

Figure S1. Superposition diagram of total ion flow diagram (TIC diagram, a) detected by mass spectrometry, MRM metabolite detection multi peak (b) and Tlc overlap diagram (c) of the mixed QC sample. The abscissa is the retention time (RT) of the metabolite detection, and the ordinate is the ion current intensity of ion detection (the intensity unit is CPS, count per second). The multi-reaction monitoring-mode MRM metabolite detection multi-peak diagram in the figure shows the substances that can be detected in the sample, and the chromatographic peaks of different colors represent different metabolites detected. The characteristic ions of each substance are screened through the triple quadrupole, and the signal strength (CPS) of the characteristic ions is obtained in the detector. The sample machine mass spectrometry file is opened with multiquant software to integrate and

[illegible]

Figure S2. The integral correction chart and variability for metabolite **semi**-quantitative analysis. (a), integral correction chart of metabolite **semi**-quantitative analysis. The figure shows the **semi**-quantitative analysis integration correction results of randomly selected metabolites in different samples. The abscissa is the retention time (min) of metabolite detection, the ordinate is the ion current intensity (CPS) of a metabolite ion detection, and the peak area represents the relative content of the substance in the sample. (b), the overall metabolic difference between samples in each group and the variability between samples in the group. (c), the variability between different groups and among samples in the group. (d), Analytical metabolome data according to oppls-da model; we may draw a score map of each group and further show the differences between each group. The prediction parameters of the evaluation model include R^2X , R^2Y and Q^2 , wherein R^2X and R^2Y , respectively represent the interpretation rate of the built model to the X and Y matrices, Q^2 represents the prediction ability of the model, the closer these three indicators are to 1, the more stable and reliable the model is. $Q^2 > 0.5$ can be considered as an effective model, and $Q^2 > 0.9$ is an excellent model. (e), the S-plot diagram of OPLS-DA; the abscissa represents the correlation coefficient between the principal component and the metabolite, and the ordinate represents the correlation coefficient between the principal component and the metabolite. The closer the metabolite is to the upper right corner and lower left corner, the more significant the difference is. The red point indicates that the VIP value of these metabolites is greater than or equal to 1, and the green point indicates that the VIP value of these metabolites is less than 1.

