

MET_CHEM_NO	CAS_UID	ONTOLOGY1_NAME	ONTOLOGY2_NAME	Comparison in CELL LINE group										supernatant													
				CELL LINE reference										KO													
				WT		WT		KO		KO		WT		WT		KO		KO		WT		WT		KO		KO	
				Ratio	Ratio	Ratio	Ratio	Ratio	Ratio	Ratio	p.value	p.value	p.value	p.value	Ratio	Ratio	Ratio	Ratio	Ratio	p.value	p.value	p.value	p.value	Ratio	Ratio	Ratio	Ratio
39980072	CAS-56-84-8	Amino acids	Amino acids, acidic	0.95	1.00	0.95	1.01	1.01	0.96	0.0795	0.9329	0.0681	0.7883	0.8501	0.1330	0.4270	0.9515	0.2783	0.9022	0.9634	0.3478	0.9698	0.3478				
39980088	CAS-56-86-0	Amino acids	Amino acids, acidic	0.90	0.94	0.96	1.50	1.60	1.45	0.0059	0.0591	0.2540	5.68E-09	8.54E-10	1.91E-08	0.2533	0.3815	0.4626	9.65E-08	1.74E-08	2.79E-07						
39980073	CAS-63-91-2	Amino acids	Amino acids, aromatic	0.99	0.97	1.01	1.00	1.00	1.00	0.0324	0.0062	0.4116	0.6215	0.0224	0.7671	0.2965	0.2094	0.6460	0.7987	0.0846	0.8598						
39980035	CAS-54-12-6, CAS-73-22-3	Amino acids	Amino acids, aromatic	1.11	1.05	1.03	1.08	0.93	1.08	0.0245	0.1030	0.4512	0.6323	0.2639	0.2412	0.2965	0.4517	0.6793	0.7987	0.5079	0.4895						
19980173	CAS-60-18-4	Amino acids	Amino acids, aromatic	1.04	1.06	0.98	1.00	0.94	0.98	0.6060	0.4036	0.7436	0.9779	0.4100	0.7343	0.8738	0.6859	0.8908	0.9779	0.5974	0.8477						
39980043	CAS-74-79-3	Amino acids	Amino acids, basic	0.99	0.93	1.06	0.93	1.00	0.98	0.6915	0.0539	0.1114	0.0603	0.9583	0.6692	0.8817	0.3815	0.3071	0.1709	0.9937	0.8282						
39980145	CAS-70-47-3, CAS-5794-13-8	Amino acids	Amino acids, basic	0.96	1.10	0.87	1.03	0.94	0.90	0.4461	0.0786	0.0179	0.5461	0.2536	0.0730	0.8738	0.3815	0.1659	0.7684	0.4974	0.2258						
39980466	CAS-71-00-1	Amino acids	Amino acids, basic	1.05	0.98	1.08	0.97	0.99	1.04	0.4705	0.7227	0.2883	0.6207	0.8738	0.5583	0.8738	0.8672	0.4983	0.7987	0.9789	0.7786						
39980013	CAS-56-87-1, CAS-39665-12-8	Amino acids	Amino acids, basic	0.99	1.01	0.98	1.02	1.01	1.01	0.3756	0.3985	0.0957	0.0360	0.1579	0.5443	0.0881	0.6459	0.2997	0.1123	0.3428	0.7325						
39980074	CAS-73-32-5	Amino acids	Amino acids, branched chain	0.99	1.01	0.98	0.99	0.98	0.97	0.6339	0.2059	0.0913	0.5989	0.0937	0.0402	0.8738	0.5677	0.2997	0.7987	0.2515	0.1323						
39980075	CAS-61-90-5	Amino acids	Amino acids, branched chain	1.00	1.01	0.99	1.00	0.99	0.98	0.8830	0.2911	0.2328	0.5499	0.1208	0.0945	0.9525	0.2772	0.4481	0.7684	0.3064	0.2754						
39980070	CAS-72-18-4, CAS-7004-03-7	Amino acids	Amino acids, branched chain	1.00	1.01	0.99	1.00	0.99	0.99	0.8872	0.2864	0.2308	0.8438	0.4095	0.3403	0.9525	0.5772	0.4481	0.9253	0.5974	0.6073						
39980003	CAS-56-41-7	Amino acids	Amino acids, neutral	0.99	1.01	0.97	1.17	1.15	1.14	0.3280	0.3002	0.0554	1.33E-08	4.25E-08	1.39E-07	0.7831	0.5772	0.2705	1.93E-07	5.42E-07	1.77E-06						
39980004	CAS-56-40-6	Amino acids	Amino acids, neutral	0.98	1.01	0.97	1.22	1.22	1.19	0.1906	0.6368	0.0843	2.13E-09	3.36E-09	1.32E-08	0.6031	0.8019	0.2997	4.35E-08	5.71E-08	2.25E-07						
39980079	CAS-147-85-3	Amino acids	Amino acids, neutral	0.98	0.98	0.99	1.09	1.11	1.08	0.0099	0.0583	0.3739	7.78E-08	8.28E-09	2.36E-07	0.2533	0.3815	0.6053	8.81E-07	1.21E-07	2.67E-06						
39980052	CAS-56-45-1	Amino acids	Amino acids, neutral	0.99	0.99	1.00	0.99	1.00	0.99	0.3547	0.2564	0.8245	0.1485	0.6946	0.2101	0.7864	0.5753	0.9246	0.3324	0.8335	0.4659						
39980006	CAS-72-19-5	Amino acids	Amino acids, neutral	1.00	1.00	1.00	1.02	1.02	1.02	0.7897	0.8155	0.9733	1.024	0.0685	0.1083	0.9477	0.9151	0.9829	0.2547	0.2116	0.2985						
39980010	CAS-52-90-4	Amino acids	Amino acids, S-containing	1.00	0.99	1.01	0.92	0.93	0.93	0.9668	0.8018	0.8340	0.0104	0.0168	0.0155	0.9879	0.9151	0.9246	0.0460	0.0683	0.0658						
39980039	CAS-63-68-3	Amino acids	Amino acids, S-containing	1.00	1.01	0.99	1.00	0.99	0.99	0.6885	0.1929	0.0973	0.8001	0.3132	0.1729	0.8817	0.5623	0.2997	0.9022	0.5566	0.4101						
39980009	CAS-98-79-3	Amino acids related	Amino acid metabolites	0.99	0.96	1.04	0.96	1.01	1.00	0.7846	0.0753	0.1227	0.1466	0.7724	0.9771	0.9477	0.3815	0.2629	0.3324	0.9056	0.9771						
