Table S9 - Biolog PM01 and PM02 area under curve and growth status for *A. baumannii* AB6870155 and *K. pneumoniae* KP6870155

PM_Plate Number	Well_ID	ID	Compound	Strain	Growth	AUC	Main Class	Sub Class
1	A1	AcB_1_A1	Negative control	AcB	no	1970.48752		
1	A2	AcB_1_A2	L-Arabinose	AcB	yes	12122.6547	sugar	saccharide
1	A3	AcB_1_A3	N-Acetyl-D-Glucosamine	AcB	no	1452.24104	sugar	saccharide
1	A4	AcB_1_A4	D-Saccharic Acid	AcB	yes	12315.2714	sugar	saccharide
1	A5	AcB_1_A5	Succinic Acid	AcB	yes	11371.2822	organic acid	organic acid
1	A6	AcB_1_A6	D-Galactose	AcB	no	2722.12026	sugar	saccharide
1	A7	AcB_1_A7	L-Aspartic Acid	AcB	yes	12027.2485	amino acid	amino acid
1	A8	AcB_1_A8	L-Proline	AcB	yes	11912.899	amino acid	amino acid
1	A9	AcB_1_A9	D-Alanine	AcB	yes	11415.884	amino acid	amino acid
1	A10	AcB_1_A10	D-Trehalose	AcB	no	1376.86815	sugar	saccharide
1	A11	AcB_1_A11	D-Mannose	AcB	no	2876.62162	sugar	saccharide
1	A12	AcB_1_A12	Dulcitol	AcB	no	2299.2411	sugar	sugar alcohol
1	B1	AcB_1_B1	D-Serine	AcB	no	1897.11442	amino acid	amino acid
1	B2	AcB_1_B2	D-Sorbitol	AcB	no	1693.98858	sugar	sugar alcohol
1	B3	AcB_1_B3	Glycerol	AcB	no	1418.74549	alcohol	alcohol
1	B4	AcB_1_B4	L-Fucose	AcB	no	1526.61746	sugar	saccharide
1	B5	AcB_1_B5	D-Glucuronic Acid	AcB	no	1339.49161	sugar	sugar acid
1	B6	AcB_1_B6	D-Gluconic Acid	AcB	no	4423.36234	sugar	saccharide
1	B7	AcB_1_B7	D,L-alpha-Glycerol-Phosphate	AcB	no	1602.49115	alcohol	alcohol
1	B8	AcB_1_B8	D-Xylose	AcB	yes	12417.6401	sugar	saccharide
1	B9	AcB_1_B9	L-Lactic Acid	AcB	yes	11420.7696	organic acid	organic acid
1	B10	AcB_1_B10	Formic Acid	AcB	no	2945.11768	organic acid	organic acid
1	B11	AcB_1_B11	D-Mannitol	AcB	no	1907.11634	sugar	sugar alcohol
1	B12	AcB_1_B12	L-Glutamic Acid	AcB	yes	12061.1186	amino acid	amino acid
1	C1	AcB_1_C1	D-Glucose-6-Phosphate	AcB	no	1862.24017	sugar	saccharide

1	C2	AcB_1_C2	D-Galactonic Acid-gamma-Lactone	AcB	no	1477.61417	sugar	saccharide
1	C3	AcB_1_C3	D,L-Malic Acid	AcB	yes	11444.2735	organic acid	organic acid
1	C4	AcB_1_C4	D-Ribose	AcB	yes	11700.9094	sugar	saccharide
1	C5	AcB_1_C5	Tween 20	AcB	yes	11904.3897	surfactant	surfactant
1	C6	AcB_1_C6	L-Rhamnose	AcB	no	1345.99647	sugar	saccharide
1	C7	AcB_1_C7	D-Fructose	AcB	no	1582.62042	sugar	saccharide
1	C8	AcB_1_C8	Acetic Acid	AcB	yes	11085.6379	organic acid	organic acid
1	C9	AcB_1_C9	Alpha-D-Glucose	AcB	yes	9031.86911	sugar	saccharide
1	C10	AcB_1_C10	Maltose	AcB	no	1856.86062	sugar	saccharide
1	C11	AcB_1_C11	D-Melibiose	AcB	no	2235.23601	sugar	saccharide
1	C12	AcB_1_C12	Thymidine	AcB	no	2325.11332	nucleic acid/nucl	nucleoside
1	D1	AcB_1_D1	L-Asparagine	AcB	yes	12501.8477	amino acid	amino acid
1	D2	AcB_1_D2	D-Aspartic Acid	AcB	no	1674.7398	amino acid	amino acid
1	D3	AcB_1_D3	D-Glucosaminic Acid	AcB	no	1776.36756	sugar	saccharide
1	D4	AcB_1_D4	1,2-Propanediol	AcB	no	1533.37314	alcohol	alcohol
1	D5	AcB_1_D5	Tween 40	AcB	yes	12129.8825	surfactant	surfactant
1	D6	AcB_1_D6	Alpha-Keto-Glutaric Acid	AcB	yes	9918.23225	organic acid	dicarboxylic acid
1	D7	AcB_1_D7	Alpha-Keto-Butyric Acid	AcB	yes	9577.25049	organic acid	organic acid
1	D8	AcB_1_D8	Alpha-Methyl-D-Galactoside	AcB	no	1430.98905	sugar	saccharide
1	D9	AcB_1_D9	Alpha-D-Lactose	AcB	no	1769.4903	sugar	saccharide
1	D10	AcB_1_D10	Lactulose	AcB	no	1597.23786	sugar	saccharide
1	D11	AcB_1_D11	Sucrose	AcB	no	1733.86998	sugar	saccharide
1	D12	AcB_1_D12	Uridine	AcB	no	2511.60953	nucleic acid/nucl	nucleic acid
1	E1	AcB_1_E1	L-Glutamine	AcB	yes	12460.7412	amino acid	amino acid
1	E2	AcB_1_E2	m-Tartaric Acid	AcB	no	1431.24629	organic acid	organic acid
1	E3	AcB_1_E3	D-Glucose-1-Phosphate	AcB	no	1510.99456	sugar	saccharide
1	E4	AcB_1_E4	D-Fructose-6-Phosphate	AcB	no	2315.60879	sugar	saccharide
1	E5	AcB_1_E5	Tween 80	AcB	yes	11668.3902	surfactant	surfactant
1	E6	AcB_1_E6	Alpha-Hydroxy Glutaric Acid-Gamma-	AcB	no	2010.48964	organic acid	organic acid
1	E7	AcB_1_E7	Alpha-Hydroxy Butyric Acid	AcB	yes	9033.12795	organic acid	organic acid

