

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.176885492573684

max MCSE = 8.21046017520036

all stationary: FALSE

burn: 0

min percent.: 4.296875

-- STATS 1D --

min ESS = 21.6366824446201

max BMK = 0.808143291687061

max MCSE = 9.96205280314916

all stationary: FALSE

burn: 1020

min percent.: 0.29296875

-- STATS 2D --

min ESS = 590.576835957535

max BMK = 0.0759300074724946

max MCSE = 4.02873834847243

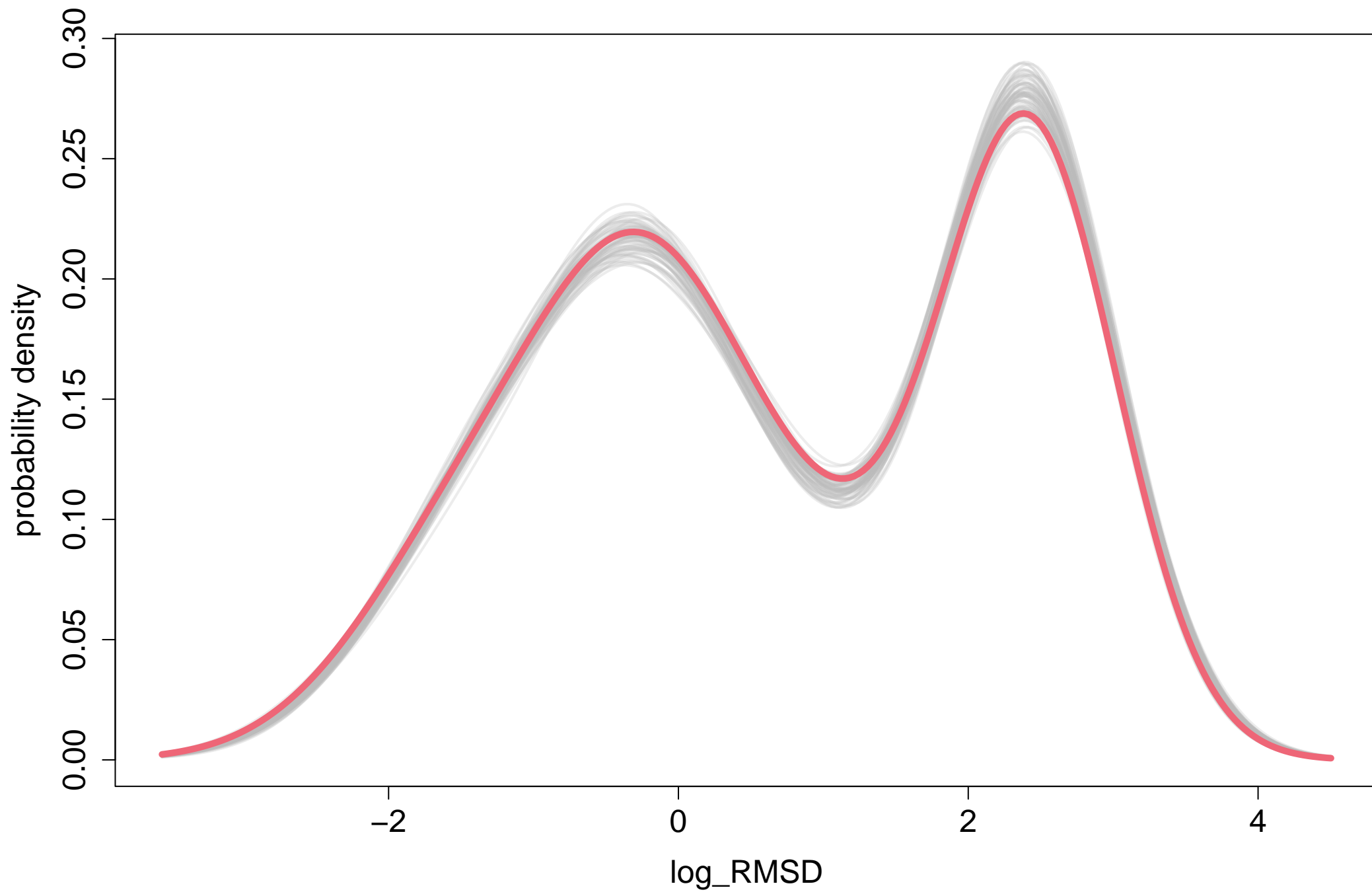
all stationary: FALSE

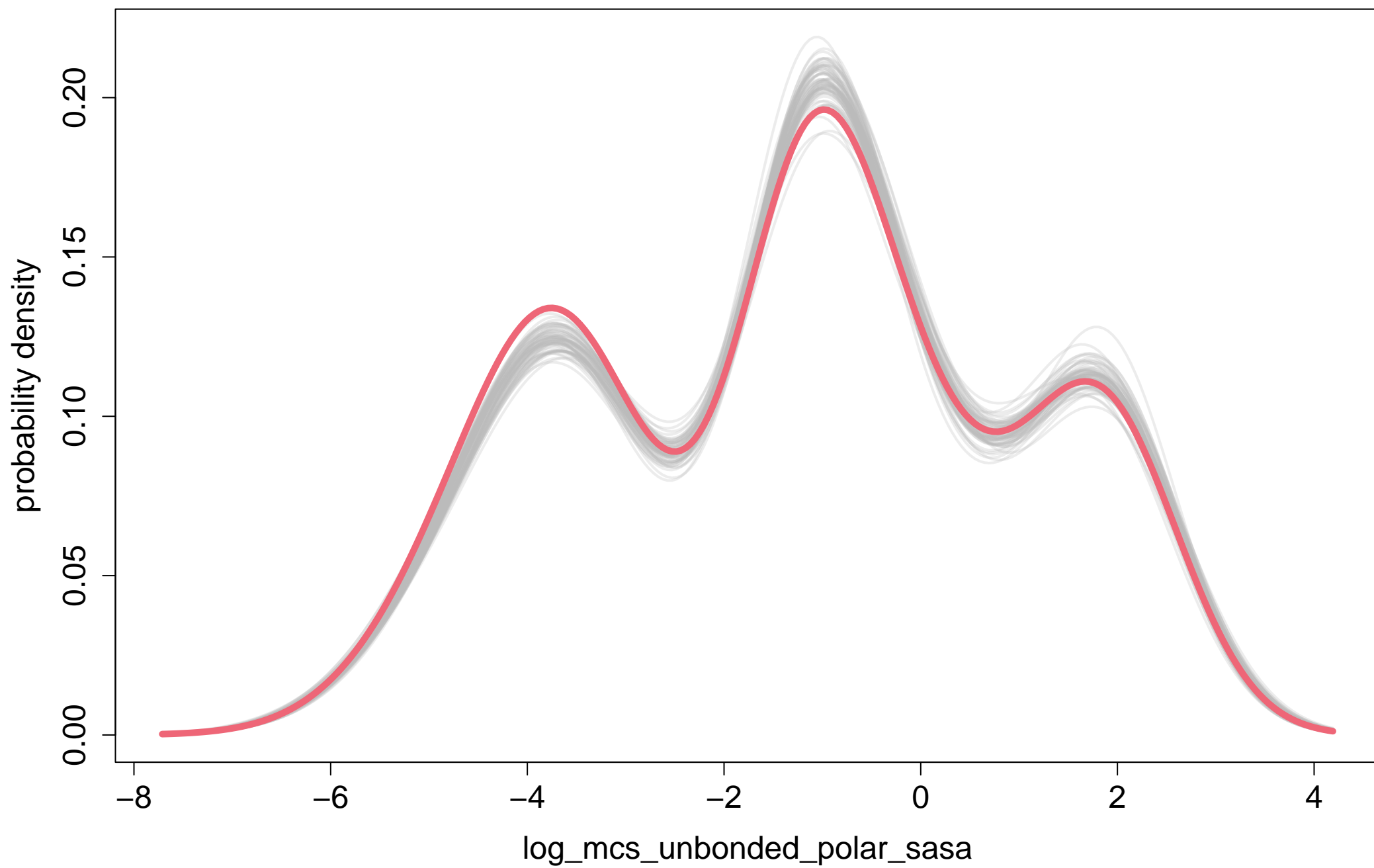
burn: 0

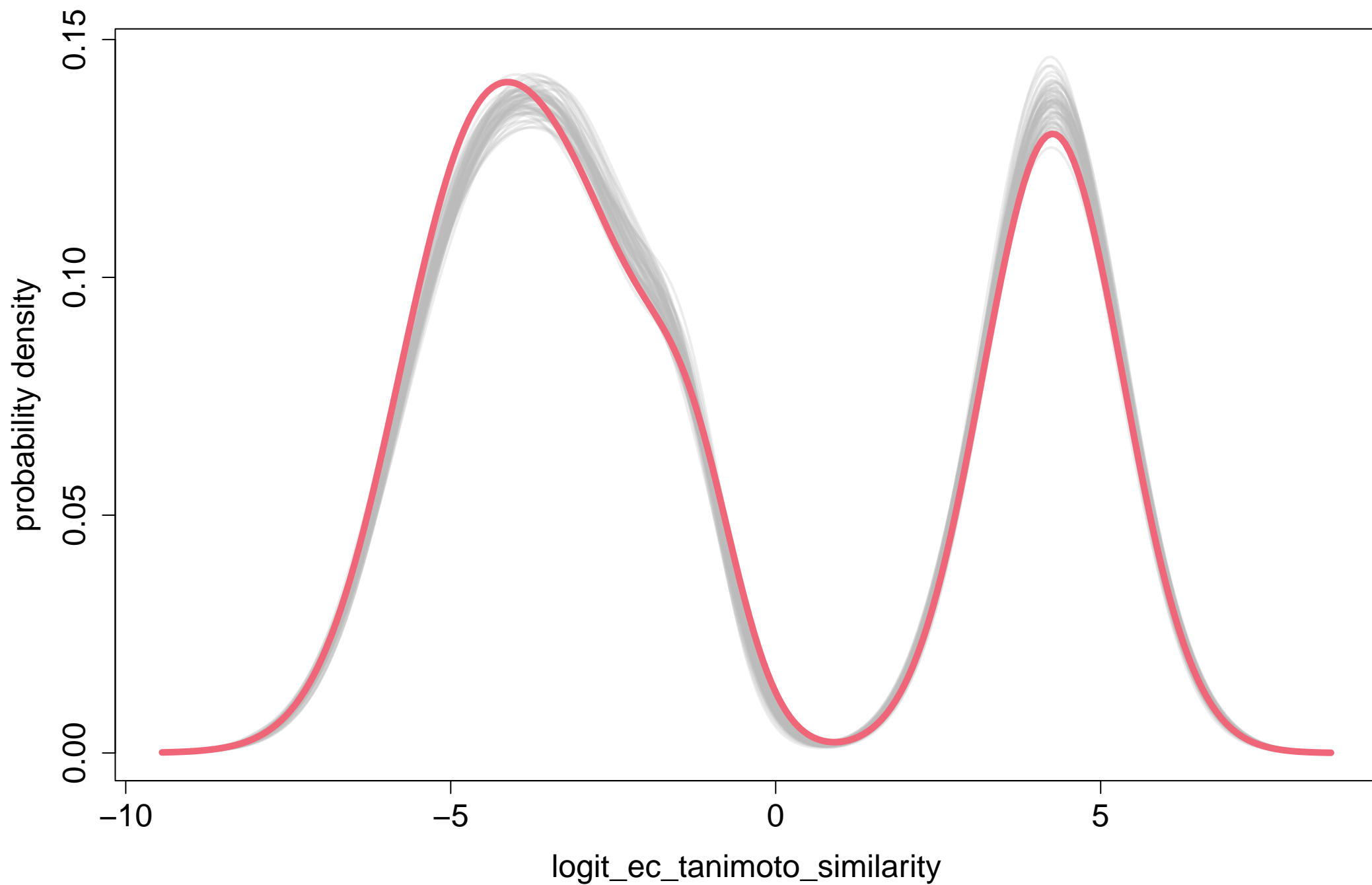
min percent.: 1.5625

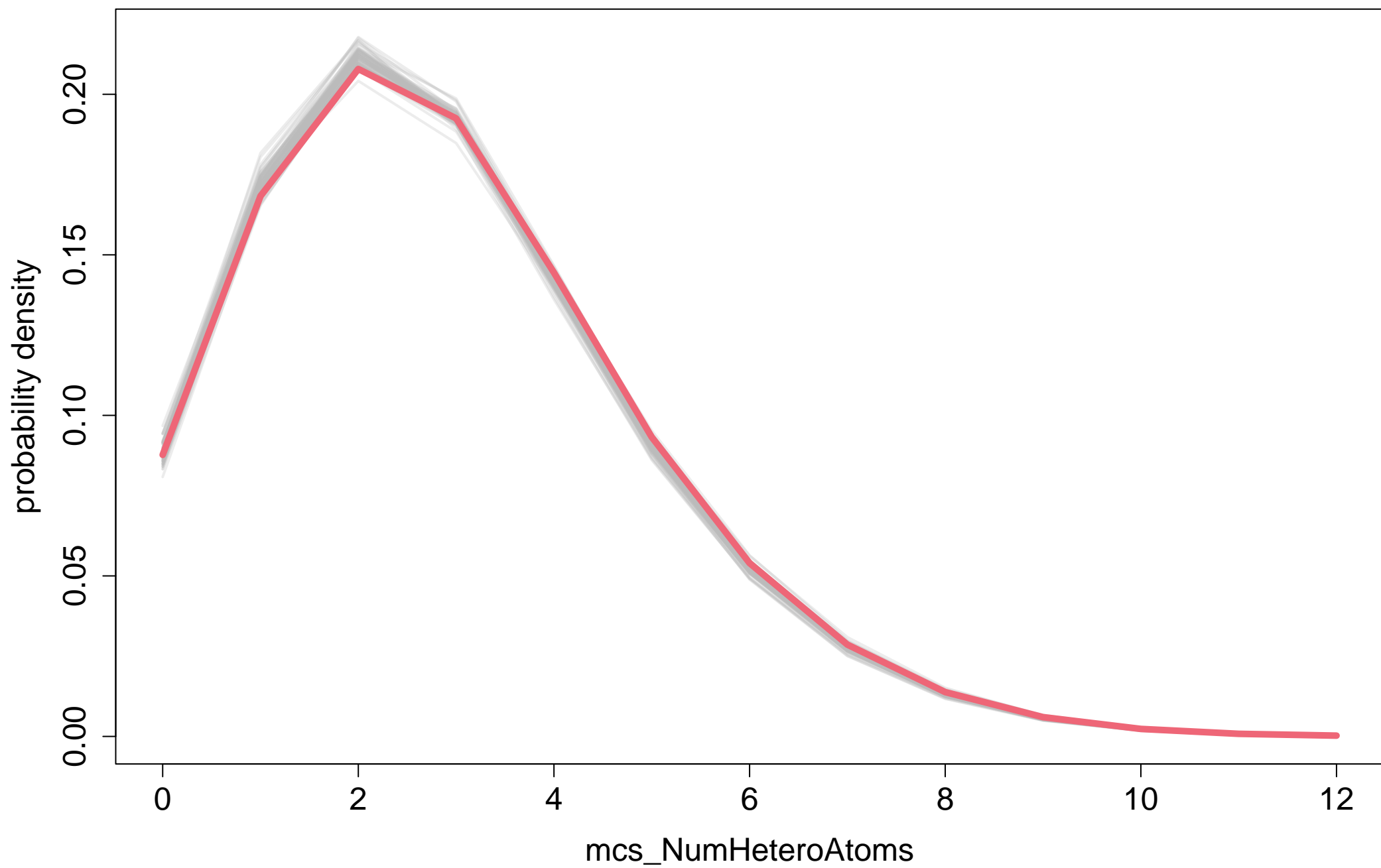
Occupied clusters: 23 of 64

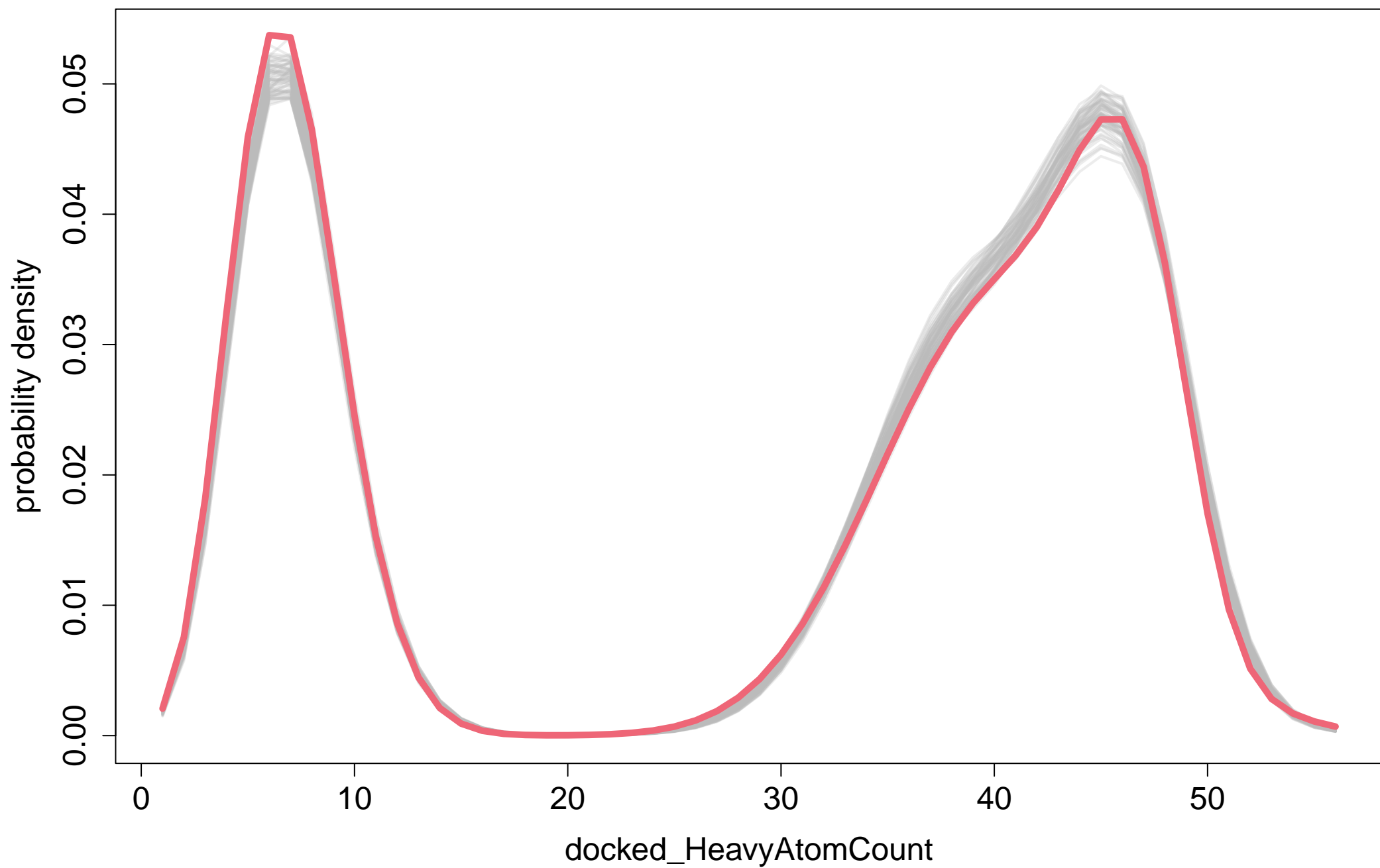
LL: -62400 +- 9.42

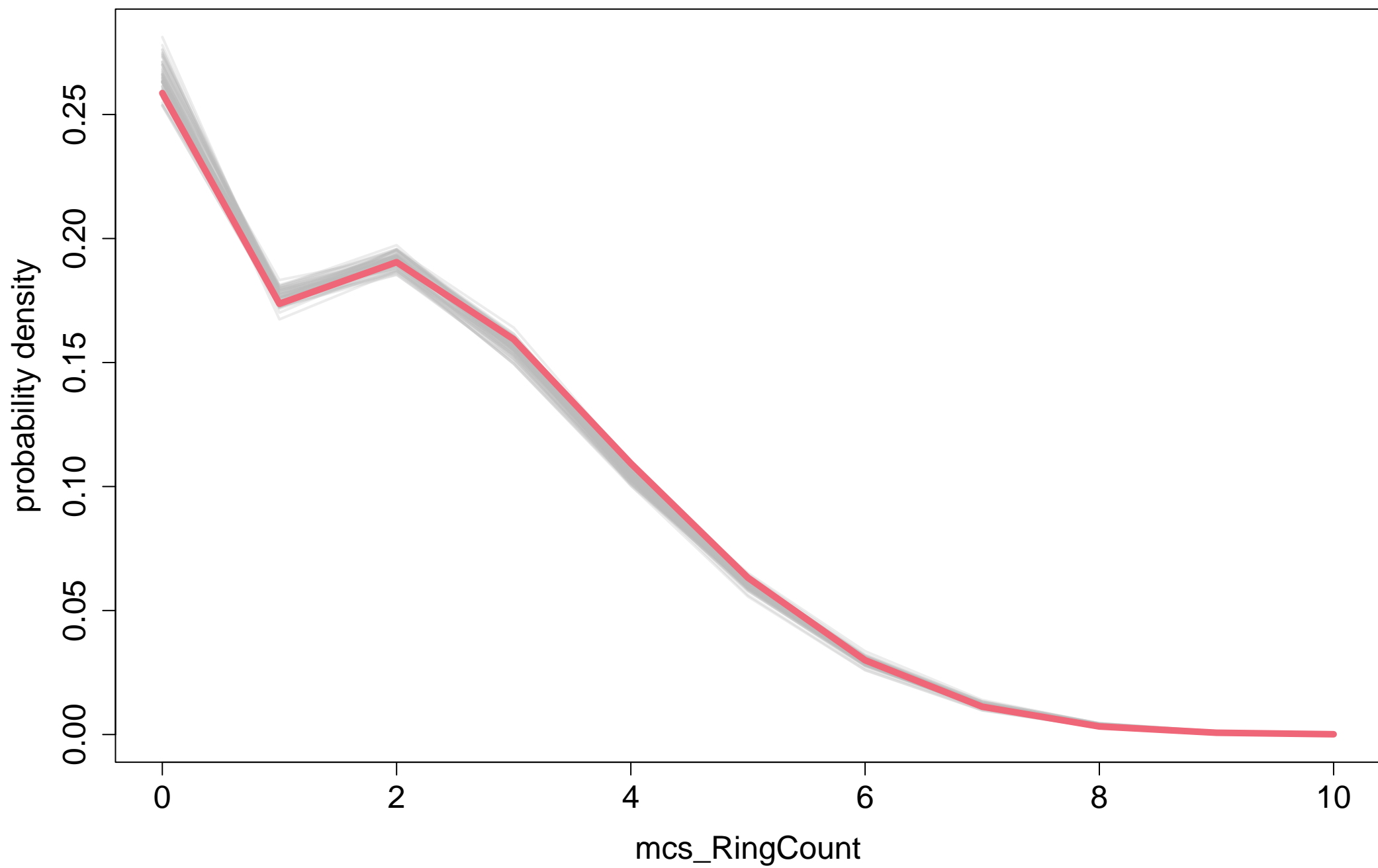


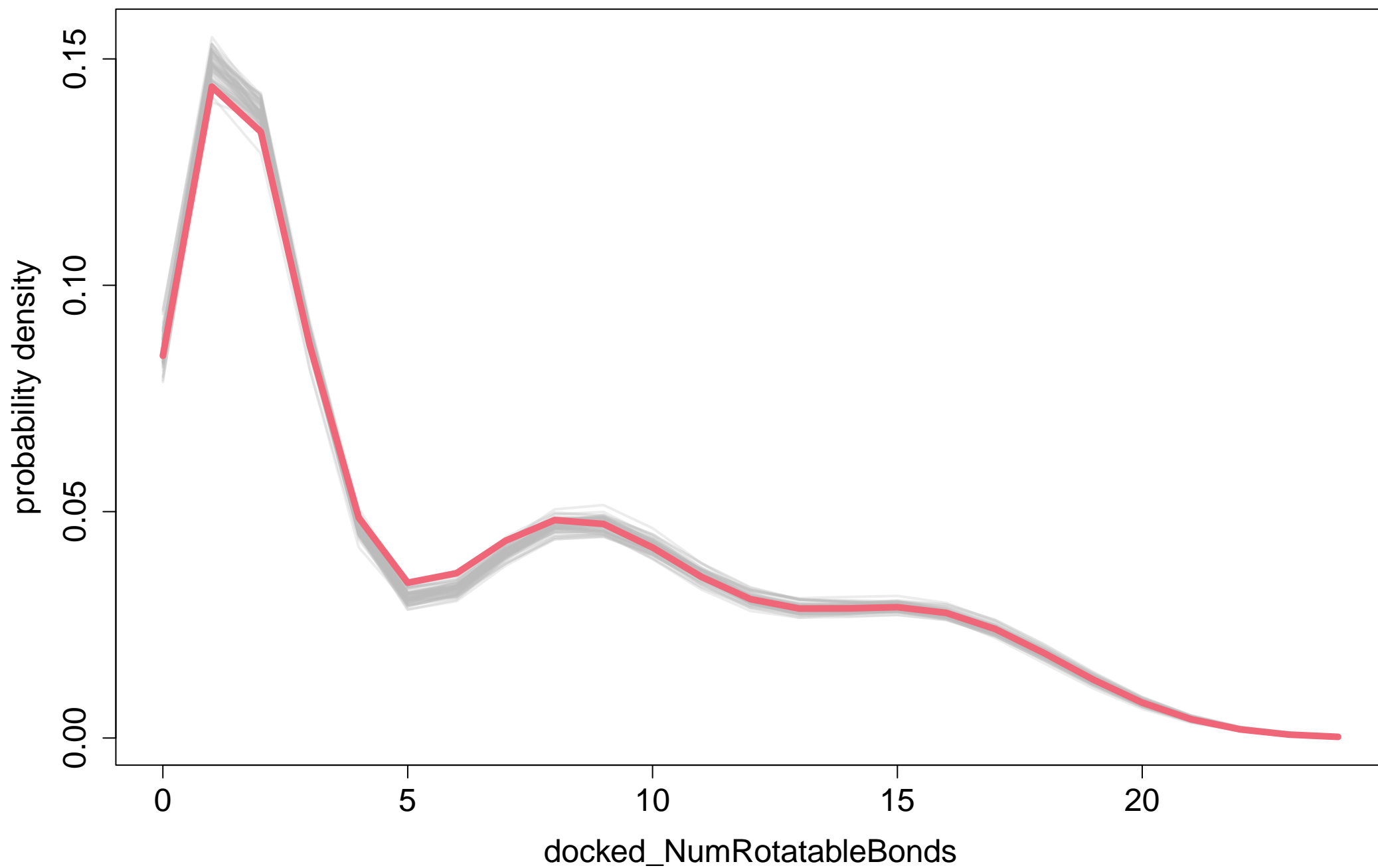


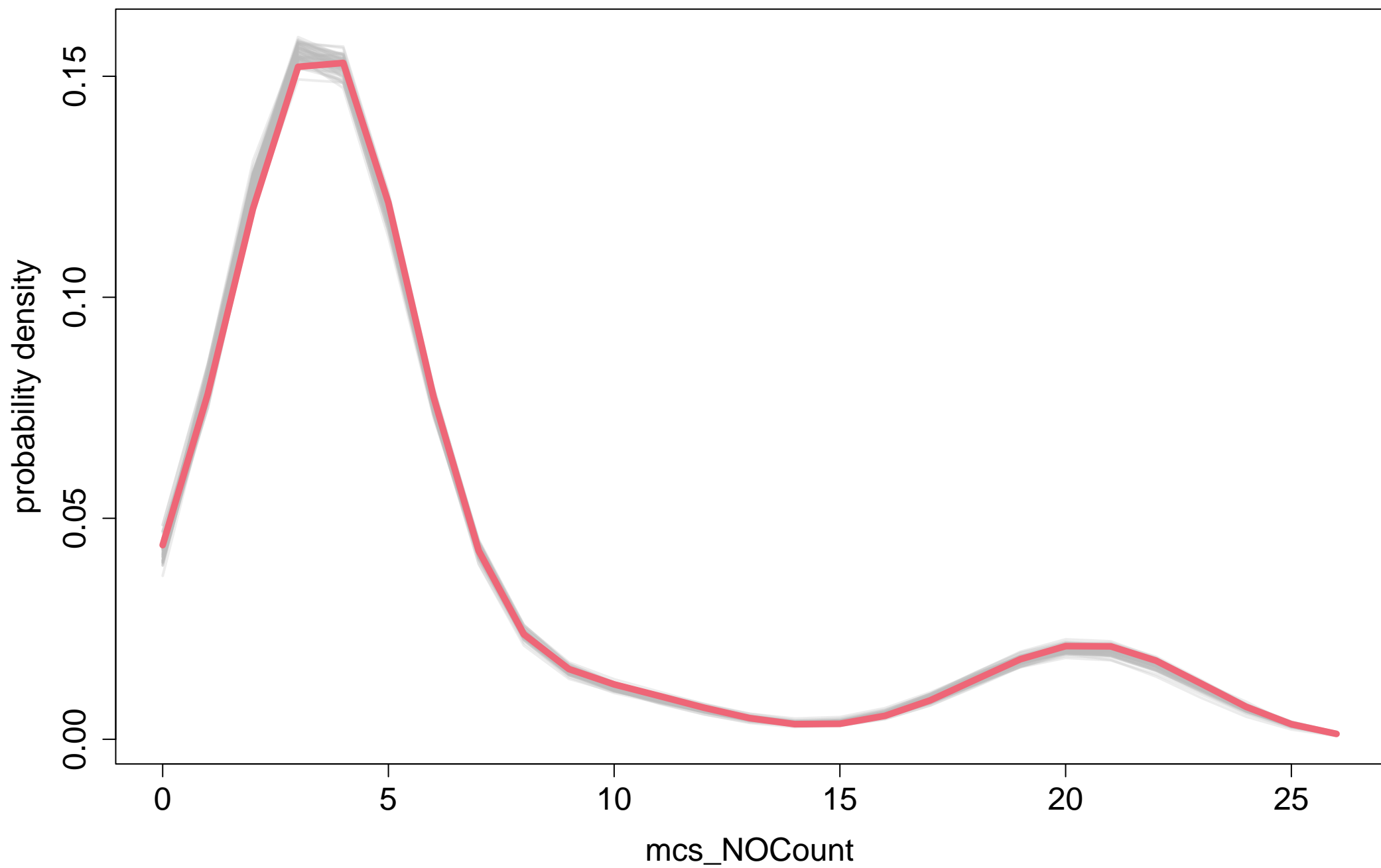


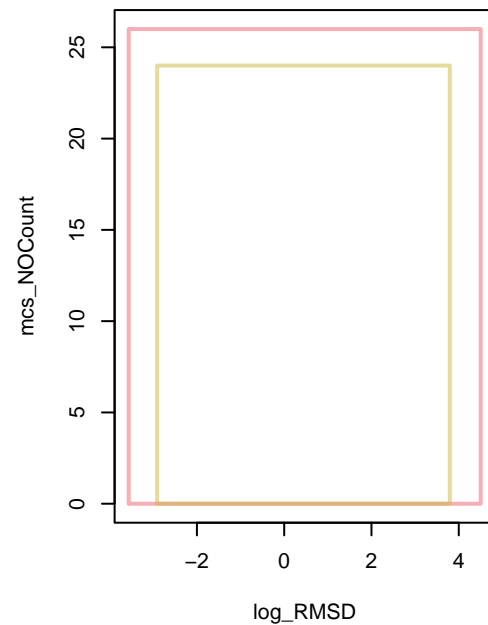
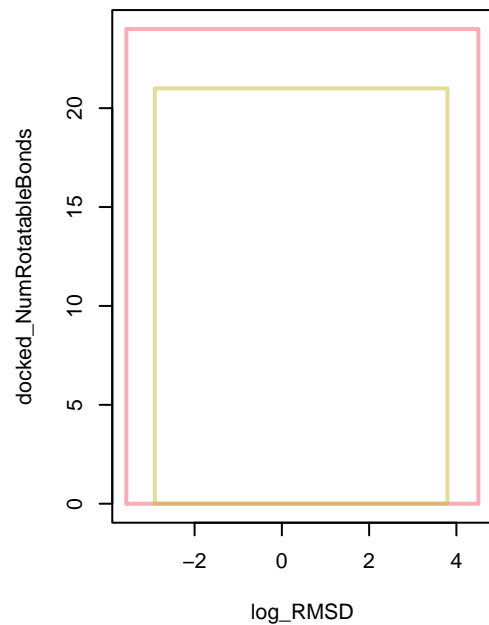
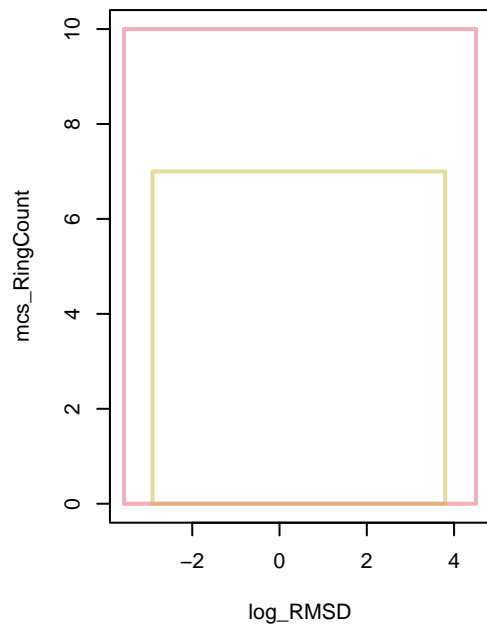
