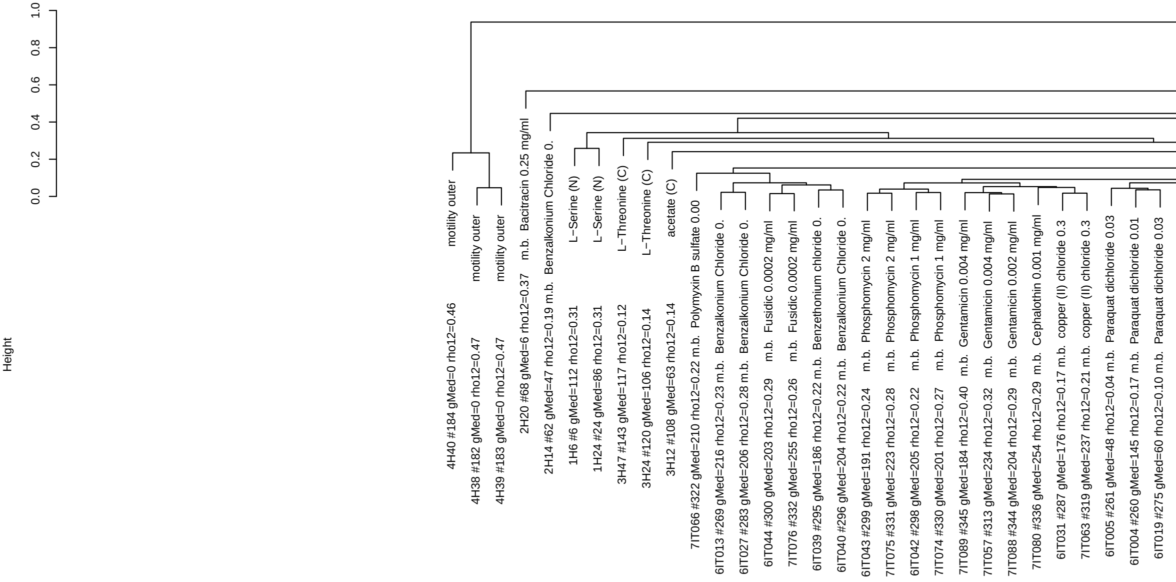

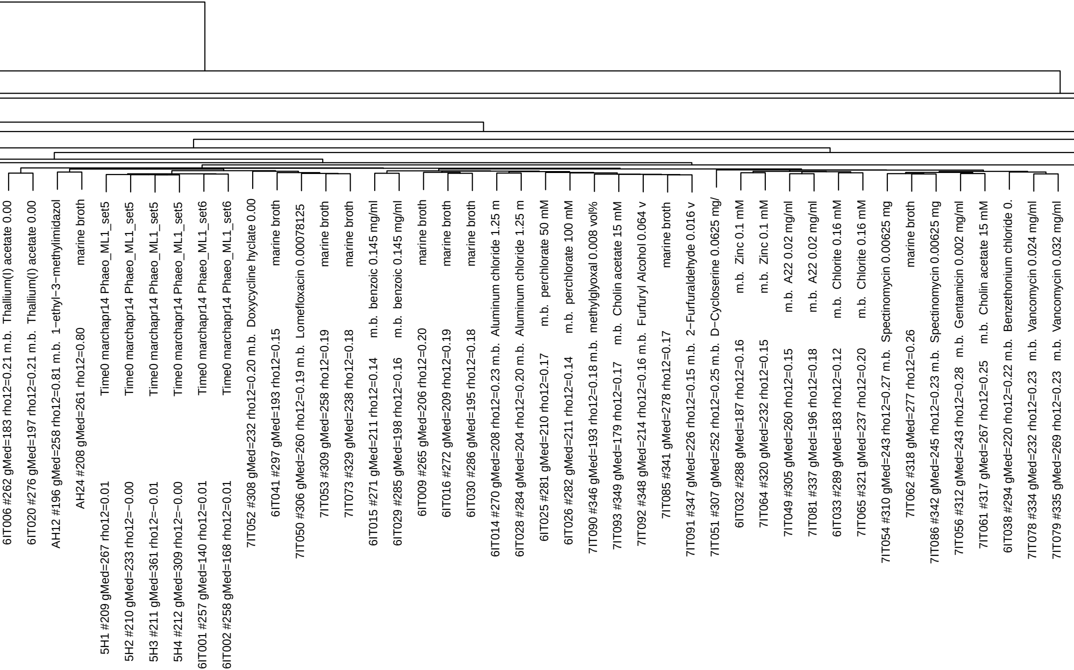

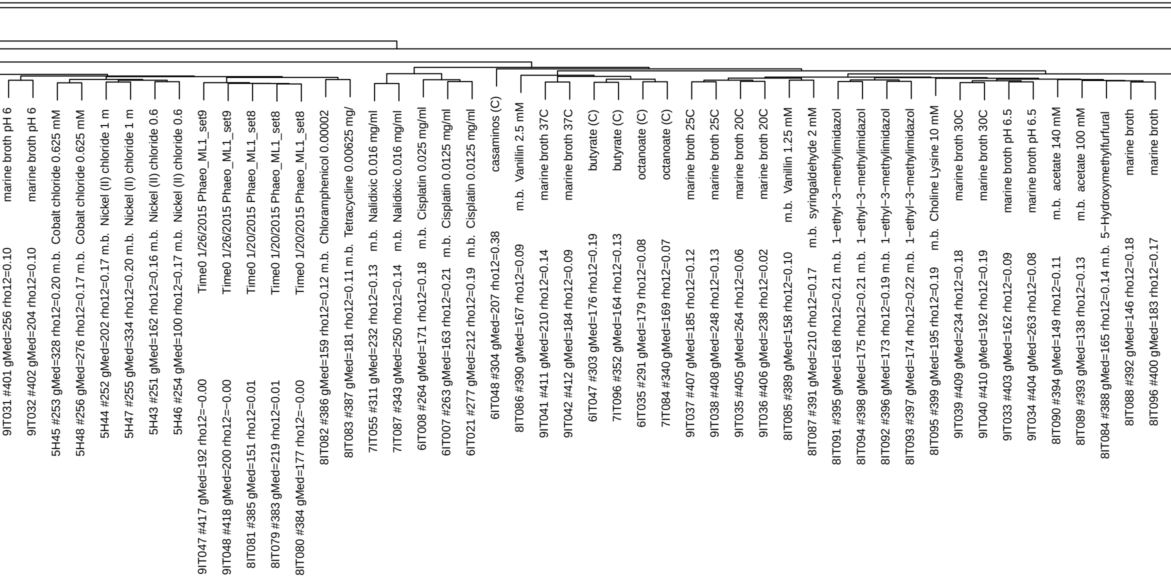

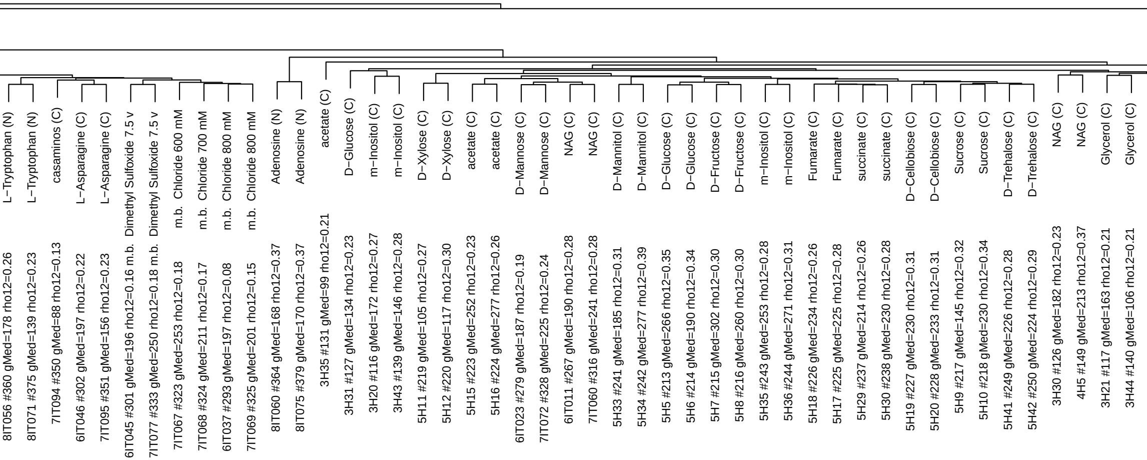

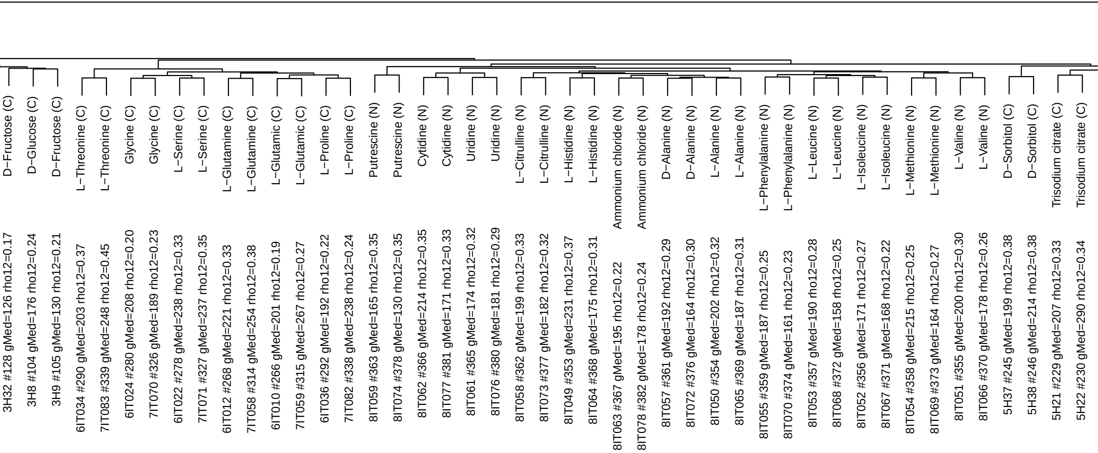

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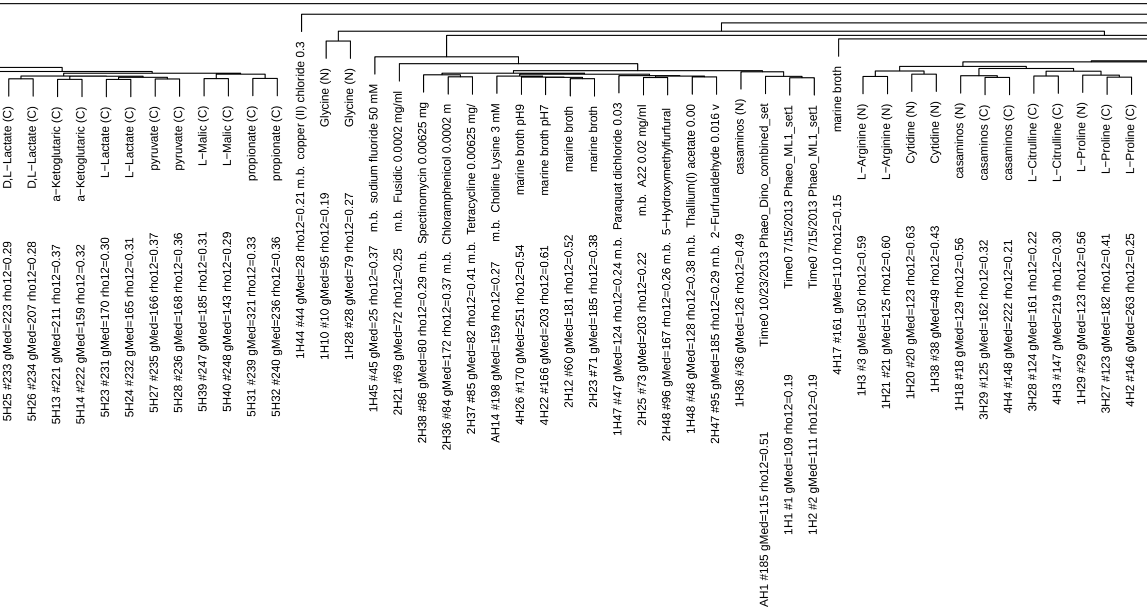
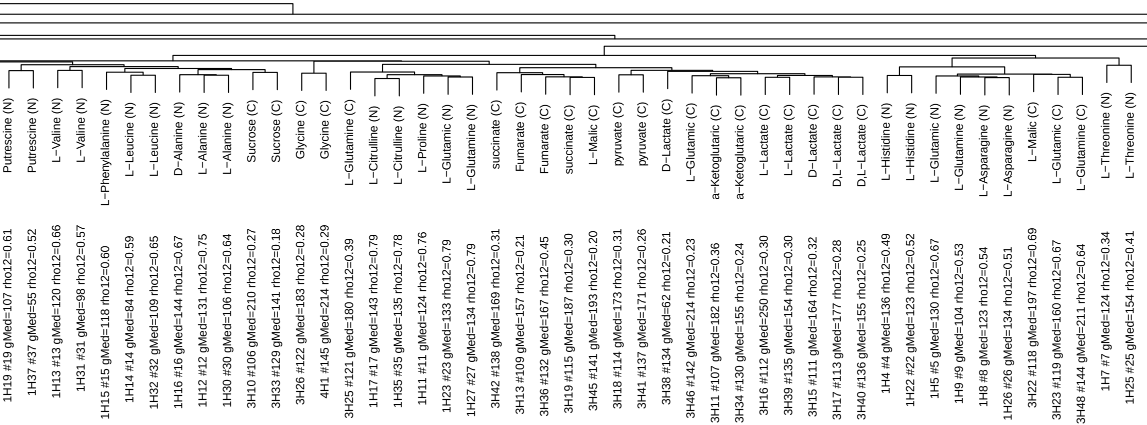
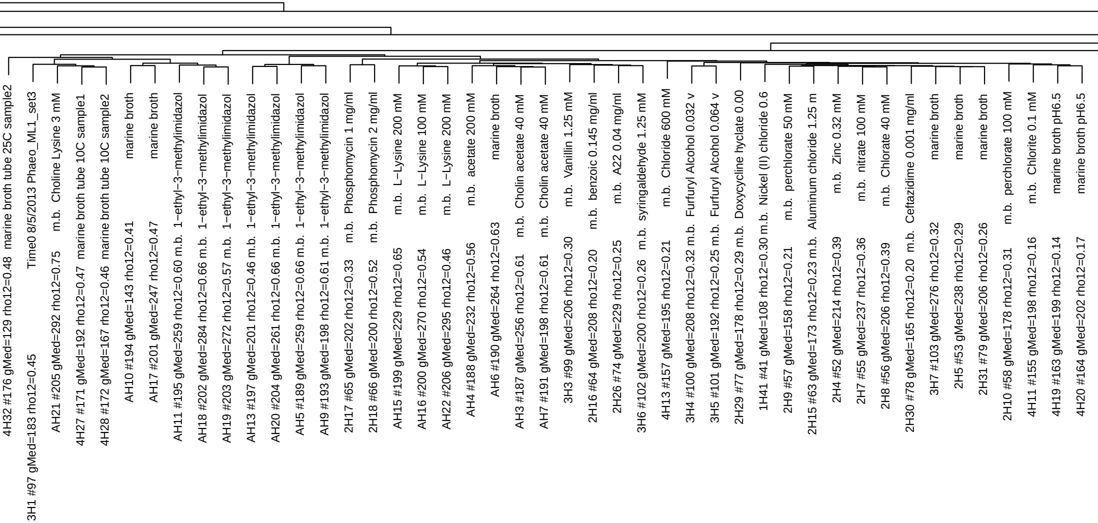
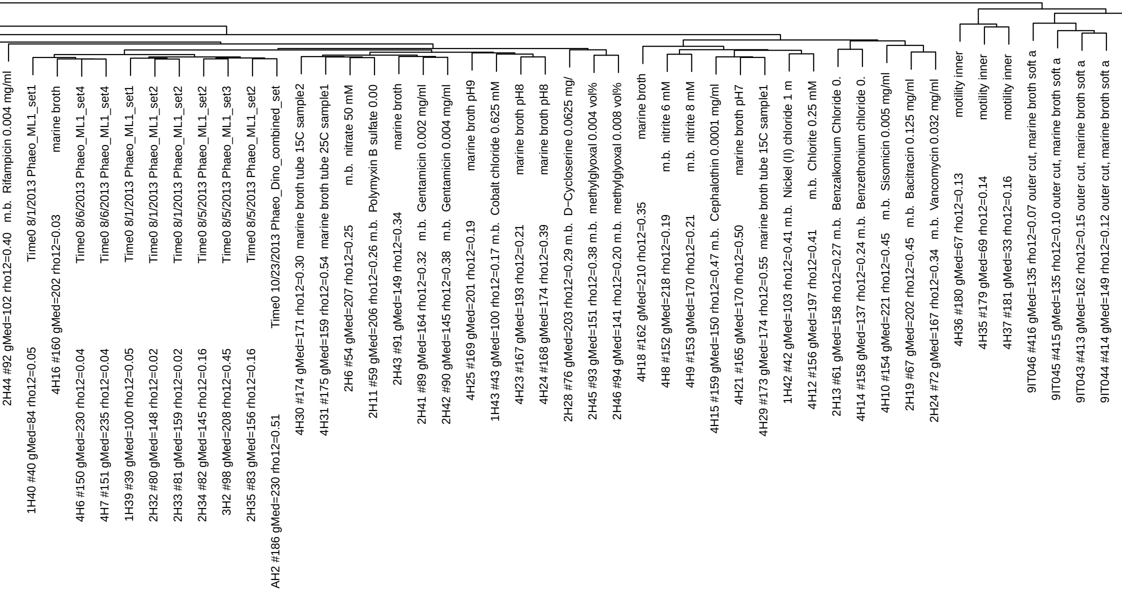

5H25 #233 gMed=223 rho12=0.29 D,L−Lactate (C)
5H26 #234 gMed=207 rho12=0.28 D,L−Lactate (C)
5H13 #221 gMed=211 rho12=0.37 a−Ketoglutaric (C)
5H14 #222 gMed=159 rho12=0.32 a−Ketoglutaric (C)
5H23 #231 gMed=170 rho12=0.30 L−Lactate (C)
5H24 #232 gMed=165 rho12=0.31 L−Lactate (C)
5H27 #235 gMed=166 rho12=0.37 pyruvate (C)
5H28 #236 gMed=168 rho12=0.36 pyruvate (C)
5H39 #247 gMed=185 rho12=0.31 L−Malic (C)
5H40 #248 gMed=143 rho12=0.29 L−Malic (C)
5H31 #239 gMed=321 rho12=0.33 propionate (C)
5H32 #240 gMed=236 rho12=0.36 propionate (C)
1H44 #44 gMed=28 rho12=0.21 m.b. copper (II) chloride 0.3
1H10 #10 gMed=95 rho12=0.19 Glycine (N)
1H28 #28 gMed=79 rho12=0.27 Glycine (N)
1H45 #45 gMed=25 rho12=0.37 m.b. sodium fluoride 50 mM
2H21 #69 gMed=72 rho12=0.25 m.b. Fusidic 0.0002 mg/ml
2H38 #86 gMed=80 rho12=0.29 m.b. Spectinomycin 0.00625 mg
