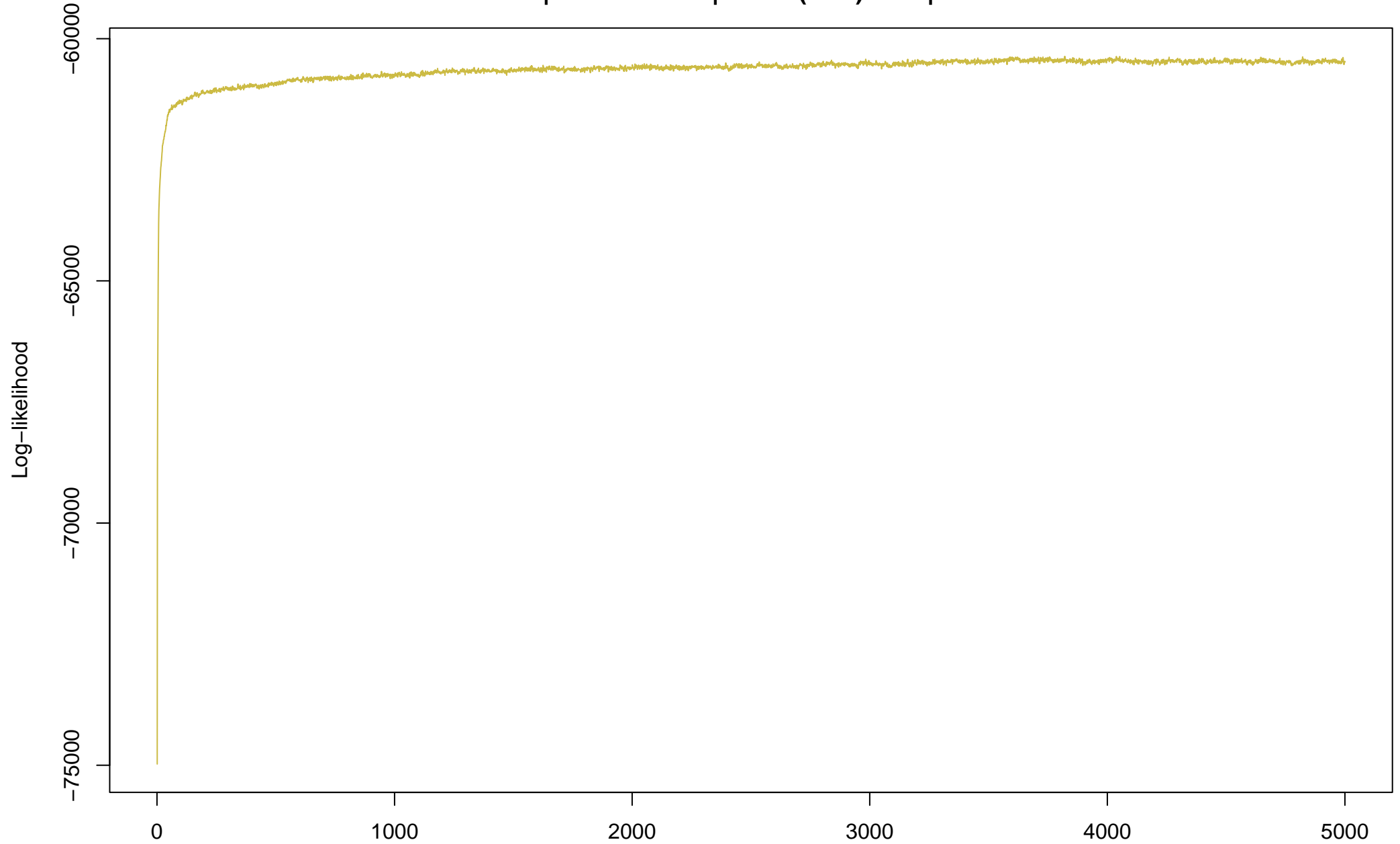


Stats

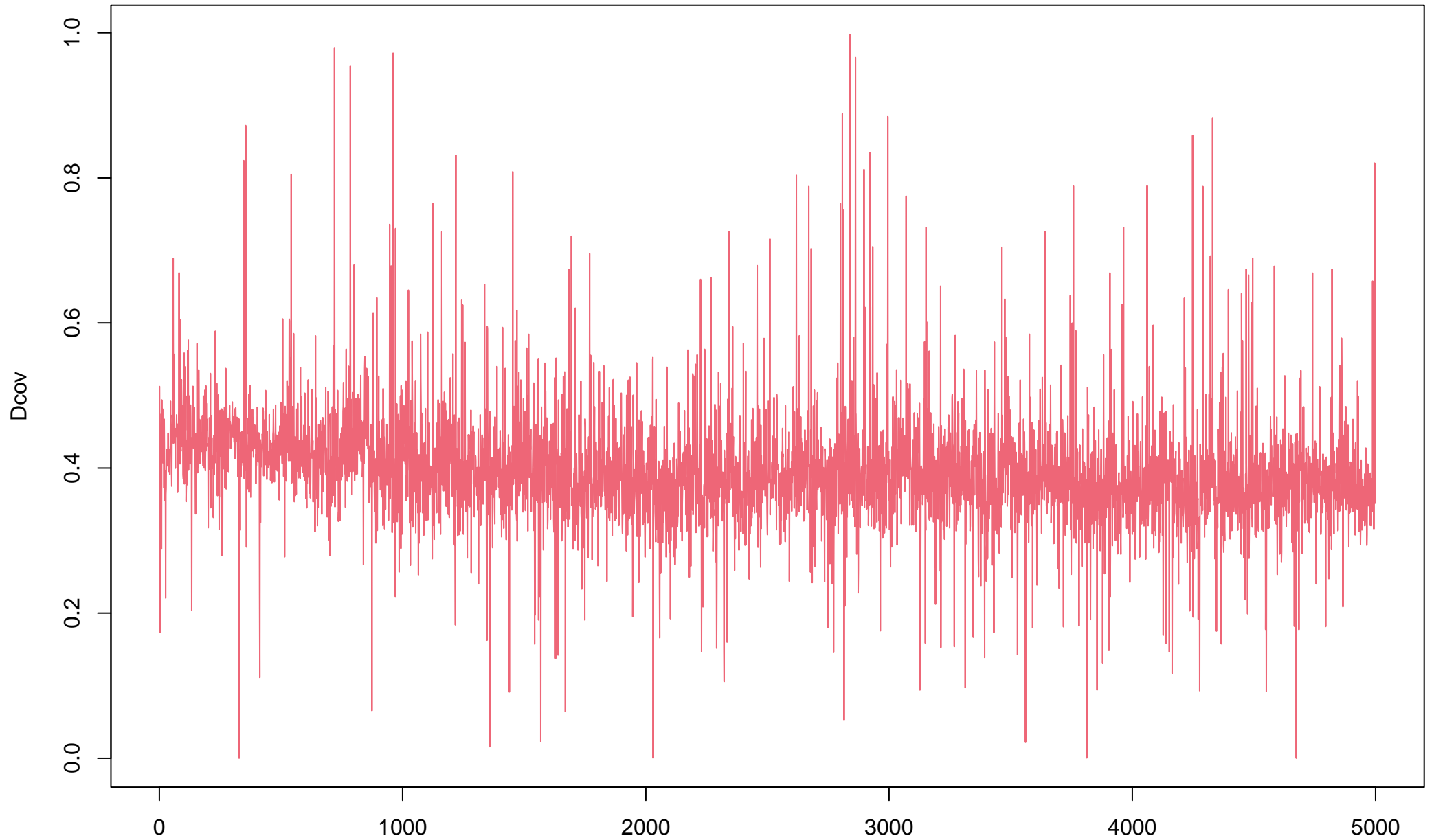
min ESS = 16.9741180604312
max BMK = 0.836055909474012
max MCSE = 12.046611831635
all stationary: FALSE

1:2

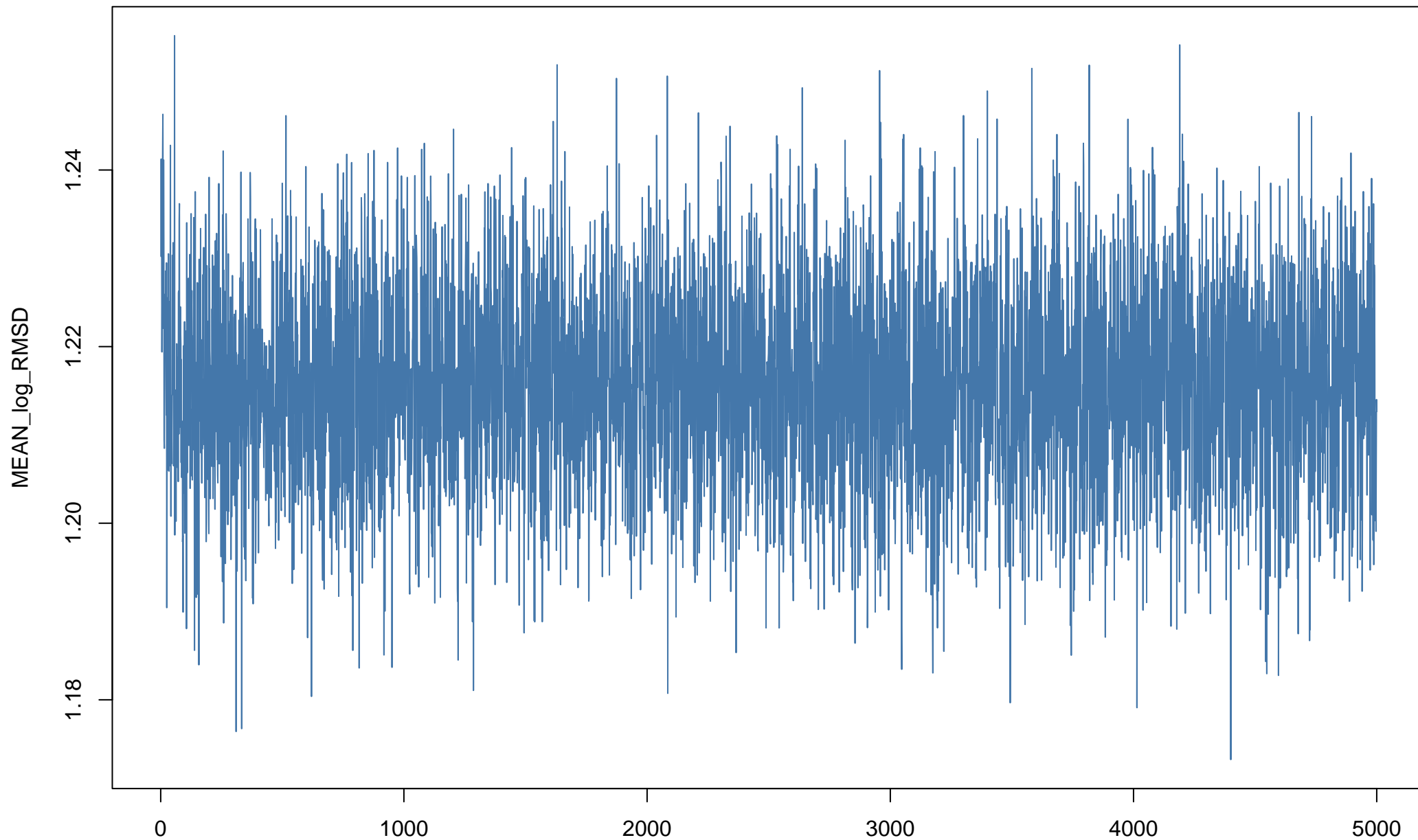
Log-likelihood
ESS = NA | BMK = 0.836 | MCSE(6.27) = 12 | stat: FALSE



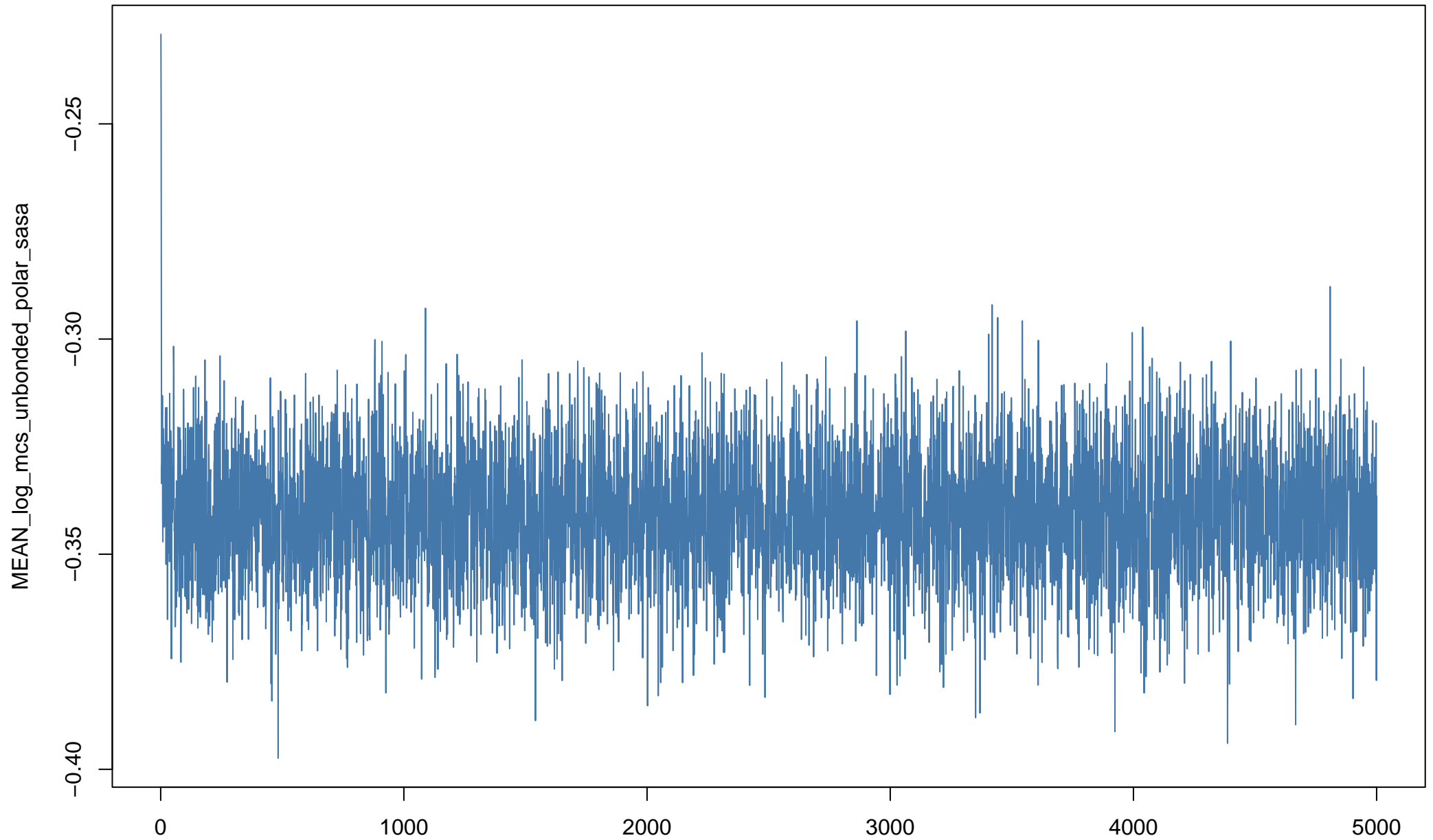
Dcov
ESS = 414 | BMK = 0.154 | MCSE(6.27) = 2.34 | stat: FALSE



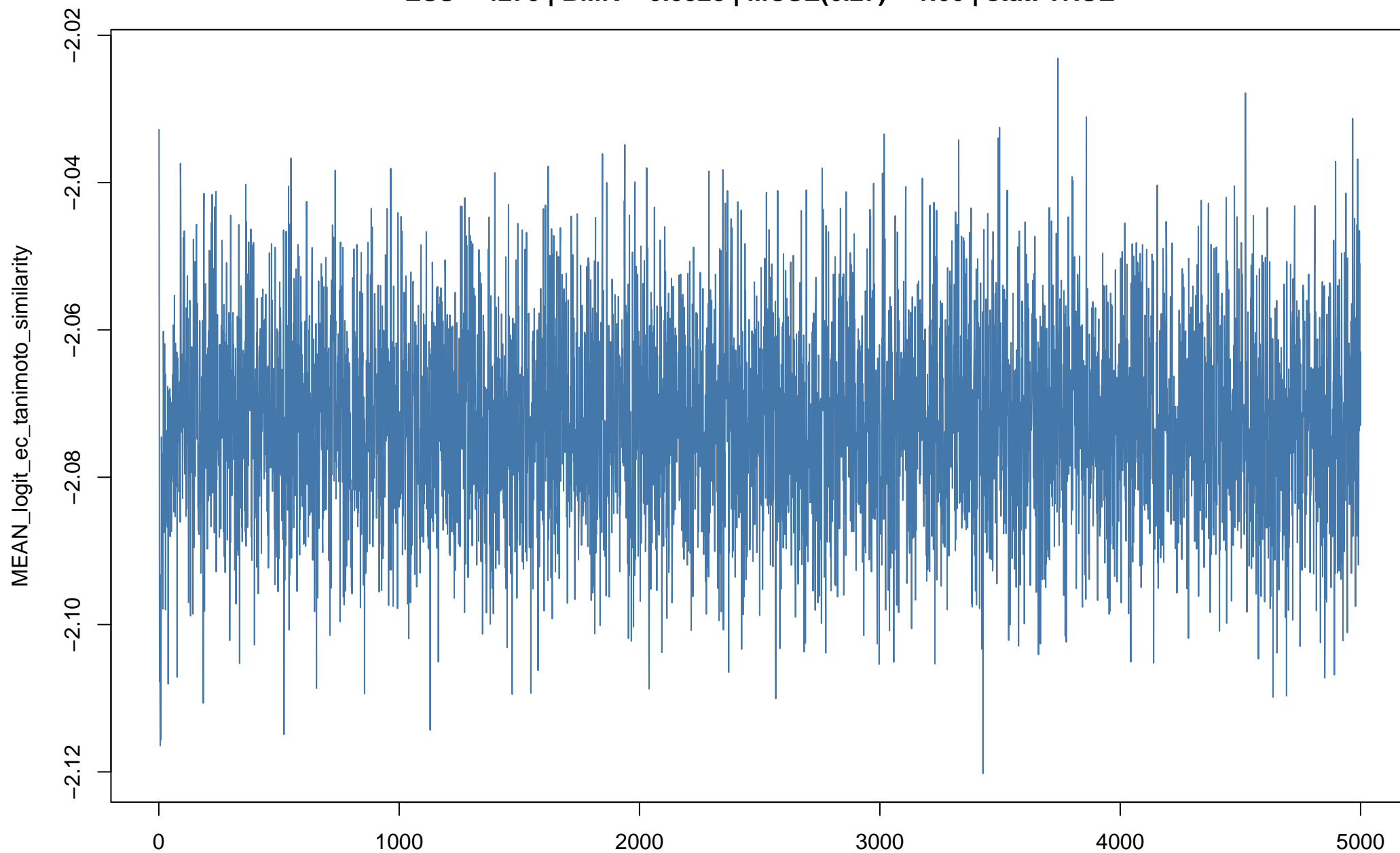
MEAN_log_RMSD
ESS = 4170 | BMK = 0.0421 | MCSE(6.27) = 1.64 | stat: TRUE



