

-- STATS maxD --

min ESS = 44.1460633638607

max BMK = 0.245881763141674

max MCSE = 14.1936653187289

all stationary: FALSE

burn: 408

-- STATS 2D --

min ESS = 1042.60559396034

max BMK = 0.0843923464581062

max MCSE = 3.18498782866714

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 127.064285634222

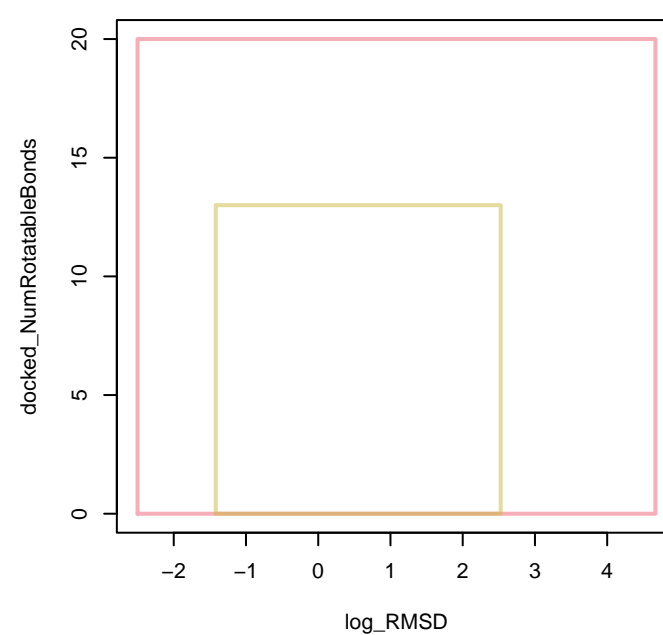
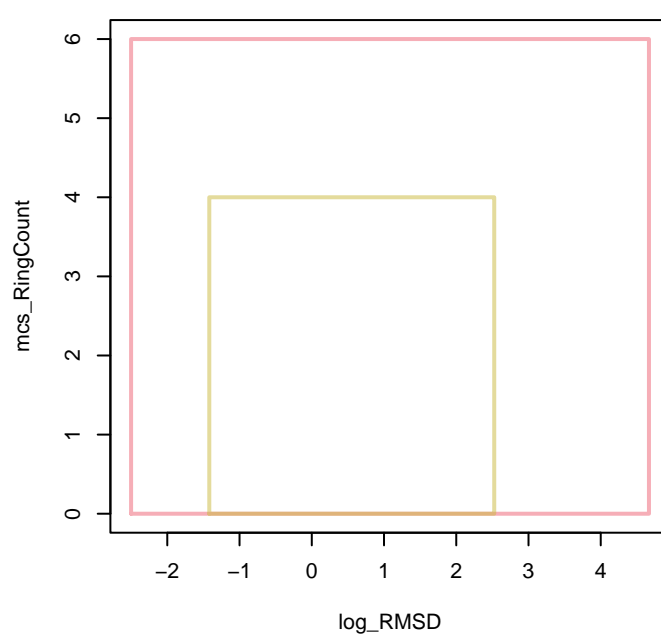
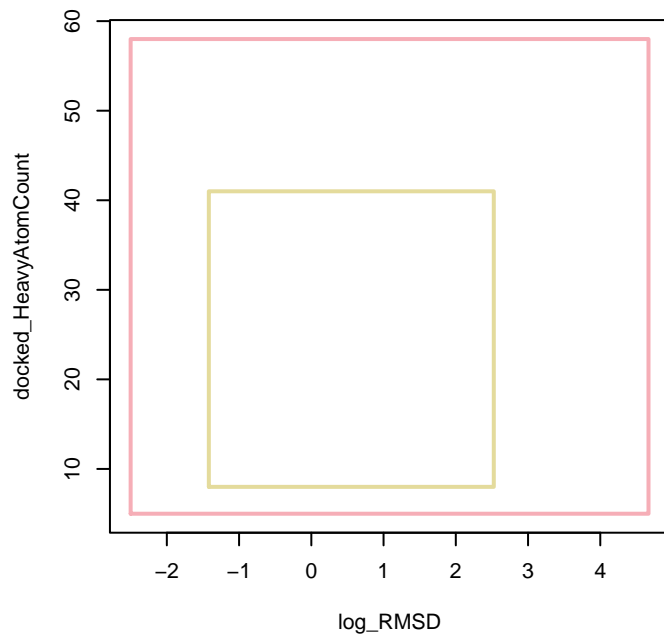
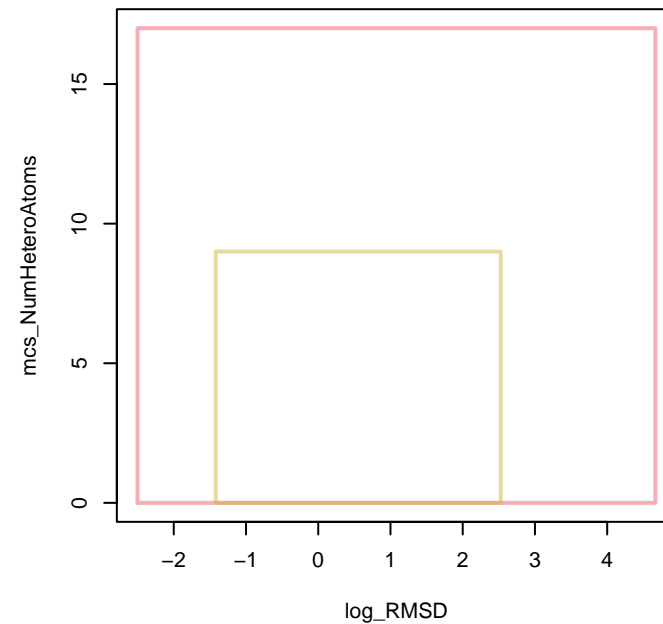
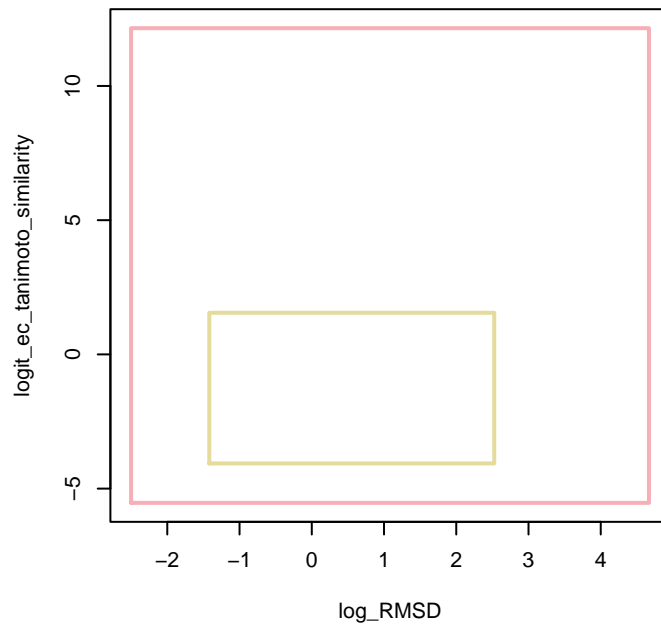
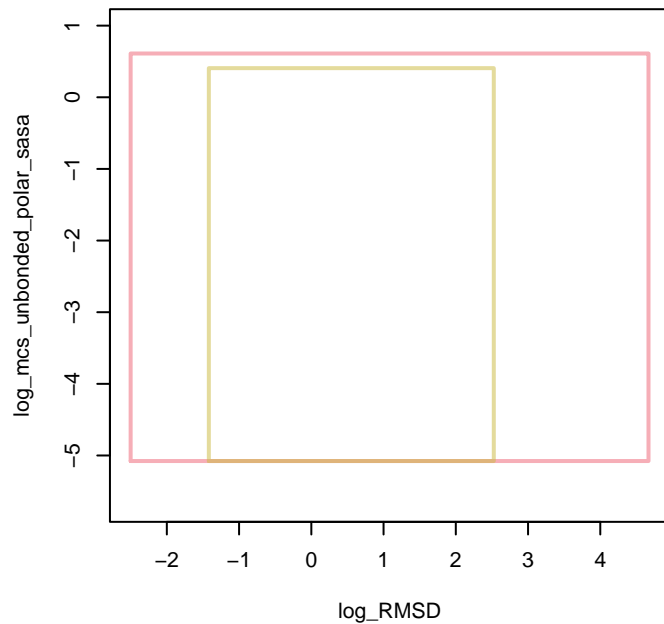
max BMK = 0.121403731829434

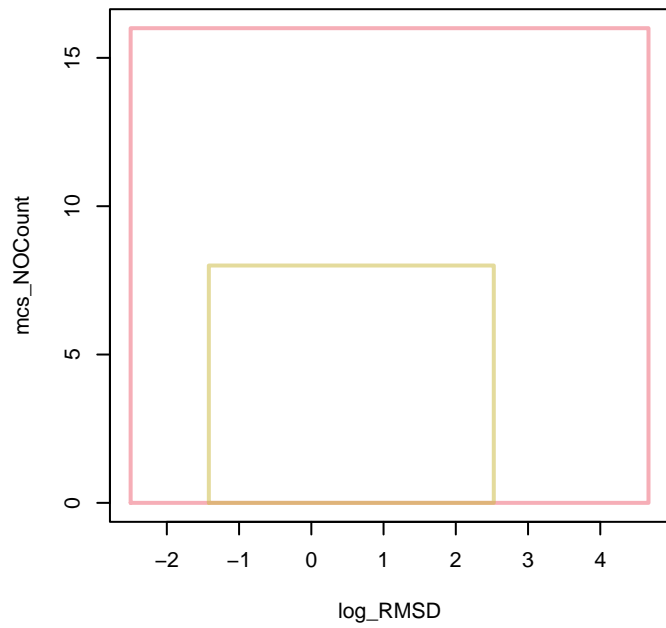
max MCSE = 3.40016247040453

all stationary: FALSE

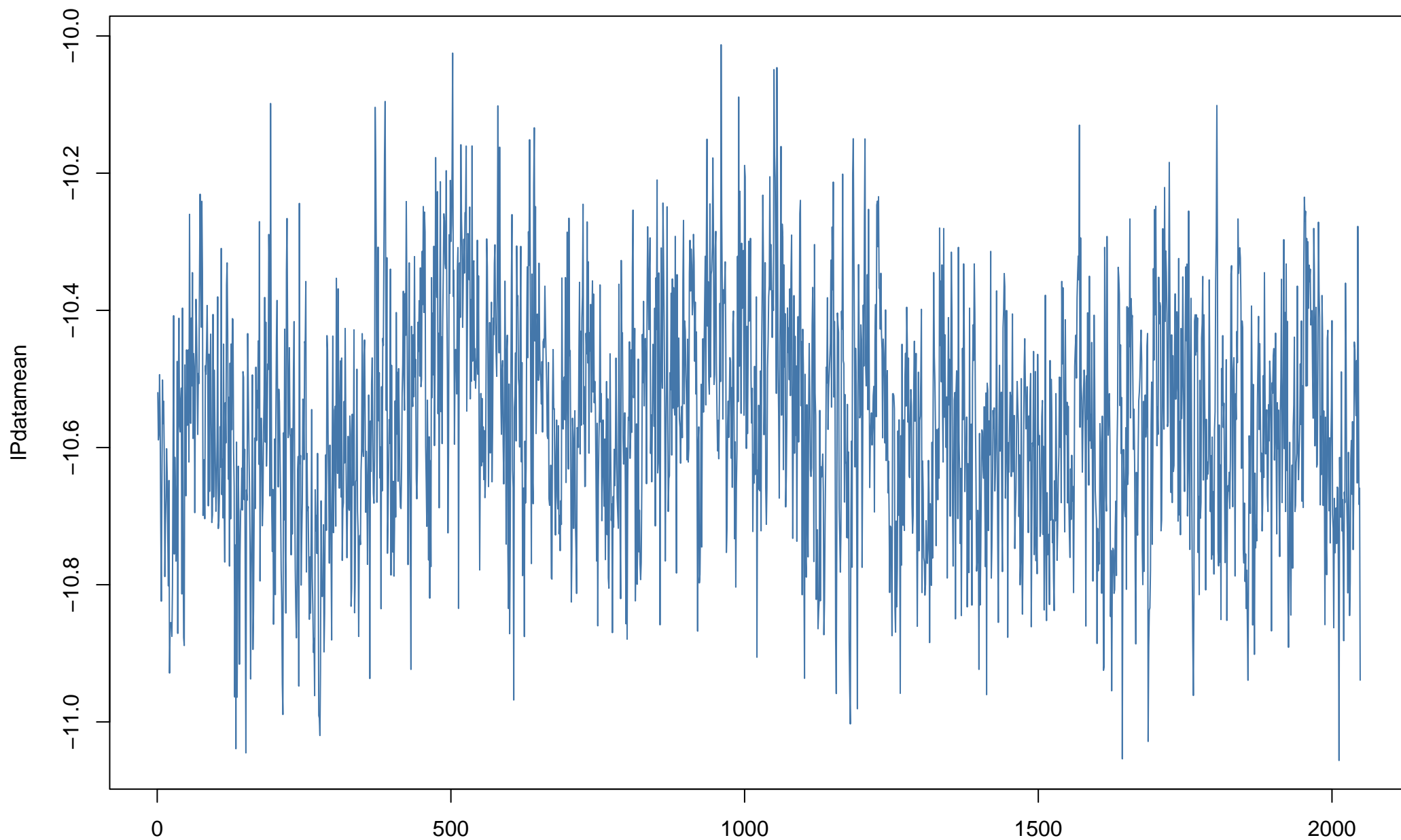
burn: 0

Occupied clusters: 20 of 64

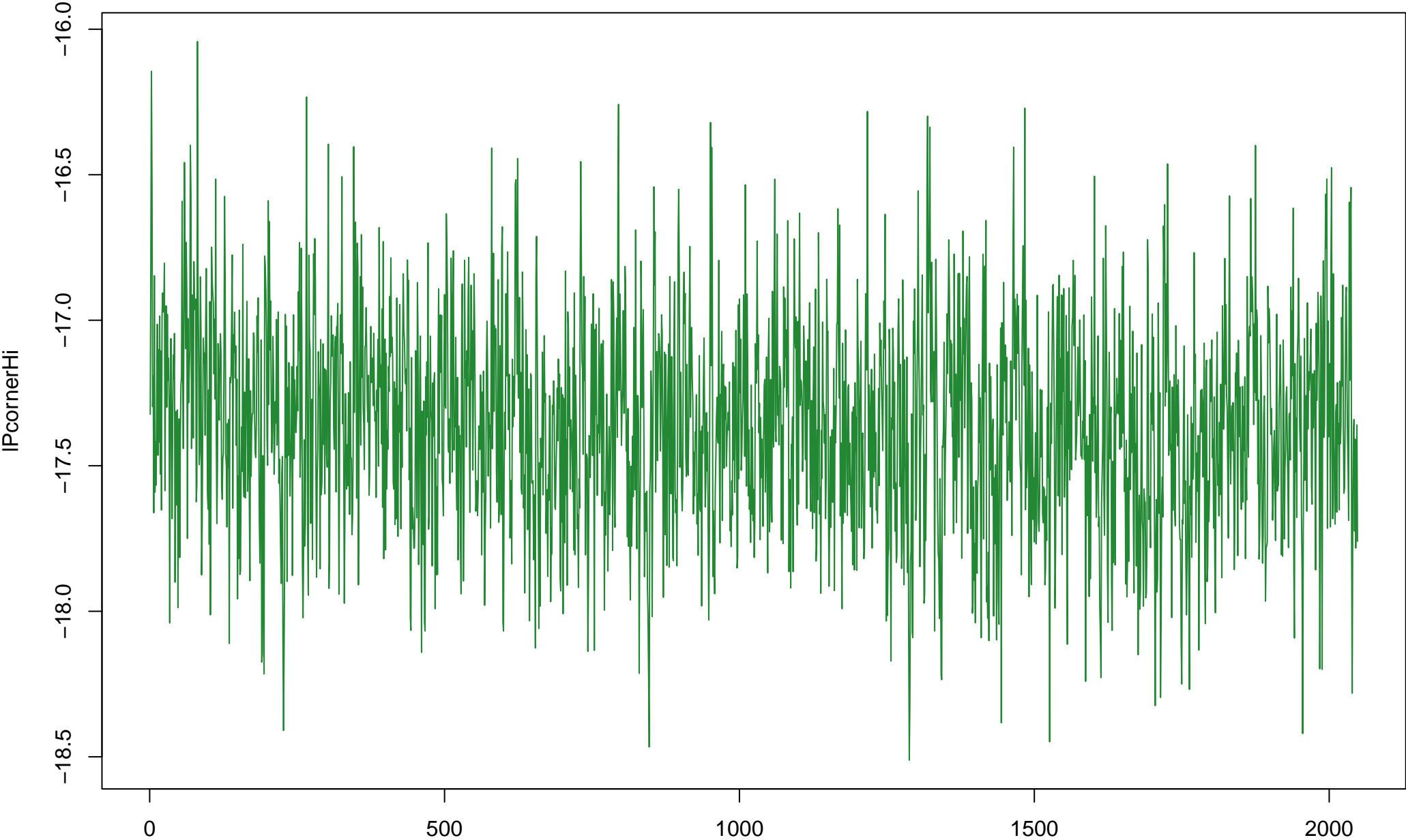




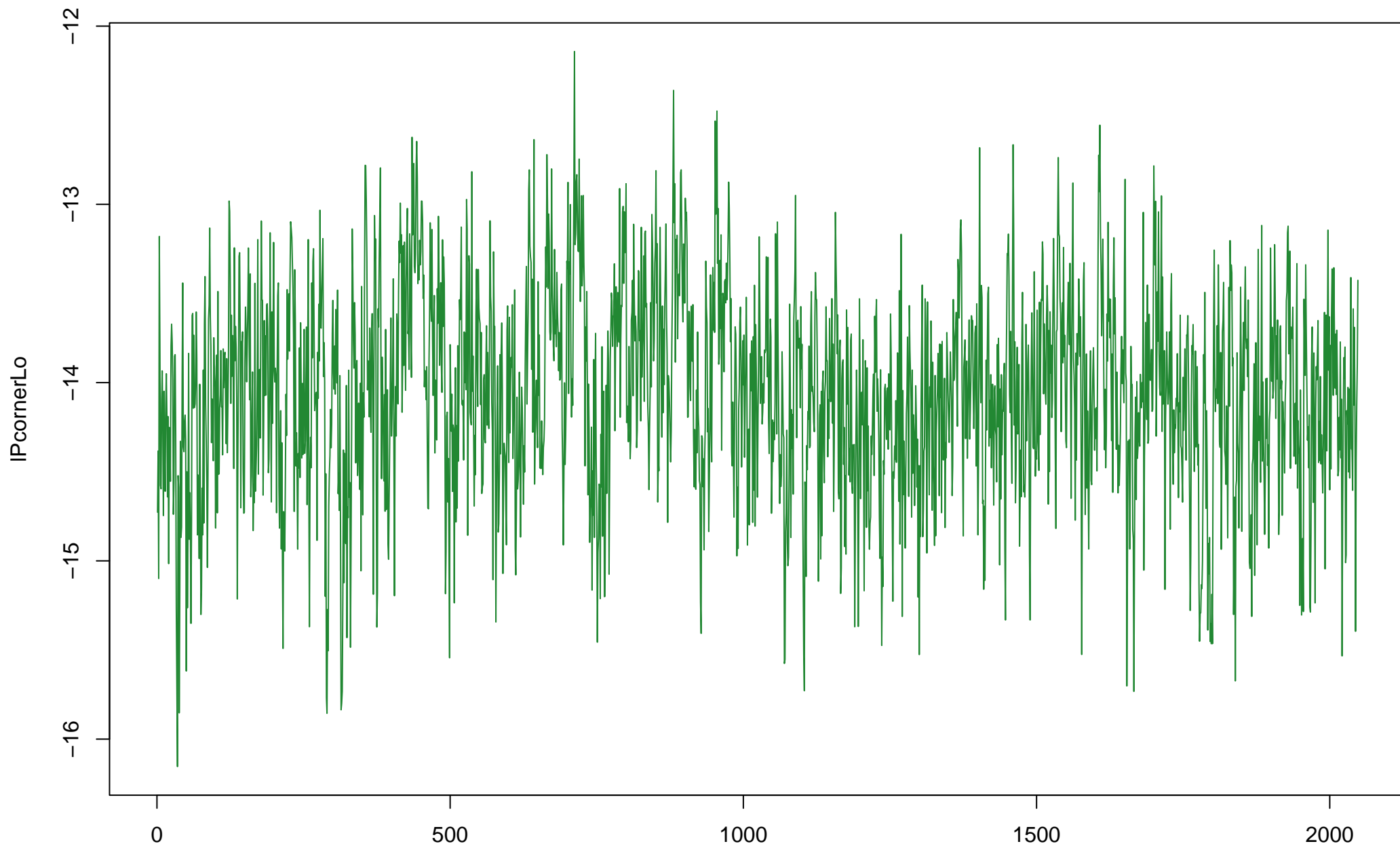
IPdatamean
ESS = 259 | BMK = 0.0636 | MCSE(6.27) = 6.5 | stat: TRUE | burn: 0



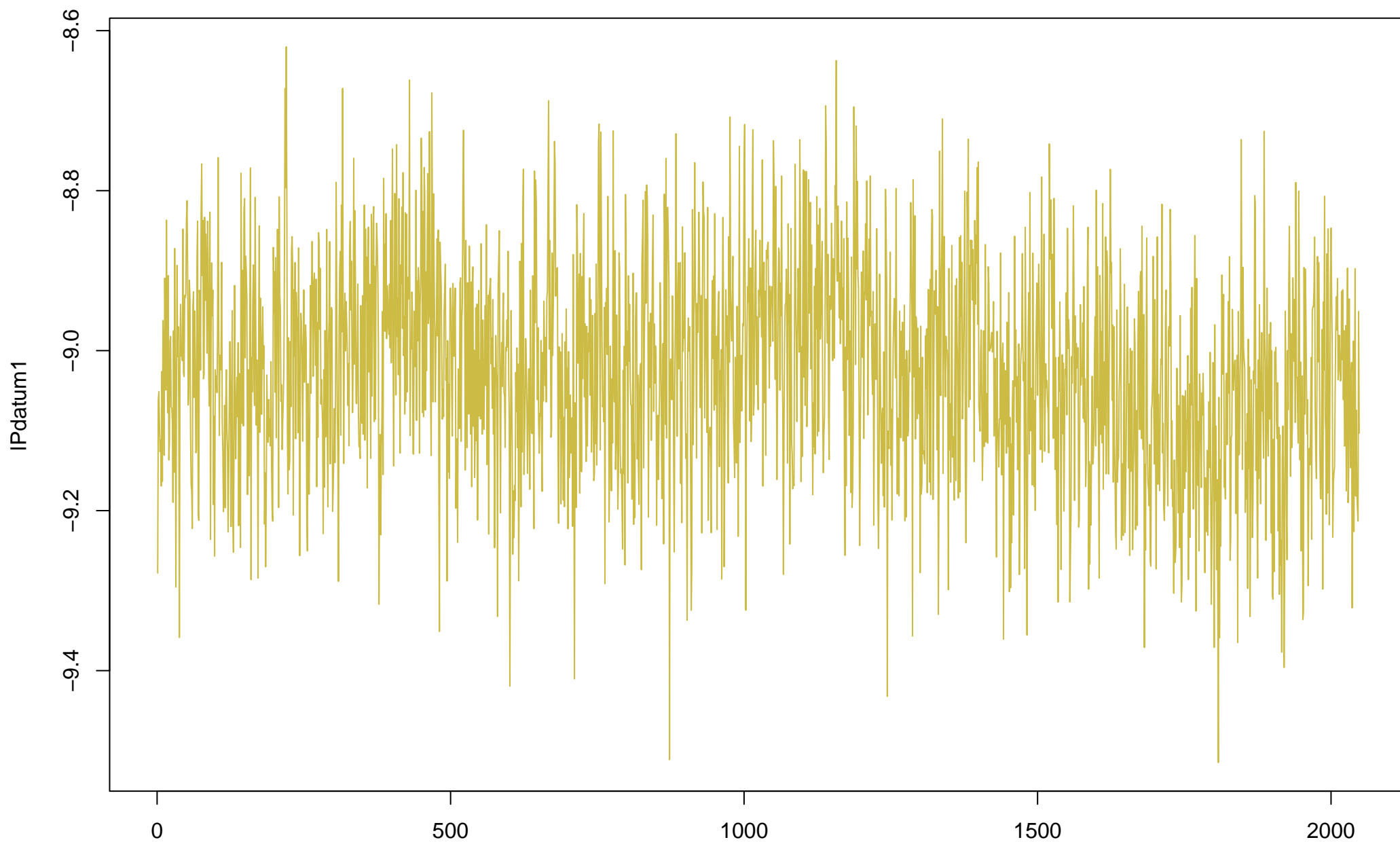
IPcornerHi
ESS = 922 | BMK = 0.062 | MCSE(6.27) = 4.26 | stat: FALSE | burn: 0



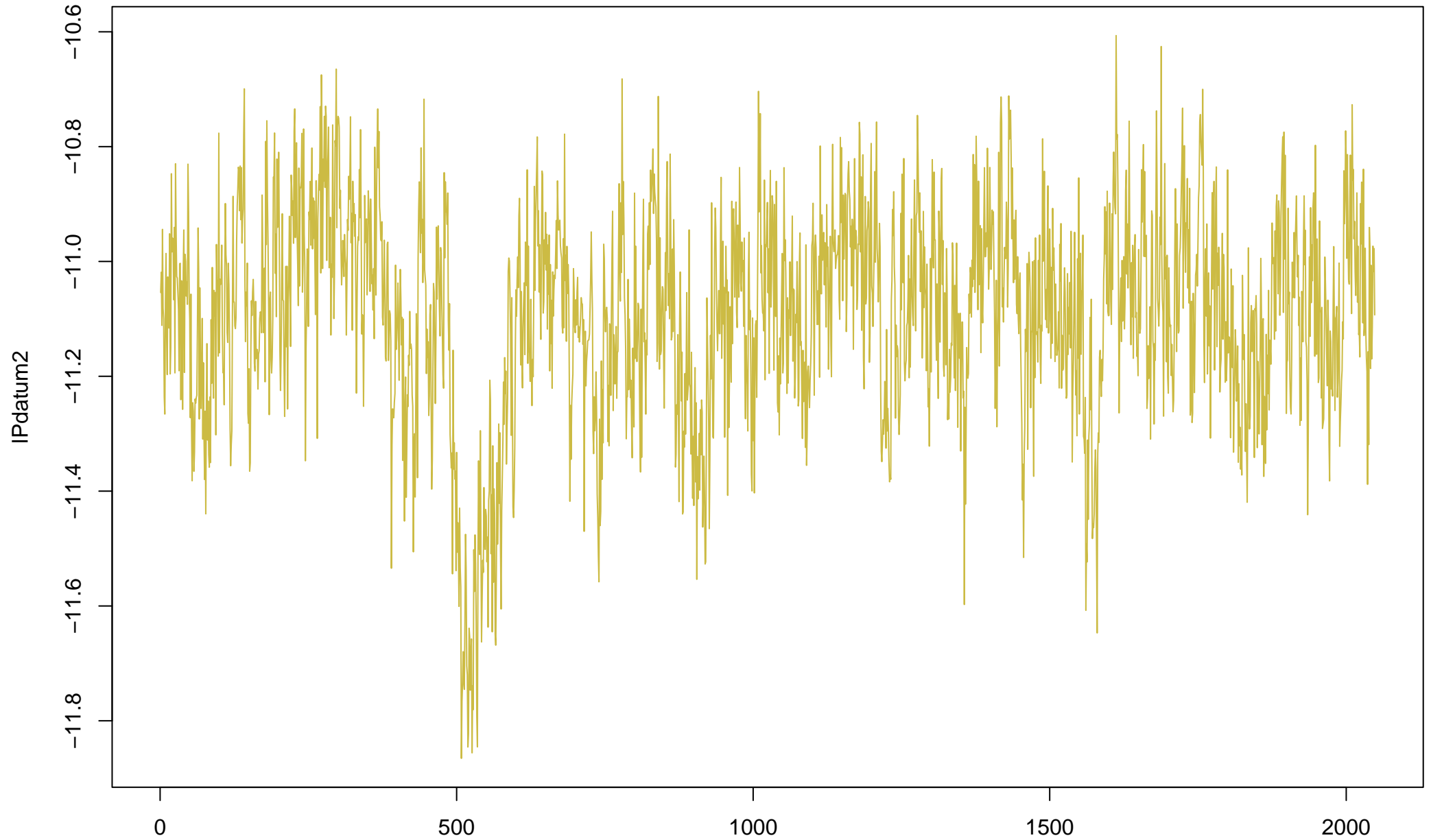
IPcornerLo
ESS = 305 | BMK = 0.136 | MCSE(6.27) = 7.55 | stat: TRUE | burn: 0



