

-- STATS maxD --

min ESS = 62.8768747791718

max BMK = 0.149181157978781

max MCSE = 11.62140624212

all stationary: FALSE

burn: 0

-- STATS 2D --

min ESS = 1093.47411822829

max BMK = 0.0608970796346531

max MCSE = 3.08192136455317

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 349.805200249436

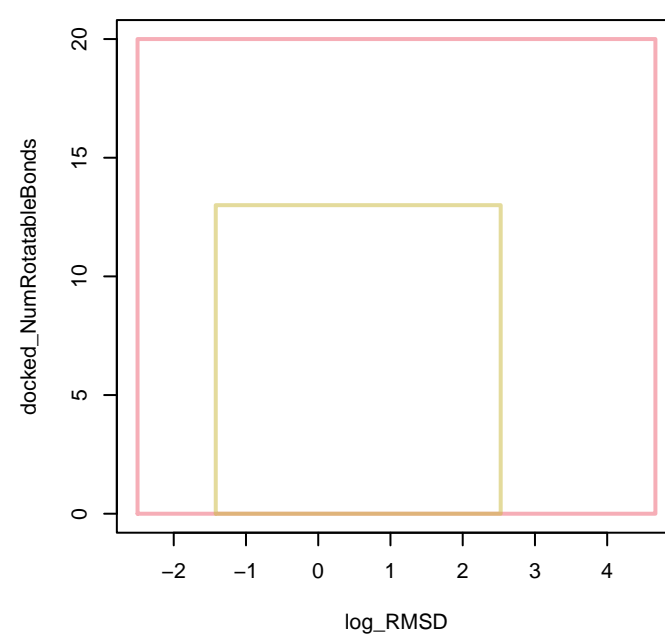
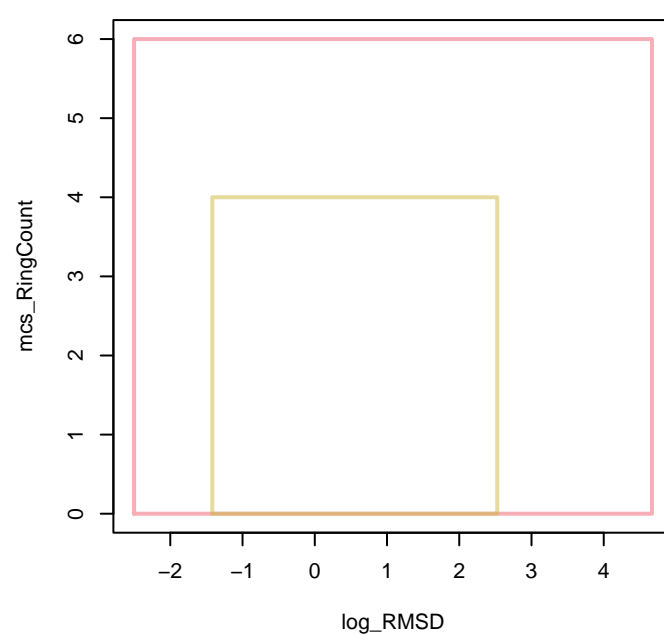
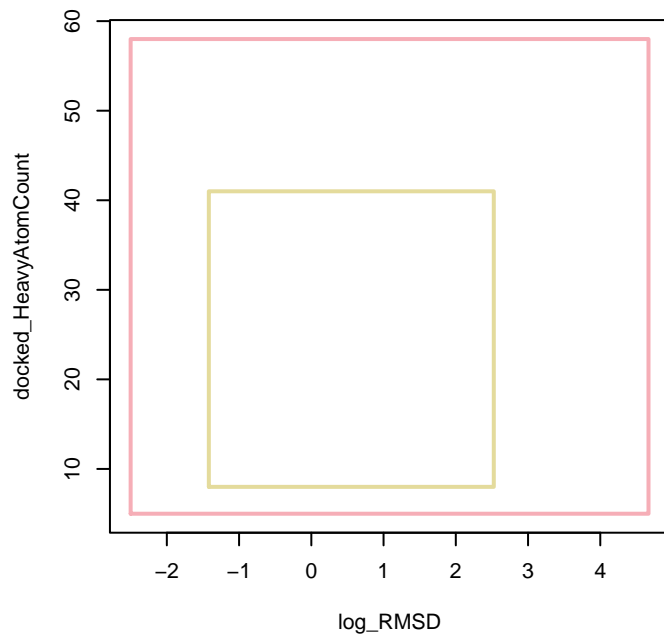
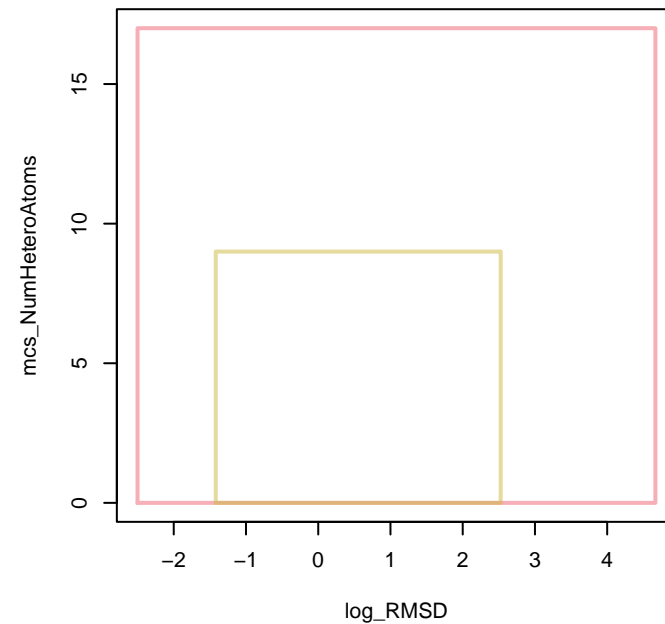
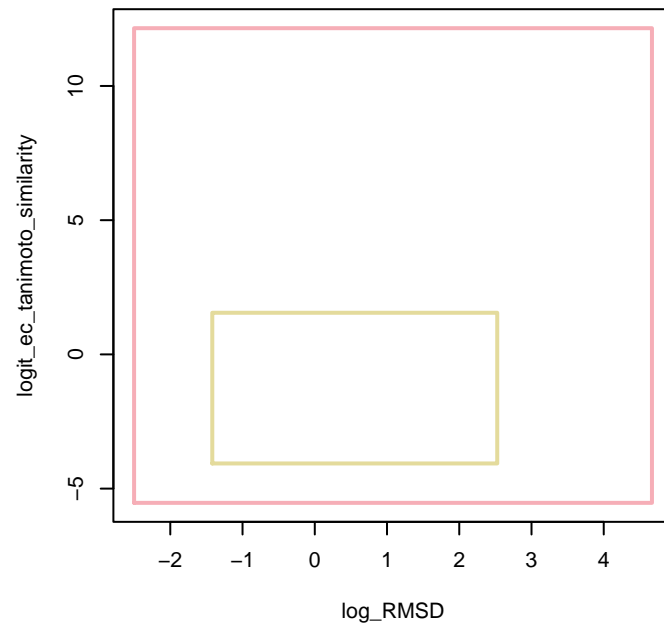
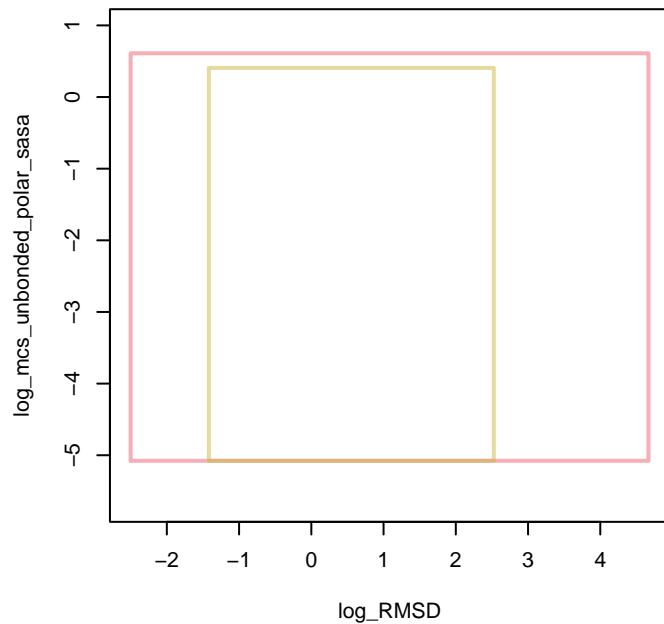
max BMK = 0.123991144767846

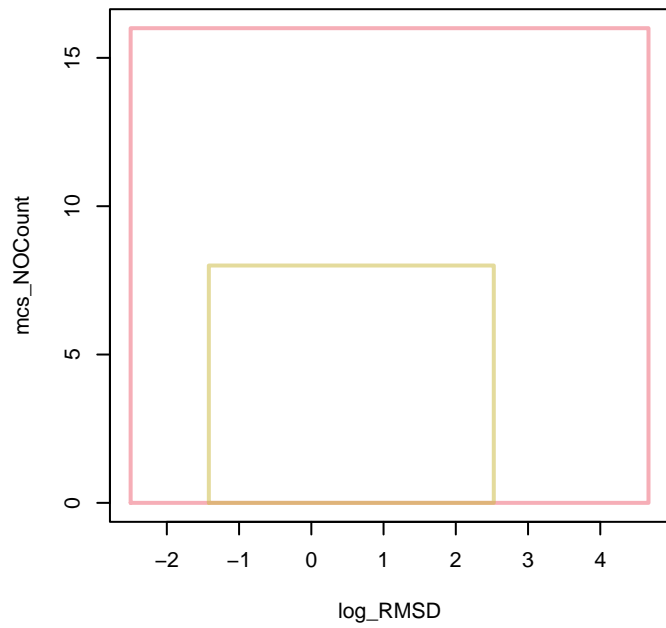
max MCSE = 3.50292388106076

all stationary: FALSE

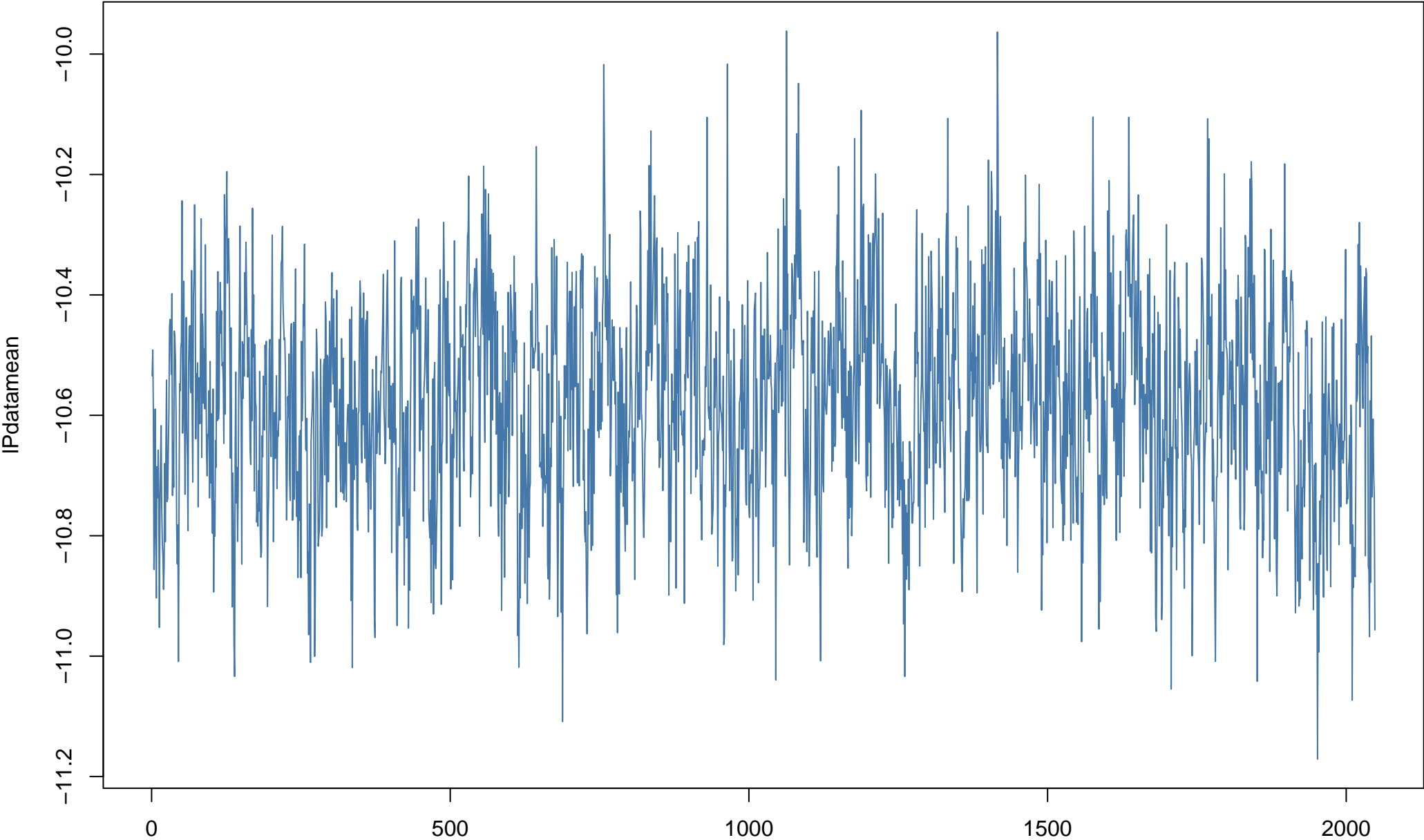
burn: 0

Occupied clusters: 20 of 64

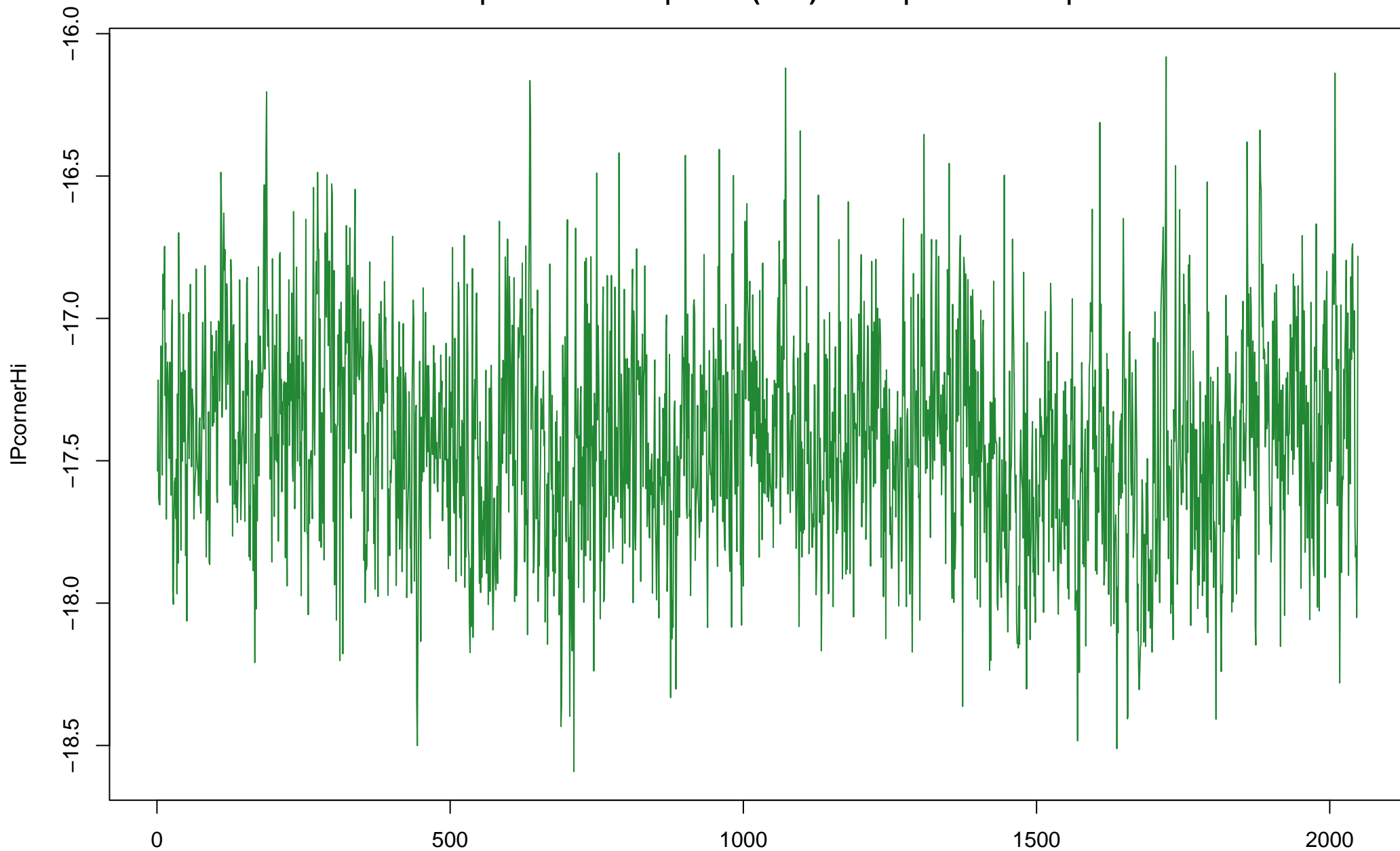




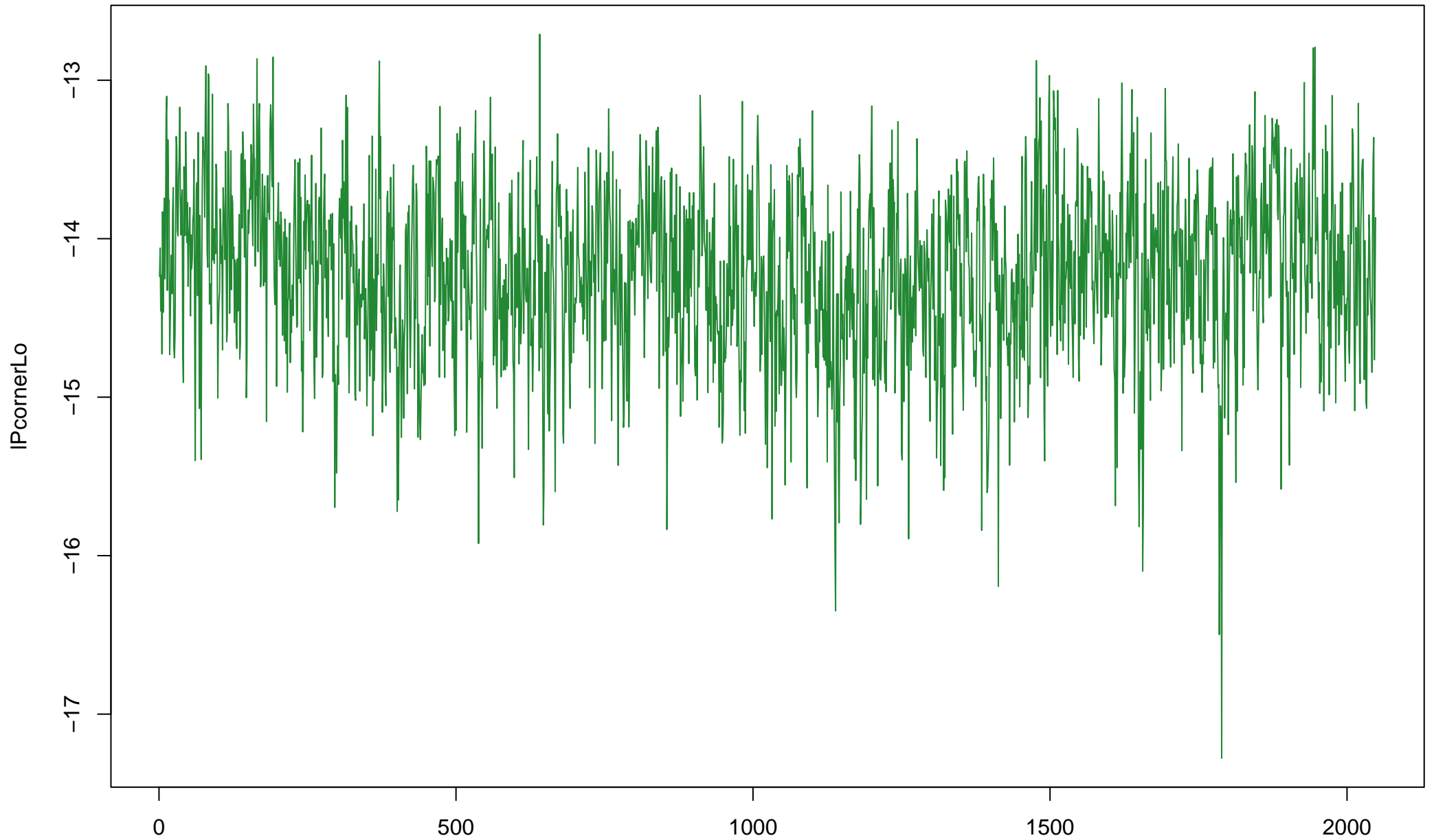
IPdatamean
ESS = 491 | BMK = 0.0514 | MCSE(6.27) = 6.54 | stat: TRUE | burn: 0



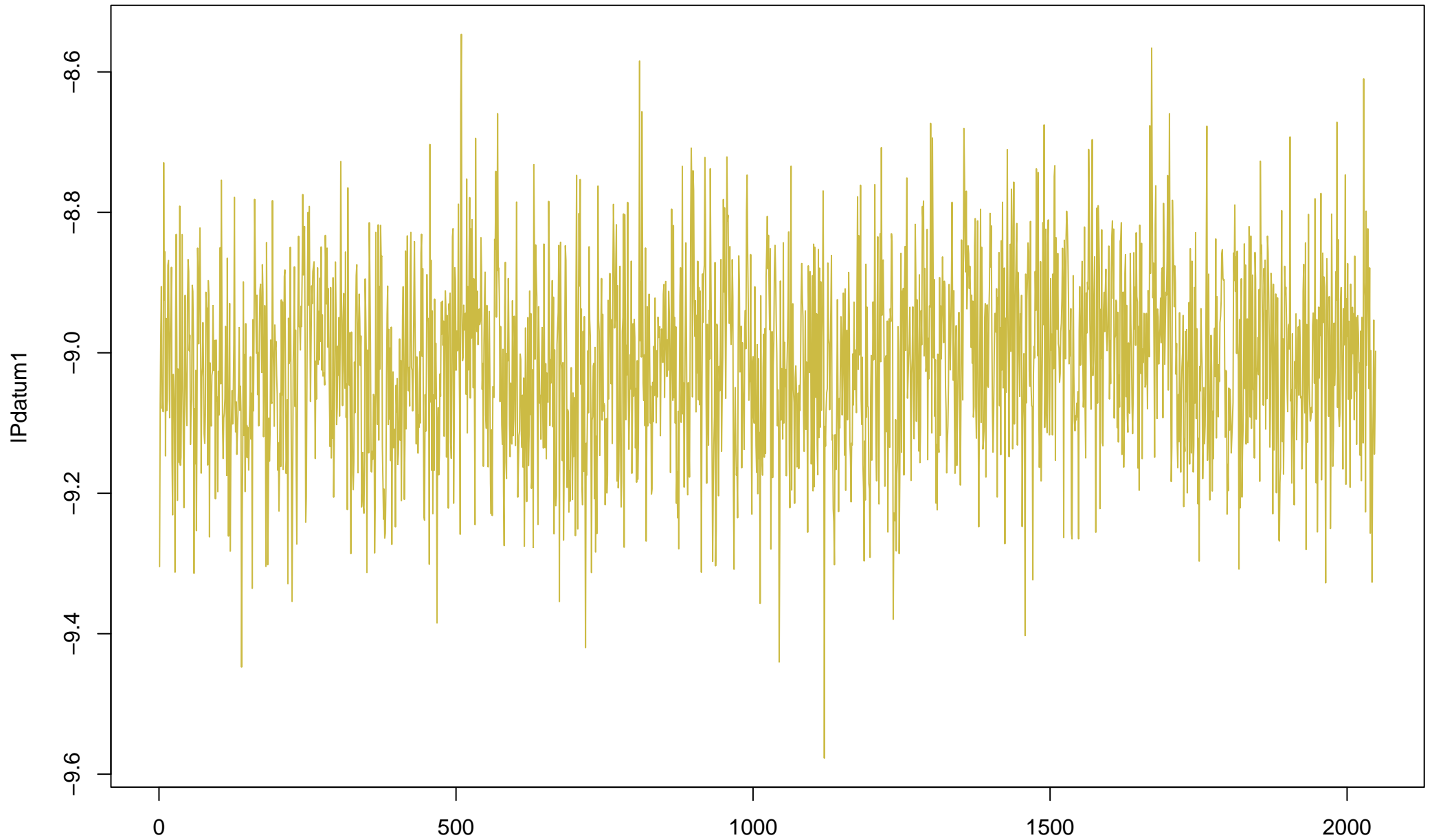
IPcornerHi
ESS = 368 | BMK = 0.0689 | MCSE(6.27) = 5.43 | stat: FALSE | burn: 0



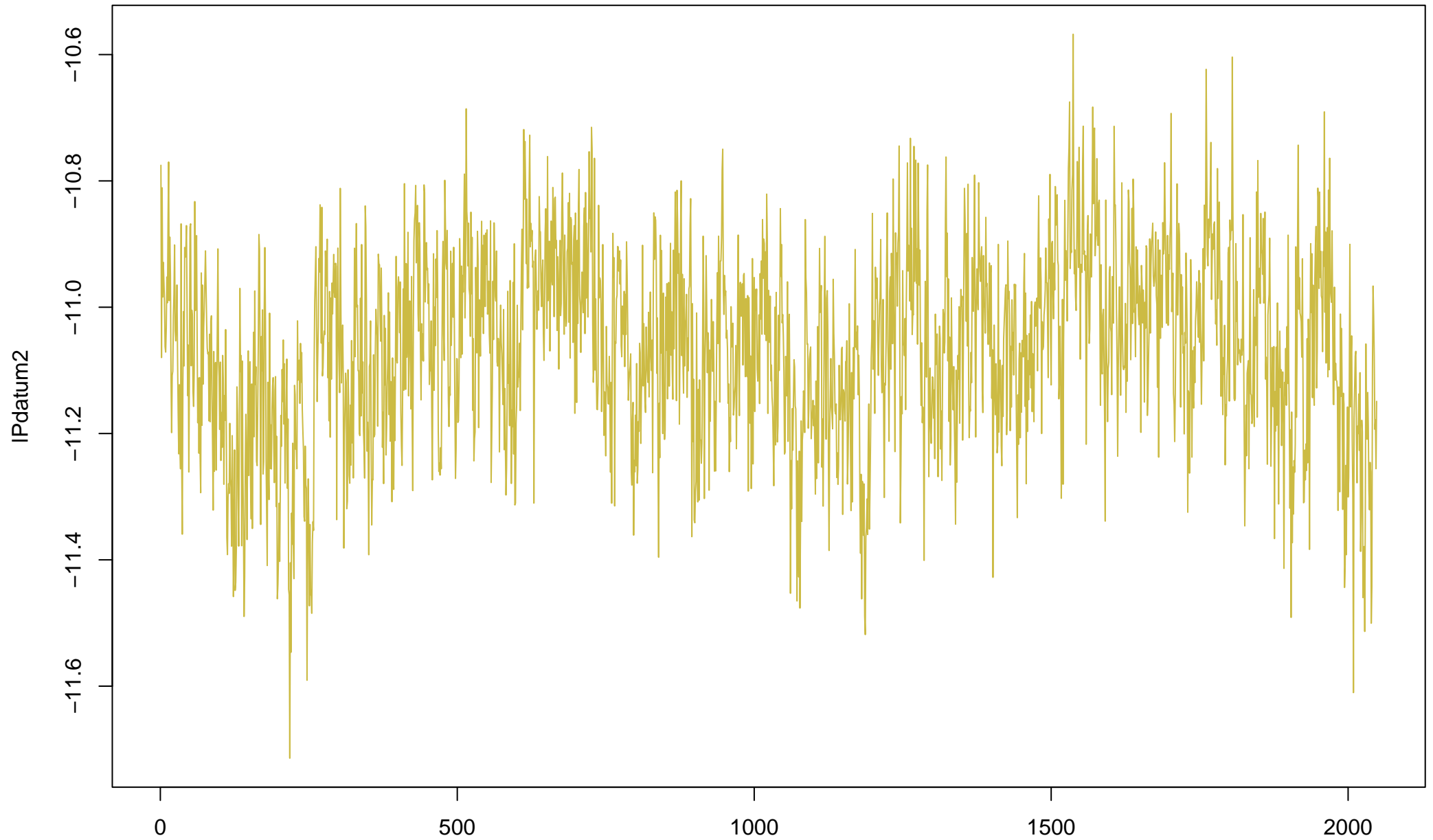
IPcornerLo
ESS = 603 | BMK = 0.0637 | MCSE(6.27) = 5.38 | stat: FALSE | burn: 0



