

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.55828285499438

max MCSE = 12.9042400601096

all stationary: FALSE

burn: 816

max rel.err.: 4.13732679039149

-- STATS 1D --

min ESS = 89.0307308637649

max BMK = 0.184844373136586

max MCSE = 5.84660440488159

all stationary: FALSE

burn: 0

max rel.err.: 1.89398535053734

-- STATS 2D --

min ESS = 916.623528830765

max BMK = 0.0792477515446058

max MCSE = 3.65089181529979

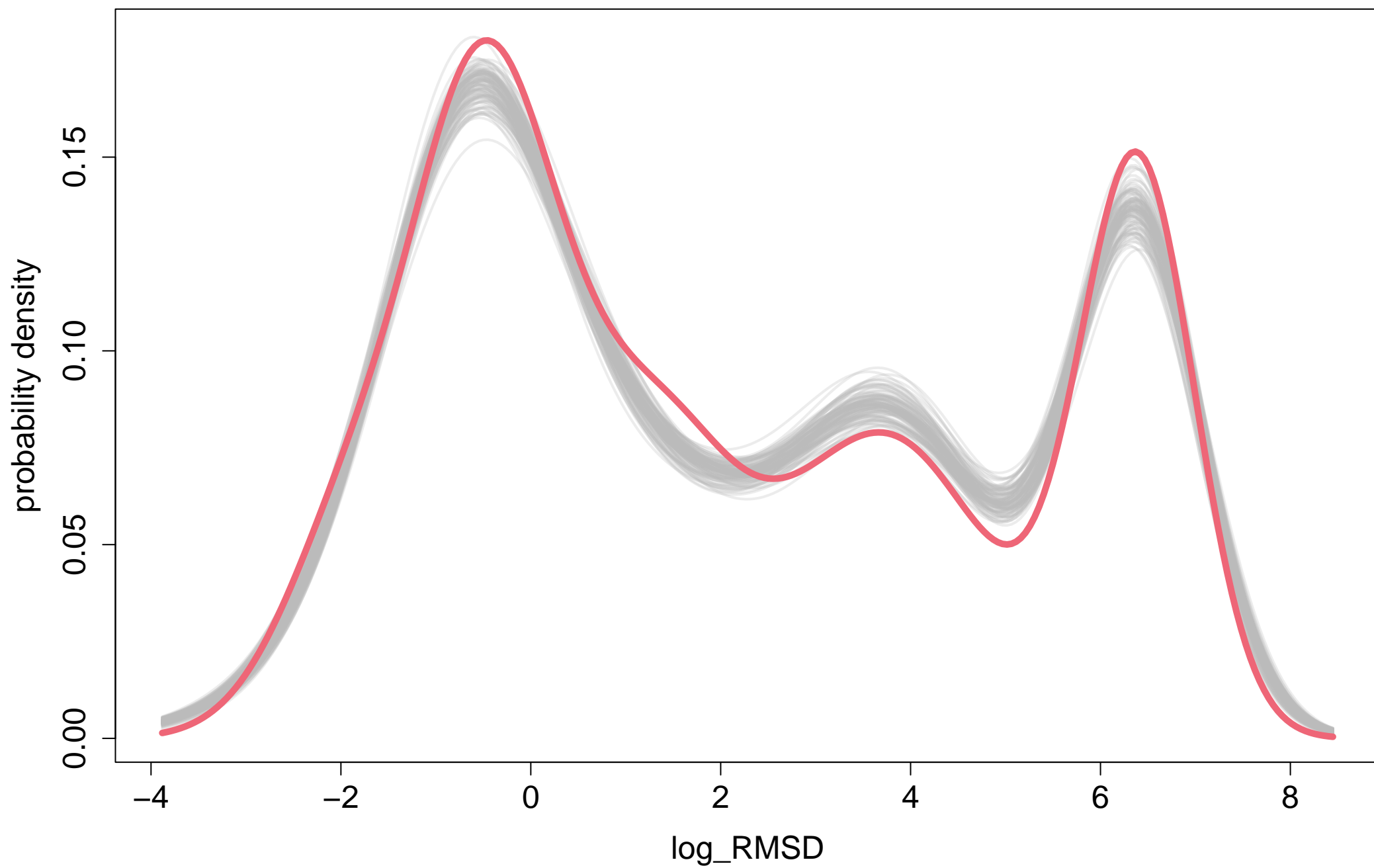
all stationary: TRUE

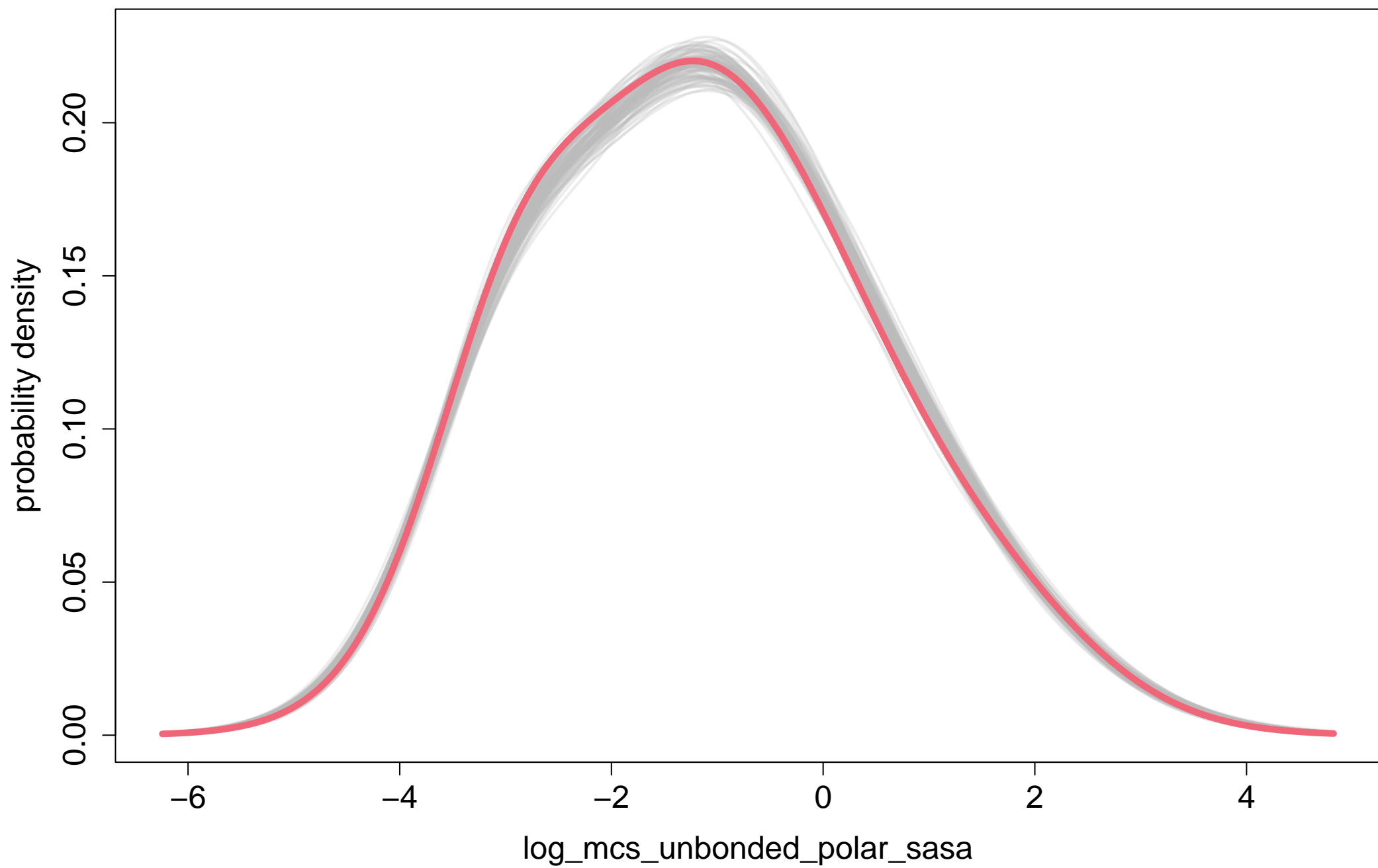
burn: 0

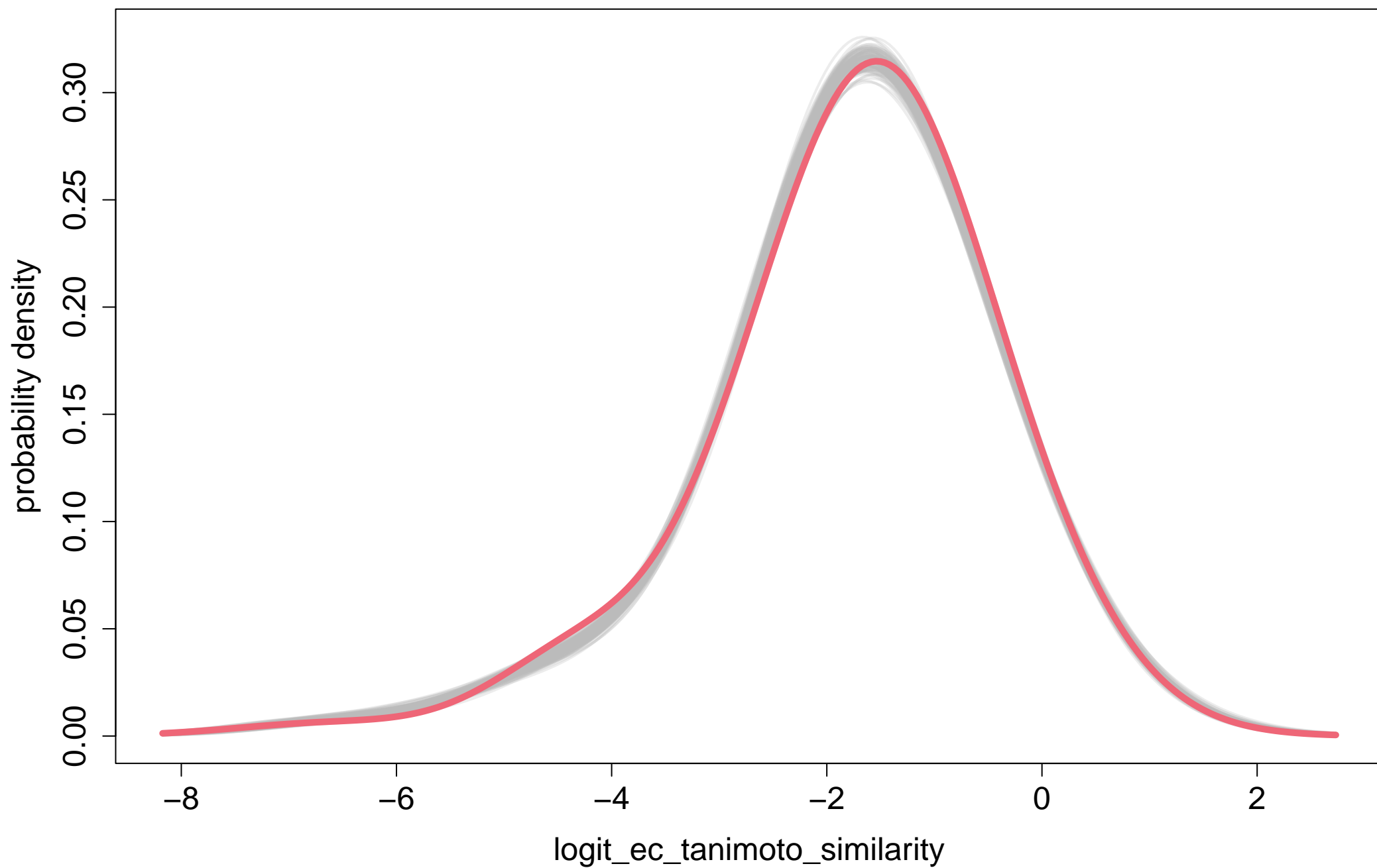
max rel.err.: 2.26011364833344

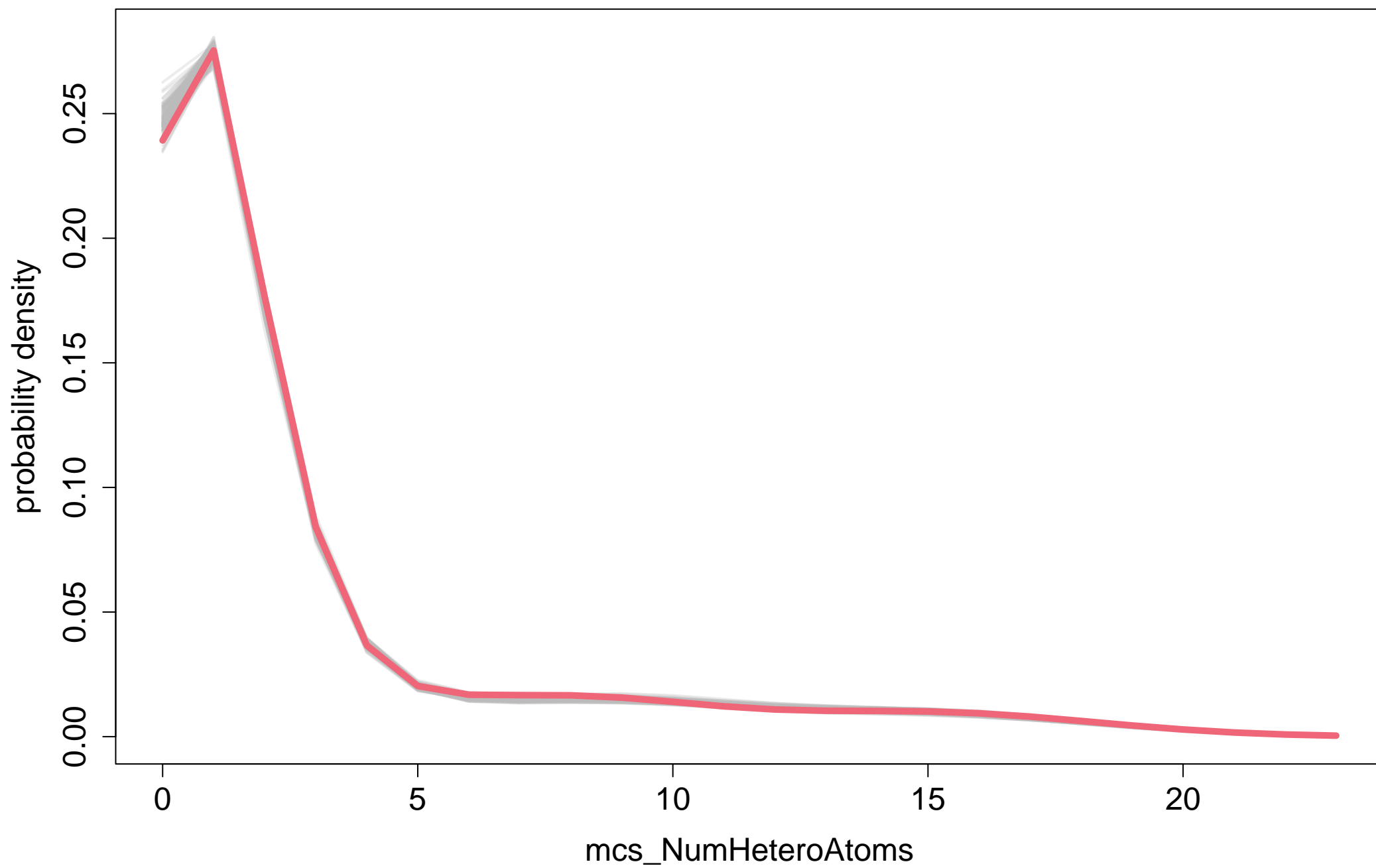
Occupied clusters: 24 of 64

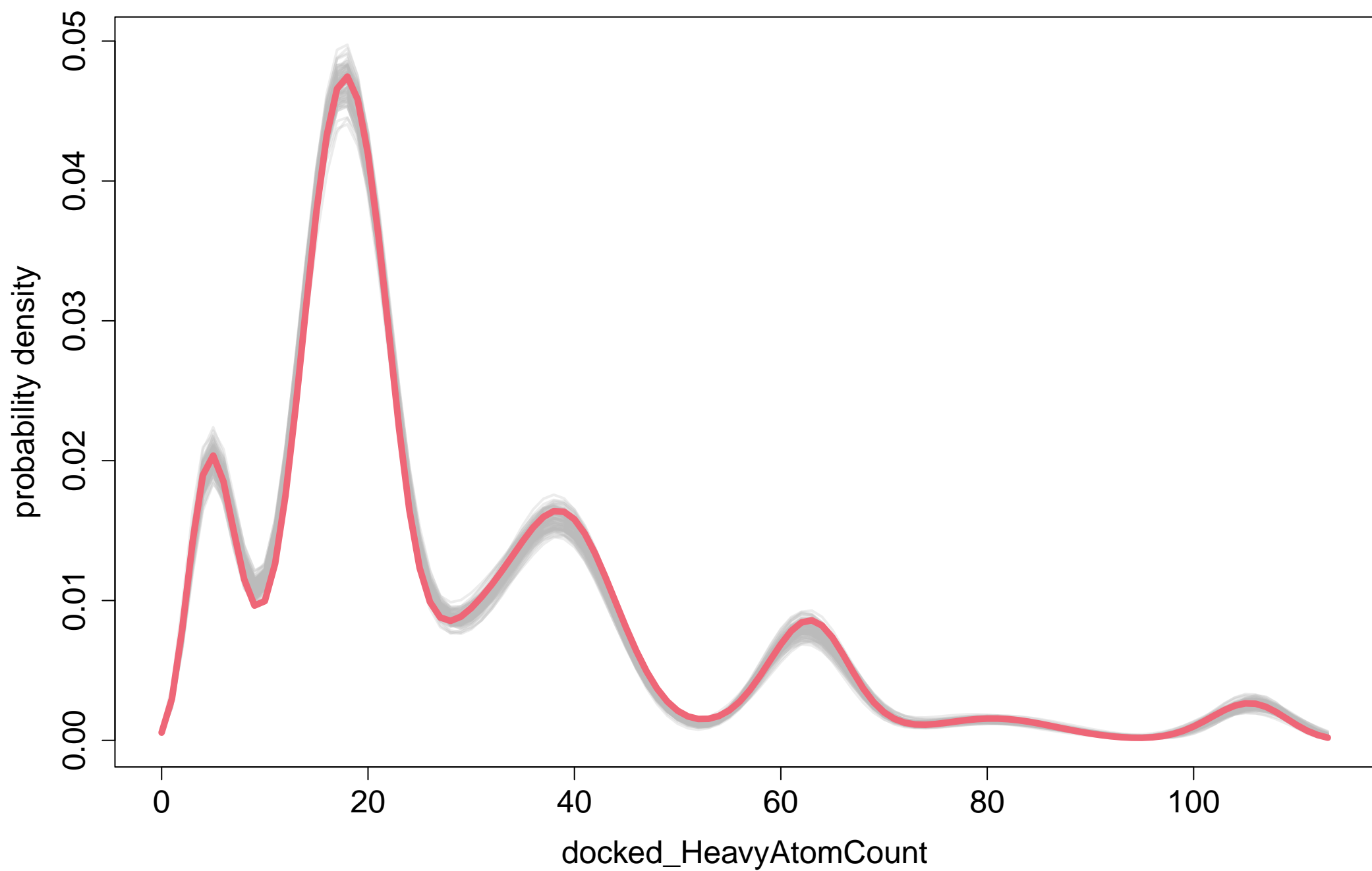
LL: -64200 +- 19.3

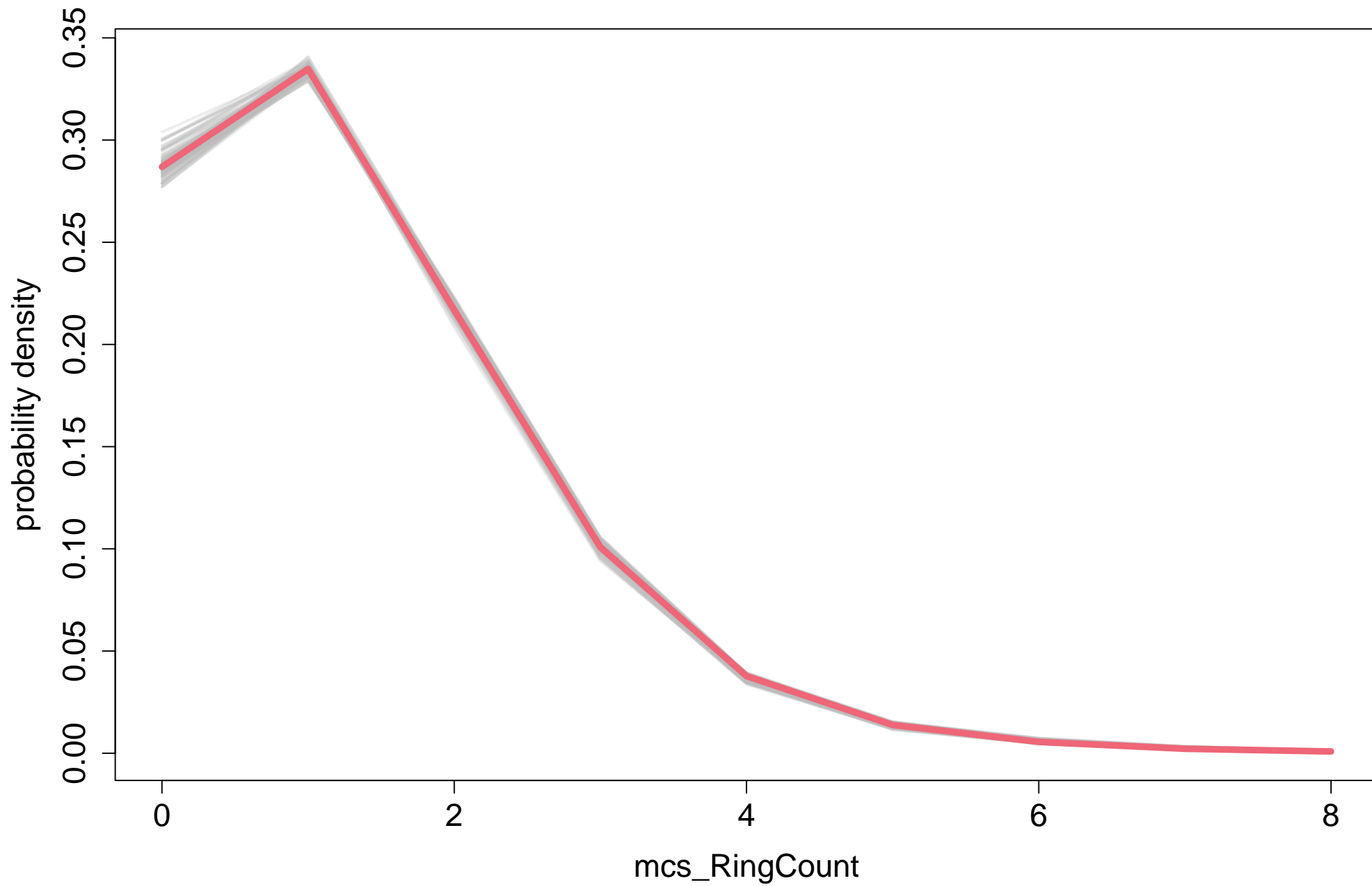


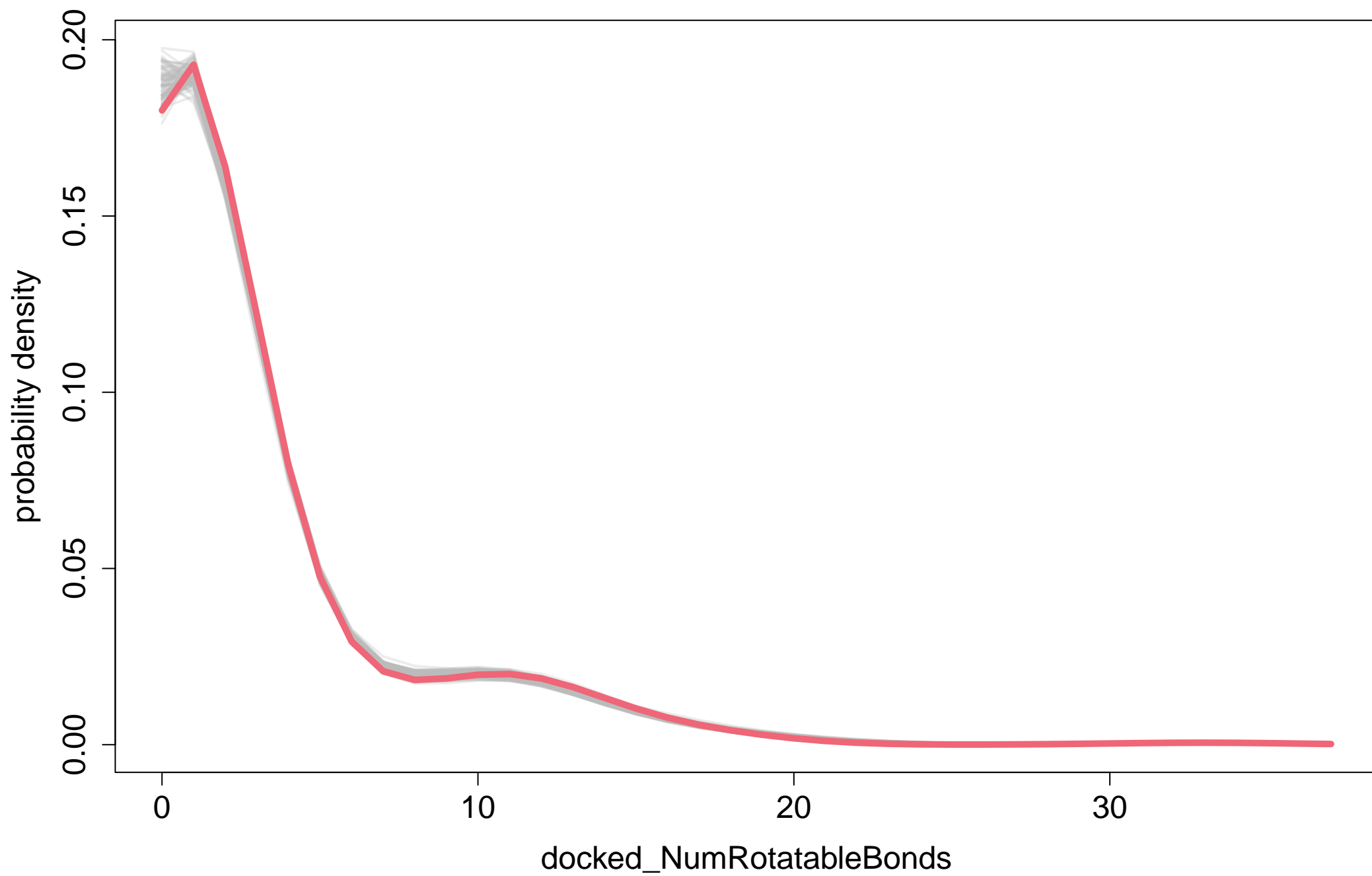


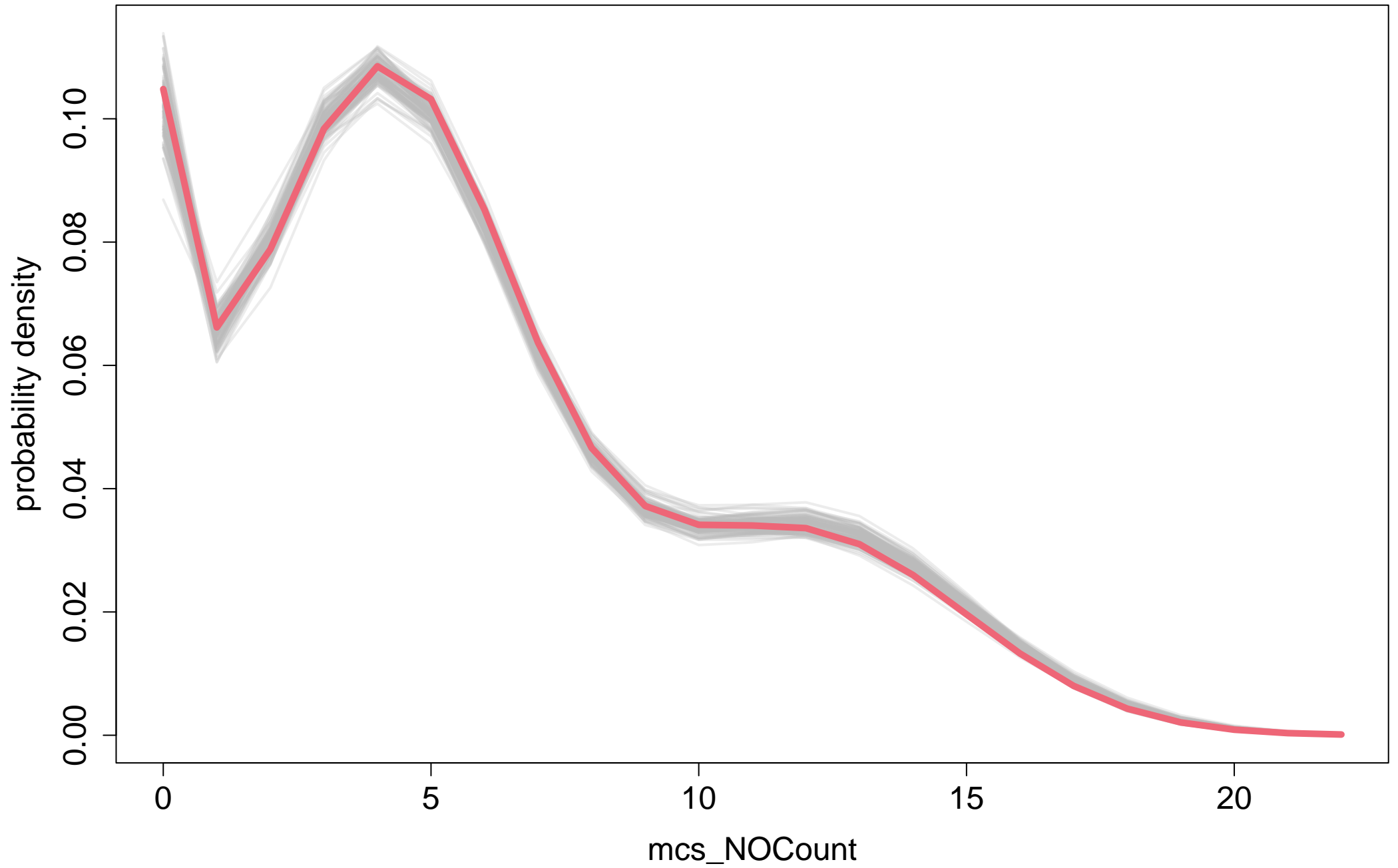


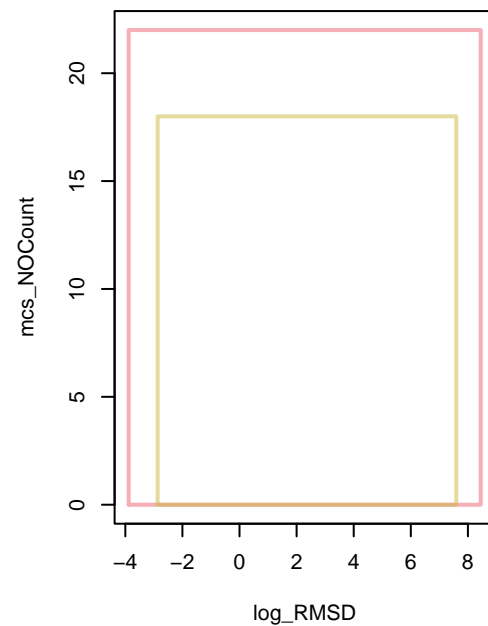
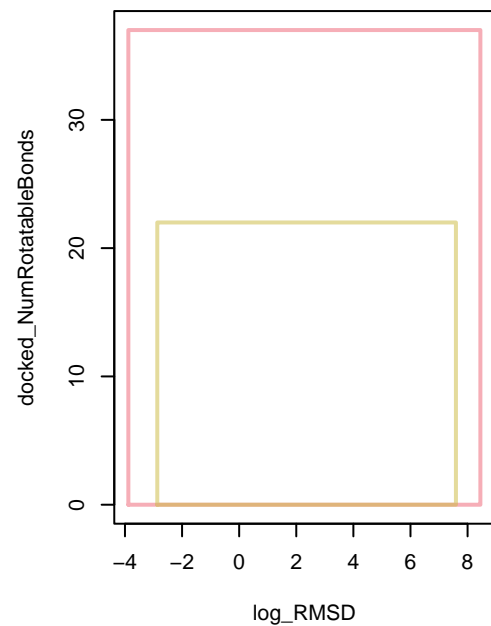
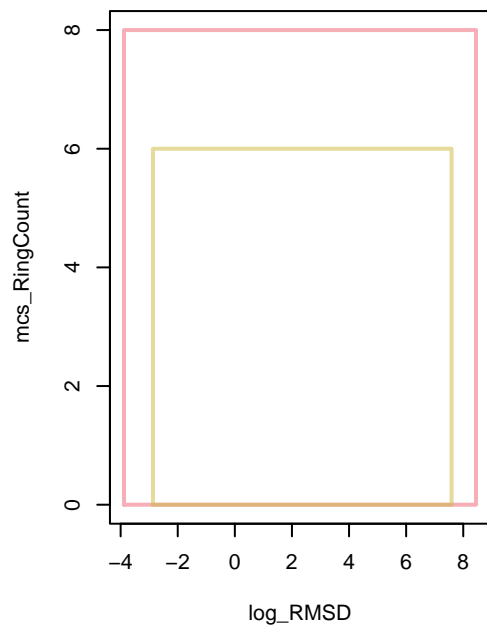