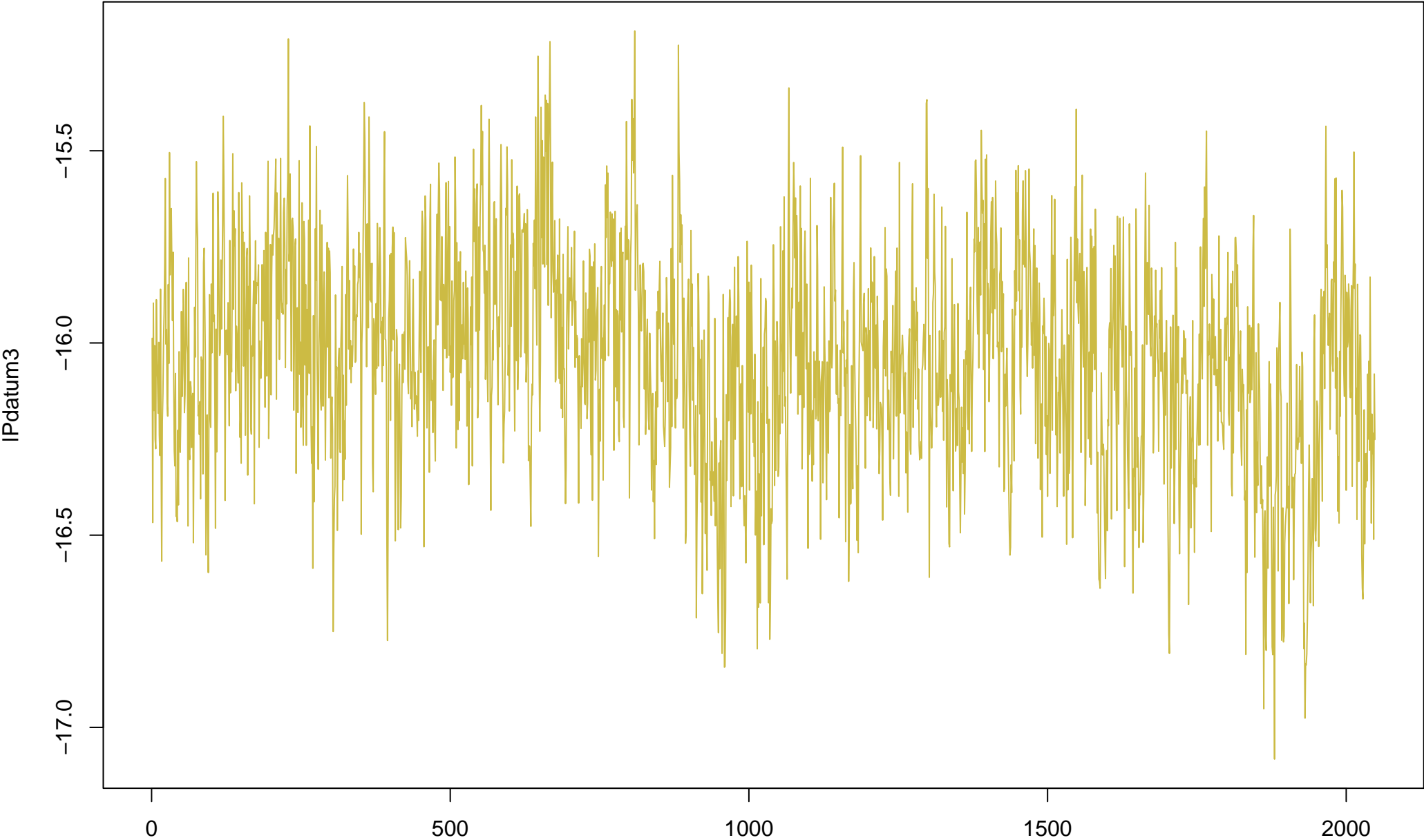
IPdatum1
ESS = 349 | BMK = 0.087 | MCSE(6.27) = 4.2 | stat: TRUE | burn: 0



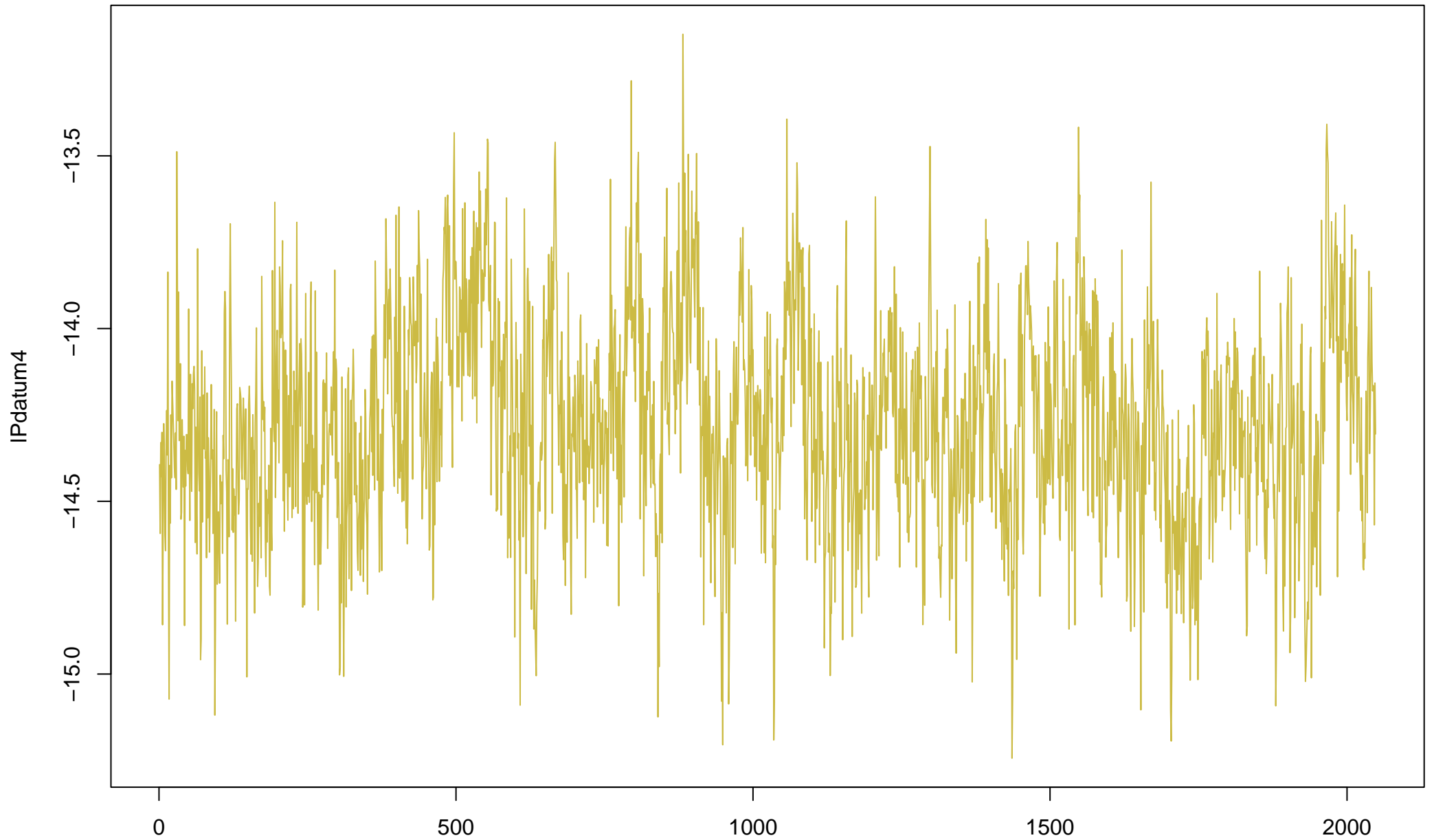
IPdatum2
ESS = 44.1 | BMK = 0.15 | MCSE(6.27) = 10.8 | stat: TRUE | burn: 408



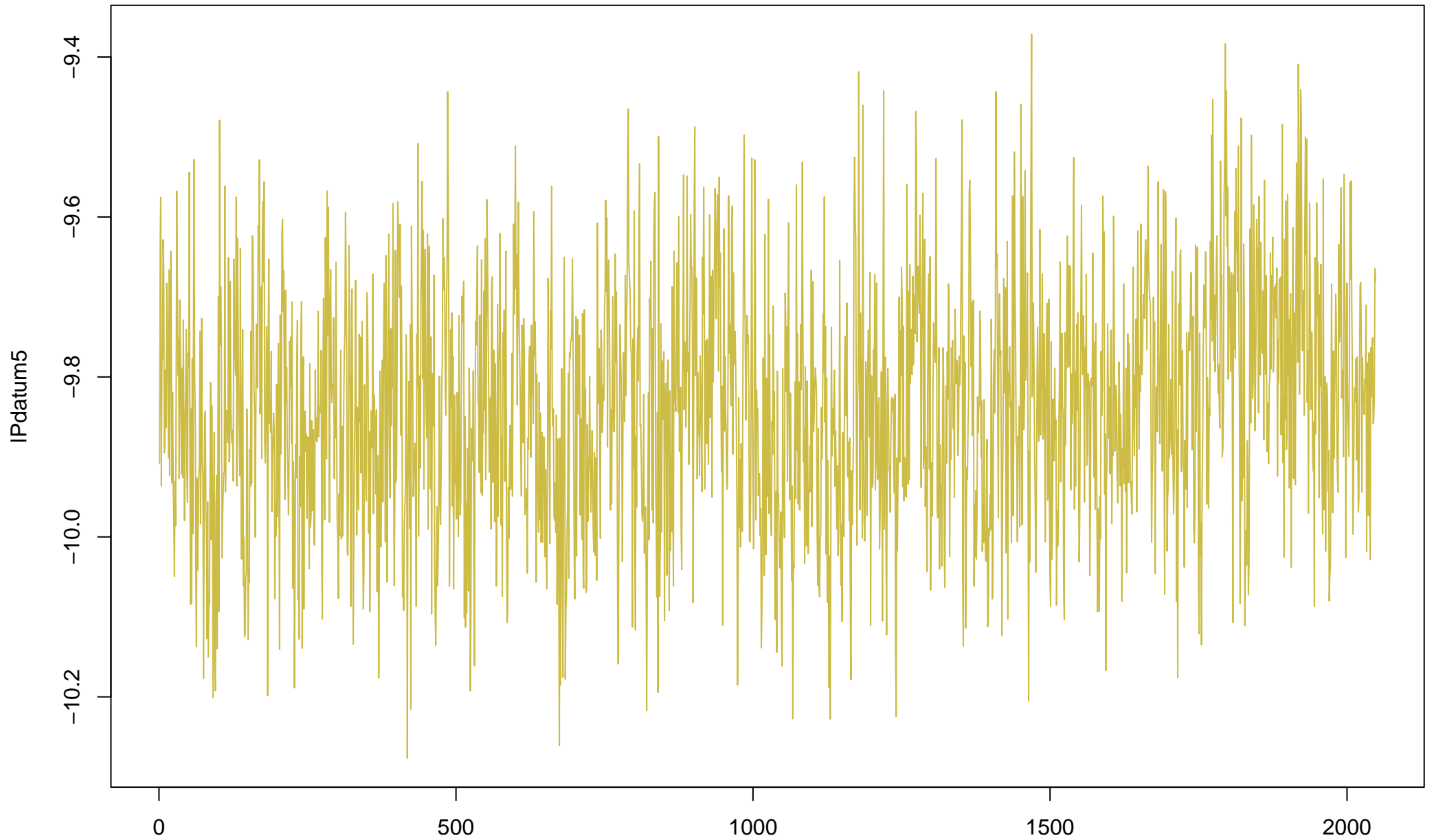
IPdatum3
ESS = 162 | BMK = 0.141 | MCSE(6.27) = 6.87 | stat: FALSE | burn: 0



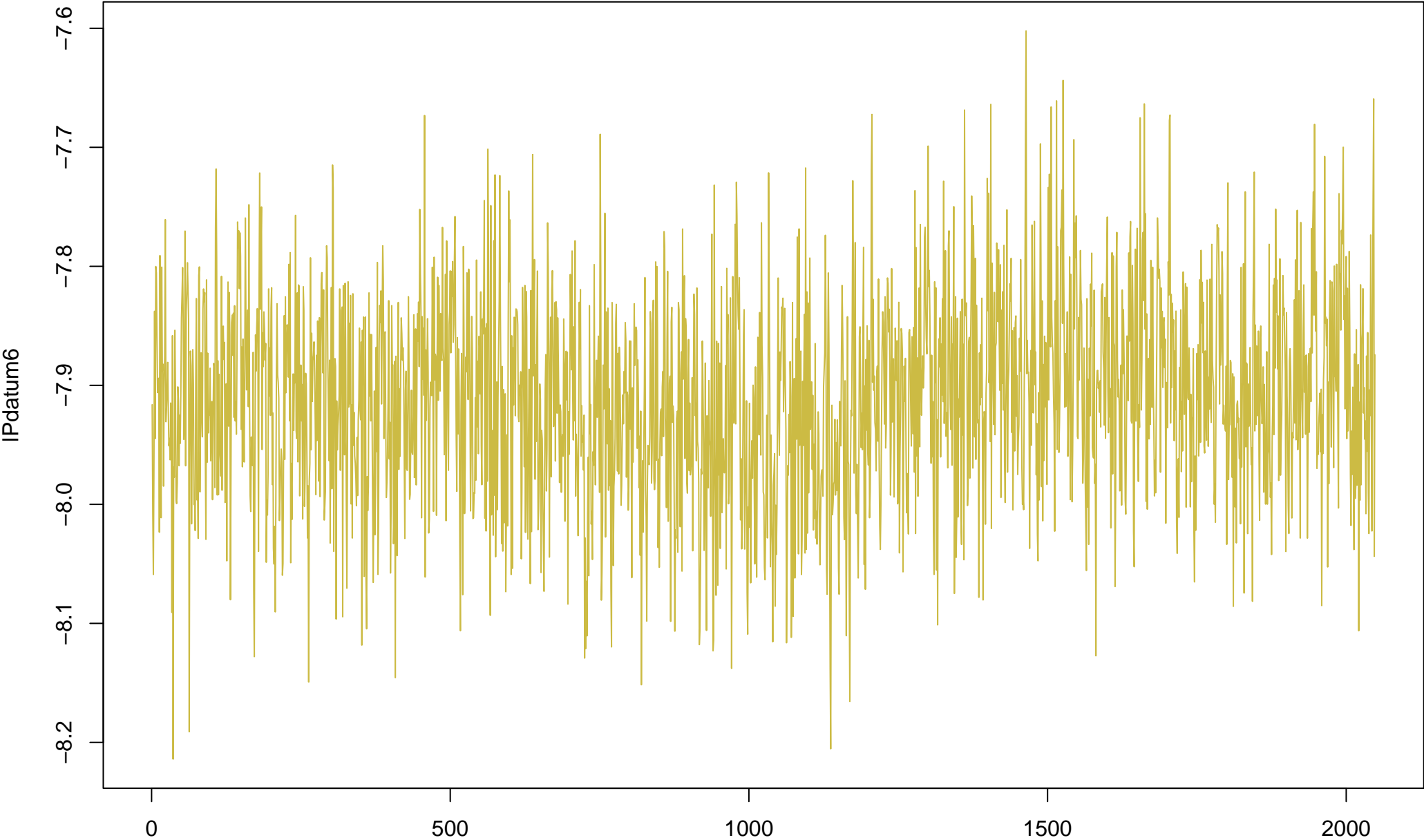
IPdatum4
ESS = 151 | BMK = 0.0788 | MCSE(6.27) = 9.06 | stat: FALSE | burn: 0



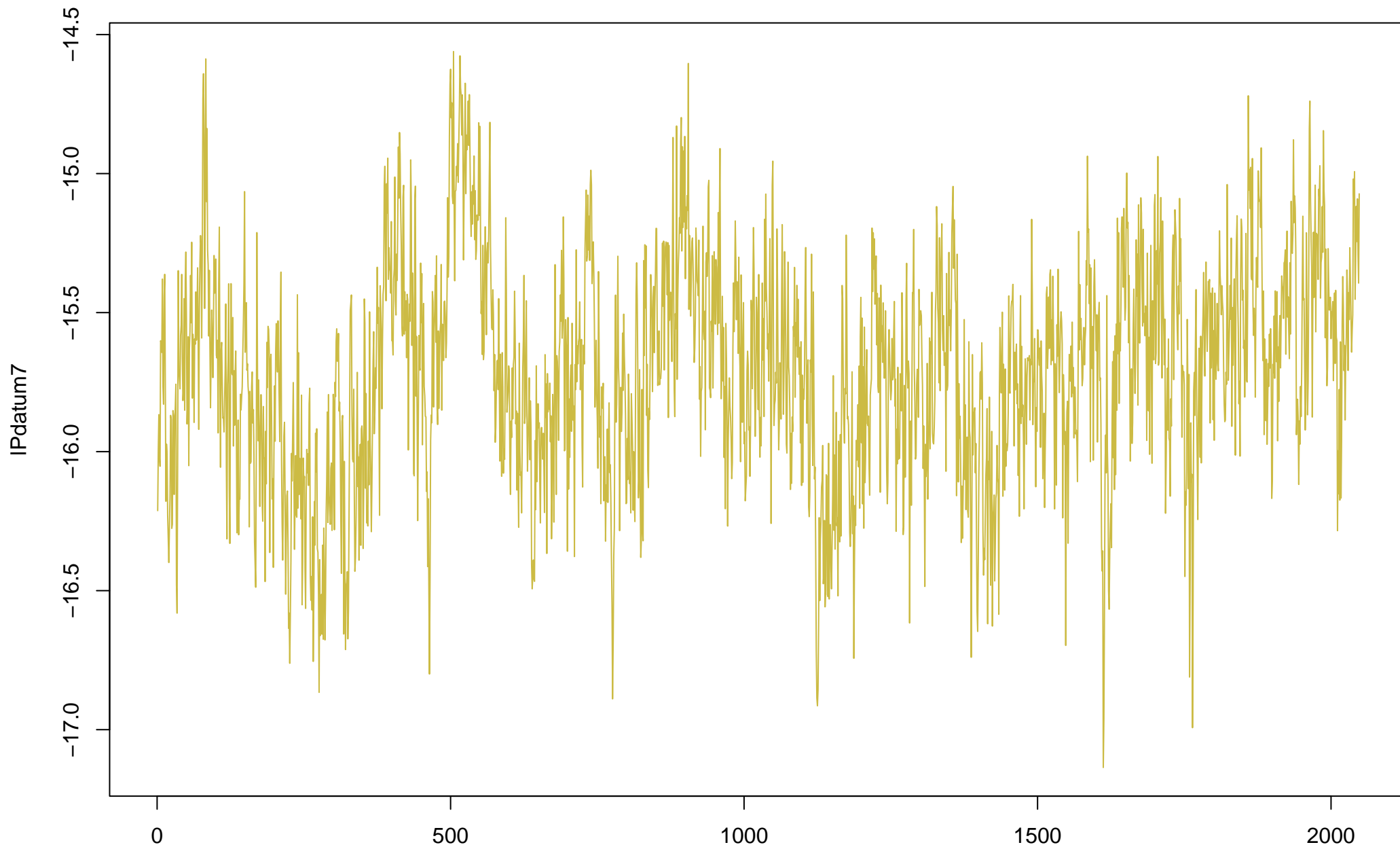
IPdatum5
ESS = 501 | BMK = 0.072 | MCSE(6.27) = 4.98 | stat: TRUE | burn: 0



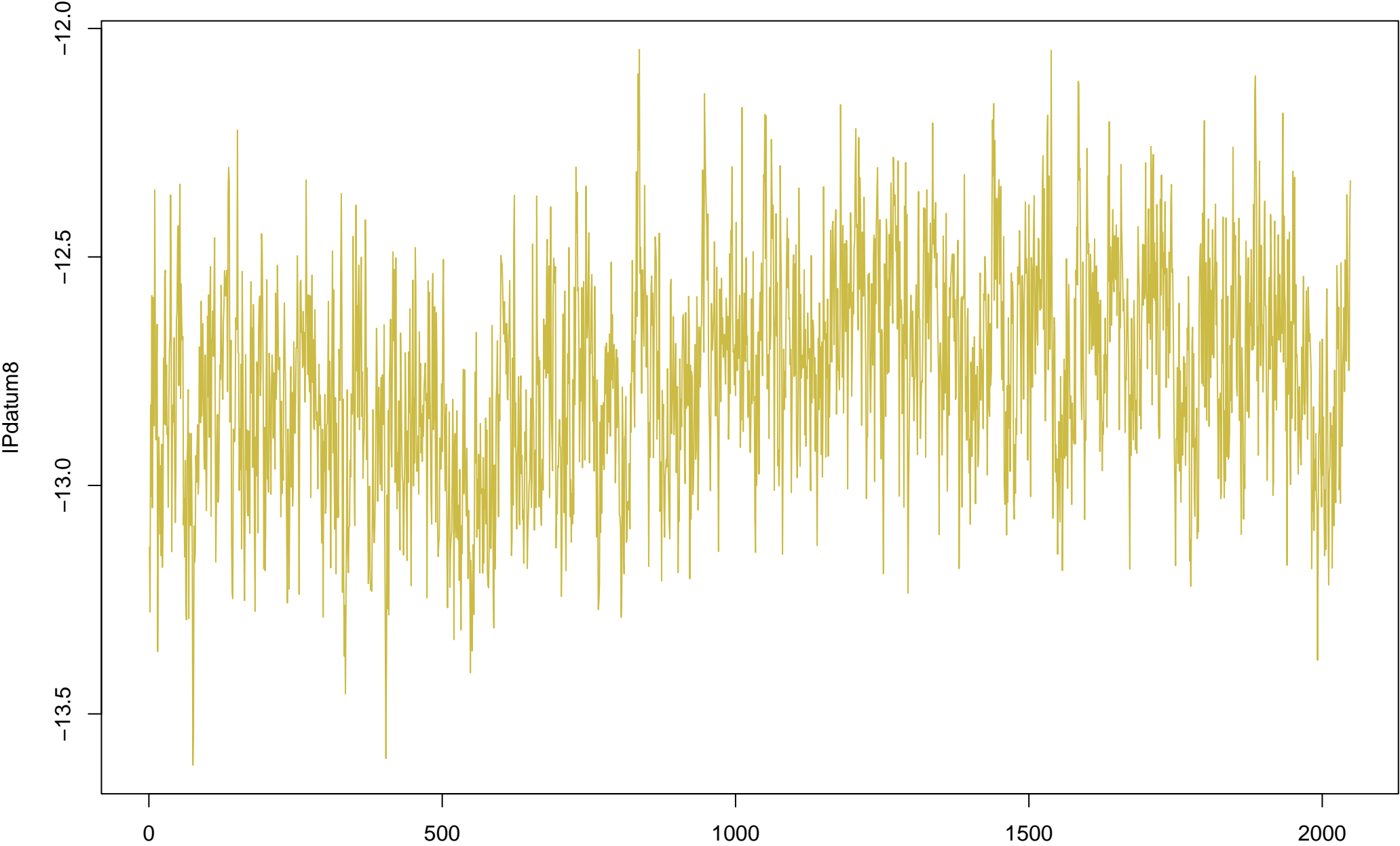
IPdatum6
ESS = 869 | BMK = 0.0863 | MCSE(6.27) = 4.24 | stat: TRUE | burn: 0



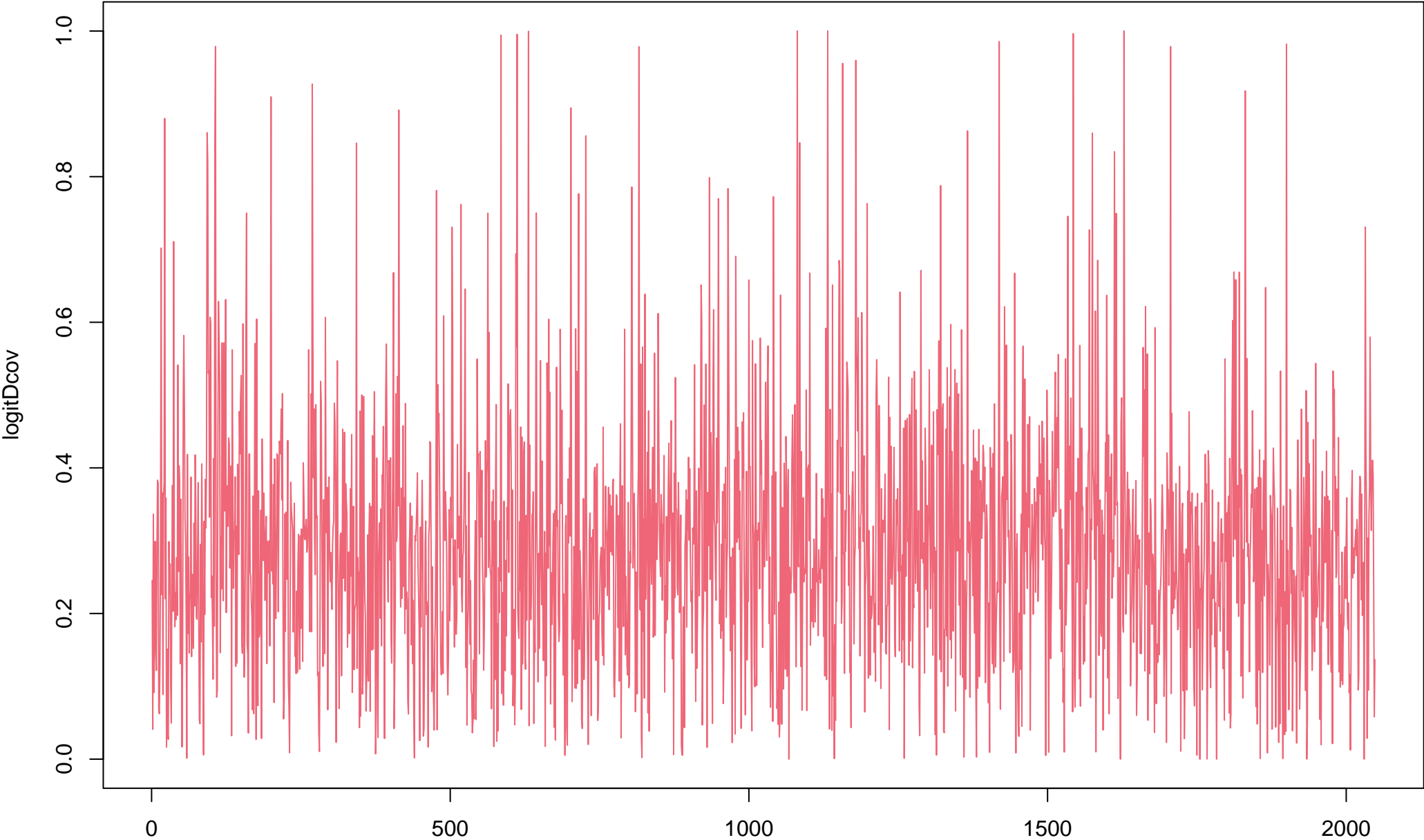
IPdatum7
ESS = 62 | BMK = 0.102 | MCSE(6.27) = 14.2 | stat: TRUE | burn: 0



