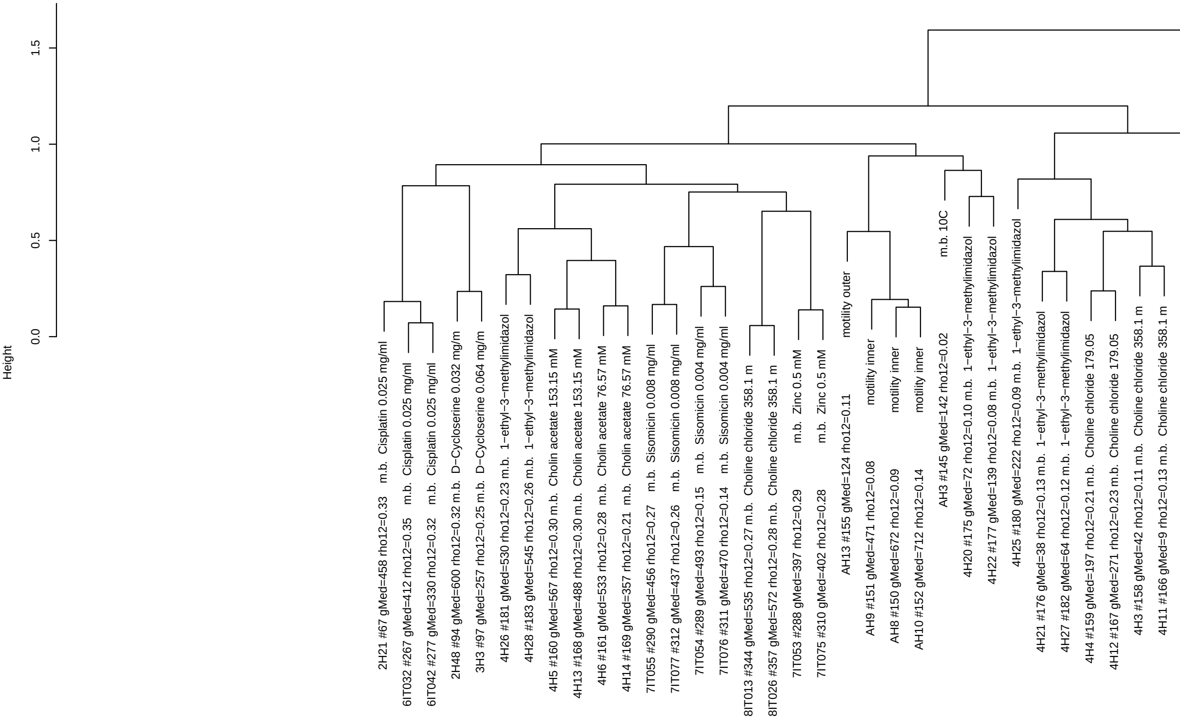
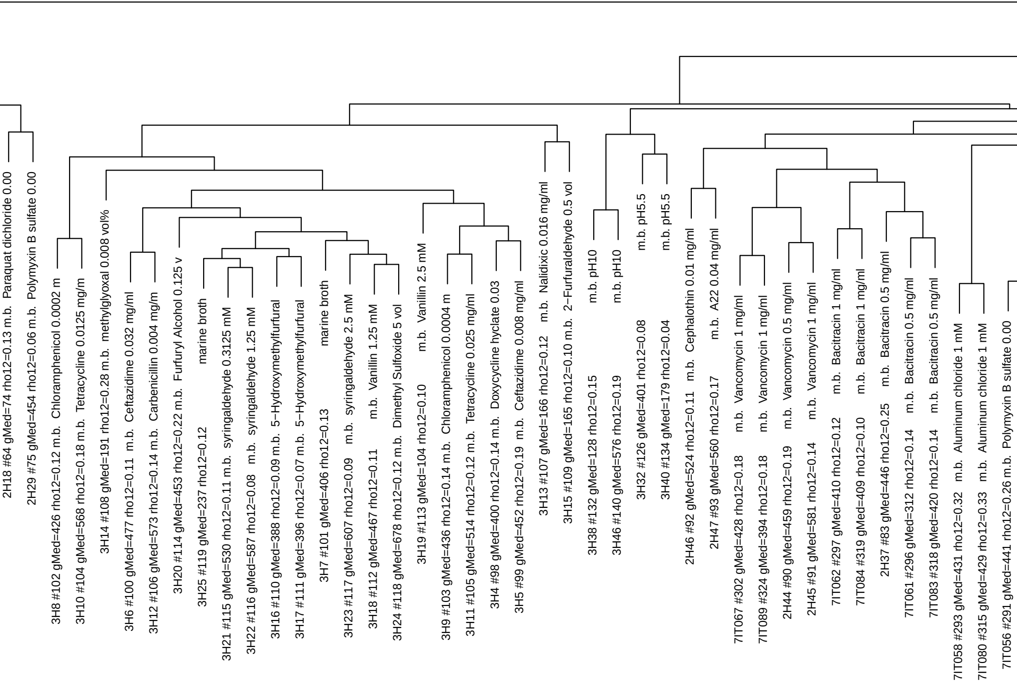
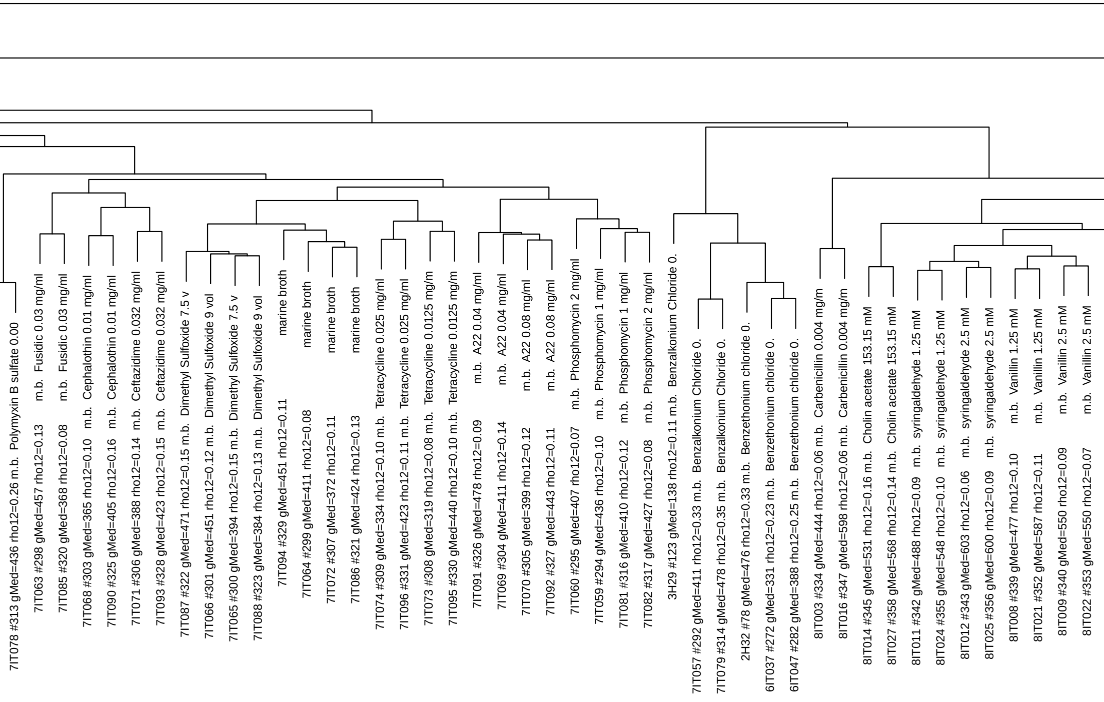
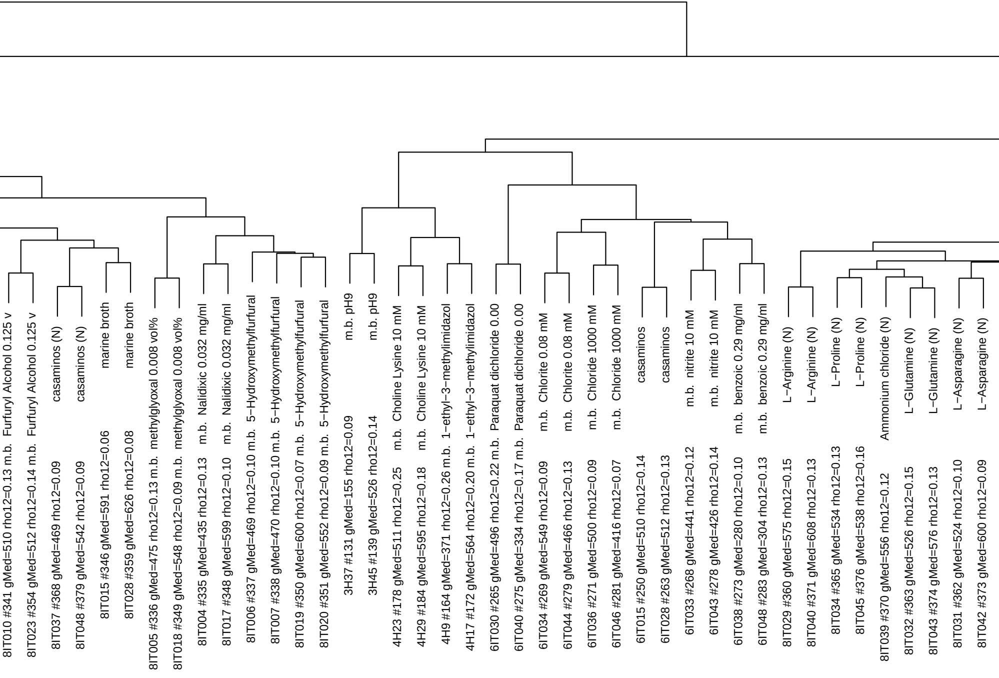
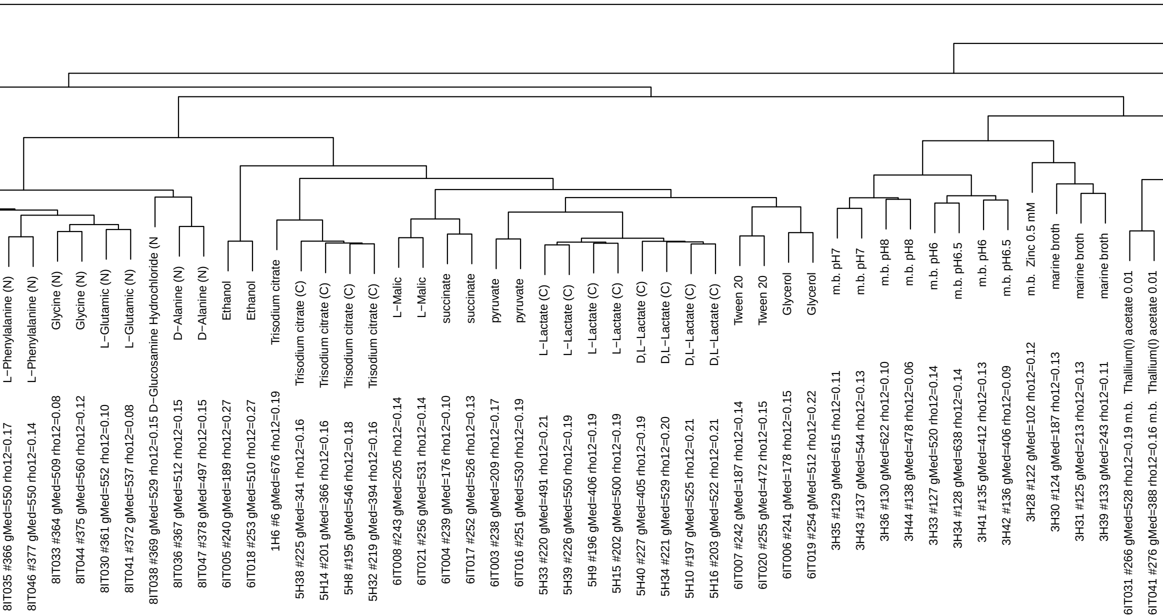





7IT078 #313 gMed=436 rho12=0.26 m.b. Polymyxin B sulfate 0.00
7IT063 #298 gMed=457 rho12=0.13 m.b. Fusidic 0.03 mg/ml
7IT085 #320 gMed=368 rho12=0.08 m.b. Fusidic 0.03 mg/ml
7IT068 #303 gMed=365 rho12=0.10 m.b. Cephalothin 0.01 mg/ml
7IT090 #325 gMed=405 rho12=0.16 m.b. Cephalothin 0.01 mg/ml
