0	1225.0

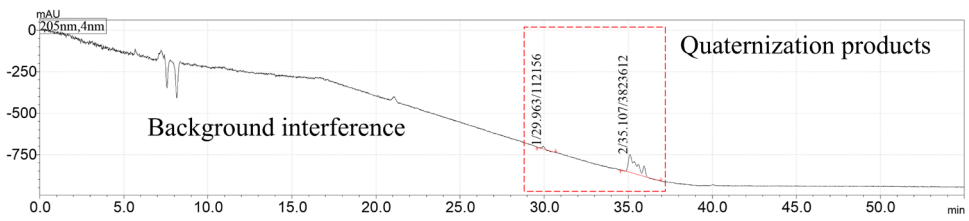

Fig. S80 Liquid chromatogram in liquid chromatography–mass spectrometry test of the first combination product derived from low-linoleic-acid-content raw materials.

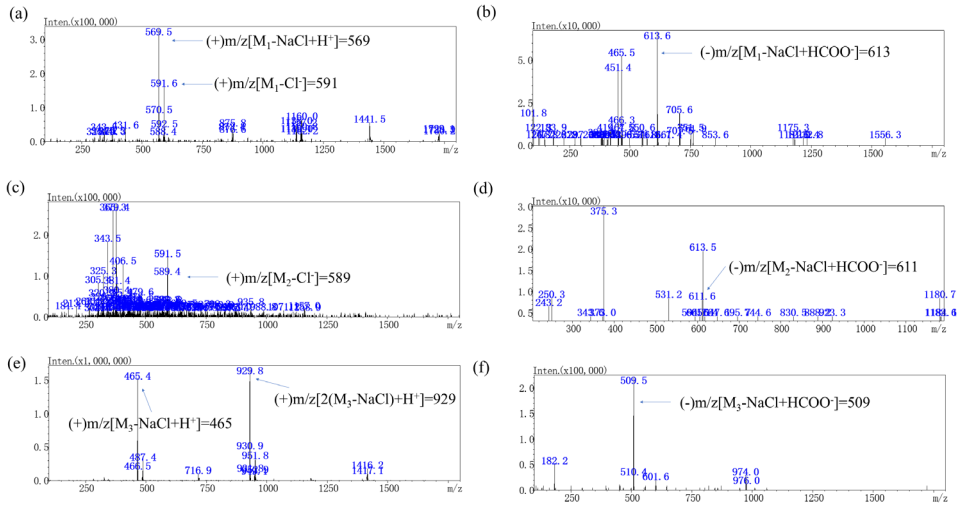

Fig. S81 Mass spectrum of the first combination product derived from moderate-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

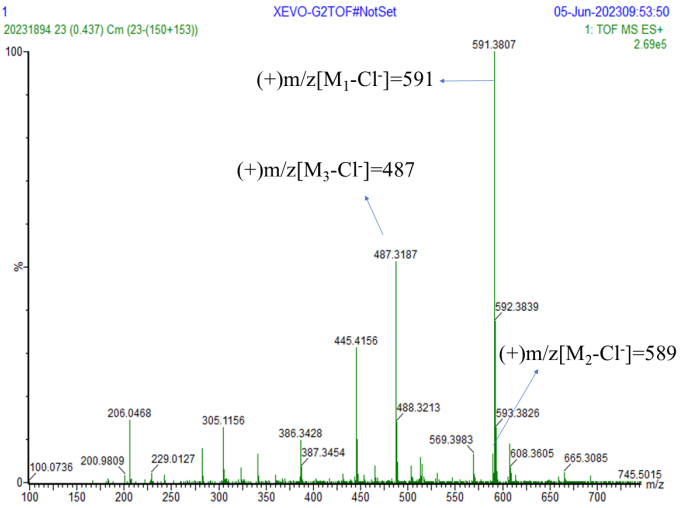

Fig. S82 Electrospray mass spectrum of the product prepared from the first combination of raw materials with a moderate linoleic acid content.

2.2.2 Combination 2: Benzene was used as the alkylation reagent, N,N-dimethyl-1,3-propanediamine as the amidation reagent, and sodium chloroacetate as the quaternization reagent

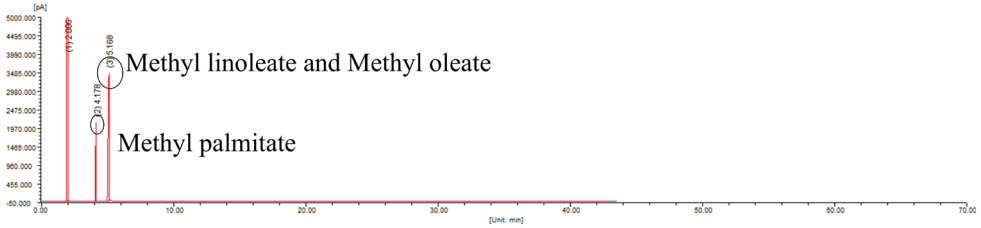

Fig. S83 Gas chromatogram of the mixed fatty acid raw materials.

Table S42 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)

Retention time/min	4.178	5.168
Integrated peak area	3971348.9	13075525.8

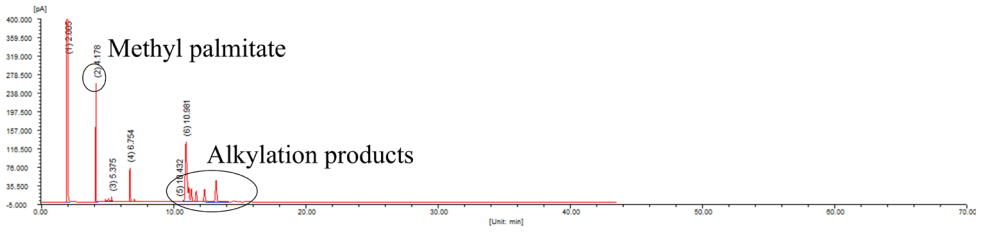

Fig. S84 Gas chromatogram of the product after the alkylation reaction.

Table S43 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.178	5.168
Integrated peak area	535842.2	116705.9

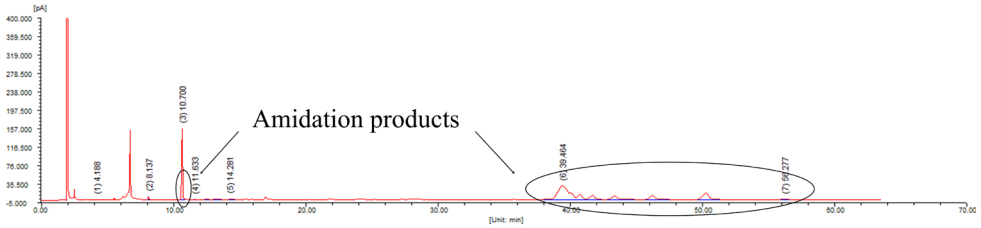

Fig. S85 Gas chromatogram of products after the amidation reaction.

Table S44 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	10.0~15.0	36.0~58.0
Integrated peak area	200861.2	3716345.2

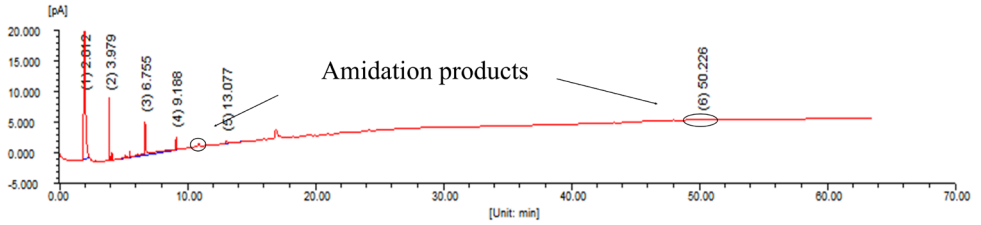

Fig. S86 Gas chromatogram of the product after the quaternization reaction.

Table S45 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~15.0	36.0~58.0
Integrated peak area	16697.4	10413.2

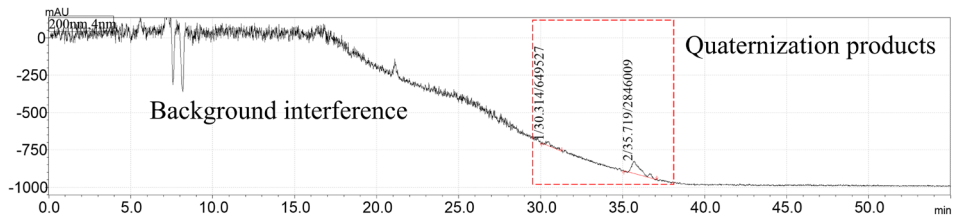

Fig. S87 Liquid chromatogram in liquid chromatography–mass spectrometry test of the second combination product derived from moderate-linoleic-acid-content raw materials.

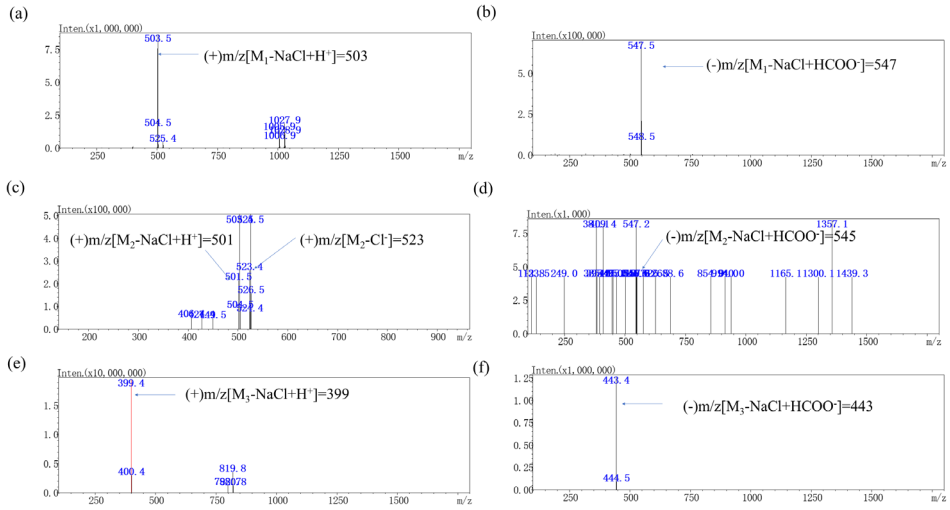

Fig. S88 Mass spectrum of the second combination product derived from moderate-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

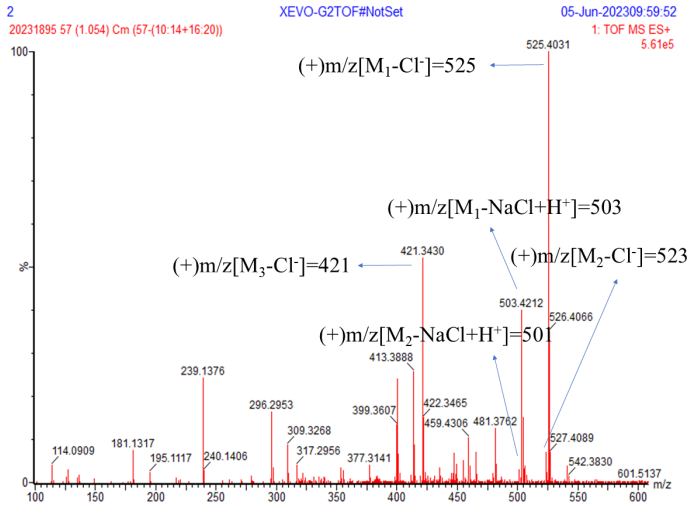

Fig. S89 Electrospray mass spectrum of the product prepared from the second combination of raw materials with a moderate linoleic acid content.

2.2.3 Combination 3: Benzene was used as the alkylation reagent, N,N-diethyl-1,3-propanediamine as the amidation reagent, and butanesultone as the quaternization reagent

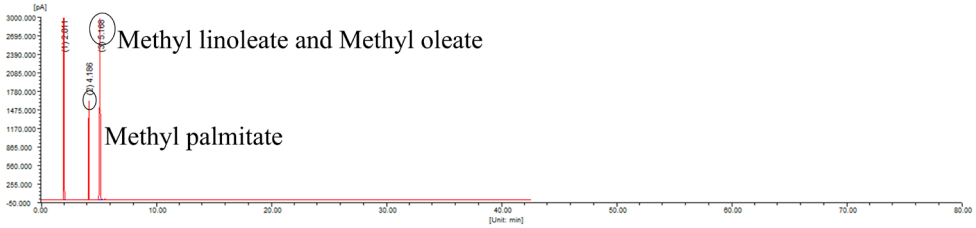

Fig. S90 Gas chromatogram of the mixed fatty acid raw materials.

Table S46 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)

Retention time/min	4.186	5.168
Integrated peak area	4148015.0	14524497.0

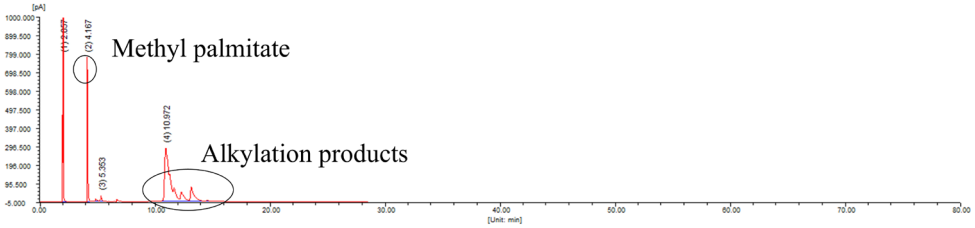

Fig. S91 Gas chromatogram of the product after the alkylation reaction.

Table S47 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.167	5.168
Integrated peak area	9274652.7	367105.8

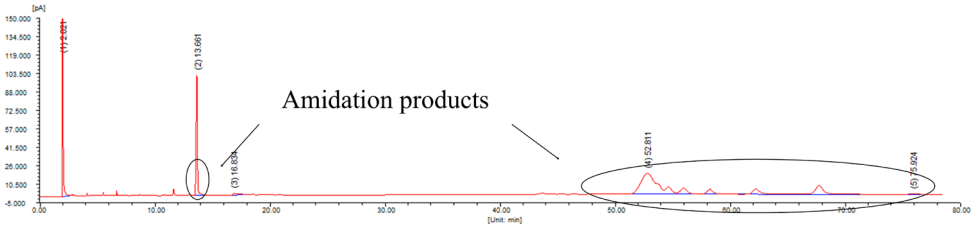

Fig. S92 Gas chromatogram of products after the amidation reaction.

Table S48 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~15.0	50.0~72.0
Integrated peak area	195278.8	2988008.4

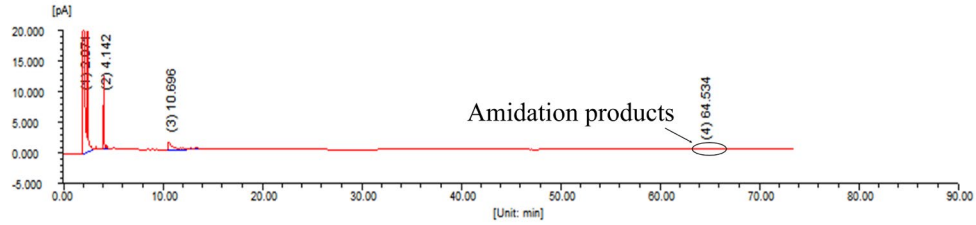

Fig. S93 Gas chromatogram of the product after the quaternization reaction.

Table S49 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~15.0	50.0~72.0
Integrated peak area	66658.4	11241.8

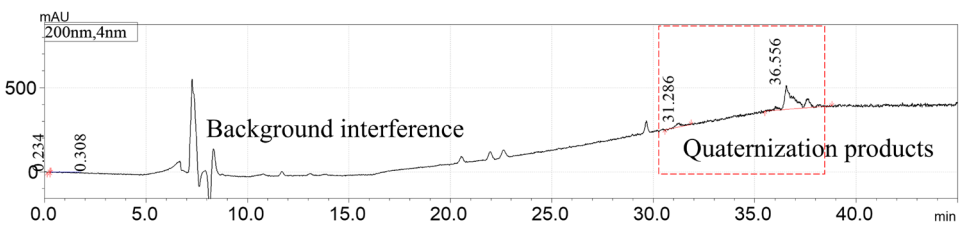

Fig. S94 Liquid chromatogram in liquid chromatography–mass spectrometry test of the third combination product derived from moderate-linoleic-acid-content raw materials.

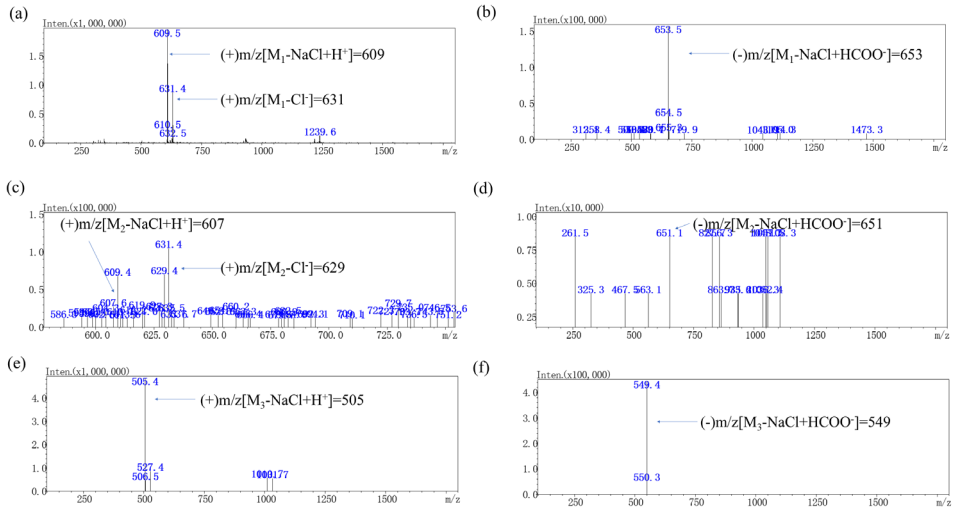

Fig. S95 Mass spectrum of the third combination product derived from moderate-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

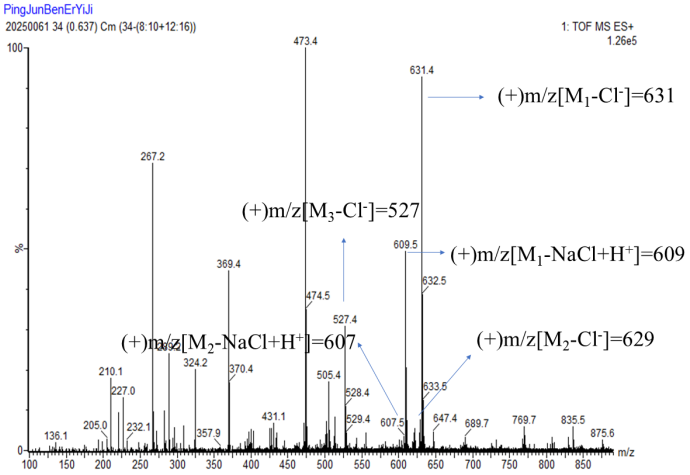

Fig. S96 Electrospray mass spectrum of the product prepared from the third combination of raw materials with a moderate linoleic acid content.

2.2.4 Combination 4: Anisole was used as the alkylation reagent, N,N-dimethylethylenediamine as the amidation reagent, and sodium chloroacetate as the quaternization reagent

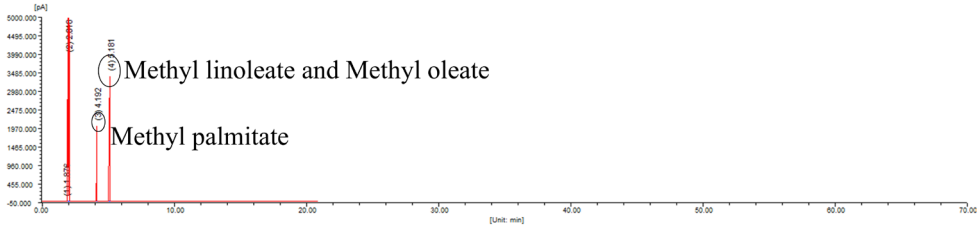

Fig. S97 Gas chromatogram of the mixed fatty acid raw materials.

Table S50 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)

Retention time/min	4.192	5.181
Integrated peak area	1398475.7	7284285.3

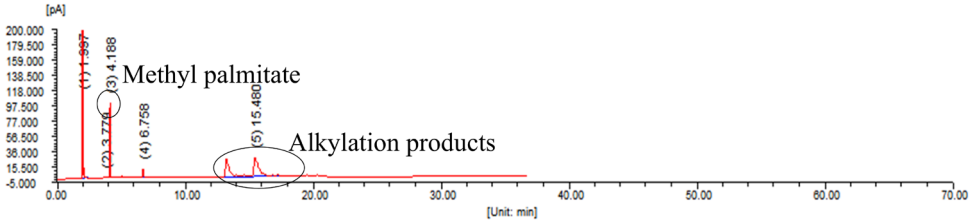

Fig. S98 Gas chromatogram of the product after the alkylation reaction.

Table S51 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.188	5.181
Integrated peak area	238376.4	15072.3

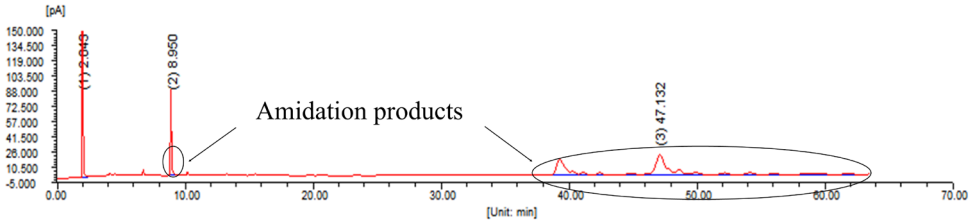

Fig. S99 Gas chromatogram of products after the amidation reaction.

Table S52 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~25.0	38.0~68.0
Integrated peak area	70424.2	3046589.4

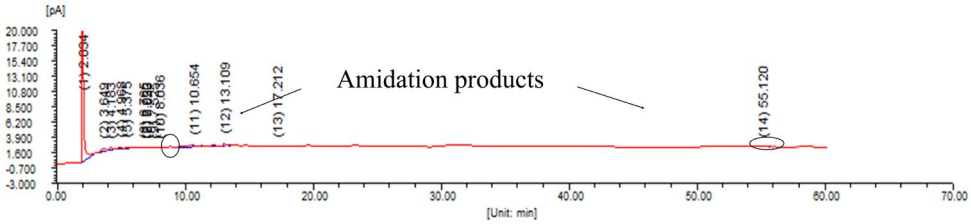

Fig. S100 Gas chromatogram of the product after the quaternization reaction.