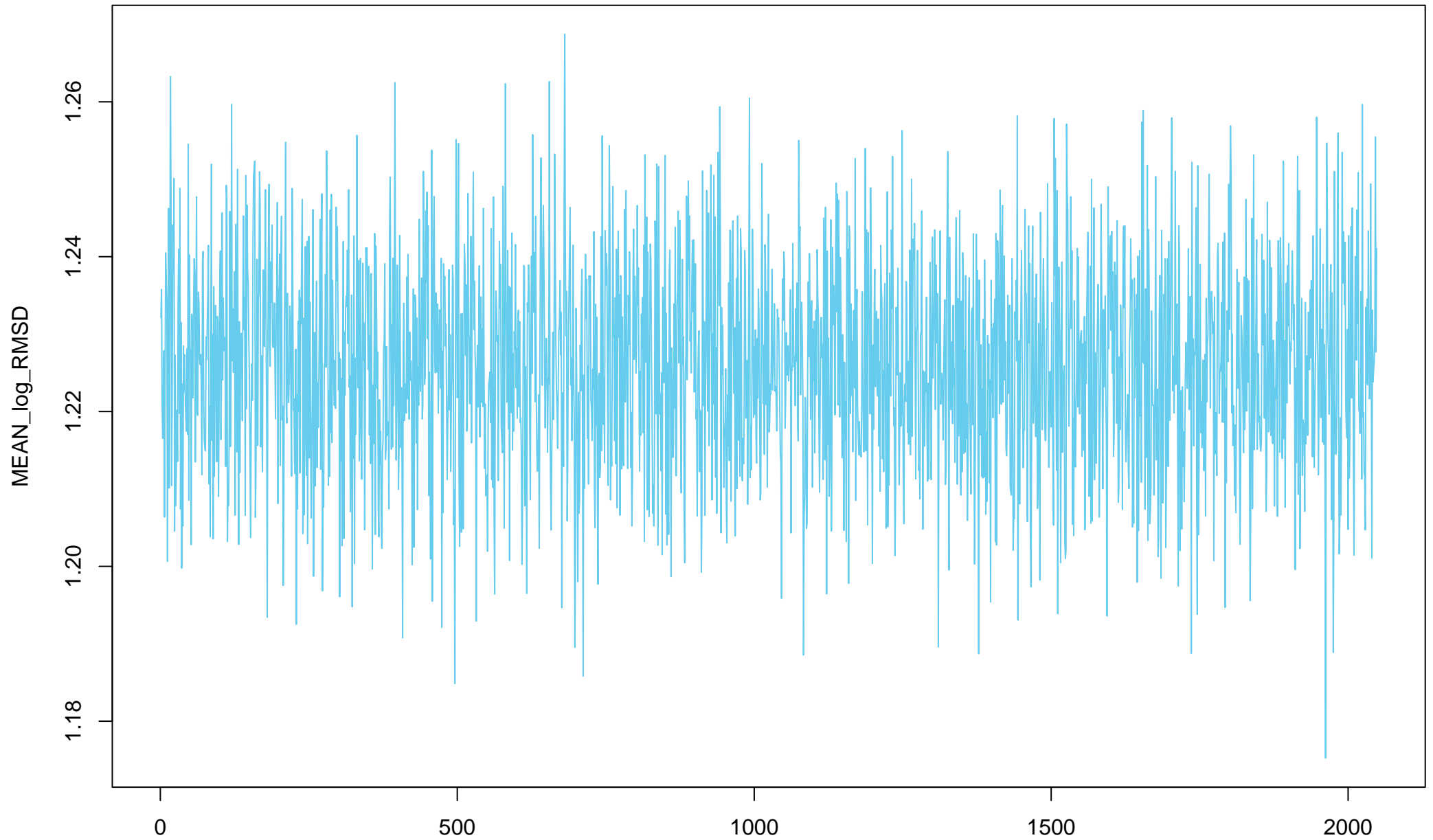
IPdatum8
ESS = 174 | BMK = 0.246 | MCSE(6.27) = 8.43 | stat: FALSE | burn: 0



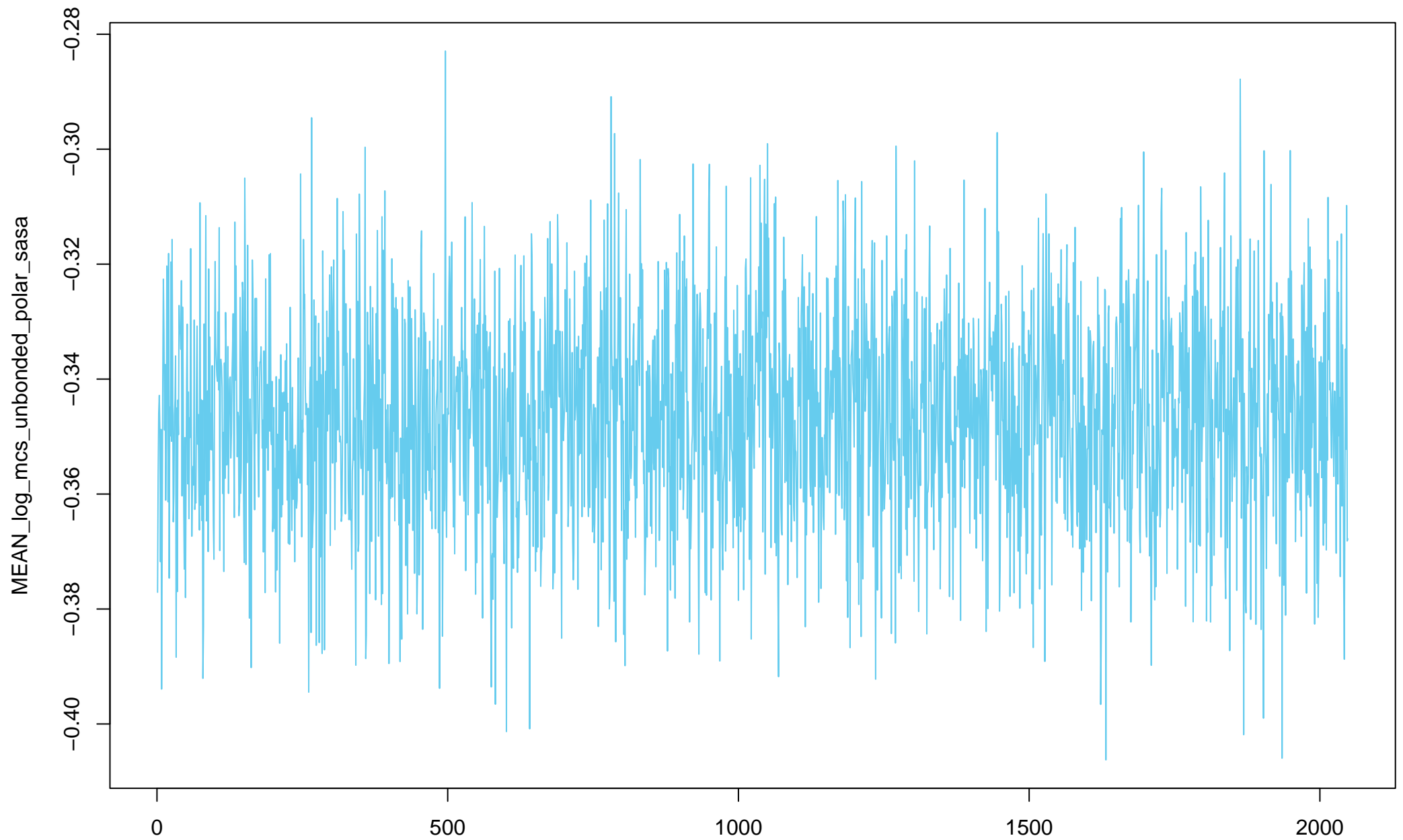
logitDcov
ESS = 1690 | BMK = 0.045 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0



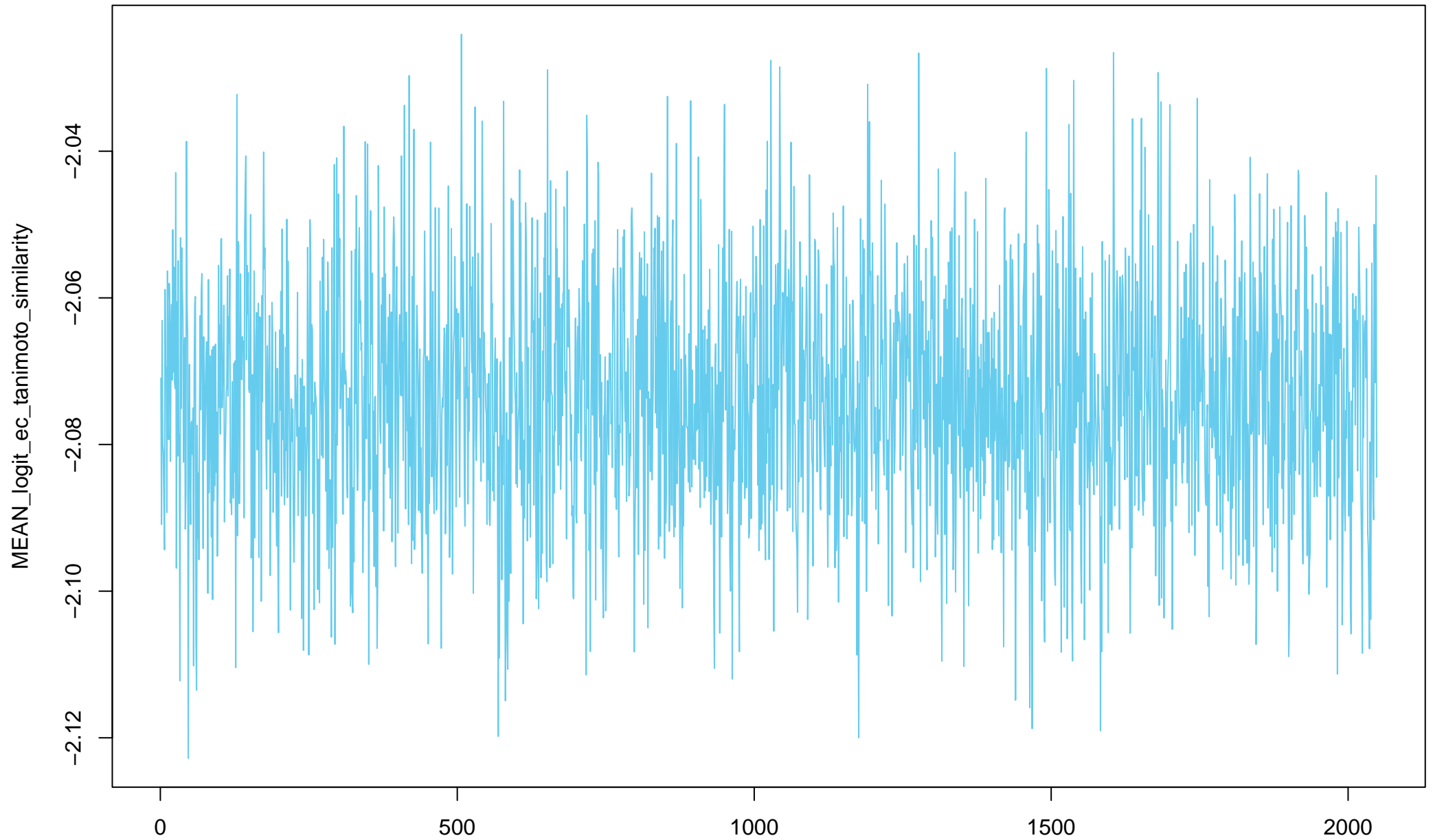
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0407 | MCSE(6.27) = 2.33 | stat: FALSE | burn: 0



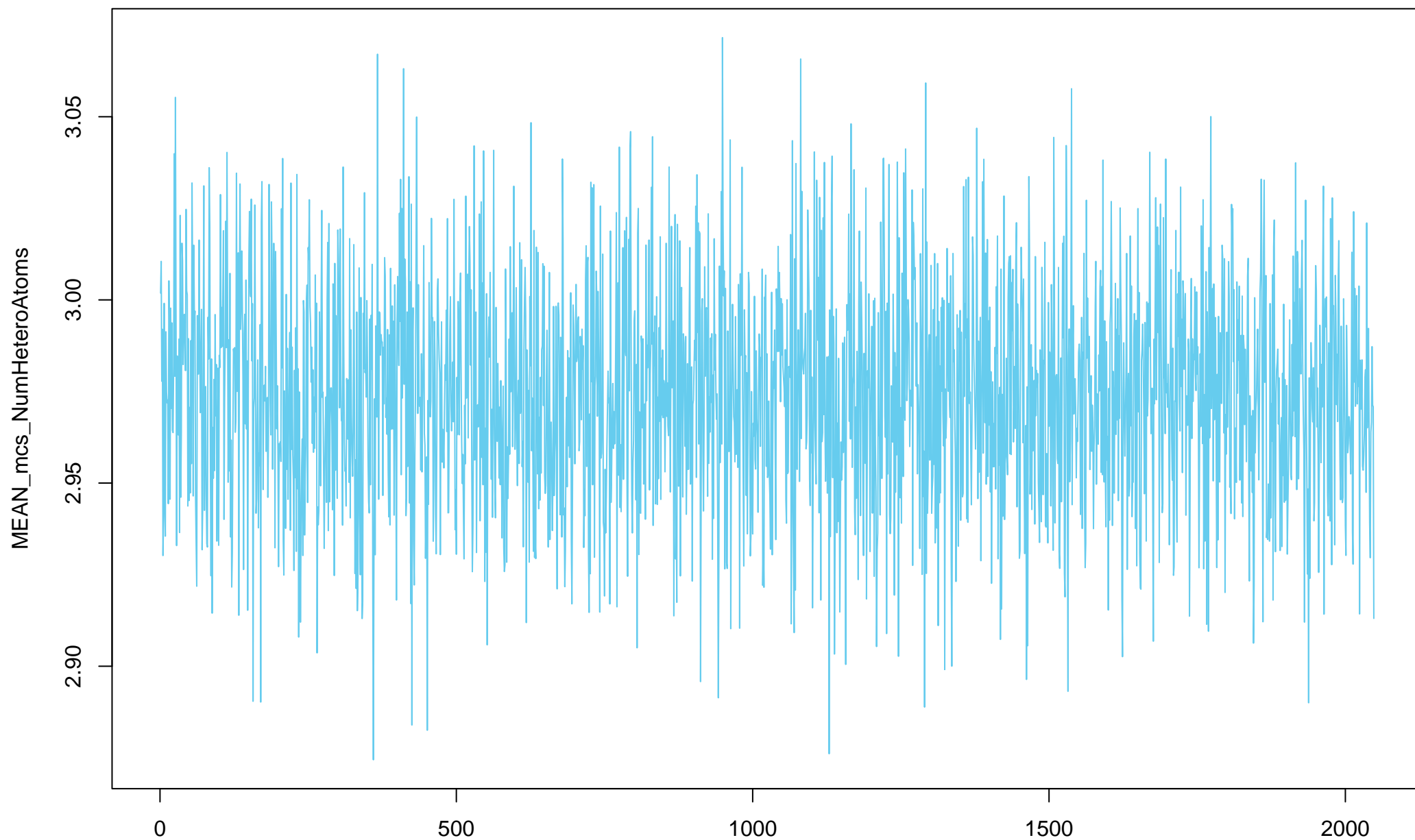
MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.044 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



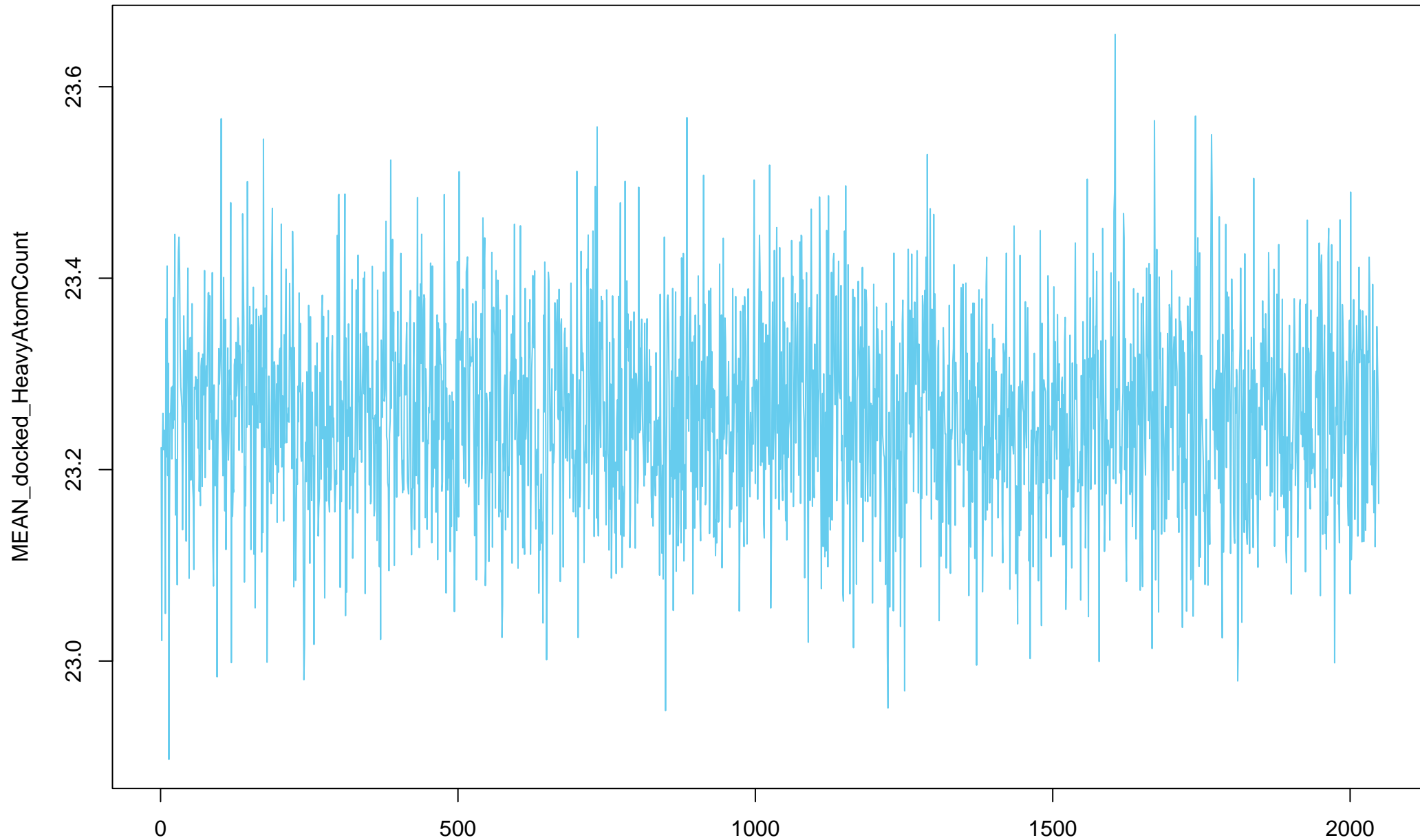
MEAN_logit_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.035 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0



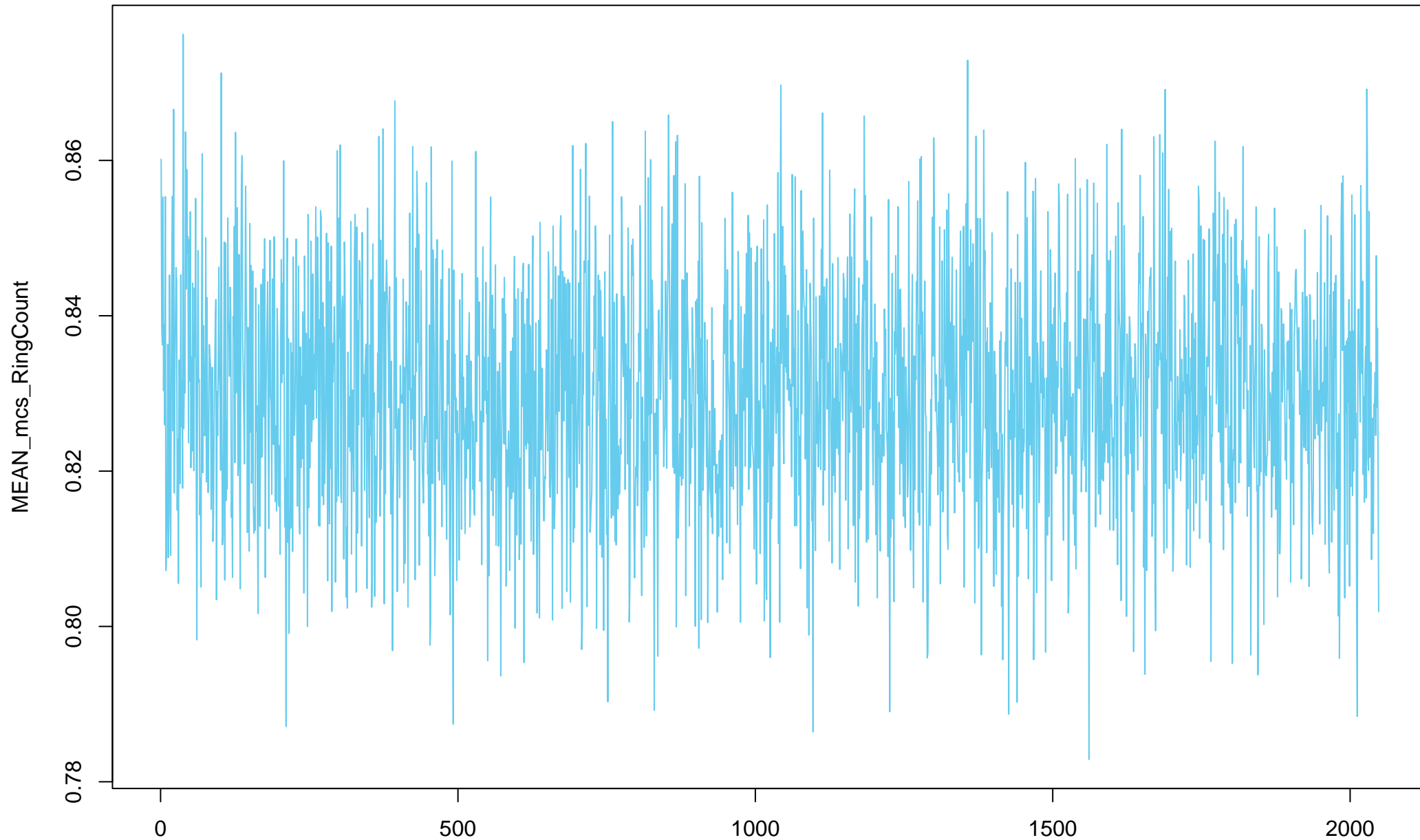
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0307 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0



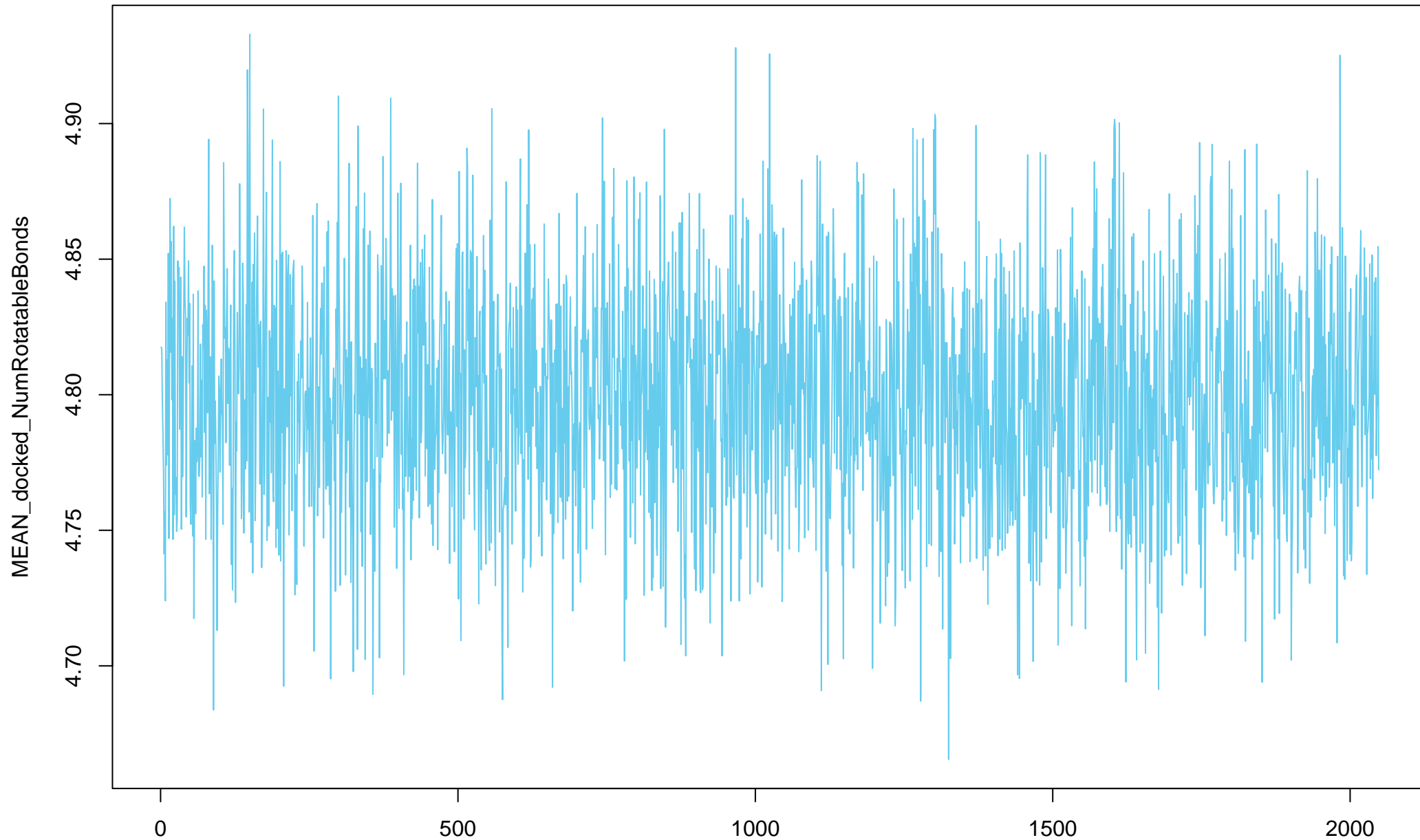
MEAN_docked_HeavyAtomCount
ESS = 1850 | BMK = 0.0379 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0