2H36 #84 gMed=172 rho12=0.37 m.b. Chloramphenicol 0.0002 m
2H37 #85 gMed=82 rho12=0.41 m.b. Tetracycline 0.00625 mg/
AH14 #198 gMed=159 rho12=0.27 m.b. Choline Lysine 3 mM
4H26 #170 gMed=251 rho12=0.54 marine broth pH9
4H22 #166 gMed=203 rho12=0.61 marine broth pH7
2H12 #60 gMed=181 rho12=0.52 marine broth
2H23 #71 gMed=185 rho12=0.38 marine broth
1H47 #47 gMed=124 rho12=0.24 m.b. Paraquat dichloride 0.03
2H25 #73 gMed=203 rho12=0.22 m.b. A22 0.02 mg/ml
2H48 #96 gMed=167 rho12=0.26 m.b. 5−Hydroxymethylfurfural
1H48 #48 gMed=128 rho12=0.38 m.b. Thallium(I) acetate 0.00
2H47 #95 gMed=185 rho12=0.29 m.b. 2−Furfuraldehyde 0.016 v
1H36 #36 gMed=126 rho12=0.49 casaminos (N)
AH1 #185 gMed=115 rho12=0.51 Time0 10/23/2013 Phaeo_Dino_combined_set
1H1 #1 gMed=109 rho12=0.19 Time0 7/15/2013 Phaeo_ML1_set1
1H2 #2 gMed=111 rho12=0.19 Time0 7/15/2013 Phaeo_ML1_set1
4H17 #161 gMed=110 rho12=0.15 marine broth
1H3 #3 gMed=150 rho12=0.59 L−Arginine (N)
1H21 #21 gMed=125 rho12=0.60 L−Arginine (N)
1H20 #20 gMed=123 rho12=0.63 Cytidine (N)
1H38 #38 gMed=49 rho12=0.43 Cytidine (N)
1H18 #18 gMed=129 rho12=0.56 casaminos (N)
3H29 #125 gMed=162 rho12=0.32 casaminos (C)
4H4 #148 gMed=222 rho12=0.21 casaminos (C)
3H28 #124 gMed=161 rho12=0.22 L−Citrulline (C)
