

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.310210582685911

max MCSE = 9.47713040444607

all stationary: FALSE

burn: 0

max rel.err.: 1.75361164335787

-- STATS 1D --

min ESS = 63.7541410298832

max BMK = 0.204113846058791

max MCSE = 8.64458661715206

all stationary: FALSE

burn: 0

max rel.err.: 2.83114152398832

-- STATS 2D --

min ESS = 729.085375684929

max BMK = 0.0757035098535914

max MCSE = 3.64185953484487

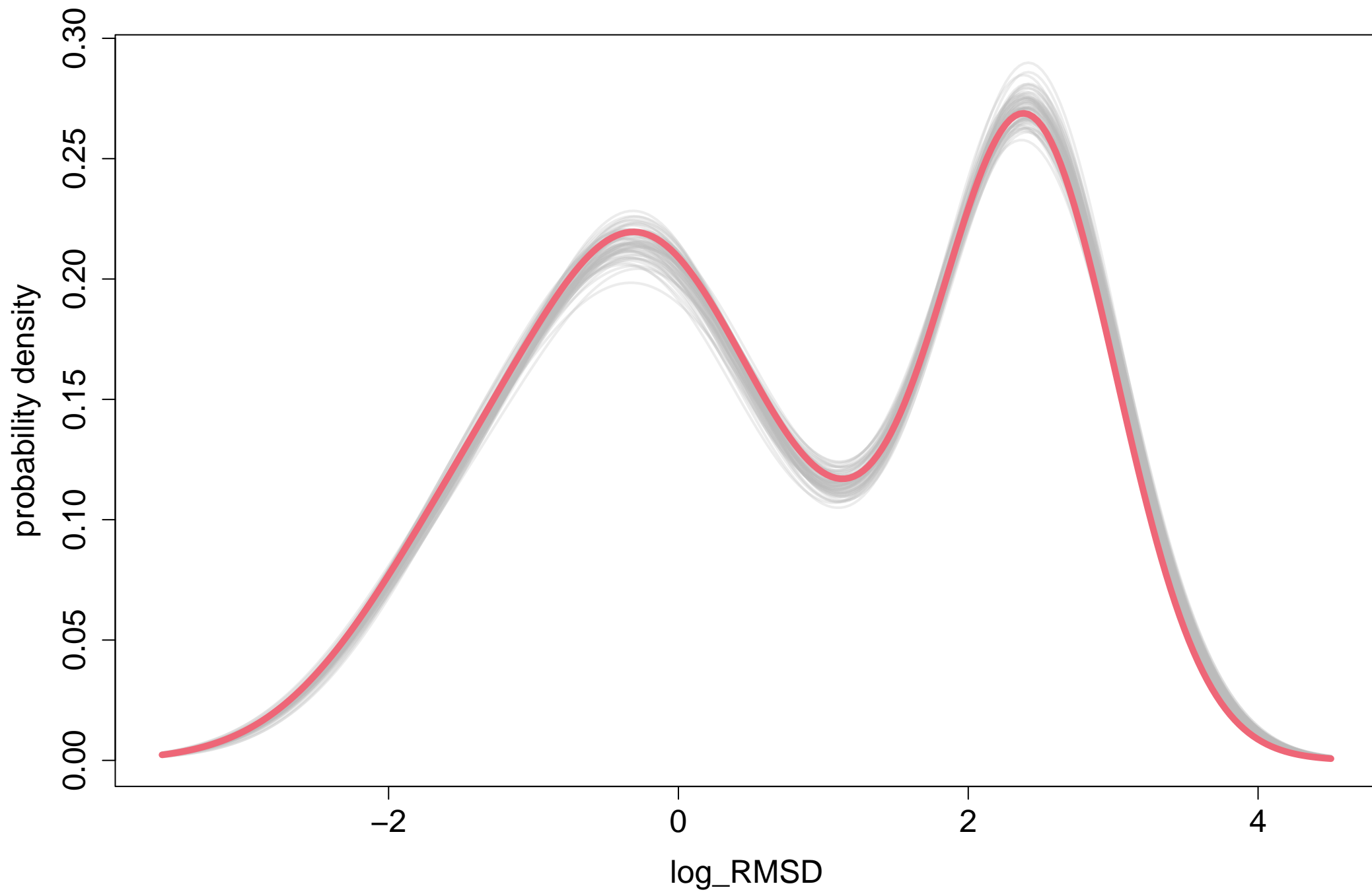
all stationary: FALSE

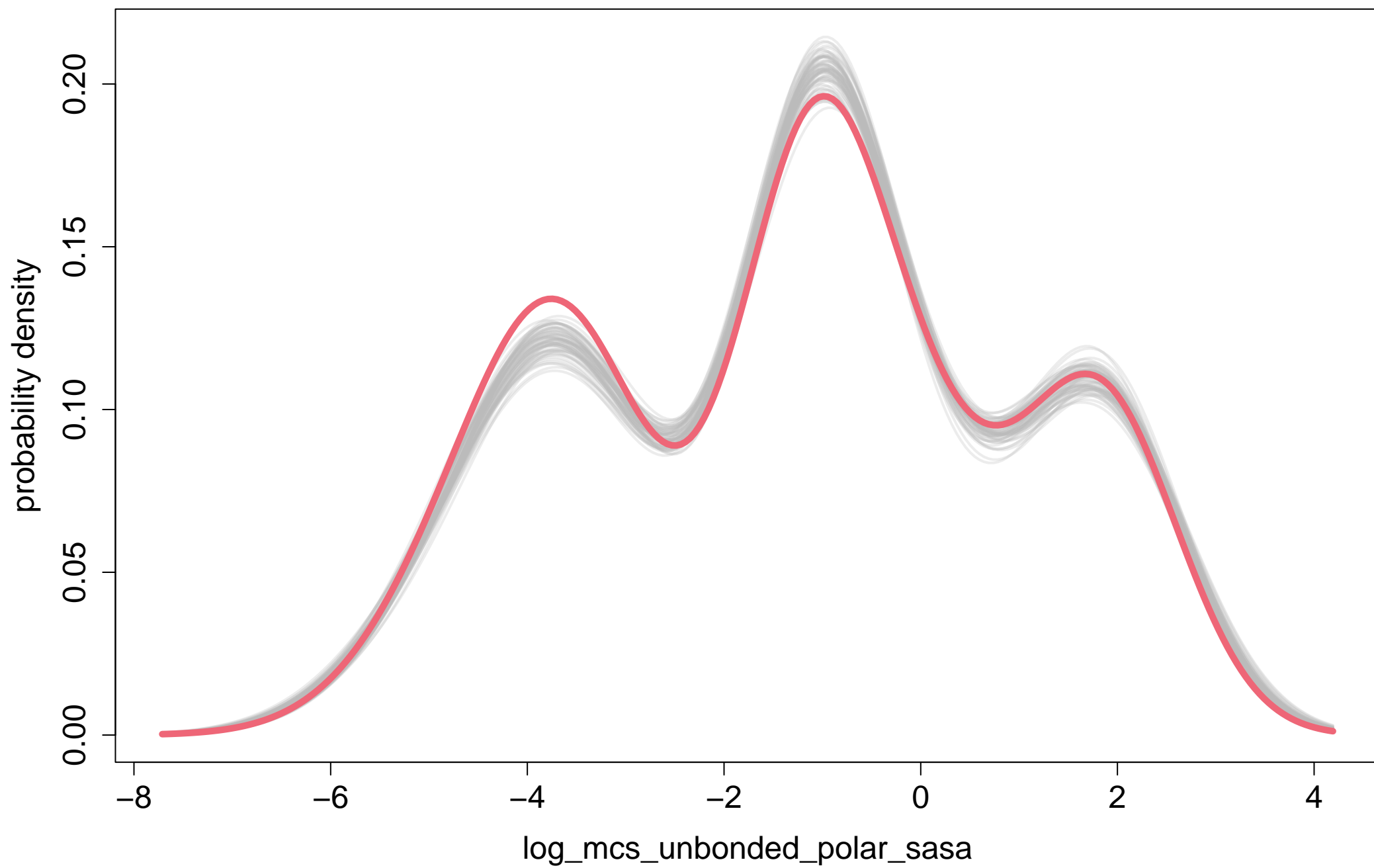
burn: 0

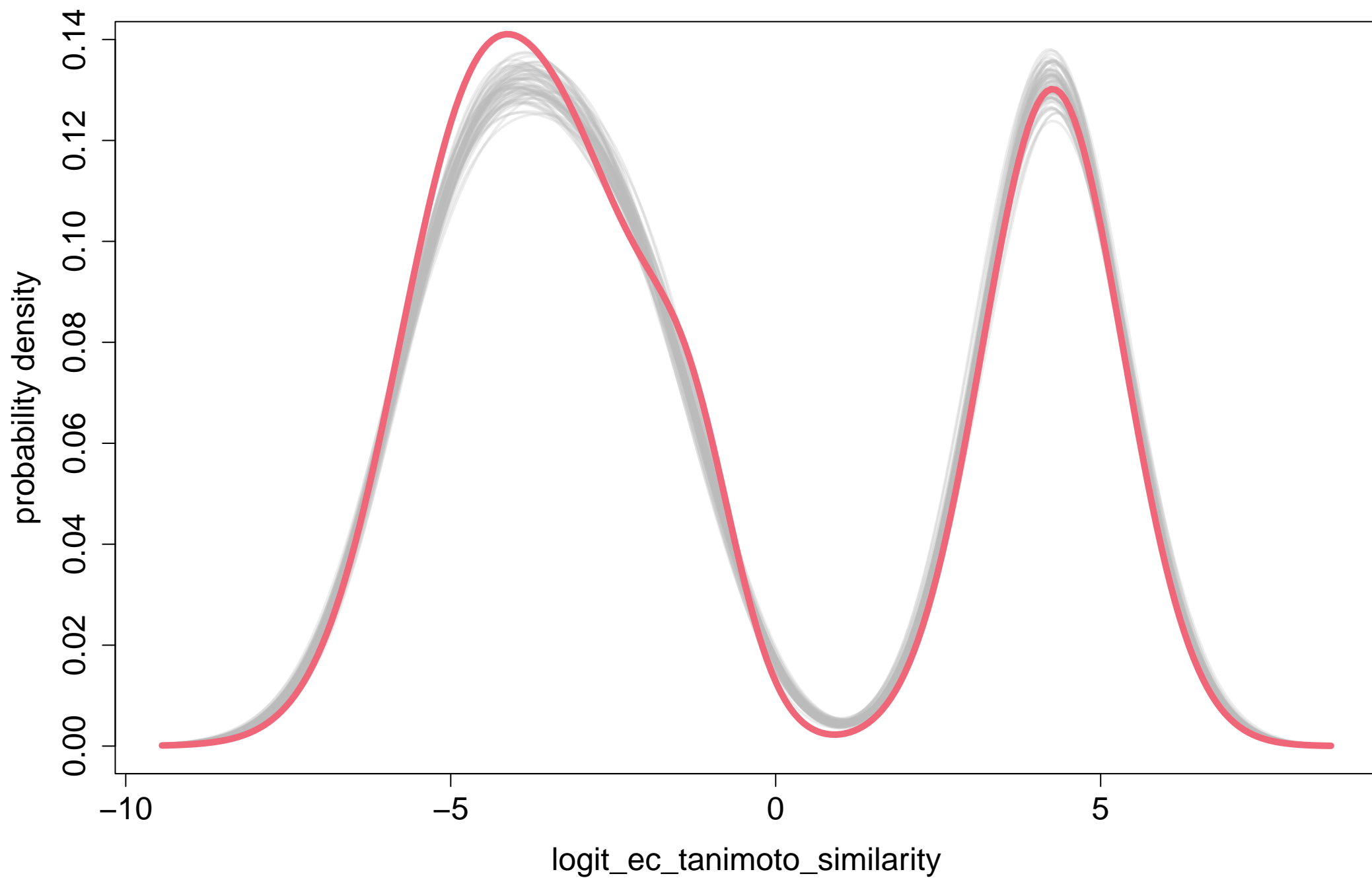
max rel.err.: 2.23289534278531

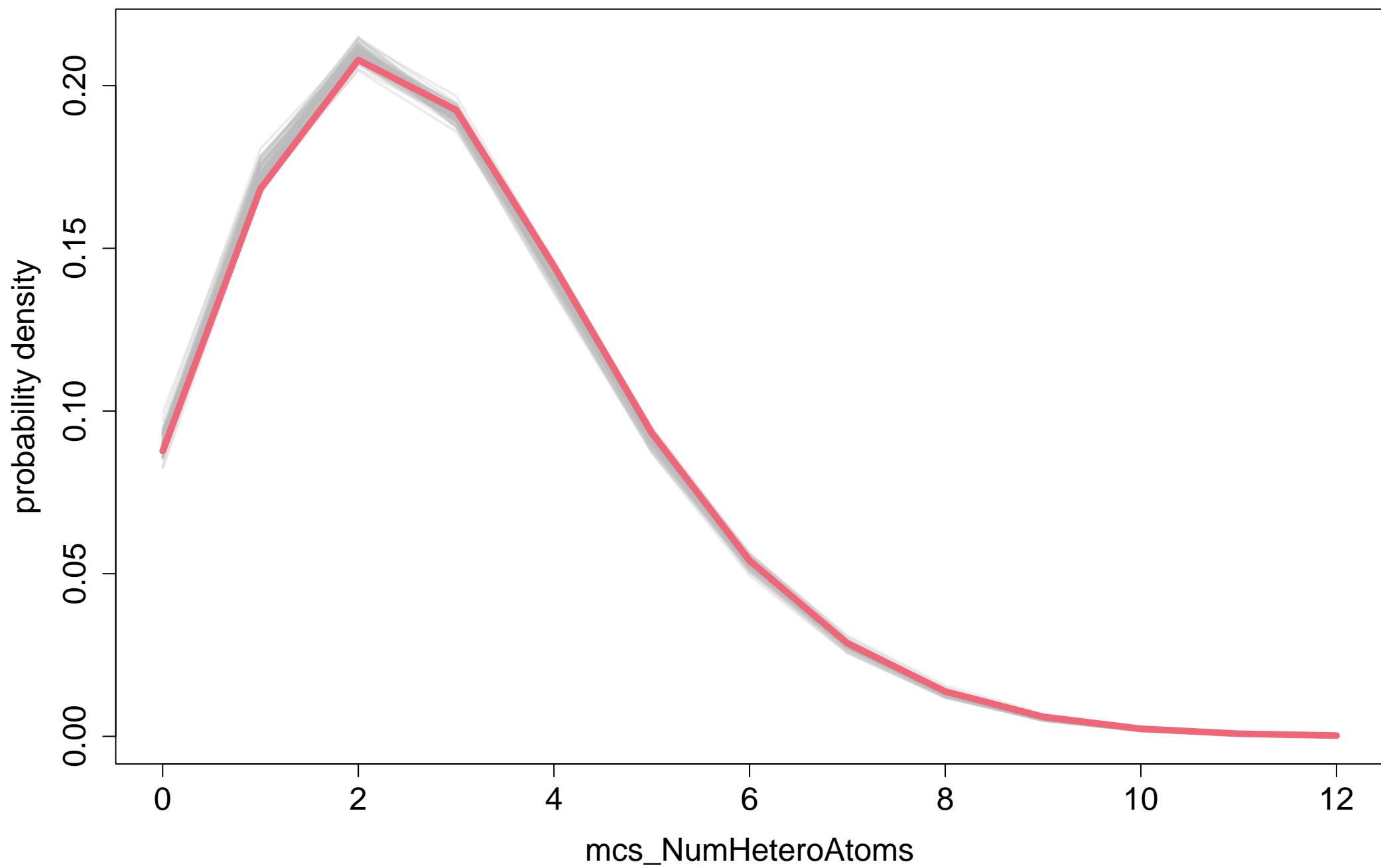
Occupied clusters: 9 of 64

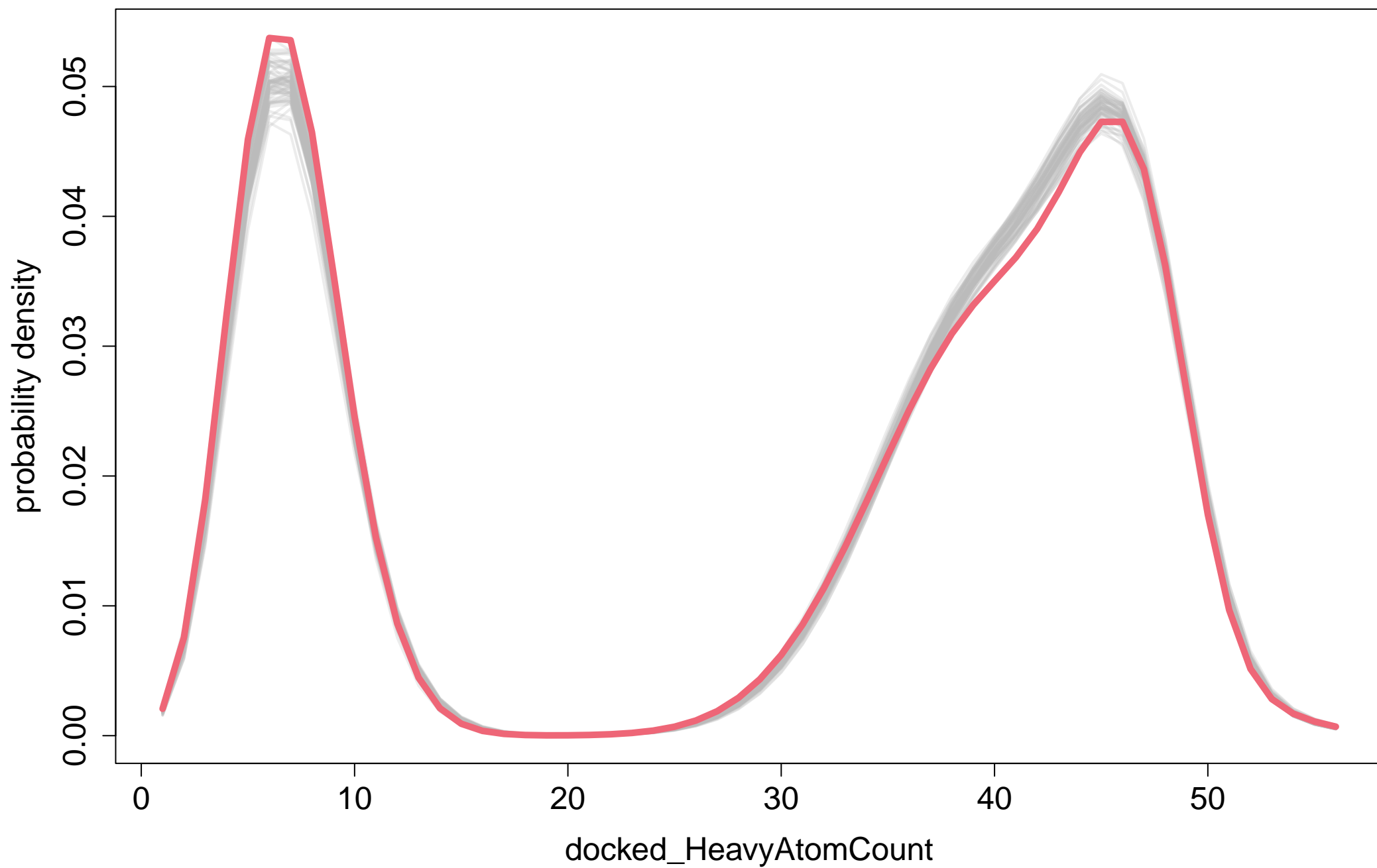
LL: -62500 +- 13.3

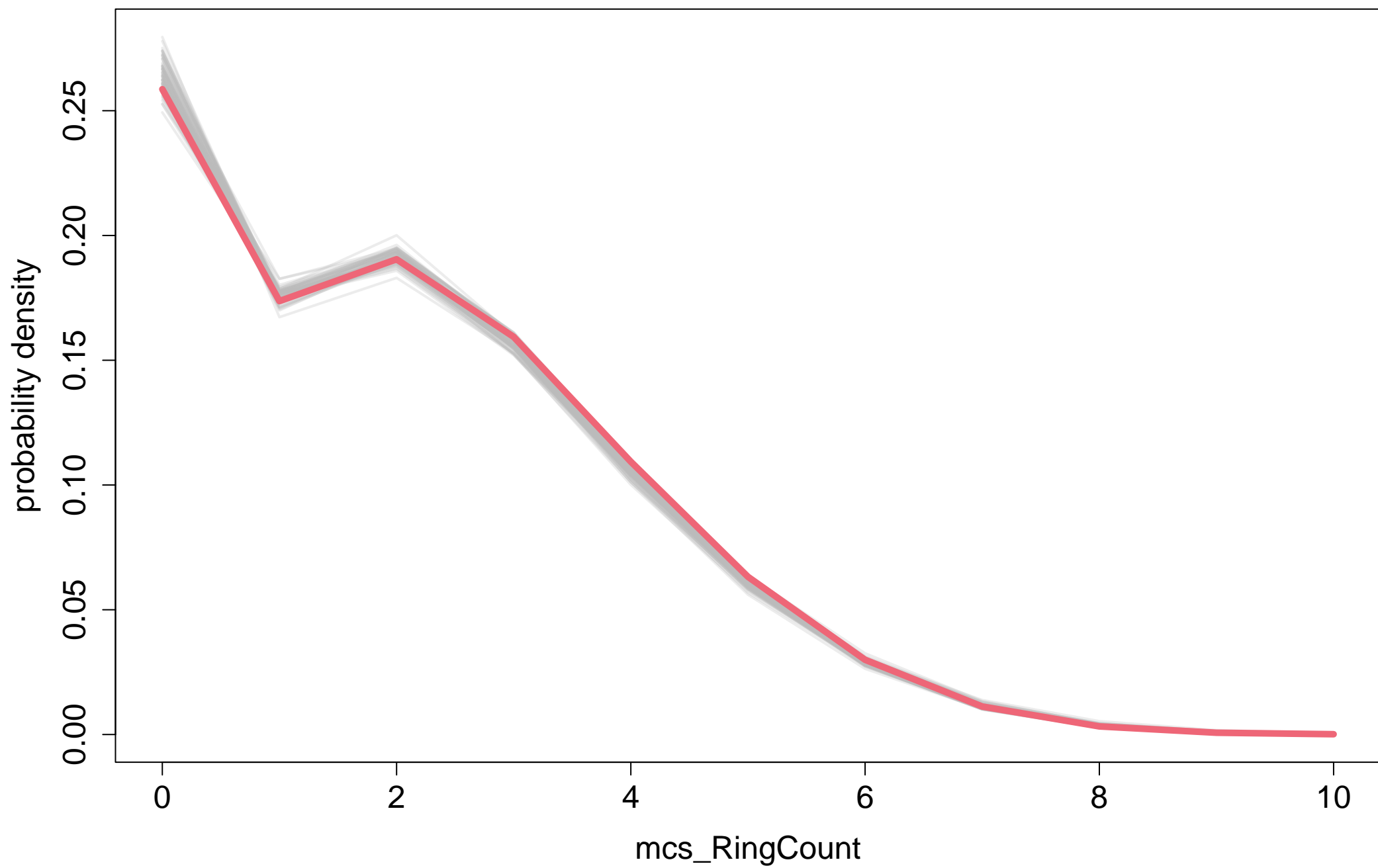


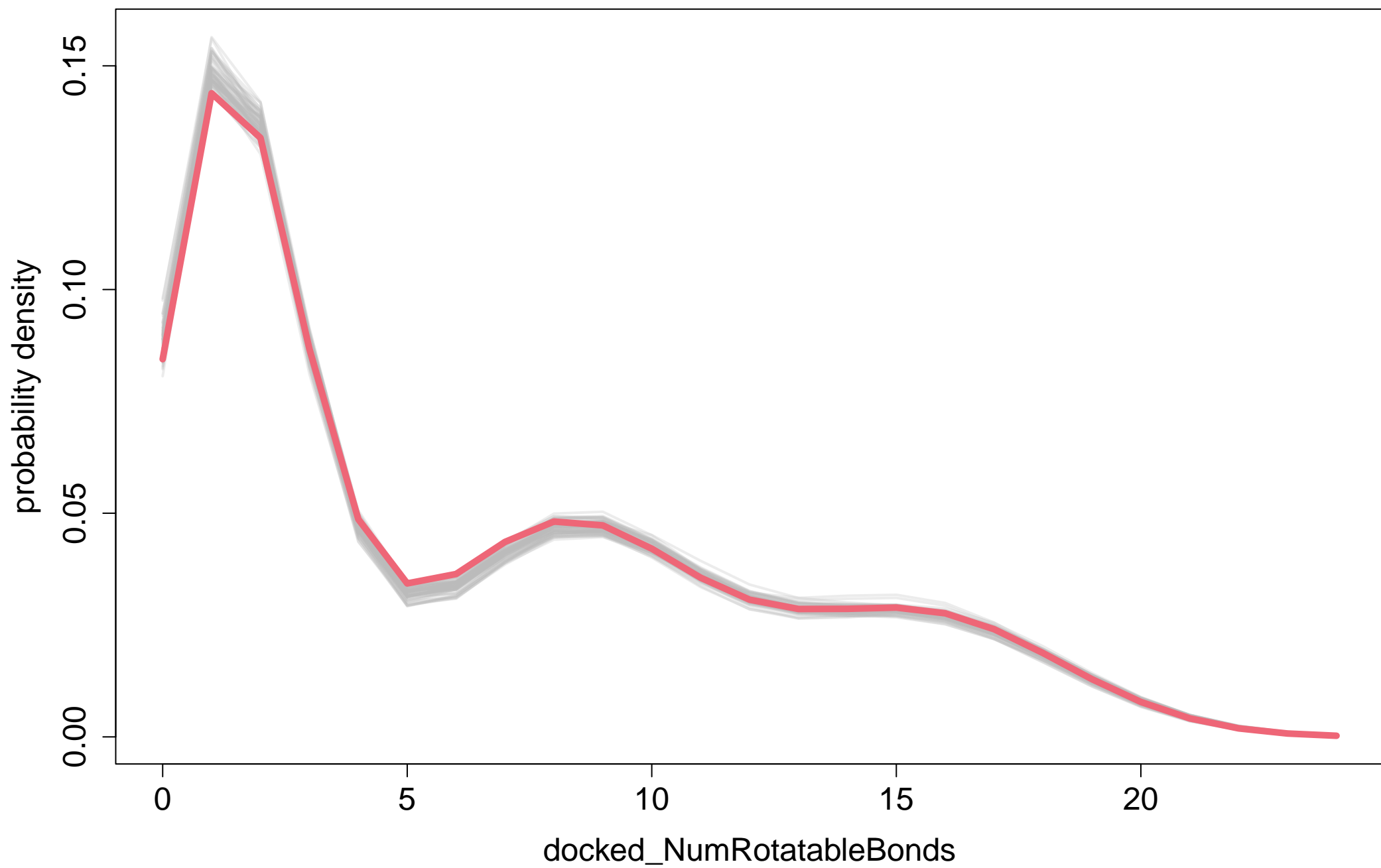


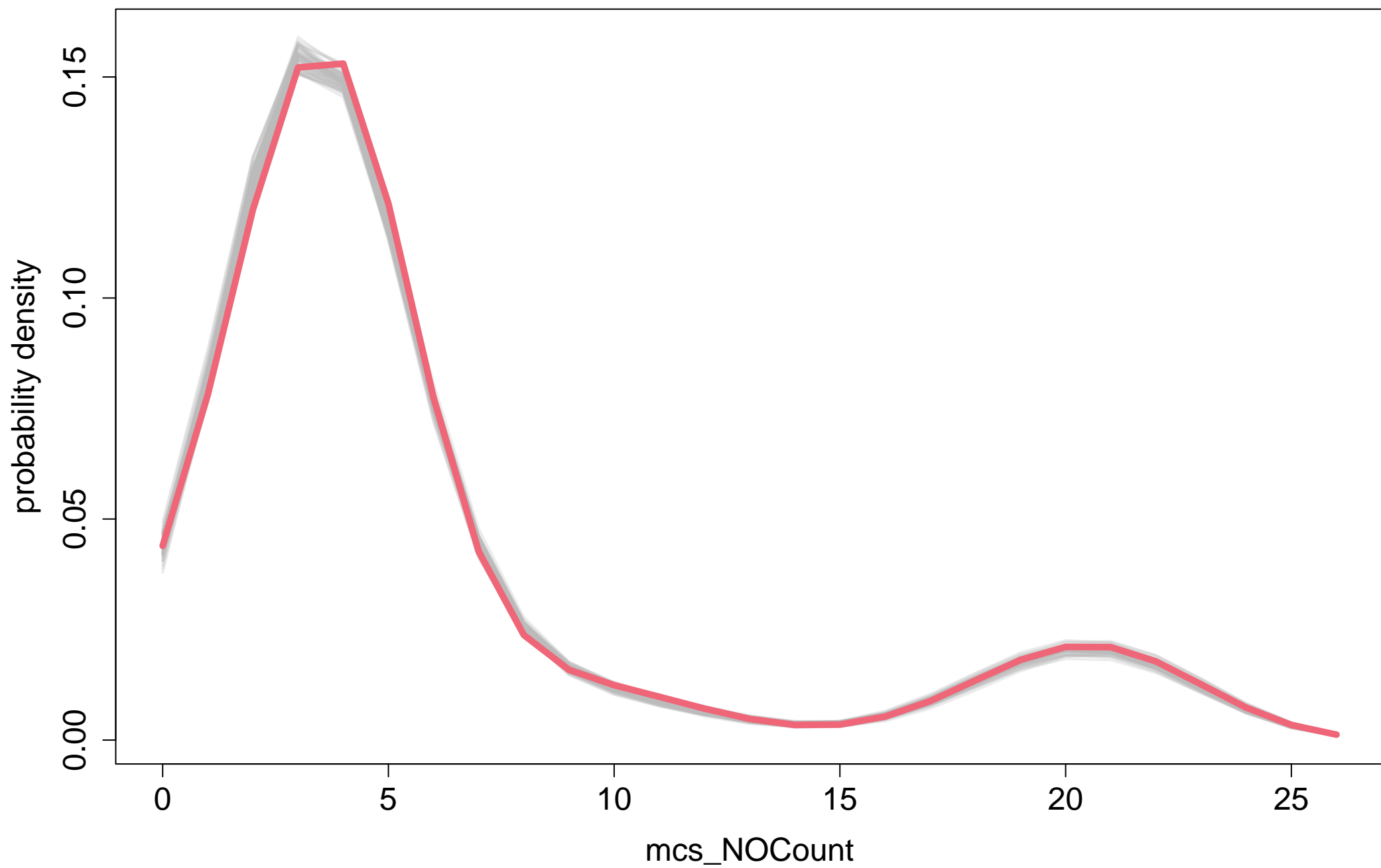


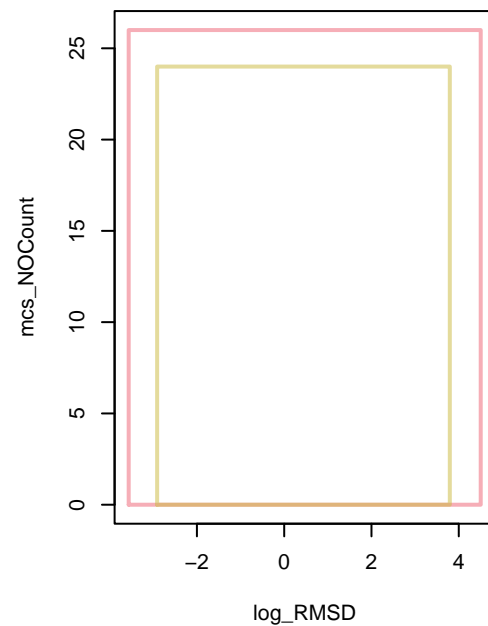
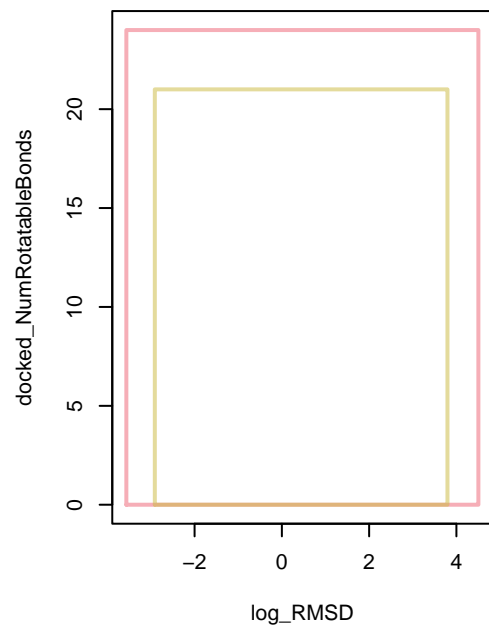
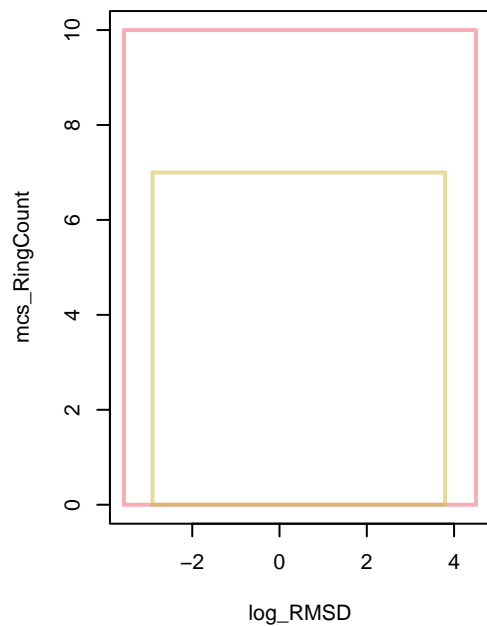
