

Analysis of the Fecal Metabolomic Profile in Breast vs. Different Formula Milk Feeding in Late Preterm Infants

Giuseppe De Bernardo ^{1,*}, Gilda D'Urso ², Simona Spadarella ¹, Maurizio Giordano ³, Giuseppina Leone ¹ and Agostino Casapullo ^{2,*}

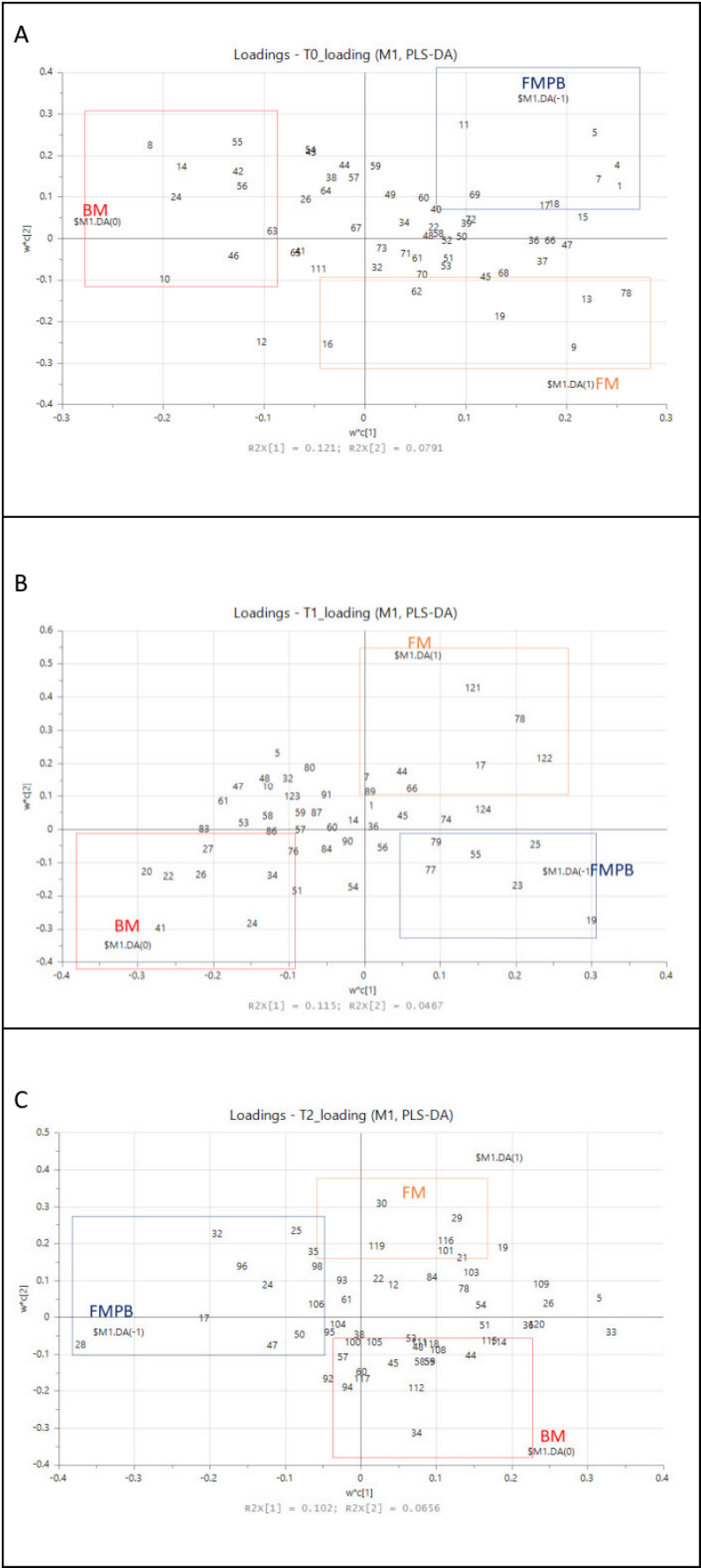
¹ Division of Pediatrics Neonatology and NICU, Ospedale Buon Consiglio Fatebenefratelli, 80123 Naples, Italy; spadarella.simona@fbfna.it (S.S.); leone.giuseppina@fbfna.it (G.L.)

