Supporting Materials

Text S1 Dose selection of nano-pollutions

Annual production level of the investigated nanomaterials. In 2018, the global production of plastic materials reached 359 million metric tons (Mai et al., 2020). Undoubtedly, nano-plastic pollution in the environment is the most serious among all the nanomaterials. In addition, during the pandemic COVID-19, personal protective equipment has driven increased plastic pollution. Packaged take-out meals and home-delivered groceries also contributed tremendously additional plastic wastes (Adyel, 2020). As for metal oxide nanomaterials, it has been calculated that the total amount of nano-TiO_2, often found in many cosmetics (e.g. suncreams, moisturizers) and has received increased attention recently from a regulatory context, reached over 45000 tons per year (Clift et al., 2020). Meanwhile, worldwide production of ZnO nanoparticles is reported to vary between 5.5–28000 tons per year (Gunasekaran et al., 2020).

By contrast, annual production levels of nano-Ag, semiconductor quantum dots (QDs) and carbon dots (CDs) are much lower. According to a previous report which provided the worldwide and Europe-wide estimates for the production and use of different engineered nanomaterials based on a survey sent to companies producing and using these nanomaterials, the estimated production level of nano-Ag and QDs was approximately one-tenth of the nano-ZnO production level (Piccinno et al., 2012). As well known, nano-silver is widely used in medicine and daily life as an effective antimicrobial material, due to its excellent and high-coverage antimicrobial property and none drug resistance (Burdușel et al., 2018). In addition, semiconductor QDs and CDs are one-dimensional nanomaterials with excellent fluorescence properties, which have widely applied in the fields of catalysis, sensing, optoelectronic devices, optical materials, biomarkers and life analysis, owing to their impressive and flexible optical properties (Goryacheva et al., 2017; Castro et al., 2021; Du et al., 2021). Since semiconductor QDs contain heavy metal ions, which contributes to their certain biotoxicity, CDs have been more and more used in biomedical fields as the substitute of QDs due to their much better biocompatibility. In fact, actual production data for nano-Ag, QDs and CDs are not publicly available. However, we can expect that with the rapid development of nanotechnology, the practical applications of these attractive functional nanomaterials will increase gradually.

Environment-relevant concentration and human risk. In a recent literature, the researchers formulated a robust model using the Human Development Index and estimated that the global plastic outflows from 1518 main rivers were in the range of 57000–265000 (median: 134000) metric tons in 2018 (Mai et al., 2020), which is 8-fold more than the values published in 2014 (plastic loads in surface waters of the global oceans were estimated to be 7000 to 35000 metric tons from 3070 surface tows worldwide) (Cózar et al., 2014). In 2015, the highest possible concentration of plastic particles in environmental water is 1 mg/L (Lenz et al., 2016; Lin et al.,

2020). It can be speculated predicatively that the environment-relevant concentration of plastic particles in some areas has exceed 1 mg/L. A recent study also declared that the human body ingests more than 100000 MPs particles per year through dietary consumption and inhalation, with the daily intake of MPs reached as much as 203–312 particles (Cox et al., 2019). The authors even claimed that their estimates of American consumption of microplastics were likely drastic underestimates overall. Therefore, 1 mg/L is not only an environment-relevant concentration but also a human-relevant level for micro- or nano-plastic pollution (Lenz et al., 2016; Lin et al., 2020; Liu et al., 2021).

Recent estimates predict high concentrations of nano-TiO_2 in the coastal waters. In summer, the concentrations of nano-TiO_2 may exceed 0.9 mg/L in the surface water near popular beaches in French (Labille et al., 2020; Luo et al., 2020). However, in the same beaches, the concentrations of nano-ZnO were much lower than those of nano-TiO_2. As the reported annual production level of nano-ZnO, the production amount varied by a large margin from 5.5 to 28000 tons per year (Sousa and Ribau Teixeira, 2020), which consequently resulted in the distinctly different environmental concentration of nano-ZnO in different areas.

The daily amount of nano-Ag derived from natural sources in food and water ingested by humans and the environmental concentration of nano-Ag is in μg/L level (Burdușel et al., 2018). Environmental concentrations of QDs and CDs have not been investigated before, which might be lower than μg/L level. However, in commercial agriculture, rapid and uniform seed germination and seedling emergence are important factors in successful stand establishment. Nano-Ag and other nanomaterials have been reported to promote seed germination, improve soil quality, decrease the residue of pesticides, protect seeds from pathogens and promote plant growth in many studies (Yang et al., 2017; Rui et al., 2018; Sotoodehnia et al., 2019). The appropriate dosage of nano-Ag was referred to its minimum inhibitory concentrations (MIC) for beneficial microbes in soil. Results in literature showed that nano-Ag colloids exhibit different antibacterial activities for each respective beneficial microbe tested with MIC varied from 12 to 40 mg/L, which means that nano-Ag concentration in soil lower than 12 mg/L would be considered as a safe concentration for agriculture practices (Sotoodehnia et al., 2019).

Dosing selection. In summary, in this study, a low dose level of 1 mg/L was set as human-/environment-relevant concentration of nano-pollutions. In fact, 1 mg/L is much higher than the real human-/environment-relevant concentration of QDs and CDs. However, in order to facilitate the horizontal comparison of the impacts of six investigated nanomaterials on microbial morphology and metabolic features, we set the same dose level for six different nanomaterials.

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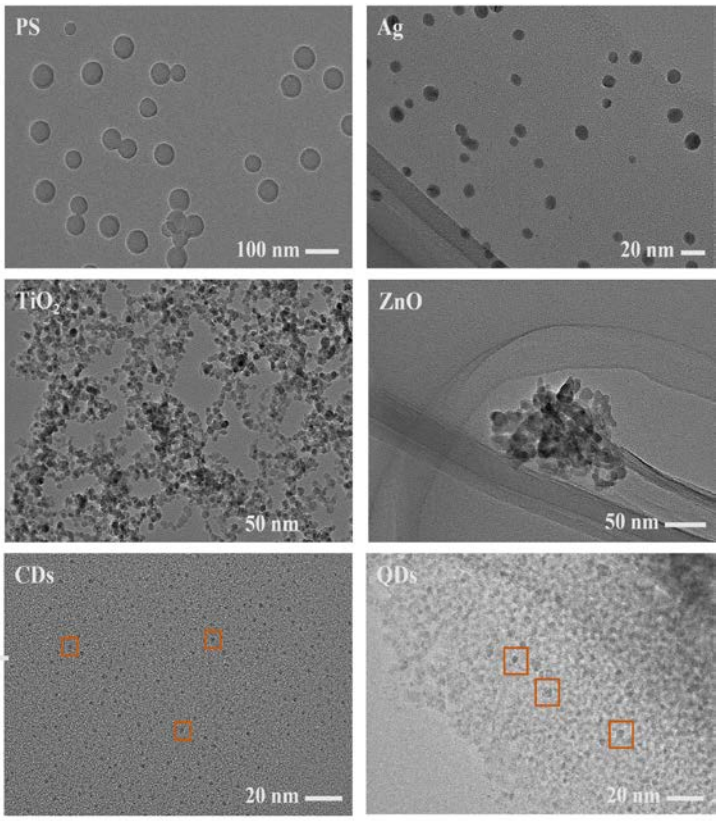

Fig. S1 TEM images of six investigated nanomaterials.

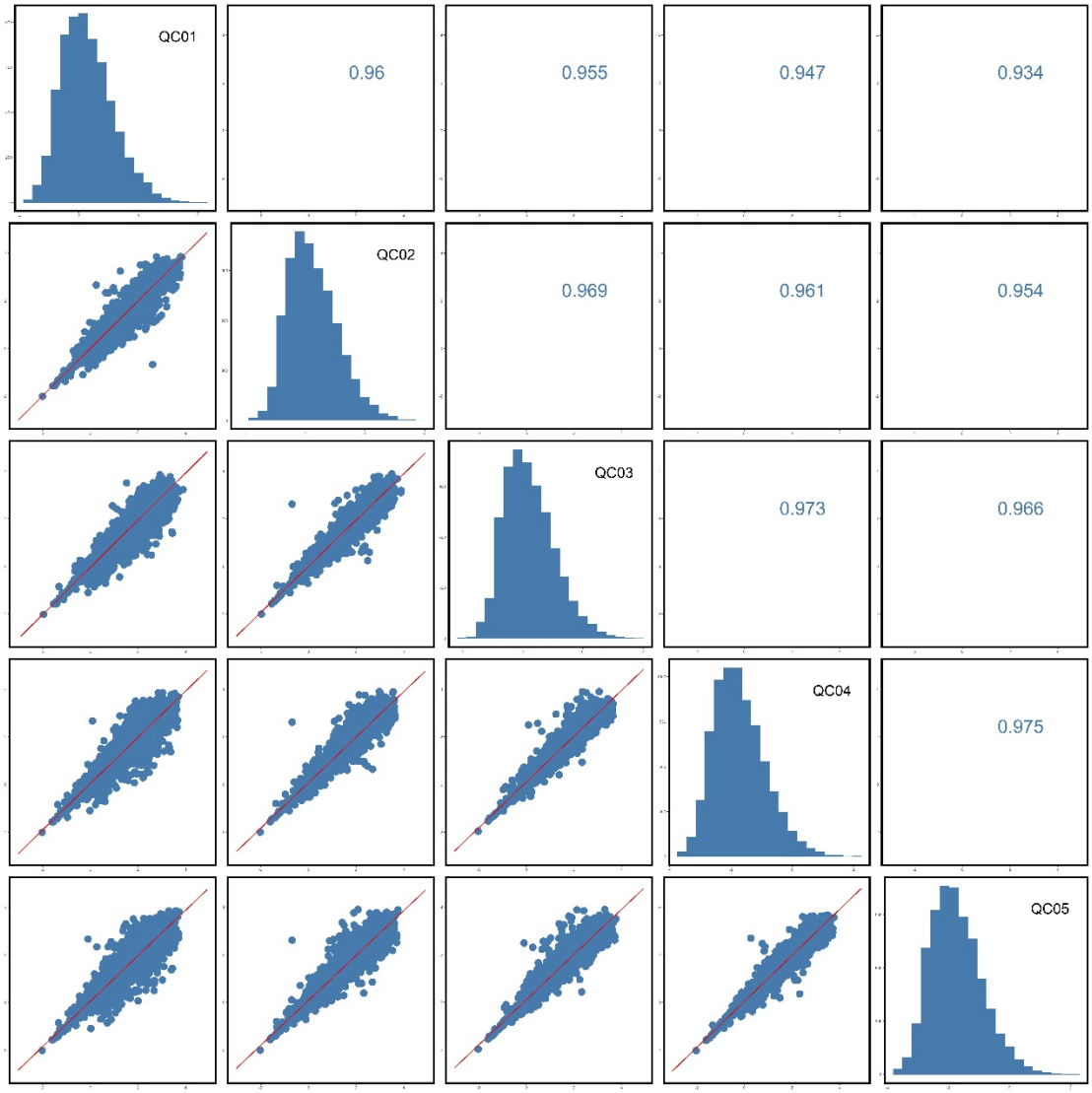

Fig. S2 Correlation analysis of QC samples under positive ion mode of LC-MS/MS analyses.

