

Supplementary Data

Phytochemical Profiling and Nutritional Assessment of Indigenous Cowpea (*Vigna unguiculata* L.) Cultivars from Bulukumba, South Sulawesi, Indonesia

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Abstract

Cowpea (*Vigna unguiculata* L.) is a leguminous crop recognized for its high nutrient density and substantial potential as a functional food. Bulukumba Regency in South Sulawesi, Indonesia, harbors two locally adapted red and white cultivars that have been traditionally cultivated and consumed as staple foods. This study aimed to evaluate their nutritional composition, antioxidant capacity, and bioactive compound profiles. Proximate composition was determined following the AOAC protocols, tannin content was quantified using a modified vanillin-HCl assay, antioxidant activity was assessed via the 2,2-diphenyl-1-picrylhydrazyl (DPPH) method, and bioactive compounds were identified through Gas Chromatography–Mass Spectrometry (GC–MS). Both cultivars exhibited high protein (20.47–21.03%) and carbohydrate (43.93–51.91%) contents, low lipid content (0.63%), and comparable ash content (3.25–3.28%). Tannin content was substantially higher in the red cowpea (465.61 µg/g) than in the white cowpea (130.43 µg/g). Antioxidant activity was significantly greater in the red cultivar (2,115.33 µg/g) compared with the white cultivar (507.18 µg/g). GC–MS analysis revealed a diverse range of bioactive compounds, including fatty acids (oleic, palmitic, and pentadecanoic acids), alcohols, esters, nitrogen-containing molecules, vitamins, terpenoids, and phenolics—many of which are reported to possess antioxidant, antimicrobial, anti-inflammatory, anticancer, and cardioprotective properties. These findings highlight the superior functional potential of the red cultivar and support the valorization of local cowpea germplasm for improved nutrition, human health, and sustainable agricultural development.

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Table S1. GC-MS analysis result showing identified compounds in red cowpea

Peak	RT (min)	Component Hit#1	Component Hit#2	Component Hit#3	Relative Area (%)
1	1.170	N-Methyltaurine	(2-Aziridinyethyl)amine	Benzeneethanamine, 2-fluoro- β ,3-dihydroxy-N-methyl	0.21
2	1.204	Hydroxylamine	1,2-Ethandiol	Difluoromethane	17.22
3	1.231	Methyl Alcohol	Acetic acid, hydroxy	Acetaldehyde, hydroxy	7.32
4	1.412	Imidazole, 2-amino-5-[(2-carboxy)vinyl]-	3,7-Diacetamido-7H-s-triazolo[5,1-c]-s-triazole	Thiophene-3-ol, tetrahydro-, 1,1-dioxide	0.50
5	1.578	DL-Arabinose	2,4,6,8-Tetraazabicyclo[3.3.0]octan-3-one, 7-nitroimino	trans-2-Aminocyclohexano	0,10
6	1.898	Imidazole, 2-amino-5-[(2-carboxy)vinyl]-	l-Gala-l-ido-octose	Benzeneethanamine, 2,5-difluoro- β ,3,4-trihydroxy-N-methyl	0.04
7	2.000	Propyl nitrite	2,2-Dimethoxybutane	Imidazole, 2-amino-5-[(2-carboxy)vinyl]-	0.04
8	2.653	Imidazole, 2-amino-5-[(2-carboxy)vinyl]-	Mannosamine	DL-Arabinose	0.03
9	3.435	Imidazole, 2-amino-5-[(2-carboxy)vinyl]-	3-Azonia-5-hexene-1-ol, N,N-dimethyl-, carbamate ester, bromide	3,6-Octadecadiynoic acid, methyl ester	0.03
10	3.609	2-Cyclopenten-1-one, 2-hydroxy-3-methyl	6-Oxa-bicyclo[3.1.0]hexan-3-one	1,2-Cyclopentanedione	1.02
11	4.404	Glycerin	Erythritol	Diglycerol	2.27
12	4.955	Glycerin	Erythritol	Glyceraldehyde	8.94
13	5.013	Glycerin	Erythritol	Glyceraldehyde	1.91
14	5.234	Glycerin	Erythritol	Glyceraldehyde	5.58
15	5.418	Glycerin	Erythritol	Glyceraldehyde	7.26
16	5.898	4,4'-Biscyclohexanone, 2,2',6,6'-tetramethyl	Methyl 6-oxoheptanoate	6-Acetyl- β -d-mannose	0.15
17	7.098	l-Gala-l-ido-octose	1-Nitro-2-acetamido-1,2-dideoxy-d-mannitol	Methyl 6-oxoheptanoate	0.09
18	7.642	9-Tetradecen-1-ol, acetate, (E)-	1,2-15,16-Diepoxyhexadecane	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1a,2a,5a)-	0.09
19	8.448	12,15-Octadecadiynoic acid, methyl ester	1-[2-Deoxy- β -d-erythro-pentofuranosyl]pyrrole-2,4-dicarboxamide	Benzenemethanol, 2-(2-aminopropoxy)-3-methyl	0.05