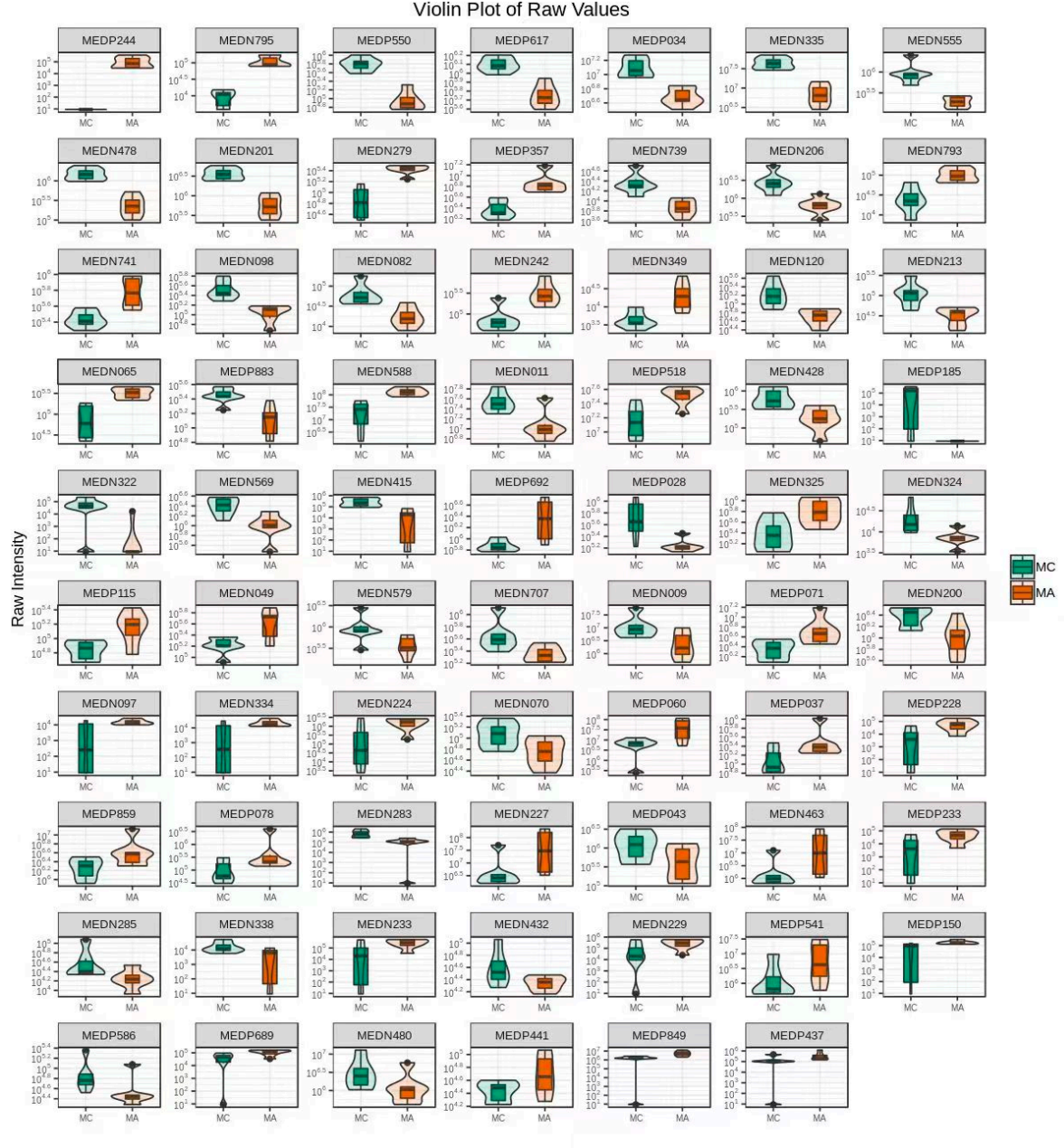
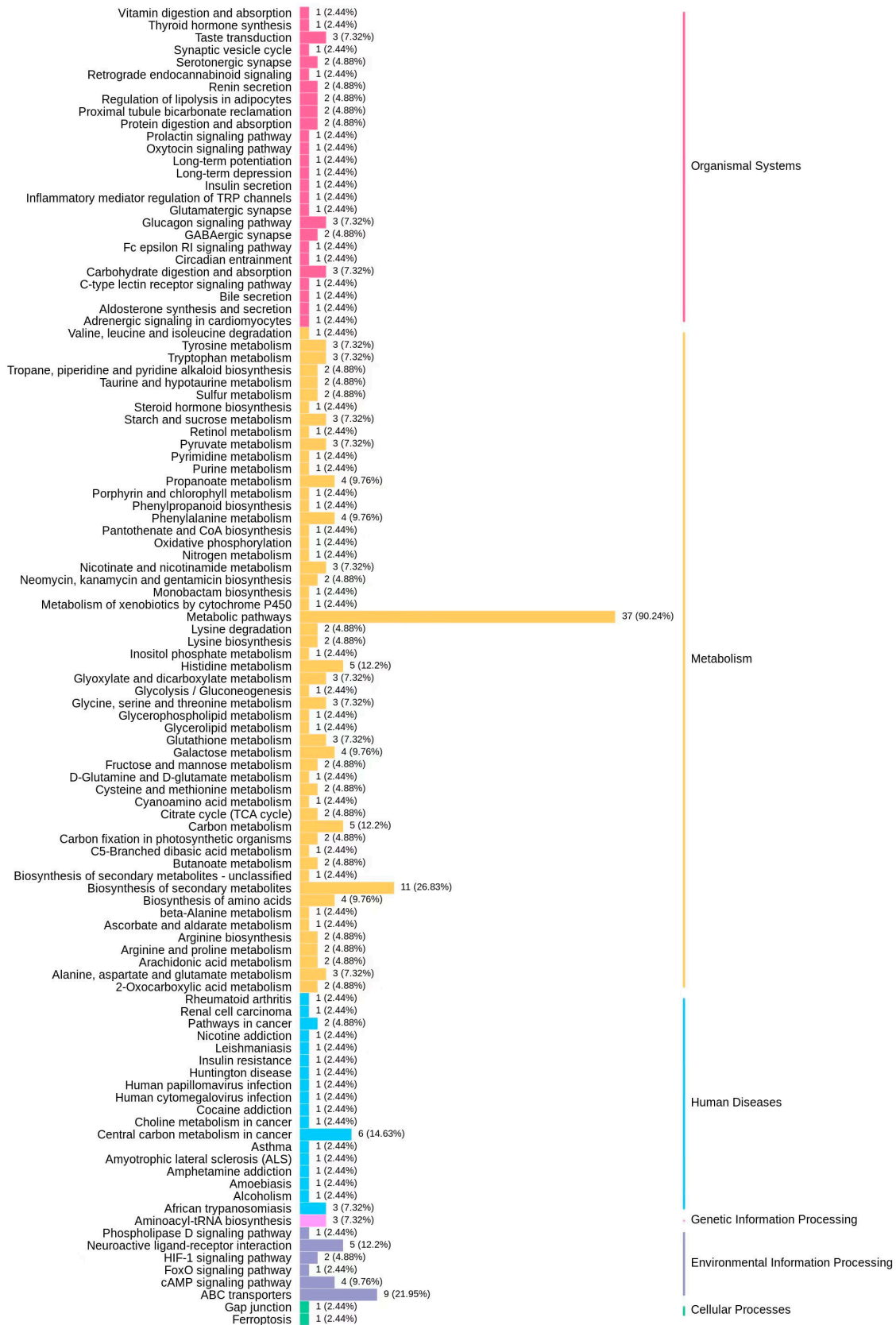