39981135	CAS-107-95-9, CAS-28854-76-4	Amino acids related	Amino acid metabolites	1.04	1.01	1.02	1.11	1.10	1.14	0.3163	0.7045	0.5248	0.0092	0.0190	0.0027	0.7831	0.8554	0.7137	0.0428	0.0746	0.0153						
39981833	CAS-816-66-0	Amino acids related	Amino acid metabolites	1.03	0.88	1.17	2.53	2.87	2.95	0.5951	0.0268	0.0092	8.96E-11	1.57E-11	1.10E-11	0.8738	0.3041	0.1359	4.57E-09	1.60E-09	1.12E-09						
39980437	CAS-51-35-4	Amino acids related	Collagen metabolism	1.00	0.99	1.01	1.10	1.11	1.11	0.9797	0.8501	0.8701	0.0081	0.0056	0.0056	0.9894	0.9324	0.9442	0.8933	0.0287	0.0201						
19980325	CAS-57-00-1	Amino acids related	Creatine metabolism	1.04	1.04	1.00	1.11	1.07	1.12	0.3459	0.3957	0.9223	0.0345	0.1544	0.0288	0.7840	0.6859	0.9693	0.1215	0.3423	0.8405						
39980321	CAS-60-27-5	Amino acids related	Creatine metabolism	1.26	1.16	1.09	0.97	0.83	1.05	0.0853	0.2505	0.5245	0.8235	0.1948	0.7021	0.4350	0.5753	0.7137	0.9131	0.4139	0.8425						
39980327	CAS-492-27-3	Amino acids related	Tryptophan metabolism	1.04	1.13	0.92	1.15	1.06	1.06	0.6629	0.2158	0.4090	0.2024	0.9208	0.6072	0.8750	0.5703	0.6460	0.4162	0.9886	0.7839						
39980159	CAS-372-75-8	Amino acids related	Urea cycle and related	0.93	0.93	1.02	0.98	1.07	0.99	0.3301	0.2355	0.8209	0.9731	0.3907	0.9416	0.7831	0.7730	0.9246	0.9022	0.5948	0.9771						
39980406	CAS-70-26-8	Amino acids related	Urea cycle and related	1.05	0.99	1.06	0.99	1.00	1.05	0.2120	0.8827	0.1668	0.8528	0.9642	0.2496	0.6169	0.3509	0.3782	0.9253	0.9937	0.4895						
29980428	CAS-57-13-6	Amino acids related	Urea cycle and related	1.08	1.06	1.01	0.87	0.82	0.88	0.4915	0.5404	0.9153	0.2040	0.0748	0.2604	0.8738	0.7253	0.9693	0.4162	0.2180	0.5012						
39981841	CAS-3416-24-8	Carbohydrates and related	Aminosugars	0.97	1.09	0.90	1.08	0.99	0.96	0.6104	0.1518	0.0610	0.2135	0.8891	0.5332	0.8738	0.5032	0.2705	0.4228	0.9789	0.7326						
39981842	CAS-2636-92-2	Carbohydrates and related	Aminosugars	0.97	1.01	0.96	1.05	1.04	1.01	0.5716	0.8892	0.4826	0.4324	0.5119	0.9057	0.8738	0.9350	0.6861	0.7001	0.7001	0.9623						
39980021	CAS-69-79-4	Carbohydrates and related	Disaccharides	0.83	0.72	1.15	1.61	2.22	1.85	0.1316	0.0141	0.2499	0.0016	1.27E-05	0.0002	0.5324	0.2242	0.4626	0.0095	0.9959	0.0011						
39982122	CAS-4084-27-9	Carbohydrates and related	Monosaccharides	1.01	0.93	1.09	0.90	0.96	0.97	0.8111	0.2642	0.1813	0.0983	0.5187	0.6739	0.9509	0.5733	0.9394	0.2547	0.7001	0.8282						
39980037	CAS-50-99-7, CAS-492-62-6	Carbohydrates and related	Monosaccharides	1.03	1.01	1.02	0.87	0.86	0.88	0.1068	0.5004	0.3198	1.91E-06	7.36E-07	8.71E-06	0.4738	0.7164	0.5437	1.77E-05	6.25E-06	6.84E-05						
39980019	CAS-50-50-6, CAS-24259-59-4	Carbohydrates and related	Nucleobase related saccharides	0.87	0.87	0.99	0.67	0.76	0.66	0.0378	0.0448	0.9295	1.88E-05	0.0008	1.63E-05	0.2965	0.3815	0.9693	0.0002	0.0052	0.0001						
39980054	CAS-149-32-6	Carbohydrates and related	Polys	0.98	1.04	0.94	1.01	0.97	0.95	0.1965	0.0154	0.0011	0.4592	0.0857	0.0074	0.6031	0.2242	0.0801	0.7206	0.2429	0.0357						
39980014	CAS-87-89-8	Carbohydrates and related	Polys	1.01	1.02	1.00	1.00	0.99	1.00	0.1434	0.0759	0.7194	0.7663	0.1501	0.9639	0.5224	0.3815	0.8841	0.9022	0.3422	0.9771						
39980033	CAS-50-70-4	Carbohydrates and related	Polys	0.96	0.89	1.07	0.97	1.08	1.03	0.6327	0.2474	0.4843	0.7344	0.4344	0.7397	0.8738	0.5753	0.9681	0.5020	0.6240	0.8477						
39980022	CAS-67-03-0	Carbohydrates and related	Polys	1.07	1.03	0.96	1.19	1.06	1.09	0.4750	0.0425	0.1565	0.1333	0.6757	0.7917	0.8738	0.3815	0.3714	0.2687	0.8205	0.8777						
39980822	CAS-13752-84-6	Carbohydrates and related	Sugar acids	1.06	0.97	1.10	1.03	1.07	1.13	0.2454	0.5079	0.0793	0.5685	0.2383	0.0316	0.6764	0.7164	0.2997	0.7837	0.4766	0.1077						
39980111	CAS-526-95-4	Carbohydrates and related	Glucuronic acid (additional: Gluconolactone)	0.98	0.98	1.00	1.01	1.03	1.01	0.1560	0.2587	0.7522	0.3498	0.0564	0.0811	0.5305	0.0753	0									

