

Supplementary Methods

Reagents and chemicals

Laboratory animal diet was purchased from Hunan SJA Laboratory Animal Co., Ltd. (Changsha, China). Fenofibrate capsules (FCs) were purchased from French Libofoni Pharmaceutical Biological Technology Co., Ltd. (Paris, France). Commercial kits for measuring total cholesterol (TC), triglyceride (TG), low-density lipoprotein cholesterol (LDL-C), high-density lipoprotein cholesterol (HDL-C), alanine transaminase (ALT), aspartate transaminase (AST), malondialdehyde (MDA), and superoxide dismutase (SOD) levels were purchased from Nanjing Jiancheng Bioengineering Institute (Nanjing, China). ELISA kits for detecting interleukin-6 (IL-6), interleukin-1 β (IL-1 β), tumor necrosis factor- α (TNF- α), rat aldehyde reductase B1 (AKR1B1), rat aldehyde reductase B10 (AKR1B10), phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit alpha (PIK3CA), and recombinant phosphoinositide-3-kinase catalytic beta (PIK3CB) were obtained from Shanghai Enzyme-linked Biotechnology Co., Ltd. (Shanghai, China). Paraformaldehyde 4% fixing solution, the hematoxylin and eosin (H&E) staining kit, and Oil Red O dye were purchased from Wuhan Servicebio Technology Co., Ltd. (Wuhan, China). The HepG2 human hepatocellular cell line was purchased from the Cell Resource Center, Institute of Basic Medical Sciences, Chinese Academy of Medical Sciences. (Beijing, China). Dulbecco's modified Eagle medium (DMEM) was purchased from Grand Island Biological Company Co., Ltd. (NY, USA). Sodium oleate was purchased from Shanghai Macklin Biochemical Co., Ltd. (Shanghai, China). Sodium palmitate (No. P9767) was purchased from Sigma-Aldrich (PA, USA). RIPA Lysis Buffer (No.240007014) was purchased from Solarbio Co., Ltd. (Beijing, China). All the other reagents were of analytical grade or higher. The PR, *Alismatis Rhizoma*, *Cinnamomi Ramulus*, *Atractylodis Macrocephalae Rhizoma*, *Glycyrrhizae Radix*, and *Zingiberis Rhizoma Recens* samples were purchased from Kunming Luosiwan Chinese Medicinal Materials Market (Kunming, China) and authenticated by Professor Xing-Xin

Yang at the Yunnan University of Chinese Medicine.

Quality control of FZD/ZD extract

To ensure the quality control of FZD/ZD extract, the contents of atractylenolide II and cinnamaldehyde were quantified by means of an Agilent 1220 Infinity II UPLC system (Agilent Technologies, CA, USA). The accurately weighed atractylenolide II reference standard was dissolved in methanol to prepare a 10 µg/mL solution. Similarly, the freeze-dried powders of FZD or ZD extract were dissolved to obtain 40 mg/mL solutions. The prepared solutions underwent ultrasonic extraction for 30 minutes, followed by filtration via a 0.22 µm microporous membrane, and were subsequently subjected to UPLC analysis. Chromatographic separation was achieved on an Agilent ZORBAX SB-C18 column (4.6×250 mm, 5 µm; Agilent Technologies, CA, USA) with a constant flow rate of 1.0 mL/min, while the column temperature was maintained at 30 °C. The injection volume was fixed at 10 µL, and the mobile phase comprised acetonitrile (phase A) and 0.1% phosphoric acid aqueous solution (phase B). The gradient elution program was detailed as below: 0-10.0 min, 19% A; 10.0-45.0 min, 30% A; 45.0-70.0 min, 45% A; 70.0-112.0 min, 70% A; 112.0-115.0 min, 70% A. The detection wavelength was set at 280 nm.

UPLC-MS analysis of Metabolomic analysis

UPLC-MS analysis was executed on a Thermo UHPLC-Q Exactive system (Thermo Scientific, MA, USA) and an ACQUITYHSS T3 column (1.8 µm, 100 mm × 2.1 mm, Waters, MA, USA). The mobile phase comprised (A) 0.1% formic acid in water: acetonitrile (95:5, v/v) and (B) 0.1% formic acid in acetonitrile: isopropanol : water (47.5:47.5:5, v/v). Chromatographic separation was achieved using the following gradient program: 0–2 min, 0% B; 2–6 min, 0–48% B; 6–10 min, 48–100% B ; 10–12 min, 100% B; 12–12.1 min, 100–0% B; and 12.1–15 min, 0% B. The sample injection volume was 4 µL, with a flow rate of 0.3 mL/min. Mass spectral signals of the samples were acquired in both the positive and negative ion scanning modes using a Thermo UHPLC-Q Exactive

Mass Spectrometer equipped with an electrospray ionization (ESI) source at a scan mass range of 75–1050 m/z. The spray voltage was 3500 V for the positive ion mode and 2800 V for the negative ion mode. The sheath gas flow rate was 40 psi, and the auxiliary gas flow rate was 10 psi. The collision energy was set to a cyclic collision energy of 20-40-60V. All samples were mixed in equal volumes to prepare quality control (QC) samples. During the detection process, one QC sample was assayed every five test samples to evaluate the repeatability of the analytical procedure.

Identification of FZD/FFZD/ZD-derived components in serum from MASLD rats

Sample preparation

For each group, 200 µL of individual serum samples was pooled, mixed with a three-fold volume of acetonitrile, and vortexed for 30 seconds, allowed to stand for 20 min at 4°C, and centrifuged (12000 rpm, 15 min, 4°C). The supernatant was collected, gently blown dry under nitrogen gas, then redissolved in 200 µL of an acetonitrile-water mixture (50:50, v/v) and filtered through a 0.22 µm microporous filter membrane for UPLC-MS analysis.

UPLC/MS conditions

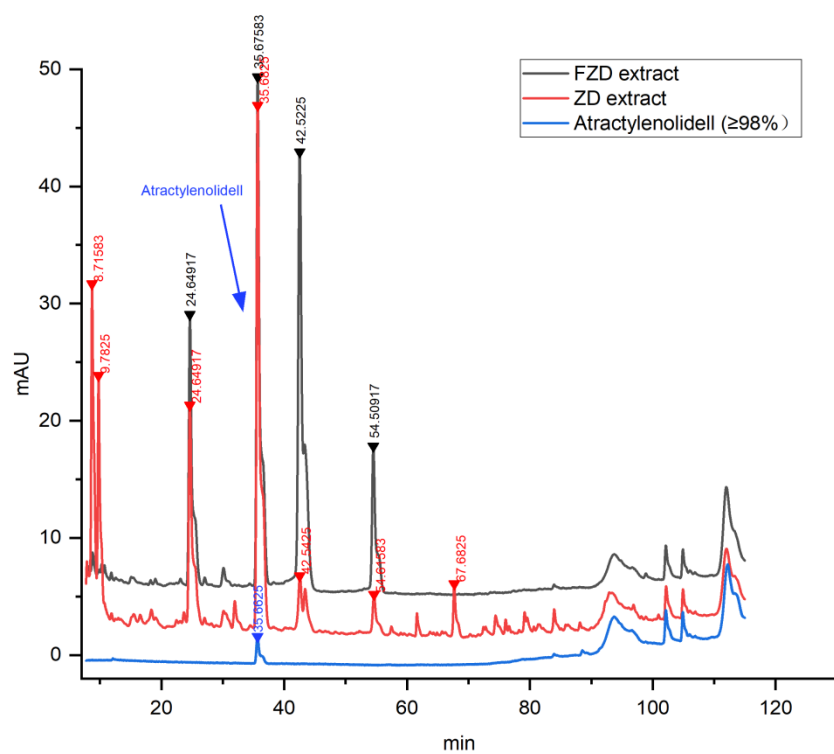
An Agilent 1290 Infinity II UPLC system (Agilent Technologies, CA, USA) was used for the analysis. Elution was performed using the Shim-pack XR-ODS column (2.0 mm × 100 mm, 2.2 µm). The flow rate was 0.2 mL/min. The column temperature was maintained at 30°C, and the injection volume was 5 µL. The mobile phase consisted of acetonitrile (A) and 0.1% formic acid in water (B) with the following gradient program: 0 min, 5% A; 20 min, 10% A; 30 min, 20% A; 40 min, 30% A; 50 min, 40% A; 60 min, 50% A; 70 min, 60% A; 80 min, 70% A; 90 min, 85% A; 100 min, 95% A; 105 min, 100% A; and 115 min, 5% A.

Mass spectrometry was performed using an Agilent G6545 Q/TOF mass spectrometer equipped with ESI (Agilent Technologies, CA, USA). Positive and

negative ion scanning were used to collect sample quality spectrum information at a scan mass range of 100–1200 m/z. The spray voltage was 3.5 kV for the positive ion mode and 2.8 kV for the negative ion mode. The capillary temperature was set at 350°C, the nebulizer gas flow was 1.5 L/min, and the heater temperature was 250°C. The collision energies were set to 35 and 40 eV.

Data processing and analysis

The acquired mass spectrometry data were processed using Qualitative Analysis B.06.00 software. First, mass spectral information on FZD, FFZD, and ZD was compared with that of the HFD group to eliminate interference from endogenous substances in the serum. Then, the FZD/ZD/FFZD-derived compounds in rat serum samples were identified based on molecular weights, MS/MS data, and the relative retention times of compounds in PR, *Alismatis Rhizoma*, *Cinnamomi Ramulus*, *Atractylodis Macrocephalae Rhizoma*, *Glycyrrhizae Radix*, and *Zingiberis Rhizoma Recens* as previously reported.



Supplementary Figure 1 UPLC chromatogram for quality control of FZD/ZD extract. FZD, Fuling Zexie Decoction; ZD, Fuling Zexie Decoction without Poria.

Supplementary Table 1 The composition of key compound groups

The key active compound ensemble of FZD (FZDC)		The key active compound ensemble of ZD (ZDC)		The key active compound ensemble of FZD that was only comprised of PR compounds (PRC)		The key active compound ensemble of FZD without PR compounds (WOC)	
Compound	Ratio	Compound	Ratio	Compound	Ratio	Compound	Ratio
Dehydrotrametenonlic acid	2.94%	Alisol F	15.06%	Dehydrotrametenonlic acid	9.20%	Alisol F	11.48%
Poricoic acid A	13.13%	Liquiritigenin	5.72%	Poricoic acid A	41.05%	Liquiritigenin	4.68%
16α-Hydroxydehydrotrametenolic acid	2.69%	Glycyrrhetic Acid	11.87%	16α-Hydroxydehydrotrametenolic acid	8.42%	Glycyrrhetic Acid	5.28%
Dehydropachymic acid	13.21%	Liquiritin	12.85%	Dehydropachymic acid	41.31%	Liquiritin	10.75%
Alisol F	7.81%	Glabrol	26.17%			Glabrol	13.88%
Liquiritigenin	3.19%	Gingerenone A	0.62%			(10)-Gingerol	10.98%
Glycyrrhetic Acid	3.59%	Cinnamic acid	0.44%			Gingerenone A	0.66%
Liquiritin	7.31%	Cinnamyl alcohol	5.41%			Cinnamic acid	21.26%
Glabrol	9.44%	Cinnamaldehyde	1.99%			Cinnamaldehyde	2.56%
(10)-Gingerol	7.47%	6-methylcoumarin	7.95%			6-methylcoumarin	8.29%
Gingerenone A	0.45%	Hydroxycinnamic acid	2.46%			Hydroxycinnamic acid	2.31%
Cinnamic acid	14.46%	7-hydroxycoumarin	2.97%			7-hydroxycoumarin	1.34%
Cinnamaldehyde	1.74%	Ligustilide	5.12%			Ligustilide	3.30%
6-methylcoumarin	5.64%	Chlorogenic Acid	1.38%			Chlorogenic Acid	0.97%
Hydroxycinnamic acid	1.57%					Diosgenin	2.25%
7-hydroxycoumarin	0.91%						
Ligustilide	2.25%						
Chlorogenic Acid	0.66%						
Diosgenin	1.53%						

FZD, Fuling Zexie Decoction; ZD, Fuling Zexie Decoction without Poria.

Supplementary Table 2 The model parameters of OPLS-DA

Sample	R ² Y	Q ²
Serum	0.930	-0.26
Liver	0.769	-0.24
Urine	0.913	-0.15
Feces	0.968	-0.14

Supplementary Table 3 The metabolites significantly-regulated by FZD in MASLD rats

Metabolite	Rt (min)	m/z	Formula	P	VIP	FZD <i>vs</i> HFD	Sample
Trimethyloxamine	1.35	76.0761	C ₃ H ₉ NO	0.0046	2.0791	↑	Serum
Hexaethylene glycol	6.63	283.1740	C ₁₂ H ₂₆ O ₇	0.0059	2.0759	↑	Serum
Indole-3-acrylic acid	9.39	186.0544	C ₁₁ H ₉ NO ₂	0.0021	2.0759	↑	Serum
Estrone glucuronide	7.66	445.1897	C ₂₄ H ₃₀ O ₈	0.0022	2.0694	↑	Serum
4-Hydroxybenzaldehyde	7.38	105.0337	C ₇ H ₆ O ₂	0.0085	2.0512	↑	Serum
Hippuric acid	7.36	178.0495	C ₉ H ₉ NO ₃	0.0090	2.0432	↑	Serum
Vanillic acid	6.48	167.0336	C ₈ H ₈ O ₄	0.0099	2.0322	↑	Serum
Cyclo(Pro-Leu)	7.94	211.1436	C ₁₁ H ₁₈ N ₂ O ₂	0.0037	2.0074	↑	Serum
1-methyl-4-(6-methylhept-5-en-2-yl)-2,3-dioxabicyclo(2.2.2)oct-5-ene	7.31	201.1631	C ₁₅ H ₂₄ O ₂	0.0142	1.9962	↑	Serum
Eudesmin	10.91	387.1781	C ₂₂ H ₂₆ O ₆	0.0041	1.9948	↑	Serum
3,5-Dihydroxyphenylvaleric acid sulfate	7.48	289.0384	C ₁₁ H ₁₄ O ₇ S	0.0143	1.9920	↑	Serum
PC(16:0/18:2)	12.32	758.5688	C ₄₂ H ₈₀ NO ₈ P	0.0049	1.9637	↓	Serum
Cinnamoylglycine	8.72	204.0654	C ₁₁ H ₁₁ NO ₃	0.0165	1.9594	↑	Serum
Glycyrrhetic acid	12.65	469.3321	C ₃₀ H ₄₆ O ₄	0.0181	1.9540	↑	Serum

Azelaic acid	8.76	187.0961	C ₉ H ₁₆ O ₄	0.0180	1.9005	↑	Serum
9-acetyl-17-hydroxy-10,14-dimethyl-20-oxahexacyclo(11.9.0.0<2,10>.0<4,9>.0<14,19>.0<19,21>)docosane	11.04	387.2885	C ₂₅ H ₃₈ O ₃	0.0351	1.8971	↓	Serum
Cinnamic acid	8.73	131.0488	C ₉ H ₈ O ₂	0.0236	1.8877	↑	Serum
Anisole	7.88	107.0486	C ₇ H ₈ O	0.0205	1.8796	↑	Serum
2,6-Diamino-9-(2-hydroxyethoxymethyl)purine	9.30	223.0965	C ₈ H ₁₂ N ₆ O ₂	0.0031	1.8739	↑	Serum
Acoric acid	10.29	267.1593	C ₁₅ H ₂₄ O ₄	0.0296	1.8516	↑	Serum
Biotin	7.44	243.0795	C ₁₀ H ₁₆ N ₂ O ₃ S	0.0149	1.8443	↓	Serum
2-Isopropylmalic acid	6.84	175.0598	C ₇ H ₁₂ O ₅	0.0280	1.8206	↑	Serum
3-Hydroxycapric acid	10.48	187.1325	C ₁₀ H ₂₀ O ₃	0.0132	1.8204	↑	Serum
Acetic acid, 2-((3-sulfooxybenzoyl)amino)-	6.12	274.0016	C ₉ H ₉ NO ₇ S	0.0118	1.8031	↑	Serum
5-Hexyltetrahydro-2-oxo-3-furancarboxylic acid	10.38	213.1116	C ₁₁ H ₁₈ O ₄	0.0389	1.7908	↑	Serum
Vaccenic acid	13.32	281.2472	C ₁₈ H ₃₄ O ₂	0.0317	1.7840	↓	Serum
Enterolactone	8.78	299.1274	C ₁₈ H ₁₈ O ₄	0.0445	1.7774	↓	Serum
Alkhanin	9.18	263.1283	C ₁₅ H ₂₀ O ₄	0.0427	1.7723	↑	Serum
3-Methylene-indolenine	9.59	130.0649	C ₉ H ₇ N	0.0162	1.7597	↑	Serum

Liquiritin apioside	7.93	549.1594	C ₂₆ H ₃₀ O ₁₃	0.0427	1.7406	↑	Serum
Abscisic acid	9.41	247.1325	C ₁₅ H ₂₀ O ₄	0.0489	1.7326	↑	Serum
3-(Indol-3-yl)propionic acid	9.59	190.0855	C ₁₁ H ₁₁ NO ₂	0.0198	1.7178	↑	Serum
10-Hydroxydecanoate	10.63	211.1318	C ₁₀ H ₂₀ O ₃	0.0267	1.6964	↑	Serum
N-epsilon-Formyl-L-lysine	1.40	175.1070	C ₇ H ₁₄ N ₂ O ₃	0.0454	1.6899	↑	Serum
gamma-Guanidinobutyric acid	2.12	146.0922	C ₅ H ₁₁ N ₃ O ₂	0.0409	1.6744	↑	Serum
cis-Dihydrocarvone	9.25	153.1271	C ₁₀ H ₁₆ O	0.0353	1.6418	↑	Serum
D-Lysine	1.12	147.1124	C ₆ H ₁₄ N ₂ O ₂	0.0433	1.6207	↓	Serum
14,15-EpETE	11.81	301.2150	C ₂₀ H ₃₀ O ₃	0.0205	1.5991	↑	Serum
Pipecolic acid	1.12	130.0861	C ₆ H ₁₁ NO ₂	0.0428	1.5932	↓	Serum
Butyrylcarnitine	6.35	232.1540	C ₁₁ H ₂₁ NO ₄	0.0368	1.5792	↑	Serum
alpha-Carboxy-delta-nonolactone	9.04	199.0963	C ₁₀ H ₁₆ O ₄	0.0236	1.5571	↑	Serum
Epoprostenol	11.04	351.2158	C ₂₀ H ₃₂ O ₅	0.0321	1.5549	↑	Serum
5-Dihydroxyhept-6-enoic acid	7.22	159.0644	C ₇ H ₁₂ O ₄	0.0495	1.3633	↑	Serum
Costunolide	10.26	233.1526	C ₁₅ H ₂₀ O ₂	0.0000	2.0369	↑	Liver
PC(18:0/18:2)	12.31	786.5969	C ₄₄ H ₈₄ NO ₈ P	0.0000	1.9828	↓	Liver
Citrazinic acid	6.62	154.0133	C ₆ H ₅ NO ₄	0.0001	1.9489	↑	Liver

Hippuric acid	7.33	178.0497	C ₉ H ₉ NO ₃	0.0001	1.9487	↑	Liver
Acoric acid	10.29	267.1602	C ₁₅ H ₂₄ O ₄	0.0001	1.9479	↑	Liver
3-Hydroxytetradecanedioic acid	9.32	273.1705	C ₁₄ H ₂₆ O ₅	0.0002	1.9302	↑	Liver
Abscisic acid	9.39	263.1287	C ₁₅ H ₂₀ O ₄	0.0004	1.9125	↑	Liver
gamma-Guanidinobutyric acid	2.12	146.0922	C ₅ H ₁₁ N ₃ O ₂	0.0005	1.8926	↑	Liver
N-Arachidonoyltaurine	12.31	412.2494	C ₂₂ H ₃₇ NO ₄ S	0.0003	1.8661	↓	Liver
Roquefortine E	10.05	456.2418	C ₂₇ H ₃₁ N ₅ O ₂	0.0008	1.8565	↑	Liver
2-Methylbenzaldehyde	7.22	119.0486	C ₈ H ₈ O	0.0010	1.8511	↑	Liver
3-Phenyllactic acid	8.19	165.0543	C ₉ H ₁₀ O ₃	0.0008	1.8423	↑	Liver
Leu ¹ ptin	12.77	427.3017	C ₂₀ H ₃₈ N ₆ O ₄	0.0005	1.8346	↓	Liver
2,3-Dimethyl-5-propylpyrazine	6.47	151.1229	C ₉ H ₁₄ N ₂	0.0013	1.8215	↑	Liver
Dibutylphthalic acid	10.07	277.1434	C ₁₆ H ₂₂ O ₄	0.0011	1.8102	↓	Liver
Trigonelline	1.40	138.0548	C ₇ H ₇ NO ₂	0.0017	1.8010	↑	Liver
Meso-Tartaric acid	0.91	149.0076	C ₄ H ₆ O ₆	0.0015	1.7829	↑	Liver
2-Methylcitric acid	3.29	205.0346	C ₇ H ₁₀ O ₇	0.0015	1.7710	↑	Liver
Glycolithocholic acid	11.89	434.3259	C ₂₆ H ₄₃ NO ₄	0.0026	1.7452	↓	Liver
Isoalantolactone	12.05	233.1526	C ₁₅ H ₂₀ O ₂	0.0031	1.7356	↑	Liver

Gingerol	9.36	277.1785	C ₁₇ H ₂₆ O ₄	0.0043	1.7344	↑	Liver
Oryzalic acid A	8.95	349.2017	C ₂₀ H ₃₀ O ₅	0.0024	1.7277	↓	Liver
Benzethonium	13.15	413.3270	C ₂₇ H ₄₂ NO ₂	0.0035	1.7248	↓	Liver
Cinnamoylglycine	8.71	204.0658	C ₁₁ H ₁₁ NO ₃	0.0034	1.7237	↑	Liver
Pyroglutamyl-Isoleucine	7.40	241.1188	C ₁₁ H ₁₈ N ₂ O ₄	0.0052	1.6751	↑	Liver
Dehydromenthofurolactone	10.43	165.0906	C ₁₀ H ₁₂ O ₂	0.0090	1.6562	↓	Liver
2-Hydroxylinolenic acid	11.75	293.2119	C ₁₈ H ₃₀ O ₃	0.0099	1.6269	↓	Liver
6-Methoxypurine	13.59	151.0612	C ₆ H ₆ N ₄ O	0.0047	1.6235	↑	Liver
(+)-Cycloolivil	9.37	375.1474	C ₂₀ H ₂₄ O ₇	0.0104	1.6221	↑	Liver
3-(2-(2,3-dihydroxy-5,6,8a-trimethyloctahydro- 2H-spiro(naphthalene-1,2'-oxiran)-5-yl)ethyl)-5- hydroxyfuran-2(5H)-one	8.13	365.1959	C ₂₀ H ₃₀ O ₆	0.0066	1.6103	↓	Liver
Perfluorooctanesulfonic Acid	11.68	498.9313	C ₈ HF ₁₇ O ₃ S	0.0080	1.6051	↓	Liver
3,4,5-Trimethylbenzaldehyde	11.79	149.0956	C ₁₀ H ₁₂ O	0.0096	1.6032	↓	Liver
Taurochenodeoxycholic acid	9.89	500.3035	C ₂₆ H ₄₅ NO ₆ S	0.0152	1.5931	↑	Liver
Glycoursodeoxycholic acid	10.86	450.3207	C ₂₆ H ₄₃ NO ₅	0.0100	1.5857	↓	Liver
Liquiritin	8.08	417.1194	C ₂₁ H ₂₂ O ₉	0.0070	1.5772	↑	Liver

3-(Indol-3-yl)propionic acid	9.57	190.0859	C ₁₁ H ₁₁ NO ₂	0.0113	1.5713	↑	Liver
8-HETE	11.96	321.2408	C ₂₀ H ₃₂ O ₃	0.0136	1.5681	↓	Liver
2-Isopropyl-5-methylpyrazine	6.18	137.1071	C ₈ H ₁₂ N ₂	0.0147	1.5663	↑	Liver
Imidazolepropionic acid	2.05	141.0654	C ₆ H ₈ N ₂ O ₂	0.0093	1.5618	↑	Liver
Sorbose	0.89	161.0442	C ₆ H ₁₂ O ₆	0.0126	1.5521	↑	Liver
Koninginin E	12.34	247.1682	C ₁₆ H ₂₆ O ₄	0.0112	1.5514	↓	Liver
Taurohyocholate	8.84	516.2973	C ₂₆ H ₄₅ NO ₇ S	0.0216	1.5488	↑	Liver
Glycocholate	9.82	504.2699	C ₂₆ H ₄₃ NO ₆	0.0106	1.5477	↑	Liver
3, 5-Tetradeciencarnitine	10.63	368.2784	C ₂₁ H ₃₇ NO ₄	0.0137	1.5454	↓	Liver
3-Hydroxycapric acid	9.23	171.1373	C ₁₀ H ₂₀ O ₃	0.0101	1.5413	↑	Liver
Leukotriene C4	9.71	624.2988	C ₃₀ H ₄₇ N ₃ O ₉ S	0.0162	1.5391	↓	Liver
Docosaehaenoic acid	12.69	329.2467	C ₂₂ H ₃₂ O ₂	0.0134	1.5369	↓	Liver
S-Adenosylhomocysteine	5.95	193.0678	C ₁₄ H ₂₀ N ₆ O ₅ S	0.0161	1.5324	↑	Liver
3-Hydroxyoctadecanoic Acid	13.00	299.2585	C ₁₈ H ₃₆ O ₃	0.0142	1.5307	↓	Liver
LPC(20:4)	13.47	544.3378	C ₂₈ H ₅₀ NO ₇ P	0.0133	1.5293	↓	Liver
Ergothioneine	1.24	228.0802	C ₉ H ₁₅ N ₃ O ₂ S	0.0126	1.5290	↓	Liver
Octadecylamine	12.36	270.3148	C ₁₈ H ₃₉ N	0.0133	1.5172	↓	Liver