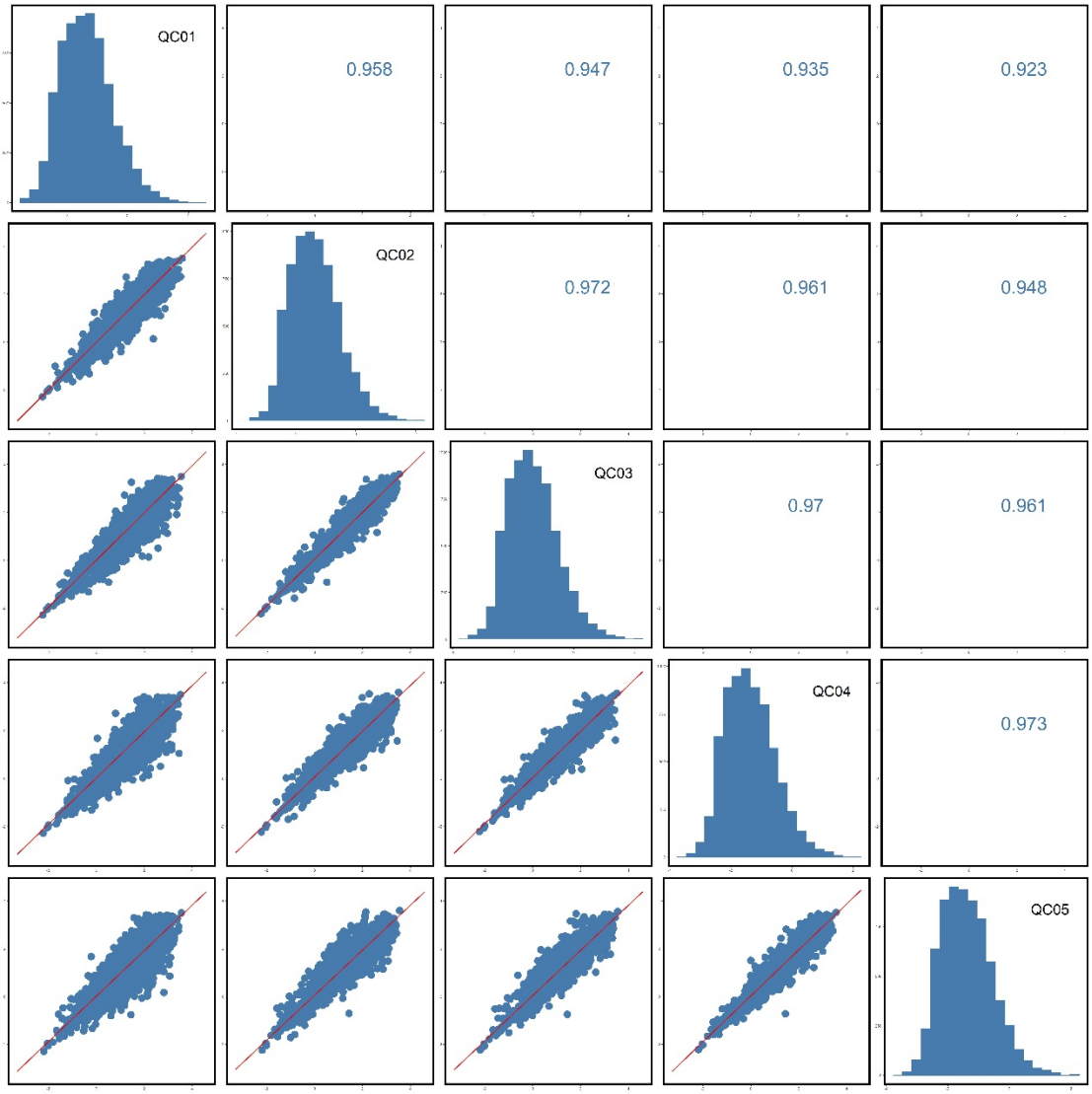

Fig. S3 Correlation analysis of QC samples under negative ion mode of LC-MS/MS analyses.

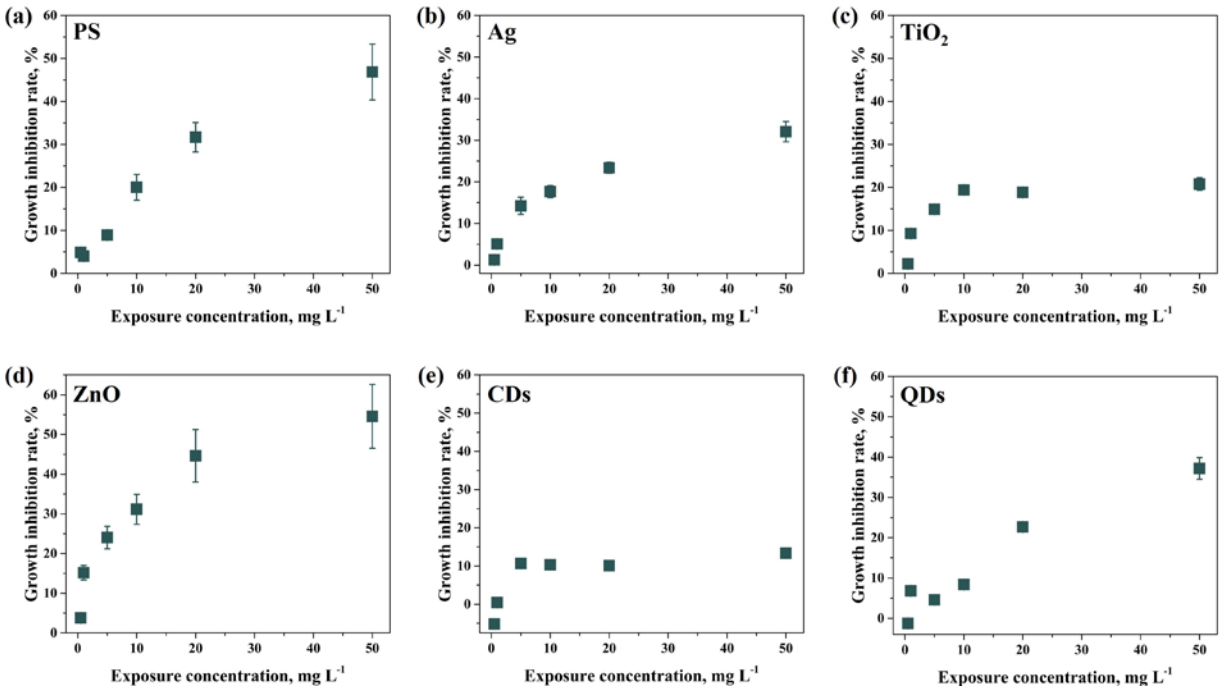

Fig. S4 Growth inhibition rates of different dose levels of nanomaterials to *E. coli* under 30 h of cultivation: (a) PS, (b) Ag, (c) TiO_2, (d) ZnO, (e) CDs, (f) QDs.

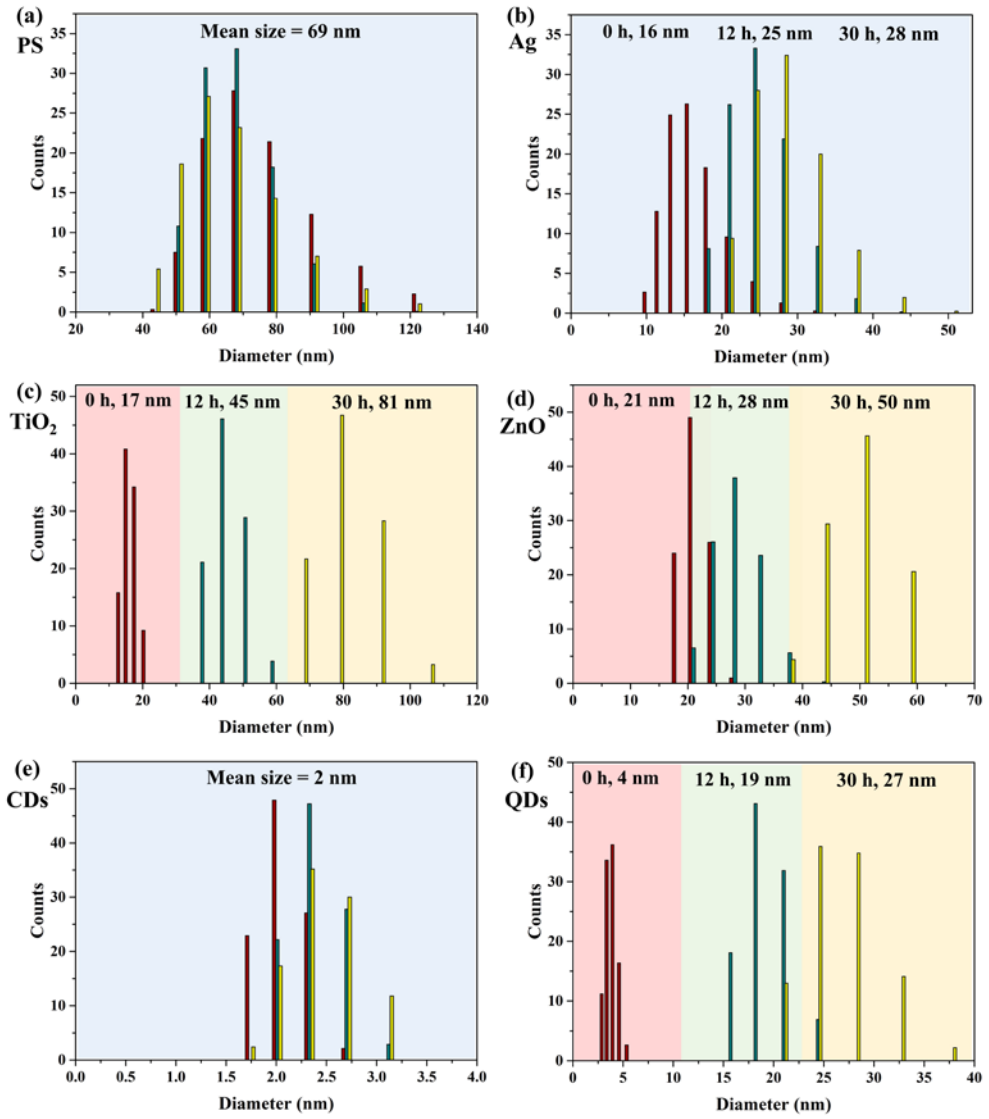

Fig. S5 Size distributions of six investigated nanomaterials in the TSB culture medium from 0 h to 30 h: (a) PS, (b) Ag, (c) TiO_2, (d) ZnO, (e) CDs, (f) QDs. Red columns: particle size distribution of the nanomaterials at 0 h; green columns: particle size distribution of the nanomaterials at 12 h; yellow columns: particle size distribution of the nanomaterials at 30 h.

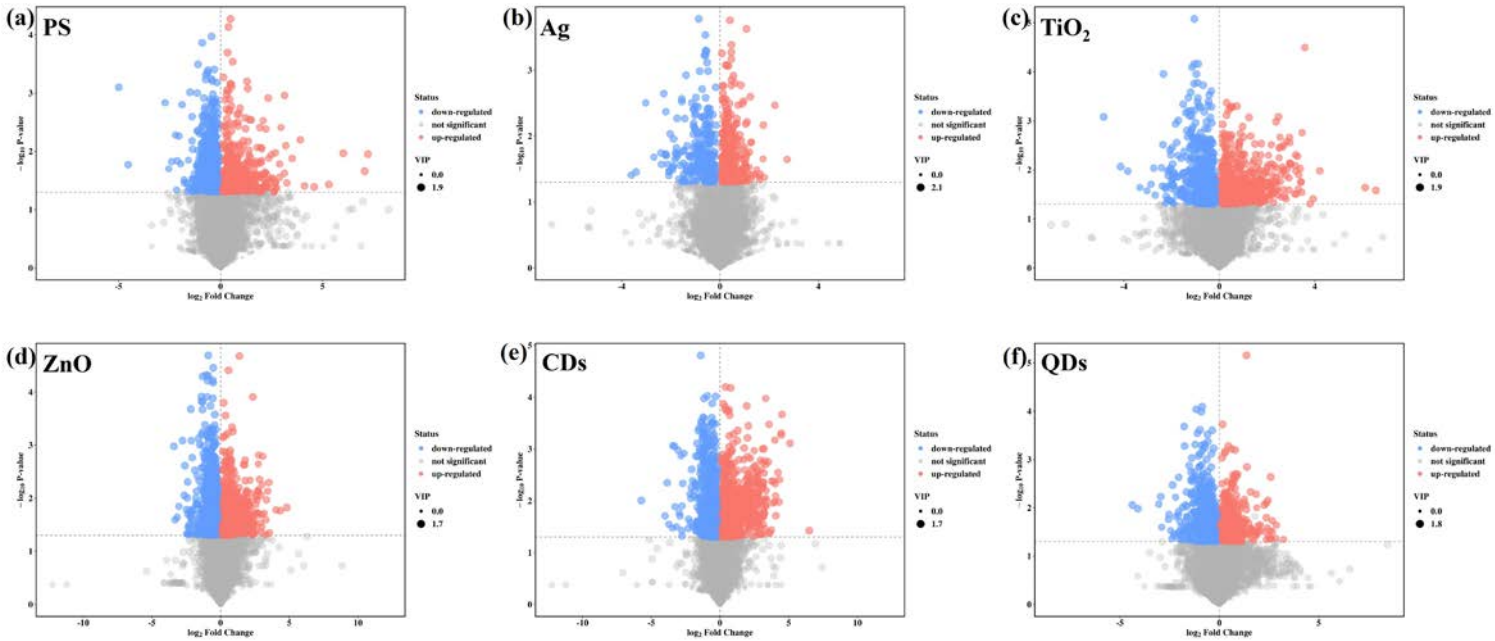

Fig. S6 Volcano plots showing metabolite features of *E. coli* induced by low exposure dose (1 mg/L) of nano-pollutions: (a) PS, (b) Ag, (c) TiO_2, (d) ZnO, (e) CDs, (f) QDs.

