

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.56241553660443

max MCSE = 8.7619816985706

all stationary: FALSE

burn: 510

max rel.err.: 1.51800971000709

-- STATS 1D --

min ESS = 78.0291677455309

max BMK = 0.153230451789123

max MCSE = 7.75401067429317

all stationary: FALSE

burn: 0

max rel.err.: 2.7155382122665

-- STATS 2D --

min ESS = 926.063160694354

max BMK = 0.0869428301742919

max MCSE = 4.34903378189725

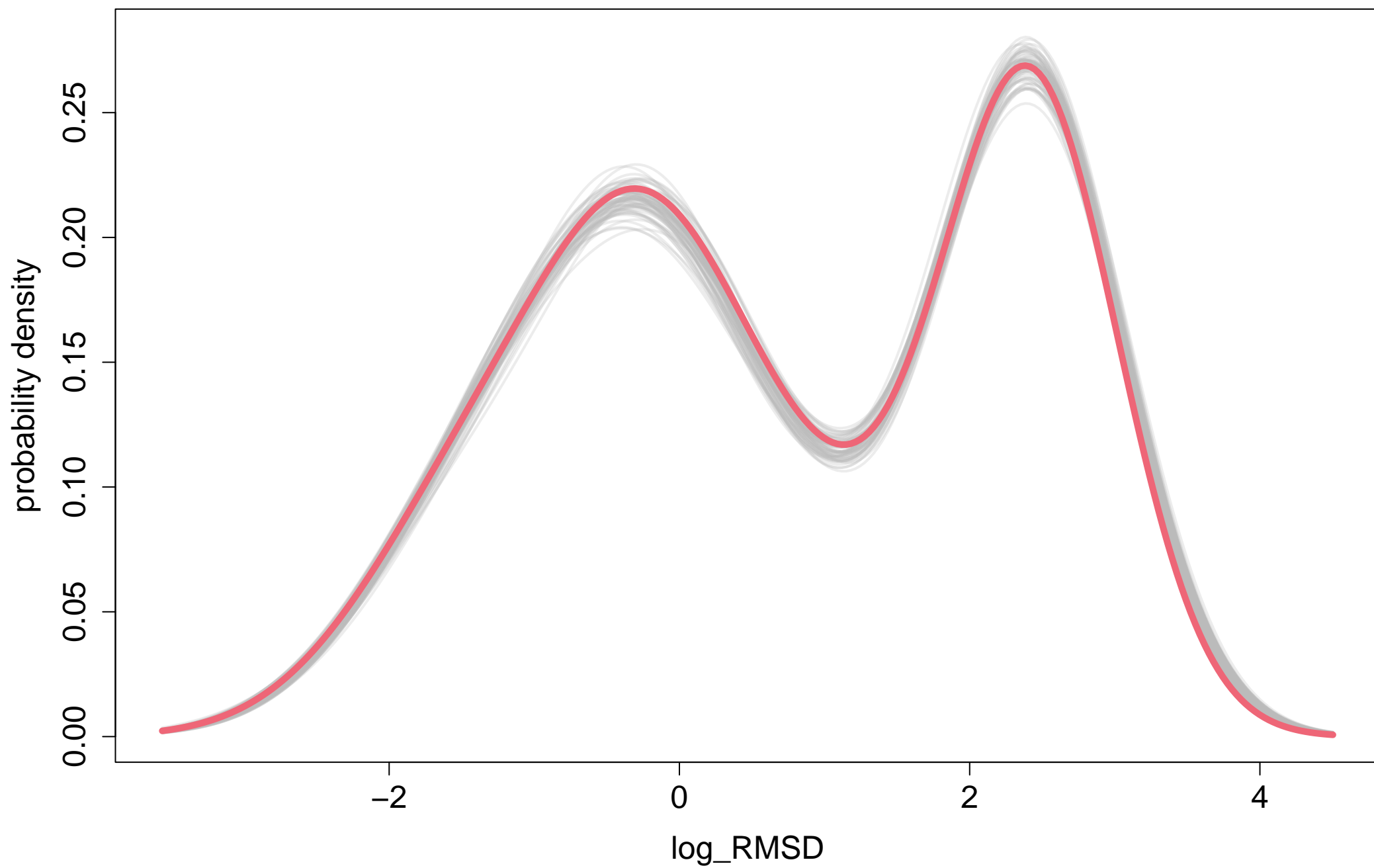
all stationary: FALSE

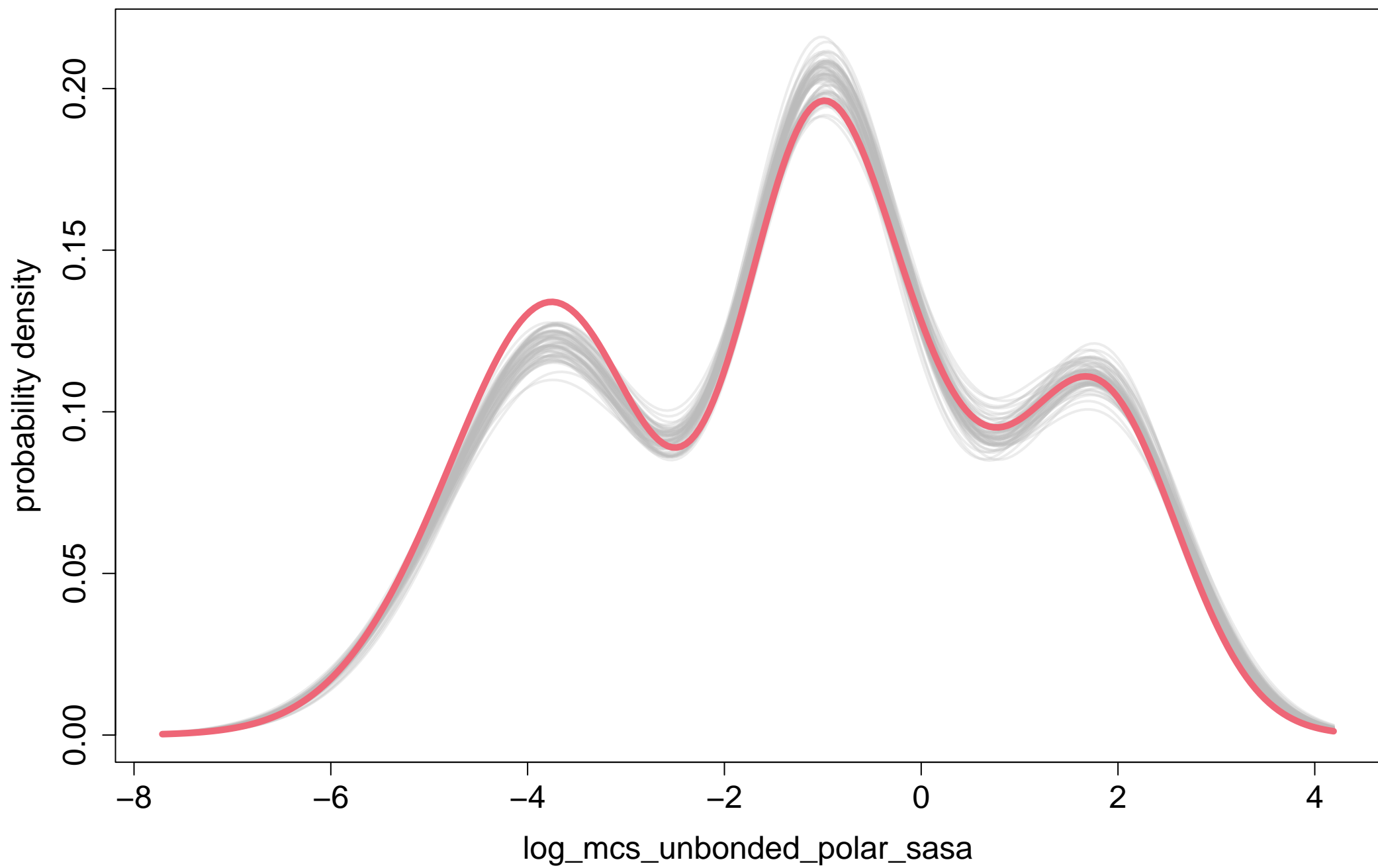
burn: 0

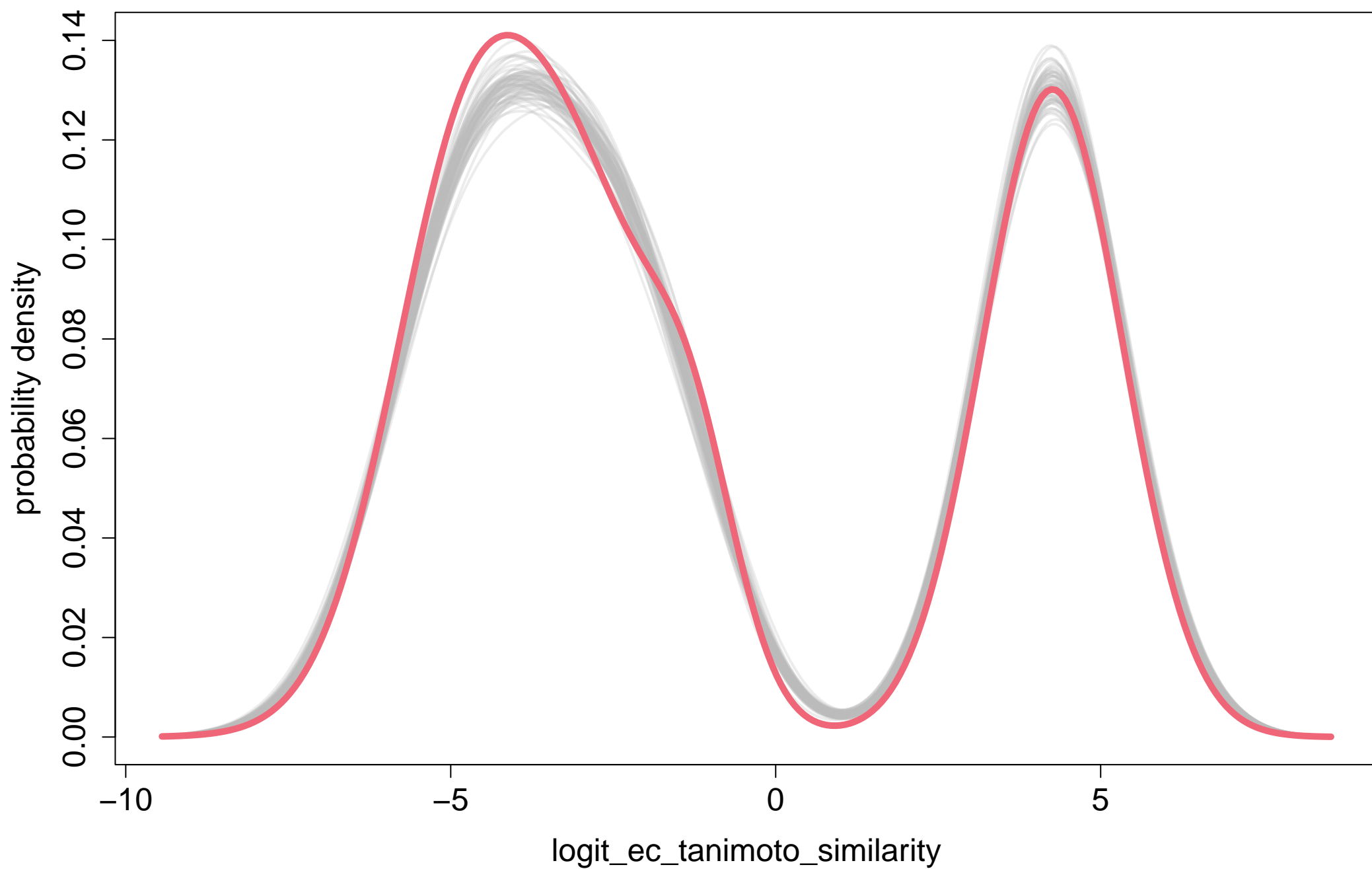
max rel.err.: 2.18000679413748

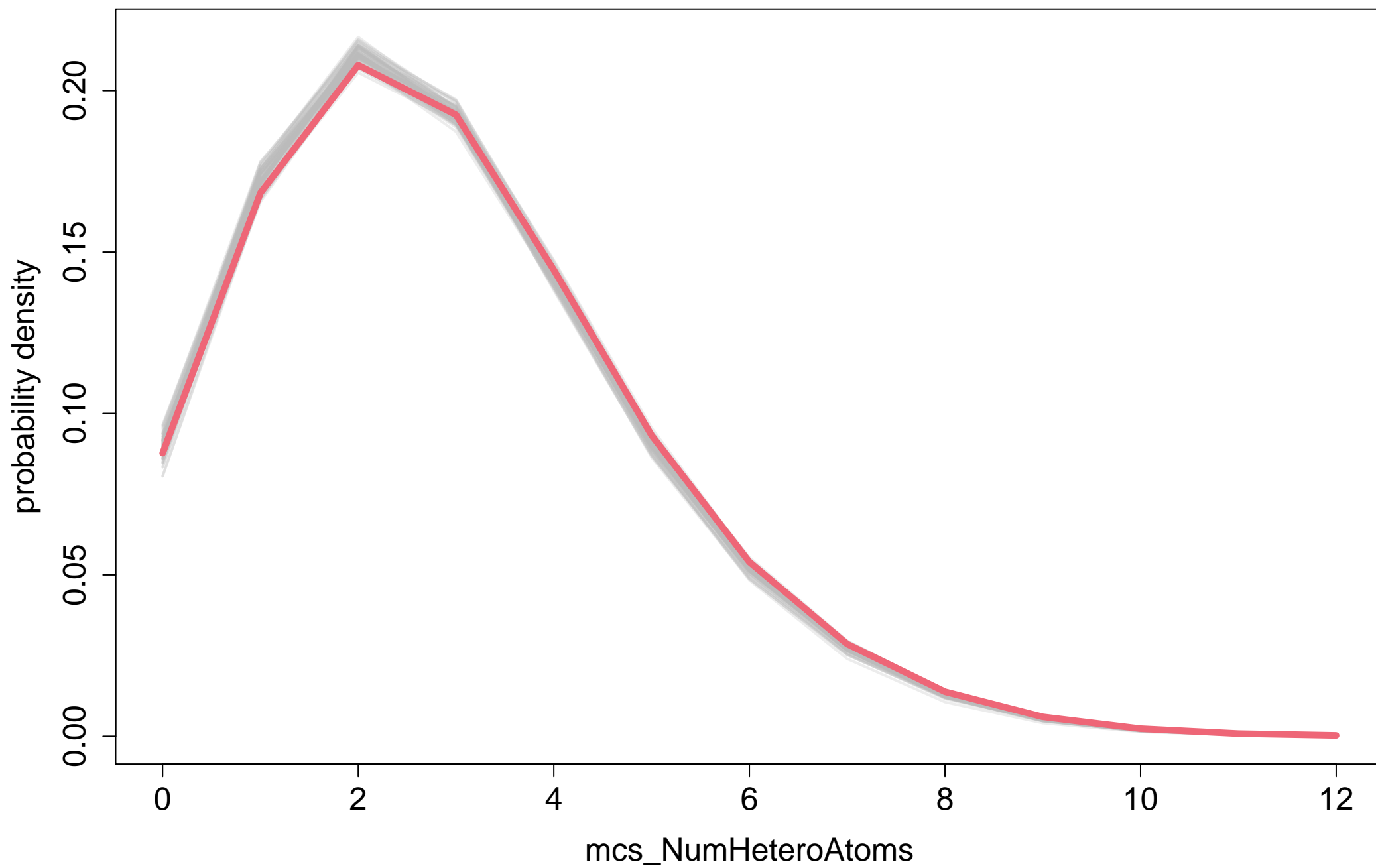
Occupied clusters: 9 of 64

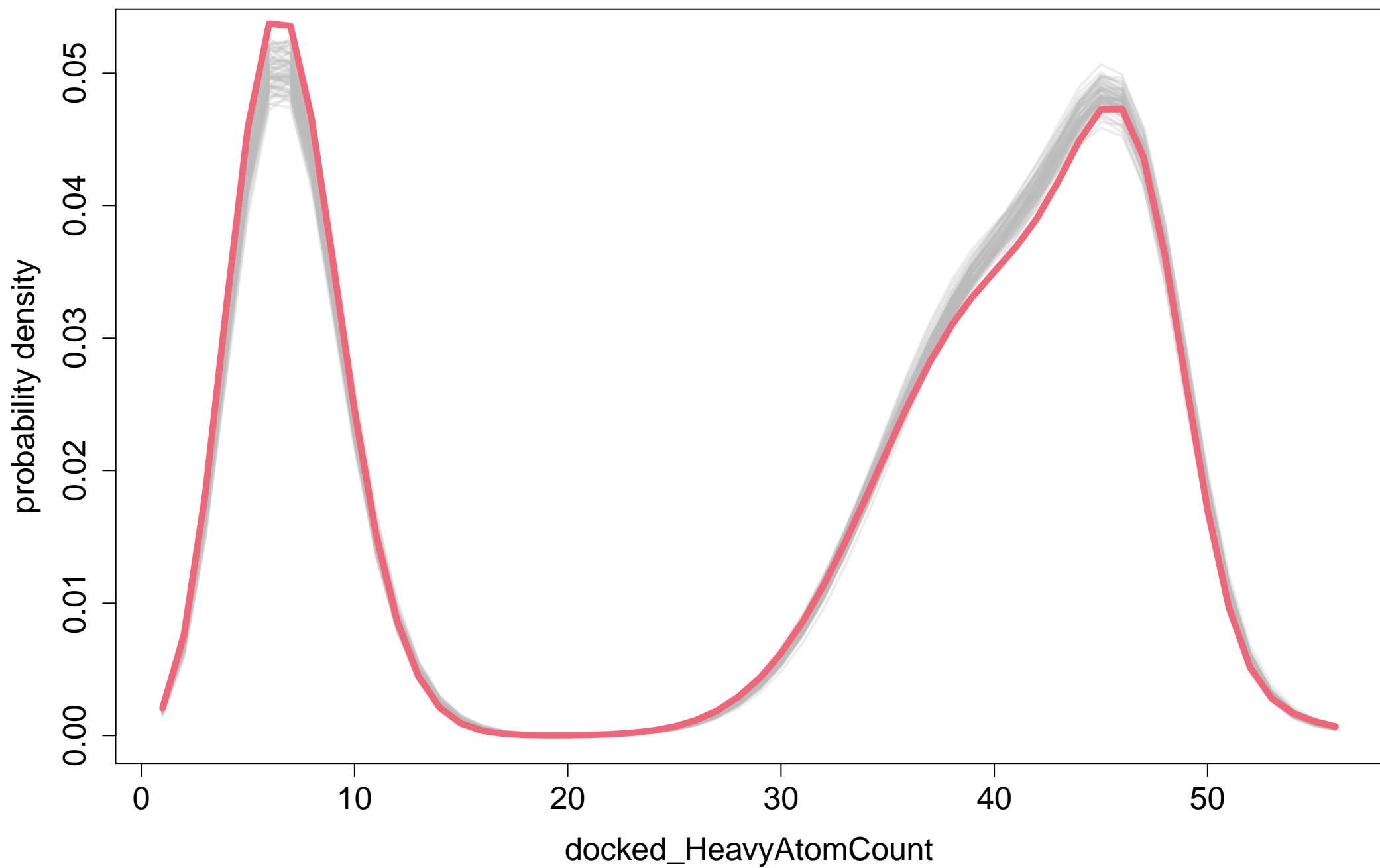
LL: -62500 +- 13.2

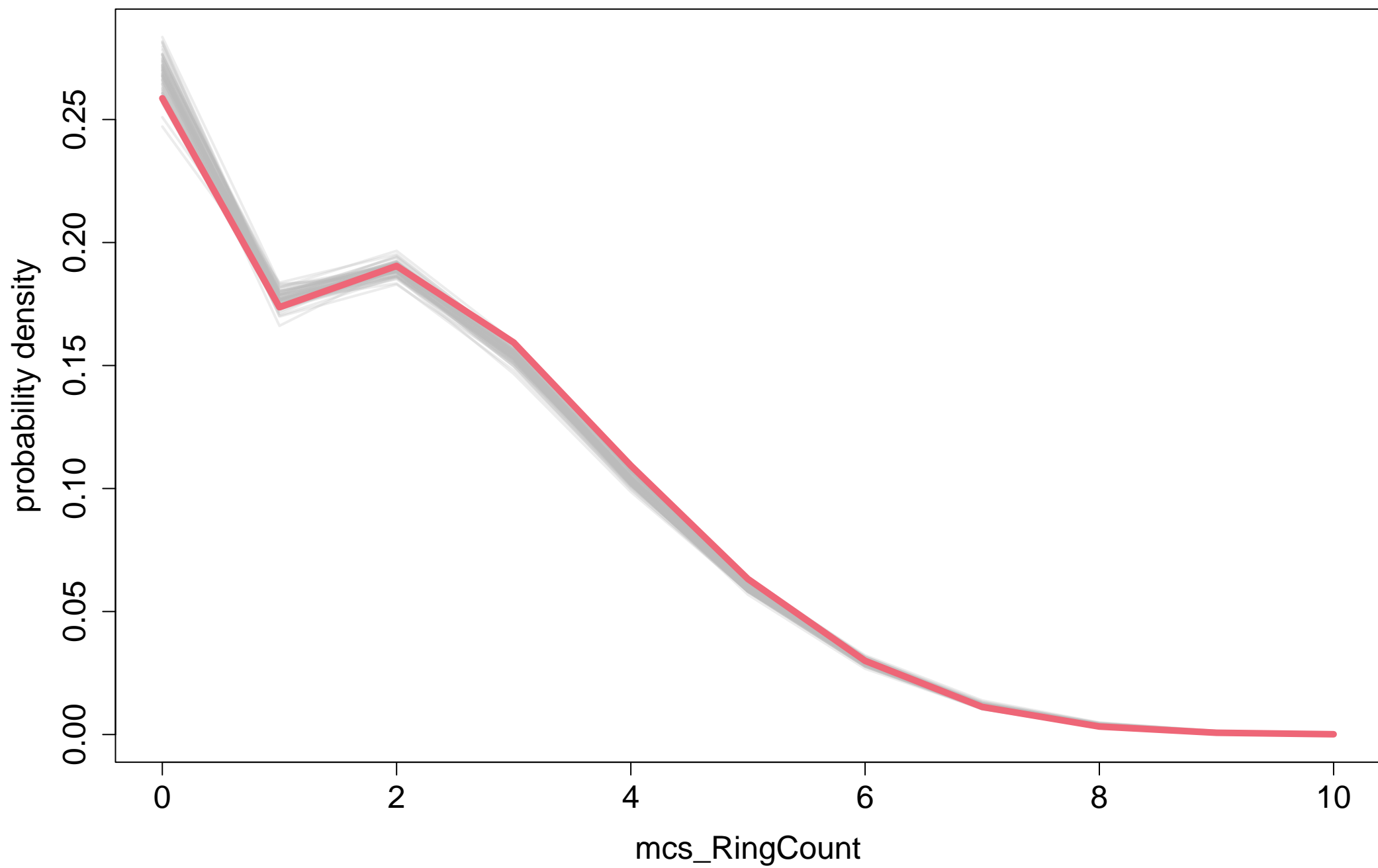


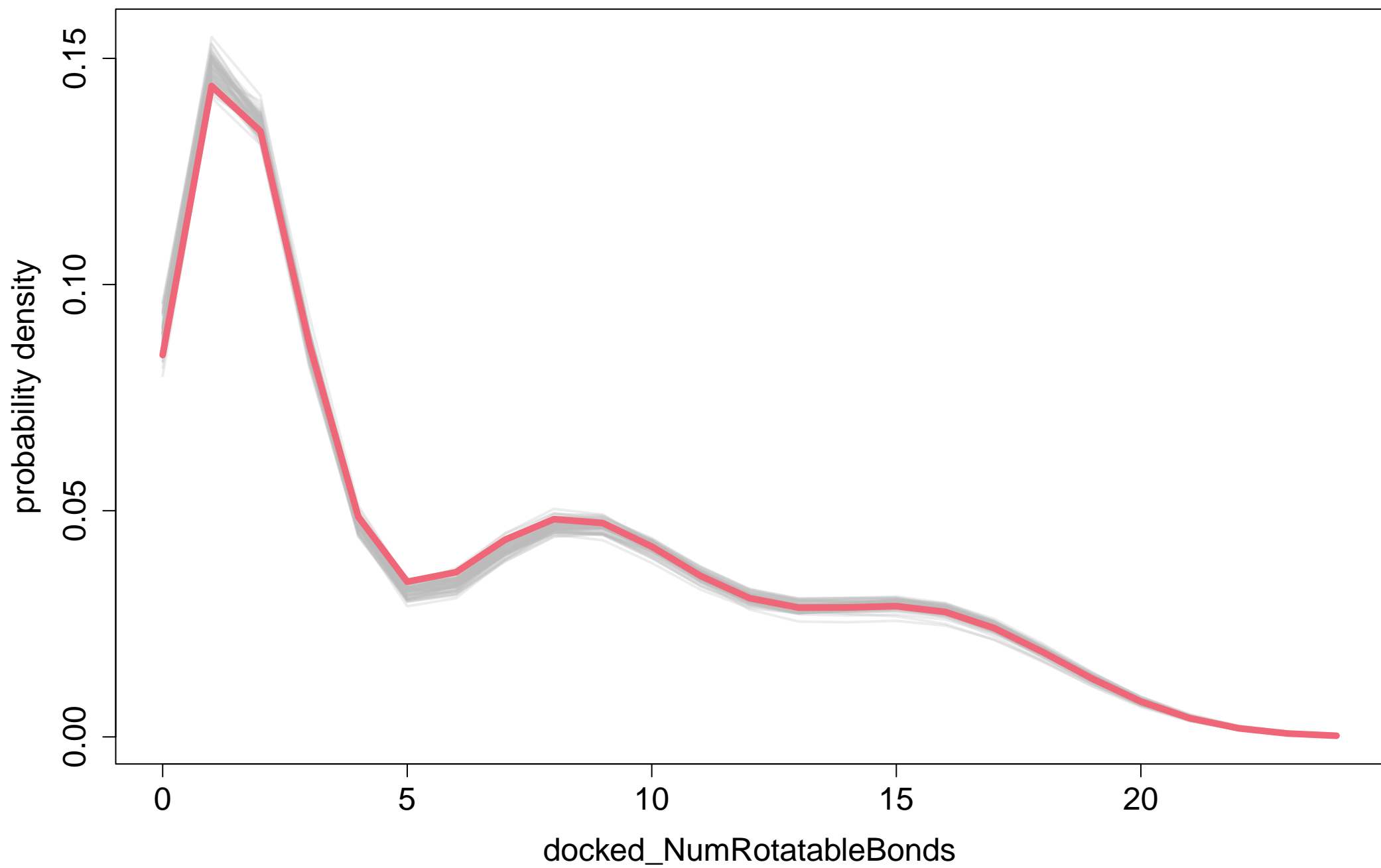


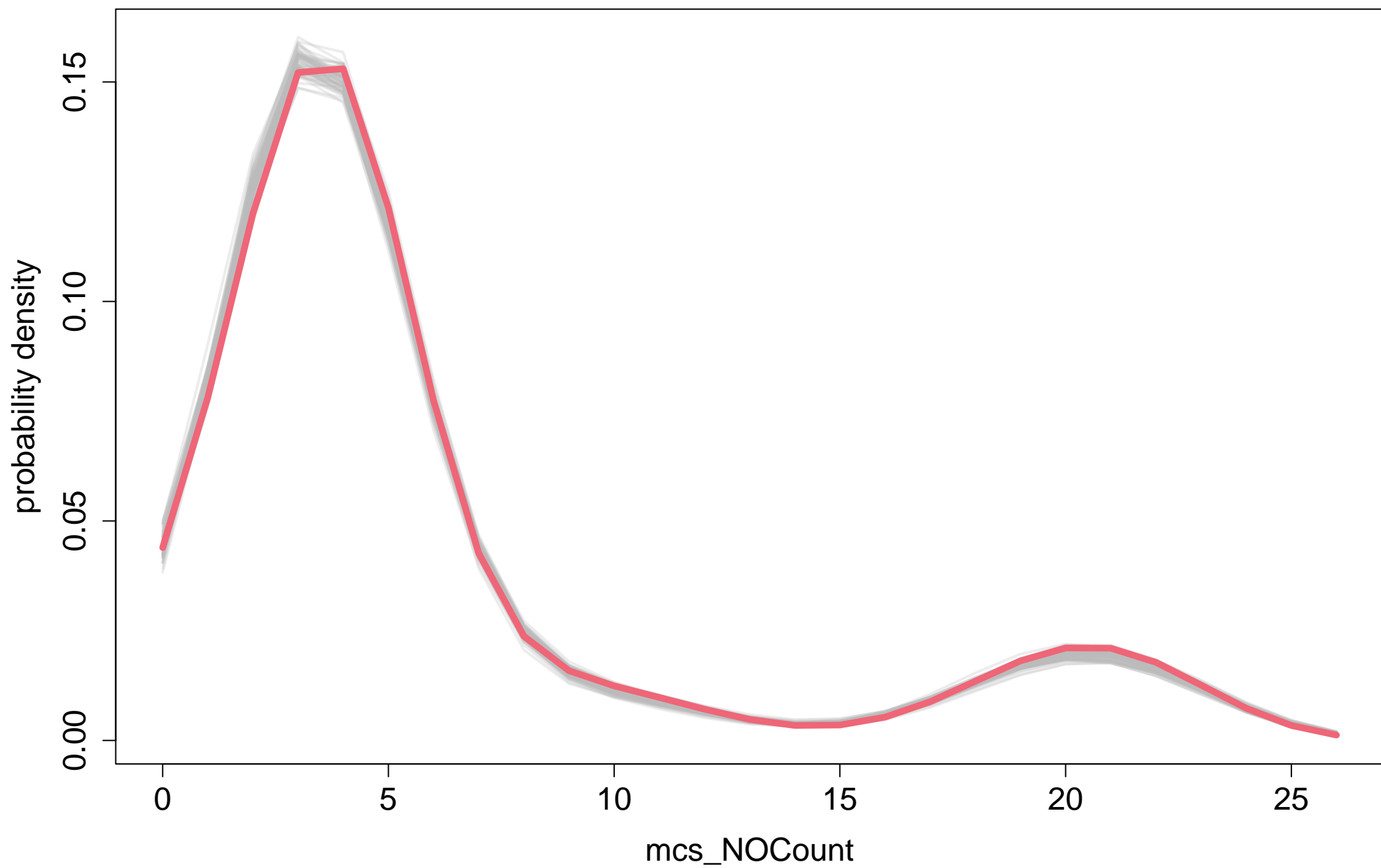


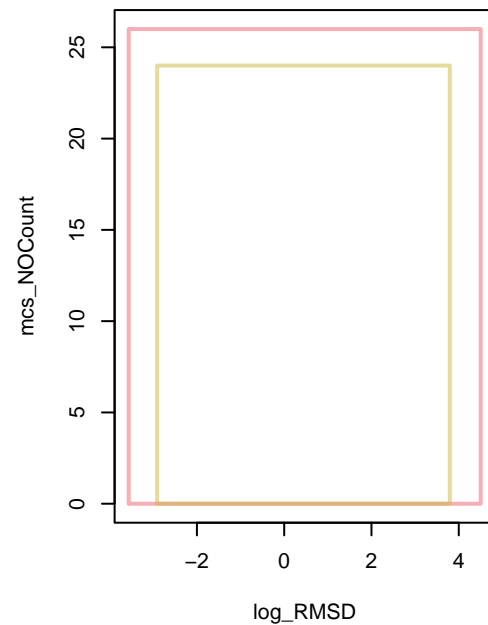
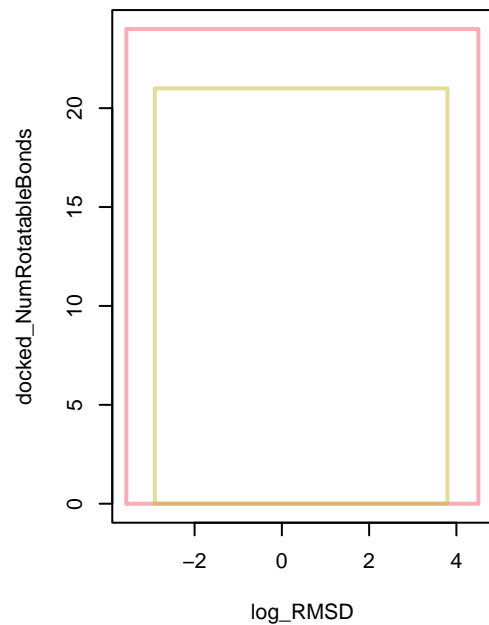
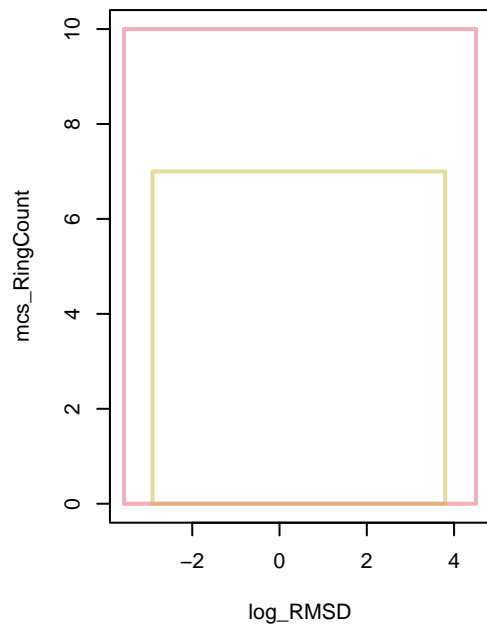