HEPES	4.29	237.0908	C ₈ H ₁₈ N ₂ O ₄ S	0.0152	1.5148	↓	Liver
Cholesterol	12.07	369.3514	C ₂₇ H ₄₆ O	0.0201	1.5085	↑	Liver
-N-(2-hydroxyethyl)octadeca-9,12,15-trienamide	12.37	322.2726	C ₂₀ H ₃₅ NO ₂	0.0215	1.4703	↓	Liver
(Z)-13-Oxo-9-octadecenoic acid	12.97	295.2279	C ₁₈ H ₃₂ O ₃	0.0228	1.4638	↓	Liver
IRB_p_329.1858_19.4	9.68	329.1827	C ₁₉ H ₂₄ N ₂ O ₃	0.0244	1.4492	↓	Liver
Glucose	0.90	179.0551	C ₆ H ₁₂ O ₆	0.0257	1.4441	↑	Liver
Kynurenine	6.10	209.0915	C ₁₀ H ₁₂ N ₂ O ₃	0.0285	1.4416	↓	Liver
(2E)-2-Propylpent-2-Enoylcarnitine	8.53	286.2000	C ₁₅ H ₂₇ NO ₄	0.0187	1.4360	↑	Liver
Pi-Methylimidazoleacetic acid	13.58	141.0653	C ₆ H ₈ N ₂ O ₂	0.0352	1.4259	↑	Liver
15-Dihydroxyeicosatrienoic acid	12.79	337.2378	C ₂₀ H ₃₄ O ₄	0.0254	1.4109	↓	Liver
4-Vinylcyclohexene	9.04	109.1013	C ₈ H ₁₂	0.0305	1.4064	↑	Liver
N-Arachidonoyl Leucine	12.77	416.3170	C ₂₆ H ₄₃ NO ₃	0.0323	1.4026	↓	Liver
Glucuronic acid	0.86	193.0340	C ₆ H ₁₀ O ₇	0.0285	1.3941	↑	Liver
Epigallocatechin	8.00	307.0826	C ₁₅ H ₁₄ O ₇	0.0359	1.3912	↓	Liver
Heliotrine N-oxide	7.33	330.1907	C ₁₆ H ₂₇ NO ₆	0.0444	1.3845	↑	Liver
Alanylglutamic acid	1.96	217.0821	C ₈ H ₁₄ N ₂ O ₅	0.0402	1.3793	↑	Liver
8,12-Octadecadienoic acid	11.77	281.2469	C ₁₈ H ₃₂ O ₂	0.0397	1.3507	↓	Liver

5-octenoylglycine	9.18	198.1126	C ₁₀ H ₁₇ NO ₃	0.0429	1.3501	↓	Liver
GABA	1.31	104.0709	C ₄ H ₉ NO ₂	0.0480	1.3455	↓	Liver
Indole-3-acrylic acid	9.38	186.0547	C ₁₁ H ₉ NO ₂	0.0399	1.3437	↑	Liver
LPC(16:0)	10.21	496.3390	C ₂₄ H ₅₀ NO ₇ P	0.0379	1.3422	↑	Liver
Vaccenic acid	13.31	281.2480	C ₁₈ H ₃₄ O ₂	0.0434	1.3248	↓	Liver
ent-1(10)-Halimene-15,19-dioic acid	12.79	335.2219	C ₂₀ H ₃₂ O ₄	0.0420	1.3245	↓	Liver
FMN	6.39	439.0995	C ₁₇ H ₂₁ N ₄ O ₉ P	0.0433	1.2976	↑	Liver
Loliolide	9.33	197.1166	C ₁₁ H ₁₆ O ₃	0.0414	1.2849	↑	Liver
3-Hydroxysebacate	7.75	217.1072	C ₁₀ H ₁₈ O ₅	0.0477	1.2609	↑	Liver
Betaine	13.43	140.0677	C ₅ H ₁₁ NO ₂	0.0472	1.2529	↓	Liver
Gentisic acid	7.13	153.0178	C ₇ H ₆ O ₄	0.0000	1.7449	↑	Urine
Bis-(acetyl)diaminopentane	6.47	187.1437	C ₉ H ₁₈ N ₂ O ₂	0.0000	1.7403	↑	Urine
1-allyl-2-hydroxy-7,8,9,10-tetrahydroazepino(2,1-b)quinazolin-12(6H)-one	7.45	271.1463	C ₁₆ H ₁₈ N ₂ O ₂	0.0000	1.7249	↓	Urine
3-Hydroxymonoethylglycinexylidide	6.29	223.1434	C ₁₂ H ₁₈ N ₂ O ₂	0.0000	1.7236	↓	Urine
(R)-Boschniakine	7.56	162.0909	C ₁₀ H ₁₁ NO	0.0001	1.7206	↓	Urine
Asarone	9.46	209.1164	C ₁₂ H ₁₆ O ₃	0.0001	1.7193	↓	Urine

Benzoic acid, 2,4-dihydroxy-6-propyl-	8.55	195.0653	C ₁₀ H ₁₂ O ₄	0.0000	1.7143	↑	Urine
2-trans,4-cis-Decadienoylcarnitine	9.16	312.2157	C ₁₇ H ₂₉ NO ₄	0.0001	1.7096	↓	Urine
N-Acetyl-L-arginine	2.30	217.1291	C ₈ H ₁₆ N ₄ O ₃	0.0001	1.6997	↓	Urine
3-Hydroxybenzyl alcohol	6.55	123.0435	C ₇ H ₈ O ₂	0.0001	1.6838	↑	Urine
10,12-dihydroxy-9-methyl-4,13-dimethylene-6-oxatricyclo(7.4.0.0<3,7>)tridecan- 5-one	8.80	247.1326	C ₁₅ H ₂₀ O ₄	0.0001	1.6829	↑	Urine
Trinexapac	9.01	223.0601	C ₁₁ H ₁₂ O ₅	0.0002	1.6828	↓	Urine
P-Menthatriene	6.94	135.1166	C ₁₀ H ₁₄	0.0001	1.6601	↑	Urine
N-Acetyl-3-methylhistidine	1.85	212.1022	C ₉ H ₁₃ N ₃ O ₃	0.0002	1.6524	↓	Urine
N-(2,4-dimethylphenyl)-N'-methylmethanimidamide	6.31	163.1224	C ₁₀ H ₁₄ N ₂	0.0002	1.6507	↑	Urine
Exemestane	6.96	319.1642	C ₂₀ H ₂₄ O ₂	0.0004	1.6484	↓	Urine
Aleuretic Acid	8.98	303.2171	C ₁₆ H ₃₂ O ₅	0.0005	1.6467	↓	Urine
N-(2-indol-3-ylethyl)(2-methylpropoxy)carboxamide	2.52	283.1392	C ₁₅ H ₂₀ N ₂ O ₂	0.0004	1.6439	↓	Urine
Atropaldehyde	9.00	133.0646	C ₉ H ₈ O	0.0002	1.6415	↑	Urine
Dropropizine	6.60	237.1593	C ₁₃ H ₂₀ N ₂ O ₂	0.0006	1.6337	↓	Urine

Aspartyl-proline	1.47	231.0969	C ₉ H ₁₄ N ₂ O ₅	0.0003	1.6285	↓	Urine
Acetaminophen	6.88	152.0701	C ₈ H ₉ NO ₂	0.0008	1.6280	↓	Urine
Tetrahydroharman-3-carboxylic acid	7.22	231.1119	C ₁₃ H ₁₄ N ₂ O ₂	0.0003	1.6279	↑	Urine
p-Coumaric acid	6.98	163.0385	C ₉ H ₈ O ₃	0.0003	1.6242	↑	Urine
1H-Indene-1,2(3H)-dione	7.34	147.0435	C ₉ H ₆ O ₂	0.0003	1.6231	↑	Urine
2,3-Dihydro-6-methyl-1H-pyrrolizine-5-carboxaldehyde	8.40	150.0910	C ₉ H ₁₁ NO	0.0008	1.6225	↓	Urine
GABA	1.62	102.0544	C ₄ H ₉ NO ₂	0.0004	1.6150	↑	Urine
Aspartylleucine	6.42	247.1280	C ₁₀ H ₁₈ N ₂ O ₅	0.0007	1.6126	↓	Urine
Corymbosin	8.99	357.1006	C ₁₉ H ₁₈ O ₇	0.0008	1.6064	↓	Urine
3-Methoxyphenylacetic acid	8.94	167.0699	C ₉ H ₁₀ O ₃	0.0012	1.6060	↓	Urine
OPFC-perfluoroalkyl_sulfate	7.13	224.9856	C ₄ H ₆ F ₄ O ₄ S	0.0007	1.6054	↑	Urine
4-Acetylanisole	8.77	151.0750	C ₉ H ₁₀ O ₂	0.0005	1.6041	↓	Urine
(S)-11,12,13-Trinor-7-calamenone	6.96	175.1113	C ₁₂ H ₁₄ O	0.0005	1.6004	↑	Urine
Lysine	1.76	129.1021	C ₆ H ₁₄ N ₂ O ₂	0.0008	1.5980	↓	Urine
11-Dehydro-2,3-dinor-txb2	9.05	339.1804	C ₁₈ H ₂₈ O ₆	0.0010	1.5966	↓	Urine

Benzoic acid, 2-hydroxy-4-methoxy-3,6-dimethyl-	7.49	195.0652	C ₁₀ H ₁₂ O ₄	0.0006	1.5947	↑	Urine
Dehydro-piliformic-acid	8.95	213.1112	C ₁₁ H ₁₆ O ₄	0.0015	1.5893	↓	Urine
4-Ethylphenylsulfate	8.59	201.0213	C ₈ H ₁₀ O ₄ S	0.0017	1.5882	↓	Urine
Pterodin B	8.95	219.1373	C ₁₄ H ₁₈ O ₂	0.0012	1.5837	↓	Urine
beta-Resorcylic acid	7.67	153.0178	C ₇ H ₆ O ₄	0.0009	1.5776	↑	Urine
3,5-Dihydroxyphenylvaleric acid sulfate	6.79	289.0383	C ₁₁ H ₁₄ O ₇ S	0.0010	1.5718	↑	Urine
6-Methoxy-9H-carbazole-3-carboxaldehyde	8.54	226.0885	C ₁₄ H ₁₁ NO ₂	0.0019	1.5680	↓	Urine
Hydroxyethyl glycine	0.85	118.0495	C ₄ H ₉ NO ₃	0.0010	1.5671	↓	Urine
Tricarballic acid	2.76	175.0236	C ₆ H ₈ O ₆	0.0014	1.5666	↑	Urine
Alkhanol	10.36	265.1444	C ₁₅ H ₂₂ O ₄	0.0014	1.5652	↑	Urine
Isoalantolactone	6.97	215.1424	C ₁₅ H ₂₀ O ₂	0.0008	1.5639	↑	Urine
2,3-Dimethyl-5-propylpyrazine	6.46	151.1226	C ₉ H ₁₄ N ₂	0.0016	1.5598	↓	Urine
2,3-Dihydrobenzofuran	8.44	121.0647	C ₈ H ₈ O	0.0010	1.5547	↓	Urine
4-methoxy-3-((4-methoxyphenoxy)methyl)benzaldehyde	8.28	137.0596	C ₁₆ H ₁₆ O ₄	0.0011	1.5534	↑	Urine
N-Acetylserine	2.83	148.0600	C ₅ H ₉ NO ₄	0.0013	1.5488	↓	Urine

3-(2-Furanyl)-2-propenal	8.55	121.0279	C ₇ H ₆ O ₂	0.0014	1.5407	↑	Urine
Flavone base + 3O, O-HexA-HexA	6.99	623.1238	C ₂₇ H ₂₆ O ₁₇	0.0025	1.5397	↓	Urine
3,5-dimethyl-7-oxo-6-oxabicyclo(3.2.1)octane-2-carboxylic acid	9.34	221.0800	C ₁₀ H ₁₄ O ₄	0.0020	1.5355	↓	Urine
Parthenolide	9.12	249.1474	C ₁₅ H ₂₀ O ₃	0.0015	1.5349	↑	Urine
Gulonolactone	1.45	177.0392	C ₆ H ₁₀ O ₆	0.0014	1.5346	↑	Urine
2-Butyl-4-methylphenol	9.63	163.1114	C ₁₁ H ₁₆ O	0.0031	1.5318	↓	Urine
Kainic acid	7.13	236.0908	C ₁₀ H ₁₅ NO ₄	0.0027	1.5277	↓	Urine
Estetrol	10.10	303.1594	C ₁₈ H ₂₄ O ₄	0.0027	1.5220	↓	Urine
3,5-Dihydroxycinnamic acid sulfate	6.60	258.9908	C ₉ H ₈ O ₇ S	0.0031	1.5163	↓	Urine
Succinylcarnitine	1.76	262.1276	C ₁₁ H ₁₉ NO ₆	0.0019	1.5159	↓	Urine
Acetamide, N-(3-amino-4-methoxyphenyl)-	6.15	181.0966	C ₉ H ₁₂ N ₂ O ₂	0.0040	1.5136	↓	Urine
3,4-Methylenepimelic acid	7.90	183.0653	C ₉ H ₁₂ O ₄	0.0031	1.5105	↓	Urine
Mannitol	0.89	227.0762	C ₆ H ₁₄ O ₆	0.0019	1.5104	↓	Urine
3,5,6-Trichloro-2-pyridinol	10.59	195.9117	C ₅ H ₂ Cl ₃ NO	0.0025	1.5053	↑	Urine
Genipin	8.88	209.0798	C ₁₁ H ₁₄ O ₅	0.0041	1.5026	↓	Urine
Artemisinin	8.80	265.1428	C ₁₅ H ₂₂ O ₅	0.0020	1.4999	↑	Urine

Cinchonine	6.01	317.1594	C ₁₉ H ₂₂ N ₂ O	0.0024	1.4991	↓	Urine
Encecalin	8.69	233.1166	C ₁₄ H ₁₆ O ₃	0.0043	1.4941	↓	Urine
Pilocarpine	6.51	209.1279	C ₁₁ H ₁₆ N ₂ O ₂	0.0054	1.4930	↓	Urine
11,12,13-Trinor-1,3,5-bisabolatrien-10-oic acid	9.20	193.1216	C ₁₂ H ₁₆ O ₂	0.0055	1.4880	↓	Urine
4',6-Dihydroxyflavone	8.36	255.0646	C ₁₅ H ₁₀ O ₄	0.0033	1.4861	↓	Urine
(2E,4E)-N-(2-(4-hydroxyphenyl)ethyl)dodeca- 2,4-dienamide	7.97	338.2069	C ₂₀ H ₂₉ NO ₂	0.0055	1.4844	↑	Urine
Resacetophenone	10.16	153.0544	C ₈ H ₈ O ₃	0.0036	1.4760	↑	Urine
Theasaponin F1	8.77	365.0687	C ₂₀ H ₁₄ O ₇	0.0063	1.4746	↓	Urine
Estriol	6.43	311.1588	C ₁₈ H ₂₄ O ₃	0.0042	1.4711	↓	Urine
5-Hydroxy-7-methoxy-2-methyl-8-(3-methyl- but-2-enyl)-chromen-4-on	10.13	275.1266	C ₁₆ H ₁₈ O ₄	0.0061	1.4697	↓	Urine
4-Amino-2-methylenebutanoic acid	2.27	116.0706	C ₅ H ₉ NO ₂	0.0057	1.4683	↑	Urine
2-Carboxy-4-dodecanolide	10.27	241.1439	C ₁₃ H ₂₂ O ₄	0.0057	1.4660	↓	Urine
1-Naphthalenecarboxylic acid, 5-((3E)-4-carboxy- 3-methyl-3-buten-1-yl)decahydro-3-hydroxy- 1,4a-dimethyl-6-methylene-	9.08	395.2074	C ₂₀ H ₃₀ O ₅	0.0073	1.4645	↓	Urine

Serine betaine	1.35	148.0963	C ₆ H ₁₄ NO ₃	0.0046	1.4603	↓	Urine
3-Oxodecanoic acid	8.79	185.1168	C ₁₀ H ₁₈ O ₃	0.0043	1.4603	↑	Urine
1-Pyrrolidinecarboxaldehyde	6.26	100.0759	C ₅ H ₉ NO	0.0079	1.4467	↑	Urine
Toddalolactone	10.05	331.1136	C ₁₆ H ₂₀ O ₆	0.0080	1.4454	↓	Urine
1,2:3,4-Di-O-isopropylidene-D-galactopyranose	7.59	283.1142	C ₁₂ H ₂₀ O ₆	0.0056	1.4443	↑	Urine
Homostachydrine	1.43	158.1171	C ₈ H ₁₅ NO ₂	0.0054	1.4441	↓	Urine
beta-Methylstyrene	7.87	119.0856	C ₉ H ₁₀	0.0077	1.4397	↑	Urine
4-(sulfooxy)-Benzonitrile	7.09	197.9852	C ₇ H ₅ NO ₄ S	0.0046	1.4332	↑	Urine
1-Pentyl-3-(1-naphthoyl) indole	7.06	342.1838	C ₂₄ H ₂₃ NO	0.0060	1.4307	↓	Urine
SDMA	1.65	203.1498	C ₈ H ₁₈ N ₄ O ₂	0.0069	1.4289	↓	Urine
Terrecyclic Acid	10.06	249.1473	C ₁₅ H ₂₀ O ₃	0.0067	1.4280	↑	Urine
4-O-Methylvanillin	7.91	167.0699	C ₉ H ₁₀ O ₃	0.0083	1.4263	↓	Urine
N-(2-octyloxyethyl)(3,4,5-trimethoxyphenyl)carboxamide	7.90	390.2272	C ₂₀ H ₃₃ NO ₅	0.0055	1.4261	↑	Urine
2-Ethyl-5-carboxypentyl phthalate	10.05	307.1179	C ₁₆ H ₂₀ O ₆	0.0095	1.4211	↓	Urine
6H-2-Benzopyran-6-one, 1,7,8,8a-tetrahydro-7,8-dihydroxy-3,5,7-trimethyl-, (7S,8S,8aS)-	8.62	225.1119	C ₁₂ H ₁₆ O ₄	0.0094	1.4145	↓	Urine

Dinitramine	1.65	321.0821	C ₁₁ H ₁₃ F ₃ N ₄ O ₄	0.0100	1.4083	↓	Urine
2-Hydroxyacetophenone sulfate	7.02	215.0013	C ₈ H ₈ O ₅ S	0.0110	1.4076	↓	Urine
2-(3-carboxypropanoylamino)-3-indol-3-ylpropanoic acid	8.32	305.1098	C ₁₅ H ₁₆ N ₂ O ₅	0.0124	1.4015	↓	Urine
3,4,5-trimethoxyphenyl 3,4,5-trimethylpyrazolyl ketone	8.56	327.1299	C ₁₆ H ₂₀ N ₂ O ₄	0.0102	1.3987	↑	Urine
Naringenin-7-O-Glucuronide	8.50	447.0927	C ₂₁ H ₂₀ O ₁₁	0.0074	1.3985	↑	Urine
(E)-7-(4-methoxy-5-methyl-6-oxopyran-2-yl)-5-methyloct-6-enoic acid	9.61	277.1429	C ₁₆ H ₂₂ O ₅	0.0084	1.3969	↓	Urine
Valine betaine	2.61	160.1326	C ₈ H ₁₇ NO ₂	0.0105	1.3959	↓	Urine
Aspergillimide	8.19	360.2274	C ₂₀ H ₂₉ N ₃ O ₃	0.0089	1.3927	↓	Urine
N-Nonanoylglycine	9.76	214.1437	C ₁₁ H ₂₁ NO ₃	0.0115	1.3885	↑	Urine
Monomethyl sebacate	9.82	199.1323	C ₁₁ H ₂₀ O ₄	0.0127	1.3876	↑	Urine
Uridine	3.16	243.0616	C ₉ H ₁₂ N ₂ O ₆	0.0085	1.3851	↓	Urine
1-Pyrrolidineethanol	1.66	116.1071	C ₆ H ₁₃ NO	0.0125	1.3832	↓	Urine
2,3-dihydro-1H-carbazol-4(9H)-one	8.88	186.0908	C ₁₂ H ₁₁ NO	0.0115	1.3824	↓	Urine

(1S,2R,4aR,8aR)-1-Acetoxy-7-isopropylidene-1,4a-dimethyl-6-oxodecahydro-2-naphthalenyl 2,3-dimethyl-2-oxiranecarboxylate	11.37	415.2091	C ₂₂ H ₃₂ O ₆	0.0089	1.3815	↑	Urine
N-(1-Adamantylmethyl)-3,4,5-Trimethoxybenzamide	9.18	360.2160	C ₂₁ H ₂₉ NO ₄	0.0086	1.3812	↓	Urine
Hexadeca-7,10,13-trienoic acid	8.97	251.1992	C ₁₆ H ₂₆ O ₂	0.0134	1.3811	↓	Urine
N-Decanoylglycine	10.19	228.1596	C ₁₂ H ₂₃ NO ₃	0.0108	1.3805	↑	Urine
1H-Pyrrole-2-carboxaldehyde	4.54	96.0448	C ₅ H ₅ NO	0.0102	1.3799	↑	Urine
1-methyl-4-(6-methylhept-5-en-2-yl)-2,3-dioxabicyclo(2.2.2)oct-5-ene	6.89	201.1632	C ₁₅ H ₂₄ O ₂	0.0084	1.3775	↑	Urine
3-Toluic acid	7.02	135.0435	C ₈ H ₈ O ₂	0.0144	1.3748	↓	Urine
1-methyl-4-methylidene-7-(propan-2-yl)-1,2,3,3a,4,5,6,8a-octahydroazulen-1-ol	8.50	203.1793	C ₁₅ H ₂₄ O	0.0096	1.3739	↑	Urine
Bavachin	9.77	347.1278	C ₂₀ H ₂₀ O ₄	0.0163	1.3712	↓	Urine
2-Ethyl-1,2,3,4-tetrahydro-isoquinoline-3-carboxylic acid	10.47	206.1168	C ₁₂ H ₁₅ NO ₂	0.0138	1.3684	↓	Urine
Mono(2-ethyl-5-hydroxyhexyl) phthalate	10.28	293.1385	C ₁₆ H ₂₂ O ₅	0.0136	1.3671	↓	Urine

Tetrahydropyridine	1.92	84.0813	C ₅ H ₉ N	0.0117	1.3638	↑	Urine
2-(3-carboxypropanoylamino)hexanoic acid	7.73	230.1026	C ₁₀ H ₁₇ NO ₅	0.0100	1.3619	↓	Urine
Glutamine	0.84	145.0602	C ₅ H ₁₀ N ₂ O ₃	0.0095	1.3599	↓	Urine
Chavicol	8.53	135.0801	C ₉ H ₁₀ O	0.0107	1.3481	↑	Urine
3,5-Diisopropylsalicylic acid	9.60	223.1323	C ₁₃ H ₁₈ O ₃	0.0188	1.3480	↓	Urine
Biotin	7.40	245.0949	C ₁₀ H ₁₆ N ₂ O ₃ S	0.0128	1.3451	↓	Urine
4-Amidinophenyl benzoate	6.88	241.0995	C ₁₄ H ₁₂ N ₂ O ₂	0.0153	1.3441	↓	Urine
(S)-Oleuropeic acid	10.35	183.1011	C ₁₀ H ₁₆ O ₃	0.0159	1.3418	↑	Urine
2,8-Quinolinediol 2-sulfate	6.37	242.0109	C ₉ H ₇ NO ₅ S	0.0206	1.3411	↓	Urine
4-Hydroxyhippuric acid	6.41	194.0448	C ₉ H ₉ NO ₄	0.0154	1.3390	↑	Urine
Tsibulin 2	10.03	181.1222	C ₁₁ H ₁₈ O ₂	0.0141	1.3356	↓	Urine
9-Decenoylcarnitine	9.52	314.2319	C ₁₇ H ₃₁ NO ₄	0.0123	1.3355	↓	Urine
Fenuron	7.80	182.1285	C ₉ H ₁₂ N ₂ O	0.0174	1.3350	↓	Urine
2,2-Dimethylglutaric acid	7.83	159.0650	C ₇ H ₁₂ O ₄	0.0096	1.3330	↑	Urine
1,2,3,4-Tetrahydroquinoline	8.80	134.0961	C ₉ H ₁₁ N	0.0165	1.3326	↓	Urine
Indole-3-carboxylic acid	7.81	144.0442	C ₉ H ₇ NO ₂	0.0209	1.3260	↓	Urine
Acoric acid	9.07	251.1634	C ₁₅ H ₂₄ O ₄	0.0203	1.3257	↑	Urine