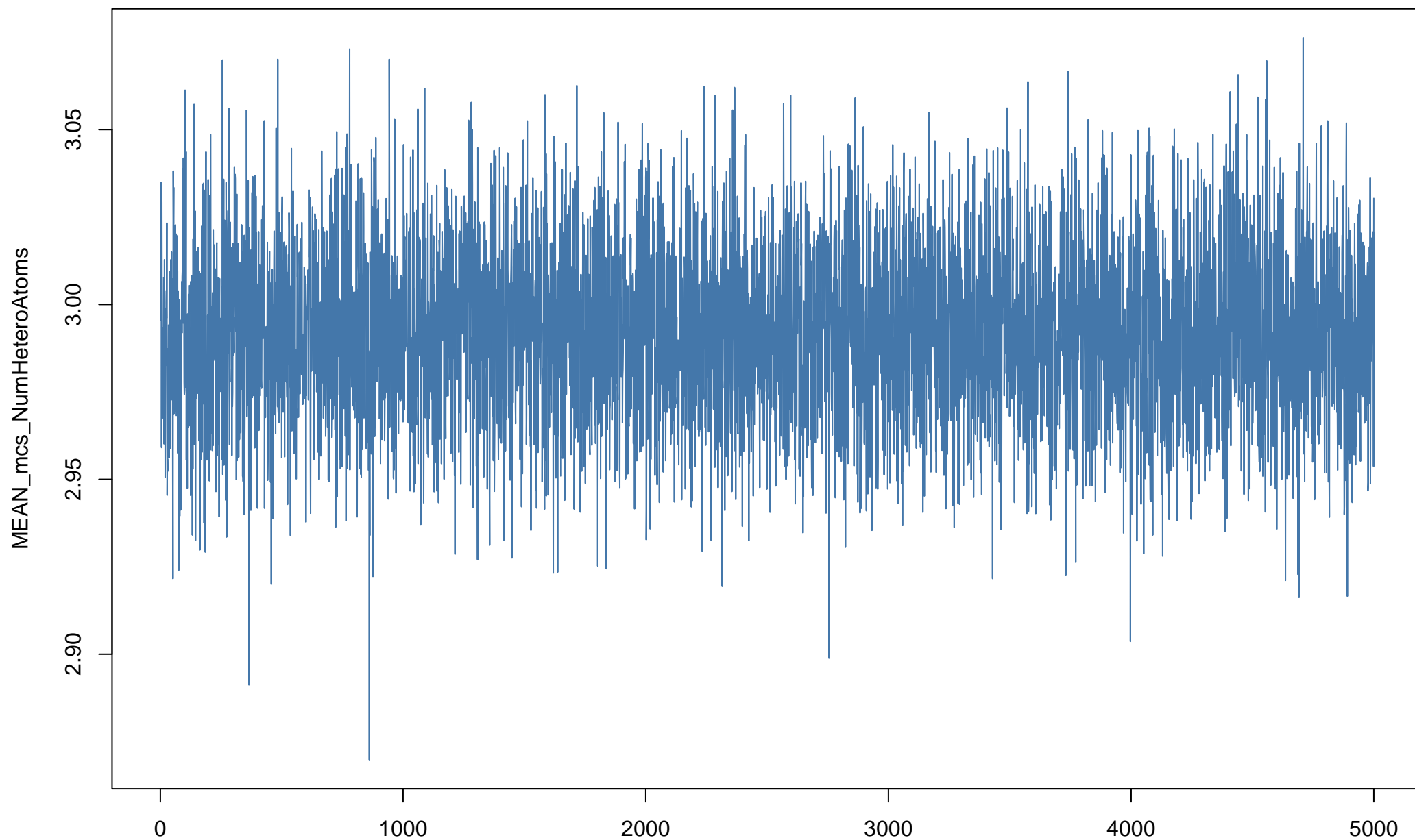
MEAN_log_mcs_unbonded_polar_sasa
ESS = 5000 | BMK = 0.0366 | MCSE(6.27) = 1.44 | stat: TRUE



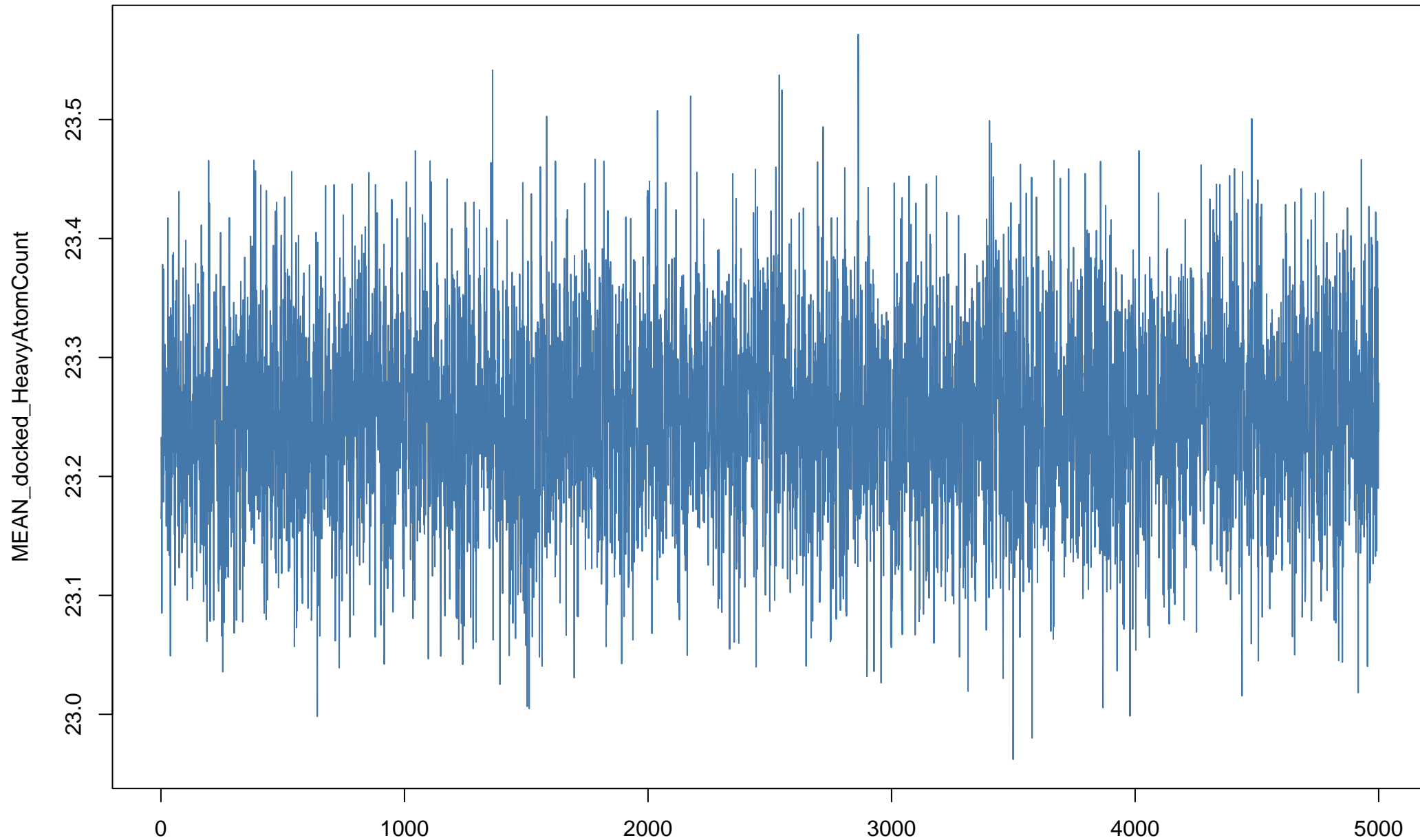
MEAN_logit_ec_tanimoto_similarity
ESS = 4270 | BMK = 0.0328 | MCSE(6.27) = 1.66 | stat: TRUE



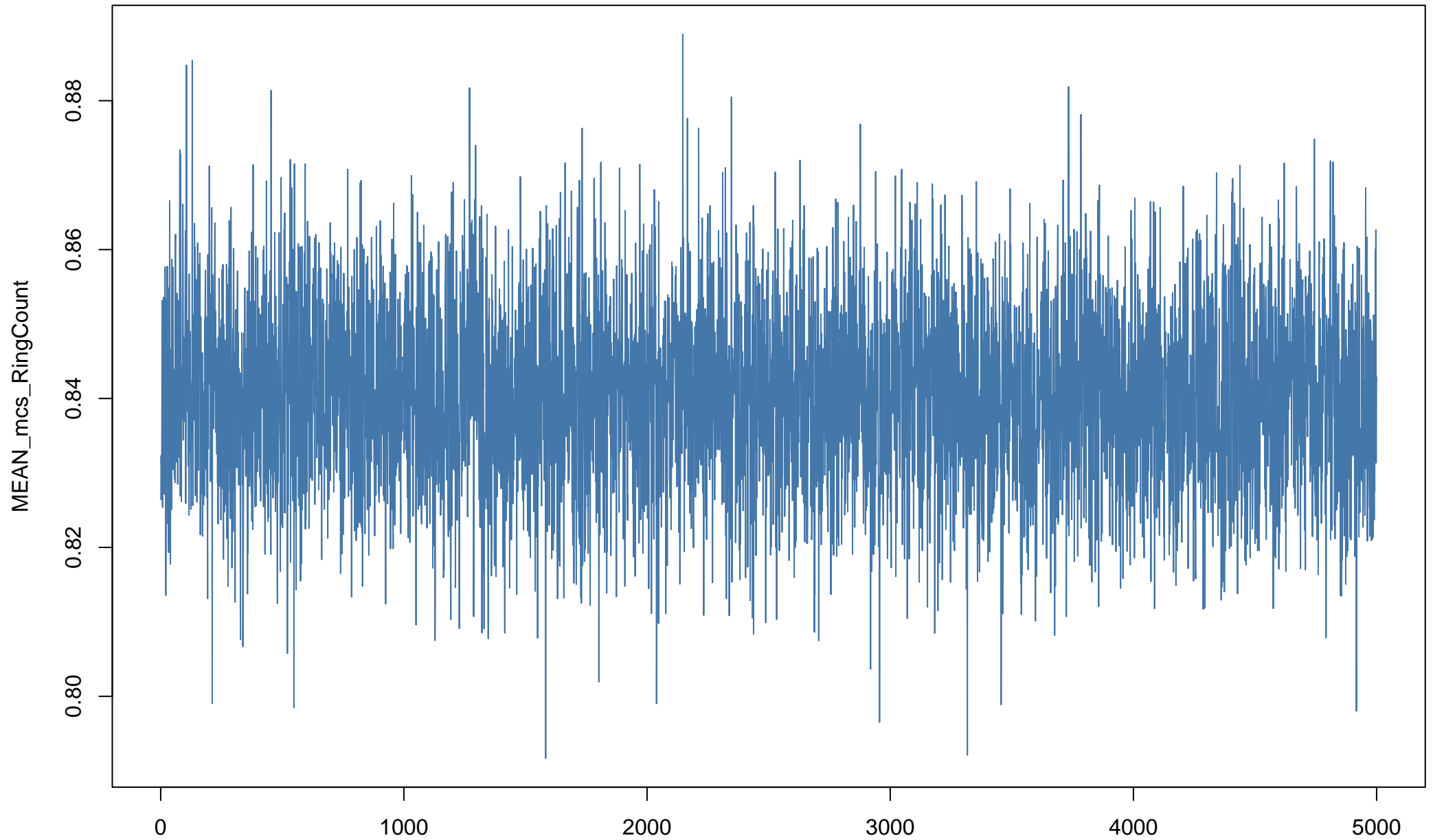
MEAN_mcs_NumHeteroAtoms
ESS = 5000 | BMK = 0.0283 | MCSE(6.27) = 1.42 | stat: TRUE



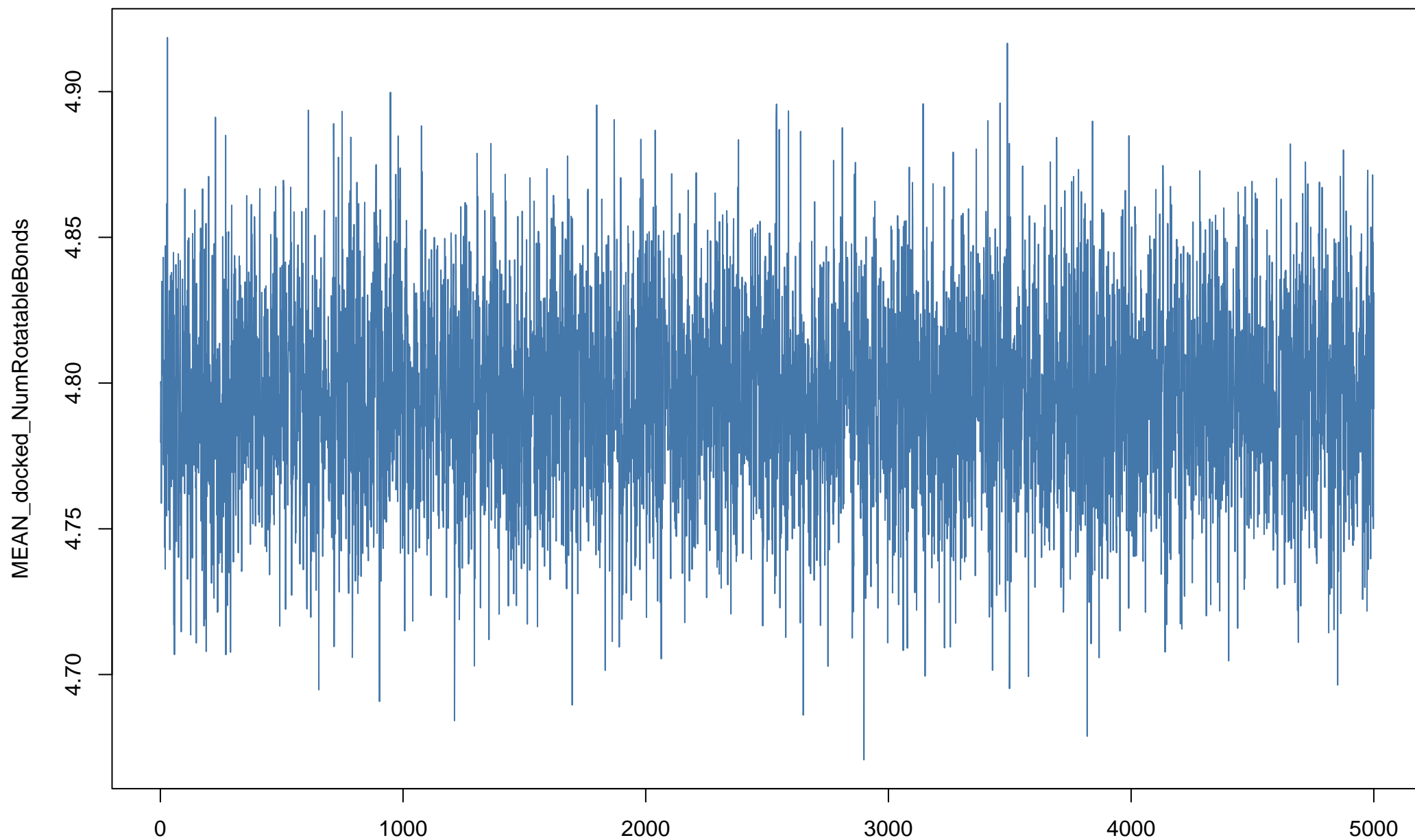
MEAN_docked_HeavyAtomCount
ESS = 5000 | BMK = 0.0284 | MCSE(6.27) = 1.46 | stat: TRUE



