

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.720885394034588

max MCSE = 13.8443325572374

all stationary: FALSE

burn: 0

min percent.: 0

-- STATS 2D --

min ESS = 4.36590855170967

max BMK = 0.483359912456478

max MCSE = 11.0164602279477

all stationary: FALSE

burn: 0

min percent.: 0.68359375

-- STATS 1D --

min ESS = 3.26817263430055

max BMK = 1

max MCSE = 12.7240763759819

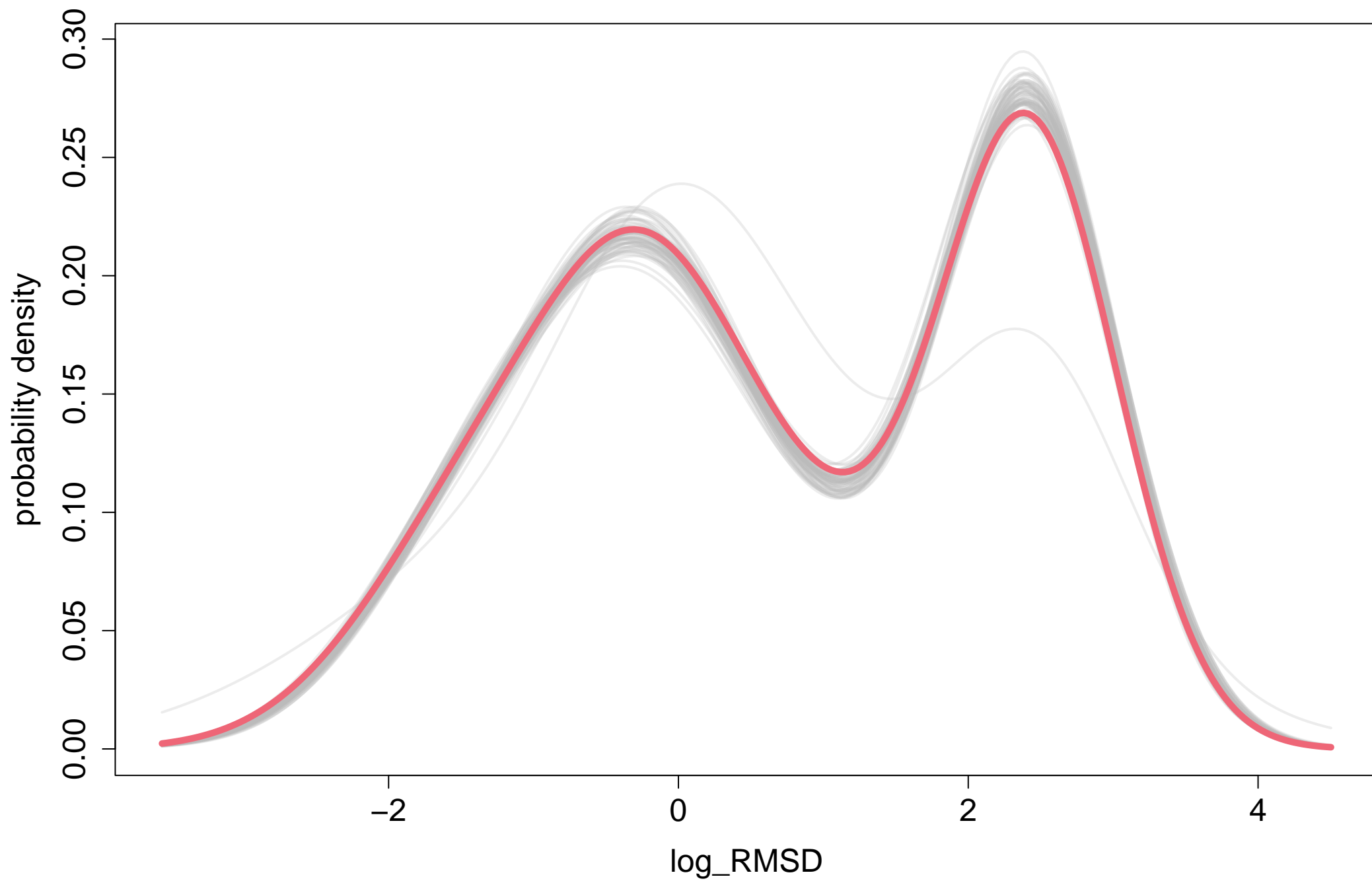
all stationary: FALSE

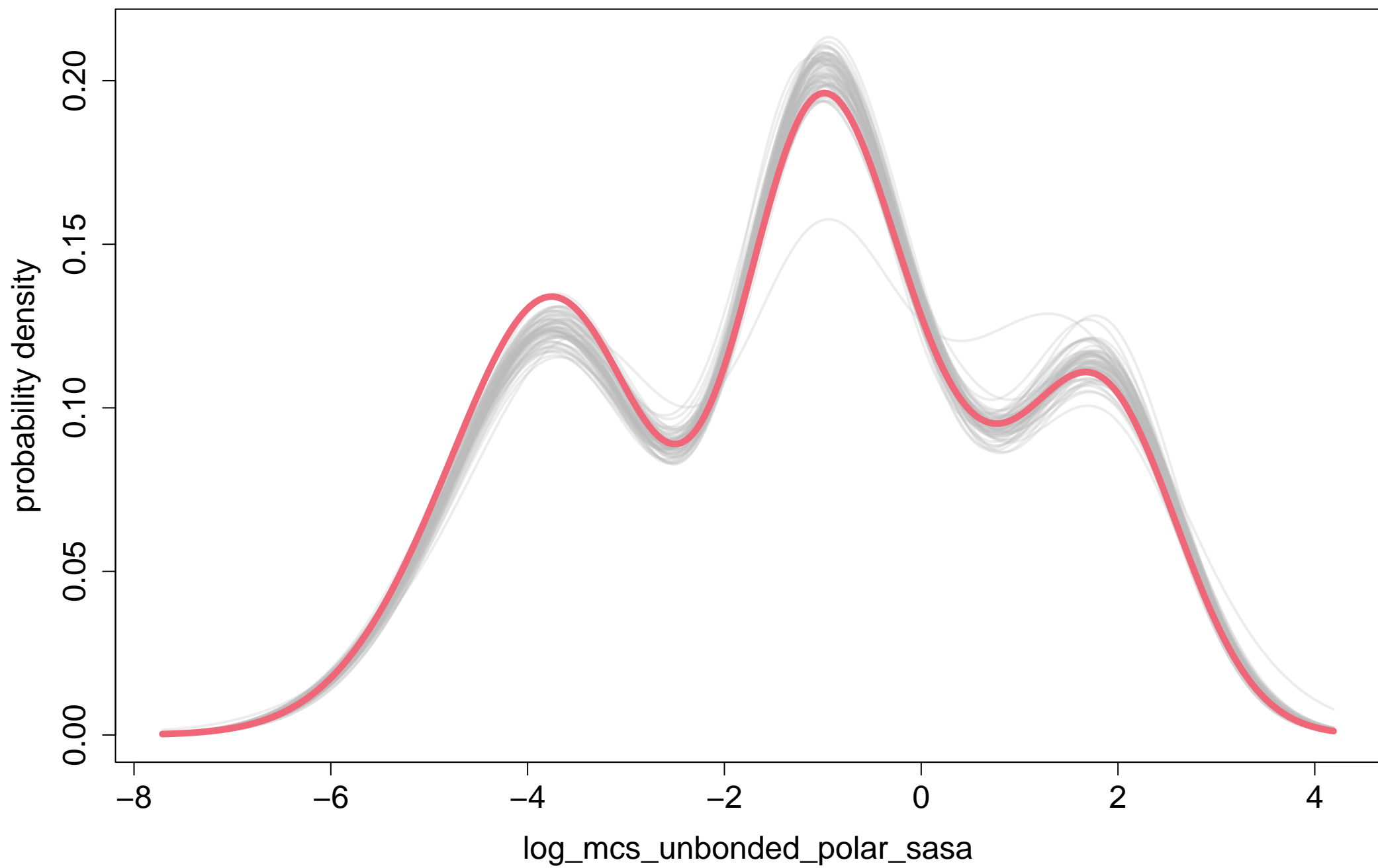
burn: 1020

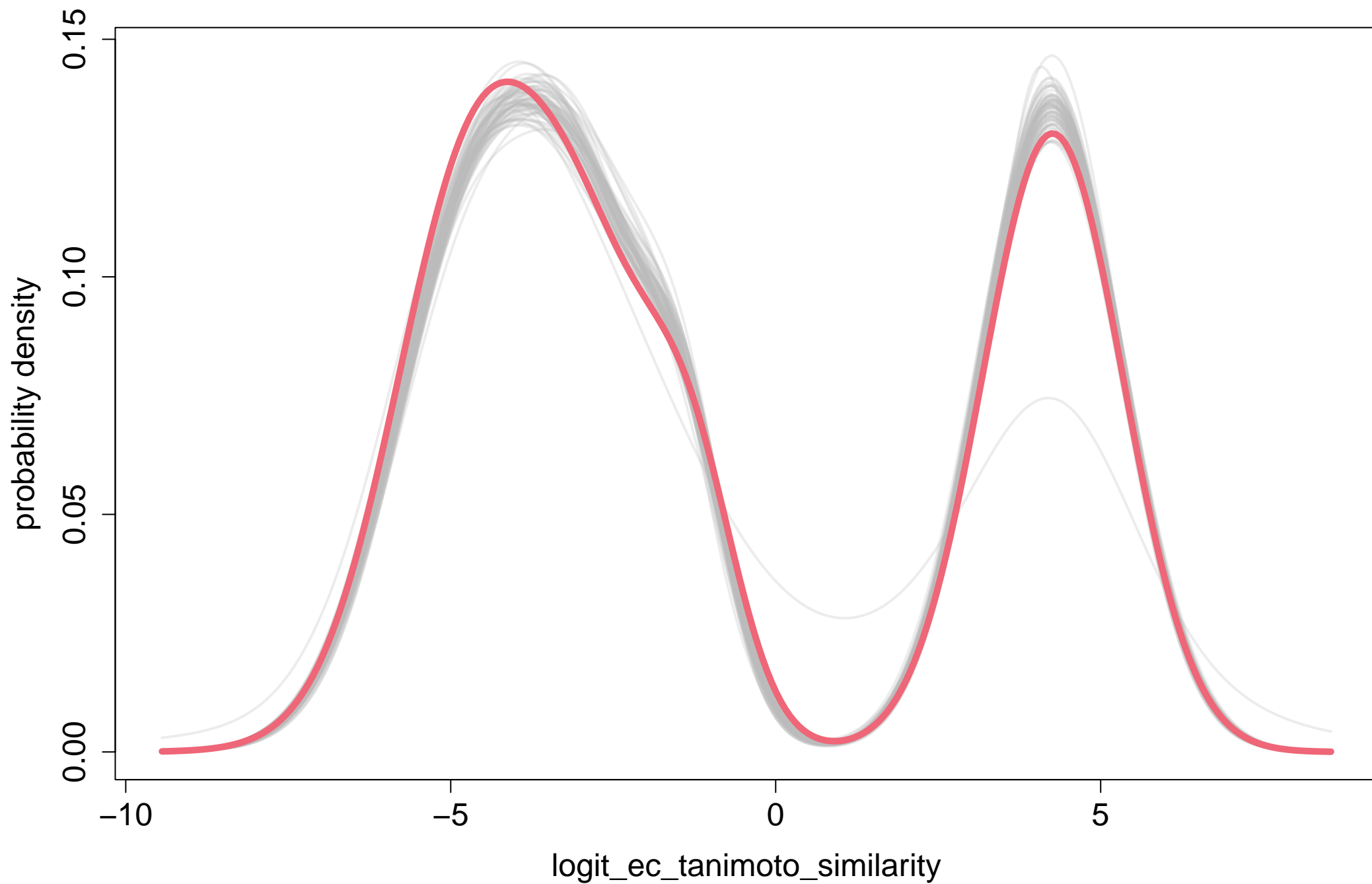