1	E8	AcB_1_E8	Beta-Methyl-D-Glucoside	AcB	no	1923.24174	sugar	saccharide
1	E9	AcB_1_E9	Adonitol	AcB	no	1539.48894	alcohol	alcohol
1	E10	AcB_1_E10	Maltotriose	AcB	no	2032.6144	sugar	saccharide
1	E11	AcB_1_E11	2-Deoxy Adenosine	AcB	no	1729.48648	nucleic acid/nucl	nucleoside
1	E12	AcB_1_E12	Adenosine	AcB	no	2356.61592	nucleic acid/nucl	nucleoside
1	F1	AcB_1_F1	Glycyl-L-Aspartic Acid	AcB	no	2564.48826	amino acid	amino acid
1	F2	AcB_1_F2	Citric Acid	AcB	yes	9469.95347	organic acid	organic acid
1	F3	AcB_1_F3	Myo-Inositol	AcB	no	1674.23814	sugar	sugar alcohol
1	F4	AcB_1_F4	D-Threonine	AcB	no	1685.6179	amino acid	amino acid
1	F5	AcB_1_F5	Fumaric Acid	AcB	yes	11539.0351	organic acid	organic acid
1	F6	AcB_1_F6	Bromo Succinic Acid	AcB	no	7556.23976	organic acid	organic acid
1	F7	AcB_1_F7	Propionic Acid	AcB	yes	10530.2443	organic acid	organic acid
1	F8	AcB_1_F8	Mucic Acid	AcB	yes	11731.5213	sugar	saccharide
1	F9	AcB_1_F9	Glycolic Acid	AcB	no	1786.61261	organic acid	organic acid
1	F10	AcB_1_F10	Glyoxylic Acid	AcB	no	1885.74363	organic acid	organic acid
1	F11	AcB_1_F11	D-Cellobiose	AcB	no	2311.98247	sugar	saccharide
1	F12	AcB_1_F12	Inosine	AcB	no	2674.61425	nucleic acid/nucl	nucleoside
1	G1	AcB_1_G1	Glycyl-L-Glutamic Acid	AcB	no	2601.23388	amino acid	amino acid
1	G2	AcB_1_G2	Tricarballylic Acid	AcB	yes	10544.7509	organic acid	organic acid
1	G3	AcB_1_G3	L-Serine	AcB	no	2722.36254	amino acid	amino acid
1	G4	AcB_1_G4	L-Threonine	AcB	no	4792.48445	amino acid	amino acid
1	G5	AcB_1_G5	L-Alanine	AcB	yes	12073.7704	amino acid	amino acid
1	G6	AcB_1_G6	L-Alanyl-Glycine	AcB	no	3016.48416	amino acid	amino acid
1	G7	AcB_1_G7	Acetoacetic Acid	AcB	no	3234.86049	organic acid	organic acid
1	G8	AcB_1_G8	N-Acetyl-Beta-D-Mannosamine	AcB	no	2497.85845	sugar	saccharide
1	G9	AcB_1_G9	Mono Methyl Succinate	AcB	no	4718.74108	organic acid	organic acid
1	G10	AcB_1_G10	Methyl Pyruvate	AcB	yes	11159.7626	organic acid	organic acid
1	G11	AcB_1_G11	D-Malic Acid	AcB	no	7720.23625	organic acid	organic acid
1	G12	AcB_1_G12	L-Malic Acid	AcB	yes	11554.7586	organic acid	organic acid
1	H1	AcB_1_H1	Glycyl-L-Proline	AcB	no	6529.11439	amino acid	amino acid