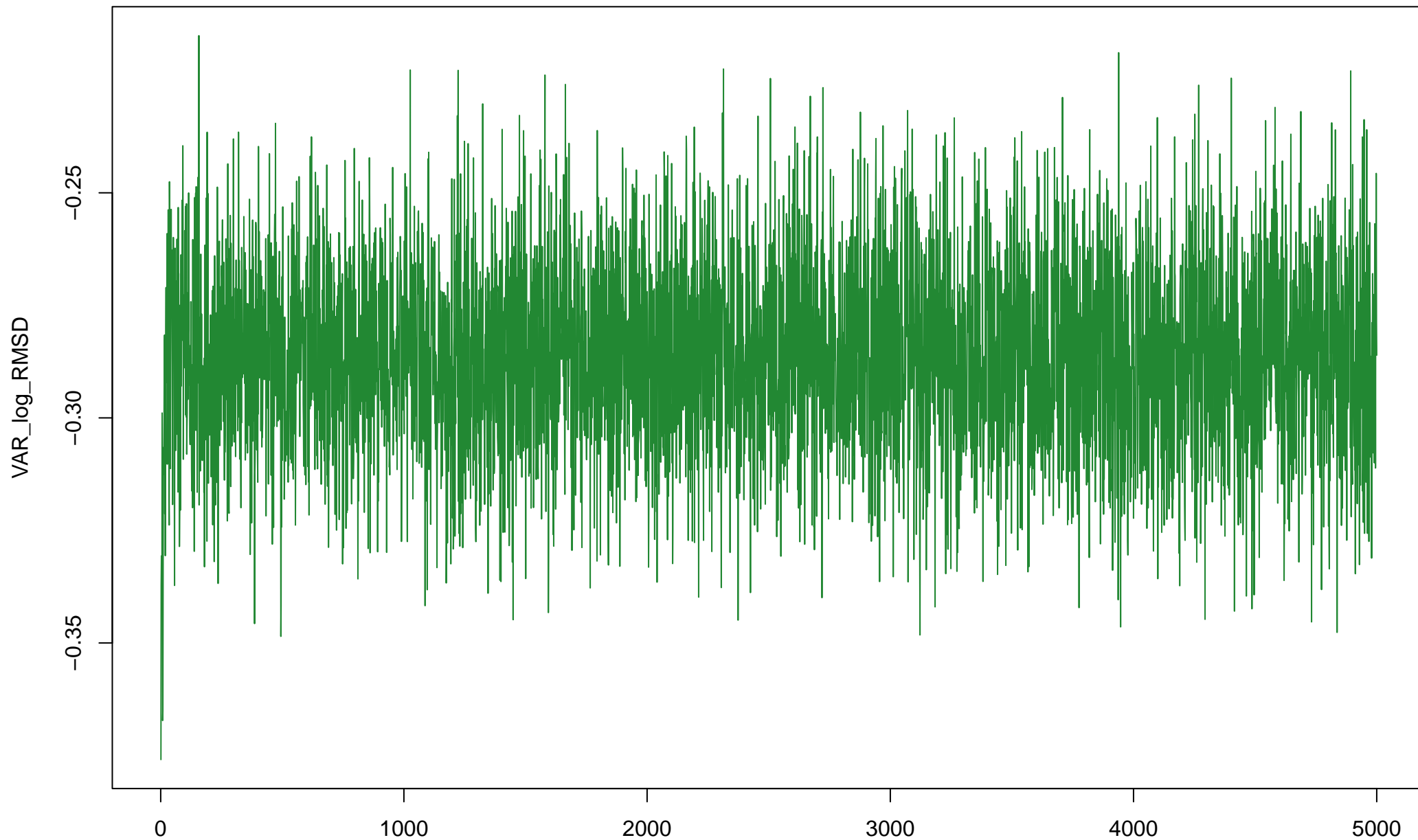
MEAN_mcs_RingCount
ESS = 4760 | BMK = 0.0396 | MCSE(6.27) = 1.48 | stat: TRUE



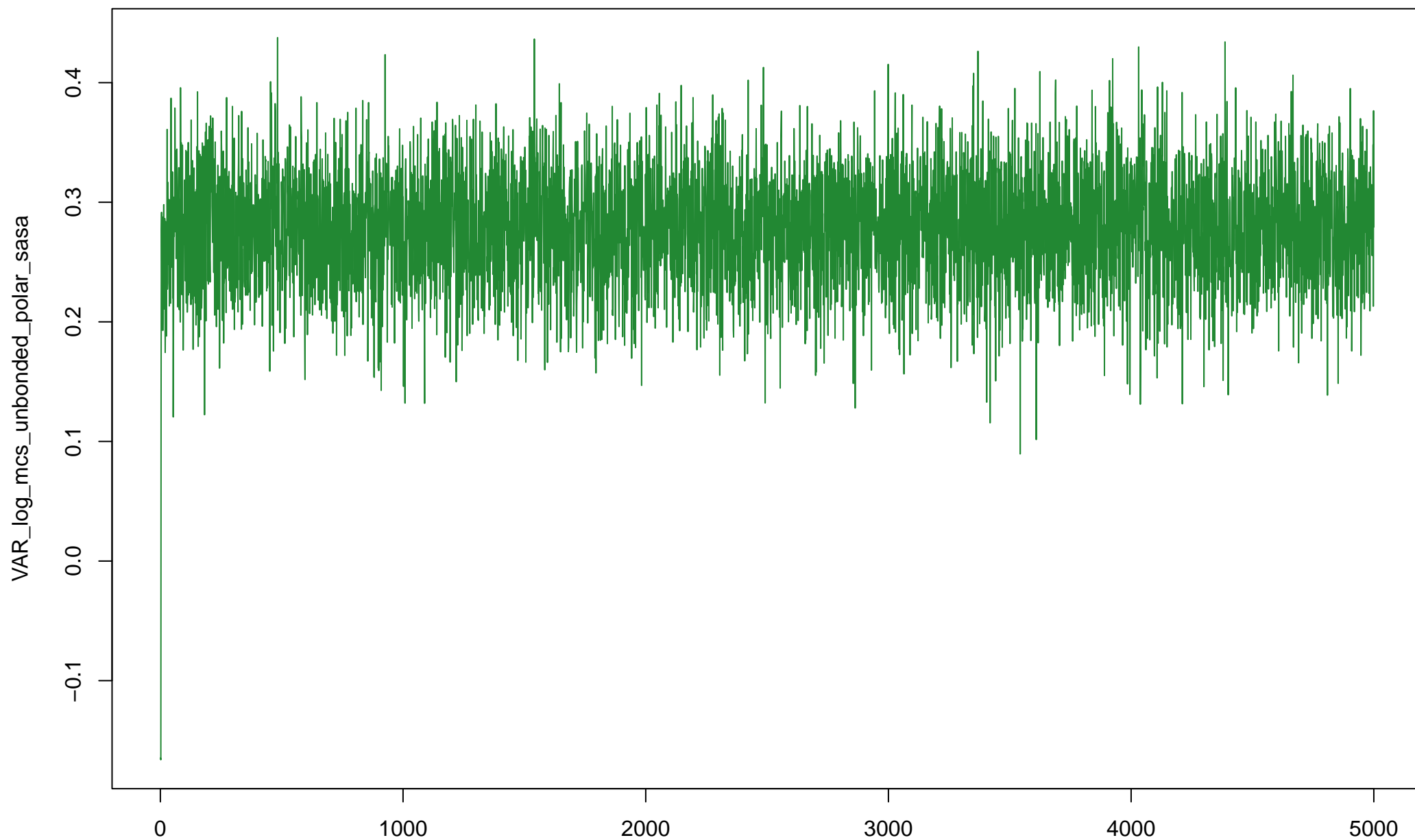
MEAN_docked_NumRotatableBonds
ESS = 4800 | BMK = 0.0171 | MCSE(6.27) = 1.46 | stat: TRUE



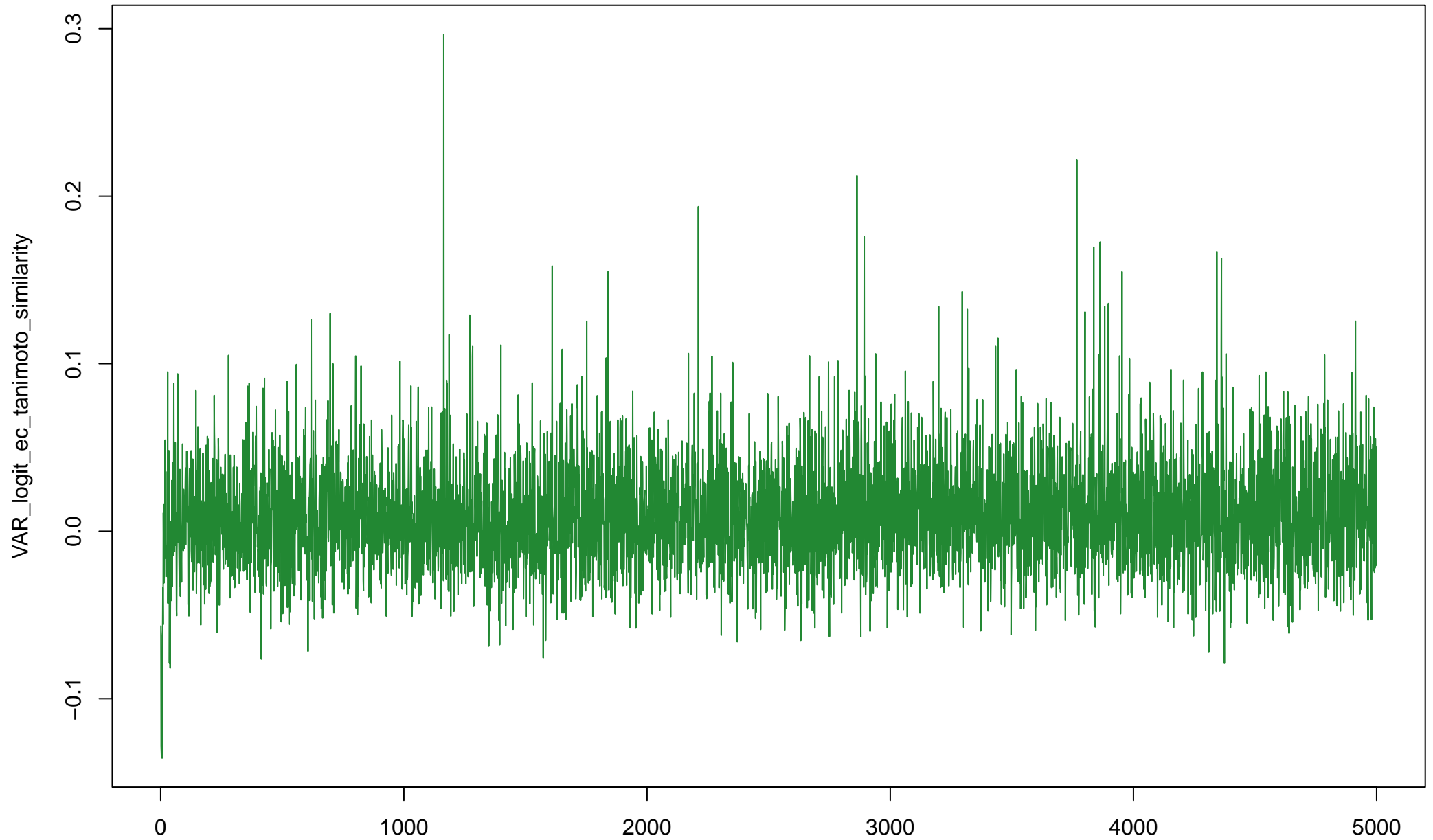
VAR_log_RMSD
ESS = 4420 | BMK = 0.0397 | MCSE(6.27) = 1.57 | stat: TRUE



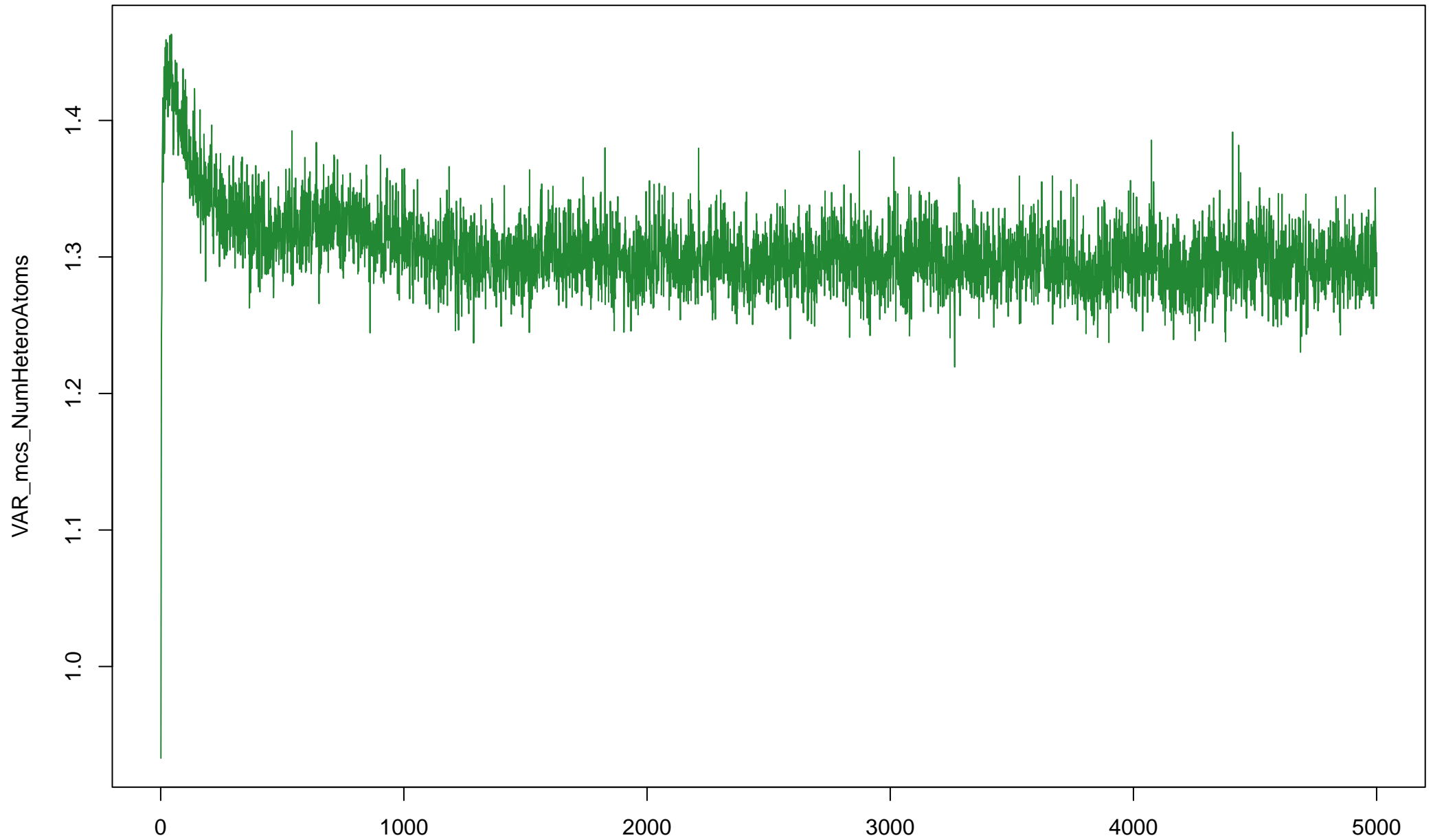
VAR_log_mcs_unbonded_polar_sasa
ESS = 5000 | BMK = 0.0345 | MCSE(6.27) = 1.45 | stat: TRUE