7IT071 #306 gMed=388 rho12=0.14 m.b. Ceftazidime 0.032 mg/ml
7IT093 #328 gMed=423 rho12=0.15 m.b. Ceftazidime 0.032 mg/ml
7IT087 #322 gMed=471 rho12=0.15 m.b. Dimethyl Sulfoxide 7.5 v
7IT066 #301 gMed=451 rho12=0.12 m.b. Dimethyl Sulfoxide 9 vol
7IT065 #300 gMed=394 rho12=0.15 m.b. Dimethyl Sulfoxide 7.5 v
7IT088 #323 gMed=384 rho12=0.13 m.b. Dimethyl Sulfoxide 9 vol
7IT094 #329 gMed=451 rho12=0.11 marine broth
7IT064 #299 gMed=411 rho12=0.08 marine broth
7IT072 #307 gMed=372 rho12=0.11 marine broth
7IT086 #321 gMed=424 rho12=0.13 marine broth
7IT074 #309 gMed=334 rho12=0.10 m.b. Tetracycline 0.025 mg/ml
7IT096 #331 gMed=423 rho12=0.11 m.b. Tetracycline 0.025 mg/ml
7IT073 #308 gMed=319 rho12=0.08 m.b. Tetracycline 0.0125 mg/m
7IT095 #330 gMed=440 rho12=0.10 m.b. Tetracycline 0.0125 mg/m
7IT091 #326 gMed=478 rho12=0.09 m.b. A22 0.04 mg/ml
7IT069 #304 gMed=411 rho12=0.14 m.b. A22 0.04 mg/ml
7IT070 #305 gMed=399 rho12=0.12 m.b. A22 0.08 mg/ml
7IT092 #327 gMed=443 rho12=0.11 m.b. A22 0.08 mg/ml
7IT060 #295 gMed=407 rho12=0.07 m.b. Phosphomycin 2 mg/ml
7IT059 #294 gMed=436 rho12=0.10 m.b. Phosphomycin 1 mg/ml
7IT081 #316 gMed=410 rho12=0.12 m.b. Phosphomycin 1 mg/ml
7IT082 #317 gMed=427 rho12=0.08 m.b. Phosphomycin 2 mg/ml
3H29 #123 gMed=138 rho12=0.11 m.b. Benzalkonium Chloride 0.
7IT057 #292 gMed=411 rho12=0.33 m.b. Benzalkonium Chloride 0.
7IT079 #314 gMed=478 rho12=0.35 m.b. Benzalkonium Chloride 0.
2H32 #78 gMed=476 rho12=0.33 m.b. Benzethonium chloride 0.
6IT037 #272 gMed=331 rho12=0.23 m.b. Benzethonium chloride 0.
6IT047 #282 gMed=388 rho12=0.25 m.b. Benzethonium chloride 0.