min percent.: 0

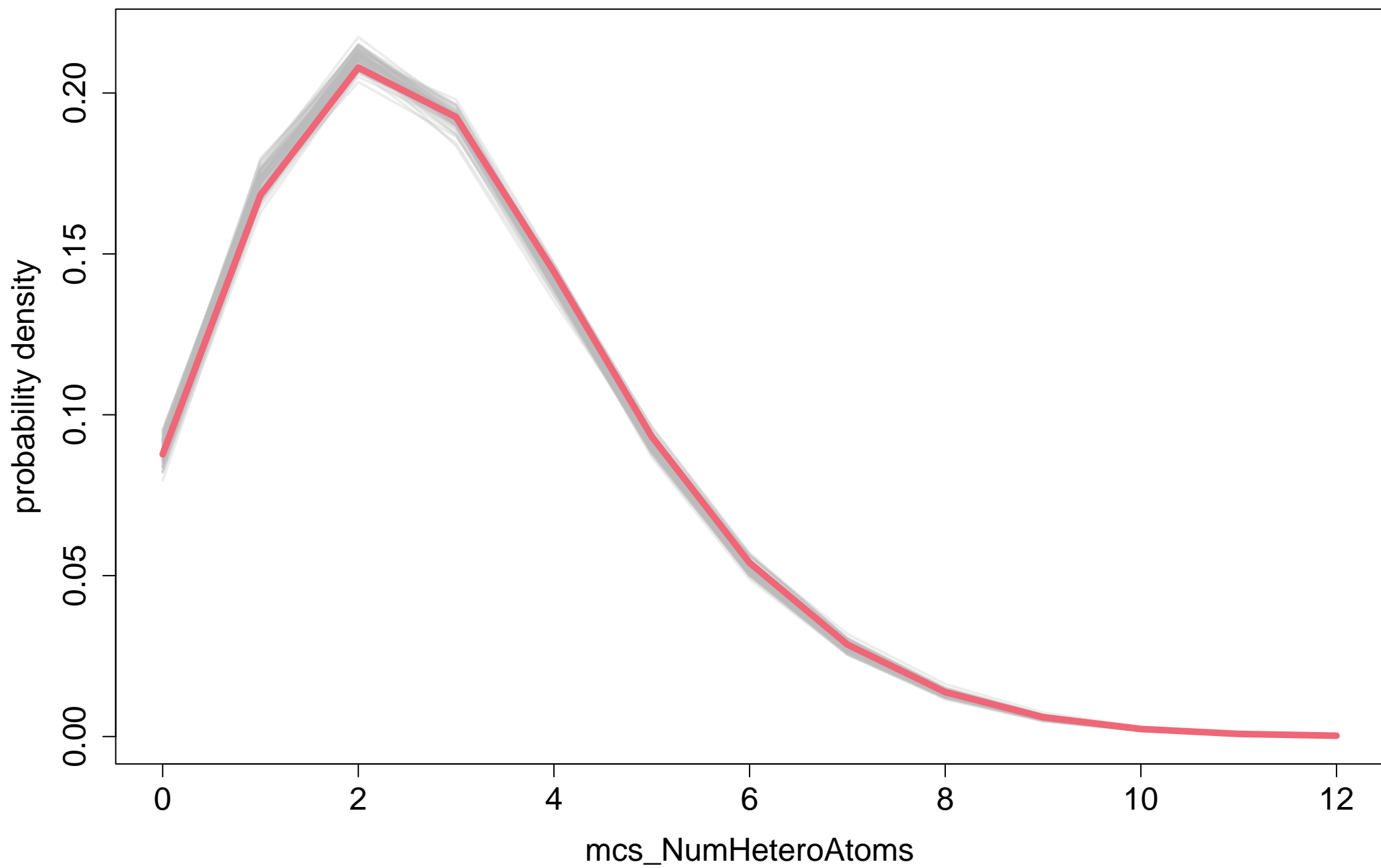
Occupied clusters: 22 of 64

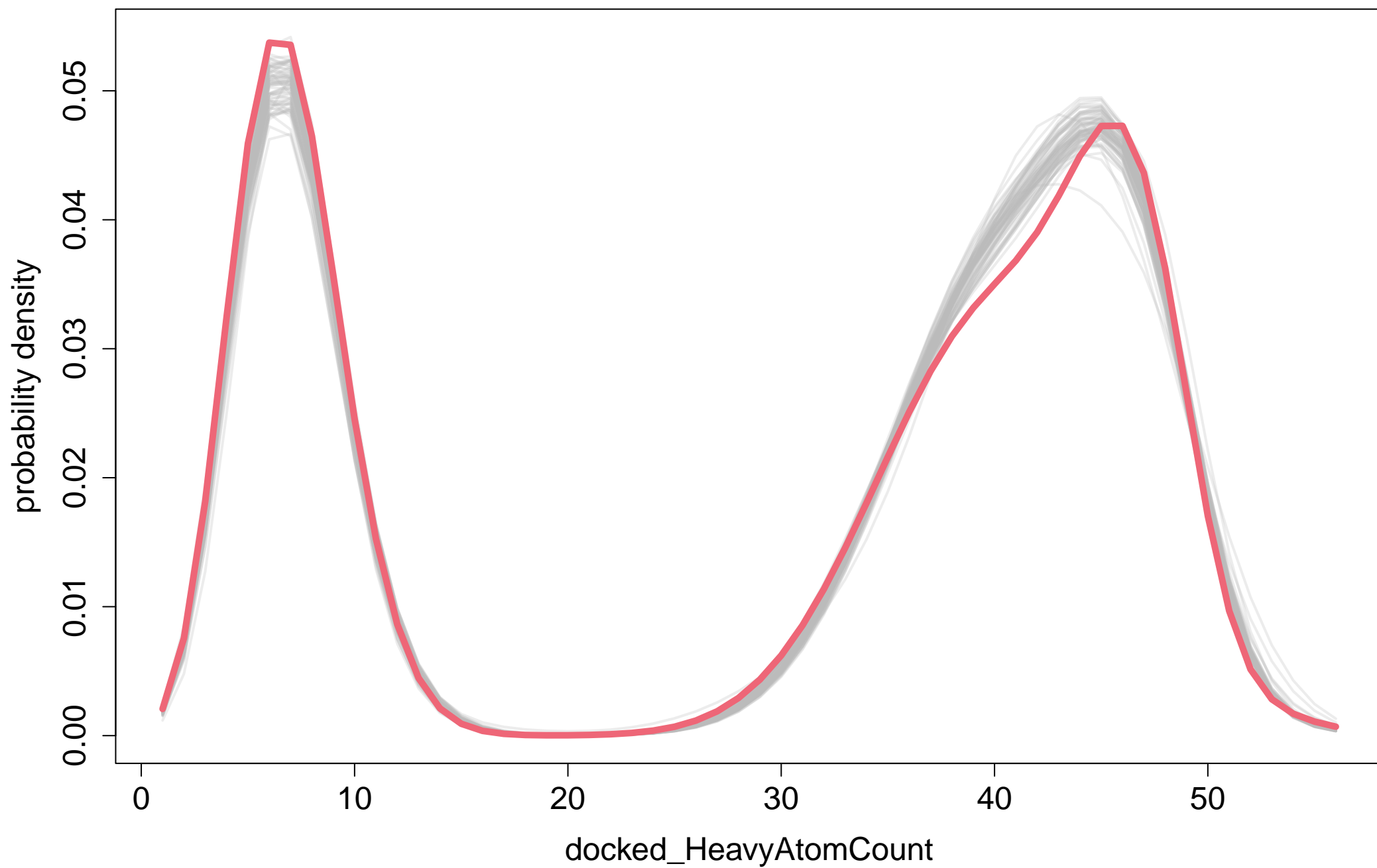
LL: -62600 +- 155

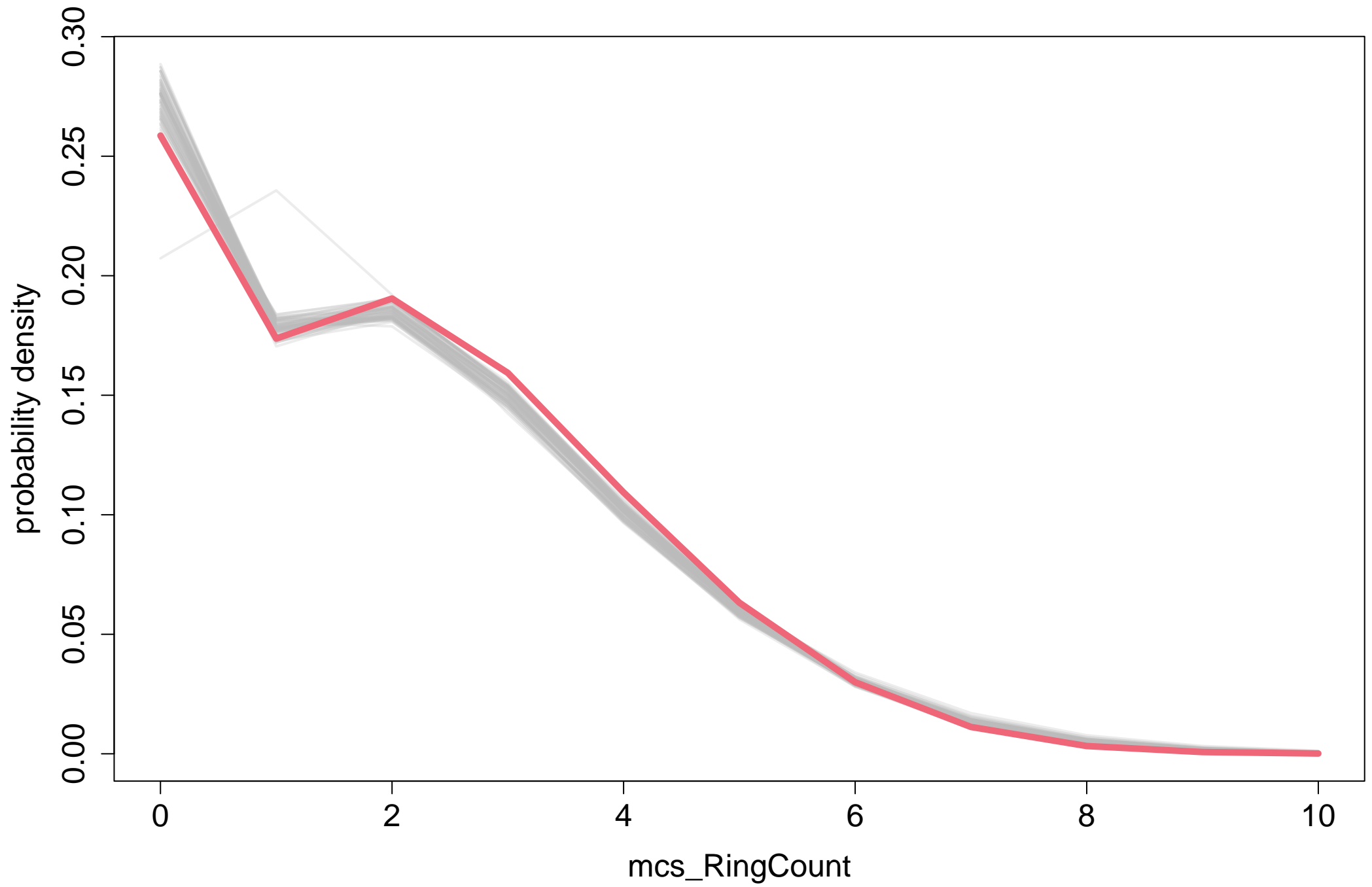


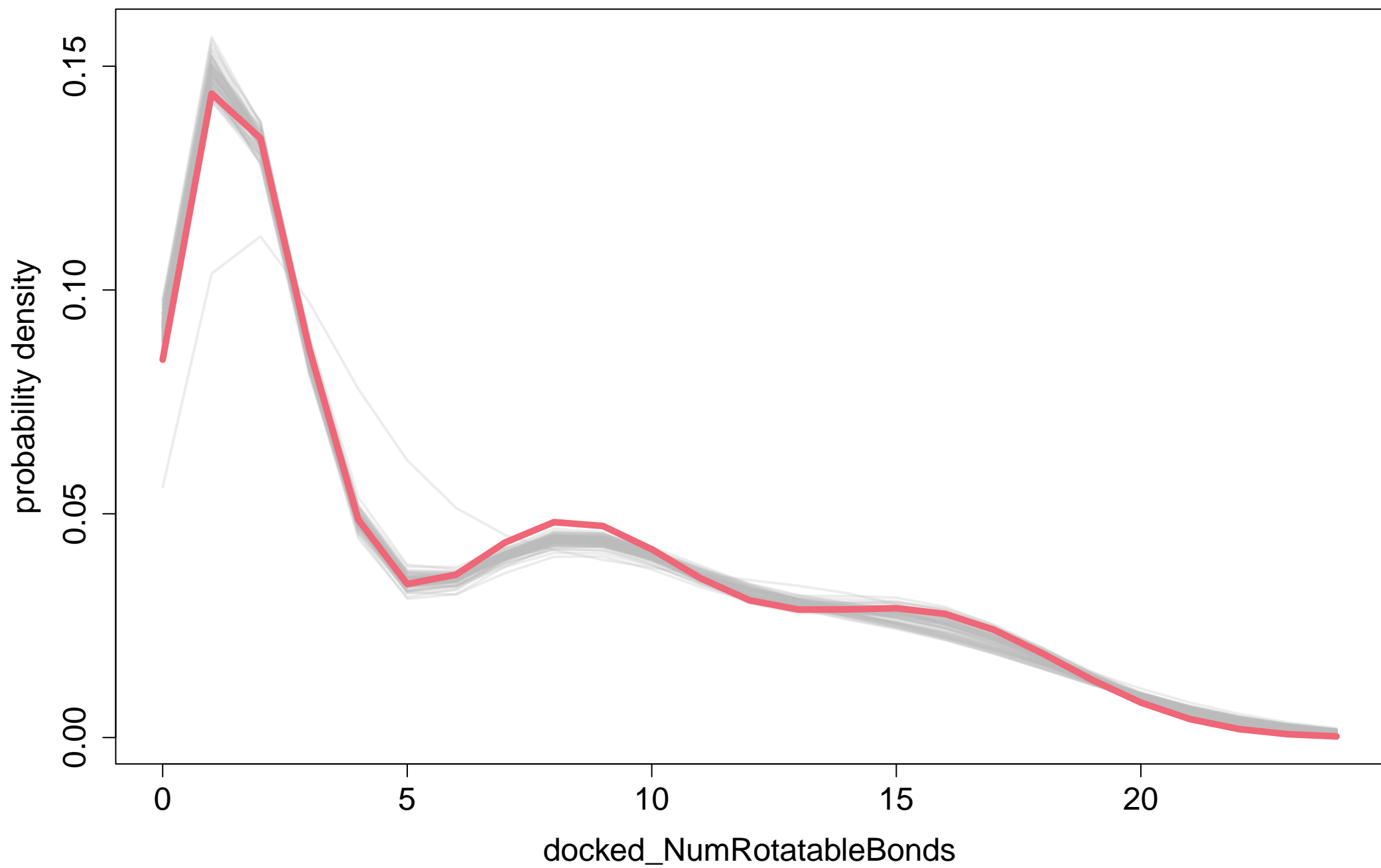


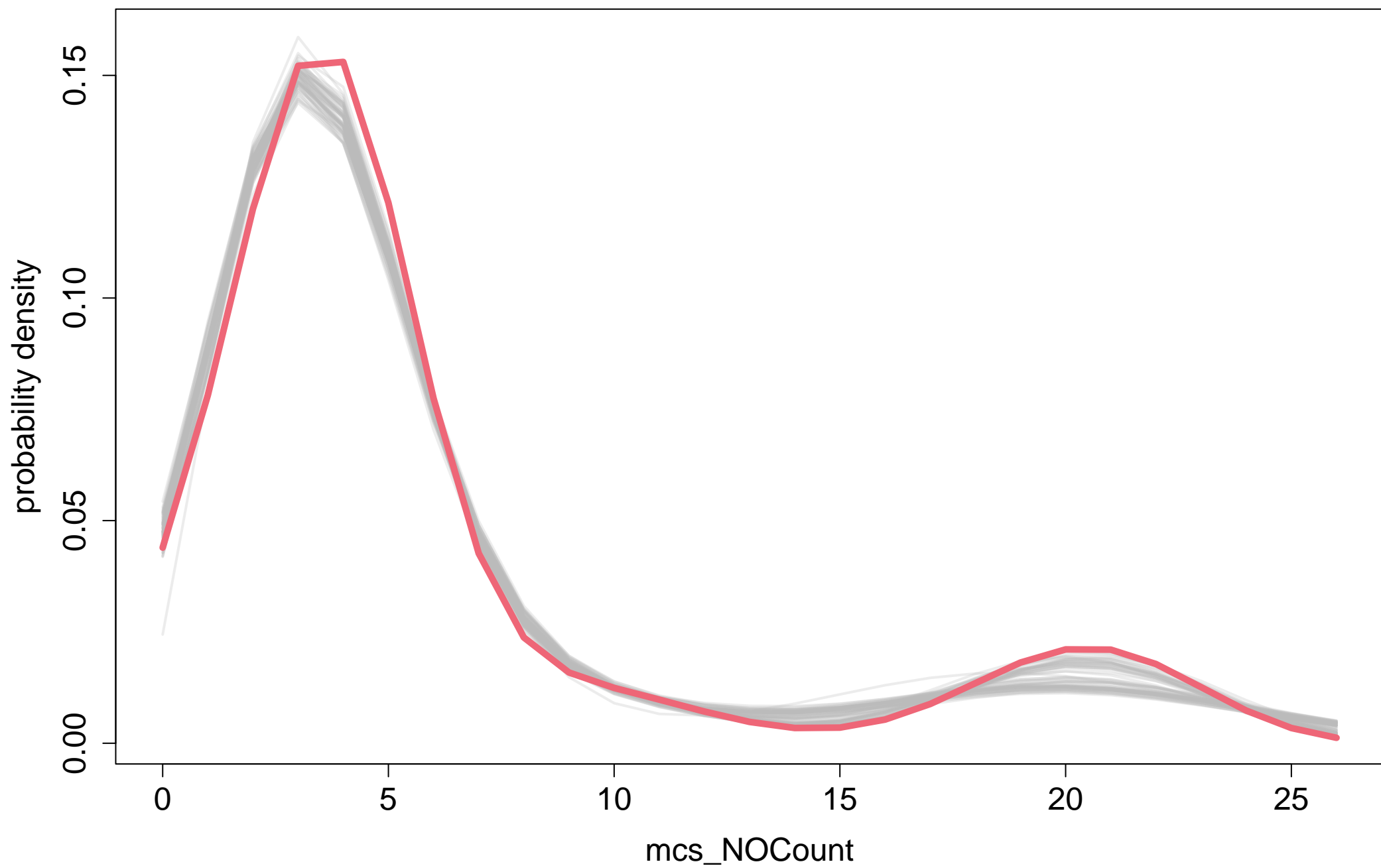


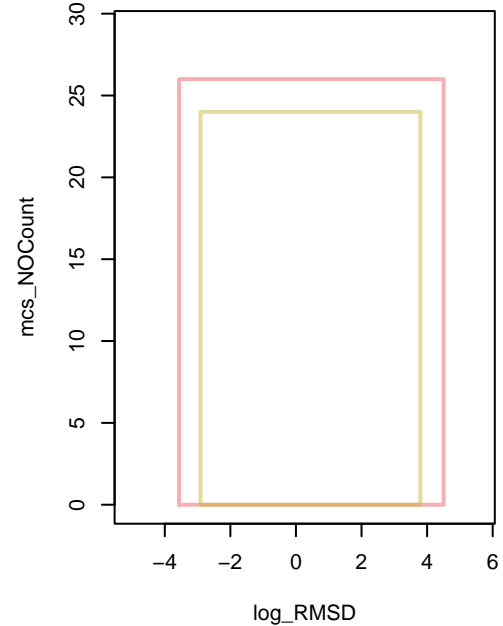
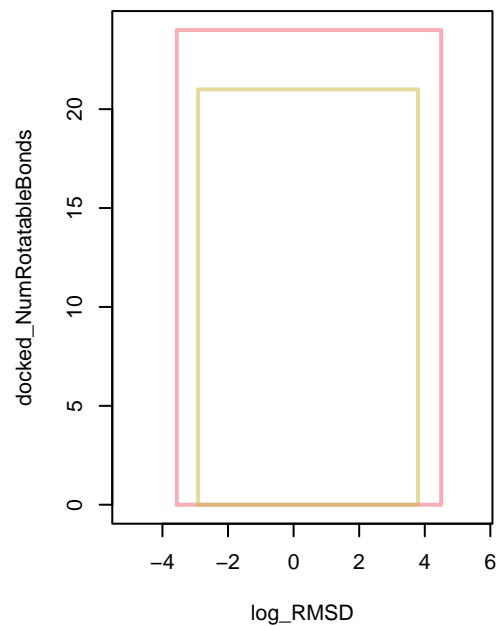
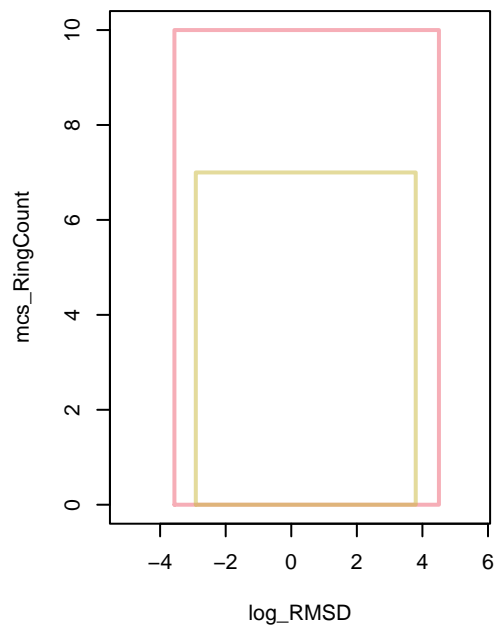
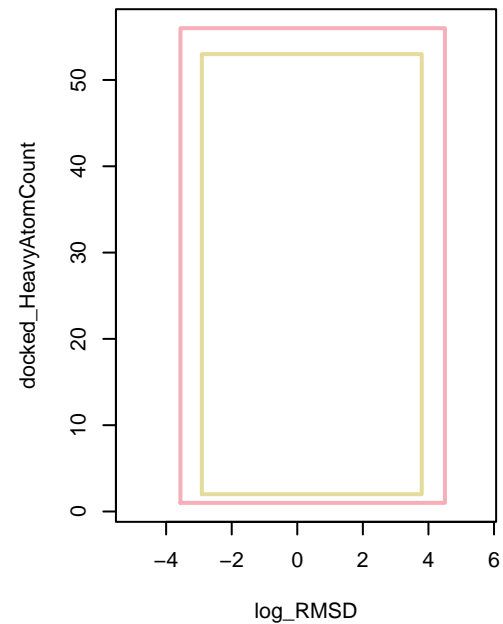
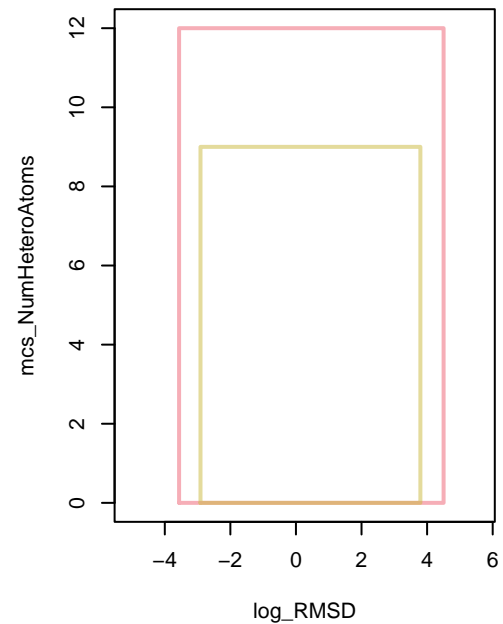
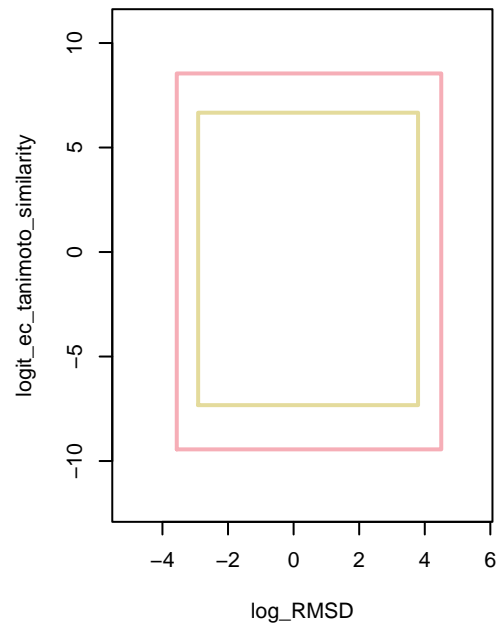
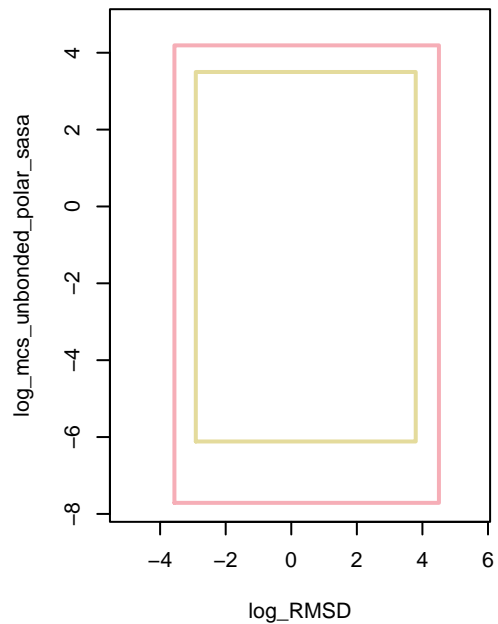