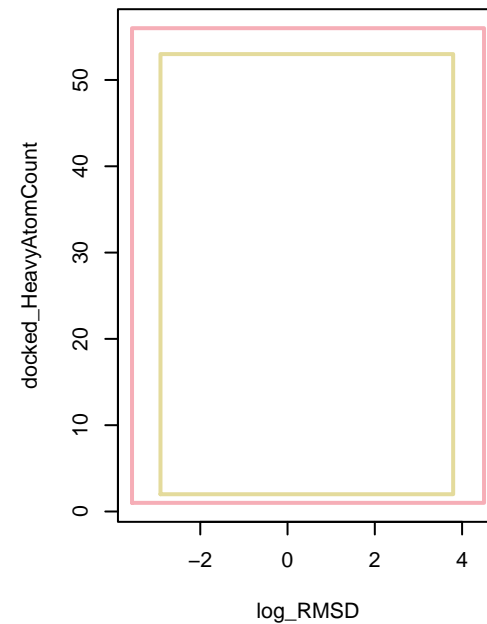
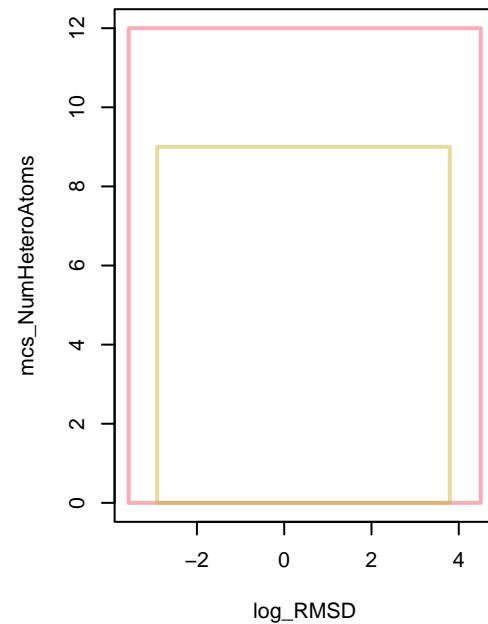
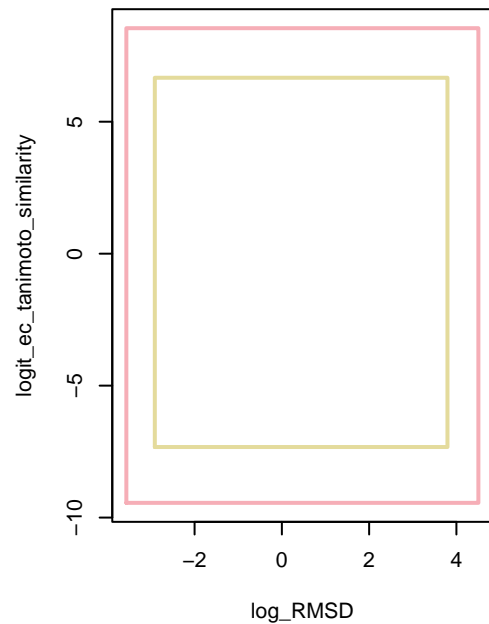
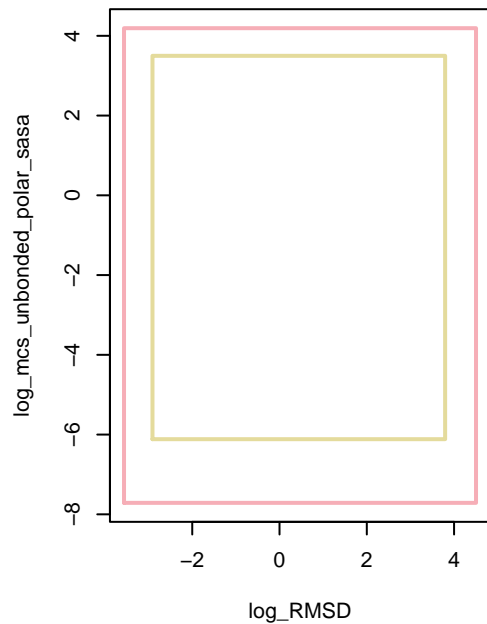




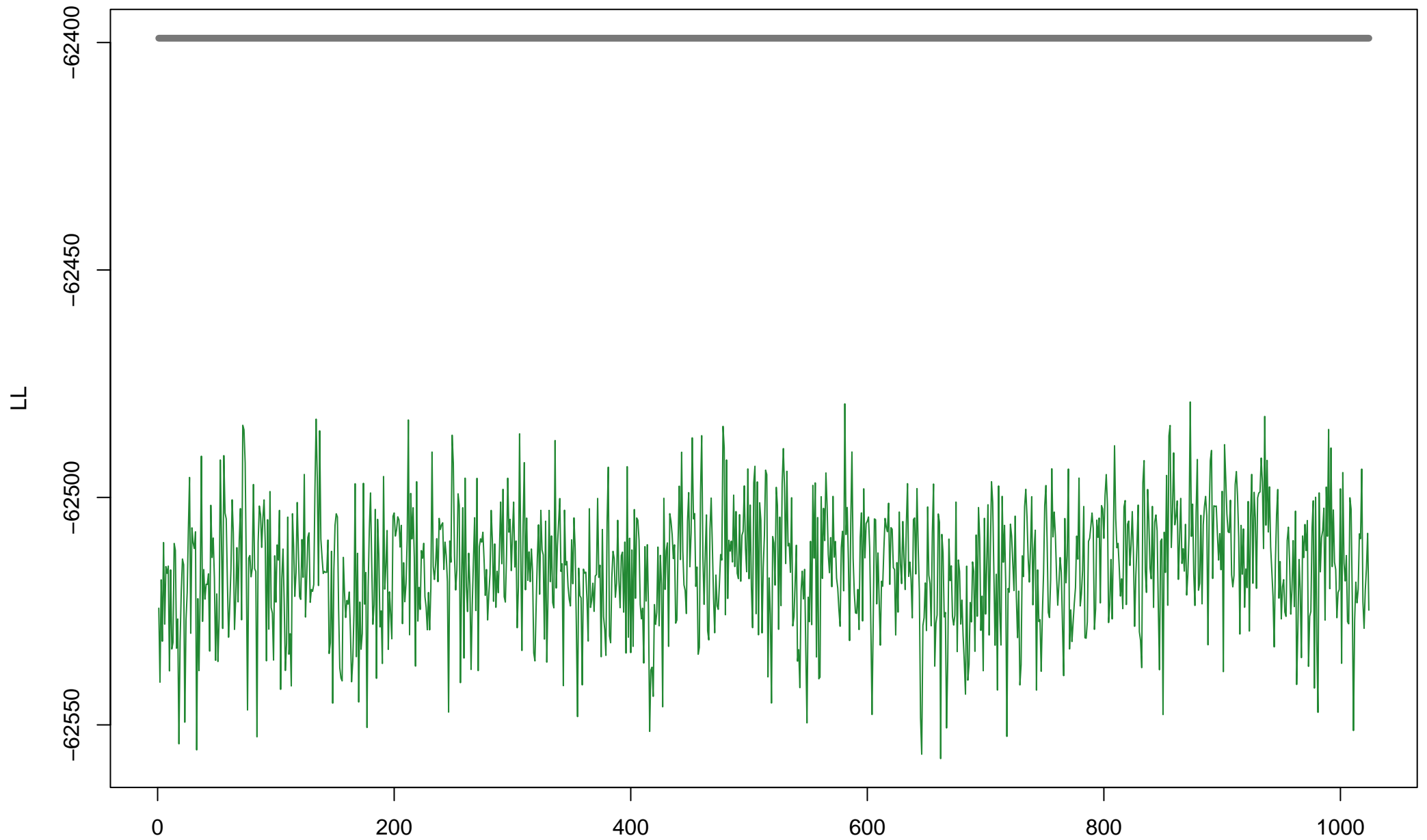






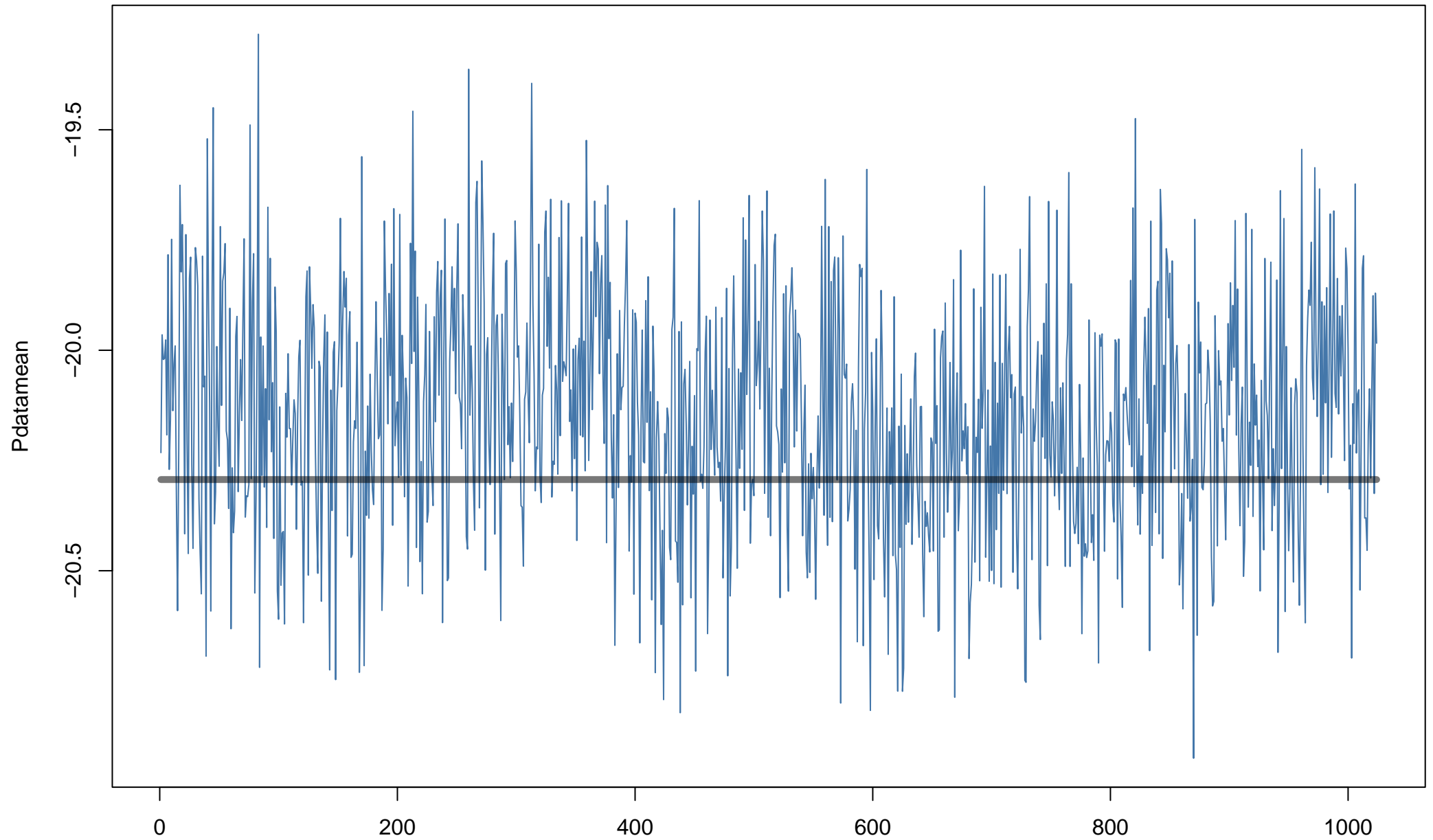


LL



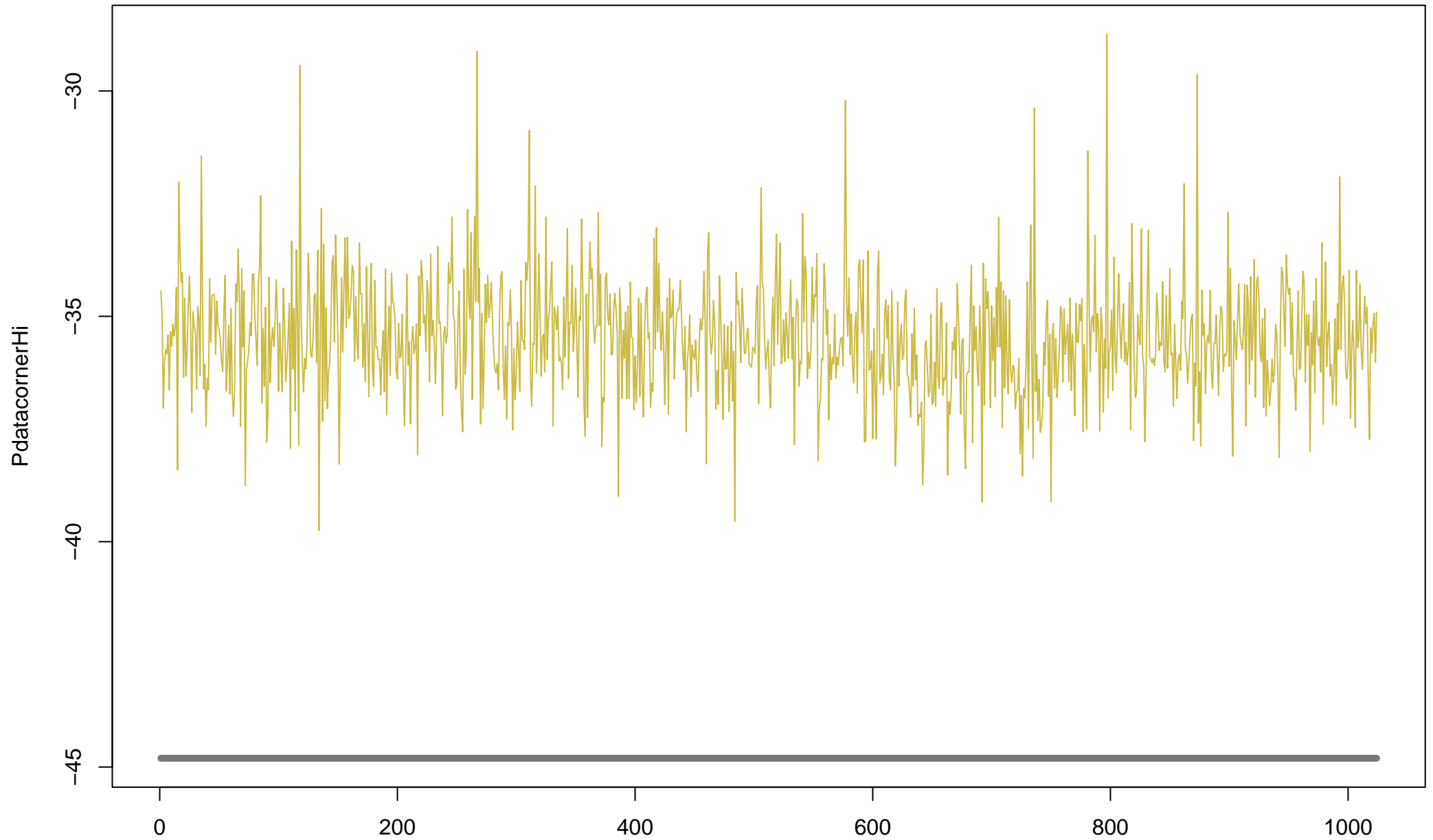
Pdatamean

ESS = 2.22e-16 | BMK = 0.101 | MCSE(6.27) = 5.42 | stat: TRUE | burn: 0 | rel.err: 0.615



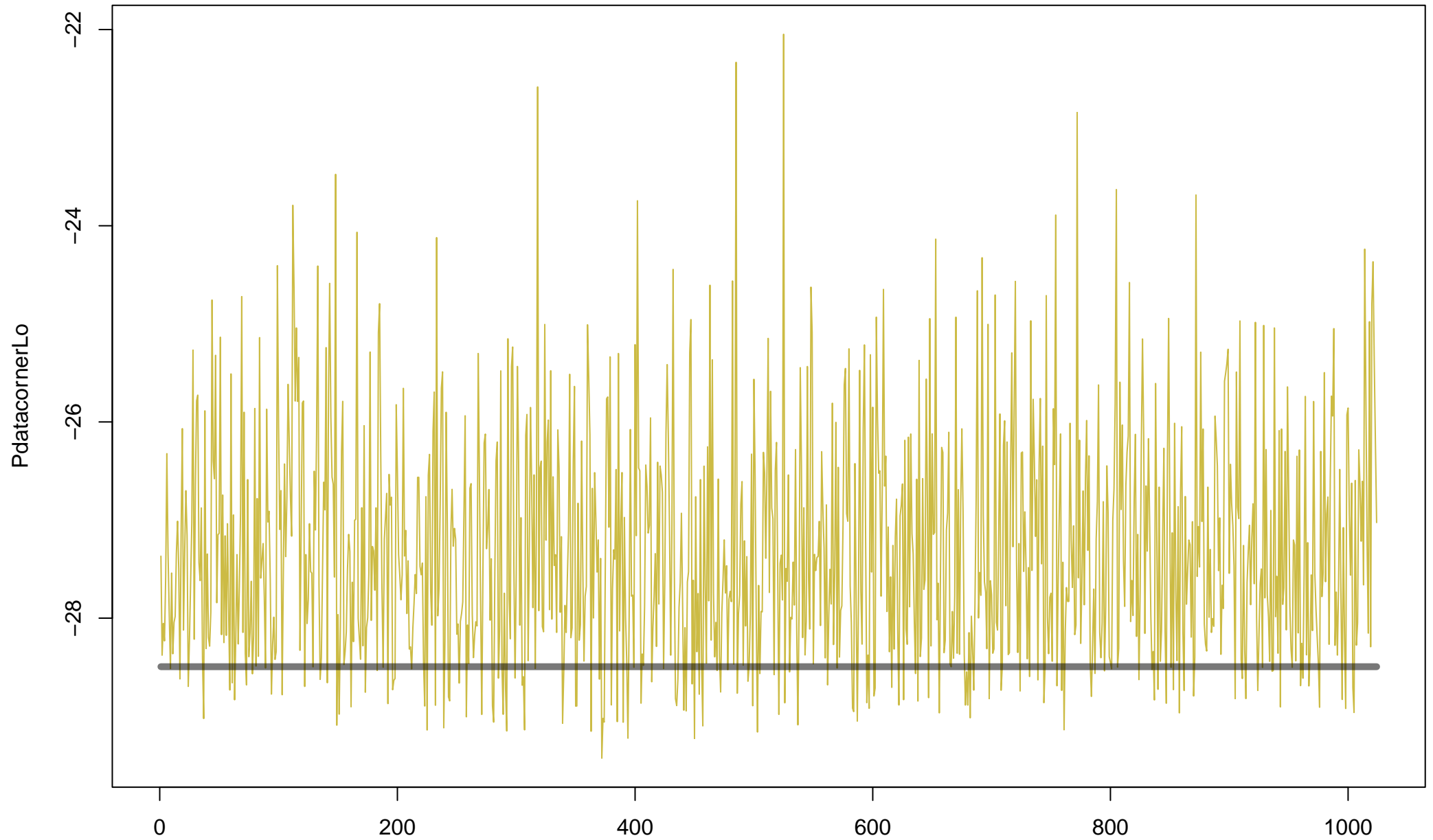
PdatacornerHi

ESS = 2.22e-16 | BMK = 0.226 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0 | rel.err: 0.122

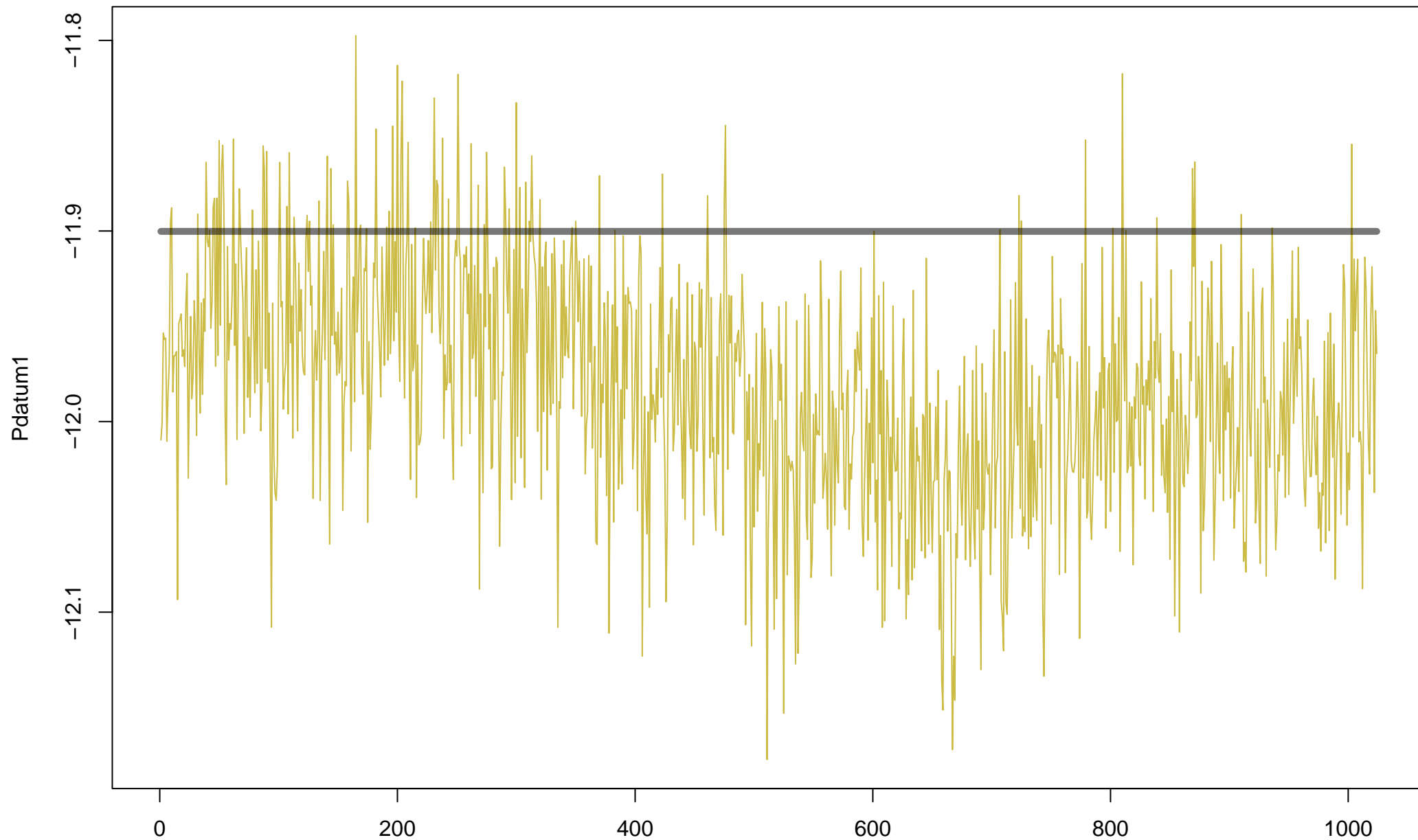


PdatacornerLo

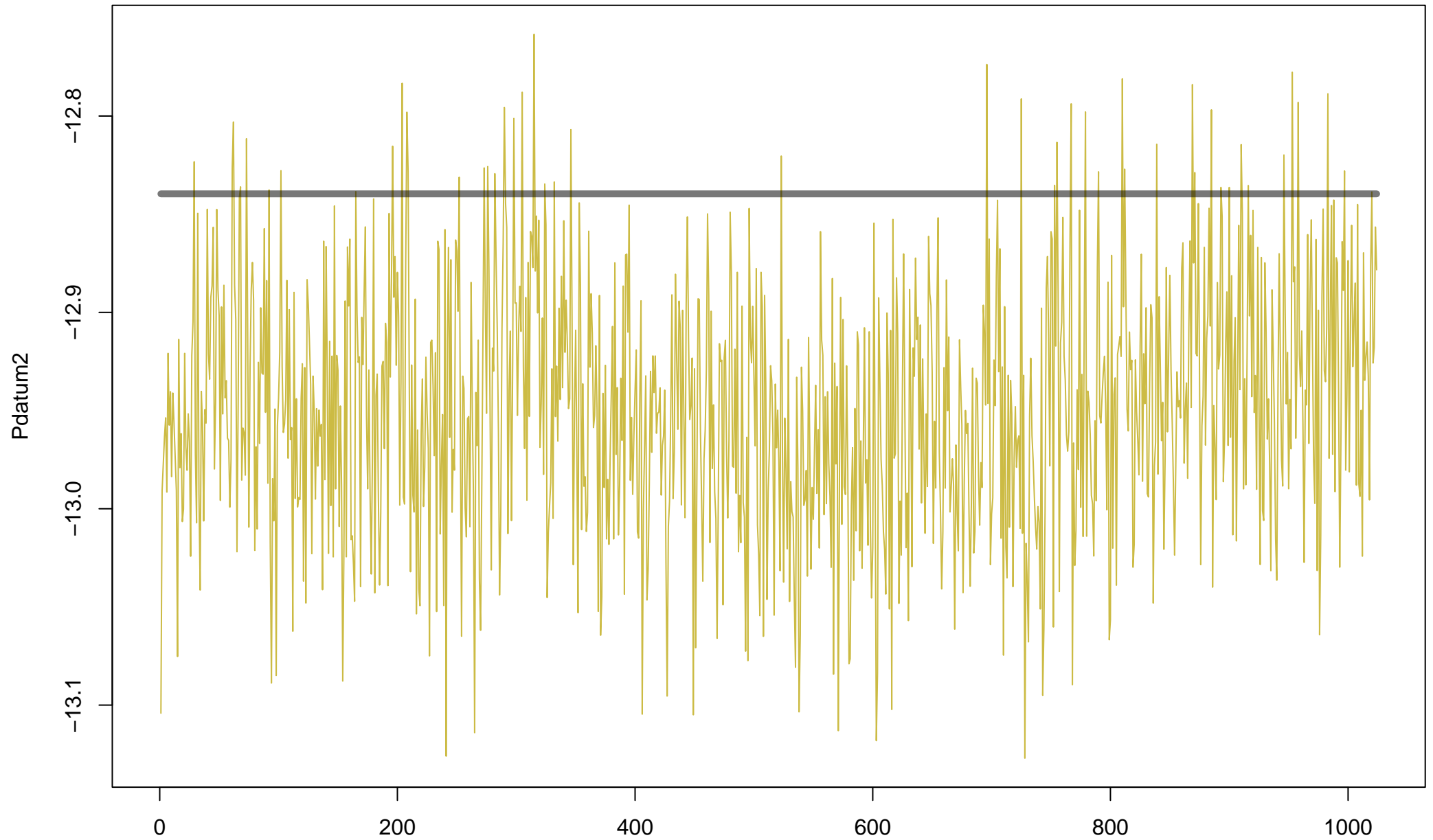
ESS = 2.22e-16 | BMK = 0.14 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0 | rel.err: 0.251



Pdatum1
ESS = 13.5 | BMK = 0.31 | MCSE(6.27) = 9.48 | stat: FALSE | burn: 0 | rel.err: -1.41

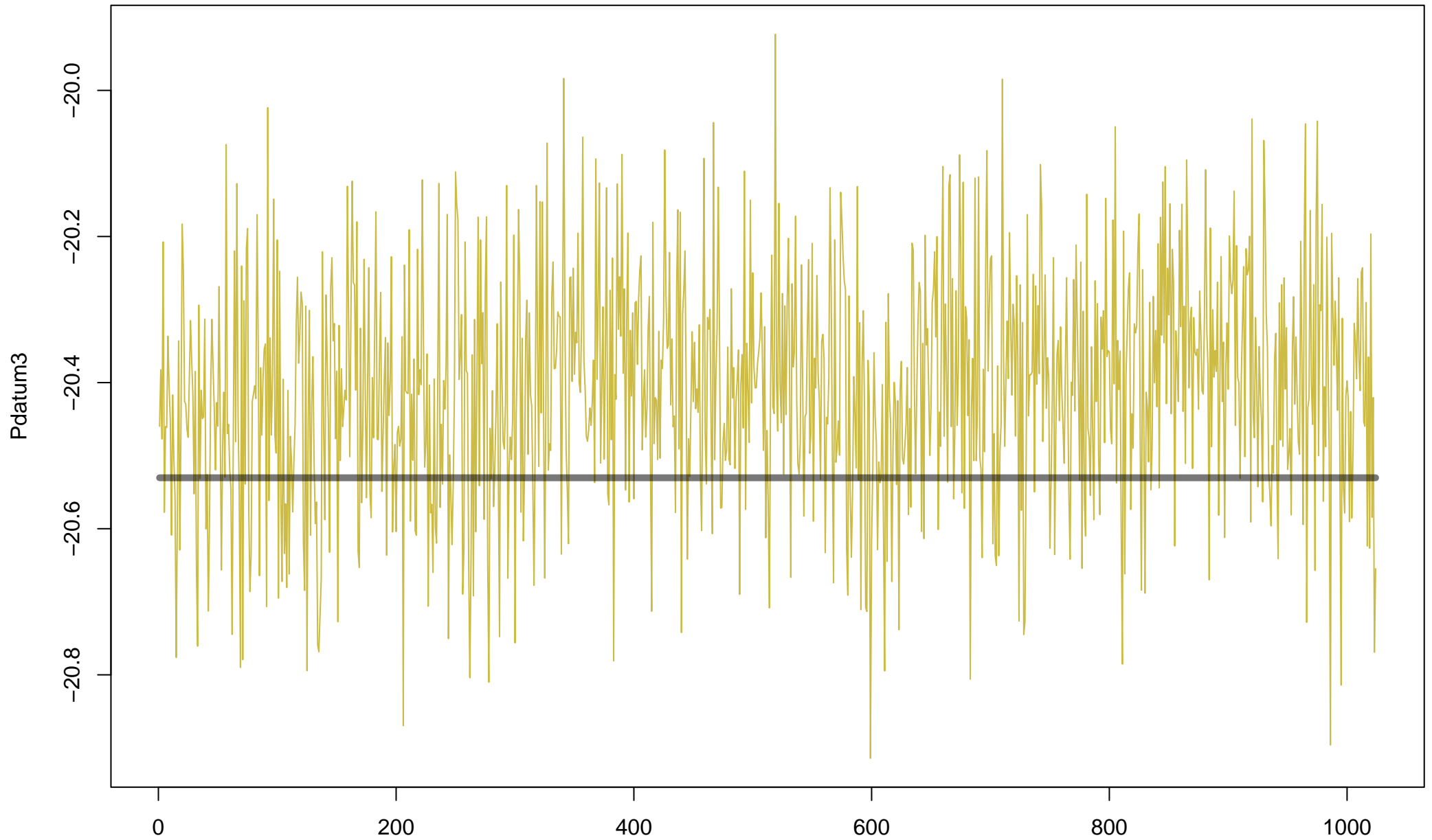


Pdatum2
ESS = 315 | BMK = 0.0324 | MCSE(6.27) = 5.65 | stat: TRUE | burn: 0 | rel.err: -1.75



