Supplementary information

Bioactive Cationic Lipidated Oligomers (CLOs) as Antimicrobial Materials: Metabolomic Insights into MRSA Membrane Disruption

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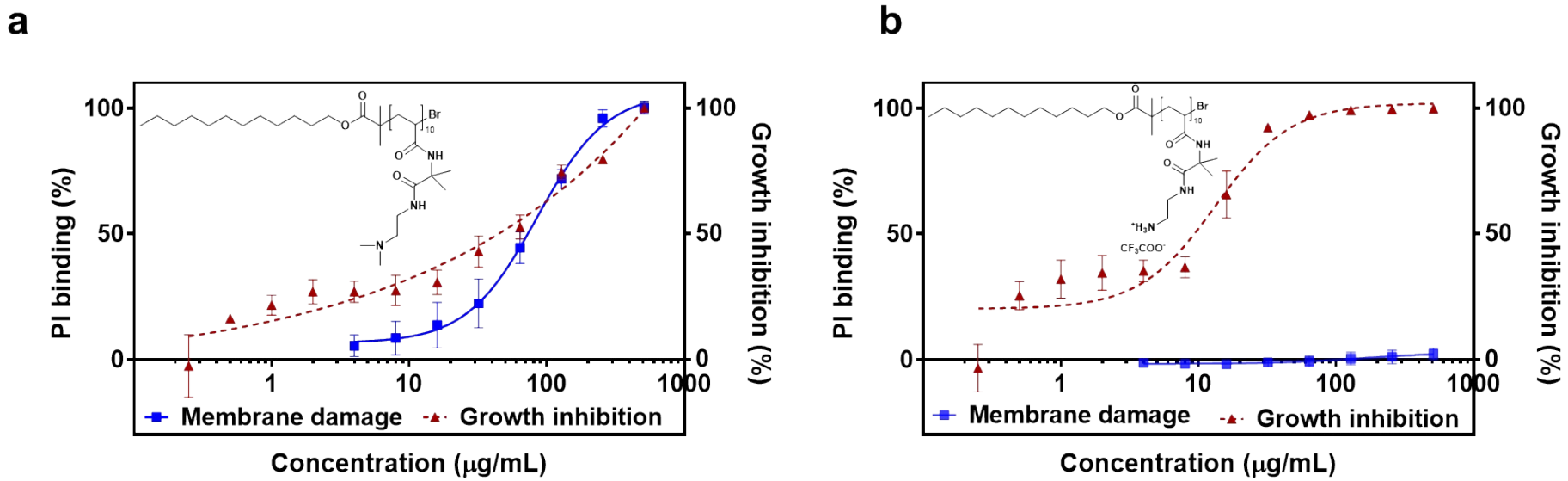

Figure S1: PI binding (%) and growth inhibition (%) assay of MRSA ATCC 43300 using **(a)** C_{12}-o-DMEN-10, **(b)** C_{12}-o-BEDA-10, over a range of oligomer concentrations. Data are presented as mean standard error of the mean (n = 6).