1	H2	AcB_1_H2	p-Hydroxy Phenyl Acetic Acid	AcB	no	2335.48849	organic acid	organic acid
1	H3	AcB_1_H3	m-Hydroxy Phenyl Acetic Acid	AcB	no	2695.2396	organic acid	organic acid
1	H4	AcB_1_H4	Tyramine	AcB	no	2920.98373	amino acid	amine
1	H5	AcB_1_H5	D-Psicose	AcB	no	2971.73255	sugar	saccharide
1	H6	AcB_1_H6	L-Lyxose	AcB	no	3386.36217	sugar	saccharide
1	H7	AcB_1_H7	Glucuronamide	AcB	no	6600.75007	sugar	saccharide
1	H8	AcB_1_H8	Pyruvic Acid	AcB	yes	11875.2498	organic acid	organic acid
1	H9	AcB_1_H9	L-Galactonic Acid-Gamma-Lactone	AcB	no	2568.23401	organic acid	lactone
1	H10	AcB_1_H10	D-Galacturonic Acid	AcB	no	3228.2362	sugar	sugar acid
1	H11	AcB_1_H11	Phenylethylamine	AcB	no	3209.86318	amino acid	amine
1	H12	AcB_1_H12	2-Aminoethanol	AcB	no	3325.60246	alcohol	alcohol
1	A1	KlP_1_A1	Negative control	KlP	no	4253.11011		
1	A2	KlP_1_A2	L-Arabinose	KlP	yes	11593.022		Saccharide
1	A3	KlP_1_A3	N-Acetyl-D-Glucosamine	KlP	yes	12791.0306		Amide (saccharide
1	A4	KlP_1_A4	D-Saccharic Acid	KlP	yes	12597.1349		saccharide
1	A5	KlP_1_A5	Succinic Acid	KlP	yes	10597.7554		organic acid
1	A6	KlP_1_A6	D-Galactose	KlP	yes	12271.5368		saccharide
1	A7	KlP_1_A7	L-Aspartic Acid	KlP	yes	11617.8837		amino acid
1	A8	KlP_1_A8	L-Proline	KlP	yes	12007.1299		amino acid
1	A9	KlP_1_A9	D-Alanine	KlP	yes	11899.6291		amino acid
1	A10	KlP_1_A10	D-Trehalose	KlP	yes	12680.6328		saccharide
1	A11	KlP_1_A11	D-Mannose	KlP	yes	12437.8978		sugar monomer
1	A12	KlP_1_A12	Dulcitol	KlP	yes	11513.3727		sugar alcohol
1	B1	KlP_1_B1	D-Serine	KlP	no	7364.65073		
1	B2	KlP_1_B2	D-Sorbitol	KlP	yes	10718.385		sugar alcohol
1	B3	KlP_1_B3	Glycerol	KlP	yes	10265.9975		sugar alcohol
1	B4	KlP_1_B4	L-Fucose	KlP	yes	10909.3756		saccharide
1	B5	KlP_1_B5	D-Glucuronic Acid	KlP	yes	12313.3791		saccharide
1	B6	KlP_1_B6	D-Gluconic Acid	KlP	yes	12392.0025		saccharide
1	B7	KlP_1_B7	D,L-alpha-Glycerol-Phosphate	KlP	yes	11255.2446		glycerophospholipi

1	B8	KlP_1_B8	D-Xylose	KlP	yes	11767.6381	saccharide
1	B9	KlP_1_B9	L-Lactic Acid	KlP	yes	10994.741	organic acid
1	B10	KlP_1_B10	Formic Acid	KlP	no	7047.74694	
1	B11	KlP_1_B11	D-Mannitol	KlP	yes	11596.6437	sugar alcohol
1	B12	KlP_1_B12	L-Glutamic Acid	KlP	yes	11172.4779	amino acid
1	C1	KlP_1_C1	D-Glucose-6-Phosphate	KlP	yes	13373.358	saccharide
1	C2	KlP_1_C2	D-Galactonic Acid-gamma-Lactone	KlP	yes	12135.6541	lactone
1	C3	KlP_1_C3	D,L-Malic Acid	KlP	yes	11138.9917	organic acid
1	C4	KlP_1_C4	D-Ribose	KlP	yes	12393.2549	saccharide
1	C5	KlP_1_C5	Tween 20	KlP	no	5524.48874	
1	C6	KlP_1_C6	L-Rhamnose	KlP	yes	10654.3829	saccharide
1	C7	KlP_1_C7	D-Fructose	KlP	yes	11828.0195	saccharide
1	C8	KlP_1_C8	Acetic Acid	KlP	yes	10289.2599	organic acid
1	C9	KlP_1_C9	Alpha-D-Glucose	KlP	yes	10837.6465	saccharide
1	C10	KlP_1_C10	Maltose	KlP	yes	11409.3809	saccharide
1	C11	KlP_1_C11	D-Melibiose	KlP	yes	10899.2666	saccharide
1	C12	KlP_1_C12	Thymidine	KlP	yes	11677.1436	nucleic acid
1	D1	KlP_1_D1	L-Asparagine	KlP	yes	11426.1214	amino acid
1	D2	KlP_1_D2	D-Aspartic Acid	KlP	no	4003.11559	
1	D3	KlP_1_D3	D-Glucosaminic Acid	KlP	no	7396.3751	
1	D4	KlP_1_D4	1,2-Propanediol	KlP	no	3685.2431	
1	D5	KlP_1_D5	Tween 40	KlP	no	5058.11596	
1	D6	KlP_1_D6	Alpha-Keto-Glutaric Acid	KlP	no	3468.11664	
1	D7	KlP_1_D7	Alpha-Keto-Butyric Acid	KlP	no	2462.61992	
1	D8	KlP_1_D8	Alpha-Methyl-D-Galactoside	KlP	yes	10879.9918	glycoside
1	D9	KlP_1_D9	Alpha-D-Lactose	KlP	yes	10883.5115	saccharide
1	D10	KlP_1_D10	Lactulose	KlP	yes	10205.2672	saccharide
1	D11	KlP_1_D11	Sucrose	KlP	yes	11654.759	saccharide
1	D12	KlP_1_D12	Uridine	KlP	yes	12188.9023	nucleic acid
1	E1	KlP_1_E1	L-Glutamine	KlP	yes	12131.6195	amino acid