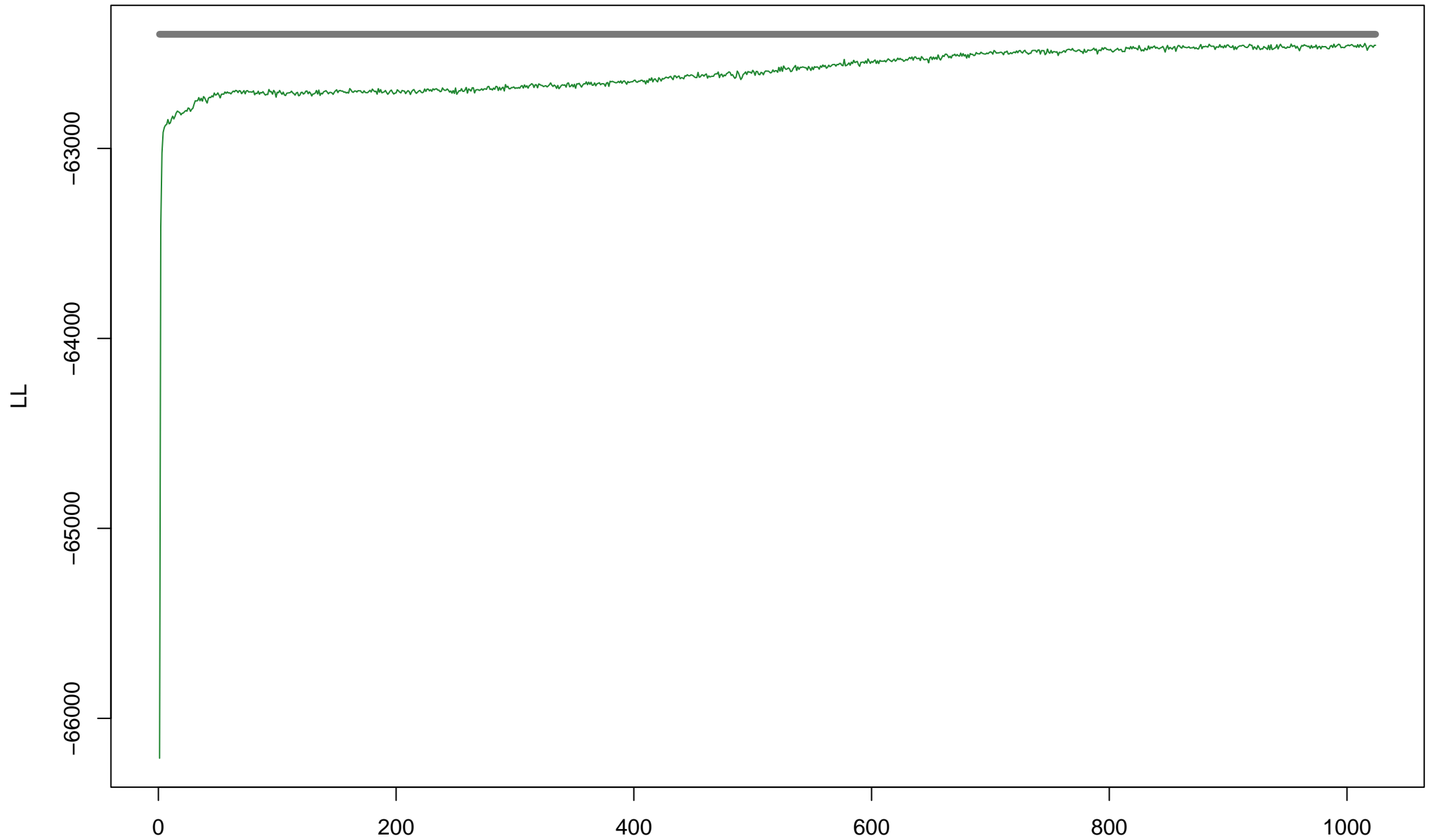






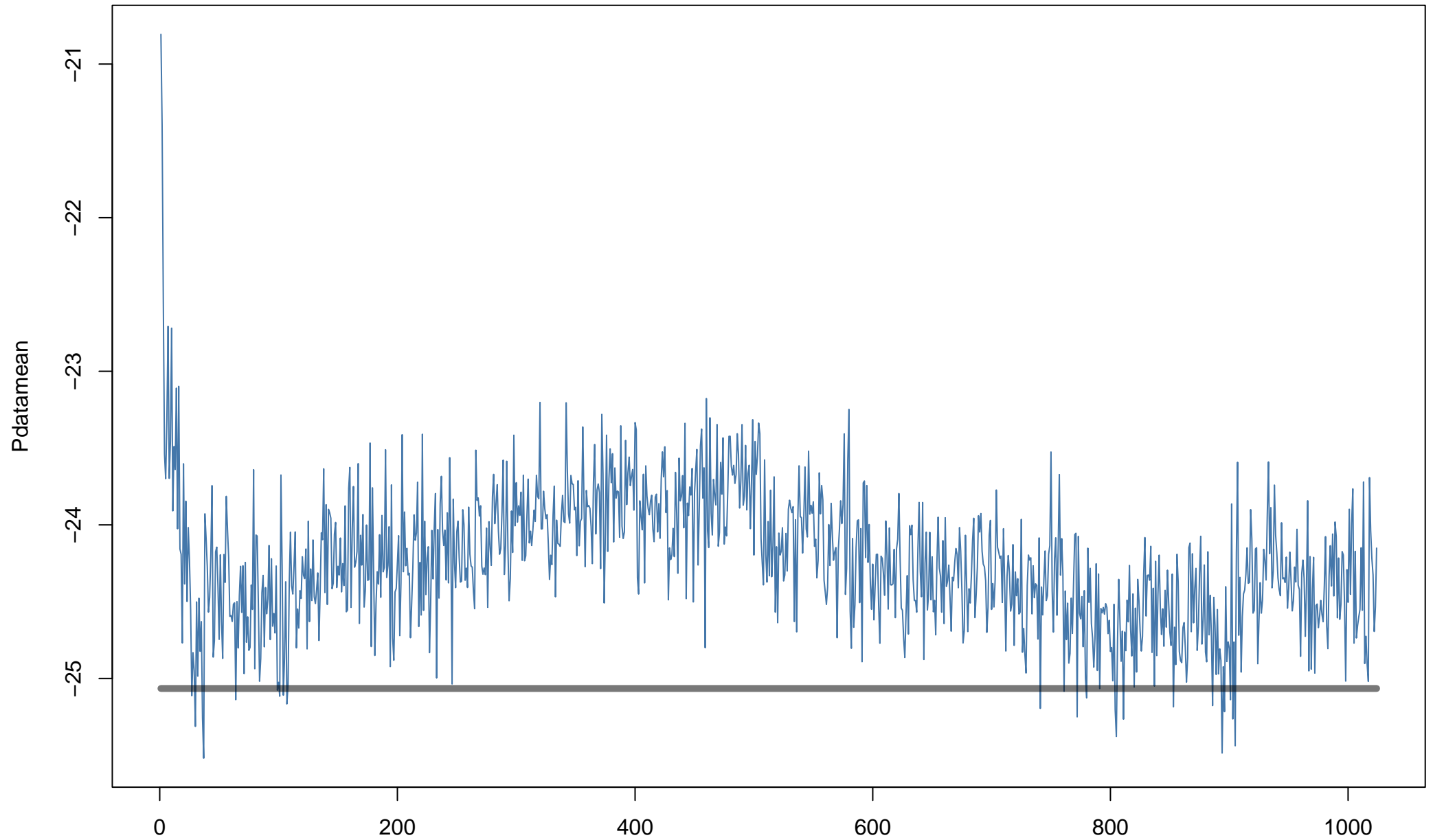


LL



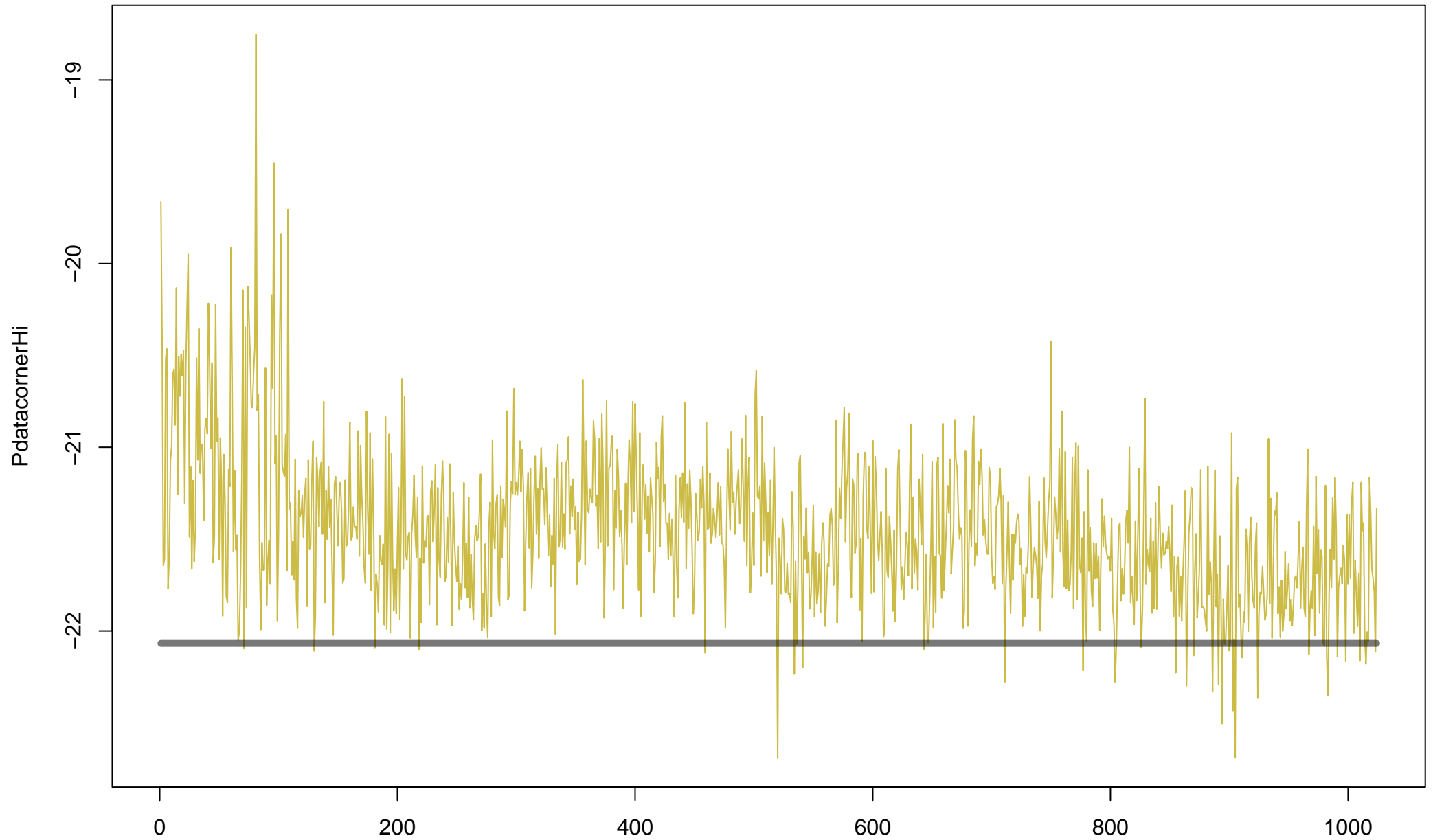
Pdatamean

ESS = 2.22e-16 | BMK = 0.294 | MCSE(6.27) = 6.94 | stat: TRUE | burn: 0 | percentile: 2.34



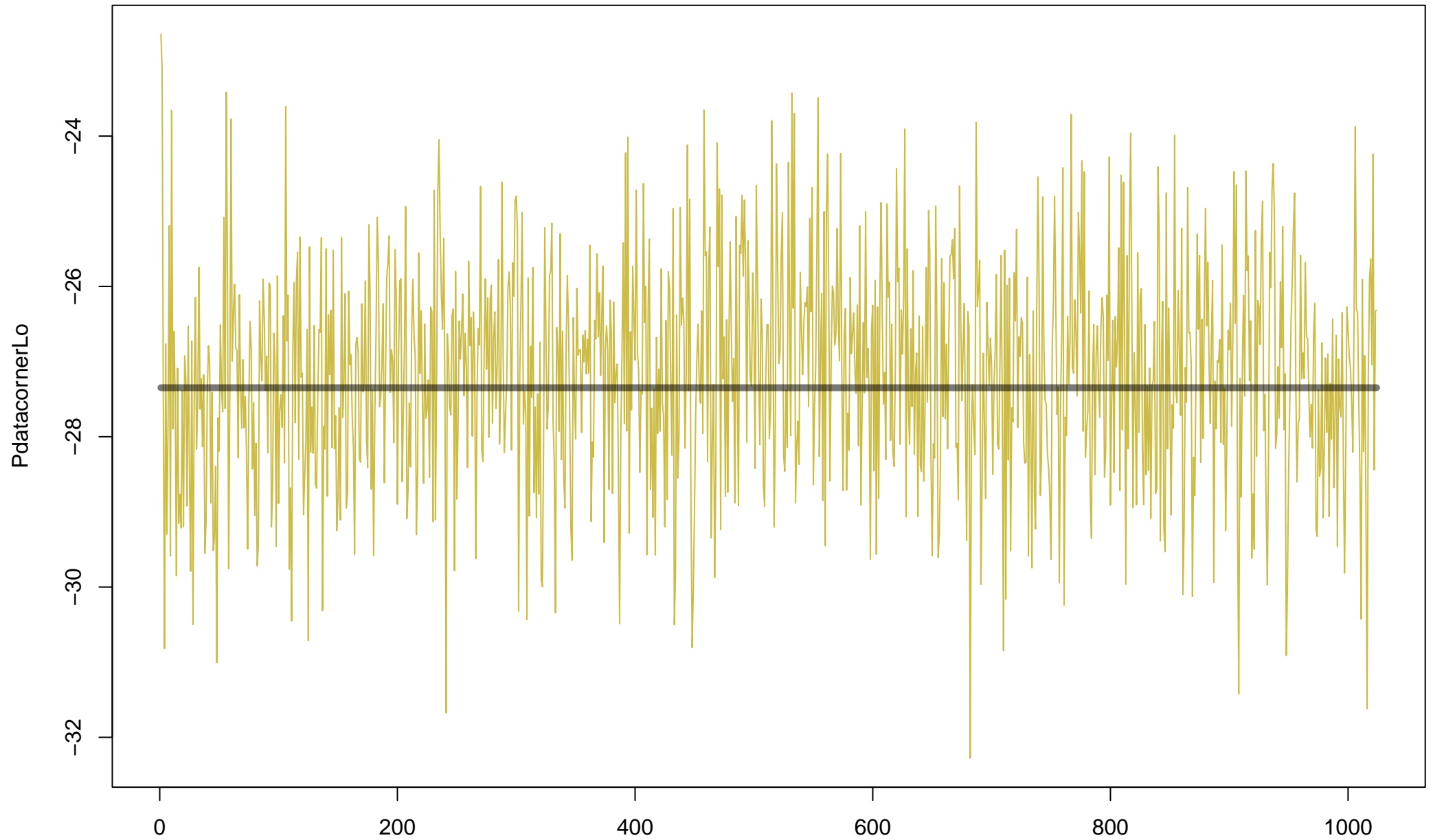
PdatacornerHi

ESS = $2.22\text{e-}16$ | BMK = 0.28 | MCSE(6.27) = 8.26 | stat: TRUE | burn: 0 | percentile: 3.52



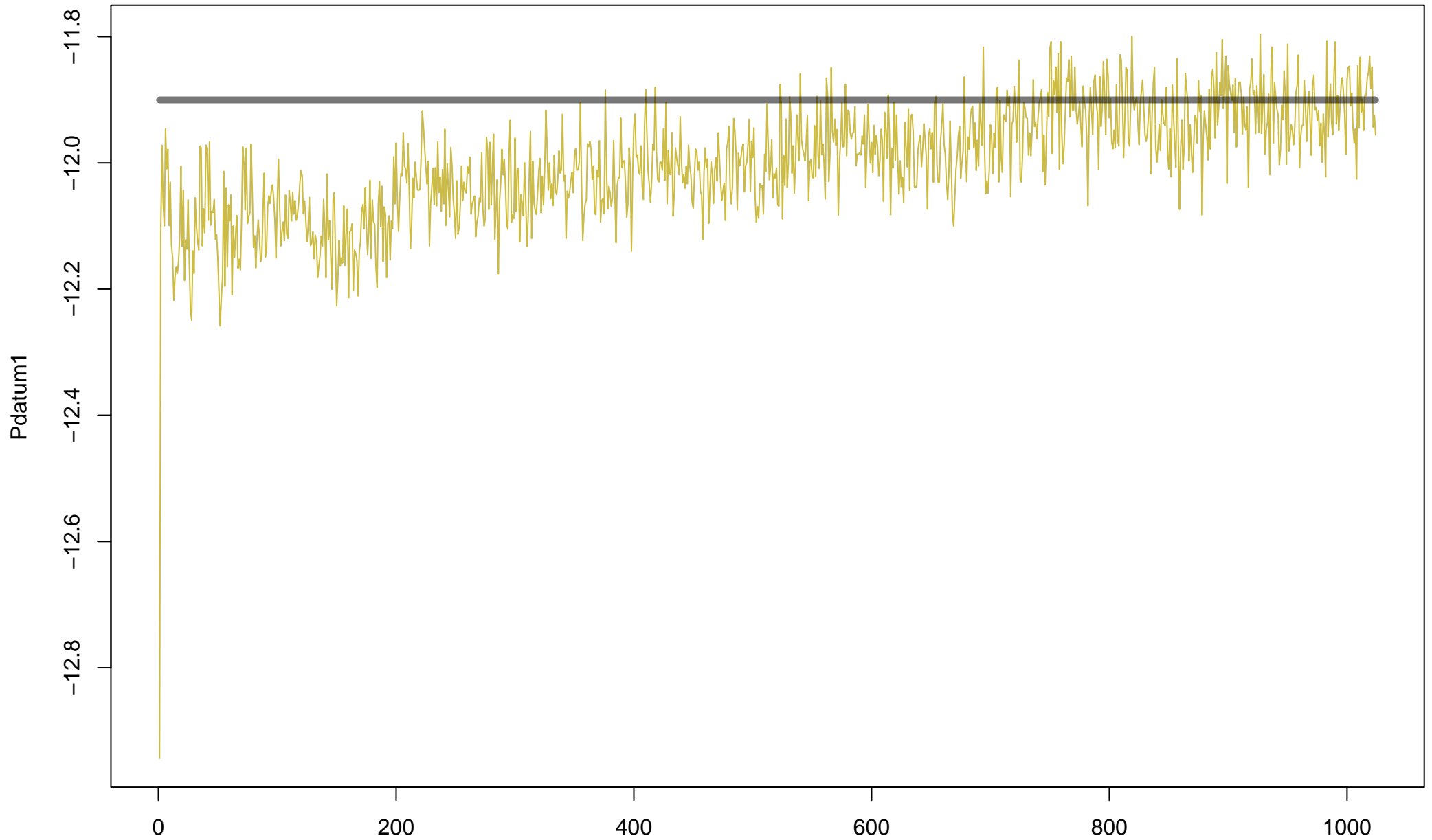
PdatacornerLo

ESS = 2.22e-16 | BMK = 0.169 | MCSE(6.27) = 3.65 | stat: TRUE | burn: 0 | percentile: 44.4

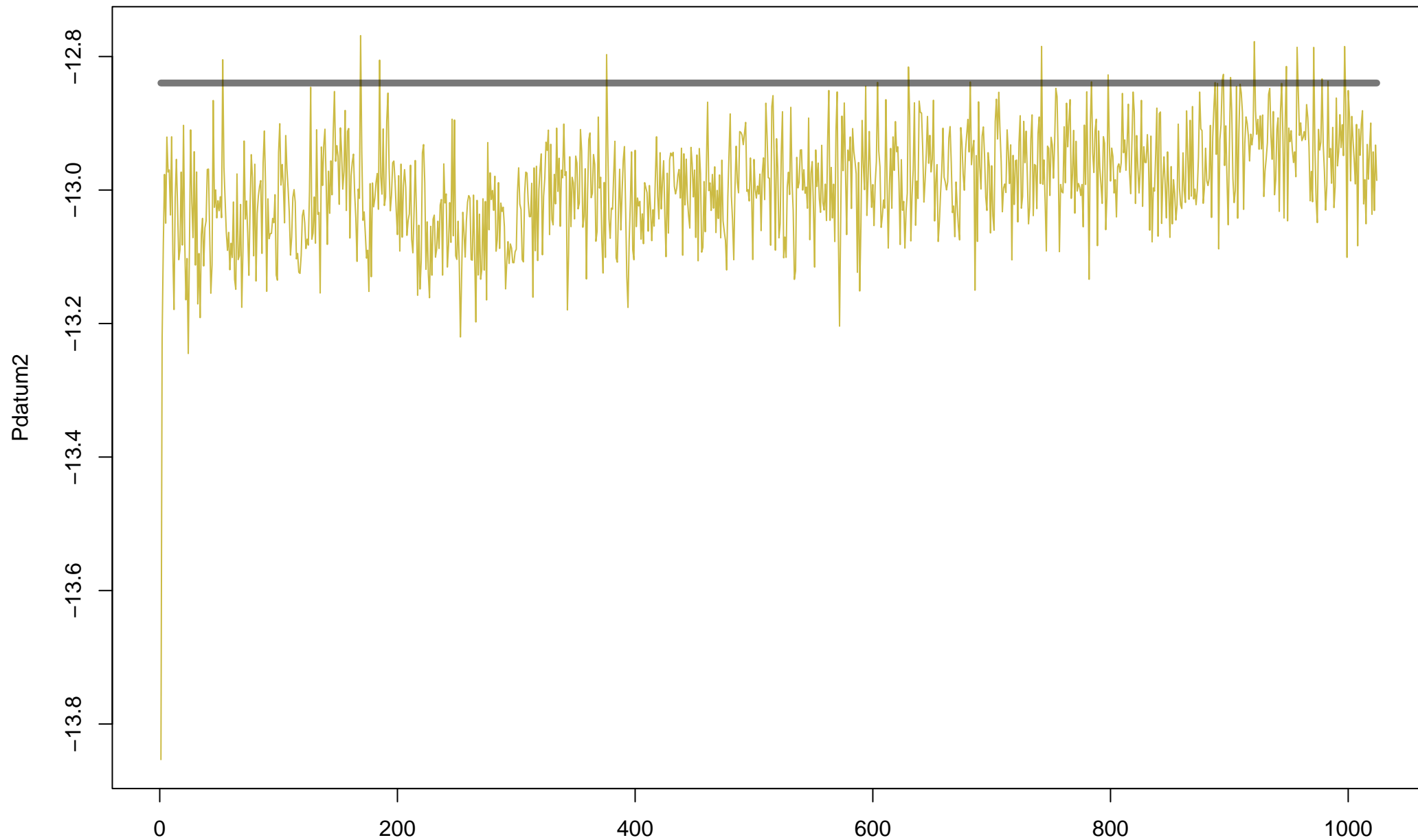


Pdatum1

ESS = 7.16 | BMK = 0.569 | MCSE(6.27) = 13.8 | stat: FALSE | burn: 0 | percentile: 86.9

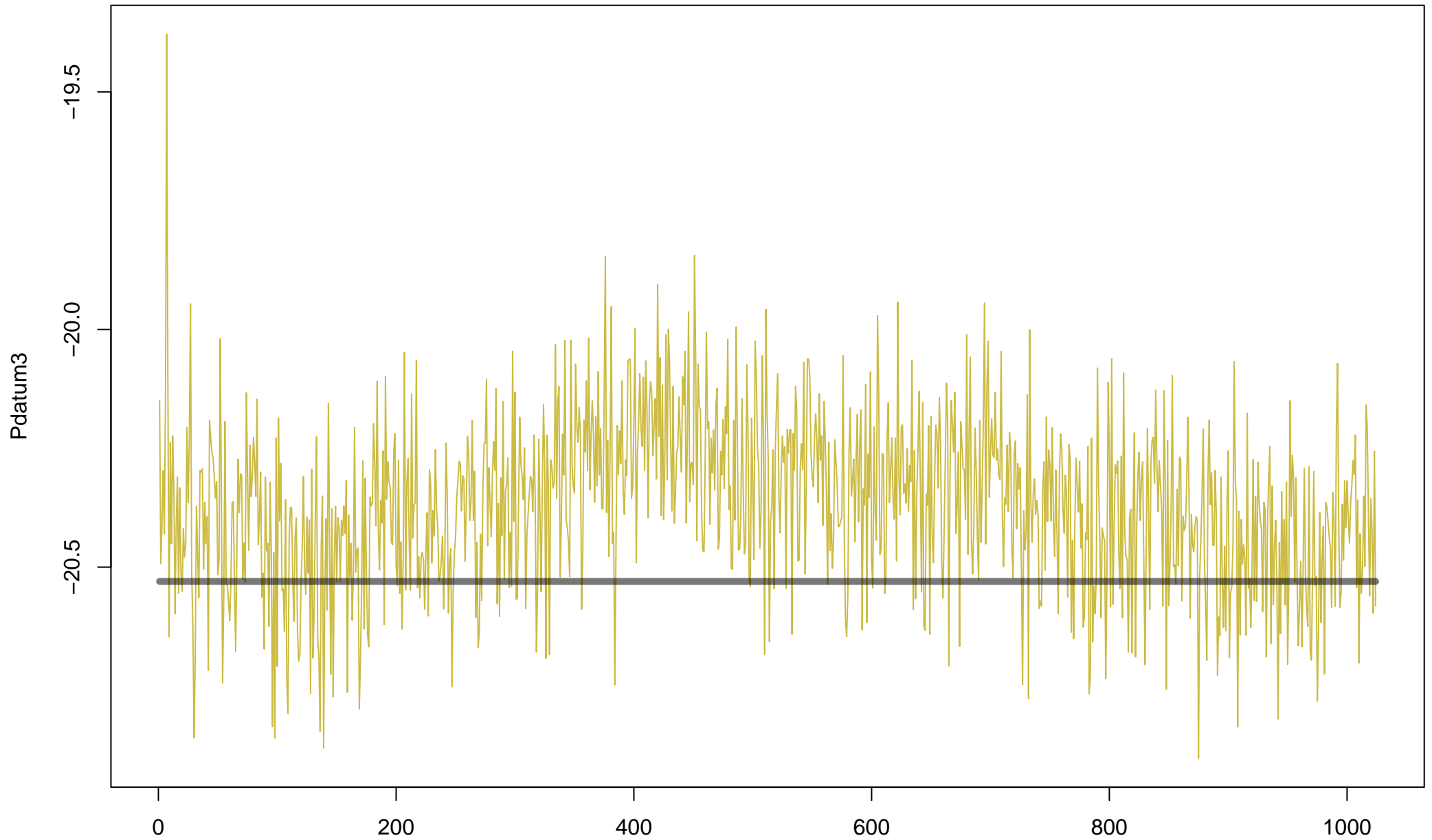


Pdatum2
ESS = 25.1 | BMK = 0.293 | MCSE(6.27) = 9 | stat: FALSE | burn: 0 | percentile: 97.9



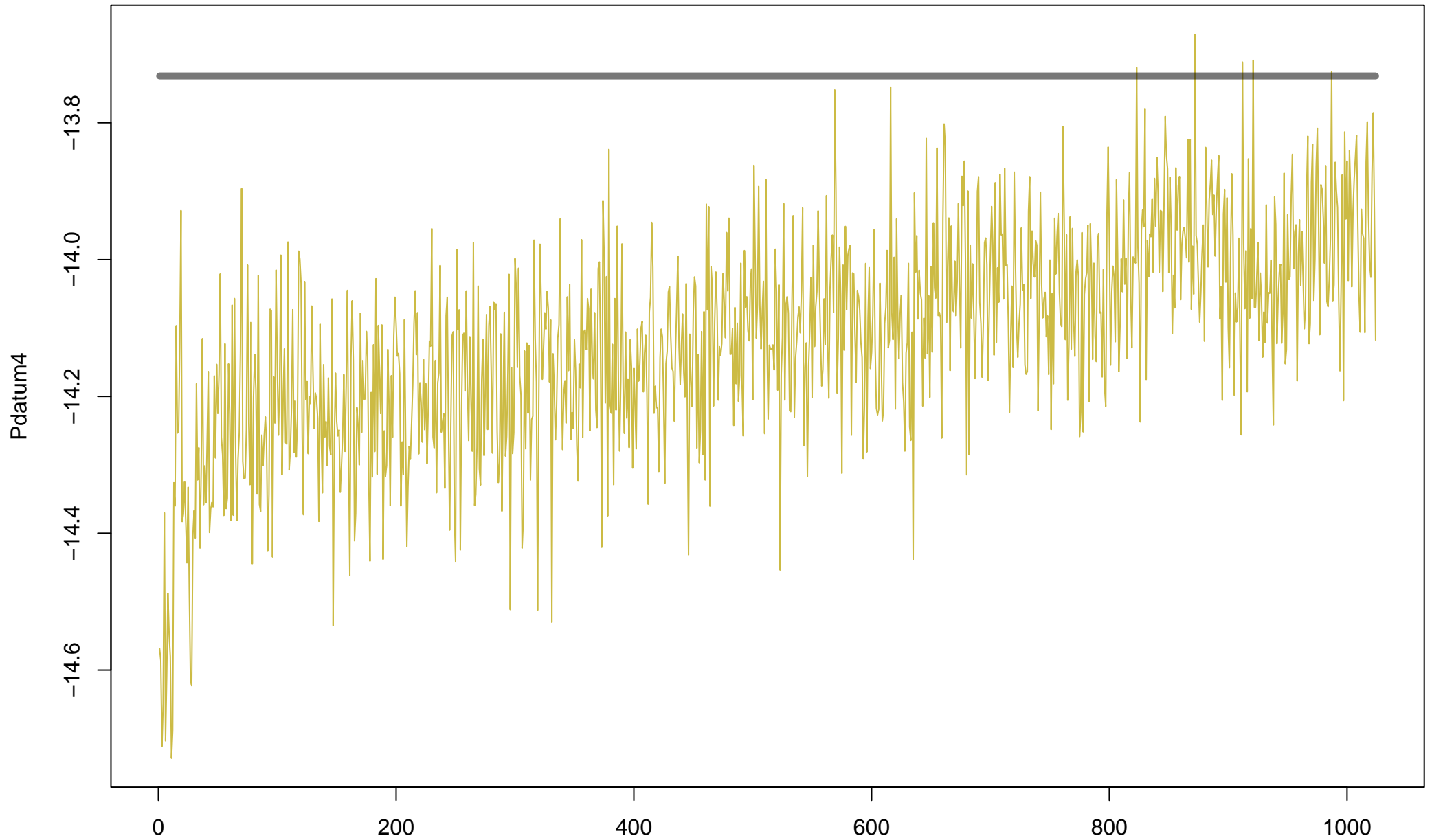
Pdatum3

ESS = $2.22\text{e-}16$ | BMK = 0.0854 | MCSE(6.27) = 7.82 | stat: TRUE | burn: 0 | percentile: 19