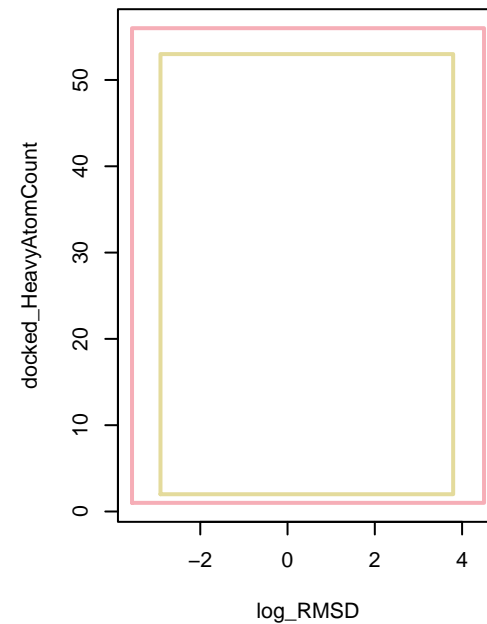
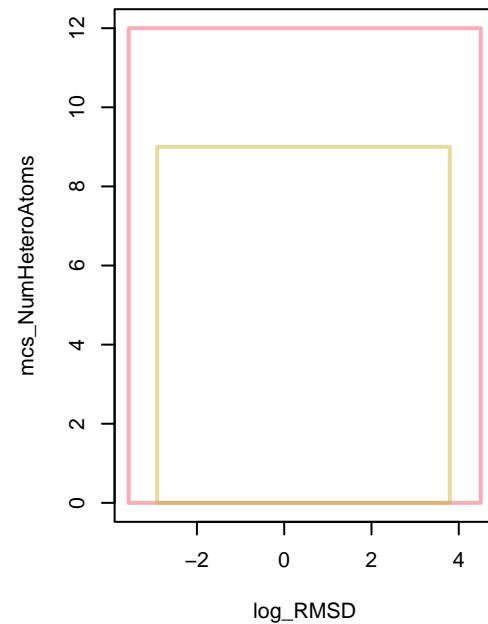
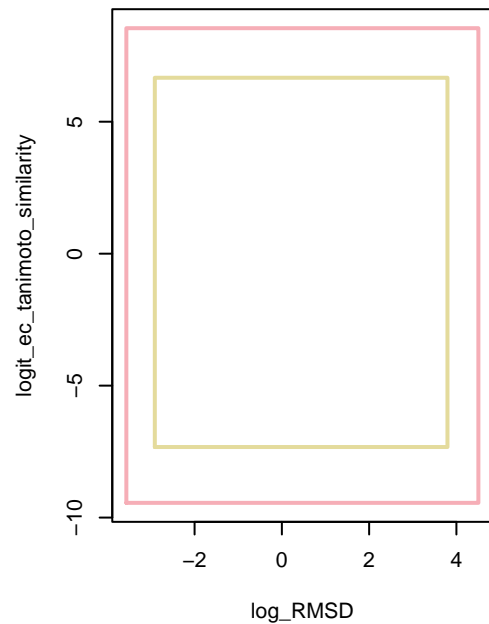
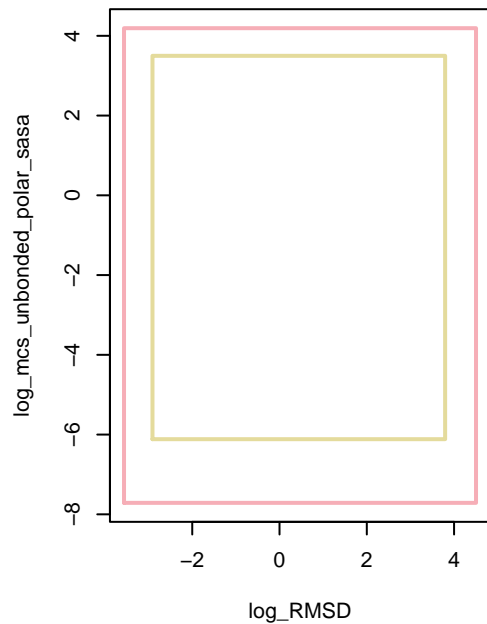




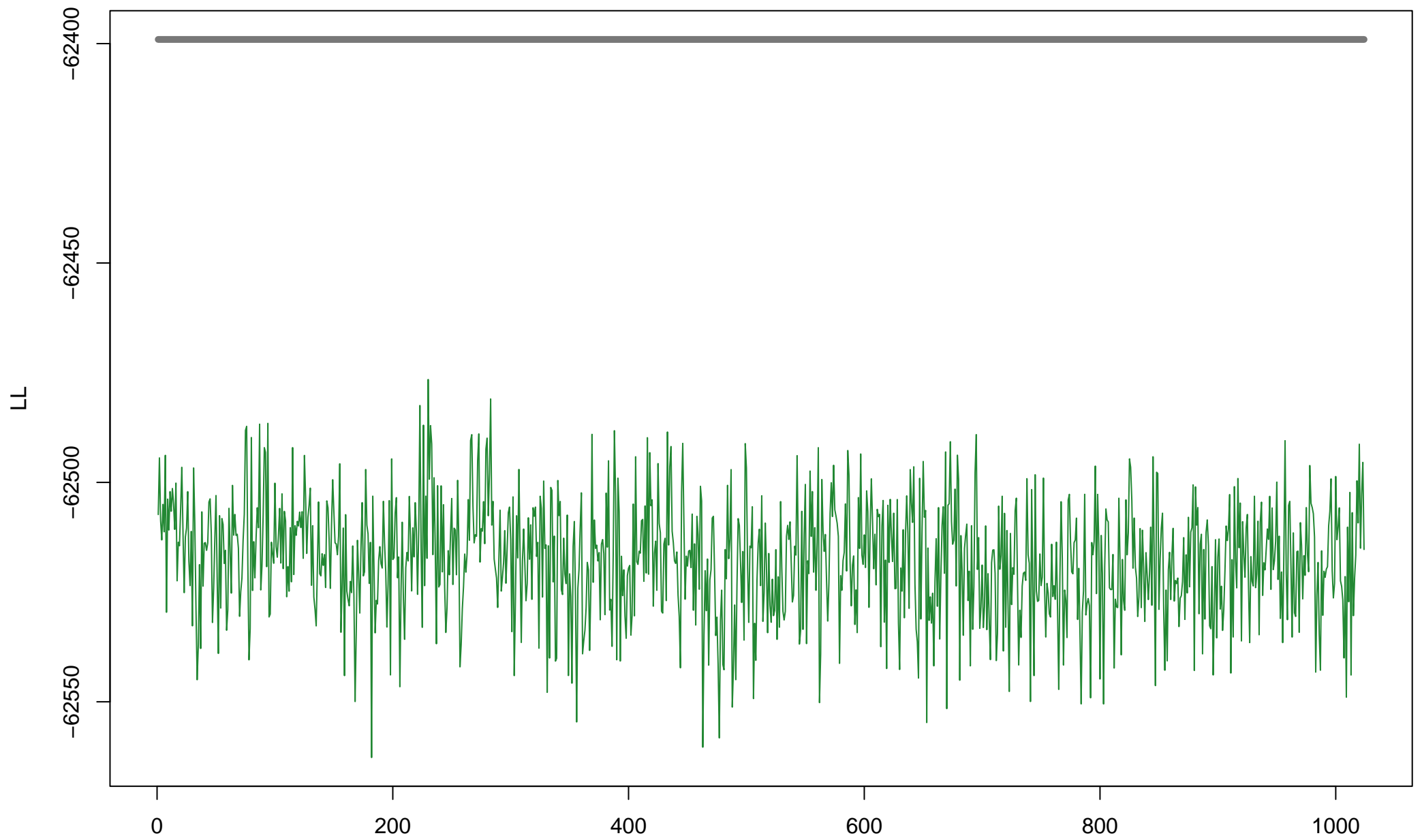






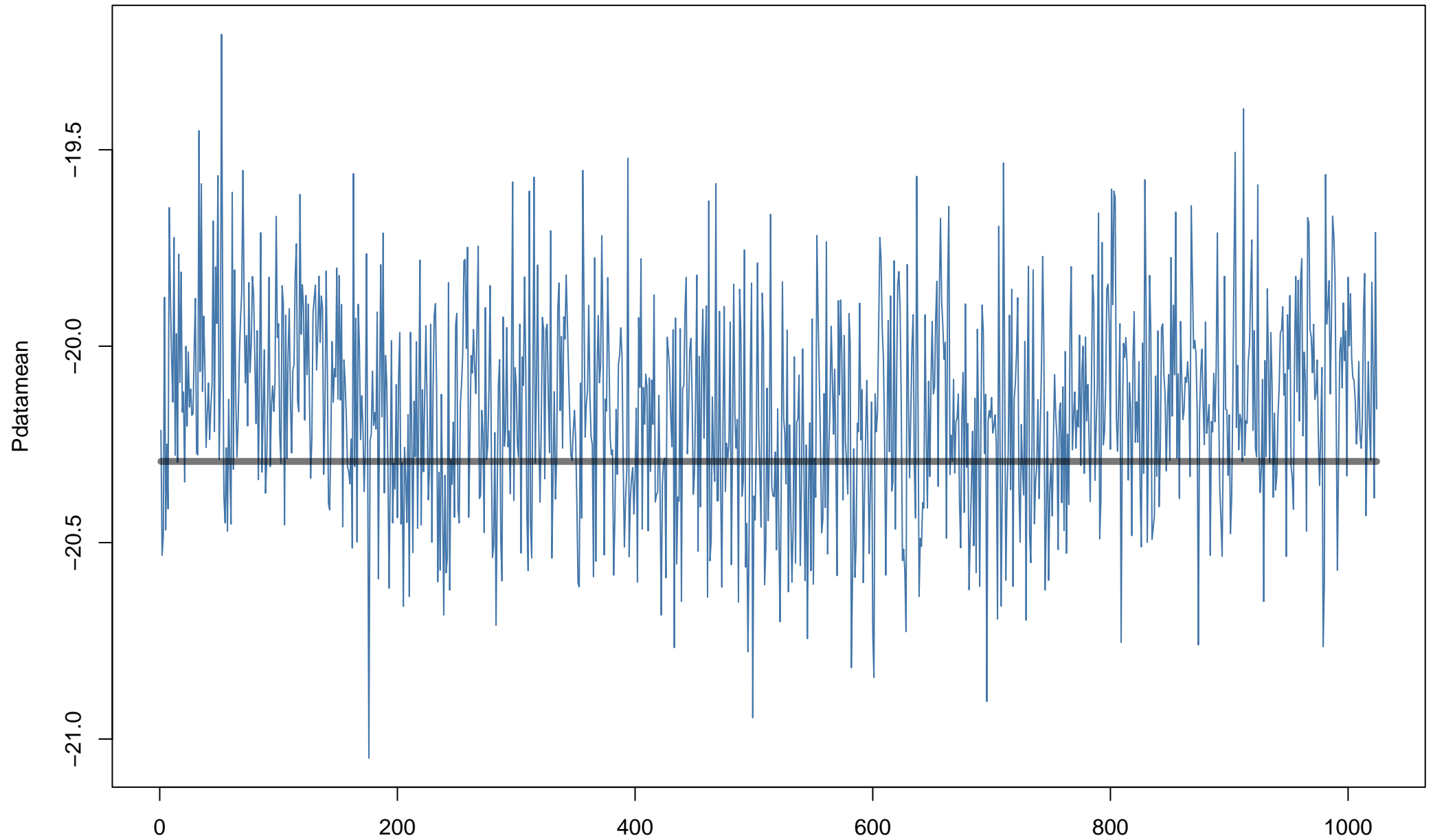


LL



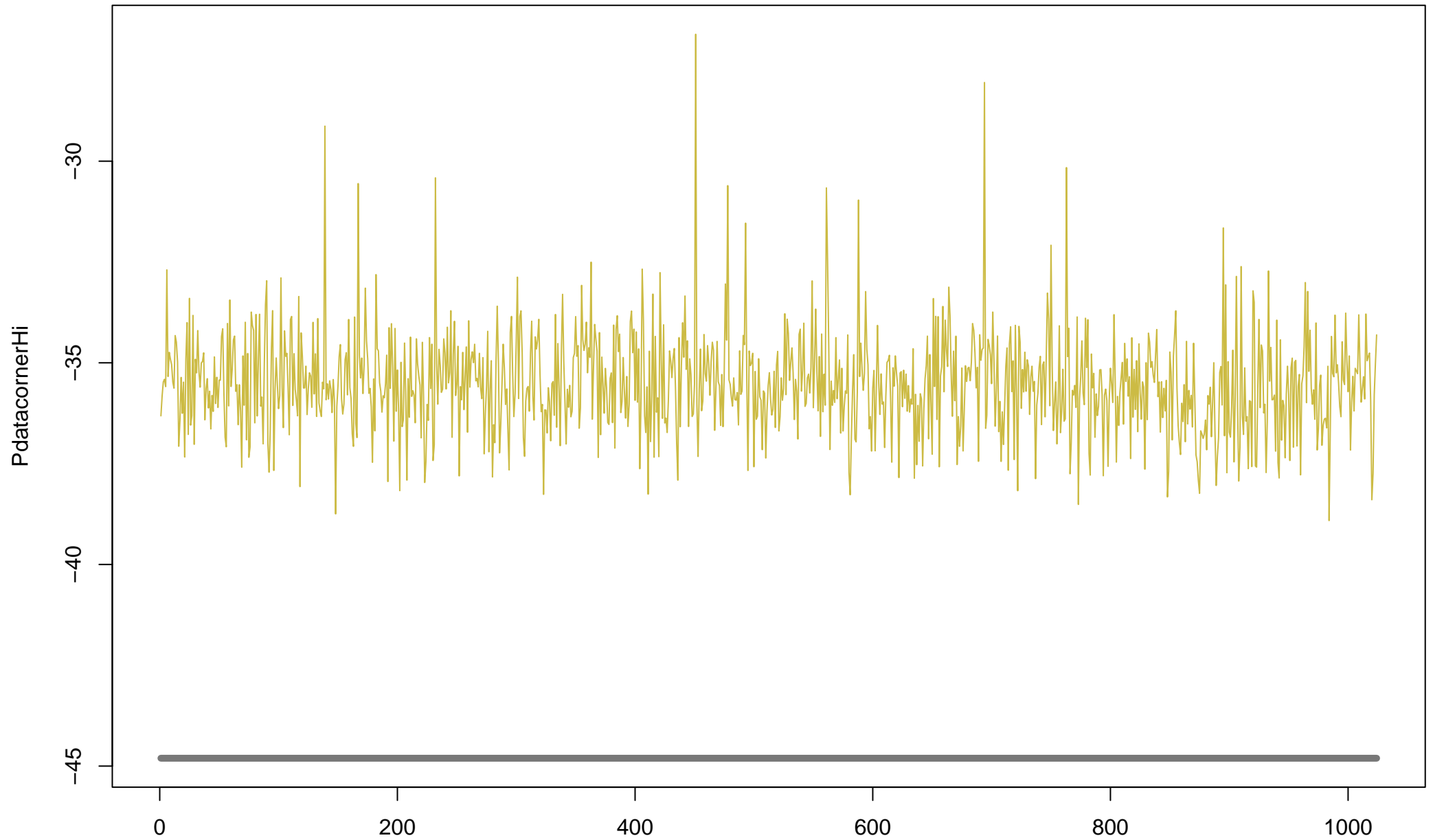
Pdatamean

ESS = 2.22e-16 | BMK = 0.0491 | MCSE(6.27) = 4.98 | stat: TRUE | burn: 0 | rel.err: 0.58



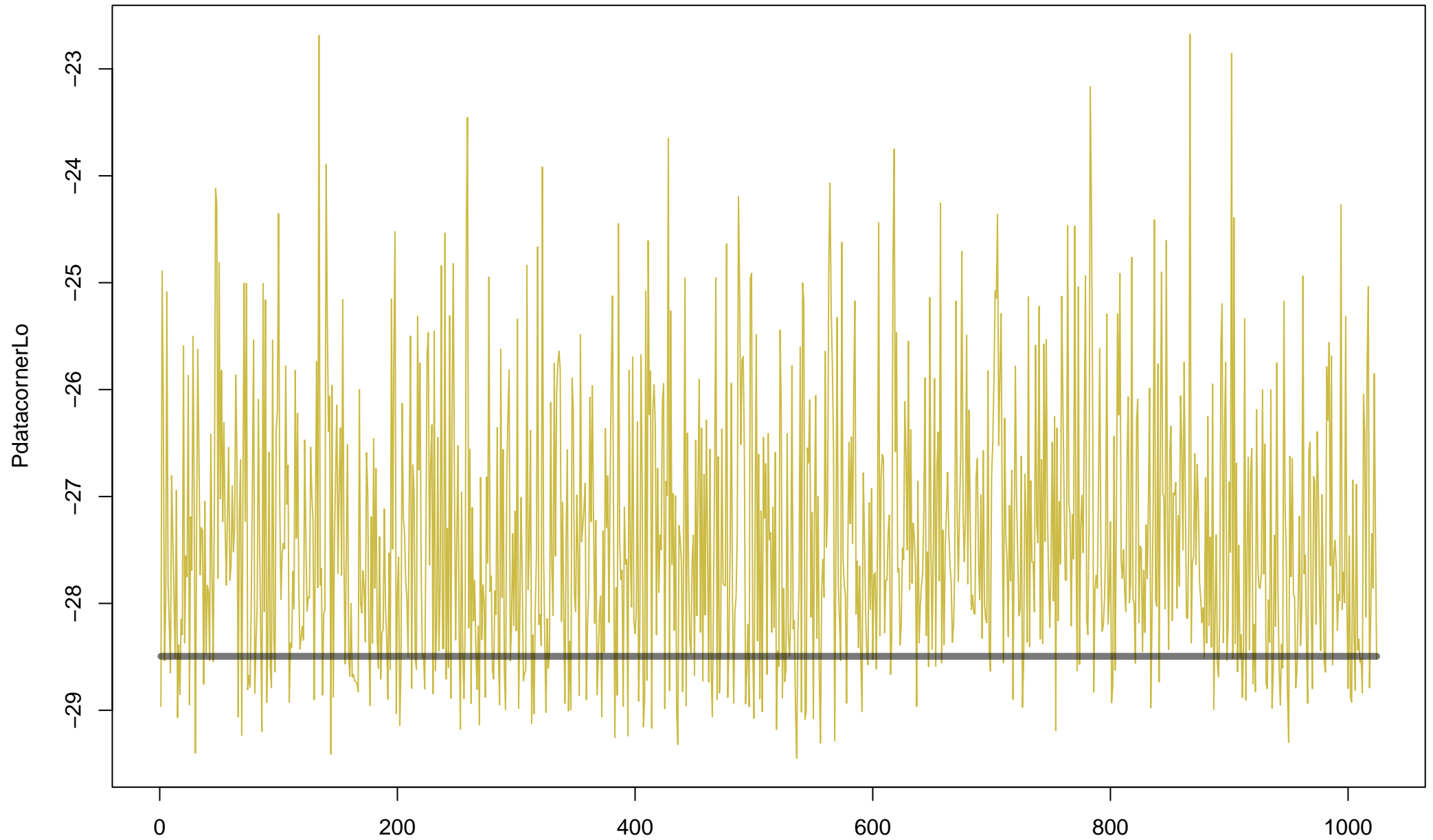
PdatacornerHi

ESS = 2.22e-16 | BMK = 0.562 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 510 | rel.err: 0.0559



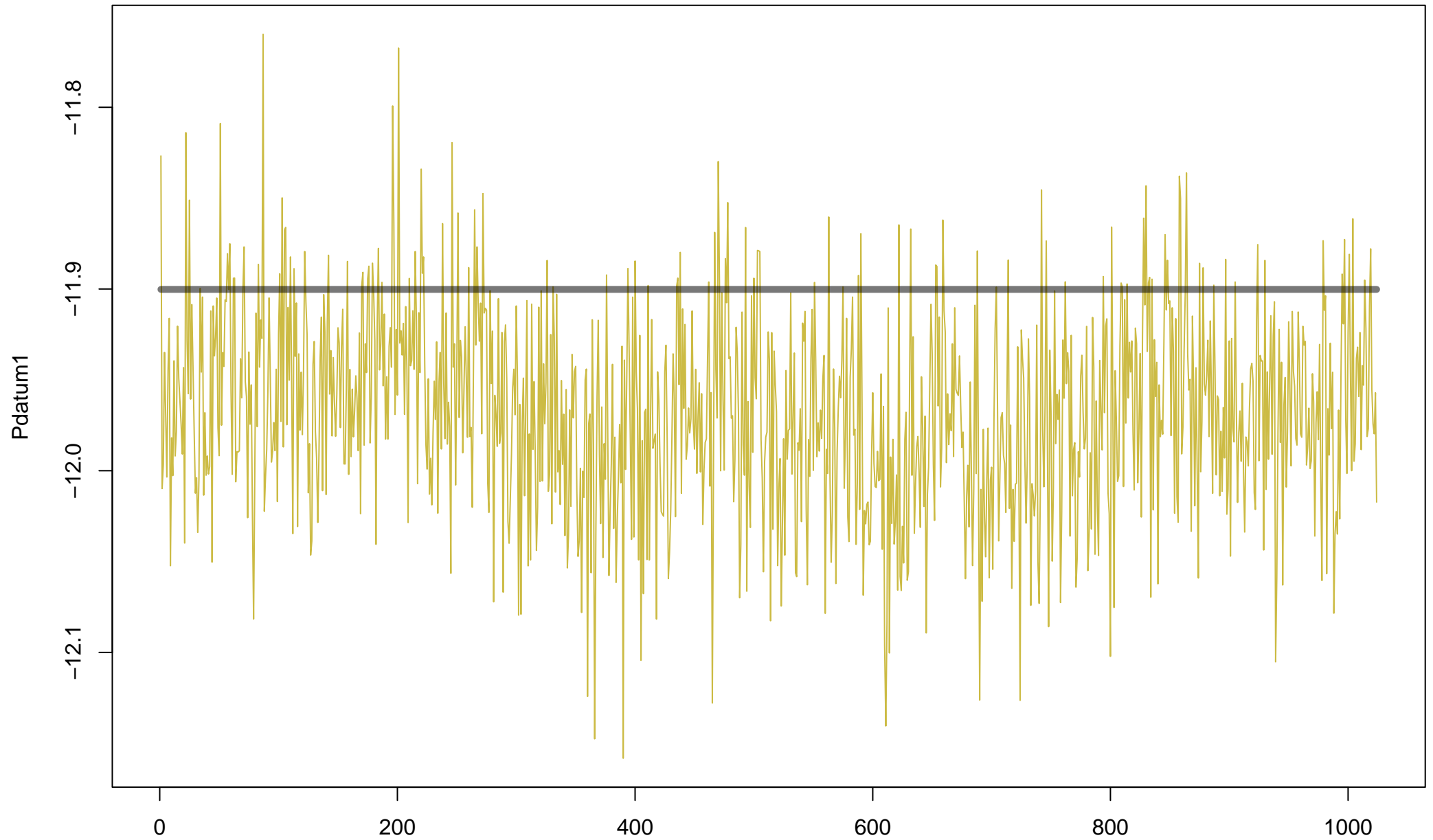
PdatacornerLo

ESS = 2.22e-16 | BMK = 0.132 | MCSE(6.27) = 2.79 | stat: TRUE | burn: 0 | rel.err: 0.322



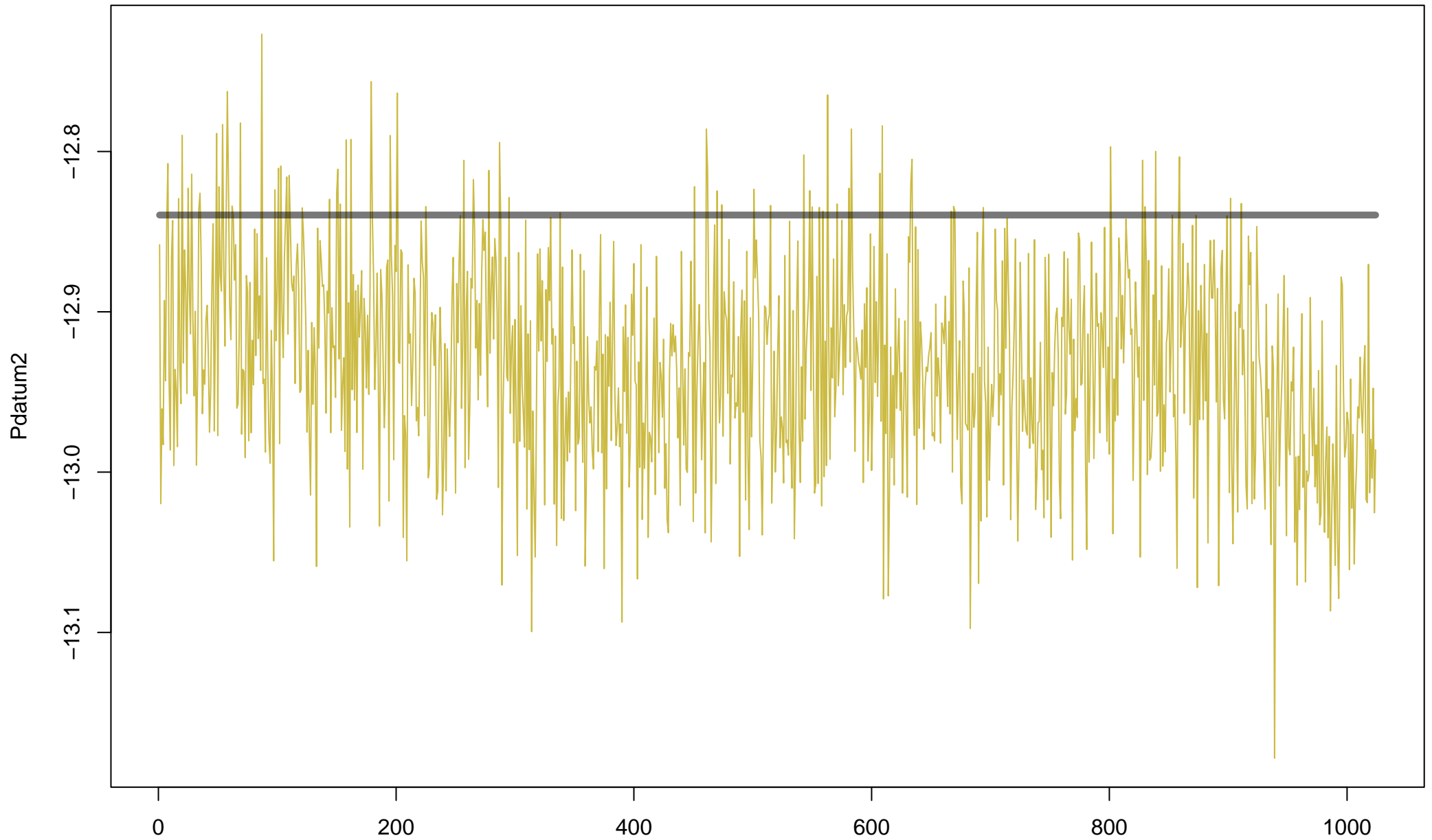
Pdatum1

ESS = 123 | BMK = 0.104 | MCSE(6.27) = 6.6 | stat: FALSE | burn: 0 | rel.err: -1.24



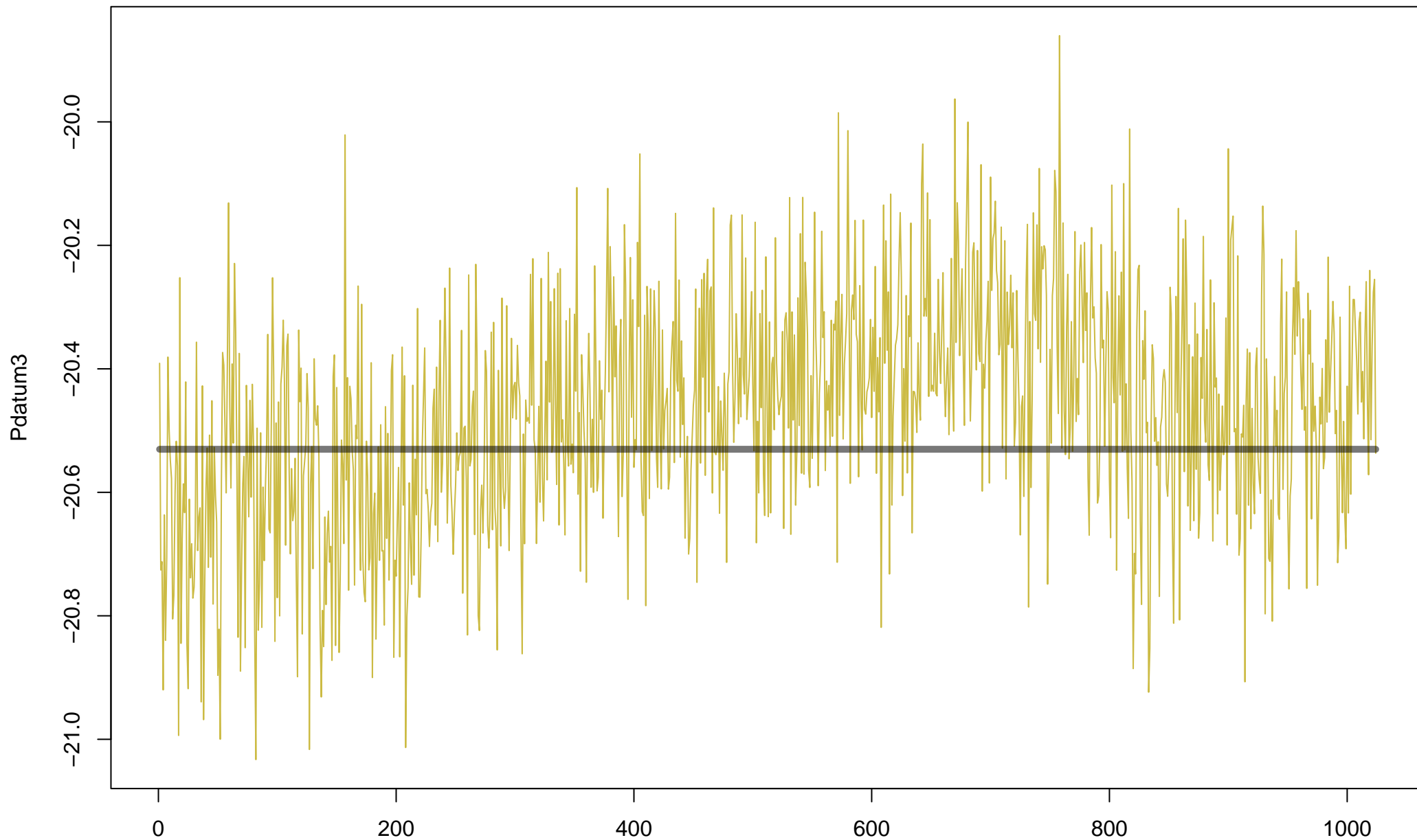
Pdatum2

ESS = 175 | BMK = 0.0993 | MCSE(6.27) = 6.84 | stat: FALSE | burn: 0 | rel.err: -1.52