2-methoxy-6-methyl-5-(phenylmethoxy)-2H-3,4,5,6-tetrahydropyran-3,4-diol	10.05	291.1186	C ₁₄ H ₂₀ O ₅	0.0166	1.3250	↓	Urine
Chelidonine	9.87	354.1326	C ₂₀ H ₁₉ NO ₅	0.0122	1.3245	↓	Urine
(R)-2-Nitro-p-mentha-1,5-diene	6.75	182.1168	C ₁₀ H ₁₅ NO ₂	0.0196	1.3240	↓	Urine
4,5-Dimethyl-3-hydroxy-2,5-dihydrofuran-2-one sulfate	6.05	206.9960	C ₆ H ₈ O ₆ S	0.0195	1.3233	↓	Urine
Carboxyethyl-hydroxychroman	9.79	221.0811	C ₁₂ H ₁₄ O ₄	0.0212	1.3230	↓	Urine
Chenodeoxycholic acid sulfate	10.57	471.2425	C ₂₄ H ₄₀ O ₇ S	0.0156	1.3149	↓	Urine
(2E,4E,7E)-Nona-2,4,7-trienedioylcarnitine	8.08	326.1585	C ₁₆ H ₂₃ NO ₆	0.0157	1.3130	↓	Urine
Butyl 4-aminobenzoate	9.08	194.1168	C ₁₁ H ₁₅ NO ₂	0.0217	1.3086	↓	Urine
2,3-Diaminotoluene	6.01	123.0916	C ₇ H ₁₀ N ₂	0.0210	1.3049	↓	Urine
JWH-073	6.61	328.1677	C ₂₃ H ₂₁ NO	0.0156	1.3015	↓	Urine
Pirimicarb-desamido	7.00	168.1127	C ₈ H ₁₃ N ₃ O	0.0226	1.2999	↓	Urine
Secobarbital	8.79	237.1238	C ₁₂ H ₁₈ N ₂ O ₃	0.0223	1.2938	↓	Urine
Maltoxazine	9.49	180.1010	C ₁₀ H ₁₃ NO ₂	0.0298	1.2902	↓	Urine
Costunolide	8.62	233.1529	C ₁₅ H ₂₀ O ₂	0.0269	1.2857	↓	Urine
7-Hydroxypestalotin	9.43	253.1036	C ₁₁ H ₁₈ O ₅	0.0233	1.2832	↑	Urine

2-Acetyl-1,2,3,4-tetrahydroisoquinoline	8.80	176.1068	C ₁₁ H ₁₃ NO	0.0229	1.2807	↓	Urine
3-(1,2-dihydroxypropyl)-1,6,8-trihydroxyanthracene-9,10-dione	8.59	329.0694	C ₁₇ H ₁₄ O ₇	0.0254	1.2806	↓	Urine
Methyl neopentyl phthalic acid	9.81	249.1122	C ₁₄ H ₁₈ O ₄	0.0280	1.2795	↓	Urine
Pantothenic acid	6.25	220.1175	C ₉ H ₁₇ NO ₅	0.0334	1.2764	↓	Urine
Topiramate	6.03	338.0913	C ₁₂ H ₂₁ NO ₈ S	0.0212	1.2740	↓	Urine
Menthol-glucoronide	9.70	315.1812	C ₁₆ H ₂₈ O ₆	0.0250	1.2737	↓	Urine
Carnosine	1.23	227.1149	C ₉ H ₁₄ N ₄ O ₃	0.0211	1.2710	↓	Urine
2-((N,N-diethylglycyl)amino)-3-methylbenzoic acid	8.08	265.1541	C ₁₄ H ₂₀ N ₂ O ₃	0.0262	1.2676	↓	Urine
2,6-Dimethylpyrazine	1.26	109.0760	C ₆ H ₈ N ₂	0.0244	1.2658	↓	Urine
2,3,5-Trimethylphenol	8.17	137.0958	C ₉ H ₁₂ O	0.0292	1.2606	↑	Urine
Sinapine	7.17	310.1644	C ₁₆ H ₂₄ NO ₅	0.0269	1.2580	↑	Urine
(8aR,12S,12aR)-12-hydroxy-4-methyl-4,5,6,7,8,8a,12,12a-octahydro-1H-3-benzoxecine-2,9-dione	10.55	253.1429	C ₁₄ H ₂₀ O ₄	0.0322	1.2564	↓	Urine
3-Hydroxy-4,5-dimethyl-2(5H)-furanone	6.33	129.0544	C ₆ H ₈ O ₃	0.0291	1.2548	↓	Urine

Liquiritigenin	9.40	255.0659	C ₁₅ H ₁₂ O ₄	0.0277	1.2548	↑	Urine
Dibutylphthalic acid	10.45	277.1436	C ₁₆ H ₂₂ O ₄	0.0285	1.2533	↓	Urine
1,2-Cyclohexanedicarboxylic acid, 4-methyl-	8.22	185.0810	C ₉ H ₁₄ O ₄	0.0299	1.2527	↓	Urine
Pi-Methylimidazoleacetic acid	1.75	141.0656	C ₆ H ₈ N ₂ O ₂	0.0341	1.2519	↓	Urine
(S)-Actinidine	7.53	148.1118	C ₁₀ H ₁₃ N	0.0299	1.2493	↓	Urine
alpha-Methyltryptamine	7.53	175.1224	C ₁₁ H ₁₄ N ₂	0.0301	1.2467	↓	Urine
3,4,5-Trimethylbenzaldehyde	7.70	149.0958	C ₁₀ H ₁₂ O	0.0309	1.2397	↓	Urine
Phenylethylmalonamide	6.32	207.1126	C ₁₁ H ₁₄ N ₂ O ₂	0.0331	1.2388	↓	Urine
Genkwanin	11.08	283.0609	C ₁₆ H ₁₂ O ₅	0.0318	1.2356	↑	Urine
2-[(4-(tert-butyl)phenyl)carbonylamino]acetic acid	6.13	258.1081	C ₁₃ H ₁₇ NO ₃	0.0285	1.2339	↑	Urine
p-tert-Butyl catechol	9.48	167.1063	C ₁₀ H ₁₄ O ₂	0.0411	1.2325	↑	Urine
7-Hydroxy-6-methoxydihydroflavonol	9.51	285.0759	C ₁₆ H ₁₄ O ₅	0.0320	1.2303	↑	Urine
N-Acetylasparagine	7.27	88.0397	C ₆ H ₁₀ N ₂ O ₄	0.0434	1.2282	↑	Urine
1-(Aminocarbonyl)-L-proline	3.23	159.0761	C ₆ H ₁₀ N ₂ O ₃	0.0329	1.2266	↓	Urine
Thunberginol A	8.91	271.0595	C ₁₅ H ₁₀ O ₅	0.0362	1.2265	↓	Urine
Ligustilide	8.20	191.1062	C ₁₂ H ₁₄ O ₂	0.0324	1.2232	↓	Urine

6-Keto-decanoylcarnitine	7.81	330.2270	C ₁₇ H ₃₁ NO ₅	0.0381	1.2197	↓	Urine
1,2,5,6-Tetrahydro-4H-pyrrolo(3,2,1-ij)quinolin-4-one	6.51	174.0906	C ₁₁ H ₁₁ NO	0.0426	1.2179	↓	Urine
alpha-(4-Fluorophenyl)-4-(5-fluoro-2-pyrimidinyl)-1-piperazine butanol	7.44	347.1702	C ₁₈ H ₂₂ F ₂ N ₄ O	0.0339	1.2176	↑	Urine
1,2,3,4-Tetrahydro-beta-carboline-3-carboxylic acid	7.05	217.0965	C ₁₂ H ₁₂ N ₂ O ₂	0.0276	1.2149	↑	Urine
(4E,7E)-3-Hydroxydeca-4,7-dienoylcarnitine	7.56	328.2114	C ₁₇ H ₂₉ NO ₅	0.0304	1.2144	↓	Urine
3-Ethylphenol	8.60	121.0642	C ₈ H ₁₀ O	0.0479	1.2105	↓	Urine
Isoliquiritigenin	9.40	257.0797	C ₁₅ H ₁₂ O ₄	0.0376	1.2085	↑	Urine
Schinifoline	6.36	280.1647	C ₁₇ H ₂₃ NO	0.0364	1.2040	↓	Urine
2-(6-Hydroxy-3,8-dimethyl-2-oxo-1,2,4,5,6,7,8,8a-octahydro-5-azulenyl)acrylic acid	8.96	247.1318	C ₁₅ H ₂₀ O ₄	0.0420	1.2021	↓	Urine
Isoimperatorin	10.48	269.0819	C ₁₆ H ₁₄ O ₄	0.0383	1.2011	↑	Urine
Dehydro-P-Cymene	7.99	133.1010	C ₁₀ H ₁₂	0.0462	1.1982	↑	Urine
Deoxycarnitine	1.40	146.1170	C ₇ H ₁₅ NO ₂	0.0377	1.1908	↓	Urine
5-(3',5')-Dihydroxyphenyl-gamma-valerolactone	8.06	209.0808	C ₁₁ H ₁₄ O ₄	0.0354	1.1870	↑	Urine

Cholic acid 7-sulfate	9.49	487.2375	C ₂₄ H ₄₀ O ₈ S	0.0324	1.1825	↓	Urine
Eremofortin A	9.96	305.1393	C ₁₇ H ₂₂ O ₅	0.0385	1.1807	↑	Urine
Ononetin	10.17	257.0811	C ₁₅ H ₁₄ O ₄	0.0382	1.1805	↑	Urine
2-(4-methoxyphenyl)propan-2-ol	7.70	167.1063	C ₁₀ H ₁₄ O ₂	0.0418	1.1803	↓	Urine
Intermedine N-oxide	8.01	316.1745	C ₁₅ H ₂₅ NO ₆	0.0356	1.1749	↑	Urine
Acetaminophen glucuronide	6.76	328.1015	C ₁₄ H ₁₇ NO ₈	0.0387	1.1727	↓	Urine
Abscisic acid	9.41	247.1326	C ₁₅ H ₂₀ O ₄	0.0359	1.1712	↑	Urine
Acetylglycine	1.61	116.0337	C ₄ H ₇ NO ₃	0.0372	1.1712	↓	Urine
Isocitric acid	0.97	191.0183	C ₆ H ₈ O ₈	0.0450	1.1680	↑	Urine
N-Propionylglycine	2.47	130.0495	C ₅ H ₉ NO ₃	0.0402	1.1679	↑	Urine
Carboxyibuprofen	8.18	219.1013	C ₁₃ H ₁₆ O ₄	0.0364	1.1663	↑	Urine
Melamine	1.64	127.0725	C ₃ H ₆ N ₆	0.0361	1.1637	↑	Urine
Amide	5.99	160.1076	C ₆ H ₁₃ N ₃ O ₂	0.0433	1.1636	↑	Urine
3,4-Diaminopyridine	1.73	110.0714	C ₅ H ₇ N ₃	0.0411	1.1616	↓	Urine
Phytosphingosine	10.90	318.2992	C ₁₈ H ₃₉ NO ₃	0.0463	1.1508	↑	Urine
N-Acetylalanine	2.78	130.0492	C ₅ H ₉ NO ₃	0.0450	1.1431	↑	Urine
Arabinosylhypoxanthine	6.00	267.0733	C ₁₀ H ₁₂ N ₄ O ₅	0.0441	1.1387	↑	Urine

Alkhanin	9.22	263.1281	C ₁₅ H ₂₀ O ₄	0.0426	1.1339	↑	Urine
5-Methoxyindoleacetic acid	7.25	206.0803	C ₁₁ H ₁₁ NO ₃	0.0439	1.1262	↑	Urine
(24E)-3-Oxolanosta-8,24-diene-21,26-dioic acid	11.15	467.3142	C ₃₀ H ₄₄ O ₅	0.0000	1.8875	↑	Fecal
Deoxycholylisoleucine	11.87	504.3698	C ₃₀ H ₅₁ NO ₅	0.0000	1.8739	↓	Fecal
4-(4-(2,3-dihydrobenzo(b)(1,4)dioxin-6-yl)-3-methyl-1H-pyrazol-5-yl)-6-propylbenzene-1,3-diol	6.91	367.1686	C ₂₁ H ₂₂ N ₂ O ₄	0.0001	1.8609	↑	Fecal
Atractylenolide III	11.27	249.1481	C ₁₅ H ₂₀ O ₃	0.0000	1.8524	↑	Fecal
Pregnanetriol 3a-O-b-D-glucuronide	8.63	511.2912	C ₂₇ H ₄₄ O ₉	0.0001	1.8411	↓	Fecal
3,6,9,12,15,18,21,24,27-Nonaoxanonacosane-1,29-diol	7.49	481.2600	C ₂₀ H ₄₂ O ₁₁	0.0001	1.8315	↑	Fecal
1-methyl-4-(6-methylhept-5-en-2-yl)-2,3-dioxabicyclo(2.2.2)oct-5-ene	7.32	201.1637	C ₁₅ H ₂₄ O ₂	0.0000	1.8313	↑	Fecal
2-(6,8-dimethyl-4-oxochromen-2-yl)benzoic acid	8.77	295.0960	C ₁₈ H ₁₄ O ₄	0.0000	1.8251	↓	Fecal
3,6,9,12,15,18,21,24,27,30-Decaoxadotriacontane-1,32-diol	7.65	503.3050	C ₂₂ H ₄₆ O ₁₂	0.0001	1.8237	↑	Fecal
Cholic acid	10.96	409.2932	C ₂₄ H ₄₀ O ₅	0.0000	1.8222	↓	Fecal

2-Aminobicyclo(3.1.0)hexane-2,6-dicarboxylic acid	1.75	186.0756	C ₈ H ₁₁ NO ₄	0.0003	1.8113	↑	Fecal
Hydroquinidine	9.44	327.2053	C ₂₀ H ₂₆ N ₂ O ₂	0.0001	1.8081	↑	Fecal
3-(dimethyl(3-((4R)-4-((3R,7R,12S,17R)-3,7,12-trihydroxy-10,13-dimethylhexadecahydro-1H-cyclopenta(a)phenanthren-17-yl)pentanamido)propyl)ammonio)-2-hydroxypropane-1-sulfonate	12.40	653.3846	C ₃₂ H ₅₈ N ₂ O ₈ S	0.0000	1.8045	↑	Fecal
Ganolucidic acid E	12.00	483.3111	C ₃₀ H ₄₄ O ₅	0.0001	1.7846	↑	Fecal
3-Hydroxylidocaine	6.57	251.1746	C ₁₄ H ₂₂ N ₂ O ₂	0.0003	1.7815	↑	Fecal
6-((2E,4E)-4,6-Dimethyl-2,4-octadienoyl)-2,3-dihydroxy-2-methylcyclohexanone	7.75	317.1737	C ₁₇ H ₂₆ O ₄	0.0005	1.7769	↑	Fecal
allo-Protolichesterinic acid	11.99	323.2221	C ₁₉ H ₃₂ O ₄	0.0002	1.7759	↓	Fecal
10,11-dihydro-20-dihydroxy-LTB ₄	8.34	369.2271	C ₂₀ H ₃₄ O ₆	0.0004	1.7757	↓	Fecal
Deoxycholyphenylalanine	11.92	540.3671	C ₃₃ H ₄₉ NO ₅	0.0002	1.7714	↓	Fecal
Deoxycholic acid	11.31	391.2843	C ₂₄ H ₄₀ O ₄	0.0002	1.7702	↓	Fecal
8,12-Octadecadienoic acid	10.95	281.2471	C ₁₈ H ₃₂ O ₂	0.0009	1.7690	↑	Fecal

6-Prenylpinocembrin	10.96	323.1288	C ₂₀ H ₂₀ O ₄	0.0005	1.7571	↑	Fecal
Nootkatone	10.30	201.1630	C ₁₅ H ₂₂ O	0.0006	1.7490	↑	Fecal
PC(18:1/18:2)	10.44	784.5819	C ₄₄ H ₈₂ NO ₈ P	0.0002	1.7489	↑	Fecal
Valerylcarnitine	7.51	246.1698	C ₁₂ H ₂₃ NO ₄	0.0012	1.7485	↑	Fecal
Valyllysine	1.36	246.1808	C ₁₁ H ₂₃ N ₃ O ₃	0.0004	1.7472	↑	Fecal
Amphetamine	7.24	158.0962	C ₉ H ₁₃ N	0.0008	1.7443	↑	Fecal
Androstane-3,17-diol 17-sulfate	11.05	371.1896	C ₁₉ H ₃₂ O ₅ S	0.0015	1.7415	↑	Fecal
1-O-hexadecyl-2-C-methyl-3-phosphatidylcholine	11.67	496.3781	C ₂₅ H ₅₄ NO ₆ P	0.0010	1.7335	↑	Fecal
Sebacic acid	7.57	185.1170	C ₁₀ H ₁₈ O ₄	0.0003	1.7327	↓	Fecal
P-Menthatriene	7.74	135.1165	C ₁₀ H ₁₄	0.0008	1.7318	↓	Fecal
7-Hydroxy-1,4a-dimethyl-9-oxo-7-propan-2-yl-2,3,4,4b,5,6,10,10a-octahydrophenanthrene-1-carboxylic acid	9.01	317.2100	C ₂₀ H ₃₀ O ₄	0.0005	1.7306	↓	Fecal
NA-135	7.97	369.2272	C ₂₀ H ₃₄ O ₆	0.0011	1.7250	↓	Fecal
Kynurenine	6.08	209.0916	C ₁₀ H ₁₂ N ₂ O ₃	0.0010	1.7229	↑	Fecal

2-(4a-Methyl-8-methylidene-4-(3-methylpentanoyloxy)-1,2,3,4,5,6,7,8a-octahydronaphthalen-2-yl)prop-2-enoic acid	7.49	349.2366	C ₂₁ H ₃₂ O ₄	0.0008	1.7223	↓	Fecal
Nadolol	7.50	310.2004	C ₁₇ H ₂₇ NO ₄	0.0011	1.7220	↑	Fecal
Wallemine	11.28	235.1688	C ₁₅ H ₂₄ O ₃	0.0010	1.7188	↓	Fecal
Chenodeoxycholic acid	11.80	357.2773	C ₂₄ H ₄₀ O ₄	0.0007	1.7183	↓	Fecal
Sinapaldehyde	9.99	209.0804	C ₁₁ H ₁₂ O ₄	0.0004	1.7161	↑	Fecal
Cediranib	7.40	451.2131	C ₂₅ H ₂₇ FN ₄ O ₃	0.0009	1.7143	↑	Fecal
3b,4b,7a,12a-Tetrahydroxy-5b-cholanoic acid	9.21	423.2755	C ₂₄ H ₄₀ O ₆	0.0013	1.7106	↓	Fecal
Isoimperatorin	10.48	269.0811	C ₁₆ H ₁₄ O ₄	0.0004	1.7098	↑	Fecal
5-hydroxycalamenene	8.68	219.1740	C ₁₅ H ₂₂ O	0.0006	1.6969	↑	Fecal
Tetrahydroharman-3-carboxylic acid	7.24	231.1125	C ₁₃ H ₁₄ N ₂ O ₂	0.0019	1.6952	↑	Fecal
Toxin T2 tetrol	8.49	297.1332	C ₁₅ H ₂₂ O ₆	0.0013	1.6939	↑	Fecal
(E)-3-(2,3-Dihydroxyphenyl)-2-propenoic acid	7.48	179.0338	C ₉ H ₈ O ₄	0.0023	1.6893	↑	Fecal
5-(1,2,4a-trimethyl-5-(3-methylbutanoyloxymethyl)-2,3,4,7,8,8a-	12.22	405.3000	C ₂₅ H ₄₂ O ₄	0.0008	1.6883	↓	Fecal

hexahydronaphthalen-1-yl)-3-methylpentanoic
acid

3-(2-Furanyl)-2-propenal	7.98	121.0280	C ₇ H ₆ O ₂	0.0011	1.6793	↓	Fecal
Norfloxacin	1.56	320.1451	C ₁₆ H ₁₈ FN ₃ O ₃	0.0033	1.6745	↑	Fecal
N-(1-(2-Methylbenzyl)-1H-Pyrazol-4-Yl)-3,4-Dihydroisoquinoline-2(1H)-Carbothioamide	6.96	363.1614	C ₂₁ H ₂₂ N ₄ S	0.0022	1.6710	↑	Fecal
N-(6-methoxyquinolin-8-yl)alanine	6.50	247.1066	C ₁₃ H ₁₄ N ₂ O ₃	0.0033	1.6680	↑	Fecal
Isoprostane F2alpha-I	10.27	353.2332	C ₂₀ H ₃₄ O ₅	0.0022	1.6645	↓	Fecal
PC(16:1/16:1)	11.84	730.5353	C ₄₀ H ₇₆ NO ₈ P	0.0010	1.6633	↓	Fecal
2-Carboxy-4-dodecanolide	10.25	241.1439	C ₁₃ H ₂₂ O ₄	0.0021	1.6607	↓	Fecal
5a-Cholestane-3a,7a,12a,23,25-pentol	12.29	451.3418	C ₂₇ H ₄₈ O ₅	0.0042	1.6597	↓	Fecal
12-Ketodeoxycholic acid	11.41	391.2837	C ₂₄ H ₃₈ O ₄	0.0020	1.6565	↓	Fecal
Pinocarvyl acetate	7.74	195.1377	C ₁₂ H ₁₈ O ₂	0.0026	1.6561	↓	Fecal
Fenofibric acid	11.47	319.0724	C ₁₇ H ₁₅ ClO ₄	0.0026	1.6552	↑	Fecal
Dehydrocholic acid	9.12	403.2470	C ₂₄ H ₃₄ O ₅	0.0043	1.6542	↓	Fecal
1,4-Benzodioxin-2(3H)-one	9.45	151.0384	C ₈ H ₆ O ₃	0.0036	1.6534	↓	Fecal
Zerumbone	11.30	201.1631	C ₁₅ H ₂₂ O	0.0012	1.6487	↓	Fecal

2-acetoxy-6-pentadecylbenzoic acid	11.17	413.2659	C ₂₄ H ₃₈ O ₄	0.0022	1.6447	↓	Fecal
Chenodeoxychollyleucine	11.87	506.3820	C ₃₀ H ₅₁ NO ₅	0.0018	1.6443	↓	Fecal
(Z)-7-((1R,2R,3R,5S)-2-(1,2-Dihydroxy-3-oxooctyl)-3,5-dihydroxycyclopentyl)hept-5-enoic acid	7.11	385.2225	C ₂₀ H ₃₄ O ₇	0.0025	1.6434	↓	Fecal
5-oxopentadecanoic Acid	12.24	255.1963	C ₁₅ H ₂₈ O ₃	0.0036	1.6428	↓	Fecal
8-Ethyl-7-Hydroxy-5-Methoxy-2-Methylchroman-4-One	7.90	235.1004	C ₁₃ H ₁₆ O ₄	0.0047	1.6407	↑	Fecal
Indane	11.80	119.0853	C ₉ H ₁₀	0.0025	1.6360	↓	Fecal
2'-Hydroxyacetophenone	8.10	135.0434	C ₈ H ₈ O ₂	0.0044	1.6302	↑	Fecal
Radiclonic acid	9.22	343.2621	C ₂₃ H ₄₀ O ₅	0.0036	1.6254	↓	Fecal
Curcumol	10.30	219.1741	C ₁₅ H ₂₄ O ₂	0.0037	1.6233	↑	Fecal
Cryptotanshinone	6.72	319.1357	C ₁₉ H ₂₀ O ₃	0.0036	1.6216	↑	Fecal
N-acetyltryptophan	7.26	229.0965	C ₁₃ H ₁₄ N ₂ O ₃	0.0067	1.6170	↑	Fecal
L↑-20(29)-ene-27,28-dioic acid, 3-oxo-, (5xi,9xi,18xi)-	10.87	485.3255	C ₃₀ H ₄₄ O ₅	0.0014	1.6158	↑	Fecal

6b-Hydroxy-8a-methoxy-7(11)-eremophilen-12,8-olide	9.70	279.1598	C ₁₆ H ₂₄ O ₄	0.0029	1.6154	↑	Fecal
Lauryl Ether Sulphate	12.25	309.1736	C ₁₄ H ₃₀ O ₅ S	0.0042	1.6138	↓	Fecal
1H-3,9a-Methanocyclopent(c)oxocin-4-carboxylic acid, octahydro-4-hydroxy-7-(2-hydroxy-1-methylethylidene)-, (7E)-	9.44	281.1390	C ₁₅ H ₂₂ O ₅	0.0042	1.6132	↓	Fecal
Dimethyl dimethoxy biphenyl	8.77	241.1226	C ₁₆ H ₁₈ O ₂	0.0024	1.6123	↓	Fecal
Penciclovir	2.32	254.1244	C ₁₀ H ₁₅ N ₅ O ₃	0.0060	1.6089	↑	Fecal
Asiatic acid	12.15	533.3482	C ₃₀ H ₄₈ O ₅	0.0024	1.6064	↑	Fecal
2-acetoxy-4-pentadecylbenzoic acid	11.42	413.2658	C ₂₄ H ₃₈ O ₄	0.0041	1.6057	↓	Fecal
Phenylacetic acid	6.89	135.0435	C ₈ H ₈ O ₂	0.0059	1.6007	↑	Fecal
N-Acetylalanine	2.78	130.0495	C ₅ H ₉ NO ₃	0.0065	1.5984	↑	Fecal
Isoferulic acid	9.99	177.0541	C ₁₀ H ₁₀ O ₄	0.0023	1.5971	↑	Fecal
Poricoic acid A	12.12	497.3265	C ₃₁ H ₄₆ O ₅	0.0058	1.5967	↑	Fecal
Ganolucidic acid A	12.24	499.3052	C ₃₀ H ₄₄ O ₆	0.0038	1.5952	↓	Fecal
Gibberellin A123	9.04	363.1809	C ₂₀ H ₂₈ O ₆	0.0029	1.5933	↓	Fecal
Arjugenin	11.86	503.3376	C ₃₀ H ₄₈ O ₆	0.0024	1.5913	↑	Fecal