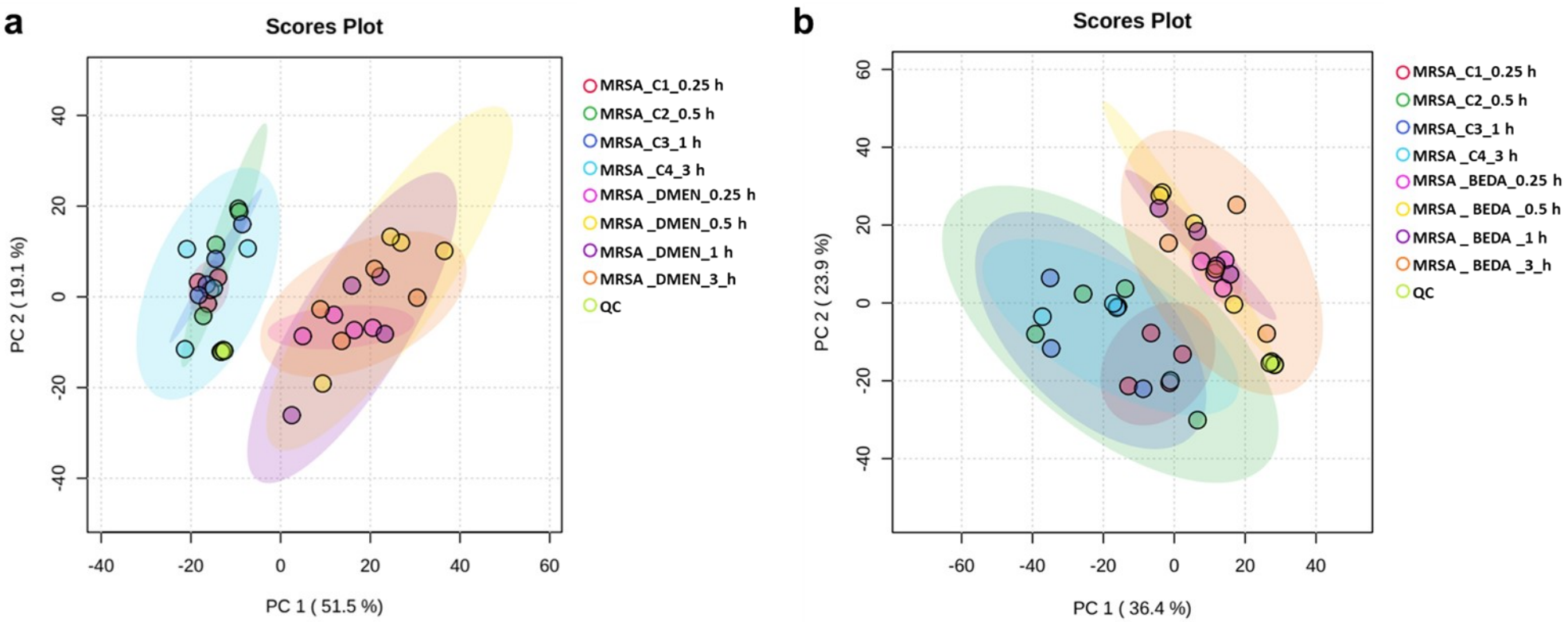

Figure S2. PCA plot of MRSA ATCC 43300 vs CLOs [C_{12}-o-DMEN-10 **(a)** and C_{12}-o-BEDA-10 **(b)**] at 0.25 h, 0.5 h, 1 h, and 3 h. DMEN= C_{12}-o-DMEN-10 and BEDA= C_{12}-o-BEDA-10.

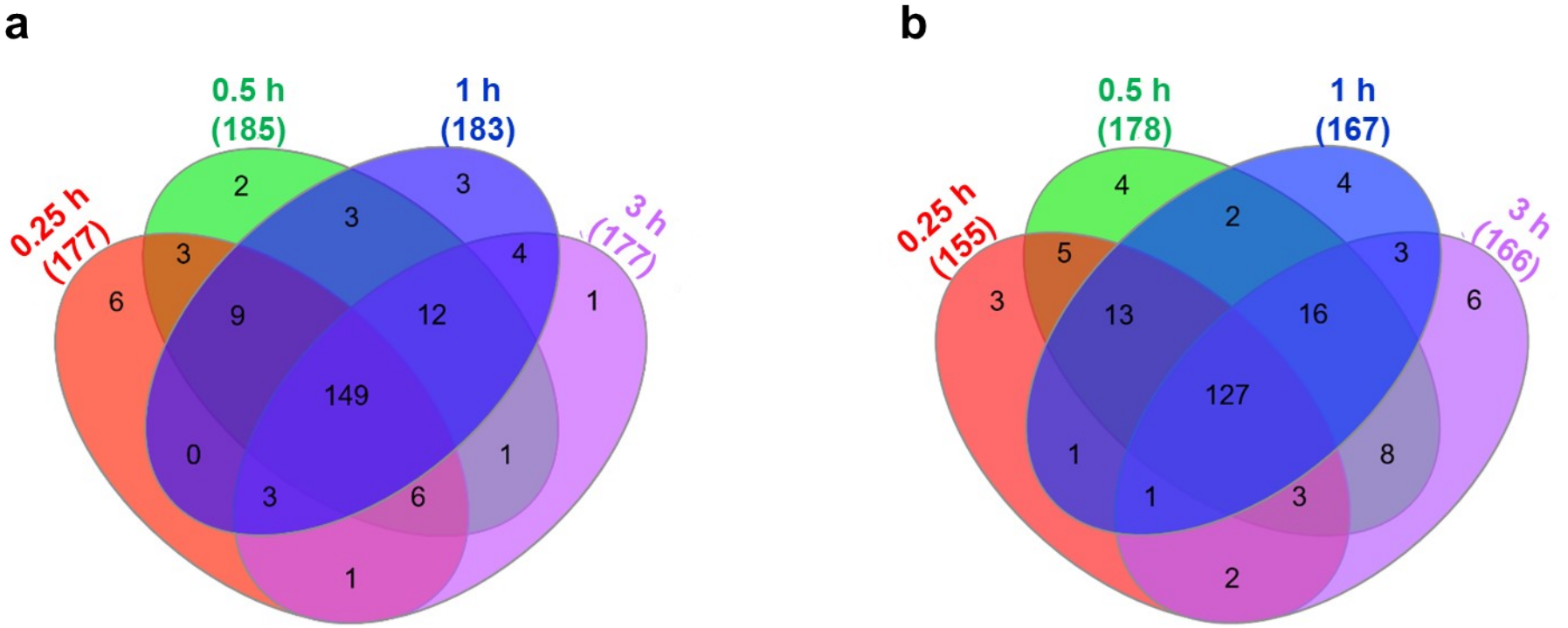

Figure S3: Venn diagram showing the number of metabolites of MRSA ATCC 43300, significantly affected by treatment with CLOs [C_{12}-o-DMEN-10 **(a)** and C_{12}-o-BEDA-10 **(b)**]. Significant metabolites were selected with (≥1-$\log_2$-FC; p<0.05).