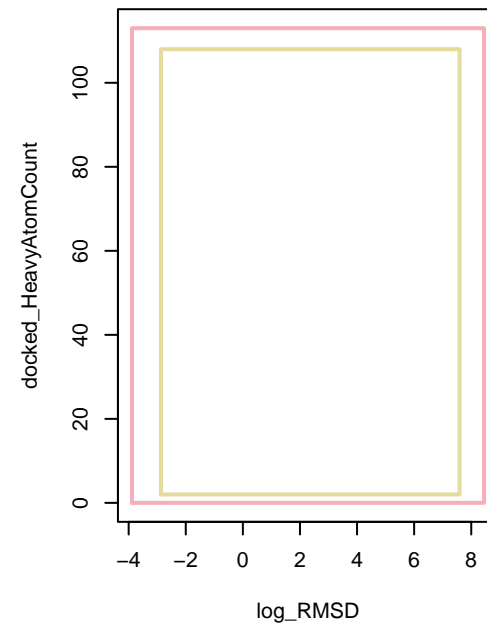
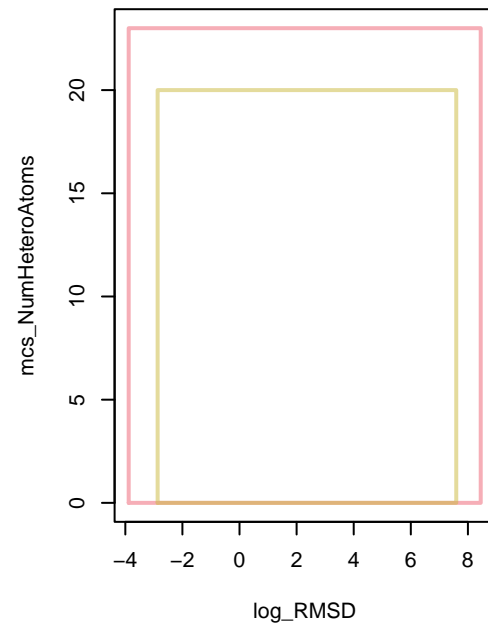
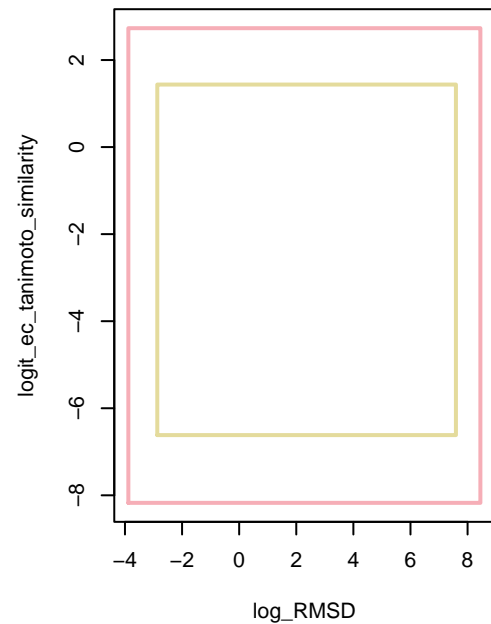
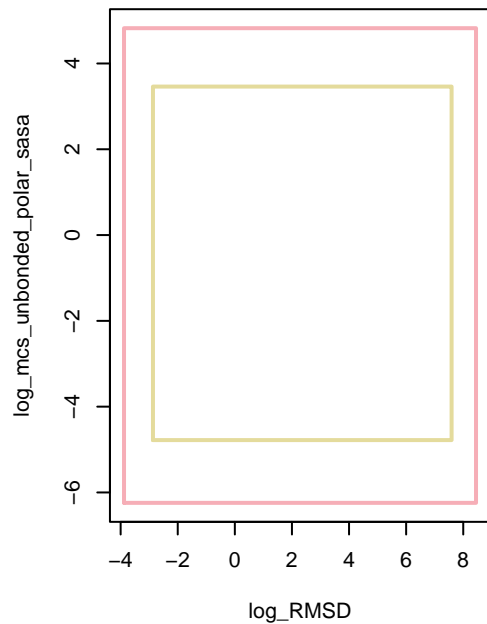




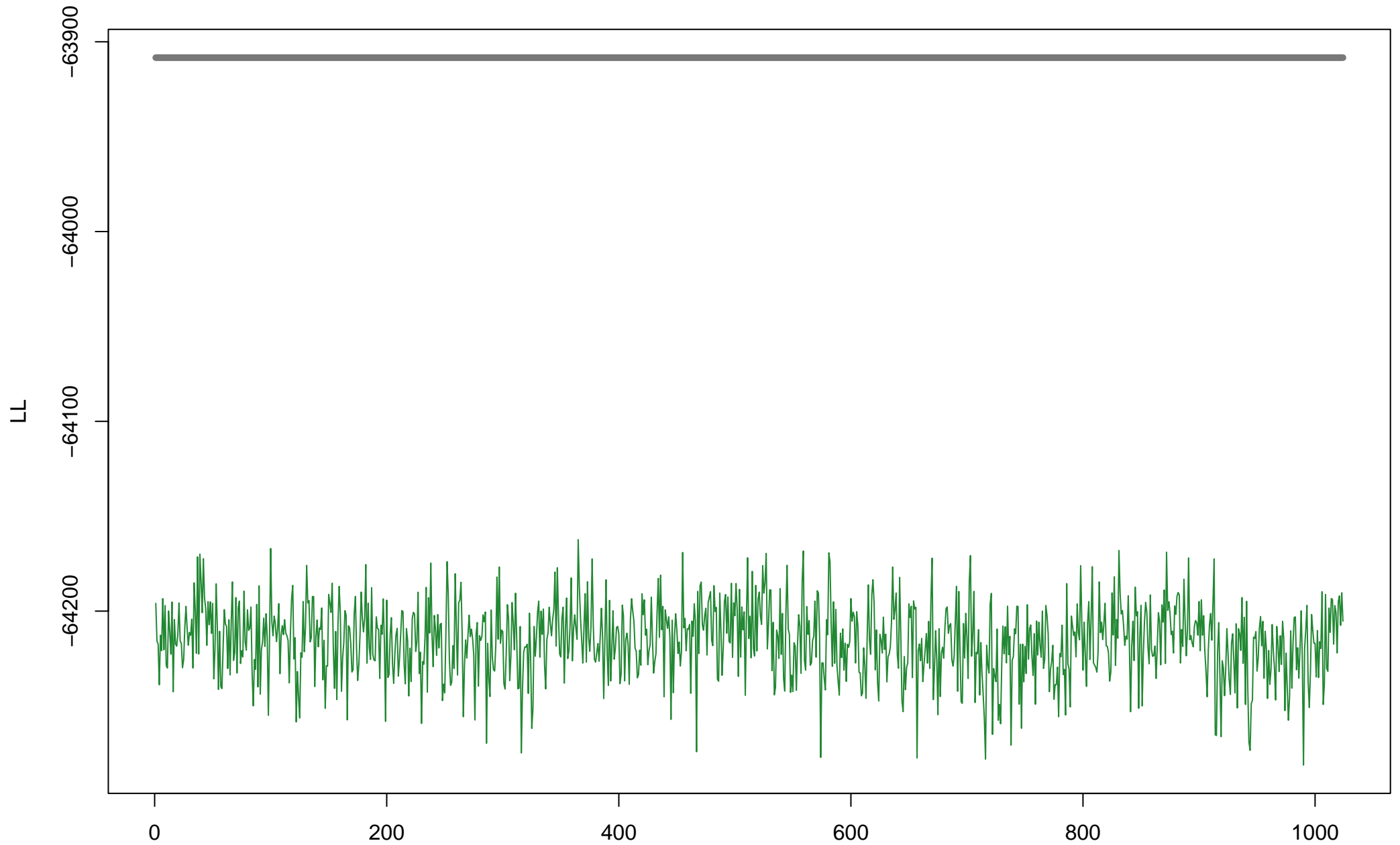






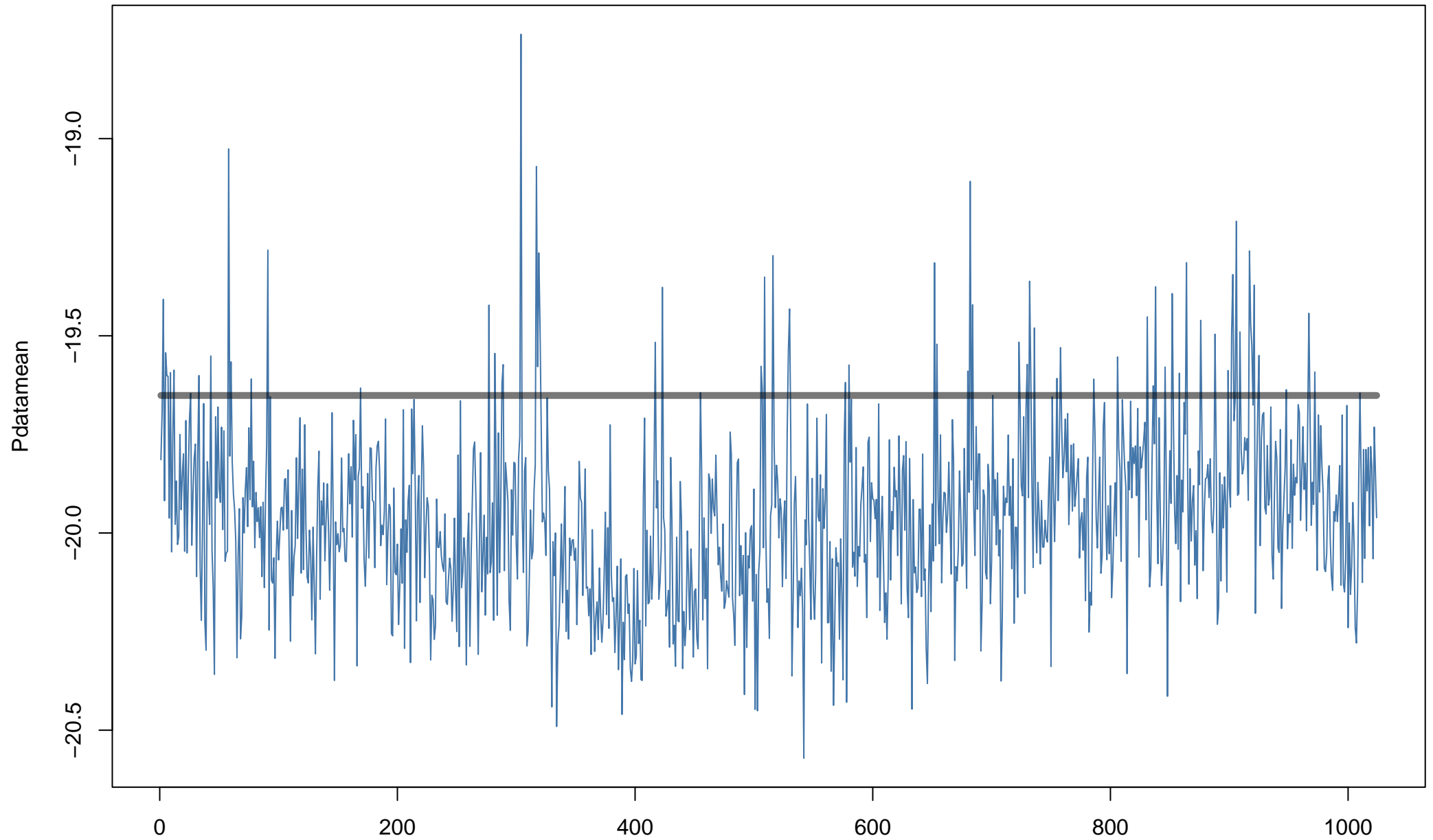


LL



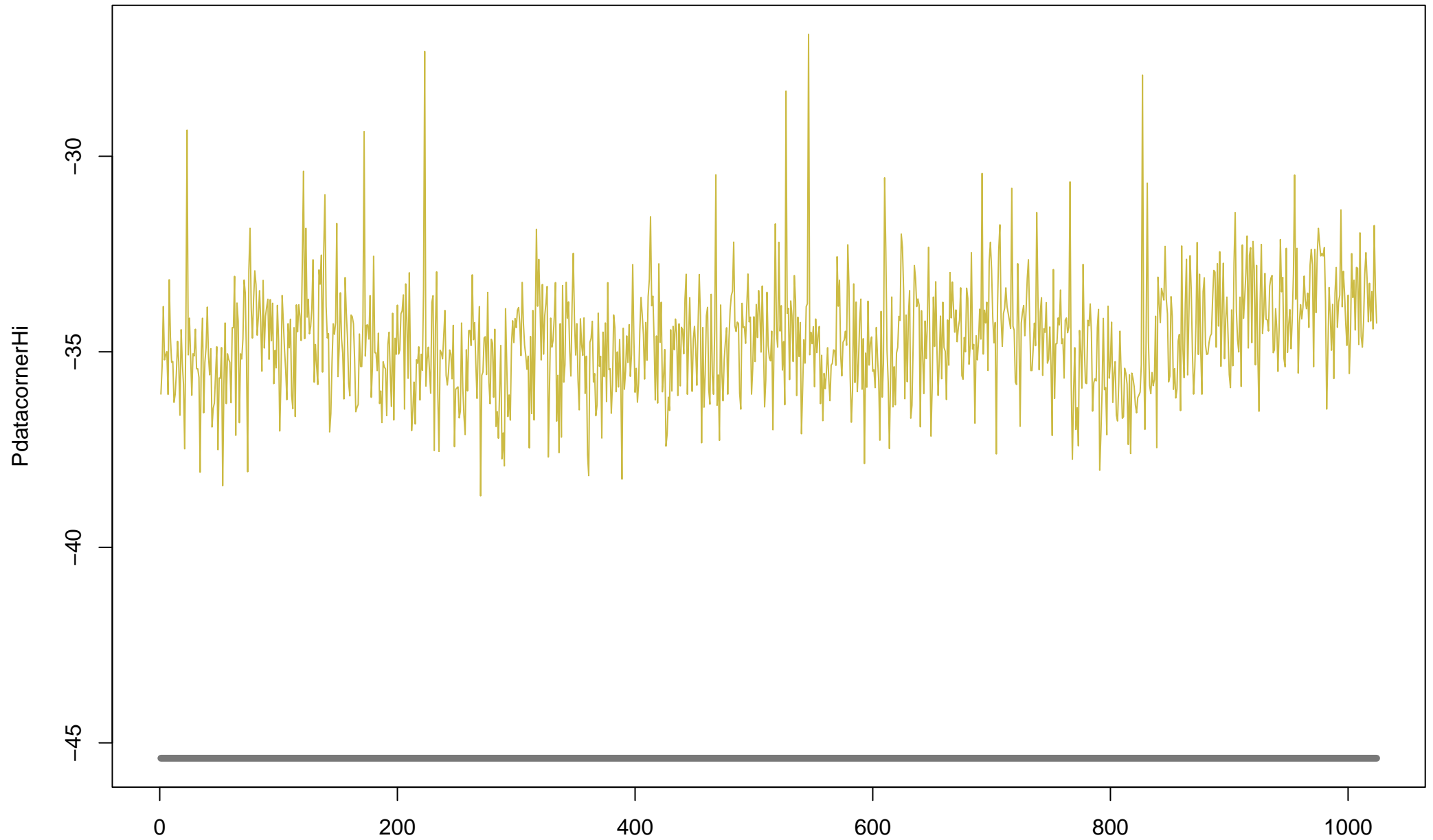
Pdatamean

ESS = 2.22e-16 | BMK = 0.169 | MCSE(6.27) = 7.35 | stat: TRUE | burn: 0 | rel.err: -1.35



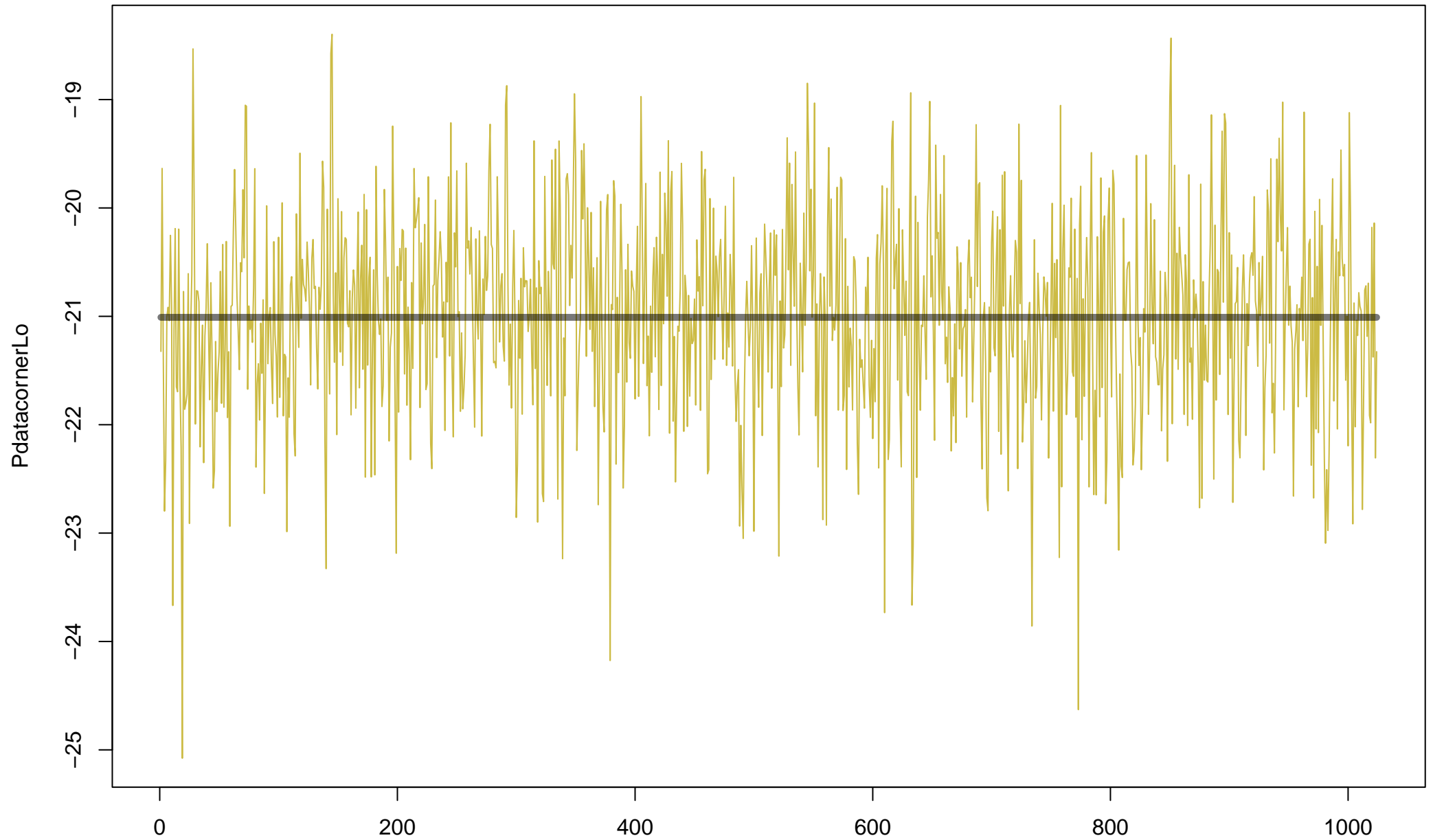
PdatacornerHi

ESS = 2.22e-16 | BMK = 0.558 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 816 | rel.err: 0.0847



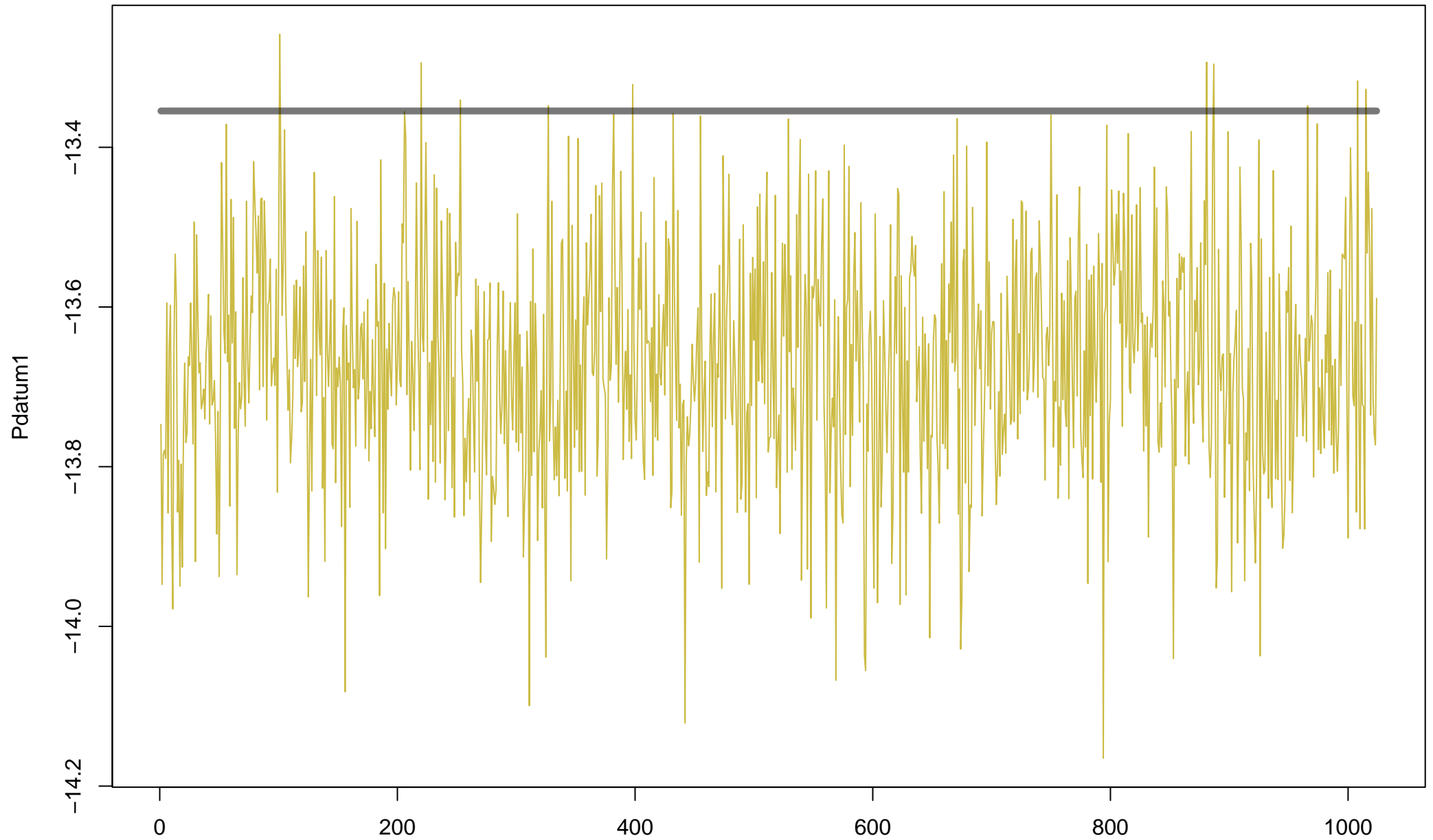
PdatacornerLo

ESS = 2.22e-16 | BMK = 0.0791 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | rel.err: 0.324



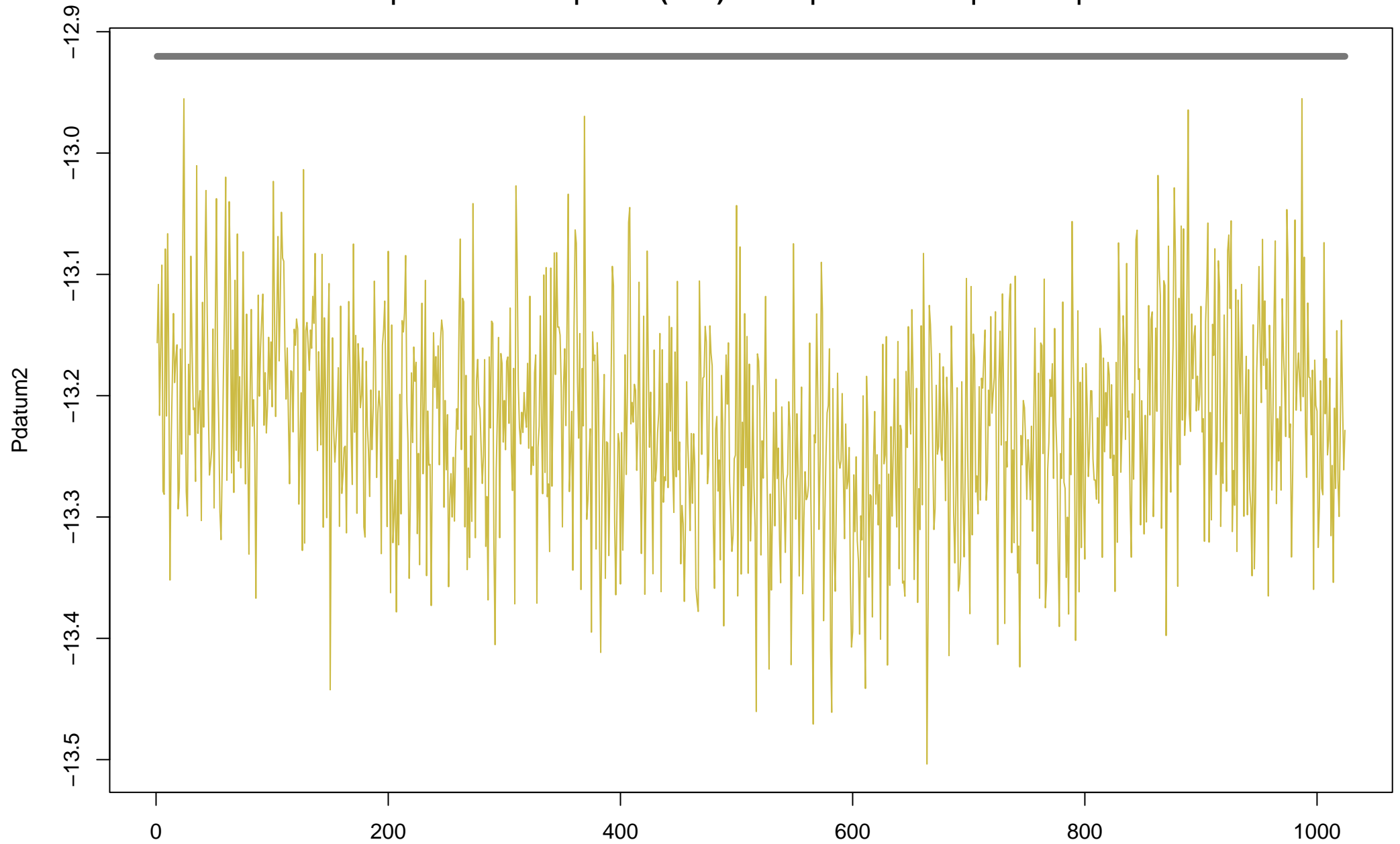
Pdatum1

ESS = 1020 | BMK = 0.0558 | MCSE(6.27) = 4.29 | stat: TRUE | burn: 0 | rel.err: -2.57



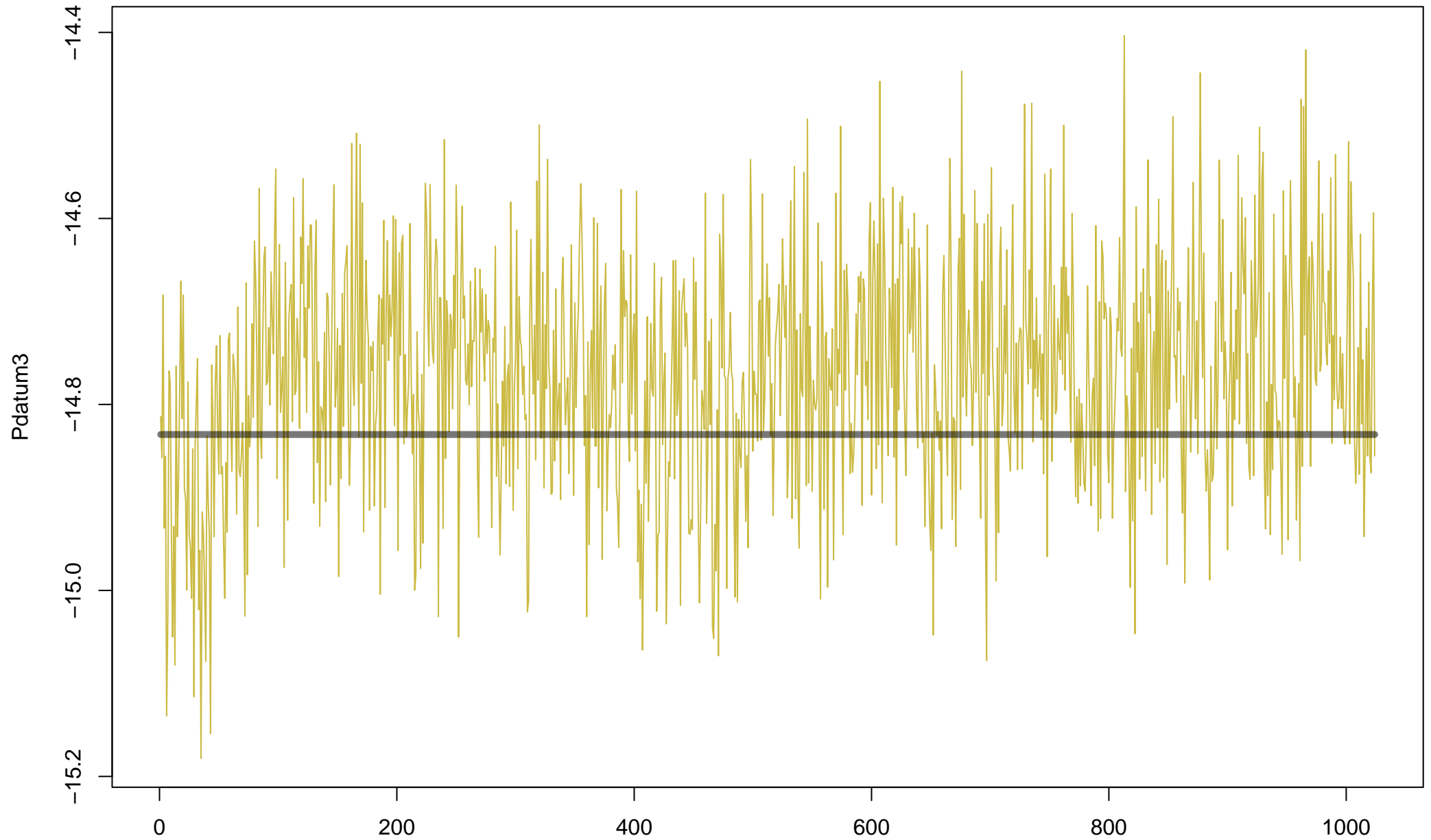
Pdatum2

ESS = 108 | BMK = 0.0972 | MCSE(6.27) = 6.51 | stat: FALSE | burn: 0 | rel.err: -4.14



