

Stats

min ESS = 16.2728105972009

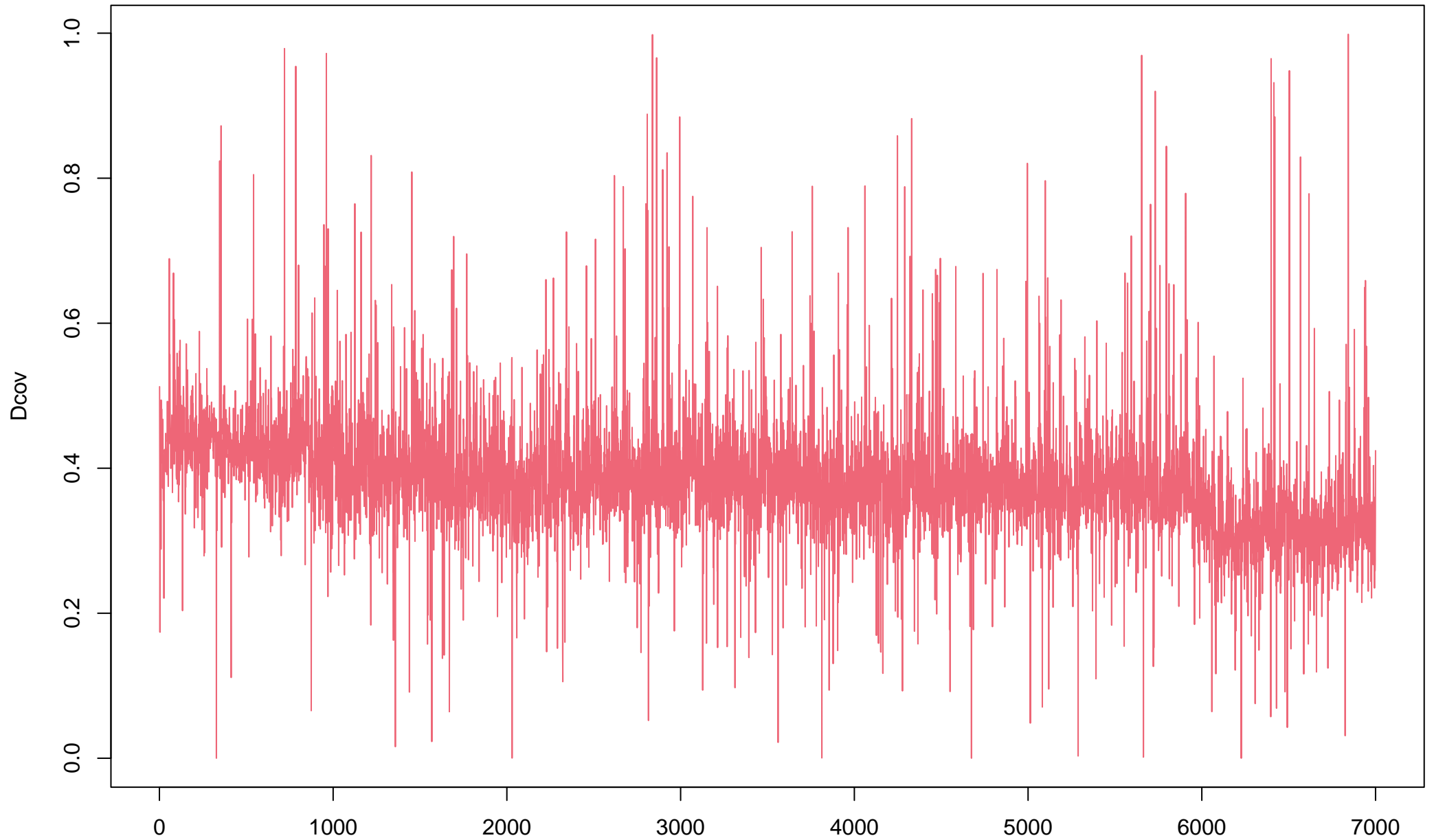
max BMK = 0.461461173474968

max MCSE = 3.25958509591864

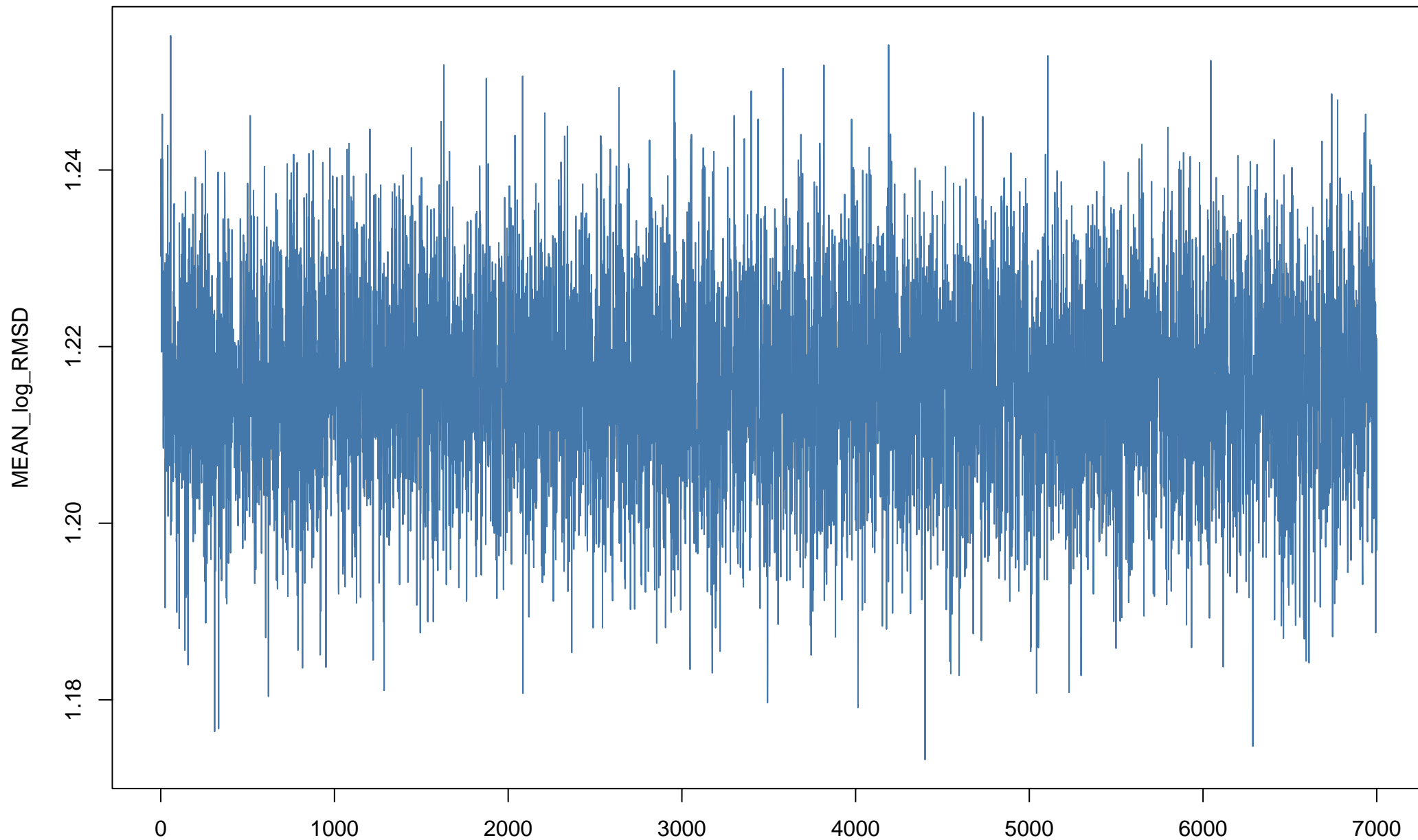
all stationary: FALSE

1:2

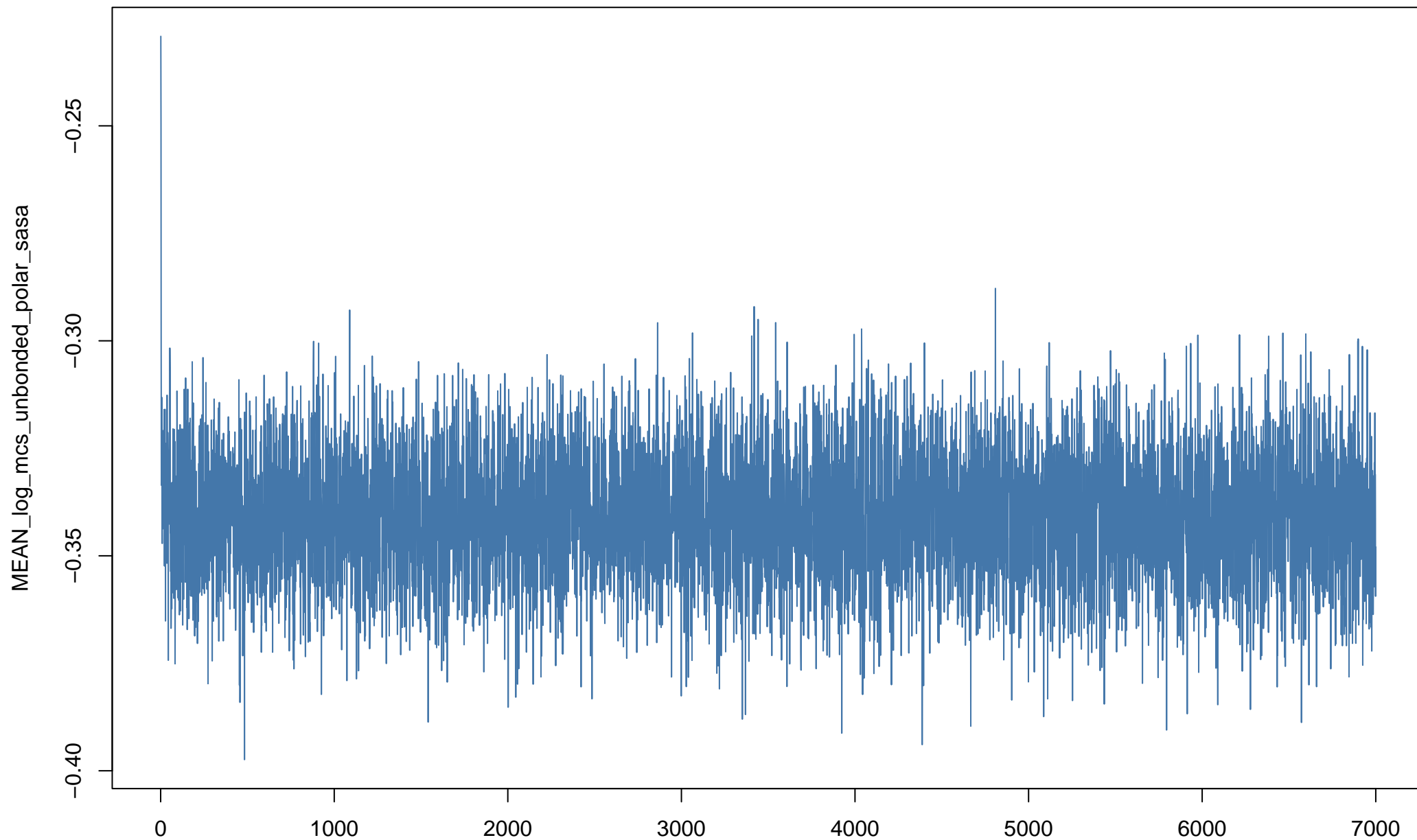
Dcov
ESS = 164 | BMK = 0.262 | MCSE(6.27) = 0.401 | stat: FALSE



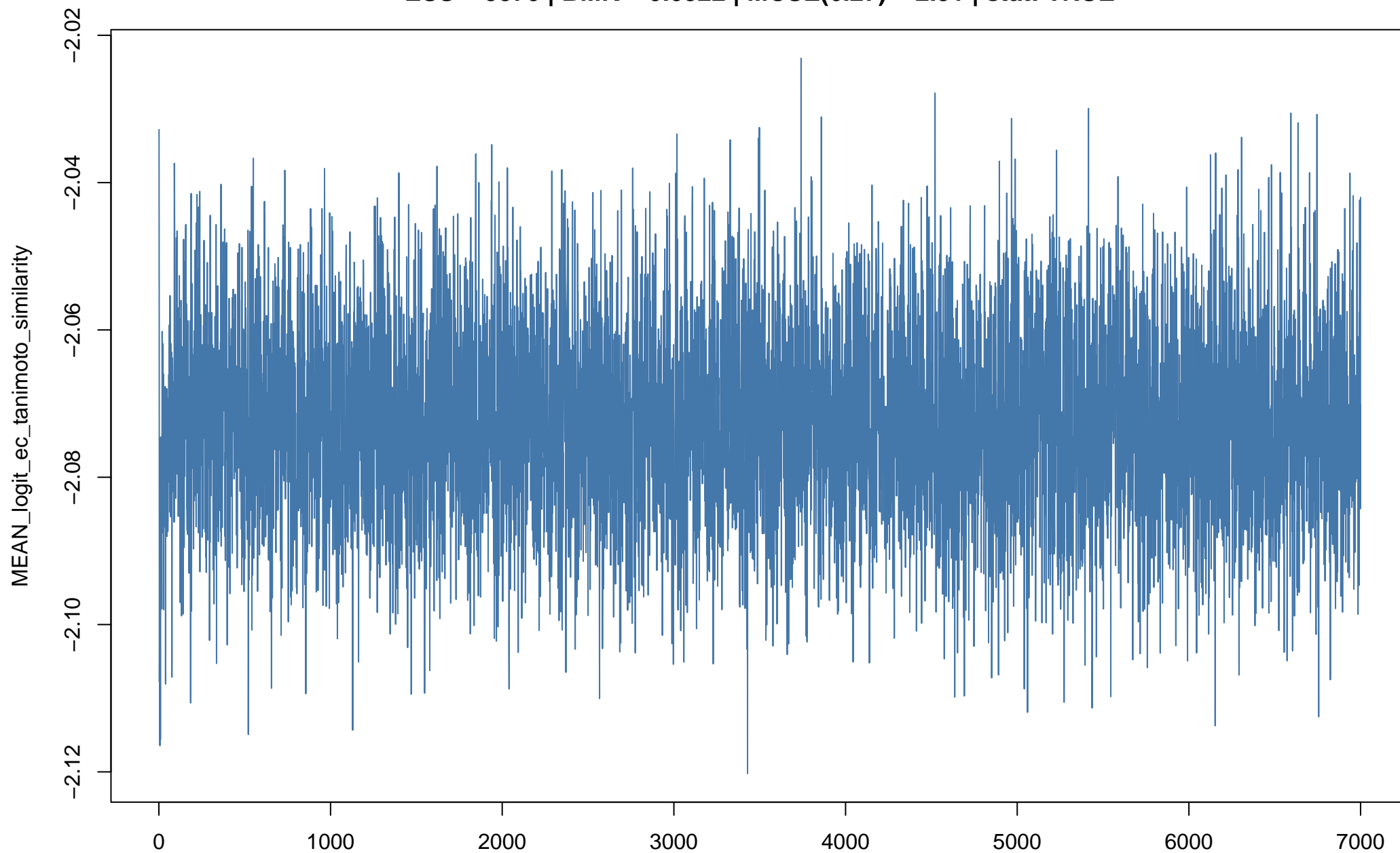
MEAN_log_RMSD
ESS = 5960 | BMK = 0.0276 | MCSE(6.27) = 2.88 | stat: TRUE