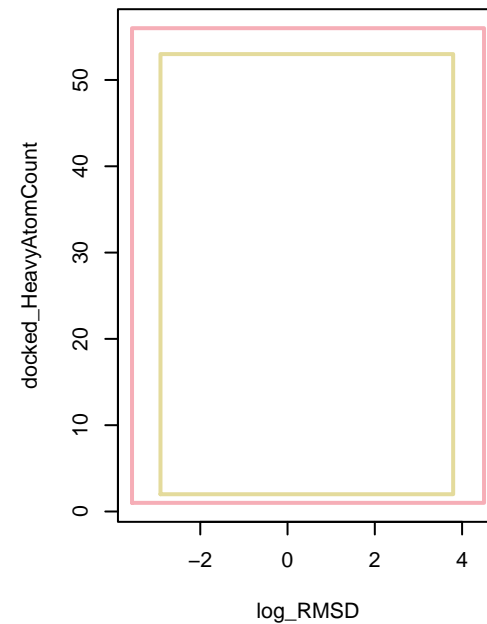
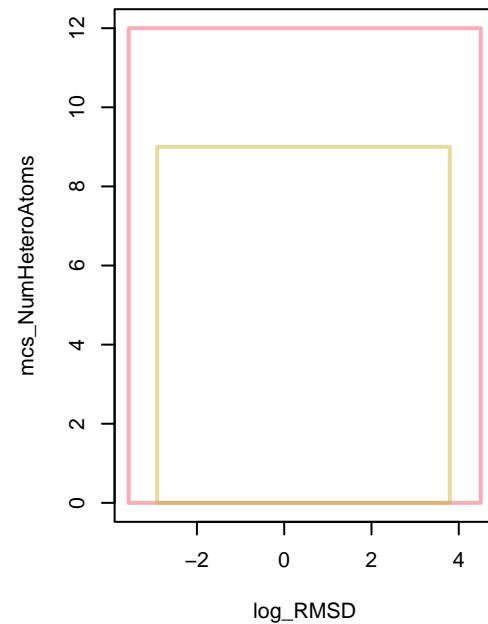
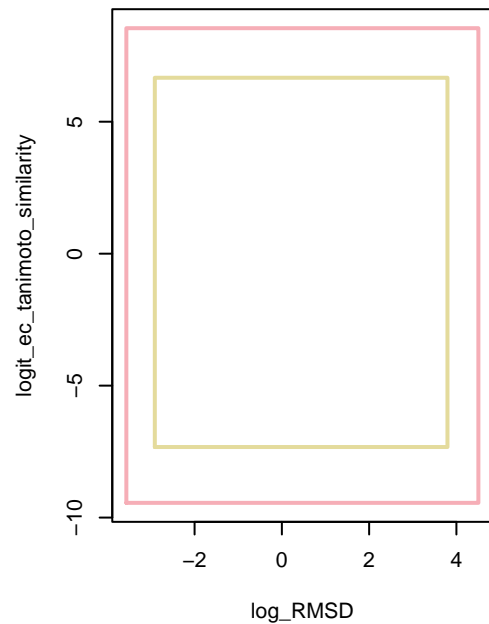
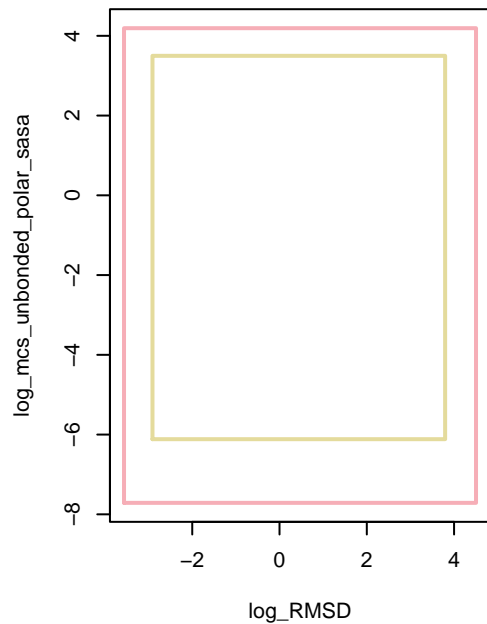




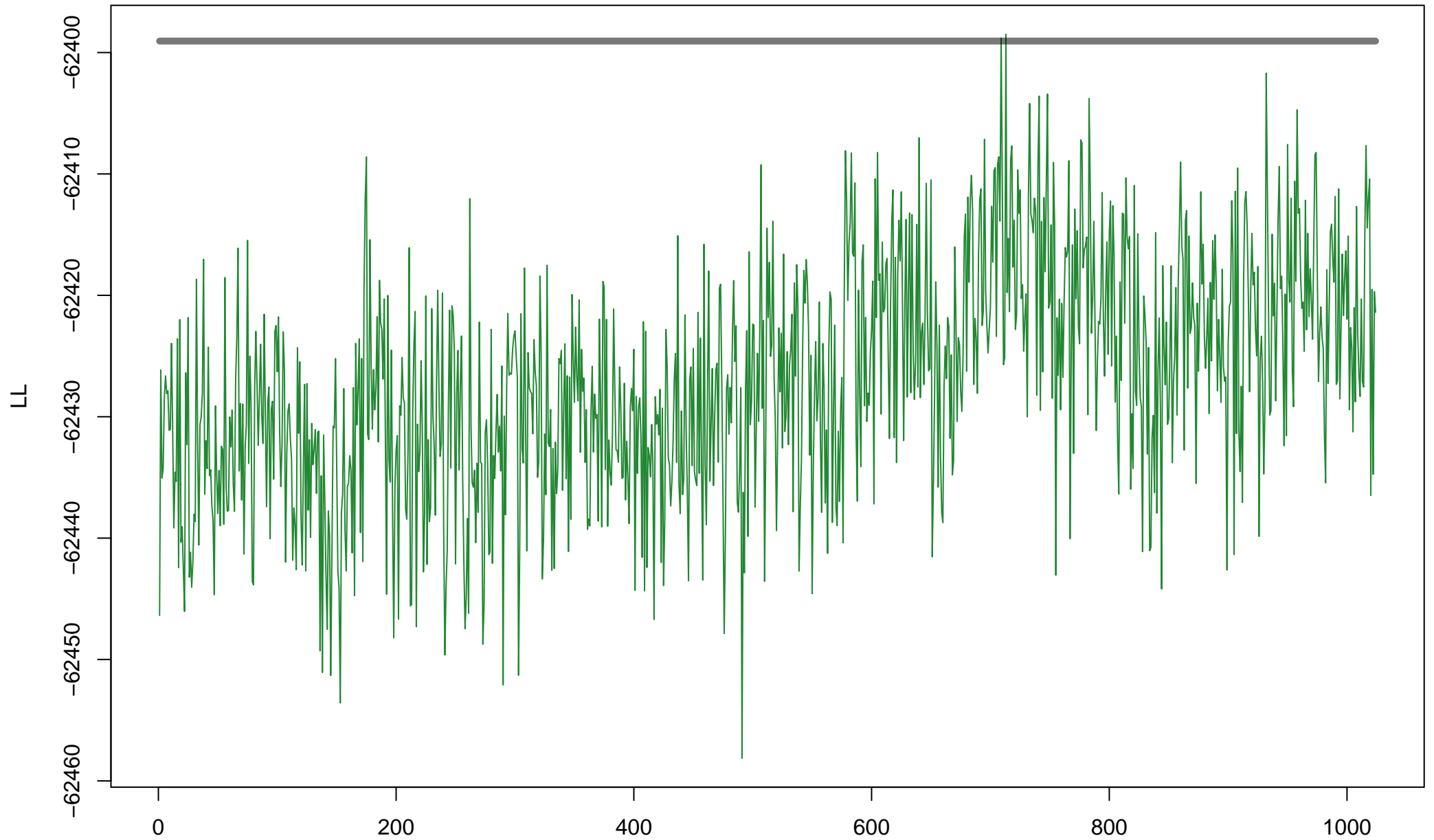






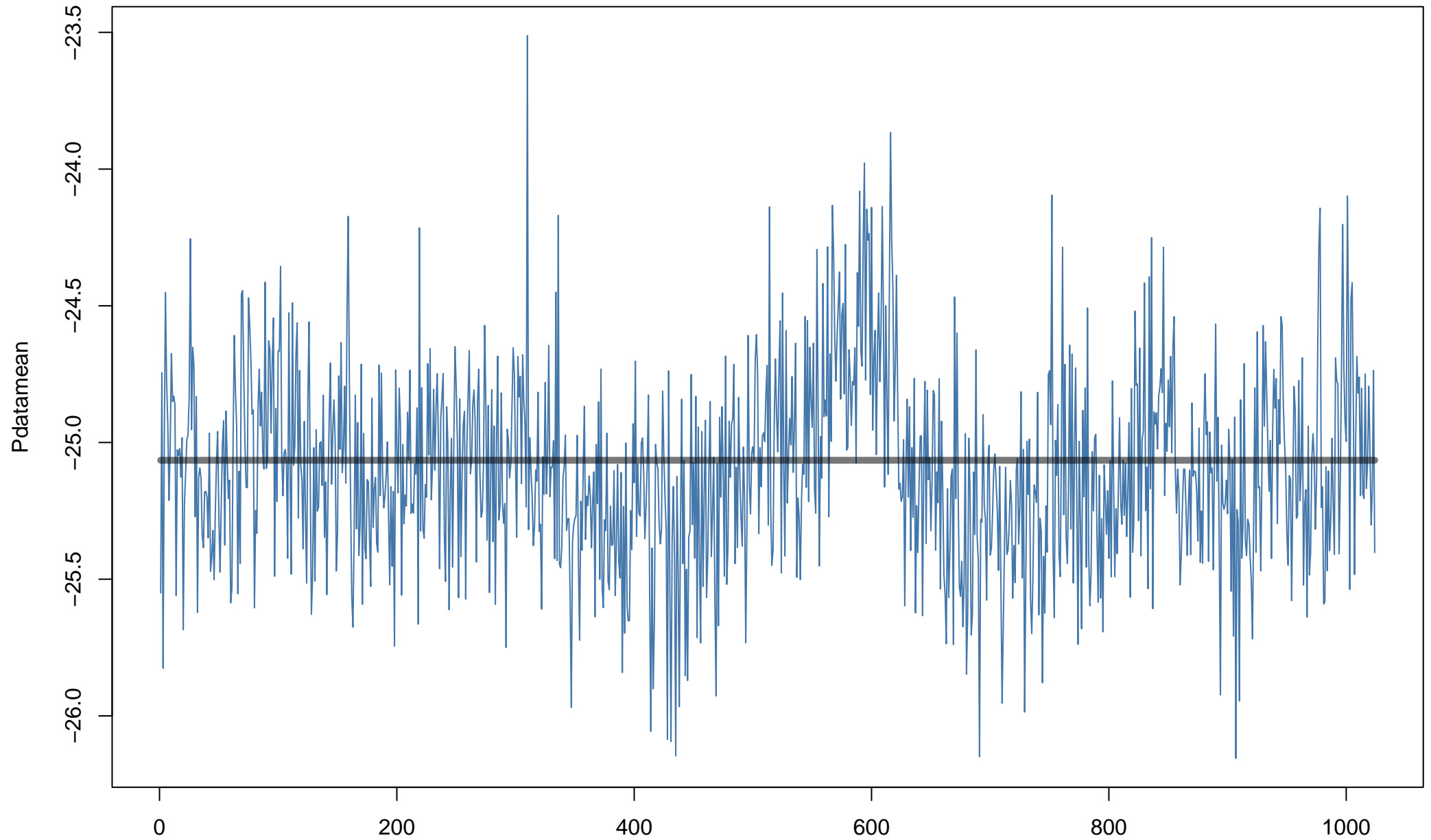


LL



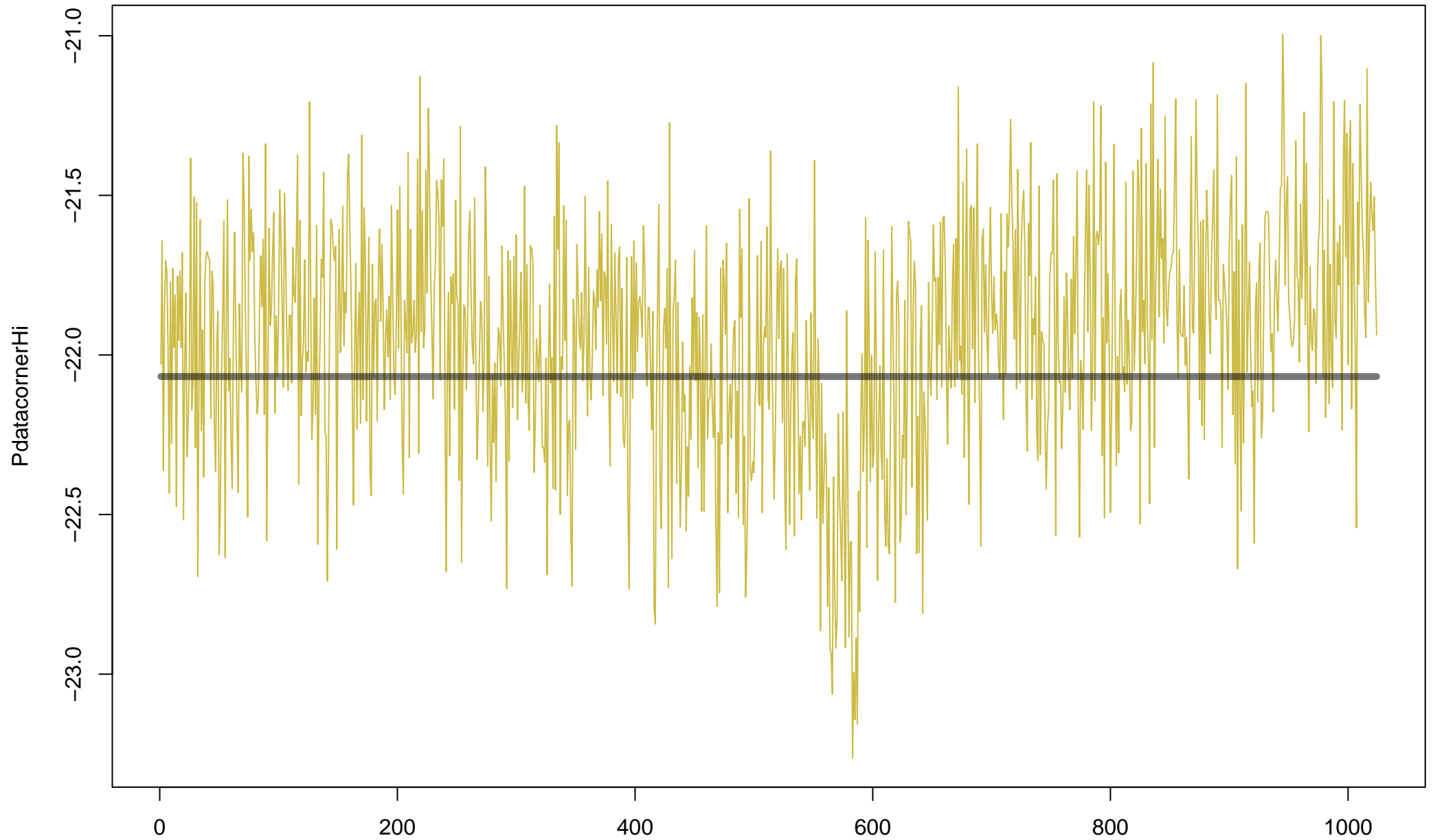
Pdatamean

ESS = 2.22e-16 | BMK = 0.124 | MCSE(6.27) = 8.21 | stat: TRUE | burn: 0 | percentile: 56.9



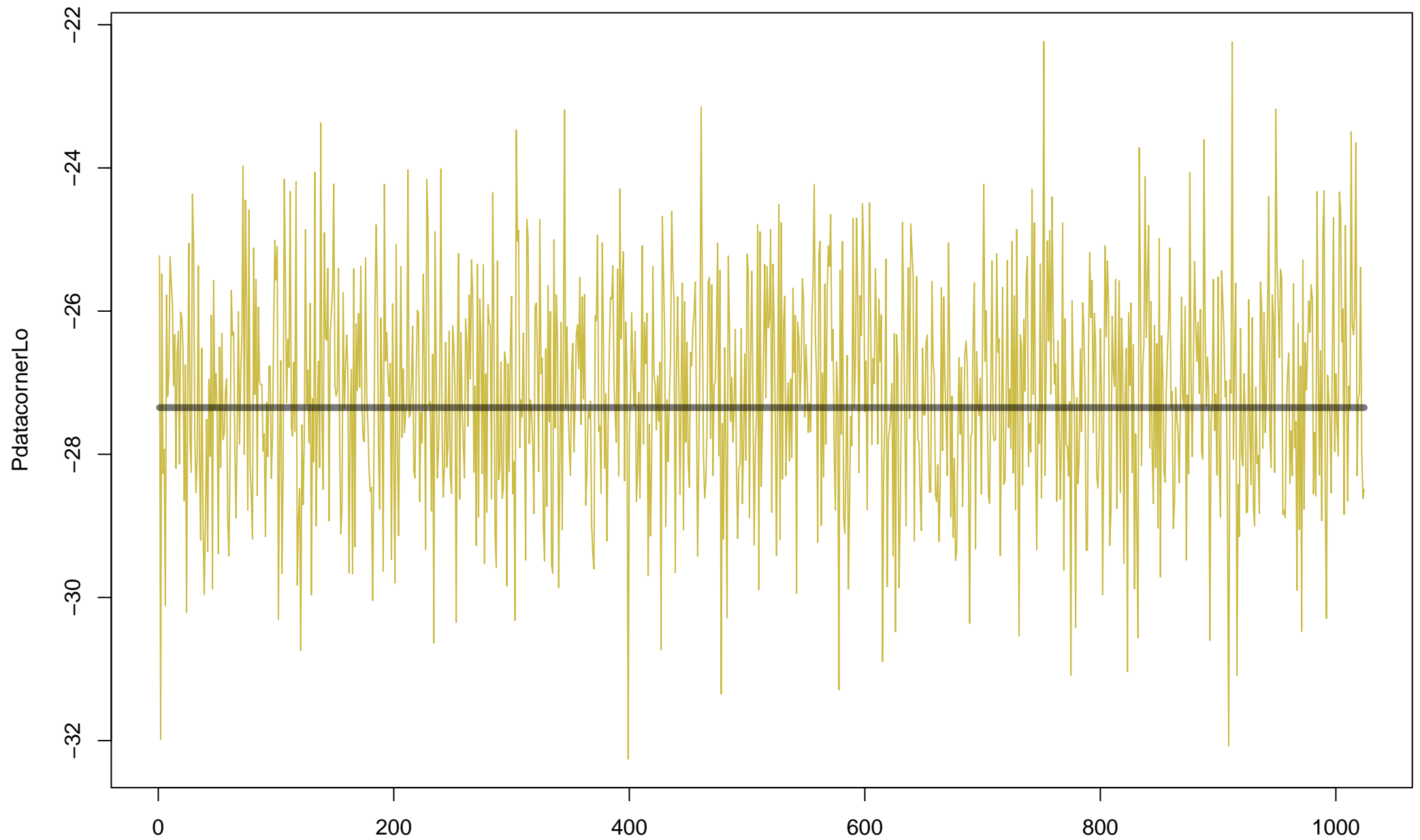
PdatacornerHi

ESS = 2.22e-16 | BMK = 0.104 | MCSE(6.27) = 7.77 | stat: TRUE | burn: 0 | percentile: 35.5

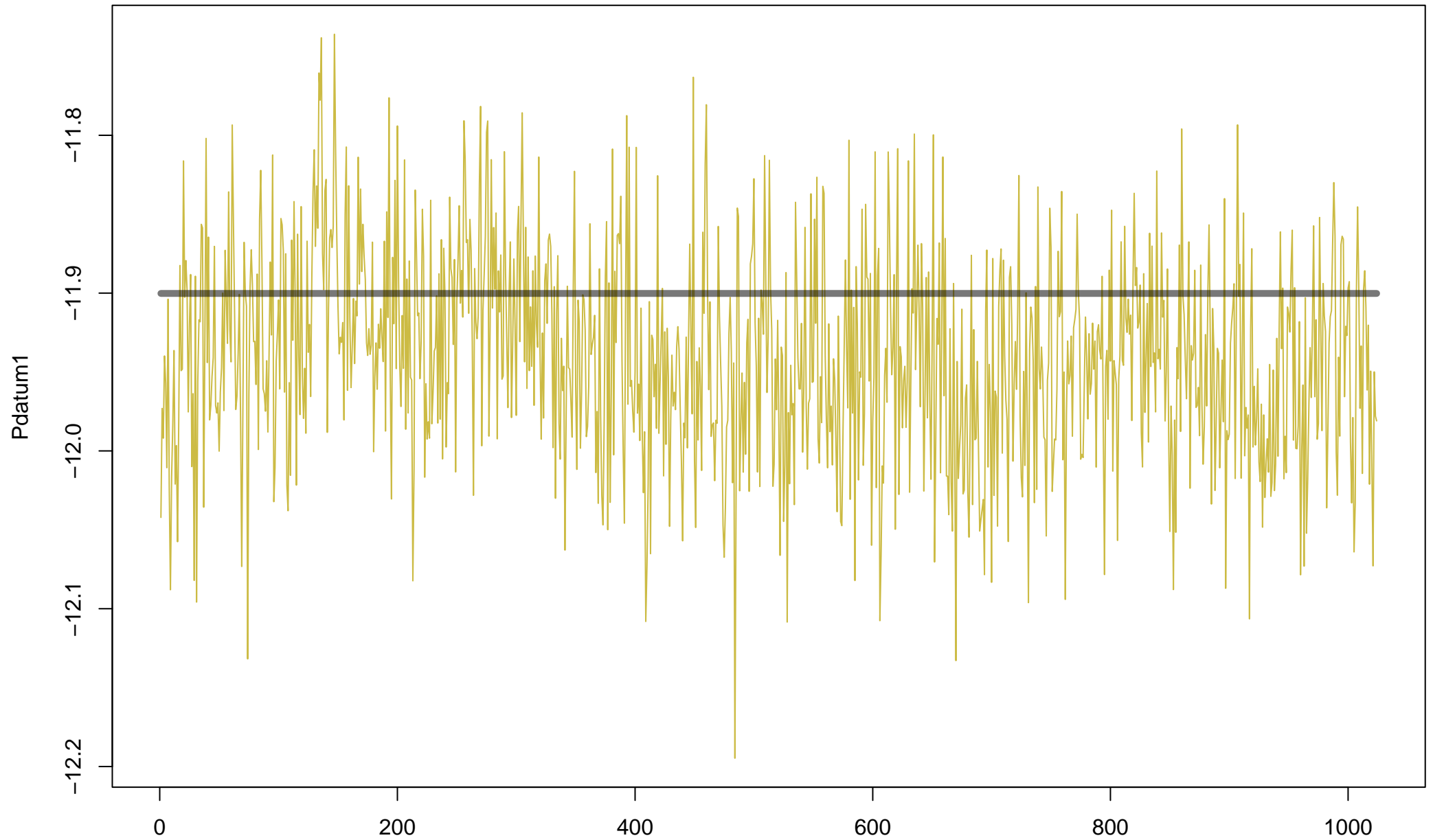


PdatacornerLo

ESS = 2.22e-16 | BMK = 0.112 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | percentile: 44.2

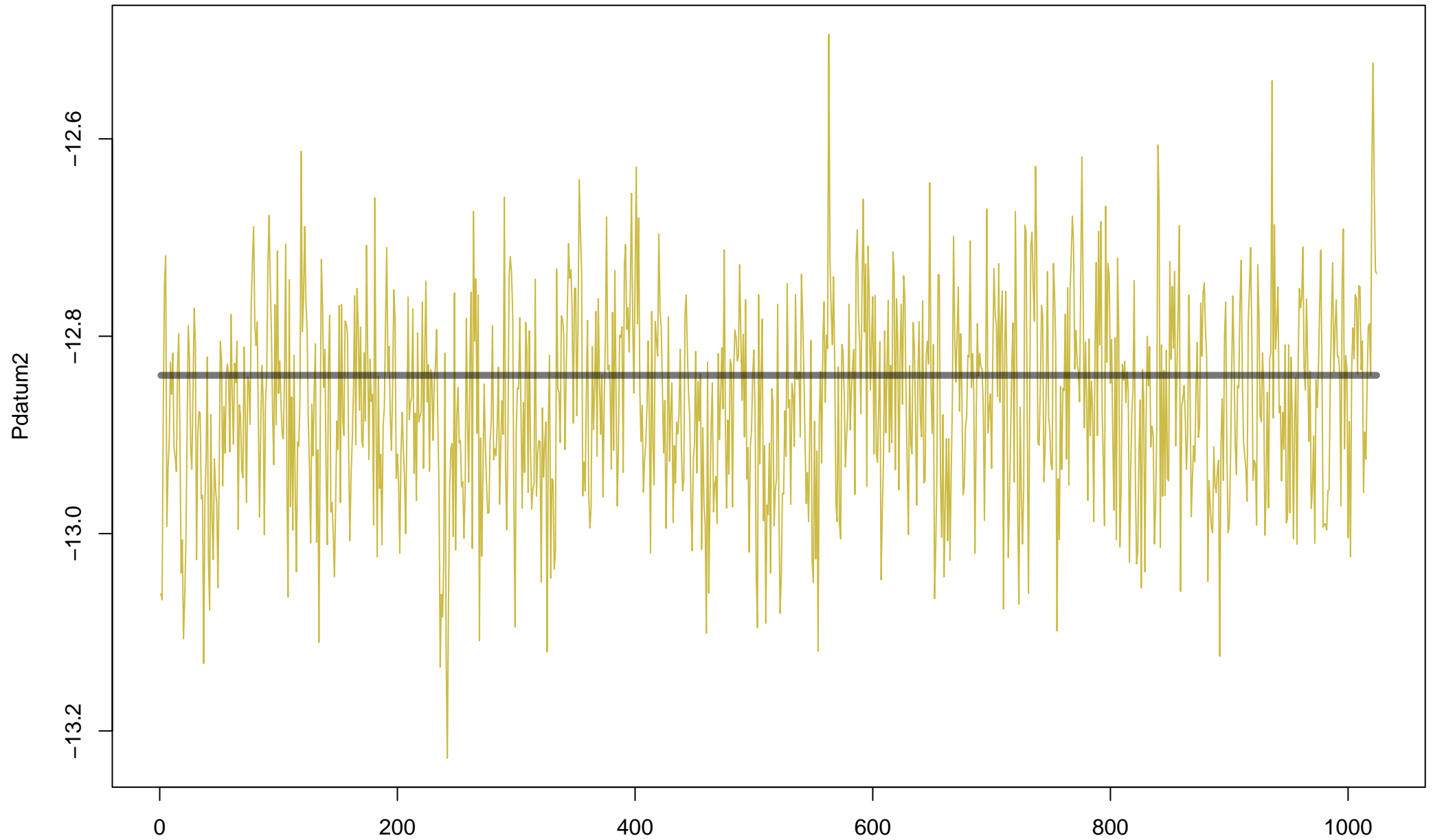


Pdatum1
ESS = 229 | BMK = 0.135 | MCSE(6.27) = 6.48 | stat: TRUE | burn: 0 | percentile: 73



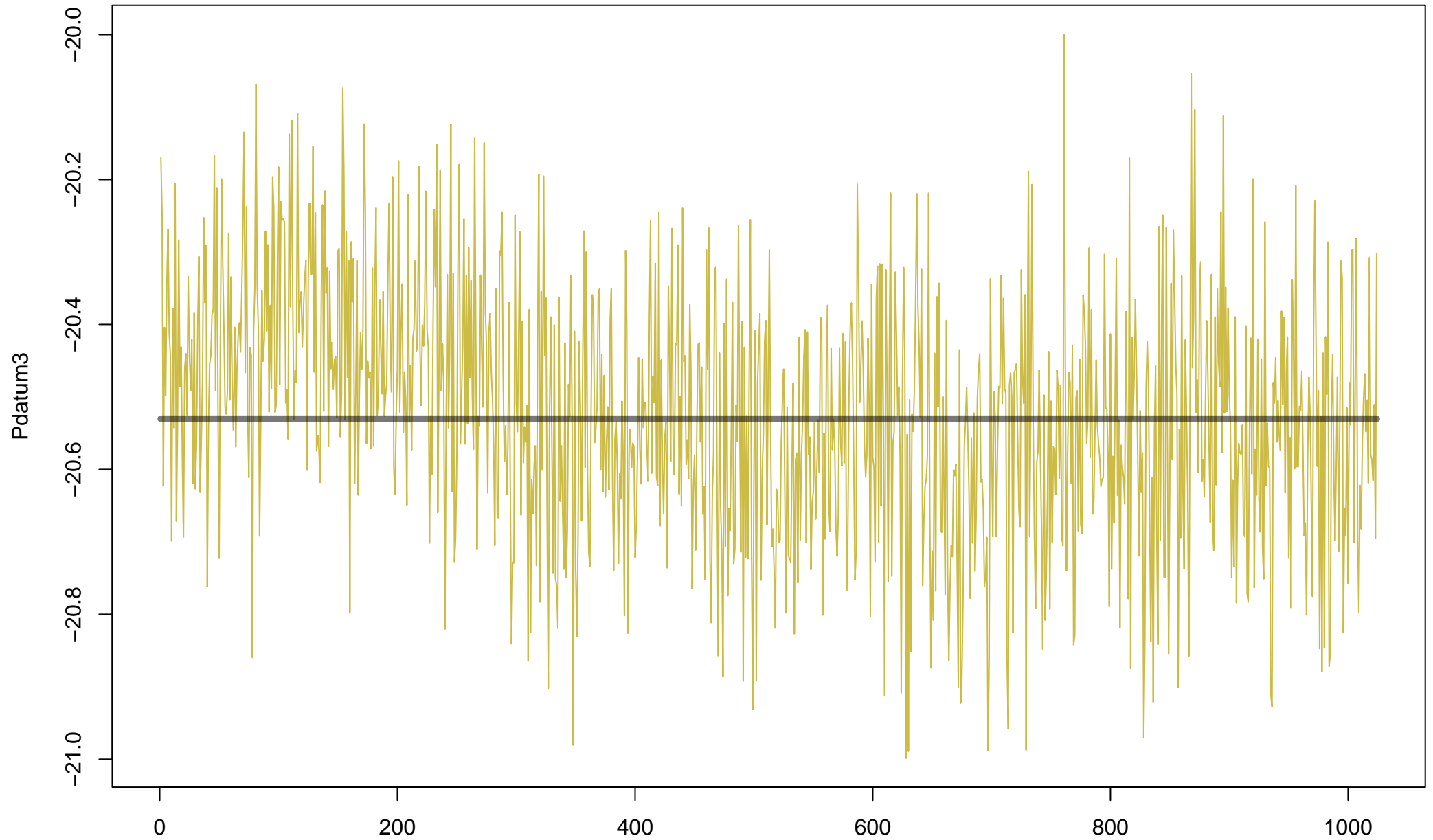
Pdatum2

ESS = 344 | BMK = 0.0957 | MCSE(6.27) = 5.14 | stat: TRUE | burn: 0 | percentile: 60.8