20	9.652	l-Gala-l-ido-octose	Tetraacetyl-d-xylonic nitrile	Pterin-6-carboxylic acid	0.58
21	9.809	1-Nitro-2-acetamido-1,2-dideoxy-d-mannitol	Pterin-6-carboxylic acid	l-Gala-l-ido-octose	0.27
22	10.020	Imidazole, 2-amino-5-[(2-carboxy)vinyl]-	l-Gala-l-ido-octose	Pterin-6-carboxylic acid	0.08
23	10.159	2-Methyl-9-β-d-ribofuranosylhypoxanthine	Ascaridole epoxide	Cyclohexanone, 2-(2-butynyl)	0.07
24	10.384	2-Methyl-9-β-d-ribofuranosylhypoxanthine	Pyrazole[4,5-b]imidazole, 1-formyl-3-ethyl-6-β-d-ribofuranosyl	d-Mannose	0.09
25	10.809	12,15-Octadecadiynoic acid, methyl ester	Phenol, 2-methoxy-5-(1-propenyl)-, (E)-	Dihydroartemisinin, 6-deshydro-5-deshydroxy-3-desoxy	0.28
26	11.594	Pterin-6-carboxylic acid	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	2,15-Octadecadiynoic acid, methyl ester	0.04
27	11.870	12-Methyl-E,E-2,13-octadecadien-1-ol	Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate	2-Methyl-Z,Z-3,13-octadecadienol	0.10
28	12.084	l-Gala-l-ido-octose	Imidazole, 2-amino-5-[(2-carboxy)vinyl]-	12,15-Octadecadiynoic acid, methyl ester	0.04
29	12.431	d-Mannose	Pterin-6-carboxylic acid	L-Glucose	0.99
30	12.550	d-Mannose	d-Glycero-d-ido-heptose	Melezitose	2.07
31	13.183	Desulphosinigrin	Pterin-6-carboxylic acid	l-Gala-l-ido-octose	0.06
32	13.622	1,3-Benzodioxole, 4-methoxy-6-(2-propenyl)-	Furan-2-carboxylic acid, 5-(1-hexynyl)-	Tricyclo[5.2.1.0(4,10)]dec-2-ene, 6,6,8-trimethoxy	0.30
33	13.826	Aminoacetamide, N-methyl-N-[4-(1-pyrrolidinyl)-2-butynyl]-	5-Aminovaleramide, N-methyl-N-[4-(1-pyrrolidinyl)-2-butynyl]-	Bicyclo[3.2.1]oct-6-ene-6,8-dimethanol, 1,7-dimethyl-4-isopropyl-, bi	0.19
34	14.115	3-Hydroxy-7,8-dihydro-β-ionol	Asarone	Pterin-6-carboxylic acid	0.13
35	14.220	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	l-Gala-l-ido-octose	Cyclopropanetetradecanoic acid, 2-octyl-, methyl ester	0.20
36	14.462	Isoamyl salicylate	Benzoic acid, 2-hydroxy-, 2-methylbutyl ester	Benzoic acid, 2-hydroxy-, heptyl ester	0.33
37	14.713	d-Mannose	d-Glycero-d-ido-heptose	L-Glucose	0.18
38	14.764	d-Mannose	d-Glycero-d-ido-heptose	Desulphosinigrin	0.31
39	14.819	Desulphosinigrin	d-Mannose	l-Gala-l-ido-octose	0.25
40	15.934	Patchouli alcohol	Aspidospermidin-17-ol, 1-acetyl-19,21-epoxy-15,16-dimethoxy	9-Hexadecenoic acid	0.19
41	16.495	Dodecanoic acid, 3-hydroxy	l-Gala-l-ido-octose	Cyclopropanetetradecanoic acid, 2-octyl-, methyl ester	0.05