² Department of Pharmacy, University of Salerno, via Giovanni Paolo II, 132, 84084, Fisciano, Italy; gidurso@unisa.it

³ Department of Clinical Medicine and Surgery, Federico II University, 80138 Naples, Italy; mauri.giordano@studenti.unina.it

* Correspondence: debernardo.giuseppe@fbfna.it (G.D.B.); casapullo@unisa.it (A.C.)

Supplementary Figure S1: Loading scatter Plot at time 0 (A), time 1 (B), time 2 (C) with variables distributed in the plot according to the distribution of samples in the score scatter plot.



FMPB: Formula milk plus post biotic (text and rectangle blue); FM: formula milk (text and rectangle orange); BM: breast milk (text and rectangle red).

1 (Porphobilinogen); 4 (1-(beta-D-ribofuranosyl) thymine); 5 (Myristyl sulfate); 7 (L-alpha-lysophosphatidylcholine); 8 (N-Acetylgalactosamine 6-sulfate); 9 (Beta-Aspartylaspartic acid); 10 (4-Undecylbenzenesulfonic acid); 11 ((1S,2R)-1-(3,4-Dihydroxyphenyl)-7-hydroxy-N,N'-bis[2-(4-hydroxyphenyl)ethyl]-6-methoxy-1,2-dihydro-2,3-naphthalenedicarboxamide); 12 (2-Dodecylbenzenesulfonic acid); 13 (N~6~-[(2R)-3,4-Dihydro-2H-pyrrol-2-ylcarbonyl]-L-lysine); 14 (17-Hydroxypregnenolone sulfate); 15 (Methyl (9E)-9-octadecenoate); 16 (1-oleoyl-sn-glycero-3-phospho-D-myoinositol); 17 (Leu-Leu); 18 (Pentadecanoic acid);

19 (3-Oxotetradecanoic acid); 20 (Taurohyocholic acid); 21 (Cholic acid), 22 (Hydroxycholic acid); 23 (Myristoleic acid); 24 (13(S)-HpOTrE); 25 (Homovanillic acid); 26 (15,16-DiHODE); 27 (3a,7a-Dihydroxycholanoic acid); 28 (Diethyl (2R,3R)-2-hydroxy-3-methylsuccinate); 29 (Reduced Glutathione); 30 (N-Acetyl-L-glutamic acid); 32 (Traumatic Acid); 33 (2-methoxyacetaminophen sulfate); 34 (Azelaic acid); 35 (N-Acetylglucosaminitol); 36 (Oleic acid); 37 (Oleoyl tyrosine);

38 (Phenylac-gln-OH); 39 (N-[(1S)-4-Carbamimidamido-1-carboxybutyl]asparaginy-beta-aspartyl-L-arginine); 40 (Leu-Val); 41 (Glycocholic acid); 42 (Glycoursodeoxycholic acid 3-sulfate); 43 (Glycochenodeoxycholic acid); 44 (Citric acid); 45 (D-Gluconic acid); 46 (D-Glucopyranuronic acid); 47 (5-Methoxy-3-indoleacetate);

48 (Sebacic acid); 49 (3-oxopalmitic acid); 50 (3-Hydroxysebacic acid); 51 (13S-hydroxyoctadecadienoic acid); 52 (Pinellic acid); 53 ((10E,15Z)-9,12,13-Trihydroxy-10,15-octadecadienoic acid); 54 (Palmitelaidic acid); 55 (Palmitic Acid); 56 (Traumatin); 57 (Phloionolic acid);

58 (12-HSA); 59 (9,10-Dihydroxystearic acid); 60 (Stearic acid); 61 (Myristic acid); 62 (Dimethyl (2E)-3-methoxy-4-oxo-5-[(8E,11E)-8,11,14-pentadecatrien-1-yl]-2-hexenedioate); 63 (Estriol); 64 (Androsterone sulfate); 65 (16alpha-hydroxydehydroepiandrosterone 3-sulfate); 66 (2-methoxy-17beta-estradiol 3-sulfate); 67 (Dehydroepiandrosterone sulfate);

68 (Tiliacorine); 69 (O-heptadecanoylcarnitine); 70 (Carbazepine); 71 (Soyasaponin I); 72 (Tomelukast); 73 (N(4)-phosphoagmatine); 74 (N-Stearoyltyrosine); 76 (Diethyl tartrate); 77 (2-methylcitric acid);