4H3 #147 gMed=219 rho12=0.30 L−Citrulline (C)
1H29 #29 gMed=123 rho12=0.56 L−Proline (N)
3H27 #123 gMed=182 rho12=0.41 L−Proline (C)
4H2 #146 gMed=263 rho12=0.25 L−Proline (C)


Putrescine (N)
1H19 #19 gMed=107 rho12=0.61
Putrescine (N)
1H37 #37 gMed=55 rho12=0.52
L−Valine (N)
1H13 #13 gMed=120 rho12=0.66
L−Valine (N)
1H31 #31 gMed=98 rho12=0.57
L−Phenylalanine (N)
1H15 #15 gMed=118 rho12=0.60
L−Leucine (N)
1H14 #14 gMed=84 rho12=0.59
L−Leucine (N)
1H32 #32 gMed=109 rho12=0.65
D−Alanine (N)
1H16 #16 gMed=144 rho12=0.67
L−Alanine (N)
1H12 #12 gMed=131 rho12=0.75
L−Alanine (N)
1H30 #30 gMed=106 rho12=0.64
Sucrose (C)
3H10 #106 gMed=210 rho12=0.27
Sucrose (C)
3H33 #129 gMed=141 rho12=0.18
Glycine (C)
3H26 #122 gMed=183 rho12=0.28
Glycine (C)
4H1 #145 gMed=214 rho12=0.29
L−Glutamine (C)
3H25 #121 gMed=180 rho12=0.39
L−Citrulline (N)
1H17 #17 gMed=143 rho12=0.79
L−Citrulline (N)
1H35 #35 gMed=135 rho12=0.78
L−Proline (N)
1H11 #11 gMed=124 rho12=0.76
L−Glutamic (N)
1H23 #23 gMed=133 rho12=0.79
L−Glutamine (N)
1H27 #27 gMed=134 rho12=0.79
succinate (C)
3H42 #138 gMed=169 rho12=0.31
Fumarate (C)
3H13 #109 gMed=157 rho12=0.21
Fumarate (C)
3H36 #132 gMed=167 rho12=0.45
succinate (C)
3H19 #115 gMed=187 rho12=0.30
L−Malic (C)
3H45 #141 gMed=193 rho12=0.20
pyruvate (C)
3H18 #114 gMed=173 rho12=0.31