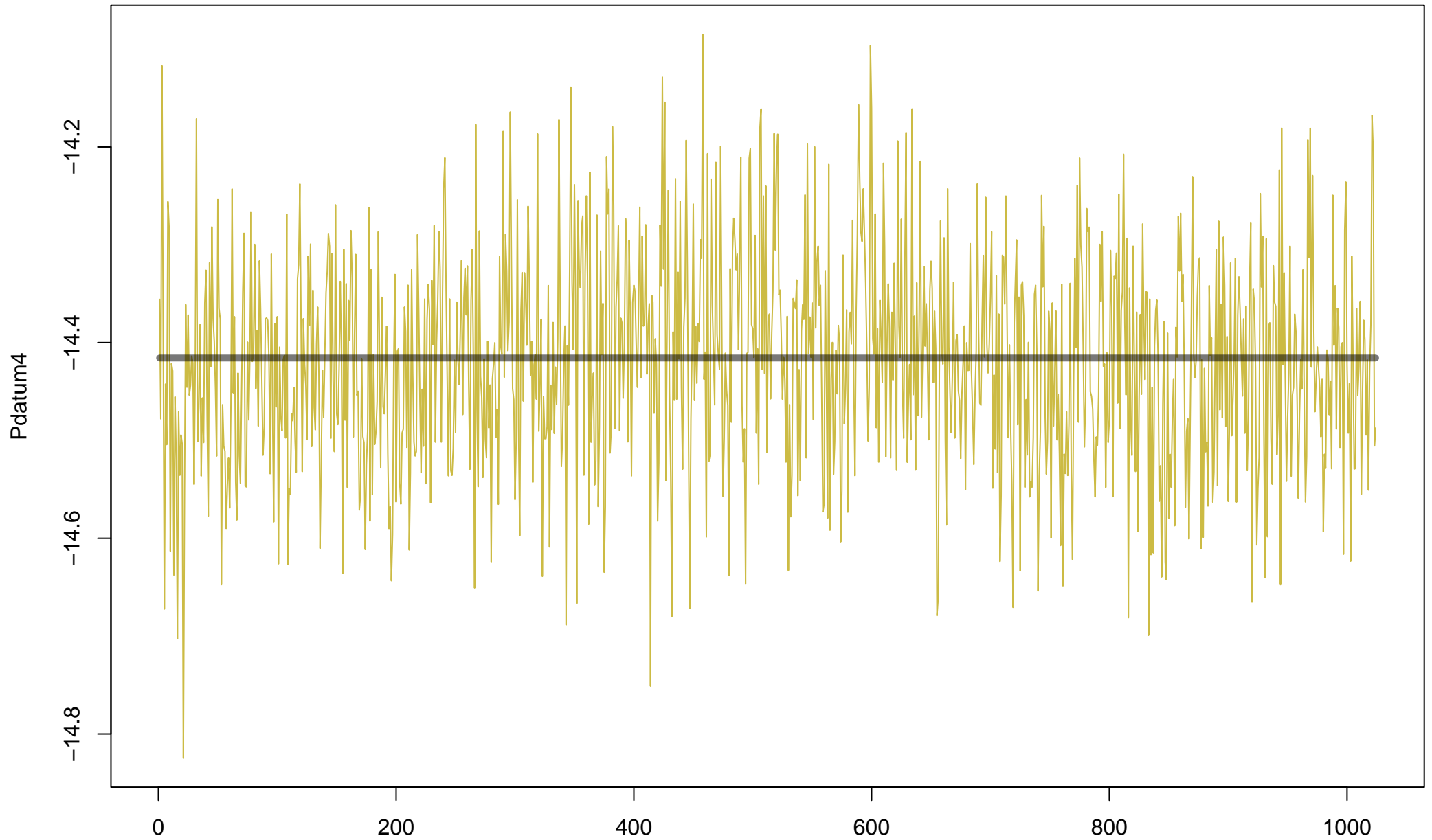
Pdatum3

ESS = 422 | BMK = 0.126 | MCSE(6.27) = 5.9 | stat: FALSE | burn: 0 | rel.err: 0.566



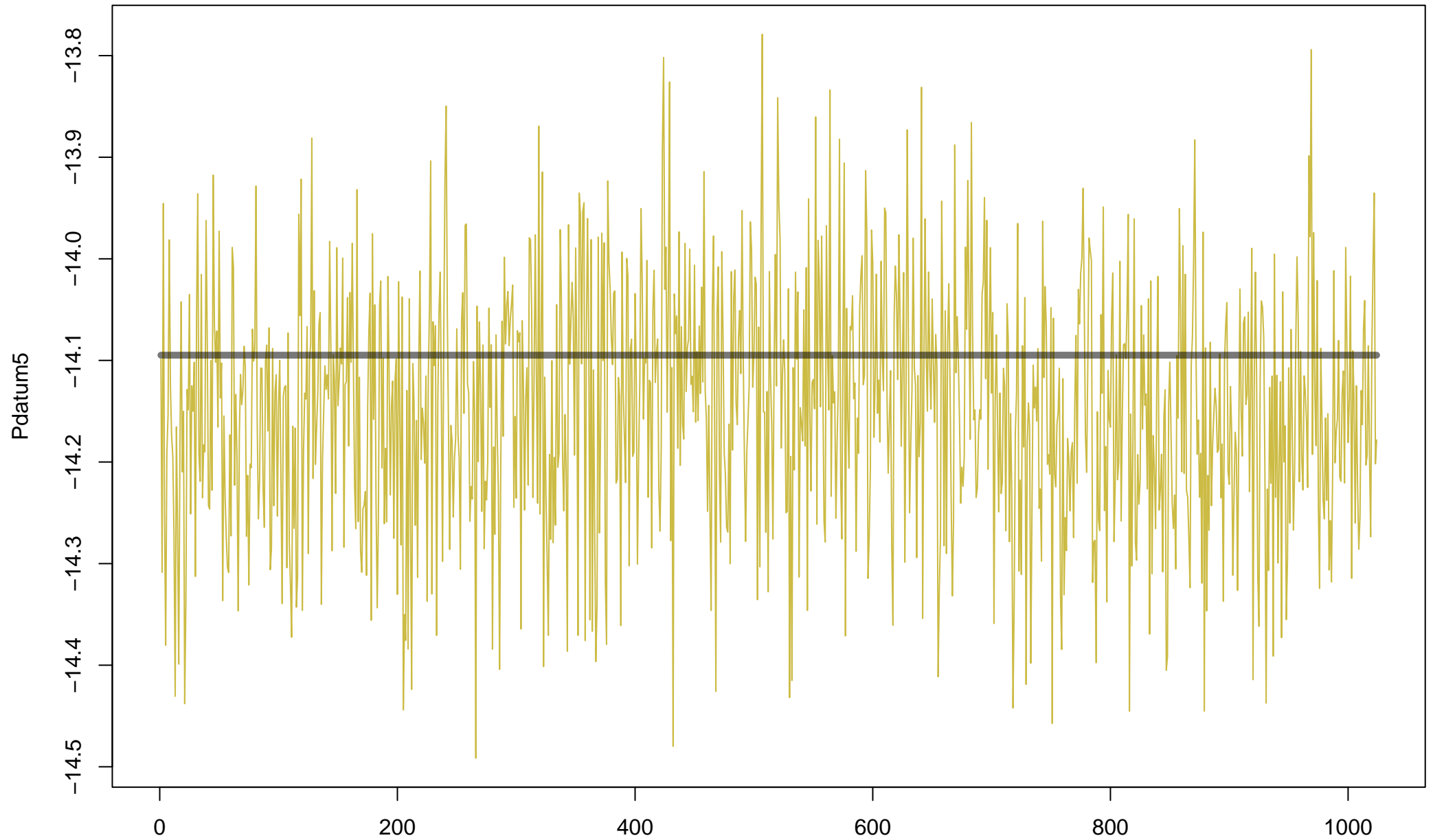
Pdatum4

ESS = 542 | BMK = 0.045 | MCSE(6.27) = 4.48 | stat: TRUE | burn: 0 | rel.err: 0.021



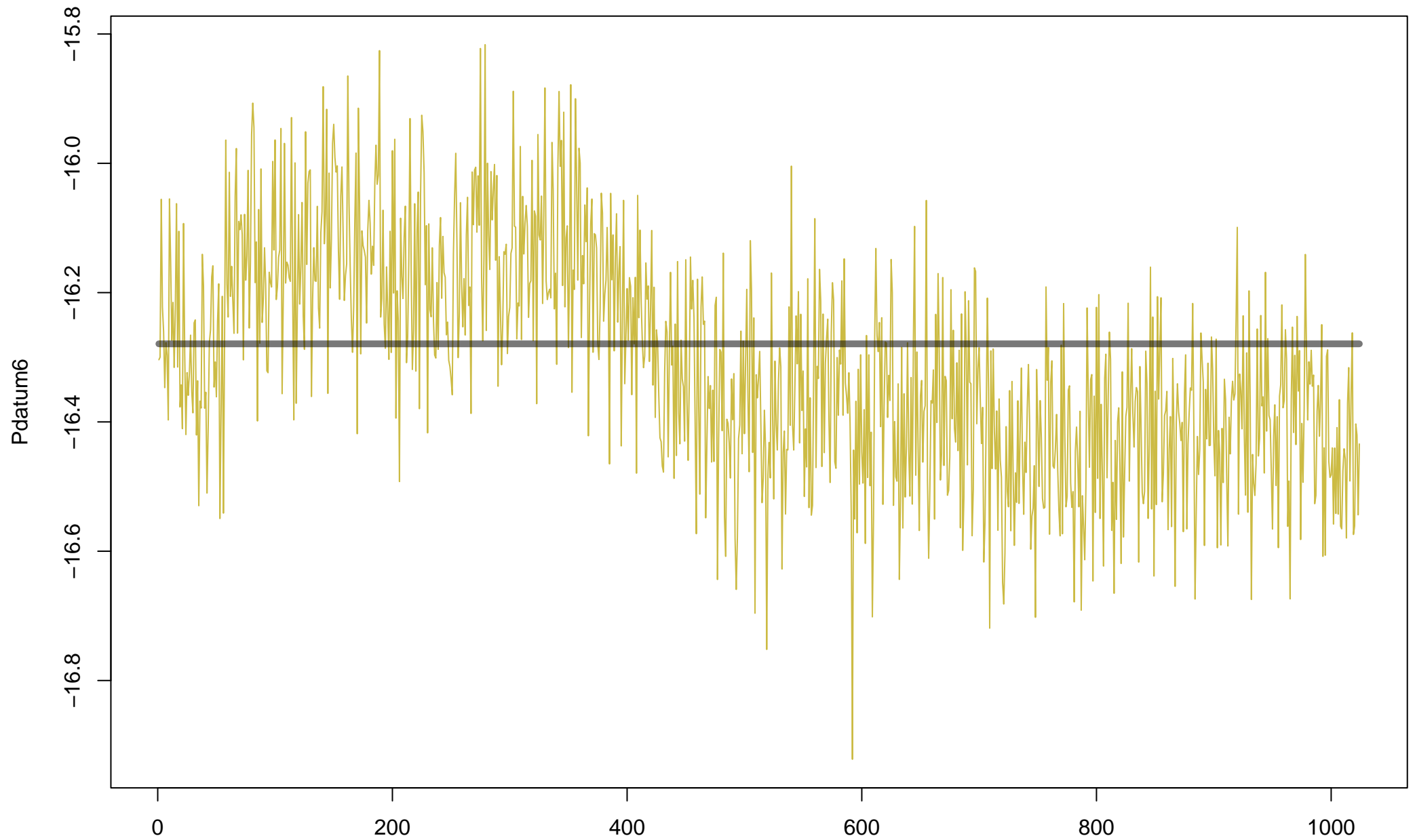
Pdatum5

ESS = 820 | BMK = 0.0501 | MCSE(6.27) = 4.43 | stat: TRUE | burn: 0 | rel.err: -0.396



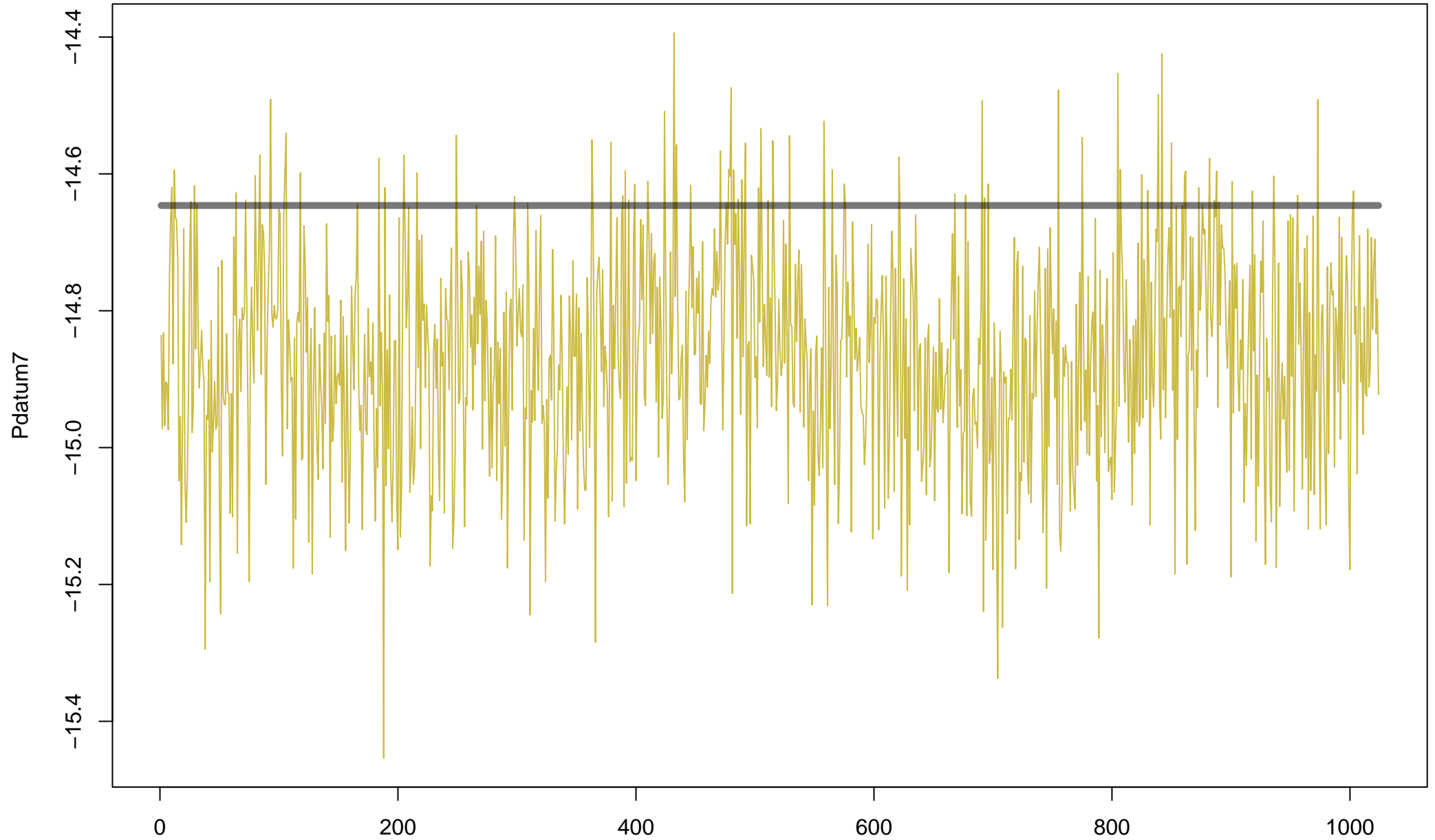
Pdatum6

ESS = 2.22e-16 | BMK = 0.488 | MCSE(6.27) = 12.9 | stat: FALSE | burn: 0 | rel.err: -0.0663



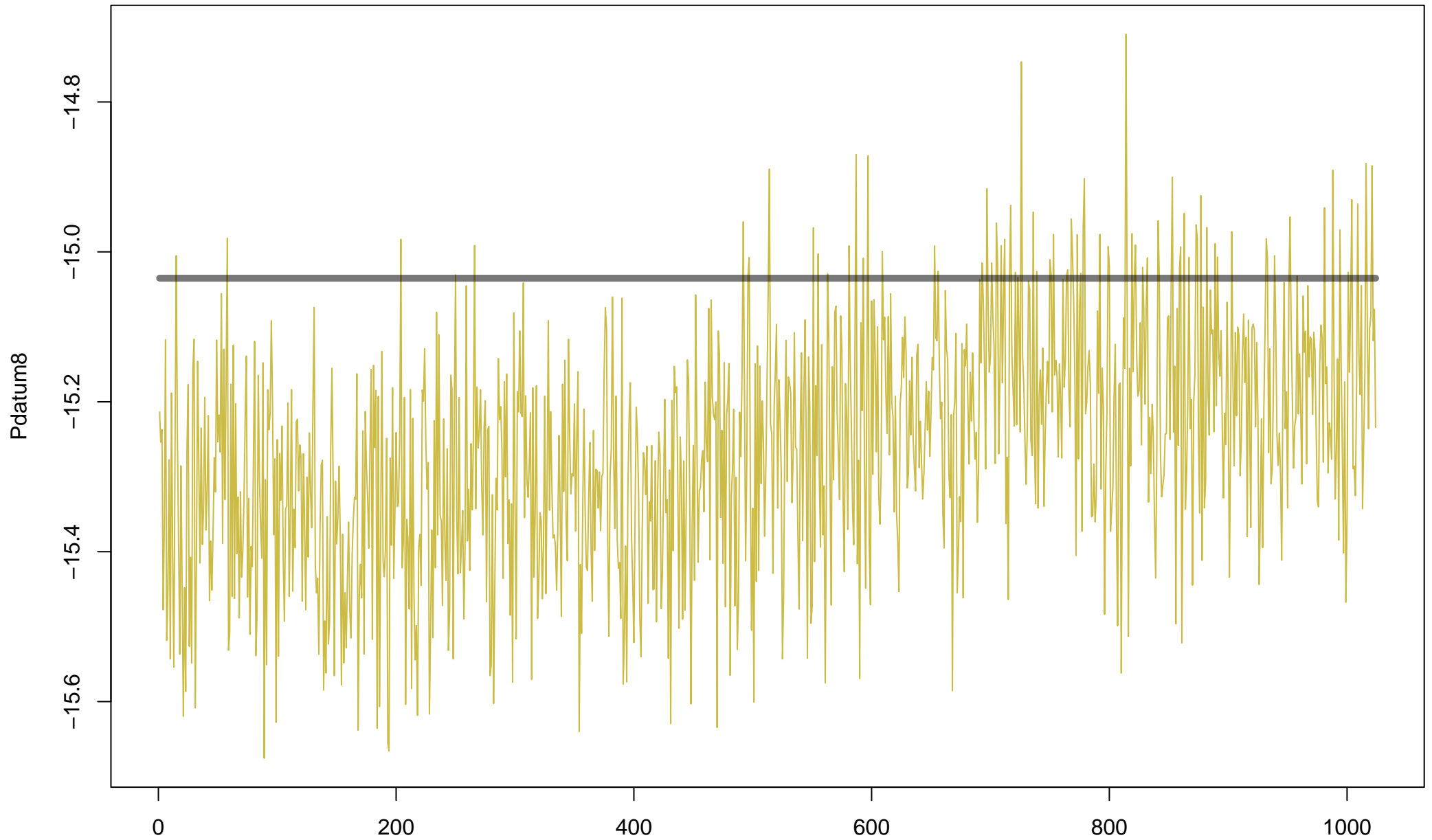
Pdatum7

ESS = 166 | BMK = 0.0444 | MCSE(6.27) = 5.47 | stat: TRUE | burn: 0 | rel.err: -1.5



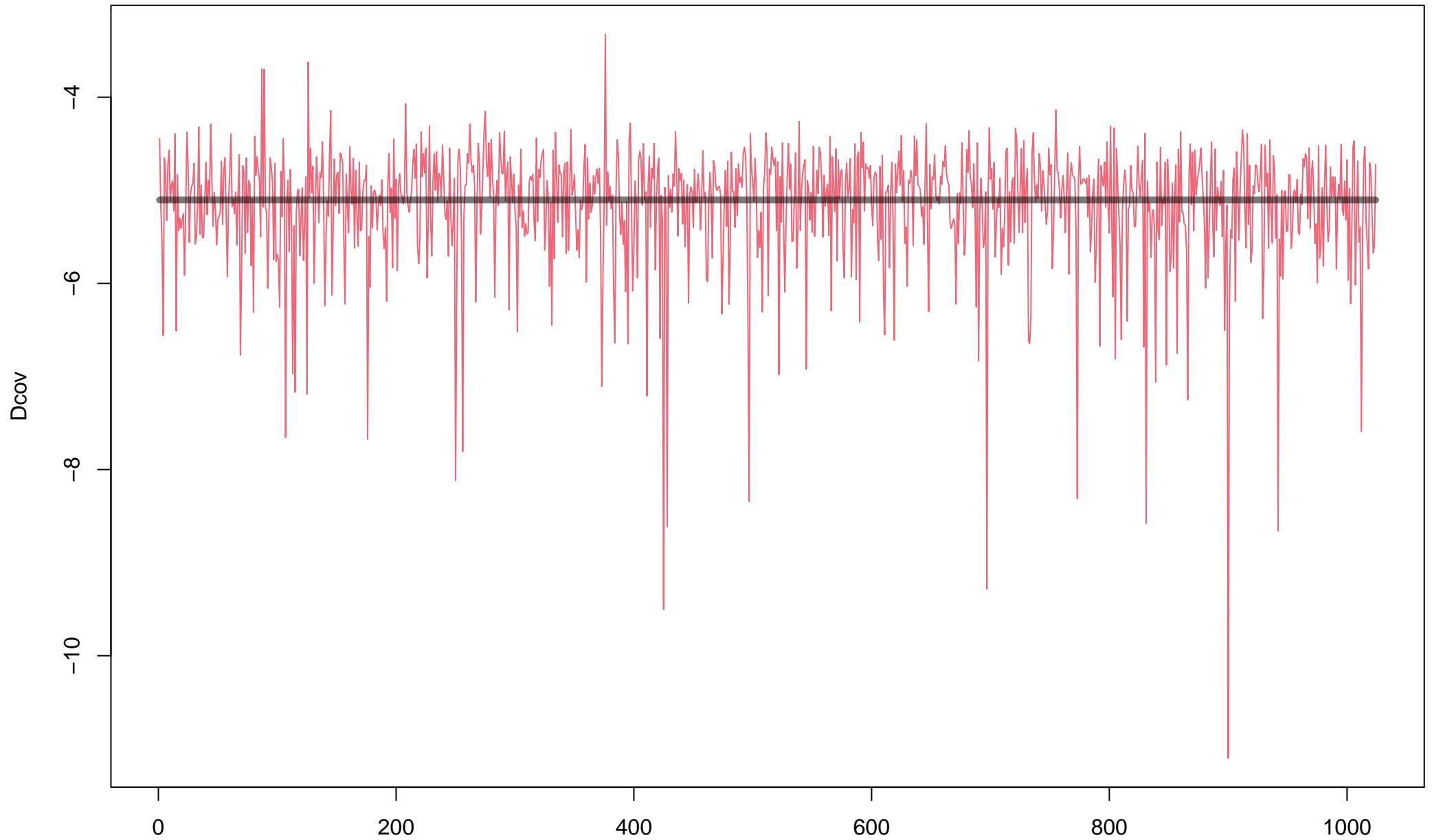
Pdatum8

ESS = 36.3 | BMK = 0.328 | MCSE(6.27) = 8.69 | stat: FALSE | burn: 0 | rel.err: -1.53

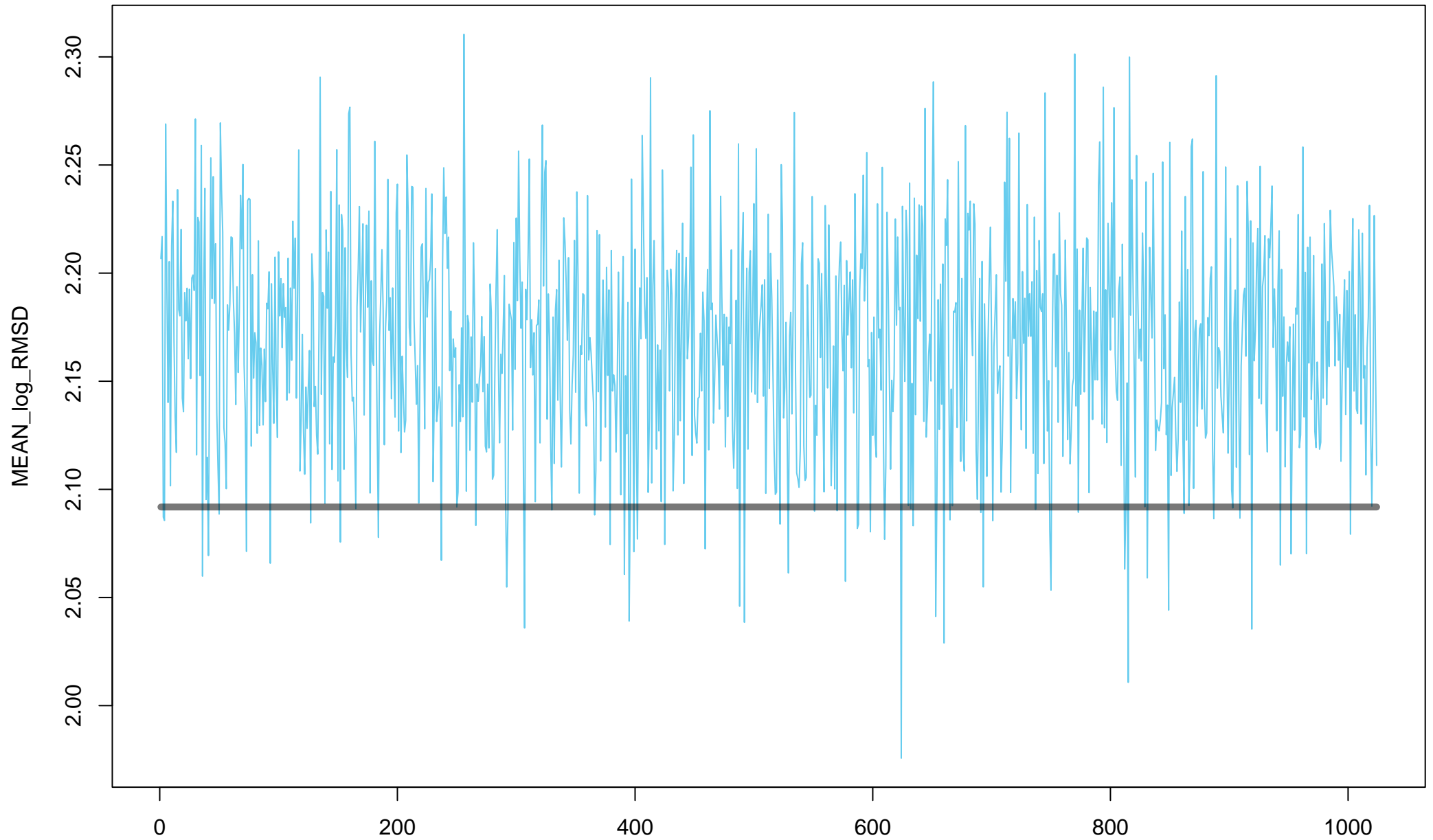


Dcov

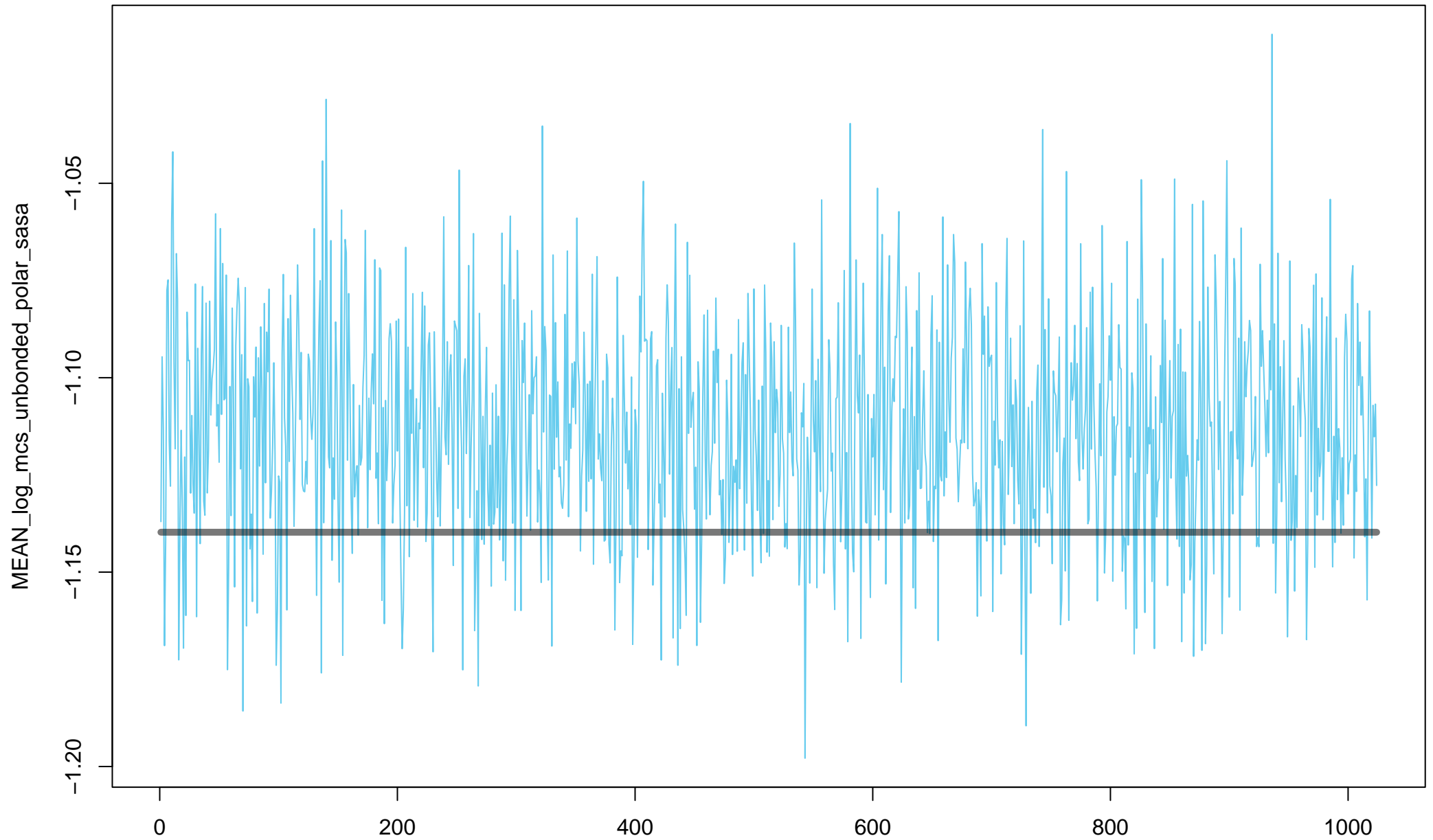
ESS = 1020 | BMK = 0.0841 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | rel.err: -0.132



