

-- STATS maxD --

min ESS = 40.5210628006377

max BMK = 0.354614719854092

max MCSE = 16.9854974259466

all stationary: FALSE

burn: 0

-- STATS 2D --

min ESS = 567.092764450263

max BMK = 0.135024329430151

max MCSE = 3.49519020133263

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 256.188878232264

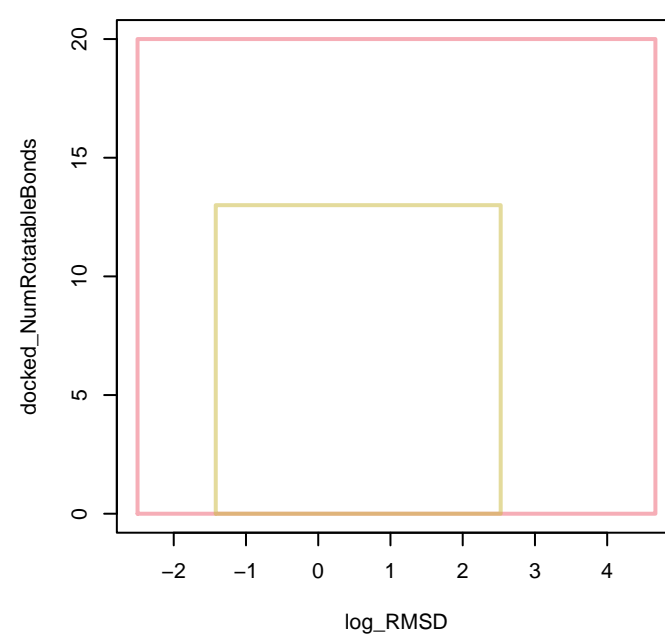
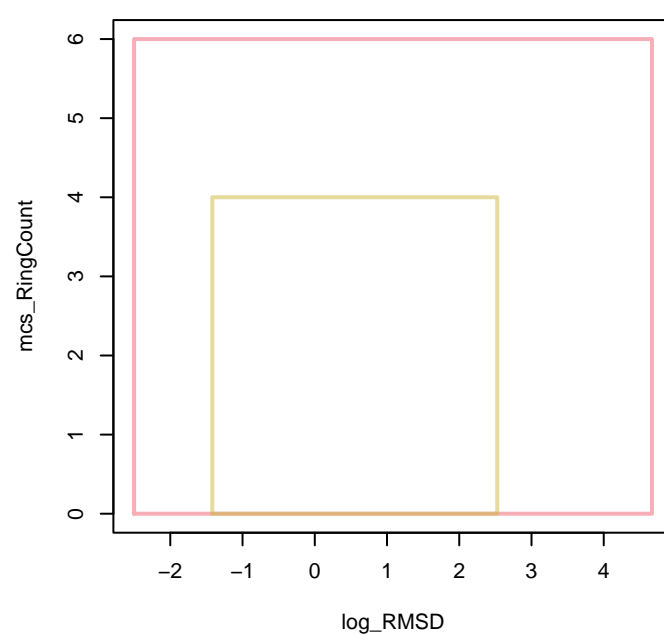
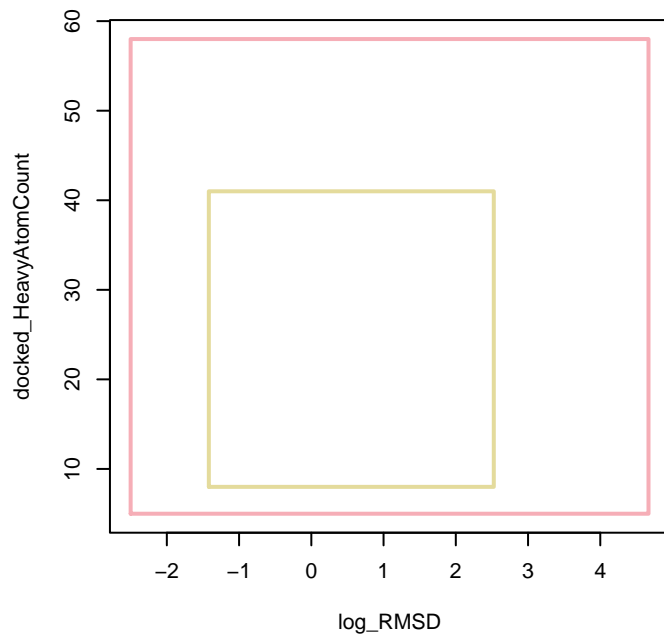
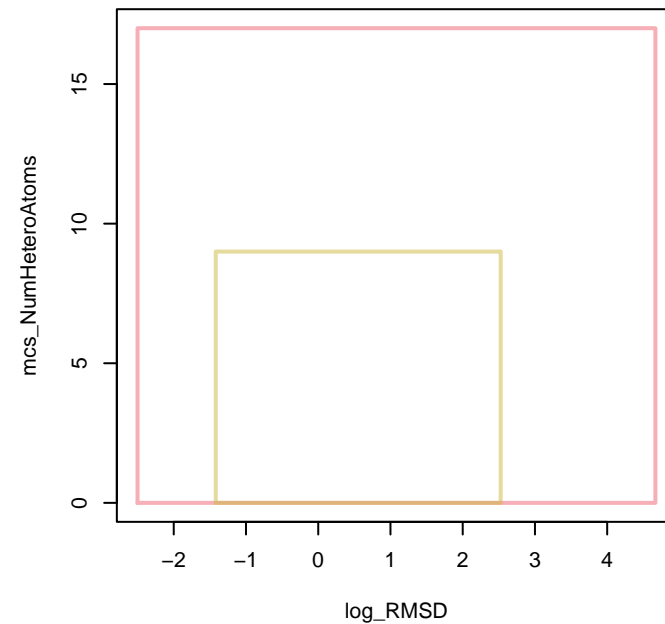
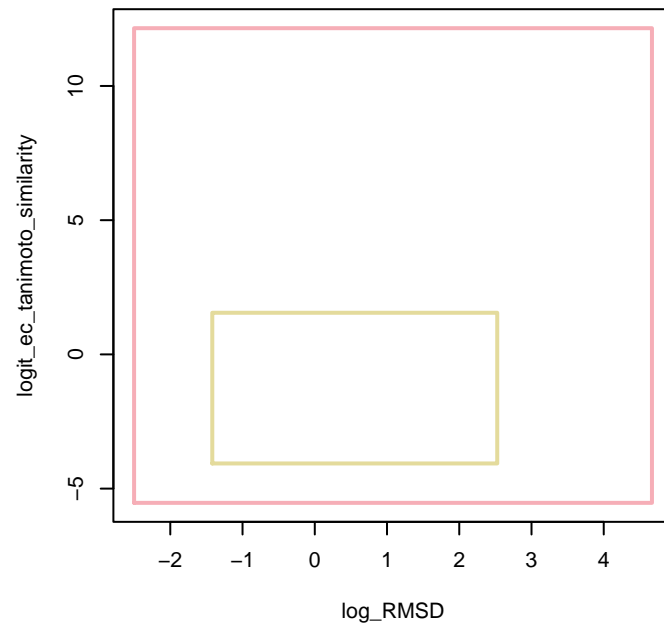
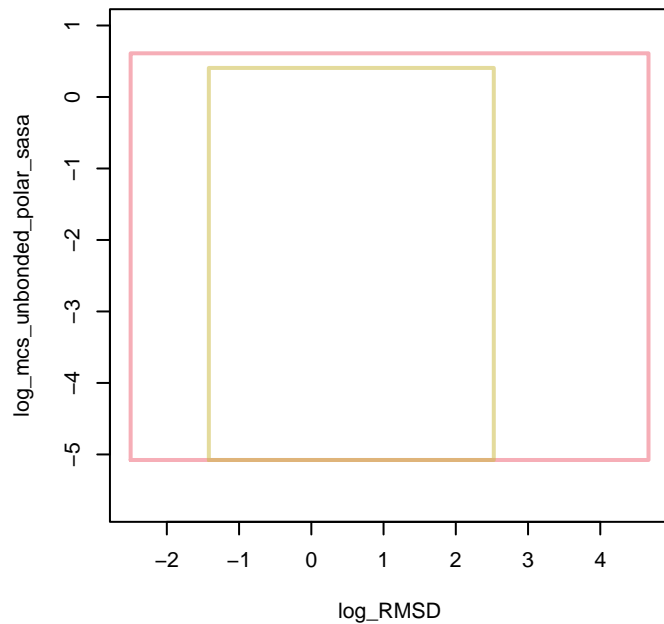
max BMK = 0.0964402588973305

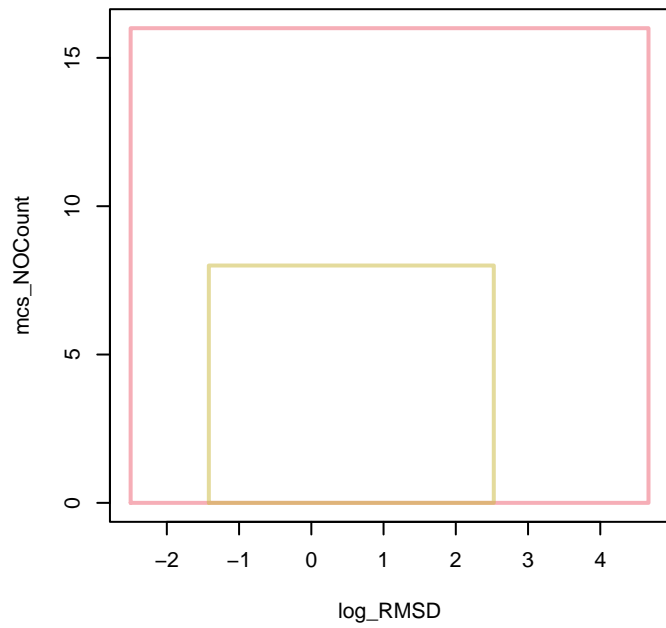
max MCSE = 3.48991066375812

all stationary: FALSE

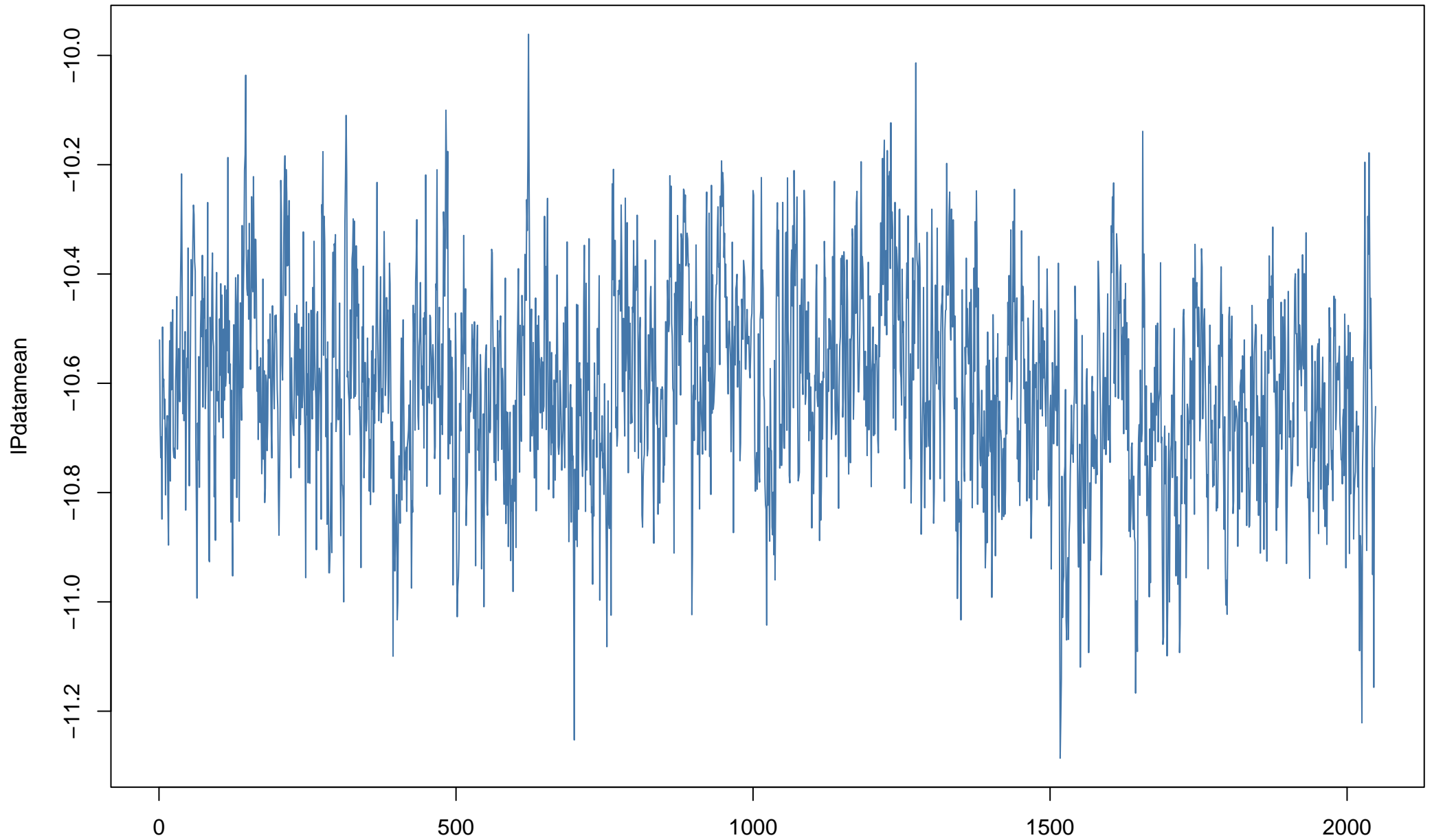
burn: 0

Occupied clusters: 20 of 64

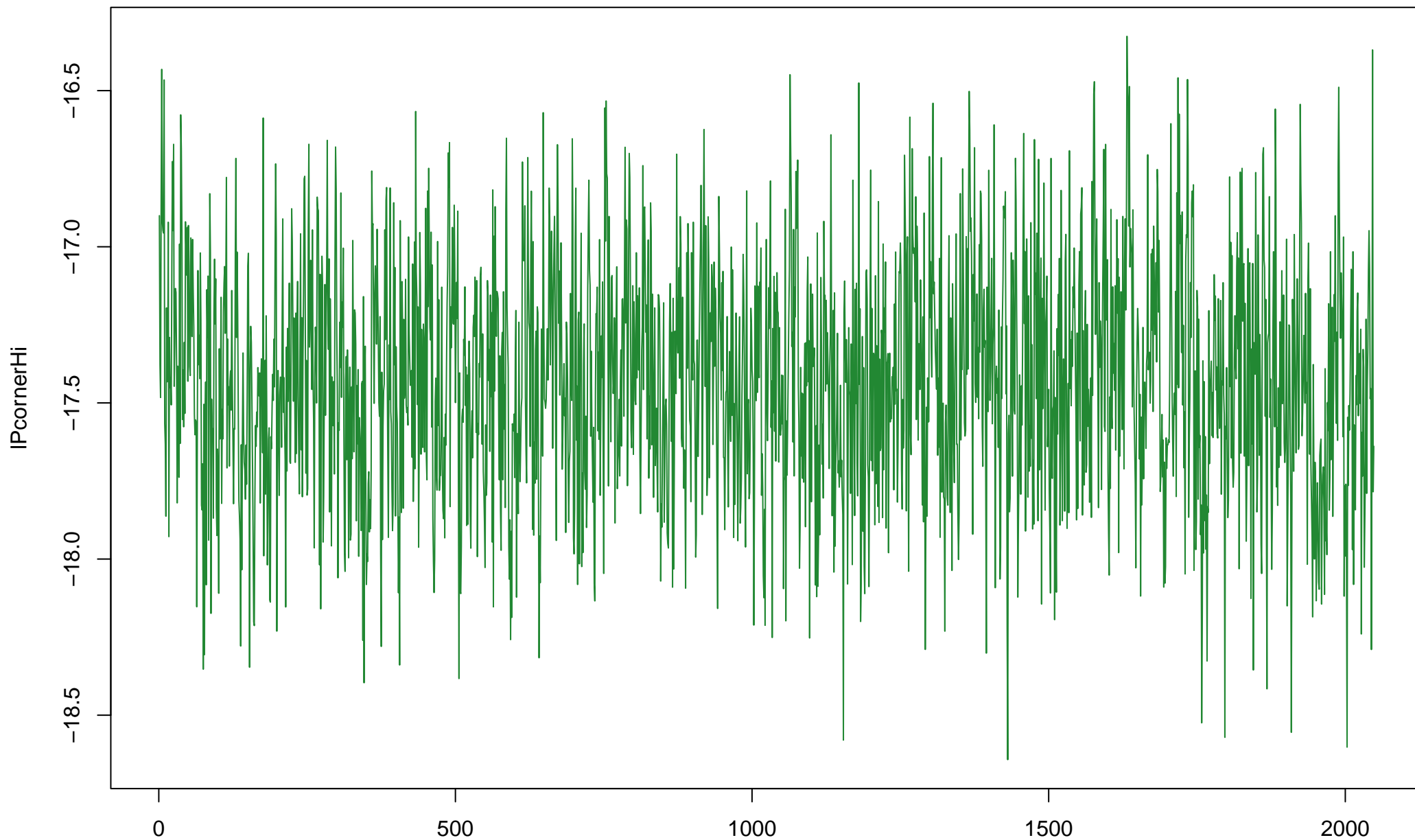




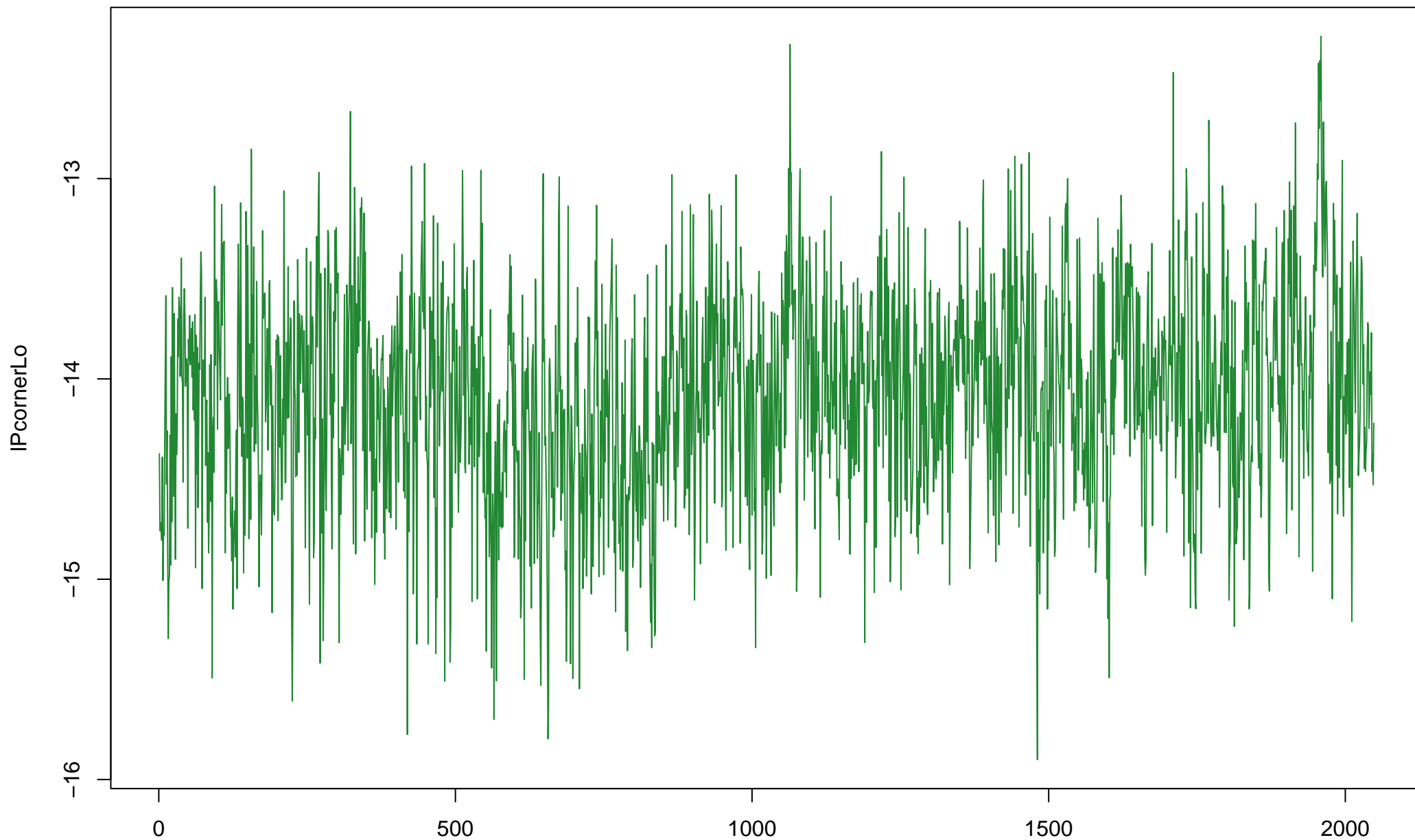
IPdatamean
ESS = 321 | BMK = 0.0878 | MCSE(6.27) = 7.72 | stat: FALSE | burn: 0



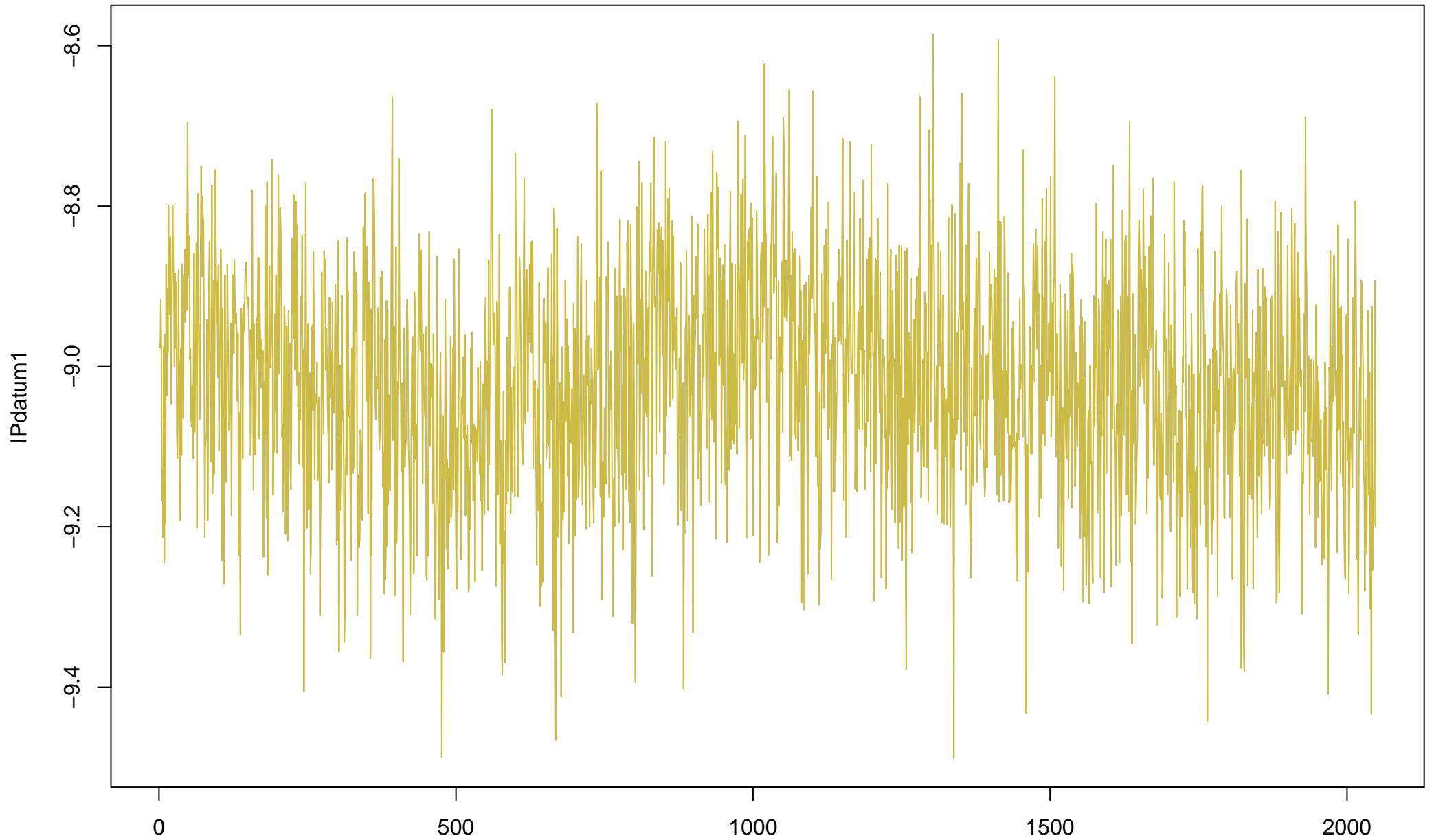
IPcornerHi
ESS = 778 | BMK = 0.051 | MCSE(6.27) = 4.3 | stat: TRUE | burn: 0



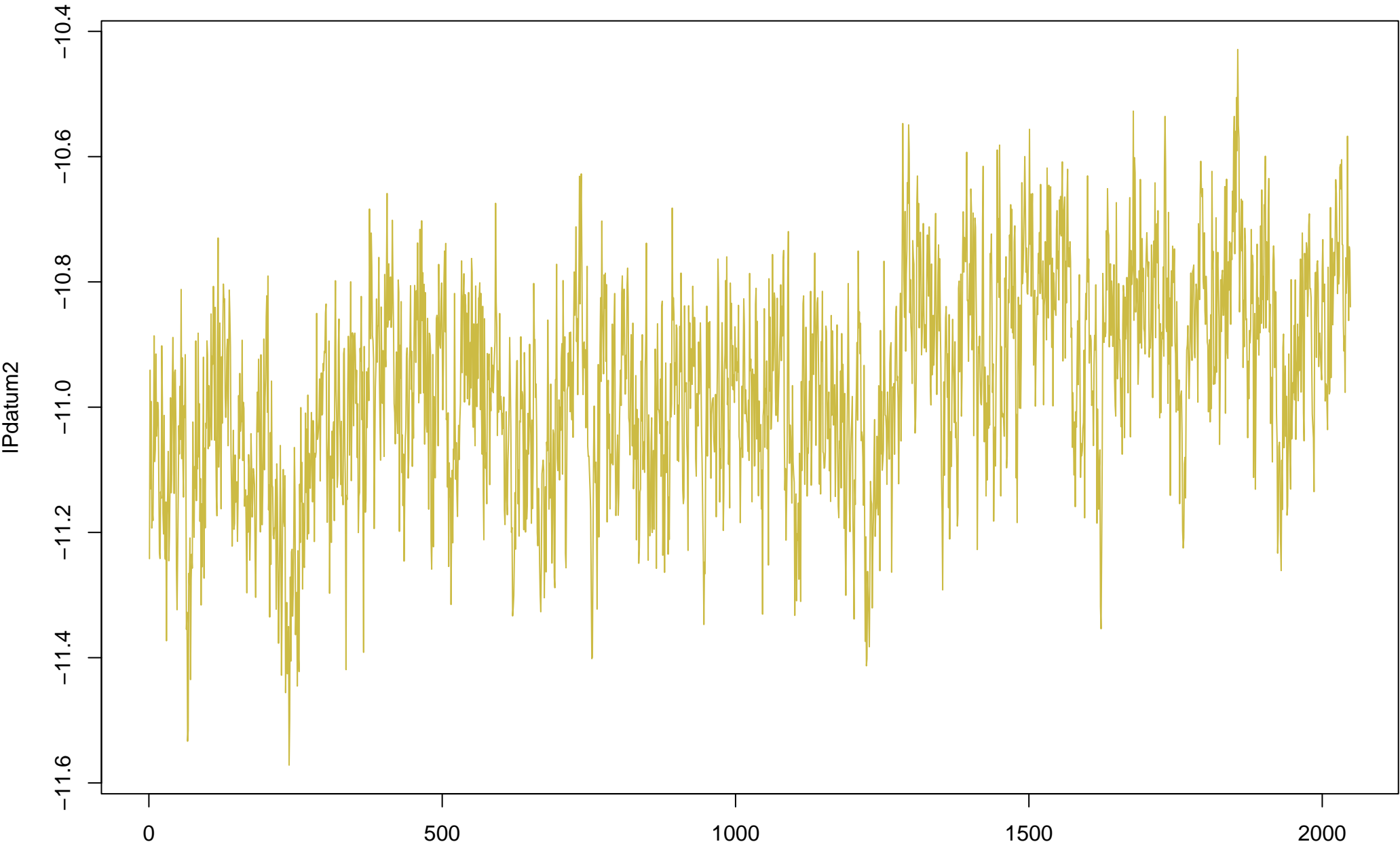
IPcornerLo
ESS = 343 | BMK = 0.13 | MCSE(6.27) = 5.22 | stat: TRUE | burn: 0



