

1 **Supporting Information**

2 Balancing trade-offs imposed by growth media and mass spectrometry for exometabolomics

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7 Content:

8 SI Figure 1 – Scans of SubTap context and analysis plates

9 SI Figure 2 – Frequency of matches to *Streptomyces*-produced compounds found in Natural

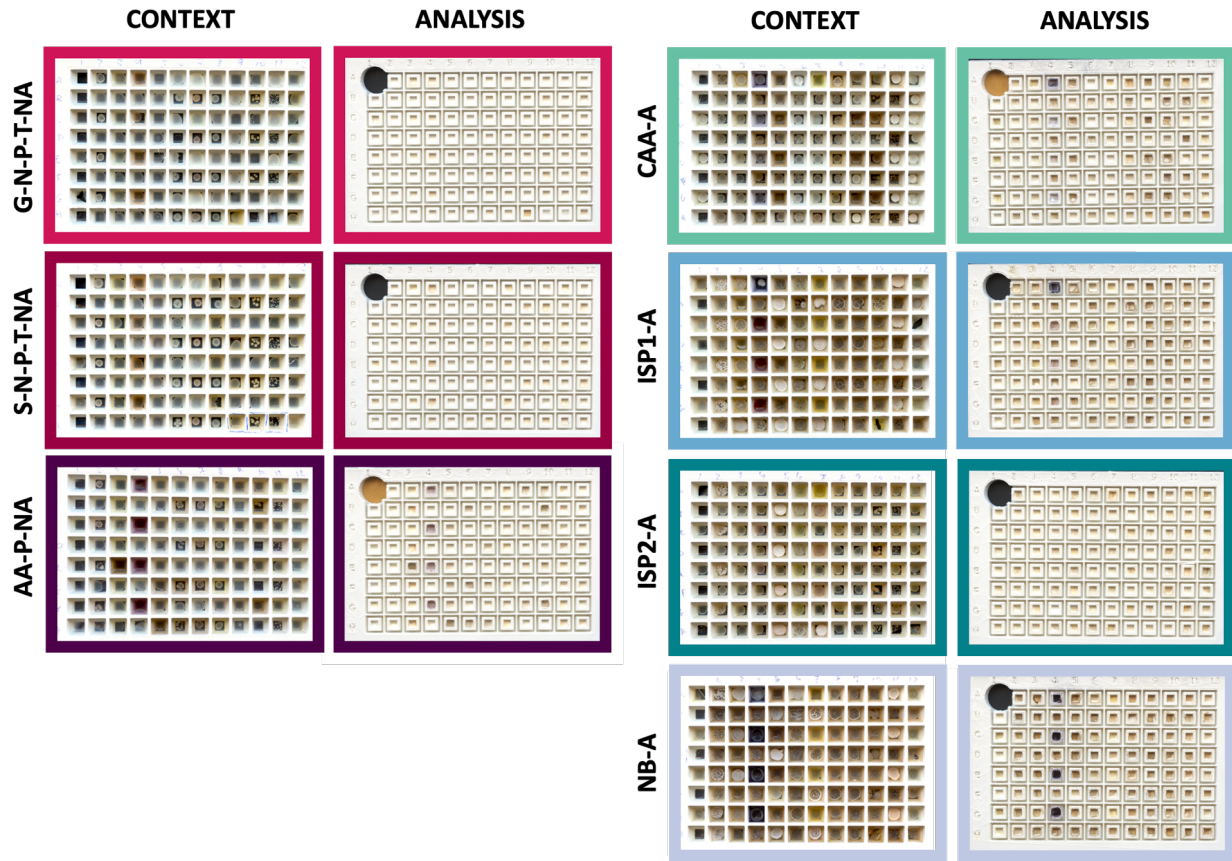