59980878		Unknown	Unknown polar	Unknown polar (59980878)	0.93	1.06	0.88	1.13	1.06	0.99	0.7701	0.8023	0.5889	0.6343	0.8095	0.9724	0.9464	0.9151	0.7867	0.7987	0.9277	0.9771
59980879		Unknown	Unknown polar	Unknown polar (59980879)	0.98	1.12	0.88	1.23	1.10	1.08	0.8464	0.3056	0.2280	0.0773	0.3872	0.4928	0.9525	0.5772	0.4481	0.2128	0.5948	0.7326
59980881		Unknown	Unknown polar	Unknown polar (59980881)	1.58	1.07	1.48	0.68	0.64	1.01	0.0082	0.6584	0.0199	0.0286	0.0124	0.9611	0.2533	0.8189	0.1690	0.1044	0.0547	0.9771
59980885		Unknown	Unknown polar	Unknown polar (59980885)	0.99	1.17	0.85	1.16	1.00	0.99	0.9580	0.3056	0.2828	0.3446	0.9745	0.9347	0.9879	0.5772	0.4973	0.6048	0.9937	0.9771
59980889		Unknown	Unknown polar	Unknown polar (59980889)	1.04	0.70	1.49	0.65	0.93	0.97	0.8516	0.1233	0.0885	0.0793	0.7432	0.8805	0.9525	0.4491	0.2997	0.2128	0.8815	0.9555
59980901		Unknown	Unknown polar	Unknown polar (59980901)	0.73	0.72	1.02	0.88	1.22	0.89	0.0999	0.0856	0.9313	0.5006	0.3018	0.5531	0.4632	0.3968	0.9693	0.7626	0.5497	0.7326
39981436	CAS-79-83-4 , CAS-137-08-6	Vitamins, cofactors and related	Acyl-carriers and related	Pantothenic acid	1.06	0.98	1.09	0.97	1.00	1.06	0.0989	0.4864	0.0263	0.4452	0.9178	0.1370	0.4632	0.7164	0.1791	0.7096	0.9886	0.3495
19980414	CAS-82-82-6	Vitamins, cofactors and related	Amino-carriers and related	4-Pyridoxic acid	1.04	1.00	1.04	1.06	1.06	1.10	0.6691	0.9880	0.6583	0.5308	0.5216	0.3012	0.8750	0.9880	0.8500	0.7626	0.7001	0.5586
19980227	CAS-65-23-6	Vitamins, cofactors and related	Amino-carriers and related	Pyridoxine	0.98	1.04	0.94	1.10	1.05	1.03	0.5527	0.2593	0.0961	0.0286	0.2067	0.4673	0.8738	0.5753	0.2997	0.1044	0.4289	0.7326
39980083	CAS-3909-12-4	Vitamins, cofactors and related	Ascorbic acid and related	Threonic acid	1.04	1.03	1.01	1.06	1.03	1.06	0.1557	0.2651	0.7391	0.0582	0.3554	0.0317	0.5305	0.5753	0.8908	0.1705	0.5847	0.1077
19980328	CAS-98-92-0	Vitamins, cofactors and related	Redox-carrier and related	Nicotinamide	0.99	1.00	1.00	0.97	0.98	0.97	0.8708	0.9202	0.9501	0.5289	0.5920	0.4915	0.9525	0.9495	0.9720	0.7626	0.7548	0.7326
29981199	CAS-59-67-6	Vitamins, cofactors and related	Redox-carrier and related	Nicotinic acid	0.98	0.96	1.02	1.00	1.04	1.02	0.6505	0.4524	0.7598	0.9293	0.4030	0.6938	0.8738	0.7164	0.8908	0.9646	0.5974	0.8425