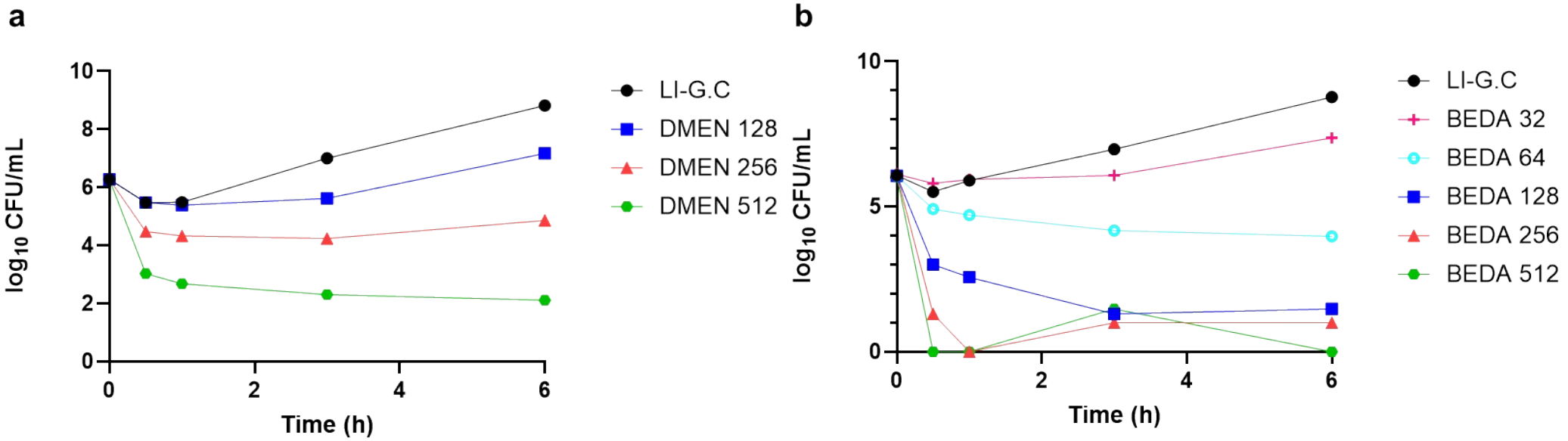

Figure S4: Killing kinetics of MRSA ATCC 43300 (initial inoculum ~10^6 $\log_{10}$ CFU/mL), after treatment with different concentrations of CLOs [**(a)** C_{12}-o-DMEN-10 (128, 256, 512 µg/mL) and **(b)** C_{12}-o-BEDA-10 (32, 64, 128, 256, 512 µg/mL)] (n=1).

Table S1: Significant metabolites putatively identified following exposure to CLOs [C_{12}-o-DMEN-10 and C_{12}-o-BEDA-10] in of methicillin-resistant *Staphylococcus aureus* (MRSA) ATCC 43300. Significant metabolites were determined using two-sample *t*-tests [(log_2fold-change [FC] ≥ 2, corresponding to a metabolite-level change of approximately 4-fold; false discovery rate [FDR] adjusted *p*-value < 0.05)].

Metabolomics changes (Log_2FC)									
Pathway	MAP	METABOLITES	C_{12}-o-DMEN-10				C_{12}-o-BEDA-10			
			0.25 h	0.5 h	1 h	3 hr	0.25 h	0.5 h	1 h	3 hr
Lipids Metabolism	Lysophospholipids	LysoPE(19:1)	1.54	1.65	0.88	1.40	1.07	1.20	0.83	1.07
		LysoPE(14:0)	0.83	1.35	0.75	0.05	0.47	0.62	0.99	0.33
		LysoPE(16:0)	-0.50	-0.80	-1.50	-1.17	0.17	0.52	0.69	1.07
		LysoPE(16:1)	0.71	0.61	-0.31	-0.29	1.94	1.60	1.23	1.50
		LysoPE(18:1)	3.45	3.32	0.69	1.36	0.79	1.73	0.45	1.01
		LysoPG(16:0)	-0.36	-0.01	-0.18	0.14	-0.86	-1.27	-0.30	0.17
		LysoPA(16:0)	-1.86	-2.25	-2.27	-0.67	-1.52	-2.01	-1.97	-0.15
		LysoPG(17:0)	-1.34	-1.36	-1.52	-1.15	-1.51	-1.77	-1.05	-1.01
	Glycerophospholipids	PE(32:1)	2.53	2.21	1.97	2.83	0.36	-1.03	2.15	0.41
		PE(34:2)	-1.69	-1.98	0.50	-0.45	-1.26	-1.94	-0.54	-0.09
		PG (28:0)	-3.45	-3.29	-2.86	-2.99	-2.41	-2.11	-2.66	-1.74
		PG(29:0)	-4.40	-4.11	-3.49	-3.47	-3.01	-2.54	-3.17	-1.90
		PG(30:0)	-5.00	-4.64	-3.83	-3.99	-3.20	-2.73	-3.49	-2.15
		PG(30:1)	-0.91	-1.05	-0.25	-0.25	-2.70	-1.05	-0.08	0.00
		PG(31:0)	-5.67	-5.34	-4.47	-4.75	-3.41	-2.83	-3.97	-2.42
		PG(31:1)	-3.65	-2.60	-3.31	-1.93	-2.85	-2.31	-3.38	-1.41
		PG(32:0)	-6.18	-5.76	-4.98	-5.16	-3.91	-3.15	-4.48	-2.59
		PG(32:2)	-2.85	0.00	0.00	0.00	-1.83	0.00	0.25	0.00