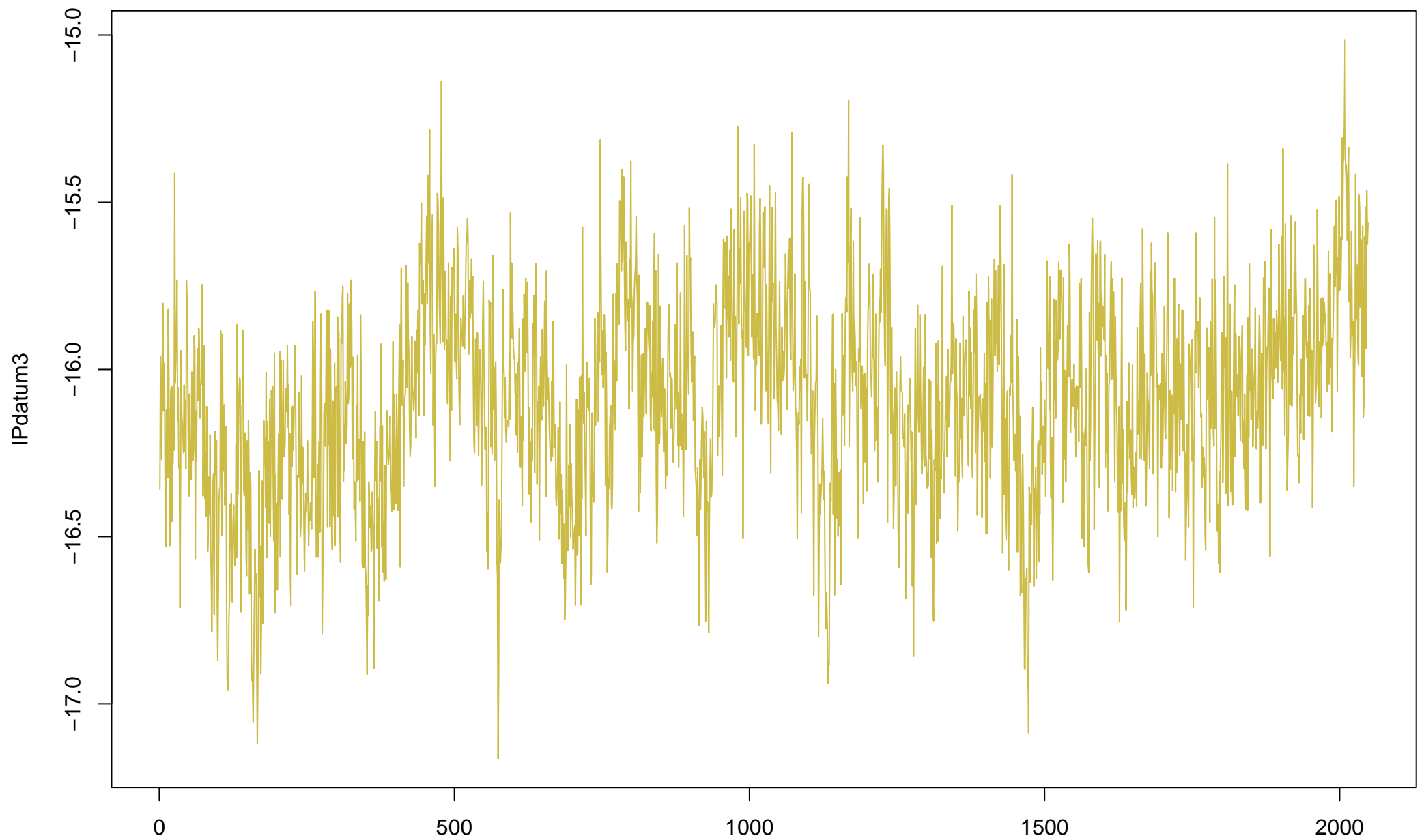
IPdatum1
ESS = 936 | BMK = 0.0728 | MCSE(6.27) = 3.96 | stat: FALSE | burn: 0



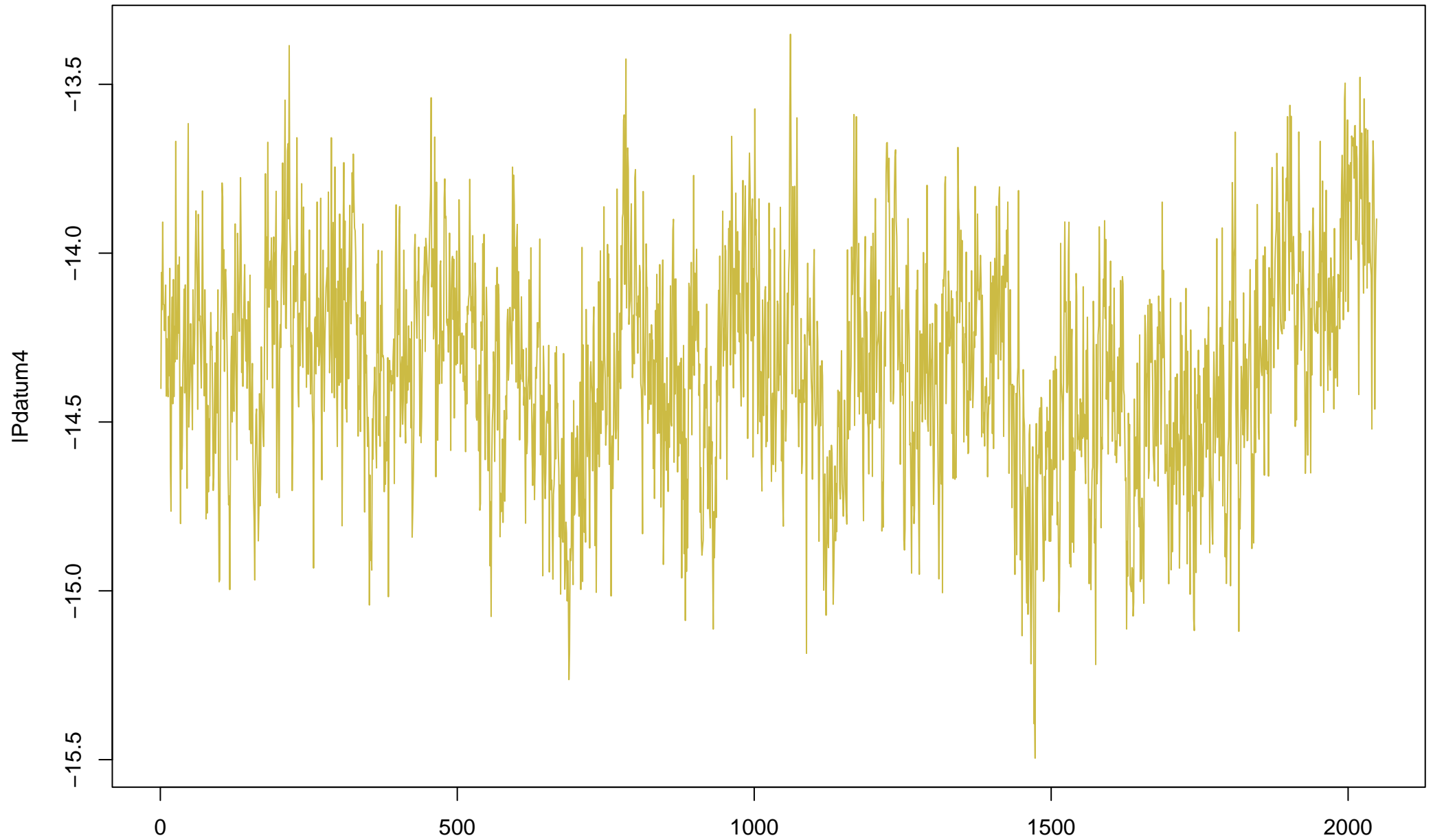
IPdatum2
ESS = 132 | BMK = 0.0591 | MCSE(6.27) = 9.95 | stat: FALSE | burn: 0



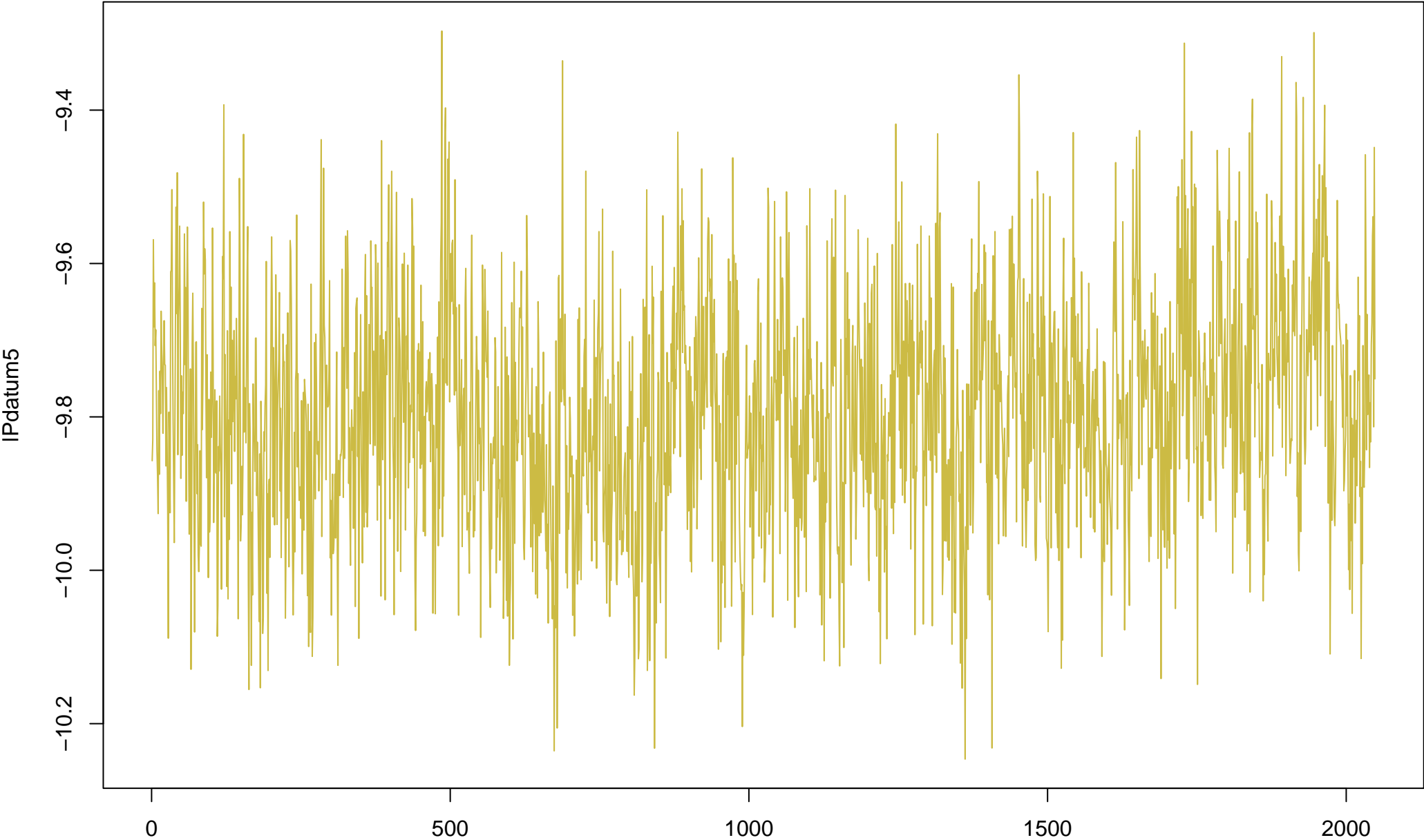
IPdatum3
ESS = 66.2 | BMK = 0.0916 | MCSE(6.27) = 8.85 | stat: FALSE | burn: 0



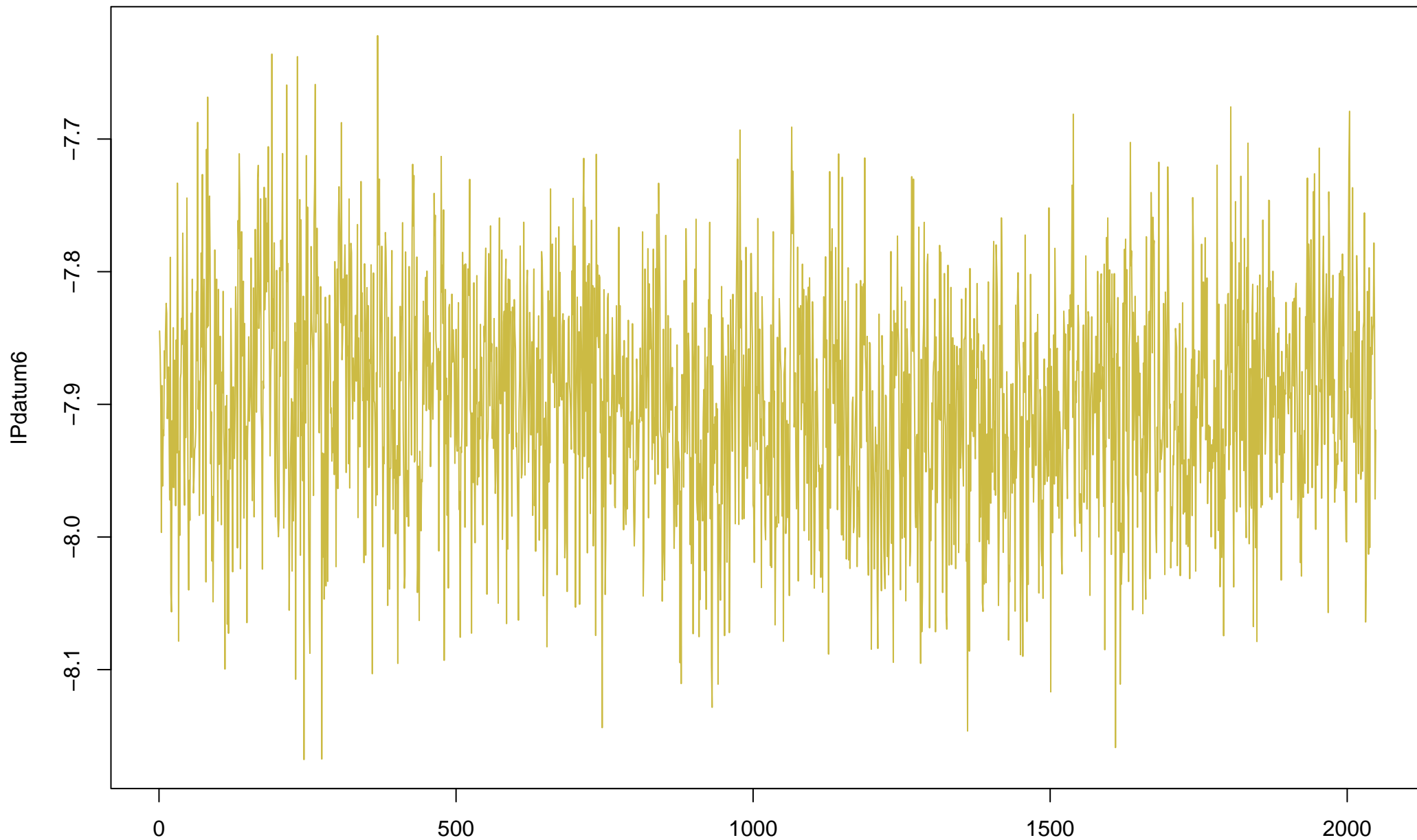
IPdatum4
ESS = 81.6 | BMK = 0.0829 | MCSE(6.27) = 10.6 | stat: TRUE | burn: 0



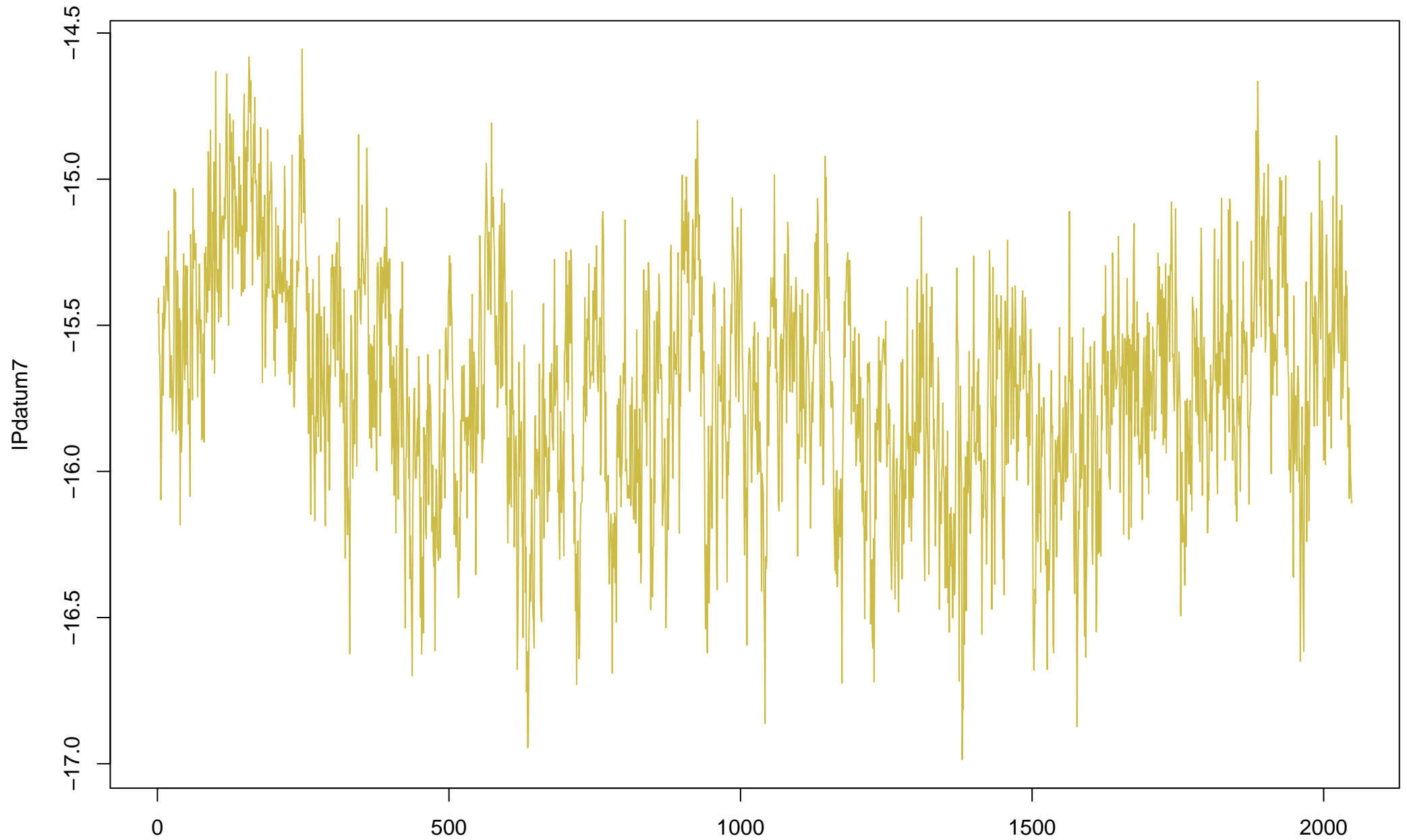
IPdatum5
ESS = 446 | BMK = 0.0928 | MCSE(6.27) = 4.83 | stat: TRUE | burn: 0



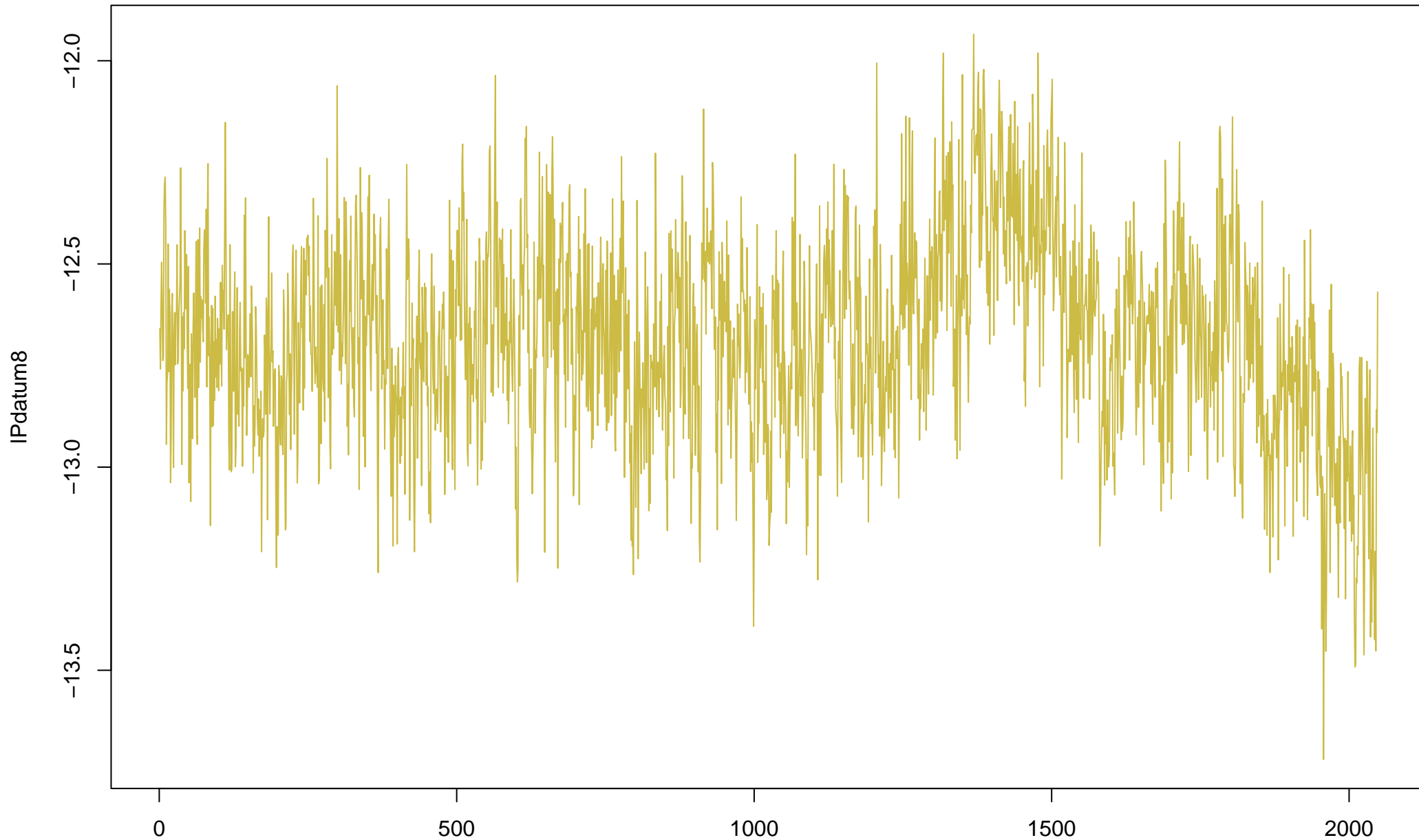
IPdatum6
ESS = 1180 | BMK = 0.0708 | MCSE(6.27) = 3.55 | stat: FALSE | burn: 0



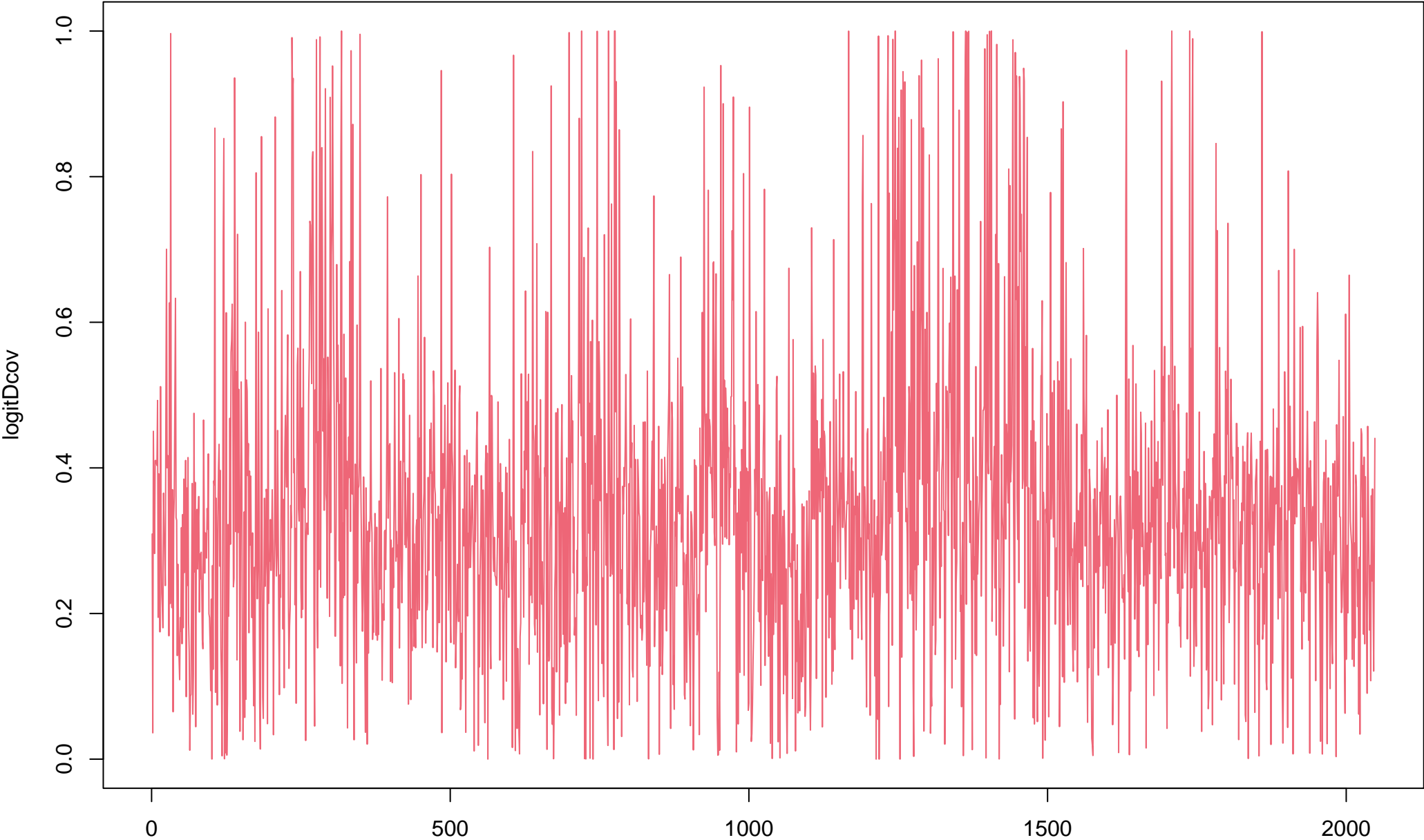
IPdatum7
ESS = 62.9 | BMK = 0.149 | MCSE(6.27) = 11.6 | stat: FALSE | burn: 0