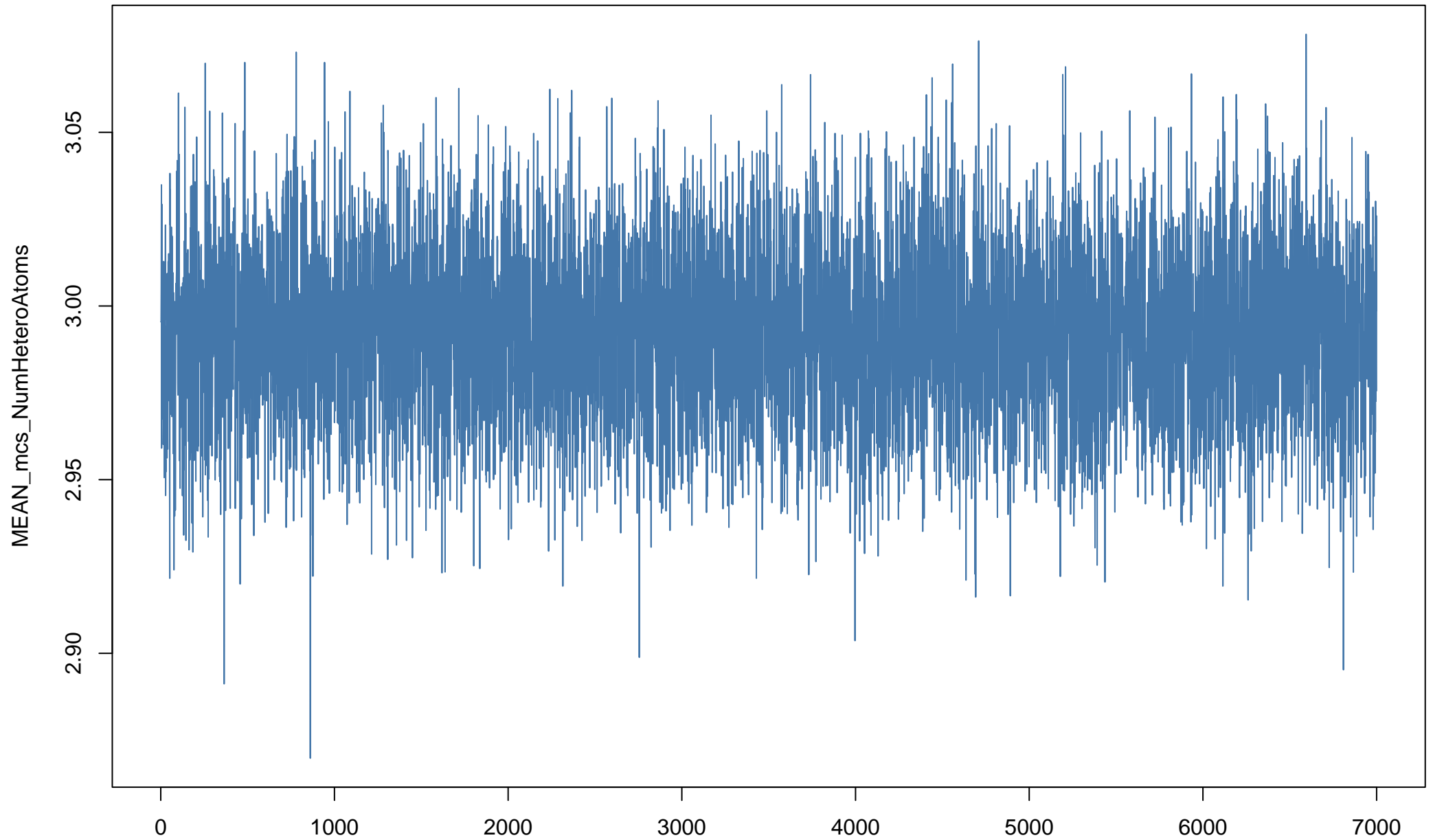
MEAN_log_mcs_unbonded_polar_sasa
ESS = 7000 | BMK = 0.0354 | MCSE(6.27) = 2.16 | stat: TRUE



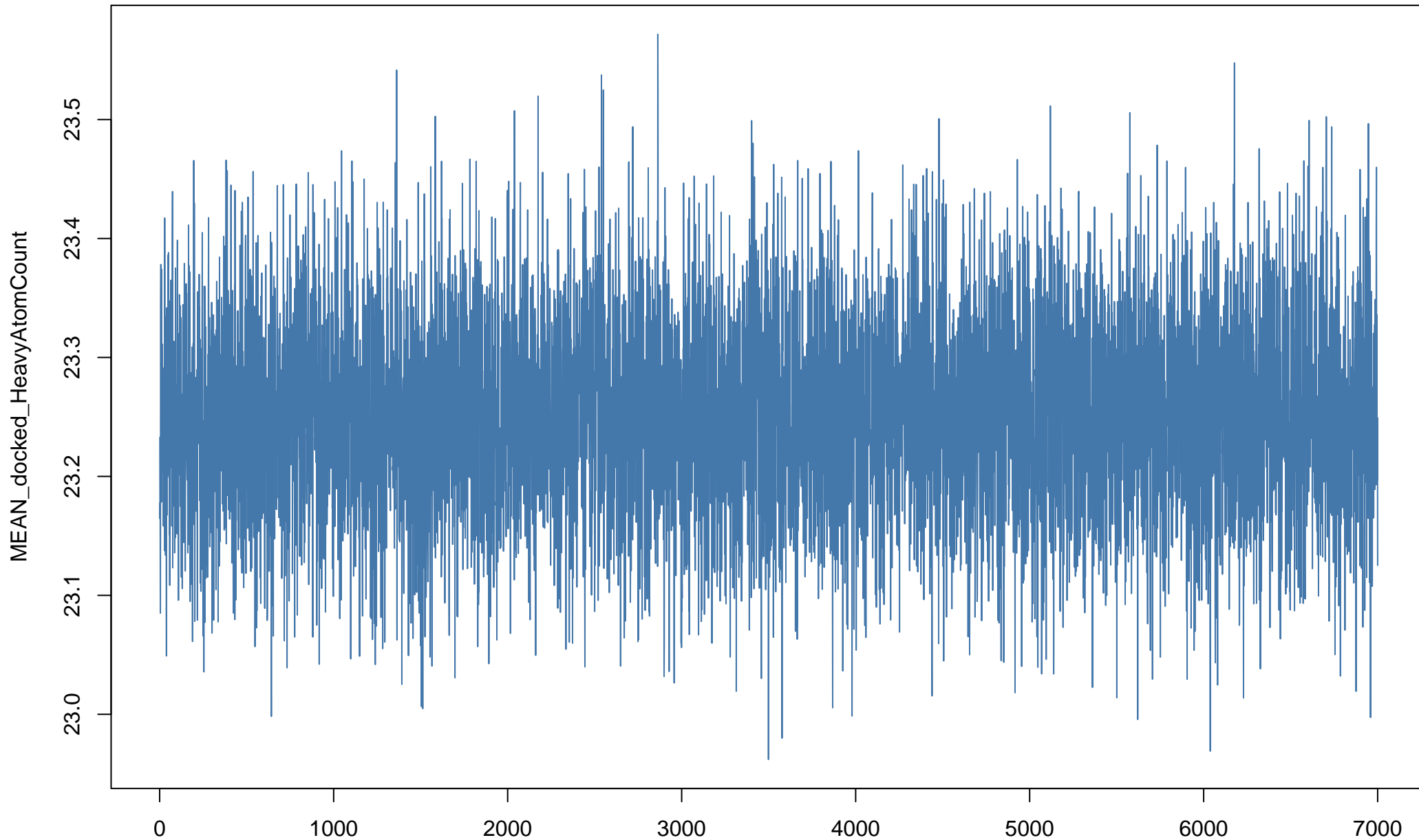
MEAN_logit_ec_tanimoto_similarity
ESS = 5870 | BMK = 0.0322 | MCSE(6.27) = 2.51 | stat: TRUE



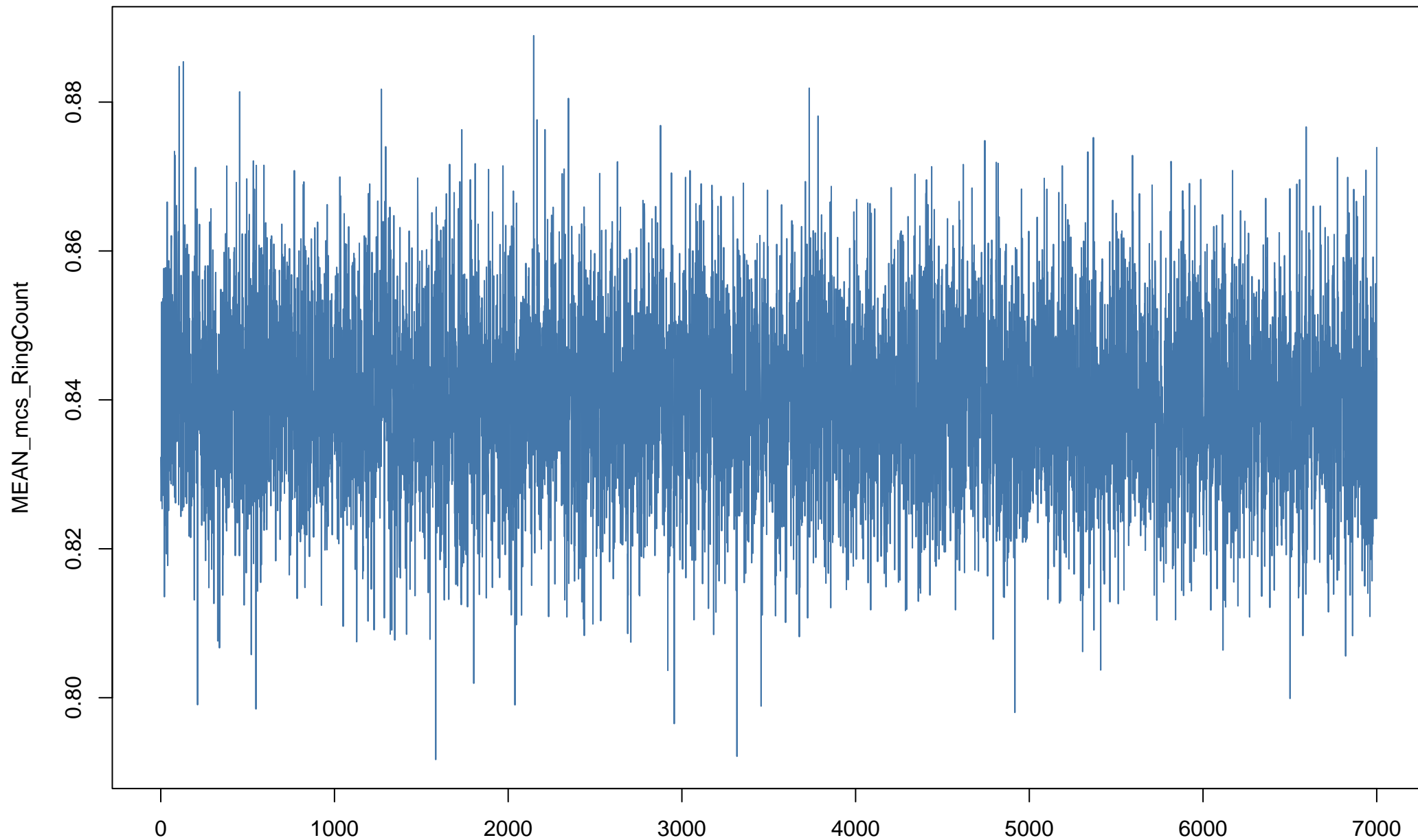
MEAN_mcs_NumHeteroAtoms
ESS = 7000 | BMK = 0.0223 | MCSE(6.27) = 1.3 | stat: TRUE



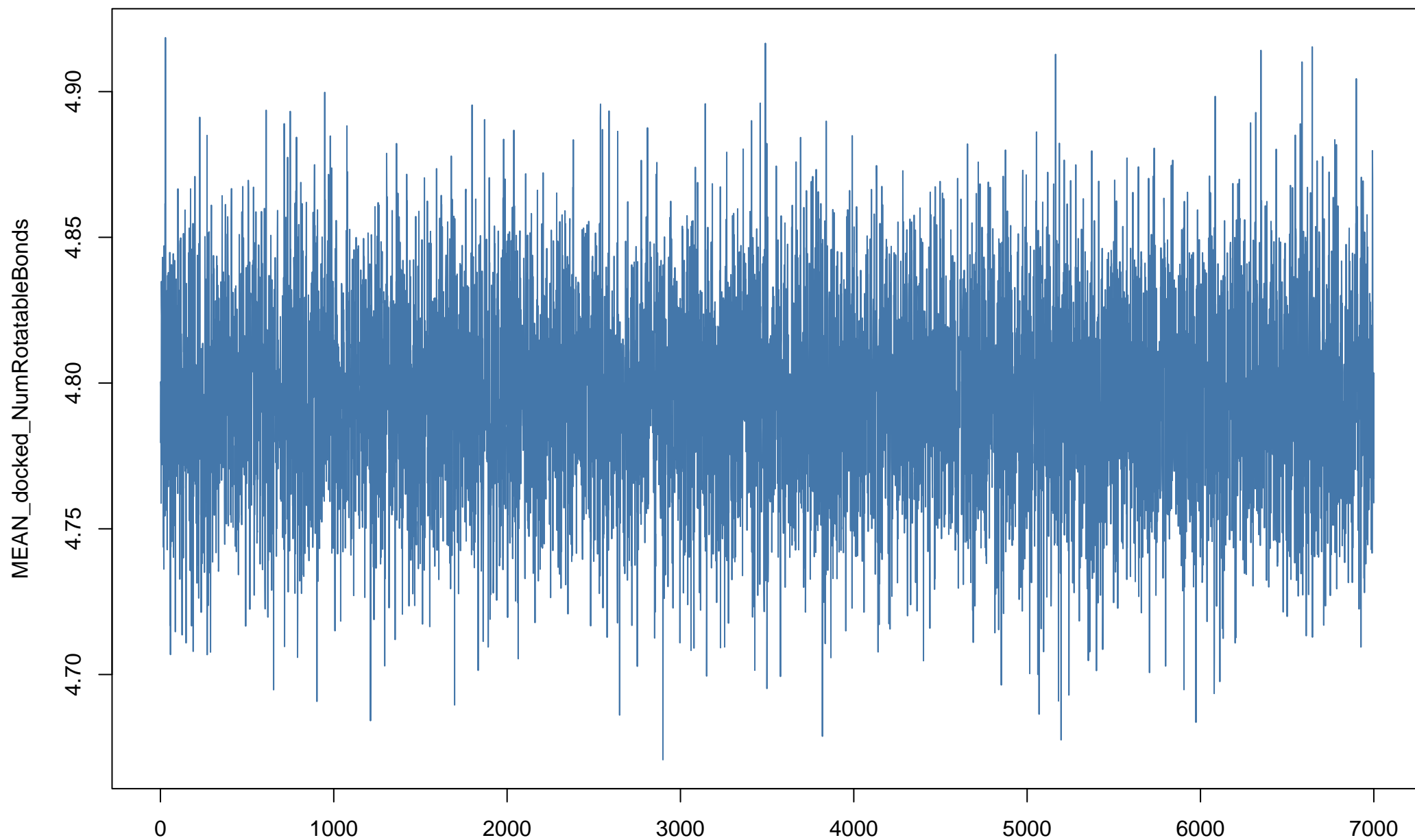
MEAN_docked_HeavyAtomCount
ESS = 7000 | BMK = 0.0286 | MCSE(6.27) = 0.392 | stat: FALSE



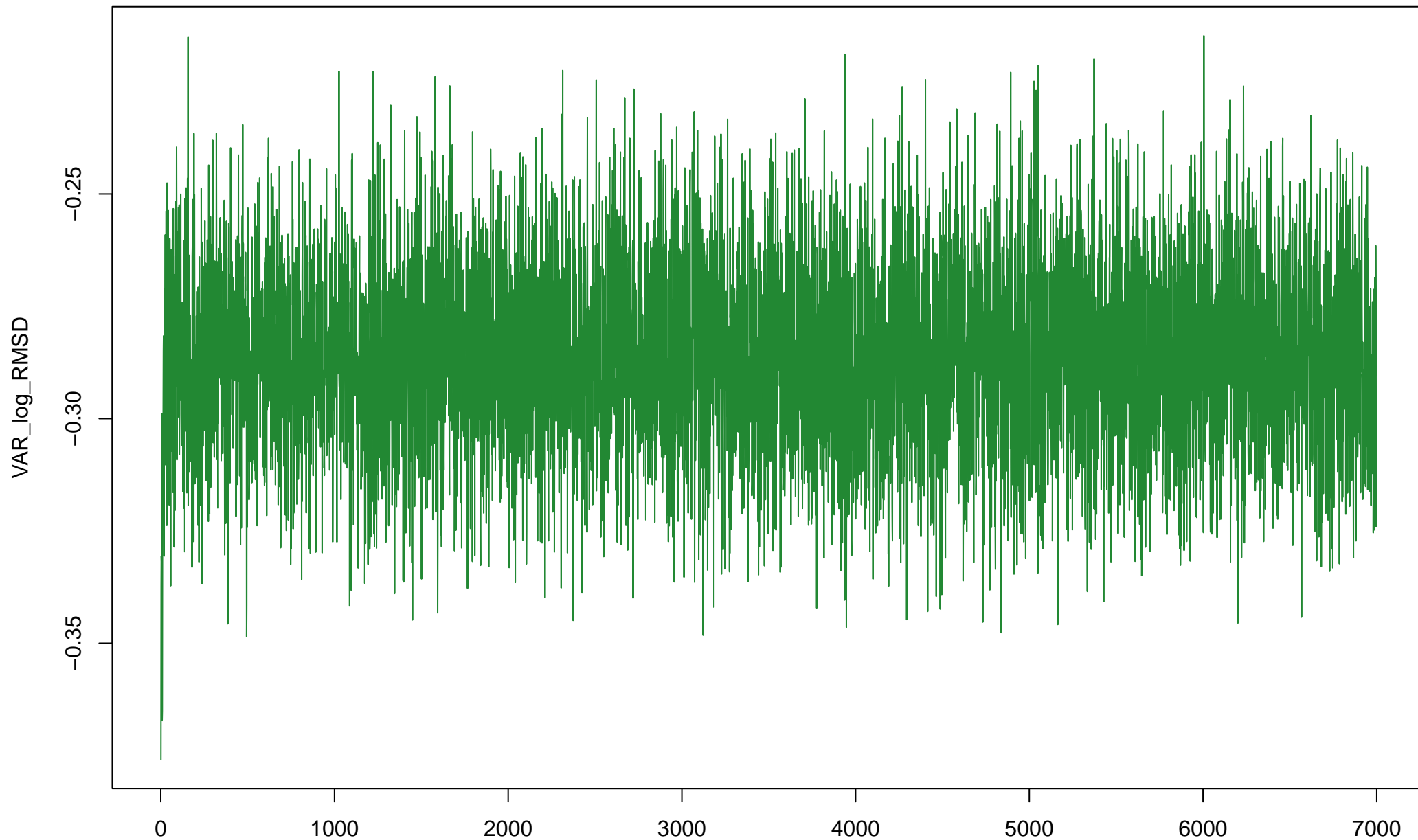
MEAN_mcs_RingCount
ESS = 7000 | BMK = 0.0448 | MCSE(6.27) = 2.67 | stat: FALSE