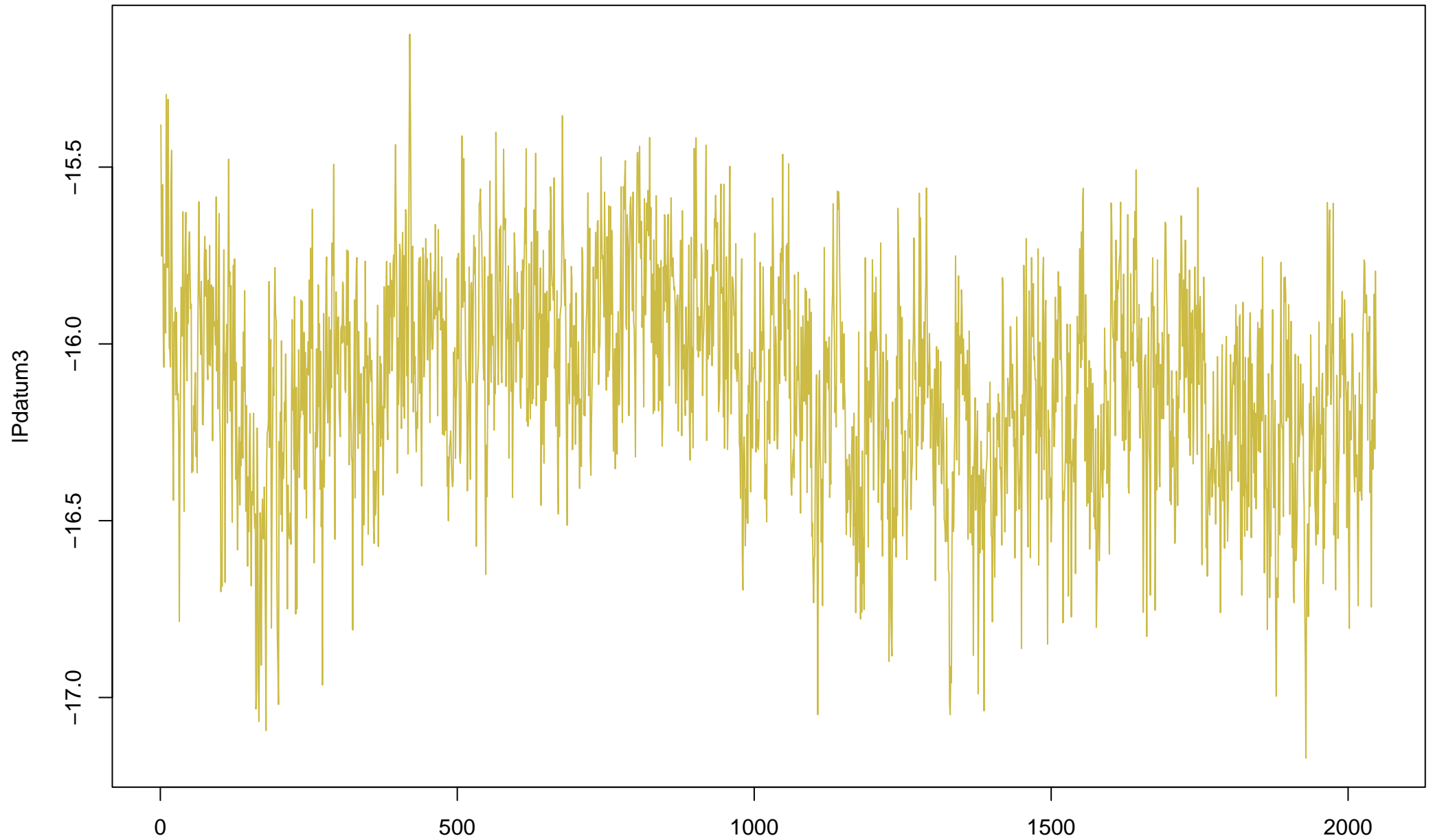
IPdatum1
ESS = 748 | BMK = 0.0414 | MCSE(6.27) = 4.75 | stat: FALSE | burn: 0



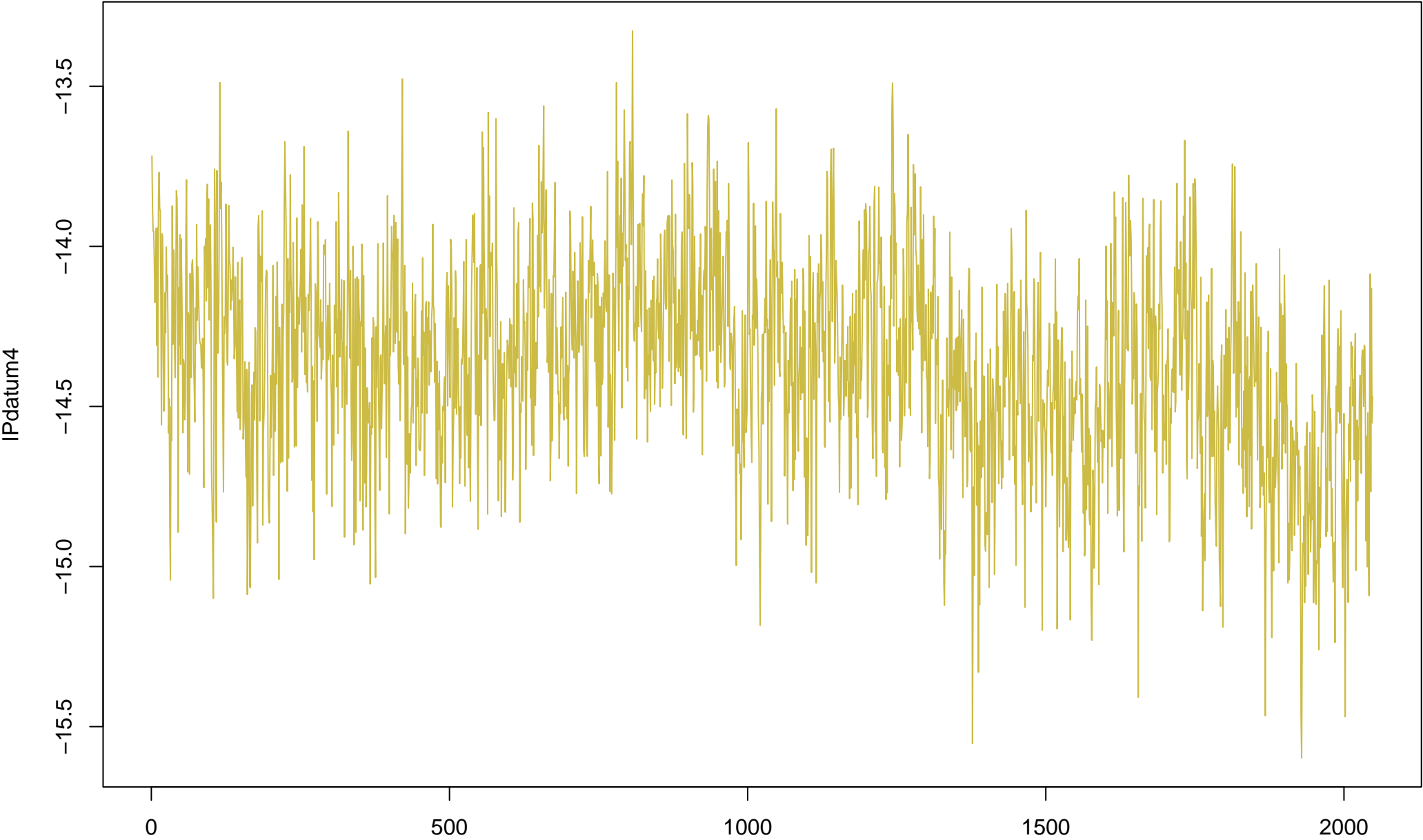
IPdatum2
ESS = 55.7 | BMK = 0.292 | MCSE(6.27) = 10.8 | stat: FALSE | burn: 0



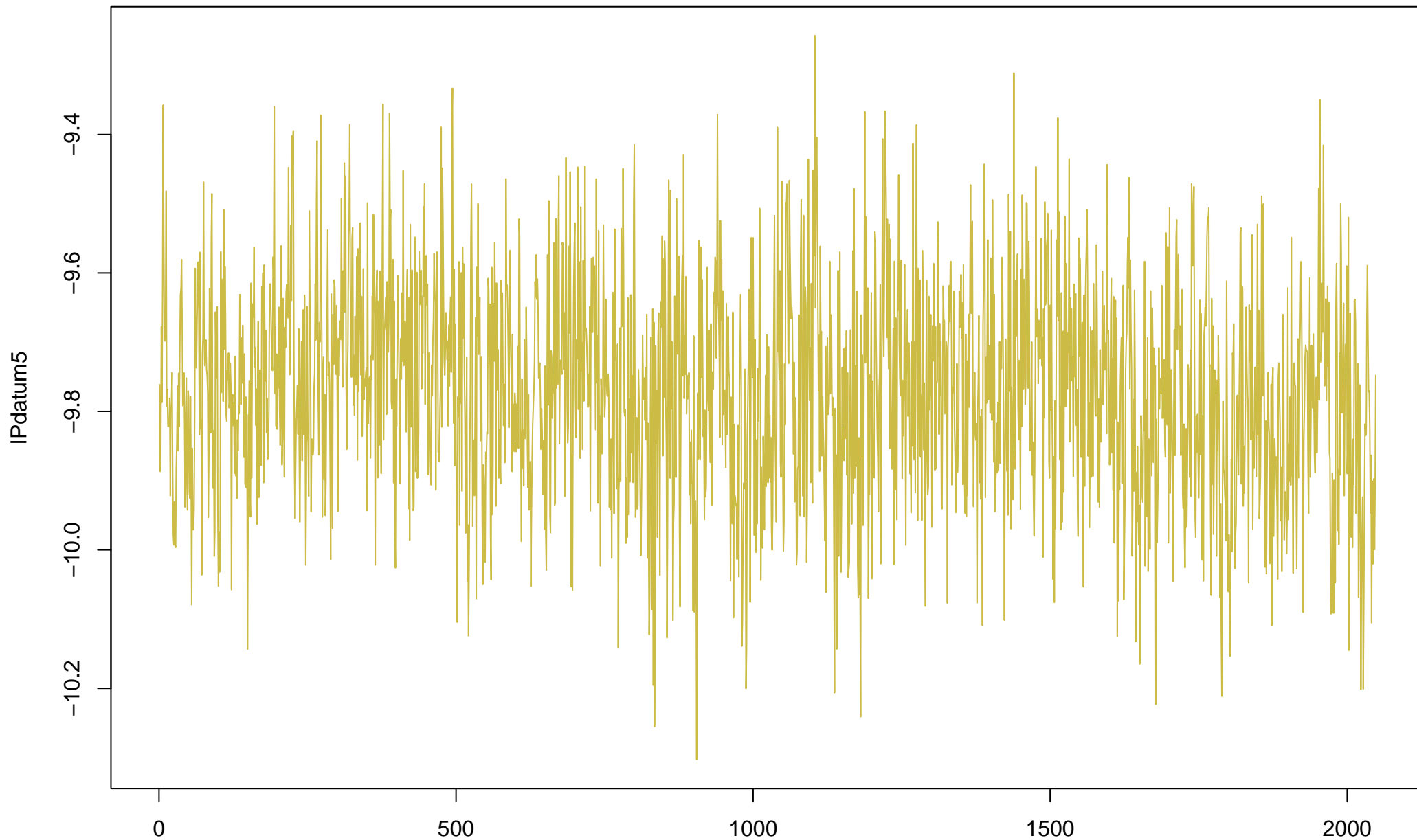
IPdatum3
ESS = 102 | BMK = 0.225 | MCSE(6.27) = 9.45 | stat: TRUE | burn: 0



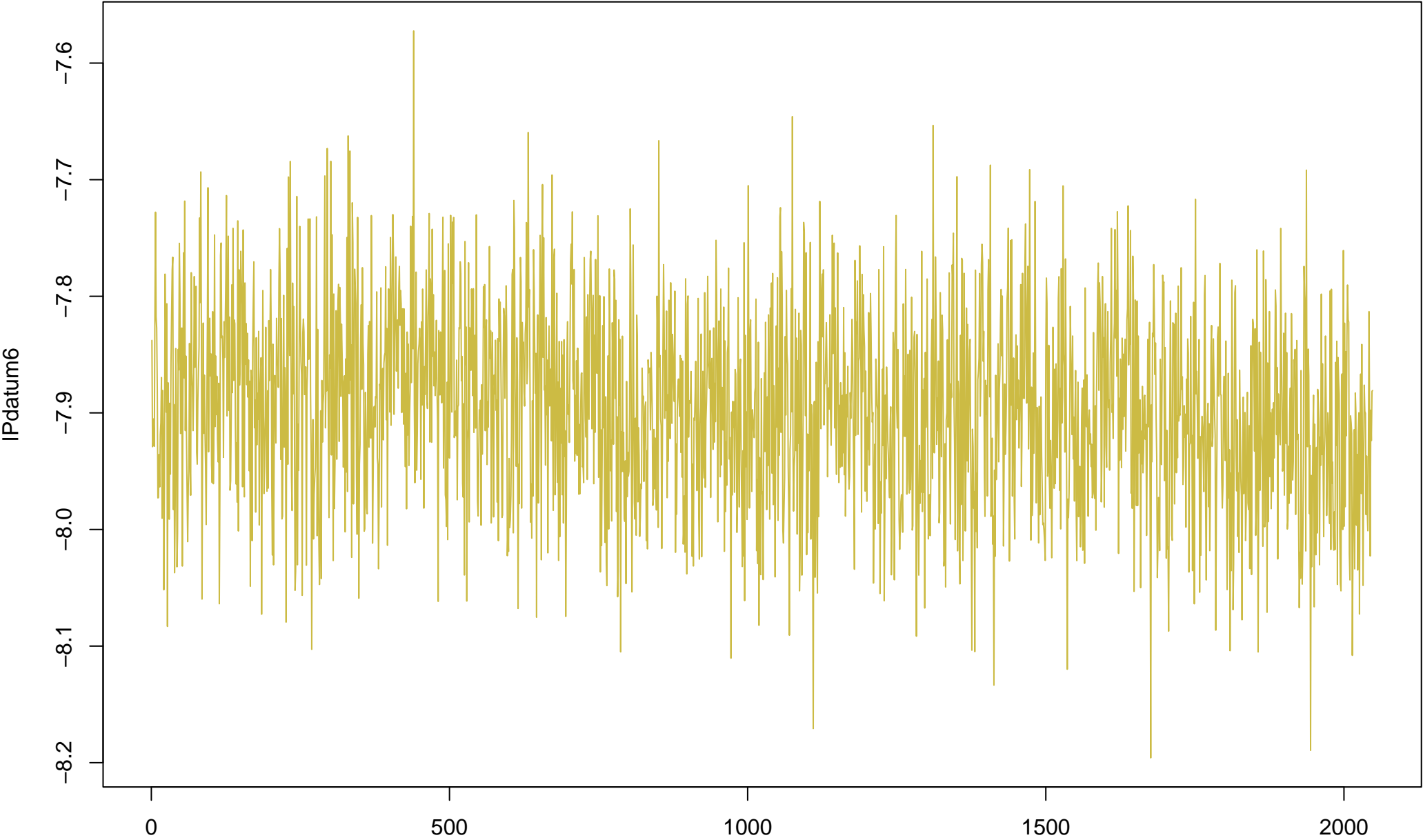
IPdatum4
ESS = 139 | BMK = 0.199 | MCSE(6.27) = 7.19 | stat: FALSE | burn: 0



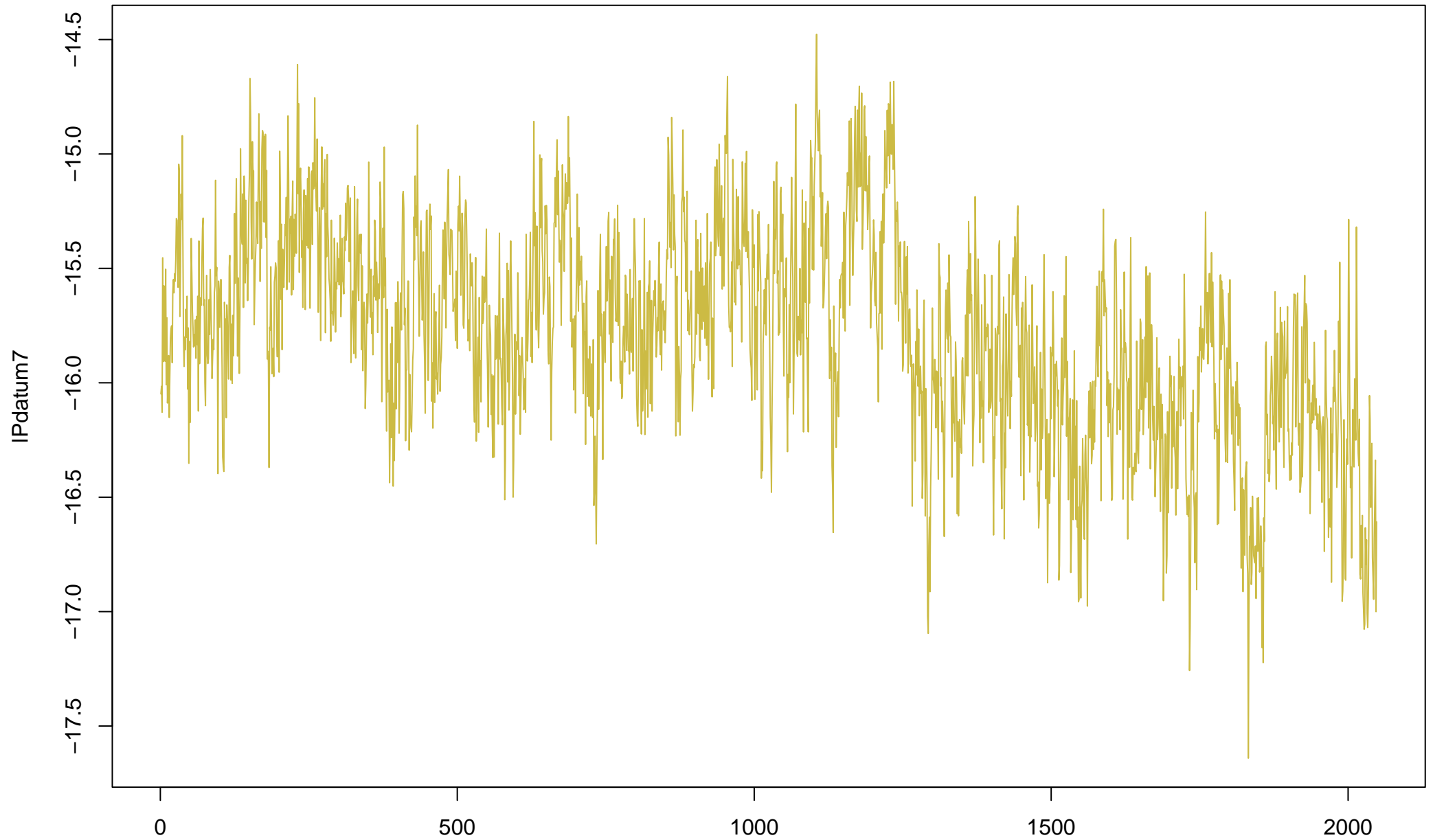
IPdatum5
ESS = 700 | BMK = 0.0689 | MCSE(6.27) = 5.1 | stat: TRUE | burn: 0



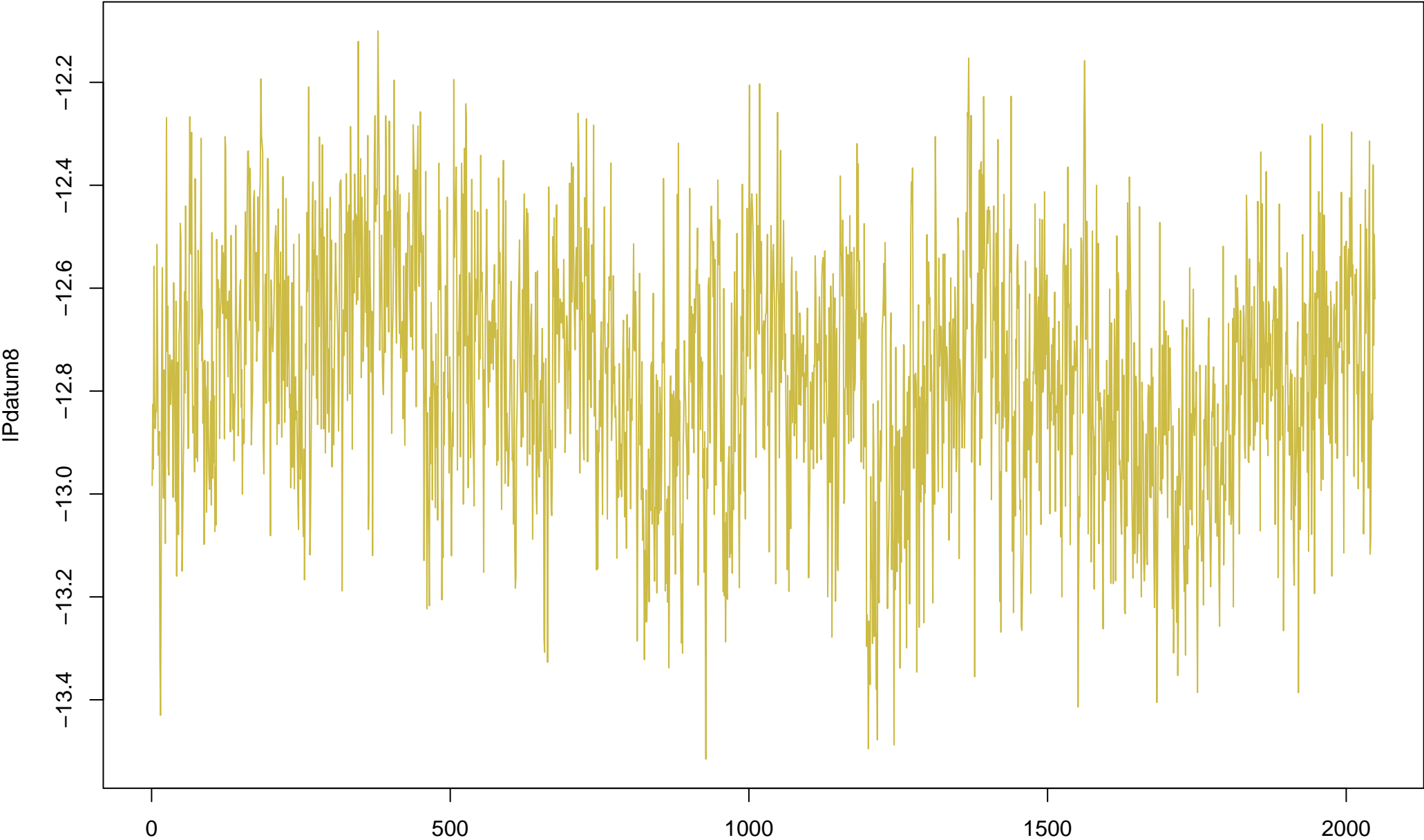
IPdatum6
ESS = 777 | BMK = 0.102 | MCSE(6.27) = 3.72 | stat: FALSE | burn: 0



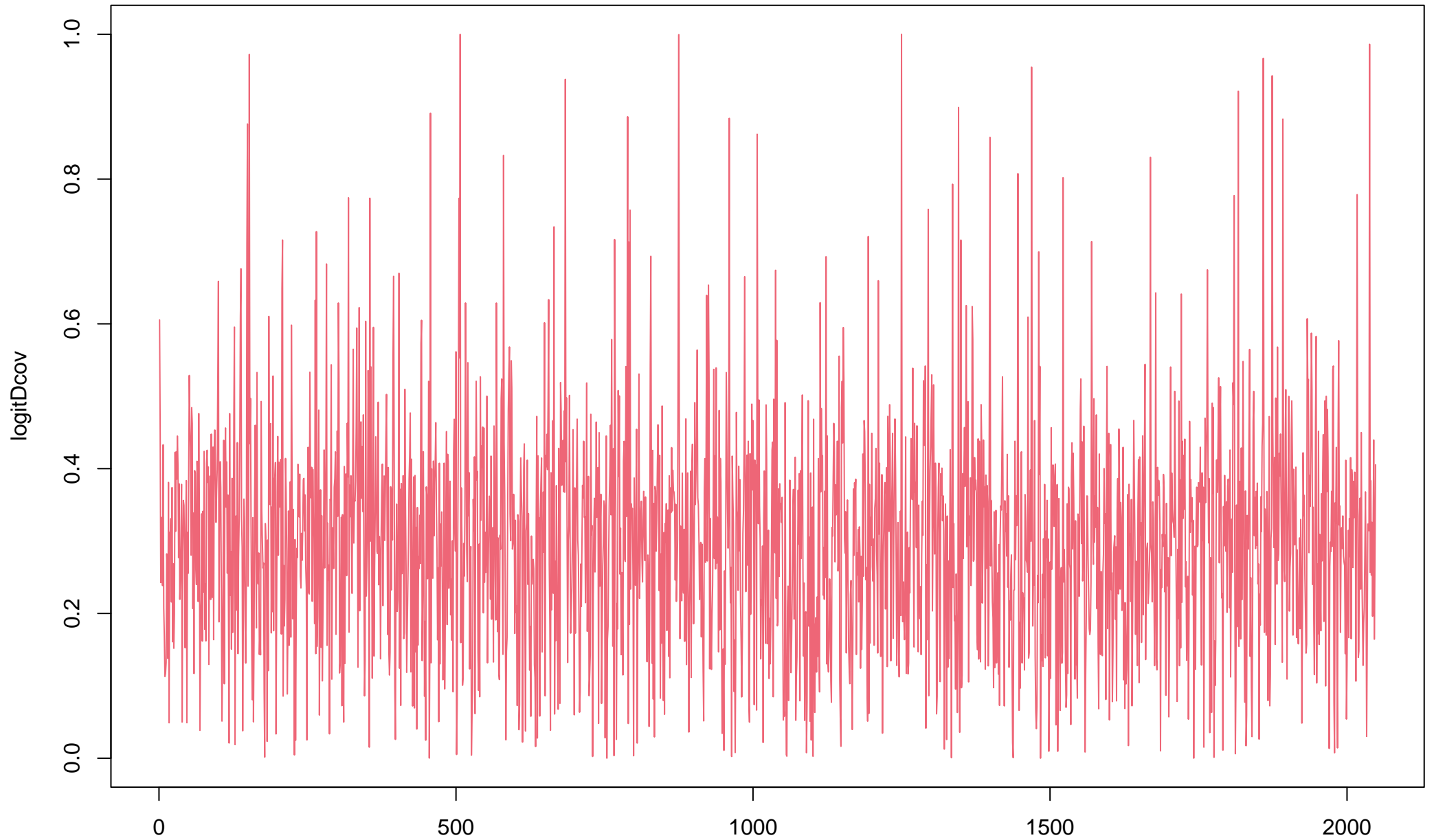
IPdatum7
ESS = 40.5 | BMK = 0.355 | MCSE(6.27) = 17 | stat: FALSE | burn: 0