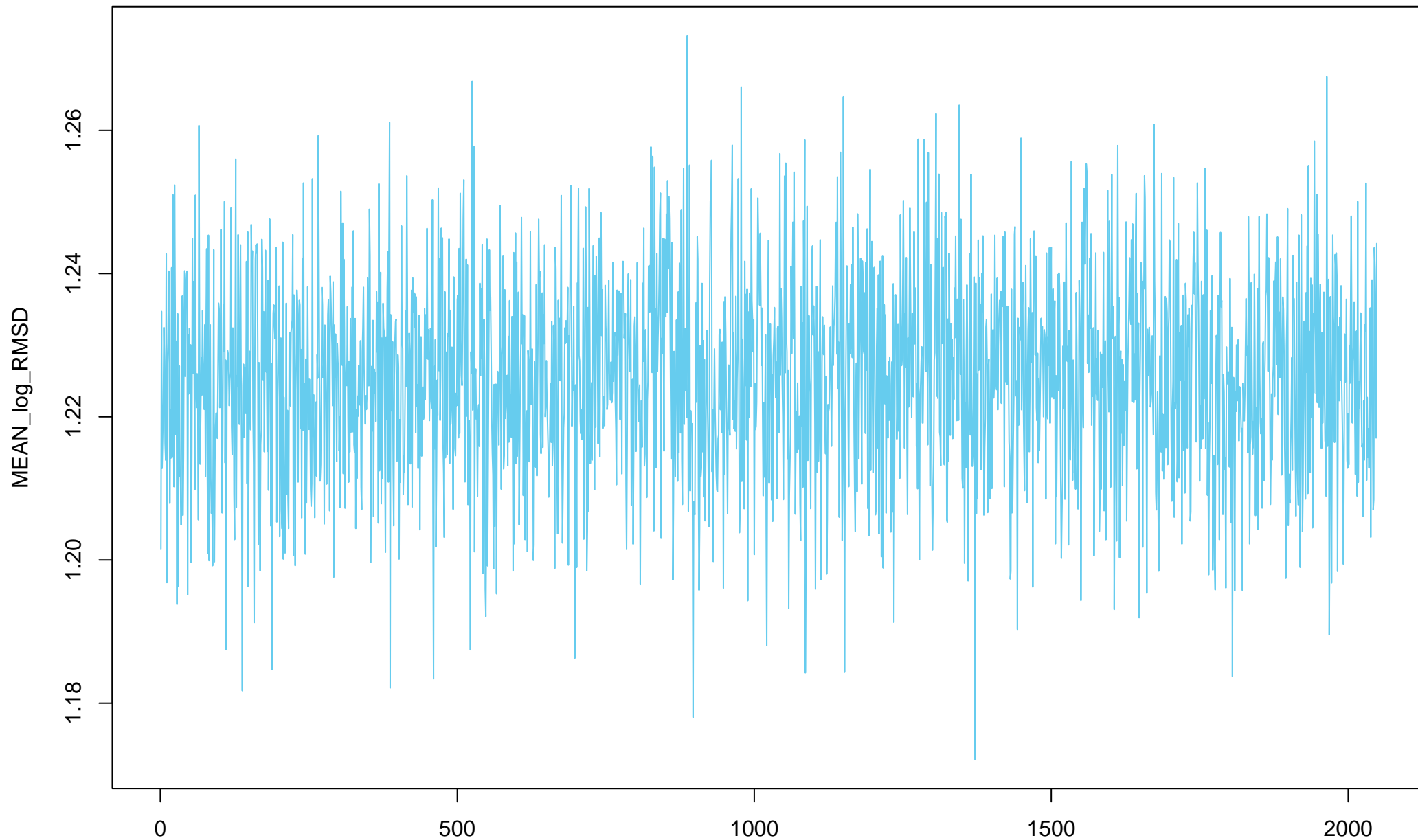
IPdatum8
ESS = 102 | BMK = 0.13 | MCSE(6.27) = 8.52 | stat: TRUE | burn: 0



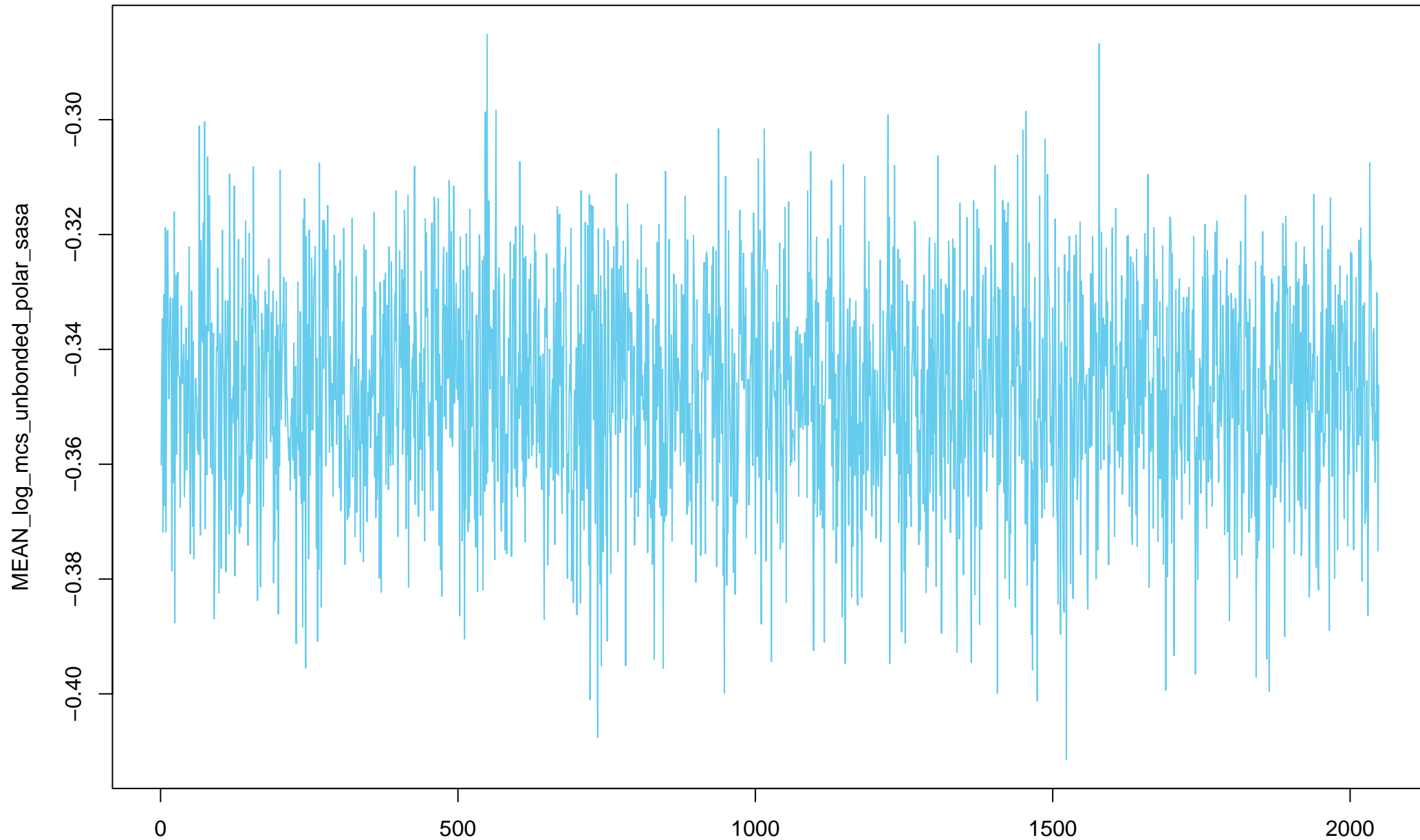
logitDcov
ESS = 352 | BMK = 0.0465 | MCSE(6.27) = 3.5 | stat: FALSE | burn: 0



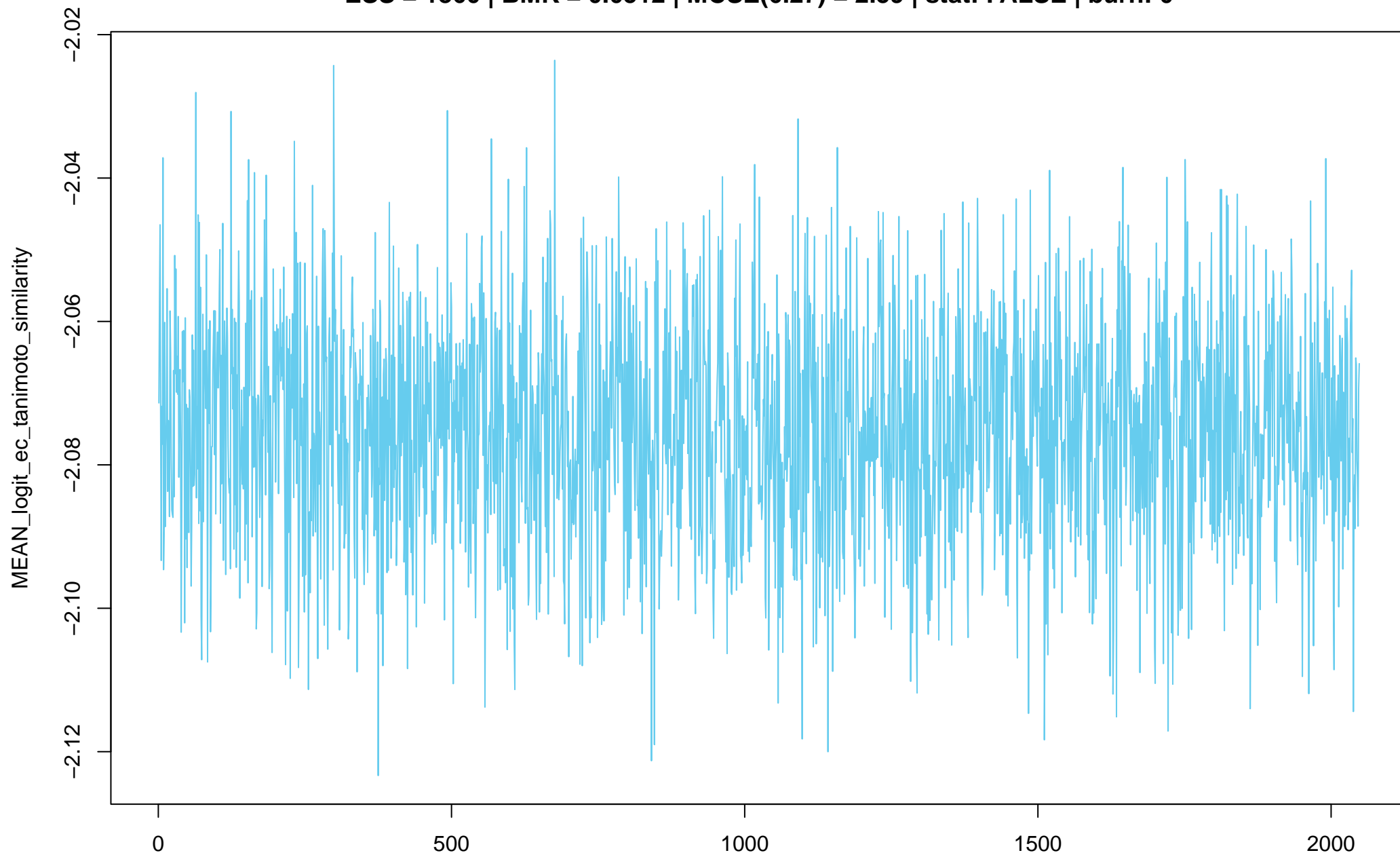
MEAN_log_RMSD
ESS = 1750 | BMK = 0.0366 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0



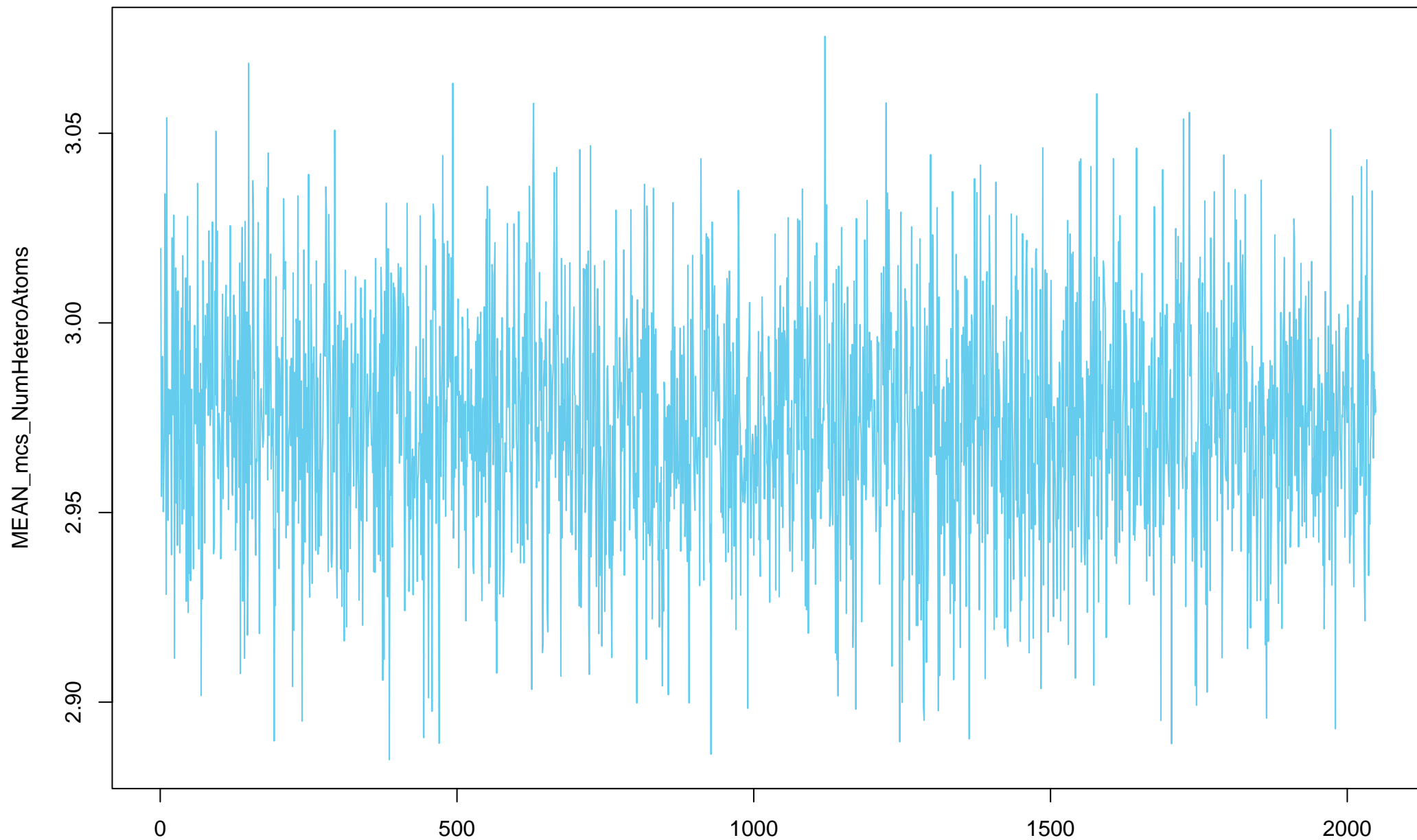
MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0435 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0



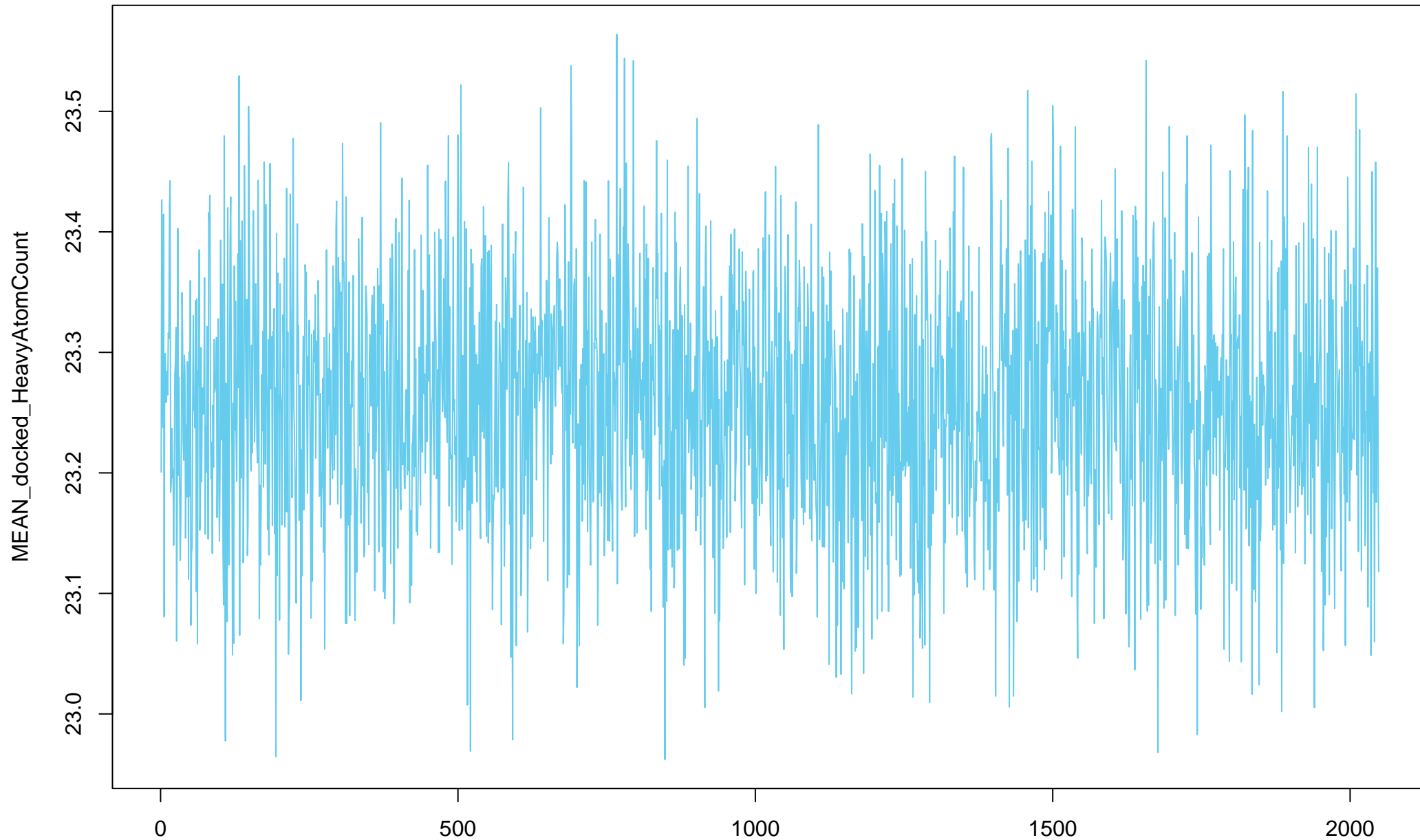
MEAN_logit_ec_tanimoto_similarity
ESS = 1860 | BMK = 0.0512 | MCSE(6.27) = 2.59 | stat: FALSE | burn: 0



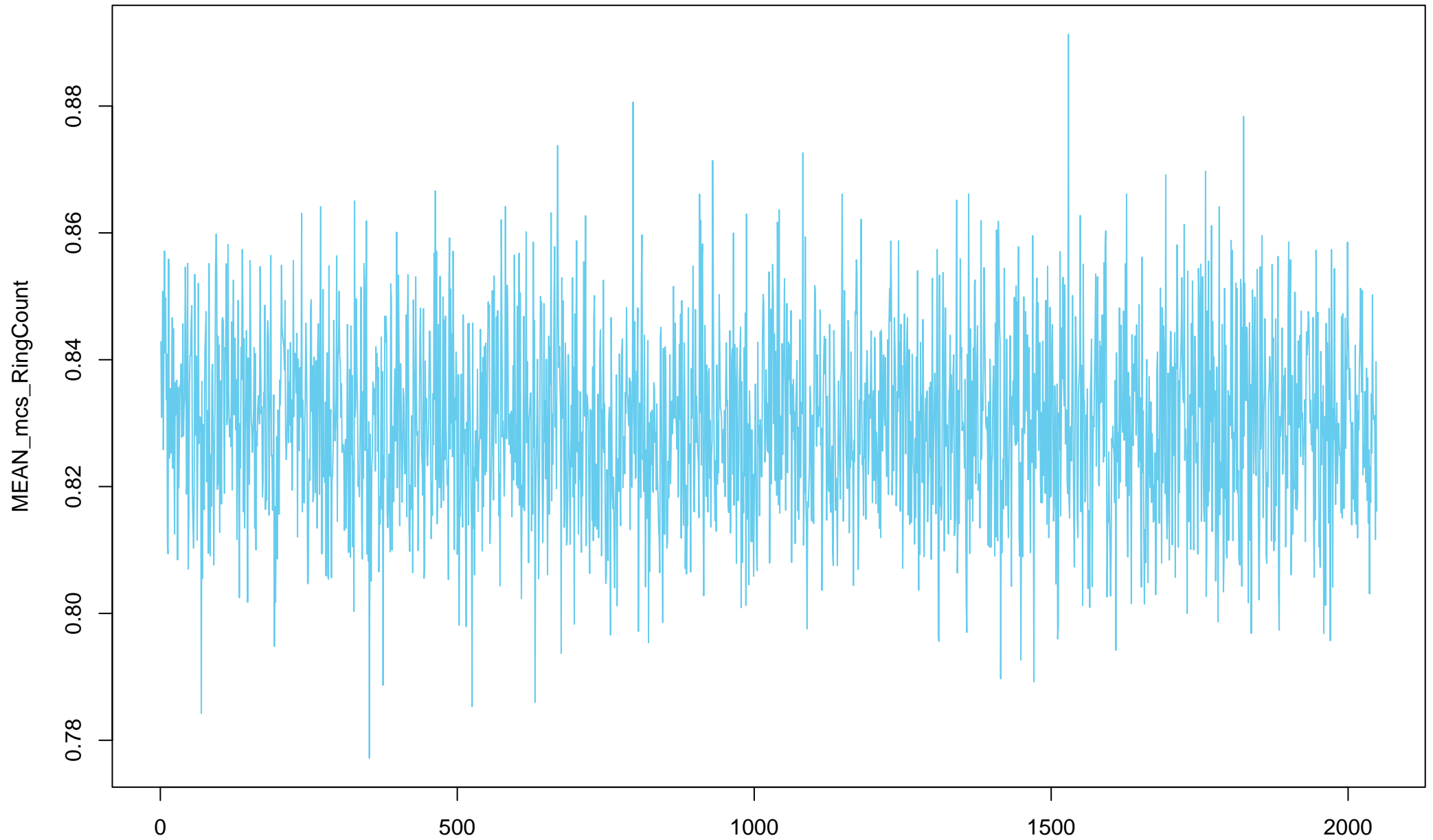
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0277 | MCSE(6.27) = 2.26 | stat: FALSE | burn: 0



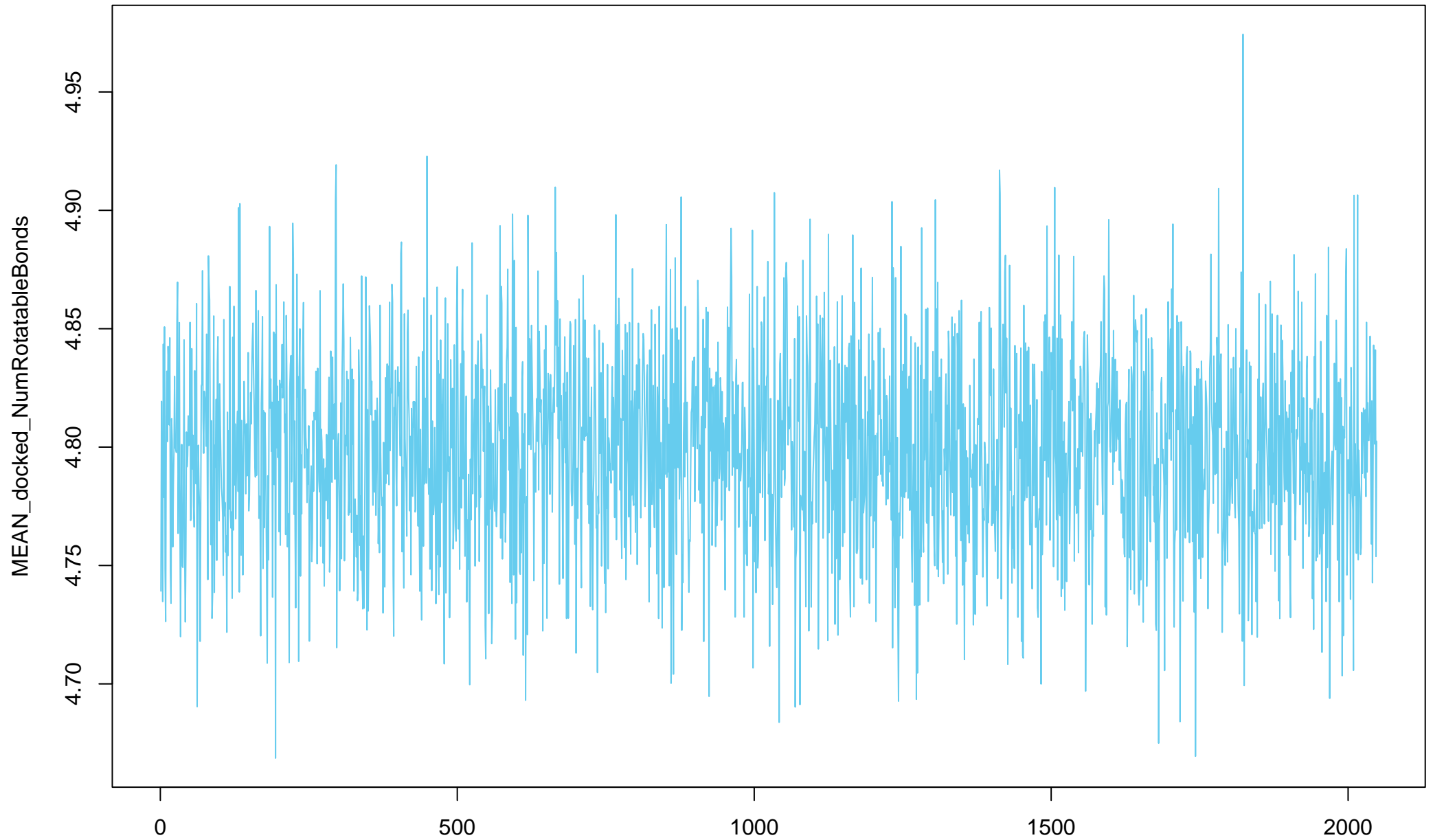
MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0479 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0



