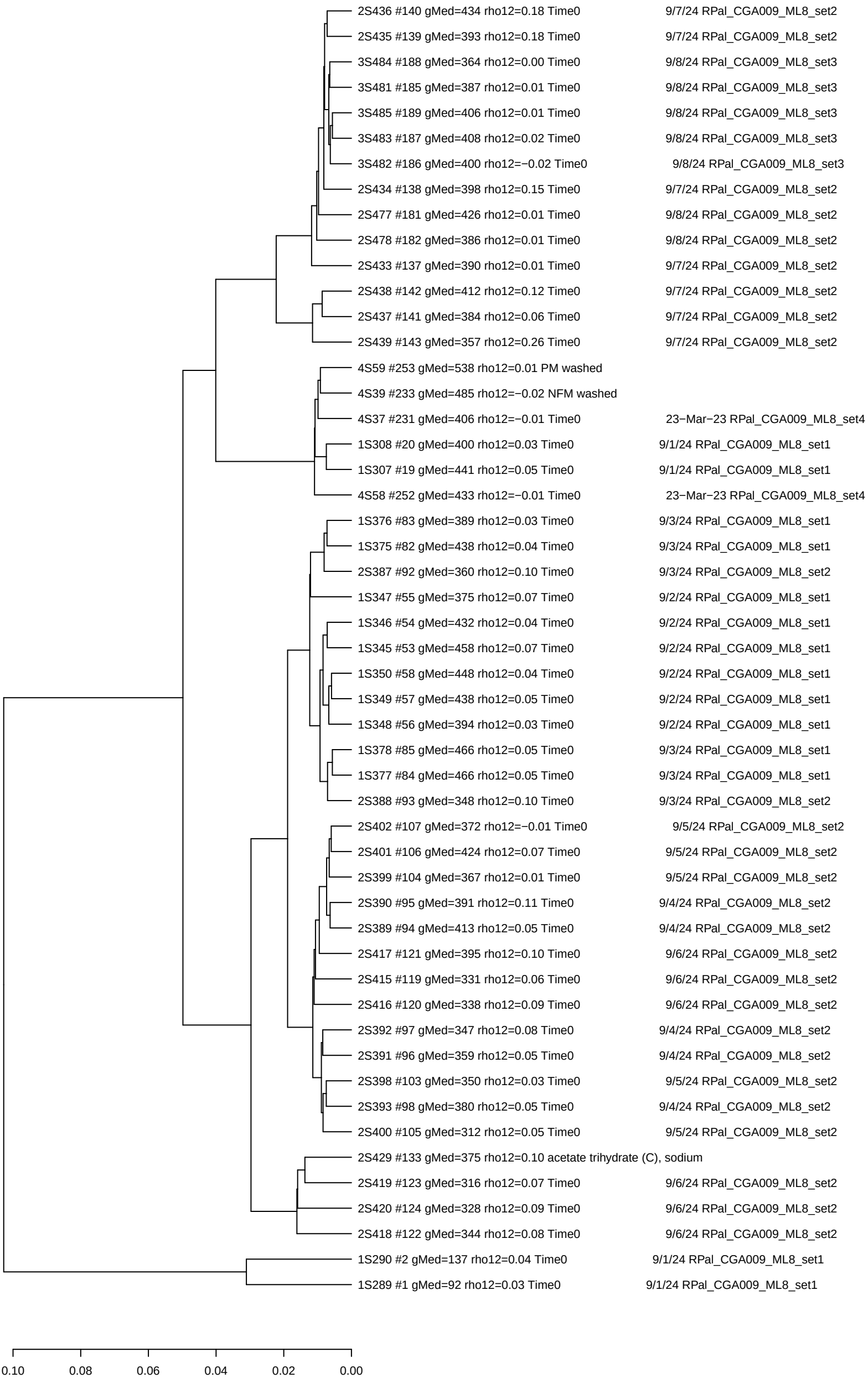
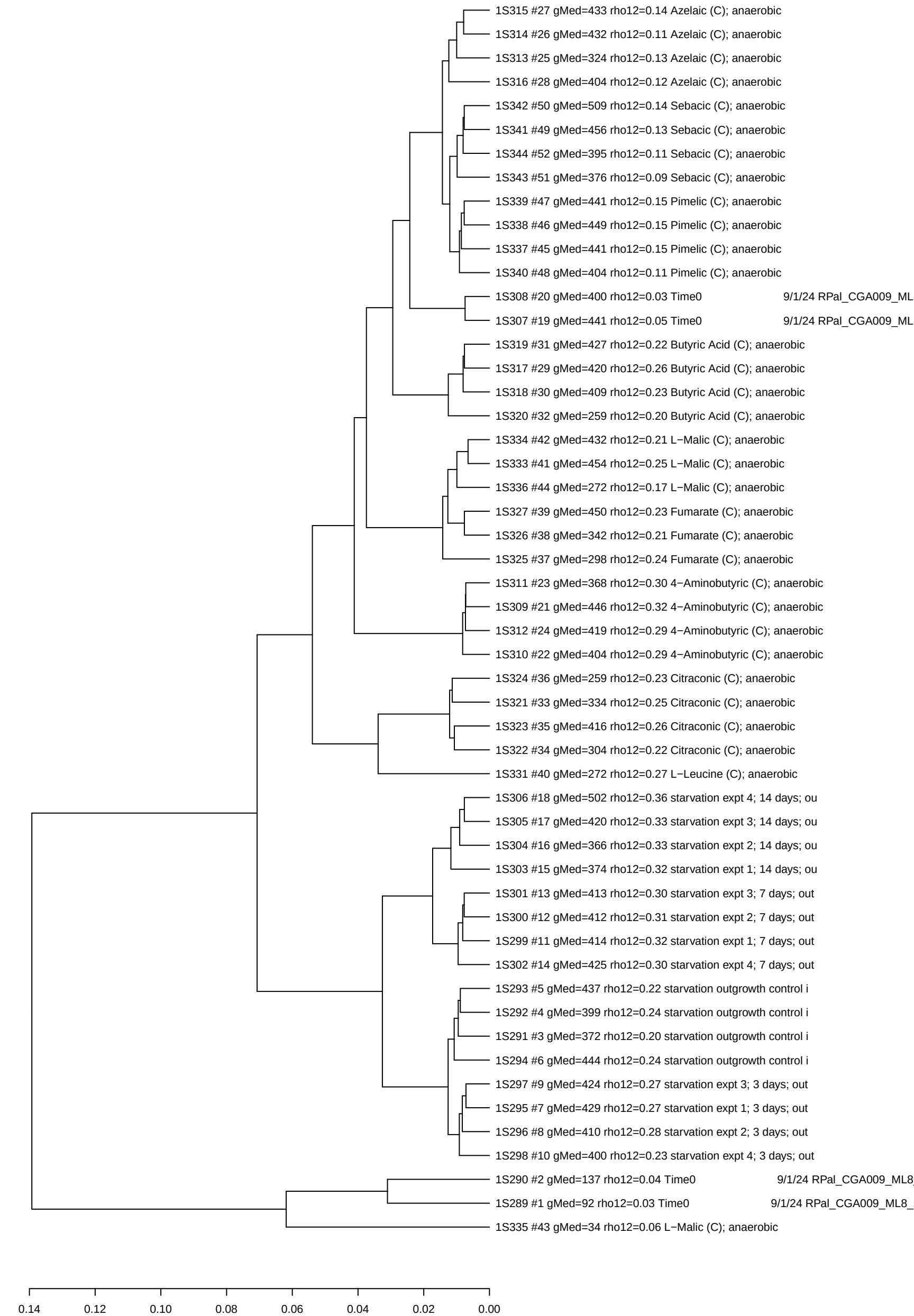
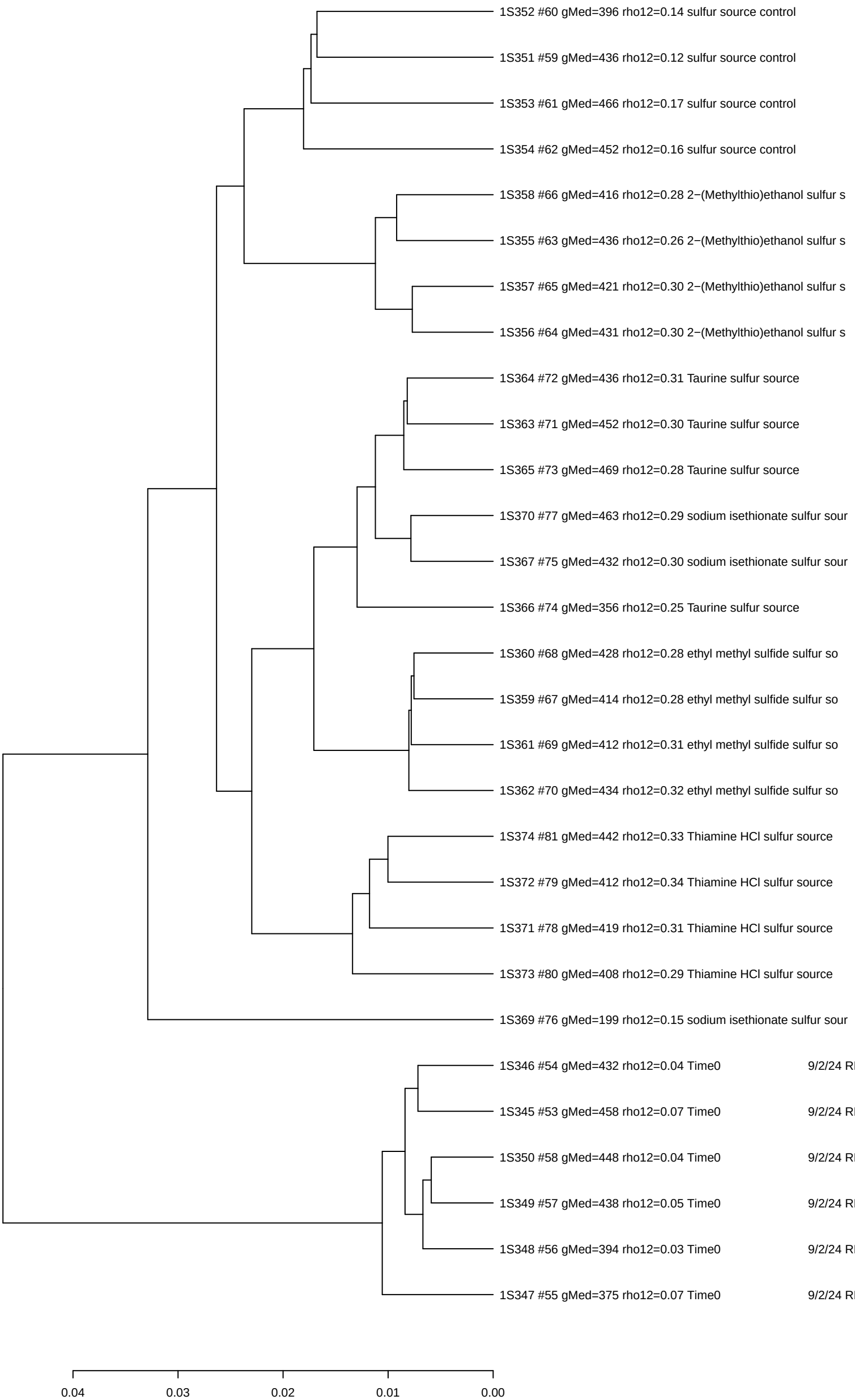
**Time0 and similar samples (clustered by log−count)**



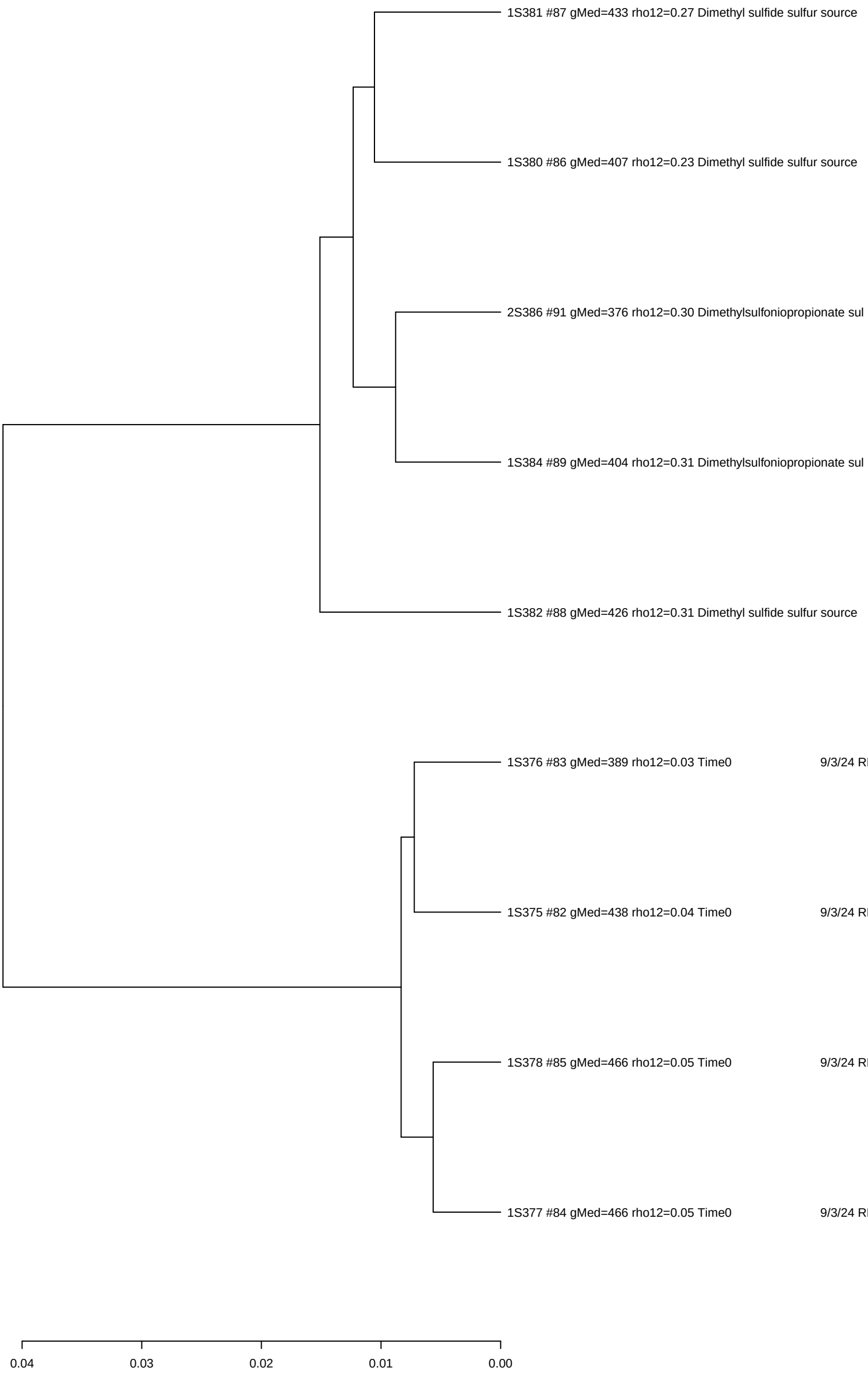
**9/1/24 RPal_CGA009_ML8_set1 and similar samples (clustered by log−count)**



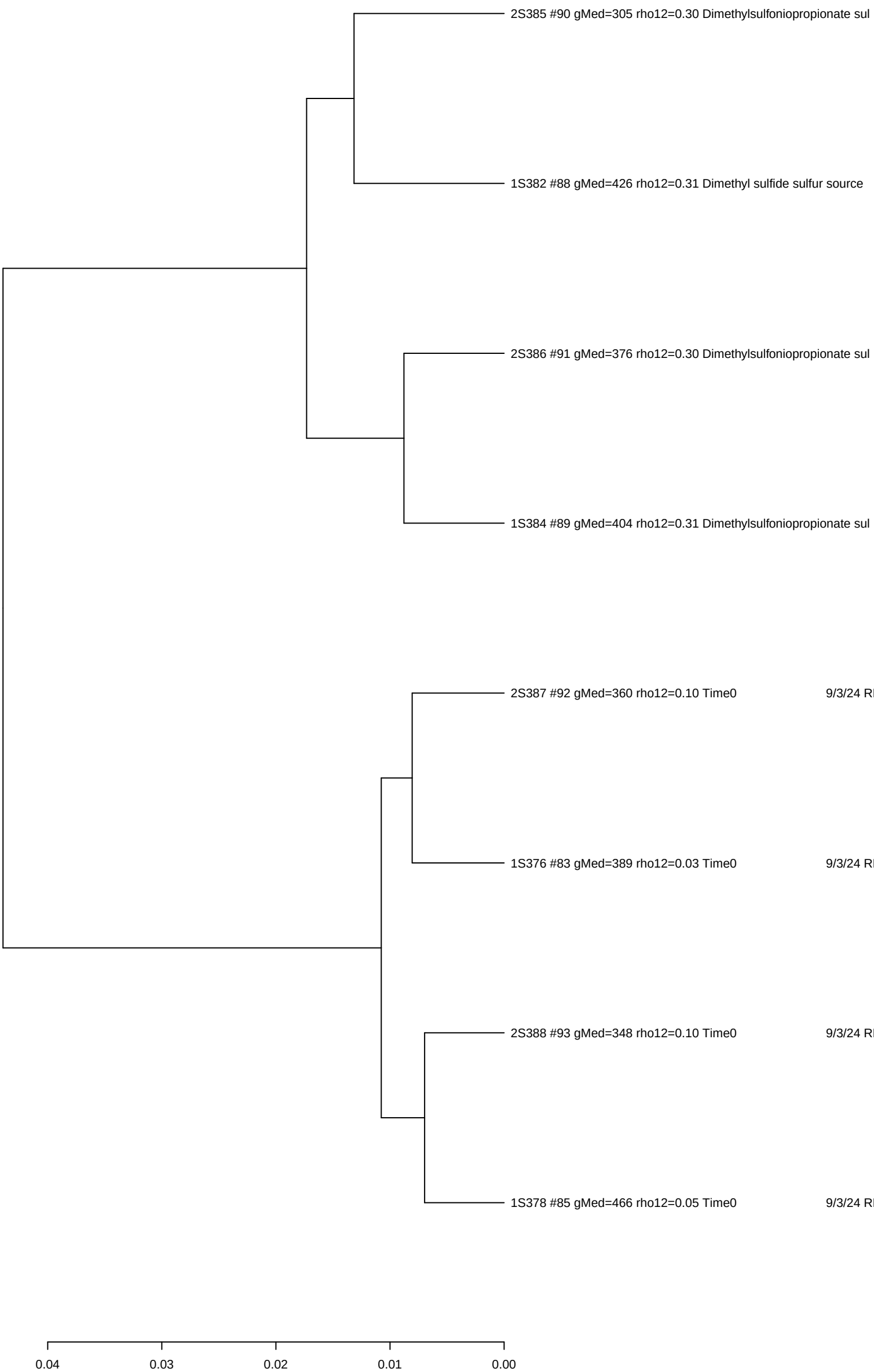
**9/2/24 RPal_CGA009_ML8_set1 and similar samples (clustered by log−count)**



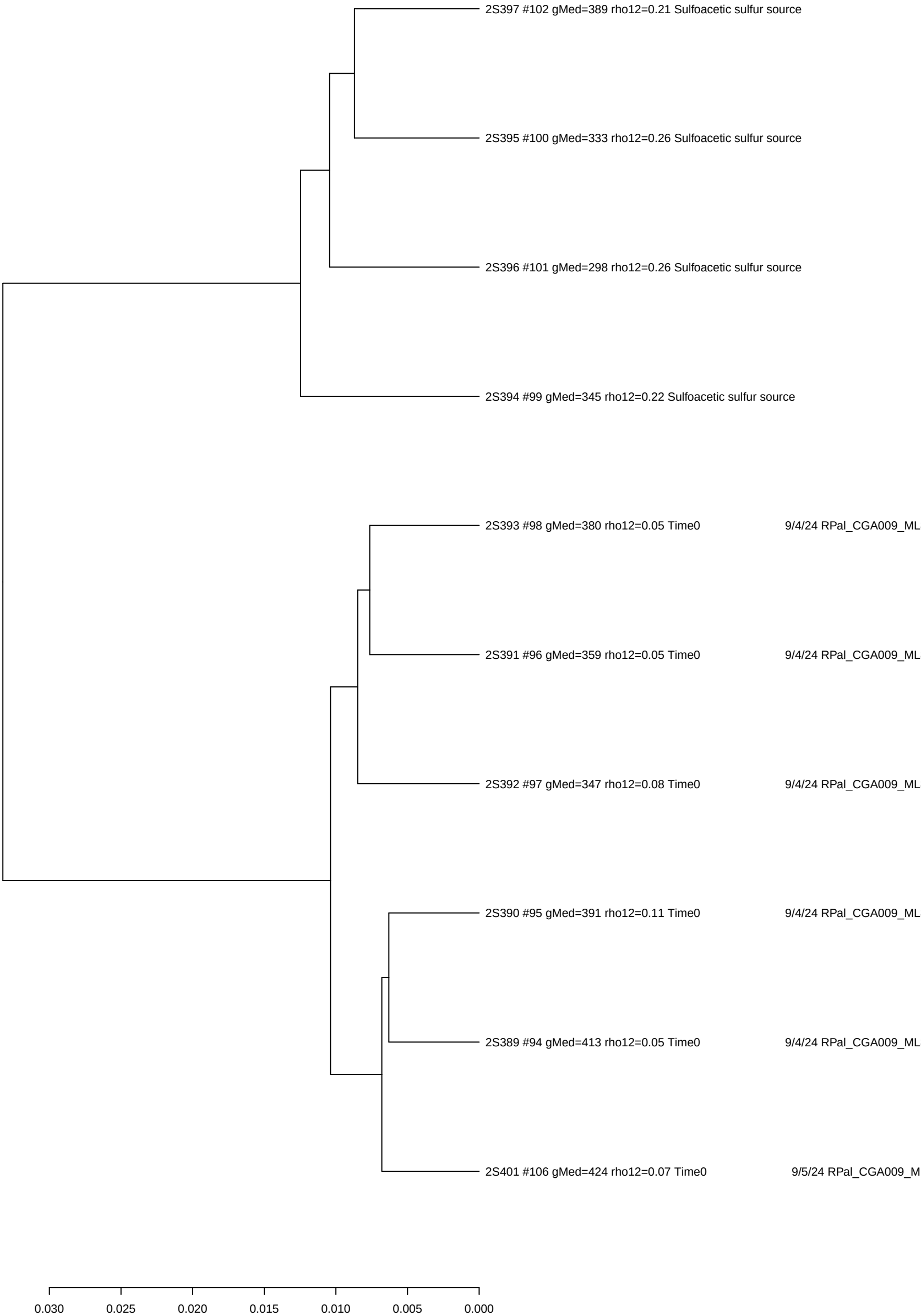