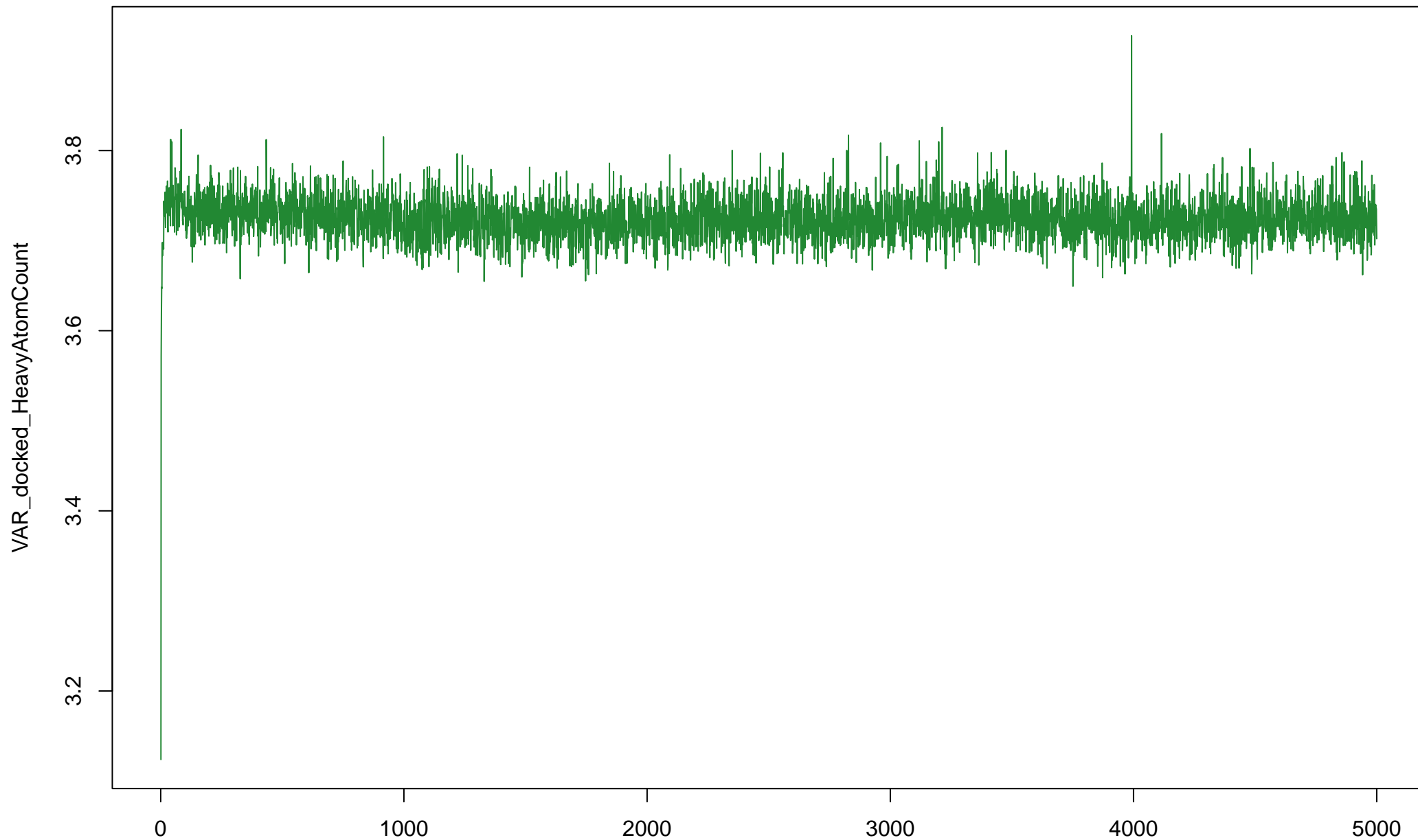
VAR_logit_ec_tanimoto_similarity
ESS = 4060 | BMK = 0.065 | MCSE(6.27) = 1.68 | stat: FALSE



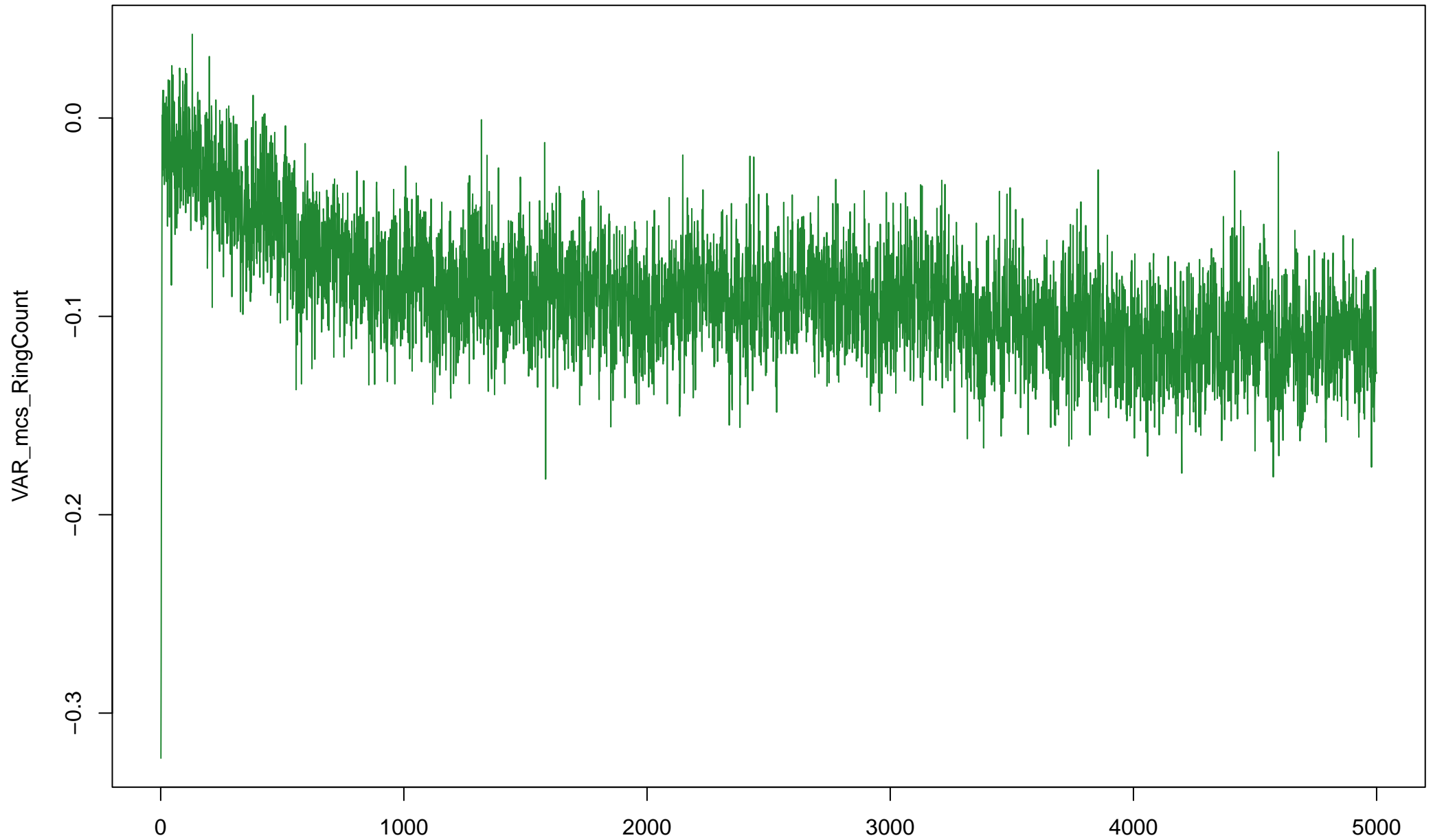
VAR_mcs_NumHeteroAtoms
ESS = 44.7 | BMK = 0.248 | MCSE(6.27) = 5.56 | stat: FALSE



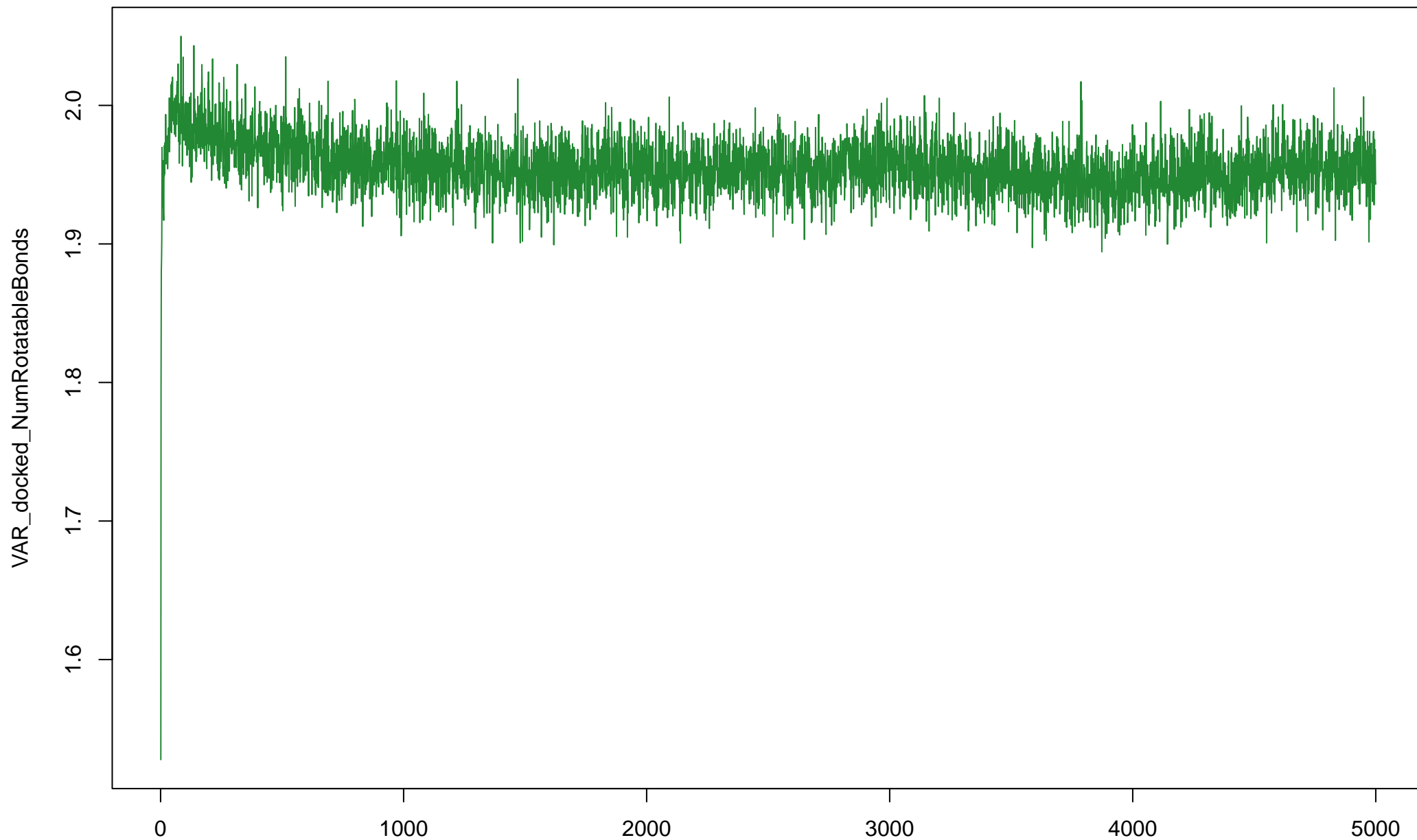
VAR_docked_HeavyAtomCount
ESS = 1900 | BMK = 0.0452 | MCSE(6.27) = 2.45 | stat: FALSE



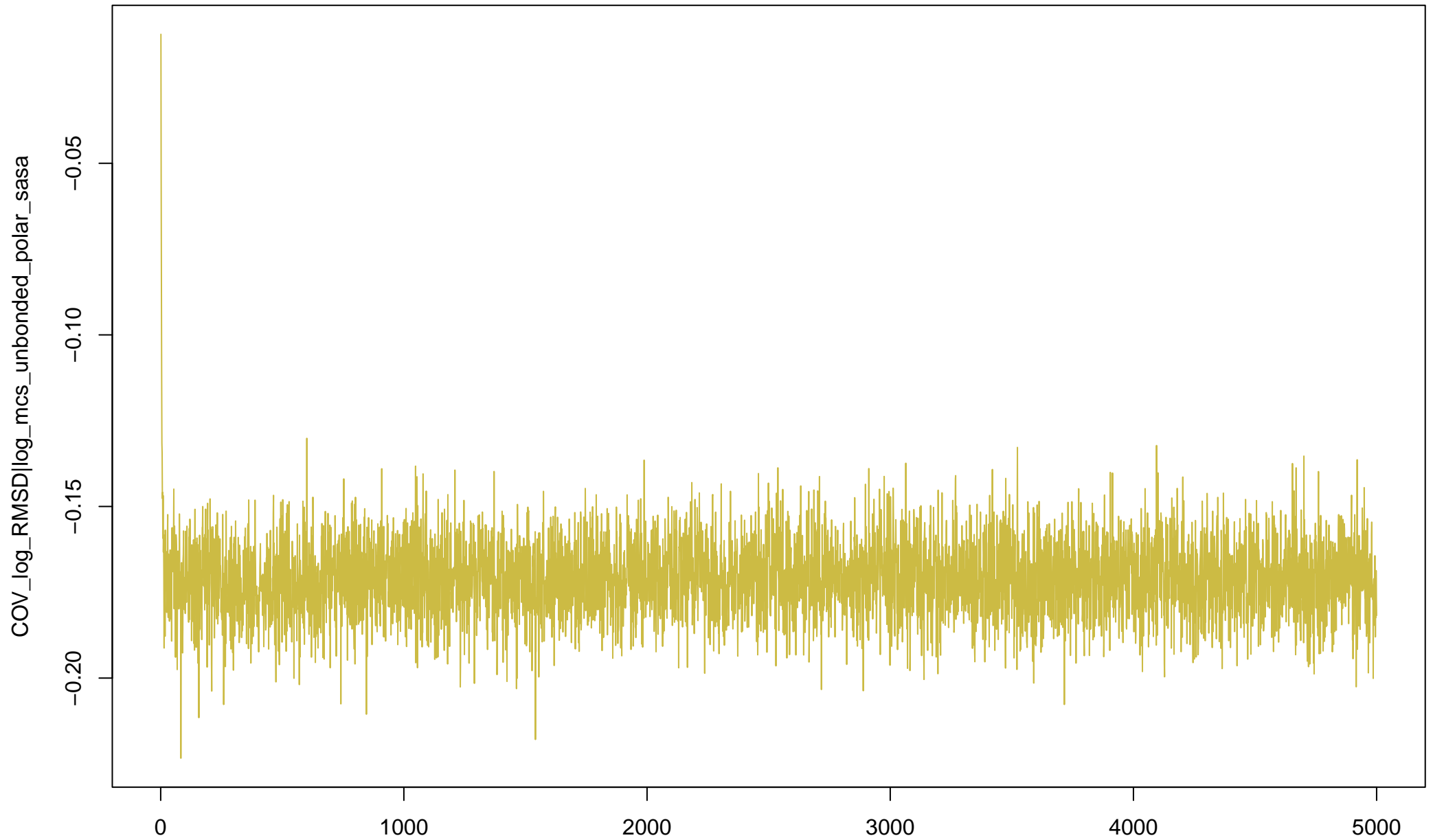
VAR_mcs_RingCount
ESS = 17 | BMK = 0.366 | MCSE(6.27) = 4.99 | stat: FALSE



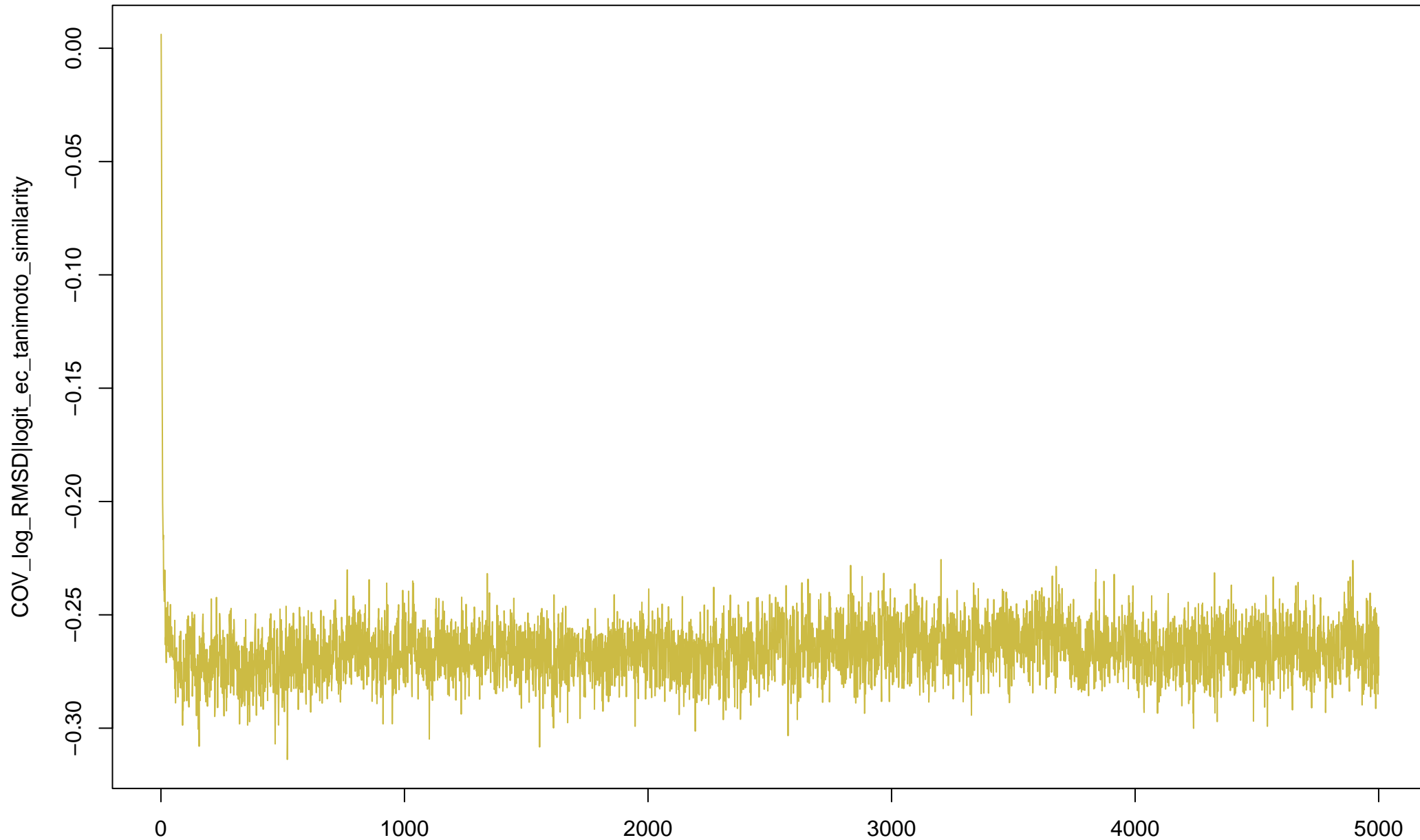
VAR_docked_NumRotatableBonds
ESS = 110 | BMK = 0.172 | MCSE(6.27) = 2.97 | stat: FALSE



