Supporting information for

Underground Reservoirs Regulate the Composition and Metabolism of Microbial Community in Coal Mine Water

Yang Li[ac*§], Min Wu[a§], Haiqin Zhang[a], Binbin Jiang[a], Yixiang Bao[a], Jie Li[ab], Jingfeng Li[a], Peng Li[b], Xinyue Yan[c], Tianqi Qin[c]

[a] *State Key Laboratory of Water Resource Protection and Utilization in Coal Mining, National Institute of Low Carbon and Clean Energy, CHN Energy, Beijing 102211, China*

[b] *Technology Research Institute, Shendong Coal Group Co., Ltd., CHN Energy, Yulin 719315, China*

[c] *State Key Laboratory of Mining Response and Disaster Prevention and Control in Deep Coal Mines, Anhui University of Science and Technology, Huainan 232001, China*

* Email: liyang20130104@163.com; liyang_aust@163.com

§ Y.L. and M.W. contributed equally to this work.

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Figures: 8

Supporting Tables

Table S1 Sampling at various coal mines

Coal mine name and GPS coordinates	Sample number	Taken position
Shangwan Coal Mine (E 110.18°-110.20°, N 39.28°-39.30°)	616A3	influent
	616A4	effluent
	616A5	effluent
Cuncaota Coal Mine II (E 109.59°-110.03°, N 39.27°-39.30°)	576A13	influent
	576A3	effluent
Cuncaota Coal Mine I (E 110.15°-110.17°, N 39.22°- 39.25°)	576A10	influent
	616A1	effluent
Buertai Coal Mine (E 109.87°-110.08°, N 39.43°-39.53°)	576A5	influent
	576A1	effluent
Wulanmulun Coal Mine (E 100.03°-110.18°, N 39.42°-39.55°)	576A6	influent
	576A7	influent
	576A2	effluent
Liuta Coal Mine (E 110.06°-110.12°, N 39.35°-39.40°)	675A3	influent
	675A4	influent
	675A5	effluent
Daluita Coal Mine (E 110.33°-110.38°, N 39.23°-39.28°)	422A2	influent
	422A1	effluent
Bulianta Coal Mine (E 109.93°-110.17°, N 39.25°-39.40°)	576A4	influent
	616A2	effluent
Shigetai Coal Mine (E 109.20°-110.22°, N 36.27°-39.28°)	528j	influent
	528	effluent
Haragou Coal Mine (E 110.09°-110.18° ,N 39.17°-39.35°)	576A16	influent
	675A1	effluent

Table S2 The compounds in mine water visibly increase and decrease after passing through underground water reservoirs.

	FC	log2(FC)	raw.pval	Chemical Compound	Molecular Formula
HMDB30931	2.9882	1.5793	0.0014133	(E)-2-Tridecene-4,6,8-triyn-1-ol	C13 H14 O
HMDB38701	8.756	3.1303	0.001425	Peltatol A	C42 H58 O4
HMDB14449	2.7599	1.4646	0.0015787	Desogestrel	C22 H30 O
HMDB14619	2.7417	1.455	0.0024898	Duloxetine	C18 H19 N O S
HMDB11280	0.27823	-1.8456	0.0025146	PC(P-18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C44 H79 N O7 P
HMDB14653	0.18147	-2.4622	0.0027981	Vancomycin	C66 H75 Cl2 N9 O24
HMDB12148	2.8479	1.5099	0.0029133	2-Hexaprenyl-6-methoxy-1,4-benzoquinol	C37 H56 O3
HMDB10666	6.2148	2.6357	0.0031878	PG(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C42 H71 O10 P
HMDB35551	0.31741	-1.6556	0.0031979	7,9-Hexacosanedione	C26 H50 O2
HMDB38026	2.999	1.5845	0.0043707	Dihydro-alpha-ionone	C13 H22 O
HMDB00089	0.16003	-2.6436	0.0048653	Cytidine	C9 H13 N3 O5
HMDB29117	2.7369	1.4525	0.0049164	Tyrosyl-Tyrosine	C18 H20 N2 O5
HMDB14592	0.40511	-1.3036	0.0054244	Dipivefrin	C19 H29 N O5
HMDB08825	0.011506	-6.4415	0.006057	PE(14:0/16:1(9Z))	C35 H68 N O8 P
HMDB09363	5.956	2.5743	0.0061898	PE(20:3(8Z,11Z,14Z)/20:2(11Z,14Z))	C45 H80 N O8 P
HMDB36320	7.7593	2.9559	0.00626	(S)-Skyrin 2-glucoside	C36 H28 O15
HMDB07866	14.347	3.8426	0.0067906	PC(14:0/14:0)	C36 H73 N O8 P
HMDB08297	7.8848	2.9791	0.0079781	PC(20:1(11Z)/15:0)	C43 H85 N O8 P
HMDB40792	0.20758	-2.2683	0.0083219	Dihydroxyacidissiminol	C25 H33 N O5
HMDB38011	5.356	2.4212	0.0084916	Malvidin 3-(6-coumaroylglucoside) 5-glucoside	C38 H41 O19