1	E2	KlP_1_E2	m-Tartaric Acid	KlP	no	3429.11954	
1	E3	KlP_1_E3	D-Glucose-1-Phosphate	KlP	yes	11745.1311	saccharide
1	E4	KlP_1_E4	D-Fructose-6-Phosphate	KlP	yes	10921.876	saccharide
1	E5	KlP_1_E5	Tween 80	KlP	no	4569.36546	
1	E6	KlP_1_E6	Alpha-Hydroxy Glutaric Acid-Gamma-	KlP	no	3086.36875	
1	E7	KlP_1_E7	Alpha-Hydroxy Butyric Acid	KlP	no	4677.98862	
1	E8	KlP_1_E8	Beta-Methyl-D-Glucoside	KlP	yes	11007.3877	saccharide
1	E9	KlP_1_E9	Adonitol	KlP	yes	11025.2403	sugar alcohol
1	E10	KlP_1_E10	Maltotriose	KlP	yes	11326.5032	saccharide
1	E11	KlP_1_E11	2-Deoxy Adenosine	KlP	yes	11826.6412	nucleic acid
1	E12	KlP_1_E12	Adenosine	KlP	yes	12105.9999	nucleic acid
1	F1	KlP_1_F1	Glycyl-L-Aspartic Acid	KlP	yes	10621.9934	amino acid
1	F2	KlP_1_F2	Citric Acid	KlP	yes	10605.8676	organic acid
1	F3	KlP_1_F3	Myo-Inositol	KlP	yes	10793.7412	saccharide
1	F4	KlP_1_F4	D-Threonine	KlP	no	3517.9897	
1	F5	KlP_1_F5	Fumaric Acid	KlP	yes	10694.5241	dicarboxylic acid
1	F6	KlP_1_F6	Bromo Succinic Acid	KlP	yes	8106.00423	organic acid
1	F7	KlP_1_F7	Propionic Acid	KlP	no	3198.36954	
1	F8	KlP_1_F8	Mucic Acid	KlP	yes	10480.7646	saccharide
1	F9	KlP_1_F9	Glycolic Acid	KlP	no	3509.61645	
1	F10	KlP_1_F10	Glyoxylic Acid	KlP	no	3377.12256	
1	F11	KlP_1_F11	D-Cellobiose	KlP	yes	10734.129	saccharide
1	F12	KlP_1_F12	Inosine	KlP	yes	12235.2437	nucleic acid
1	G1	KlP_1_G1	Glycyl-L-Glutamic Acid	KlP	yes	10861.736	amino acid
1	G2	KlP_1_G2	Tricarballylic Acid	KlP	no	4012.36887	
1	G3	KlP_1_G3	L-Serine	KlP	yes	10907.9956	amino acid
1	G4	KlP_1_G4	L-Threonine	KlP	yes	9029.23499	amino acid
1	G5	KlP_1_G5	L-Alanine	KlP	yes	11121.7538	amino acid
1	G6	KlP_1_G6	L-Alanyl-Glycine	KlP	yes	11034.6275	dipeptide
1	G7	KlP_1_G7	Acetoacetic Acid	KlP	no	4633.73611	