Table S53 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~25.0	38.0~68.0
Integrated peak area	22166.7	25206.3

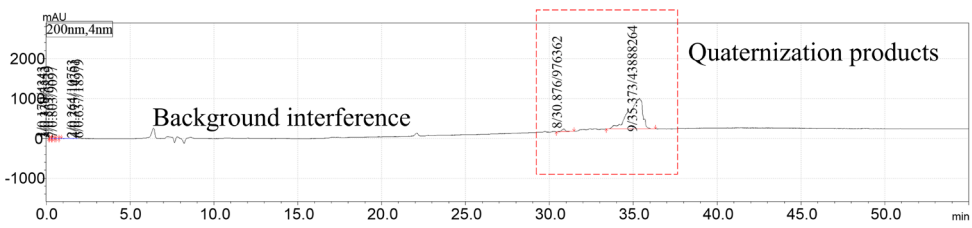

Fig. S101 Liquid chromatogram in liquid chromatography–mass spectrometry test of the fourth combination product derived from moderate-linoleic-acid-content raw materials.

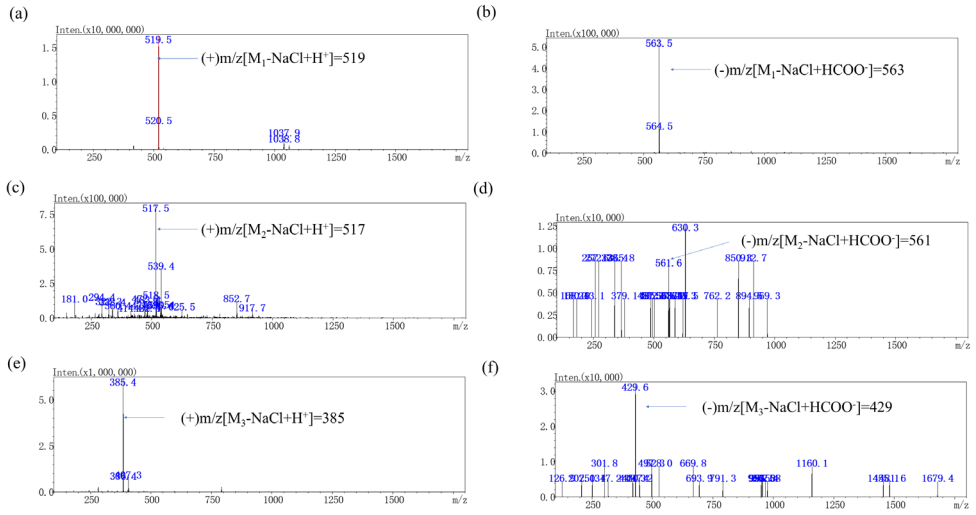

Fig. S102 Mass spectrum of the fourth combination product derived from moderate-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

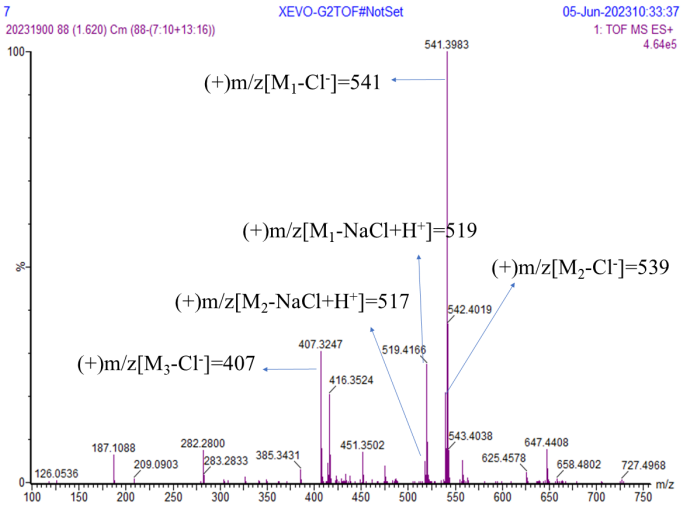

Fig. S103 Electrospray mass spectrum of the product prepared from the fourth combination of raw materials with a moderate linoleic acid content.

2.2.5 Combination 5: Anisole was used as the alkylation reagent, N,N-dimethyl-1,3-propanediamine as the amidation reagent, and butanesultone as the quaternization reagent

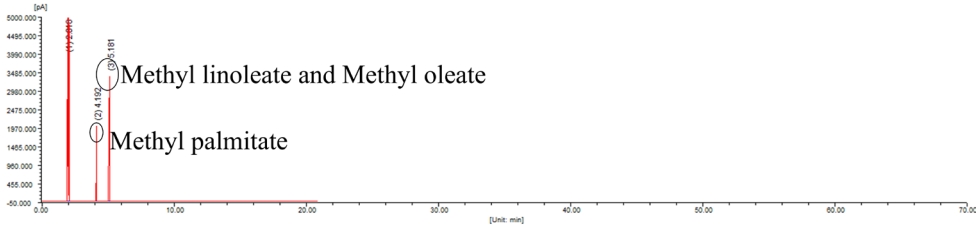

Fig. S104 Gas chromatogram of the mixed fatty acid raw materials.

Table S54 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)

Retention time/min	4.192	5.181
Integrated peak area	1398475.7	7284285.3

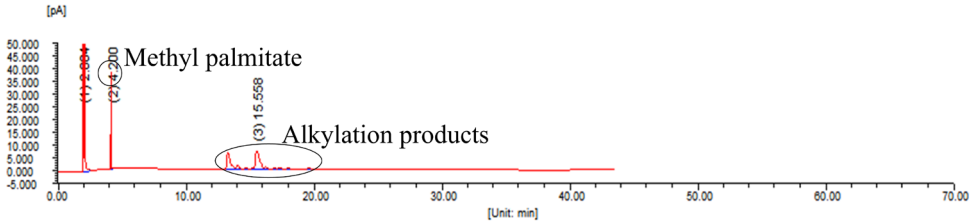

Fig. S105 Gas chromatogram of the product after the alkylation reaction.

Table S55 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.200	5.181
Integrated peak area	77445.4	2160.6

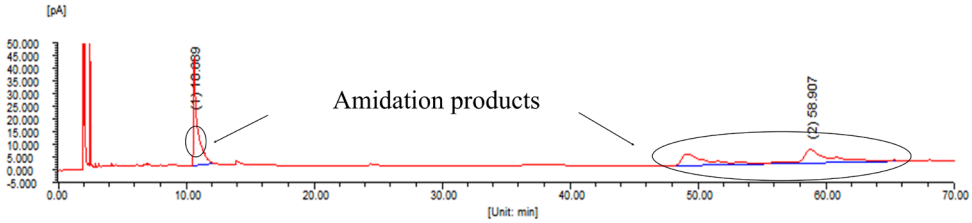

Fig. S106 Gas chromatogram of products after the amidation reaction.

Table S56 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	12.0~20.0	44.0~80.0
Integrated peak area	54502.7	1994282.2

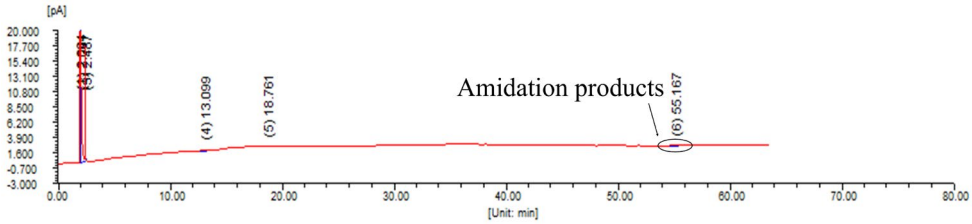

Fig. S107 Gas chromatogram of the product after the quaternization reaction.

Table S57 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	12.0~20.0	44.0~80.0
Integrated peak area	10603.2	9845.6

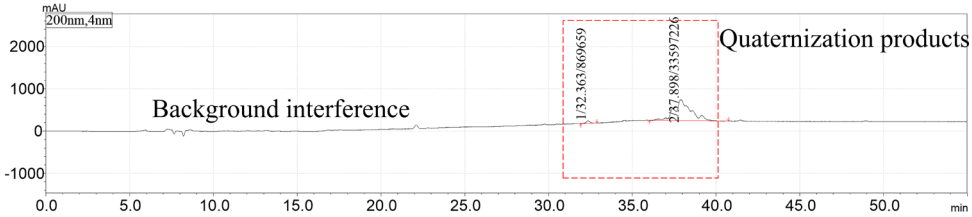

Fig. S108 Liquid chromatogram in liquid chromatography–mass spectrometry test of the fifth combination product derived from moderate-linoleic-acid-content raw materials.

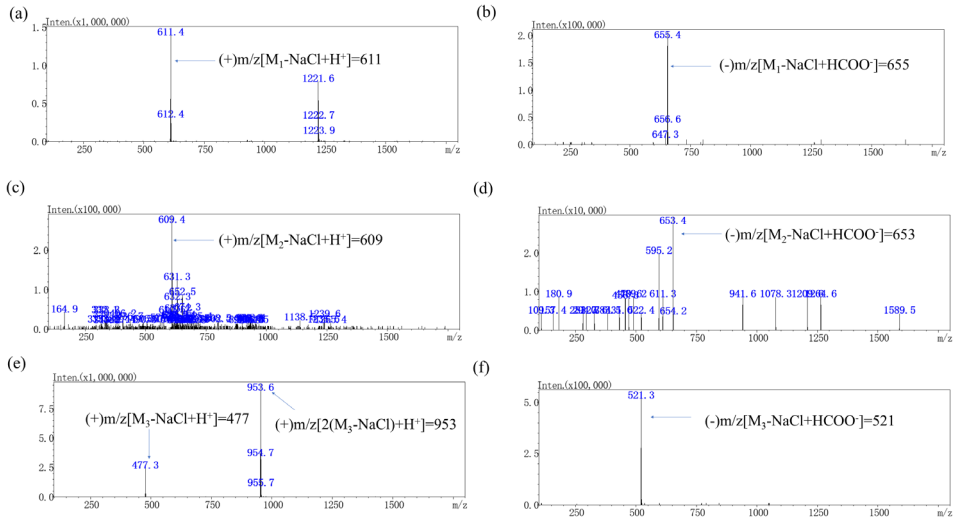

Fig. S109 Mass spectrum of the fifth combination product derived from moderate-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

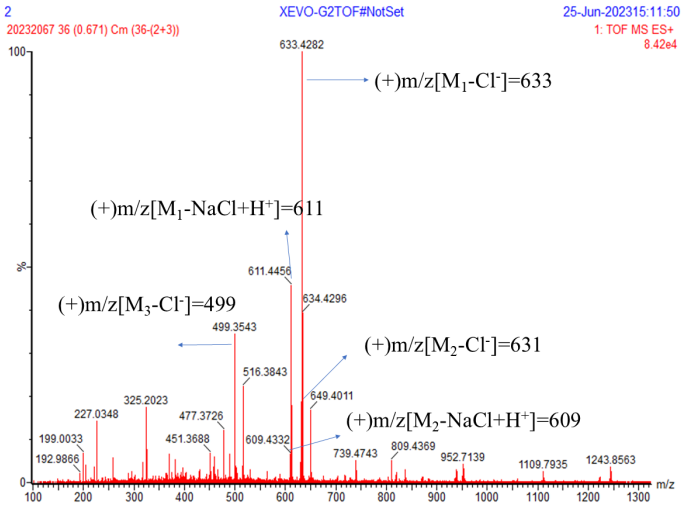

Fig. S110 Electrospray mass spectrum of the product prepared from the fifth combination of raw materials with a moderate linoleic acid content.

2.2.6 Combination 6: Anisole was used as the alkylation reagent, N,N-diethyl-1,3-propanediamine as the amidation reagent, and sodium 3-chloro-2-hydroxypropane sulfonate as the quaternization reagent

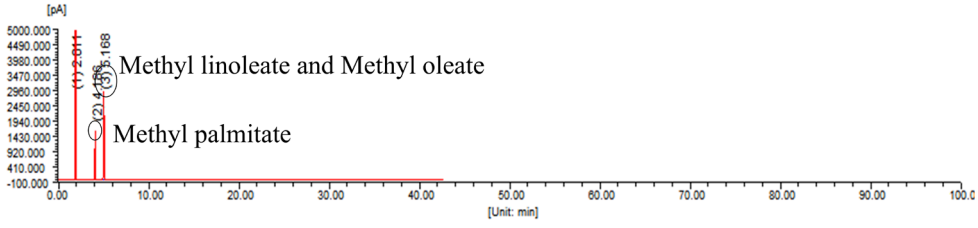

Fig. S111 Gas chromatogram of the mixed fatty acid raw materials.

Table S58 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)

Retention time/min	4.186	5.168
Integrated peak area	1641426.5	13112204.6

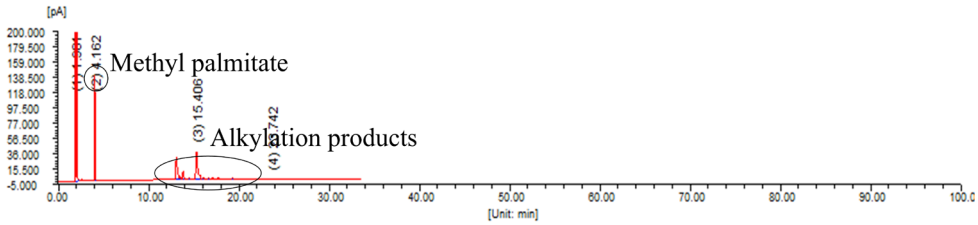

Fig. S112 Gas chromatogram of the product after the alkylation reaction.

Table S59 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.162	5.168
Integrated peak area	262184.4	3316.8

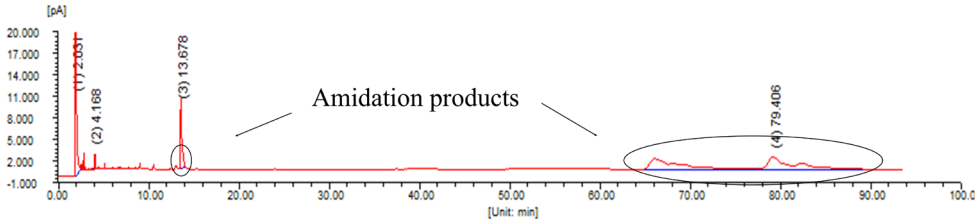

Fig. S113 Gas chromatogram of products after the amidation reaction.

Table S60 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~25.0	65.0~90.0
Integrated peak area	12949.0	760850.8

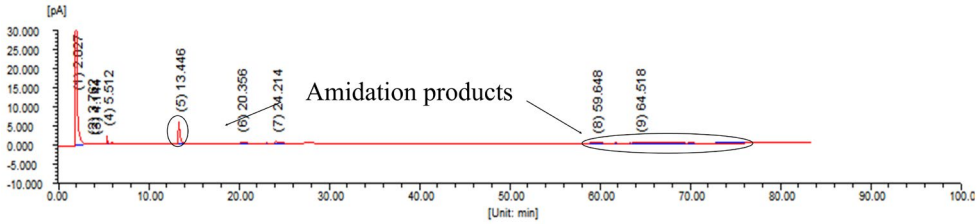

Fig. S114 Gas chromatogram of the product after the quaternization reaction.

Table S61 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	12.0~25.0	66.0~90.0
Integrated peak area	56832.3	111517.7

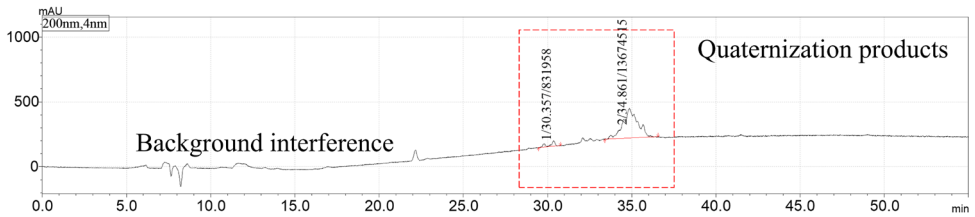

Fig. S115 Liquid chromatogram in liquid chromatography–mass spectrometry test of the sixth combination product derived from moderate-linoleic-acid-content raw materials.

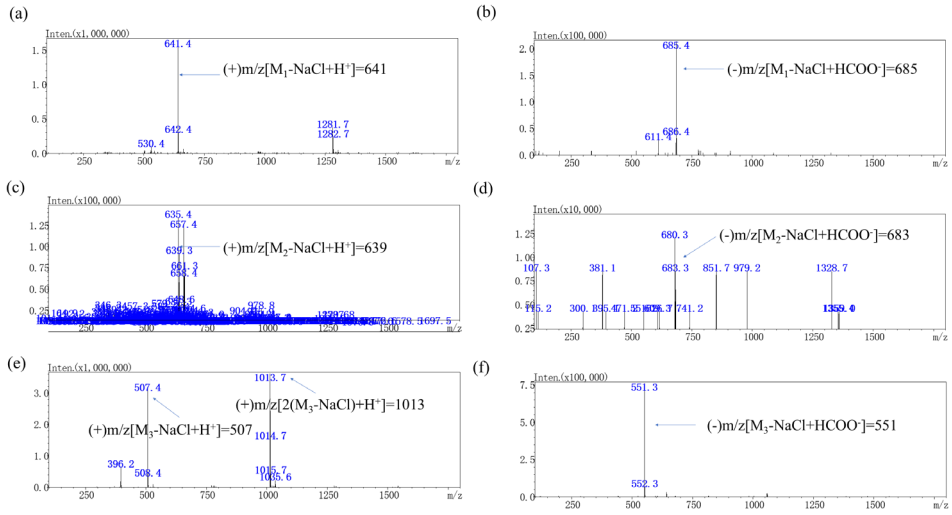

Fig. S116 Mass spectrum of the sixth combination product derived from moderate-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

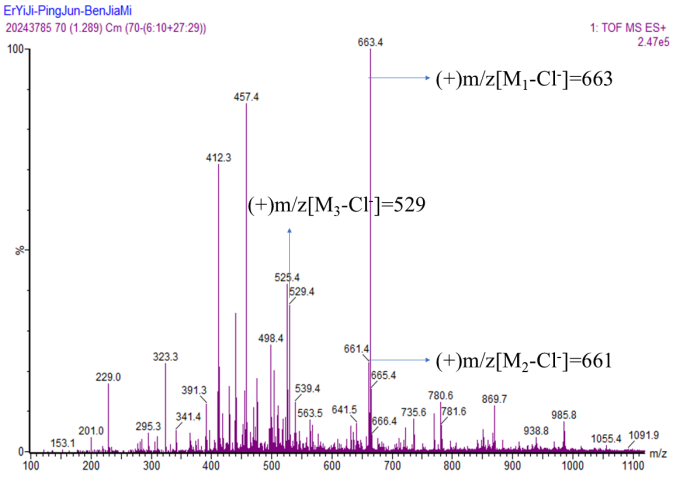

Fig. S117 Mass spectrum of the sixth combination product derived from moderate-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

2.2.7 Combination 7: Toluene was used as the alkylation reagent, N,N-dimethylethylenediamine as the amidation reagent, and butanesultone as the quaternization reagent

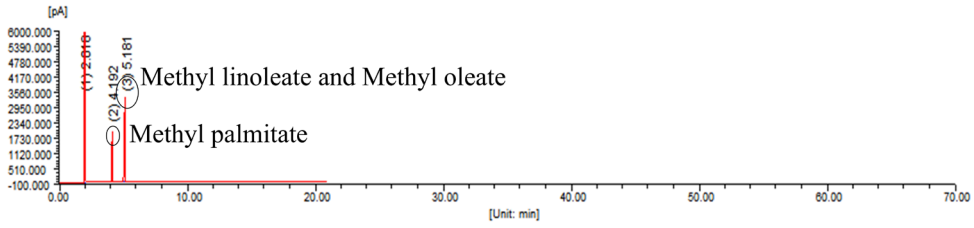

Fig. S118 Gas chromatogram of the mixed fatty acid raw materials.

Table S62 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)

Retention time/min	4.192	5.181
Integrated peak area	4169885.6	14562204.0

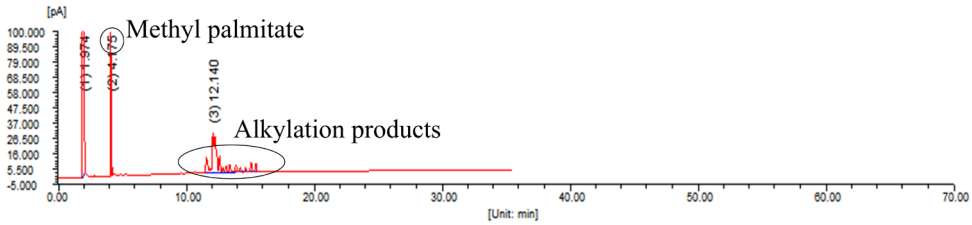

Fig. S119 Gas chromatogram of the product after the alkylation reaction.

Table S63 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.175	5.181
Integrated peak area	195662.7	13832.4

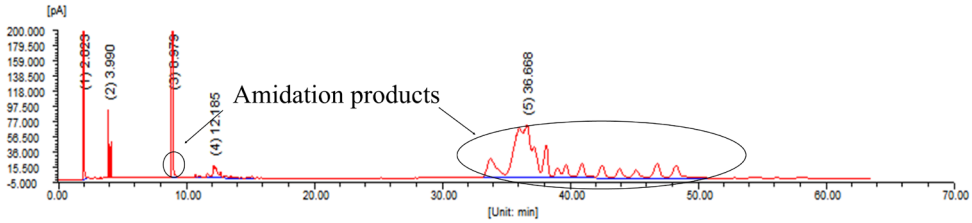

Fig. S120 Gas chromatogram of products after the amidation reaction.

Table S64 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~20.0	32.0~60.0
Integrated peak area	810877.1	13870671.4

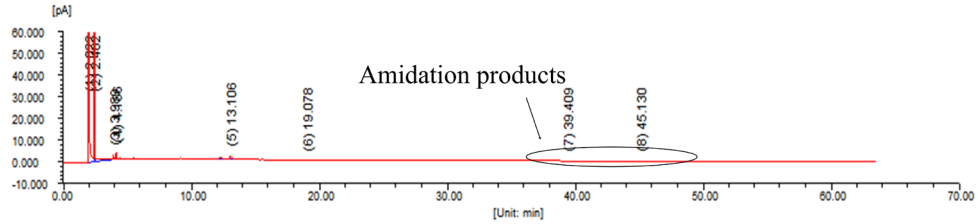

Fig. S121 Gas chromatogram of the product after the quaternization reaction.

Table S65 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~20.0	32.0~60.0
Integrated peak area	70093.6	1278.0

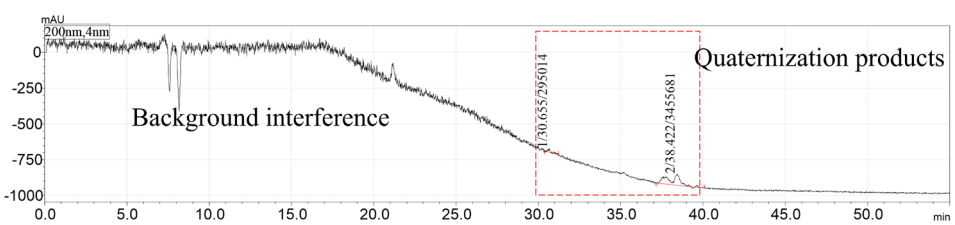

Fig. S122 Liquid chromatogram in liquid chromatography–mass spectrometry test of the seventh combination product derived from moderate-linoleic-acid-content raw materials.