pyruvate (C)
3H41 #137 gMed=171 rho12=0.26
D−Lactate (C)
3H38 #134 gMed=62 rho12=0.21
L−Glutamic (C)
3H46 #142 gMed=214 rho12=0.23
a−Ketoglutaric (C)
3H11 #107 gMed=182 rho12=0.36
a−Ketoglutaric (C)
3H34 #130 gMed=155 rho12=0.24
L−Lactate (C)
3H16 #112 gMed=250 rho12=0.30
L−Lactate (C)
3H39 #135 gMed=154 rho12=0.30
D−Lactate (C)
3H15 #111 gMed=164 rho12=0.32
D,L−Lactate (C)
3H17 #113 gMed=177 rho12=0.28
D,L−Lactate (C)
3H40 #136 gMed=155 rho12=0.25
L−Histidine (N)
1H4 #4 gMed=136 rho12=0.49
L−Histidine (N)
1H22 #22 gMed=123 rho12=0.52
L−Glutamic (N)
1H5 #5 gMed=130 rho12=0.67
L−Glutamine (N)
1H9 #9 gMed=104 rho12=0.53
L−Asparagine (N)
1H8 #8 gMed=123 rho12=0.54
L−Asparagine (N)
1H26 #26 gMed=134 rho12=0.51
L−Malic (C)
3H22 #118 gMed=197 rho12=0.69
L−Glutamic (C)
3H23 #119 gMed=160 rho12=0.67
L−Glutamine (C)
3H48 #144 gMed=211 rho12=0.64
L−Threonine (N)
1H7 #7 gMed=124 rho12=0.34
L−Threonine (N)
1H25 #25 gMed=154 rho12=0.41


4H32 #176 gMed=129 rho12=0.48 marine broth tube 25C sample2
3H1 #97 gMed=183 rho12=0.45 Time0 8/5/2013 Phaeo_ML1_set3
AH21 #205 gMed=292 rho12=0.75 m.b. Choline Lysine 3 mM
4H27 #171 gMed=192 rho12=0.47 marine broth tube 10C sample1
4H28 #172 gMed=167 rho12=0.46 marine broth tube 10C sample2
AH10 #194 gMed=143 rho12=0.41 marine broth