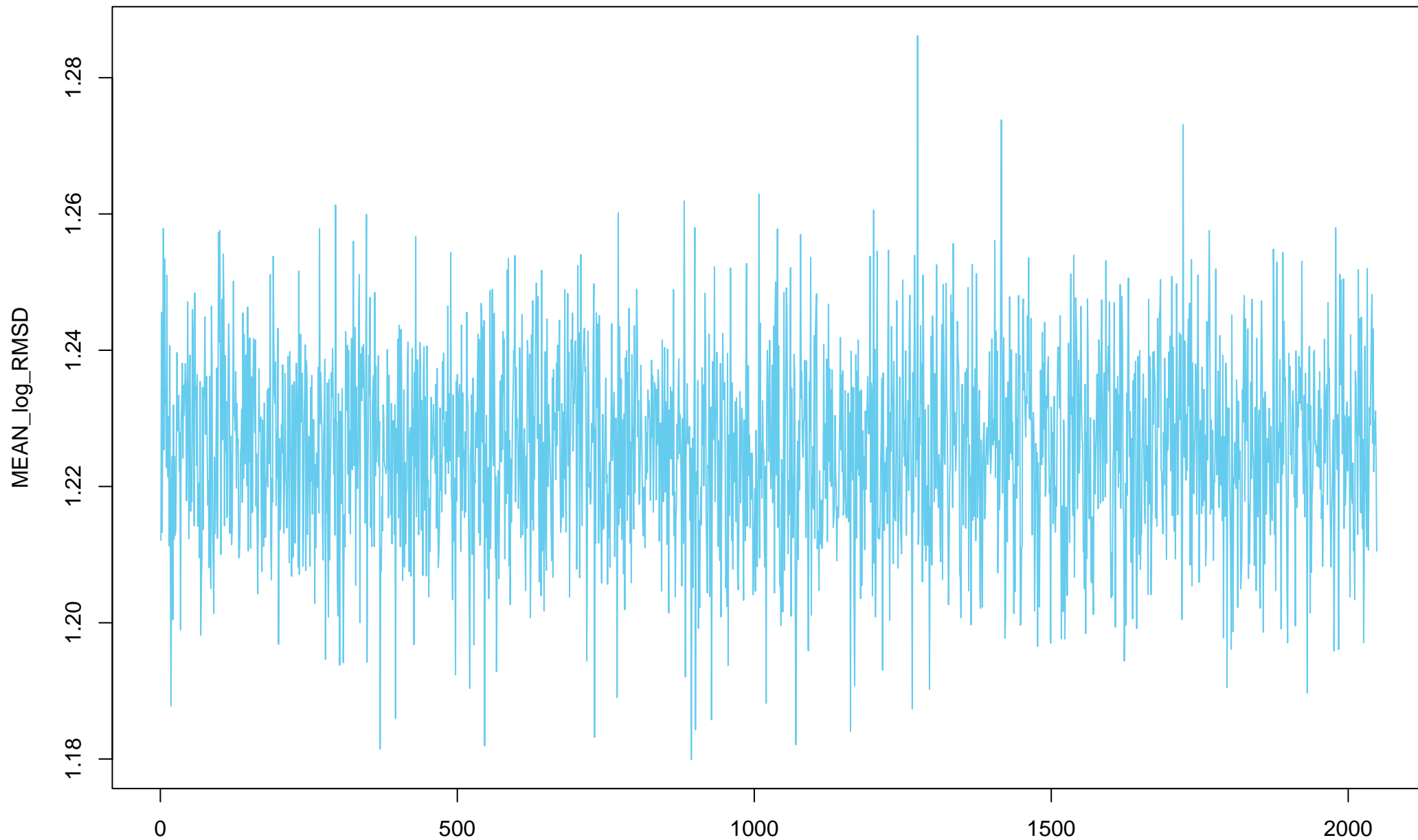
IPdatum8
ESS = 161 | BMK = 0.121 | MCSE(6.27) = 6.72 | stat: FALSE | burn: 0



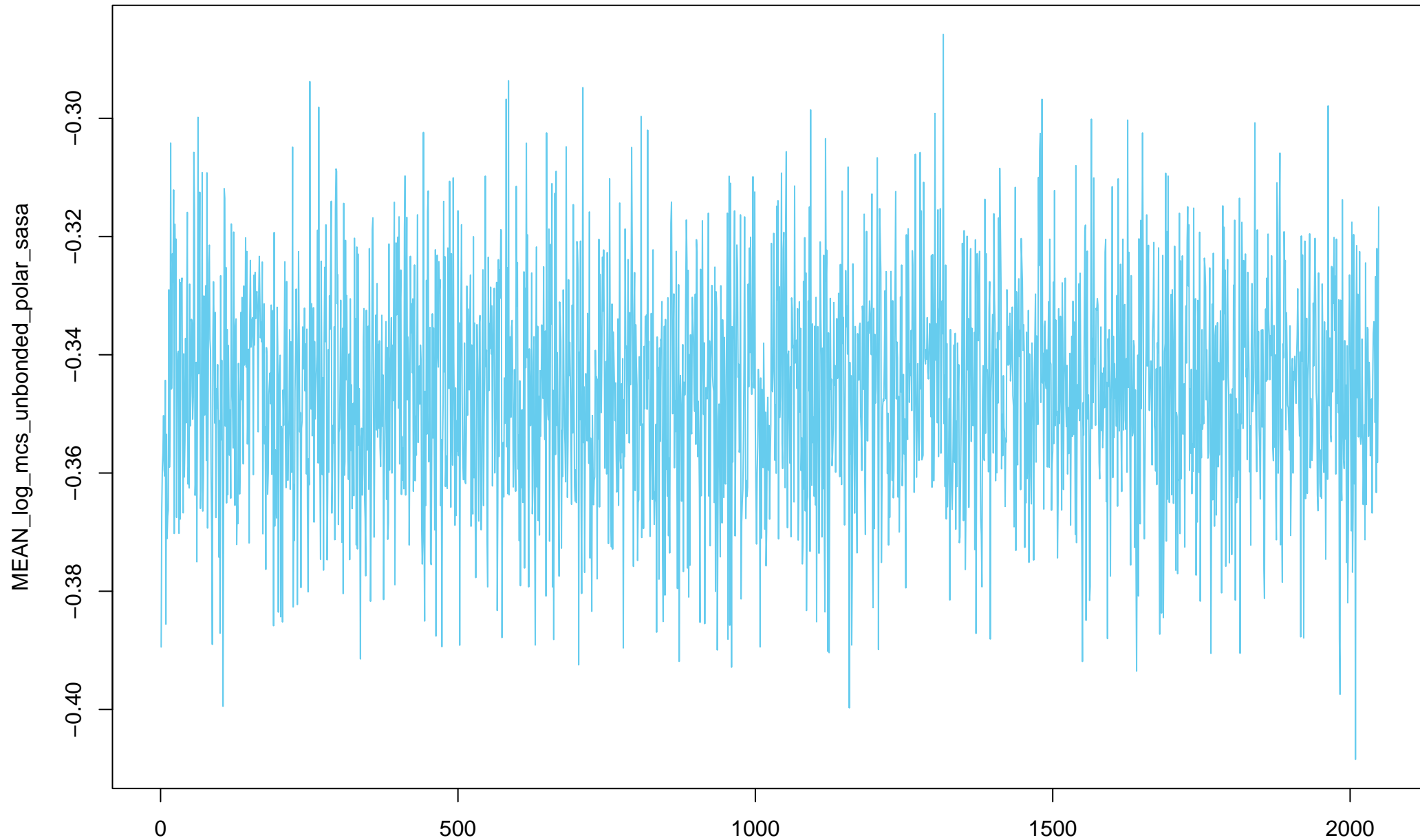
logitDcov
ESS = 1720 | BMK = 0.0504 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0



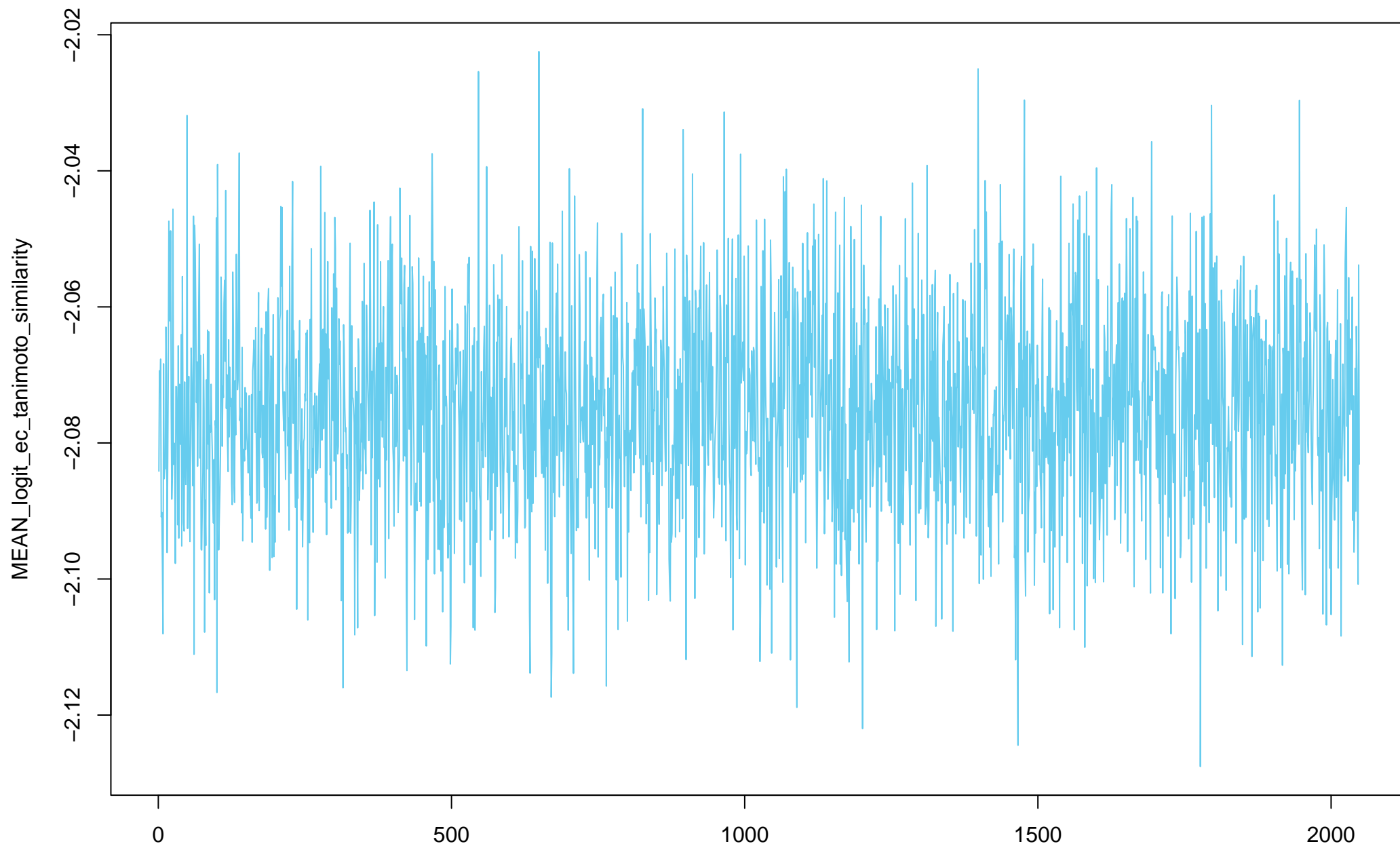
MEAN_log_RMSD
ESS = 1870 | BMK = 0.0669 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0



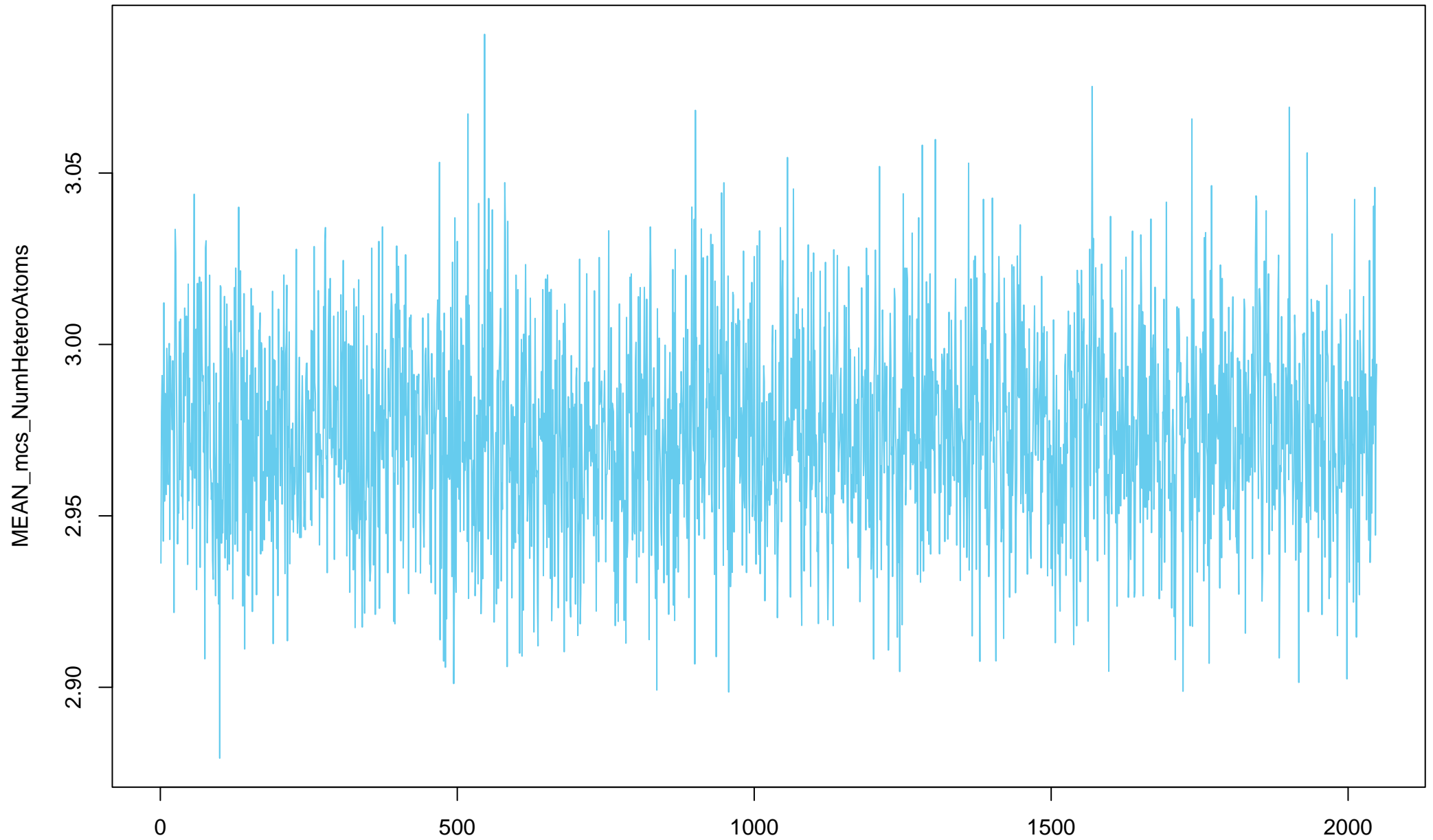
MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0487 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0



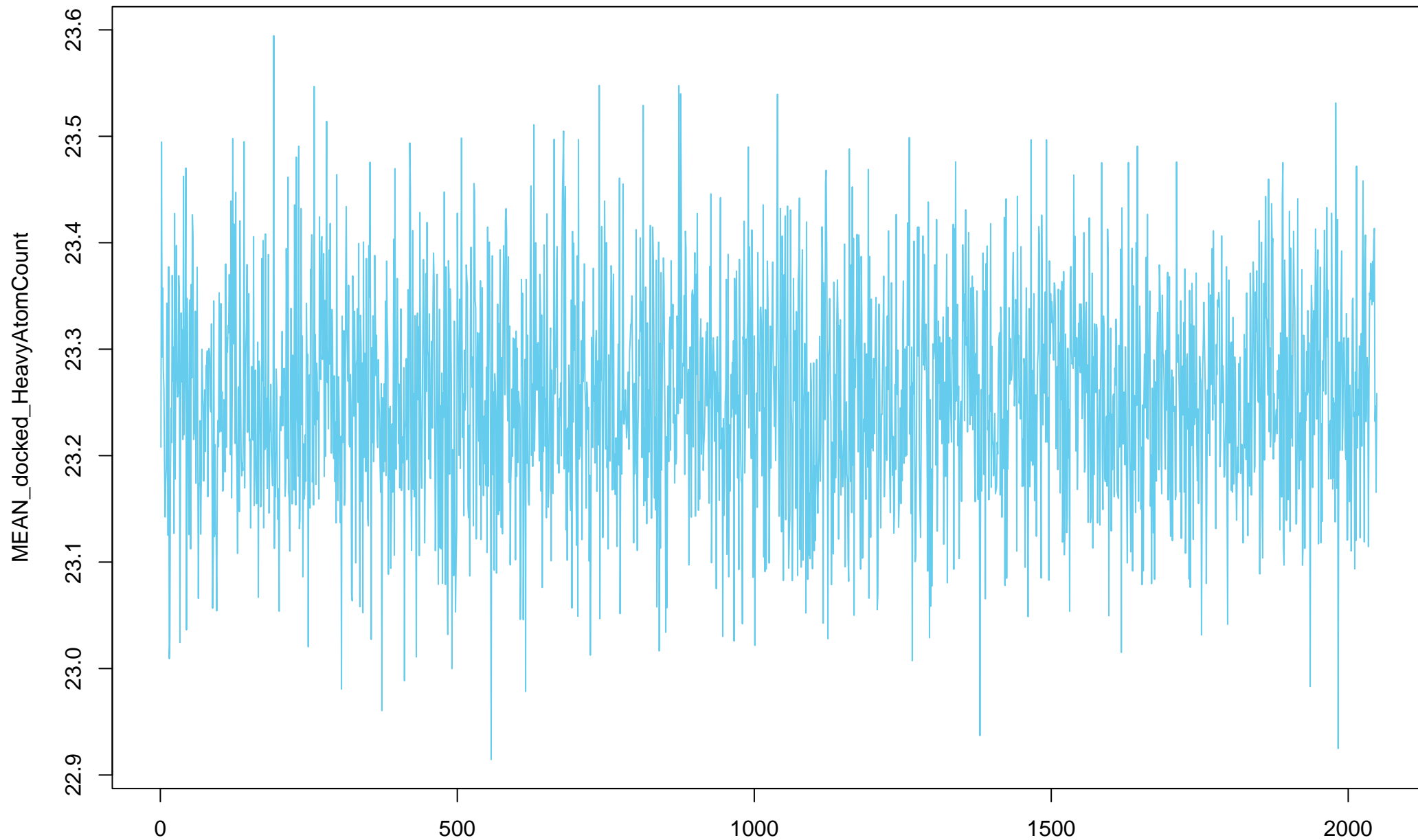
MEAN_logit_ec_tanimoto_similarity
ESS = 1890 | BMK = 0.0506 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0



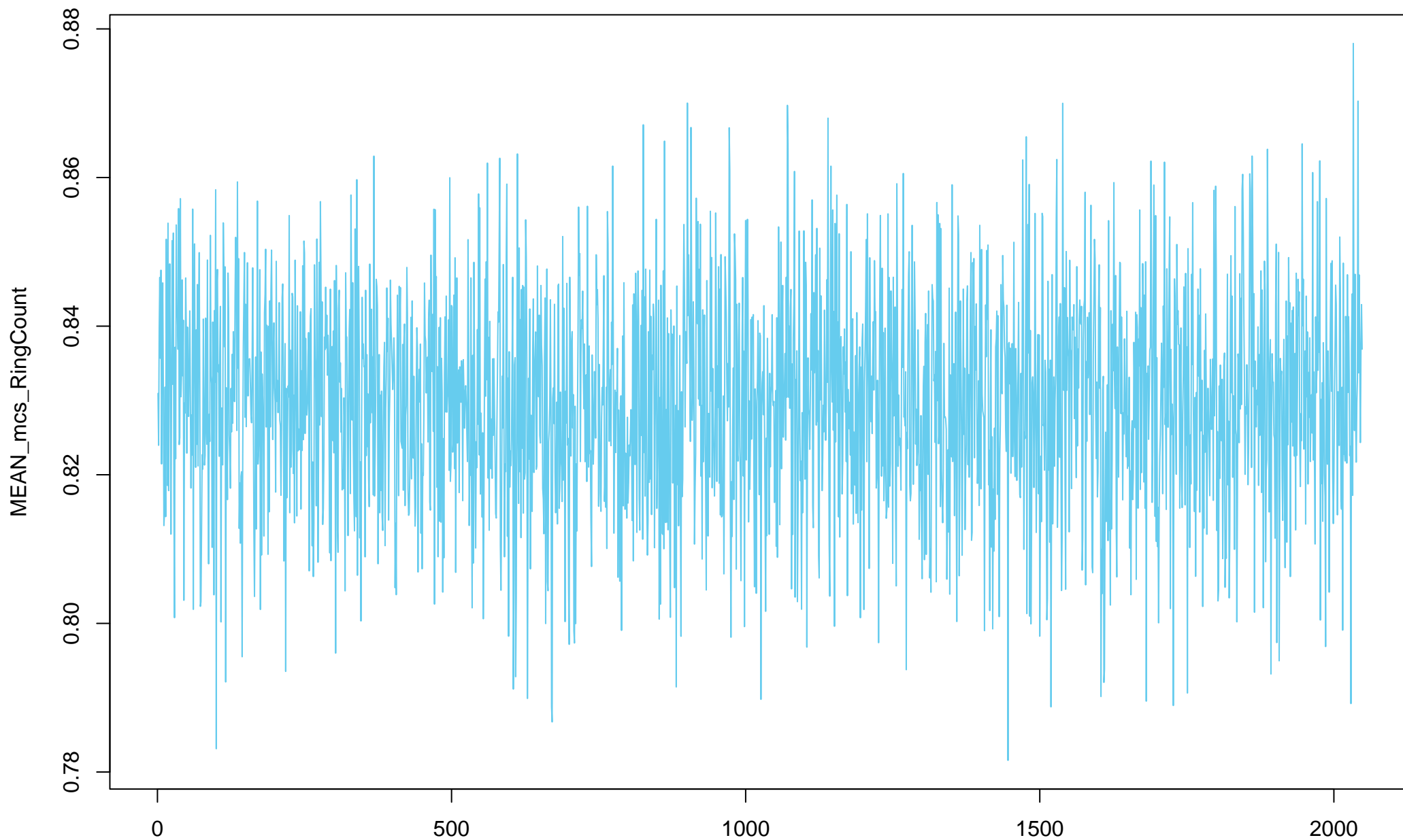
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.048 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0



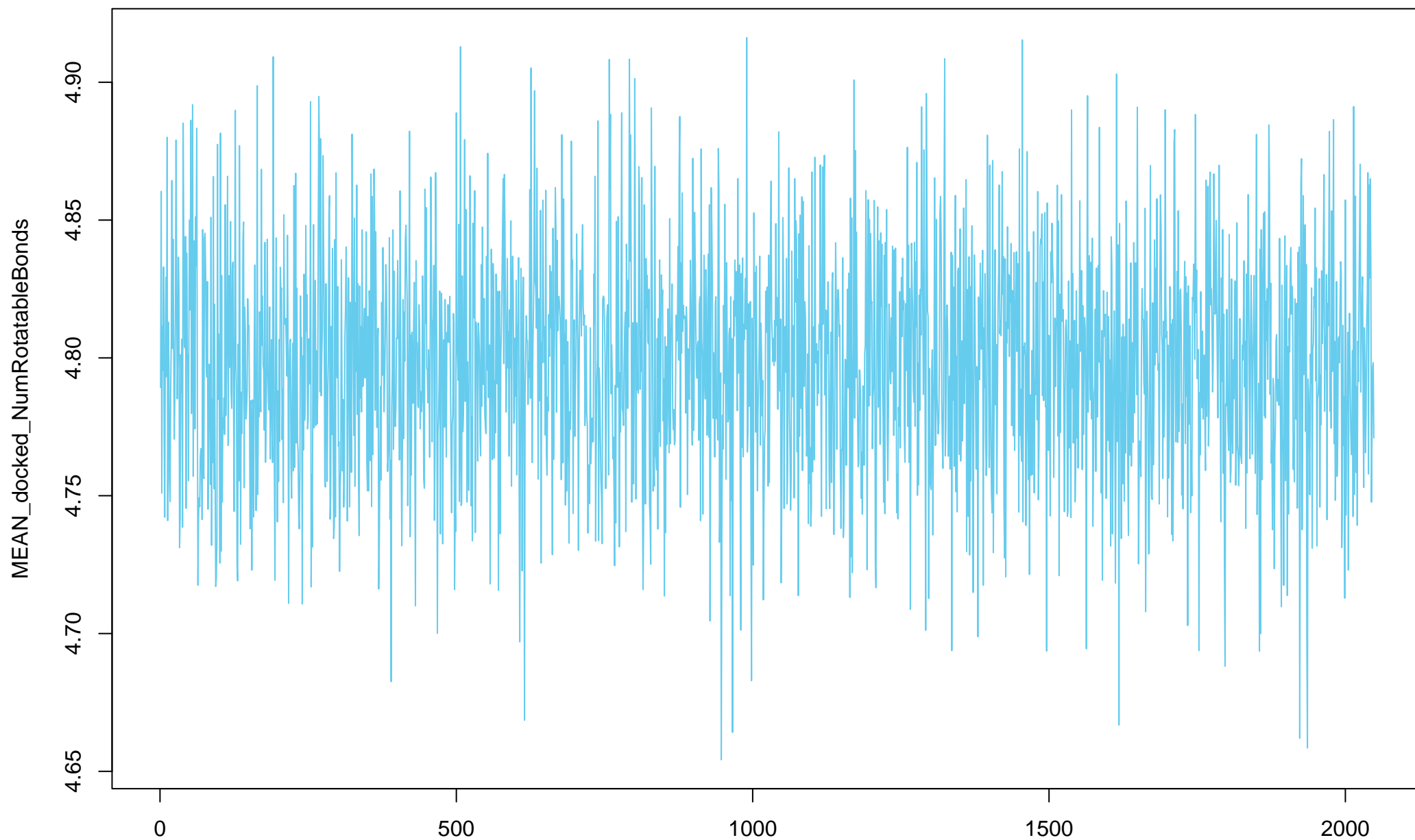
MEAN_docked_HeavyAtomCount
ESS = 1970 | BMK = 0.0583 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0