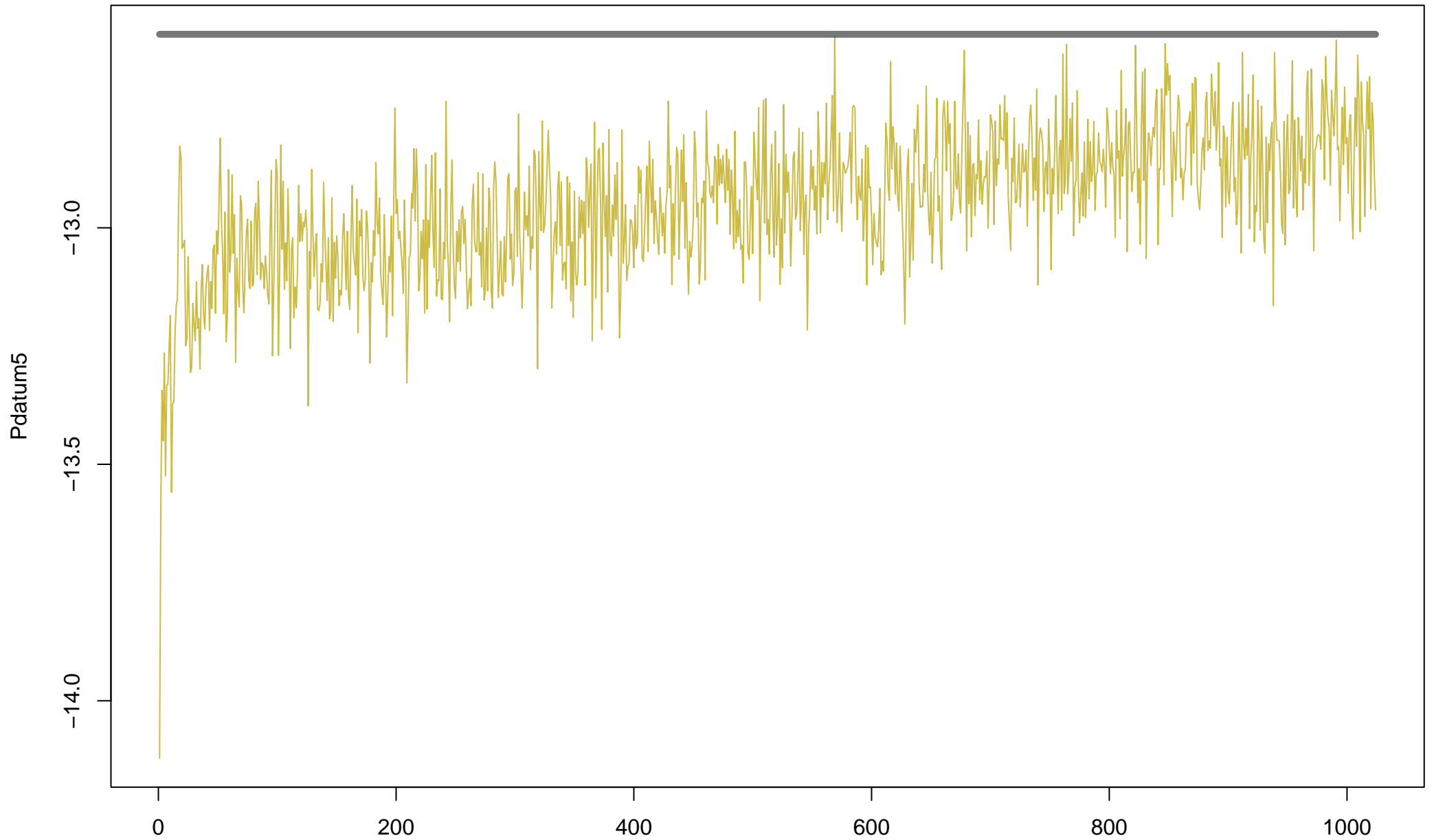
Pdatum4

ESS = 11.9 | BMK = 0.433 | MCSE(6.27) = 12.1 | stat: FALSE | burn: 0 | percentile: 99.5



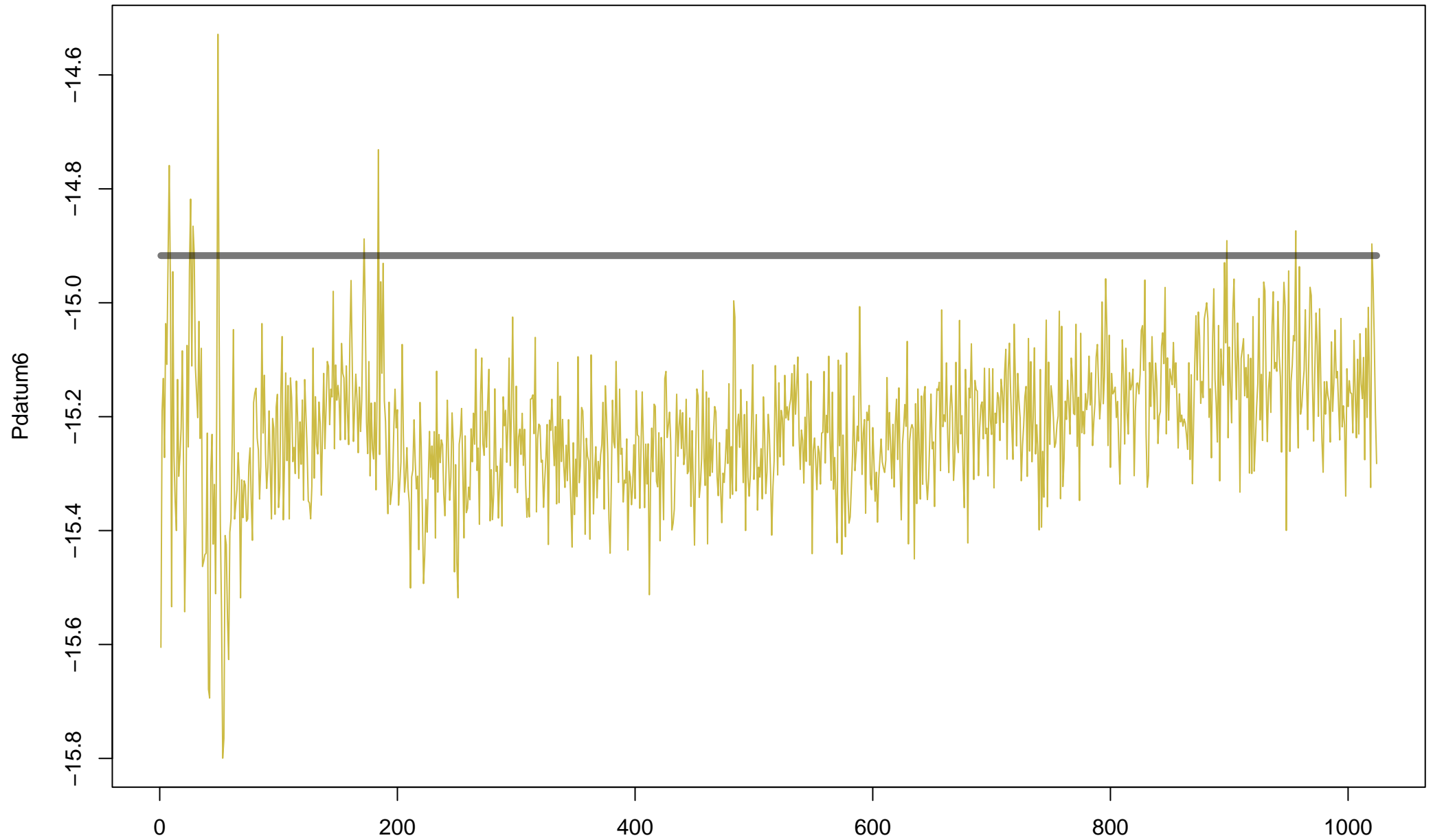
Pdatum5

ESS = 26.7 | BMK = 0.45 | MCSE(6.27) = 12.1 | stat: FALSE | burn: 0 | percentile: 100



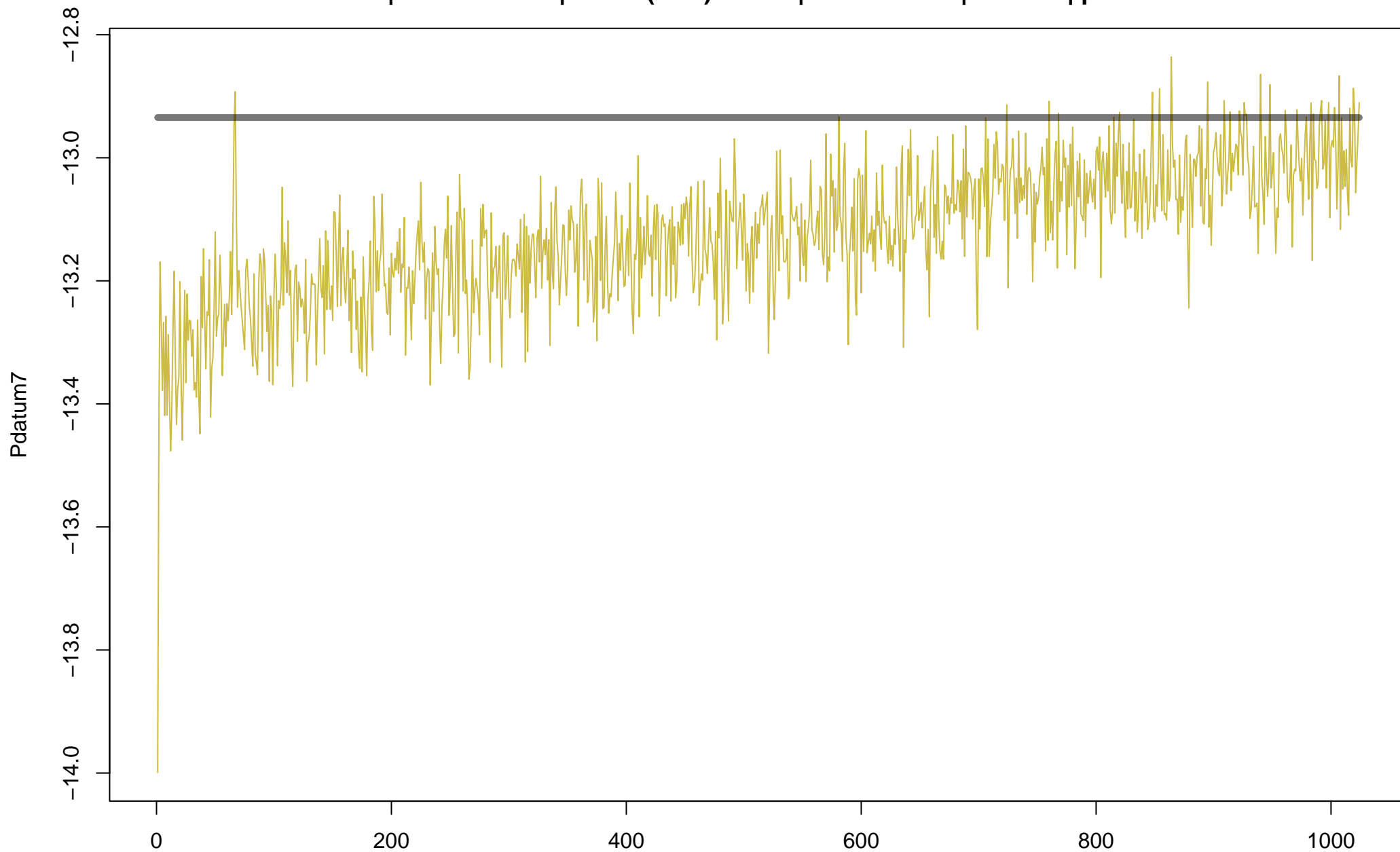
Pdatum6

ESS = 35.4 | BMK = 0.264 | MCSE(6.27) = 8.98 | stat: TRUE | burn: 0 | percentile: 99



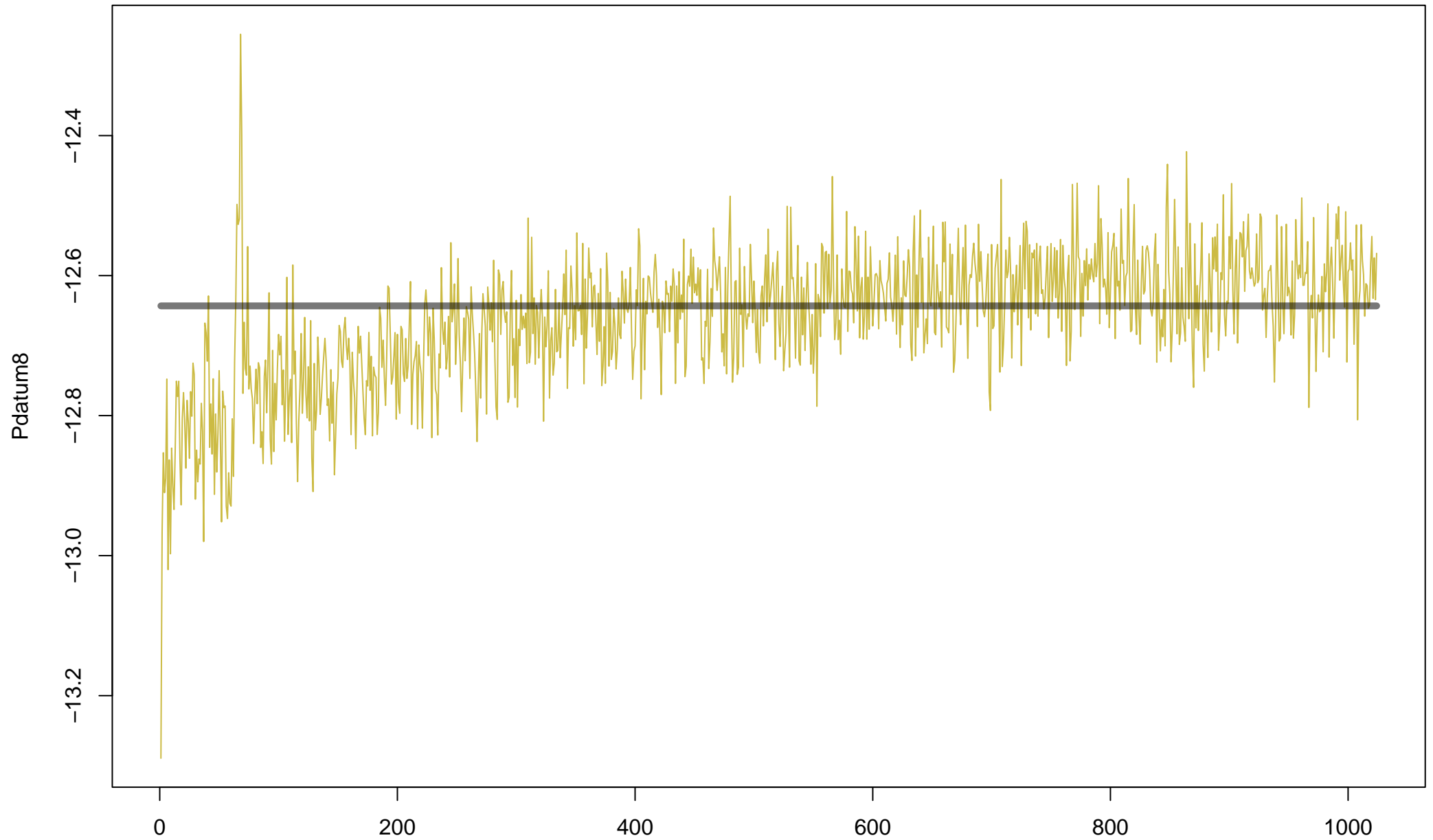
Pdatum7

ESS = 5.58 | BMK = 0.535 | MCSE(6.27) = 13.7 | stat: FALSE | burn: 0 | percentile: 96.8



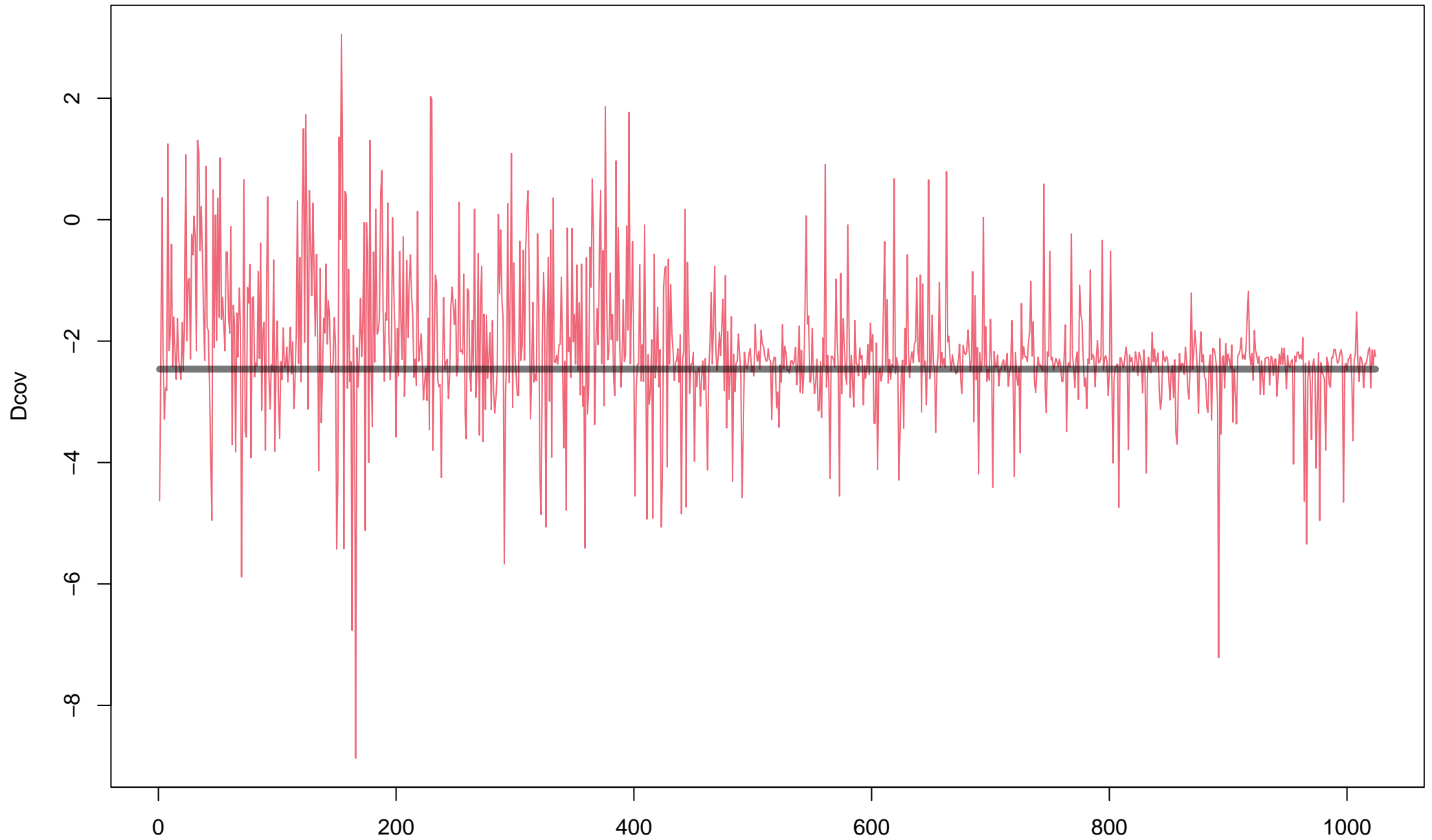
Pdatum8

ESS = 10.7 | BMK = 0.415 | MCSE(6.27) = 12.1 | stat: FALSE | burn: 0 | percentile: 53.3



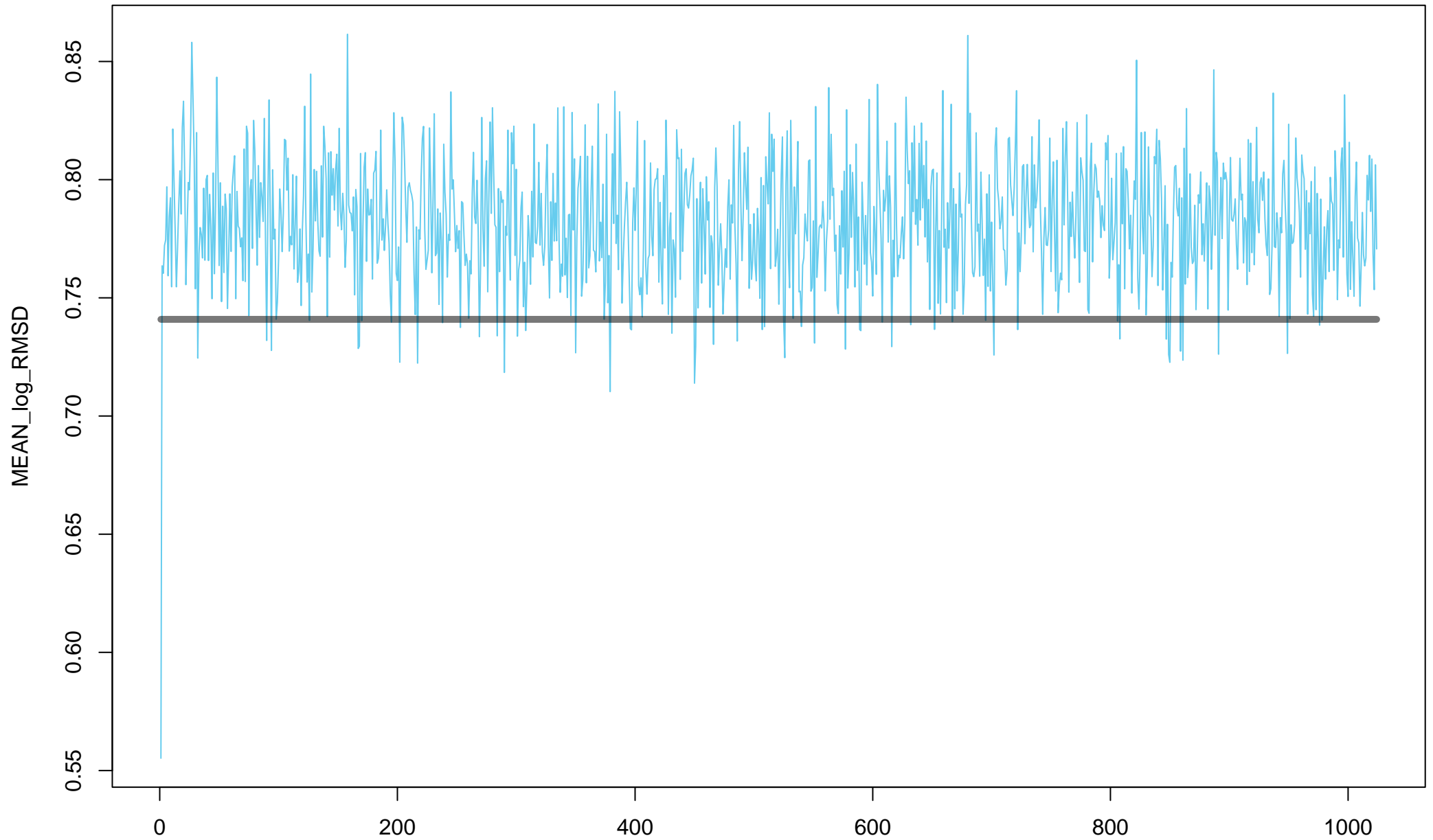
Dcov

ESS = 1020 | BMK = 0.721 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | percentile: 57.3

