

Table S8. Statistically significant phenomena, after Benjamini Hochberg correction of p-value. Column legend (in order of appearance): set; data-minimum experiment type; Can be one of p1corrd, c (correlation between fungal data and sPCA scores of chemical data), p1corrd.f (correlation between chemical data and sPCA scores of fungal data), p2corrd.f (correlation between chemical data and sPCA scores of fungal data), p2corrd (correlation between sPCA scores of fungal and sPCA scores of chemical data), pccm (statistical difference between accessions for sPCA scores of chemical data), pccrsts, t (statistical difference between sample types in sPCA scores of fungal chemical data), rawcorrd (correlation between chemical data and fungal data), type diversity (significant differences among diversity indices); mcol, ID of chemical in selected core chemical data or number of chemical sPCA PC; k, level of aggregation for fungal data (1 = phylum-level aggregation, 2 = order-level aggregates, 3 = genus-level data, 4 = diversity indices); Icol, ID of fungal feature or number of fungal sPCA PC; covr, Spearman correlation value; effect size, difference between Q1 and Q4 subset of fungal abundance, binned along chemical data; pval, p-value after Benjamini Hochberg correction; sigxt, significance (***, padj < 0.001, **, padj < 0.01, *, padj < 0.05); abslowerCI, lower edge of 95% confidence interval for bootstrapped Spearman correlation value (n = 250); fungal, part, fungal taxon used in correlation in UNITE notation ("p_...", phylum; "o_...", order; "c_...", class; "f_...", family; "g_...", genus) or sPCA principal component number; mzm, m/z of chemical feature in correlation; rtm, retention time of chemical feature in correlation; polarity, 1 or -1 denotes hydrophilic or hydrophobic; putative, putative identification; manual class, manual classification; canopus class, canopus classification; canopus, class and CSI: Fingerprint suggestions; canopus_class, "most specific class" suggestion in the Classifyer hierarchy by the canopus algorithm; id, compound id as plotted in Fig. 3; identified compounds appear as class, m_x, unknown as m_x, f_t, unknown as m_x, f_t.																
set	mcol	k	pcal	covr	effect size	pval	sigxt	abslowerCI	fungal part	nmzed	rtmed	polarity	putative identification	manual class	canopus class	id
p1corrd.c	1	2	2	0.42459484017734	0.735495484017734	0.0358626153239792	***	0.2248017819096139	lungal part	NA	NA	NA	NA	Glucosinolates	Canopus class	sinigrin
p1corrd.c	1	2	1	0.583213134145841	-2.05131272033939	0.00047375022300972	***	0.3887536340504602	Xyariales	NA	NA	NA	NA	Glucosinolates	Canopus class	sinigrin
p1corrd.c	1	3	8	0.433049415635823	-1.44388564054217	0.029364712848756	***	0.221035931216462	Morphaeaceae	NA	NA	NA	NA	Glucosinolates	Canopus class	sinigrin
p1corrd.f	6	2	2	0.57385511355311	-1.49422398626309	0.000952136004935233	***	0.40010996441003	PC2 2	287.0559	12.86	-1	other compounds	Organotin compounds	other compounds	287.0559 12.86
p1corrd.f	6	2	2	0.6310439566439566	1.90643043026059	0.00014779518610128	***	0.457143448741813	PC2 2	204.0158	11.29	-1	other compounds	Organotin compounds	other compounds	204.0158 11.29