42	16.740	12,15-Octadecadiynoic acid, methyl ester	10-Heptadecen-8-ynoic acid, methyl ester, (E)-	l-Gala-l-ido-octose	0.03
43	17.057	12,15-Octadecadiynoic acid, methyl ester	Ethyl iso-allocholate	Cucurbitacin b, 25-desacetoxy	0.05
44	17.172	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	Cyclopropanetetradecanoic acid, 2-octyl-, methyl ester	Estra-1,3,5(10)-trien-17 β -ol	0.52
45	17.475	12,15-Octadecadiynoic acid, methyl ester	Tetraacetyl-d-xylonic nitrile	Cucurbitacin b, 25-desacetoxy	0.03
46	17.699	l-Gala-l-ido-octose	Tertbutyloxyformamide, N-methyl-N-[4-(1-pyrrolidiny)-2-butynyl]-	Pterin-6-carboxylic acid	0.09
47	18.791	Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	12,15-Octadecadiynoic acid, methyl ester	Cyclopropanedodecanoic acid, 2-octyl-, methyl ester	0.14
48	19.084	Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	Cyclopropanedodecanoic acid, 2-octyl-, methyl ester	Oxiraneundecanoic acid, 3-pentyl-, methyl ester, cis	0.53
49	19.403	Hexadecanoic acid, methyl ester	Pentadecanoic acid, 14-methyl-, methyl ester	Pentadecanoic acid, methyl ester	3.86
50	19.682	Ethyl iso-allocholate	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	9,10-Secocholesta-5,7,10(19)-triene-3,24,25-triol, (3 β ,5Z,7E)	0.09
51	19.907	n-Hexadecanoic acid	l-(+)-Ascorbic acid 2,6-dihexadecanoate	Pentadecanoic acid	3.88
52	20.264	Estra-1,3,5(10)-trien-17 β -ol	Cyclopropanetetradecanoic acid, 2-octyl-, methyl ester	l-(+)-Ascorbic acid 2,6-dihexadecanoate	0.04
53	20.339	Estra-1,3,5(10)-trien-17 β -ol	Cyclopropanetetradecanoic acid, 2-octyl-, methyl ester	Ethyl iso-allocholate	0.08
54	20.781	Ethyl iso-allocholate	Cyclopropanetetradecanoic acid, 2-octyl-, methyl ester	13-Heptadecyn-1-ol	0.08
55	21.267	Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate	Estra-1,3,5(10)-trien-17 β -ol	Z-8-Methyl-9-tetradecenoic acid	0,11
56	21.396	9-Hexadecenoic acid	12-Methyl-E,E-2,13-octadecadien-1-ol	Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate	0.11
57	21.546	Methyl 10-trans,12-cis-octadecadienoate	9,12-Octadecadienoic acid, methyl ester, (E,E)-	Methyl 9-cis,11-trans-octadecadienoate	0,65
58	21.618	trans-13-Octadecenoic acid, methyl ester	9-Octadecenoic acid (Z)-, methyl ester	cis-13-Octadecenoic acid, methyl ester	5.91
59	21.679	10-Octadecenoic acid, methyl ester	11-Octadecenoic acid, methyl ester	16-Octadecenoic acid, methyl ester	0.49