10 Products Atlas, by media type

11 SI Figure 3 - Correlation of Natural Products Atlas hits to *Streptomyces* isolate genetic

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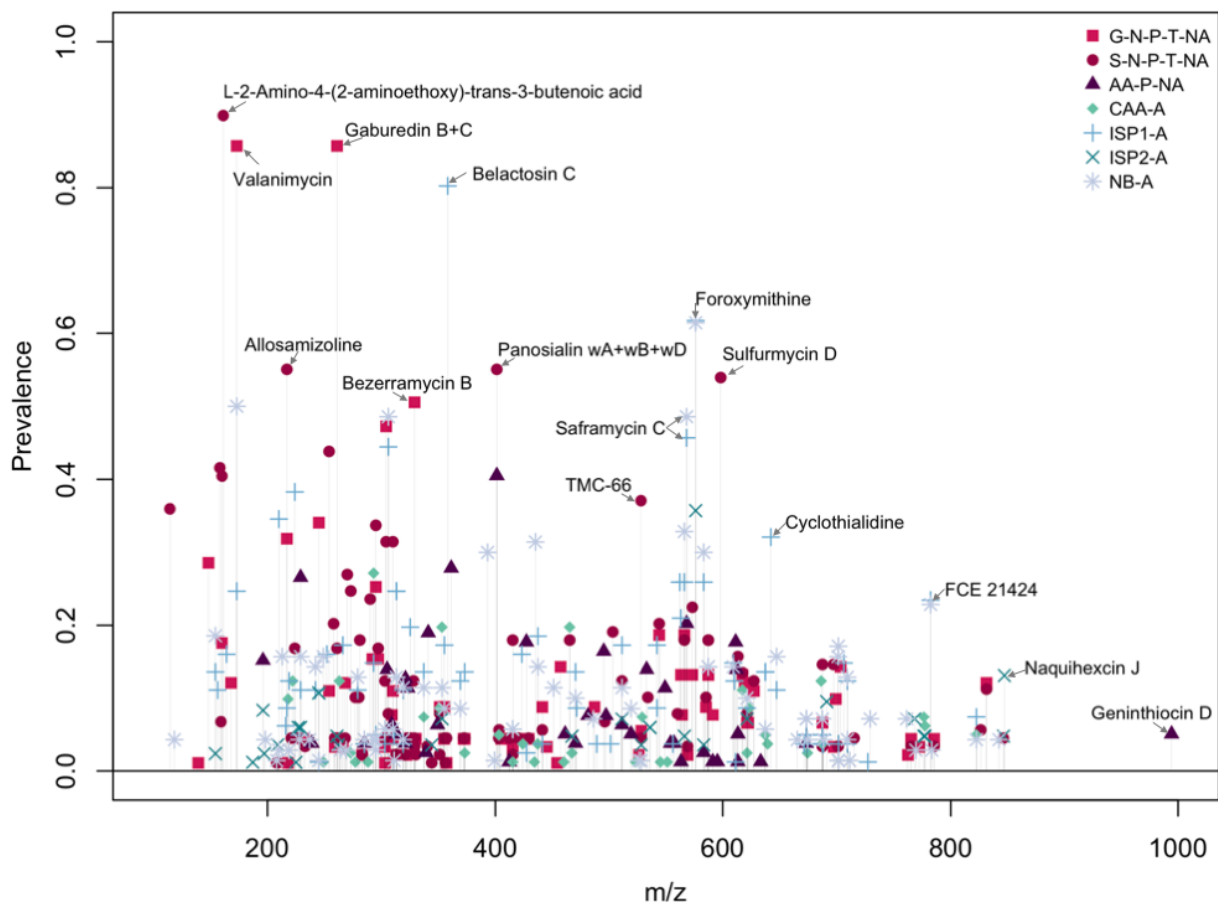
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SI Figure 1. Pictures of SubTap analysis plates used in this study.