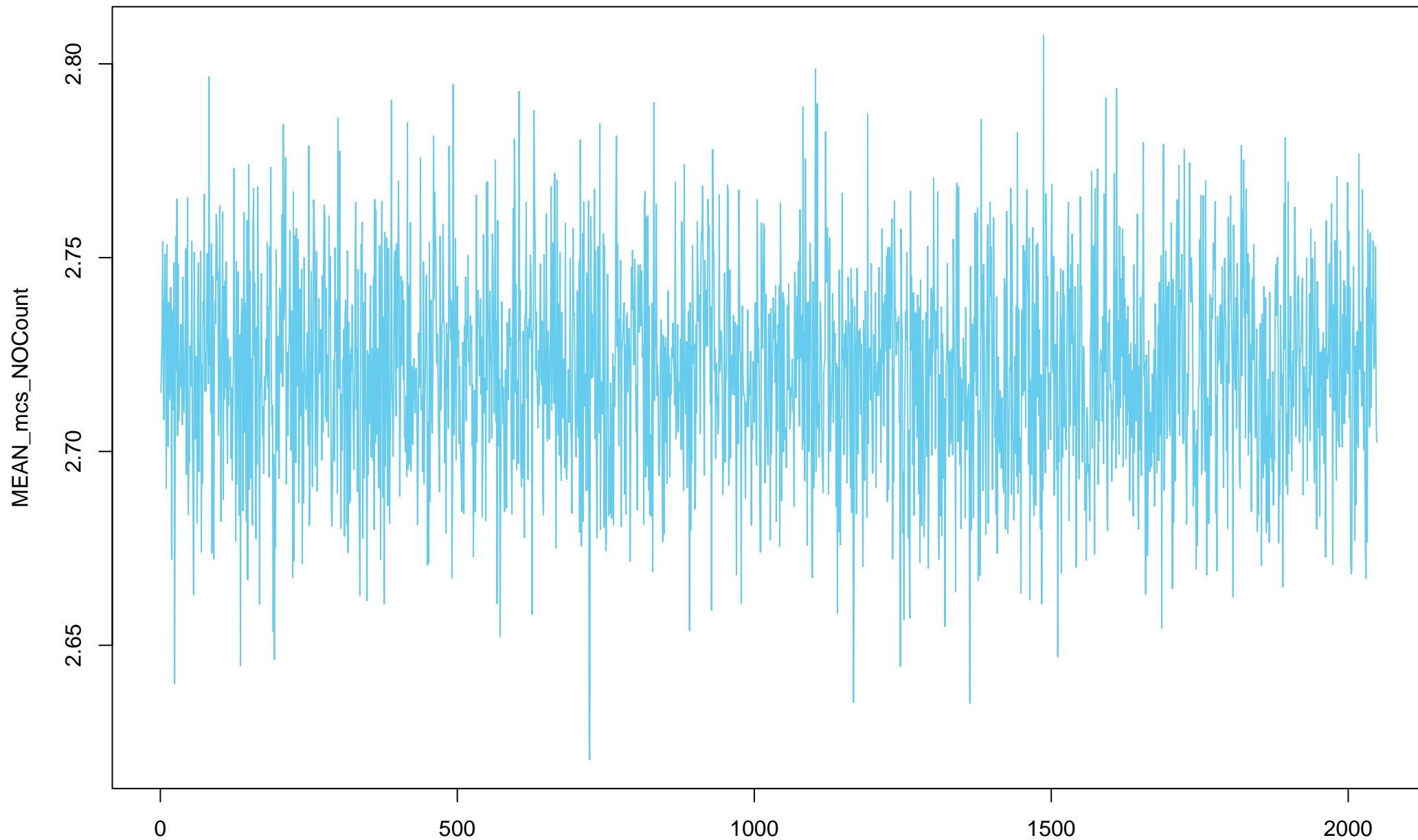
MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0428 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0



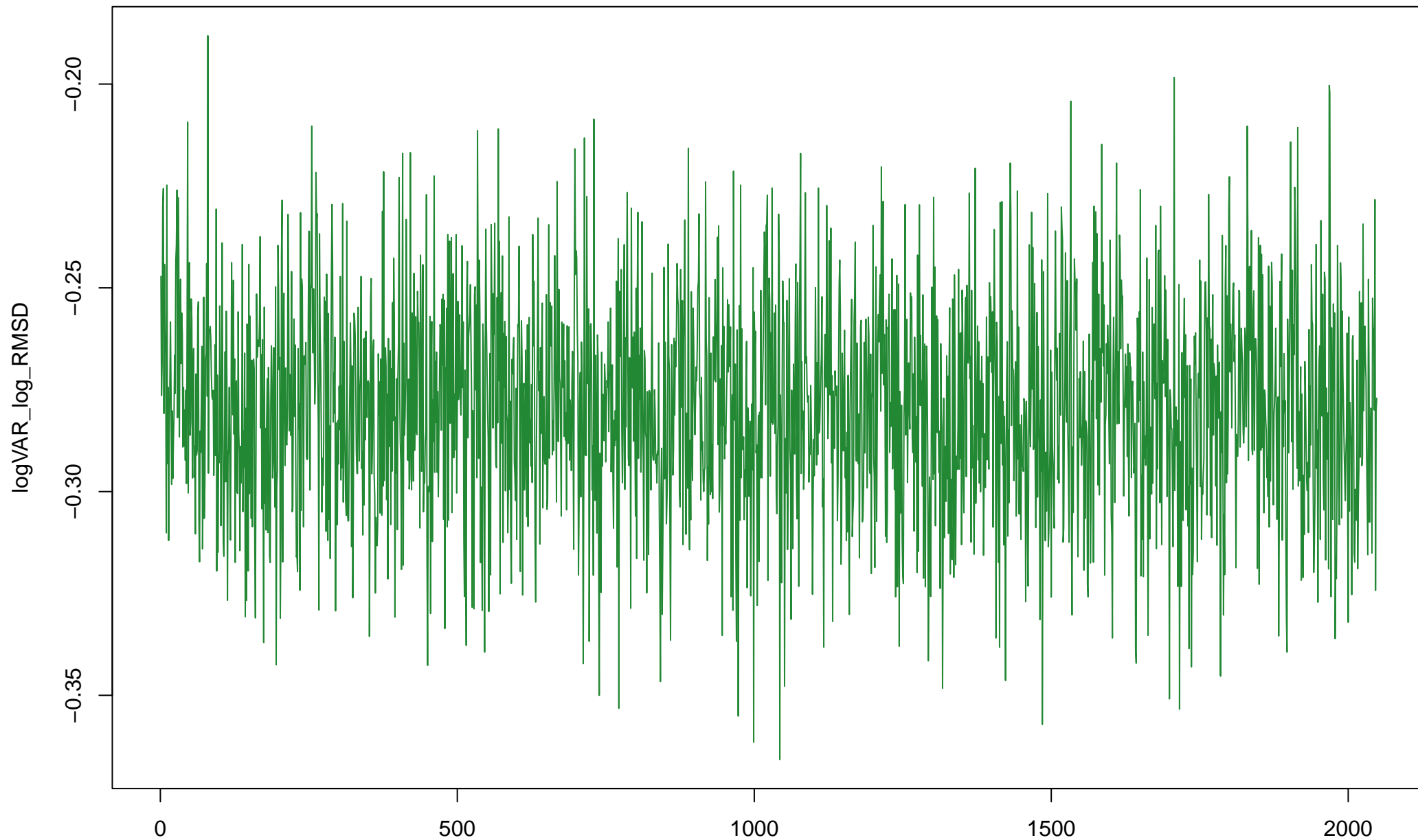
MEAN_docked_NumRotatableBonds
ESS = 2050 | BMK = 0.041 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0



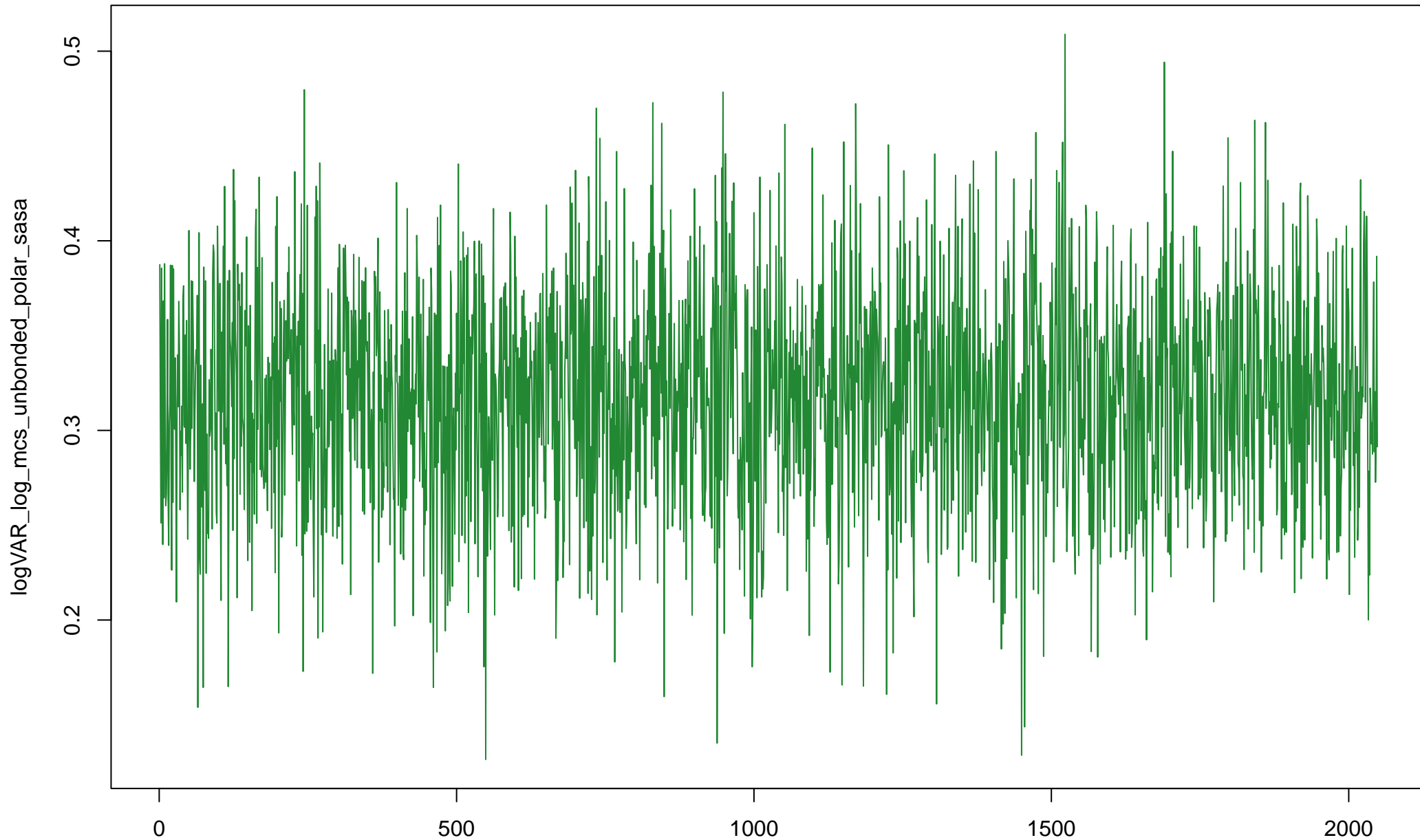
MEAN_mcs_NOCount
ESS = 2050 | BMK = 0.0451 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0



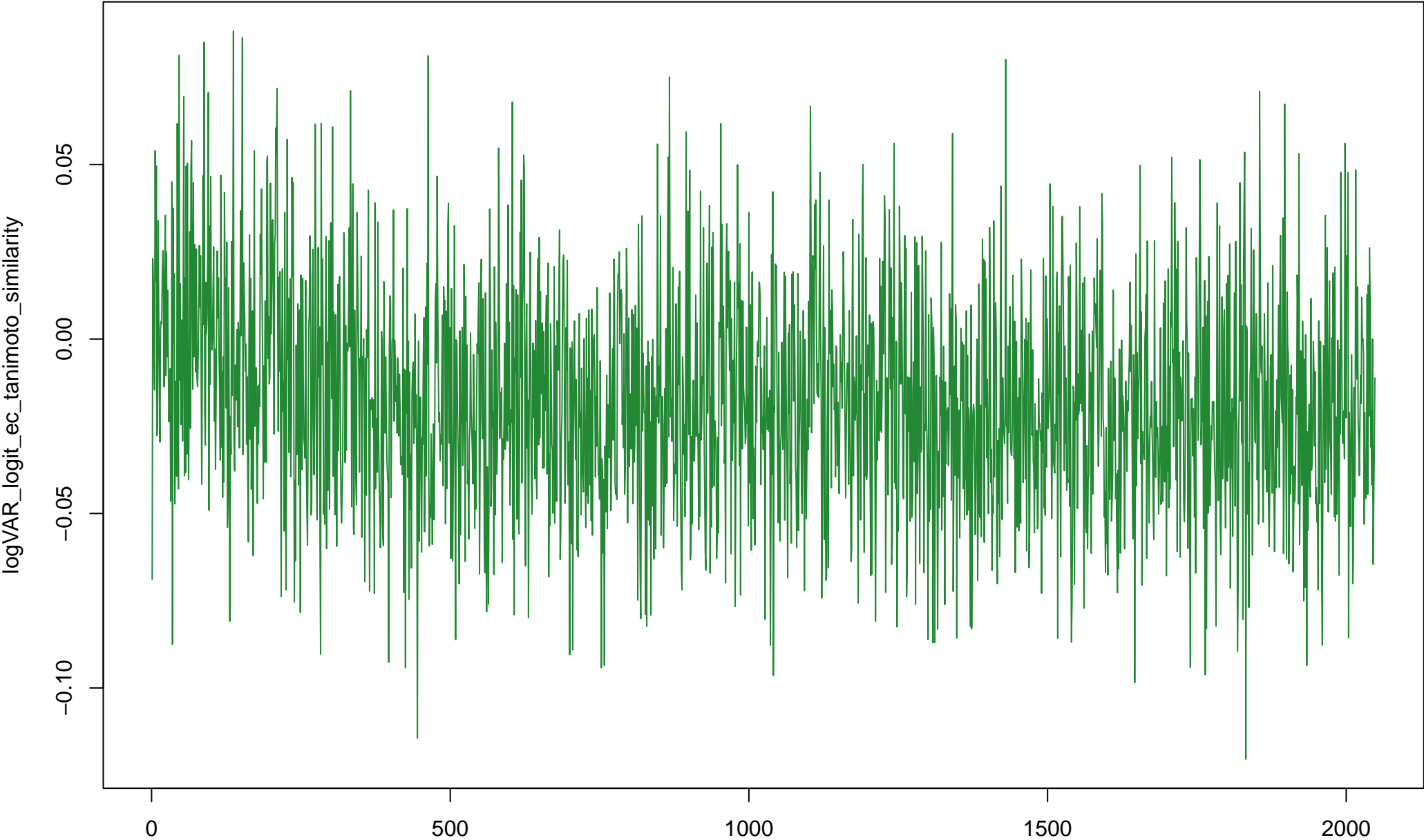
logVAR_log_RMSD
ESS = 1860 | BMK = 0.0346 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0



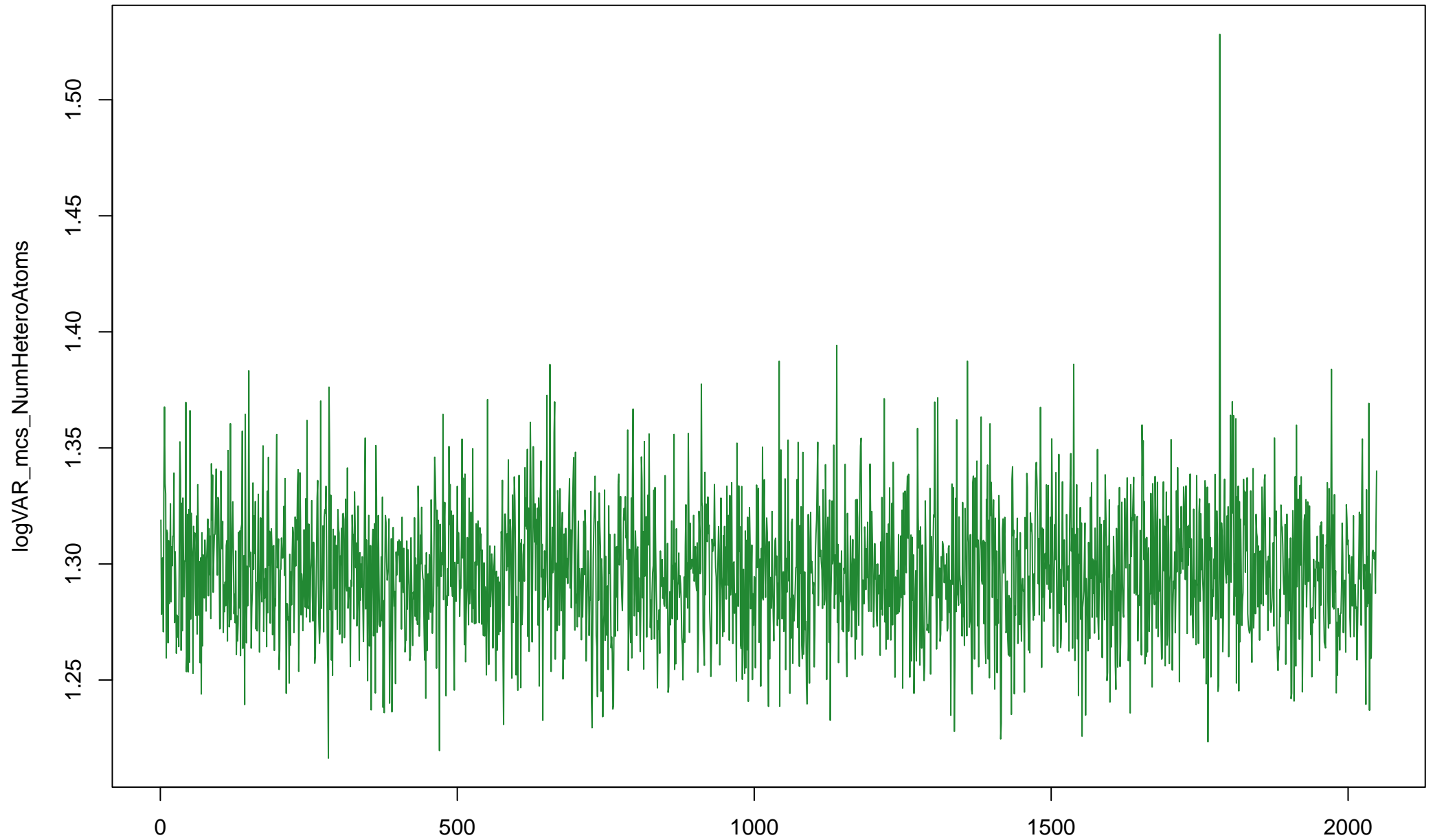
logVAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0429 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



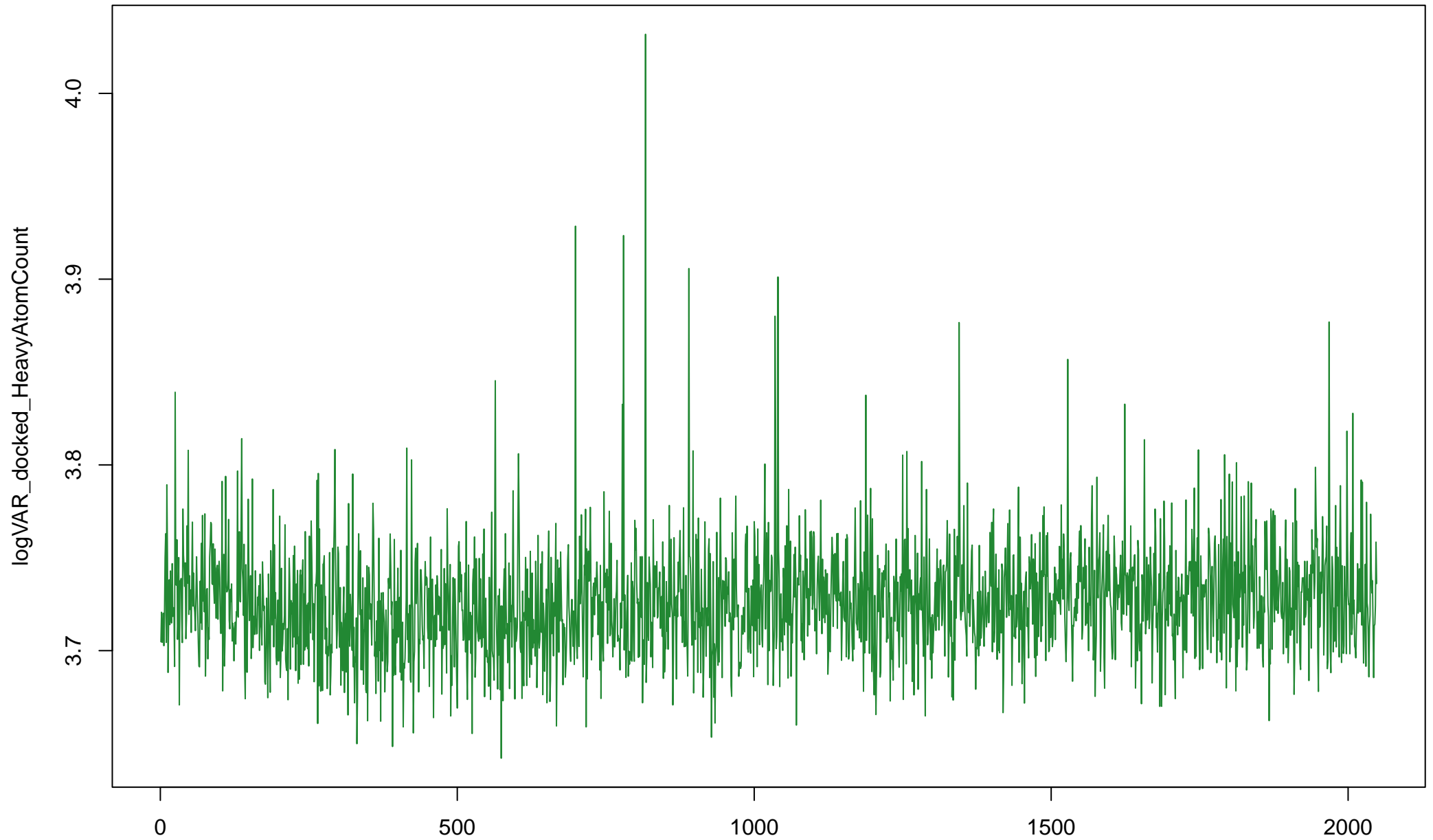
logVAR_logit_ec_tanimoto_similarity
ESS = 822 | BMK = 0.0752 | MCSE(6.27) = 2.9 | stat: FALSE | burn: 0



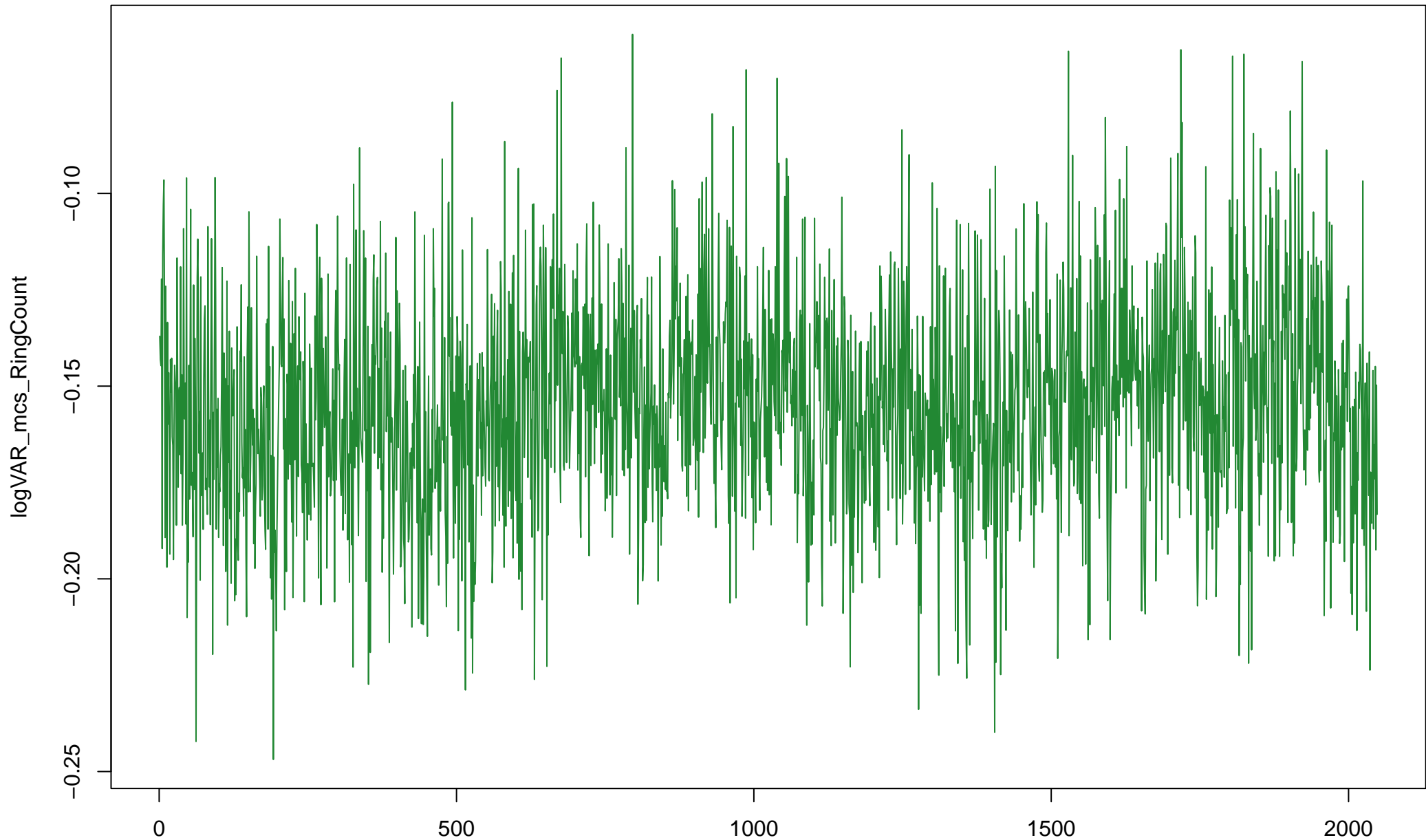
logVAR_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.036 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0