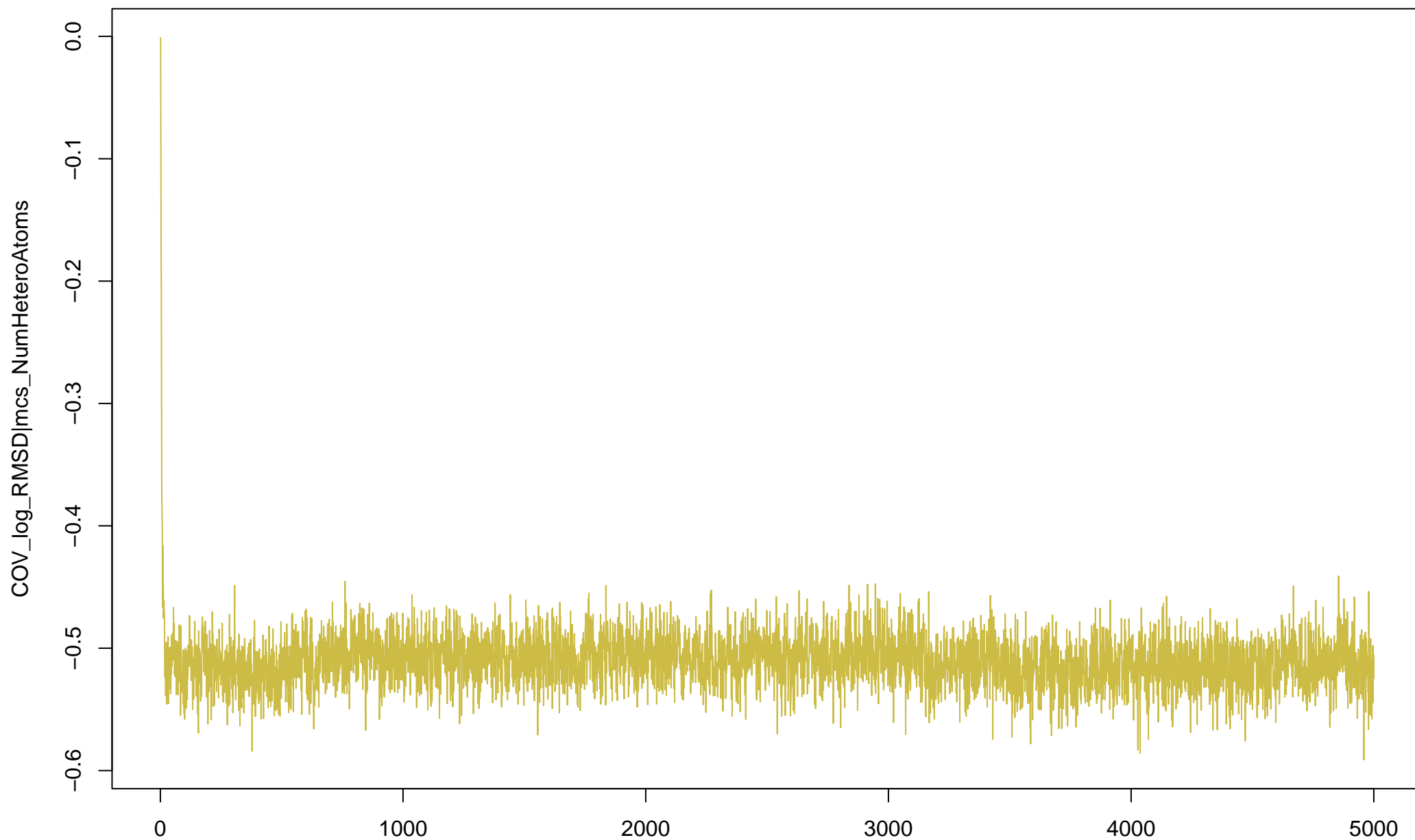
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3300 | BMK = 0.0452 | MCSE(6.27) = 1.8 | stat: TRUE



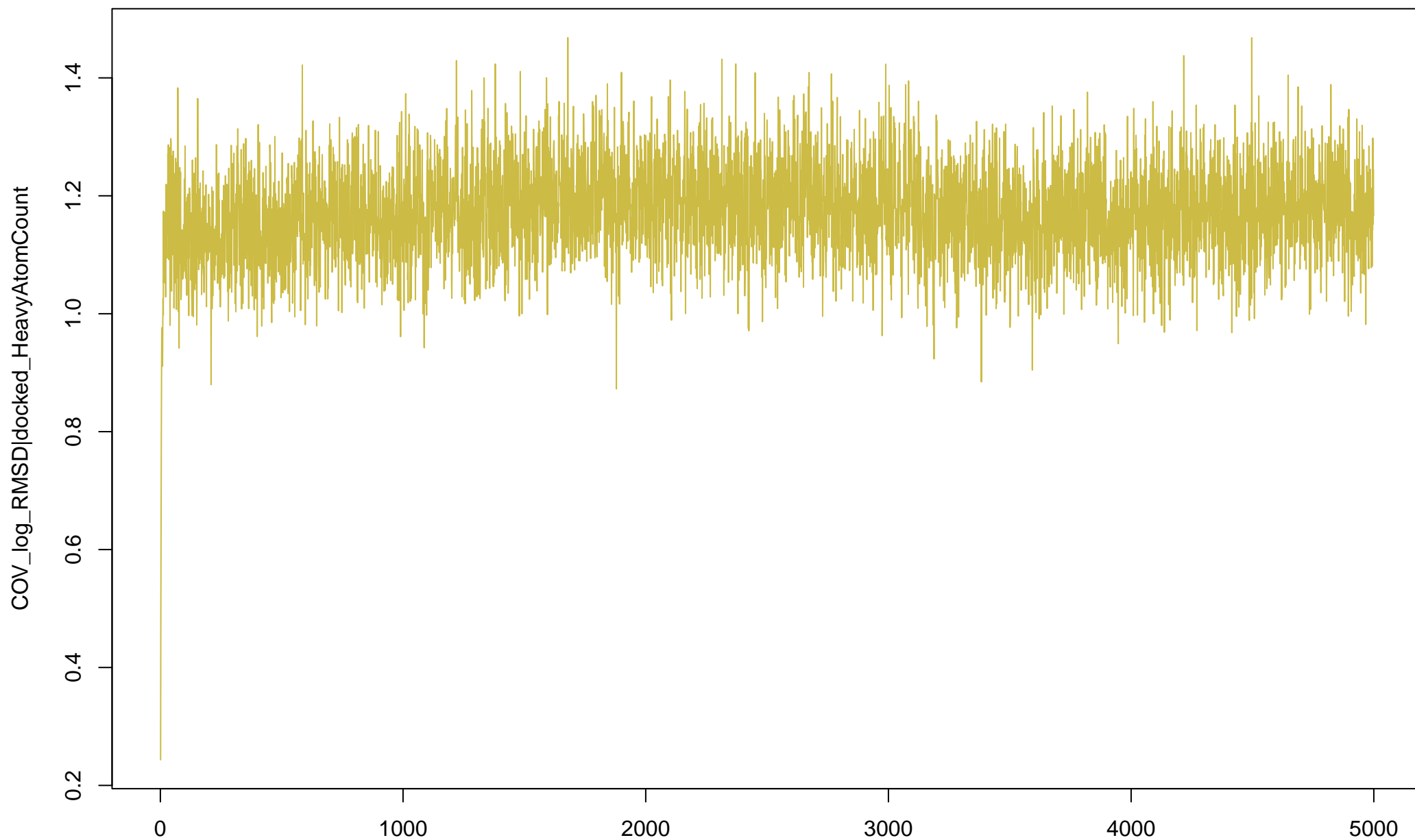
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 707 | BMK = 0.147 | MCSE(6.27) = 4.07 | stat: TRUE



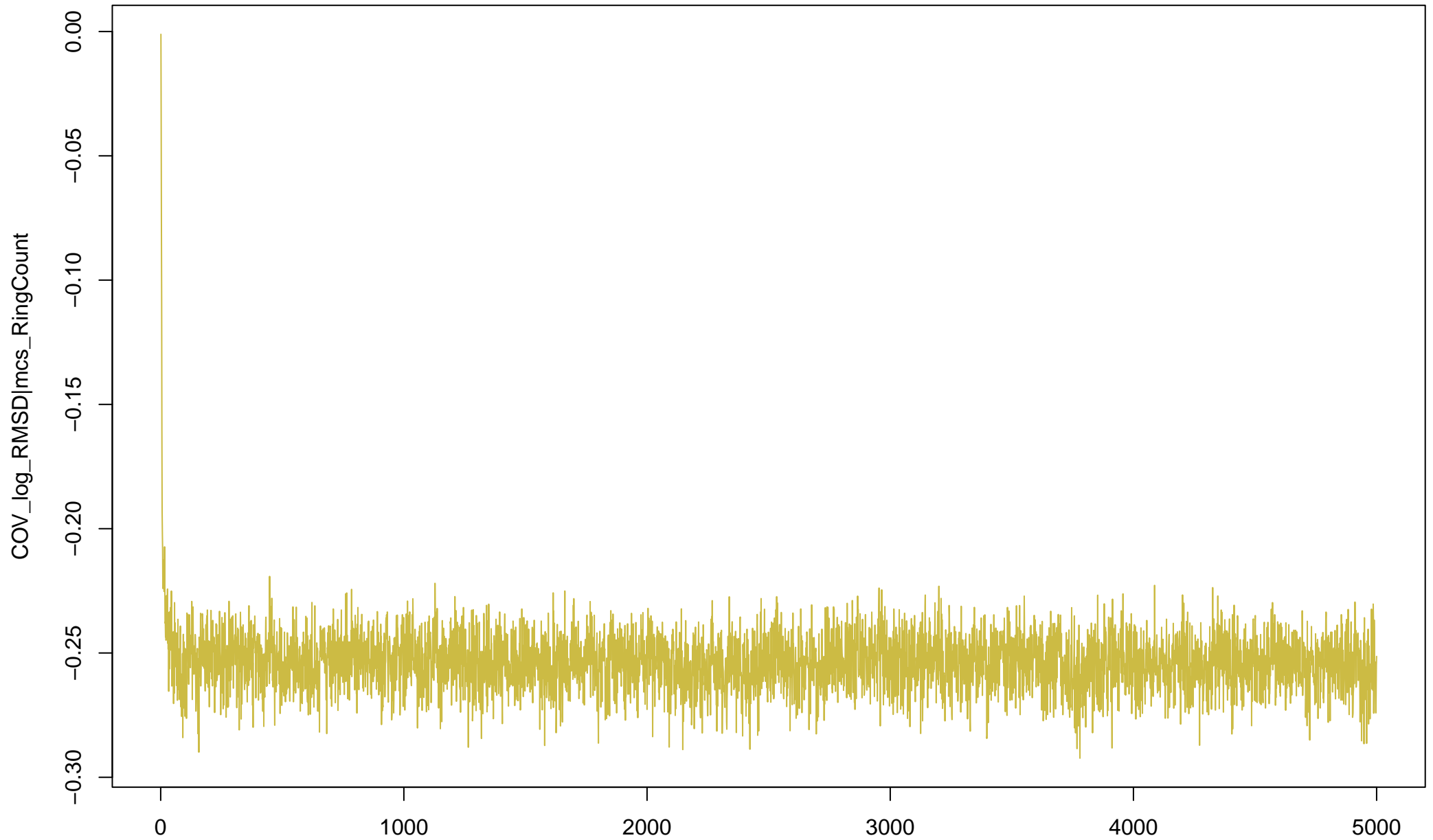
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 902 | BMK = 0.0793 | MCSE(6.27) = 3.99 | stat: TRUE



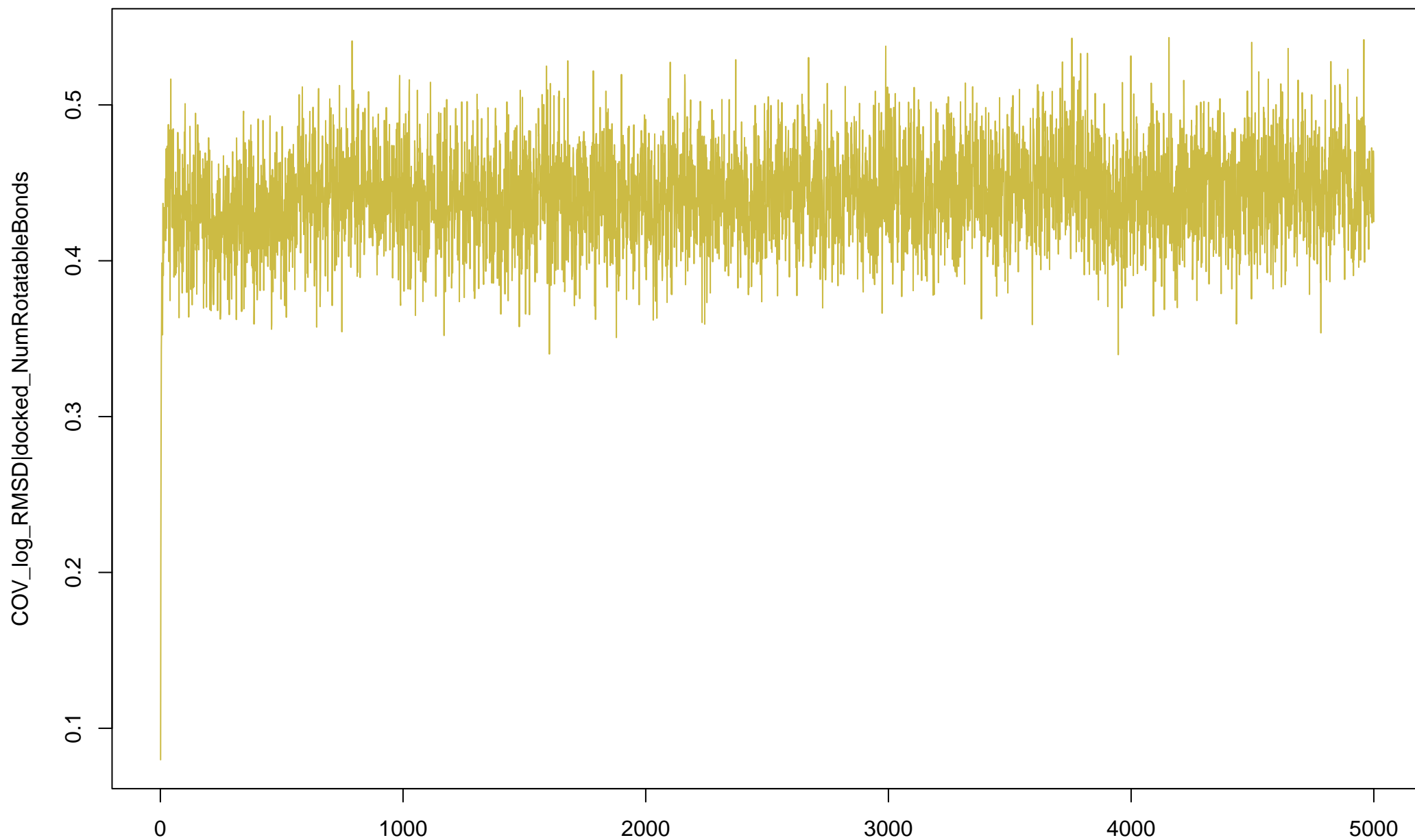
COV_log_RMSD|docked_HeavyAtomCount
ESS = 805 | BMK = 0.0403 | MCSE(6.27) = 2.38 | stat: FALSE