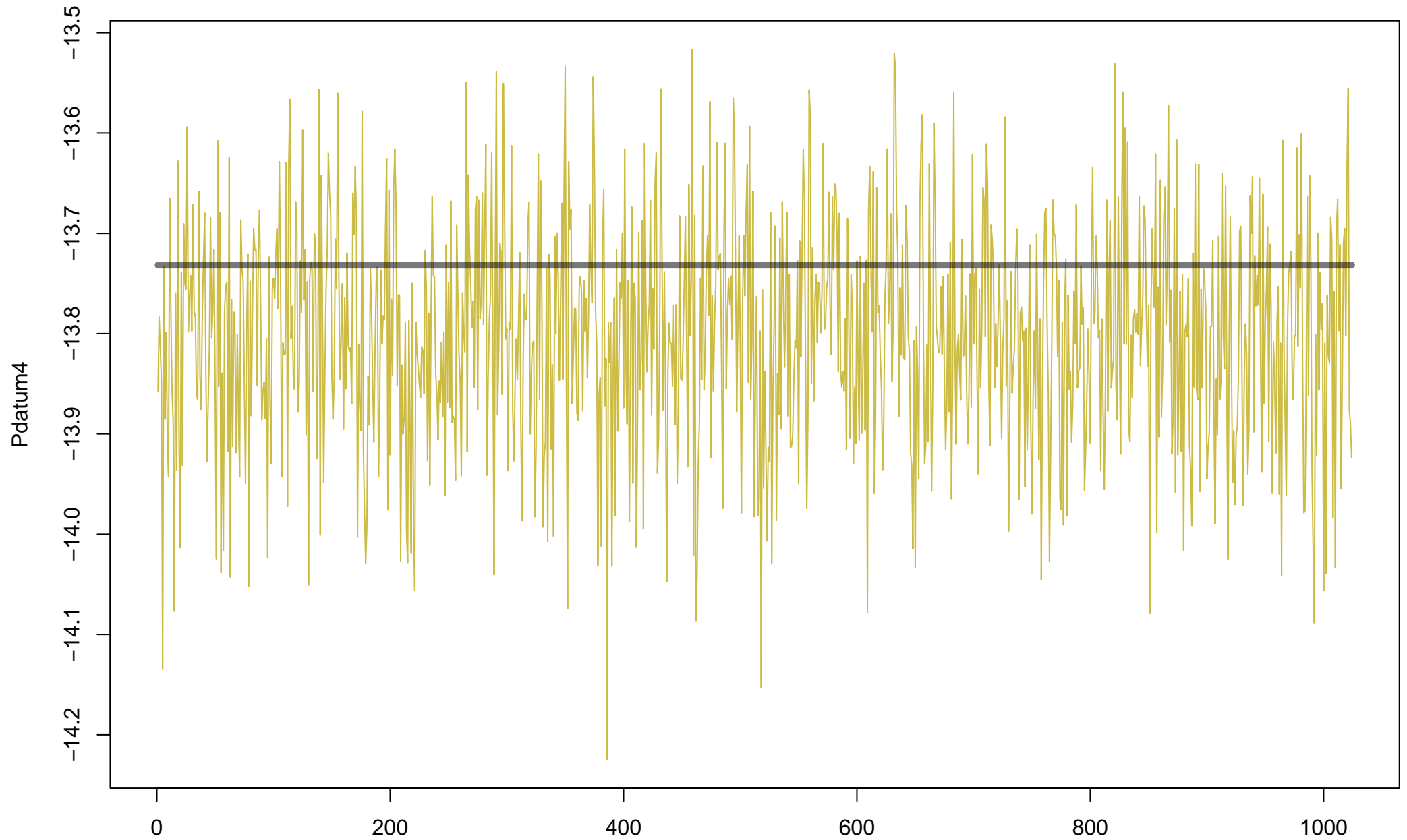
Pdatum3

ESS = 2.22e-16 | BMK = 0.234 | MCSE(6.27) = 8.76 | stat: TRUE | burn: 0 | rel.err: 0.399



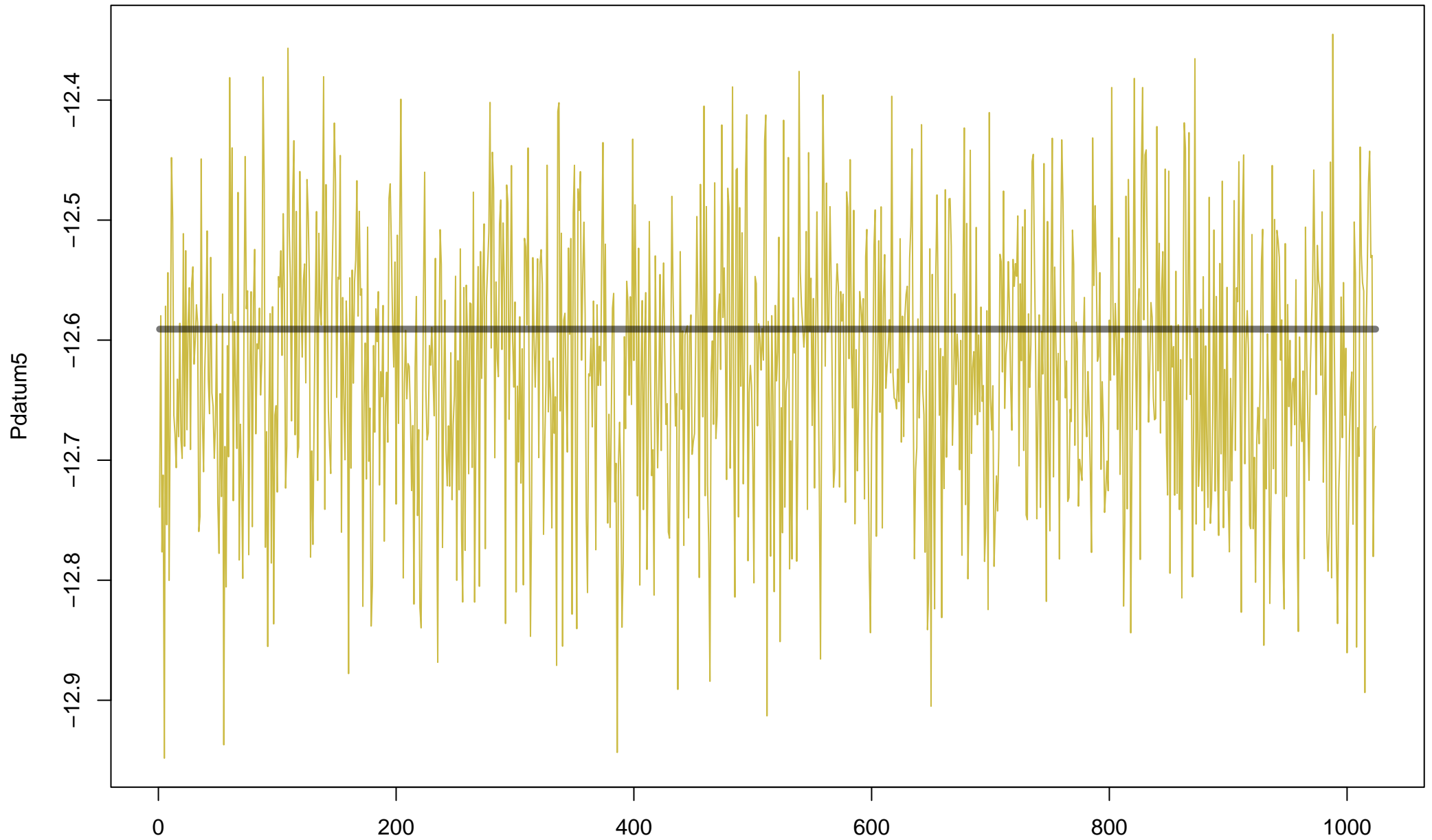
Pdatum4

ESS = 625 | BMK = 0.0516 | MCSE(6.27) = 3.91 | stat: TRUE | burn: 0 | rel.err: -0.611



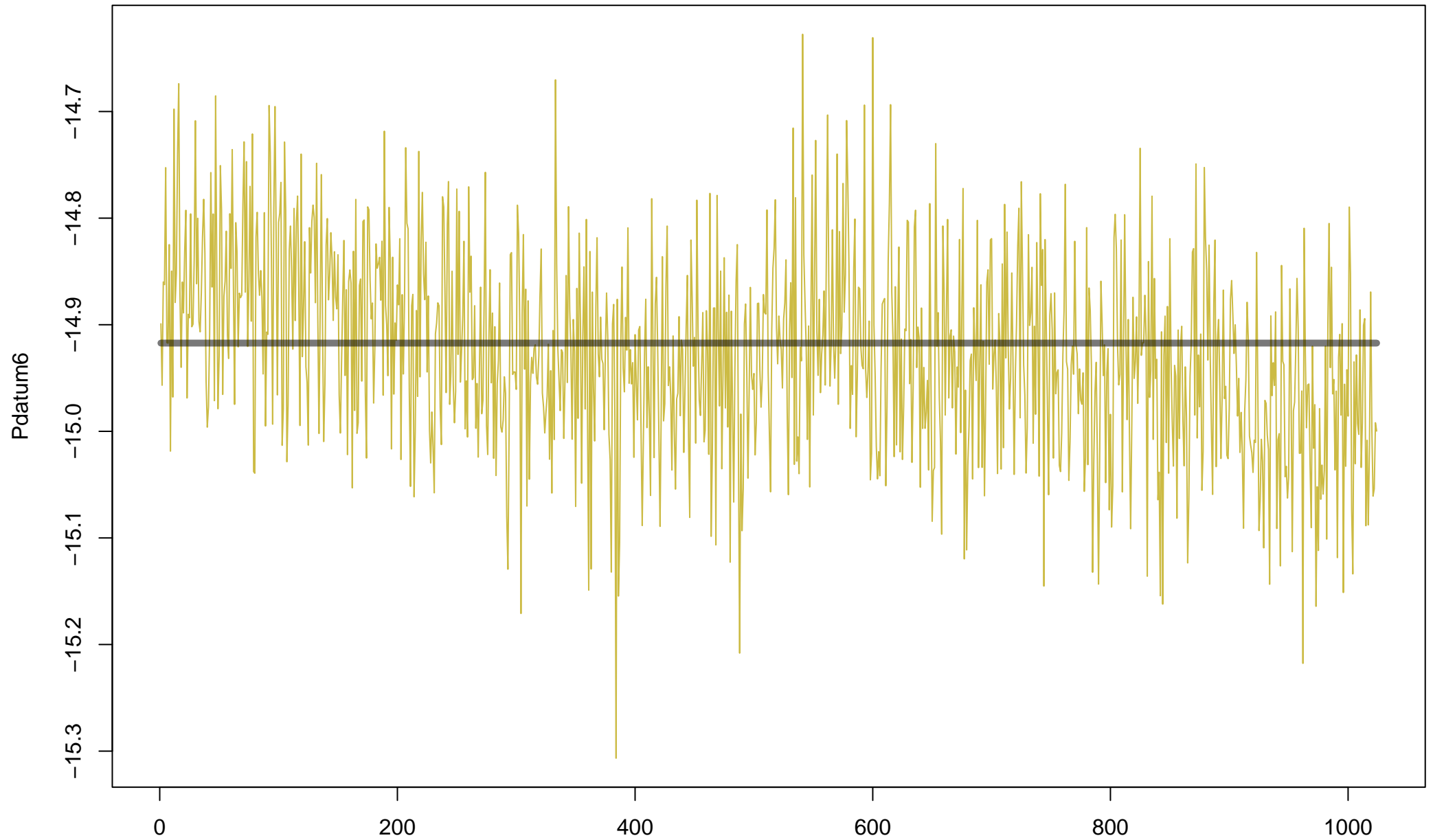
Pdatum5

ESS = 1020 | BMK = 0.0347 | MCSE(6.27) = 3.28 | stat: TRUE | burn: 0 | rel.err: -0.258



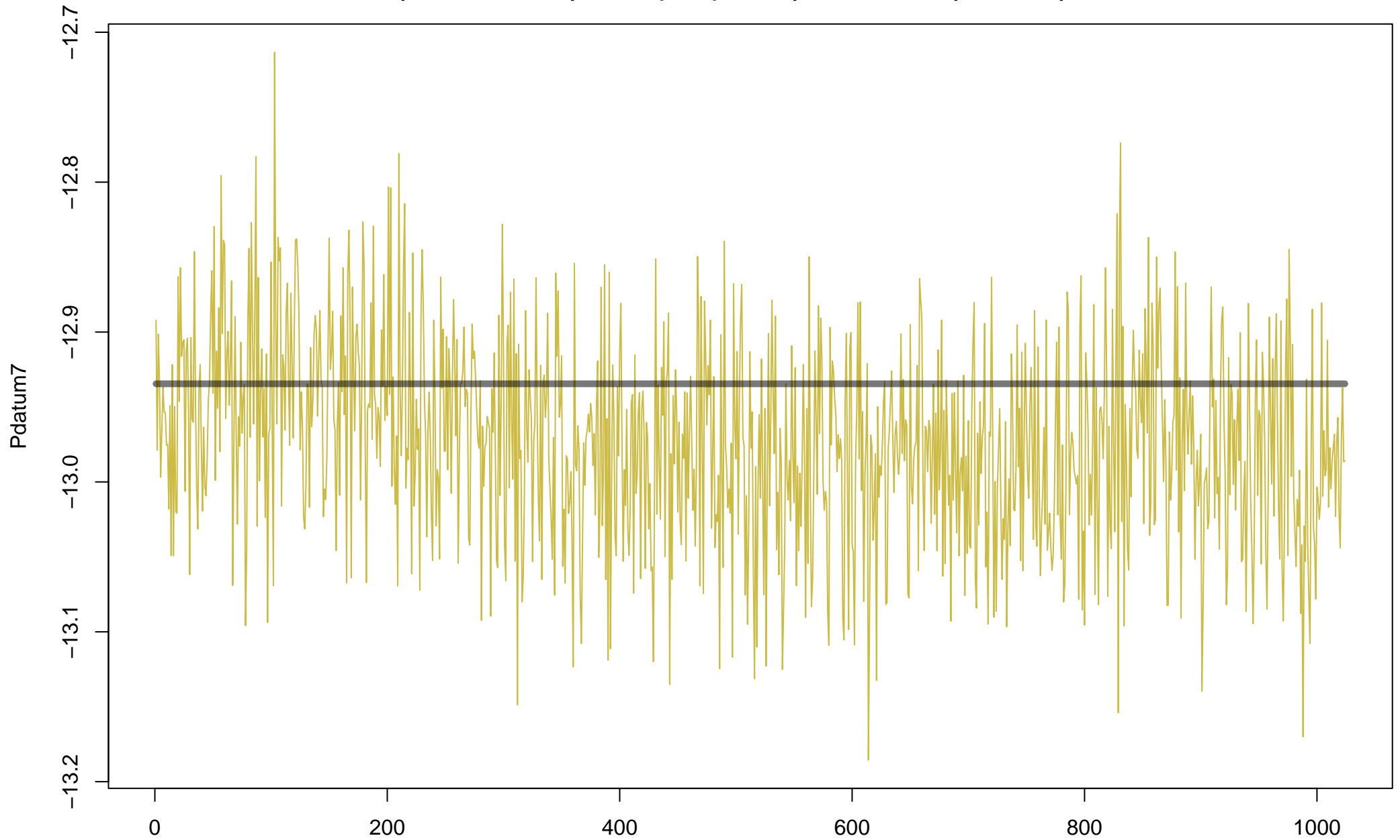
Pdatum6

ESS = 43.3 | BMK = 0.144 | MCSE(6.27) = 7.37 | stat: FALSE | burn: 0 | rel.err: -0.0523



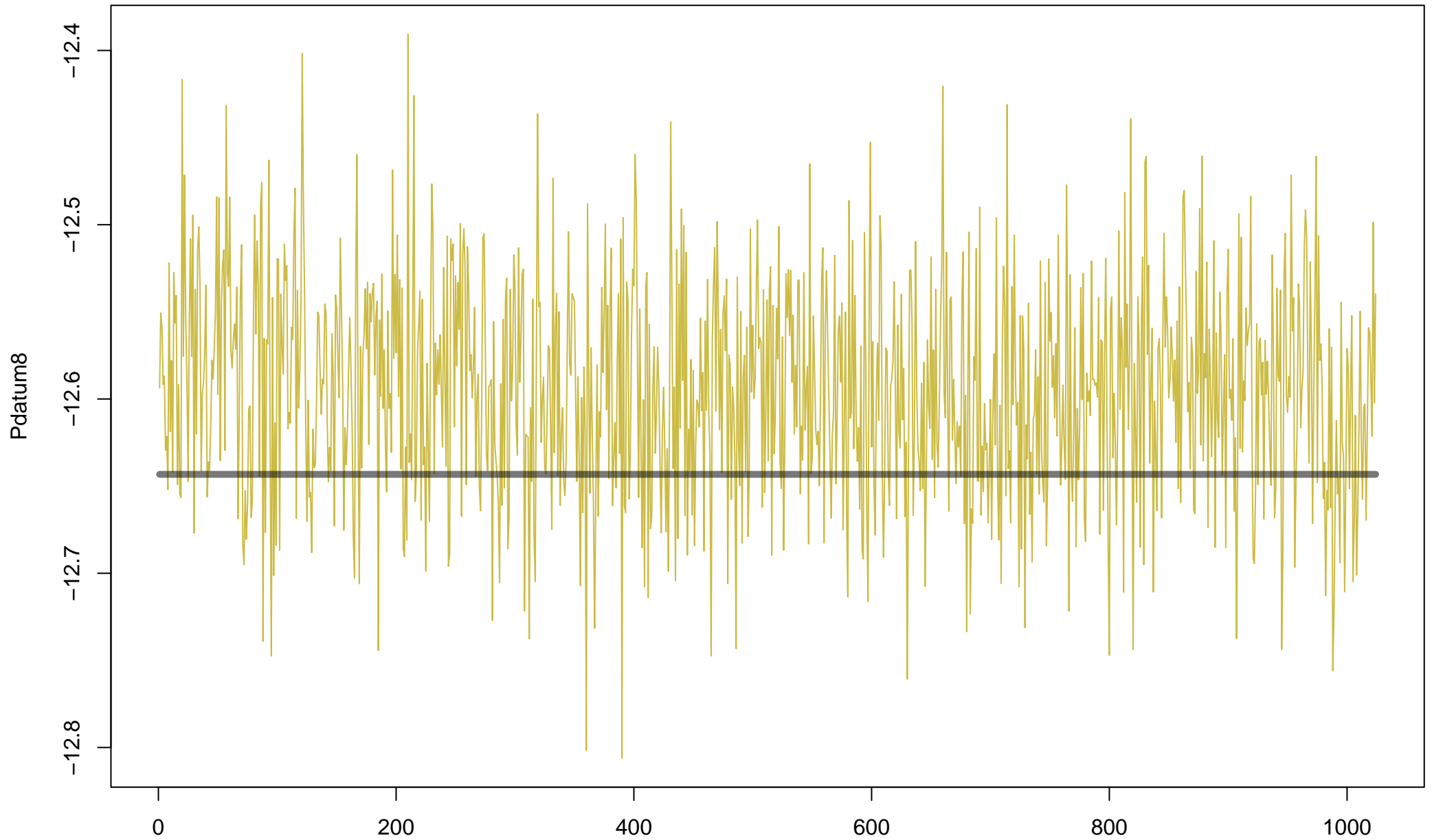
Pdatum7

ESS = 77.9 | BMK = 0.152 | MCSE(6.27) = 6.1 | stat: FALSE | burn: 0 | rel.err: -0.551



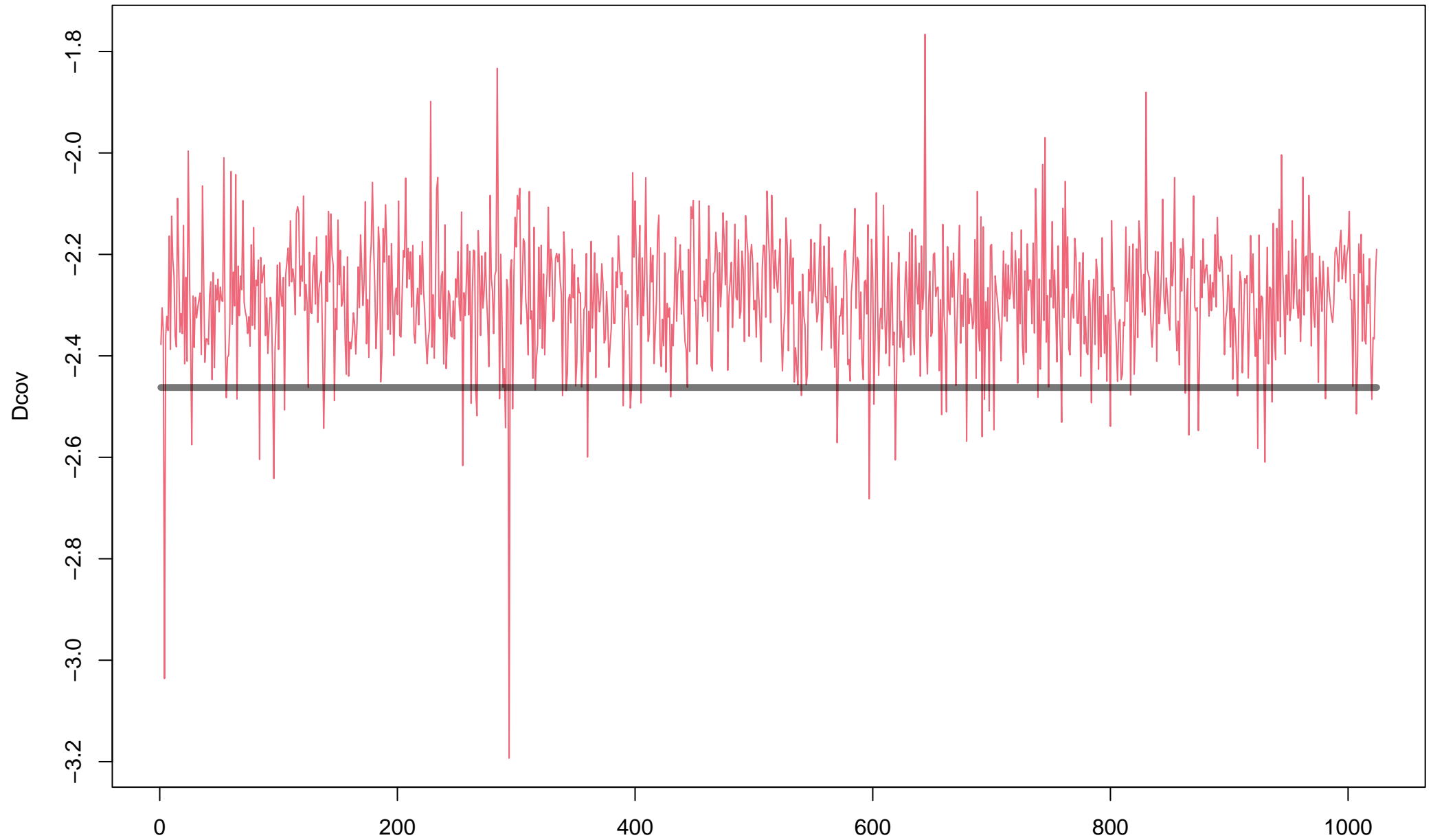
Pdatum8

ESS = 1020 | BMK = 0.061 | MCSE(6.27) = 3.36 | stat: FALSE | burn: 0 | rel.err: 0.788

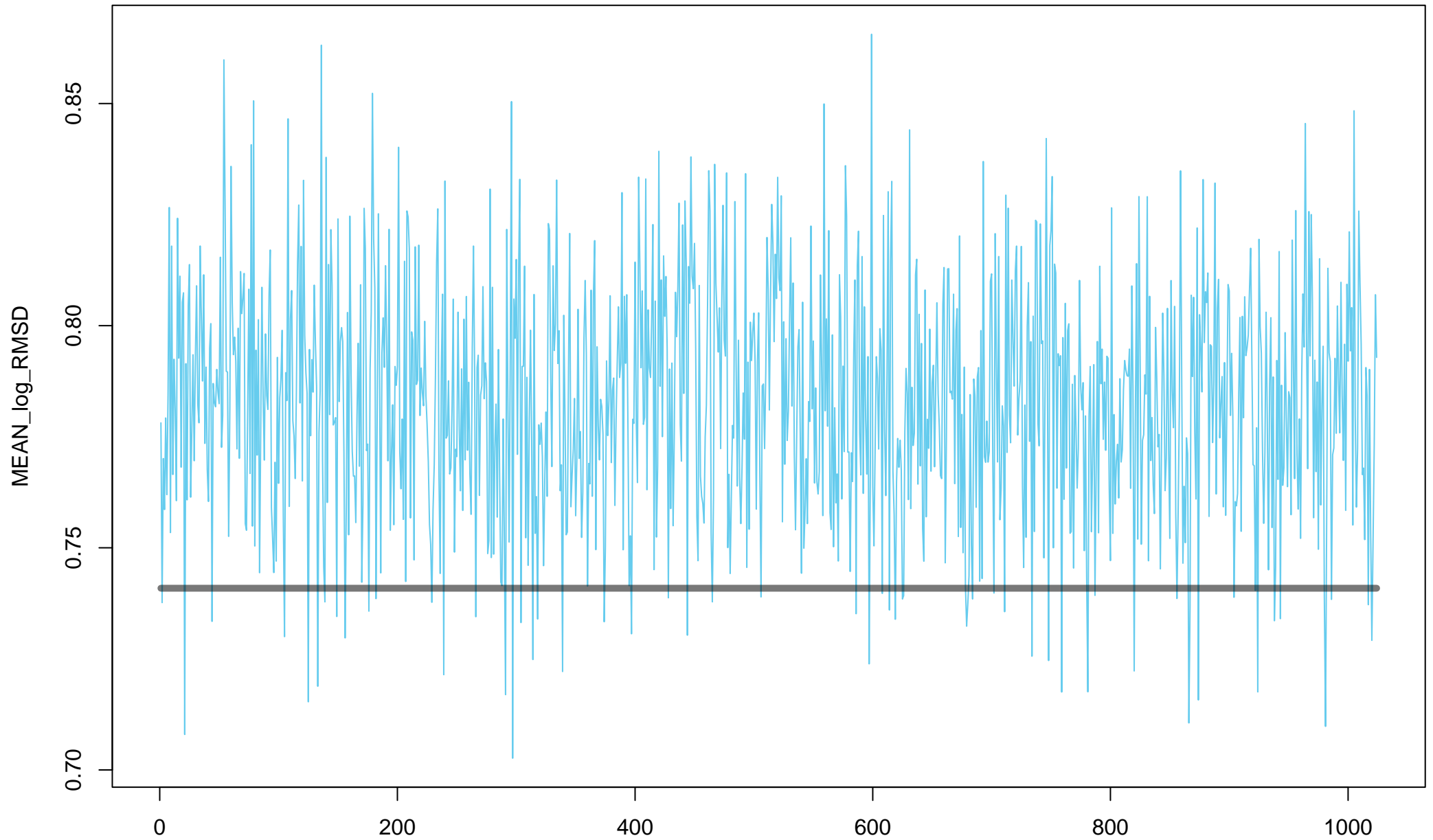


Dcov

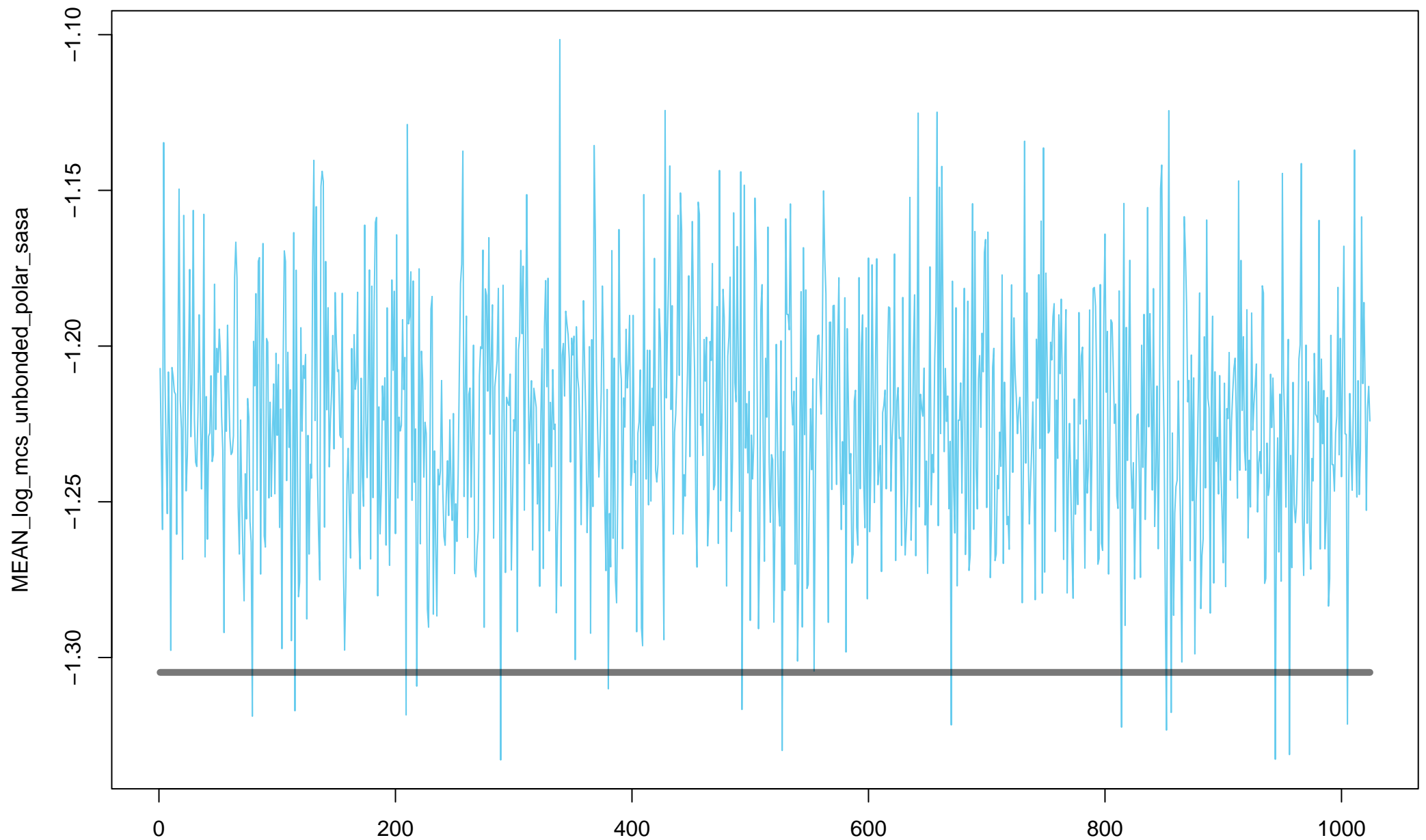
ESS = 1020 | BMK = 0.0772 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0 | rel.err: -1.47



