

Figure S1 Assessment of QC samples.

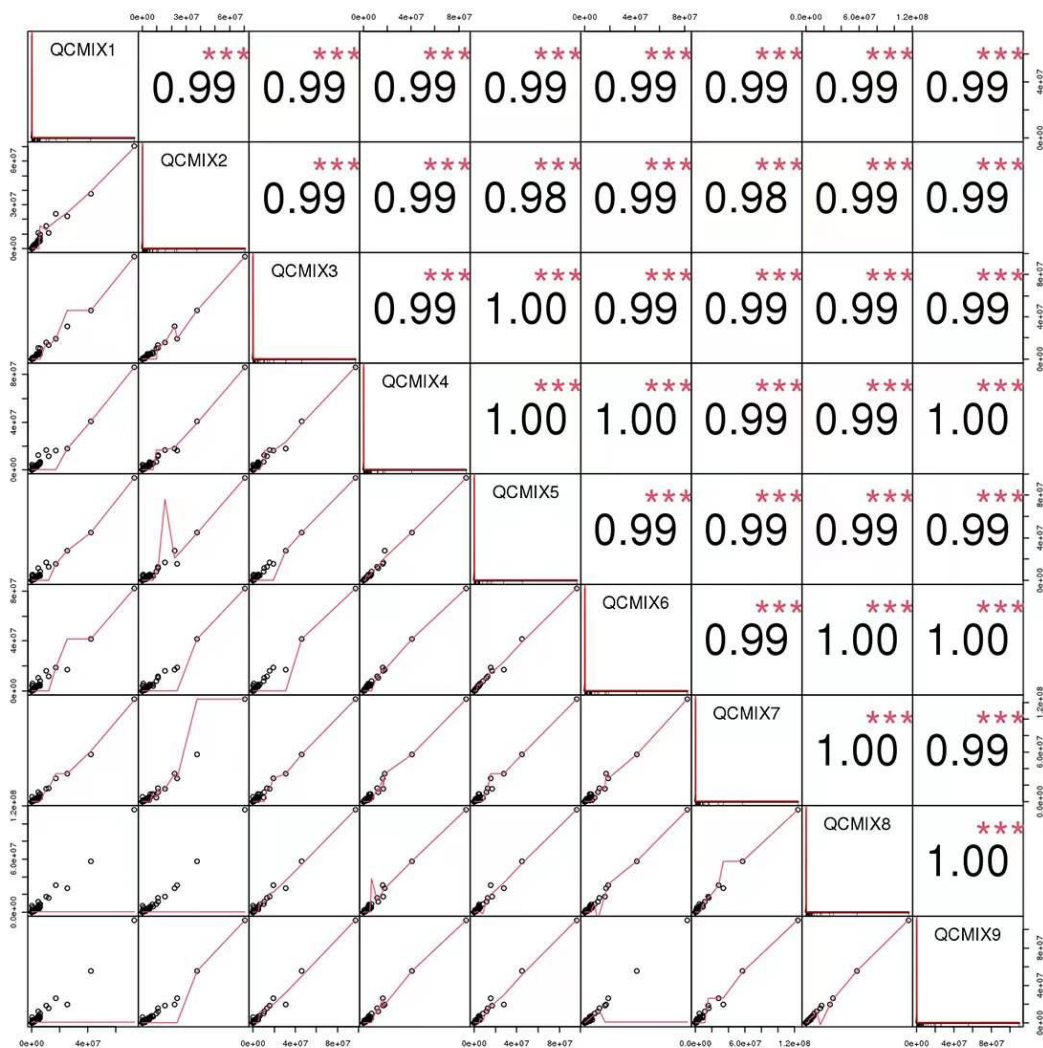


Figure S2 LC/MS serum chromatogram of QC sample

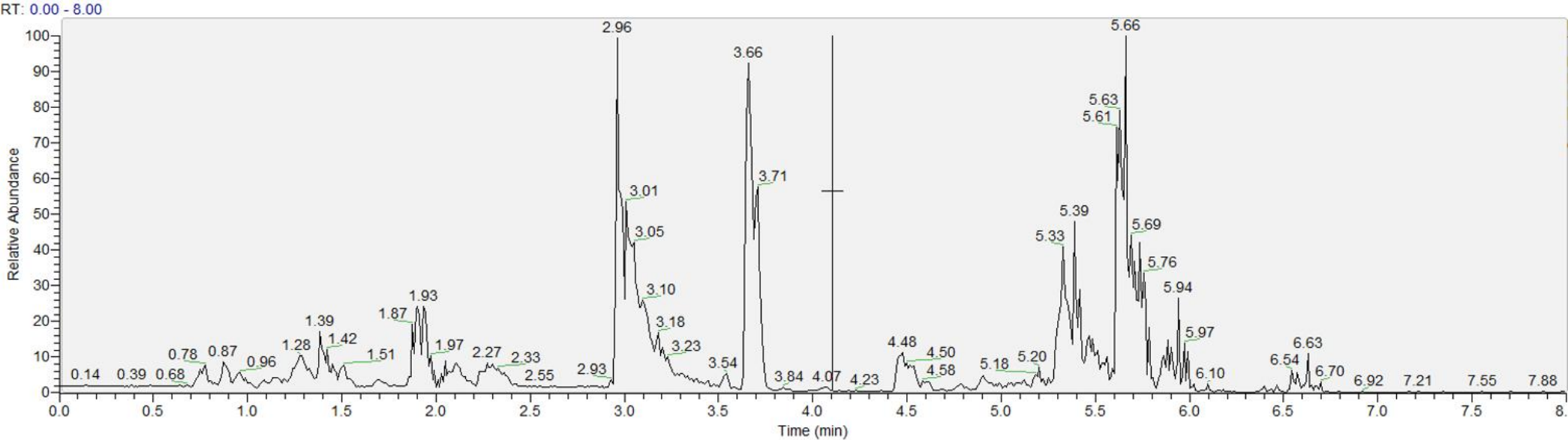


Figure S3 Metabolic profiling variation. **(a)** Score plot of the unsupervised PCA model among the CRC and HC. **(b)** One hundred permutation tests of the OPLS-DA model based on CRC and HC serum metabolome. $R^2=(0.0,0.815)$ $Q^2=(0.0,-0.421)$.