**9/3/24 RPal_CGA009_ML8_set1 and similar samples (clustered by log−count)**



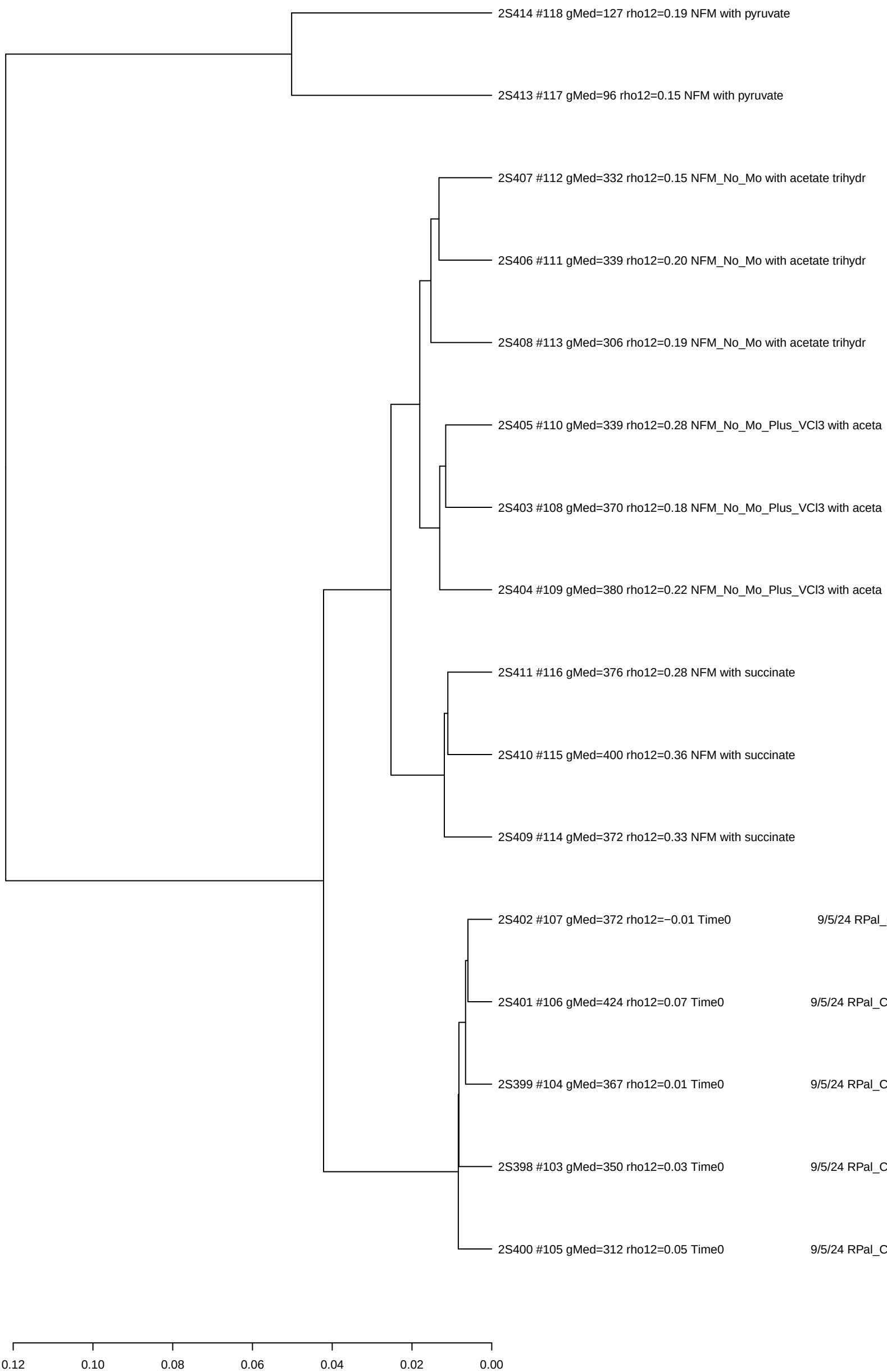
**9/3/24 RPal_CGA009_ML8_set2 and similar samples (clustered by log−count)**



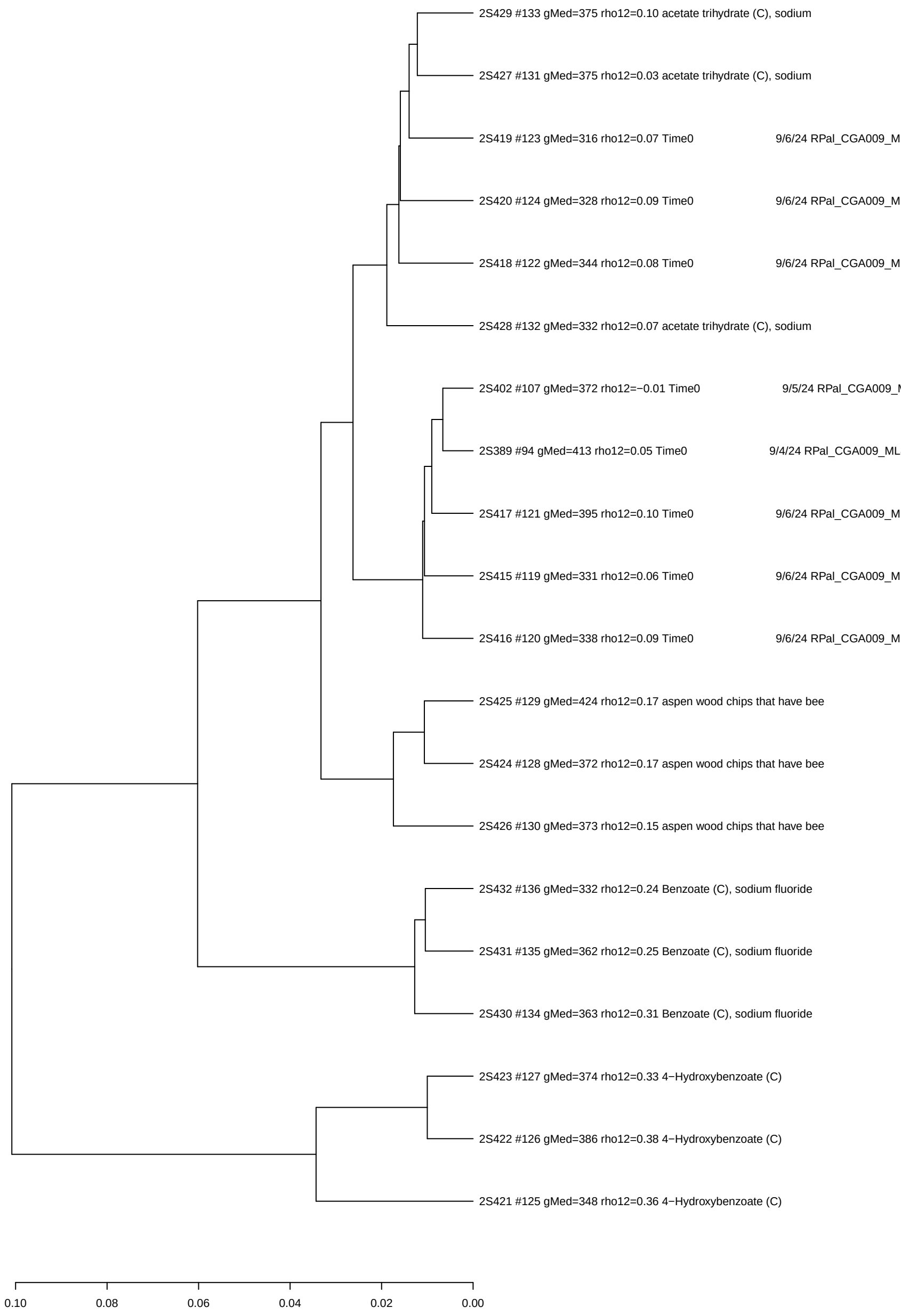
**9/4/24 RPal_CGA009_ML8_set2 and similar samples (clustered by log−count)**



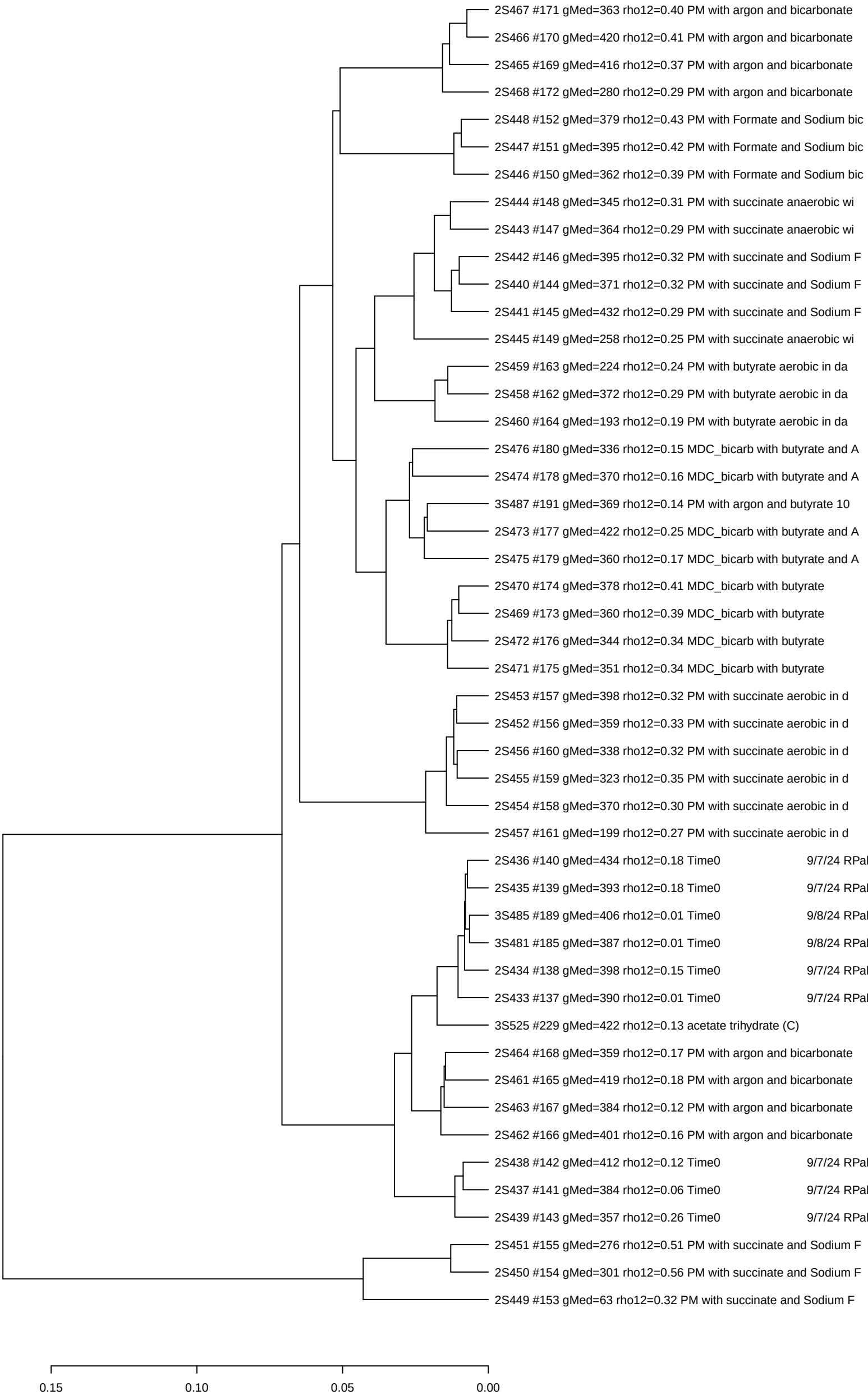