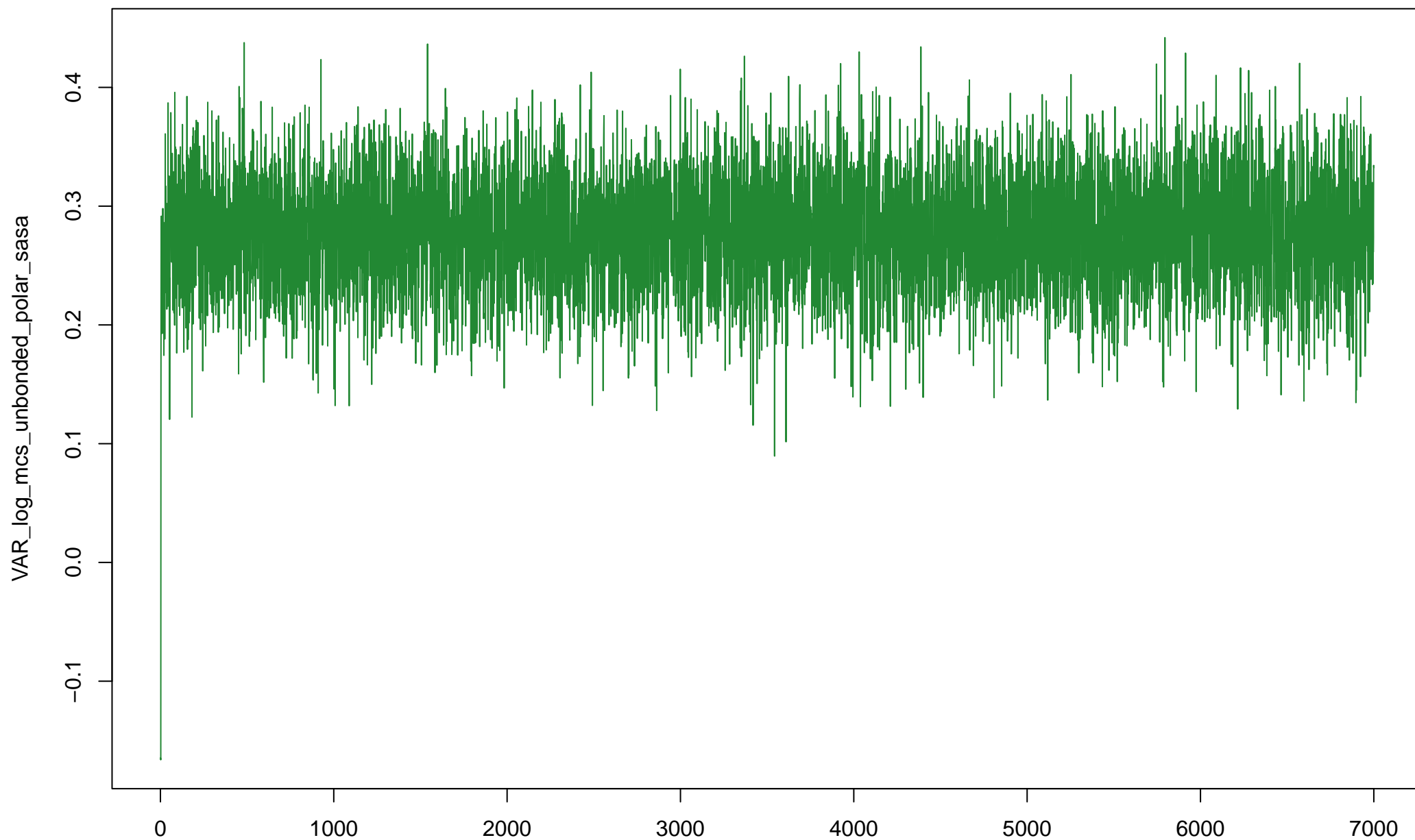
MEAN_docked_NumRotatableBonds
ESS = 7000 | BMK = 0.0267 | MCSE(6.27) = 0.948 | stat: TRUE



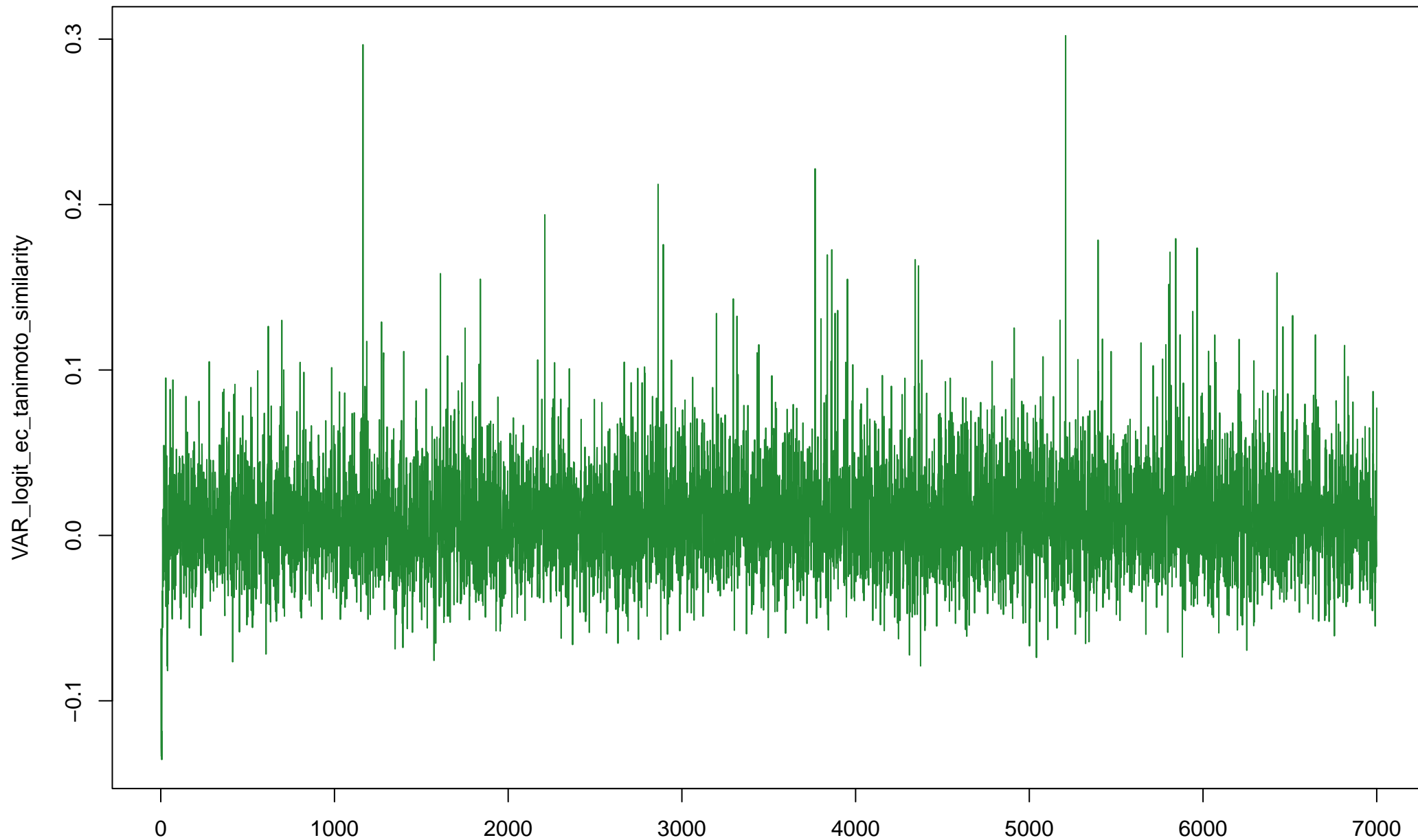
VAR_log_RMSD
ESS = 6200 | BMK = 0.0344 | MCSE(6.27) = 1.59 | stat: TRUE



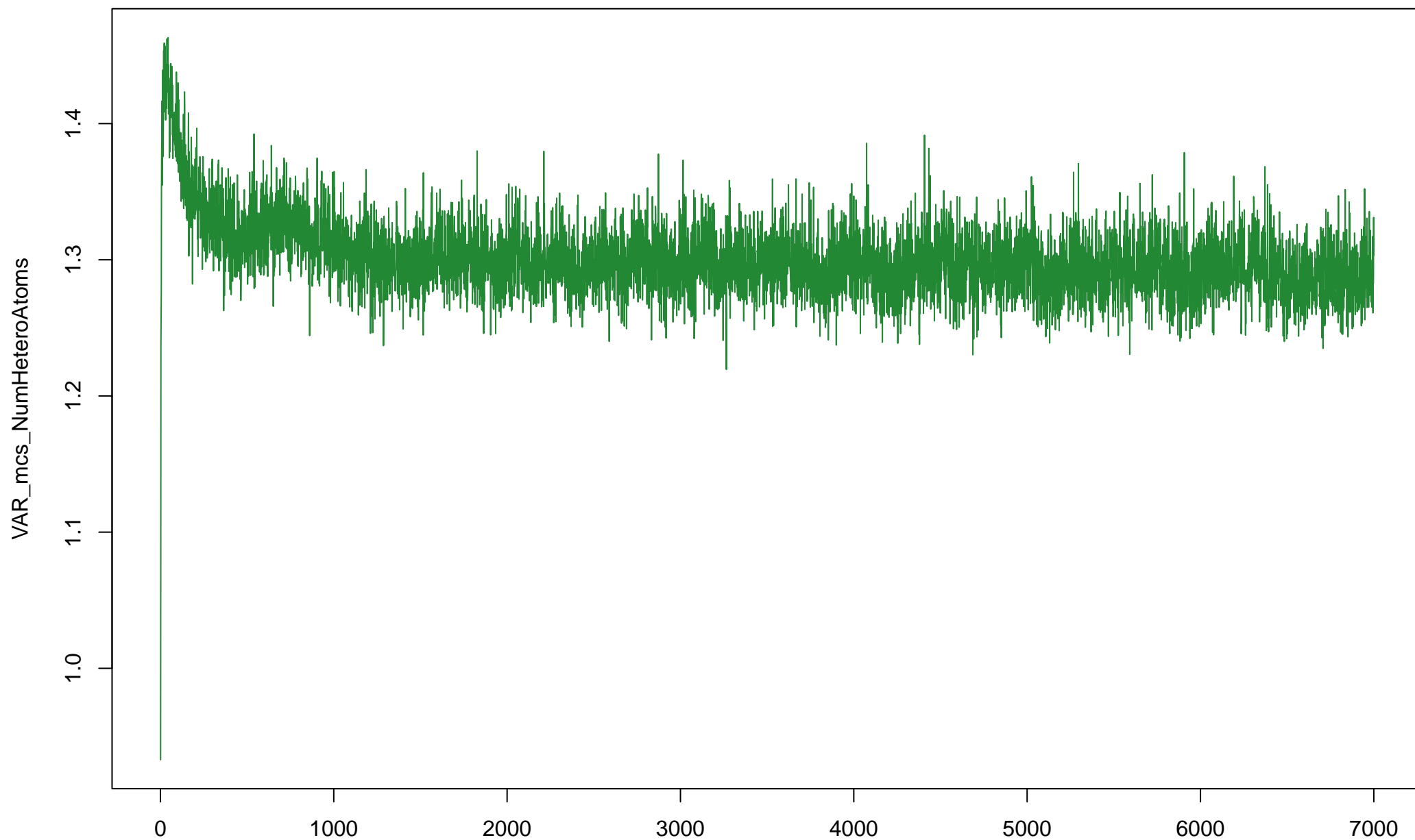
VAR_log_mcs_unbonded_polar_sasa
ESS = 7000 | BMK = 0.0325 | MCSE(6.27) = 0.674 | stat: TRUE



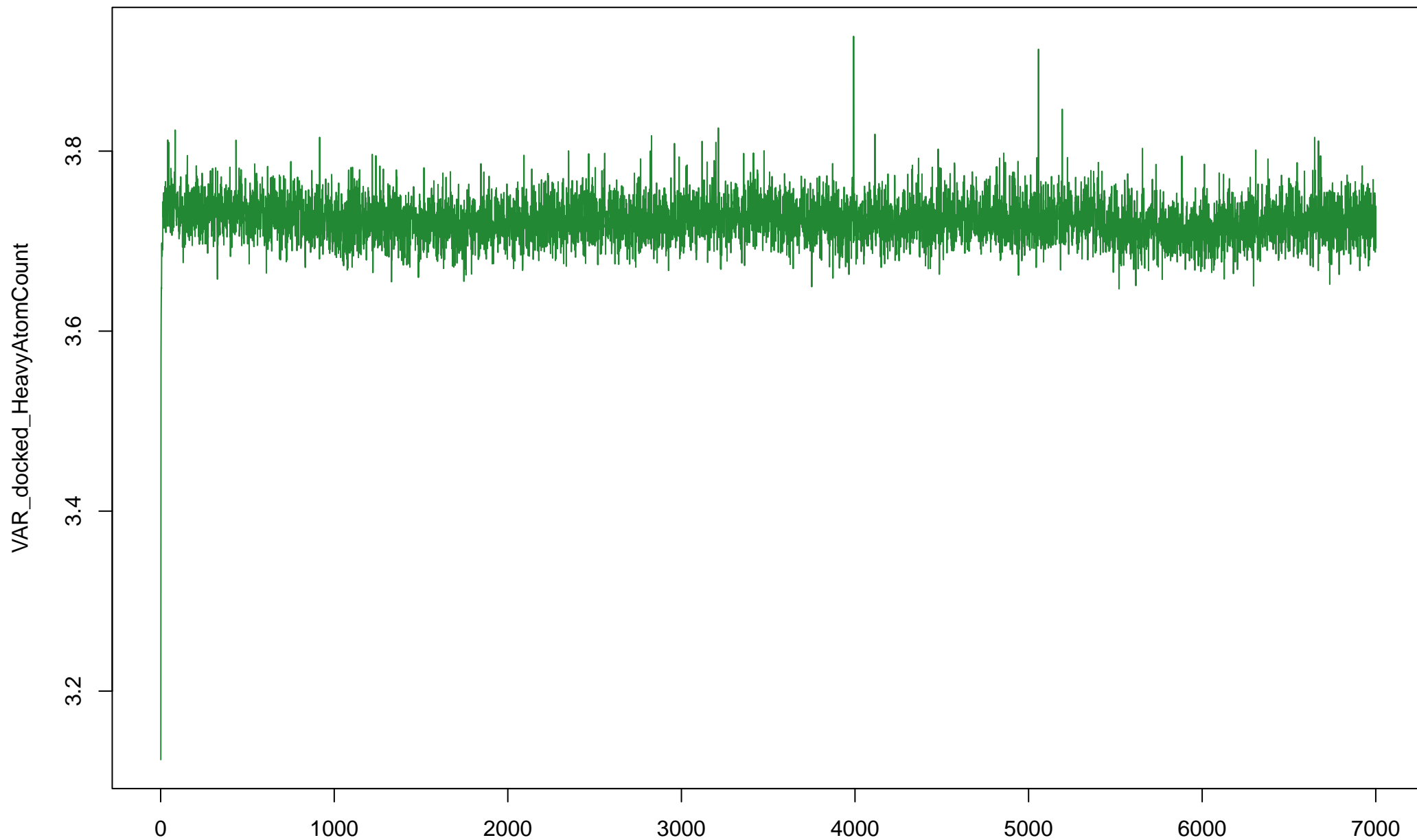
VAR_logit_ec_tanimoto_similarity
ESS = 5890 | BMK = 0.0463 | MCSE(6.27) = 1.02 | stat: FALSE