AH17 #201 gMed=247 rho12=0.47 marine broth
AH11 #195 gMed=259 rho12=0.60 m.b. 1−ethyl−3−methylimidazol
AH18 #202 gMed=284 rho12=0.66 m.b. 1−ethyl−3−methylimidazol
AH19 #203 gMed=272 rho12=0.57 m.b. 1−ethyl−3−methylimidazol
AH13 #197 gMed=201 rho12=0.46 m.b. 1−ethyl−3−methylimidazol
AH20 #204 gMed=261 rho12=0.66 m.b. 1−ethyl−3−methylimidazol
AH5 #189 gMed=259 rho12=0.66 m.b. 1−ethyl−3−methylimidazol
AH9 #193 gMed=198 rho12=0.61 m.b. 1−ethyl−3−methylimidazol
2H17 #65 gMed=202 rho12=0.33 m.b. Phosphomycin 1 mg/ml
2H18 #66 gMed=200 rho12=0.52 m.b. Phosphomycin 2 mg/ml
AH15 #199 gMed=229 rho12=0.65 m.b. L−Lysine 200 mM
AH16 #200 gMed=270 rho12=0.54 m.b. L−Lysine 100 mM
AH22 #206 gMed=295 rho12=0.46 m.b. L−Lysine 200 mM
AH4 #188 gMed=232 rho12=0.56 m.b. acetate 200 mM
AH6 #190 gMed=264 rho12=0.63 marine broth
AH3 #187 gMed=256 rho12=0.61 m.b. Cholin acetate 40 mM
AH7 #191 gMed=198 rho12=0.61 m.b. Cholin acetate 40 mM
3H3 #99 gMed=206 rho12=0.30 m.b. Vanillin 1.25 mM
2H16 #64 gMed=208 rho12=0.20 m.b. benzoic 0.145 mg/ml
2H26 #74 gMed=229 rho12=0.25 m.b. A22 0.04 mg/ml
3H6 #102 gMed=200 rho12=0.26 m.b. syringaldehyde 1.25 mM
4H13 #157 gMed=195 rho12=0.21 m.b. Chloride 600 mM
3H4 #100 gMed=208 rho12=0.32 m.b. Furfuryl Alcohol 0.032 v