p1corrd.f	6	2	2	0.42701971904719	-0.3358671532972	0.000810510656371	***	0.200810510656371	PC2 2	204.0158	11.29	-1	other compounds	Organotin compounds	other compounds	204.0158 11.29
p1corrd.f	18	2	2	0.547619047619048	-1.41562790106602	0.00121696586666357	***	0.3411296547280121	PC2 2	449.1098	13.51	-1	Kaempferol-hexoside	flavonoid glycosides	Kaempferol-hexoside	287.0559 12.86
p1corrd.f	21	2	2	0.56048547985348	-1.7552746139664	0.00136694095964666	***	0.363997216028201	PC2 2	287.0559	12.86	-1	other compounds	Organotin compounds	other compounds	287.0559 12.86
p1corrd.f	26	2	2	0.462454212454212	-1.08403191827347	0.0171281171269551	***	0.24388453981427	PC2 2	268.0562	9.72	-1	other compounds	Organotin compounds	other compounds	268.0562 9.72
p1corrd.f	31	2	2	0.520591575091575	1.90190626887971	0.003858886792747	***	0.32824572829681	PC2 2	471.1058	11.06	-1	GSH + 3-methylsulfinylpropyl ITC	Peptides	Gamma-glutamyl peptides	GSH + 3-methylsulfinylpropyl ITC
p1corrd.f	35	2	2	0.421336996336996	1.26830704271791	0.0149296666666666	***	0.178947440023242	PC2 2	351.1564	13.41	-1	other compounds	Organotin compounds	other compounds	351.1564 13.41
p1corrd.f	35	2	2	0.54807140888929	1.78015921781461	0.0035921781461	***	0.36841408888929	PC2 2	617.1558	12.86	-1	Kaempferol-dihexoside	flavonoid glycosides	Flavonoid-3-O-glycosides	Kaempferol-dihexoside
p1corrd.f	41	2	2	0.515338872388872	1.26400904322477	0.0049680566666666	***	0.301269022490381	PC2 2	325.0474	12.98	-1	other aromatic compounds	Benzenoids	other aromatic compounds	325.0474 12.98
p1corrd.f	49	2	2	0.50947801978022	1.2100082204841	0.0057062432654137	***	0.288652504209666	PC2 2	322.1888	12.41	-1	other compounds	Organotin compounds	other compounds	322.1888 12.41
p1corrd.f	50	2	2	0.589194139194139	1.8059266649151	0.0005640809655349	***	0.396584179316211	PC2 2	272.5316	13.25	-1	other compounds	Organotin compounds	other compounds	272.5316 13.25
p1corrd.f	52	2	2	0.495628448484503	1.5311689512788	0.0068646999898505	***	0.292145860654599	PC2 2	314.1836	9.93	-1	other compounds	Organotin compounds	other compounds	314.1836 9.93
p1corrd.f	55	2	2	0.529388273388273	1.55959638274024	0.0176539174654564	***	0.2403626533239792	PC2 2	285.1863	9.54	-1	Lipids and lipid-like molecules	Glycerolipids	Lipids and lipid-like molecules	285.1863 9.54
p1corrd.f	64	2	2	0.403461361963619	-1.403461361963619	0.003555337957	***	0.2727434972443	PC2 2	455.1615	12.79	-1	Amino acid derivatives and peptides	N-acetyl-alpha amino acids and derivatives	Amino acid derivatives and peptides	455.1615 12.79
p1corrd.f	69	2	2	0.579166666666667	1.60274831405405	0.0073953611860002	***	0.330850163629655	PC2 2	277.1058	12.32	-1	other compounds	Organotin compounds	other compounds	277.1058 12.32
p1corrd.f	84	2	2	0.593438352847334	2.26640093927982	0.0034078126998933	***	0.409686391531759	PC2 2	423.1387	12.58	-1	Cys Cys Pro Thr	Peptides	Cys Cys Pro Thr	423.1387 12.58
p1corrd.f	88	2	2	0.5992739927399	1.8874706134634	0.00376615104050379	***	0.39729394774603	PC2 2	262.0753	12.32	-1	other compounds	Organotin compounds	other compounds	262.0753 12.32
p1corrd.f	90	2	2	0.54025178021978	1.32741647807717	0.0271112001186002	***	0.25490969245332	PC2 2	272.1729	10.84	-1	Indol-3-ylmethyl amino derivative	Amino acid derivatives and peptides	Alpha amino acids	Indol-3-ylmethyl amino derivative