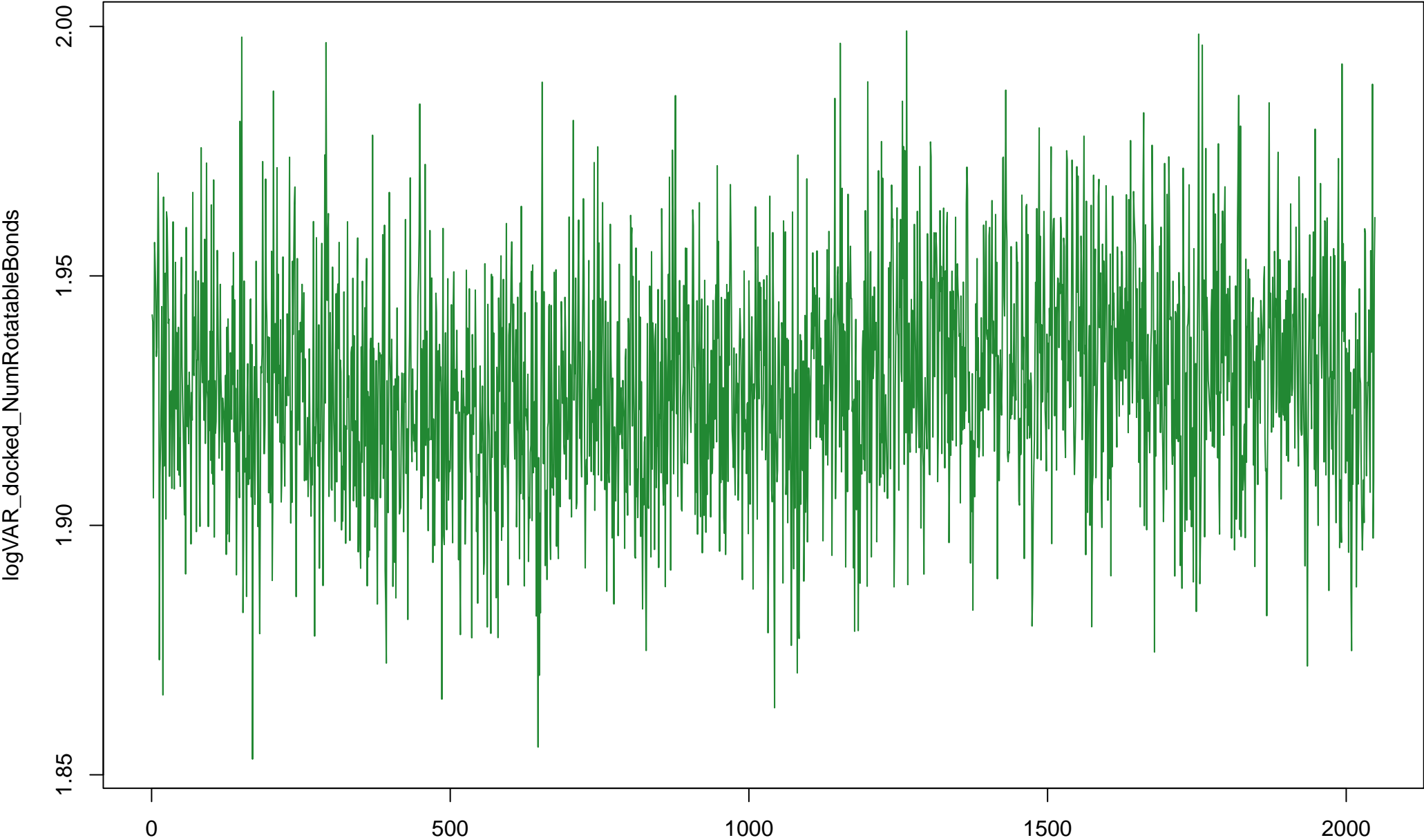
logVAR_docked_HeavyAtomCount
ESS = 1820 | BMK = 0.124 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0



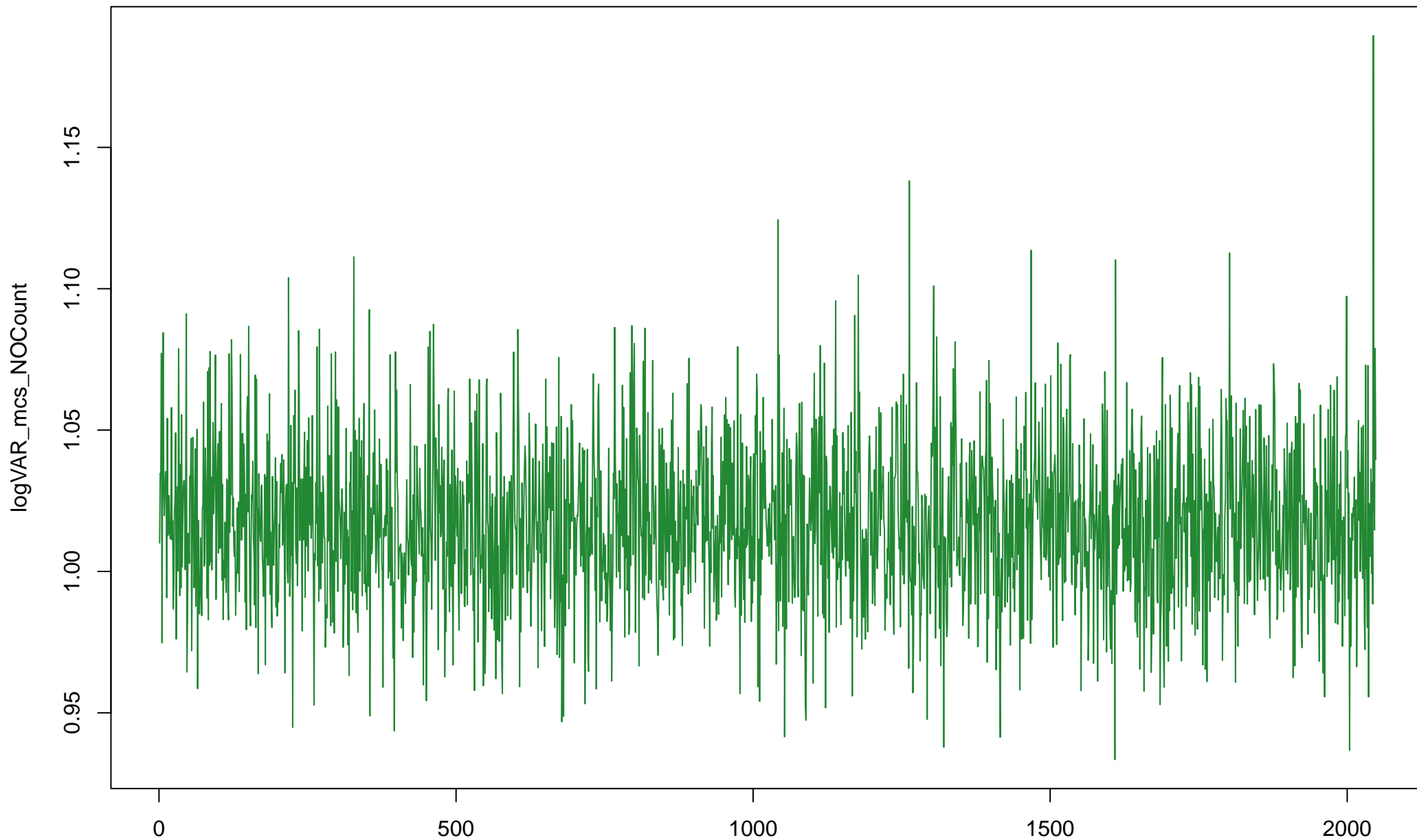
logVAR_mcs_RingCount
ESS = 350 | BMK = 0.0535 | MCSE(6.27) = 3.23 | stat: FALSE | burn: 0



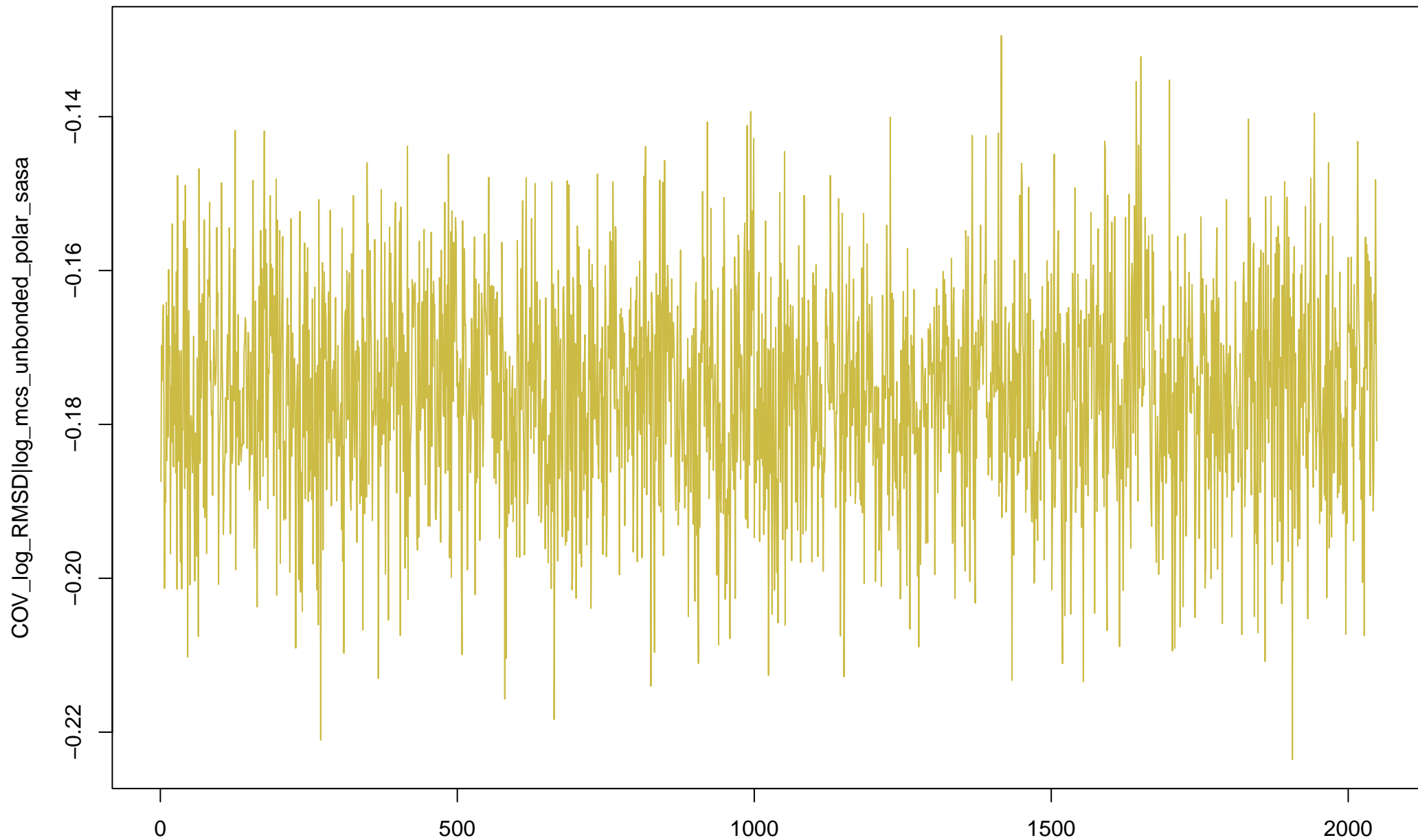
logVAR_docked_NumRotatableBonds
ESS = 401 | BMK = 0.124 | MCSE(6.27) = 3.36 | stat: FALSE | burn: 0



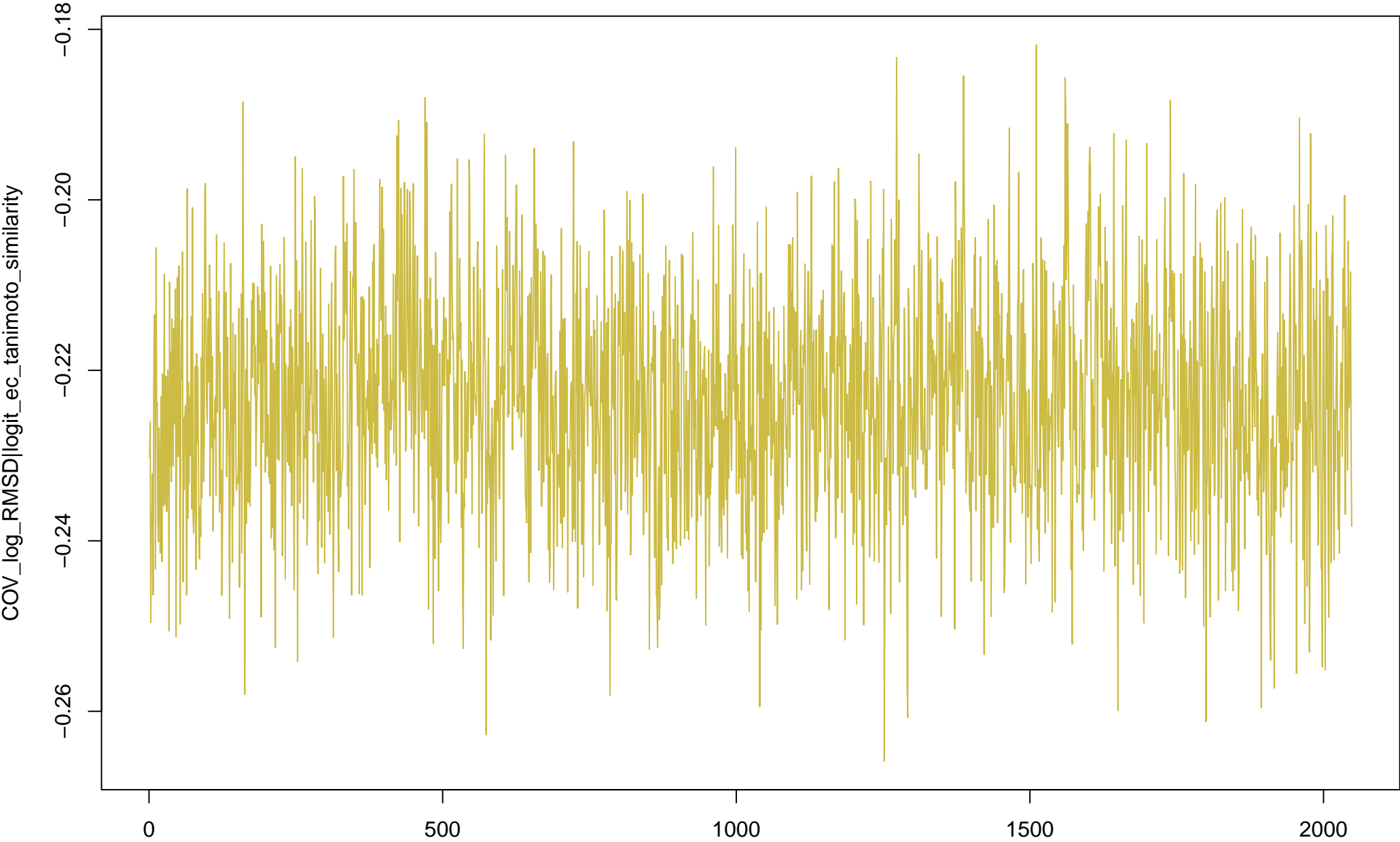
logVAR_mcs_NOCount
ESS = 2050 | BMK = 0.0607 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0



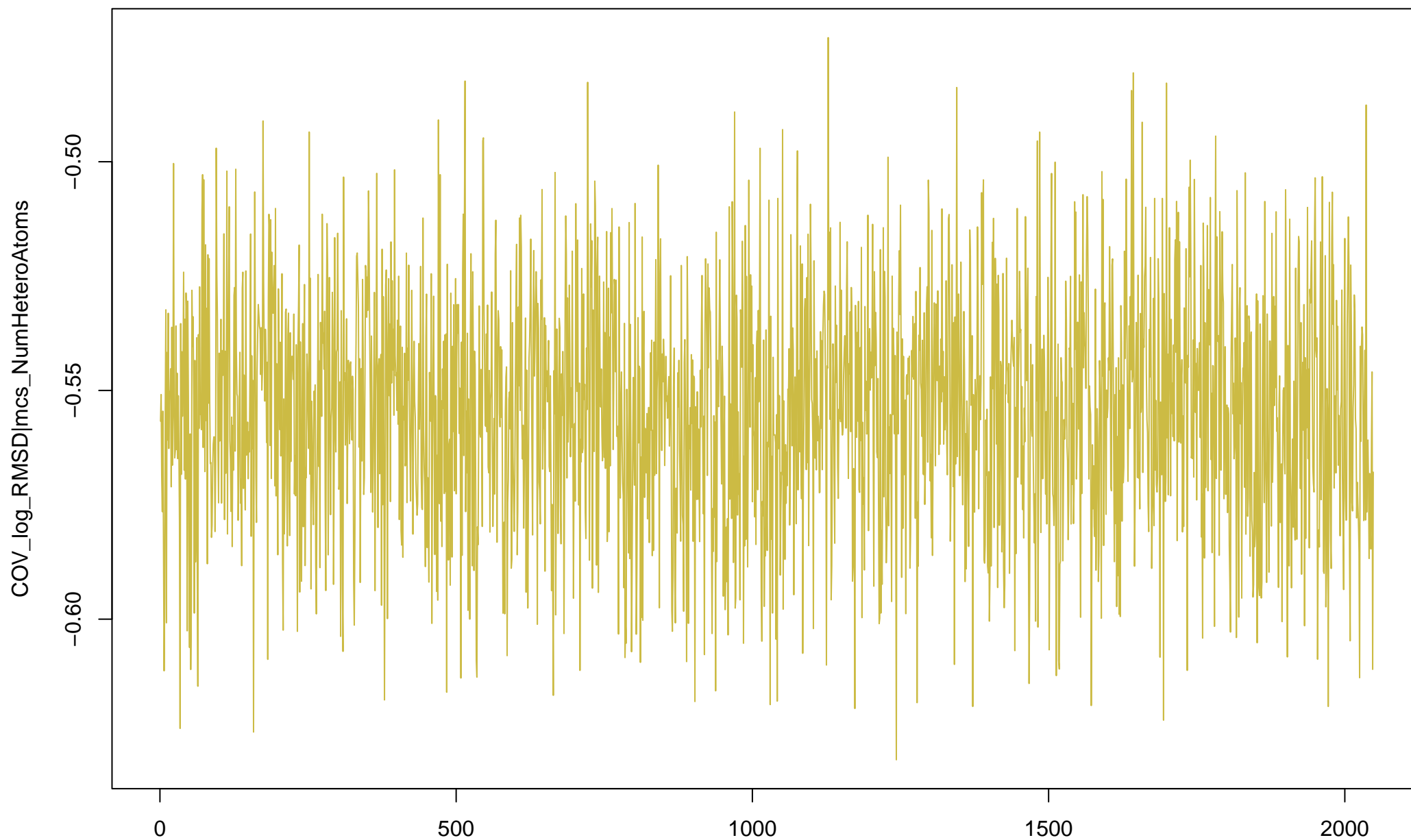
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1280 | BMK = 0.0478 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0



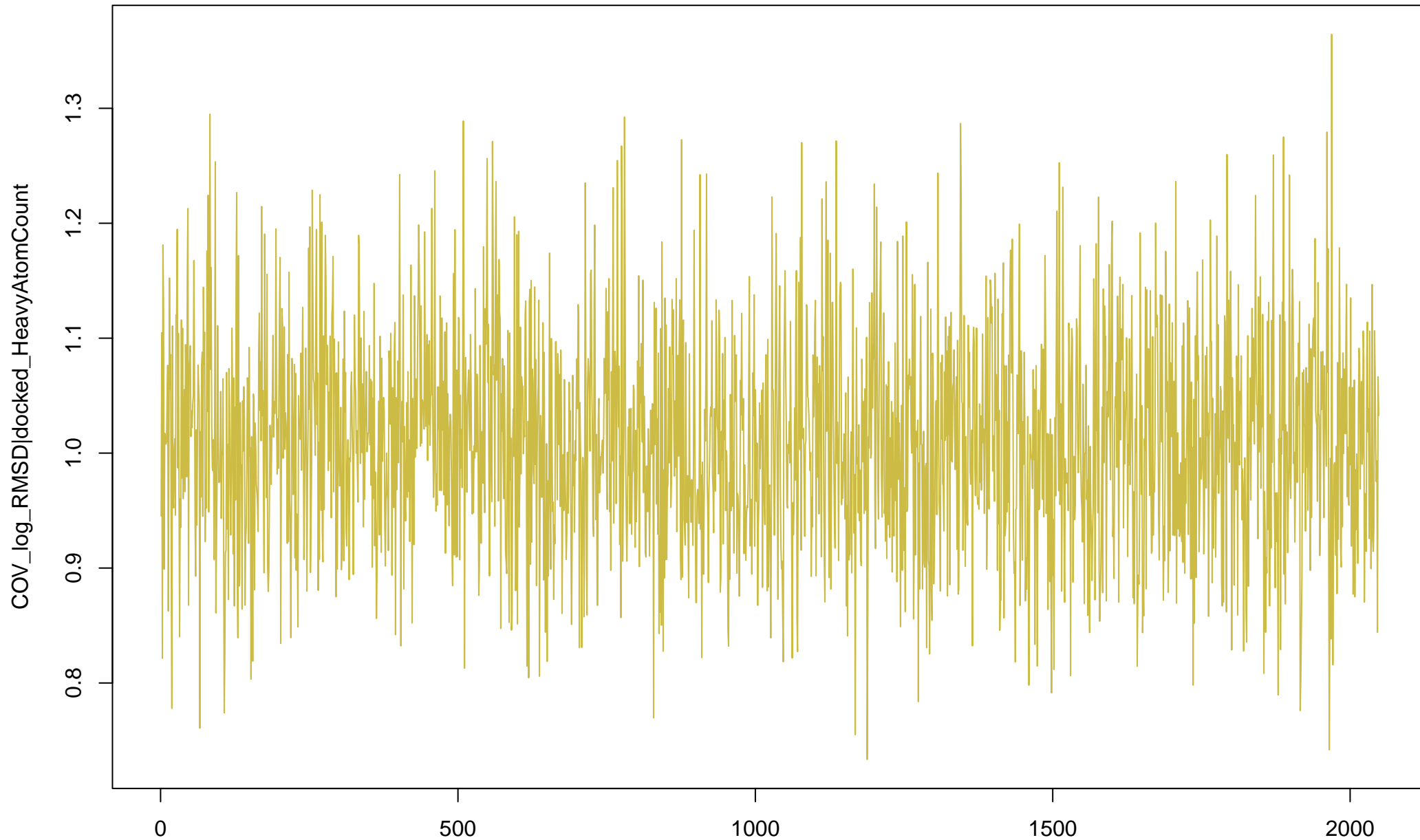
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1130 | BMK = 0.038 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 0



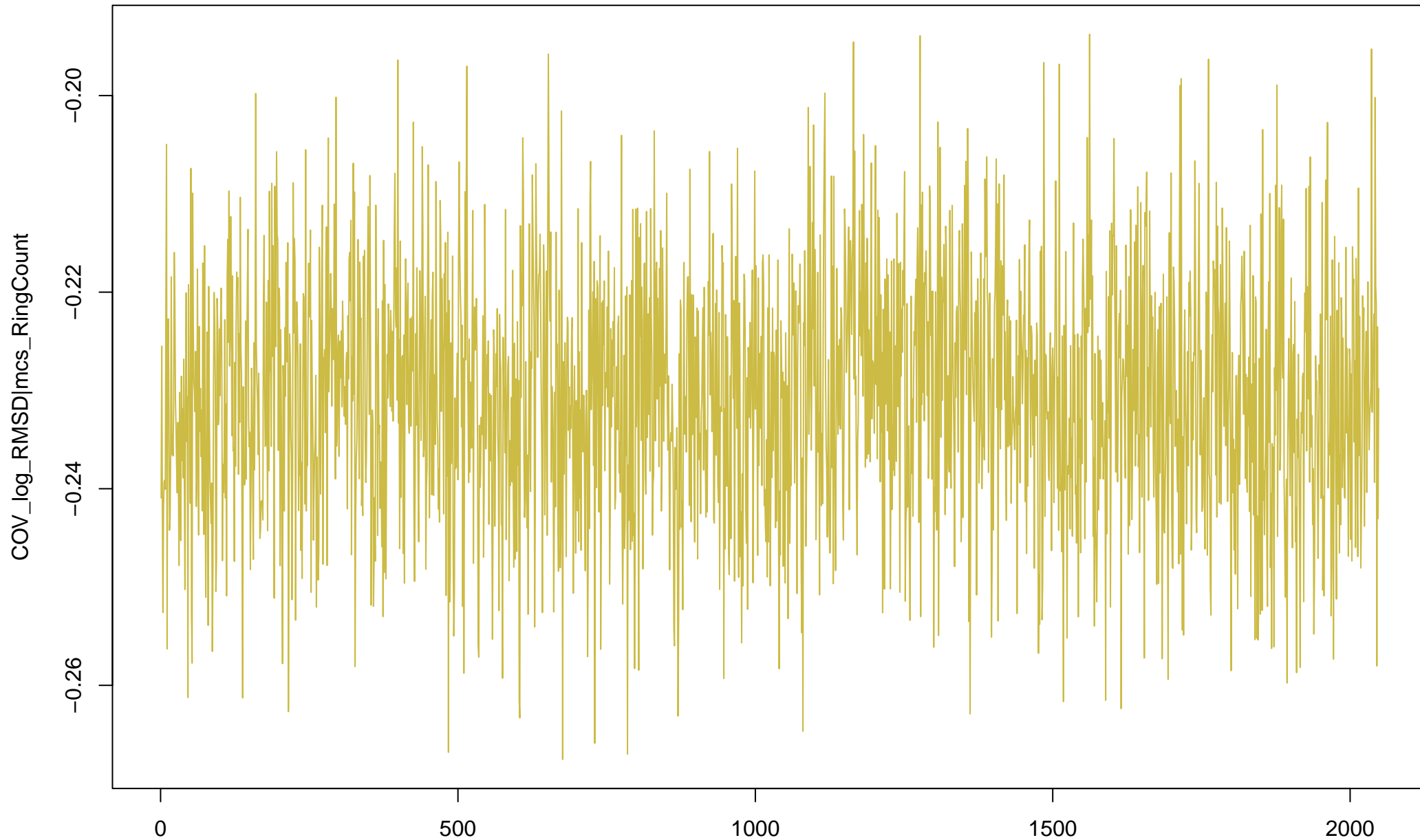
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1780 | BMK = 0.0333 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0



