

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.808492560459473

max MCSE = 8.76782022412296

all stationary: FALSE

burn: 1020

max rel.err.: 2.68916963668643

-- STATS 1D --

min ESS = 422.283802155624

max BMK = 0.0915434211850822

max MCSE = 5.25629342841456

all stationary: FALSE

burn: 0

max rel.err.: 1.98183914562511

-- STATS 2D --

min ESS = 768.491819695418

max BMK = 0.0875242192977565

max MCSE = 3.74690222722519

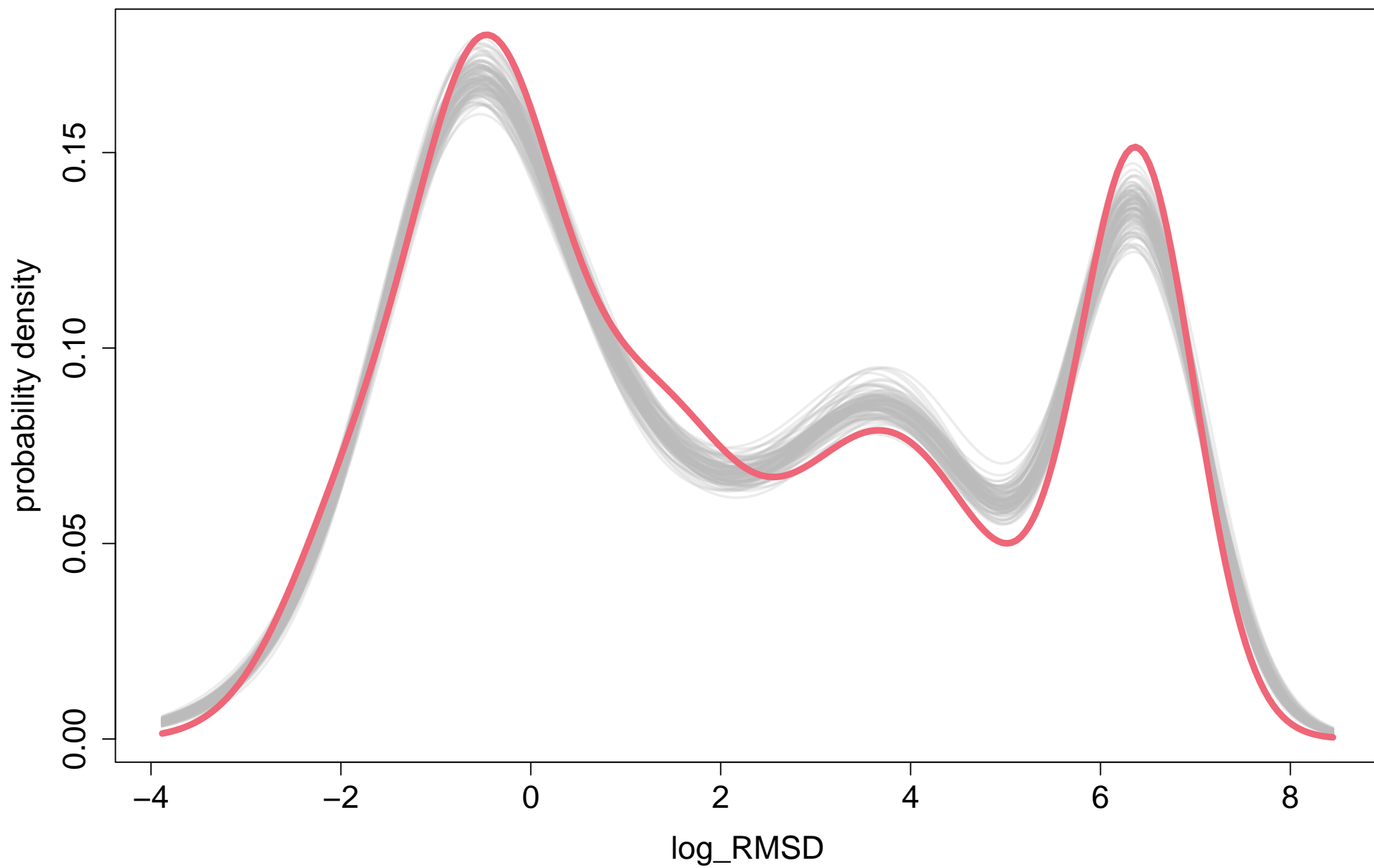
all stationary: FALSE

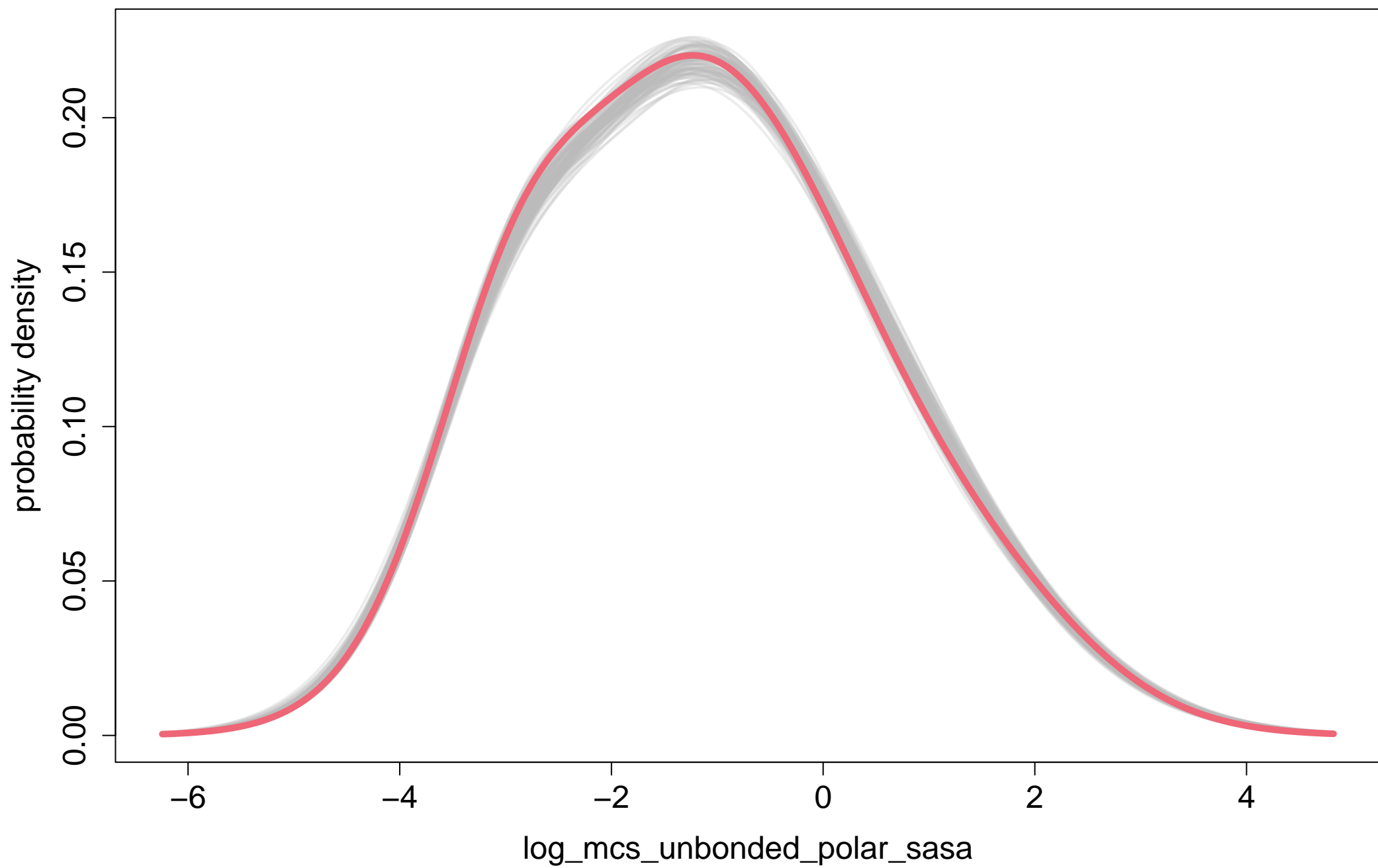
burn: 0

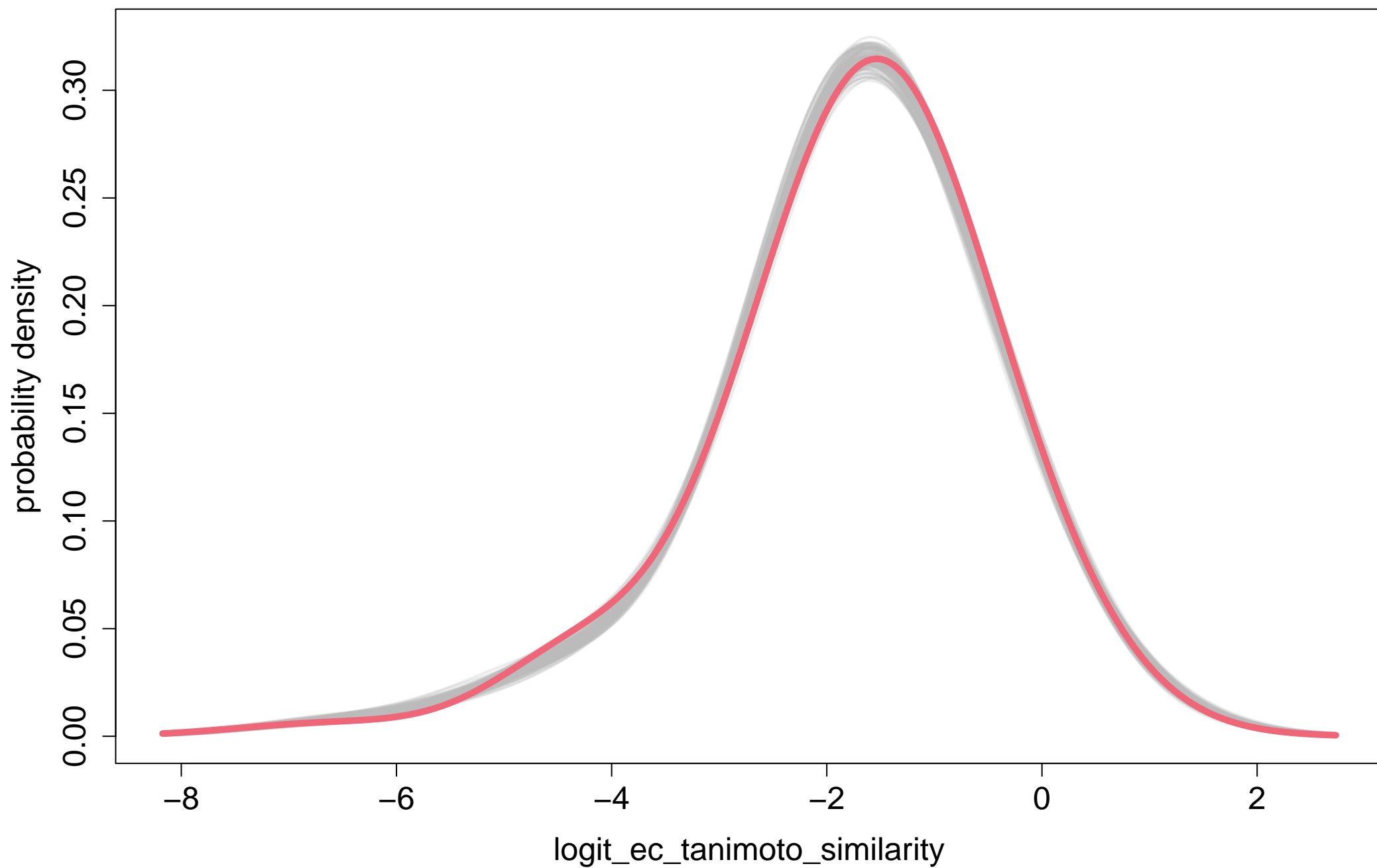
max rel.err.: 2.26905805916358

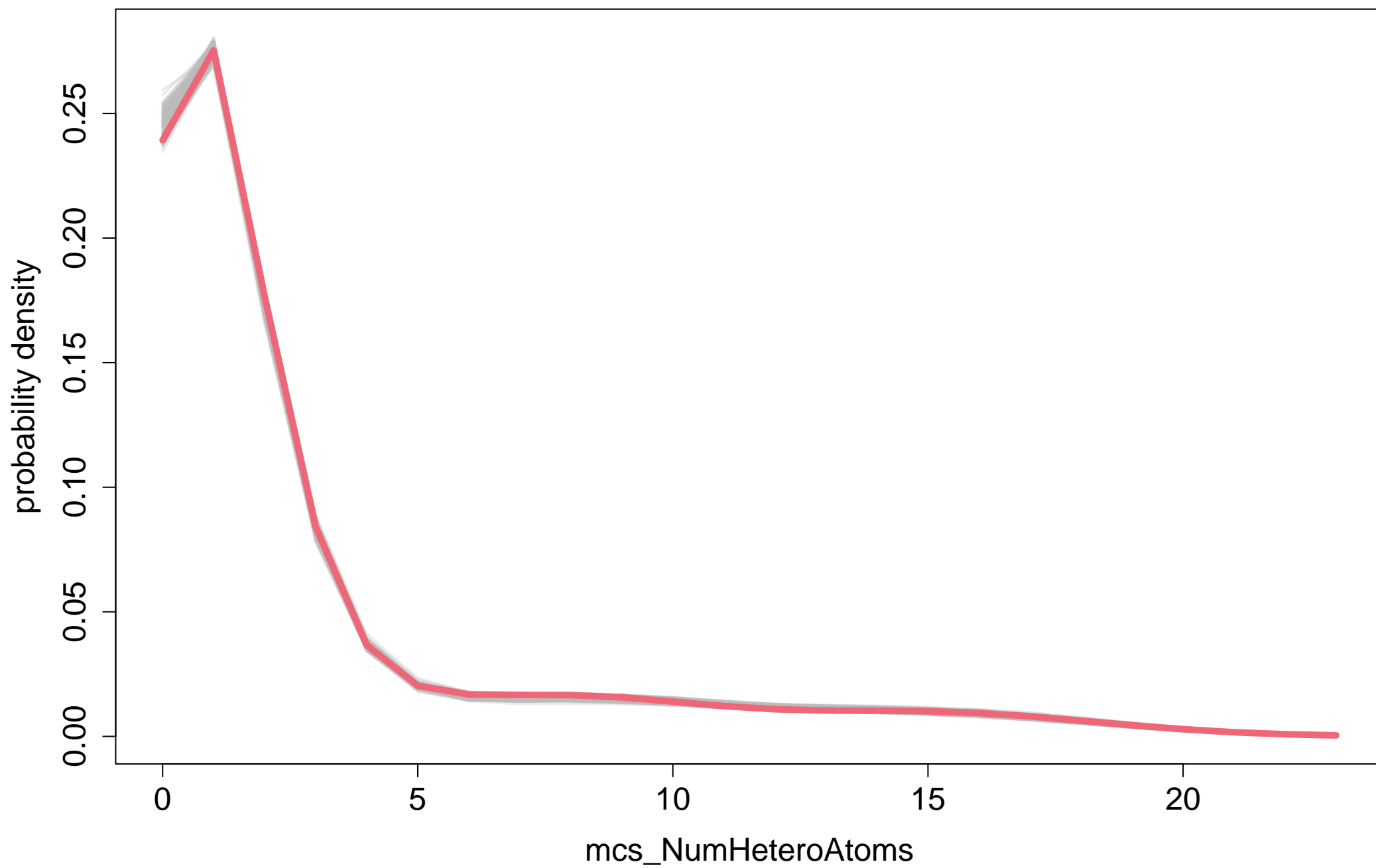
Occupied clusters: 24 of 64

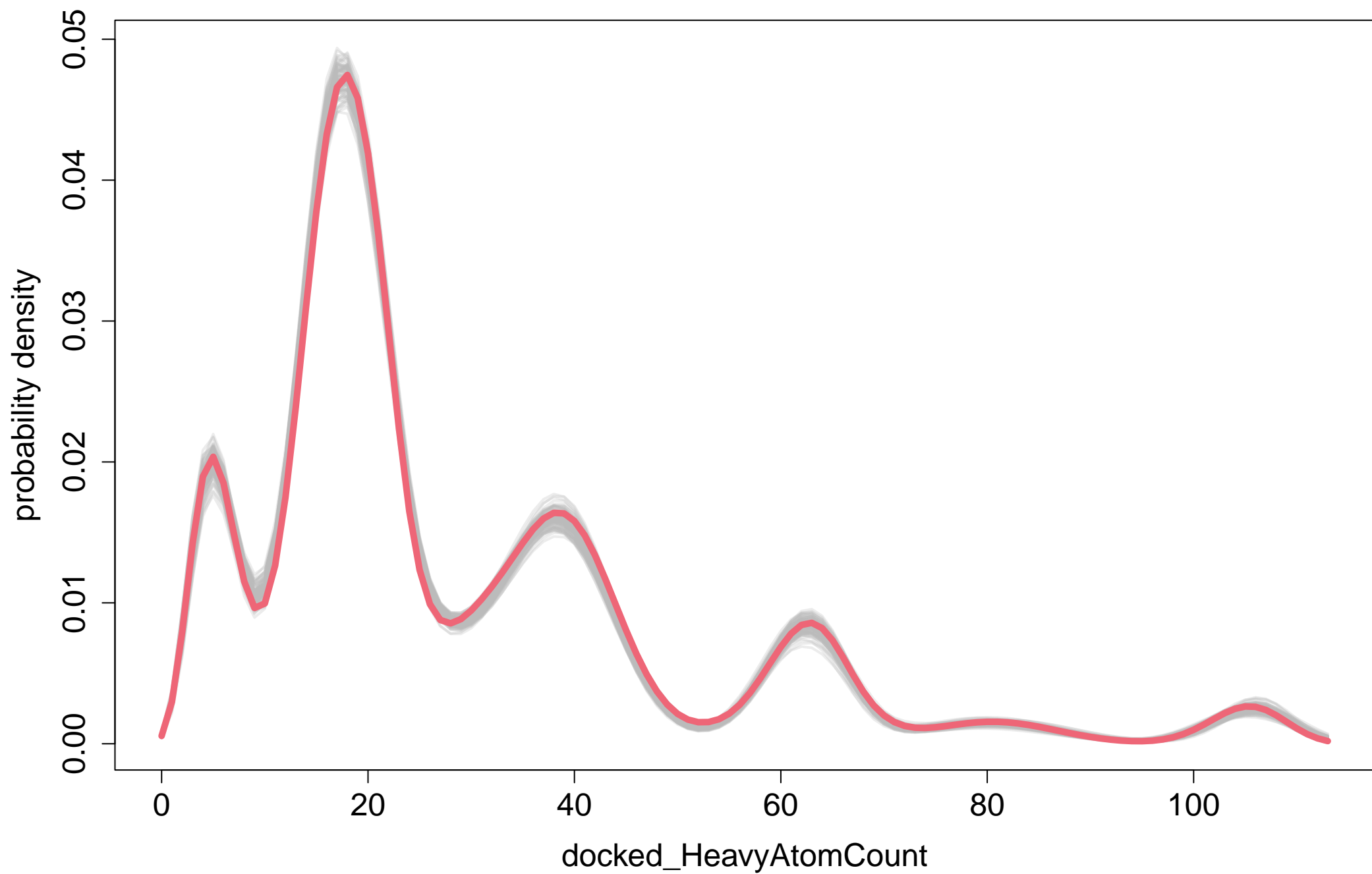
LL: -64200 +- 19.1

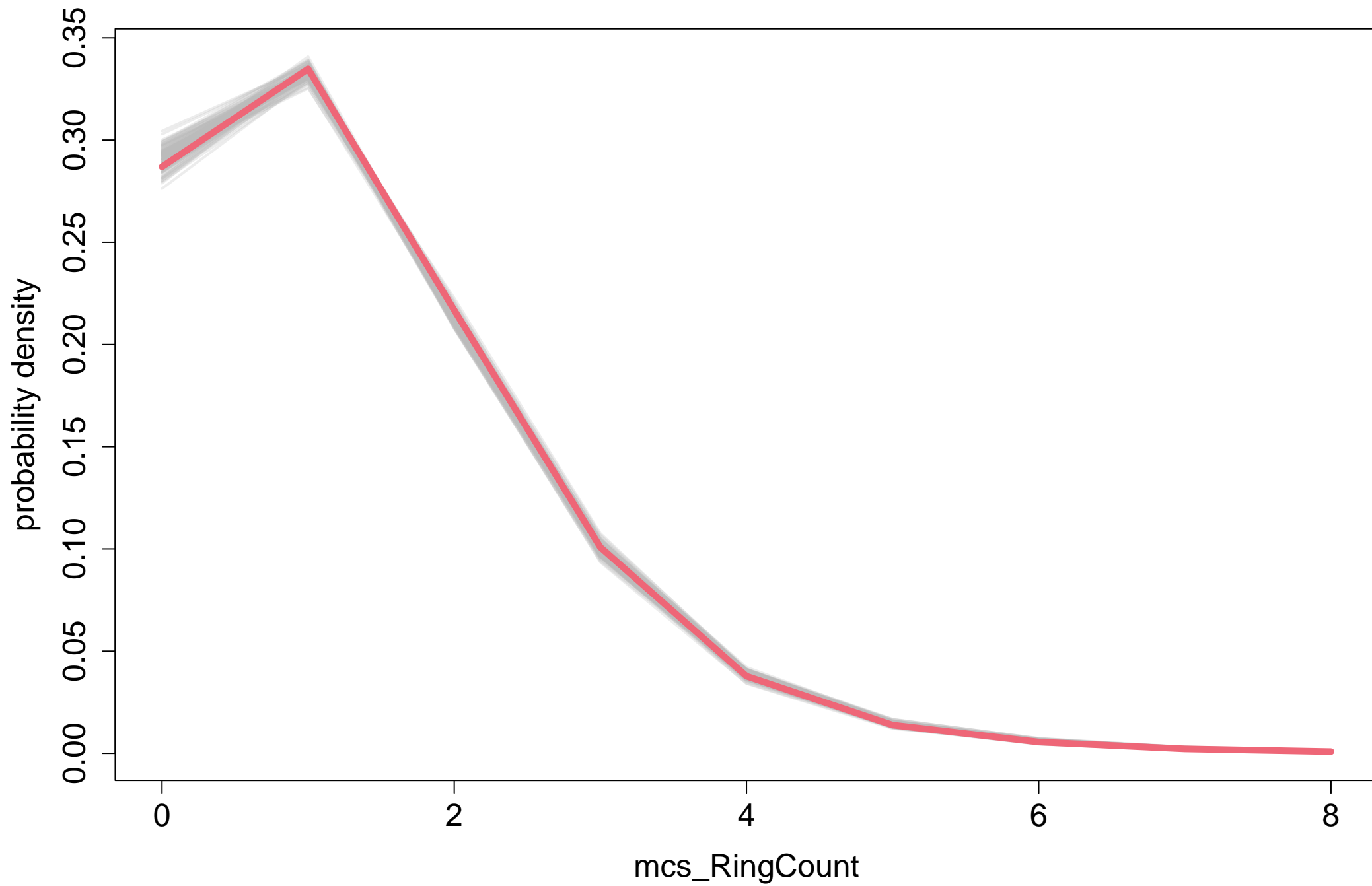


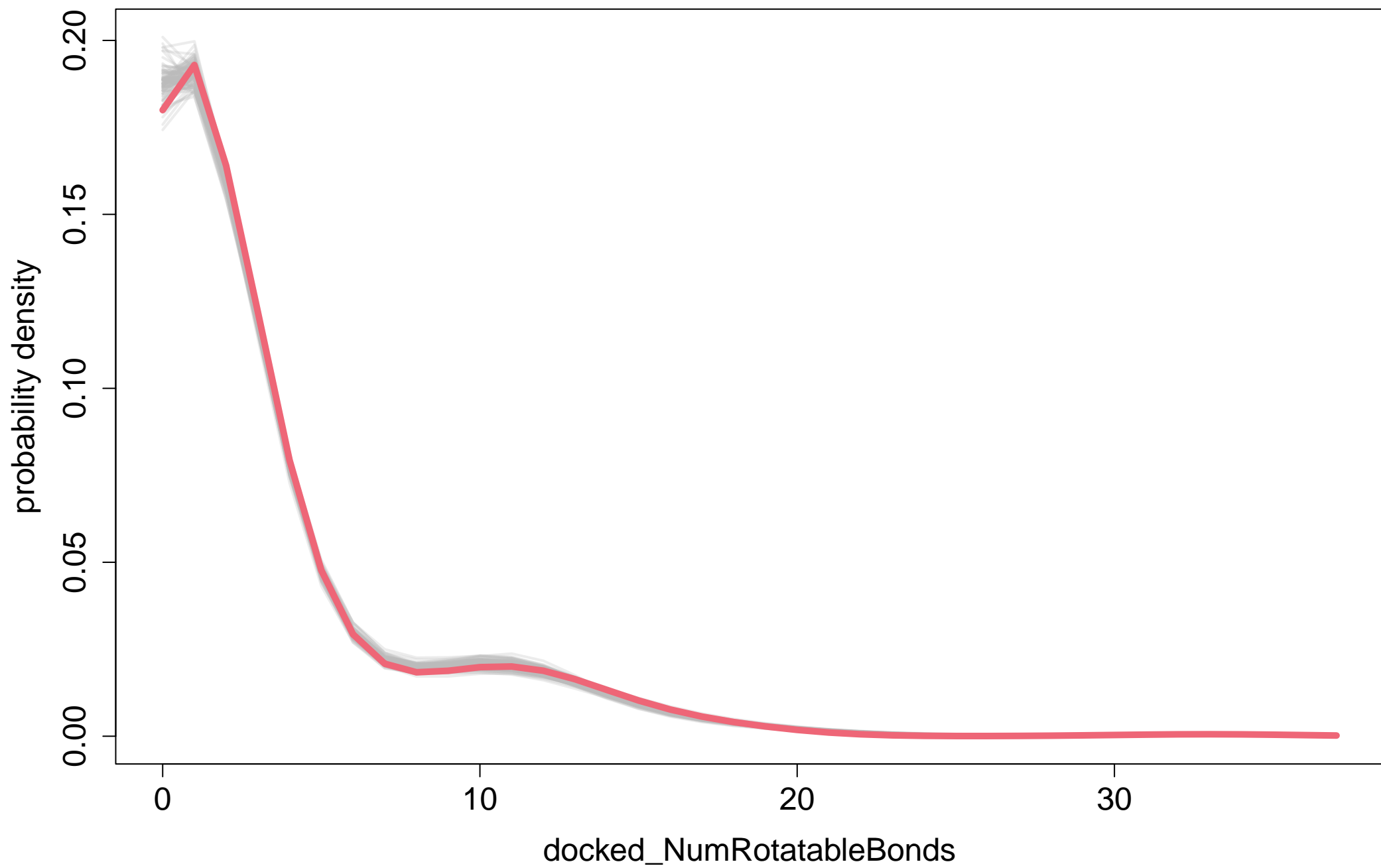


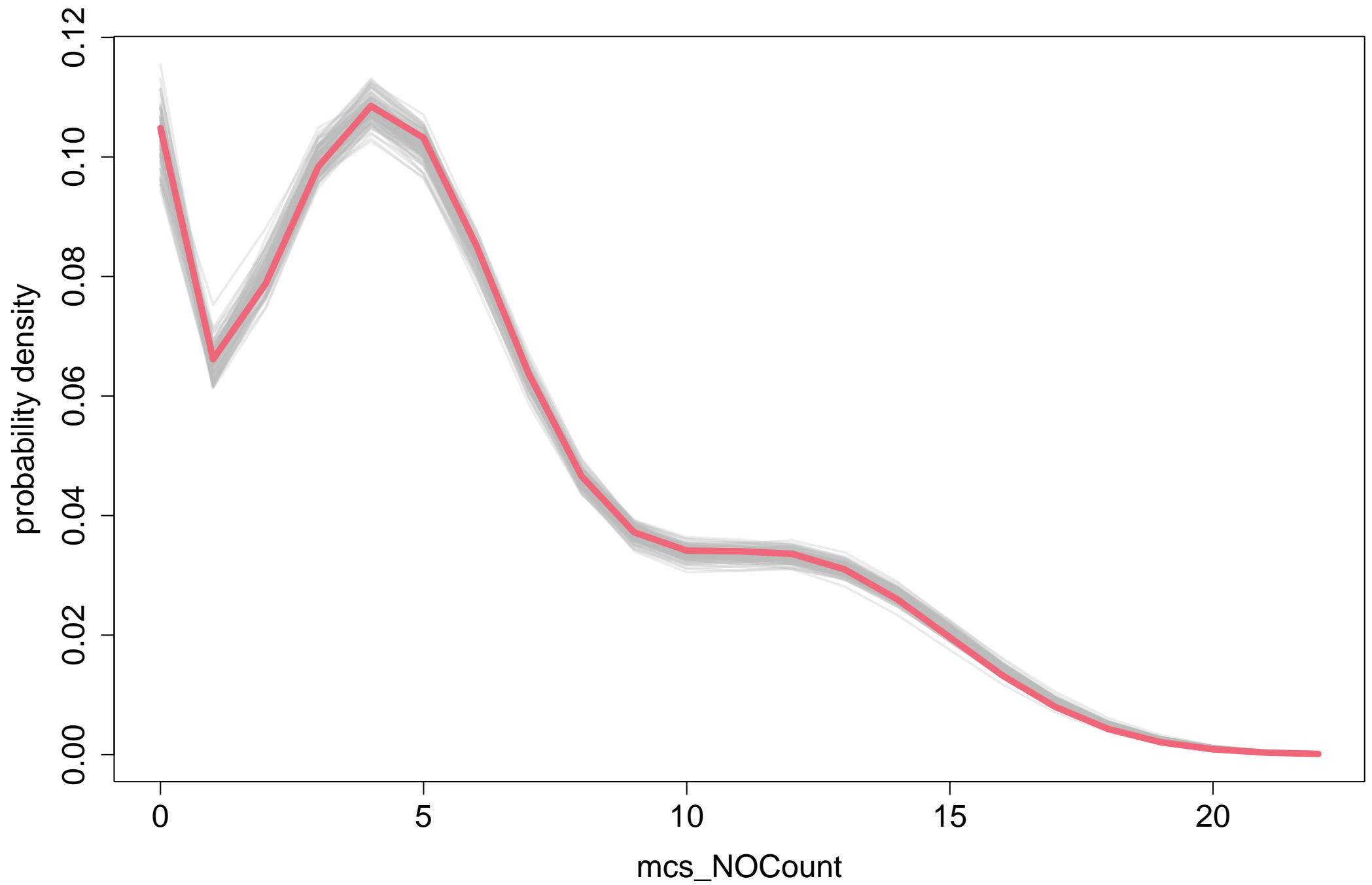


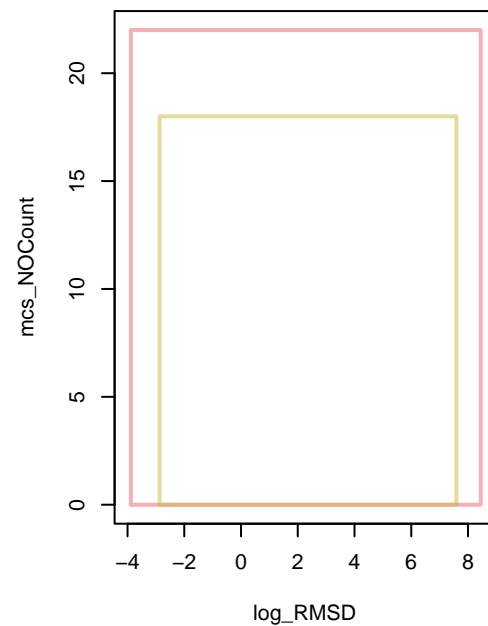
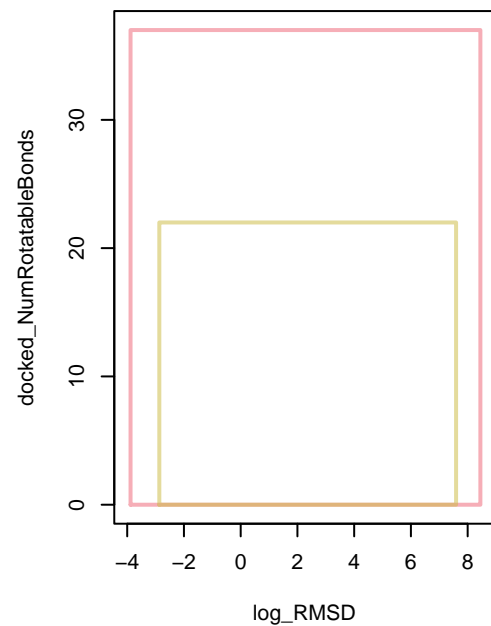