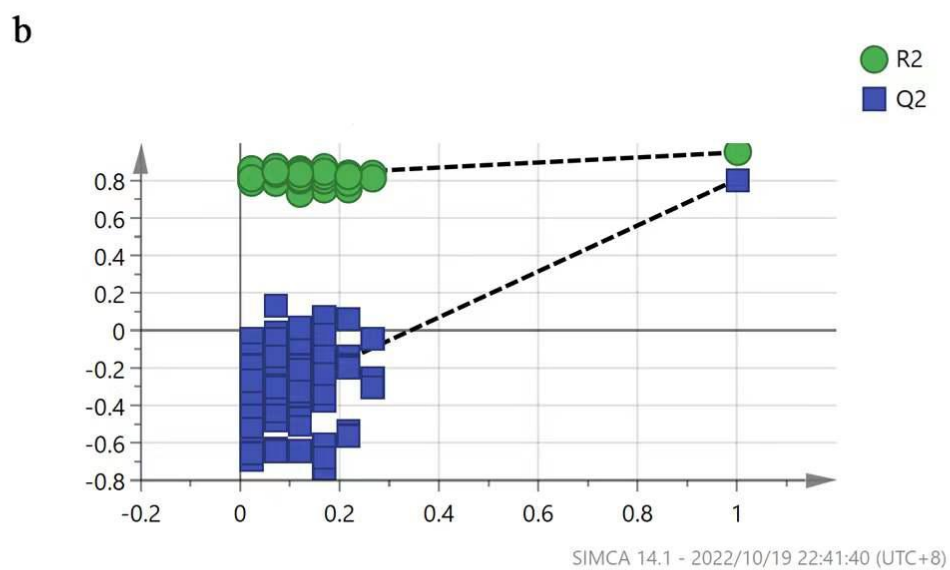
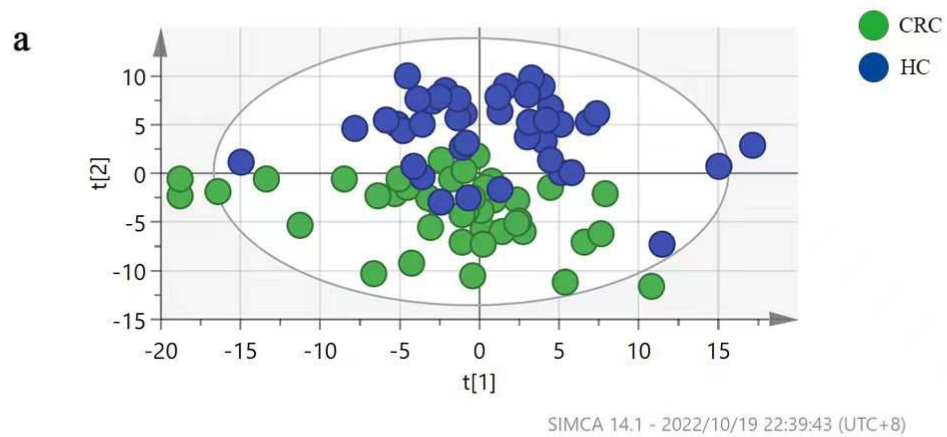
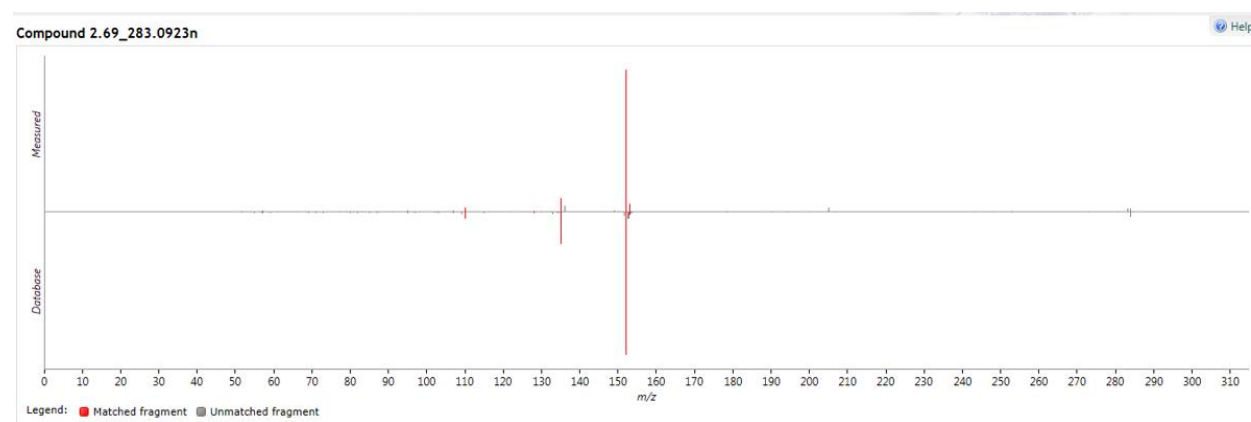