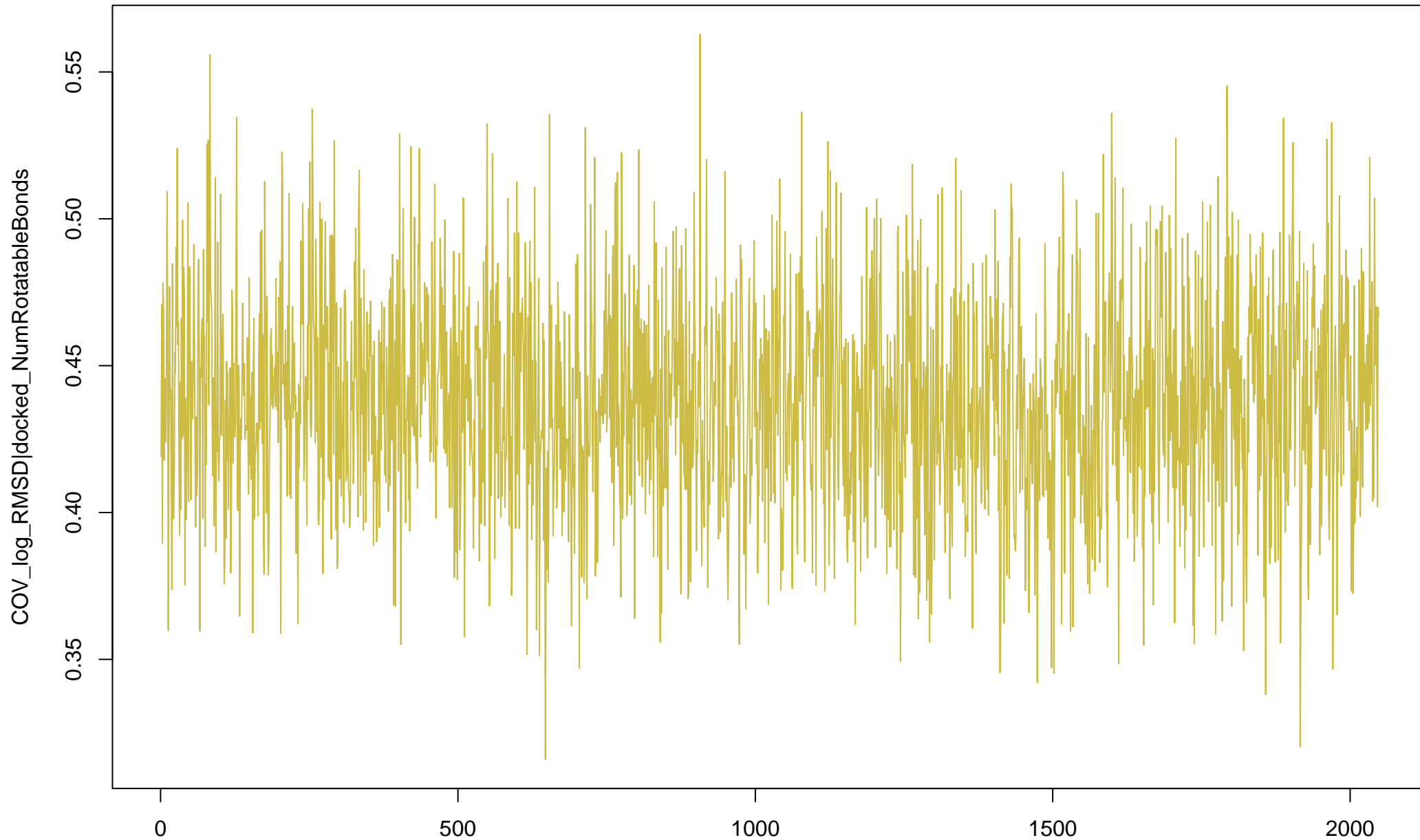
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1710 | BMK = 0.0448 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0



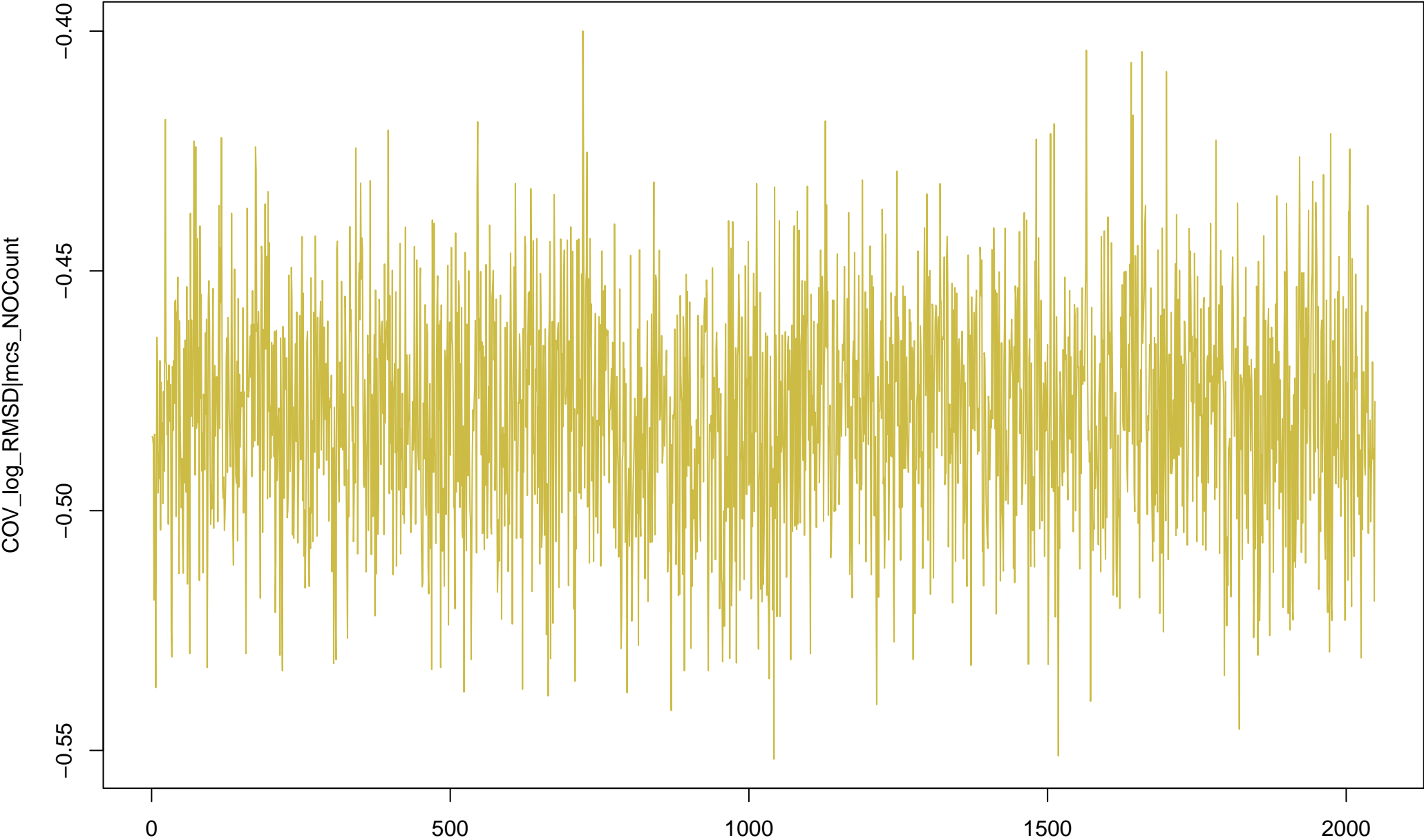
COV_log_RMSD|mcs_RingCount
ESS = 1680 | BMK = 0.0399 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0



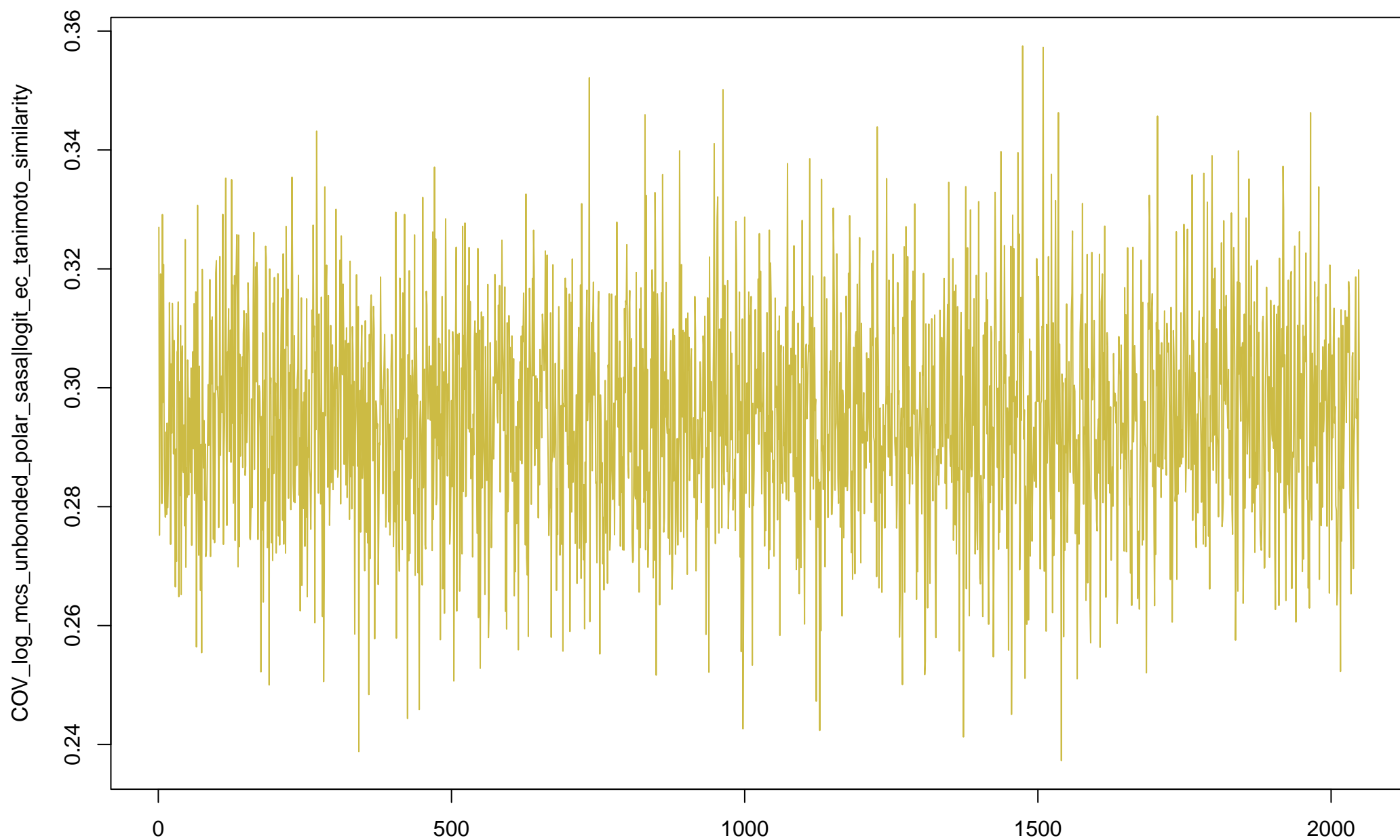
COV_log_RMSD|docked_NumRotatableBonds
ESS = 1640 | BMK = 0.0559 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0



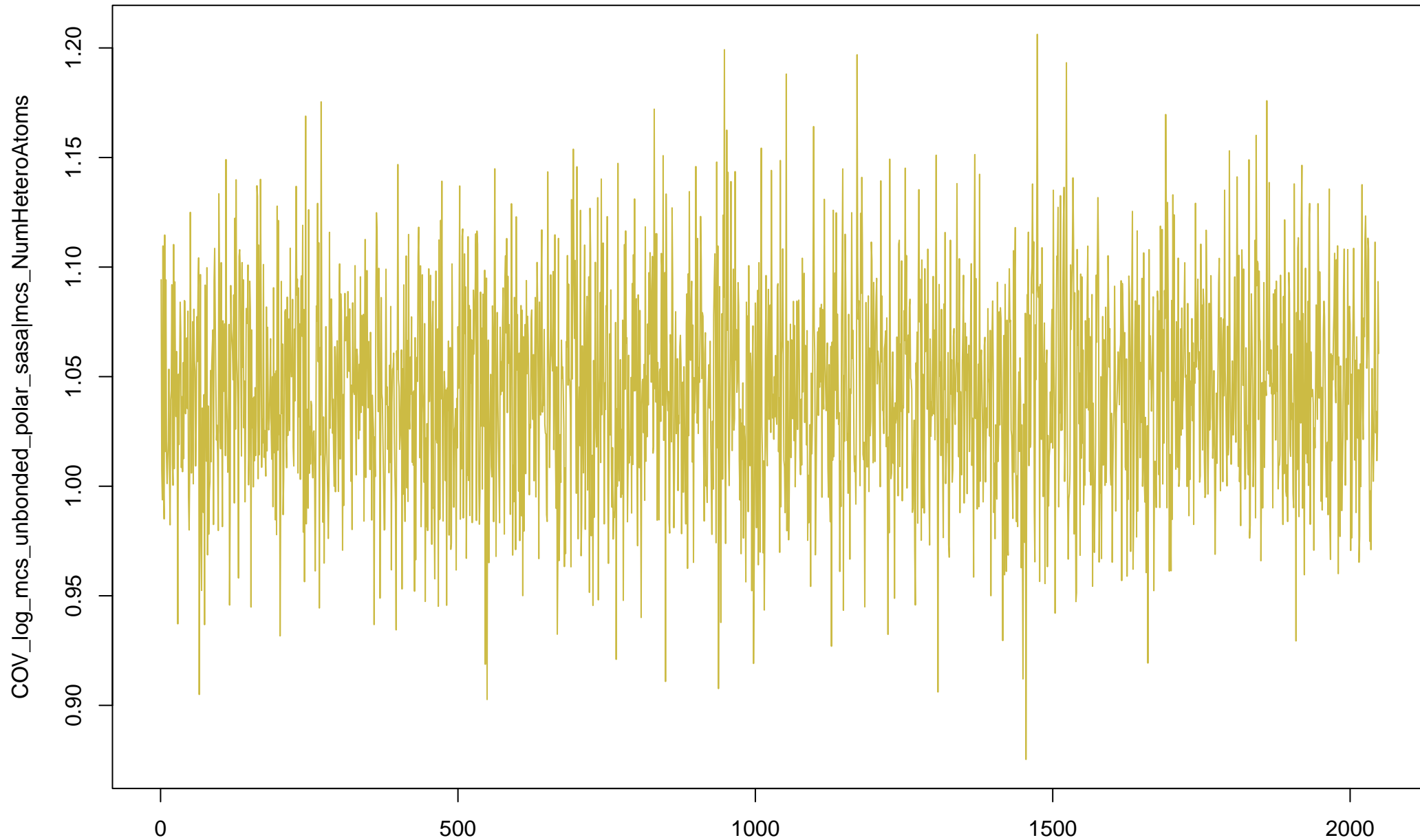
COV_log_RMSD|mcs_NOCount
ESS = 1330 | BMK = 0.0481 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0



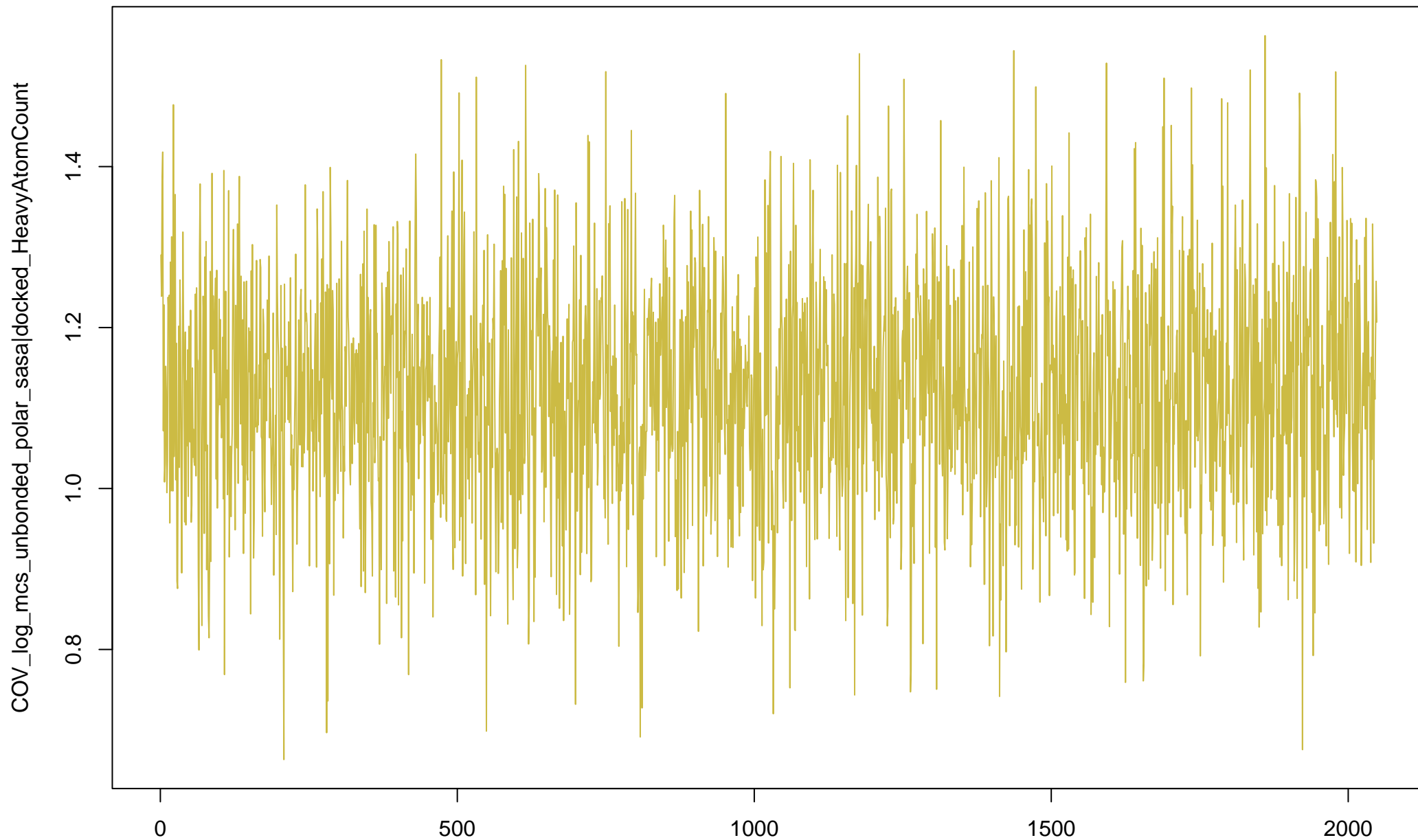
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0434 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



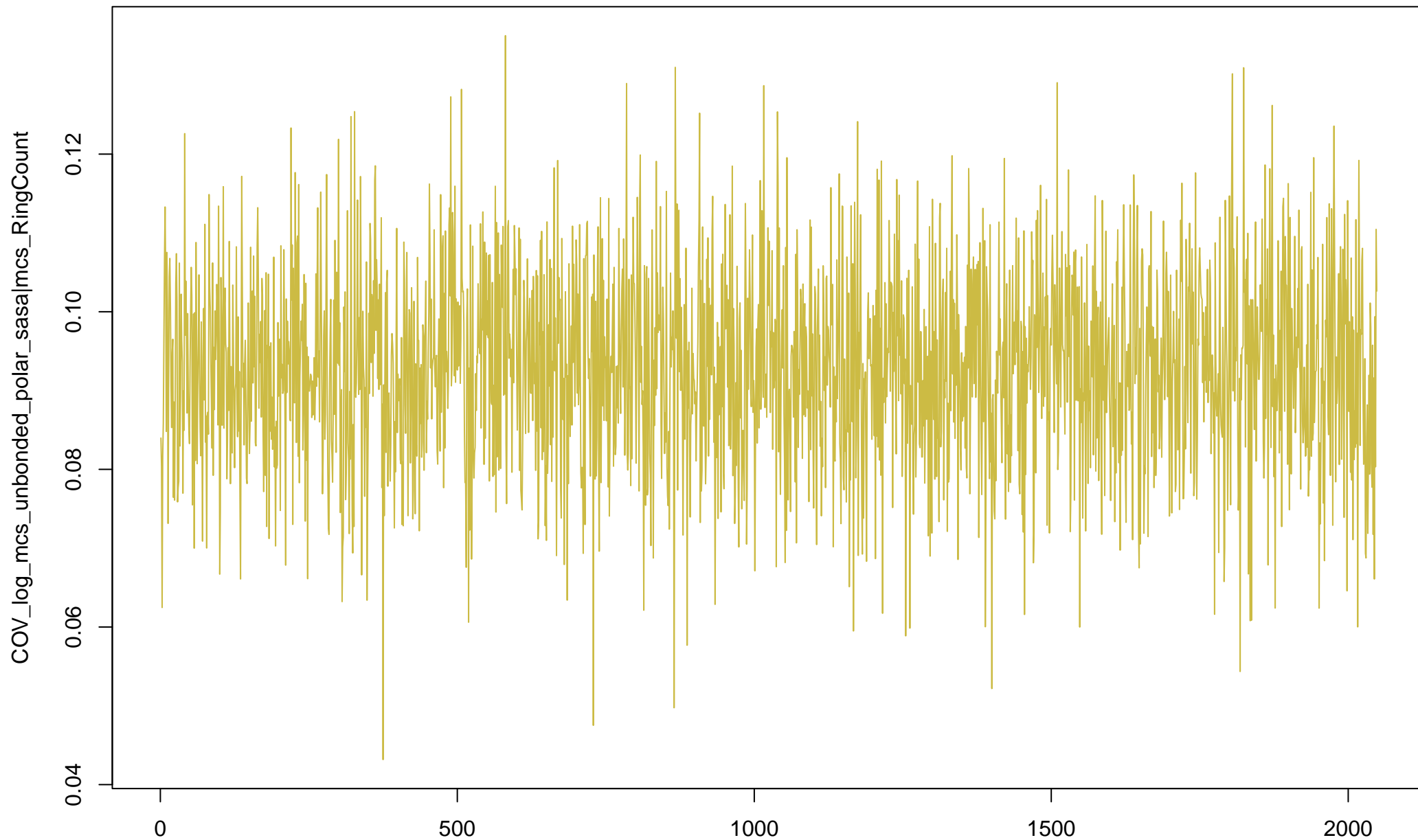
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0353 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0



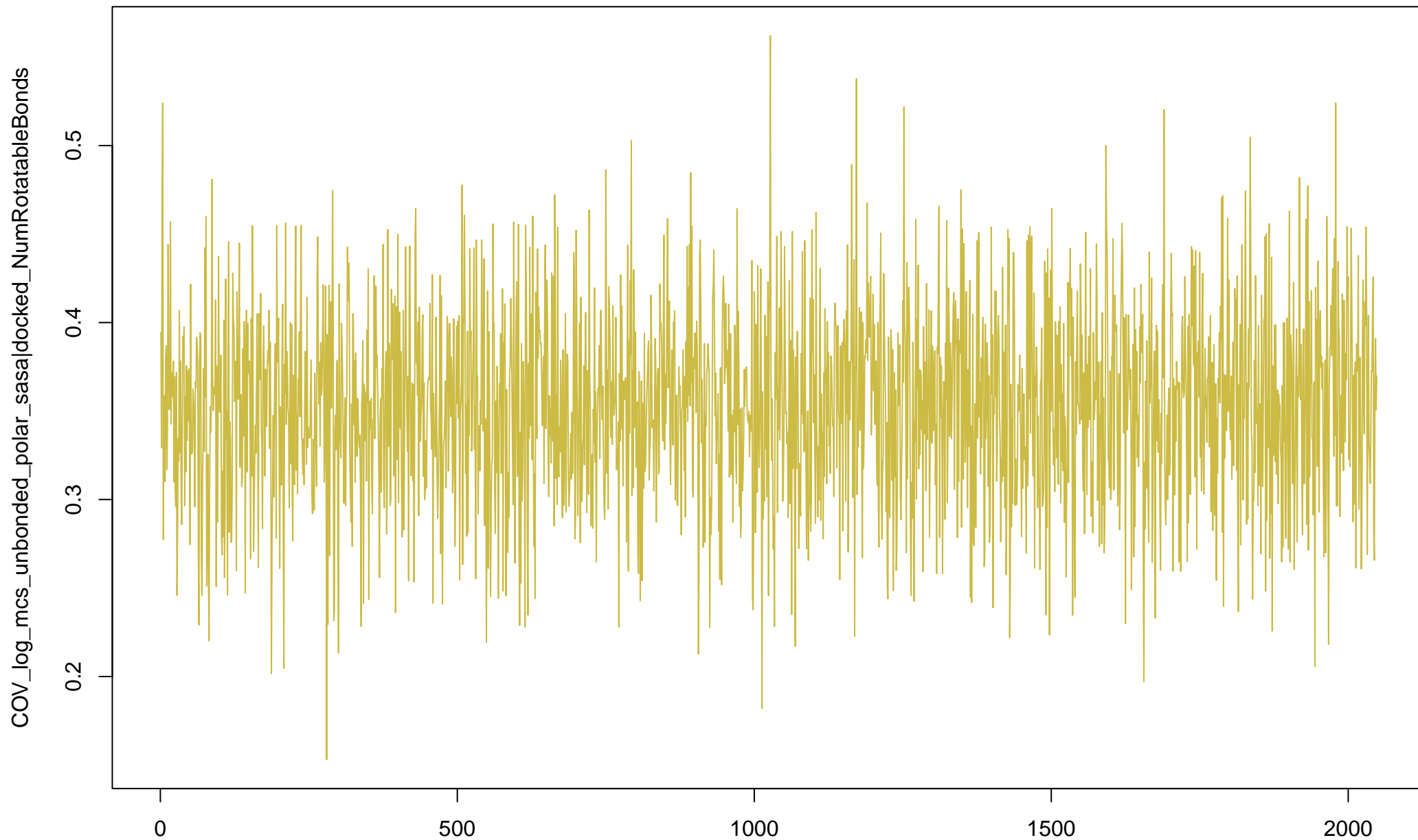
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0471 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0



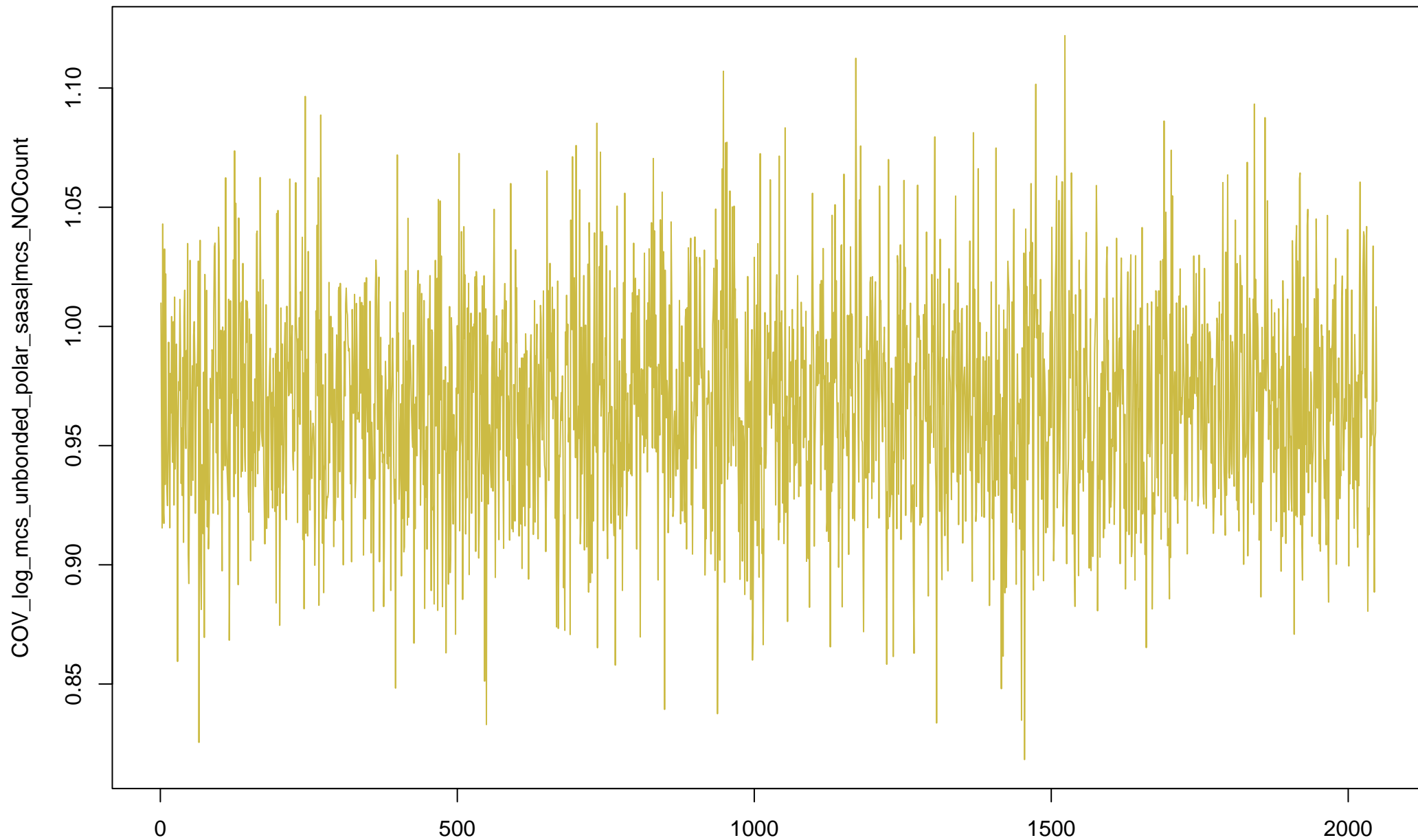
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1900 | BMK = 0.0428 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0



