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Icescape scale metabolomics reveals cyanobacteria and solar radiation influence core
biochemical pathways in the cryoconite ecosystem of an Arctic ice cap

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SUPPLEMENTARY TABLE 1: Core and keystone* OTUs based on Greengenes identification defined from Gokul et al (2016) used to predict regression patterns on cryoconite metabolome and metabolic pathways.

Taxon	% Relative Abundance	Phylum	Class	Order	Family	Genus	BLAST ID
denovo4 0205*	12.95	<i>Cyanobacteria</i>	<i>Synechococcyphycideae</i>	<i>Pseudanabaenales</i>	<i>Pseudanabaenaceae</i>	<i>Leptolyngbya</i>	<i>Phormidesmis priestleyi</i> ANT.L66.
denovo3 2521	4.59	<i>Actinobacteria</i>	<i>Actinobacteria</i>	<i>Actinomycetales</i>	<i>Microbacteriaceae</i>	-	<i>Frigoribacterium</i> sp. MP117
denovo5 709	4.50	<i>Proteobacteria</i>	<i>Betaproteobacteria</i>	Ellin6067	-	-	<i>Massilia</i> sp. 4106
denovo5 9904	2.89	<i>Gemmatimonadetes</i>	<i>Gemmatimonadetes</i>	Gemmatimonadales	Ellin5301	-	Ellin5220
denovo3 7757*	2.77	<i>Chloroflexi</i>	C0119	-	-	-	<i>Azospirillum</i> sp. YM195
denovo5 3430*	2.14	Unassigned	-	-	-	-	<i>Rhizobium</i> sp. AC86c1
denovo1 1564	1.88	<i>Proteobacteria</i>	<i>Alphaproteobacteria</i>	<i>Sphingomonadales</i>	<i>Sphingomonadaceae</i>	-	<i>Novosphingobium</i> sp. R1-11
denovo1 447*	1.73	<i>Actinobacteria</i>	<i>Actinobacteria</i>	<i>Actinomycetales</i>	<i>Intrasporangiaceae</i>	-	<i>Eubacterium</i> sp. 4c
denovo4 6072	1.71	<i>Actinobacteria</i>	<i>Actinobacteria</i>	<i>Actinomycetales</i>	<i>Intrasporangiaceae</i>	-	<i>Oryzihumus</i> sp. aerobe-19
denovo5 3638*	1.67	<i>Actinobacteria</i>	<i>Actinobacteria</i>	<i>Actinomycetales</i>	<i>Intrasporangiaceae</i>	-	<i>Ornithinimicrobium tianjinense</i>
denovo2 7964*	1.44	<i>Actinobacteria</i>	<i>Actinobacteria</i>	<i>Actinomycetales</i>	<i>Intrasporangiaceae</i>	-	<i>Humibacter albus</i>
denovo1 0679	1.34	<i>Proteobacteria</i>	<i>Betaproteobacteria</i>	Ellin6067	-	-	<i>Telluria mixta</i>
denovo4 5763	1.14	<i>Cyanobacteria</i>	<i>Oscillatoriophyycideae</i>	<i>Oscillatoriales</i>	<i>Phormidiaceae</i>	<i>Phormidium</i>	<i>Phormidium autumnale</i> Ant-Ph68
denovo5 1358	1.14	<i>Proteobacteria</i>	<i>Gammaproteobacteria</i>	<i>Xanthomonadales</i>	<i>Xanthomonadaceae</i>	-	<i>Pseudoxanthomonas sacheonensis</i>
denovo2 2304	1.06	<i>Proteobacteria</i>	<i>Betaproteobacteria</i>	<i>Burkholderiales</i>	<i>Comamonadaceae</i>	-	<i>Curvibacter</i>
denovo6 1341	1.00	<i>Bacteroidetes</i>	<i>Sphingobacteriia</i>	<i>Sphingobacteriales</i>	<i>Sphingobacteriaceae</i>	-	<i>Pedobacter daechungensis</i>
denovo6 1555*	0.60	<i>Actinobacteria</i>	<i>Acidimicrobiia</i>	<i>Acidimicrobiales</i>	C111	-	<i>Iamia</i> sp. T2-YC6790
denovo4 1255*	0.29	<i>Actinobacteria</i>	<i>Actinobacteria</i>	<i>Actinomycetales</i>	<i>Intrasporangiaceae</i>	-	<i>Arsenicicoccus</i> sp. 12-2
denovo4 8894*	0.20	<i>Actinobacteria</i>	<i>Acidimicrobiia</i>	<i>Acidimicrobiales</i>	EB1017	-	Ellin7143
denovo5 1679*	0.14	<i>Gemmatimonadetes</i>	<i>Gemmatimonadetes</i>	<i>Gemmatimonadales</i>	Ellin5301	-	Ellin5220