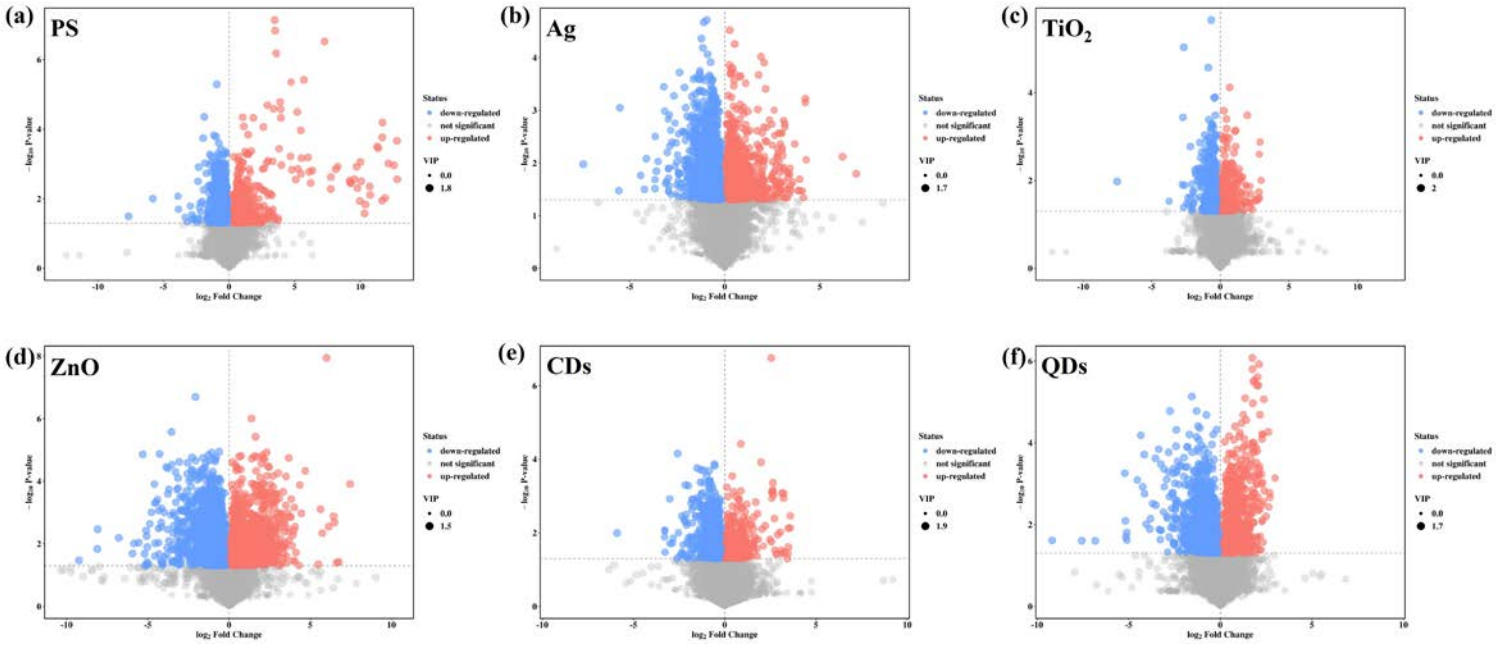

Fig. S7 Volcano plots showing metabolite features of *E. coli* induced by high exposure dose (20 mg/L) of nano-pollutions: (a) PS, (b) Ag, (c) TiO_2, (d) ZnO, (e) CDs, (f) QDs.

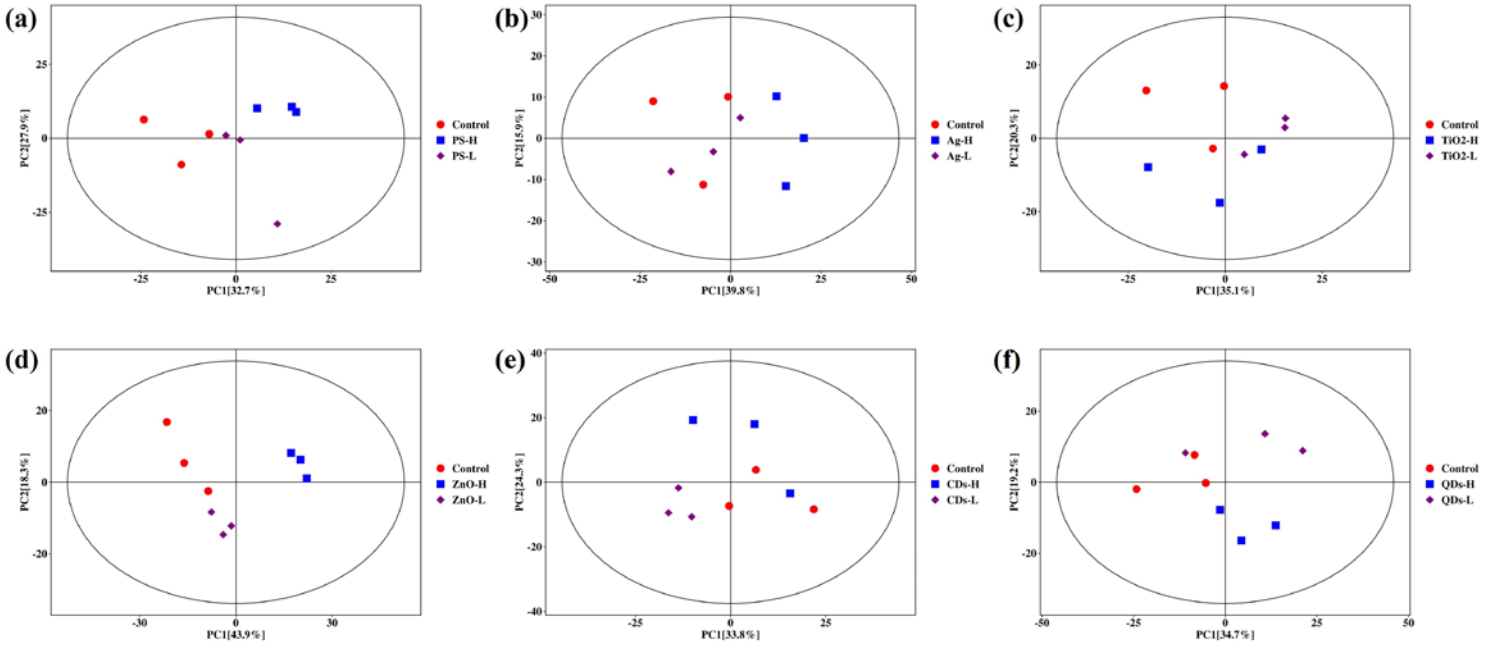

Fig. S8 PCA score plots of significant metabolite features of *E. coli* in exposure to six nano-pollutions at low and high dose levels: (a) PS, (b) Ag, (c) TiO_2, (d) ZnO, (e) CDs, (f) QDs. PS-L, Ag-L, TiO_2-L, ZnO-L, CDs-L, QDs-L represent microbial groups cultured under each nanomaterial at low dose level (1 mg/L) while PS-H, Ag-H, TiO_2-H, ZnO-H, CDs-H, QDs-H represent microbial groups cultured under each nanomaterial at high dose level (20 mg/L).

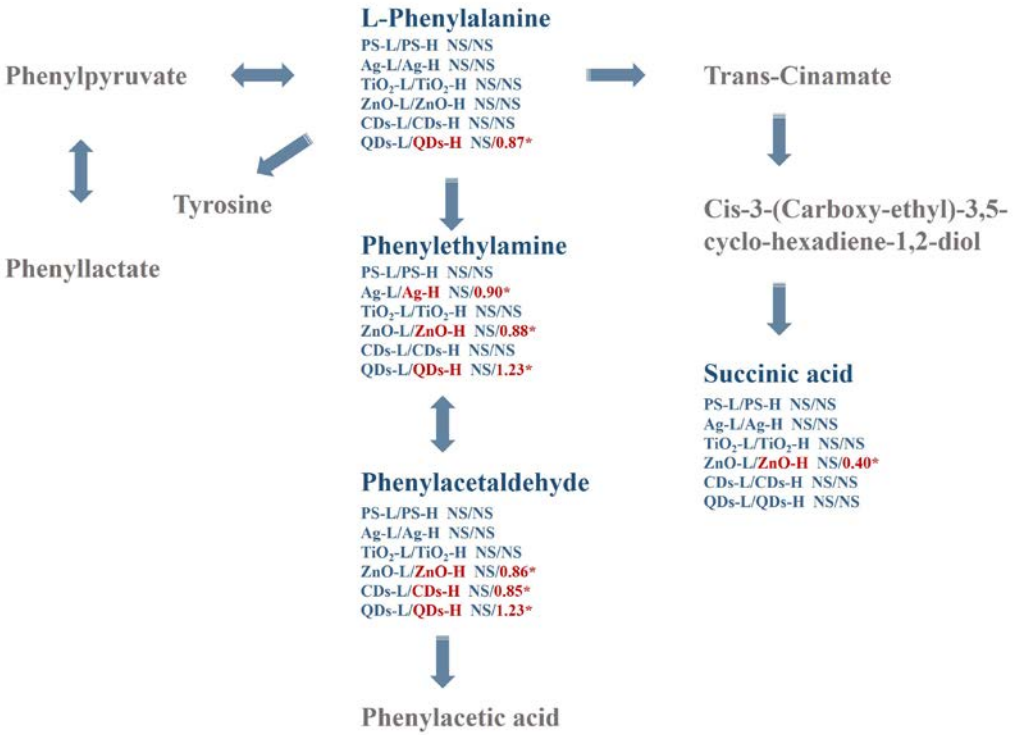

Fig. S9 Metabolites involved in phenylalanine metabolism in *E. coli*. The values in red text were fold changes of metabolites (*$p < 0.05$). NS means the metabolite in the contaminated *E. coli* is not significant ($p > 0.05$) compared with the control group. Metabolites in grey text are undetected compounds.

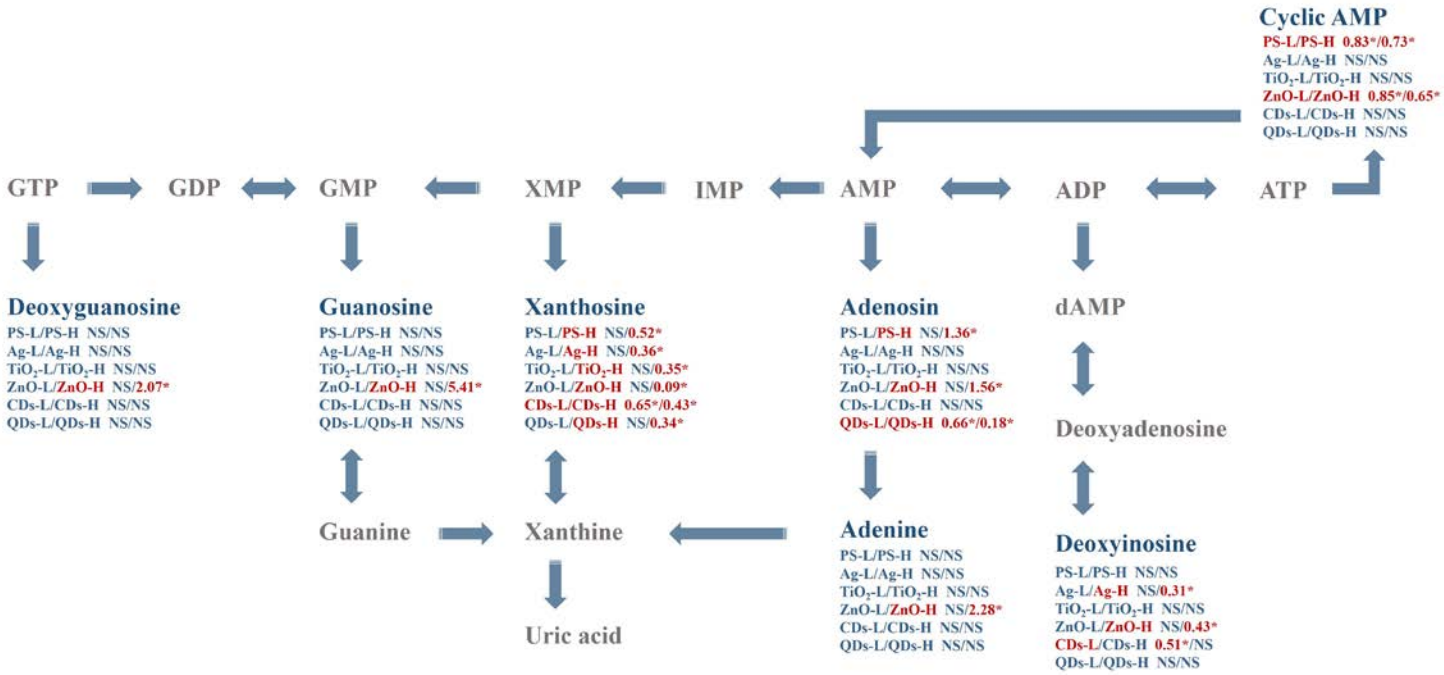

Fig. S10 Metabolites involved in purine metabolism in *E. coli*. The values in red text were fold changes of metabolites (*$p < 0.05$). NS means the metabolite in the contaminated *E. coli* is not significant ($p > 0.05$) compared with the control group. Metabolites in grey text are undetected compounds.