60	21.920	Heptadecanoic acid, 16-methyl-, methyl ester	Methyl stearate	Heptadecanoic acid, 10-methyl-, methyl ester	0.41
61	22.032	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	12-Methyl-E,E-2,13-octadecadien-1-ol	0.24
62	22.141	Oleic Acid	trans-13-Octadecenoic acid	cis-Vaccenic acid	7.05
63	22.376	trans-13-Octadecenoic acid, methyl ester	Oleic Acid	cis-Vaccenic acid	7.08
64	22.628	Oleic Acid	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	cis-Vaccenic acid	0.64
65	23.090	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	trans-13-Octadecenoic acid	cis-Vaccenic acid	1.42
66	23.379	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	Oleic Acid	0.21
67	23.747	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	9-Hexadecenoic acid	12-Methyl-E,E-2,13-octadecadien-1-ol	0.09
69	23.893	Glycidyl palmitoleate	trans-13-Octadecenoic acid	cis-Vaccenic acid	0.26
70	24.097	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	Oleic Acid	12-Methyl-E,E-2,13-octadecadien-1-ol	0.03
71	24.648	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	trans-13-Octadecenoic acid	0.07
72	25.651	Ethyl iso-allocholate	1,2-15,16-Diepoxyhexadecane	7,11-Hexadecadienal	0.18
73	25.855	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	0.10
74	25.906	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	Glycidyl palmitoleat	Glycidyl (Z)-9-Heptadecenoate	0.41
75	26.216	Ethyl iso-allocholate	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	9-Hexadecenoic acid	0.04
76	26.328	Hexadecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	Glycerol 1-palmitate	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	0.36

77	26.454	Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopro	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	0.11
78	26.872	3',8,8'-Trimethoxy-3-piperidyl-2,2'-binaphthalene-1,1',4,4'-tetron	9-(2',2'-Dimethylpropanoilhydrazono)-3,6-dichloro-2,7-bis-[2-(diethylamino)-ethoxy]fluorene	12-Methyl-E,E-2,13-octadecadien-1-ol	0.39
79	29.148	Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]	Ethyl iso-allocholate	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	0.17
80	29.216	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester (0,67 %)	9-Octadecenoic acid, 1,2,3-propanetriyl ester, (E,E,E)-	2,3-Dihydroxypropyl elaidate	0.67

Table S2. GC-MS analysis results showing identified compounds in white cowpea

Peak	RT (min)	Component Hit#1	Component Hit#2	Component Hit#3	Relative Area (%)
1	1.170	Benzeneethanamine, 2-fluoro- β ,3-dihydroxy-N-methyl	Benzeneethanamine, 2-fluoro- β ,5-dihydroxy-N-methyl	Hydrazinecarboxamide	0.24
2	1.204	Hydroxylamine	1,2-Ethandiol	Hydroxyurea	23.25
3	1.252	Acetic acid, hydroxy	2-Formylhistamine	Semicarbazide	2.13
4	1.415	DL-Arabinose	Cyclohexan-1,4,5-triol-3-one-1-carboxylic acid	Propanal, 2,3-dihydroxy-, (S)-	0.61
5	1.558	DL-Arabinose	l-Gala-l-ido-octose	3,7-Diacetamido-7H-s-triazolo[5,1-c]-s-triazole	0.05
6	1.595	DL-Arabinose	l-Gala-l-ido-octose	d-Glycero-d-ido-heptose	0.04
7	1.912	Imidazole, 2-amino-5-[(2-carboxy)vin	DL-Arabinose	Cyclohexan-1,4,5-triol-3-one-1-carboxylic acid	0.06
8	2.010	Propyl nitrite	2,2-Dimethoxybutane	DL-Arabinose	0.06
9	2.157	1,2,3-Butanetriol	(3-Methyl-oxiran-2-yl)-methanol	1,3-Butanediol, (S)-	0.06
10	2.221	L-Talose, 6-deoxy-3-C-methyl-2-O-methyl	DL-Arabinose	Cyclohexan-1,4,5-triol-3-one-1-carboxylic acid	0.04
11	2.674	1,3,5-Pentanetriol, 3-methyl	DL-Arabinose	1-Nitro-2-acetamido-1,2-dideoxy-d-mannitol	0.02
12	3.616	1H-Pyrrole, 2,5-dihydro-1-nitroso	3-Azabutyl-1-ol, 4-cyclopropyl-3,3-dimethyl-, bromide	3-Azabutyl-1-ol, O-acetyl-4-cyclopropyl-N,N-dimethyl-, bromide	0.16
13	4.480	Glycerin	Erythritol	DL-Arabinose	2.48
14	6.554	6-Acetyl- β -d-mannose	4,4'-Biscyclohexanone, 2,2',6,6'-tetramethyl	Methyl 6-oxoheptanoate	0.07
15	7.316	l-Gala-l-ido-octose	Glucopyranuronamide, 1-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1,4-dideoxy-4-(D-2-(2-(methylamino)acetamido)hydracrylamido)-, β -	Imidazole, 2-amino-5-[(2-carboxy)vinyl]-	0.05
16	7.513	Imidazole, 2-amino-5-[(2-carboxy)vinyl]-	l-Gala-l-ido-octose	4-Cyclopropylcarbonyloxytetradecane	0.05