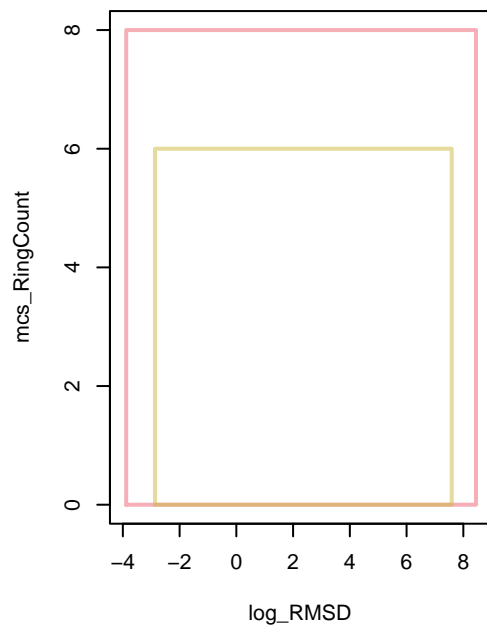
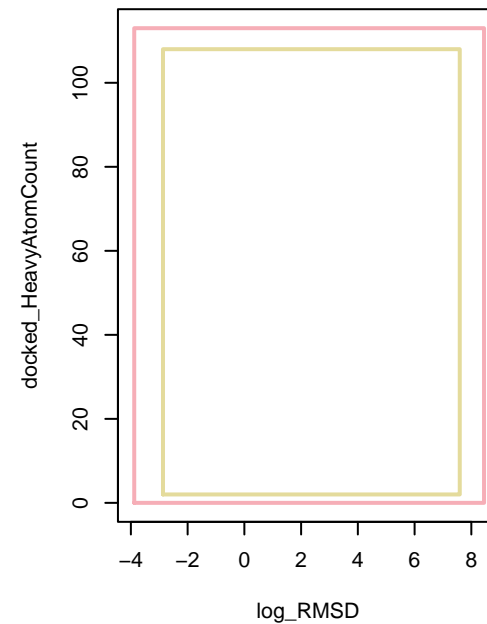
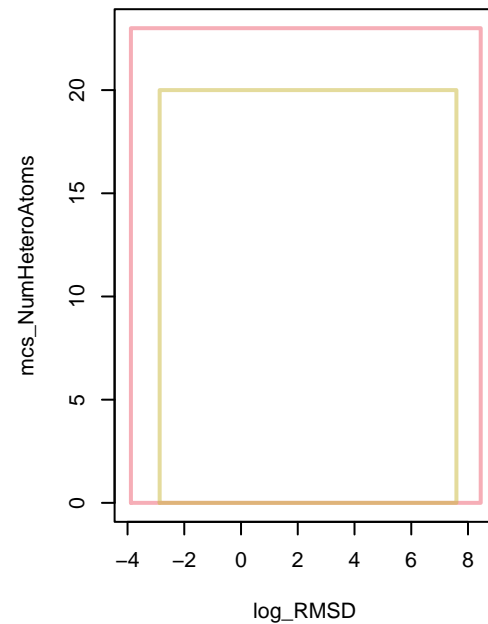
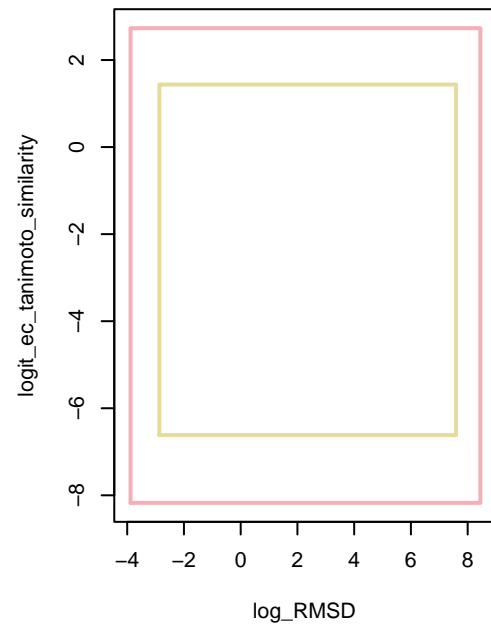
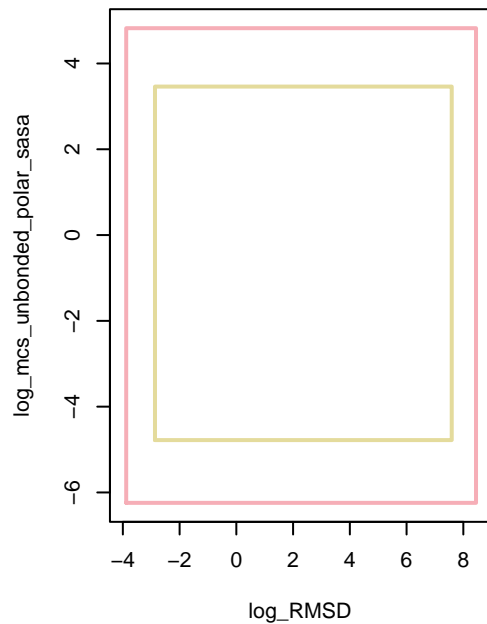




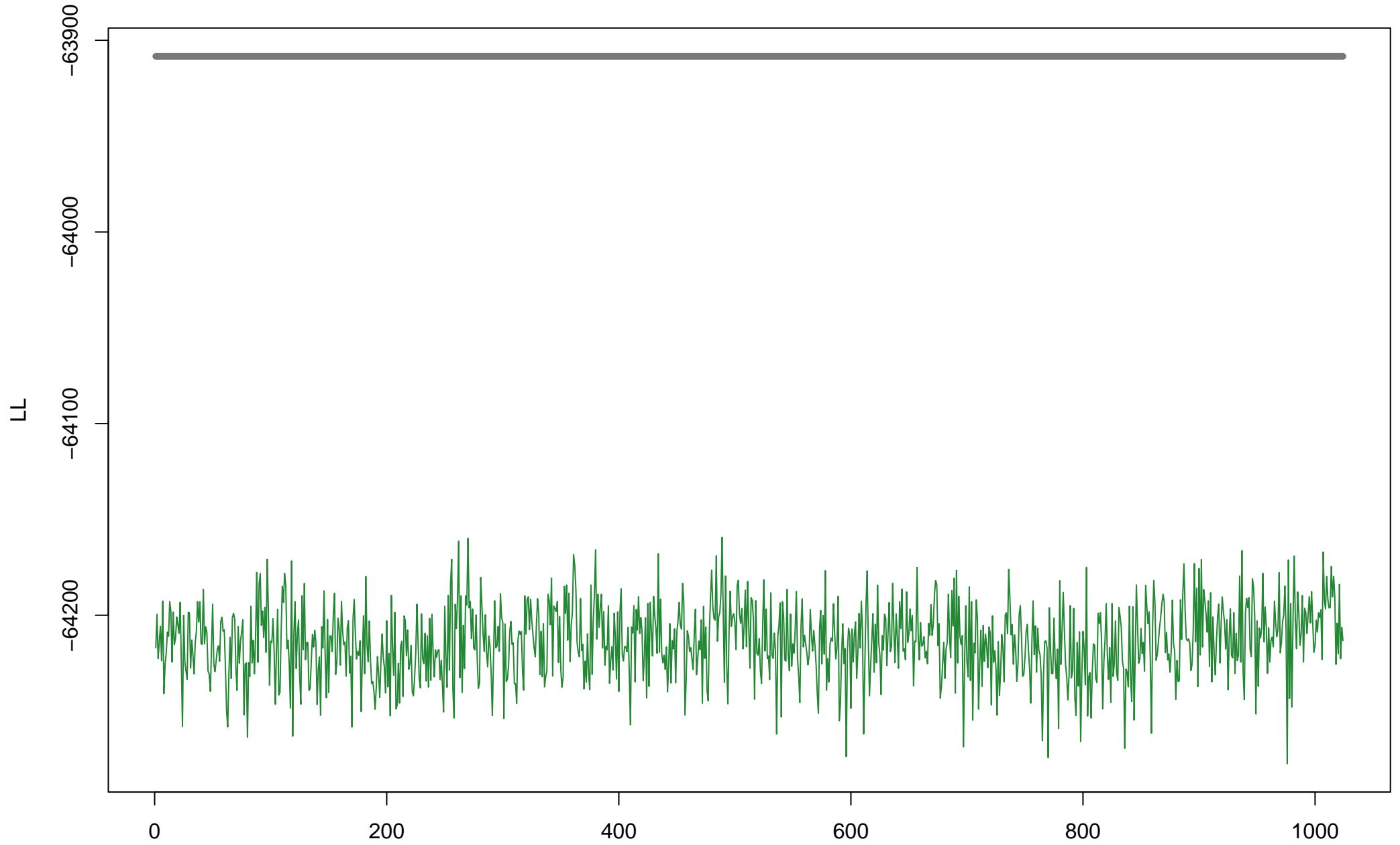






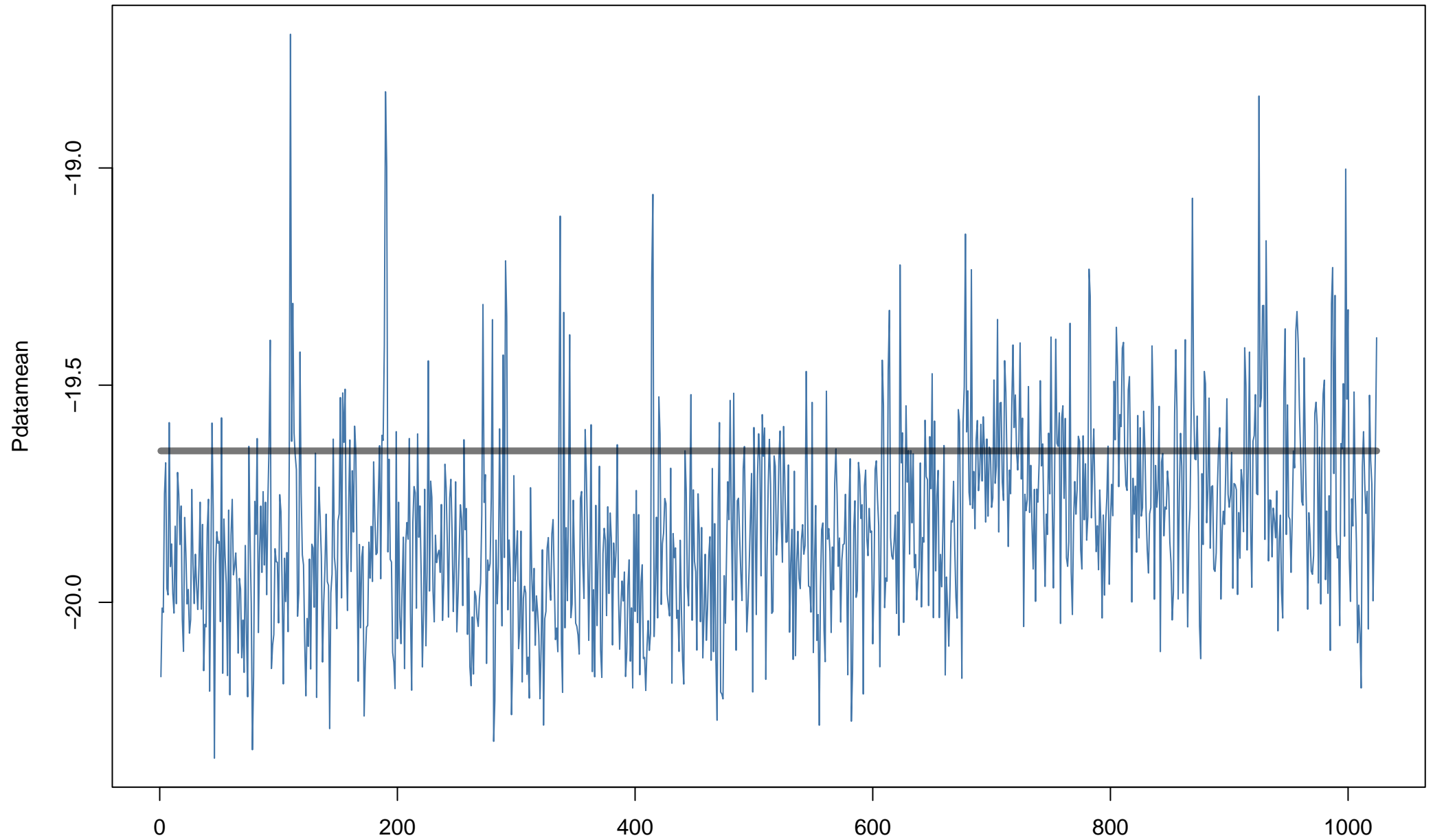


LL



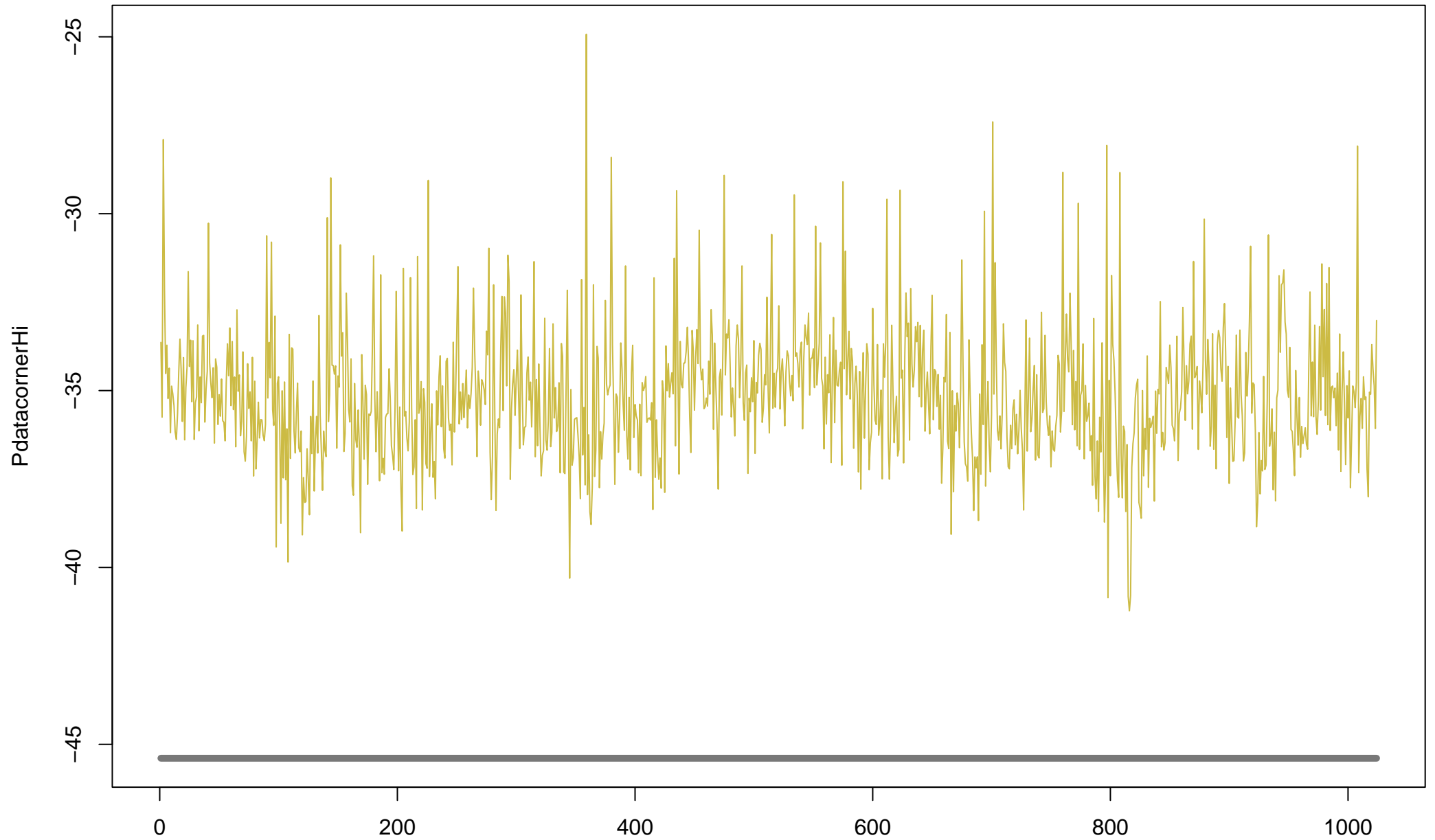
Pdatamean

ESS = 2.22e-16 | BMK = 0.267 | MCSE(6.27) = 6.91 | stat: TRUE | burn: 0 | rel.err: -0.642



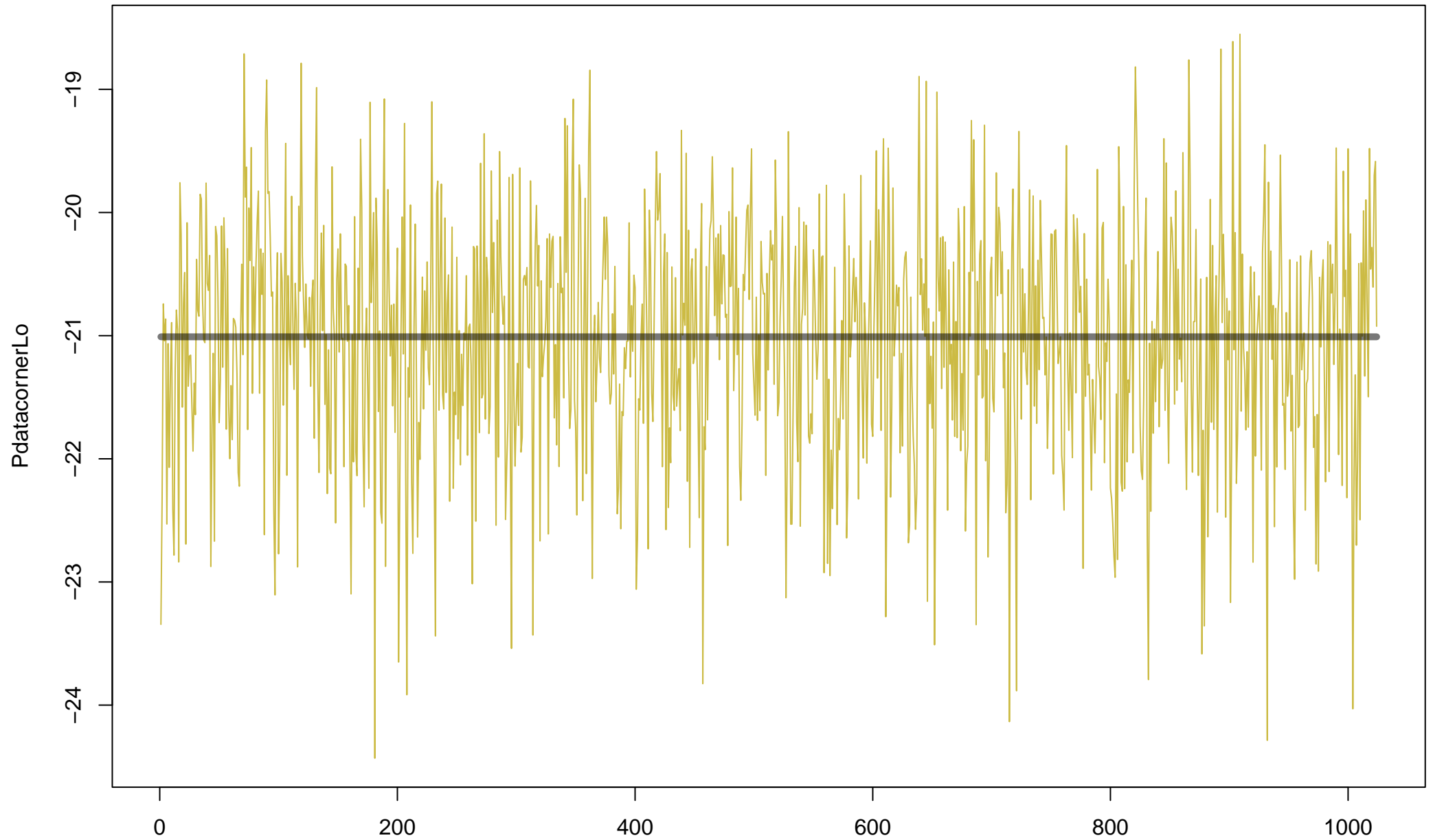
PdatacornerHi

ESS = 2.22e-16 | BMK = 0.808 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 1020 | rel.err: 0.0487

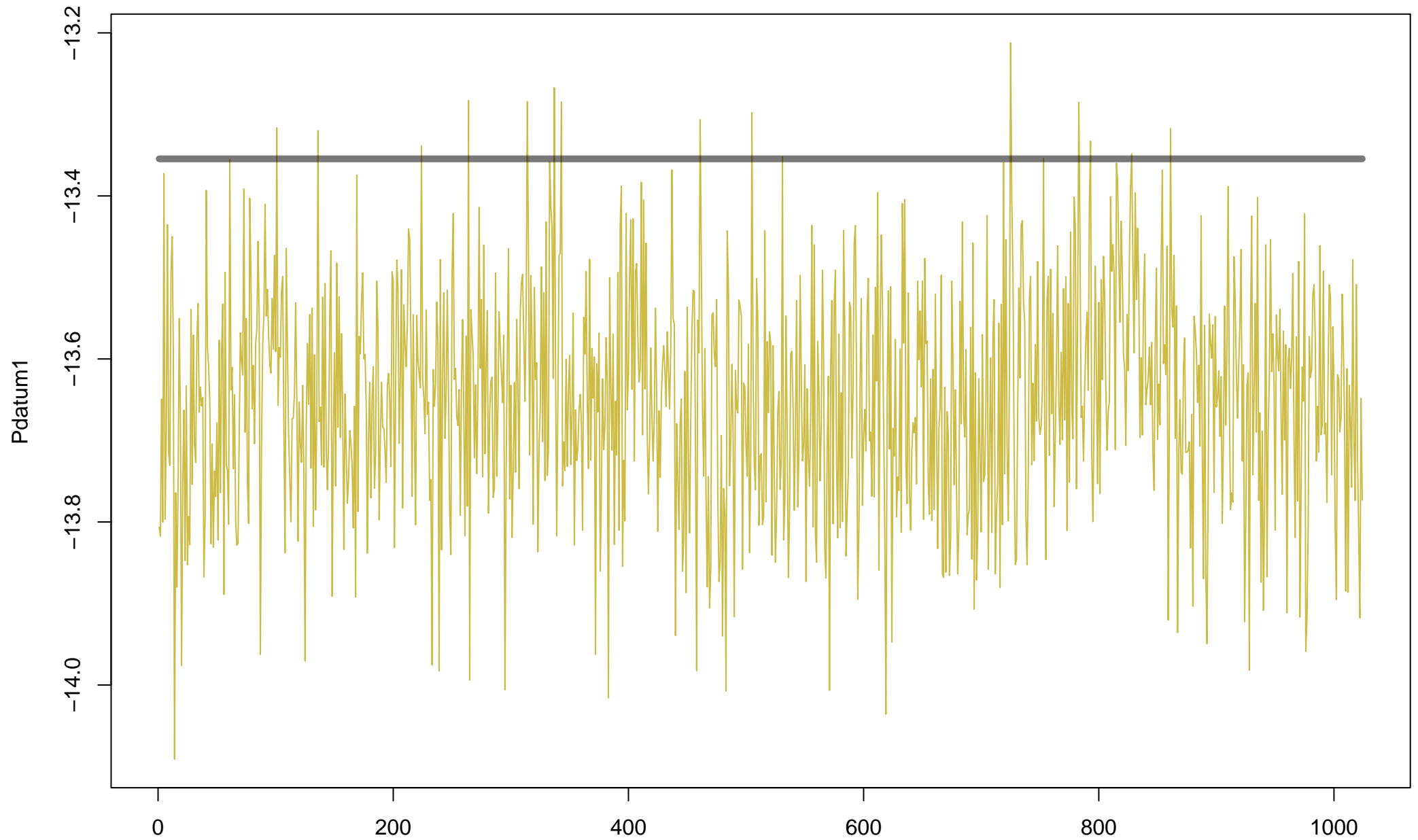


PdatacornerLo

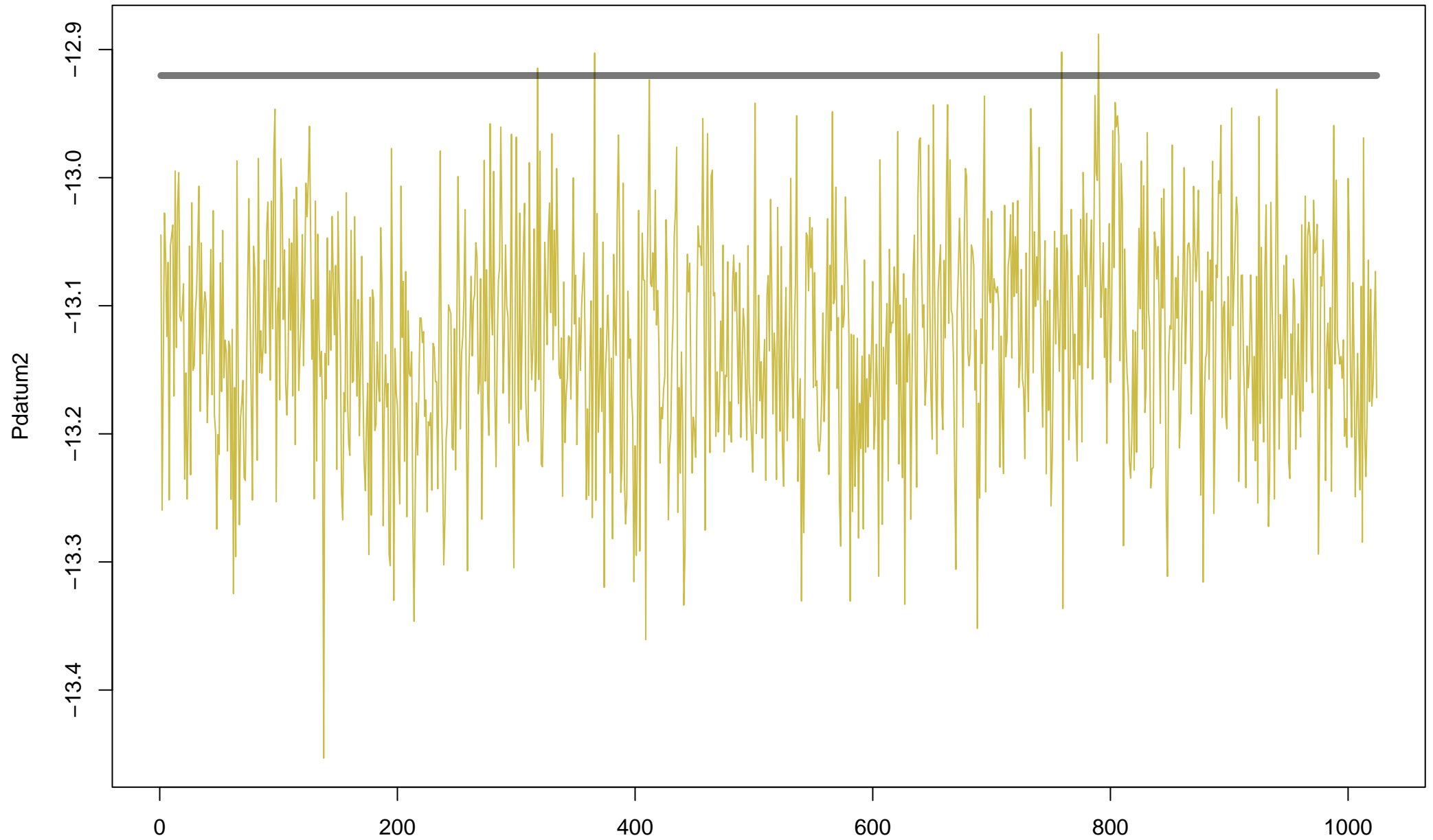
ESS = 2.22e-16 | BMK = 0.0789 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0 | rel.err: 0.307



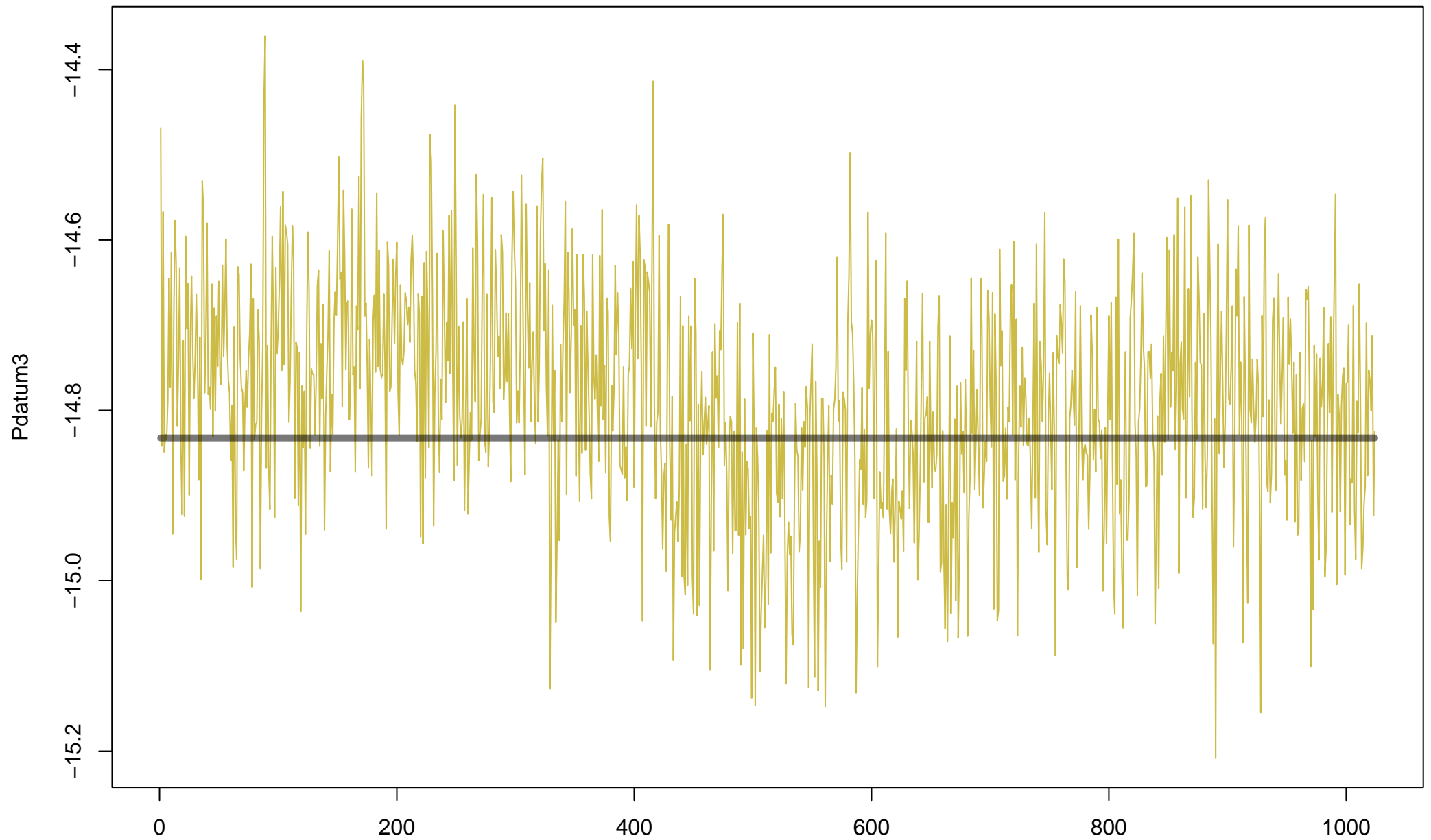
Pdatum1
ESS = 368 | BMK = 0.0652 | MCSE(6.27) = 5 | stat: TRUE | burn: 0 | rel.err: -2.41