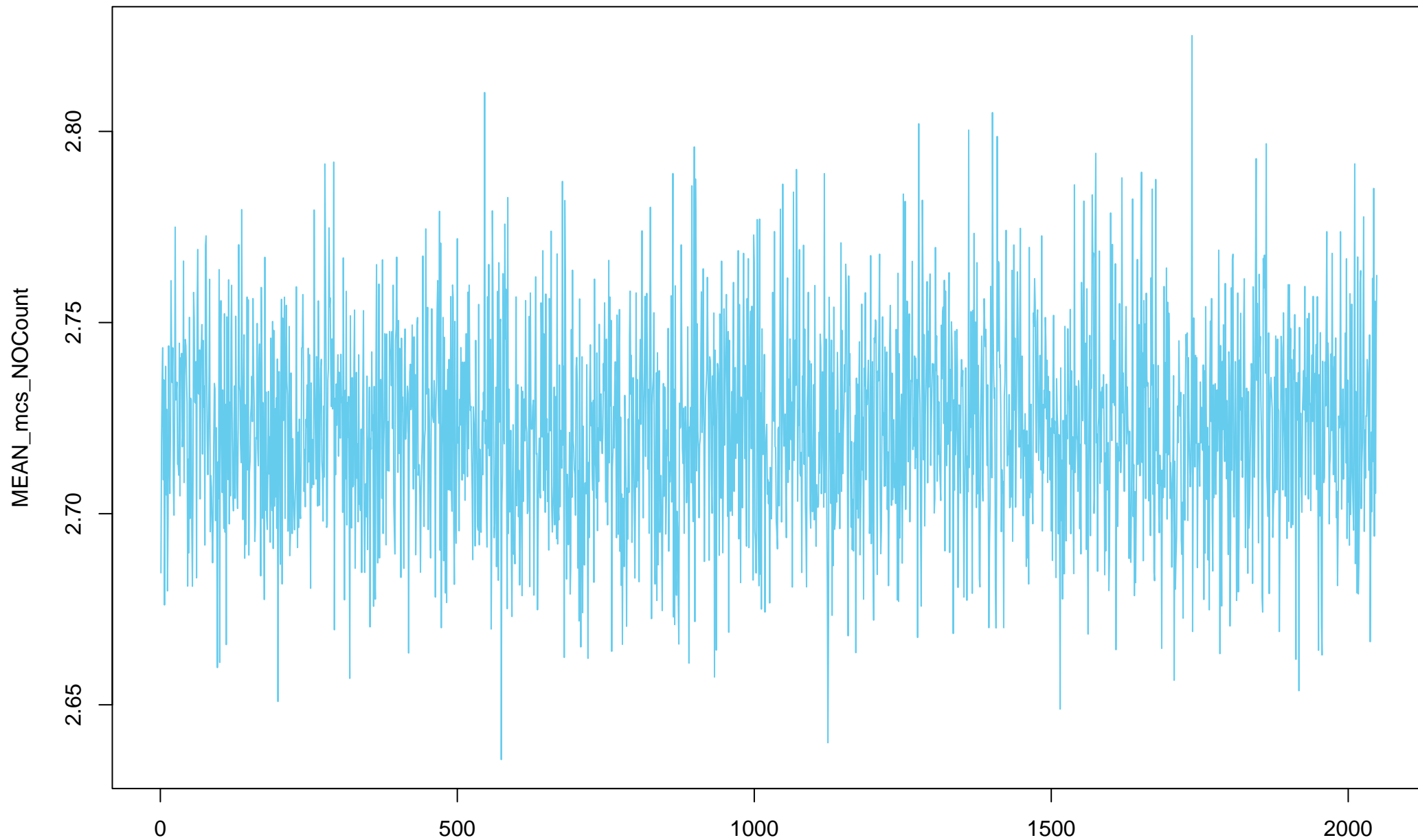
MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0416 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



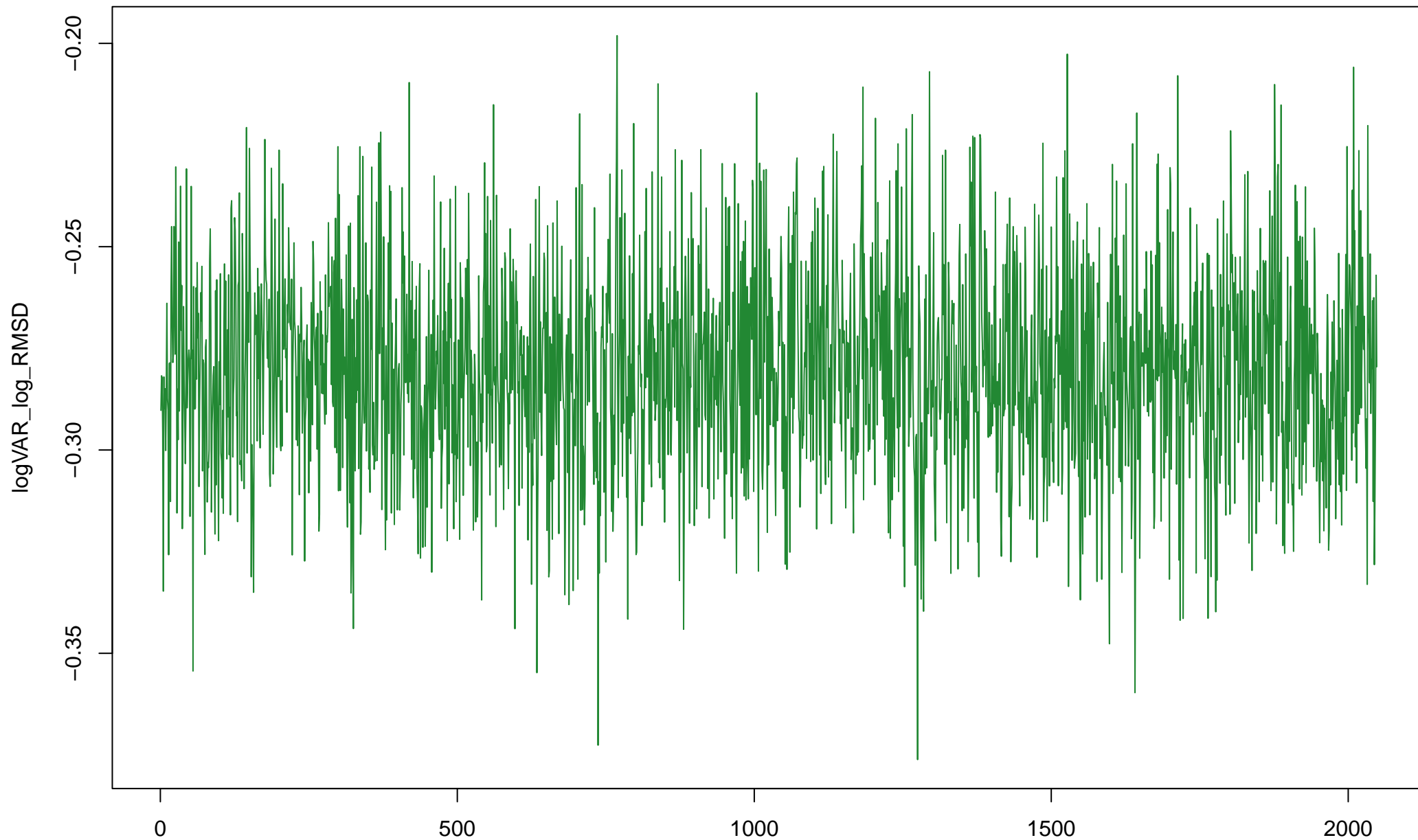
MEAN_docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0384 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0



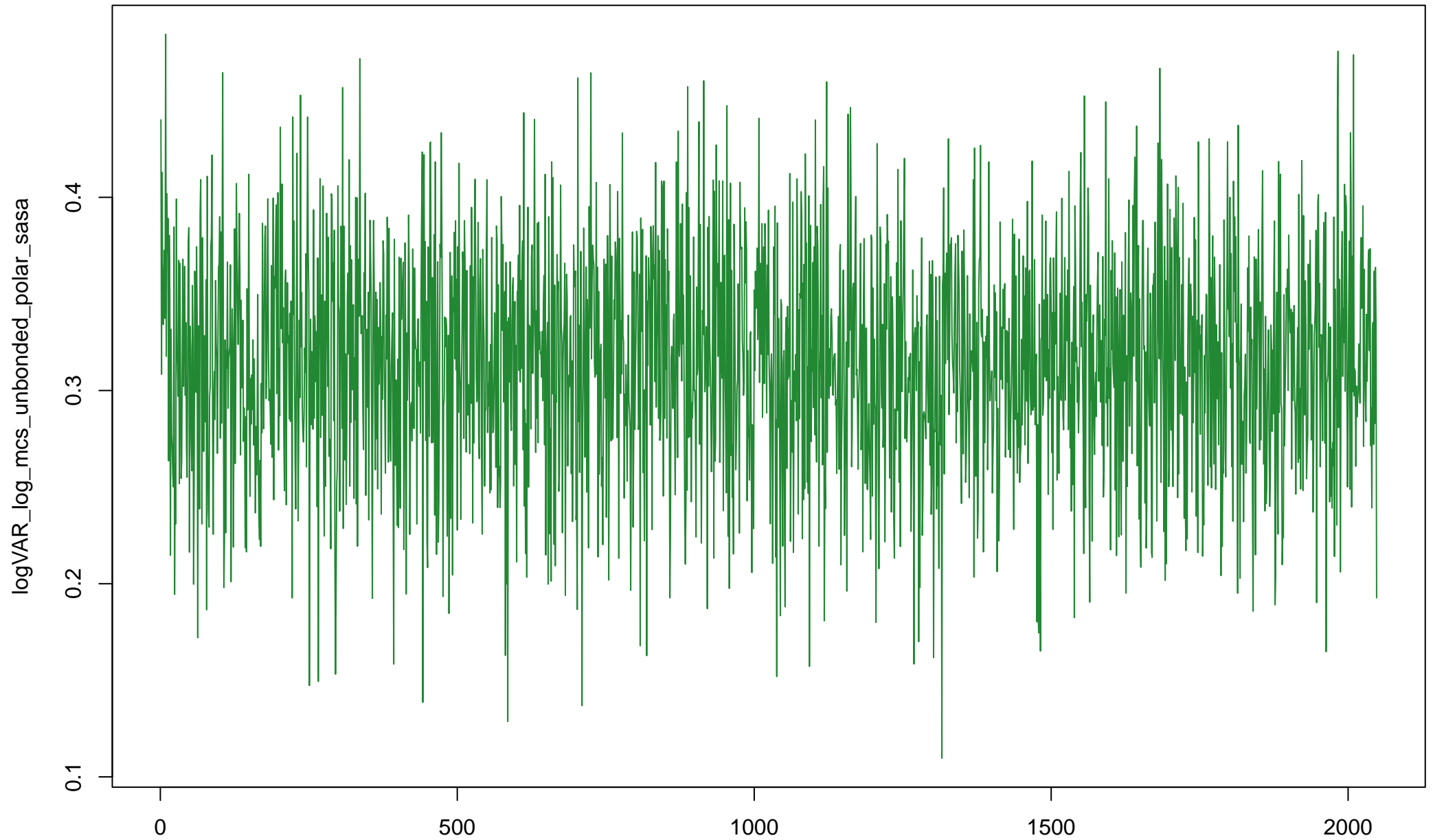
MEAN_mcs_NOCount
ESS = 2050 | BMK = 0.0426 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0



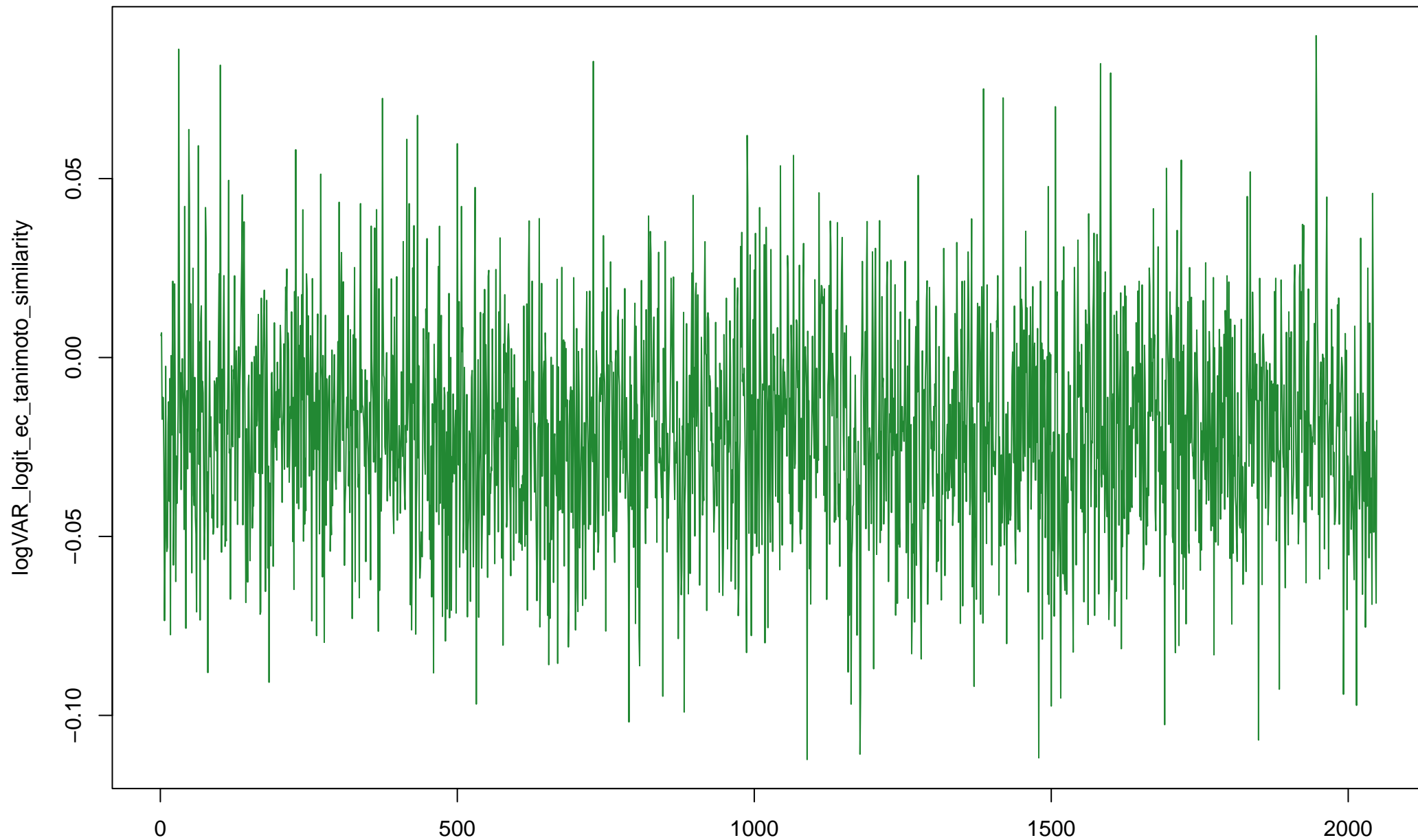
logVAR_log_RMSD
ESS = 1900 | BMK = 0.0317 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0



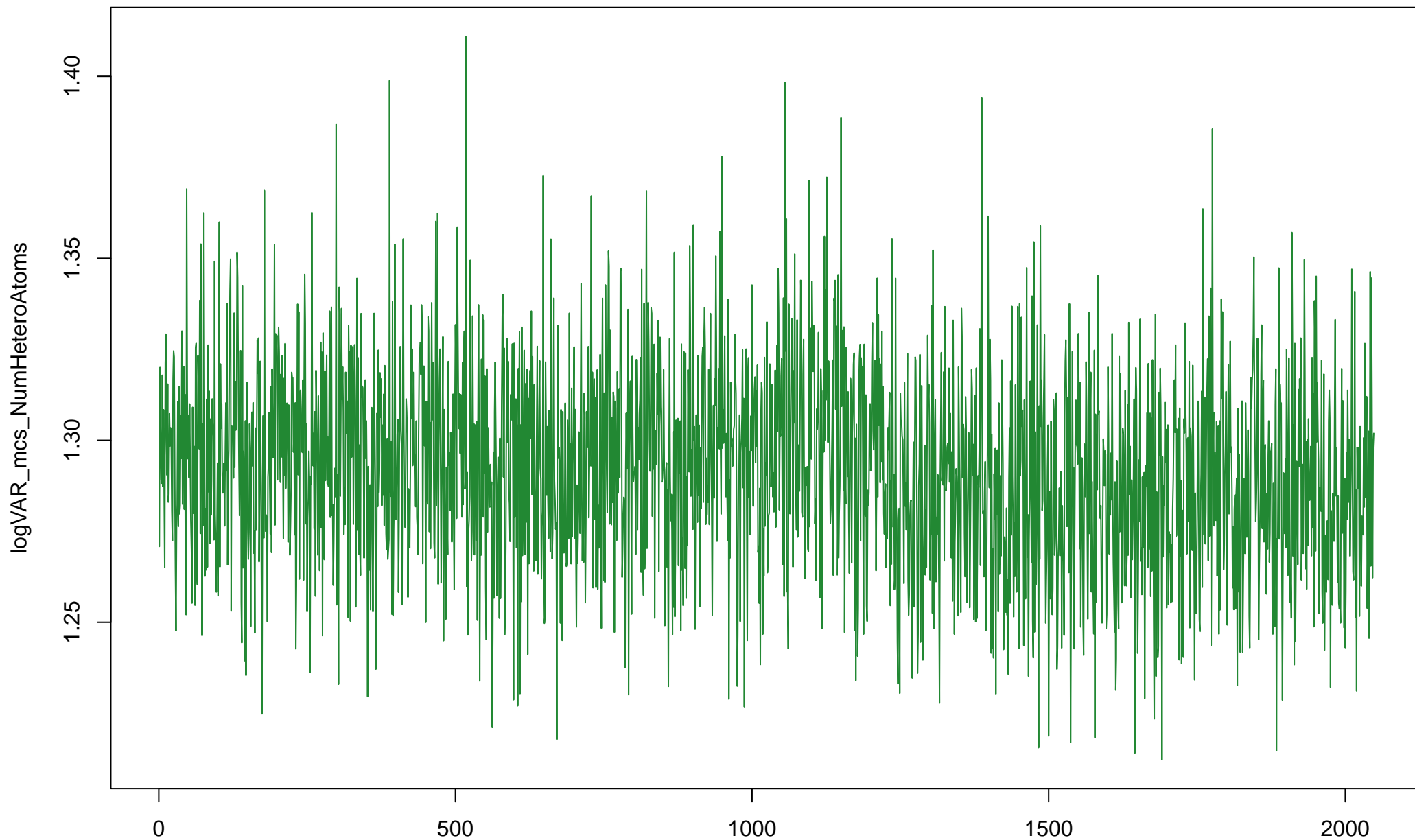
logVAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.048 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0



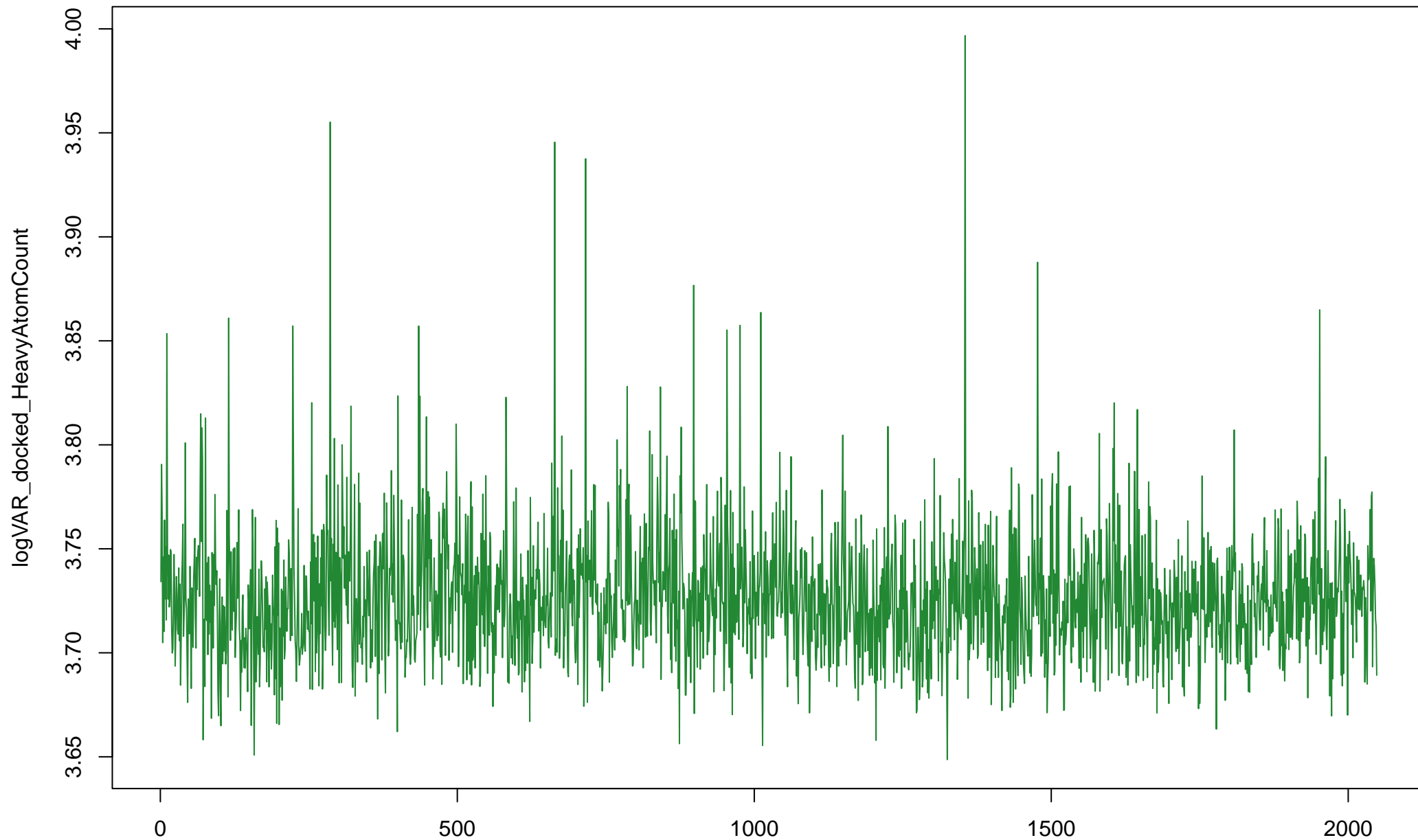
logVAR_logit_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0515 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0



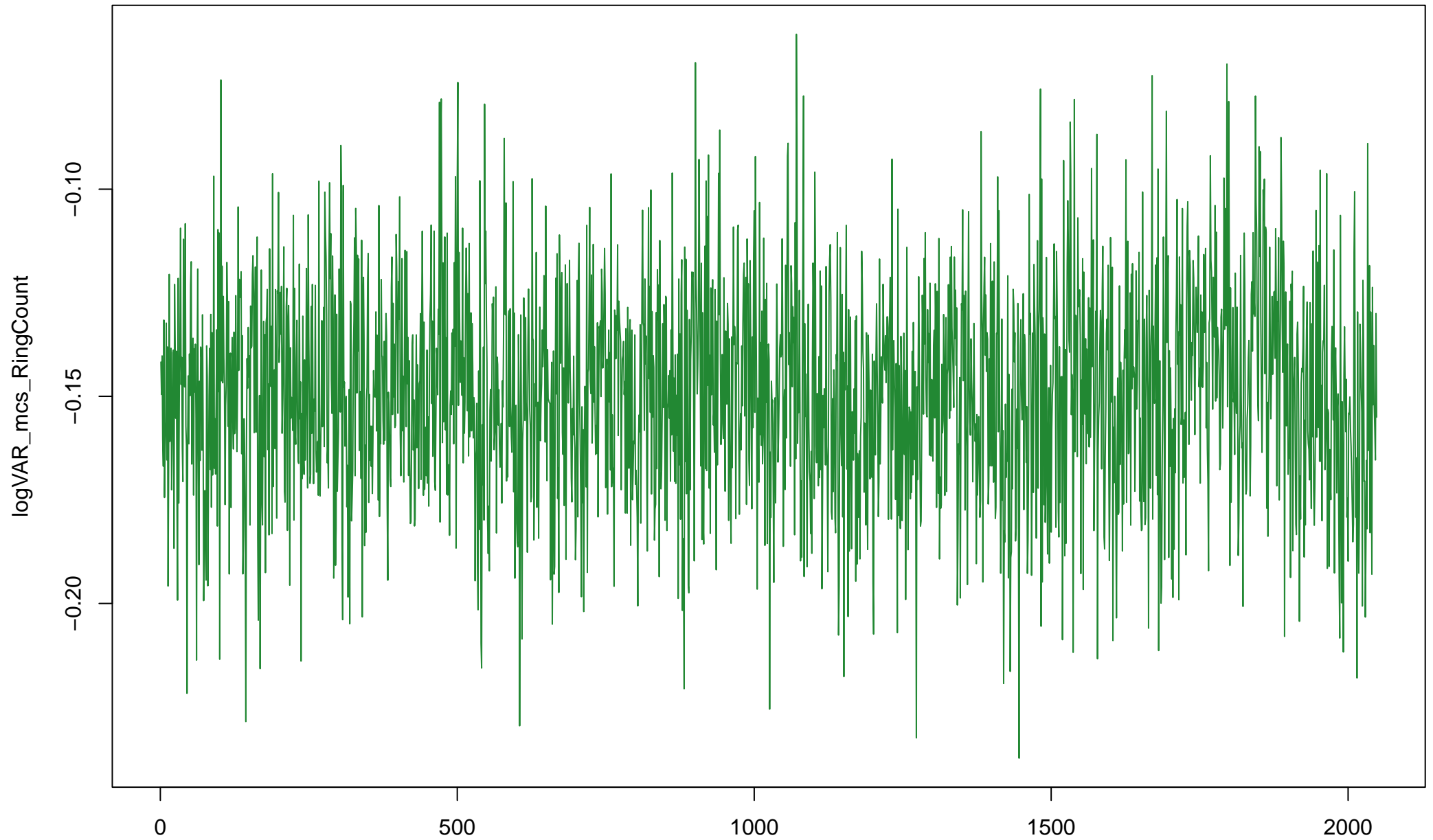
logVAR_mcs_NumHeteroAtoms
ESS = 507 | BMK = 0.0964 | MCSE(6.27) = 2.53 | stat: FALSE | burn: 0