Figure S3. The data distribution and its probability density via the violin diagram. The middle box represents the quartile range, the thin line extending from it represents the 95% confidence interval, the black horizontal line in the middle is the median, and the outer shape represents the distribution density of the data.

KEGG Classification



0 6 12 20 28 36 44 52 60 68 76 84 92
Percent (%)

Figure S4. A metabolite with significant difference; the classification diagram is made according to the types of pathways in KEGG, according to the annotation results of KEGG. The ordinate is the name of the KEGG metabolic pathway, and the abscissa is the number of metabolites annotated to the pathway and its proportion to the total number of metabolites annotated.

Table S1. The numbers of the significant expression metabolites and partial calculation results of orthogonal partial least squares discriminant analysis (OPLS-DA) metabolite database mapping table.

Index	Compounds	Class	VIP/ty pe	KEG G CID	HMDB	Pubch em CID
003	MEDN Glycine	Amino acid metabolom ics	1.165	C000 37	HMDB00 123	750
005	MEDN L- Threonine	Amino acid metabolom ics	0.556	C001 88	HMDB00 167	6288
009	MEDN L- Aspartic Acid	Amino acid metabolom ics	1.489 ↓	C000 49	HMDB00 191	5960
011	MEDN L- Glutamic Acid	Amino acid metabolom ics	1.675 ↓	C000 25	HMDB00 148	33032
012	MEDN L- Histidine	Amino acid metabolom ics	0.059	C001 35	HMDB00 177	6274
013	MEDN L- Isoleucine	Amino acid metabolom ics	1.196	C004 07	HMDB00 172	6306
018	MEDN L-Serine	Amino acid metabolom ics	0.310	C000 65	HMDB00 187	5951

Index	Compounds	Class	VIP/typ	KEGG G CID	HMDB	Pubchem CID
		Amino				
019	MEDN L-Tryptophan	acid metabolomics	0.519	C00078	HMDB00929	6305
		Amino				
028	MEDN 4-Hydroxy-L-Glutamic Acid	acid metabolomics	0.329	C03079	HMDB02273	5460078
		Organic acid and its derivatives				
032	MEDN Allantoin	c acid and its derivatives	0.193	C01551	HMDB00462	204

Note: PLS-DA based on the results of opsls-da, the obtained multivariable analysis of the variable importance in projection (VIP) of the opsls-da model.