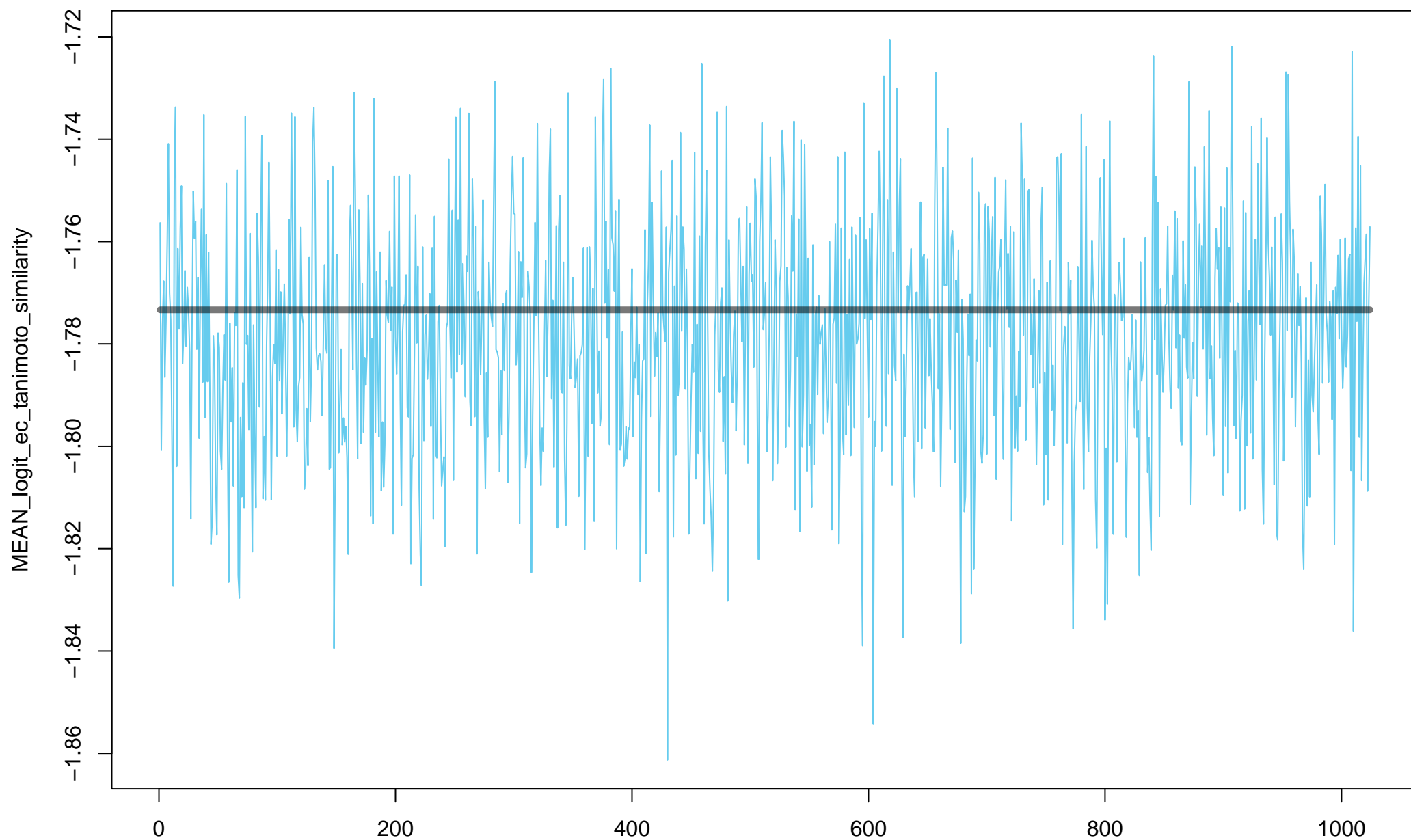
MEAN_log_RMSD
ESS = 1020 | BMK = 0.0443 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0 | rel.err: 1.54



MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0462 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | rel.err: 0.938

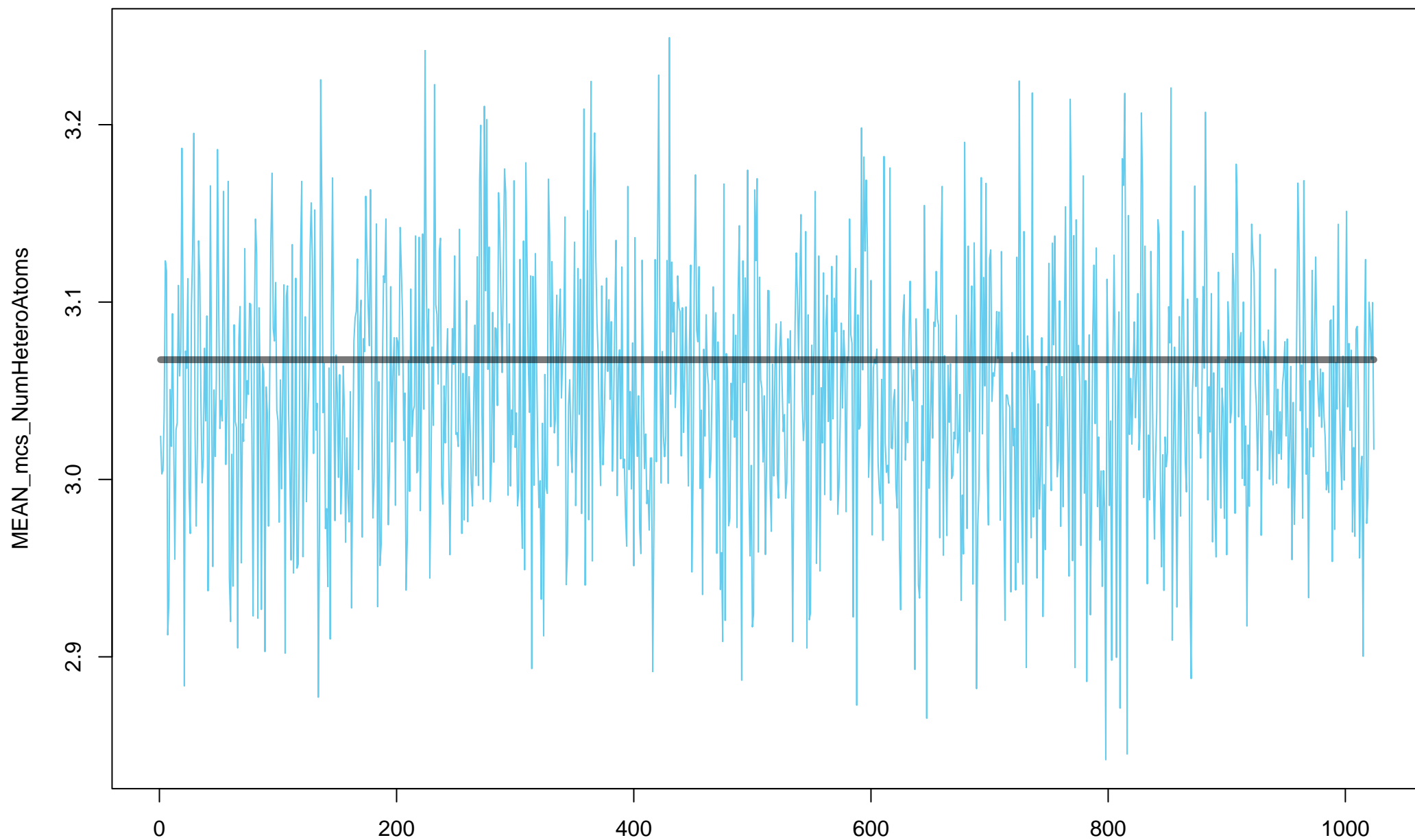


MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0507 | MCSE(6.27) = 3.35 | stat: TRUE | burn: 0 | rel.err: -0.244



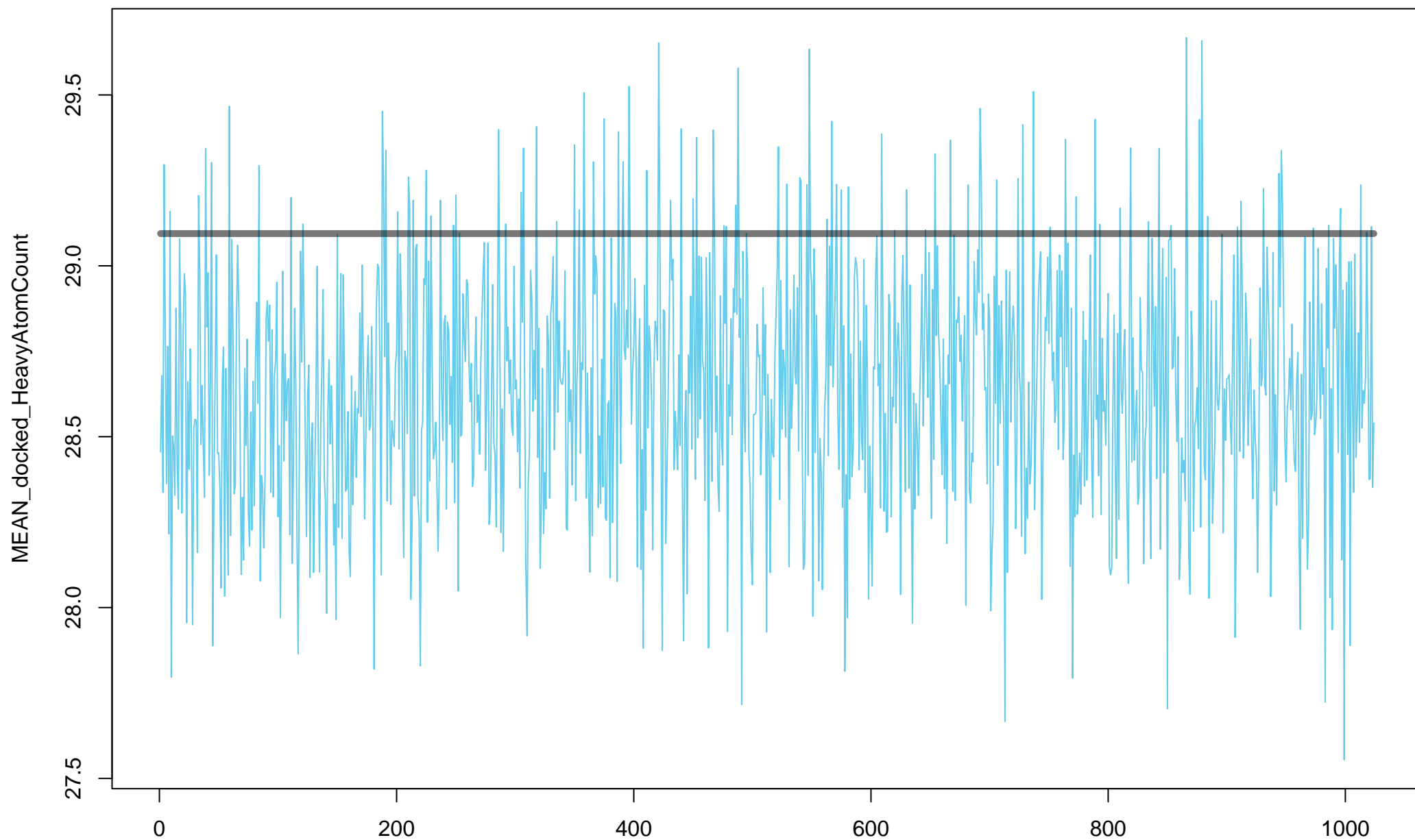
MEAN_mcs_NumHeteroAtoms

ESS = 1020 | BMK = 0.0554 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0 | rel.err: -0.295

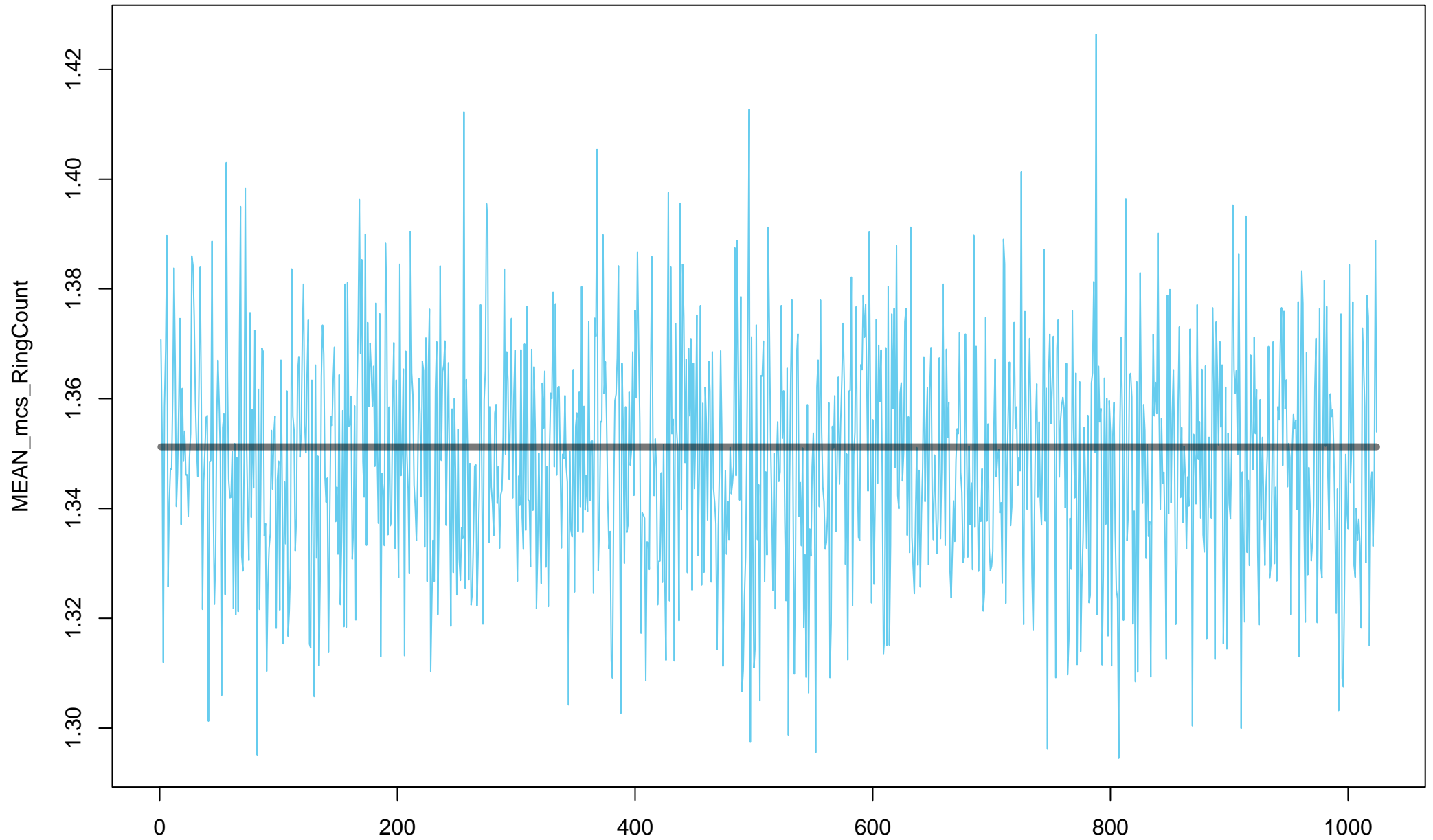


MEAN_docked_HeavyAtomCount

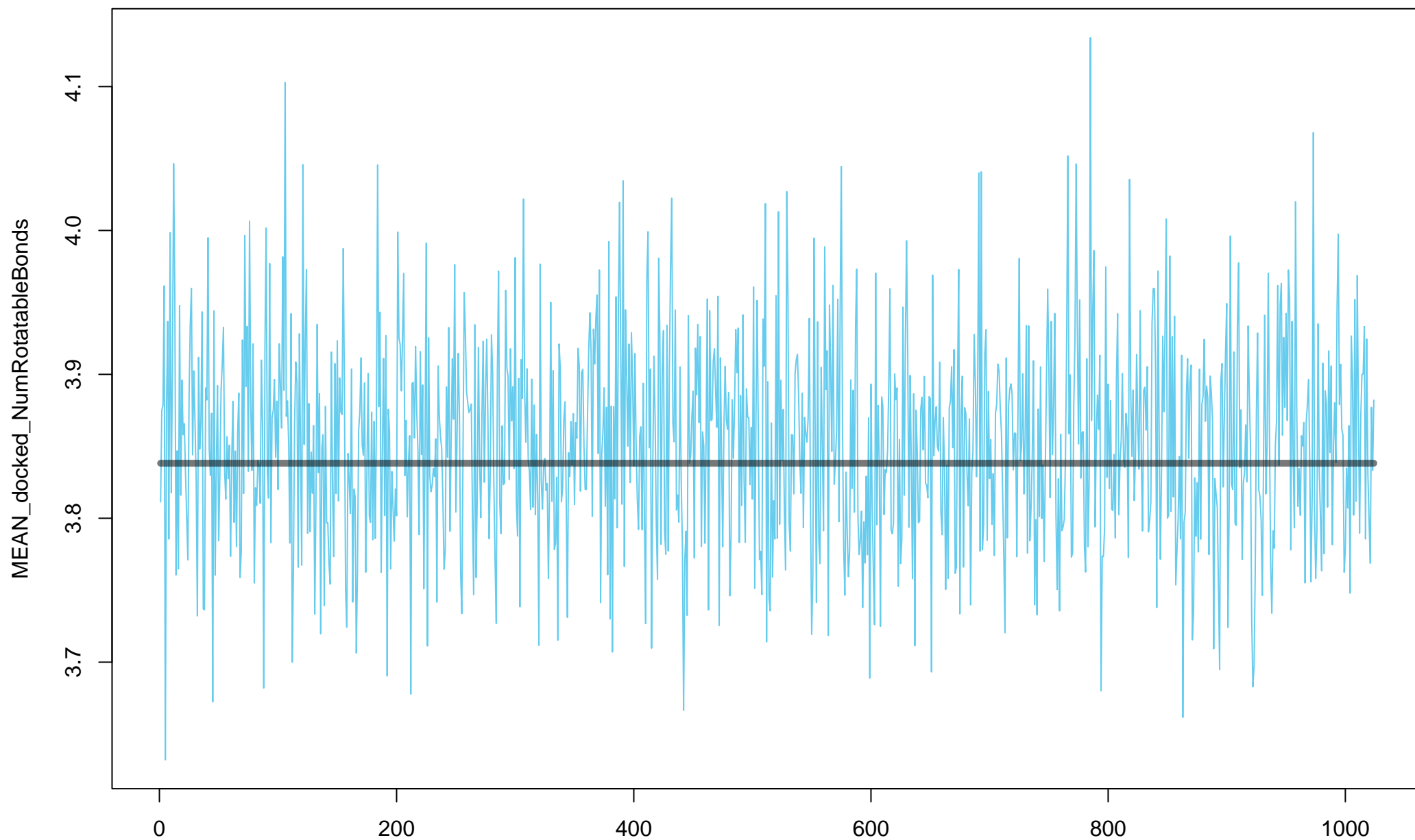
ESS = 1020 | BMK = 0.0403 | MCSE(6.27) = 3.04 | stat: FALSE | burn: 0 | rel.err: -1.3



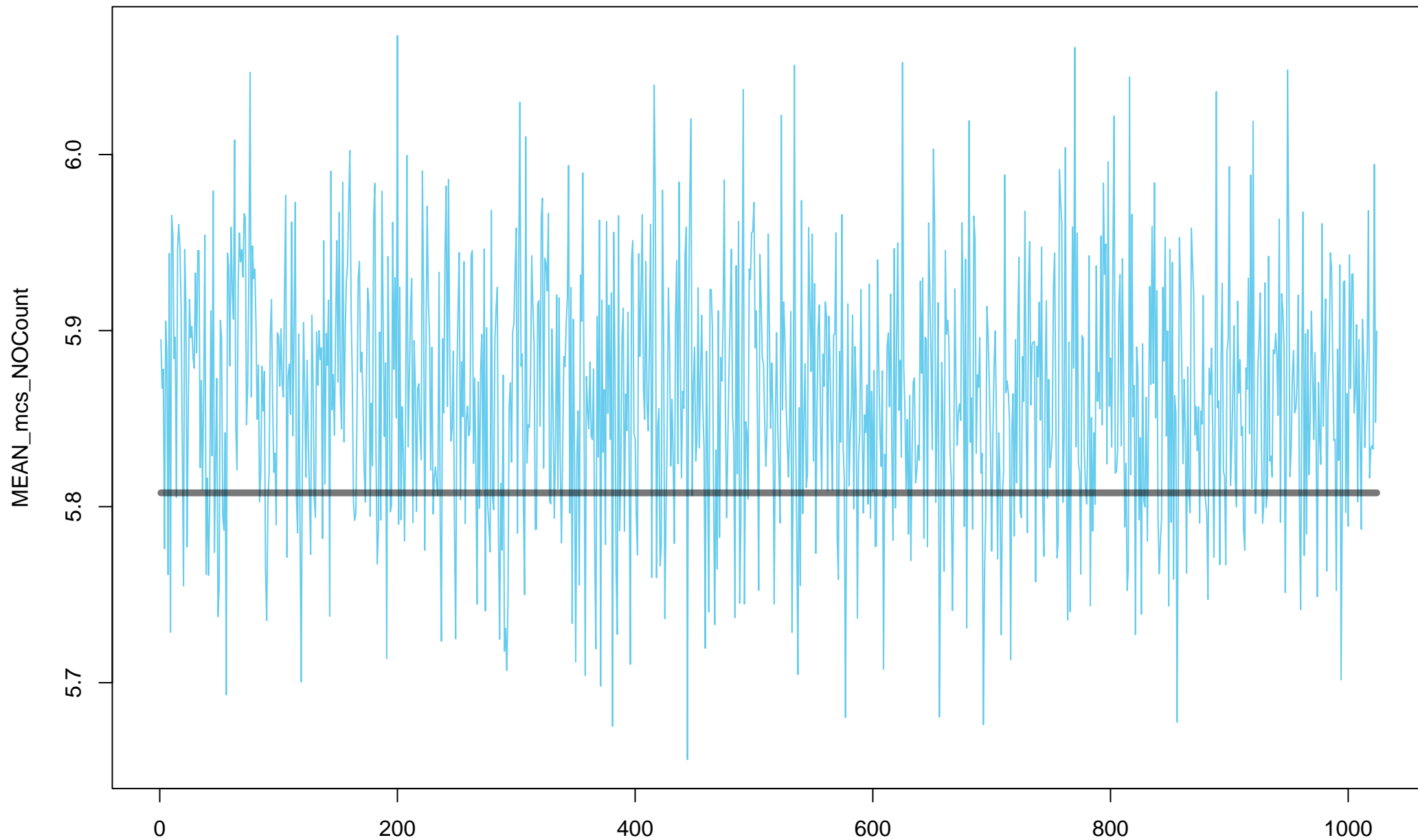
MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0524 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0 | rel.err: -0.124



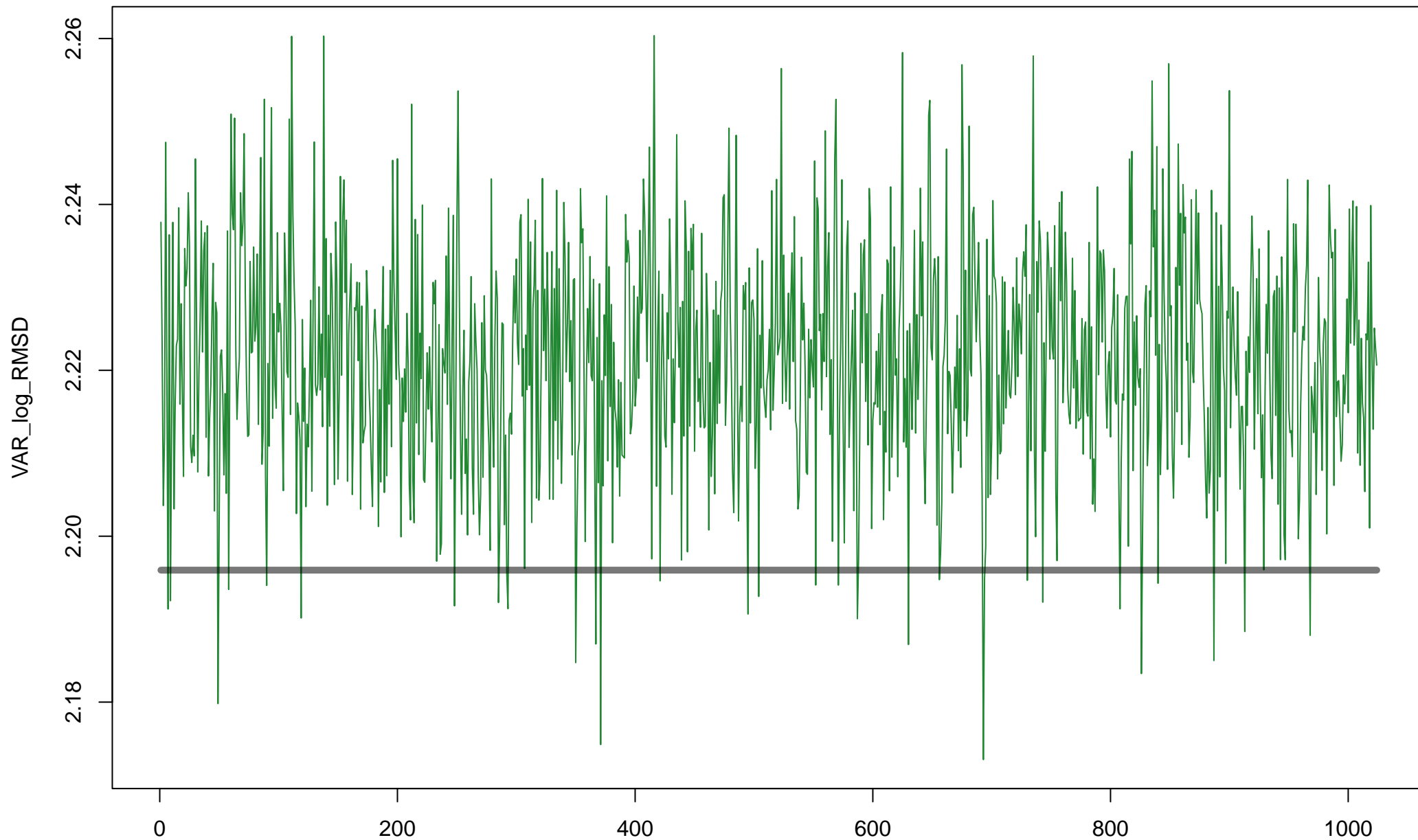
MEAN_docked_NumRotatableBonds
ESS = 993 | BMK = 0.0504 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0 | rel.err: 0.208



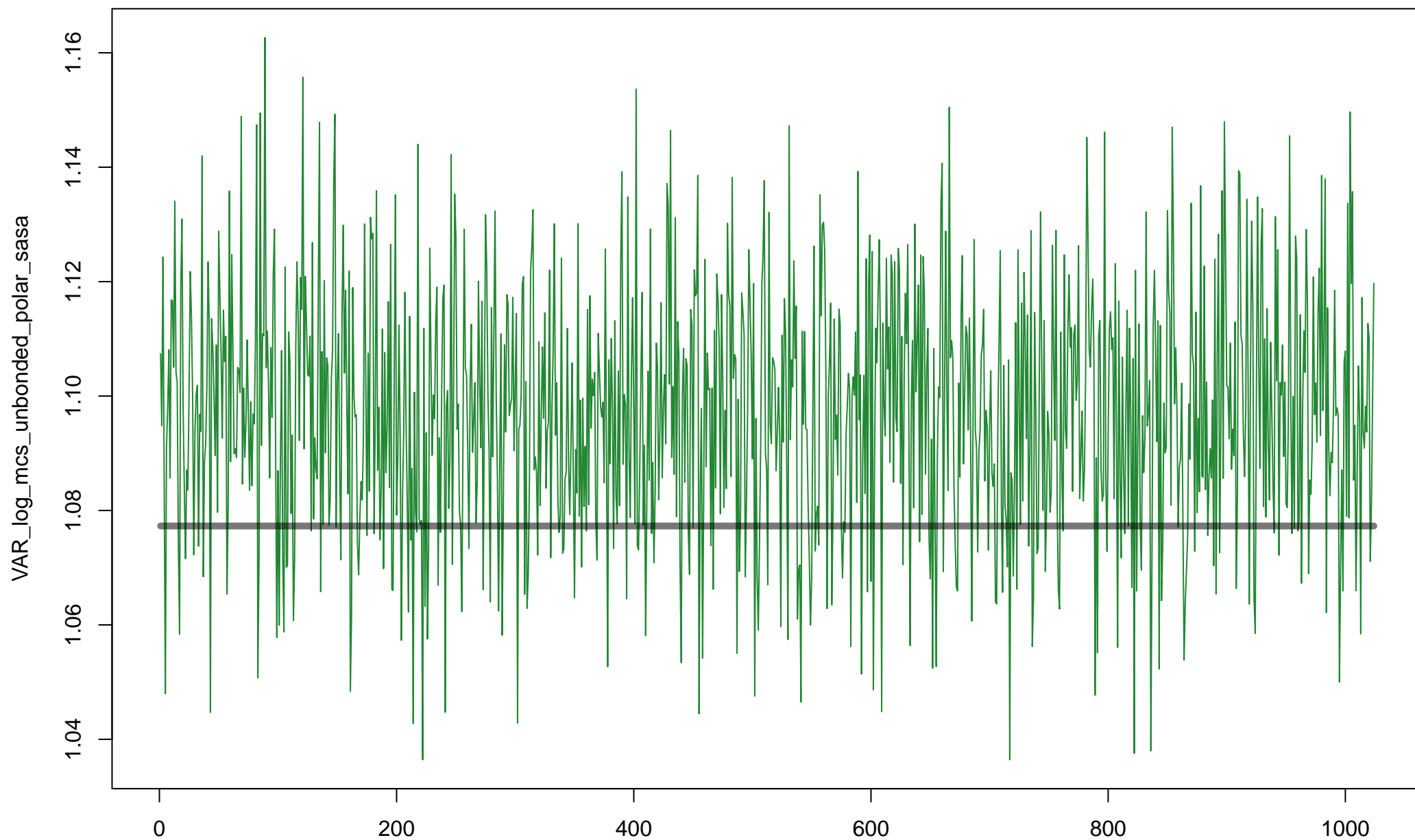
MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0877 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0 | rel.err: 0.791