78 (laurilsulfate); 79 (1,1'-monoglyceride citrate); 80 (1-stearyl estercitric acid); 83 (Juniperic acid); 84 (6-Hydroxy-5-methyl-4,11-dioxoundecanoic acid); 86 (1-linoleoyl-sn-glycero-3-phosphoethanolamine); 87 (1-Glyceryl stearate);

89 (phyllanthin); 90 (Pirsidomine); 91 (Omacetaxine mepesuccinate); 92 (L-gamma-Glutamyl-L-leucine); 93 (Fructoselysine); 94 (N-tert-Butyloxycarbonyl-deacetyl-leupeptin); 95 (3-Hydroxyhexadecanoylcarnitine); 96 (4-(Trimethylammonio)-3-(undecanoyloxy)butanoate);

98 (7-ketodeoxycholic acid); 100 (Glucoheptonic Acid); 101 (5-Dibutyl 2-deoxy-3-C-(methoxycarbonyl)pentarate); 103 (Ascorbyl stearate); 104 (10,16-Dihydroxyhexadecanoic acid); 105 (7-Mercaptoheptanoylthreonine); 106 (1-Stearoyl-2-hydroxy-sn-glycero-3-PE);

108 (Patrinolide); 109 (Rehmanolide C); 111 (Glucopyranosyloxyjasmonic acid); 112 ((2-Hydroxy-2-oxido-1,3,2-dioxaphospholan-4-yl)methyl palmitate); 114 (1,3-Dihydroxy-2-propenyl (9Z)-9-tetradecenoate); 115 (Istamycin B3); 116 (Bafilomycin A1); 117 (Eriogonolide B);

118 (Precorrin-5); 119 (Ubiquinol 10); 120 (D-Pantothenic acid); 121 (3-Hydroxy carbofuran); 122 (9,10-Epoxyoctadecanoic acid); 123 (1,3-Dimethyluric acid); 124 (dibutyl decanedioate)

Supplementary Table S1: Common metabolites (T0) among the different diet regimens (Formula milk plus Post biotics (FMPB); Breast Milk (BM); Formula Milk (FM)) grouped based on their belonging class.

Metabolites	FMPB	BM	FM
	Median (25-75)	Median (25-75)	Median (25-75)
<i>Amminoacids and derivatives</i>			
Oleoyl tyrosine	0.3 (0.3-0.3)	0.3 (0.3-1.4)	0.3 (0.3-0.3)
Phenylac-gln-OH	2.95 (0.3-6.45)	0.3 (0.3-5.38)	0.3 (0.3-6.25)
N-[(1S)-4-Carbamimidamido-1-carboxybutyl]asparaginyL-beta-aspartyl-L-arginine	4.4 (1.9-5.8)	4.1 (2.15-5.2)	3.6 (0.3-5)
Leu-Val	0.3 (0.3-4.88)	0.3 (0.3-2.05)	0.3 (0.3-1.85)
<i>Bile acid and derivatives</i>			
11 ² -Hydroxycholic acid	0.3 (0.3-5.88)	2.45 (0.3-4.65)	0.3 (0.3-4.65)
Glycocholic acid	0.3 (0.3-1.05)	0.3 (0.3-5.25)	0.3 (0.3-5.2)
Glycoursodeoxycholic acid 3-sulfate	1 (0.3-4.78)	0.3 (0.3-0.3)	2.8 (0.3-6.4)
Glycochenodeoxycholic acid	2.75 (0.3-6.1)	0.3 (0.3-0.3)	0.3 (0.3-5.55)
<i>Organic acid</i>			
Citric acid	5.5 (4.3-6.13)	5.3 (0.3-5.8)	5.4 (2.1-6.2)
Traumatic Acid	5 (2.3-5.25)	5 (3.7-5.4)	5 (3.35-5.4)
D-Gluconic acid	5.65 (0.3-6.03)	5.4 (5-5.45)	5.4 (0.3-6)
D-Glucopyranuronic acid	0.3 (0.3-5.58)	0.3 (0.3-6.5)	6.1 (0.3-6.15)
5-Methoxy-3-indoleacetate	2.9 (0.3-5.88)	0.3 (0.3-6.25)	0.3 (0.3-0.3)
<i>Fatty acid and derivatives</i>			
Azelaic acid	5.65 (3.9-6.6)	5.35 (4.2-6.2)	5.8 (4.1-6.2)
Sebacic acid	4.3 (4.1-5.25)	4.6 (3.78-6.2)	4.1 (4-5.95)
15,16-DiHODE	5.2 (3.28-5.28)	4.1 (2.2-4.78)	4.7 (3.6-5.7)
3-oxopalmitic acid	4.8 (1.95-4.9)	2.05 (0.3-4.8)	3.3 (0.3-5.3)
3-Hydroxysebacic acid	5.6 (5.35-6.1)	5.6 (5.05-6.03)	5.8 (4.3-6.1)
13S-hydroxyoctadecadienoic acid	2.4 (2.03-5)	3.45 (1.68-5.2)	2.4 (1.4-4.55)
Pinellic acid	3.7 (3.65-5.2)	4.15 (2.57-5.5)	3.9 (0.3-5.2)
(10E,15Z)-9,12,13-Trihydroxy-10,15-octadecadienoic acid	2.1 (0.3-4.03)	2.3 (1.8-3.68)	2 (0.3-3.9)
3-Oxotetradecanoic acid	0.3 (0.3-4.6)	2.9 (0.3-6.2)	0.3 (0.3-2.75)
Palmitelaidic acid	5.1 (4.28-5.45)	3.15 (0.3-5.6)	4.8 (3.6-5.55)
Palmitic Acid	5 (3.9-5.4)	2.1 (0.3-5.2)	5 (3.6-5.6)
Traumatol	5 (0.3-5.7)	3.7 (0.3-4.35)	5.2 (3.6-5.6)
13(S)-HpOTrE	2.15 (0.3-5.1)	1.1 (0.3-4.5)	4.5 (2.15-5.5)
Oleic acid	5.8 (5.5-6.6)	6 (5.5-7)	5.8 (5.5-5.8)