		PG(33:0)	-6.52	-5.84	-5.07	-3.14	-4.06	-3.12	-4.79	-0.81
		PG(33:1)	0.25	0.25	1.15	0.25	0.90	0.77	0.70	0.25
		PG(34:0)	-7.12	-6.24	-5.53	-5.30	-4.57	-3.60	-5.29	-2.78
		PG(34:1)	-4.41	-3.67	-2.93	-2.28	-4.32	-2.46	-4.06	-2.77
		PG(34:2)	-1.21	-0.25	-0.25	-1.40	-1.21	-0.25	-0.13	-1.10
		PG(35:0)	-7.04	-6.44	-5.45	-5.53	-5.00	-3.68	-5.76	-3.81
		PG(35:1)	-5.86	-4.10	-4.79	-1.77	-4.26	-2.88	-4.88	-2.58
		PG(35:2)	-2.02	-0.76	-1.66	1.76	-4.75	-1.29	-2.81	0.00
		PG(36:0)	-5.14	-3.21	-3.24	-4.85	-5.47	-3.21	-5.57	-3.22
		PI(22:0)	-1.31	-1.05	-0.95	-2.04	-0.33	-0.72	0.23	-0.50
		PS(32:0)	0.74	0.25	0.62	0.80	2.07	2.60	2.05	1.39
		PS(34:0)	-1.35	-0.94	0.06	-0.12	-1.36	-0.42	-0.80	0.06
	FA metabolism	(9xi,10xi,12xi)-9,10-Dihydroxy-12-octadecenoic acid	2.45	2.57	3.31	2.83	4.28	4.35	4.31	3.24
		2(R)-hydroxydocosanoic acid	1.90	0.25	1.26	1.88	2.66	3.16	3.03	2.29
		2-Hydroxyhexadecanoic acid	1.39	1.19	1.45	0.76	1.27	0.94	1.03	0.75
		2-Hydroxymyristoylcarnitine	5.20	5.05	4.37	3.90	1.11	2.35	0.15	0.78
		2-Hydroxystearic acid	1.13	1.21	1.57	0.78	1.26	1.39	1.26	1.36
		3-Hydroxy-octadecenoylcarnitine	1.10	7.39	1.63	8.35	1.86	2.13	1.41	1.11
		3-Oxooctadecanoic acid	0.97	1.12	1.62	0.87	0.91	1.24	1.20	1.17
		FA hydroxy(15:0)	1.23	1.73	1.98	2.24	1.13	1.50	1.57	2.01
		FA hydroxy(18:1)	-1.13	-0.14	-0.39	-0.03	-0.88	0.47	-0.46	0.17
		FA oxo(16:0)	0.94	1.00	1.25	1.09	0.93	1.05	0.97	1.00
		Heptadecanoic acid	-1.27	-0.32	0.30	0.14	-0.79	0.56	0.09	1.49
		Hexacosanedioic acid	7.01	5.51	5.34	4.88	10.98	10.03	5.81	8.26
		Hexadecanedioic acid mono-L-carnitine ester	1.92	2.34	2.21	1.62	1.81	1.27	1.51	1.16
		Myristic acid	0.93	0.83	1.66	0.32	1.06	1.08	1.29	0.90
		N-Heptanoylglycine	4.61	3.62	4.65	4.33	-0.91	-0.66	-1.04	-1.09