1	G8	KlP_1_G8	N-Acetyl-Beta-D-Mannosamine	KlP	yes	8938.33257	saccharide
1	G9	KlP_1_G9	Mono Methyl Succinate	KlP	no	6011.86866	
1	G10	KlP_1_G10	Methyl Pyruvate	KlP	yes	10517.2641	organic acid
1	G11	KlP_1_G11	D-Malic Acid	KlP	no	7184.36667	
1	G12	KlP_1_G12	L-Malic Acid	KlP	yes	11205.7401	organic acid
1	H1	KlP_1_H1	Glycyl-L-Proline	KlP	yes	10946.1212	dipeptide
1	H2	KlP_1_H2	p-Hydroxy Phenyl Acetic Acid	KlP	yes	11087.7443	chemical compour
1	H3	KlP_1_H3	m-Hydroxy Phenyl Acetic Acid	KlP	yes	11141.6284	chemical compour
1	H4	KlP_1_H4	Tyramine	KlP	yes	10415.7532	amine
1	H5	KlP_1_H5	D-Psicose	KlP	yes	10822.1469	saccharide
1	H6	KlP_1_H6	L-Lyxose	KlP	yes	10038.016	saccharide
1	H7	KlP_1_H7	Glucuronamide	KlP	yes	8521.98733	saccharide
1	H8	KlP_1_H8	Pyruvic Acid	KlP	yes	11598.254	keto acid
1	H9	KlP_1_H9	L-Galactonic Acid-Gamma-Lactone	KlP	yes	8341.5003	lactone
1	H10	KlP_1_H10	D-Galacturonic Acid	KlP	yes	11417.0076	saccharide
1	H11	KlP_1_H11	Phenylethylamine	KlP	no	5426.11747	
1	H12	KlP_1_H12	2-Aminoethanol	KlP	no	5151.11367	
2	A1	AcB_2_A1	Negative control	AcB	no	2194.49124	
2	A2	AcB_2_A2	Chondroitin Sulfate C	AcB	no	1922.73966	
2	A3	AcB_2_A3	Alpha-Cyclodextrin	AcB	no	2100.3678	
2	A4	AcB_2_A4	Beta-Cyclodextrin	AcB	no	1934.74093	
2	A5	AcB_2_A5	Gamma-Cyclodextrin	AcB	no	2093.24143	
2	A6	AcB_2_A6	Dextrin	AcB	no	5685.61866	
2	A7	AcB_2_A7	Gelatin	AcB	no	2151.9911	
2	A8	AcB_2_A8	Glycogen	AcB	no	2586.23977	
2	A9	AcB_2_A9	Inulin	AcB	no	2307.86389	
2	A10	AcB_2_A10	Laminarin	AcB	no	2557.73941	
2	A11	AcB_2_A11	Mannan	AcB	no	2577.24629	
2	A12	AcB_2_A12	Pectin	AcB	no	3770.48951	
2	B1	AcB_2_B1	N-Acetyl-D-Galactosamine	AcB	no	2004.61441	

2	B2	AcB_2_B2	N-Acetyl-Neuraminic Acid	AcB	no	1538.36961
2	B3	AcB_2_B3	Beta-D-Allose	AcB	no	3036.74651
2	B4	AcB_2_B4	Amygdalin	AcB	no	1474.99415
2	B5	AcB_2_B5	D-Arabinose	AcB	no	1619.1212
2	B6	AcB_2_B6	D-Arabitol	AcB	no	1605.36327
2	B7	AcB_2_B7	L-Arabitol	AcB	no	1629.36839
2	B8	AcB_2_B8	Arbutin	AcB	no	1706.49621
2	B9	AcB_2_B9	2-Deoxy-D-Ribose	AcB	no	1904.24549
2	B10	AcB_2_B10	i-Erythritol	AcB	no	2145.48967
2	B11	AcB_2_B11	D-Fucose	AcB	no	3590.61972
2	B12	AcB_2_B12	3-0-Beta-D-Galactopyranosyl-D-Arabi	AcB	no	2929.36766
2	C1	AcB_2_C1	Gentiobiose	AcB	no	2662.36514
2	C2	AcB_2_C2	L-Glucose	AcB	no	1579.61689
2	C3	AcB_2_C3	Lactitol	AcB	no	1559.62118
2	C4	AcB_2_C4	D-Melezitose	AcB	no	1520.24528
2	C5	AcB_2_C5	Maltitol	AcB	no	1375.87253
2	C6	AcB_2_C6	Alpha-Methyl-D-Glucoside	AcB	no	1577.49084
2	C7	AcB_2_C7	Beta-Methyl-D-Galactoside	AcB	no	1521.99423
2	C8	AcB_2_C8	3-Methyl Glucose	AcB	no	1924.24121
2	C9	AcB_2_C9	Beta-Methyl-D-Glucuronic Acid	AcB	no	1641.11627
2	C10	AcB_2_C10	Alpha-Methyl-D-Mannoside	AcB	no	1574.49415
2	C11	AcB_2_C11	Beta-Methyl-D-Xyloside	AcB	no	1928.86785
2	C12	AcB_2_C12	Palatinose	AcB	no	2640.98902
2	D1	AcB_2_D1	D-Raffinose	AcB	no	1983.24384
2	D2	AcB_2_D2	Salicin	AcB	no	1434.86876
2	D3	AcB_2_D3	Sedoheptulosan	AcB	no	1417.74432
2	D4	AcB_2_D4	L-Sorbose	AcB	no	1548.86635
2	D5	AcB_2_D5	Stachyose	AcB	no	1441.37447
2	D6	AcB_2_D6	D-Tagatose	AcB	no	1788.62137
2	D7	AcB_2_D7	Turanose	AcB	no	2031.87089