VAR_log_RMSD
ESS = 898 | BMK = 0.0398 | MCSE(6.27) = 3.21 | stat: TRUE | burn: 0 | rel.err: 1.89

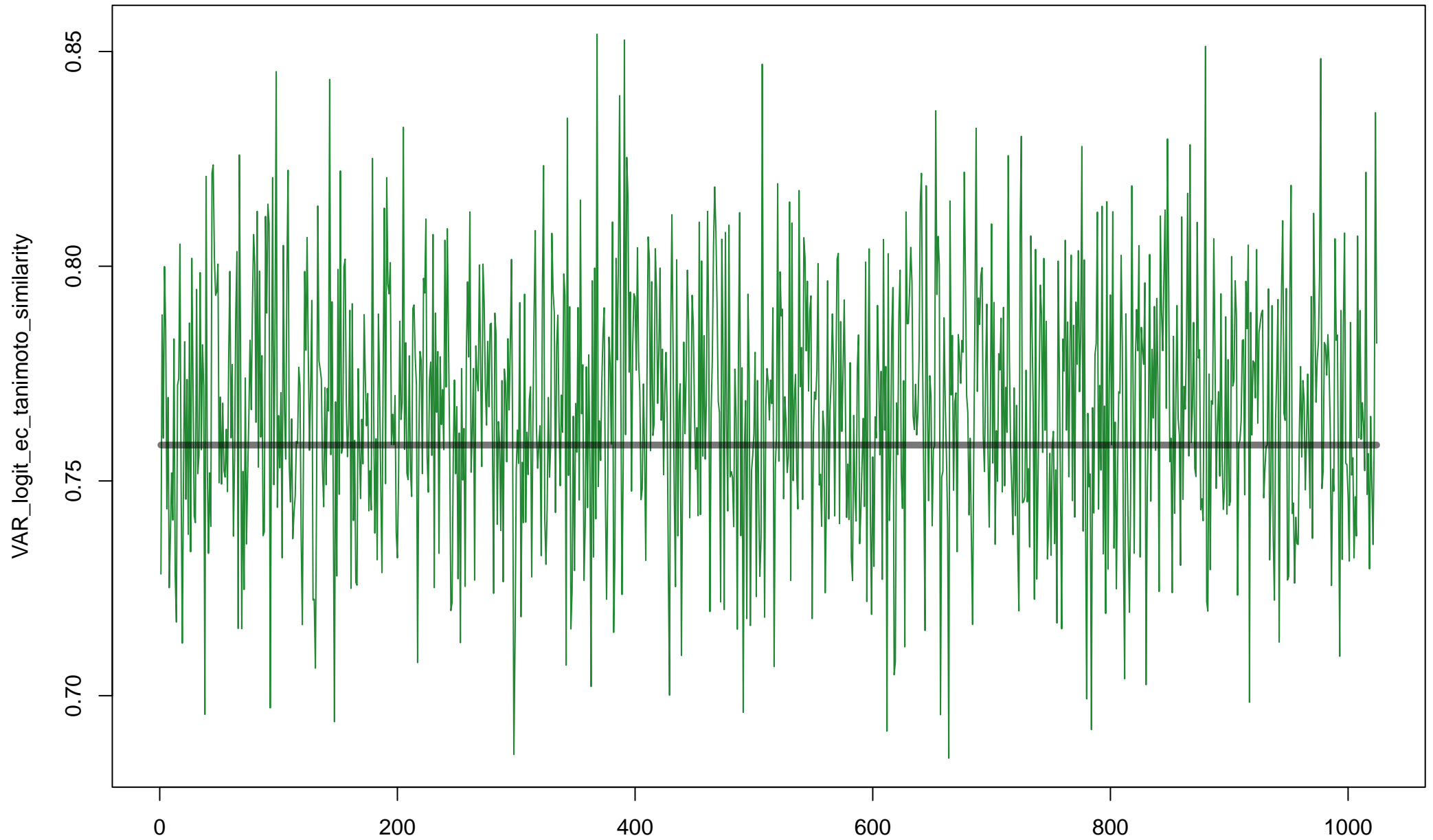


VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0331 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0 | rel.err: 0.911

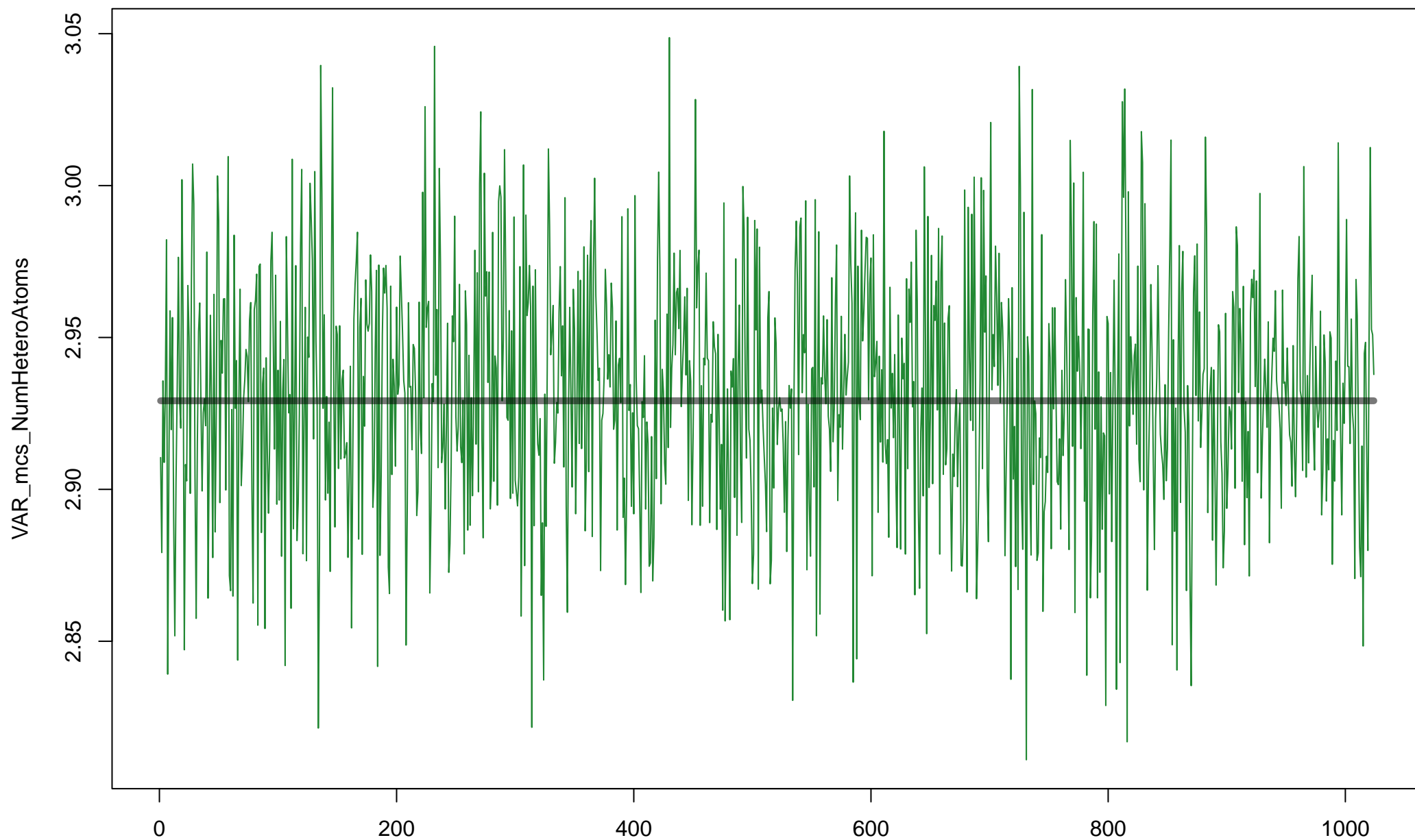


VAR_logit_ec_tanimoto_similarity

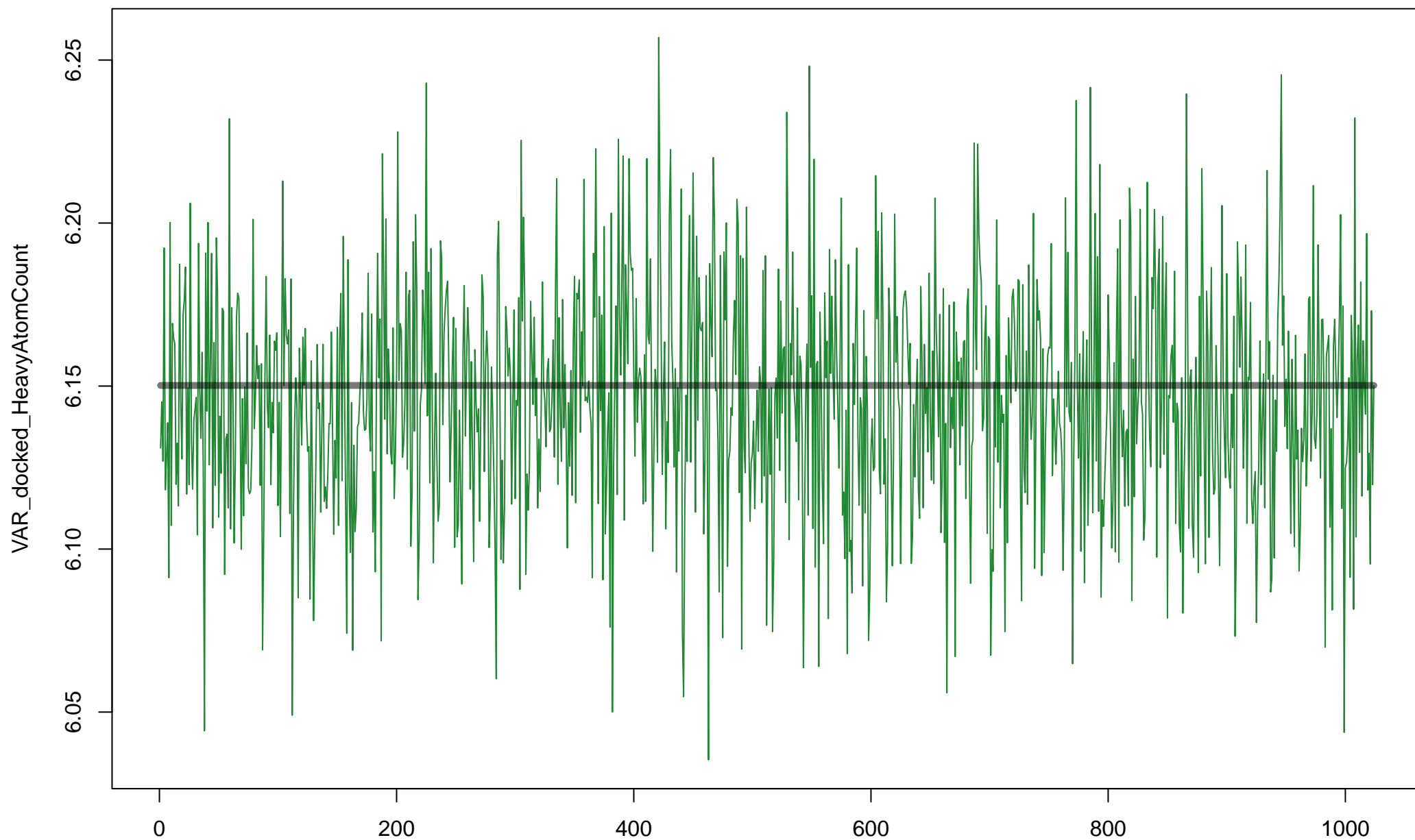
ESS = 1020 | BMK = 0.0375 | MCSE(6.27) = 3.39 | stat: TRUE | burn: 0 | rel.err: 0.316



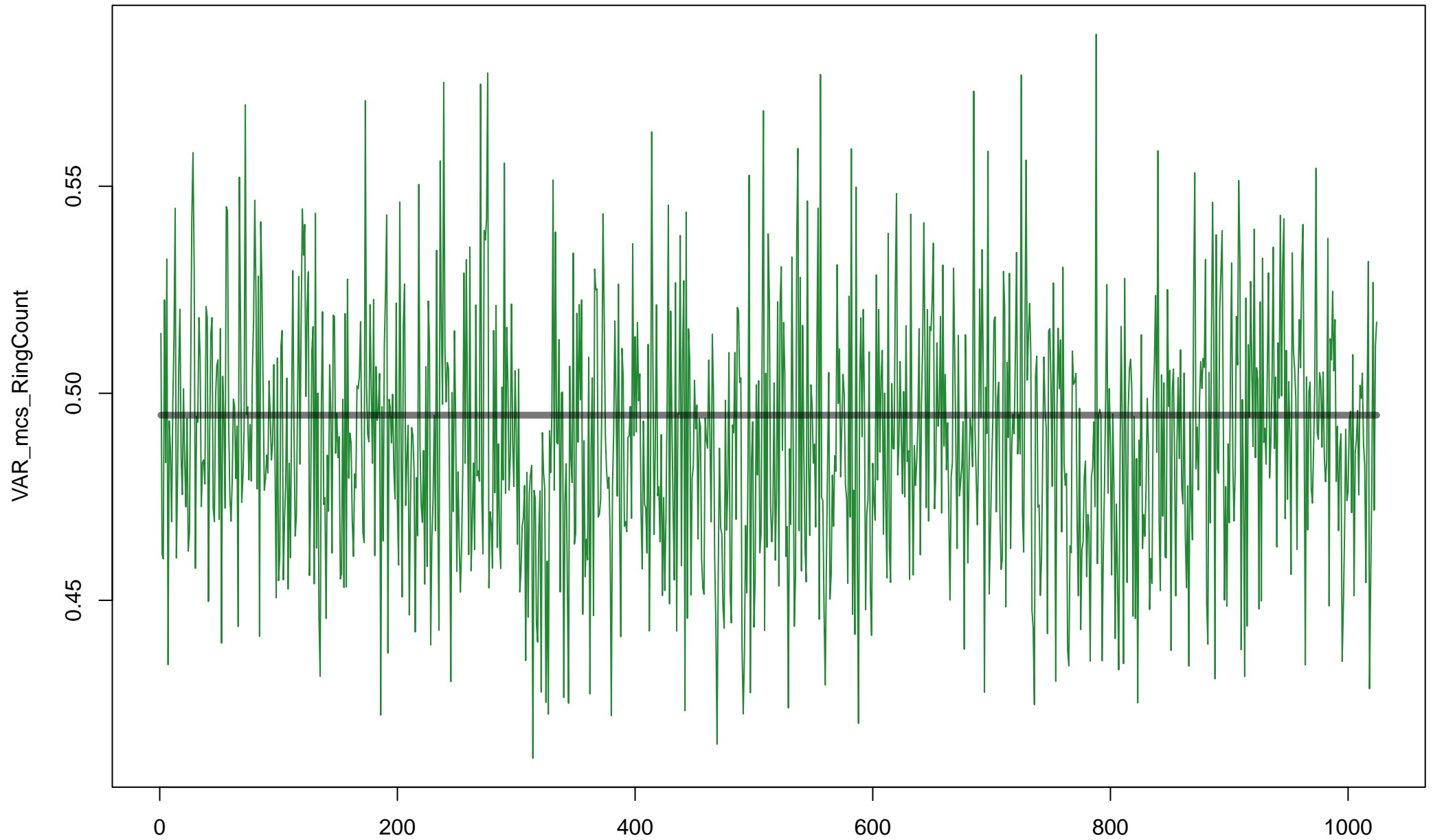
VAR_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0543 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0 | rel.err: 0.0874



VAR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0553 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0 | rel.err: -0.116

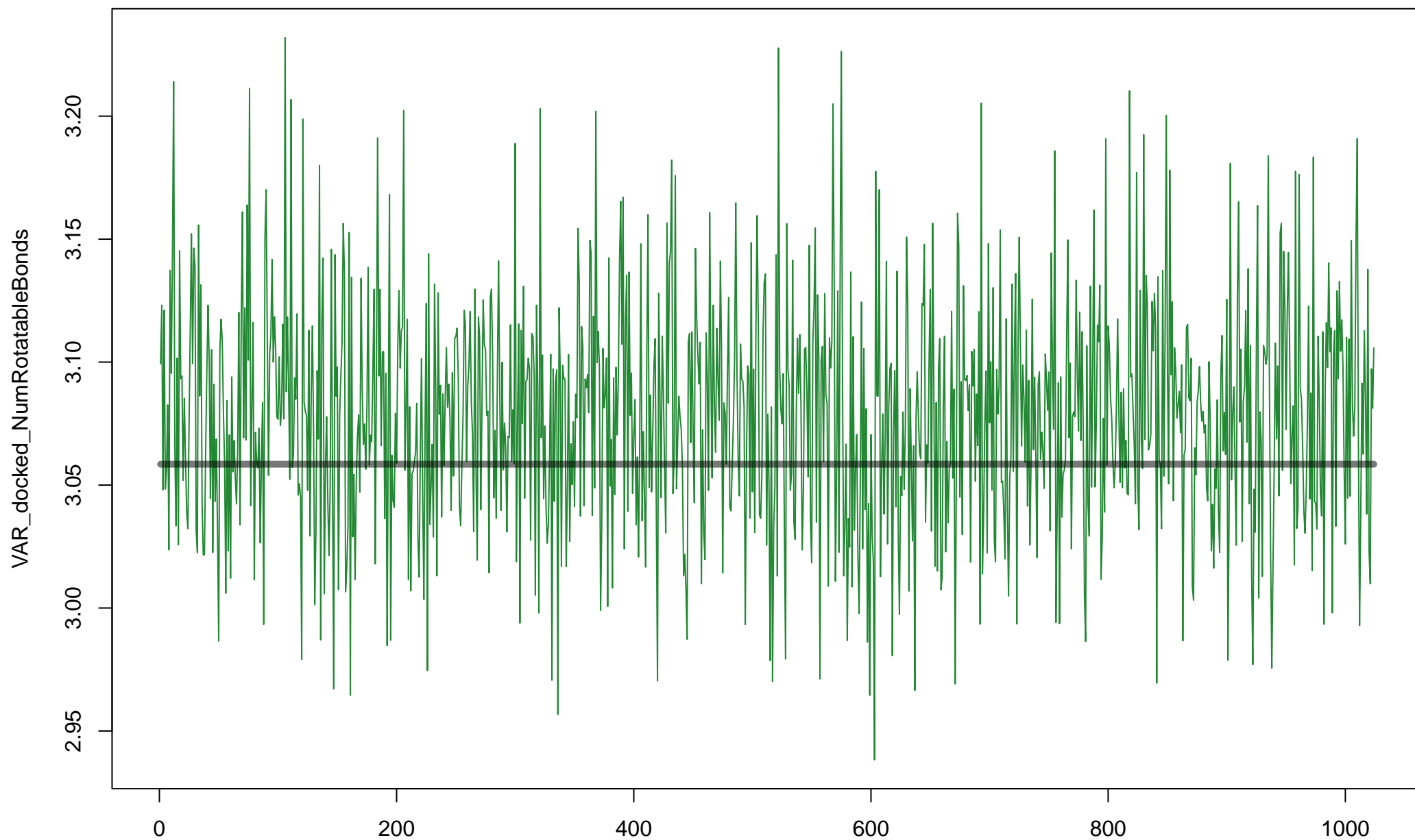


VAR_mcs_RingCount
ESS = 1020 | BMK = 0.0482 | MCSE(6.27) = 3.81 | stat: TRUE | burn: 0 | rel.err: -0.193

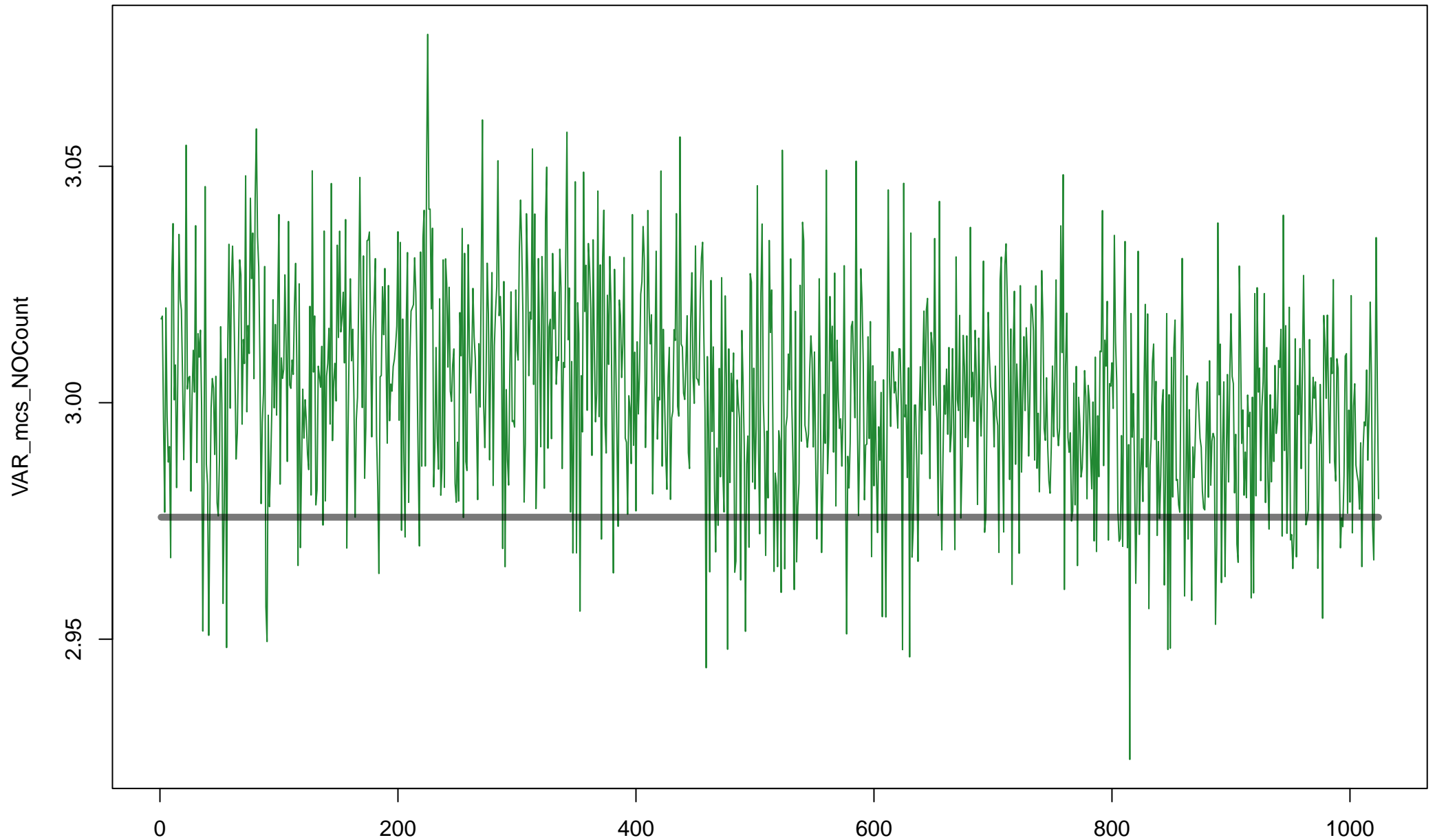


VAR_docked_NumRotatableBonds

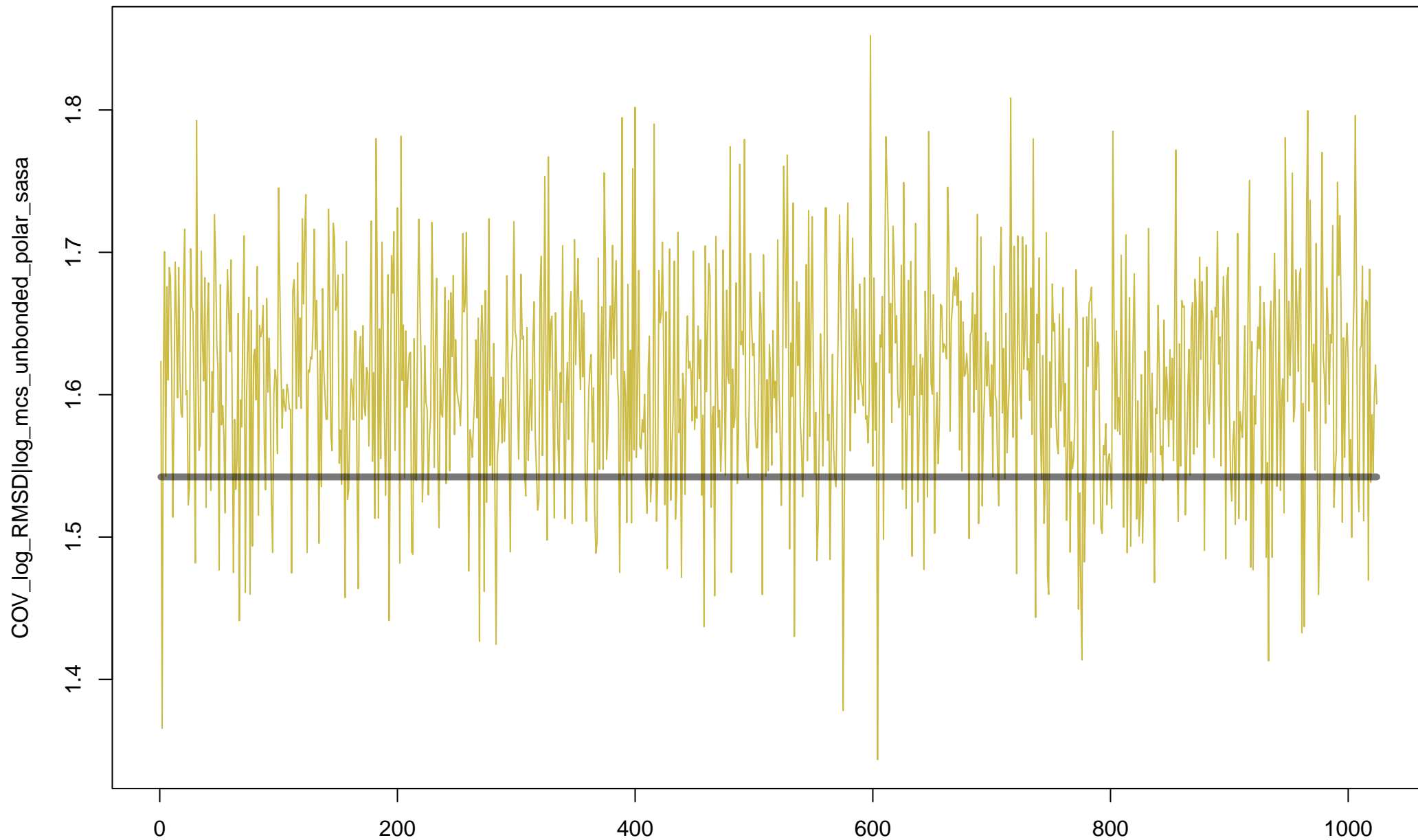
ESS = 1020 | BMK = 0.0363 | MCSE(6.27) = 3.45 | stat: TRUE | burn: 0 | rel.err: 0.441



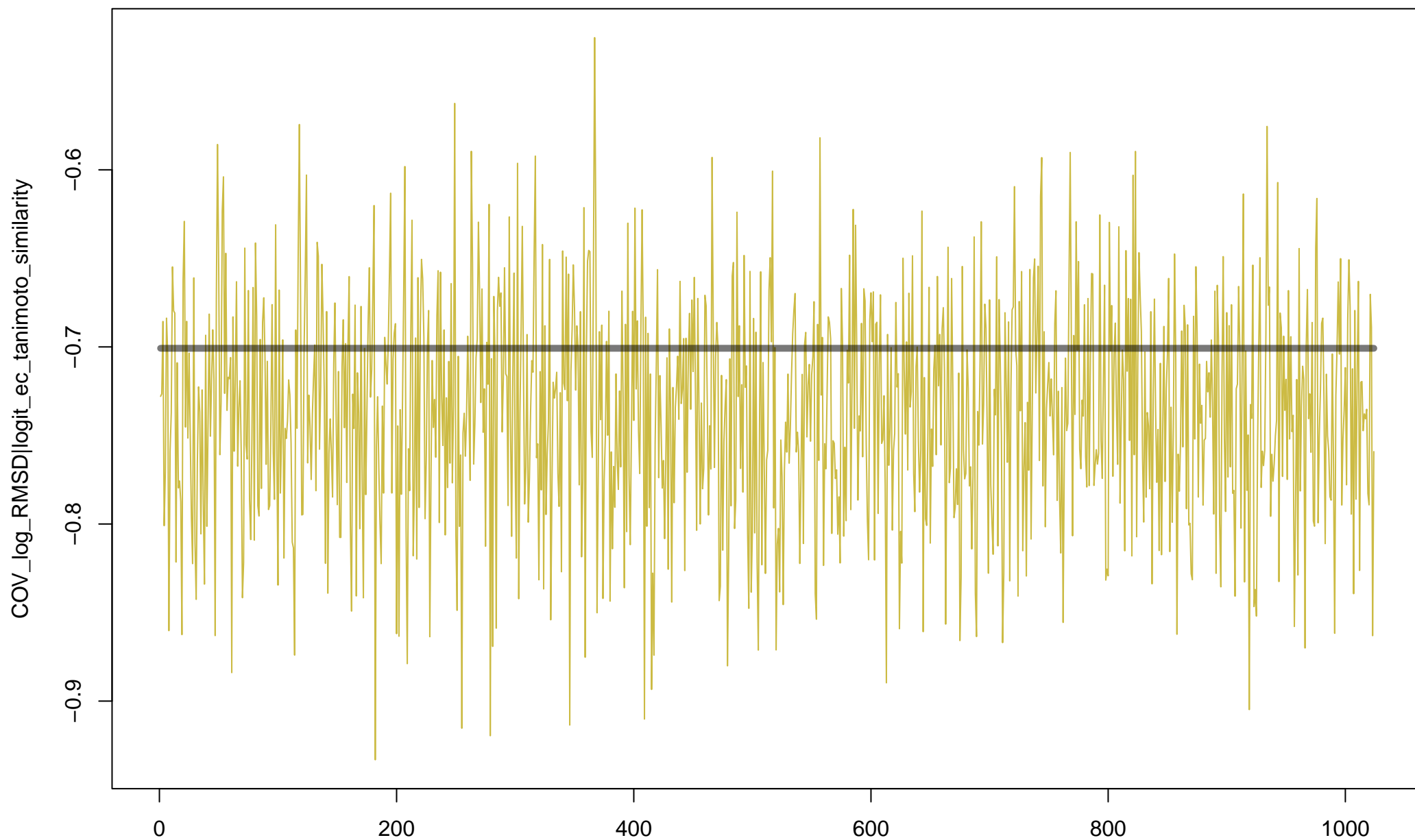
VAR_mcs_NOCount
ESS = 89 | BMK = 0.185 | MCSE(6.27) = 5.85 | stat: FALSE | burn: 0 | rel.err: 1.21