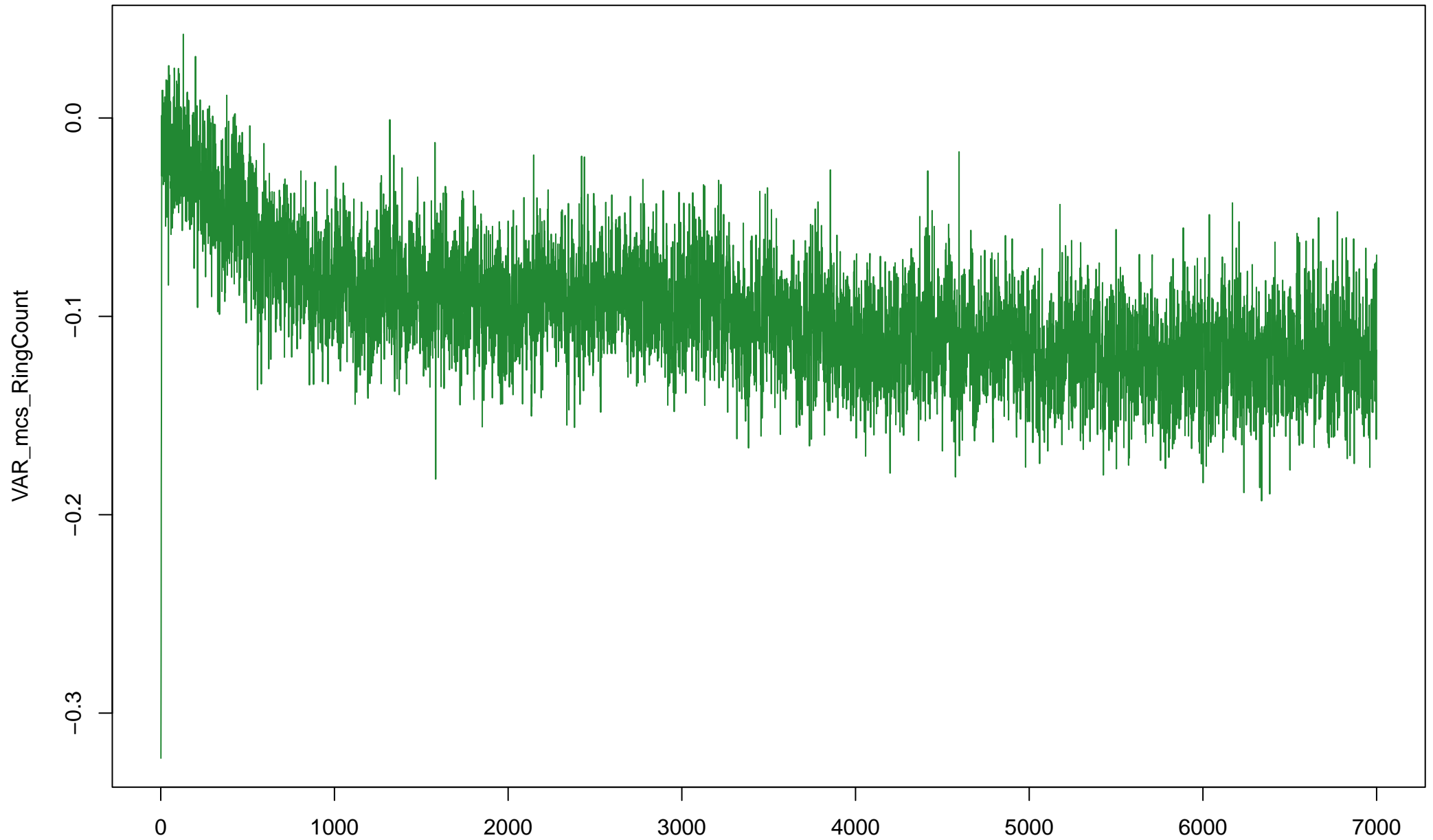
VAR_mcs_NumHeteroAtoms
ESS = 65.9 | BMK = 0.24 | MCSE(6.27) = 1.16 | stat: FALSE



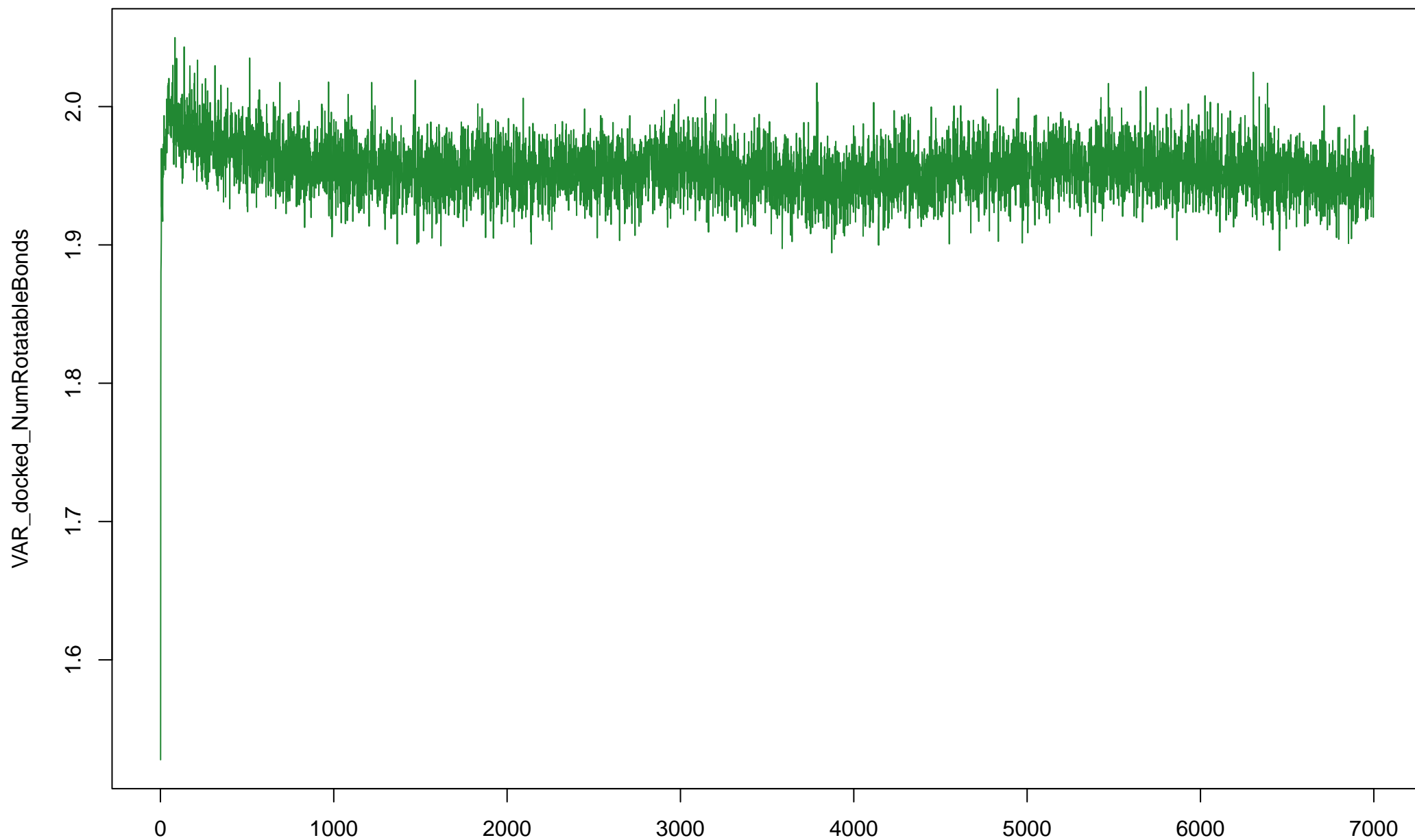
VAR_docked_HeavyAtomCount
ESS = 1620 | BMK = 0.0634 | MCSE(6.27) = 1.35 | stat: FALSE



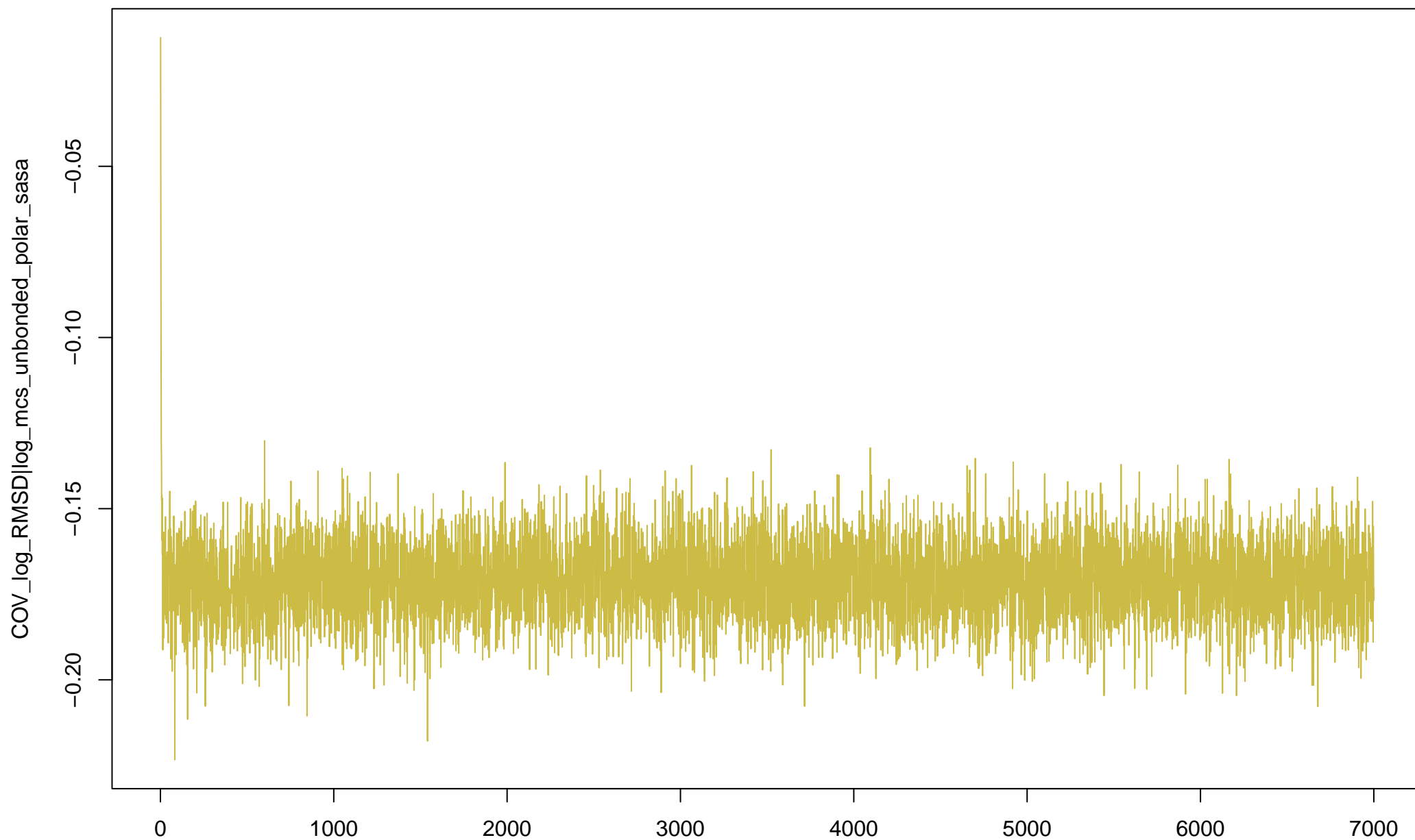
VAR_mcs_RingCount
ESS = 16.3 | BMK = 0.461 | MCSE(6.27) = 0.984 | stat: FALSE



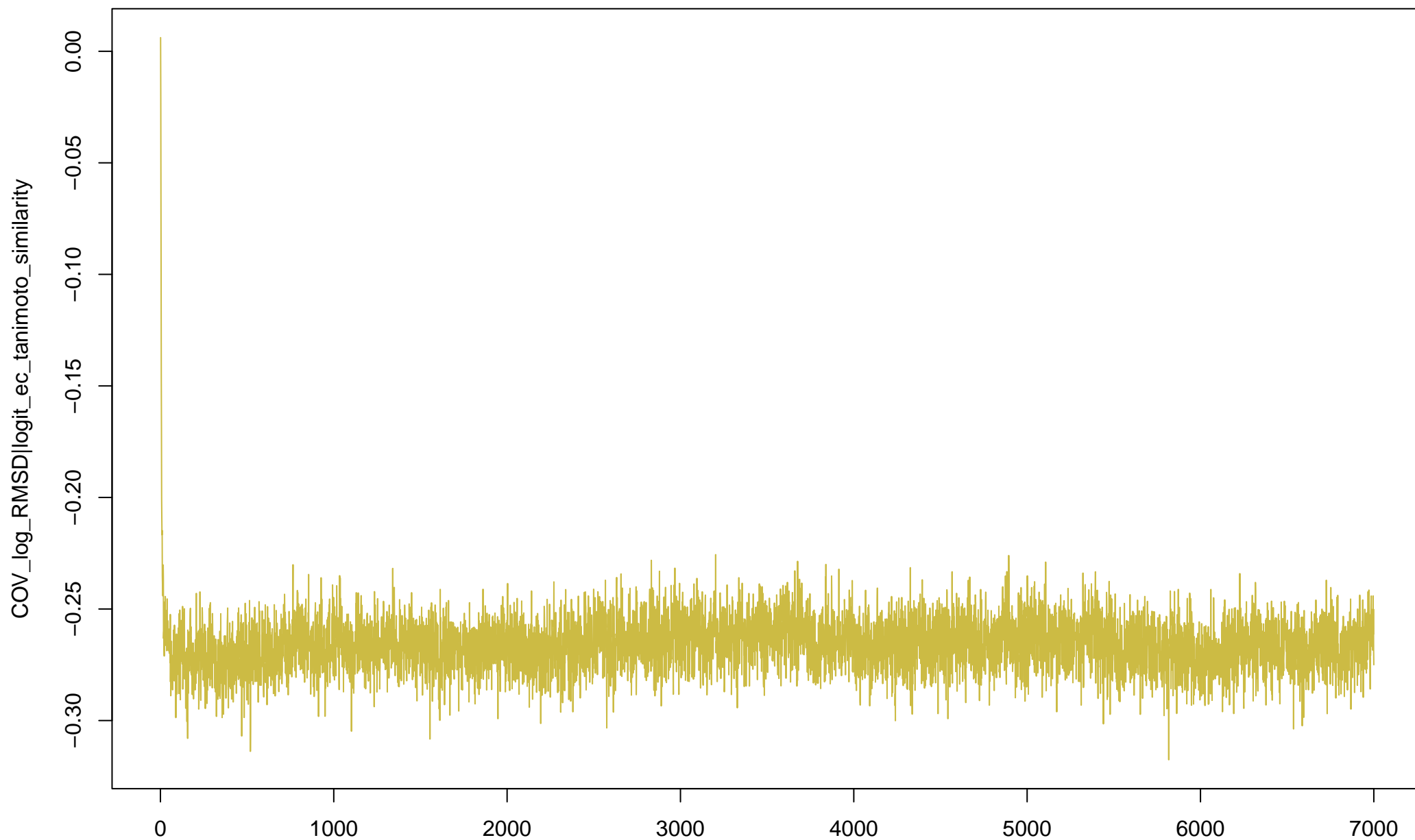
VAR_docked_NumRotatableBonds
ESS = 178 | BMK = 0.14 | MCSE(6.27) = 1.64 | stat: FALSE