HMDB38922	0.12873	-2.9576	0.0092665	(7'R)-(+)-Lyoniresinol 9'-glucoside	C28 H38 O13
HMDB40688	3.991	1.9968	0.009823	(3x,5x,10x)-9,10-Didehydroisohumbertiol O-[rhamnopyranosyl-(1->4)-rhamnopyranosyl-(1->2)-[(E)-feruloyl-(->4)-rhamnosyl-(1->6)]-glucoside]	C49 H70 O21
HMDB10380	3.2086	1.6819	0.0098863	LysoPC(14:1(9Z))	C22 H45 N O7 P
HMDB15026	3.5977	1.8471	0.0099966	Granisetron	C18 H24 N4 O
HMDB09606	5.3274	2.4134	0.010284	PE(22:4(7Z,10Z,13Z,16Z)/24:0)	C51 H94 N O8 P
HMDB29949	0.22952	-2.1233	0.010525	Pangamic acid	C20 H40 N2 O8
HMDB35565	0.26584	-1.9114	0.010849	4,6-Tricosanedione	C23 H44 O2
HMDB41911	2.8564	1.5142	0.012606	isepamicin	C22 H43 N5 O12
HMDB59699	4.7874	2.2592	0.013445	Procerin	C15 H18 O2
HMDB40697	0.31264	-1.6774	0.013496	Oblongine	C19 H24 N O3
HMDB33356	0.32193	-1.6352	0.014135	Xanthoplanine	C21 H26 N O4
HMDB10343	3.3278	1.7346	0.014657	1-(alpha-Methyl-4-(2-methylpropyl)benzeneacetate)-beta-D-Glucopyranuronic acid	C19 H26 O8
HMDB39962	3.6213	1.8565	0.014992	N1,N5,N10-Tris-trans-p-coumaroylspermine	C37 H44 N4 O6
HMDB39432	0.22379	-2.1598	0.016117	1,2,4,5,7,8-Hexathionane	C3 H6 S6
HMDB36298	3.2279	1.6906	0.016374	Cyclopassifloic acid E	C31 H52 O8
HMDB01898	3.4384	1.7817	0.016644	Mesobilirubinogen	C33 H44 N4 O6
HMDB07784	2.7193	1.4433	0.016652	DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:2(13Z,16Z)/0:0)	C47 H76 O5
HMDB41052	2.7213	1.4443	0.016711	Ajocysteine	C9 H15 N O3 S3
HMDB12006	2.6712	1.4175	0.016814	Ganglioside GT1c (d18:0/26:1(17Z))	C104 H182 N4 O47
HMDB39804	2.6444	1.4029	0.016838	3-Hexylpyridine	C11 H17 N