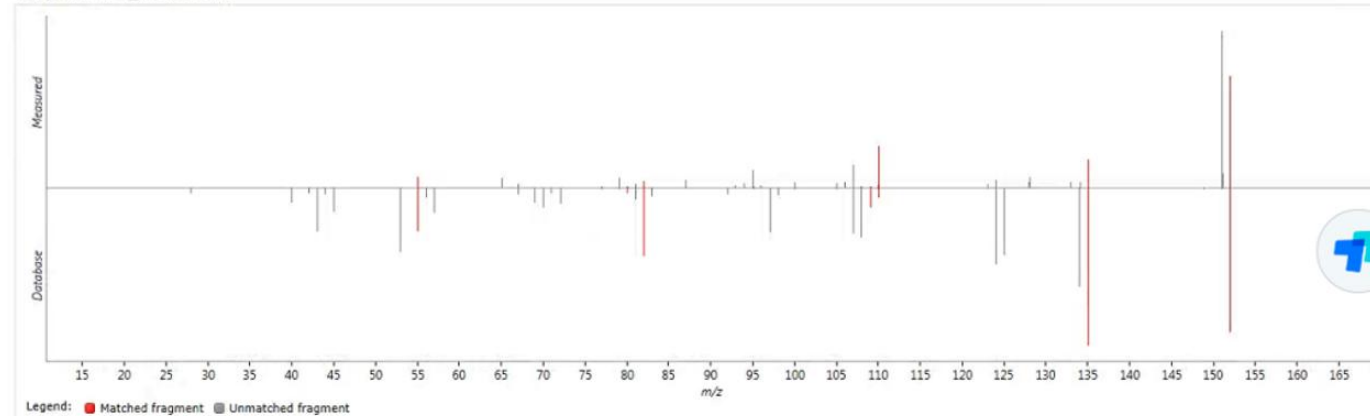
Figure S4 Mass spectra of 9 metabolites

Metabolite	Compound	Compound ID	Adducts	Formula	Score	Fragmentation Score
Guanosine	2.69_283.0923n	HMDB0000133	M+H, M+Na	C10H13N5O5	52	69.8



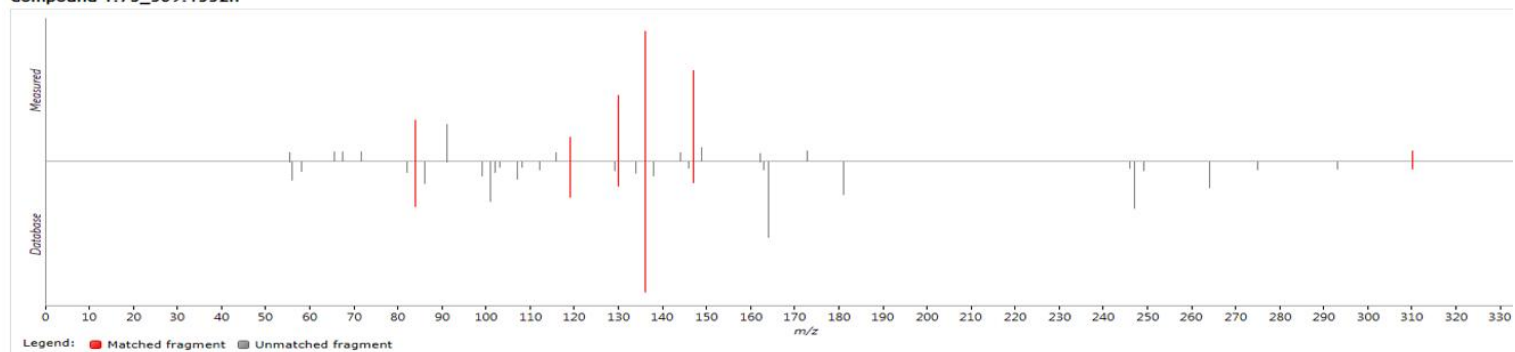
Metabolite	Compound	Compound ID	Adducts	Formula	Score	Fragmentation Score