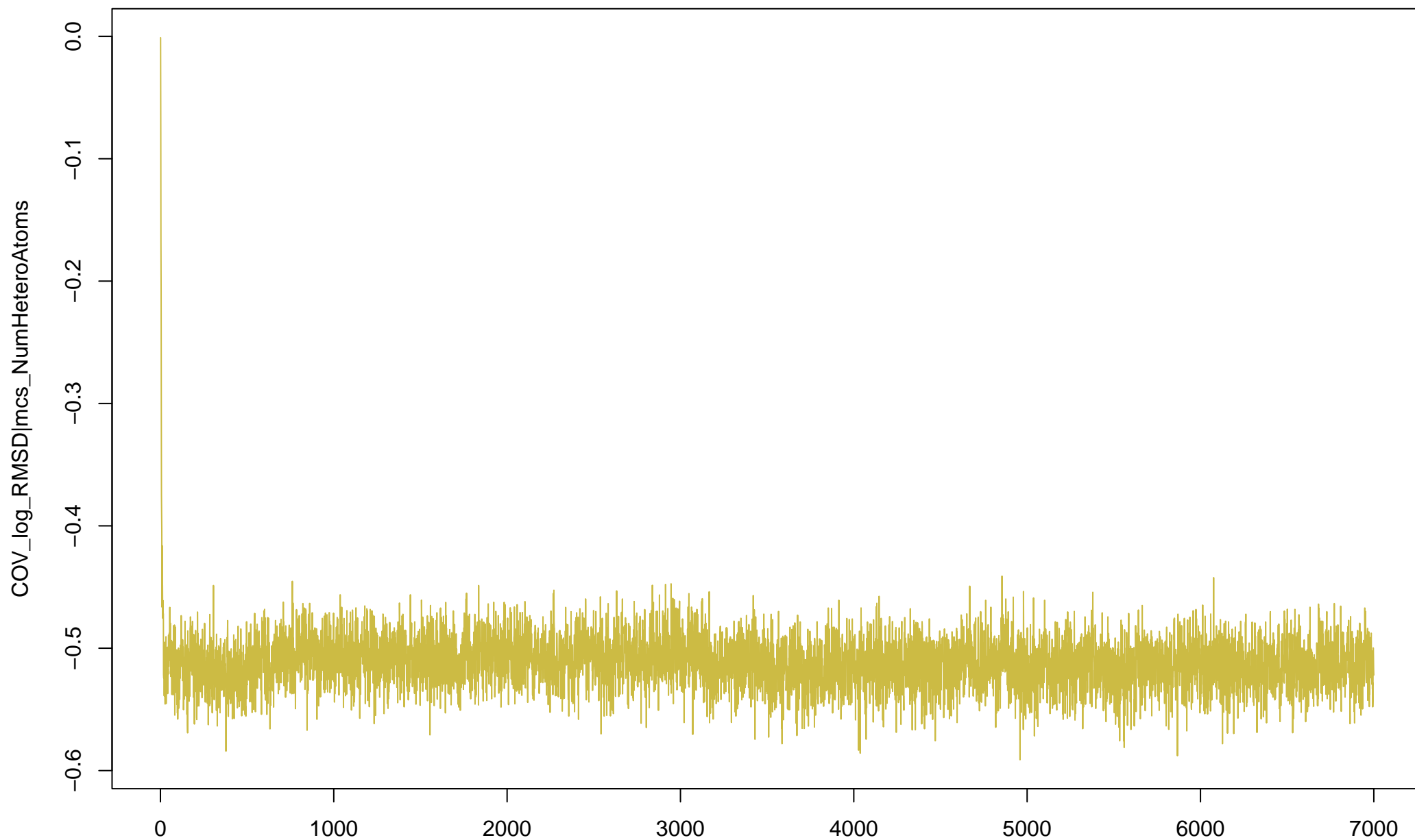
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 4920 | BMK = 0.0413 | MCSE(6.27) = 2.88 | stat: TRUE



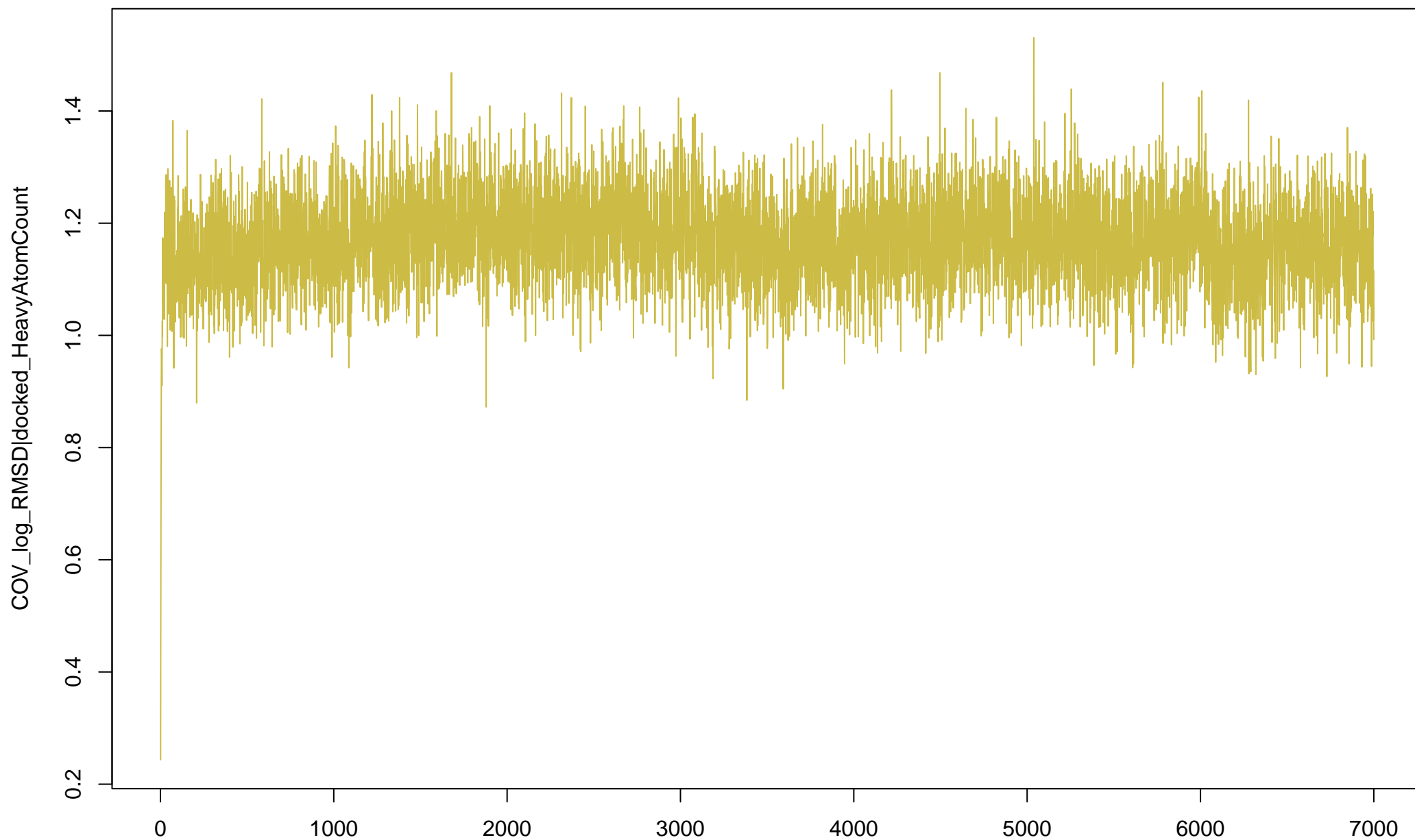
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1090 | BMK = 0.0539 | MCSE(6.27) = 2.54 | stat: TRUE



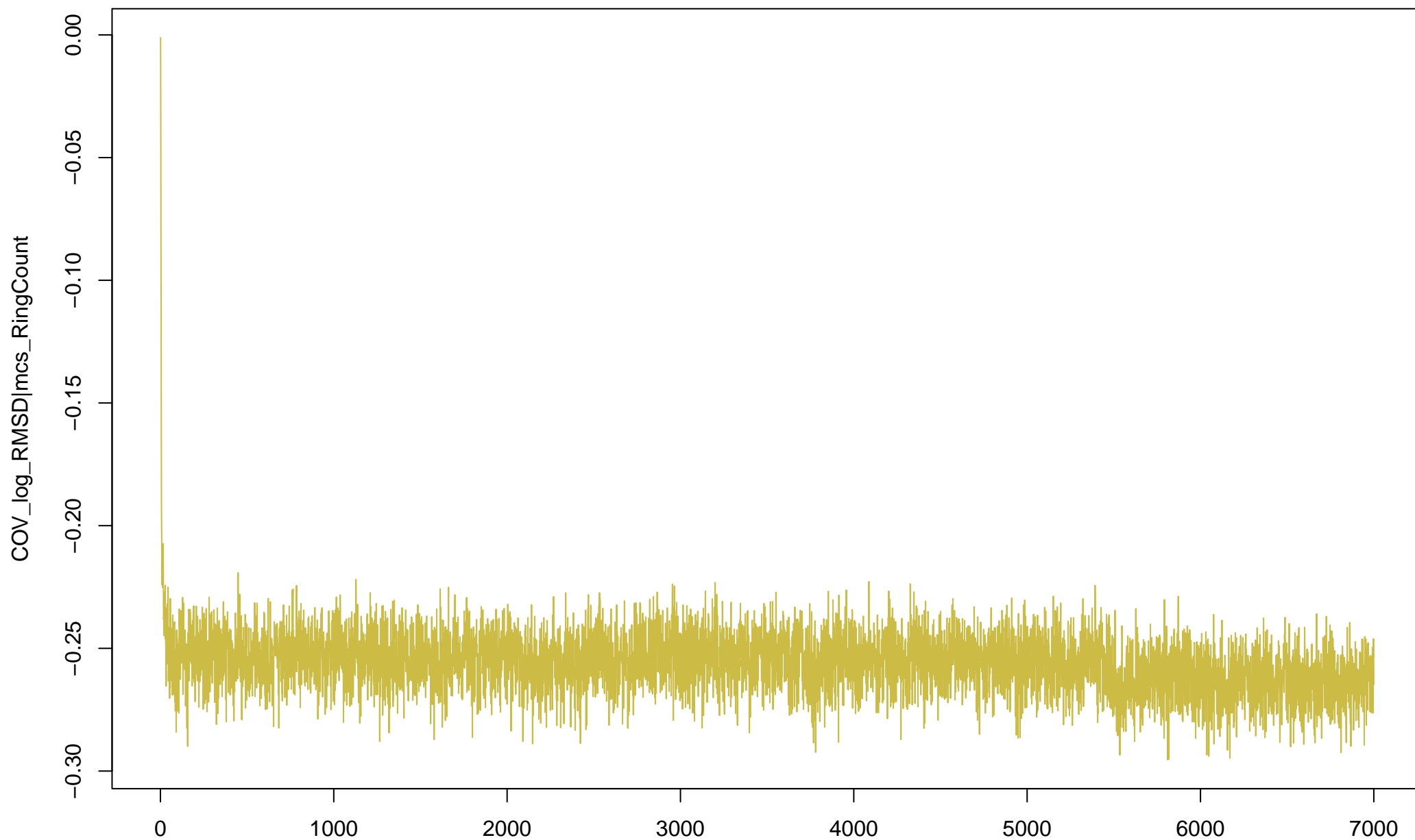
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1420 | BMK = 0.117 | MCSE(6.27) = 1.43 | stat: TRUE



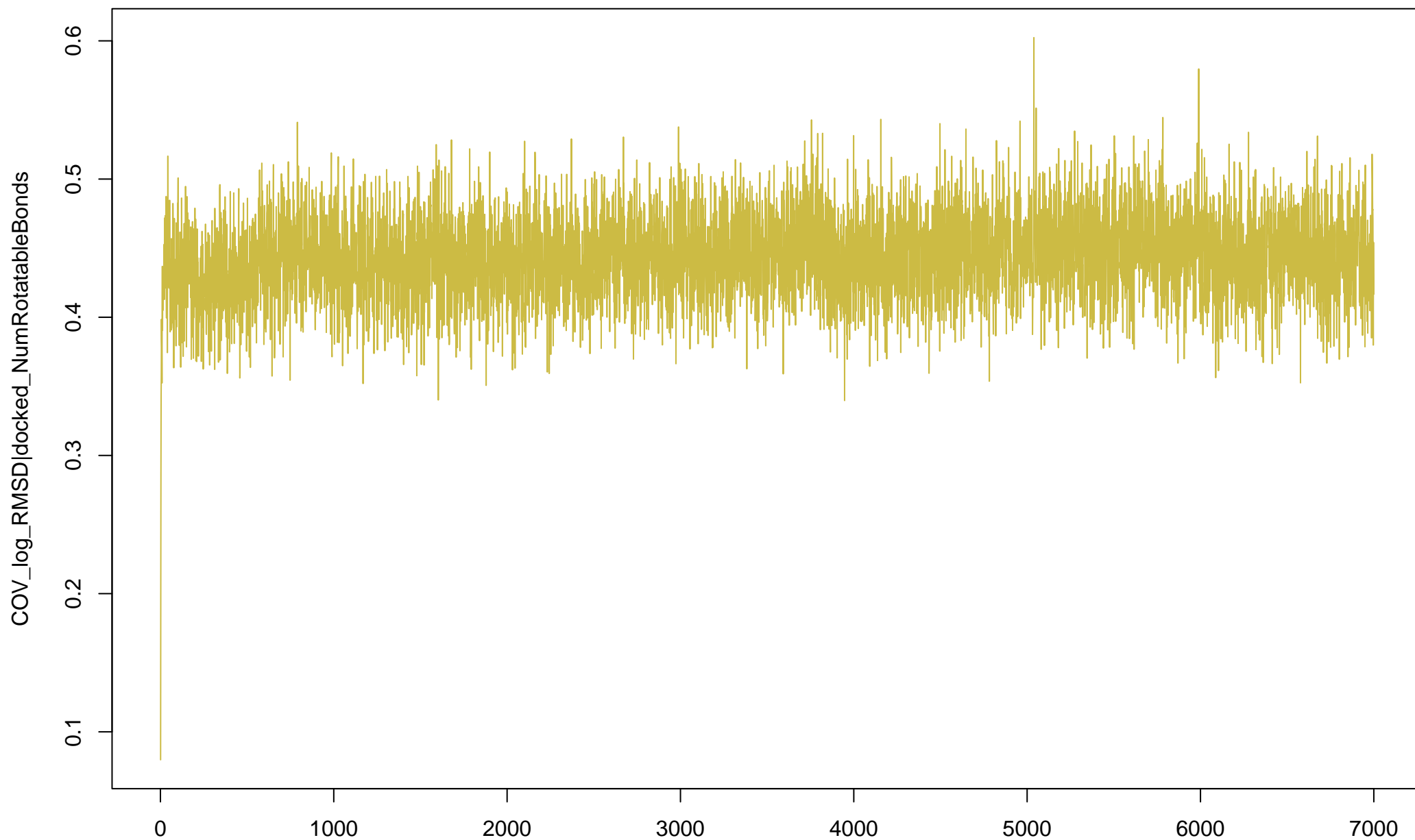
COV_log_RMSD|docked_HeavyAtomCount
ESS = 923 | BMK = 0.0603 | MCSE(6.27) = 0.402 | stat: FALSE



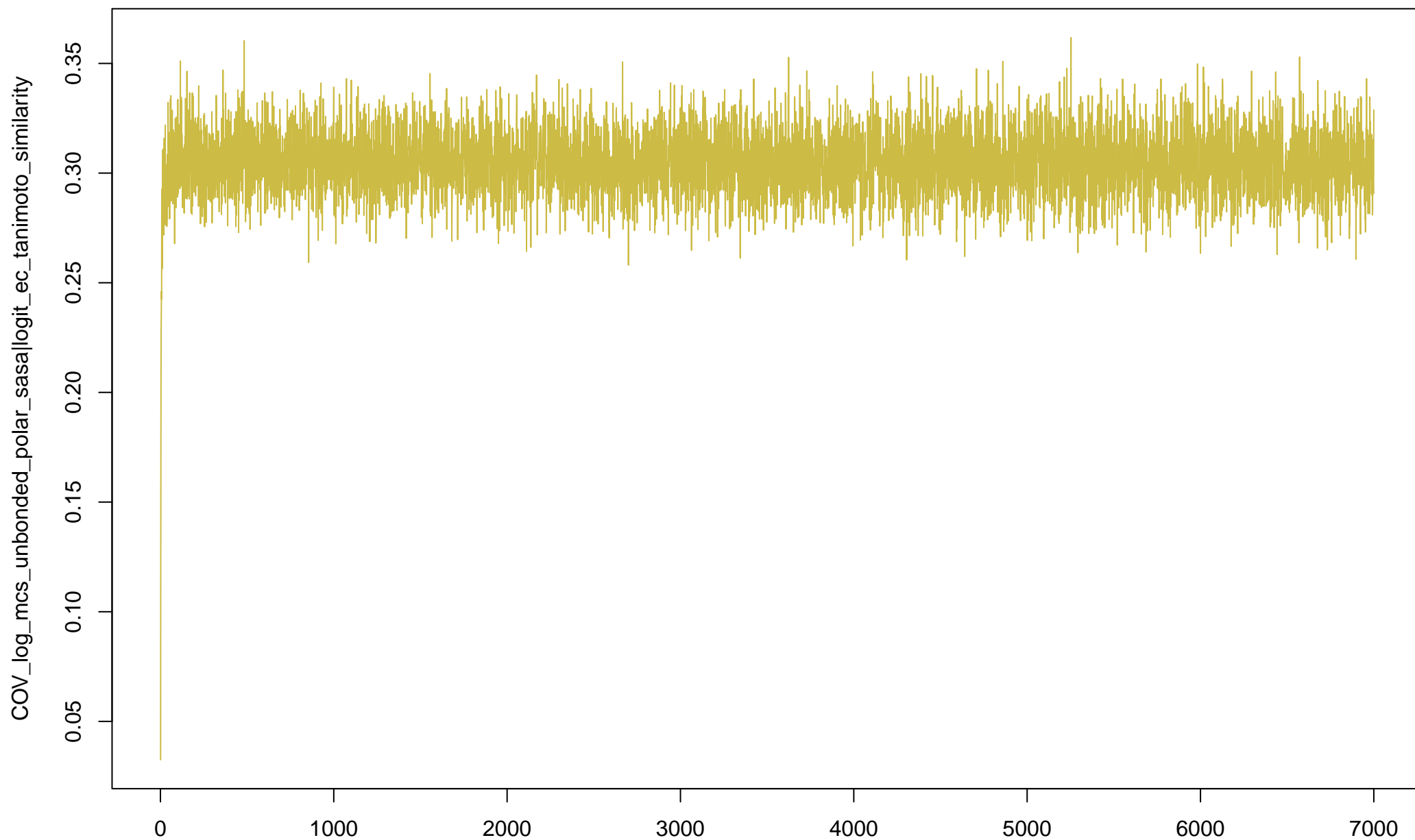
COV_log_RMSD|mcs_RingCount
ESS = 297 | BMK = 0.17 | MCSE(6.27) = 2.6 | stat: FALSE