HMDB38452	3.0382	1.6032	0.017165	28-Glucosylpomolate	C36 H58 O9
HMDB32293	0.35274	-1.5033	0.017202	N-Gluconyl ethanolamine	C8 H17 N O7
HMDB12078	2.7941	1.4824	0.017572	Ganglioside GT3 (d18:1/24:1(15Z))	C87 H152 N4 O37
HMDB29154	14.938	3.9009	0.017886	Gamma-glutamyl-Lysine	C11 H22 N4 O4
HMDB12033	2.9752	1.573	0.017917	Ganglioside GT2 (d18:0/24:1(15Z))	C96 H168 N4 O42
HMDB01969	2.8935	1.5328	0.017991	Dolichol	C100 H164 O
HMDB28712	4.5475	2.1851	0.018419	Arginyl-Isoleucine	C12 H25 N5 O3
HMDB33625	3.1273	1.6449	0.018593	(3R,7R)-1,3,7-Octanetriol	C8 H18 O3
HMDB33799	3.0599	1.6135	0.018951	26-Desglucoavenacoside A	C45 H72 O18
HMDB39636	2.8953	1.5337	0.019053	Abscisic alcohol 11-glucoside	C21 H32 O8
HMDB32800	2.3699	1.2448	0.019797	Feruloylcholine	C15 H22 N O4
HMDB32719	5.0643	2.3403	0.020252	Isofumonisin B1	C34 H59 N O15
HMDB11528	2.8917	1.5319	0.020444	LysoPE(24:1(15Z)/0:0)	C29 H58 N O7 P
HMDB29083	3.3387	1.7393	0.020513	Tryptophyl-Glycine	C13 H15 N3 O3
HMDB15147	4.7263	2.2407	0.021139	Cinacalcet	C22 H22 F3 N
HMDB31716	3.2312	1.6921	0.021231	3-(Methylthio)-1-propanol	C4 H10 O S
HMDB40188	0.19692	-2.3443	0.022982	1,1-Dibromo-2-propanone	C3 H4 Br2 O
HMDB38244	0.3213	-1.638	0.0234	Panaxatriol	C30 H52 O4
HMDB32315	2.3262	1.218	0.023752	Hexanal butane-2,3-diol acetal	C10 H20 O2
HMDB38286	0.3376	-1.5666	0.023857	Eujambin	C30 H26 O17
HMDB01345	2.0775	1.0548	0.023963	4-Trimethylammoniobutanal	C7 H16 N O
HMDB28818	2.2279	1.1557	0.023982	Glutamyl-glutamate	C10 H15 N2 O7

HMDB29356	3.2853	1.716	0.024161	N-Feruloylglycyl-L-phenylalanine	C21 H22 N2 O6
HMDB39728	2.2112	1.1448	0.024783	b-D-Glucuronopyranosyl-(1->3)-a-D-galacturonopyranosyl-(1->2)-L-rhamnose	C18 H28 O17
HMDB06288	0.35275	-1.5033	0.02525	All trans decaprenyl diphosphate	C50 H90 O7 P2
HMDB04898	0.42625	-1.2302	0.025514	Ganglioside GA2 (d18:1/25:0)	C63 H118 N2 O18
HMDB00636	2.1613	1.1119	0.026338	Dioleoylphosphatidic acid	C39 H73 O8 P
HMDB28732	0.39087	-1.3552	0.026422	Asparaginyl-Hydroxyproline	C9 H15 N3 O5
HMDB40672	0.13169	-2.9248	0.026426	3-Oxo-alpha-ionol 9-[apiosyl-(1->6)-glucoside]	C24 H38 O11
HMDB29973	0.37098	-1.4306	0.026612	Simonin I	C69 H112 O21
HMDB39695	0.22661	-2.1417	0.027006	4,7-Didehydroneophysalin B	C28 H28 O9
HMDB15416	3.6751	1.8778	0.027039	Fosamprenavir	C25 H36 N3 O9 P S
HMDB09791	0.2448	-2.0303	0.027092	PI(16:0/22:2(13Z,16Z))	C47 H87 O13 P
HMDB29237	2.882	1.527	0.027199	Cyanidin 3-(6''-succinyl-glucoside)	C25 H25 O14
HMDB12357	2.4244	1.2776	0.027459	PS(16:0/18:1(9Z))	C40 H76 N O10 P
HMDB28990	5.781	2.5313	0.027536	Phenylalanyl-Asparagine	C13 H17 N3 O4
HMDB35996	2.3861	1.2546	0.027606	2-(Methylthio)-3H-phenoxazin-3-one	C13 H9 N O2 S
HMDB41632	2.4398	1.2867	0.027996	5alpha-Cholestane	C27 H48
HMDB09597	5.085	2.3463	0.028108	PE(22:4(7Z,10Z,13Z,16Z)/20:4(8Z,11Z,14Z,17Z))	C47 H78 N O8 P
HMDB37420	0.27124	-1.8824	0.028333	Maysin 3'-methyl ether	C28 H30 O14
HMDB40133	0.30613	-1.7078	0.028849	Pectenotoxin 2 secoacid	C47 H72 O15
HMDB41826	0.3015	-1.7298	0.029734	amifloxacin	C16 H19 F N4 O3
HMDB09195	0.078383	-3.6733	0.030129	PE(18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C41 H66 N O8 P