2-Hydroxyadenine	2.69_152.0569m/z	HMDB0000403	M+H	C5H5N5O	42.7	18.6

Compound 2.69_152.0569m/z



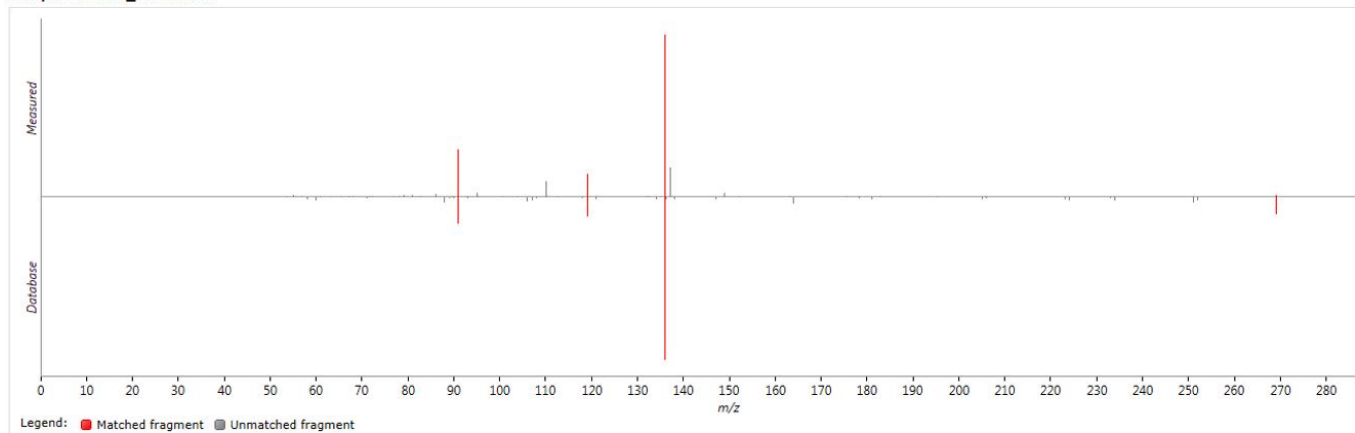
Metabolite	Compound	Compound ID	Adducts	Formula	Score	Fragmentation Score
Tyrosyl-Gamma-glutamate	1.75_309.1332n	HMDB0029119	M+H, M+Na	C14H19N3O5	43.3	26.7