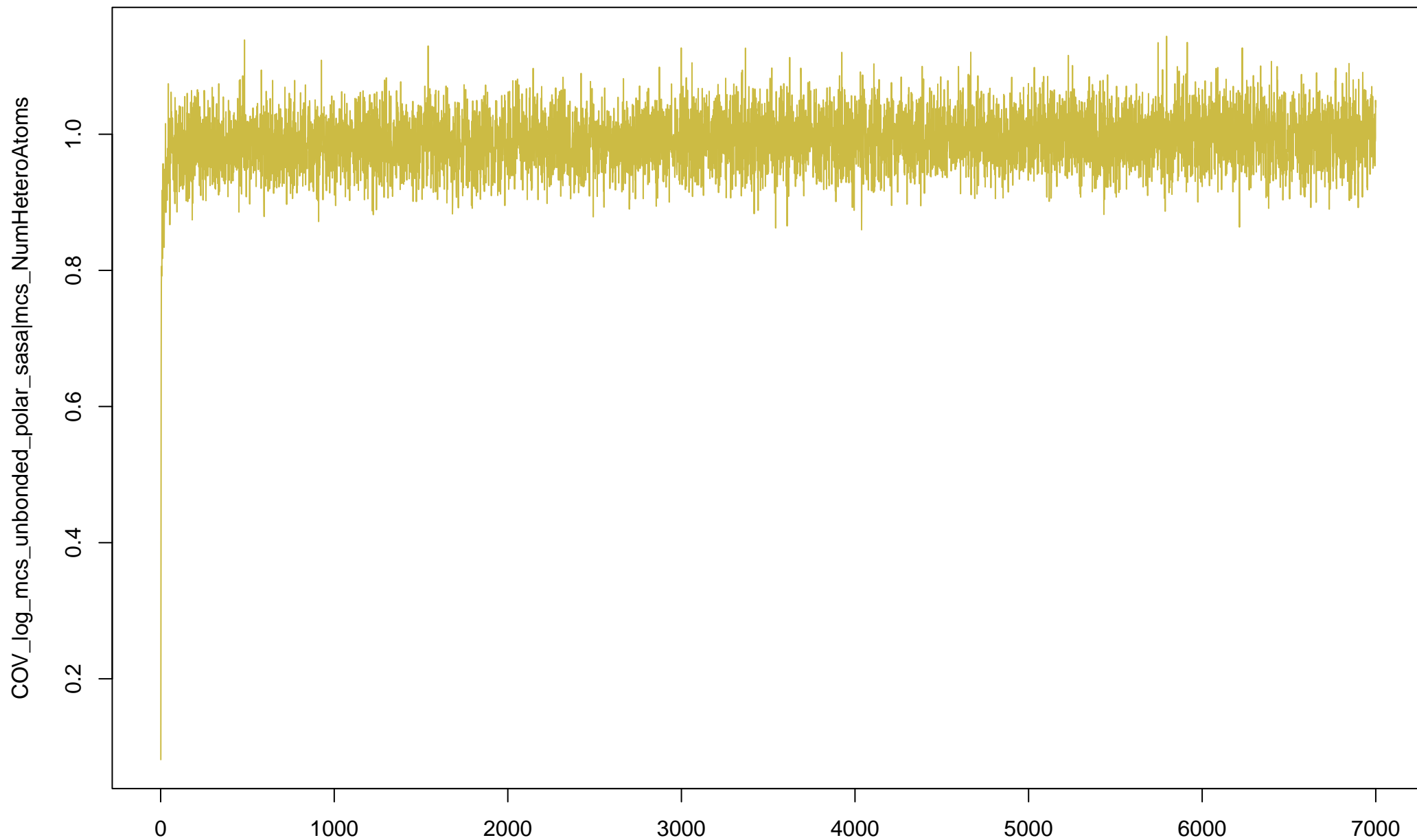
COV_log_RMSD|docked_NumRotatableBonds
ESS = 1840 | BMK = 0.0917 | MCSE(6.27) = 1.05 | stat: FALSE



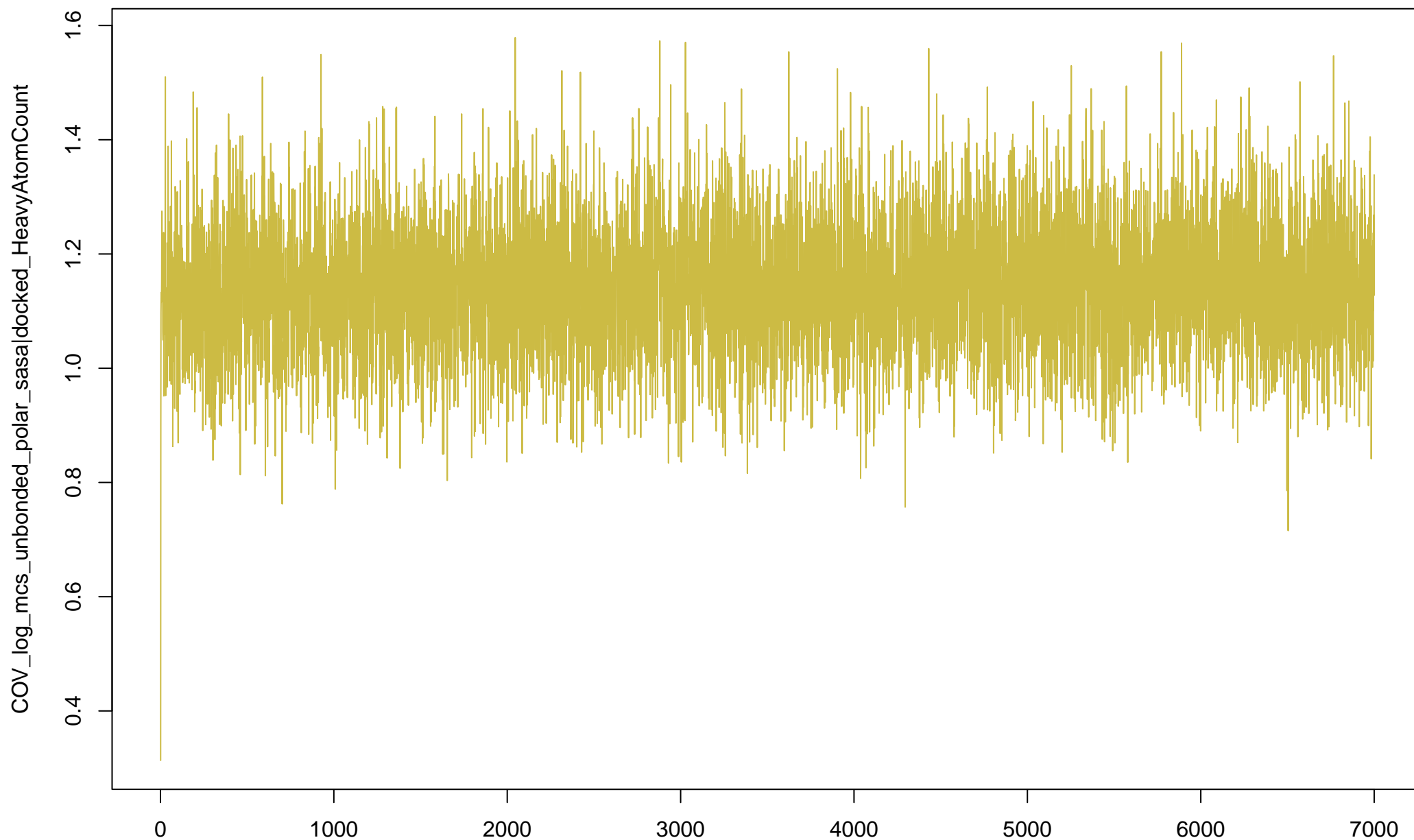
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 4030 | BMK = 0.0555 | MCSE(6.27) = 2.2 | stat: TRUE



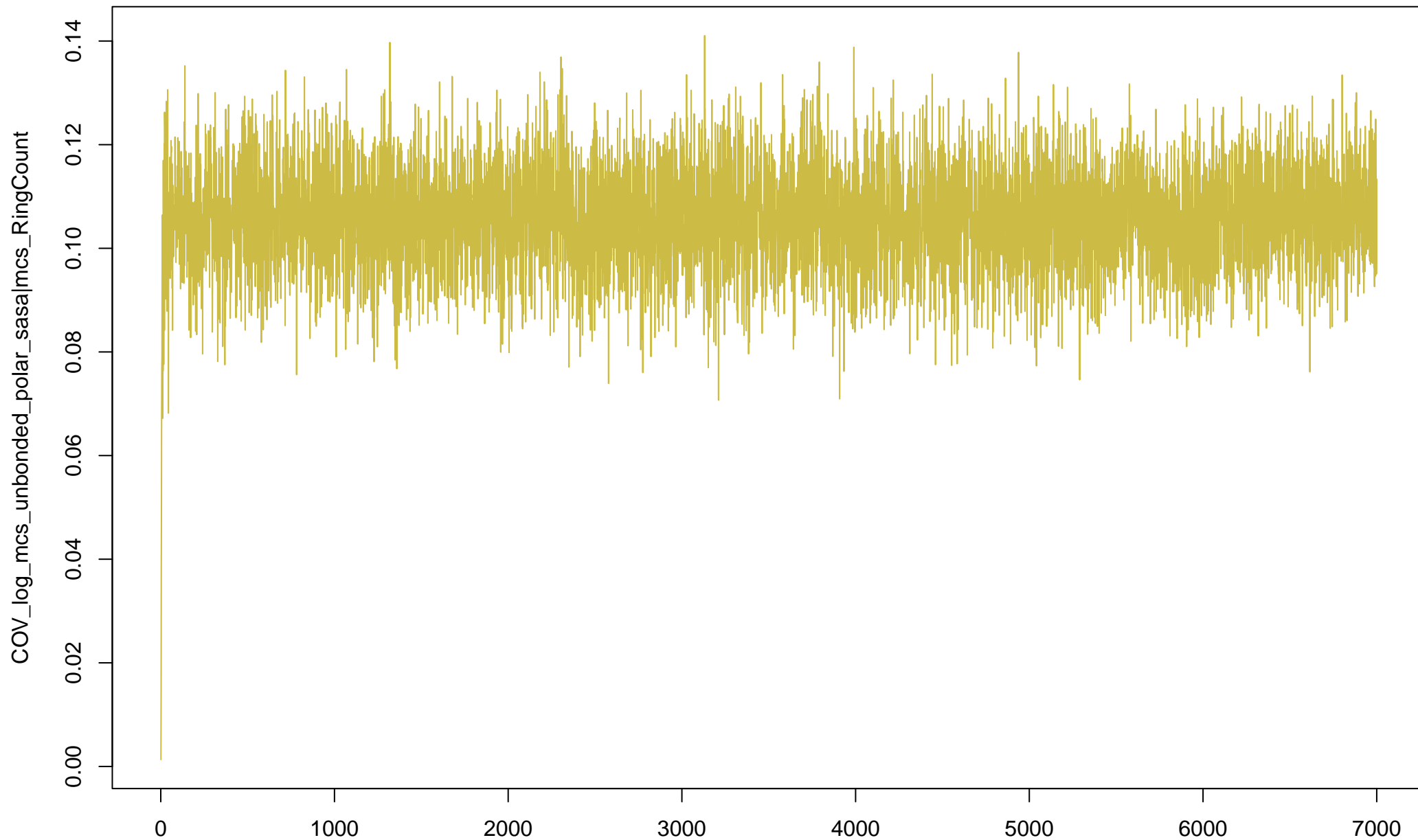
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1350 | BMK = 0.0975 | MCSE(6.27) = 0.784 | stat: FALSE



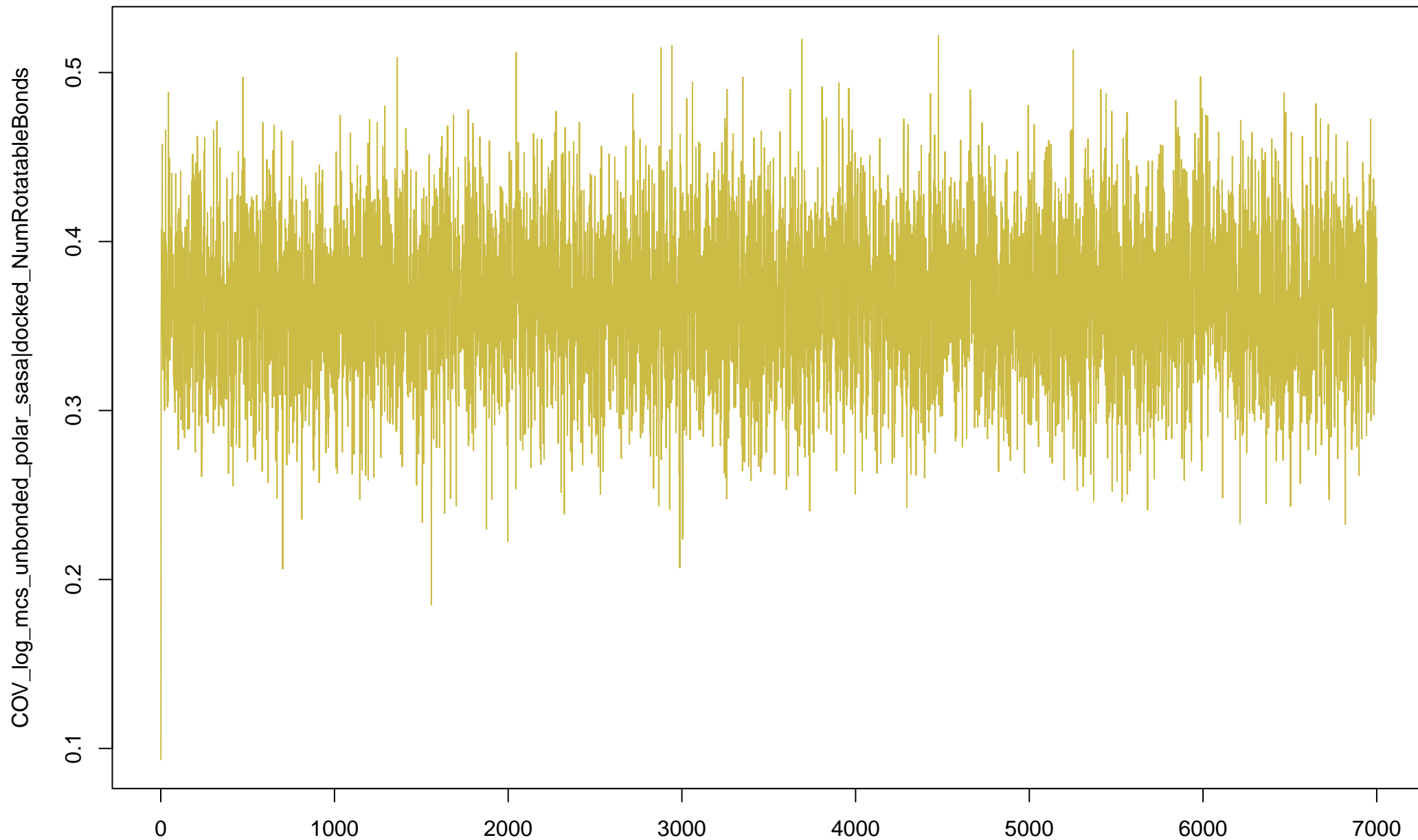
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 6760 | BMK = 0.0453 | MCSE(6.27) = 0.278 | stat: FALSE