3H5 #101 gMed=192 rho12=0.25 m.b. Furfuryl Alcohol 0.064 v
2H29 #77 gMed=178 rho12=0.29 m.b. Doxycycline hyclate 0.00
1H41 #41 gMed=108 rho12=0.30 m.b. Nickel (II) chloride 0.6
2H9 #57 gMed=158 rho12=0.21 m.b. perchlorate 50 mM
2H15 #63 gMed=173 rho12=0.23 m.b. Aluminum chloride 1.25 m
2H4 #52 gMed=214 rho12=0.39 m.b. Zinc 0.32 mM
2H7 #55 gMed=237 rho12=0.36 m.b. nitrate 100 mM
2H8 #56 gMed=206 rho12=0.39 m.b. Chlorate 40 mM
2H30 #78 gMed=165 rho12=0.20 m.b. Ceftazidime 0.001 mg/ml
3H7 #103 gMed=276 rho12=0.32 marine broth
2H5 #53 gMed=238 rho12=0.29 marine broth
2H31 #79 gMed=206 rho12=0.26 marine broth
2H10 #58 gMed=178 rho12=0.31 m.b. perchlorate 100 mM
4H11 #155 gMed=198 rho12=0.16 m.b. Chlorite 0.1 mM
4H19 #163 gMed=199 rho12=0.14 marine broth pH6.5
4H20 #164 gMed=202 rho12=0.17 marine broth pH6.5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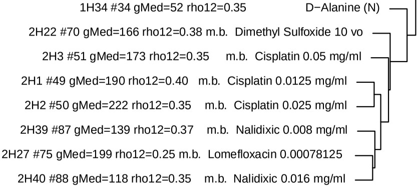
1H40 #40 gMed=84 rho12=0.05 Time0 8/1/2013 Phaeo_ML1_set1
4H16 #160 gMed=202 rho12=0.03 marine broth
4H6 #150 gMed=230 rho12=0.04 Time0 8/6/2013 Phaeo_ML1_set4
4H7 #151 gMed=235 rho12=0.04 Time0 8/6/2013 Phaeo_ML1_set4
1H39 #39 gMed=100 rho12=0.05 Time0 8/1/2013 Phaeo_ML1_set1
2H32 #80 gMed=148 rho12=0.02 Time0 8/1/2013 Phaeo_ML1_set2
2H33 #81 gMed=159 rho12=0.02 Time0 8/1/2013 Phaeo_ML1_set2