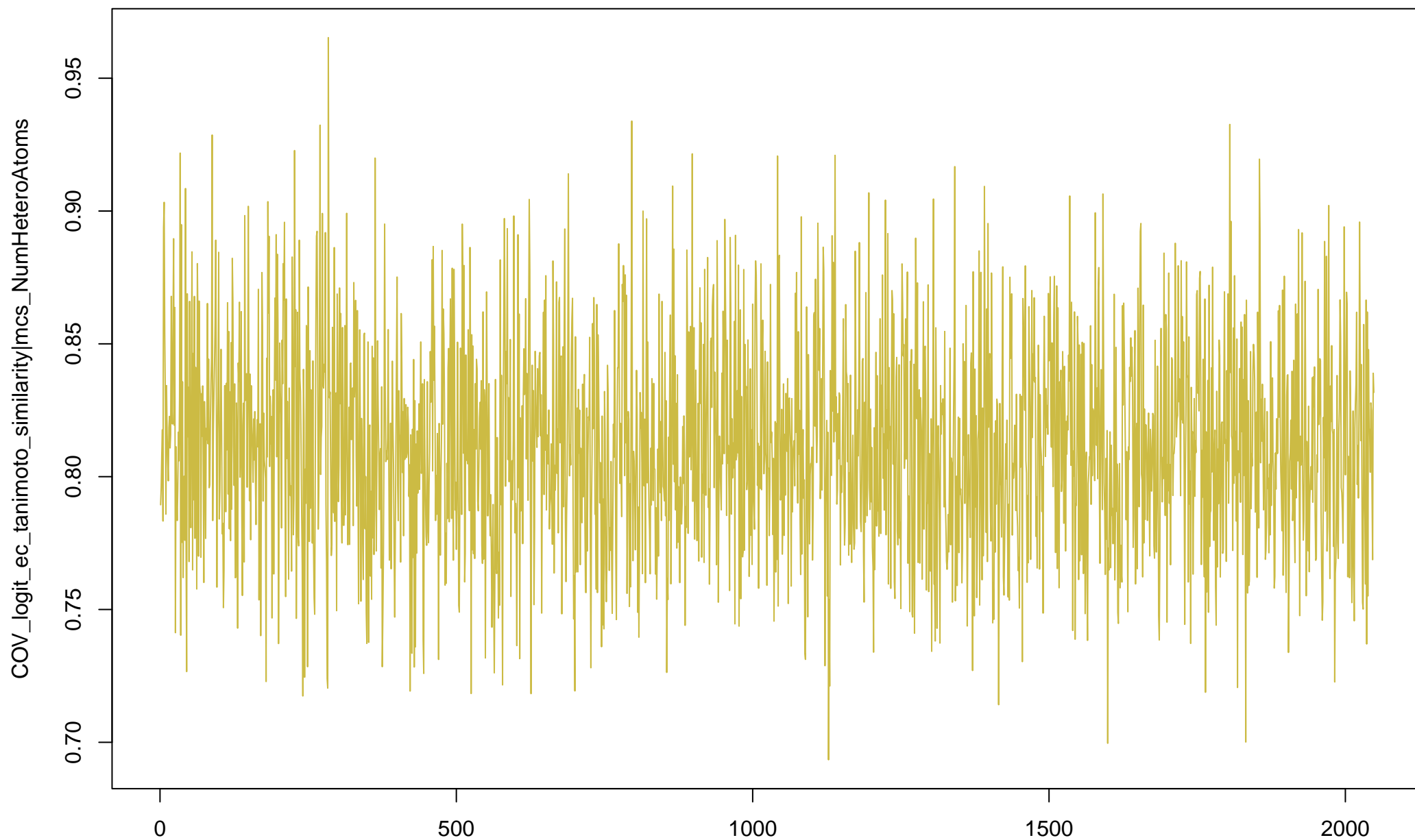
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0609 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0



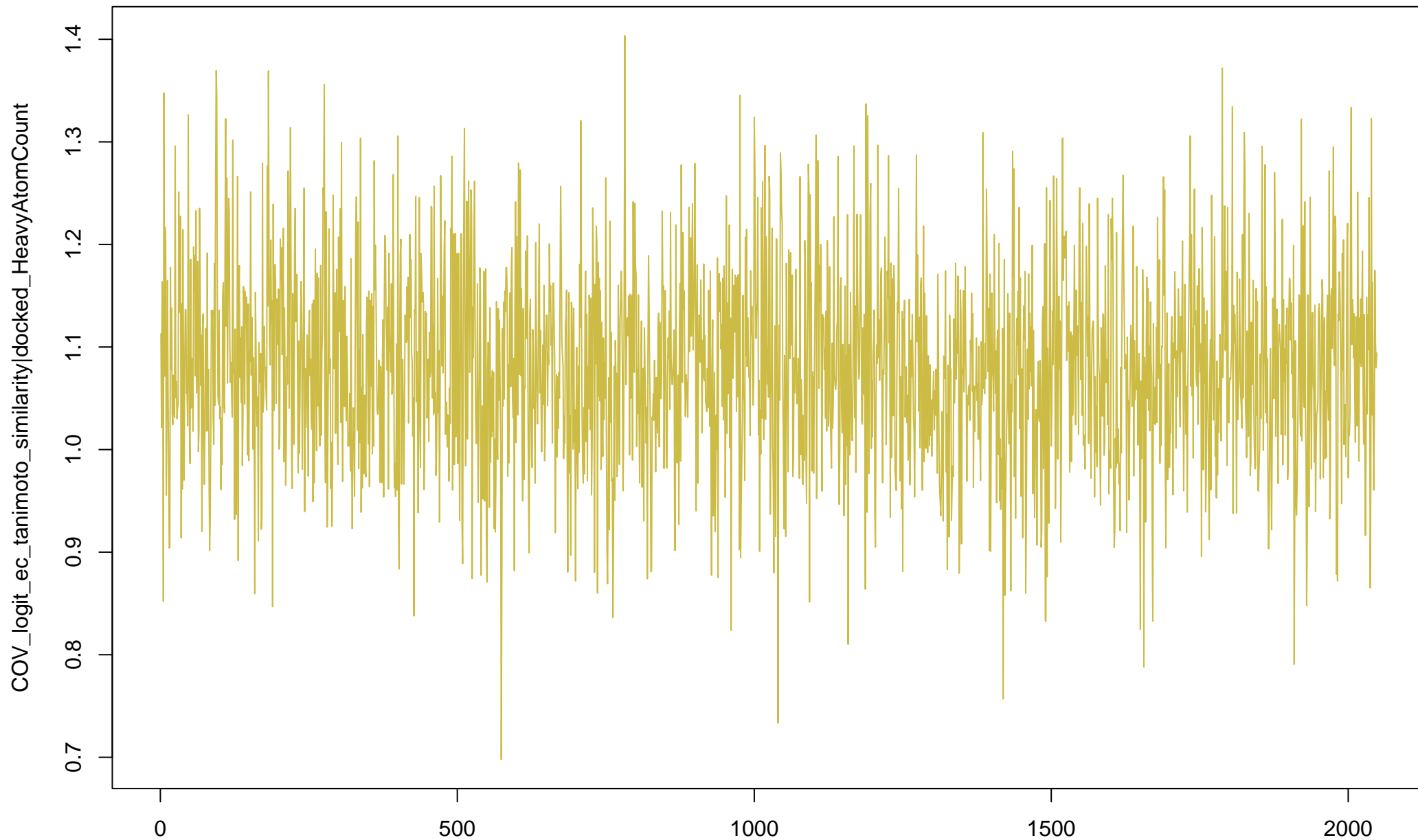
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 2050 | BMK = 0.0386 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0



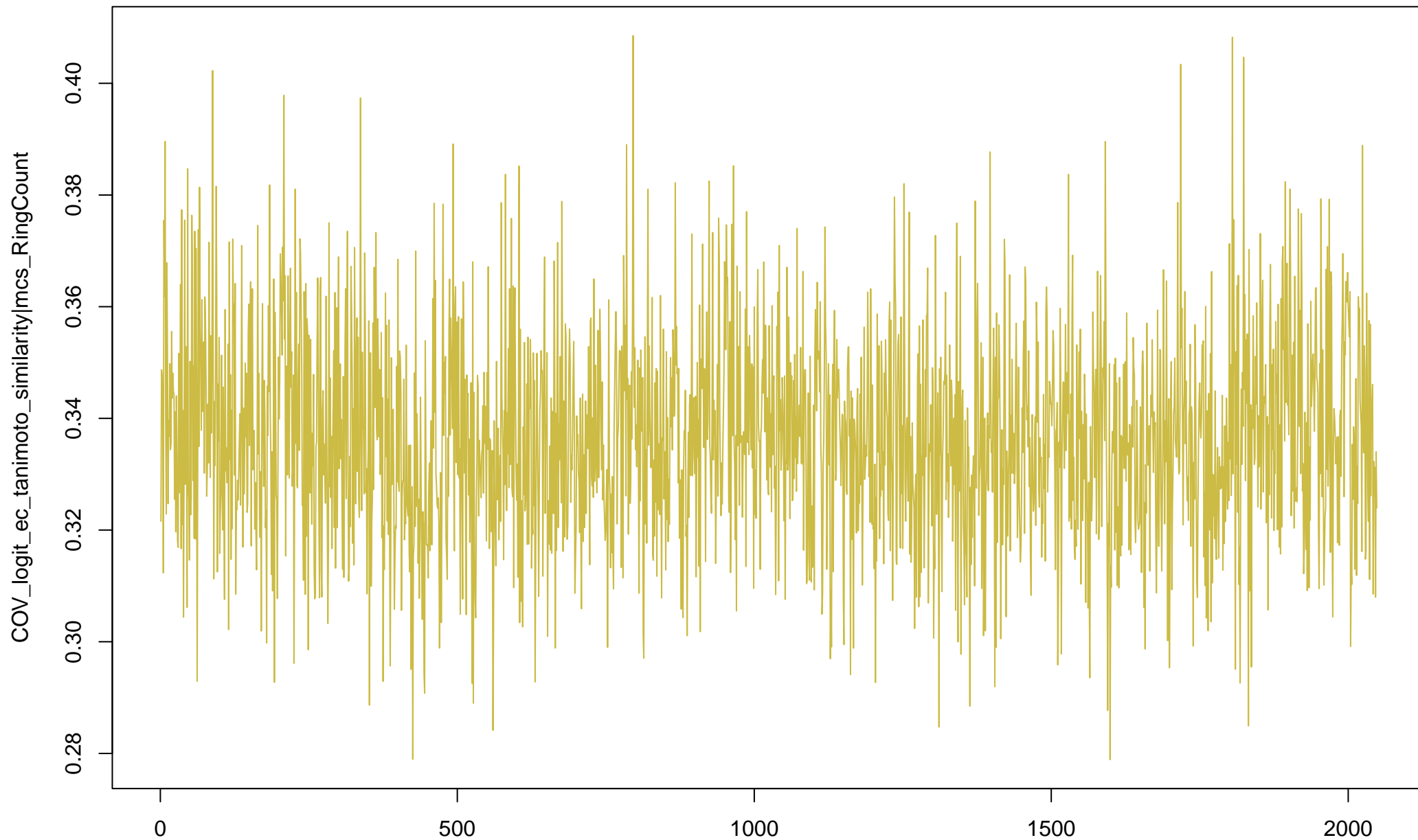
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1860 | BMK = 0.0478 | MCSE(6.27) = 2.46 | stat: FALSE | burn: 0



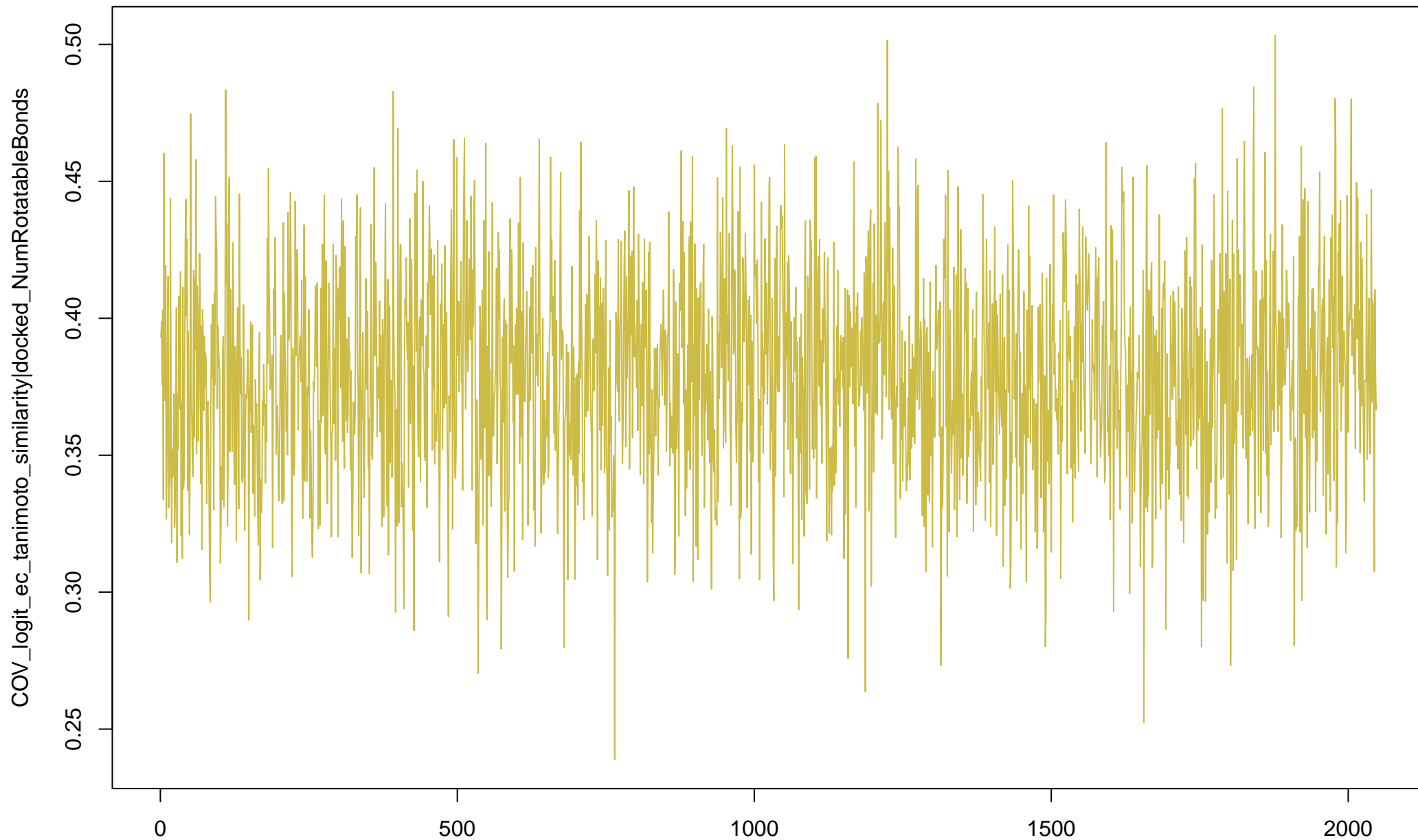
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1690 | BMK = 0.0534 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0



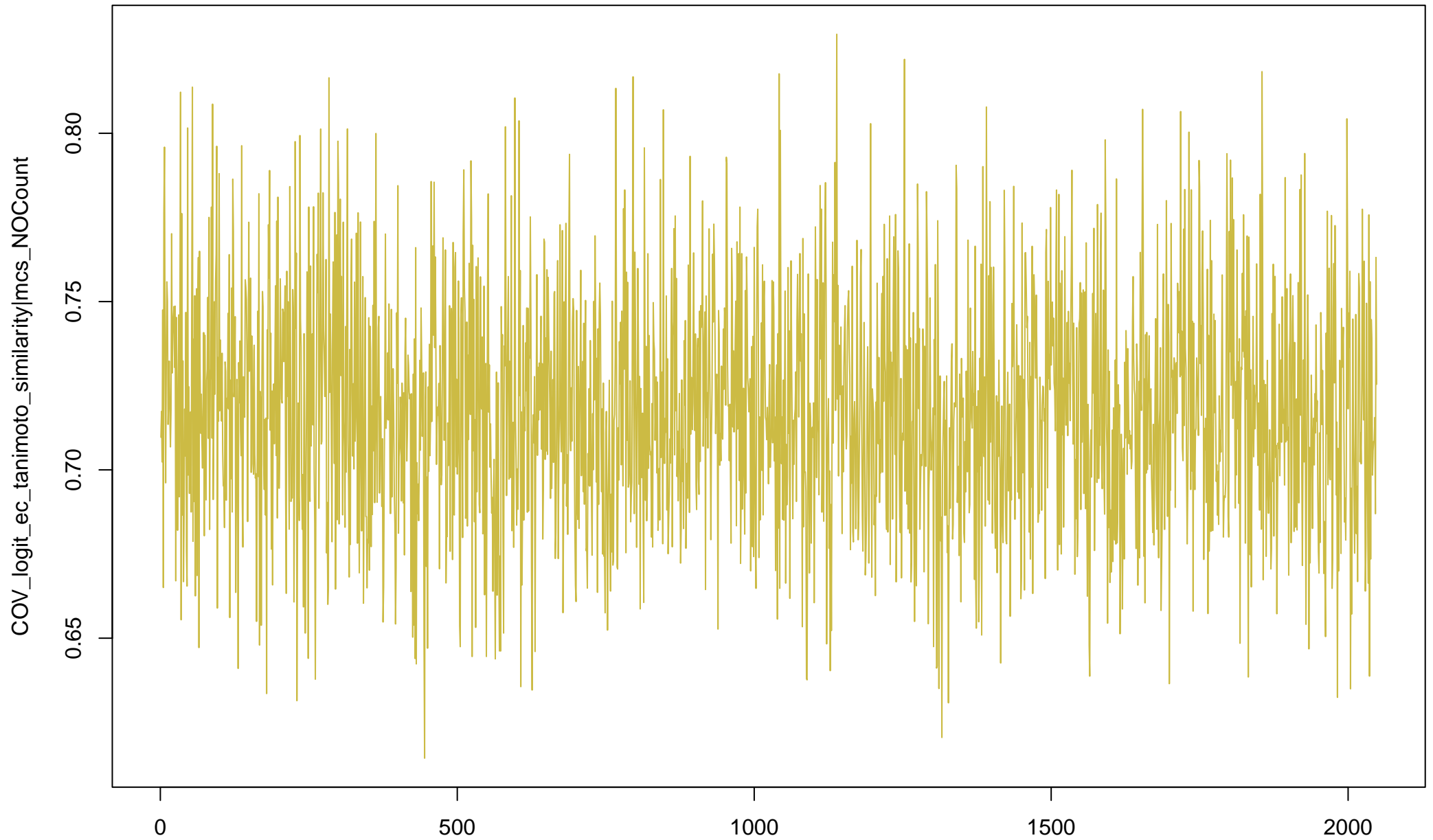
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1090 | BMK = 0.0485 | MCSE(6.27) = 3.08 | stat: FALSE | burn: 0



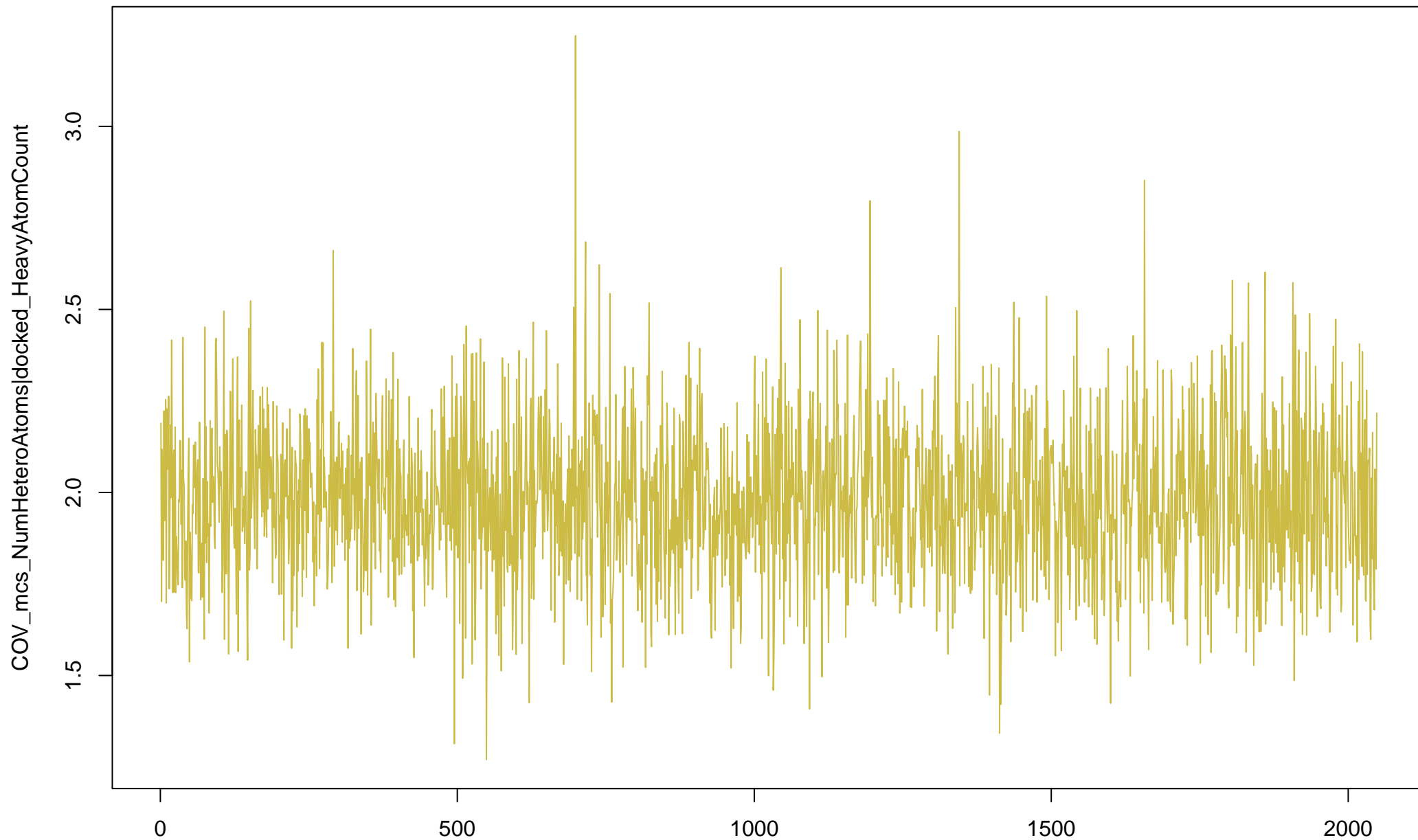
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1460 | BMK = 0.0408 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0



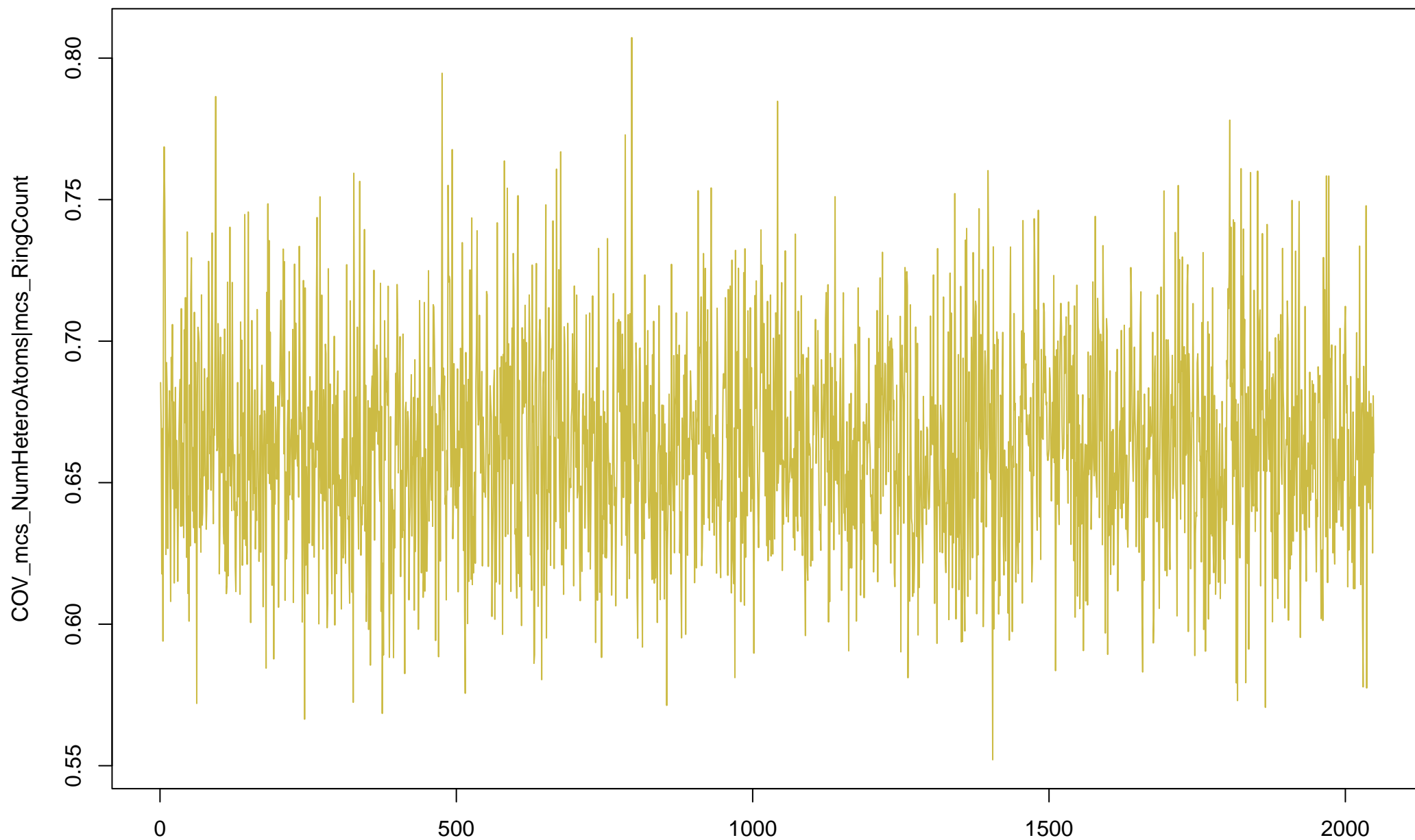
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1590 | BMK = 0.0381 | MCSE(6.27) = 2.46 | stat: FALSE | burn: 0