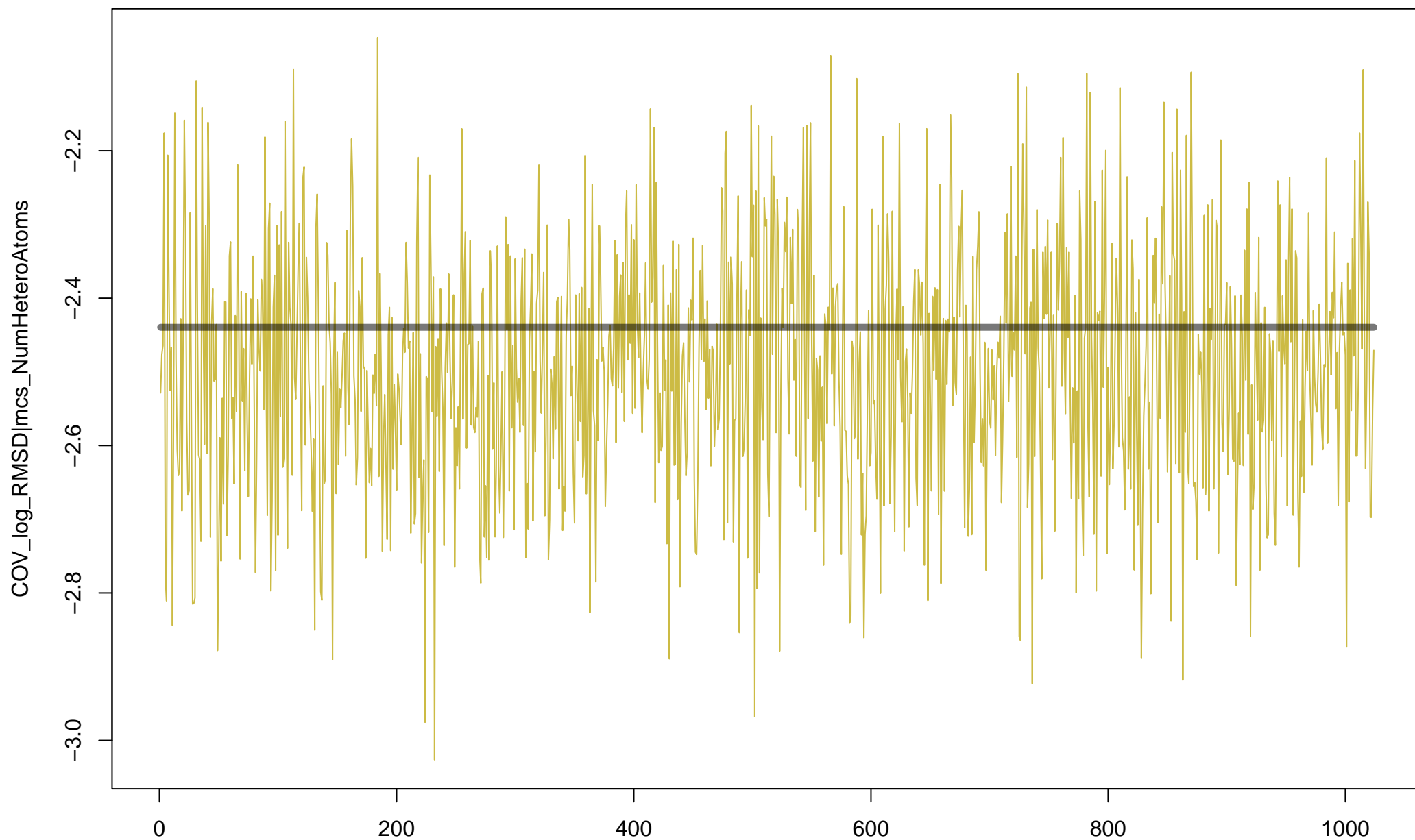
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.04 | MCSE(6.27) = 3.53 | stat: TRUE | burn: 0 | rel.err: 0.936



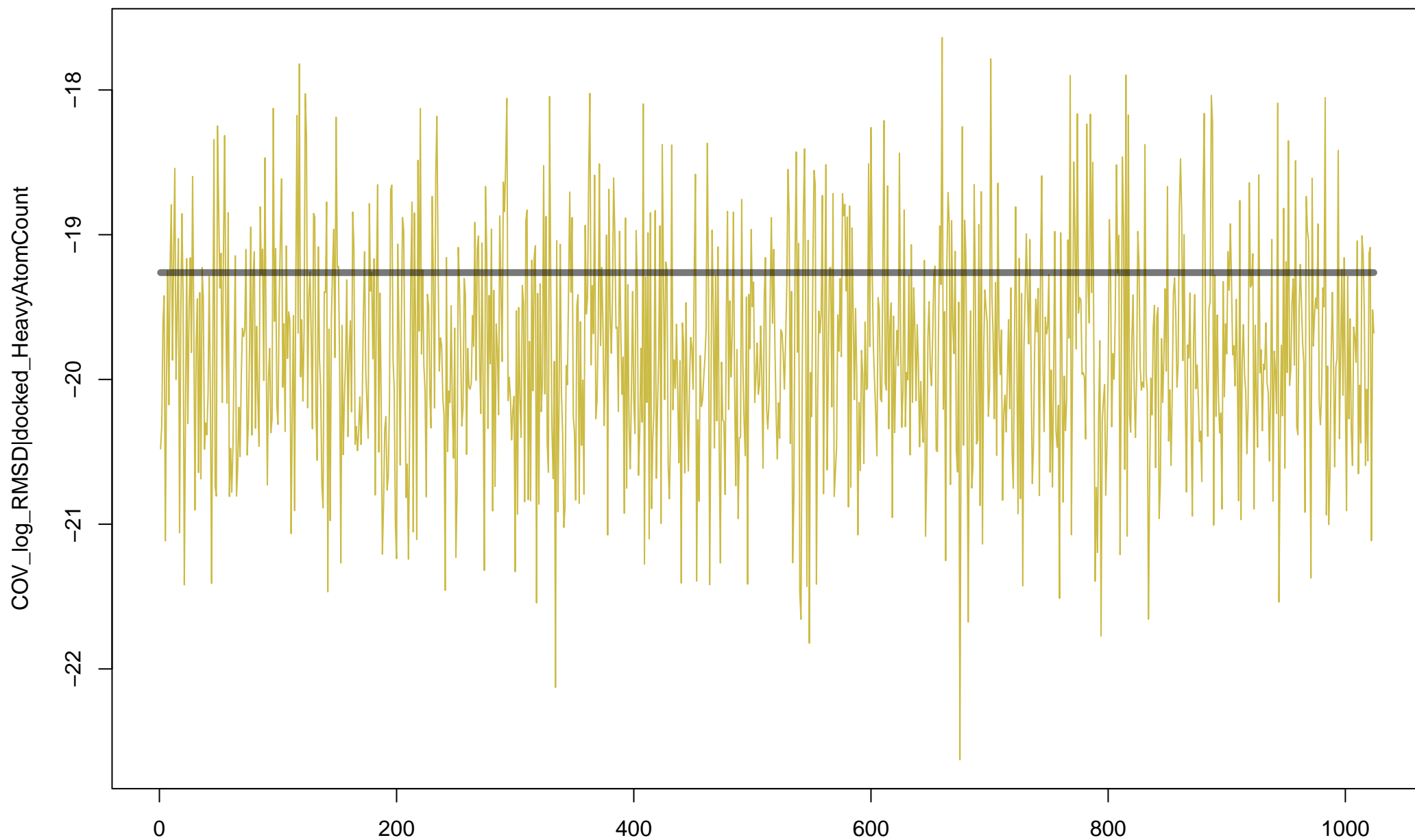
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0585 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0 | rel.err: -0.573



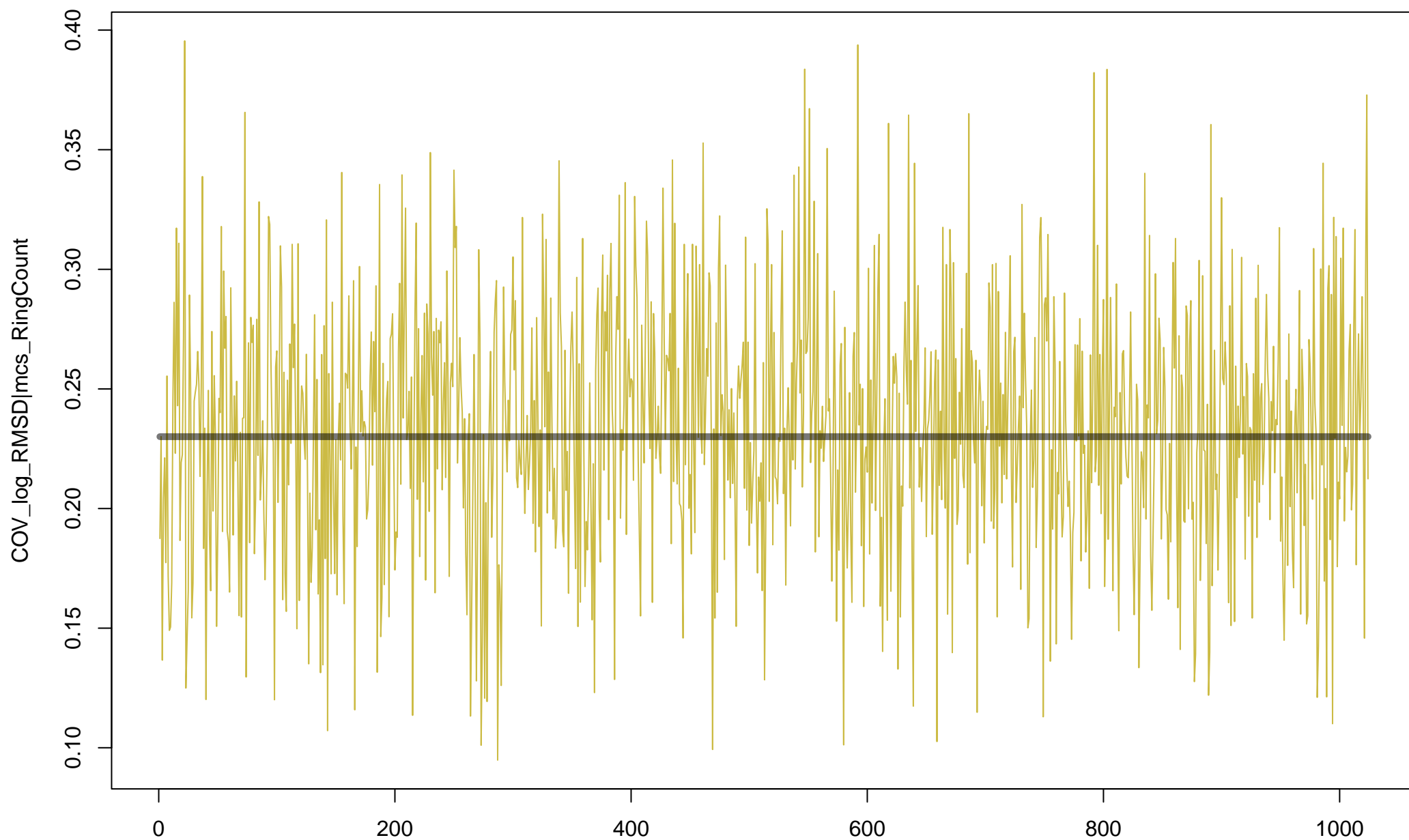
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0539 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0 | rel.err: -0.352



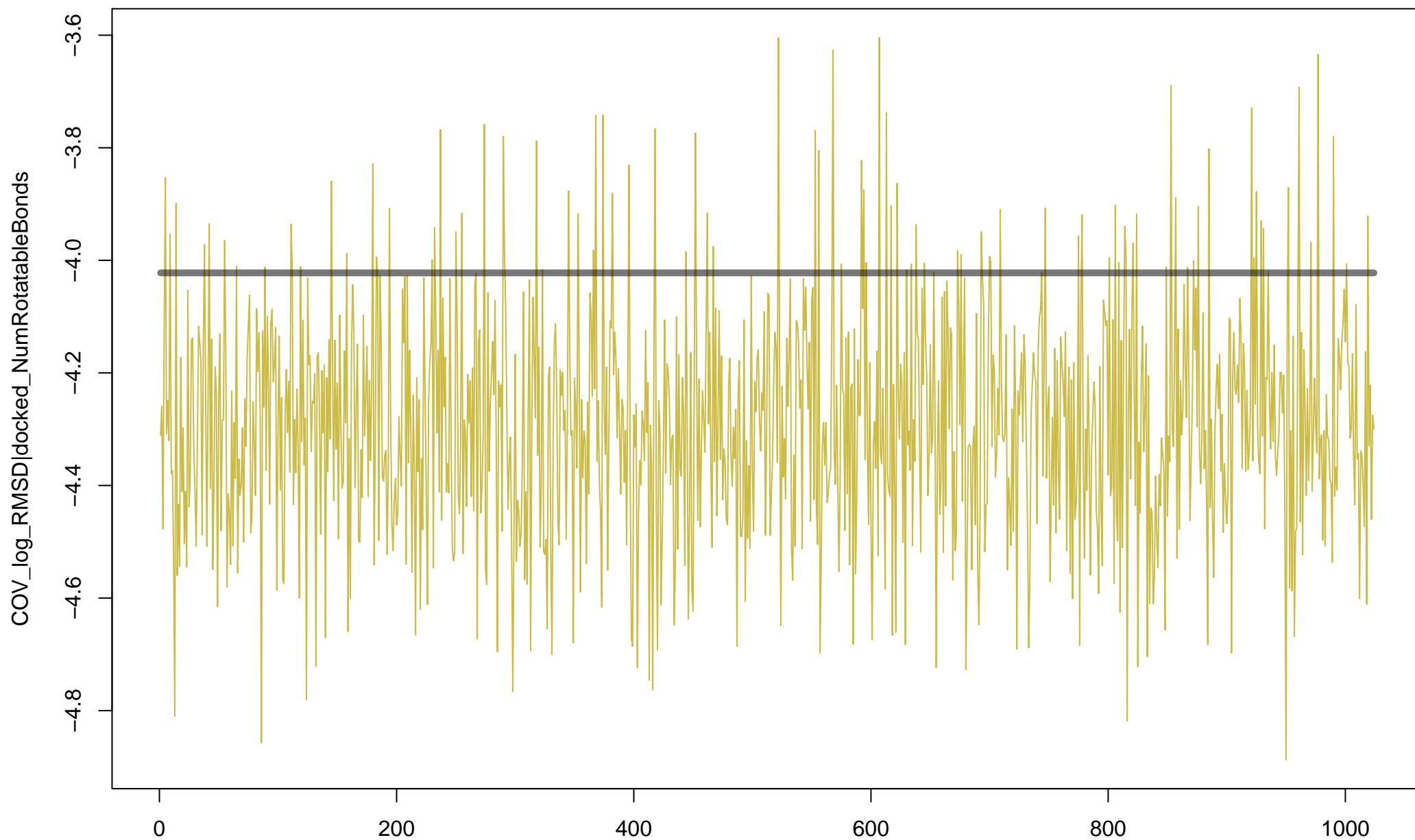
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0545 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | rel.err: -0.728



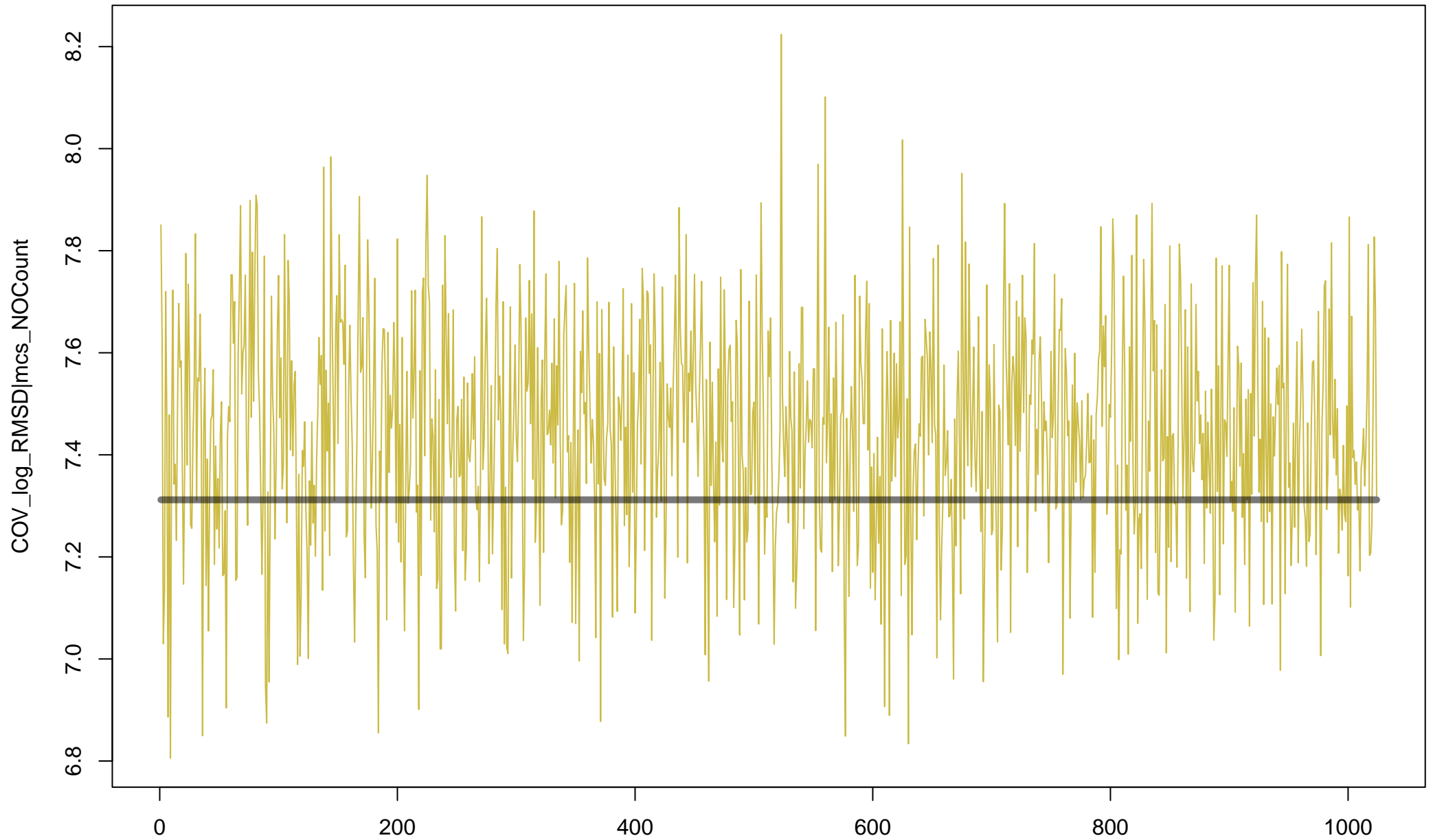
COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.057 | MCSE(6.27) = 3.64 | stat: TRUE | burn: 0 | rel.err: 0.0582



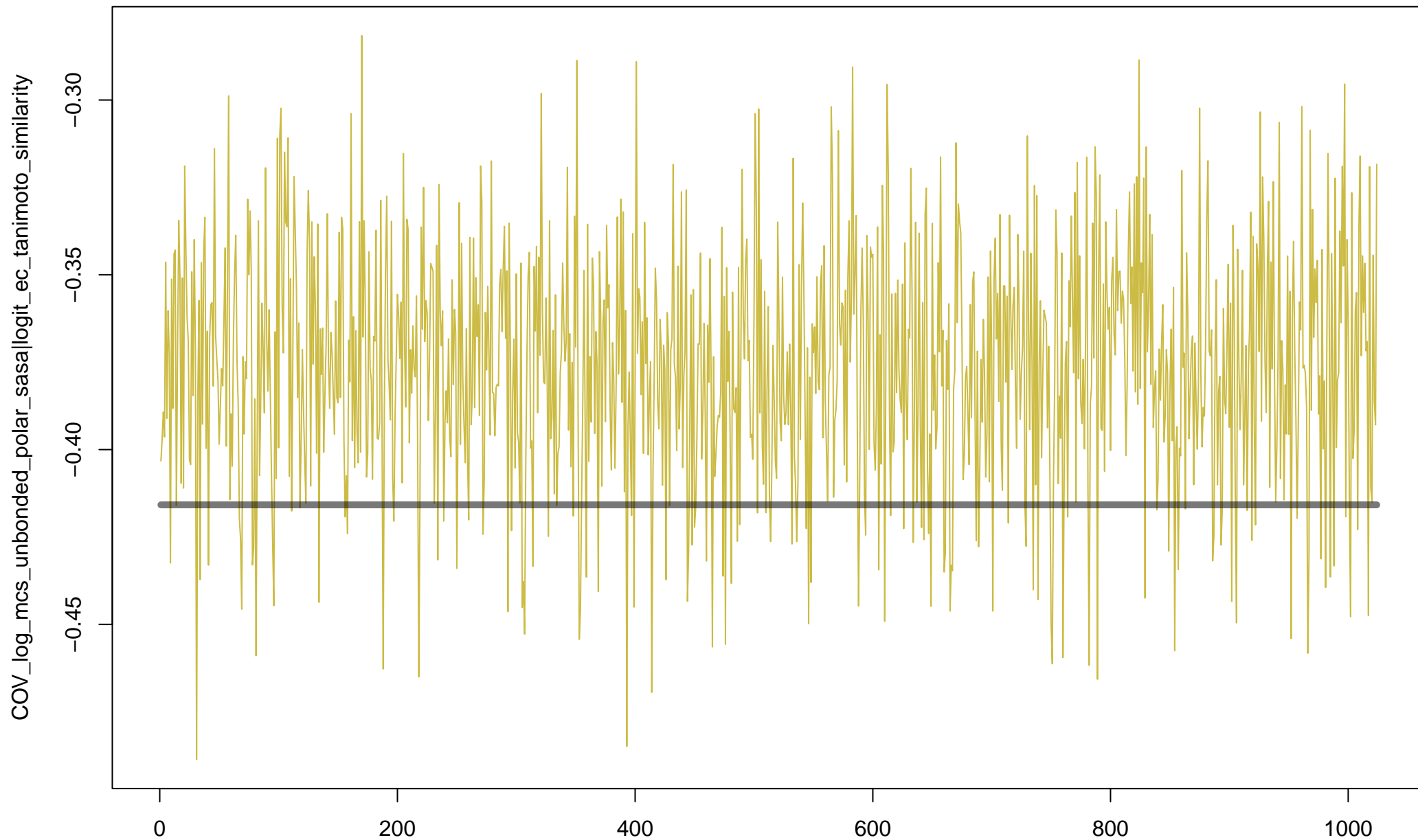
COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0542 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0 | rel.err: -1.33



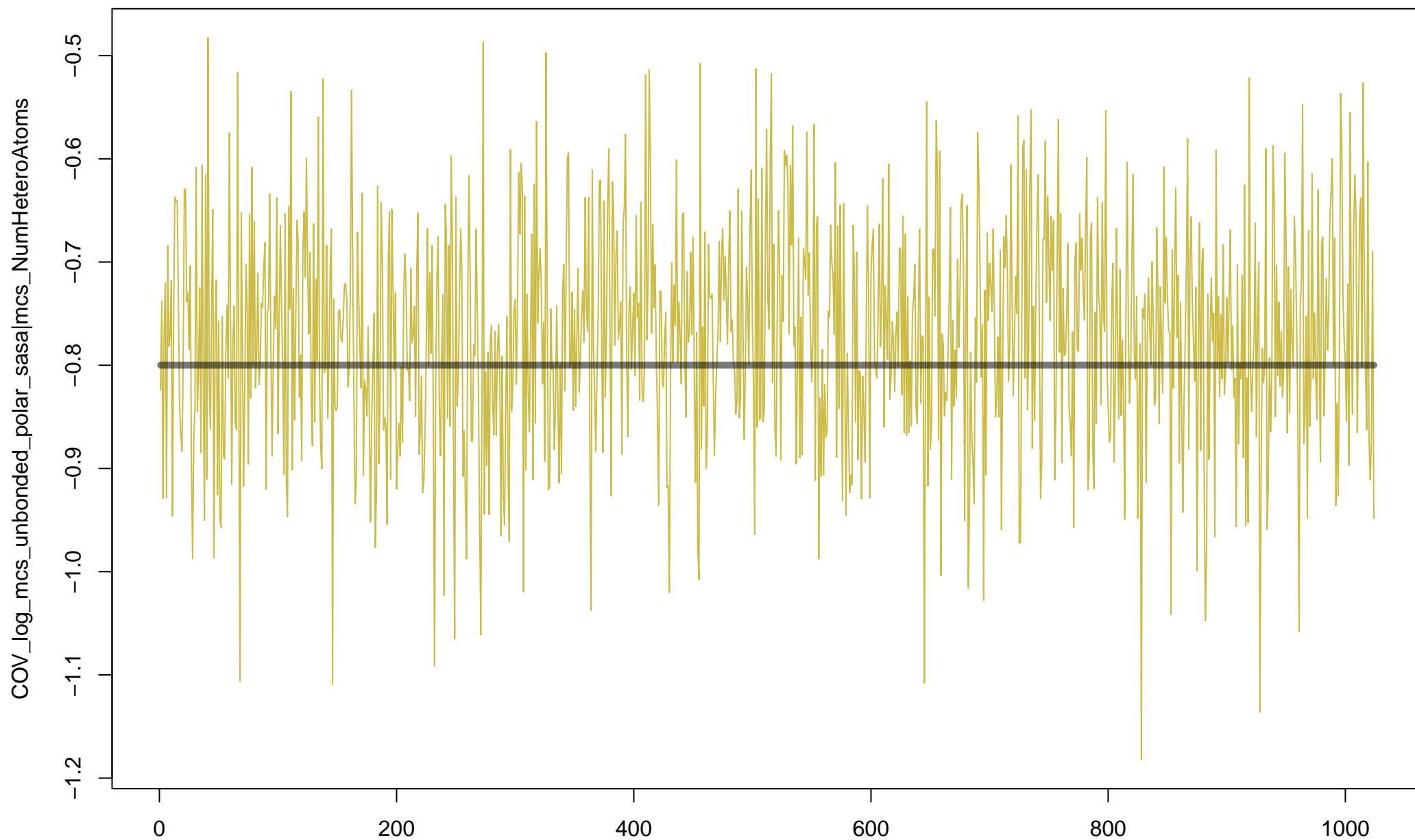
COV_log_RMSD|mcs_NOCount
ESS = 917 | BMK = 0.0763 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0 | rel.err: 0.591



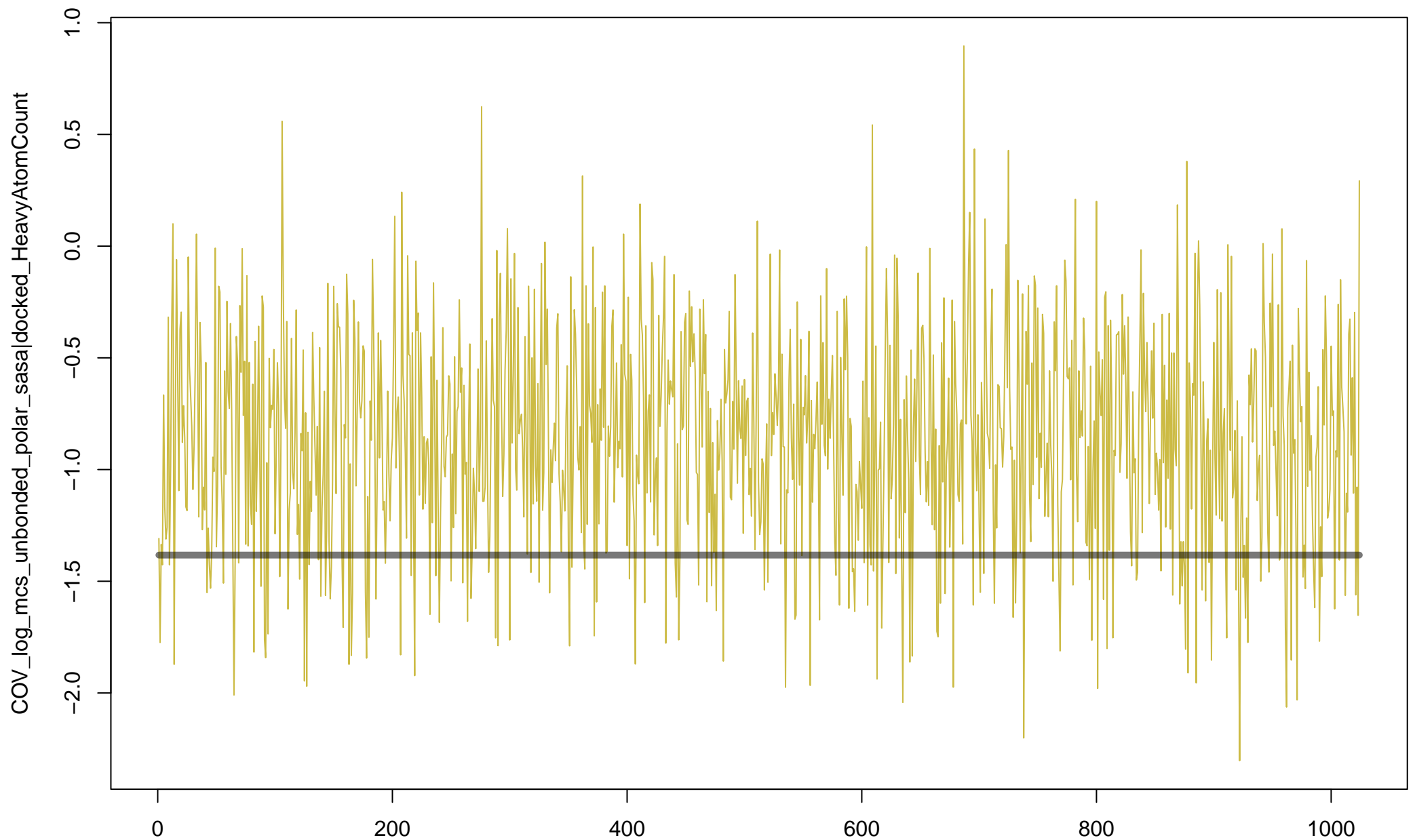
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0476 | MCSE(6.27) = 3.61 | stat: TRUE | burn: 0 | rel.err: 1.17



