

Stats

min ESS = 220.932958735695

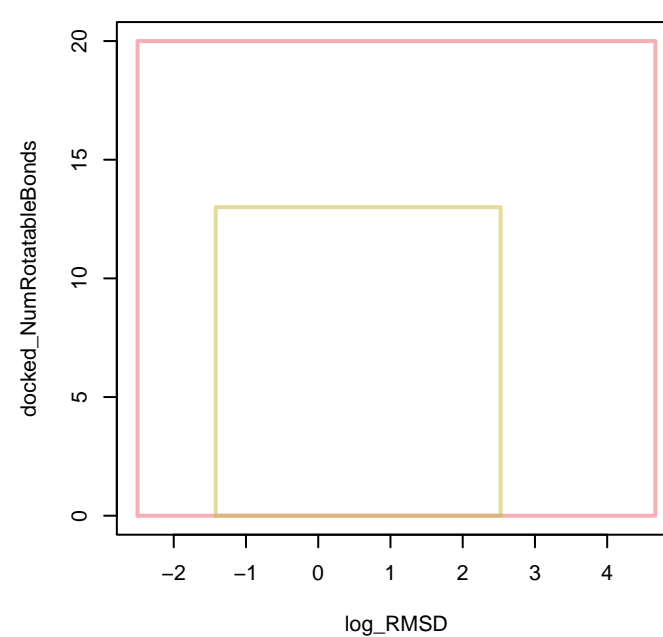
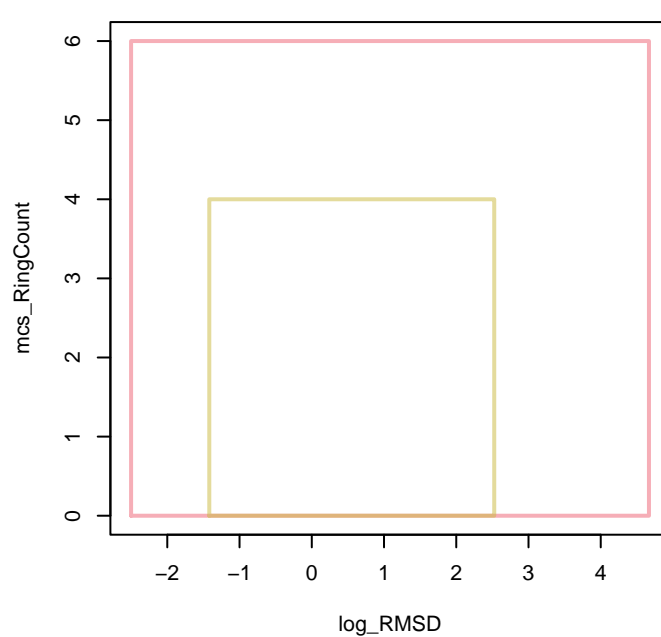
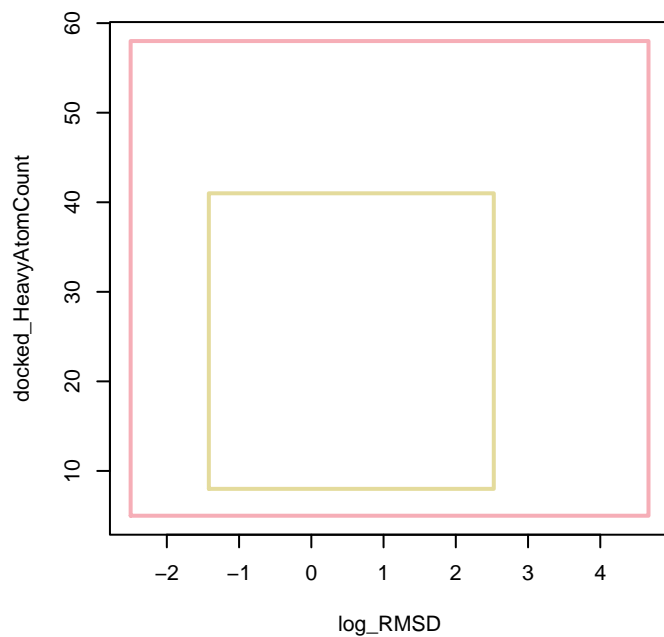
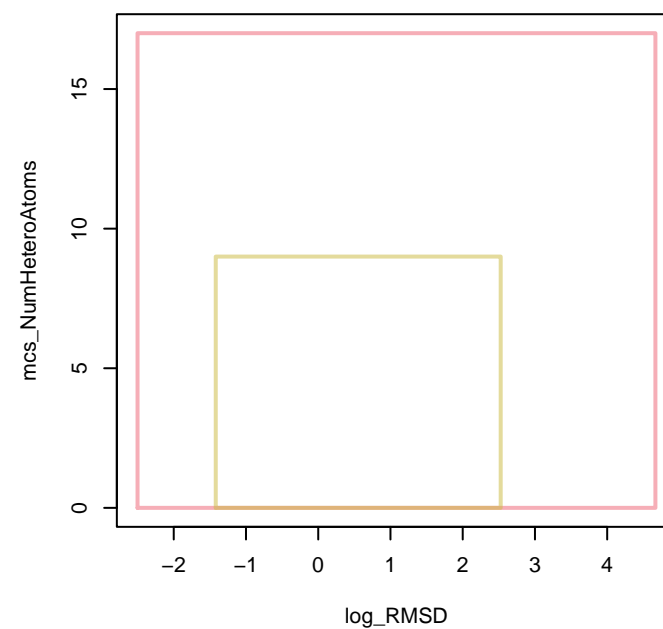
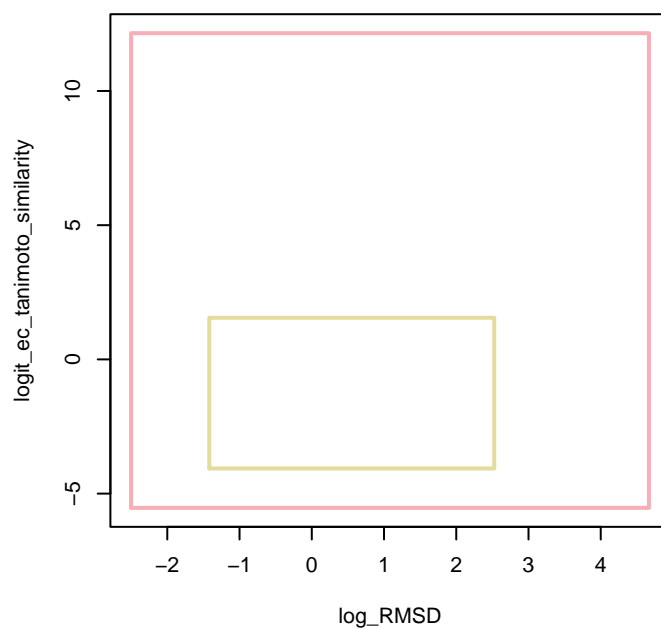
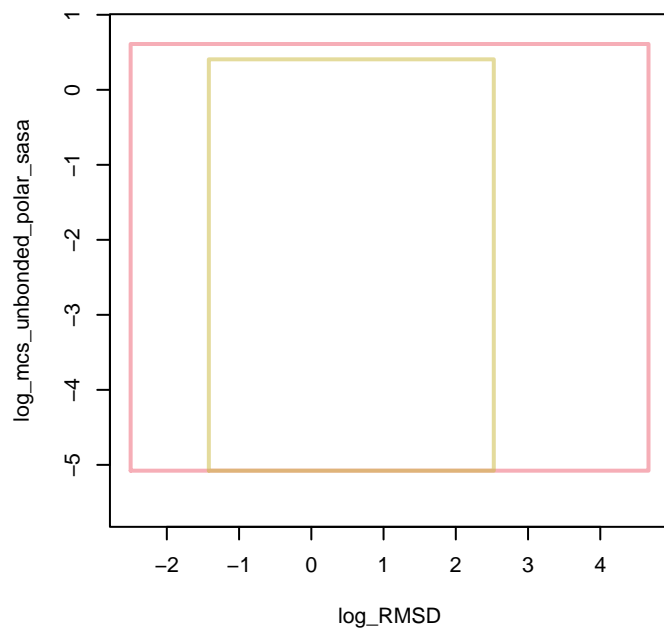
max BMK = 0.205529327084652

max MCSE = 21.7464542279339

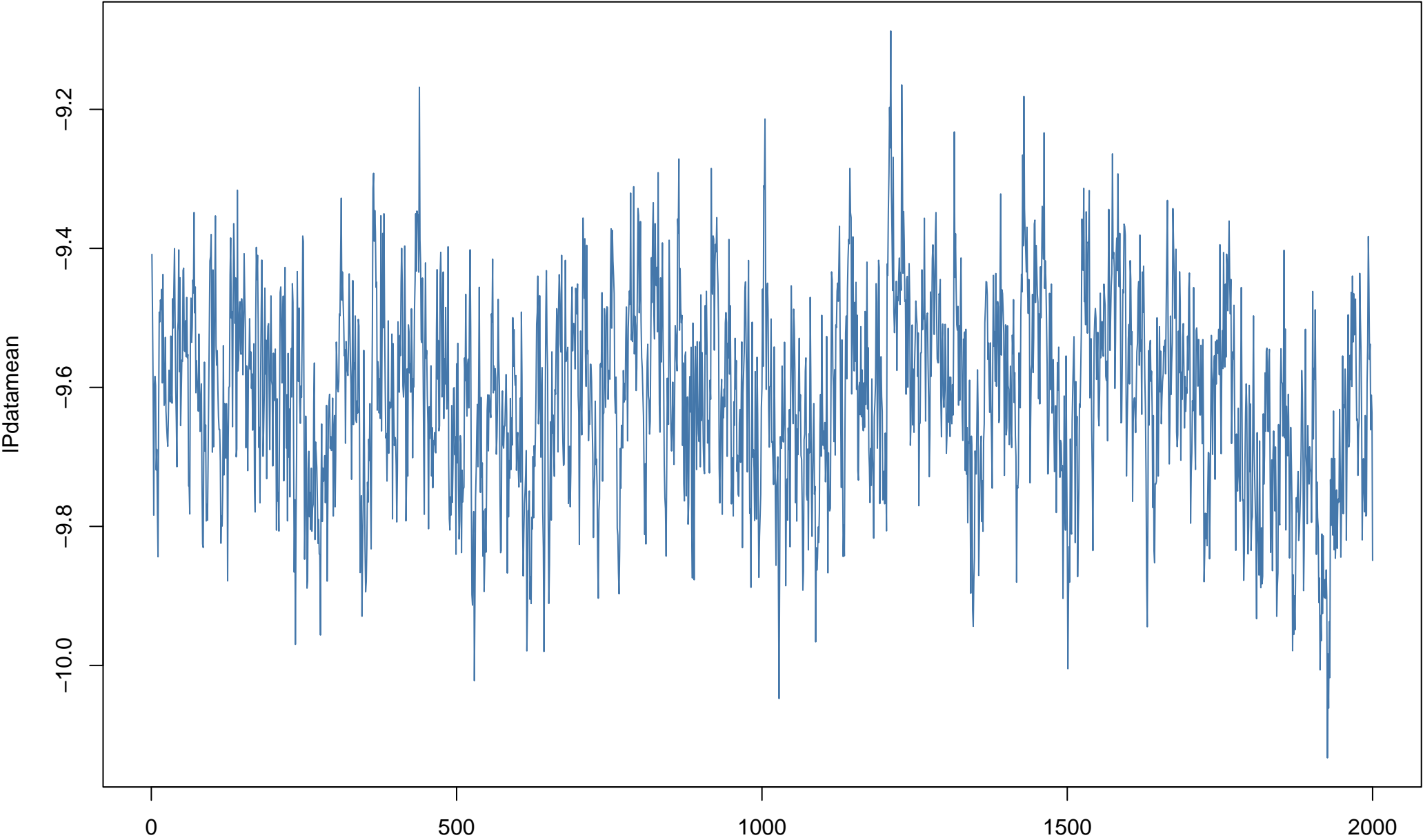
all stationary: FALSE

burn: 0

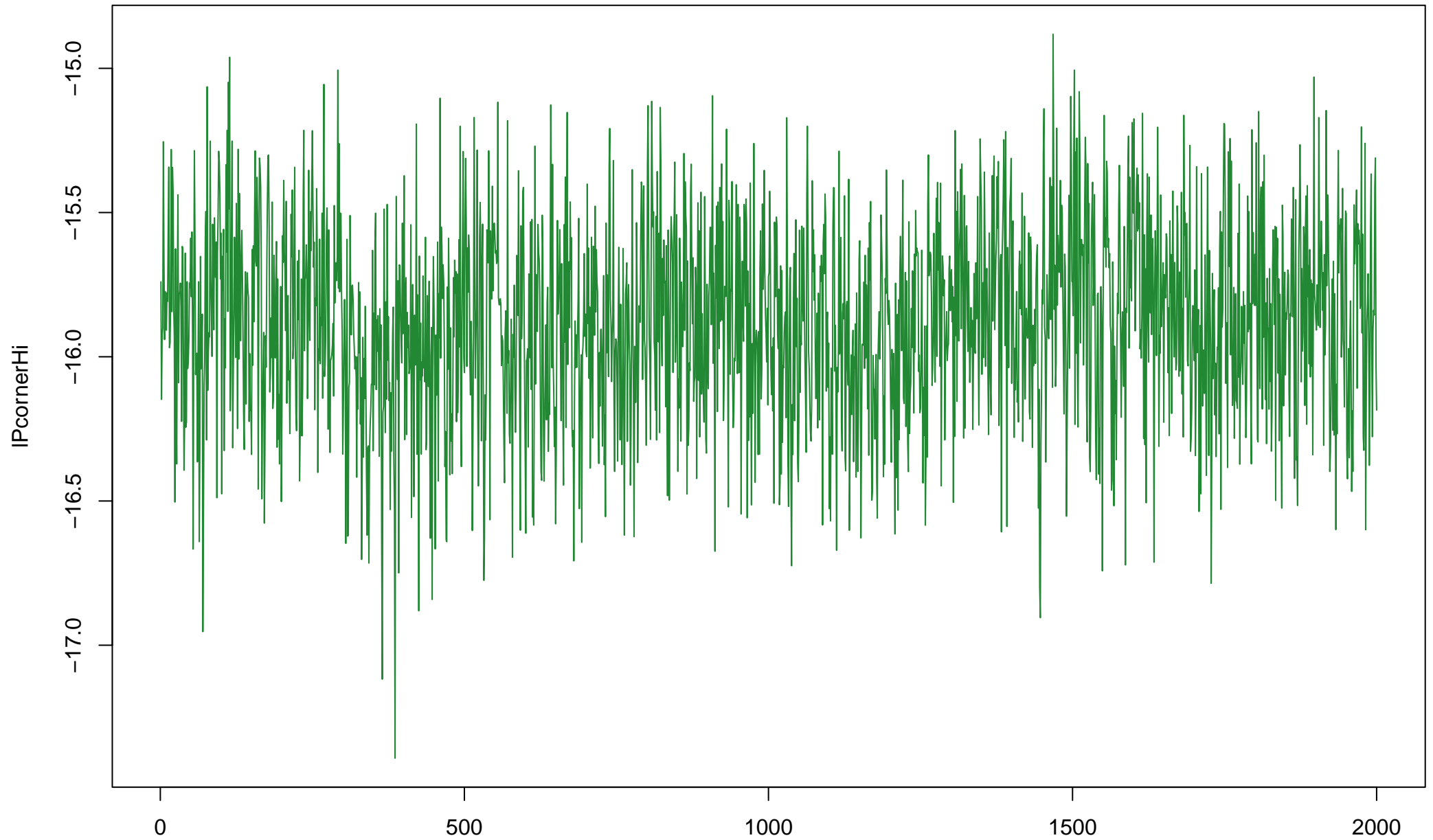
1:2



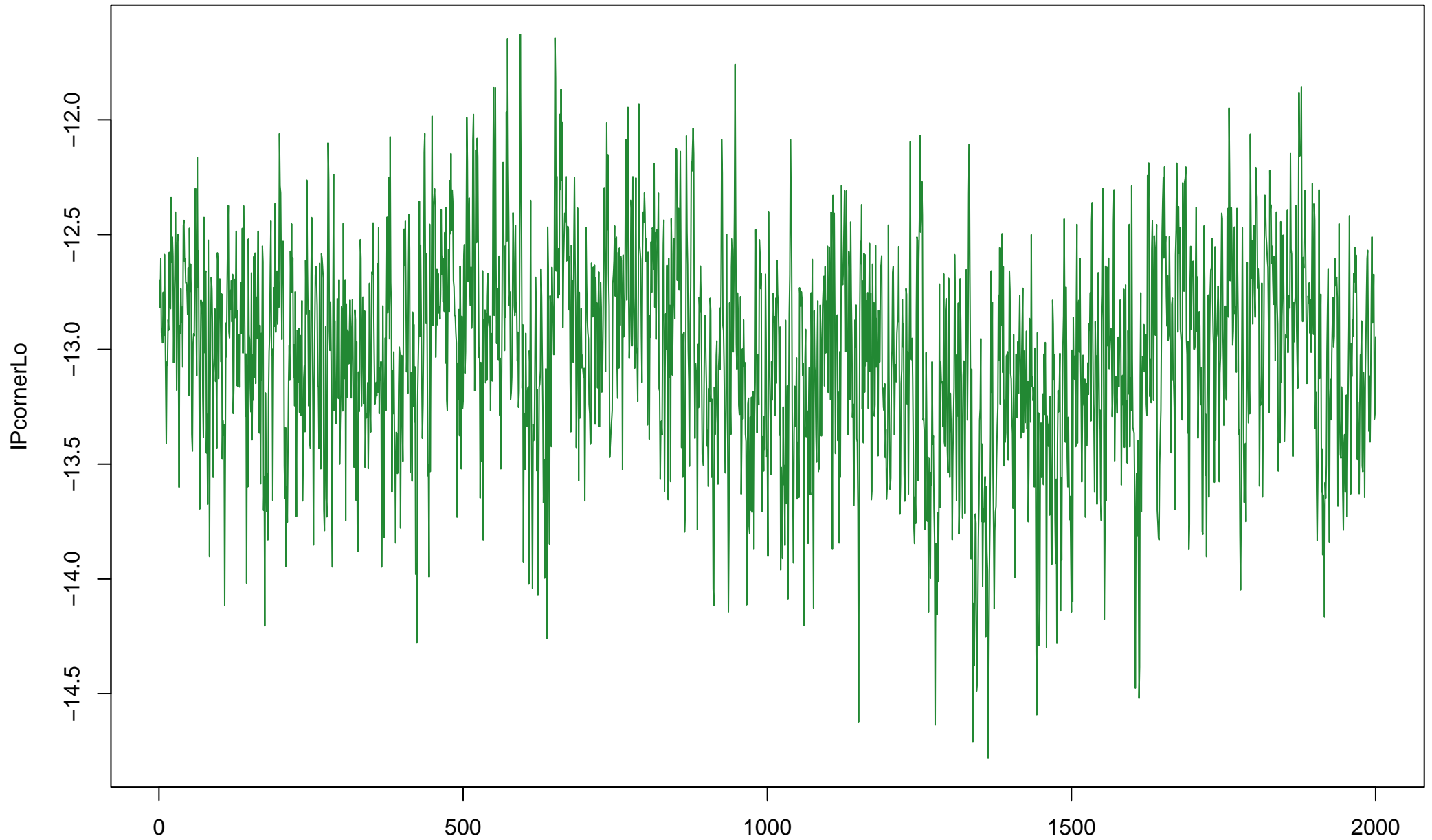
IPdatamean
ESS = 221 | BMK = 0.0708 | MCSE(6.27) = 1.39 | stat: TRUE | burn: 0



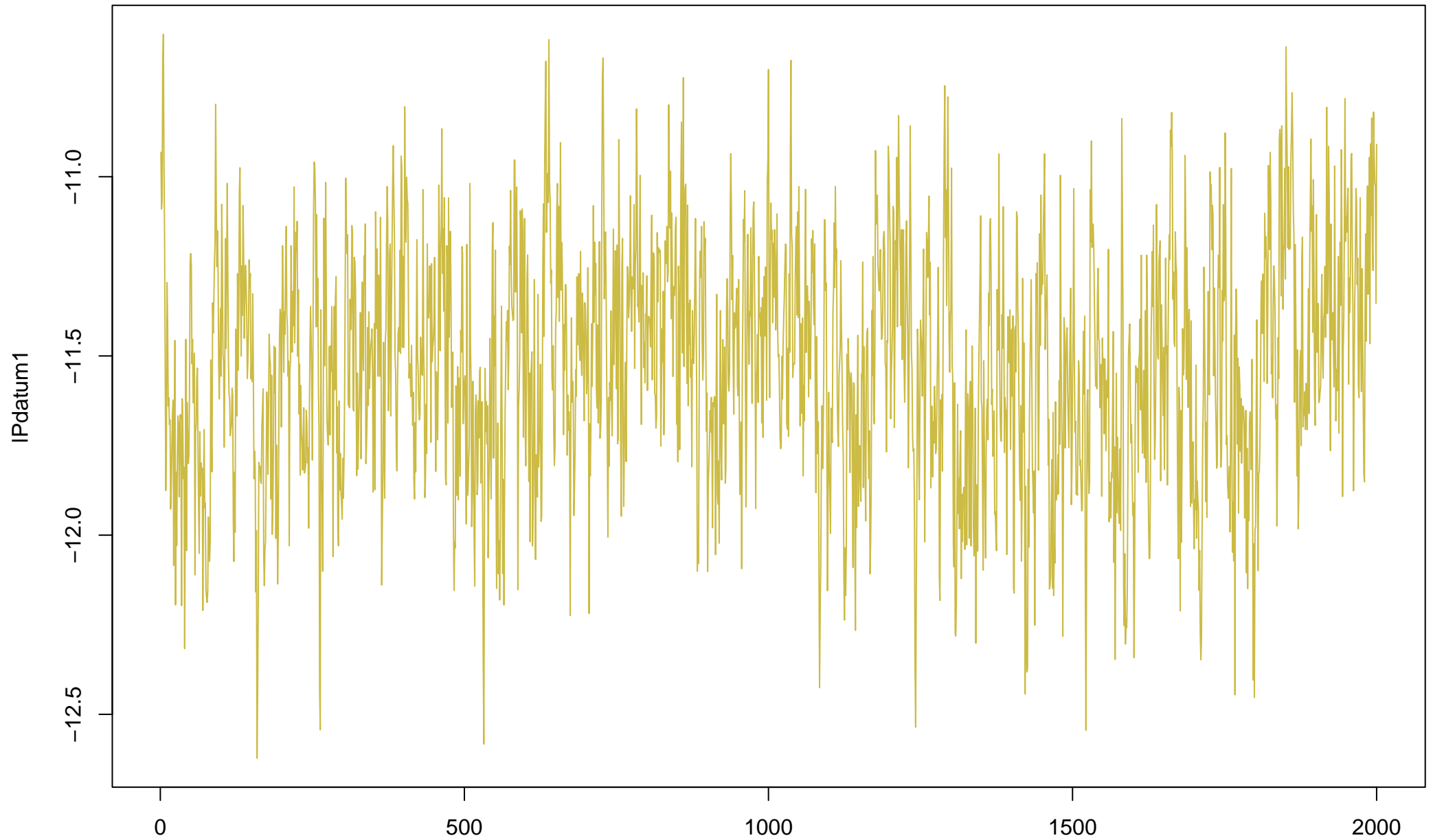
IPcornerHi
ESS = 818 | BMK = 0.053 | MCSE(6.27) = 0.575 | stat: TRUE | burn: 0