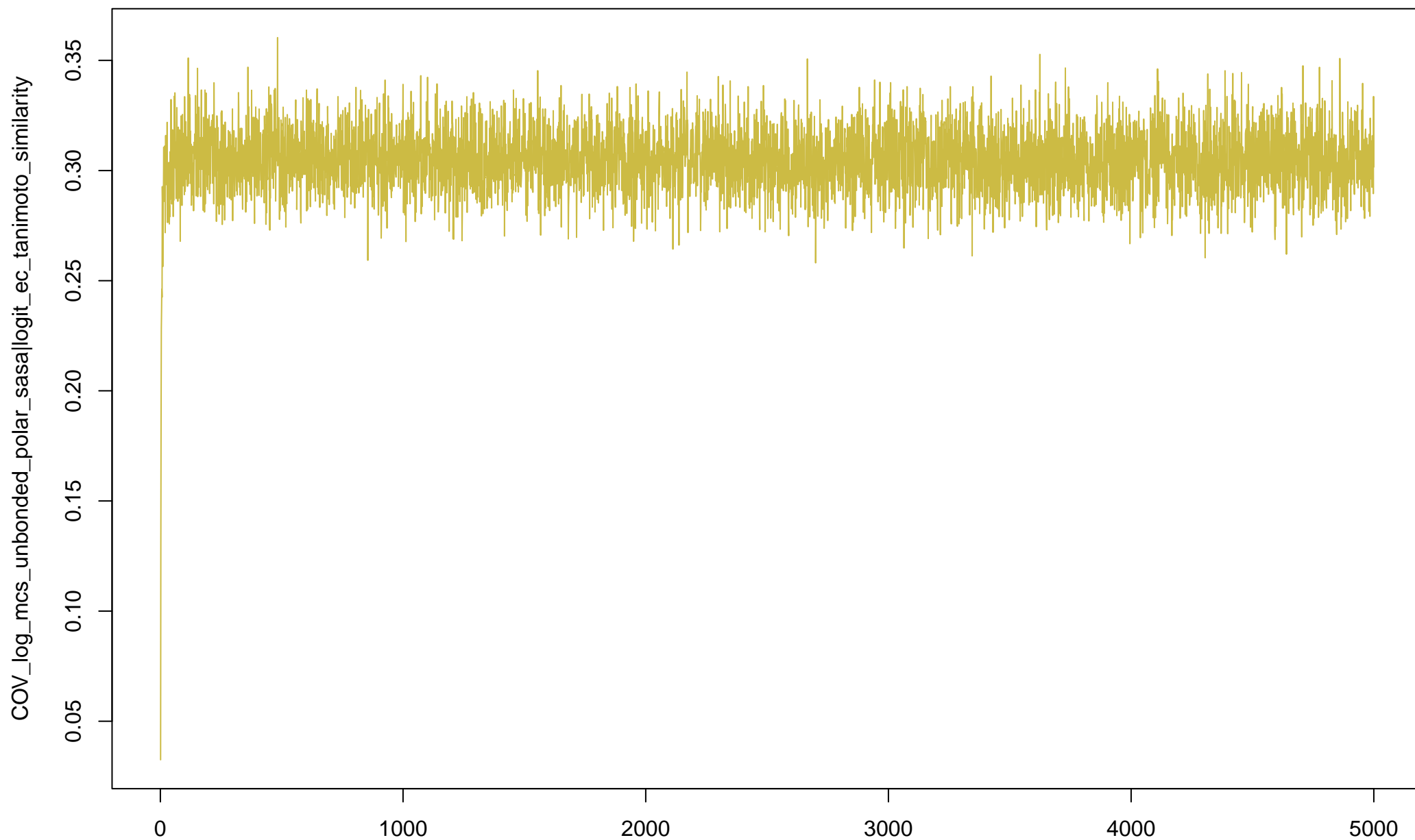
COV_log_RMSD|mcs_RingCount
ESS = 959 | BMK = 0.0649 | MCSE(6.27) = 3.34 | stat: FALSE



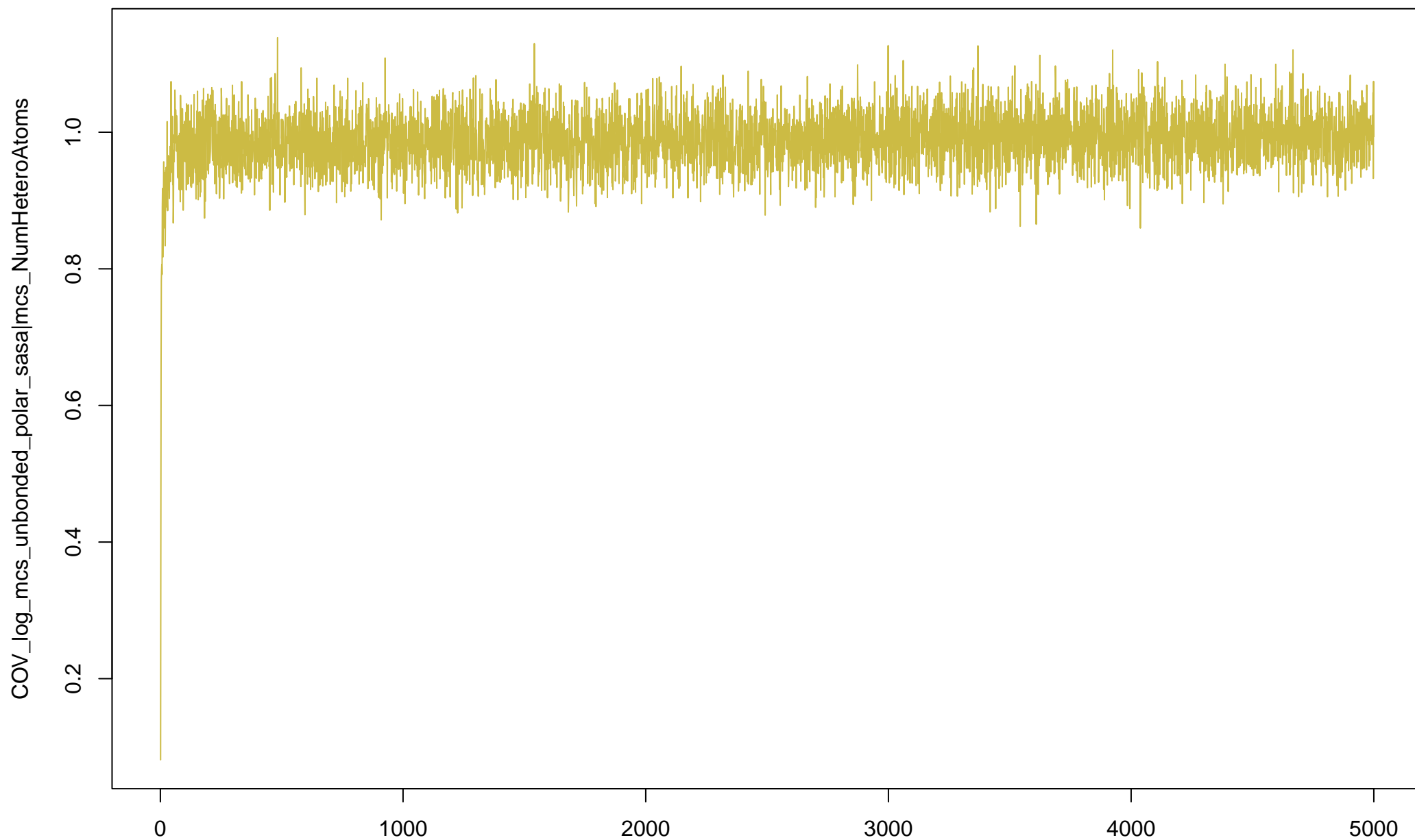
COV_log_RMSD|docked_NumRotatableBonds
ESS = 1410 | BMK = 0.0998 | MCSE(6.27) = 2.45 | stat: FALSE



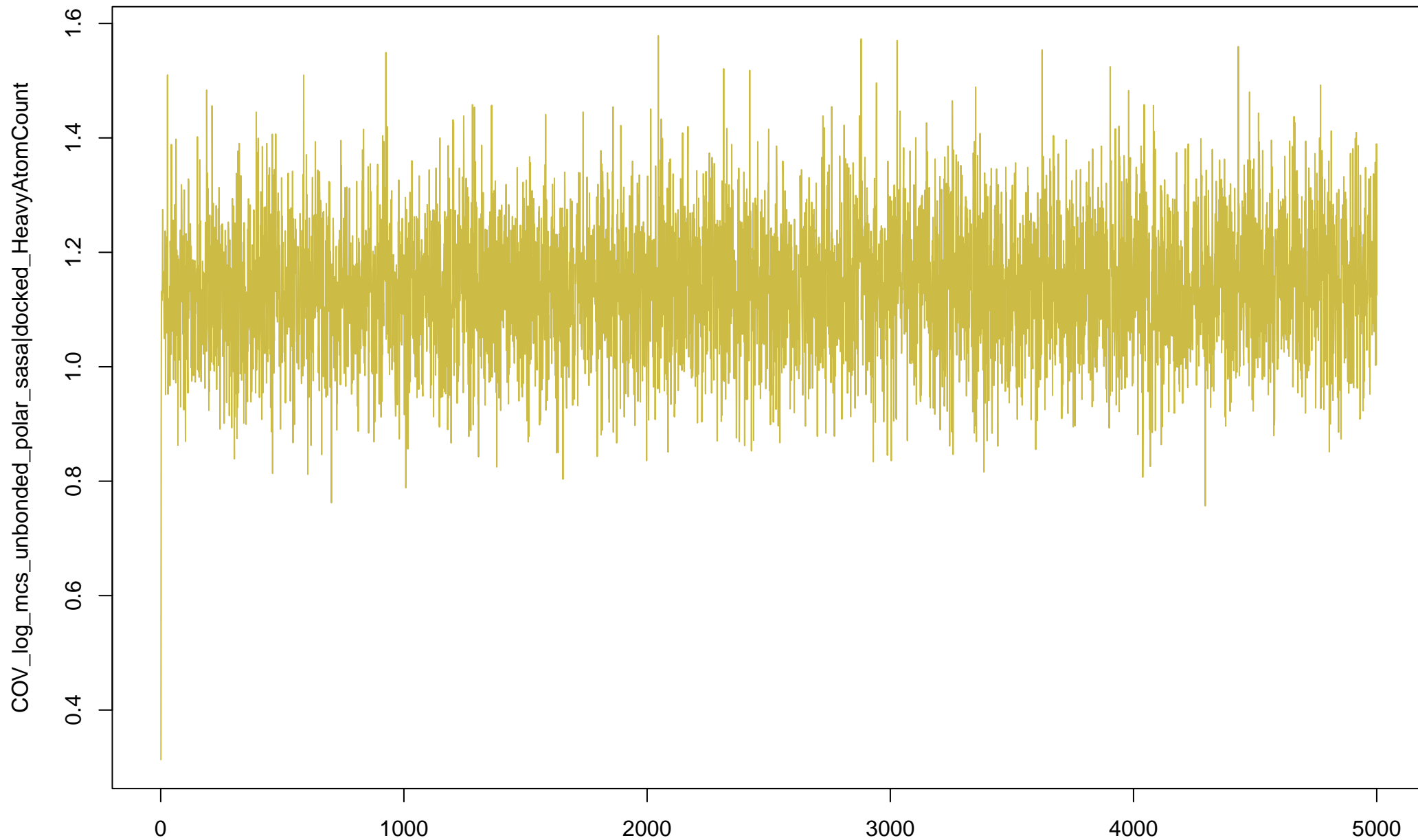
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 2490 | BMK = 0.0635 | MCSE(6.27) = 2.18 | stat: TRUE



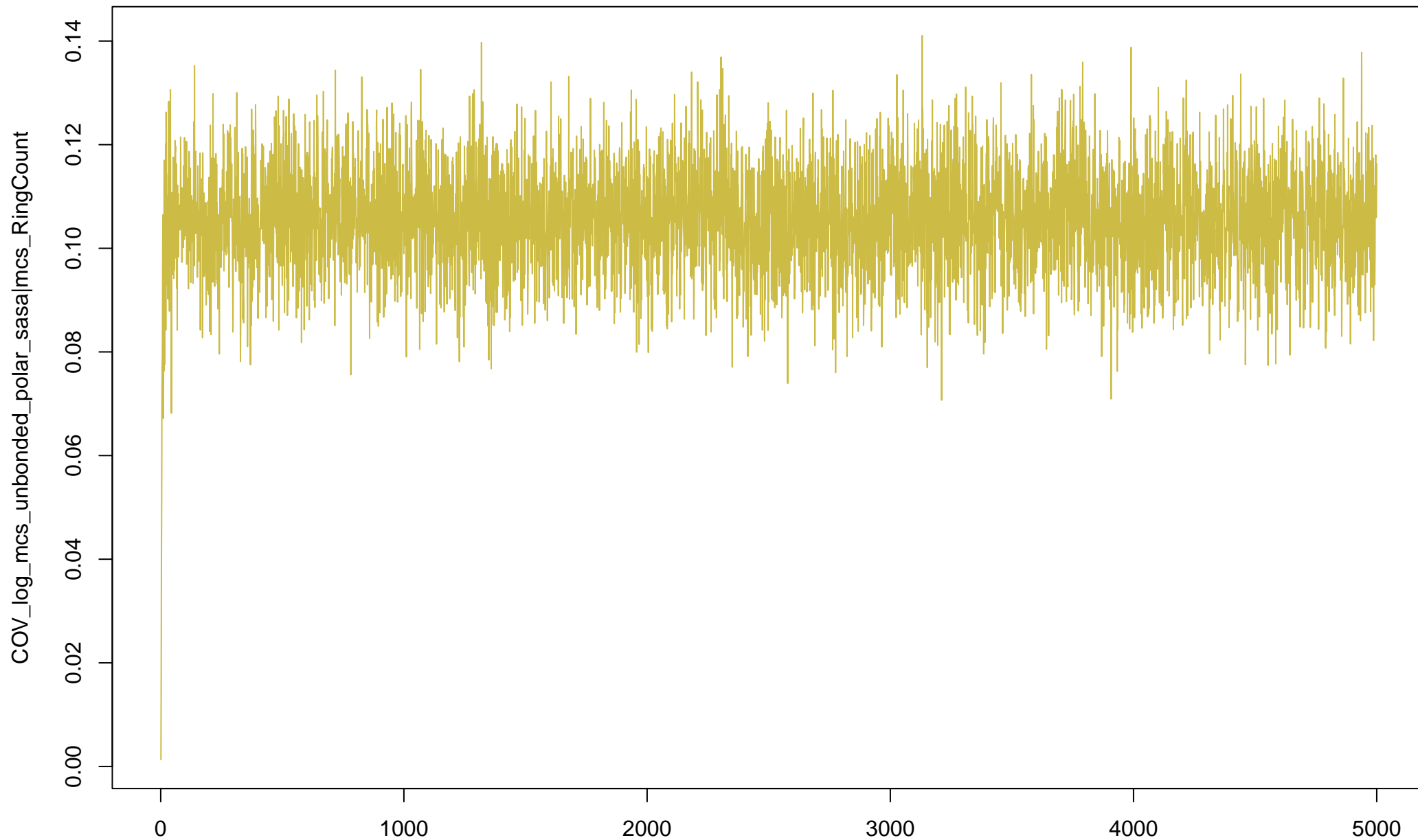
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1140 | BMK = 0.1 | MCSE(6.27) = 2.16 | stat: FALSE



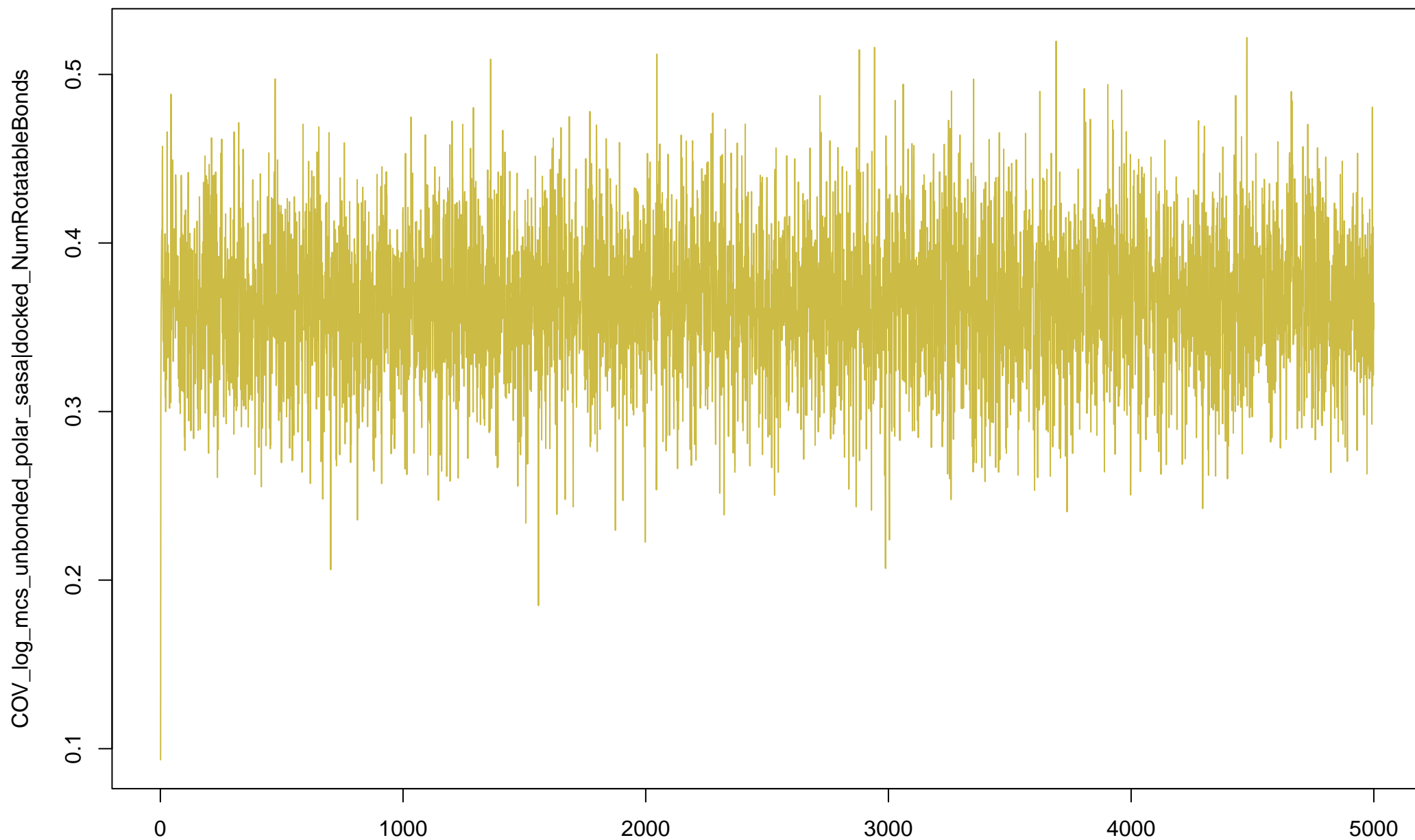
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 4780 | BMK = 0.0433 | MCSE(6.27) = 1.48 | stat: FALSE