**9/5/24 RPal_CGA009_ML8_set2 and similar samples (clustered by log−count)**



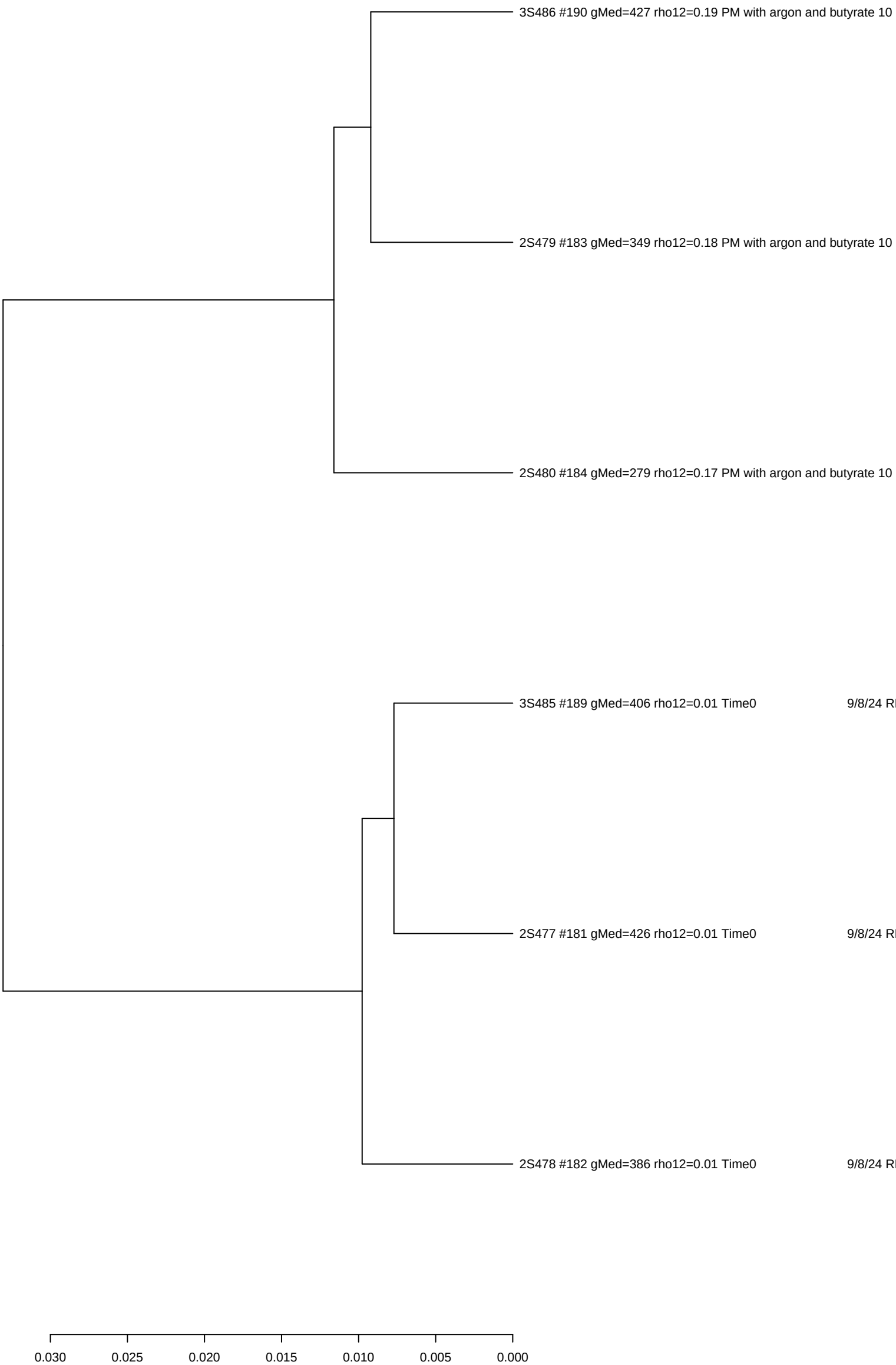
**9/6/24 RPal_CGA009_ML8_set2 and similar samples (clustered by log−count)**



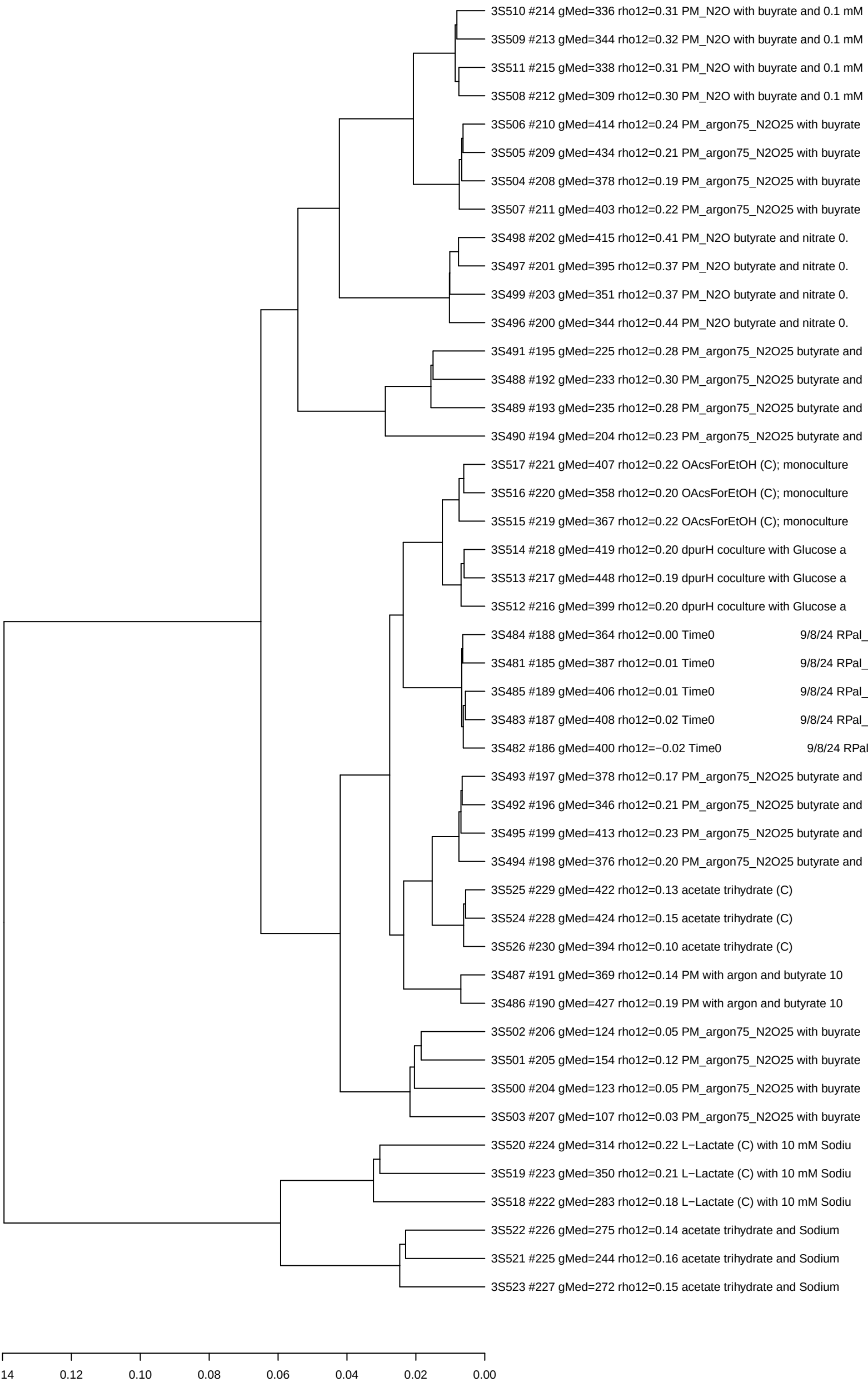
**9/7/24 RPal_CGA009_ML8_set2 and similar samples (clustered by log−count)**



**9/8/24 RPal_CGA009_ML8_set2 and similar samples (clustered by log−count)**



**9/8/24 RPal_CGA009_ML8_set3 and similar samples (clustered by log−count)**