		N-Oleoylethanolamine	0.28	10.07	-1.15	10.27	0.25	1.20	0.25	-0.51
		N-palmitoyl threonine	1.29	5.54	1.63	7.13	1.62	1.62	1.31	7.37
		N-palmitoyl tryptophan	1.57	7.89	8.52	9.51	0.55	1.38	1.26	1.45
		Oleamide	2.06	1.71	2.07	3.18	3.96	4.38	4.09	5.07
		Palmitoleic acid	1.03	1.06	1.14	-0.53	0.71	0.69	0.52	0.42
		Palmitoylethanolamide	1.75	1.55	1.61	2.16	-0.09	0.81	-0.29	0.30
		Stearic acid	-1.35	-0.97	-0.66	-0.74	-0.64	-0.03	-0.79	0.36
		Stearoylglycine	4.05	3.44	4.82	4.48	0.44	0.94	-0.06	0.77
		Tridecanoic acid	0.77	1.23	1.40	1.60	0.58	1.06	1.20	1.16
Membrane Biosynthesis	**Amino sugar and sugar nucleotides**	UDP-*N*-acetyl-D-galactosamine	-1.70	-2.31	-2.06	-1.69	-1.50	-2.34	-1.82	-1.88
		N-Acetylneuraminate	-3.71	-4.62	-4.81	-2.34	-2.67	-3.15	-3.01	-2.07
		D-Mannose 1-phosphate	-3.70	-4.08	-4.62	-3.56	-3.18	-3.44	-3.15	-3.15
		UDP-glucose	-2.07	-2.67	-3.41	-2.62	-0.84	-1.67	-1.75	-1.92
		2-C-Methyl-D-erythritol 4-phosphate	-0.45	-1.62	-1.95	-1.98	-0.13	-0.58	-0.40	-1.36
		alpha-D-Glucosamine 1-phosphate	-1.66	-2.33	-4.18	-3.17	-1.27	-2.74	-2.87	-3.16
		N-Acetyl-D-glucosamine 6-phosphate	-1.01	-2.67	-1.12	-1.49	-0.50	-2.02	-1.25	-1.80
	Peptidoglycan biosynthesis	UDP-*N*-acetylmuramate	-1.60	-2.24	-2.73	-1.64	-0.07	-0.75	-1.44	-0.76
		UDP-*N*-acetylmuramoyl-L-alanyl-D-glutamate	2.91	0.13	-3.00	-3.38	3.16	0.01	-1.26	-1.50
		UDP-*N*-acetyl-2-amino-2-deoxy-D-glucuronate	-3.25	-3.52	-3.46	-2.69	-2.18	-2.76	-2.28	-1.23
		D-Alanyl-D-alanine	-2.57	-3.61	-4.00	-5.21	-1.79	-2.72	-2.21	-3.91
		UDPMurNAc(oyl-L-Ala-D-gamma-Glu-L-Lys-D-Ala-D-Ala)	-1.16	-1.63	-2.38	-1.12	0.40	-0.45	-1.28	-0.27
		L-Alanine	-1.67	-2.78	-2.57	-2.90	-1.11	-2.48	-1.15	-2.66
		D-Glutamate	-2.71	-3.71	-3.96	-2.99	-1.90	-2.92	-2.55	-2.73
		D-Aspartate	-3.06	-3.88	-4.26	-3.29	-2.26	-3.29	-2.88	-3.44
	Teichoic Acid	CDP-ribitol	-3.04	-3.57	-3.75	-2.02	-1.70	-2.55	-2.30	-1.35
		CDP-glycerol	-2.85	-2.84	-4.10	-2.61	-1.58	-2.08	-2.39	-1.83

	Lysine biosynthesis	D-Lysine	-1.89	-3.17	-3.66	-1.24	-1.33	-2.69	-2.50	-1.09
		L-2-Aminoadipate	-2.31	-2.37	-2.45	-3.55	-2.00	-2.03	-2.12	-3.52
		N6-Acetyl-L-lysine	-2.76	-3.35	-3.67	-1.42	-1.90	-2.87	-2.78	-0.61
		Protein N6,N6-dimethyl-L-lysine	-3.20	-2.87	-3.06	-3.07	-1.87	-2.59	-2.66	-3.20
		meso-2,6-Diaminoheptanedioate	0.03	-2.81	-1.08	-1.87	-0.62	-2.67	-1.08	-1.87
		(2R,4S)-2,4-Diaminopentanoate	-0.98	-1.64	-2.31	-1.59	-0.57	-1.61	-1.43	-1.82
		5-Acetamidopentanoate	-4.41	-4.76	-4.60	-3.04	-3.49	-4.44	-3.68	-2.12
	Mevalonic acid Pathway	farnesyl phosphate	2.16	1.89	1.70	0.17	2.98	1.03	0.92	0.01
		Mevalonic acid-5P	-2.56	-2.95	-6.79	-4.78	-4.40	-3.19	-2.63	-3.07
Amino acid metabolism		Glycine	-1.16	-1.70	-1.94	-2.22	-0.83	-1.51	-1.08	-2.29
		2-Aminoheptanoate	-3.74	-4.81	-5.30	-6.82	-2.99	-4.41	-5.06	-5.24
		L-Aspartate 4-semialdehyde	-3.87	-4.57	-4.94	-4.48	-3.14	-3.71	-3.46	-3.55
		L-Glutamine	-3.92	-5.05	-5.51	-2.99	-3.31	-4.37	-4.22	-2.73
		L-Methionine	-1.56	-2.24	-1.94	-1.35	-1.01	-1.71	-0.86	-1.29
		L-Valine	-2.50	-3.20	-3.57	-0.18	-1.68	-2.93	-2.33	-0.15
		4-Aminobutanoate	-2.00	-2.47	-1.92	-3.84	-2.10	-3.14	-2.64	-3.44
		O-Phospho-L-homoserine	-1.16	-1.79	-2.04	-3.25	-0.52	-1.04	-1.06	-2.61
		Iminoglycine	-1.92	-1.85	-3.44	-2.91	-1.77	-2.65	-1.66	-2.37
		N-Formyl-L-methionine	-4.04	-4.10	-3.78	-4.84	-2.87	-3.04	-2.37	-3.70
		L-Asparagine	-2.01	-2.79	-0.94	-2.71	-2.58	-2.68	-0.87	-3.66
		N-Acetyl-L-aspartic acid	-3.86	-5.73	-5.60	-8.50	-2.81	-4.11	-3.85	-6.65
		malyl alpha-D-glucosaminide	-2.80	-3.88	-4.47	-3.93	-1.63	-2.65	-2.91	-2.36
		malyl N-acetyl-alpha-D-glucosaminide	-1.84	-2.25	-3.30	-2.93	-1.19	-1.88	-2.76	-1.91
		Glutamate methylester	-4.11	-4.86	-5.38	-5.33	-3.28	-3.90	-3.68	-3.71
DNA and RNA biosynthesis	**Purines biosynthesis**	ATP	-2.84	-4.52	-4.95	-3.14	-2.63	-3.86	-3.85	-2.82
		ADP	-4.01	-4.82	-4.48	-4.08	-3.07	-3.54	-3.19	-3.62
		dADP	-3.08	-4.42	-2.70	-3.85	-2.43	-3.30	-3.11	-4.86
		dAMP	-2.71	-4.00	-5.40	-3.07	-1.89	-2.64	-3.10	-3.70
		Adenine	-2.07	-2.08	-2.62	-1.78	-1.06	-1.39	-1.08	-1.06