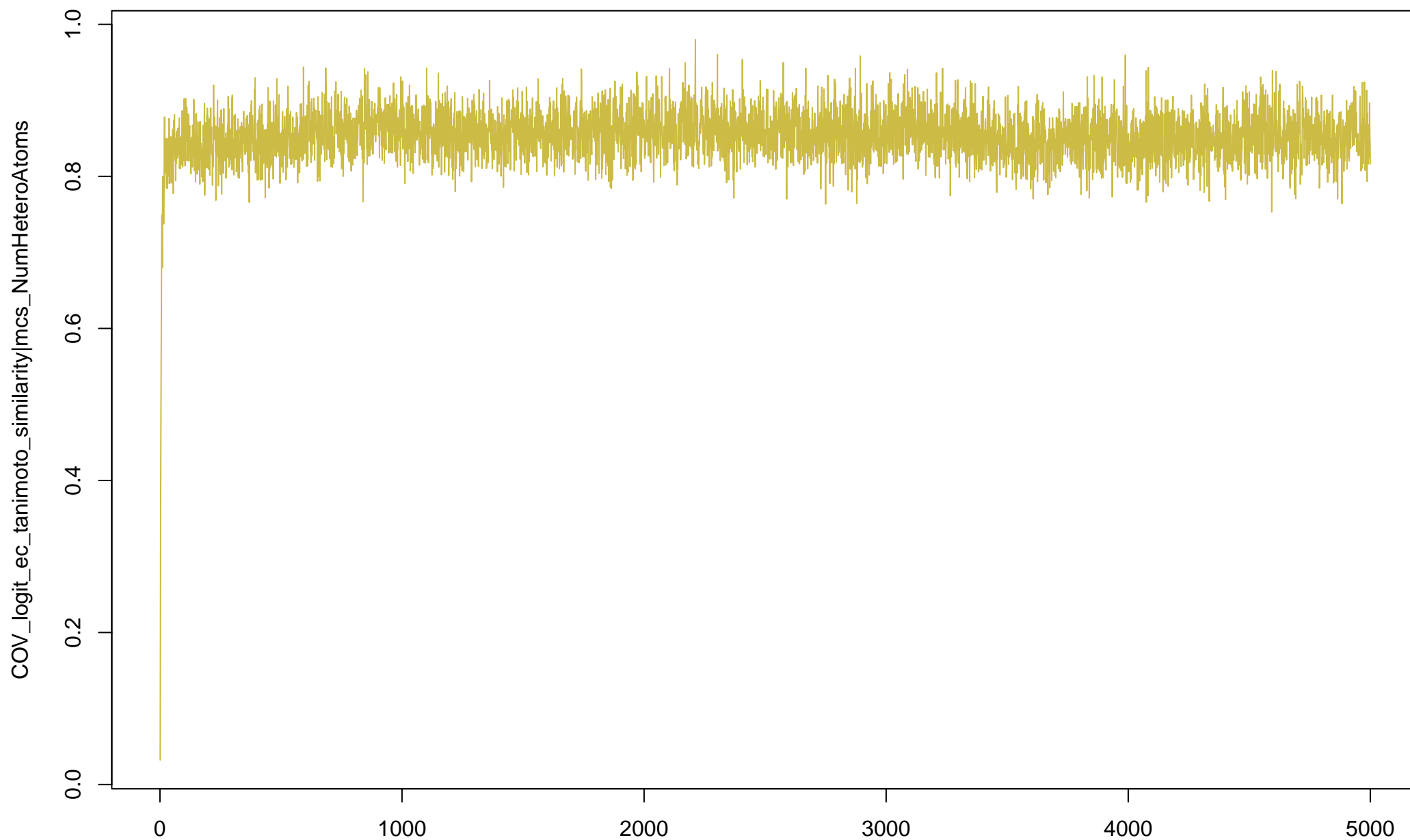
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 3370 | BMK = 0.0425 | MCSE(6.27) = 1.79 | stat: TRUE



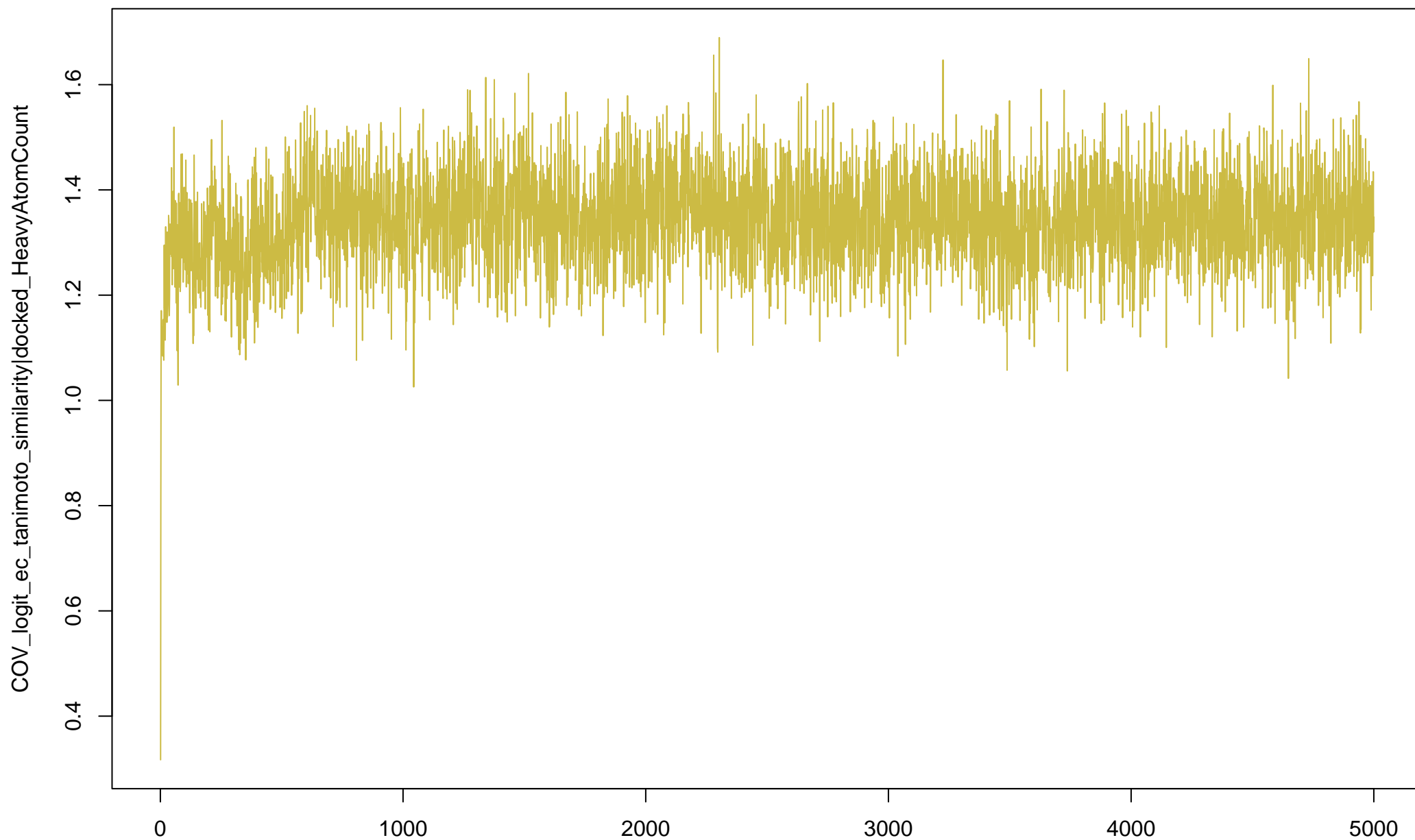
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 4730 | BMK = 0.0314 | MCSE(6.27) = 1.51 | stat: TRUE



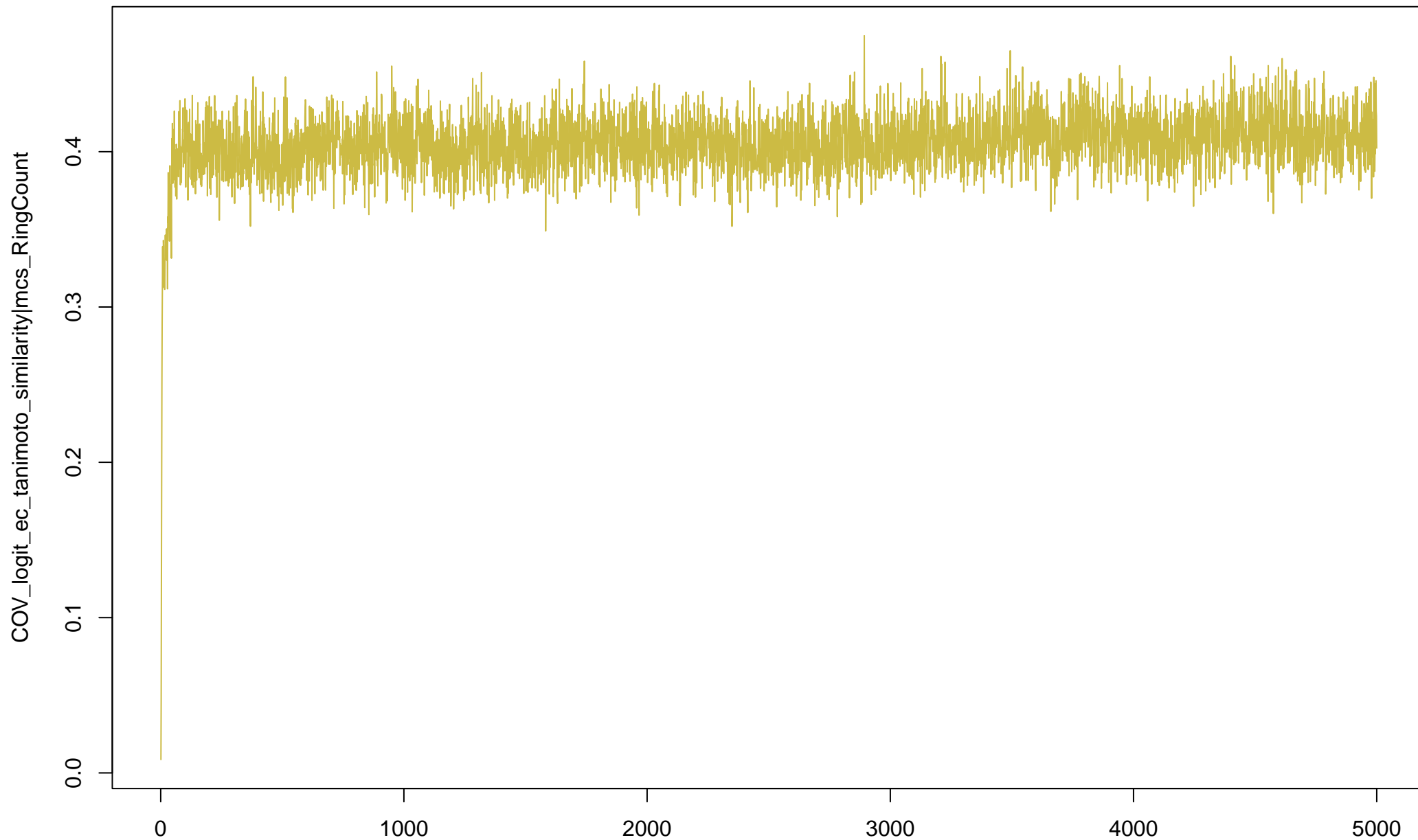
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 850 | BMK = 0.071 | MCSE(6.27) = 3.76 | stat: FALSE



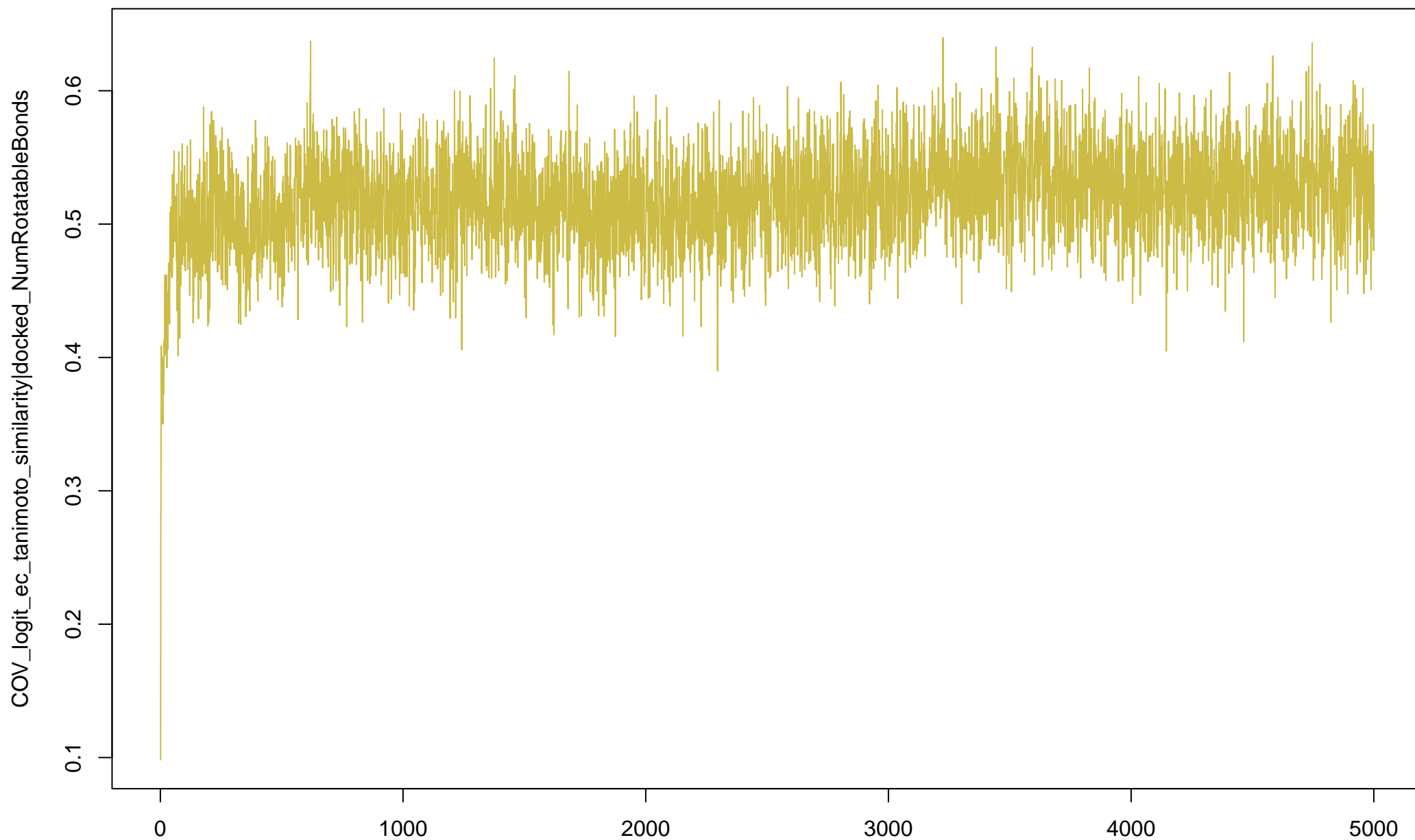
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 458 | BMK = 0.0543 | MCSE(6.27) = 2.59 | stat: FALSE



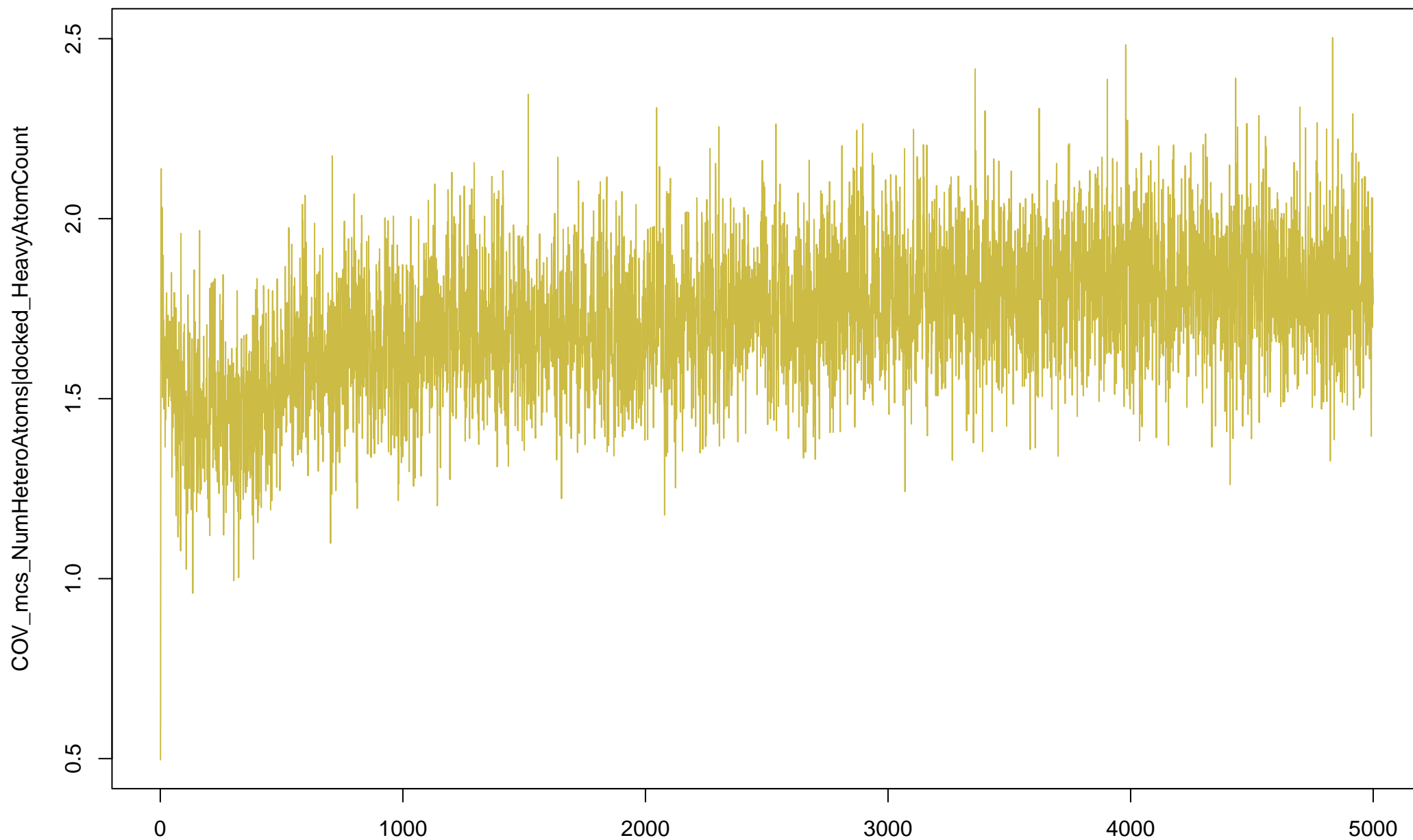
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 401 | BMK = 0.163 | MCSE(6.27) = 4.5 | stat: FALSE