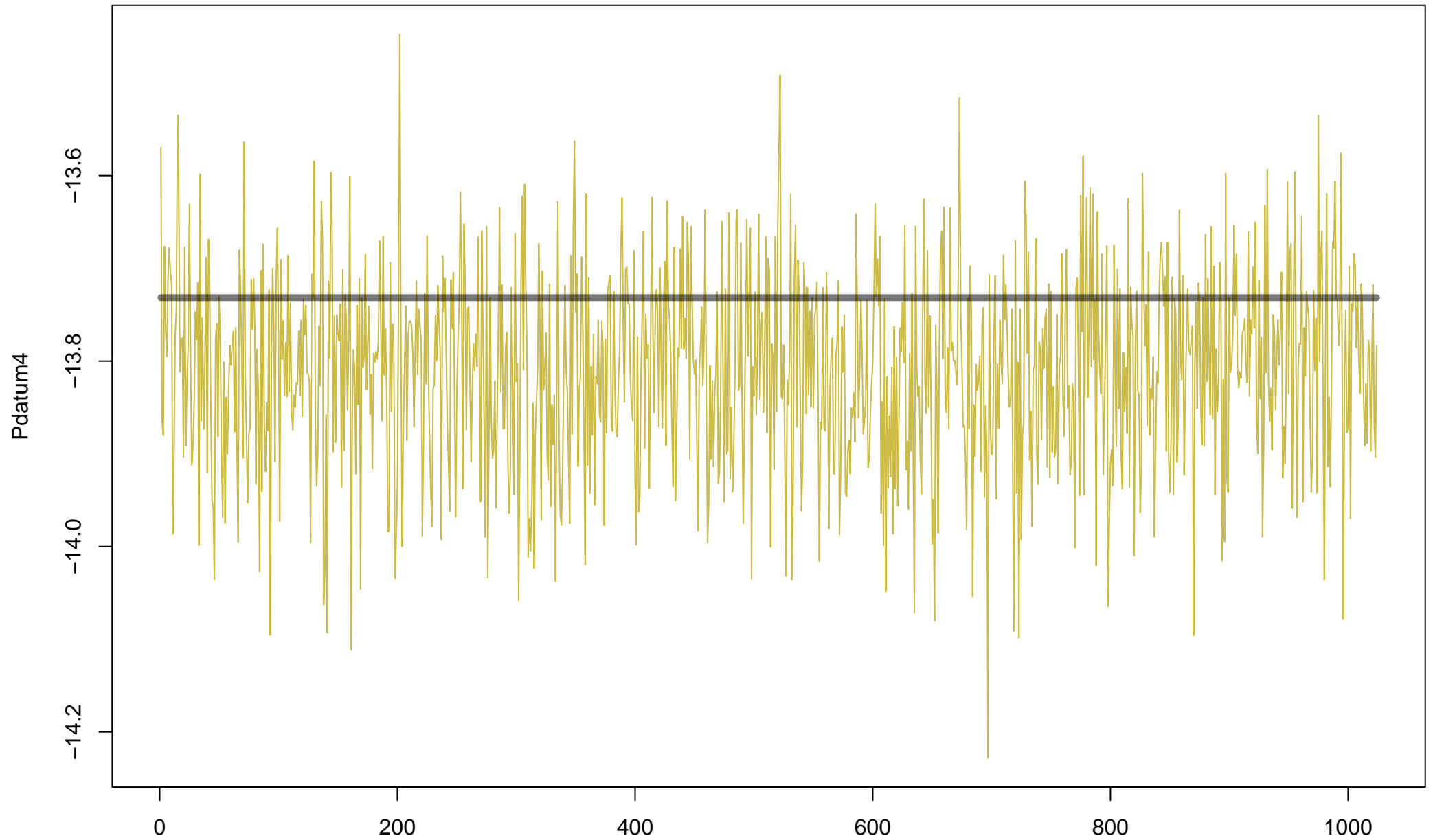
Pdatum3

ESS = 2.22e-16 | BMK = 0.0645 | MCSE(6.27) = 4.53 | stat: TRUE | burn: 0 | rel.err: 0.799



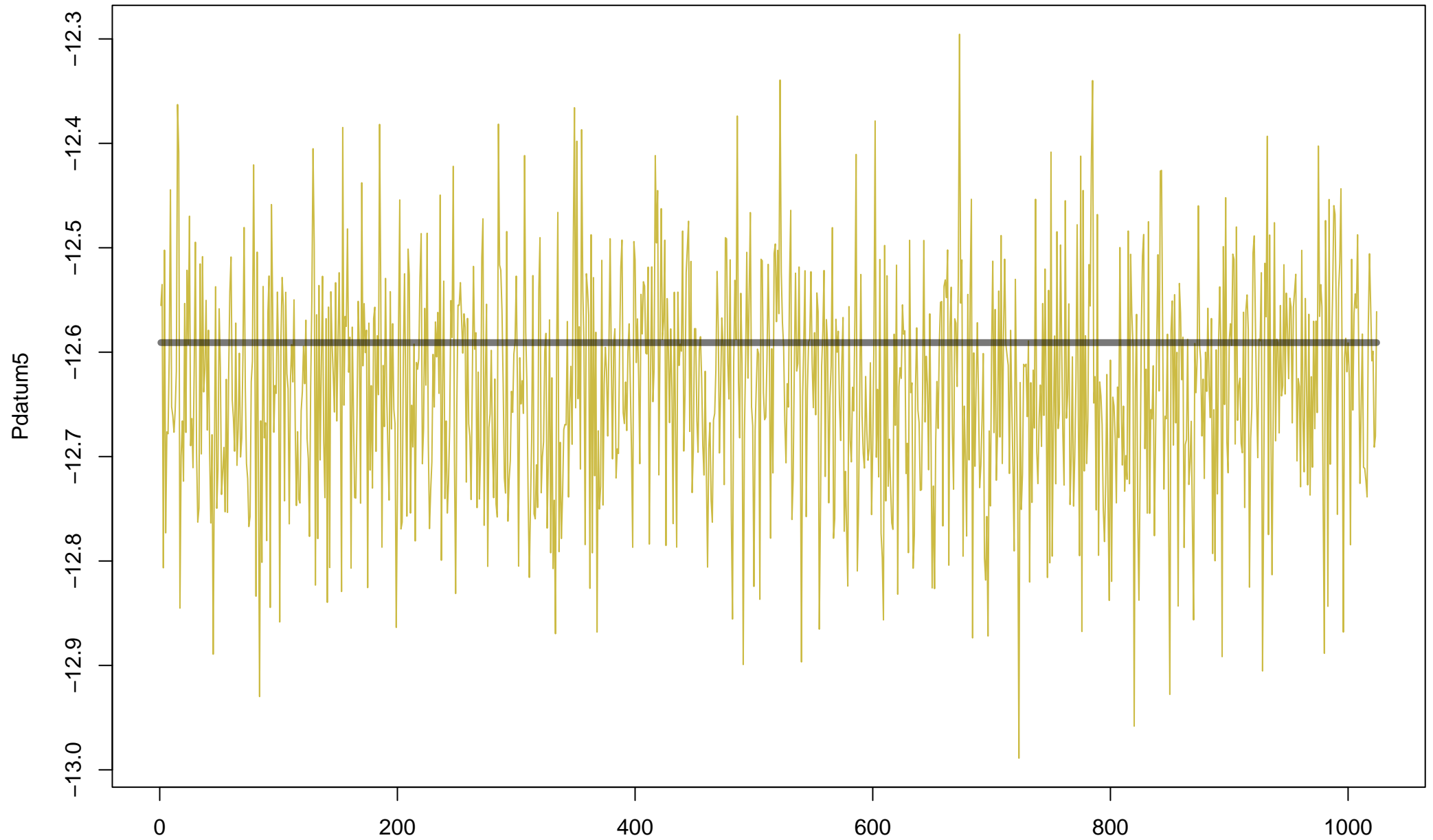
Pdatum4

ESS = 1020 | BMK = 0.0384 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0 | rel.err: -0.719



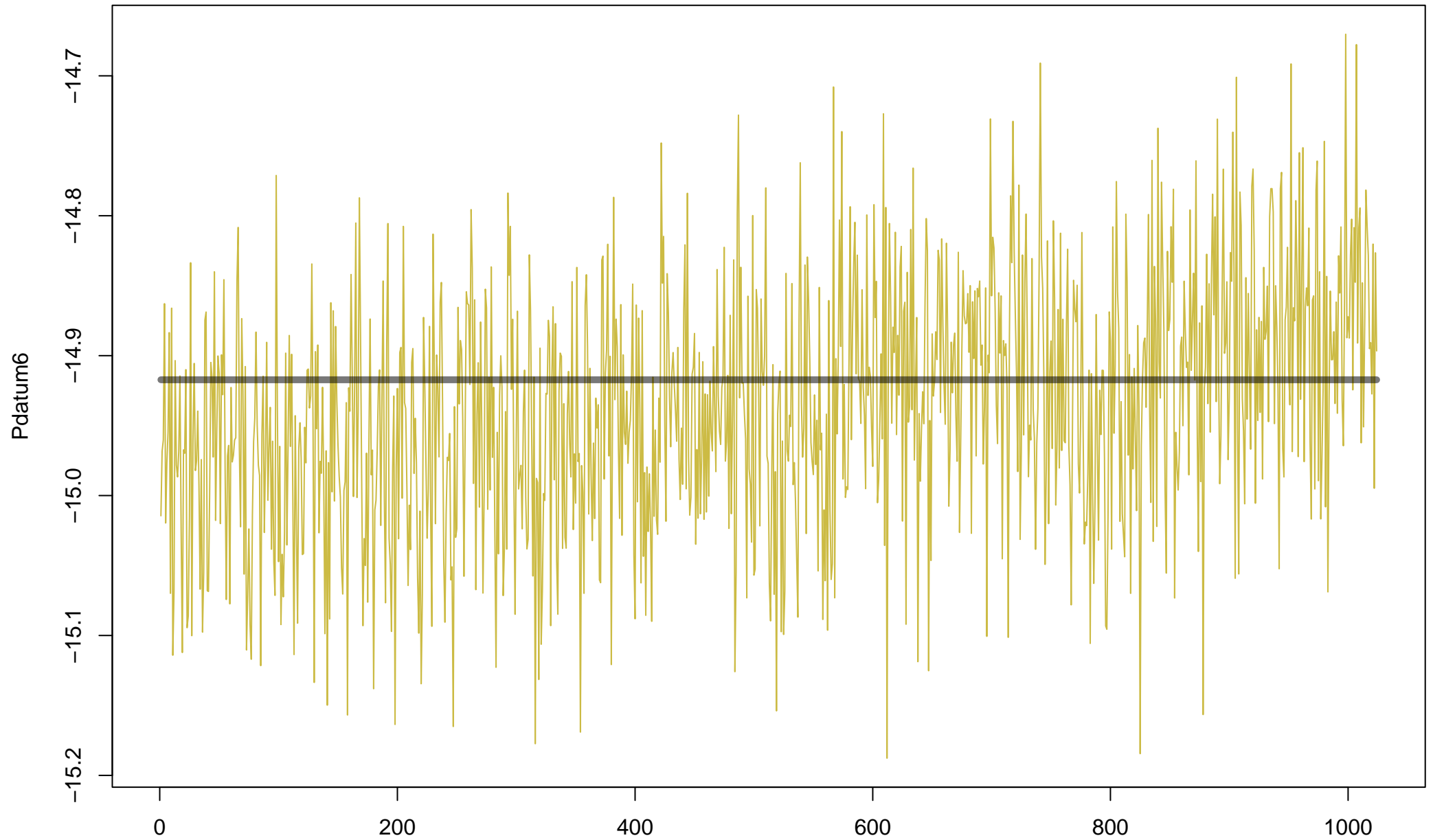
Pdatum5

ESS = 1020 | BMK = 0.0453 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0 | rel.err: -0.387



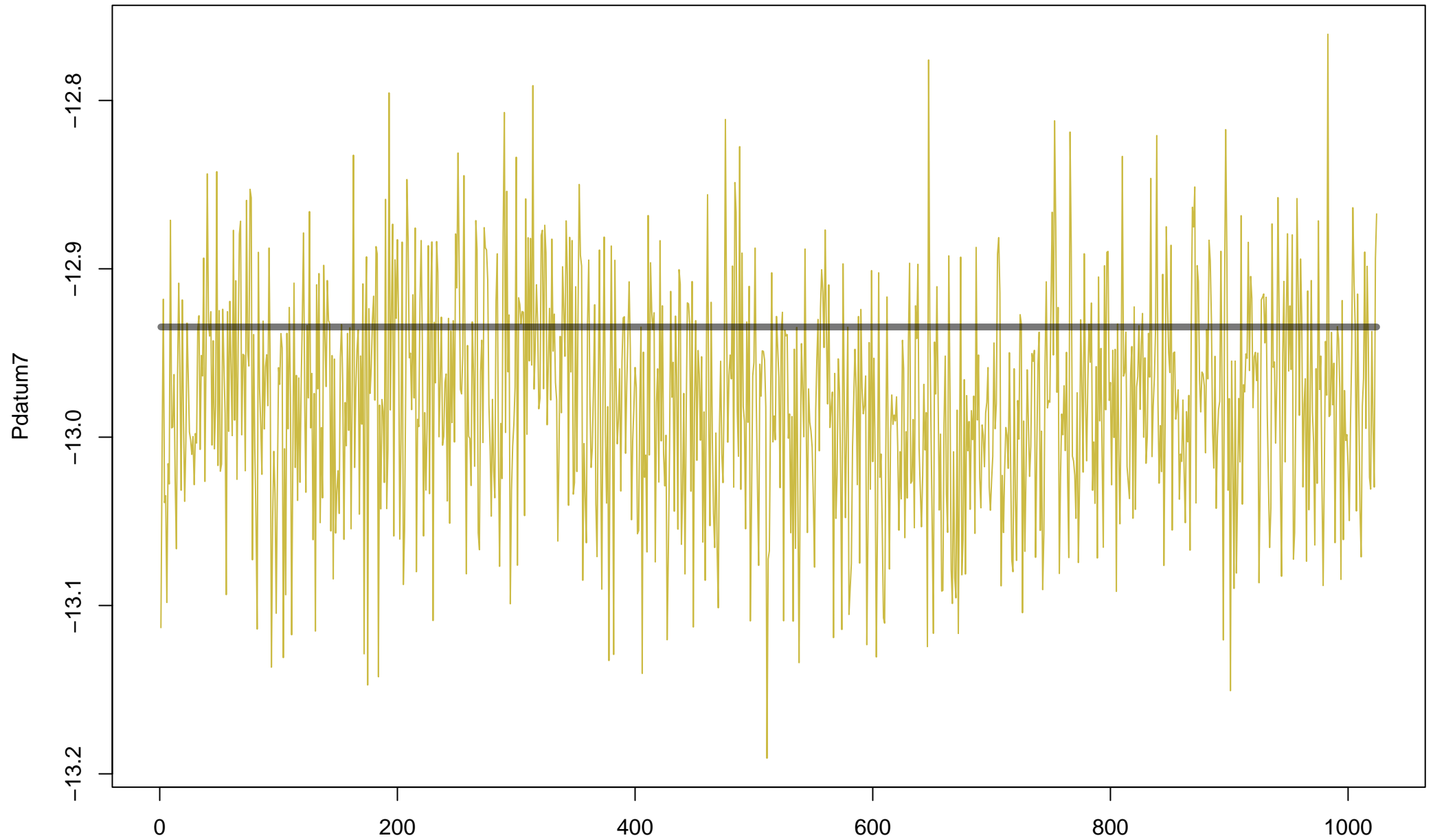
Pdatum6

ESS = 74.5 | BMK = 0.217 | MCSE(6.27) = 7.36 | stat: FALSE | burn: 0 | rel.err: -0.183

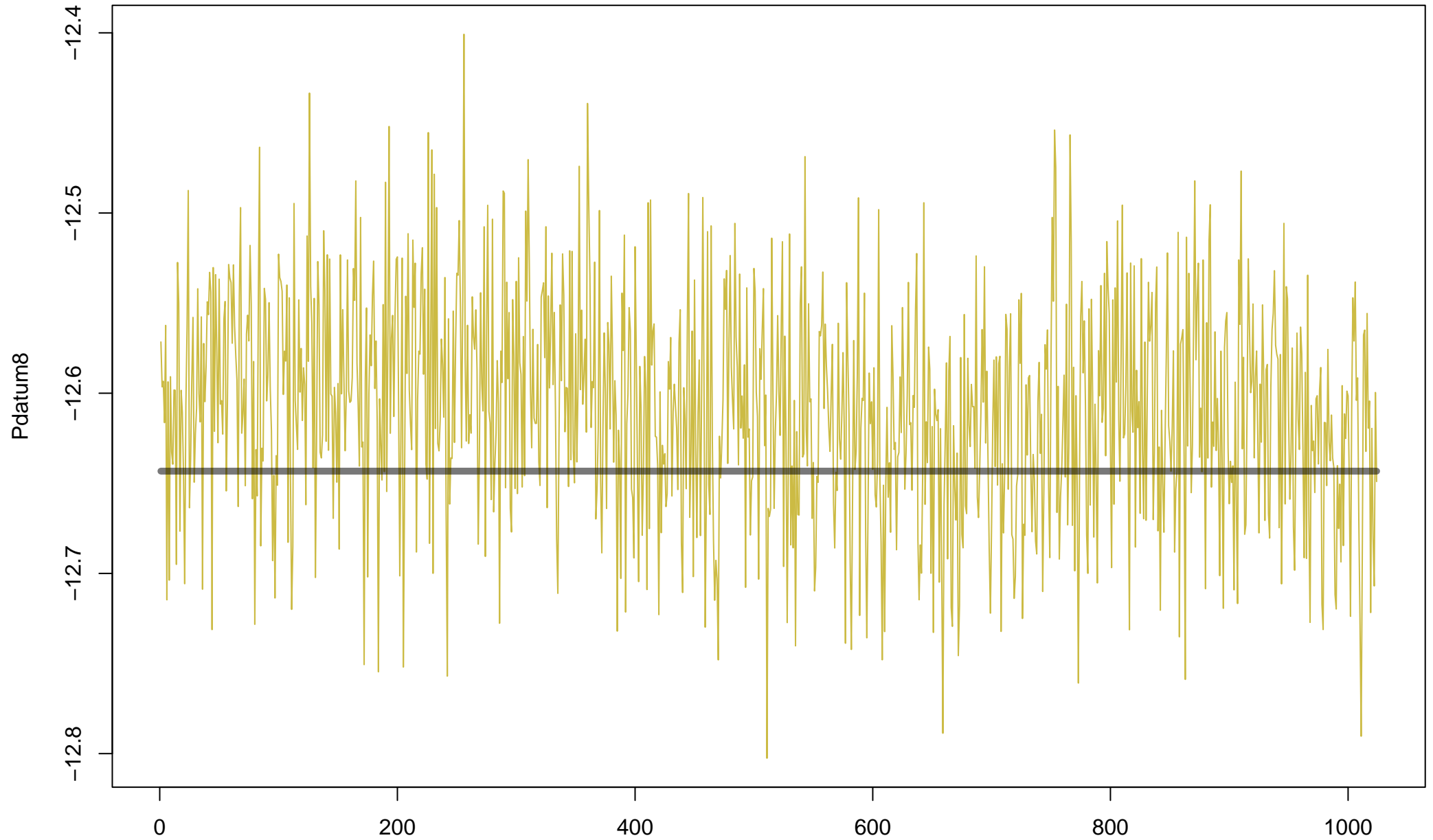


Pdatum7

ESS = 892 | BMK = 0.0852 | MCSE(6.27) = 4.64 | stat: TRUE | burn: 0 | rel.err: -0.655

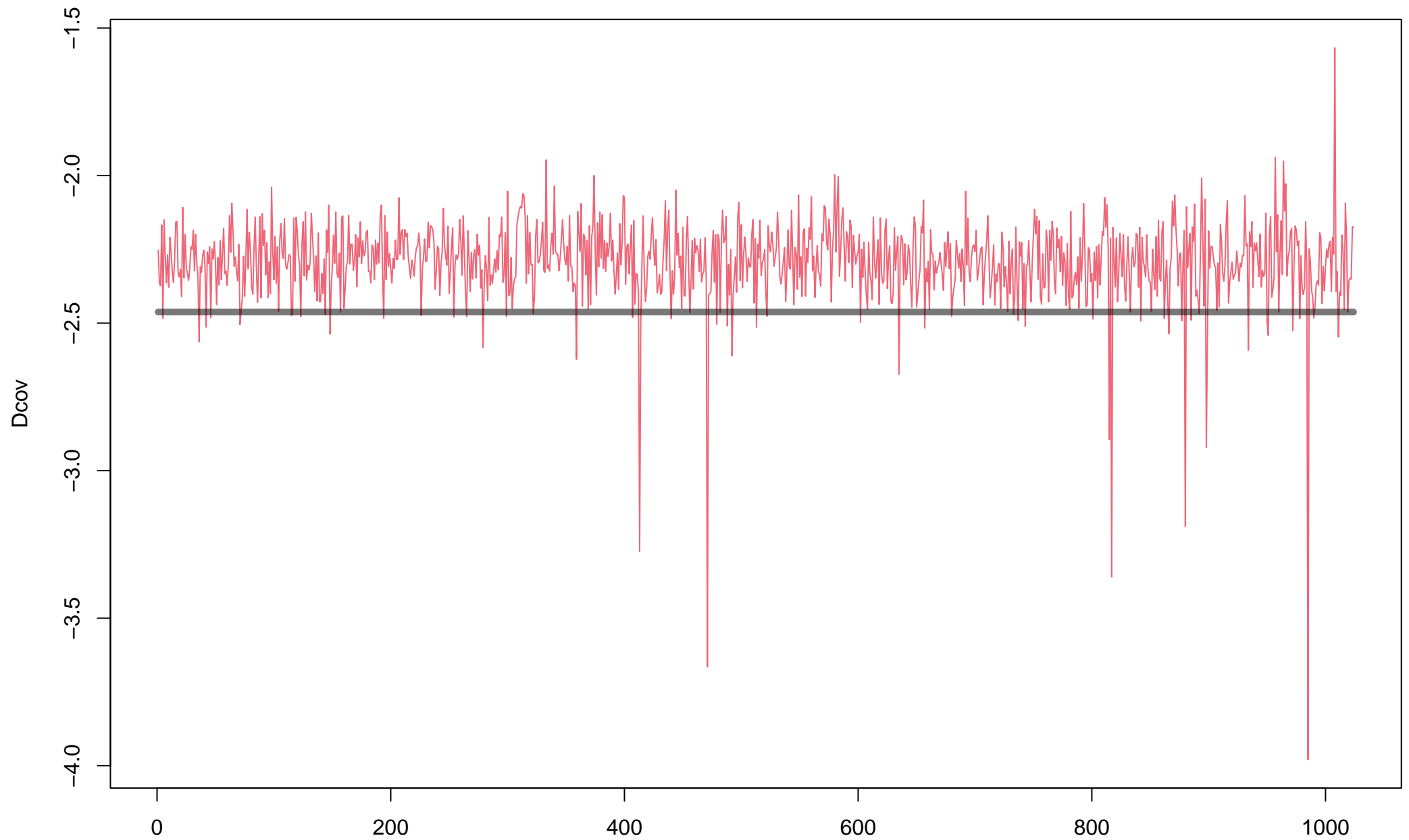


Pdatum8
ESS = 210 | BMK = 0.131 | MCSE(6.27) = 5.15 | stat: FALSE | burn: 0 | rel.err: 0.587

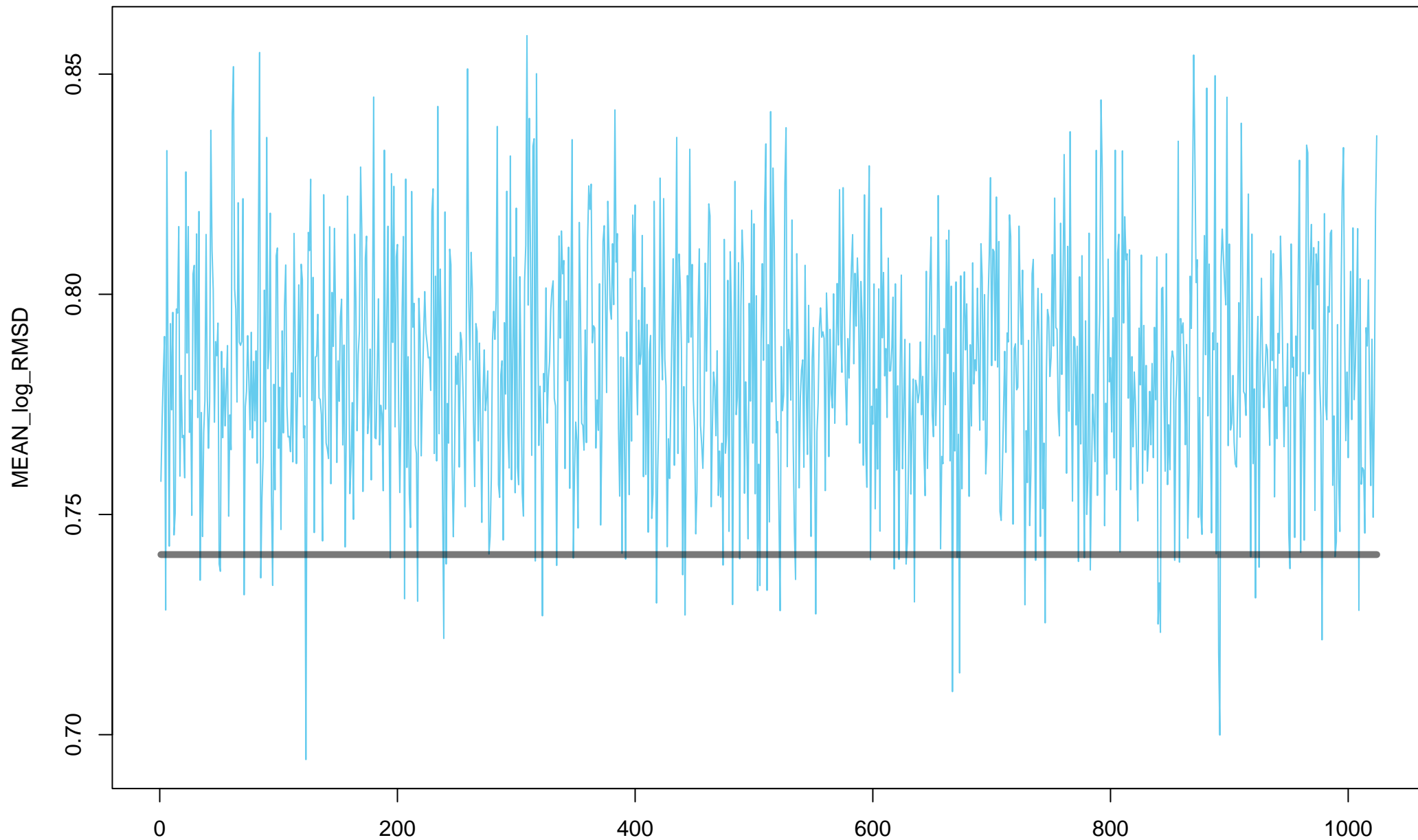


Dcov

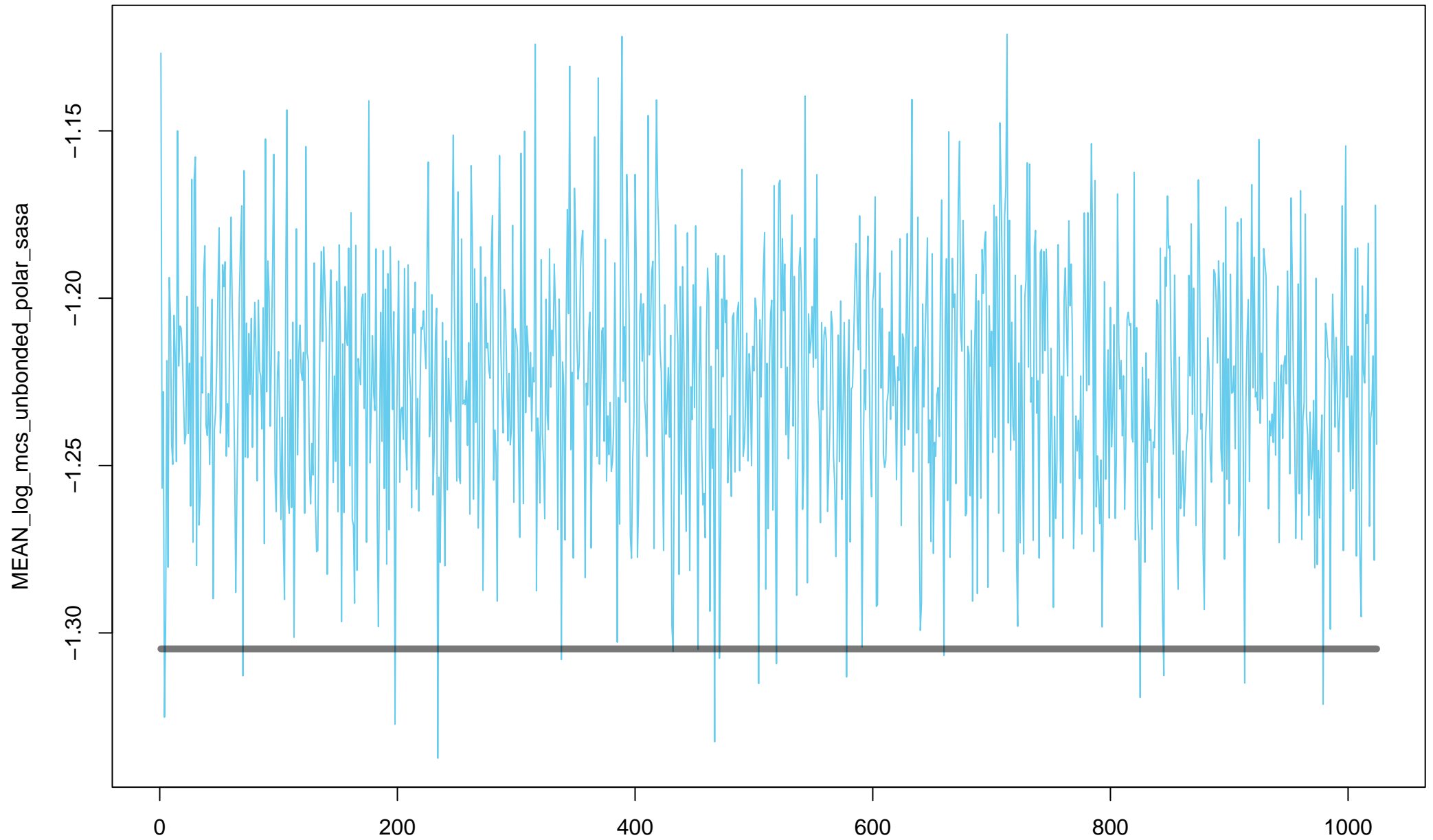
ESS = 815 | BMK = 0.0981 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0 | rel.err: -1.14