Pdatum2
ESS = 189 | BMK = 0.0651 | MCSE(6.27) = 4.87 | stat: TRUE | burn: 0 | rel.err: -2.69

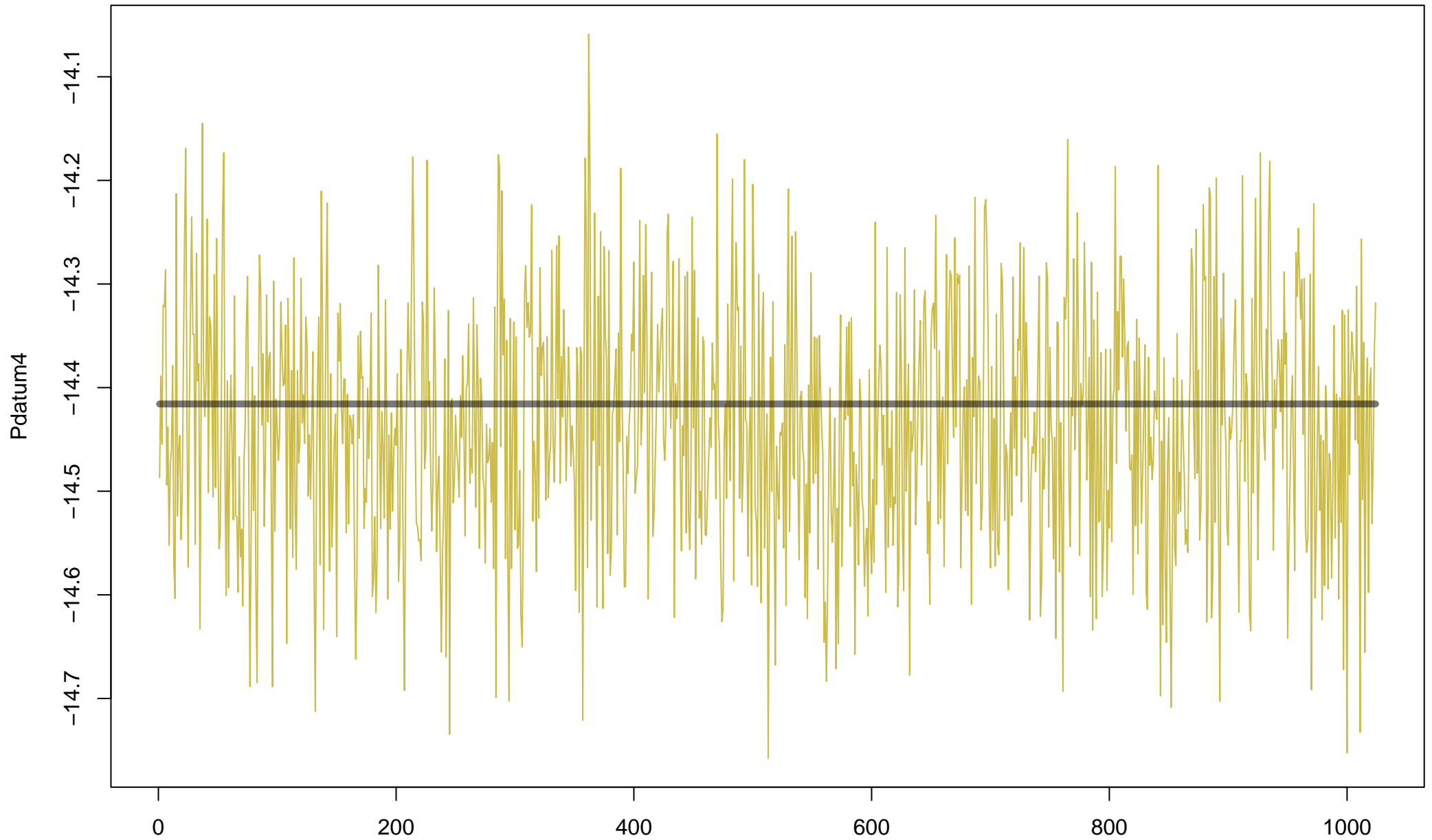


Pdatum3
ESS = 60.5 | BMK = 0.19 | MCSE(6.27) = 7.78 | stat: FALSE | burn: 0 | rel.err: 0.374



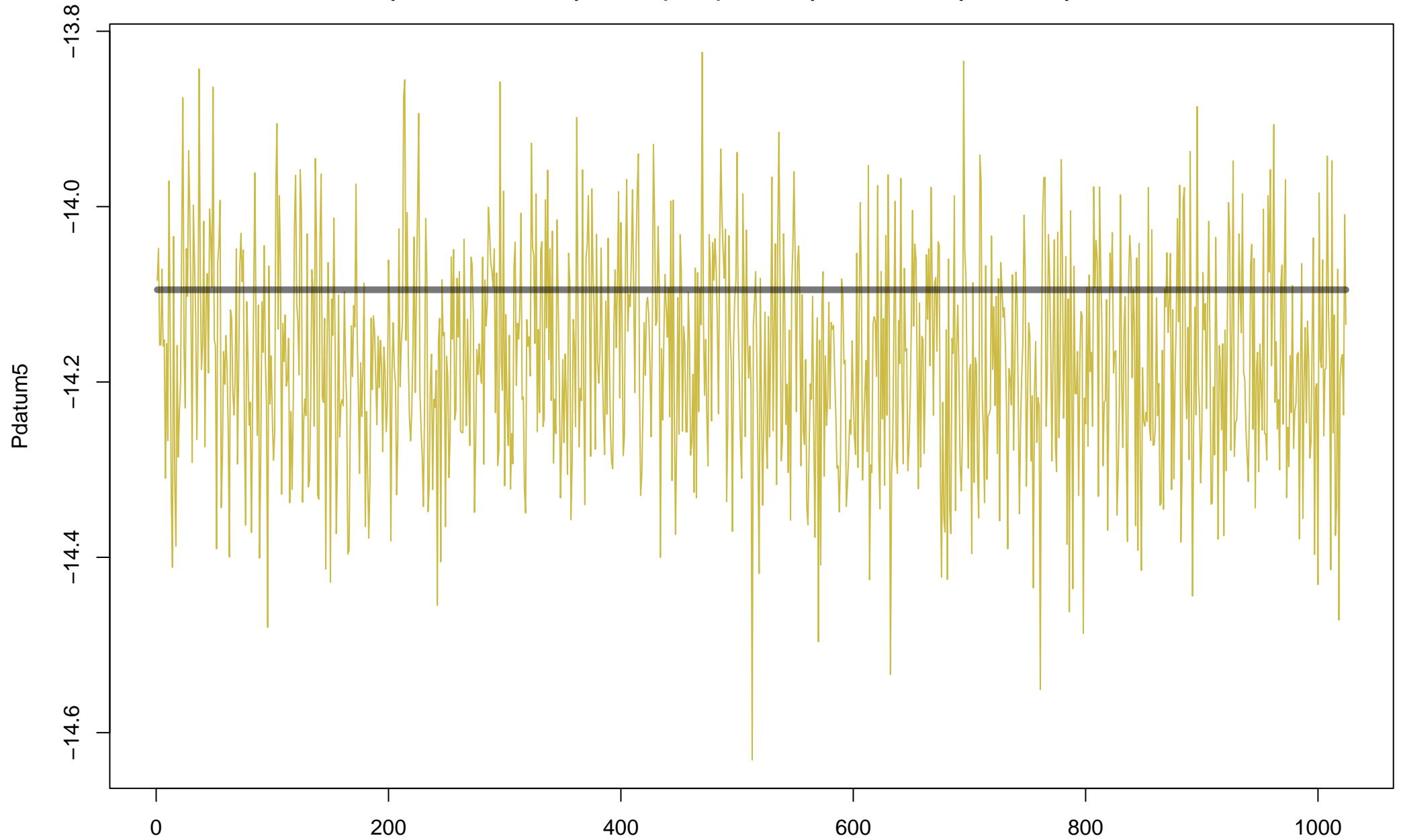
Pdatum4

ESS = 887 | BMK = 0.0461 | MCSE(6.27) = 4 | stat: TRUE | burn: 0 | rel.err: -0.141



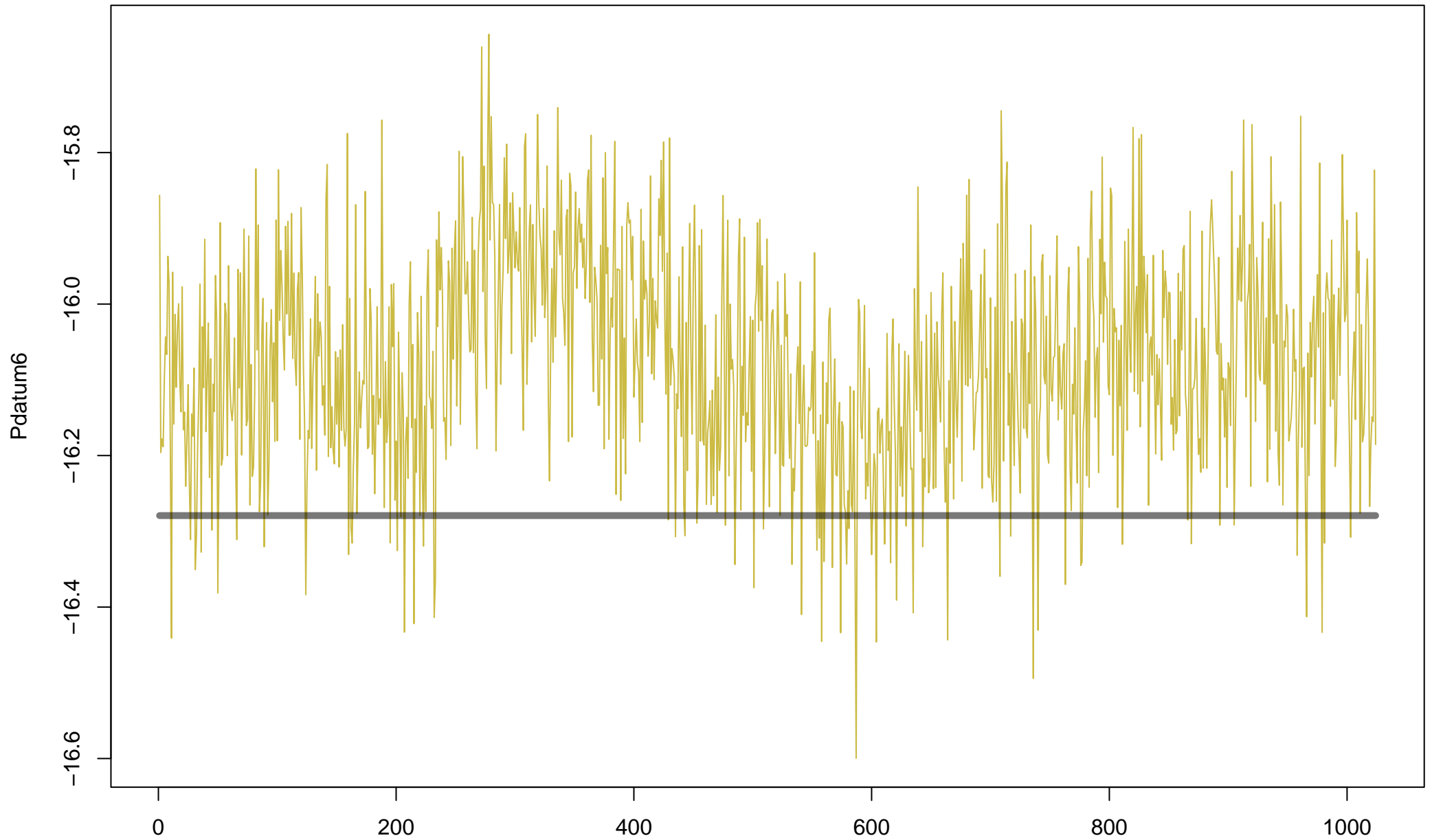
Pdatum5

ESS = 956 | BMK = 0.0865 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0 | rel.err: -0.628



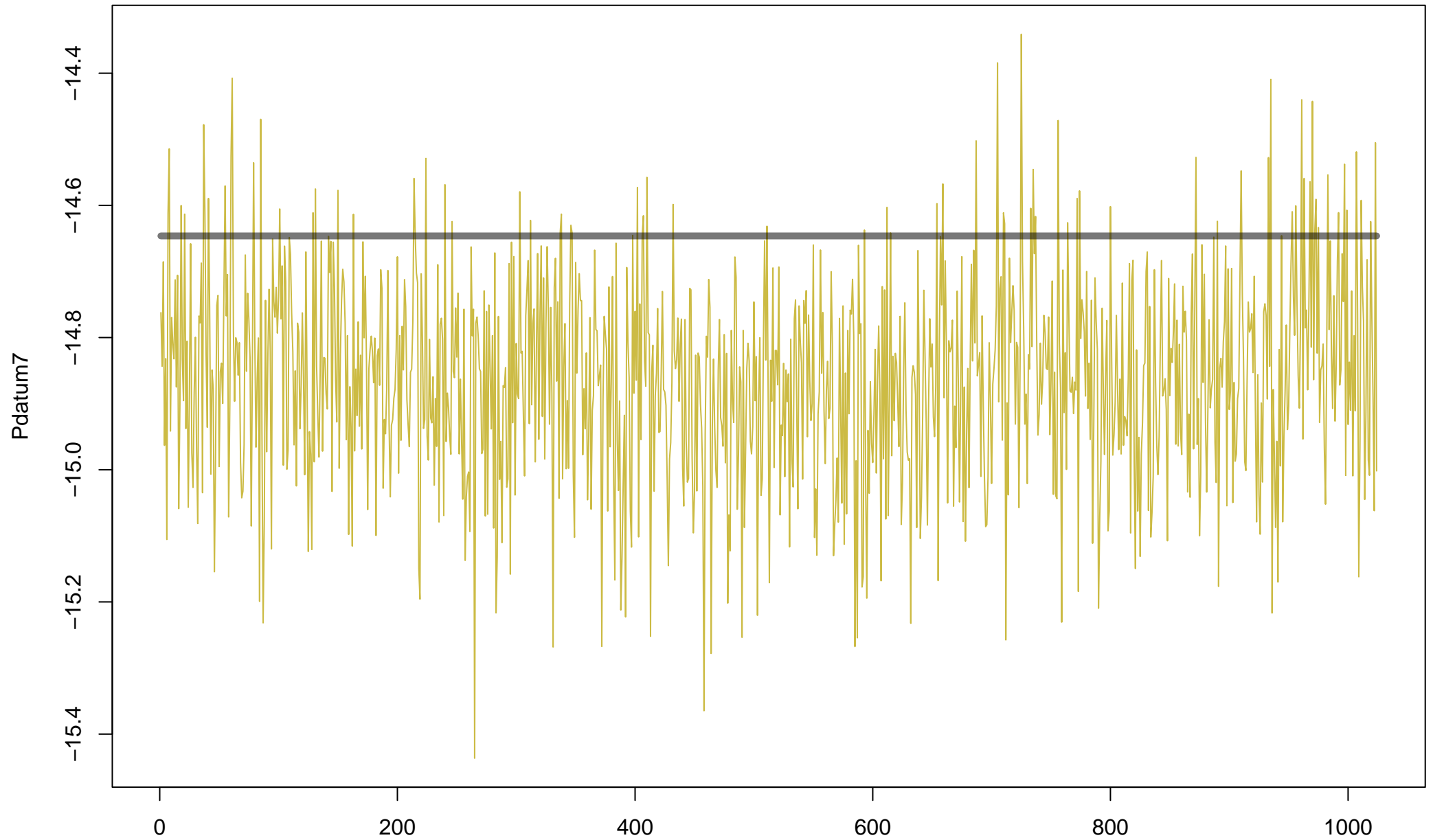
Pdatum6

ESS = 2.22e-16 | BMK = 0.128 | MCSE(6.27) = 8.28 | stat: TRUE | burn: 0 | rel.err: 1.36



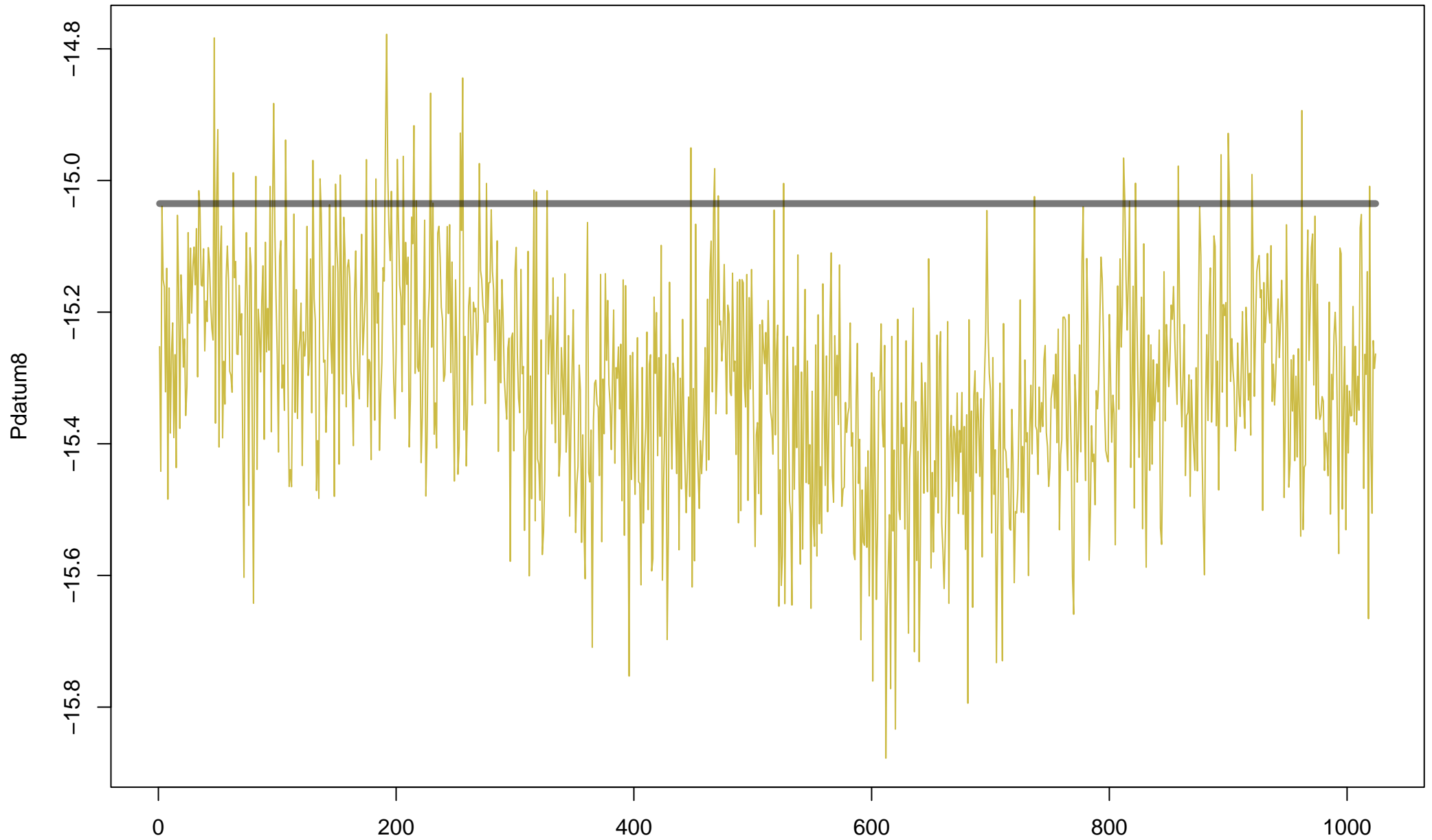
Pdatum7

ESS = 1020 | BMK = 0.0496 | MCSE(6.27) = 4.81 | stat: TRUE | burn: 0 | rel.err: -1.47



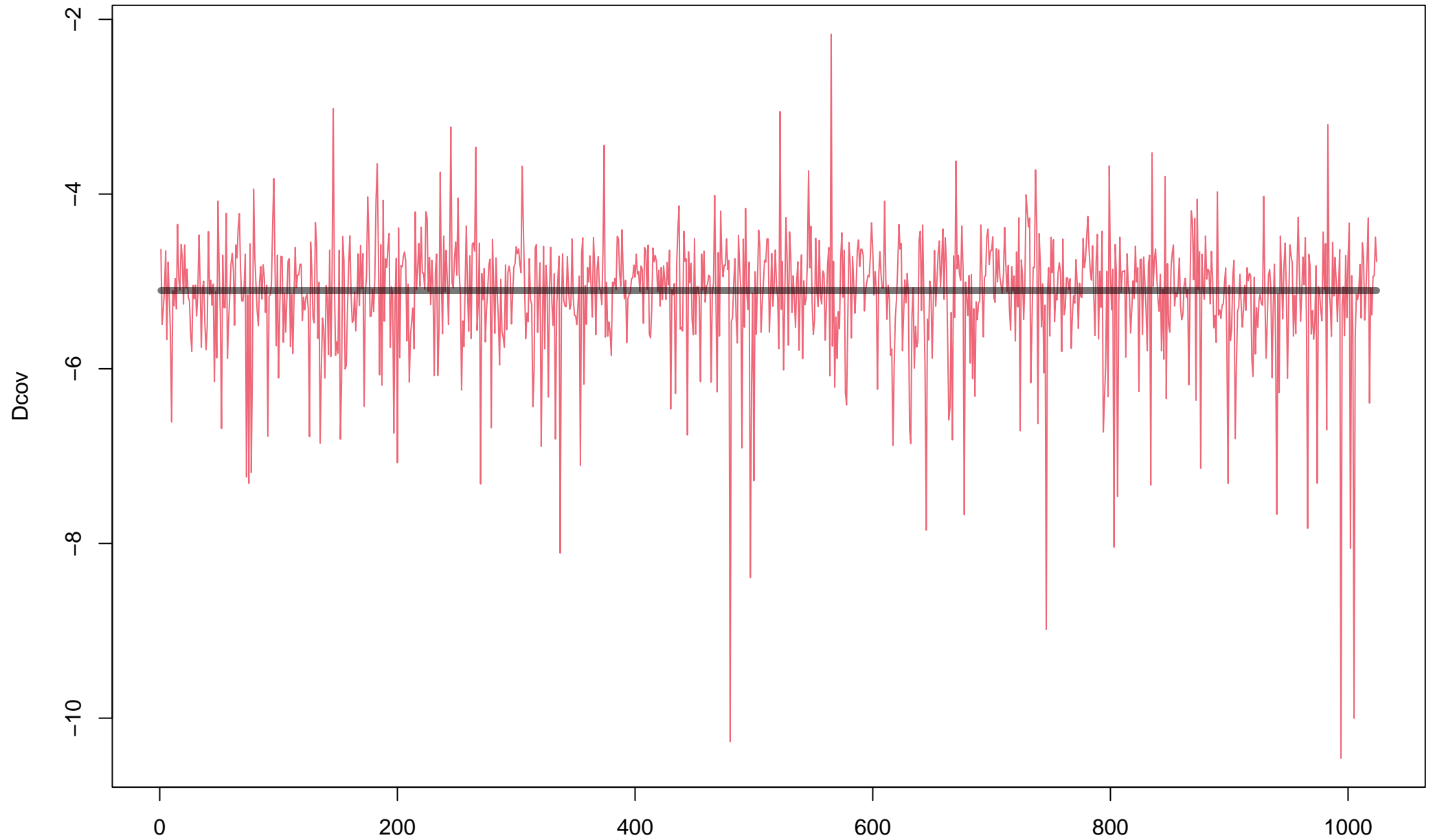
Pdatum8

ESS = 44.3 | BMK = 0.189 | MCSE(6.27) = 8.77 | stat: FALSE | burn: 0 | rel.err: -1.81



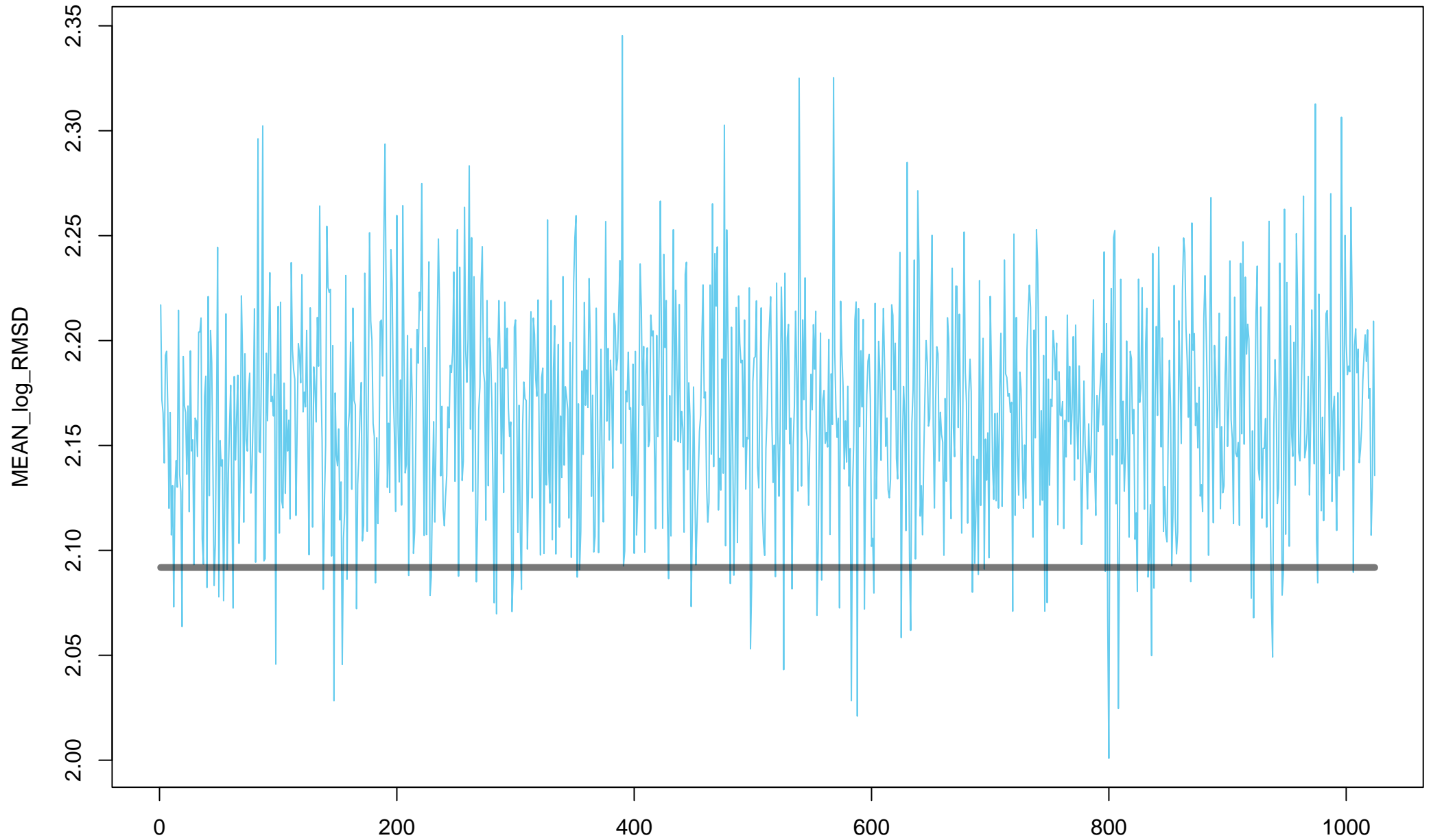
Dcov

ESS = 1020 | BMK = 0.114 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0 | rel.err: -0.0695