SUPPLEMENTARY TABLE 2: Marginal tests of core taxa, keystone taxa and environmental parameters in redundancy analysis of total metabolites.

Variable	SS(trace)	Pseudo-F	P	Prop.
E	4.062	12.721	0.001	0.27227
N	0.96025	2.3389	0.043	6.44E-02
Chl A	0.91475	2.2208	0.061	6.13E-02
Z	2.7508	7.6861	0.001	0.18438
SLOPE	0.32971	0.76837	0.565	2.21E-02
ASPECT	2.0849	5.5233	0.002	0.13975
FAA	1.2423	3.0884	0.021	8.33E-02
FLOWLENGTH	1.2694	3.1619	0.023	8.51E-02
CURVATURE	0.51477	1.215	0.257	3.45E-02
WETNESS	0.28162	0.65415	0.61	1.89E-02
PDDs	2.115	5.6162	0.001	0.14177
PositiveHrs	2.8478	8.0212	0.001	0.19088
PDH	2.7162	7.5679	0.002	0.18206
IR (W)	2.0253	5.3406	0.002	0.13575
IRh (hrs)	0.6513	1.552	0.151	4.37E-02
IR (kW)	2.0253	5.3406	0.001	0.13575
Irhrs	0.65002	1.5488	0.174	4.36E-02
ACA	0.61076	1.4513	0.196	4.09E-02
<i>O. tianjinense</i>-53638	1.2475	3.1024	0.033	8.36E-02
<i>H. albus</i>-27964	1.341	3.3579	0.028	8.99E-02
<i>Iamia</i>-61555	1.1912	2.9501	0.035	7.98E-02
<i>Azospirillum</i> -37757	0.84626	2.0446	0.067	5.67E-02
<i>Eubacterium</i> -1447	0.44452	1.0441	0.356	2.98E-02
<i>Ellin5220</i> -51679	0.45973	1.081	0.34	3.08E-02
<i>Rhizobium</i> -53430	0.79849	1.9226	0.089	5.35E-02
<i>Ellin7143</i> -48894	0.13981	0.32164	0.926	9.37E-03
<i>P. priestleyi</i> -40205	0.59489	1.412	0.195	3.99E-02
<i>Frigoribacterium</i> -32521	0.65665	1.5654	0.155	4.40E-02
<i>Massilia</i> -5709	0.7295	1.748	0.11	4.89E-02
<i>Ellin5220</i>-59904	1.9105	4.9933	0.001	0.12806
<i>Novosphingobium</i> -11564	0.17951	0.41406	0.889	1.20E-02
<i>Oryzihumus</i> -46072	0.40736	0.95441	0.403	2.73E-02
<i>T. mixta</i>-10679	1.5161	3.846	0.015	0.10162
<i>Arsenicococcus</i>-41255	1.2565	3.1269	0.025	8.42E-02
<i>P. daechungensis</i>-61341	1.4666	3.7066	0.01	9.83E-02
<i>P. autumnale</i>-45763	0.53015	1.2527	0.224	3.55E-02
<i>P. sacheonensis</i>-51358	0.42883	1.0062	0.409	2.87E-02
<i>Curvibacter</i>-22304	0.71958	1.723	0.124	4.82E-02

SUPPLEMENTARY TABLE 3: Sequential tests of core taxa, keystone taxa (*) and environmental parameters in redundancy analysis of total metabolites.