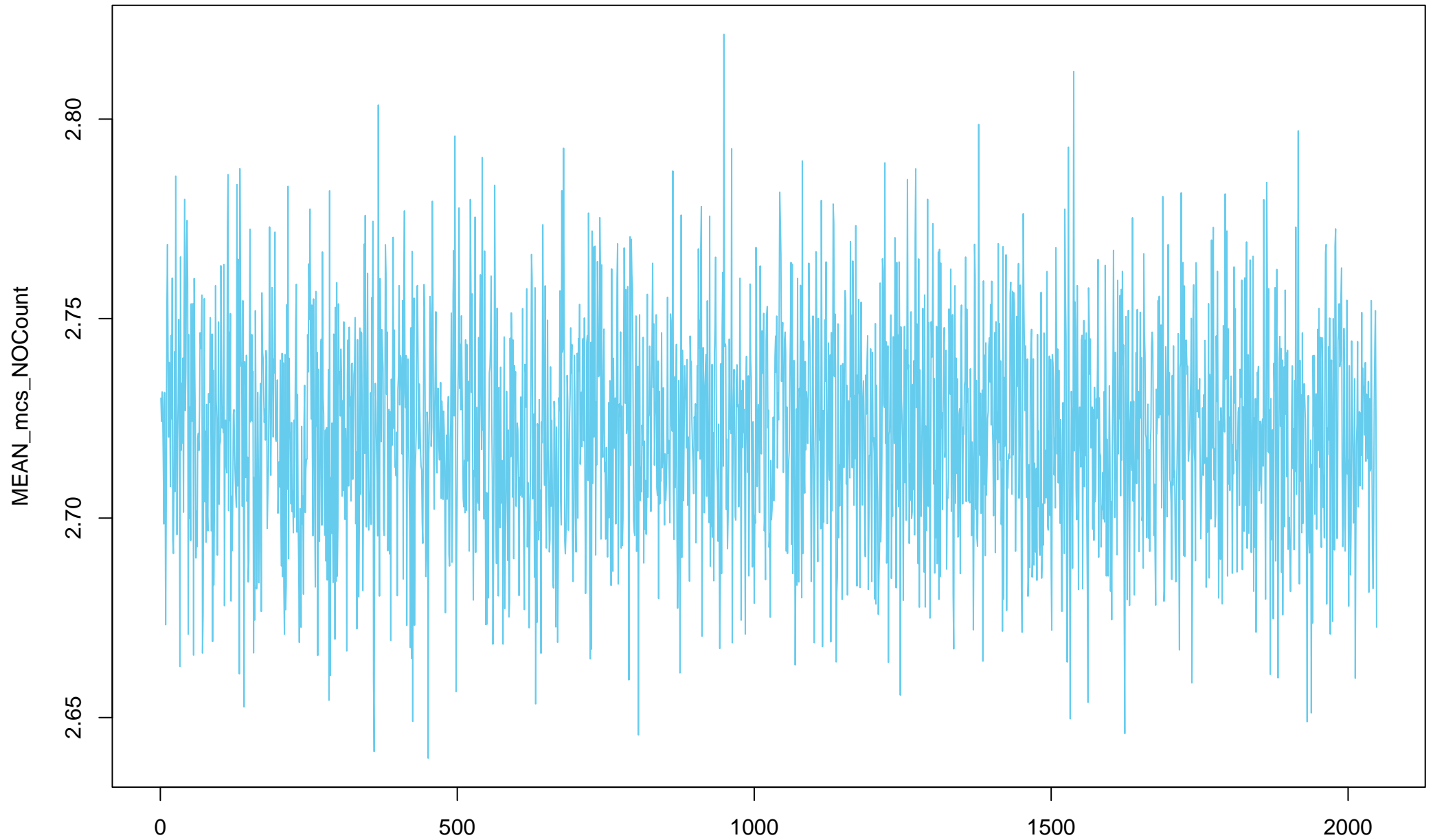
MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0508 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



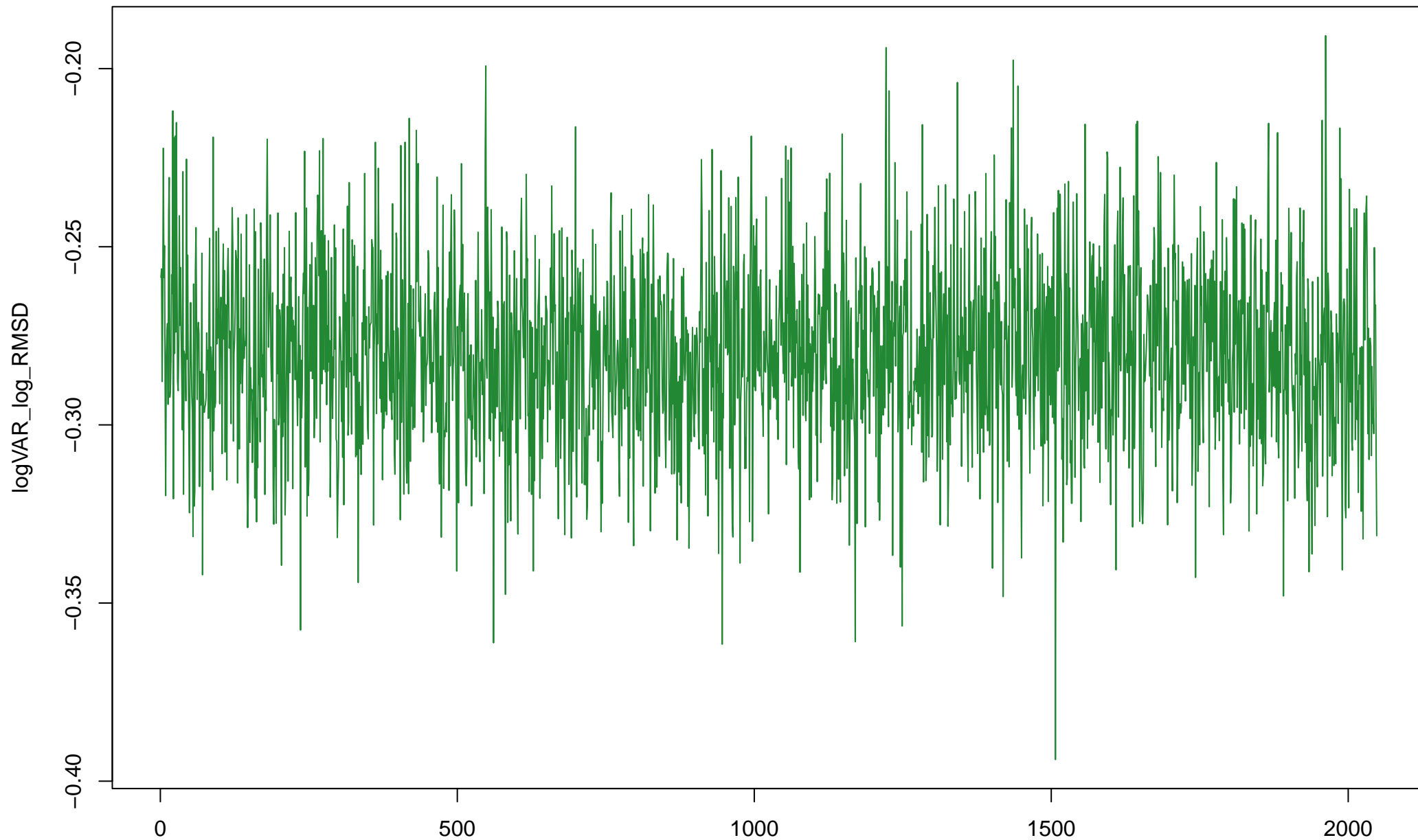
MEAN_docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0353 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



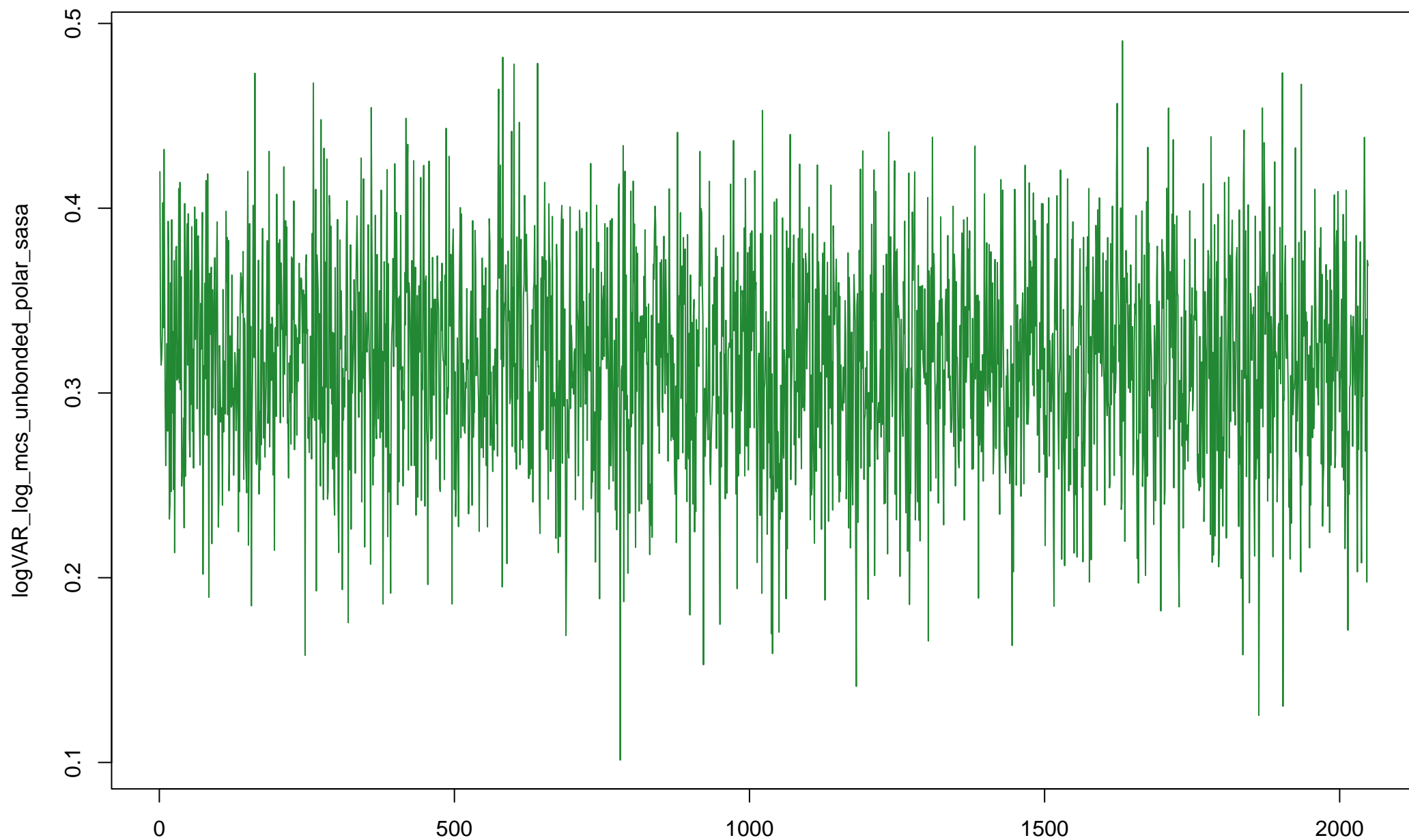
MEAN_mcs_NOCount
ESS = 2050 | BMK = 0.0378 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0



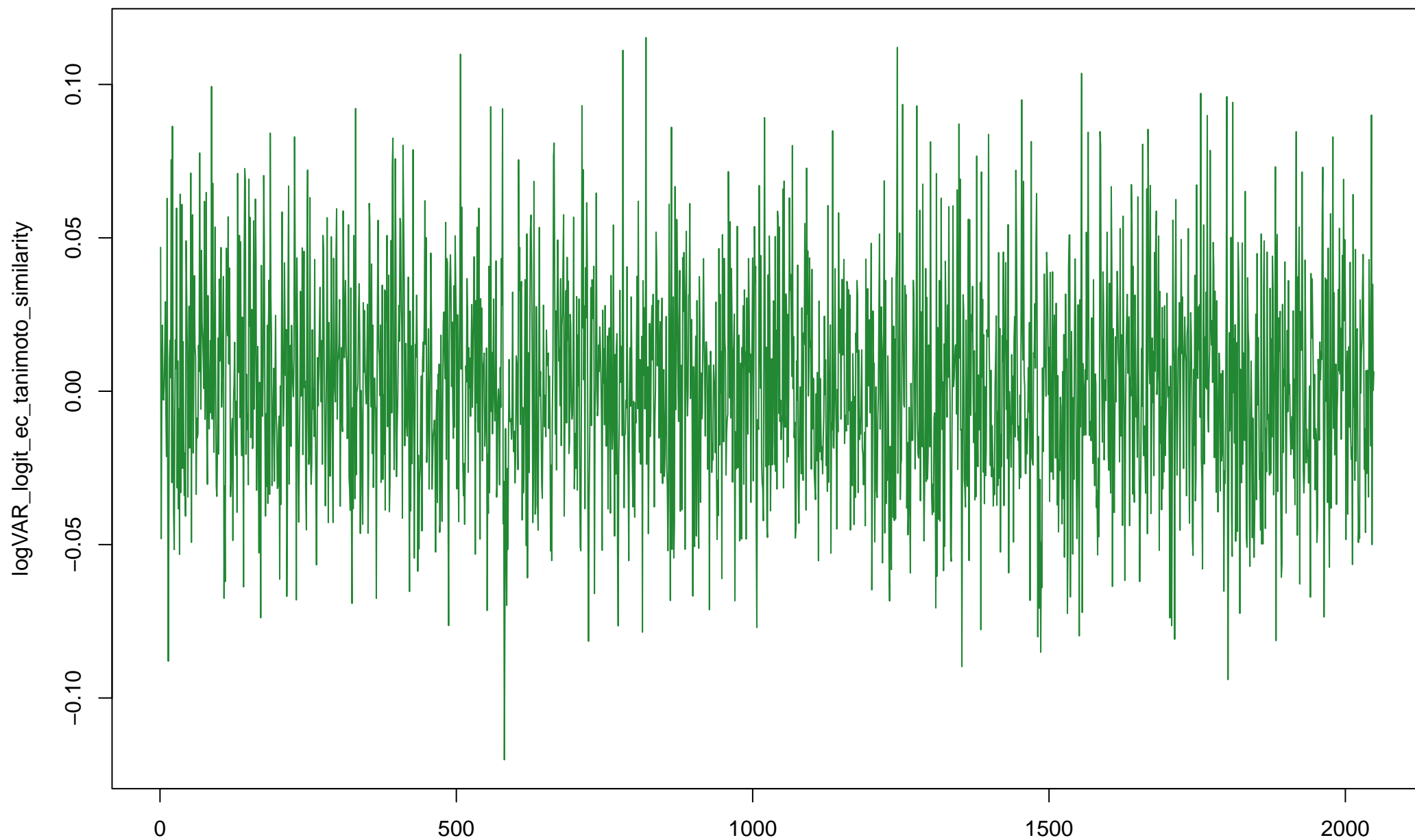
logVAR_log_RMSD
ESS = 1880 | BMK = 0.0429 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0



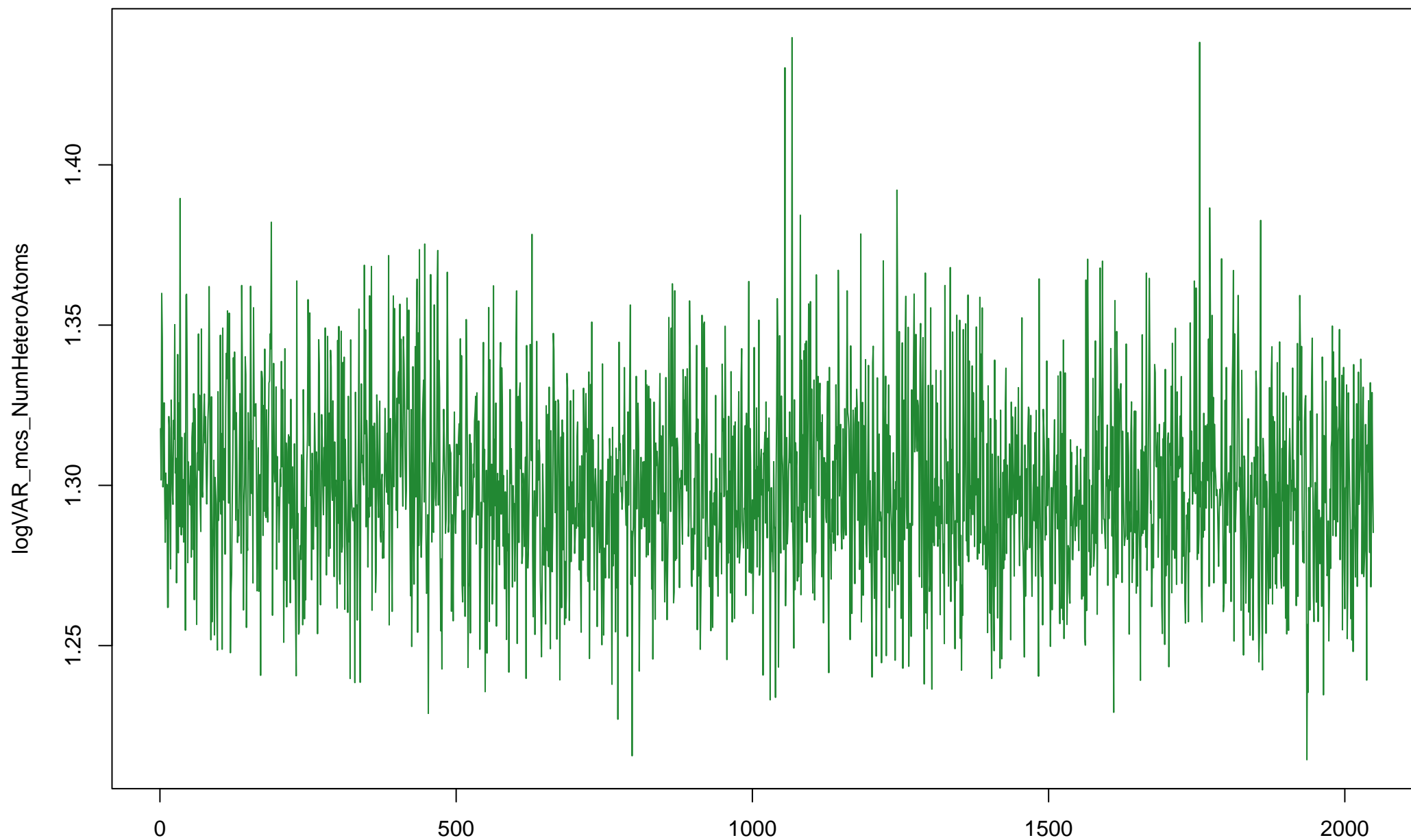
logVAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0445 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0



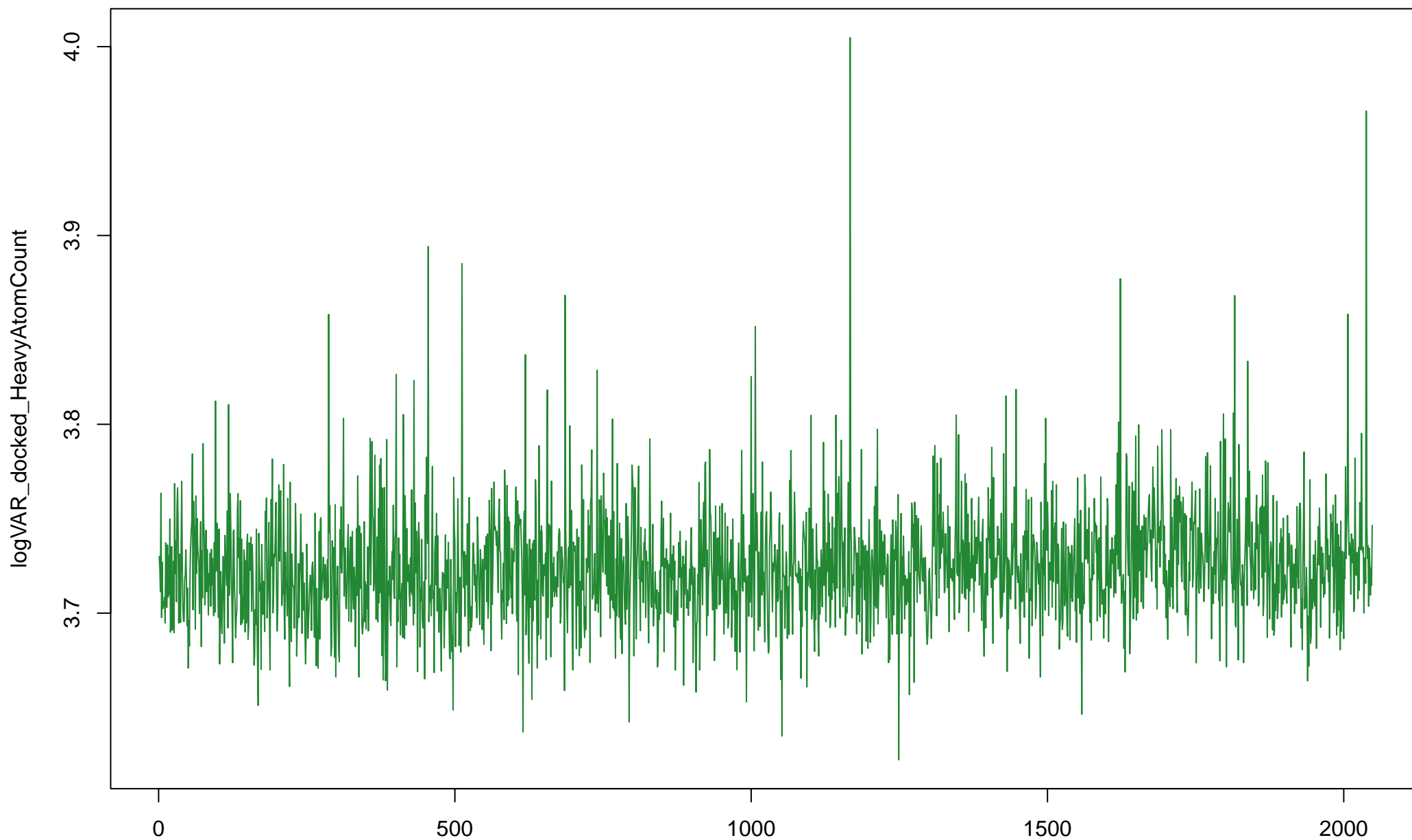
logVAR_logit_ec_tanimoto_similarity
ESS = 1880 | BMK = 0.0458 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0



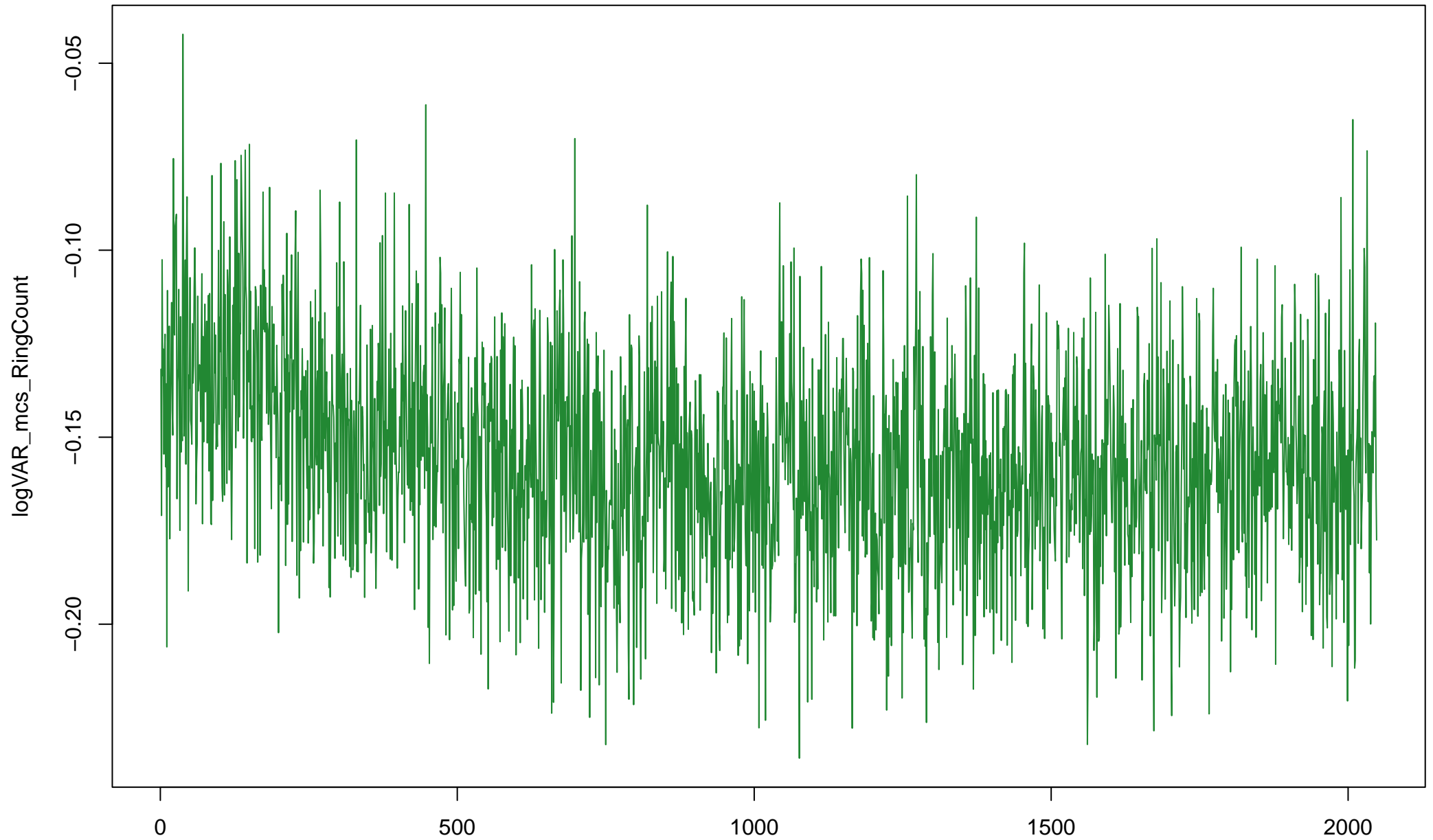
logVAR_mcs_NumHeteroAtoms
ESS = 1690 | BMK = 0.0558 | MCSE(6.27) = 2.31 | stat: FALSE | burn: 0