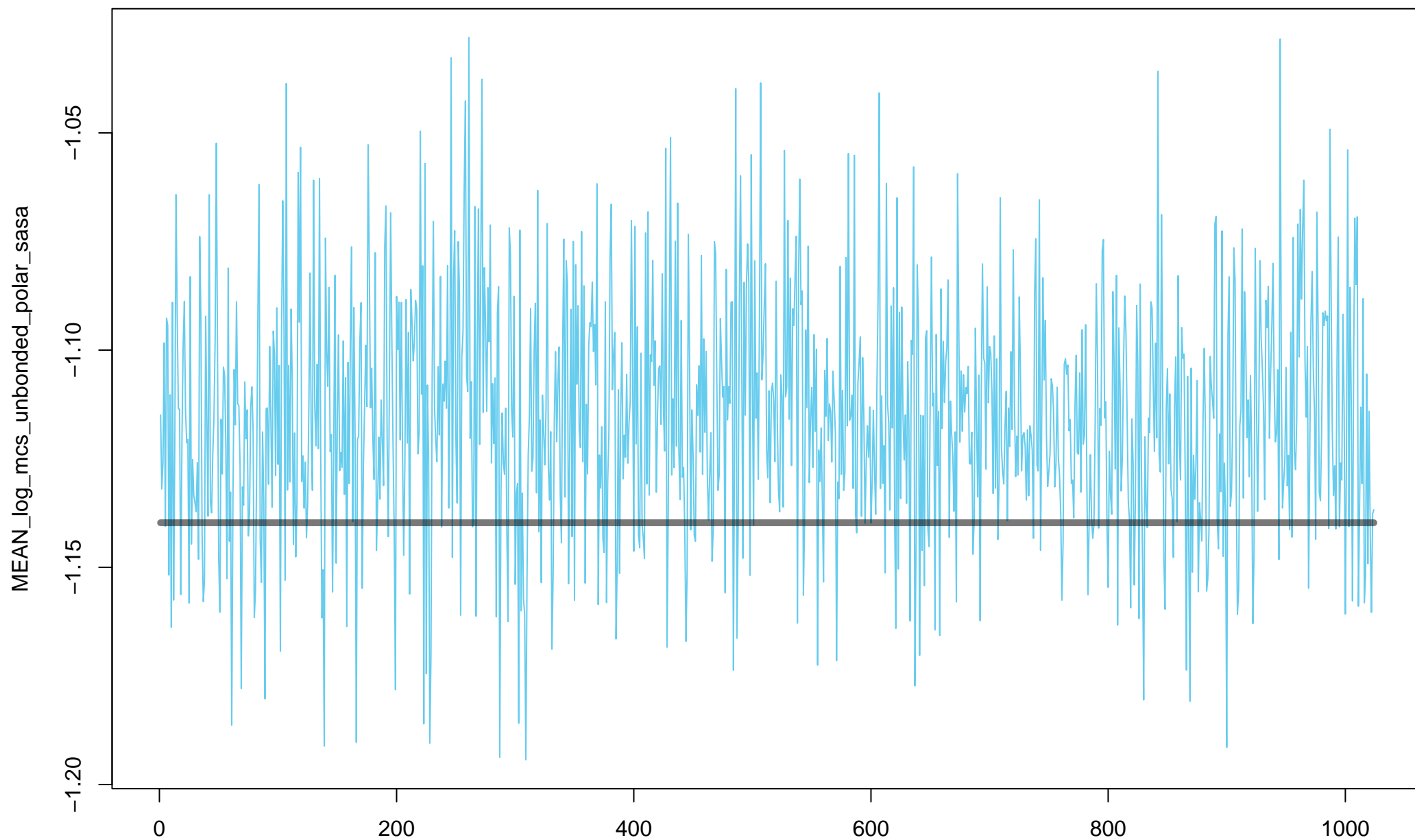


MEAN_log_RMSD

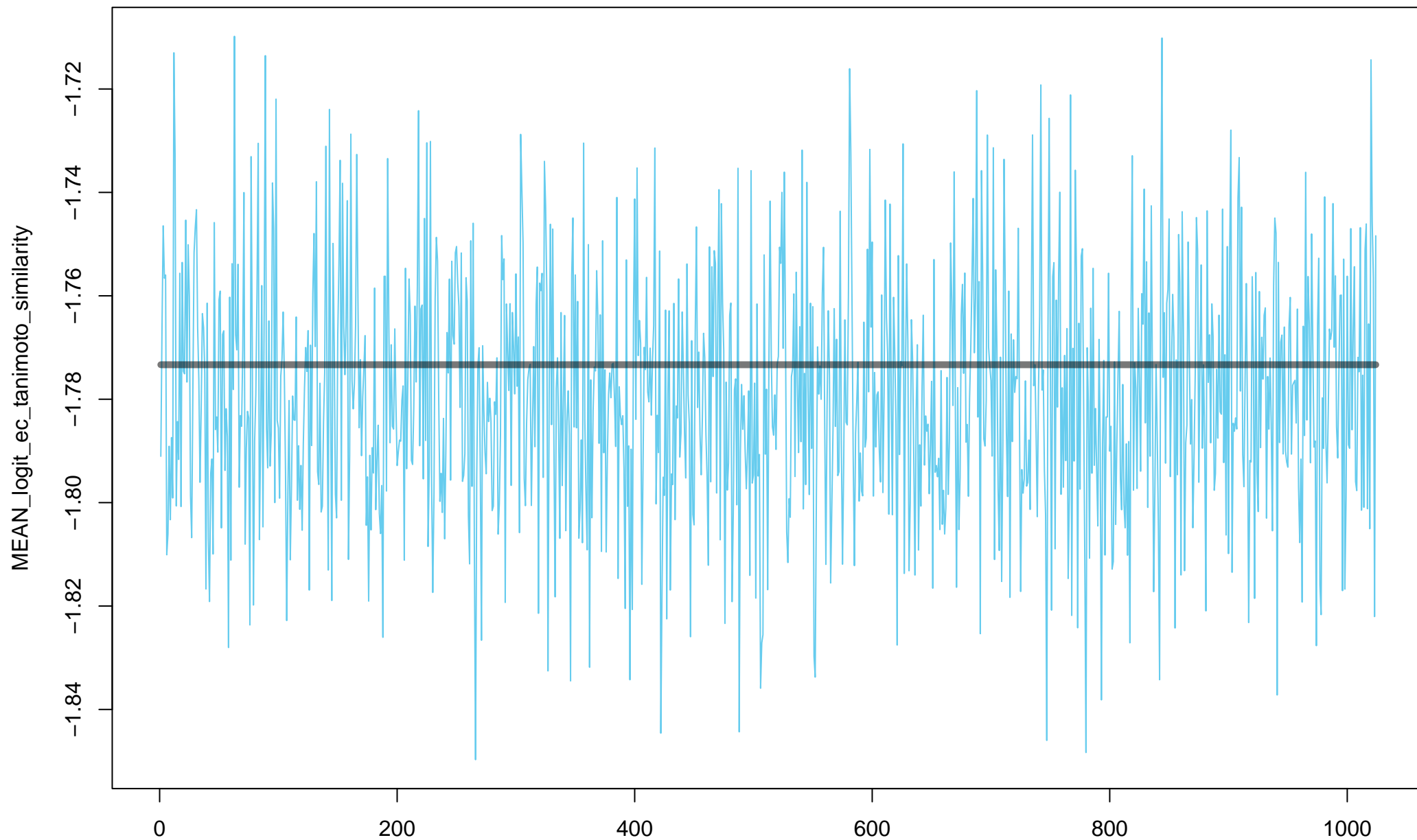
ESS = 1020 | BMK = 0.0566 | MCSE(6.27) = 3.08 | stat: FALSE | burn: 0 | rel.err: 1.51



MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0797 | MCSE(6.27) = 3.99 | stat: TRUE | burn: 0 | rel.err: 0.892

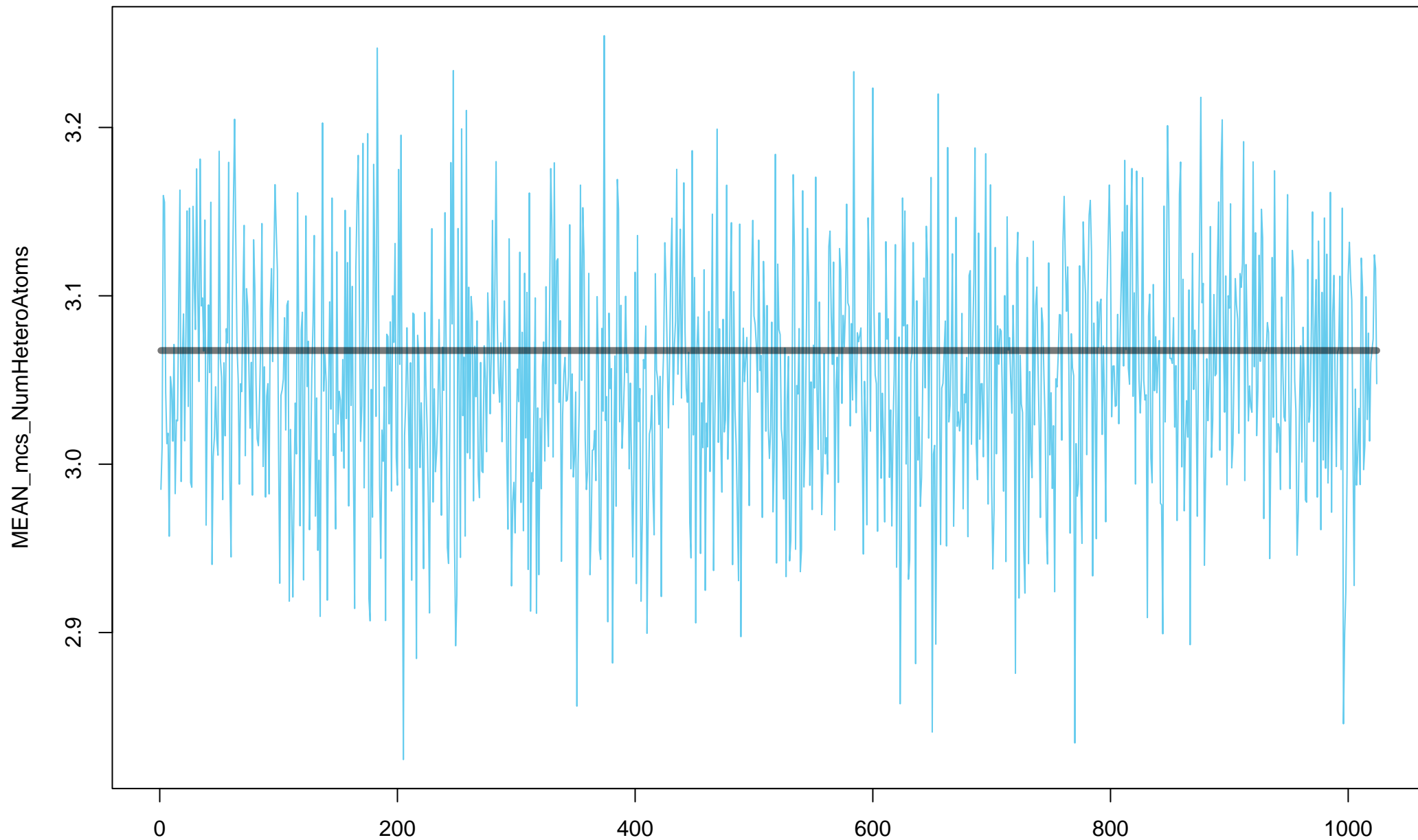


MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0209 | MCSE(6.27) = 3.56 | stat: TRUE | burn: 0 | rel.err: -0.258

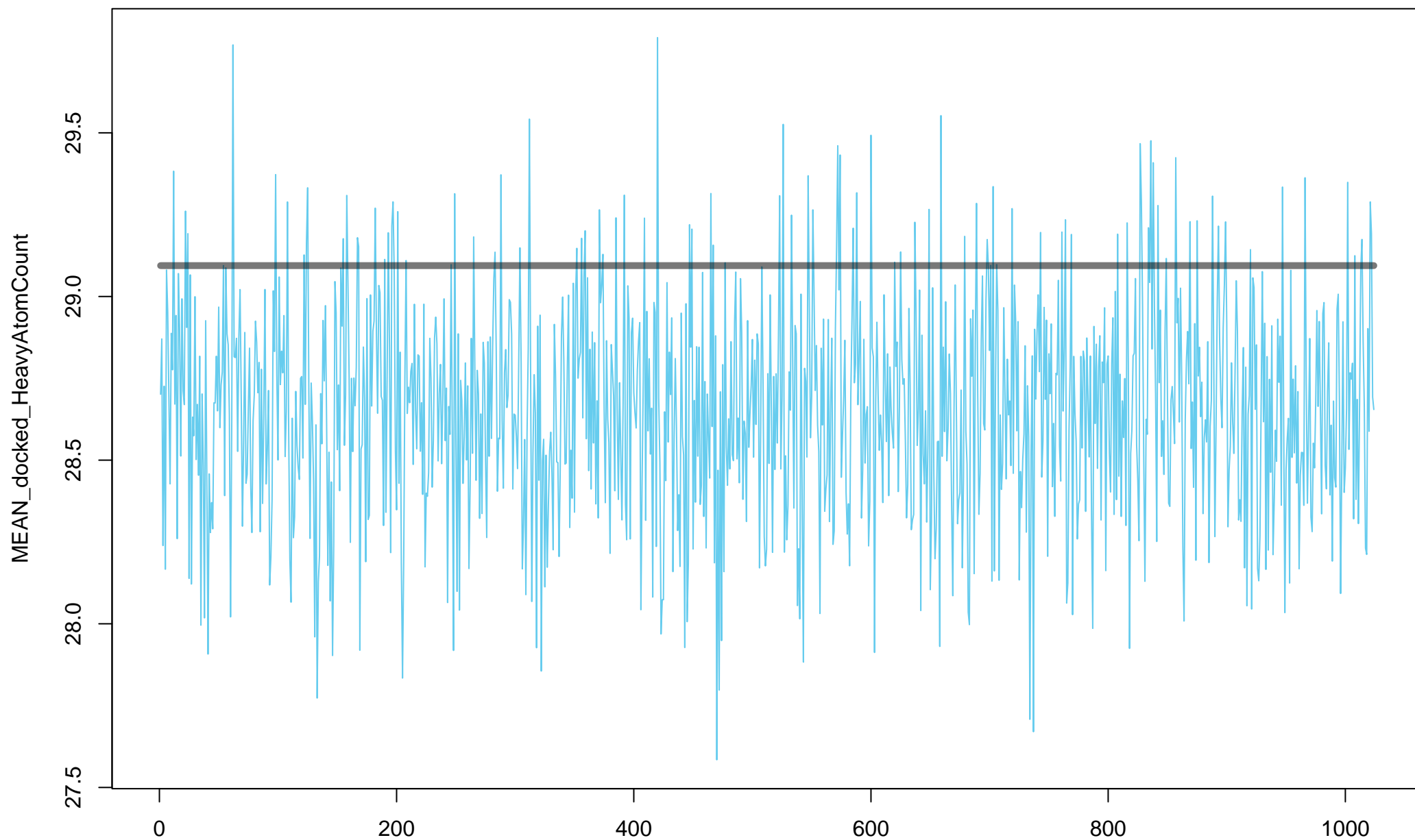


MEAN_mcs_NumHeteroAtoms

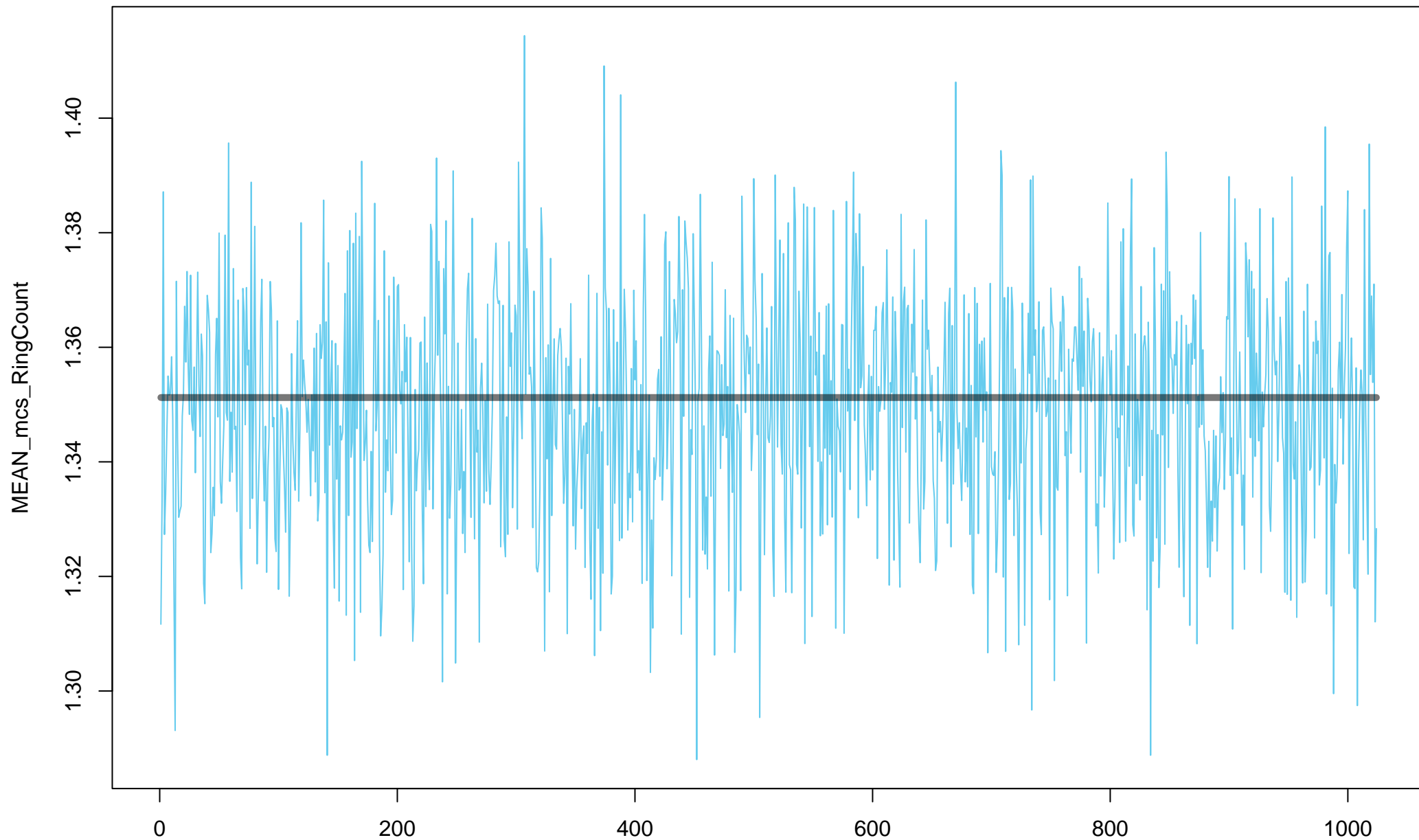
ESS = 1020 | BMK = 0.0687 | MCSE(6.27) = 3.64 | stat: TRUE | burn: 0 | rel.err: -0.247



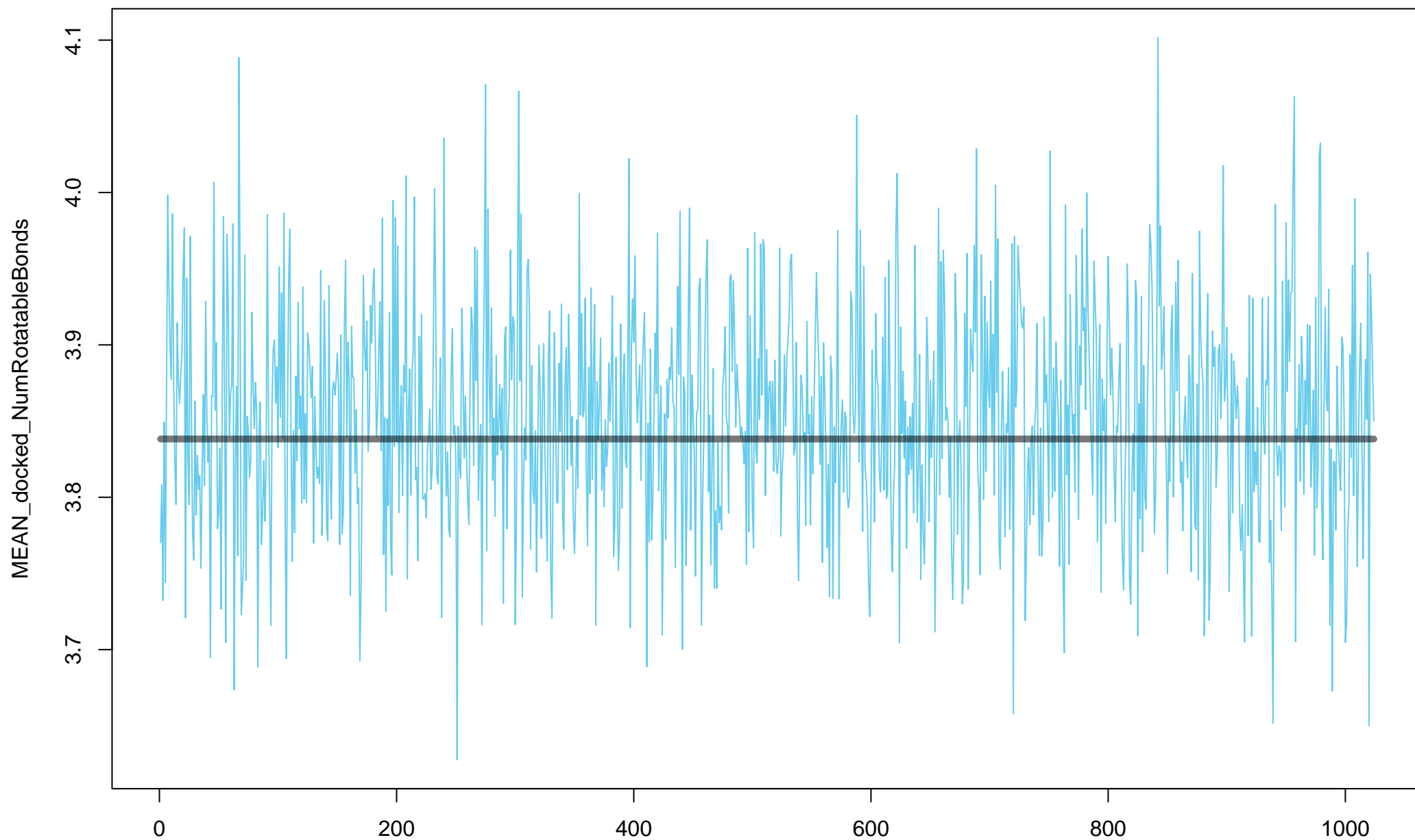
MEAN_docked_HeavyAtomCount
ESS = 880 | BMK = 0.0574 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | rel.err: -1.33



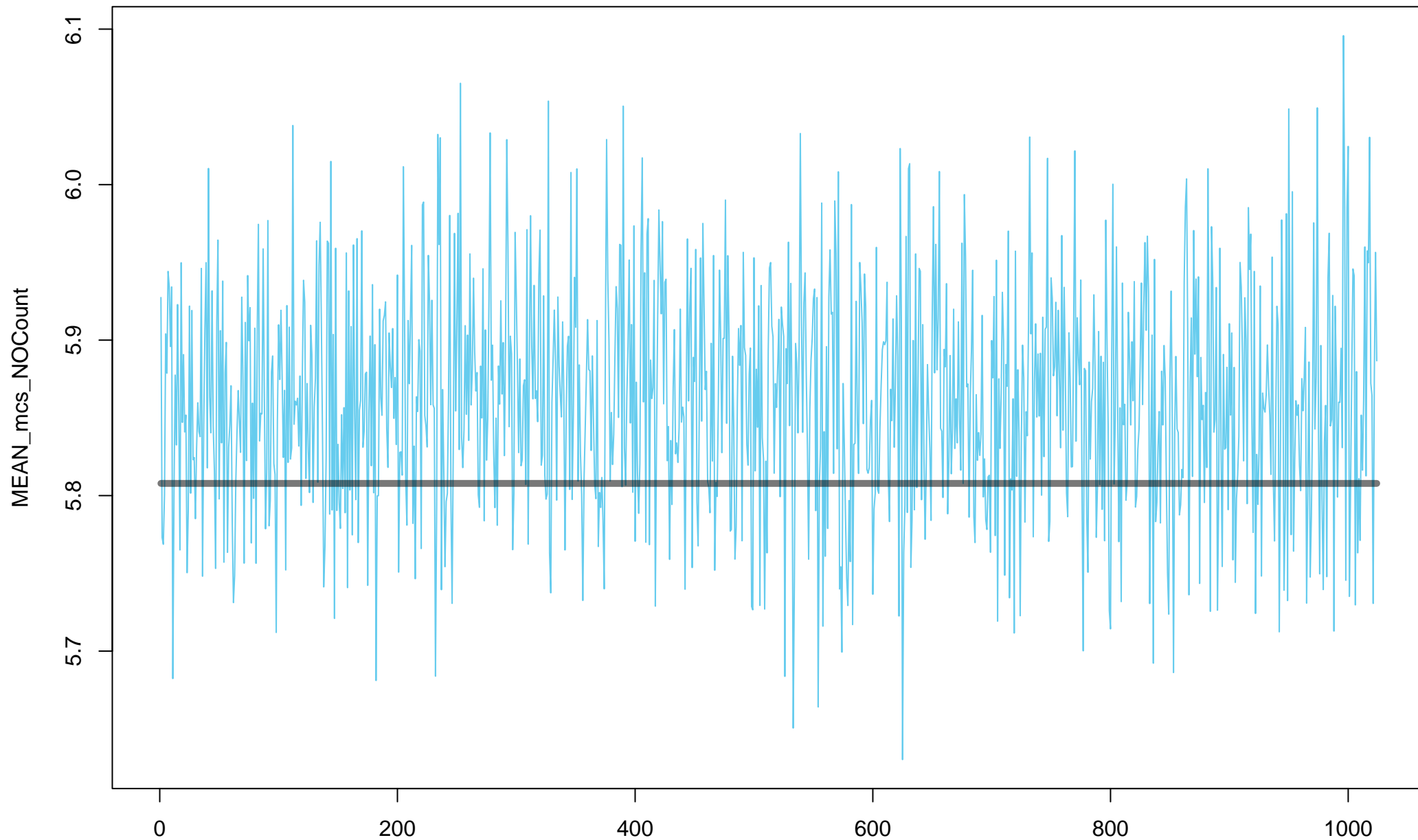
MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0454 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0 | rel.err: -0.119



MEAN_docked_NumRotatableBonds
ESS = 924 | BMK = 0.0333 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | rel.err: 0.2

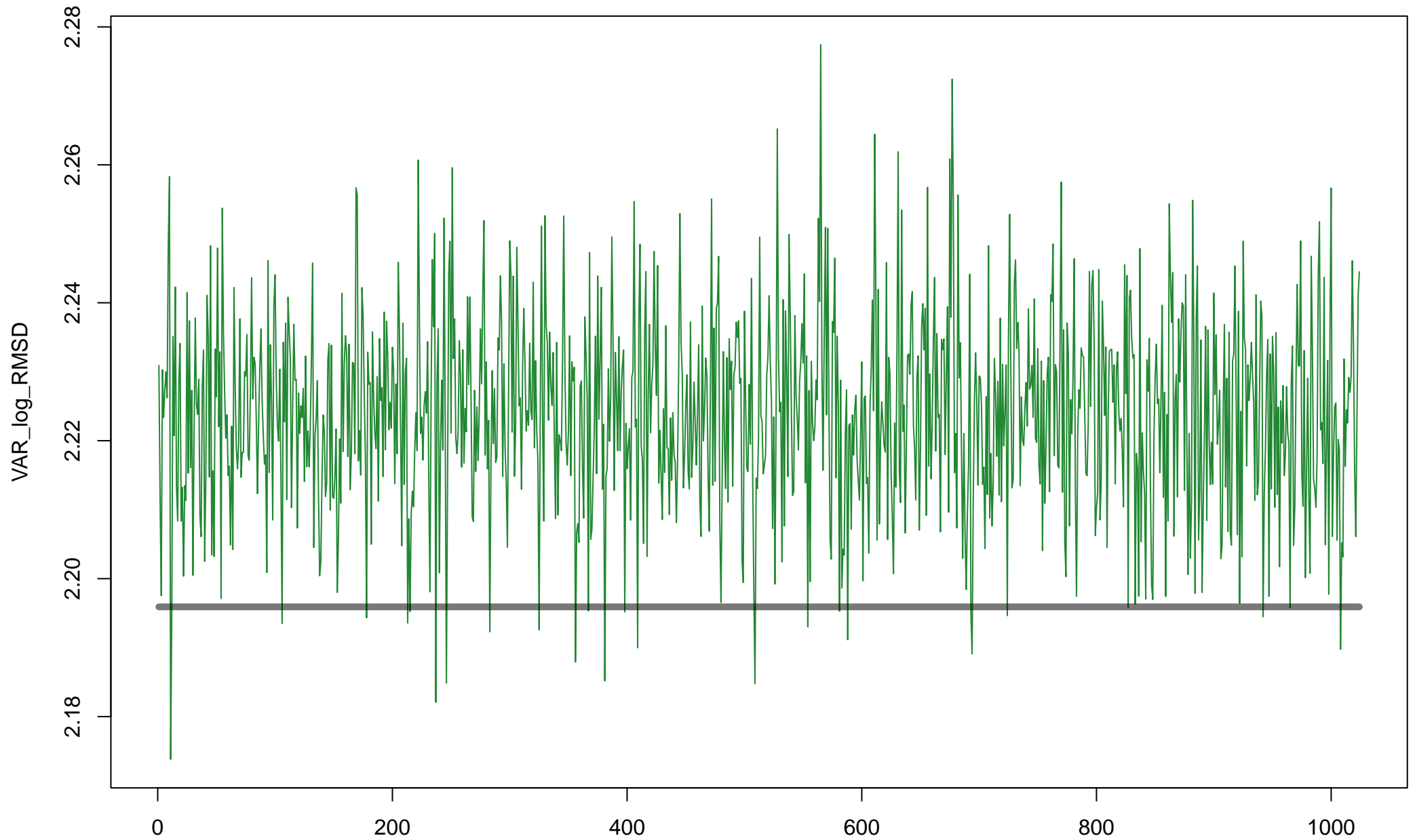


MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0615 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0 | rel.err: 0.733