Statistical quantities	Explanation
Ratio	ANOVA estimate of effect on ratio scale (transformed Estimate: 10*Est.log)
p-value	p-value of ANOVA t-statistics
t-value	ANOVA t-statistics
Est.log	ANOVA contrast estimate (on log10-scale)
Std.Err	Standard error of ANOVA contrast estimate (on log10-scale)
DF	Degrees of freedom for contrast estimate
q value	Benjamini-Hochberg multiple comparisons q-value (= False-discovery rate/FDR)

Coloring of ratios:
ratio > 1 & p-value < 0.01
ratio > 1 & 0.01 ≤ p-value < 0.05
ratio > 1 & 0.05 ≤ p-value < 0.10
ratio < 1 & 0.05 ≤ p-value < 0.10
ratio < 1 & 0.01 ≤ p-value < 0.05
ratio < 1 & p-value < 0.01

Font style of ratios:
bold: (ratio < 0.5) or (ratio > 2
normal: (ratio > 0.5) or (ratio < 2)

Coloring of p-values:
0.05 ≤ p < 0.10
0.01 ≤ p < 0.05
p < 0.01

METABOLITE_NAME contains an "Additional ": Quantitation can be disturbed by metabolites exhibiting identical analytical characteristics with respect to quantitation method. Literature data and/or comparison with alternative methods (e.g. LC-MS/MS, GC-MS) suggest that disturbing metabolite is present at minor levels only.

CAS_UID: Numerical identifier for chemical elements, compounds and polymers assigned by the American Chemical Society (Chemical Abstracts Service).

MET_CHEM_NO: Internal metabolite identification number used by metanomics GmbH.

Data normalized to the Metabolite Median