17	7.653	Cyclohexanol, 1-methyl-4-(1-methylethyl)-	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1 α ,2 β ,5 α)-(\pm)-	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1 α ,2 β ,5 β)-	1.08
18	8.459	Paromomycin	12,15-Octadecadiynoic acid, methyl ester	N-Chloroacetyl-3,6,9,12-tetraoxapentadec-14-yn-1-amine	0.08
19	9.660	Anethole	Benzene, 1-methoxy-4-(1-propenyl)-, (Z)-	Anethole	0.93
20	10.166	3,5-Heptadienal, 2-ethylidene-6-methyl	Cyclohexanone, 2-(2-butyryl)-	Ascaridole epoxide	0.17
21	12.734	d-Mannose	Sucrose	Melezitose	4.83
22	12.795	d-Mannose	Melezitose	Sucrose	2.68
23	13.476	Paromomycin	D-Streptamine, O-6-amino-6-deoxy-a-D-glucopyranosyl-(1-4)-O-(3-deoxy-4-C-methyl-3-(methylamino)- β -L-arabinopyranosyl-(1-6))-2-deoxy	Pterin-6-carboxylic acid	0.06
24	14.231	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	Cyclopropanetetradecanoic acid, 2-octyl-, methyl ester	l-Gala-l-ido-octose	0.17
25	14.771	Desulphosinigrin	d-Mannose	Melezitose	0.22
26	14.826	Desulphosinigrin	d-Mannose	Melezitose	1.40
27	17.183	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	Tetradecanoic acid	Cyclopropanetetradecanoic acid, 2-octyl-, methyl ester	0.45
28	17.703	7-Methyl-Z-tetradecen-1-ol acetate	Acetamide, N-methyl-N-[4-(3-hydroxypyrrolidinyl)-2-butyryl]-	Cyclopropanetetradecanoic acid, 2-octyl-, methyl ester	0.07
29	19.040	1-Indolinecarboxaldehyde, 2-hydroxy-5-methoxy	Pyrazole[4,5-b]imidazole, 1-formyl-3-ethyl-6- β -d-ribofuranosyl	Benzoisofuran-1-one, 1,3-dihydro-6,7-dimethoxy-3-(4,5,6,7-tetrahydrobenzothiazol-2-yl)amino	0.25
30	19.407	Hexadecanoic acid, methyl ester	Pentadecanoic acid, 14-methyl-, methyl ester	Hexadecanoic acid, 15-methyl-, methyl ester	1.18
31	19.686	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	2,6-Dimethyl-N-[3-(trimethylsilyl)-1,3-thiazinan-2-ylidene]aniline	2-Cyclohexen-1-one, 3-methoxy-2-(2,4,5-trimethoxyphenyl)-	0.40
32	19.934	n-Hexadecanoic acid	l-(+)-Ascorbic acid 2,6-dihexadecanoate	Pentadecanoic acid	12.29