2H34 #82 gMed=145 rho12=0.16 Time0 8/5/2013 Phaeo_ML1_set2
3H2 #98 gMed=208 rho12=0.45 Time0 8/5/2013 Phaeo_ML1_set3
2H35 #83 gMed=156 rho12=0.16 Time0 8/5/2013 Phaeo_ML1_set2
AH2 #186 gMed=230 rho12=0.51 Time0 10/23/2013 Phaeo_Dino_combined_set
4H30 #174 gMed=171 rho12=0.30 marine broth tube 15C sample2
4H31 #175 gMed=159 rho12=0.54 marine broth tube 25C sample1
2H6 #54 gMed=207 rho12=0.25 m.b. nitrate 50 mM
2H11 #59 gMed=206 rho12=0.26 m.b. Polymyxin B sulfate 0.00
2H43 #91 gMed=149 rho12=0.34 marine broth
2H41 #89 gMed=164 rho12=0.32 m.b. Gentamicin 0.002 mg/ml
2H42 #90 gMed=145 rho12=0.38 m.b. Gentamicin 0.004 mg/ml
4H25 #169 gMed=201 rho12=0.19 marine broth pH9
1H43 #43 gMed=100 rho12=0.17 m.b. Cobalt chloride 0.625 mM
4H23 #167 gMed=193 rho12=0.21 marine broth pH8
4H24 #168 gMed=174 rho12=0.39 marine broth pH8
2H28 #76 gMed=203 rho12=0.29 m.b. D−Cycloserine 0.0625 mg/
2H45 #93 gMed=151 rho12=0.38 m.b. methylglyoxal 0.004 vol%
2H46 #94 gMed=141 rho12=0.20 m.b. methylglyoxal 0.008 vol%
4H18 #162 gMed=210 rho12=0.35 marine broth
4H8 #152 gMed=218 rho12=0.19 m.b. nitrite 6 mM
4H9 #153 gMed=170 rho12=0.21 m.b. nitrite 8 mM
4H15 #159 gMed=150 rho12=0.47 m.b. Cephalothin 0.0001 mg/ml
4H21 #165 gMed=170 rho12=0.50 marine broth pH7