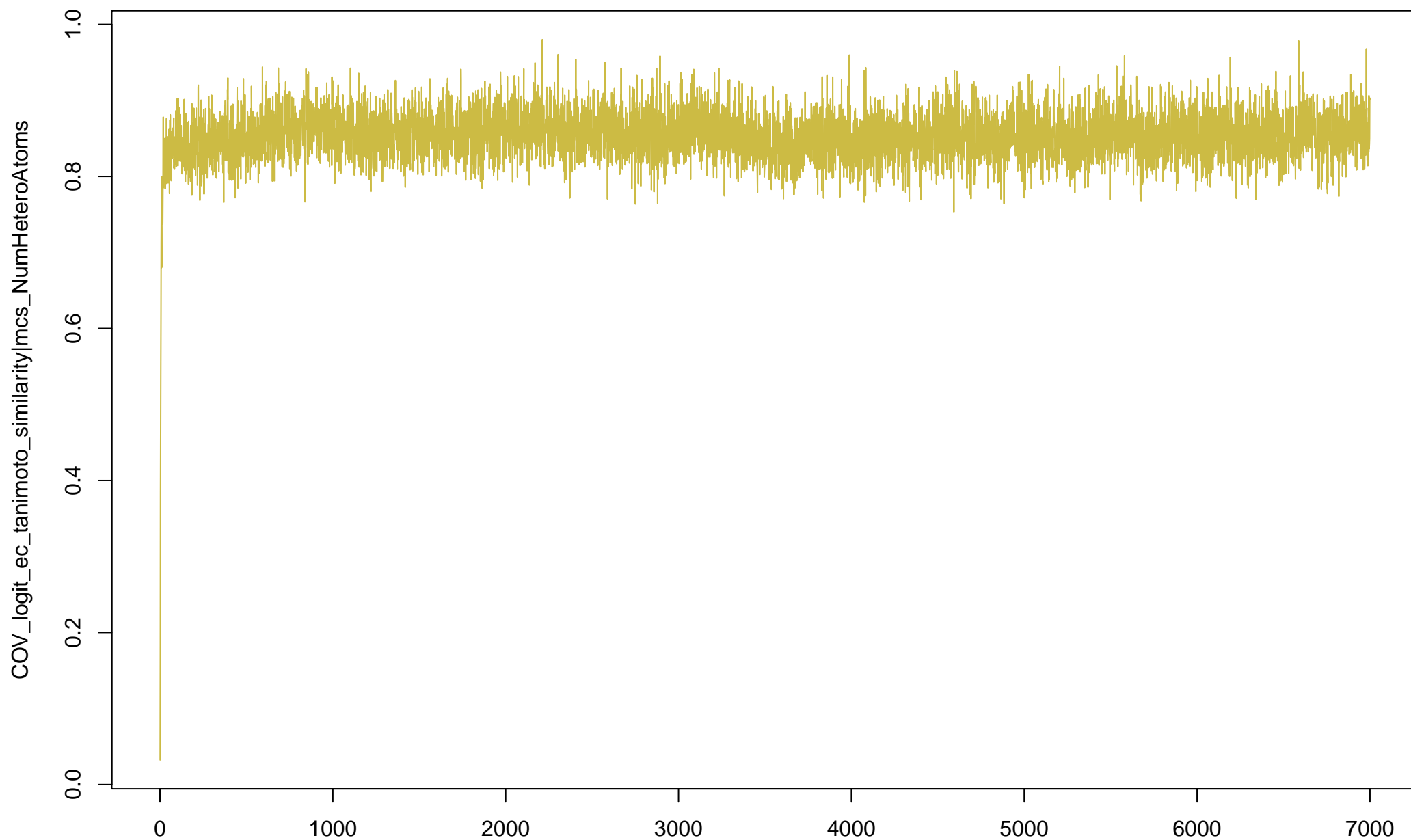
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 5890 | BMK = 0.0424 | MCSE(6.27) = 3.26 | stat: TRUE



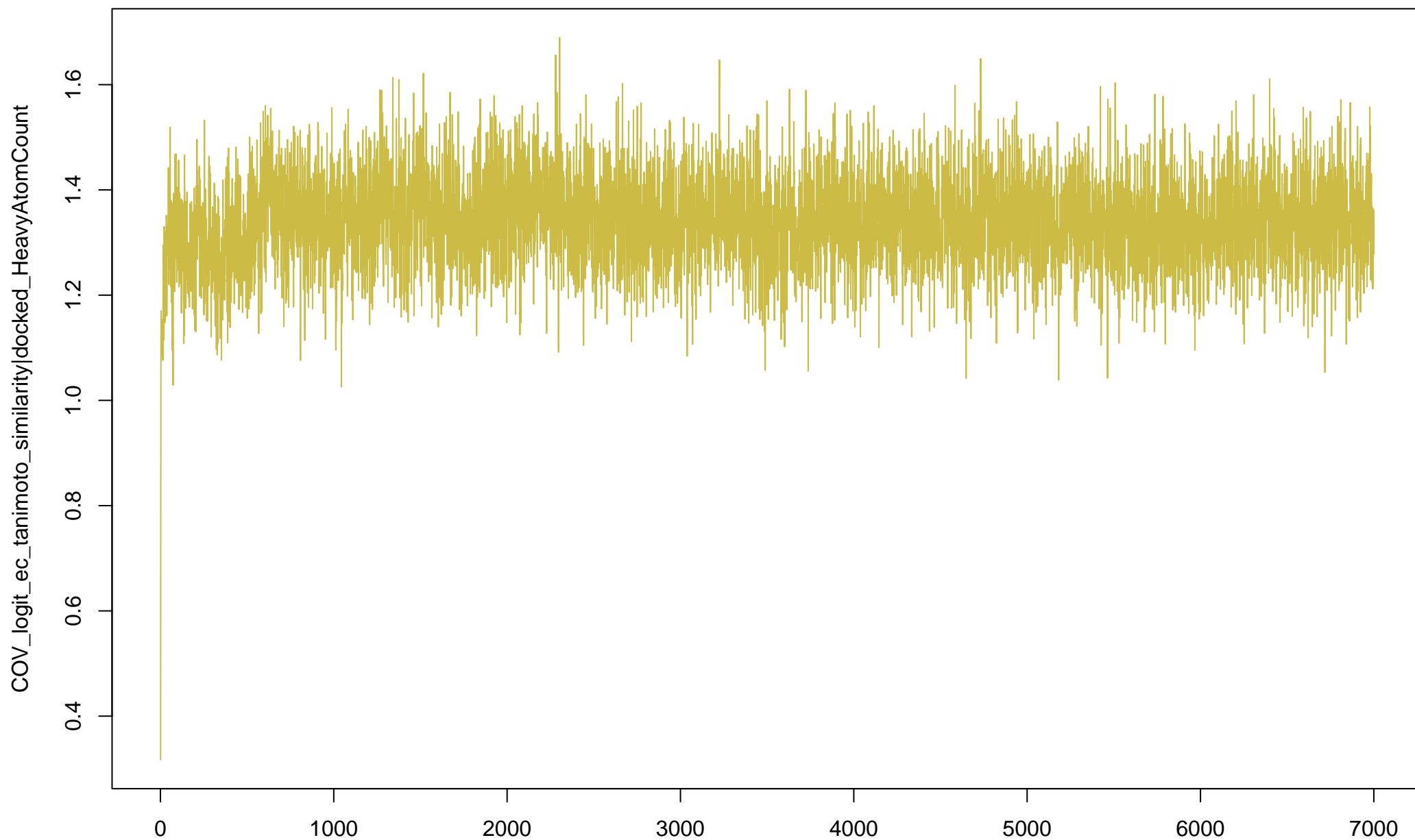
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 6910 | BMK = 0.0336 | MCSE(6.27) = 0.743 | stat: TRUE



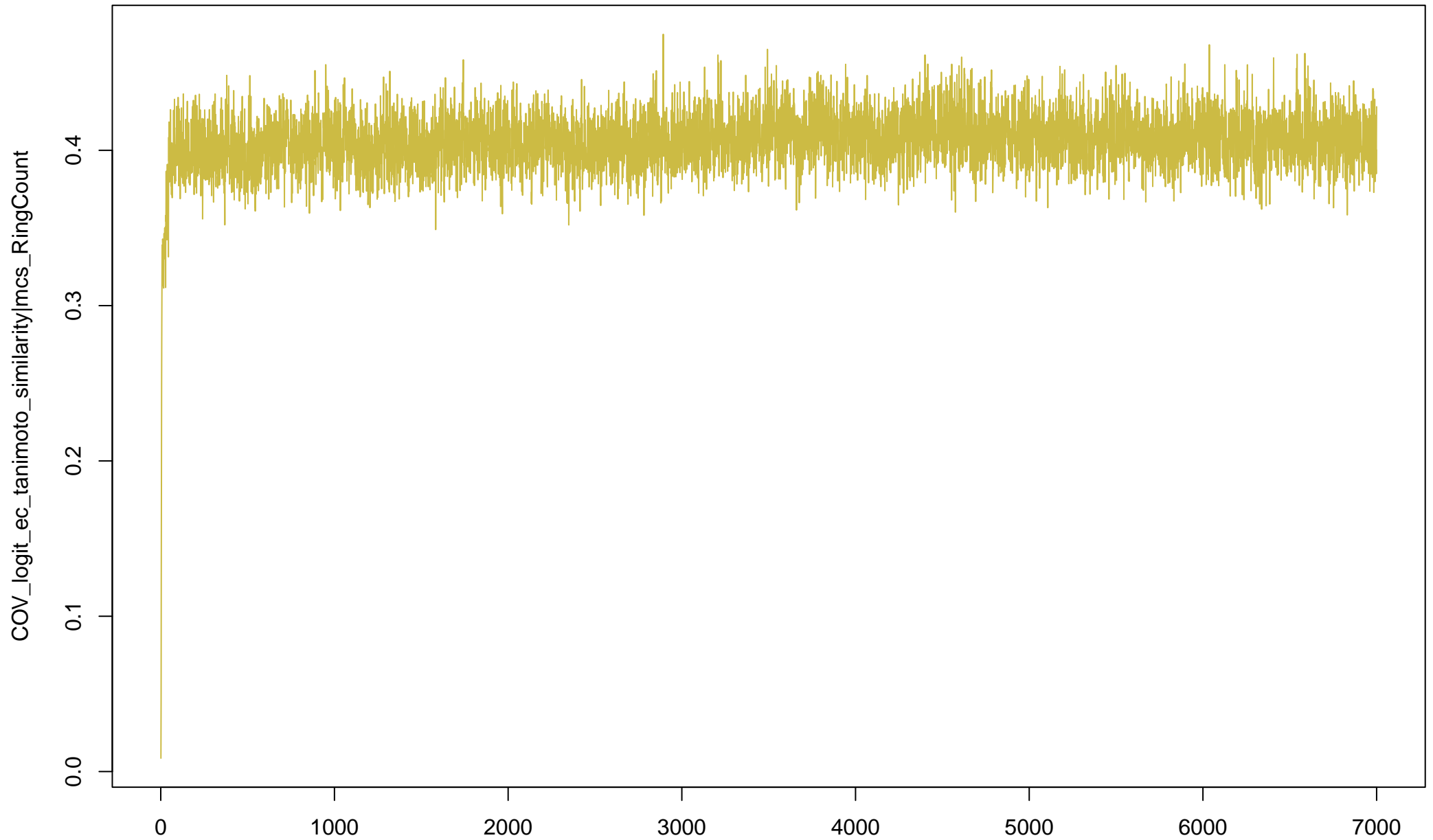
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1440 | BMK = 0.0689 | MCSE(6.27) = 0.96 | stat: TRUE



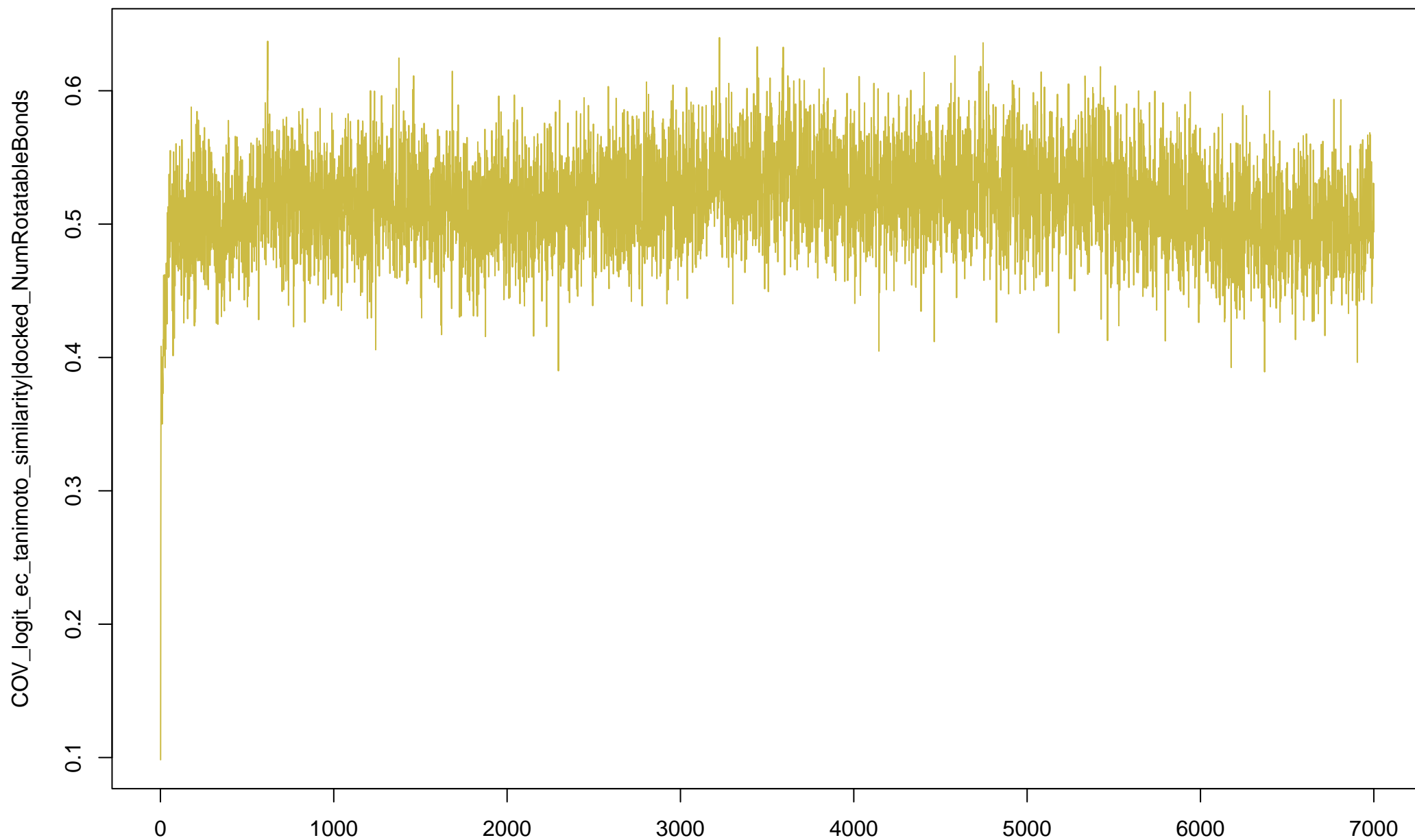
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 888 | BMK = 0.0526 | MCSE(6.27) = 0.372 | stat: FALSE



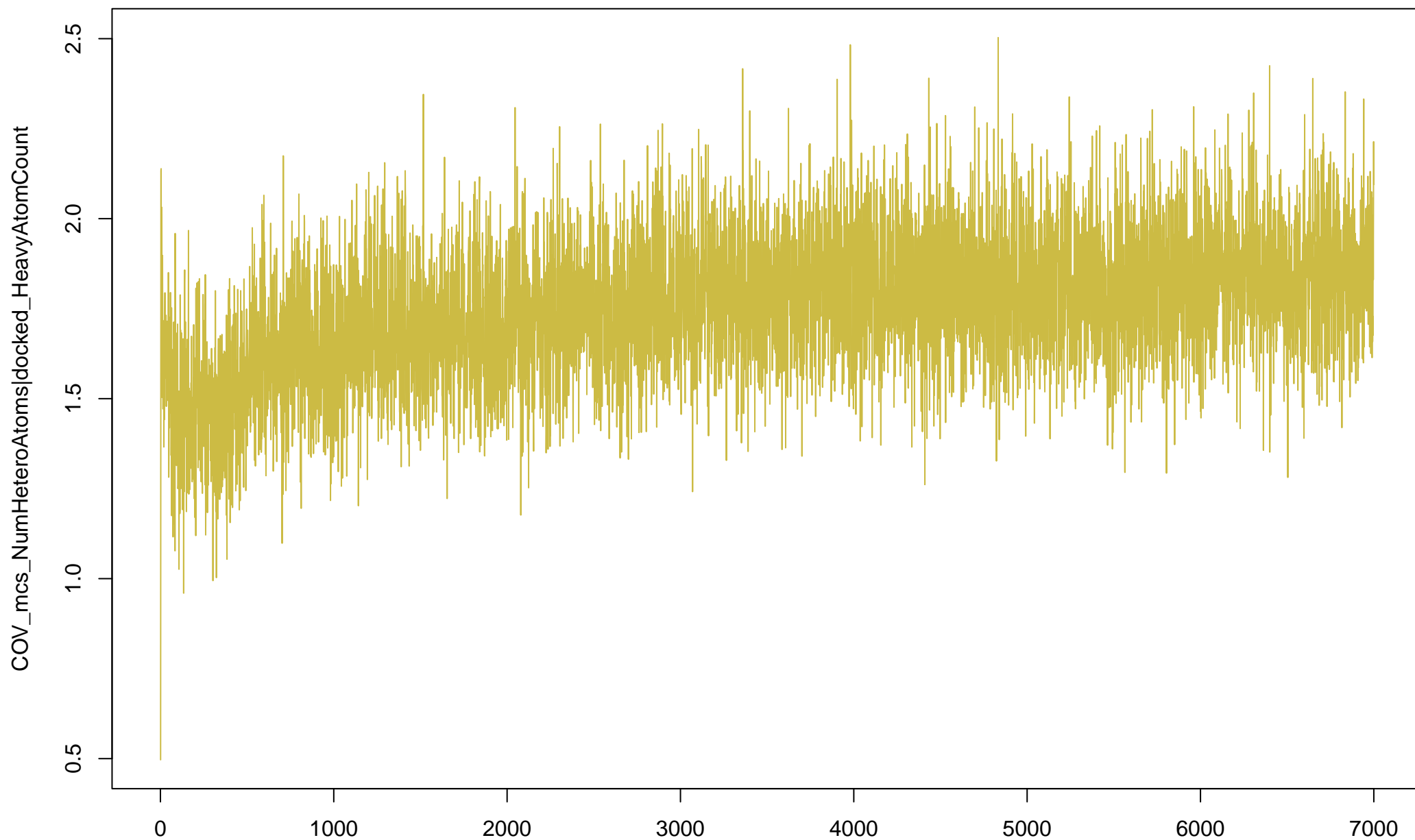
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 544 | BMK = 0.148 | MCSE(6.27) = 1.73 | stat: FALSE