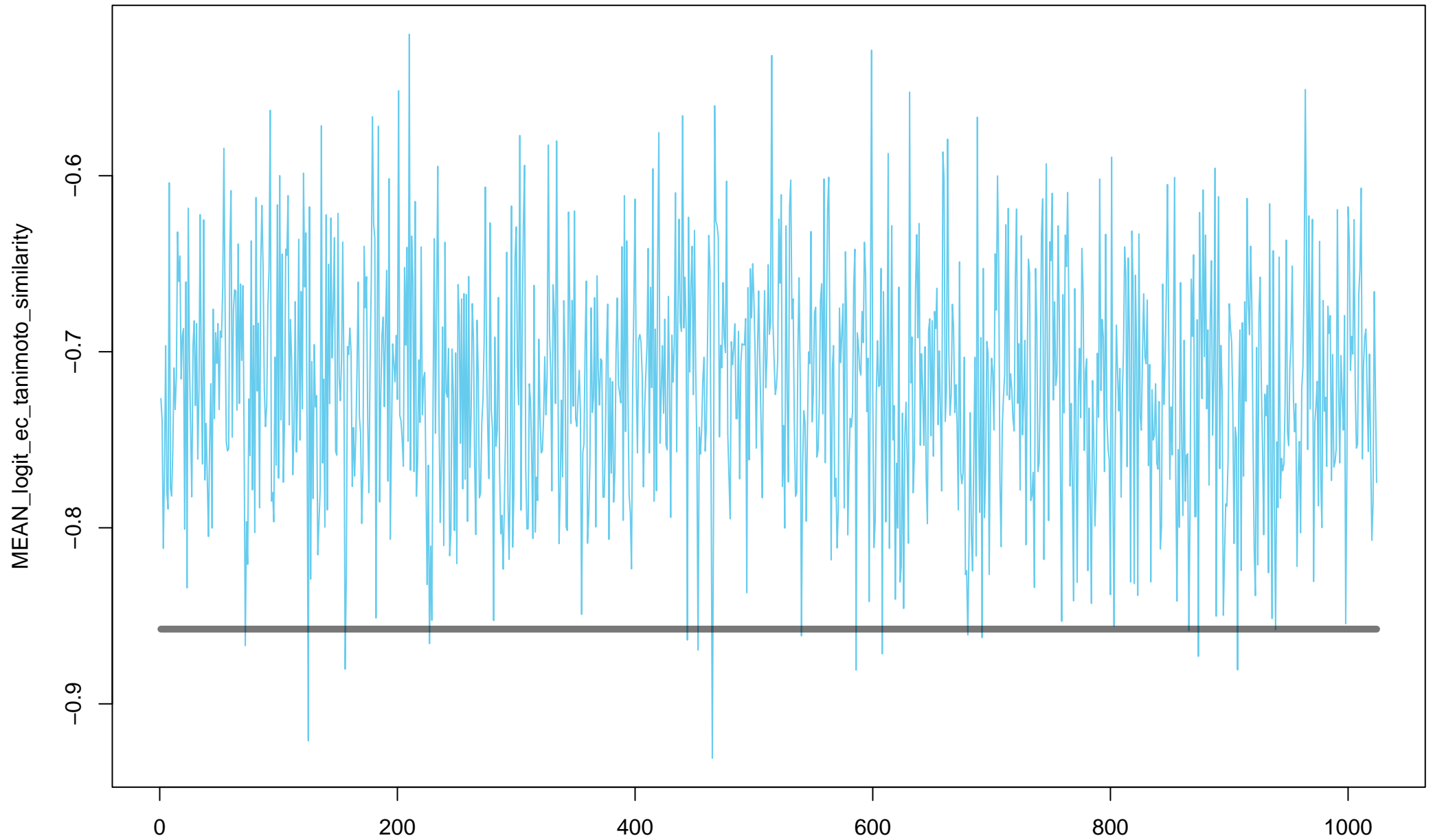
MEAN_log_RMSD
ESS = 1020 | BMK = 0.0386 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0 | rel.err: 1.58



MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0587 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0 | rel.err: 2.19

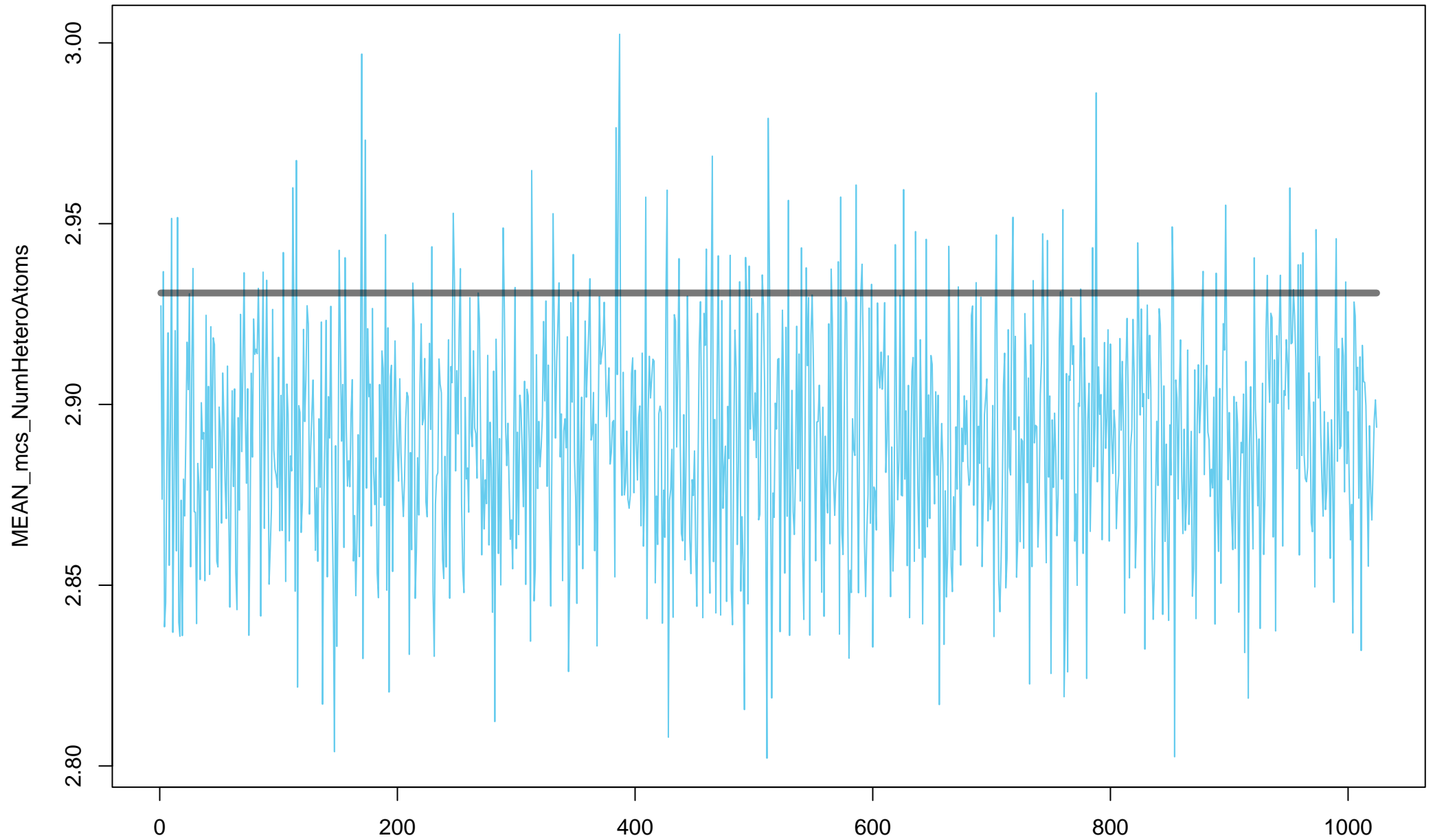


MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0678 | MCSE(6.27) = 3.76 | stat: TRUE | burn: 0 | rel.err: 2.14

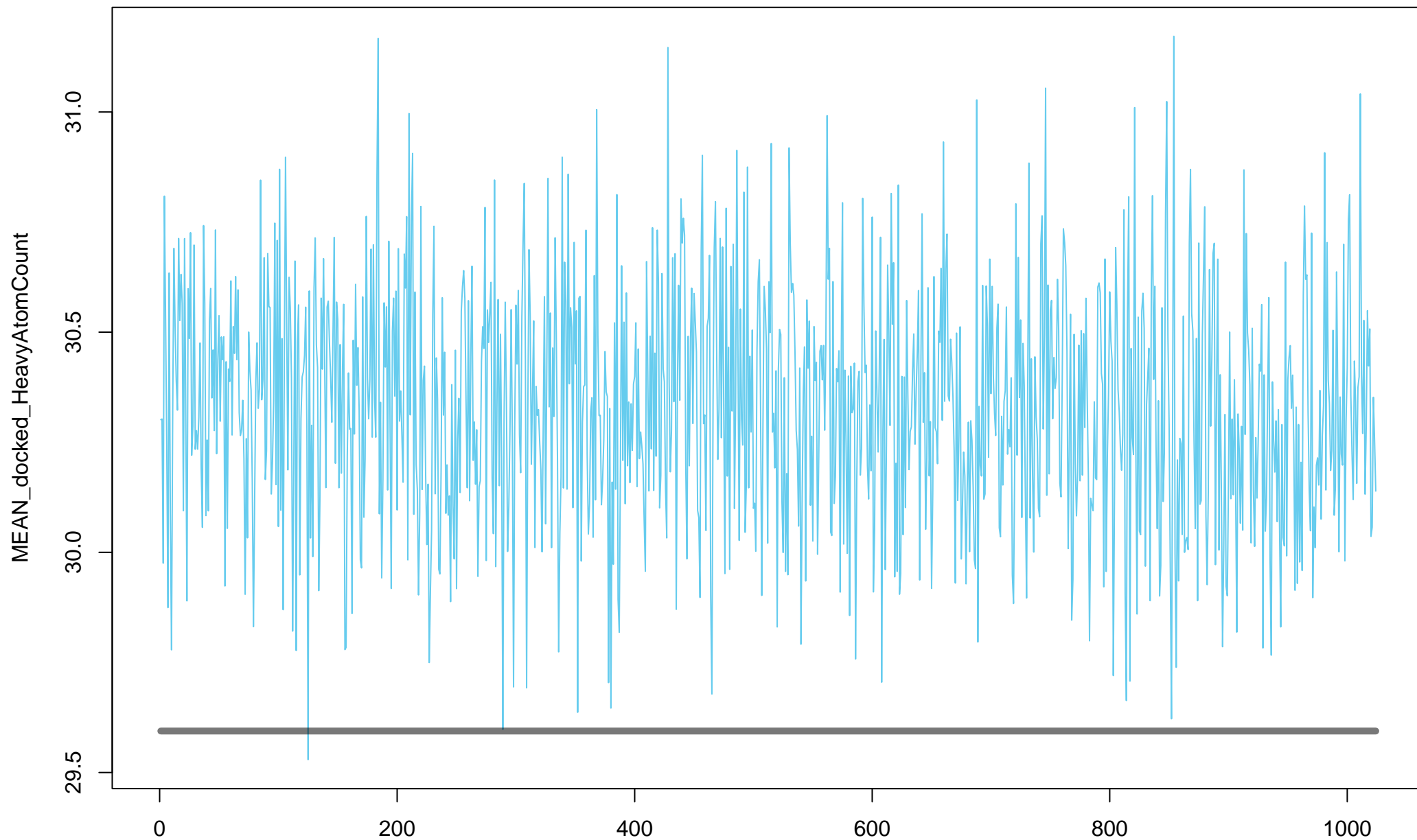


MEAN_mcs_NumHeteroAtoms

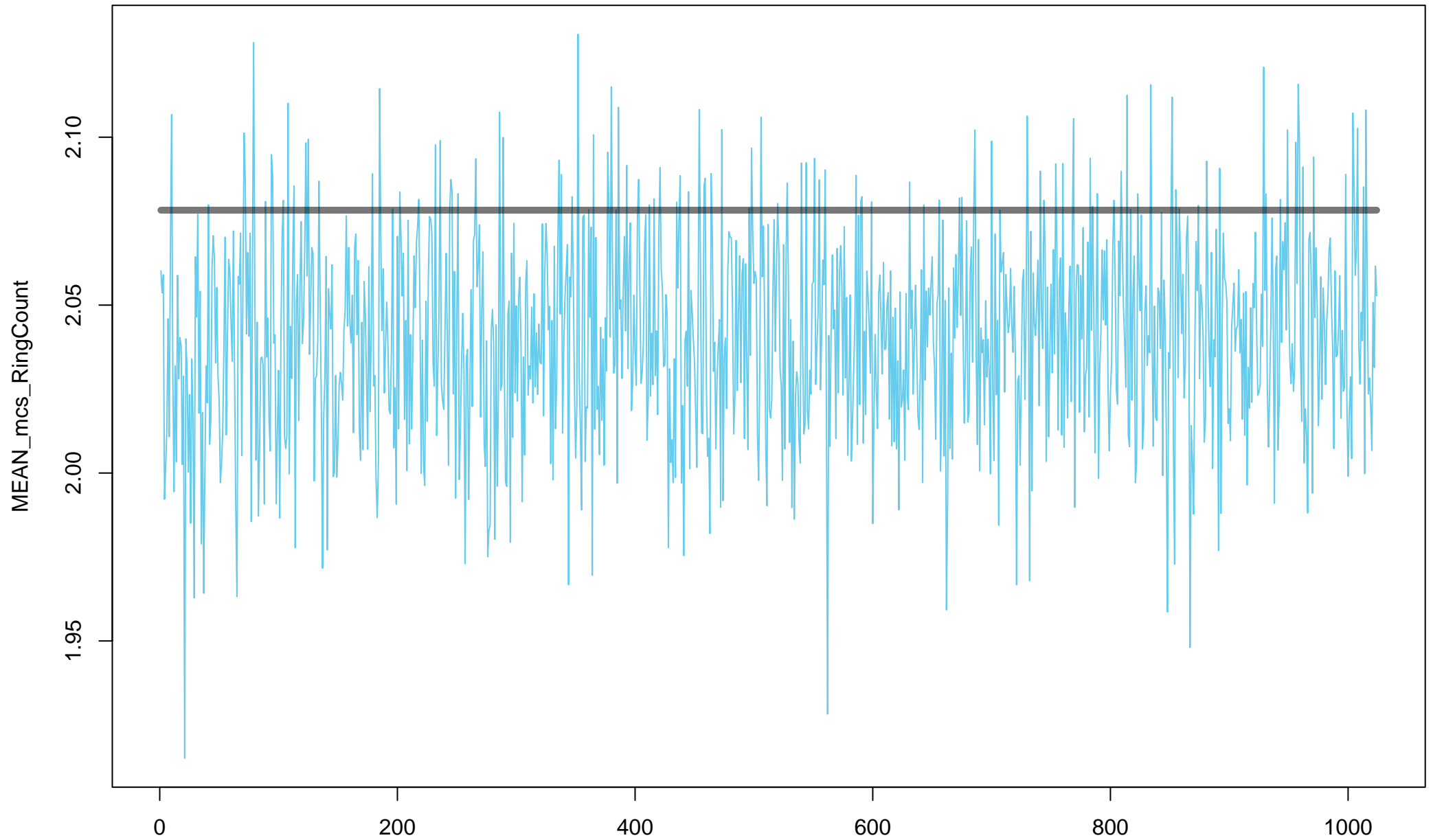
ESS = 1020 | BMK = 0.0515 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0 | rel.err: -1.31



MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0721 | MCSE(6.27) = 3.4 | stat: FALSE | burn: 0 | rel.err: 2.72

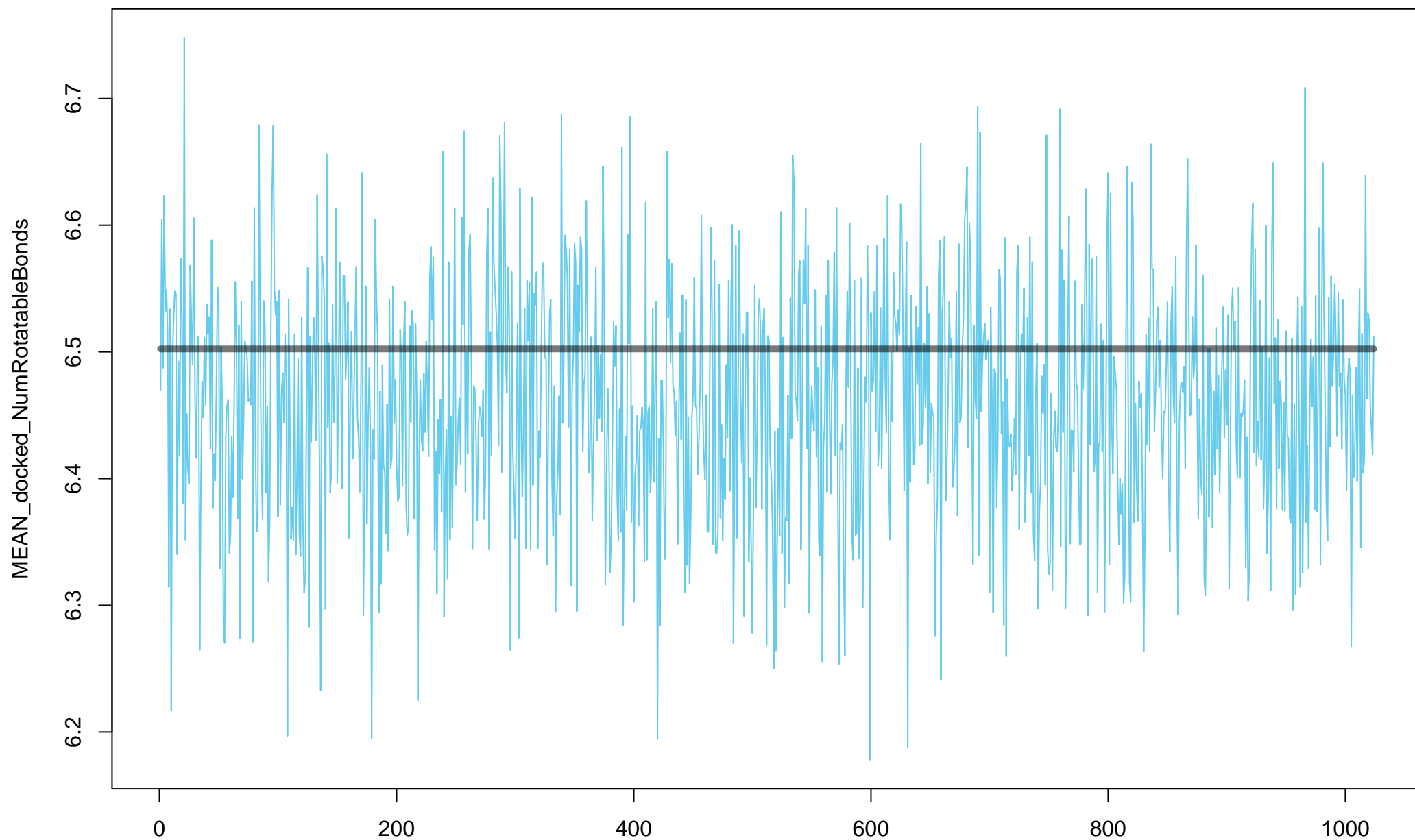


MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0807 | MCSE(6.27) = 3.36 | stat: FALSE | burn: 0 | rel.err: -1.25

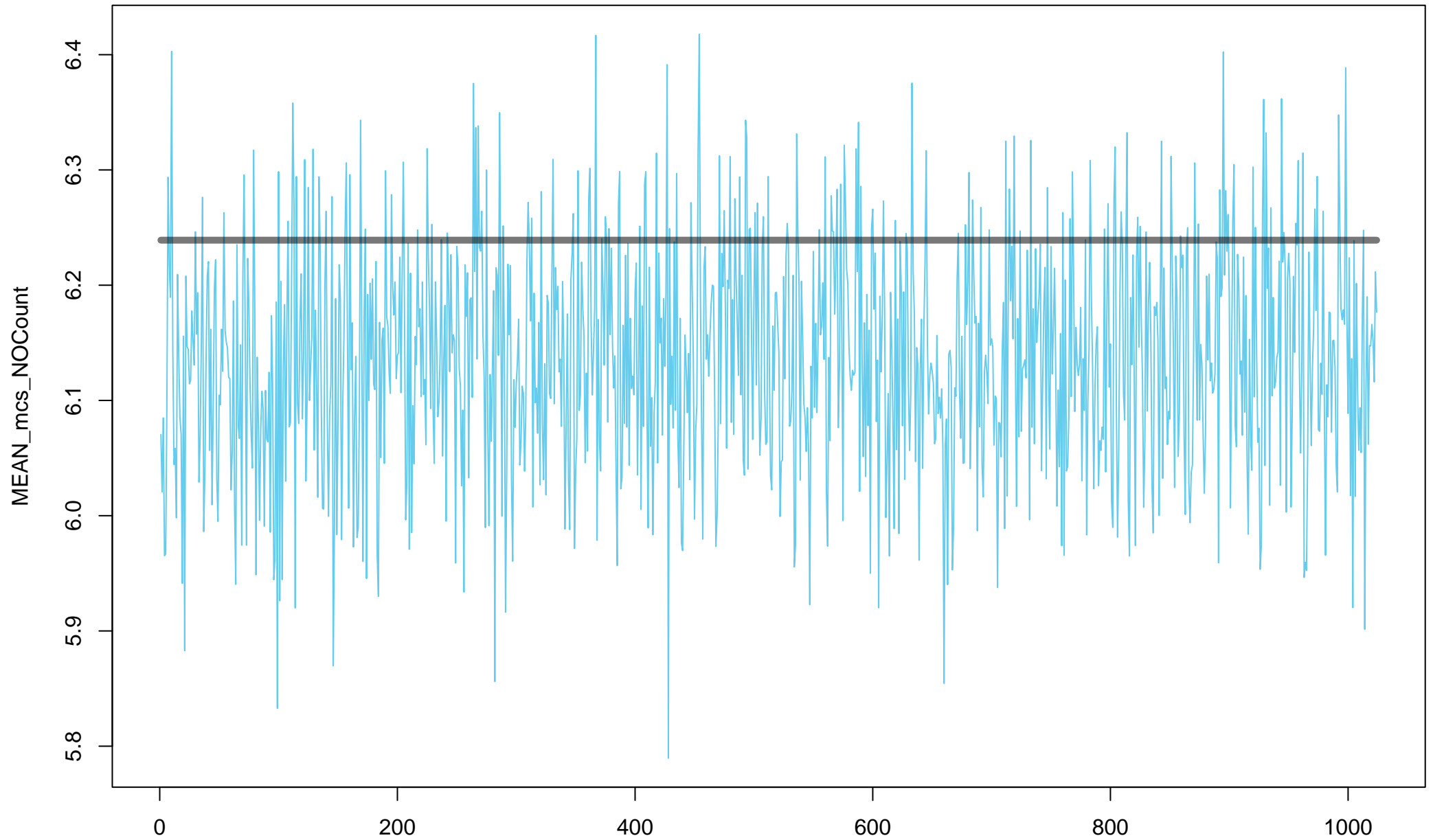


MEAN_docked_NumRotatableBonds

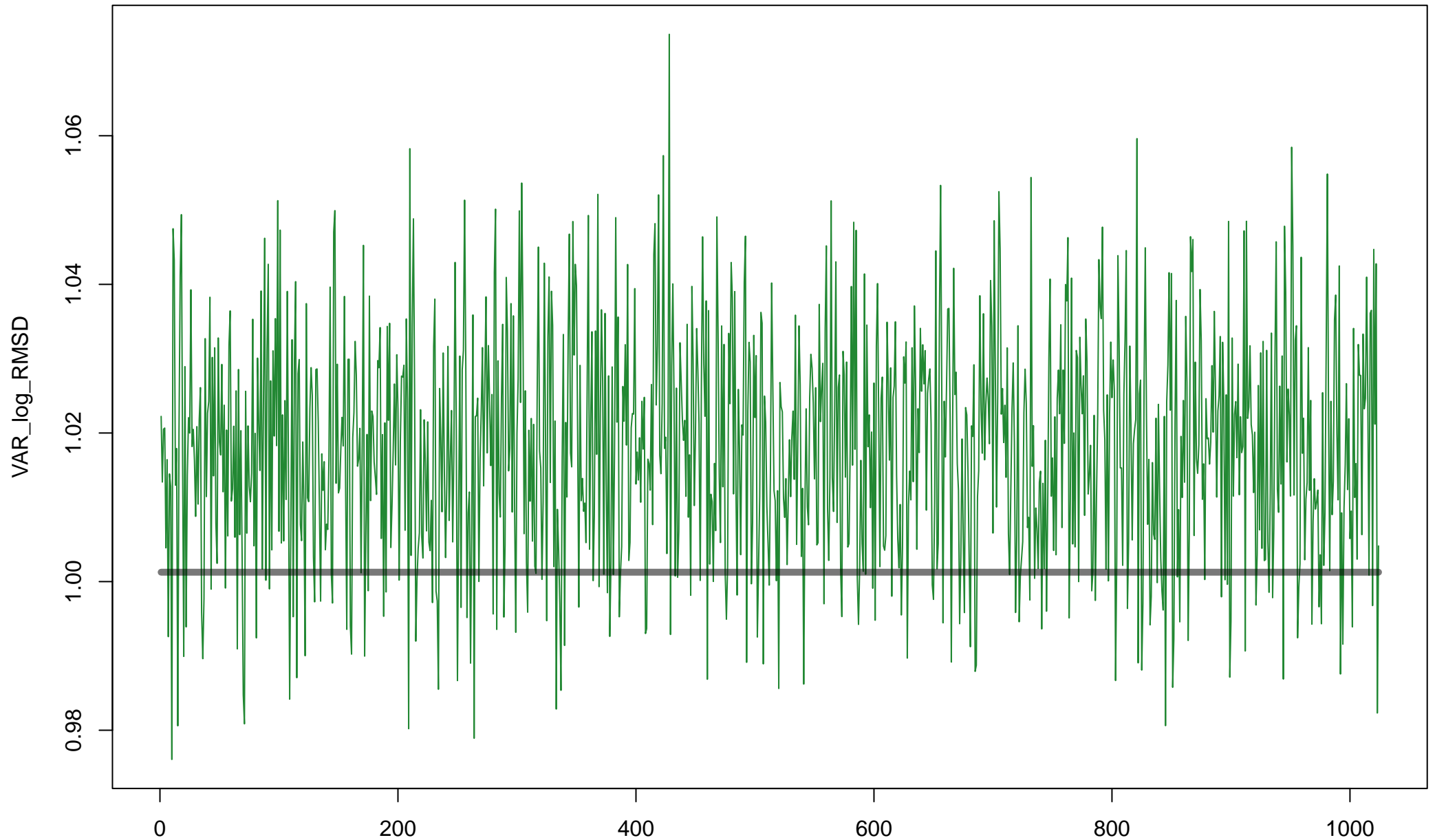
ESS = 1020 | BMK = 0.0338 | MCSE(6.27) = 3.51 | stat: TRUE | burn: 0 | rel.err: -0.467



MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0418 | MCSE(6.27) = 3.13 | stat: FALSE | burn: 0 | rel.err: -1.04

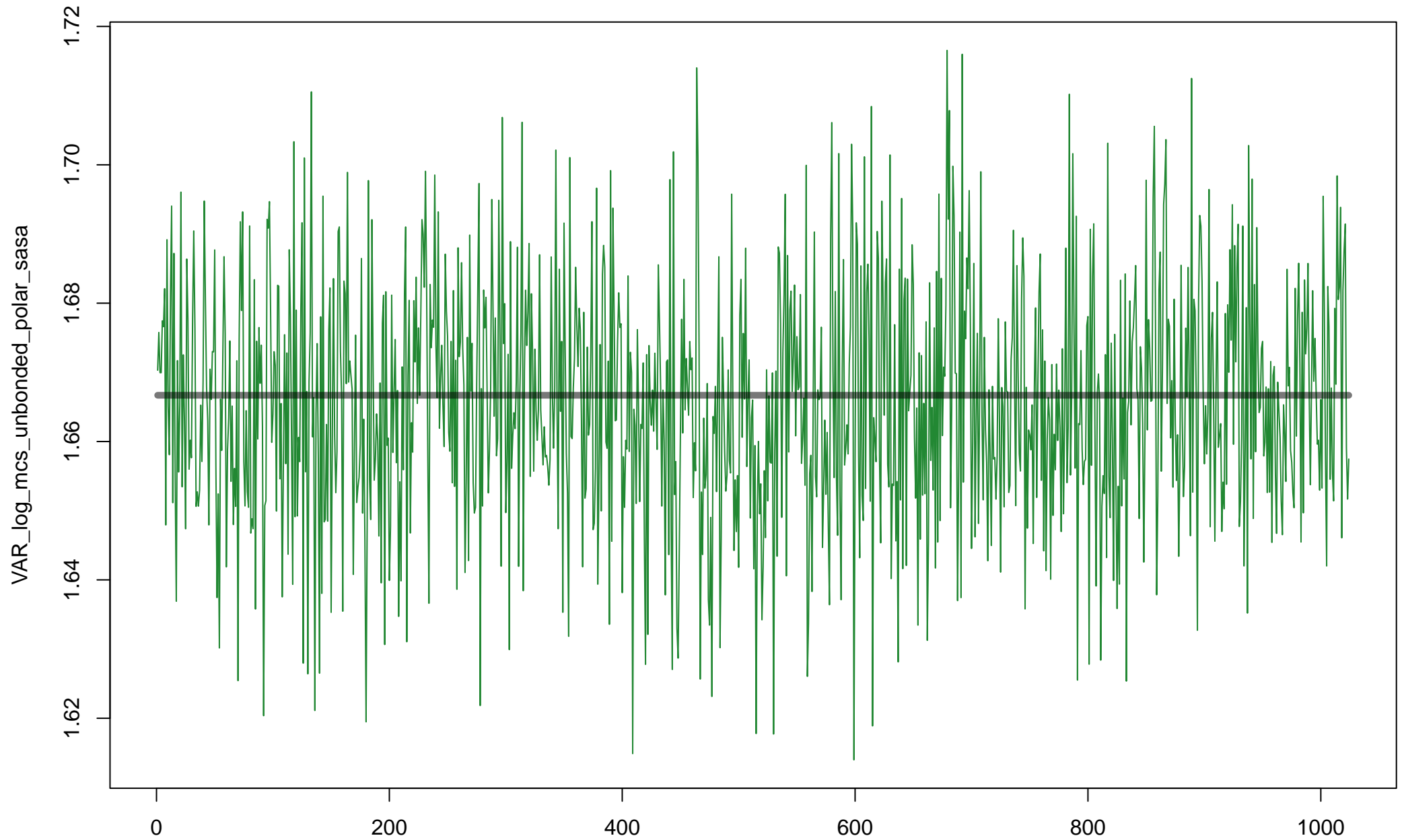


VAR_log_RMSD
ESS = 1020 | BMK = 0.0412 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0 | rel.err: 1.08