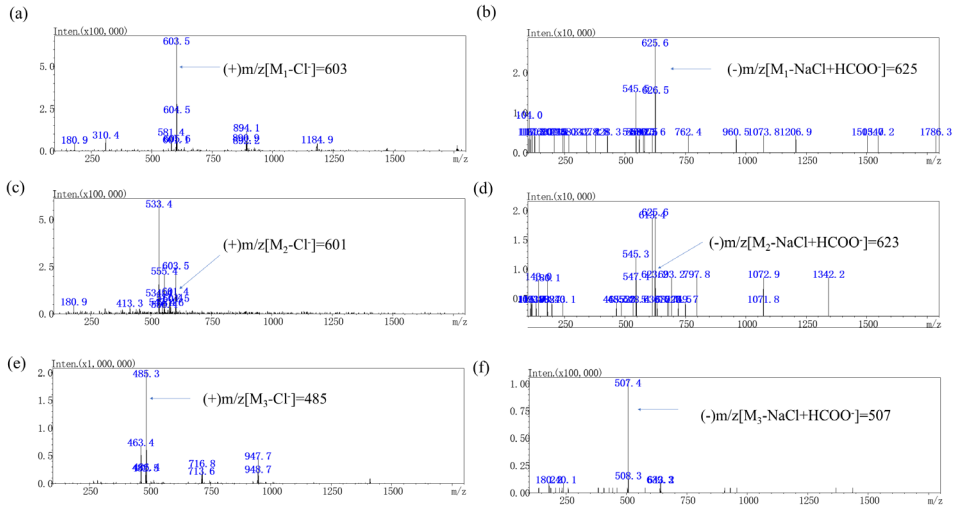

Fig. S123 Mass spectrum of the seventh combination product derived from moderate-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

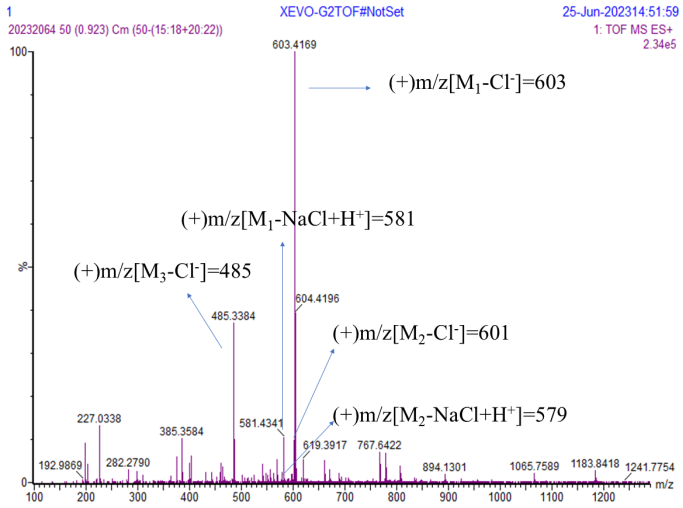

Fig. S124 Electrospray mass spectrum of the product prepared from the seventh combination of raw materials with a moderate linoleic acid content.

2.2.8 Combination 8: Toluene was used as the alkylation reagent, N,N-dimethyl-1,3-propanediamine as the amidation reagent, and sodium 3-chloro-2-hydroxypropane sulfonate as the quaternization reagent

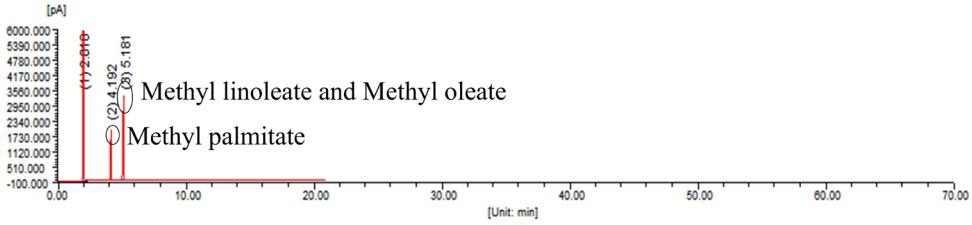

Fig. S125 Gas chromatogram of the mixed fatty acid raw materials.

Table S66 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)

Retention time/min	4.192	5.181
Integrated peak area	4176362.0	14594542.2

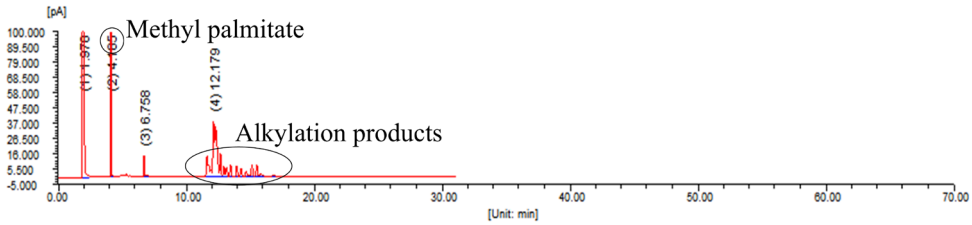

Fig. S126 Gas chromatogram of the product after the alkylation reaction.

Table S67 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.165	5.181
Integrated peak area	290726.1	20548.3

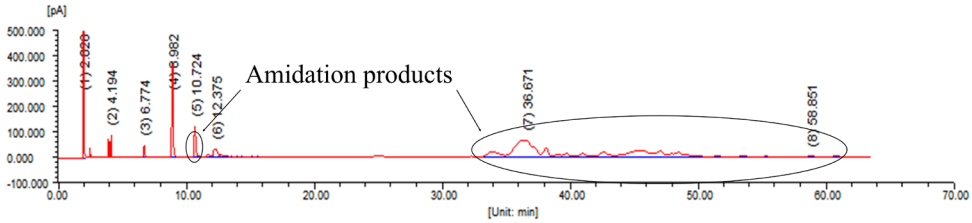

Fig. S127 Gas chromatogram of products after the amidation reaction.

Table S68 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~20.0	38.0~65.0
Integrated peak area	1550720.2	17748724.4

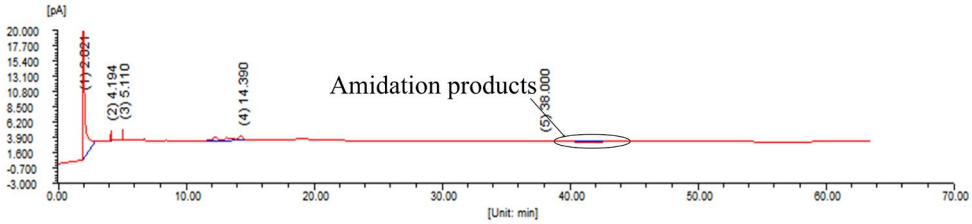

Fig. S128 Gas chromatogram of the product after the quaternization reaction.

Table S69 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~20.0	38.0~65.0
Integrated peak area	61803.6	12861.3

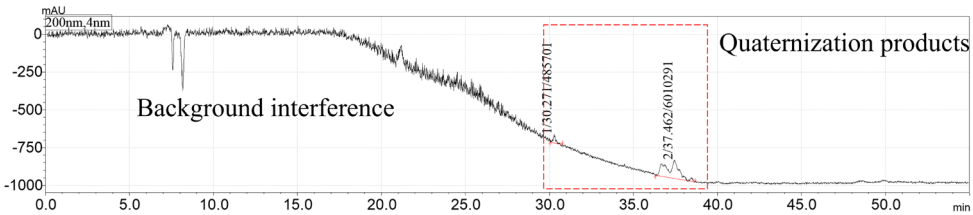

Fig. S129 Liquid chromatogram in liquid chromatography–mass spectrometry test of the eighth combination product derived from moderate-linoleic-acid-content raw materials.

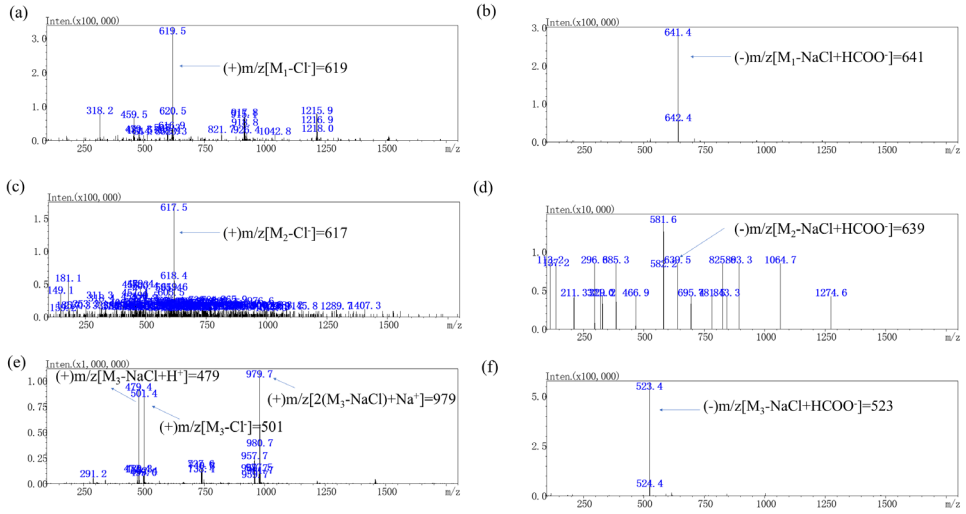

Fig. S130 Mass spectrum of the eighth combination product derived from moderate-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

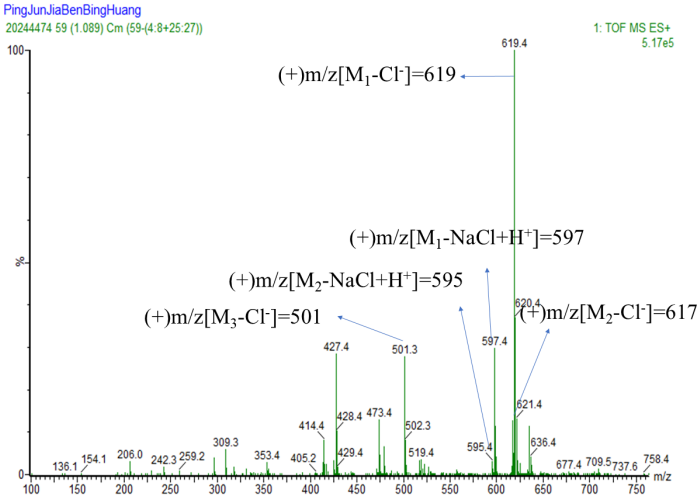

Fig. S131 Electrospray mass spectrum of the product prepared from the eighth combination of raw materials with a moderate linoleic acid content.

2.2.9 Combination 9: Toluene was used as the alkylation reagent, N,N-diethyl-1,3-propanediamine as the amidation reagent, and sodium chloroacetate as the quaternization reagent

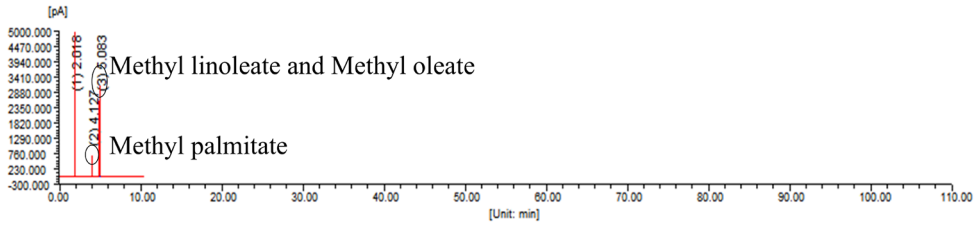

Fig. S132 Gas chromatogram of the mixed fatty acid raw materials.

Table S70 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)

Retention time/min	4.127	5.083
Integrated peak area	747836.1	12645918.3

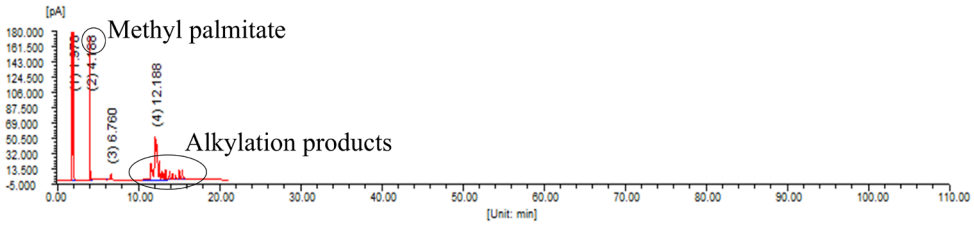

Fig. S133 Gas chromatogram of the product after the alkylation reaction.

Table S71 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.188	5.083
Integrated peak area	361894.6	23112.7

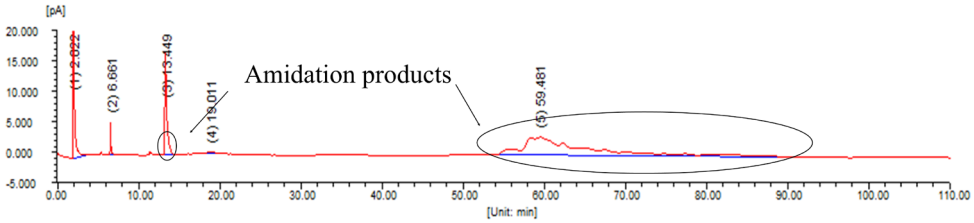

Fig. S134 Gas chromatogram of products after the amidation reaction.

Table S72 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~20.0	54.0~90.0
Integrated peak area	62175.1	2107452.4

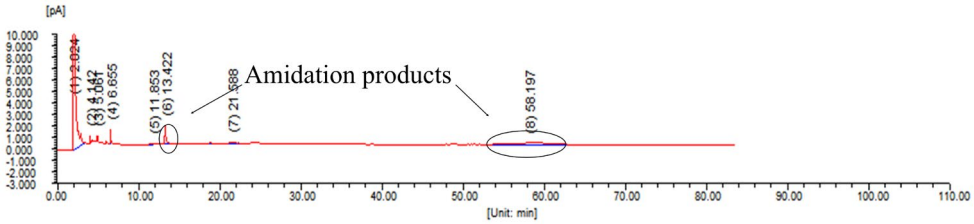

Fig. S135 Gas chromatogram of the product after the quaternization reaction.

Table S73 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~20.0	54.0~90.0
Integrated peak area	16674.7	56360.6

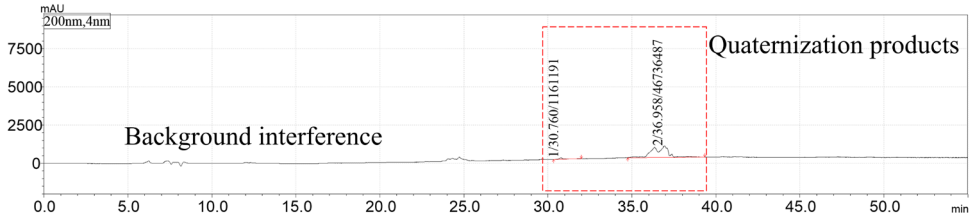

Fig. S136 Liquid chromatogram in liquid chromatography–mass spectrometry test of the ninth combination product derived from moderate-linoleic-acid-content raw materials.

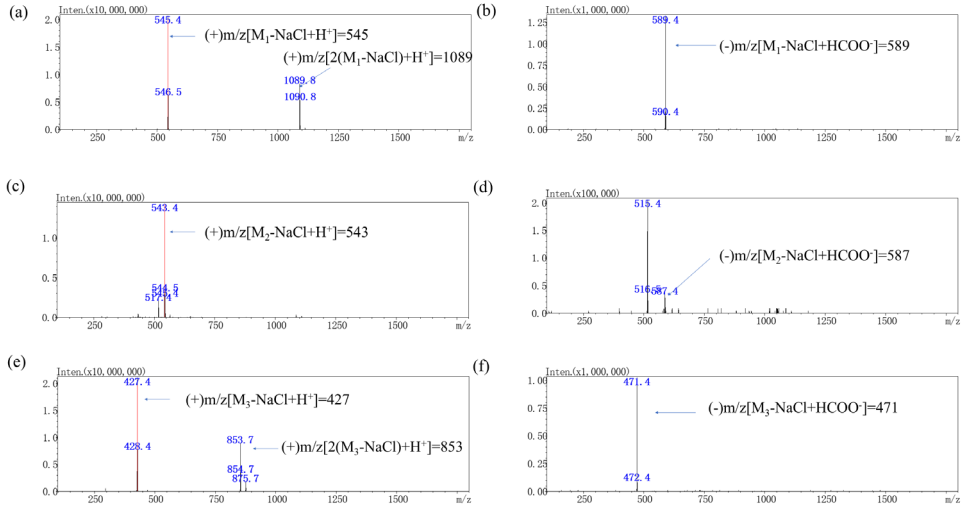

Fig. S137 Mass spectrum of the ninth combination product derived from moderate-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

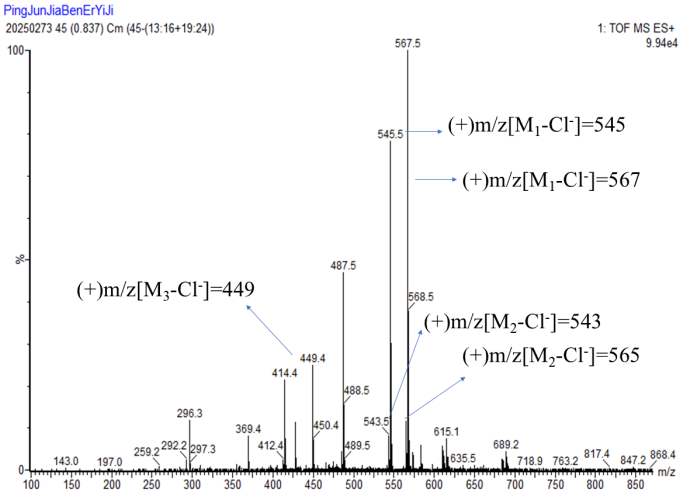

Fig. S138 Electrospray mass spectrum of the product prepared from the ninth combination of raw materials with a moderate linoleic acid content.

2.3 The GC-MS, HPLC-MS, and ESI-MS spectra of products synthesized from raw materials with a high linoleic/oleic acid ratio

2.3.1 Combination 1: Benzene as the alkylation reagent, N,N-dimethylethylenediamine as the amidation reagent, and sodium 3-chloro-2-hydroxypropane sulfonate as the quaternization reagent

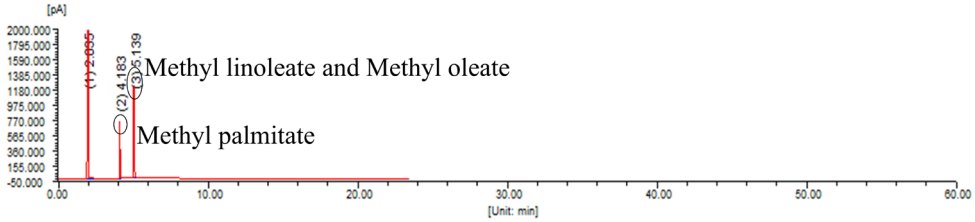

Fig. S139 Gas chromatogram of the mixed fatty acid raw materials.

Table S74 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.183	5.139
Integrated peak area	1616571.6	6138457.9

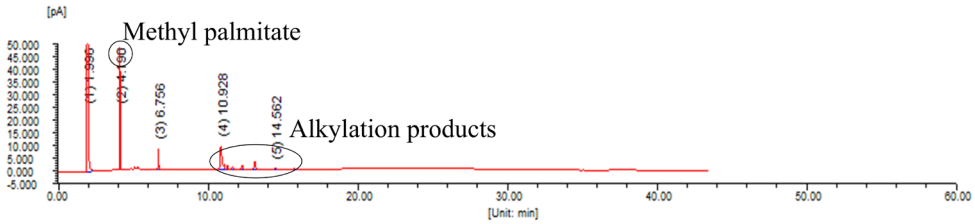

Fig. S140 Gas chromatogram of the product after the alkylation reaction.

Table S75 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.190	5.139
Integrated peak area	90718.9	18362.3

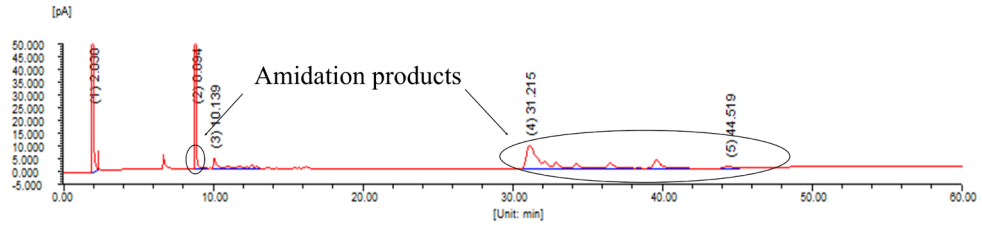

Fig. S141 Gas chromatogram of products after the amidation reaction.

Table S76 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~15.0	25.0~46.0
Integrated peak area	100732.1	1016922.0

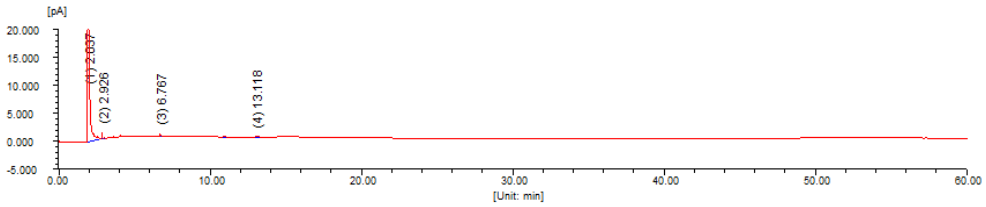

Fig. S142 Gas chromatogram of the product after the quaternization reaction.

Table S77 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~15.0	25.0~46.0
Integrated peak area	4370.4	2812.3

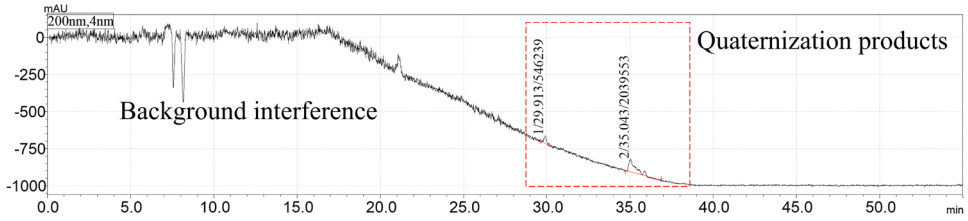

Fig. S143 Liquid chromatogram in liquid chromatography–mass spectrometry test of the first combination product derived from high-linoleic-acid-content raw materials.