Dihydrocorticosterone	8.62	349.2365	C ₂₁ H ₃₂ O ₄	0.0021	1.5899	↓	Fecal
Acaranoic Acid	9.34	297.2062	C ₁₇ H ₃₀ O ₄	0.0042	1.5864	↓	Fecal
Gibberellin A12 aldehyde	10.25	317.2099	C ₂₀ H ₂₈ O ₃	0.0049	1.5835	↓	Fecal
Nonanoic acid	8.28	157.1218	C ₉ H ₁₈ O ₂	0.0056	1.5803	↑	Fecal
Metenolone acetate	12.34	343.2300	C ₂₂ H ₃₂ O ₃	0.0035	1.5800	↓	Fecal
11'-Carboxy-alpha-chromanol	12.55	417.2998	C ₂₆ H ₄₂ O ₄	0.0051	1.5787	↓	Fecal
4,5-Dimethyl-3-hydroxy-2,5-dihydrofuran-2-one sulfate	0.96	206.9960	C ₆ H ₈ O ₆ S	0.0099	1.5696	↑	Fecal
3-(2-(2,3-dihydroxy-5,6,8a-trimethyloctahydro-2H-spiro(naphthalene-1,2'-oxiran)-5-yl)ethyl)-5-hydroxyfuran-2(5H)-one	9.31	365.1960	C ₂₀ H ₃₀ O ₆	0.0041	1.5674	↓	Fecal
Dehydromenthofurolactone	7.68	165.0907	C ₁₀ H ₁₂ O ₂	0.0037	1.5638	↓	Fecal
Lumiflavin	6.80	255.0873	C ₁₃ H ₁₂ N ₄ O ₂	0.0081	1.5597	↑	Fecal
1,7-Bis(4-hydroxyphenyl)-3,5-heptanediol	9.47	315.1589	C ₁₉ H ₂₄ O ₄	0.0073	1.5582	↑	Fecal
Isoliquiritigenin	7.39	255.0654	C ₁₅ H ₁₂ O ₄	0.0109	1.5545	↑	Fecal
Fraxinellone	8.02	233.1164	C ₁₄ H ₁₆ O ₃	0.0068	1.5515	↑	Fecal
3alpha,7alpha-Dihydroxycoprostanic acid	12.14	433.3311	C ₂₇ H ₄₆ O ₄	0.0069	1.5392	↓	Fecal

3-(2-methylpropyl)-3a,4,5,6-tetrahydro-2-benzofuran-1(3h)-one	7.74	177.1267	C ₁₂ H ₁₈ O ₂	0.0087	1.5382	↓	Fecal
Glycylglutamine	1.31	204.0976	C ₇ H ₁₃ N ₃ O ₄	0.0096	1.5354	↑	Fecal
Mannosamine	1.28	180.0860	C ₆ H ₁₃ NO ₅	0.0158	1.5310	↑	Fecal
Bisnorcholic acid	9.37	379.2474	C ₂₂ H ₃₆ O ₅	0.0099	1.5266	↓	Fecal
9H-xanthen-9-one, 1,3,6-trihydroxy-8-methyl-	6.39	257.0480	C ₁₄ H ₁₀ O ₅	0.0097	1.5245	↑	Fecal
Brefeldin A	10.32	279.1588	C ₁₆ H ₂₄ O ₄	0.0042	1.5241	↑	Fecal
GlcNAc	0.91	256.0590	C ₈ H ₁₅ NO ₆	0.0102	1.5231	↓	Fecal
Benzoxazine-6-carboxylic acid	6.60	178.0492	C ₉ H ₇ NO ₃	0.0075	1.5175	↓	Fecal
ethyl 2-((3-methylphenyl)carbonylamino)acetate	7.28	244.0961	C ₁₂ H ₁₅ NO ₃	0.0155	1.5171	↑	Fecal
Sebuthylazine	5.59	230.1127	C ₉ H ₁₆ ClN ₅	0.0159	1.5104	↑	Fecal
Isohomovanillic acid	7.18	181.0489	C ₉ H ₁₀ O ₄	0.0095	1.5102	↑	Fecal
3-O-Acetyl-16alpha-hydroxytrametenolic acid	12.63	513.3561	C ₃₂ H ₅₀ O ₅	0.0135	1.5100	↑	Fecal
Chenodeoxycholyphenylalanine	11.90	538.3544	C ₃₃ H ₄₉ NO ₅	0.0071	1.5060	↓	Fecal
Eicosanedioic acid	12.60	341.2693	C ₂₀ H ₃₈ O ₄	0.0068	1.5054	↓	Fecal
GalNAc	1.32	222.0966	C ₈ H ₁₅ NO ₆	0.0076	1.5014	↓	Fecal
N-Acetyl-5-aminosalicylic acid	7.00	196.0600	C ₉ H ₉ NO ₄	0.0160	1.4961	↑	Fecal

(6E,8E,10R,12Z)-10-Hydroxy-3-oxooctadecatrienoic acid	11.71	307.1917	C ₁₈ H ₂₈ O ₄	0.0104	1.4944	↓	Fecal
Ceanothic acid	11.17	487.3397	C ₃₀ H ₄₆ O ₅	0.0078	1.4925	↑	Fecal
(2R,3R,4S,6R)-6-((10-formyl-5,14-dihydroxy-13-methyl-17-(5-oxo-2,5-dihydrofuran-3-yl)hexadecahydro-1H-cyclopenta(a)phenanthren-3-yl)oxy)-4-methoxy-2-methyltetrahydro-2H-pyran-3-yl acetate	12.74	613.2982	C ₃₂ H ₄₆ O ₁₀	0.0094	1.4916	↑	Fecal
2-Ethylpropanedioylcarnitine	6.11	276.1441	C ₁₂ H ₂₁ NO ₆	0.0182	1.4903	↑	Fecal
N-Benzylpiperazine	6.62	177.1384	C ₁₁ H ₁₆ N ₂	0.0146	1.4902	↑	Fecal
Methoxyphenylacetic acid	6.94	165.0545	C ₉ H ₁₀ O ₃	0.0172	1.4899	↑	Fecal
Terpestacin	10.26	403.2833	C ₂₅ H ₃₈ O ₄	0.0100	1.4892	↓	Fecal
Dodecanedioic acid	10.23	213.1479	C ₁₂ H ₂₂ O ₄	0.0107	1.4859	↓	Fecal
Corynoxene	8.49	383.1981	C ₂₂ H ₂₆ N ₂ O ₄	0.0119	1.4783	↓	Fecal
Indole-3-acetyl-valine	7.41	273.1239	C ₁₅ H ₁₈ N ₂ O ₃	0.0132	1.4743	↓	Fecal
Oxysophocarpine	6.11	285.1547	C ₁₅ H ₂₂ N ₂ O ₂	0.0186	1.4736	↑	Fecal
Dopaminechrome	6.42	148.0388	C ₈ H ₇ NO ₂	0.0150	1.4704	↓	Fecal

Caulophylline	7.65	205.1330	C ₁₂ H ₁₆ N ₂ O	0.0164	1.4685	↑	Fecal
Coprocholic acid	11.23	449.3252	C ₂₇ H ₄₆ O ₅	0.0093	1.4648	↓	Fecal
Adrenic acid	13.14	333.2782	C ₂₂ H ₃₆ O ₂	0.0166	1.4631	↓	Fecal
Pregnanetriolone	10.62	349.2377	C ₂₁ H ₃₄ O ₄	0.0140	1.4556	↓	Fecal
5-((1-Iminoethyl)amino)-2-aminopentanoic acid	5.19	174.1232	C ₇ H ₁₅ N ₃ O ₂	0.0147	1.4521	↓	Fecal
3-(sec-butyl)-2-hydroxy-3H-benzo(e)(1,4)diazepin-5(4H)-one	6.78	233.1283	C ₁₃ H ₁₆ N ₂ O ₂	0.0196	1.4521	↓	Fecal
4-(3-Pyridyl)-3-butenic acid	7.44	162.0546	C ₉ H ₉ NO ₂	0.0143	1.4510	↓	Fecal
Equilin	12.26	267.1417	C ₁₈ H ₂₀ O ₂	0.0147	1.4508	↓	Fecal
9-acetyl-10,14-dimethyl-20-oxahexacyclo(11.9.0.0<2,10>.0<4,9>.0<14,19>.0<19,21>)docos-17-yl acetate	9.20	411.2890	C ₂₇ H ₄₀ O ₄	0.0205	1.4485	↓	Fecal
Isorhynchophylline	8.96	383.1972	C ₂₂ H ₂₈ N ₂ O ₄	0.0090	1.4476	↑	Fecal
N-(((1S,9aR)-octahydro-1H-quinolizin-1-yl)methyl)-5-(pyridin-3-yl)-1H-pyrazole-3-carboxamide	7.15	340.2114	C ₁₉ H ₂₅ N ₅ O	0.0140	1.4472	↓	Fecal
Isobutyryl-Carnitine	2.92	232.1541	C ₁₁ H ₂₁ NO ₄	0.0162	1.4449	↓	Fecal

5-Hydroxyferulic acid	6.94	209.0441	C ₁₀ H ₁₀ O ₅	0.0235	1.4438	↑	Fecal
6,7-Dimethoxy-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid	4.14	238.1067	C ₁₂ H ₁₅ NO ₄	0.0162	1.4420	↓	Fecal
Oseltamivir acid	6.93	285.1798	C ₁₄ H ₂₄ N ₂ O ₄	0.0158	1.4401	↓	Fecal
Arctigenin	10.50	371.1523	C ₂₁ H ₂₄ O ₆	0.0146	1.4389	↓	Fecal
6,10a-Dihydroxy-4-(hydroxymethyl)-4,7,11b-trimethyl-1,2,3,4a,5,6,6a,7,11,11a-decahydronaphtho(2,1-)(1)benzouran-9-one	10.21	349.2021	C ₂₀ H ₃₀ O ₅	0.0136	1.4380	↓	Fecal
Bilirubin	12.86	585.2709	C ₃₃ H ₃₆ N ₄ O ₆	0.0192	1.4358	↓	Fecal
Cycluron	10.55	199.1801	C ₁₁ H ₂₂ N ₂ O	0.0233	1.4353	↑	Fecal
Traumatic acid	8.71	229.1425	C ₁₂ H ₂₀ O ₄	0.0207	1.4345	↑	Fecal
Muricholic Acid	10.36	407.2787	C ₂₄ H ₄₀ O ₅	0.0173	1.4323	↓	Fecal
3-(Indol-3-yl)propionic acid	9.59	190.0859	C ₁₁ H ₁₁ NO ₂	0.0102	1.4319	↑	Fecal
Abscisic acid	9.45	247.1324	C ₁₅ H ₂₀ O ₄	0.0260	1.4305	↓	Fecal
5-Hydroxyindoleacetate	7.70	192.0650	C ₁₀ H ₉ NO ₃	0.0195	1.4283	↓	Fecal
N-Acetylserine	1.26	192.0235	C ₅ H ₉ NO ₄	0.0274	1.4265	↓	Fecal
13-Hydroxyl↑anine	7.61	265.1907	C ₁₅ H ₂₄ N ₂ O ₂	0.0194	1.4260	↓	Fecal

(2E)-2-Propylpent-2-Enoylcarnitine	6.68	286.2009	C ₁₅ H ₂₇ NO ₄	0.0274	1.4239	↑	Fecal
2,3-Dinor-TXB2	9.74	341.1961	C ₁₈ H ₃₀ O ₆	0.0143	1.4233	↓	Fecal
Sapogenins	13.33	401.3414	C ₂₇ H ₄₄ O ₂	0.0118	1.4212	↓	Fecal
OPFC-perfluoroalkyl_sulfate	7.21	224.9857	C ₄ H ₆ F ₄ O ₄ S	0.0242	1.4192	↑	Fecal
Glu-CA	9.67	536.3225	C ₂₉ H ₄₇ NO ₈	0.0150	1.4190	↑	Fecal
5-HEPE	11.99	317.2117	C ₂₀ H ₃₀ O ₃	0.0246	1.4179	↑	Fecal
(E)-N-(4-acetamidobutyl)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide	6.03	329.1450	C ₁₆ H ₂₂ N ₂ O ₄	0.0166	1.4173	↑	Fecal
Perindopril	12.29	369.2409	C ₁₉ H ₃₂ N ₂ O ₅	0.0196	1.4161	↓	Fecal
Coumarin	9.62	147.0438	C ₉ H ₆ O ₂	0.0154	1.4140	↑	Fecal
6-Methyl-2-pyridinecarboxylic acid	6.56	138.0549	C ₇ H ₇ NO ₂	0.0124	1.4136	↑	Fecal
Neotrehalose	1.54	341.1079	C ₁₂ H ₂₂ O ₁₁	0.0209	1.4107	↑	Fecal
5,6-Dihydroxyprostaglandin F1a	9.74	387.2380	C ₂₀ H ₃₆ O ₇	0.0164	1.4090	↓	Fecal
Sclareolide	12.23	251.2001	C ₁₆ H ₂₆ O ₂	0.0170	1.4072	↓	Fecal
Ursonic acid	13.22	477.3334	C ₃₀ H ₄₆ O ₃	0.0251	1.4028	↓	Fecal
1,10-Epoxygermacrone	12.26	235.1688	C ₁₅ H ₂₂ O ₂	0.0194	1.4004	↓	Fecal
Am-3102	13.11	340.3197	C ₂₁ H ₄₁ NO ₂	0.0254	1.3993	↓	Fecal

PC(18:2/18:2)	12.27	782.5694	C ₄₄ H ₈₀ NO ₈ P	0.0214	1.3937	↓	Fecal
beta-D-Fucose	0.98	163.0596	C ₆ H ₁₂ O ₅	0.0236	1.3918	↑	Fecal
4-[(5-(7-Hydroxy-5,5,8a-trimethyl-2-methylenedecahydro-1-naphthalenyl)-3-methylpentyl)oxy]-4-oxobutanoic acid	10.35	431.2757	C ₂₄ H ₄₀ O ₅	0.0281	1.3895	↓	Fecal
Myoinositol	0.94	179.0547	C ₆ H ₁₂ O ₆	0.0238	1.3875	↑	Fecal
5-(3-Pyridyl)-2-hydroxytetrahydrofuran	2.54	166.0860	C ₉ H ₁₁ NO ₂	0.0290	1.3870	↑	Fecal
PI(16:0/18:2)	10.75	833.5148	C ₄₃ H ₇₉ O ₁₃ P	0.0186	1.3864	↓	Fecal
5'-Amino-5'-deoxyadenosine	7.75	267.1191	C ₁₀ H ₁₄ N ₆ O ₃	0.0179	1.3843	↓	Fecal
4(5)-EpDPE methyl ester	10.48	341.2461	C ₂₃ H ₃₄ O ₃	0.0243	1.3839	↓	Fecal
Dimethyl phthalate	10.21	195.0645	C ₁₀ H ₁₀ O ₄	0.0184	1.3797	↓	Fecal
3-Hydroxyoctadecanoic Acid	12.47	299.2587	C ₁₈ H ₃₆ O ₃	0.0278	1.3794	↑	Fecal
Clozapine	7.08	327.1365	C ₁₈ H ₁₉ ClN ₄	0.0270	1.3786	↓	Fecal
4,8,12,15-Octadecatetraenoic acid	9.65	277.2158	C ₁₈ H ₂₈ O ₂	0.0321	1.3778	↑	Fecal
2,6-bis((4-methoxyphenyl)methylene)-4-ethylcyclohexan-1-one	6.79	363.1909	C ₂₄ H ₂₆ O ₃	0.0263	1.3748	↓	Fecal
N-Acetyltyrosine	6.81	224.0912	C ₁₁ H ₁₃ NO ₄	0.0197	1.3743	↑	Fecal

(6)-Gingerdione	10.47	291.1600	C ₁₇ H ₂₄ O ₄	0.0288	1.3709	↓	Fecal
1-Pentyl-3-(1-naphthoyl) indole	7.05	342.1834	C ₂₄ H ₂₃ NO	0.0228	1.3653	↑	Fecal
12-Hydroxy-8,10-octadecadienoic acid	11.39	297.2411	C ₁₈ H ₃₂ O ₃	0.0299	1.3625	↑	Fecal
Heliotrine	8.13	314.1946	C ₁₆ H ₂₇ NO ₅	0.0342	1.3602	↑	Fecal
Hydroxy Tyrosol -Acetate	6.35	226.1070	C ₁₁ H ₁₅ NO ₄	0.0282	1.3600	↓	Fecal
Tryptophenolide	7.11	335.1587	C ₂₀ H ₂₄ O ₃	0.0326	1.3581	↓	Fecal
Indole-3-acetyl-leucine	7.77	289.1535	C ₁₆ H ₂₀ N ₂ O ₃	0.0307	1.3563	↓	Fecal
L-2,3-Dihydrodipicolinic acid	0.84	168.0262	C ₇ H ₇ NO ₄	0.0420	1.3509	↓	Fecal
25-Methyldolichosterone	12.20	475.3413	C ₂₉ H ₄₈ O ₅	0.0276	1.3494	↓	Fecal
(Z)-5-((2R,3S,4S)-4-Hydroxy-2-((E)-3-hydroxyoct-1-enyl)oxan-3-yl)pent-3-enoic acid	10.27	325.2016	C ₁₈ H ₃₀ O ₅	0.0191	1.3491	↓	Fecal
Dihydrotestosterone	6.91	313.2107	C ₁₉ H ₃₀ O ₂	0.0306	1.3447	↓	Fecal
Palmatine	10.34	352.1565	C ₂₁ H ₂₂ NO ₄ ⁺	0.0325	1.3418	↓	Fecal
Fructose lactate	0.96	267.0713	C ₉ H ₁₆ O ₉	0.0229	1.3398	↑	Fecal
1-O-Acetyllycorine	6.50	330.1357	C ₁₈ H ₁₉ NO ₅	0.0313	1.3388	↓	Fecal
Soyasapogenol A	12.92	497.3581	C ₃₀ H ₅₀ O ₄	0.0292	1.3370	↓	Fecal
Medicagenic acid	11.32	501.3219	C ₃₀ H ₄₆ O ₆	0.0286	1.3330	↓	Fecal

Tridecanedioic acid	10.64	243.1595	C ₁₃ H ₂₄ O ₄	0.0288	1.3320	↓	Fecal
Bicine	1.30	164.0915	C ₆ H ₁₃ NO ₄	0.0463	1.3320	↑	Fecal
Naringenin	8.34	273.0744	C ₁₅ H ₁₂ O ₅	0.0320	1.3301	↑	Fecal
Phe-CA	11.00	538.3532	C ₃₃ H ₄₉ NO ₆	0.0237	1.3286	↑	Fecal
Leucyl-Isoleucine	7.84	245.1855	C ₁₂ H ₂₄ N ₂ O ₃	0.0202	1.3282	↑	Fecal
Mevinolinic acid	10.58	445.2549	C ₂₄ H ₃₈ O ₆	0.0382	1.3282	↓	Fecal
Dihydromelilotoside	7.34	327.1081	C ₁₅ H ₂₀ O ₈	0.0383	1.3266	↑	Fecal
Uzarigenin	9.16	375.2519	C ₂₃ H ₃₄ O ₄	0.0284	1.3258	↓	Fecal
8-Hydroxy-9,10-epoxystearic acid	12.28	315.2525	C ₁₈ H ₃₄ O ₄	0.0310	1.3234	↓	Fecal
Estriol	6.95	311.1587	C ₁₈ H ₂₄ O ₃	0.0348	1.3197	↓	Fecal
O-Desmethyl tramadol	7.69	250.1799	C ₁₅ H ₂₃ NO ₂	0.0387	1.3171	↓	Fecal
Phenylalanine butyl ester	6.50	222.1485	C ₁₃ H ₁₉ NO ₂	0.0414	1.3168	↓	Fecal
Sucrose	5.98	325.1118	C ₁₂ H ₂₂ O ₁₁	0.0336	1.3145	↑	Fecal
2,8-Dihydroxyquinoline	7.77	162.0547	C ₉ H ₇ NO ₂	0.0349	1.3136	↓	Fecal
1-allyl-2-hydroxy-7,8,9,10-tetrahydroazepino(2,1-b)quinazolin-12(6H)-one	7.42	271.1473	C ₁₆ H ₁₈ N ₂ O ₂	0.0403	1.3117	↓	Fecal
16-HDoHE	12.07	343.2271	C ₂₂ H ₃₂ O ₃	0.0187	1.3115	↑	Fecal

5-Hydroxyindole	6.42	132.0440	C ₈ H ₇ NO	0.0371	1.3098	↓	Fecal
Cholylasparagine	9.45	523.3364	C ₂₈ H ₄₆ N ₂ O ₇	0.0214	1.3059	↑	Fecal
3-Hydroxymonoethylglycinexylidide	6.27	223.1432	C ₁₂ H ₁₈ N ₂ O ₂	0.0465	1.3051	↓	Fecal
1-Tetradecanol hydrogen sulfate	12.47	293.1788	C ₁₄ H ₃₀ O ₄ S	0.0426	1.3014	↓	Fecal
Imidocarb	6.91	349.1748	C ₁₉ H ₂₀ N ₆ O	0.0272	1.3002	↑	Fecal
(-)-Camphanic acid	8.70	197.0808	C ₁₀ H ₁₄ O ₄	0.0330	1.2987	↓	Fecal
Magnoflorine	7.25	343.1675	C ₂₀ H ₂₄ NO ₄ ⁺	0.0413	1.2917	↓	Fecal
(2E)-3-(1-ethyl-3-methylpyrazol-4-yl)-1-(4-hydroxyphenyl)prop-2-en-1-one	6.91	257.1314	C ₁₅ H ₁₆ N ₂ O ₂	0.0422	1.2910	↓	Fecal
Piperine	7.19	286.1426	C ₁₇ H ₁₉ NO ₃	0.0488	1.2898	↓	Fecal
N-Acetylornithine	1.37	175.1074	C ₇ H ₁₄ N ₂ O ₃	0.0403	1.2897	↓	Fecal
Polyporusterone D	11.44	459.3102	C ₂₈ H ₄₄ O ₅	0.0389	1.2880	↓	Fecal
1-Phenanthrenecarboxylic acid,	7.22	337.1753	C ₂₀ H ₂₆ O ₃	0.0370	1.2853	↓	Fecal
1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-9-oxo-ethyl (2E)-3-(4-(diethylamino)phenyl)-2-cyanoprop-2-enoate	8.19	295.1429	C ₁₆ H ₂₀ N ₂ O ₂	0.0482	1.2823	↓	Fecal

Cholyltyrosine	10.17	570.3434	C ₃₃ H ₄₉ NO ₇	0.0248	1.2810	↑	Fecal
(2E,8E)-10-hydroxydeca-2,8-dien-4-ynoylcarnitine	8.43	324.1798	C ₁₇ H ₂₅ NO ₅	0.0471	1.2774	↑	Fecal
Avenoleic acid	11.22	297.2421	C ₁₈ H ₃₂ O ₃	0.0480	1.2767	↑	Fecal
9-hydroxy-5b,8,11a-trimethyl-1-prop-1-en-2-yl-1,2,3,4,5,6,7,7a,9,10,11,11b,12,13,13a,13b-hexadecahydrocyclopenta(a)chrysene-3a,5a,8-tricarboxylic acid	10.83	517.3144	C ₃₀ H ₄₄ O ₇	0.0229	1.2641	↑	Fecal
Monoketocholic acid	10.52	421.2592	C ₂₄ H ₃₈ O ₆	0.0413	1.2609	↓	Fecal
Cholyllysine	8.95	537.3890	C ₃₀ H ₅₂ N ₂ O ₆	0.0406	1.2568	↑	Fecal
CID 75411918	11.13	485.3257	C ₃₀ H ₄₆ O ₆	0.0318	1.2557	↑	Fecal
5b-Cyprinol sulfate	10.97	531.2990	C ₂₇ H ₄₈ O ₈ S	0.0476	1.2545	↓	Fecal
2-heptylhexanedioic acid	8.11	243.1594	C ₁₃ H ₂₄ O ₄	0.0354	1.2536	↓	Fecal
Trachelanthine	6.22	324.1799	C ₁₅ H ₂₇ NO ₅	0.0487	1.2528	↓	Fecal
4-Oxo-L-proline	3.04	130.0498	C ₅ H ₇ NO ₃	0.0395	1.2511	↓	Fecal
5-Hydroxy-7-methoxy-2-methyl-8-(3-methyl-but-2-enyl)-chromen-4-on	10.15	275.1265	C ₁₆ H ₁₈ O ₄	0.0436	1.2381	↓	Fecal

7-Ketodeoxycholic acid	9.64	407.2781	C ₂₄ H ₃₈ O ₅	0.0471	1.2328	↓	Fecal
Chenodeoxycholytryptophan	11.69	579.3774	C ₃₅ H ₅₀ N ₂ O ₅	0.0466	1.2325	↓	Fecal
Methionylleucine	6.96	263.1418	C ₁₁ H ₂₂ N ₂ O ₃ S	0.0380	1.2325	↑	Fecal
5-Hydroxyculmorin	8.22	237.1843	C ₁₅ H ₂₆ O ₃	0.0404	1.2245	↑	Fecal
Gibberellin A55	9.31	363.1447	C ₁₉ H ₂₄ O ₇	0.0483	1.2182	↓	Fecal
13-OxoODE	12.25	295.2258	C ₁₈ H ₃₀ O ₃	0.0407	1.2143	↓	Fecal
(2E,6E,10E)-4-hydroxy-3-(3,7,11,15-tetramethyl- hexadeca-2,6,10,14-tetraenyl)-benzoic acid	11.64	411.2888	C ₂₇ H ₃₈ O ₃	0.0457	1.2117	↓	Fecal
22-Hydroxy-2-hopen-1-one	13.18	441.3709	C ₃₀ H ₄₈ O ₂	0.0403	1.2099	↑	Fecal
Acetaminophen	1.89	152.0705	C ₈ H ₉ NO ₂	0.0456	1.1995	↓	Fecal
Lathyrol	11.70	335.2199	C ₂₀ H ₃₀ O ₄	0.0481	1.1452	↓	Fecal

FZD, Fuling Zexie Decoction; HFD, high-fat diet.