Compound 1.75_309.1332n



Metabolite	Compound	Compound ID	Adducts	Formula	Score	Fragmentation Score
Tyr Ser	1.60_268.1064n	METLIN23814	M+H, M+Na	C12H16N2O5	49.6	56

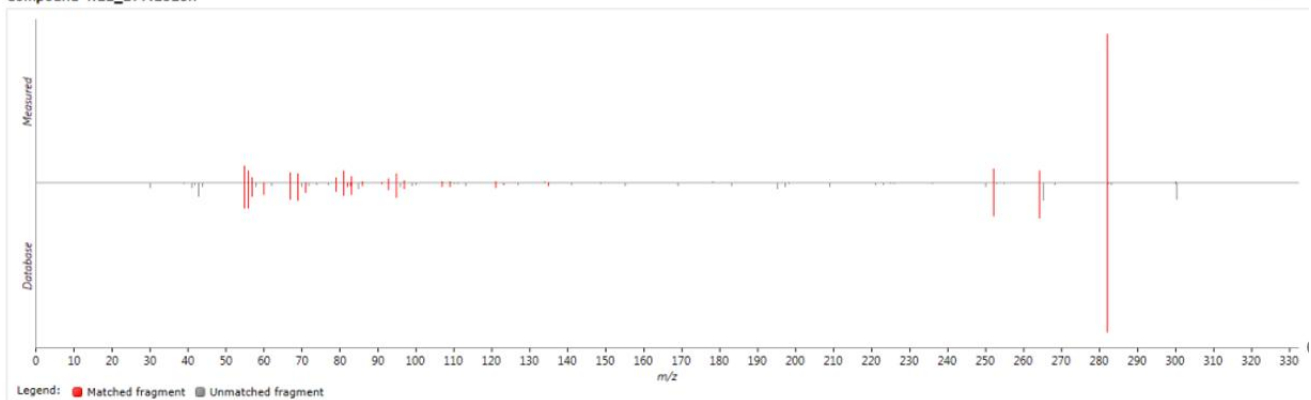
Compound 1.60_268.1064n



Metabolite	Compound	Compound ID	Adducts	Formula	Score	Fragmentation Score
Sphingosine	4.22_299.2828n	HMDB0000252	M+H-H ₂ O, M+H	C ₁₈ H ₃₇ NO ₂	51.5	63.1