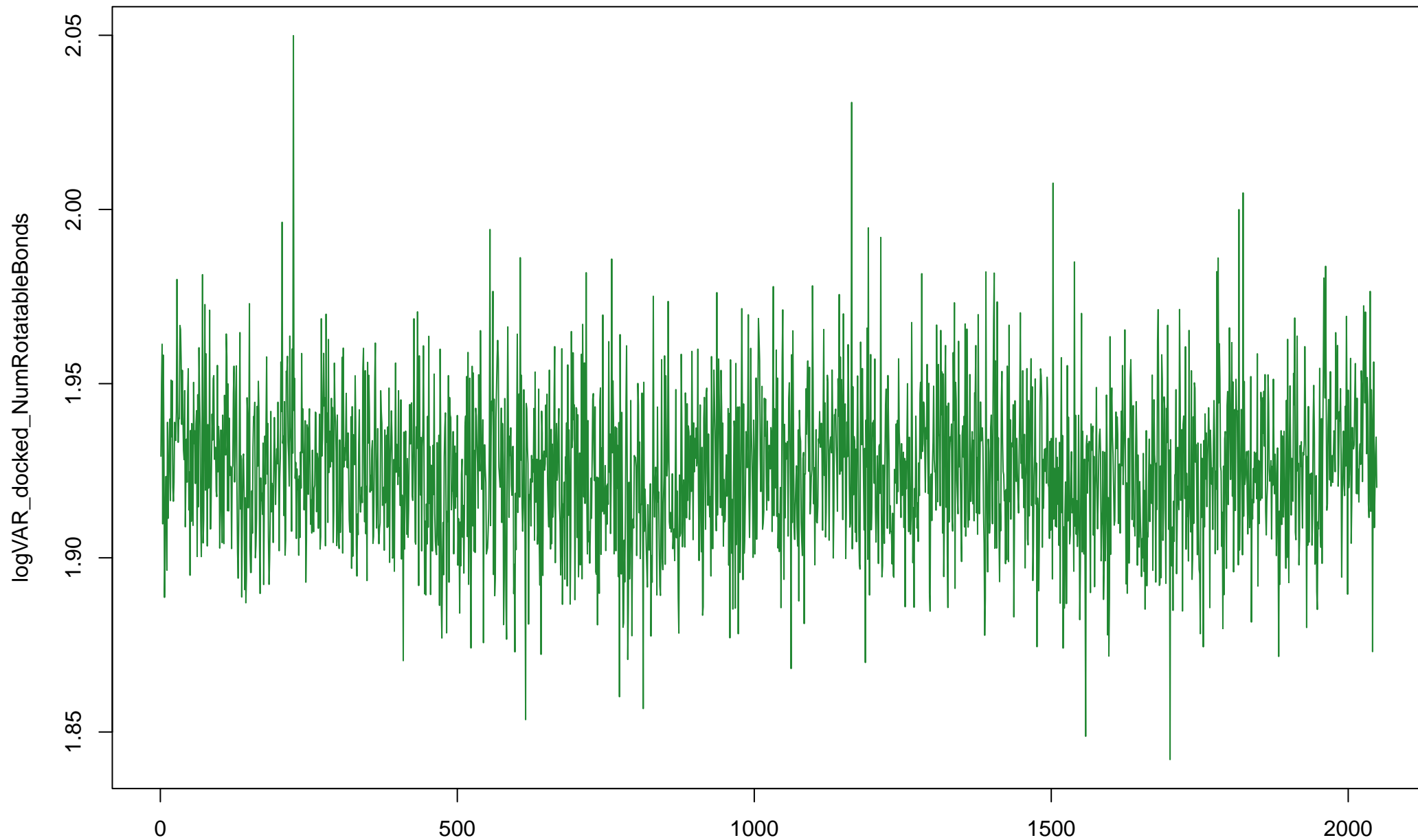
logVAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.105 | MCSE(6.27) = 2.35 | stat: FALSE | burn: 0



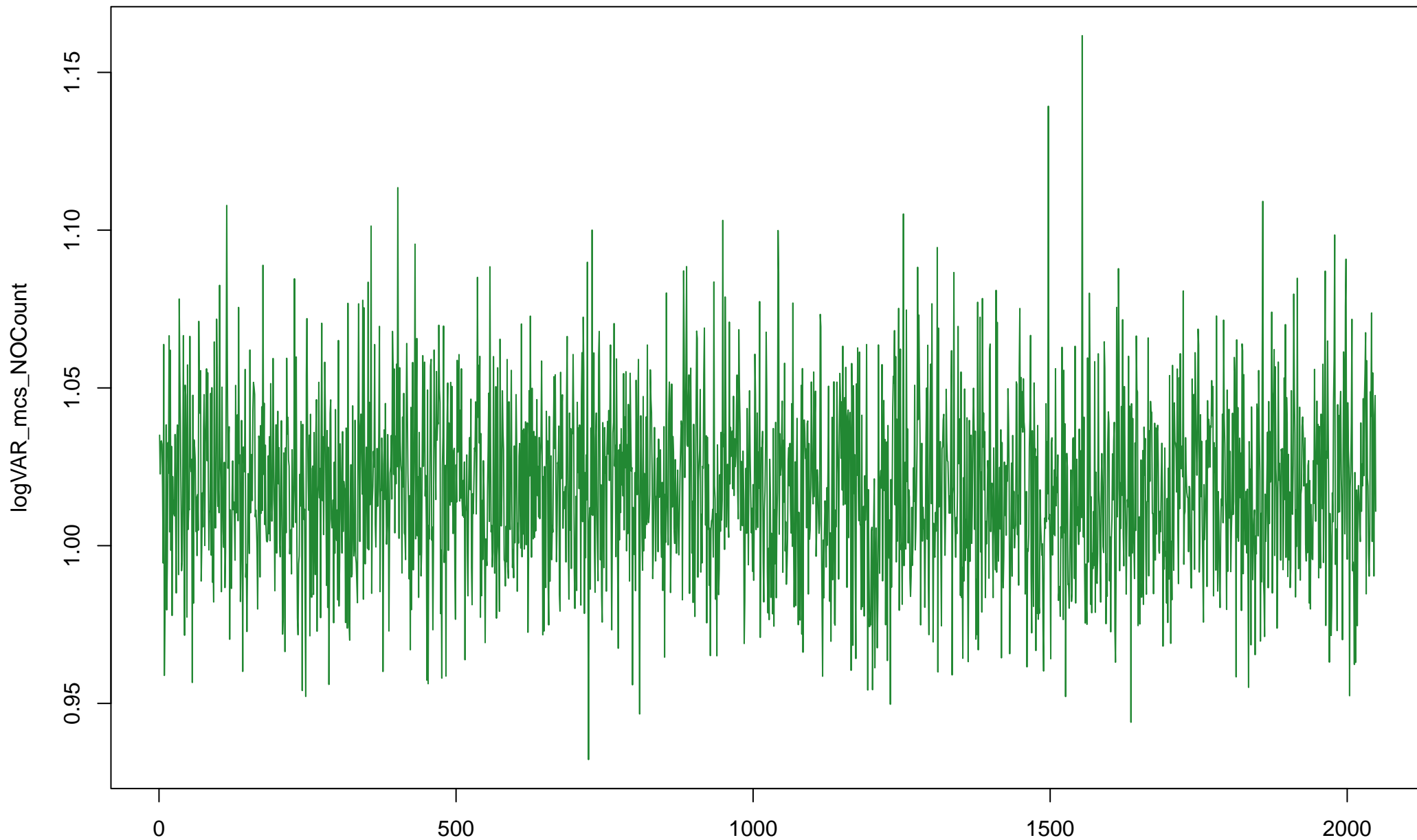
logVAR_mcs_RingCount
ESS = 127 | BMK = 0.121 | MCSE(6.27) = 3.4 | stat: FALSE | burn: 0



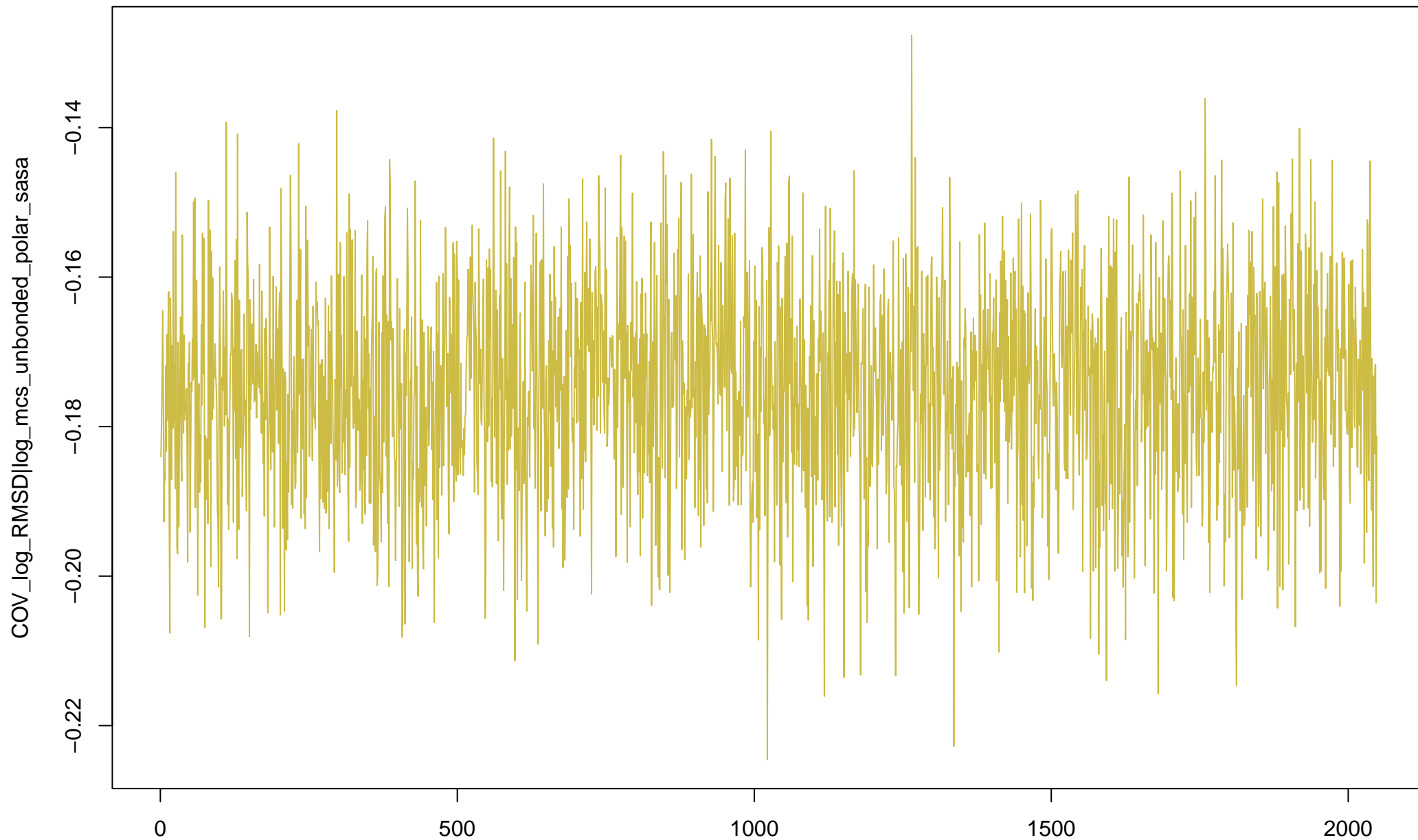
logVAR_docked_NumRotatableBonds
ESS = 1190 | BMK = 0.0579 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0



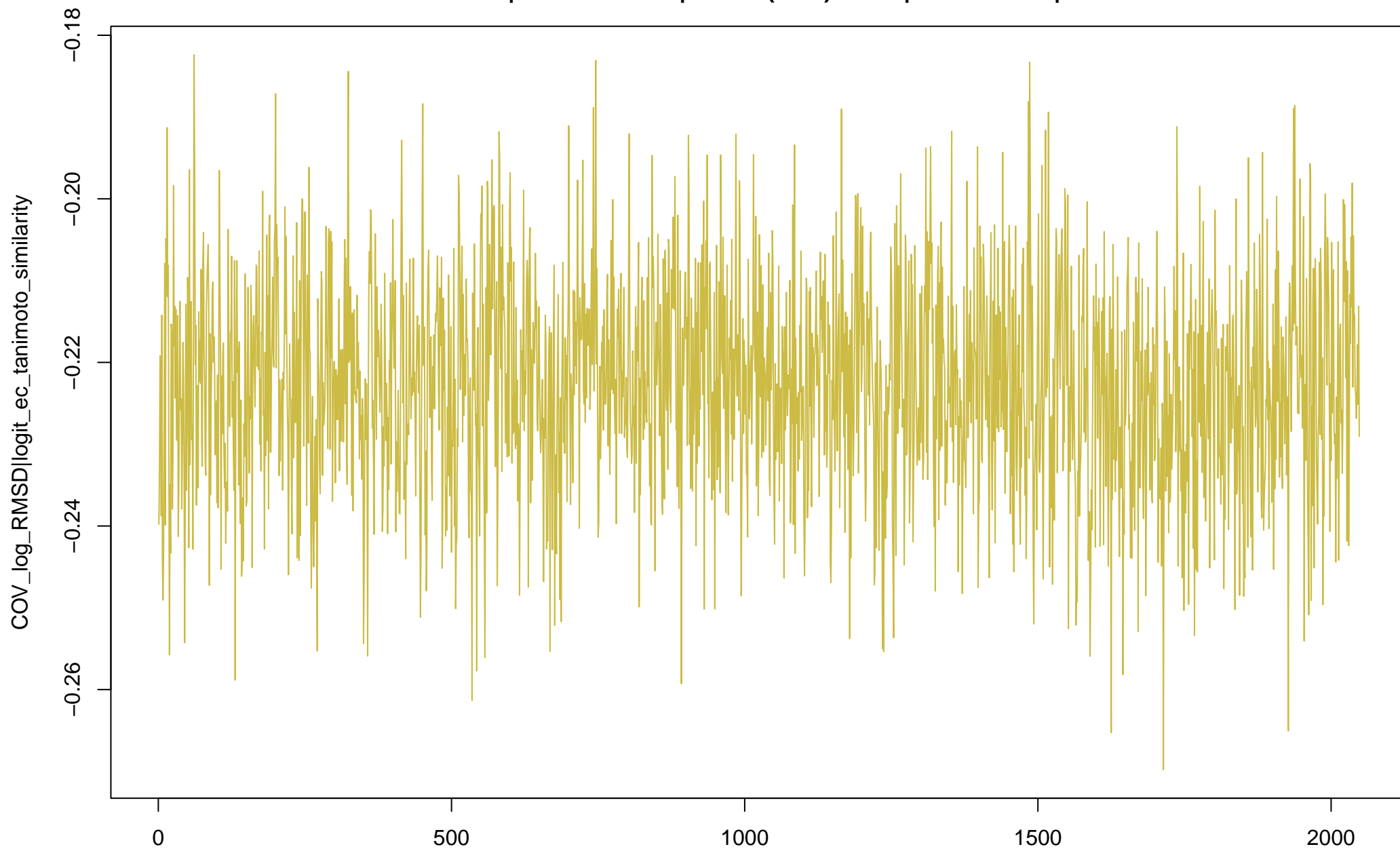
logVAR_mcs_NOCount
ESS = 2050 | BMK = 0.0674 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0



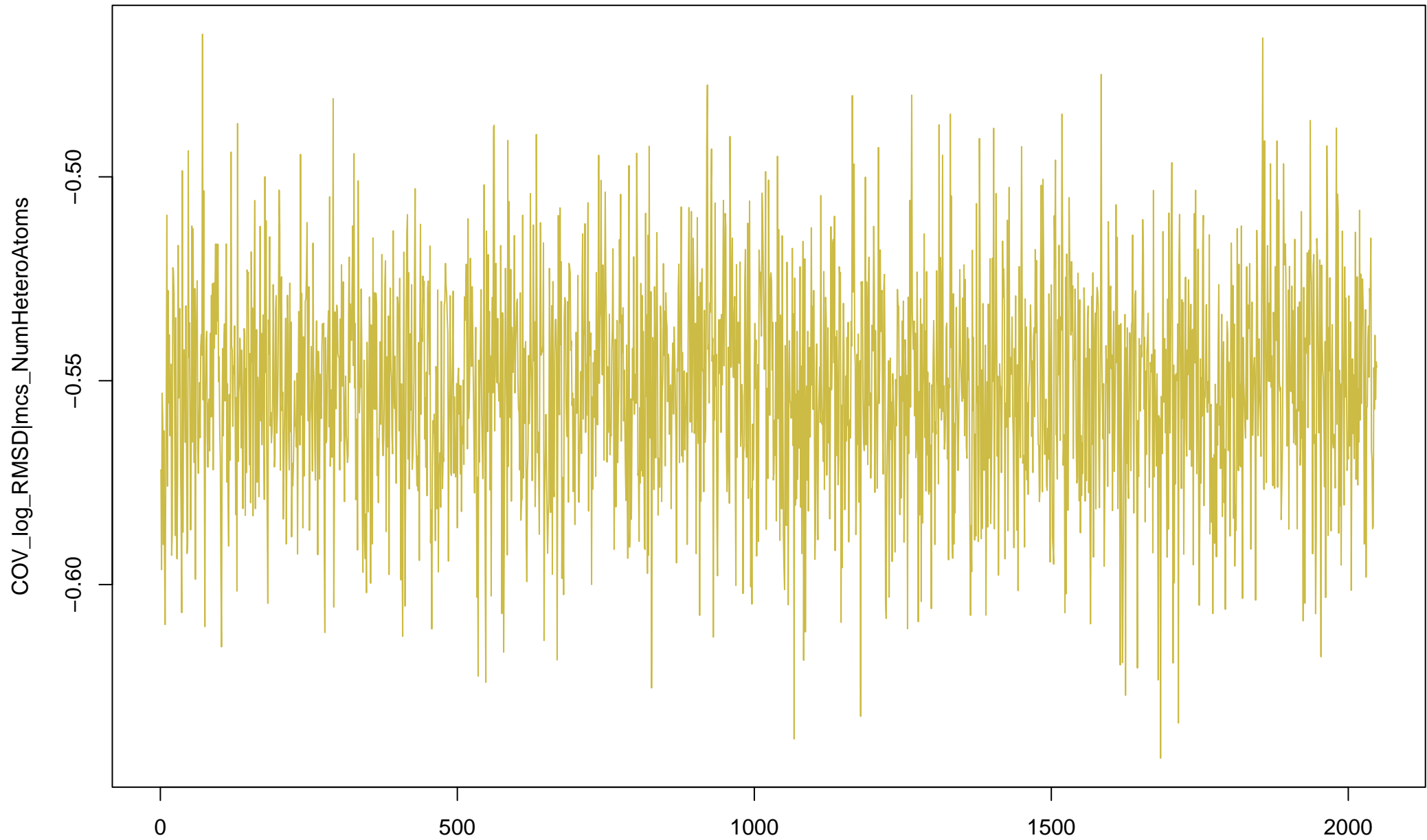
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1760 | BMK = 0.0504 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0



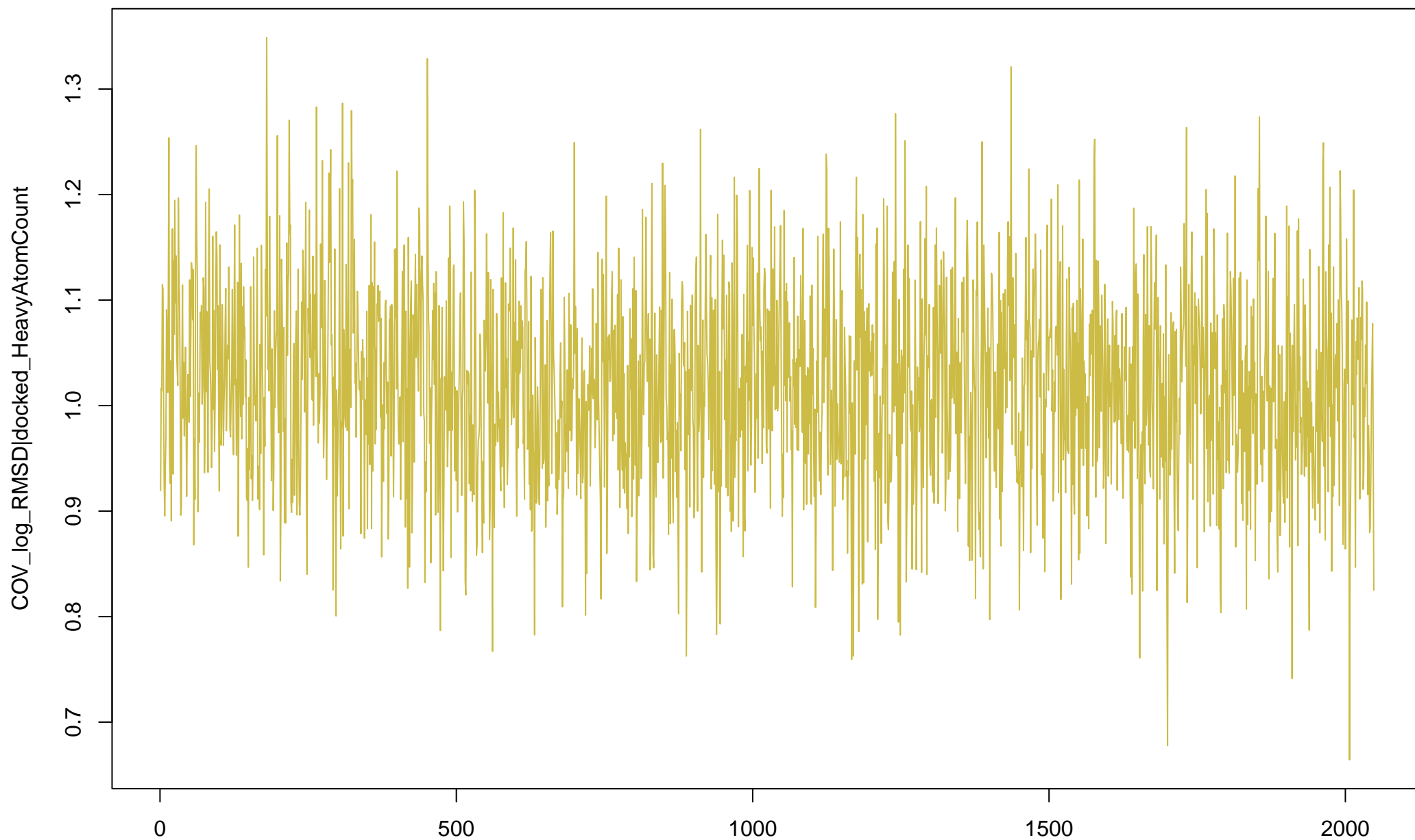
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1180 | BMK = 0.054 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0



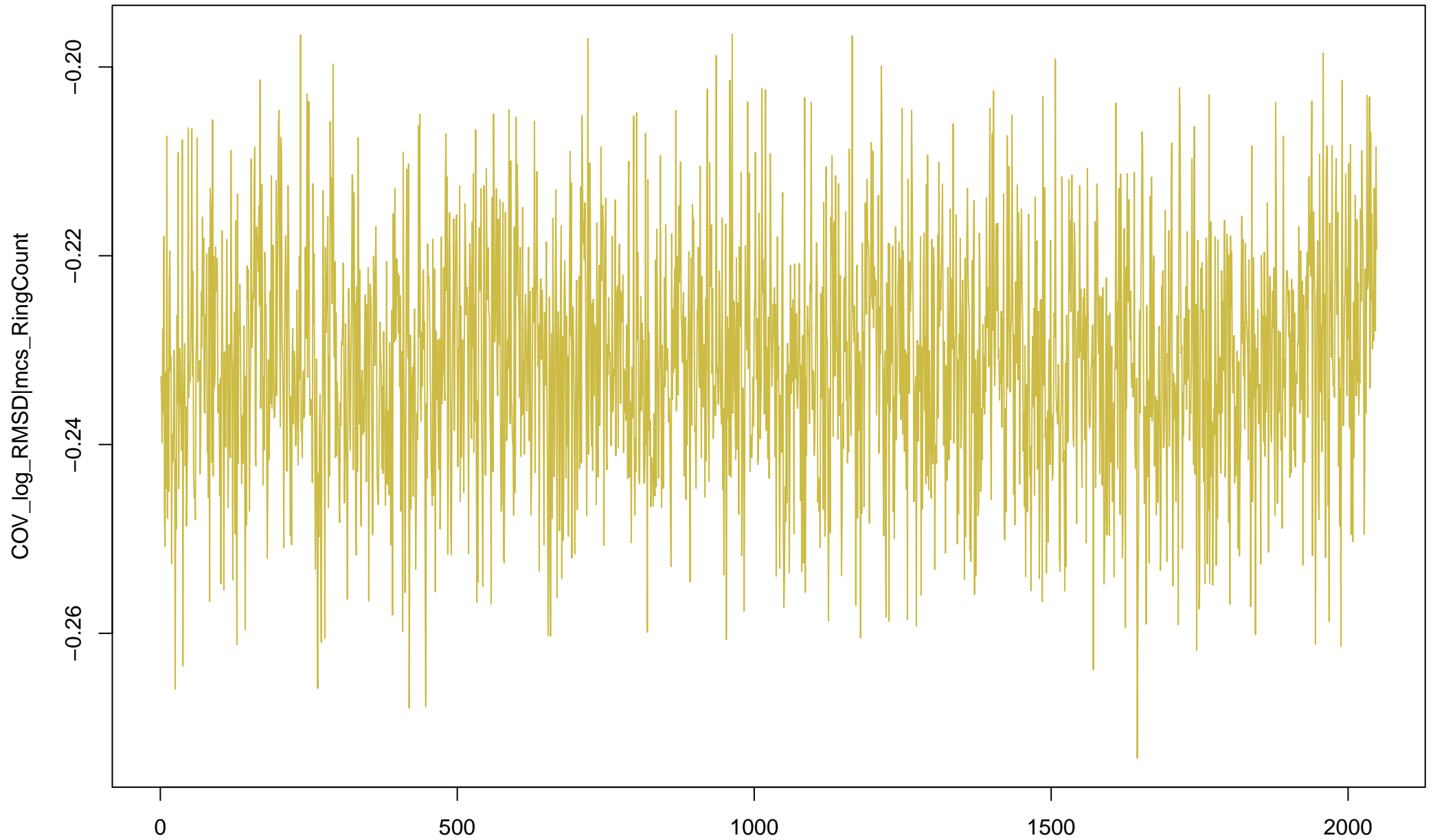
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1840 | BMK = 0.0404 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0



