

Supplementary Table S1. Differential abundant metabolites identified after 14 days treatment of AKBA

Metabolite	m/z_ retention time (min)	I/D	P- Value	Possible formula	Possible compound	Possible formula	Possible compound
<i>Male Feature Level</i>							
<u>1</u>	163.0594__184.36	Decrease	1.08E-05	C ₄ H ₁₀ N ₃ O ₄	2-(3-Amino-3-carboxypropyl)-1-hydroxy-1-oxohydrazinium; 1,1-Bis(2-hydroxyethyl)-3-oxo-2-triazanolate; N-[bis(2-hydroxyethyl)amino]-N-oxidonitrous amide	C ₁₀ H ₁₂ S	¹ Unidentifiable; 205 results found
2	174.0438__92.03	Increase	1.08E-05	C ₉ H ₇ N ₂ O ₂	¹ Unidentifiable; 23 results found	C ₇ H ₇ N ₅ O	5-(3-amino-1H-1,2,4-triazol-5-yl)pyridine-3-ol
3	179.1289__271.38	Increase	0.00032	C ₈ H ₂₀ O ₄	2-[2-(2-Methoxyethoxy)ethoxy]ethanol - methane (1:1); di(propylene glycol) methyl ether	C ₉ H ₁₆ N ₄	N2-[2-(dimethylamino)ethyl]pyridine-2,5-diamine
4	148.0612__50.23	Decrease	0.00049	C ₅ H ₁₁ NO ₄	¹ Unidentifiable; 351 results found	C ₃ H ₉ N ₄ O ₃	1-Hydroxy-2-[N'-(2-hydroxyethyl)carbamidoyl]-1-oxohydrazinium
<i>Female Feature Level</i>							
1	126.9198__34.12	Decrease	4.33E-05	Unidentifiable	Unidentifiable		
2	151.058__178.14	Decrease	8.66E-05	C ₃ H ₁₀ N ₃ O ₄	Unidentifiable		
3	217.1336__196.45	Increase	0.00015	C ₁₁ H ₁₆ N ₅	5-(2,2-Dimethylcyclopropyl)imidazo[4,5-b]pyridine-3-ium-1,3-diamine	C ₁₀ H ₂₀ NO ₄	Aclatonium; (propionyloxy)-1-propanaminium
4	118.0548__32.78	Decrease	0.00015	C ₇ H ₆ N ₂	Benzimidazole; Indazole; Phenylidiazomethane, (Diazomethyl) benzene		
5	155.0301__33.31	Decrease	0.00025	Unidentifiable	Unidentifiable		
<u>6</u>	163.0594__184.36	Decrease	0.00025	C ₄ H ₁₀ N ₃ O ₄	2-(3-Amino-3-carboxypropyl)-1-hydroxy-1-oxohydrazinium; 1,1-Bis(2-hydroxyethyl)-3-oxo-2-triazanolate; N-[bis(2-hydroxyethyl)amino]-N-oxidonitrous amide	C ₁₀ H ₁₂ S	¹ Unidentifiable; 205 results found
7	107.0627__177.89	Decrease	0.00025	Unidentifiable	Unidentifiable		
8	146.0783__172.75	Decrease	0.00065	C ₇ H ₁₅ OS	Dimethyl(tetrahydro-2-furanyl)methyl)sulfonium; 1-Isopropoxytetrahydrothiophenium		
9	202.1322__184.9	Decrease	0.00065	C ₉ H ₁₉ N ₂ O ₃	¹ Unidentifiable; 14 results found		
10	164.0912__80.22	Decrease	0.00065	C ₆ H ₁₅ NO ₄	¹ Unidentifiable; 38 results found		
11	190.0734__173.21	Decrease	0.00097	C ₁₀ H ₁₁ N ₂ O ₂	¹ Unidentifiable; 62 results found	C ₃ H ₁₁ N ₈ S	Unidentifiable
12	200.0341__204.76	Increase	0.00145	C ₉ H ₅ N ₄ O ₂	3-Cyano-7-methylpyrazolo[1,5-a]pyrimidine-6-carboxylate; 5-(5H-Tetrazol-5-ylidene)-3,5-dihydro-2-benzofuran-1-olate	C ₉ H ₁₃ OS ₂	¹ Unidentifiable; 46 results found

¹ Unidentifiable with more than 4 results via ChemSpider databases are linked in supplementary data