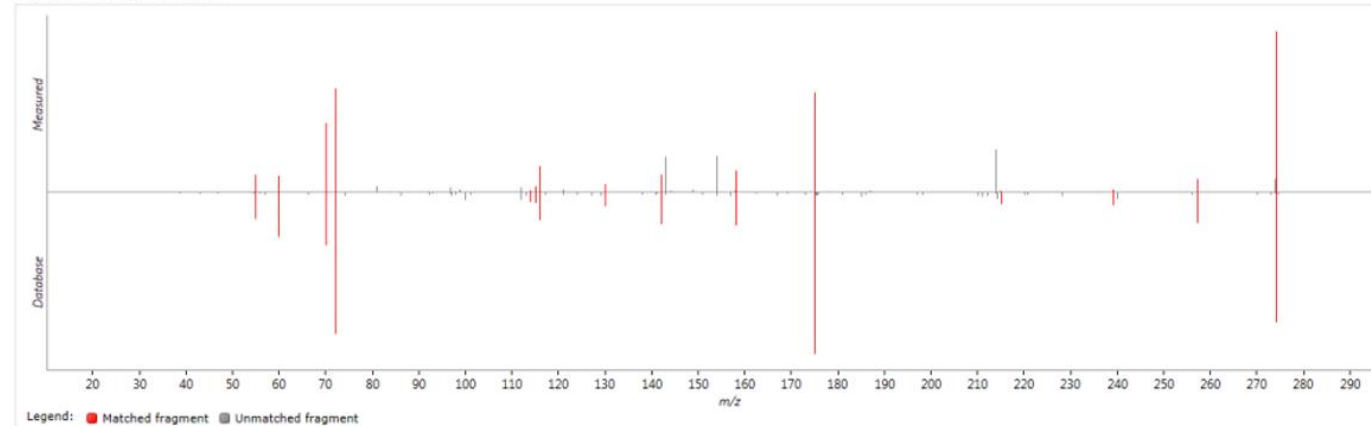
Compound 4.22_299.2828n

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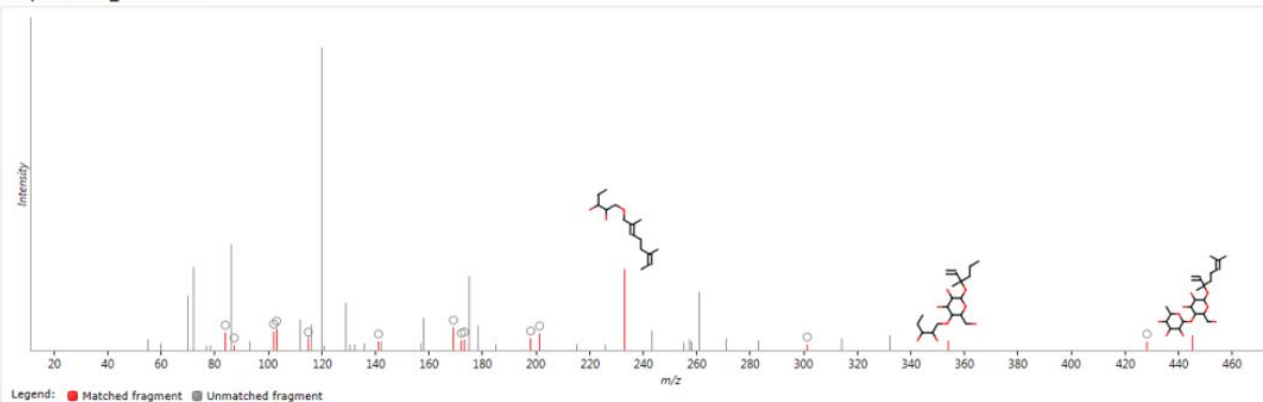
Metabolite	Compound	Compound ID	Adducts	Formula	Score	Fragmentation Score
Val Arg	0.94_273.1806n	METLIN23912	M+H, M+Na	C ₁₁ H ₂₃ N ₅ O ₃	49.3	56

Compound 0.94_273.1806n



Metabolite	Compound	Compound ID	Adducts	Formula	Score	Fragmentation Score
Lyciumoside VI	2.99_905.4851m/z	HMDB0033500	M+H-H ₂ O	C ₄₄ H ₇₄ O ₂₀	44	48.4