2	D8	AcB_2_D8	Xylitol	AcB	no	1593.12356	
2	D9	AcB_2_D9	N-Acetyl-D-Glucosaminitol	AcB	no	1733.99454	
2	D10	AcB_2_D10	Gamma-Amino Butyric Acid	AcB	yes	11250.412	amino acid
2	D11	AcB_2_D11	Delta-Amino Valeric Acid	AcB	no	1646.4924	
2	D12	AcB_2_D12	Butyric Acid	AcB	yes	9929.86882	organic acid
2	E1	AcB_2_E1	Capric Acid	AcB	no	1805.37	
2	E2	AcB_2_E2	Caproic Acid	AcB	yes	10396.3867	fatty acid
2	E3	AcB_2_E3	Citraconic Acid	AcB	yes	8201.99819	organic acid
2	E4	AcB_2_E4	Citramalic Acid	AcB	yes	10086.6558	organic acid
2	E5	AcB_2_E5	D-Glucosamine	AcB	no	4295.00027	
2	E6	AcB_2_E6	2-Hydroxy Benzoic Acid	AcB	no	684.246599	
2	E7	AcB_2_E7	4-Hydroxy Benzoic Acid	AcB	yes	10129.1359	phenolic acid
2	E8	AcB_2_E8	Beta-Hydroxy Butyric Acid	AcB	yes	11411.149	beta-hydroxy acid
2	E9	AcB_2_E9	Glycolic Acid	AcB	no	1930.74222	
2	E10	AcB_2_E10	Alpha-Keto-Valeric Acid	AcB	yes	10824.0187	keto acid
2	E11	AcB_2_E11	Itaconic Acid	AcB	no	1401.24353	
2	E12	AcB_2_E12	5-Keto-D-Gluconic Acid	AcB	no	3001.37018	
2	F1	AcB_2_F1	D-Lactic Acid Methyl Ester	AcB	yes	8926.63297	organic acid
2	F2	AcB_2_F2	Malonic Acid	AcB	no	6080.49526	
2	F3	AcB_2_F3	Melibionic Acid	AcB	no	1545.99679	
2	F4	AcB_2_F4	Oxalic Acid	AcB	no	1758.61647	
2	F5	AcB_2_F5	Oxalomalic Acid	AcB	no	2019.99545	
2	F6	AcB_2_F6	Quinic Acid	AcB	yes	10646.891	organic acid
2	F7	AcB_2_F7	D-Ribono-1,4-Lactone	AcB	yes	10682.3965	lactone
2	F8	AcB_2_F8	Sebacic Acid	AcB	yes	10247.1433	dicarboxylic acid
2	F9	AcB_2_F9	Sorbic Acid	AcB	yes	10951.0247	organic acid
2	F10	AcB_2_F10	Succinamic Acid	AcB	no	4106.23208	
2	F11	AcB_2_F11	D-Tartaric Acid	AcB	no	2521.98855	
2	F12	AcB_2_F12	L-Tartaric Acid	AcB	no	2525.86698	
2	G1	AcB_2_G1	Acetamide	AcB	no	1791.99088	

2	G2	AcB_2_G2	L-Alaninamide	AcB	no	2582.37031	
2	G3	AcB_2_G3	N-Acetyl-L-Glutamic Acid	AcB	no	1425.74602	
2	G4	AcB_2_G4	L-Arginine	AcB	yes	11173.8997	amino acid
2	G5	AcB_2_G5	Glycine	AcB	no	575.249331	
2	G6	AcB_2_G6	L-Histidine	AcB	yes	11140.9131	amino acid
2	G7	AcB_2_G7	L-Homoserine	AcB	no	1235.86749	
2	G8	AcB_2_G8	Hydroxy-L-Proline	AcB	yes	11708.0328	amino acid
2	G9	AcB_2_G9	L-Isoleucine	AcB	no	4017.23352	
2	G10	AcB_2_G10	L-Leucine	AcB	no	6478.24656	
2	G11	AcB_2_G11	L-Lysine	AcB	no	1920.23608	
2	G12	AcB_2_G12	L-Methionine	AcB	no	1869.98934	
2	H1	AcB_2_H1	L-Ornithine	AcB	yes	11090.2427	amino acid
2	H2	AcB_2_H2	L-Phenylalanine	AcB	yes	11372.3831	amino acid
2	H3	AcB_2_H3	L-Pyroglutamic Acid	AcB	yes	12122.9213	amino acid
2	H4	AcB_2_H4	L-Valine	AcB	no	1785.11961	
2	H5	AcB_2_H5	D,L-Carnitine	AcB	no	2459.87278	
2	H6	AcB_2_H6	Sec-Butylamine	AcB	no	1496.247	
2	H7	AcB_2_H7	D,L-Octopamine	AcB	no	1305.74225	
2	H8	AcB_2_H8	Putrescine	AcB	yes	12984.4113	amine
2	H9	AcB_2_H9	Dihydroxy Acetone	AcB	no	3353.87121	
2	H10	AcB_2_H10	2,3-Butanediol	AcB	no	7487.36874	
2	H11	AcB_2_H11	2,3-Butanedione	AcB	no	1778.36691	
2	H12	AcB_2_H12	3-Hydroxy-2-Butanone	AcB	no	2796.73639	
2	A1	KlP_2_A1	Negative control	KlP	no	3977.85591	
2	A2	KlP_2_A2	Chondroitin Sulfate C	KlP	no	3754.35726	
2	A3	KlP_2_A3	Alpha-Cyclodextrin	KlP	no	4331.23142	
2	A4	KlP_2_A4	Beta-Cyclodextrin	KlP	no	4371.10727	
2	A5	KlP_2_A5	Gamma-Cyclodextrin	KlP	no	4544.48288	
2	A6	KlP_2_A6	Dextrin	KlP	yes	10813.8551	saccharide
2	A7	KlP_2_A7	Gelatin	KlP	no	4212.73432	