Table S1 Size and morphology information of six investigated nanomaterials in this study. The measured morphologies and mean sizes were obtained from TEM images and size distribution results. The theoretical sizes were obtained from reagent instructions or literatures of the nanomaterials

Nanomaterial	Theoretical size (nm)	Mean size (nm)	Measured morphology
PS	50–100 [a)]	69	Bead
Ag	10–15 [b)]	16	Particle
TiO_2	40 [c)]	17	Particle
ZnO	50 ± 10 [d)]	21	Nanoaggregate
CDs	2–3 [e)]	2	Dot
QDs	~5 [f)]	4	Dot

Notes: a) PS nano-plastic aqueous dispersion was brought from Aladin (Shanghai, China): 2.5% w/v in water, diameter 0.05–0.1 μm, latex beads, product number P107772. b) Nano silver aqueous solution was brought from Aladin (Shanghai, China): concentration 1000 mg/L, 10–15 nm, product number N196422. c) TiO_2 powder was brought from Aladin (Shanghai, China): 99.8% metals basis, 40 nm, anatase, product number T104937. d) ZnO powder was brought from Aladin (Shanghai, China): 99.8% metals basis, 50 ± 10 nm, product number Z112849. e) CDs were synthesized by a microwave-assisted pyrolysis method according to the reference: Zhai X, Zhang P, Liu C, Bai T, Li W, Dai L, Liu W (2012). Highly luminescent carbon nanodots by microwave-assisted pyrolysis. Chemical Communications, 48(64): 7955–7957. The reported size of the CDs was 2.2–3.0 nm. f) CdTe QDs were synthesized through a one-pot method according to the reference: Wu S, Dou J, Zhang J, Zhang S (2012). A simple and economical one-pot method to synthesize high-quality water soluble CdTe QDs. Journal of Materials Chemistry, 22(29): 14573. The reported size of the QDs was about 5 nm.

Table S2 Summary of microbial groups and their treated conditions

Microbial group	Microbial treatment
Control	*E. coli* cultured under untreated culture medium
PS-L	*E. coli* cultured under PS nanoplastic at low dose level (1 mg/L)
PS-H	*E. coli* cultured under PS nanoplastic at high dose level (20 mg/L)
Ag-L	*E. coli* cultured under nanosilver at low dose level (1 mg/L)
Ag-H	*E. coli* cultured under nanosilver at high dose level (20 mg/L)
TiO_2-L	*E. coli* cultured under nano-TiO_2 at low dose level (1 mg/L)
TiO_2-H	*E. coli* cultured under nano-TiO_2 at high dose level (20 mg/L)
ZnO-L	*E. coli* cultured under nano-ZnO at low dose level (1 mg/L)
ZnO-H	*E. coli* cultured under nano-ZnO at high dose level (20 mg/L)
CDs-L	*E. coli* cultured under CDs at low dose level (1 mg/L)

CDs-H	*E. coli* cultured under CDs at high dose level (20 mg/L)
QDs-L	*E. coli* cultured under CdTe QDs at low dose level (1 mg/L)
QDs-H	*E. coli* cultured under CdTe QDs at high dose level (20 mg/L)

Table S3 Metabolite extraction and profiling conditions

Procedure	Step	Operational content
Extraction	Step 1	100 μL of ultrapure water was added to each 1×10^{10} bacterial cells, followed by a 30 s vortex and a 5 min sonication at ice-water bath.
	Step 2	50 μL of the Step 1 sample was added with 950 μL of extraction solution (acetonitrile/methanol/water, 2/2/1, v/v/v, with isotopically-labelled internal standard mixture), followed by a 30 s vortex, a 4 min homogenization (35 Hz) and a 5 min sonication at ice-water bath.
	Step 3	Repeat homogenization and sonication cycle for 3 times, keep the samples at –40 ℃ for 1 h before centrifugation under 12000 r/min for 15 min at 4 ℃.
LC-MS/MS analyses	Mobile phase A	Aqueous solution consisted of 25 mmol/L ammonium acetate and 25 mmol/L ammonia hydroxide (pH = 9.75).
	Mobile phase B	Acetonitrile.
	Elution gradient	0–0.5 min, 95% B; 0.5–7.0 min, 95%–65% B; 7.0–8.0 min, 65%–40% B; 8.0–9.0 min, 40% B; 9.0–9.1 min, 40%–95% B; 9.1–12.0 min, 95% B.
	ESI source conditions	Sheath gas flow rate: 50 Arb, Aux gas flow rate: 10 Arb, capillary temperature: 320 ℃, full MS resolution: 60000, MS/MS resolution: 7500, collision energy: 10/30/60 in NCE mode, spray Voltage: 3.5 kV (positive) or –3.2 kV (negative).

Table S4 Growth inhibition rates (the mean ± SD, n = 8) of different dose levels of nanomaterials to *E. coli* under 30 h of cultivation. Significant difference between the control and the treatment was represented as $*p < 0.05$

Exposure dosage	PS	Ag	TiO_2	ZnO	CDs	QDs
0.5 mg/L	4.9% ± 0.3%	1.3% ± 0.1%	2.2% ± 0.2%	3.8% ± 0.5%	–5.2% ± 0.4%	–1.3% ± 0.1%
1 mg/L	**4.0% ± 0.4%**	**5.1% ± 0.3%***	**9.3% ± 1.1%***	**15.2% ± 1.8%***	**0.4% ± 0.04%**	**6.8% ± 0.4%**
5 mg/L	8.9% ± 1.0%*	14.2% ± 2.1%*	14.9% ± 0.9%*	24.0% ± 2.8%*	10.6% ± 0.7%*	4.6% ± 0.2%
10 mg/L	20.0% ± 3.0%*	17.6% ± 1.5%*	19.4% ± 0.9%*	31.1% ± 3.8%*	10.3% ± 1.1%*	8.4% ± 0.4%
20 mg/L	**31.7% ± 3.4%***	**23.4% ± 1.3%***	**18.8% ± 0.6%***	**44.6% ± 6.6%***	**10.1% ± 0.8%***	**22.7% ± 0.8%***
50 mg/L	46.8% ± 6.5%*	32.1% ± 2.4%*	20.8% ± 1.5%*	54.6% ± 8.0%*	13.3% ± 1.2%*	37.2% ± 2.7%*

Table S5 Information of 293 identified metabolites in *E. coli*, and respective fold change of each metabolite at different nano-pollution exposures

Metabolite	KEGG	RT	MSI	m/z	Fold change (the ratio of metabolic expression level between the nanomaterial contaminated group and the control group)											
					PS-L	PS-H	Ag-L	Ag-H	TiO_2-L	TiO_2-H	ZnO-L	ZnO-H	CDs-L	CDs-H	QDs-L	QDs-H
Isobutyric acid	C02632	104.45	[M-H]-	87.0444	1.20	0.81	0.88	0.94	0.86	0.76	0.97	0.95	0.81	0.84	0.83	0.92
L-Leucine	C00123	282.8485	[M+H]+	132.1021	0.82	0.82	0.95	0.80	1.06	0.98	0.77	0.69	0.98	0.71	0.91	0.96
Propionic acid	C00163	395.0555	[M-H]-	73.0288	0.85	1.15	0.95	0.85	1.02	0.81	1.11	0.44	0.91	0.96	0.97	1.28
Pyruvic acid	C00022	181.047	[M-H]-	87.0082	1.08	0.93	1.20	1.07	1.05	1.25	0.97	0.92	1.17	1.05	0.98	0.99
Uracil	C00106	511.154	[M-H]-	111.0194	0.79	0.78	0.90	0.86	0.81	0.89	0.82	0.82	1.32	0.81	1.08	0.84
3,3,5-triiodo-L-thyronine-beta-D-glucuronoside	C16439	293.654	[M+H]+	132.1022	0.93	0.97	0.97	0.91	0.95	0.98	0.90	0.71	1.10	0.82	1.02	0.87
1H-Indole-3-carboxaldehyde	C08493	60.0522	[M-H]-	144.0450	0.97	0.86	1.00	0.85	0.94	1.20	0.85	1.02	0.95	0.84	1.00	0.68
L-Norleucine	C01933	293.2895	[M-H]-	130.0869	0.93	0.94	0.91	0.90	0.88	0.93	0.89	0.73	1.06	0.79	1.01	0.85
Adenine	C00147	284.665	[M+H]+	136.0618	1.17	1.27	0.79	1.18	0.92	1.34	0.91	2.28	1.23	0.83	0.93	1.00
Oleic acid	C00712	38.6073	[M-H]-	281.2491	1.40	0.86	1.75	1.50	0.85	2.40	1.67	1.54	1.18	1.31	1.29	0.85
Tridecanoic acid	C17076	35.46345	[M-H]-	213.1861	1.16	0.99	1.74	1.31	1.52	1.30	1.52	1.26	1.91	1.30	1.08	1.20
Pelargonic acid	C01601	51.288845	[M-H]-	157.1228	0.94	0.84	1.05	1.08	1.10	1.05	1.07	1.09	1.01	1.03	1.04	0.93

16-Methylheptadecanoic acid		38.0649	[M-H]-	283.2642	1.60	1.75	1.32	1.53	1.88	1.71	2.23	2.29	1.52	1.78	1.75	2.05
Dodecanoic acid	C02679	46.8809	[M-H]-	199.1704	1.11	1.00	1.23	1.53	1.26	1.76	1.18	1.23	1.24	1.40	1.05	0.98
Hypoxanthine	C00262	231.285	[M+H]+	137.0458	0.52	0.81	1.19	4.80	0.66	0.98	0.83	0.49	0.50	0.75	0.43	0.51
Caprylic acid	C06423	45.1688	[M-H]-	143.1071	0.89	0.82	0.86	1.06	0.99	0.95	0.91	0.96	0.86	1.08	0.89	1.01
2,6-Dimethylpyrazine		268.5355	[M+H]+	109.0765	0.84	0.75	0.94	0.83	0.94	0.90	0.94	1.01	0.99	0.83	0.93	0.79
2-Methyl-6-(2-propenyl)pyrazine		232.7355	[M+H]+	135.0920	1.03	1.12	1.22	1.15	1.18	1.05	1.15	0.99	1.27	1.21	1.25	0.96
Thymine		66.3308	[M-H]-	125.0352	0.86	0.86	1.02	0.79	0.89	0.89	0.92	0.47	0.84	0.88	0.87	0.66
2-Methyl-3-(2-propenyl)pyrazine		258.251	[M+H]+	135.0920	0.93	0.92	1.21	0.93	0.98	1.02	1.02	1.24	1.01	0.97	1.05	1.16
Deoxyguanosine	C00330	216.6805	[M+H]+	268.1041	8.60	11.86	10.05	0.63	0.67	11.87	0.89	2.07	0.90	0.86	0.75	0.64
Creatinine	C00791	179.158	[M+H]+	114.0666	0.97	0.92	1.06	1.13	1.14	1.14	0.93	1.28	1.07	1.11	1.08	1.01
Stearic acid	C01530	713.021	[M-H]-	283.2642	0.89	0.80	0.86	0.95	0.89	0.94	0.80	0.95	0.88	1.11	1.14	0.87
Adenosine	C00212	272.674	[M-H]-	266.0900	0.96	1.36	1.07	0.88	0.99	1.25	1.08	1.56	1.08	1.07	0.66	0.18
3-Methyl-2-oxovaleric acid	C03465	37.9746	[M-H]-	129.0552	1.17	1.02	0.71	0.91	0.67	0.97	0.99	6.20	1.47	0.61	0.91	0.32
Betaine	C00719	290.08	[M+H]+	118.0863	0.92	0.91	0.99	0.98	0.98	0.97	0.90	0.96	0.93	0.99	0.99	1.15
Isopropylpyrazine		257.981	[M+H]+	123.0919	0.82	0.79	0.95	0.77	0.89	0.94	0.95	0.98	0.88	0.86	0.99	1.05
Choline	C00114	293.661	[M+H]+	104.1072	0.93	0.95	1.03	0.94	0.98	1.02	0.98	0.99	0.98	0.99	0.98	0.80
Nicotinic acid	C00253	228.492	[M+H]+	124.0395	0.94	1.03	1.26	0.81	0.99	0.73	0.75	0.09	0.63	1.19	0.87	0.92
Harman	C09209	44.0252	[M+H]+	183.0920	0.83	0.99	0.99	0.97	0.88	0.90	0.79	1.06	0.82	0.94	0.85	0.83
Guanine	C00242	143.1045	[M+H]+	152.0568	0.74	1.30	0.51	0.56	0.38	1.20	0.75	1.06	1.04	0.48	0.60	0.51
Valeric acid	C00803	84.005	[M-H]-	101.0601	1.24	1.26	1.63	1.30	1.32	1.27	1.32	1.51	1.34	1.36	1.28	1.13
2-Methyl-3-propylpyrazine		99.4142	[M+H]+	137.1074	0.87	0.83	1.04	0.86	1.01	0.98	1.06	1.65	1.11	0.94	0.97	0.93
4-Hydroxymandelonitrile		108.609	[M+H]+	150.0552	1.08	1.06	1.34	1.12	1.17	1.17	1.11	1.06	1.06	1.26	1.17	1.58
Diethanolamine	C06772	330.72	[M+H]+	106.0866	1.38	0.79	0.77	1.14	0.78	1.00	1.09	1.24	1.37	1.98	1.09	1.33