Phloionolic acid	5 (2.55-5.83)	3.6 (1.8-5)	4.6 (2.65-5.5)
12-HSA	5.45 (1.93-6.4)	5.45 (2.85-6.2)	4.3 (0.4-6.2)
9,10-Dihydroxystearic acid	3.3 (1.28-4.05)	0.3 (0.3-2.08)	1.8 (0.3-3.6)
Stearic acid	5.8 (4.3-5.8)	5.1 (4.3-5.8)	4.7 (4.3-5.8)
Myristic acid	5.3 (4.25-6.03)	5.7 (4.9-6.35)	5.8 (5.2-6.2)
Dimethyl (2E)-3-methoxy-4-oxo-5-[(8E,11E)-8,11,14-pentadecatrien-1-yl]-2-hexenedioate	0.3 (0.3-5.63)	5.3 (1.65-5.65)	0.3 (0.3-6.3)
<i>Steroids</i>			
Estriol	0.3 (0.3-1.7)	0.3 (0.3-1.7)	0.3 (0.3-6.5)
Androsterone sulfate	4.8 (0.3-5.8)	0.3 (0.3-4.9)	4.8 (0.3-5.7)
16alpha-hydroxydehydroepiandrosterone 3-sulfate	0.3 (0.3-1.63)	0.3 (0.3-3.6)	0.3 (0.3-4.8)
2-methoxy-17beta-estradiol 3-sulfate	4.95 (3.53-6.03)	4.8 (2.45-6.5)	3.3 (0.5-5.2)
Dehydroepiandrosterone sulfate	3.15 (0.3-5.2)	2 (0.3-5.2)	3.3 (0.3-5.3)
<i>Other organic compounds</i>			
Tiliacorine	5.6 (0.3-6.2)	6 (3.3-6.23)	4.3 (0.3-5.8)
O-heptadecanoylcarnitine	0.3 (0.3-5.7)	0.3 (0.3-0.3)	0.3 (0.3-0.3)
Carbazeran	5.6 (5.1-5.8)	5.6 (5.4-5.8)	5.6 (4.8-5.9)
Soyasaponin I	0.3 (0.3-0.3)	0.3 (0.3-0.3)	0.3 (0.3-0.3)
Tomelukast	5.1 (5-5.25)	5 (3.68-5.45)	5 (2.95-5.3)
N(4)-phosphoagmatine	5.6 (4.6-6.4)	6.3 (4.25-6.7)	6.2 (5.8-6.6)

Data are expressed as peak rating.