HMDB07910	3.3535	1.7457	0.030397	PC(14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C40 H71 N O8 P
HMDB02706	2.0532	1.0379	0.030979	L-Canavanine	C5 H12 N4 O3
HMDB15277	0.068429	-3.8693	0.032194	Diphenylpyraline	C19 H23 N O
HMDB34248	2.7082	1.4373	0.032646	Pyropheophytin b	C53 H70 N4 O4
HMDB00777	0.35153	-1.5083	0.032863	N-Acrylylglycine methyl ester	C6 H9 N O3
HMDB35732	2.4315	1.2819	0.033145	Dukunolide D	C26 H28 O8
HMDB07955	5.7588	2.5258	0.033482	PC(15:0/22:4(7Z,10Z,13Z,16Z))	C45 H83 N O8 P
HMDB06970	4.4872	2.1658	0.033896	CDP-DG(16:0/18:1(11Z))	C46 H83 N3 O15 P2
HMDB35459	2.4715	1.3054	0.034192	YGM 1A	C49 H51 O26
HMDB33336	2.007	1.005	0.034894	Antibiotic X 14889A	C33 H60 O8
HMDB33887	0.35092	-1.5108	0.035371	Chondrillasterol 3-[glucosyl-(1->2)-glucosyl-(1->2)-glucoside]	C47 H78 O16
HMDB00827	0.10149	-3.3006	0.035876	Stearic acid	C18 H36 O2
HMDB28912	3.4023	1.7665	0.036687	Isoleucyl-Lysine	C12 H25 N3 O3
HMDB02139	2.7113	1.439	0.036726	Ubisemiquinone	C59 H90 O4
HMDB37158	0.34576	-1.5322	0.036802	3-[(2-Methyl-3-furanyl)thio]-4-heptanone	C12 H18 O2 S
HMDB29045	0.27824	-1.8456	0.037546	Serinyl-Methionine	C8 H16 N2 O4 S
HMDB00798	2.1844	1.1272	0.037625	Ethyl heptanoate	C9 H18 O2
HMDB09457	2.7032	1.4346	0.037921	PE(20:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C43 H70 N O8 P
HMDB14931	2.2887	1.1945	0.037998	Haloprogin	C9 H4 Cl3 I O
HMDB32023	0.1802	-2.4724	0.038854	3-Epidemissidine	C27 H45 N O
HMDB31252	9.4825	3.2453	0.039652	3-Iodopropanoic acid	C3 H5 I O2

HMDB10379	3.3395	1.7396	0.040616	LysoPC(14:0)	C22 H47 N O7 P
HMDB41519	2.9131	1.5426	0.041032	Nb-Feruloyltryptamine	C20 H20 N2 O3
HMDB40059	2.3564	1.2366	0.041112	(±)-2-(2-Furanyl)pyrrolidine	C8 H11 N O
HMDB15608	0.096162	-3.3784	0.041722	Indacaterol	C24 H28 N2 O3
HMDB41723	0.46042	-1.119	0.042158	Dihydroferulic acid 4-O-glucuronide	C16 H20 O10
HMDB39138	0.0035437	-8.1405	0.042199	Hericenone C	C35 H54 O6
HMDB02818	5.2757	2.3994	0.042817	Alloxan	C4 H2 N2 O4
HMDB30833	2.3411	1.2272	0.043222	Bilobetin	C31 H20 O10
HMDB10551	7.5262	2.9119	0.043482	TG(22:5(7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))[iso6]	C67 H100 O6
HMDB34557	0.29688	-1.752	0.043807	8,8-Diethoxy-2,6-dimethyl-2-octanol	C14 H30 O3
HMDB32419	3.9466	1.9806	0.043817	2-(4-Methyl-5-thiazolyl)ethyl decanoate	C16 H27 N O2 S
HMDB41129	2.6853	1.4251	0.043959	6''-O-(3-Hydroxy-3-methylglutaroyl)astragalin	C27 H28 O15
HMDB37162	2.1039	1.0731	0.043979	1,2,3-Tris(1-ethoxyethoxy)propane	C15 H32 O6
HMDB40744	3.4149	1.7718	0.044006	Polypodoside B	C39 H62 O13
HMDB15057	0.33131	-1.5937	0.044126	Buprenorphine	C29 H41 N O4
HMDB32739	2.3503	1.2328	0.044302	S-Methyl methanesulfinothioate	C2 H6 O S2
HMDB15686	6.1234	2.6143	0.044646	Pipazethate	C21 H25 N3 O3 S
HMDB36593	2.4998	1.3218	0.045108	Validamycin B	C20 H35 N O14
HMDB29044	2.1308	1.0914	0.045317	Serinyl-Lysine	C9 H19 N3 O4
HMDB38779	2.1076	1.0756	0.04614	4'-Methylisoscutellarein 8-(2''-sulfoglucoside)	C22 H22 O14 S
HMDB41048	0.21701	-2.2041	0.046204	Physagulin B	C30 H39 Cl O7

