Similarity clustering ../run 2.1/Final/M00000328 FIT.sdf ../run 4.0/Final/M00000145 FIT.sdf ../run_3.0/Final/M00000207_FIT.sdf ../run_3.0/Final/M00000240_FIT.sdf ../run_3.0/Final/M00000238_FIT.sdf ../run_4.0/Final/M00000180_FIT.sdf ../run_4.1/Final/M00000205_FIT.sdf ../run_4.1/Final/M00000231_FIT.sdf ../run_4.1/Final/M00000217_FIT.sdf ../run 2.2/Final/M00000092 FIT.sdf ../run_2.2/Final/M00000085_FIT.sdf ../run 2.2/Final/M00000200 FIT.sdf ../run_2.2/Final/M00000190 FIT.sdf ../run_2.2/Final/M00000144_FIT.sdf ../run_2.2/Final/M00000097_FIT.sdf ../run_2.1/Final/M00000263_FIT.sdf ../run_2.1/Final/M00000301_FIT.sdf ../run_2.2/Final/M00000113 FIT.sdf ../run 2.2/Final/M00000099 FIT.sdf ../run_2.2/Final/M00000087_FIT.sdf ../run_2.1/Final/M00000267_FIT.sdf ../run_2.1/Final/M00000245_FIT.sdf ../run_2.2/Final/M00000046 FIT.sdf ../run_2.1/Final/M00000309 FIT.sdf ../run_2.1/Final/M00000298_FIT.sdf ../run 2.1/Final/M00000259 FIT.sdf ../run_2.1/Final/M00000308_FIT.sdf ../run 2.2/Final/M00000160 FIT.sdf ../run_2.2/Final/M00000174 FIT.sdf ../run_2.2/Final/M00000105_FIT.sdf ../run_2.2/Final/M00000141_FIT.sdf ../run_2.2/Final/M00000202_FIT.sdf ../run_4.0/Final/M00000214 FIT.sdf ../run_2.1/Final/M00000182_FIT.sdf ../run_2.1/Final/M00000258_FIT.sdf ../run_2.1/Final/M00000253_FIT.sdf ../run_2.1/Final/M00000178_FIT.sdf ../run 2.2/Final/M00000180 FIT.sdf ../run_2.1/Final/M00000193_FIT.sdf ../run_2.1/Final/M00000275_FIT.sdf ../run_2.1/Final/M00000243_FIT.sdf ../run_2.1/Final/M00000157_FIT.sdf ../run_2.1/Final/M00000201_FIT.sdf ../run_2.1/Final/M00000284_FIT.sdf ../run_2.1/Final/M00000322_FIT.sdf ../run_2.1/Final/M00000257_FIT.sdf ../run_2.1/Final/M00000295_FIT.sdf ../run 2.2/Final/M00000183 FIT.sdf ../run 2.2/Final/M00000101_FIT.sdf ../run_2.1/Final/M00000116_FIT.sdf ../run 2.1/Final/M00000107 FIT.sdf ../run_4.1/Final/M00000075_FIT.sdf ../run 4.0/Final/M00000217 FIT.sdf ../run 4.0/Final/M00000200_FIT.sdf ../run_2.1/Final/M00000292_FIT.sdf ../run_4.0/Final/M00000097_FIT.sdf ../run 4.0/Final/M00000174 FIT.sdf ../run_4.0/Final/M00000137_FIT.sdf ../run_4.0/Final/M00000222 FIT.sdf ../run 4.0/Final/M00000216 FIT.sdf ../run_2.0/Final/M00000482_FIT.sdf ../run_2.0/Final/M00000512_FIT.sdf ../run_2.0/Final/M00000386_FIT.sdf ../run 2.0/Final/M00000217 FIT.sdf ../run_2.0/Final/M00000181 FIT.sdf ../run_1.1/Final/M00000254_FIT.sdf ../run_2.0/Final/M00000459_FIT.sdf ../run_2.0/Final/M00000362_FIT.sdf ../run 1.1/Final/M00000332 FIT.sdf ../run_2.0/Final/M00000410_FIT.sdf ../run_2.0/Final/M00000317_FIT.sdf ../run_2.0/Final/M00000285_FIT.sdf ../run_2.0/Final/M00000167_FIT.sdf ../run 1.1/Final/M00000299 FIT.sdf ../run 1.1/Final/M00000267 FIT.sdf ../run_2.0/Final/M00000179_FIT.sdf ../run_1.1/Final/M00000274_FIT.sdf ../run_2.0/Final/M00000340_FIT.sdf ../run_1.1/Final/M00000359_FIT.sdf ../run 1.1/Final/M00000318 FIT.sdf ../run_1.1/Final/M00000288 FIT.sdf ../run 1.1/Final/M00000320 FIT.sdf ../run_1.1/Final/M00000302_FIT.sdf ../run 1.1/Final/M00000297 FIT.sdf ../run 1.1/Final/M00000289 FIT.sdf ../run_1.1/Final/M00000310_FIT.sdf ../run_1.1/Final/M00000300_FIT.sdf ../run_1.1/Final/M00000281_FIT.sdf ../run_2.0/Final/M00000545_FIT.sdf ../run_1.1/Final/M00000330 FIT.sdf ./run_2.0/Final/M00000407_FIT.sdf ../run_2.0/Final/M00000472_FIT.sdf ../run_1.1/Final/M00000370_FIT.sdf ../run_1.1/Final/M00000381_FIT.sdf ../run_2.0/Final/M00000258 FIT.sdf ../run_2.0/Final/M00000228 FIT.sdf ../run_1.1/Final/M00000401_FIT.sdf ../run 1.1/Final/M00000369 FIT.sdf ../run 1.1/Final/M00000306 FIT.sdf ../run_2.0/Final/M00000370 FIT.sdf ../run_1.1/Final/M00000340 FIT.sdf ../run_1.1/Final/M00000341_FIT.sdf ../run 1.1/Final/M00000405 FIT.sdf ../run 4.1/Final/M00000200 FIT.sdf ../run_1.1/Final/M00000406 FIT.sdf ../run_2.0/Final/M00000214 FIT.sdf ../run_2.0/Final/M00000306_FIT.sdf 1.4 1.2 1.0 8.0 0.6 0.4 0.2 0.0