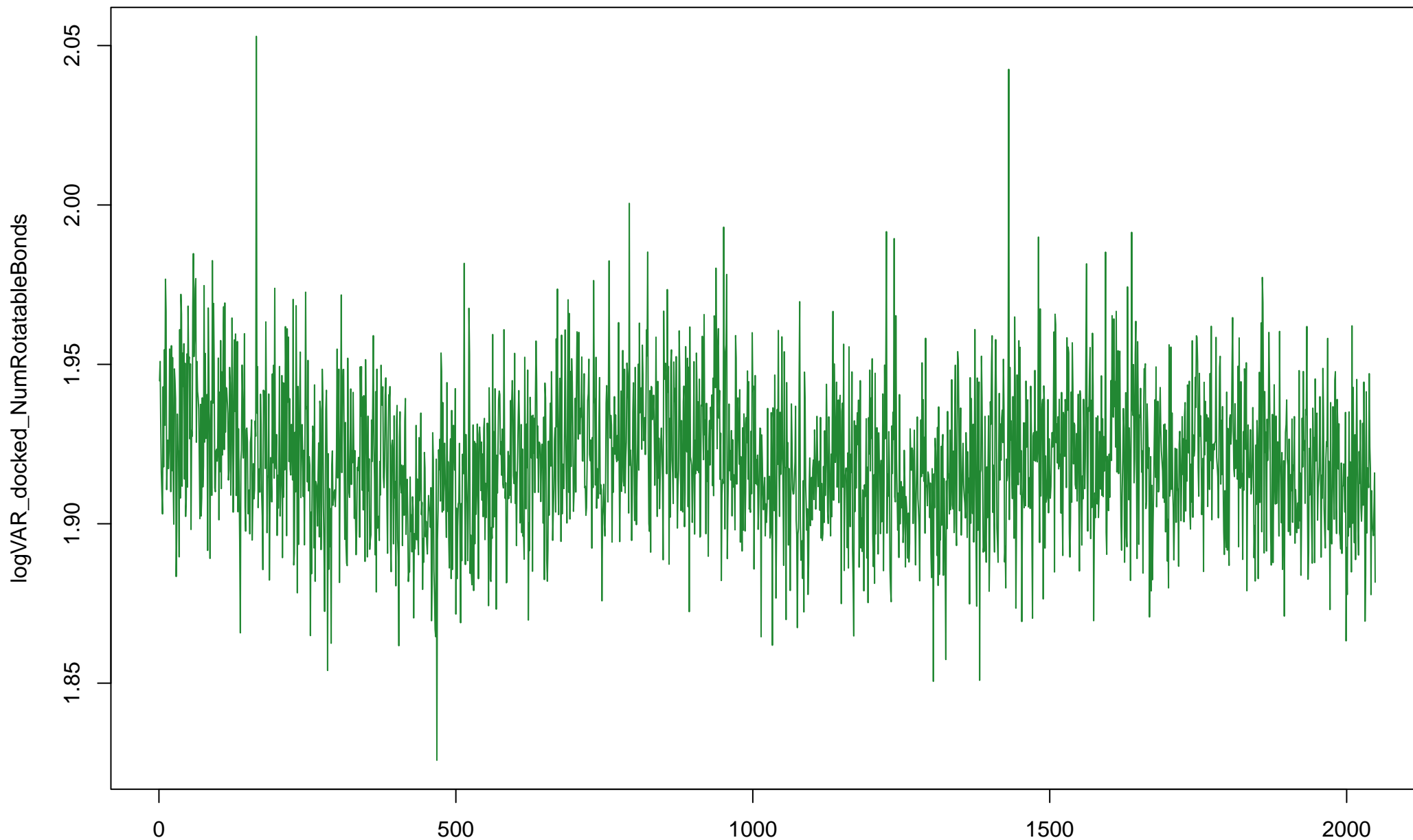
logVAR_docked_HeavyAtomCount
ESS = 1310 | BMK = 0.0883 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0



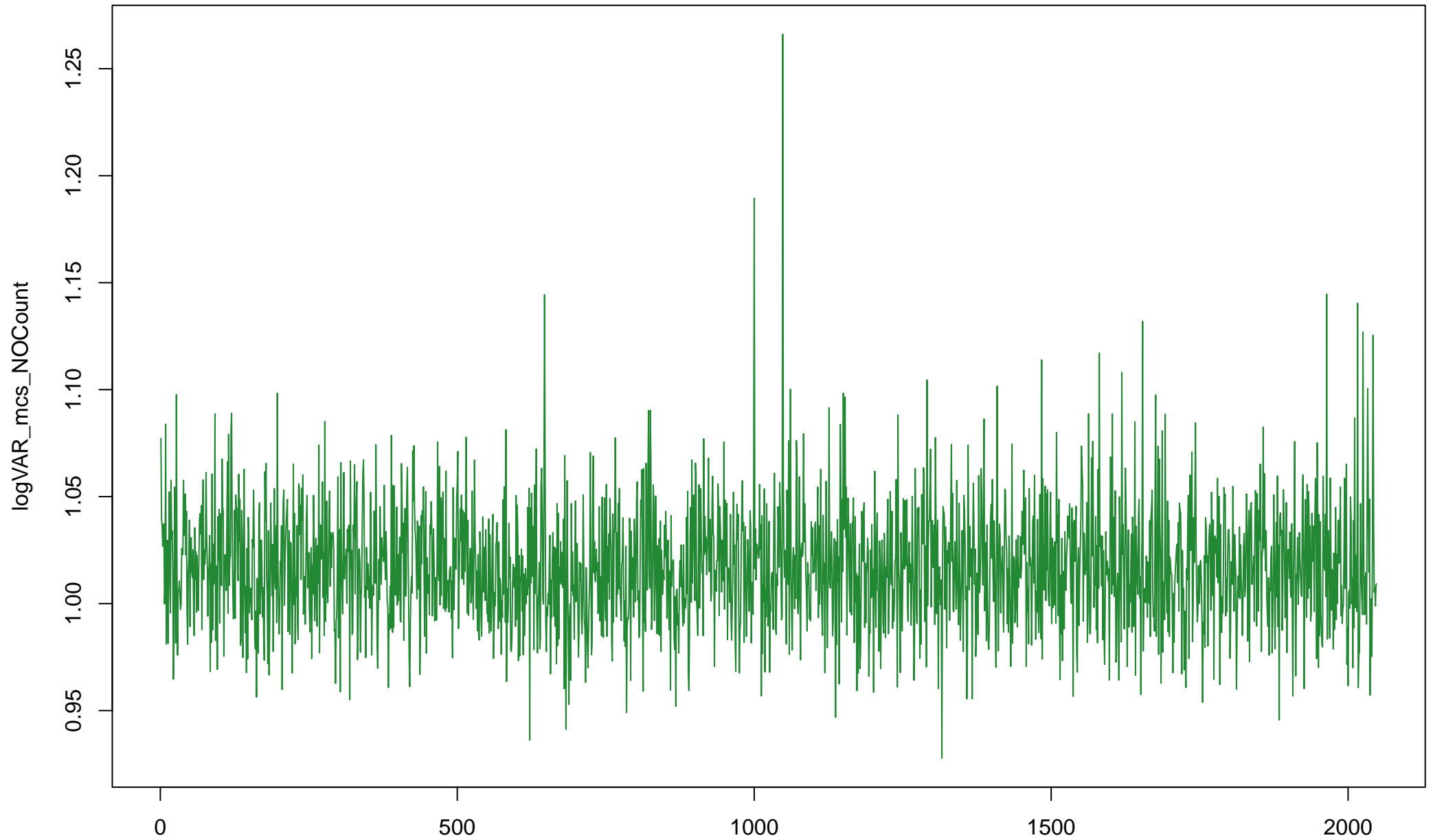
logVAR_mcs_RingCount
ESS = 1050 | BMK = 0.0396 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0



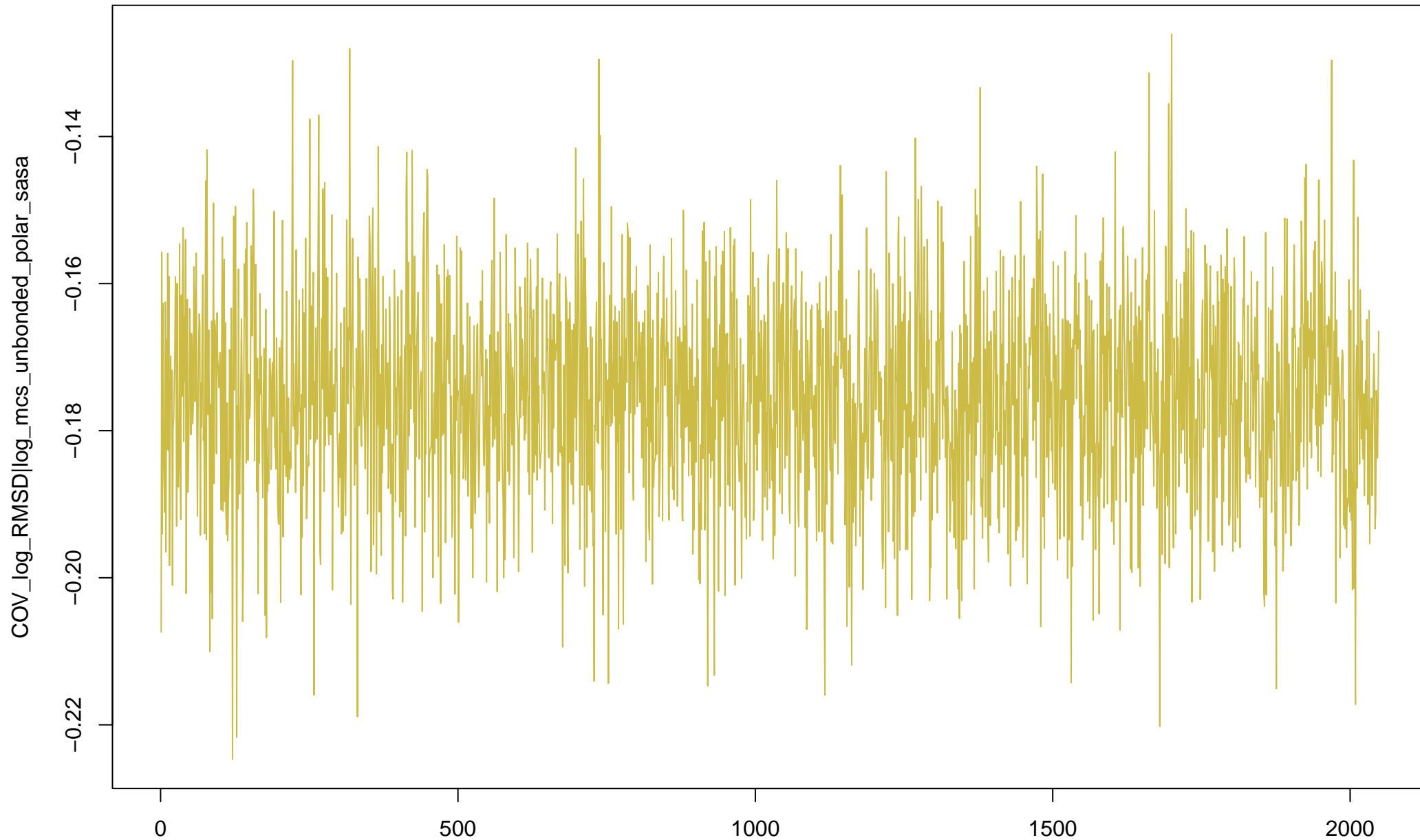
logVAR_docked_NumRotatableBonds
ESS = 256 | BMK = 0.0784 | MCSE(6.27) = 3.49 | stat: FALSE | burn: 0



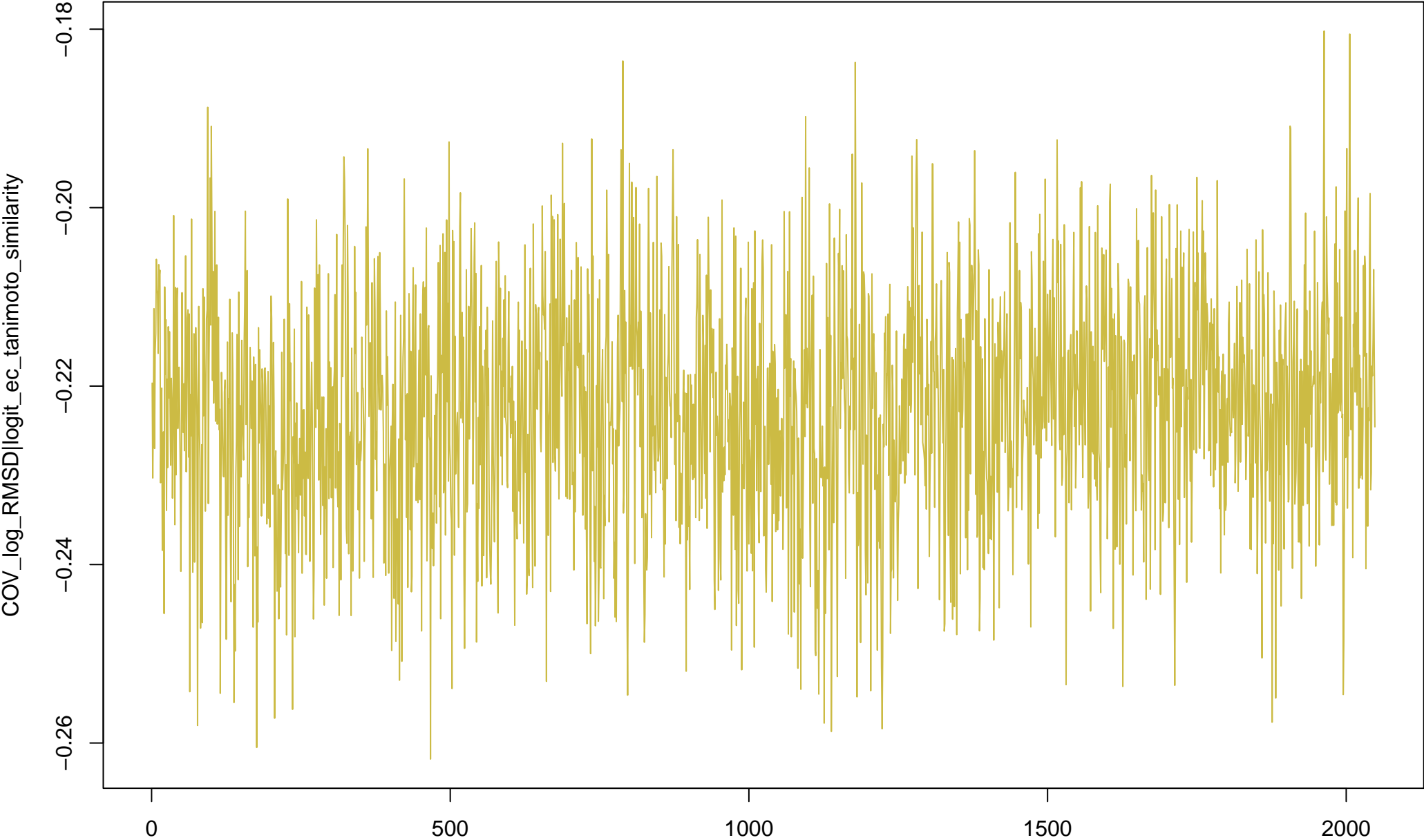
logVAR_mcs_NOCount
ESS = 2050 | BMK = 0.069 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0



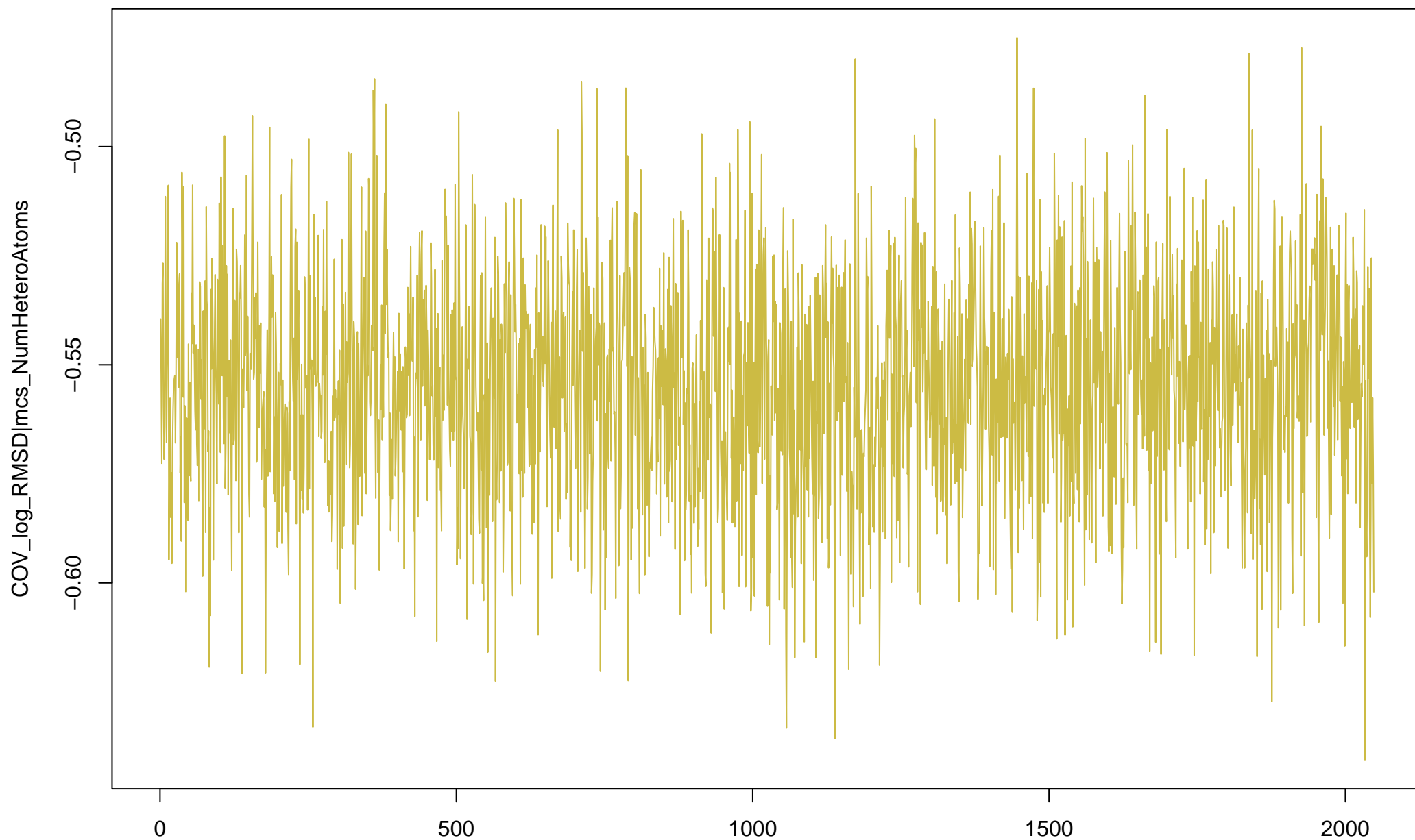
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1740 | BMK = 0.0351 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0



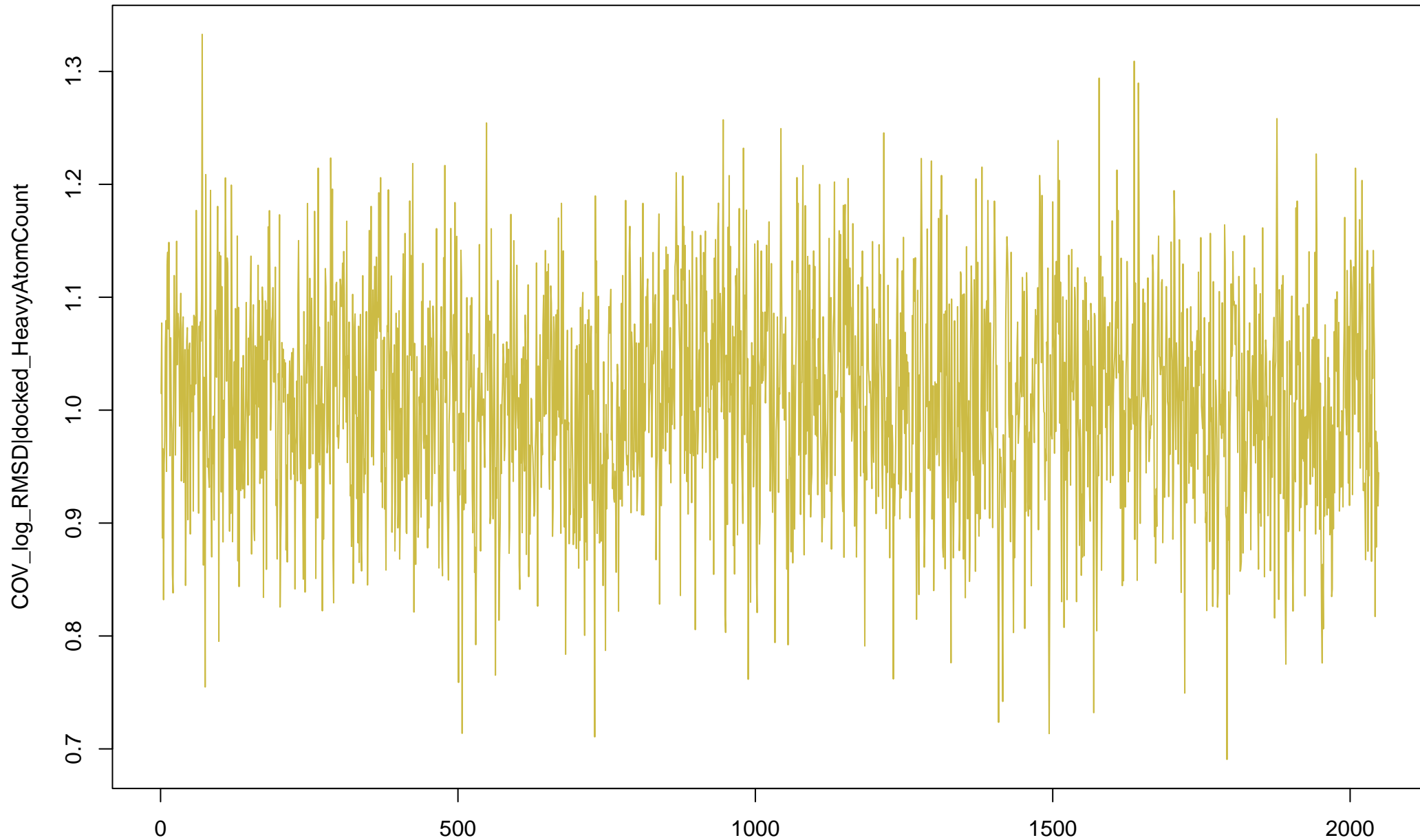
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 944 | BMK = 0.0571 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0



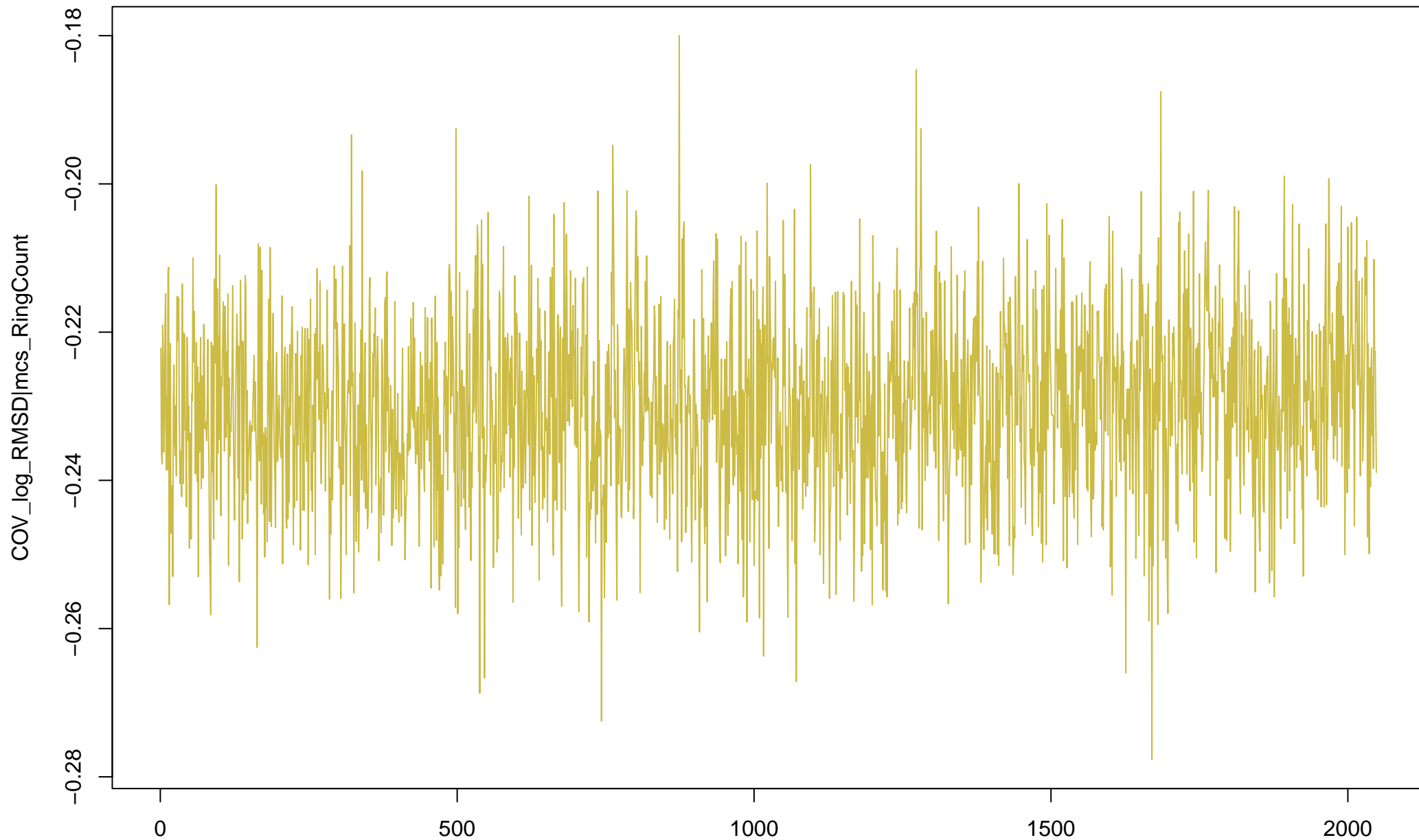
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1710 | BMK = 0.0492 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0