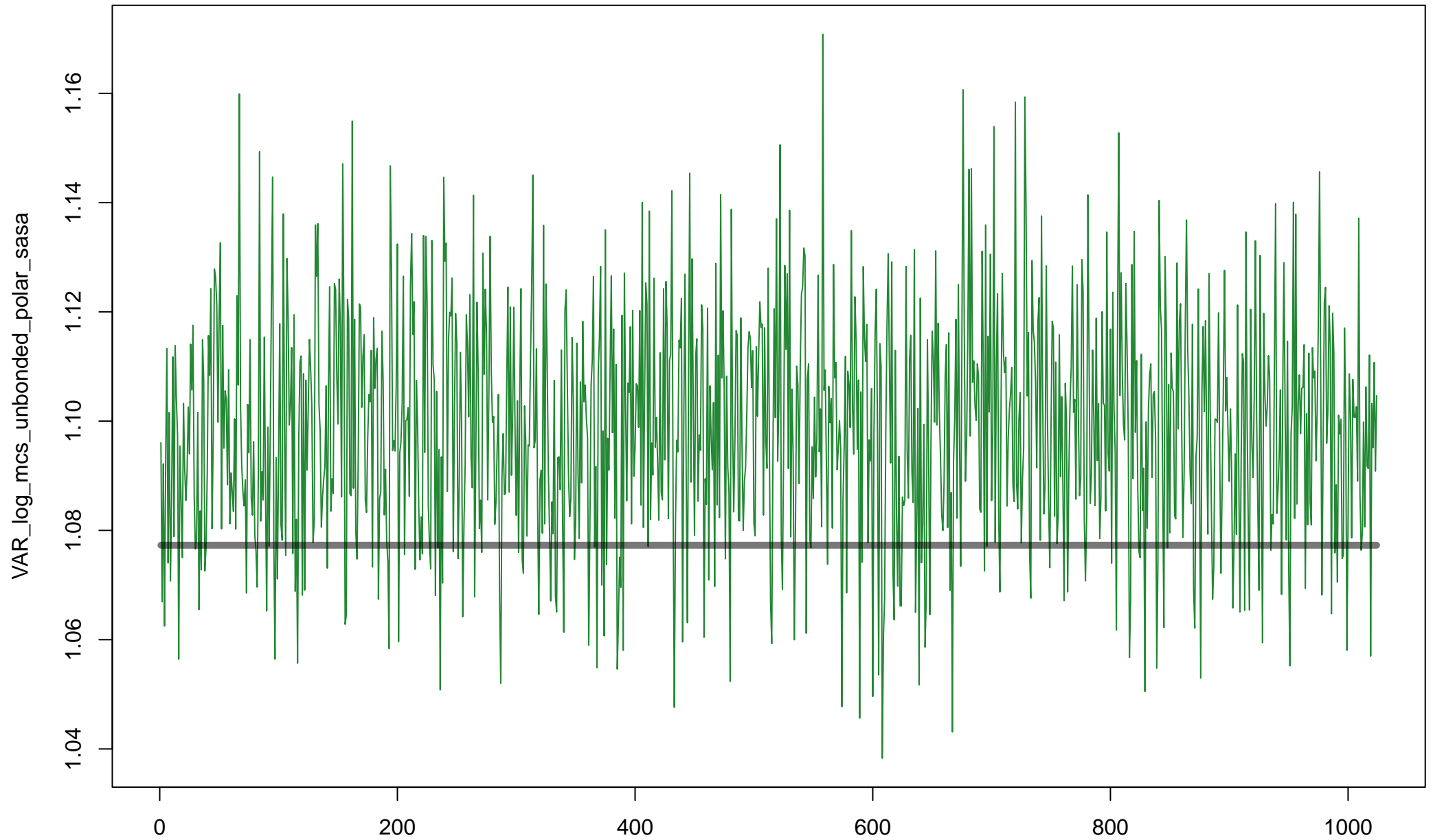


VAR_log_RMSD

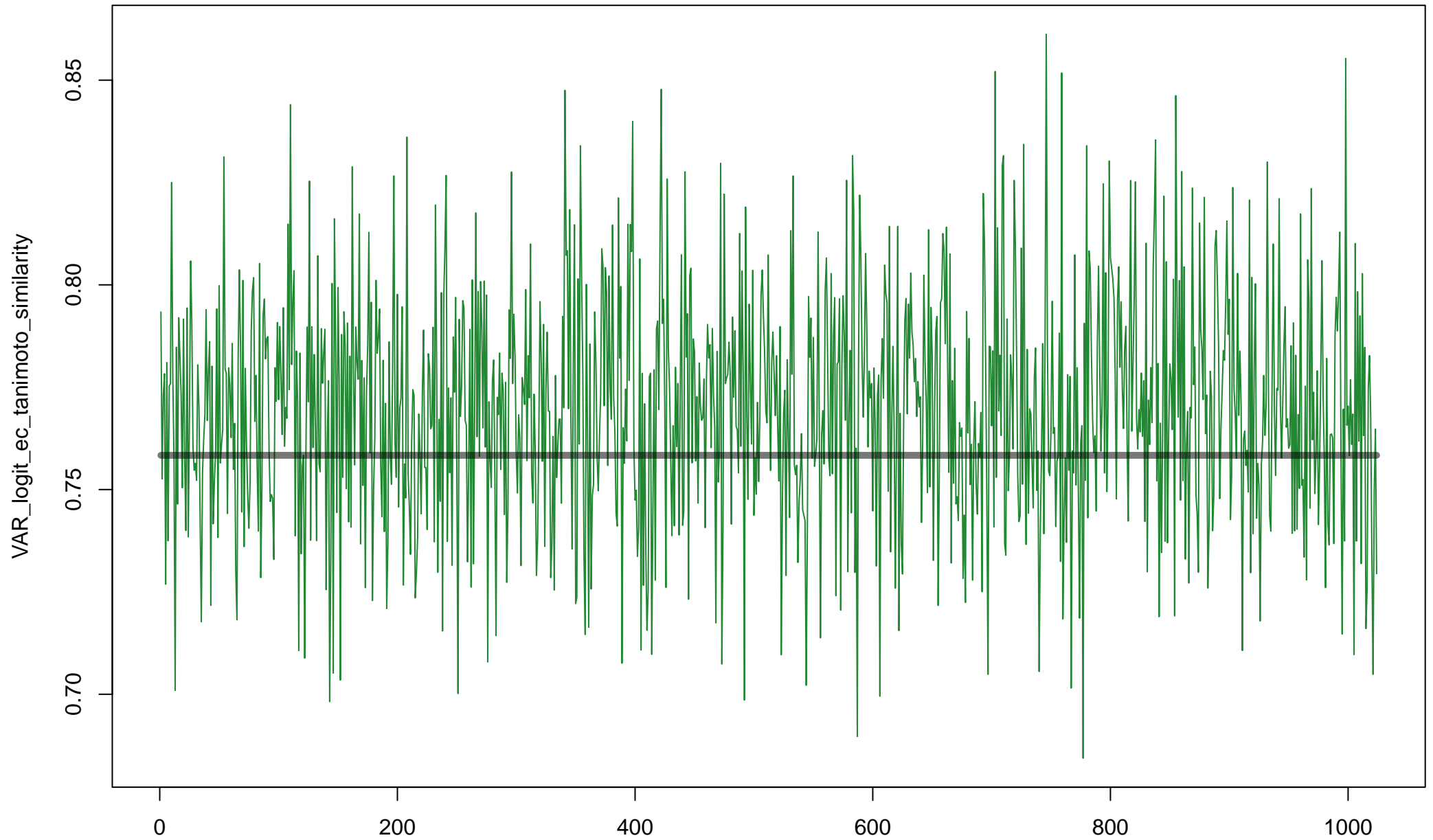
ESS = 935 | BMK = 0.0915 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0 | rel.err: 1.98



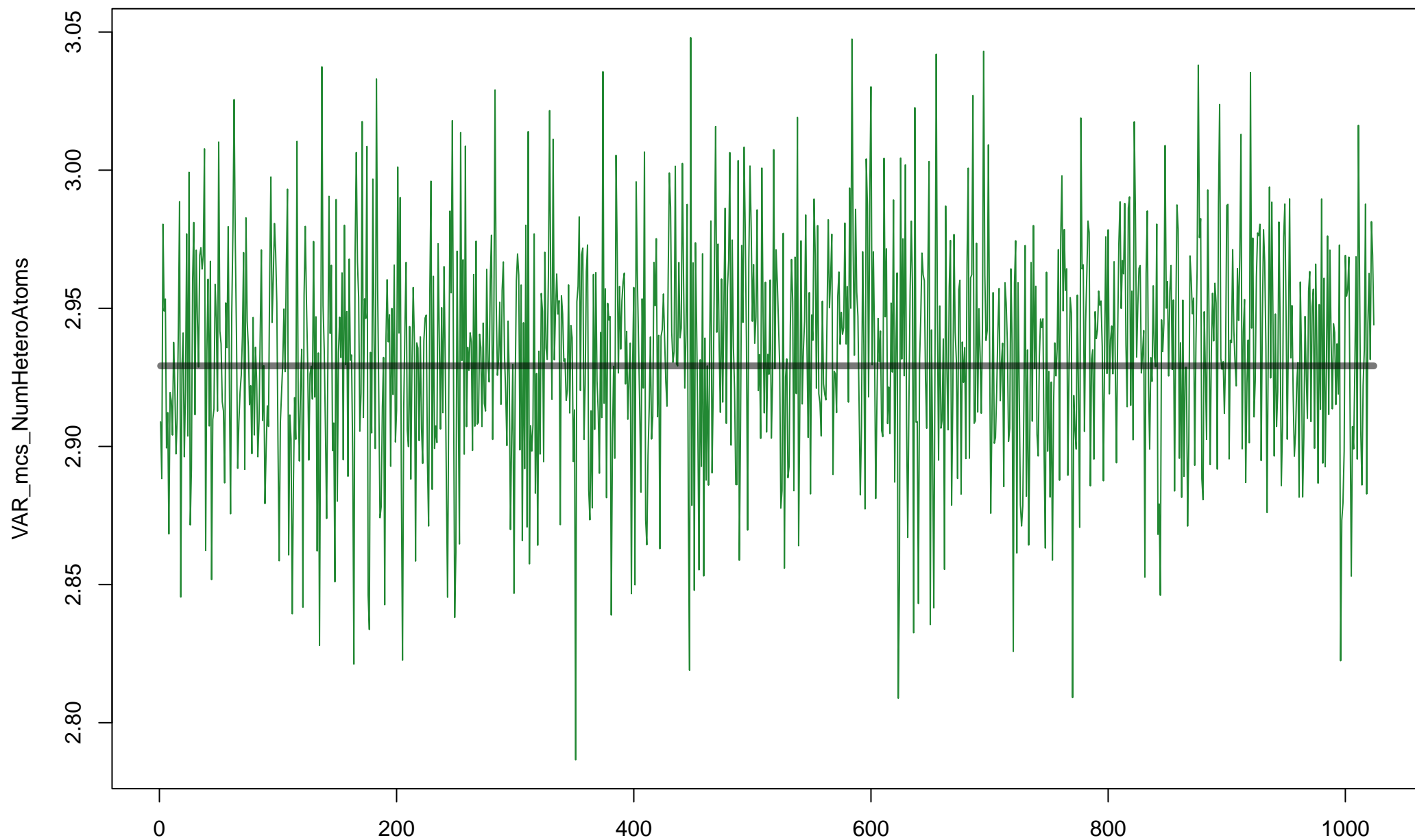
VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0622 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0 | rel.err: 1.02



VAR_logit_ec_tanimoto_similarity
ESS = 937 | BMK = 0.0532 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0 | rel.err: 0.418

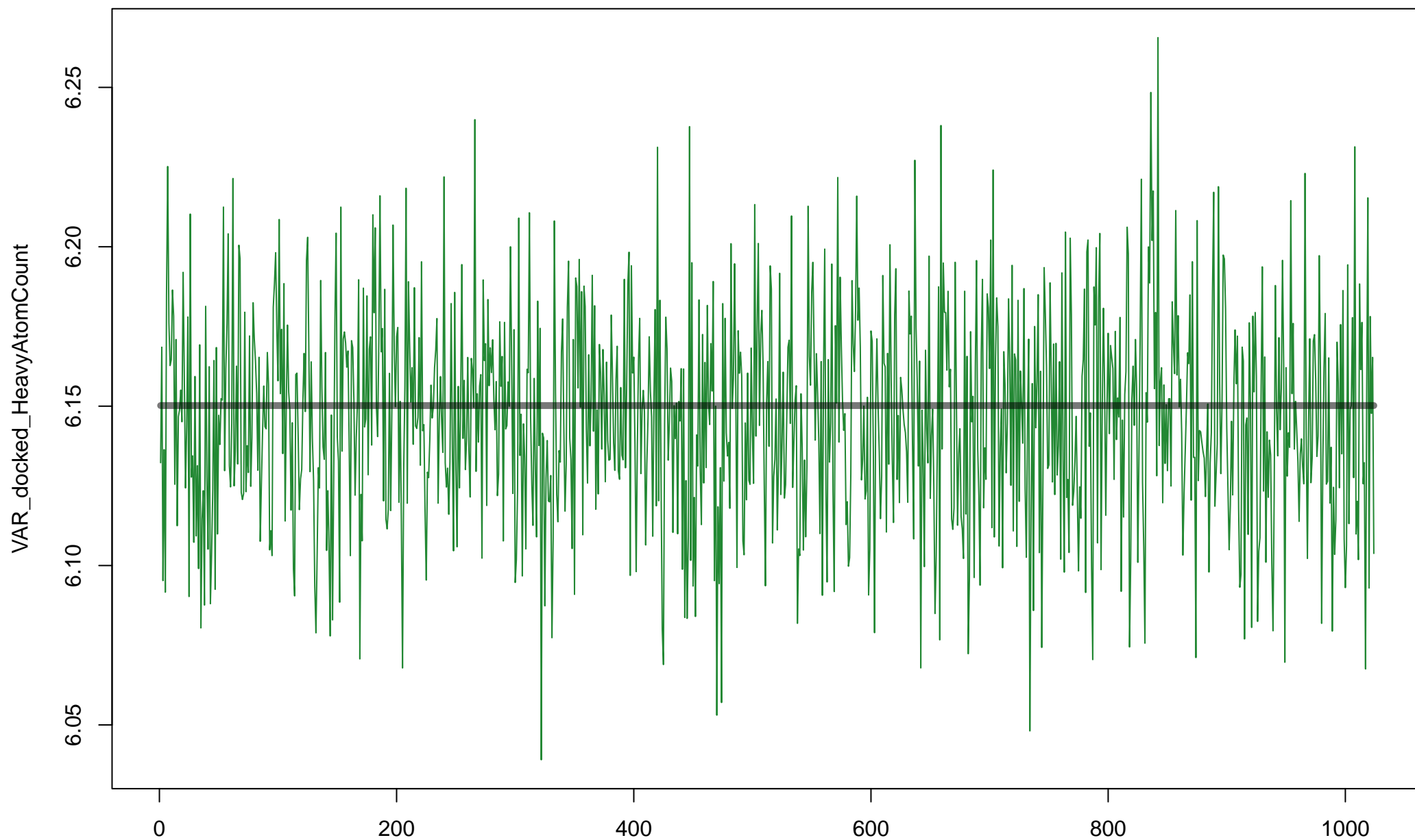


VAR_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0682 | MCSE(6.27) = 3.42 | stat: TRUE | burn: 0 | rel.err: 0.138

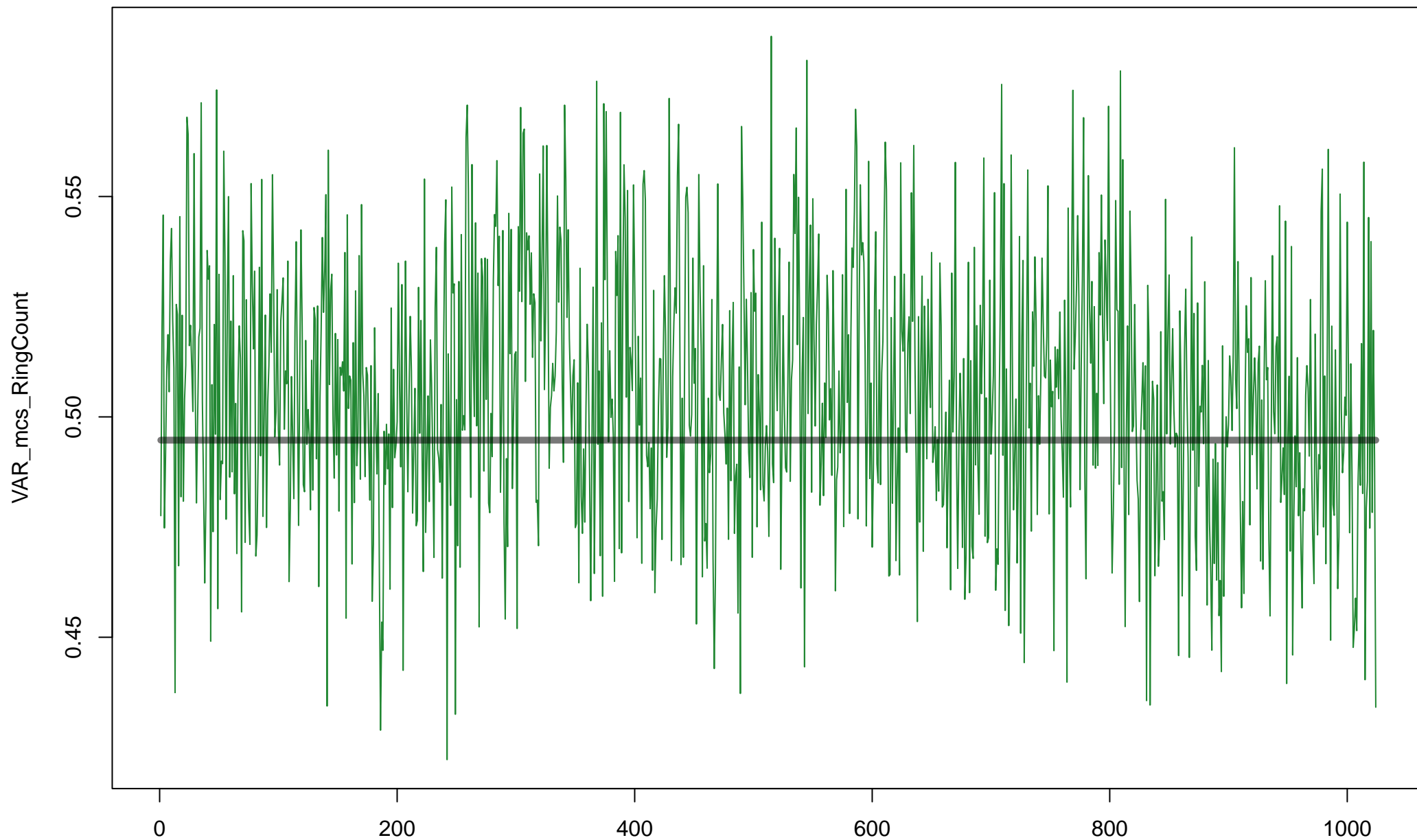


VAR_docked_HeavyAtomCount

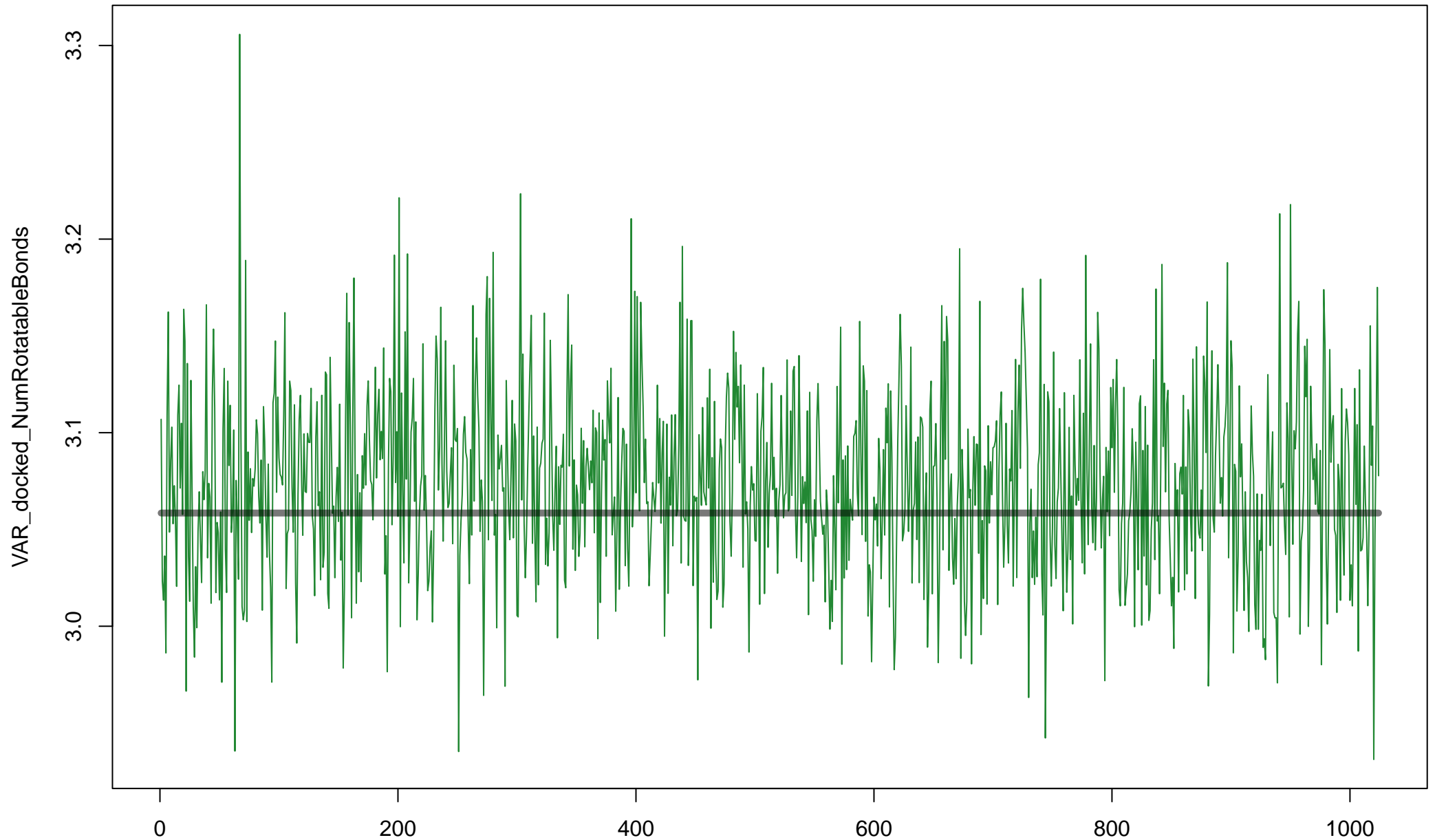
ESS = 1020 | BMK = 0.0474 | MCSE(6.27) = 3.22 | stat: TRUE | burn: 0 | rel.err: -0.0988



VAR_mcs_RingCount
ESS = 422 | BMK = 0.0677 | MCSE(6.27) = 5.26 | stat: FALSE | burn: 0 | rel.err: 0.374

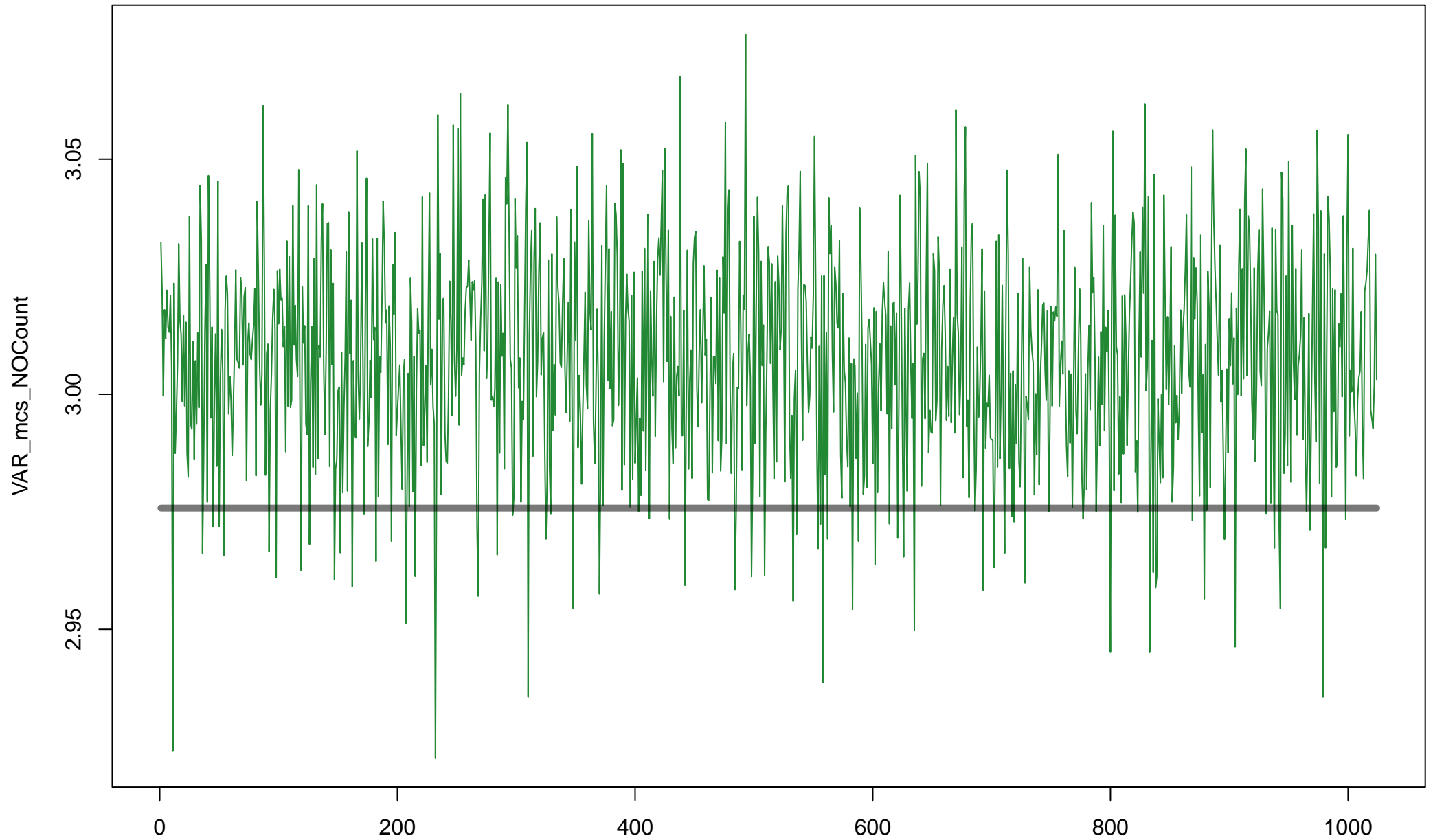


VAR_docked_NumRotatableBonds
ESS = 936 | BMK = 0.0605 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | rel.err: 0.343

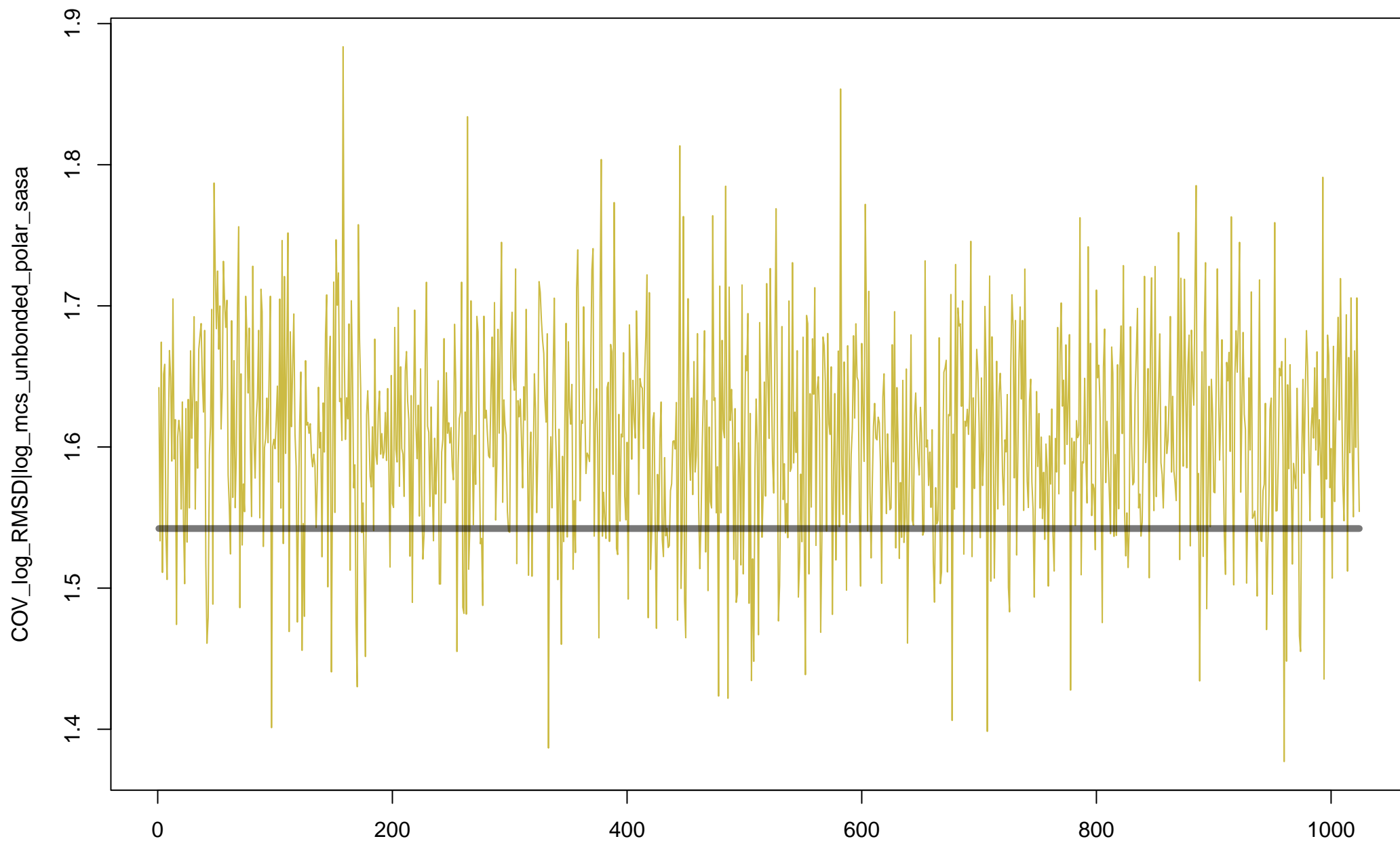


VAR_mcs_NOCount

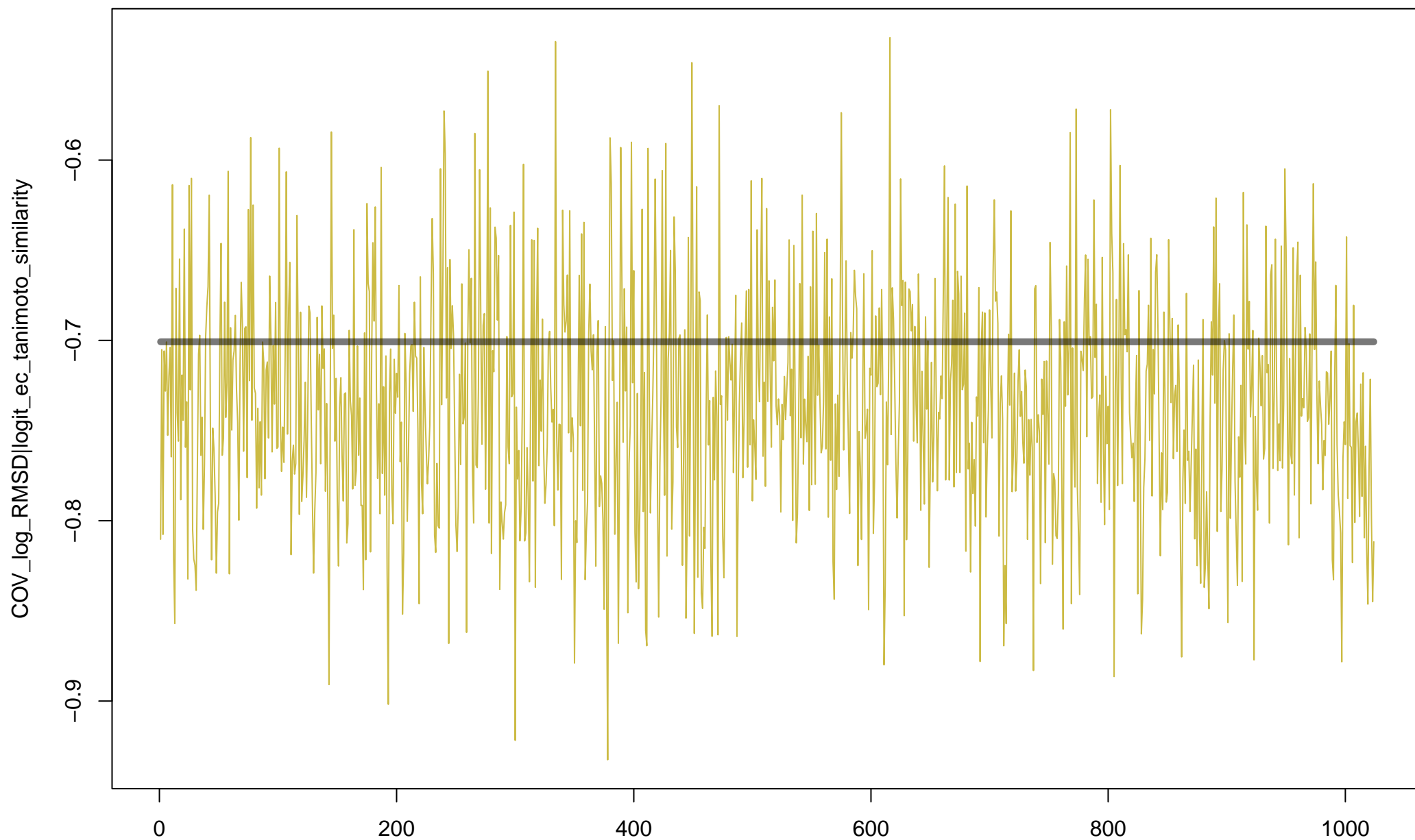
ESS = 1020 | BMK = 0.0539 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0 | rel.err: 1.39



