

**Supporting Information Table 3. Results of anionic metabolites at T-0.5 B. subtilis 168 cells by CE-MS**

From molecular weight, <sup>13</sup>C contributions<sup>25</sup> and LIGAND database<sup>22</sup>, compound names are designated in parentheses and estimated formulas ranking first are listed.

Compound	Identified, estimated compound name or fomula	m/z	MT	MT/MT(IS)	Area	Area/Area(IS)
UA73, 0.799		73	9.393	0.7985	18058	0.0240
UA79, 0.796		79	9.361	0.7958	4025	0.0054
UA79, 0.798		79	9.382	0.7976	4693	0.0062
UA79, 0.858		79	10.098	0.8585	108033	0.1437
UA79, 0.871		79	10.25	0.8714	6969	0.0093
UA79, 0.883		79	10.385	0.8829	39808	0.0530
UA79, 0.974		79	11.452	0.9736	6592	0.0088
UA83, 0.662		83	7.785	0.6618	3474	0.0046
UA85, 1.108		85	13.032	1.1079	7384	0.0098
UA87, 0.946	Pyruvate	87	11.123	0.9456	167435	0.2227
UA87, 1.108	Butyrate	87	13.035	1.1081	20095	0.0267
UA88, 1.133		88	13.332	1.1334	15886	0.0211
UA89, 1.038	Lactate	89	12.207	1.0377	1661780	2.2107
UA91, 1.141		91	13.42	1.1409	7217	0.0096
UA93, 0.581		93	6.832	0.5808	13793	0.0183
UA97, 0.640		97	7.529	0.6401	218248	0.2903
UA97, 0.859		97	10.1	0.8586	1427040	1.8984
UA99, 1.127	Tiglate	99	13.273	1.1272	14332	0.0168
UA103, 0.731	Malonate	103	8.61	0.7312	21221	0.0248
UA103, 1.100	$\beta$ -Hydroxypropyruvate	103	12.953	1.1000	13593	0.0159
UA103, 1.122	2-Hydroxypropanoate	103	13.216	1.1224	22381	0.0262
UA105, 1.068	Glycerate	105	12.577	1.0681	21781	0.0255
UA107, 0.908		107	10.69	0.9079	39441	0.0461
UA108, 0.754		108	8.878	0.7540	1279	0.0015
UA111, 0.870		111	10.248	0.8703	37265	0.0436
UA115, 0.762		115	8.967	0.7615	12919	0.0151
UA115, 0.770	Fumarate	115	9.062	0.7696	15181	0.0178
UA115, 1.080	3-Methyl-2-oxobutanoate	115	12.719	1.0802	62730	0.0733
UA115, 1.111		115	13.082	1.1110	17805	0.0208
UA115, 1.145		115	13.48	1.1448	5306	0.0062
UA117, 0.798	Succinate	117	9.391	0.7975	319367	0.3734
UA117, 1.141		117	13.441	1.1415	99973	0.1169
UA121, 1.104	Benzoate	121	12.994	1.1035	53108	0.0621
UA122, 1.102	Nicotinate	122	12.976	1.1020	14009	0.0164
UA125, 0.996		125	11.733	0.9964	4296	0.0050
UA126, 1.145		126	13.485	1.1452	2253	0.0026
UA128, 1.125		128	13.253	1.1250	391916	0.5618
UA129, 0.858	Itaconate	129	10.105	0.8578	14423	0.0207
UA129, 1.122	C <sub>5</sub> H <sub>6</sub> O <sub>4</sub>	129	13.219	1.1222	261327	0.3746
UA129, 1.143	4-Methyl-2-oxovalerate	129	13.459	1.1425	59538	0.0854
UA131, 1.127		131	13.279	1.1272	43197	0.0619
UA132, 1.134	(Aspartate)	132	13.354	1.1336	851753	1.2210
UA133, 0.793	Malate	133	9.339	0.7928	29363	0.0421
UA133, 1.142		133	13.455	1.1422	35197	0.0505
UA135, 1.141	Toluate	135	13.441	1.1410	570241	0.8175
UA136, 0.512		136	6.028	0.5117	2348	0.0034
UA137, 0.959	(Urocanate)	137	11.3	0.9593	22366	0.0321
UA137, 1.132	<i>p</i> -Hydroxybenzoate	137	13.329	1.1315	11760	0.0169
UA139, 0.883	Acetylphosphate	139	10.396	0.8825	8110	0.0116
UA145, 0.793	2-Oxoglutarate	145	9.335	0.7924	103253	0.1480
UA147, 0.612		147	7.206	0.6117	36698	0.0526
UA149, 0.999		149	11.772	0.9993	14079	0.0202
UA149, 1.128		149	13.289	1.1281	10764	0.0154
UA150, 1.000	2-Carboxybenzaldehyde	150	11.778	0.9998	687633	0.9858
UA153, 1.126	Protocatechurate	153	13.269	1.1264	10322	0.0148
UA163, 0.931	C <sub>9</sub> H <sub>8</sub> O <sub>3</sub> or C <sub>10</sub> H <sub>12</sub> O <sub>2</sub>	163	11.244	0.9309	27523	0.0356
UA163, 0.958	C <sub>9</sub> H <sub>8</sub> O <sub>3</sub> or C <sub>10</sub> H <sub>12</sub> O <sub>2</sub>	163	11.566	0.9576	19412	0.0251
UA165, 0.878		165	10.607	0.8782	28183	0.0364
UA167, 0.792	Phosphoenolpyruvate	167	9.557	0.7913	101404	0.1311
UA169, 0.893		169	10.788	0.8932	36223	0.0468
UA169, 0.952	Dihydroxyacetone phosphate	169	11.502	0.9523	75835	0.0980
UA171, 0.950		171	11.471	0.9497	10418	0.0135
UA171, 0.972	Glycerophosphate	171	11.744	0.9723	323203	0.4177
UA171, 1.041		171	12.573	1.0410	21466	0.0277
UA171, 1.112		171	13.425	1.1115	148240	0.1916