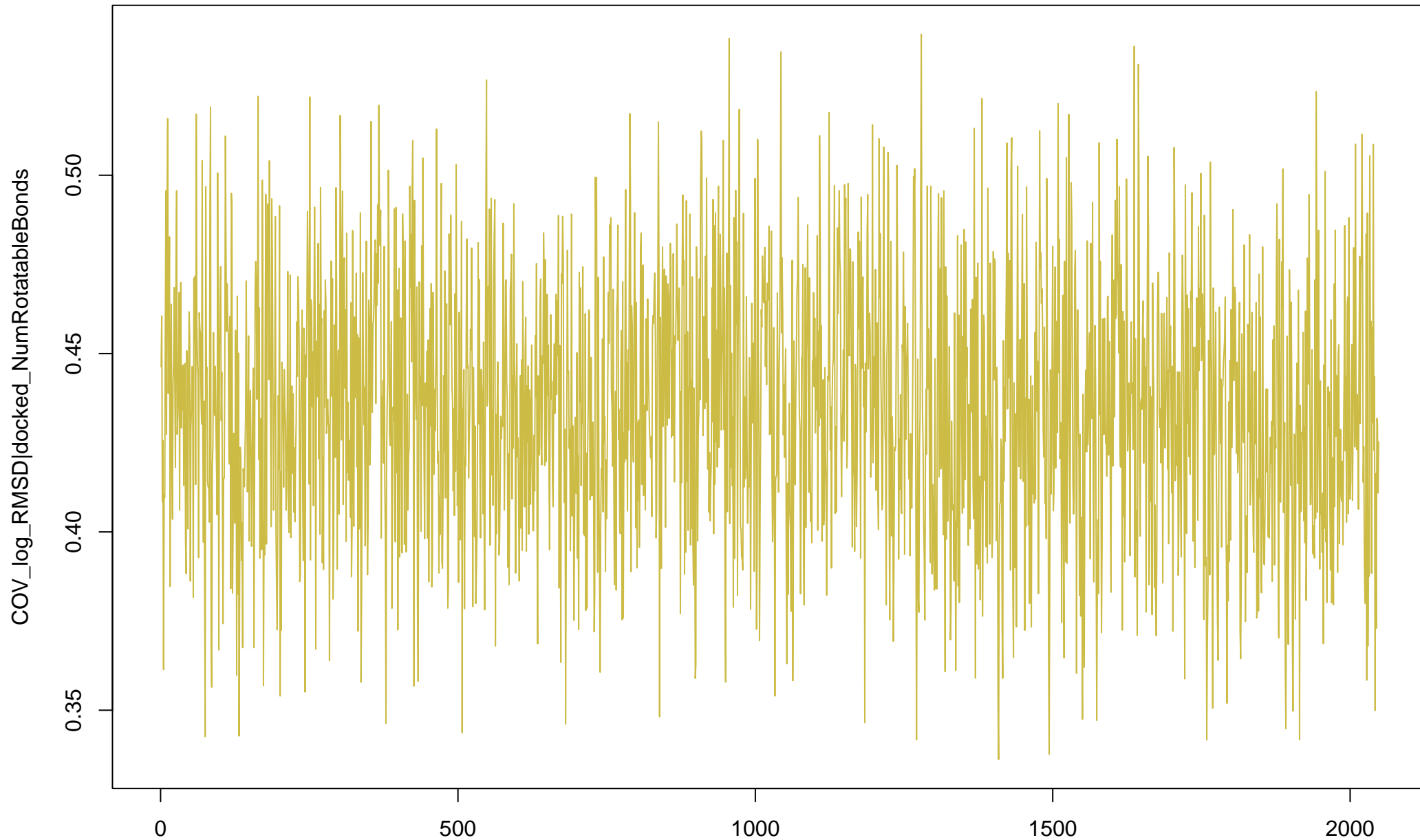
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1470 | BMK = 0.0392 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0



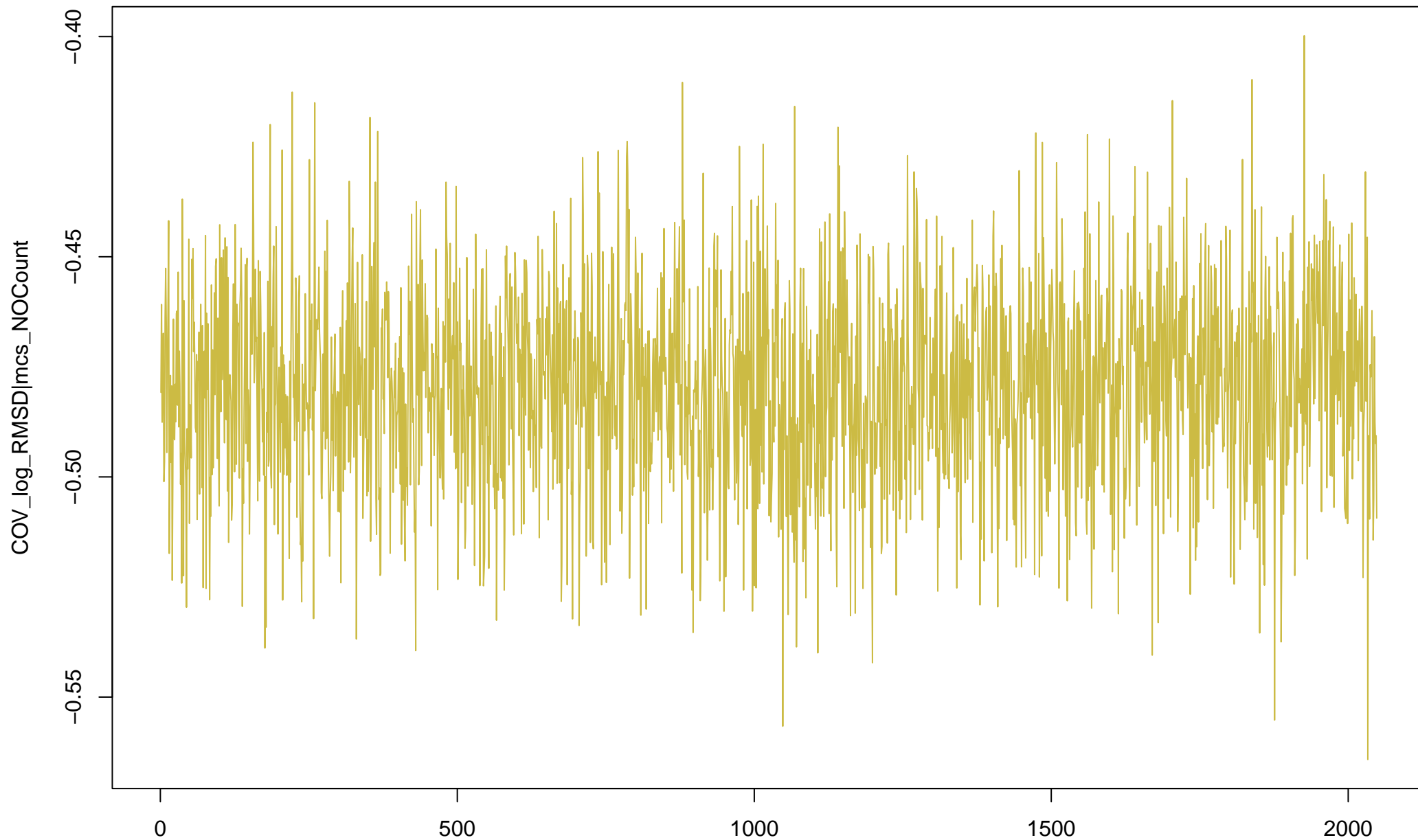
COV_log_RMSD|mcs_RingCount
ESS = 1400 | BMK = 0.064 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0



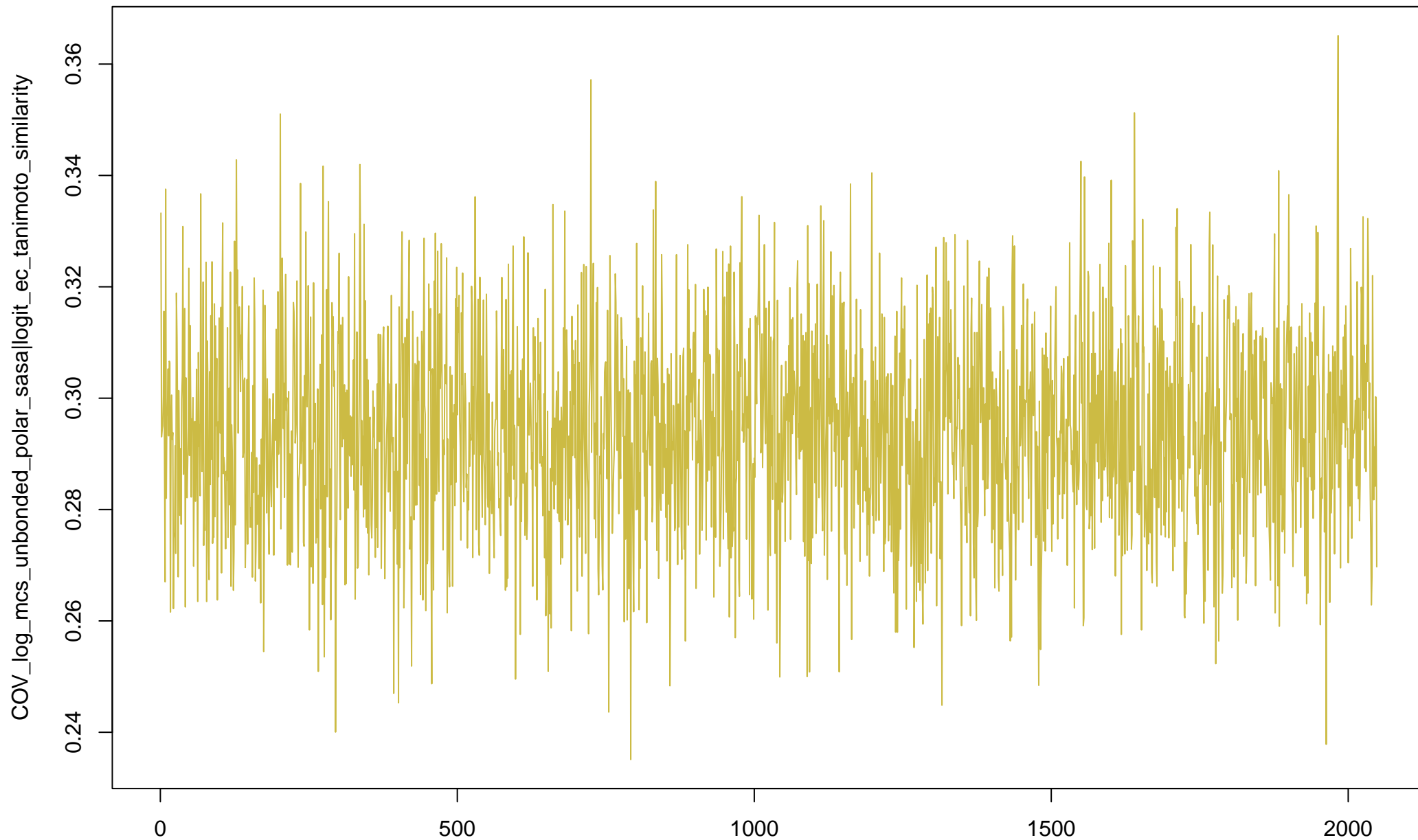
COV_log_RMSD|docked_NumRotatableBonds
ESS = 1540 | BMK = 0.0563 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0



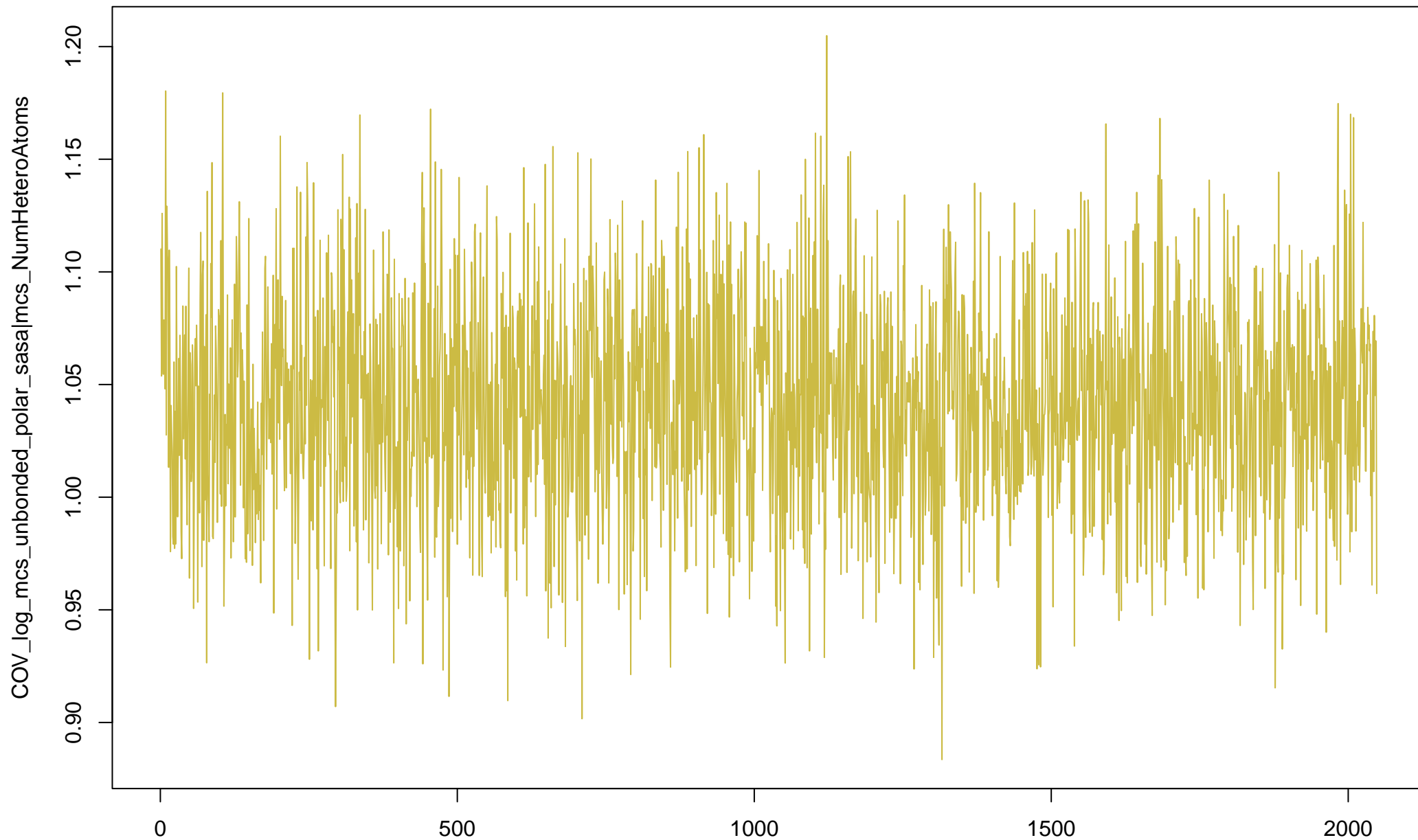
COV_log_RMSD|mcs_NOCount
ESS = 1730 | BMK = 0.0554 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0



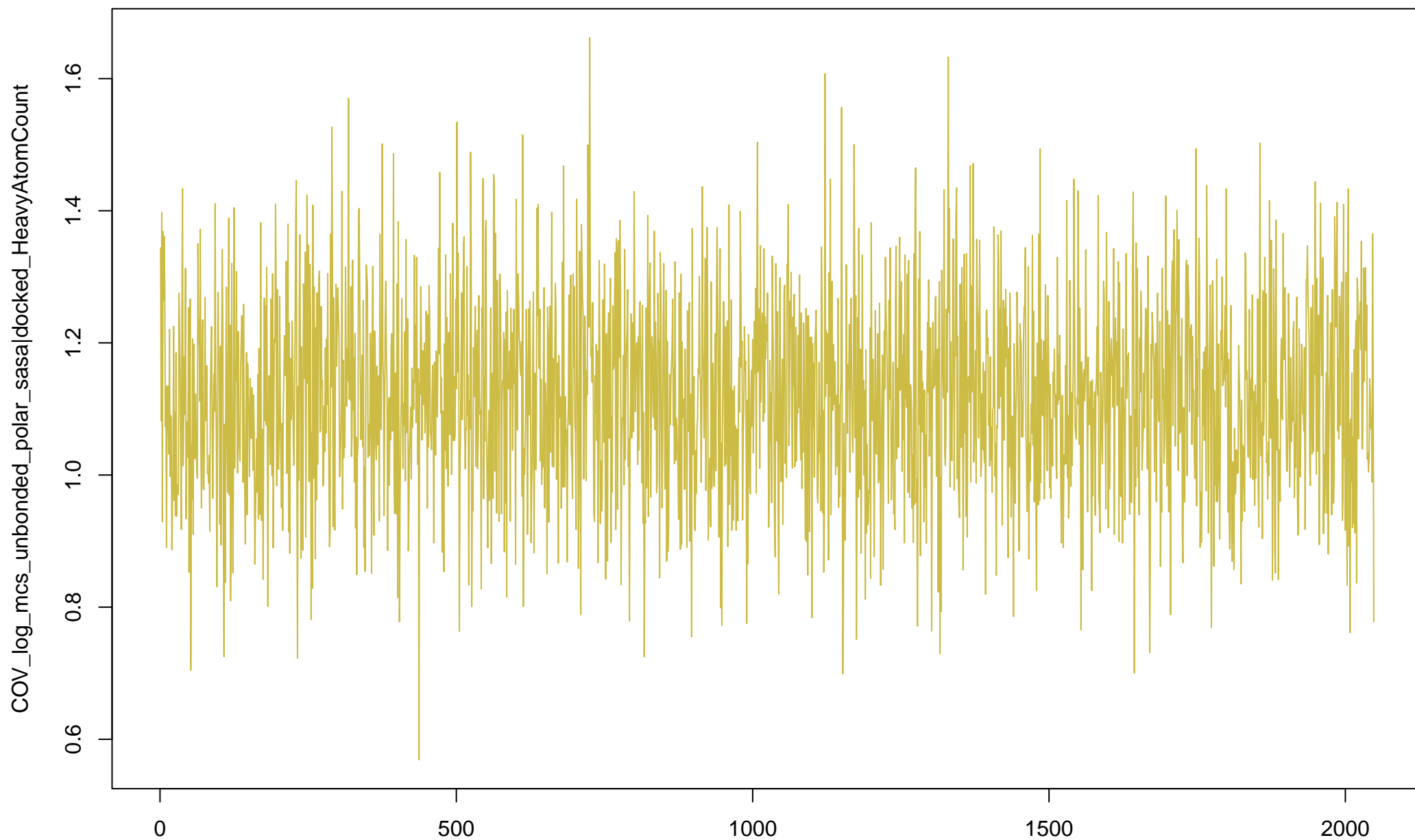
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0352 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0



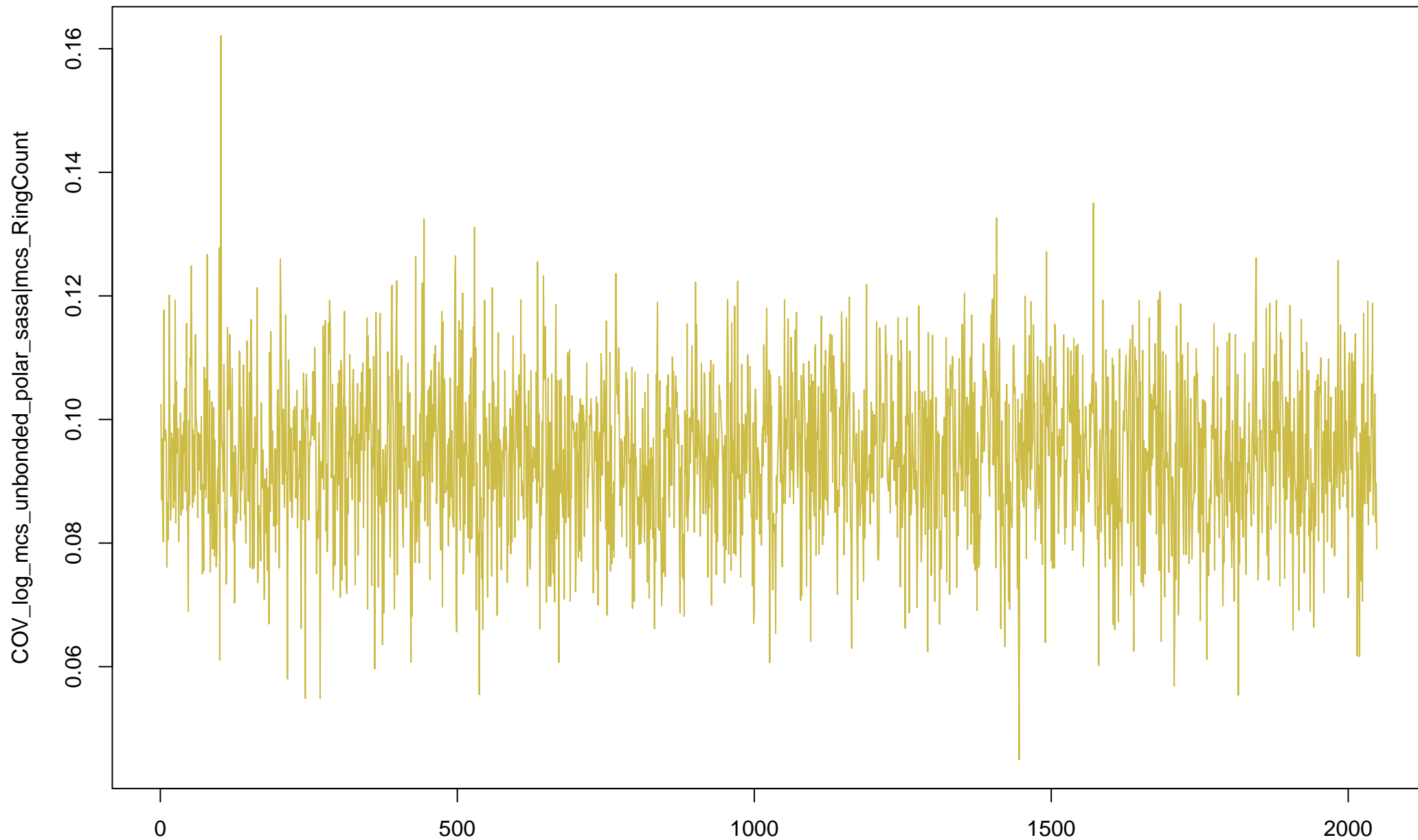
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0462 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0



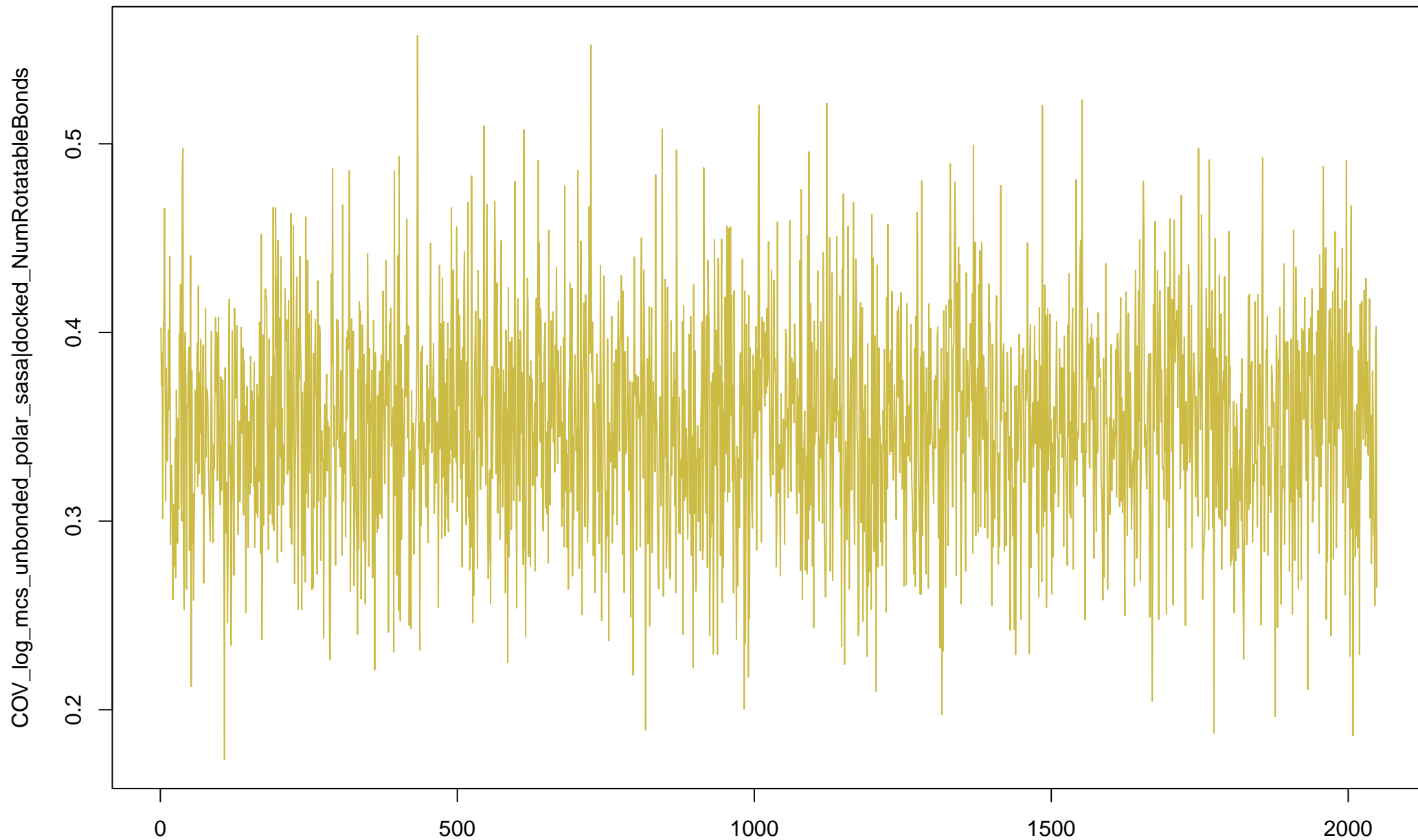
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0272 | MCSE(6.27) = 2.19 | stat: FALSE | burn: 0



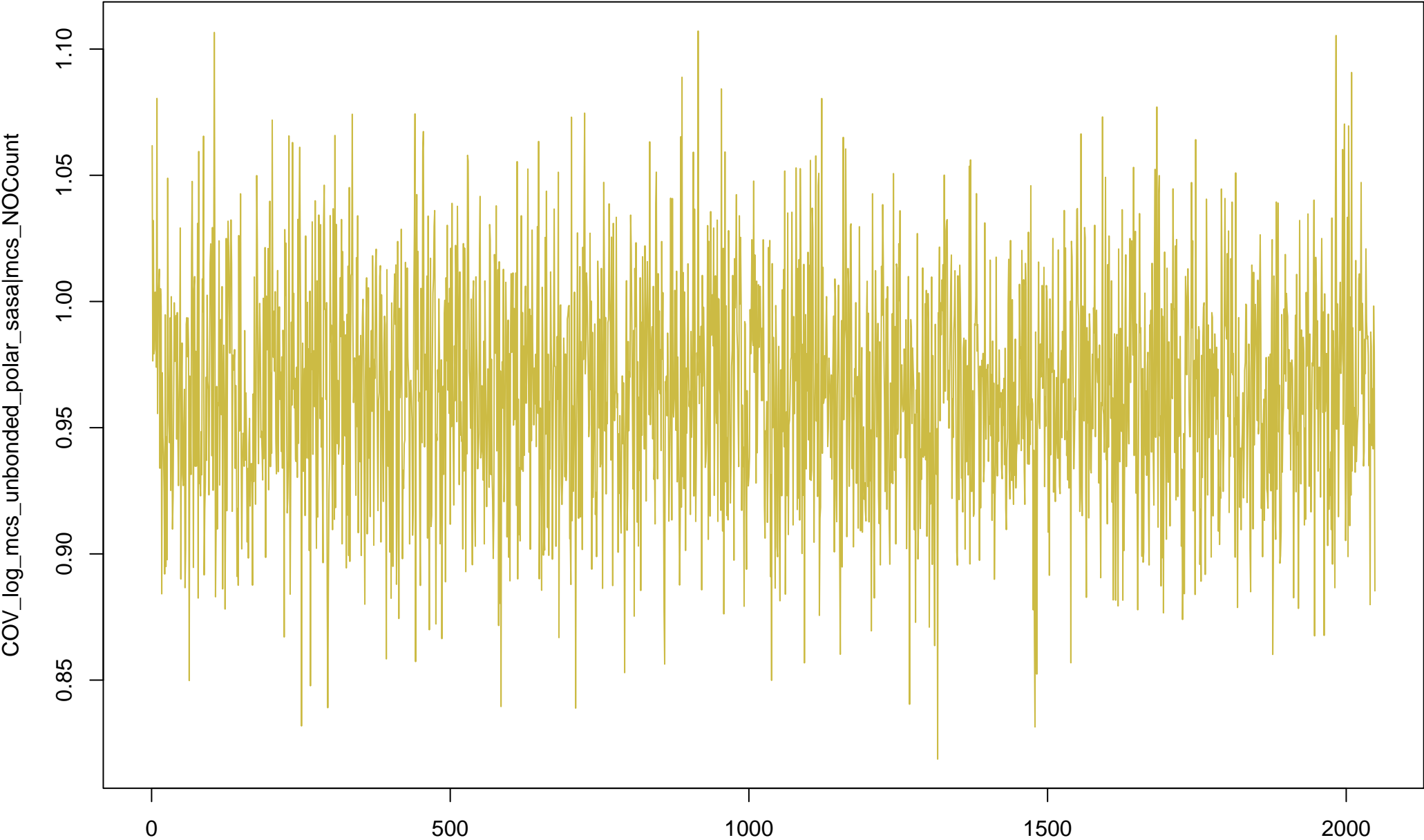
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1740 | BMK = 0.0604 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0