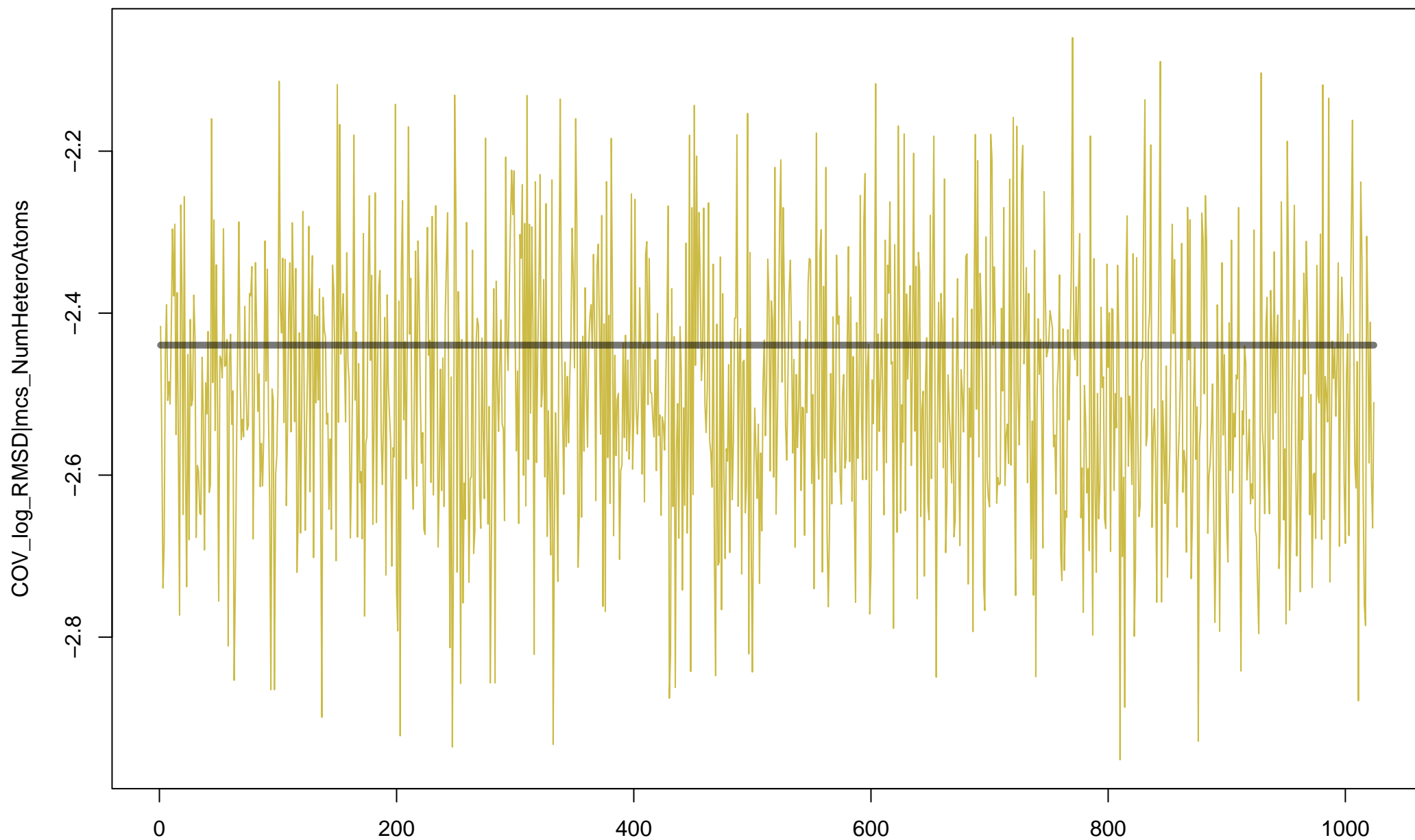
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0634 | MCSE(6.27) = 3.51 | stat: TRUE | burn: 0 | rel.err: 0.918



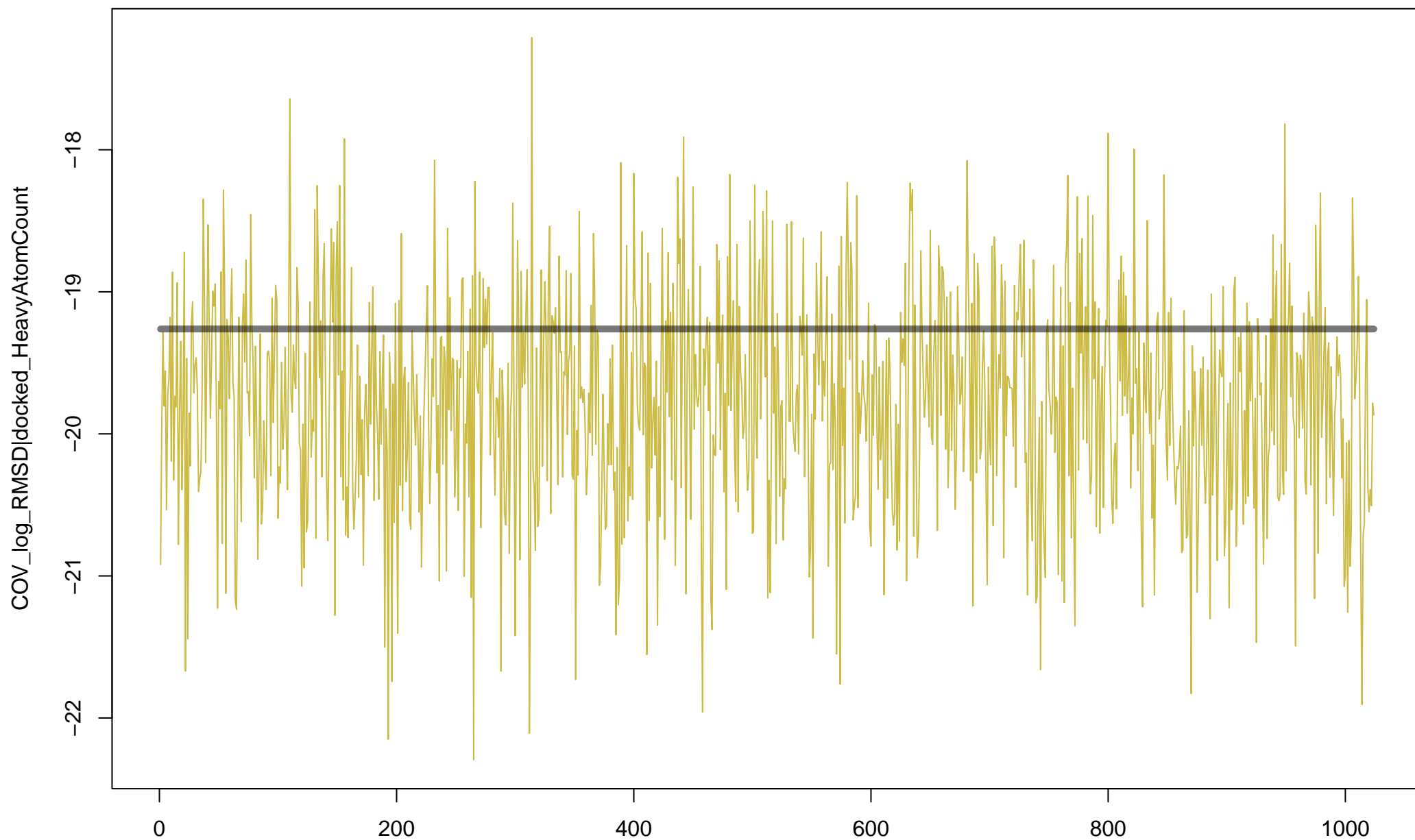
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0827 | MCSE(6.27) = 3.46 | stat: TRUE | burn: 0 | rel.err: -0.556



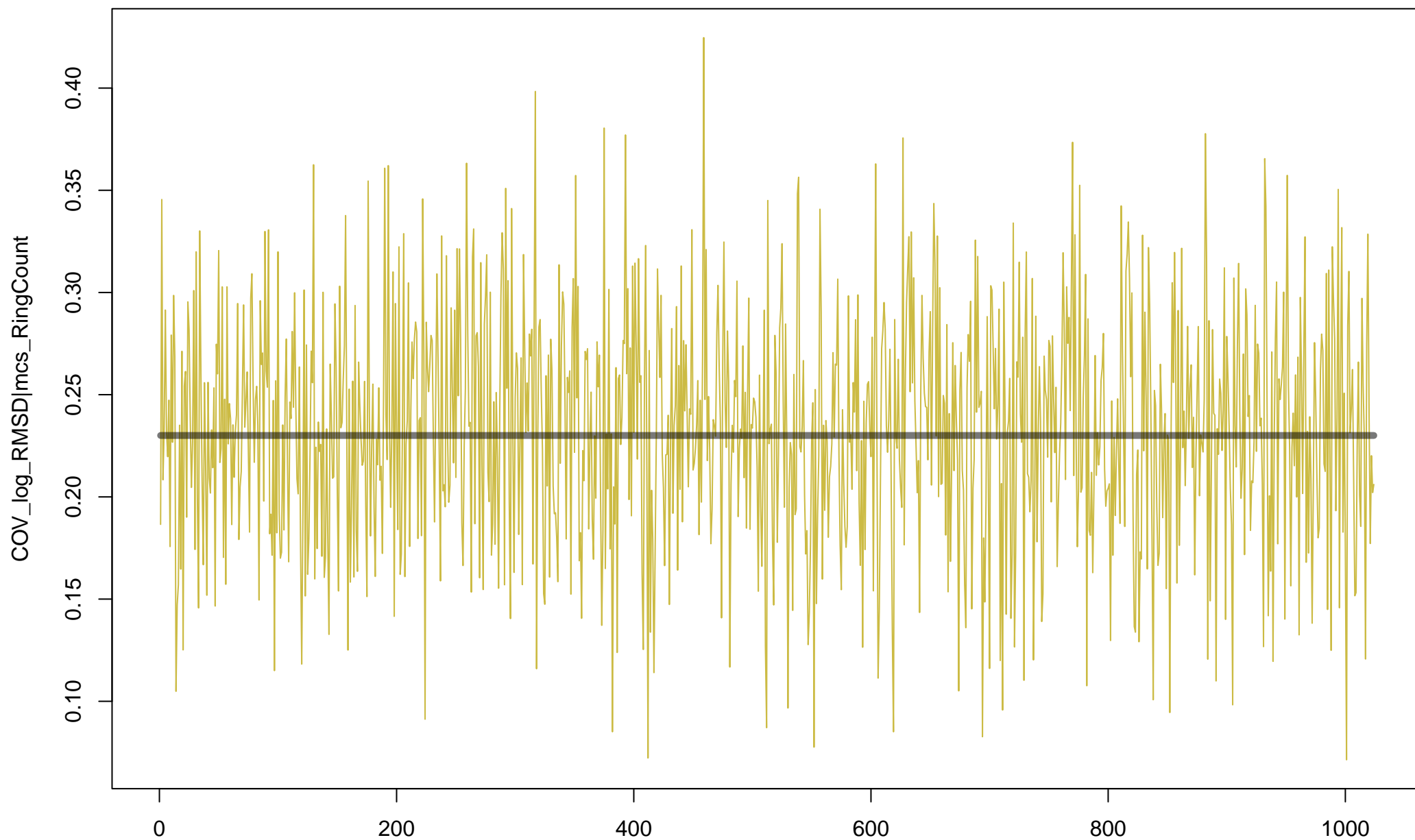
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0483 | MCSE(6.27) = 3.21 | stat: TRUE | burn: 0 | rel.err: -0.381



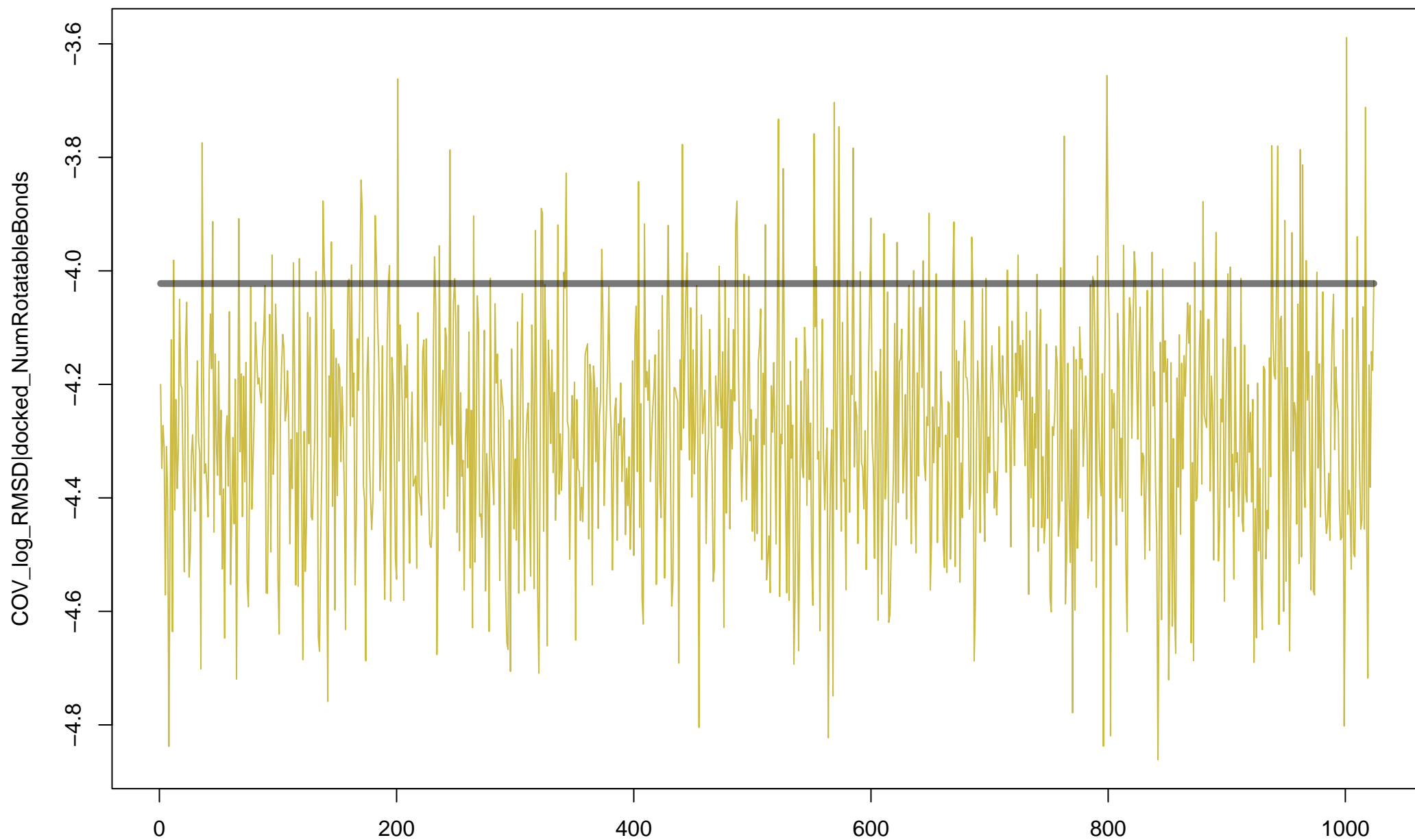
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0438 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 0 | rel.err: -0.685



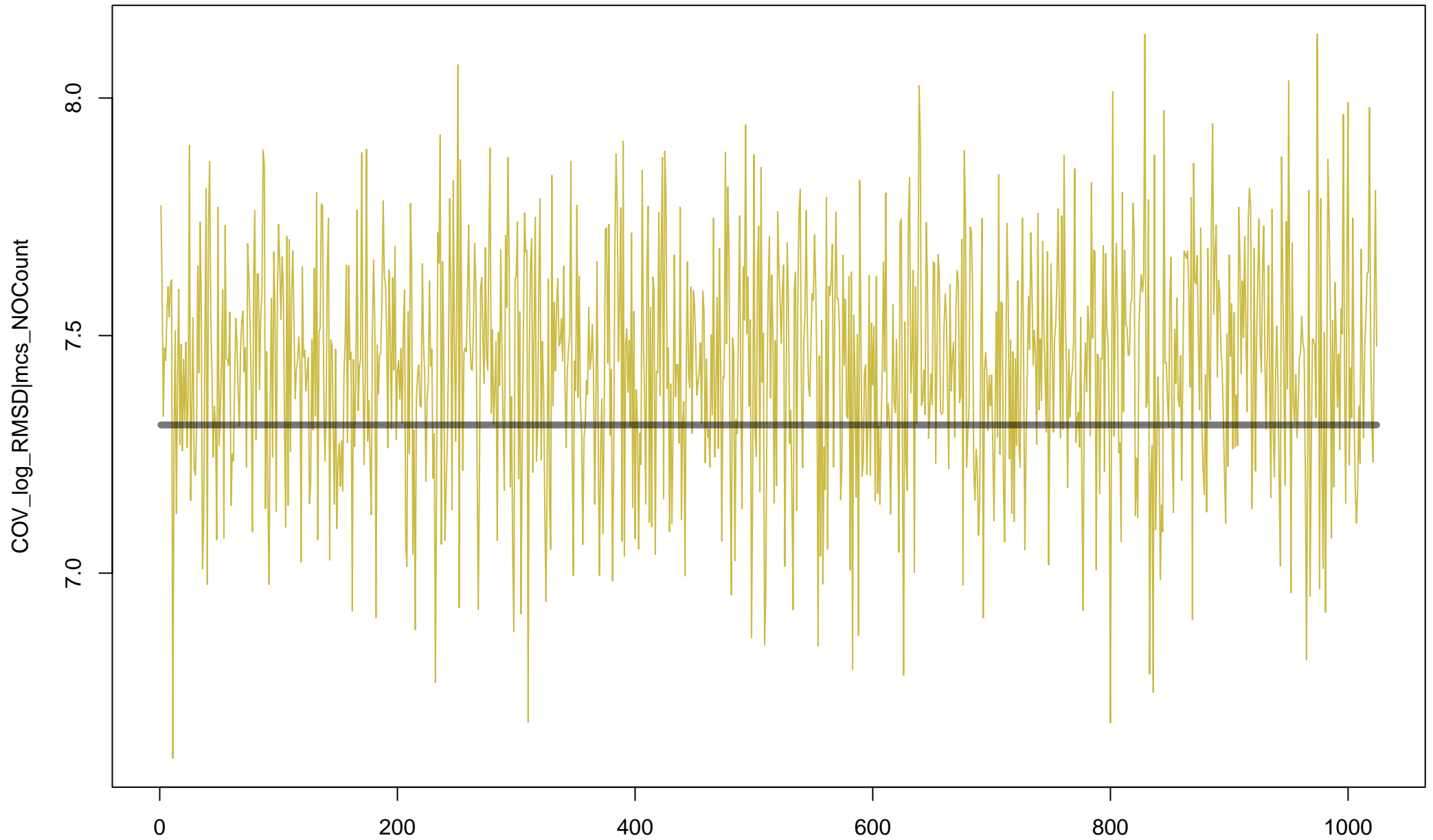
COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0632 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0 | rel.err: 0.0516



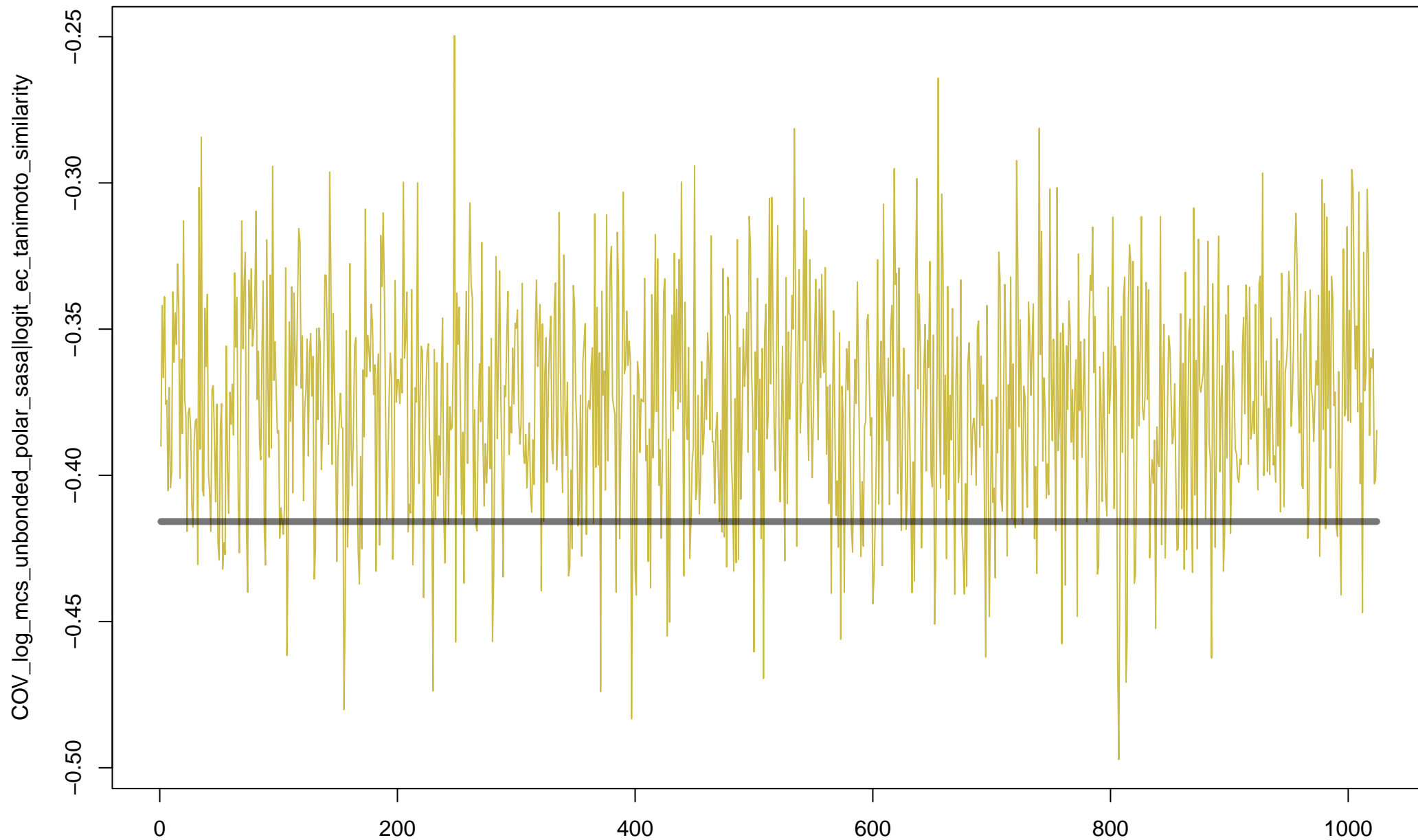
COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0581 | MCSE(6.27) = 2.67 | stat: TRUE | burn: 0 | rel.err: -1.29



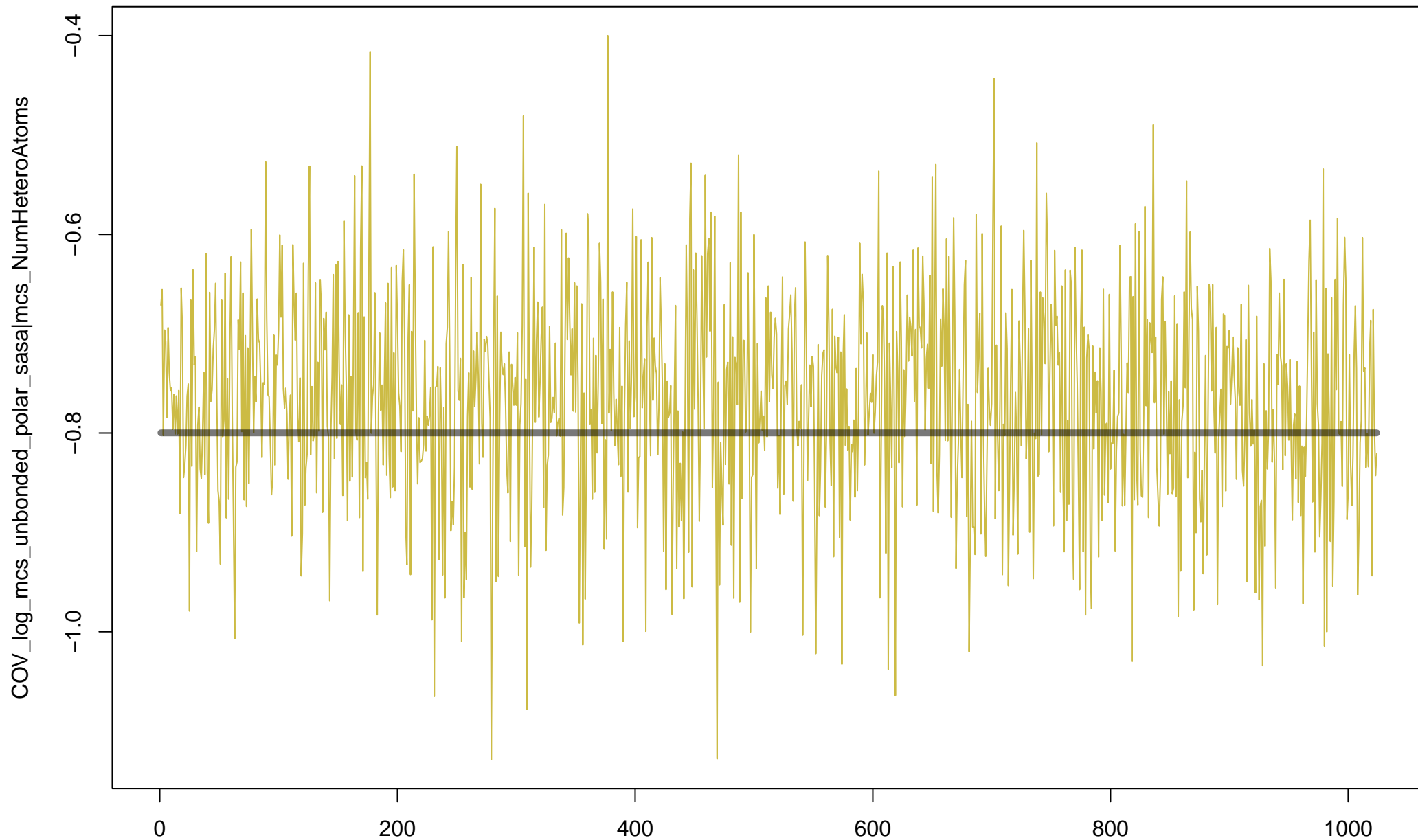
COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0538 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0 | rel.err: 0.523



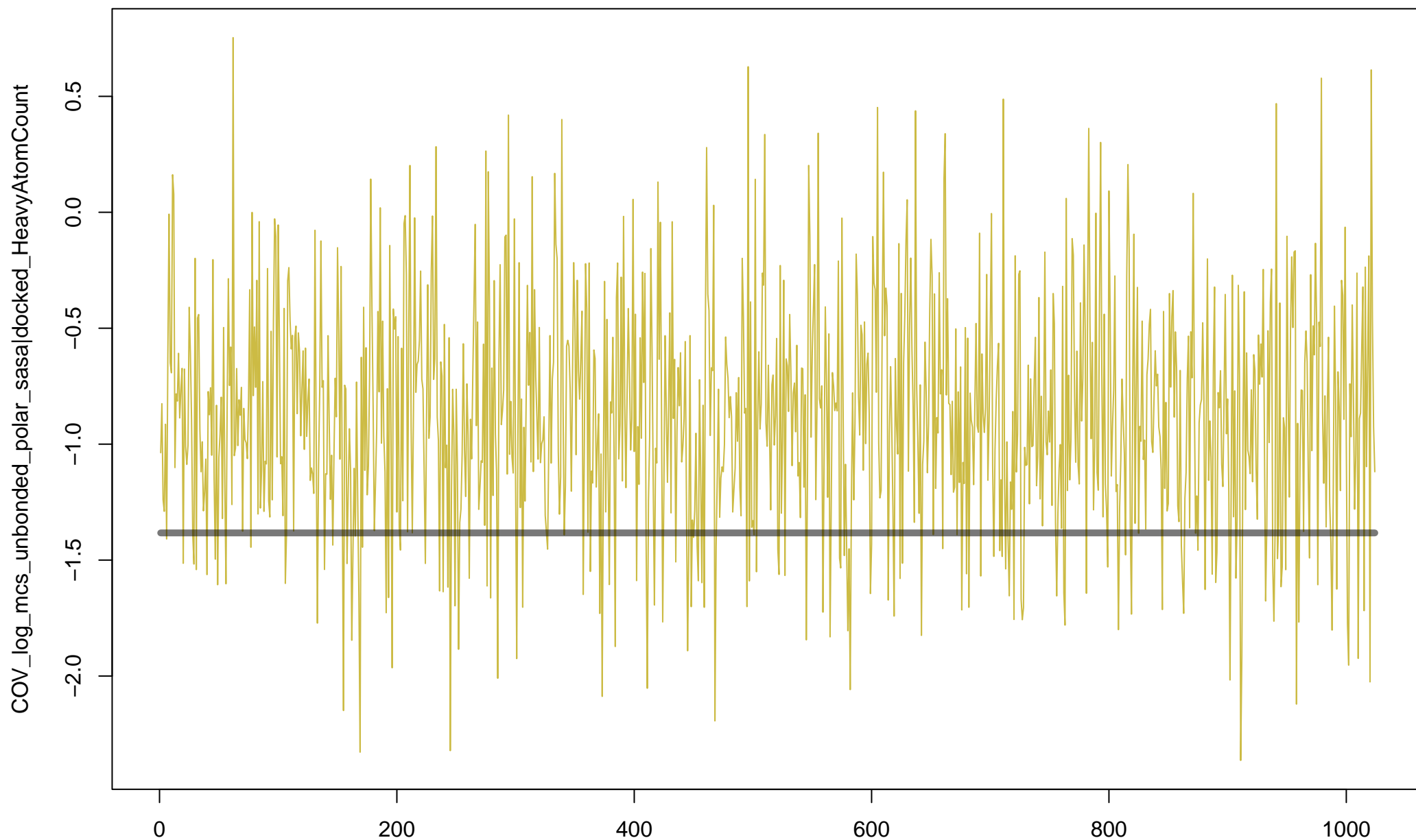
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 928 | BMK = 0.0417 | MCSE(6.27) = 3.39 | stat: TRUE | burn: 0 | rel.err: 1.11