N-Acetylserine		311.574	[M-H]-	146.0453	1.00	0.76	1.06	1.34	0.95	0.78	0.89	1.27	1.27	1.03	1.28	0.78
Succinic acid semialdehyde	C00232	271.547	[M-H]-	101.0238	2.08	0.00	1.47	0.61	2.50	0.00	0.00	5.24	0.00	3.74	2.52	2.63
Zymonic acid		179.157	[M+H]+	159.0279	0.64	0.63	0.99	0.61	0.80	0.74	0.70	0.31	0.54	0.72	0.54	0.67
2-Amino-4-ethoxy-3-hydroxybutanoic acid		61.6105	[M+H]+	164.0931	0.84	0.84	1.12	0.78	0.94	0.88	1.09	0.27	0.86	0.76	0.83	0.80
Linoleic acid	C01595	43.278	[M-H]-	279.2331	0.78	0.70	0.86	0.62	0.76	3.67	0.73	0.72	0.49	0.73	0.97	0.48
Metenamine		285.5595	[M+H]+	141.1134	1.08	1.01	1.09	1.18	1.08	1.14	1.19	1.21	1.05	1.20	1.02	0.92
Sphinganine	C00836	41.4402	[M+H]+	302.3047	1.37	1.02	0.86	1.08	1.01	0.85	1.00	1.03	0.91	0.96	0.95	0.87
7-Methyladenine		166.125	[M+H]+	150.0774	0.96	1.20	1.13	0.91	1.03	1.06	0.99	0.37	1.00	1.09	0.82	0.48
Sarcosine	C00213	364.217	[M-H]-	88.0397	0.85	1.02	0.83	0.65	0.82	0.90	0.89	0.42	0.99	0.60	0.84	0.82
L-Carnitine	C00318	392.571	[M+H]+	162.1127	0.79	1.16	1.55	0.91	1.28	1.20	0.82	0.55	0.99	1.27	1.06	1.55
4-Guanidinobutanoic acid	C01035	378.292	[M+H]+	146.0923	0.93	0.87	1.07	1.00	1.02	0.99	0.91	1.31	1.04	0.94	1.07	1.04
Succinic acid	C00042	395.0295	[M-H]-	117.0186	0.97	1.43	1.14	1.04	1.19	0.91	1.38	0.40	1.04	1.01	1.15	1.49
Melleolide M		38.5321	[M+H]+	453.1682	0.76	0.29	0.49	0.72	0.35	0.33	0.54	0.90	0.32	0.46	0.33	0.26
gamma-Aminobutyric acid		392.636	[M+H]+	104.0710	0.81	0.84	1.03	0.84	0.92	0.81	0.79	0.66	0.86	0.84	0.76	1.33
2-Ethyl-2-Hydroxybutyric acid		124.722	[M-H]-	131.0709	1.09	0.92	1.02	0.95	1.03	0.90	0.80	1.23	0.88	1.02	0.99	0.72
Creatine	C00300	368.266	[M+H]+	132.0769	1.02	0.89	1.04	1.04	1.01	0.93	0.93	0.99	1.05	0.98	1.05	0.48
Saccharin	C12283	31.01965	[M-H]-	181.9914	1.53	1.04	1.35	1.16	1.21	1.03	1.56	1.38	0.99	1.26	1.27	2.22
1-Methyladenosine	C02494	268.206	[M+H]+	282.1201	0.85	1.02	1.15	0.81	0.97	0.89	0.97	0.36	0.93	0.86	0.86	0.68
Dethiobiotin	C01909	306.425	[M+H]+	215.1393	0.90	1.19	0.90	0.92	0.83	1.44	0.90	1.44	1.56	0.81	0.85	0.47
3-Dehydroxycarnitine	C05543	398.0455	[M+H]+	146.1175	0.75	0.77	0.97	0.62	0.78	0.80	0.76	0.56	0.68	0.84	0.87	1.25
Pyrrolidine		476.36	[M+H]+	72.0814	1.18	0.60	0.73	0.93	0.52	0.73	0.88	0.80	1.41	1.01	0.59	0.91
4-Dodecylbenzenesulfonic Acid		716.004	[M-H]-	325.1844	1.04	0.90	1.01	1.14	1.28	0.91	1.20	1.06	0.74	0.98	1.36	0.95

Capric acid	C01571	48.64365	[M-H]-	171.1386	0.96	0.68	1.07	1.09	0.98	1.08	0.89	1.09	0.85	1.03	0.86	0.91
D-alpha-Aminobutyric acid		342.2545	[M+H]+	104.0710	0.80	0.79	0.92	0.38	0.83	0.59	0.74	0.42	0.62	0.72	0.74	0.92
6-Methylquinoline		246.785	[M+H]+	144.0811	0.88	0.98	0.97	0.83	1.01	0.89	0.91	0.90	1.00	0.89	0.99	1.27
Phenylethylamine	C05332	194.985	[M+H]+	122.0967	0.80	0.98	1.04	0.90	0.94	0.94	0.93	0.88	0.91	0.96	0.94	1.23
Terephthalic acid	C06337	435.239	[M-H]-	165.0190	1.11	0.91	1.11	1.08	1.40	1.03	1.00	1.01	0.97	0.98	1.02	0.93
Tyramine	C00483	246.9775	[M+H]+	138.0915	0.92	1.00	0.97	0.89	0.97	0.94	0.91	0.85	0.98	0.87	1.00	1.27
Acrylic acid	C00511	180.148	[M-H]-	71.0131	0.68	0.71	0.87	0.77	0.84	0.85	0.69	0.89	0.75	0.93	0.74	0.91
Histamine	C00388	300.932	[M+H]+	112.0871	0.93	0.98	0.82	0.94	0.94	1.17	0.72	2.10	1.06	1.23	1.13	0.91
Palmitic amide		33.5392	[M+H]+	256.2634	0.88	1.03	1.13	0.96	1.02	0.97	1.13	0.99	1.01	1.13	1.01	1.07
L-trans-4-Methyl-2-pyrrolidinecarboxylic acid		65.10895	[M+H]+	130.0864	0.91	0.99	0.93	0.84	1.11	0.95	0.79	0.84	0.79	0.99	1.11	1.53
p-Toluenesulfonic acid	C06677	39.71755	[M-H]-	171.0119	0.82	1.39	1.13	3.15	0.80	1.05	1.19	1.23	1.40	1.42	6.73	0.93
Pyroglutamic acid	C01879	312.435	[M-H]-	128.0346	1.09	0.86	1.14	1.06	1.18	0.95	1.14	1.19	1.31	0.91	1.27	0.62
Phthalic acid	C01606	341.0335	[M-H]-	165.0192	0.91	0.85	1.09	1.25	0.94	1.00	1.20	0.99	1.16	0.93	1.20	0.95
Undecanoic acid	C17715	36.2186	[M-H]-	185.1545	1.12	0.83	1.21	1.30	1.35	1.25	1.29	1.13	1.17	1.32	1.18	0.99
Cyclamic acid	C02824	59.1752	[M-H]-	178.0542	118.41	5.56	0.25	0.56	77.67	0.73	1.42	0.33	0.42	6.27	0.74	0.35
5'-Methylthioadenosine	C00170	86.7076	[M-H]-	296.0825	0.85	0.63	0.87	0.67	0.88	0.76	0.78	0.55	0.78	0.66	0.96	0.83
Benzoic acid	C00180	109.479	[M-H]-	121.0288	0.93	1.03	1.22	1.13	1.18	1.23	1.32	1.28	1.23	1.11	1.16	0.95
6-Dimethylaminopurine		81.92495	[M+H]+	164.0931	0.80	0.77	0.95	0.65	0.75	0.72	0.86	0.51	0.80	0.65	0.64	0.68
4-Hydroxyproline	C01157	364.081	[M-H]-	130.0504	0.92	0.94	0.88	0.97	0.88	0.84	0.86	0.66	0.87	0.82	0.95	1.44
2,5-Dihydro-2,4-dimethyloxazole		52.87365	[M+H]+	100.0761	0.93	0.87	0.93	1.07	0.97	1.04	0.92	1.18	1.06	0.95	1.04	0.91
Ketoleucine	C00233	57.53165	[M-H]-	129.0552	1.14	1.10	0.91	1.03	0.91	1.18	1.09	3.98	1.55	0.82	1.09	0.59
Maleic acid	C01384	45.078	[M-H]-	115.0032	1.41	1.00	1.89	2.38	1.53	1.14	2.57	1.66	1.41	1.90	1.58	0.34

N-Nitroso-pyrrolidine	C19285	348.69	[M+H]+	101.0714	0.99	1.06	1.09	1.08	0.88	0.92	1.08	0.66	0.71	0.98	1.00	1.16
9,10-DHOME	C14828	55.6838	[M-H]-	313.2387	0.93	1.05	1.16	1.58	0.97	1.31	1.04	0.79	1.13	1.09	0.87	0.62
L-Arginine	C00062	541.3355	[M+H]+	175.1189	1.84	2.19	1.11	2.56	1.73	2.52	1.48	5.93	3.07	1.40	2.78	2.90
L-Proline	C00148	328.1075	[M-H]-	114.0554	1.04	1.18	1.09	1.03	1.04	1.06	1.03	0.33	1.14	0.92	1.12	1.90
Nicotinic acid mononucleotide	C01185	343.957	[M+H]+	256.0813	0.54	0.31	1.80	0.40	1.19	0.40	0.61	0.08	0.31	0.81	0.43	0.23
Imidazoleacetic acid	C02835	46.1415	[M-H]-	125.0352	1.13	0.80	1.05	1.21	1.03	0.80	0.86	1.14	1.11	0.70	1.07	1.23
Isokobusone		56.638	[M-H]-	221.1547	1.00	0.69	1.04	1.44	1.47	1.03	0.91	1.29	0.90	1.12	1.51	0.70
Ethyl tetradecanoate		84.83385	[M-H]-	255.2328	1.20	1.10	1.25	1.44	1.21	1.28	1.14	1.17	1.25	1.29	1.13	1.84
Uridine	C00299	167.172	[M-H]-	243.0626	0.95	1.34	0.70	0.50	0.48	1.62	0.76	3.68	1.11	0.80	0.62	0.73
Phytosphingosine	C12144	45.6752	[M+H]+	318.3005	1.00	0.93	0.79	0.98	0.89	0.87	0.89	0.98	0.91	0.86	0.86	0.77
PS(16:1(9Z)/20:4(5Z,8Z,11Z,14Z))		167.057	[M+H]+	782.5075	1.14	0.98	0.90	0.86	0.93	0.66	0.80	0.72	0.96	1.13	0.88	0.76
Artocarpin		38.7296	[M+H]+	437.1939	1.53	1.02	1.89	1.11	0.84	1.03	1.26	1.77	1.10	1.47	1.08	1.39
Dihydrouracil	C00429	139.701	[M-H]-	113.0350	1.06	0.84	1.02	1.07	1.07	0.82	0.86	0.95	1.22	0.94	1.26	1.13
LysoPE (16:0/0:0)		223.952	[M+H]+	454.2930	0.86	1.27	0.78	0.85	0.65	1.29	0.86	1.61	1.00	0.71	0.76	0.85
O-Arachidonoyl Ethanolamine		35.2674	[M+H]+	348.2879	1.06	1.03	1.06	1.44	1.43	1.52	0.99	1.34	1.09	1.24	1.30	1.13
m-Coumaric acid	C12621	37.0723	[M-H]-	163.0395	0.86	0.61	0.69	0.80	0.41	0.71	1.00	2.83	1.25	0.32	0.61	0.23
Polyoxyethylene dioleate		169.634	[M+H]+	591.5368	1.01	0.99	1.06	0.93	1.00	0.88	0.93	0.98	0.92	1.27	1.00	1.35
PC(20:3(5Z,8Z,11Z)/16:0)		29.8013	[M+H]+	784.5860	0.90	0.77	1.33	1.03	0.97	1.06	1.39	0.75	1.00	1.28	0.86	1.46
(Â±)-2-(1-Methylpropyl)-4,6-dinitrophenol		22.4404	[M-H]-	239.0672	9.93	7.45	1.29	1.71	1.24	1.44	1.29	1.19	1.45	1.44	1.32	1.16
Methyl jasmonate	C11512	32.76435	[M-H]-	223.1341	0.85	0.64	0.90	1.00	0.80	0.80	0.80	0.80	0.89	0.77	0.85	0.83
Xanthine	C00385	225.008	[M-H]-	151.0256	0.99	1.29	0.89	0.96	0.86	1.30	1.12	0.79	1.05	0.96	0.88	1.13
(Z)-15-Oxo-11-eicosenoic acid		217.481	[M+H]+	325.2737	0.73	1.25	0.60	0.53	0.44	1.18	0.87	1.11	0.81	0.72	0.58	1.08