Variable	R²	SS(trace)	Pseudo-F	P	Prop.	Cumul.
E	0.27227	4.062	12.721	0.001	0.27227	0.27227
N	0.35699	1.264	4.3482	0.001	8.47E-02	0.35699
PDDs	0.42278	0.98143	3.6469	0.008	6.58E-02	0.42278
Chl A	0.46117	0.57279	2.2088	0.033	3.84E-02	0.46117
<i>Novosphingobium</i> -11564	0.6549	0.41633	1.8598	0.056	2.79E-02	0.6549
IRh (hrs)	0.84165	0.4329	2.3822	0.057	2.90E-02	0.84165
Irhrs	0.86736	0.3836	2.3263	0.058	2.57E-02	0.86736
<i>Ellin5220</i> -59904	0.89	0.33764	2.263	0.077	2.26E-02	0.89
<i>Massilia</i> -5709	0.49017	0.43268	1.7065	0.09	2.90E-02	0.49017
<i>Eubacterium</i> -1447	0.56796	0.39378	1.6495	0.11	2.64E-02	0.56796
<i>Ellin5220</i> -51679	0.9084	0.27457	2.0091	0.113	1.84E-02	0.9084
ASPECT	0.51627	0.38945	1.565	0.118	2.61E-02	0.51627
<i>P. priestleyi</i> -40205	0.54156	0.3773	1.5446	0.128	2.53E-02	0.54156
<i>Iamia</i> -61555	0.95299	0.23322	1.9951	0.133	1.56E-02	0.95299
FAA	0.76487	0.33053	1.6018	0.145	2.22E-02	0.76487
<i>O. tianjinense</i> -53638	0.74272	0.34034	1.596	0.153	2.28E-02	0.74272
Z	0.99765	0.17174	4.9011	0.189	1.15E-02	0.99765
<i>P. daechungensis</i> -61341	0.60961	0.30927	1.3275	0.201	2.07E-02	0.60961
<i>Curvibacter</i> -22304	0.58888	0.31216	1.3232	0.223	2.09E-02	0.58888
SLOPE	0.81264	0.25743	1.2893	0.254	1.73E-02	0.81264
ACA	0.67304	0.27061	1.2205	0.275	1.81E-02	0.67304
<i>H. albus</i> -27964	0.97164	0.15243	1.4411	0.294	1.02E-02	0.97164
PositiveHrs	0.79538	0.25426	1.2493	0.294	1.70E-02	0.79538
<i>Oryzihumus</i> -46072	0.92751	0.17609	1.3026	0.299	1.18E-02	0.92751
<i>Rhizobium</i> -53430	0.68979	0.24992	1.134	0.333	1.68E-02	0.68979
CURVATURE	0.9806	0.13363	1.385	0.336	8.96E-03	0.9806
<i>Frigoribacterium</i> -32521	0.62699	0.25935	1.1185	0.349	1.74E-02	0.62699
WETNESS	0.71991	0.24141	1.0976	0.35	1.62E-02	0.71991
<i>P. autumnale</i> -45763	0.93736	0.14694	1.1006	0.373	9.85E-03	0.93736
<i>Azospirillum</i> -37757	0.96143	0.12586	1.0934	0.385	8.44E-03	0.96143
<i>Ellin7143</i> -48894	0.77834	0.20091	0.97202	0.429	1.35E-02	0.77834
<i>P. sacheonensis</i> -51358	0.70373	0.2079	0.94069	0.482	1.39E-02	0.70373
IR (W)	0.98614	8.27E-02	0.79967	0.5	5.54E-03	0.98614
FLOWLENGTH	0.91571	0.109	0.78002	0.521	7.31E-03	0.91571
IR(kW)	0.99765	8.98E-14	0	1	6.02E-15	0.99765