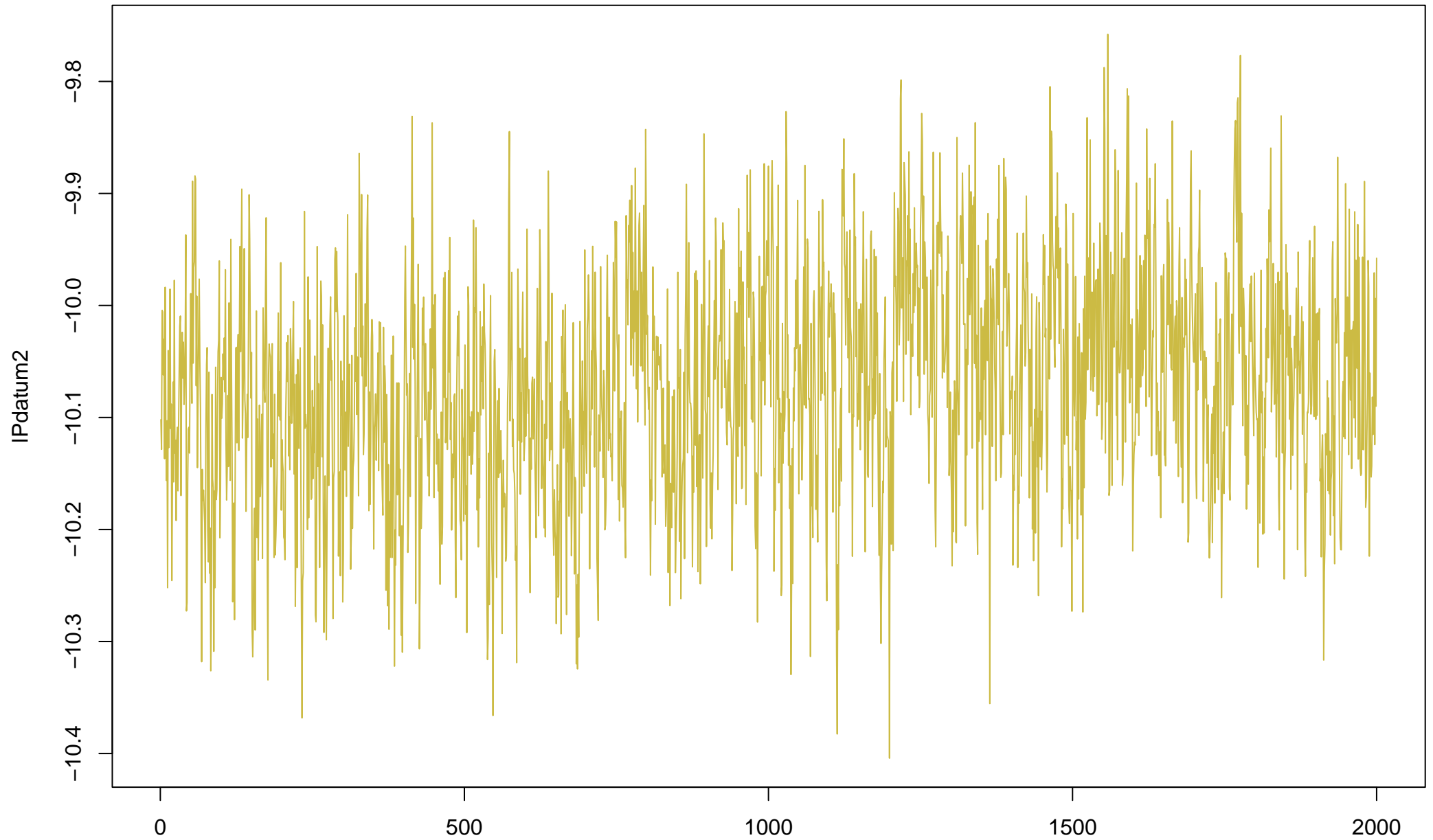
IPcornerLo
ESS = 270 | BMK = 0.138 | MCSE(6.27) = 0.419 | stat: FALSE | burn: 0



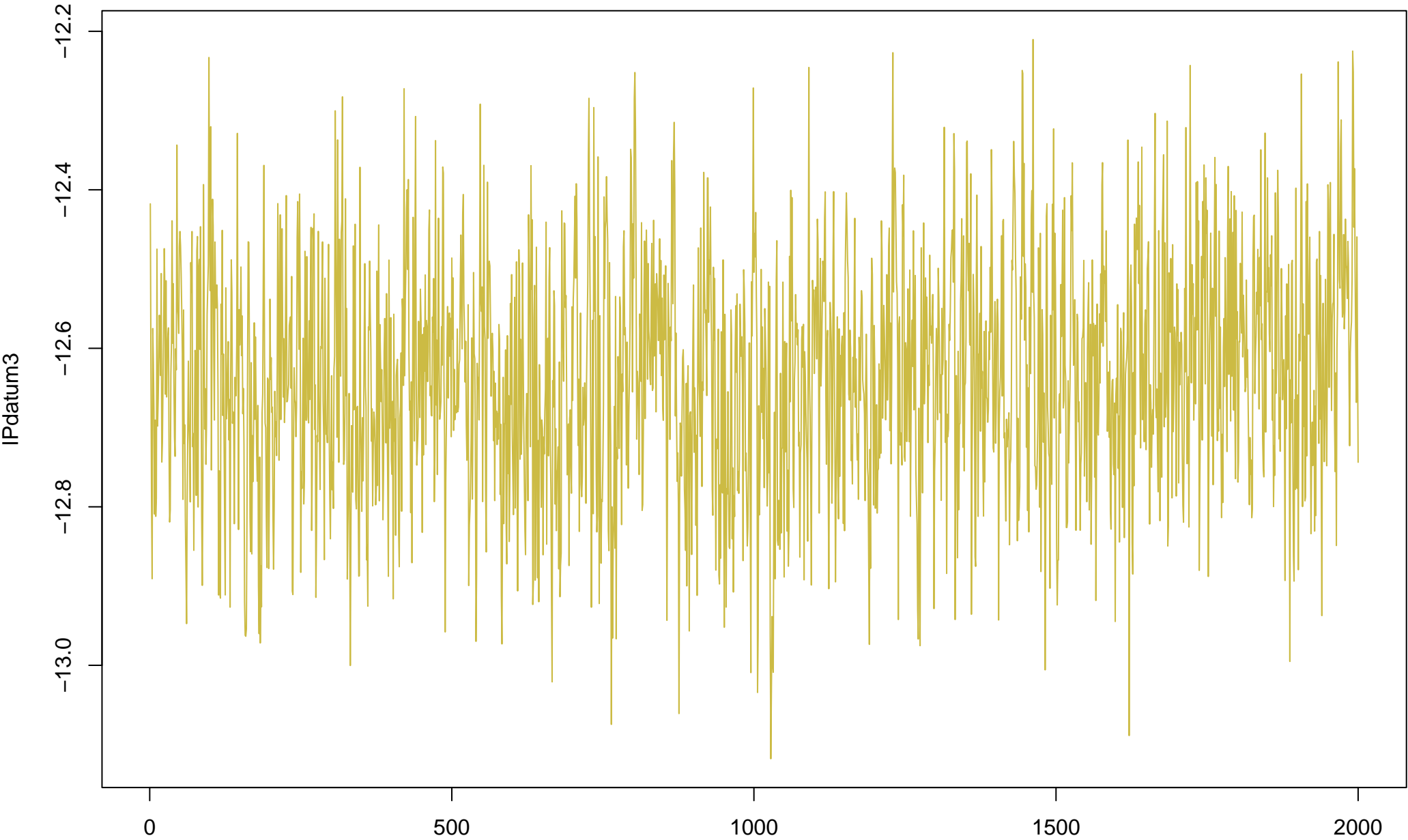
IPdatum1
ESS = 263 | BMK = 0.0745 | MCSE(6.27) = 0.602 | stat: TRUE | burn: 0



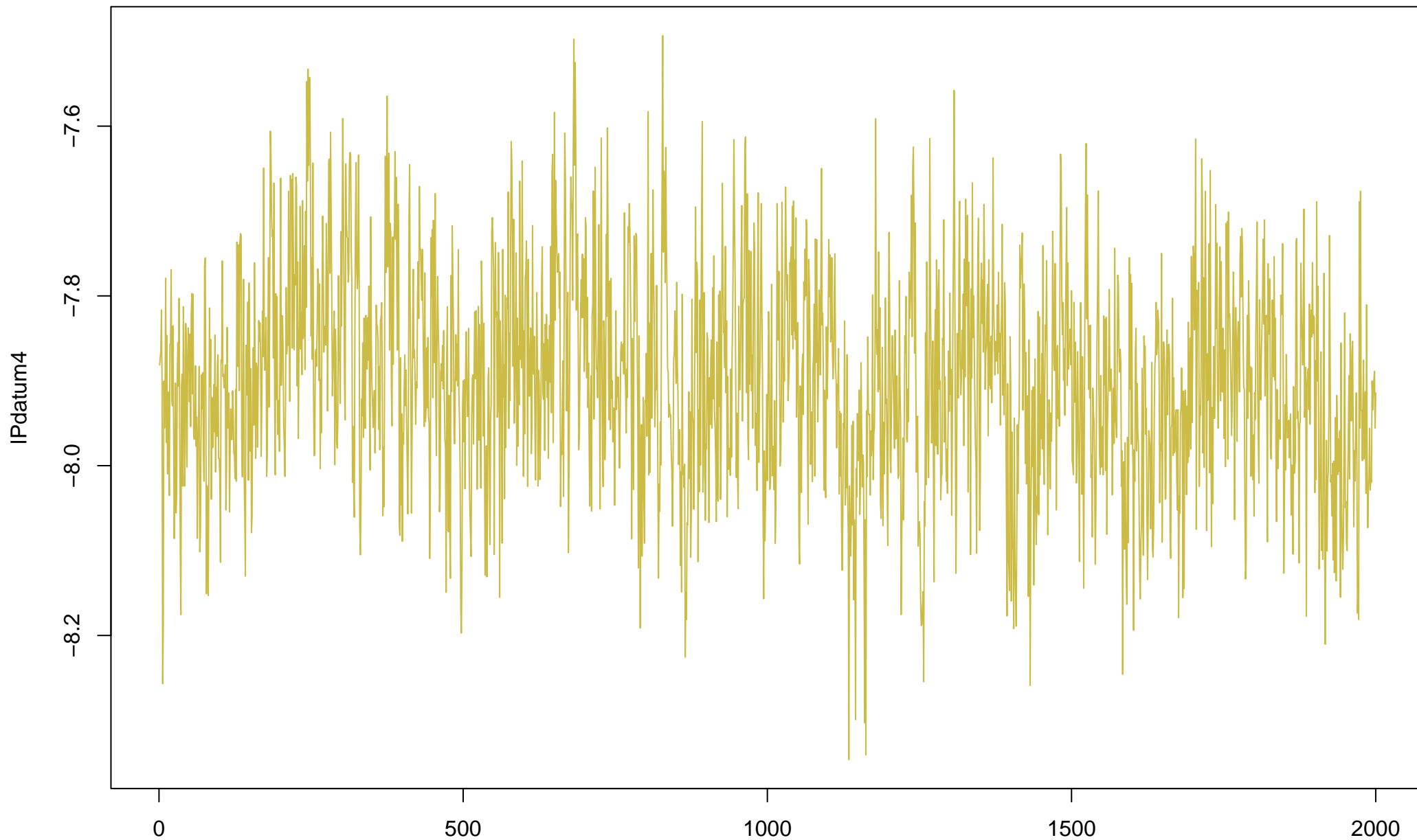
IPdatum2
ESS = 342 | BMK = 0.18 | MCSE(6.27) = 1.96 | stat: FALSE | burn: 0



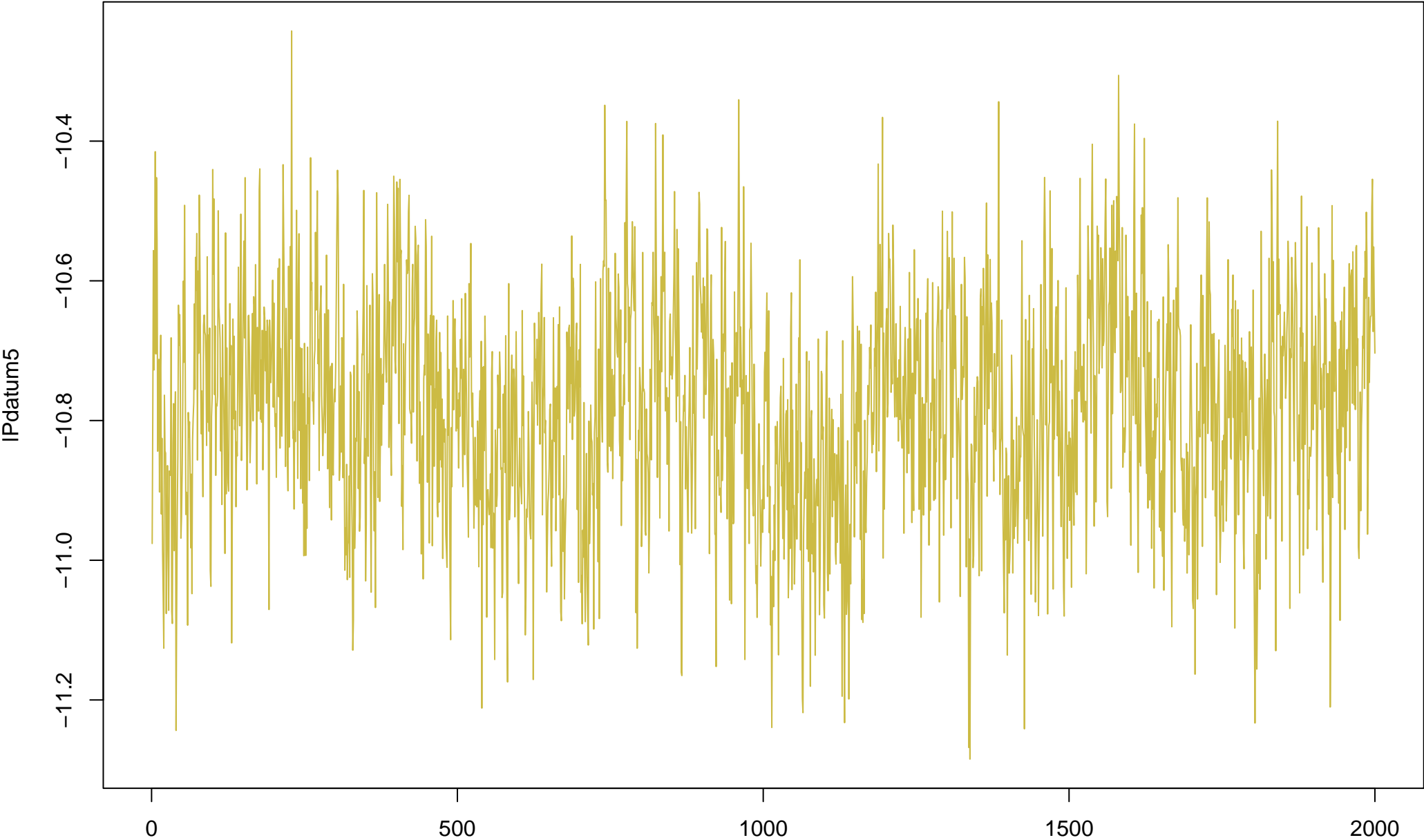
IPdatum3
ESS = 748 | BMK = 0.0733 | MCSE(6.27) = 1.36 | stat: TRUE | burn: 0



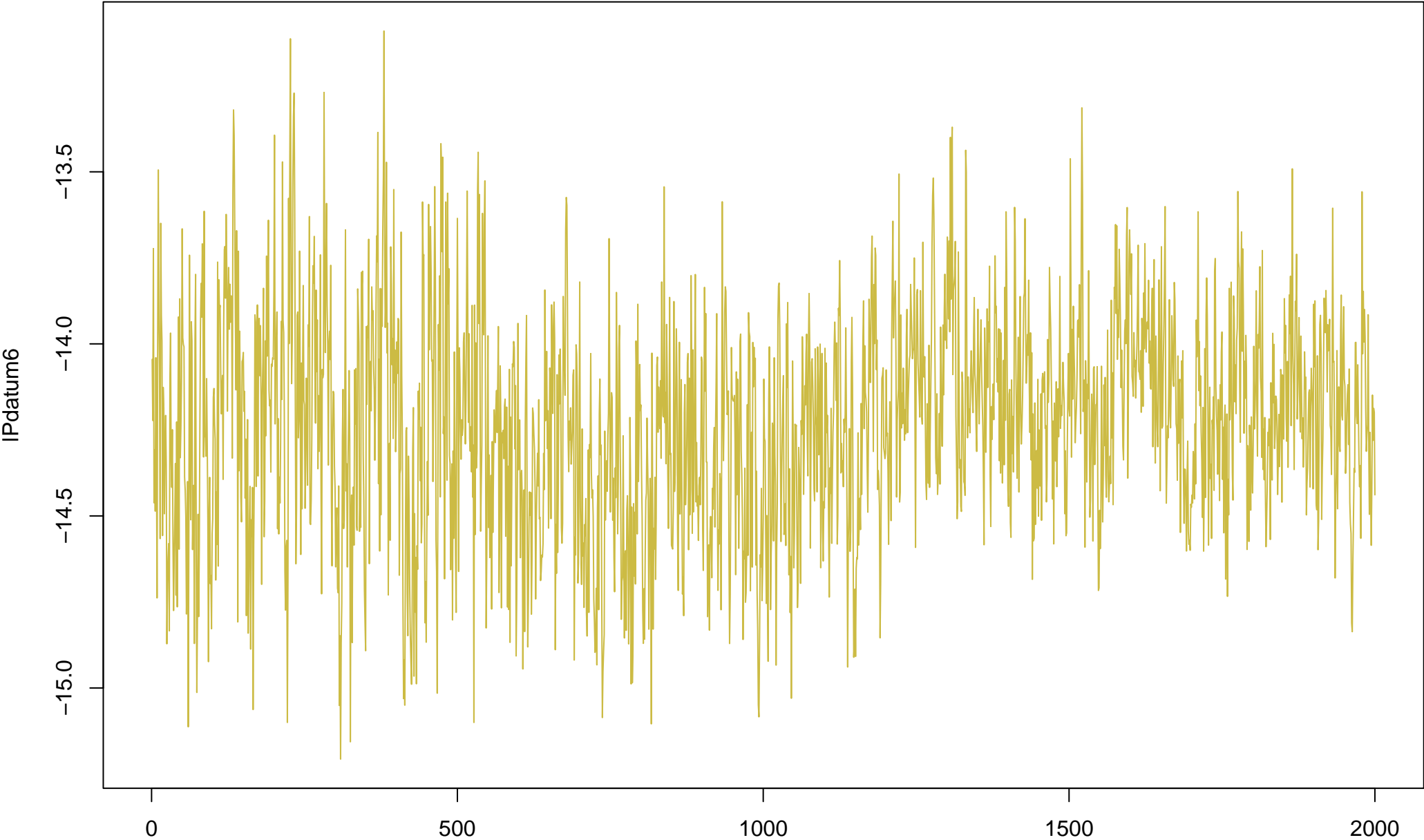
IPdatum4
ESS = 307 | BMK = 0.127 | MCSE(6.27) = 1.57 | stat: TRUE | burn: 0



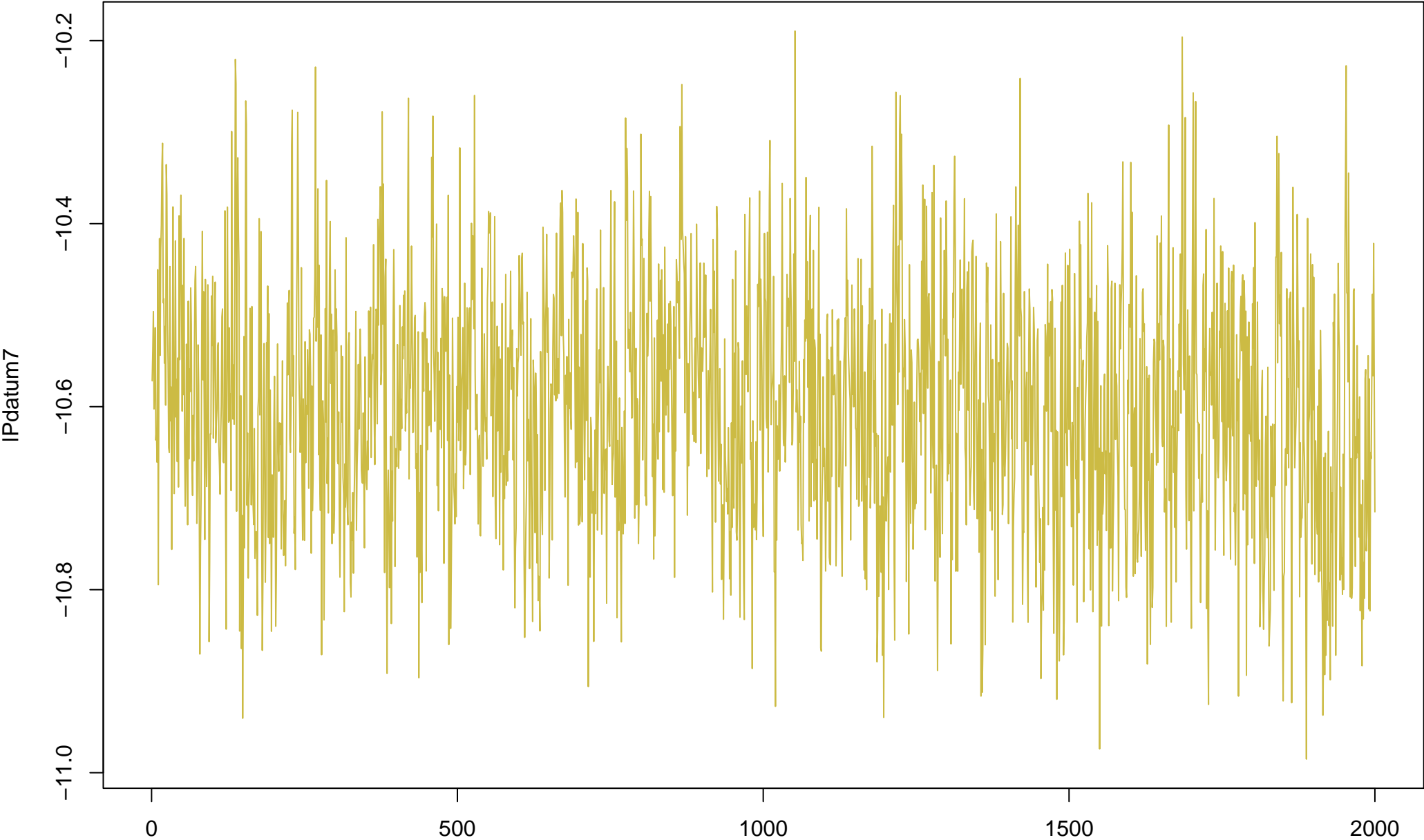
IPdatum5
ESS = 256 | BMK = 0.0466 | MCSE(6.27) = 1.26 | stat: TRUE | burn: 0