Neotrehalose		382.067	[M+Na]1+	365.1061	0.73	0.68	0.91	0.59	0.81	0.72	0.67	0.66	0.69	0.70	0.90	1.51
Cohibin A		58.97925	[M+H]+	549.4874	0.92	1.17	1.02	1.02	1.04	0.95	0.91	0.94	1.01	0.94	0.91	1.30
N-Acetylcadaverine		335.831	[M+H]+	145.1336	0.94	0.61	0.98	0.63	0.92	0.73	0.93	0.43	0.86	0.76	1.12	1.34
Emodin	C10343	115.5615	[M-H]-	269.0460	0.86	1.08	0.99	1.18	0.96	1.19	0.90	1.46	0.85	1.13	0.92	0.86
Palmitic acid	C00249	70.72165	[M-H]-	255.2327	1.65	0.90	0.97	2.22	1.61	2.93	0.94	1.05	0.98	2.08	0.95	0.95
5-Aminopentanamide	C00990	406.332	[M+H]+	117.1027	1.15	0.94	1.07	1.33	0.99	1.12	1.18	1.22	0.88	3.92	0.95	1.07
Guanosine	C00387	281.475	[M-H]-	282.0843	1.05	1.28	0.61	0.58	0.37	0.90	0.83	5.41	1.48	0.71	0.63	0.62
Phenylacetaldehyde	C00601	246.902	[M+H]+	121.0649	0.92	1.01	0.97	0.88	0.95	0.92	0.90	0.86	0.96	0.85	0.97	1.23
Indoleacetaldehyde	C00637	59.3581	[M-H]-	158.0606	0.88	0.81	0.88	0.90	1.03	0.88	0.87	0.82	1.02	1.06	0.96	0.92
L-Tyrosine	C00082	321.456	[M-H]-	180.0668	0.74	0.79	0.82	0.68	0.74	0.83	0.77	0.70	0.90	0.58	0.84	0.96
Phenyllactic acid	C01479	101.849	[M-H]-	165.0552	1.06	0.85	1.08	1.10	1.15	0.82	1.07	1.29	1.26	0.84	1.21	0.79
Leucinic acid		98.1933	[M-H]-	131.0709	0.85	0.70	1.05	1.00	1.00	0.85	1.00	0.78	0.98	1.09	0.93	0.81
Undecylenic acid	C13910	49.6426	[M-H]-	183.1388	1.24	0.85	1.31	1.06	1.24	1.75	1.32	1.51	1.32	1.05	1.03	0.69
3,5-Dimethyl-2-propylpyrazine		204.771	[M+H]+	151.1232	0.87	1.04	0.97	0.76	0.93	0.87	0.91	0.83	0.98	0.87	1.02	0.86
Ethyl dodecanoate		195.07	[M-H]-	227.2017	0.83	1.15	0.79	0.80	0.70	1.54	1.06	2.28	1.24	0.62	0.76	0.59
PS(20:4(5Z,8Z,11Z,14Z)/15:0)		45.9946	[M+H]+	770.5105	0.65	1.42	0.91	1.00	1.38	0.68	0.98	1.18	0.75	1.65	2.00	1.90
Cosmosiin	C04608	164.307	[M-H]-	431.0994	0.87	1.07	0.95	1.15	0.92	1.09	0.86	1.37	0.82	1.07	0.86	0.89
D-Linalool 3-(6''-malonylglucoside)		115.318	[M+H]+	403.1939	0.71	0.64	0.89	0.53	0.76	0.64	0.55	0.60	0.61	0.64	0.60	0.78
Hexadecanedioic acid	C19615	446.602	[M-H]-	285.2076	0.99	1.03	1.11	1.27	1.17	1.07	1.03	1.02	1.22	0.97	1.04	0.84
Cyclic AMP	C00575	62.6846	[M-H]-	328.0461	0.83	0.73	0.99	0.83	0.87	0.83	0.85	0.65	0.83	0.85	0.88	0.88
N-Acetylputrescine	C02714	302.083	[M+H]+	131.1180	0.98	0.92	1.05	0.94	0.97	0.84	1.03	0.72	0.94	0.89	1.00	1.43
2-Hydroxyvaleric acid		361.1045	[M-H]-	117.0553	1.35	0.90	1.30	1.89	0.87	1.63	1.45	1.42	1.39	1.91	1.08	1.09
L-Malic acid	C00149	207.7225	[M-H]-	133.0137	1.06	0.45	0.74	0.34	0.56	1.35	0.71	0.91	1.44	0.90	0.60	0.85

Inosine	C00294	514.8325	[M-H]-	267.0738	0.50	0.77	1.11	0.35	0.61	0.96	0.78	0.62	0.49	0.69	0.41	0.52
3-Methylguanine	C02230	231.34	[M+H]+	166.0724	0.81	1.12	1.42	0.84	1.22	0.85	0.75	0.30	0.72	1.22	0.69	0.61
Dimethyl dialkyl ammonium chloride		144.237	[M+H]+	304.3001	1.48	0.55	0.66	0.69	1.12	0.48	0.97	6.91	1.75	1.14	0.91	0.82
4-[(E)-2-(3,5-dimethoxyphenyl)ethenyl]phenol		51.28	[M-H]-	255.1005	0.98	0.80	0.76	1.07	1.14	0.96	0.97	0.99	0.98	0.95	1.07	0.91
PE(20:2(11Z,14Z)/15:0)		169.588	[M+H]+	730.5385	0.85	1.00	0.96	0.95	0.93	0.86	0.85	0.65	0.93	1.08	0.81	0.82
N-Acetylglutamic acid	C00624	396.8415	[M-H]-	188.0562	0.68	0.62	0.87	0.55	0.78	0.67	0.64	0.66	0.58	0.78	0.86	2.09
2-Hydroxystearic acid		50.3769	[M-H]-	299.2598	1.07	1.13	2.07	1.31	1.13	0.95	1.12	1.17	1.15	1.28	1.05	0.89
xi-5-Hydroxydecanoic acid		38.75275	[M+H]+	189.1485	0.66	0.54	0.82	0.65	0.73	0.75	0.88	0.87	0.75	0.77	0.87	0.72
L-Phenylalanine	C00079	277.5215	[M-H]-	164.0714	0.92	0.89	0.98	0.84	0.92	0.90	0.90	0.81	1.06	0.80	1.02	0.87
Prostaglandin D2	C00696	44.163	[M-H]-	351.2217	0.81	1.09	0.70	0.73	0.71	1.15	0.96	1.45	1.04	0.59	0.73	0.69
Daidzin	C10216	154.0185	[M-H]-	415.1043	0.86	0.88	1.01	1.03	0.98	1.10	0.86	1.31	0.90	1.01	0.87	0.66
Diethylcarbamazine N-oxide		356.187	[M+H]+	216.1706	1.01	0.79	0.58	1.07	0.72	0.90	0.71	0.61	0.84	0.57	0.88	0.99
Xanthosine	C01762	323.42	[M-H]-	283.0684	0.69	0.52	1.10	0.36	1.00	0.35	0.79	0.09	0.65	0.43	0.67	0.34
L-Valine	C00183	318.035	[M-H]-	116.0711	0.96	0.98	0.89	0.96	0.87	0.99	0.91	0.79	1.12	0.79	1.03	0.90
Sucrose	C00089	382.574	[M-H]-	341.1094	0.75	0.71	0.93	0.70	0.85	0.77	0.50	0.74	0.82	0.79	0.96	1.52
Heptanoic acid	C17714	33.1236	[M-H]-	129.0915	1.42	0.96	0.92	1.09	1.25	1.31	1.26	1.02	1.18	1.47	1.44	1.22
Homocysteine thiolactone		183.5535	[M+H]+	118.0324	1.12	1.51	1.05	0.90	0.93	1.23	0.96	0.68	1.05	0.96	0.95	0.88
Dehydroepiandrosterone sulfate	C04555	29.3498	[M-H]-	367.1585	1.05	0.88	1.14	1.07	1.01	1.25	0.91	1.20	1.02	1.05	1.18	0.95
PE(22:4(7Z,10Z,13Z,16Z)/15:0)		58.15125	[M+H]+	754.5495	0.94	0.88	0.97	0.94	0.96	0.89	0.63	0.96	0.65	0.86	0.87	0.96
1-Methylnicotinamide	C02918	66.9331	[M+H]+	138.0775	1.05	0.79	1.02	1.11	0.91	0.96	0.91	1.19	1.05	0.95	1.00	0.71
Racemethionine		302.759	[M+H]+	150.0585	0.87	1.10	0.90	0.66	0.57	0.97	0.88	0.53	1.07	0.65	0.86	0.87
2-Acetylpyrrolidine		361.0165	[M+H]+	114.0917	0.97	0.94	1.05	0.94	0.95	0.87	1.01	0.72	0.96	0.86	1.00	1.44

Cohibin C		58.1235	[M+H]+	577.5196	0.95	1.20	1.03	0.79	1.03	1.06	0.99	1.01	1.07	1.11	1.04	1.41
Aminoadipic acid	C00956	422.9	[M-H]-	160.0610	0.85	1.30	1.00	1.06	0.83	1.22	1.07	1.20	0.82	0.91	0.81	1.07
LysoPE(0:0/18:3(6Z,9Z,12Z))		224.584	[M+H]+	476.2747	0.85	1.35	1.01	0.73	0.62	1.39	0.90	1.47	0.95	0.97	0.68	0.87
PE(22:5(4Z,7Z,10Z,13Z,16Z)/16:0)		167.917	[M+H]+	766.5369	1.03	0.97	1.14	0.74	0.99	1.01	0.85	0.80	1.02	1.16	0.78	1.04
Isoleucyl-Glycine		379.2465	[M+H]+	189.1234	0.75	0.77	0.65	0.77	0.57	0.79	0.58	0.46	0.56	0.68	0.64	0.67
(±)-erythro-Isoleucine		332.2245	[M+H]+	132.1021	0.94	0.68	0.89	0.75	0.91	0.16	0.91	0.77	0.85	0.77	0.43	0.71
2-Ethylacrylic acid		405.433	[M+H]+	101.0601	0.85	0.68	1.01	0.66	0.90	0.81	0.78	0.46	0.78	0.87	0.98	1.24
Oleamide	C19670	77.6652	[M+H]+	282.2793	0.90	1.04	0.99	0.87	0.99	0.87	0.95	0.88	0.91	0.97	0.85	3.36
PE(20:4(5Z,8Z,11Z,14Z)/15:0)		171.361	[M+H]+	726.5056	1.06	0.93	1.25	1.01	1.03	1.06	0.95	1.00	1.03	1.15	0.93	0.82
Petasitenine	C10359	335.8455	[M+H]+	382.1831	0.98	0.98	1.05	0.84	1.06	0.88	0.87	0.88	0.91	0.98	0.93	0.86
Pentadecanoic acid	C16537	35.1064	[M-H]-	241.2174	1.14	1.08	1.50	1.26	1.59	1.72	1.40	1.11	1.93	1.47	0.88	1.35
Montecristin		128.359	[M+H]+	575.5057	1.04	0.80	0.54	0.59	0.63	0.54	0.69	0.47	0.61	0.64	0.36	0.70
4-Methoxybenzyl propanoate		400.858	[M+H]+	195.1010	1.00	0.86	1.09	1.01	1.00	0.96	0.92	0.95	0.97	0.98	0.93	1.03
Artesunate		446.6055	[M+H]+	385.1830	0.73	0.71	0.92	0.61	0.80	0.72	0.64	0.70	0.65	0.72	0.70	0.77
1,5-Octadien-3-one		34.1703	[M+H]+	125.0962	1.41	1.03	1.19	1.33	1.43	1.21	1.49	1.34	1.25	3.96	1.62	1.32
alpha-Methylstyrene	C14395	35.0915	[M+H]+	119.0857	1.29	1.02	1.32	1.08	1.11	1.11	1.18	1.20	1.14	1.15	1.13	1.13
2'-Methoxy-3-(2,4-dihydroxyphenyl)-1,2-propanediol 4'-glucoside		453.9985	[M+H]+	361.1473	0.83	0.87	1.08	0.70	0.87	0.72	0.65	0.73	0.75	0.87	0.71	0.93
LysoPE(18:1(9Z)/0:0)		222.2085	[M-H]-	478.2937	0.71	1.58	0.65	1.66	0.54	2.12	0.82	1.58	0.84	0.92	0.85	1.25
Acetone cyanohydrin		82.8884	[M+H]+	86.0606	0.93	1.02	0.99	1.06	0.99	0.92	0.96	0.65	0.95	1.03	1.19	1.43
Isobornyl propionate		378.3065	[M+H]+	144.1020	0.76	0.80	0.99	0.67	0.82	0.83	0.81	0.66	0.70	0.86	0.93	1.24