2	A8	KlP_2_A8	Glycogen	KlP	no	5722.34719	
2	A9	KlP_2_A9	Inulin	KlP	no	4177.23642	
2	A10	KlP_2_A10	Laminarin	KlP	no	4863.35782	
2	A11	KlP_2_A11	Mannan	KlP	no	4847.4747	
2	A12	KlP_2_A12	Pectin	KlP	yes	8905.22566	saccharide
2	B1	KlP_2_B1	N-Acetyl-D-Galactosamine	KlP	no	4156.35298	
2	B2	KlP_2_B2	N-Acetyl-Neuraminic Acid	KlP	no	3553.3562	
2	B3	KlP_2_B3	Beta-D-Allose	KlP	no	3108.86078	
2	B4	KlP_2_B4	Amygdalin	KlP	no	5351.9906	
2	B5	KlP_2_B5	D-Arabinose	KlP	no	4374.8543	
2	B6	KlP_2_B6	D-Arabitol	KlP	yes	12313.8559	sugar alcohol
2	B7	KlP_2_B7	L-Arabitol	KlP	no	4183.72803	
2	B8	KlP_2_B8	Arbutin	KlP	yes	12601.2757	saccharide
2	B9	KlP_2_B9	2-Deoxy-D-Ribose	KlP	no	3266.36352	
2	B10	KlP_2_B10	i-Erythritol	KlP	no	4067.98234	
2	B11	KlP_2_B11	D-Fucose	KlP	no	4225.23383	
2	B12	KlP_2_B12	3-0-Beta-D-Galactopyranosyl-D-Arabi	KlP	yes	10671.6139	glycosylarabinose
2	C1	KlP_2_C1	Gentiobiose	KlP	yes	12326.0036	saccharide
2	C2	KlP_2_C2	L-Glucose	KlP	no	3601.48586	
2	C3	KlP_2_C3	Lactitol	KlP	yes	9516.58628	sugar alcohol
2	C4	KlP_2_C4	D-Melezitose	KlP	no	4069.23135	
2	C5	KlP_2_C5	Maltitol	KlP	yes	10745.5182	sugar alcohol
2	C6	KlP_2_C6	Alpha-Methyl-D-Glucoside	KlP	no	4823.47941	
2	C7	KlP_2_C7	Beta-Methyl-D-Galactoside	KlP	yes	11287.8619	saccharide
2	C8	KlP_2_C8	3-Methyl Glucose	KlP	no	3874.72788	
2	C9	KlP_2_C9	Beta-Methyl-D-Glucuronic Acid	KlP	no	3673.10872	
2	C10	KlP_2_C10	Alpha-Methyl-D-Mannoside	KlP	no	4163.85303	
2	C11	KlP_2_C11	Beta-Methyl-D-Xyloside	KlP	no	4257.85404	
2	C12	KlP_2_C12	Palatinose	KlP	yes	10848.6304	saccharide
2	D1	KlP_2_D1	D-Raffinose	KlP	yes	11932.4988	saccharide