UA173, 0.948	Phenyl phosphate	173	11.455	0.9484	15628	0.0202
UA174, 0.894	C <sub>6</sub> H <sub>7</sub> O <sub>6</sub> or C <sub>6</sub> H <sub>9</sub> NO <sub>5</sub>	174	10.792	0.8935	8809	0.0114
UA175, 0.873	N-Carbamoyl-L-aspartate	175	10.548	0.8733	23889	0.0309
UA175, 0.918		175	11.084	0.9177	10430	0.0135
UA177, 0.854		177	10.313	0.8539	52526	0.0679
UA179, 0.632		179	7.636	0.6322	8854	0.0114
UA179, 0.854		179	10.31	0.8536	60743	0.0785
UA179, 0.958		179	11.576	0.9584	9054	0.0117
UA179, 1.040	(2-Deoxy-D-gluconate)	179	12.558	1.0397	54021	0.0698
UA181, 0.931	(4-Hydroxyphthalate)	181	11.248	0.9313	55729	0.0720

UA184, 0.809		184	9.773	0.8092	7343	0.0095
UA184, 0.901		184	10.88	0.9008	74383	0.0961
UA184, 0.971	o-Phospho-L-Serine	184	11.723	0.9706	16237	0.0210
UA185, 0.811	3-Phosphoglycerate	185	9.79	0.8106	1132480	1.4636
UA186, 0.821		186	9.211	0.8206	29926	0.0335
UA187, 0.975	Azelate	187	10.948	0.9753	38583	0.0432
UA187, 1.036		187	11.624	1.0355	28866	0.0323
UA188, 0.937	N-Acetyl-L-glutamate	188	10.517	0.9369	47030	0.0527
UA191, 0.825	iso-Citrate	191	9.265	0.8254	38632	0.0433
UA191, 0.853	Citrate	191	9.569	0.8525	39634	0.0444
UA191, 1.000		191	11.223	0.9998	21284	0.0238
UA195, 0.647		195	7.257	0.6465	35731	0.0400
UA195, 0.861		195	9.666	0.8611	1007320	1.1281
UA196, 0.584		196	6.552	0.5837	508290	0.5693
UA196, 0.617	(Phosphoguanidinoacetate)	196	6.922	0.6167	38412	0.0430
UA198, 0.587		198	6.59	0.5871	551231	0.6173
UA198, 0.618		198	6.932	0.6176	57838	0.0648
UA198, 1.002		198	11.251	1.0023	169068	0.1893
UA199, 0.926		199	10.39	0.9256	18472	0.0207
UA199, 0.987	Erythrose 4-phosphate	199	11.074	0.9865	31376	0.0351
UA200, 0.580		200	6.514	0.5803	159068	0.1781
UA200, 0.589		200	6.606	0.5885	90658	0.1015
UA200, 0.616		200	6.914	0.6159	27254	0.0305
UA201, 1.036	Sebacate	201	11.628	1.0359	29217	0.0327
UA203, 1.117		203	12.541	1.1172	33513	0.0375
UA203, 1.124		203	12.616	1.1239	11998	0.0134
UA207, 0.820		207	9.209	0.8204	47884	0.0536
UA207, 0.961	Benzylsuccinate	207	10.784	0.9607	393994	0.4412
UA207, 1.133	(Dihydroliipoate)	207	12.721	1.1333	24939	0.0279
UA213, 0.856		213	9.606	0.8558	24530	0.0275
UA213, 1.014	2-Deoxyribose 5-phosphate	213	11.38	1.0138	108699	0.1217
UA214, 1.126		214	12.64	1.1261	48192	0.0540
UA214, 1.135		214	12.745	1.1354	14678	0.0164
UA215, 1.024		215	12.539	1.0243	14886	0.0198
UA215, 1.049		215	12.843	1.0491	18950	0.0252
UA217, 0.630		217	7.707	0.6296	18220	0.0242
UA217, 0.847		217	10.375	0.8475	75188	0.0999
UA217, 1.148		217	14.057	1.1483	16046	0.0213
UA218, 0.969	4-Nitrophenyl phosphate	218	11.865	0.9692	5495	0.0073
UA218, 1.039		218	12.721	1.0391	119058	0.1581
UA219, 0.731		219	8.946	0.7308	2954	0.0039
UA219, 0.878		219	10.75	0.8781	3682	0.0049
UA220, 0.996		220	12.198	0.9964	10543	0.0140
UA223, 0.604		223	7.391	0.6037	15300	0.0203
UA225, 0.604		225	7.391	0.6037	16257	0.0216
UA225, 0.957		225	11.717	0.9571	6559	0.0087
UA226, 0.604		226	7.391	0.6037	11645	0.0155
UA229, 1.031	Ribulose 5-phosphate	229	12.619	1.0308	228916	0.3041
UA229, 1.055	Ribose 5-phosphate	229	12.919	1.0553	66191	0.0879
UA232, 1.043	(2-Hydroxy-6-oxo-(2'-aminophenyl)-hexa-2,4-dienoate)	232	12.766	1.0428	8739	0.0116
UA232, 1.141		232	13.973	1.1414	14948	0.0199
UA239, 0.878		239	10.752	0.8783	5769	0.0077
UA240, 0.999		240	12.229	0.9989	4881	0.0065
UA241, 0.604		241	7.391	0.6037	32353	0.0430
UA241, 0.973		241	11.911	0.9730	16190	0.0215
UA241, 1.049		241	12.836	1.0485	20872	0.0277
UA243, 1.073		243	13.137	1.0731	24158	0.0321
UA244, 0.602		244	7.401	0.6021	53590	0.0697
UA247, 0.958	(Pyridoxamine phosphate)	247	11.772	0.9577	16770	0.0218
UA250, 0.603		250	7.408	0.6027	11652	0.0152
UA251, 0.952		251	11.7	0.9518	4628	0.0060
UA252, 0.603		252	7.409	0.6027	7223	0.0094
UA253, 0.872	C7H11O8P, C7H14N2O6S, C7H14N2O4S2 or C6H15N	253	10.72	0.8721	355457	0.4622
UA253, 0.971		253	11.941	0.9714	12142	0.0158
UA253, 1.503	(Palmitoleate)	253	18.47	1.5026	157748	0.2051