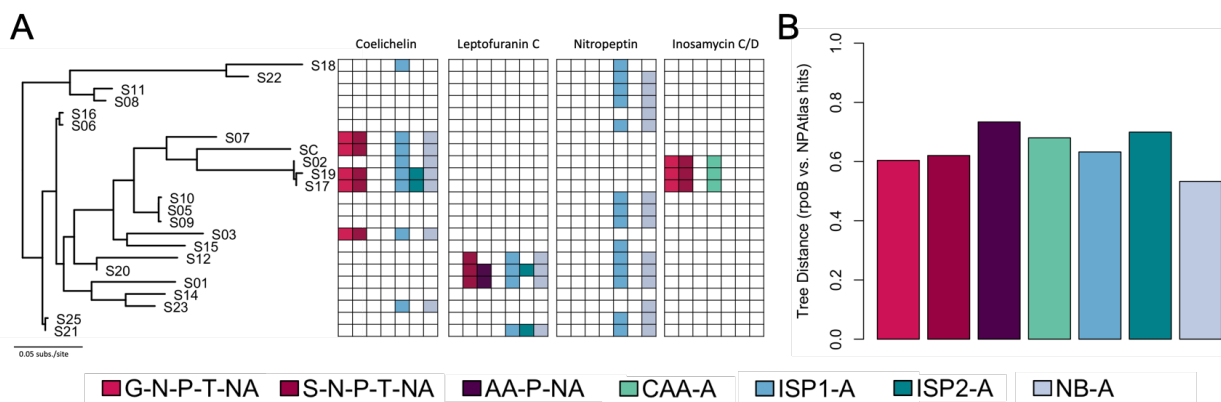
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SI Figure 2. Frequency of matches to *Streptomyces*-produced compounds found in the Natural Products Atlas, by media type. Named compounds depicted in figure are putatively annotated – level 3 (as defined in Sumner *et. al.*¹). See **SI Table 1** for additional information.

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SI Figure 3. Correlation of Natural Products Atlas hits to *Streptomyces* isolate relatedness. **(A)** *Streptomyces* phylogenetic tree based on the *rpoB* gene, and detection of four *Streptomyces*-produced compounds: coelichelin, leptofuranin C, nitropeptin and inosamycin C/D, by media and isolate. **(B)** Distance between the *rpoB* tree and Natural Products Atlas hit tree (see methods); lower value indicates closer match.

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21 **SI Table 1.** Putative annotations (level 3) of 19 compounds named in **SI Figs. 2 and 3**. Compound
 22 names are reported as listed in the Natural Products Atlas.
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Compound Name	Molecular Formula	Monoisotopic Mass	Medium	Adduct	Measured m/z	Error (ppm)
L-2-amino-4-pentynoic acid	C5H7NO2	113.0477	S-N-P-T-NA	M+H	114.0547	1.9
				M+K	152.0105	2.3
Valanimycin	C7H12N2O3	172.0848	G-N-P-T-NA	M+H	173.0921	0.4
				M+Na	195.0740	0.2
				M+K	211.0480	0.4
			ISP1-A	M+Na	195.0735	2.5
				M+K	211.0474	2.6
			NB-A	M+H	173.0916	2.6
				M+Na	195.0735	2.5
				M+K	211.0475	2.4
Allosamizoline	C9H16N2O4	216.1110	G-N-P-T-NA	M+H	217.1185	0.9
				M+K	255.0742	0.2
			S-N-P-T-NA	M+H	217.1178	2.1
				M+Na	239.0997	2.3
				M+K	255.0736	2.2
Gaburedin B; Gaburedin C	C11H20N2O5	260.1372	G-N-P-T-NA	M+H	261.1445	0.1
				M+K	299.1004	0.1
			S-N-P-T-NA	M+H	261.1439	2.4
				M+Na	283.1281	5.9
Nitropeptin	C11H19N3O7	305.1223	ISP1-A	M+Na	328.1108	2.2
				M+K	344.0847	2.4
			NB-A	M+Na	328.1107	2.5
				M+K	344.0846	2.5
Bezerramycin B	C16H12N2O6	328.0695	G-N-P-T-NA	M+H	329.0745	7.0
				M+K	367.0304	6.2
Belactosin C	C16H27N3O6	357.1900	ISP1-A	M+Na	380.1784	2.1
				M+K	396.1522	2.3
Panosialin wD; Panosialin wA; Panosialin wB	C21H36O5S	400.2284	S-N-P-T-NA	M+H	401.2383	6.7
				M+K	439.1941	6.0
			AA-P-NA	M+H	401.2342	3.6
				M+K	439.1895	4.5
Leptofuranin C	C32H46O5	510.3345	S-N-P-T-NA	M+H	511.3444	5.2
				M+Na	533.3262	4.5
				M+K	549.3003	4.7
			AA-P-NA	M+H	511.3390	5.4
				M+Na	533.3221	3.0
				M+K	549.2944	6.0
			ISP1-A	M+H	511.3444	5.2
				M+Na	533.3262	4.5
				M+K	549.3002	4.5
			ISP2-A	M+H	511.3439	4.1
				M+Na	533.3269	5.9
				M+K	549.2996	3.4
			NB-A	M+H	511.3446	5.5
				M+K	549.3003	4.8
			TMC-66	C29H21NO9	527.1216	S-N-P-T-NA
M+K	566.0867	3.3				