		Adenosine	-3.72	-3.57	-4.60	-5.48	-2.25	-2.65	-2.62	-3.08
		Deoxyadenosine	-3.35	-3.30	-2.51	-3.40	-1.19	-1.80	-1.58	-2.70
		GDP	-3.68	-4.27	-4.91	-6.42	-3.32	-4.77	-4.19	-5.80
		GTP	-3.13	-4.85	-5.64	-5.90	-3.53	-5.70	-5.41	-5.71
		GMP	-1.20	-4.64	-4.85	-6.31	-2.78	-4.01	-3.34	-4.85
		dGDP	-2.71	-4.24	-4.69	-2.86	-2.61	-3.66	-3.46	-2.45
		Guanine	1.55	1.14	-0.17	-2.51	2.01	0.74	0.27	-2.49
		8-Hydroxyadenine	-4.16	-3.55	-1.44	-1.92	-2.01	-3.62	-3.12	-4.05
		N-Formiminoglycine	-2.87	-3.67	-4.43	-4.34	-1.77	-2.71	-2.95	-3.23
		5'-Phosphoribosyl-N-formylglycinamide	-5.98	-2.90	-2.98	-5.49	-3.90	-5.12	-5.03	-4.57
		1-(5'-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole	-3.27	-5.61	-3.48	-3.35	-3.96	-5.81	-5.12	-4.51
	Pyrimidines biosynthesis	CMP	-3.11	-2.91	-3.22	-3.98	-3.32	-3.51	-2.99	-3.86
		CTP	-4.29	-4.32	-5.75	-3.02	-3.51	-5.83	-6.32	0.00
		CDP	-3.96	-4.82	-4.98	-2.90	-3.12	-4.22	-3.71	-2.46
		dCMP	-2.63	-2.69	0.00	-0.25	-2.78	-2.84	0.00	-0.25
		dCTP	-2.88	-3.74	-4.92	-2.33	-2.55	-3.97	-4.49	-2.23
		UDP	-4.88	-5.65	-5.87	-4.89	-3.74	-4.52	-4.02	-4.26
		UTP	-5.67	-6.76	-7.62	-5.32	-5.00	-6.30	-6.35	-4.77
		UMP	-5.11	-5.29	-5.07	-3.92	-3.61	-3.74	-2.83	-3.50
		Uracil	-1.63	-1.38	-2.03	-1.33	-0.88	-1.13	-1.07	-1.35
		Thymine	-1.74	-2.21	-2.79	-1.70	-1.31	-2.00	-2.33	-1.72
		dTDP	-3.76	-4.68	-5.30	-4.64	-3.13	-3.13	-2.65	-3.30
		dTTP	-2.38	-2.57	-5.50	-2.56	-2.40	-2.64	-3.13	-3.88
		Uridine	-0.90	-1.38	-1.45	-1.39	-1.19	-1.59	-1.08	-1.34
		Orotate	-0.44	-0.94	-2.76	-0.11	0.65	-0.76	-1.70	0.00
		(S)-Dihydroorotate	-2.77	-4.19	-5.57	-2.74	-1.76	-4.14	-4.78	-1.75
		N-Carbamoyl-L-aspartate	-3.72	-5.22	-6.62	-2.24	-2.54	-4.70	-5.07	-1.16
	Glycolysis	Phosphoenolpyruvate	-2.81	-4.37	-4.62	-4.67	-2.75	-3.57	-4.03	-3.29