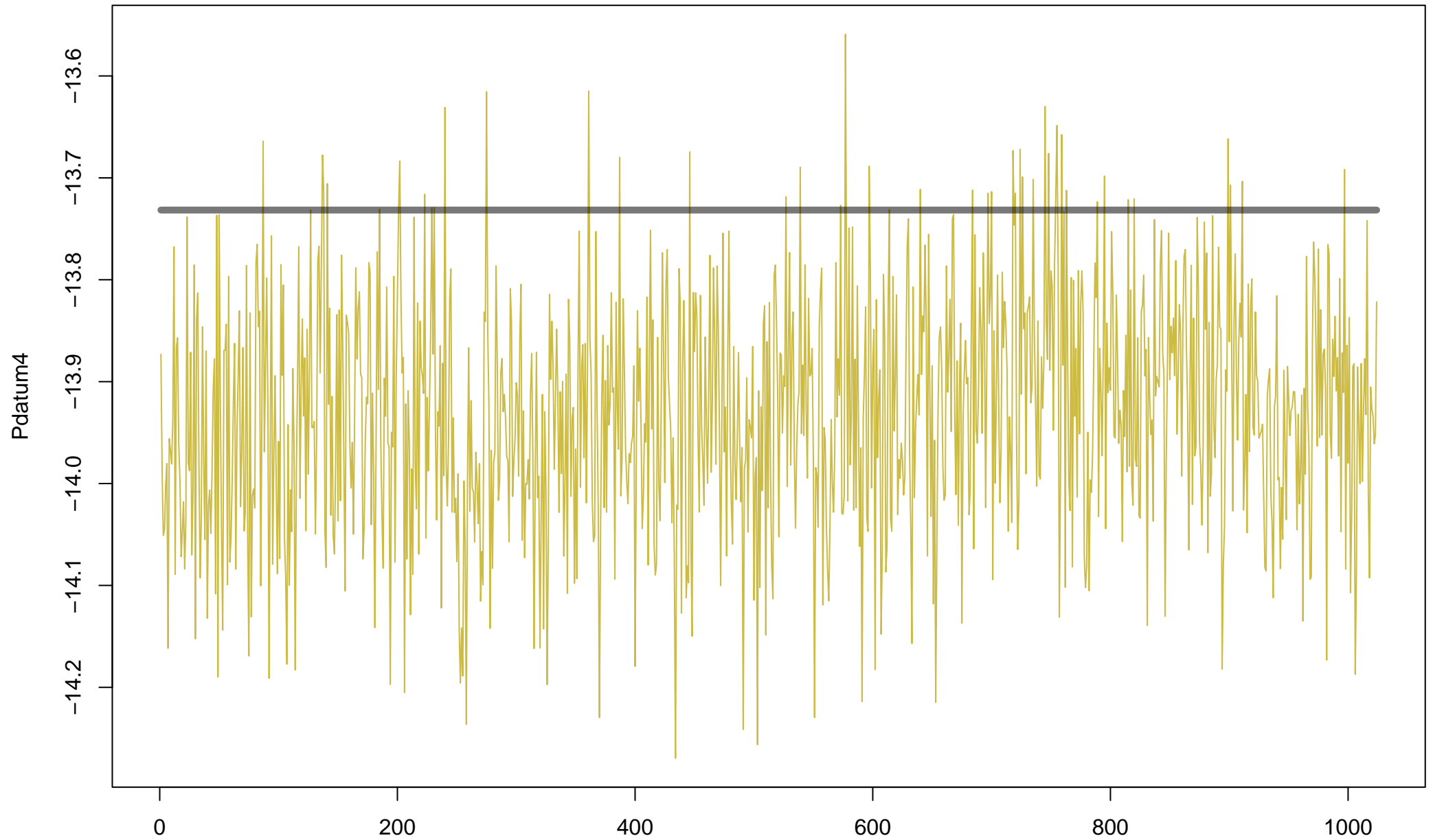
Pdatum3

ESS = 2.22e-16 | BMK = 0.177 | MCSE(6.27) = 7.47 | stat: TRUE | burn: 0 | percentile: 47.9



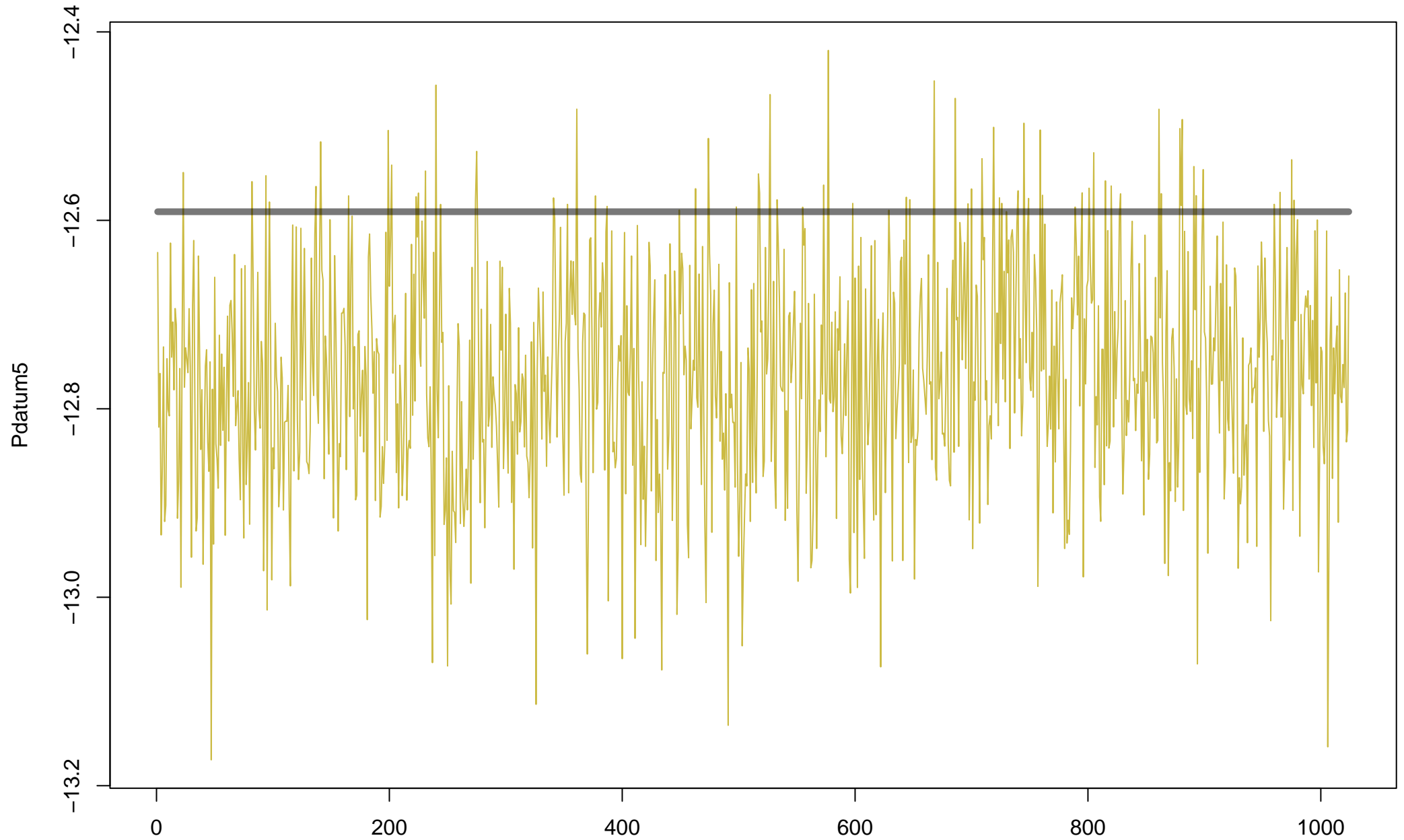
Pdatum4

ESS = 554 | BMK = 0.115 | MCSE(6.27) = 4.95 | stat: FALSE | burn: 0 | percentile: 95.7



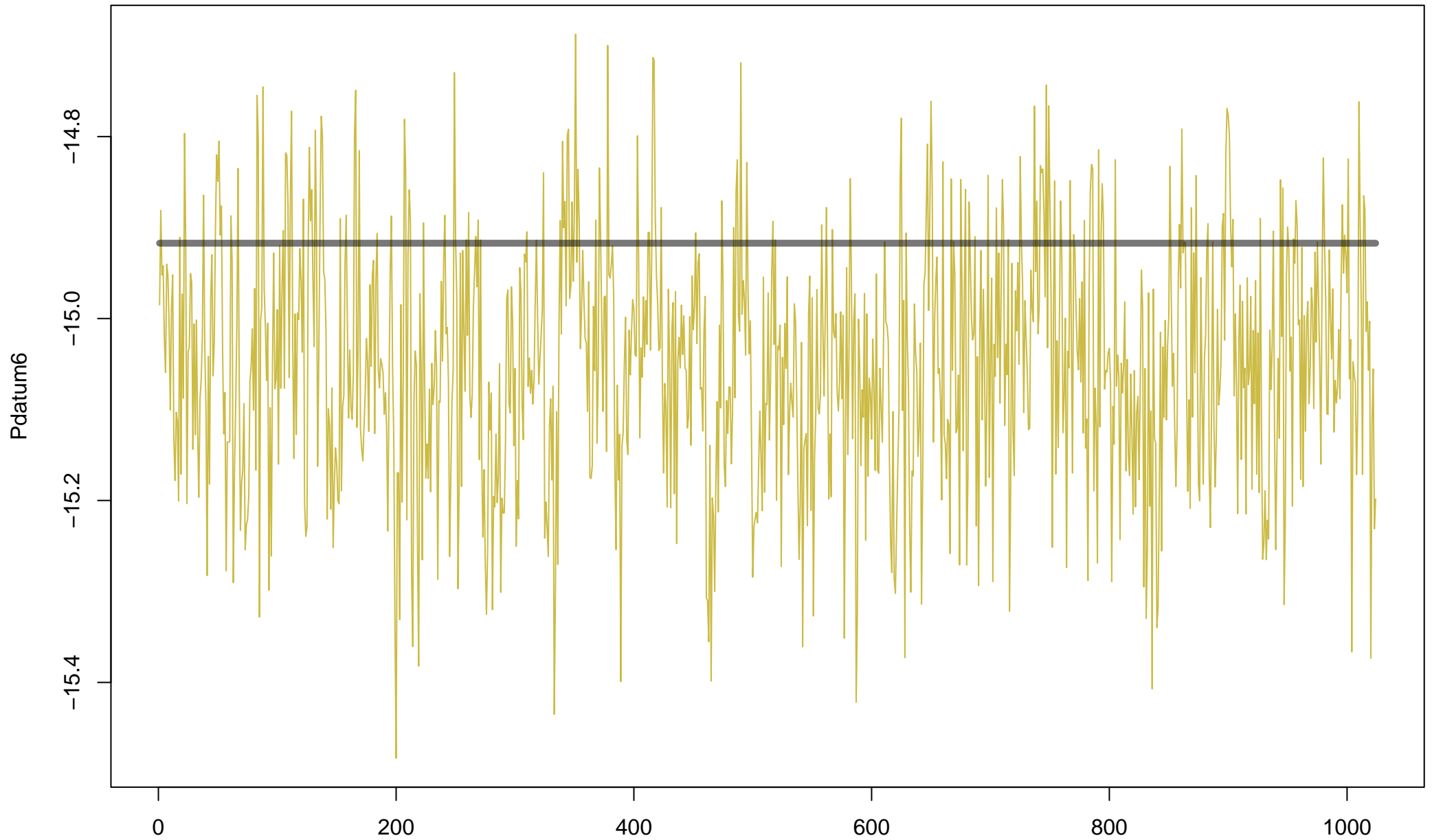
Pdatum5

ESS = 606 | BMK = 0.0919 | MCSE(6.27) = 4.41 | stat: FALSE | burn: 0 | percentile: 93.3



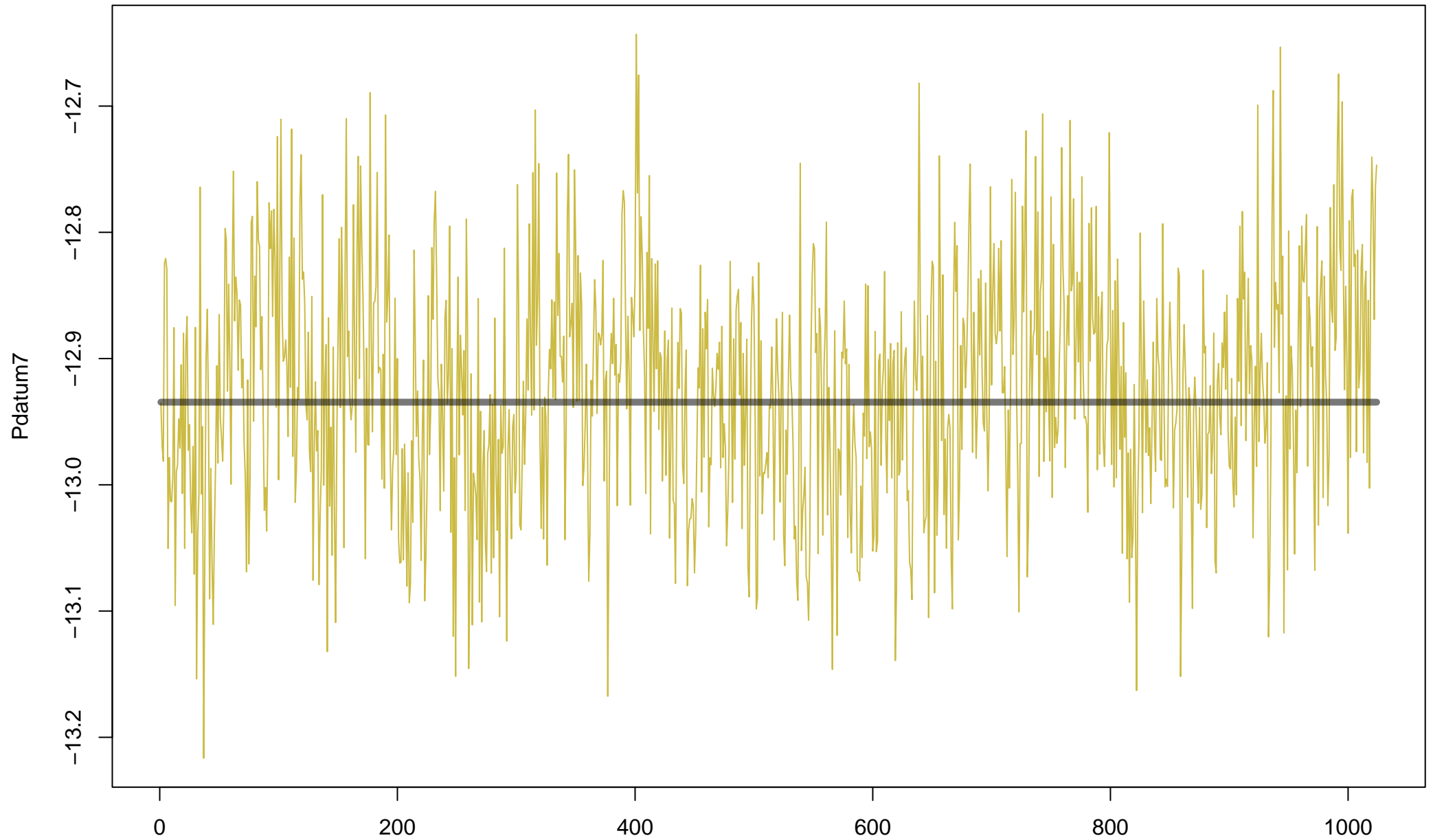
Pdatum6

ESS = 312 | BMK = 0.0514 | MCSE(6.27) = 4.72 | stat: TRUE | burn: 0 | percentile: 83.6



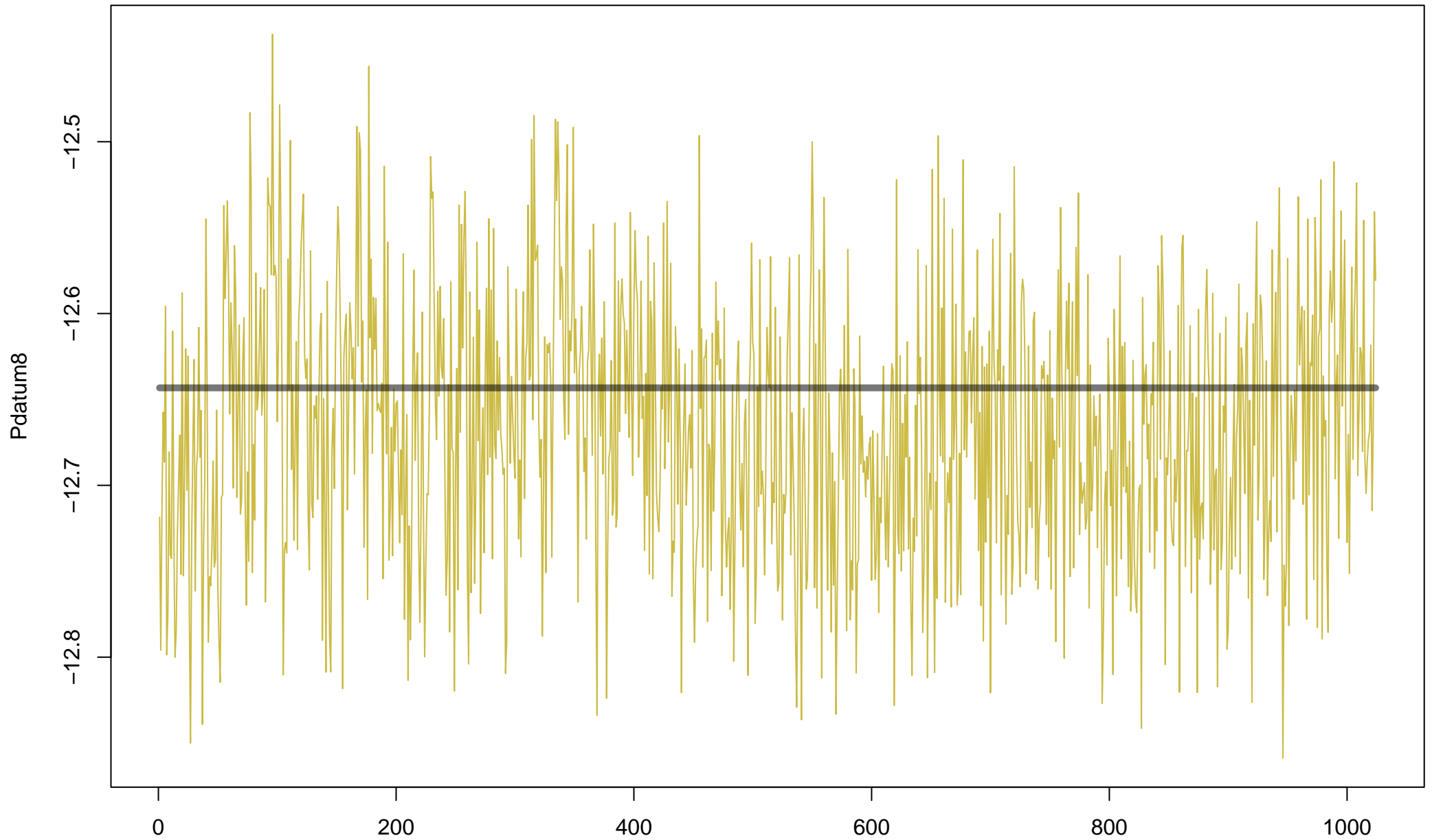
Pdatum7

ESS = 122 | BMK = 0.0334 | MCSE(6.27) = 7.21 | stat: TRUE | burn: 0 | percentile: 46.4



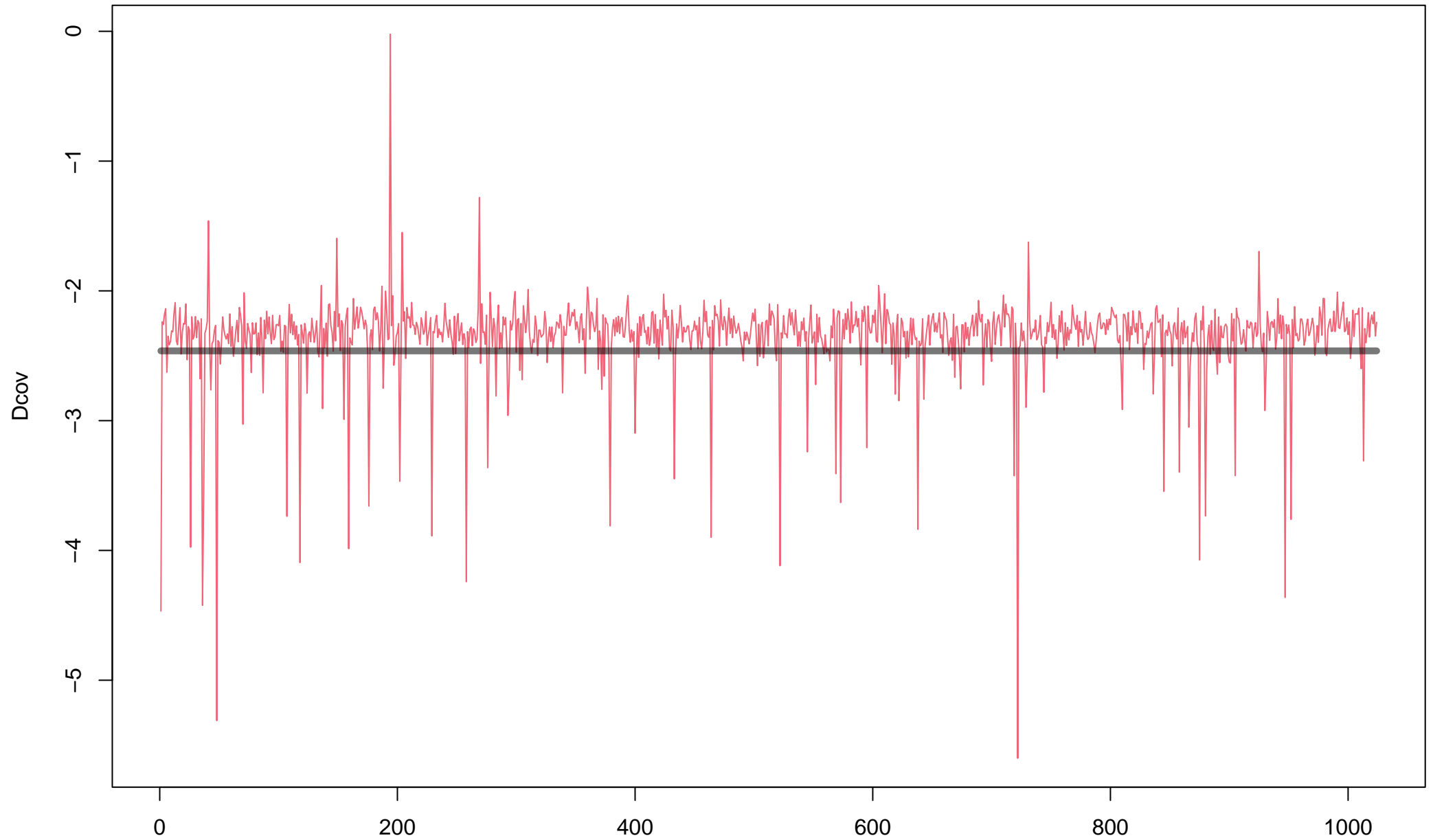
Pdatum8

ESS = 168 | BMK = 0.0941 | MCSE(6.27) = 5.65 | stat: TRUE | burn: 0 | percentile: 61.3



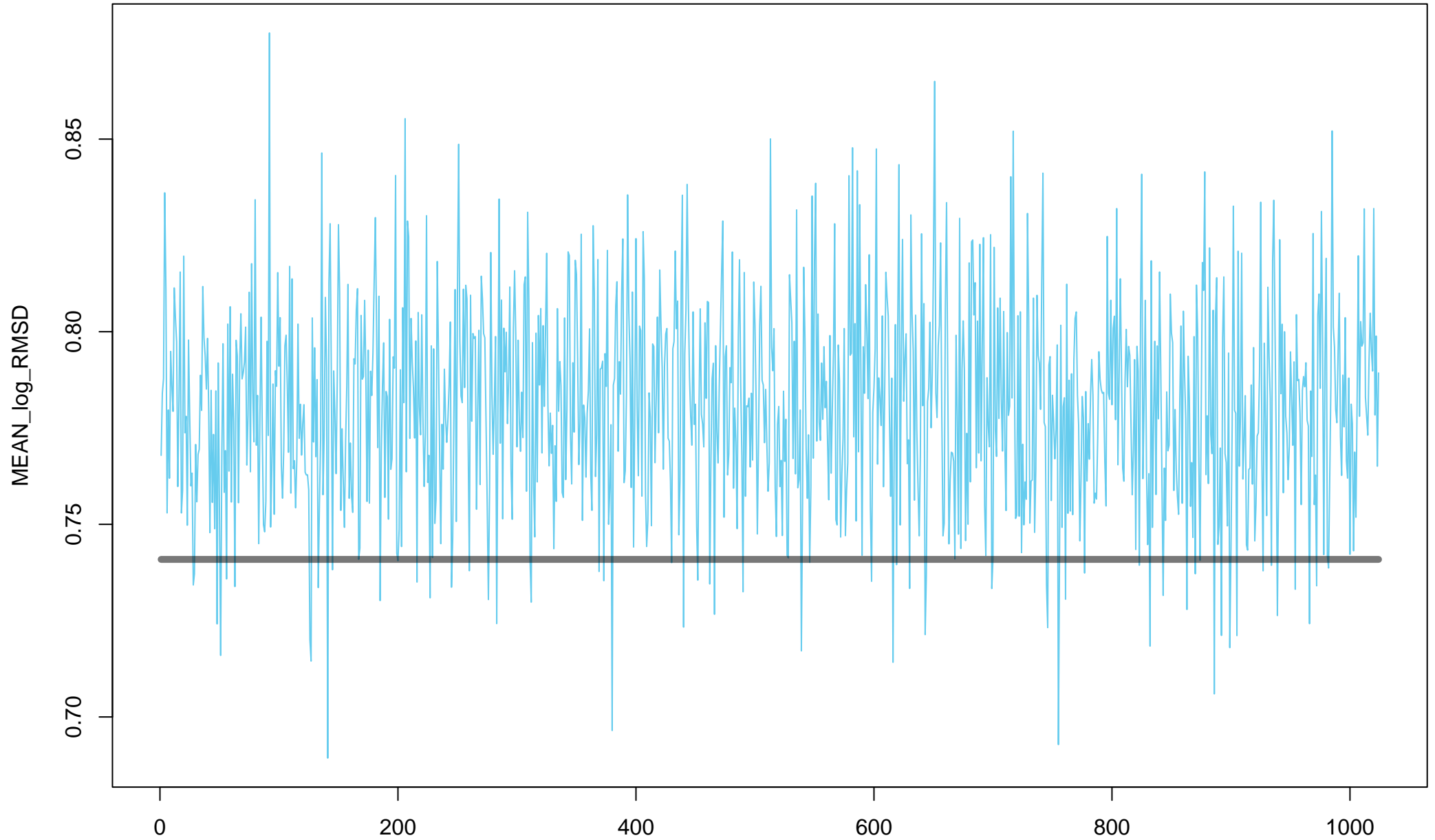
Dcov

ESS = 1020 | BMK = 0.103 | MCSE(6.27) = 3.42 | stat: TRUE | burn: 0 | percentile: 85.8