8IT003 #334 gMed=444 rho12=0.06 m.b. Carbenicillin 0.004 mg/m
8IT016 #347 gMed=598 rho12=0.06 m.b. Carbenicillin 0.004 mg/m
8IT014 #345 gMed=531 rho12=0.16 m.b. Cholin acetate 153.15 mM
8IT027 #358 gMed=568 rho12=0.14 m.b. Cholin acetate 153.15 mM
8IT011 #342 gMed=488 rho12=0.09 m.b. syringaldehyde 1.25 mM
8IT024 #355 gMed=548 rho12=0.10 m.b. syringaldehyde 1.25 mM
8IT012 #343 gMed=603 rho12=0.06 m.b. syringaldehyde 2.5 mM
8IT025 #356 gMed=600 rho12=0.09 m.b. syringaldehyde 2.5 mM
8IT008 #339 gMed=477 rho12=0.10 m.b. Vanillin 1.25 mM
8IT021 #352 gMed=587 rho12=0.11 m.b. Vanillin 1.25 mM
8IT009 #340 gMed=550 rho12=0.09 m.b. Vanillin 2.5 mM
8IT022 #353 gMed=550 rho12=0.07 m.b. Vanillin 2.5 mM





as.dist(1 − cor(fit$lrn[, as.character(fit$q$name)[use]], use = "p"))
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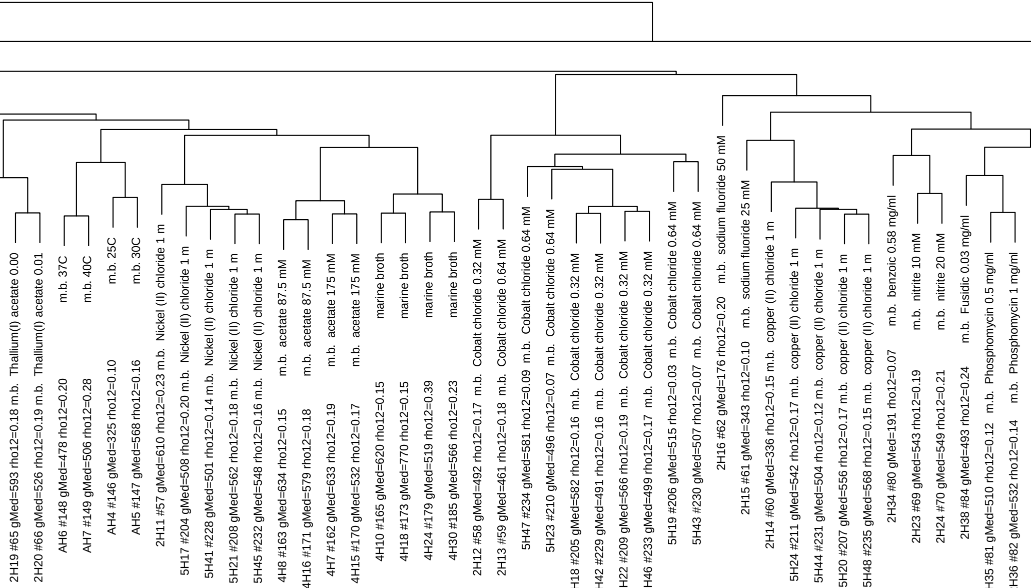
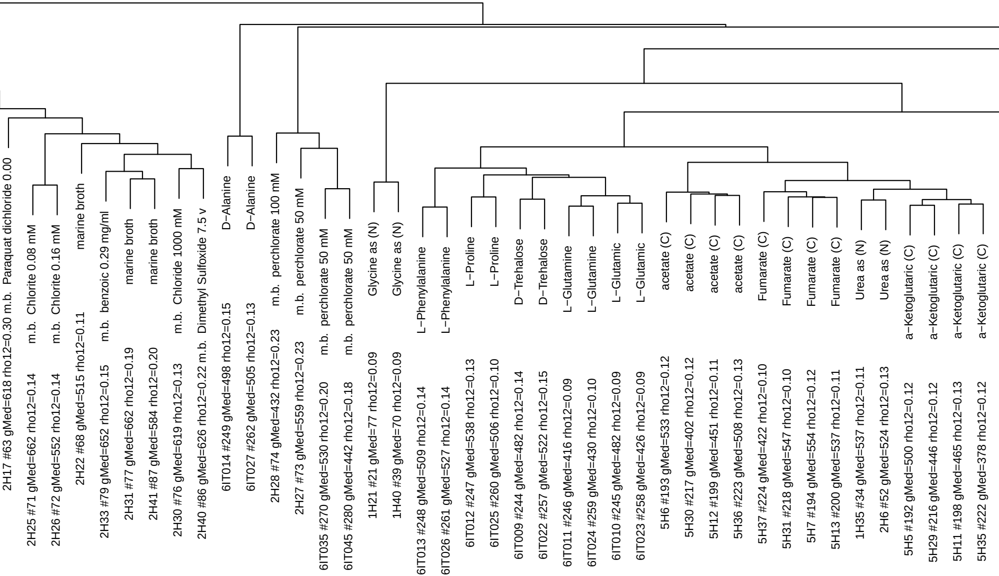
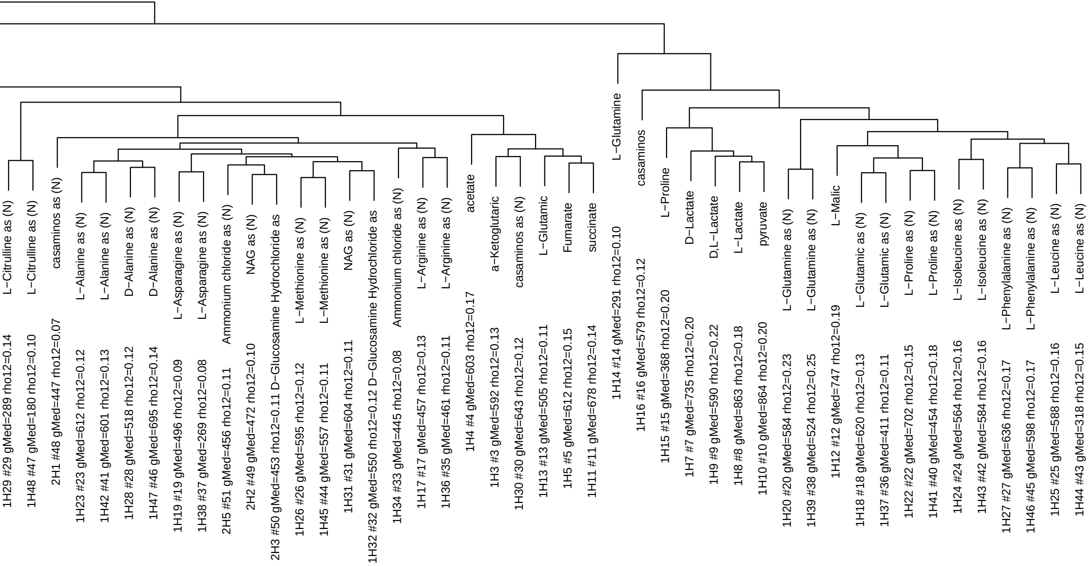

2H19 #65 gMed=593 rho12=0.18 m.b. Thallium(I) acetate 0.00
2H20 #66 gMed=526 rho12=0.19 m.b. Thallium(I) acetate 0.01
AH6 #148 gMed=478 rho12=0.20 m.b. 37C
AH7 #149 gMed=506 rho12=0.28 m.b. 40C
AH4 #146 gMed=325 rho12=0.10 m.b. 25C
AH5 #147 gMed=568 rho12=0.16 m.b. 30C
2H11 #57 gMed=610 rho12=0.23 m.b. Nickel (II) chloride 1 m
5H17 #204 gMed=508 rho12=0.20 m.b. Nickel (II) chloride 1 m
5H41 #228 gMed=501 rho12=0.14 m.b. Nickel (II) chloride 1 m
5H21 #208 gMed=562 rho12=0.18 m.b. Nickel (II) chloride 1 m
5H45 #232 gMed=548 rho12=0.16 m.b. Nickel (II) chloride 1 m
4H8 #163 gMed=634 rho12=0.15 m.b. acetate 87.5 mM
4H16 #171 gMed=579 rho12=0.18 m.b. acetate 87.5 mM
4H7 #162 gMed=633 rho12=0.19 m.b. acetate 175 mM
4H15 #170 gMed=532 rho12=0.17 m.b. acetate 175 mM
4H10 #165 gMed=620 rho12=0.15 marine broth
4H18 #173 gMed=770 rho12=0.15 marine broth