UA257, 1.133		257	13.923	1.1327	36017	0.0468
UA258, 1.154		258	14.186	1.1541	15535	0.0202
UA259, 1.047	Glucose 1-phosphate	259	12.875	1.0474	156642	0.2037
UA259, 1.077	Fructose 6-phosphate	259	13.232	1.0765	362429	0.4713
UA259, 1.107	Glucose 6-phosphate	259	13.605	1.1068	363418	0.4726
UA261, 0.930		261	11.433	0.9301	19534	0.0254
UA261, 1.076		261	13.232	1.0765	19284	0.0251
UA261, 1.094		261	13.452	1.0944	24757	0.0322
UA261, 1.107		261	13.602	1.1066	33069	0.0430
UA268, 0.973	(N-Acetyl-L-glutamate 5-phosphate)	268	11.956	0.9727	11265	0.0146
UA269, 0.972		269	11.95	0.9722	9545	0.0124
UA271, 0.710		271	8.722	0.7096	3989	0.0052
UA271, 0.972		271	11.952	0.9723	15750	0.0205
UA273, 1.117		273	13.83	1.1171	14111	0.0169
UA274, 1.157		274	14.325	1.1571	2519	0.0030

UA275, 0.872		275	10.792	0.8717	16364	0.0196
UA275, 0.888	(2-Carboxy-D-arabinitol 1-phosphate)	275	10.994	0.8880	58406	0.0699
UA275, 0.939	6-Phosphogluconate	275	11.625	0.9390	80474	0.0963
UA275, 1.045		275	12.937	1.0450	47867	0.0573
UA275, 1.076		275	13.322	1.0761	13689	0.0164
UA277, 0.975		277	12.072	0.9751	695521	0.8319
UA279, 0.877		279	10.852	0.8766	11822	0.0141
UA279, 1.134		279	14.038	1.1339	9958	0.0119
UA283, 0.807		283	9.99	0.8069	14706	0.0176
UA283, 0.892		283	11.041	0.8918	5199	0.0062
UA285, 0.806	(N-Glucosylnicotinate)	285	9.979	0.8061	45001	0.0538
UA286, 0.807		286	9.994	0.8073	7335	0.0088
UA287, 0.927	C7H13O10P	287	11.472	0.9267	146959	0.1758
UA287, 1.036	C7H13O10P	287	12.827	1.0361	10401	0.0124
UA287, 1.143		287	14.152	1.1431	28484	0.0341
UA288, 0.958		288	11.862	0.9582	5209	0.0062
UA288, 1.124		288	13.917	1.1242	7675	0.0092
UA289, 1.028		289	12.727	1.0280	33282	0.0398
UA289, 1.123		289	13.898	1.1226	904352	1.0817
UA291, 0.864		291	10.702	0.8645	16427	0.0196
UA291, 1.123	(Sedoheptulose 7-phosphate)	291	13.908	1.1234	22780	0.0272
UA291, 1.134		291	14.034	1.1336	16864	0.0202
UA293, 0.851		293	10.532	0.8507	512393	0.6129
UA294, 1.164		294	14.411	1.1641	126929	0.1518
UA294, 1.296		294	16.04	1.2956	138694	0.1659
UA298, 0.807		298	9.985	0.8065	28417	0.0340
UA298, 0.935		298	11.571	0.9347	20881	0.0250
UA298, 0.973		298	12.048	0.9732	11737	0.0140
UA299, 0.808		299	10.001	0.8078	18188	0.0218
UA299, 0.976		299	12.084	0.9761	27378	0.0327
UA299, 1.000		299	12.374	0.9995	16890	0.0202
UA300, 0.976	C18H20O4, C18H36O3 or C20H28O2	300	12.082	0.9759	5683	0.0068
UA300, 1.129		300	13.977	1.1290	58859	0.0704
UA300, 1.139		300	14.105	1.1393	4937	0.0059
UA300, 1.151		300	14.244	1.1506	5649	0.0068
UA303, 1.000	N2-[1,3-Dicarboxypropyl]-L-arginine	303	12.336	1.0004	96093	0.1009
UA303, 1.135		303	13.995	1.1349	13269	0.0139
UA304, 0.766		304	9.443	0.7658	14708	0.0154
UA304, 1.001		304	12.339	1.0006	13674	0.0144
UA305, 1.142		305	14.076	1.1415	4101	0.0043
UA306, 1.114	dCMP	306	13.736	1.1139	26072	0.0274
UA307, 1.098	dUMP	307	13.541	1.0981	12658	0.0133
UA309, 0.867		309	10.687	0.8667	13337	0.0140
UA309, 0.927		309	11.437	0.9275	15223	0.0160
UA309, 1.005		309	12.394	1.0051	20365	0.0214
UA309, 1.027		309	12.667	1.0272	42049	0.0442
UA311, 1.031		311	12.71	1.0307	13522	0.0142
UA313, 1.123	(Geranyl diphosphate)	313	13.847	1.1229	64616	0.0679
UA315, 0.629		315	7.759	0.6292	5697	0.0060
UA315, 0.853		315	10.515	0.8527	123811	0.1300
UA315, 0.875		315	10.794	0.8754	4238	0.0045
UA315, 1.139		315	14.039	1.1385	17317	0.0182
UA317, 0.940		317	11.589	0.9398	19194	0.0202
UA317, 1.057		317	13.034	1.0570	30997	0.0326
UA318, 1.142		318	14.082	1.1420	7945	0.0083
UA319, 1.140		319	14.054	1.1397	120199	0.1262
UA321, 1.126		321	13.89	1.1264	35710	0.0375
UA321, 1.142	TMP	321	14.081	1.1419	36521	0.0384
UA322, 1.125	CMP	322	13.873	1.1250	87329	0.0917
UA323, 0.822	C9H13N2O9P or C10H13O10P	323	10.135	0.8219	196989	0.2069
UA323, 1.001	C9H13N2O9P or C10H13O10P	323	12.339	1.0006	75818	0.0796
UA323, 1.109	C9H13N2O9P or C10H13O10P	323	13.671	1.1087	222355	0.2335
UA323, 1.125	UMP	323	13.867	1.1246	8746	0.0092