2	D2	KlP_2_D2	Salicin	KlP	yes	11480.3925	saccharide
2	D3	KlP_2_D3	Sedoheptulosan	KlP	no	3250.60837	
2	D4	KlP_2_D4	L-Sorbose	KlP	no	2821.23632	
2	D5	KlP_2_D5	Stachyose	KlP	yes	11901.7526	saccharide
2	D6	KlP_2_D6	D-Tagatose	KlP	yes	11522.3657	saccharide
2	D7	KlP_2_D7	Turanose	KlP	yes	10302.4247	saccharide
2	D8	KlP_2_D8	Xylitol	KlP	no	4959.0813	
2	D9	KlP_2_D9	N-Acetyl-D-Glucosaminitol	KlP	no	3931.1058	
2	D10	KlP_2_D10	Gamma-Amino Butyric Acid	KlP	yes	10934.7286	amino acid
2	D11	KlP_2_D11	Delta-Amino Valeric Acid	KlP	no	4622.98641	
2	D12	KlP_2_D12	Butyric Acid	KlP	no	4125.10762	
2	E1	KlP_2_E1	Capric Acid	KlP	no	3171.12289	
2	E2	KlP_2_E2	Caproic Acid	KlP	no	2678.11601	
2	E3	KlP_2_E3	Citraconic Acid	KlP	no	3192.48662	
2	E4	KlP_2_E4	Citramalic Acid	KlP	no	3467.23489	
2	E5	KlP_2_E5	D-Glucosamine	KlP	yes	12503.8928	amino sugar
2	E6	KlP_2_E6	2-Hydroxy Benzoic Acid	KlP	no	1102.99693	
2	E7	KlP_2_E7	4-Hydroxy Benzoic Acid	KlP	yes	9346.8528	phenolic acid
2	E8	KlP_2_E8	Beta-Hydroxy Butyric Acid	KlP	yes	10919.3818	beta-hydroxy acid
2	E9	KlP_2_E9	Glycolic Acid	KlP	no	3798.98303	
2	E10	KlP_2_E10	Alpha-Keto-Valeric Acid	KlP	no	3093.23574	
2	E11	KlP_2_E11	Itaconic Acid	KlP	no	1705.9937	
2	E12	KlP_2_E12	5-Keto-D-Gluconic Acid	KlP	no	5186.9784	
2	F1	KlP_2_F1	D-Lactic Acid Methyl Ester	KlP	yes	10568.3806	organic acid
2	F2	KlP_2_F2	Malonic Acid	KlP	no	3193.98176	
2	F3	KlP_2_F3	Melibionic Acid	KlP	yes	11415.2522	saccharide
2	F4	KlP_2_F4	Oxalic Acid	KlP	no	4039.4807	
2	F5	KlP_2_F5	Oxalomalic Acid	KlP	no	4311.48397	
2	F6	KlP_2_F6	Quinic Acid	KlP	yes	11453.3659	organic acid
2	F7	KlP_2_F7	D-Ribono-1,4-Lactone	KlP	no	2724.36532	

2	F8	KlP_2_F8	Sebacic Acid	KlP	no	2895.9877	
2	F9	KlP_2_F9	Sorbic Acid	KlP	no	3710.73609	
2	F10	KlP_2_F10	Succinamic Acid	KlP	no	5172.10158	
2	F11	KlP_2_F11	D-Tartaric Acid	KlP	no	3588.98806	
2	F12	KlP_2_F12	L-Tartaric Acid	KlP	yes	10679.7376	organic acid
2	G1	KlP_2_G1	Acetamide	KlP	no	3959.10792	
2	G2	KlP_2_G2	L-Alaninamide	KlP	no	4974.97852	
2	G3	KlP_2_G3	N-Acetyl-L-Glutamic Acid	KlP	no	3237.36065	
2	G4	KlP_2_G4	L-Arginine	KlP	yes	9315.48672	amino acid
2	G5	KlP_2_G5	Glycine	KlP	no	3327.99173	
2	G6	KlP_2_G6	L-Histidine	KlP	yes	11946.502	amino acid
2	G7	KlP_2_G7	L-Homoserine	KlP	no	3197.11027	
2	G8	KlP_2_G8	Hydroxy-L-Proline	KlP	yes	11316.256	amino acid
2	G9	KlP_2_G9	L-Isoleucine	KlP	no	3170.11146	
2	G10	KlP_2_G10	L-Leucine	KlP	no	3571.47968	
2	G11	KlP_2_G11	L-Lysine	KlP	no	4145.73425	
2	G12	KlP_2_G12	L-Methionine	KlP	no	4710.73083	
2	H1	KlP_2_H1	L-Ornithine	KlP	no	5672.73094	
2	H2	KlP_2_H2	L-Phenylalanine	KlP	no	7576.25385	
2	H3	KlP_2_H3	L-Pyroglutamic Acid	KlP	no	3882.85842	
2	H4	KlP_2_H4	L-Valine	KlP	no	3649.23629	
2	H5	KlP_2_H5	D,L-Carnitine	KlP	no	3197.48438	
2	H6	KlP_2_H6	Sec-Butylamine	KlP	no	4323.60596	
2	H7	KlP_2_H7	D,L-Octopamine	KlP	yes	11261.1211	amine
2	H8	KlP_2_H8	Putrescine	KlP	yes	12274.1512	amine
2	H9	KlP_2_H9	Dihydroxy Acetone	KlP	yes	12138.5408	saccharide
2	H10	KlP_2_H10	2,3-Butanediol	KlP	no	4145.35416	
2	H11	KlP_2_H11	2,3-Butanedione	KlP	no	2589.86481	
2	H12	KlP_2_H12	3-Hydroxy-2-Butanone	KlP	no	4839.47983	

+ organic acid)

id

ıd
ıd