IPdatum6
ESS = 243 | BMK = 0.206 | MCSE(6.27) = 0.615 | stat: TRUE | burn: 0

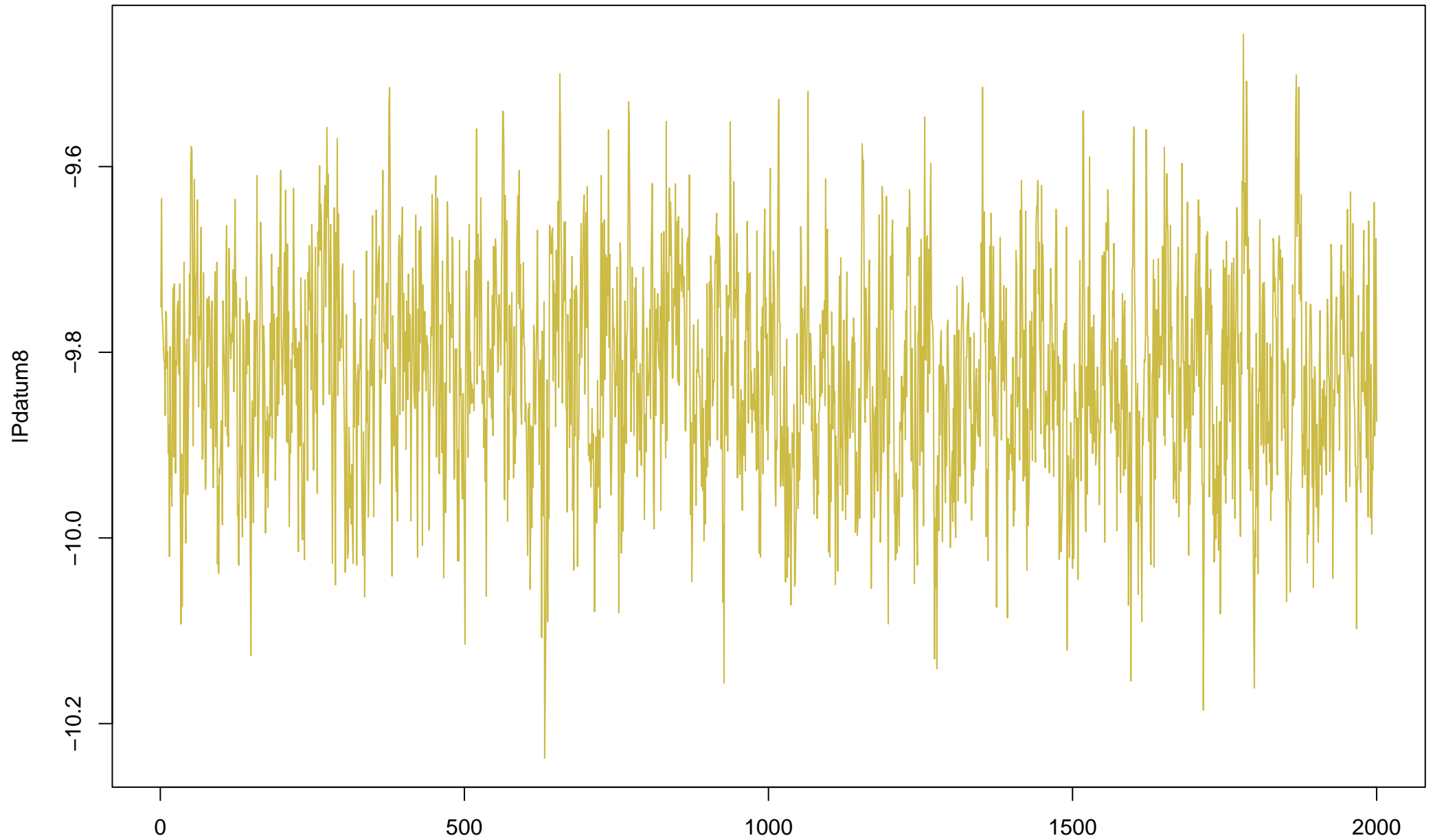


IPdatum7
ESS = 608 | BMK = 0.0836 | MCSE(6.27) = 1.51 | stat: TRUE | burn: 0

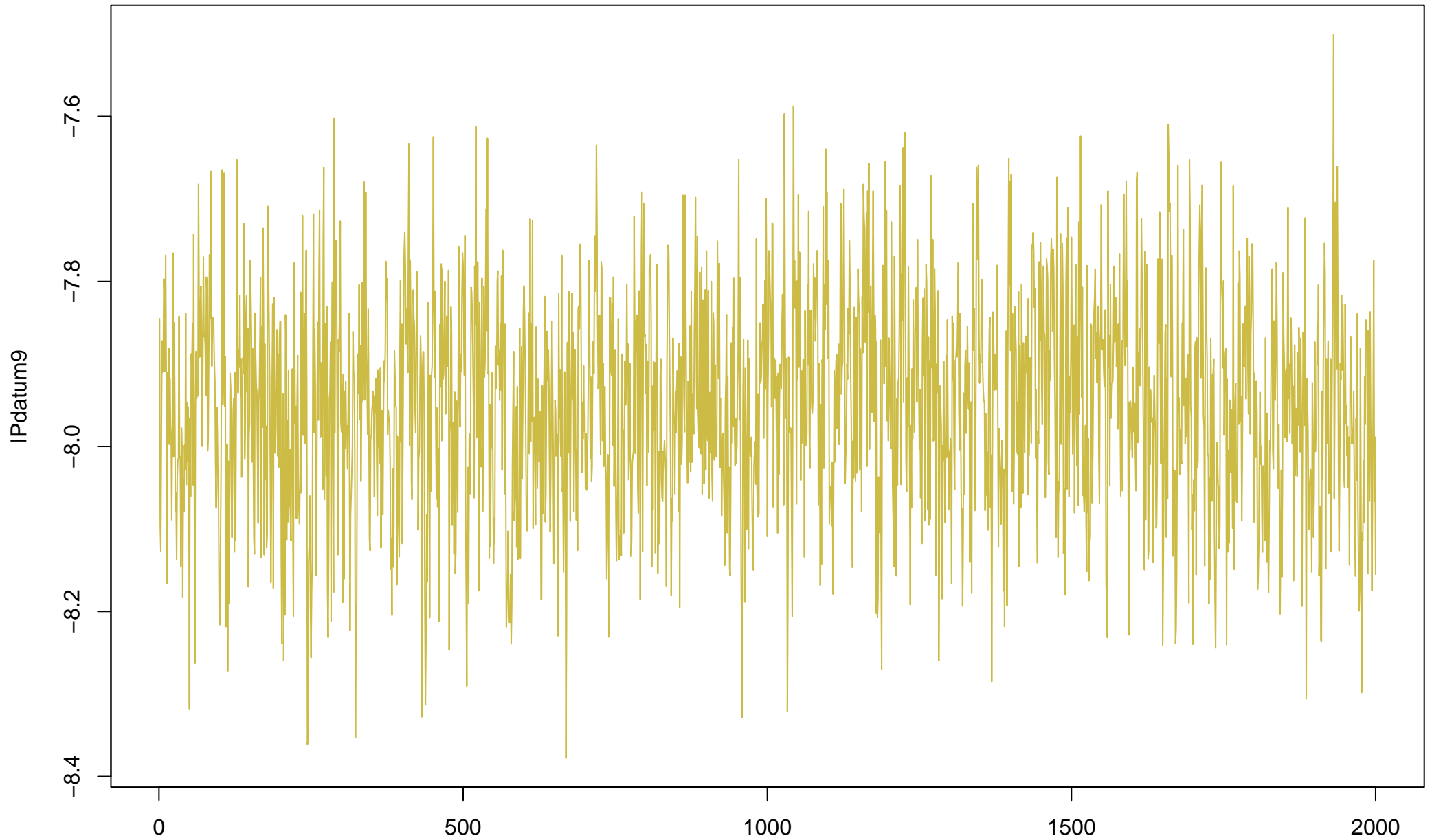


IPdatum8

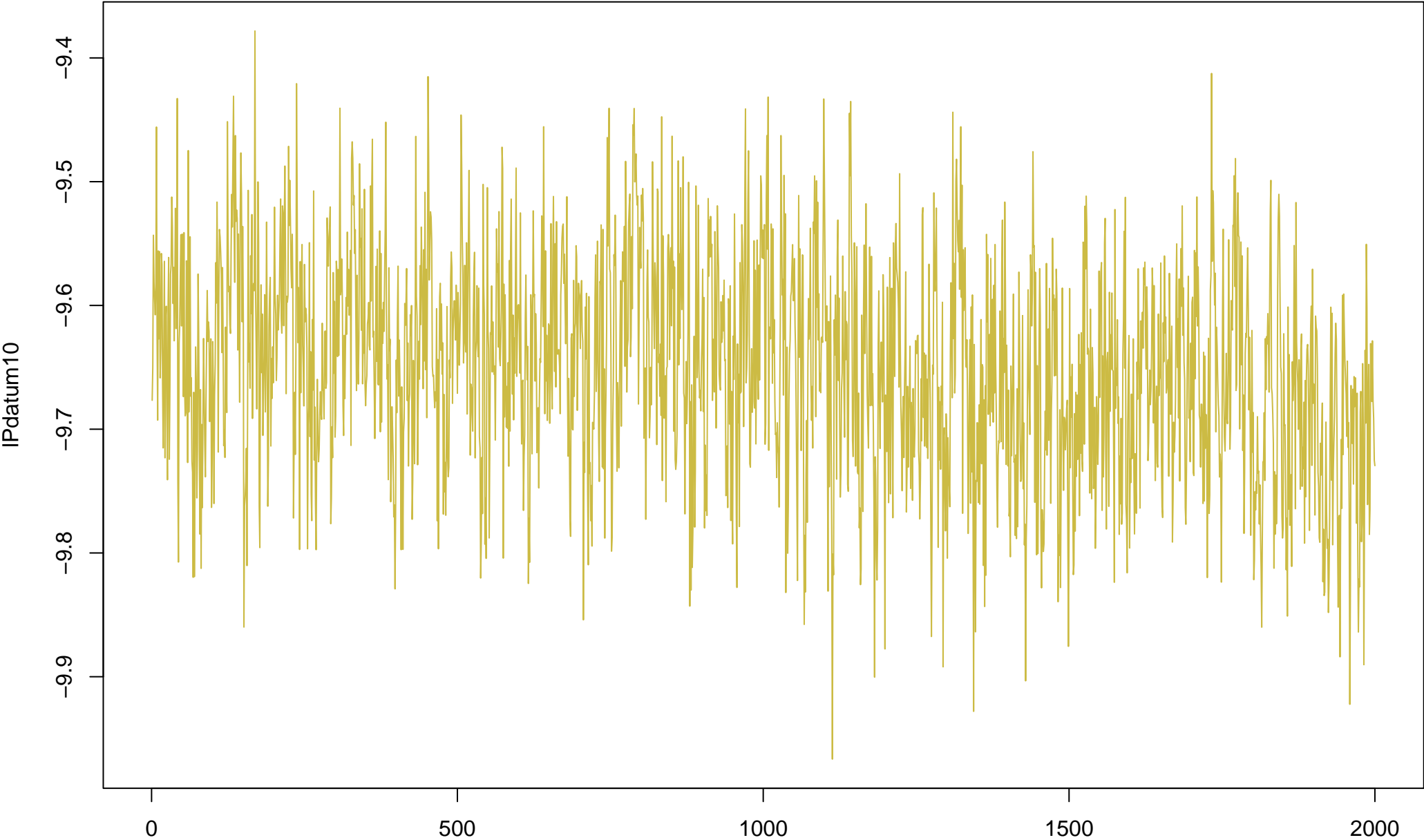
ESS = 479 | BMK = 0.0933 | MCSE(6.27) = 1.72 | stat: TRUE | burn: 0



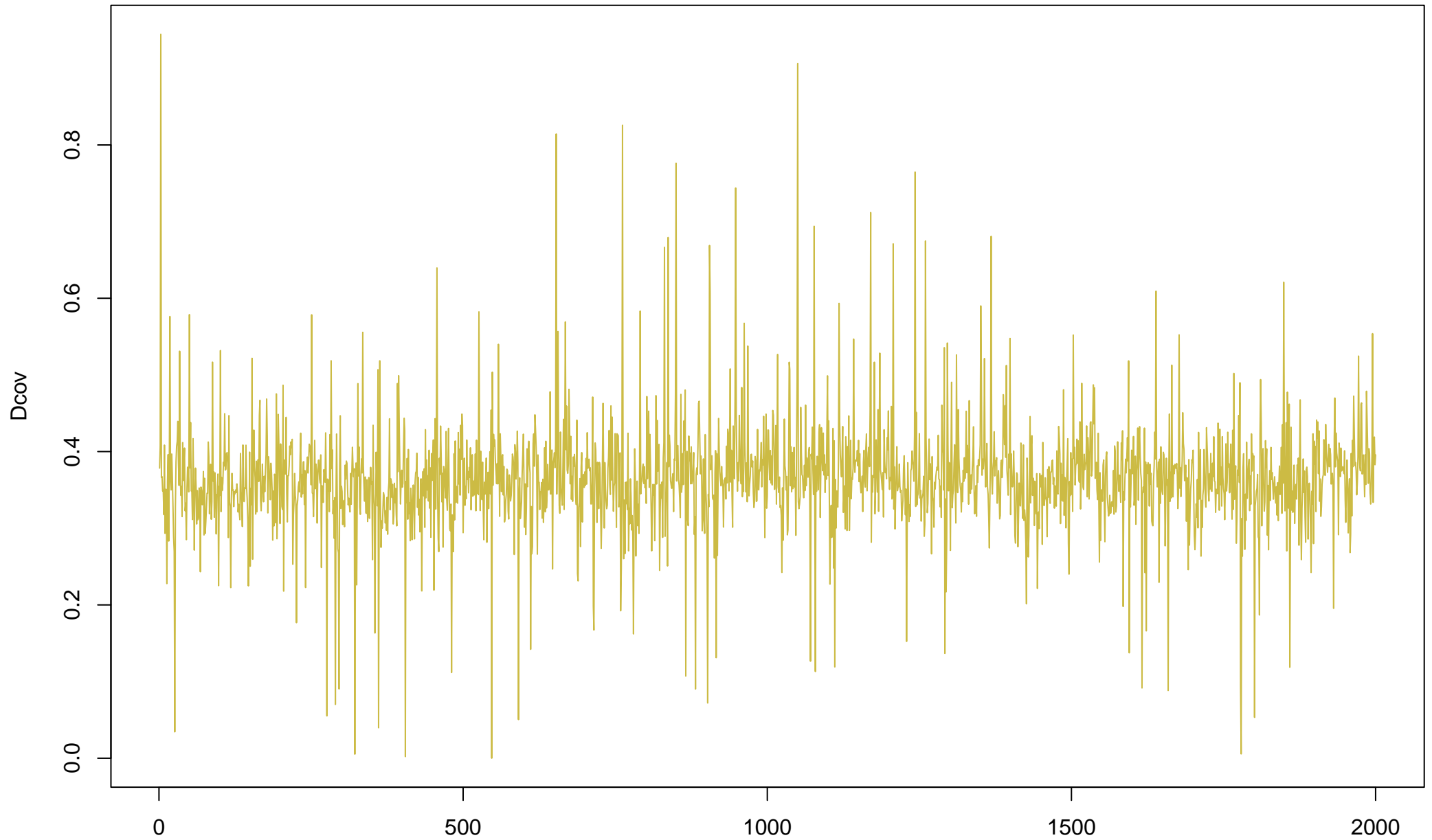
IPdatum9
ESS = 694 | BMK = 0.071 | MCSE(6.27) = 1.49 | stat: TRUE | burn: 0



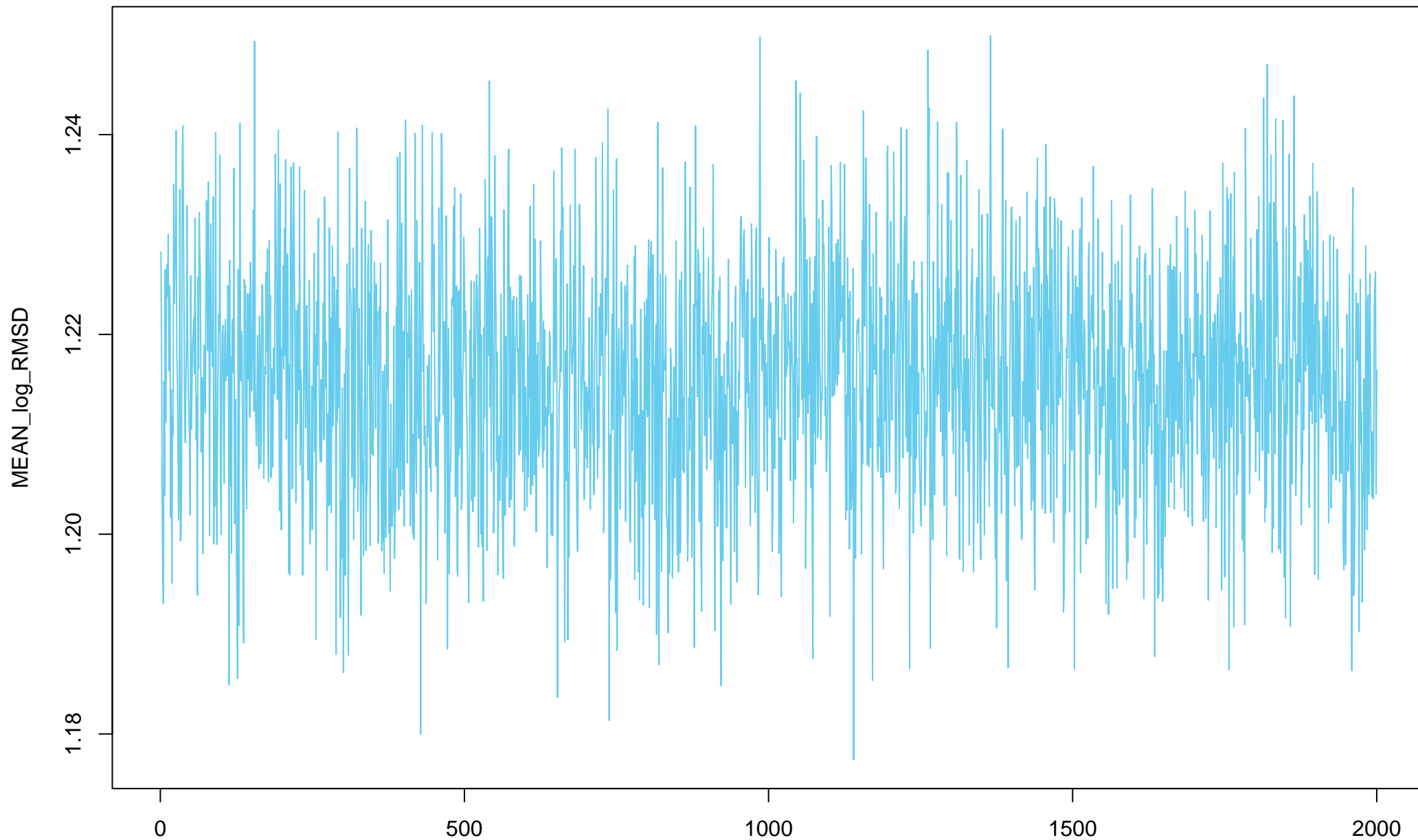
IPdatum10
ESS = 264 | BMK = 0.181 | MCSE(6.27) = 2.26 | stat: FALSE | burn: 0



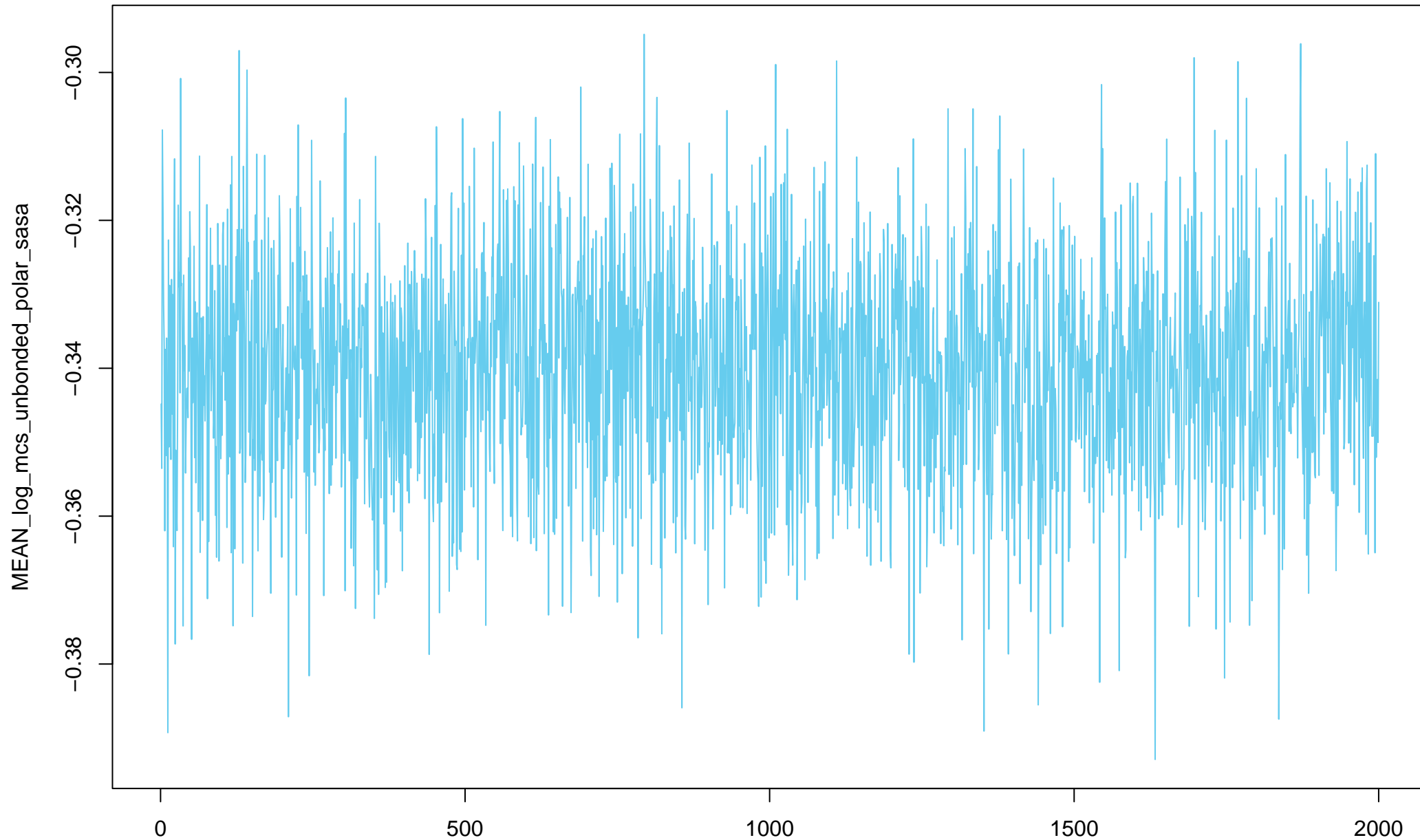
Dcov
ESS = 1700 | BMK = 0.0907 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0



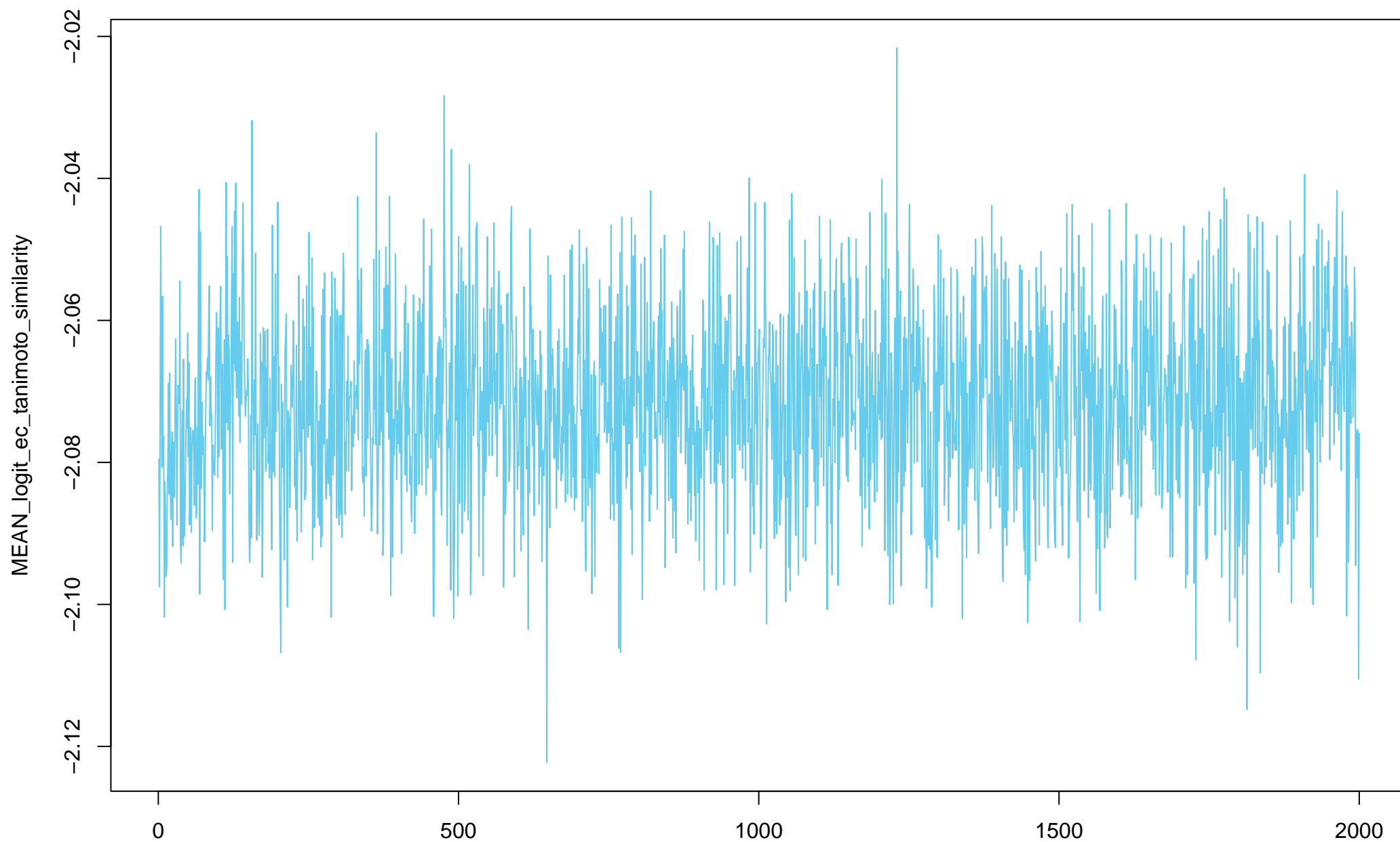
MEAN_log_RMSD
ESS = 1710 | BMK = 0.0497 | MCSE(6.27) = 17 | stat: TRUE | burn: 0