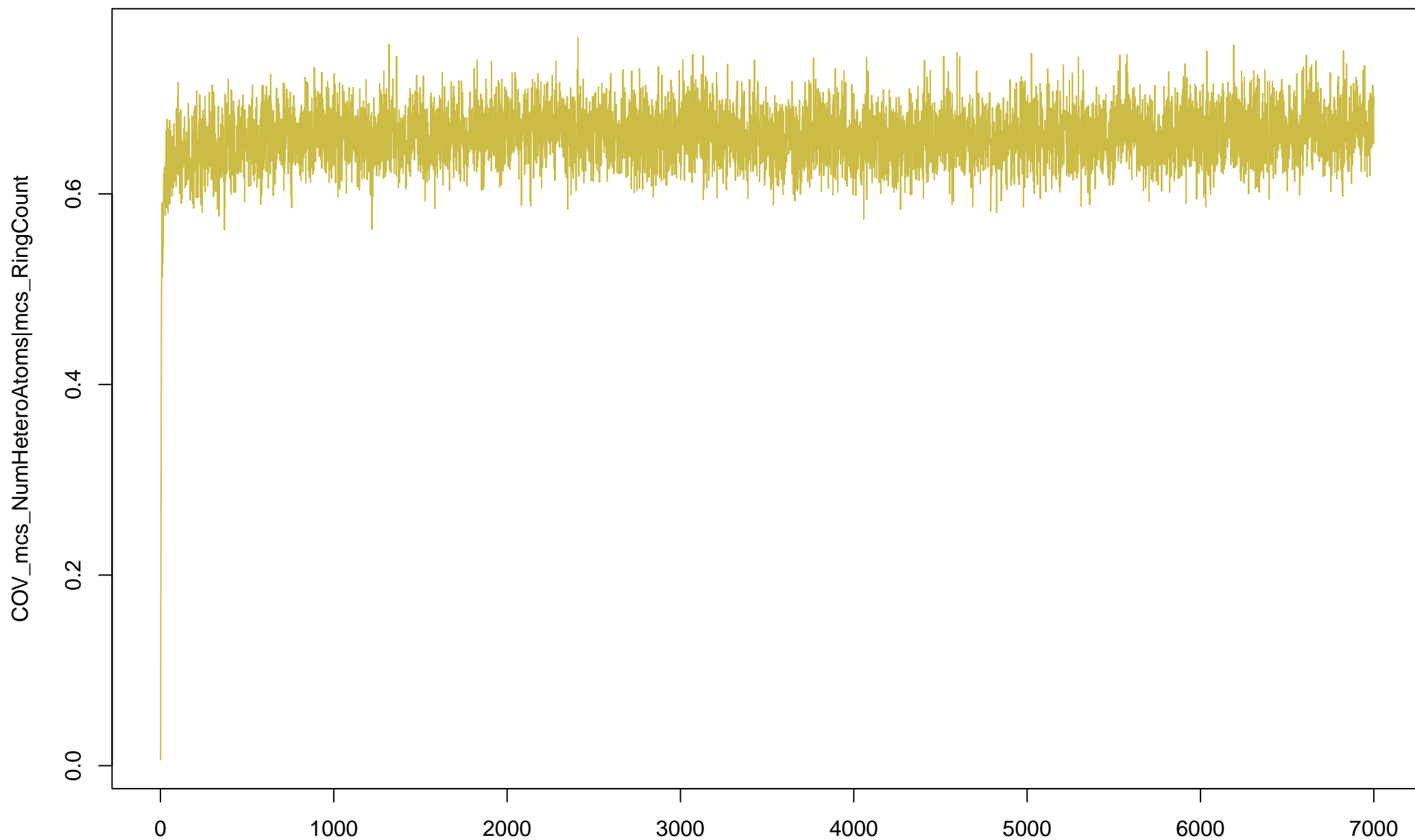
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 249 | BMK = 0.0555 | MCSE(6.27) = 0.908 | stat: FALSE



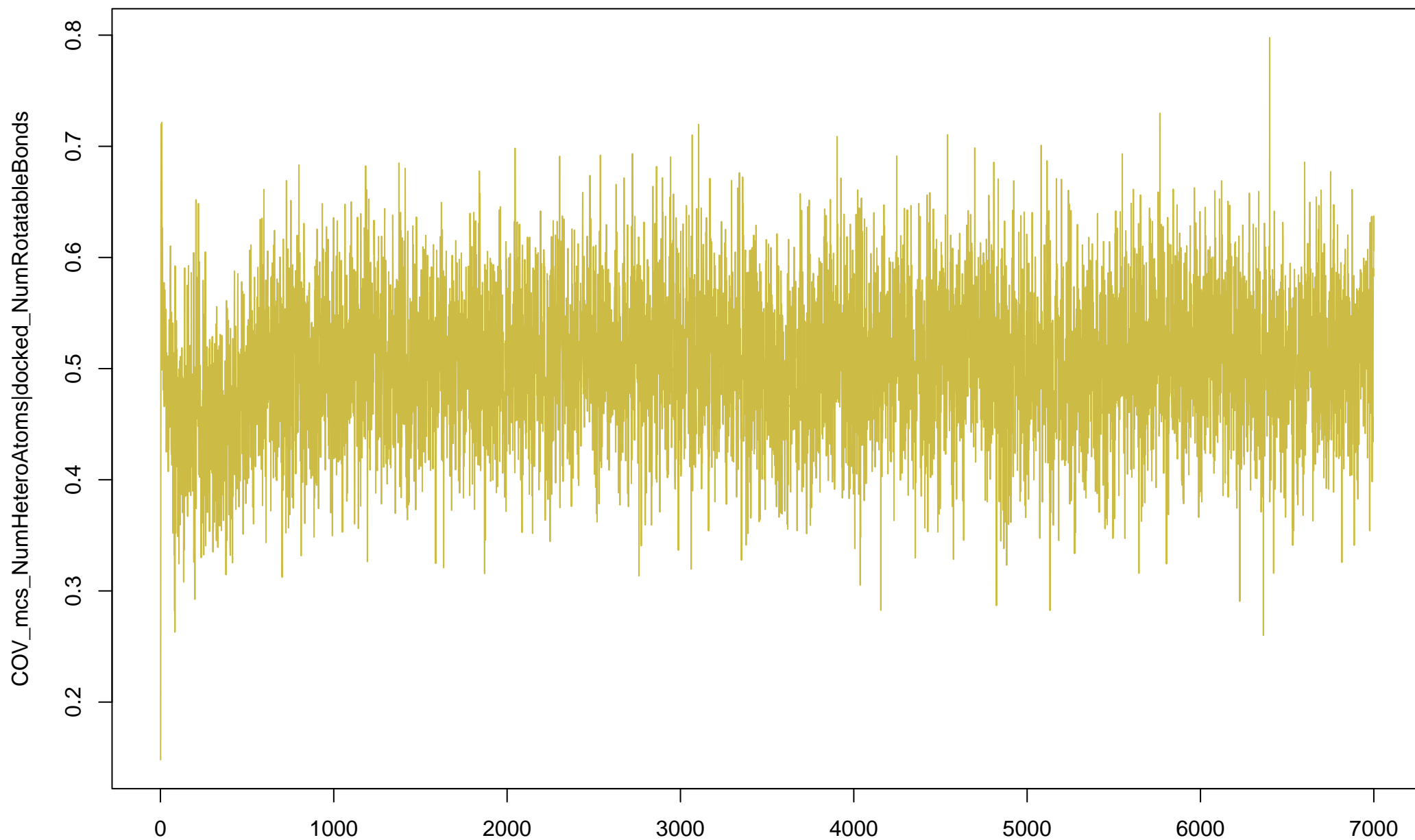
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 49.8 | BMK = 0.28 | MCSE(6.27) = 0.165 | stat: FALSE



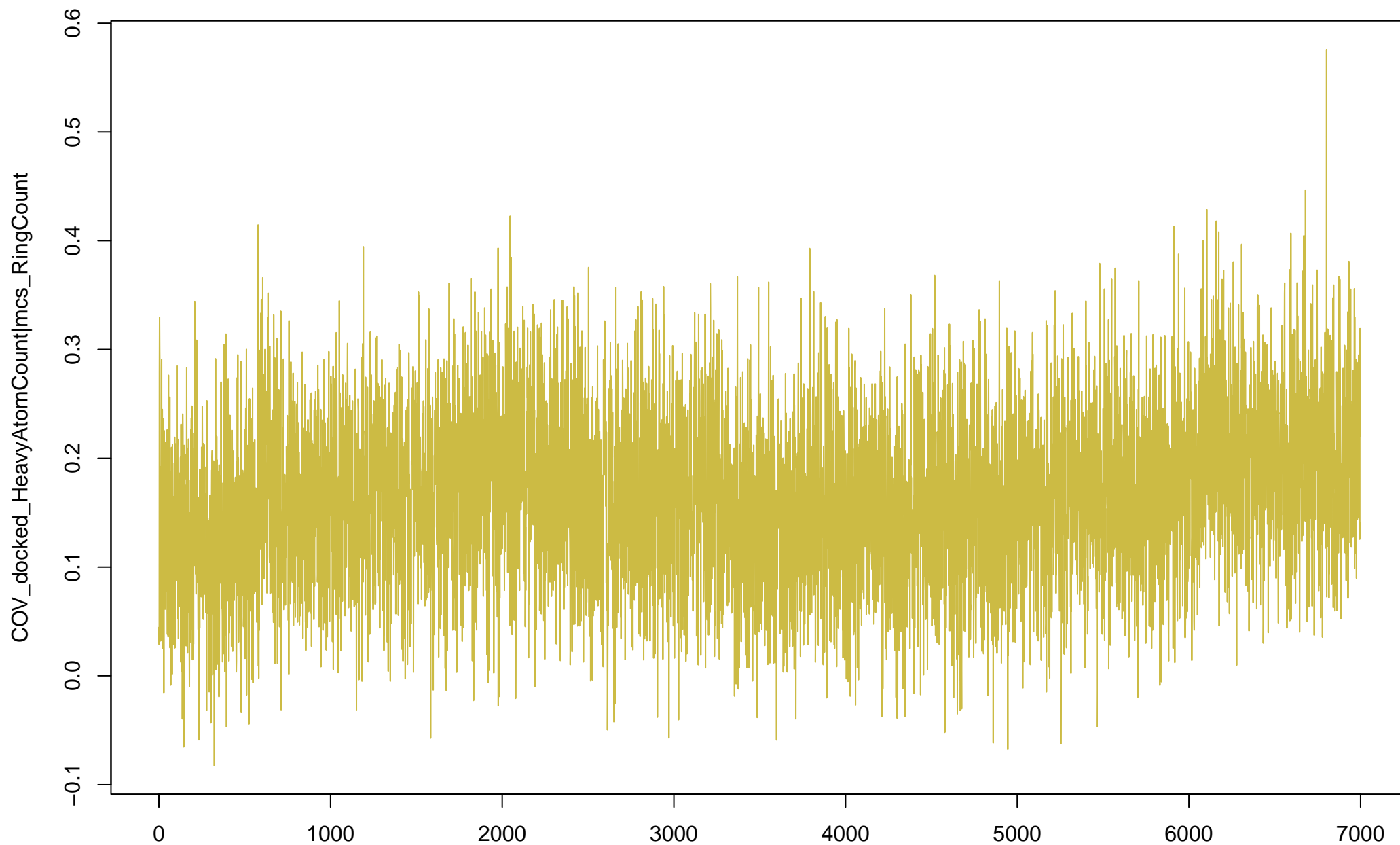
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 782 | BMK = 0.0605 | MCSE(6.27) = 1.06 | stat: FALSE



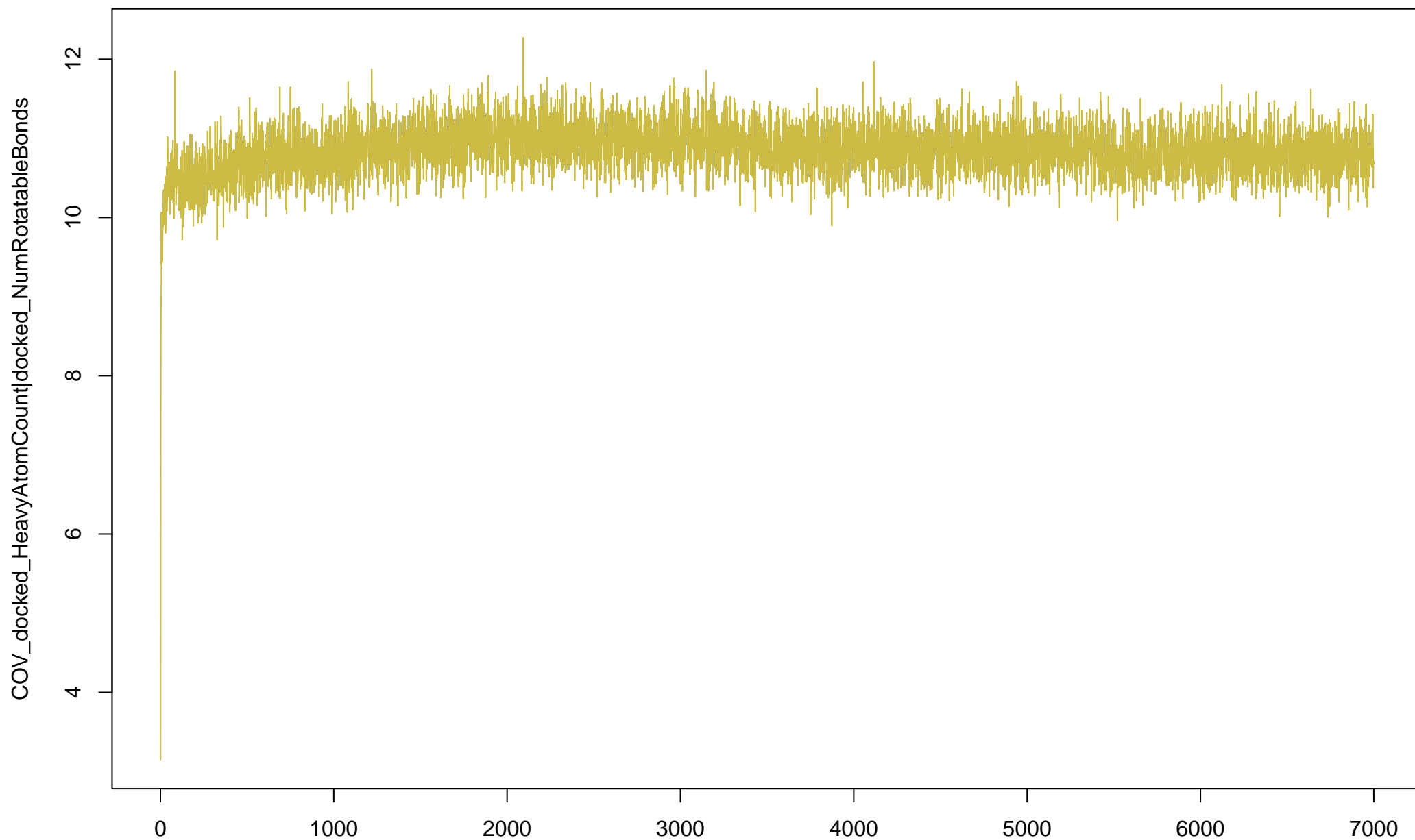
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1000 | BMK = 0.0545 | MCSE(6.27) = 0.506 | stat: FALSE



COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 420 | BMK = 0.0509 | MCSE(6.27) = 0.426 | stat: FALSE



COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 204 | BMK = 0.121 | MCSE(6.27) = 0.102 | stat: FALSE



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 2210 | BMK = 0.0235 | MCSE(6.27) = 1.15 | stat: FALSE