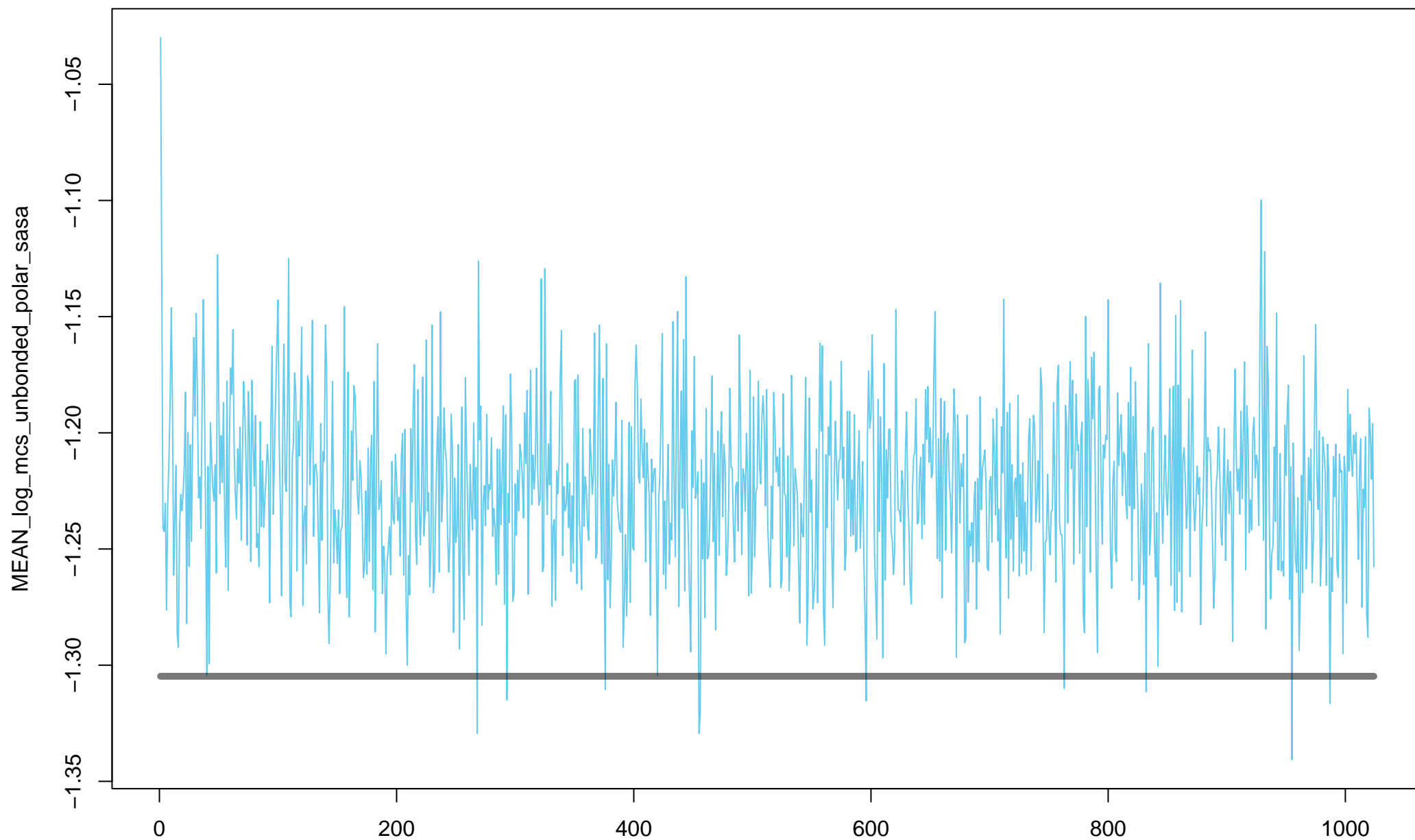


MEAN_log_RMSD

ESS = 1020 | BMK = 0.0446 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0 | percentile: 5.27

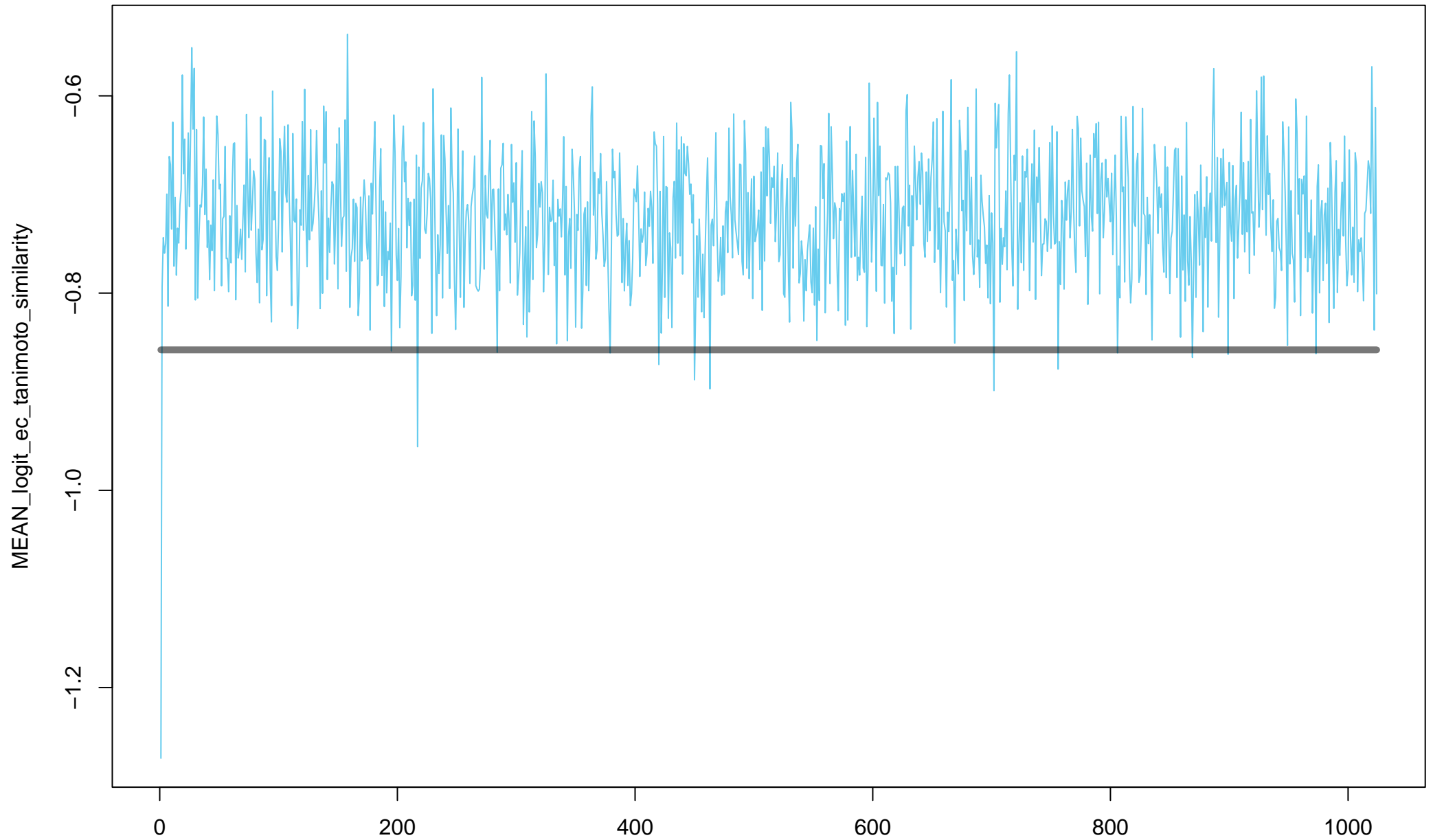


MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0666 | MCSE(6.27) = 3.19 | stat: FALSE | burn: 0 | percentile: 0.977



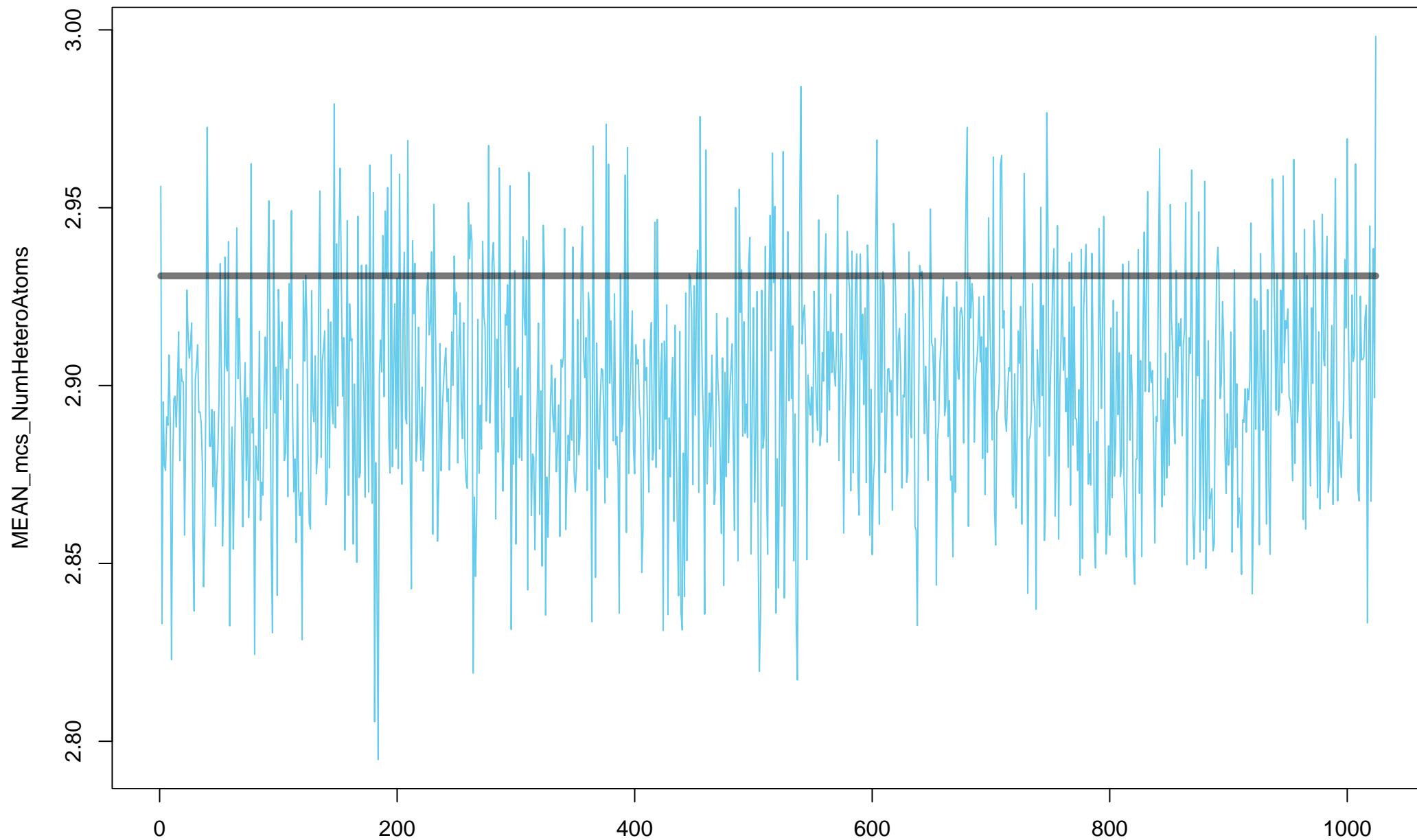
MEAN_logit_ec_tanimoto_similarity

ESS = 1020 | BMK = 0.0504 | MCSE(6.27) = 2.79 | stat: TRUE | burn: 0 | percentile: 1.37



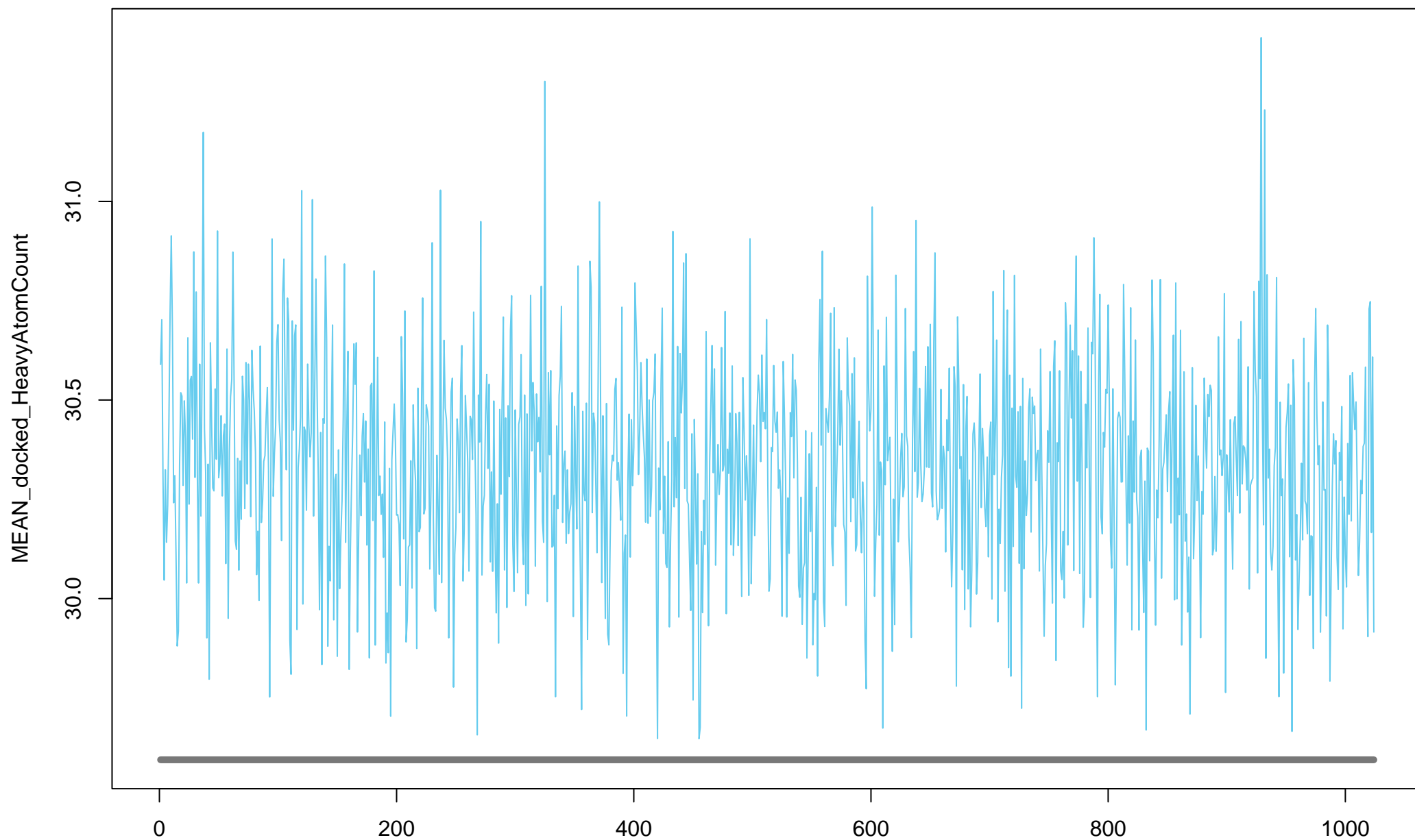
MEAN_mcs_NumHeteroAtoms

ESS = 1020 | BMK = 0.0862 | MCSE(6.27) = 3.57 | stat: FALSE | burn: 0 | percentile: 84.5

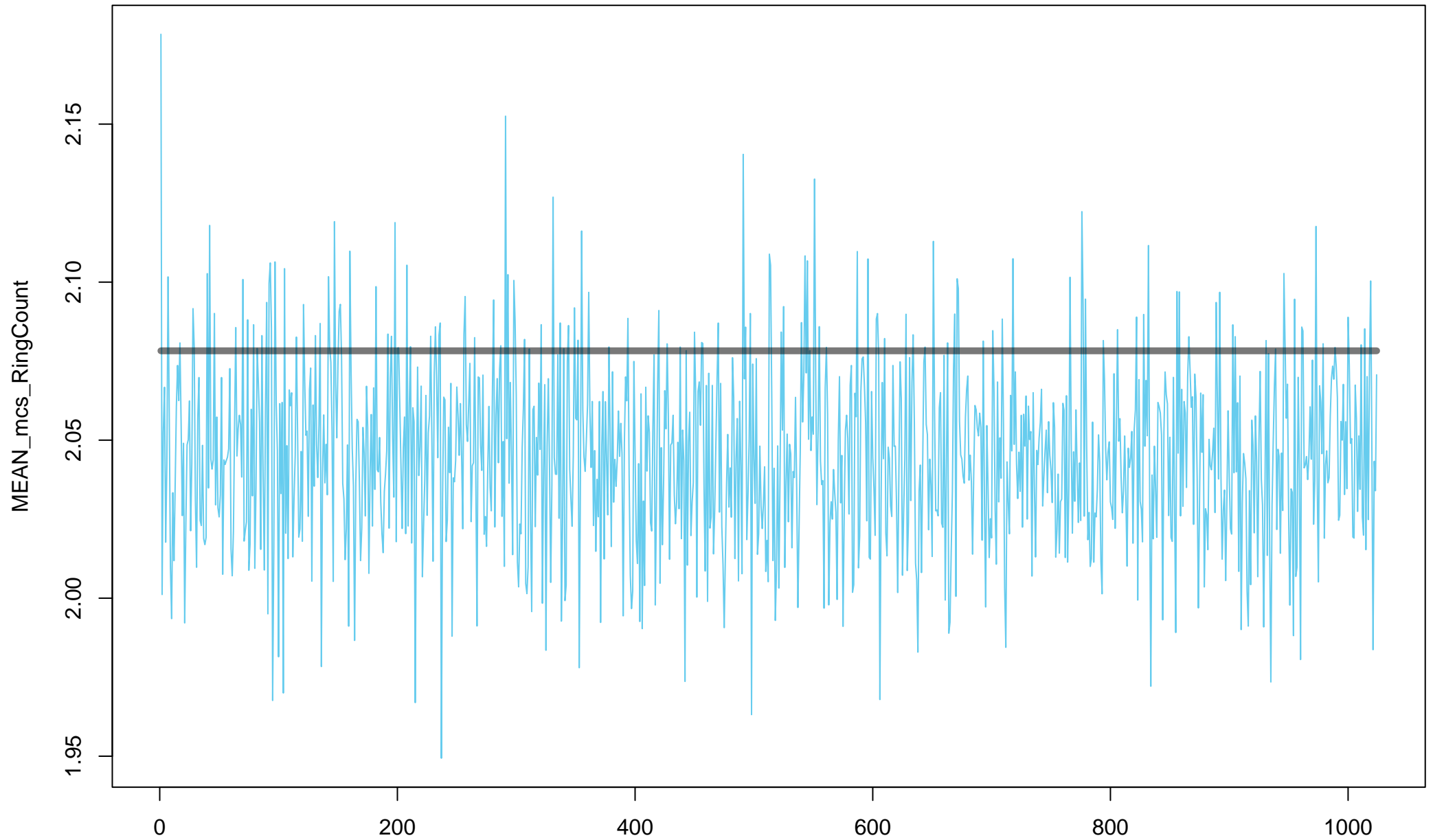


MEAN_docked_HeavyAtomCount

ESS = 1020 | BMK = 0.0529 | MCSE(6.27) = 2.97 | stat: FALSE | burn: 0 | percentile: 0