4H24 #179 gMed=519 rho12=0.39 marine broth
4H30 #185 gMed=566 rho12=0.23 marine broth
2H12 #58 gMed=492 rho12=0.17 m.b. Cobalt chloride 0.32 mM
2H13 #59 gMed=461 rho12=0.18 m.b. Cobalt chloride 0.64 mM
5H47 #234 gMed=581 rho12=0.09 m.b. Cobalt chloride 0.64 mM
5H23 #210 gMed=496 rho12=0.07 m.b. Cobalt chloride 0.64 mM
5H18 #205 gMed=582 rho12=0.16 m.b. Cobalt chloride 0.32 mM
5H42 #229 gMed=491 rho12=0.16 m.b. Cobalt chloride 0.32 mM
5H22 #209 gMed=566 rho12=0.19 m.b. Cobalt chloride 0.32 mM
5H46 #233 gMed=499 rho12=0.17 m.b. Cobalt chloride 0.32 mM
5H19 #206 gMed=515 rho12=0.03 m.b. Cobalt chloride 0.64 mM
5H43 #230 gMed=507 rho12=0.07 m.b. Cobalt chloride 0.64 mM
2H16 #62 gMed=176 rho12=0.20 m.b. sodium fluoride 50 mM
2H15 #61 gMed=343 rho12=0.10 m.b. sodium fluoride 25 mM
2H14 #60 gMed=336 rho12=0.15 m.b. copper (II) chloride 1 m
5H24 #211 gMed=542 rho12=0.17 m.b. copper (II) chloride 1 m
5H44 #231 gMed=504 rho12=0.12 m.b. copper (II) chloride 1 m
5H20 #207 gMed=556 rho12=0.17 m.b. copper (II) chloride 1 m
5H48 #235 gMed=568 rho12=0.15 m.b. copper (II) chloride 1 m
2H34 #80 gMed=191 rho12=0.07 m.b. benzoic 0.58 mg/ml
2H23 #69 gMed=543 rho12=0.19 m.b. nitrite 10 mM
2H24 #70 gMed=549 rho12=0.21 m.b. nitrite 20 mM
2H38 #84 gMed=493 rho12=0.24 m.b. Fusidic 0.03 mg/ml
2H35 #81 gMed=510 rho12=0.12 m.b. Phosphomycin 0.5 mg/ml
2H36 #82 gMed=532 rho12=0.14 m.b. Phosphomycin 1 mg/ml


2H17 #63 gMed=618 rho12=0.30 m.b. Paraquat dichloride 0.00
2H25 #71 gMed=662 rho12=0.14 m.b. Chlorite 0.08 mM
2H26 #72 gMed=552 rho12=0.14 m.b. Chlorite 0.16 mM
2H22 #68 gMed=515 rho12=0.11 marine broth
2H33 #79 gMed=652 rho12=0.15 m.b. benzoic 0.29 mg/ml
2H31 #77 gMed=662 rho12=0.19 marine broth
2H41 #87 gMed=584 rho12=0.20 marine broth