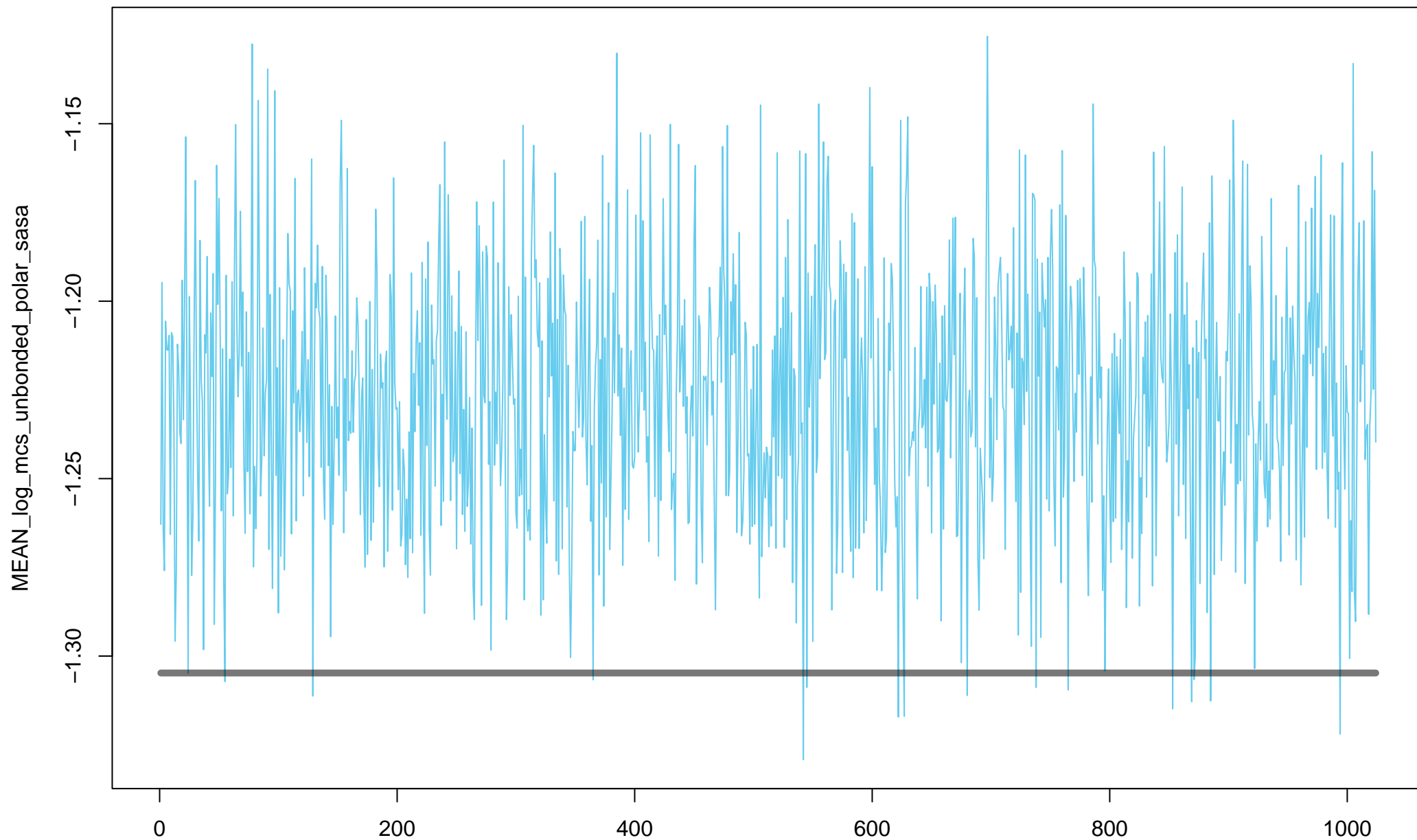


MEAN_log_RMSD

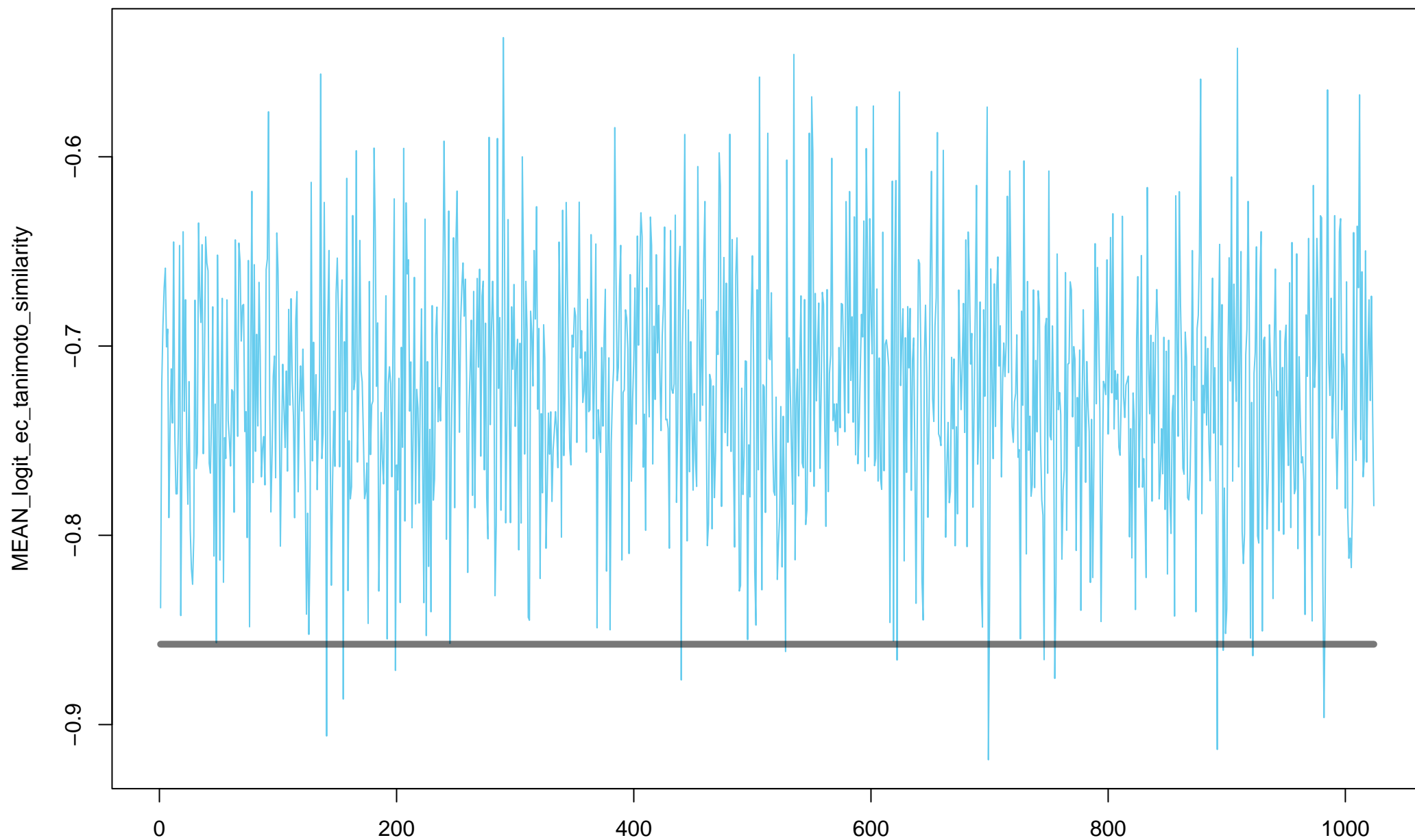
ESS = 1020 | BMK = 0.0615 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0 | percentile: 5.96



MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0688 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0 | percentile: 1.56

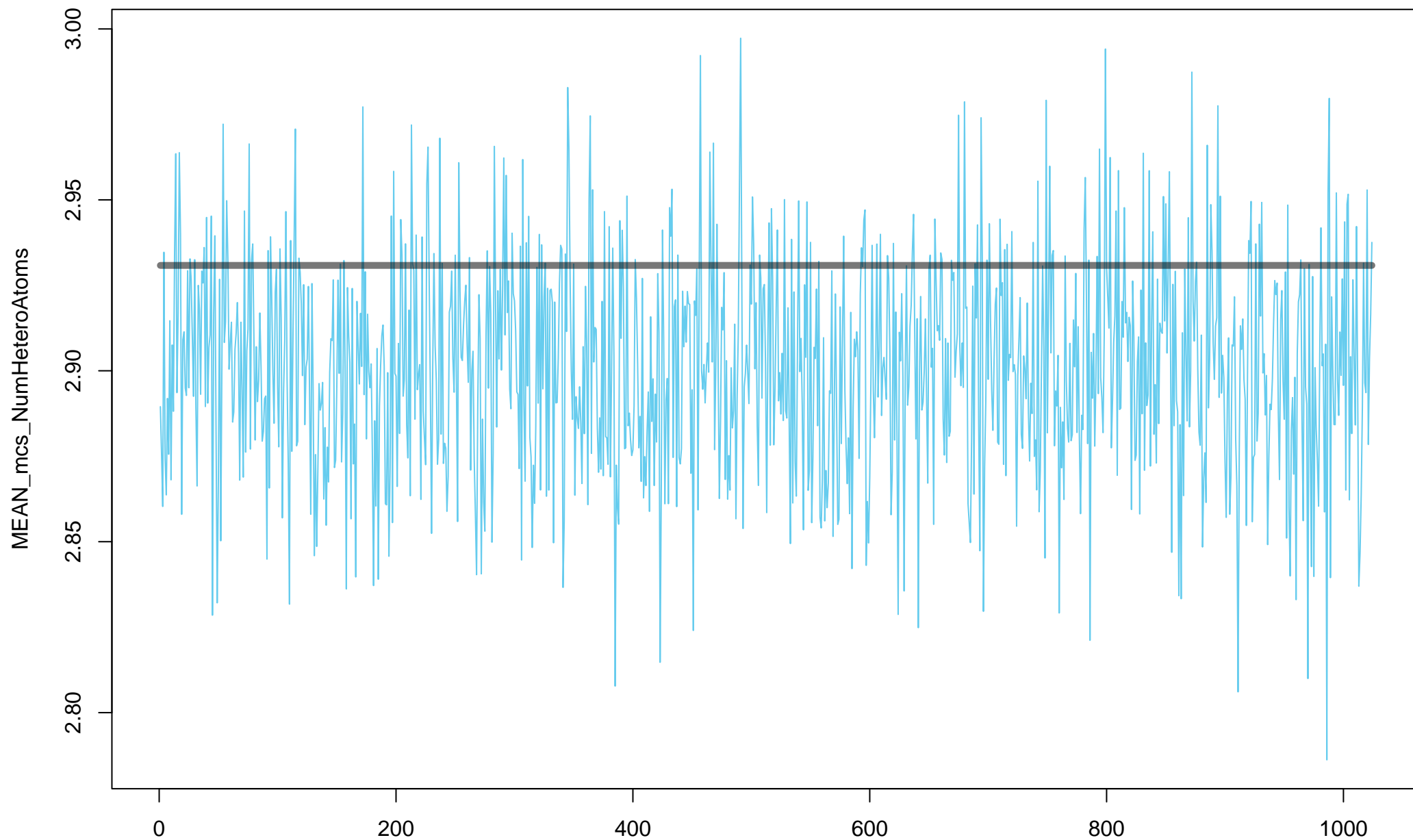


MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0424 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | percentile: 1.27



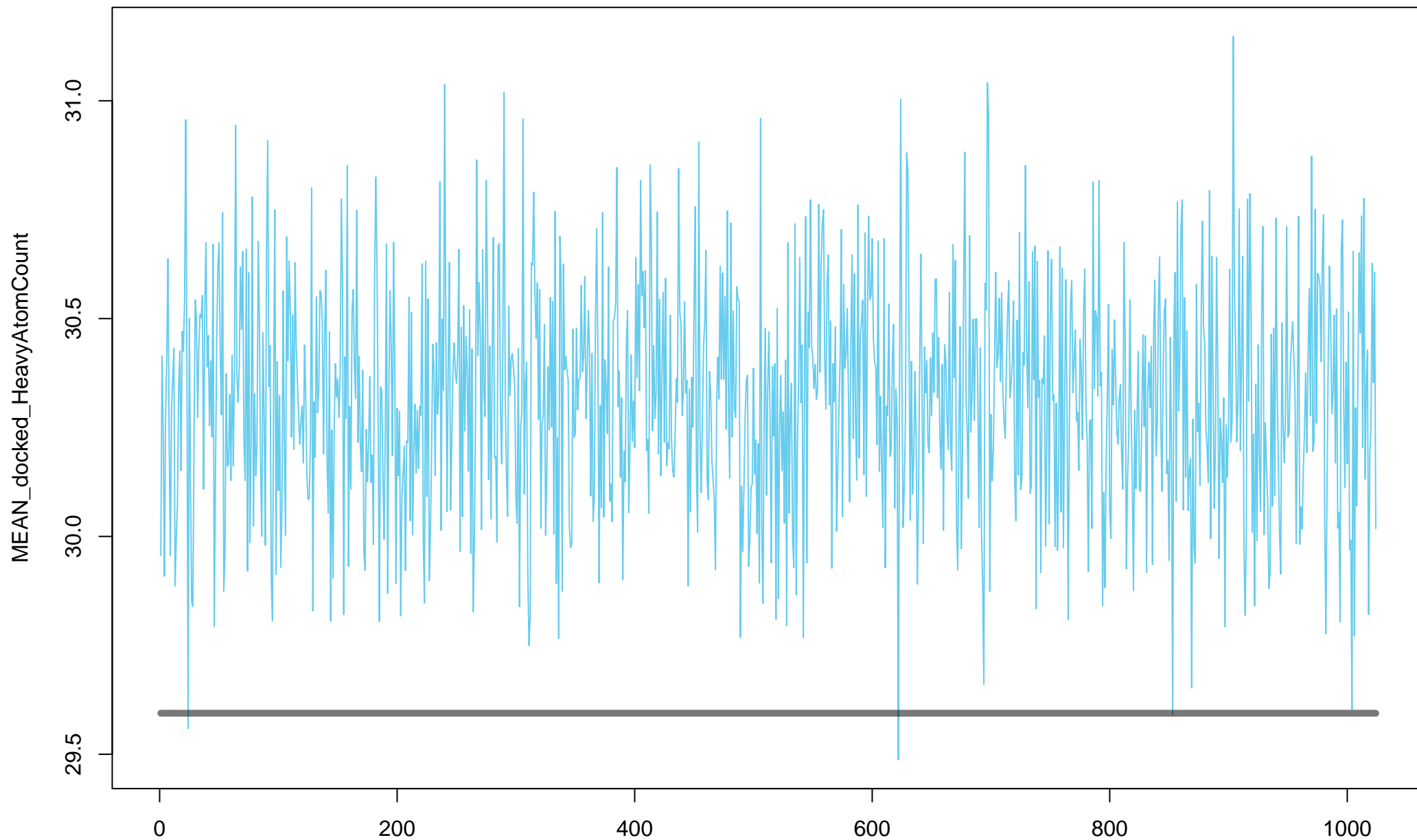
MEAN_mcs_NumHeteroAtoms

ESS = 1020 | BMK = 0.045 | MCSE(6.27) = 3.26 | stat: TRUE | burn: 0 | percentile: 82.7



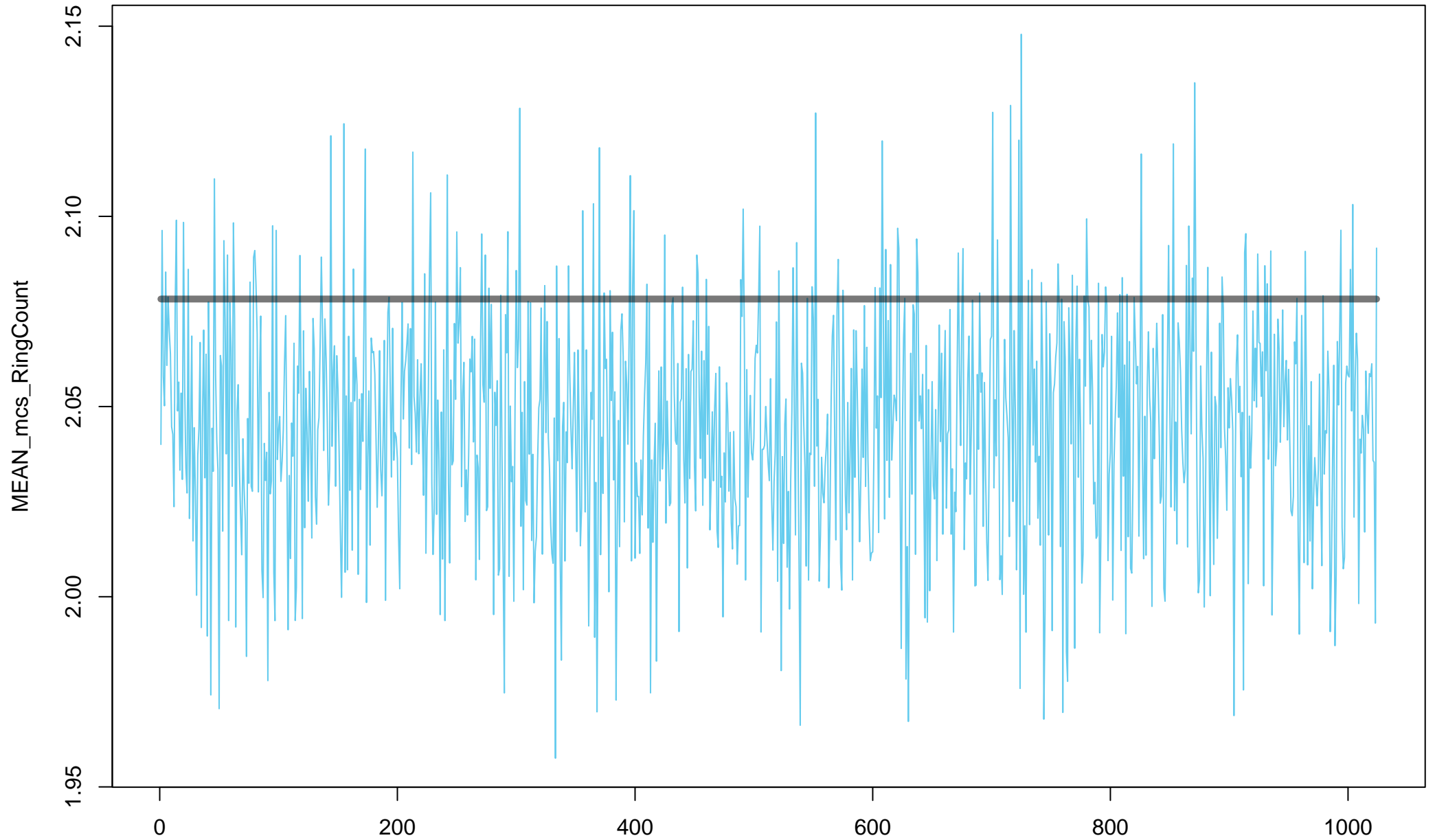
MEAN_docked_HeavyAtomCount

ESS = 1020 | BMK = 0.0431 | MCSE(6.27) = 3.29 | stat: TRUE | burn: 0 | percentile: 0.293



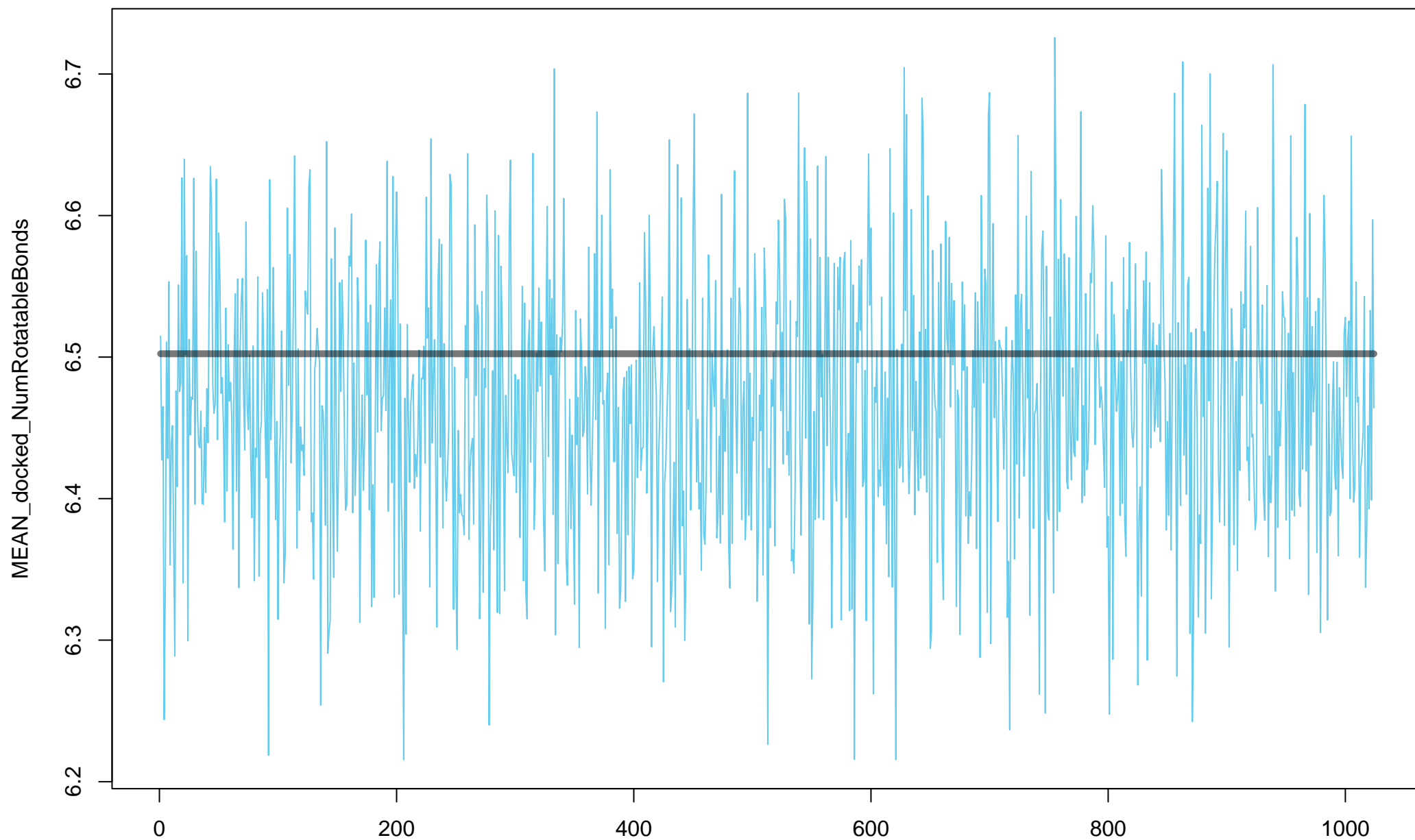
MEAN_mcs_RingCount

ESS = 1020 | BMK = 0.0577 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0 | percentile: 88.2



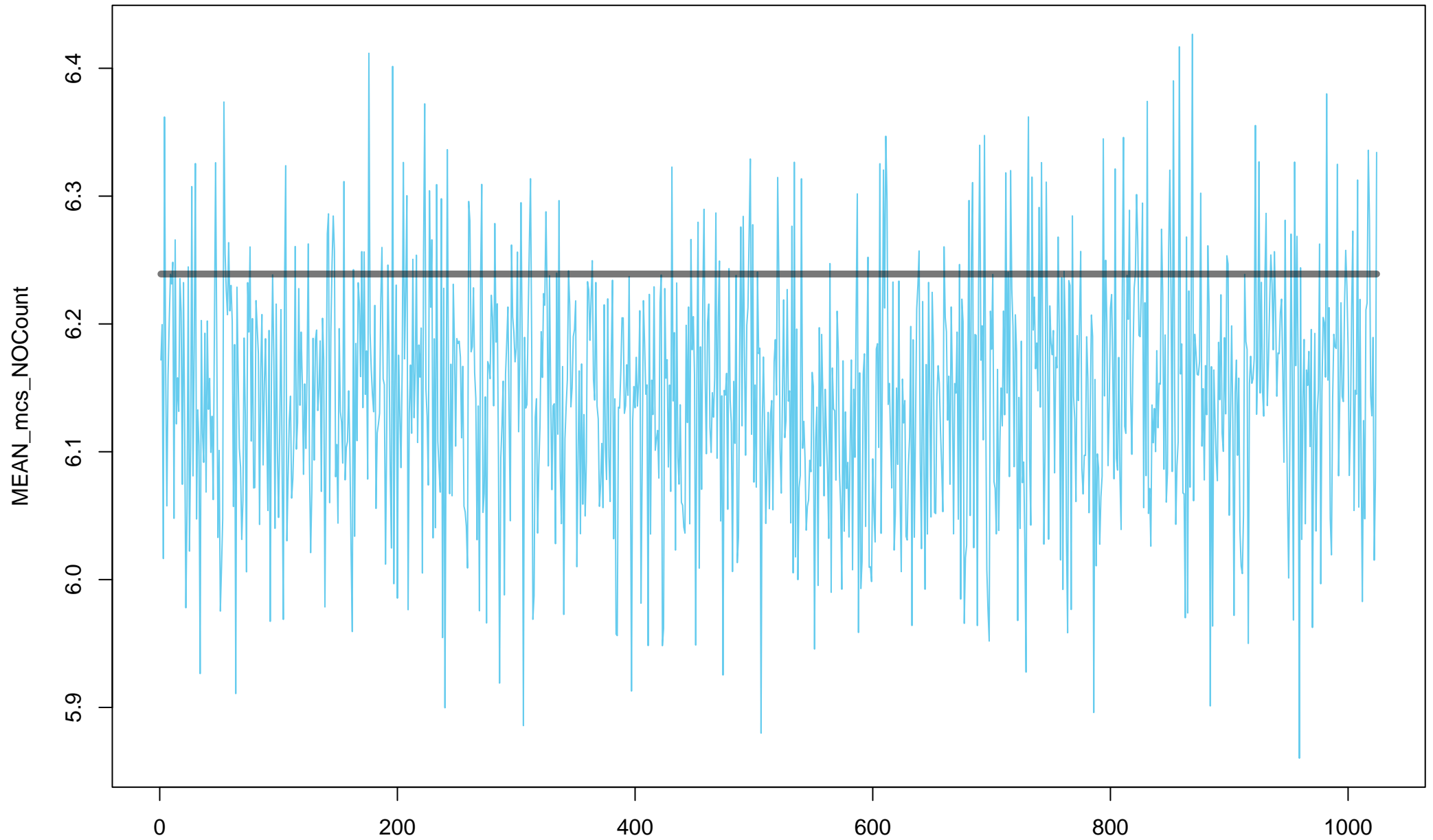
MEAN_docked_NumRotatableBonds

ESS = 1020 | BMK = 0.0686 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0 | percentile: 65.5



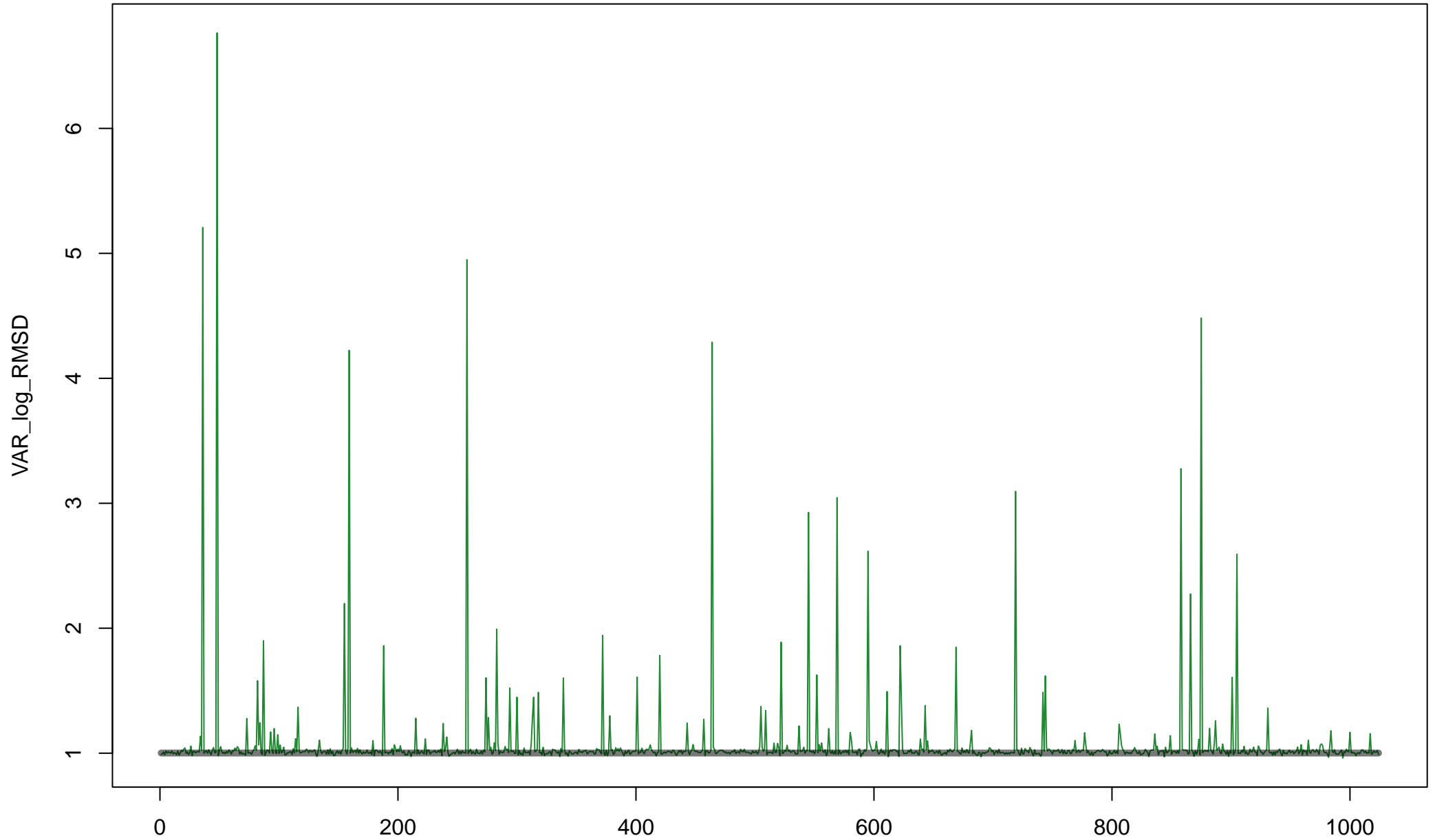
MEAN_mcs_NOCount

ESS = 1020 | BMK = 0.0621 | MCSE(6.27) = 3.21 | stat: TRUE | burn: 0 | percentile: 86.6



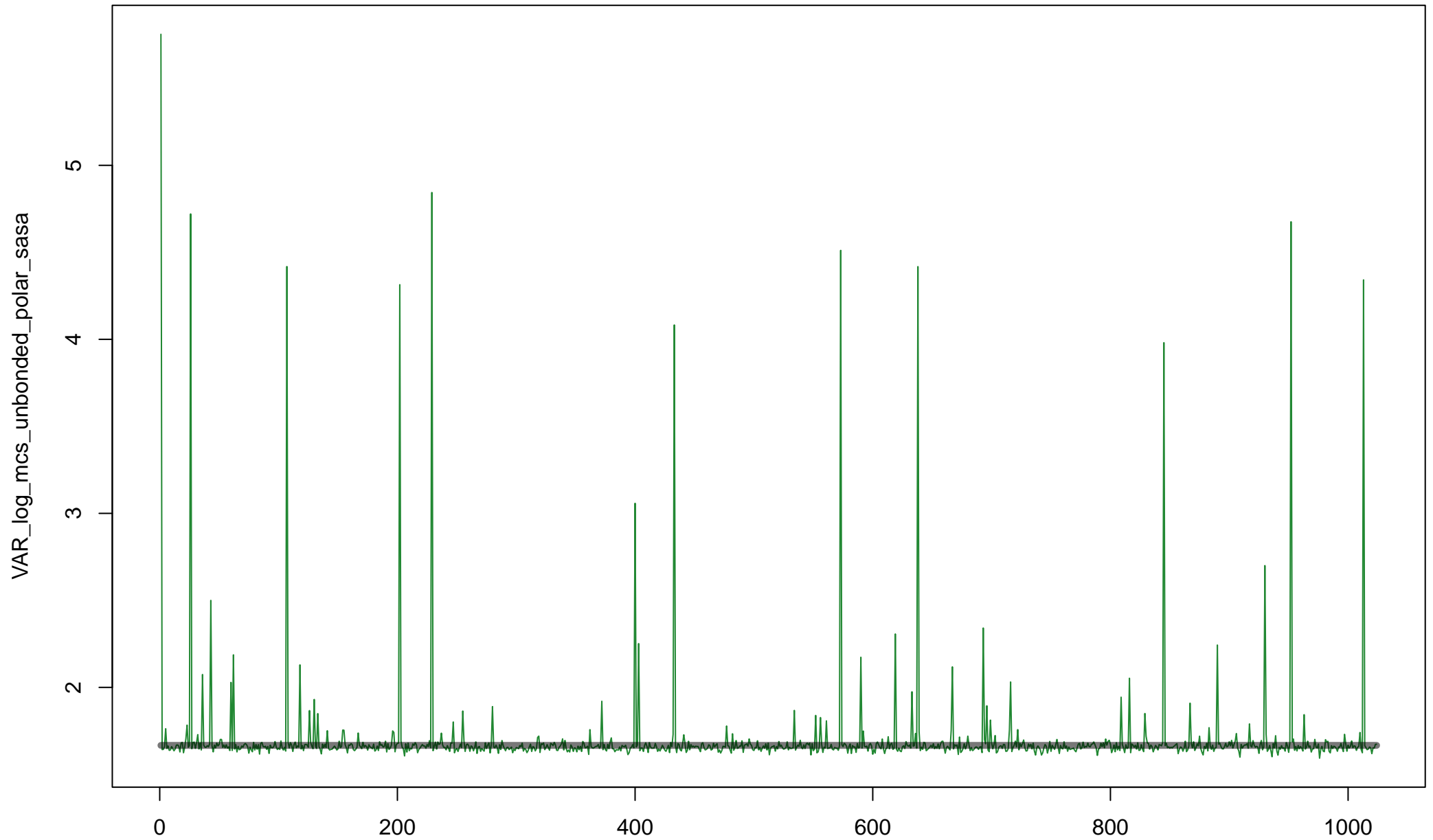
VAR_log_RMSD

ESS = 739 | BMK = 0.808 | MCSE(6.27) = 3.61 | stat: TRUE | burn: 204 | percentile: 28.4