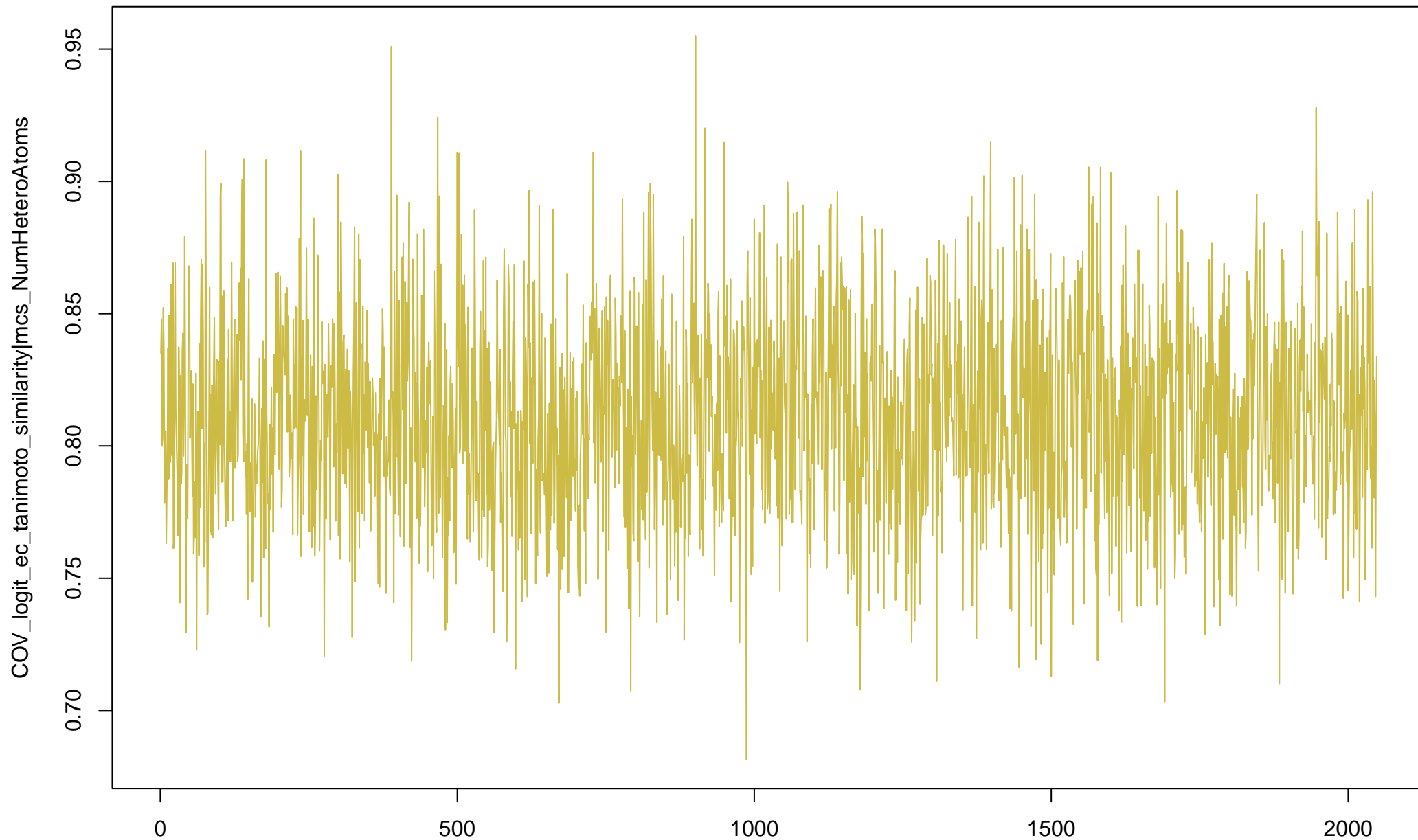
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 2050 | BMK = 0.032 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0



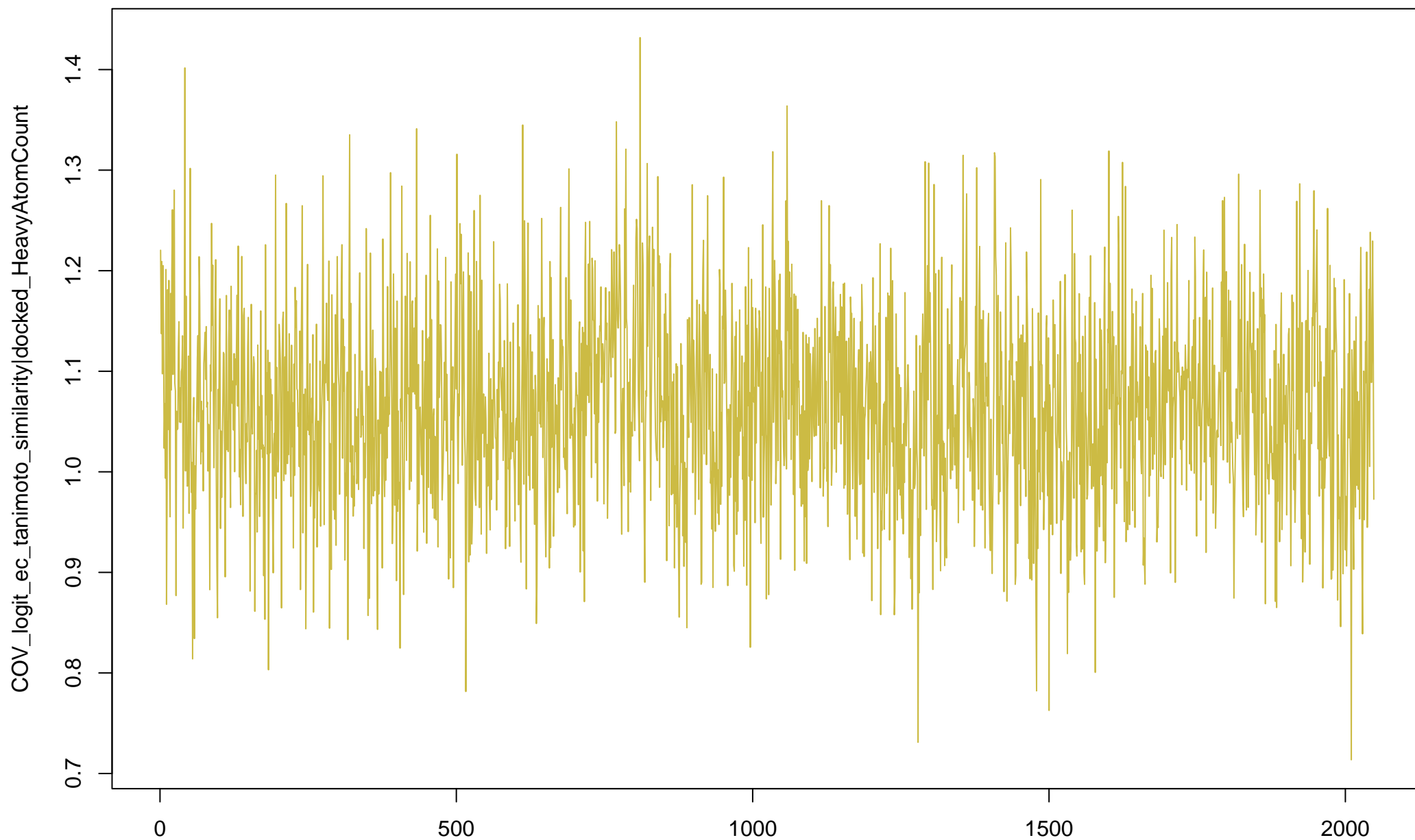
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 2050 | BMK = 0.045 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0



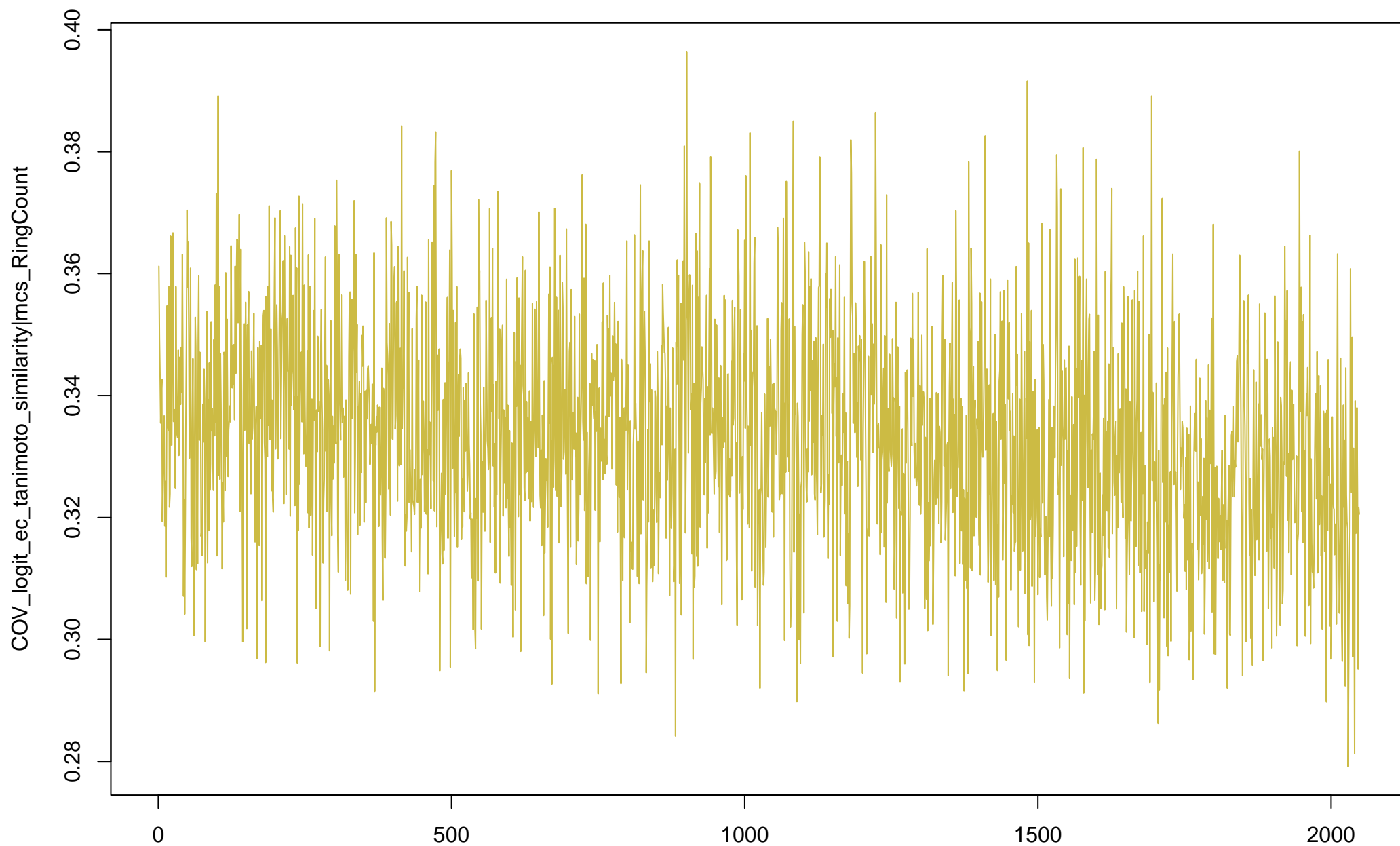
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1760 | BMK = 0.0607 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0



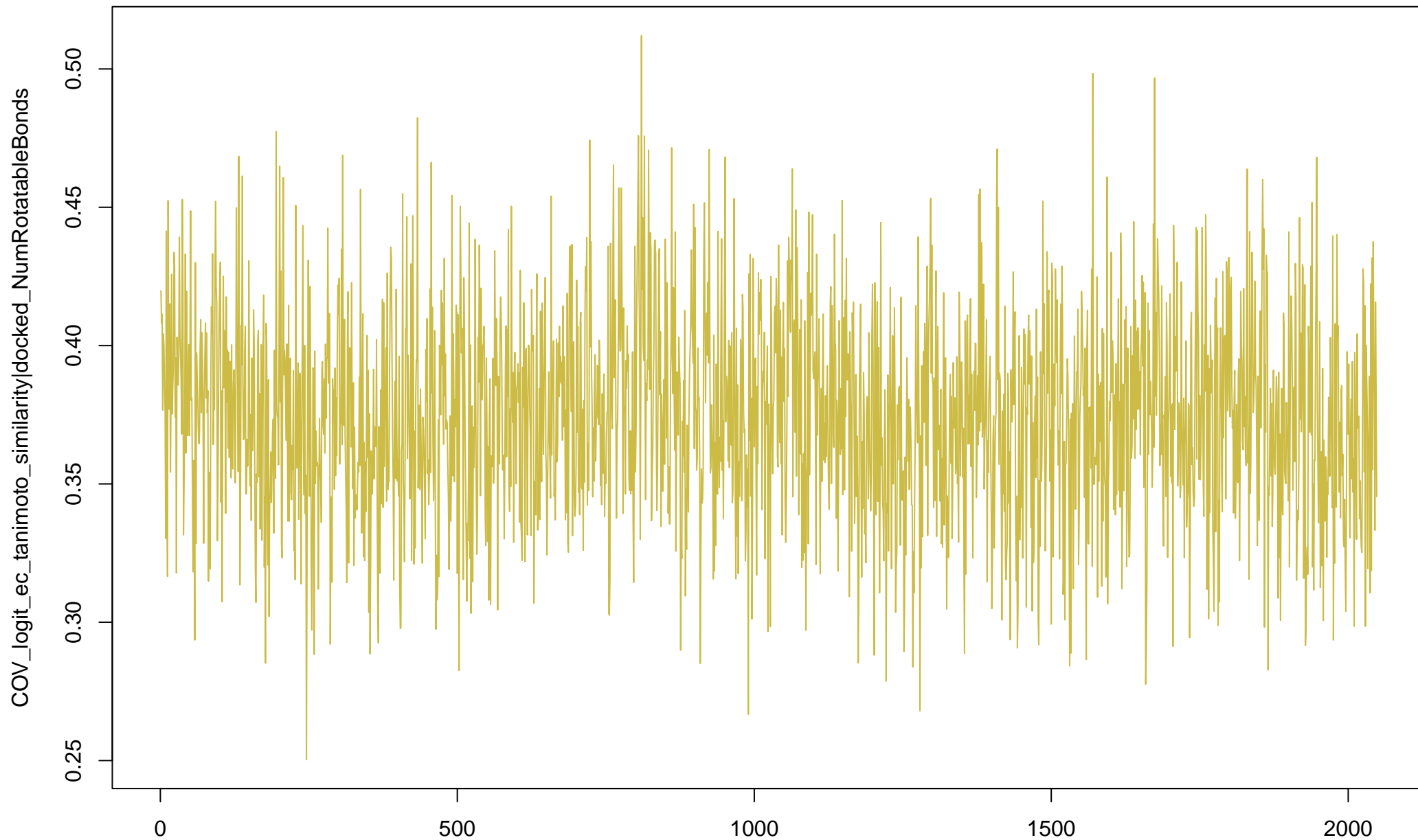
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1240 | BMK = 0.0527 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0



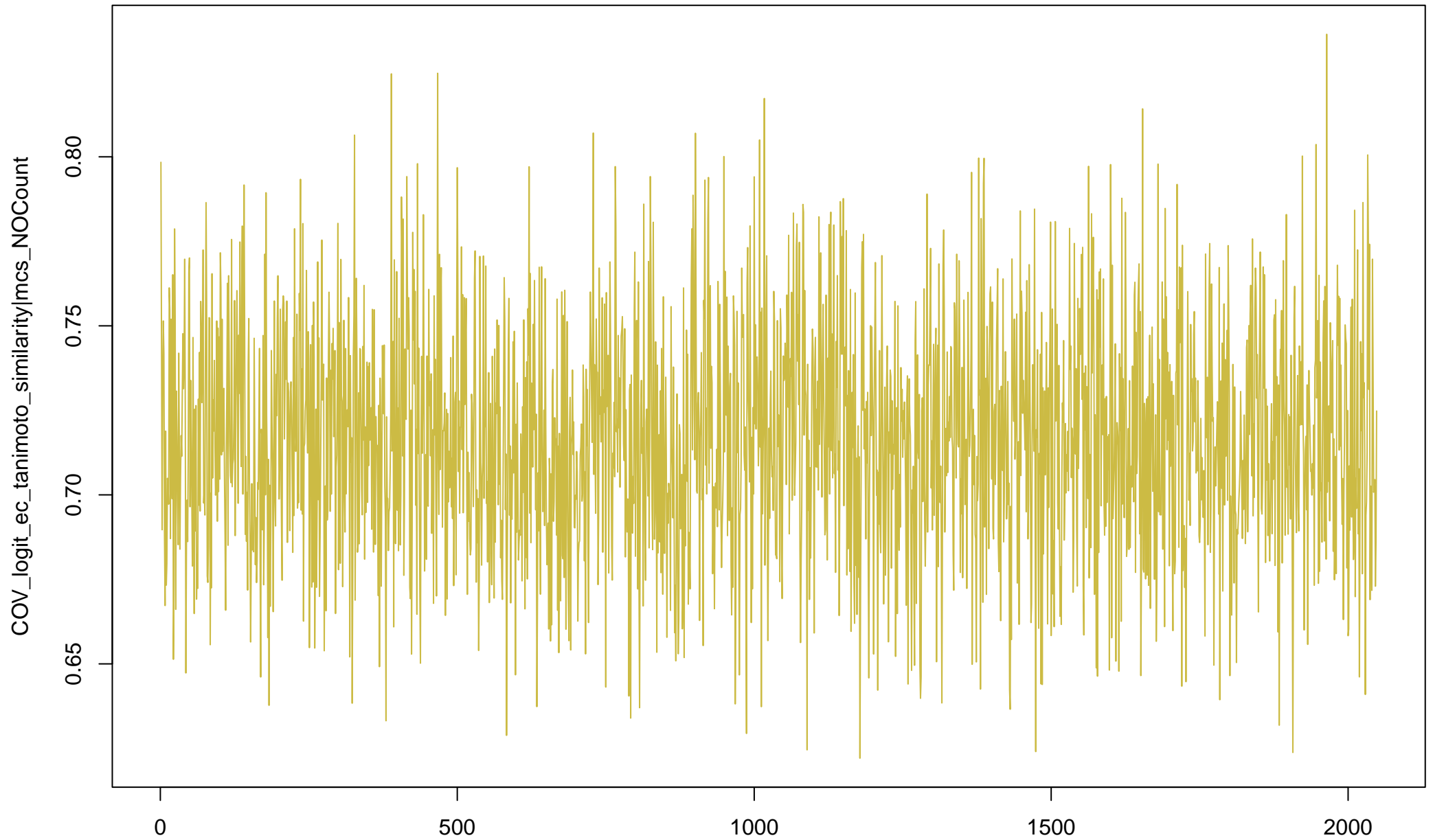
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 567 | BMK = 0.135 | MCSE(6.27) = 3.5 | stat: FALSE | burn: 0



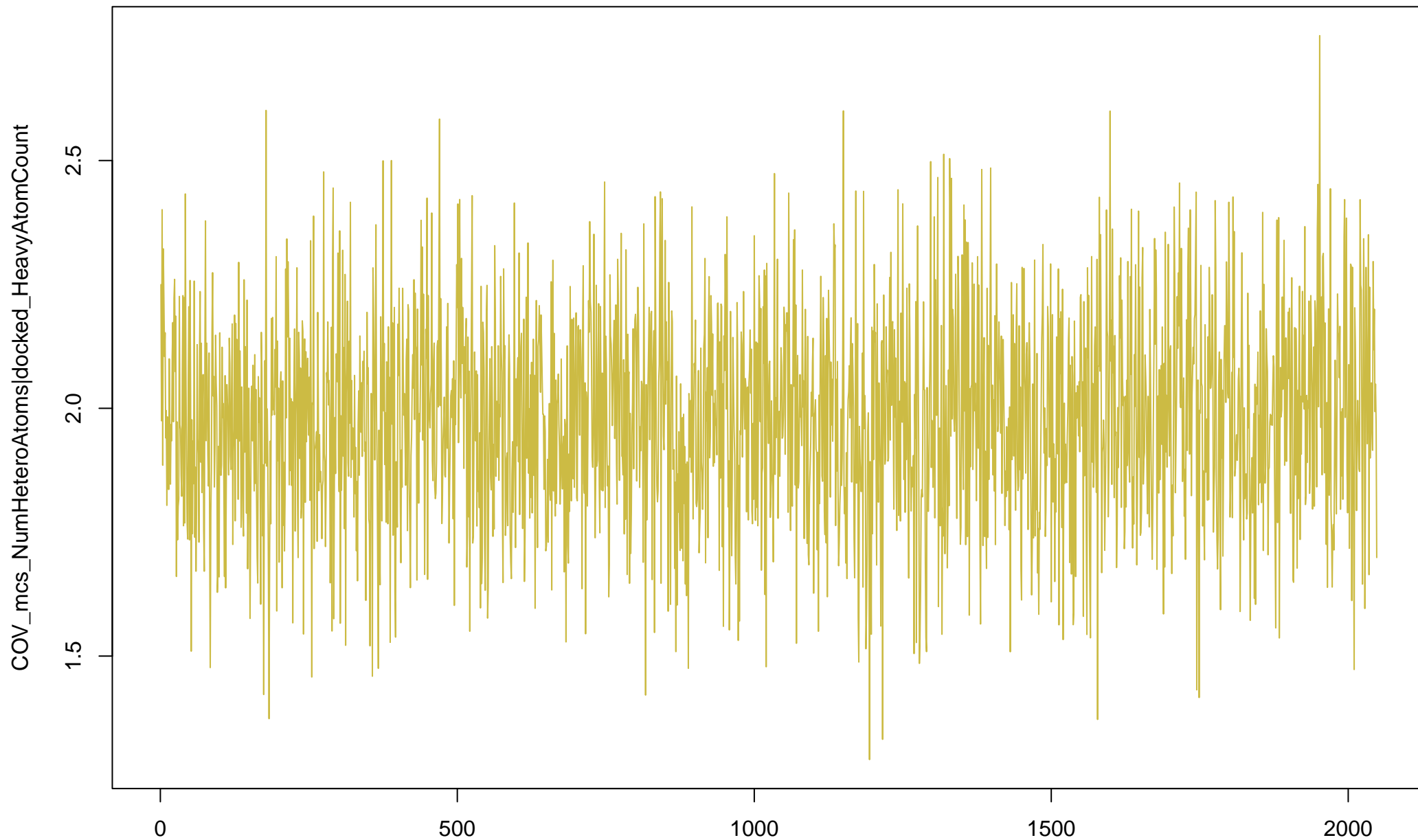
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1280 | BMK = 0.064 | MCSE(6.27) = 3.32 | stat: FALSE | burn: 0



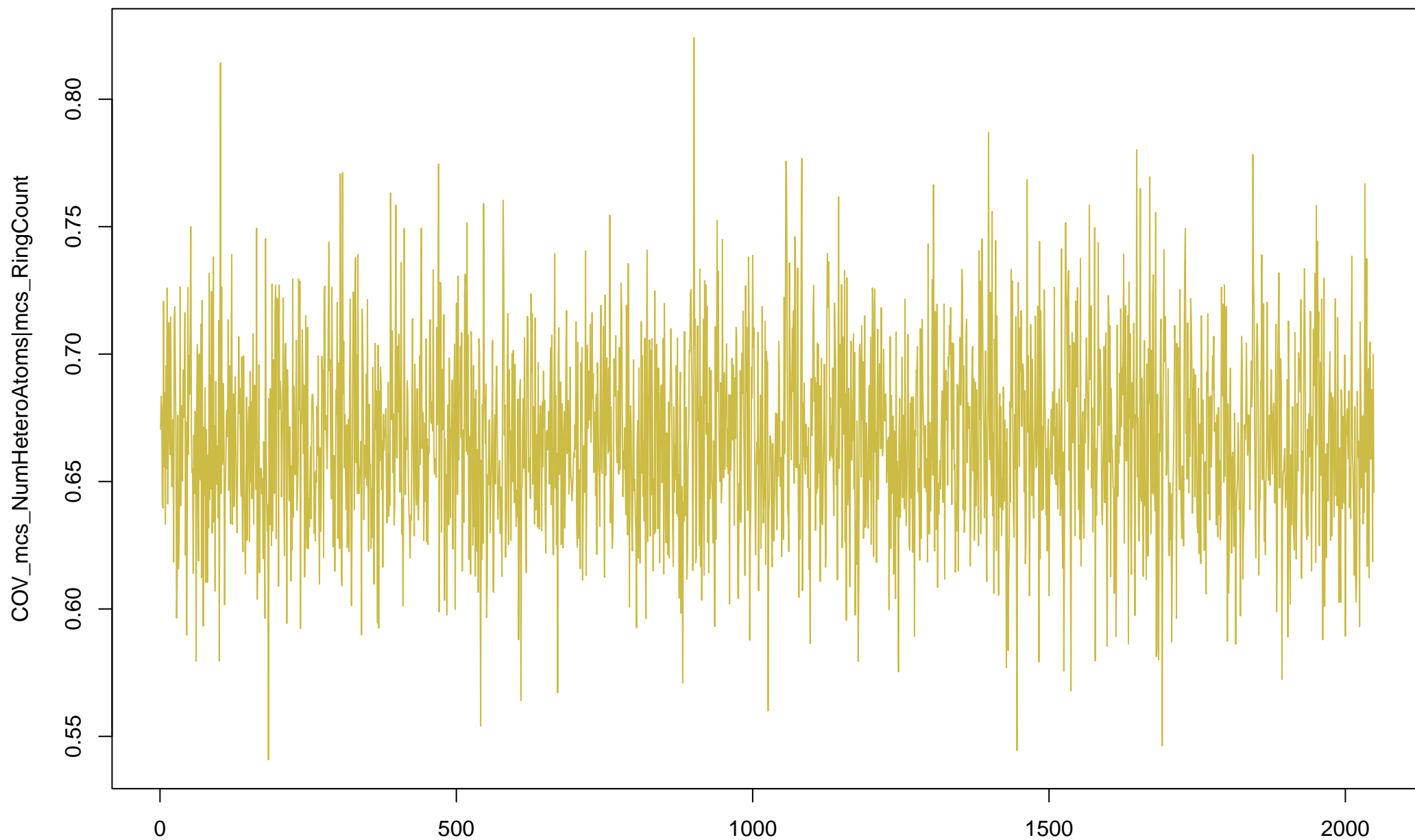
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1830 | BMK = 0.0476 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0