Table S2. The shared and specific proteins in the detected tissues of the ‘iron prawn’ *M. rosenbergii*.

Comparison group	Index	Compounds	Class	L og2FC	T ype
MA vs. MB	ME	Epinephrine	Hormones	19	u
	DP185			.36	p
	ME	4-Pyridoxic Acid	Pyridine and pyridine derivatives	16	u
	DP118			.31	p
	ME	N1-Acetylspermine	Organic acid and its derivatives	6.	u
	DP576			85	p
	ME	5-Aminovaleric Acid	Organic acid and its derivatives	3.	u
	DP297			18	p
	ME	(5-L-Glutamyl)-L-Amino Acid	Amino acid metabolomics	3.	u
	DP028			16	p
	ME	Guanidineacetic Acid	Organic acid and its derivatives	2.	u
	DP313			97	p
	ME	8-Hydroxyguanosine	Nucleotide metabolomics	2.	u
	DP158			92	p
	ME	Indoleacrylic acid	Organic acid and its derivatives	2.	u
	DN551			57	p
	ME	Kinurenine	Organic acid and its derivatives	2.	u
	DN322			50	p
	ME	D-Fructose-1,6-Biphosphate-Trisodium Salt	Carbohydrate metabolomics	2.	u
	DN485			04	p
	ME	Lysopc 18:0	Lipids others phospholipid	-	d
	DP342			2.00	own
	ME	Cysteine glutathione disulfide	Amino acid metabolomics	-	d
	DN822			2.11	own
	ME	Lysopc 17:0	Lipids others phospholipid	-	d
	DP434			2.30	own
	ME	Lysopc 20:2	Lipids others phospholipid	-	d
	DP352			2.33	own

MC vs. MA	ME	Lysopc 20:1	Lipids	others	-	d
	DP350		phospholipid		2.37	own
	ME	Guanosine	3',5'-Cyclic	Nucleotide	-	d
	DN161	Monophosphate	metabolomics		2.69	own
	ME	Sn-Glycero-3-Phosphocholine	Cholines		-	d
	DP442				2.81	own
	ME	Phe-Phe	Amino	acid	-	d
	DP078		metabolomics		2.88	own
	ME	δ-Valerolactam	Pyridine	and	-	d
	DP541		pyridine derivatives		3.00	own
	ME	Ginkgoic acid	Organic	acid and	-	d
	DN636		its derivatives		3.07	own
	ME	L- tyrosine methyl ester	Amino	acid	-	d
	DP664		metabolomics		3.46	own
	ME	N-Acetyl-5-Hydroxytryptamine	Tryptamines	and	-	d
	DP212		its derivatives		3.66	own
	ME	S-Sulfo-L-Cysteine	Amino	acid	-	d
	DN071		metabolomics		11.86	own
	ME	All-Trans-13,14-Dihydroretinol	Coothersenzyme		13	u
	DP244		factor and vitamin		.89	p
	ME	PGF2α [9α,11α,15S-trihydroxy- prosta-5Z,13E-dien-1-oic acid]	Oxidized lipid		3.	u
	DN795				54	p
	ME	D-Fructose	6-Phosphate-	Carbohydrate	3.	u
	DN463	Disodium Salt	metabolomics		45	p
	ME	D-Glucose 6-Phosphate	Carbohydrate		3.	u
	DN227		metabolomics		11	p
	ME	Methionine Sulfoxide	Amino	acid	3.	u
	DP060		metabolomics		00	p
	ME	Phe-Phe	Amino	acid	2.	u
	DP078		metabolomics		79	p
	ME	D-Melezitose	Carbohydrate		2.	u
	DP228		metabolomics		51	p
	ME	PGD2 [9α,15S-dihydroxy-11-oxo- prosta-5Z,13E-dien-1-oic acid]	Oxidized lipid		2.	u
	DN349				50	p
	ME	Glycerol 3-phosphate	Lipids_fatty acids		2.	u
	DN588				32	p
	ME	δ-Valerolactam	Pyridine	and	2.	u
	DP541		pyridine derivatives		31	p
	ME	Raffinose	Carbohydrate		2.	u
	DP233		metabolomics		01	p
	ME	L-Aspartic Acid	Amino	acid	-	d
	DN009		metabolomics		2.23	own
	ME	Citramalic Acid	Amino	acid	-	d
	DN206		metabolomics		2.26	own
	ME	Hydroxyphenyllactic acid	Carbohydrate		-	d
	DN555		metabolomics		2.43	own
	ME	Aminomalonic Acid	Organic	acid and	-	d
	DN478		its derivatives		2.56	own
	ME	Methylmalonic Acid	Organic	acid and	-	d
	DN335		its derivatives		2.59	own
	ME	Succinic Acid	Amino	acid	-	d
	DN201		metabolomics		2.59	own
	ME	18-Hydroxycorticosterone	Lipids		-	d
	DP550				2.72	own