HMDB39904	2.1485	1.1033	0.046444	3'-Methoxytricetin 7-glucuronide	C22 H20 O13
HMDB29795	0.43662	-1.1956	0.046514	Montecristin	C37 H66 O4
HMDB33133	2.1464	1.1019	0.046634	2-Acetylthiophene	C6 H6 O S
HMDB36479	2.2053	1.141	0.046926	Cyclolinopeptide F	C55 H73 N9 O10 S2
HMDB10411	2.2279	1.1557	0.047101	TG(16:0/14:0/16:0)[iso3]	C49 H94 O6
HMDB11558	2.2524	1.1715	0.047233	MG(0:0/24:0/0:0)	C27 H54 O4
HMDB11898	2.272	1.184	0.047502	Ganglioside GM2 (d18:0/18:1(11Z))	C68 H122 N2 O26
HMDB29948	2.3052	1.2049	0.047962	Scleroglucan	C24 H44 O20 P2
HMDB11806	2.3117	1.209	0.048132	Ganglioside GD1a (d18:1/26:1(17Z))	C93 H163 N3 O39
HMDB29243	2.484	1.3126	0.048257	Cyanidin 3-O-(6''-malonyl-arabinoside)	C23 H21 O13
HMDB00244	0.40052	-1.3201	0.048385	Riboflavin	C17 H20 N4 O6
HMDB31778	3.0216	1.5953	0.048616	Diflubenzuron	C14 H9 Cl F2 N2 O2
HMDB31041	4.5406	2.1829	0.049095	(8E,15E)-1,8,15-Heptadecatriene-11,13-diyne	C17 H22
HMDB11810	2.3803	1.2512	0.04926	Ganglioside GD1b (d18:0/18:0)	C85 H151 N3 O39
HMDB06890	2.2797	1.1888	0.049362	3a,7a,12a,24-Tetrahydroxy-5b-cholestanoyl-CoA	C48 H80 N7 O21 P3 S
HMDB31083	0.32033	-1.6424	0.049367	(E)-7-Pentadecene	C15 H30
HMDB15179	2.4497	1.2926	0.049976	Rifampin	C43 H58 N4 O12

Supporting Figures

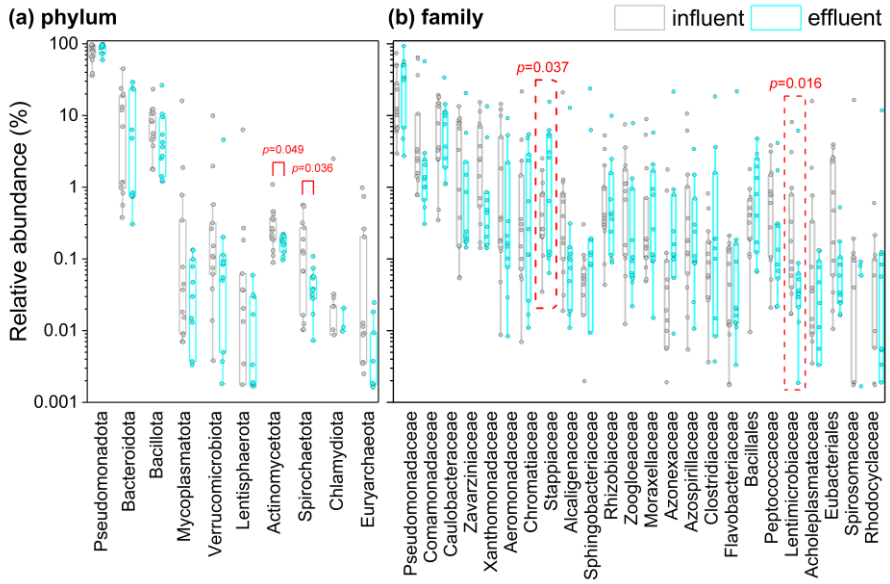

Figure S1 The dominant taxa at phylum (a) and family (b) levels.