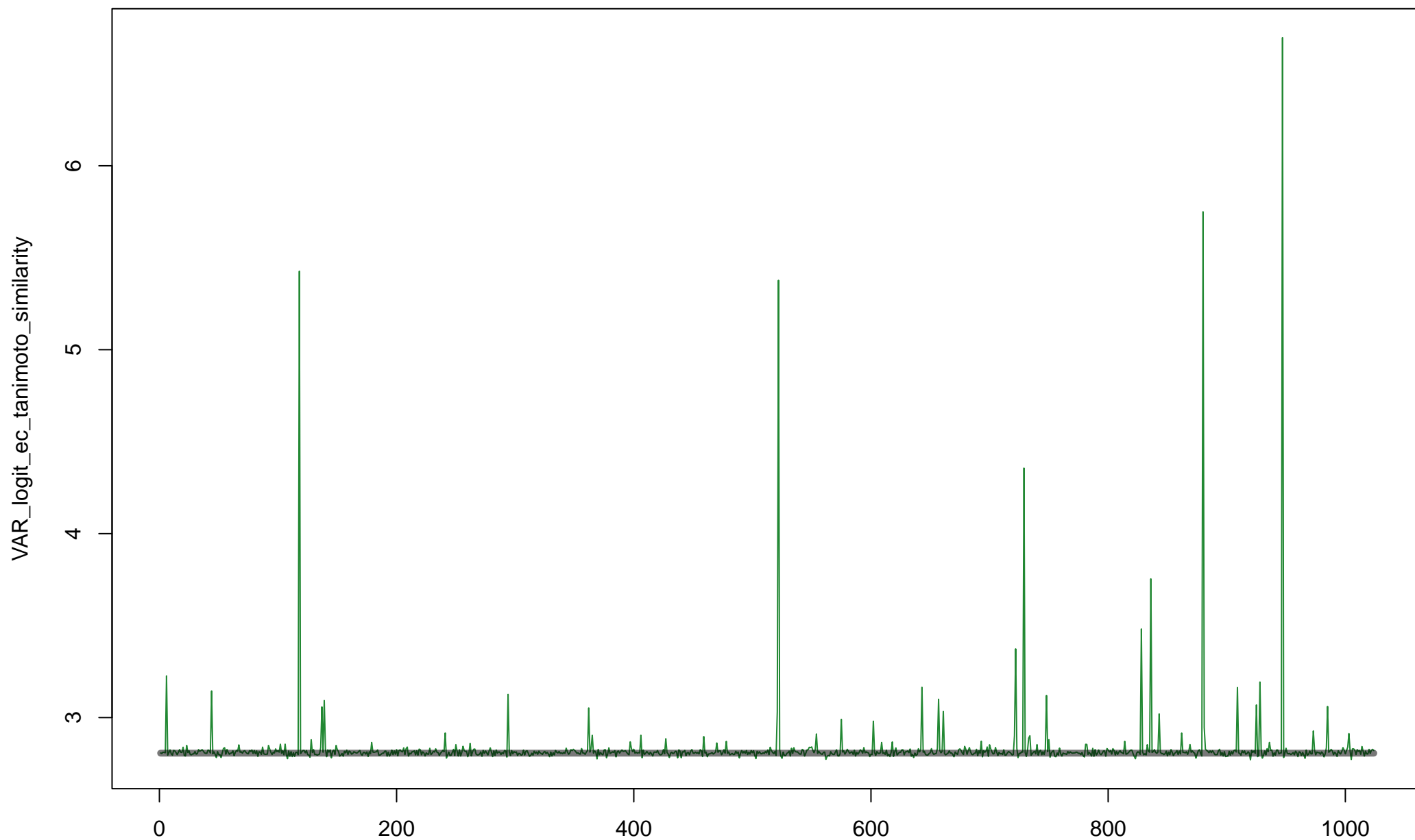
VAR_log_mcs_unbonded_polar_sasa

ESS = 1020 | BMK = 0.342 | MCSE(6.27) = 3.42 | stat: TRUE | burn: 0 | percentile: 65.4

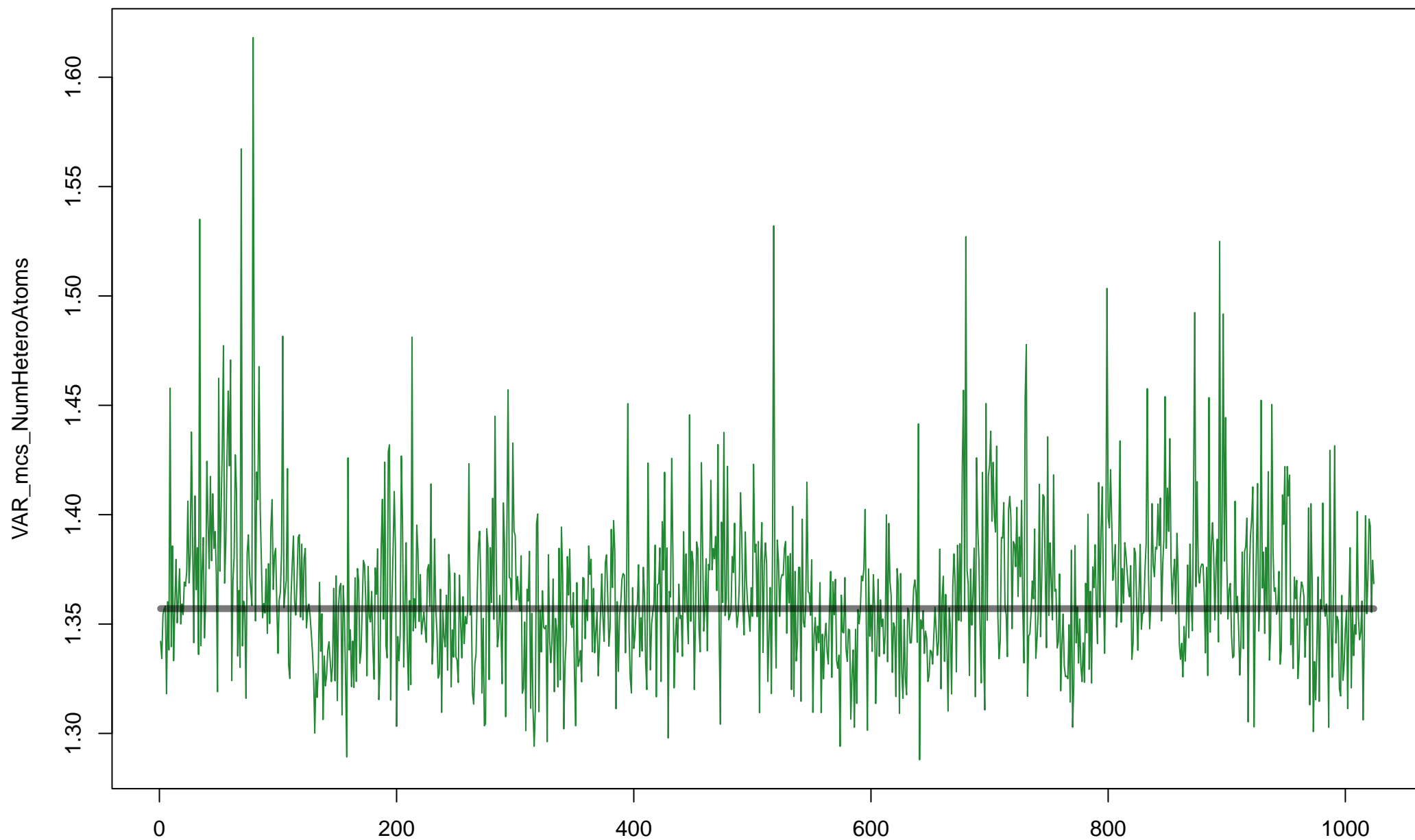


VAR_logit_ec_tanimoto_similarity

ESS = 1020 | BMK = 0.377 | MCSE(6.27) = 3 | stat: TRUE | burn: 1020 | percentile: 40.6

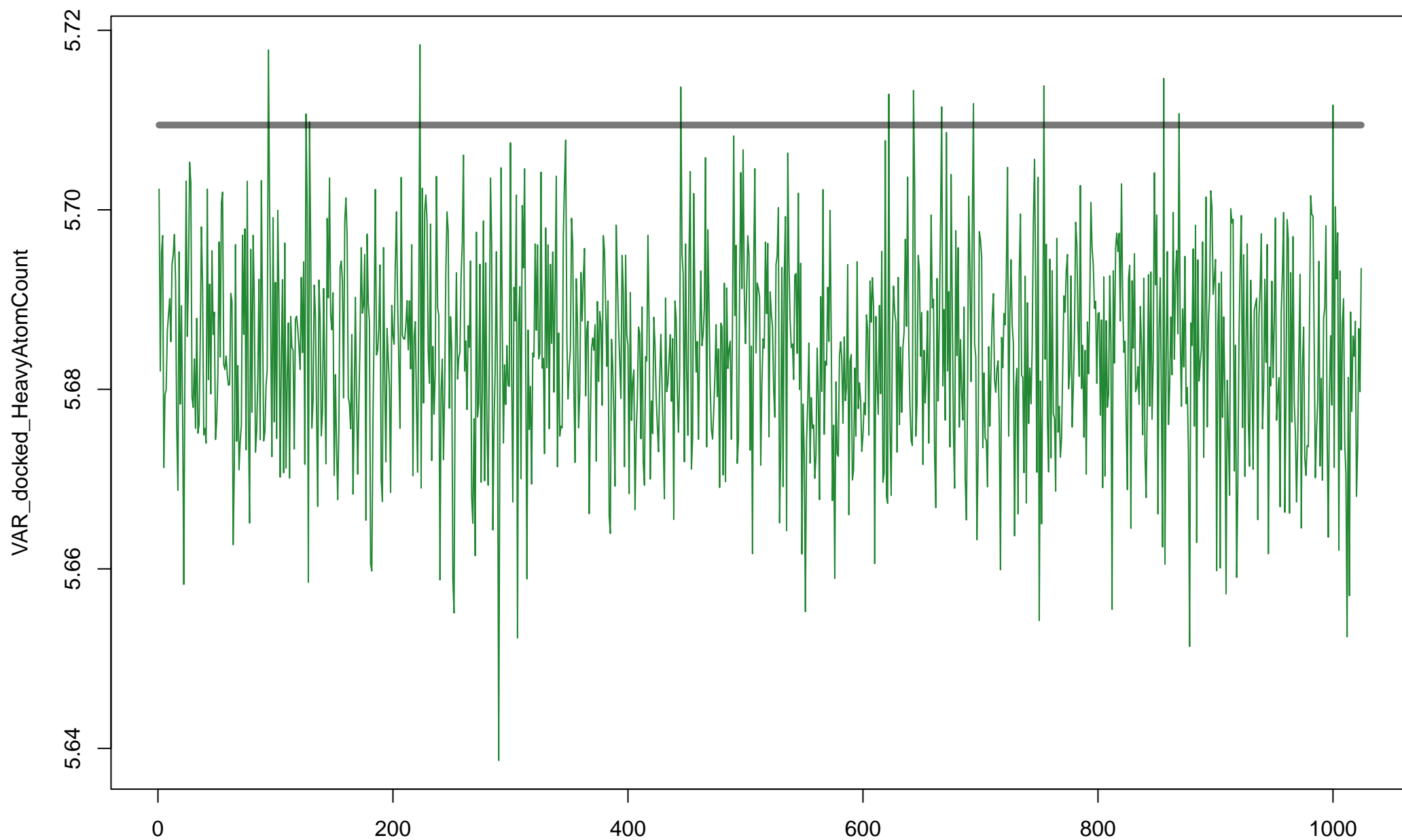


VAR_mcs_NumHeteroAtoms
ESS = 168 | BMK = 0.0805 | MCSE(6.27) = 6.75 | stat: FALSE | burn: 0 | percentile: 46.9

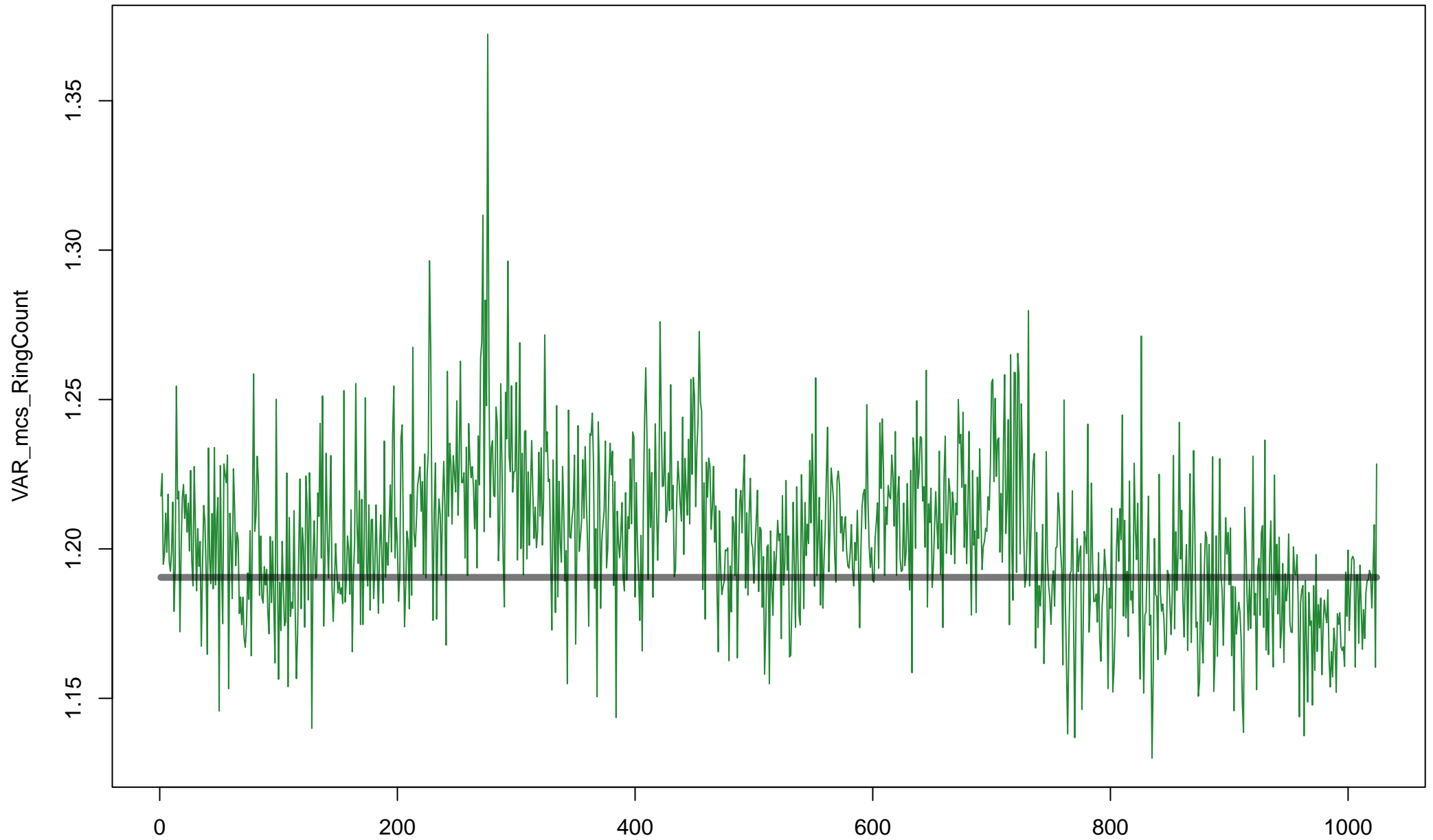


VAR_docked_HeavyAtomCount

ESS = 1020 | BMK = 0.0621 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | percentile: 98.7

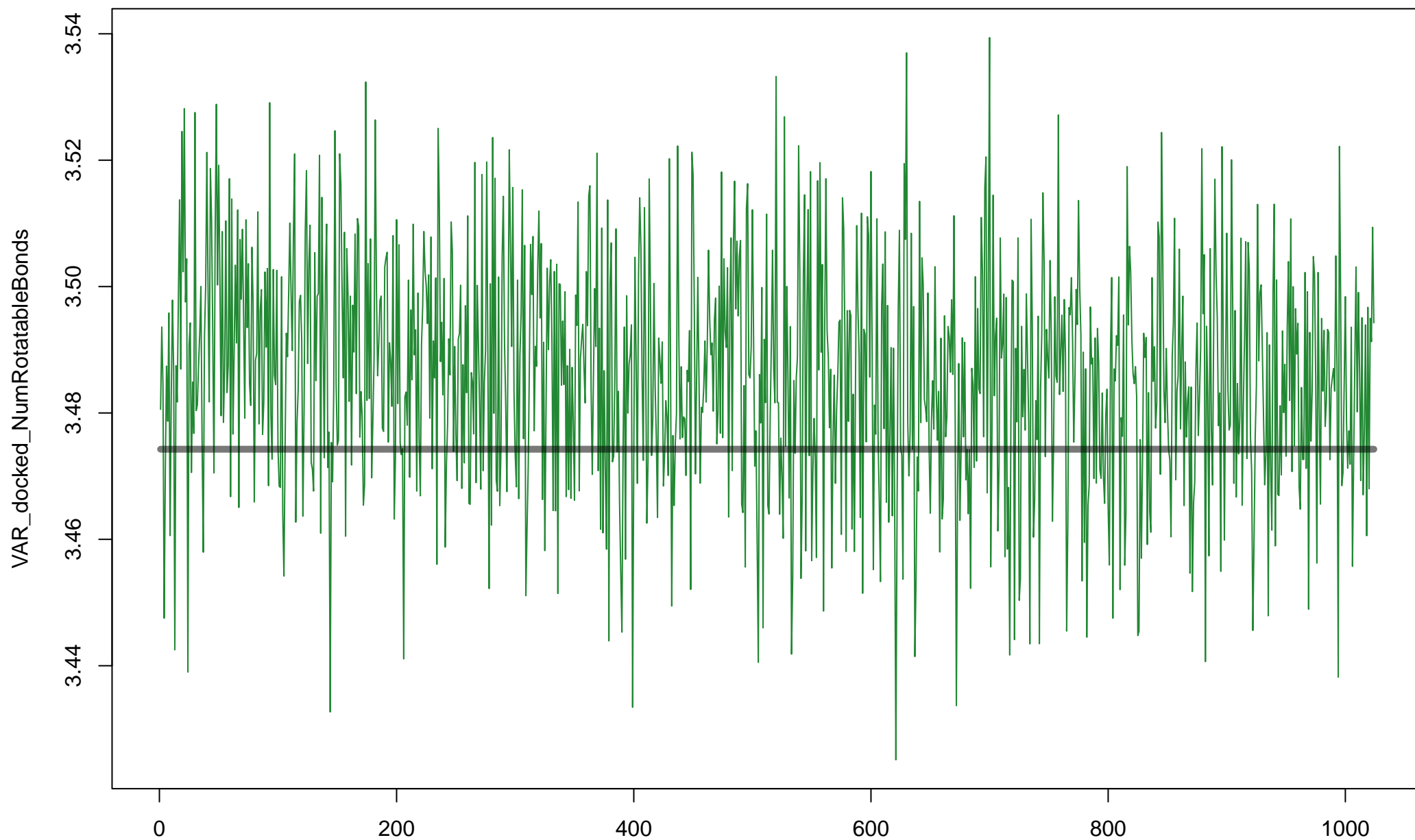


VAR_mcs_RingCount
ESS = 21.6 | BMK = 0.183 | MCSE(6.27) = 9.96 | stat: TRUE | burn: 0 | percentile: 32.2



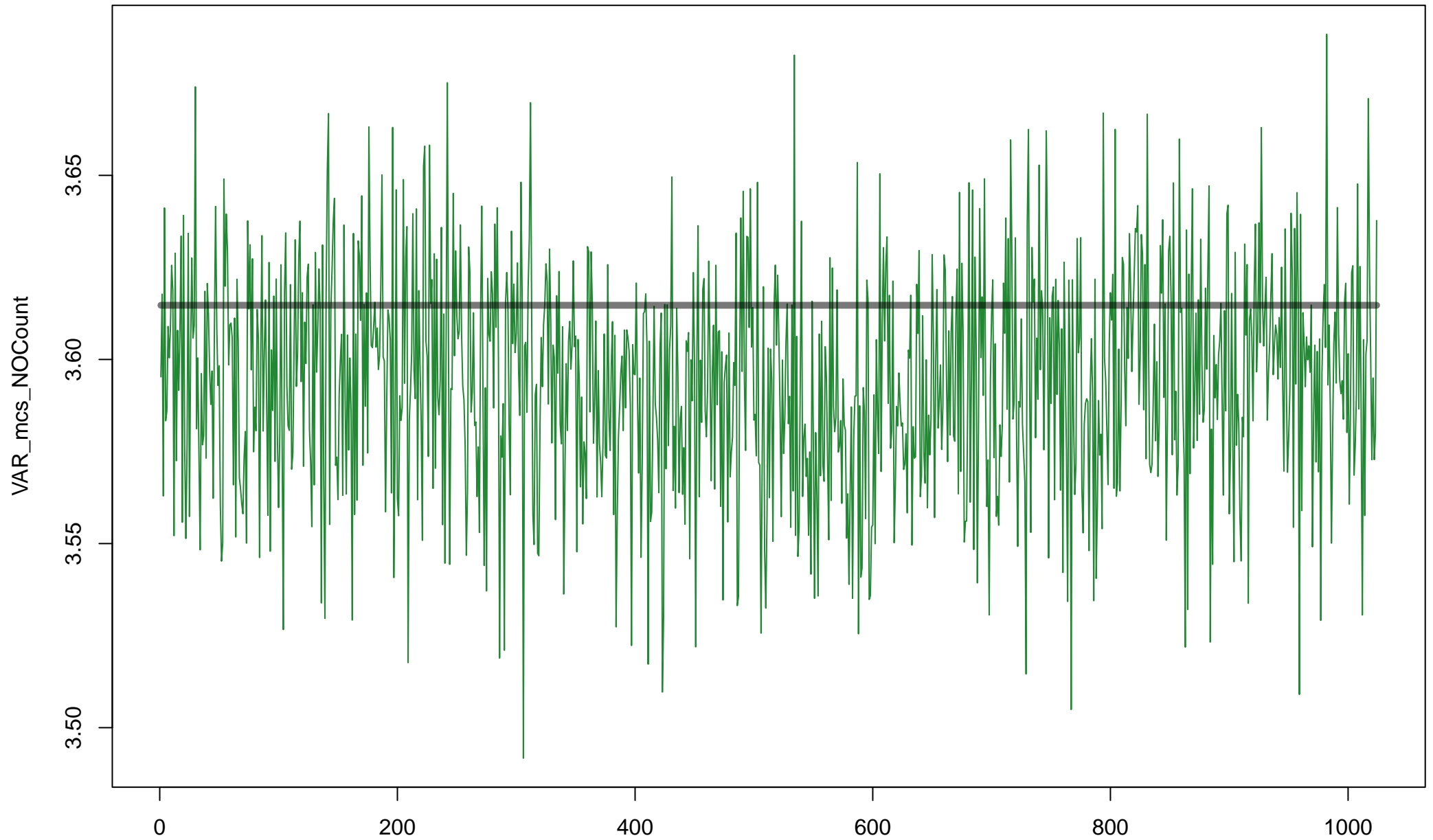
VAR_docked_NumRotatableBonds

ESS = 1020 | BMK = 0.104 | MCSE(6.27) = 3.56 | stat: FALSE | burn: 0 | percentile: 26.3

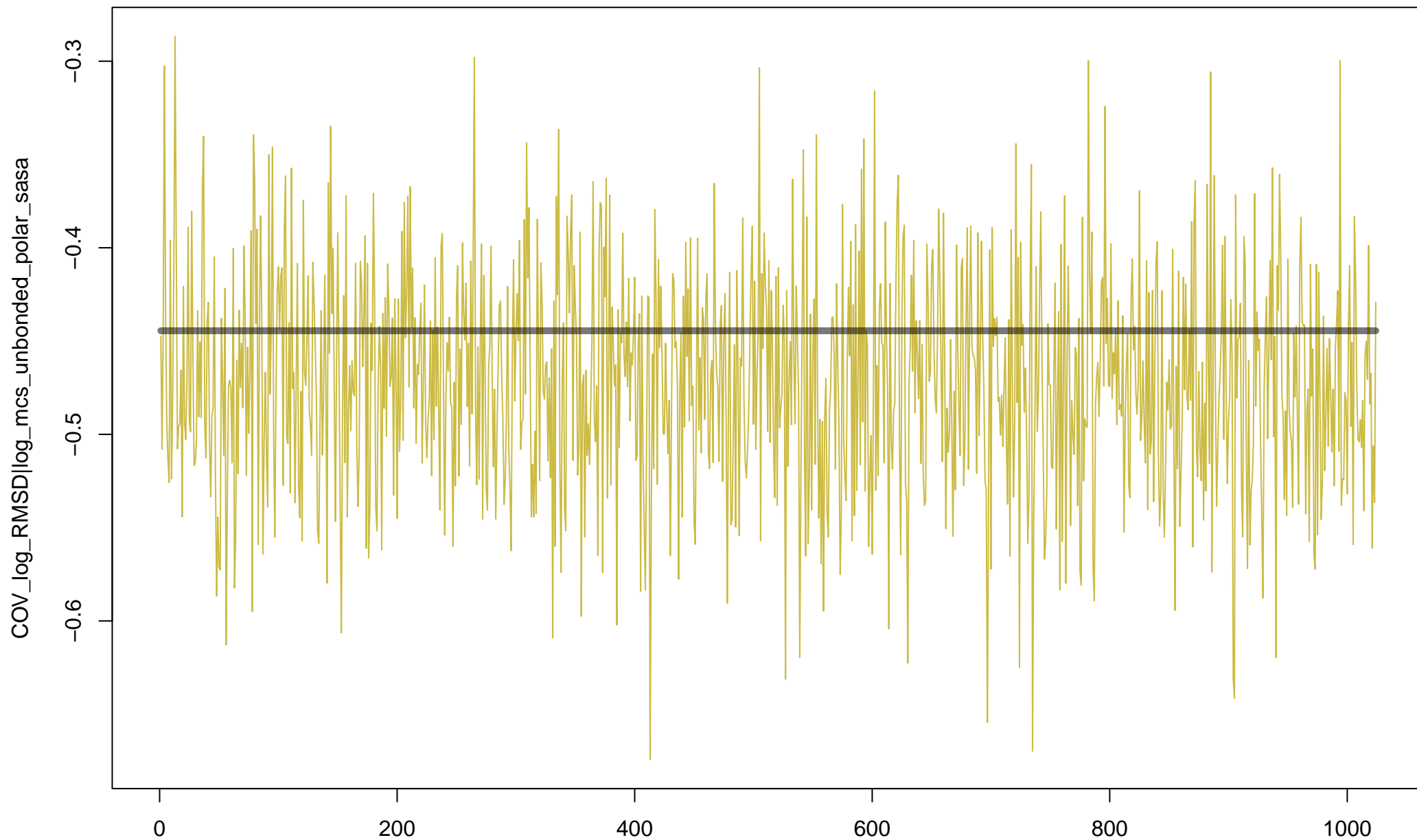


VAR_mcs_NOCount

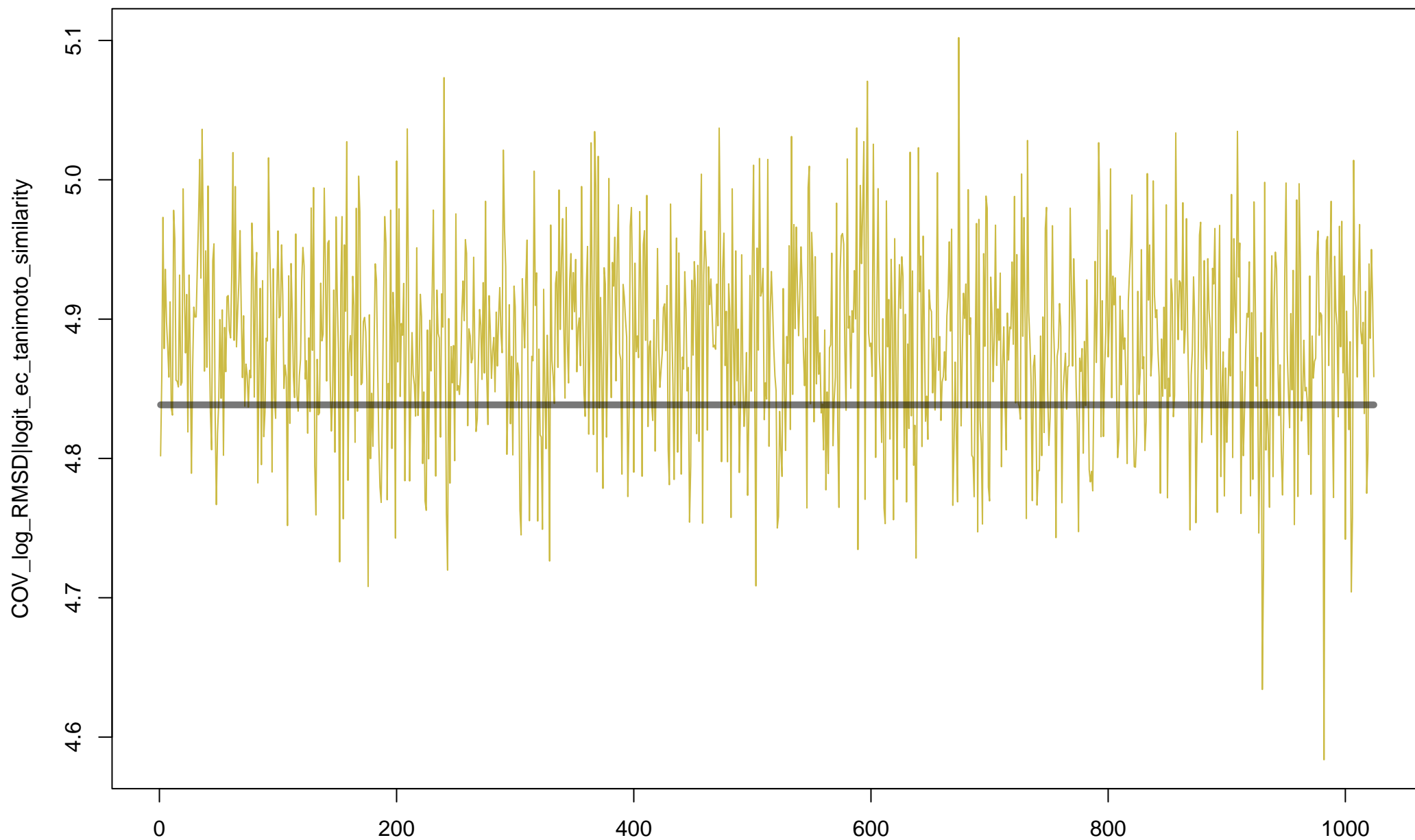
ESS = 1020 | BMK = 0.0499 | MCSE(6.27) = 4.14 | stat: TRUE | burn: 0 | percentile: 74.7



COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.058 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0 | percentile: 68.5

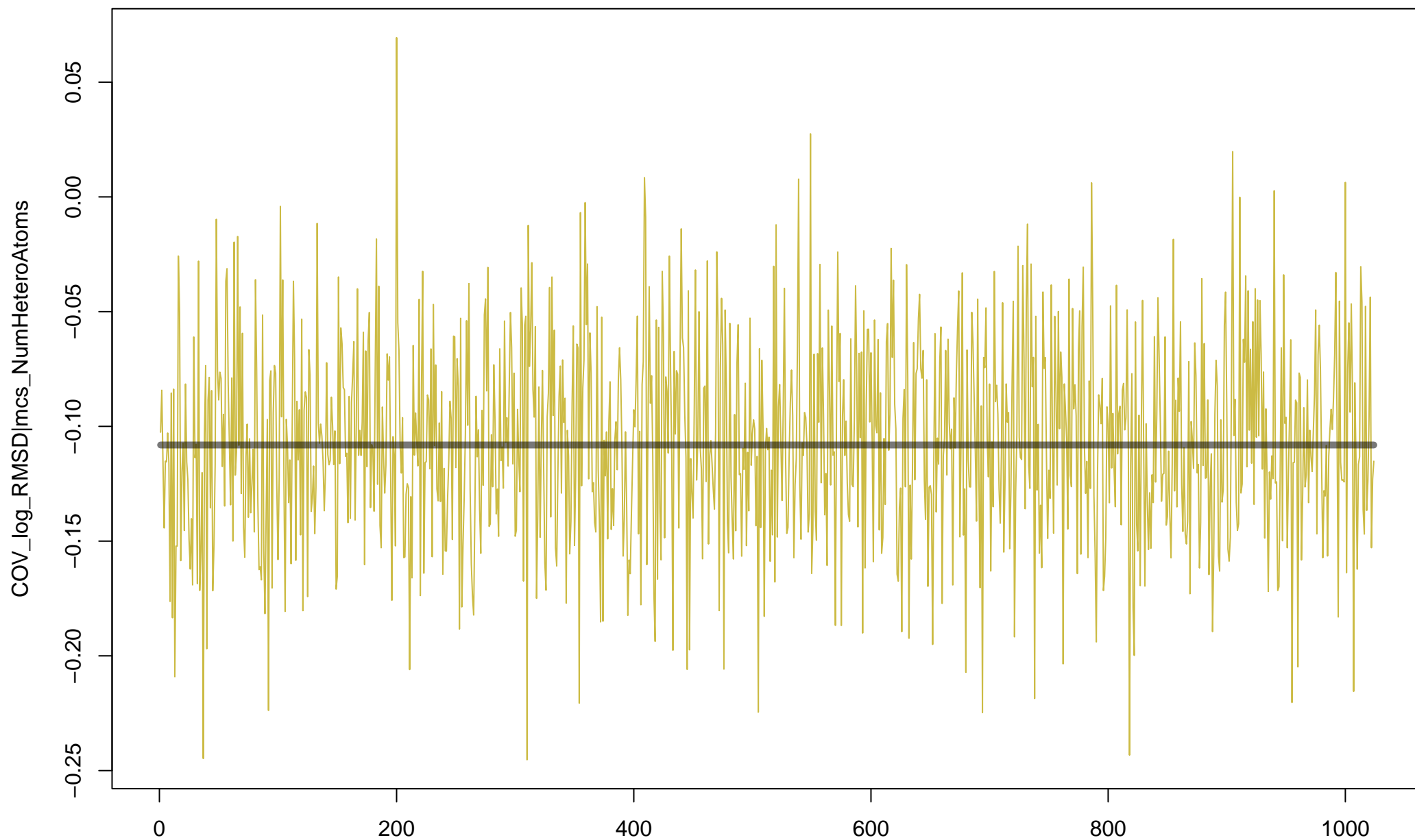


COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0643 | MCSE(6.27) = 3.31 | stat: FALSE | burn: 0 | percentile: 24.4



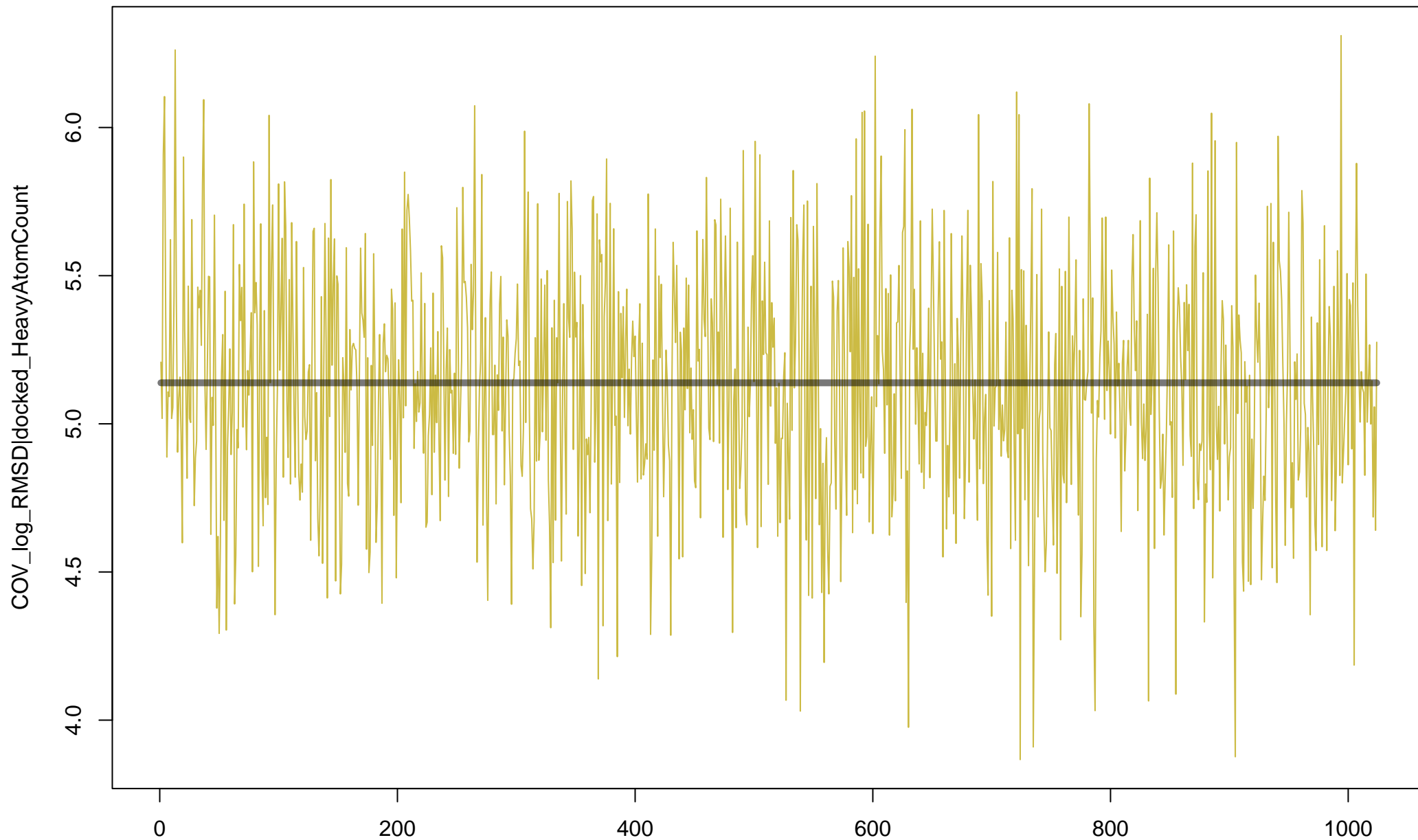
COV_log_RMSD|mcs_NumHeteroAtoms

ESS = 1020 | BMK = 0.0527 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0 | percentile: 50.3



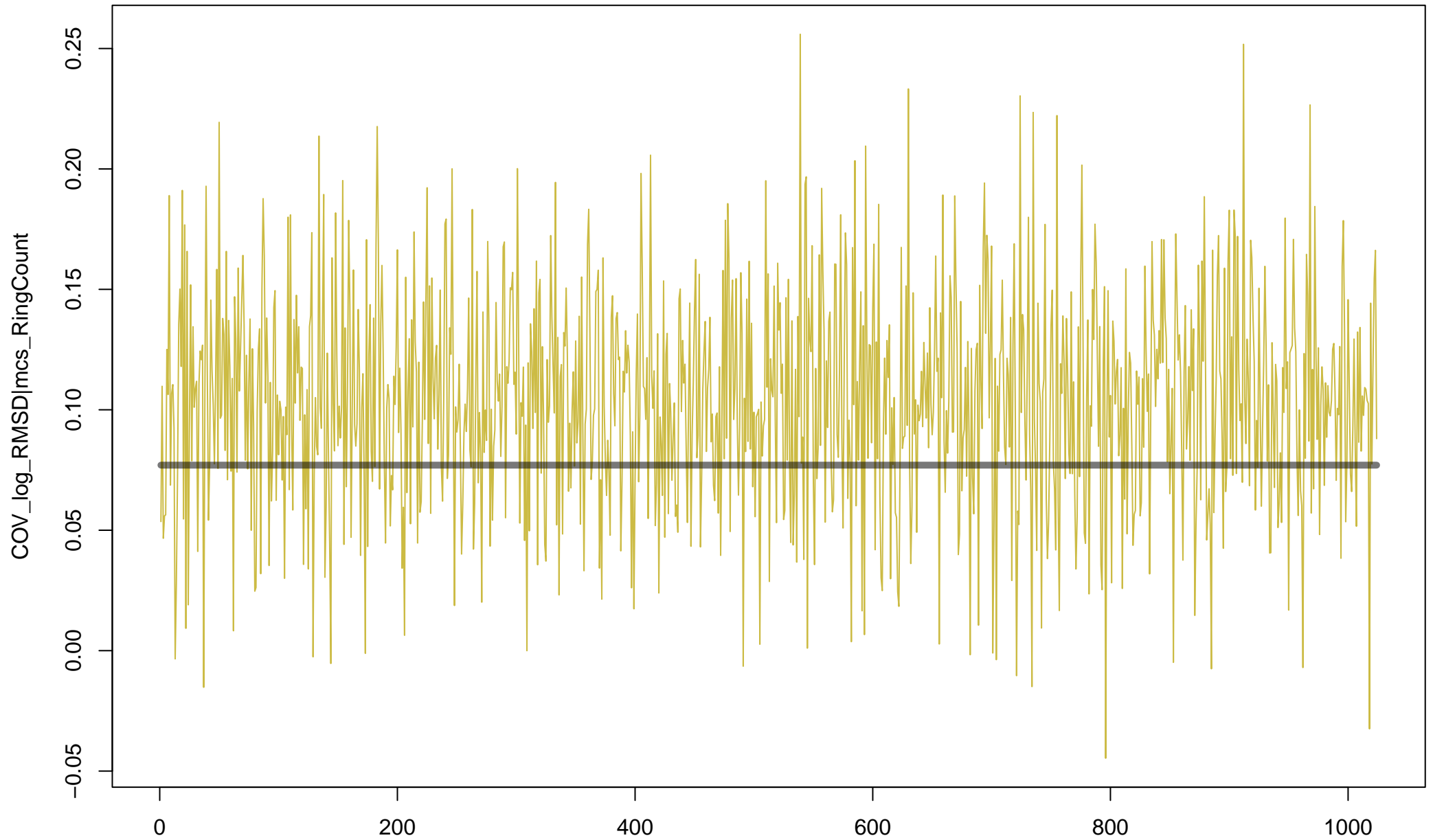
COV_log_RMSD|docked_HeavyAtomCount

ESS = 1020 | BMK = 0.0759 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0 | percentile: 51.7

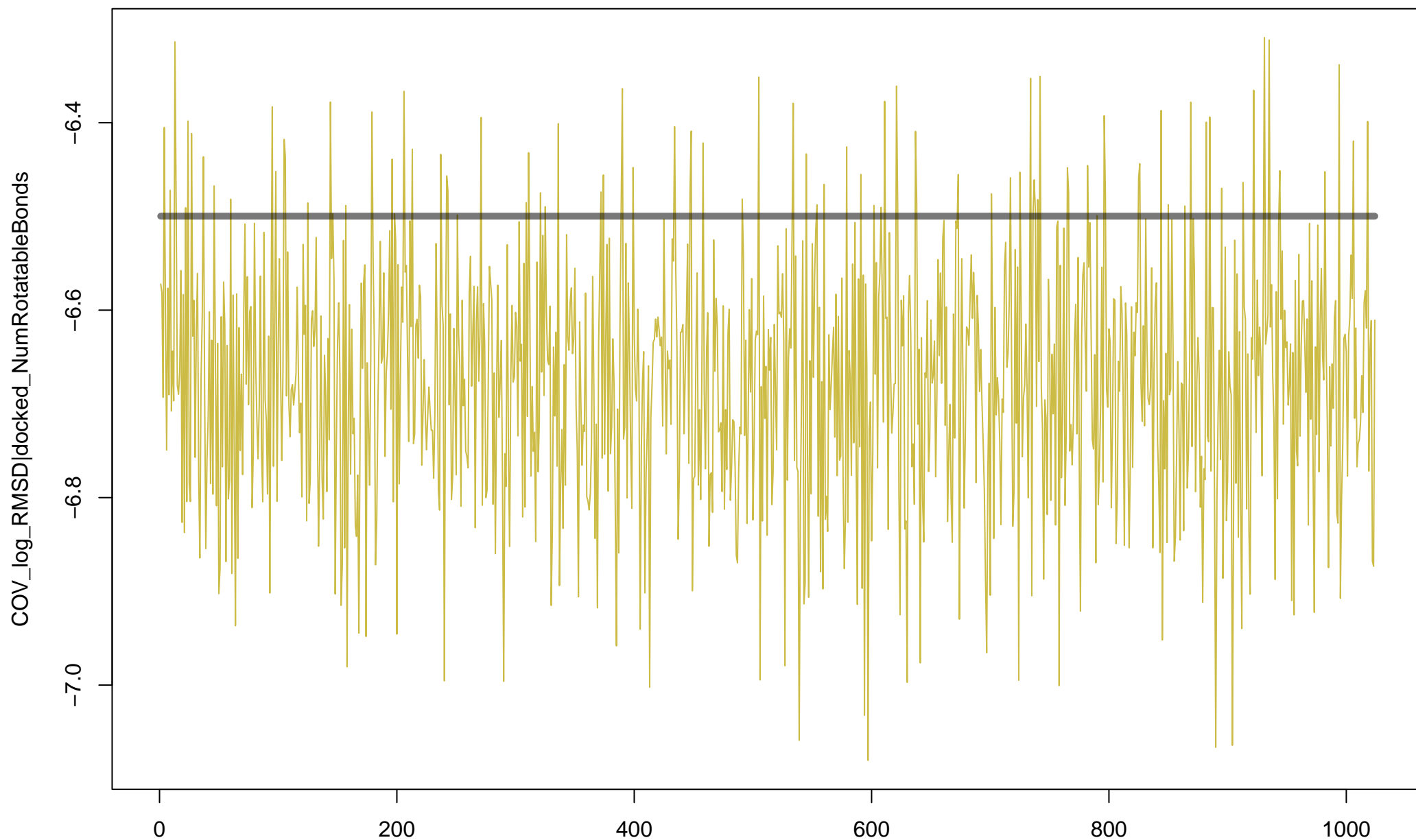


COV_log_RMSD|mcs_RingCount

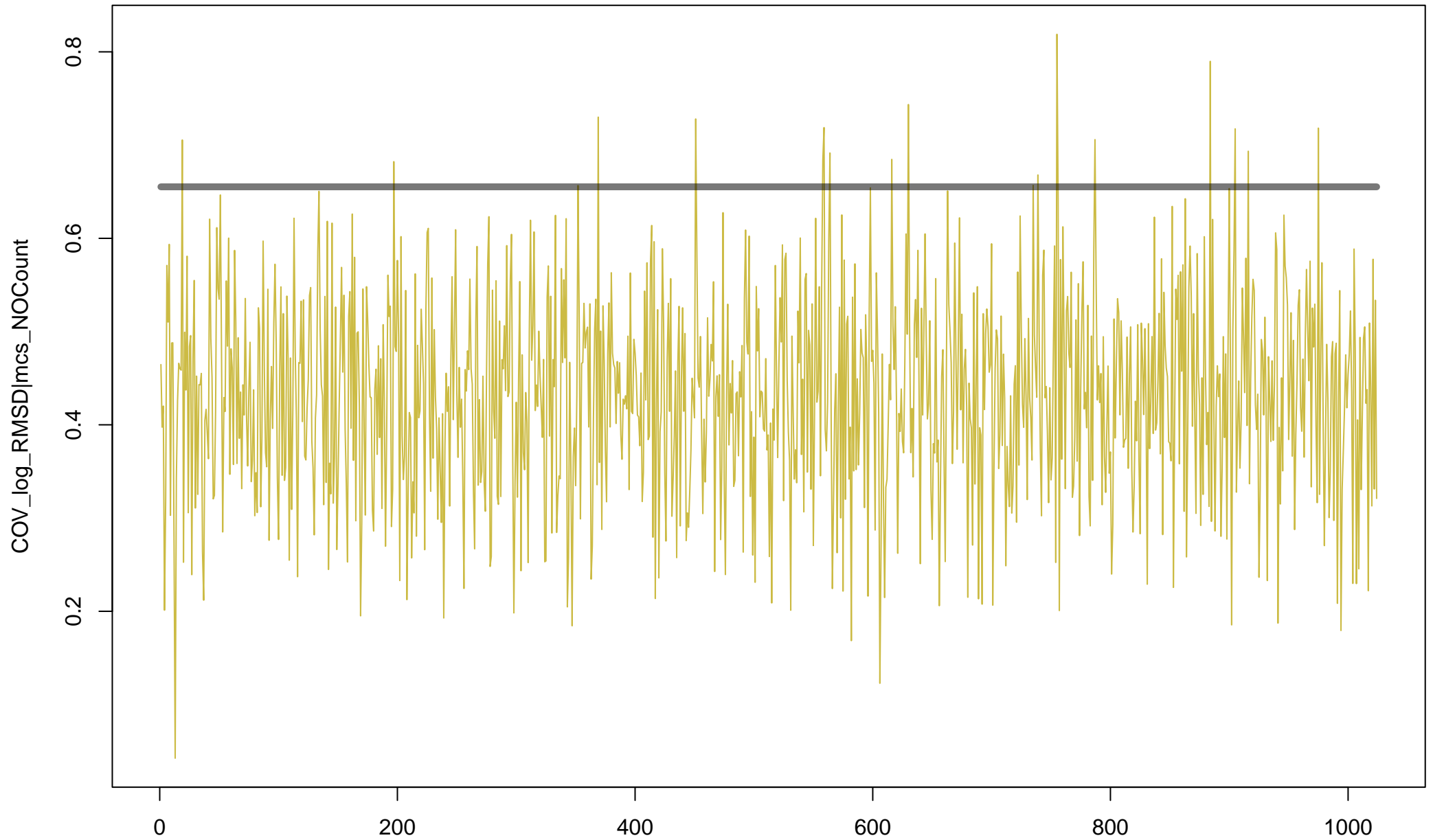
ESS = 1020 | BMK = 0.0599 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0 | percentile: 25.7



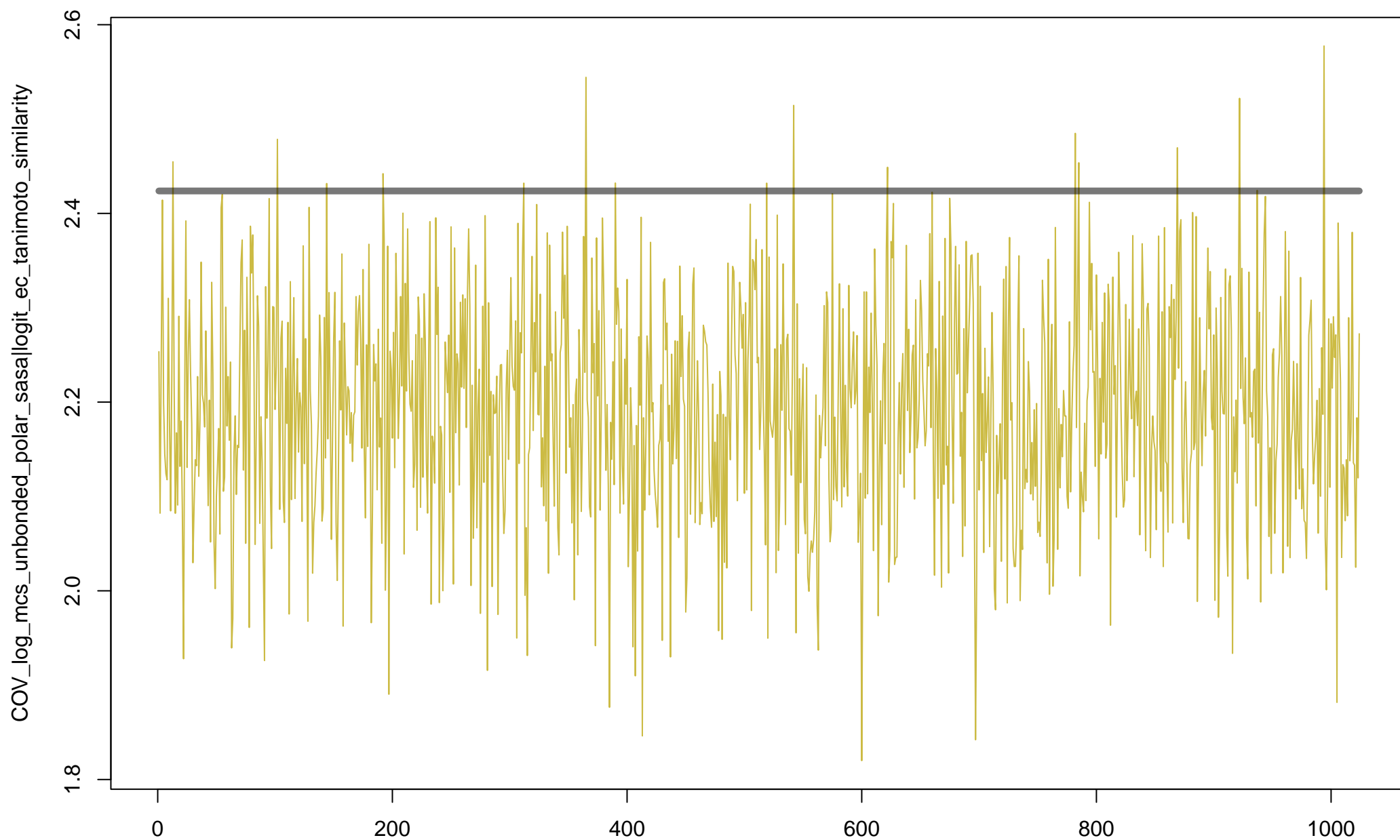
COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0498 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 0 | percentile: 91.1



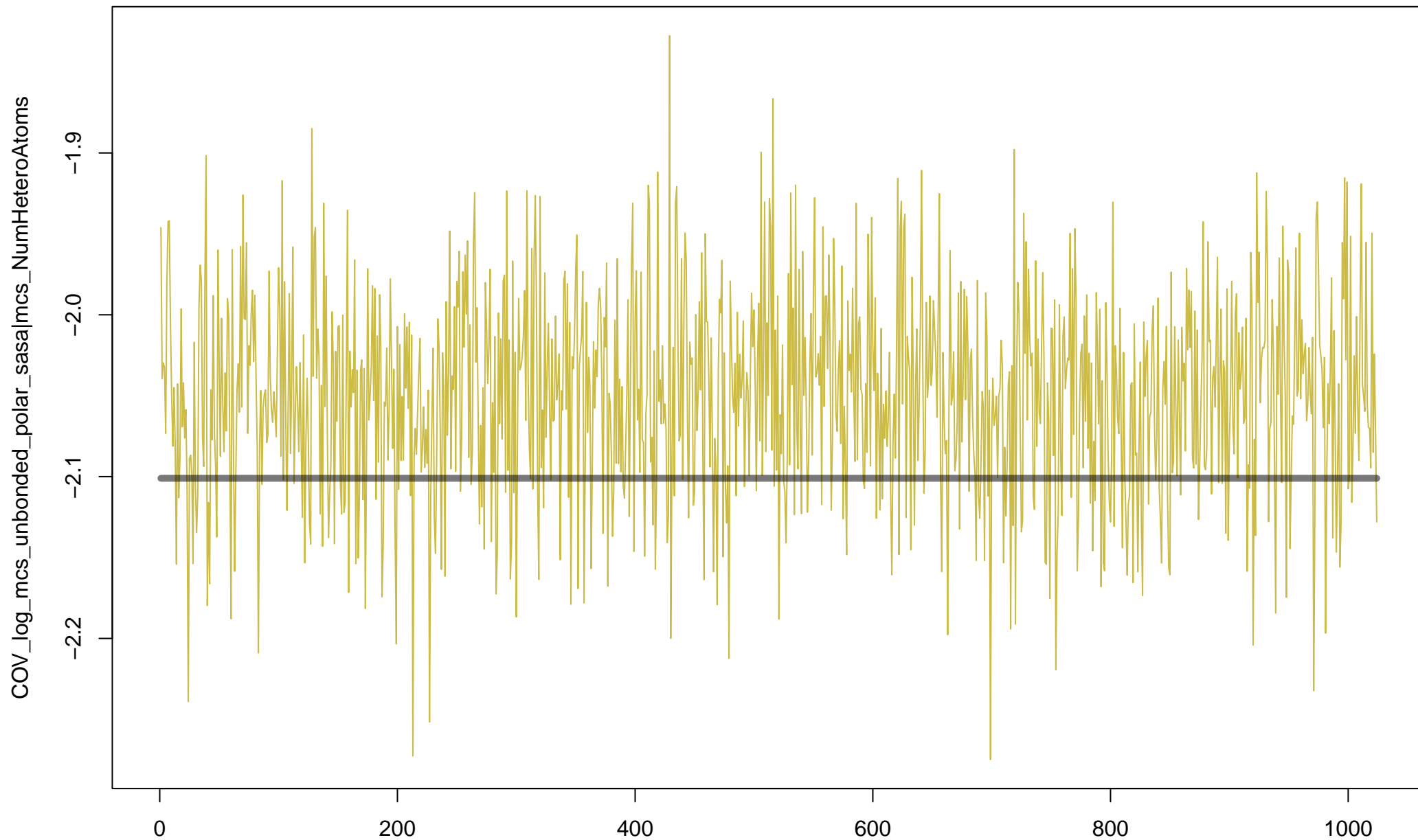
COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0659 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0 | percentile: 98.2



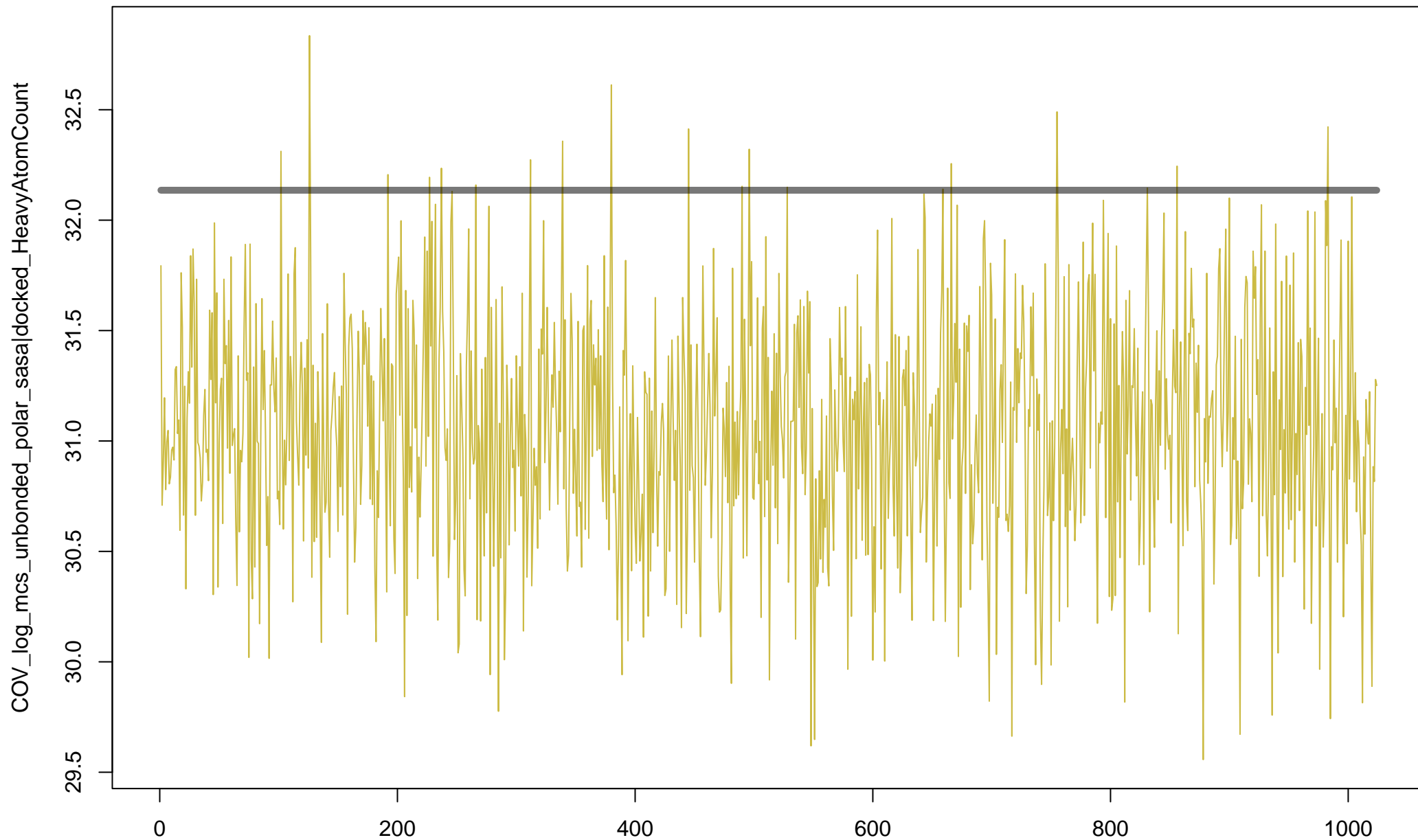
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0723 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | percentile: 98.4