UA323, 1.142		323	14.082	1.1420	11934	0.0125
UA324, 0.821		324	10.122	0.8209	22334	0.0235
UA325, 0.957	(Glucosyl-2-hydroxycinnamate)	325	11.806	0.9574	27773	0.0292
UA325, 0.958		325	11.813	0.9580	5042	0.0053
UA328, 1.061		328	13.081	1.0608	30188	0.0317
UA329, 0.932		329	11.492	0.9320	44933	0.0472
UA329, 1.032		329	12.726	1.0320	12450	0.0131
UA330, 1.138	dAMP	330	14.032	1.1379	28468	0.0299
UA331, 0.853		331	10.522	0.8533	20733	3.8407
UA331, 1.138	dIMP	331	14.037	1.1384	5398	0.0057
UA334, 1.121		334	13.941	1.1207	7305	0.0074
UA335, 0.788		335	9.804	0.7882	9366	0.0095
UA336, 1.105	(5-Hydroxymethyldeoxycytidylate)	336	13.739	1.1045	599339	0.6088
UA337, 0.627		337	7.796	0.6267	4306	0.0044
UA337, 1.134		337	14.103	1.1338	8664	0.0088
UA338, 1.071		338	13.317	1.0706	13609	0.0138
UA338, 1.089		338	13.543	1.0888	10853	0.0110

UA338, 1.105		338	13.741	1.1047	17813	0.0181
UA339, 0.892	Fructose 1,6-diphosphate	339	11.092	0.8917	454125	0.4613
UA339, 0.911		339	11.33	0.9108	23047	0.0234
UA339, 1.089	C6H14O12P2	339	13.542	1.0887	56246	0.0571
UA341, 0.892		341	11.093	0.8918	10740	0.0109
UA341, 1.077		341	13.392	1.0766	14668	0.0149
UA341, 1.106		341	13.76	1.1062	12200	0.0124
UA342, 1.121		342	13.95	1.1215	5065	0.0051
UA343, 0.972		343	12.085	0.9715	85334	0.0867
UA343, 1.140		343	14.175	1.1396	3534	0.0036
UA344, 1.724		344	21.448	1.7243	33791	0.0343
UA346, 1.144	AMP	346	14.228	1.1440	68404	0.6949
UA347, 1.123	IMP	347	13.973	1.1233	112473	0.1143
UA347, 1.144		347	14.229	1.1439	84077	0.0854
UA348, 1.124		348	13.976	1.1236	13503	0.0137
UA348, 1.145		348	14.237	1.1445	14115	0.0143
UA351, 0.873		351	10.86	0.8731	8915	0.0091
UA354, 1.155		354	14.372	1.1554	23801	0.0242
UA355, 1.155		355	14.373	1.1555	11584	0.0118
UA356, 0.972		356	12.085	0.9715	4785	0.0049
UA356, 1.156		356	14.374	1.1556	9888	0.0100
UA357, 1.077		357	13.398	1.0771	5778	0.0059
UA357, 1.155		357	14.373	1.1555	4690	0.0048
UA358, 0.930		358	11.574	0.9305	21756	0.0221
UA359, 1.077	C18H16O6	359	13.401	1.0773	17959	0.0182
UA360, 1.155		360	14.365	1.1548	7032	0.0071
UA361, 0.901		361	10.244	0.9011	17308	0.0166
UA362, 1.136	GMP	362	12.913	1.1360	44086	0.0424
UA363, 0.998	Xanthosine 5-monophosphate	363	11.349	0.9983	13715	0.0132
UA363, 1.136		363	12.911	1.1357	5742	0.0055
UA364, 0.872		364	9.915	0.8722	52444	0.0504
UA365, 0.974		365	11.071	0.9739	6017	0.0058
UA365, 1.083		365	12.314	1.0832	11081	0.0106
UA366, 0.860		366	9.777	0.8600	20197	0.0194
UA366, 0.872		366	9.915	0.8722	6370	0.0061
UA366, 0.881		366	10.018	0.8812	11008	0.0106
UA367, 0.881		367	10.015	0.8810	9782	0.0094
UA369, 0.908	(Sedoheptulose 1,7-bisphosphate)	369	10.325	0.9083	194906	0.1873
UA371, 0.822		371	9.342	0.8218	130894	0.1258
UA371, 1.111		371	12.633	1.1113	24049	0.0231
UA372, 0.861		372	9.789	0.8611	12608	0.0121
UA372, 1.070		372	12.164	1.0700	5683	0.0055
UA374, 1.106		374	12.577	1.1064	105639	0.1015
UA375, 0.978		375	11.121	0.9783	9963	0.0096
UA377, 0.979	(7-Methylguanosine 5'-phosphate)	377	11.126	0.9787	15416	0.0148
UA378, 1.111		378	12.631	1.1111	6319	0.0061
UA380, 0.940	(N-Acetyl-D-glucosamine 1,6-bisphosphate)	380	10.685	0.9399	88145	0.0847
UA382, 0.861		382	9.793	0.8615	16739	0.0161
UA382, 1.125		382	12.79	1.1251	19559	0.0188
UA385, 0.862		385	9.799	0.8620	11241	0.0108
UA386, 1.004	dCDP	386	11.415	1.0041	11354	0.0109
UA387, 0.858		387	9.754	0.8580	17370	0.0167
UA387, 1.111		387	12.632	1.1112	11095	0.0107
UA389, 0.882	Ribose 1,5-diphosphate	389	10.029	0.8822	11408	0.0110
UA389, 1.111		389	12.633	1.1113	21753	0.0209
UA390, 0.858		390	10.801	0.8582	3438	0.0033
UA390, 0.960		390	12.078	0.9597	6268	0.0060
UA390, 0.978		390	12.313	0.9784	9580	0.0092
UA390, 1.124		390	14.143	1.1238	7164	0.0069
UA391, 0.899		391	11.314	0.8990	31008	0.0298
UA391, 1.160		391	14.601	1.1602	32707	0.0314
UA392, 0.892		392	11.22	0.8915	18464	0.0177
UA392, 0.997		392	12.545	0.9968	3879	0.0037
UA393, 0.807		393	10.15	0.8065	42973	0.0413