DL-2-Aminooctanoic acid		405.433	[M+H]+	160.1335	0.93	0.95	1.06	0.85	0.93	1.09	0.93	0.96	0.98	0.95	1.07	0.92
Mesylate		116.4635	[M-H]-	94.9801	1.69	0.86	0.92	1.60	1.28	1.03	0.96	1.41	1.26	0.89	1.40	0.96
4-Methylbenzaldehyde	C06758	35.9706	[M+H]+	121.0649	1.62	1.26	1.47	1.32	1.43	1.47	1.54	1.59	1.15	1.56	1.93	1.42
5-Aminopentanoic acid	C00431	405.433	[M+H]+	118.0863	0.85	0.69	0.99	0.66	0.90	0.79	0.78	0.46	0.78	0.87	0.99	1.23
2-Methylguanosine		215.031	[M-H]-	296.1002	0.75	0.80	1.05	0.60	1.04	0.59	0.77	0.41	0.77	0.88	0.65	0.57
Camelledionol		179.1665	[M+H]+	441.3325	0.50	0.79	0.74	0.86	0.63	0.72	0.78	0.92	0.68	0.74	0.76	0.59
Asparaginyl-Proline		344.194	[M+H]+	230.1140	1.11	0.99	1.37	1.22	1.17	1.14	1.08	0.87	1.06	1.08	1.24	0.86
Pyro-L-glutaminyl-L-glutamine		344.187	[M+H]+	258.1087	0.96	0.91	1.03	0.98	1.04	0.88	0.92	0.71	1.00	0.92	1.18	1.29
Tromethamine		19.3439	[M+H]+	122.0814	0.98	0.83	1.07	1.44	1.09	0.99	0.95	1.04	1.04	1.04	1.03	1.03
L-Pipecolic acid	C00408	296.35	[M+H]+	130.0977	1.25	0.53	1.10	0.62	0.68	0.63	1.35	2.57	0.75	0.70	0.94	0.87
6-Deoxocastasterone	C15802	181.779	[M+H]+	451.3791	0.76	0.87	0.97	0.89	0.80	0.72	0.80	0.52	0.73	0.76	0.82	0.65
3-Amino-2-piperidone		265.3125	[M+H]+	115.0869	0.76	0.85	0.80	0.76	0.81	0.83	0.83	0.72	0.77	0.79	0.64	1.70
N-Acetylleucine	C02710	206.058	[M-H]-	172.0975	0.88	0.79	1.02	0.84	0.97	0.80	0.98	0.73	0.95	0.82	1.06	0.96
12-Hydroxydodecanoic acid	C08317	71.15445	[M-H]-	215.1651	0.85	0.86	0.90	1.03	0.63	0.99	1.08	0.96	0.96	0.80	0.84	0.65
Homo-L-arginine	C01924	304.584	[M+H]+	189.1346	0.93	1.24	0.71	0.72	0.68	1.30	0.89	0.96	1.00	1.05	0.95	0.89
Myzodendrone		400.845	[M+H]+	343.1359	0.89	0.92	1.09	0.80	0.92	0.80	0.79	0.70	0.82	0.95	0.80	0.93
Leukotriene D4	C05951	332.156	[M+H]+	497.2725	1.12	1.13	1.23	1.25	1.13	0.97	1.06	0.65	1.52	0.75	1.13	0.64
Isopentyl beta-D-glucoside		151.9595	[M+H]+	251.1502	0.97	0.90	1.03	0.94	1.00	0.90	0.89	1.05	1.01	0.98	1.07	0.90
Leukotriene E4	C05952	330.3035	[M+H]+	440.2513	0.98	0.91	1.05	1.03	1.06	0.89	0.90	0.68	1.28	0.83	1.14	0.78
N-Acetyl-L-alanine		261.03	[M-H]-	130.0504	1.03	0.90	1.01	1.21	1.10	1.10	1.04	1.31	1.22	1.01	1.18	0.90
Nepetaside		473.5525	[M+H]+	347.1674	0.82	0.77	0.92	0.71	0.85	0.77	0.71	0.65	0.80	0.77	0.78	0.76

Pantothenic acid	C00864	284.058	[M-H]-	218.1033	1.27	1.12	1.15	1.13	1.20	1.18	1.00	0.91	1.18	1.21	1.39	1.12
Shikimic acid	C00493	155.765	[M-H]-	173.0450	1.28	1.02	1.14	1.40	1.22	1.60	1.25	1.24	1.29	1.25	1.31	1.19
Isoleucyl-Alanine		373.453	[M+H]+	203.1391	0.91	0.87	1.03	0.93	0.84	0.84	0.83	0.87	0.84	0.91	0.81	0.83
5Z-Dodecenoic acid		47.73065	[M-H]-	197.1546	1.26	1.12	1.79	1.76	0.96	4.53	1.68	1.29	1.45	1.33	1.22	1.00
Cer(d18:0/14:0)		31.27975	[M+H]+	512.5041	1.18	1.20	0.99	0.96	0.96	0.95	1.04	0.96	1.14	1.25	1.15	1.36
3-Methyluridine		76.949	[M-H]-	257.0782	0.91	1.00	1.05	0.87	1.01	0.91	0.96	0.68	0.93	1.01	0.98	1.03
(3S,6E,10E)-1,6,10,14-Phytatetraen-3-ol		34.1746	[M+H]+	291.2683	0.71	0.92	0.79	1.09	1.11	0.98	0.69	0.98	1.02	0.83	0.89	1.28
2-Oxovaleric acid	C06255	67.9769	[M-H]-	115.0396	0.89	1.14	0.88	0.83	0.86	0.91	0.89	2.99	1.04	0.83	1.04	0.73
Ethyl oleate	C03425	41.52665	[M-H]-	309.2807	0.65	0.66	0.96	1.05	0.60	1.00	1.01	0.80	1.07	0.68	0.53	0.60
LysoPC(16:1(9Z)/0:0)	C04230	220.2065	[M+H]+	494.3236	0.78	1.09	0.66	0.64	0.52	1.31	0.69	2.67	0.81	0.82	0.79	0.59
2-Aminoheptanedioic acid		360.82	[M+H]+	176.0918	0.82	0.83	1.00	0.81	0.91	0.89	0.86	0.70	0.85	0.81	0.87	1.36
Ethyl stearate		41.62185	[M-H]-	311.2954	1.20	1.59	1.20	1.26	1.56	2.17	1.91	2.57	1.37	1.27	1.19	1.57
2-Phenylethyl beta-D-glucopyranoside		156.3515	[M+H]+	285.1350	0.98	0.82	1.00	0.91	1.03	0.92	0.90	1.21	1.02	0.92	1.07	0.86
Triethanolamine	C06771	307.367	[M+H]+	150.1127	0.98	0.54	0.70	0.91	0.81	0.89	0.92	1.04	1.28	1.10	0.79	0.84
benzene-1,2,4-triol		128.201	[M-H]-	125.0240	0.47	0.74	0.90	0.53	0.61	0.92	0.69	0.84	0.76	0.73	0.50	0.47
DG(18:2(9Z,12Z)/15:0/0:0)		186.143	[M+H]+	579.4989	0.60	0.76	0.80	0.90	0.78	0.67	0.69	0.47	0.73	0.83	0.75	0.81
PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:3(8Z,11Z,14Z))		230.3065	[M+H]+	858.5269	0.90	0.92	0.93	0.84	0.74	1.01	0.86	0.12	1.03	0.73	0.61	0.19
Hydroxykynurenine	C02794	65.2836	[M-H]-	223.0823	0.53	0.39	0.90	0.39	0.55	1.30	0.83	1.11	0.57	0.41	0.39	0.59
PE(20:5(5Z,8Z,11Z,14Z,17Z)/15:0)		173.947	[M+H]+	724.4928	0.62	0.32	0.80	0.69	0.61	0.53	0.49	0.56	0.56	0.69	0.46	0.57
L-Agaridoxin		442.889	[M+H]+	255.0952	0.72	0.59	0.88	0.55	0.69	0.58	0.66	0.27	0.70	0.80	0.85	2.01
LysoPC(18:4(6Z,9Z,12Z,15Z))	C04230	214.068	[M+H]+	516.3070	0.81	1.24	0.75	0.61	0.48	1.29	0.96	1.34	0.75	0.81	0.70	1.00
Sciadonic acid		34.1921	[M+H]+	307.2627	0.96	1.06	0.97	1.19	1.16	1.07	0.96	0.89	1.15	1.00	1.01	1.19

Nicotinamide riboside	C03150	442.632	[M-H]-	253.0805	0.86	0.93	1.07	0.86	1.05	0.83	1.00	0.11	0.80	0.84	1.14	3.38
6,10,14-Trimethyl-5,9,13-pentadecatrien-2-one		34.2113	[M+H]+	263.2368	0.86	0.88	0.97	1.00	1.11	1.04	0.98	0.99	0.86	0.91	1.00	0.89
Indole	C00463	34.9533	[M+H]+	118.0652	1.06	0.94	1.01	1.02	1.05	1.04	1.08	1.02	0.94	1.19	1.19	0.95
PE(15:0/14:1(9Z))		143.6985	[M+H]+	648.4607	0.89	0.80	0.81	0.80	0.71	0.38	0.76	0.48	0.61	0.73	0.58	0.45
5-Methylcytidine		229.3225	[M-H]-	256.0941	0.83	1.07	1.03	0.81	0.80	0.94	1.01	0.60	0.88	0.98	0.80	0.95
L-Lactic acid	C00186	69.9165	[M-H]-	89.0237	1.04	0.90	1.02	0.95	1.06	1.08	0.99	1.08	1.05	1.00	1.01	0.95
Gingerol	C10462	24.7497	[M-H]-	293.1789	5.13	37.92	0.78	1.07	0.88	0.92	1.08	0.59	1.04	1.38	0.59	0.72
L-cis-3-Amino-2-pyrrolidinecarboxylic acid		396.23	[M+H]+	131.0816	0.91	1.14	1.10	0.94	0.89	0.99	0.94	0.65	0.86	1.05	0.90	1.26
PE(18:2(9Z,12Z)/15:0)		171.356	[M+H]+	702.5086	0.83	0.88	0.87	0.83	0.87	0.89	0.81	0.67	0.81	0.78	0.74	0.86
Succinic anhydride	C19524	61.8233	[M-H]-	99.0081	1.07	1.18	0.79	0.79	0.74	1.11	1.07	1.88	1.32	0.76	0.86	0.50
O-Acetylethanolamine		47.9171	[M+H]+	104.0709	0.77	0.62	0.94	0.65	1.08	0.59	0.64	0.33	0.61	1.02	0.95	1.28
Fragransin B2		35.9309	[M+H-H2O]1+	387.1796	1.12	0.88	1.03	0.98	1.01	1.06	1.05	1.06	0.89	1.16	1.36	1.04
2-Phenylpropionate		82.2269	[M-H]-	149.0602	0.69	0.58	0.80	0.83	0.75	0.70	0.83	1.16	0.86	0.90	0.84	0.71
D-Alanyl-D-alanine	C00993	336.225	[M-H]-	159.0771	0.77	0.49	0.69	0.78	0.96	0.64	0.84	0.34	0.58	0.73	0.95	0.68
LysoPC(14:1(9Z))	C04230	221.775	[M+H]+	466.2934	0.84	1.48	0.79	0.82	0.57	1.46	0.81	2.23	0.99	1.24	0.73	0.67
(R)-3-Hydroxy-tetradecanoic acid		61.8213	[M-H]-	243.1969	0.87	1.25	0.67	0.77	0.54	1.26	0.93	0.76	1.19	0.68	0.71	0.48
Deoxyinosine	C05512	191.6895	[M-H]-	251.0788	0.56	0.77	1.01	0.31	0.47	0.90	1.02	0.43	0.51	0.75	0.56	0.64
Hydroxyphenyllactic acid	C03672	199.665	[M-H]-	181.0506	0.90	0.86	0.94	0.71	1.03	0.70	0.81	0.90	0.97	0.79	0.92	0.67
PE(20:0/18:2(9Z,12Z))		167.9095	[M+H]+	772.5852	0.88	0.79	1.09	0.62	0.94	0.79	0.83	0.83	0.84	1.22	0.88	1.13
LysoPE(0:0/14:0)		223.892	[M+H]+	426.2625	0.70	1.17	0.69	0.61	0.42	1.07	0.97	1.18	0.75	0.71	0.56	0.72
3,5,8-Megastigmatrien-7-one		32.5134	[M+H]+	191.1433	1.11	0.69	0.49	0.94	0.64	1.49	1.08	0.34	0.82	1.31	1.49	0.76
3-Aminocaproic acid		36.8616	[M+H]+	132.1020	0.74	0.97	0.82	0.78	0.92	0.86	0.98	1.03	0.90	0.49	0.54	0.43