Supplementary Table 4 The metabolites significantly-regulated by ZD in MASLD rats

Metabolite name	Rt (min)	m/z	Formula	P	VIP	ZD <i>vs</i> HFD	Sample
1-Methylcyclohexane-1,2-dicarboxylic acid	9.30	185.0804	C ₉ H ₁₄ O ₄	0.0003	2.1880	↑	Serum
Glycyrrhetinic acid	12.65	469.3321	C ₃₀ H ₄₆ O ₄	0.0003	2.1750	↑	Serum
Liquiritin apioside	7.93	549.1594	C ₂₆ H ₃₀ O ₁₃	0.0005	2.1170	↑	Serum
5-Hexyltetrahydro-2-oxo-3-furancarboxylic acid	10.38	213.1116	C ₁₁ H ₁₈ O ₄	0.0015	2.0502	↑	Serum
2-Isopropylmalic acid	6.84	175.0598	C ₇ H ₁₂ O ₅	0.0008	2.0447	↑	Serum
Alkhanin	9.18	263.1283	C ₁₅ H ₂₀ O ₄	0.0013	2.0323	↑	Serum
3,5-Dihydroxyphenylvaleric acid sulfate	7.48	289.0384	C ₁₁ H ₁₄ O ₇ S	0.0017	1.9971	↑	Serum
6-Prenylnaringenin	10.20	339.1267	C ₂₀ H ₂₀ O ₅	0.0060	1.9500	↑	Serum
Vanillic acid	6.48	167.0336	C ₈ H ₈ O ₄	0.0026	1.9224	↑	Serum
Hippuric acid	7.36	178.0495	C ₉ H ₉ NO ₃	0.0051	1.8666	↑	Serum
Wogonoside	8.32	459.0933	C ₂₂ H ₂₀ O ₁₁	0.0087	1.8581	↑	Serum
9-acetyl-17-hydroxy-10,14-dimethyl-20-oxahexacyclo docosane	11.04	387.2885	C ₂₅ H ₃₈ O ₃	0.0109	1.8567	↓	Serum
Enterolactone	8.78	299.1274	C ₁₈ H ₁₈ O ₄	0.0117	1.8553	↓	Serum
N-palmitoyl-phosphoethanolamine	11.02	378.2405	C ₁₈ H ₃₈ NO ₅ P	0.0113	1.8485	↓	Serum

Azelaic acid	8.76	187.0961	C ₉ H ₁₆ O ₄	0.0077	1.8384	↑	Serum
Acoric acid	10.29	267.1593	C ₁₅ H ₂₄ O ₄	0.0097	1.8070	↑	Serum
Gingerol	10.99	293.1751	C ₁₇ H ₂₆ O ₄	0.0126	1.7949	↓	Serum
Glycoursodeoxycholic acid	10.86	450.3211	C ₂₆ H ₄₃ NO ₅	0.0151	1.7949	↓	Serum
Cinnamoylglycine	8.72	204.0654	C ₁₁ H ₁₁ NO ₃	0.0114	1.7444	↑	Serum
2-Pyrrolidinecarboxamide	1.11	115.0865	C ₅ H ₁₀ N ₂ O	0.0072	1.7386	↑	Serum
2-Hydroxy-3-Methylvaleric Acid	7.55	131.0696	C ₆ H ₁₂ O ₃	0.0240	1.7351	↓	Serum
Eicosatetraenoic acid	12.80	303.2320	C ₂₀ H ₃₂ O ₂	0.0243	1.7286	↑	Serum
2-Hydroxystearic acid	13.16	299.2576	C ₁₈ H ₃₆ O ₃	0.0110	1.7186	↓	Serum
3-Hydroxy-2-methyl-4-pyrone sulfate	6.41	204.9801	C ₆ H ₆ O ₆ S	0.0202	1.7144	↓	Serum
Glycocholate	10.92	448.3044	C ₂₆ H ₄₃ NO ₆	0.0227	1.6937	↓	Serum
1-methyl-4-(6-methylhept-5-en-2-yl)-2,3-dioxabicyclo(2.2.2)oct-5-ene	7.31	201.1631	C ₁₅ H ₂₄ O ₂	0.0169	1.6720	↑	Serum
3,4,5-Trimethylbenzaldehyde	11.80	149.0958	C ₁₀ H ₁₂ O	0.0373	1.6678	↓	Serum
Indole-3-acrylic acid	9.39	186.0544	C ₁₁ H ₉ NO ₂	0.0152	1.6265	↑	Serum
2-Methylbutyrylglycine	6.67	158.0805	C ₇ H ₁₃ NO ₃	0.0341	1.6264	↓	Serum
Arachidoyl Ethanolamide	11.63	356.3504	C ₂₂ H ₄₅ NO ₂	0.0144	1.6216	↓	Serum

Anisole	7.88	107.0486	C ₇ H ₈ O	0.0311	1.6188	↑	Serum
Sphinganine 1-phosphate	11.22	380.2565	C ₁₈ H ₄₀ NO ₅ P	0.0272	1.6092	↓	Serum
15-Methylheptadecanoylcarnitine	12.27	428.3729	C ₂₅ H ₄₉ NO ₄	0.0283	1.6056	↓	Serum
Hexaethylene glycol	6.63	283.1740	C ₁₂ H ₂₆ O ₇	0.0223	1.5953	↑	Serum
Dehydromenthofurolactone	10.45	165.0907	C ₁₀ H ₁₂ O ₂	0.0299	1.5900	↓	Serum
Abscisic acid	9.42	263.1283	C ₁₅ H ₂₀ O ₄	0.0331	1.5851	↑	Serum
4-Hydroxybenzaldehyde	7.38	105.0337	C ₇ H ₆ O ₂	0.0229	1.5841	↑	Serum
Ornithine	1.11	133.0969	C ₅ H ₁₂ N ₂ O ₂	0.0210	1.5584	↑	Serum
4-Ethoxybenzaldehyde	10.08	151.0750	C ₉ H ₁₀ O ₂	0.0345	1.5572	↓	Serum
Corymbosin	8.99	357.1008	C ₁₉ H ₁₈ O ₇	0.0419	1.5370	↓	Serum
delta-Valerolactone	6.25	101.0598	C ₅ H ₈ O ₂	0.0380	1.5346	↓	Serum
Cinnamic acid	8.73	131.0488	C ₉ H ₈ O ₂	0.0303	1.5346	↑	Serum
ent-1(10)-Halimene-15,19-dioic acid	11.82	335.2220	C ₂₀ H ₃₂ O ₄	0.0403	1.5202	↑	Serum
4-Acetylanisole	8.76	151.0749	C ₉ H ₁₀ O ₂	0.0427	1.5084	↓	Serum
Docosaheenoicacid(DHA)	12.70	327.2325	C ₂₂ H ₃₂ O ₂	0.0411	1.4411	↑	Serum
Trimethyloxamine	1.35	76.0761	C ₃ H ₉ NO	0.0402	1.3860	↑	Serum
PC(18:0/18:2)	12.31	233.1526	C ₄₄ H ₈₄ NO ₈ P	0.0000	1.9716	↓	Liver

Le [↑] eptin	12.77	786.5969	C ₂₀ H ₃₈ N ₆ O ₄	0.0000	1.9227	↓	Liver
Loliolide	9.33	154.0133	C ₁₁ H ₁₆ O ₃	0.0003	1.8783	↑	Liver
2-Isopropyl-5-methylpyrazine	6.18	178.0497	C ₈ H ₁₂ N ₂	0.0004	1.8736	↑	Liver
Liquiritin	8.08	267.1602	C ₂₁ H ₂₂ O ₉	0.0003	1.8644	↑	Liver
Glycolithocholic acid	11.89	273.1705	C ₂₆ H ₄₃ NO ₄	0.0004	1.8549	↓	Liver
Abscisic acid	9.39	263.1287	C ₁₅ H ₂₀ O ₄	0.0005	1.8542	↑	Liver
Gingerol	9.36	146.0922	C ₁₇ H ₂₆ O ₄	0.0005	1.8524	↑	Liver
Docosaehaenoic acid	12.69	412.2494	C ₂₂ H ₃₂ O ₂	0.0005	1.8418	↓	Liver
Benzethonium	13.15	456.2418	C ₂₇ H ₄₂ NO ₂	0.0009	1.8154	↓	Liver
Leukotriene C4	9.71	119.0486	C ₃₀ H ₄₇ N ₃ O ₉ S	0.0011	1.8074	↓	Liver
Citrazinic acid	6.62	165.0543	C ₆ H ₅ NO ₄	0.0012	1.8031	↑	Liver
2-Methylbenzaldehyde	7.22	427.3017	C ₈ H ₈ O	0.0006	1.8016	↑	Liver
Cinnamoylglycine	8.71	151.1229	C ₁₁ H ₁₁ NO ₃	0.0007	1.7994	↑	Liver
Betaine	13.43	277.1434	C ₅ H ₁₁ NO ₂	0.0014	1.7441	↓	Liver
gamma-Guanidinobutyric acid	2.12	138.0548	C ₅ H ₁₁ N ₃ O ₂	0.0026	1.7398	↑	Liver
Maritimetin	1.11	149.0076	C ₁₅ H ₁₀ O ₆	0.0030	1.7330	↑	Liver
Trigonelline	1.40	205.0346	C ₇ H ₇ NO ₂	0.0034	1.7136	↑	Liver

Roquefortine E	10.05	434.3259	C ₂₇ H ₃₁ N ₅ O ₂	0.0036	1.7107	↑	Liver
Meso-Tartaric acid	0.91	233.1526	C ₄ H ₆ O ₆	0.0038	1.7062	↑	Liver
beta-D-Glucopyranosiduronic acid, 4-methylphenyl	7.79	277.1785	C ₁₃ H ₁₆ O ₇	0.0027	1.7061	↓	Liver
(6E,8E,10R,12Z)-10-Hydroxy-3-oxooctadecatrienoic acid	11.72	349.2017	C ₁₈ H ₂₈ O ₄	0.0081	1.6852	↓	Liver
LPC(20:4)	13.47	413.3270	C ₂₈ H ₅₀ NO ₇ P	0.0033	1.6834	↓	Liver
4-Vinylcyclohexene	9.04	204.0658	C ₈ H ₁₂	0.0044	1.6799	↑	Liver
Glycoursodeoxycholic acid	10.86	241.1188	C ₂₆ H ₄₃ NO ₅	0.0028	1.6796	↓	Liver
Dehydromenthofurolactone	10.43	165.0906	C ₁₀ H ₁₂ O ₂	0.0043	1.6789	↓	Liver
Taurohyocholate	8.84	293.2119	C ₂₆ H ₄₅ NO ₇ S	0.0049	1.6725	↑	Liver
Hippuric acid	7.33	151.0612	C ₉ H ₉ NO ₃	0.0045	1.6552	↑	Liver
Oryzalic acid A	8.95	375.1474	C ₂₀ H ₃₀ O ₅	0.0061	1.6448	↓	Liver
Indole-3-acrylic acid	9.38	365.1959	C ₁₁ H ₉ NO ₂	0.0065	1.6411	↑	Liver
Ergothioneine	1.24	498.9313	C ₉ H ₁₅ N ₃ O ₂ S	0.0098	1.6159	↓	Liver
4-(Decan-4-yl)benzenesulfonic acid	11.70	149.0956	C ₁₆ H ₂₆ O ₃ S	0.0130	1.6148	↓	Liver
Tryptophenolide	12.14	500.3035	C ₂₀ H ₂₄ O ₃	0.0143	1.6139	↓	Liver
Costunolide	10.26	450.3207	C ₁₅ H ₂₀ O ₂	0.0080	1.6055	↑	Liver
LPC(22:4)	11.40	417.1194	C ₃₀ H ₅₄ NO ₇ P	0.0156	1.5975	↓	Liver

3,4,5-Trimethylbenzaldehyde	11.79	190.0859	C ₁₀ H ₁₂ O	0.0106	1.5863	↓	Liver
3-(2-(2,3-dihydroxy-5,6,8a-trimethyloctahydro-2H-spiro(naphthalene-1,2'-oxiran)-5-yl)ethyl)-5-hydroxyfuran-2(5H)-one	8.13	321.2408	C ₂₀ H ₃₀ O ₆	0.0096	1.5682	↓	Liver
3-Hydroxytetradecanedioic acid	9.32	137.1071	C ₁₄ H ₂₆ O ₅	0.0114	1.5549	↑	Liver
2-Hydroxylinolenic acid	11.75	141.0654	C ₁₈ H ₃₀ O ₃	0.0107	1.5546	↓	Liver
Sumaresinolic acid	12.88	161.0442	C ₃₀ H ₄₈ O ₄	0.0114	1.5533	↓	Liver
6-Methoxypurine	13.59	247.1682	C ₆ H ₆ N ₄ O	0.0156	1.5378	↑	Liver
IRB_p_329.1858_19.4	9.68	516.2973	C ₁₉ H ₂₄ N ₂ O ₃	0.0206	1.5246	↓	Liver
Peracetic acid	0.86	504.2699	C ₂ H ₄ O ₃	0.0123	1.5122	↑	Liver
(Z)-13-Oxo-9-octadecenoic acid	12.97	368.2784	C ₁₈ H ₃₂ O ₃	0.0168	1.5114	↓	Liver
Retinal	13.23	171.1373	C ₂₀ H ₂₈ O	0.0109	1.5102	↓	Liver
Norleucine	6.18	624.2988	C ₆ H ₁₃ NO ₂	0.0150	1.4978	↑	Liver
Pterosin A	9.61	329.2467	C ₁₅ H ₂₀ O ₃	0.0162	1.4833	↑	Liver
2,6,10,14-Hexadecatetraenoic acid, 3,7,11,15-tetramethyl-, (Z,E,E)-	12.79	193.0678	C ₂₀ H ₃₂ O ₂	0.0160	1.4781	↓	Liver
Taurochenodeoxycholic acid	9.88	299.2585	C ₂₆ H ₄₅ NO ₆ S	0.0194	1.4655	↑	Liver

6-Keto-decanoylcarnitine	8.16	544.3378	C ₁₇ H ₃₁ NO ₅	0.0219	1.4480	↑	Liver
Alanylglutamic acid	1.96	228.0802	C ₈ H ₁₄ N ₂ O ₅	0.0259	1.4396	↑	Liver
2,3-Dimethyl-5-propylpyrazine	6.47	270.3148	C ₉ H ₁₄ N ₂	0.0291	1.4327	↑	Liver
Isoalantolactone	12.05	237.0908	C ₁₅ H ₂₀ O ₂	0.0270	1.4268	↑	Liver
Corymbosin	8.38	369.3514	C ₁₉ H ₁₈ O ₇	0.0295	1.4255	↓	Liver
Phosphoric acid	2.54	322.2726	H ₃ O ₄ P	0.0260	1.4174	↓	Liver
Cucurbitic acid	10.86	295.2279	C ₁₂ H ₂₀ O ₃	0.0411	1.4159	↓	Liver
2-Methylcitric acid	3.29	329.1827	C ₇ H ₁₀ O ₇	0.0382	1.4064	↑	Liver
Glucose	0.90	179.0551	C ₆ H ₁₂ O ₆	0.0300	1.4038	↑	Liver
Koninginin E	12.34	209.0915	C ₁₆ H ₂₆ O ₄	0.0192	1.4034	↓	Liver
3, 5-Tetradecadiencarnitine	10.63	286.2000	C ₂₁ H ₃₇ NO ₄	0.0351	1.4009	↓	Liver
Trachelanthine	6.57	141.0653	C ₁₅ H ₂₇ NO ₅	0.0282	1.3986	↑	Liver
3-(Indol-3-yl)propionic acid	9.57	337.2378	C ₁₁ H ₁₁ NO ₂	0.0403	1.3921	↑	Liver
1,10-Epoxygermacrone	12.25	109.1013	C ₁₅ H ₂₂ O ₂	0.0383	1.3864	↓	Liver
Aspterric acid	10.89	416.3170	C ₁₅ H ₂₂ O ₄	0.0386	1.3849	↑	Liver
Acoric acid	10.29	193.0340	C ₁₅ H ₂₄ O ₄	0.0310	1.3796	↑	Liver
3-Methylazelaic acid	8.25	307.0826	C ₁₀ H ₁₈ O ₄	0.0256	1.3786	↑	Liver

Uridine	3.56	330.1907	C ₉ H ₁₂ N ₂ O ₆	0.0379	1.3758	↑	Liver
Isonerylgeraniol-18-oic acid	12.66	217.0821	C ₂₀ H ₃₂ O ₃	0.0225	1.3757	↓	Liver
Phenylacetyl glycine	7.73	281.2469	C ₁₀ H ₁₁ NO ₃	0.0301	1.3755	↓	Liver
Pi-Methylimidazoleacetic acid	13.58	198.1126	C ₆ H ₈ N ₂ O ₂	0.0334	1.3736	↓	Liver
3-Phenyllactic acid	8.19	104.0709	C ₉ H ₁₀ O ₃	0.0341	1.3715	↑	Liver
Levocetirizine	8.69	186.0547	C ₂₁ H ₂₅ ClN ₂ O ₃	0.0468	1.3606	↓	Liver
1,2:3,4-Di-O-isopropylidene-D-galactopyranose	7.58	496.3390	C ₁₂ H ₂₀ O ₆	0.0395	1.3551	↑	Liver
FMN	6.71	281.2480	C ₁₇ H ₂₁ N ₄ O ₉ P	0.0423	1.3546	↓	Liver
-N-(2-hydroxyethyl)octadeca-9,12,15-trienamide	12.37	335.2219	C ₂₀ H ₃₅ NO ₂	0.0370	1.3496	↓	Liver
S-Adenosylhomocysteine	5.95	439.0995	C ₁₄ H ₂₀ N ₆ O ₅ S	0.0416	1.3480	↑	Liver
(7Z,10Z,13E)-Docosa-7,10,13-trienoylcarnitine	12.31	197.1166	C ₂₉ H ₅₁ NO ₄	0.0379	1.3402	↓	Liver
Gly-Tyr	5.21	217.1072	C ₁₁ H ₁₄ N ₂ O ₄	0.0362	1.3222	↑	Liver
LPC(22:5)	13.48	140.0677	C ₃₀ H ₅₂ NO ₇ P	0.0456	1.3080	↑	Liver
20-Hydroxy-5,8,11,14-eicosatetraenoic acid	12.59	233.1526	C ₂₀ H ₃₂ O ₃	0.0380	1.3077	↓	Liver
1-Carboxyethylphenylalanine	8.31	786.5969	C ₁₂ H ₁₅ NO ₄	0.0477	1.2894	↑	Liver
Gentisic acid	7.13	153.0178	C ₇ H ₆ O ₄	0.0000	1.9290	↑	Urine
N-(2,4-dimethylphenyl)-N'-methylmethanimidamide	6.31	163.1224	C ₁₀ H ₁₄ N ₂	0.0000	1.8738	↑	Urine

OPFC-perfluoroalkyl_sulfate	7.13	224.9856	C ₄ H ₆ F ₄ O ₄ S	0.0001	1.8633	↑	Urine
P-Menthatriene	6.94	135.1166	C ₁₀ H ₁₄	0.0001	1.8581	↑	Urine
1-allyl-2-hydroxy-7,8,9,10-tetrahydroazepino(2,1-b)quinazolin-12(6H)-one	7.45	271.1463	C ₁₆ H ₁₈ N ₂ O ₂	0.0001	1.8550	↓	Urine
Parthenolide	9.12	249.1474	C ₁₅ H ₂₀ O ₃	0.0001	1.8525	↑	Urine
4,5-Dimethyl-3-hydroxy-2,5-dihydrofuran-2-one sulfate	6.05	206.9960	C ₆ H ₈ O ₆ S	0.0001	1.8506	↓	Urine
1H-Indene-1,2(3H)-dione	7.34	147.0435	C ₉ H ₆ O ₂	0.0001	1.8495	↑	Urine
4-methoxy-3-((4-methoxyphenoxy)methyl)benzaldehyde	8.28	137.0596	C ₁₆ H ₁₆ O ₄	0.0001	1.8371	↑	Urine
Tetrahydroharman-3-carboxylic acid	7.22	231.1119	C ₁₃ H ₁₄ N ₂ O ₂	0.0002	1.8274	↑	Urine
(R)-Boschniakine	7.56	162.0909	C ₁₀ H ₁₁ NO	0.0001	1.8266	↓	Urine
Tricarballic acid	2.76	175.0236	C ₆ H ₈ O ₆	0.0002	1.8256	↑	Urine
(S)-11,12,13-Trinor-7-calamenone	6.96	175.1113	C ₁₂ H ₁₄ O	0.0002	1.8246	↑	Urine
4-Amino-2-methylenebutanoic acid	2.27	116.0706	C ₅ H ₉ NO ₂	0.0002	1.8189	↑	Urine
Benzoic acid, 2-hydroxy-4-methoxy-3,6-dimethyl-	7.49	195.0652	C ₁₀ H ₁₂ O ₄	0.0003	1.8080	↑	Urine
4-Ethylphenylsulfate	8.59	201.0213	C ₈ H ₁₀ O ₄ S	0.0003	1.7999	↓	Urine
2,3-Dihydro-6-methyl-1H-pyrrolizine-5-carboxaldehyde	8.40	150.0910	C ₉ H ₁₁ NO	0.0003	1.7981	↓	Urine

5-Methoxyindoleacetic acid	7.25	206.0803	C ₁₁ H ₁₁ NO ₃	0.0005	1.7834	↑	Urine
3,5-Dihydroxycinnamic acid sulfate	6.60	258.9908	C ₉ H ₈ O ₇ S	0.0005	1.7823	↓	Urine
3-Hydroxymonoethylglycinexylidide	6.29	223.1434	C ₁₂ H ₁₈ N ₂ O ₂	0.0005	1.7803	↓	Urine
Atropaldehyde	9.00	133.0646	C ₉ H ₈ O	0.0005	1.7794	↑	Urine
Carboxyibuprofen	8.18	219.1013	C ₁₃ H ₁₆ O ₄	0.0006	1.7674	↑	Urine
Naringenin-7-O-Glucuronide	8.50	447.0927	C ₂₁ H ₂₀ O ₁₁	0.0008	1.7610	↑	Urine
10,12-dihydroxy-9-methyl-4,13-dimethylene-6-oxatricyclo(7.4.0.0<3,7>)tridecan- 5-one	8.80	247.1326	C ₁₅ H ₂₀ O ₄	0.0008	1.7575	↑	Urine
N-Acetyl-L-arginine	2.30	217.1291	C ₈ H ₁₆ N ₄ O ₃	0.0009	1.7570	↓	Urine
Benzoic acid, 2,4-dihydroxy-6-propyl-	8.55	195.0653	C ₁₀ H ₁₂ O ₄	0.0008	1.7566	↑	Urine
Bis-(acetyl)diaminopentane	6.47	187.1437	C ₉ H ₁₈ N ₂ O ₂	0.0008	1.7542	↑	Urine
Exemestane	6.96	319.1642	C ₂₀ H ₂₄ O ₂	0.0009	1.7478	↓	Urine
11-Dehydro-2,3-dinor-txb2	9.05	339.1804	C ₁₈ H ₂₈ O ₆	0.0007	1.7473	↓	Urine
p-Coumaric acid	6.98	163.0385	C ₉ H ₈ O ₃	0.0009	1.7465	↑	Urine
Scaposin	8.52	389.0911	C ₁₉ H ₁₈ O ₉	0.0007	1.7459	↑	Urine
Isoalantolactone	6.97	215.1424	C ₁₅ H ₂₀ O ₂	0.0009	1.7444	↑	Urine
Serine betaine	1.35	148.0963	C ₆ H ₁₄ NO ₃	0.0008	1.7443	↓	Urine