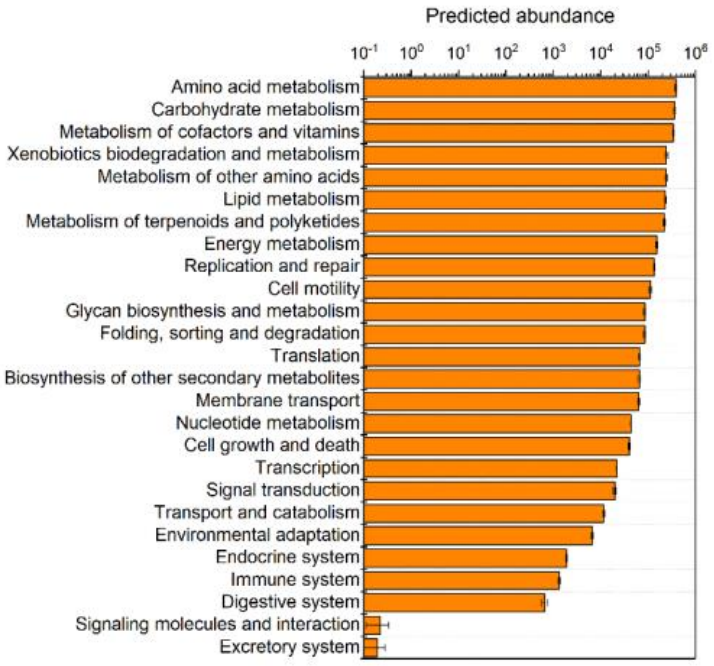

Figure S2 Predictive functional gene analysis of the underground water reservoir at level 2.

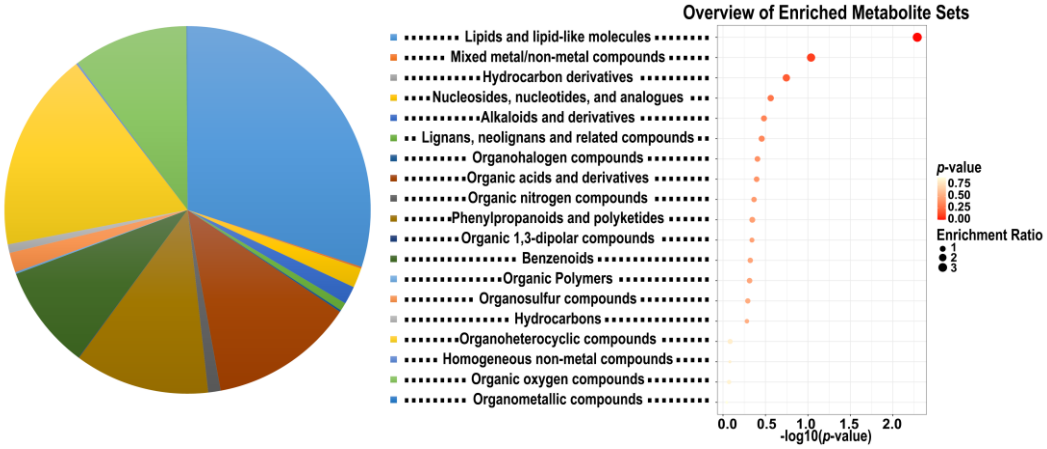

Figure S3 The component of metabolites in the water samples and the enriched components in the effluent water samples.