		D-Fructose 1,6-bisphosphate	-3.55	-3.15	-4.97	-3.40	-3.79	-2.96	-4.03	-3.88
		D-Glyceraldehyde 3-phosphate	-3.81	-3.47	-2.54	-3.86	-3.29	-4.35	-4.72	-4.46
		Glucose 6-phosphate	-2.21	-2.61	-3.29	-2.65	-1.41	-1.81	-1.95	-2.29
		Mannitol	-3.29	-3.57	-3.20	-3.72	-2.55	-2.46	-2.62	-4.59
		Serine	-0.65	-1.73	-2.49	-0.33	0.01	-1.24	-0.86	-0.12
		3-Phospho-D-glycerate	-2.16	-3.47	-3.54	-3.86	-2.15	-3.50	-3.43	-2.16
		D-Fructose	-0.99	-2.07	-2.69	-2.06	-0.33	-1.53	-1.26	-1.87
		Hydroxypyruvate	-2.48	-4.33	-4.27	-2.22	-2.21	-3.94	-3.43	-0.21
	Tricarboxylic Acid (TCA) cycle	b-aminoisobutyric acid	-1.15	-1.40	-1.48	-1.71	-0.81	-1.07	-0.79	-1.58
		Acetyl-CoA	-2.92	-3.30	-4.33	-4.39	-2.98	-3.71	-3.29	-2.57
		Thiamin diphosphate	-3.05	-3.64	-3.52	-2.41	-2.36	-2.86	-2.55	-1.67
		Propanoyl-CoA	8.34	4.72	11.52	7.84	0.48	-0.88	2.70	-0.98
		2-Oxoglutarate	-0.58	-1.68	-1.76	-0.68	-0.28	-0.94	-0.52	-1.43
		CoA	-5.75	-4.18	-6.72	-5.93	-3.16	-3.90	-3.81	-3.79
		(S)-Malate	-0.92	-2.04	-2.67	-2.99	-1.16	-2.57	-1.84	-1.57
		(S)-2-Hydroxyglutarate	-2.87	-3.34	-3.22	-4.47	-2.12	-2.53	-2.05	-4.31
		Citrate	-0.40	-0.88	-1.15	-1.44	-0.32	-1.38	-0.64	-1.58
		4-Oxoglutaramate	-1.51	-1.88	-2.47	-1.95	-0.86	-1.57	-1.51	-1.80
	Pentose phosphate pathway (PPP)	6-Phospho-D-gluconate	-2.72	-3.48	-4.43	-3.50	-2.17	-3.30	-3.20	-3.05
		Sedoheptulose 1,7-bisphosphate	-2.96	-3.37	-5.86	-4.93	-2.83	-3.26	-4.57	-4.79
		D-Glucono-1,5-lactone 6-phosphate	-3.77	-2.57	-3.23	-3.95	-2.45	-2.49	-3.27	-3.86
		2-Deoxy-D-ribose 5-phosphate	-2.31	-2.56	-3.11	-3.13	-1.64	-3.54	-5.51	-1.93
		Sedoheptulose	-3.45	-3.34	-4.91	-4.19	-2.17	-2.61	-4.10	-4.62
		D-Glucono-1,5-lactone6-phosphate	-3.25	-1.19	-1.83	-2.39	-2.51	-2.49	-1.83	-2.39
		D-Ribose	0.60	0.56	0.11	0.25	1.02	-0.01	0.67	-0.03
		Deoxyribose	-3.79	-3.51	-2.59	-4.29	-3.14	-3.28	-1.63	-4.61
		Sedoheptulose 7-phosphate	-1.78	-3.07	-2.94	-4.74	-2.16	-2.79	-2.75	-3.26
Shikimic Acid Pathway Metabolism		(10aS)-10,10a-dihydrophenazine-1-carboxylate	1.36	1.72	0.37	0.46	2.95	2.99	2.72	1.51

		(1R*,3R*,3'S*)-1,2,3,4-Tetrahydro-1-(2-thio-3-pyrrolidinyl)-beta-carboline-3-carboxylic acid	-6.24	-2.86	-3.35	-5.04	-5.21	-6.09	-5.58	-5.34
		2-O-methyl cyclic 3-deoxy-D-arabino-heptulosonate 7-phosphate	-3.23	-4.13	-4.73	-4.00	-2.60	-3.77	-3.29	-3.18
		alpha-(2,6-anhydro-3-deoxy-D-arabino-heptulopyranosid)onate 7-phosphate	-2.03	-3.47	-3.19	-4.12	-1.35	-2.83	-3.60	-4.69
		2-keto-4-hydroxy-5-phosphopentanoate	-3.38	-4.93	-5.24	-6.62	-1.95	-2.58	-2.72	-4.57
Energy Metabolism	**Arginine biosynthesis**	L-Ornithine	-3.57	-5.58	-5.54	-3.95	-2.37	-4.17	-3.14	-1.97
		N-Acetylornithine	-3.52	-5.23	-5.22	-4.07	-2.42	-3.61	-3.17	-1.67
		N-Acetyl-L-glutamate	-4.03	-5.20	-5.91	-5.26	-2.59	-3.29	-5.66	-3.63
		4-Guanidinobutanal	-0.97	-0.16	-0.10	-1.29	-0.26	-1.19	-0.90	-1.52
		Arginine	-0.95	-1.59	-2.11	-1.57	-0.57	-1.50	-1.29	-1.74
		N2-Succinyl-L-arginine	-2.36	-3.08	-3.44	-1.62	-1.23	-2.84	-2.28	-1.29
		N2-Succinyl-L-ornithine	-2.16	-3.05	-0.25	-2.45	0.00	-2.03	0.00	-2.81
		N-Succinyl-L-glutamate	-4.45	-4.54	-5.17	-2.94	-2.43	-4.06	-4.48	-2.63
		L-Citrulline	-2.43	-4.04	-3.90	-4.90	-1.83	-3.31	-2.14	-2.99
	Histidine biosynthesis	*N*-Formimino-L-glutamate	-3.31	-3.42	-3.39	-2.73	-2.60	-2.93	-1.86	-0.29
		N-Acetylhistidine	-2.95	-3.53	-3.27	-2.18	-1.70	-2.17	-1.67	-0.62
		Histidine	-2.59	-3.93	-3.52	-2.18	-1.75	-3.60	-2.28	-2.63
		Ergothioneine	-2.91	-3.44	-2.83	-0.93	-2.35	-2.90	-1.69	-0.40
	Vitamins biosynthesis	FAD	-0.93	-1.17	-1.28	-1.57	-0.73	-1.07	-0.76	-1.97
		FMN	-0.86	-2.80	-2.07	-4.06	-0.86	-1.61	-1.23	-3.57
		5-Aminolevulinate	-1.89	-2.35	-2.52	-5.04	-1.39	-1.65	-1.94	-4.65
		2-(Hydroxymethyl)-3-(acetamidomethylene)succinate	-2.69	-3.10	-2.88	-2.34	-0.02	-2.58	-2.35	-0.68
		Pyridoxine	-1.67	-4.22	-3.38	-3.20	-2.86	-3.04	-2.94	-3.03
		Pantothenate	-1.10	-1.78	-1.91	-2.35	0.09	-1.31	-1.11	-1.40
		Pantetheine 4'-phosphate	-3.57	-3.21	-3.90	-4.81	-2.13	-2.83	-2.56	-3.76