2-(3-carboxypropanoylamino)-3-indol-3-ylpropanoic acid	8.32	305.1098	C ₁₅ H ₁₆ N ₂ O ₅	0.0011	1.7297	↓	Urine
beta-Resorcylic acid	7.67	153.0178	C ₇ H ₆ O ₄	0.0012	1.7281	↑	Urine
3-Toluic acid	7.02	135.0435	C ₈ H ₈ O ₂	0.0013	1.7253	↓	Urine
Acetaminophen	6.88	152.0701	C ₈ H ₉ NO ₂	0.0012	1.7235	↓	Urine
Aspartylleucine	6.42	247.1280	C ₁₀ H ₁₈ N ₂ O ₅	0.0013	1.7224	↓	Urine
2-Hydroxyacetophenone sulfate	7.02	215.0013	C ₈ H ₈ O ₅ S	0.0012	1.7204	↓	Urine
1-Pyrrolidinecarboxaldehyde	6.26	100.0759	C ₅ H ₉ NO	0.0012	1.7185	↑	Urine
4-Acetylanisole	8.77	151.0750	C ₉ H ₁₀ O ₂	0.0016	1.7184	↓	Urine
Dropropizine	6.60	237.1593	C ₁₃ H ₂₀ N ₂ O ₂	0.0014	1.7148	↓	Urine
Chavicol	8.53	135.0801	C ₉ H ₁₀ O	0.0018	1.7066	↑	Urine
Acoric acid	9.07	251.1634	C ₁₅ H ₂₄ O ₄	0.0015	1.7045	↑	Urine
N-(2-octyloxyethyl)(3,4,5-trimethoxyphenyl)carboxamide	7.90	390.2272	C ₂₀ H ₃₃ NO ₅	0.0017	1.7044	↑	Urine
Imidazooxazole	6.75	108.0200	C ₄ H ₃ N ₃ O	0.0016	1.7018	↓	Urine
Flavone base + 3O, O-HexA-HexA	6.99	623.1238	C ₂₇ H ₂₆ O ₁₇	0.0019	1.6912	↓	Urine
Artemisinin	8.80	265.1428	C ₁₅ H ₂₂ O ₅	0.0025	1.6775	↑	Urine

Absciscic acid	9.41	247.1326	C ₁₅ H ₂₀ O ₄	0.0028	1.6695	↑	Urine
2-{{4-(tert-butyl)phenyl}carbonylamino}acetic acid	6.13	258.1081	C ₁₃ H ₁₇ NO ₃	0.0025	1.6653	↑	Urine
Alkhanin	9.22	263.1281	C ₁₅ H ₂₀ O ₄	0.0029	1.6624	↑	Urine
Kainic acid	7.13	236.0908	C ₁₀ H ₁₅ NO ₄	0.0022	1.6574	↓	Urine
Estriol	6.43	311.1588	C ₁₈ H ₂₄ O ₃	0.0028	1.6561	↓	Urine
Carnosine	1.23	227.1149	C ₉ H ₁₄ N ₄ O ₃	0.0030	1.6506	↓	Urine
Pterosin B	8.95	219.1373	C ₁₄ H ₁₈ O ₂	0.0027	1.6472	↓	Urine
Sinapine	7.17	310.1644	C ₁₆ H ₂₄ NO ₅	0.0040	1.6347	↑	Urine
Imidazolepropionic acid	2.06	141.0656	C ₆ H ₈ N ₂ O ₂	0.0031	1.6317	↑	Urine
3,6,9,12-Tetraoxatetradecane-1,14-diol	6.41	239.1487	C ₁₀ H ₂₂ O ₆	0.0041	1.6257	↑	Urine
4',6-Dihydroxyflavone	8.36	255.0646	C ₁₅ H ₁₀ O ₄	0.0037	1.6256	↓	Urine
Aleuretic Acid	8.98	303.2171	C ₁₆ H ₃₂ O ₅	0.0040	1.6219	↓	Urine
N-Acetyl-3-methylhistidine	1.85	212.1022	C ₉ H ₁₃ N ₃ O ₃	0.0049	1.6217	↓	Urine
Ligustilide	8.20	191.1062	C ₁₂ H ₁₄ O ₂	0.0048	1.6186	↑	Urine
Secobarbital	8.79	237.1238	C ₁₂ H ₁₈ N ₂ O ₃	0.0042	1.6158	↓	Urine
GABA	1.62	102.0544	C ₄ H ₉ NO ₂	0.0044	1.6104	↑	Urine
2,6-Dimethylpyrazine	1.26	109.0760	C ₆ H ₈ N ₂	0.0057	1.6038	↓	Urine

6-Methoxy-9H-carbazole-3-carboxaldehyde	8.54	226.0885	C ₁₄ H ₁₁ NO ₂	0.0058	1.5962	↓	Urine
3-(2-Furanyl)-2-propenal	7.54	121.0279	C ₇ H ₆ O ₂	0.0052	1.5949	↑	Urine
Valine betaine	2.61	160.1326	C ₈ H ₁₇ NO ₂	0.0059	1.5939	↓	Urine
beta-Methylstyrene	7.87	119.0856	C ₉ H ₁₀	0.0050	1.5924	↑	Urine
3,4-Diaminopyridine	1.73	110.0714	C ₅ H ₇ N ₃	0.0062	1.5889	↓	Urine
1-Pentyl-3-(1-naphthoyl) indole	7.06	342.1838	C ₂₄ H ₂₃ NO	0.0058	1.5886	↓	Urine
3-Hydroxy-4,5-dimethyl-2(5H)-furanone	6.33	129.0544	C ₆ H ₈ O ₃	0.0071	1.5818	↓	Urine
3-Ethylphenol	8.60	121.0642	C ₈ H ₁₀ O	0.0065	1.5806	↓	Urine
Isovalerylcarnitine	7.17	246.1700	C ₁₂ H ₂₃ NO ₄	0.0061	1.5681	↑	Urine
Pilocarpine	6.51	209.1279	C ₁₁ H ₁₆ N ₂ O ₂	0.0065	1.5664	↓	Urine
Acetamide, N-(3-amino-4-methoxyphenyl)-	6.15	181.0966	C ₉ H ₁₂ N ₂ O ₂	0.0059	1.5648	↓	Urine
Gulonolactone	1.45	177.0392	C ₆ H ₁₀ O ₆	0.0074	1.5629	↑	Urine
Genkwanin	11.08	283.0609	C ₁₆ H ₁₂ O ₅	0.0066	1.5626	↑	Urine
11,12,13-Trinor-1,3,5-bisabolatrien-10-oic acid	9.20	193.1216	C ₁₂ H ₁₆ O ₂	0.0062	1.5596	↓	Urine
N-(2-indol-3-ylethyl)(2-methylpropoxy)carboxamide	2.52	283.1392	C ₁₅ H ₂₀ N ₂ O ₂	0.0088	1.5479	↓	Urine
Homoarecoline	7.64	170.1171	C ₉ H ₁₅ NO ₂	0.0083	1.5447	↓	Urine
JWH-073	6.61	328.1677	C ₂₃ H ₂₁ NO	0.0078	1.5439	↓	Urine

1,2,3,4-Tetrahydroquinoline	8.80	134.0961	C ₉ H ₁₁ N	0.0085	1.5415	↓	Urine
2,3-dihydro-1H-carbazol-4(9H)-one	8.88	186.0908	C ₁₂ H ₁₁ NO	0.0086	1.5411	↓	Urine
Alkhanol	10.36	265.1444	C ₁₅ H ₂₂ O ₄	0.0085	1.5392	↑	Urine
1,3-Benzodioxole	7.32	123.0440	C ₇ H ₆ O ₂	0.0079	1.5339	↑	Urine
Trimethyllysine	1.24	189.1592	C ₉ H ₂₀ N ₂ O ₂	0.0091	1.5335	↓	Urine
Piconol	2.94	110.0600	C ₆ H ₇ NO	0.0090	1.5298	↓	Urine
Lysine	1.76	129.1021	C ₆ H ₁₄ N ₂ O ₂	0.0098	1.5254	↓	Urine
Schinifoline	6.36	280.1647	C ₁₇ H ₂₃ NO	0.0098	1.5244	↓	Urine
4,1-Benzoxazepine	9.93	146.0596	C ₉ H ₇ NO	0.0096	1.5227	↑	Urine
Resacetophenone	10.16	153.0544	C ₈ H ₈ O ₃	0.0102	1.5154	↑	Urine
2-Ethyl-1,2,3,4-tetrahydro-isoquinoline-3-carboxylic acid	10.47	206.1168	C ₁₂ H ₁₅ NO ₂	0.0106	1.5140	↓	Urine
Pirimicarb-desamido	7.00	168.1127	C ₈ H ₁₃ N ₃ O	0.0113	1.5099	↓	Urine
4-Amidinophenyl benzoate	6.88	241.0995	C ₁₄ H ₁₂ N ₂ O ₂	0.0113	1.5066	↓	Urine
(8aR,12S,12aR)-12-hydroxy-4-methyl-4,5,6,7,8,8a,12,12a-octahydro-1H-3-benzoxecine-2,9-dione	10.55	253.1429	C ₁₄ H ₂₀ O ₄	0.0101	1.5065	↓	Urine
Dehydro-piliformic-acid	8.95	213.1112	C ₁₁ H ₁₆ O ₄	0.0102	1.5049	↓	Urine
Isoliquiritigenin	9.40	257.0797	C ₁₅ H ₁₂ O ₄	0.0111	1.5031	↑	Urine

3,5,6-Trichloro-2-pyridinol	10.59	195.9117	C ₅ H ₂ Cl ₃ NO	0.0115	1.5012	↑	Urine
Cinnamic acid	8.72	131.0490	C ₉ H ₈ O ₂	0.0102	1.4998	↓	Urine
DL-Cycloserine	8.72	103.0543	C ₃ H ₆ N ₂ O ₂	0.0102	1.4995	↓	Urine
Theasaponin F1	8.77	365.0687	C ₂₀ H ₁₄ O ₇	0.0104	1.4983	↓	Urine
2-Methylbenzaldehyde	8.41	119.0485	C ₈ H ₈ O	0.0122	1.4973	↓	Urine
(6R,8Z)-6-Hydroxy-3-oxotetradecenoic acid	10.60	255.1597	C ₁₄ H ₂₄ O ₄	0.0113	1.4962	↑	Urine
Fenuron	7.80	182.1285	C ₉ H ₁₂ N ₂ O	0.0129	1.4946	↓	Urine
(S)-Actinidine	7.53	148.1118	C ₁₀ H ₁₃ N	0.0130	1.4905	↓	Urine
2,3-Dimethyl-5-propylpyrazine	6.46	151.1226	C ₉ H ₁₄ N ₂	0.0127	1.4885	↓	Urine
3,5-Dihydroxyphenylvaleric acid sulfate	6.79	289.0383	C ₁₁ H ₁₄ O ₇ S	0.0123	1.4873	↑	Urine
FA 9:2+1O	10.28	169.0858	C ₉ H ₁₄ O ₃	0.0141	1.4872	↑	Urine
Asarone	9.46	209.1164	C ₁₂ H ₁₆ O ₃	0.0123	1.4867	↓	Urine
7-Hydroxy-6-methoxydihydroflavonol	9.51	285.0759	C ₁₆ H ₁₄ O ₅	0.0135	1.4839	↑	Urine
Butyl 4-aminobenzoate	9.08	194.1168	C ₁₁ H ₁₅ NO ₂	0.0134	1.4828	↓	Urine
Pi-Methylimidazoleacetic acid	1.75	141.0656	C ₆ H ₈ N ₂ O ₂	0.0146	1.4807	↓	Urine
Amide	5.99	160.1076	C ₆ H ₁₃ N ₃ O ₂	0.0131	1.4804	↑	Urine
3-Hydroxybenzyl alcohol	6.46	107.0493	C ₇ H ₈ O ₂	0.0125	1.4781	↑	Urine

2-Butyl-4-methylphenol	9.63	163.1114	C ₁₁ H ₁₆ O	0.0141	1.4780	↓	Urine
Acetaminophen glucuronide	6.76	328.1015	C ₁₄ H ₁₇ NO ₈	0.0129	1.4777	↓	Urine
alpha-Methyltryptamine	7.53	175.1224	C ₁₁ H ₁₄ N ₂	0.0143	1.4766	↓	Urine
Fructosyl-lysine	1.27	309.1643	C ₁₂ H ₂₄ N ₂ O ₇	0.0149	1.4686	↓	Urine
Costunolide	8.62	233.1529	C ₁₅ H ₂₀ O ₂	0.0134	1.4636	↓	Urine
Cinchonine	6.01	317.1594	C ₁₉ H ₂₂ N ₂ O	0.0160	1.4594	↓	Urine
Corymbosin	8.99	357.1006	C ₁₉ H ₁₈ O ₇	0.0154	1.4482	↓	Urine
Chelidonine	9.87	354.1326	C ₂₀ H ₁₉ NO ₅	0.0169	1.4480	↓	Urine
4,4alpha,5,6-Tetrahydro-7-methyl-2(3H)-naphthalenone	8.55	163.1115	C ₁₁ H ₁₄ O	0.0186	1.4441	↑	Urine
2-((N,N-diethylglycyl)amino)-3-methylbenzoic acid	8.08	265.1541	C ₁₄ H ₂₀ N ₂ O ₃	0.0169	1.4433	↓	Urine
1,2,5,6-Tetrahydro-4H-pyrrolo(3,2,1-ij)quinolin-4-one	6.51	174.0906	C ₁₁ H ₁₁ NO	0.0184	1.4408	↓	Urine
3-Aminopicolinaldehyde	3.26	123.0553	C ₆ H ₆ N ₂ O	0.0170	1.4395	↑	Urine
Cinnamoylglycine	8.71	204.0654	C ₁₁ H ₁₁ NO ₃	0.0163	1.4298	↓	Urine
2-Acetyl-1,2,3,4-tetrahydroisoquinoline	8.80	176.1068	C ₁₁ H ₁₃ NO	0.0193	1.4287	↓	Urine
9-Decenoylcarnitine	9.52	314.2319	C ₁₇ H ₃₁ NO ₄	0.0214	1.4248	↓	Urine
2,8-Quinolinediol 2-sulfate	6.37	242.0109	C ₉ H ₇ NO ₅ S	0.0193	1.4247	↓	Urine
Estetrol	10.10	303.1594	C ₁₈ H ₂₄ O ₄	0.0216	1.4215	↓	Urine

2-trans,4-cis-Decadienoylcarnitine	9.16	312.2157	C ₁₇ H ₂₉ NO ₄	0.0200	1.4181	↓	Urine
Tetrahydropyridine	1.92	84.0813	C ₅ H ₉ N	0.0208	1.4174	↑	Urine
Liquiritigenin	9.40	255.0659	C ₁₅ H ₁₂ O ₄	0.0206	1.4173	↑	Urine
Succinylcarnitine	1.76	262.1276	C ₁₁ H ₁₉ NO ₆	0.0218	1.4163	↓	Urine
Hexaethylene glycol	6.62	283.1740	C ₁₂ H ₂₆ O ₇	0.0231	1.4078	↑	Urine
Homostachydrine	1.43	158.1171	C ₈ H ₁₅ NO ₂	0.0228	1.4064	↓	Urine
N-Acetylalanine	2.78	130.0492	C ₅ H ₉ NO ₃	0.0229	1.3981	↑	Urine
Methyl trans-p-methoxycinnamate	11.34	193.0853	C ₁₁ H ₁₂ O ₃	0.0238	1.3953	↑	Urine
4-(sulfooxy)-Benzonitrile	7.09	197.9852	C ₇ H ₅ NO ₄ S	0.0246	1.3949	↑	Urine
Melamine	1.64	127.0725	C ₃ H ₆ N ₆	0.0261	1.3934	↑	Urine
Ononetin	10.17	257.0811	C ₁₅ H ₁₄ O ₄	0.0242	1.3909	↑	Urine
2,2-Dimethylglutaric acid	7.83	159.0650	C ₇ H ₁₂ O ₄	0.0249	1.3908	↑	Urine
Indole-3-acetyl-glutamic acid	8.13	305.1121	C ₁₅ H ₁₆ N ₂ O ₅	0.0240	1.3892	↓	Urine
5-Hydroxy-7-methoxy-2-methyl-8-(3-methyl-but-2-enyl)-chromen-4-on	10.13	275.1266	C ₁₆ H ₁₈ O ₄	0.0232	1.3870	↓	Urine
Midazolam	8.84	326.0871	C ₁₈ H ₁₃ ClFN ₃	0.0273	1.3848	↓	Urine
1-(Aminocarbonyl)-L-proline	3.23	159.0761	C ₆ H ₁₀ N ₂ O ₃	0.0271	1.3837	↓	Urine

Phosphoric acid	14.17	96.9680	H ₃ O ₄ P	0.0246	1.3815	↓	Urine
Hydroxyethyl glycine	0.85	118.0495	C ₄ H ₉ NO ₃	0.0254	1.3769	↓	Urine
alpha-(4-Fluorophenyl)-4-(5-fluoro-2-pyrimidinyl)-1-piperazine butanol	7.44	347.1702	C ₁₈ H ₂₂ F ₂ N ₄ O	0.0274	1.3696	↑	Urine
Indole-3-ethanol	8.71	160.0753	C ₁₀ H ₁₁ NO	0.0241	1.3682	↓	Urine
Dinitramine	1.65	321.0821	C ₁₁ H ₁₃ F ₃ N ₄ O ₄	0.0308	1.3590	↓	Urine
3,4,5-trimethoxyphenyl 3,4,5-trimethylpyrazolyl ketone	8.56	327.1299	C ₁₆ H ₂₀ N ₂ O ₄	0.0316	1.3531	↑	Urine
PharmaGSID_47333	12.67	381.2305	C ₂₂ H ₃₀ N ₄ O ₂	0.0329	1.3481	↑	Urine
2,3-Dihydrobenzofuran	8.44	121.0647	C ₈ H ₈ O	0.0346	1.3409	↓	Urine
3-Hydroxyoctadecanoic Acid	12.46	299.2585	C ₁₈ H ₃₆ O ₃	0.0309	1.3340	↑	Urine
1-methyl-4-(6-methylhept-5-en-2-yl)-2,3-dioxabicyclo(2.2.2)oct-5-ene	6.89	201.1632	C ₁₅ H ₂₄ O ₂	0.0337	1.3254	↑	Urine
2,3-Diaminotoluene	6.01	123.0916	C ₇ H ₁₀ N ₂	0.0382	1.3206	↓	Urine
Cortisol	8.61	363.2156	C ₂₁ H ₃₀ O ₅	0.0414	1.3105	↓	Urine
2H-1-Benzopyran-2-one, 7-(ethylamino)-4-methyl-	8.74	204.1013	C ₁₂ H ₁₃ NO ₂	0.0403	1.3100	↓	Urine
Thunberginol A	8.91	271.0595	C ₁₅ H ₁₀ O ₅	0.0393	1.3055	↓	Urine

ethyl 2-(8,8-dimethyl-7,8,9-trihydro-2H,3H-1,4-dioxano(5,6-g)isoquinolin-6-ylidene)acetate	9.96	326.1390	C ₁₇ H ₂₁ NO ₄	0.0421	1.3050	↓	Urine
LPC(20:4)	12.07	544.3381	C ₂₈ H ₅₀ NO ₇ P	0.0421	1.3030	↑	Urine
3alpha-Hydroxyoreadone	9.62	251.1280	C ₁₄ H ₂₀ O ₄	0.0404	1.3006	↓	Urine
(E)-7-(4-methoxy-5-methyl-6-oxopyran-2-yl)-5-methyloct-6-enoic acid	9.61	277.1429	C ₁₆ H ₂₂ O ₅	0.0412	1.2971	↓	Urine
Trachelanthine	6.64	302.1956	C ₁₅ H ₂₇ NO ₅	0.0441	1.2943	↑	Urine
Bavachin	9.77	347.1278	C ₂₀ H ₂₀ O ₄	0.0403	1.2939	↓	Urine
Acedoben	7.57	180.0649	C ₉ H ₉ NO ₃	0.0428	1.2880	↓	Urine
2-amino-4,6-dimethylpyridine-3-carboxylic acid	6.99	167.0812	C ₈ H ₁₀ N ₂ O ₂	0.0448	1.2814	↓	Urine
Isocitric acid	0.97	191.0183	C ₆ H ₈ O ₈	0.0445	1.2794	↑	Urine
Eremofortin A	9.96	305.1393	C ₁₇ H ₂₂ O ₅	0.0435	1.2735	↑	Urine
3-Hydroxytetradecanedioic acid	9.10	273.1699	C ₁₄ H ₂₆ O ₅	0.0420	1.2726	↓	Urine
SDMA	1.65	203.1498	C ₈ H ₁₈ N ₄ O ₂	0.0449	1.2693	↓	Urine
3-Hydroxy-2H-pyran-2-one	5.99	111.0070	C ₅ H ₄ O ₃	0.0457	1.2690	↓	Urine
4-(Formyl(6-Methoxyquinolin-8-yl)Amino)Pentanoic Acid	8.81	303.1307	C ₁₆ H ₁₈ N ₂ O ₄	0.0491	1.2640	↓	Urine

(2E,4E)-N-(2-(4-hydroxyphenyl)ethyl)dodeca-2,4-dienamide	7.97	338.2069	C ₂₀ H ₂₉ NO ₂	0.0454	1.2634	↑	Urine
Indole-3-carboxylic acid	7.81	144.0442	C ₉ H ₇ NO ₂	0.0483	1.2540	↓	Urine
Maltoxazine	9.49	180.1010	C ₁₀ H ₁₃ NO ₂	0.0476	1.2497	↓	Urine
(6E,10E,14E,18E)-2,6,10,15,19,23-hexamethyltetracos-6,10,14,18-tetraene-1,2,3,22,23-pentol	12.96	459.3829	C ₃₀ H ₅₄ O ₅	0.0000	1.9020	↓	Fecal
2-(6,8-dimethyl-4-oxochromen-2-yl)benzoic acid	8.77	295.0960	C ₁₈ H ₁₄ O ₄	0.0000	1.8993	↓	Fecal
3-Hydroxysebacate	7.72	217.1075	C ₁₀ H ₁₈ O ₅	0.0001	1.8919	↓	Fecal
1,2-Cyclohexanedicarboxylic acid, 4-methyl-	8.40	185.0809	C ₉ H ₁₄ O ₄	0.0001	1.8879	↓	Fecal
Deoxycholylisoleucine	11.87	504.3698	C ₃₀ H ₅₁ NO ₅	0.0001	1.8863	↓	Fecal
Isoprostane F2alpha-I	10.27	353.2332	C ₂₀ H ₃₄ O ₅	0.0001	1.8744	↓	Fecal
Geranic acid	12.92	169.1217	C ₁₀ H ₁₆ O ₂	0.0001	1.8692	↓	Fecal
5-(1,2,4a-trimethyl-5-(3-methylbutanoyloxymethyl)-2,3,4,7,8,8a-hexahydronaphthalen-1-yl)-3-methylpentanoic acid	12.22	405.3000	C ₂₅ H ₄₂ O ₄	0.0002	1.8660	↓	Fecal
3-(dimethyl(3-((4R)-4-((3R,7R,12S,17R)-3,7,12-trihydroxy-10,13-dimethylhexadecahydro-1H-	12.40	653.3846	C ₃₂ H ₅₈ N ₂ O ₈ S	0.0001	1.8570	↑	Fecal

cyclopenta(a)phenanthren-17-
yl)pentanamido)propyl)ammonio)-2-hydroxypropane-
1-sulfonate

L-Monomenthyl glutarate	10.89	269.1752	C ₁₅ H ₂₆ O ₄	0.0002	1.8352	↓	Fecal
allo-Protolichesterinic acid	11.99	323.2221	C ₁₉ H ₃₂ O ₄	0.0002	1.8269	↓	Fecal
Coumarin	9.62	147.0438	C ₉ H ₆ O ₂	0.0003	1.8268	↑	Fecal
(R)-2-Hydroxycaprylic acid	8.01	159.1011	C ₈ H ₁₆ O ₃	0.0003	1.8264	↓	Fecal
Cholic acid	10.96	409.2932	C ₂₄ H ₄₀ O ₅	0.0004	1.8152	↓	Fecal
Deoxycholic acid	11.31	391.2843	C ₂₄ H ₄₀ O ₄	0.0003	1.8146	↓	Fecal
Phe-CA	10.98	520.3406	C ₃₃ H ₄₉ NO ₆	0.0004	1.8035	↑	Fecal
2-Carboxy-4-dodecanolide	10.25	241.1439	C ₁₃ H ₂₂ O ₄	0.0008	1.8007	↓	Fecal
Chenodeoxycholic acid	11.80	357.2773	C ₂₄ H ₄₀ O ₄	0.0005	1.7930	↓	Fecal
Coprocholic acid	11.23	449.3252	C ₂₇ H ₄₆ O ₅	0.0004	1.7889	↓	Fecal
Soyasapogenol A	12.92	497.3581	C ₃₀ H ₅₀ O ₄	0.0006	1.7885	↓	Fecal
Dehydromenthofurolactone	7.68	165.0907	C ₁₀ H ₁₂ O ₂	0.0007	1.7862	↓	Fecal
Dihydrocorticosterone	8.62	349.2365	C ₂₁ H ₃₂ O ₄	0.0007	1.7730	↓	Fecal