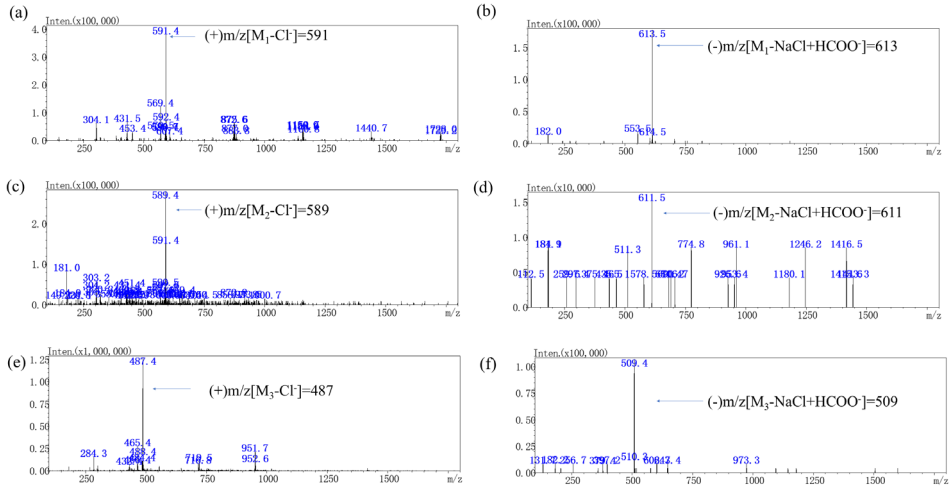

Fig. S144 Mass spectrum of the first combination product derived from high-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

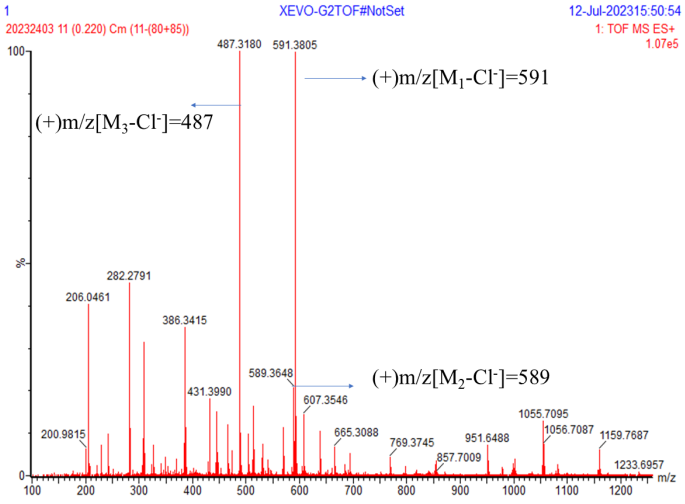

Fig. S145 Electrospray mass spectrum of the product prepared from the first combination of raw materials with a high linoleic acid content.

2.3.2 Combination 2: Benzene was used as the alkylation reagent, N,N-dimethyl-1,3-propanediamine as the amidation reagent, and sodium chloroacetate as the quaternization reagent

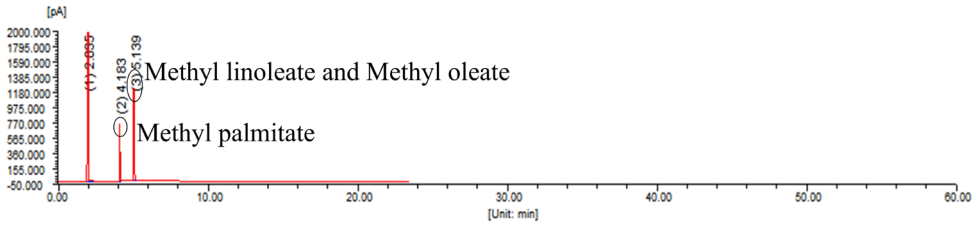

Fig. S146 Gas chromatogram of the mixed fatty acid raw materials.

Table S78 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.183	5.139
Integrated peak area	1618489.2	6239668.1

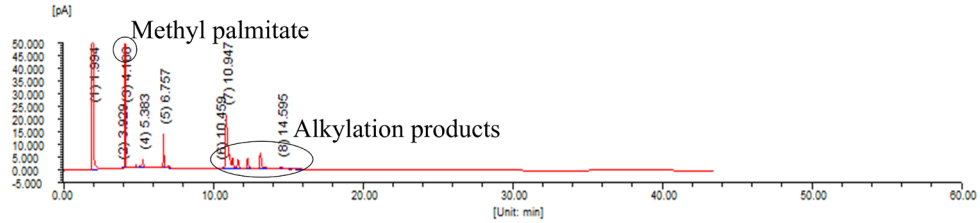

Fig. S147 Gas chromatogram of the product after the alkylation reaction.

Table S79 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.180	5.139
Integrated peak area	96923.3	21723.2

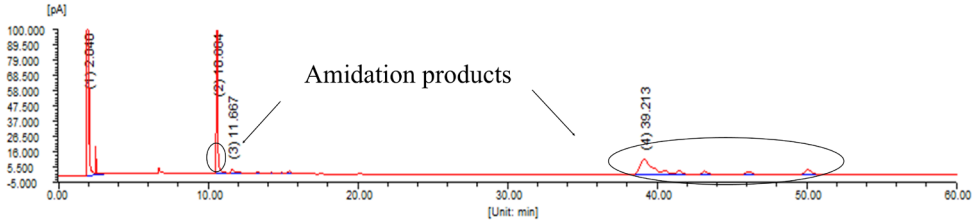

Fig. S148 Gas chromatogram of products after the amidation reaction.

Table S80 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~15.0	38.0~58.0
Integrated peak area	123664.9	1292556.2

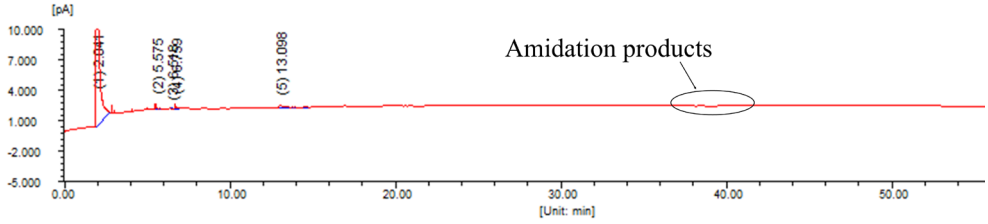

Fig. S149 Gas chromatogram of the product after the quaternization reaction.

Table S81 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~15.0	38.0~58.0
Integrated peak area	18718.5	19363.4

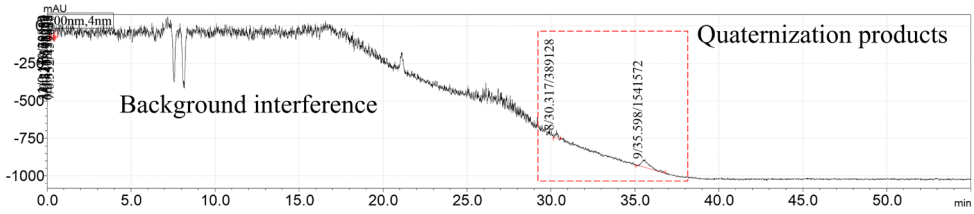

Fig. S150 Liquid chromatogram in liquid chromatography–mass spectrometry test of the second combination product derived from high-linoleic-acid-content raw materials.

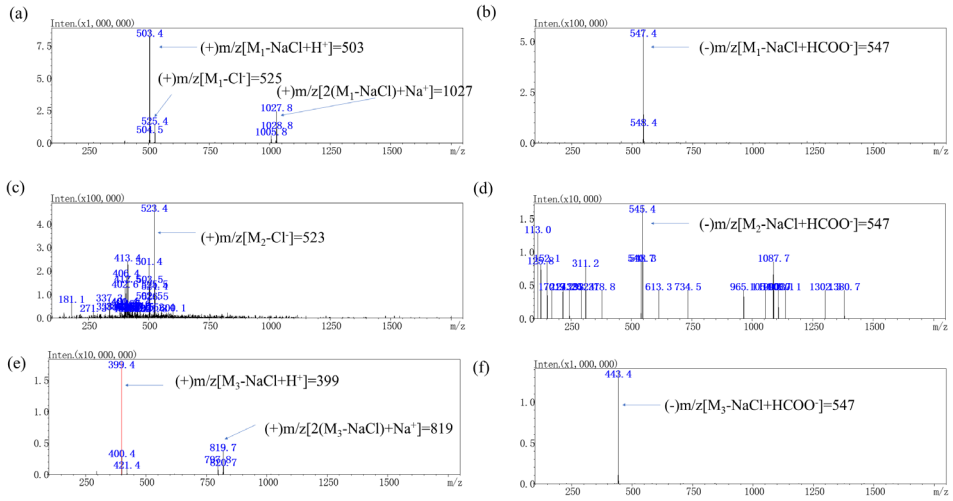

Fig. S151 Mass spectrum of the second combination product derived from high-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

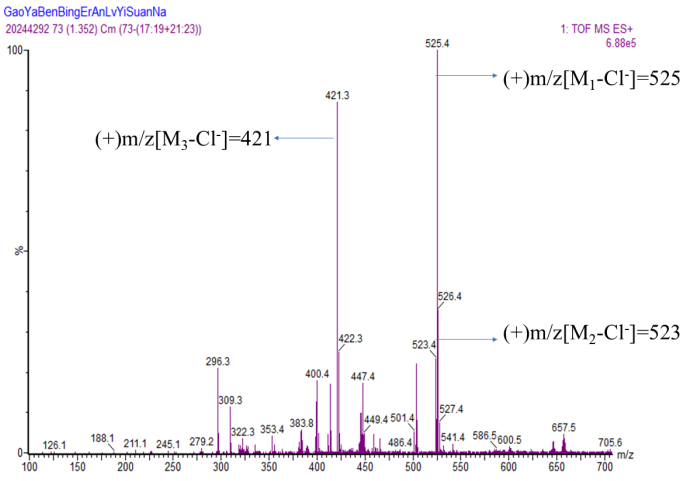

Fig. S152 Electrospray mass spectrum of the product prepared from the second combination of raw materials with a high linoleic acid content.

2.3.3 Combination 3: Benzene was used as the alkylation reagent, N,N-diethyl-1,3-propanediamine as the amidation reagent, and butanesultone as the quaternization reagent

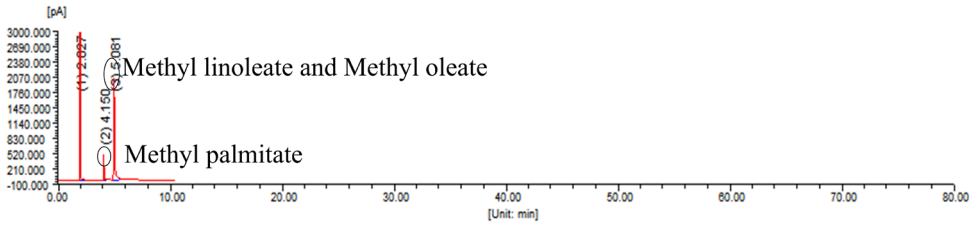

Fig. S153 Gas chromatogram of the mixed fatty acid raw materials.

Table S82 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.150	5.081
Integrated peak area	2126530.6	13513226.6

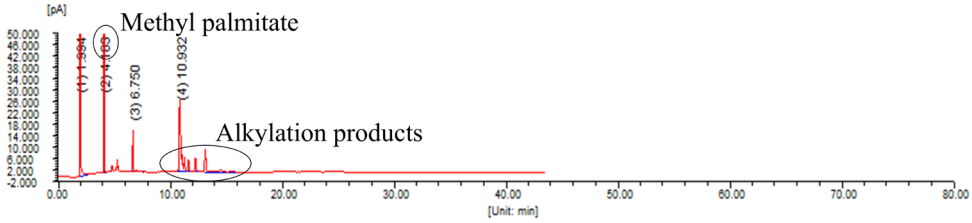

Fig. S154 Gas chromatogram of the product after the alkylation reaction.

Table S83 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.160	5.081
Integrated peak area	237075.7	45248.6

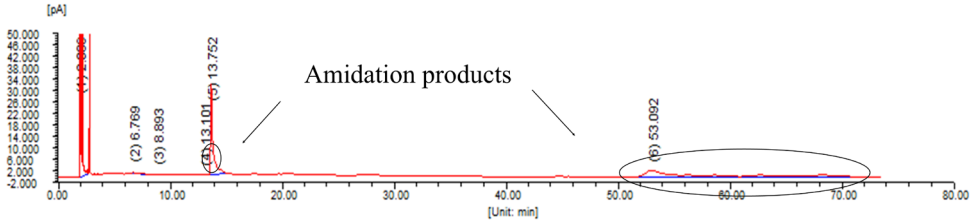

Fig. S155 Gas chromatogram of products after the amidation reaction.

Table S84 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~15.0	50.0~72.0
Integrated peak area	56576.6	584655.8

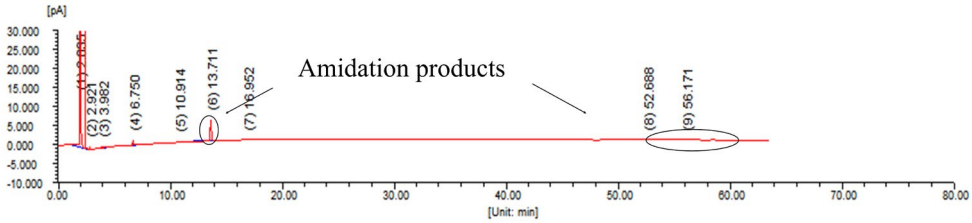

Fig. S156 Gas chromatogram of the product after the quaternization reaction.

Table S85 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~15.0	50.0~72.0
Integrated peak area	19324.5	18719.6

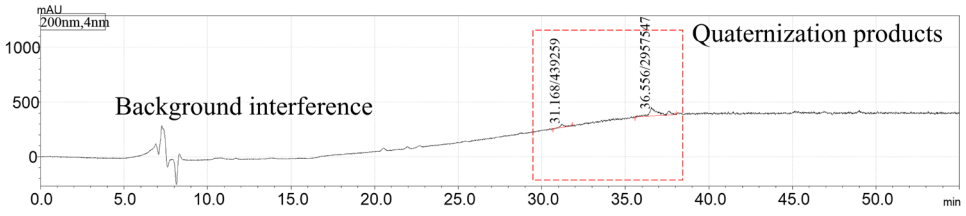

Fig. S157 Liquid chromatogram in liquid chromatography–mass spectrometry test of the third combination product derived from high-linoleic-acid-content raw materials.

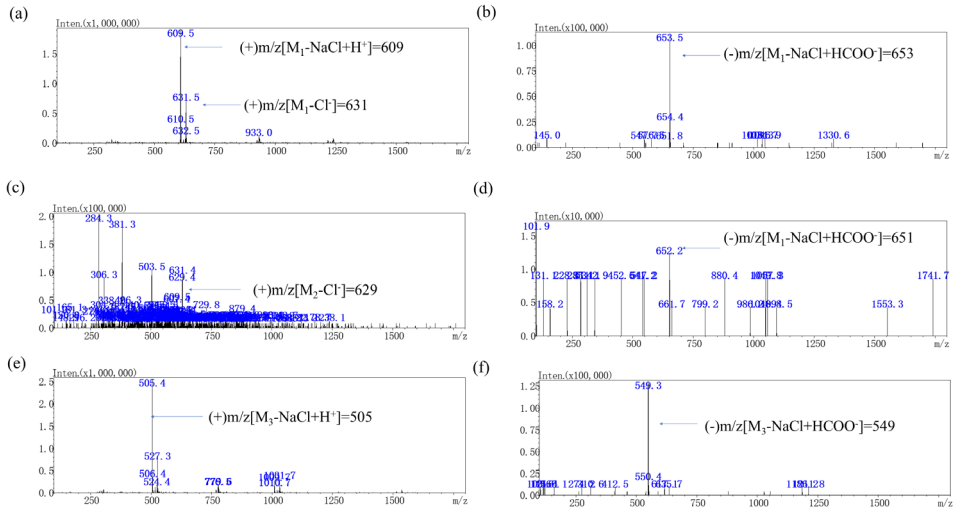

Fig. S158 Mass spectrum of the third combination product derived from high-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

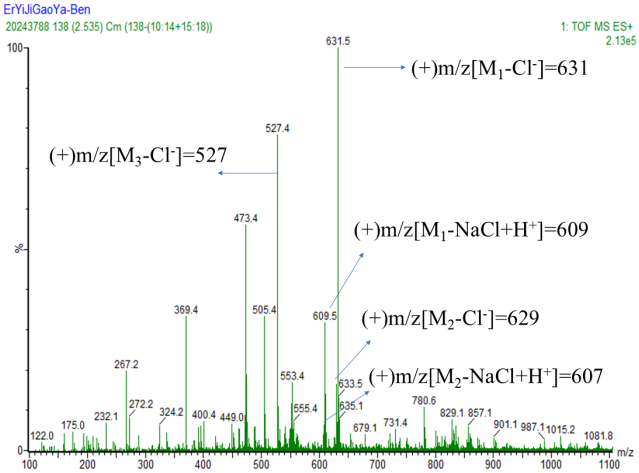

Fig. S159 Electrospray mass spectrum of the product prepared from the third combination of raw materials with a high linoleic acid content.

2.3.4 Combination 4: Anisole was used as the alkylation reagent, N,N-dimethylethylenediamine as the amidation reagent, and sodium chloroacetate as the quaternization reagent

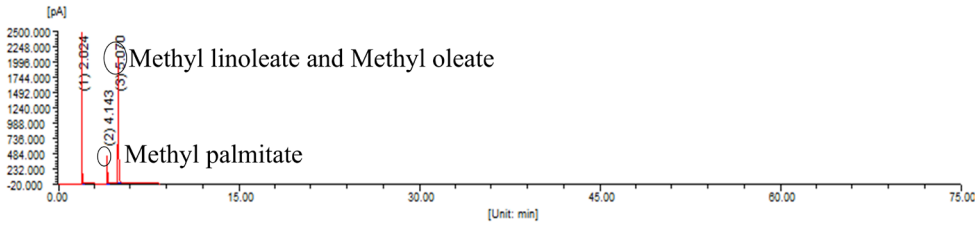

Fig. S160 Gas chromatogram of the mixed fatty acid raw materials.

Table S86 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.143	5.070
Integrated peak area	1665863.3	16232728.3

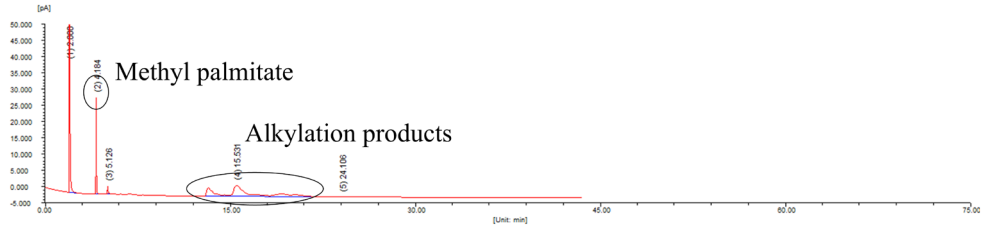

Fig. S161 Gas chromatogram of the product after the alkylation reaction.

Table S87 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.184	5.070
Integrated peak area	80950.0	15478.6

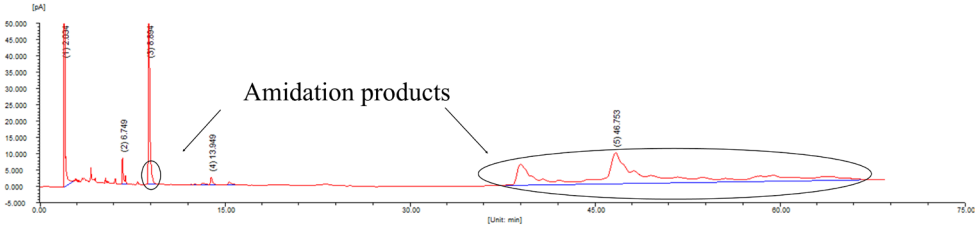

Fig. S162 Gas chromatogram of products after the amidation reaction.

Table S88 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~25.0	38.0~68.0
Integrated peak area	112152.1	2829990.2

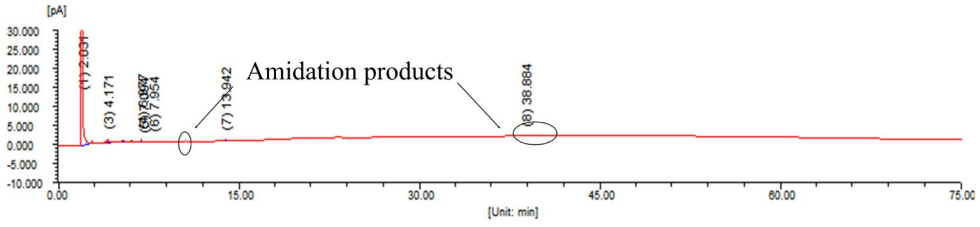

Fig. S163 Gas chromatogram of the product after the quaternization reaction.

Table S89 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~25.0	38.0~68.0
Integrated peak area	9533.4	5895.1

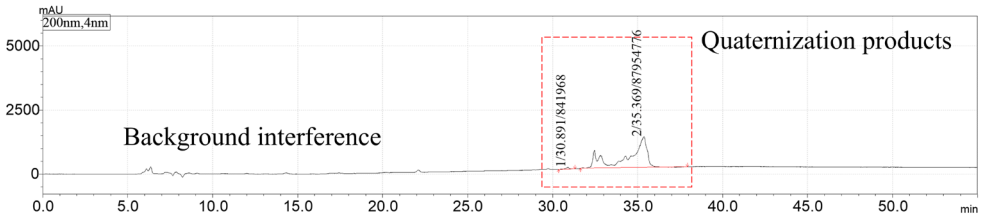

Fig. S164 Liquid chromatogram in liquid chromatography–mass spectrometry test of the fourth combination product derived from high-linoleic-acid-content raw materials.