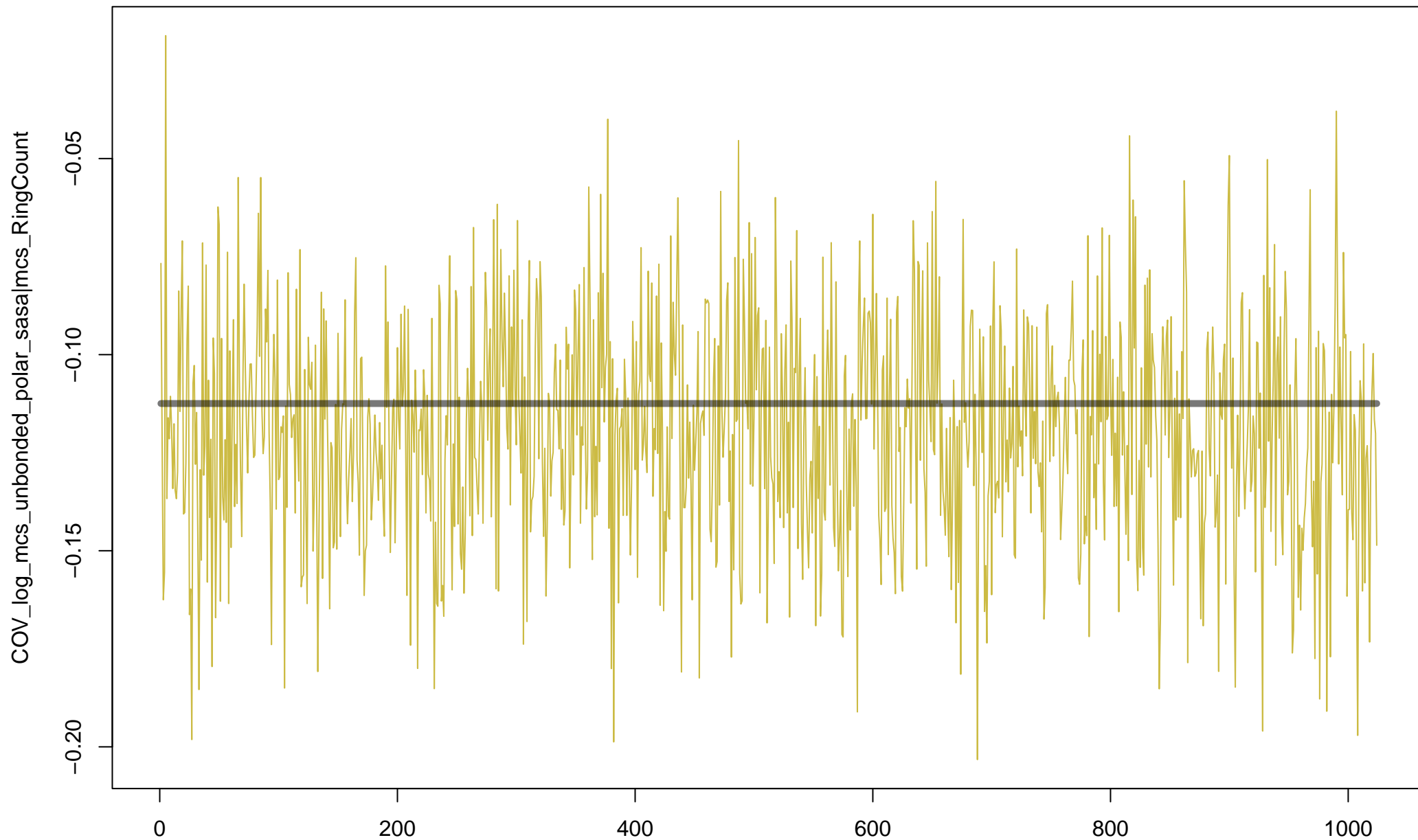
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0627 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | rel.err: 0.309



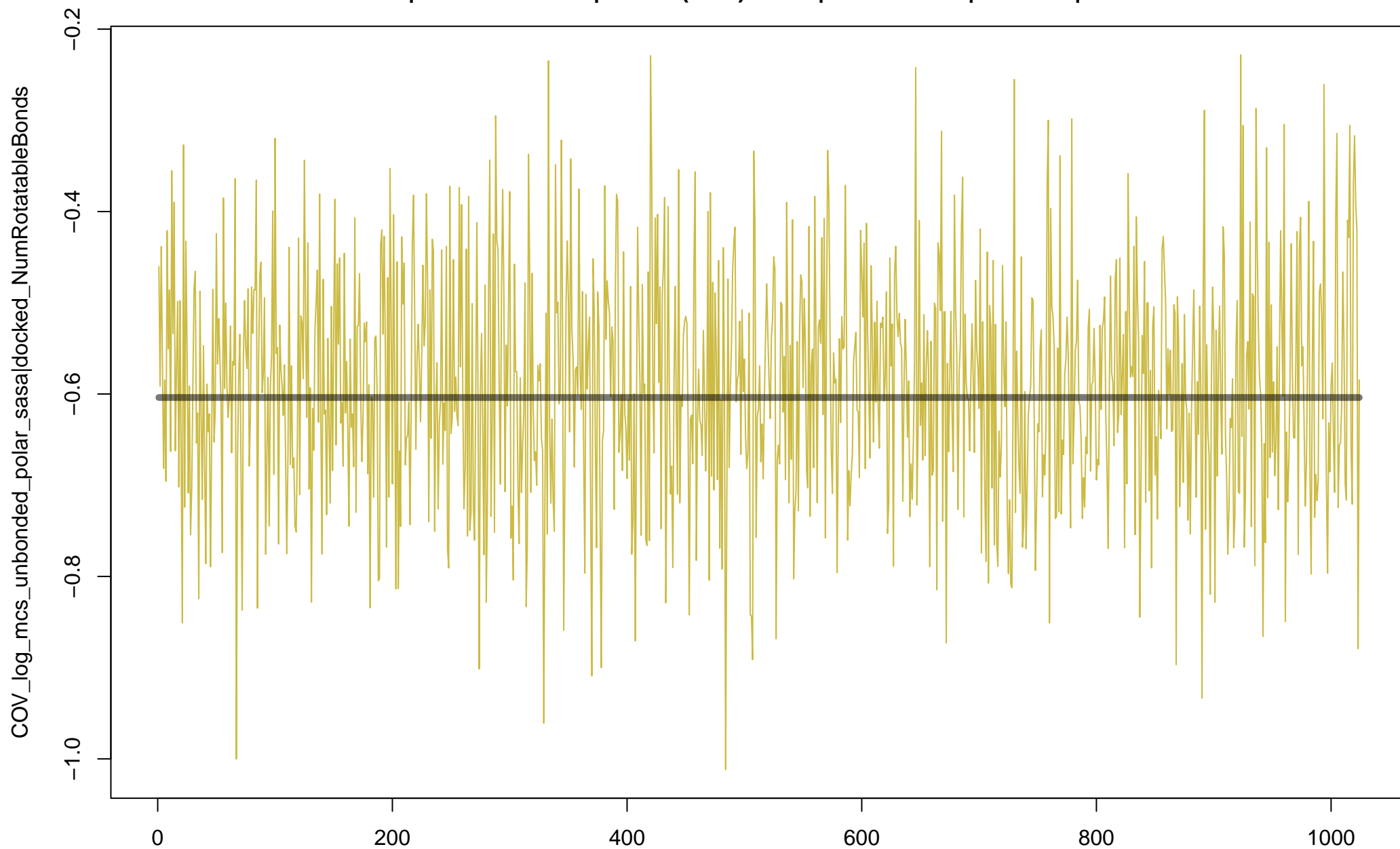
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0557 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0 | rel.err: 1.02



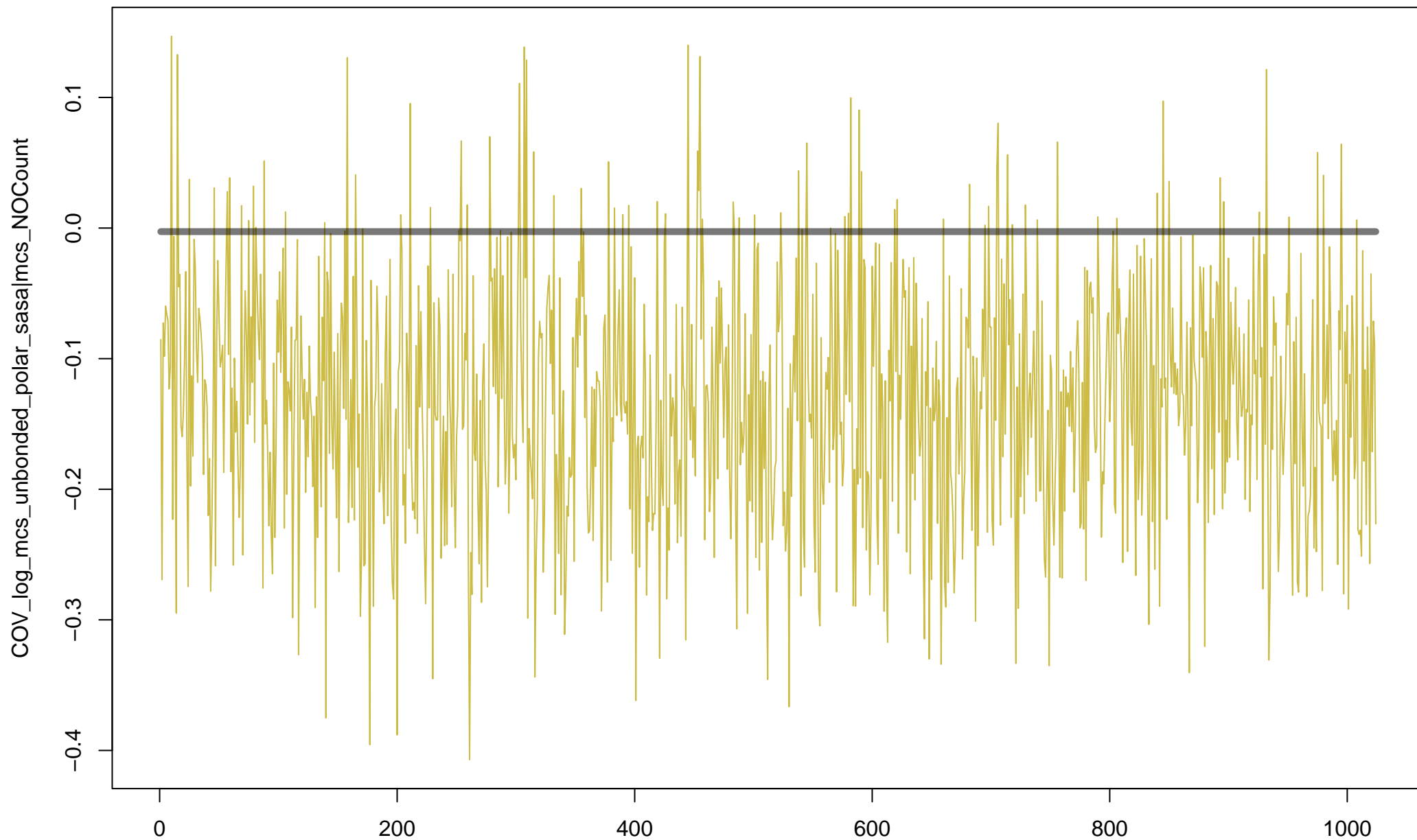
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 914 | BMK = 0.0472 | MCSE(6.27) = 3.33 | stat: TRUE | burn: 0 | rel.err: -0.257



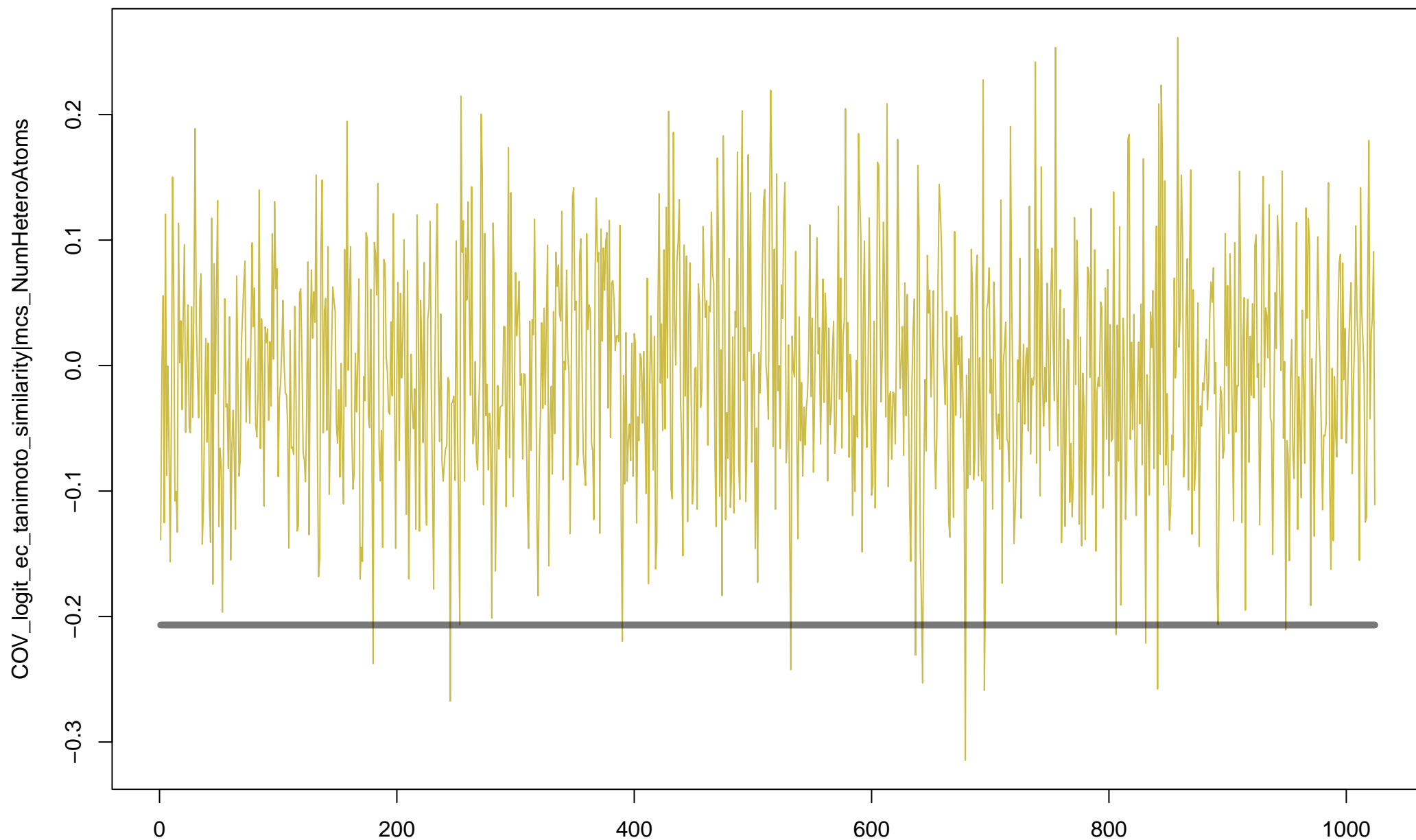
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0756 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0 | rel.err: 0.0988



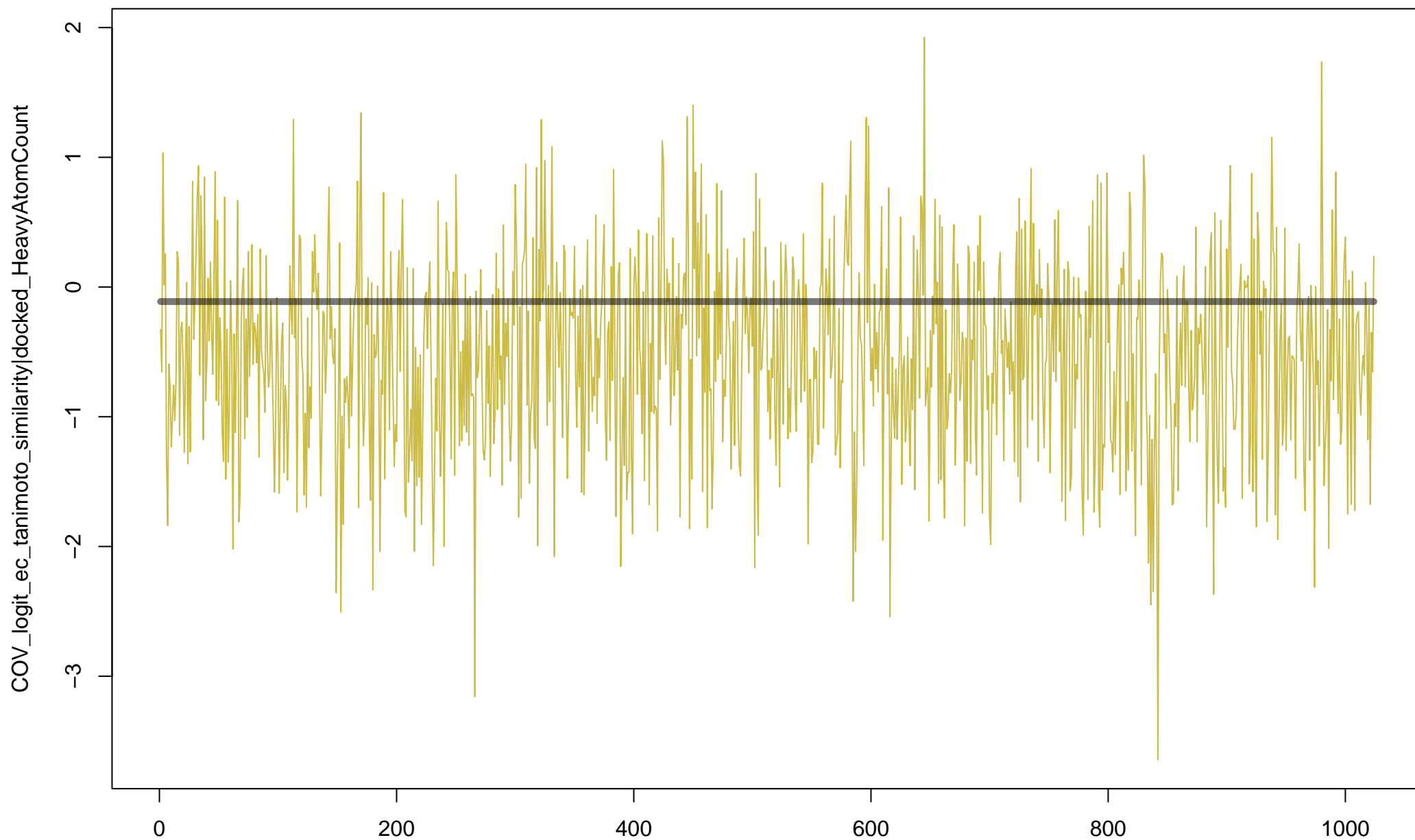
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 768 | BMK = 0.0477 | MCSE(6.27) = 3.46 | stat: FALSE | burn: 0 | rel.err: -1.42



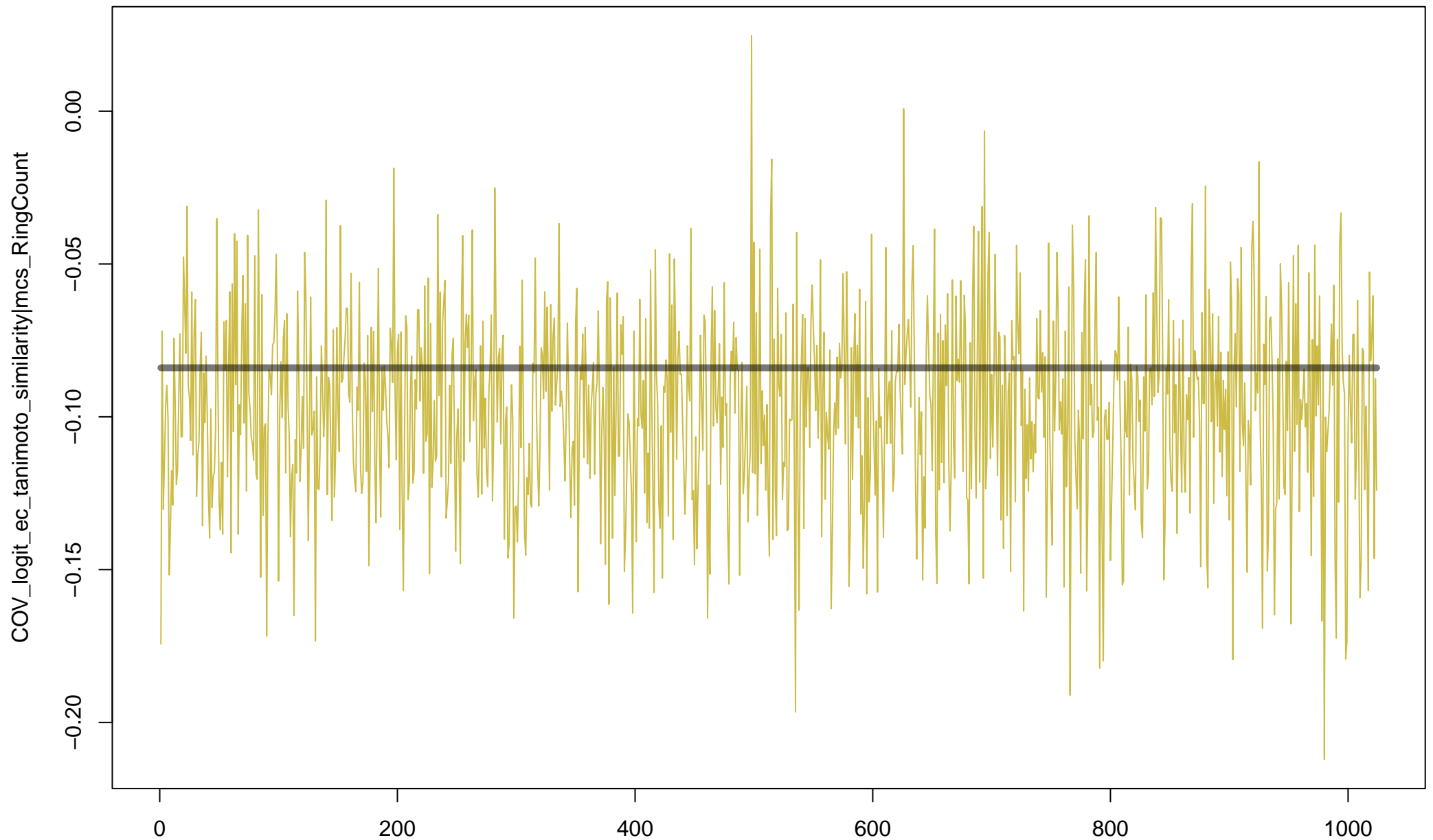
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0597 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0 | rel.err: 2.27



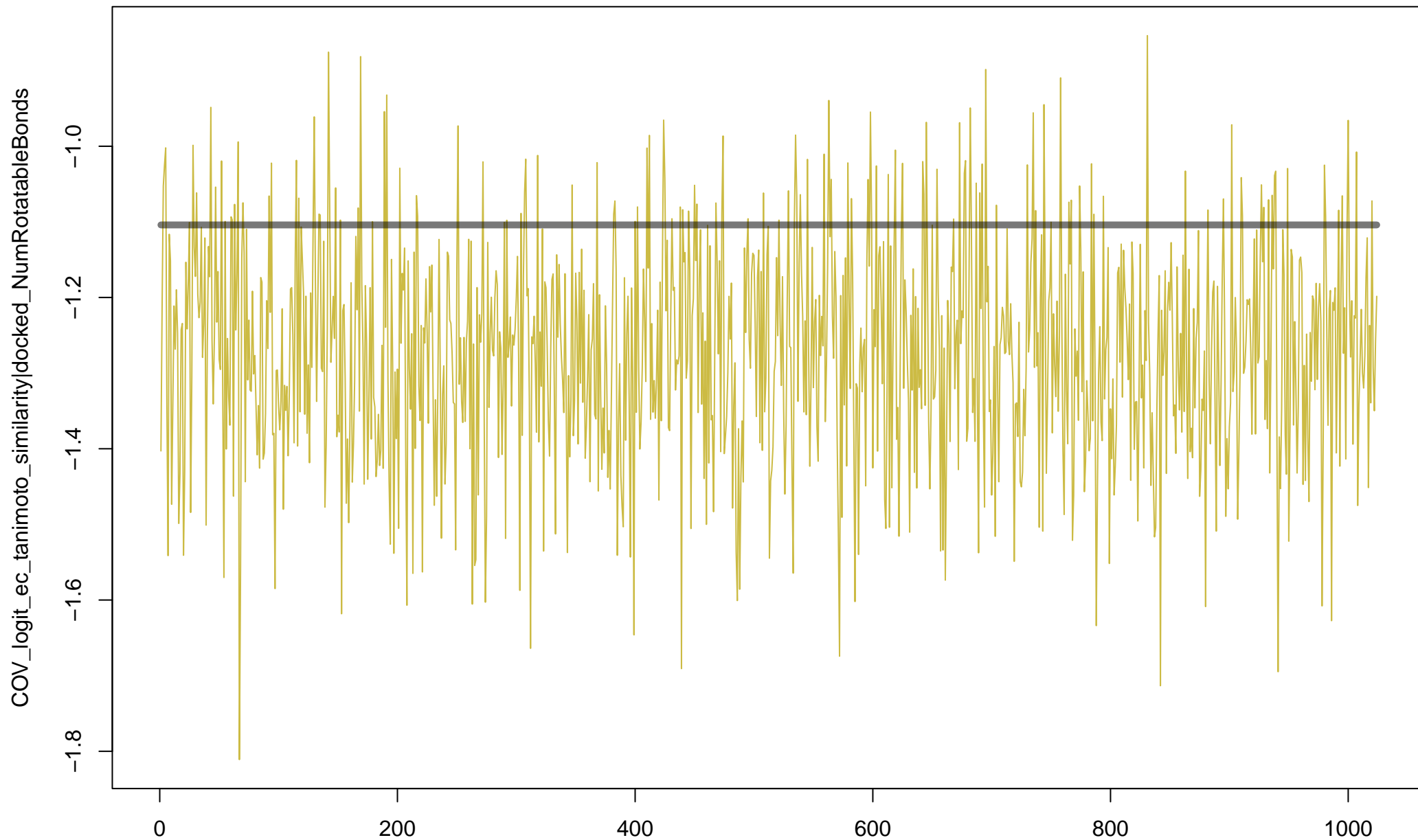
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0455 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0 | rel.err: -0.557



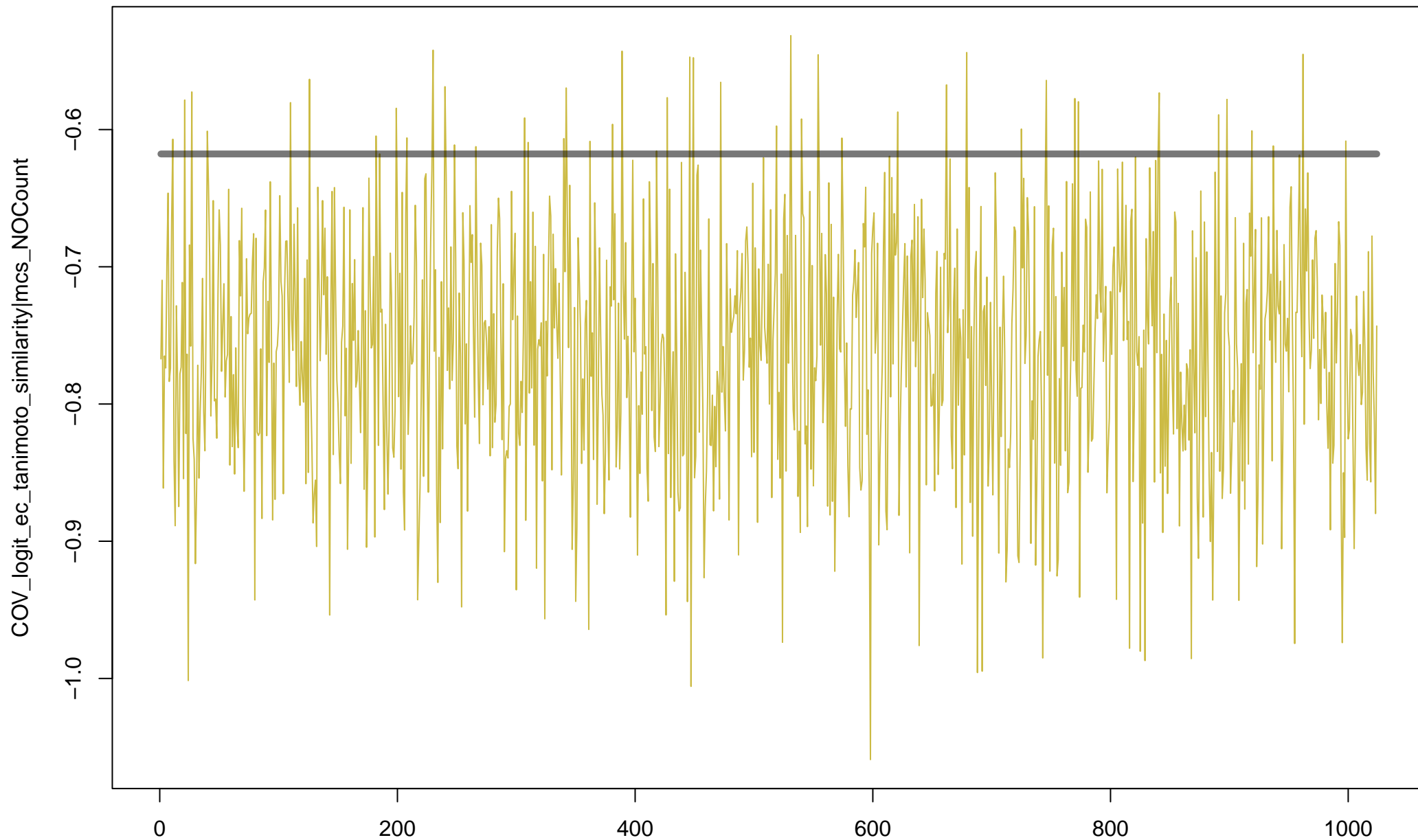
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0875 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0 | rel.err: -0.439



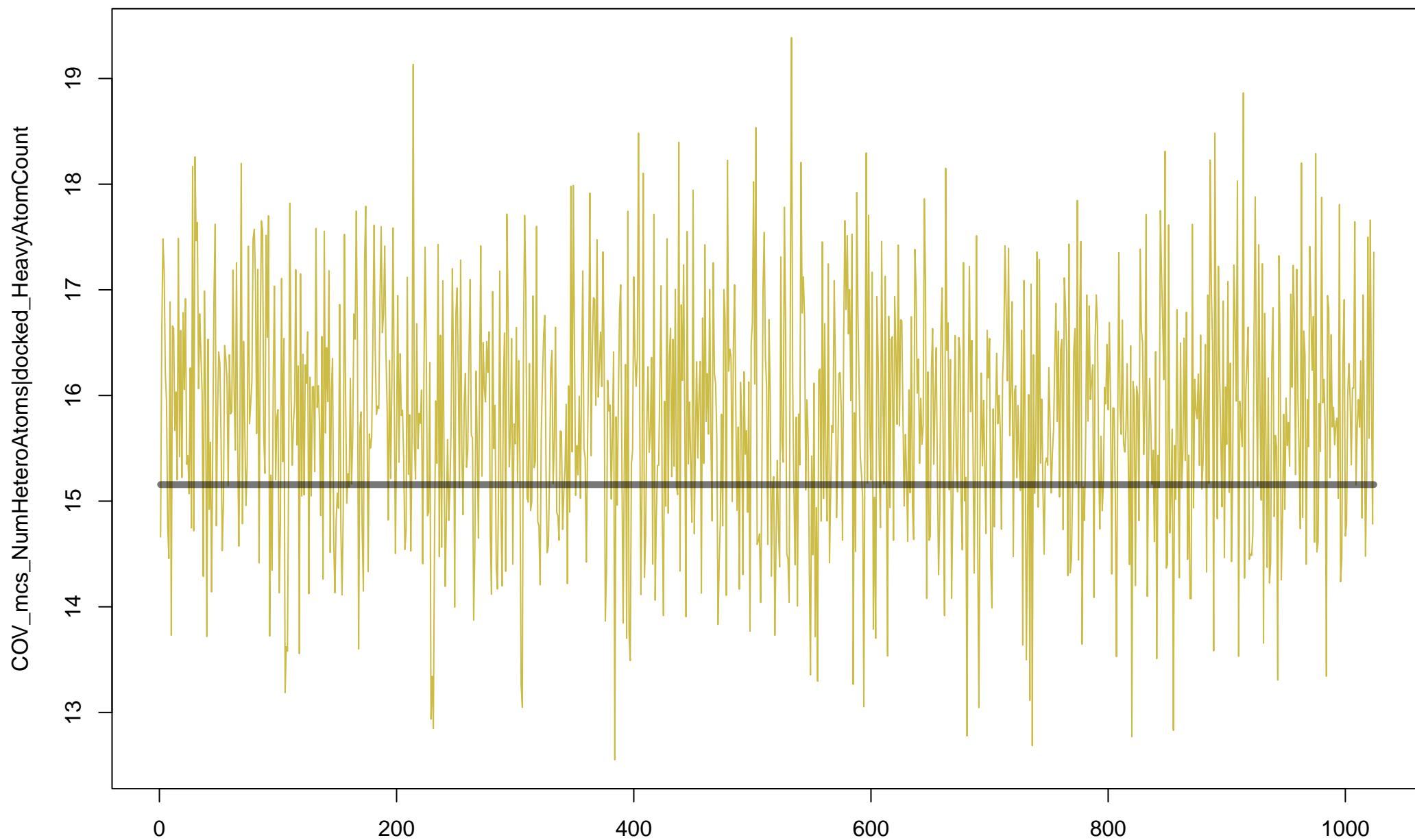
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 935 | BMK = 0.0435 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0 | rel.err: -1.17