33	21.271	9-Hexadecenoic acid	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate	0.07
34	21.550	9,12-Octadecadienoic acid, methyl ester, (E,E)-	7,10-Octadecadienoic acid, methyl ester	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	0.43
35	21.621	10-Octadecenoic acid, methyl ester	trans-13-Octadecenoic acid, methyl ester	11-Octadecenoic acid, methyl ester	1.64
36	21.921	Cyclopropanebutanoic acid, 2-[[2-[[2-(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	Oxiraneundecanoic acid, 3-pentyl-, methyl ester, cis	Cyclopropanepentanoic acid, 2-undecyl-, methyl ester, trans	0.15
37	22.148	Oleic Acid	trans-13-Octadecenoic acid	cis-Vaccenic acid	11.80
38	22.172	Oleic Acid	trans-13-Octadecenoic acid	cis-Vaccenic acid	9.16
39	22.213	trans-13-Octadecenoic acid	Oleic Acid	cis-Vaccenic acid	9.29
40	22.397	Oleic Acid	trans-13-Octadecenoic acid	cis-Vaccenic acid	0.88
41	22.638	Oleic Acid	17-Octadecynoic acid	cis-Vaccenic acid	1.34
42	23.108	17-Octadecynoic acid	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	cis-Vaccenic acid	0.37
43	23.182	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	Oleic Acid	17-Octadecynoic acid	0.22
44	23.638	cis-Vaccenic acid	17-Octadecynoic acid	Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate	0.06
45	23.696	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	2-Methyl-E,E-2,13-octadecadien-1-ol	trans-13-Octadecenoic acid	0.02
46	23.757	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	12-Methyl-E,E-2,13-octadecadien-1-ol	Oleic Acid	0.92
47	23.900	Glycidyl palmitoleate	cis-Vaccenic acid	9-Hexadecenoic acid	0.94
48	24.101	9-Hexadecenoic acid	trans-13-Octadecenoic acid	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	0.30
49	24.186	trans-13-Octadecenoic acid	trans-13-Octadecenoic acid	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	0.06
50	24.461	12-Methyl-E,E-2,13-octadecadien-1-ol	7-Methyl-Z-tetradecen-1-ol acetate	2-Methyl-Z,Z-3,13-octadecadienol	0.39

51	24.645	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	trans-13-Octadecenoic acid	Cyclopropanebutanoic acid, 2-[[2-[[2-[[2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	0.11
52	25.652	2-(Dimethylamino)ethyl (9Z,12Z)-octadeca-9,12-dienoate	Cholestan-3-ol, 2-methylene-, (3 β ,5 α)-	1,2-15,16-Diepoxylhexadecane	0.52
53	25.750	Ethyl iso-allocholate	1,2-15,16-Diepoxylhexadecane	7,11-Hexadecadienal	0.13
54	25.852	9,12,15-Octadecatrienoic acid, 2,3-dihydroxypropyl ester, (Z,Z,Z)-	Cyclopropanebutanoic acid, 2-[[2-[[2-[[2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	0.25
55	25.903	Glycidyl palmitoleate	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	Glycidyl (Z)-9-Heptadecenoate	0.65
56	26.335	Glycerol 1-palmitate	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	Hexadecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	0.90
57	26.818	Cyclopropanebutanoic acid, 2-[[2-[[2-[[2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	0.21
58	26.879	3',8,8'-Trimethoxy-3-piperidyl-2,2'-binaphthalene-1,1',4,4'-tetrone	Isopropyl linoleate	17-Octadecynoic acid	0.81
59	29.165	9,12-Octadecadienoic acid (Z,Z)-, 2,3-dihydroxypropyl ester	9,12-Octadecadienoic acid (Z,Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	9,12,15-Octadecatrienoic acid, 2,3-dihydroxypropyl ester, (Z,Z,Z)-	0.78
60	29.223	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	Cyclopropanebutanoic acid, 2-[[2-[[2-[[2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	9-Octadecenoic acid, 1,2,3-propanetriyl ester, (E,E,E)-	1.96