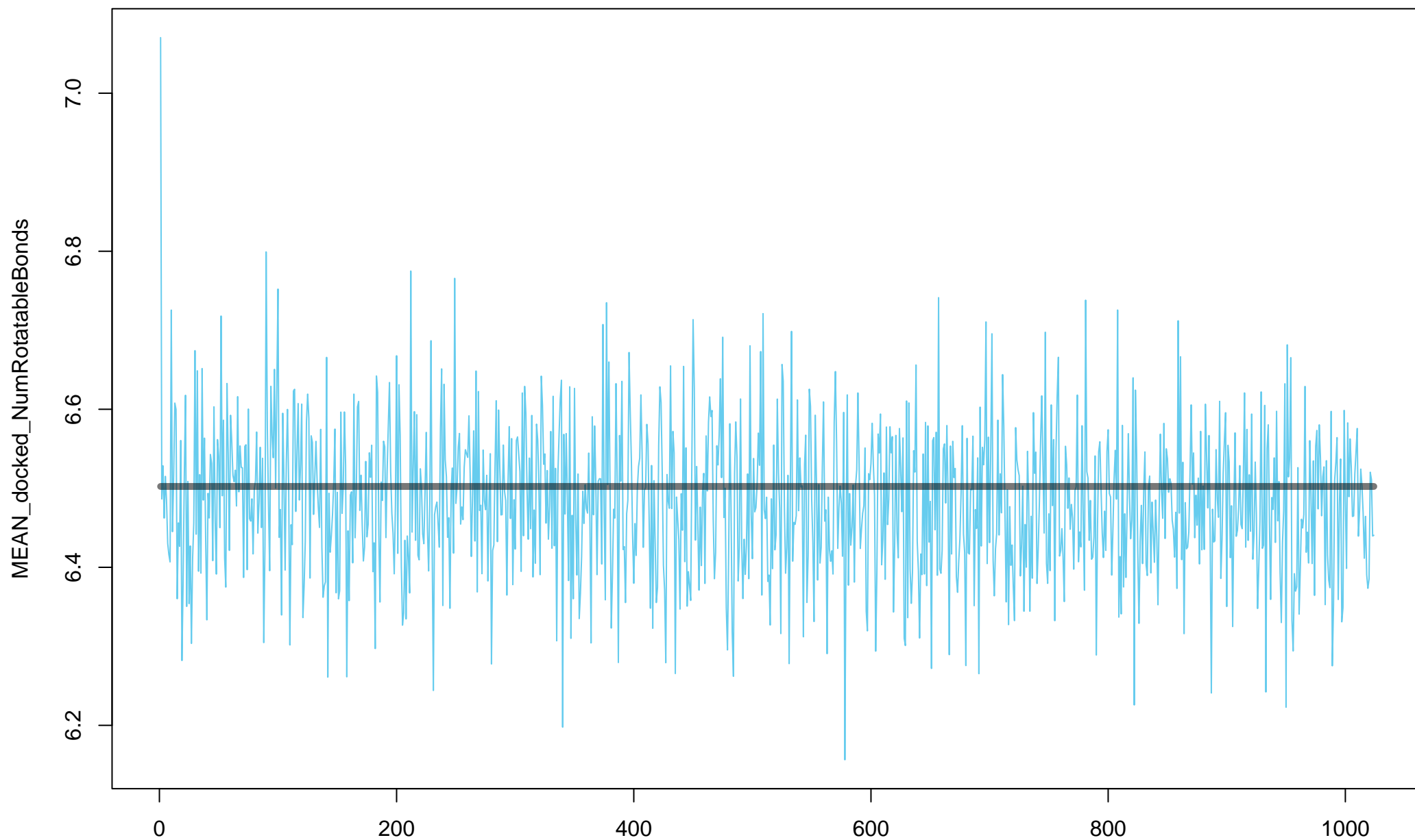


MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0612 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0 | percentile: 87

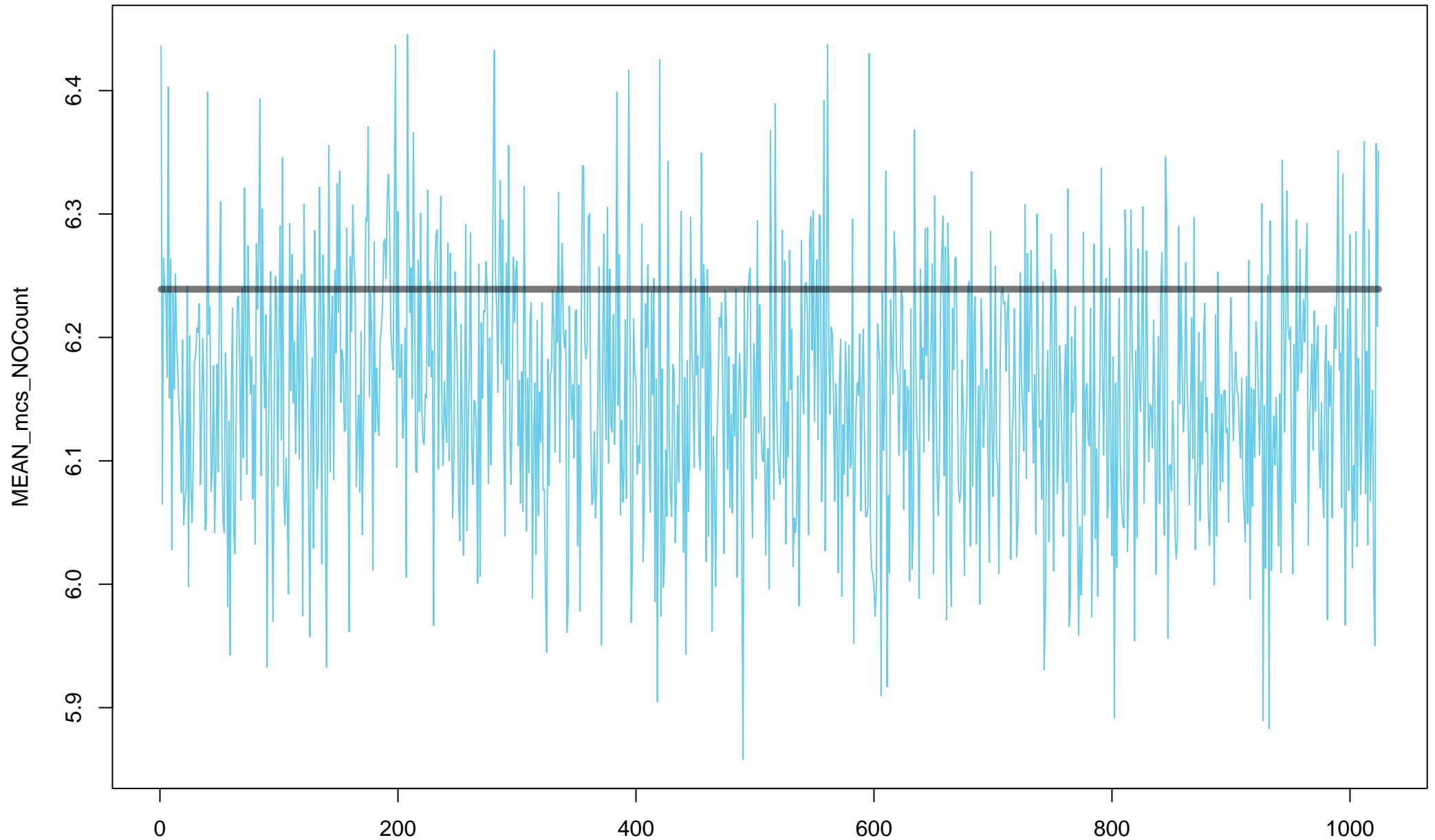


MEAN_docked_NumRotatableBonds

ESS = 1020 | BMK = 0.0804 | MCSE(6.27) = 2.66 | stat: FALSE | burn: 0 | percentile: 58.7

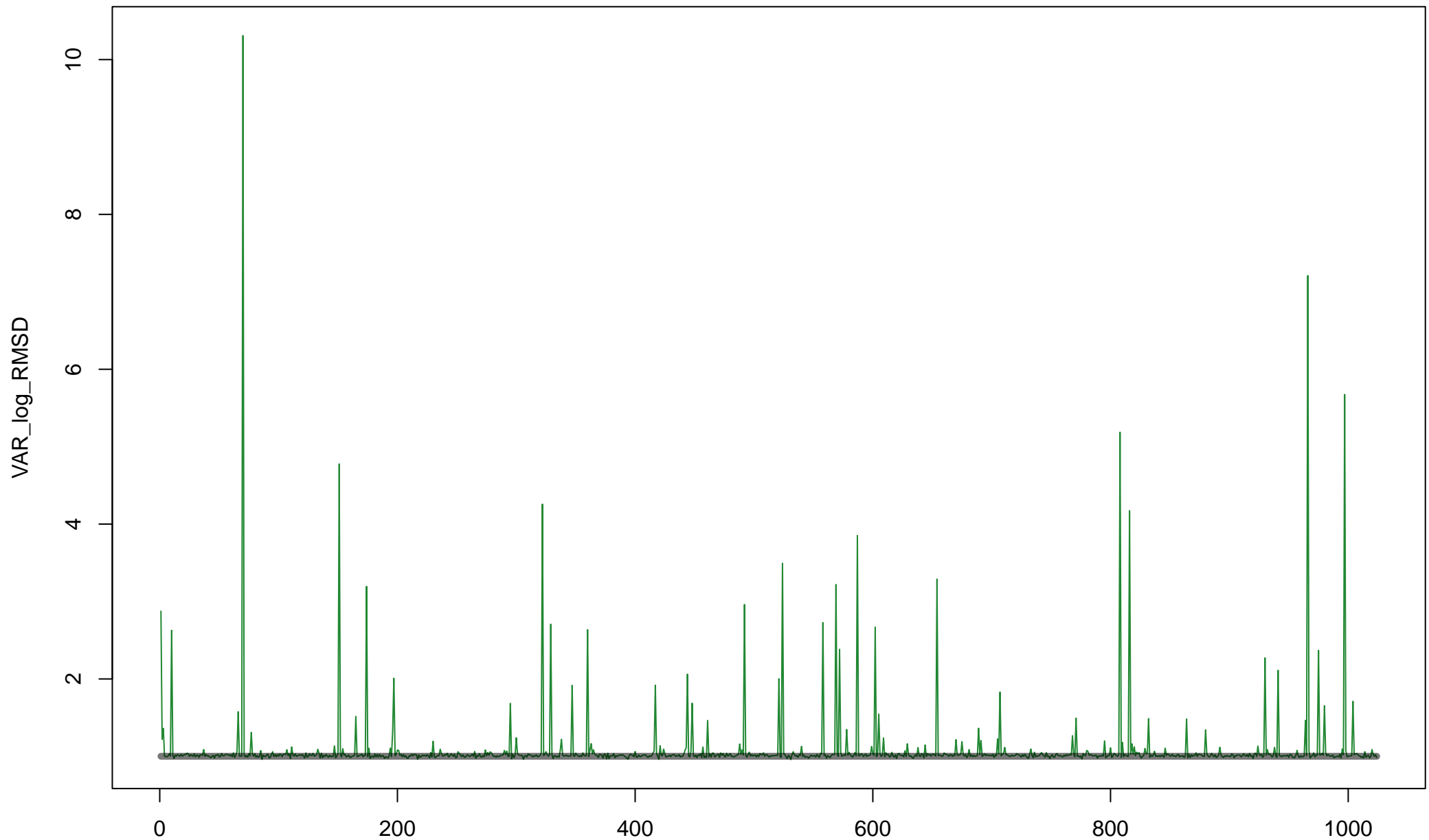


MEAN_mcs_NOCount
ESS = 566 | BMK = 0.0699 | MCSE(6.27) = 4.01 | stat: TRUE | burn: 0 | percentile: 80.4

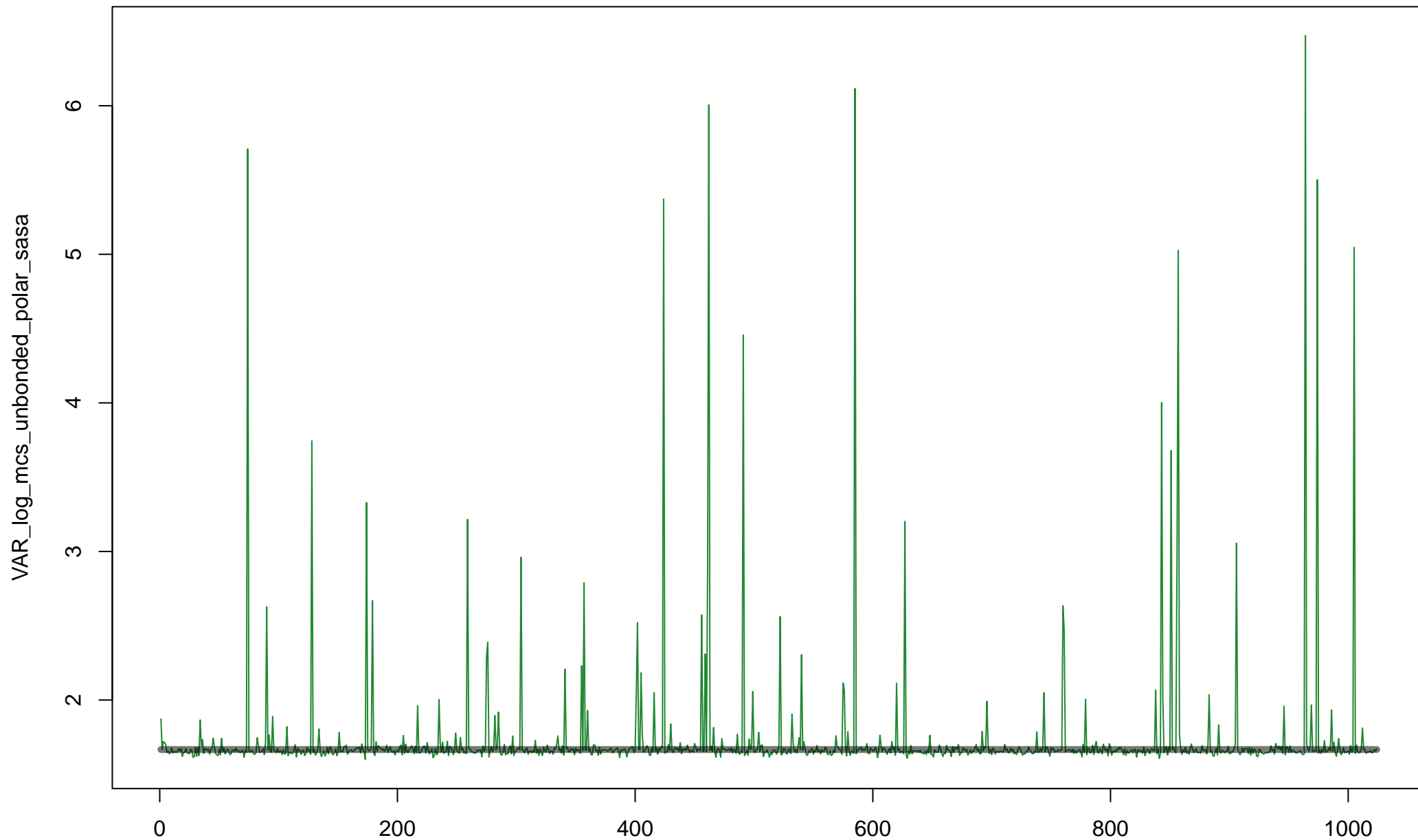


VAR_log_RMSD

ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 1020 | percentile: 26.5

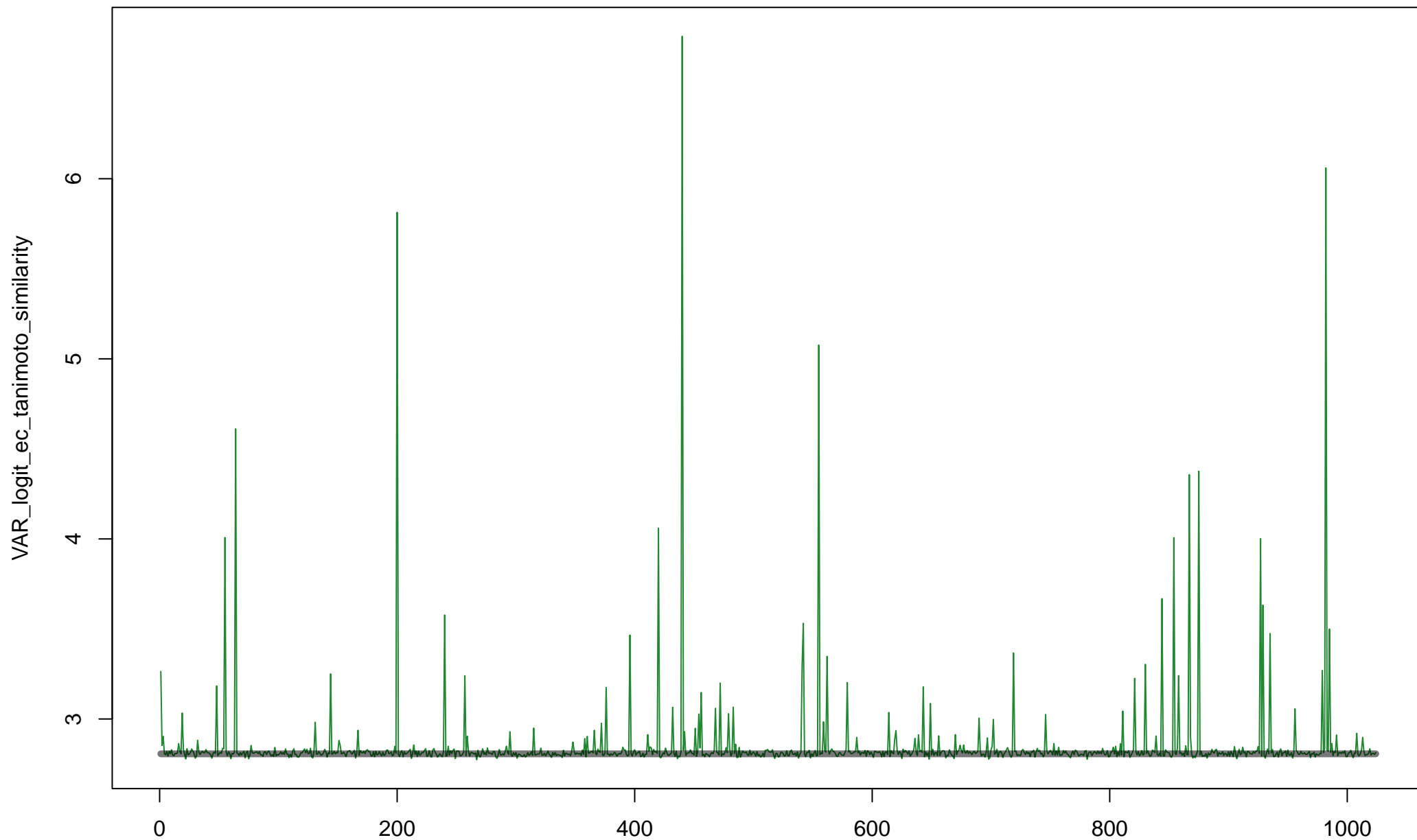


VAR_log_mcs_unbonded_polar_sasa
ESS = 847 | BMK = 0.549 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 1020 | percentile: 62.5

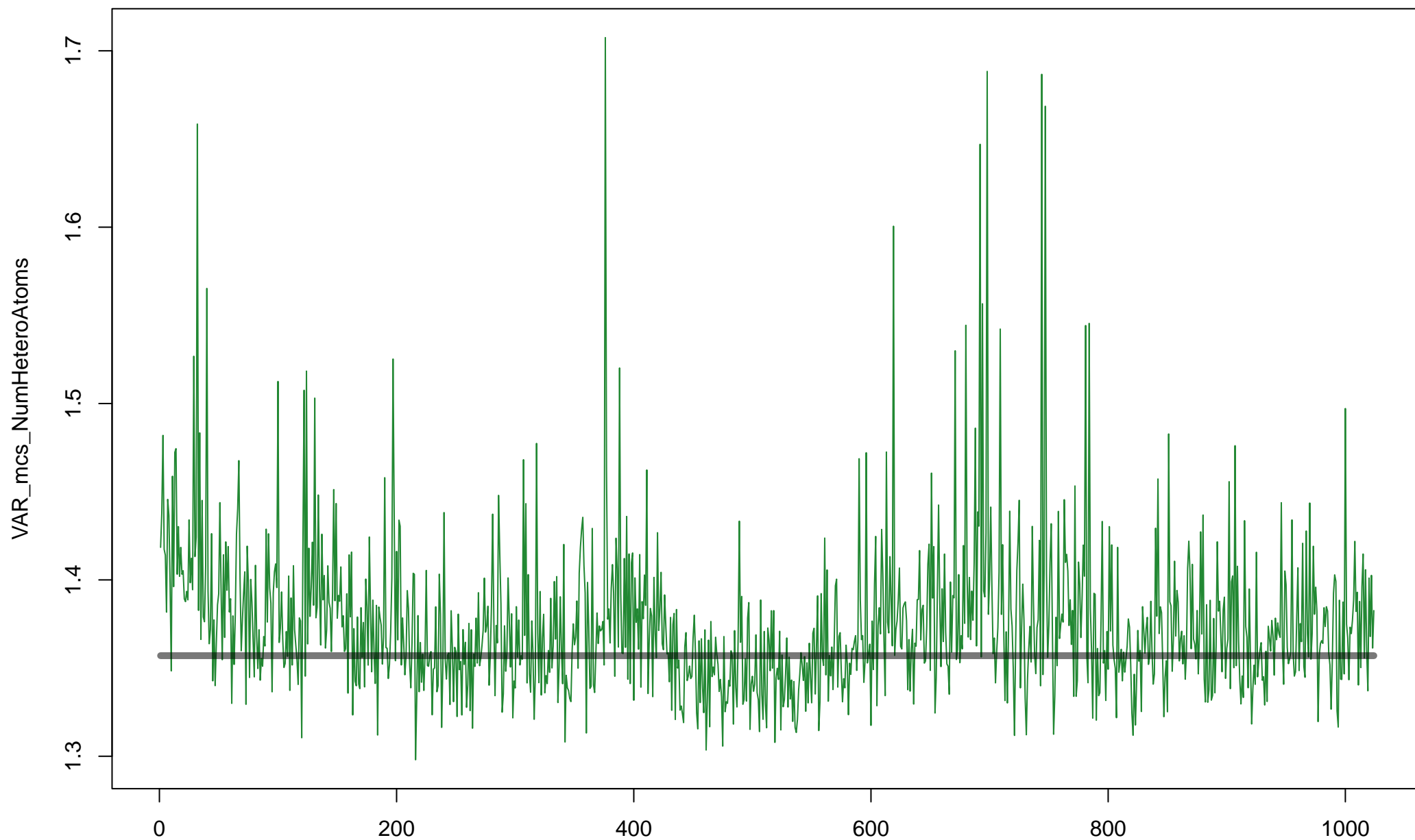


VAR_logit_ec_tanimoto_similarity

ESS = 1020 | BMK = 0.356 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 510 | percentile: 39.5