MC vs. MD	ME DN283	2-Hydroxybutanoic Acid	Organic acid and its derivatives	- 2.85	d own
	ME DN415	2-(Formylamino)Benzoic Acid	Benzene and substituted derivatives	- 3.85	d own
	ME DN322	Kinurenine	Organic acid and its derivatives	- 4.70	d own
	ME DP185	Epinephrine	Hormones	- 14.08	d own
	ME DP244	All-Trans-13,14-Dihydroretinol	Coothersenzyme factor and vitamin	11 .58	u p
	ME DP233	Raffinose	Carbohydrate metabolomics	2. 51	u p
	ME DN224	D-Trehalose	Carbohydrate metabolomics	2. 50	u p
	ME DN229	Lactose	Carbohydrate metabolomics	2. 41	u p
	ME DP028	(5-L-Glutamyl)-L-Amino Acid	Amino acid metabolomics	2. 34	u p
	ME DN283	2-Hydroxybutanoic Acid	Organic acid and its derivatives	- 2.04	d own
MD vs. MB	ME DP391	Menaquinone	Coothersenzyme factor and vitamin	- 2.36	d own
	ME DN487	Allysine	Organic acid and its derivatives	- 2.61	d own
	ME DN109	Hyodeoxycholic Acid	Bile acids	- 2.80	d own
	ME DP630	Methyl jasmonate	Lipids_fatty acids	- 2.96	d own
	ME DN225	D-Xylose	Carbohydrate metabolomics	- 3.31	d own
	ME DP576	N1-Acetylspermine	Organic acid and its derivatives	- 10.21	d own
	ME DP576	N1-Acetylspermine	Organic acid and its derivatives	15 .79	u p
	ME DN551	Indoleacrylic acid	Organic acid and its derivatives	5. 67	u p
	ME DP313	Guanidineacetic Acid	Organic acid and its derivatives	4. 01	u p
	ME DP297	5-Aminovaleric Acid	Organic acid and its derivatives	3. 89	u p
	ME DP384	Isoxanthopterin	Pteridines and derivatives	3. 39	u p
	ME DN225	D-Xylose	Carbohydrate metabolomics	3. 27	u p
	ME DP689	TranexamicAcid	Organic acid and its derivatives	3. 06	u p
	ME DP296	4-Guanidinobutyric Acid	Organic acid and its derivatives	3. 03	u p
	ME DN109	Hyodeoxycholic Acid	Bile acids	2. 97	u p
	ME DP630	Methyl jasmonate	Lipids_fatty acids	2. 90	u p
	ME DP123	Acetylcholine Chloride	Cholines	2. 78	u p