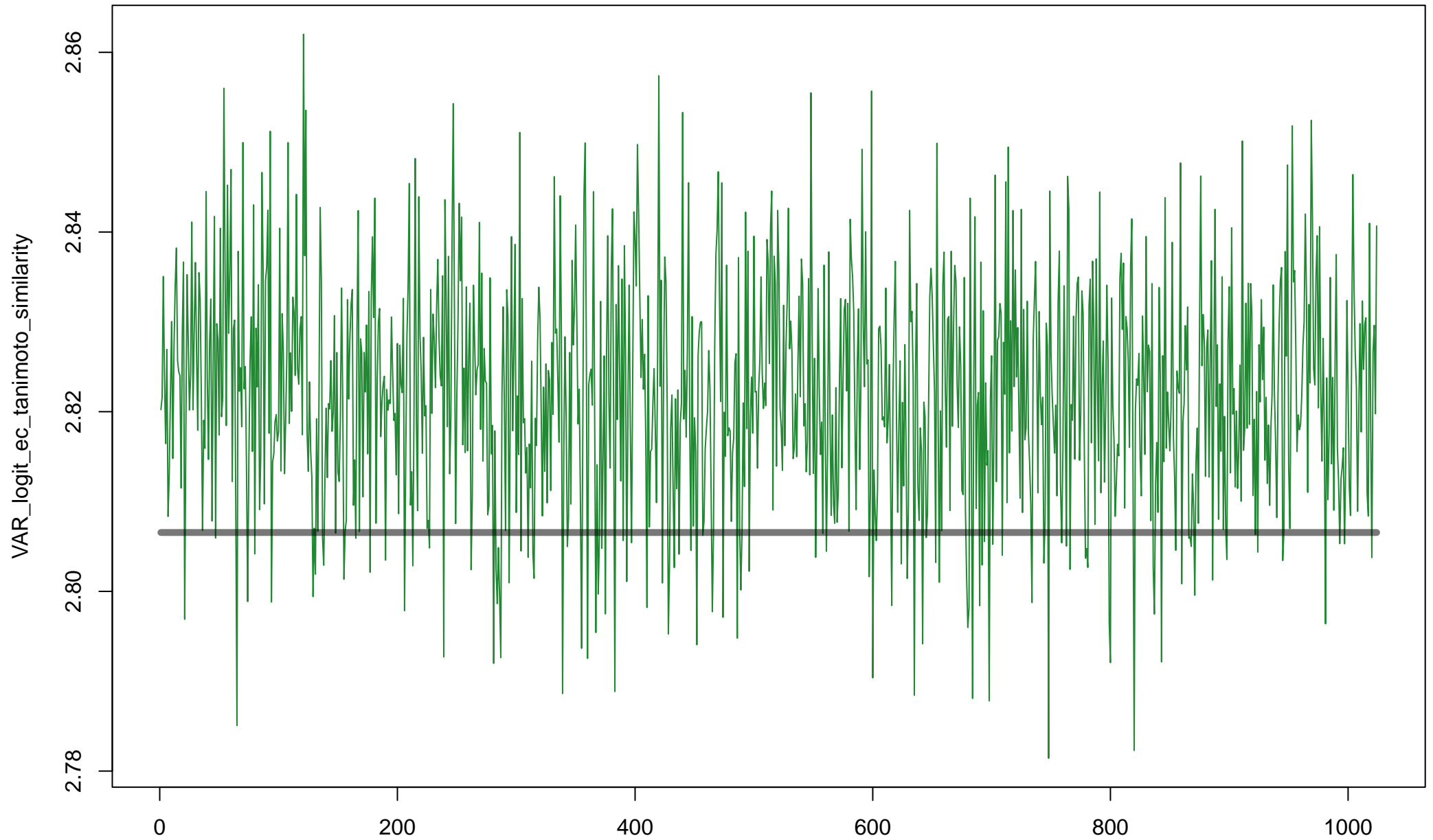


VAR_log_mcs_unbonded_polar_sasa

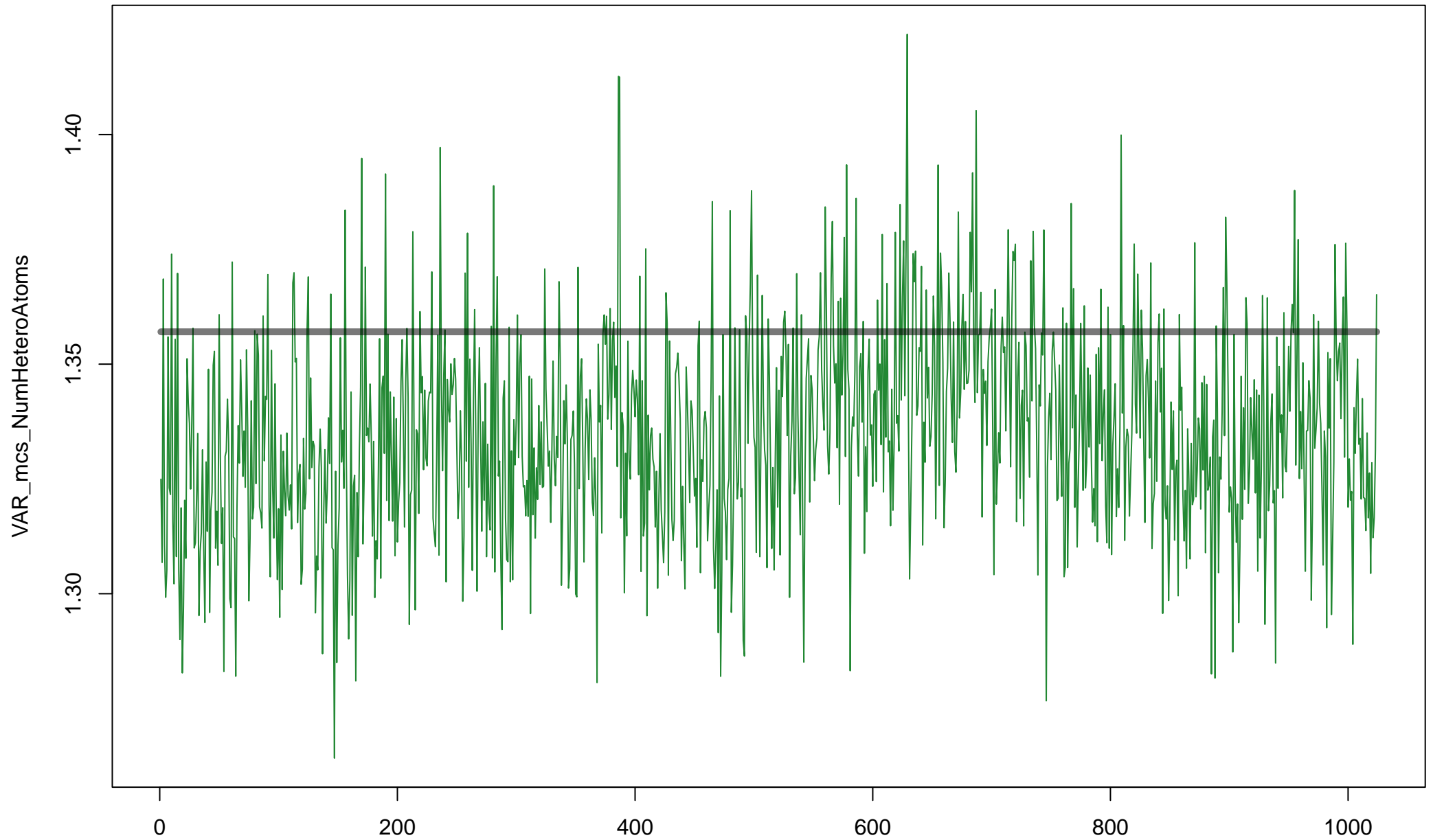
ESS = 1020 | BMK = 0.0592 | MCSE(6.27) = 3.76 | stat: TRUE | burn: 0 | rel.err: -0.0532



VAR_logit_ec_tanimoto_similarity
ESS = 924 | BMK = 0.0572 | MCSE(6.27) = 3.71 | stat: FALSE | burn: 0 | rel.err: 1.22

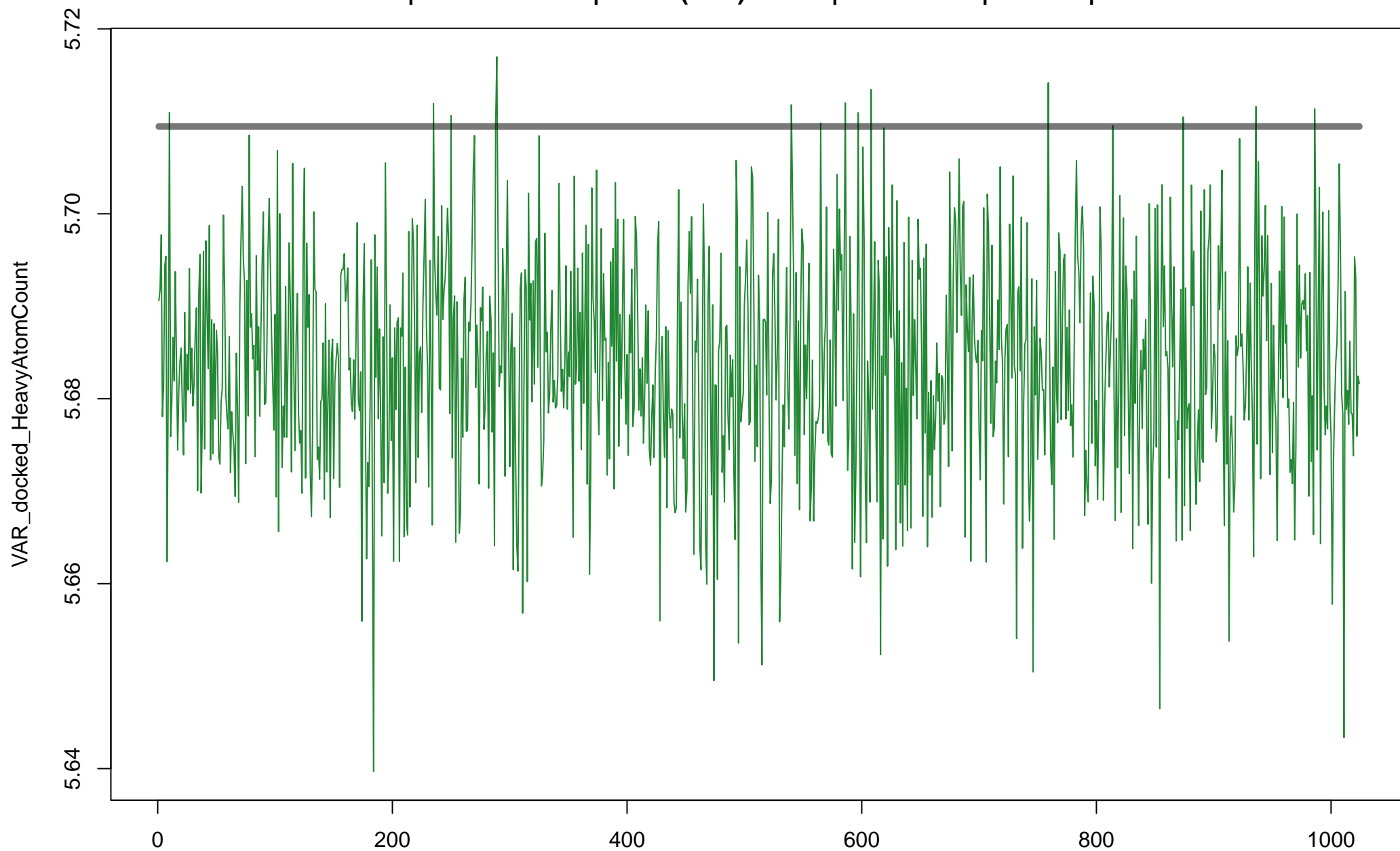


VAR_mcs_NumHeteroAtoms
ESS = 121 | BMK = 0.153 | MCSE(6.27) = 6.22 | stat: FALSE | burn: 0 | rel.err: -1.01

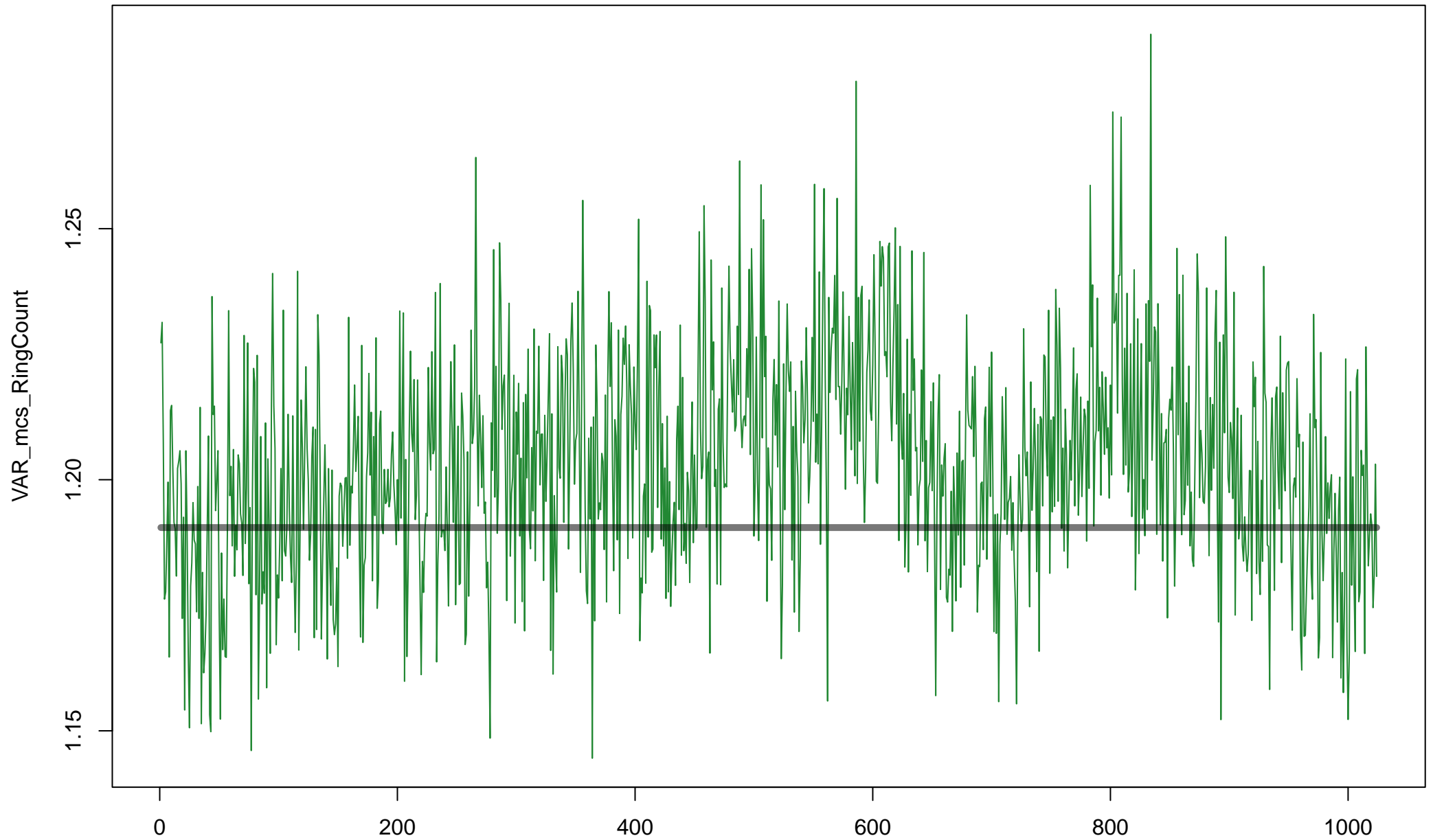


VAR_docked_HeavyAtomCount

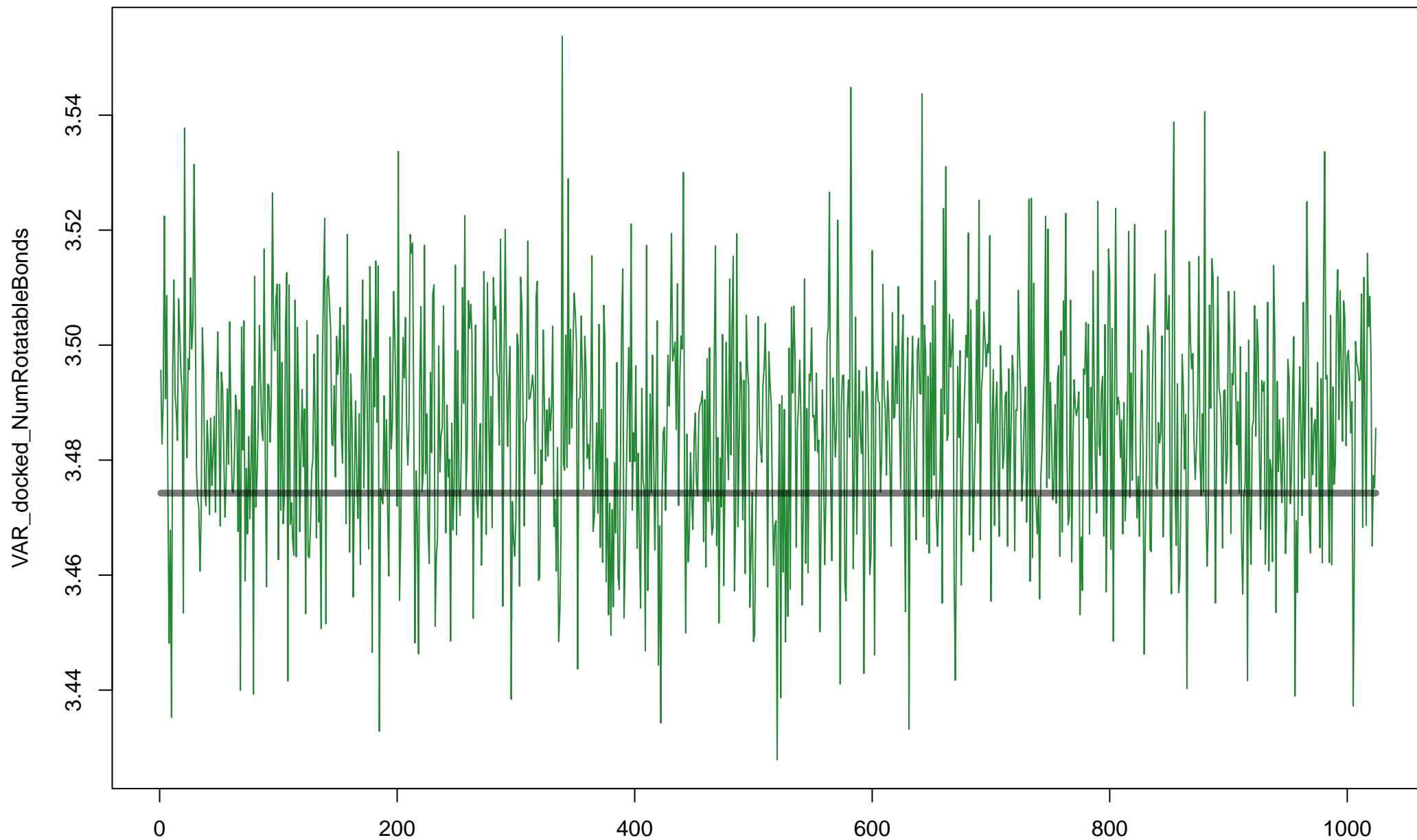
ESS = 1020 | BMK = 0.0518 | MCSE(6.27) = 3.32 | stat: TRUE | burn: 0 | rel.err: -2.23



VAR_mcs_RingCount
ESS = 78 | BMK = 0.0936 | MCSE(6.27) = 7.75 | stat: FALSE | burn: 0 | rel.err: 0.596

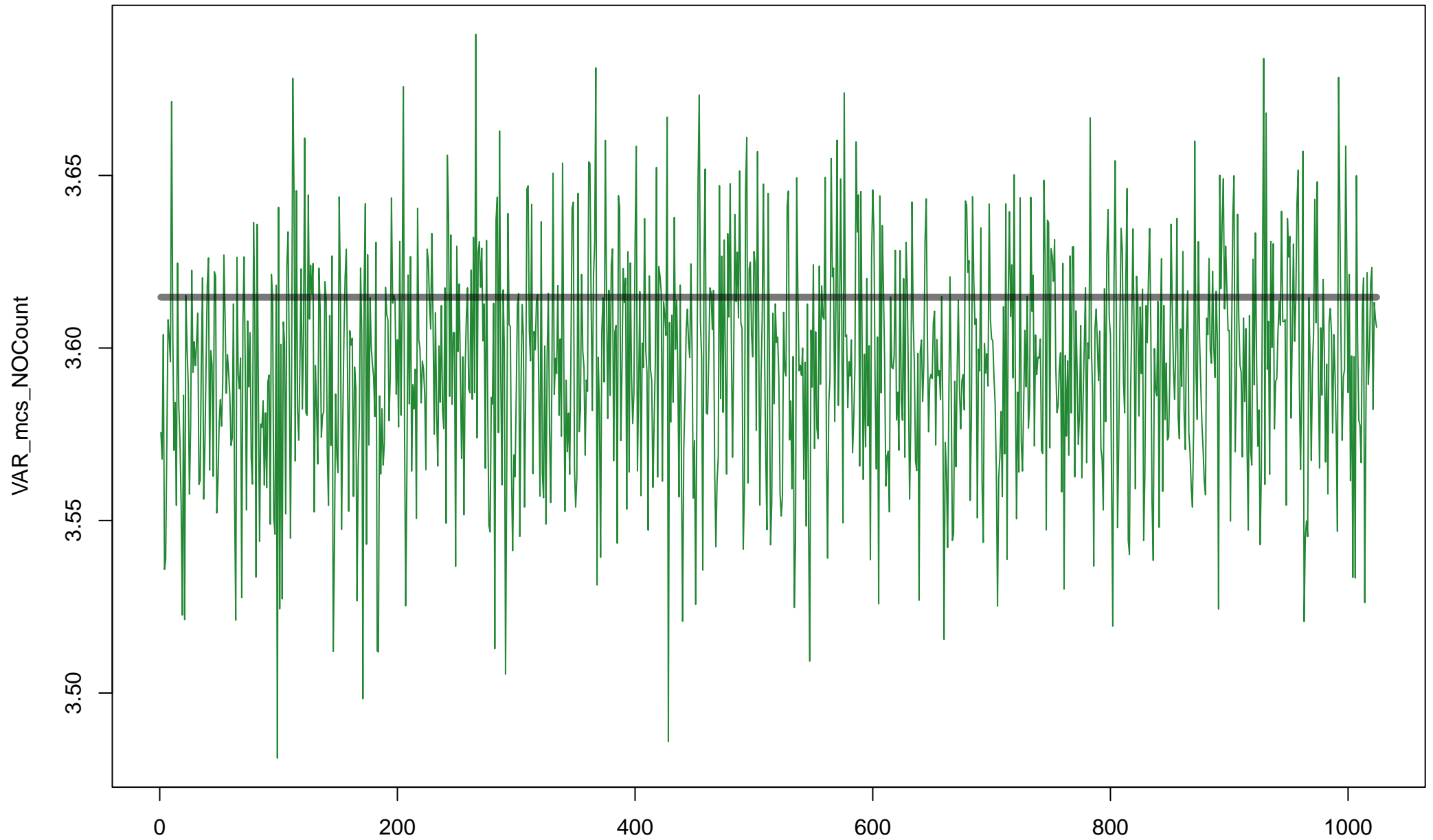


VAR_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0632 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0 | rel.err: 0.6

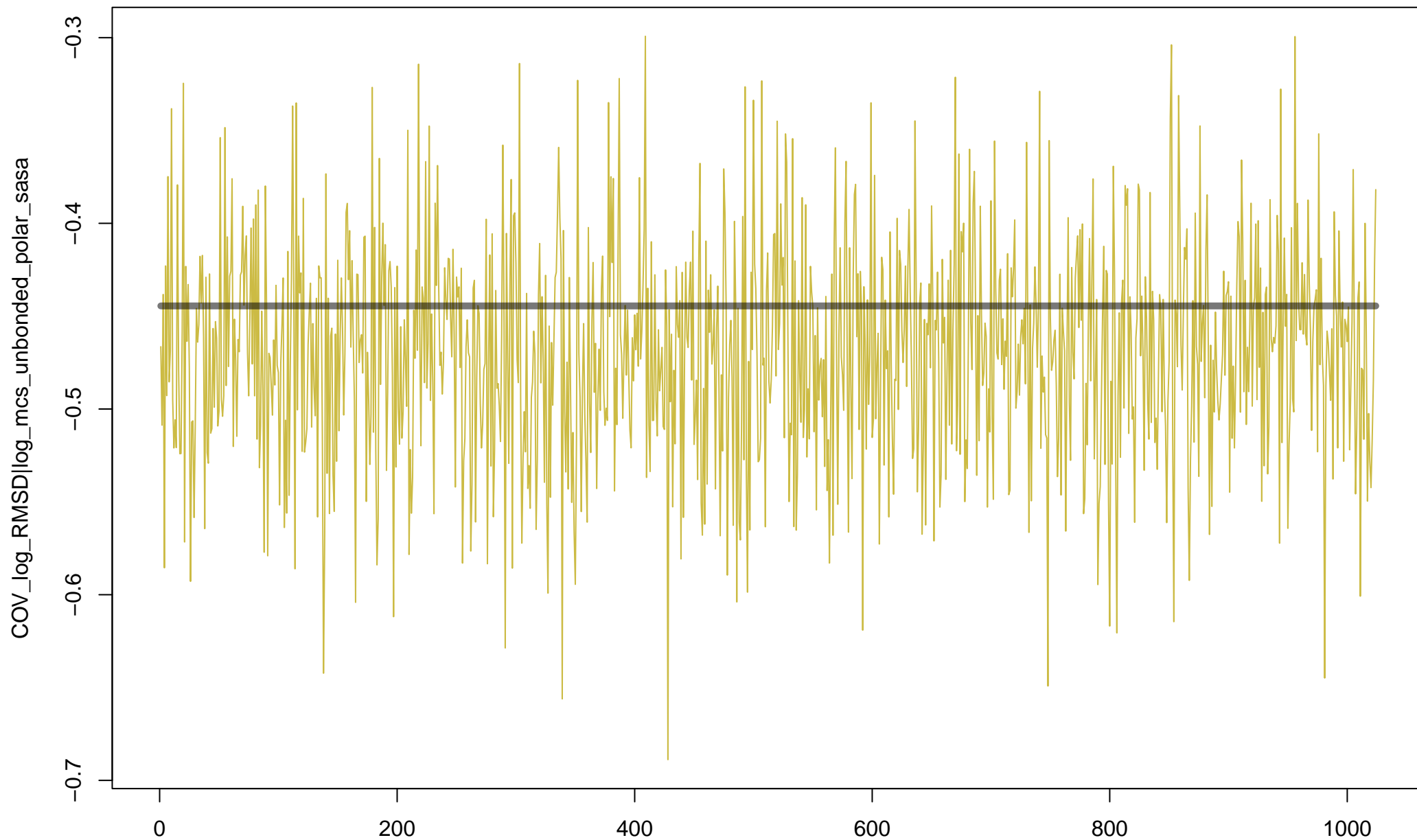


VAR_mcs_NOCount

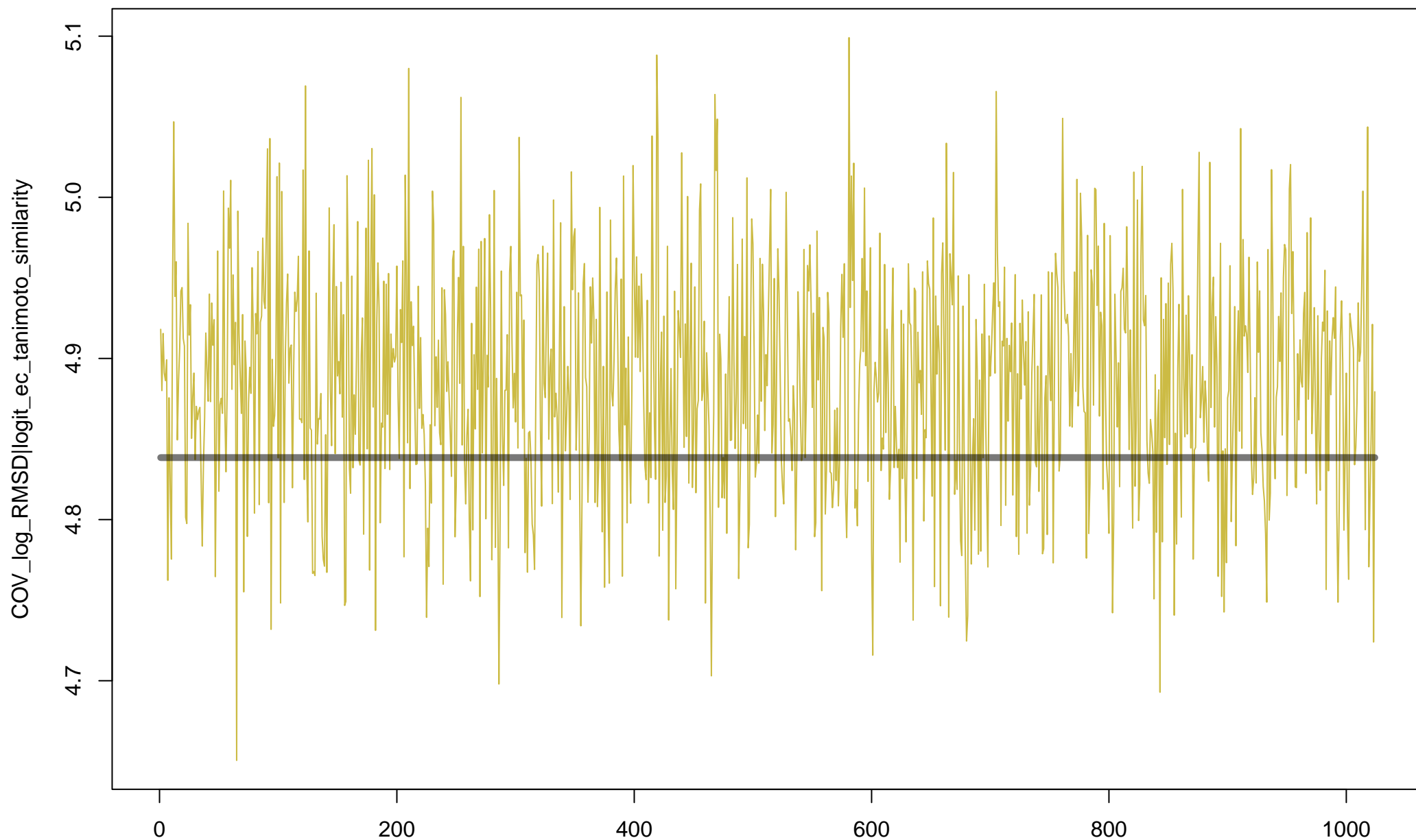
ESS = 1020 | BMK = 0.0581 | MCSE(6.27) = 3.46 | stat: FALSE | burn: 0 | rel.err: -0.615