UA393, 0.876	(5'-Butyrylphosphouridine)	393	11.027	0.8762	25314	0.0243
UA396, 1.095		396	13.782	1.0951	1428700	1.3729
UA397, 0.998		397	12.559	0.9979	104607	0.1005
UA397, 1.151		397	14.48	1.1506	47767	0.0459
UA398, 1.097		398	13.808	1.0972	26036	0.0250
UA399, 0.806		399	10.149	0.8064	7186	0.0069
UA399, 0.851		399	10.716	0.8515	29331	0.0282
UA399, 0.918	(Bis(Glycerophospho)-glycerol)	399	11.554	0.9181	139083	0.1337
UA399, 0.972		399	12.236	0.9723	7436	0.0071
UA399, 1.000		399	12.587	1.0002	8236	0.0079
UA401, 1.000		401	12.586	1.0001	23558	0.0226
UA401, 1.014	TDP	401	12.761	1.0140	39894	0.0383
UA402, 0.933		402	11.741	0.9329	13826	0.0133
UA402, 1.005	CDP	402	12.654	1.0050	43728	0.0420
UA403, 0.974		403	12.261	0.9743	36639	0.0352
UA403, 0.996		403	12.529	0.9956	87683	0.0843

UA403, 1.029		403	12.948	1.0288	7855	0.0075
UA404, 0.985	UDP	404	12.4	0.9853	24182	0.0232
UA404, 0.995		404	12.527	0.9954	24920	0.0239
UA404, 1.079		404	13.585	1.0795	363733	0.3495
UA406, 0.979		406	12.315	0.9785	5444	0.0052
UA407, 1.095	(Palmitoylglycerone phosphate)	407	13.786	1.0954	82636	0.0794
UA409, 0.807		409	10.157	0.8071	8935	0.0086
UA409, 1.140		409	14.348	1.1401	170259	0.1636
UA410, 1.034	dADP	410	13.019	1.0345	47297	0.0455
UA410, 1.076		410	13.545	1.0763	6426	0.0062
UA410, 1.085		410	13.652	1.0848	4341	0.0042
UA411, 0.858		411	10.804	0.8585	6494	0.0062
UA411, 1.095		411	13.777	1.0947	63585	0.0611
UA412, 1.094		412	13.771	1.0942	38179	0.0367
UA413, 0.851		413	10.716	0.8515	150252	0.1444
UA413, 1.095		413	13.779	1.0949	14810	0.0142
UA414, 0.937		414	11.792	0.9370	12451	0.0120
UA414, 1.146		414	14.426	1.1463	5516	0.0053
UA415, 0.806		415	10.14	0.8057	6622	0.0064
UA415, 0.958		415	12.054	0.9578	7422	0.0071
UA415, 1.080		415	13.598	1.0805	12674	0.0122
UA415, 1.095		415	13.776	1.0946	22490	0.0216
UA416, 0.936		416	11.776	0.9357	4402	0.0042
UA417, 1.083		417	13.626	1.0827	22562	0.0217
UA418, 1.000		418	12.58	0.9996	4232	0.0041
UA418, 1.095	(myo-Inositol triphosphate)	418	13.784	1.0953	62474	0.0600
UA419, 0.999		419	12.527	0.9990	5275	0.0051
UA419, 1.080		419	13.536	1.0795	7991	0.0077
UA419, 1.094		419	13.718	1.0940	16175	0.0156
UA420, 1.078		420	13.522	1.0784	7619	0.0073
UA421, 0.831	C12H23O14P	421	10.419	0.8309	16169	0.0156
UA421, 0.918		421	11.505	0.9175	13197	0.0127
UA422, 0.898		422	11.259	0.8979	21107	0.0203
UA423, 1.096		423	13.745	1.0962	19744	0.0190
UA423, 1.152		423	14.443	1.1518	162869	0.1570
UA424, 0.805		424	10.1	0.8055	21006	0.0203
UA424, 1.095		424	13.724	1.0945	68928	0.0665
UA425, 0.972		425	12.186	0.9718	3692	0.0036
UA425, 0.995		425	12.476	0.9950	4391	0.0042
UA425, 1.096		425	13.737	1.0955	35011	0.0338
UA425, 1.110		425	13.917	1.1099	21754	0.0210
UA425, 1.141		425	14.312	1.1414	17357	0.0167
UA425, 1.152		425	14.443	1.1518	13141	0.0127
UA426, 1.038	ADP	426	13.019	1.0380	52804	0.5091
UA427, 1.015	IDP	427	12.729	1.0152	11706	0.0113
UA427, 1.038		427	13.02	1.0384	70158	0.0676
UA428, 1.147		428	14.383	1.1471	13235	0.0128
UA429, 0.850		429	10.663	0.8504	25752	0.0248
UA429, 0.870		429	10.914	0.8704	8263	0.0080
UA429, 0.942		429	11.814	0.9422	12485	0.0120
UA429, 1.026	(CMP-2-aminoethylphosphate)	429	12.866	1.0261	36305	0.0350
UA429, 1.083		429	13.583	1.0833	15667	0.0151
UA429, 1.094		429	13.716	1.0939	11750	0.0113
UA430, 1.081		430	13.551	1.0807	198588	0.1915
UA432, 1.033		432	12.955	1.0332	4125	0.0040
UA432, 1.092		432	13.694	1.0921	23068	0.0222
UA432, 1.157		432	14.507	1.1570	3366	0.0032
UA433, 0.957		433	12.002	0.9572	3060	0.0029
UA433, 1.005		433	12.6	1.0049	4730	0.0046
UA435, 0.849		435	10.645	0.8490	13679	0.0132
UA436, 1.107		436	13.884	1.1073	10931	0.0105
UA436, 1.145		436	14.355	1.1448	2910	0.0028
UA437, 0.890		437	11.162	0.8902	3380	0.0033
UA437, 1.157		437	14.503	1.1566	21988	0.0212
UA438, 1.037		438	13.009	1.0375	7508	0.0072
UA439, 1.002		439	12.565	1.0021	11099	0.0107
UA439, 1.038		439	13.014	1.0379	65327	0.0630