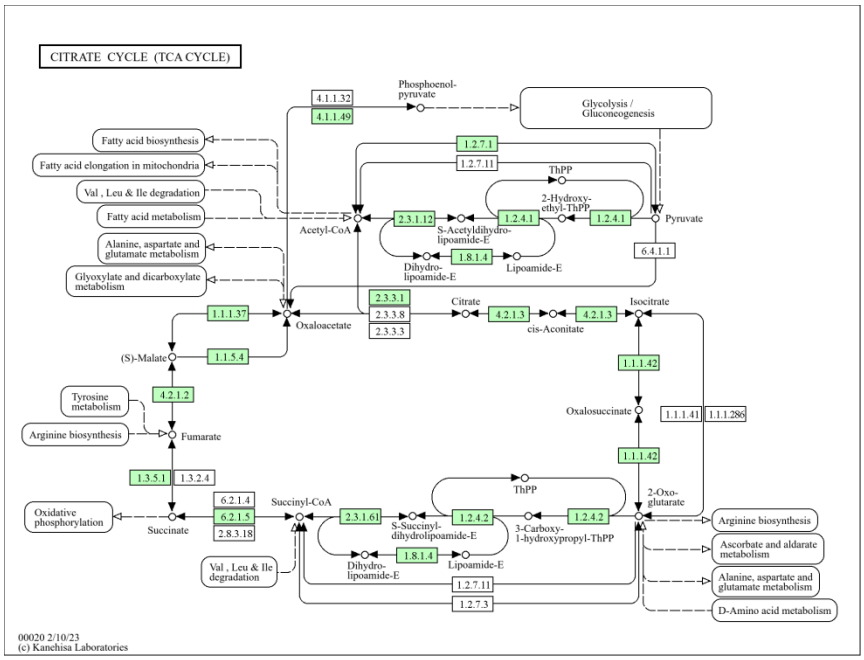

Figure S4 The Citrate cycle (TCA cycle) in the aquifer.

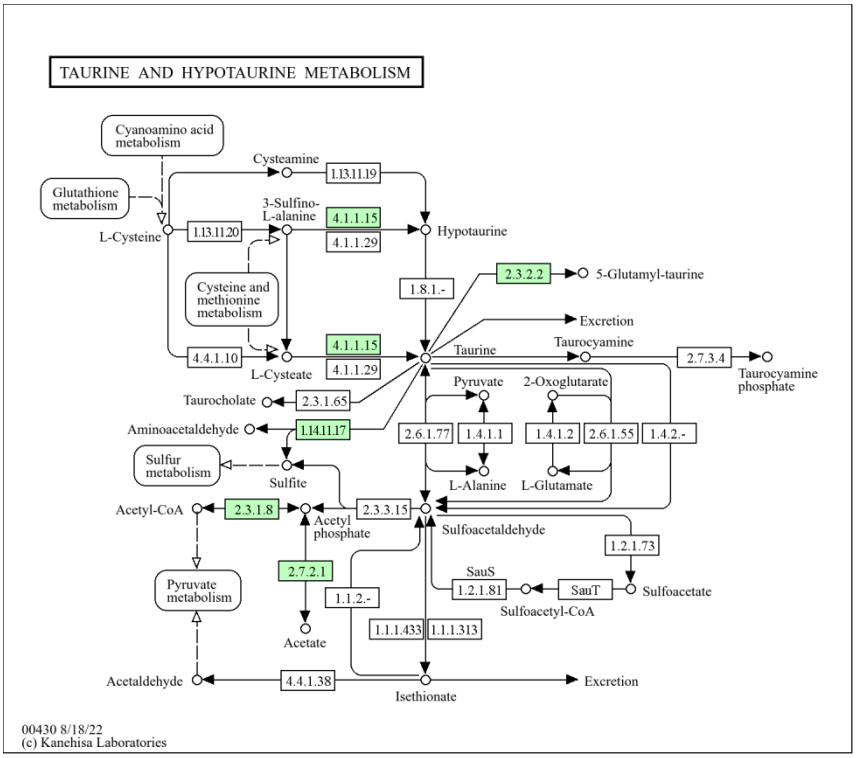

Figure S5 The Taurine and hypotaurine metabolism in the aquifer.