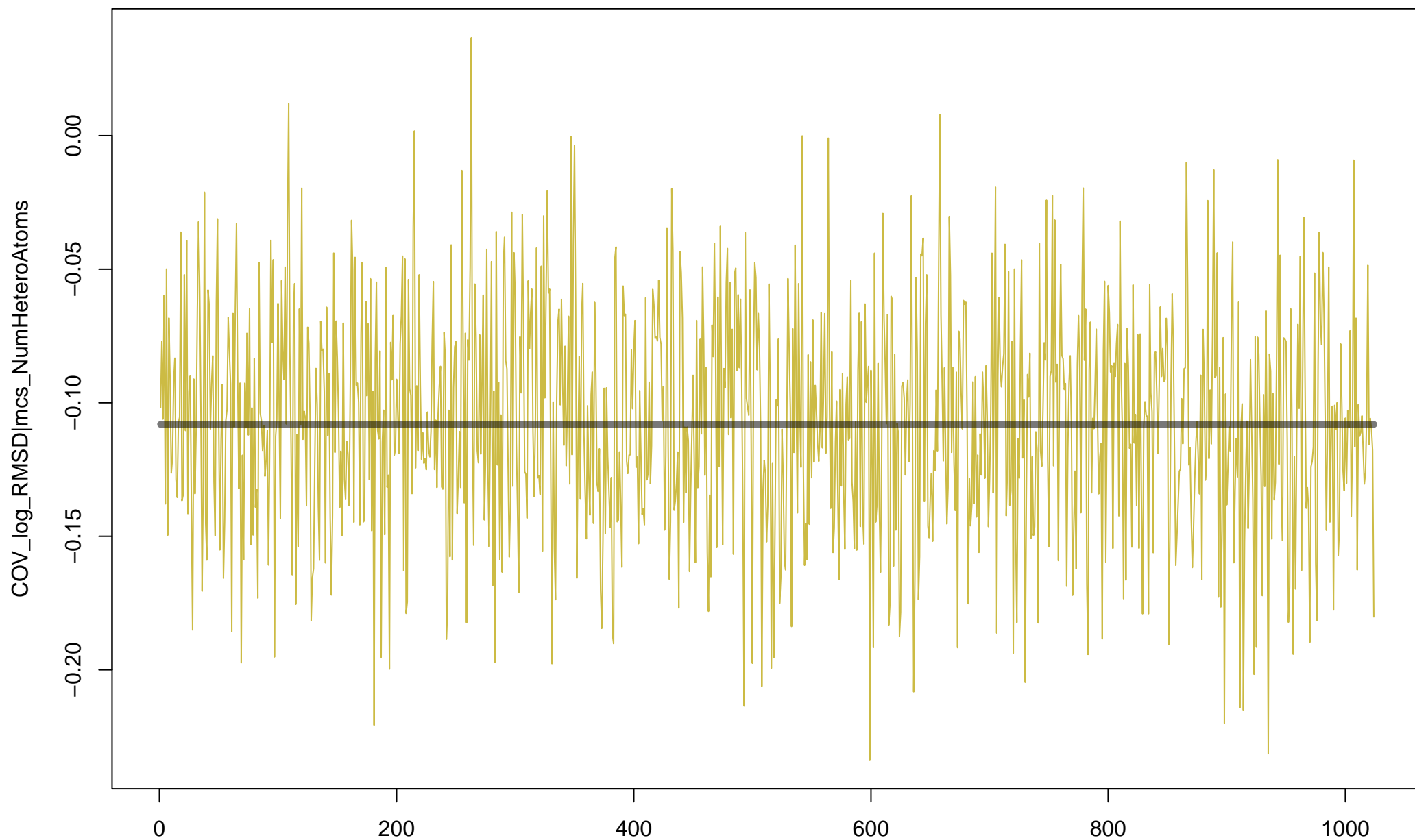
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 963 | BMK = 0.0635 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0 | rel.err: -0.432



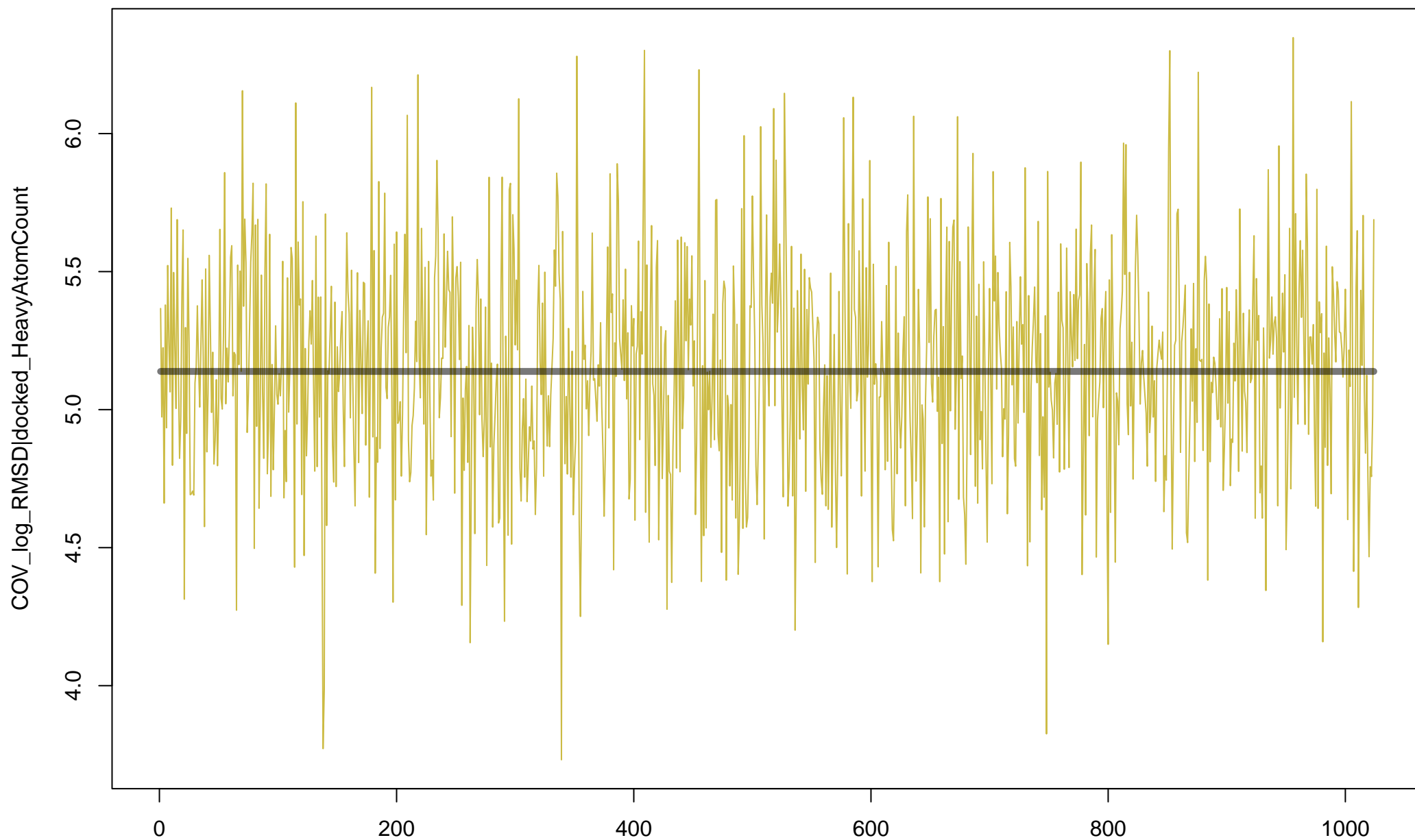
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0562 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0 | rel.err: 0.667



COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0779 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0 | rel.err: 0.0282

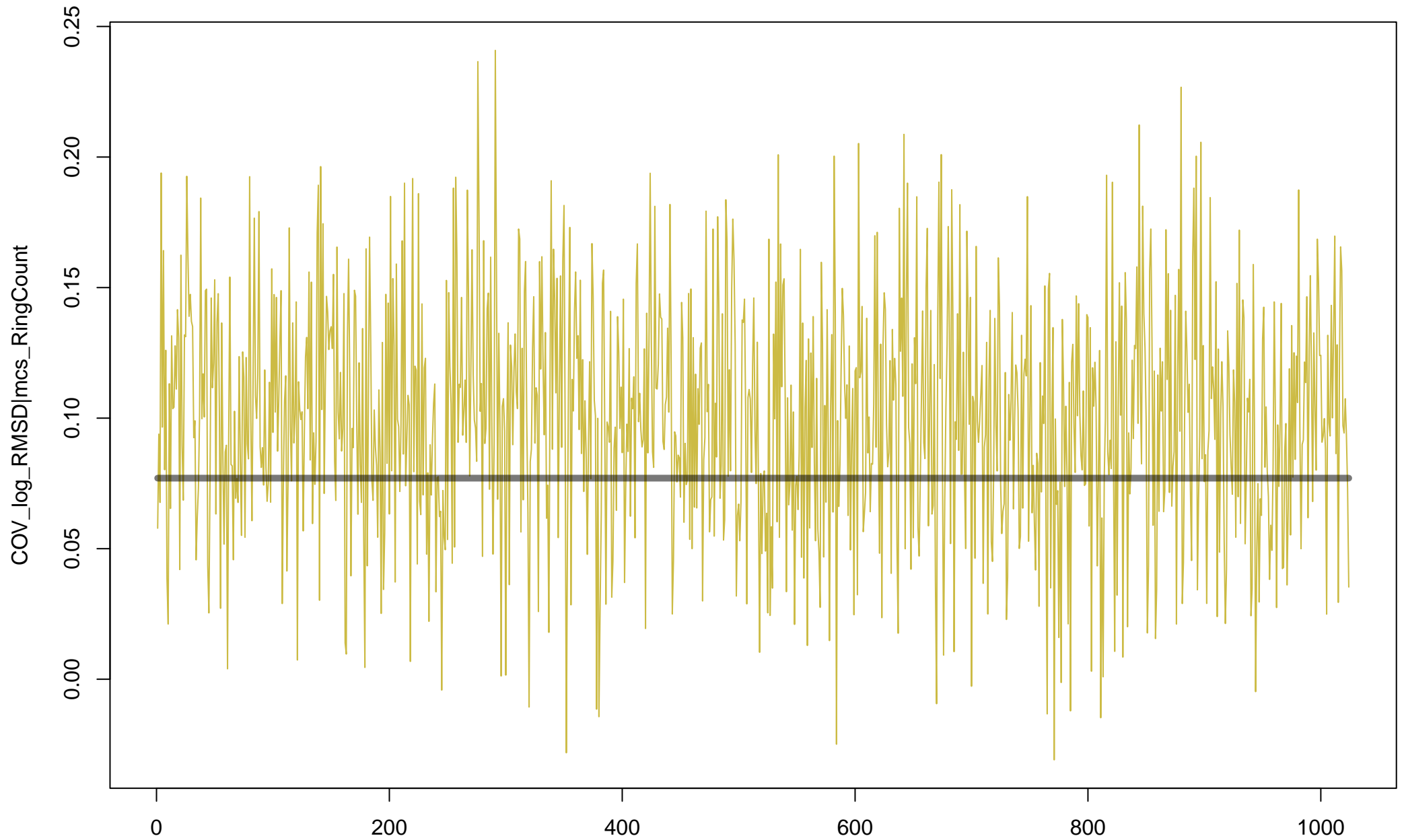


COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0468 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0 | rel.err: 0.0262

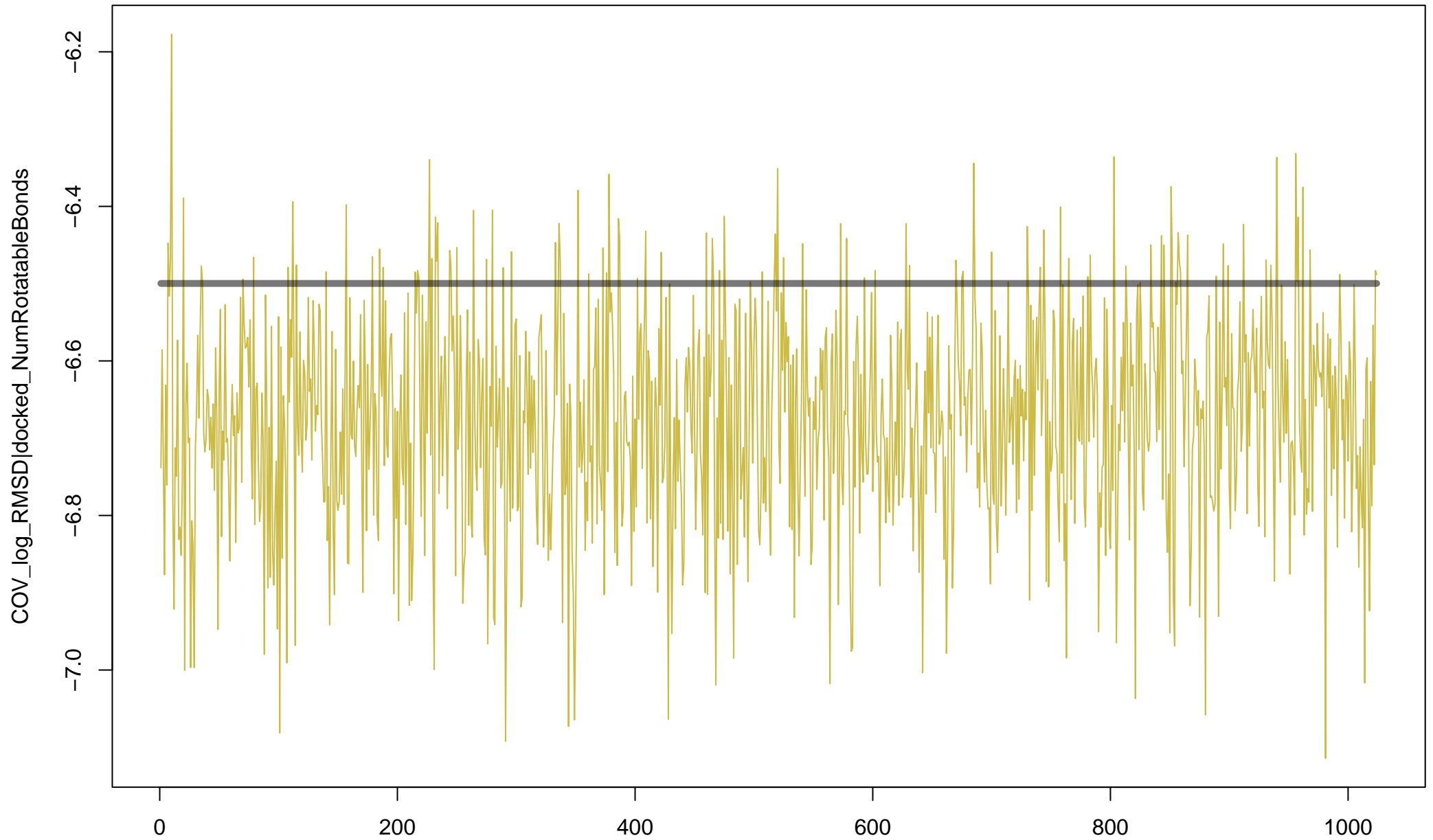


COV_log_RMSD|mcs_RingCount

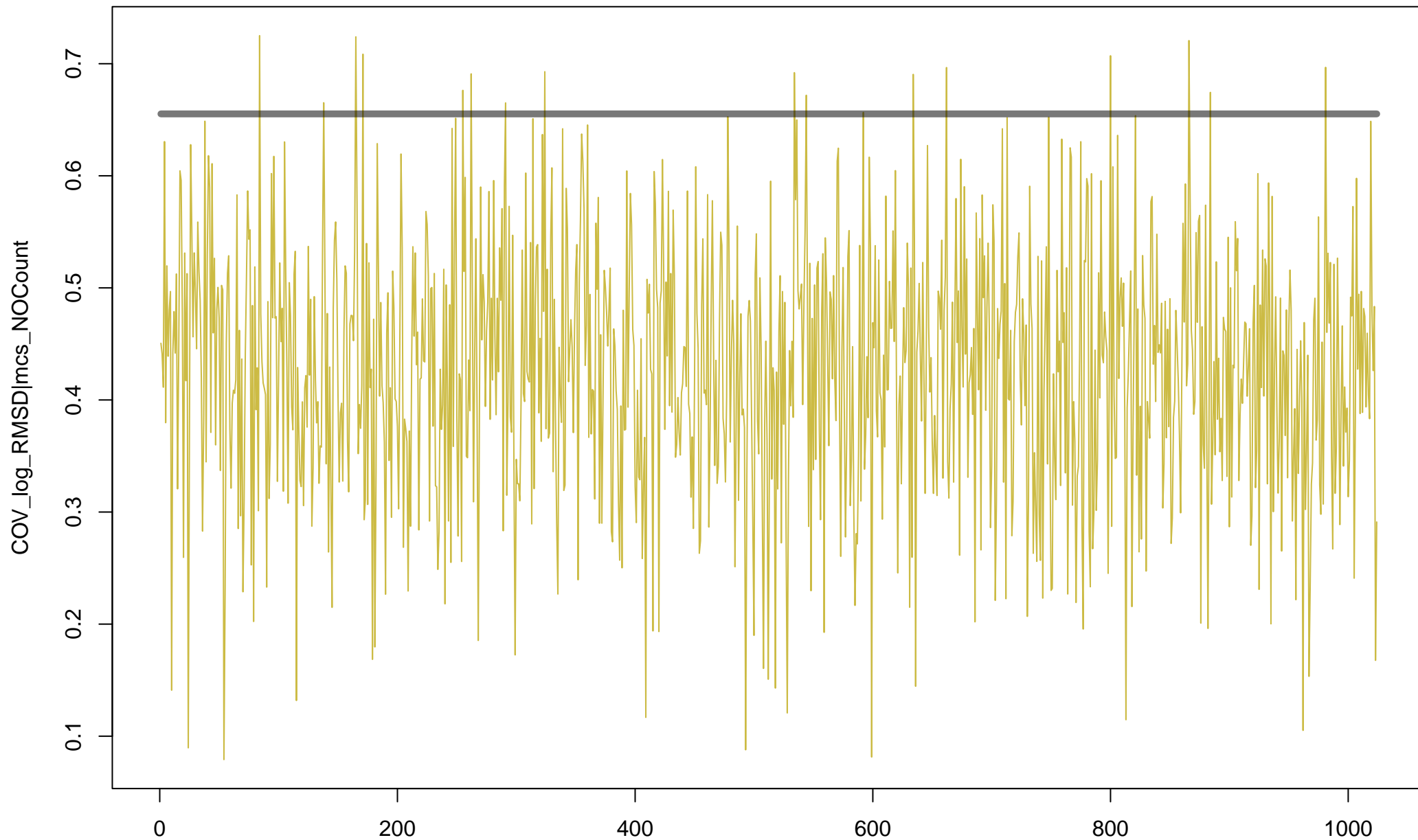
ESS = 1020 | BMK = 0.0757 | MCSE(6.27) = 3.65 | stat: TRUE | burn: 0 | rel.err: 0.517



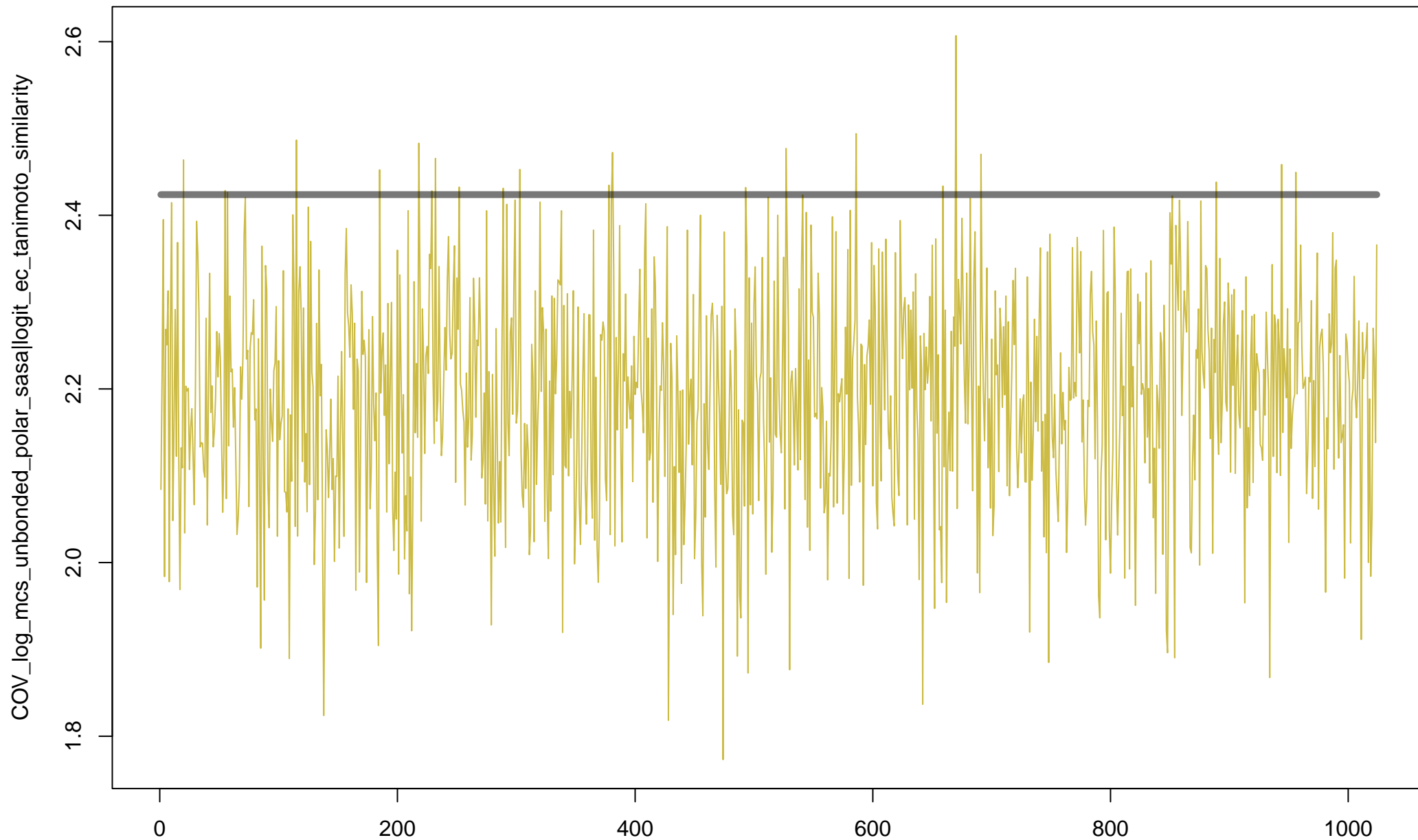
COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0749 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | rel.err: -1.3



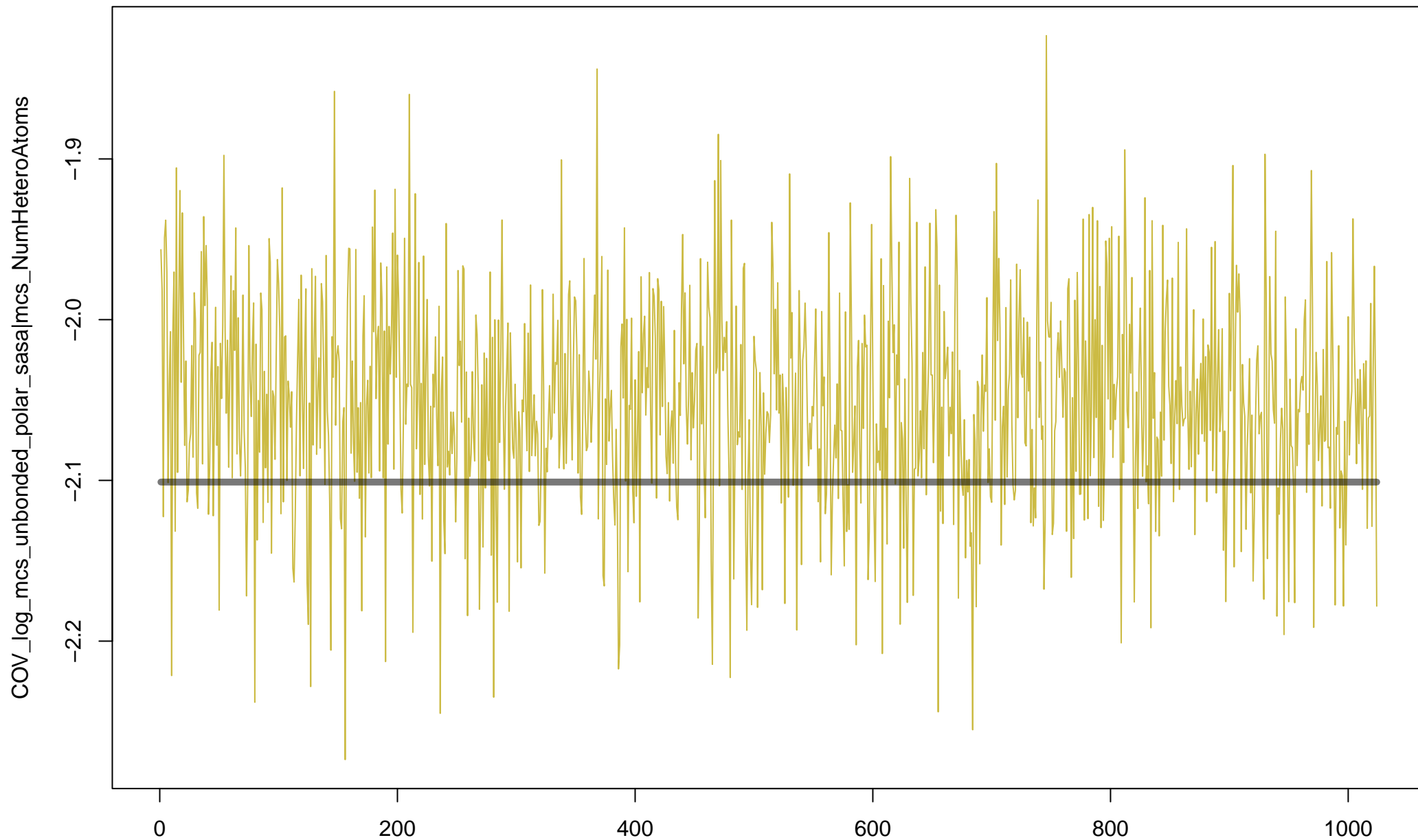
COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0434 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0 | rel.err: -2.04



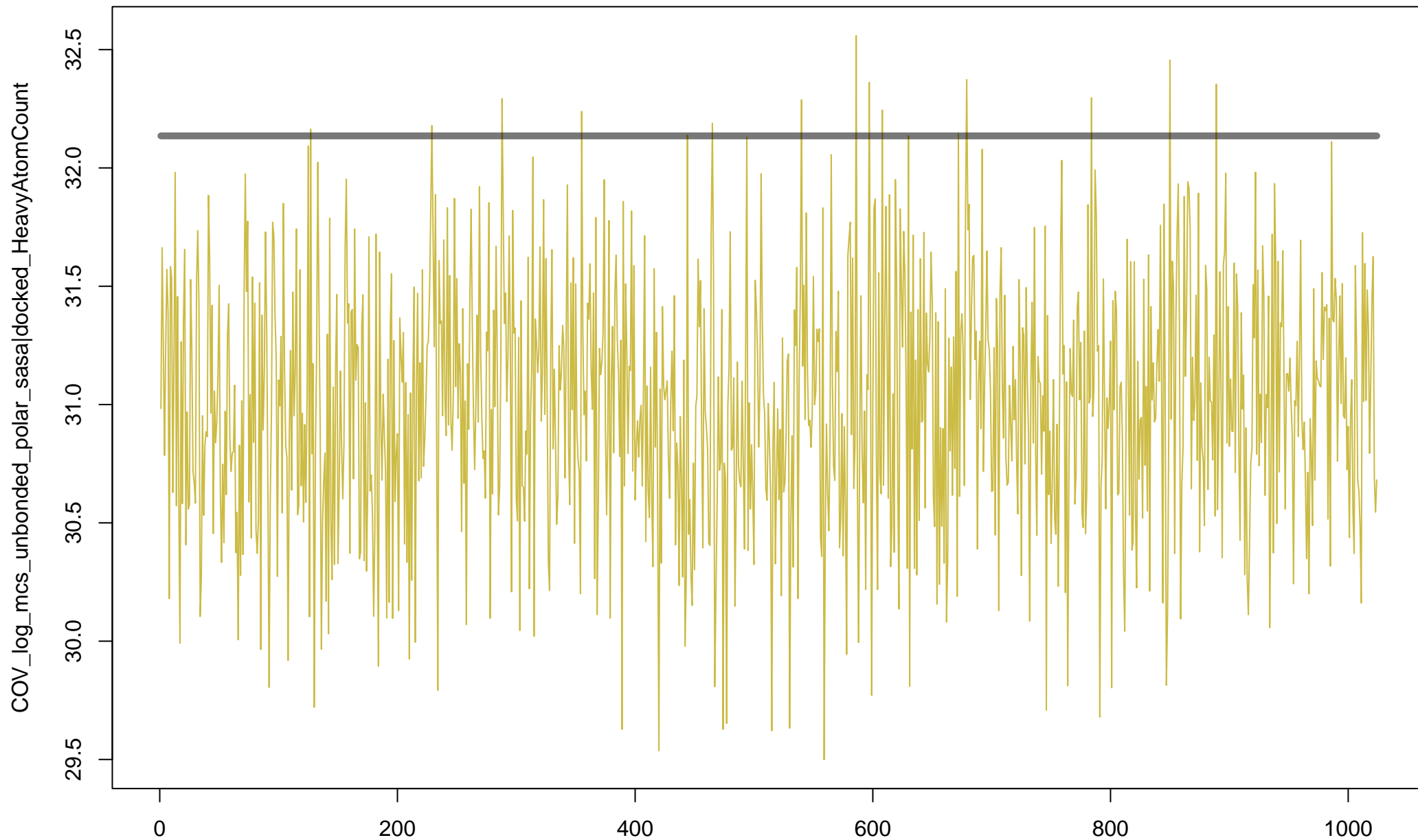
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0748 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0 | rel.err: -1.92