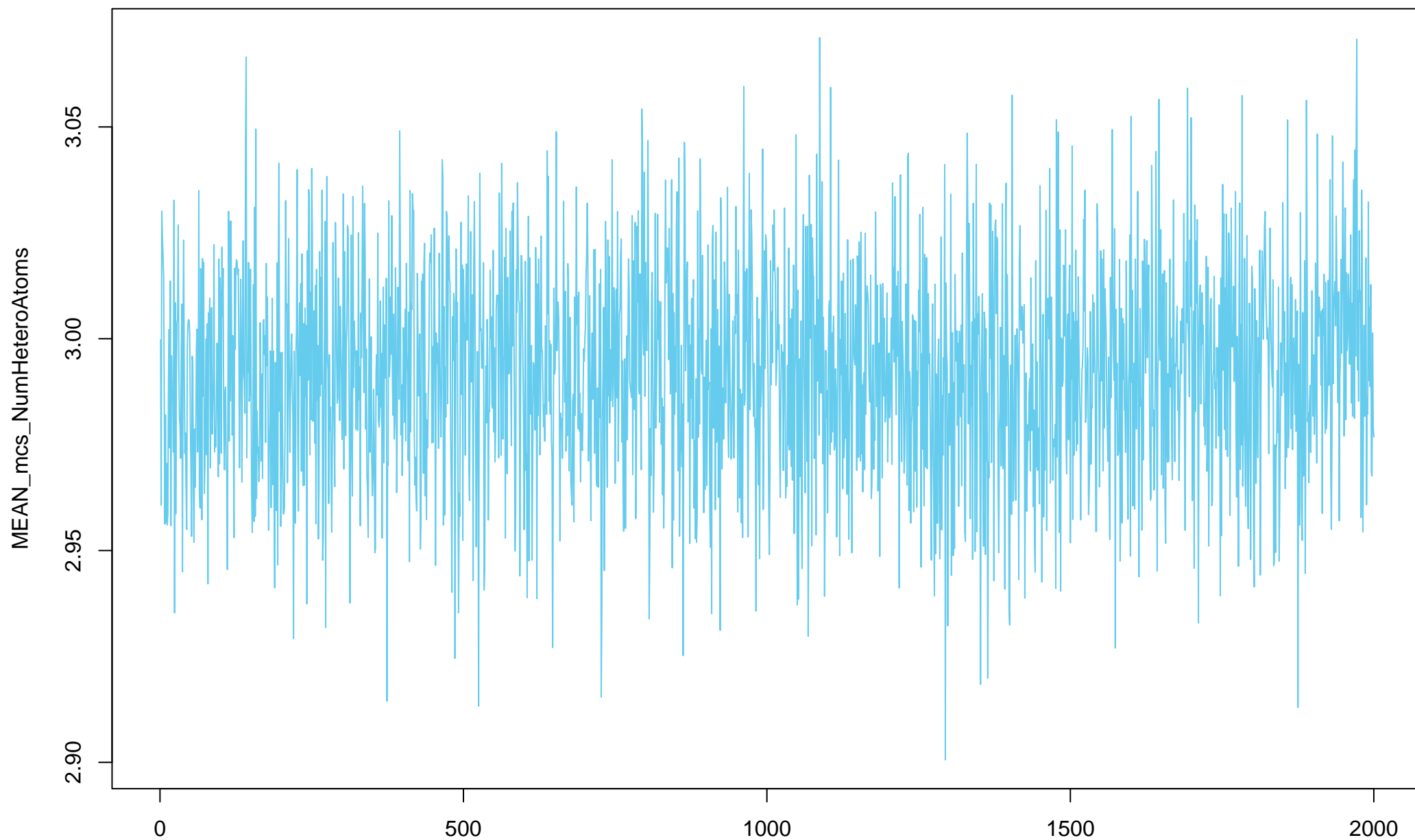
MEAN_log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0444 | MCSE(6.27) = 12.9 | stat: TRUE | burn: 0



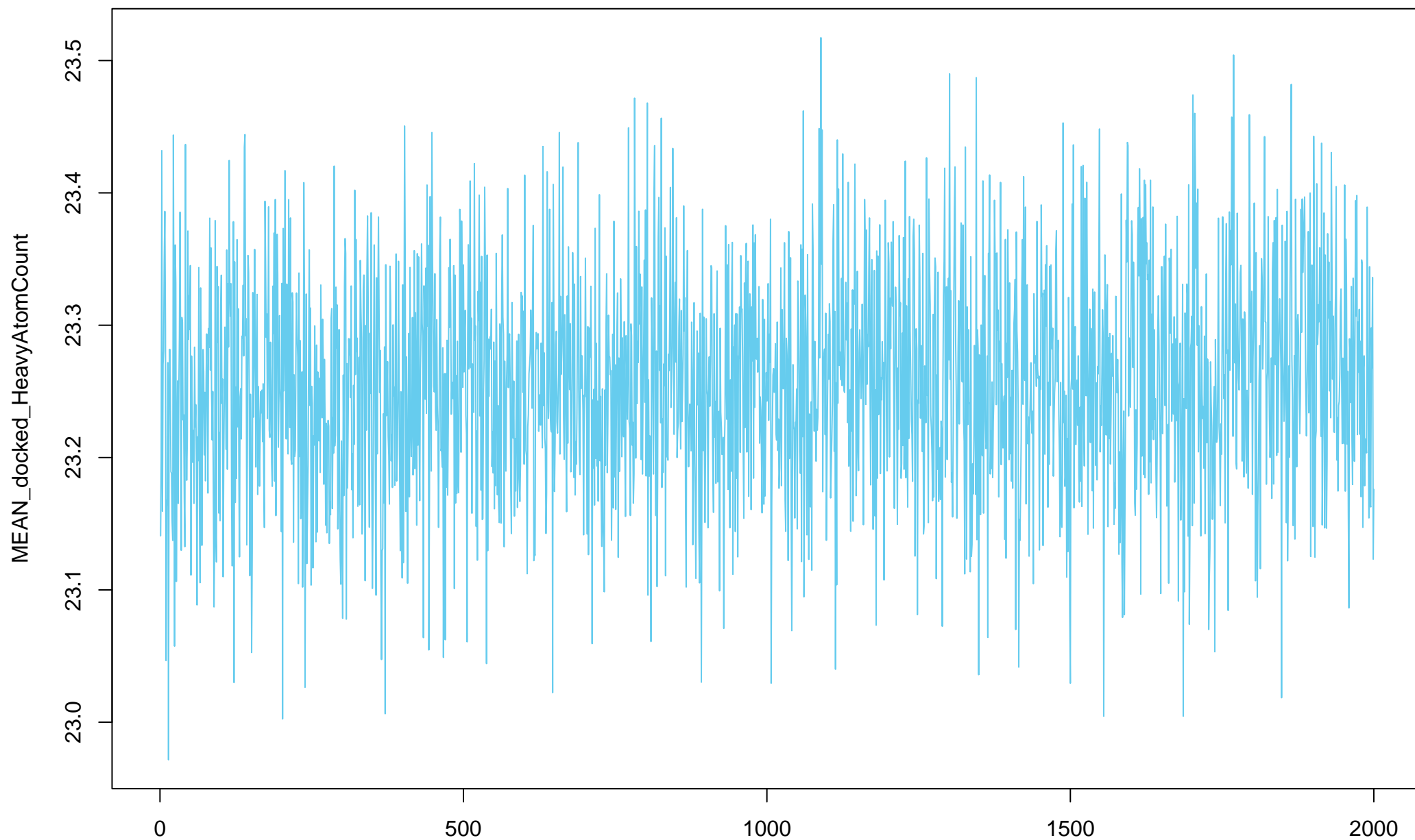
MEAN_logit_ec_tanimoto_similarity
ESS = 1660 | BMK = 0.0677 | MCSE(6.27) = 14.9 | stat: TRUE | burn: 0



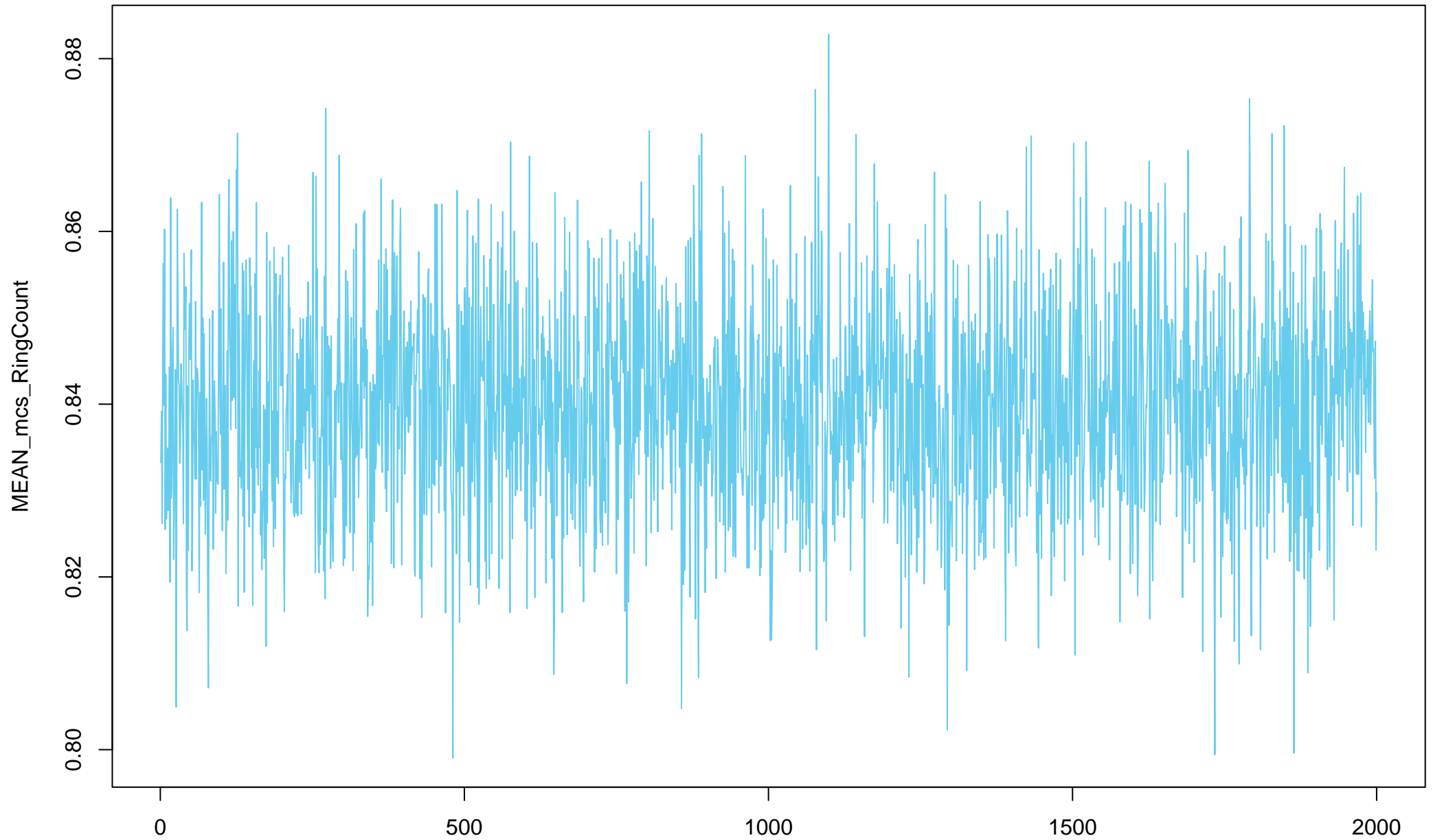
MEAN_mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0512 | MCSE(6.27) = 7.83 | stat: TRUE | burn: 0



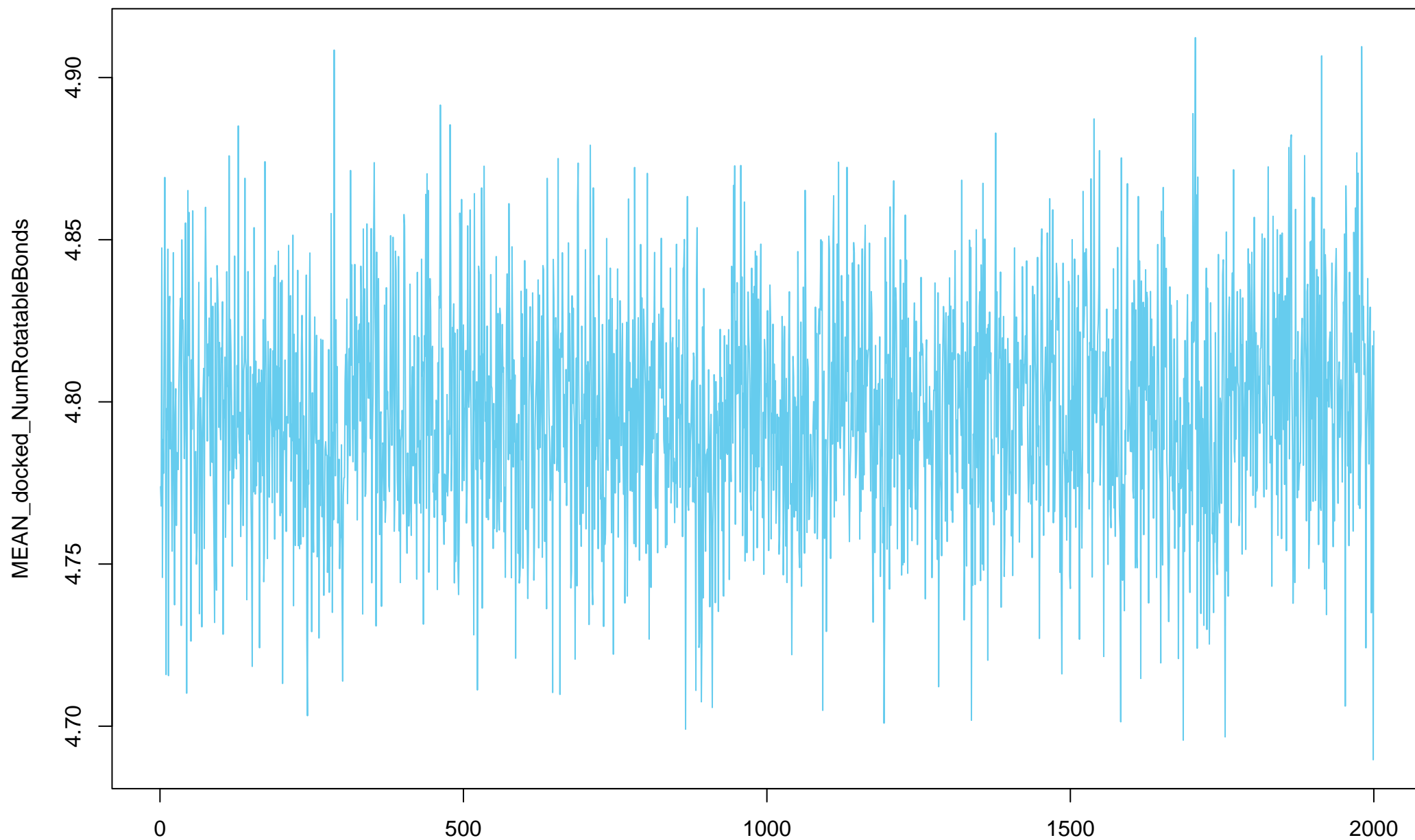
MEAN_docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0651 | MCSE(6.27) = 2.34 | stat: FALSE | burn: 0



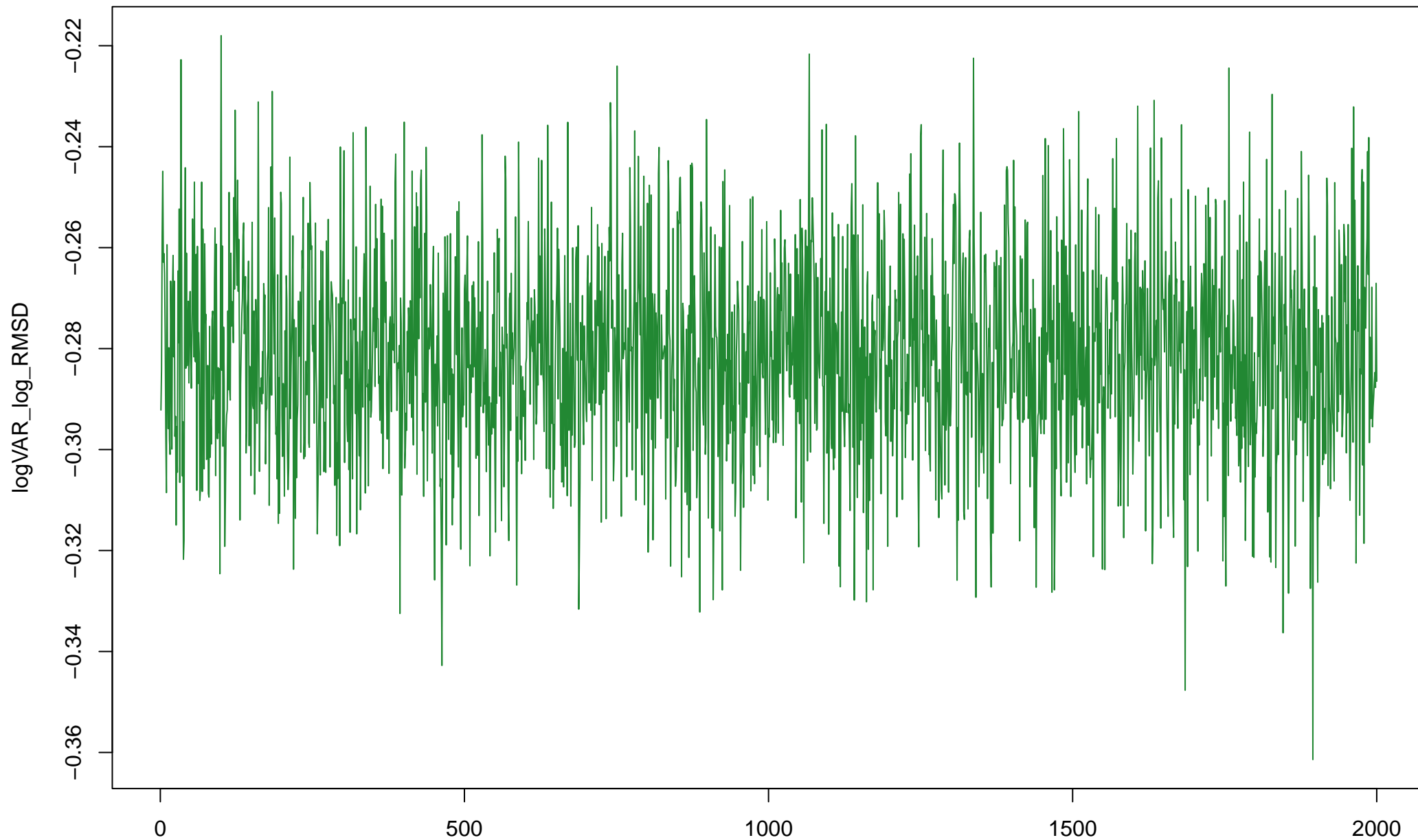
MEAN_mcs_RingCount
ESS = 2000 | BMK = 0.0399 | MCSE(6.27) = 16.2 | stat: TRUE | burn: 0



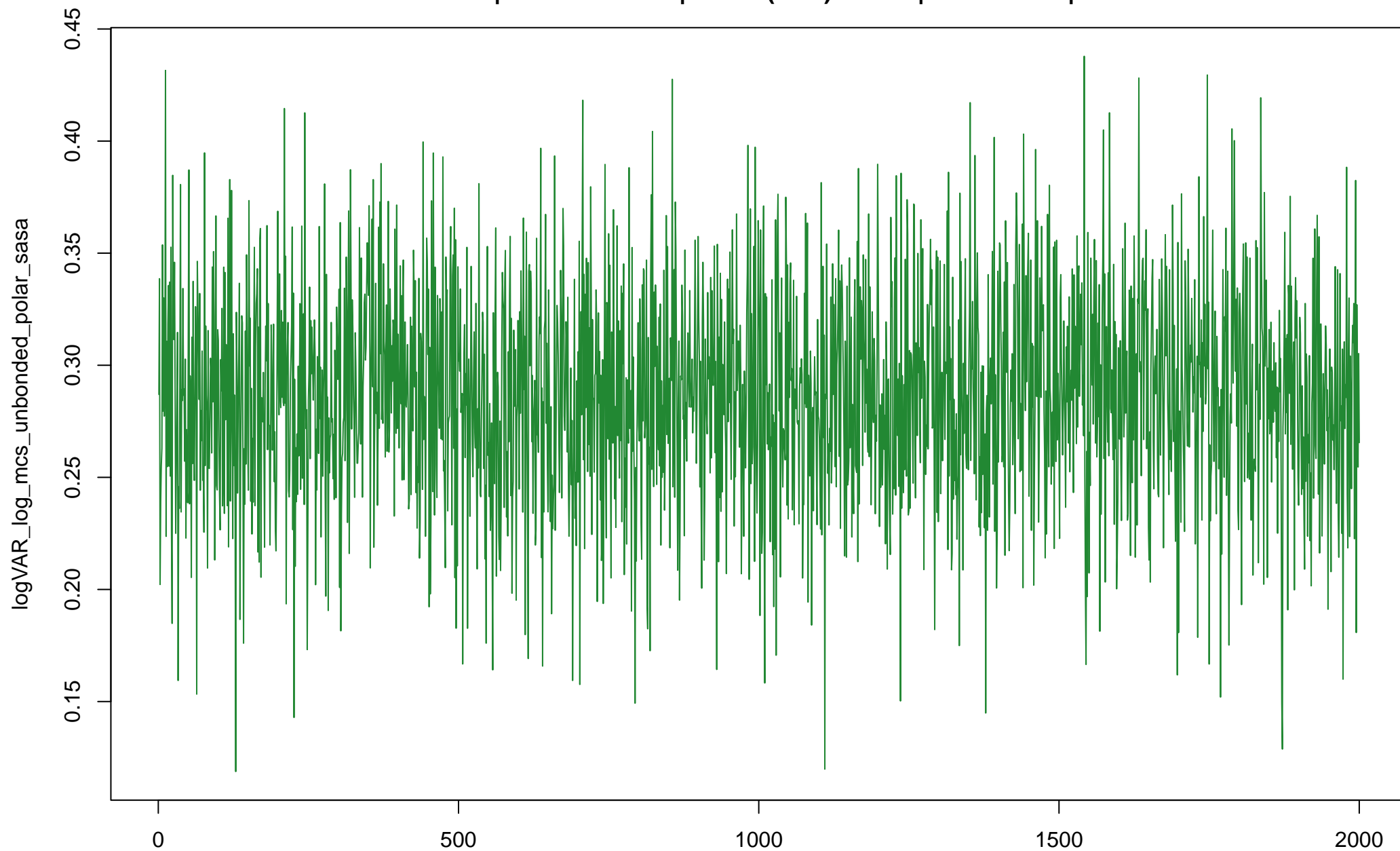
MEAN_docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0505 | MCSE(6.27) = 5.68 | stat: TRUE | burn: 0