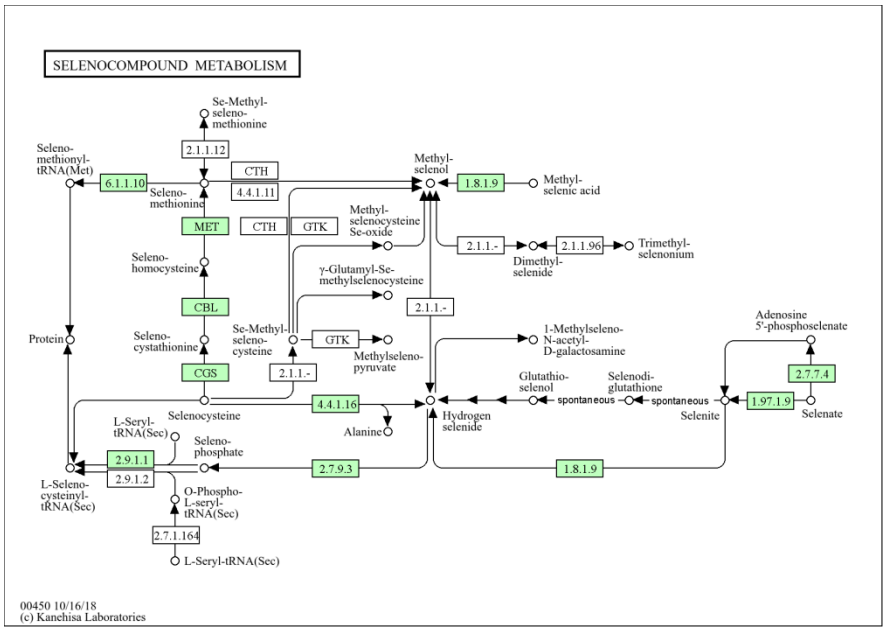

Figure S6 The Selenocompound metabolism in the aquifer.

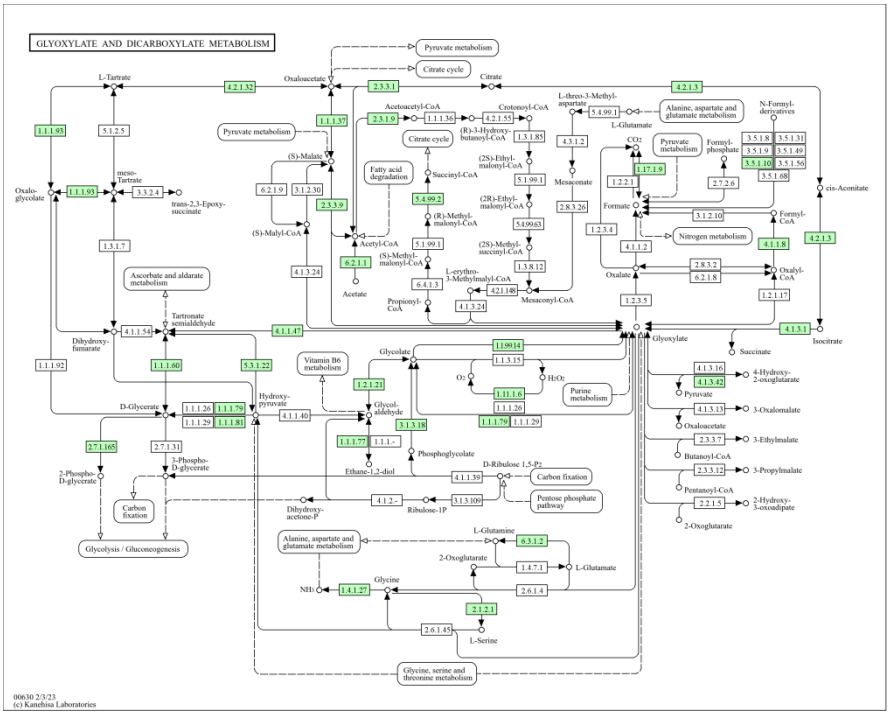

Figure S7 The Glyoxylate and dicarboxylate metabolism in the aquifer.

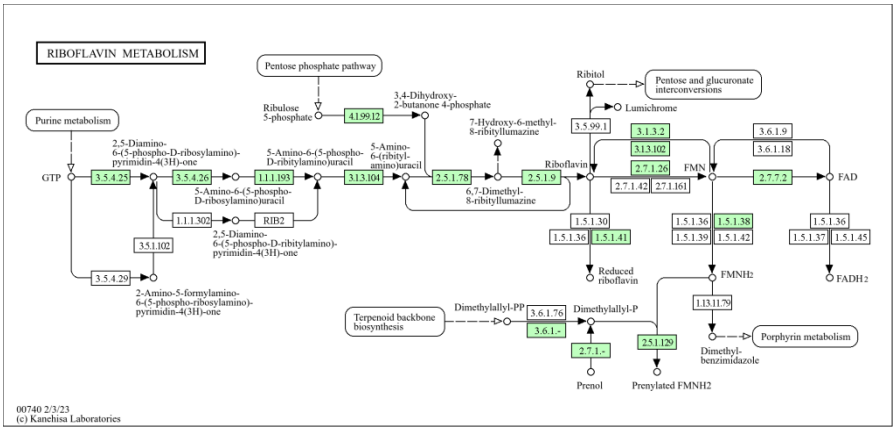

Figure S8 The Riboflavin metabolism in the aquifer.