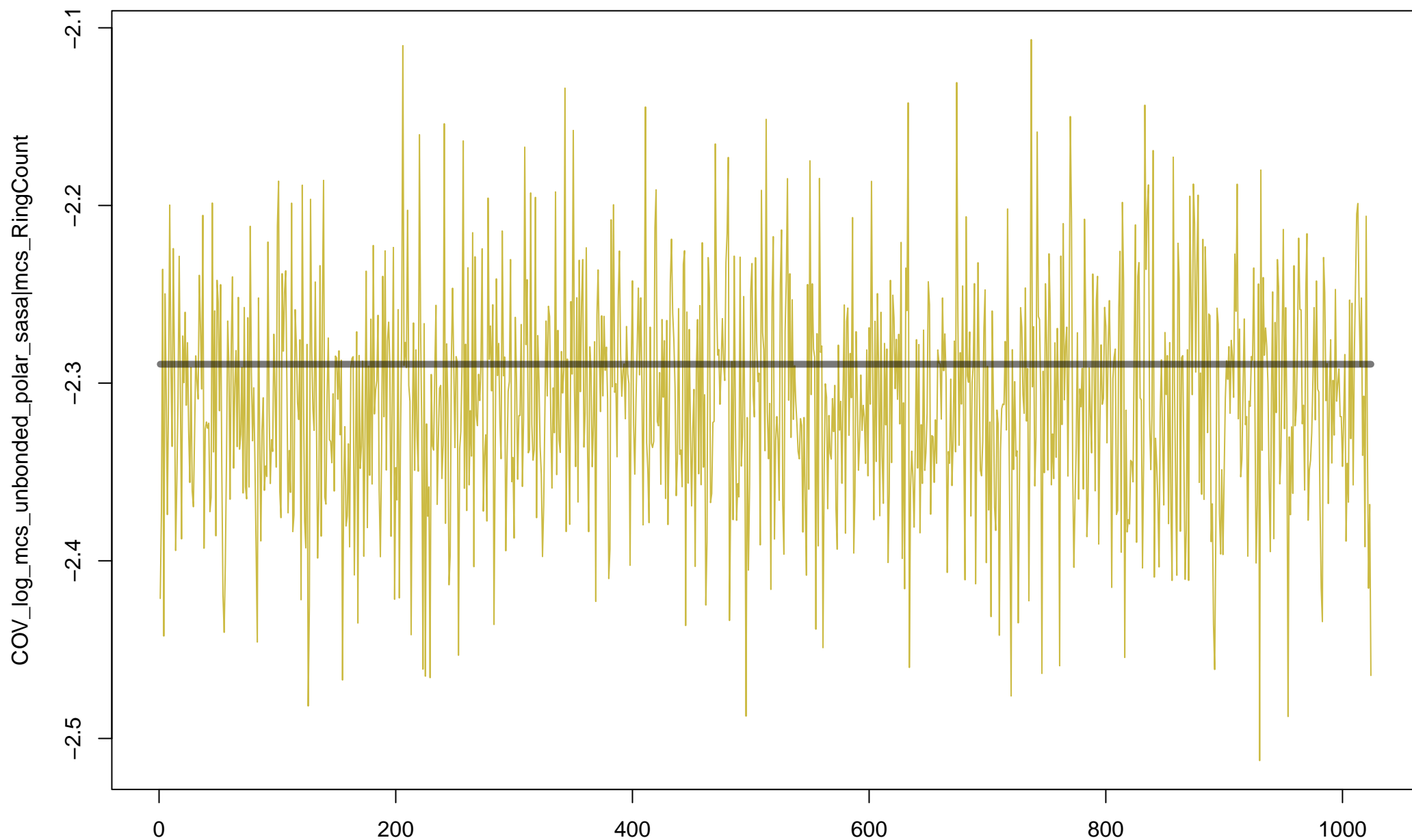
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0304 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0 | percentile: 20.8



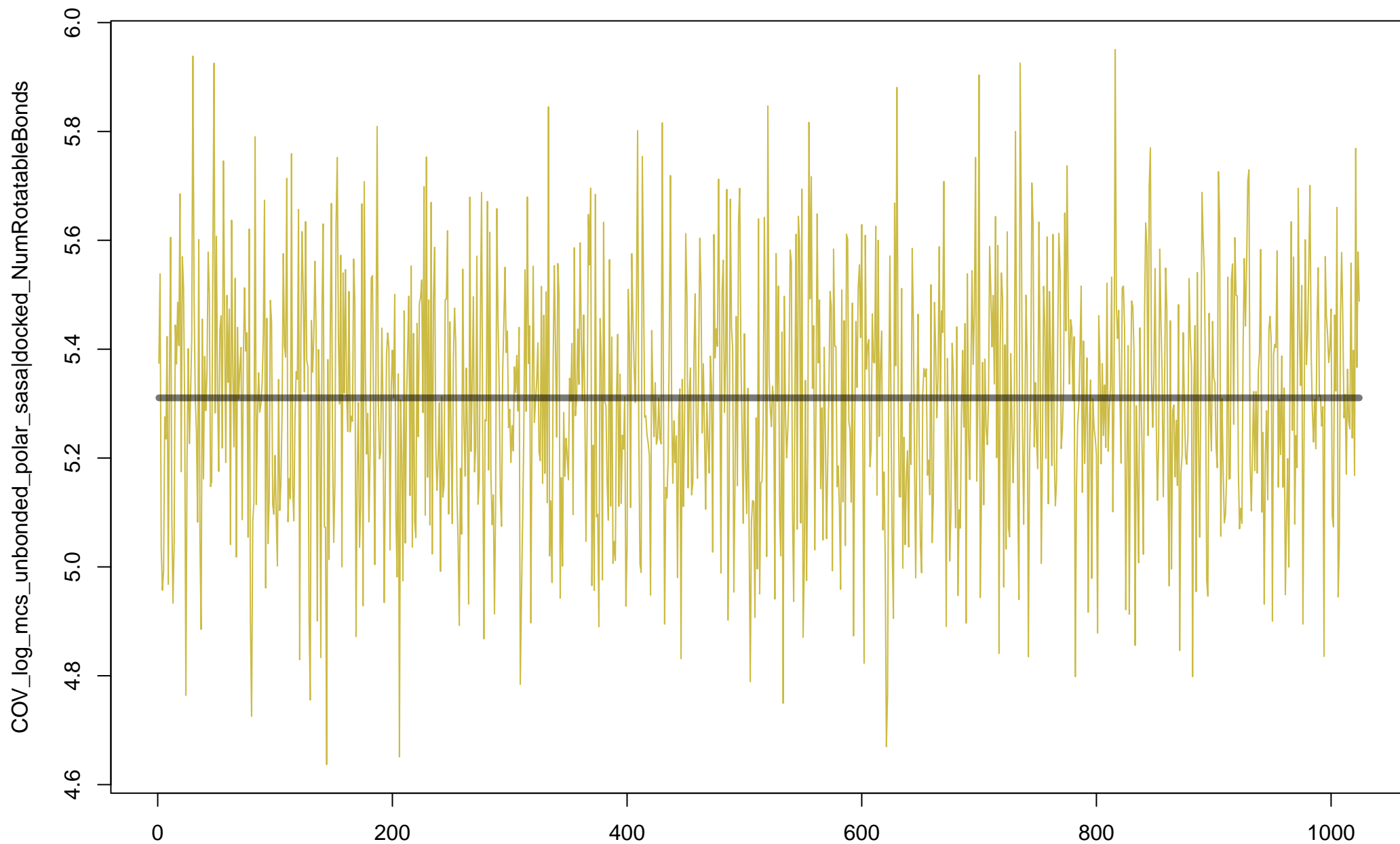
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0632 | MCSE(6.27) = 3.32 | stat: TRUE | burn: 0 | percentile: 98.1



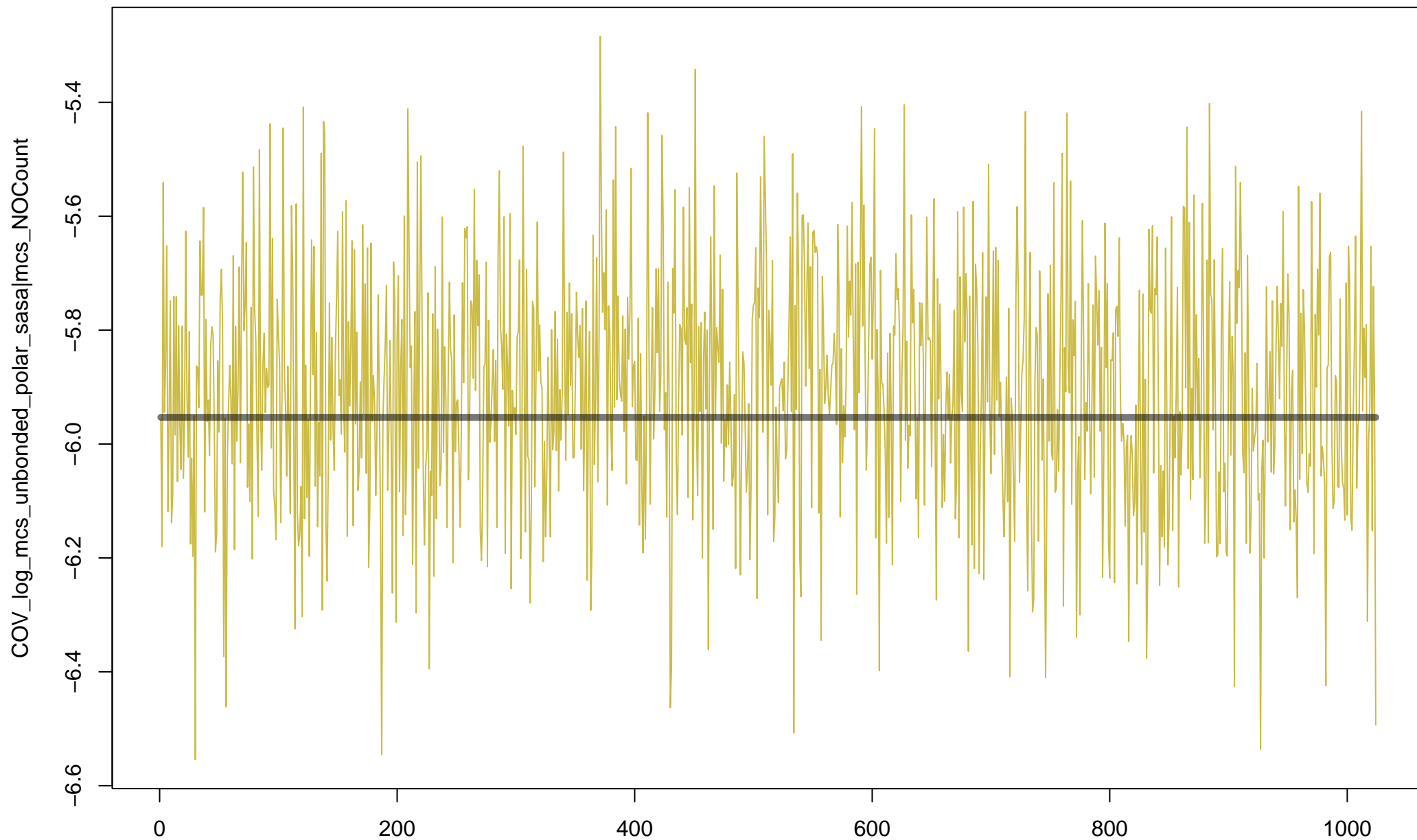
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0253 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | percentile: 63.6



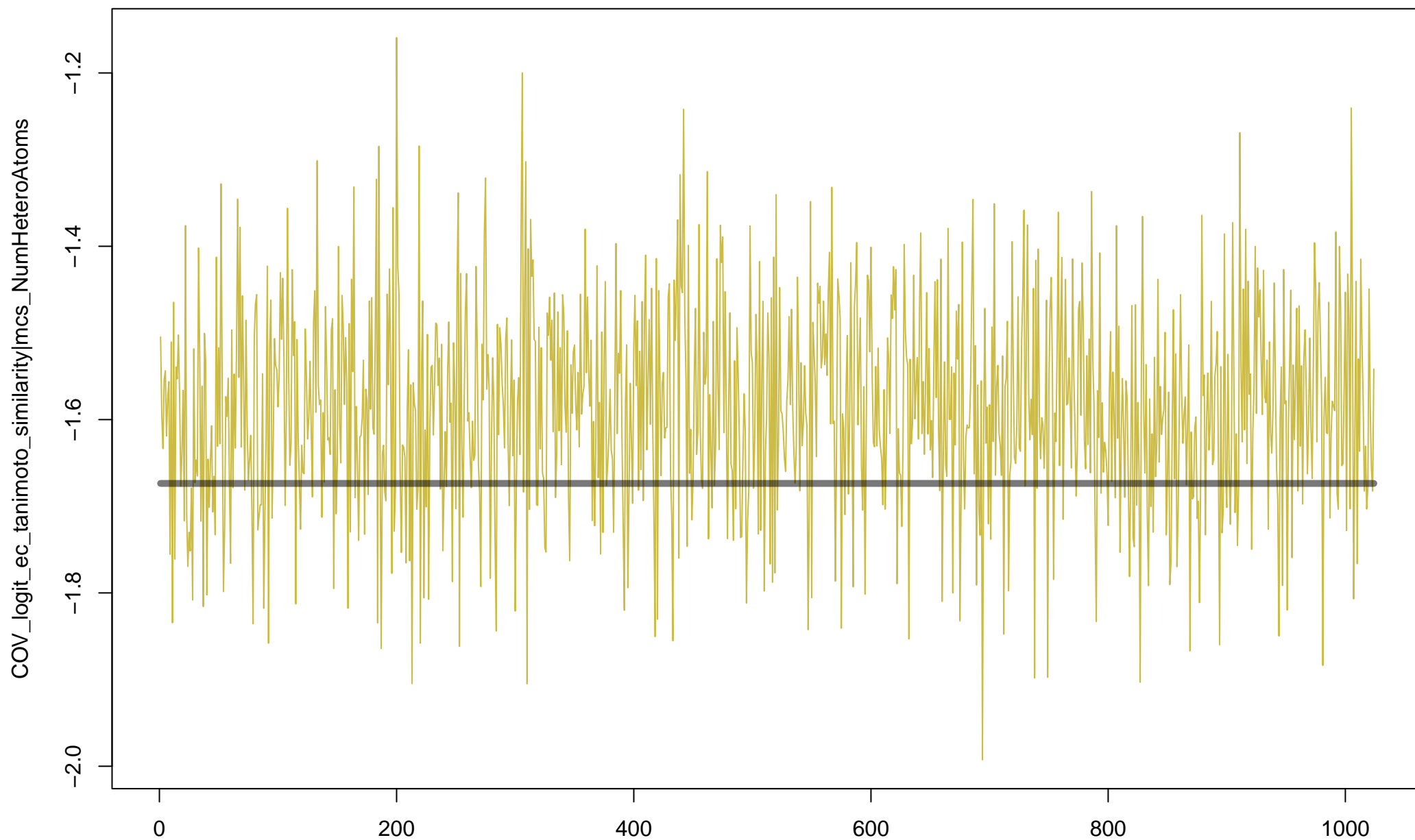
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0412 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | percentile: 51.5



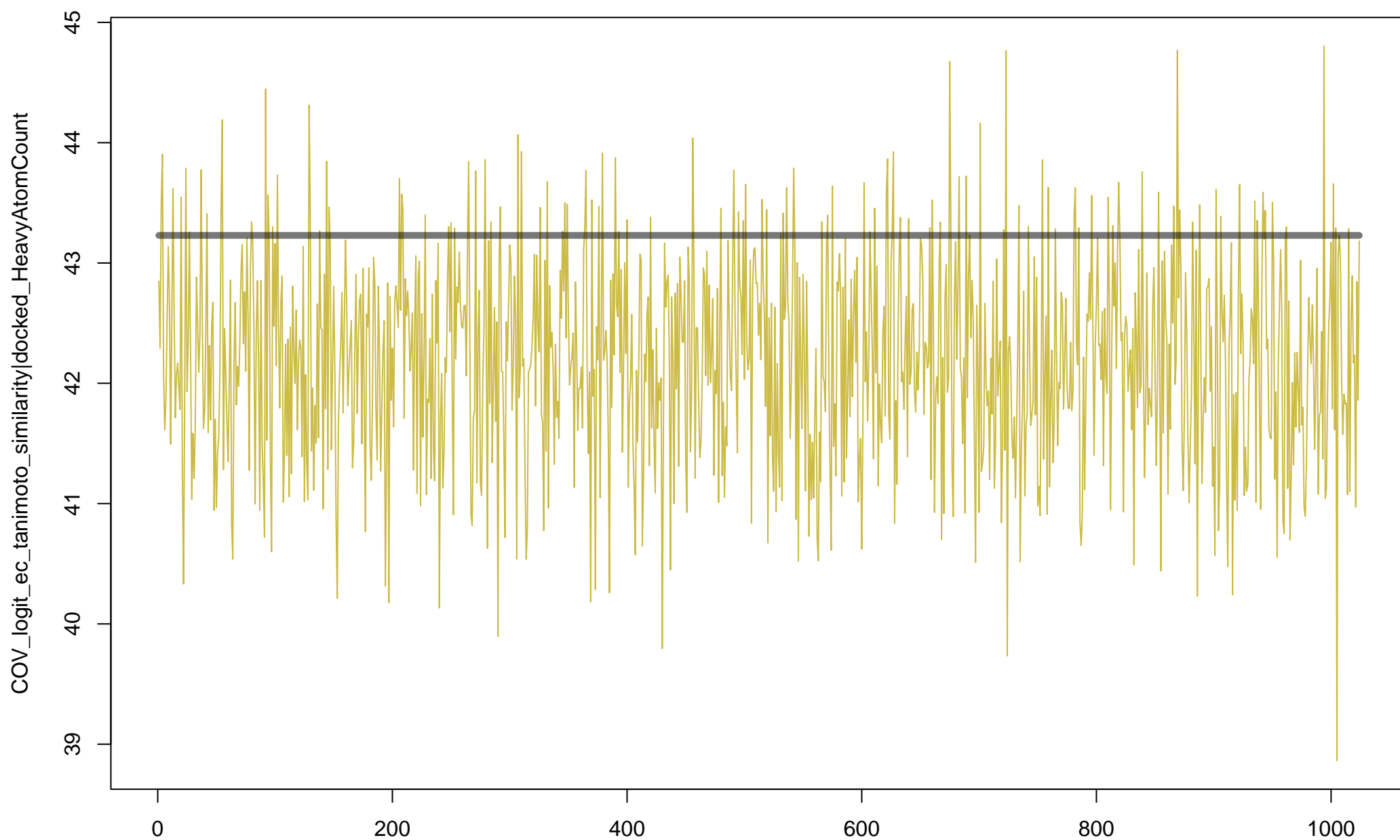
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0447 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0 | percentile: 39.8



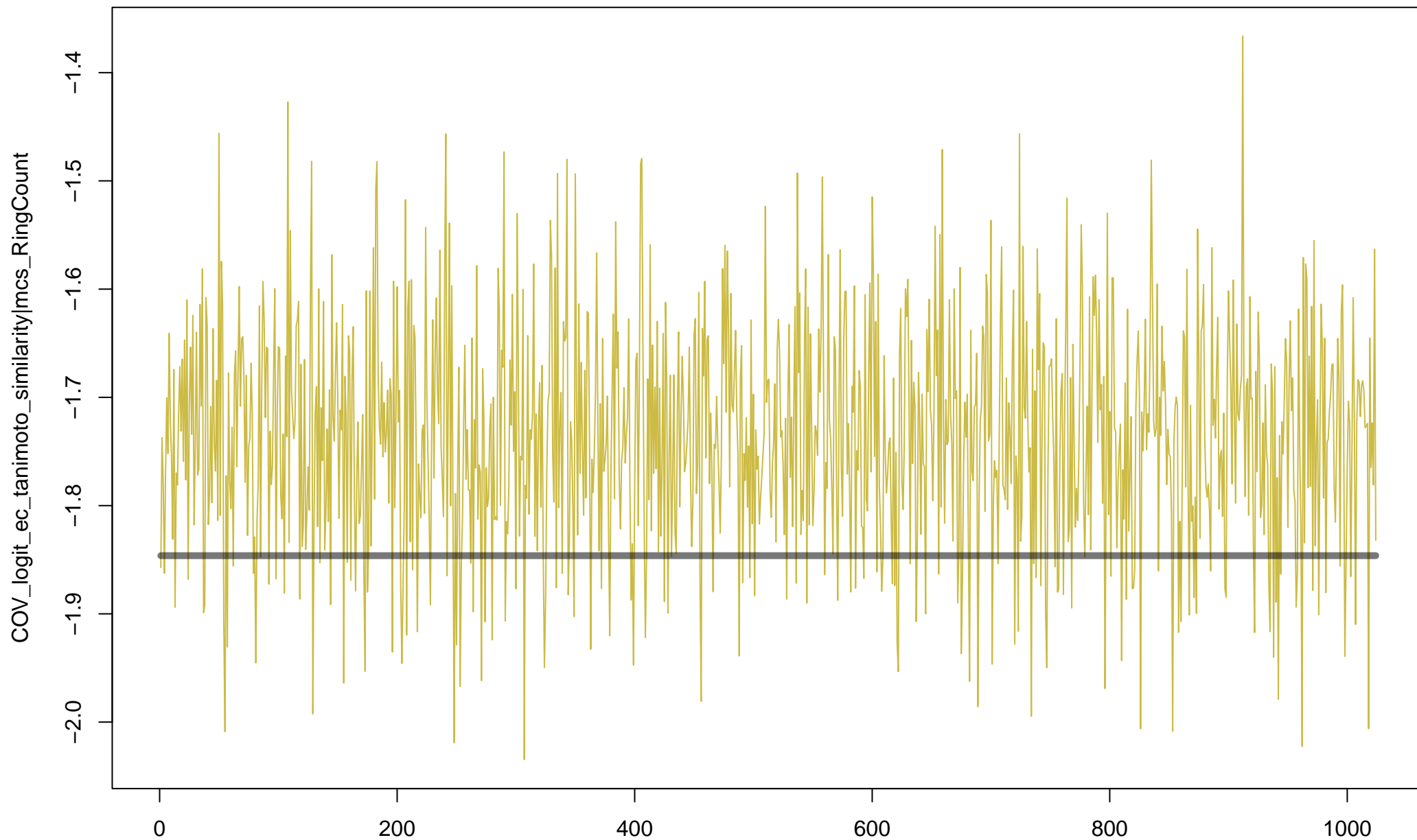
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0717 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | percentile: 21.9



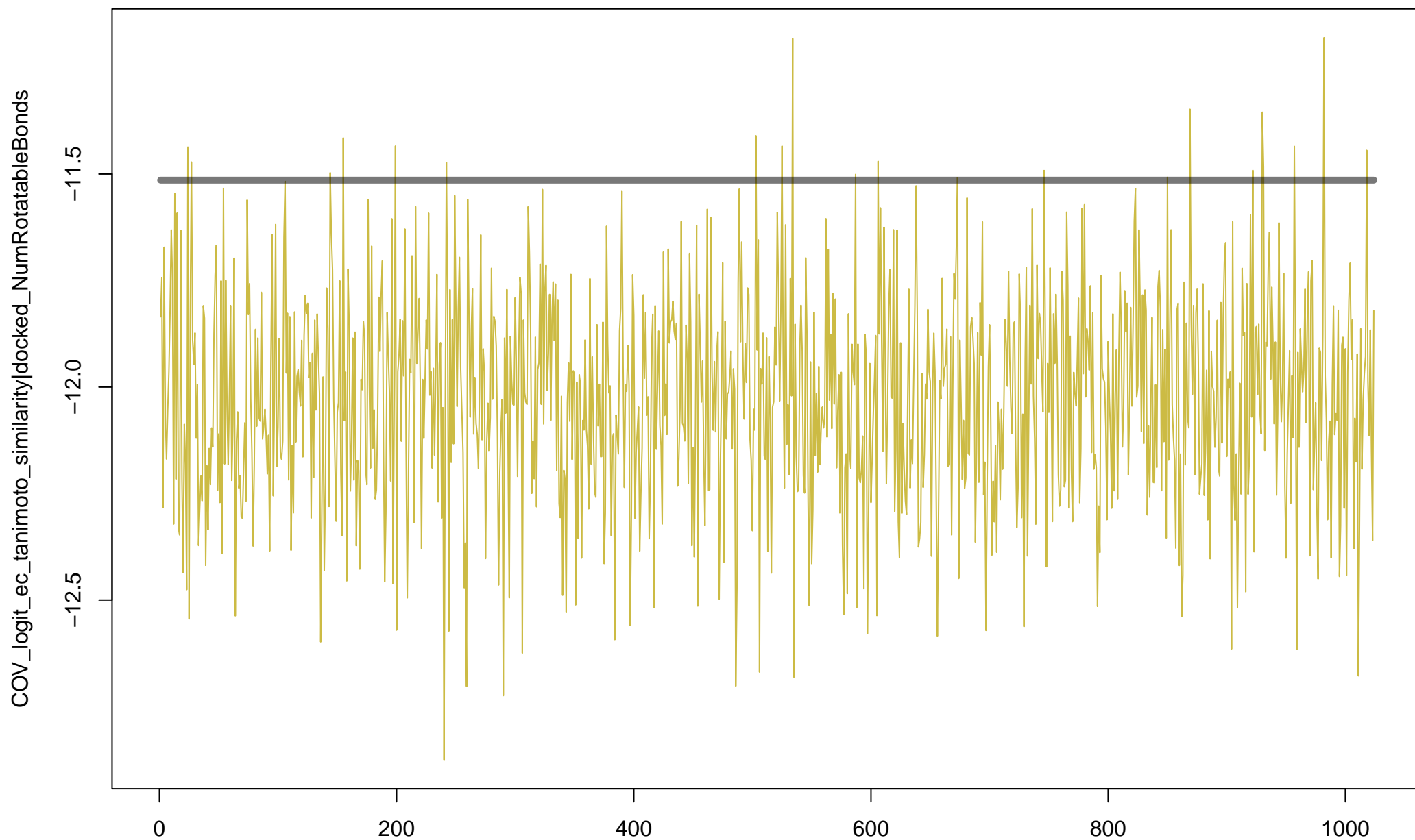
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0716 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0 | percentile: 88.8



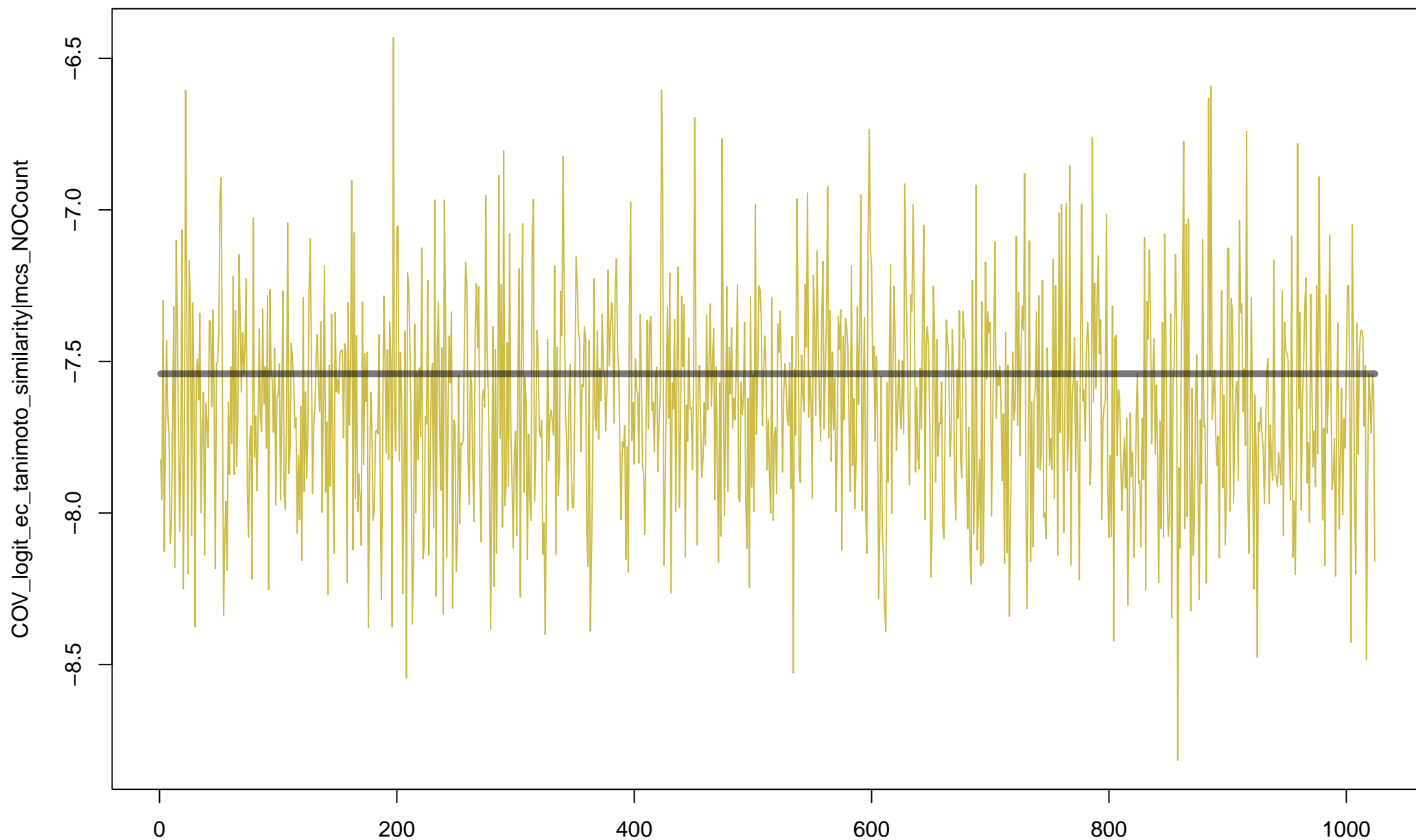
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0458 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0 | percentile: 14.4



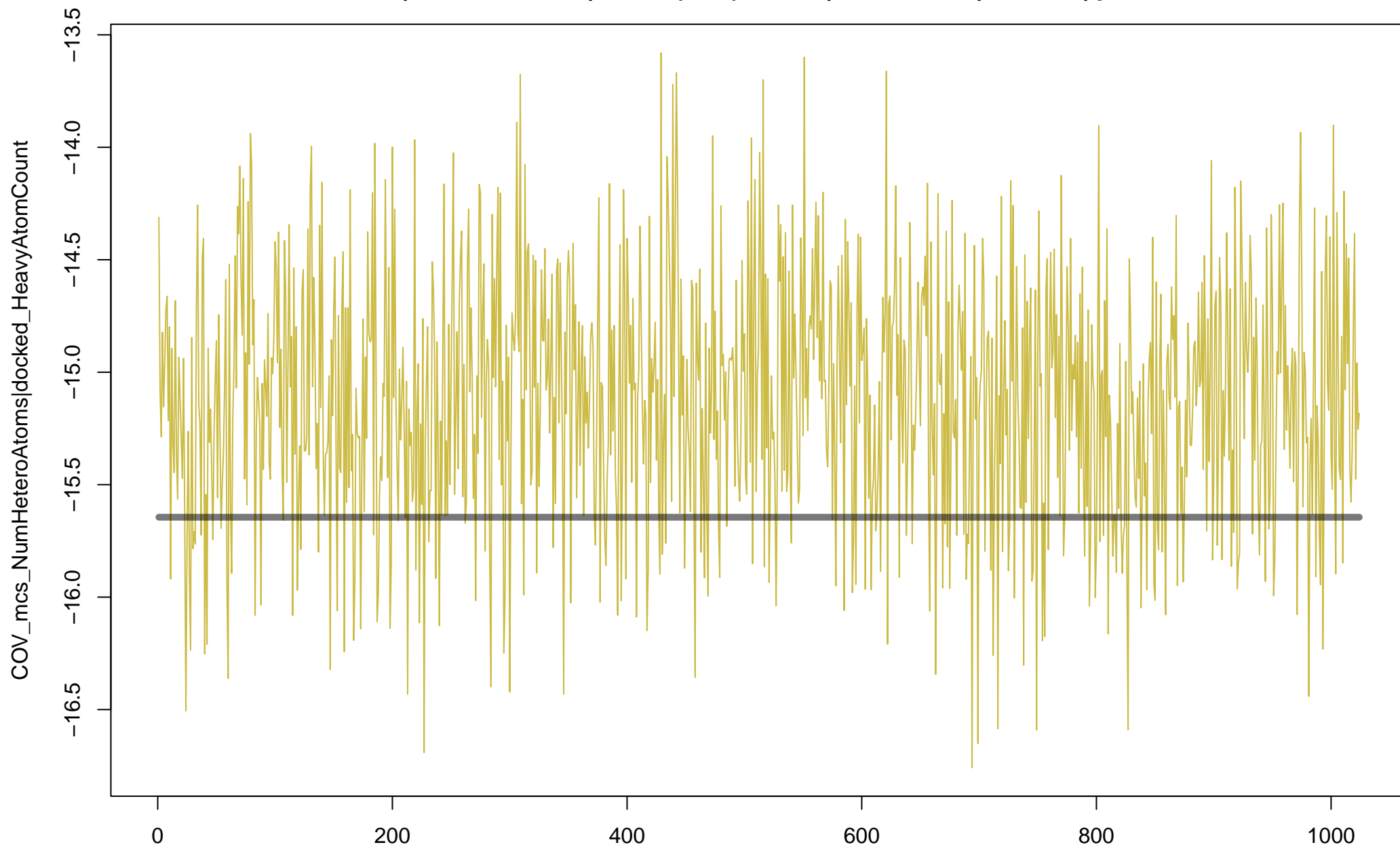
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0518 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0 | percentile: 97.9