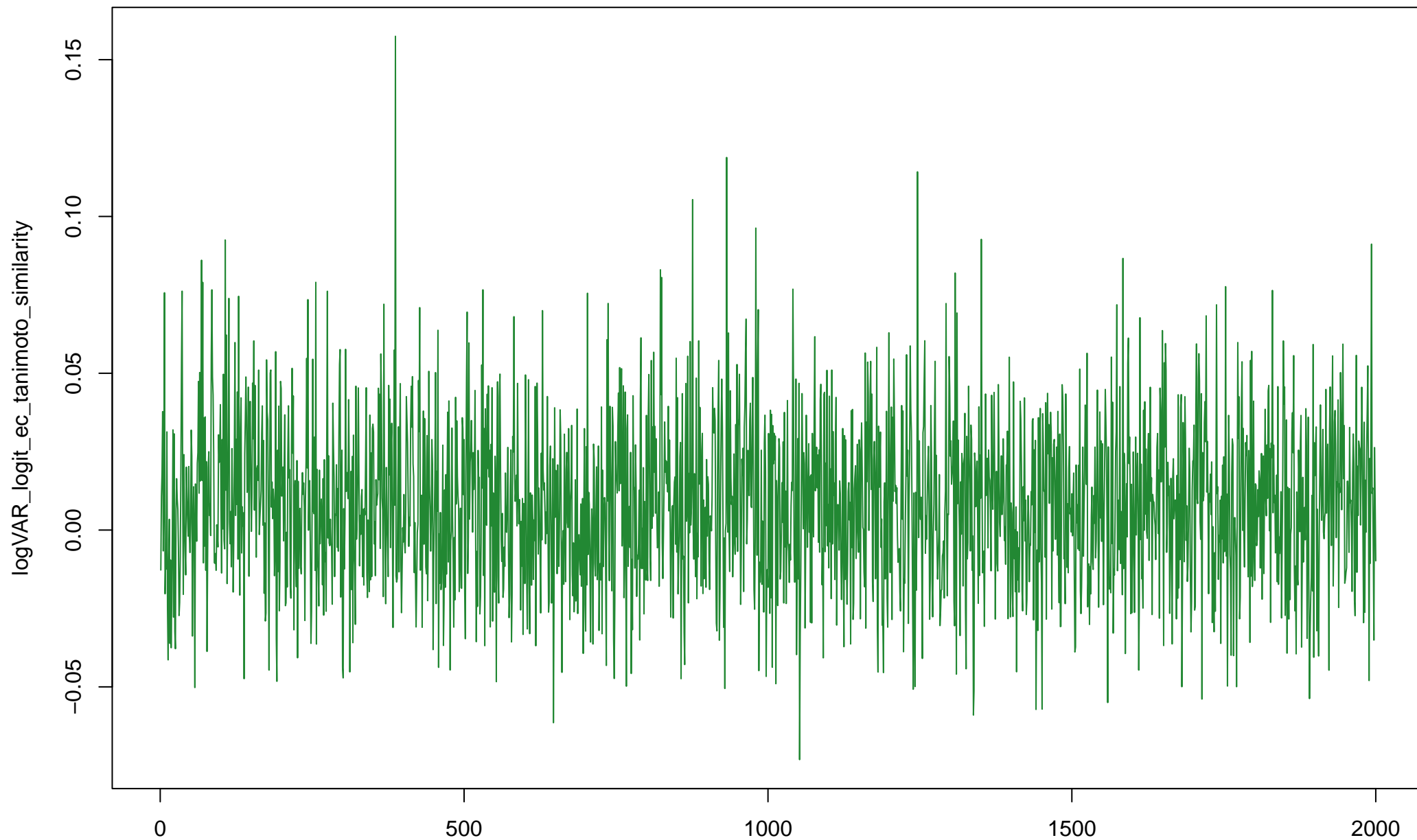
logVAR_log_RMSD
ESS = 1660 | BMK = 0.0473 | MCSE(6.27) = 9.94 | stat: TRUE | burn: 0



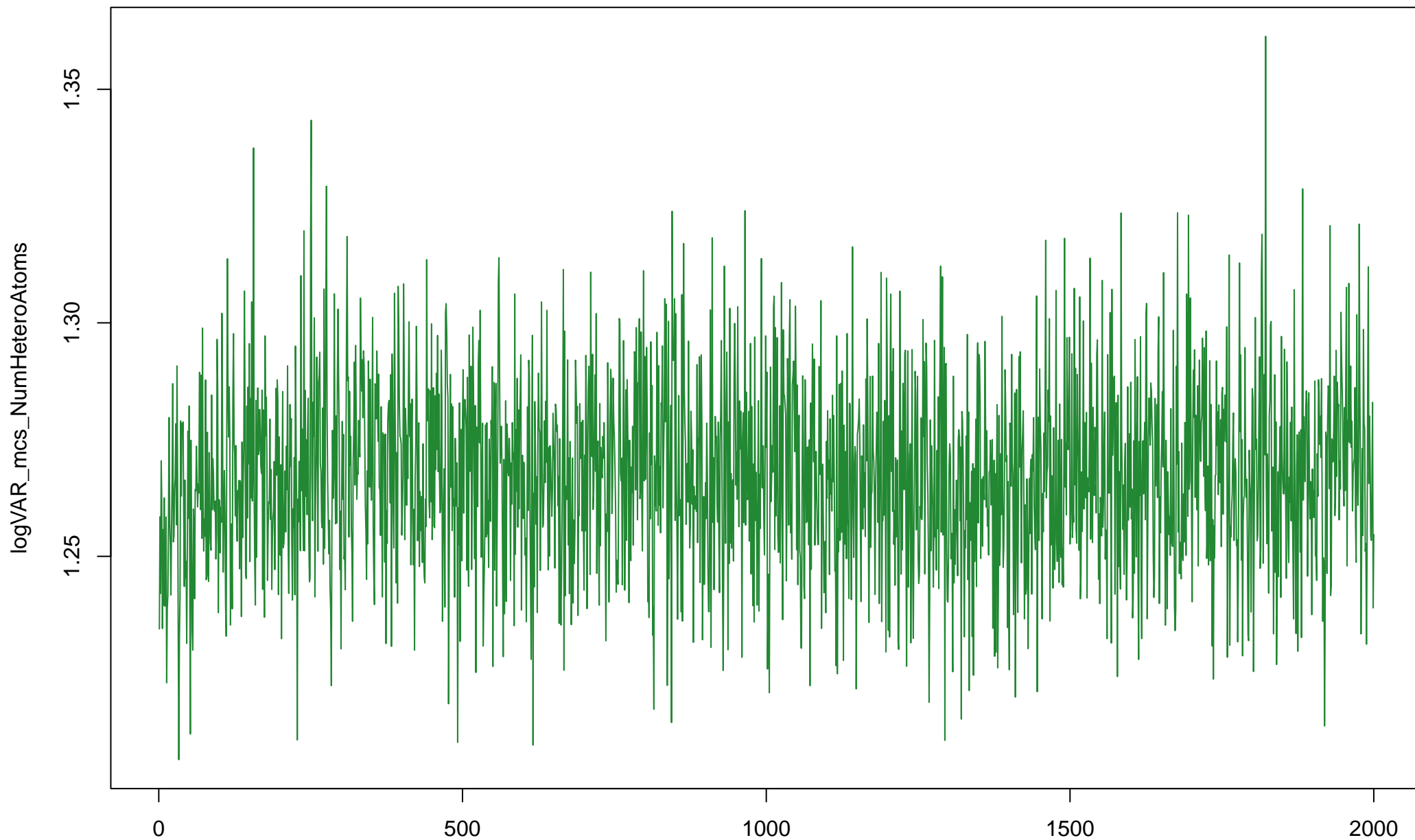
logVAR_log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0301 | MCSE(6.27) = 4.09 | stat: TRUE | burn: 0



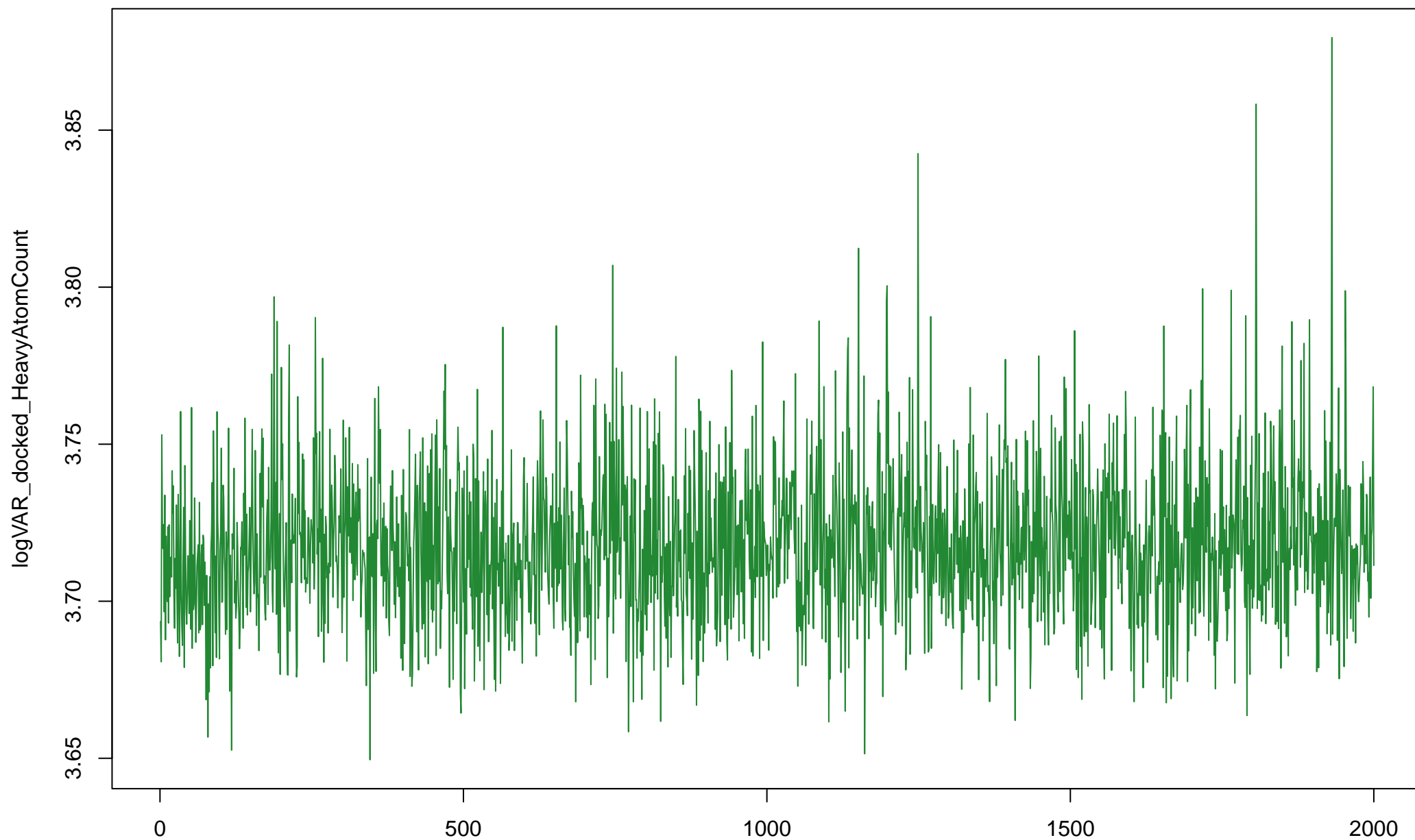
logVAR_logit_ec_tanimoto_similarity
ESS = 2000 | BMK = 0.0567 | MCSE(6.27) = 7.32 | stat: TRUE | burn: 0



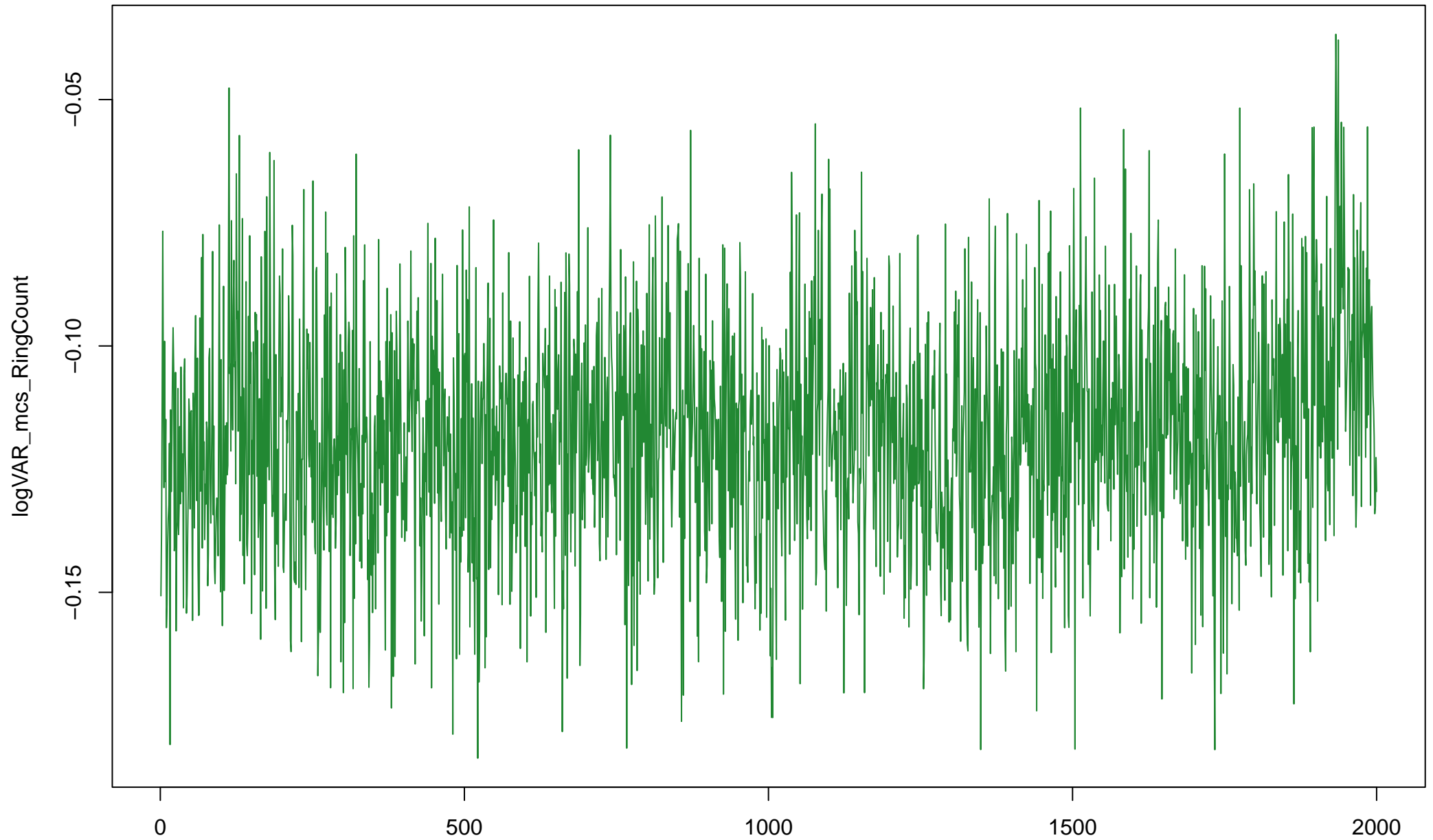
logVAR_mcs_NumHeteroAtoms
ESS = 1770 | BMK = 0.051 | MCSE(6.27) = 9.81 | stat: FALSE | burn: 0



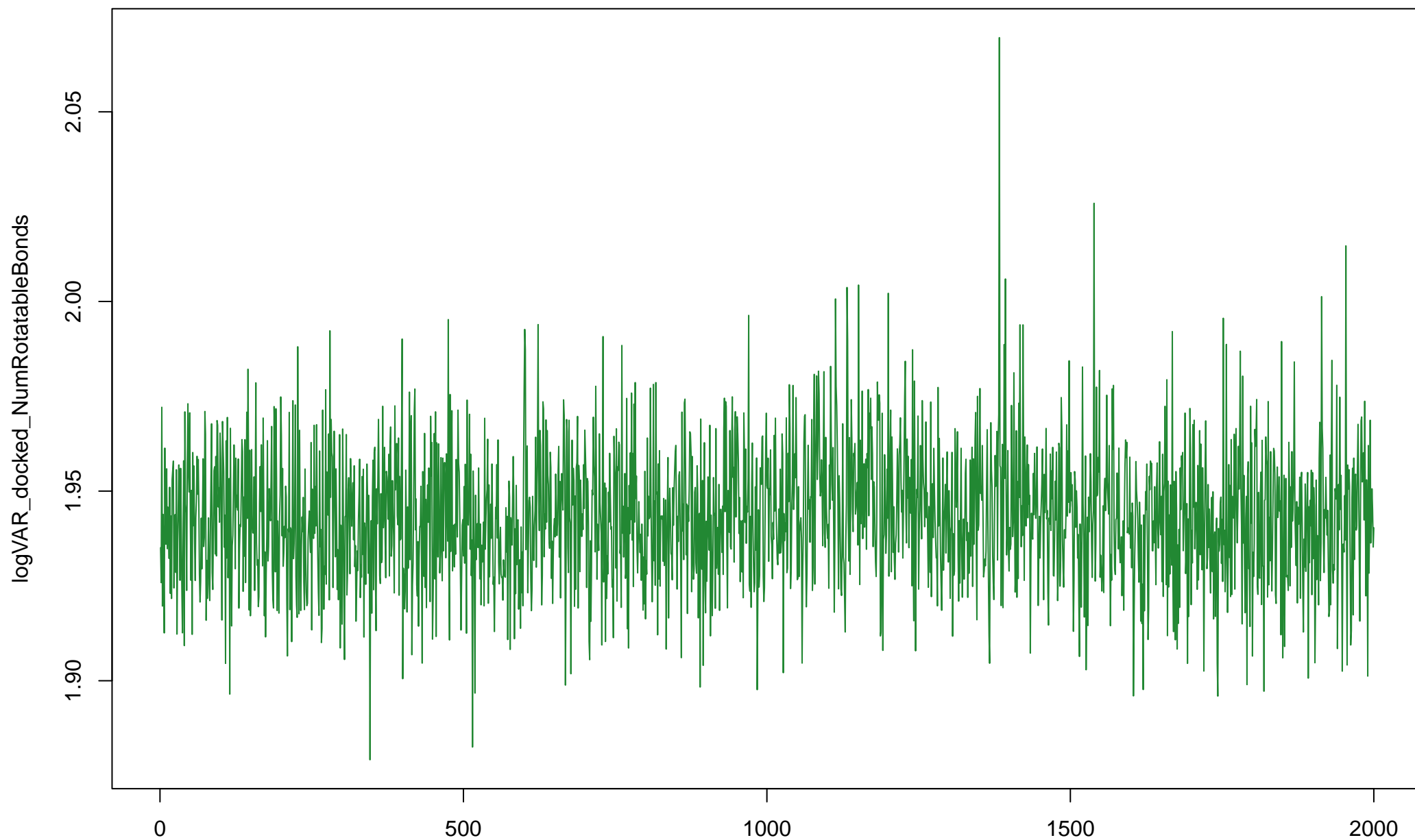
logVAR_docked_HeavyAtomCount
ESS = 1870 | BMK = 0.0644 | MCSE(6.27) = 8.12 | stat: FALSE | burn: 0



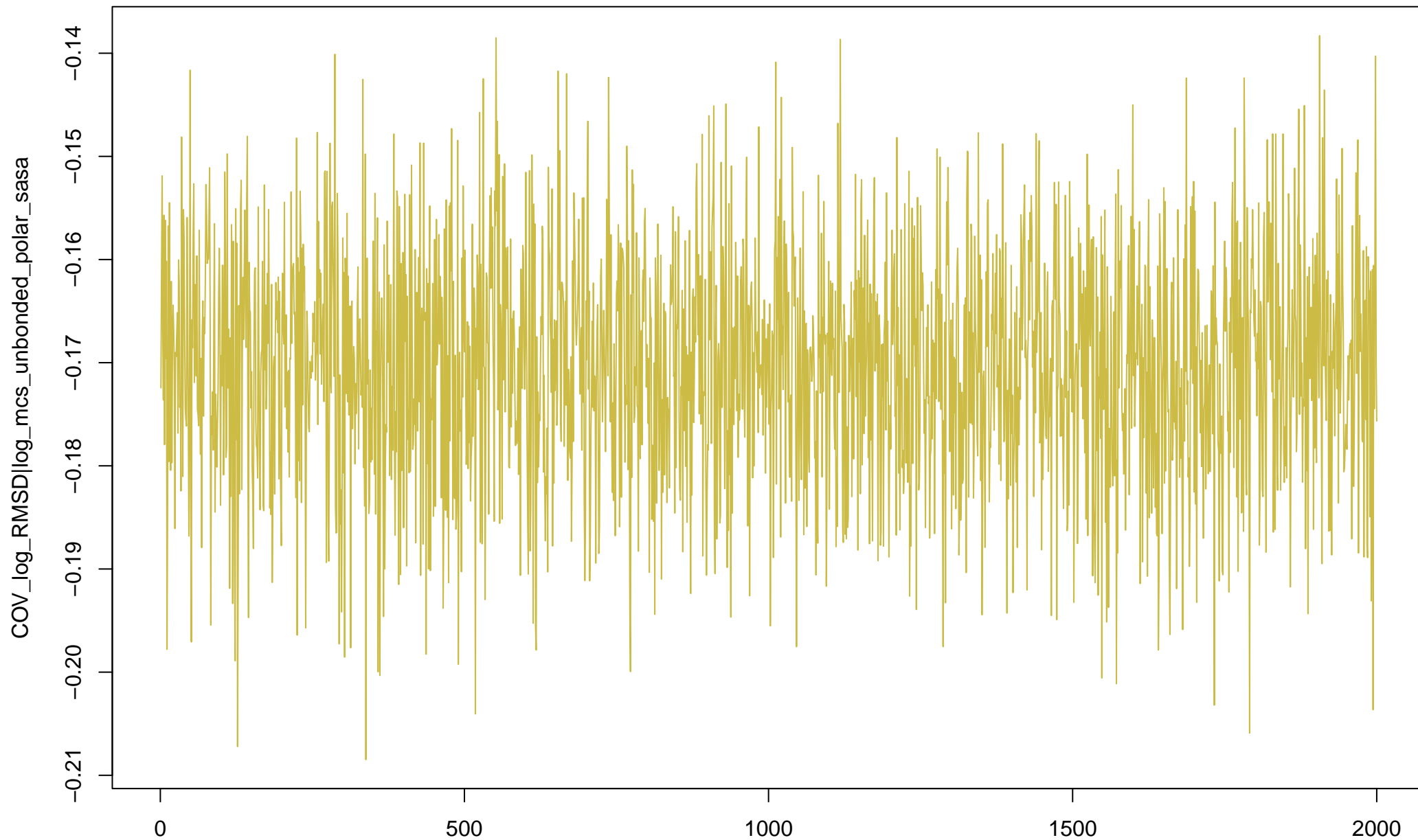
logVAR_mcs_RingCount
ESS = 666 | BMK = 0.058 | MCSE(6.27) = 8.55 | stat: TRUE | burn: 0