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Compound Name	Molecular Formula	Monoisotopic Mass	Medium	Adduct	Measured m/z	Error (ppm)
Coelichelin	C21H39N7O11	565.2708	G-N-P-T-NA	M+H	566.2778	0.5
				M+K	604.2337	0.3
			S-N-P-T-NA	M+H	566.2762	3.2
				M+K	604.2320	3.1
			ISP1-A	M+H	566.2766	2.5
				M+Na	588.2586	2.4
			ISP2-A	M+K	604.2326	2.2
				M+H	566.2758	4.0
			NB-A	M+Na	588.2577	3.9
				M+K	604.2315	4.0
				M+H	566.2765	2.8
				M+Na	588.2583	2.9
	M+K	604.2324	2.4			
Saframycin C	C29H33N3O9	567.2217	ISP1-A	M+H	568.2323	5.9
				M+Na	590.2142	5.6
				M+K	606.1881	5.4
			NB-A	M+H	568.2322	5.7
				M+Na	590.2141	5.3
Foroxymithine	C22H37N7O11	575.2551	ISP1-A	M+H	576.2609	2.6
				M+Na	598.2428	2.6
			ISP2-A	M+K	614.2167	2.6
				M+Na	598.2420	3.9
			NB-A	M+K	614.2159	3.9
				M+H	576.2608	2.7
				M+Na	598.2427	2.7
				M+K	614.2166	2.7
Sulfurmycin D	C31H35NO11	597.2210	S-N-P-T-NA	M+H	598.2298	2.6
				M+K	636.1856	2.3
Inosamycin D; Inosamycin C	C23H44N4O15	616.2803	G-N-P-T-NA	M+H	617.2886	1.6
				M+Na	639.2707	1.8
				M+K	655.2445	1.5
			CAA-A	M+H	617.2872	0.6
				M+Na	639.2691	0.7
Cyclothialidine	C26H35N5O12S	641.2003	ISP1-A	M+H	642.2066	1.5
				M+K	680.1624	1.5
FCE 21424	C38H43N3O15	781.2694	ISP1-A	M+H	782.2773	0.8
				M+Na	804.2592	0.6
			NB-A	M+H	782.2769	0.2
				M+Na	804.2588	0.2
Naquihexcin J	C39H42O19S	846.2041	ISP2-A	M+H	847.2101	1.5
				M+Na	869.1920	1.5
				M+K	885.1658	1.6
Geninthiocin D	C44H43N13O13S	993.2824	AA-P-NA	M+H	994.2923	2.6
				M+Na	1016.2732	1.6
				M+K	1032.2467	1.1

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30 **SI REFERENCES**

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