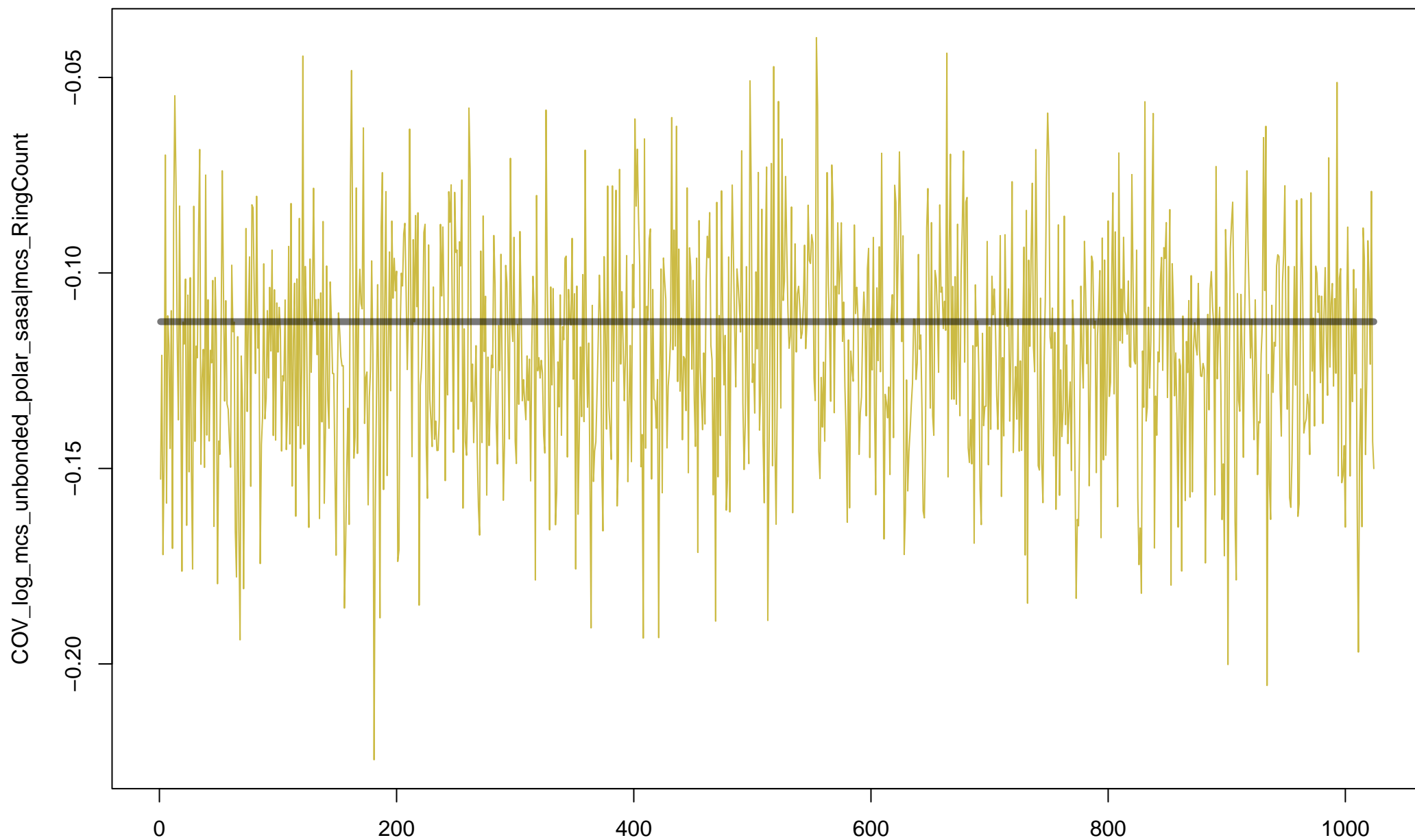
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0525 | MCSE(6.27) = 3.52 | stat: TRUE | burn: 0 | rel.err: 0.253



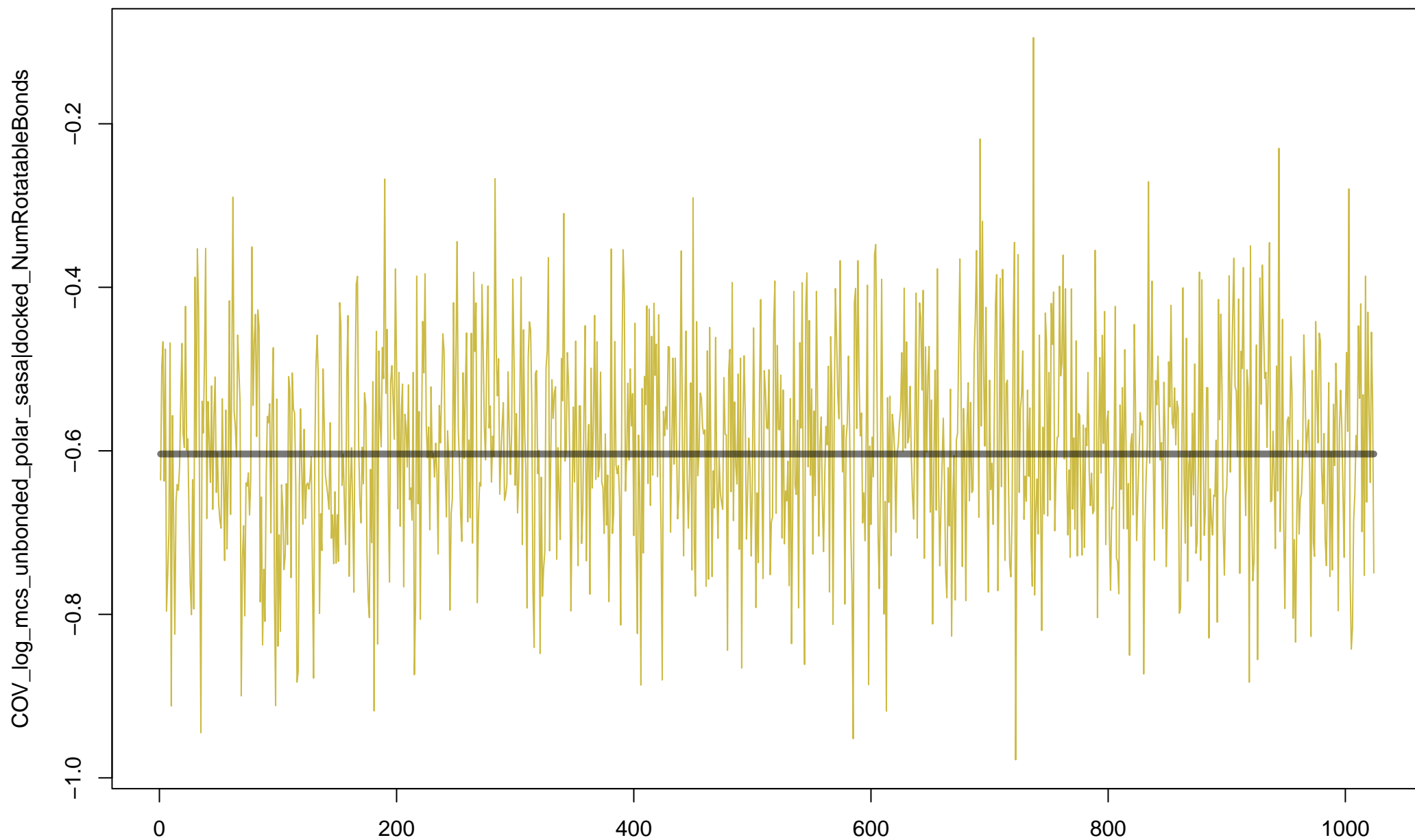
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0495 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | rel.err: 1.06



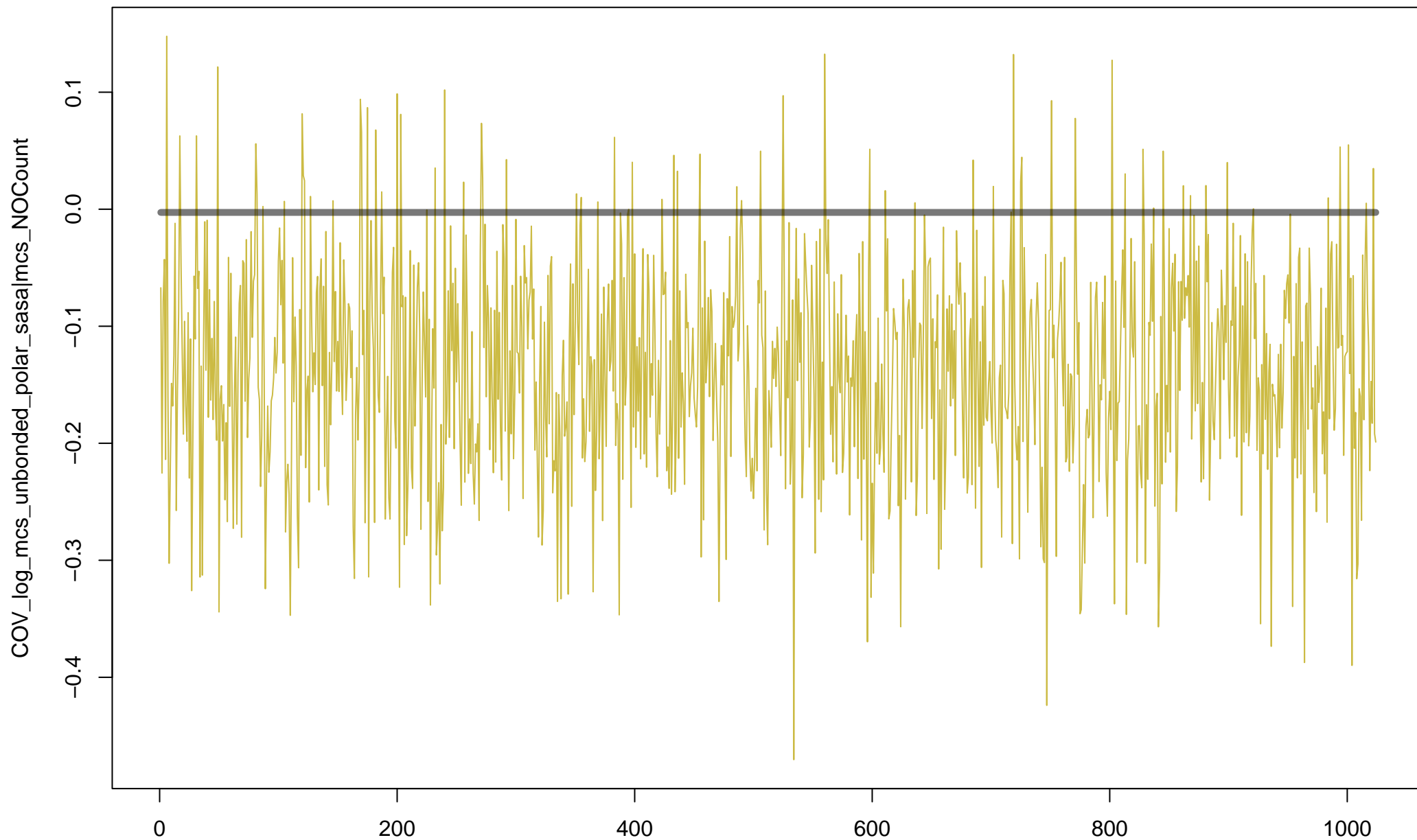
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1010 | BMK = 0.0496 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | rel.err: -0.278



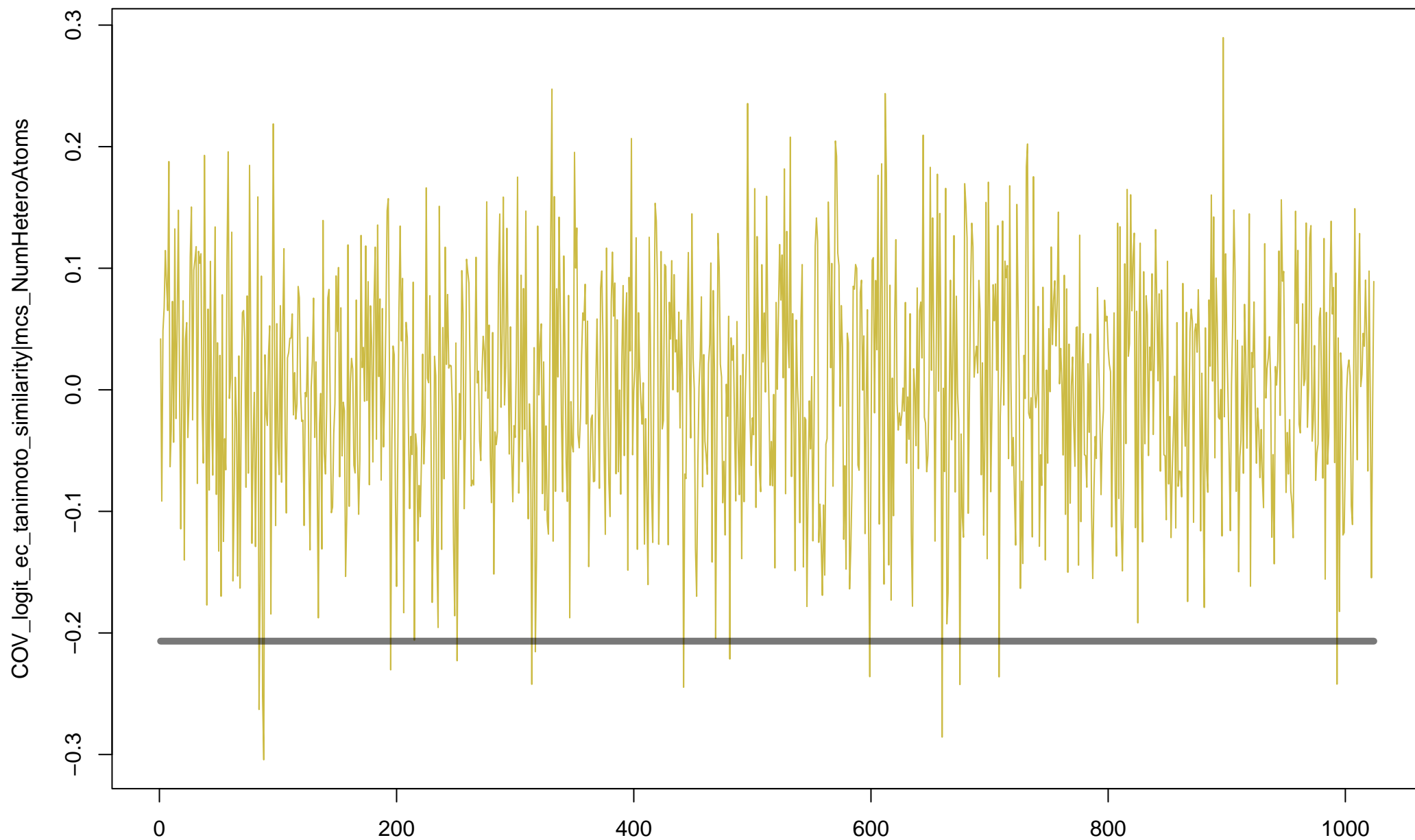
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0677 | MCSE(6.27) = 3.49 | stat: TRUE | burn: 0 | rel.err: 0.0639



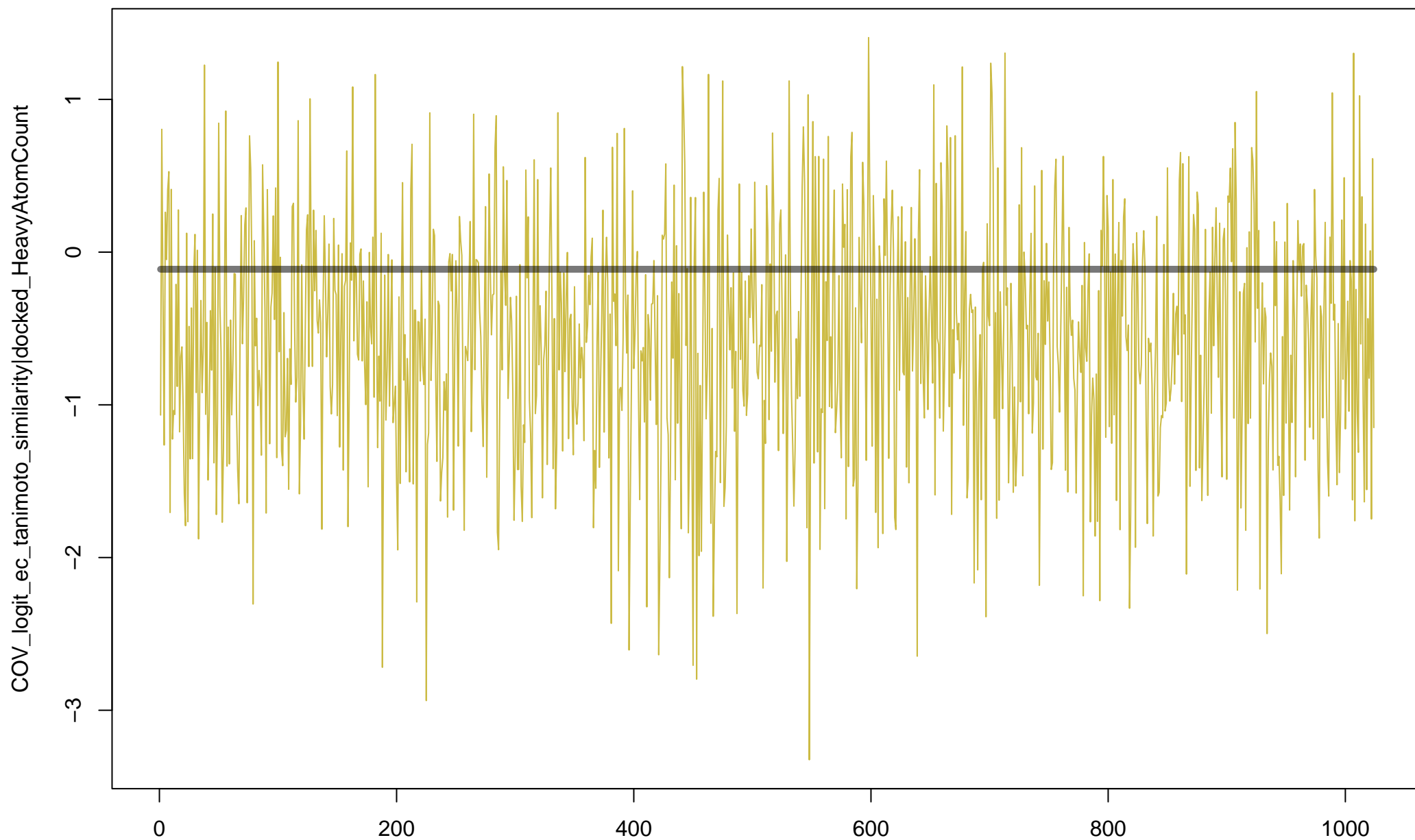
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0658 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0 | rel.err: -1.47



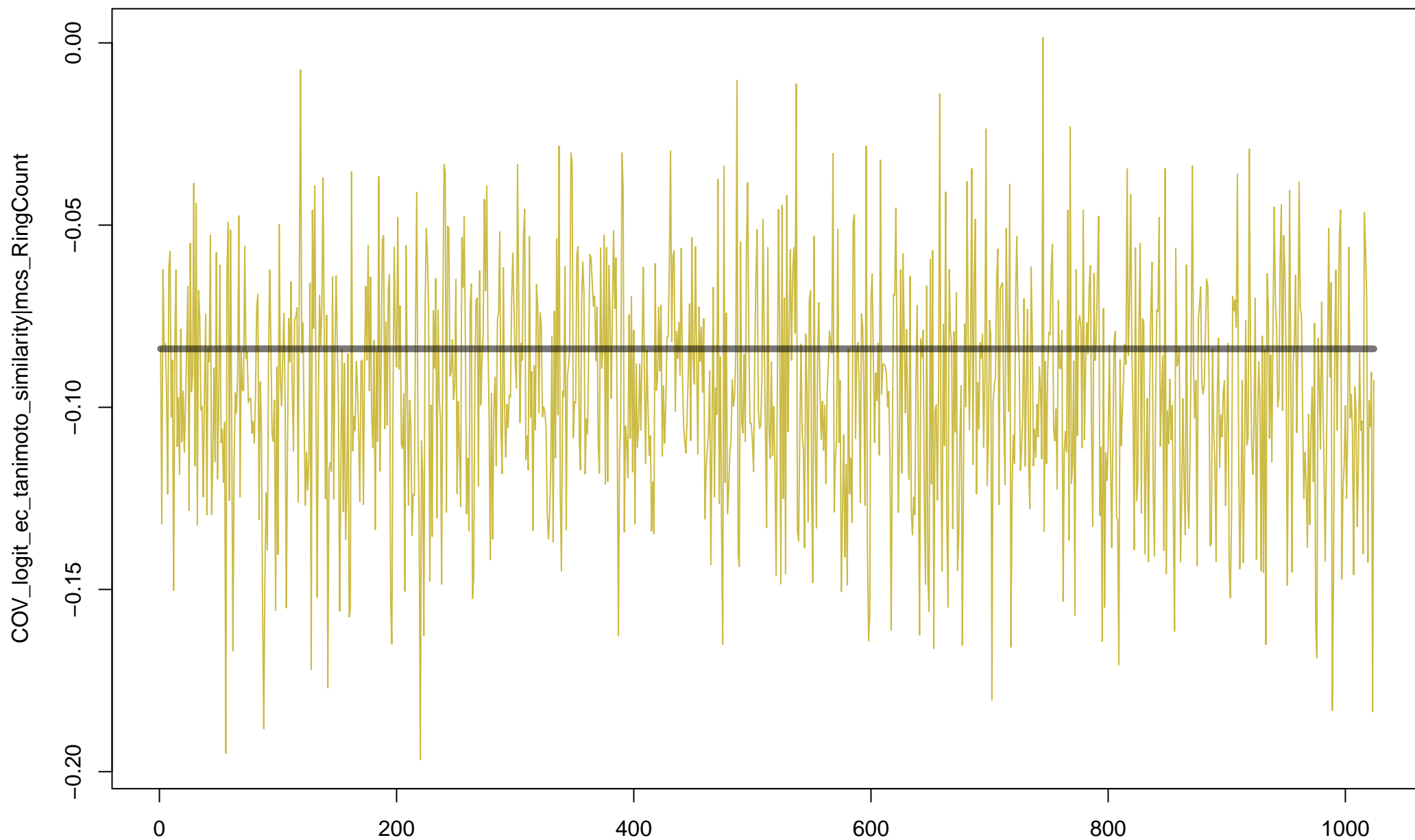
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0403 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0 | rel.err: 2.26



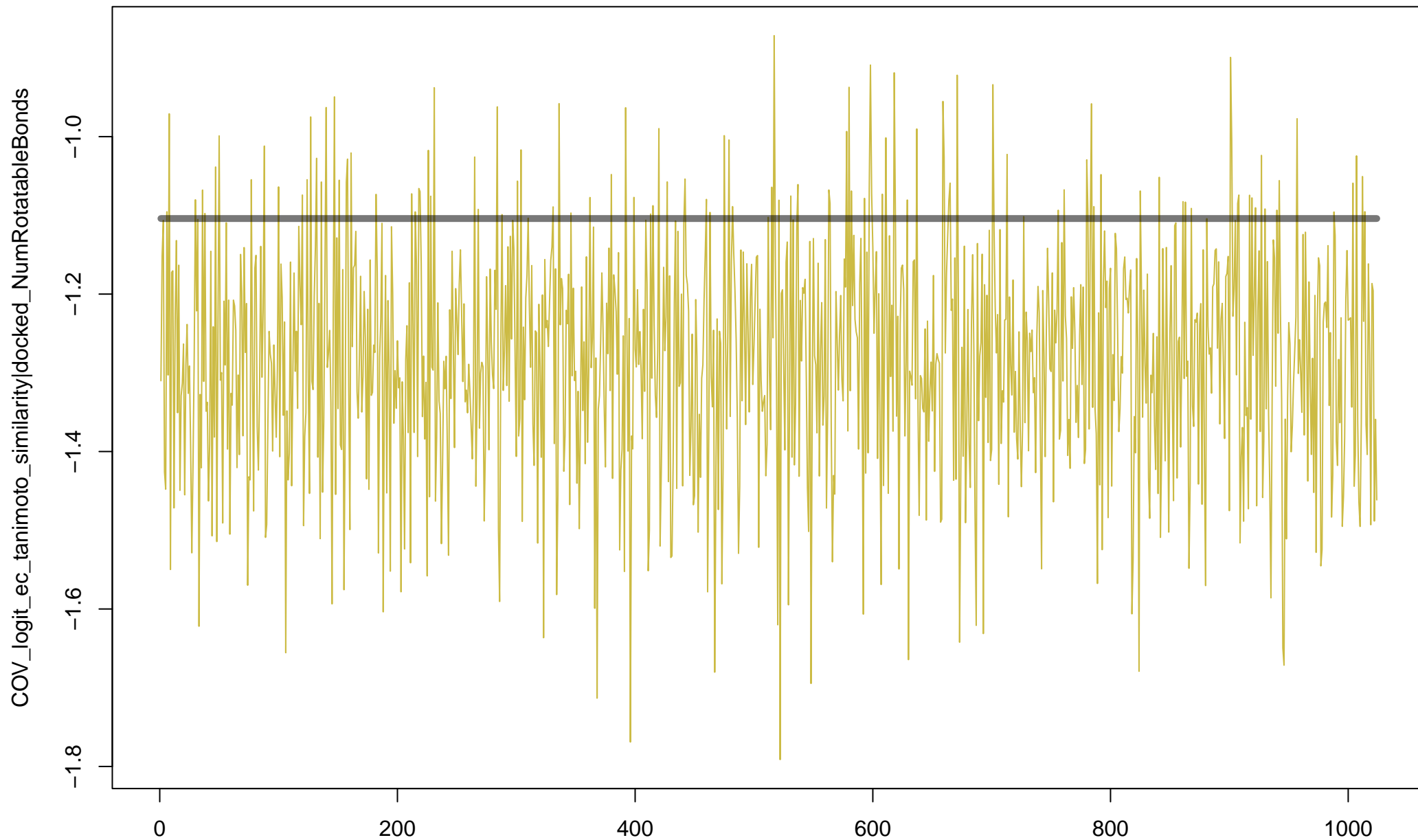
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0612 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | rel.err: -0.613



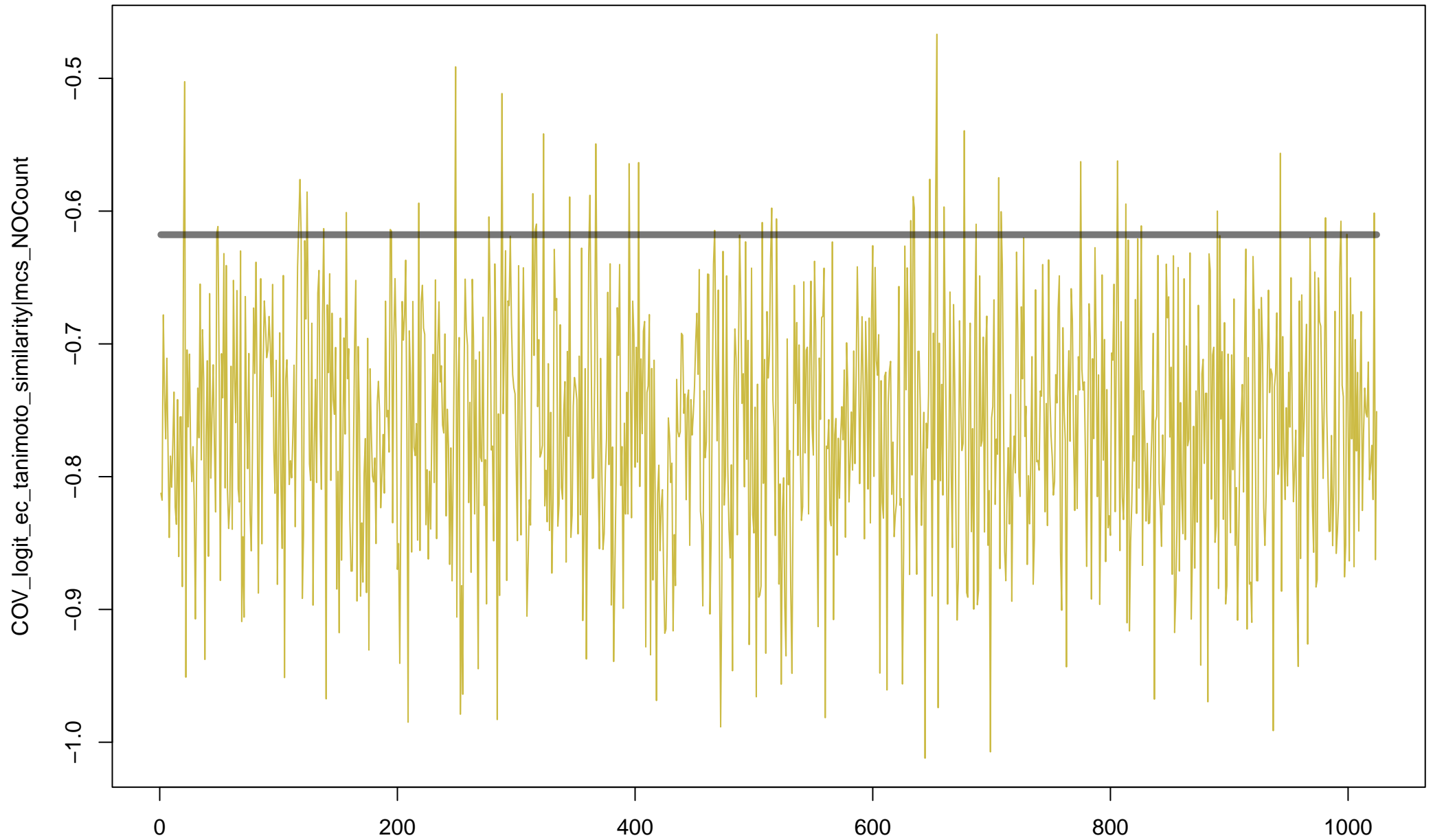
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0703 | MCSE(6.27) = 3.14 | stat: TRUE | burn: 0 | rel.err: -0.385



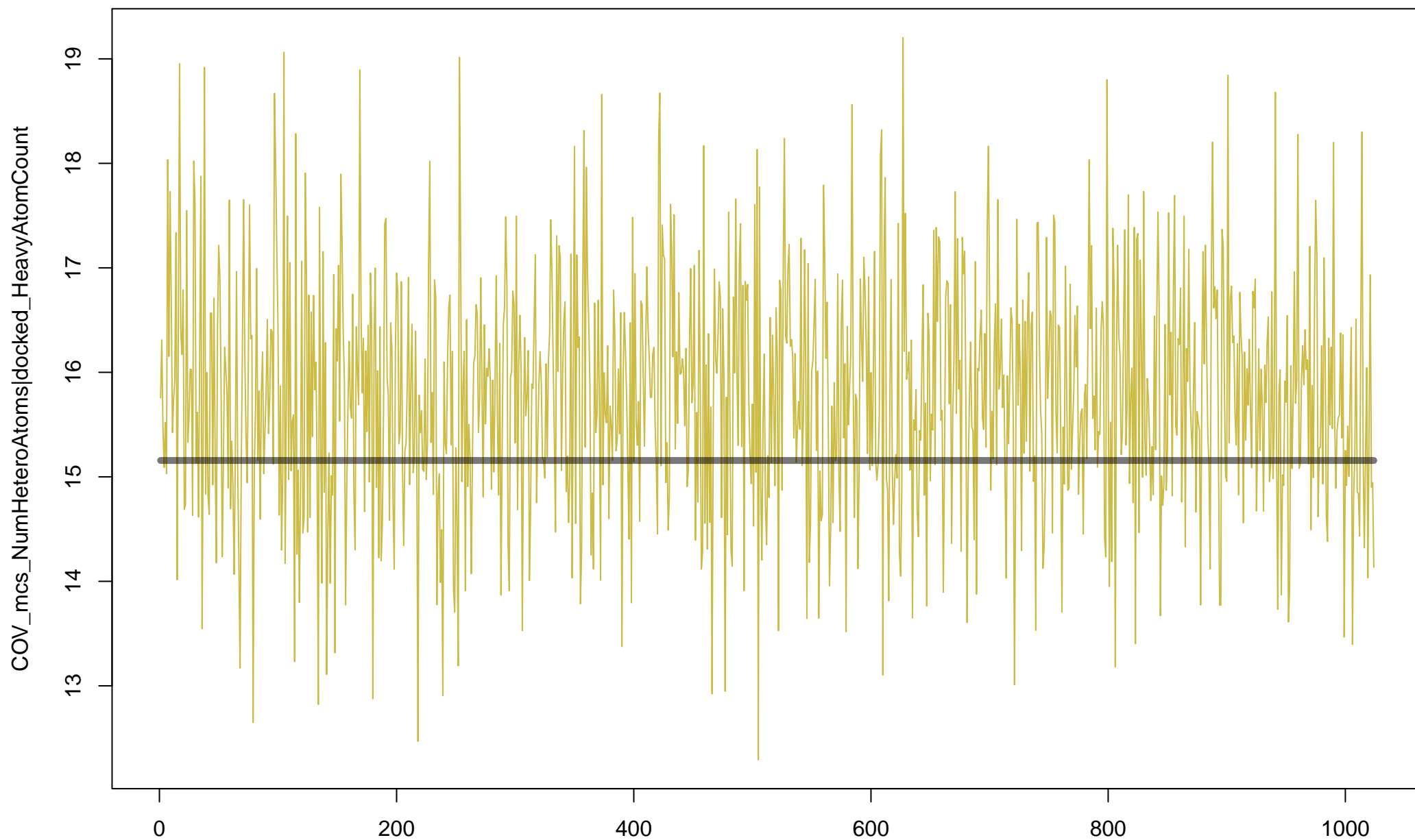
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0503 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0 | rel.err: -1.23