Supplementary Table S2: Common metabolites (T1) among the different diet regimens (Formula milk plus Post biotics (FMPB); Breast Milk (BM); Formula Milk (FM)) grouped based on their belonging class.

Metabolites	FMPB	FM	BM
	Median (25-75)	Median (25-75)	Median (25-75)
<i>Ammiinoacids and derivatives</i>			
N-Stearoyltyrosine	0.3 (0.3-0.3)	0.3 (0.3-0.3)	0.3 (0.3-0.3)
Leu-Leu	3.9 (0.3-5.2)	0.6 (0.3-4.85)	4.3 (0.9-5.1)
Leu-Asn	0.3 (0.3-3.9)	0.3 (0.3-5.65)	0.3 (0.3-1.6)
<i>Organic acid</i>			
Diethyl tartrate	0.3 (0.3-0.3)	0.3 (0.3-5.2)	0.3 (0.3-0.3)
2-methylcitric acid	0.3 (0.3-6)	0.3 (0.3-5.5)	0.3 (0.3-0.3)
Citric acid	5.6 (0.3-6.4)	2.9 (0.3-6.4)	5.8 (0.3-6.1)
D-Gluconic acid	5.2 (0.3-6.1)	4 (0.3-6.05)	4.6 (0.3-5.8)
laurilsulfate	4.3 (4.3-4.7)	0.3 (0.3-4.7)	4.7 (4.3-6.2)
porphobilinogen	0.3 (0.3-0.3)	0.3 (0.3-0.4)	0.3 (0.3-2.7)
Undecylbenzenesulfonic acid	0.3 (0.3-2)	2.2 (0.3-3.75)	2 (0.3-3.6)
1,1'-monoglyceride citrate	0.3 (0.3-6.6)	0.3 (0.3-5.6)	0.3 (0.3-5.2)
<i>Fatty acids and derivatives</i>			
1-stearyl estercitric acid	0.3 (0.3-0.3)	0.3 (0.3-2)	0.3 (0.3-4.3)
Traumatic Acid	0.3 (0.3-0.3)	0.3 (0.3-5.15)	0.3 (0.3-6)
Azelaic acid	0.3 (0.3-4.8)	4.35 (0.3-6.6)	0.3 (0.3-6.2)
Sebacic acid	0.5 (0.3-3.5)	3.05 (0.7-4.3)	2 (0.3-5.6)
9,10-Epoxy stearic acid	5.2 (3.9-5.5)	5.35 (5.1-5.8)	3.9 (0.3-5.5)
Dibutyl sebacate	2 (0.3-5)	0.3 (0.3-3.15)	0.3 (0.3-2.4)
13S-hydroxyoctadecadienoic acid	2.2 (0.3-4.1)	3.15 (1.3-4.75)	0.7 (0.3-4.3)
(10E,15Z)-9,12,13-Trihydroxy-10,15-octadecadienoic acid	0.3 (0.3-2)	4.45 (0.3-5.5)	3.5 (0.3-5)
Palmitic Acid	0.3 (0.3-0.3)	0.3 (0.3-0.3)	0.3 (0.3-0.3)
Palmitelaidic acid	4.8 (0.3-5.2)	3.7 (0.3-5.15)	0.3 (0.3-3)
Traumatins	5 (3.3-6)	5.2 (1.85-6)	4.8 (2.2-5.6)