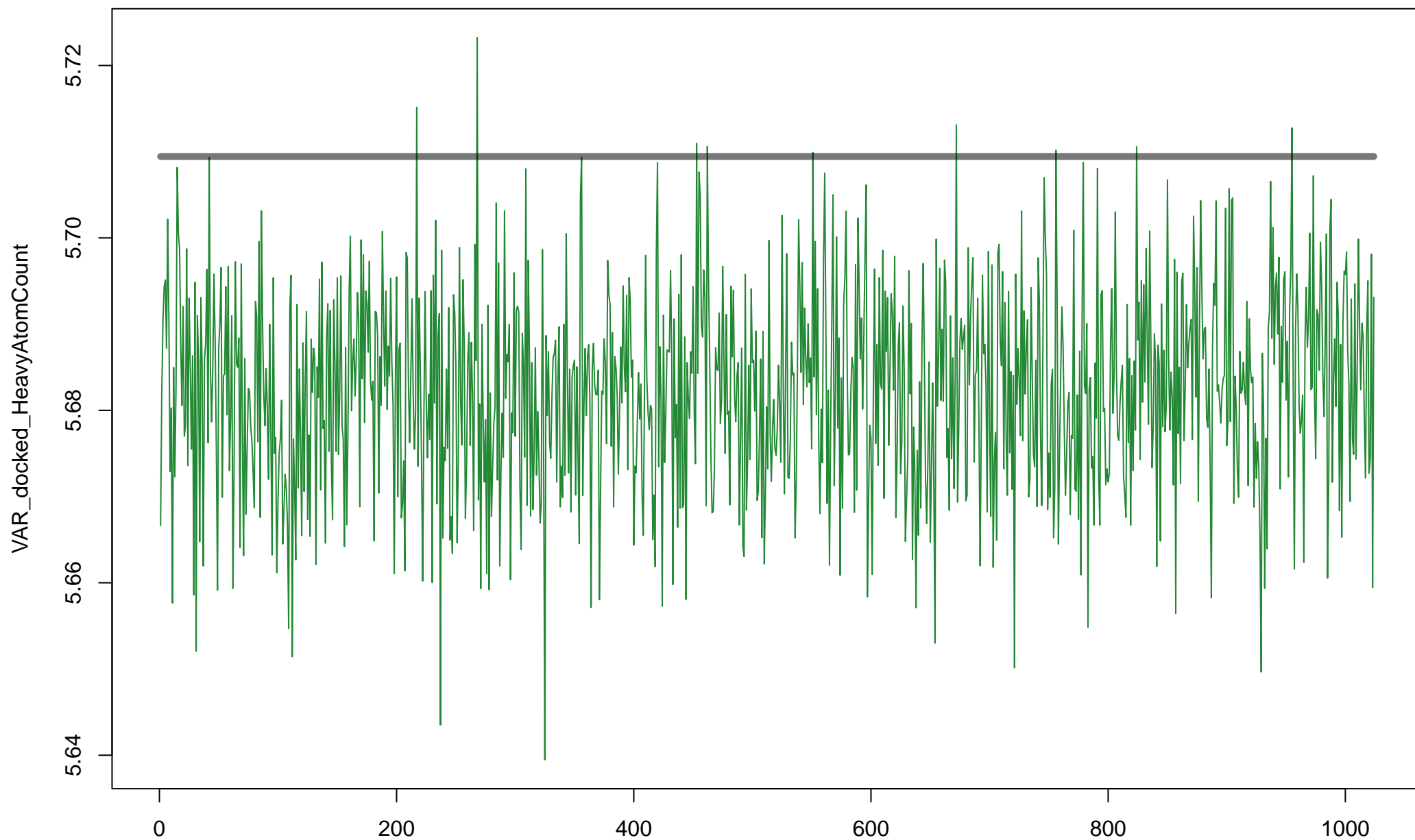


VAR_mcs_NumHeteroAtoms
ESS = 140 | BMK = 0.105 | MCSE(6.27) = 7.22 | stat: FALSE | burn: 0 | percentile: 35.4

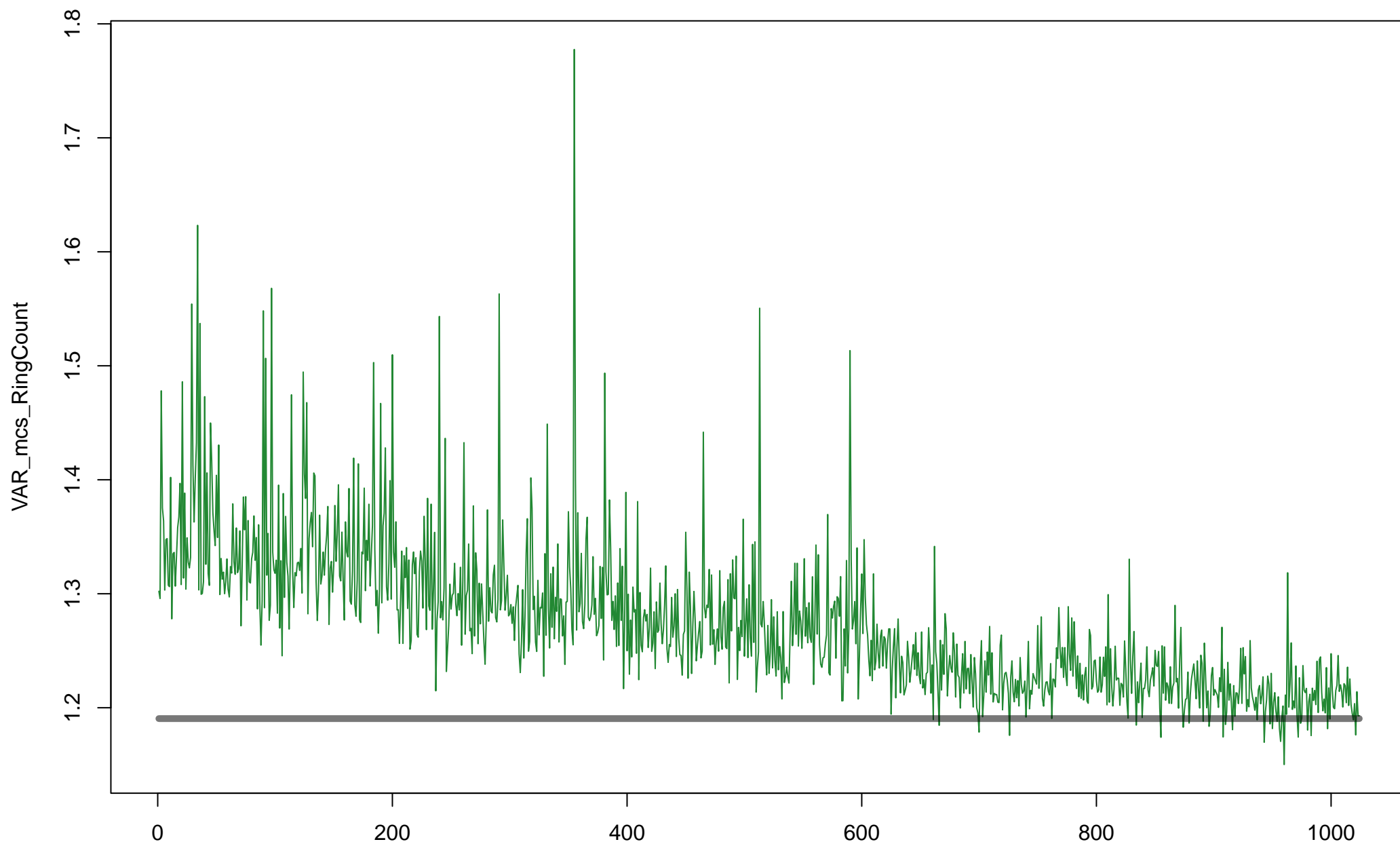


VAR_docked_HeavyAtomCount

ESS = 1020 | BMK = 0.0751 | MCSE(6.27) = 3.92 | stat: TRUE | burn: 0 | percentile: 99.1

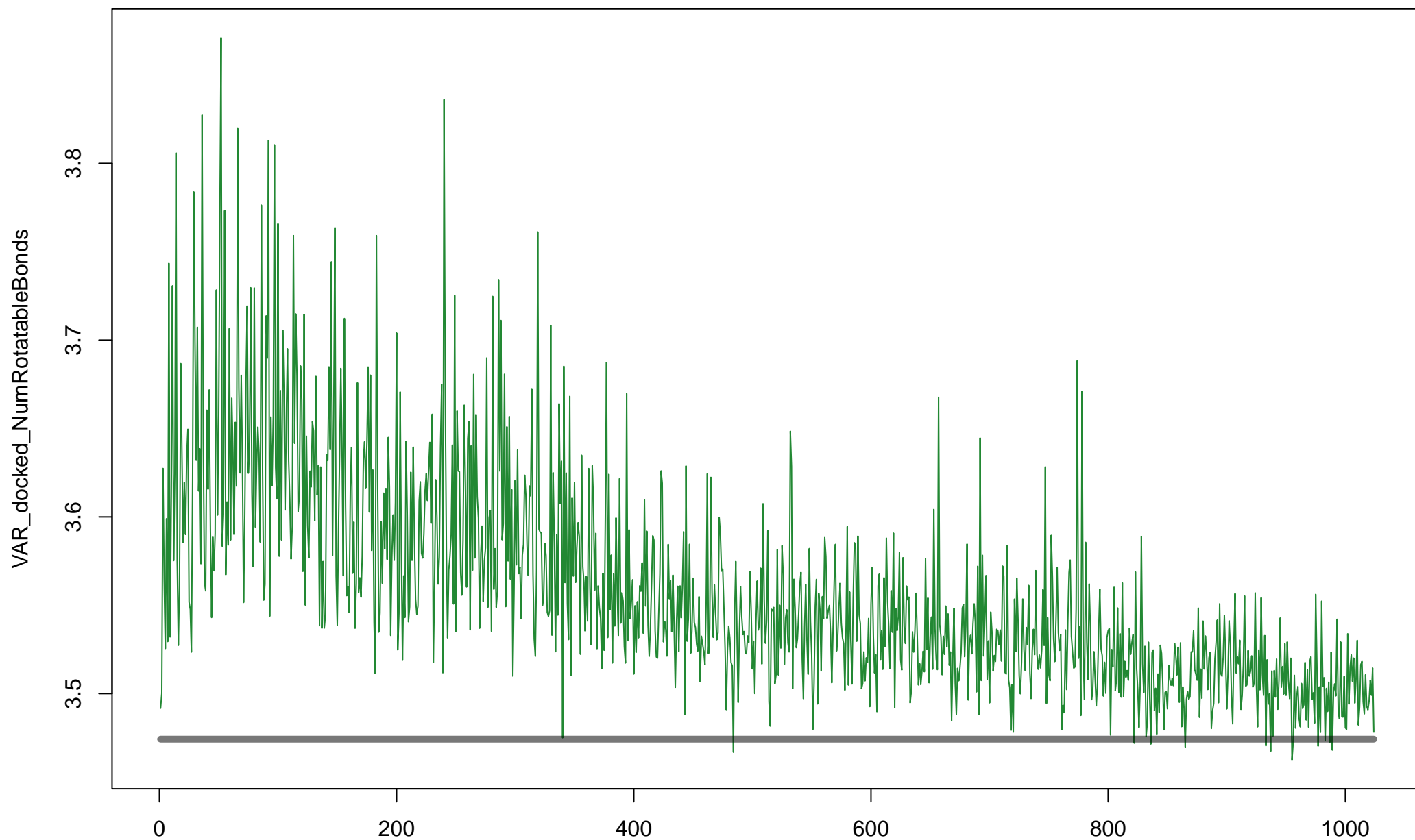


VAR_mcs_RingCount
ESS = 8.13 | BMK = 0.612 | MCSE(6.27) = 12.5 | stat: FALSE | burn: 0 | percentile: 2.83



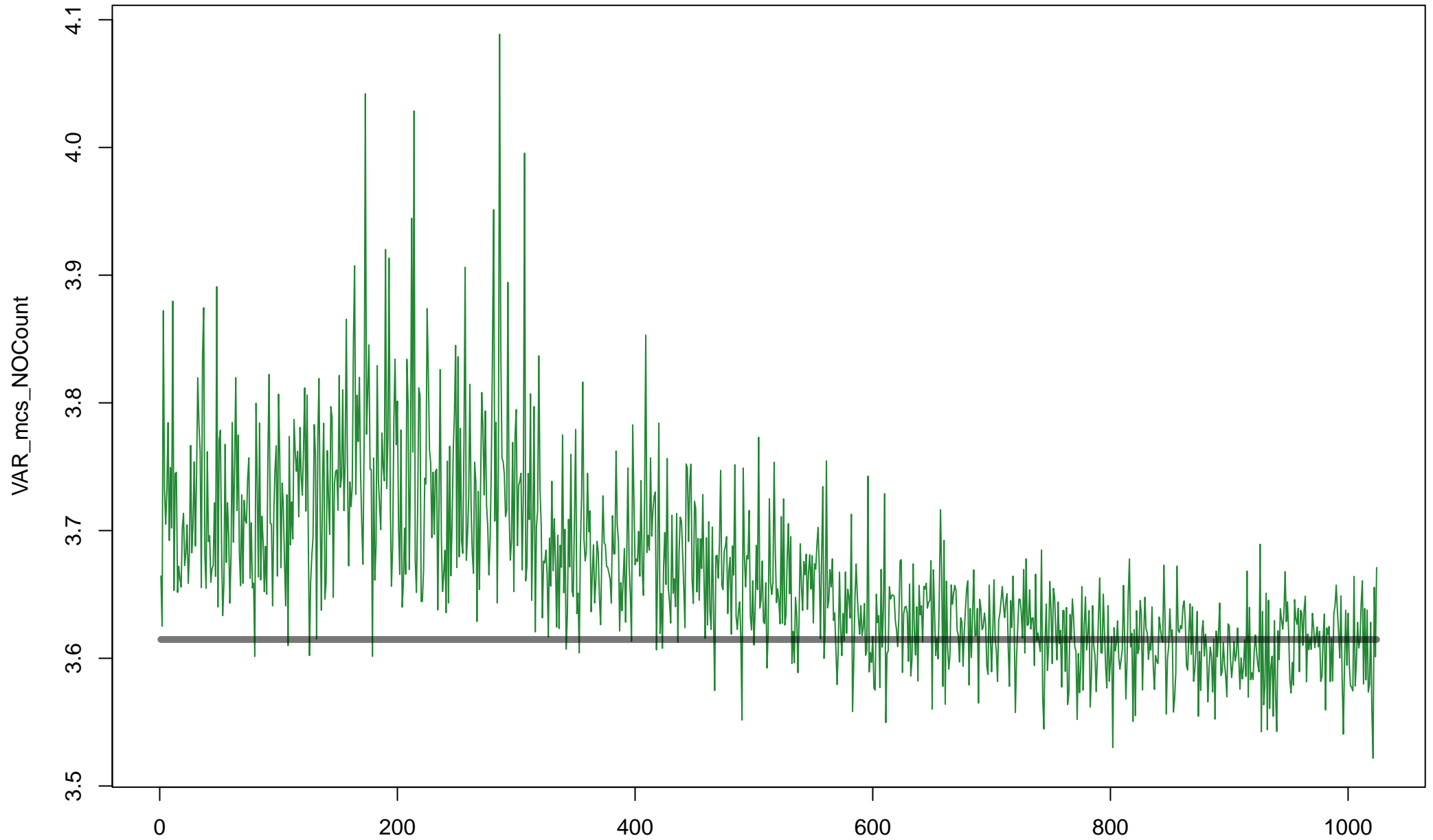
VAR_docked_NumRotatableBonds

ESS = 3.72 | BMK = 0.511 | MCSE(6.27) = 12.6 | stat: FALSE | burn: 0 | percentile: 1.17

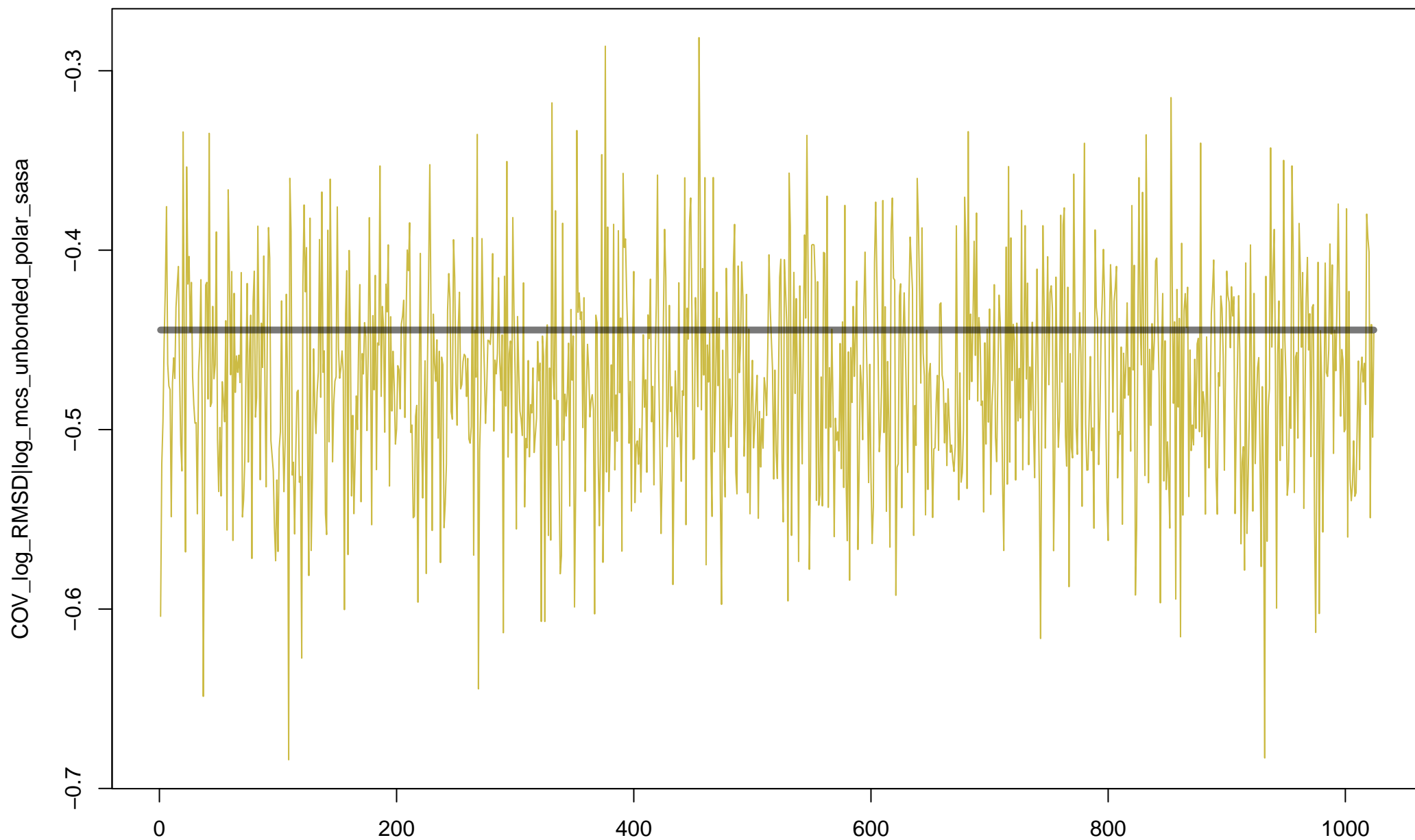


VAR_mcs_NOCount

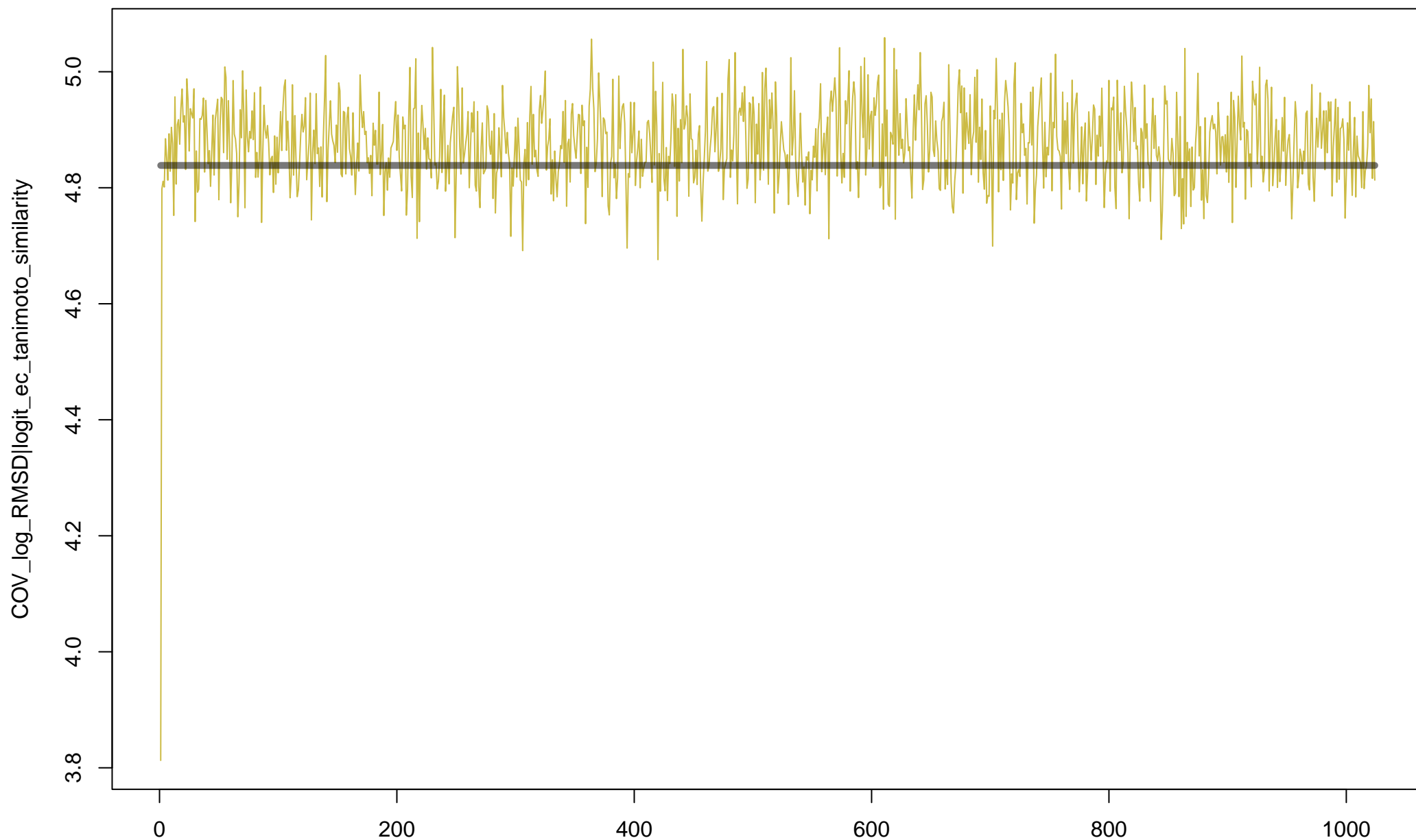
ESS = 3.27 | BMK = 0.583 | MCSE(6.27) = 12.7 | stat: FALSE | burn: 0 | percentile: 22.1