UA439, 1.102		439	13.824	1.1025	14063	0.0136
UA439, 1.141		439	14.304	1.1408	17973	0.0173
UA439, 1.153		439	14.453	1.1526	13116	0.0126
UA440, 1.140		440	14.296	1.1401	4279	0.0041
UA442, 1.039		442	13.027	1.0389	7300	0.0070
UA442, 1.055	GDP	442	13.227	1.0550	30058	0.0290
UA442, 1.099		442	13.775	1.0986	2973	0.0029
UA443, 0.858		443	10.761	0.8582	9629	0.0093
UA443, 1.034		443	12.97	1.0344	5325	0.0051
UA443, 1.156		443	14.499	1.1563	3664	0.0035
UA446, 1.148		446	14.39	1.1476	9696	0.0093
UA447, 0.848		447	10.637	0.8483	15118	0.0146
UA447, 1.105		447	13.855	1.1050	13442	0.0130

UA447, 1.154		447	14.47	1.1540	16978	0.0164
UA448, 1.038		448	13.037	1.0384	17571	0.0172
UA448, 1.080		448	13.562	1.0802	7350	0.0072
UA449, 0.850		449	10.672	0.8500	5879	0.0057
UA449, 0.973		449	12.215	0.9729	11095	0.0109
UA449, 1.081		449	13.571	1.0809	4072	0.0040
UA449, 1.126		449	14.132	1.1256	3668	0.0036
UA449, 1.156		449	14.508	1.1556	15638	0.0153
UA451, 1.111		451	13.953	1.1114	13807	0.0135
UA451, 1.157		451	14.524	1.1568	10318	0.0101
UA452, 0.916		452	11.506	0.9164	11645	0.0114
UA452, 0.985		452	12.362	0.9846	19820	0.0194
UA453, 0.918		453	11.521	0.9176	6959	0.0068
UA453, 1.141		453	14.327	1.1411	9390	0.0092
UA453, 1.153		453	14.477	1.1531	3679	0.0036
UA453, 1.158		453	14.541	1.1582	3102	0.0030
UA454, 1.080		454	13.565	1.0804	5883	0.0058
UA454, 1.158		454	14.539	1.1580	2806	0.0027
UA459, 1.032		459	12.963	1.0325	39669	0.0388
UA460, 1.154	(3-Phosphoglycerol-glutathione)	460	14.489	1.1540	111553	0.1091
UA461, 1.081		461	13.568	1.0807	7620	0.0075
UA461, 1.123		461	14.105	1.1235	20530	0.0201
UA462, 0.916	Adenylosuccinate	462	11.505	0.9164	15506	0.0152
UA465, 1.159		465	14.545	1.1585	2776	0.0027
UA466, 0.986	dCTP	466	12.375	0.9857	24944	0.0244
UA467, 1.143		467	14.354	1.1433	20615	0.0202
UA467, 1.158		467	14.544	1.1584	34348	0.0336
UA469, 1.123		469	14.102	1.1232	3396	0.0033
UA469, 1.159		469	14.548	1.1587	5558	0.0054
UA471, 0.973		471	12.217	0.9731	8525	0.0083
UA476, 1.157	(Phosphatidylinositol phosphate)	476	14.53	1.1573	1066080	1.0426
UA477, 0.974		477	12.332	0.9739	19367	0.0186
UA477, 1.158		477	14.668	1.1583	167115	0.1603
UA481, 1.002	TTP	481	12.694	1.0024	49625	0.0476
UA482, 0.998	CTP	482	12.632	0.9980	41064	0.0394
UA482, 1.155		482	14.627	1.1551	4105	0.0039
UA483, 0.977	UTP	483	12.372	0.9770	135181	0.1297
UA485, 0.980		485	12.415	0.9804	6131	0.0059
UA485, 1.160		485	14.683	1.1595	2882	0.0028
UA486, 1.080		486	13.676	1.0800	3747	0.0036
UA487, 1.083		487	13.718	1.0833	24080	0.0231
UA488, 0.996		488	12.616	0.9963	5376	0.0052
UA488, 1.081		488	13.692	1.0813	9154	0.0088
UA490, 1.014	dATP	490	12.842	1.0141	10506	0.0101
UA492, 1.158		492	14.668	1.1583	4336	0.0042
UA493, 0.932		493	11.805	0.9322	10491	0.0101
UA496, 1.081		496	13.69	1.0811	9510	0.0091
UA498, 1.159	C26H45NO6S	498	14.671	1.1586	33518	0.0322
UA500, 1.000		500	12.658	0.9996	32916	0.0316
UA500, 1.043		500	13.208	1.0430	3642	0.0035
UA500, 1.160		500	14.685	1.1597	2507	0.0024
UA501, 1.148		501	14.539	1.1481	11477	0.0110
UA502, 0.857		502	10.856	0.8573	7383	0.0071
UA502, 1.007		502	12.754	1.0072	3238	0.0031
UA502, 1.159		502	14.681	1.1594	1401	0.0013
UA503, 1.003		503	12.697	1.0027	3976	0.0038
UA503, 1.159		503	14.673	1.1587	3301	0.0032
UA504, 1.159		504	14.677	1.1590	5283	0.0051
UA505, 0.889		505	11.263	0.8894	5015	0.0048
UA505, 0.977		505	12.376	0.9773	12772	0.0123
UA506, 1.011	ATP	506	12.878	1.0110	306182	0.2687
UA507, 0.870	ITP	507	11.078	0.8697	8626	0.0076
UA508, 1.010		508	12.867	1.0101	9856	0.0086
UA508, 1.114		508	14.186	1.1137	6406	0.0056
UA508, 1.145		508	14.59	1.1454	1264	0.0011
UA508, 1.160		508	14.775	1.1599	2911	0.0026
UA509, 0.981		509	12.498	0.9812	4390	0.0039
UA509, 1.145		509	14.582	1.1448	3791	0.0033
UA513, 0.847		513	10.794	0.8474	7786	0.0068
UA513, 1.038		513	13.224	1.0382	2932	0.0026
UA514, 1.160		514	14.771	1.1596	4010	0.0035