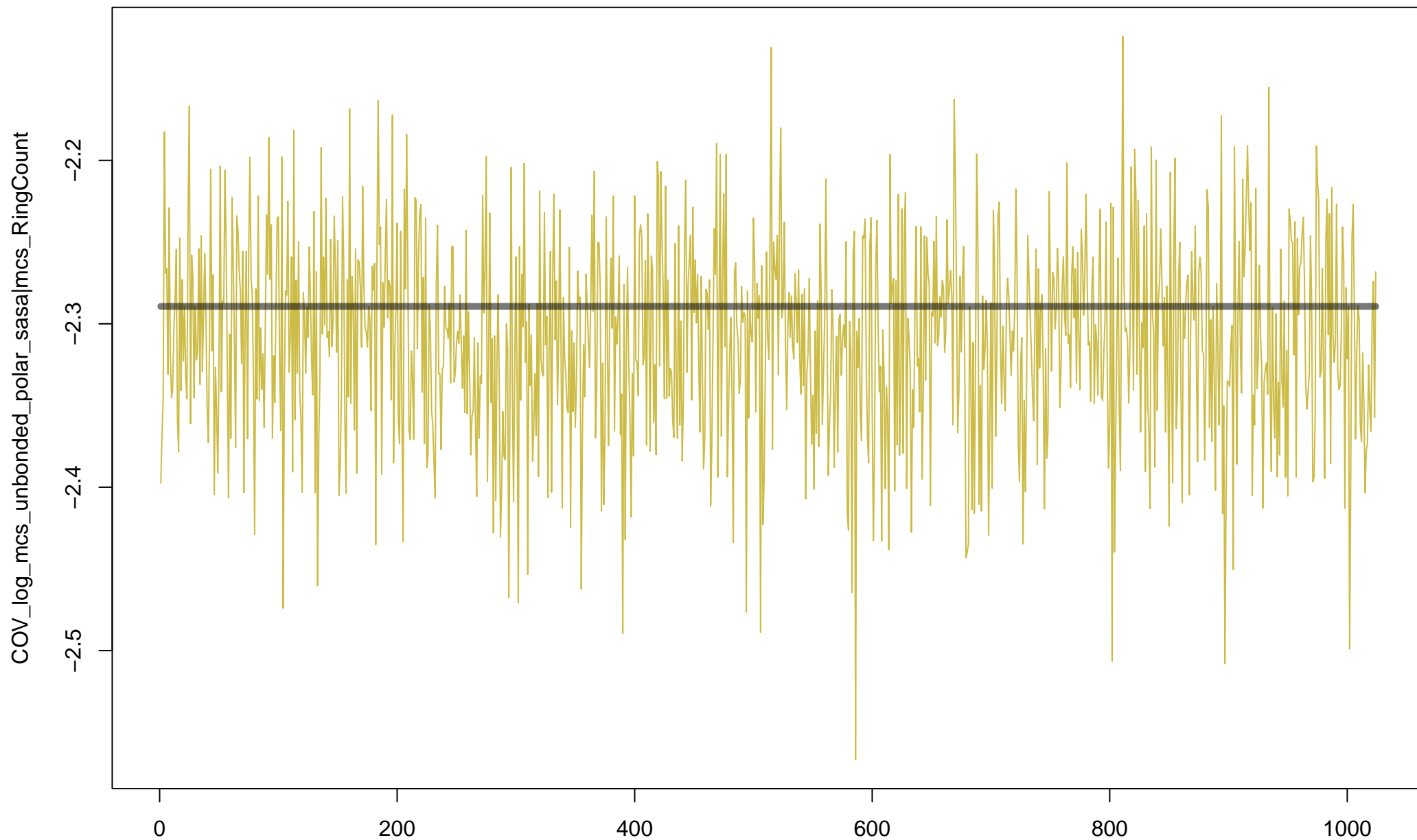
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0689 | MCSE(6.27) = 3.45 | stat: FALSE | burn: 0 | rel.err: 0.743



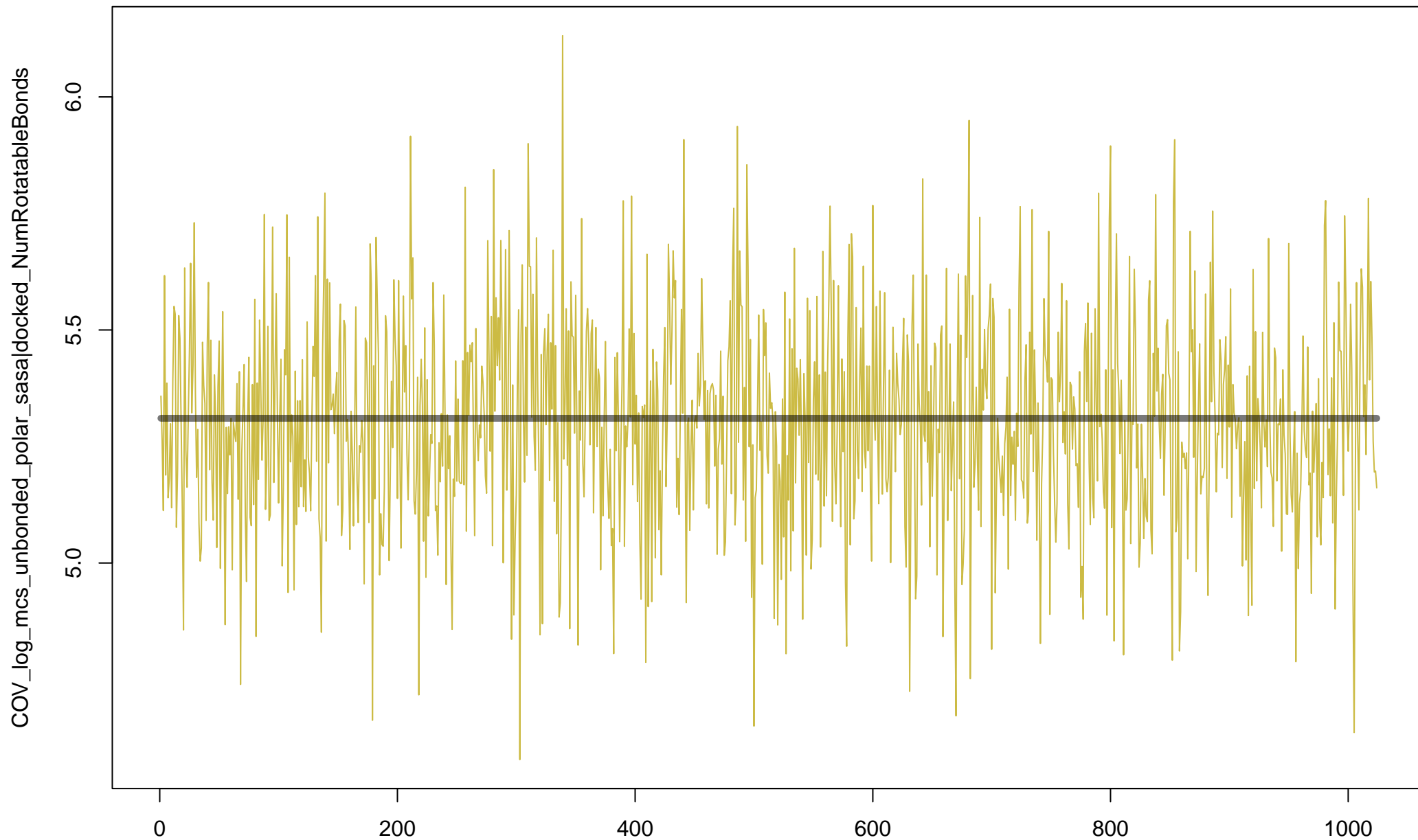
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0445 | MCSE(6.27) = 3.77 | stat: TRUE | burn: 0 | rel.err: -2.18



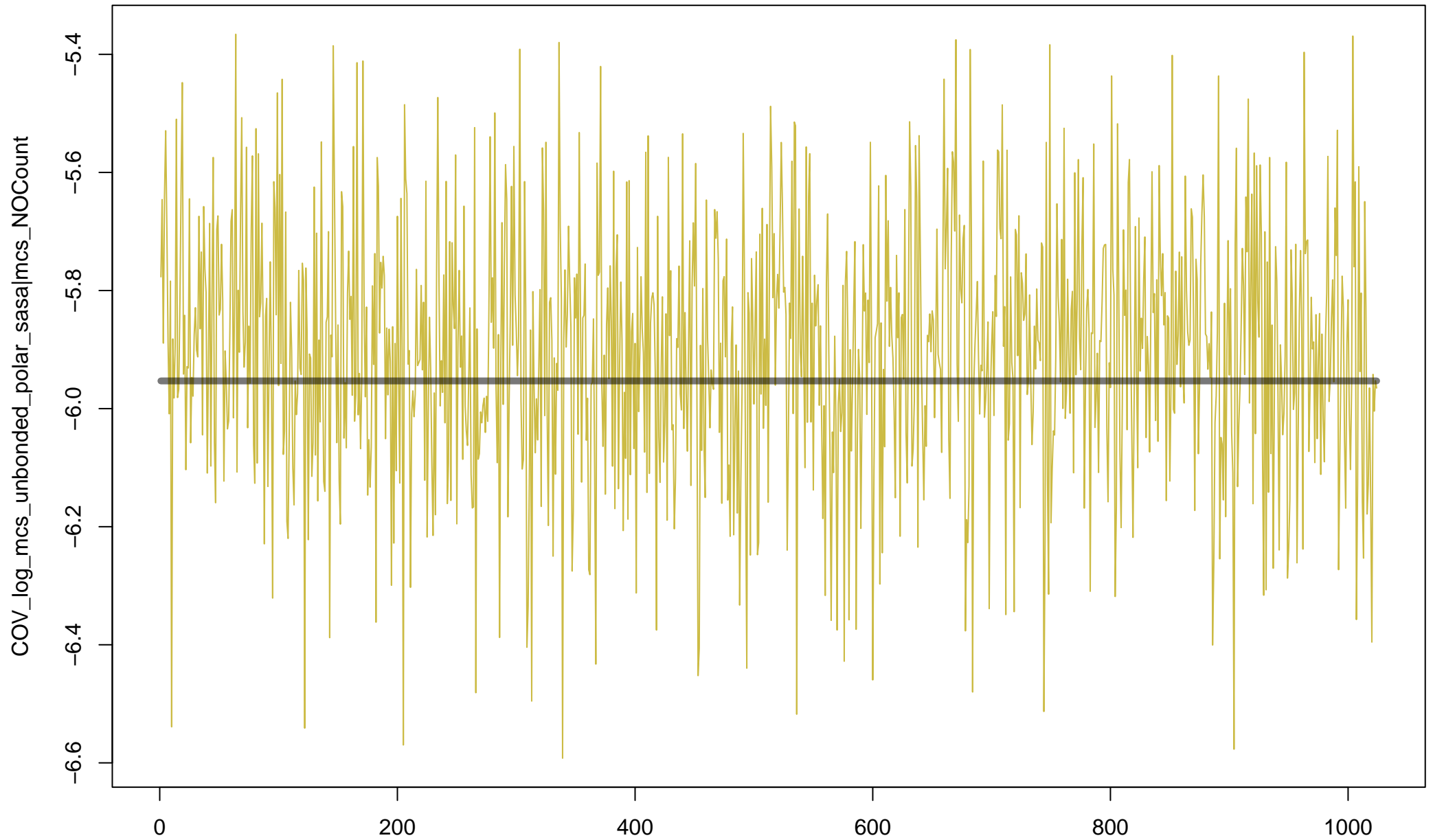
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0576 | MCSE(6.27) = 3.86 | stat: TRUE | burn: 0 | rel.err: -0.335



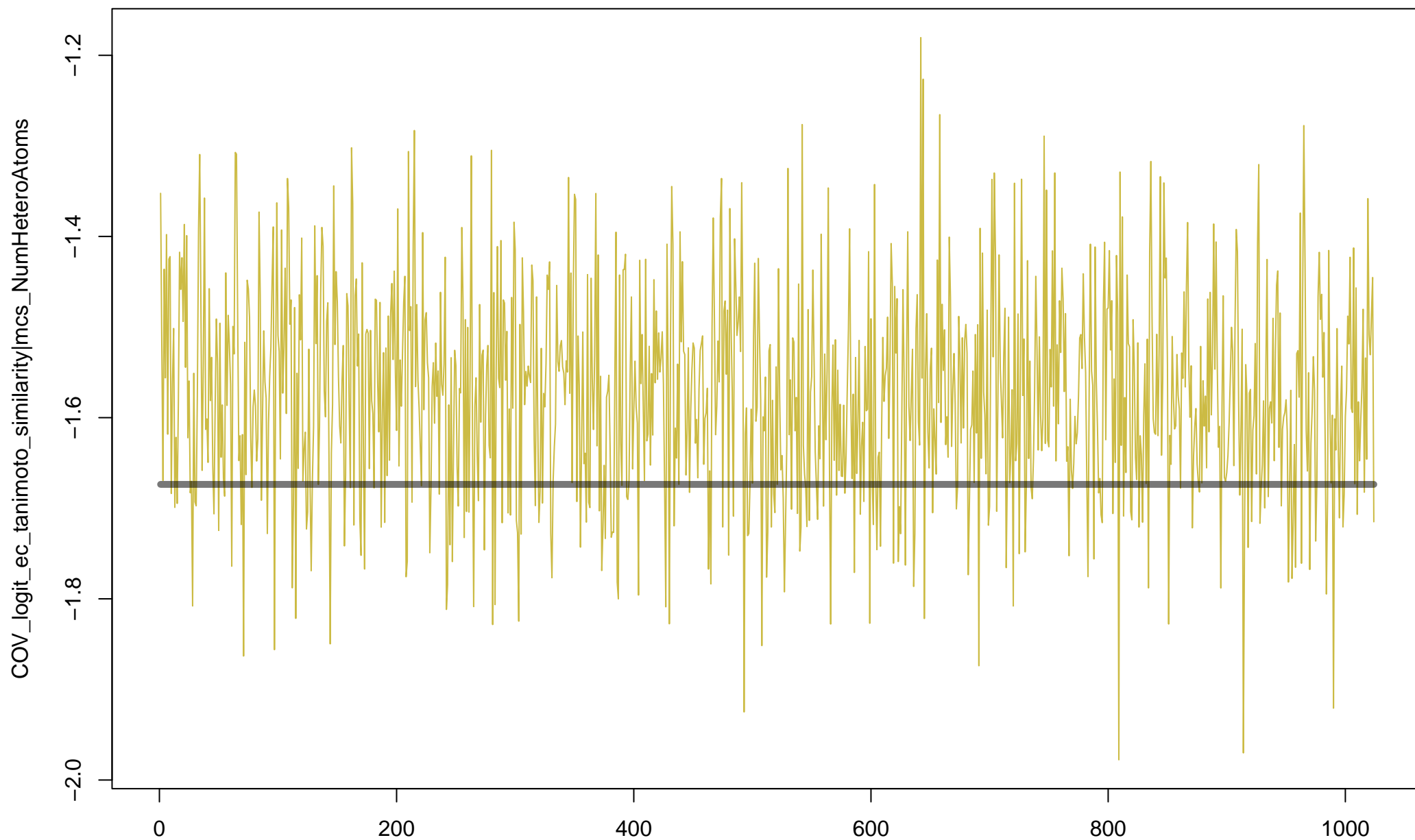
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0384 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | rel.err: -0.0457



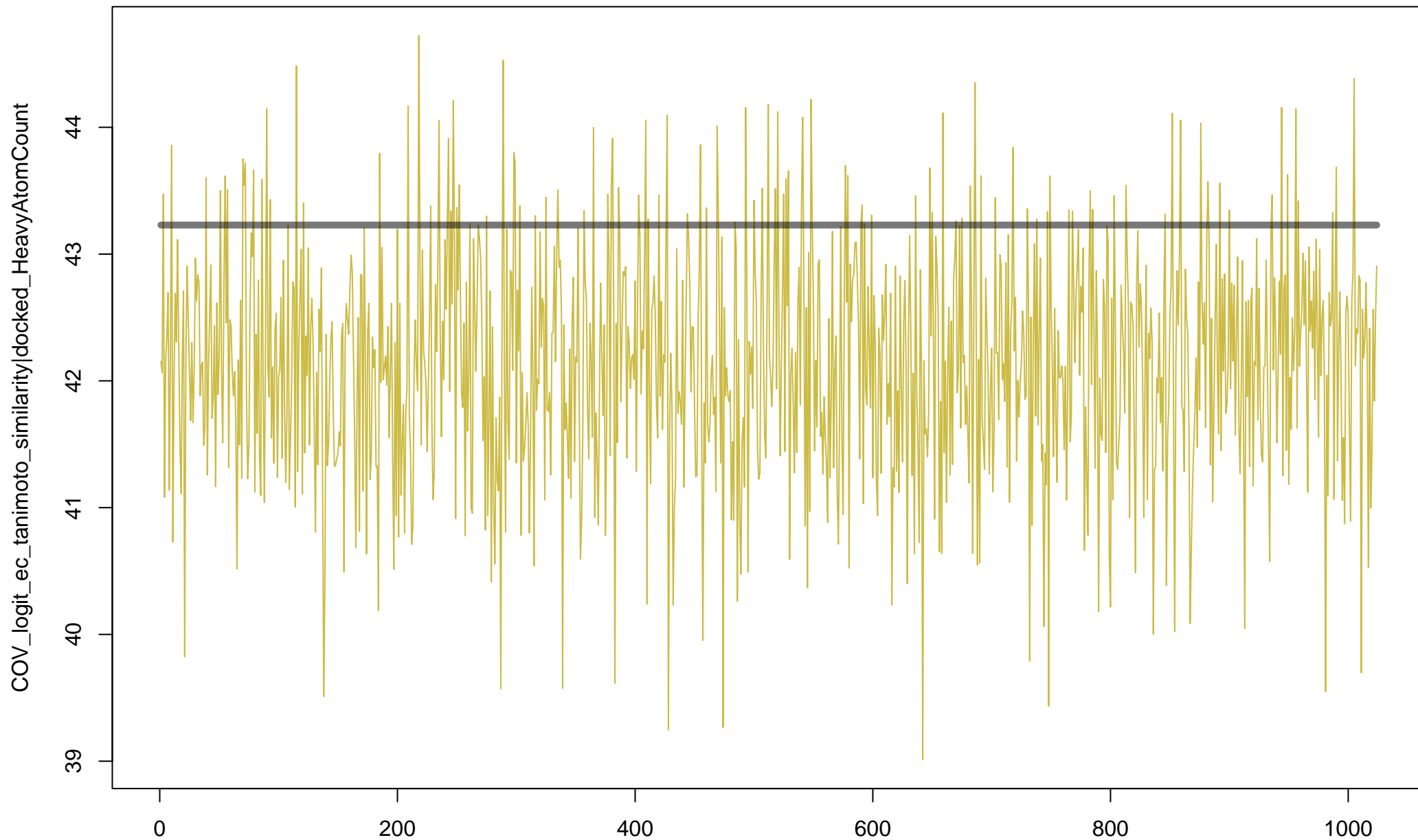
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0495 | MCSE(6.27) = 3.49 | stat: FALSE | burn: 0 | rel.err: 0.238



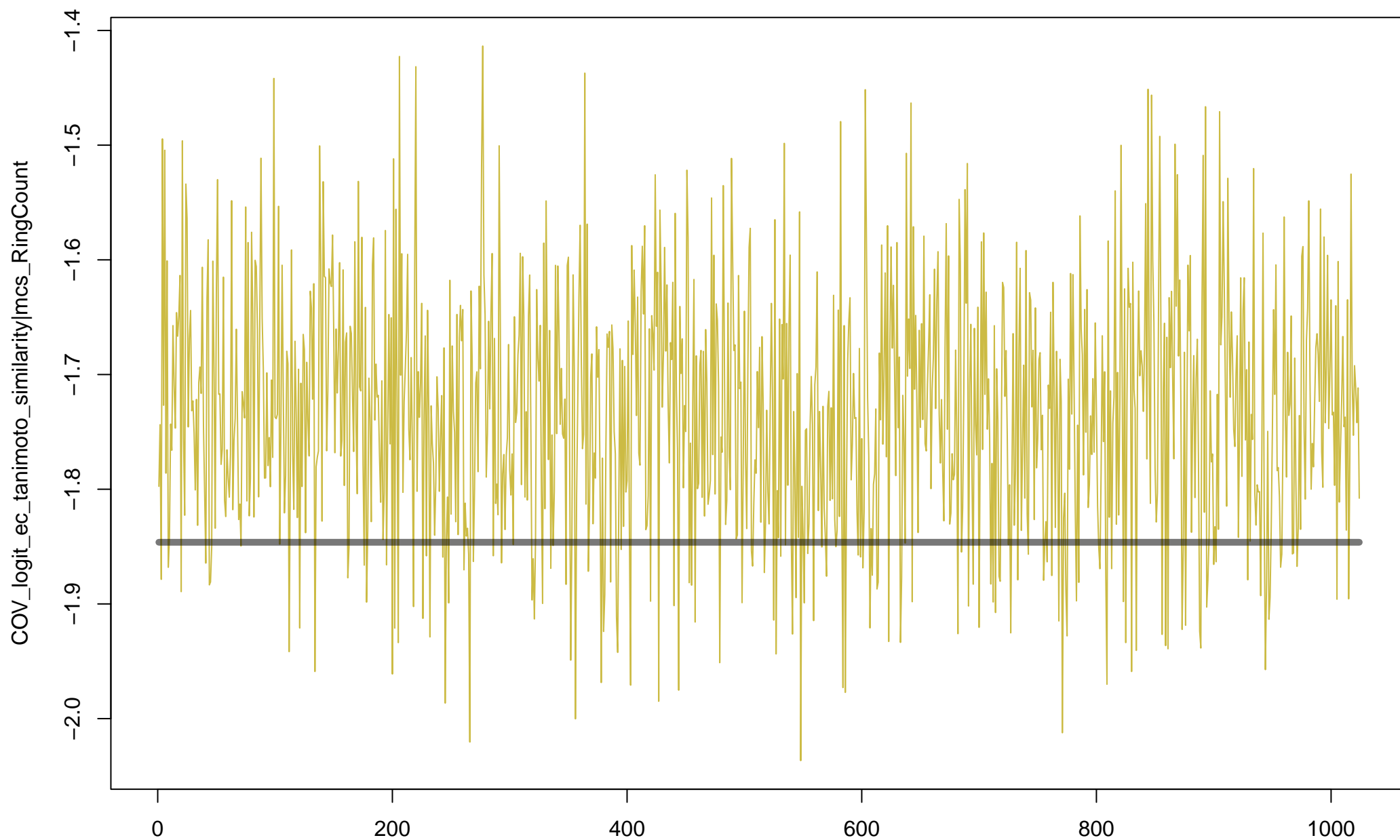
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0869 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0 | rel.err: 0.864



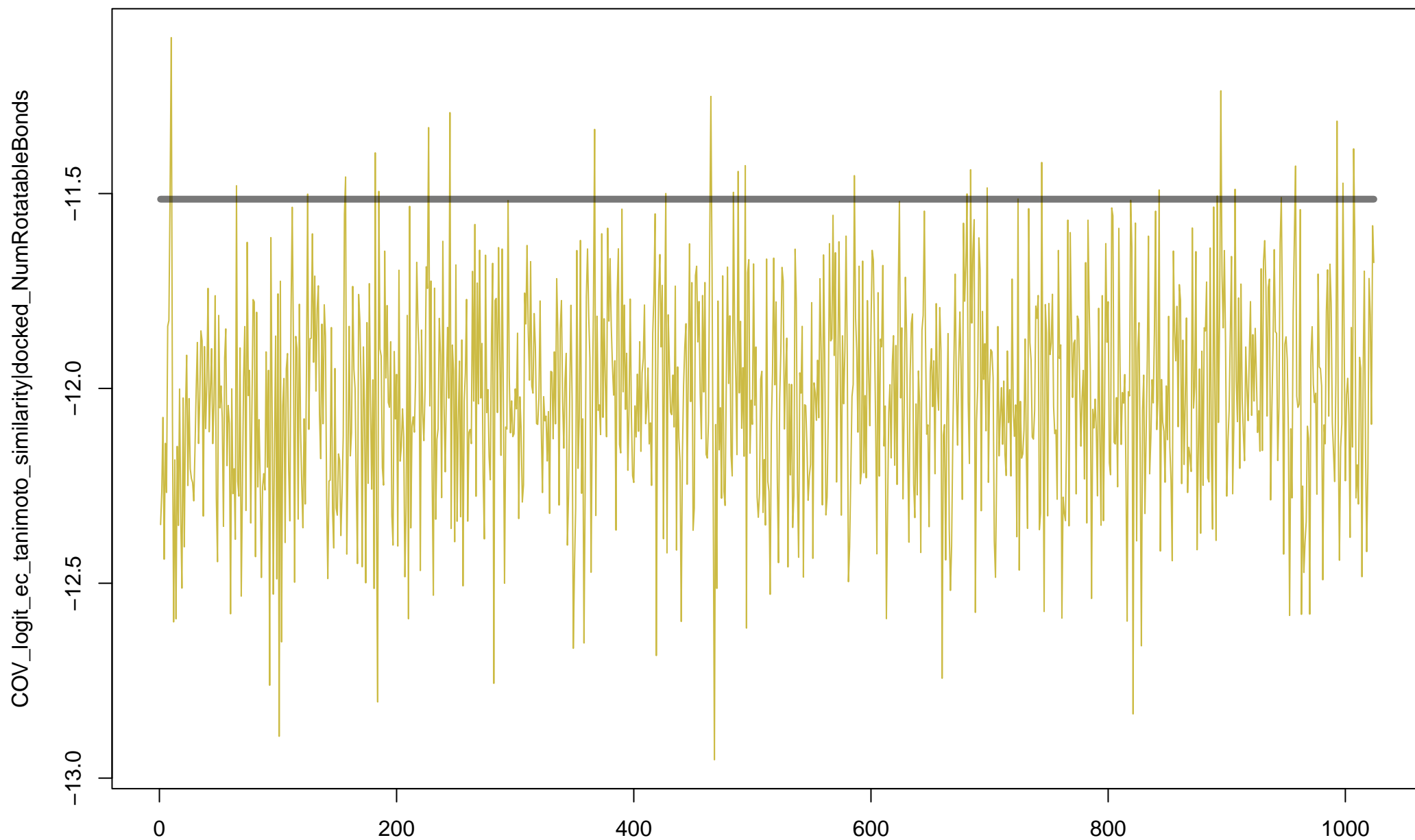
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0465 | MCSE(6.27) = 3.33 | stat: TRUE | burn: 0 | rel.err: -1.24



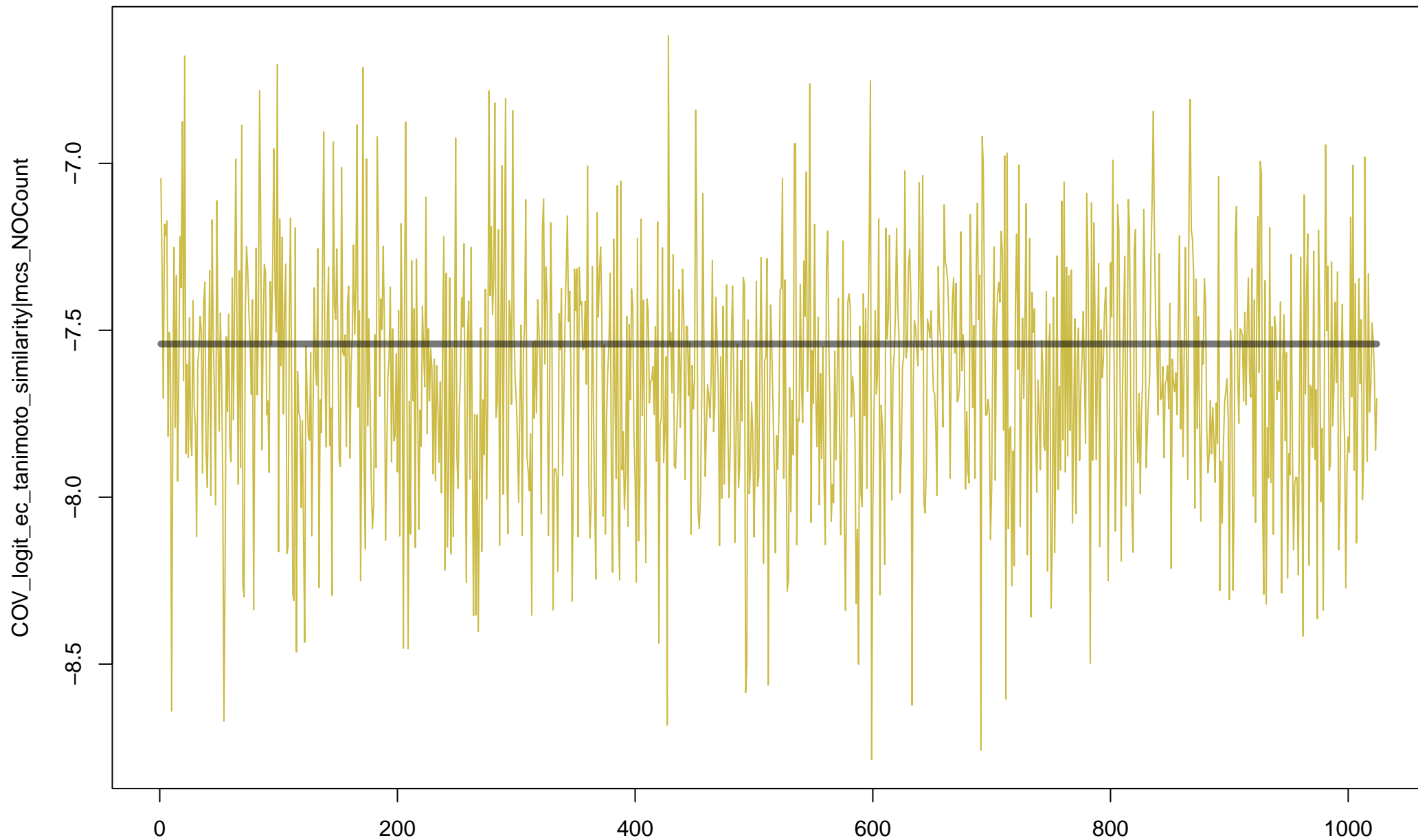
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0591 | MCSE(6.27) = 3.72 | stat: FALSE | burn: 0 | rel.err: 1.06



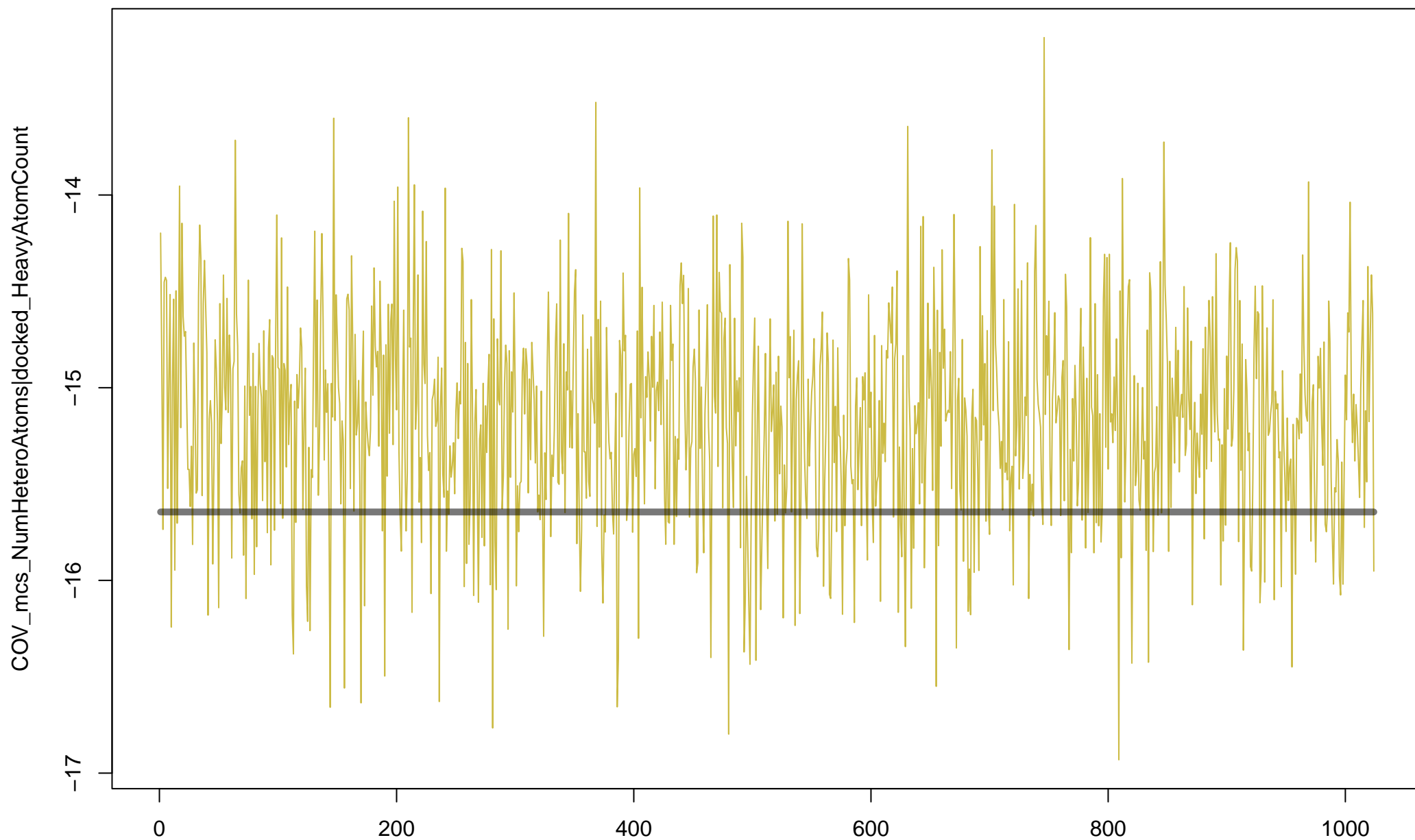
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.055 | MCSE(6.27) = 3.36 | stat: FALSE | burn: 0 | rel.err: -1.89