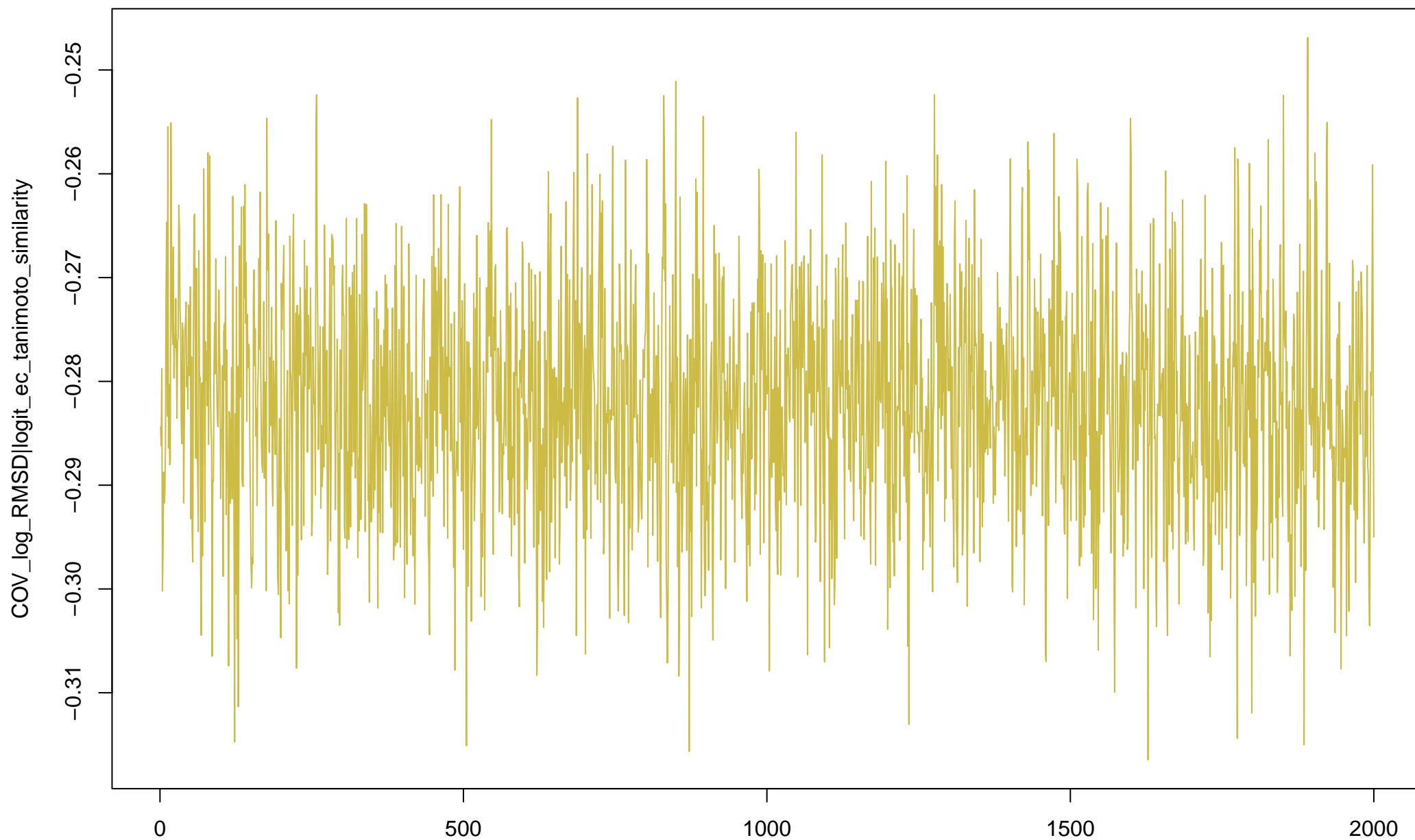
logVAR_docked_NumRotatableBonds
ESS = 1780 | BMK = 0.0826 | MCSE(6.27) = 10.8 | stat: TRUE | burn: 0



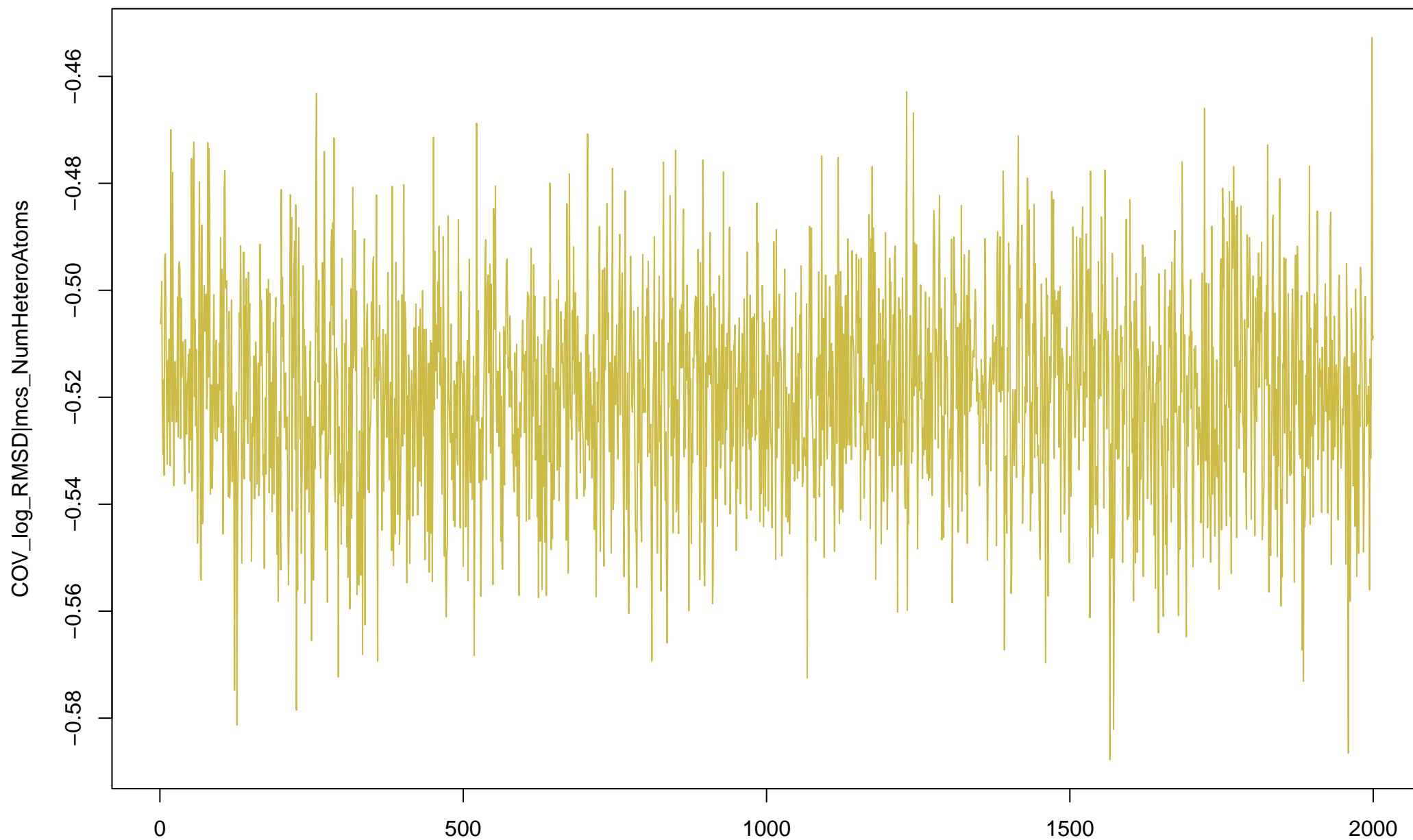
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0295 | MCSE(6.27) = 17.4 | stat: TRUE | burn: 0



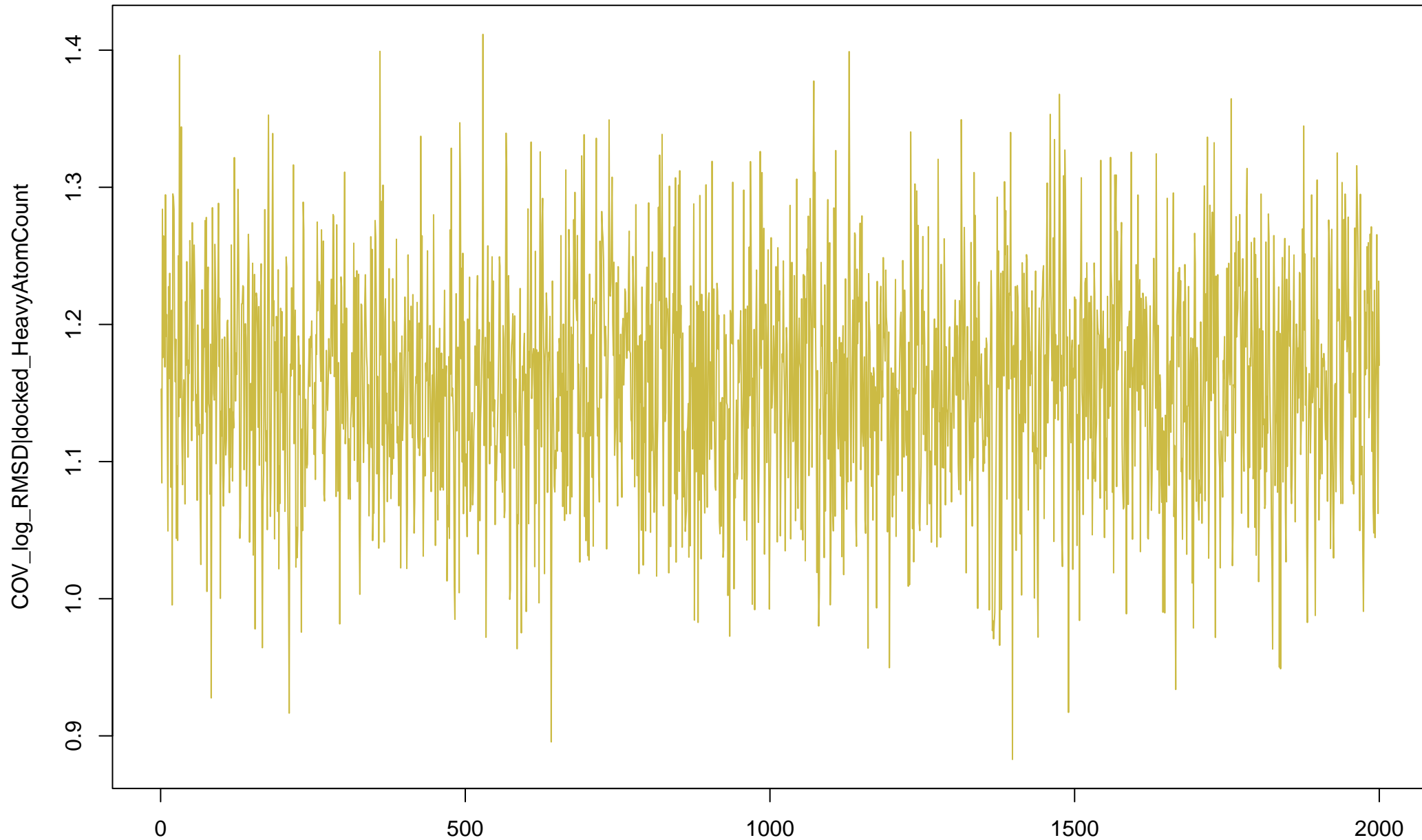
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1410 | BMK = 0.0328 | MCSE(6.27) = 18.3 | stat: TRUE | burn: 0



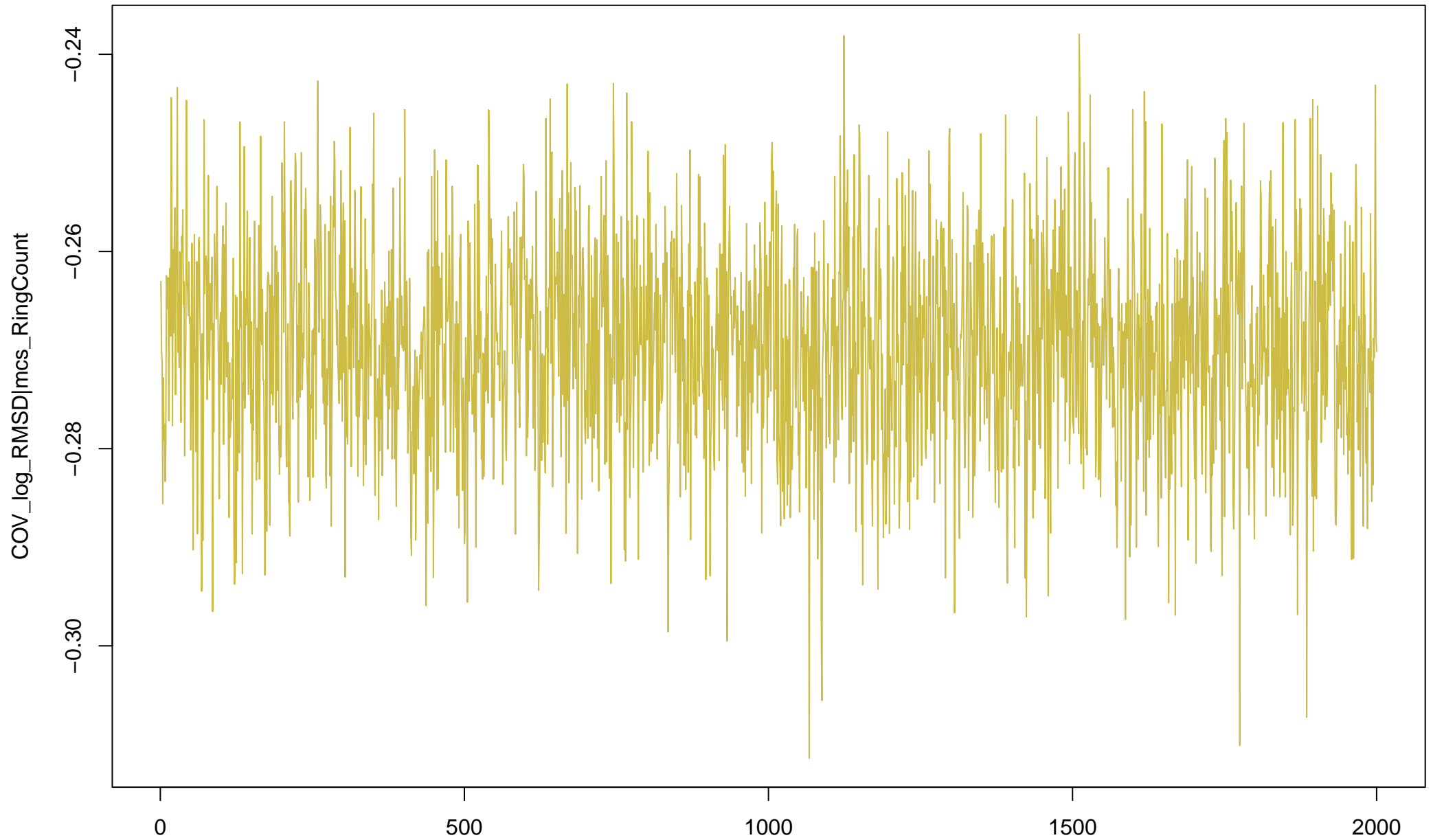
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1510 | BMK = 0.0523 | MCSE(6.27) = 10.3 | stat: TRUE | burn: 0



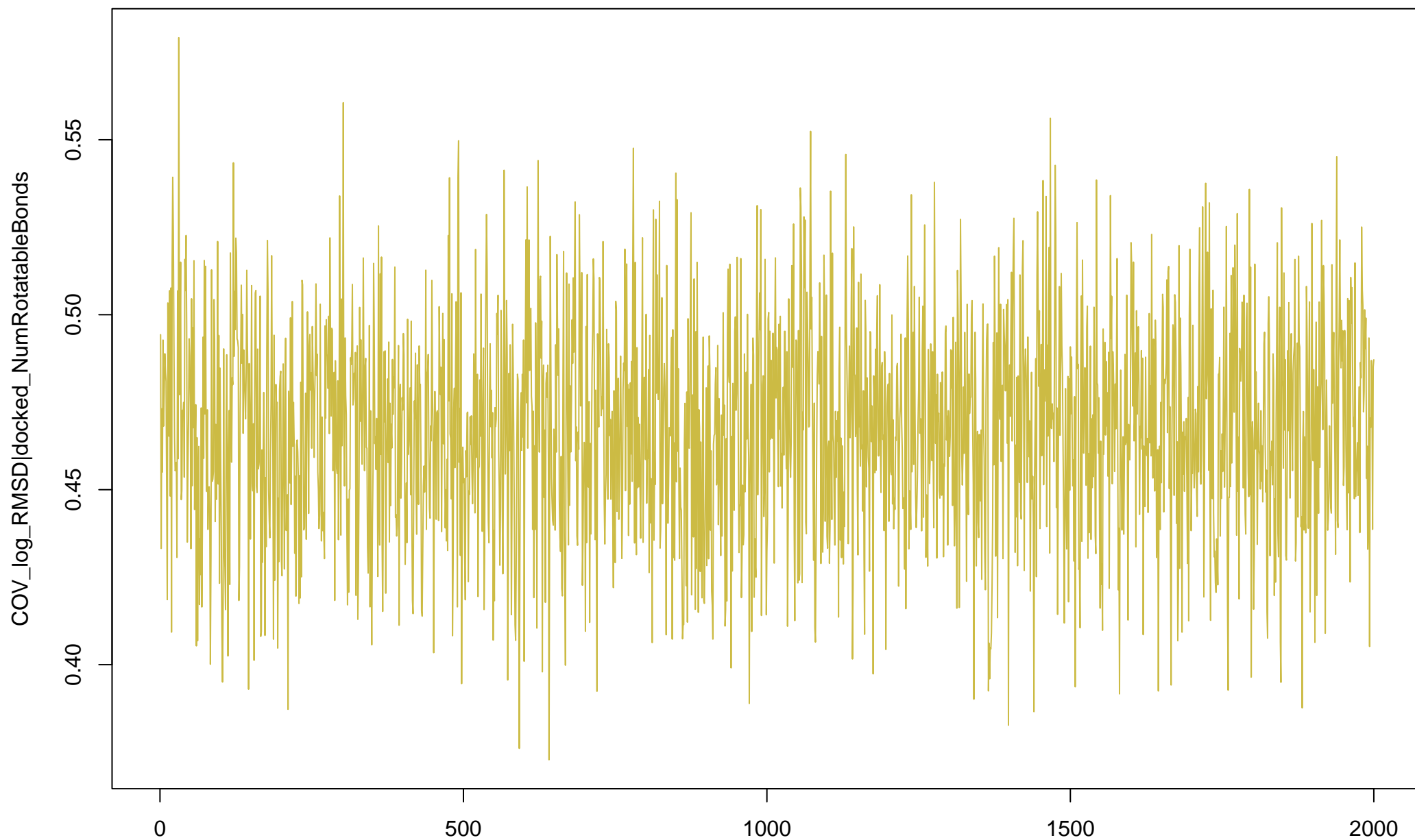
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1510 | BMK = 0.0327 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0



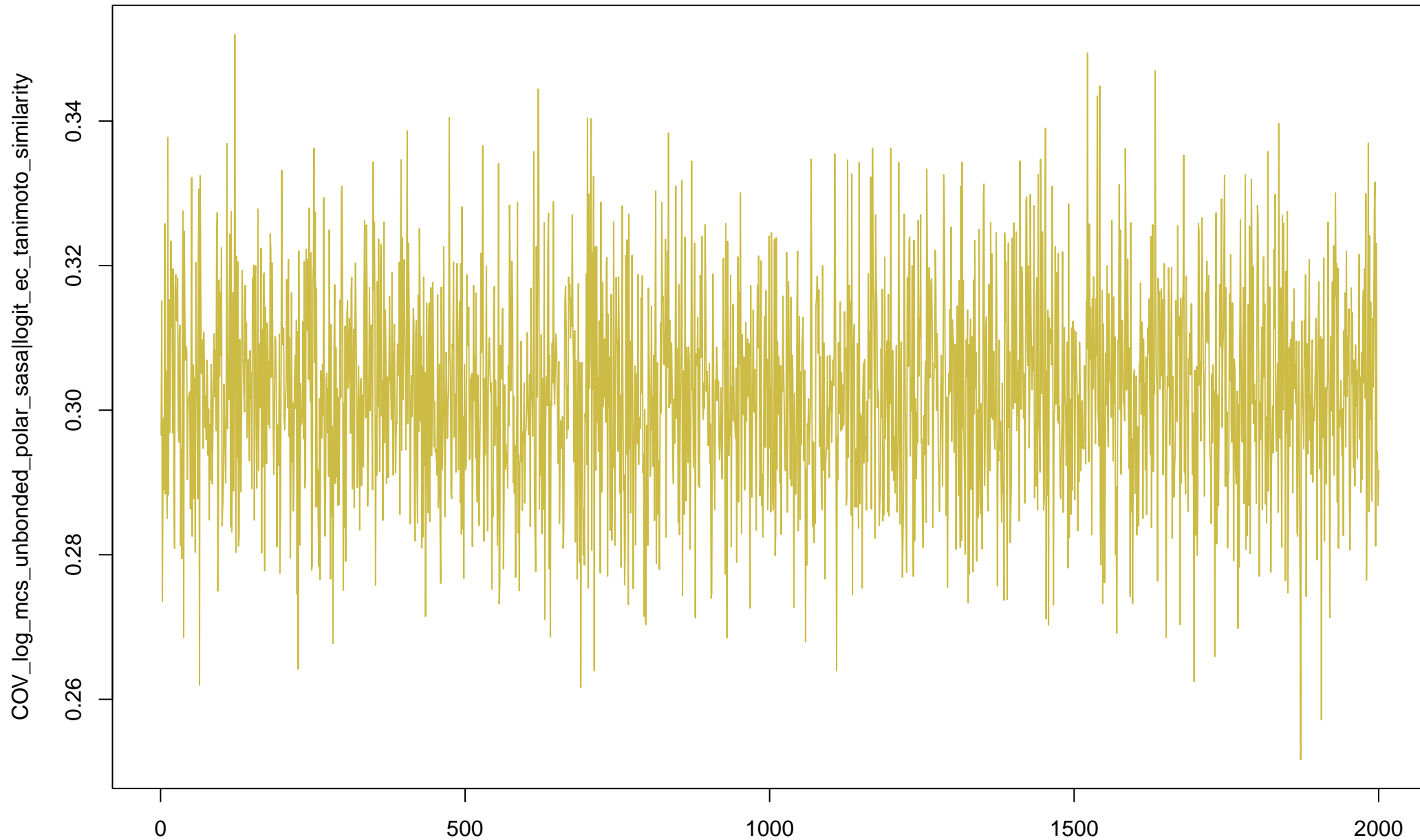
COV_log_RMSD|mcs_RingCount
ESS = 1550 | BMK = 0.0622 | MCSE(6.27) = 18.8 | stat: TRUE | burn: 0