4H29 #173 gMed=174 rho12=0.55 marine broth tube 15C sample1
1H42 #42 gMed=103 rho12=0.41 m.b. Nickel (II) chloride 1 m
4H12 #156 gMed=197 rho12=0.41 m.b. Chlorite 0.25 mM
2H13 #61 gMed=158 rho12=0.27 m.b. Benzalkonium Chloride 0.
4H14 #158 gMed=137 rho12=0.24 m.b. Benzethonium chloride 0.
4H10 #154 gMed=221 rho12=0.45 m.b. Sisomicin 0.005 mg/ml
2H19 #67 gMed=202 rho12=0.45 m.b. Bacitracin 0.125 mg/ml
2H24 #72 gMed=167 rho12=0.34 m.b. Vancomycin 0.032 mg/ml
4H36 #180 gMed=67 rho12=0.13 motility inner
4H35 #179 gMed=69 rho12=0.14 motility inner
4H37 #181 gMed=33 rho12=0.16 motility inner
9IT046 #416 gMed=135 rho12=0.07 outer cut, marine broth soft a
9IT045 #415 gMed=135 rho12=0.10 outer cut, marine broth soft a
9IT043 #413 gMed=162 rho12=0.15 outer cut, marine broth soft a
9IT044 #414 gMed=149 rho12=0.12 outer cut, marine broth soft a


1H34 #34 gMed=52 rho12=0.35 D−Alanine (N)
2H22 #70 gMed=166 rho12=0.38 m.b. Dimethyl Sulfoxide 10 vo
2H3 #51 gMed=173 rho12=0.35 m.b. Cisplatin 0.05 mg/ml
2H1 #49 gMed=190 rho12=0.40 m.b. Cisplatin 0.0125 mg/ml
2H2 #50 gMed=222 rho12=0.35 m.b. Cisplatin 0.025 mg/ml
2H39 #87 gMed=139 rho12=0.37 m.b. Nalidixic 0.008 mg/ml
2H27 #75 gMed=199 rho12=0.25 m.b. Lomefloxacin 0.00078125
2H40 #88 gMed=118 rho12=0.35 m.b. Nalidixic 0.016 mg/ml