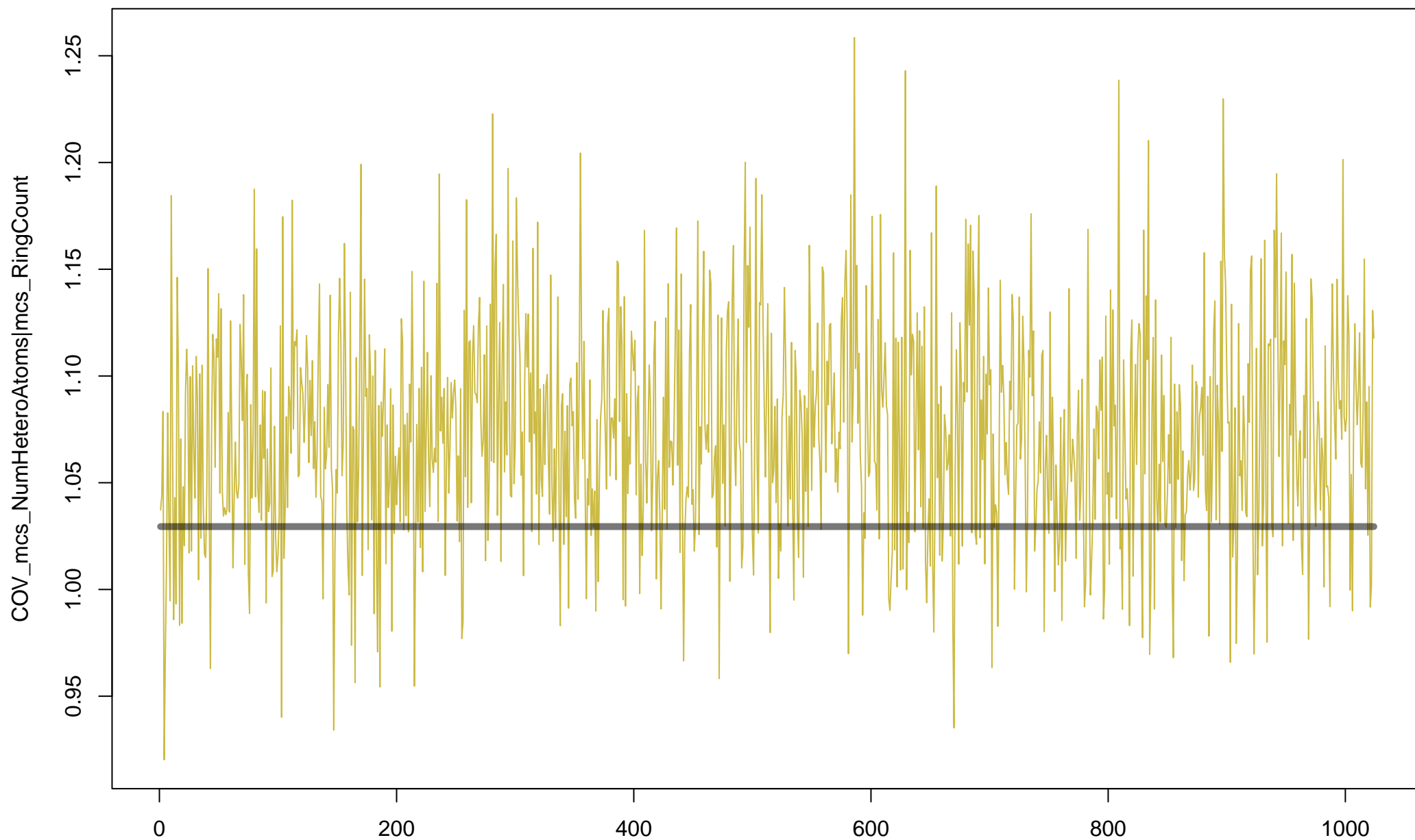
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0538 | MCSE(6.27) = 3.21 | stat: TRUE | burn: 0 | rel.err: -0.305



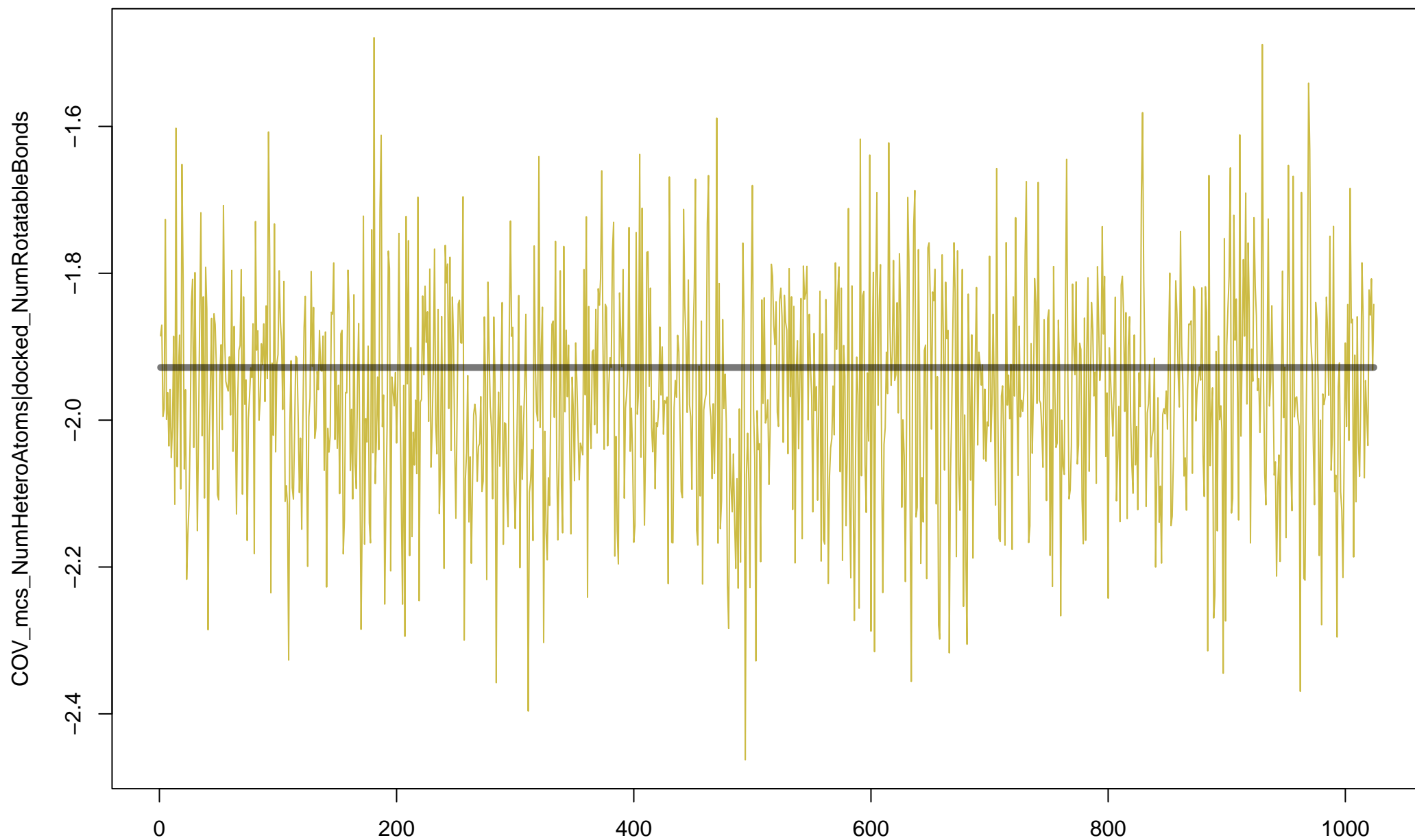
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0674 | MCSE(6.27) = 3.41 | stat: FALSE | burn: 0 | rel.err: 0.878



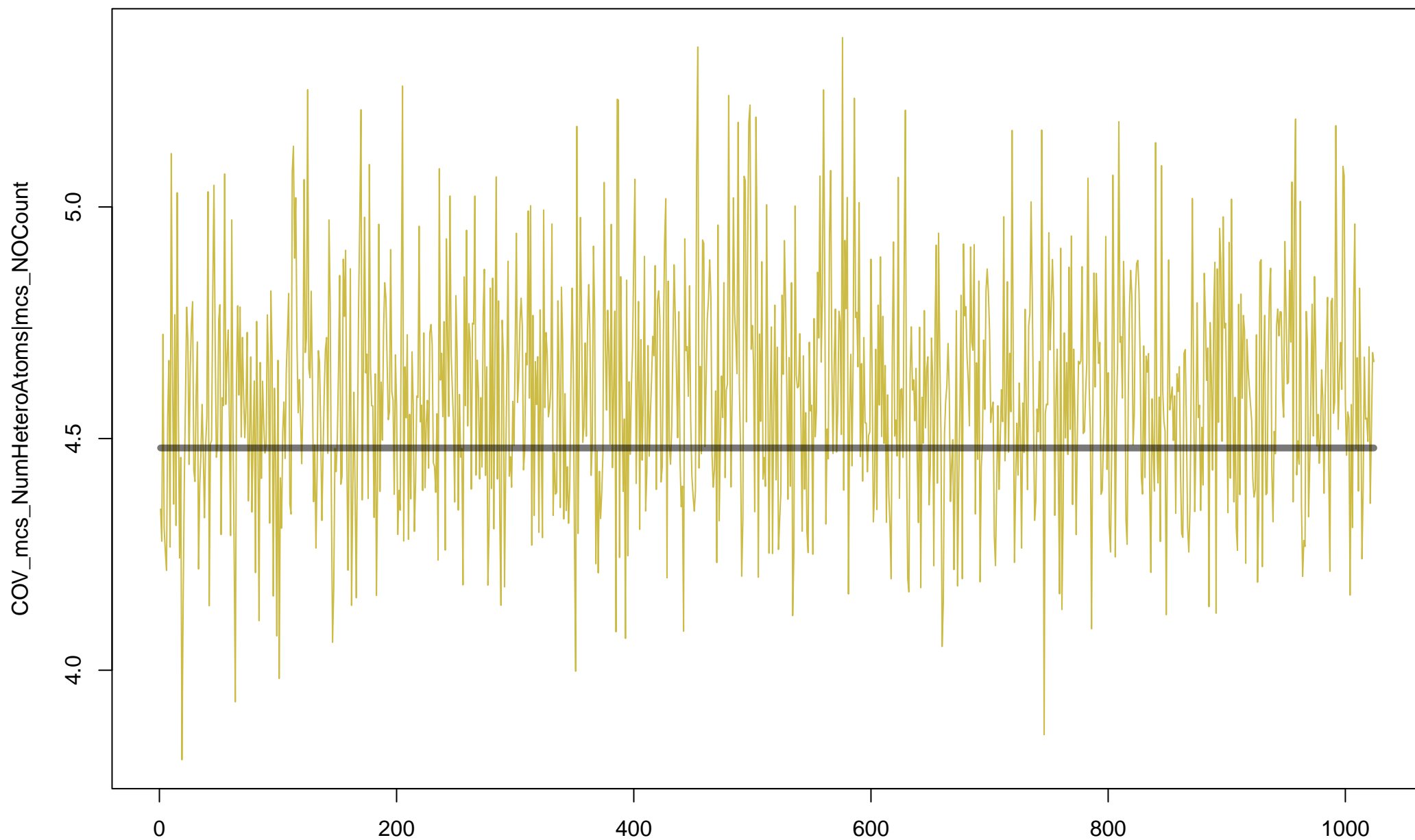
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0568 | MCSE(6.27) = 4.35 | stat: FALSE | burn: 0 | rel.err: 0.859



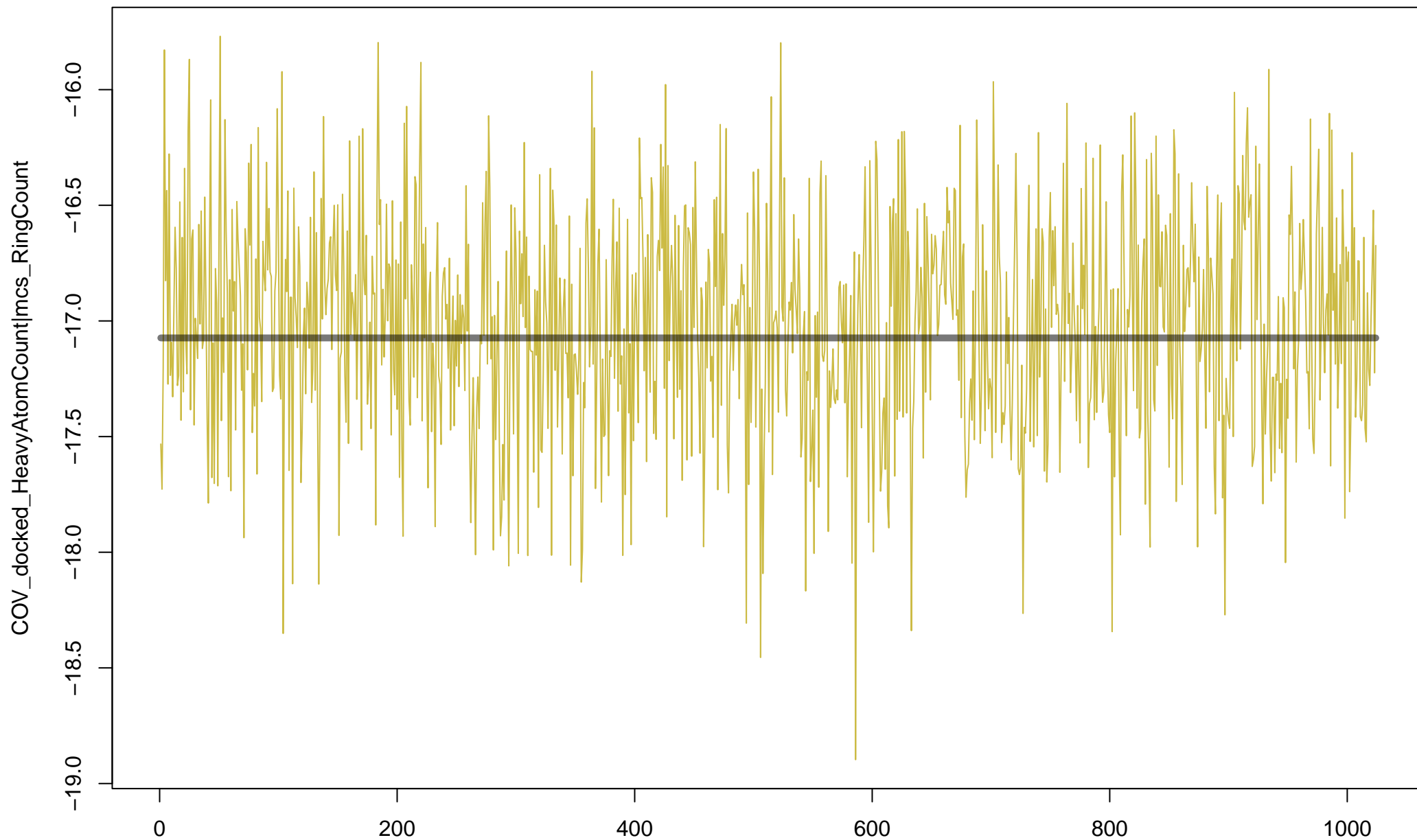
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0622 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0 | rel.err: -0.271



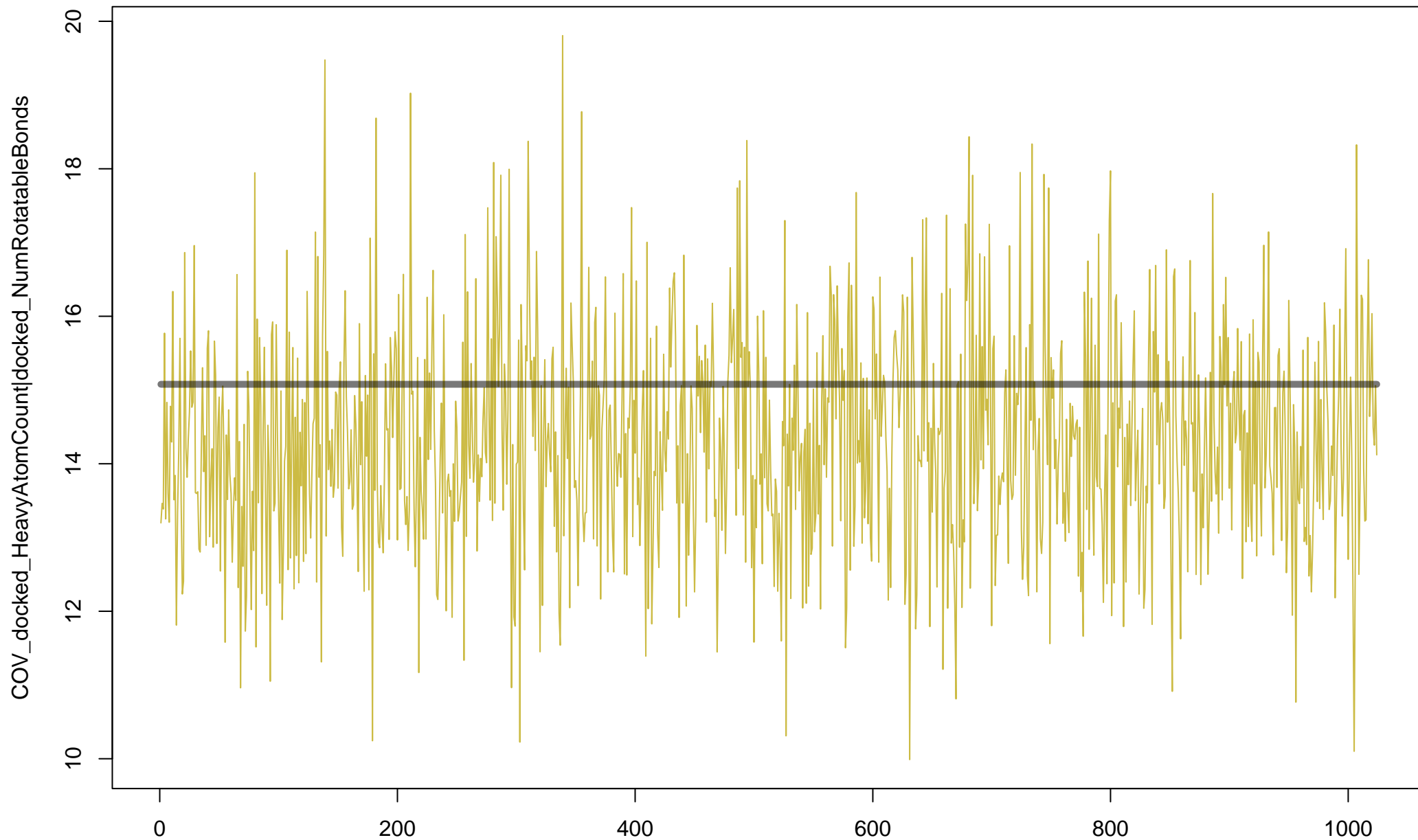
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 926 | BMK = 0.0555 | MCSE(6.27) = 3.29 | stat: FALSE | burn: 0 | rel.err: 0.485



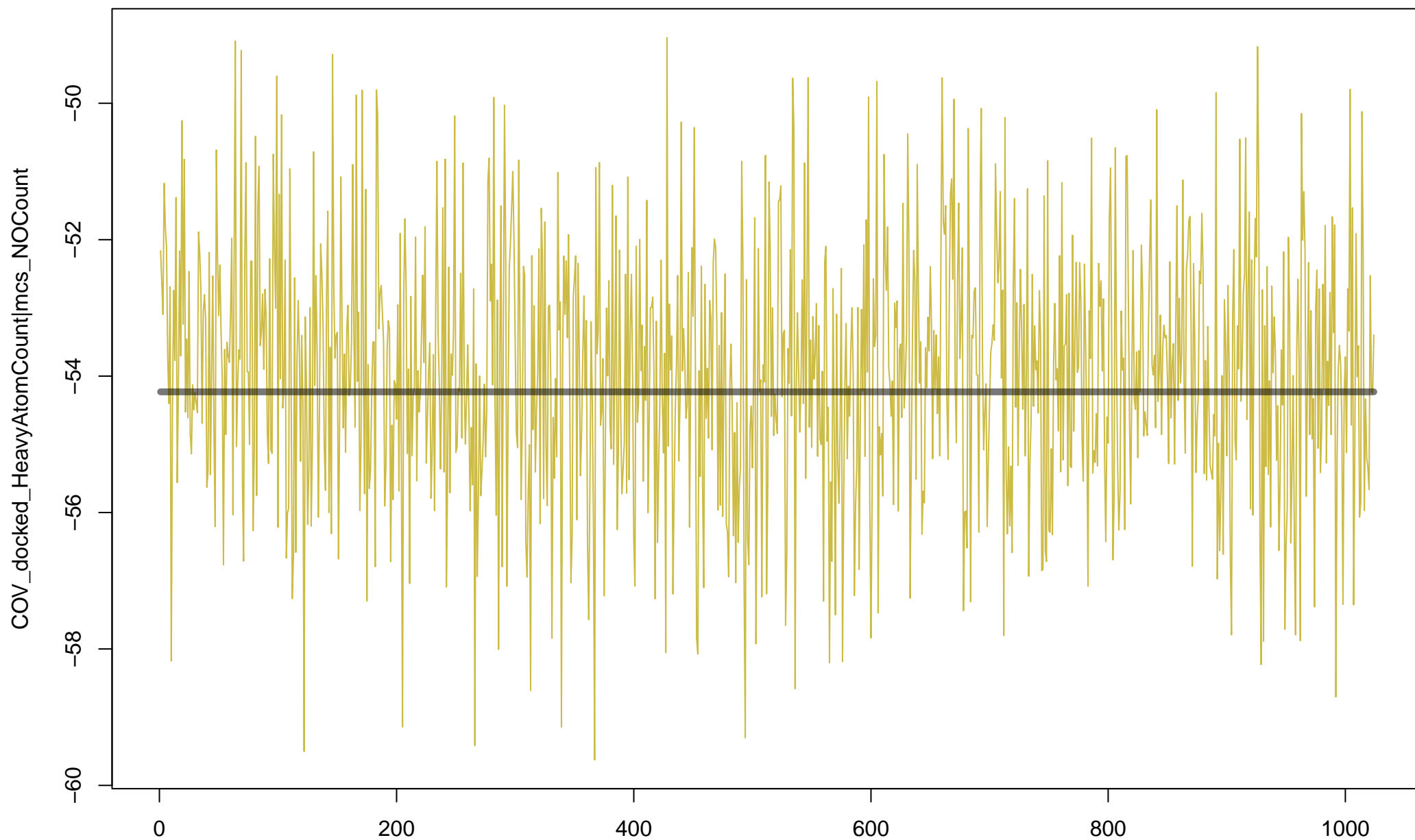
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0603 | MCSE(6.27) = 3.67 | stat: FALSE | burn: 0 | rel.err: 0.12



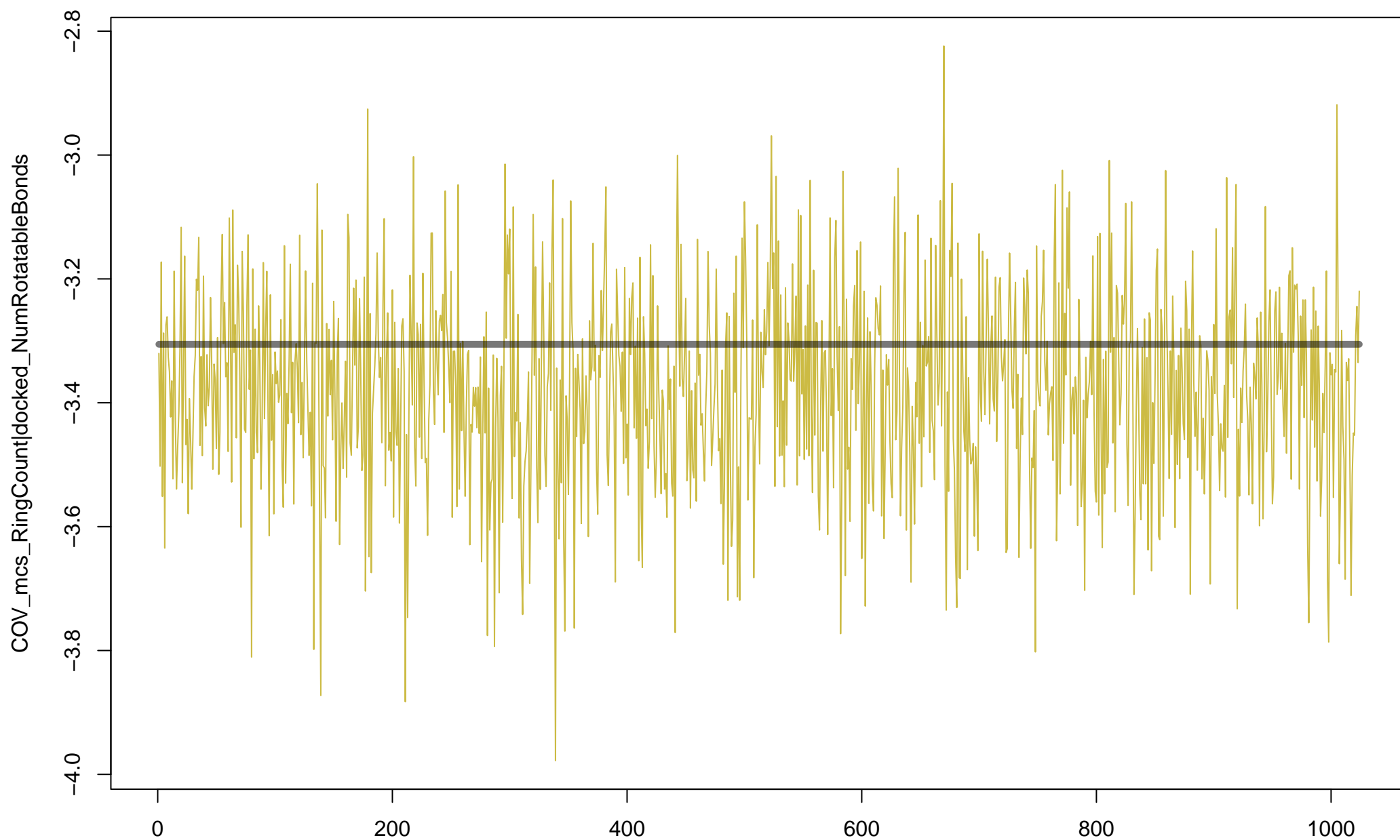
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0588 | MCSE(6.27) = 3.27 | stat: FALSE | burn: 0 | rel.err: -0.533



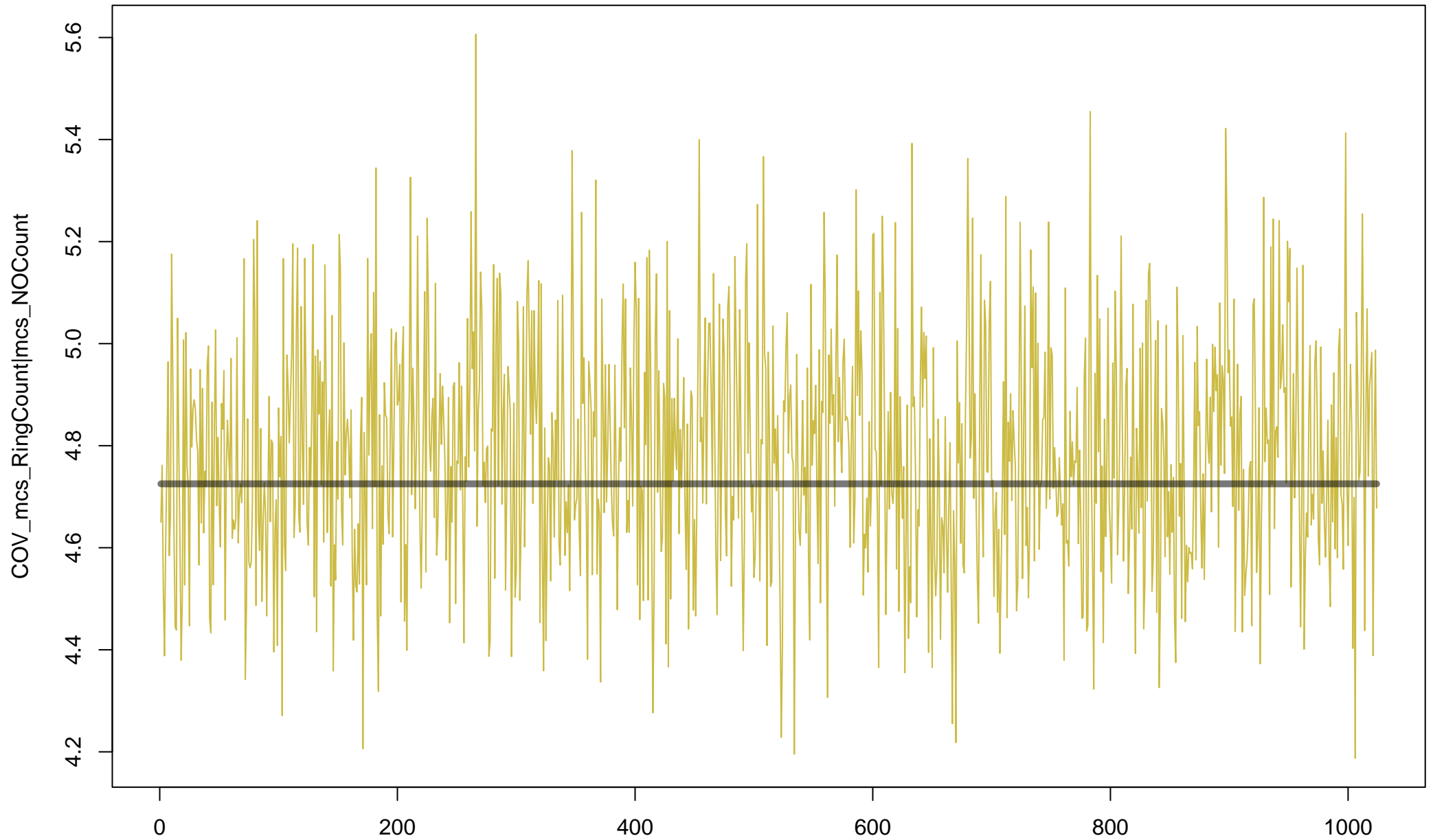
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0423 | MCSE(6.27) = 3.63 | stat: FALSE | burn: 0 | rel.err: 0.148



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0615 | MCSE(6.27) = 3.26 | stat: TRUE | burn: 0 | rel.err: -0.462



COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.0353 | MCSE(6.27) = 3.74 | stat: FALSE | burn: 0 | rel.err: 0.262



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0438 | MCSE(6.27) = 3.18 | stat: FALSE | burn: 0 | rel.err: 1.03