**23−Mar−23 RPal_CGA009_ML8_set4 and similar samples (clustered by log−count)**

4S54 #248 gMed=467 rho12=0.31 PM with 4−Hydroxybenzoic Acid
4S53 #247 gMed=452 rho12=0.30 PM with 4−Hydroxybenzoic Acid
4S75 #268 gMed=434 rho12=0.32 PM with 4−Hydroxybenzoic Acid
4S73 #266 gMed=463 rho12=0.30 PM with 4−Hydroxybenzoic Acid
4S74 #267 gMed=480 rho12=0.29 PM with 4−Hydroxybenzoic Acid
4S52 #246 gMed=352 rho12=0.29 PM with 4−Hydroxybenzoic Acid
4S71 #264 gMed=494 rho12=0.34 PM with p−Coumaric (C)
4S51 #245 gMed=402 rho12=0.33 PM with p−Coumaric (C)
4S50 #244 gMed=437 rho12=0.33 PM with p−Coumaric (C)
4S72 #265 gMed=376 rho12=0.34 PM with p−Coumaric (C)
4S70 #263 gMed=426 rho12=0.35 PM with p−Coumaric (C)
4S49 #243 gMed=458 rho12=0.35 PM with p−Coumaric (C)
4S77 #270 gMed=480 rho12=0.12 NFM with acetate (C)
4S57 #251 gMed=462 rho12=0.12 NFM with acetate (C)