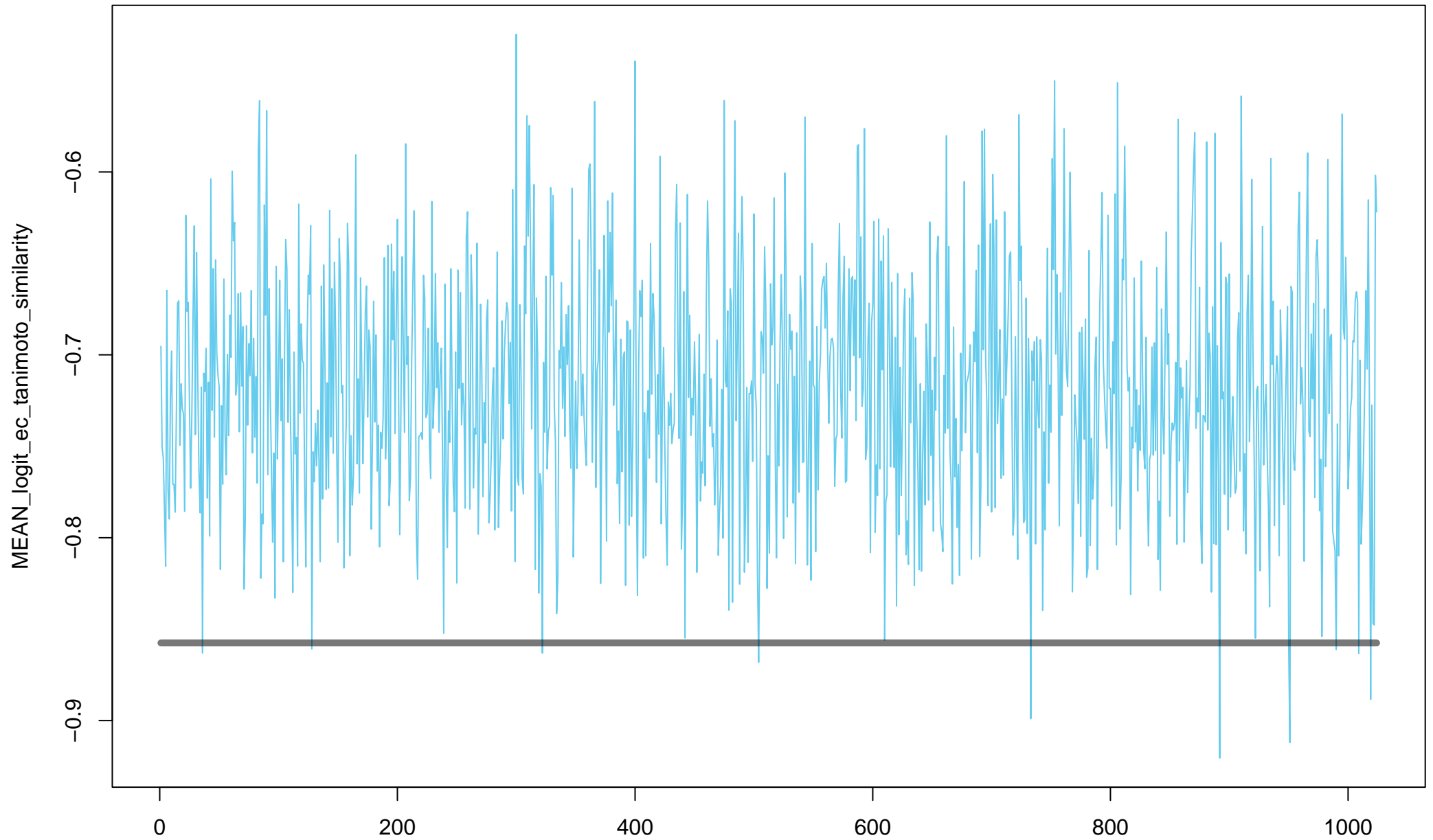
MEAN_log_RMSD
ESS = 1020 | BMK = 0.0548 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0 | rel.err: 1.62



MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0519 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0 | rel.err: 2.26

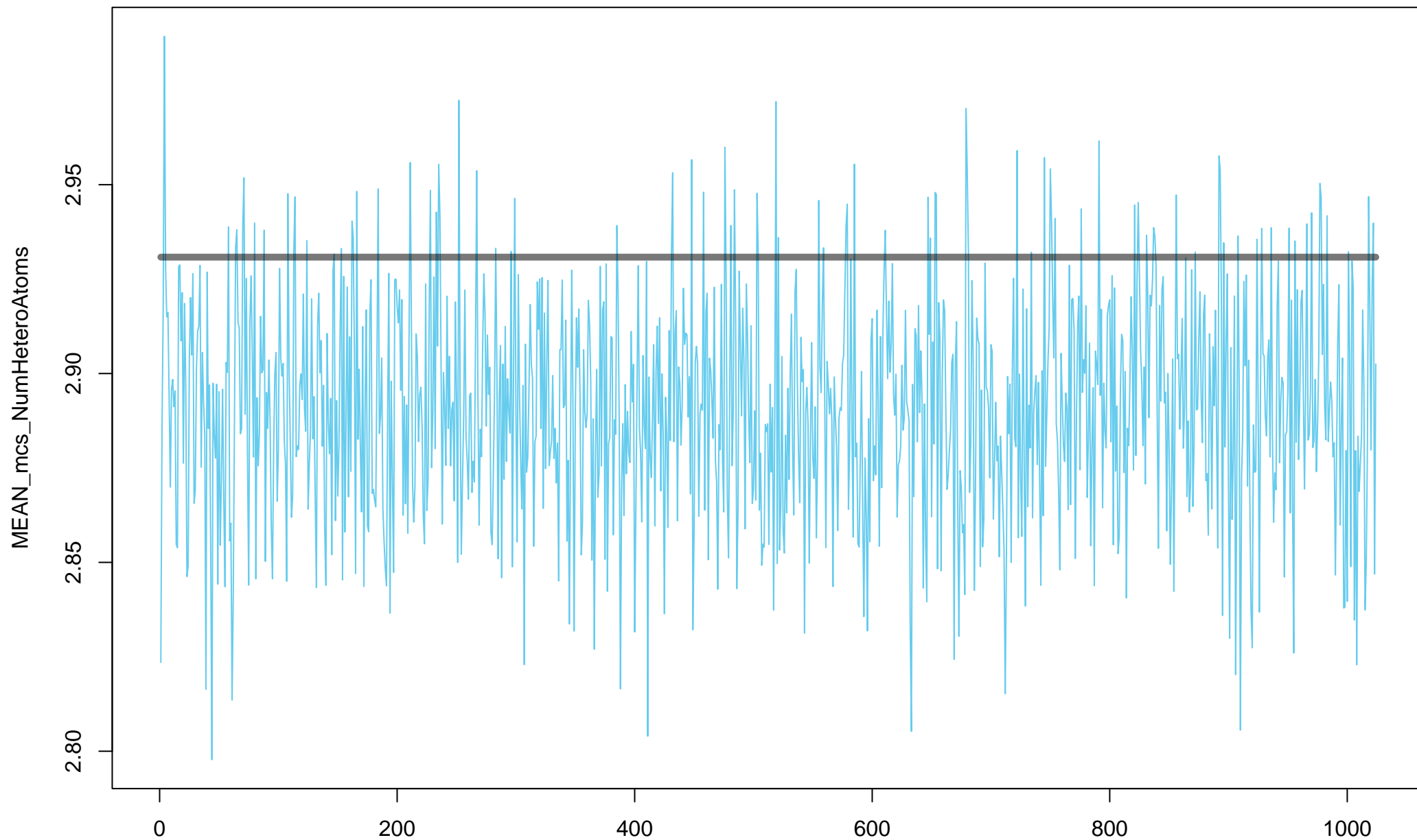


MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0571 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0 | rel.err: 2.18

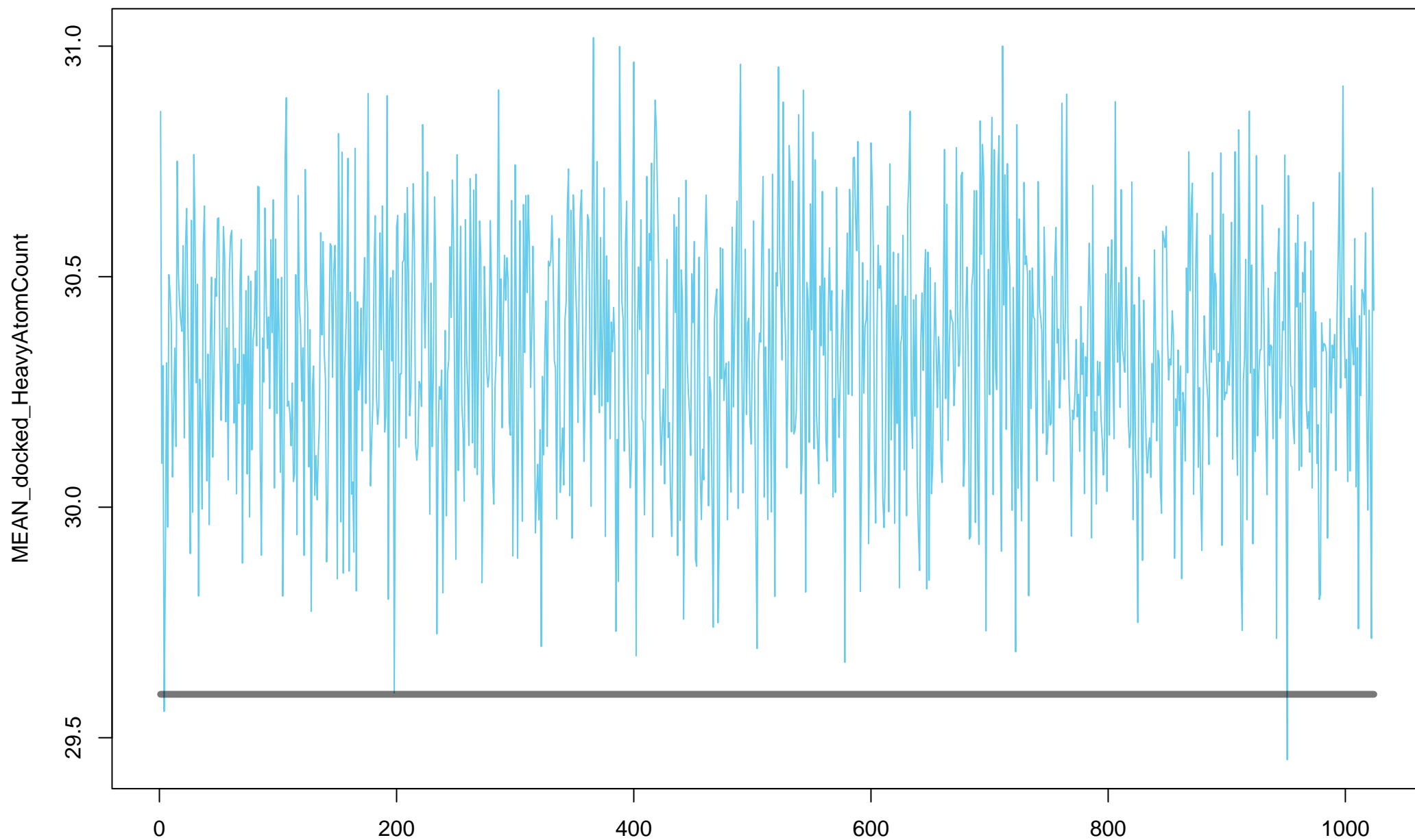


MEAN_mcs_NumHeteroAtoms

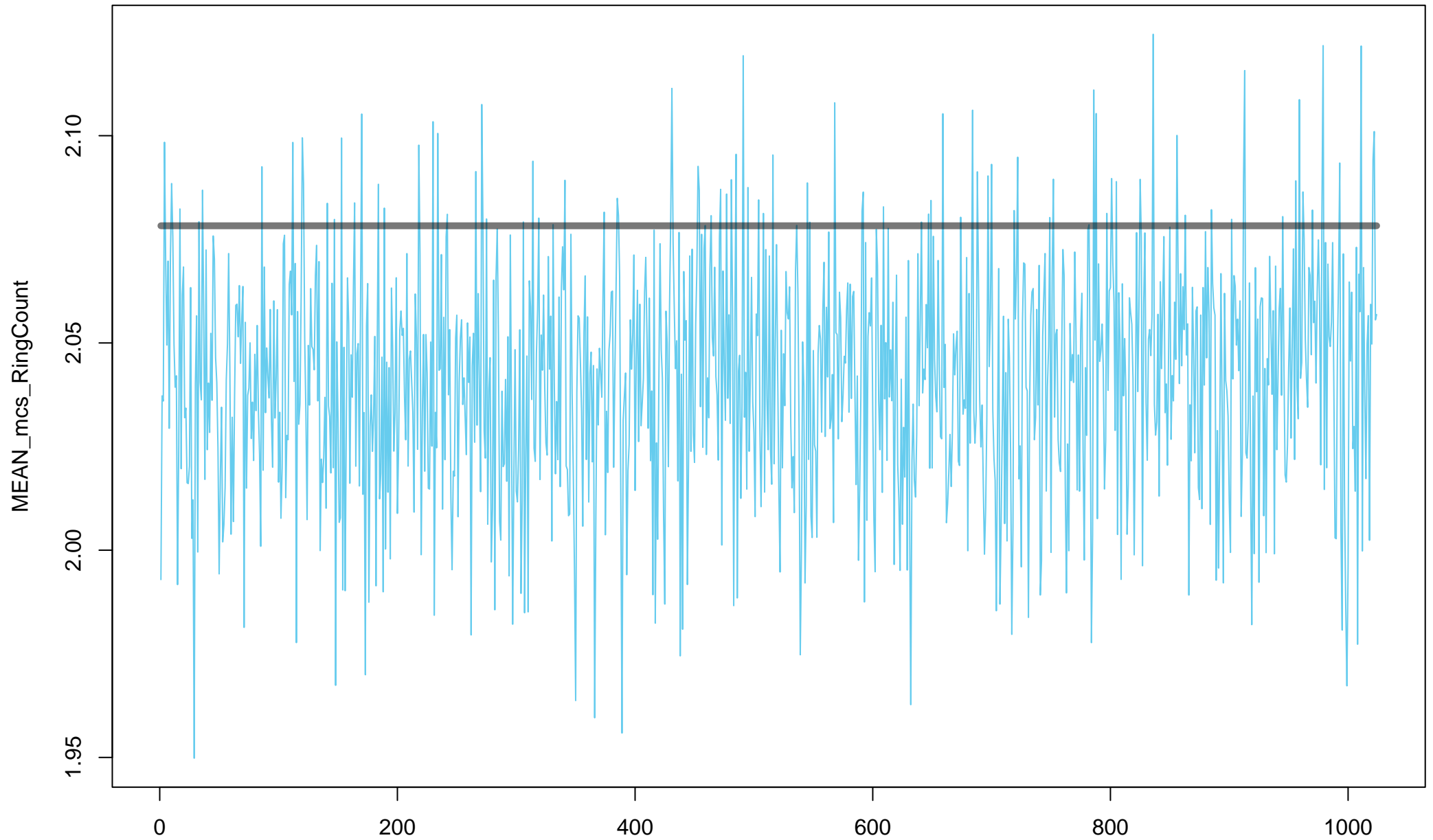
ESS = 1020 | BMK = 0.0366 | MCSE(6.27) = 3.33 | stat: TRUE | burn: 0 | rel.err: -1.37



MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0593 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0 | rel.err: 2.83

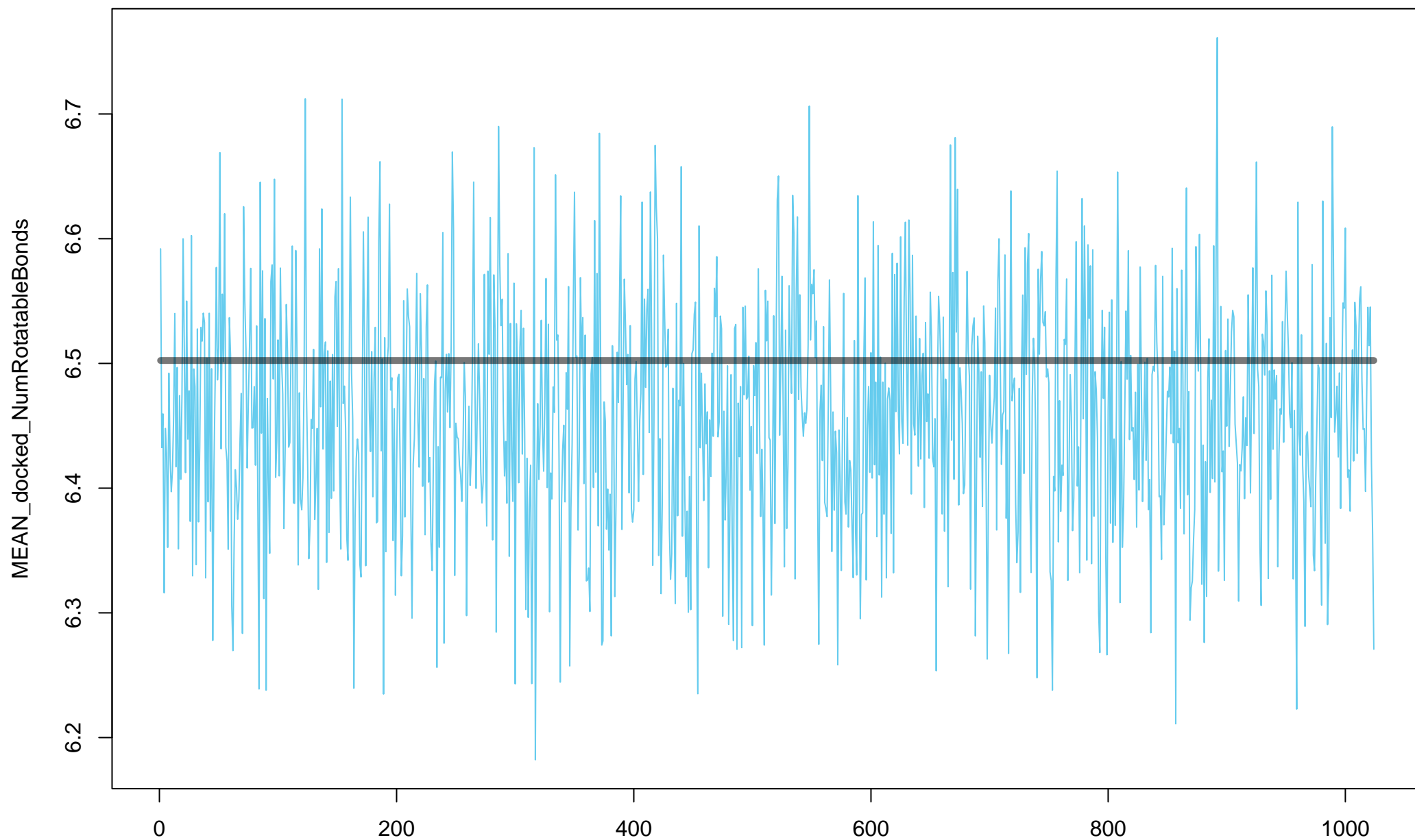


MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.058 | MCSE(6.27) = 3.21 | stat: TRUE | burn: 0 | rel.err: -1.32

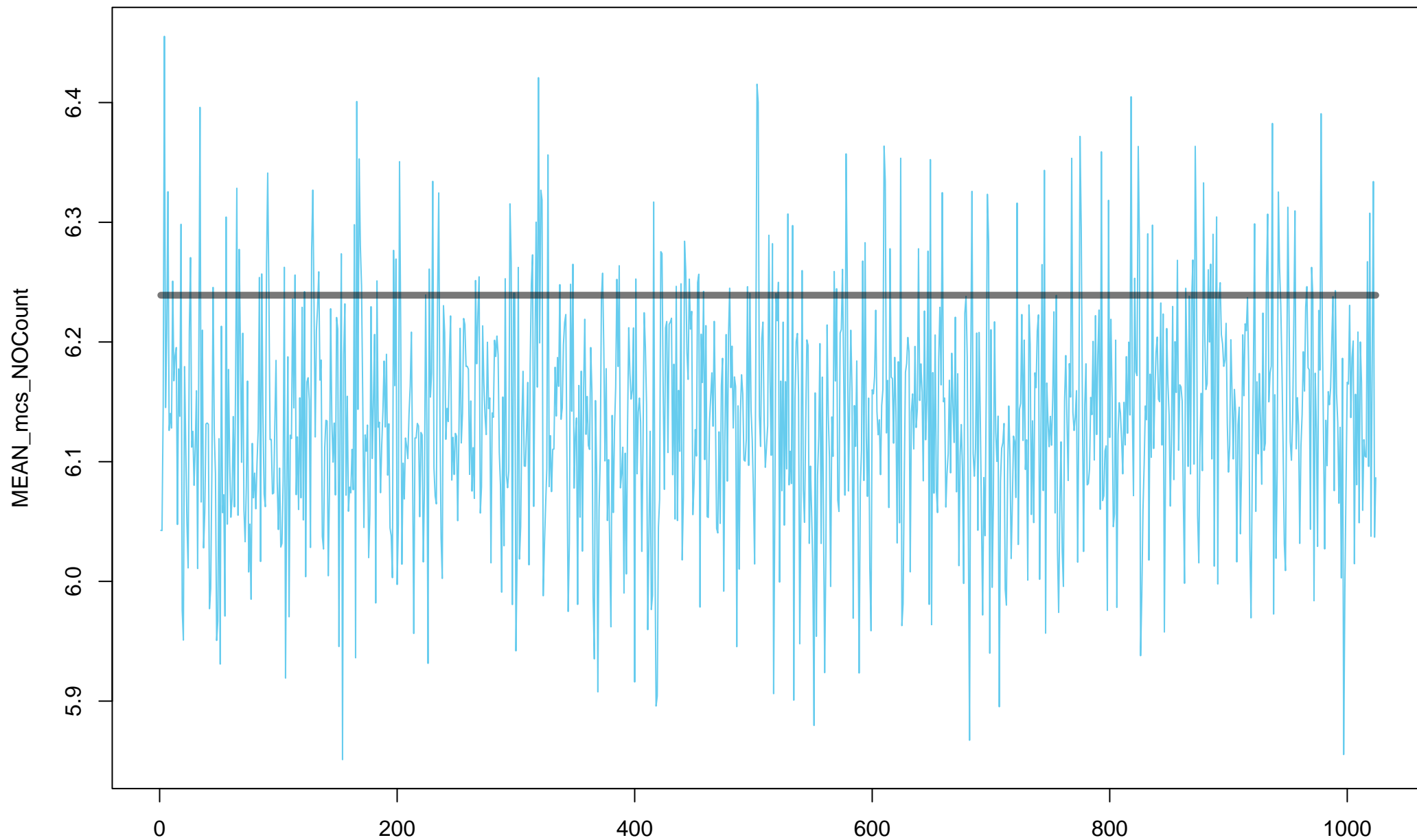


MEAN_docked_NumRotatableBonds

ESS = 1020 | BMK = 0.0455 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0 | rel.err: -0.48

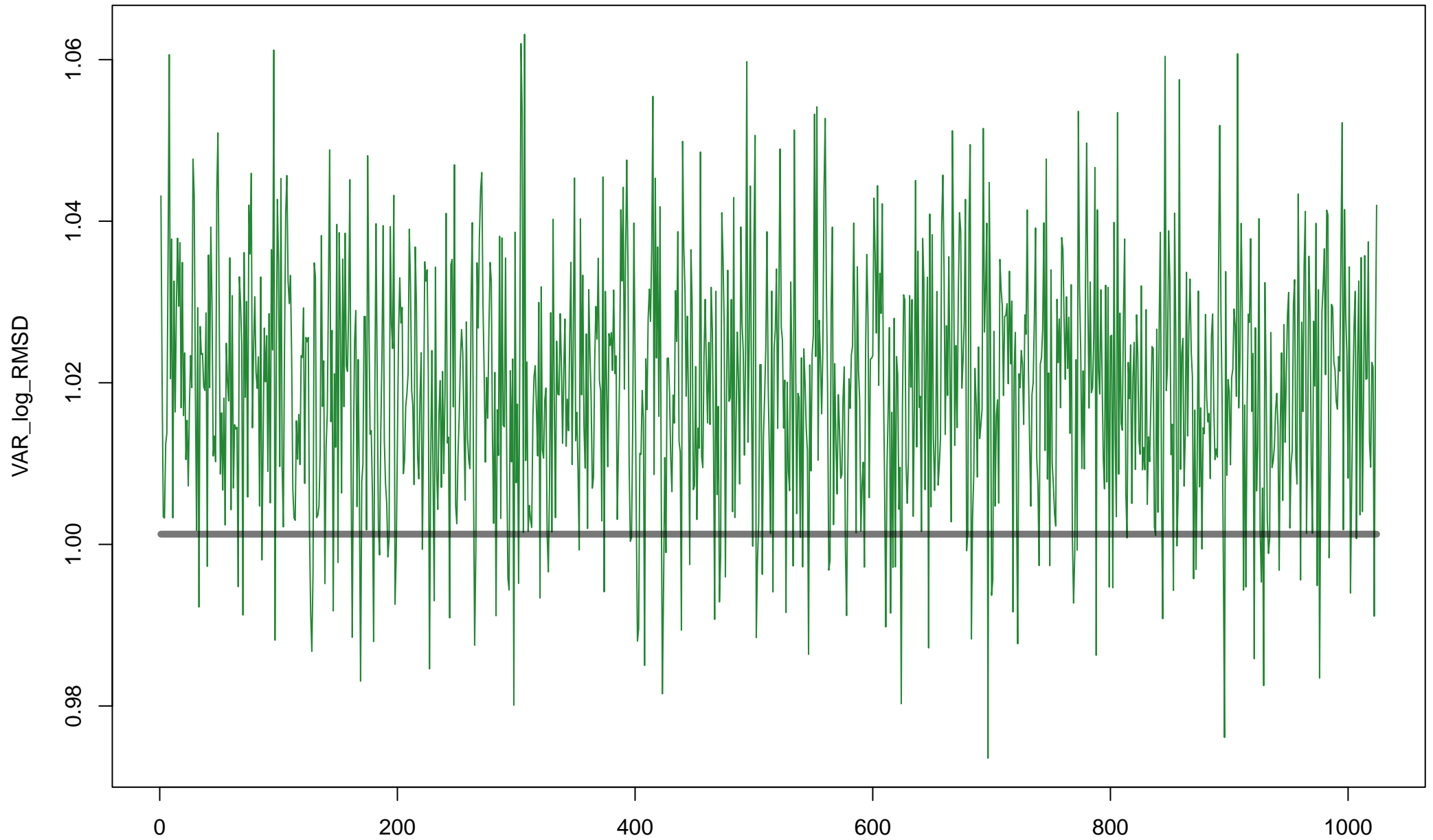


MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0649 | MCSE(6.27) = 3.45 | stat: TRUE | burn: 0 | rel.err: -1.08



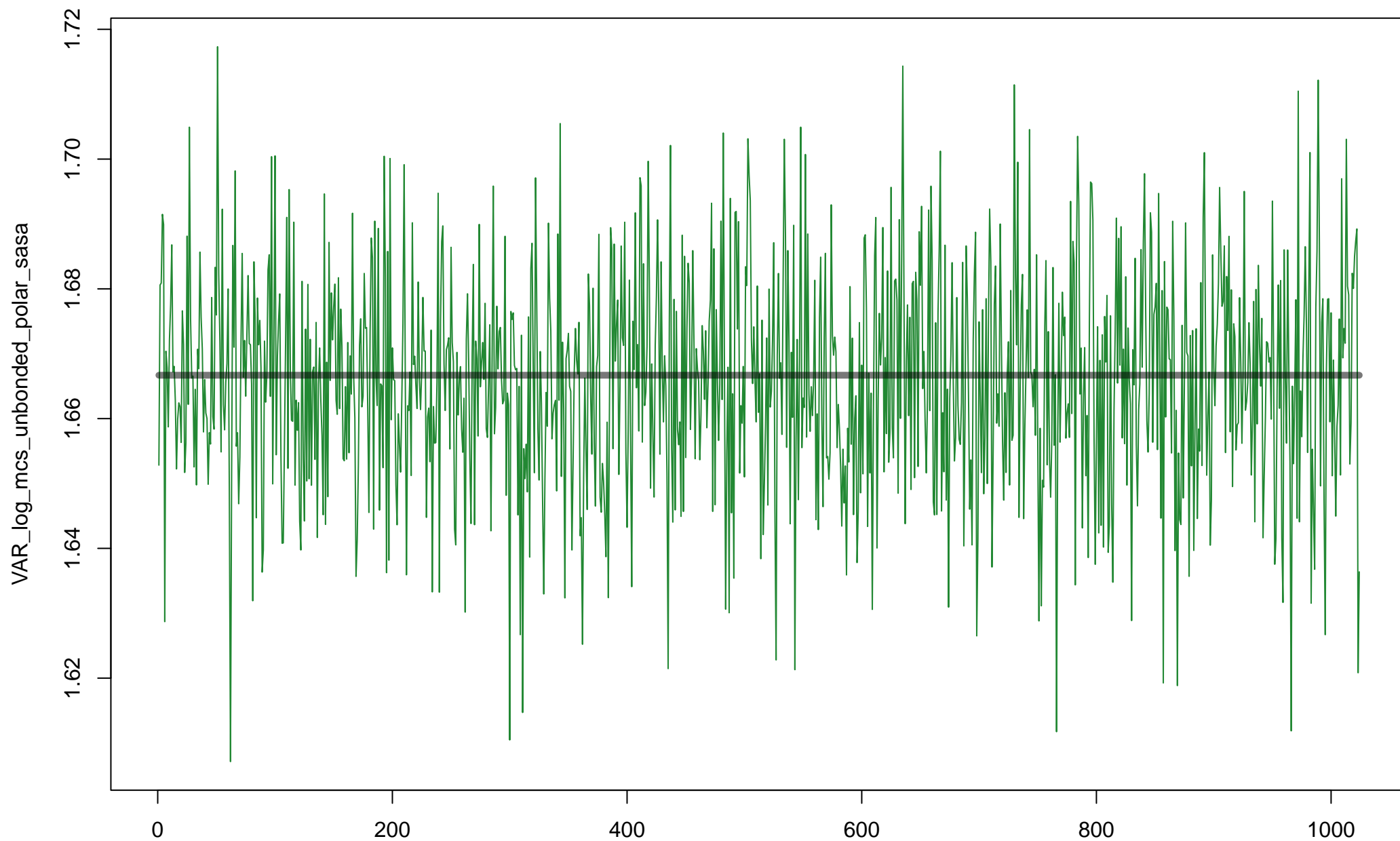
VAR_log_RMSD

ESS = 1020 | BMK = 0.0451 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | rel.err: 1.21