2H30 #76 gMed=619 rho12=0.13 m.b. Chloride 1000 mM
2H40 #86 gMed=626 rho12=0.22 m.b. Dimethyl Sulfoxide 7.5 v
6IT014 #249 gMed=498 rho12=0.15 D−Alanine
6IT027 #262 gMed=505 rho12=0.13 D−Alanine
2H28 #74 gMed=432 rho12=0.23 m.b. perchlorate 100 mM
2H27 #73 gMed=559 rho12=0.23 m.b. perchlorate 50 mM
6IT035 #270 gMed=530 rho12=0.20 m.b. perchlorate 50 mM
6IT045 #280 gMed=442 rho12=0.18 m.b. perchlorate 50 mM
1H21 #21 gMed=77 rho12=0.09 Glycine as (N)
1H40 #39 gMed=70 rho12=0.09 Glycine as (N)
6IT013 #248 gMed=509 rho12=0.14 L−Phenylalanine
6IT026 #261 gMed=527 rho12=0.14 L−Phenylalanine
6IT012 #247 gMed=538 rho12=0.13 L−Proline
6IT025 #260 gMed=506 rho12=0.10 L−Proline
6IT009 #244 gMed=482 rho12=0.14 D−Trehalose
6IT022 #257 gMed=522 rho12=0.15 D−Trehalose
6IT011 #246 gMed=416 rho12=0.09 L−Glutamine
6IT024 #259 gMed=430 rho12=0.10 L−Glutamine
6IT010 #245 gMed=482 rho12=0.09 L−Glutamic
6IT023 #258 gMed=426 rho12=0.09 L−Glutamic
5H6 #193 gMed=533 rho12=0.12 acetate (C)
5H30 #217 gMed=402 rho12=0.12 acetate (C)
5H12 #199 gMed=451 rho12=0.11 acetate (C)
5H36 #223 gMed=508 rho12=0.13 acetate (C)
5H37 #224 gMed=422 rho12=0.10 Fumarate (C)
5H31 #218 gMed=547 rho12=0.10 Fumarate (C)
5H7 #194 gMed=554 rho12=0.12 Fumarate (C)
5H13 #200 gMed=537 rho12=0.11 Fumarate (C)
1H35 #34 gMed=537 rho12=0.11 Urea as (N)
2H6 #52 gMed=524 rho12=0.13 Urea as (N)
5H5 #192 gMed=500 rho12=0.12 a−Ketoglutaric (C)
5H29 #216 gMed=446 rho12=0.12 a−Ketoglutaric (C)
5H11 #198 gMed=465 rho12=0.13 a−Ketoglutaric (C)
5H35 #222 gMed=378 rho12=0.12 a−Ketoglutaric (C)


L−Citrulline as (N)
1H29 #29 gMed=289 rho12=0.14
L−Citrulline as (N)
1H48 #47 gMed=180 rho12=0.10
casaminos as (N)
2H1 #48 gMed=447 rho12=0.07
L−Alanine as (N)
1H23 #23 gMed=612 rho12=0.12
L−Alanine as (N)
1H42 #41 gMed=601 rho12=0.13
D−Alanine as (N)