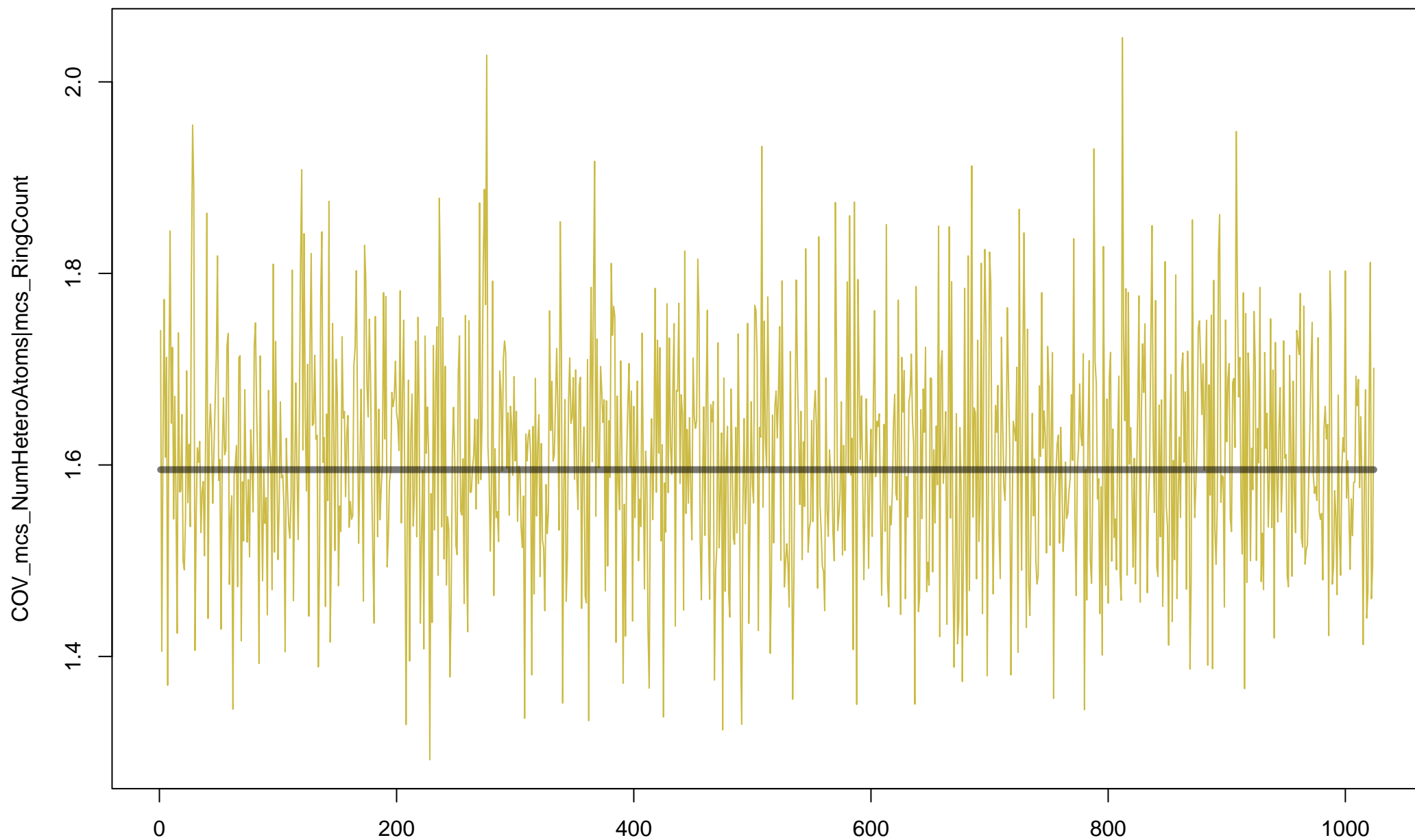
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0343 | MCSE(6.27) = 2.9 | stat: TRUE | burn: 0 | rel.err: -1.62



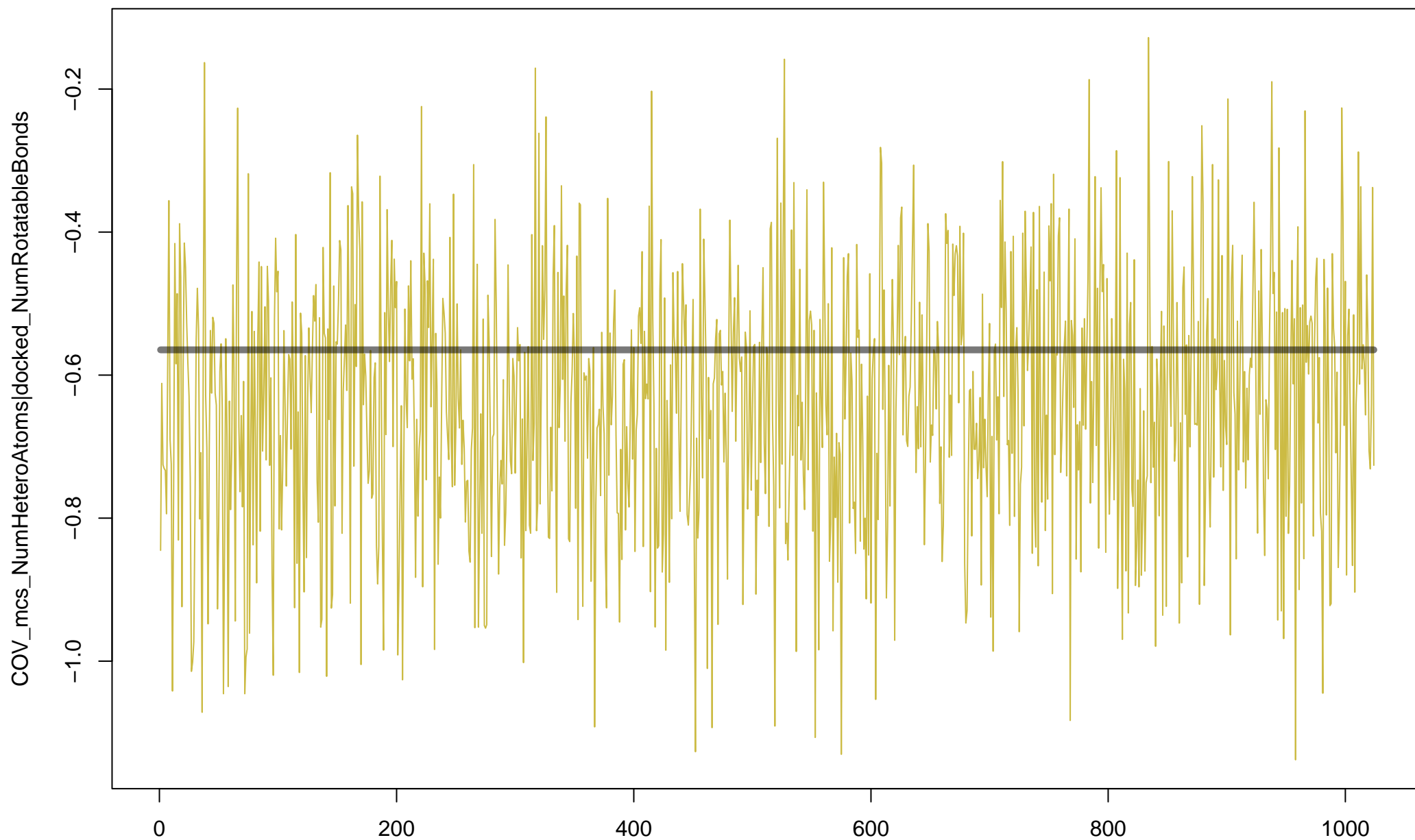
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0669 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0 | rel.err: 0.559



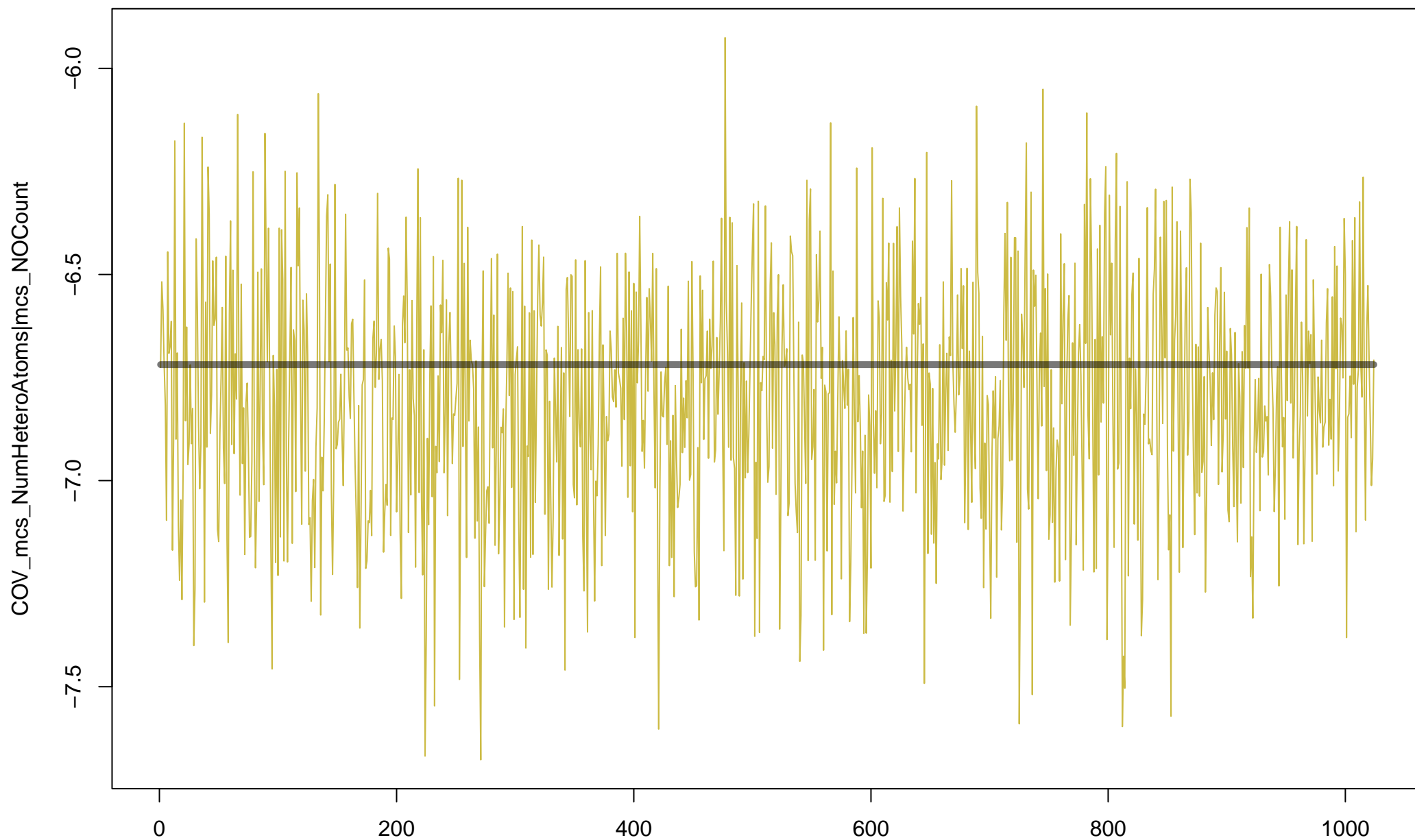
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0674 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0 | rel.err: 0.119



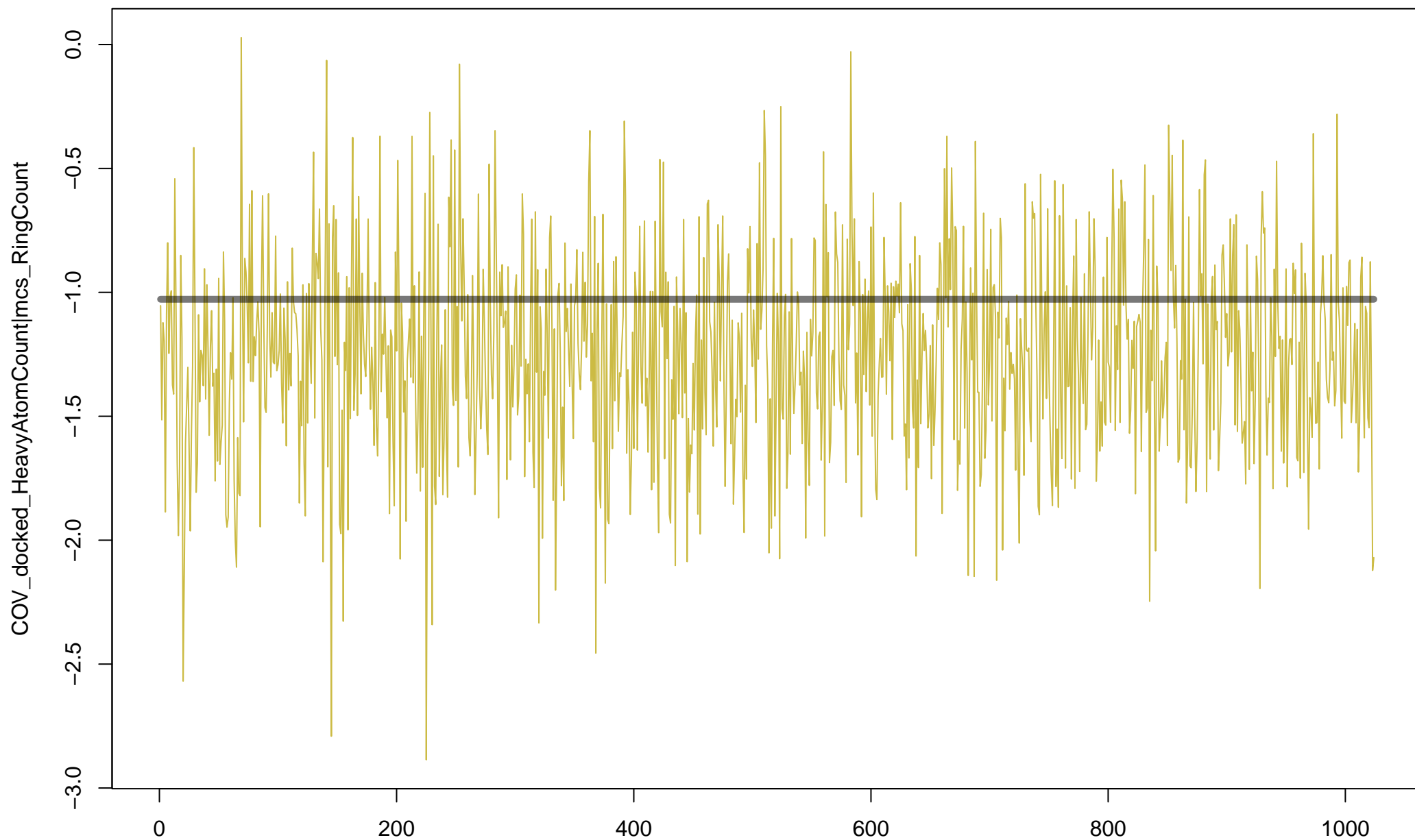
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0676 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0 | rel.err: -0.424



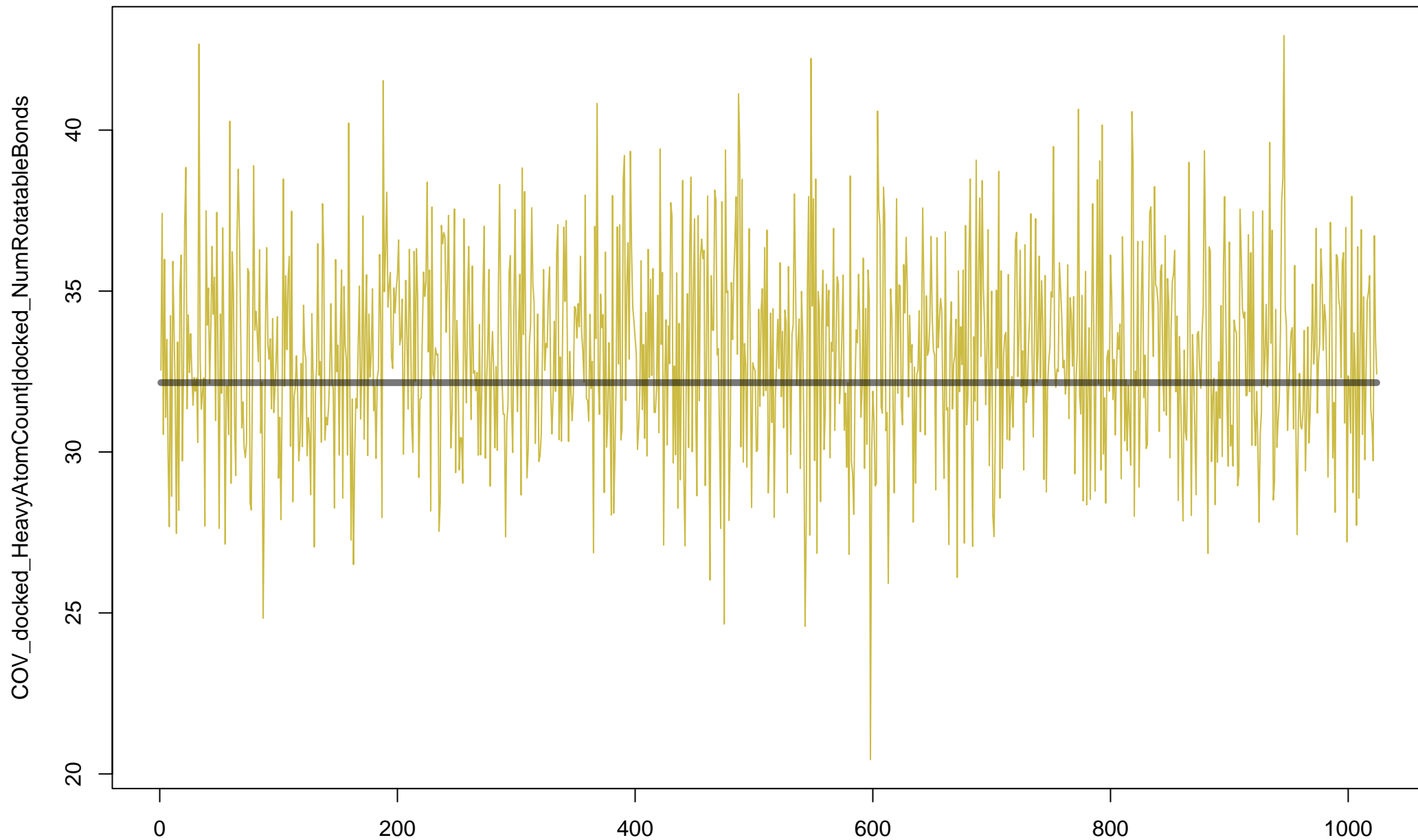
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0546 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | rel.err: -0.307



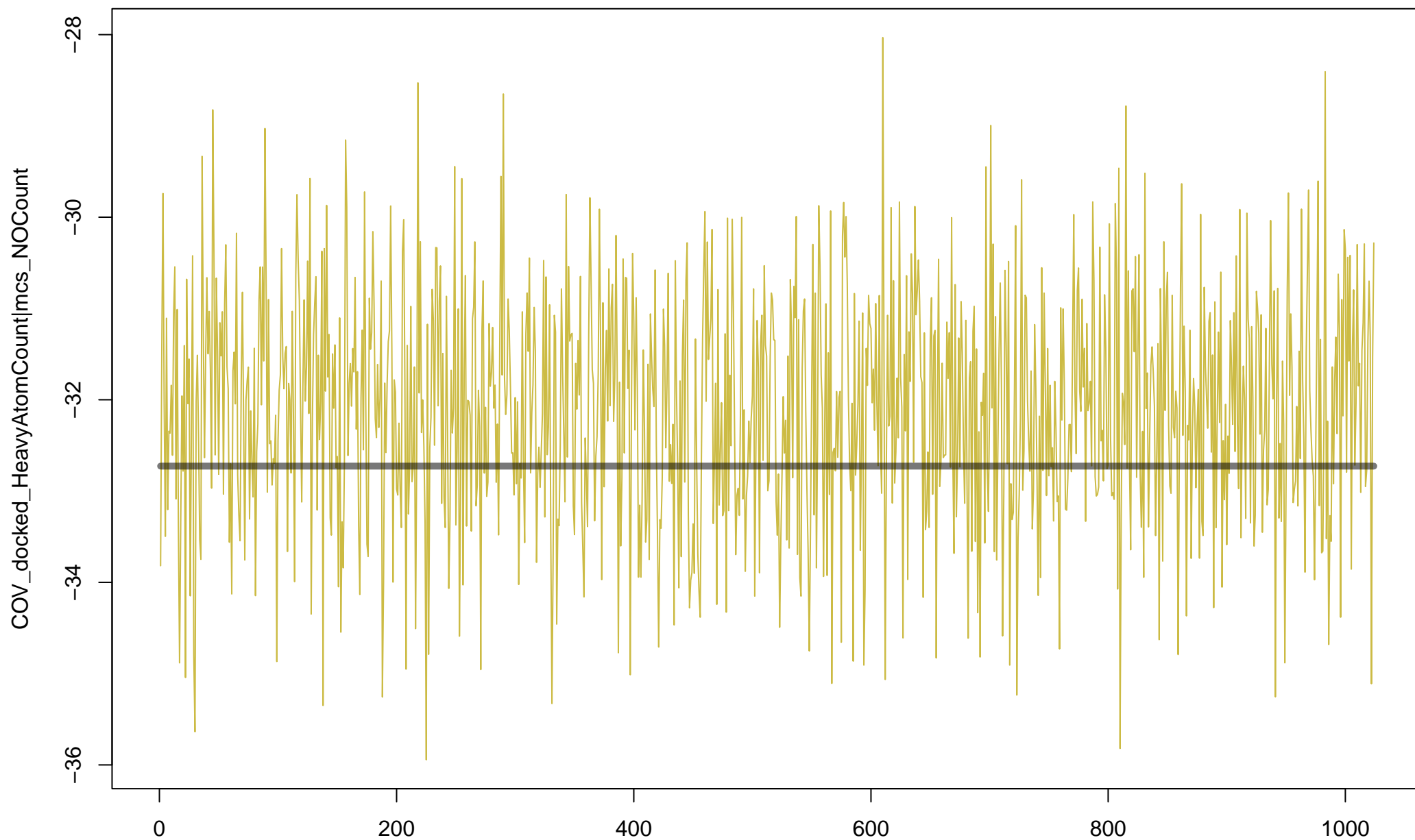
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0792 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0 | rel.err: -0.558



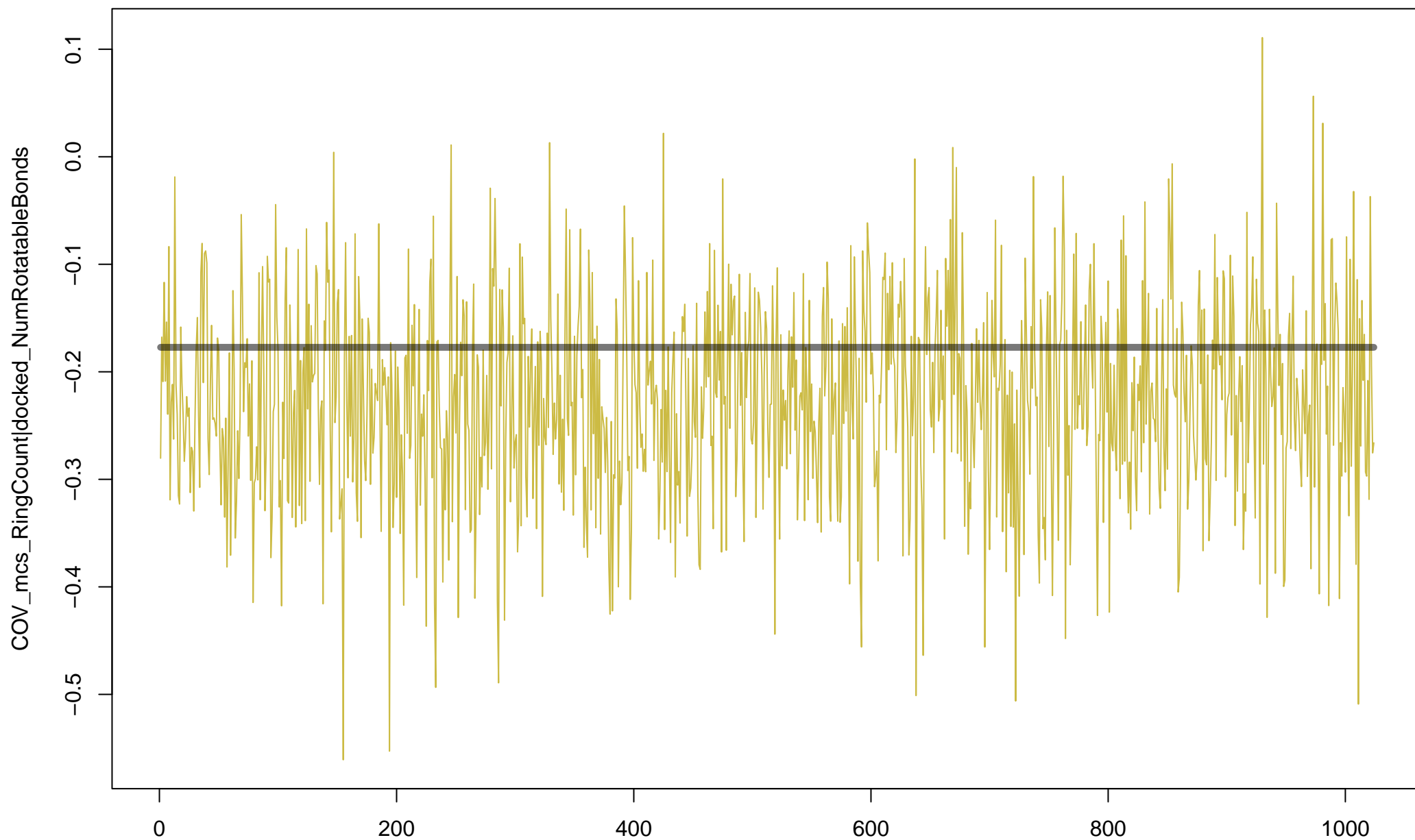
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.035 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0 | rel.err: 0.304



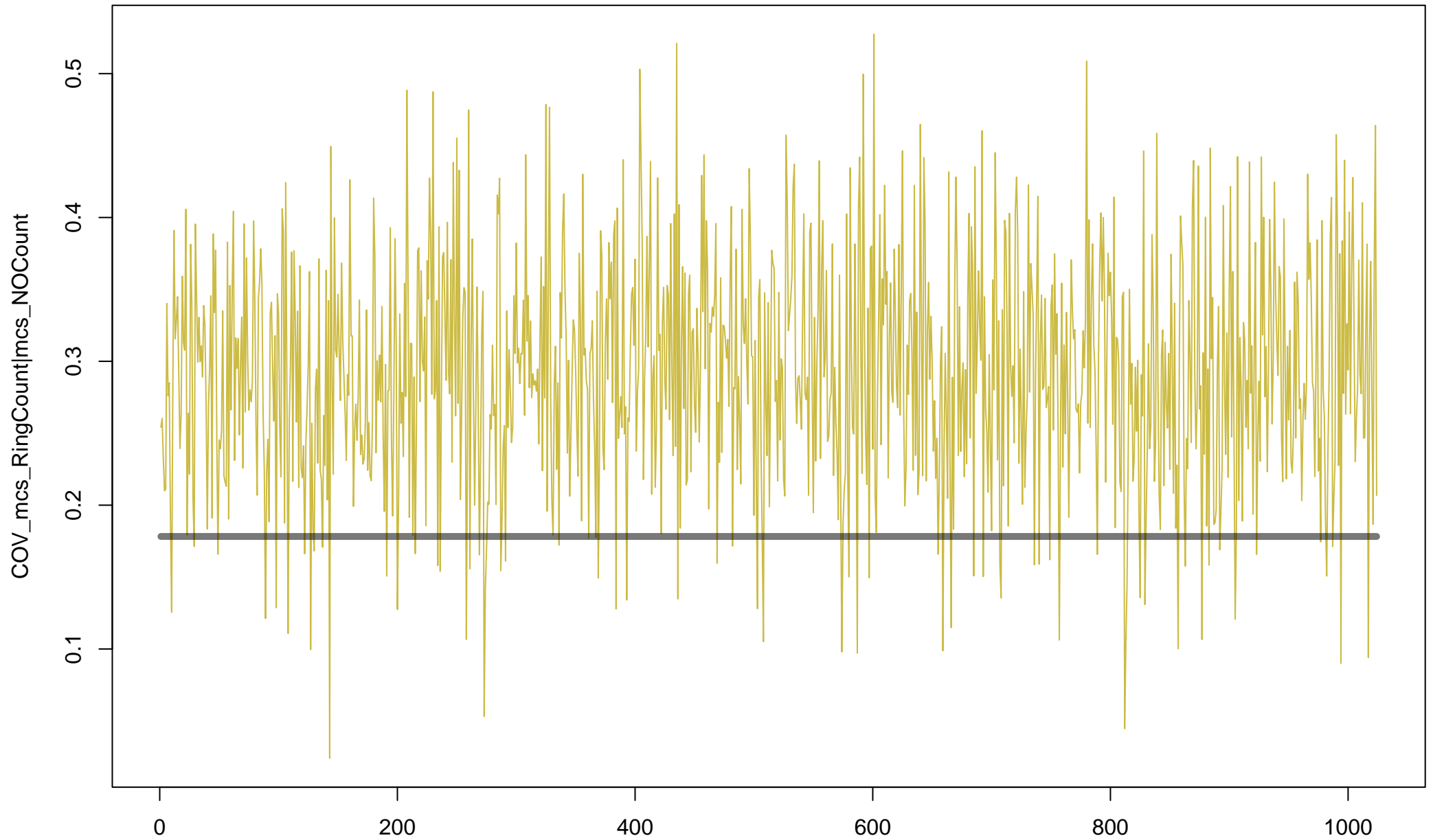
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0371 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0 | rel.err: 0.492



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0571 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0 | rel.err: -0.529



COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.0545 | MCSE(6.27) = 3.65 | stat: TRUE | burn: 0 | rel.err: 1.45



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0501 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 0 | rel.err: -1.78