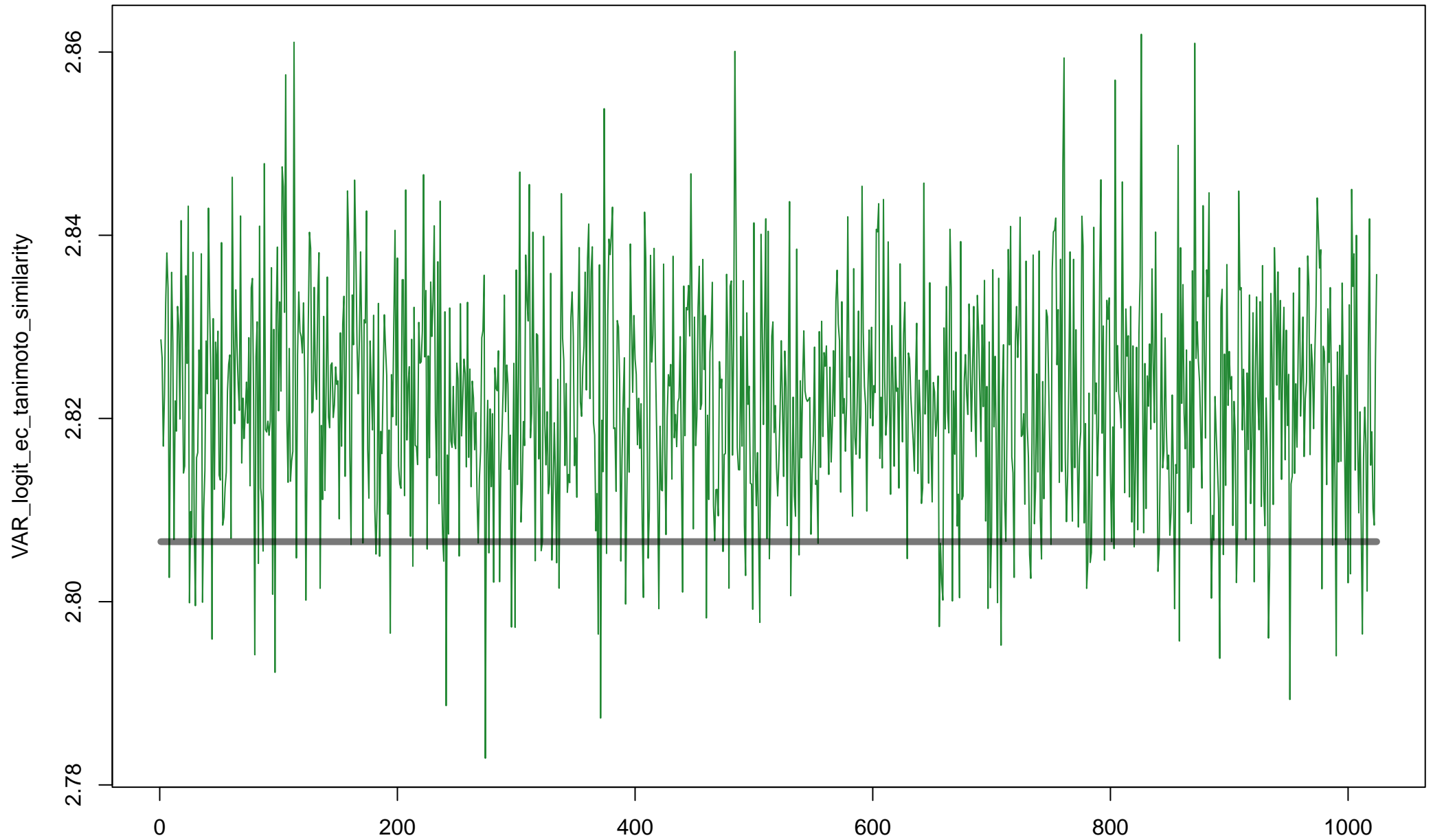


VAR_log_mcs_unbonded_polar_sasa

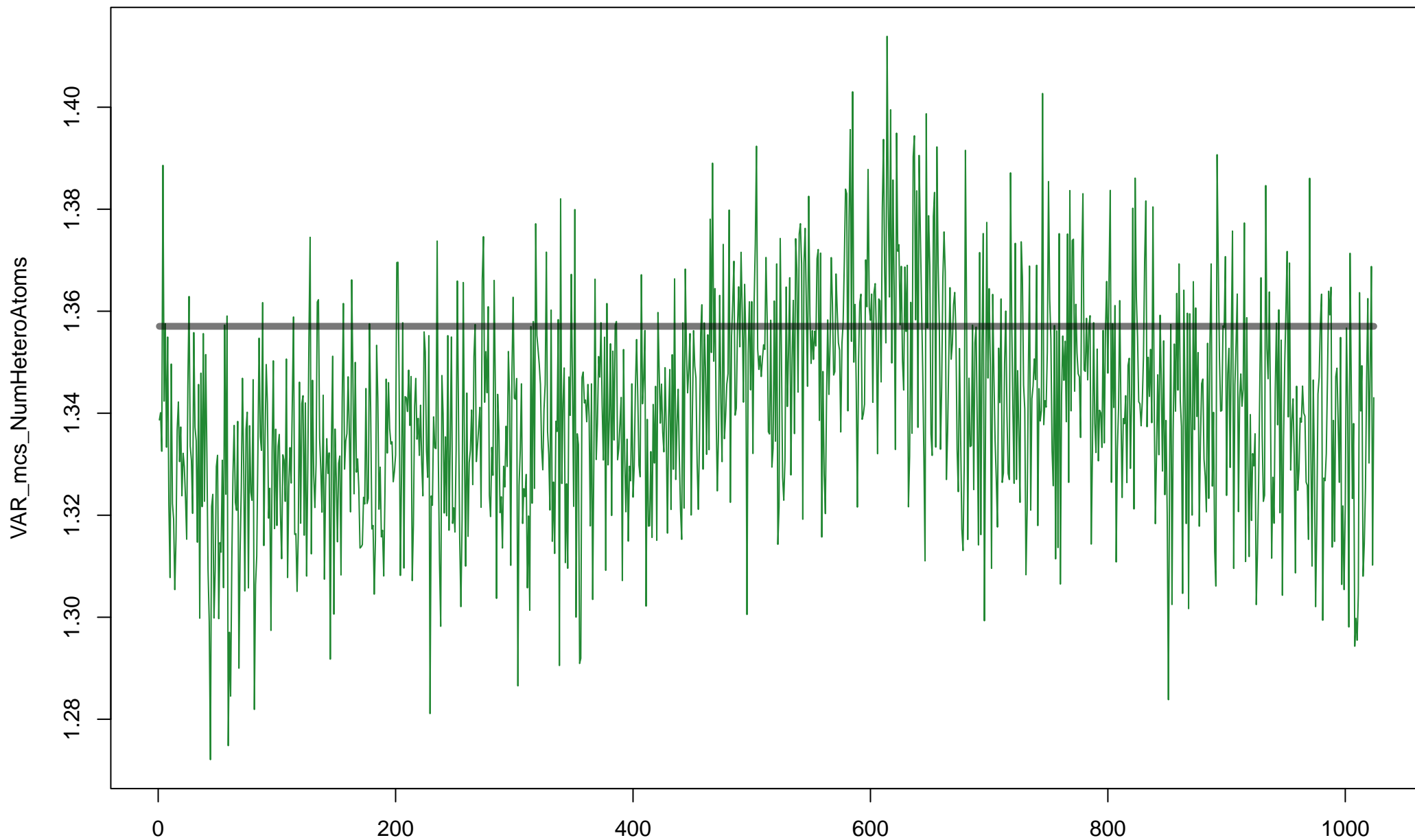
ESS = 1020 | BMK = 0.0764 | MCSE(6.27) = 3.42 | stat: TRUE | burn: 0 | rel.err: -0.0435



VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0421 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | rel.err: 1.31

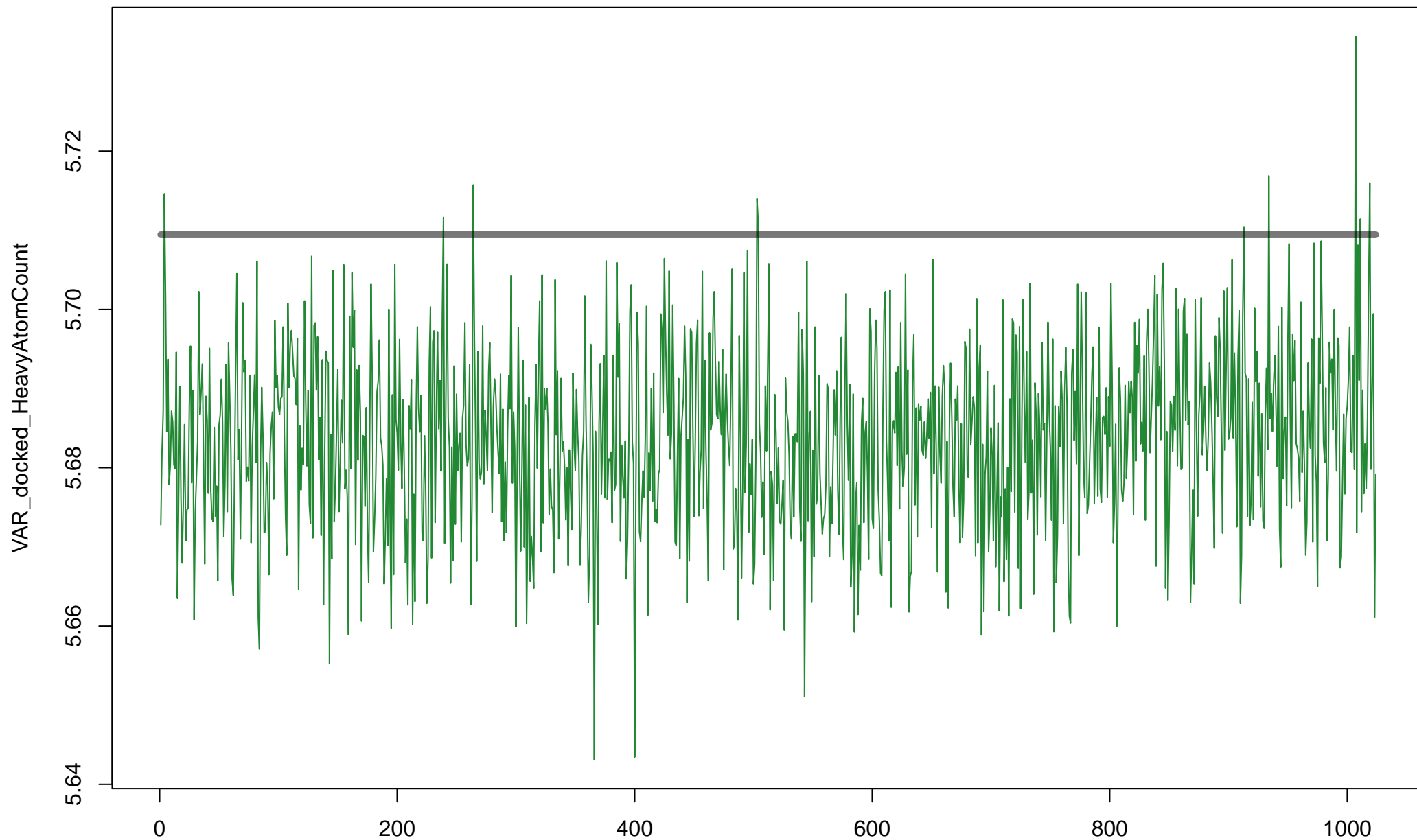


VAR_mcs_NumHeteroAtoms
ESS = 63.8 | BMK = 0.204 | MCSE(6.27) = 8.64 | stat: FALSE | burn: 0 | rel.err: -0.765

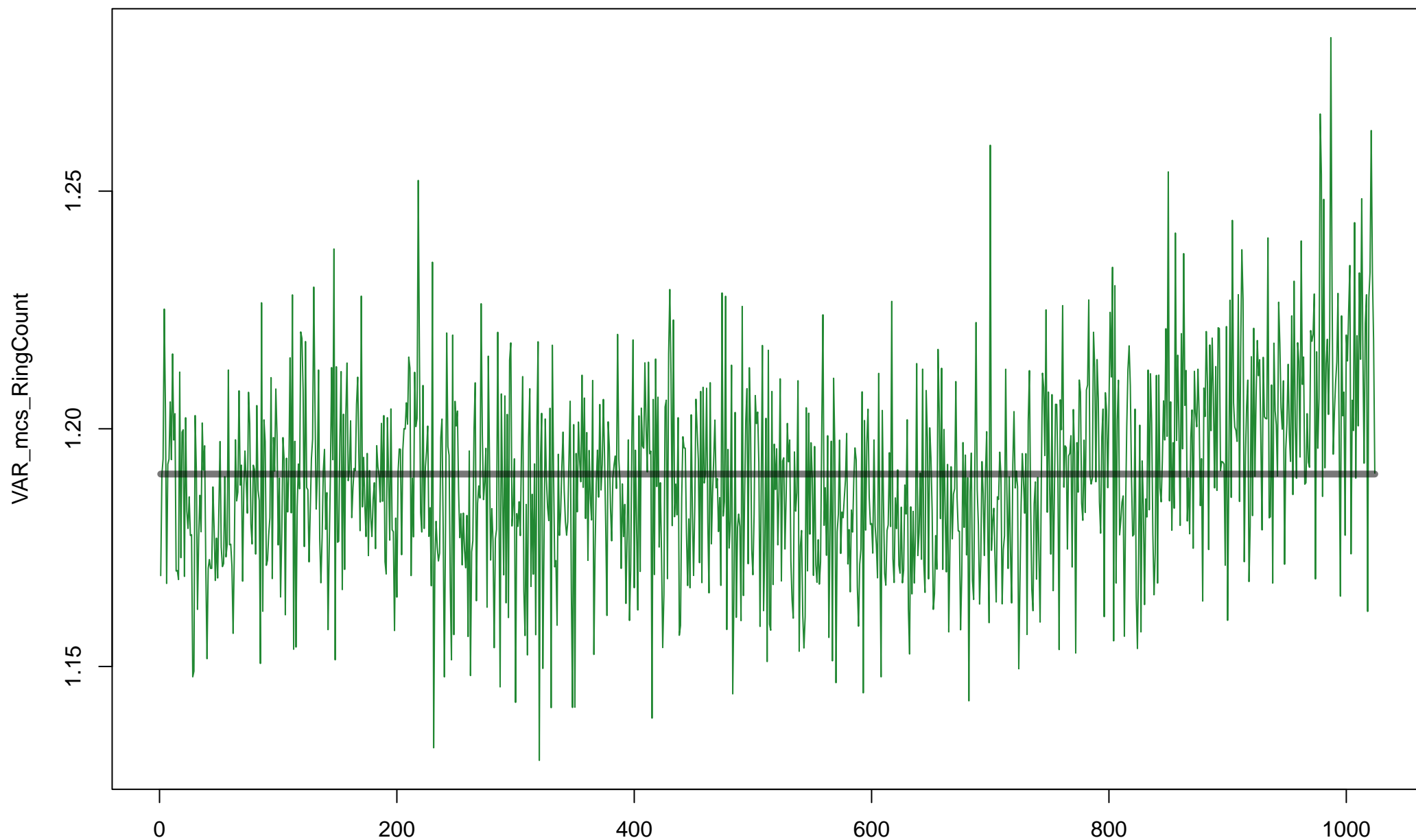


VAR_docked_HeavyAtomCount

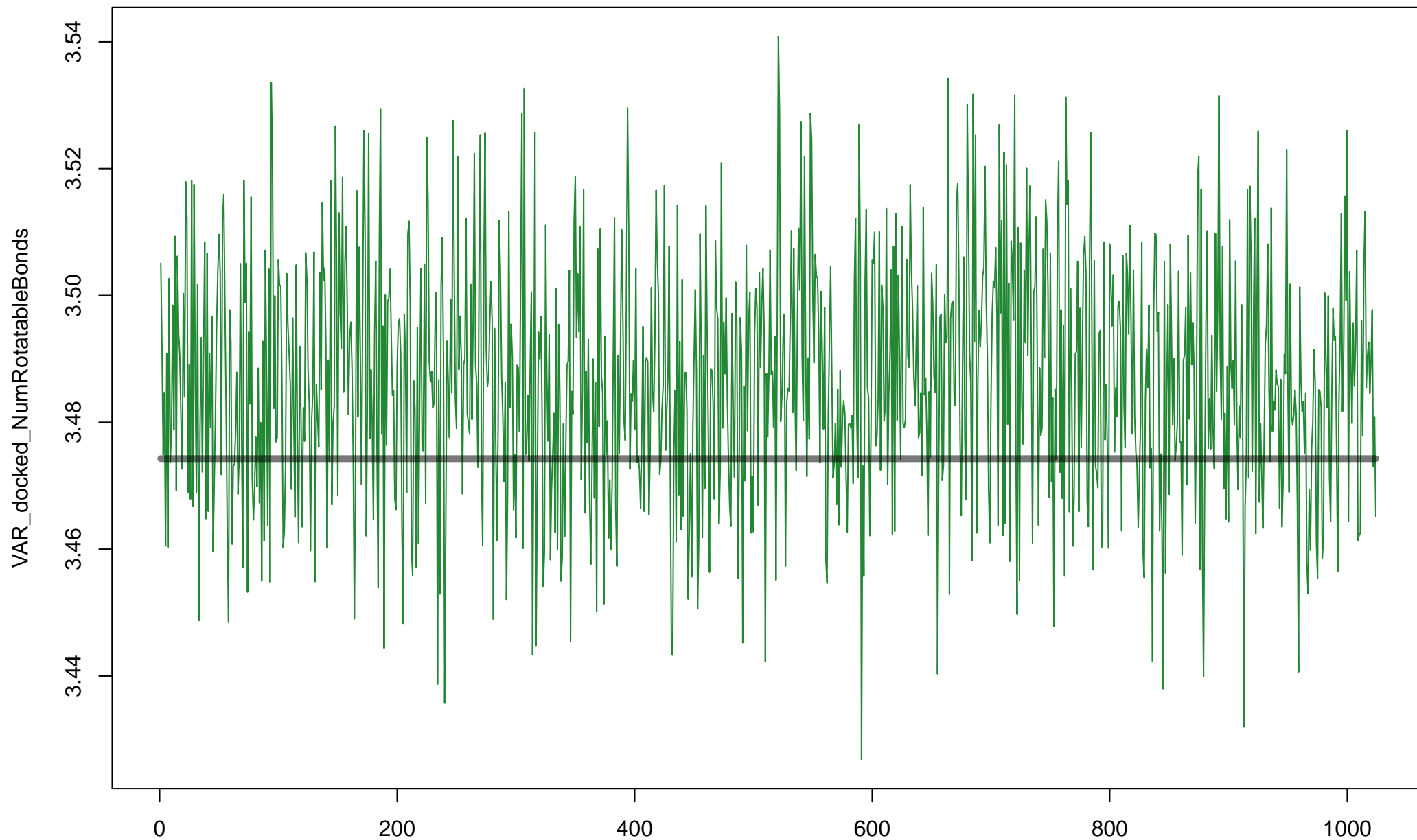
ESS = 1020 | BMK = 0.0477 | MCSE(6.27) = 3.94 | stat: TRUE | burn: 0 | rel.err: -2.28



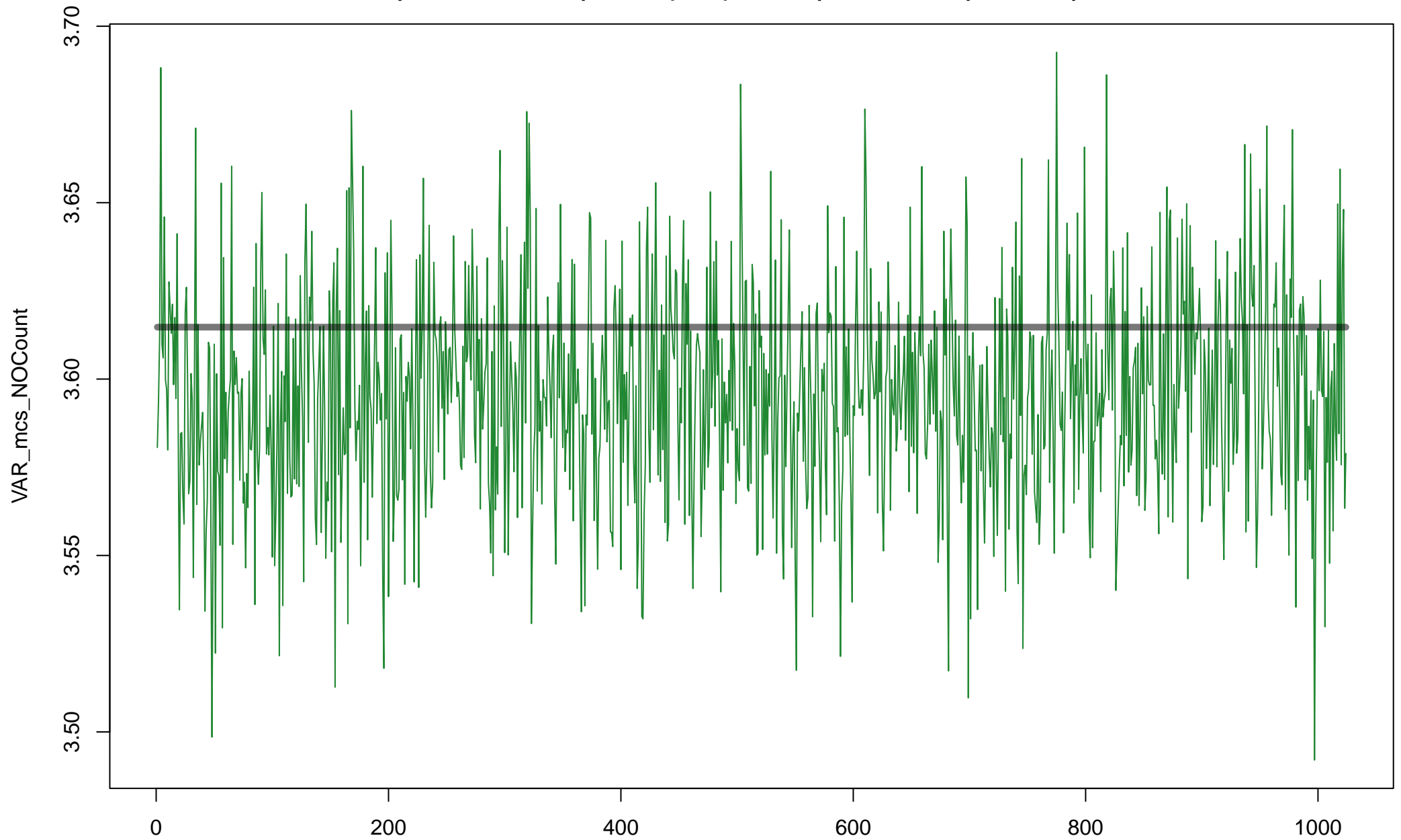
VAR_mcs_RingCount
ESS = 77.8 | BMK = 0.128 | MCSE(6.27) = 7.7 | stat: FALSE | burn: 0 | rel.err: -0.0232



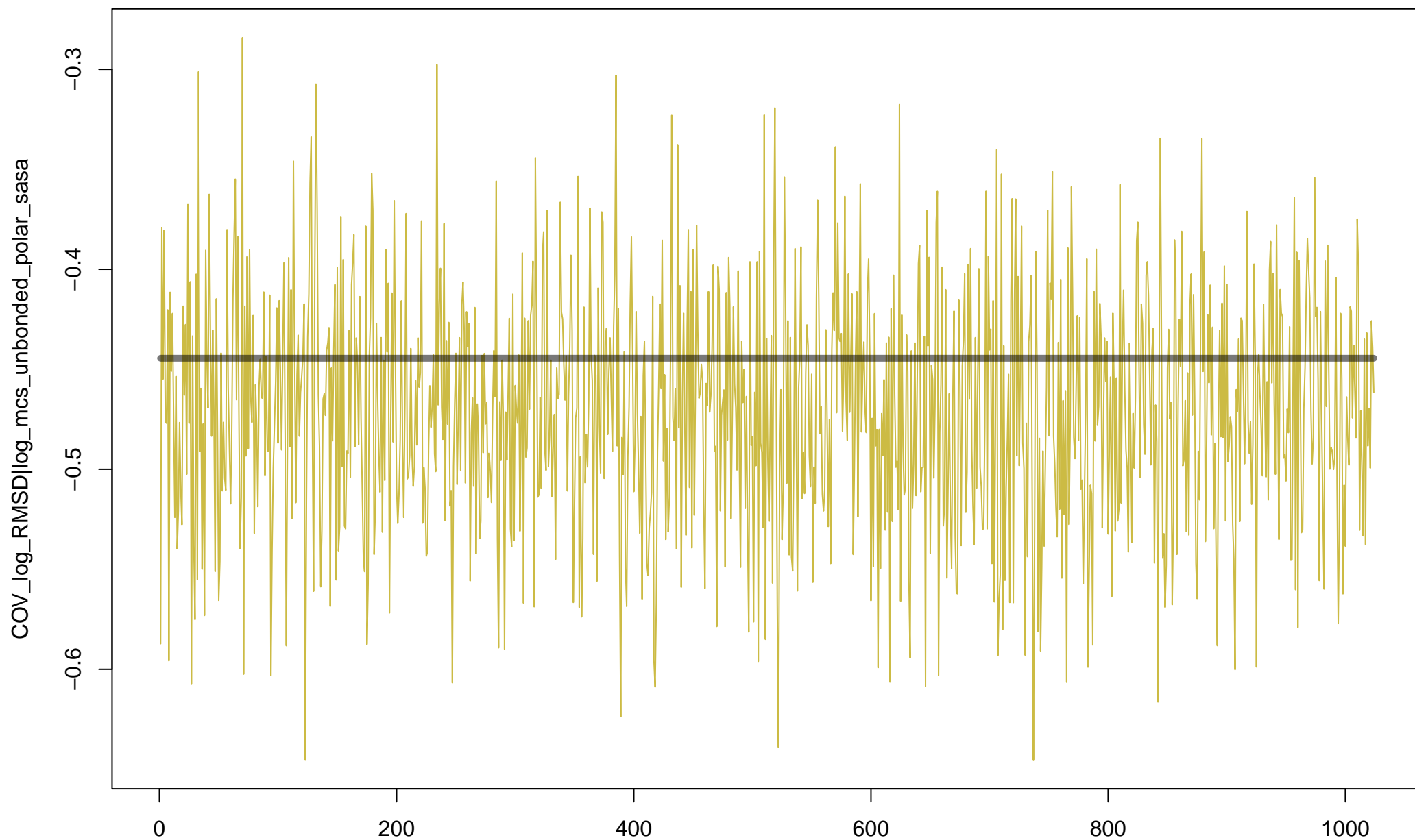
VAR_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0584 | MCSE(6.27) = 3.81 | stat: TRUE | burn: 0 | rel.err: 0.653



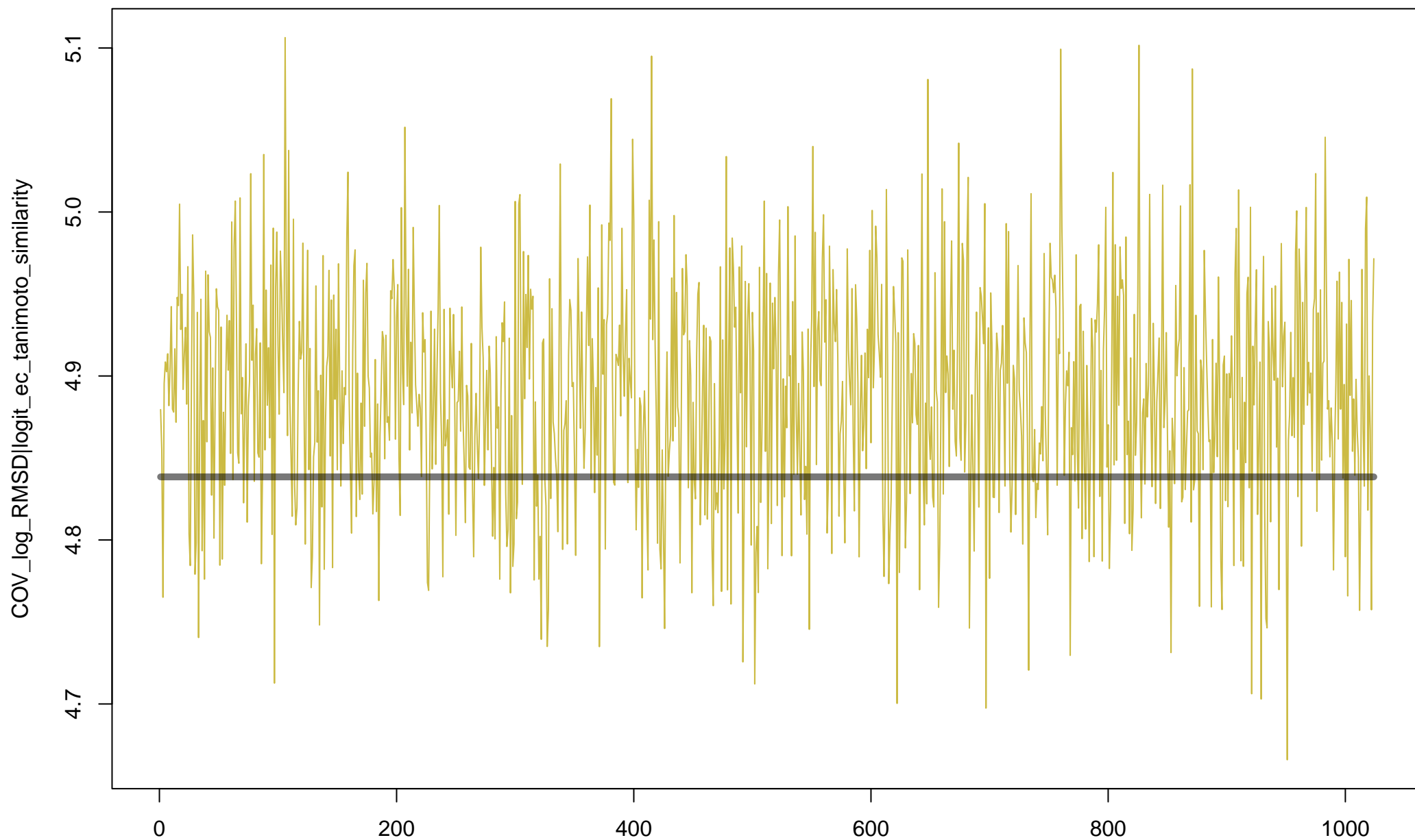
VAR_mcs_NOCount
ESS = 1020 | BMK = 0.0487 | MCSE(6.27) = 3.61 | stat: TRUE | burn: 0 | rel.err: -0.633