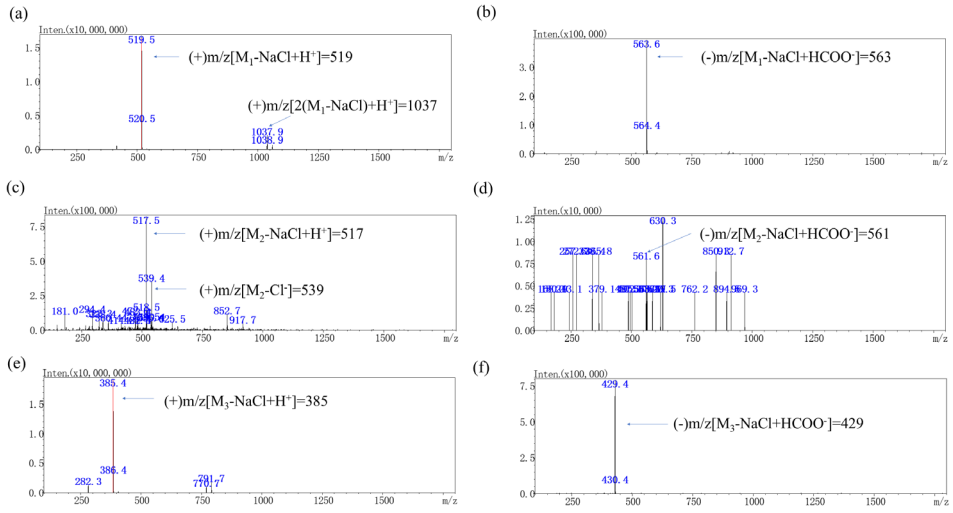

Fig. S165 Mass spectrum of the fourth combination product derived from high-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

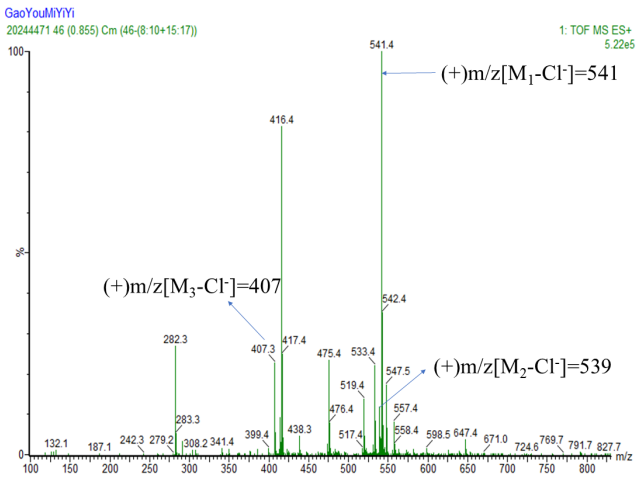

Fig. S166 Electrospray mass spectrum of the product prepared from the fourth combination of raw materials with a high linoleic acid content.

2.3.5 Combination 5: Anisole was used as the alkylation reagent, N,N-dimethyl-1,3-propanediamine as the amidation reagent, and butanesultone as the quaternization reagent

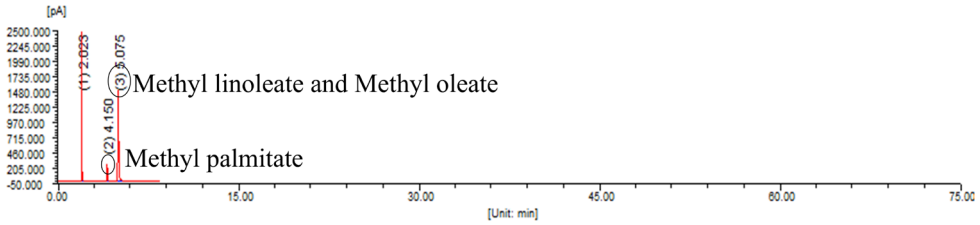

Fig. S167 Gas chromatogram of the mixed fatty acid raw materials.

Table S90 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.150	5.075
Integrated peak area	1374356.9	10688654.5

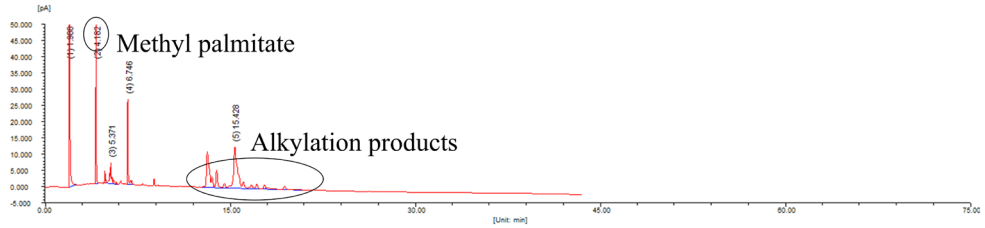

Fig. S168 Gas chromatogram of the product after the alkylation reaction.

Table S91 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.182	5.075
Integrated peak area	360874.9	69950.5

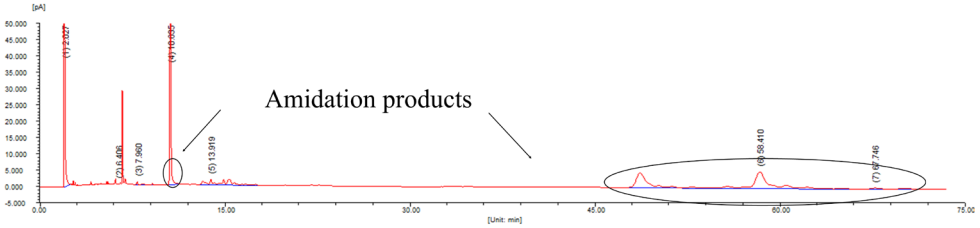

Fig. S169 Gas chromatogram of products after the amidation reaction.

Table S92 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~25.0	44.0~80.0
Integrated peak area	91374.6	822371.5

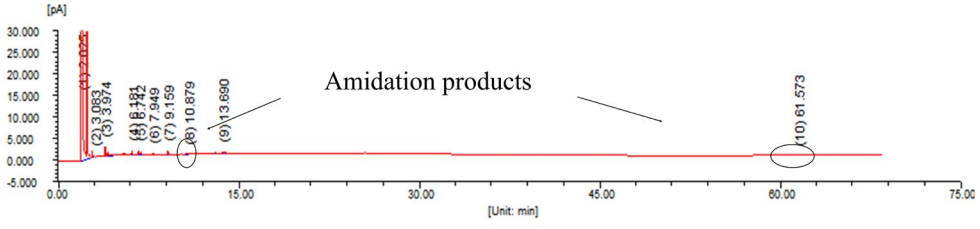

Fig. S170 Gas chromatogram of the product after the quaternization reaction.

Table S93 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~25.0	44.0~80.0
Integrated peak area	17547.7	5525.7

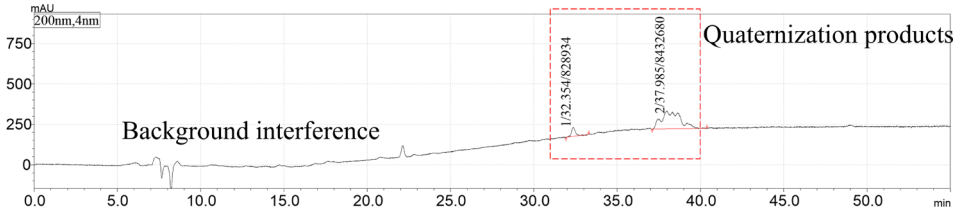

Fig. S171 Liquid chromatogram in liquid chromatography–mass spectrometry test of the fifth combination product derived from high-linoleic-acid-content raw materials.

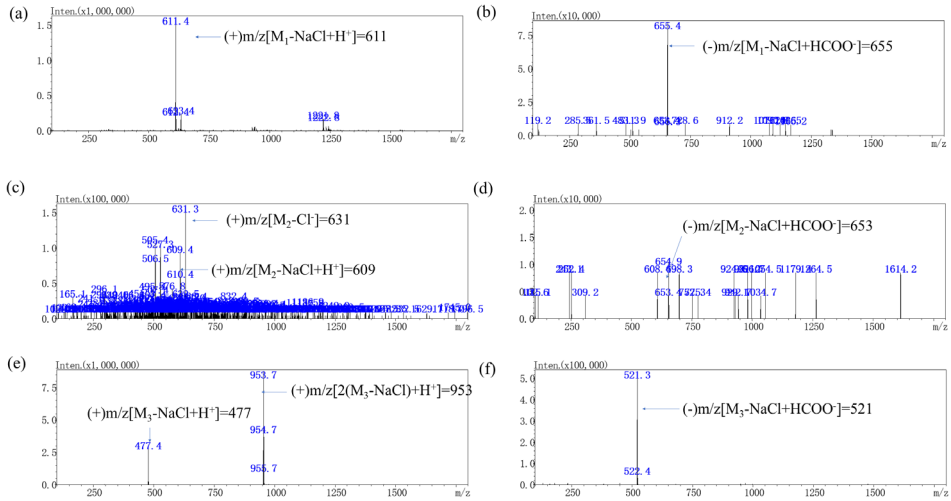

Fig. S172 Mass spectrum of the fifth combination product derived from high-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

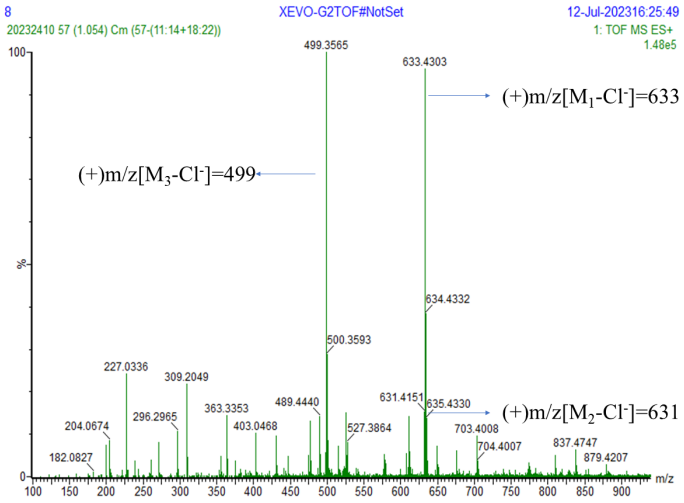

Fig. S173 Electrospray mass spectrum of the product prepared from the fifth combination of raw materials with a high linoleic acid content.

2.3.6 Combination 6: Anisole was used as the alkylation reagent, N,N-diethyl-1,3-propanediamine as the amidation reagent, and sodium 3-chloro-2-hydroxypropane sulfonate as the quaternization reagent

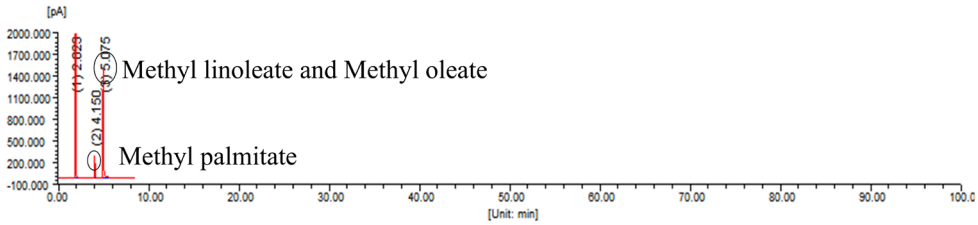

Fig. S174 Gas chromatogram of the mixed fatty acid raw materials.

Table S94 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.150	5.075
Integrated peak area	1057763.2	8122036.7

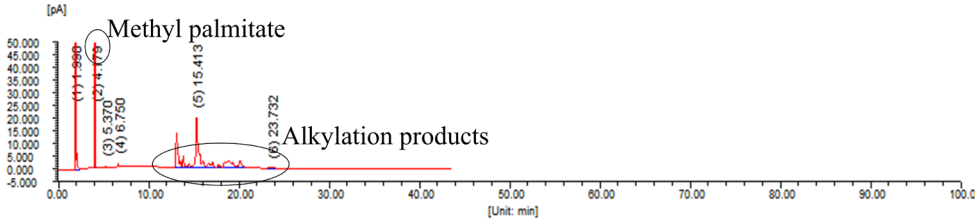

Fig. S175 Gas chromatogram of the product after the alkylation reaction.

Table S95 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.179	5.075
Integrated peak area	218756.3	7513.2

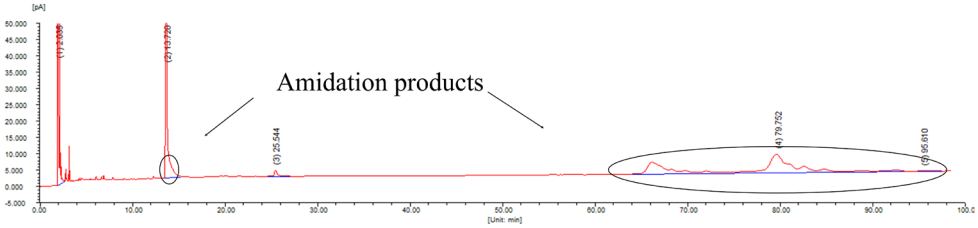

Fig. S176 Gas chromatogram of products after the amidation reaction.

Table S96 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~25.0	65.0~95.0
Integrated peak area	120444.9	1768769.5

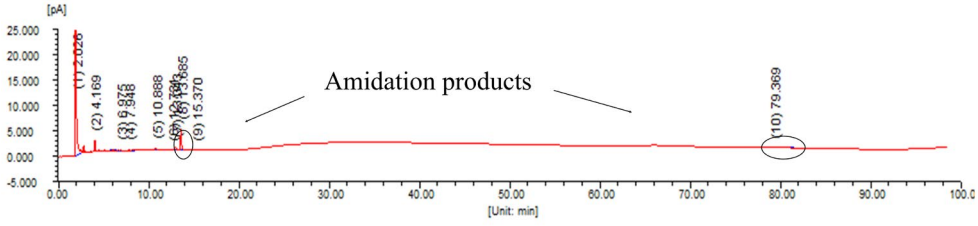

Fig. S177 Gas chromatogram of the product after the quaternization reaction.

Table S97 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~25.0	65.0~95.0
Integrated peak area	54098.5	75632.6

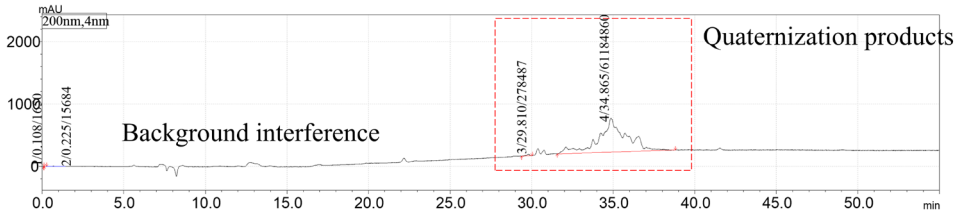

Fig. S178 Liquid chromatogram in liquid chromatography–mass spectrometry test of the sixth combination product derived from high-linoleic-acid-content raw materials.

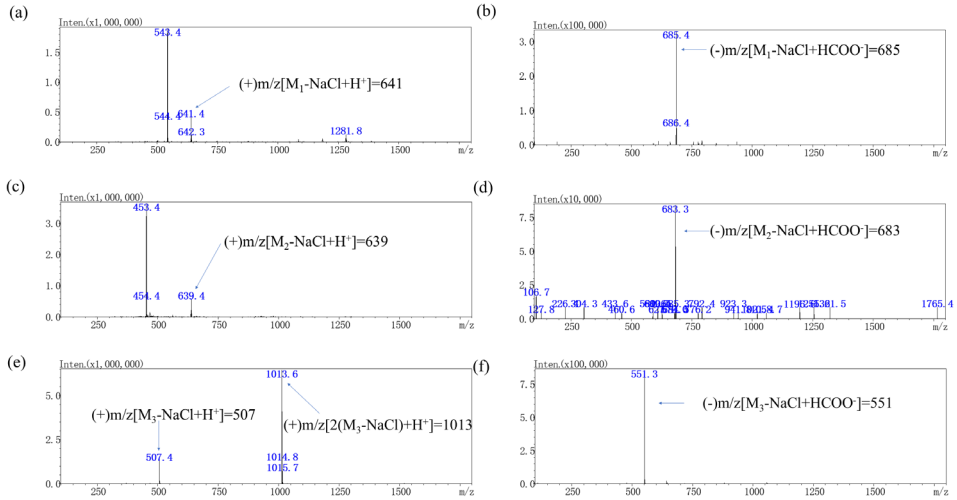

Fig. S179 Mass spectrum of the sixth combination product derived from high-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

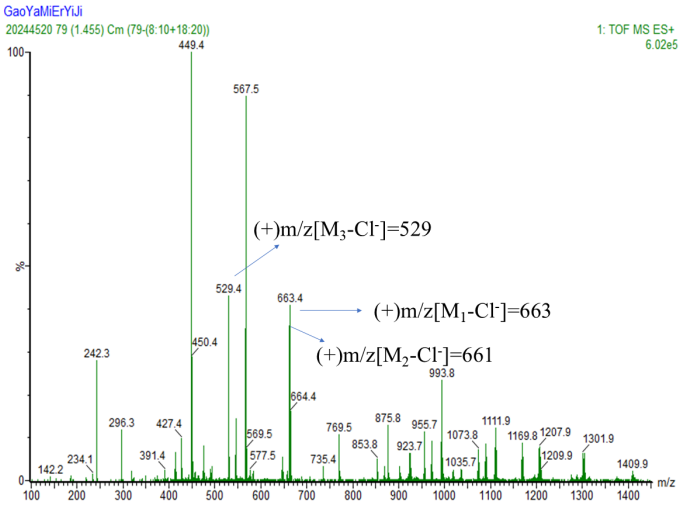

Fig. S180 Electrospray mass spectrum of the product prepared from the sixth combination of raw materials with a high linoleic acid content.

2.3.7 Combination 7: Toluene was used as the alkylation reagent, N,N-dimethylethylenediamine as the amidation reagent, and butanesultone as the quaternization reagent

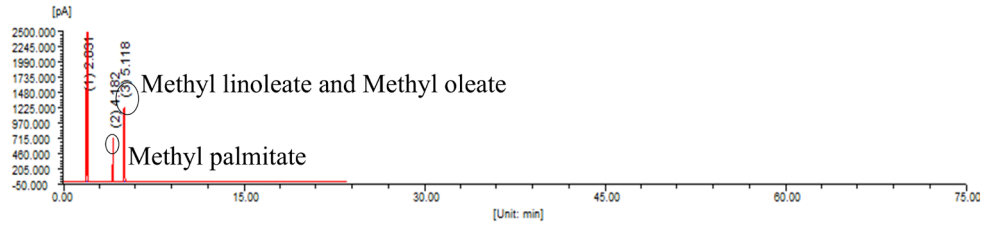

Fig. S181 Gas chromatogram of the mixed fatty acid raw materials.

Table S98 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.182	5.118
Integrated peak area	1535414.4	6112370.0

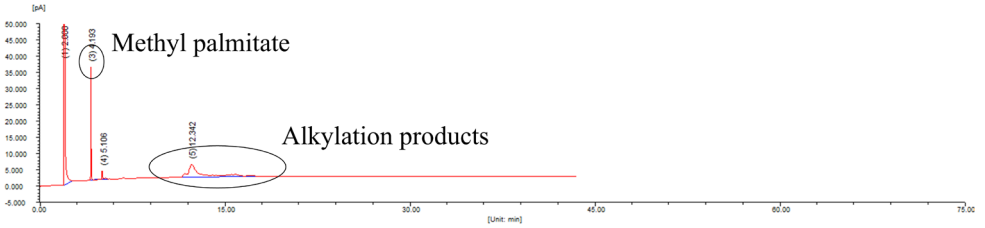

Fig. S182 Gas chromatogram of the product after the alkylation reaction.

Table S99 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.193	5.108
Integrated peak area	85892.7	16364.0

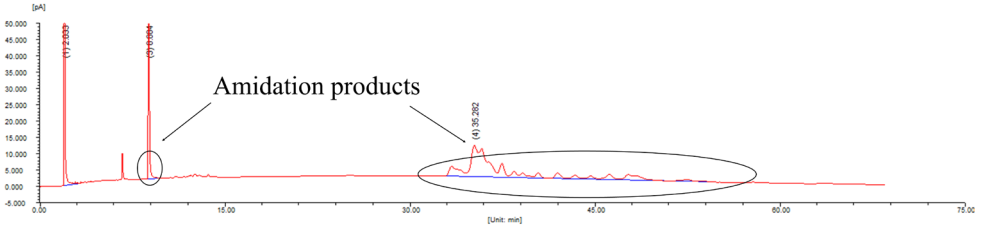

Fig. S183 Gas chromatogram of products after the amidation reaction.

Table S100 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~20.0	32.0~60.0
Integrated peak area	53939.7	1734143.3

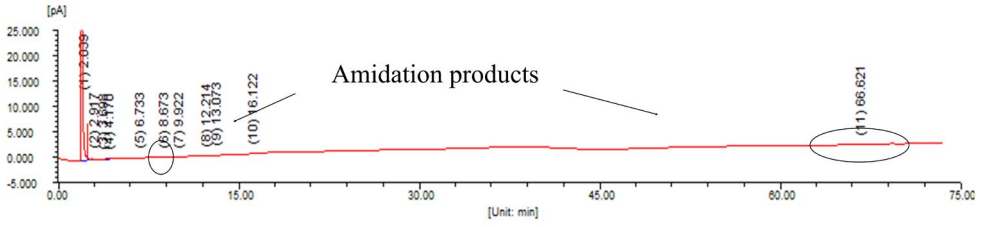

Fig. S184 Gas chromatogram of the product after the quaternization reaction.

Table S101 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~20.0	32.0~60.0
Integrated peak area	4117.6	9433.1

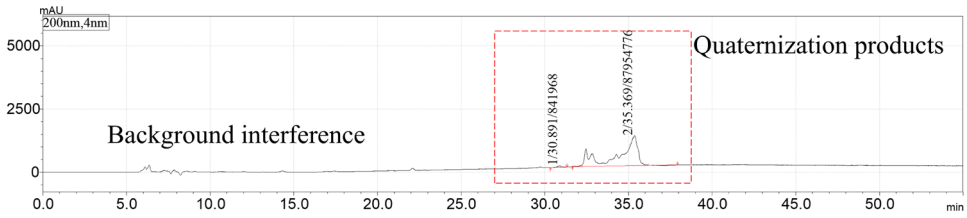

Fig. S185 Liquid chromatogram in liquid chromatography–mass spectrometry test of the seventh combination product derived from high-linoleic-acid-content raw materials.