Oleic acid	5.8 (4.3-5.8)	5.65 (4-6)	5.8 (3.9-5.8)
Juniperic acid	0.3 (0.3-0.3)	0.3 (0.3-5.6)	0.3 (0.3-2.7)
Phloionolic acid	5 (2.3-5.4)	4.75 (3.8-5.5)	5.4 (4.5-5.8)
6-Hydroxy-5-methyl-4,11-dioxoundecanoic acid	1.2 (0.3-4.8)	4.3 (0.3-4.8)	0.3 (0.3-4.3)
12-HSA	0.3 (0.3-0.3)	0.3 (0.3-6.2)	0.3 (0.3-4.7)
9,10-Dihydroxystearic acid	0.3 (0.3-2)	2.2 (0.3-4.1)	1.1 (0.3-4.2)
Stearic acid	3.6 (0.3-3.9)	4.3 (2.65-4.9)	4.2 (1.7-5.5)
Myristic acid	0.3 (0.3-0.3)	0.3 (0.3-5.4)	0.3 (0.3-4.8)
Myristyl sulfate	0.3 (0.3-0.3)	0.3 (0.3-2.3)	0.3 (0.3-4.1)
Glycerol trihexanoate	3.9 (0.3-5.6)	3.05 (0.3-5.5)	0.3 (0.3-4.8)
L-alpha-lysophosphatidylcholine	0.3 (0.3-0.3)	0.3 (0.3-0.3)	0.3 (0.3-5.4)
1-linoleoyl-sn-glycero-3-phosphoethanolamine	0.3 (0.3-0.3)	0.3 (0.3-0.3)	0.3 (0.3-0.3)
1-Glyceryl stearate	0.3 (0.3-0.3)	0.3 (0.3-0.3)	0.3 (0.3-0.3)
<i>Steroids</i>			
2-methoxy-17beta-estradiol 3-sulfate	0.3 (0.3-0.3)	0.3 (0.3-0.3)	0.3 (0.3-0.3)
17-Hydroxypregnenolone sulfate	3.9 (0.3-5.4)	3.95 (0.3-5.3)	4.1 (0.3-5.6)
<i>Other organic compounds</i>			
5-Methoxy-3-indoleacetate	0.3 (0.3-0.3)	0.3 (0.3-2.5)	0.3 (0.3-0.3)
phyllanthin	0.3 (0.3-0.3)	0.3 (0.3-0.3)	0.3 (0.3-6)
Pirsidomine	5.2 (0.3-6)	4.15 (0.3-5.8)	4.8 (0.3-5.8)
Omacetaxine mepesuccinate	0.3 (0.3-0.3)	0.3 (0.3-0.3)	0.3 (0.3-0.3)

Data are expressed as peak rating.

Supplementary Table S3: Common metabolites (T2) among the different diet regimens (Formula milk plus Post biotics (FMPB); Breast Milk (BM); Formula Milk (FM)) grouped based on their belonging class.

Metabolites	FMPB	FM	BM
	Median (25-75)	Median (25-75)	Median (25-75)
<i>Aminoacids and derivatives</i>			
L-gamma-Glutamyl-L-leucine	2.9 (0.3-4.55)	2.25 (0.75-3.8)	0.3 (0.3-2.5)
Fructoselysine	4.5 (0.3-5.5)	1.25 (0.3-4.9)	3.4 (0.3-5.5)
N-tert-Butyloxycarbonyl-deacetyl-leupeptin	6 (5.65-6.2)	6.2 (5.8-6.4)	5.8 (5.8-6)
3-Hydroxyhexadecadienoylcarnitine	4.25 (0.3-5.35)	1.8 (0.3-4.8)	0.3 (0.3-5.15)
4-(Trimethylammonio)-3-(undecanoyloxy)butanoate	0.3 (0.3-4.1)	0.3 (0.3-0.3)	0.3 (0.3-0.3)
<i>Bile acids and derivatives</i>			
1β-Hydroxycholic acid	1.2 (0.3-5)	0.3 (0.3-4.95)	4.05 (0.3-5)
7-ketodeoxycholic acid	6.2 (5.8-6.85)	6.15 (5.5-6.65)	6.45 (5.8-6.6)
Cholic acid	0.3 (0.3-5.35)	3.1 (0.3-5.6)	5.4 (4.4-5.65)
<i>Organic acids</i>			
Citric acid	5.35 (3-6.2)	5.9 (4.3-6.65)	5.15 (4.3-6.2)
Glucoheptonic Acid	5.4 (4-6.3)	5.55 (4.75-5.8)	4.95 (2.75-6.05)
1,5-Dibutyl 2-deoxy-3-C-(methoxycarbonyl)pentarate	3.5 (2.75-4.9)	3.8 (2.7-4.8)	4.25 (3.7-5.2)
D-Gluconic acid	5.5 (5-5.8)	5.9 (5.5-6.5)	5.7 (4.85-5.8)
5-Methoxy-3-indoleacetate	6.2 (6.15-6.6)	6.35 (0.3-7)	6 (0.3-6.6)
<i>Fatty acid derivatives</i>			
Sebacic acid	4.3 (4.3-4.75)	4.3 (4.3-6.2)	4.3 (4.3-4.7)
9,10-Epoxystearic acid	5.5 (4.7-5.5)	5.5 (5.1-5.65)	5.5 (5.1-5.8)
Ascorbyl stearate	3.8 (1.85-4.9)	4.8 (4.35-4.9)	4.7 (4.3-5.1)
Dibutyl sebacate	5 (4-5.65)	5.5 (4.7-5.8)	5.65 (4.3-6.2)
10,16-Dihydroxyhexadecanoic acid	5.8 (4.55-6.35)	5.35 (3.7-5.75)	5.1 (3.4-5.65)
13S-hydroxyoctadecadienoic acid	5.1 (4.7-5.7)	5.5 (5.3-5.7)	5.5 (4.85-5.55)
3-Hydroxysebacic acid	6.05 (5.3-7.4)	6.05 (4.8-6.8)	4.8 (4.8-7.1)