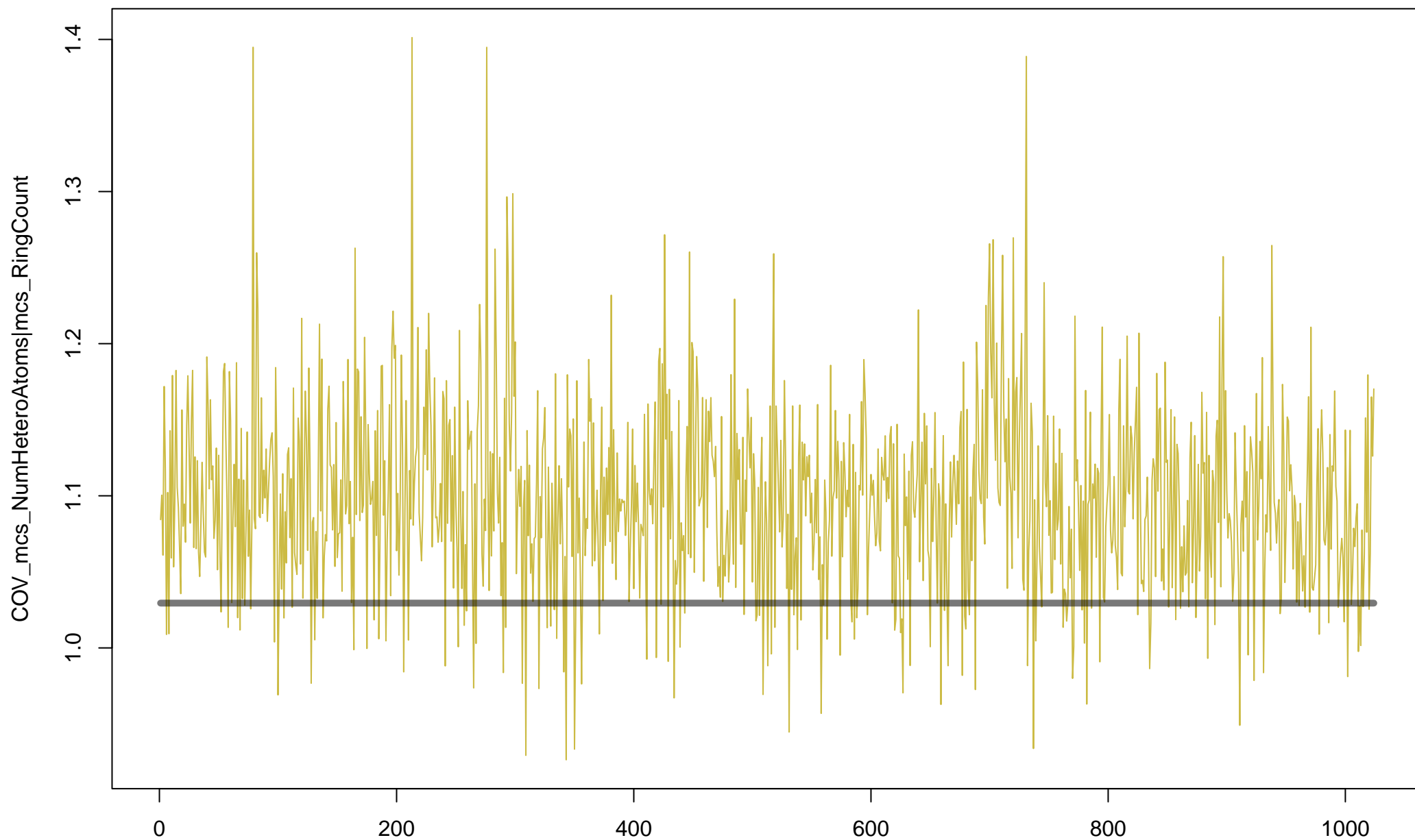
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.043 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0 | percentile: 62.5



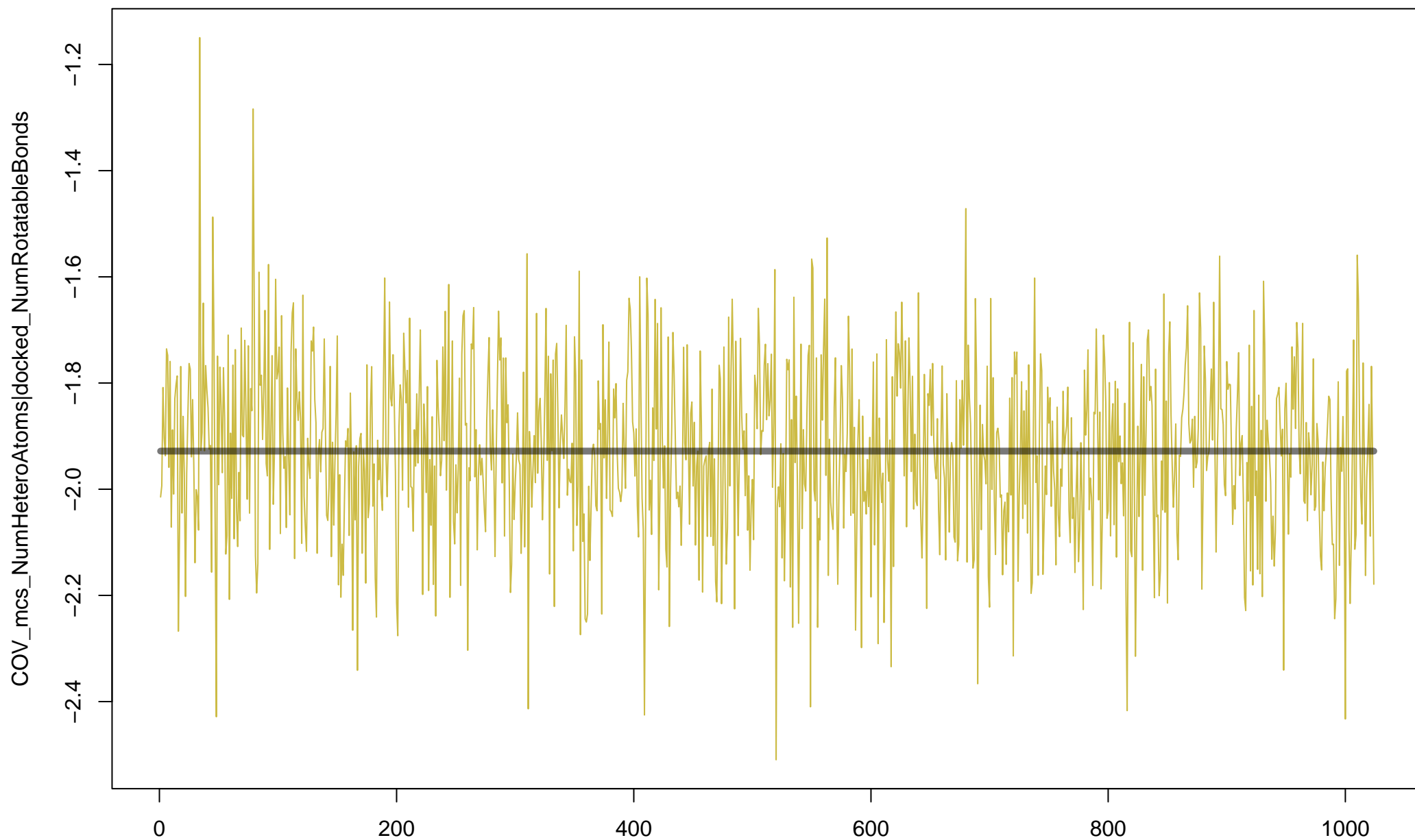
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0564 | MCSE(6.27) = 3.67 | stat: TRUE | burn: 0 | percentile: 17



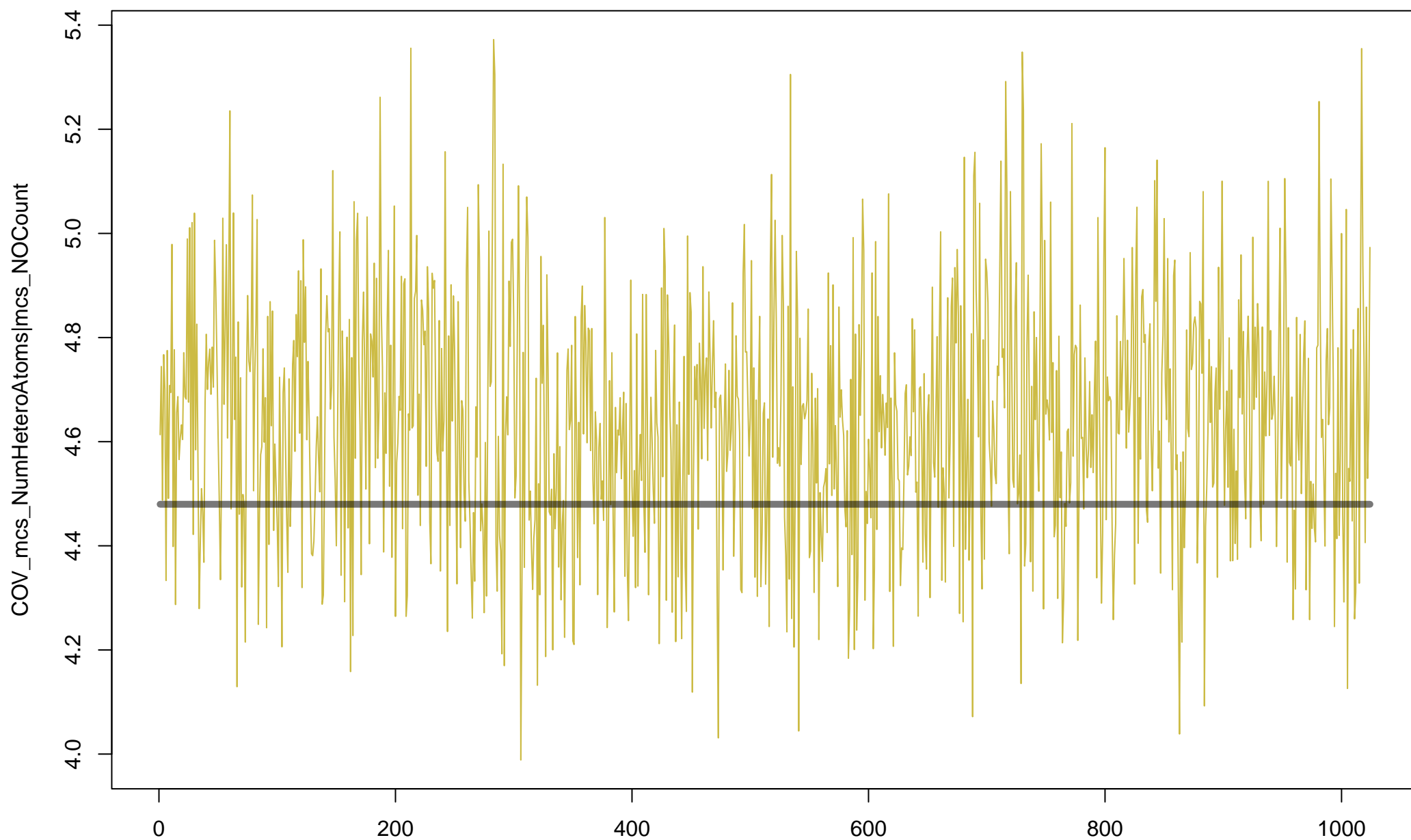
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 591 | BMK = 0.0709 | MCSE(6.27) = 4.03 | stat: TRUE | burn: 0 | percentile: 12.5



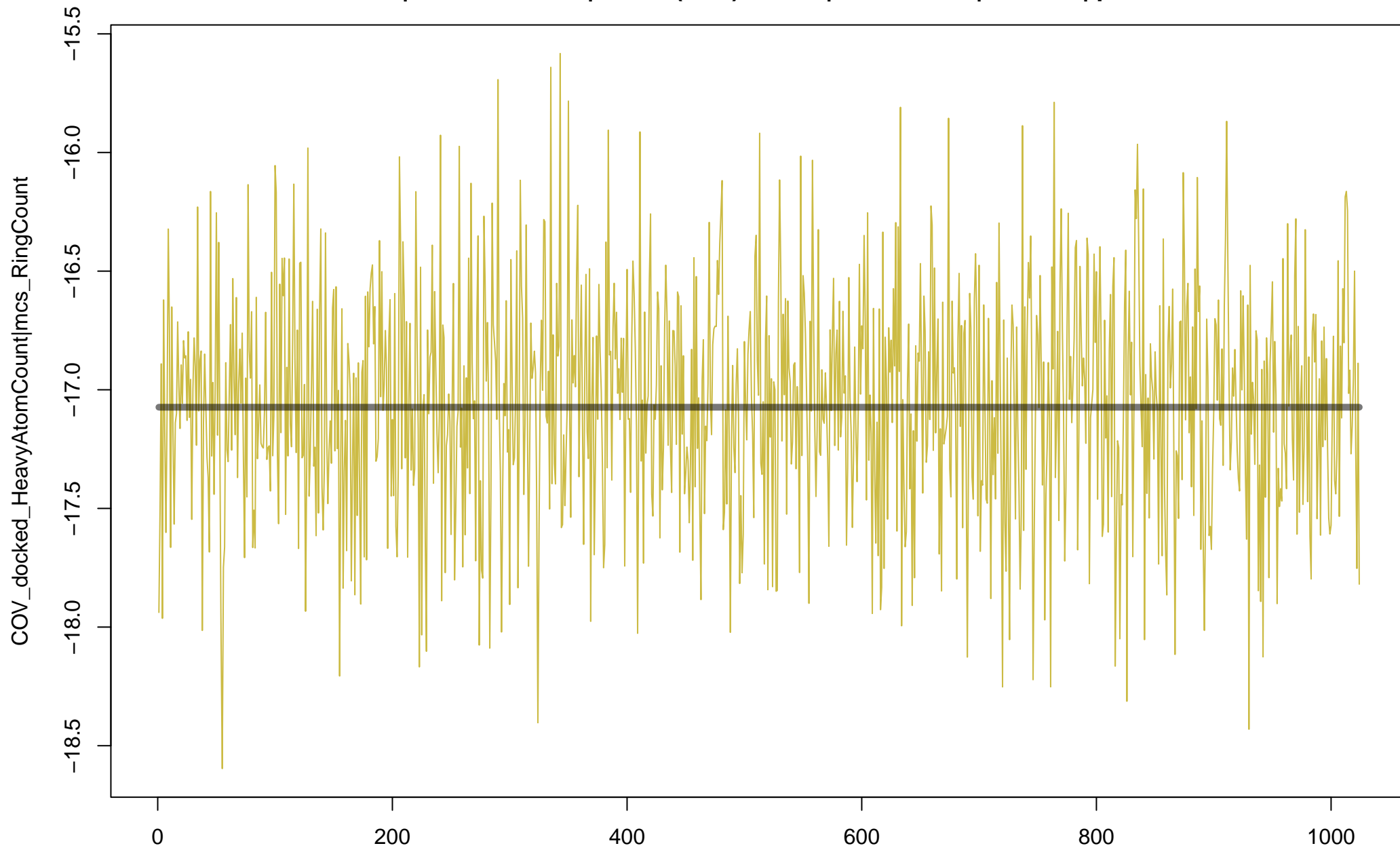
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0668 | MCSE(6.27) = 3.75 | stat: FALSE | burn: 0 | percentile: 50.8



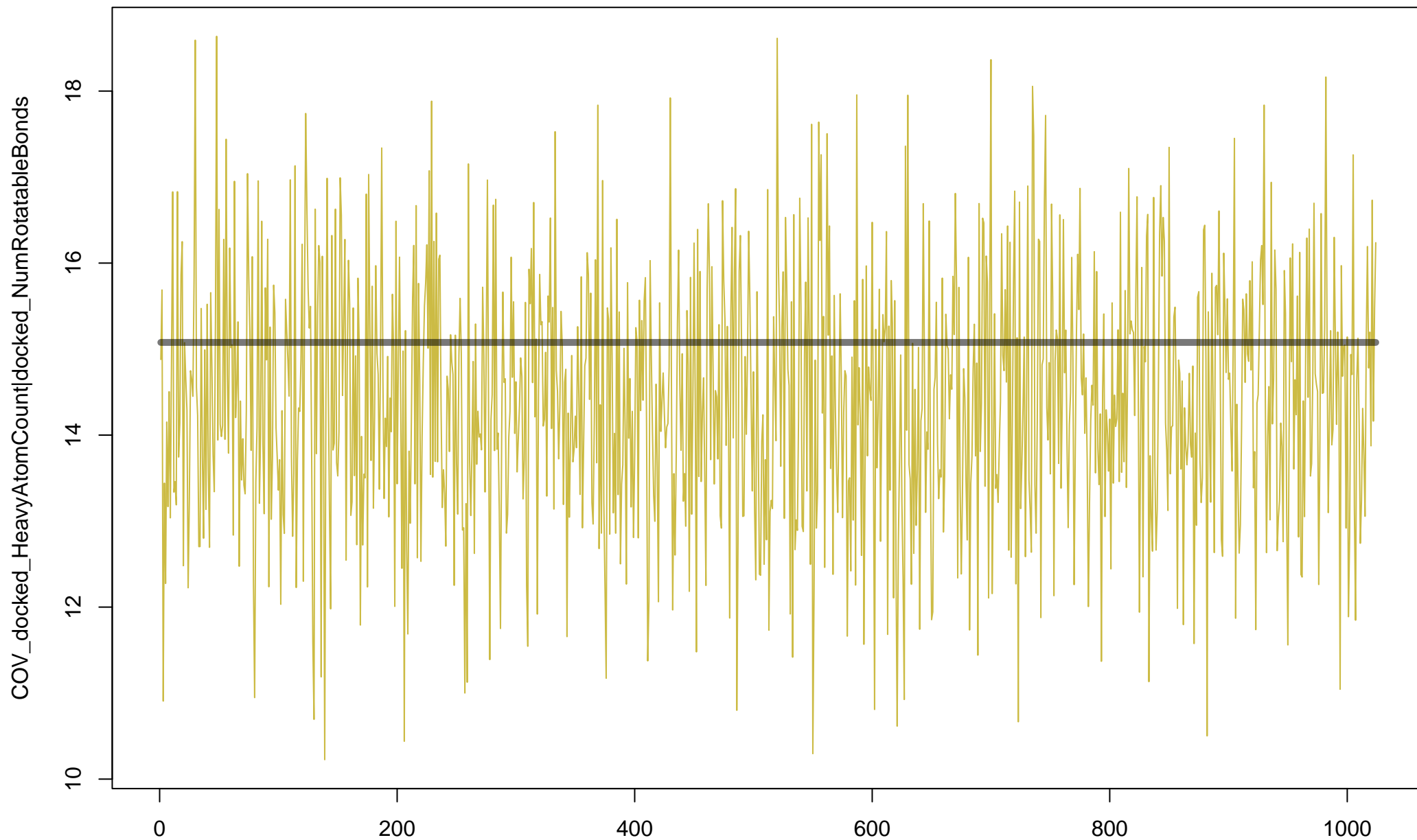
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0446 | MCSE(6.27) = 3.46 | stat: TRUE | burn: 0 | percentile: 24.8



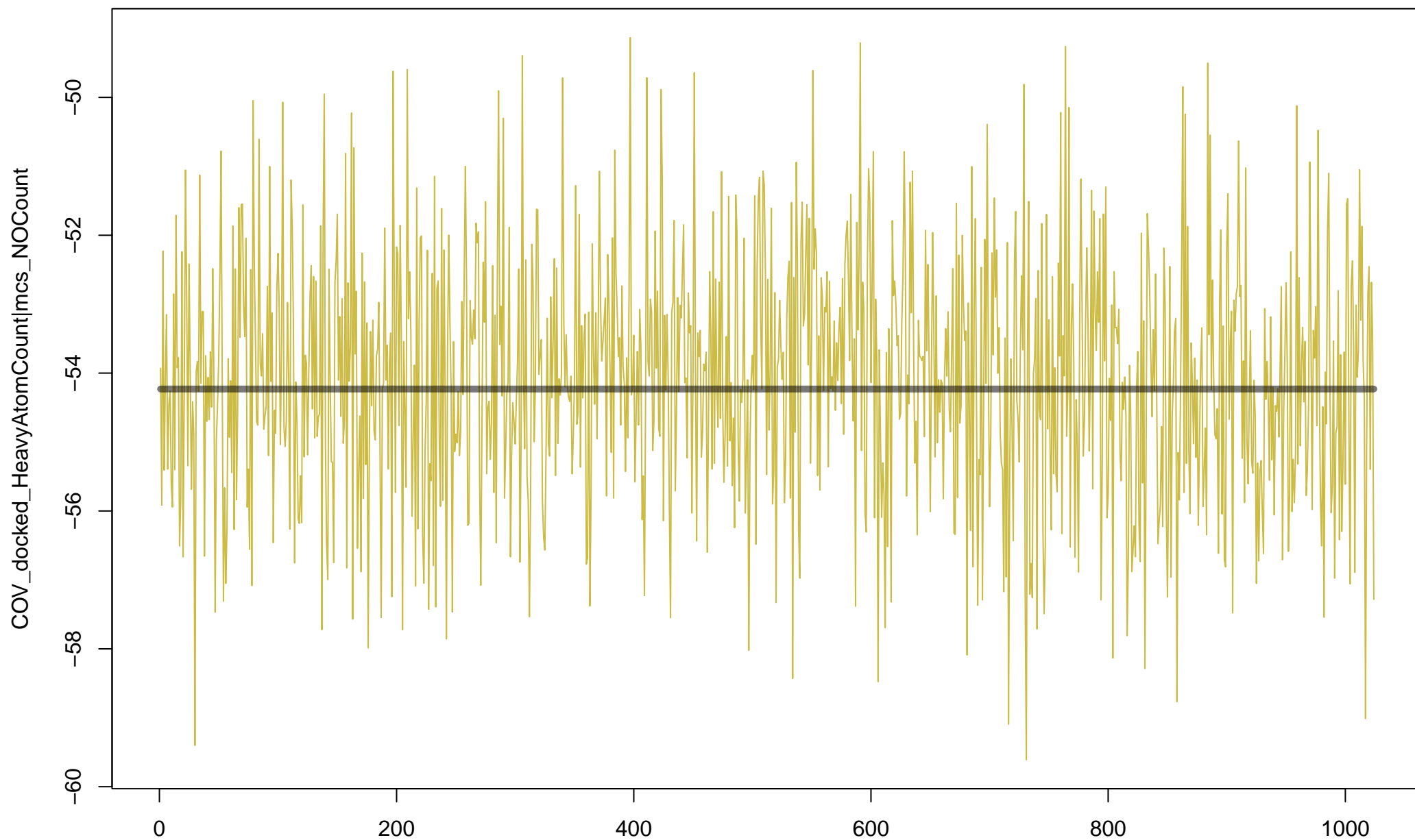
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0387 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | percentile: 48



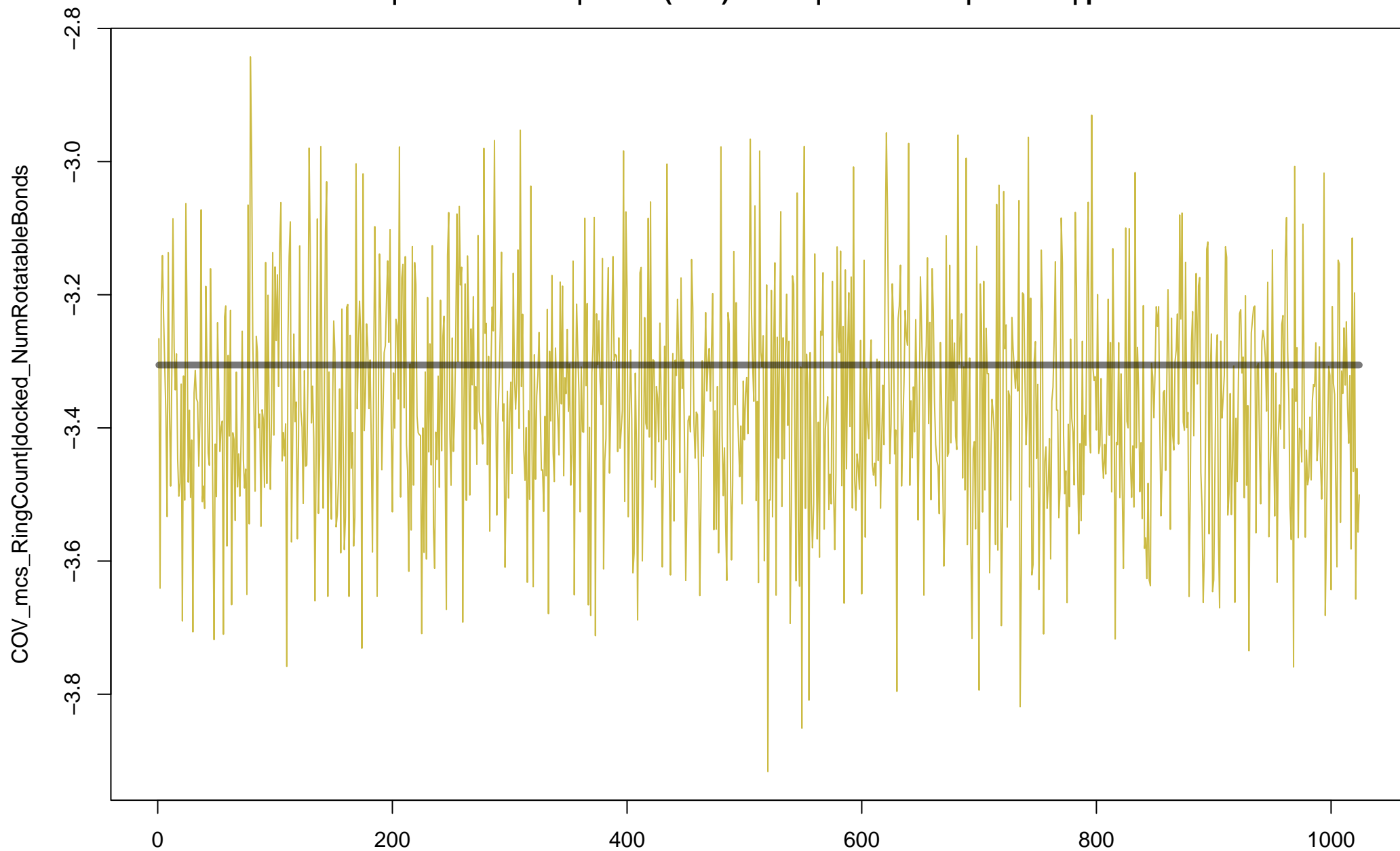
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0394 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0 | percentile: 68.3



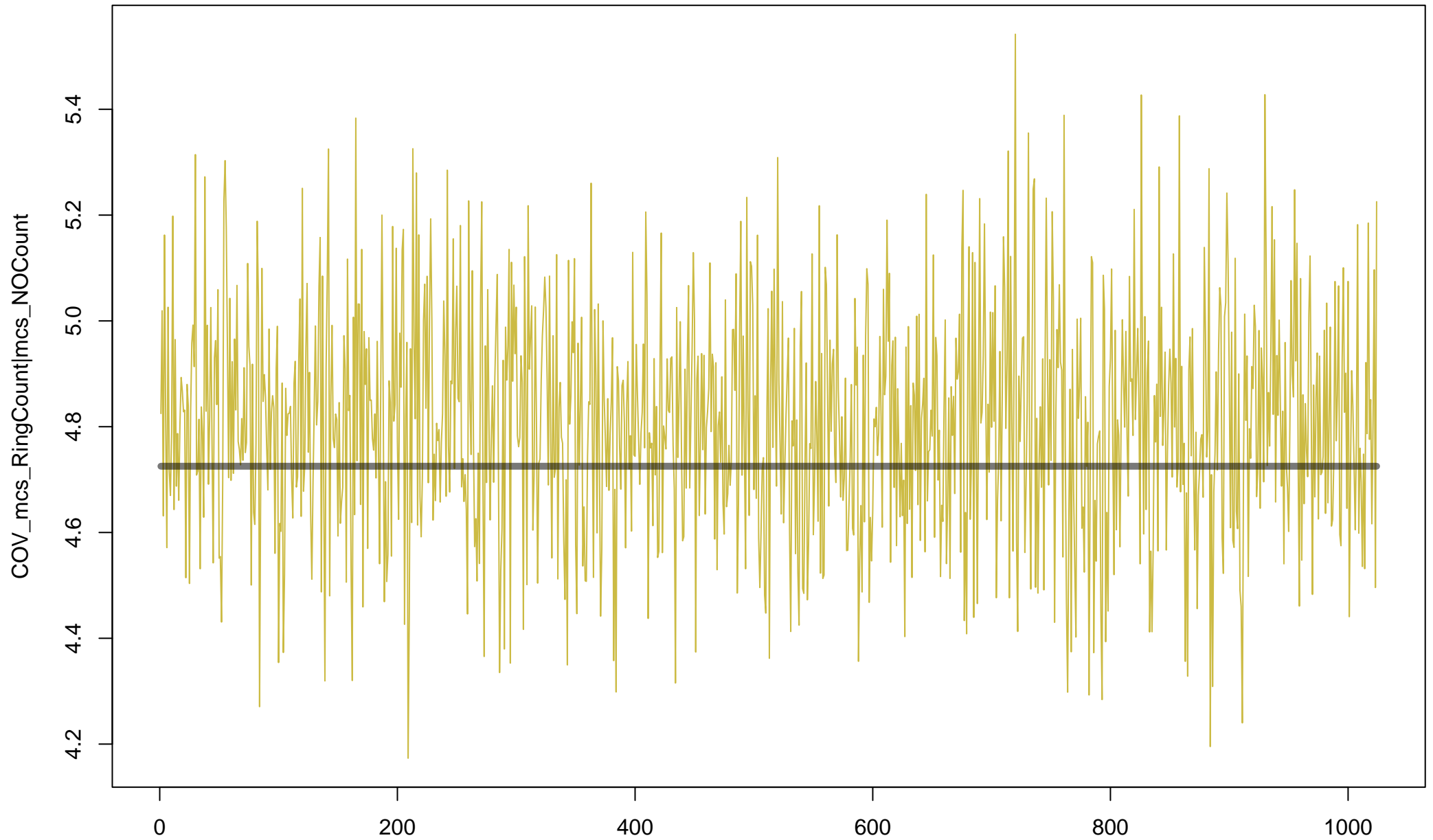
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0577 | MCSE(6.27) = 3.35 | stat: TRUE | burn: 0 | percentile: 45.1



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0714 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0 | percentile: 65.1



COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.0539 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0 | percentile: 35



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0377 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | percentile: 16.8