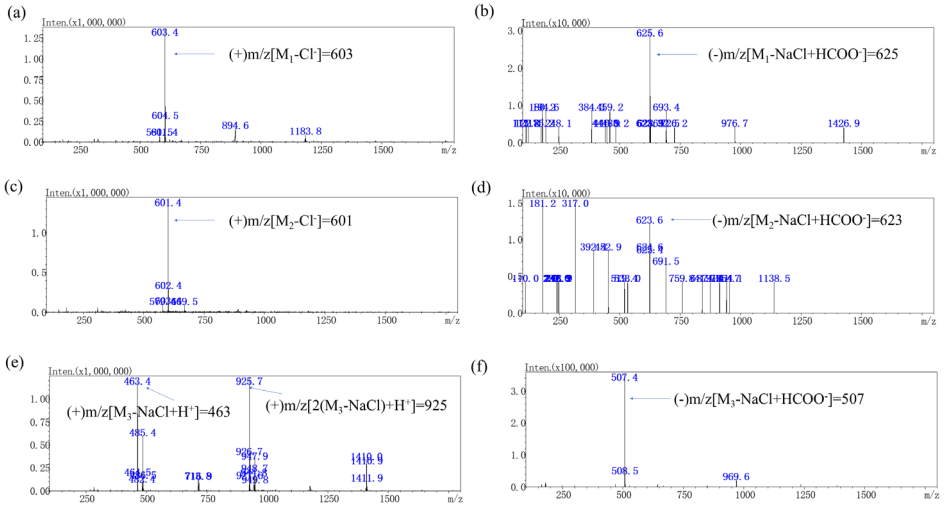

Fig. S186 Mass spectrum of the seventh combination product derived from high-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

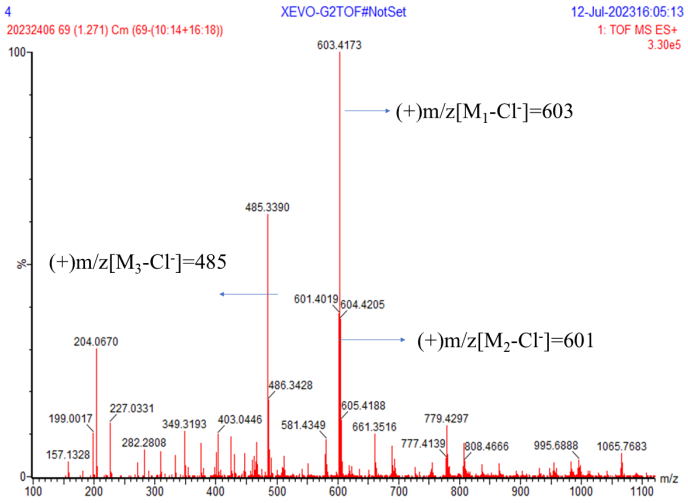

Fig. S187 Electrospray mass spectrum of the product prepared from the seventh combination of raw materials with a high linoleic acid content.

2.3.8 Combination 8: Toluene was used as the alkylation reagent, N,N-dimethyl-1,3-propanediamine as the amidation reagent, and sodium 3-chloro-2-hydroxypropane sulfonate as the quaternization reagent

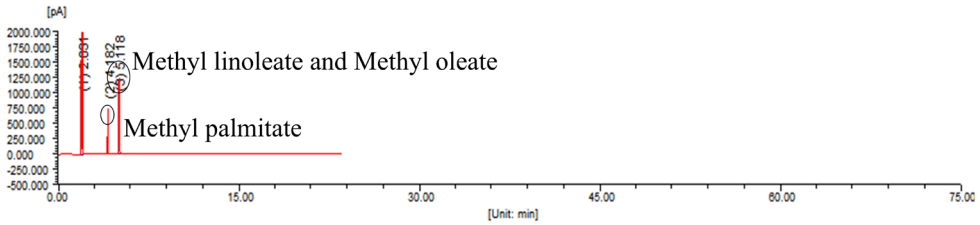

Fig. S188 Gas chromatogram of the mixed fatty acid raw materials.

Table S102 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.182	5.118
Integrated peak area	1520170.2	5860201.7

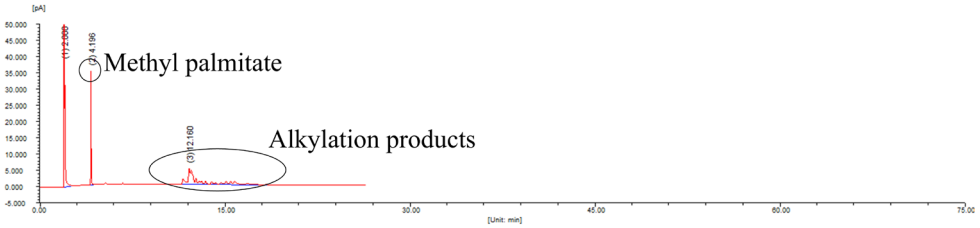

Fig. S189 Gas chromatogram of the product after the alkylation reaction.

Table S103 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.196	5.118
Integrated peak area	95658.1	10777.1

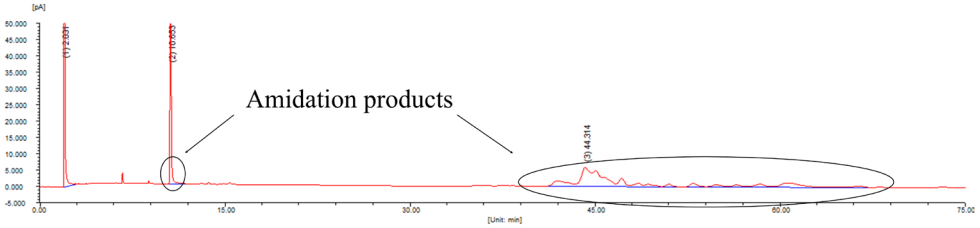

Fig. S190 Gas chromatogram of products after the amidation reaction.

Table S104 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~20.0	40.0~70.0
Integrated peak area	41802.1	1306201.2

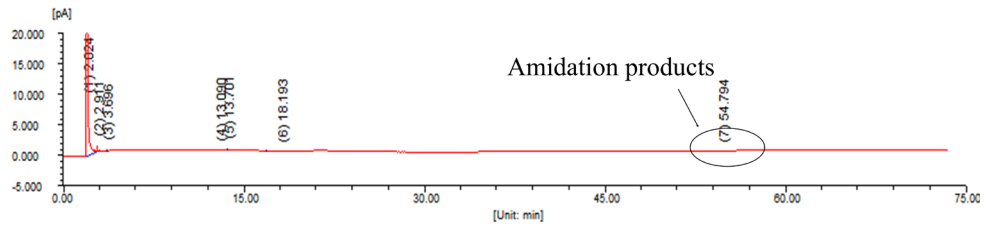

Fig. S191 Gas chromatogram of the product after the quaternization reaction.

Table S105 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~20.0	40.0~70.0
integrated peak area	2858.7	610.7

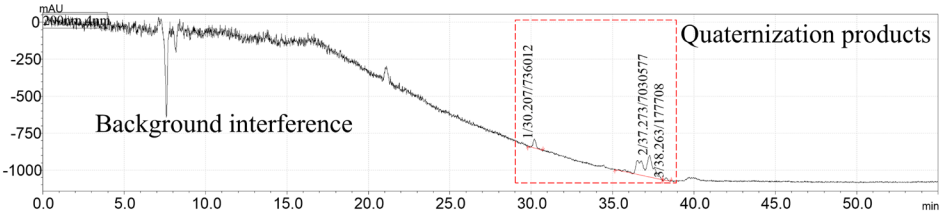

Fig. S192 Liquid chromatogram in liquid chromatography–mass spectrometry test of the eighth combination product derived from high-linoleic-acid-content raw materials.

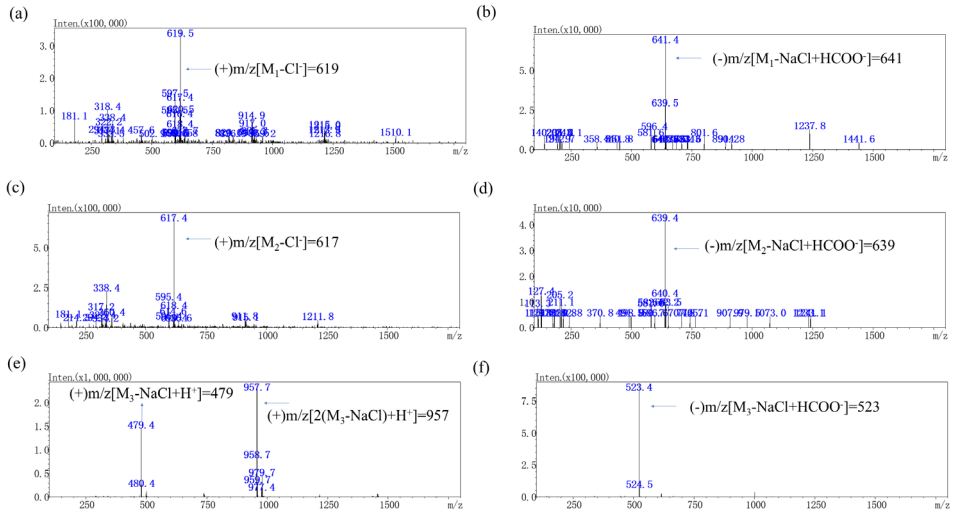

Fig. S193 Mass spectrum of the eighth combination product derived from high-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

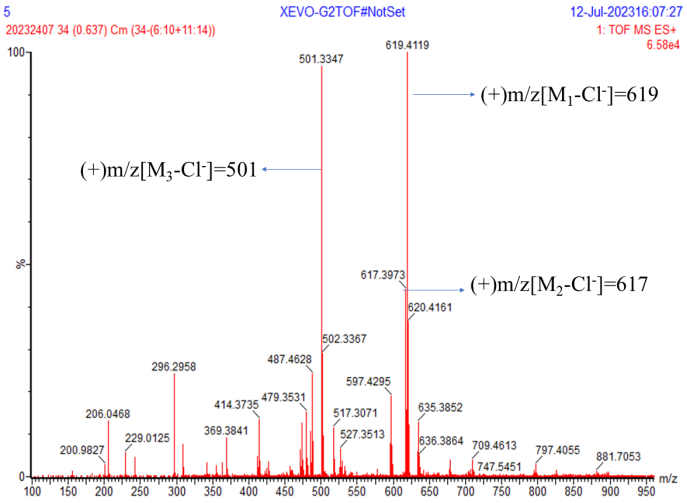

Fig. S194 Electrospray mass spectrum of the product prepared from the eighth combination of raw materials with a high linoleic acid content.

2.3.9 Combination 9: Toluene was used as the alkylation reagent, N,N-diethyl-1,3-propanediamine as the amidation reagent, and sodium chloroacetate as the quaternization reagent

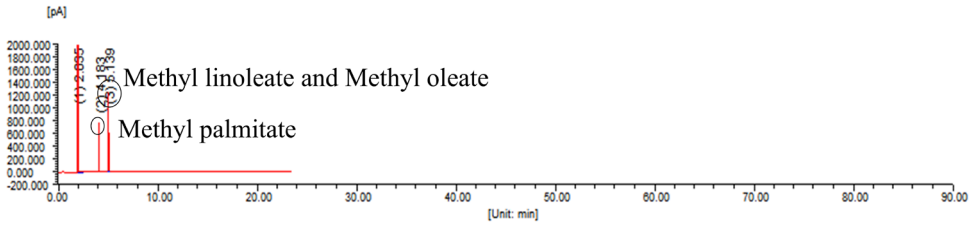

Fig. S195 Gas chromatogram of the mixed fatty acid raw materials.

Table S106 GC peak area of raw materials for conversion rate calculation.

Main component	Methyl palmitate (pre-reaction)	Methyl oleate and methyl linoleate (pre-reaction)
Retention time/min	4.183	5.139
Integrated peak area	1489369.7	6083304.7

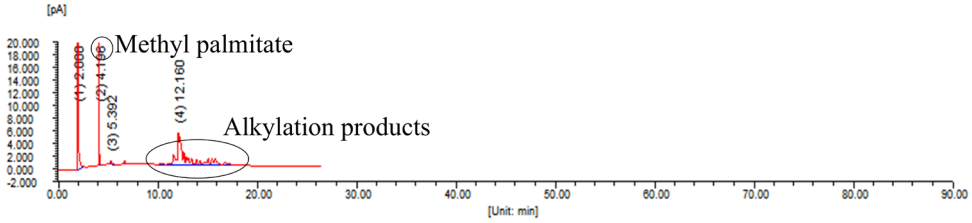

Fig. S196 Gas chromatogram of the product after the alkylation reaction.

Table S107 GC peak area of the alkylation reaction for conversion rate calculation.

Main component	Methyl palmitate (post-alkylation reaction)	Methyl oleate and methyl linoleate (post-alkylation reaction)
Retention time/min	4.196	5.139
Integrated peak area	96899.8	8336.8

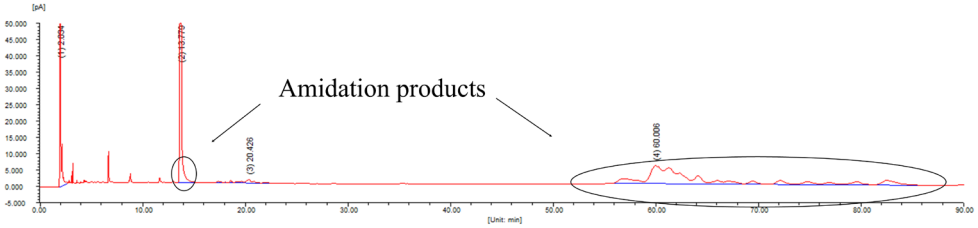

Fig. S197 Gas chromatogram of products after the amidation reaction.

Table S108 GC peak area of the amidation reaction for conversion rate calculation.

Main component	Alkylation products (post-amidation reaction)	Amidation products (post-amidation reaction)
Retention time/min	10.0~20.0	50.0~90.0
Integrated peak area	122389.5	2222827.1

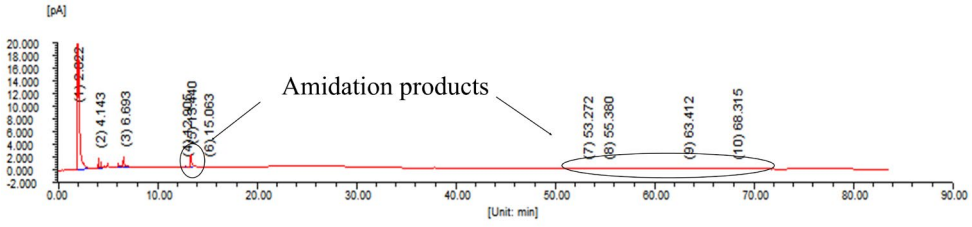

Fig. S198 Gas chromatogram of the product after the quaternization reaction.

Table S109 GC peak area of the quaternization reaction for conversion rate calculation.

Main component	Alkylation products (post-quaternization reaction)	Amidation products (post-quaternization reaction)
Retention time/min	10.0~20.0	50.0~90.0
Integrated peak area	3939.8	4944.1

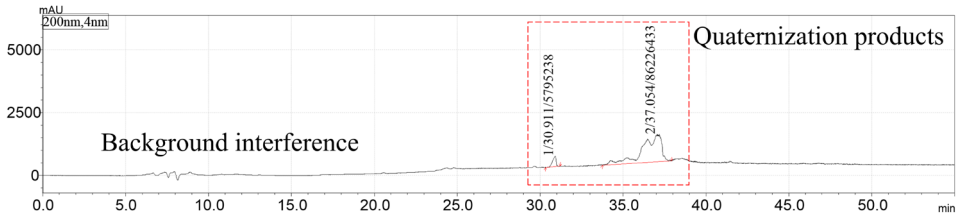

Fig. S199 Liquid chromatogram in liquid chromatography–mass spectrometry test of the ninth combination product derived from high-linoleic-acid-content raw materials.

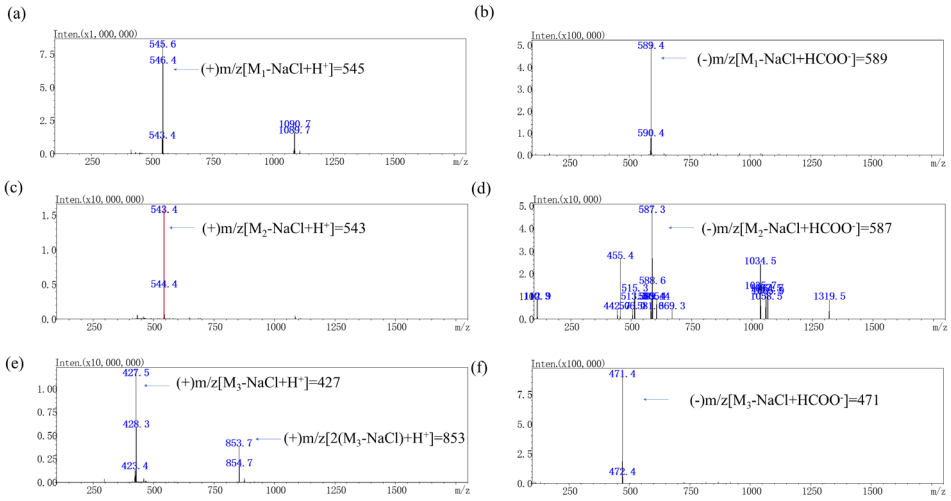

Fig. S200 Mass spectrum of the ninth combination product derived from high-linoleic-acid-content raw materials in liquid chromatography–mass spectrometry testing.

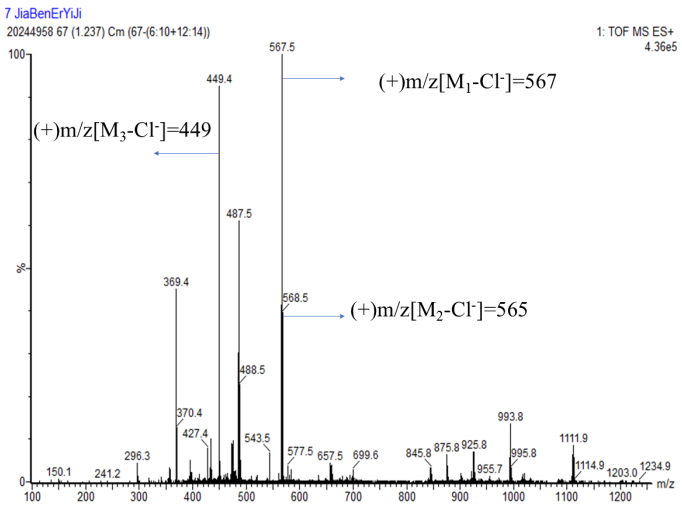

Fig. S201 Electrospray mass spectrum of the product prepared from the ninth combination of raw materials with a high linoleic acid content.

3 GC-MS, HPLC-MS, and ESI-MS spectra of surfactants synthesized from mixed fatty acids with varying PUFA contents using the optimal combination (phenyl methyl ether/N,N-

dimethylethylenediamine/sodium 3-chloro-2-hydroxypropane sulfonate)

3.1 GC, HPLC-MS, and ESI-MS of the surfactants synthesized from mixed fatty acid methyl esters with a low ratio of linoleic acid to oleic acid as raw materials (M_1, M_2, and M_3 represent products derived from methyl oleate, methyl linoleate, and methyl palmitate, respectively—note that M_1, M_2, and M_3 refer to different products in each step, with varying structures and molecular weights, although they originate from the same raw materials)

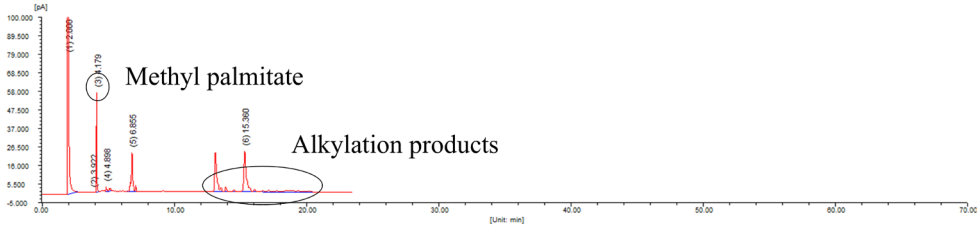

Fig. S202 Gas chromatogram of the product after the alkylation reaction.

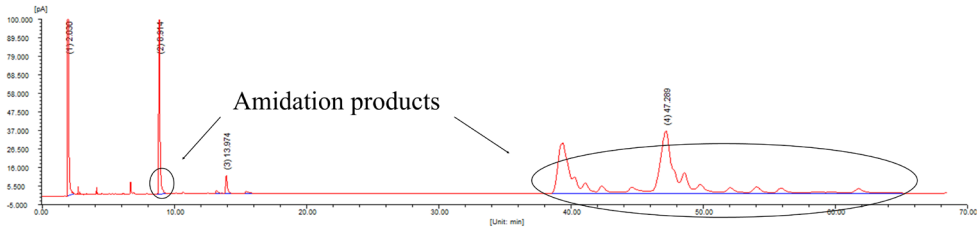

Fig. S203 Gas chromatogram of the product after the amidation reaction.

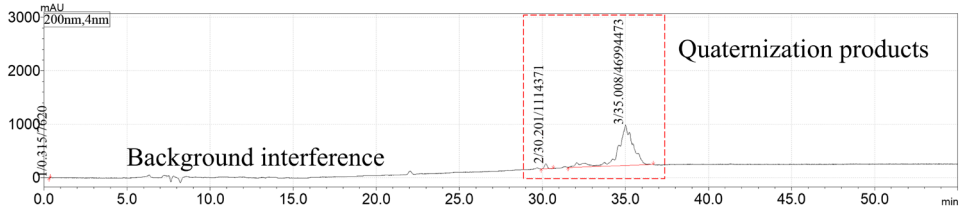

Fig. S204 Liquid chromatography profile of surfactants synthesized from raw materials with a low ratio of linoleic acid to oleic acid using the optimal reagent combination.

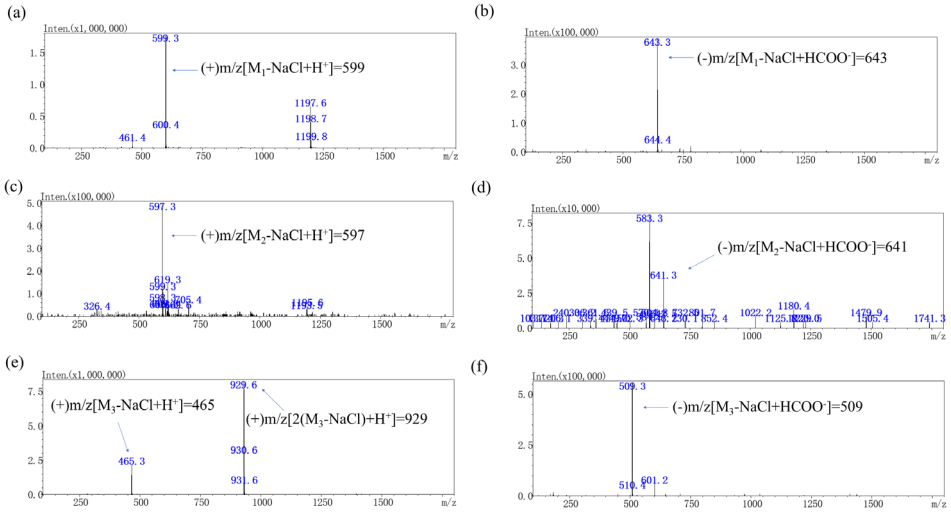

Fig. S205 Mass spectrum of surfactants synthesized from raw materials with a low ratio of linoleic acid to oleic acid using the optimal reagent combination.