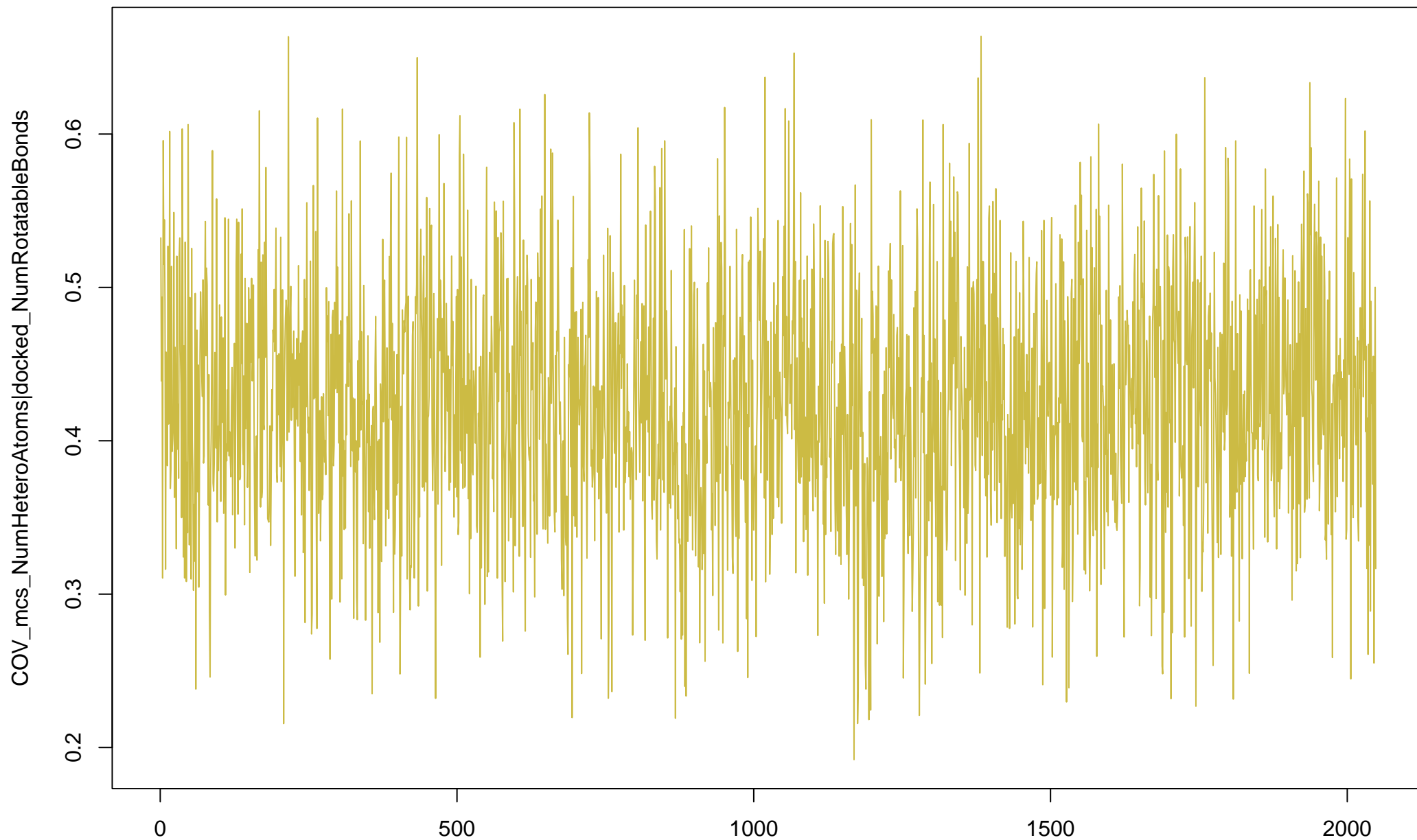
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1830 | BMK = 0.0494 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0



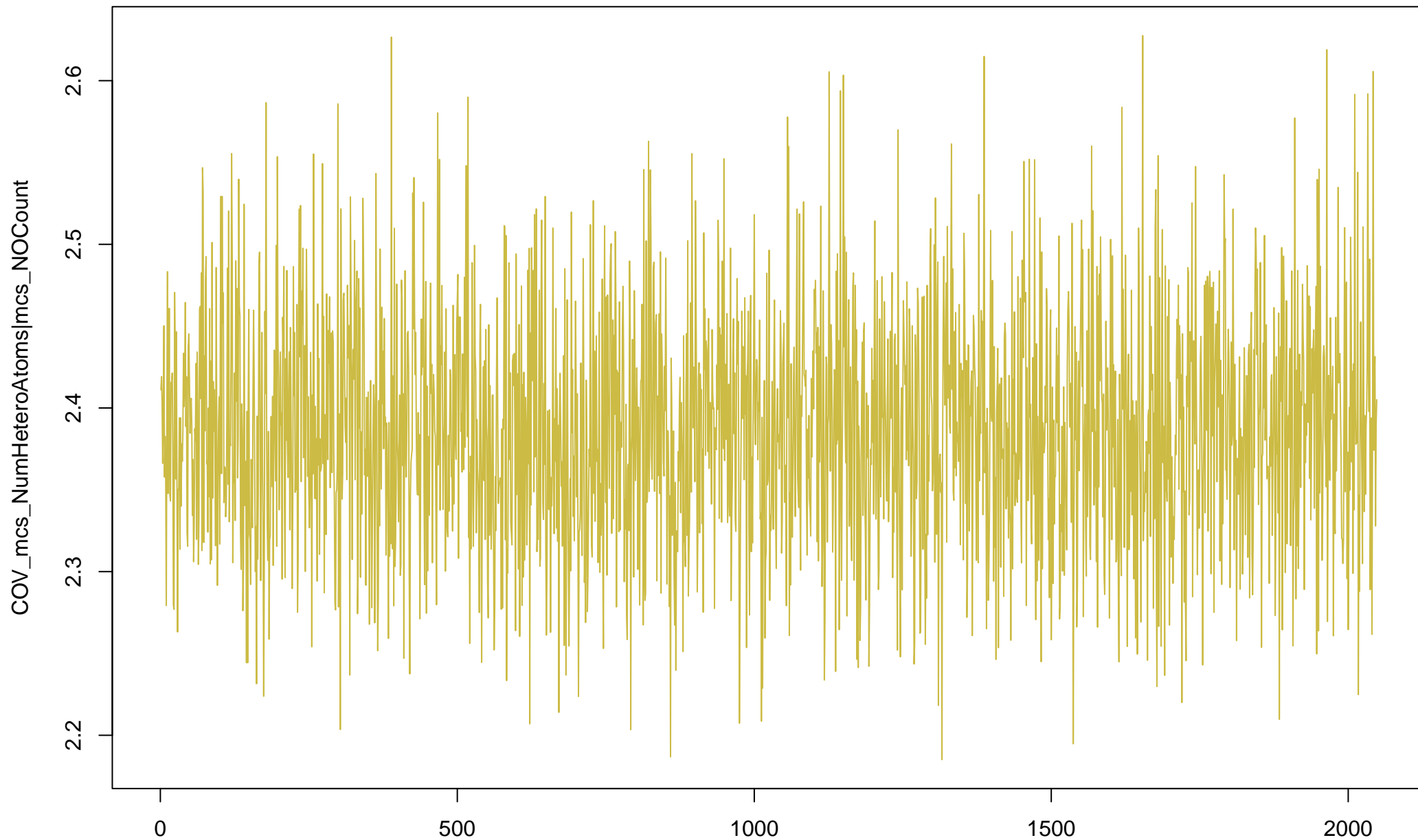
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 2050 | BMK = 0.0509 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0



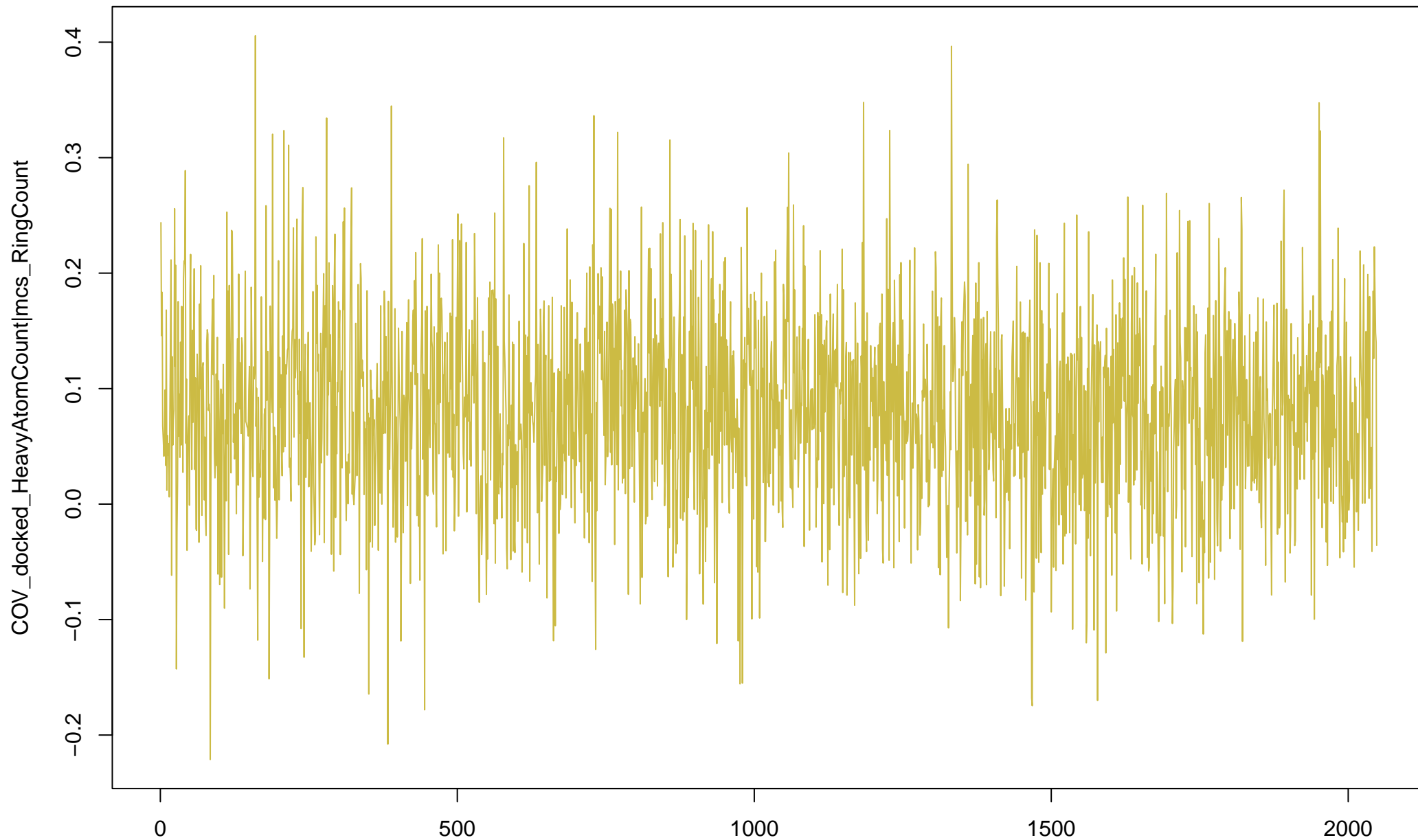
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1870 | BMK = 0.034 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0



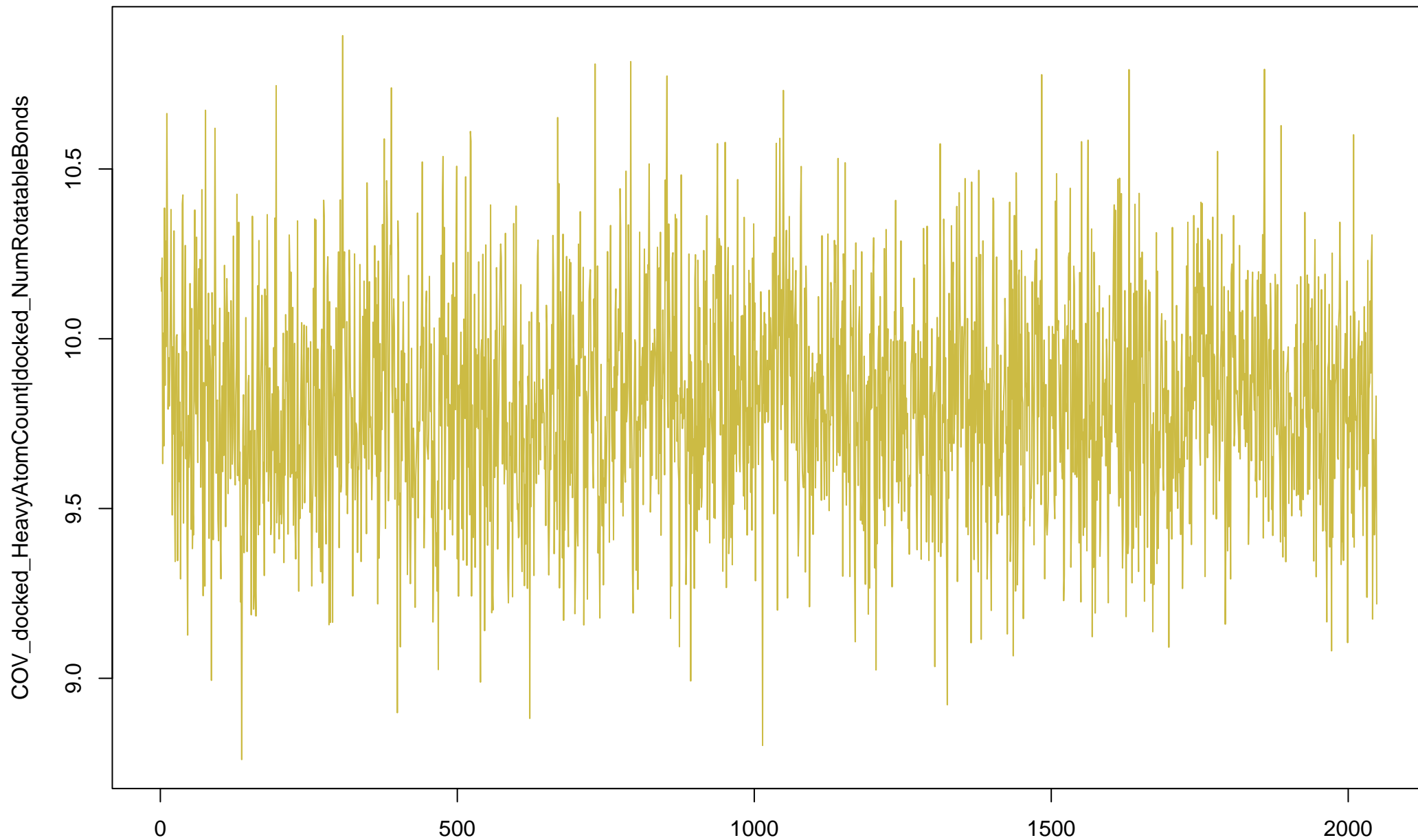
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1990 | BMK = 0.0491 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0



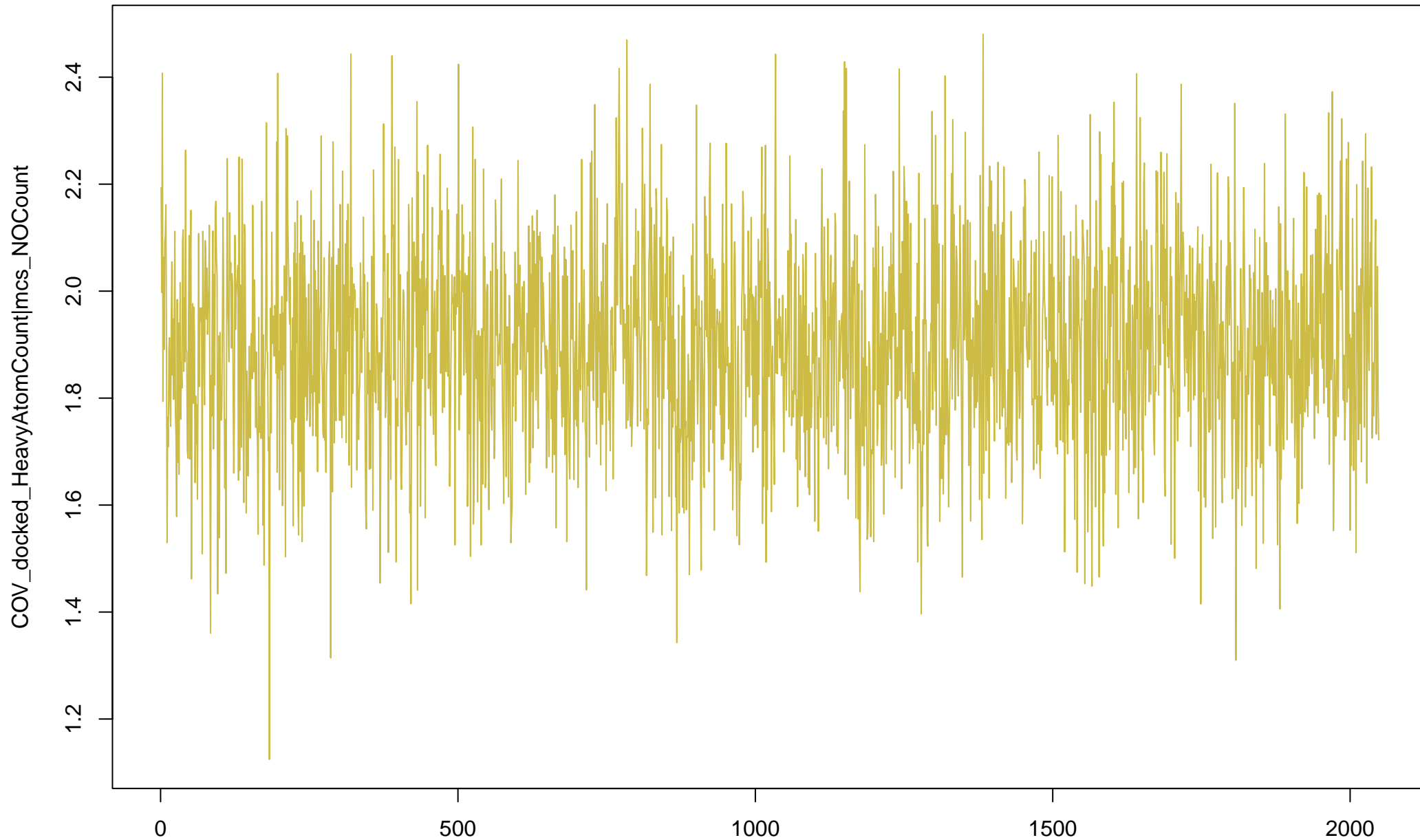
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1850 | BMK = 0.054 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0



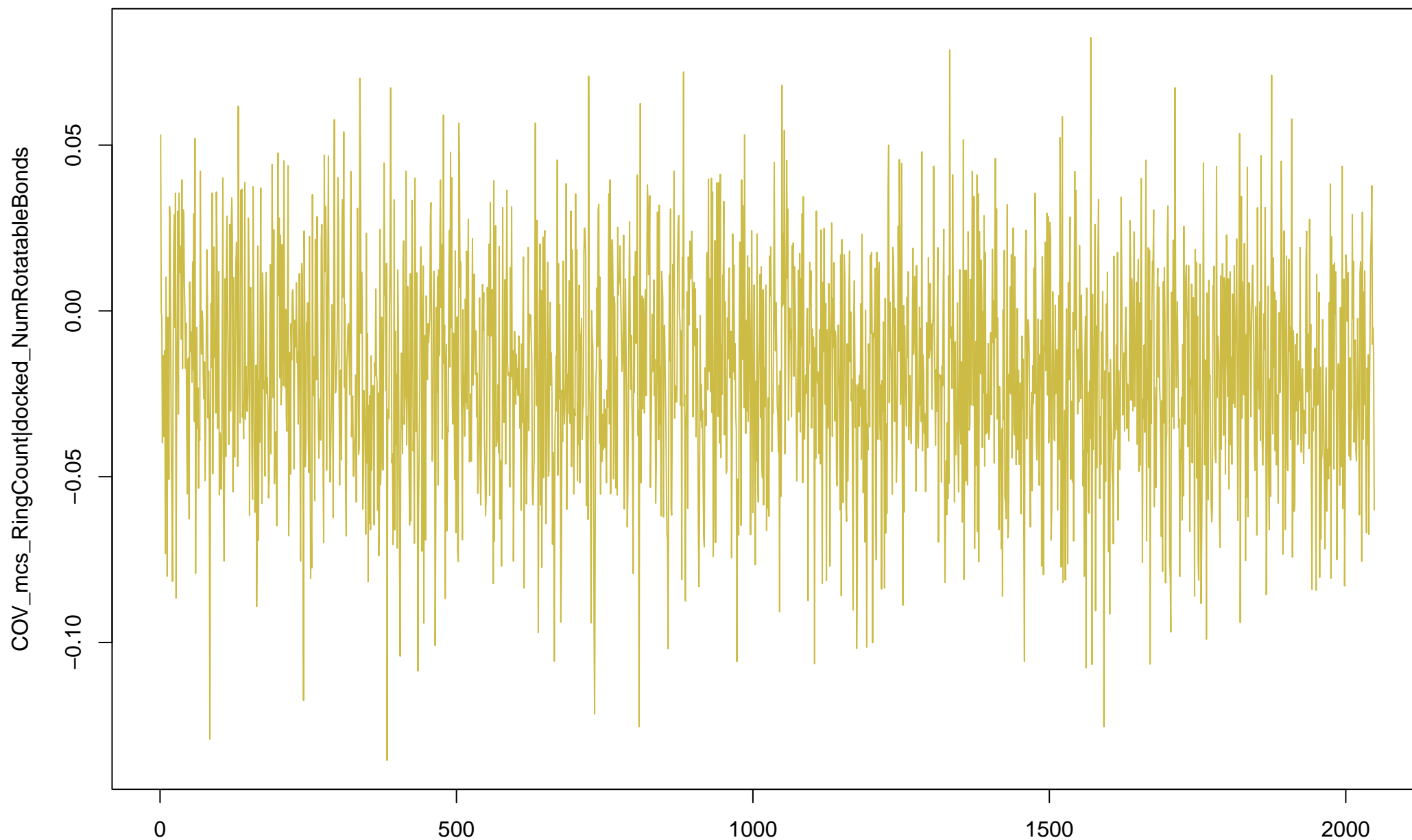
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1910 | BMK = 0.0438 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0



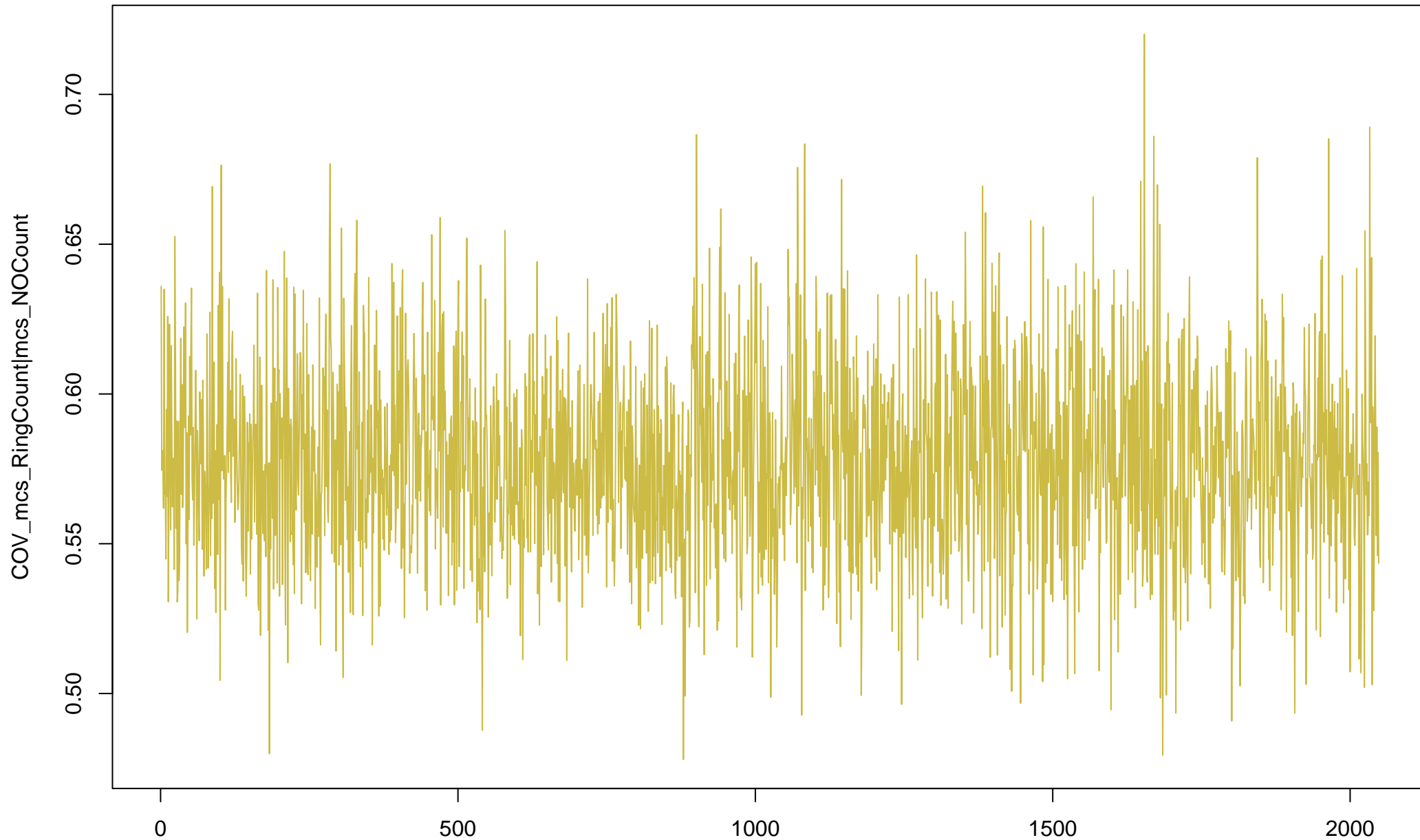
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1920 | BMK = 0.0383 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1840 | BMK = 0.0584 | MCSE(6.27) = 2.46 | stat: FALSE | burn: 0



COV_mcs_RingCount|mcs_NOCount
ESS = 2050 | BMK = 0.0626 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1770 | BMK = 0.0367 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0