		4-Methyl-5-(2-phosphooxyethyl)thiazole	-2.32	-3.16	-3.53	-2.60	-1.55	-2.48	-2.45	-3.74
		6,7-Dimethyl-8-(D-ribityl)lumazine	-3.57	-4.34	-4.43	-3.64	-2.38	-2.77	-2.03	-1.59
Stress and homeostasis Metabolism	**Osmotic stress**	*N*-Acetylputrescine	-0.07	-0.05	-0.63	0.00	-0.10	-1.10	-0.05	0.13
		Cyclic ADP-ribose	-2.30	-3.19	-1.68	-3.15	-1.81	-2.68	-2.35	-1.98
		Carnitine	-3.64	-4.63	-5.30	-6.92	-3.06	-4.34	-4.97	-5.24
		N-acetyl-L-glutaminyl-L-glutamine amide	-1.37	-1.52	-1.55	-0.92	-0.72	-1.50	-0.20	-1.15
		lauryl sulfobetaine	3.35	0.25	0.00	0.60	2.48	4.60	2.75	2.83
		2-O-(beta-D-mannosyl)-bis(myo-inositol) 1,3'-phosphate	-2.40	-2.15	-2.20	-2.38	-1.76	-1.93	-1.03	-1.59
		Feruloylputrescine	-1.64	-1.24	-1.47	-0.98	0.00	0.00	0.46	-0.54
		Choline sulfate	-2.37	-2.58	-2.48	-1.72	-1.39	-2.28	-1.44	-0.59
		L-Proline	-0.37	-1.00	-0.67	-1.98	-0.34	-0.77	-0.10	-1.18
		Trehalose 6-phosphate	-1.62	-1.50	-3.35	-3.39	-0.66	-0.83	-1.91	-2.58
	Oxidative stress	CoA-glutathione	-1.98	-2.35	-3.66	-3.98	-1.34	-2.66	-2.29	-5.02
		N-hydroxy-N-succinylcadaverine	-1.35	-1.15	-1.83	-1.38	-0.12	-0.88	-0.46	-1.14
		NADPH	-4.88	-5.31	-6.11	-5.63	-4.02	-5.12	-3.67	-3.33
		NADP+	-2.90	-3.49	-3.77	-3.05	-2.19	-2.83	-2.72	-2.56
		Ophthalmic acid	-1.53	-2.66	-2.45	-3.76	-1.75	-2.28	-2.45	-4.99
		N4-acetyl-N4-hydroxy-1-aminopropane	-2.34	-3.54	-3.44	-4.28	-1.68	-3.17	-1.51	-2.55
		L-Cystathionine	-3.63	-4.56	-4.89	-4.07	-2.66	-3.67	-3.03	-2.39
		O-Acetyl-L-serine	-2.95	-3.26	-3.34	-2.12	-2.18	-2.52	-2.01	-0.71
	Redox stress	Succinate semialdehyde	-3.63	-3.91	-5.08	-1.26	-2.90	-4.08	-4.23	-5.01
		(R)-Lactate	-4.38	-4.40	-4.90	-4.64	-3.69	-3.97	-4.15	-3.89
	Membrane lipid remodelling	2-Hydroxymyristoylcarnitine	5.20	5.05	4.37	4.14	1.11	2.35	0.15	0.81
		HpOTrE	-0.29	-0.58	-1.40	-2.65	0.14	0.47	-0.04	0.15
		N-Gluconyl ethanolamine phosphate	0.00	0.00	-3.72	-3.70	0.00	0.00	-2.15	-2.10

	Quorum sensing	*N*-(butyryl)-L-homoserine	-3.66	-4.37	-4.45	-4.25	-2.92	-4.04	-3.48	-3.05
		P-DPD	-3.54	-4.41	-5.24	-6.62	-1.95	-2.58	-2.72	-4.57
	Misc.	dTDP-D-desosamine	-3.09	-3.88	-5.18	-1.59	-2.66	-3.89	-4.06	-5.64
		mycaminose	-2.72	-3.32	-5.02	-7.03	-2.31	-2.72	-4.33	-6.42