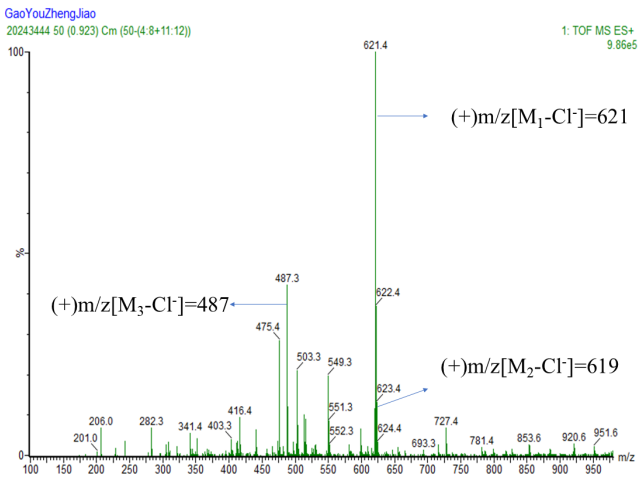

Fig. S206 Electrospray mass spectrum of surfactants synthesized from raw materials with a low ratio of linoleic acid to oleic acid using the optimal reagent combination.

3.2 GC, HPLC-MS, and ESI-MS of the surfactants synthesized from mixed fatty acid methyl esters with a moderate ratio of linoleic acid to oleic acid as raw materials (M_1, M_2, and M_3 represent products derived from methyl oleate, methyl linoleate, and methyl palmitate, respectively—note that M_1, M_2, and M_3 refer to different products in each step, with varying structures and molecular weights, although they originate from the same raw materials)

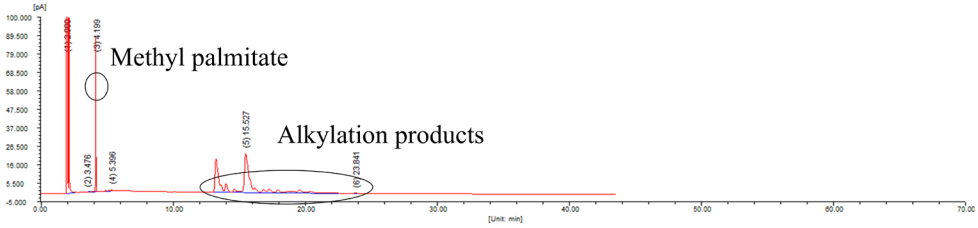

Fig. S207 Gas chromatogram of the product after the alkylation reaction.

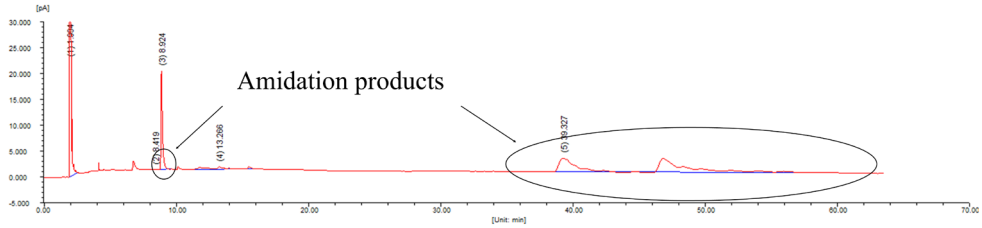

Fig. S208 Gas chromatogram of the product after the amidation reaction.

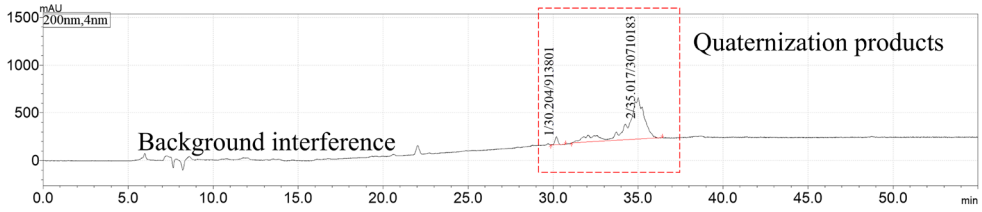

Fig. S209 Liquid chromatography profile of surfactants synthesized from raw materials with a moderate ratio of linoleic acid to oleic acid using the optimal reagent combination.

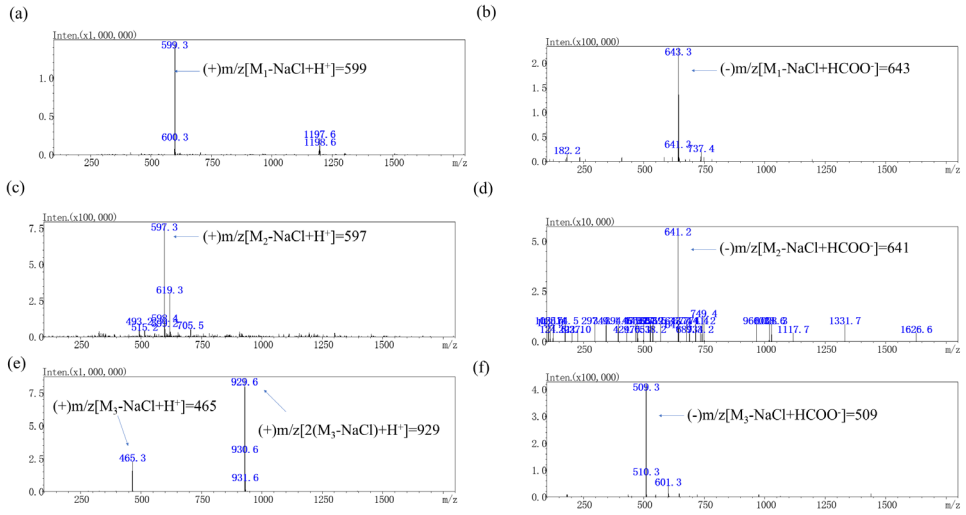

Fig. S210 Mass spectrum of surfactants synthesized from raw materials with a moderate ratio of linoleic acid to oleic acid using the optimal reagent combination.

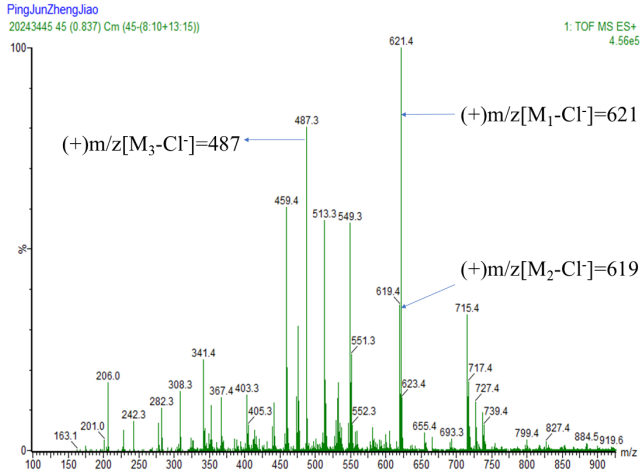

Fig. S211 Interfacial tension profile of surfactants synthesized from raw materials with a moderate ratio of linoleic acid to oleic acid using the optimal reagent combination.

3.3 ***GC, HPLC-MS, and ESI-MS of the surfactants synthesized from mixed fatty acid methyl esters with a high ratio of linoleic acid to oleic acid as raw materials (M1, M2, and M3 represent products derived from methyl oleate, methyl linoleate, and methyl palmitate, respectively—note that M1, M2, and M3 refer to different products in each step, with varying structures and molecular weights, although they originate from the same raw materials)***

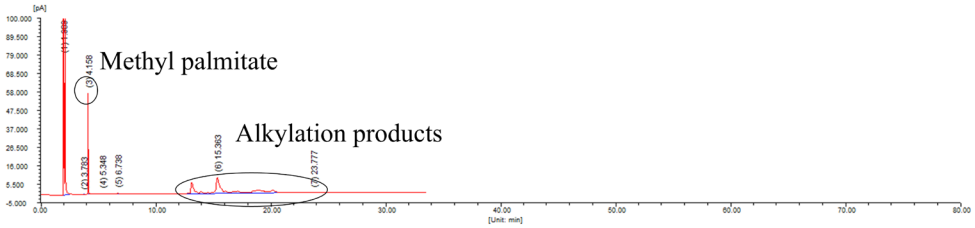

Fig. S212 Gas chromatogram of the product after the alkylation reaction.

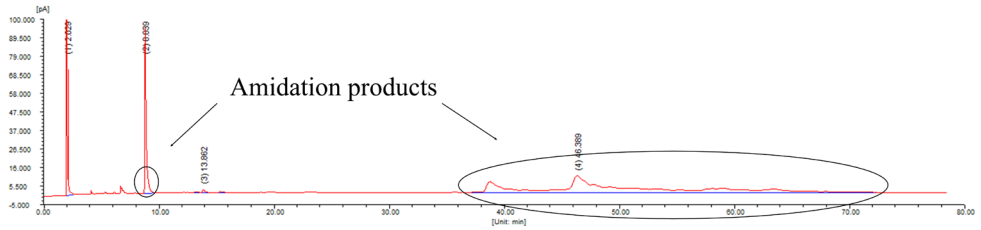

Fig. S213 Gas chromatogram of the product after the amidation reaction.

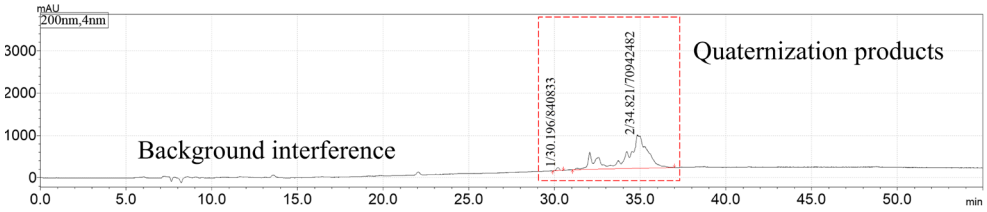

Fig. S214 Liquid chromatography profile of surfactants synthesized from raw materials with a high ratio of linoleic acid to oleic acid using the optimal reagent combination.

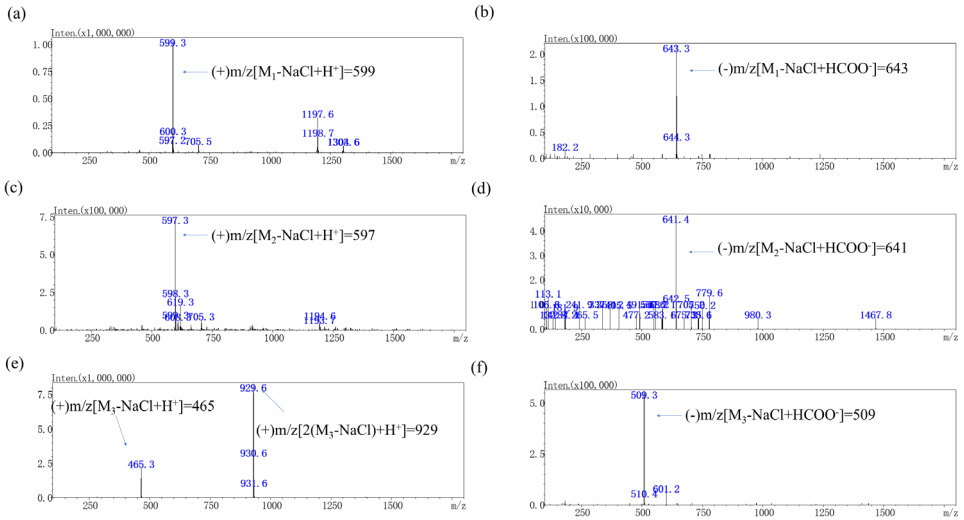

Fig. S215 Mass spectrum of surfactants synthesized from raw materials with a high ratio of linoleic acid to oleic acid using the optimal reagent combination.

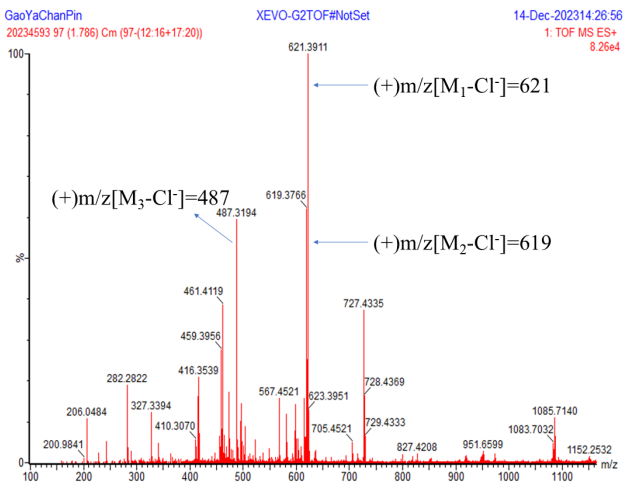

Fig. S216 Interfacial tension profile of surfactants synthesized from raw materials with a high ratio of

linoleic acid to oleic acid using the optimal reagent combination.

4 GC-MS, HPLC-MS, and ESI-MS spectra of surfactants synthesized from different waste oils using the optimal combination (phenyl methyl ether/N,N-dimethylethylenediamine/sodium 3-chloro-2-hydroxypropane sulfonate)

4.1 GC-MS, HPLC-MS, and ESI-MS spectra of surfactants synthesized from waste rapeseed oil (M_1–M_4 correspond to products derived from methyl oleate, methyl linoleate, methyl palmitate, and methyl stearate, respectively; GC conditions: 260 °C for 2 min, heated at 20 °C/min to 290 °C, then held as shown in each figure)

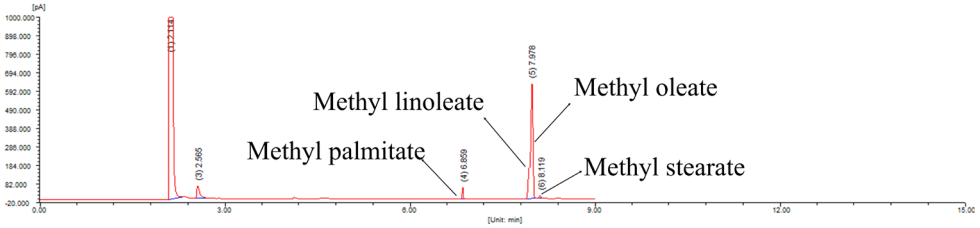

Fig. S217 Gas chromatography profile of mixed fatty acid methyl esters obtained from the transesterification of waste rapeseed oil (initial temperature is set to 200 °C for 2 minutes, followed by a temperature ramp to 290 °C at a rate of 20 °C/min for 10 minutes).

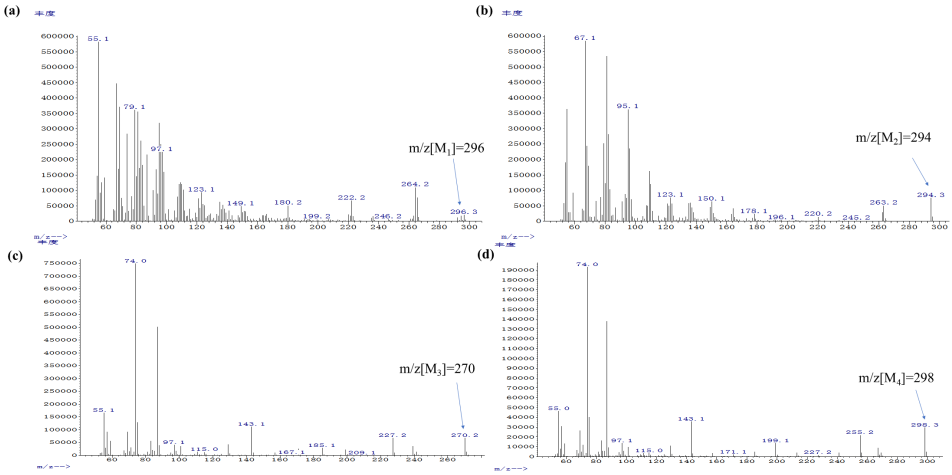

Fig. S218 Mass spectrum of mixed fatty acid methyl esters obtained from the transesterification of waste rapeseed oil.

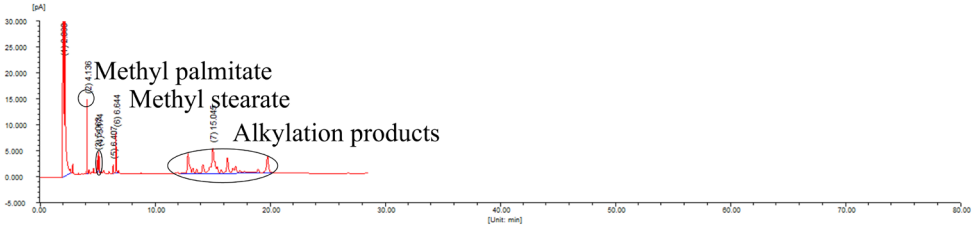

Fig. S219 Gas chromatography profile of the alkylated raw materials after transesterification of waste rapeseed oil.

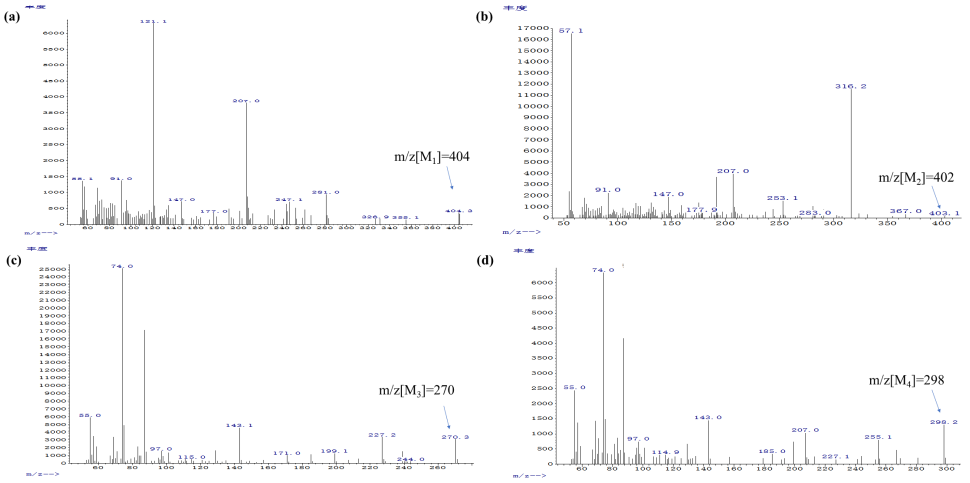

Fig. S220 Mass spectrum of the alkylated raw materials after transesterification of waste rapeseed oil.

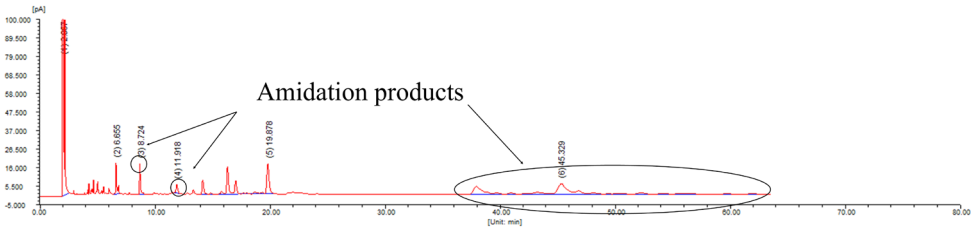

Fig. S221 The gas chromatography profile of the transesterified raw materials after amidation.

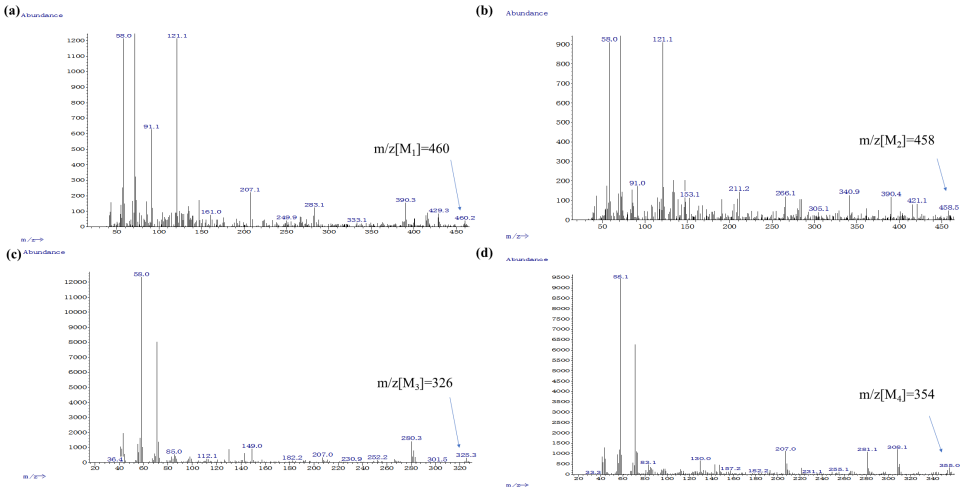

Fig. S222 Mass spectrum of the transesterified raw materials after amidation.

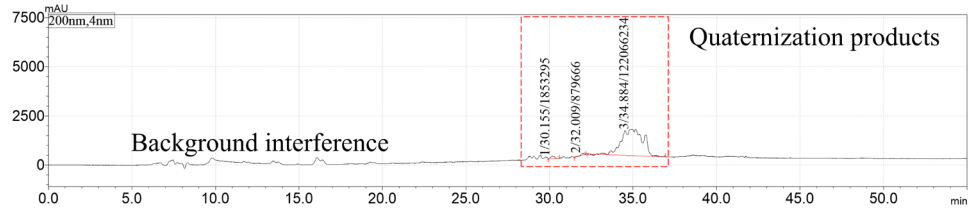

Fig. S223 Liquid chromatography profile of surfactants synthesized from waste rapeseed oil as the raw material using the optimal reagent combination.

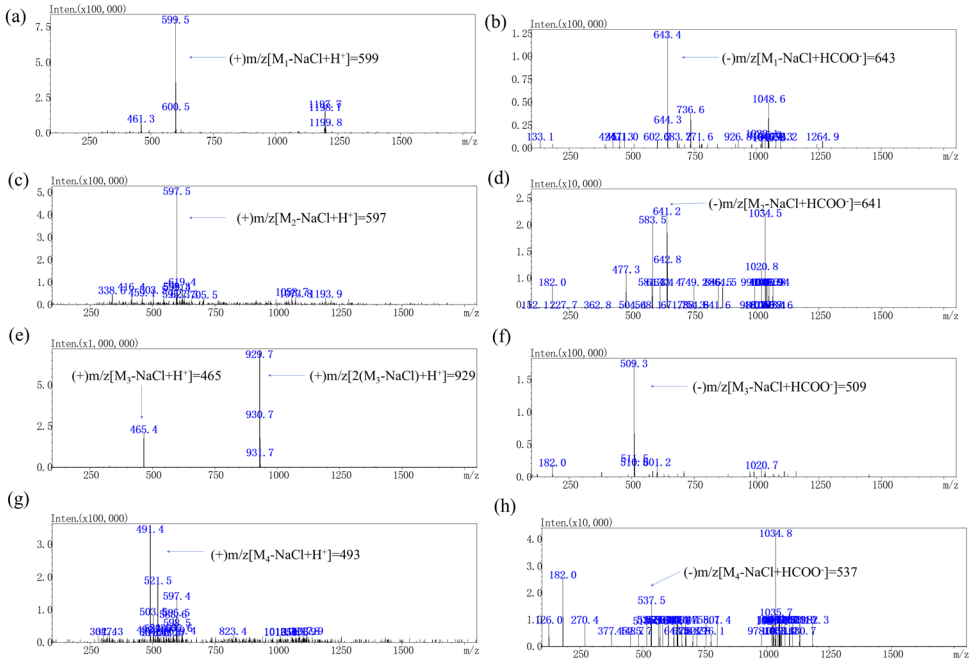

Fig. S224 Mass spectrum of surfactants synthesized from waste rapeseed oil as the raw material using the optimal reagent combination.