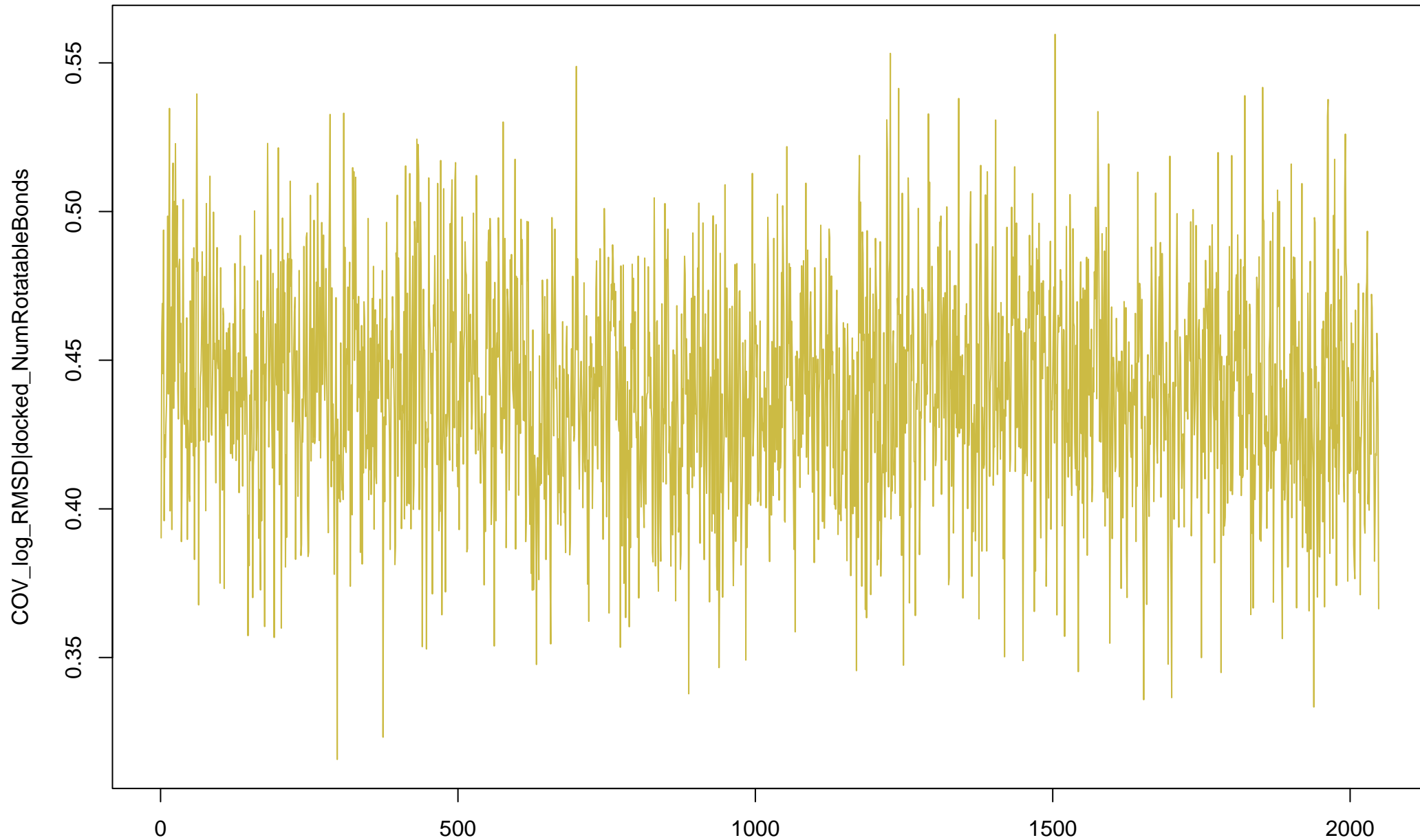
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1600 | BMK = 0.0475 | MCSE(6.27) = 2.78 | stat: FALSE | burn: 0



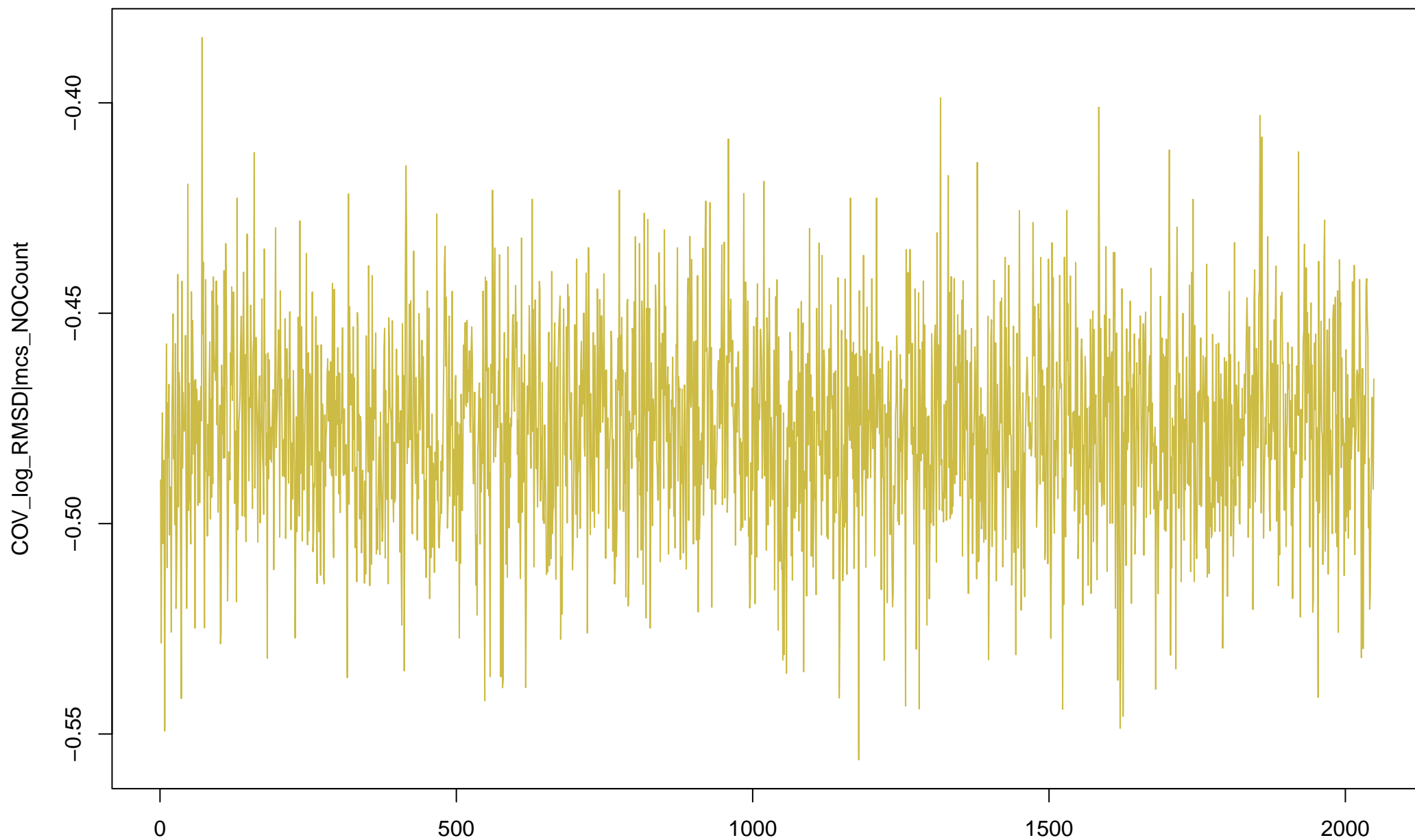
COV_log_RMSD|mcs_RingCount
ESS = 1440 | BMK = 0.0508 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0



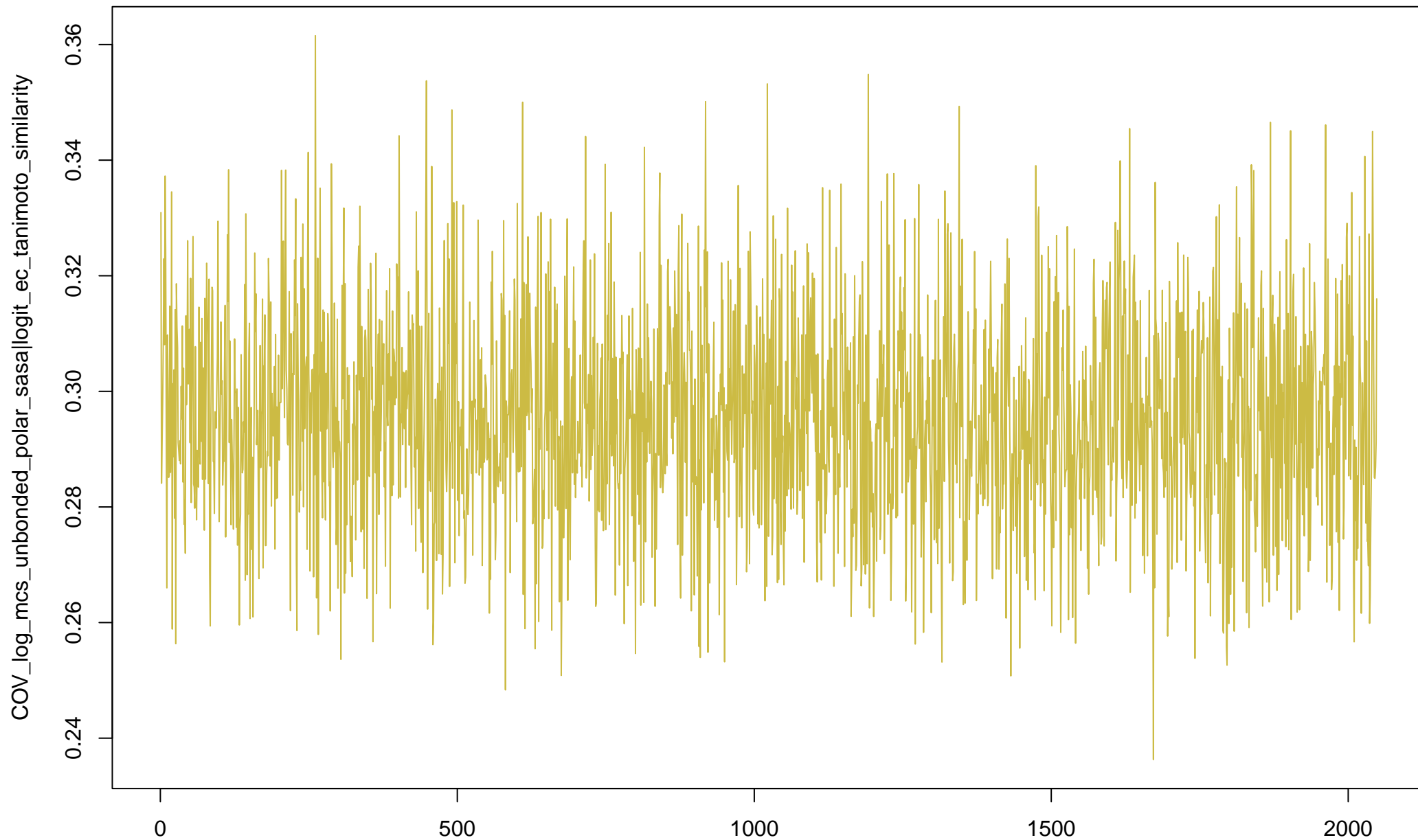
COV_log_RMSD|docked_NumRotatableBonds
ESS = 1550 | BMK = 0.0441 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0



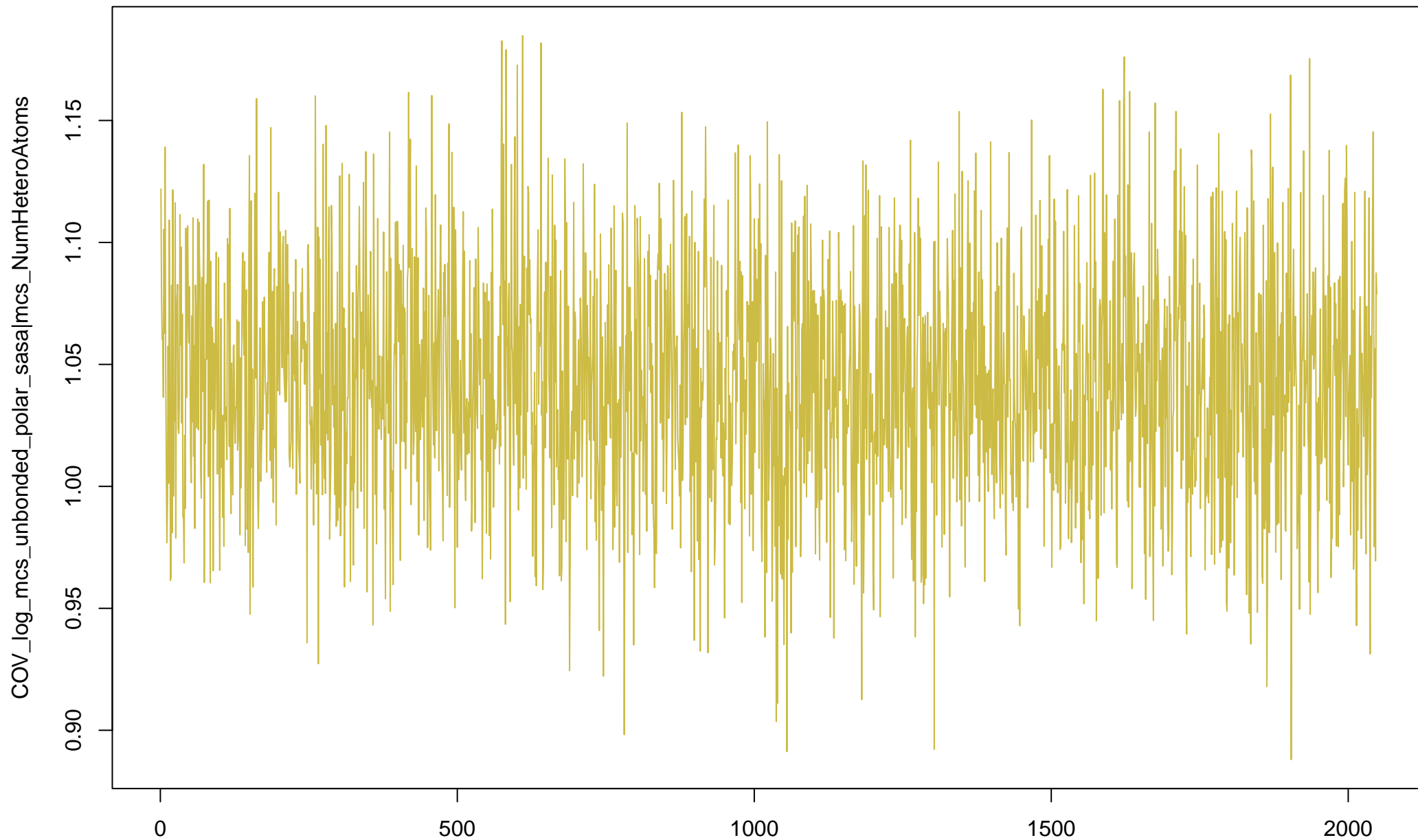
COV_log_RMSD|mcs_NOCount
ESS = 1840 | BMK = 0.0418 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0



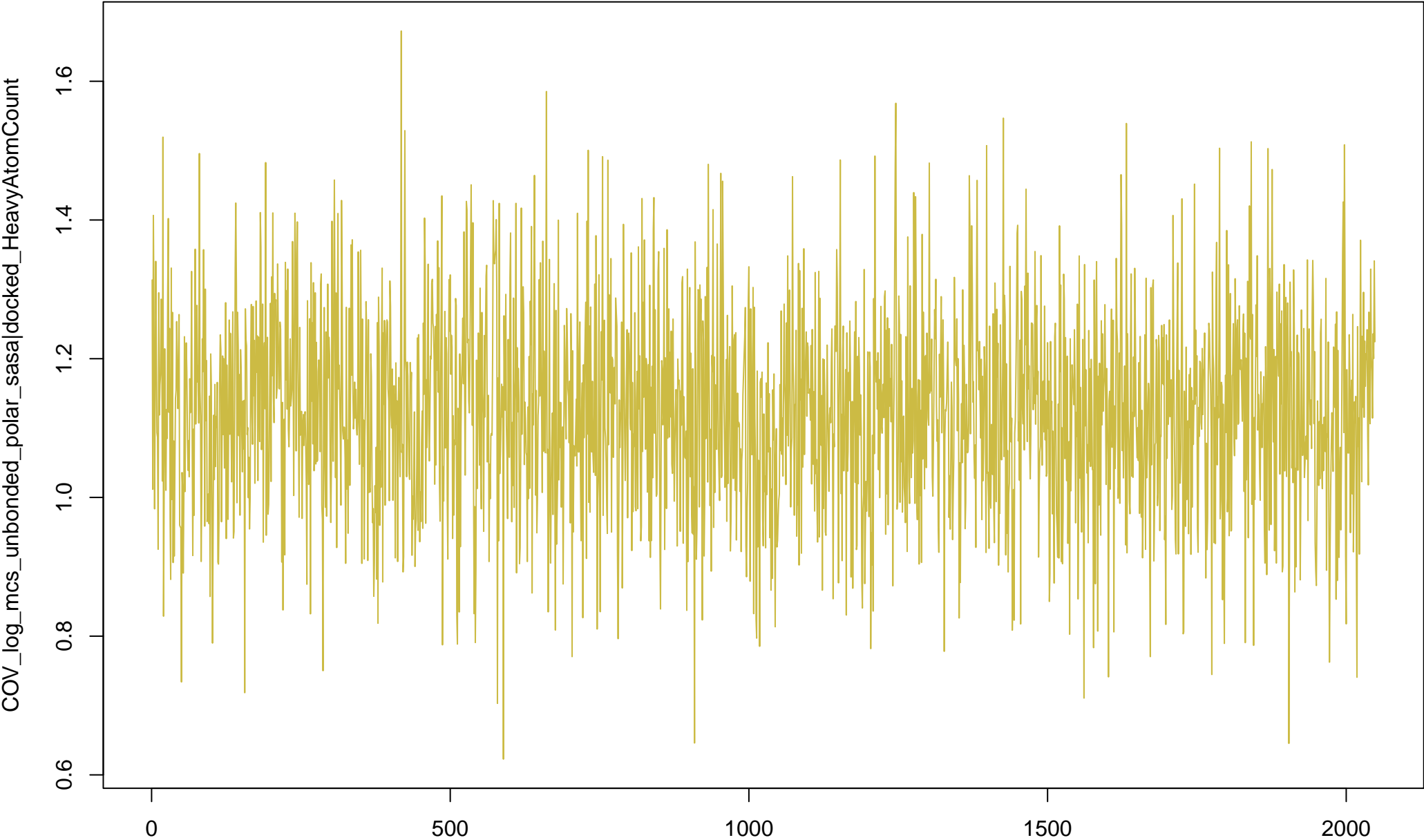
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1840 | BMK = 0.0473 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0



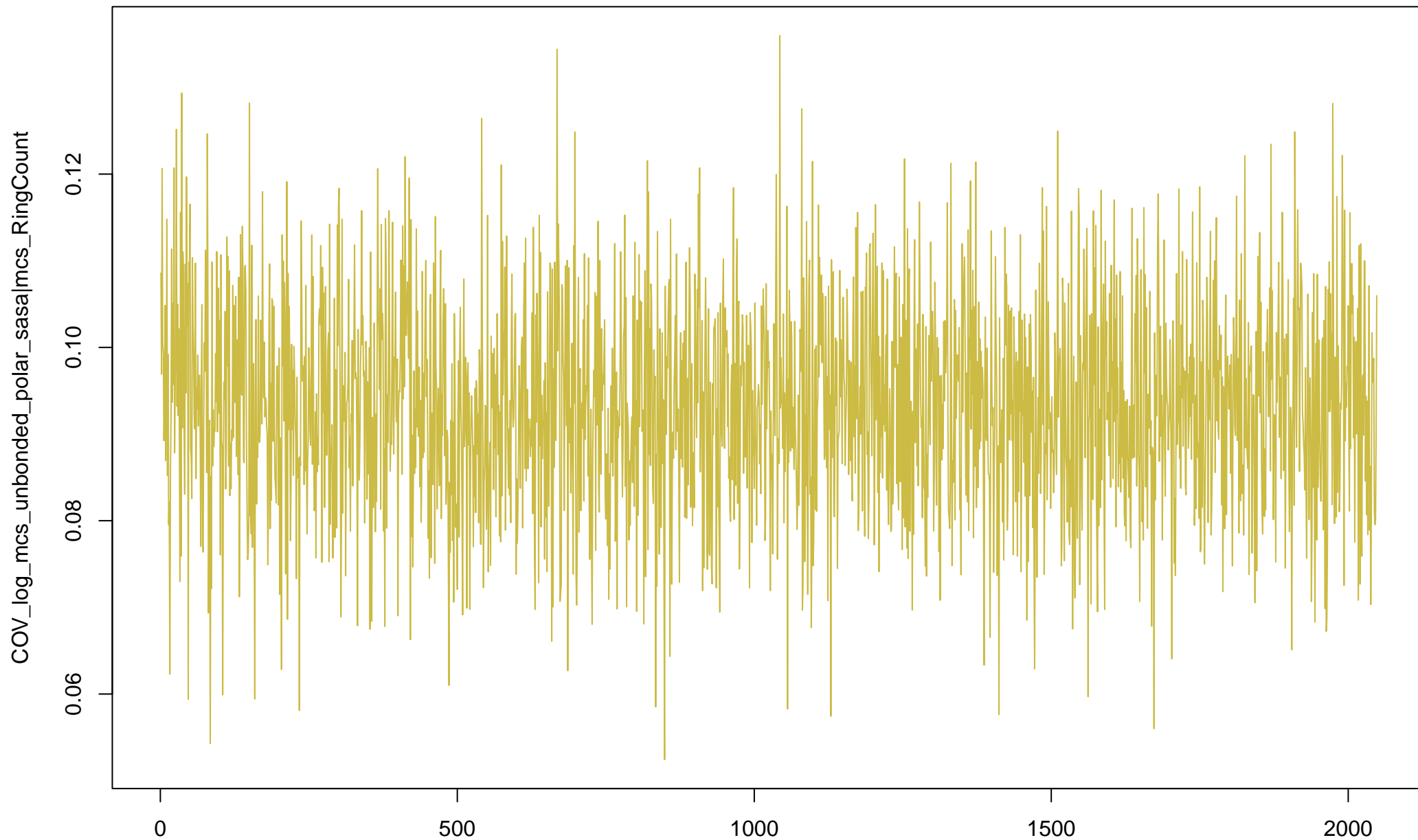
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0501 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0



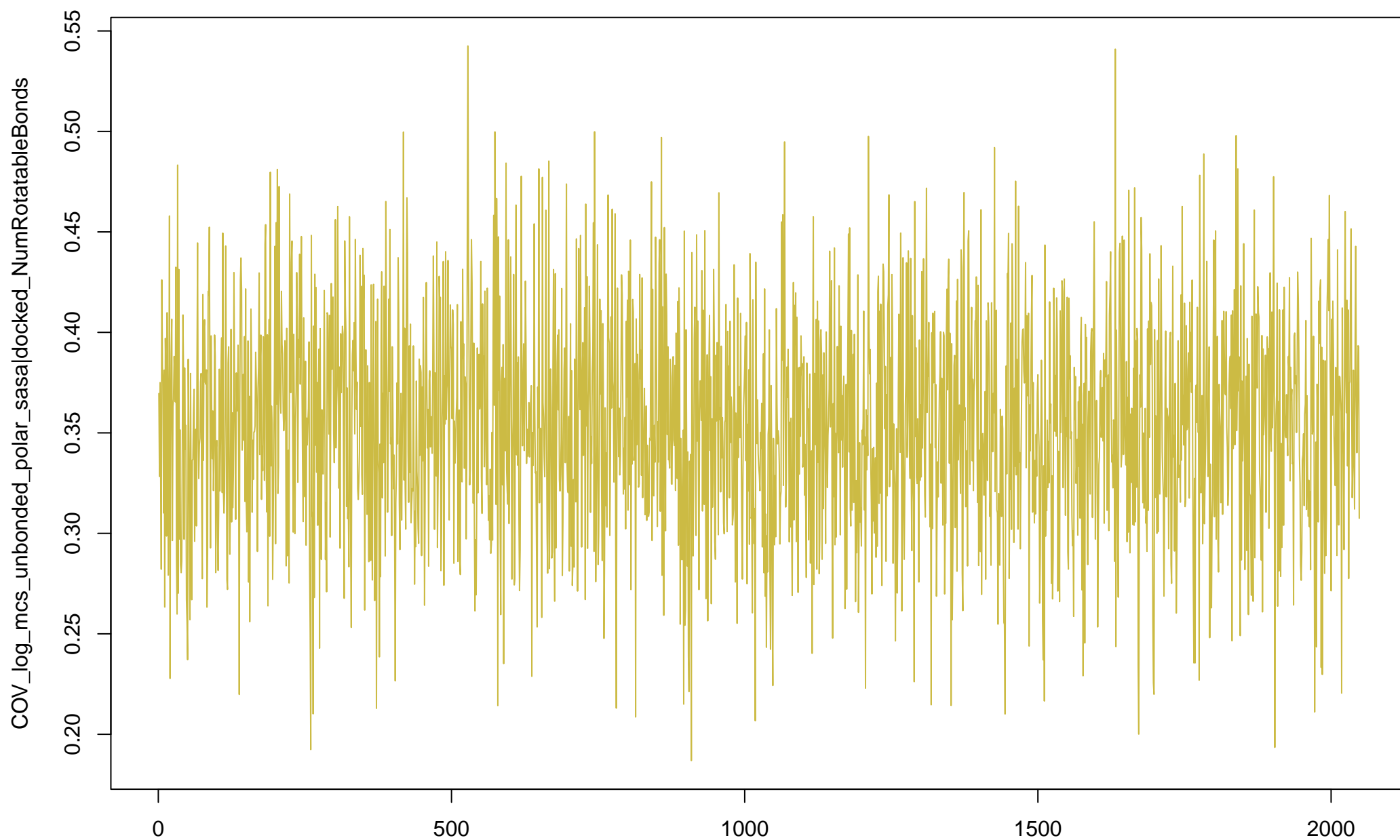
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1890 | BMK = 0.057 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0



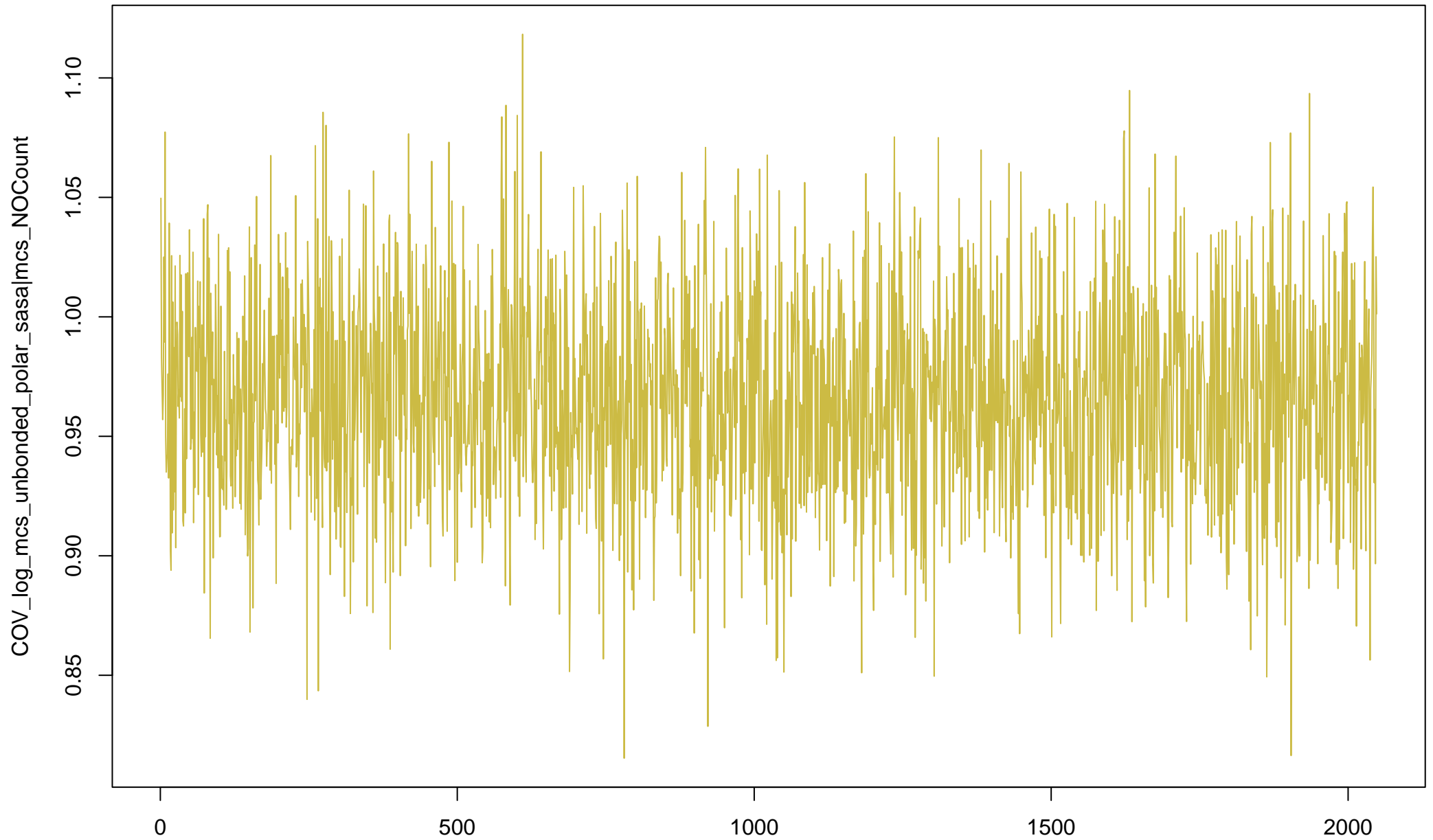
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 2050 | BMK = 0.0344 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0