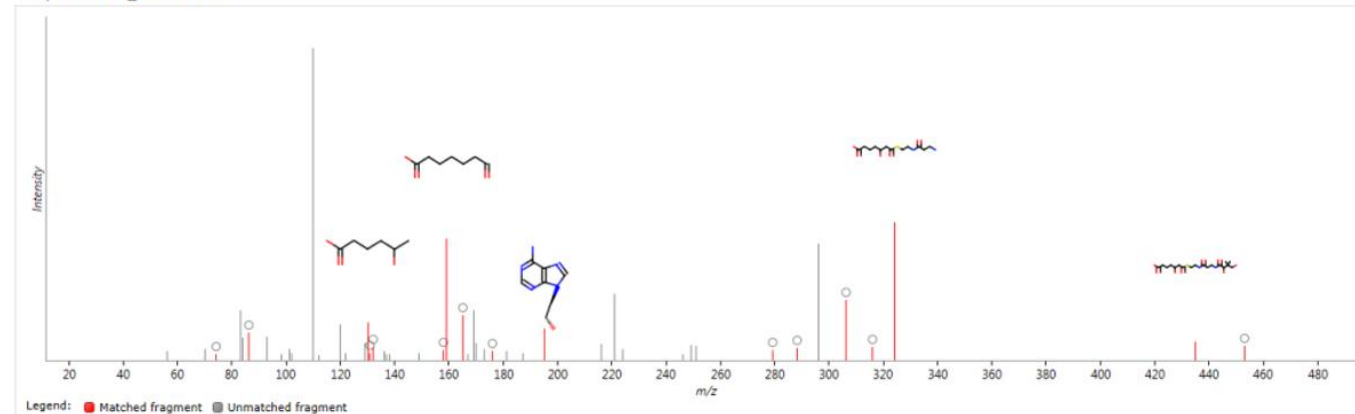
Compound 2.99_905.4851m/z



Metabolite	Compound	Compound ID	Adducts	Formula	Score	Fragmentation Score
3-Hydroxypimelyl-CoA	3.03_943.2078m/z	HMDB0012155	M+NH4	C ₂₈ H ₄₆ N ₇ O ₂₀ P ₃ S	46	66.4

Compound 3.03_943.2078m/z

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Metabolite	Compound	Compound ID	Adducts	Formula	Score	Fragmentation Score
N-Phenylacetylaspartic acid	2.93_251.0804n	HMDB0029355	M+H, M+NH4	C ₁₂ H ₁₃ NO ₅	45.1	34.5

Compound 2.93_251.0804n

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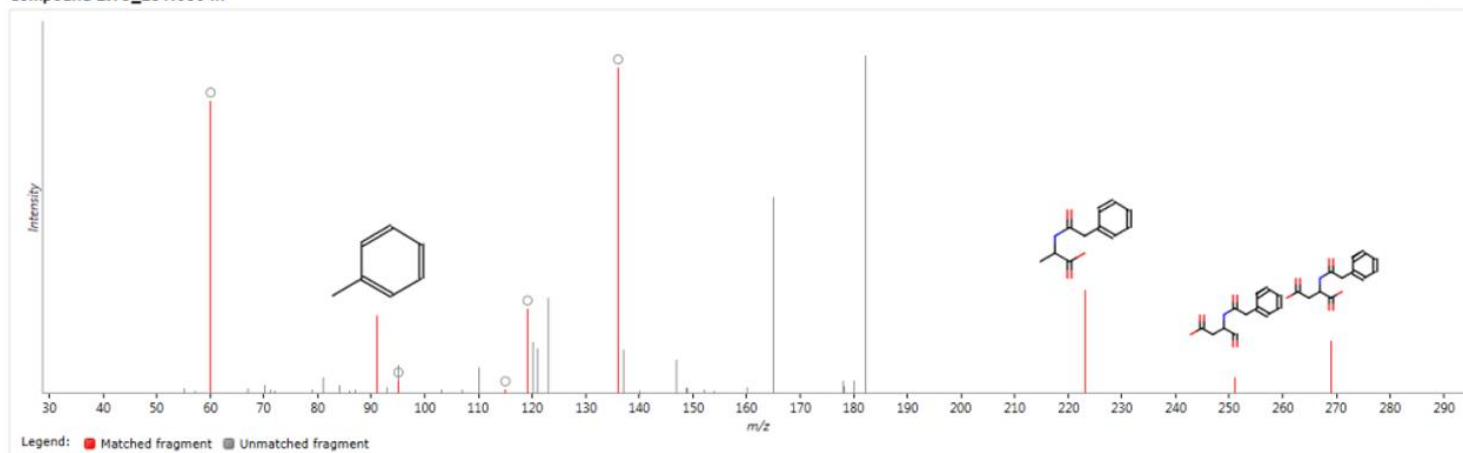


Figure S5 Box plots of 6 typical differential metabolites: **(a)** Guanosine, **(b)** 2-Hydroxyadenine, **(c)** Lyciumoside VI, **(d)** 3-Hydroxypimelyl-CoA, **(e)** Val Arg; "***"p < 0.001,"*"p < 0.05.