7-Mercaptoheptanoylthreonine	4.3 (0.3-5.65)	3.5 (0.3-6.25)	2.9 (0.3-4.35)
(10E,15Z)-9,12,13-Trihydroxy-10,15-octadecadienoic acid	4.2 (2.7-5.3)	4.7 (3.45-5.5)	4.6 (2.9-5.5)
1-Stearoyl-2-hydroxy-sn-glycero-3-PE	5.4 (4.95-5.8)	5.2 (0.3-5.25)	5.2 (2-5.5)
Palmitic Acid	5.65 (5.5-6.6)	6 (5.8-6.6)	5.85 (5.5-6.2)
Palmitelaidic acid	4.5 (2.95-5.35)	5.45 (4.6-5.55)	5.3 (4.8-5.7)
13(S)-HpOTrE	4.25 (1.95-4.65)	2.1 (1.1-2.25)	2 (1.85-4.5)
12-HSA	6.2 (5.25-6.4)	6.2 (5.75-7)	5.8 (4.5-7)
9,10-Dihydroxystearic acid	5.65 (5.5-6.6)	6 (5.8-6.6)	5.85 (5.5-6.2)
Stearic acid	5.6 (4.6-5.7)	5.8 (4.95-5.8)	4.95 (4.4-5.35)
Myristic acid	5.5 (5.2-5.9)	5.7 (5.2-5.9)	5.8 (5.5-6.05)
<i>Terpenes</i>			
Patrinoside	4.6 (2.15-5.1)	5 (3.7-5.3)	4.9 (2-5)
Rehmaionoside C	0.55 (0.3-5)	5 (2.5-5.2)	5 (4.25-5.2)
<i>Other compounds</i>			
12-O-Î²-D-Glucopyranosyloxyjasmonic acid	0.3 (0.3-5.6)	2.4 (0.3-5.2)	0.3 (0.3-5.2)
(2-Hydroxy-2-oxido-1,3,2-dioxaphospholan-4-yl)methyl palmitate	0.3 (0.3-4.3)	1.9 (0.3-4.65)	0.3 (0.3-1.9)
2-Dodecylbenzenesulfonic acid	3.2 (2.9-4.3)	3.7 (2.9-4.25)	4.1 (3.5-4.45)
3-Hydroxycarbofuran	0.3 (0.3-1)	0.3 (0.3-5.2)	4.45 (0.3-6.15)
1,3-Dihydroxy-2-propanyl (9Z)-9-tetradecenoate	3.6 (0.3-5.1)	5.2 (4.55-5.4)	4.35 (3-5.15)
Istamycin B3	2 (1.3-3.75)	4 (2.2-5.2)	4.35 (1.5-5.2)
Bafilomycin A1	2.4 (1.9-5)	4 (1.7-5.5)	5.2 (3.6-6.2)
Phenylac-gln-OH	5.7 (0.3-6.1)	4.95 (0.3-5.95)	2.9 (0.3-6.1)
Eriojaposide B	4.2 (3-5.65)	4.5 (3.8-5.8)	3.85 (3.1-4.4)
Precorrin-5	0.3 (0.3-3.9)	2.1 (0.3-5.5)	0.3 (0.3-4.8)
Ubiquinol 10	2.9 (0.3-5.85)	0.3 (0.3-5.8)	5.35 (2.75-5.75)
D-Pantothenic acid	1.5 (0.3-5.8)	5.5 (5.4-5.6)	5.5 (2.85-5.8)

Data are expressed as peak rating.