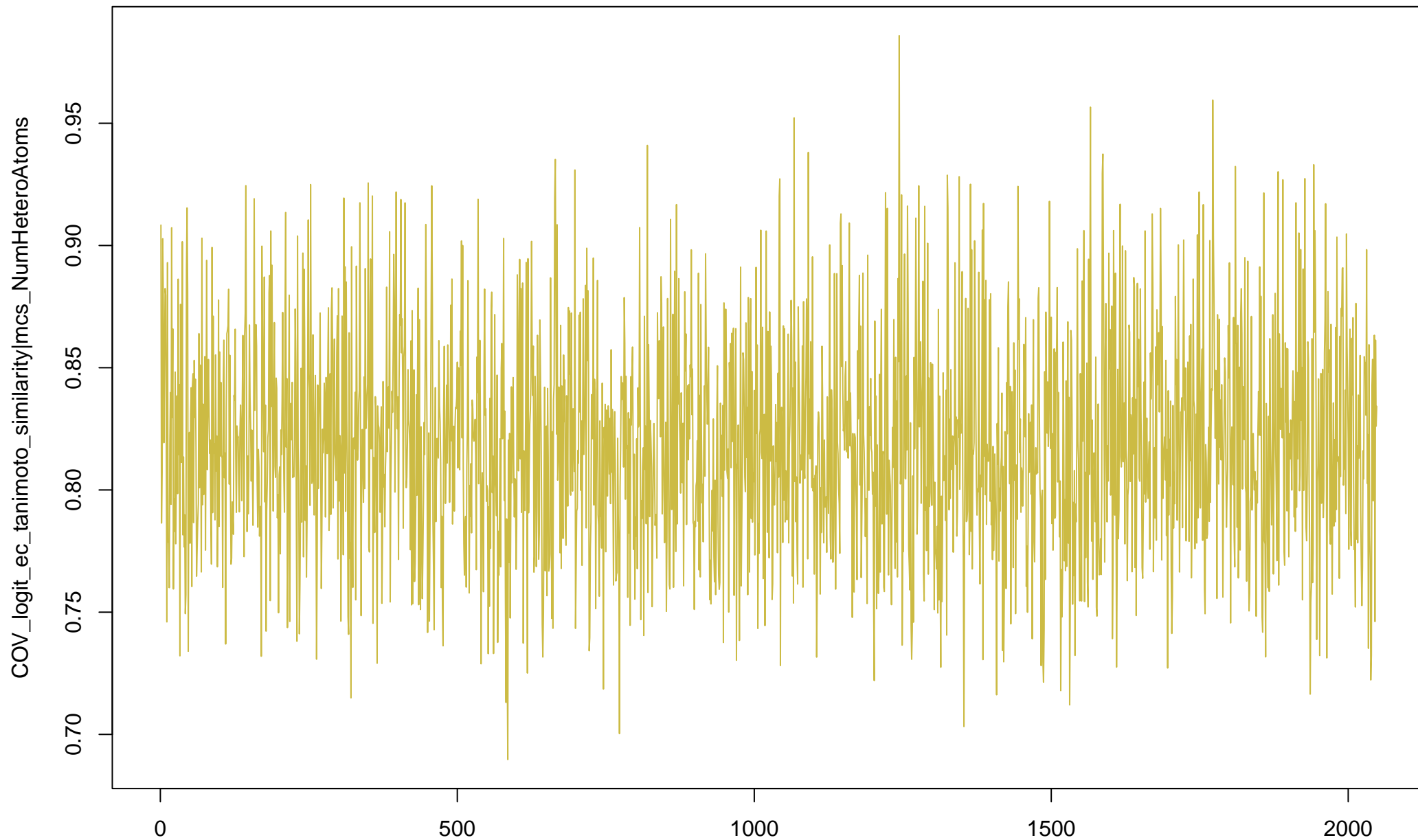
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0363 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0



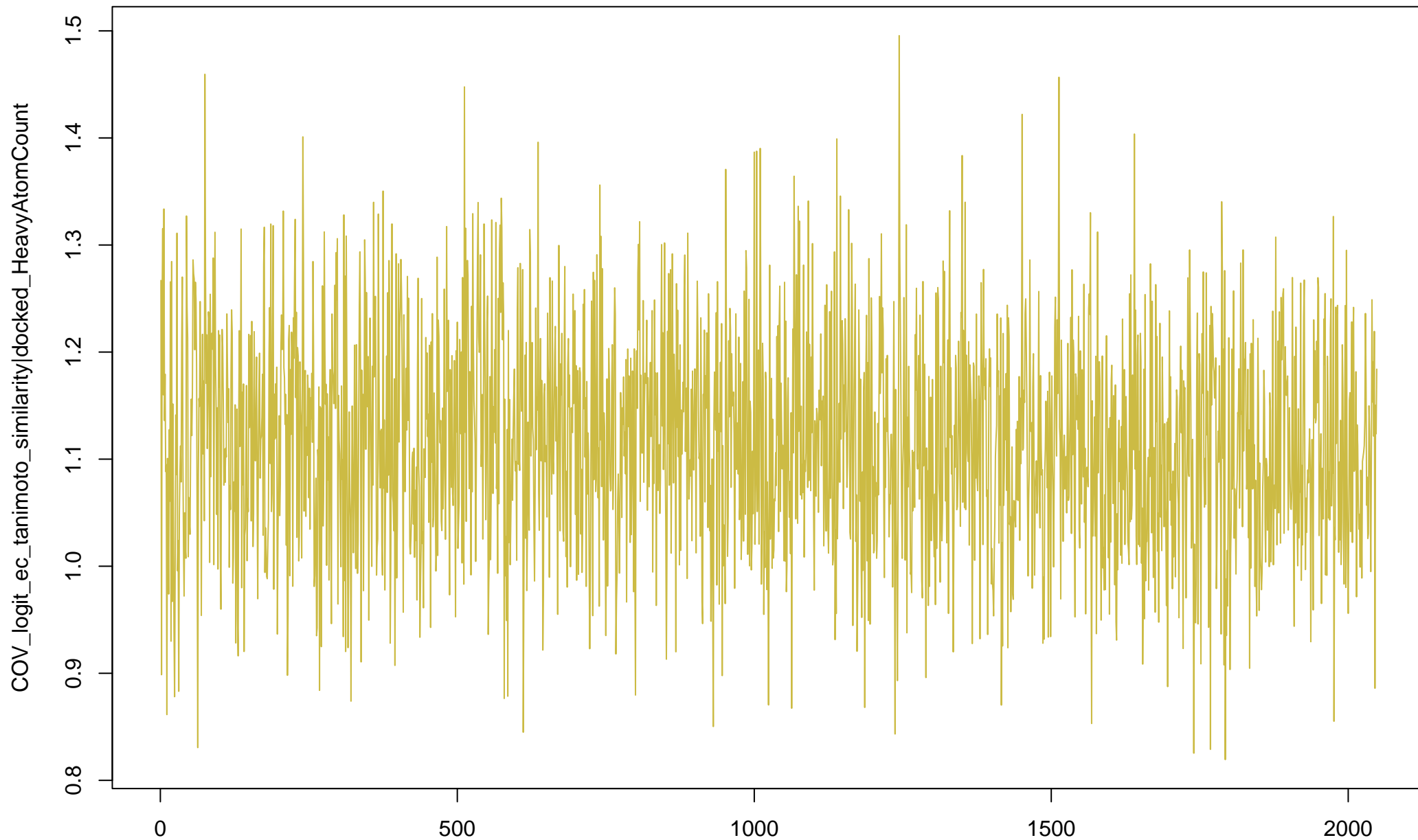
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 2050 | BMK = 0.0528 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0



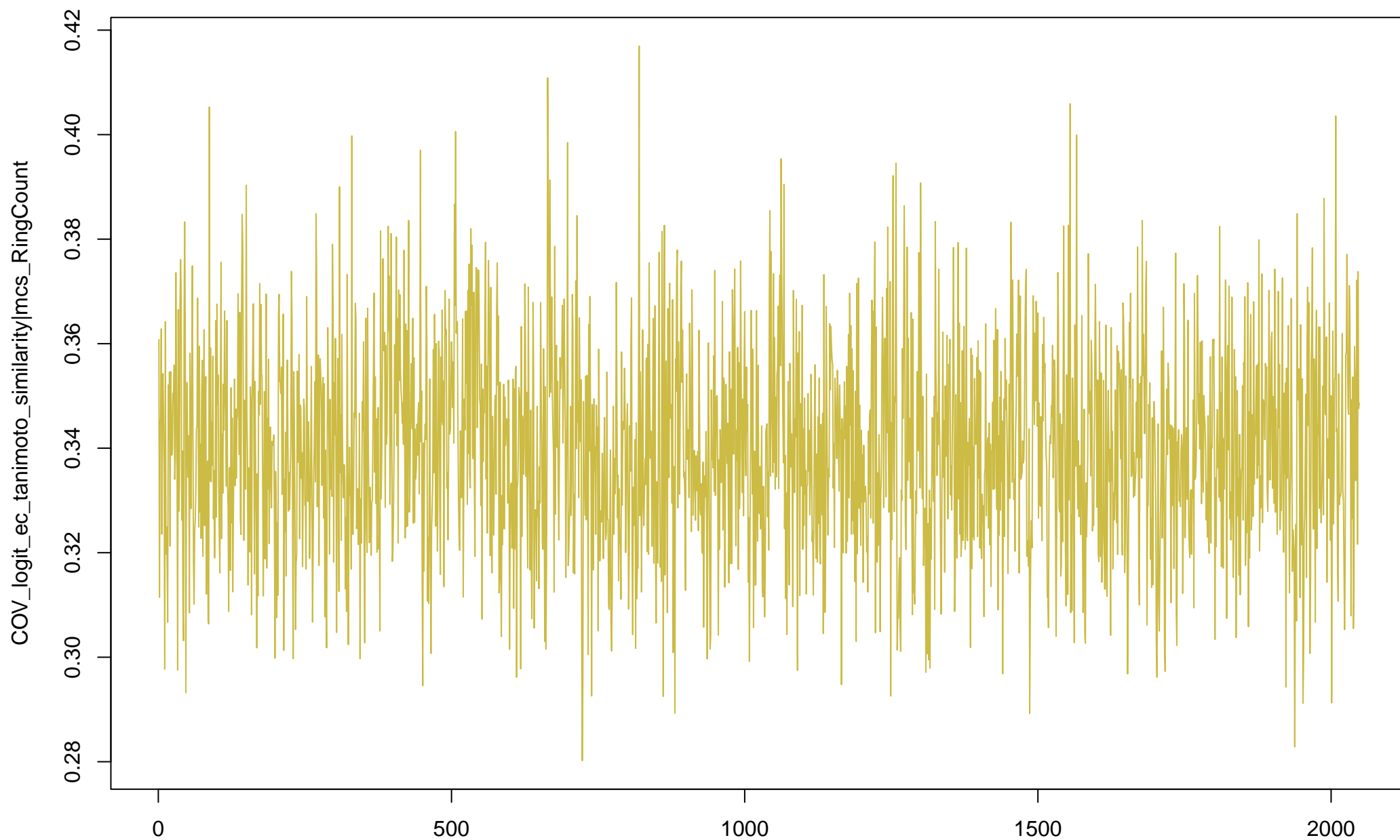
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1750 | BMK = 0.0589 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0



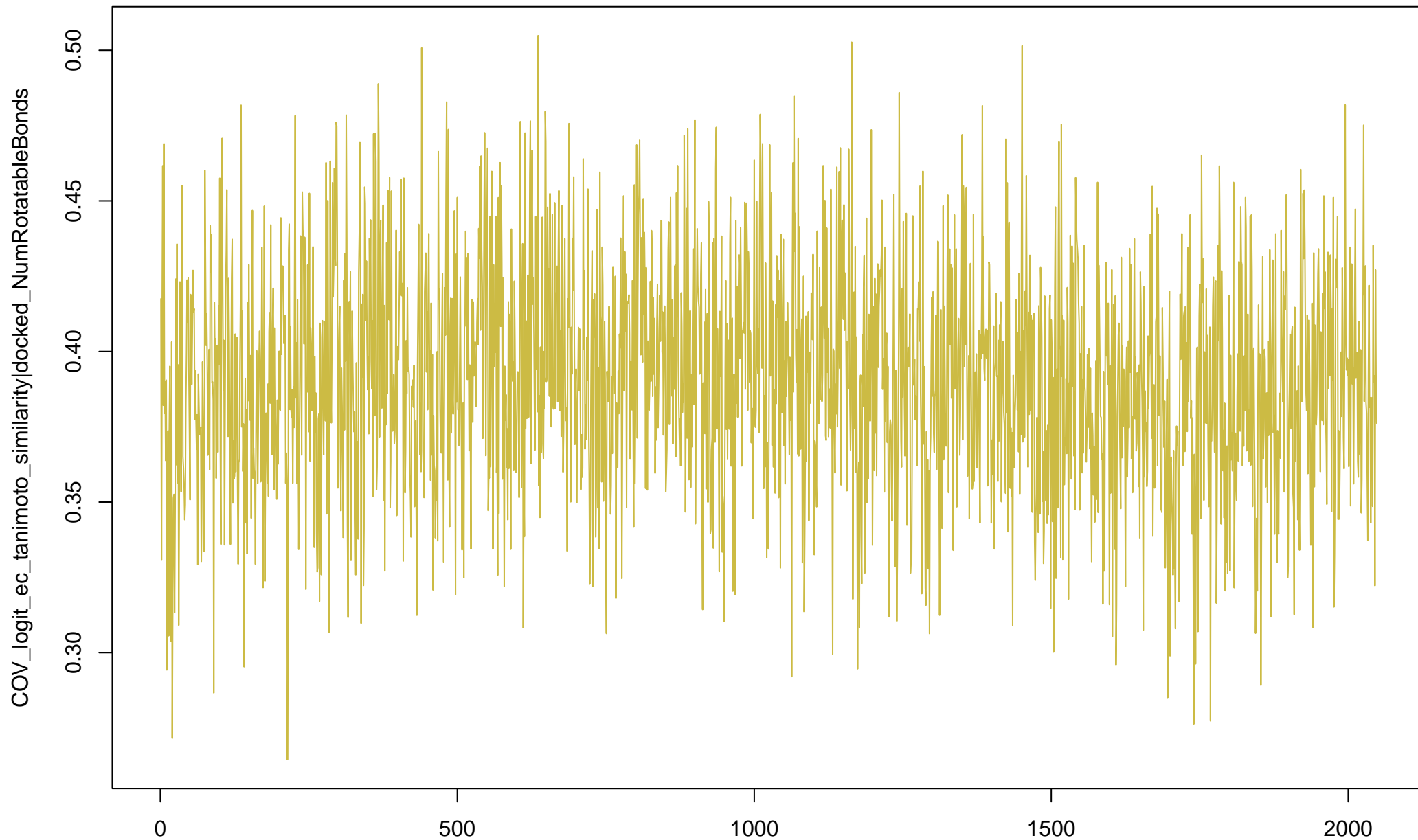
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1490 | BMK = 0.0844 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0



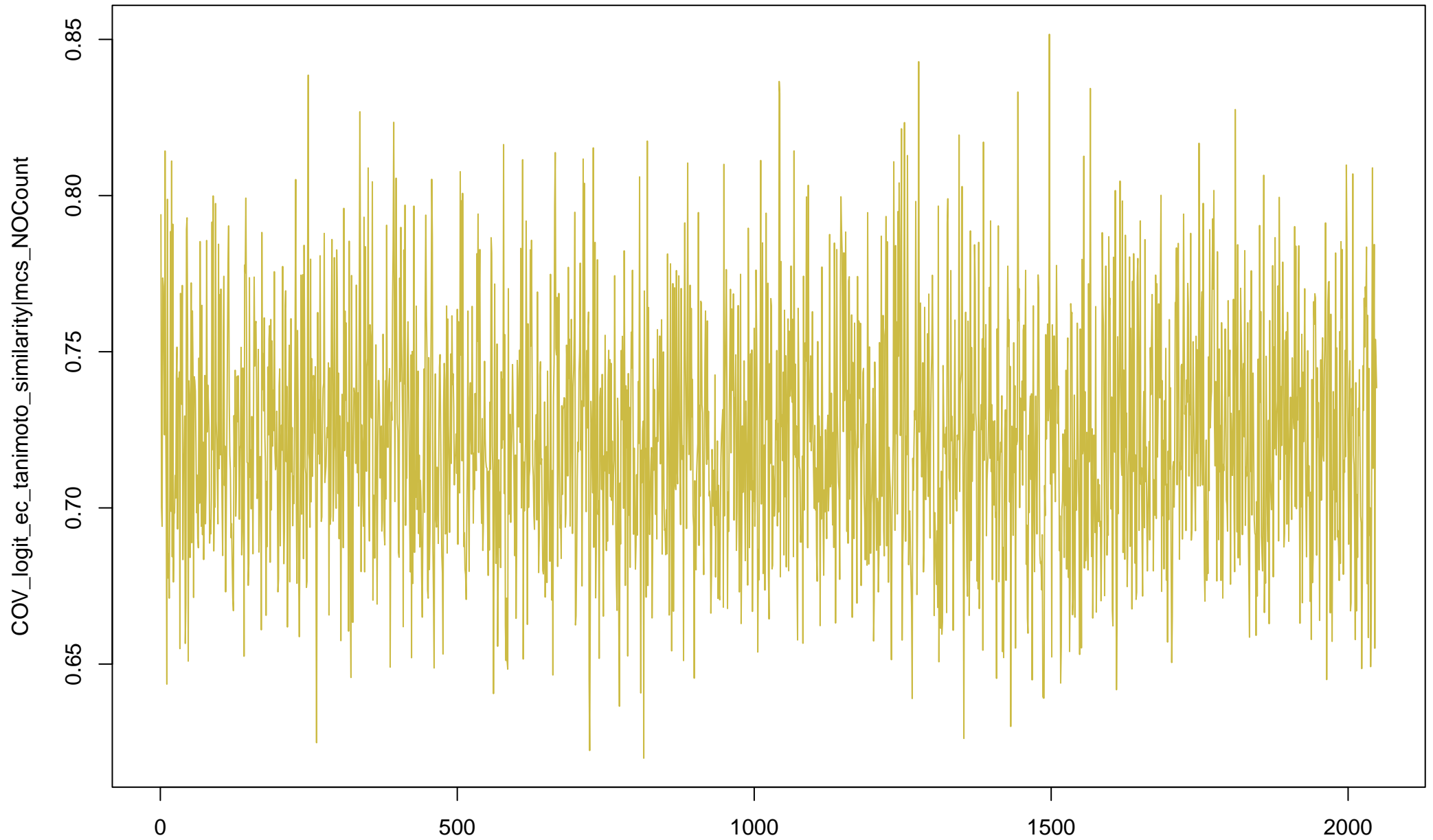
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1530 | BMK = 0.0282 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0



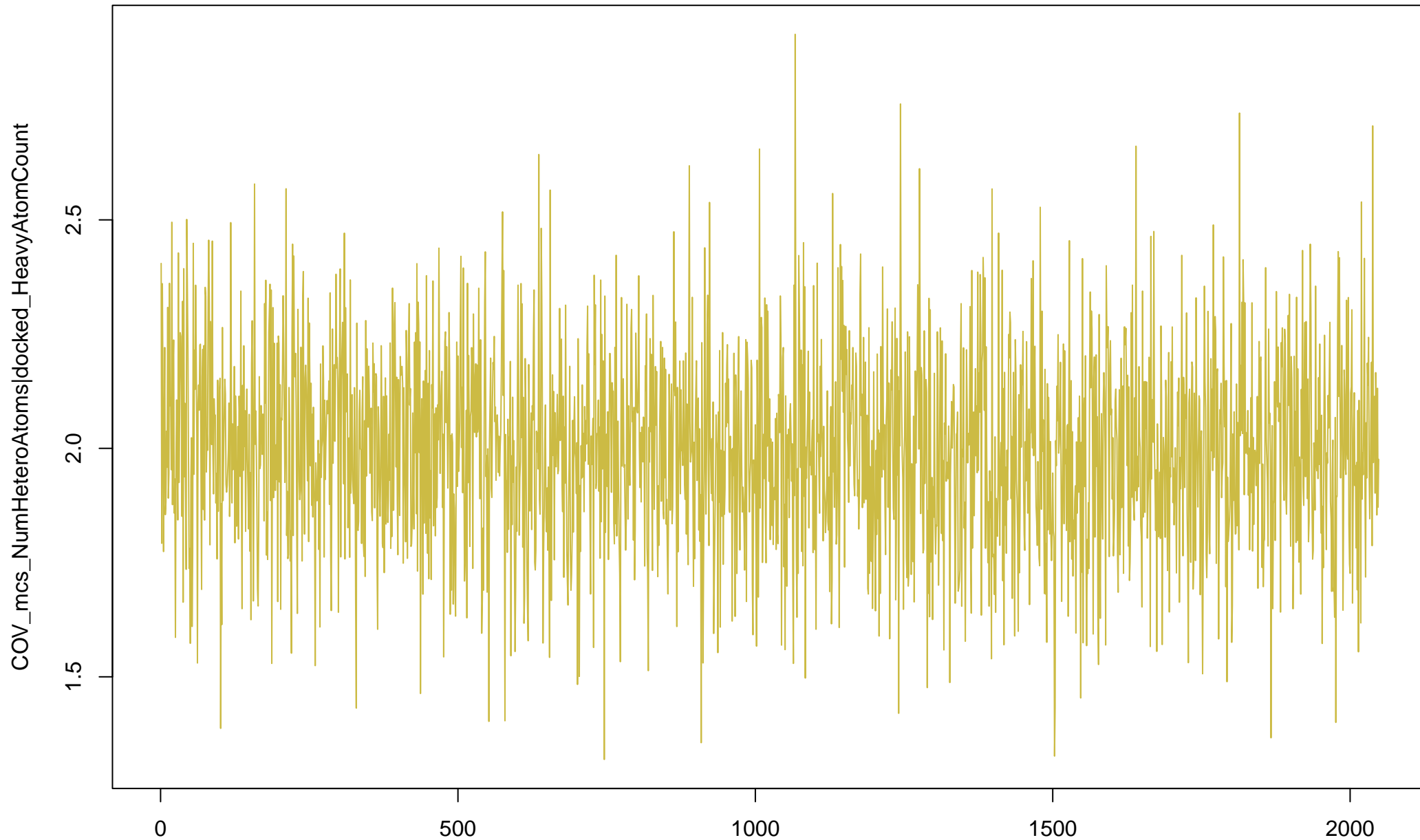
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1040 | BMK = 0.0734 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0



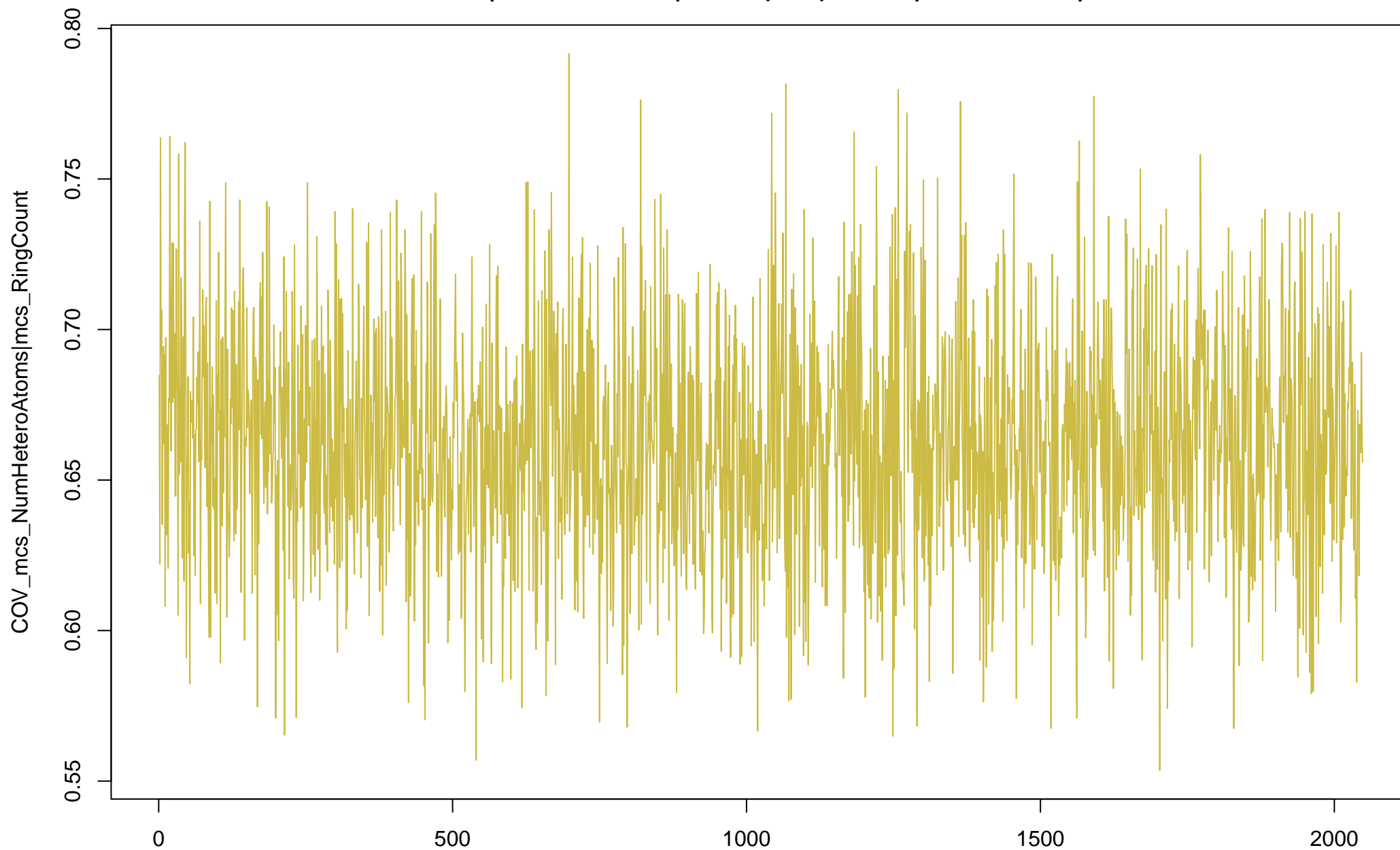
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1730 | BMK = 0.0403 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0