4S55 #249 gMed=360 rho12=0.09 NFM with acetate (C)
4S76 #269 gMed=428 rho12=0.11 NFM with acetate (C)
4S56 #250 gMed=438 rho12=0.08 NFM with acetate (C)
4S59 #253 gMed=538 rho12=0.01 PM washed
4S39 #233 gMed=485 rho12=−0.02 NFM washed
4S38 #232 gMed=415 rho12=−0.01 PM washed
4S37 #231 gMed=406 rho12=−0.01 Time0 23−Mar−23 RPal_CGA00
4S58 #252 gMed=433 rho12=−0.01 Time0 23−Mar−23 RPal_CGA00
4S63 #256 gMed=524 rho12=0.12 PM with acetate (C)
4S41 #235 gMed=424 rho12=0.11 PM with acetate (C)
4S40 #234 gMed=502 rho12=0.14 PM with acetate (C)
4S62 #255 gMed=430 rho12=0.13 PM with acetate (C)
4S42 #236 gMed=366 rho12=0.11 PM with acetate (C)
4S61 #254 gMed=391 rho12=0.11 PM with acetate (C)
4S64 #257 gMed=478 rho12=0.16 PM with succinate (C)
4S43 #237 gMed=459 rho12=0.18 PM with succinate (C)
4S65 #258 gMed=465 rho12=0.16 PM with succinate (C)
4S44 #238 gMed=481 rho12=0.18 PM with succinate (C)
4S66 #259 gMed=418 rho12=0.14 PM with succinate (C)
4S45 #239 gMed=488 rho12=0.14 PM with succinate (C)
4S69 #262 gMed=468 rho12=0.21 PM with benzoic (C)
4S46 #240 gMed=436 rho12=0.20 PM with benzoic (C)
4S48 #242 gMed=386 rho12=0.18 PM with benzoic (C)
4S67 #260 gMed=386 rho12=0.19 PM with benzoic (C)
4S47 #241 gMed=453 rho12=0.23 PM with benzoic (C)
4S68 #261 gMed=373 rho12=0.19 PM with benzoic (C)