ME	8-Hydroxyguanosine	Nucleotide	2.	u
DP158		metabolomics	63	p
ME	DI-Glyceraldehyde3-Phosphate	Organic acid and	2.	u
DN480		its derivatives	60	p
ME	Urocanic Acid	Organic acid and	2.	u
DP357		its derivatives	41	p
ME	Creatine	Organic acid and	2.	u
DN305		its derivatives	30	p
ME	2-Methylbutyroylcarnitine	Lipids_fatty acids	2.	u
DP618			19	p
ME	D-Glucose 6-Phosphate	Carbohydrate	2.	u
DN227		metabolomics	13	p
ME	D-Fructose 6-Phosphate-	Carbohydrate	2.	u
DN463	Disodium Salt	metabolomics	02	p
ME	Lysope 18:1	Lipids others	-	d
DN362		phospholipid	2.07	own
ME	Cysteine glutathione disulfide	Amino acid	-	d
DN822		metabolomics	2.09	own
ME	Lysope 14:0	Lipids others	-	d
DN368		phospholipid	2.16	own
ME	Lysopc 18:3	Lipids others	-	d
DP498		phospholipid	2.16	own
ME	Lysopa 16:0	Lipids others	-	d
DN372		phospholipid	2.23	own
ME	Methylmalonic Acid	Organic acid and	-	d
DN335		its derivatives	2.27	own
ME	Lysopc 18:2	Lipids others	-	d
DP346		phospholipid	2.28	own
ME	Lysopc 16:0	Lipids others	-	d
DP338		phospholipid	2.29	own
ME	Succinic Acid	Amino acid	-	d
DN201		metabolomics	2.30	own
ME	Riboflavin	Coothersenzym	-	d
DP250		factor and vitamin	2.31	own
ME	Aminomalonic Acid	Organic acid and	-	d
DN478		its derivatives	2.31	own
ME	Lysopc 17:0	Lipids others	-	d
DP434		phospholipid	2.33	own
ME	Lysope 16:0	Lipids others	-	d
DN366		phospholipid	2.36	own
ME	L-Aspartic Acid	Amino acid	-	d
DN009		metabolomics	2.37	own
ME	Kinurenine	Organic acid and	-	d
DN322		its derivatives	2.49	own
ME	LysoPE(16:1(9Z)-0:0)	Lipids_fatty acids	-	d
DP638			2.51	own
ME	Lysopc 15:0	Lipids others	-	d
DP494		phospholipid	2.57	own
ME	Ginkgoic acid	Organic acid and	-	d
DN636		its derivatives	2.62	own
ME	Lysopc 18:1	Lipids others	-	d
DP344		phospholipid	2.63	own
ME	PAF C-16	Lipids	-	d
DP537			2.75	own

ME	Lysopc 18:0	Lipids	others	-	d
DP342		phospholipid		2.78	own
ME	Lysopc 14:0	Lipids	others	-	d
DP336		phospholipid		3.00	own
ME	18-Hydroxycorticosterone	Lipids		-	d
DP550				3.01	own
ME	Lysopc 20:2	Lipids	others	-	d
DP352		phospholipid		3.14	own
ME	Lysopc 16:1	Lipids	others	-	d
DP340		phospholipid		3.16	own
ME	N-Acetyl-5-Hydroxytryptamine	Tryptamines	and	-	d
DP212		its derivatives		3.40	own
ME	N6-Succinyl Adenosine	Nucleotide		-	d
DN428		metabolomics		4.07	own
ME	Lysopc 20:1	Lipids	others	-	d
DP350		phospholipid		4.44	own
ME	S-Sulfo-L-Cysteine	Amino	acid	-	d
DN071		metabolomics		12.61	own