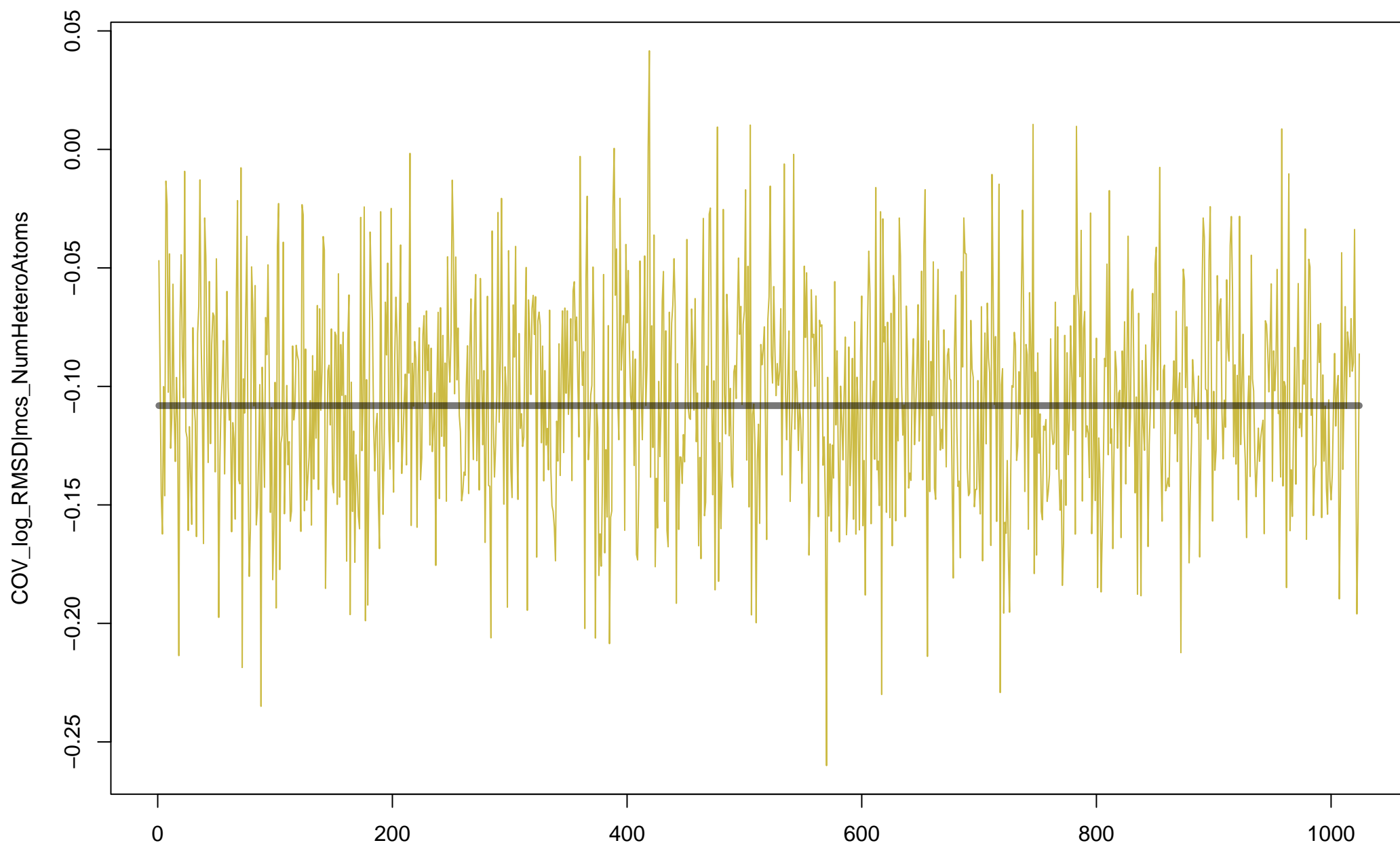
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0487 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0 | rel.err: -0.448



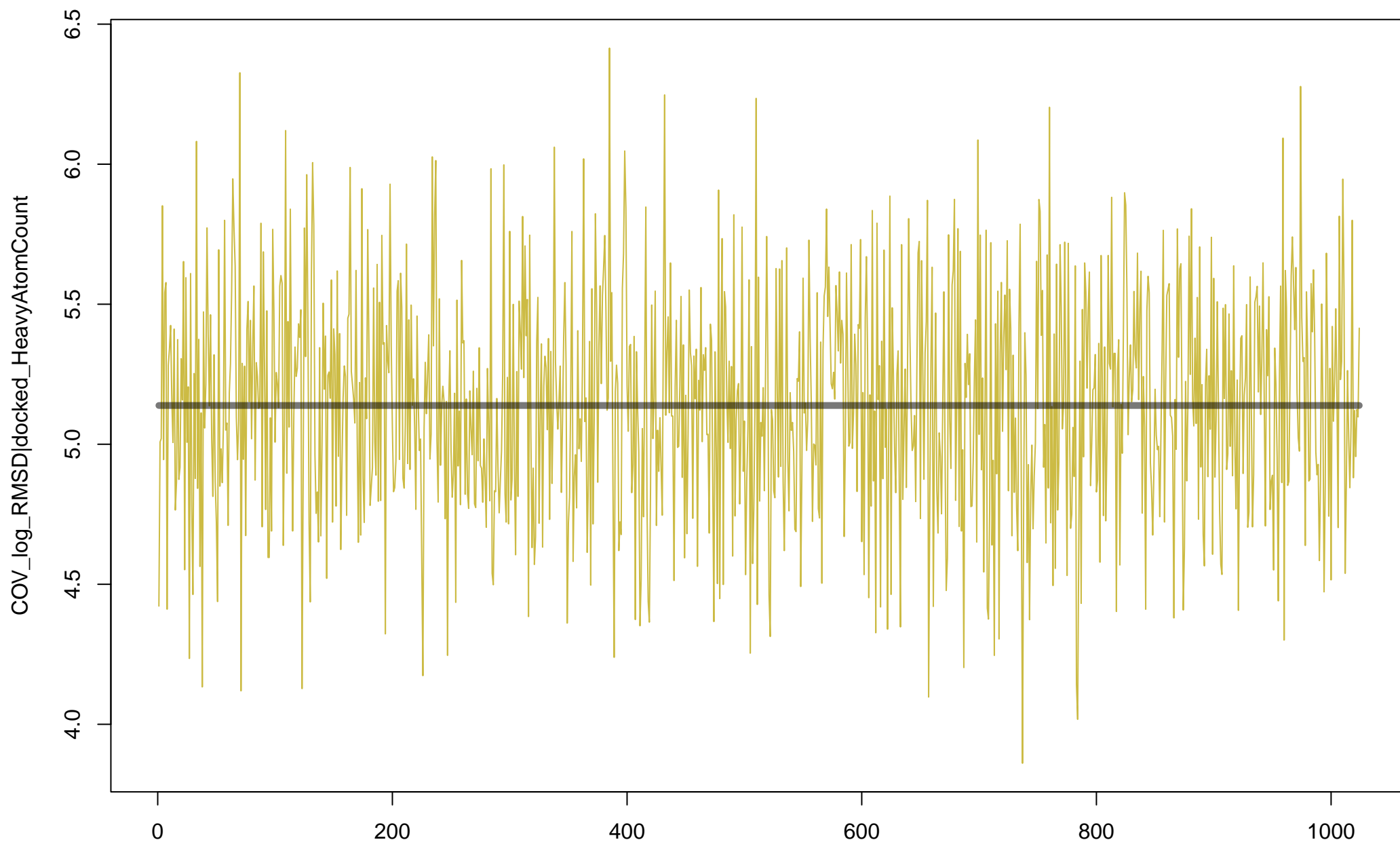
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0432 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0 | rel.err: 0.742



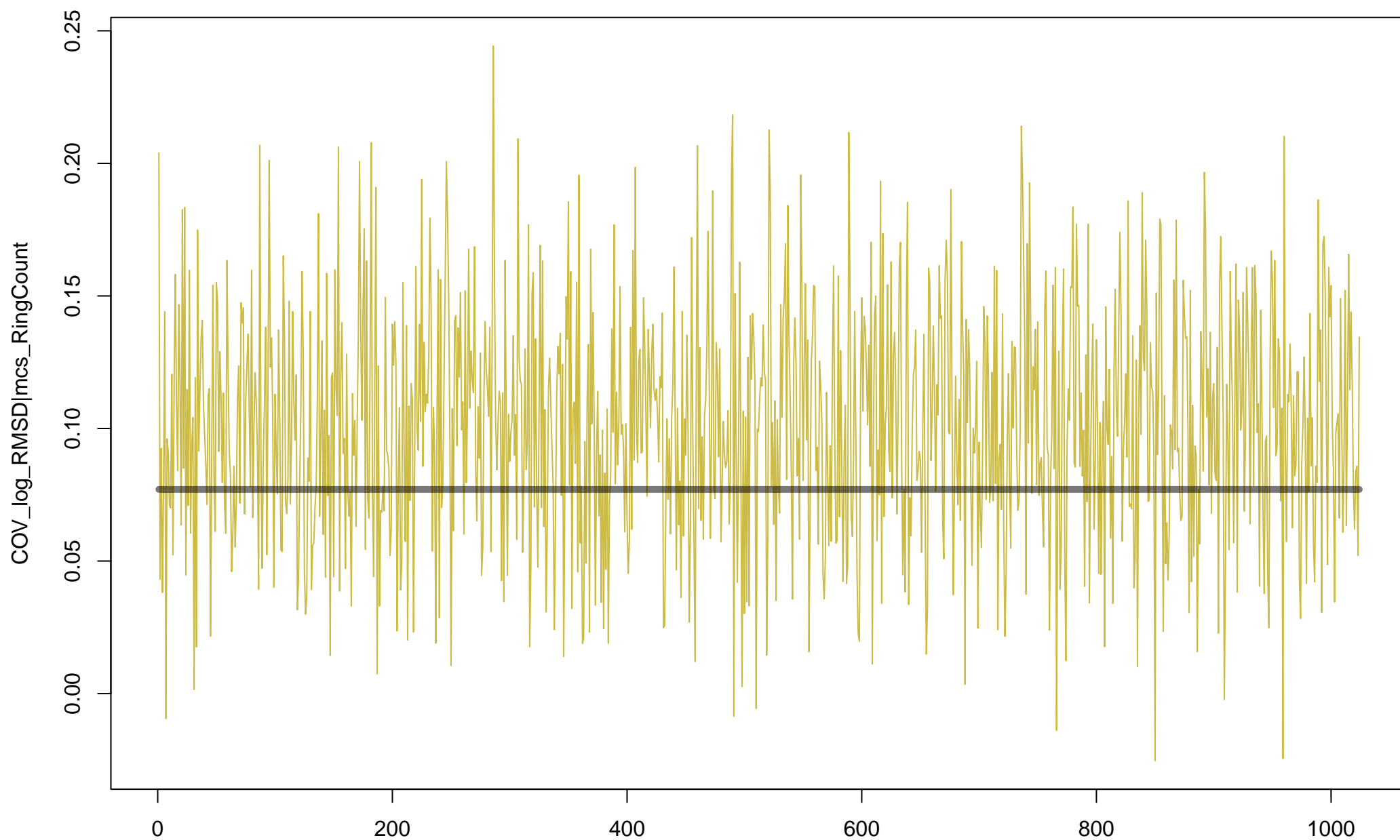
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.06 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | rel.err: 0.0672



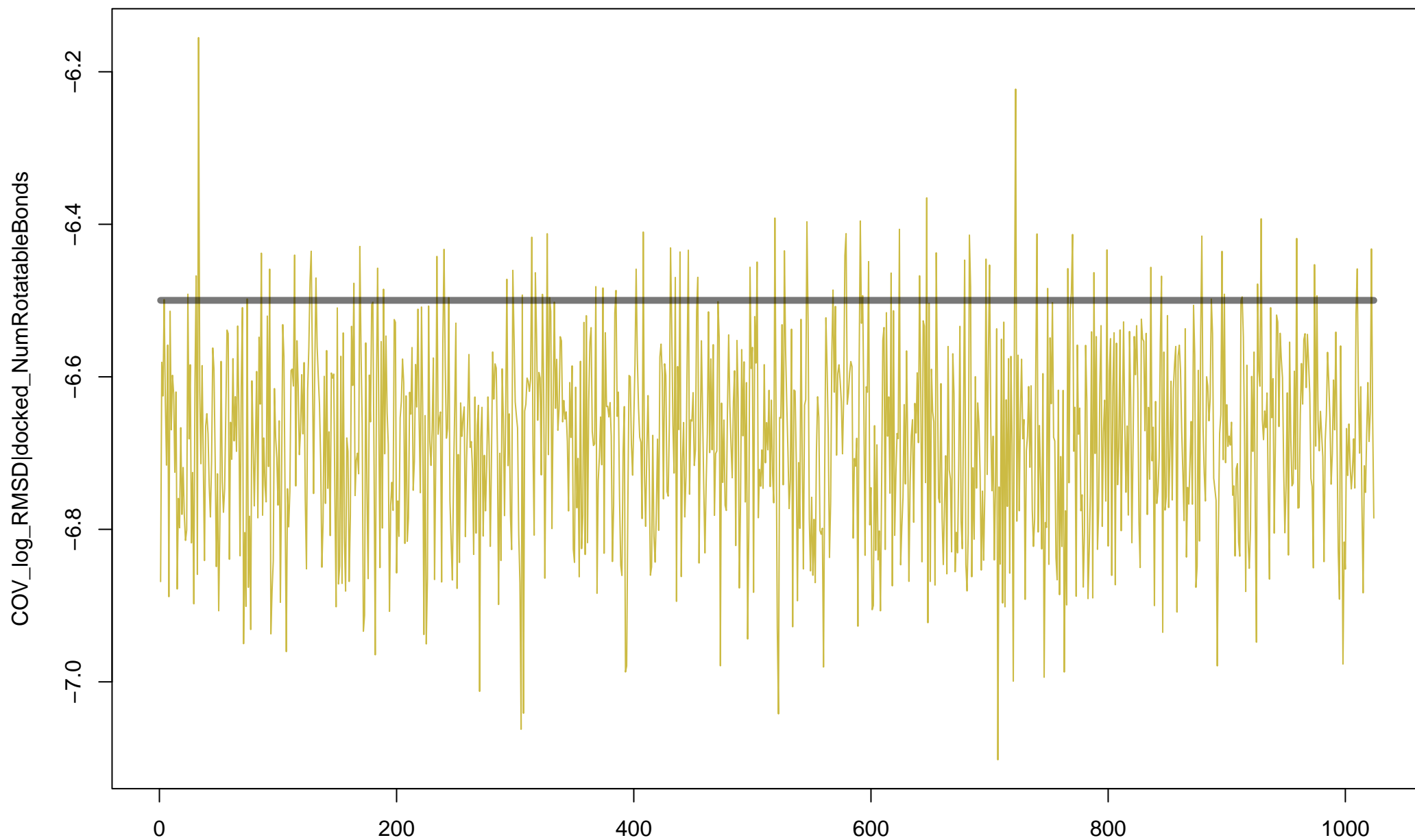
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0661 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0 | rel.err: 0.0152



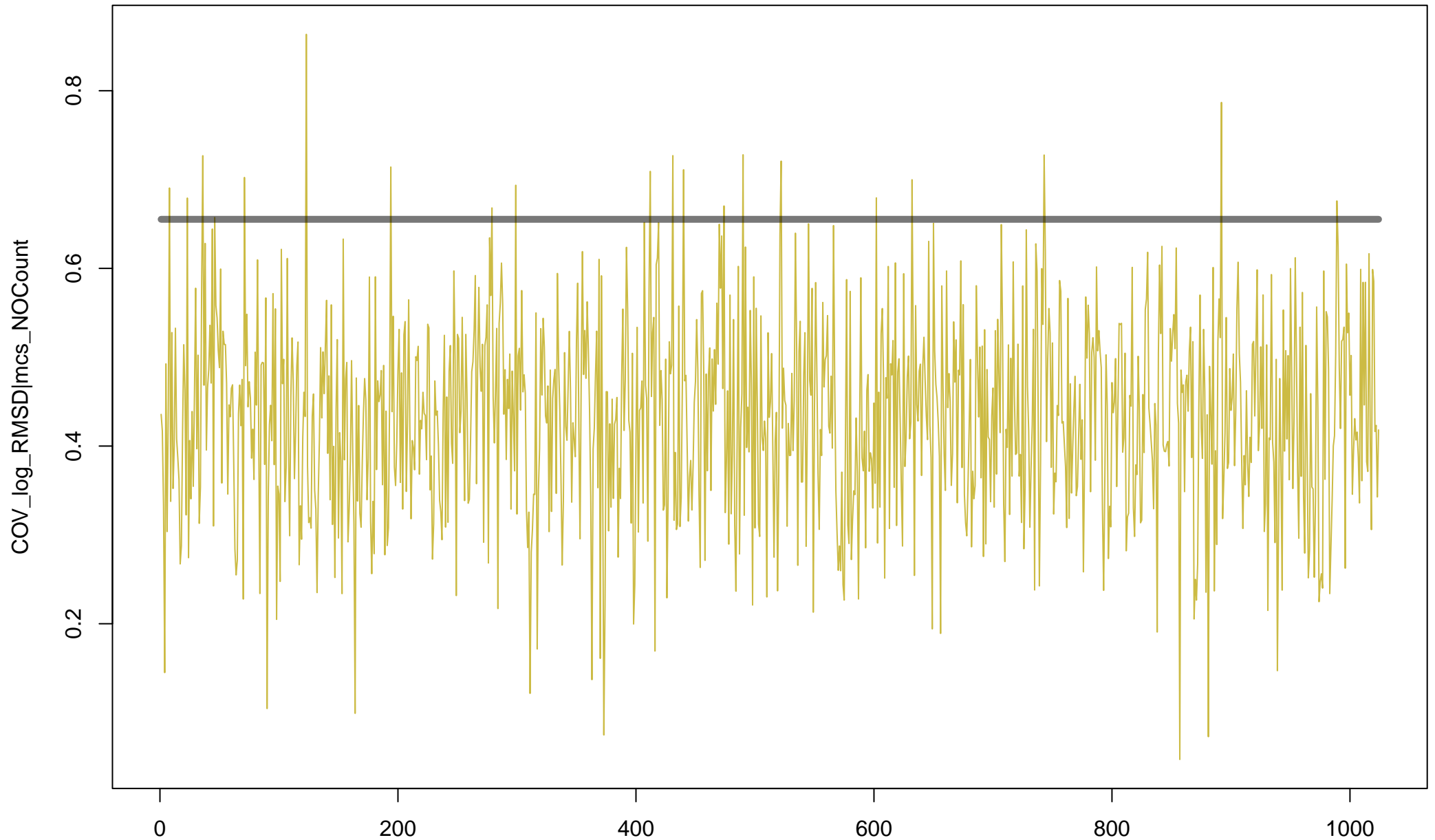
COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0549 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0 | rel.err: 0.558



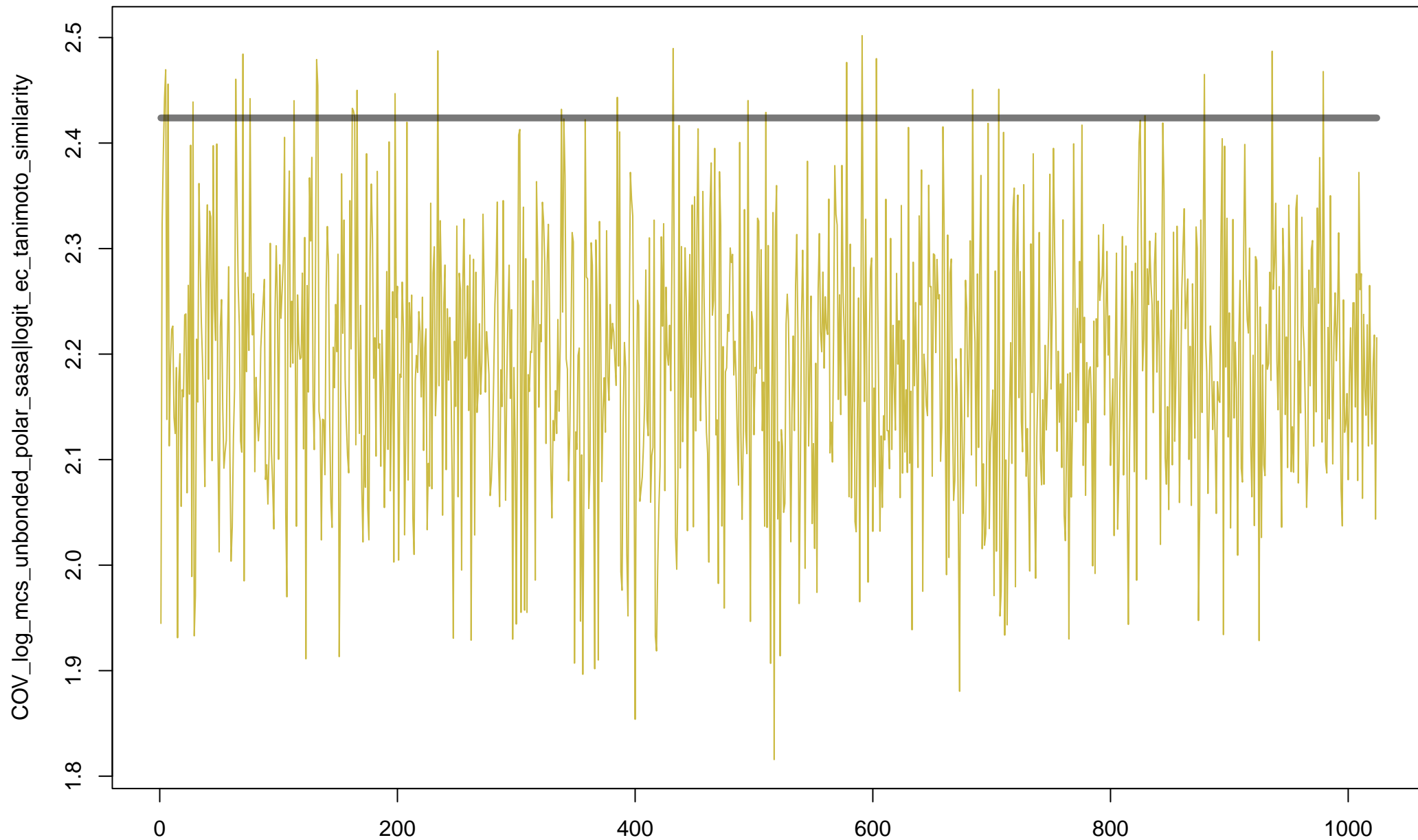
COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0551 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0 | rel.err: -1.41



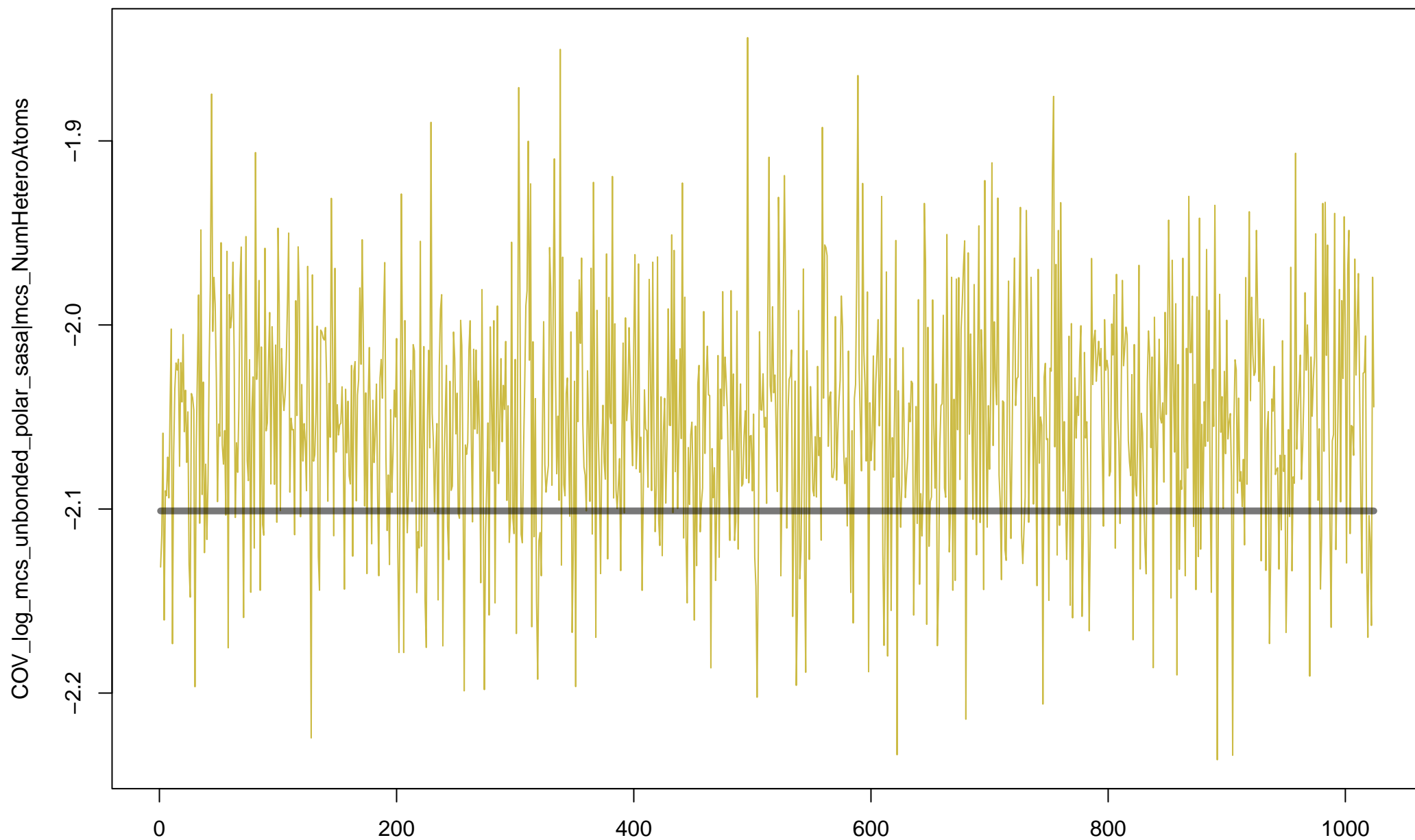
COV_log_RMSD|mcs_NOCount
ESS = 852 | BMK = 0.0721 | MCSE(6.27) = 3.41 | stat: TRUE | burn: 0 | rel.err: -2.01



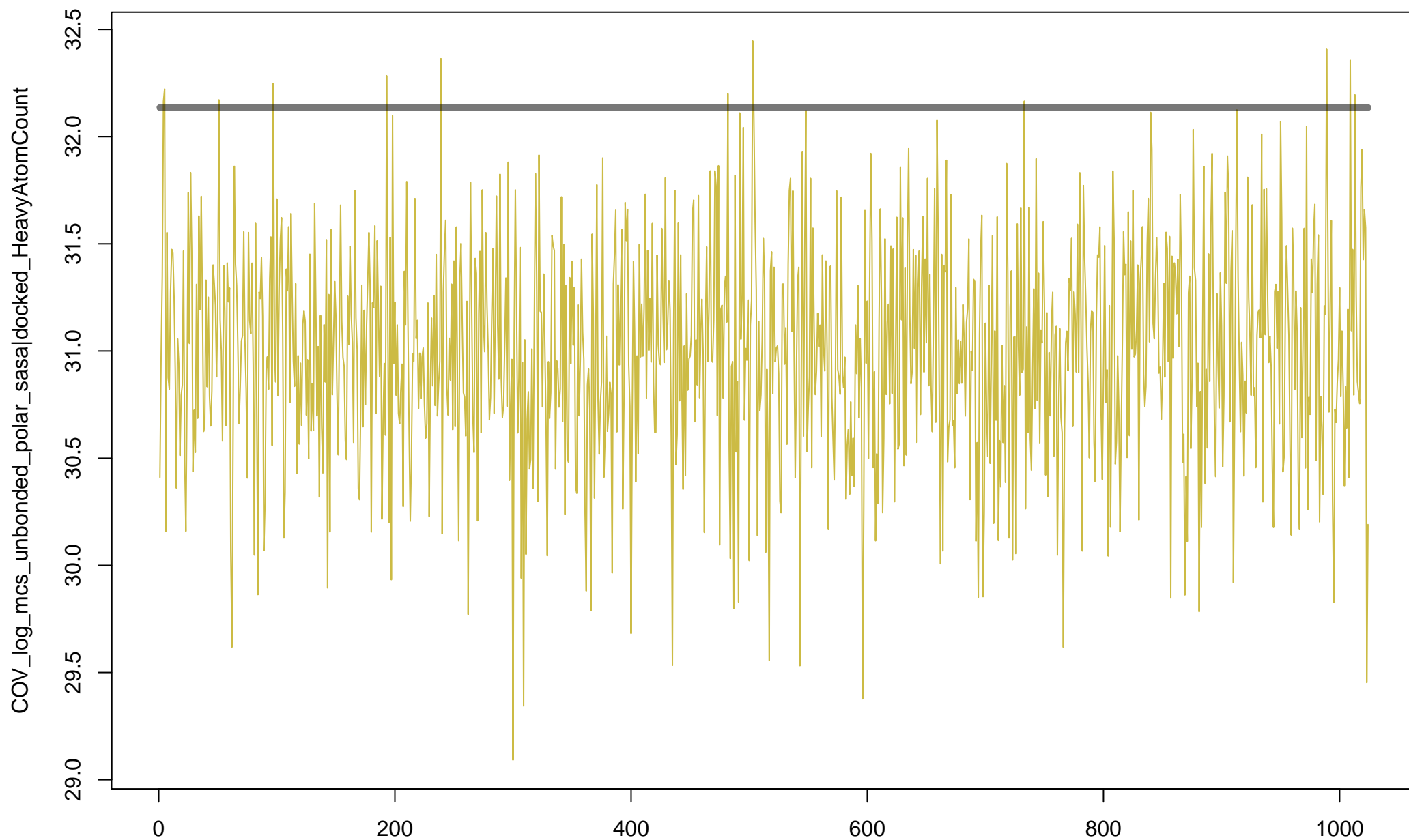
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0571 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | rel.err: -1.94