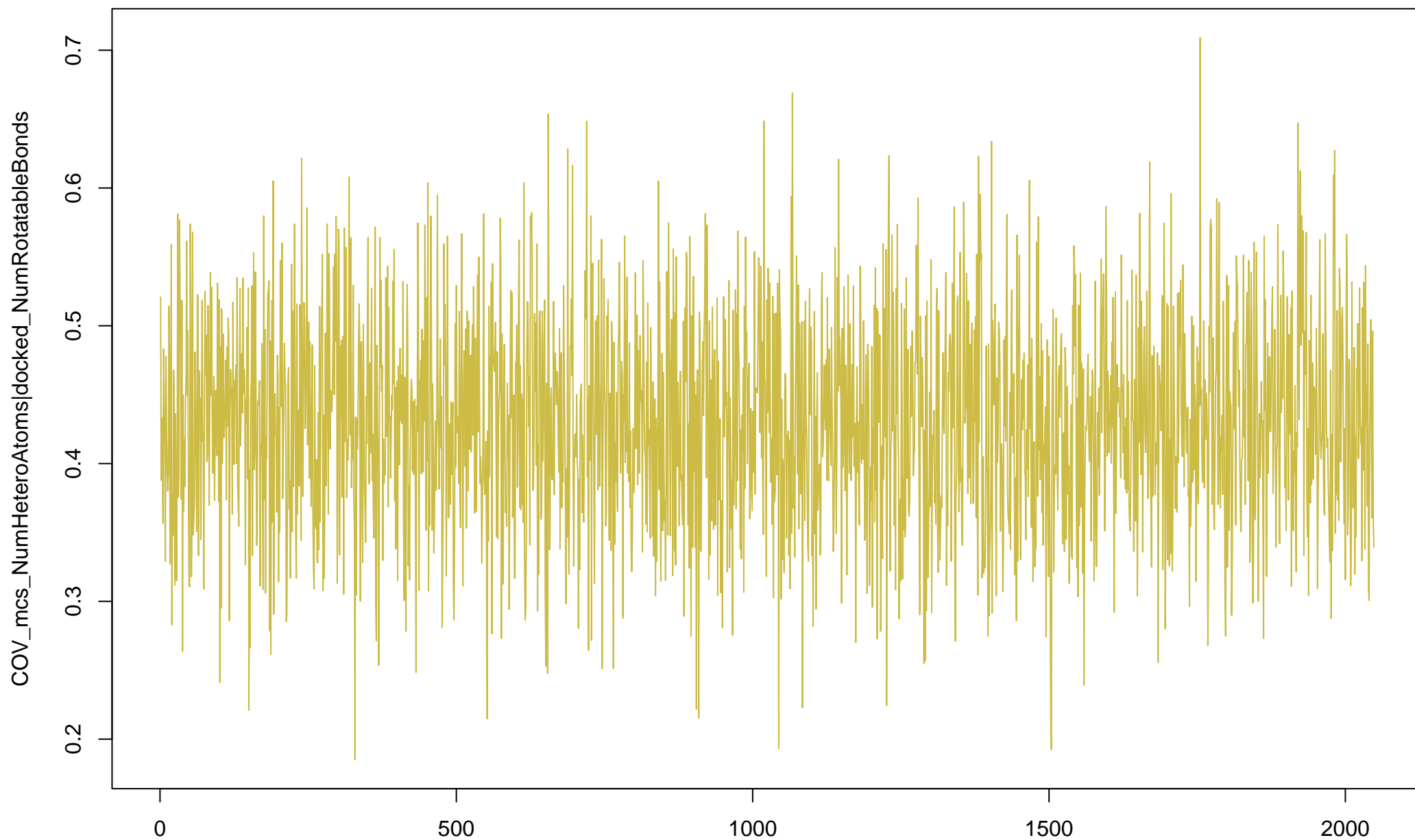
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0508 | MCSE(6.27) = 2.32 | stat: FALSE | burn: 0



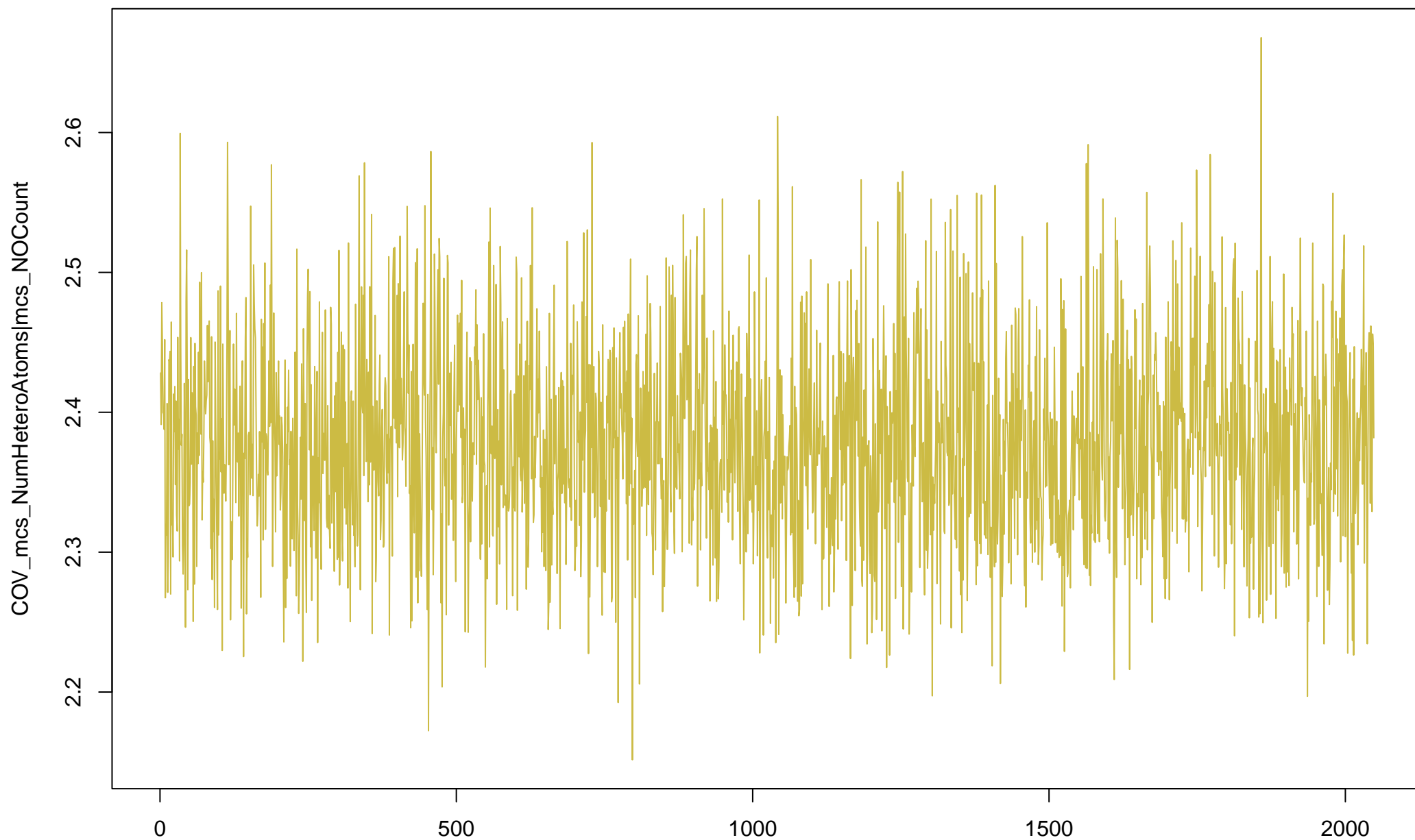
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 2050 | BMK = 0.0389 | MCSE(6.27) = 2.28 | stat: FALSE | burn: 0



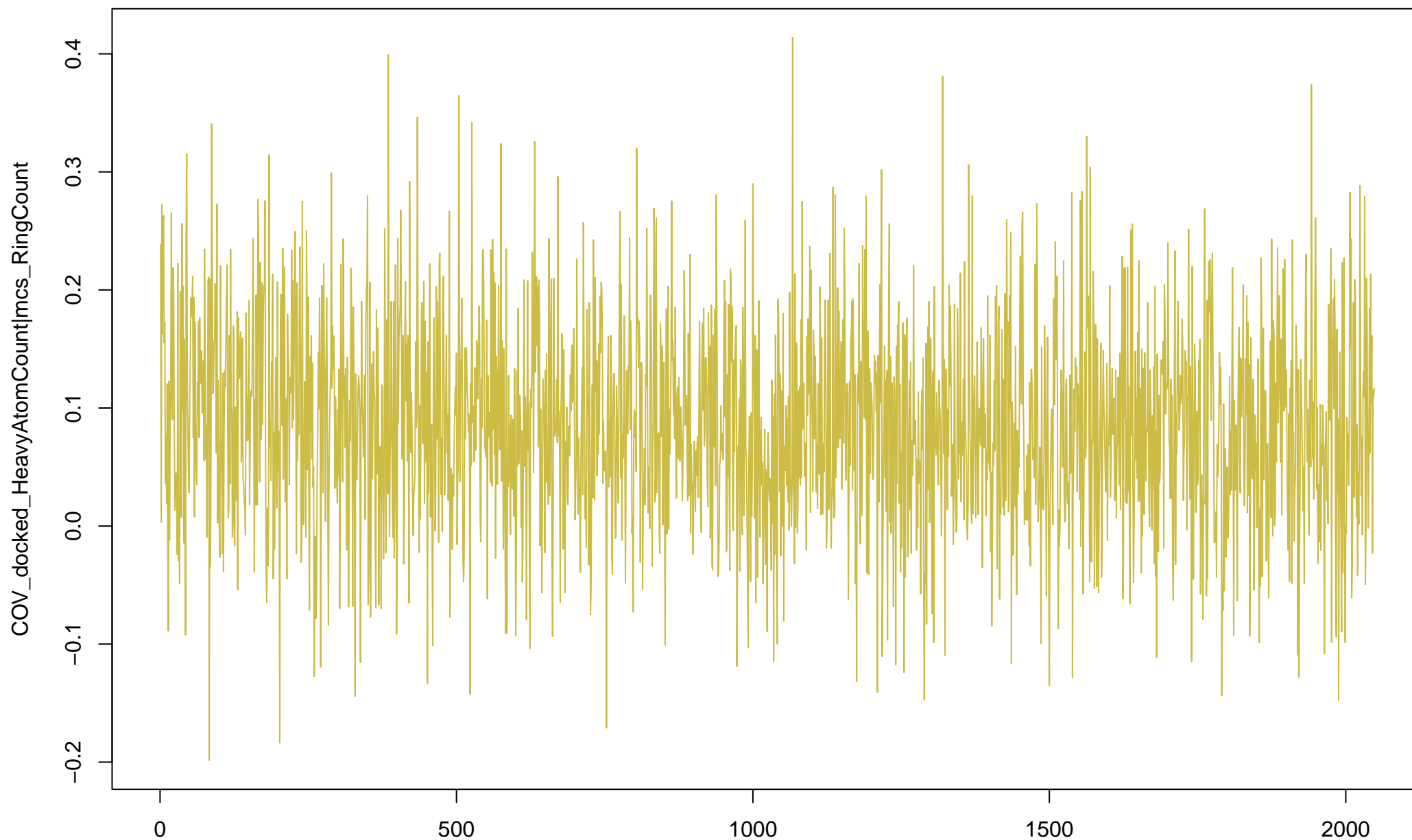
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0393 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0



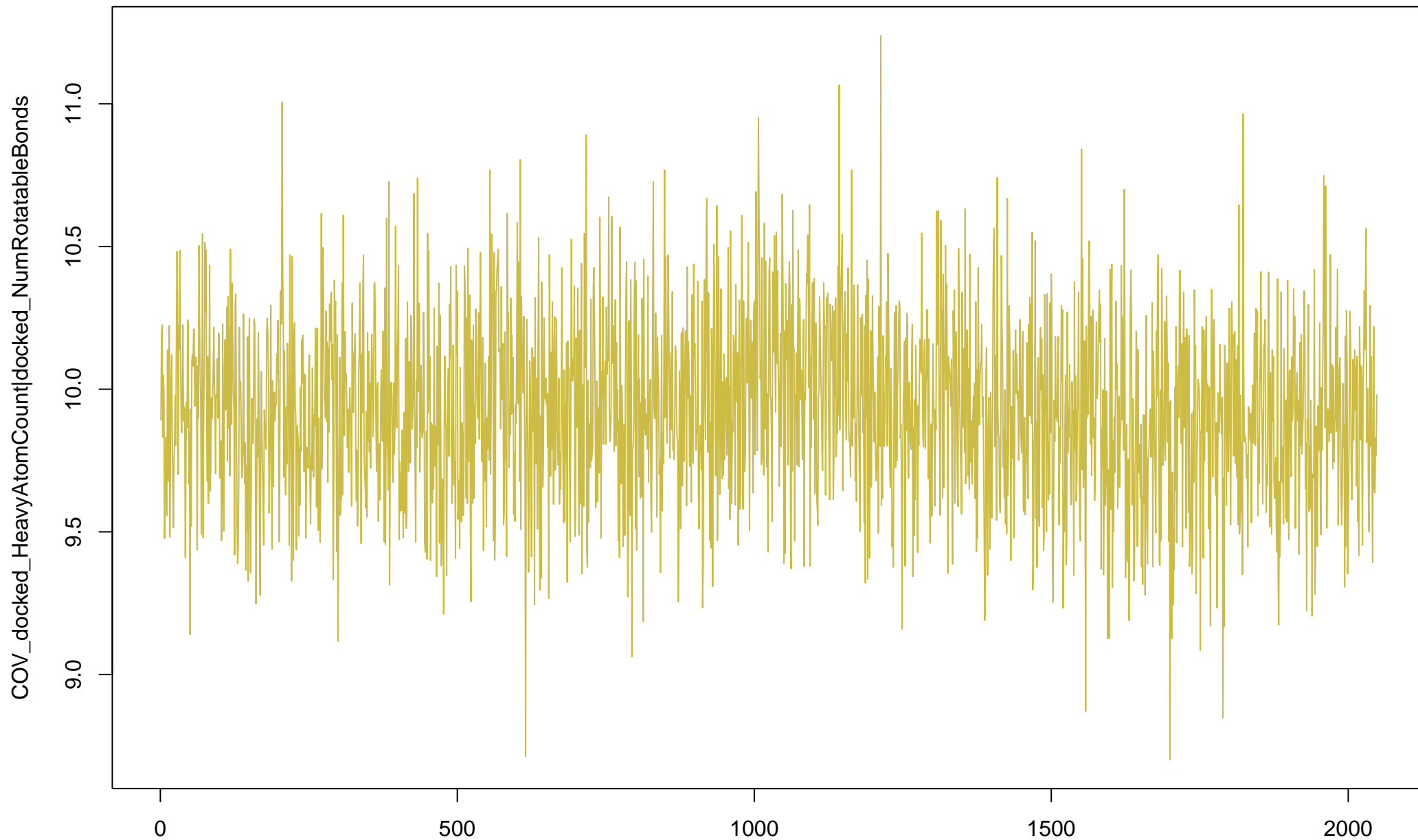
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 2050 | BMK = 0.0444 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0



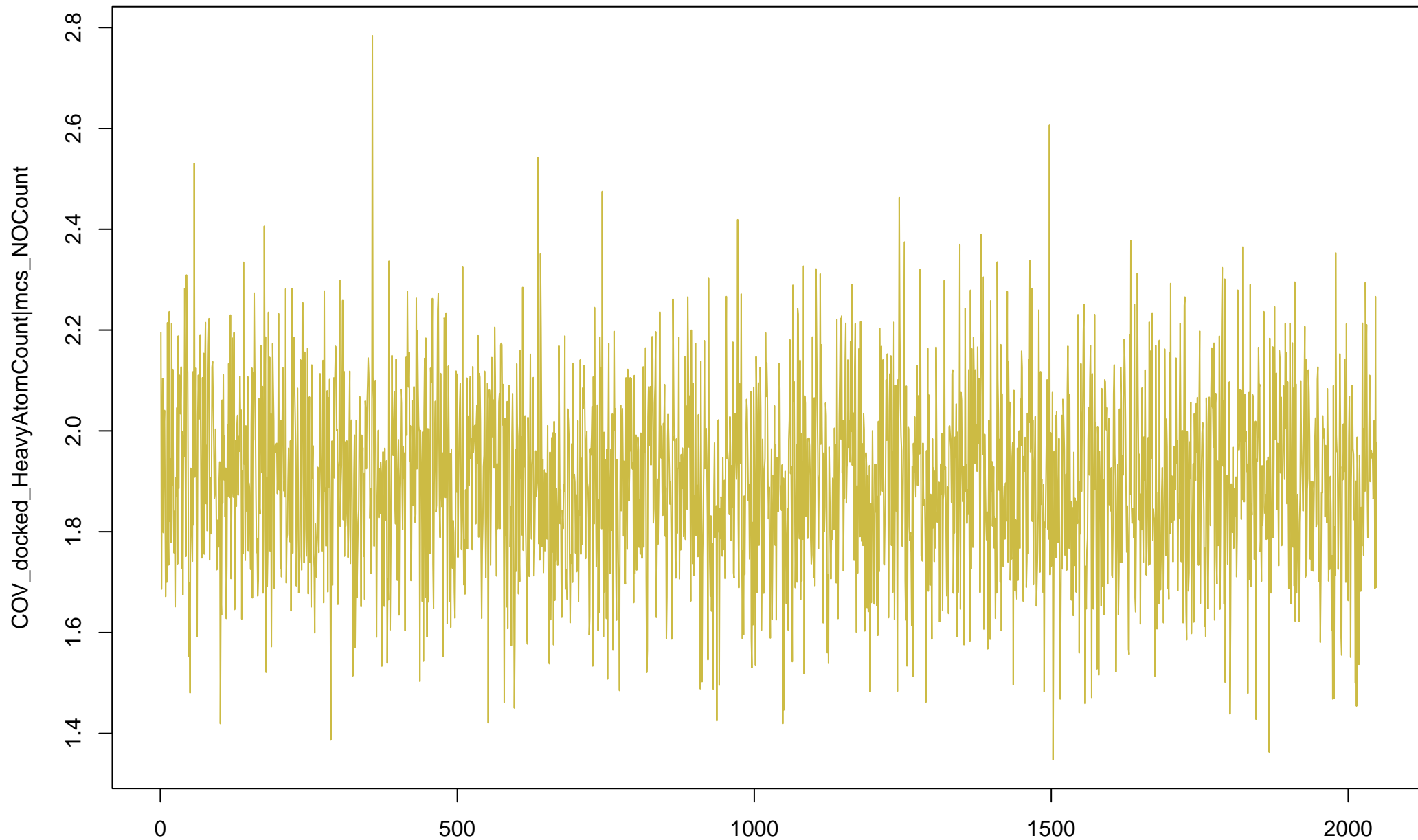
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1840 | BMK = 0.0611 | MCSE(6.27) = 2.39 | stat: FALSE | burn: 0



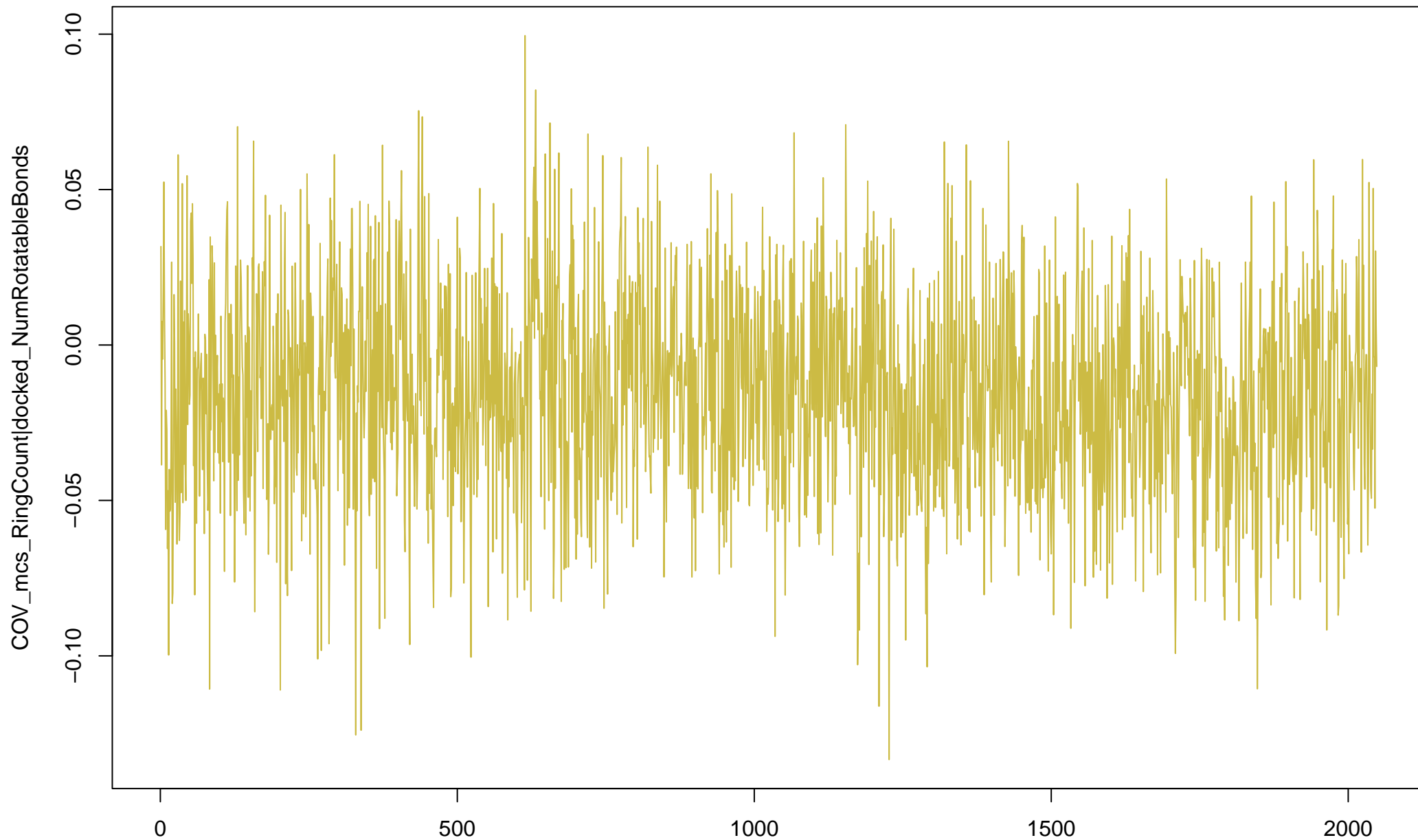
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1810 | BMK = 0.0478 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0



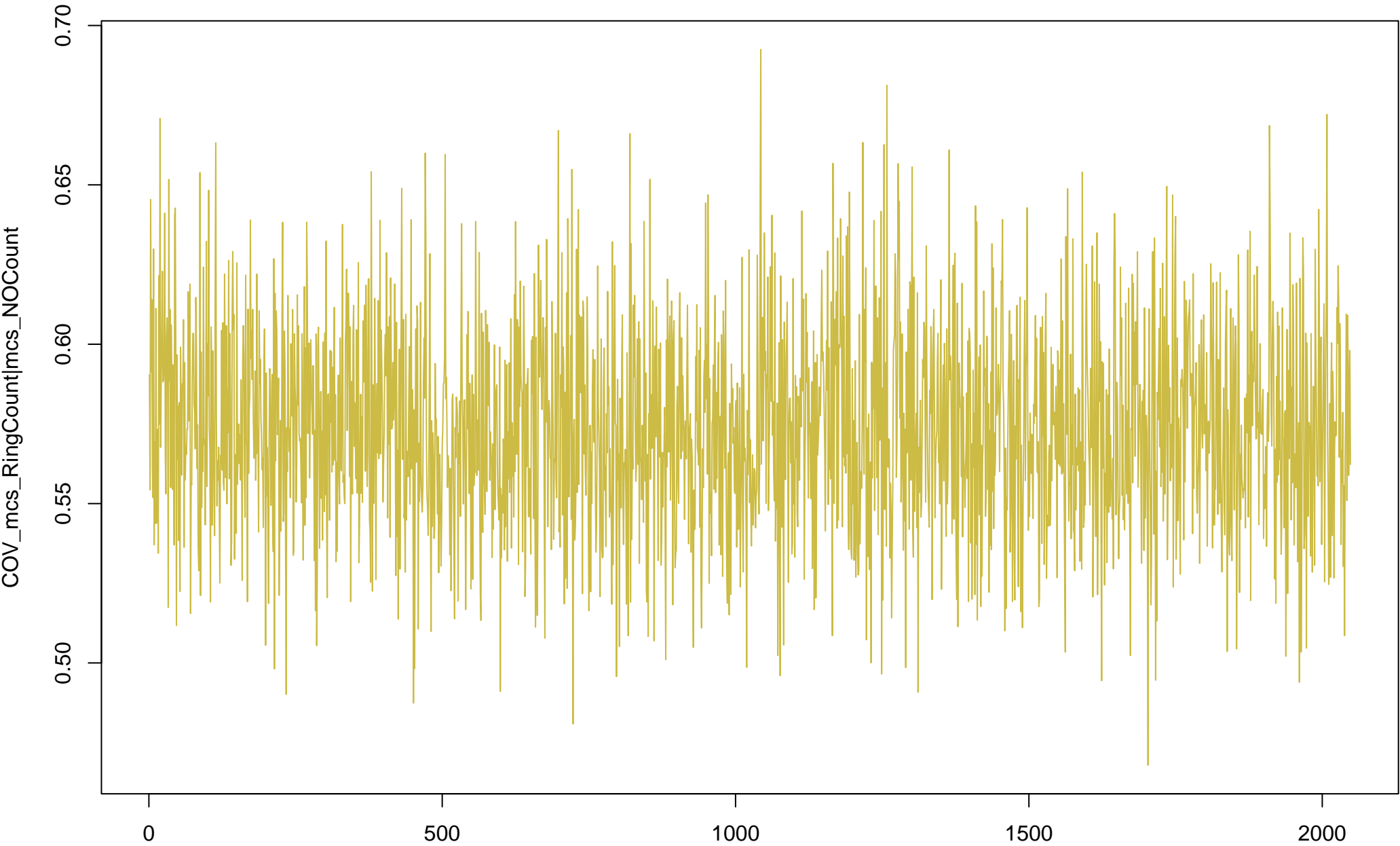
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1750 | BMK = 0.0477 | MCSE(6.27) = 2.49 | stat: FALSE | burn: 0



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1210 | BMK = 0.0725 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0



COV_mcs_RingCount|mcs_NOCount
ESS = 2050 | BMK = 0.036 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 2050 | BMK = 0.0368 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0