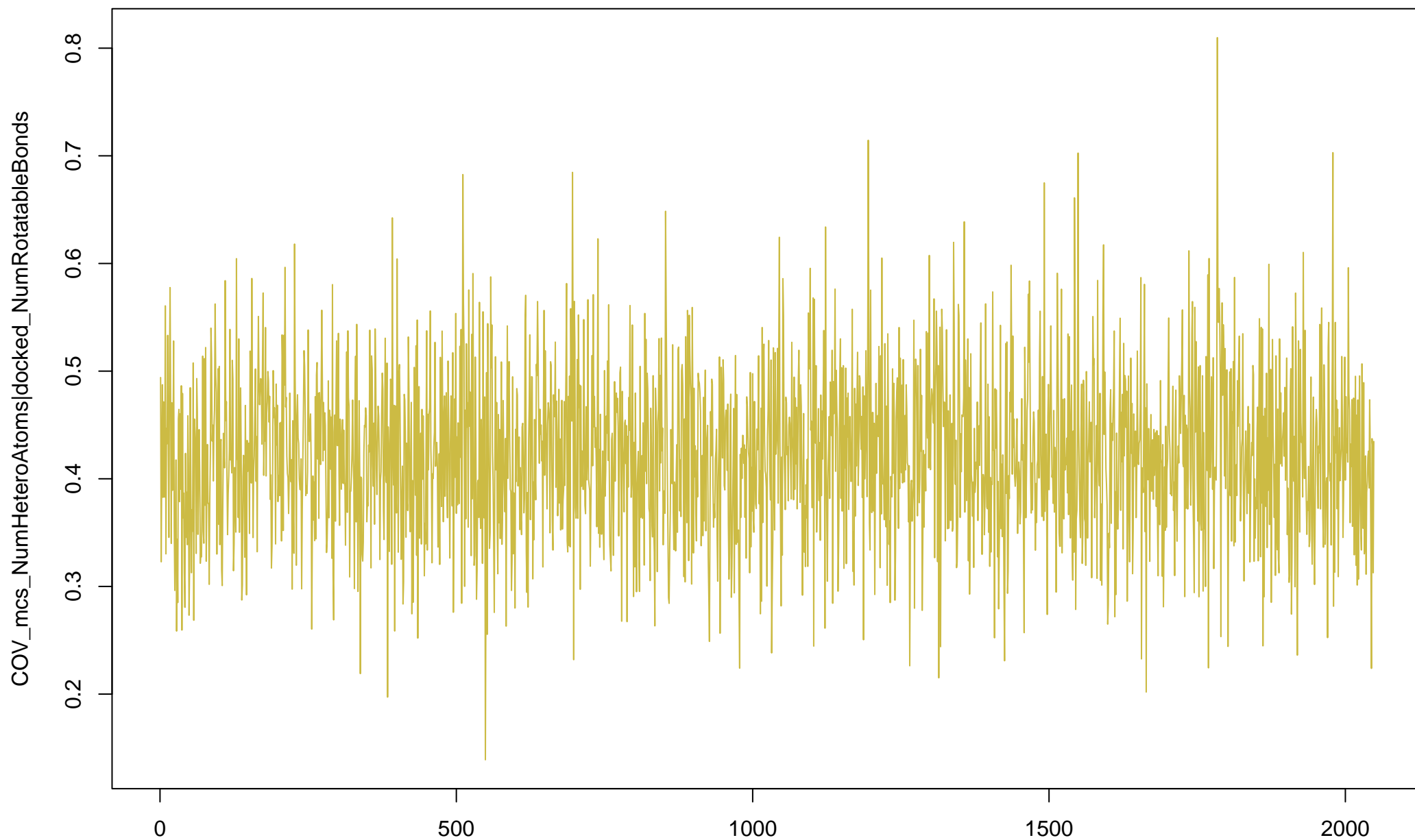
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0597 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0



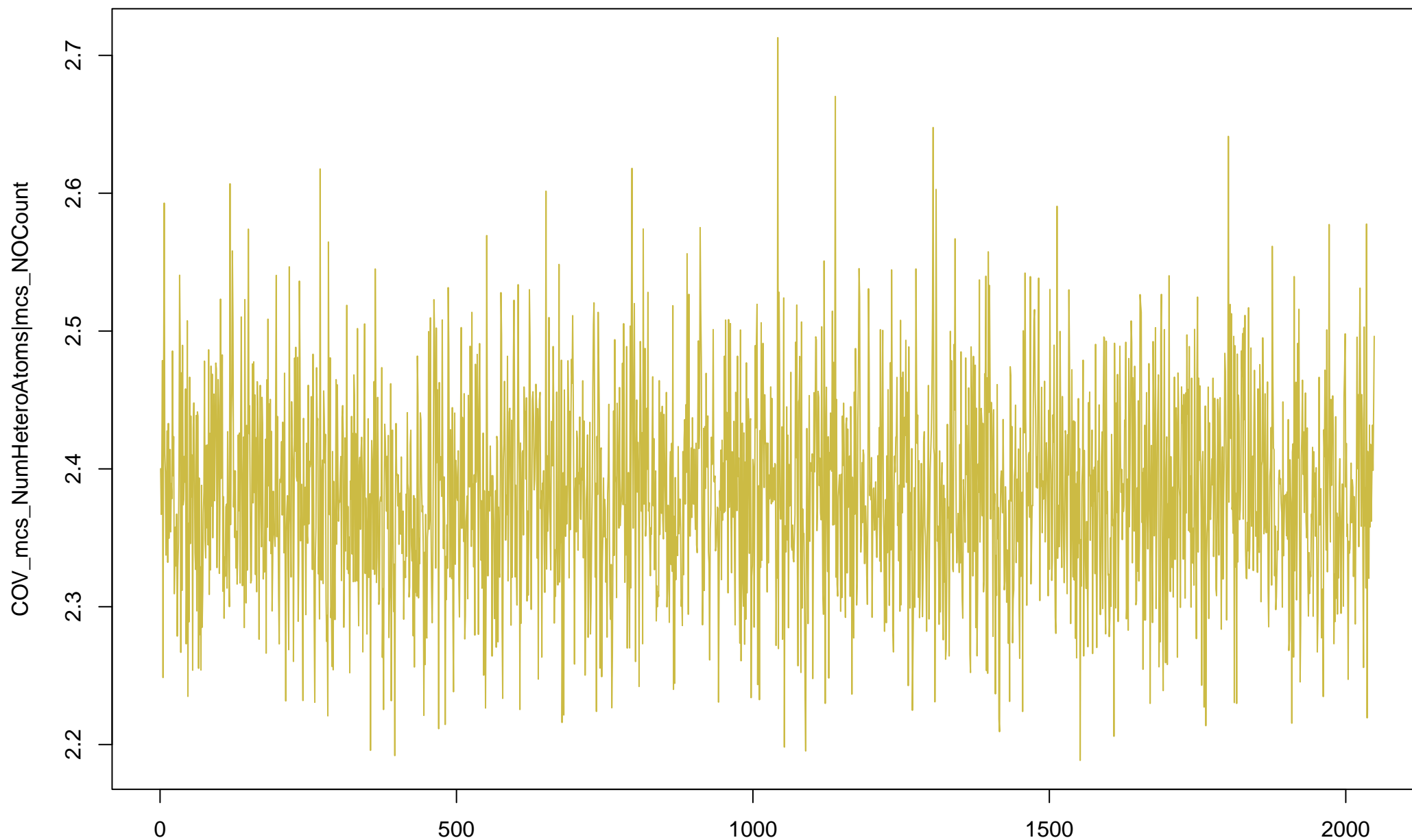
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 2050 | BMK = 0.0292 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0



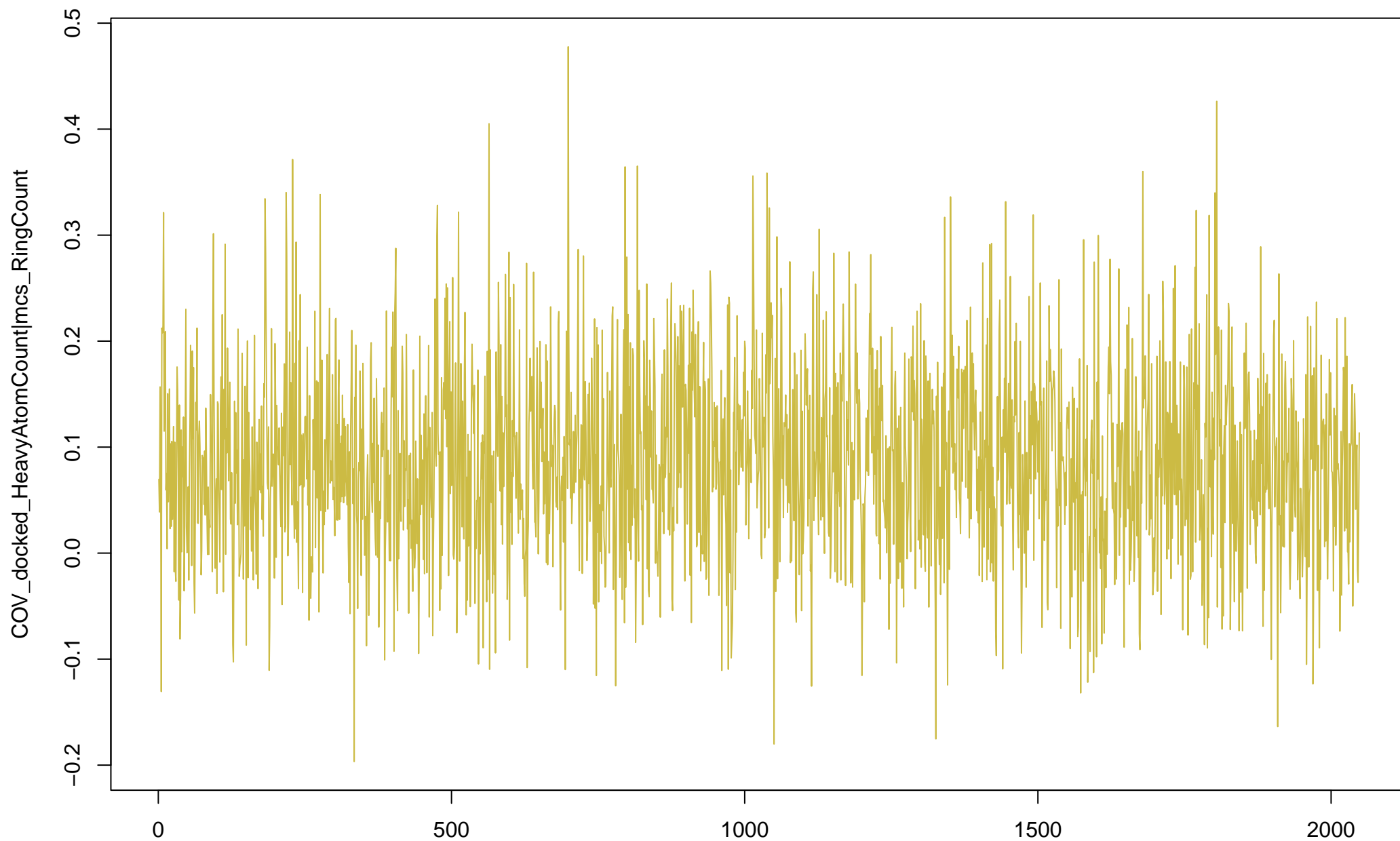
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0519 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0



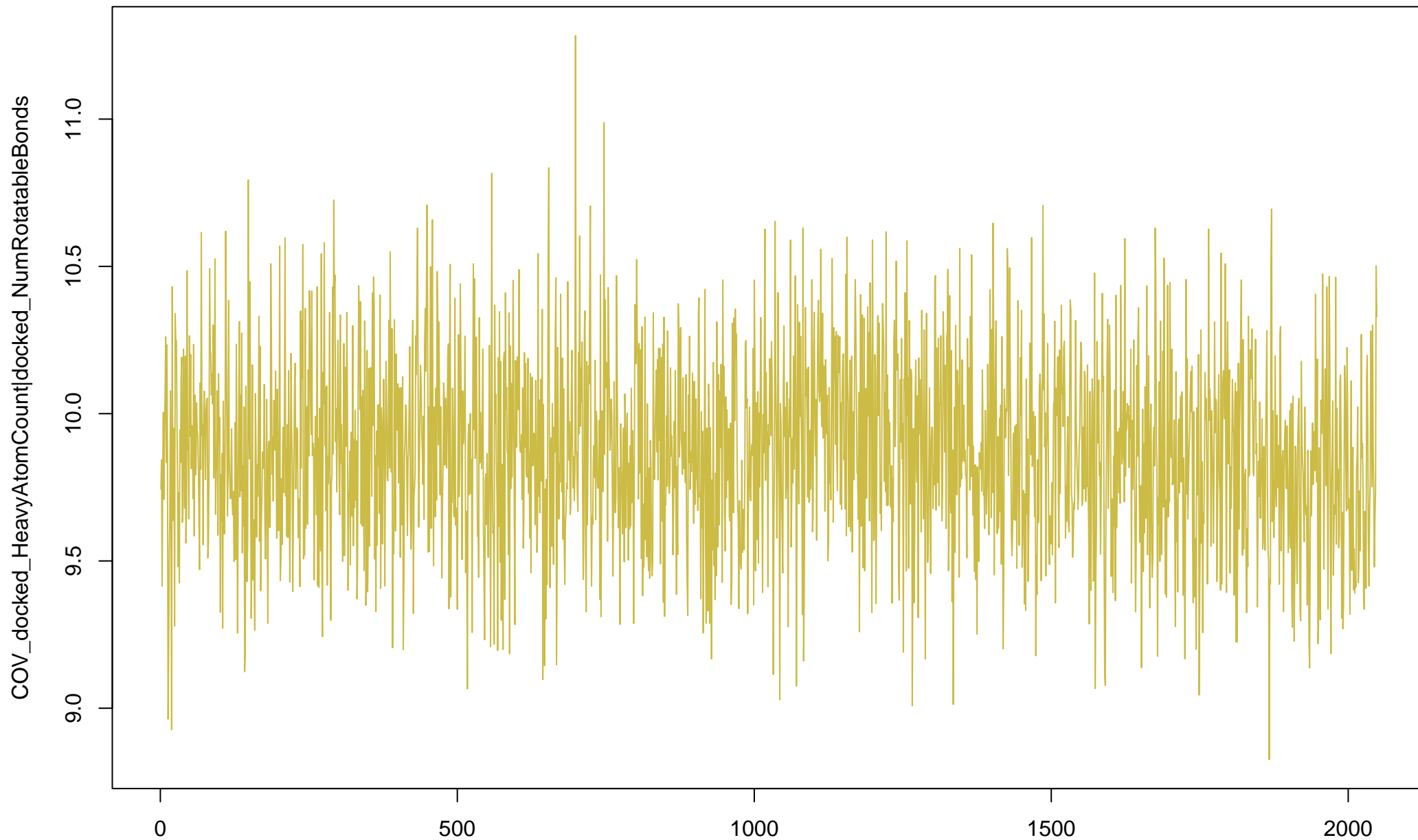
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 2050 | BMK = 0.0422 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0



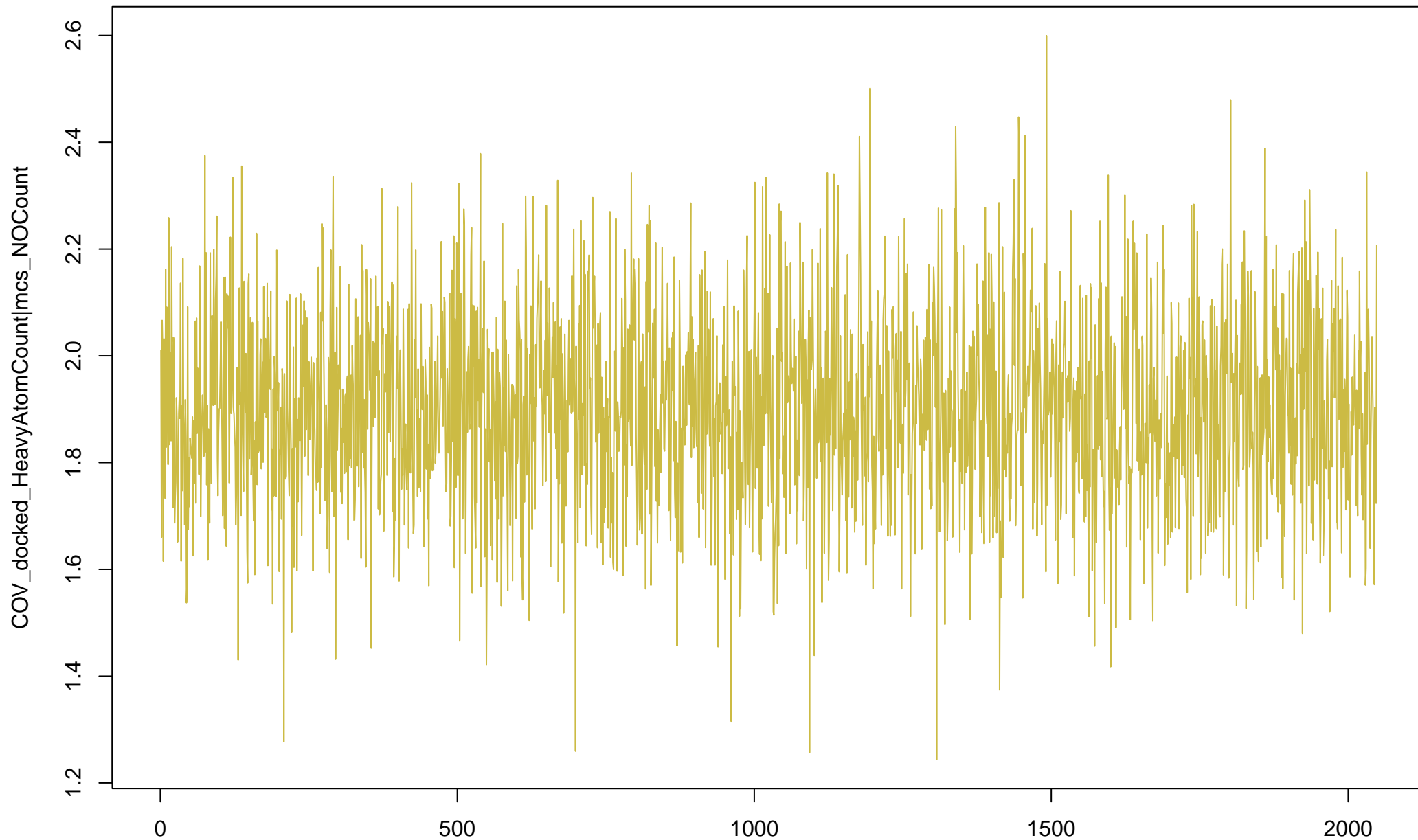
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1660 | BMK = 0.0462 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0



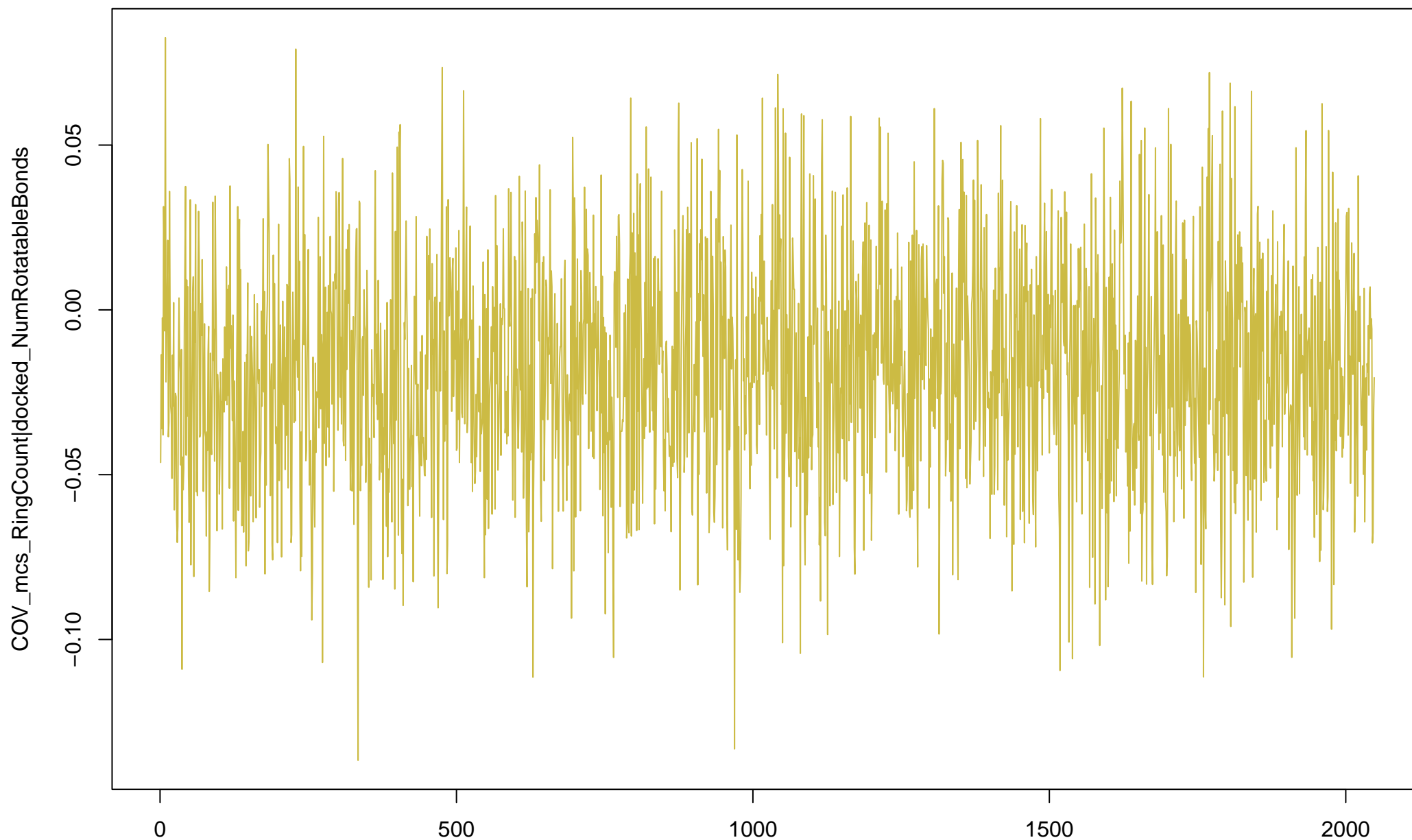
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1780 | BMK = 0.0449 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0



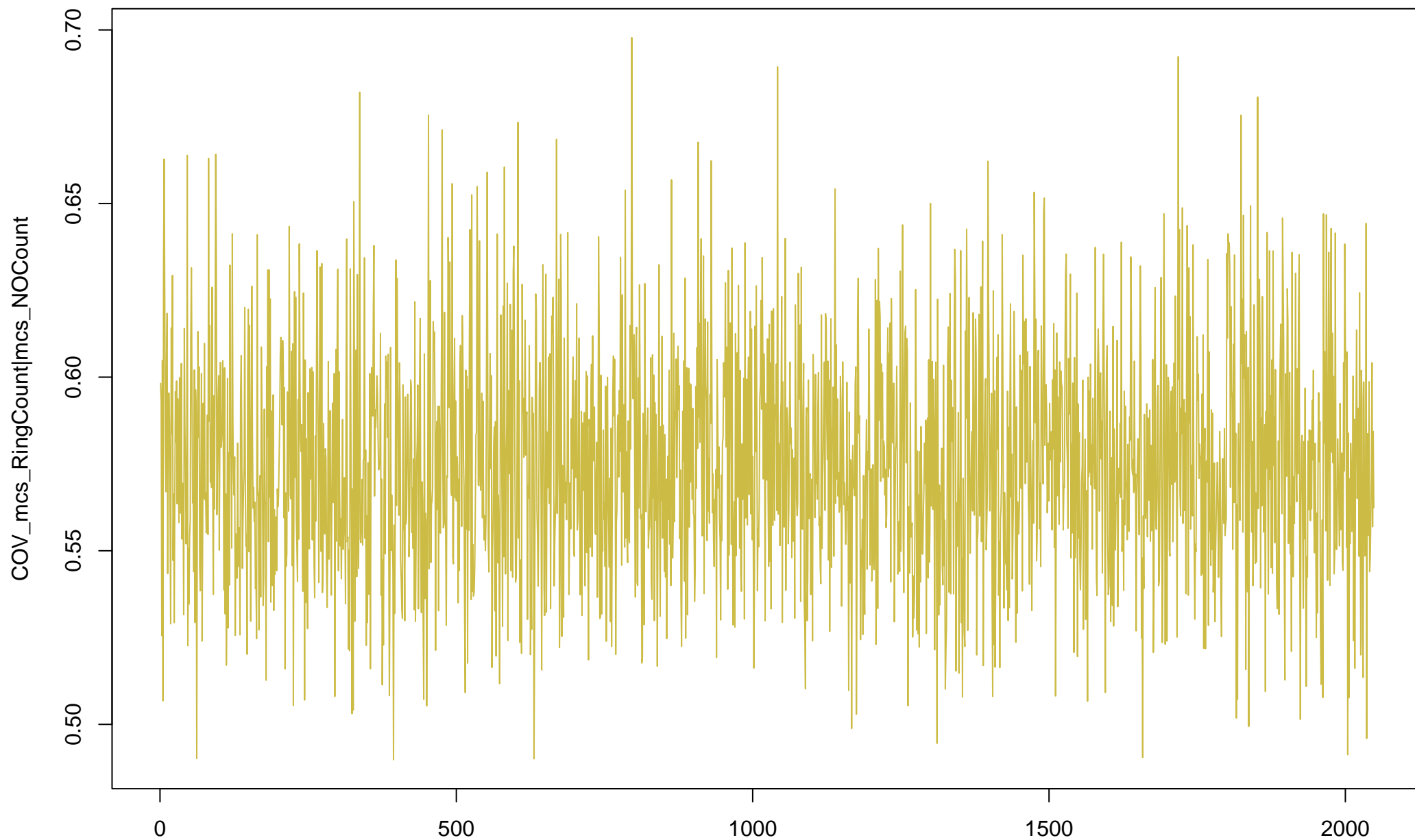
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 2050 | BMK = 0.0495 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1580 | BMK = 0.0526 | MCSE(6.27) = 2.58 | stat: FALSE | burn: 0



COV_mcs_RingCount|mcs_NOCount
ESS = 2050 | BMK = 0.0502 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 2050 | BMK = 0.0521 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0