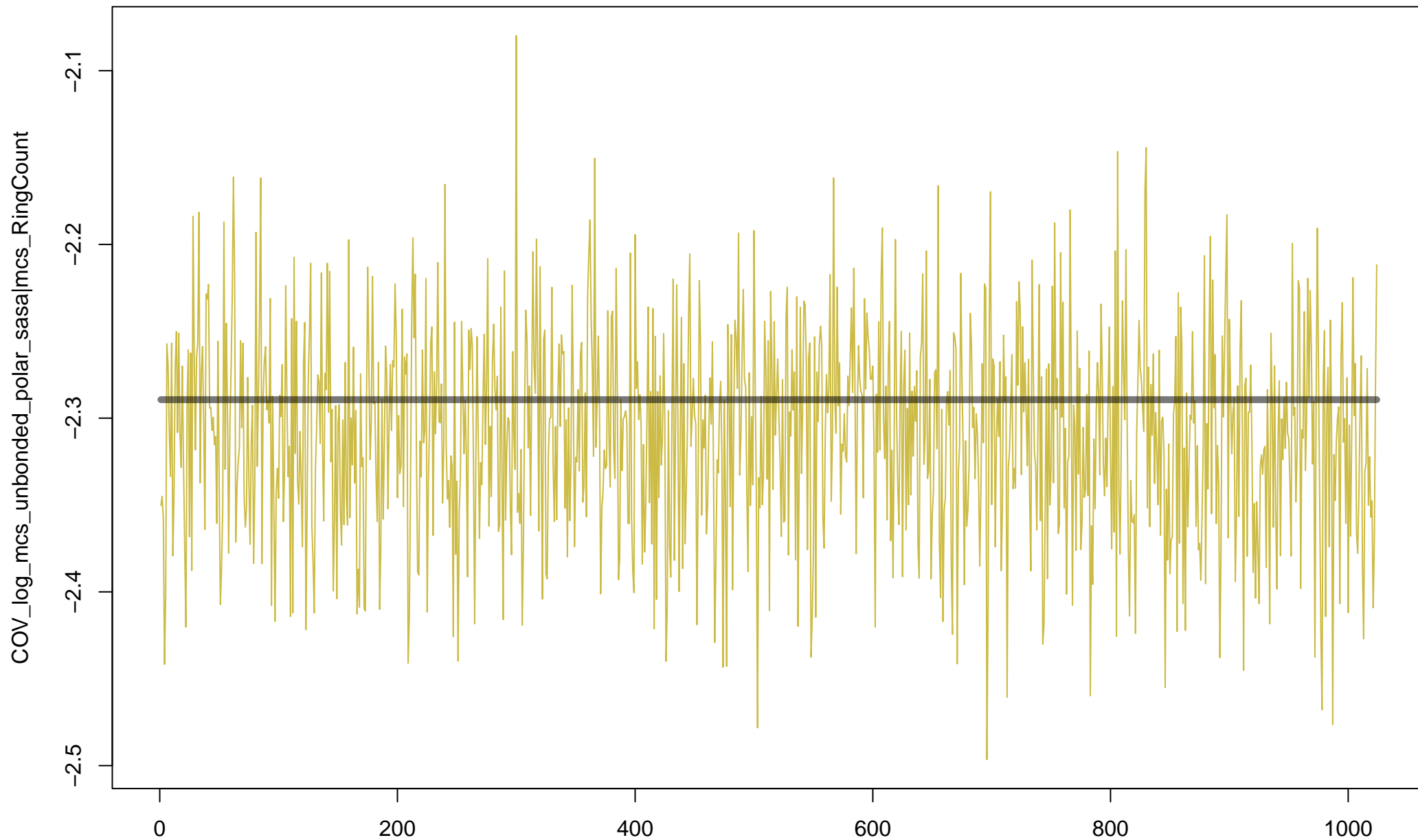
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.062 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0 | rel.err: 0.792



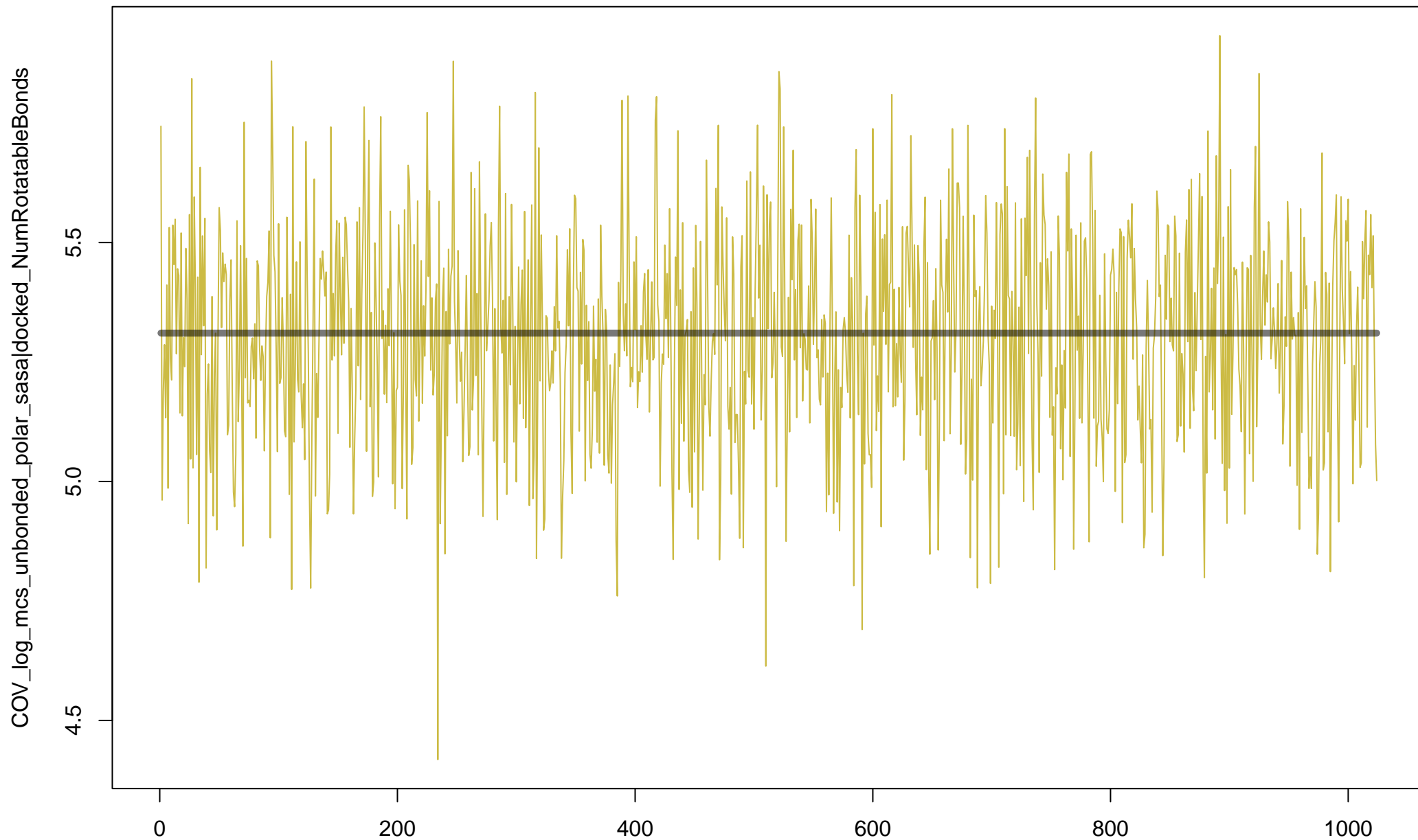
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.059 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0 | rel.err: -2.23



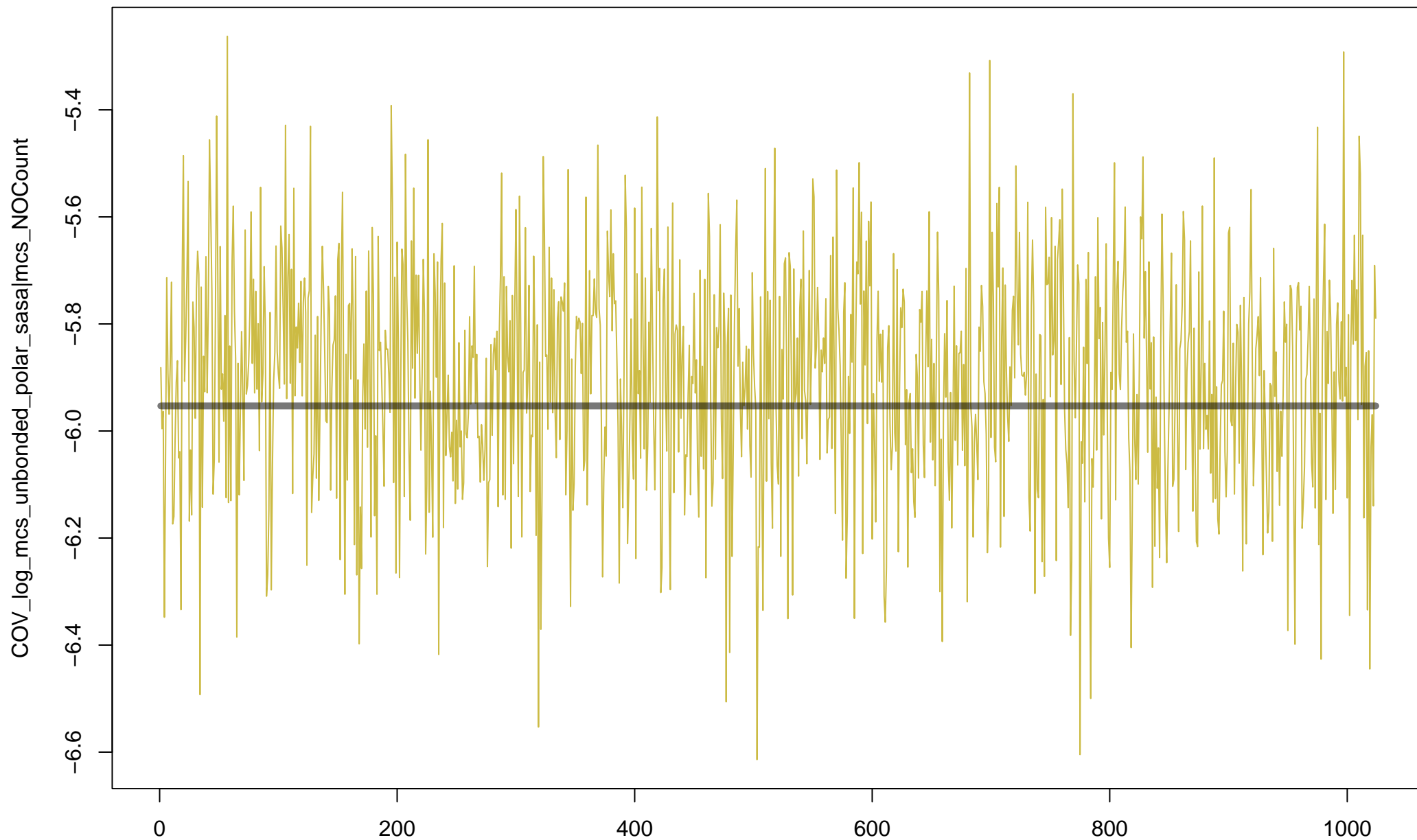
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0436 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0 | rel.err: -0.342



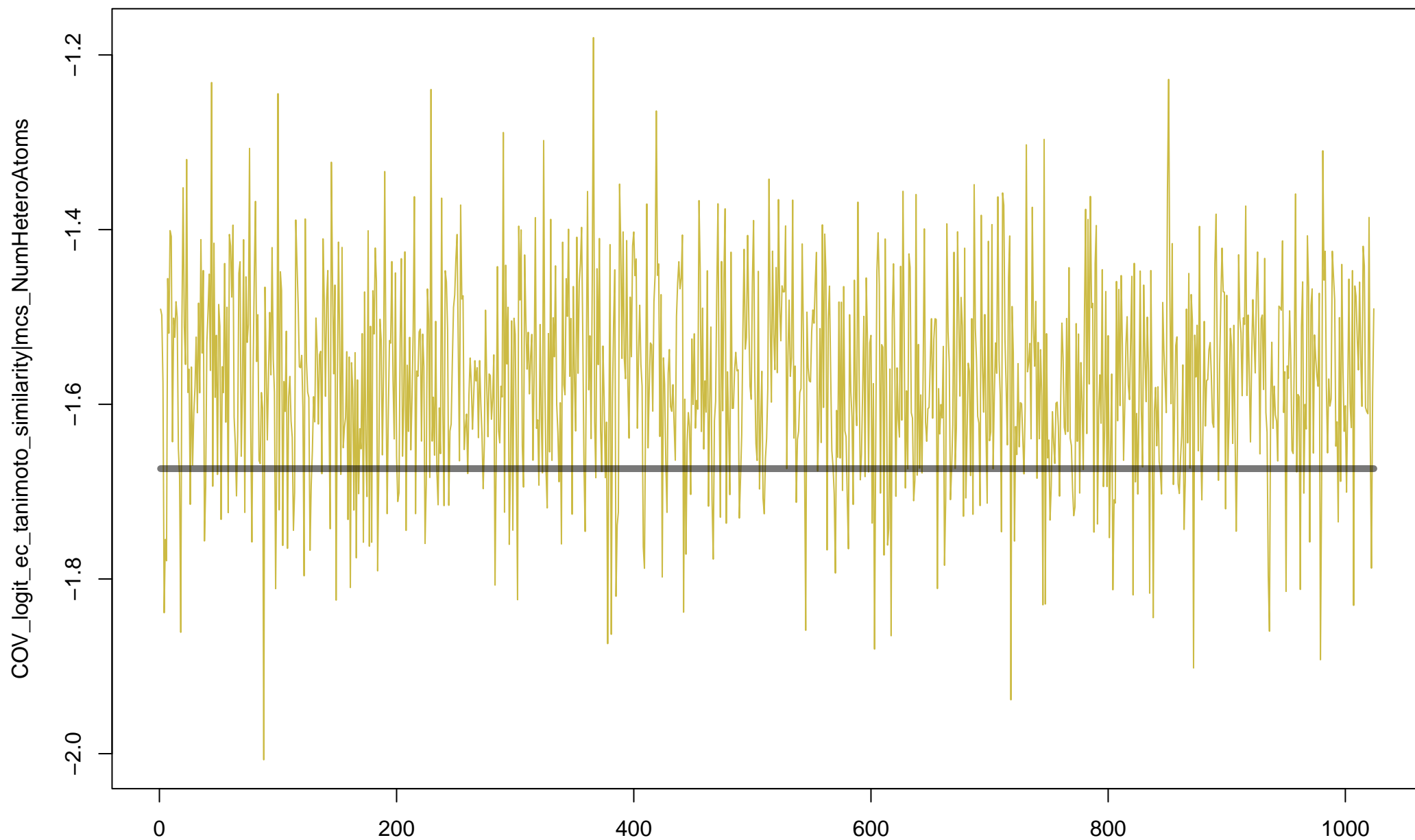
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0582 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0 | rel.err: -0.0417



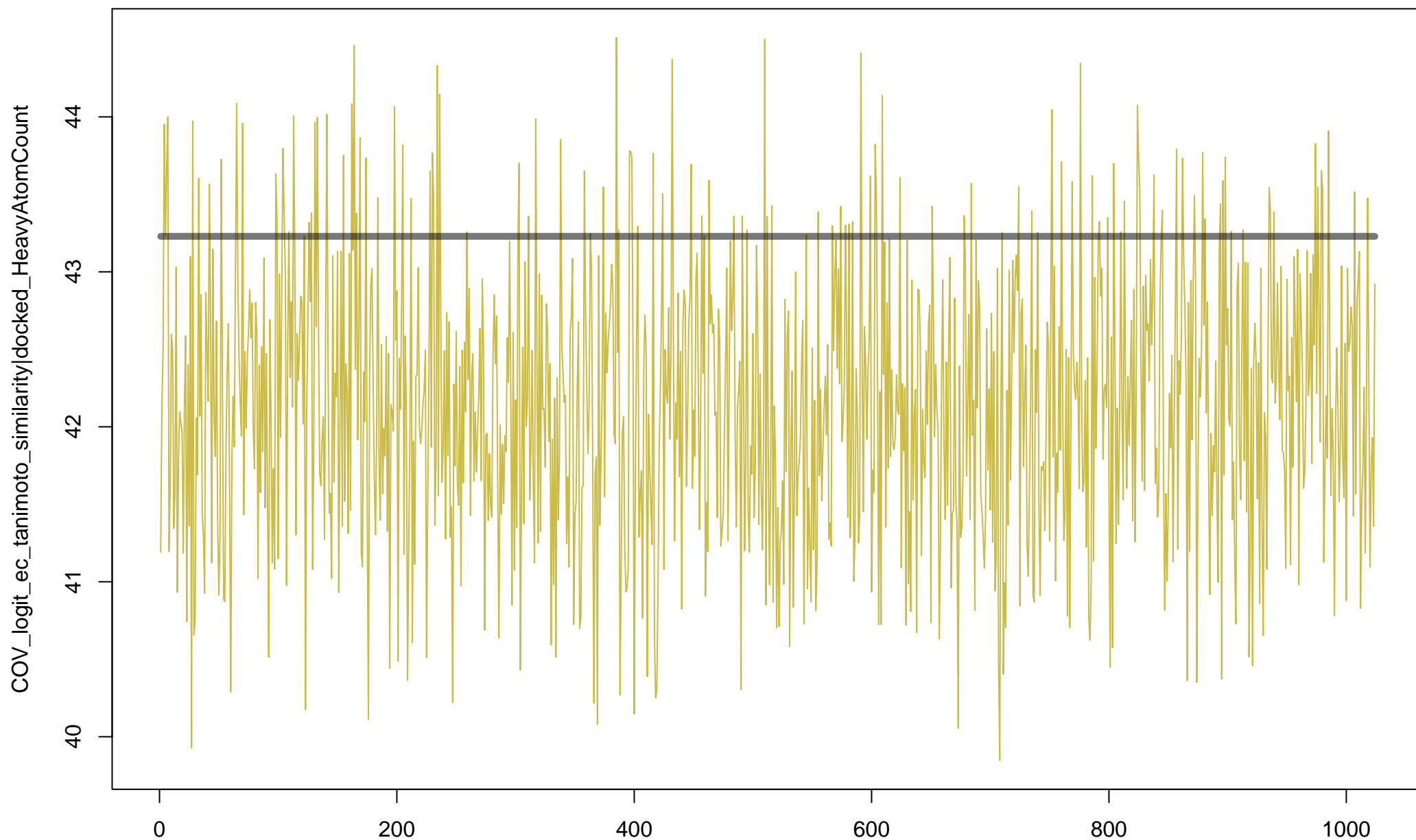
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0359 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0 | rel.err: 0.241



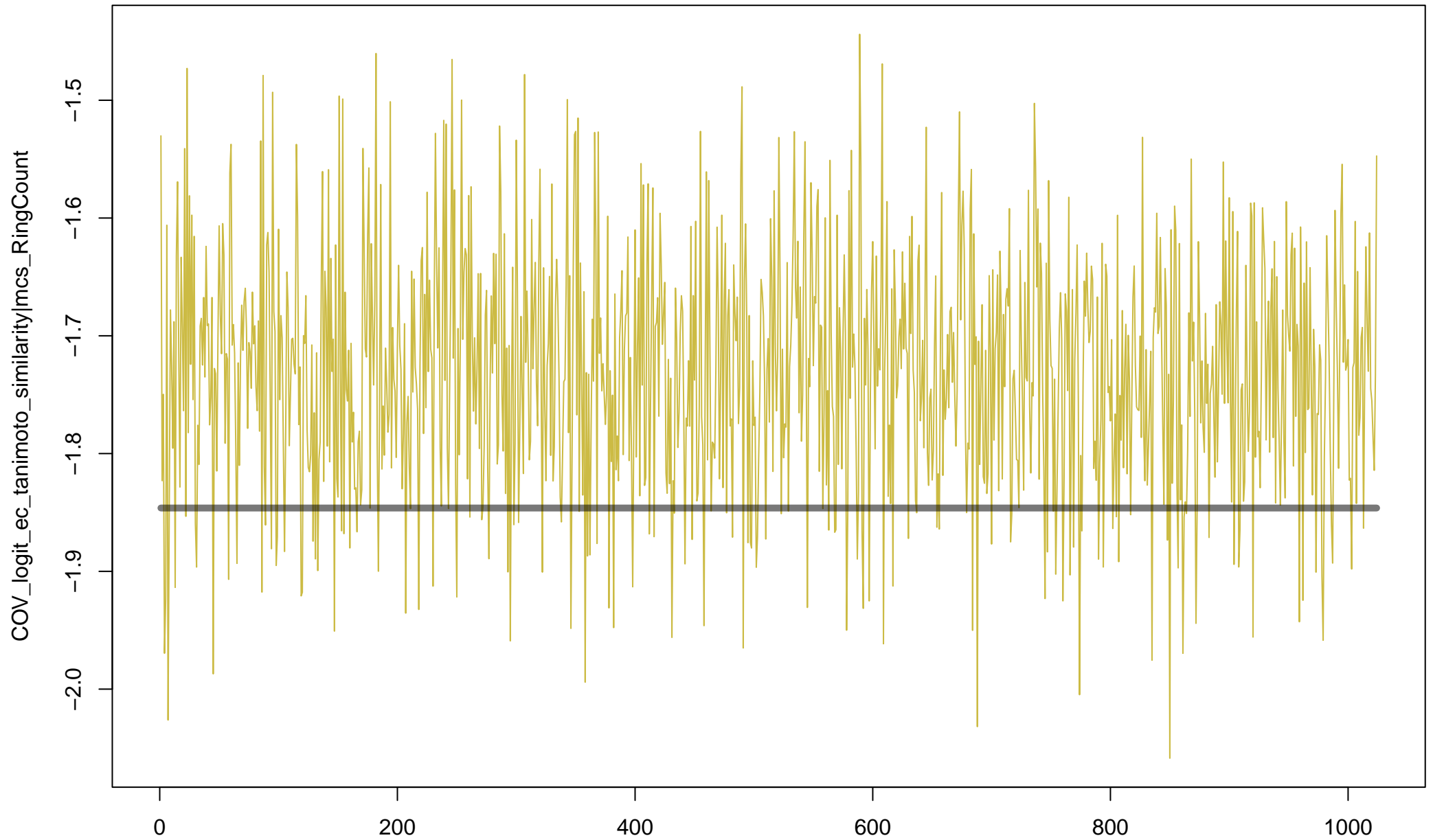
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0613 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | rel.err: 0.888



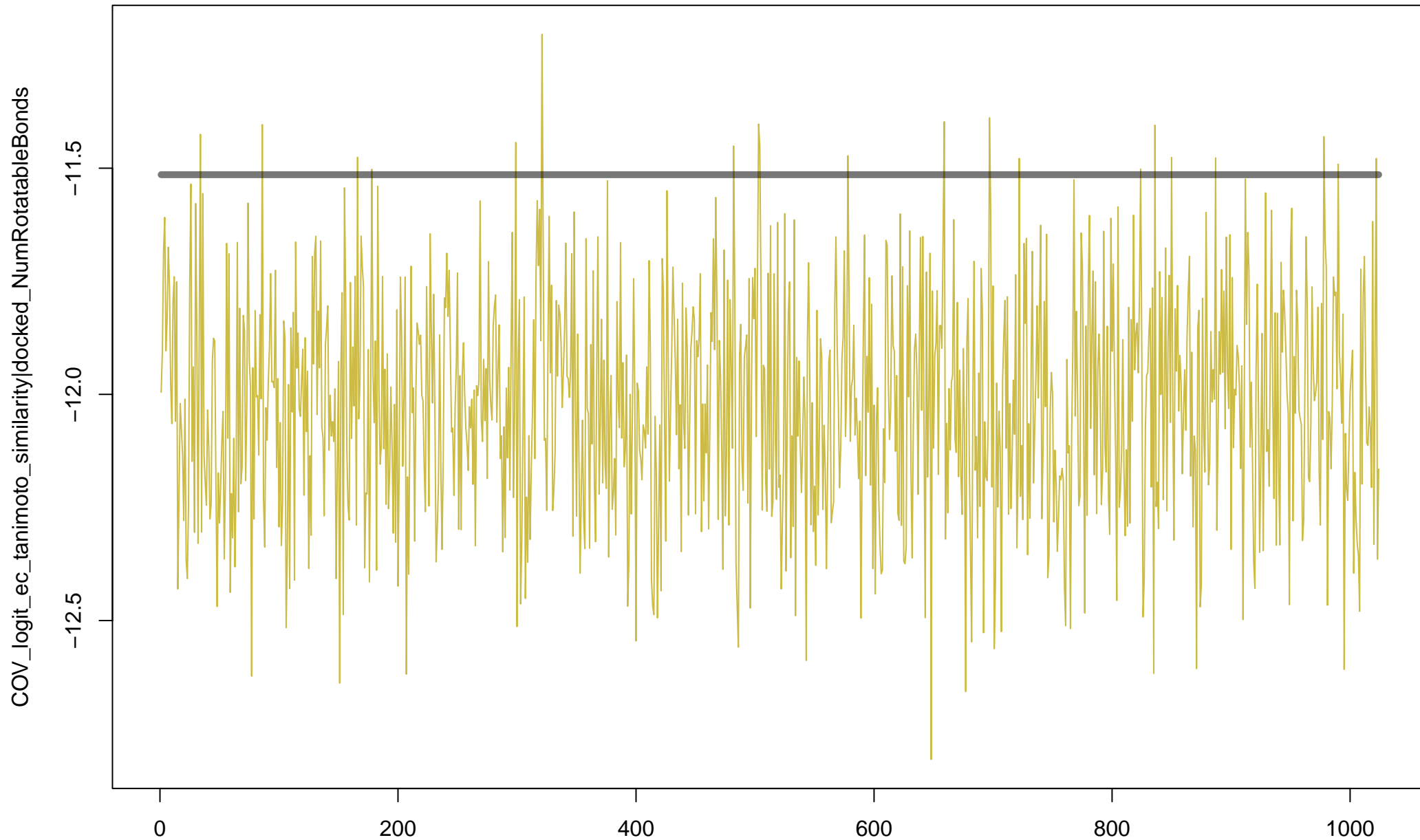
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 729 | BMK = 0.0667 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | rel.err: -1.25



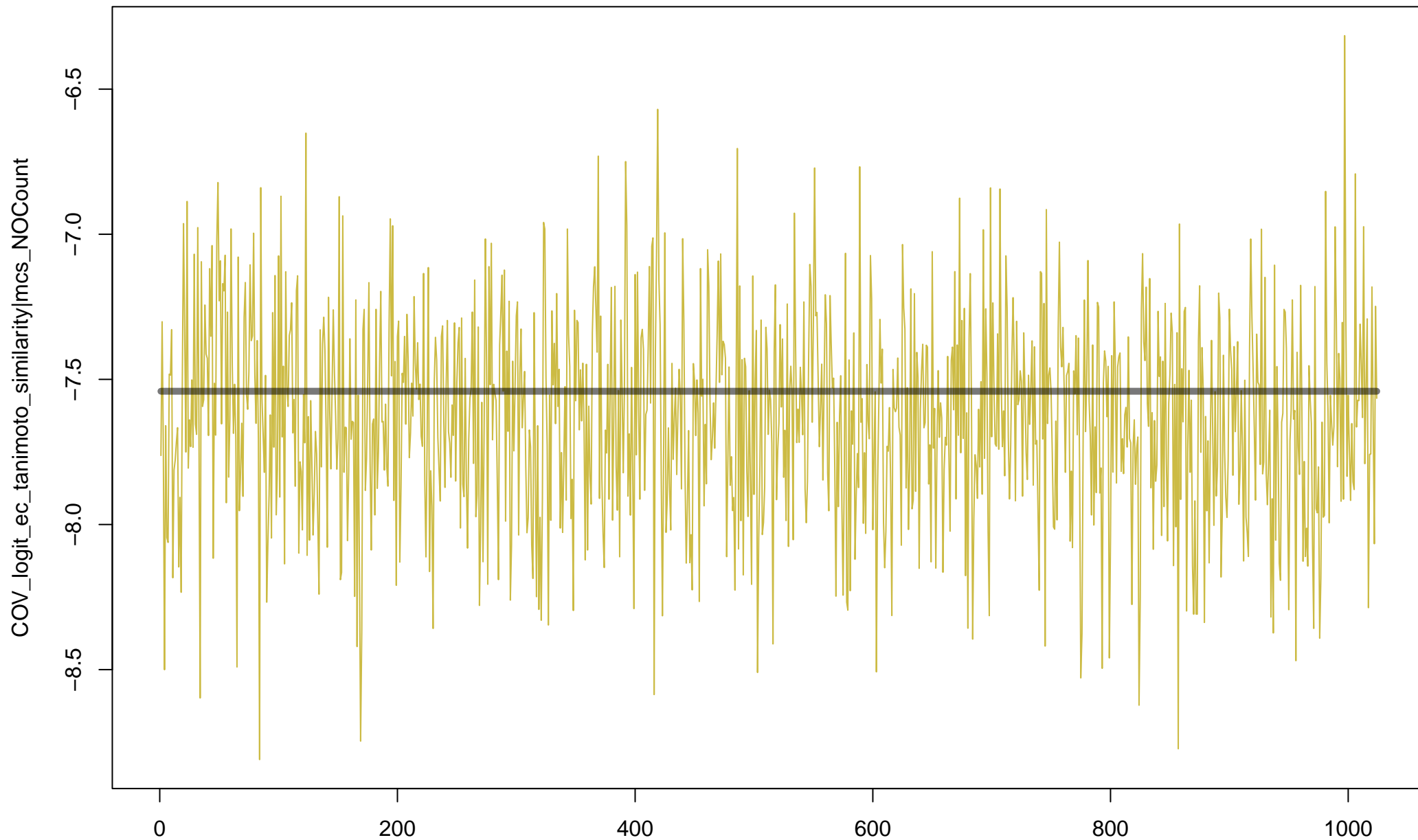
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0681 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0 | rel.err: 1.14



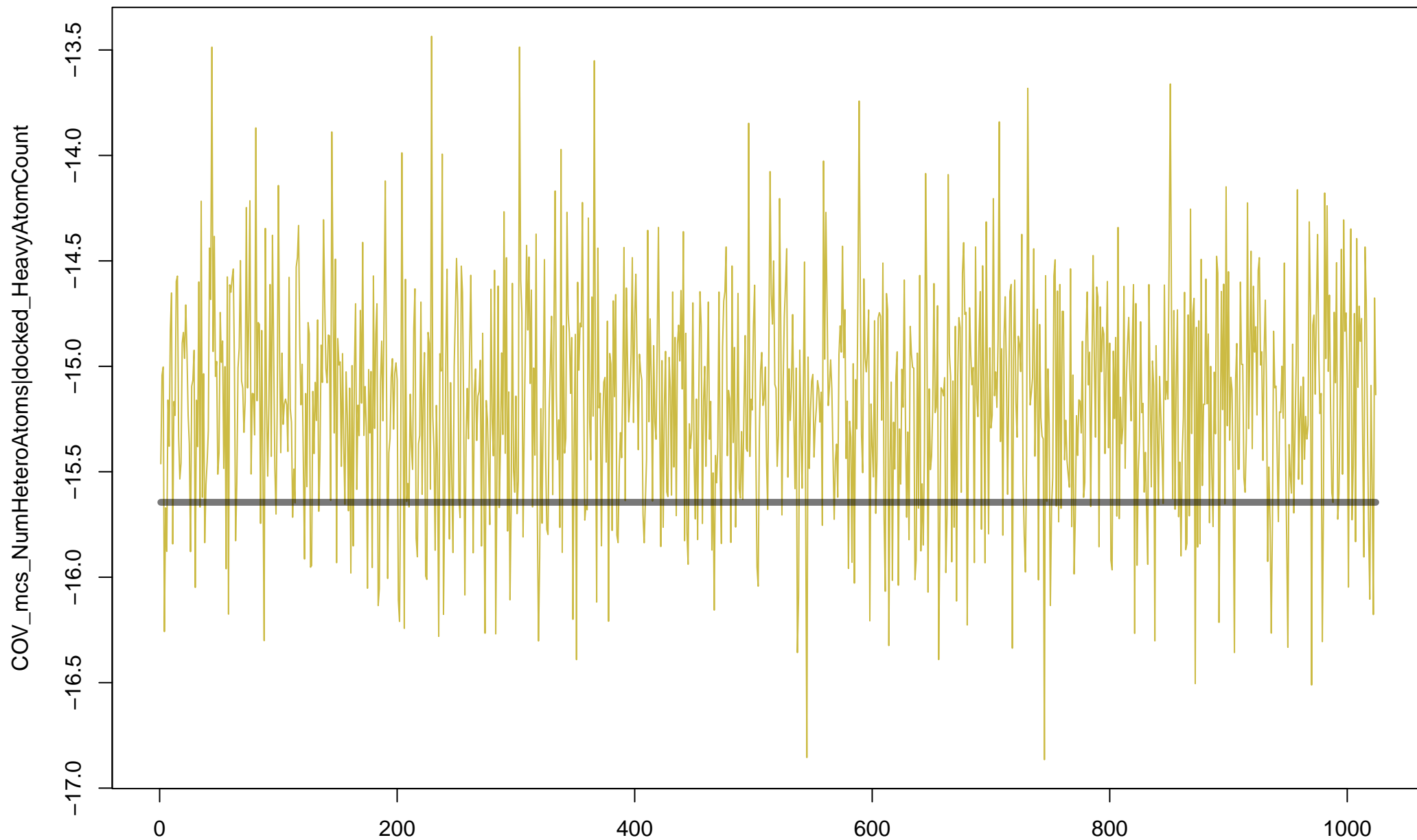
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0401 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0 | rel.err: -2.07