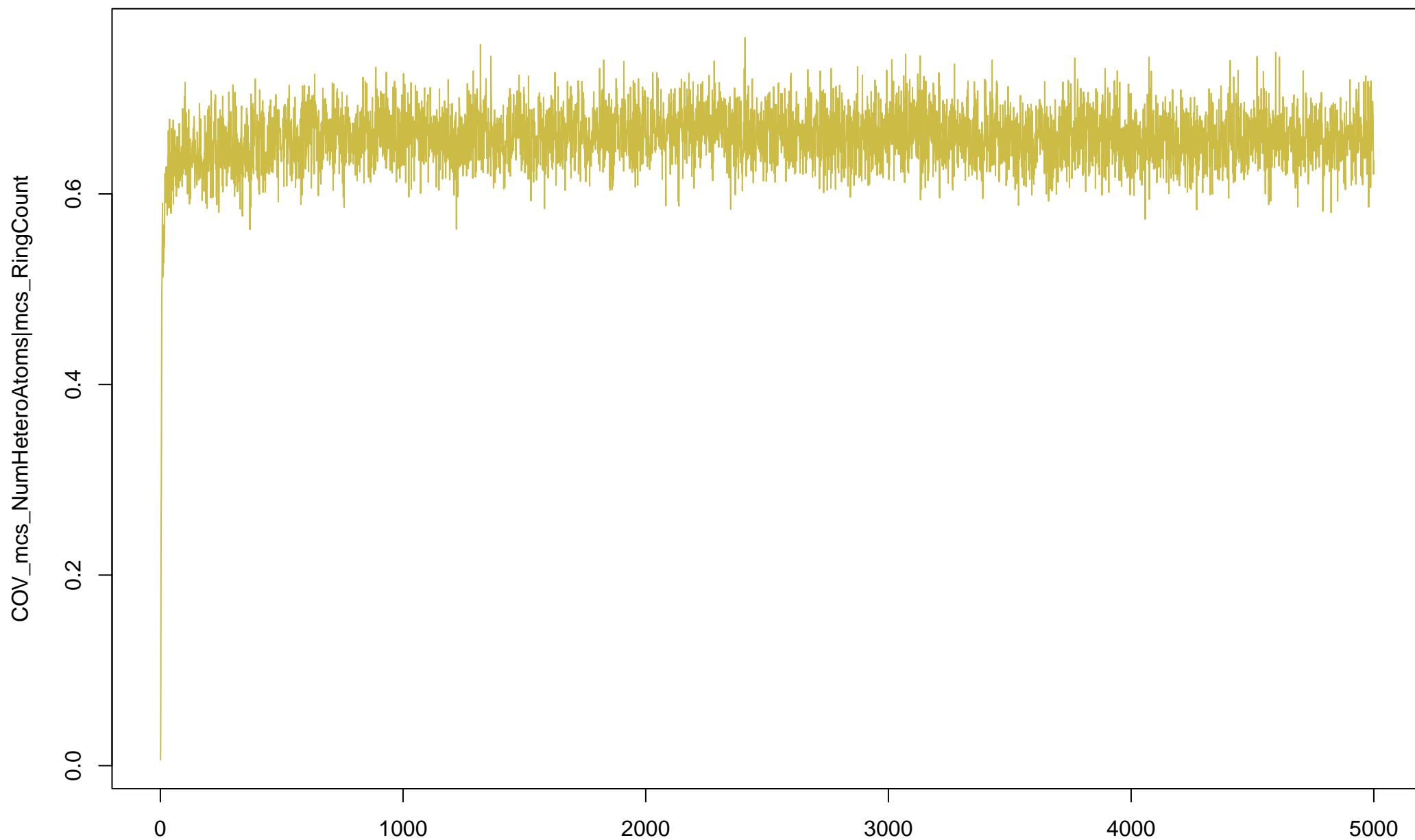
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 323 | BMK = 0.188 | MCSE(6.27) = 3.55 | stat: FALSE



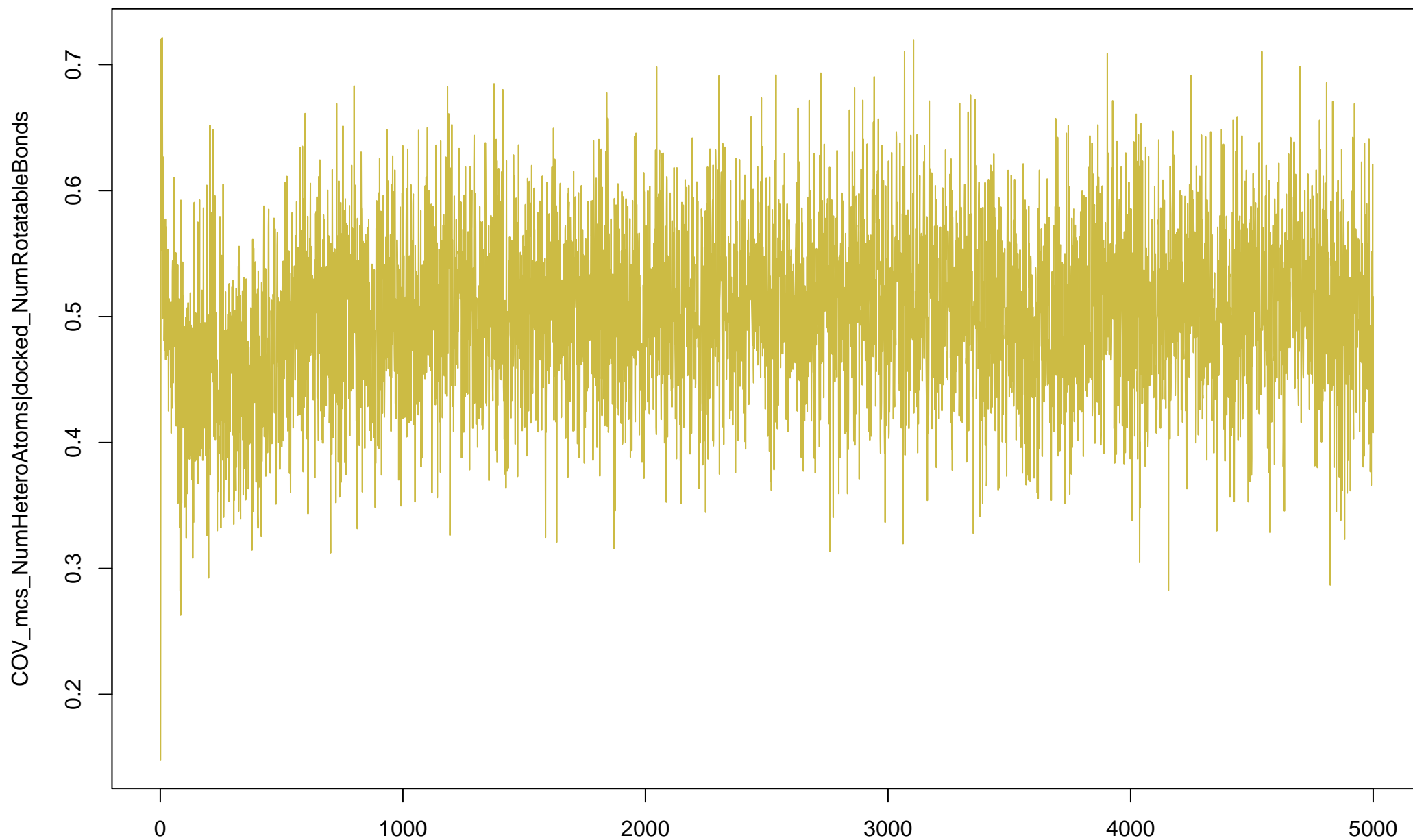
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 37.4 | BMK = 0.303 | MCSE(6.27) = 4.03 | stat: FALSE



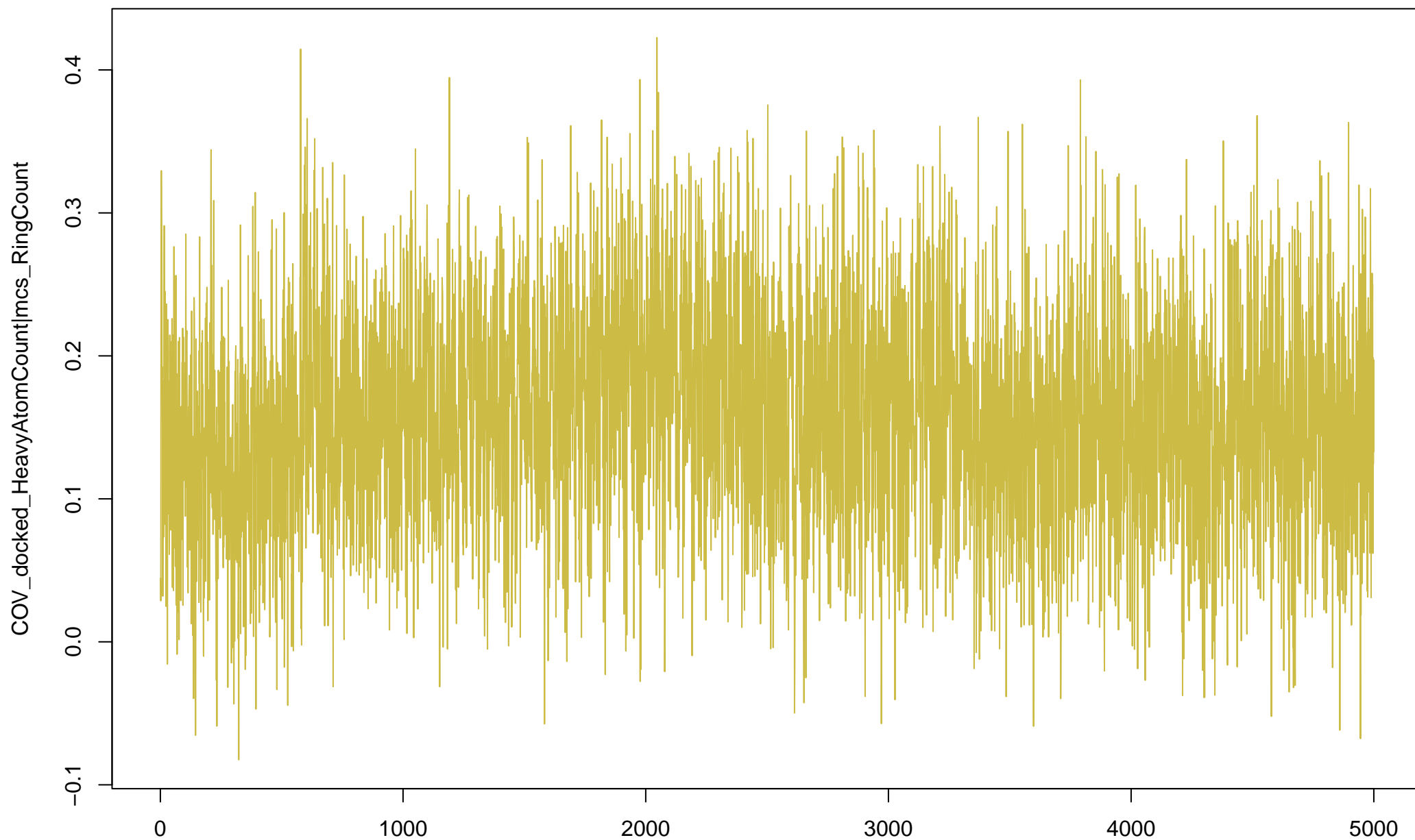
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 730 | BMK = 0.0709 | MCSE(6.27) = 3.38 | stat: FALSE



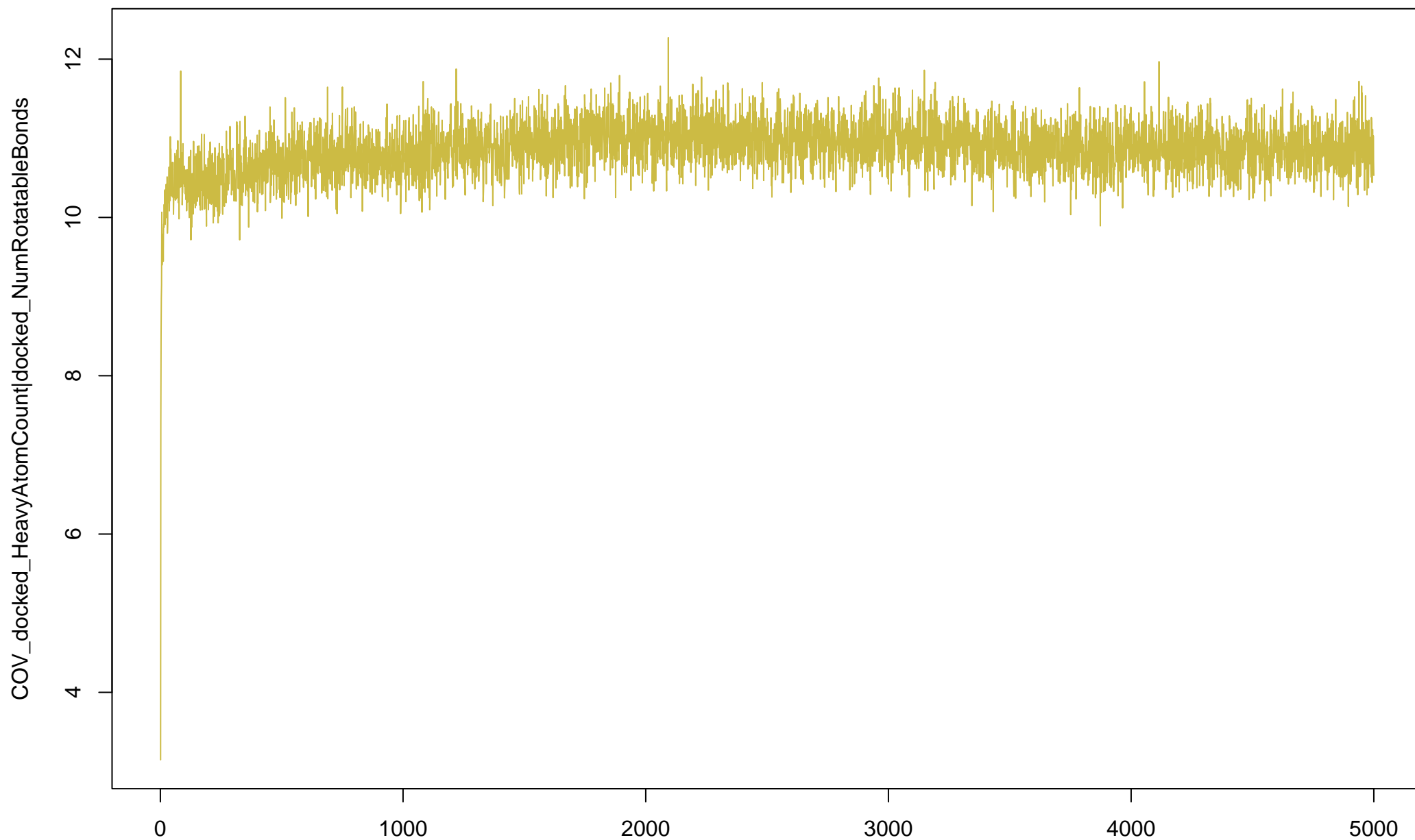
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 533 | BMK = 0.0646 | MCSE(6.27) = 2.12 | stat: FALSE



COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 654 | BMK = 0.044 | MCSE(6.27) = 1.89 | stat: FALSE



COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 122 | BMK = 0.139 | MCSE(6.27) = 3.33 | stat: FALSE



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 2990 | BMK = 0.0611 | MCSE(6.27) = 1.87 | stat: FALSE