UA514, 1.871		514	23.838	1.8714	64390	0.0565
UA515, 1.039		515	13.24	1.0394	3164	0.0028
UA516, 0.996		516	12.685	0.9958	6137	0.0054
UA516, 1.164		516	14.831	1.1643	19601	0.0172
UA517, 1.085		517	13.819	1.0849	4219	0.0037
UA517, 1.162		517	14.803	1.1621	6356	0.0056
UA519, 0.848		519	10.806	0.8483	5711	0.0050
UA519, 0.971		519	12.371	0.9712	3011	0.0026
UA519, 0.992		519	12.641	0.9924	6838	0.0060

UA519, 1.039		519	13.231	1.0387	2693	0.0024
UA519, 1.080		519	13.751	1.0795	17805	0.0156
UA519, 1.111		519	14.151	1.1109	10783	0.0095
UA520, 1.146		520	14.596	1.1459	4968	0.0044
UA521, 1.080		521	13.757	1.0800	2569	0.0023
UA521, 1.146		521	14.601	1.1463	3550	0.0031
UA522, 1.001		522	12.754	1.0013	3399	0.0030
UA522, 1.046	GTP	522	13.329	1.0460	20072	0.0176
UA523, 0.929		523	11.837	0.9293	37568	0.0330
UA524, 1.040		524	13.242	1.0396	7757	0.0068
UA524, 1.146		524	14.601	1.1463	2939	0.0026
UA525, 1.131		525	14.401	1.1306	17092	0.0150
UA525, 1.146		525	14.597	1.1459	4367	0.0038
UA525, 1.160		525	14.777	1.1601	2881	0.0025
UA527, 0.848		527	10.804	0.8482	8872	0.0078
UA528, 1.011		528	12.88	1.0111	17810	0.0156
UA529, 1.160		529	14.776	1.1600	8439	0.0074
UA532, 0.850		532	10.824	0.8497	9529	0.0084
UA532, 1.150		532	14.644	1.1496	3715	0.0033
UA533, 0.849		533	10.813	0.8489	18716	0.0164
UA533, 1.150		533	14.646	1.1498	4006	0.0035
UA534, 1.005		534	12.804	1.0052	22909	0.0201
UA535, 0.897		535	11.359	0.8970	7474	0.0067
UA535, 1.004		535	12.716	1.0041	9866	0.0088
UA535, 1.146		535	14.514	1.1461	4485	0.0040
UA536, 0.980	(CDPribitol)	536	12.414	0.9803	47423	0.0425
UA539, 1.084		539	13.726	1.0839	9690	0.0087
UA540, 1.039		540	13.16	1.0392	11116	0.0100
UA540, 1.925		540	24.38	1.9251	1185260	1.0631
UA542, 0.849	(CMP-3-deoxy-D-Manno-octulosonate)	542	10.753	0.8491	24537	0.0220
UA543, 0.804		543	10.183	0.8041	5498	0.0049
UA546, 0.969		546	12.272	0.9690	5709	0.0051
UA549, 0.845		549	10.702	0.8451	4979	0.0045
UA552, 1.081		552	13.694	1.0813	10413	0.0093
UA553, 1.082		553	13.704	1.0821	10511	0.0094
UA555, 0.976		555	12.358	0.9758	62404	0.0560
UA556, 1.000		556	12.663	0.9999	4540	0.0041
UA559, 1.012	(ADPribitol)	559	12.813	1.0118	86216	0.0773
UA560, 1.012		560	12.813	1.0118	63844	0.0573
UA560, 1.080		560	13.678	1.0801	10689	0.0096
UA561, 1.014		561	12.84	1.0139	15012	0.0135
UA561, 1.081		561	13.693	1.0813	10529	0.0094
UA562, 0.559		562	7.075	0.5587	6342	0.0057
UA562, 1.012		562	12.82	1.0123	27579	0.0247
UA562, 1.159		562	14.673	1.1586	1667	0.0015
UA562, 1.927		562	24.405	1.9271	44999	0.0404
UA564, 0.850		564	10.723	0.8504	5058	0.0043
UA564, 1.010		564	12.741	1.0105	8038	0.0069
UA567, 1.004		567	12.657	1.0038	3661	0.0031
UA567, 1.040		567	13.109	1.0397	4953	0.0042
UA569, 0.980		569	12.362	0.9804	10849	0.0093
UA569, 1.040		569	13.114	1.0401	11857	0.0102
UA570, 1.005		570	12.673	1.0051	5547	0.0048
UA572, 0.982		572	12.383	0.9821	7868	0.0067
UA572, 1.040		572	13.111	1.0398	4711	0.0040
UA574, 0.983		574	12.395	0.9830	6367	0.0055
UA574, 1.156		574	14.573	1.1558	3270	0.0028
UA575, 1.052		575	13.264	1.0519	17014	0.0146
UA575, 1.156		575	14.582	1.1565	1891	0.0016
UA576, 1.048		576	13.218	1.0483	6461	0.0055
UA576, 1.156		576	14.58	1.1563	3934	0.0034
UA577, 1.011	C16H24N2O17P2	577	12.753	1.0114	16047	0.0137
UA578, 1.048		578	13.213	1.0479	8485	0.0073
UA579, 0.806		579	10.158	0.8056	8662	0.0074
UA579, 0.990		579	12.486	0.9902	10177	0.0087
UA579, 1.029	UDP-glucuronate	579	12.98	1.0294	68784	0.0589
UA580, 1.124		580	14.171	1.1239	9405	0.0081
UA581, 1.041		581	13.12	1.0405	29102	0.0249
UA581, 1.080		581	13.616	1.0799	7729	0.0066
UA582, 1.080		582	13.623	1.0804	12912	0.0111
UA583, 1.110		583	13.998	1.1102	6482	0.0056
UA587, 1.079		587	13.605	1.0790	5915	0.0051
UA588, 0.972		588	12.257	0.9721	3027	0.0026
UA589, 1.151	(UDP-2-acetamido-4-amino-2,4,6-trideoxyglucose)	589	14.509	1.1507	16603	0.0142
UA590, 1.126		590	14.195	1.1258	4421	0.0038
UA590, 1.156		590	14.575	1.1559	4593	0.0039