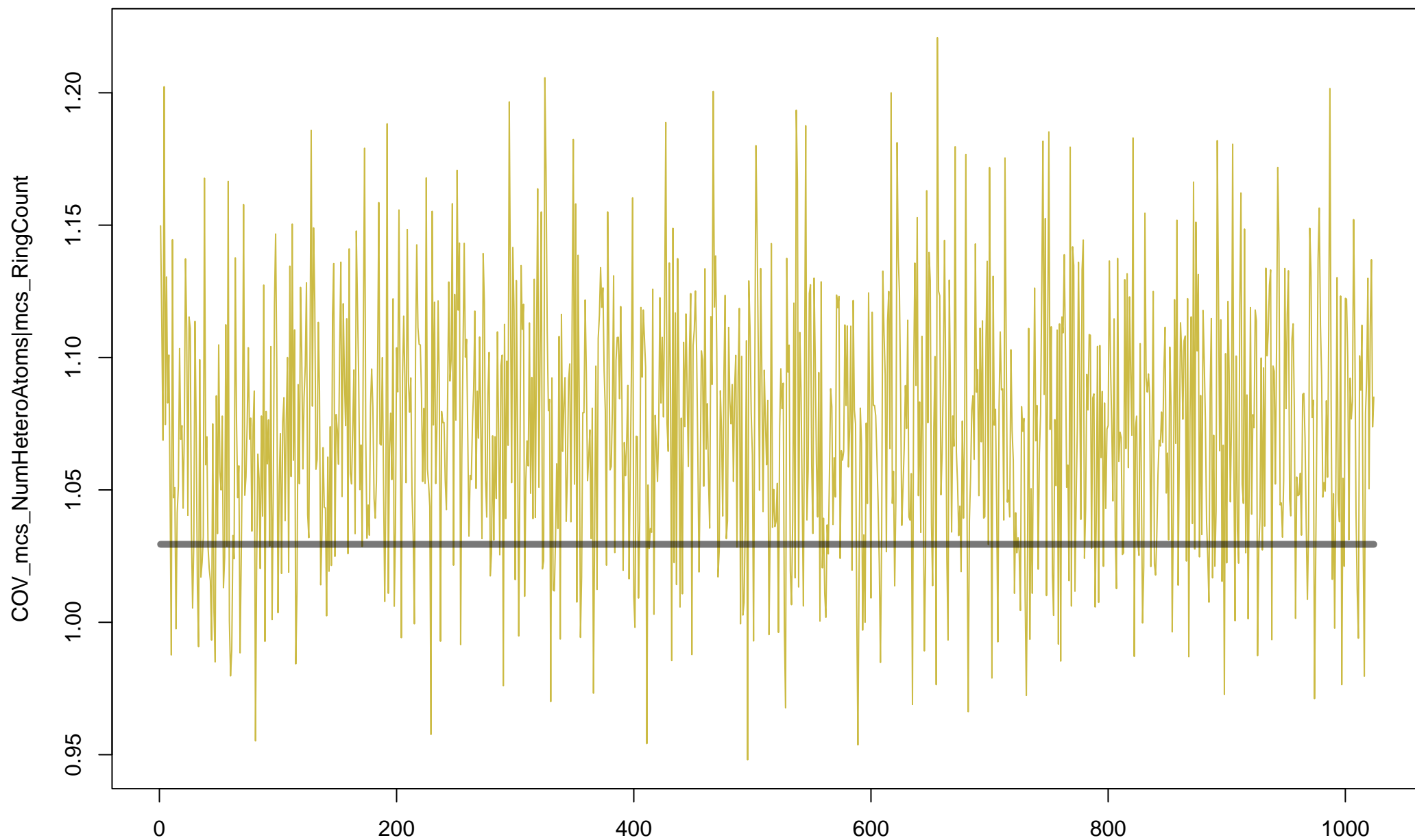
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0672 | MCSE(6.27) = 3.46 | stat: TRUE | burn: 0 | rel.err: -0.267



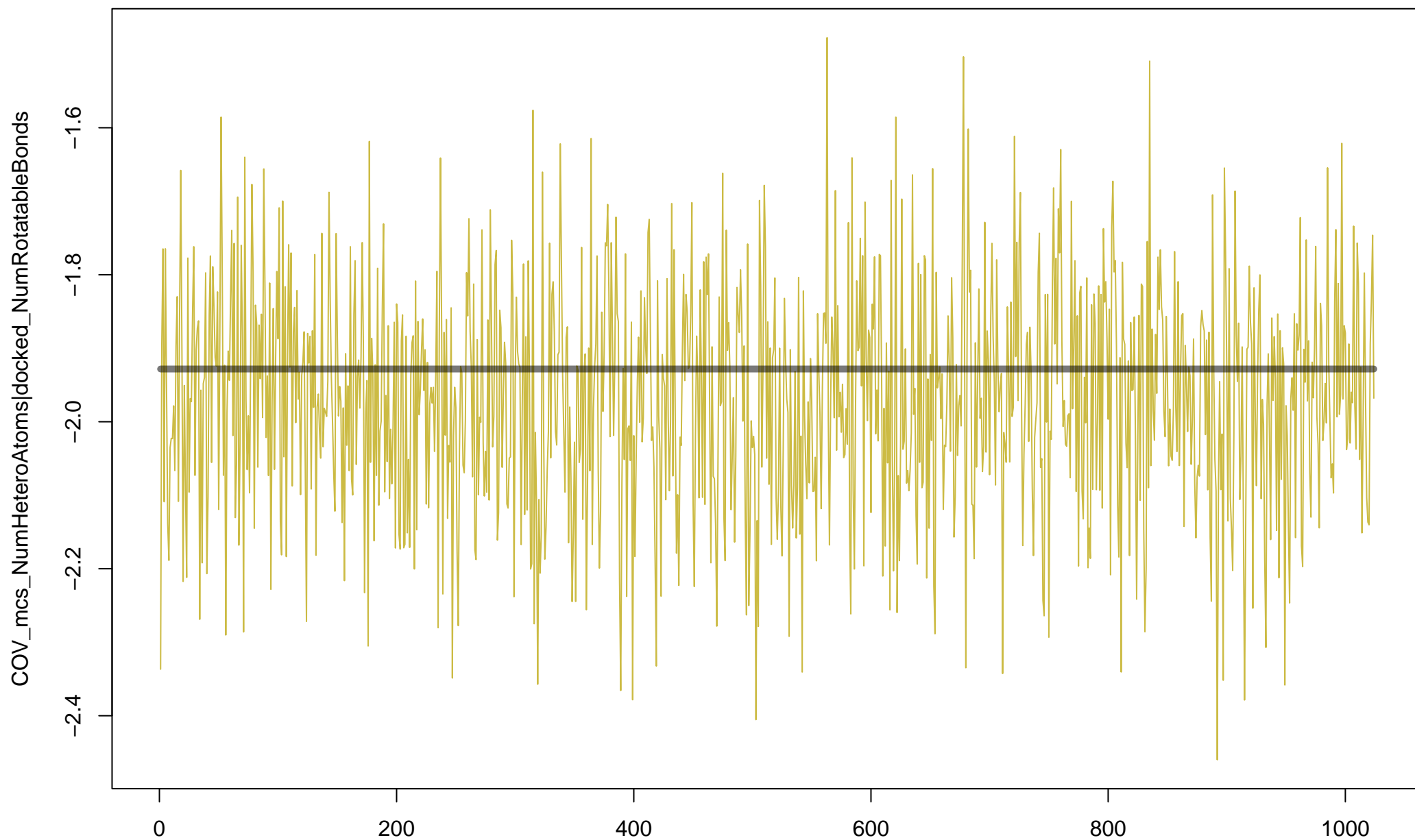
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0552 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0 | rel.err: 0.926



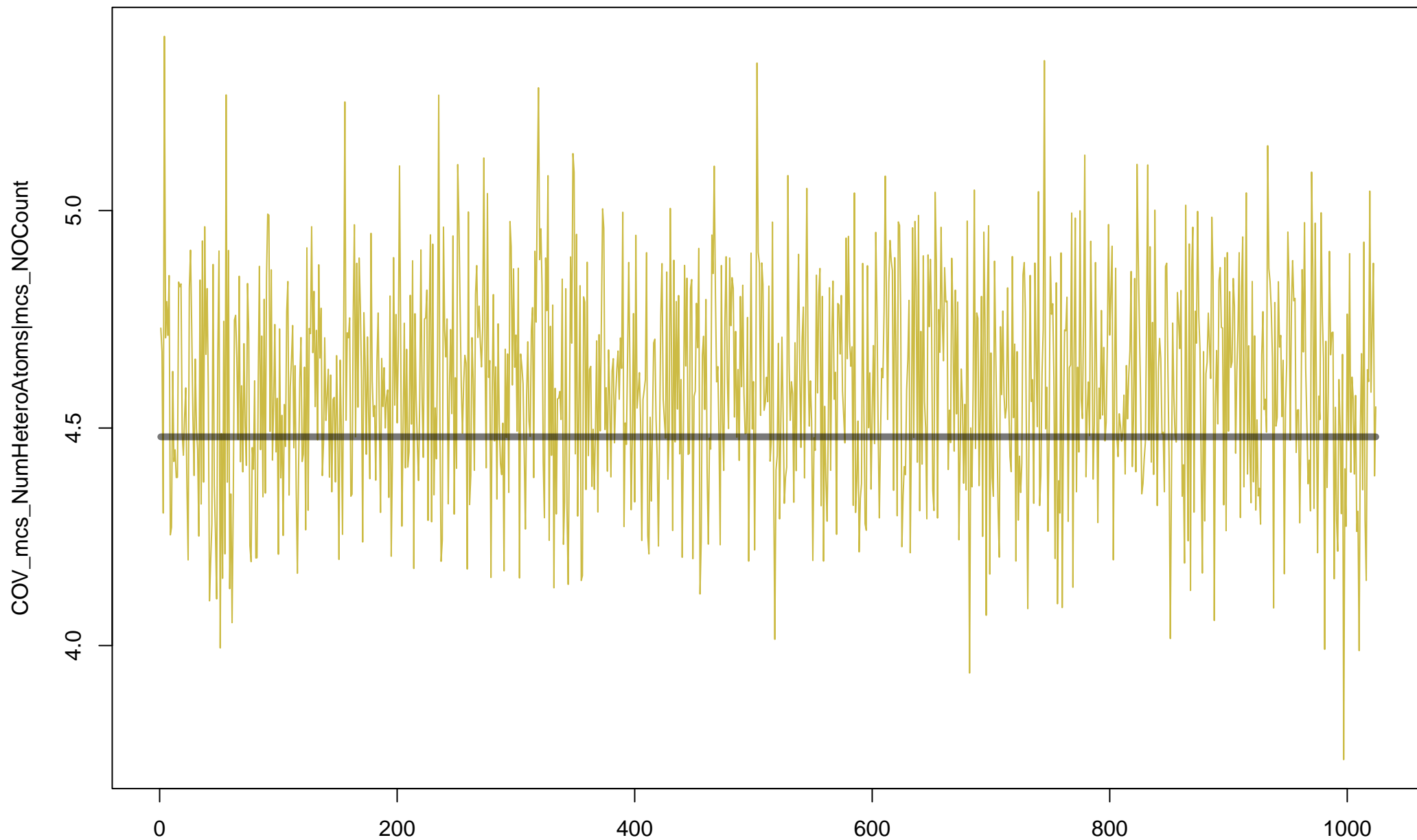
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0406 | MCSE(6.27) = 3.36 | stat: FALSE | burn: 0 | rel.err: 0.921



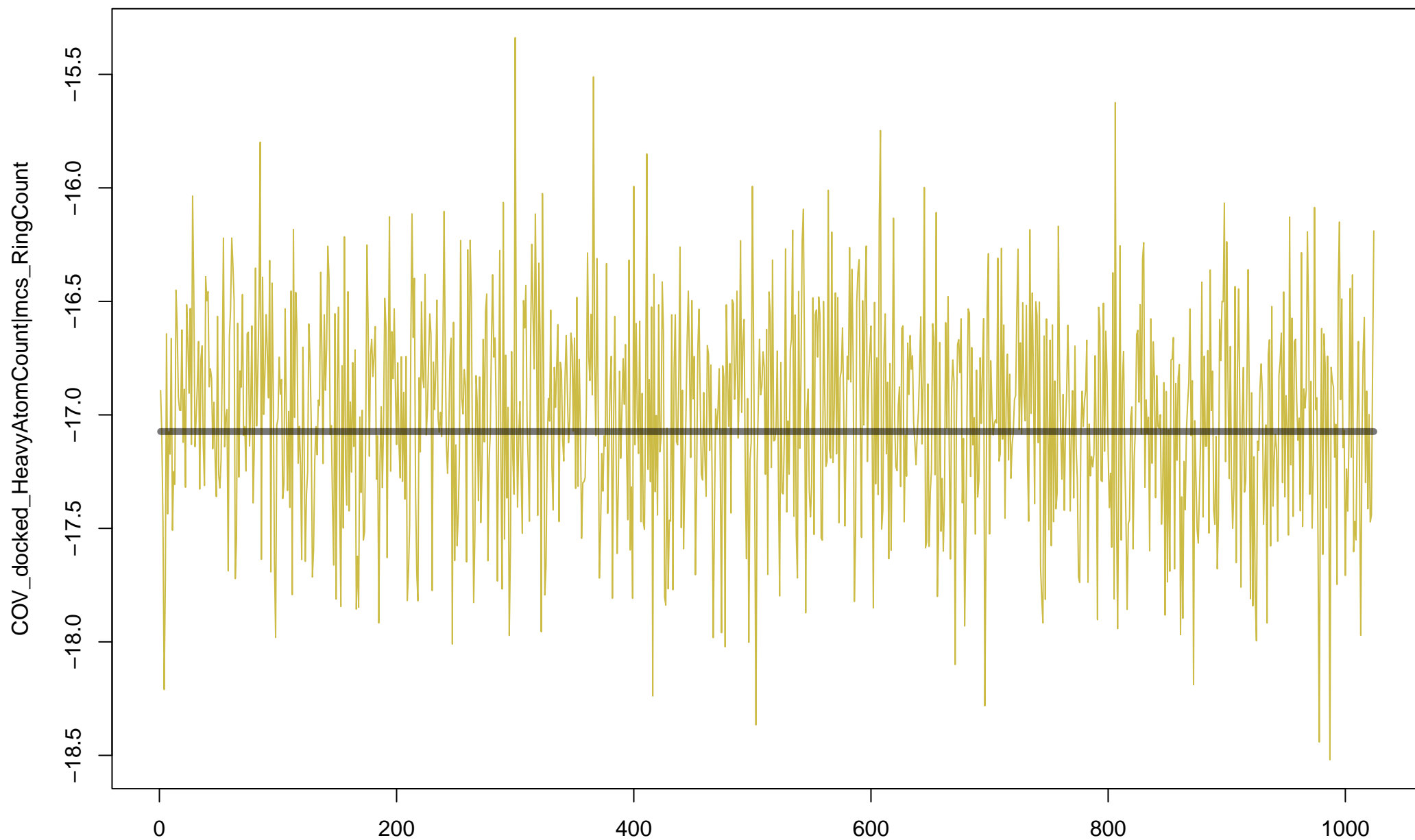
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0417 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0 | rel.err: -0.276



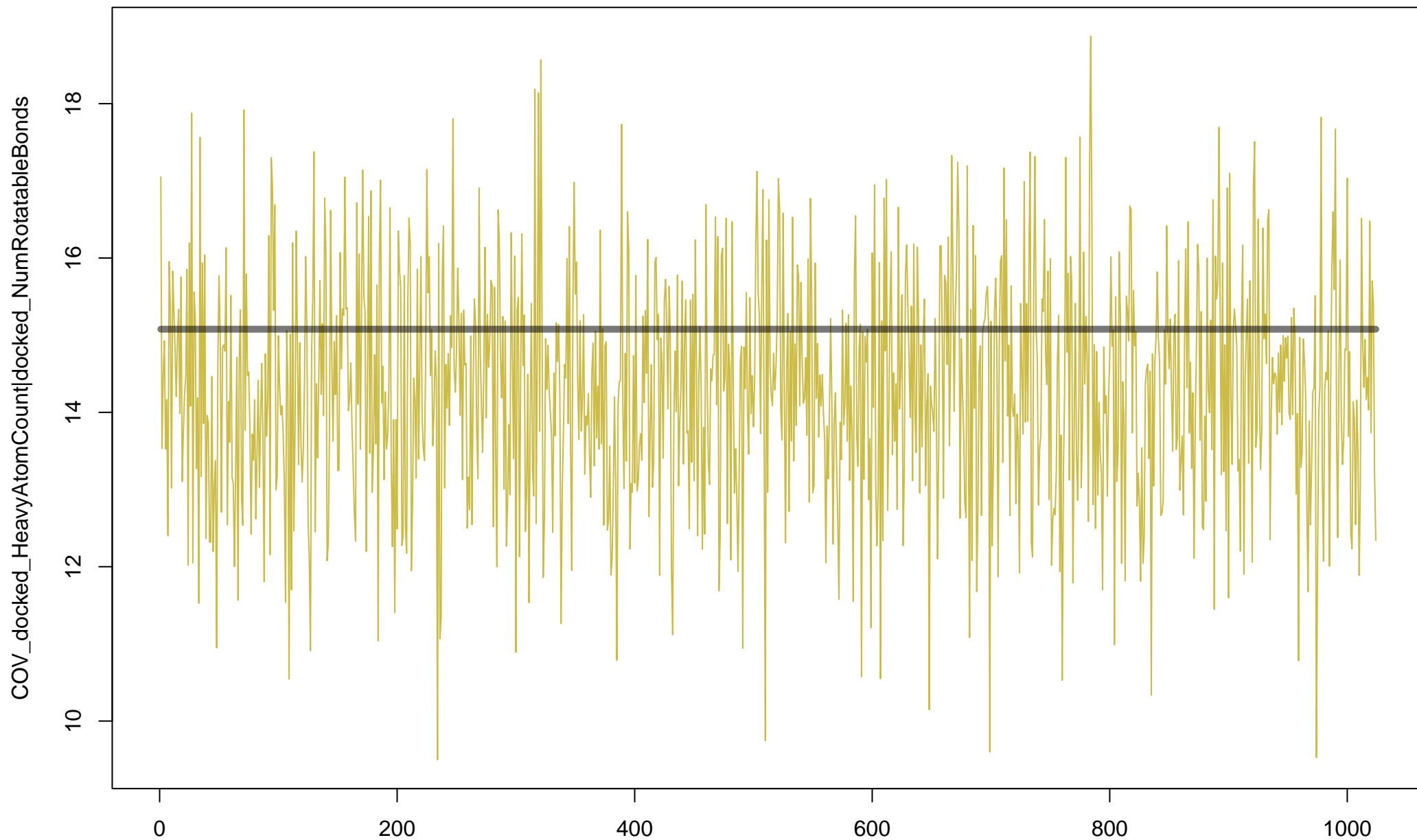
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0699 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | rel.err: 0.481



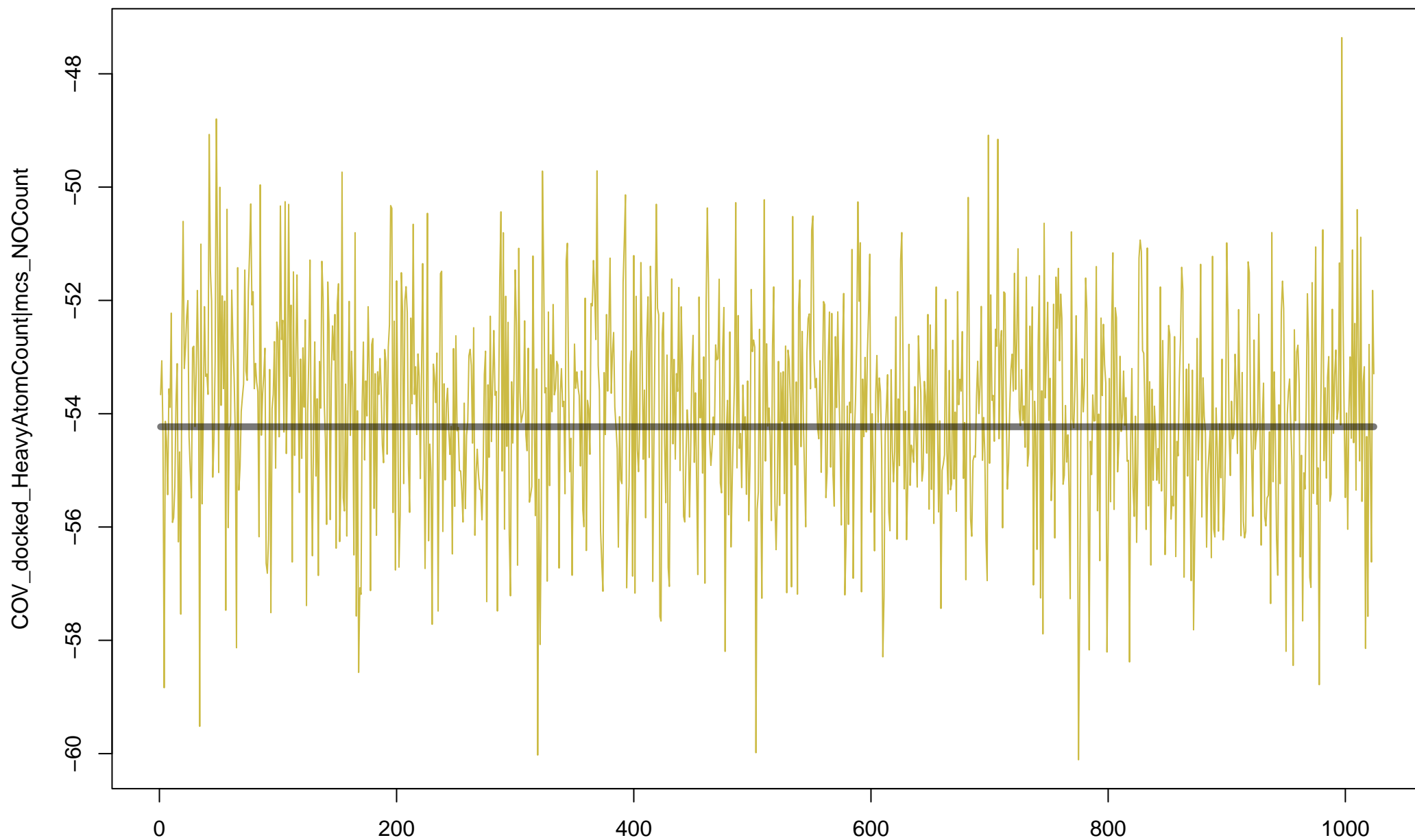
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0468 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0 | rel.err: 0.145



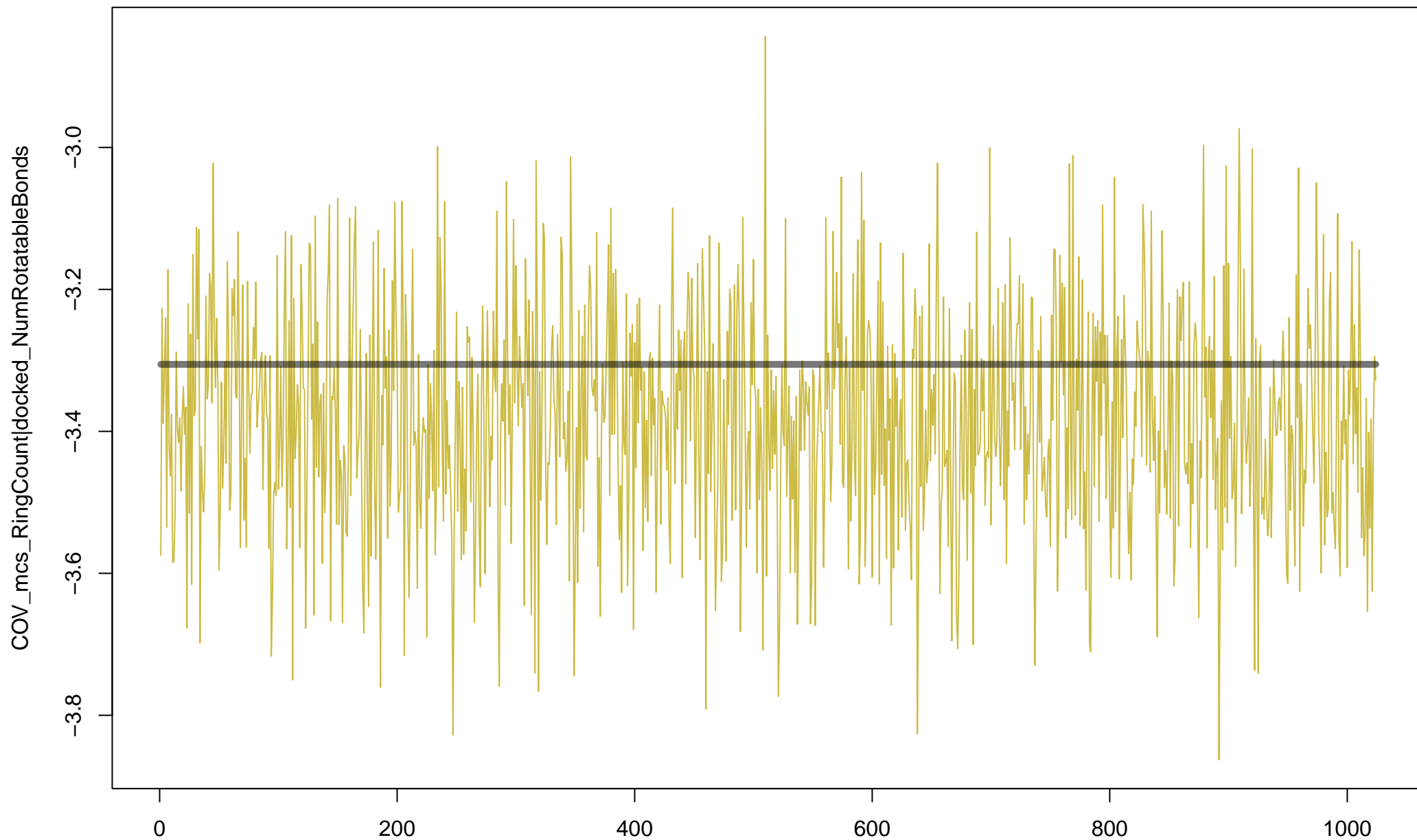
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0399 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | rel.err: -0.532



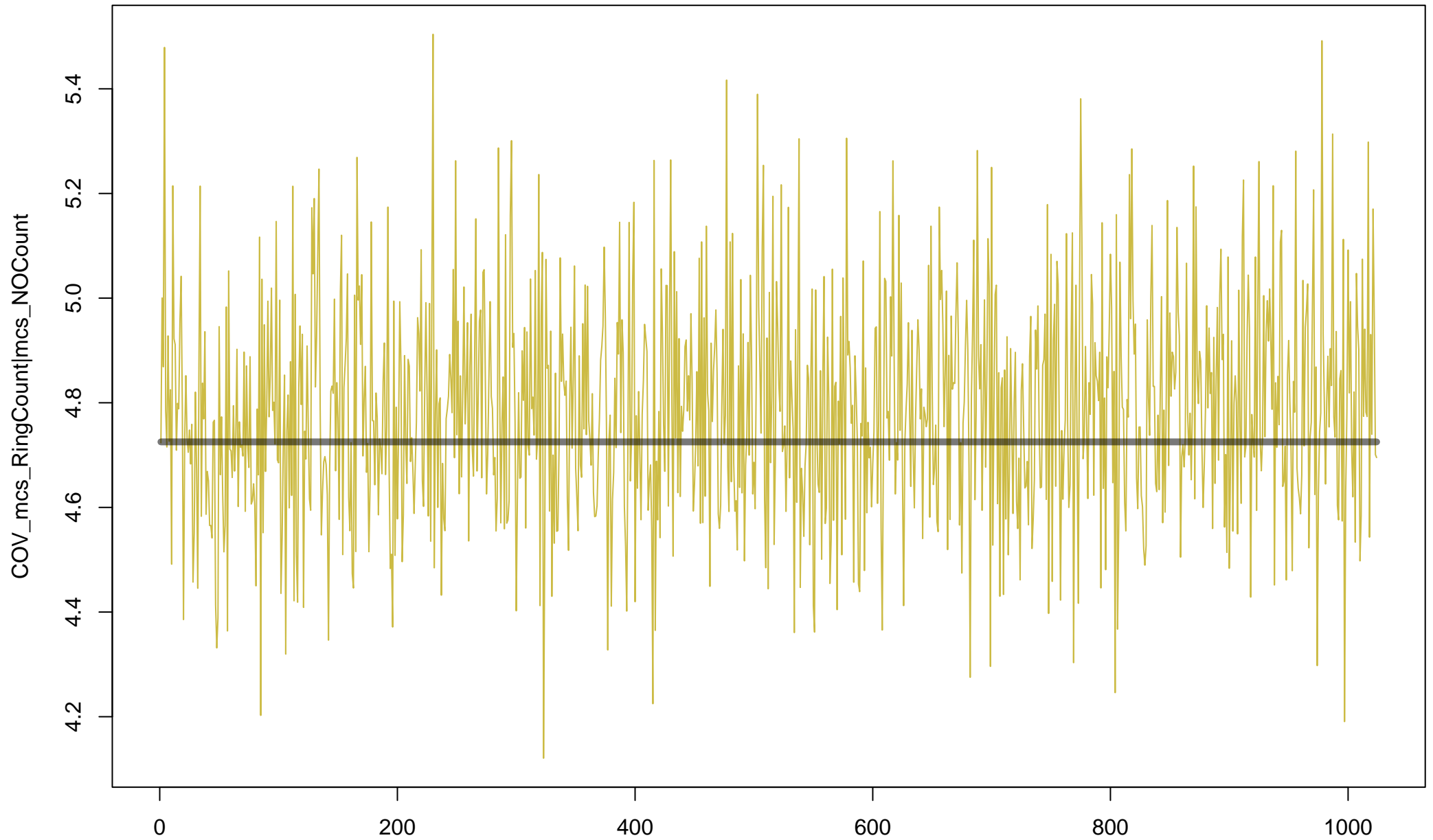
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0757 | MCSE(6.27) = 3.64 | stat: FALSE | burn: 0 | rel.err: 0.15



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0634 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0 | rel.err: -0.501



COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.0503 | MCSE(6.27) = 3.14 | stat: FALSE | burn: 0 | rel.err: 0.294



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0504 | MCSE(6.27) = 3.46 | stat: TRUE | burn: 0 | rel.err: 1.05