p1corrd.f	96	2	2	0.456504659341	1.44021930459341	0.0163902174609	***	0.270710517499915	PC2 2	258.1573	9.67	-1	other compounds	Organotin compounds	other compounds	258.1573 9.67
p1corrd.f	97	2	2	0.576810810715916	-1.5147221161416	0.00058983327795724	***	0.37029698306883	PC2 2	307.0939	12.49	-1	Kaempferol derivate	flavonoid glycosides	Flavonoid-3-O-glycosides	Kaempferol derivate
p1corrd.f	98	2	2	0.56767399267399	-1.89116613439081	0.0012365400354162	***	0.409076065166961	PC2 2	307.0939	12.49	-1	Amino acid derivatives and peptides	Alpha amino acids and derivatives	Amino acid derivatives and peptides	307.0939 12.49
p1corrd.f	102	2	2	0.5147036939662	-1.5011269110303	0.0042248604454719	***	0.2848378099337	PC2 2	325.5489	12.98	-1	other compounds	Organotin compounds	other compounds	325.5489 12.98
p1corrd.f	107	2	2	0.427838827388827	1.1888574905968	0.0358626153239792	***	0.190498419328113	PC2 2	382.1149	11.31	-1	Glycosides	O-glycosyl compounds	Glycosides	382.1149 11.31
p1corrd.f	110	2	2	0.50425178021978	-1.50425178021978	0.013555337957	***	0.408172727272727	PC2 2	271.058	12.32	-1	other compounds	Organotin compounds	other compounds	271.058 12.32
p1corrd.f	111	2	2	0.6030318128309	-1.8385756383807	0.8963367817851105	***	0.454781697143151	PC2 2	539.0059	13.25	-1	other compounds	Organotin compounds	other compounds	539.0059 13.25
p1corrd.f	113	2	2	0.565247252747253	1.7034301086807	0.0012810254961322	***	0.355987091062945	PC2 2	273.0328	12.32	-1	other compounds	Organotin compounds	other compounds	273.0328 12.32
p1corrd.f	117	2	2	0.473443223443223	1.3742195088329	0.139882158053529	***	0.252480212881612	PC2 2	298.1156	10.61	-1	Nucleotide derivatives	Purine nucleosides	Nucleotide derivatives	298.1156 10.61
p1corrd.f	131	2	2	0.452518315018315	-1.4012518711564	0.002789288667243	***	0.276932869474403	PC2 2	388.0748	11.52	-1	pentyl GSL	Glucosinolates	pentyl GSL	388.0748 11.52
p1corrd.f	132	2	2	0.475293882738827	1.26830704271791	0.0149296666666666	***	0.249342055393638	PC2 2	226.1081	12.68	-1	other compounds	Organotin compounds	other compounds	226.1081 12.68
p1corrd.f	136	2	2	0.438033633363336	1.09470821268404	0.02890924540347	***	0.15747721726934	PC2 2	307.0939	12.41	-1	other compounds	Organotin compounds	other compounds	307.0939 12.41
p1corrd.f	139	2	2	0.525549455054945	-1.5654515834265	0.003858886792747	***	0.321262238295363	PC2 2	549.1256	13.13	-1	Kaempferol-dipentose	flavonoid glycosides	Flavonoid-3-O-glycosides	Kaempferol-dipentose
p1corrd.f	159	2	2	0.529487179487179	-1.4228270664981	0.0036732140479801	***	0.294224105233379	PC2 2	417.0833	13.42	-1	other compounds	Organotin compounds	other compounds	417.0833 13.42
p1corrd.f	163	2	2	0.445558608680868	1.28639653045502	0.0245912679295426	***	0.238571072994668	PC2 2	282.085	9.84	-1	other compounds	Organotin compounds	other compounds	282.085 9.84
p1corrd.f	163	2	2	0.473901089091089	-1.29663708013814	0.013985142857143	***	0.267662299174603	PC2 2	225.9845	12.66	-1	other compounds	Organotin compounds	other compounds	225.9845 12.66
p1corrd.f	6	3	2	0.427103296703297	1.5498676880729	0.01686823329964	***	0.202399953036693	PC3 1	287.0559	12.86	-1	other compounds	Organotin compounds	other compounds	287.0559 12.86