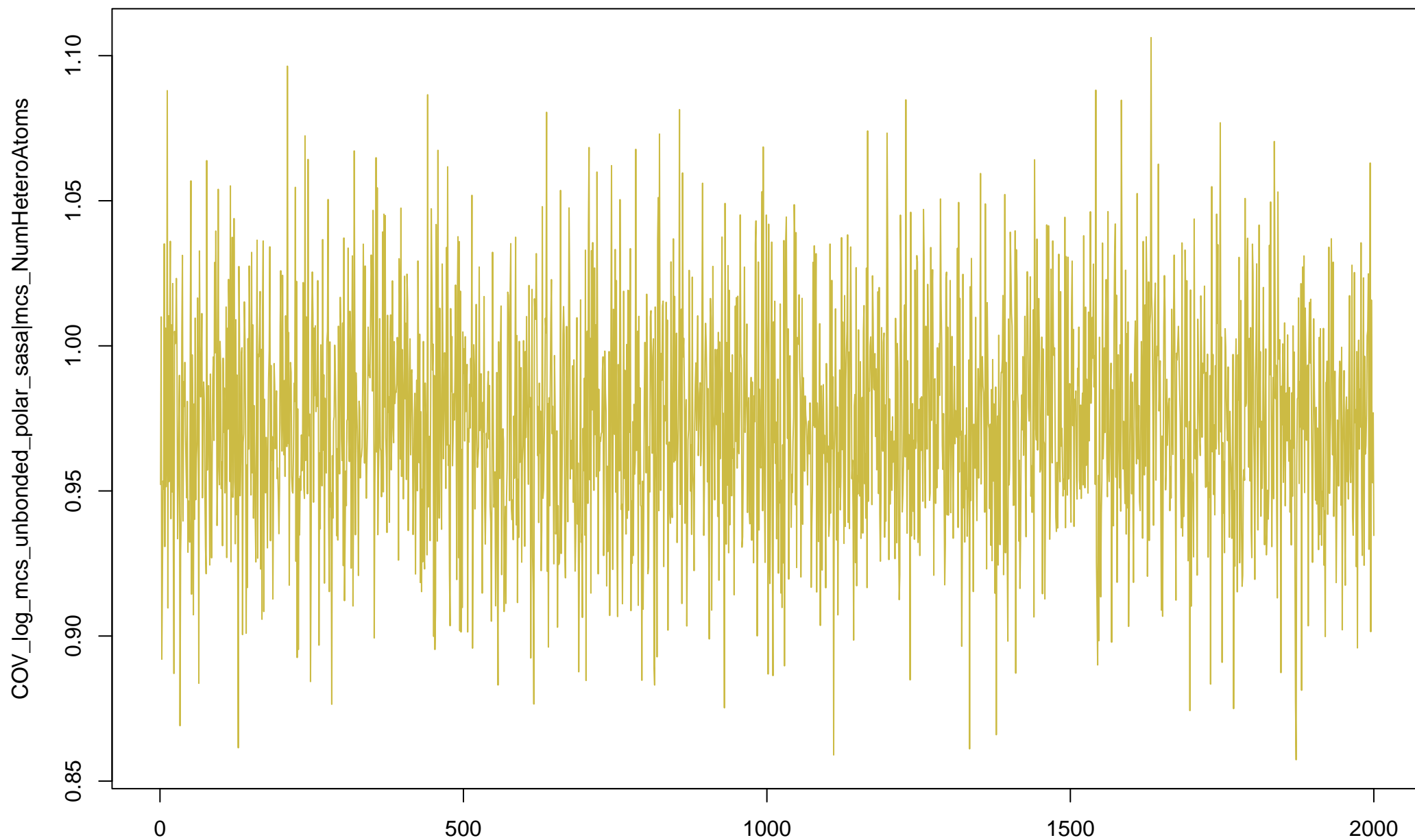
COV_log_RMSD|docked_NumRotatableBonds
ESS = 1510 | BMK = 0.0548 | MCSE(6.27) = 6.4 | stat: TRUE | burn: 0



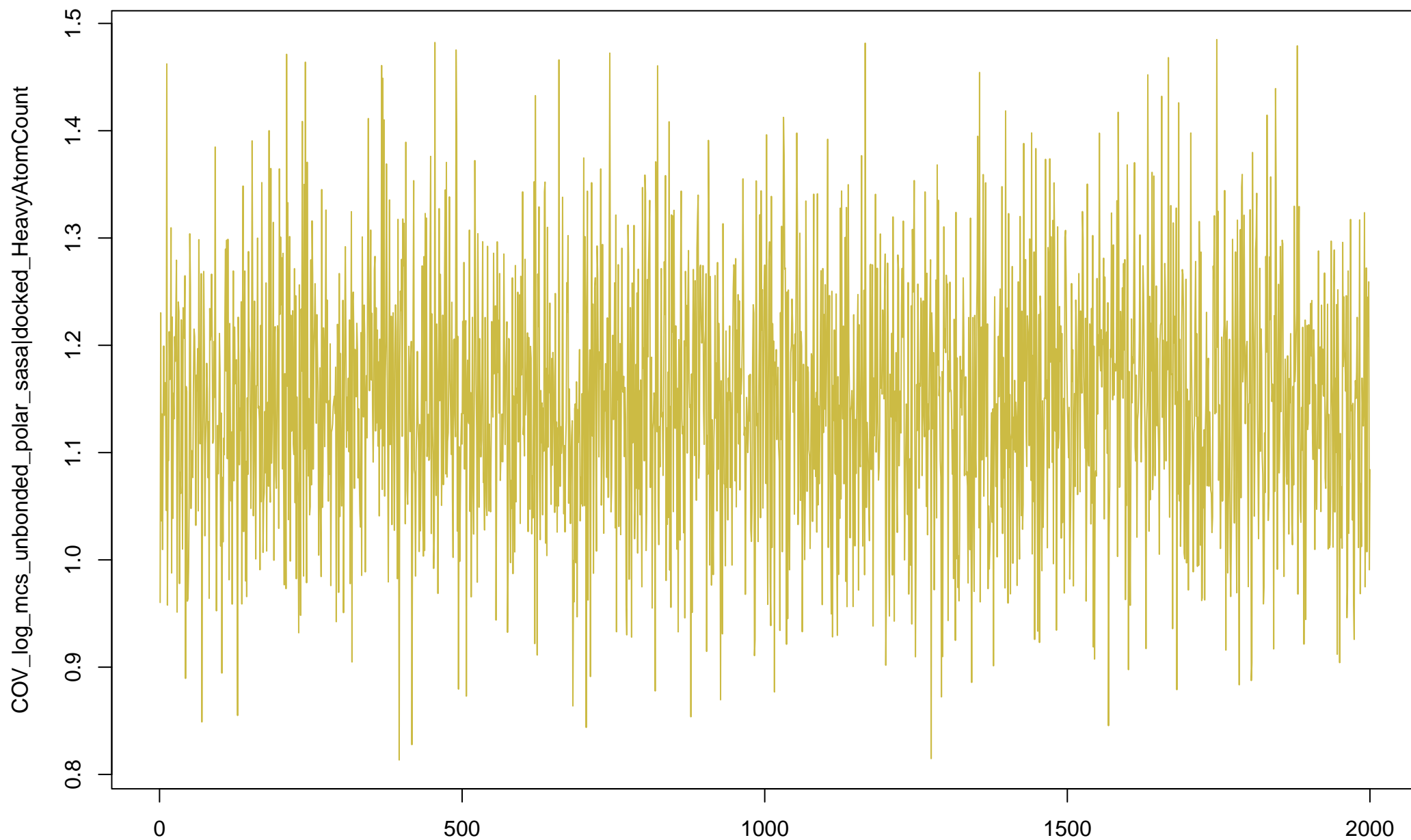
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 2000 | BMK = 0.0326 | MCSE(6.27) = 13.6 | stat: TRUE | burn: 0



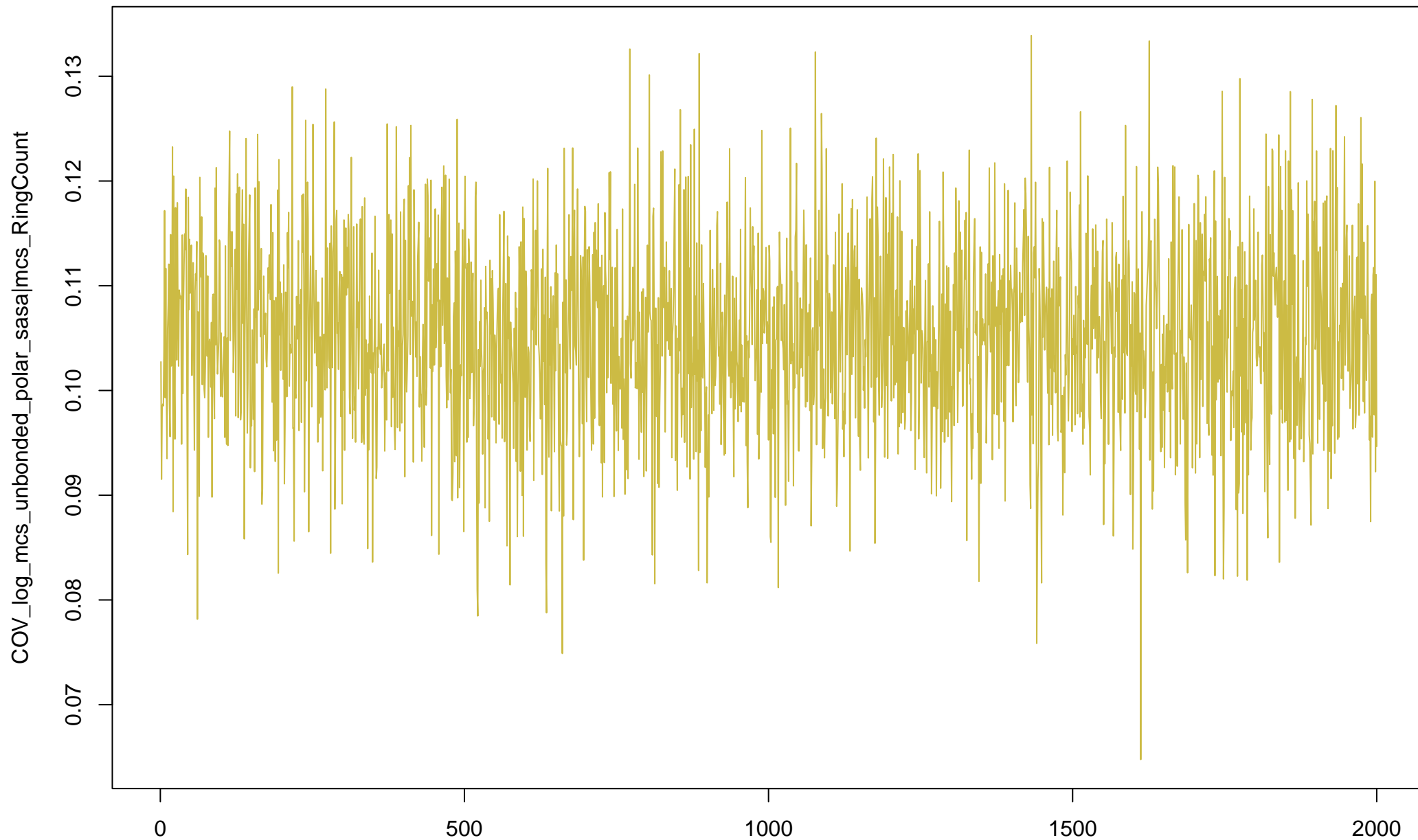
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0465 | MCSE(6.27) = 5.13 | stat: TRUE | burn: 0



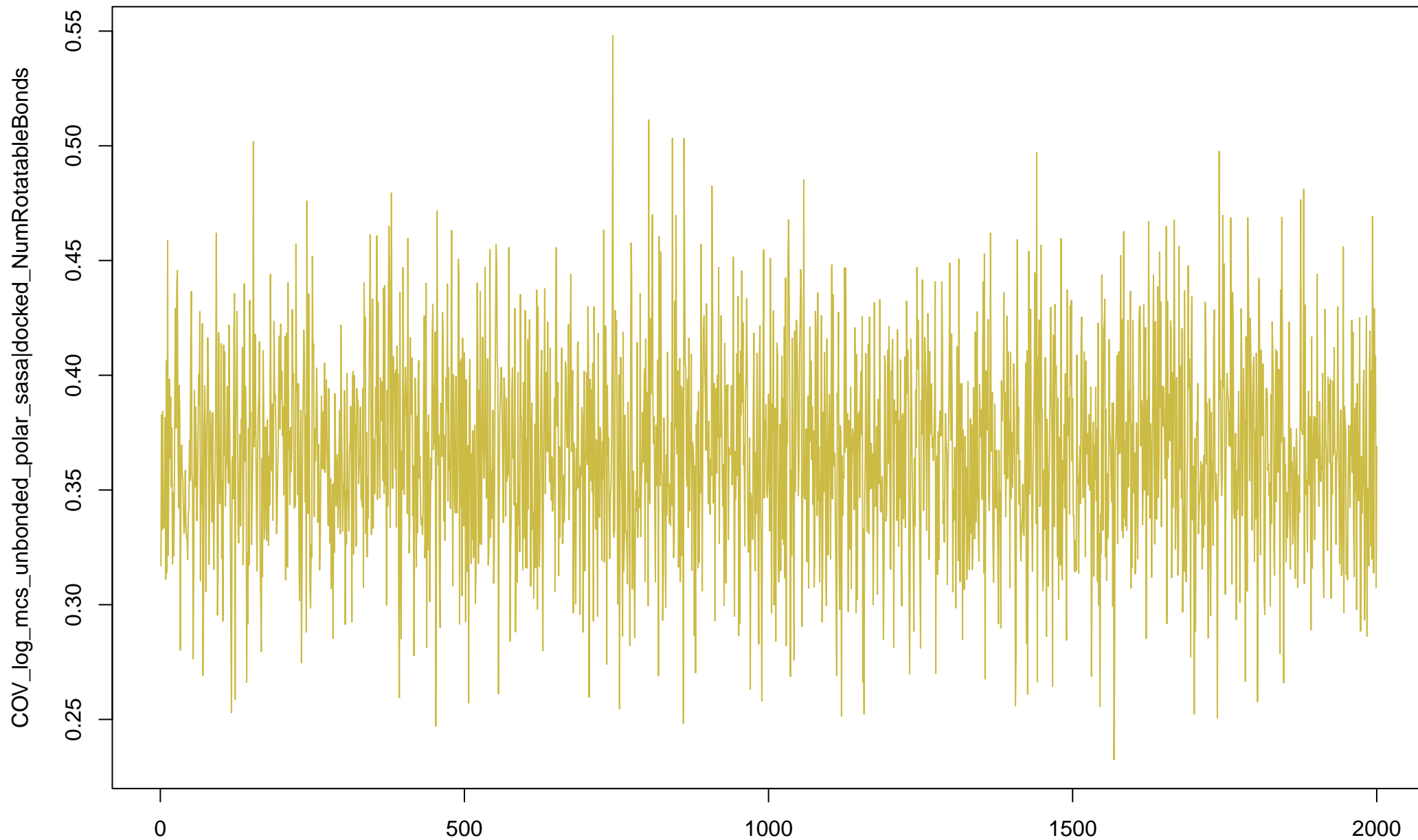
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0432 | MCSE(6.27) = 1.72 | stat: TRUE | burn: 0



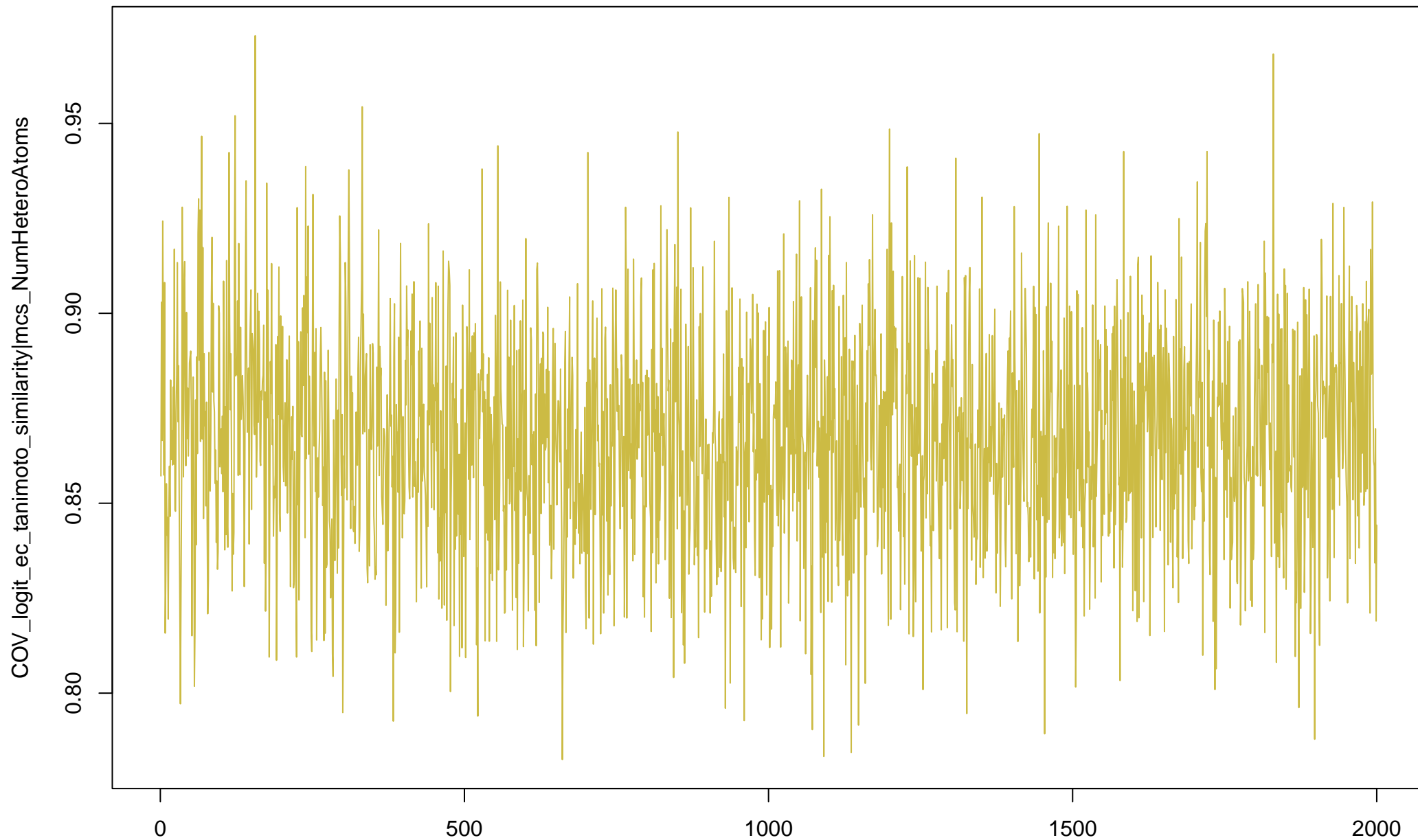
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 2000 | BMK = 0.0295 | MCSE(6.27) = 21.7 | stat: TRUE | burn: 0



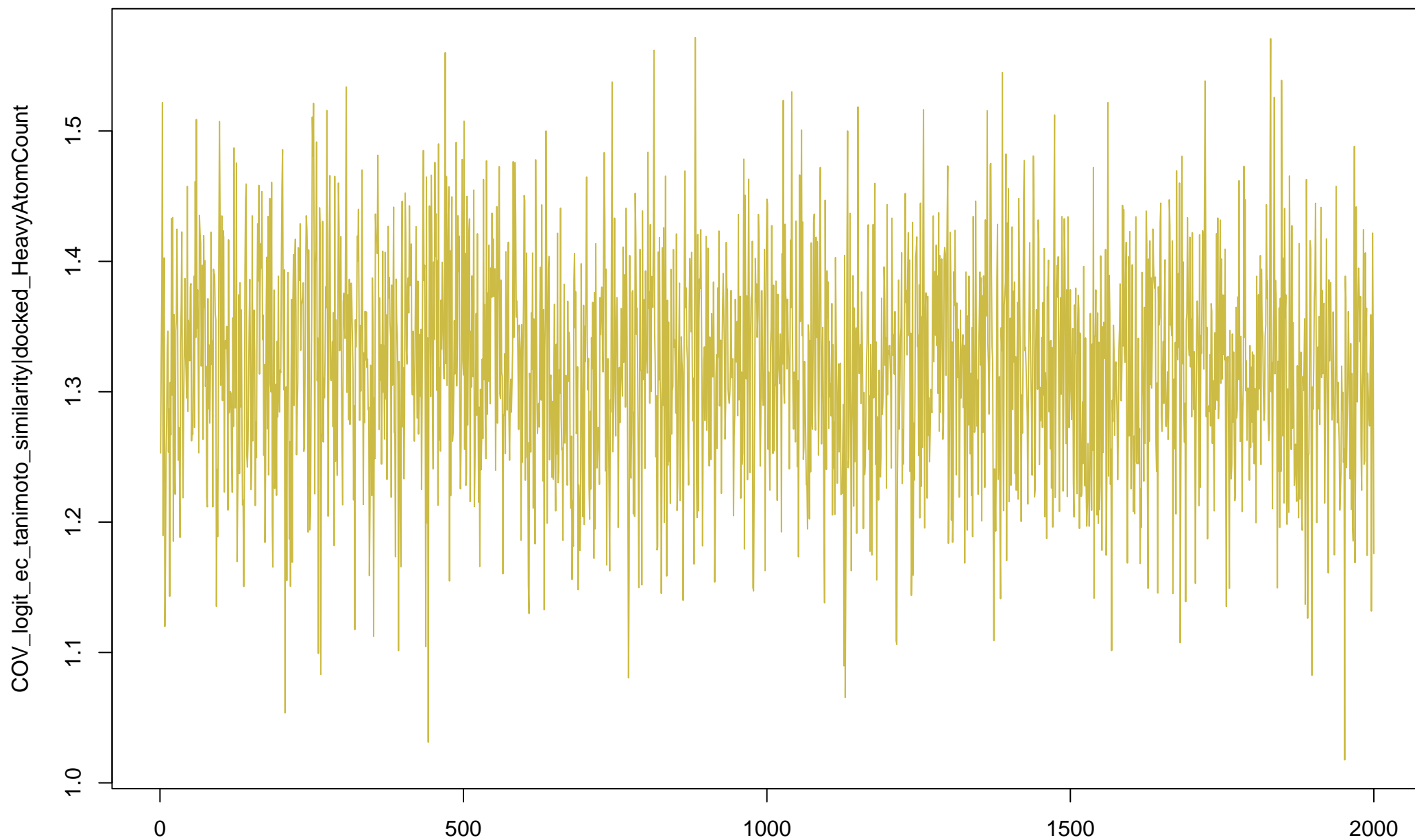
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0431 | MCSE(6.27) = 4.5 | stat: TRUE | burn: 0



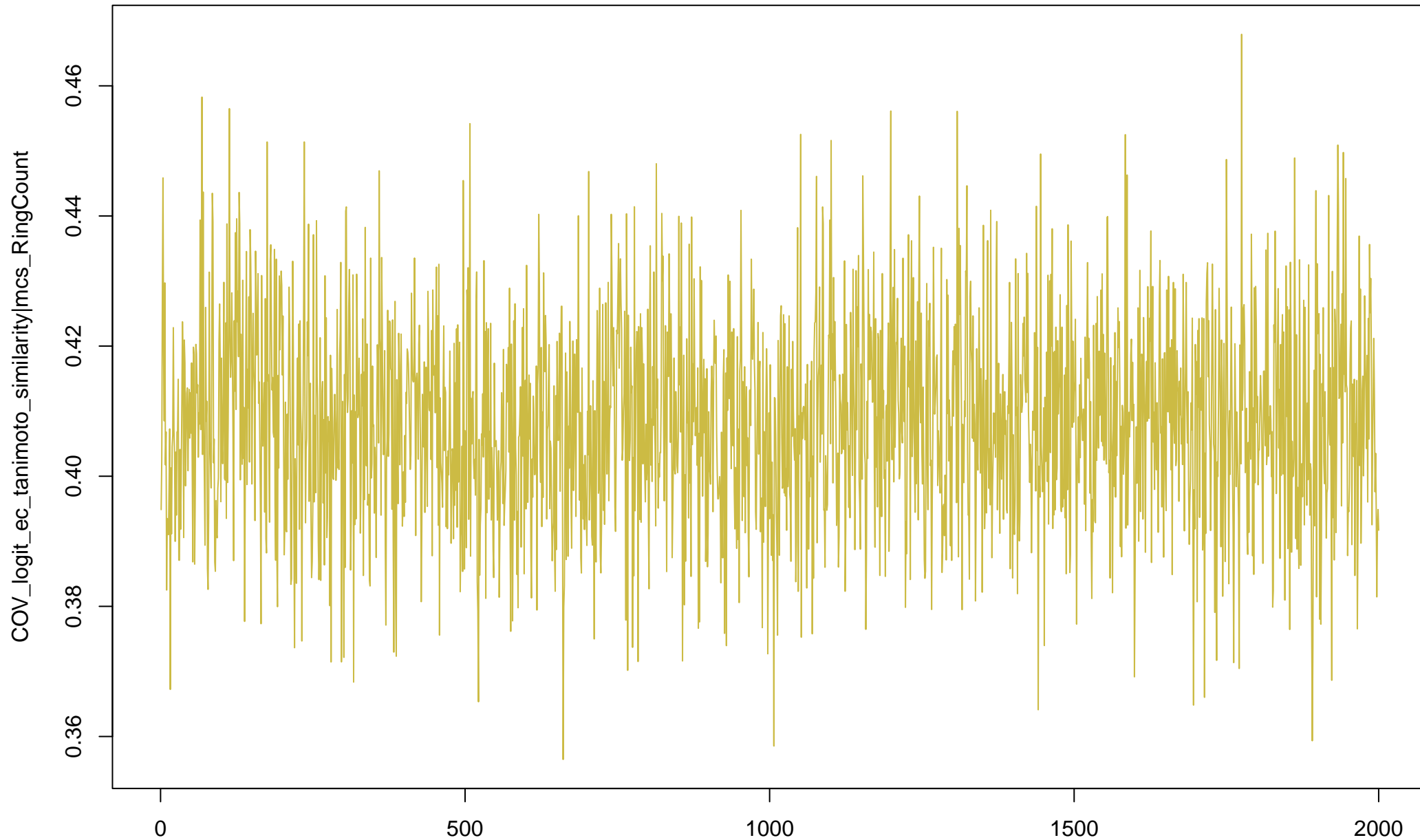
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1750 | BMK = 0.035 | MCSE(6.27) = 6.89 | stat: FALSE | burn: 0