L-Threonine	C00188	60.73755	[M+H]+	120.0658	0.99	1.23	0.73	0.75	0.81	1.44	0.86	1.09	1.18	0.79	1.03	1.03
Asparaginyl-Arginine		460.44	[M+H]+	289.1620	0.90	0.96	1.13	0.80	0.98	0.81	0.80	0.80	0.80	0.95	0.82	0.95
3-(5-Methyl-2-furanyl)butanal		46.6348	[M+H]+	153.1024	0.84	0.85	1.19	0.84	0.75	0.96	0.97	1.37	1.09	0.70	1.19	0.74
Thymidine	C00214	326.21	[M-H]-	241.0832	1.03	0.97	1.06	1.13	1.10	1.24	0.95	1.42	1.25	1.00	1.25	0.81
PE(14:1(9Z)/18:0)		134.2785	[M+H]+	690.5076	1.12	1.00	1.28	0.72	0.78	0.88	0.90	0.84	0.76	1.04	0.69	1.23
PE(22:2(13Z,16Z)/14:0)		168.775	[M+H]+	744.5562	0.87	0.82	1.02	0.65	0.97	0.81	0.78	0.72	0.87	1.12	0.81	0.97
Deoxyadenosine	C00559	143.375	[M+H]+	252.1093	0.69	1.14	0.70	0.54	0.44	1.23	0.76	0.88	0.92	0.52	0.60	0.51
gamma-Glutamylvaline		443.794	[M+H]+	247.1291	0.82	0.82	0.96	0.83	0.94	0.76	0.65	0.31	0.75	0.68	0.75	1.64
Diethyl phthalic acid		61.8536	[M-H]-	221.0818	1.20	1.12	1.10	1.43	0.72	5.39	1.43	1.29	1.77	1.05	1.22	0.91
N-Carboxyethyl-g-aminobutyric acid		360.4425	[M-H]-	174.0767	0.79	0.84	0.98	0.78	0.85	0.88	0.86	0.70	0.81	0.81	0.88	1.52
PE(22:2(13Z,16Z)/15:0)		167.9035	[M+H]+	758.5720	0.98	0.94	1.03	0.87	0.99	0.83	0.78	0.91	0.89	1.24	0.83	1.03
2-Dodecanone	C14996	221.97	[M+H]+	285.2423	0.65	1.11	0.67	0.61	0.40	1.03	0.76	1.15	0.70	0.67	0.53	0.70
Biotin	C00120	60.9364	[M-H]-	243.0810	1.01	0.87	1.01	1.08	1.11	0.98	0.96	1.08	1.15	0.88	1.24	0.91
Pyridoxine	C00314	76.61035	[M+H]+	170.0816	0.88	0.93	1.02	0.91	0.93	0.96	0.98	0.80	1.01	0.82	0.93	1.21
N-Acetyl-L-aspartic acid	C01042	403.22	[M-H]-	174.0404	0.80	0.91	0.81	0.68	0.74	0.65	0.68	0.55	0.74	0.77	0.91	1.24
Sissotrin		115.052	[M+FA-H]1-	491.1194	0.83	1.09	0.96	1.10	0.96	1.07	0.86	1.37	0.82	1.11	0.86	0.86
Oxoglutaric acid		378.896	[M-H]-	145.0137	0.90	0.44	1.19	0.78	1.44	0.83	0.50	10.53	0.28	1.45	1.13	2.05
Hypogeic acid		37.0723	[M-H]-	253.2176	0.95	1.04	0.89	1.06	0.68	6.12	1.15	1.11	1.27	0.91	0.89	0.84
15-Methylpalmitate		40.1773	[M-H]-	269.2486	3.69	1.57	3.36	0.89	0.93	1.85	1.39	1.25	1.12	0.90	0.90	1.00
4-Oxo-2-nonenal		35.2778	[M+H]+	155.1066	1.94	1.07	1.16	1.51	1.54	1.24	1.46	1.44	1.19	3.55	2.07	1.22
Thiomorpholine 3-carboxylate	C03901	346.184	[M+H]+	148.0429	0.95	1.07	0.91	0.76	0.79	1.05	0.99	0.60	1.01	0.75	0.90	0.87
Beta-D-Galactose	C00962	69.84215	[M-H]-	179.0558	0.86	0.59	0.80	0.93	0.86	1.03	0.83	1.30	1.26	1.80	1.11	0.84
Hydroxyoctanoic acid		121.261	[M-H]-	159.1022	2.95	0.83	1.94	2.14	0.97	1.27	1.53	0.98	0.94	2.35	0.91	0.86

Parabanic Acid		33.60135	[M-H]-	112.9987	0.82	0.76	0.72	0.84	0.79	0.89	0.81	0.84	0.87	0.86	0.79	0.79
3-(3,4-Dihydroxy-5-methoxy)-2-propenoic acid	C05619	33.5876	[M-H]-	209.0457	1.02	0.87	1.12	1.23	1.42	1.17	0.87	1.30	1.30	1.27	1.02	1.21
PE(20:1(11Z)/15:0)		169.635	[M+H]+	732.5549	1.06	0.94	1.03	0.91	1.01	0.87	0.91	0.97	0.89	1.25	0.99	1.28
Gibberellin A39		371.146	[M+H]+	395.1676	0.76	0.44	0.90	0.65	0.89	0.69	0.74	0.37	0.47	0.89	0.71	0.64
L-Tryptophan	C00078	70.7555	[M-H]-	203.0826	0.99	0.93	1.08	1.03	1.07	1.00	0.95	1.17	1.12	0.93	1.21	0.73
Prolylhydroxyproline		252.416	[M-H]-	227.1034	1.07	0.96	1.03	1.11	1.15	0.93	0.94	1.17	1.19	0.95	1.31	0.76
Monomethyl glutaric acid		137.985	[M-H]-	145.0503	0.89	0.80	0.94	0.83	0.99	0.98	1.04	1.02	0.92	0.84	0.89	0.97
PE(14:0/16:1(9Z))		136.7875	[M+H]+	662.4760	0.68	0.71	0.92	0.99	0.76	0.67	0.71	0.83	0.58	0.60	0.61	0.54
N-Acetylvaline		200.6965	[M-H]-	158.0820	0.88	0.80	0.68	0.99	0.72	0.93	0.69	0.85	0.86	0.68	0.86	0.53
(R)-Pelletierine		34.1919	[M+H]+	142.1227	1.14	1.04	1.15	1.20	1.34	1.14	1.29	1.16	1.23	2.20	1.35	1.11
16-Hydroxy hexadecanoic acid		59.1507	[M-H]-	271.2281	0.95	1.60	0.57	0.79	0.59	1.67	1.13	0.53	1.53	0.49	0.86	0.56
5-Aminoimidazole-4-carboxamide	C04051	369.108	[M+H]+	127.0618	0.92	1.07	1.14	1.17	0.94	1.38	0.73	3.00	1.30	0.97	1.19	1.44
5-Hydroxy-L-tryptophan	C01017	91.47935	[M-H]-	219.0775	0.94	0.82	0.97	0.97	0.96	0.95	0.90	1.00	1.03	0.85	1.09	0.80
Goyaglycoside c		604.9885	[M+H]+	663.4557	0.90	0.82	1.40	1.06	1.42	1.17	0.89	0.80	1.43	0.95	0.88	1.28
Cellulose, microcrystalline		357.149	[M+H]+	371.1567	0.88	0.83	0.98	1.03	0.96	0.59	0.80	0.49	1.03	0.83	0.96	1.04
Dihydrojasmonic acid		54.8498	[M-H]-	211.1341	2.18	1.11	1.60	1.42	1.57	1.42	1.95	4.29	1.59	1.58	1.22	1.40
8,9-DiHETrE	C14773	8.217605	[M-H]-	337.2363	1.01	1.57	0.59	1.55	1.15	1.76	1.37	1.64	1.61	1.29	1.36	1.33
PE(18:1(9Z)/16:0)		169.649	[M+H]+	718.5390	0.96	1.19	1.03	0.82	1.05	0.92	1.01	0.86	0.96	1.21	1.10	1.49
p-Cresol sulfate		23.8679	[M-H]-	187.0070	1.10	0.75	1.08	1.12	1.10	0.98	1.05	1.26	1.29	0.91	1.23	0.77
3,4-Methylenedioxybenzoic acid		22.1015	[M+H]+	165.0190	0.90	0.77	1.02	0.98	0.94	1.25	0.87	0.86	0.91	0.82	0.84	0.96
3,5-Dimethyl-2-vinylpyrazine		7.625995	[M-H]-	135.0920	0.91	0.73	0.88	1.04	0.92	0.98	0.84	0.98	0.78	0.87	0.79	0.64
Pipericine		33.5537	[M+H]+	336.3261	0.93	0.71	1.17	1.48	1.26	1.22	1.07	1.05	1.34	1.42	0.87	1.14

1-Methyluric acid	C16359	15.5206	[M-H]-	181.0364	1.16	1.08	1.27	1.30	1.01	1.25	1.19	1.24	1.11	1.30	1.23	1.07
Diacetone alcohol		33.6234	[M-H]-	115.0758	2.01	1.05	1.62	1.46	1.75	1.40	1.78	1.20	2.03	2.47	1.73	1.92
Isonicotinic acid	C07446	227.965	[M-H]-	122.0241	0.91	1.16	1.24	0.74	0.91	0.73	0.74	0.09	0.61	1.17	0.78	0.87
5,6-DHET	C14772	44.3245	[M-H]-	337.2363	0.99	1.30	0.74	0.79	0.74	1.04	1.10	1.56	1.02	0.61	0.94	0.89
Homoarecoline		226.632	[M+H]+	170.1178	1.50	1.26	1.16	1.41	1.18	1.22	2.00	1.65	1.22	2.29	1.57	1.26
UDP-N-acetylmuraminate	C01050	448.207	[M-H]-	678.0981	0.62	0.55	0.76	0.55	0.63	0.75	0.62	0.64	0.58	0.56	0.61	0.47
PS(20:2(11Z,14Z)/15:0)		215.919	[M+H]+	774.5294	0.92	1.90	1.24	0.80	1.15	0.80	1.05	0.58	0.88	0.94	1.08	1.32
N-methyl-L-glutamic Acid	C01046	268.8575	[M-H]-	160.0611	0.95	0.72	0.98	0.91	1.05	1.03	0.97	1.23	1.07	0.95	1.22	0.66
Eicosapentaenoic acid	C06428	34.91355	[M-H]-	301.2177	2.75	0.16	0.13	2.33	0.11	0.15	0.11	0.97	0.17	0.57	0.26	0.20
Phenylacetylglycine	C05598	185.424	[M-H]-	192.0664	0.87	0.72	0.64	0.94	0.65	0.83	0.63	0.78	0.77	0.58	0.80	0.50
Deoxycholic acid	C04483	49.25355	[M+Na]1+	415.2804	301.19	80.75	1.05	316.09	114.91	139.41	457.57	228.55	174.85	595.83	353.17	114.86
Aspartyl-Valine		442.887	[M+H]+	233.1130	0.90	0.76	1.04	0.77	1.02	0.73	0.80	0.18	0.89	0.74	0.97	3.35
Linoleoyl ethanolamide		34.4013	[M+H]+	324.2899	0.84	0.98	0.86	1.10	1.09	1.00	0.91	0.84	1.04	0.97	0.95	1.05
PS(16:0/22:0)		57.2819	[M+H]+	820.6080	0.78	0.74	0.90	0.77	0.94	0.82	0.78	0.79	0.79	0.93	0.74	0.89
D-1-Amino-2-pyrrolidinecarboxylic acid		34.4608	[M+H]+	131.0856	1.17	0.41	0.93	0.83	1.15	0.98	0.94	0.89	1.03	1.45	1.37	0.80
N-Acetyl-L-phenylalanine	C03519	190.798	[M-H]-	206.0822	0.89	0.68	0.91	0.92	0.93	0.82	0.83	0.84	0.96	0.79	1.01	0.69

Table S6 Pathway impact analysis of significant metabolic pathways in model bacteria under low and high level of nanomaterial exposures. Data analysis was conducted by the open source platform MetaboAnalyst

Dysregulated pathway	**Dysregulated metabolites (KEGG ID)**	**Pathway impact**											
		PS-L	**PS-H**	**Ag-L**	**Ag-H**	**TiO_2-L**	**TiO_2-H**	**ZnO-L**	**ZnO-H**	**CDs-L**	**CDs-H**	**QDs-L**	**QDs-H**
Arginine and proline metabolism	N-Acetyl-L-alanine (C00624); L-Arginine (C00062); L-Proline (C00148); Hydroxyproline (C01157); N-Acetylputrescine (C02714)	0.062	0.062		0.062		0.038	0.038	0.038	0.062			0.062

Biotin metabolism	Dethiobiotin (C01909); Biotin (C00120)							0.214	0.214			0.214
Cysteine and methionine metabolism	5'-Methylthioadenosine (C00170)		0.031	0.031		0.031	0.031	0.031	0.031	0.031		
Nicotinate and nicotinamide metabolism	Nicotinamide riboside (C03150)	0.028		0.028				0.028	0.028			0.028
Peptidoglycan biosynthesis	D-Alanyl-D-alanine (C00993)	0.066	0.066	0.066		0.066		0.066		0.066		
Phenylalanine metabolism	Phenylethylamine (C05332); Phenylacetaldehyde (C00601); Succinic acid (C00042); L-Phenylalanine (C00079)							0.006		0.006		0.006
Purine metabolism	Deoxyinosine (C05512); Xanthosine (C01762); Adenosine (C00212); Adenine (C00147); Deoxyguanosine (C00330); Guanosine (C00387); Cyclic AMP (C00575)		0.001	0.004				0.016	0.004		0.001	0.001
Pyrimidine metabolism	Uridine (C00299); Thymidine (C00214)				0.011			0.055	0.044			
Pyruvate metabolism	L-Lactic acid (C00186)		0.073					0.073				
Tryptophan metabolism	L-Tryptophan (C00078)							0.200	0.200			0.200
Vitamin B6 metabolism	Pyridoxine (C00314)									0.046		0.046