UA591, 1.011		591	12.754	1.0115	24368	0.0209
UA592, 1.012		592	12.757	1.0117	12496	0.0107
UA594, 1.004		594	12.737	1.0039	6553	0.0063
UA596, 0.980		596	12.436	0.9802	17993	0.0172

UA596, 1.152		596	14.613	1.1518	795830	0.7610
UA599, 0.980		599	12.438	0.9804	5438	0.0052
UA600, 0.977		600	12.397	0.9771	6181	0.0059
UA601, 0.978		601	12.413	0.9784	3722	0.0036
UA601, 1.029		601	13.056	1.0291	3652	0.0035
UA601, 1.123		601	14.251	1.1233	7221	0.0069
UA602, 0.806		602	10.223	0.8058	9698	0.0093
UA602, 1.152		602	14.62	1.1524	2911	0.0028
UA603, 1.000		603	12.692	1.0004	19026	0.0182
UA603, 1.124		603	14.26	1.1240	5529	0.0053
UA604, 1.152		604	14.62	1.1524	6860	0.0066
UA607, 1.041		607	13.211	1.0413	8830	0.0084
UA607, 1.152		607	14.613	1.1518	34147	0.0327
UA609, 1.040		609	13.198	1.0403	1774	0.0017
UA610, 0.805		610	10.209	0.8047	4092	0.0039
UA611, 1.126		611	14.289	1.1263	2692	0.0026
UA611, 1.151		611	14.598	1.1506	4452	0.0043
UA612, 1.125		612	14.273	1.1250	4806	0.0046
UA612, 1.153		612	14.631	1.1532	5015	0.0048
UA615, 0.889		615	11.282	0.8893	3240	0.0031
UA615, 1.152		615	14.617	1.1521	9166	0.0088
UA618, 0.980		618	12.432	0.9799	5073	0.0049
UA618, 1.082		618	13.73	1.0822	5578	0.0053
UA618, 1.152		618	14.621	1.1524	2776	0.0027
UA619, 1.012		619	12.835	1.0117	6006	0.0057
UA620, 1.140		620	14.467	1.1403	12365	0.0118
UA621, 1.153		621	14.622	1.1525	9579	0.0092
UA622, 1.010		622	12.917	1.0095	7125	0.0074
UA622, 1.078		622	13.792	1.0779	3341	0.0035
UA622, 1.152		622	14.746	1.1525	71421	0.0745
UA622, 1.349		622	17.259	1.3489	2539	0.0026
UA623, 0.998		623	12.769	0.9980	2986	0.0031
UA623, 1.153		623	14.752	1.1530	21878	0.0228
UA624, 0.932		624	11.92	0.9316	1359	0.0014
UA624, 1.153		624	14.758	1.1534	15590	0.0163
UA625, 1.000		625	12.8	1.0004	8796	0.0092
UA631, 1.148		631	14.683	1.1476	3280	0.0034
UA631, 1.157		631	14.805	1.1571	2736	0.0029
UA632, 1.029		632	13.166	1.0290	1834	0.0019
UA632, 1.125		632	14.39	1.1247	2854	0.0030
UA632, 1.157		632	14.808	1.1573	1527	0.0016
UA633, 1.153		633	14.759	1.1535	7232	0.0075
UA635, 1.056		635	13.51	1.0559	15780	0.0165
UA637, 1.126		637	14.408	1.1261	3459	0.0036
UA640, 0.850		640	10.882	0.8505	5869	0.0061
UA646, 1.153		646	14.749	1.1527	4119	0.0043
UA648, 1.154		648	14.77	1.1544	4135	0.0043
UA649, 1.153		649	14.759	1.1535	11340	0.0118
UA650, 1.155		650	14.772	1.1545	3474	0.0036
UA658, 1.136		658	12.877	1.1358	9539	0.0115
UA662, 1.767	NAD	662	20.027	1.7670	535564	0.6455
UA665, 1.138		665	12.906	1.1384	6796	0.0082
UA676, 1.068		676	12.111	1.0683	5994	0.0072
UA678, 1.083	(UDP-N-acetylmuramate)	678	12.274	1.0826	25199	0.0304
UA684, 1.157		684	15.028	1.1573	9850	0.0123
UA685, 1.157		685	15.022	1.1569	2738	0.0034
UA692, 2.017		692	26.192	2.0171	99942	0.1253
UA700, 1.094		700	14.201	1.0936	4170	0.0052
UA726, 1.040		726	13.601	1.0404	2744	0.0035
UA728, 1.040		728	13.602	1.0405	1748	0.0022
UA742, 1.150	NADP	742	15.021	1.1500	44802	0.0565
UA749, 1.124		749	14.679	1.1239	6863	0.0087
UA750, 1.123		750	14.673	1.1234	2149	0.0027
UA760, 0.844		760	11.026	0.8442	1752	0.0022
UA764, 1.150		764	15.018	1.1498	3954	0.0050
UA769, 1.164		769	15.383	1.1638	5290	0.0069
UA770, 1.164		770	15.385	1.1639	4143	0.0054
UA772, 1.154		772	15.254	1.1540	4261	0.0056
UA793, 1.104		793	14.589	1.1037	38136	0.0499
UA794, 1.102		794	14.57	1.1023	12938	0.0169
UA795, 1.104		795	14.589	1.1037	6180	0.0081
UA795, 1.154		795	15.254	1.1540	2741	0.0036
UA796, 1.166		796	15.545	1.1657	1402	0.0018
UA808, 1.086		808	14.476	1.0856	8464	0.0108
UA815, 1.108		815	14.777	1.1081	3166	0.0040
UA835, 1.088		835	14.53	1.0881	2806	0.0039
UA846, 1.105		846	14.75	1.1046	3767	0.0052
UA854, 1.069		854	10.482	1.0695	1532	0.0018
UA854, 1.111		854	10.886	1.1107	1038	0.0012
UA861, 1.064		861	10.43	1.0642	6214	0.0072



UA861, 1.112	861	10.896	1.1117	2891	0.0033
UA862, 1.062	862	10.413	1.0624	1990	0.0023

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