1H28 #28 gMed=518 rho12=0.12
D−Alanine as (N)
1H47 #46 gMed=695 rho12=0.14
L−Asparagine as (N)
1H19 #19 gMed=496 rho12=0.09
L−Asparagine as (N)
1H38 #37 gMed=269 rho12=0.08
Ammonium chloride as (N)
2H5 #51 gMed=456 rho12=0.11
NAG as (N)
2H2 #49 gMed=472 rho12=0.10
2H3 #50 gMed=453 rho12=0.11 D−Glucosamine Hydrochloride as
L−Methionine as (N)
1H26 #26 gMed=595 rho12=0.12
L−Methionine as (N)
1H45 #44 gMed=557 rho12=0.11
NAG as (N)
1H31 #31 gMed=604 rho12=0.11
1H32 #32 gMed=550 rho12=0.12 D−Glucosamine Hydrochloride as
Ammonium chloride as (N)
1H34 #33 gMed=445 rho12=0.08
L−Arginine as (N)
1H17 #17 gMed=457 rho12=0.13
L−Arginine as (N)
1H36 #35 gMed=461 rho12=0.11
acetate
1H4 #4 gMed=603 rho12=0.17
a−Ketoglutaric
1H3 #3 gMed=592 rho12=0.13
casaminos as (N)
1H30 #30 gMed=643 rho12=0.12
L−Glutamic
1H13 #13 gMed=505 rho12=0.11
Fumarate
1H5 #5 gMed=612 rho12=0.15
succinate
1H11 #11 gMed=678 rho12=0.14
L−Glutamine
1H14 #14 gMed=291 rho12=0.10
casaminos
1H16 #16 gMed=579 rho12=0.12
L−Proline
1H15 #15 gMed=368 rho12=0.20
D−Lactate
1H7 #7 gMed=735 rho12=0.20
D,L−Lactate
1H9 #9 gMed=590 rho12=0.22
L−Lactate
1H8 #8 gMed=863 rho12=0.18
pyruvate
1H10 #10 gMed=864 rho12=0.20
L−Glutamine as (N)
1H20 #20 gMed=584 rho12=0.23
L−Glutamine as (N)
1H39 #38 gMed=524 rho12=0.25
L−Malic
1H12 #12 gMed=747 rho12=0.19
L−Glutamic as (N)
1H18 #18 gMed=620 rho12=0.13
L−Glutamic as (N)
1H37 #36 gMed=411 rho12=0.11
L−Proline as (N)
1H22 #22 gMed=702 rho12=0.15
L−Proline as (N)
1H41 #40 gMed=454 rho12=0.18
L−Isoleucine as (N)
1H24 #24 gMed=564 rho12=0.16
L−Isoleucine as (N)
1H43 #42 gMed=584 rho12=0.16
L−Phenylalanine as (N)
1H27 #27 gMed=636 rho12=0.17
L−Phenylalanine as (N)
1H46 #45 gMed=598 rho12=0.17
L−Leucine as (N)
1H25 #25 gMed=588 rho12=0.16
L−Leucine as (N)
1H44 #43 gMed=318 rho12=0.15