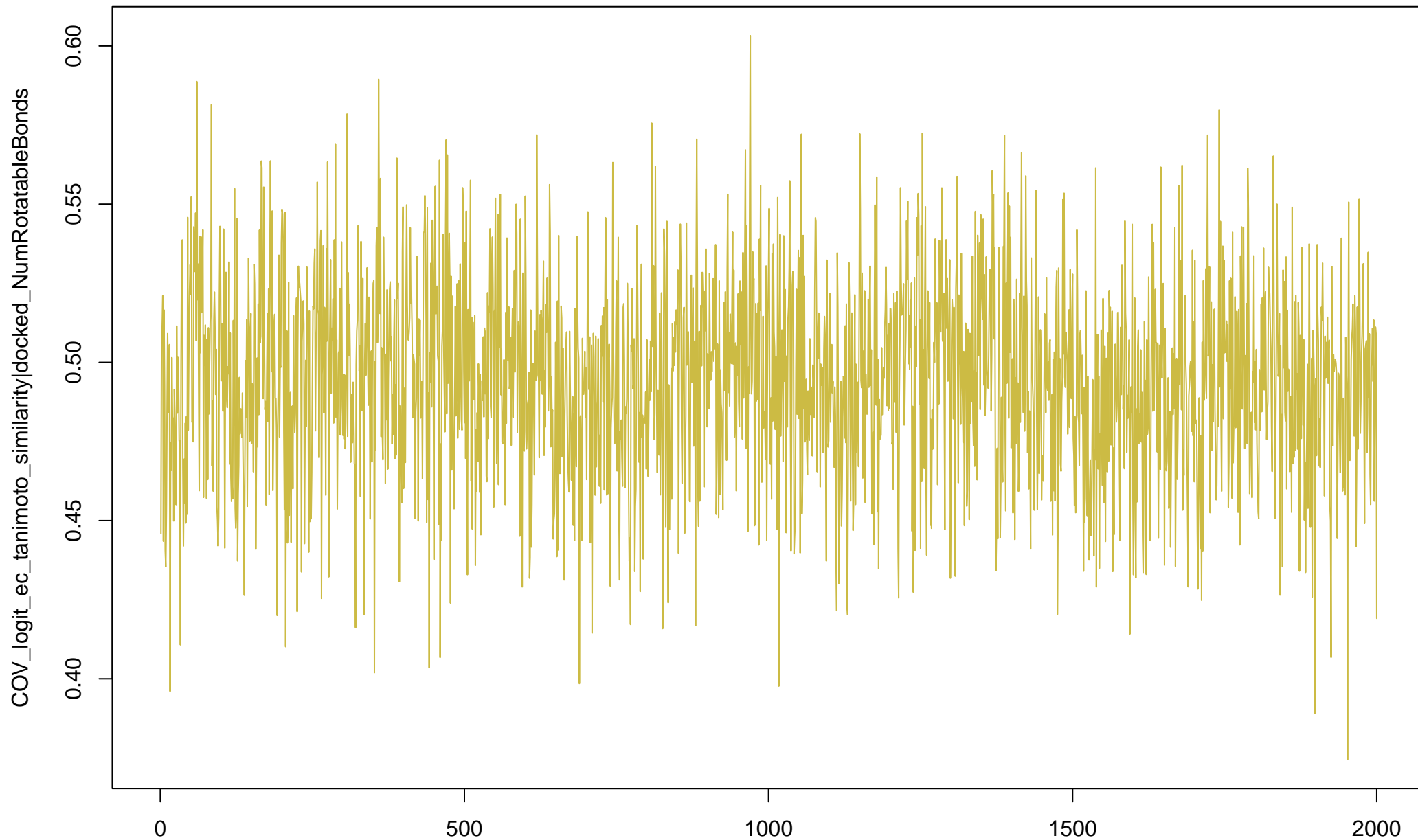
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1700 | BMK = 0.0564 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0



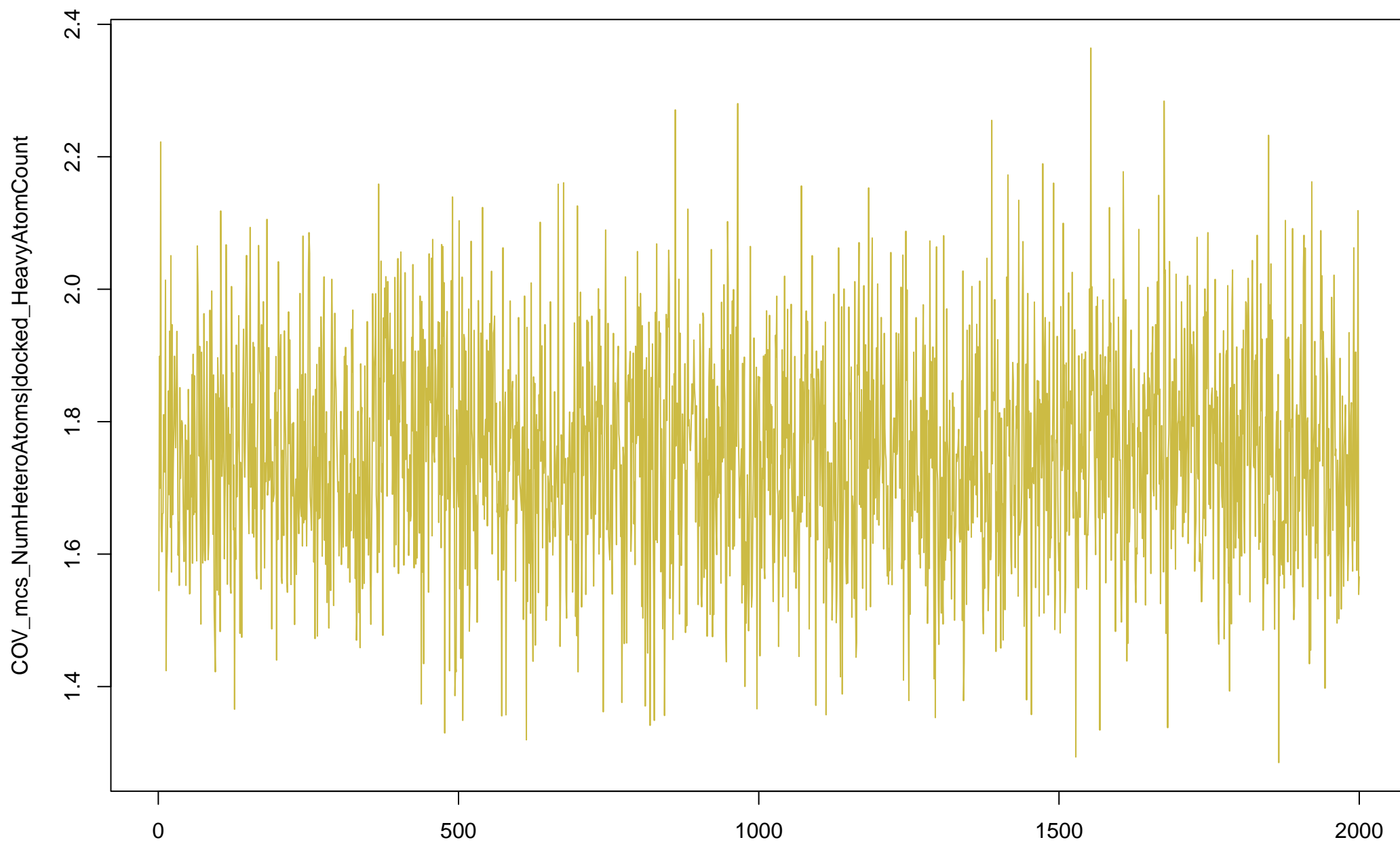
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1580 | BMK = 0.0397 | MCSE(6.27) = 12.6 | stat: TRUE | burn: 0



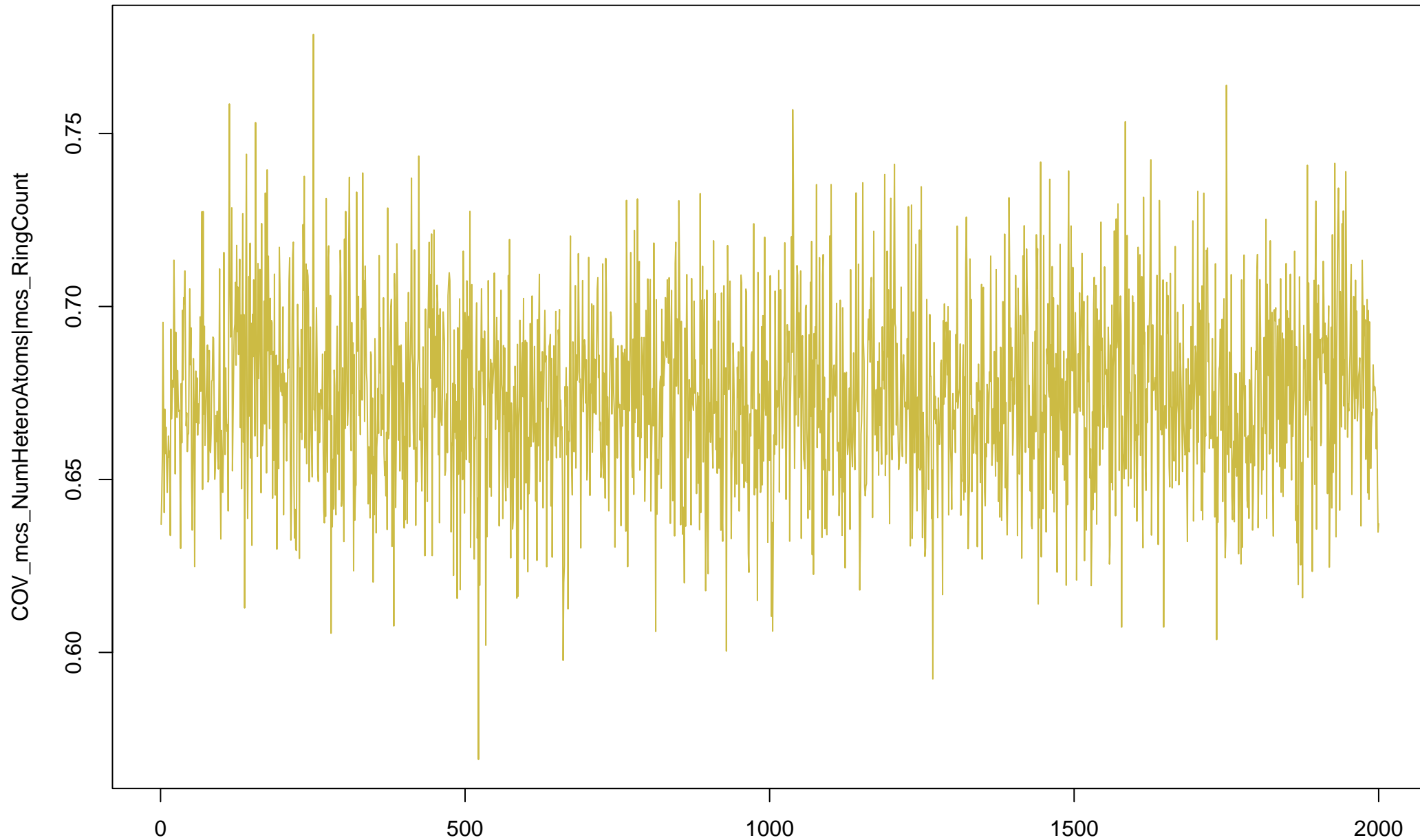
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1140 | BMK = 0.0535 | MCSE(6.27) = 6.23 | stat: TRUE | burn: 0



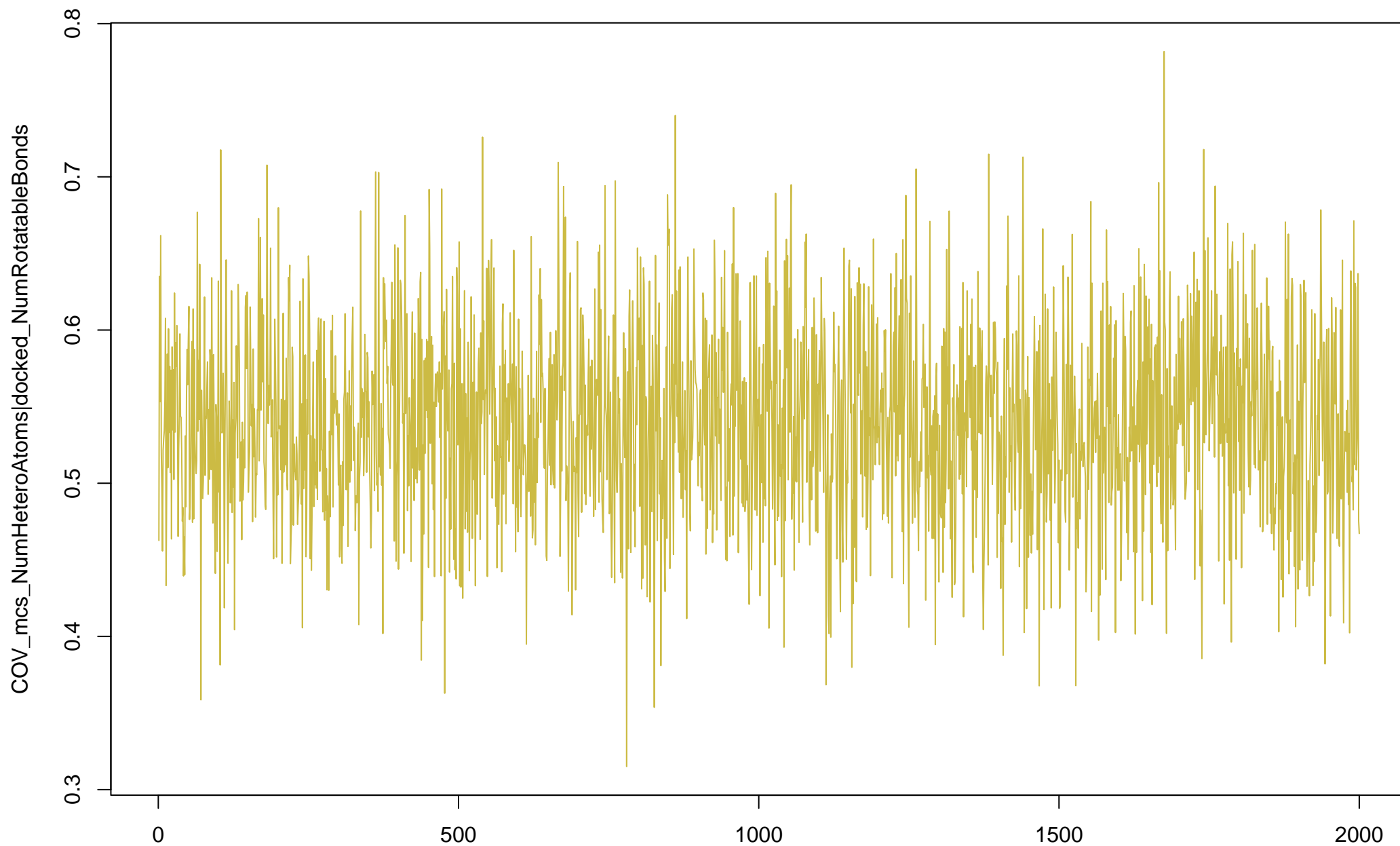
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0331 | MCSE(6.27) = 1.2 | stat: TRUE | burn: 0



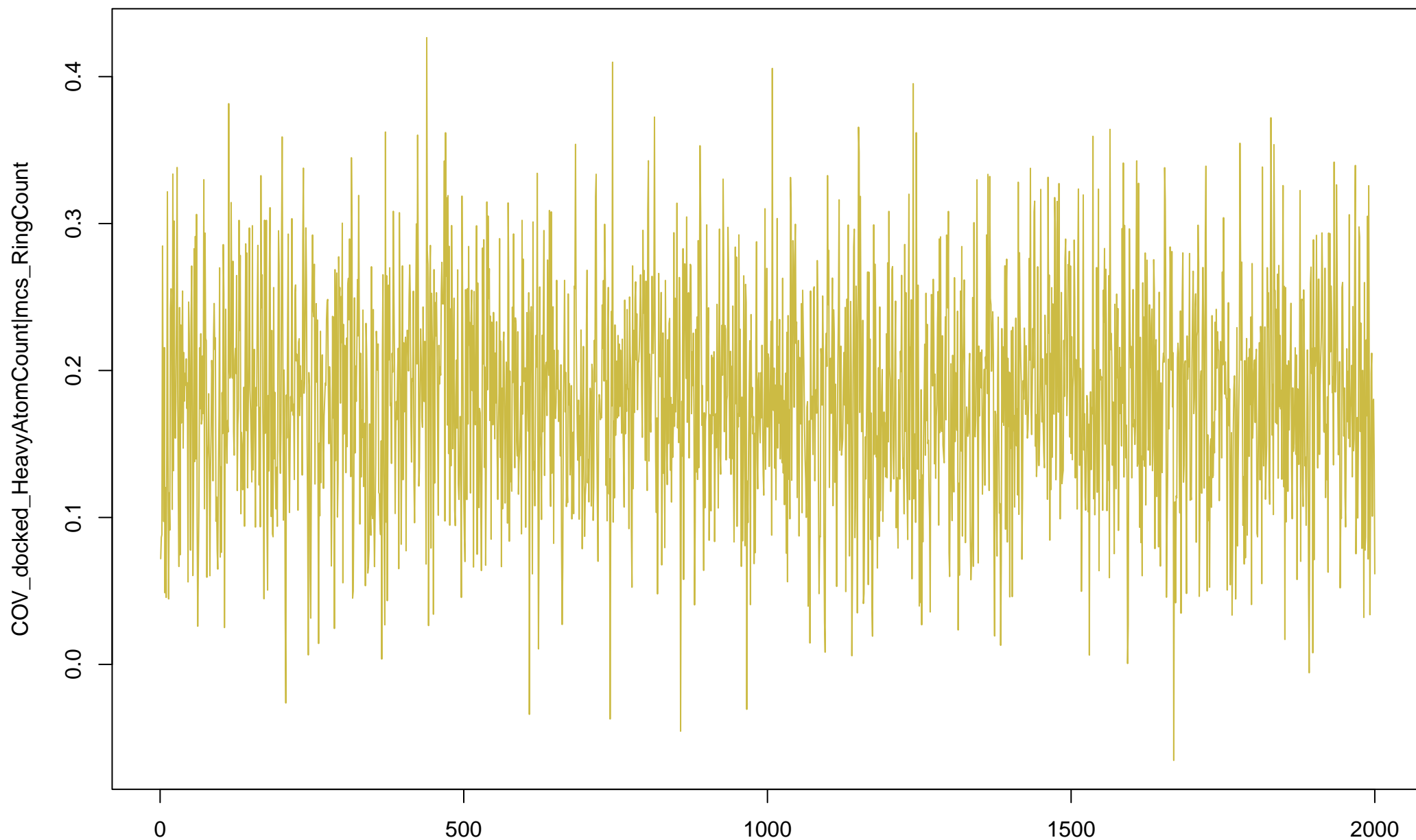
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1770 | BMK = 0.0422 | MCSE(6.27) = 7.53 | stat: TRUE | burn: 0



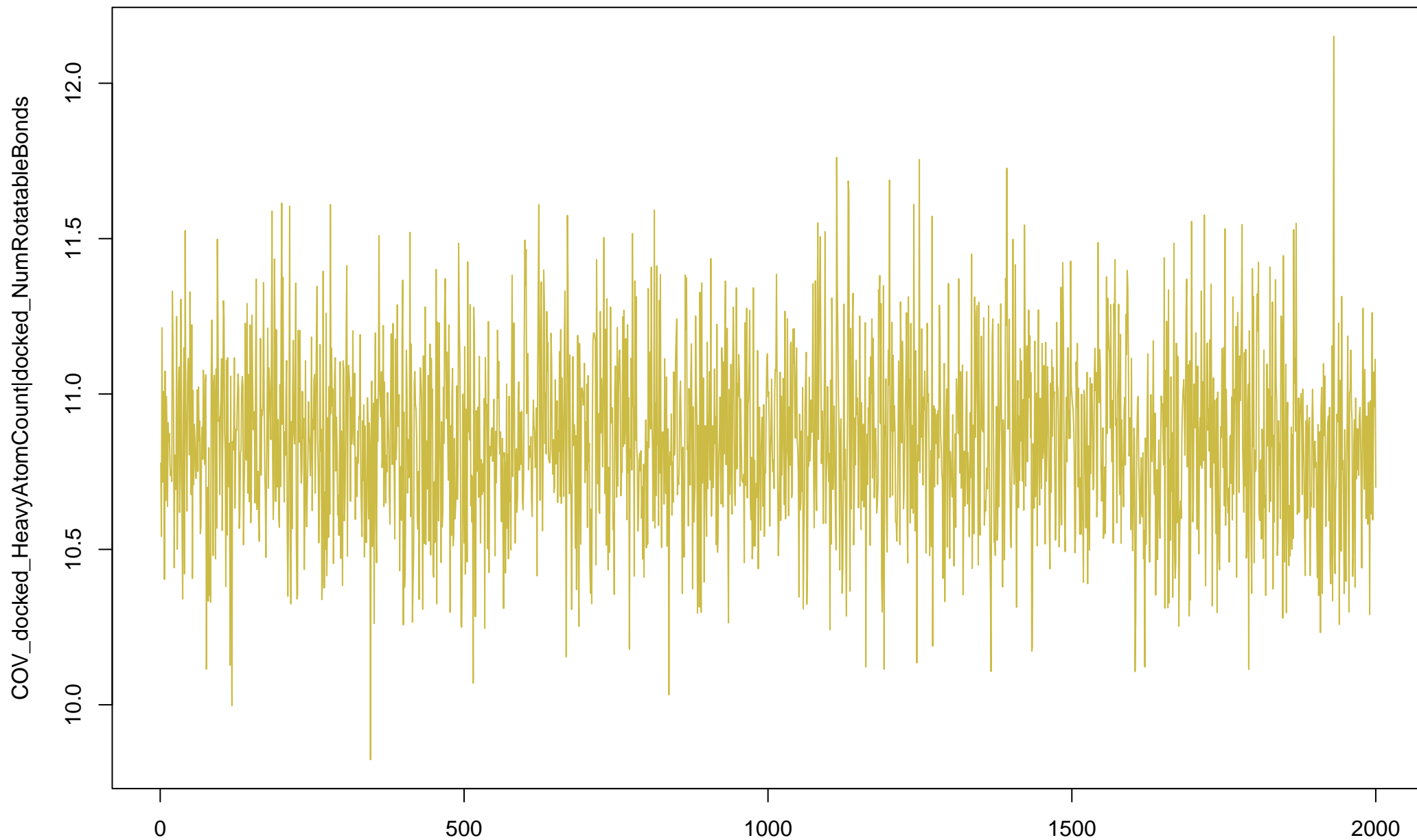
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0548 | MCSE(6.27) = 3.14 | stat: TRUE | burn: 0



COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1880 | BMK = 0.0456 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0



COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1810 | BMK = 0.0497 | MCSE(6.27) = 0.694 | stat: TRUE | burn: 0



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1720 | BMK = 0.0576 | MCSE(6.27) = 6.87 | stat: TRUE | burn: 0