3,5-dimethyl-7-oxo-6-oxabicyclo(3.2.1)octane-2-carboxylic acid	8.28	199.0962	C ₁₀ H ₁₄ O ₄	0.0010	1.7698	↓	Fecal
Eicosanedioic acid	12.60	341.2693	C ₂₀ H ₃₈ O ₄	0.0008	1.7629	↓	Fecal
Betulonaldehyde	12.66	439.3571	C ₃₀ H ₄₆ O ₂	0.0008	1.7612	↓	Fecal
Sebacic acid	9.25	201.1125	C ₁₀ H ₁₈ O ₄	0.0013	1.7573	↓	Fecal
Radiclonic acid	9.22	343.2621	C ₂₃ H ₄₀ O ₅	0.0013	1.7462	↓	Fecal
Mono(2-ethyl-5-hydroxyhexyl) phthalate	10.29	293.1397	C ₁₆ H ₂₂ O ₅	0.0012	1.7449	↓	Fecal
(-)-Camphanic acid	8.70	197.0808	C ₁₀ H ₁₄ O ₄	0.0012	1.7436	↓	Fecal
Gibberellin A123	9.04	363.1809	C ₂₀ H ₂₈ O ₆	0.0009	1.7425	↓	Fecal
Tetradecanedioic acid	11.03	257.1750	C ₁₄ H ₂₆ O ₄	0.0011	1.7369	↓	Fecal
11'-Carboxy-alpha-chromanol	12.55	417.2998	C ₂₆ H ₄₂ O ₄	0.0012	1.7345	↓	Fecal
2-(4a-Methyl-8-methylidene-4-(3-methylpentanoyloxy)-1,2,3,4,5,6,7,8a-octahydronaphthalen-2-yl)prop-2-enoic acid	7.49	349.2366	C ₂₁ H ₃₂ O ₄	0.0009	1.7328	↓	Fecal
2-acetoxy-4-pentadecylbenzoic acid	11.42	413.2658	C ₂₄ H ₃₈ O ₄	0.0012	1.7325	↓	Fecal
Uvaol	13.06	443.3872	C ₃₀ H ₅₀ O ₂	0.0017	1.7304	↓	Fecal
Dimethyl dimethoxy biphenyl	8.77	241.1226	C ₁₆ H ₁₈ O ₂	0.0015	1.7250	↓	Fecal

6b-Hydroxy-8a-methoxy-7(11)-eremophilen-12,8-olide	9.70	279.1598	C ₁₆ H ₂₄ O ₄	0.0010	1.7237	↑	Fecal
10,11-dihydro-20-dihydroxy-LTB ₄	8.34	369.2271	C ₂₀ H ₃₄ O ₆	0.0016	1.7159	↓	Fecal
(E)-3-(2,3-Dihydroxyphenyl)-2-propenoic acid	7.48	179.0338	C ₉ H ₈ O ₄	0.0020	1.7088	↑	Fecal
Uzarigenin	9.16	375.2519	C ₂₃ H ₃₄ O ₄	0.0019	1.7047	↓	Fecal
Roccellic Acid	12.05	299.2220	C ₁₇ H ₃₂ O ₄	0.0014	1.7028	↓	Fecal
7(14)-Bisabolene-2,3,10,11-tetrol	11.39	271.1906	C ₁₅ H ₂₈ O ₄	0.0014	1.7024	↓	Fecal
12-Ketodeoxycholic acid	11.41	391.2837	C ₂₄ H ₃₈ O ₄	0.0020	1.7006	↓	Fecal
9-acetyl-10,14-dimethyl-20-oxahexacyclo(11.9.0.0<2,10>.0<4,9>.0<14,19>.0<19,21>) docos-17-yl acetate	9.20	429.2990	C ₂₇ H ₄₀ O ₄	0.0029	1.6945	↓	Fecal
Ganolucidic acid A	12.24	499.3052	C ₃₀ H ₄₄ O ₆	0.0022	1.6905	↓	Fecal
NA-135	7.97	369.2272	C ₂₀ H ₃₄ O ₆	0.0021	1.6903	↓	Fecal
9(11)-Dehydromanogenin	8.54	445.2929	C ₂₇ H ₄₀ O ₅	0.0028	1.6887	↓	Fecal
Biliverdin	10.59	583.2549	C ₃₃ H ₃₄ N ₄ O ₆	0.0026	1.6861	↓	Fecal
N-Acetylserine	1.26	192.0235	C ₅ H ₉ NO ₄	0.0026	1.6846	↓	Fecal
2-acetoxy-6-pentadecylbenzoic acid	11.17	413.2659	C ₂₄ H ₃₈ O ₄	0.0022	1.6811	↓	Fecal
Quebrachitol	0.96	193.0705	C ₇ H ₁₄ O ₆	0.0029	1.6808	↑	Fecal

3alpha,7alpha-Dihydroxycoprostanic acid	12.14	433.3311	C ₂₇ H ₄₆ O ₄	0.0025	1.6796	↓	Fecal
Gibberellin A12 aldehyde	10.25	317.2099	C ₂₀ H ₂₈ O ₃	0.0032	1.6761	↓	Fecal
Dehydroepiandrosterone	10.95	289.2153	C ₁₉ H ₂₈ O ₂	0.0027	1.6757	↓	Fecal
3alpha-Hydroxyoreadone	9.63	251.1280	C ₁₄ H ₂₀ O ₄	0.0023	1.6704	↓	Fecal
Chenodeoxycholylleucine	11.87	506.3820	C ₃₀ H ₅₁ NO ₅	0.0038	1.6636	↓	Fecal
(Z)-5-((2R,3S,4S)-4-Hydroxy-2-((E)-3-hydroxyoct-1-enyl)oxan-3-yl)pent-3-enoic acid	10.27	325.2016	C ₁₈ H ₃₀ O ₅	0.0029	1.6634	↓	Fecal
beta-D-Fucose	0.98	163.0596	C ₆ H ₁₂ O ₅	0.0031	1.6596	↑	Fecal
PC(16:1/16:1)	11.84	730.5353	C ₄₀ H ₇₆ NO ₈ P	0.0023	1.6555	↓	Fecal
7-Hydroxy-1,4a-dimethyl-9-oxo-7-propan-2-yl-2,3,4,4b,5,6,10,10a-octahydrophenanthrene-1-carboxylic acid	9.01	317.2100	C ₂₀ H ₃₀ O ₄	0.0044	1.6553	↓	Fecal
5a-Cholestane-3a,7a,12a,23,25-pentol	12.29	451.3418	C ₂₇ H ₄₈ O ₅	0.0042	1.6502	↓	Fecal
L-2,3-Dihydrodipicolinic acid	0.84	168.0262	C ₇ H ₇ NO ₄	0.0035	1.6483	↓	Fecal
19-Hydroxydeoxycorticosterone	11.04	347.2211	C ₂₁ H ₃₀ O ₄	0.0039	1.6461	↓	Fecal
delta-CEHC	9.44	249.1124	C ₁₄ H ₁₈ O ₄	0.0044	1.6445	↓	Fecal

3-(2-(2,3-dihydroxy-5,6,8a-trimethyloctahydro-2H-spiro(naphthalene-1,2'-oxiran)-5-yl)ethyl)-5-hydroxyfuran-2(5H)-one	9.31	365.1960	C ₂₀ H ₃₀ O ₆	0.0045	1.6366	↓	Fecal
4(5)-EpDPE methyl ester	10.48	341.2461	C ₂₃ H ₃₄ O ₃	0.0039	1.6342	↓	Fecal
Tridecanedioic acid	10.64	243.1595	C ₁₃ H ₂₄ O ₄	0.0048	1.6222	↓	Fecal
Adrenic acid	13.14	333.2782	C ₂₂ H ₃₆ O ₂	0.0058	1.6213	↓	Fecal
Glycylglutamine	1.31	204.0976	C ₇ H ₁₃ N ₃ O ₄	0.0040	1.6129	↑	Fecal
7-Ketodeoxycholic acid	9.64	407.2781	C ₂₄ H ₃₈ O ₅	0.0074	1.6098	↓	Fecal
Terpestacin	10.26	403.2833	C ₂₅ H ₃₈ O ₄	0.0062	1.6076	↓	Fecal
Jasmine lactone	8.99	169.1218	C ₁₀ H ₁₆ O ₂	0.0068	1.6054	↓	Fecal
Phenylacetic acid	6.89	135.0435	C ₈ H ₈ O ₂	0.0063	1.6001	↑	Fecal
Indane	11.80	119.0853	C ₉ H ₁₀	0.0068	1.5947	↓	Fecal
1,7-Bis(4-hydroxyphenyl)-3,5-heptanediol	9.47	315.1589	C ₁₉ H ₂₄ O ₄	0.0059	1.5938	↑	Fecal
Cryptotanshinone	6.72	319.1357	C ₁₉ H ₂₀ O ₃	0.0056	1.5873	↑	Fecal
N-Acetylsphinganine	12.81	344.3154	C ₂₀ H ₄₁ NO ₃	0.0085	1.5868	↓	Fecal
Pregnanetriol 3a-O-b-D-glucuronide	8.63	511.2912	C ₂₇ H ₄₄ O ₉	0.0065	1.5792	↓	Fecal

N-(1-(2-Methylbenzyl)-1H-Pyrazol-4-yl)-3,4-Dihydroisoquinoline-2(1H)-Carbothioamide	6.96	363.1614	C ₂₁ H ₂₂ N ₄ S	0.0065	1.5785	↑	Fecal
(2E,6E,10E)-4-hydroxy-3-(3,7,11,15-tetramethyl-hexadeca-2,6,10,14-tetraenyl)-benzoic acid	11.64	411.2888	C ₂₇ H ₃₈ O ₃	0.0080	1.5780	↓	Fecal
Dodecanedioic acid	10.19	231.1583	C ₁₂ H ₂₂ O ₄	0.0078	1.5693	↓	Fecal
Cediranib	7.40	451.2131	C ₂₅ H ₂₇ FN ₄ O ₃	0.0075	1.5648	↑	Fecal
Dopaminechrome	6.42	148.0388	C ₈ H ₇ NO ₂	0.0073	1.5583	↓	Fecal
4-Methylene-2-octyl-5-oxotetrahydrofuran-3-carboxylic acid	10.44	253.1444	C ₁₄ H ₂₂ O ₄	0.0064	1.5575	↓	Fecal
16-HDoHE	12.07	343.2271	C ₂₂ H ₃₂ O ₃	0.0108	1.5536	↑	Fecal
Ciprostene	12.17	363.2531	C ₂₂ H ₃₆ O ₄	0.0074	1.5484	↓	Fecal
Bisnorcholic acid	9.37	379.2474	C ₂₂ H ₃₆ O ₅	0.0090	1.5479	↓	Fecal
Altenuene	6.79	291.0905	C ₁₅ H ₁₆ O ₆	0.0098	1.5463	↓	Fecal
Carboxyethyl-hydroxychroman	9.22	221.0806	C ₁₂ H ₁₄ O ₄	0.0109	1.5432	↓	Fecal
3-(sec-butyl)-2-hydroxy-3H-benzo(e)(1,4)diazepin-5(4H)-one	6.78	233.1283	C ₁₃ H ₁₆ N ₂ O ₂	0.0108	1.5402	↓	Fecal
Cholyllysine	8.95	537.3890	C ₃₀ H ₅₂ N ₂ O ₆	0.0108	1.5394	↑	Fecal

4-(3-Pyridyl)-3-butenic acid	7.44	162.0546	C ₉ H ₉ NO ₂	0.0097	1.5382	↓	Fecal
Cartorimine	7.01	289.0707	C ₁₅ H ₁₄ O ₆	0.0099	1.5379	↓	Fecal
Testosterone	11.54	289.2152	C ₁₉ H ₂₈ O ₂	0.0089	1.5367	↓	Fecal
1,10-Epoxygermacrone	12.26	235.1688	C ₁₅ H ₂₂ O ₂	0.0098	1.5331	↓	Fecal
5'-Amino-5'-deoxyadenosine	7.75	267.1191	C ₁₀ H ₁₄ N ₆ O ₃	0.0092	1.5312	↓	Fecal
Zerumbone	11.30	201.1631	C ₁₅ H ₂₂ O	0.0099	1.5306	↓	Fecal
N-Acetylalanine	2.78	130.0495	C ₅ H ₉ NO ₃	0.0106	1.5303	↑	Fecal
Lumichrome	8.73	243.0873	C ₁₂ H ₁₀ N ₄ O ₂	0.0122	1.5281	↓	Fecal
3-(2-Furanyl)-2-propenal	7.98	121.0280	C ₇ H ₆ O ₂	0.0077	1.5276	↓	Fecal
3-(5-Acetyl-2-furyl)-5-methoxy-2-benzofuran-1(3H)-one	9.07	271.0605	C ₁₅ H ₁₂ O ₅	0.0116	1.5235	↓	Fecal
Ceanothic acid	12.08	485.3255	C ₃₀ H ₄₆ O ₅	0.0099	1.5188	↑	Fecal
(6E,8E,10R,12Z)-10-Hydroxy-3-oxooctadecatrienoic acid	11.71	307.1917	C ₁₈ H ₂₈ O ₄	0.0103	1.5157	↓	Fecal
Acaranoic Acid	9.34	297.2062	C ₁₇ H ₃₀ O ₄	0.0110	1.5102	↓	Fecal
N-Acetyltyrosine	6.78	222.0760	C ₁₁ H ₁₃ NO ₄	0.0129	1.5071	↑	Fecal
(10betaH,11xi)-11-Hydroxy-13-nor-6-eremophilen-8-one	12.13	221.1537	C ₁₄ H ₂₂ O ₂	0.0129	1.5047	↑	Fecal
Fenofibric acid	11.47	319.0724	C ₁₇ H ₁₅ ClO ₄	0.0129	1.5041	↑	Fecal
Valyllysine	1.36	246.1808	C ₁₁ H ₂₃ N ₃ O ₃	0.0142	1.5035	↑	Fecal

6,10a-Dihydroxy-4-(hydroxymethyl)-4,7,11b-trimethyl-1,2,3,4a,5,6,6a,7,11,11a-decahydronaphtho(2,1-)(1)benzouran-9-one	10.21	349.2021	C ₂₀ H ₃₀ O ₅	0.0150	1.5017	↓	Fecal
P-Menthatriene	7.74	135.1165	C ₁₀ H ₁₄	0.0137	1.4970	↓	Fecal
Indole-3-acetyl-valine	7.41	273.1239	C ₁₅ H ₁₈ N ₂ O ₃	0.0119	1.4957	↓	Fecal
Toxin T2 tetrol	8.49	297.1332	C ₁₅ H ₂₂ O ₆	0.0130	1.4919	↑	Fecal
2-(3-methoxy-4-(sulfooxy)phenyl)acetic acid	1.97	261.0067	C ₉ H ₁₀ O ₇ S	0.0122	1.4869	↑	Fecal
Citrinin hydrate	6.49	267.0901	C ₁₃ H ₁₆ O ₆	0.0189	1.4847	↓	Fecal
Pinocarvyl acetate	7.74	195.1377	C ₁₂ H ₁₈ O ₂	0.0158	1.4793	↓	Fecal
Isobutyryl-Carnitine	2.92	232.1541	C ₁₁ H ₂₁ NO ₄	0.0150	1.4741	↓	Fecal
3,4,5-Trimethylbenzaldehyde	7.47	149.0957	C ₁₀ H ₁₂ O	0.0162	1.4738	↓	Fecal
(2E,8E)-10-hydroxydeca-2,8-dien-4-ynoylcarnitine	8.43	324.1798	C ₁₇ H ₂₅ NO ₅	0.0138	1.4698	↑	Fecal
beta-Methylstyrene	7.75	119.0855	C ₉ H ₁₀	0.0193	1.4690	↓	Fecal
Am-3102	13.11	340.3197	C ₂₁ H ₄₁ NO ₂	0.0195	1.4684	↓	Fecal
Ganolucidic acid E	12.00	483.3111	C ₃₀ H ₄₄ O ₅	0.0127	1.4667	↑	Fecal
Deoxycholylyphenylalanine	11.92	540.3671	C ₃₃ H ₄₉ NO ₅	0.0190	1.4651	↓	Fecal
Heptadecanoyl Ethanolamide	13.36	314.3044	C ₁₉ H ₃₉ NO ₂	0.0178	1.4602	↓	Fecal

3,6,9,12,15,18,21,24,27,30-Decaoxadotriacontane-1,32-diol	7.65	503.3050	C ₂₂ H ₄₆ O ₁₂	0.0155	1.4600	↑	Fecal
2,8-Dihydroxyquinoline	6.42	160.0388	C ₉ H ₇ NO ₂	0.0171	1.4545	↓	Fecal
(Z)-7-((1R,4S,5R,6S)-5-((E,3R)-3-Hydroxyoct-1-enyl)-2-oxabicyclo(2.2.1)heptan-6-yl)hept-5-enoic acid	11.93	349.2376	C ₂₁ H ₃₄ O ₄	0.0139	1.4535	↓	Fecal
L↑-20(29)-ene-27,28-dioic acid, 3-oxo-, (5xi,9xi,18xi)-	10.87	485.3255	C ₃₀ H ₄₄ O ₅	0.0150	1.4498	↑	Fecal
8-Hydroxy-9,10-epoxystearic acid	12.28	315.2525	C ₁₈ H ₃₄ O ₄	0.0188	1.4479	↓	Fecal
Isoliquiritigenin	7.39	255.0654	C ₁₅ H ₁₂ O ₄	0.0239	1.4417	↑	Fecal
Thr-Pro	1.74	217.1177	C ₉ H ₁₆ N ₂ O ₄	0.0172	1.4399	↑	Fecal
3,14-Dihydroxy-11,13-dihydrocostunolide	10.02	265.1445	C ₁₅ H ₂₂ O ₄	0.0238	1.4389	↑	Fecal
Arctigenin	10.50	371.1523	C ₂₁ H ₂₄ O ₆	0.0167	1.4374	↓	Fecal
(6)-Gingerdione	10.47	291.1600	C ₁₇ H ₂₄ O ₄	0.0188	1.4297	↓	Fecal
2-Phenylpyridine	6.93	156.0805	C ₁₁ H ₉ N	0.0222	1.4293	↓	Fecal
Methoxyphenylacetic acid	6.94	165.0545	C ₉ H ₁₀ O ₃	0.0209	1.4215	↑	Fecal
Menthol-glucoronide	9.23	315.1801	C ₁₆ H ₂₈ O ₆	0.0239	1.4196	↓	Fecal
1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-9-oxo-	7.22	337.1753	C ₂₀ H ₂₆ O ₃	0.0228	1.4180	↓	Fecal

5-Hydroxyferulic acid	6.94	209.0441	C ₁₀ H ₁₀ O ₅	0.0215	1.4177	↑	Fecal
3,6,9,12,15,18,21,24,27-Nonaoxanonacosane-1,29-diol	7.49	481.2600	C ₂₀ H ₄₂ O ₁₁	0.0204	1.4159	↑	Fecal
1-methyl-4-(6-methylhept-5-en-2-yl)-2,3-dioxabicyclo(2.2.2)oct-5-ene	7.32	201.1637	C ₁₅ H ₂₄ O ₂	0.0200	1.4147	↑	Fecal
Dihydroferulic acid	7.30	195.0653	C ₁₀ H ₁₂ O ₄	0.0236	1.4115	↑	Fecal
6-Prenylpinocembrin	10.96	323.1288	C ₂₀ H ₂₀ O ₄	0.0260	1.4106	↑	Fecal
Oseltamivir acid	6.93	285.1798	C ₁₄ H ₂₄ N ₂ O ₄	0.0223	1.4097	↓	Fecal
1,2,4-Tris(methylene)cyclohexane	7.75	121.1010	C ₉ H ₁₂	0.0230	1.4092	↓	Fecal
Clozapine	7.08	327.1365	C ₁₈ H ₁₉ ClN ₄	0.0255	1.4077	↓	Fecal
Brefeldin A	10.04	263.1628	C ₁₆ H ₂₄ O ₄	0.0256	1.4014	↓	Fecal
Myristoylglycine	12.27	284.2219	C ₁₆ H ₃₁ NO ₃	0.0299	1.3989	↑	Fecal
Equilin	12.26	267.1417	C ₁₈ H ₂₀ O ₂	0.0266	1.3981	↓	Fecal
9-hydroxy-5b,8,11a-trimethyl-1-prop-1-en-2-yl-1,2,3,4,5,6,7,7a,9,10,11,11b,12,13,13a,13b-hexadecahydrocyclopenta(a)chrysene-3a,5a,8-tricarboxylic acid	10.52	515.3034	C ₃₀ H ₄₄ O ₇	0.0283	1.3961	↓	Fecal

2,6-bis((4-methoxyphenyl)methylene)-4-ethylcyclohexan-1-one	6.79	363.1909	C ₂₄ H ₂₆ O ₃	0.0254	1.3948	↓	Fecal
5,7-Dimethoxy-4'-hydroxyflavanone	8.25	299.0954	C ₁₇ H ₁₆ O ₅	0.0251	1.3930	↓	Fecal
OPFC-perfluoroalkyl_sulfate	7.21	224.9857	C ₄ H ₆ F ₄ O ₄ S	0.0239	1.3883	↑	Fecal
5,6-Dihydroxyprostaglandin F1a	9.74	387.2380	C ₂₀ H ₃₆ O ₇	0.0216	1.3875	↓	Fecal
Corynoxine	8.49	383.1981	C ₂₂ H ₂₆ N ₂ O ₄	0.0262	1.3861	↓	Fecal
1H-3,9a-Methanocyclopent(c)oxocin-4-carboxylic acid, octahydro-4-hydroxy-7-(2-hydroxy-1-methylethylidene)-, (7E)-	9.44	281.1390	C ₁₅ H ₂₂ O ₅	0.0289	1.3809	↓	Fecal
3b,4b,7a,12a-Tetrahydroxy-5b-cholanoic acid	9.21	423.2755	C ₂₄ H ₄₀ O ₆	0.0245	1.3778	↓	Fecal
Epicatechin	6.87	289.0745	C ₁₅ H ₁₄ O ₆	0.0324	1.3764	↓	Fecal
(Z)-2,4-Dihydroxy-6-(8-pentadecenyl)benzoic acid	12.15	361.2374	C ₂₂ H ₃₄ O ₄	0.0294	1.3720	↓	Fecal
4,4'-Dimethoxychalcone	9.68	269.1165	C ₁₇ H ₁₆ O ₃	0.0286	1.3696	↓	Fecal
(Z)-7-((1R,2R,3R,5S)-2-(1,2-Dihydroxy-3-oxooctyl)-3,5-dihydroxycyclopentyl)hept-5-enoic acid	7.11	385.2225	C ₂₀ H ₃₄ O ₇	0.0289	1.3694	↓	Fecal
5-hydroxycalamenene	8.68	219.1740	C ₁₅ H ₂₂ O	0.0271	1.3681	↑	Fecal
Sclareolide	12.23	251.2001	C ₁₆ H ₂₆ O ₂	0.0271	1.3647	↓	Fecal

Bilirubin	12.86	585.2709	C ₃₃ H ₃₆ N ₄ O ₆	0.0340	1.3626	↓	Fecal
Tropisetron	7.88	285.1629	C ₁₇ H ₂₀ N ₂ O ₂	0.0291	1.3623	↓	Fecal
Valerylcarnitine	7.51	246.1698	C ₁₂ H ₂₃ NO ₄	0.0300	1.3601	↑	Fecal
13-Hydroxyl↑anine	7.61	265.1907	C ₁₅ H ₂₄ N ₂ O ₂	0.0323	1.3565	↓	Fecal
Lysine	7.82	147.1124	C ₆ H ₁₄ N ₂ O ₂	0.0366	1.3537	↓	Fecal
Monoketocholic acid	10.52	421.2592	C ₂₄ H ₃₈ O ₆	0.0353	1.3532	↓	Fecal
Tenuazonic acid	6.75	198.1121	C ₁₀ H ₁₅ NO ₃	0.0354	1.3528	↓	Fecal
Prostaglandin F1a	10.97	355.2491	C ₂₀ H ₃₆ O ₅	0.0291	1.3524	↓	Fecal
Nootkatone	10.30	201.1630	C ₁₅ H ₂₂ O	0.0311	1.3518	↑	Fecal
Sinapaldehyde	9.99	209.0804	C ₁₁ H ₁₂ O ₄	0.0289	1.3513	↑	Fecal
6,7-Dimethoxy-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid	4.14	238.1067	C ₁₂ H ₁₅ NO ₄	0.0326	1.3489	↓	Fecal
Cholytyrosine	10.17	570.3434	C ₃₃ H ₄₉ NO ₇	0.0362	1.3478	↑	Fecal
Hydroxy Tyrosol -Acetate	6.35	226.1070	C ₁₁ H ₁₅ NO ₄	0.0339	1.3455	↓	Fecal
ethyl (2E)-3-(4-(diethylamino)phenyl)-2-cyanoprop-2-enoate	8.19	295.1429	C ₁₆ H ₂₀ N ₂ O ₂	0.0338	1.3435	↓	Fecal
Ferulic acid	9.22	177.0536	C ₁₀ H ₁₀ O ₄	0.0331	1.3435	↑	Fecal