p1corrd.f	6	3	2	0.479166666666667	1.021771258231	0.010724602545892	***	0.284727122459281	PC3 1	258.1573	9.67	-1	other compounds	Organotin compounds	other compounds	258.1573 9.67
p1corrd.f	8	3	2	0.5653388131868	-1.3077092343304	0.006171881866201	***	0.29724145988159	PC3 1	204.0158	11.29	-1	other compounds	Organotin compounds	other compounds	204.0158 11.29
p1corrd.f	8	3	2	0.405338827388273	1.41609292170087	0.014646497448857	***	0.254225427526338	PC3 1	204.0158	11.29	-1	other compounds	Organotin compounds	other compounds	204.0158 11.29
p1corrd.f	18	3	2	0.42226995970666	1.4042221969102	0.041175354360322	***	0.213116240045079	PC3 1	449.1098	12.86	-1	Kaempferol-hexoside	flavonoid glycosides	Flavonoid-3-O-glycosides	Kaempferol-hexoside
p1corrd.f	18	3	2	0.428113563135631	1.05270323394413	0.0358626153239792	***	0.200959545284357	PC3 1	449.1098	12.86	-1	Kaempferol-hexoside	flavonoid glycosides	Flavonoid-3-O-glycosides	Kaempferol-hexoside
p1corrd.f	21	3	2	0.471428571428571	1.24283101892837	0.0143730749880326	***	0.226656205939498	PC3 2	287.0559	13.25	-1	other compounds	Organotin compounds	other compounds	287.0559 13.25
p1corrd.f	24	3	2	0.524917595471759	-1.4531555437609	0.003555337957	***	0.333555437609	PC3 2	423.1387	12.58	-1	other compounds	Organotin compounds	other compounds	423.1387 12.58
p1corrd.f	26	3	2	0.525257472527473	1.44221880912678	0.004941960544673	***	0.3152224511513	PC3 2	272.5316	12.32	-1	other compounds	Organotin compounds	other compounds	272.5316 12.32
p1corrd.f	55	3	2	0.525257472527473	-1.85564648188217	0.03965558546422	***	0.192421181908198	PC3 1	285.1863	9.54	-1	Lipids and lipid-like molecules	Glycerolipids	Lipids and lipid-like molecules	285.1863 9.54
p1corrd.f	59	3	2	0.500854997998668	-1.6046734470082	0.006066267852576	***	0.286110914833001	PC3 1	357.9849	12.13	-1	other aromatic compounds	Benzenesulfonamides	other aromatic compounds	357.9849 12.13
p1corrd.f	59	3	2	0.561743534435344	-1.4095030987738	0.00136694095964666	***	0.316791748065009	PC3 1	357.9849	12.13	-1	other aromatic compounds	Benzenesulfonamides	other aromatic compounds	357.9849 12.13
p1corrd.f	64	3	2	0.501501831051831	-1.52780136939785	0.01335435849006	***	0.29447898238951	PC3 2	455.1615	12.79	-1	Amino acid derivatives and peptides	N-acetyl-alpha amino acids and derivatives	Amino acid derivatives and peptides	455.1615 12.79
p1corrd.f	69	3	2	0.5380366303663	-1.53701023610827	0.0021385987966	***	0.3040002116983	PC3 2	277.1058	12.32	-1	other compounds	Organotin compounds	other compounds	277.1058 12.32
p1corrd.f	84	3	2	0.4924859387434	-1.3660663205388	0.007588713258314	***	0.278810556123274	PC3 1	423.1387	12.58	-1	Cys Cys Pro Thr	Peptides	Cys Cys Pro Thr	423.1387 12.58
p1corrd.f	84	3	2	0.431422880343685	-1.5762711880420	0.03070503061706	***	0.2020436908216	PC3 2	423.1387	12.58	-1	Cys Cys Pro Thr	Peptides	Cys Cys Pro Thr	423.1387 12.58
p1corrd.f	94	3	2	0.508608658086580	-1.434375743208	0.0057062432654137	***	0.326149514904065	PC3 2	262.0753	12.32	-1	other compounds	Organotin compounds	other compounds	262.0753 12.32
p1corrd.f	94	3	2	0.420375547303058	-1.30271758231	0.0057062432654137	***	0.266136774678426	PC3 2	247.1451	12.32	-1	Indol-3-ylmethyl amino derivative	Amino acid derivatives and peptides	Alpha amino acids	Indol-3-ylmethyl amino derivative