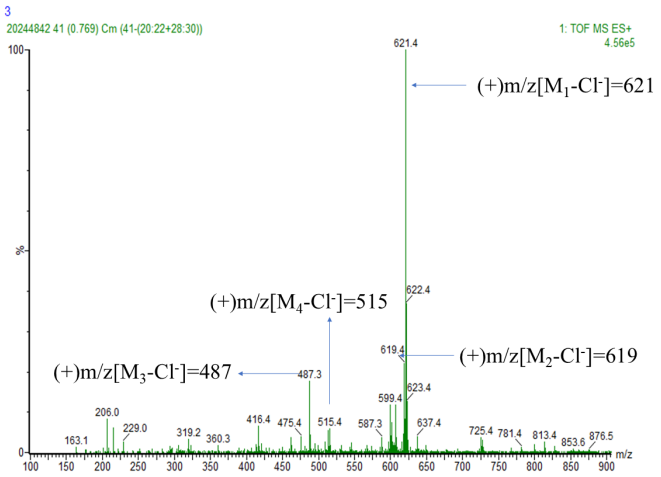

Fig. S225 Electrospray mass spectrum of surfactants synthesized from waste rapeseed oil as the raw material using the optimal reagent combination.

4.2 GC-MS, HPLC-MS, and ESI-MS spectra of surfactants synthesized from waste cooking oil (M1–M4 correspond to products derived from methyl oleate, methyl linoleate, methyl palmitate, and methyl stearate, respectively; GC conditions: 260 °C for 2 min, heated at 20 °C/min to 290 °C, then held as shown in each figure)

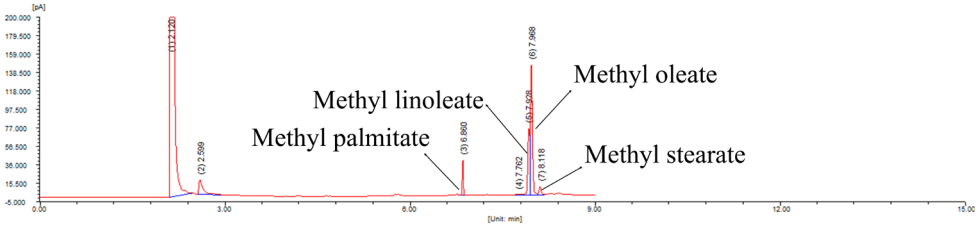

Fig. S226 Gas chromatography profile of mixed fatty acid methyl esters obtained from the transesterification of waste cooking oil (initial temperature is set to 200 °C for 2 minutes, followed by a temperature ramp to 290 °C at a rate of 20 °C/min for 10 minutes).

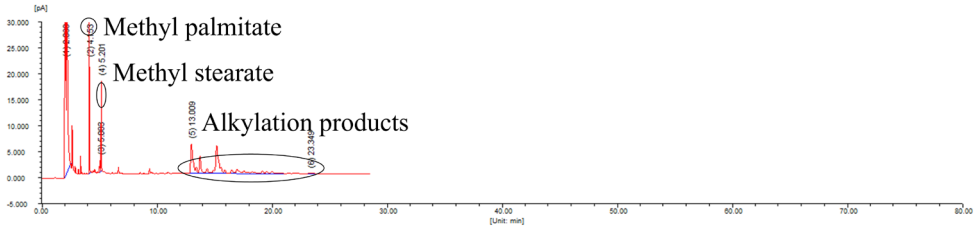

Fig. S227 Gas chromatography profile of the alkylated raw materials after transesterification of waste cooking oil.

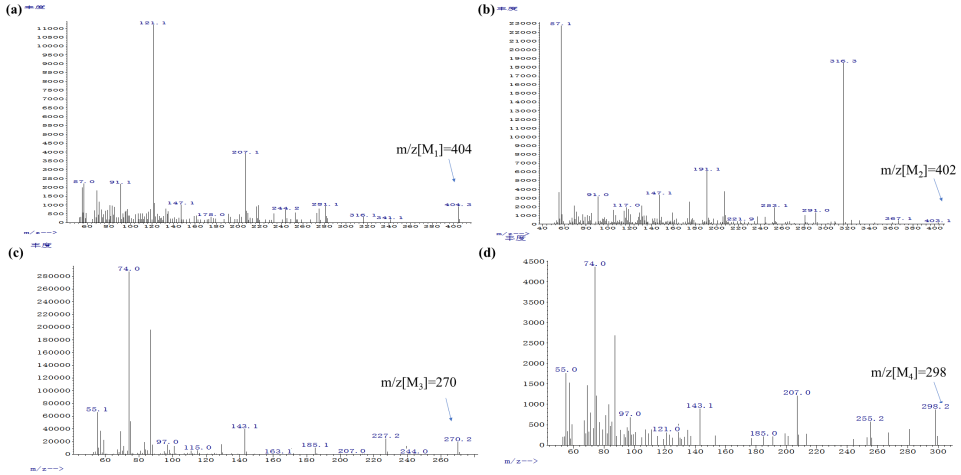

Fig. S228 Mass spectrum of the alkylated raw materials after transesterification of waste cooking oil.

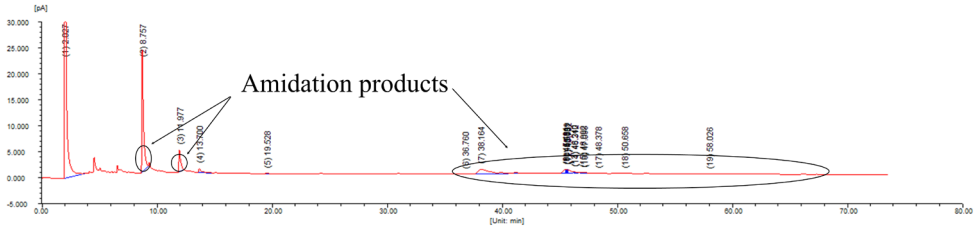

Fig. S229 The gas chromatography profile of the transesterified raw materials after amidation.

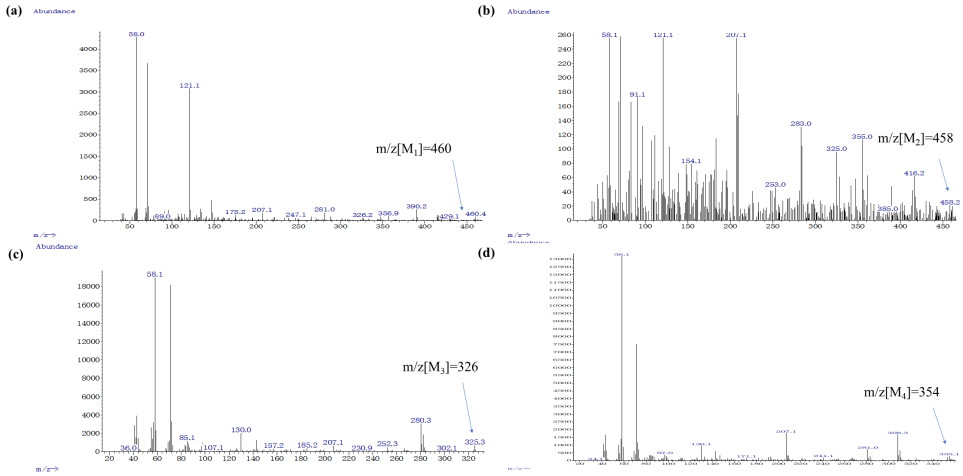

Fig. S230 Mass spectrum of the transesterified raw materials after amidation.

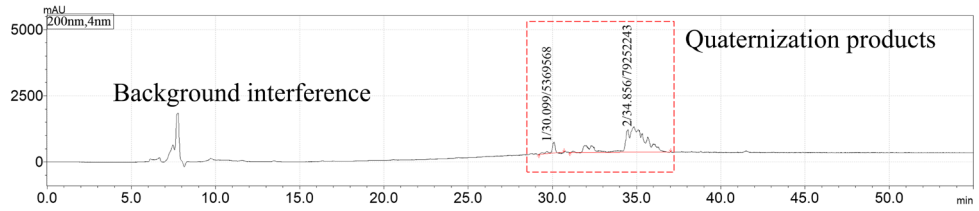

Fig. S231 Liquid chromatography profile of surfactants synthesized from waste cooking oil as the raw material using the optimal reagent combination.

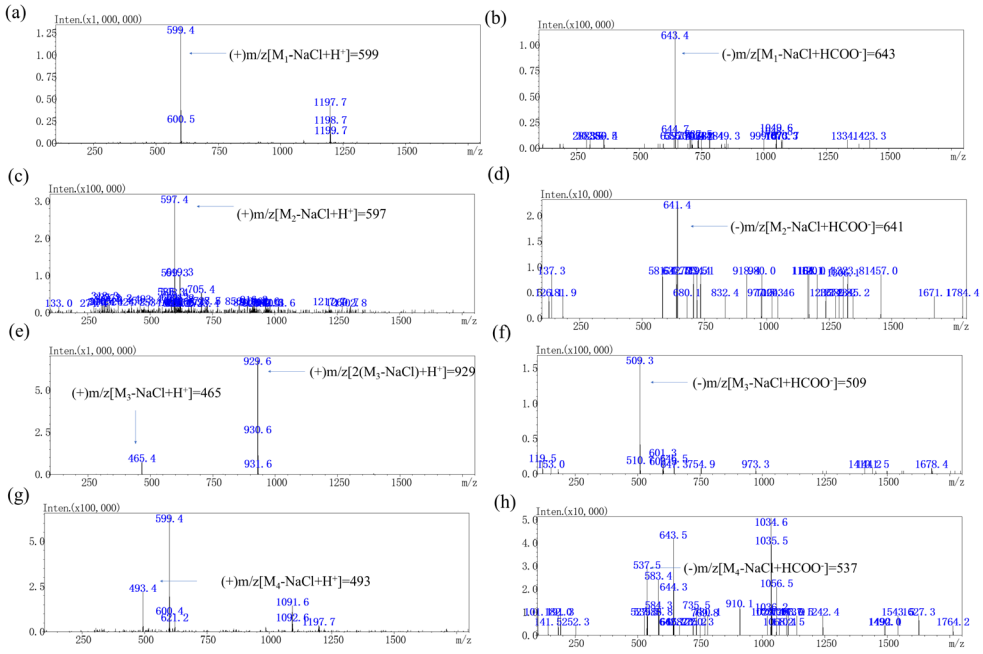

Fig. S232 Mass spectrum of surfactants synthesized from waste cooking oil as the raw material using the optimal reagent combination.

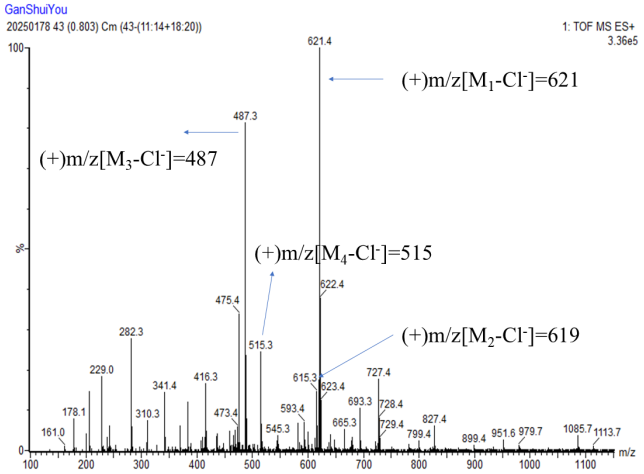

Fig. S233 Electrospray mass spectrum of surfactants synthesized from waste cooking oil as the raw material using the optimal reagent combination.

4.3 GC-MS, HPLC-MS, and ESI-MS spectra of surfactants synthesized from waste soybean oil (M_1–M_4 correspond to products derived from methyl oleate, methyl linoleate, methyl palmitate, and methyl

stearate, respectively; GC conditions: 260 °C for 2 min, heated at 20 °C/min to 290 °C, then held as shown in each figure)

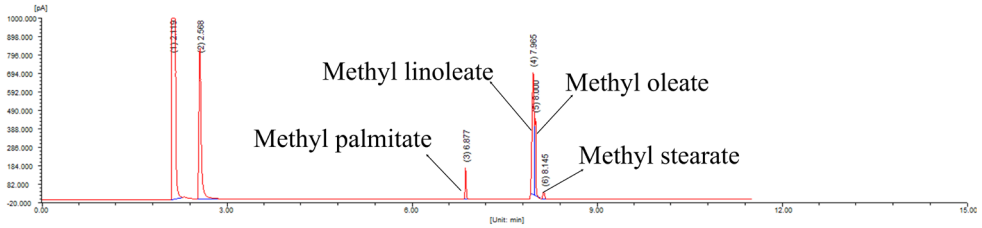

Fig. S234 Gas chromatography profile of mixed fatty acid methyl esters obtained from the transesterification of waste soybean oil (initial temperature is set to 200 °C for 2 minutes, followed by a temperature ramp to 290 °C at a rate of 20 °C/min for 10 minutes).

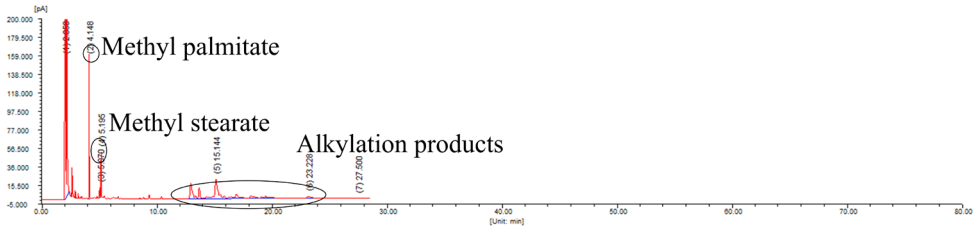

Fig. S235 Gas chromatography profile of the alkylated raw materials after transesterification of waste soybean oil.

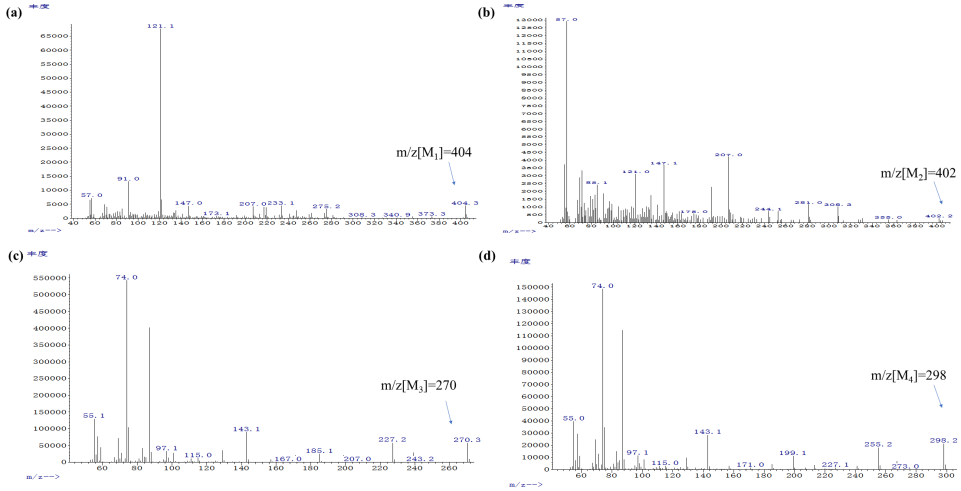

Fig. S236 Mass spectrum of the alkylated raw materials after transesterification of waste soybean oil.

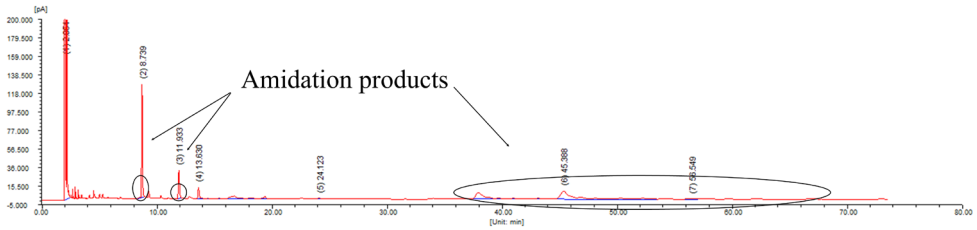

Fig. S237 The gas chromatography profile of the transesterified raw materials after amidation.

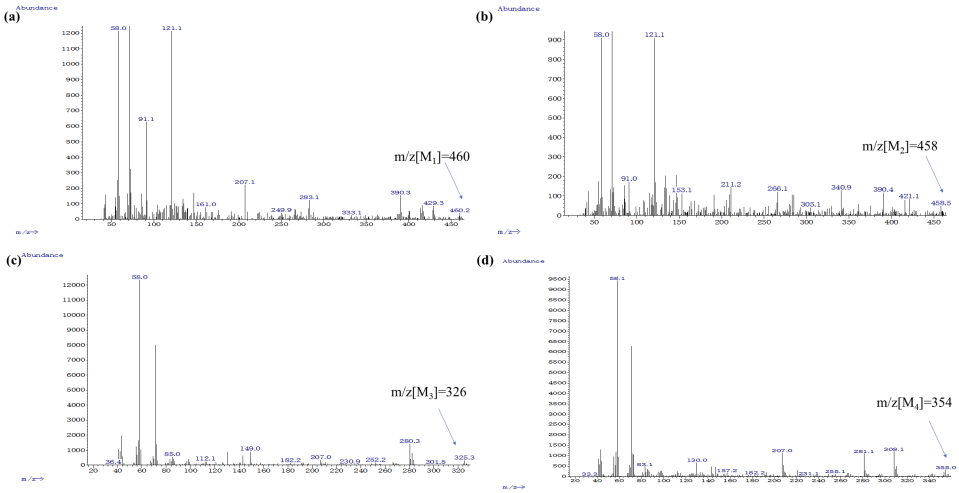

Fig. S238 Mass spectrum of the transesterified raw materials after amidation.

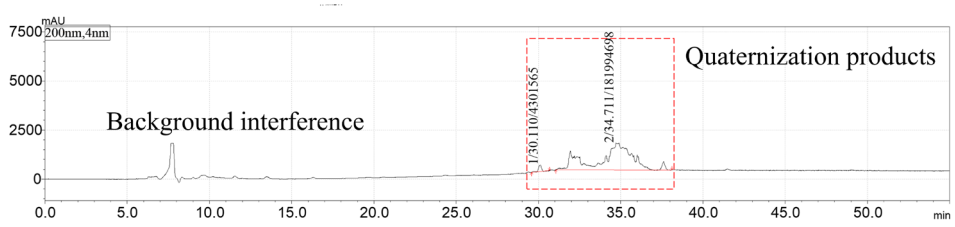

Fig.S239 Liquid chromatography profile of surfactants synthesized from waste soybean oil as the raw material using the optimal reagent combination.

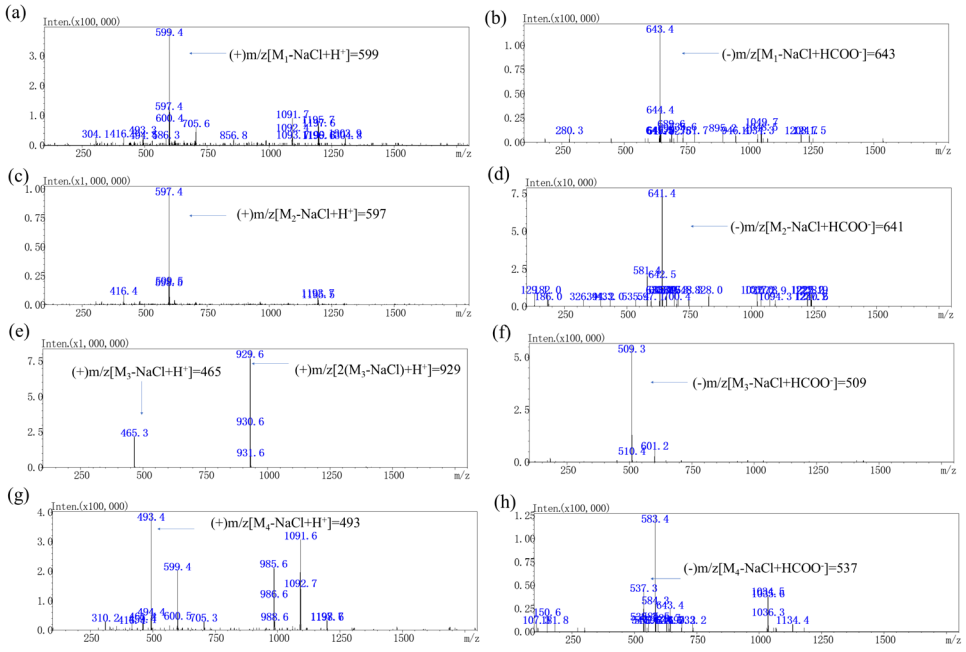

Fig. S240 Mass spectrum of surfactants synthesized from waste soybean oil as the raw material using the optimal reagent combination.

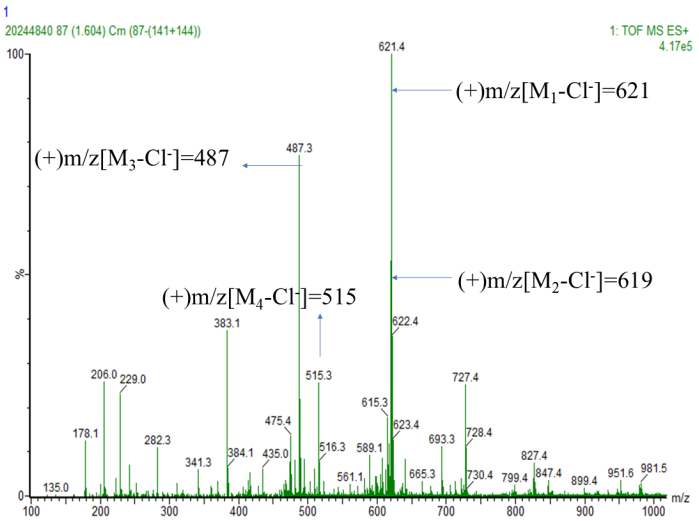

Fig. S241 Electrospray mass spectrum of surfactants synthesized from waste soybean oil as the raw material using the optimal reagent combination.