3,7,11-Trimethyldodeca-2,6,10-trienoic acid	12.08	237.1842	C ₁₅ H ₂₄ O ₂	0.0296	1.3432	↓	Fecal
ent-1(10)-Halimene-15,19-dioic acid	11.65	335.2222	C ₂₀ H ₃₂ O ₄	0.0265	1.3427	↓	Fecal
4-methoxyquinoline-2-carboxylic acid	6.62	204.0652	C ₁₁ H ₉ NO ₃	0.0358	1.3408	↓	Fecal
Isoferulic acid	9.99	177.0541	C ₁₀ H ₁₀ O ₄	0.0316	1.3368	↑	Fecal
Glu-CA	9.67	536.3225	C ₂₉ H ₄₇ NO ₈	0.0430	1.3360	↑	Fecal
3-Hydroxymonoethylglycinexylidide	6.27	223.1432	C ₁₂ H ₁₈ N ₂ O ₂	0.0390	1.3333	↓	Fecal
5-((1-Iminoethyl)amino)-2-aminopentanoic acid	5.19	174.1232	C ₇ H ₁₅ N ₃ O ₂	0.0359	1.3309	↓	Fecal
Polyporusterone D	11.44	459.3102	C ₂₈ H ₄₄ O ₅	0.0340	1.3278	↓	Fecal
Fraxinellone	8.02	233.1164	C ₁₄ H ₁₆ O ₃	0.0348	1.3273	↑	Fecal
Suberic acid	8.15	157.0854	C ₈ H ₁₄ O ₄	0.0459	1.3238	↓	Fecal
Riboflavin	7.22	421.1363	C ₁₇ H ₂₀ N ₄ O ₆	0.0419	1.3177	↑	Fecal
Cyproterone	6.00	373.1614	C ₂₂ H ₂₇ ClO ₃	0.0366	1.3159	↓	Fecal
Mannitol	13.49	183.0857	C ₆ H ₁₄ O ₆	0.0360	1.3121	↓	Fecal
4,4alpha,5,6-Tetrahydro-7-methyl-2(3H)-naphthalenone	7.75	163.1114	C ₁₁ H ₁₄ O	0.0396	1.3119	↓	Fecal
Curcumol	10.30	219.1741	C ₁₅ H ₂₄ O ₂	0.0370	1.3094	↑	Fecal
(2E)-2-Propylpent-2-Enoylcarnitine	6.68	286.2009	C ₁₅ H ₂₇ NO ₄	0.0398	1.3060	↑	Fecal
Triptophenolide	7.11	335.1587	C ₂₀ H ₂₄ O ₃	0.0431	1.3051	↓	Fecal

PC(18:2/18:2)	12.27	782.5694	C ₄₄ H ₈₀ NO ₈ P	0.0386	1.3032	↓	Fecal
Chenodeoxycholyphenylalanine	11.90	538.3544	C ₃₃ H ₄₉ NO ₅	0.0446	1.3000	↓	Fecal
N,N-Dimethylarginine	1.61	203.1496	C ₈ H ₁₈ N ₄ O ₂	0.0462	1.2994	↑	Fecal
Estriol	6.95	311.1587	C ₁₈ H ₂₄ O ₃	0.0464	1.2894	↓	Fecal
Dihydrotestosterone	6.91	313.2107	C ₁₉ H ₃₀ O ₂	0.0467	1.2877	↓	Fecal
Asiatic acid	12.15	533.3482	C ₃₀ H ₄₈ O ₅	0.0498	1.2864	↑	Fecal
Sarsasapogenin	12.41	399.3246	C ₂₇ H ₄₄ O ₃	0.0395	1.2862	↓	Fecal
12-Hydroxy-13-(hydroxymethyl)-3,5,7-trimethyl-2,4-tetradecadienedioic acid	9.98	325.1996	C ₁₈ H ₃₀ O ₆	0.0483	1.2847	↓	Fecal
Kynurenic acid	8.42	188.0340	C ₁₀ H ₇ NO ₃	0.0448	1.2807	↓	Fecal
2,3-Dinor-TXB2	9.74	341.1961	C ₁₈ H ₃₀ O ₆	0.0475	1.2804	↓	Fecal
3-O-Acetyl-16alpha-hydroxytrametenolic acid	12.63	513.3561	C ₃₂ H ₅₀ O ₅	0.0473	1.2779	↑	Fecal
(3E,5Z)-1,3,5-Heptatriene	10.95	95.0856	C ₇ H ₁₀	0.0445	1.2753	↓	Fecal
4-cholesten	12.30	431.3147	C ₂₇ H ₄₄ O ₄	0.0415	1.2752	↓	Fecal
PC(16:0/18:1)	12.27	760.5839	C ₄₂ H ₈₂ NO ₈ P	0.0440	1.2749	↓	Fecal
3, 5-Tetradeciencarnitine	10.53	368.2785	C ₂₁ H ₃₇ NO ₄	0.0464	1.2732	↑	Fecal
Fructose lactate	0.96	267.0713	C ₉ H ₁₆ O ₉	0.0493	1.2687	↑	Fecal

Medicagenic acid	11.32	501.3219	C ₃₀ H ₄₆ O ₆	0.0439	1.2648	↓	Fecal
6-Hydroxypentadecanedioic acid	9.63	287.1864	C ₁₅ H ₂₈ O ₅	0.0492	1.2640	↓	Fecal
Nadolol	7.50	310.2004	C ₁₇ H ₂₇ NO ₄	0.0460	1.2631	↑	Fecal
6-((2E,4E)-4,6-Dimethyl-2,4-octadienoyl)-2,3-dihydroxy-2-methylcyclohexanone	7.75	317.1737	C ₁₇ H ₂₆ O ₄	0.0484	1.2597	↑	Fecal
Deferiprone	2.01	140.0705	C ₇ H ₉ NO ₂	0.0486	1.2511	↓	Fecal
2,3-Dimethyl-2-cyclohexen-1-one	12.86	125.0960	C ₈ H ₁₂ O	0.0497	1.2483	↓	Fecal

ZD, Fuling Zexie Decoction without Poria; HFD, high-fat diet.

Supplementary Table 5 The metabolites exclusively-regulated by FZD

Metabolite name	P	VIP	Formula	NC <i>vs</i> HFD	FZD <i>vs</i> HFD	Sample
PR(16:0/18:2)	0.022	1.560	C ₄₂ H ₈₀ NO ₈ P	↓	↓	Serum
Vaccenic acid	0.024	1.478	C ₁₈ H ₃₄ O ₂	↓	↓	Serum
D-Lysine	0.016	1.471	C ₆ H ₁₄ N ₂ O ₂	↓	↓	Serum
Pipecolic acid	0.018	1.444	C ₆ H ₁₁ NO ₂	↓	↓	Serum
N-epsilon-Formyl-L-lysine	0.000	1.903	C ₇ H ₁₄ N ₂ O ₃	↑	↑	Serum
14,15-EpETE	0.002	1.750	C ₂₀ H ₃₀ O ₃	↑	↑	Serum
Eudesmin	0.004	1.685	C ₂₂ H ₂₆ O ₆	↑	↑	Serum
Epoprostenol	0.010	1.597	C ₂₀ H ₃₂ O ₅	↑	↑	Serum
10-Hydroxydecanoate	0.009	1.571	C ₁₀ H ₂₀ O ₃	↑	↑	Serum
5-Dihydroxyhept-6-enoic acid	0.007	1.563	C ₇ H ₁₂ O ₄	↑	↑	Serum
cis-Dihydrocarvone	0.008	1.523	C ₁₀ H ₁₆ O	↑	↑	Serum
3-Methylene-indolenine	0.017	1.492	C ₉ H ₇ N	↑	↑	Serum
3-(Indol-3-yl)propionic acid	0.019	1.473	C ₁₁ H ₁₁ NO ₂	↑	↑	Serum
Estrone glucuronide	0.018	1.470	C ₂₄ H ₃₀ O ₈	↑	↑	Serum
Butyrylcarnitine	0.023	1.459	C ₁₁ H ₂₁ NO ₄	↑	↑	Serum
3-Hydroxycapric acid	0.023	1.414	C ₁₀ H ₂₀ O ₃	↑	↑	Serum
Cyclo(Pro-Leu)	0.029	1.376	C ₁₁ H ₁₈ N ₂ O ₂	↑	↑	Serum
Acetic acid, 2-((3-sulfooxybenzoyl)amino)-	0.028	1.366	C ₉ H ₉ NO ₇ S	↑	↑	Serum
alpha-Carboxy-delta-nonalactone	0.034	1.350	C ₁₀ H ₁₆ O ₄	↑	↑	Serum
2,6-Diamino-9-(2-hydroxyethoxymethyl)purine	0.036	1.331	C ₈ H ₁₂ N ₆ O ₂	↑	↑	Serum
gamma-Guanidinobutyric acid	0.038	1.252	C ₅ H ₁₁ N ₃ O ₂	↑	↑	Serum
Perfluorooctanesulfonic Acid	0.000	1.995	C ₈ HF ₁₇ O ₃ S	↓	↓	Liver
8,12-Octadecadienoic acid	0.000	1.844	C ₁₈ H ₃₂ O ₂	↓	↓	Liver
Octadecylamine	0.002	1.726	C ₁₈ H ₃₉ N	↓	↓	Liver
Vaccenic acid	0.014	1.515	C ₁₈ H ₃₄ O ₂	↓	↓	Liver

GABA	0.015	1.477	C ₄ H ₉ NO ₂	↓	↓	Liver
5-octenoylglycine	0.022	1.433	C ₁₀ H ₁₇ NO ₃	↓	↓	Liver
Epigallocatechin	0.046	1.314	C ₁₅ H ₁₄ O ₇	↓	↓	Liver
(+)-Cycloolivil	0.002	1.658	C ₂₀ H ₂₄ O ₇	↑	↑	Liver
LPR(16:0)	0.013	1.536	C ₂₄ H ₅₀ NO ₇ P	↑	↑	Liver
Heliotrine N-oxide	0.017	1.471	C ₁₆ H ₂₇ NO ₆	↑	↑	Liver
(2E)-2-Propylpent-2-Enoylcarnitine	0.025	1.391	C ₁₅ H ₂₇ NO ₄	↑	↑	Liver
3-Hydroxycapric acid	0.030	1.331	C ₁₀ H ₂₀ O ₃	↑	↑	Liver
(4E,7E)-3-Hydroxydeca-4,7-dienoylcarnitine	0.000	1.857	C ₁₇ H ₂₉ NO ₅	↓	↓	Urine
Carboxyethyl-hydroxychroman	0.000	1.836	C ₁₂ H ₁₄ O ₄	↓	↓	Urine
Trinexapac	0.000	1.815	C ₁₁ H ₁₂ O ₅	↓	↓	Urine
3,4-Methylenepimelic acid	0.000	1.784	C ₉ H ₁₂ O ₄	↓	↓	Urine
Dibutylphthalic acid	0.000	1.744	C ₁₆ H ₂₂ O ₄	↓	↓	Urine
4-O-Methylvanillin	0.000	1.740	C ₉ H ₁₀ O ₃	↓	↓	Urine
N-(1-Adamantylmethyl)-3,4,5-Trimethoxybenzamide	0.001	1.705	C ₂₁ H ₂₉ NO ₄	↓	↓	Urine
Menthol-glucoronide	0.001	1.703	C ₁₆ H ₂₈ O ₆	↓	↓	Urine
Aspergillimide	0.001	1.699	C ₂₀ H ₂₉ N ₃ O ₃	↓	↓	Urine
Methyl neopentyl phthalic acid	0.001	1.673	C ₁₄ H ₁₈ O ₄	↓	↓	Urine
1-Naphthalenecarboxylic acid, 5-[(3E)-4-carboxy-3-methyl-3-buten-1-yl]decahydro-3-hydroxy-1,4a-dimethyl-6-methylene-3,5-dimethyl-7-oxo-6-oxabicyclo[3.2.1]octane-2-carboxylic acid	0.003	1.626	C ₂₀ H ₃₀ O ₅	↓	↓	Urine
Glutamine	0.004	1.601	C ₅ H ₁₀ N ₂ O ₃	↓	↓	Urine

2-(3-carboxypropanoylamino)hexanoic acid	0.005	1.570	C ₁₀ H ₁₇ NO ₅	↓	↓	Urine
6-Keto-decanoylcarnitine	0.008	1.491	C ₁₇ H ₃₁ NO ₅	↓	↓	Urine
Phenylethylmalonamide	0.011	1.488	C ₁₁ H ₁₄ N ₂ O ₂	↓	↓	Urine
Chenodeoxycholic acid sulfate	0.012	1.476	C ₂₄ H ₄₀ O ₇ S	↓	↓	Urine
2-(6-Hydroxy-3,8-dimethyl-2-oxo-1,2,4,5,6,7,8,8a-octahydro-5-azulenyl)acrylic acid	0.012	1.471	C ₁₅ H ₂₀ O ₄	↓	↓	Urine
Aspartyl-proline	0.010	1.455	C ₉ H ₁₄ N ₂ O ₅	↓	↓	Urine
Mannitol	0.014	1.434	C ₆ H ₁₄ O ₆	↓	↓	Urine
Cholic acid 7-sulfate	0.020	1.389	C ₂₄ H ₄₀ O ₈ S	↓	↓	Urine
Deoxycarnitine	0.028	1.355	C ₇ H ₁₅ NO ₂	↓	↓	Urine
3-Methoxyphenylacetic acid	0.028	1.338	C ₉ H ₁₀ O ₃	↓	↓	Urine
N-Acetylserine	0.028	1.328	C ₅ H ₉ NO ₄	↓	↓	Urine
Acetylglycine	0.029	1.299	C ₄ H ₇ NO ₃	↓	↓	Urine
5-(3',5')-Dihydroxyphenyl-gamma-valerolactone	0.000	1.803	C ₁₁ H ₁₄ O ₄	↑	↑	Urine
1,2,3,4-Tetrahydro-beta-carboline-3-carboxylic acid	0.001	1.722	C ₁₂ H ₁₂ N ₂ O ₂	↑	↑	Urine
N-Decanoylglycine	0.001	1.668	C ₁₂ H ₂₃ NO ₃	↑	↑	Urine
3-Oxodecanoic acid	0.004	1.589	C ₁₀ H ₁₈ O ₃	↑	↑	Urine
1,2:3,4-Di-O-isopropylidene-D-galactopyranose	0.003	1.582	C ₁₂ H ₂₀ O ₆	↑	↑	Urine
Phytosphingosine	0.009	1.515	C ₁₈ H ₃₉ NO ₃	↑	↑	Urine
Dehydro-P-Cymene	0.016	1.449	C ₁₀ H ₁₂	↑	↑	Urine
Isoimperatorin	0.015	1.440	C ₁₆ H ₁₄ O ₄	↑	↑	Urine
1H-Pyrrole-2-carboxaldehyde	0.021	1.406	C ₅ H ₅ NO	↑	↑	Urine
2,3,5-Trimethylphenol	0.029	1.374	C ₉ H ₁₂ O	↑	↑	Urine

N-Nonanoylglycine	0.027	1.365	C ₁₁ H ₂₁ NO ₃	↑	↑	Urine
(1S,2R,4aR,8aR)-1-Acetoxy-7-isopropylidene-1,4a-dimethyl-6-oxodecahydro-2-naphthalenyl 2,3-dimethyl-2-oxiranecarboxylate	0.032	1.348	C ₂₂ H ₃₂ O ₆	↑	↑	Urine
p-tert-Butyl catechol	0.032	1.346	C ₁₀ H ₁₄ O ₂	↑	↑	Urine
Monomethyl sebacate	0.038	1.313	C ₁₁ H ₂₀ O ₄	↑	↑	Urine
7-Hydroxypestalotin	0.037	1.307	C ₁₁ H ₁₈ O ₅	↑	↑	Urine
Intermedine N-oxide	0.045	1.281	C ₁₅ H ₂₅ NO ₆	↑	↑	Urine
1-methyl-4-methylidene-7-(propan-2-yl)-1,2,3,3a,4,5,6,8a-octahydroazulen-1-ol	0.041	1.239	C ₁₅ H ₂₄ O	↑	↑	Urine
Arabinosylhypoxanthine	0.049	1.209	C ₁₀ H ₁₂ N ₄ O ₅	↑	↑	Urine
Wallemine	0.000	1.854	C ₁₅ H ₂₄ O ₃	↓	↓	Fecal
1,4-Benzodioxin-2(3H)-one	0.000	1.777	C ₈ H ₆ O ₃	↓	↓	Fecal
PI(16:0/18:2)	0.000	1.744	C ₄₃ H ₇₉ O ₁₃ P	↓	↓	Fecal
Muricholic Acid	0.000	1.701	C ₂₄ H ₄₀ O ₅	↓	↓	Fecal
Abscisic acid	0.001	1.648	C ₁₅ H ₂₀ O ₄	↓	↓	Fecal
5-Hydroxyindole	0.001	1.644	C ₈ H ₇ NO	↓	↓	Fecal
Indole-3-acetyl-leucine	0.001	1.634	C ₁₆ H ₂₀ N ₂ O ₃	↓	↓	Fecal
Ursonic acid	0.001	1.621	C ₃₀ H ₄₆ O ₃	↓	↓	Fecal
Palmatine	0.002	1.600	C ₂₁ H ₂₂ NO ₄ ⁺	↓	↓	Fecal
Magnoflorine	0.003	1.580	C ₂₀ H ₂₄ NO ₄ ⁺	↓	↓	Fecal
1-allyl-2-hydroxy-7,8,9,10-tetrahydroazepino[2,1-b]quinazolin-12(6H)-one	0.004	1.561	C ₁₆ H ₁₈ N ₂ O ₂	↓	↓	Fecal
Sapogenins	0.004	1.531	C ₂₇ H ₄₄ O ₂	↓	↓	Fecal
N-Acetylornithine	0.006	1.507	C ₇ H ₁₄ N ₂ O ₃	↓	↓	Fecal

Mevinolinic acid	0.006	1.491	C ₂₄ H ₃₈ O ₆	↓	↓	Fecal
O-Desmethyl tramadol	0.010	1.474	C ₁₅ H ₂₃ NO ₂	↓	↓	Fecal
(2E)-3-(1-ethyl-3-methylpyrazol-4-yl)-1-(4-hydroxyphenyl)prop-2-en-1-one	0.011	1.462	C ₁₅ H ₁₆ N ₂ O ₂	↓	↓	Fecal
5b-Cyprinol sulfate	0.018	1.421	C ₂₇ H ₄₈ O ₈ S	↓	↓	Fecal
Piperine	0.022	1.391	C ₁₇ H ₁₉ NO ₃	↓	↓	Fecal
Phenylalanine butyl ester	0.020	1.385	C ₁₃ H ₁₉ NO ₂	↓	↓	Fecal
1-O-Acetyllycorine	0.021	1.373	C ₁₈ H ₁₉ NO ₅	↓	↓	Fecal
Dehydrocholic acid	0.024	1.329	C ₂₄ H ₃₄ O ₅	↓	↓	Fecal
Benzoxazine-6-carboxylic acid	0.022	1.324	C ₉ H ₇ NO ₃	↓	↓	Fecal
Chenodeoxycholytryptophan	0.028	1.309	C ₃₅ H ₅₀ N ₂ O ₅	↓	↓	Fecal
4-[5-(7-Hydroxy-5,5,8a-trimethyl-2-methylenedecahydro-1-naphthalenyl)-3-methylpentyl]oxy-4-oxobutanoic acid	0.026	1.306	C ₂₄ H ₄₀ O ₅	↓	↓	Fecal
4-Oxo-L-proline	0.026	1.295	C ₅ H ₇ NO ₃	↓	↓	Fecal
5-oxopentadecanoic Acid	0.050	1.239	C ₁₅ H ₂₈ O ₃	↓	↓	Fecal
Sucrose	0.000	1.727	C ₁₂ H ₂₂ O ₁₁	↑	↑	Fecal
ethyl 2-[(3-methylphenyl)carbonylamino]acetate	0.000	1.726	C ₁₂ H ₁₅ NO ₃	↑	↑	Fecal
2-Aminobicyclo[3.1.0]hexane-2,6-dicarboxylic acid	0.000	1.715	C ₈ H ₁₁ NO ₄	↑	↑	Fecal
Heliotrine	0.000	1.694	C ₁₆ H ₂₇ NO ₅	↑	↑	Fecal
Neotrehalose	0.000	1.692	C ₁₂ H ₂₂ O ₁₁	↑	↑	Fecal
Amphetamine	0.000	1.692	C ₉ H ₁₃ N	↑	↑	Fecal

Tetrahydroharman-3-carboxylic acid	0.000	1.690	C ₁₃ H ₁₄ N ₂ O ₂	↑	↑	Fecal
Mannosamine	0.001	1.615	C ₆ H ₁₃ NO ₅	↑	↑	Fecal
Cycluron	0.003	1.597	C ₁₁ H ₂₂ N ₂ O	↑	↑	Fecal
N-acetyltryptophan	0.002	1.566	C ₁₃ H ₁₄ N ₂ O ₃	↑	↑	Fecal
Norfloxacin	0.005	1.566	C ₁₆ H ₁₈ FN ₃ O	↑	↑	Fecal
3						
5-(3-Pyridyl)-2-hydroxytetrahydrofuran	0.004	1.545	C ₉ H ₁₁ NO ₂	↑	↑	Fecal
Penciclovir	0.003	1.541	C ₁₀ H ₁₅ N ₅ O ₃	↑	↑	Fecal
6-Methyl-2-pyridinecarboxylic acid	0.004	1.541	C ₇ H ₇ NO ₂	↑	↑	Fecal
Androstane-3,17-diol 17-sulfate	0.005	1.517	C ₁₉ H ₃₂ O ₅ S	↑	↑	Fecal
2-Ethylpropanedioylcarnitine	0.007	1.514	C ₁₂ H ₂₁ NO ₆	↑	↑	Fecal
12-Hydroxy-8,10-octadecadienoic acid	0.007	1.511	C ₁₈ H ₃₂ O ₃	↑	↑	Fecal
Leucyl-Isoleucine	0.008	1.510	C ₁₂ H ₂₄ N ₂ O ₃	↑	↑	Fecal
2'-Hydroxyacetophenone	0.010	1.478	C ₈ H ₈ O ₂	↑	↑	Fecal
(E)-N-(4-acetamidobutyl)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide	0.011	1.433	C ₁₆ H ₂₂ N ₂ O ₄	↑	↑	Fecal
4,8,12,15-Octadecatetraenoic acid	0.013	1.430	C ₁₈ H ₂₈ O ₂	↑	↑	Fecal
Arjugenin	0.016	1.415	C ₃₀ H ₄₈ O ₆	↑	↑	Fecal
Dihydromelilotoside	0.017	1.404	C ₁₅ H ₂₀ O ₈	↑	↑	Fecal
Cholylasparagine	0.016	1.371	C ₂₈ H ₄₆ N ₂ O ₇	↑	↑	Fecal
Hydroquinidine	0.018	1.371	C ₂₀ H ₂₆ N ₂ O ₂	↑	↑	Fecal
4,5-Dimethyl-3-hydroxy-2,5-dihydrofuran-2-one sulfate	0.018	1.370	C ₆ H ₈ O ₆ S	↑	↑	Fecal
Imidocarb	0.017	1.358	C ₁₉ H ₂₀ N ₆ O	↑	↑	Fecal

N-(6-methoxyquinolin-8-yl)alanine	0.023	1.327	C ₁₃ H ₁₄ N ₂ O ₃	↑	↑	Fecal
Avenoleic acid	0.031	1.318	C ₁₈ H ₃₂ O ₃	↑	↑	Fecal
8-Ethyl-7-Hydroxy-5-Methoxy-2-Methylchroman-4-One	0.025	1.309	C ₁₃ H ₁₆ O ₄	↑	↑	Fecal
Poricoic acid A	0.028	1.302	C ₃₁ H ₄₆ O ₅	↑	↑	Fecal
3-(Indol-3-yl)propionic acid	0.040	1.299	C ₁₁ H ₁₁ NO ₂	↑	↑	Fecal
Sebuthylazine	0.024	1.294	C ₉ H ₁₆ ClN ₅	↑	↑	Fecal
Isoimperatorin	0.034	1.289	C ₁₆ H ₁₄ O ₄	↑	↑	Fecal
N-Acetyl-5-aminosalicylic acid	0.034	1.282	C ₉ H ₉ NO ₄	↑	↑	Fecal
Kynurenine	0.029	1.276	C ₁₀ H ₁₂ N ₂ O ₃	↑	↑	Fecal
8,12-Octadecadienoic acid	0.042	1.272	C ₁₈ H ₃₂ O ₂	↑	↑	Fecal
Lumiflavin	0.045	1.266	C ₁₃ H ₁₂ N ₄ O ₂	↑	↑	Fecal
Myoinositol	0.028	1.265	C ₆ H ₁₂ O ₆	↑	↑	Fecal
PR(18:1/18:2)	0.033	1.262	C ₄₄ H ₈₂ NO ₈ P	↑	↑	Fecal
3-Hydroxyoctadecanoic Acid	0.031	1.259	C ₁₈ H ₃₆ O ₃	↑	↑	Fecal
Bicine	0.034	1.240	C ₆ H ₁₃ NO ₄	↑	↑	Fecal
Brefeldin A	0.037	1.235	C ₁₆ H ₂₄ O ₄	↑	↑	Fecal
1-O-hexadecyl-2-C-methyl-3-phosphatidylcholine	0.031	1.223	C ₂₅ H ₅₄ NO ₆ P	↑	↑	Fecal
Methionylleucine	0.044	1.213	C ₁₁ H ₂₂ N ₂ O ₃	↑	↑	Fecal
S						
Isohomovanillic acid	0.049	1.188	C ₉ H ₁₀ O ₄	↑	↑	Fecal