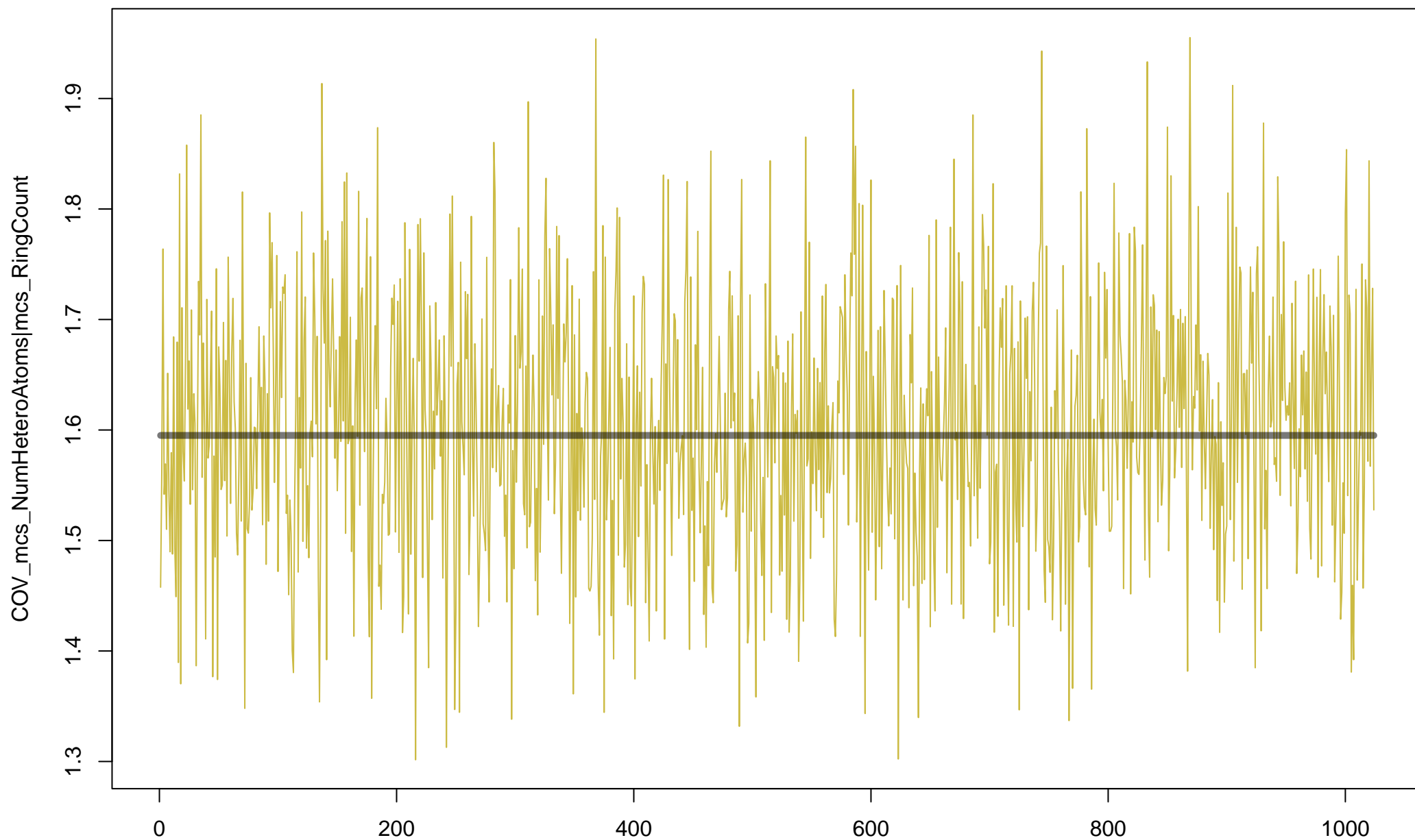
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0451 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0 | rel.err: -1.65



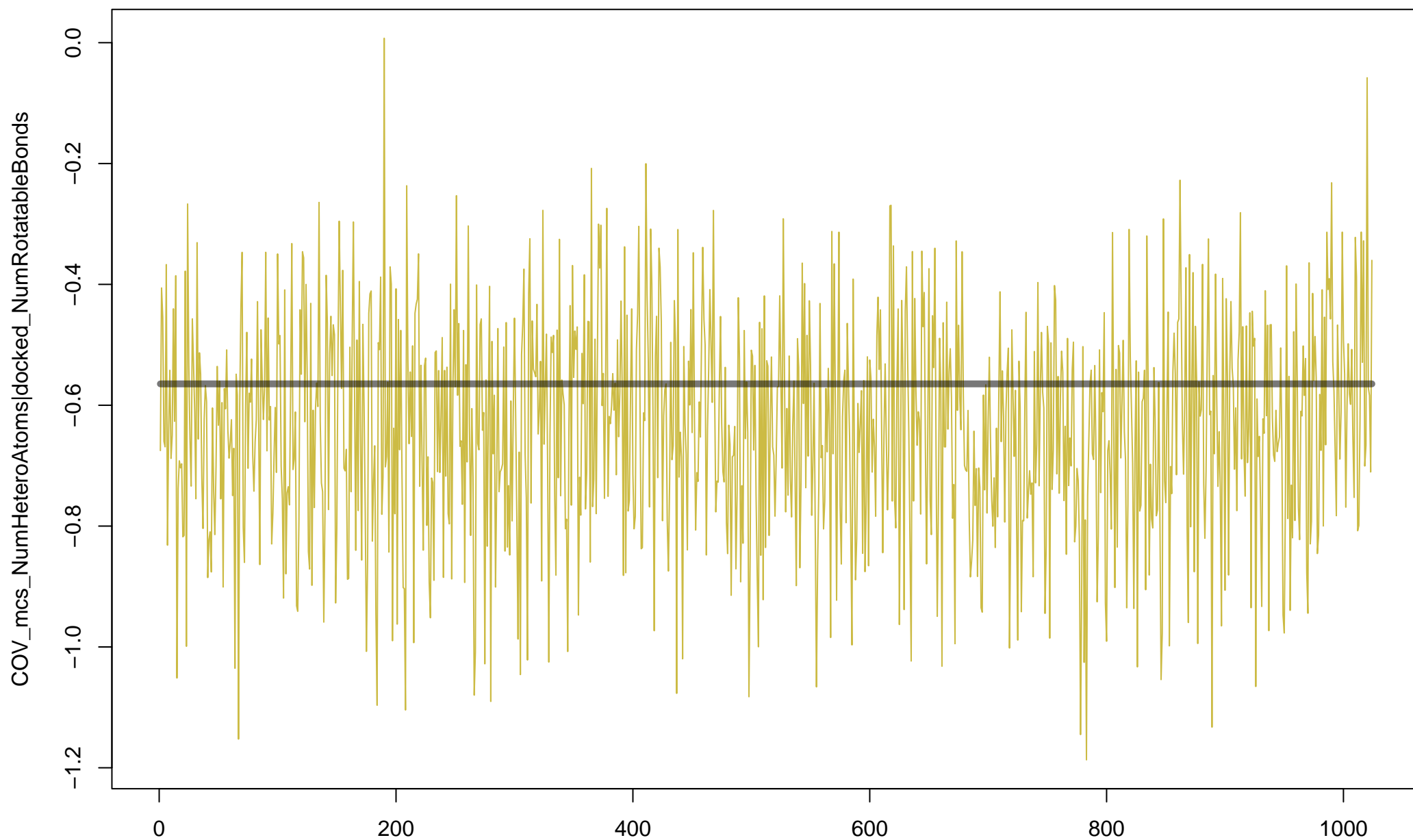
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0331 | MCSE(6.27) = 2.92 | stat: FALSE | burn: 0 | rel.err: 0.558



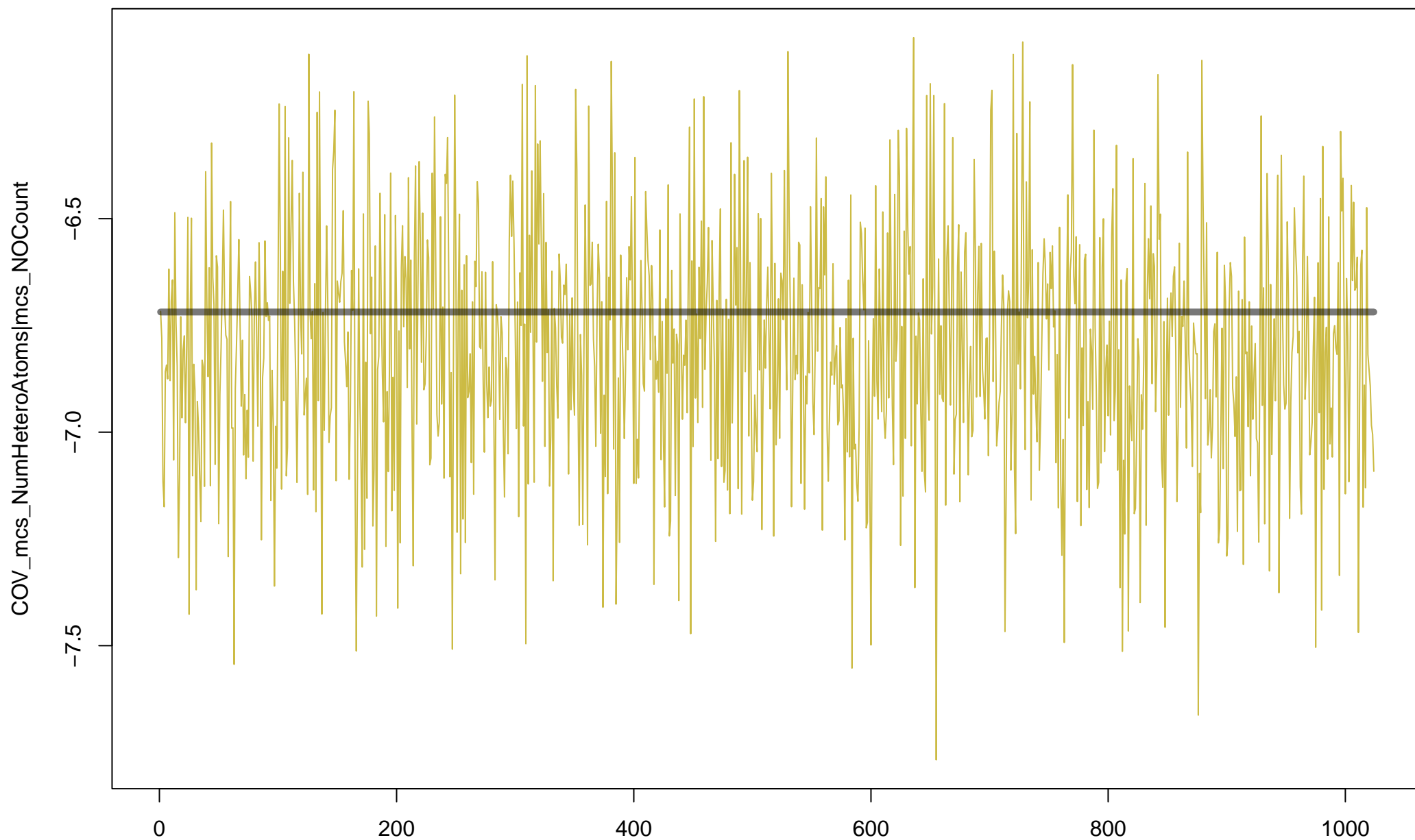
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0504 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | rel.err: 0.0785



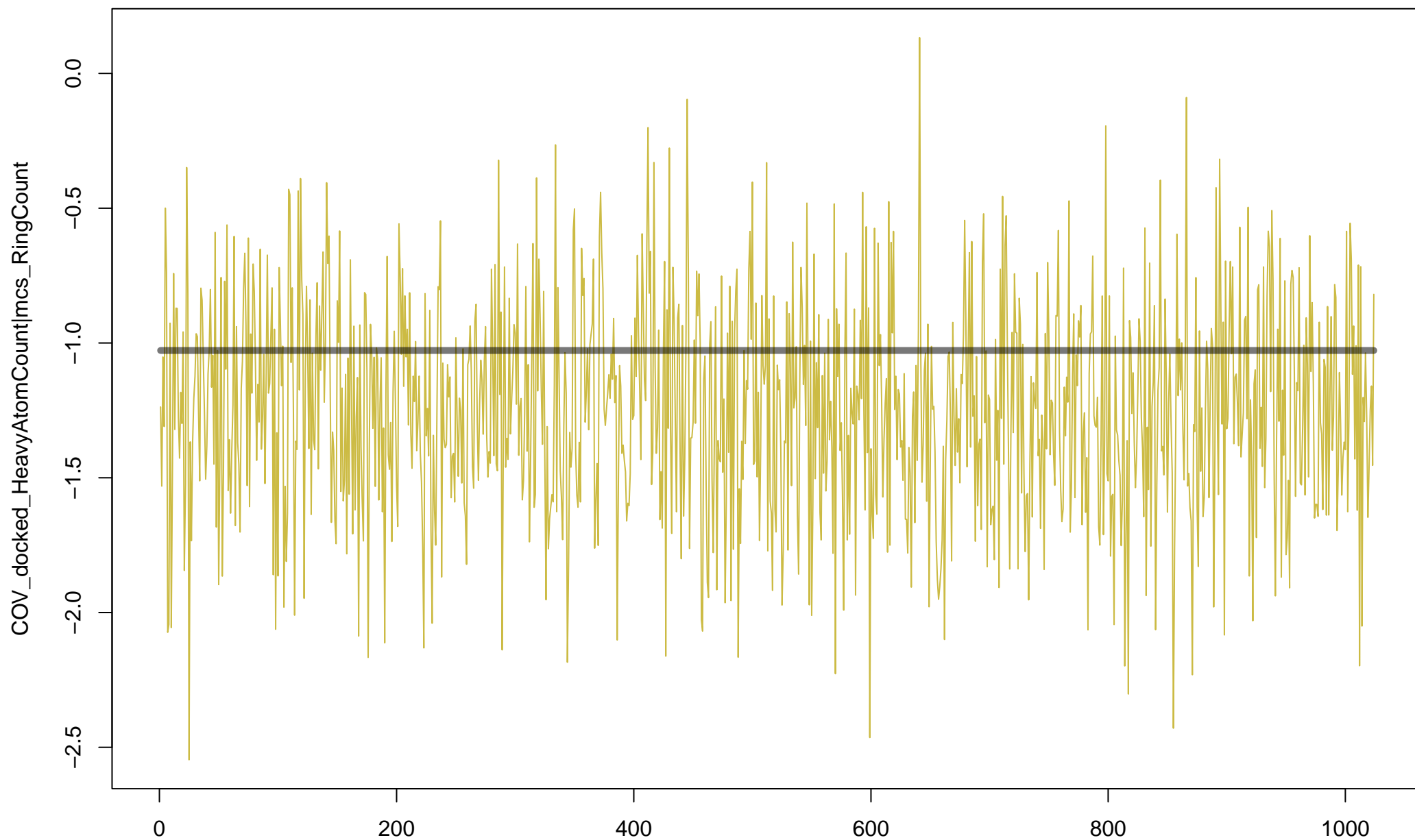
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0457 | MCSE(6.27) = 3.54 | stat: TRUE | burn: 0 | rel.err: -0.411



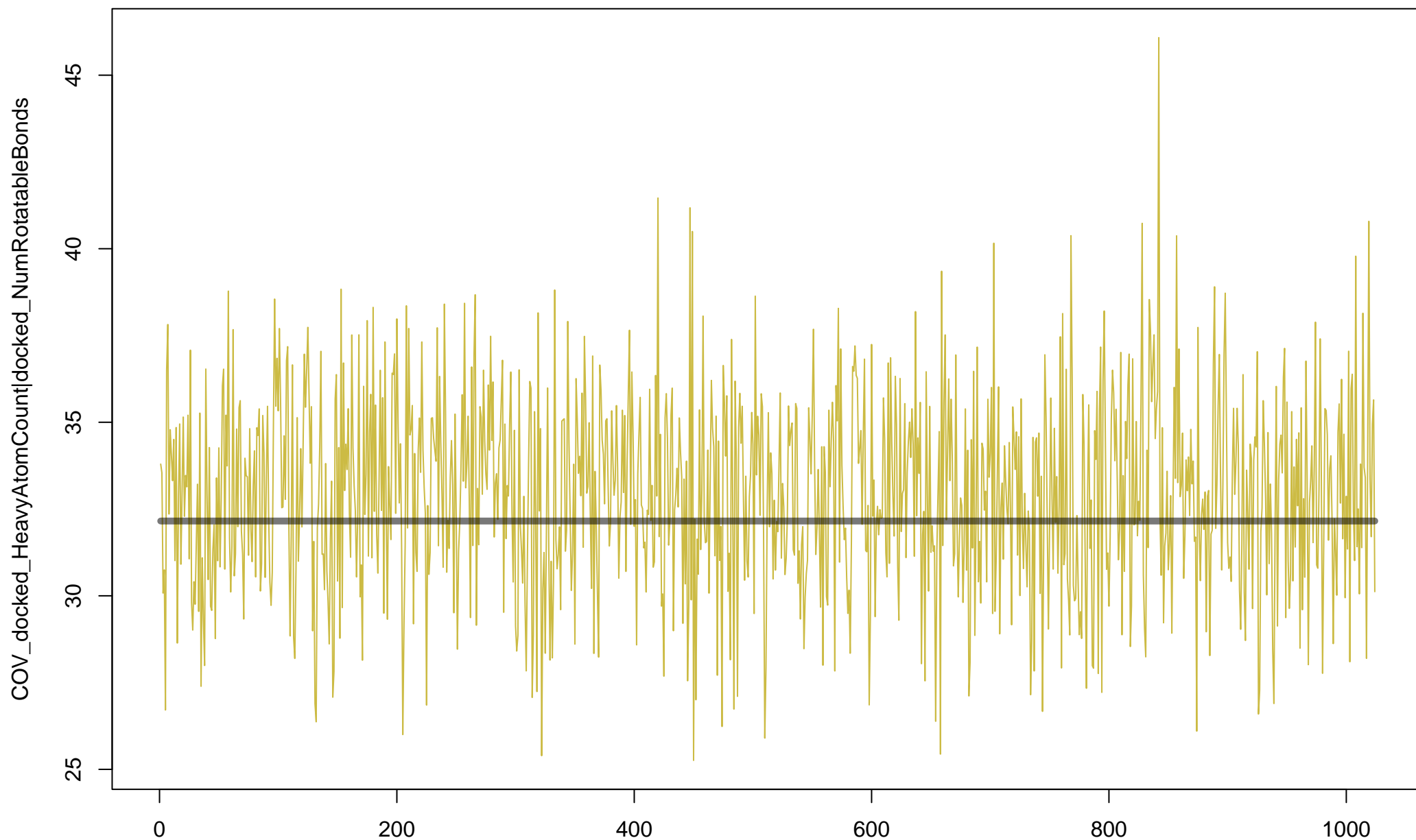
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0545 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0 | rel.err: -0.318



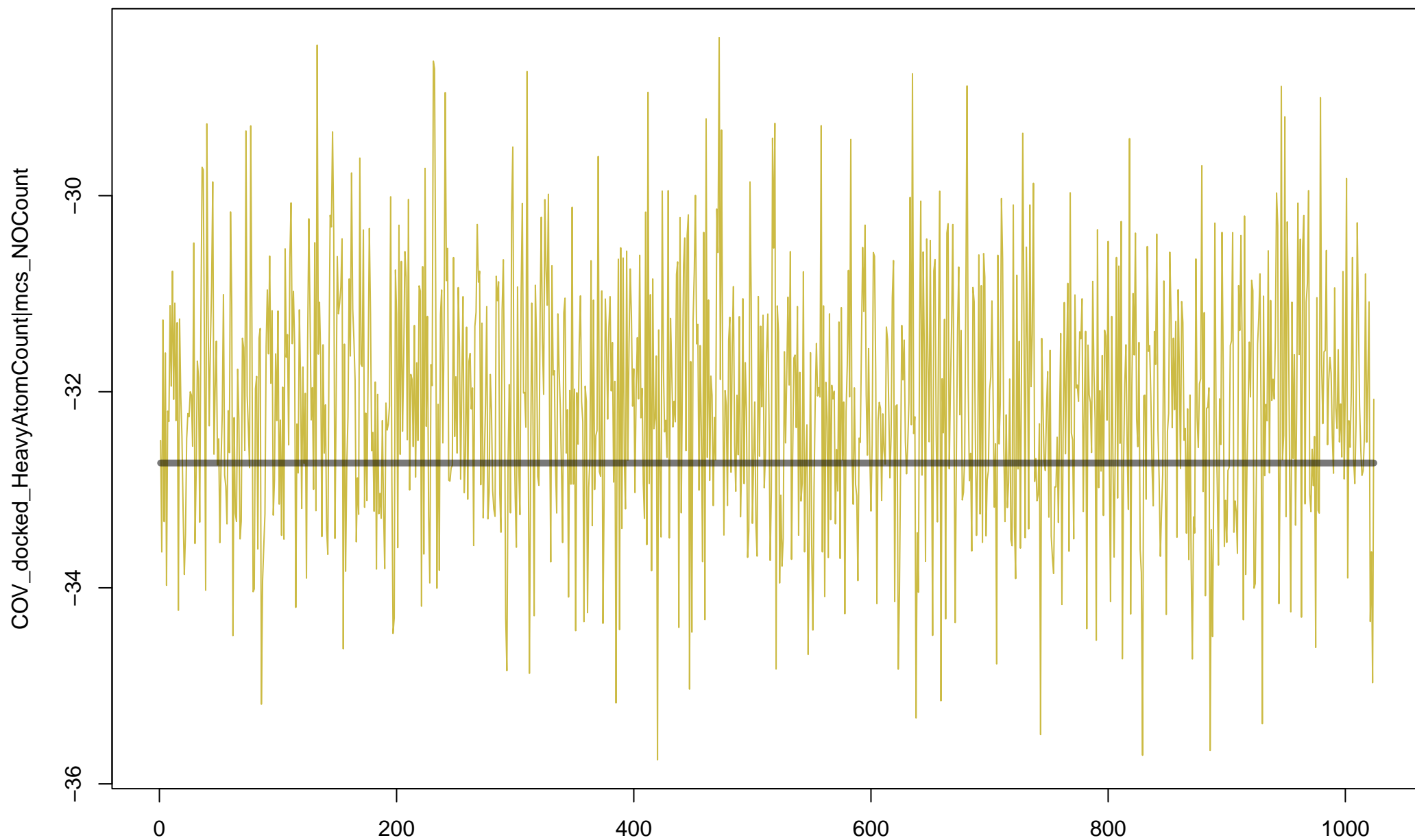
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.066 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 0 | rel.err: -0.548



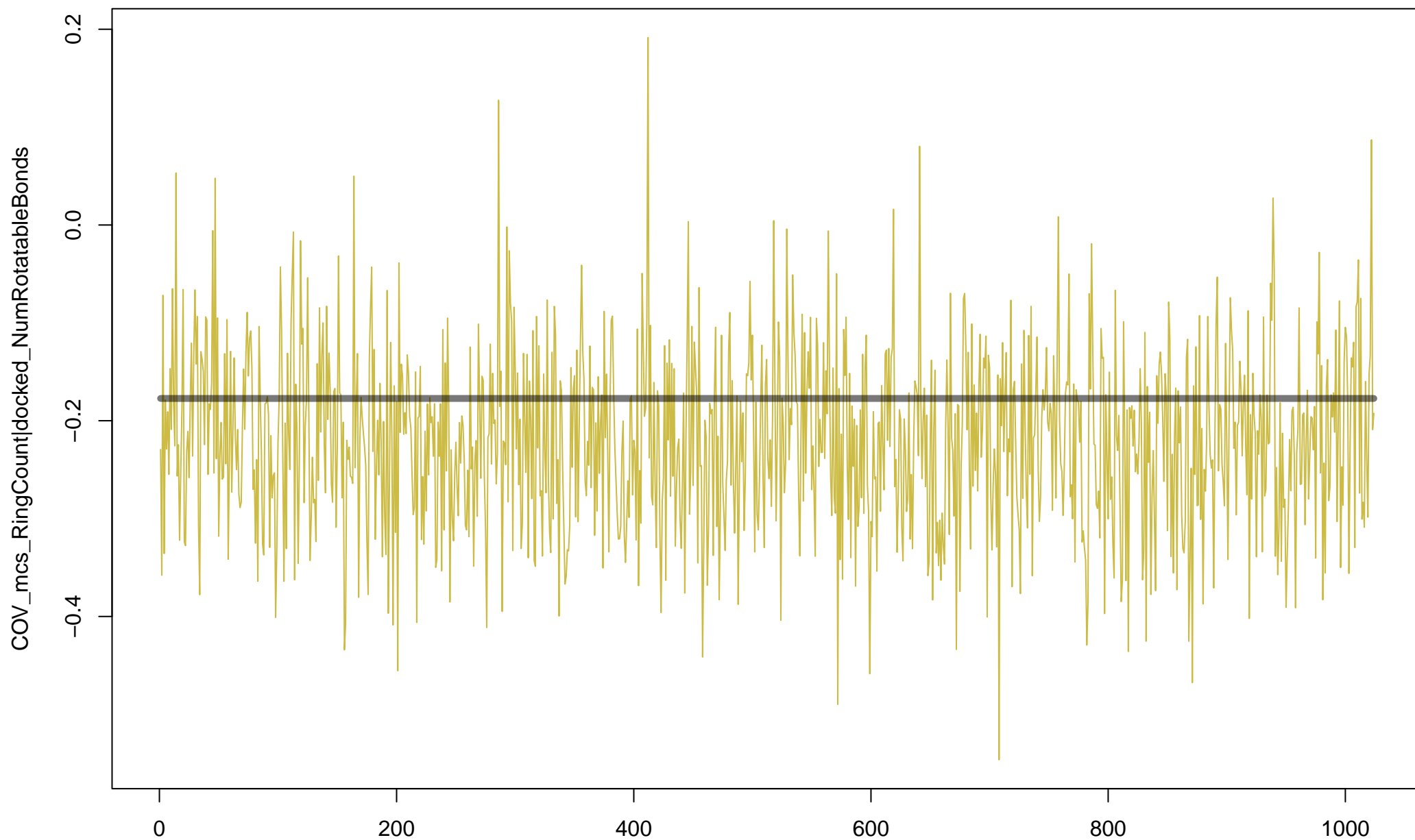
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0463 | MCSE(6.27) = 3.75 | stat: TRUE | burn: 0 | rel.err: 0.277



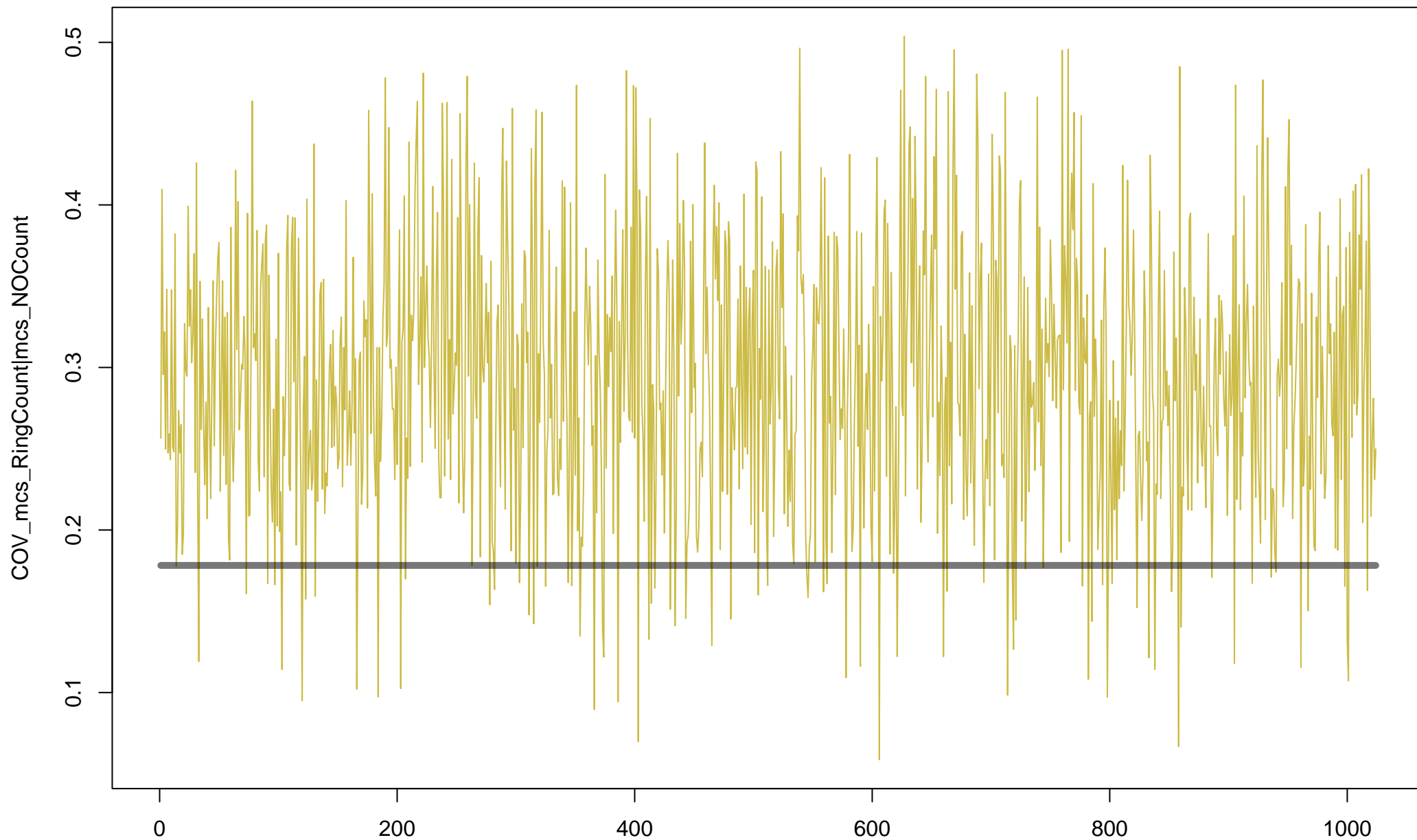
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0517 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | rel.err: 0.491



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 787 | BMK = 0.0521 | MCSE(6.27) = 3.42 | stat: TRUE | burn: 0 | rel.err: -0.464



COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.0273 | MCSE(6.27) = 3.35 | stat: TRUE | burn: 0 | rel.err: 1.4



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 910 | BMK = 0.0518 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | rel.err: -1.68