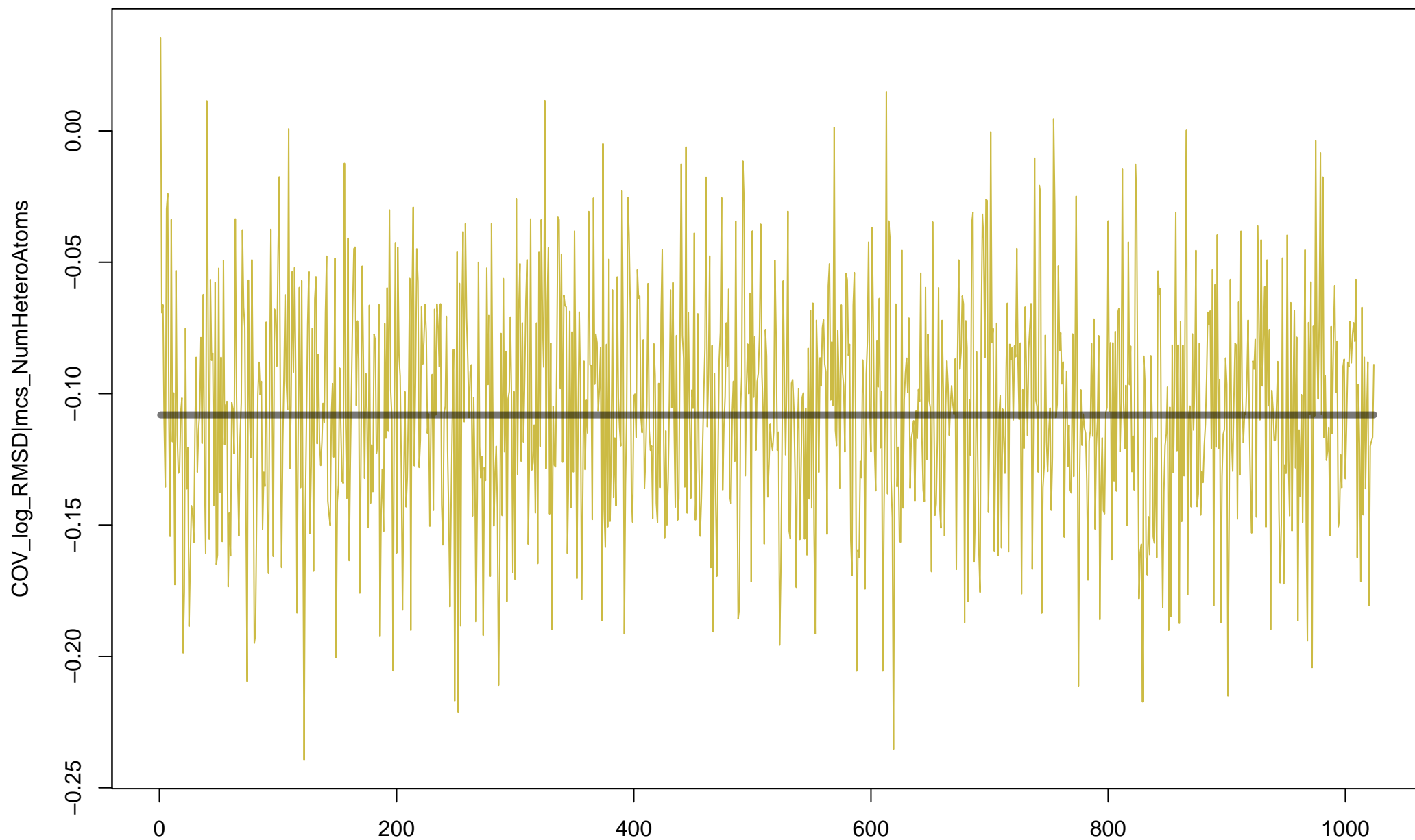
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0664 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | percentile: 68.8



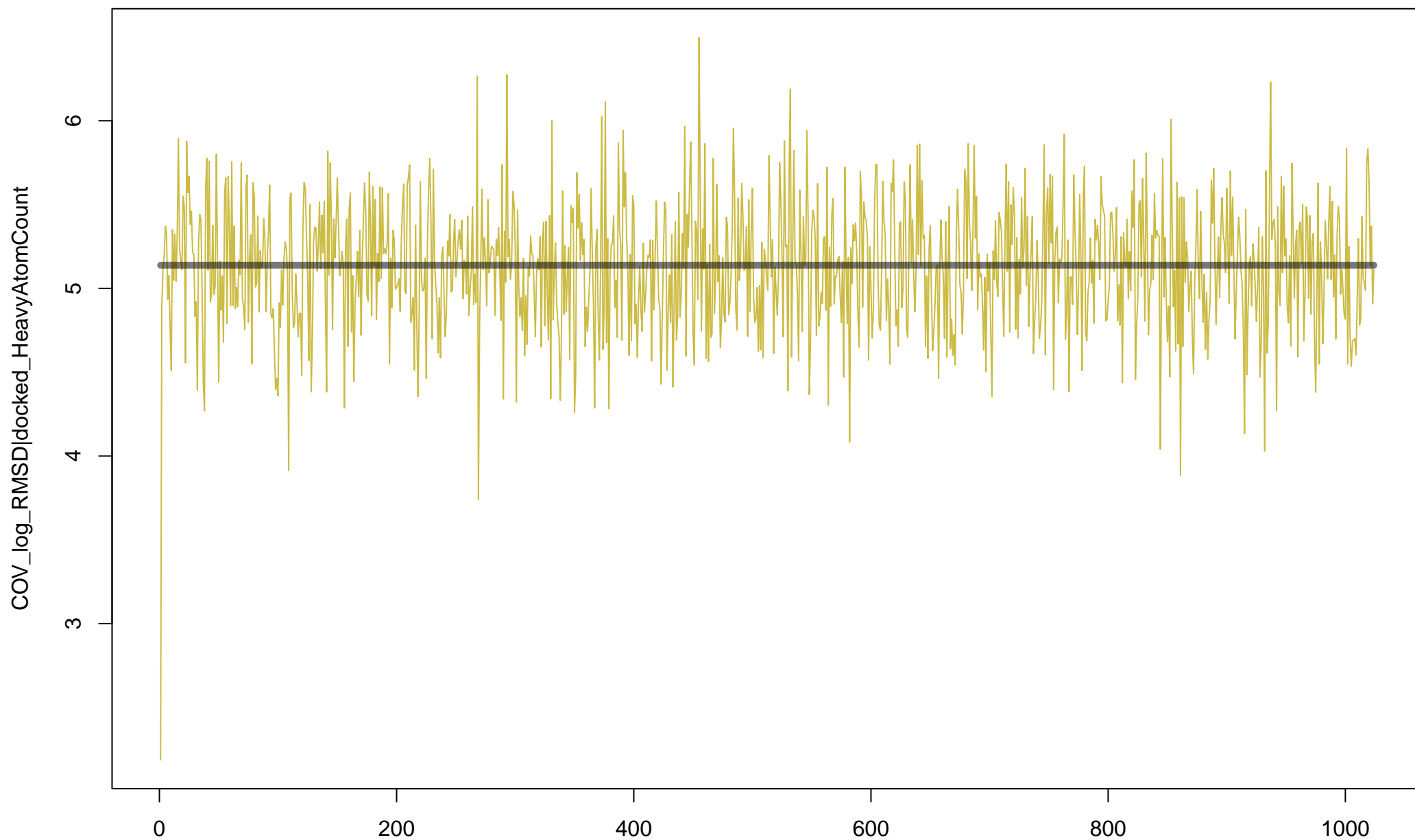
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 915 | BMK = 0.0534 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0 | percentile: 29.1



COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0602 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0 | percentile: 47

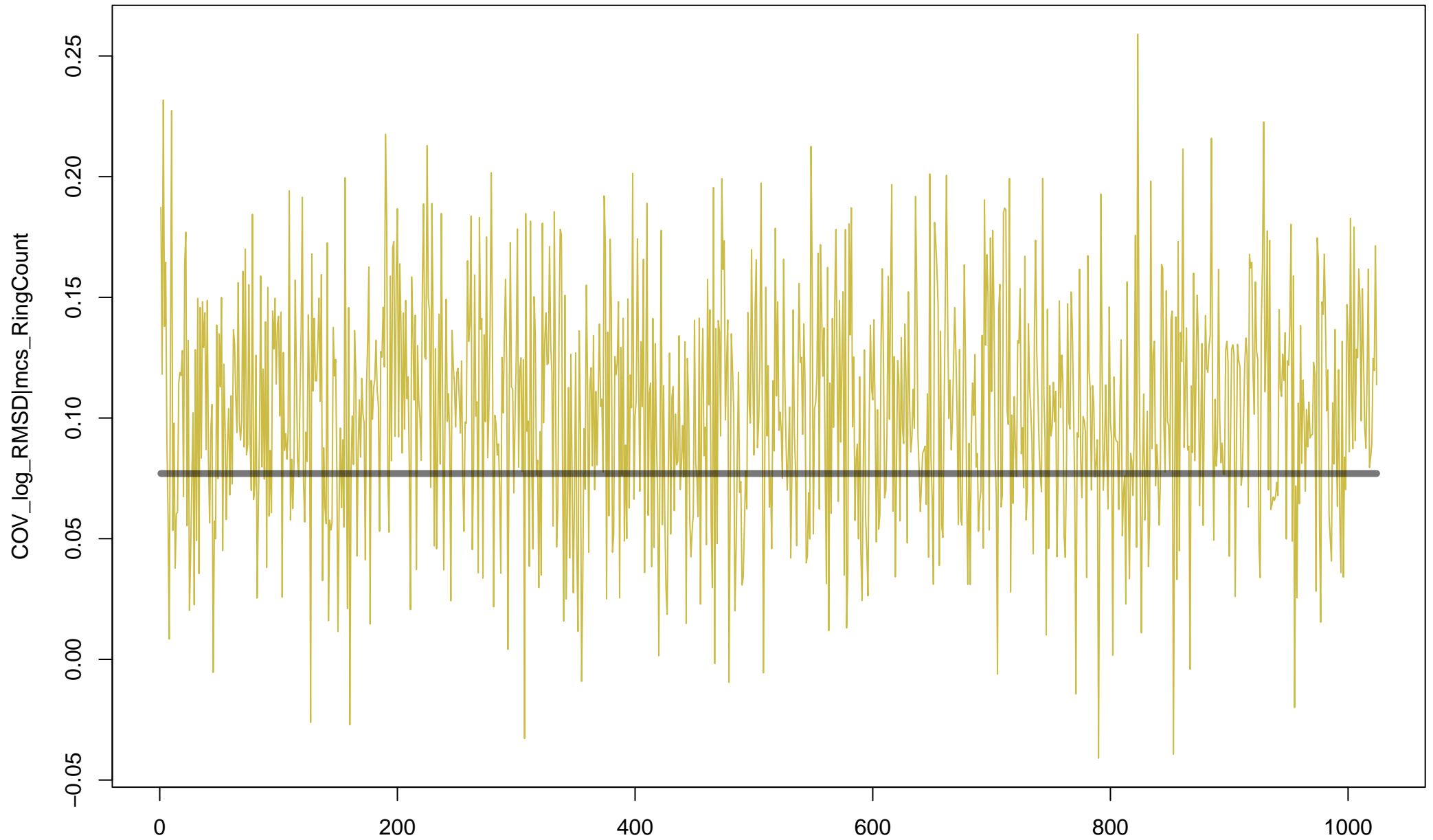


COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0623 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | percentile: 50.3

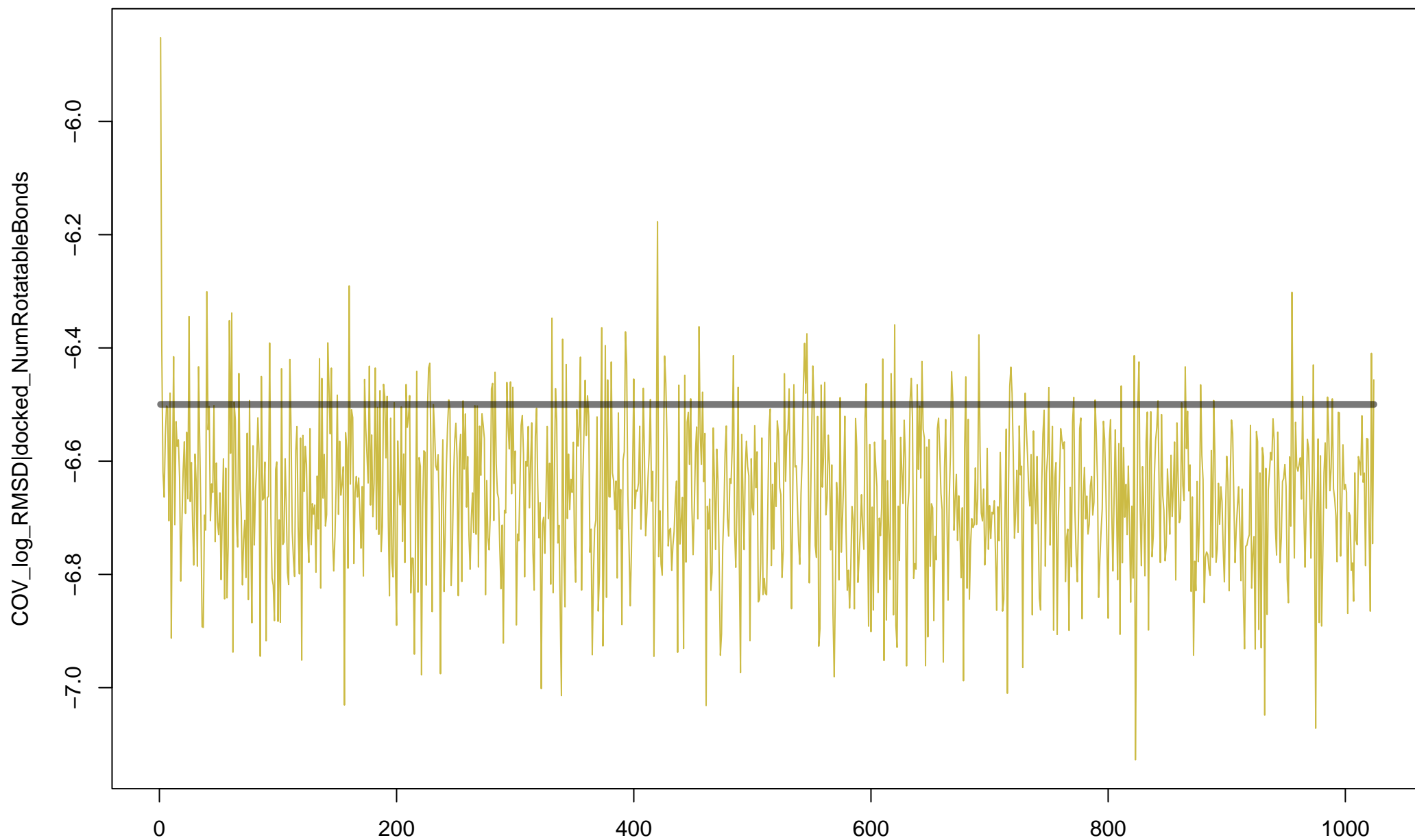


COV_log_RMSD|mcs_RingCount

ESS = 1020 | BMK = 0.0536 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0 | percentile: 28.7

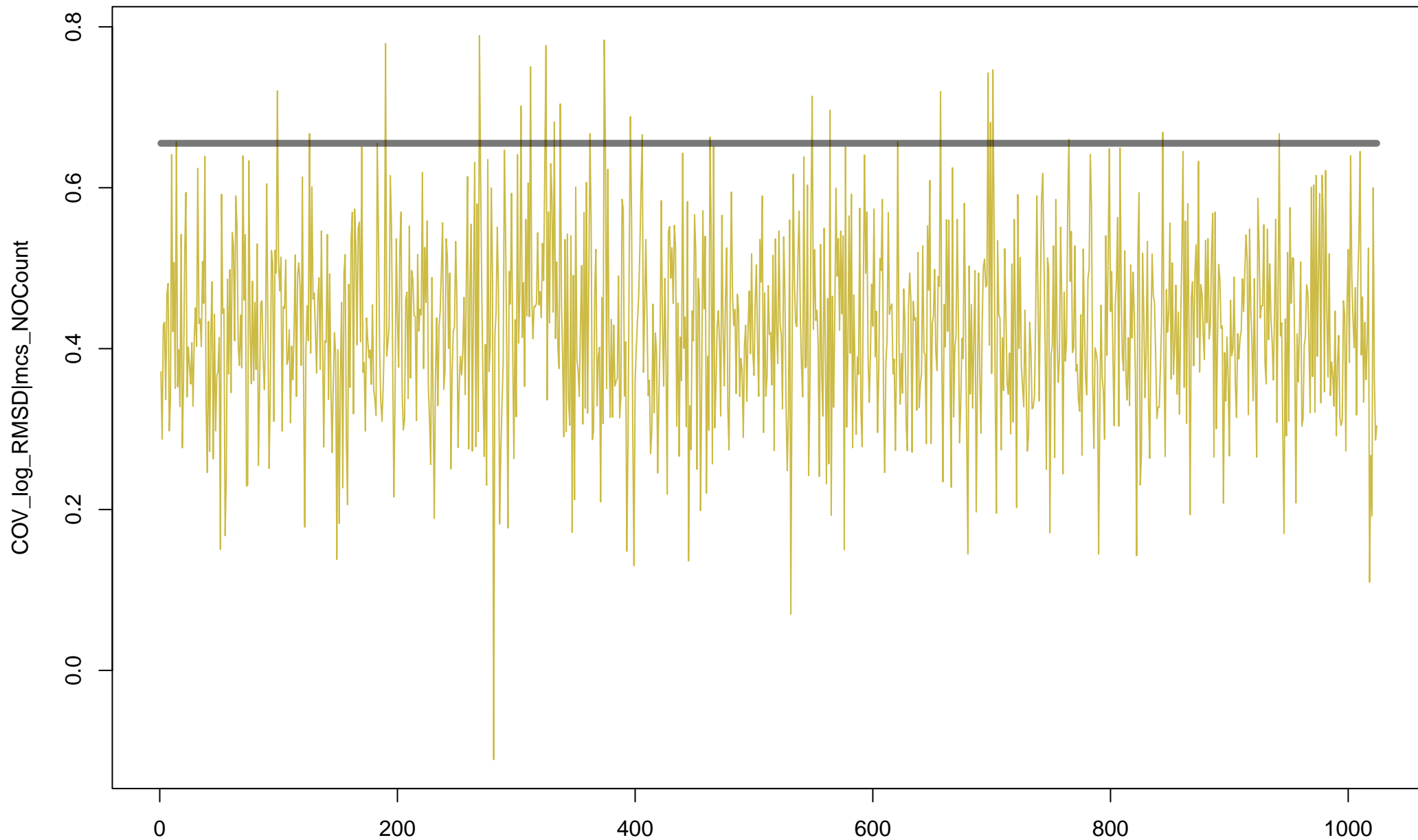


COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0787 | MCSE(6.27) = 3.47 | stat: TRUE | burn: 0 | percentile: 88.8

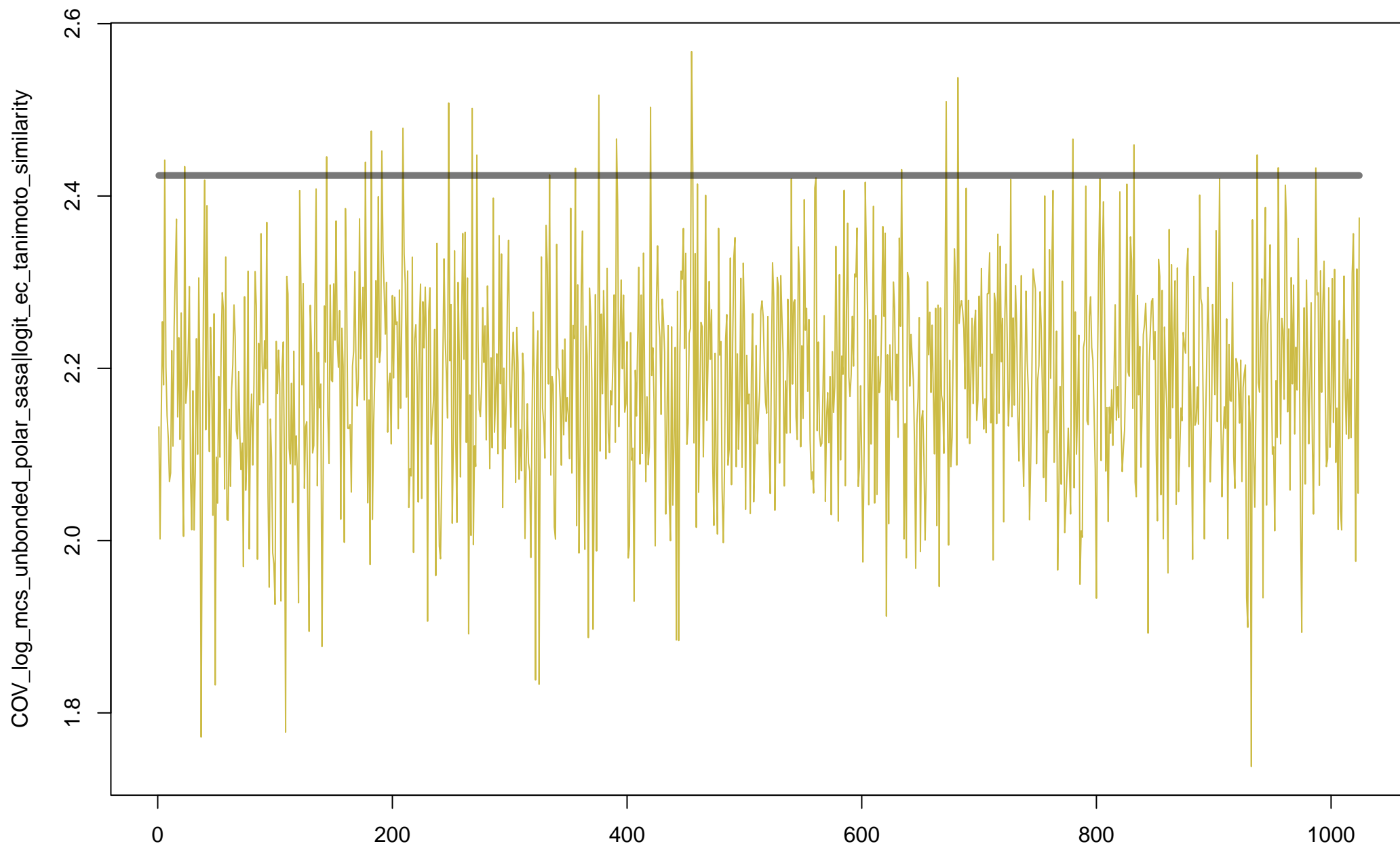


COV_log_RMSD|mcs_NOCount

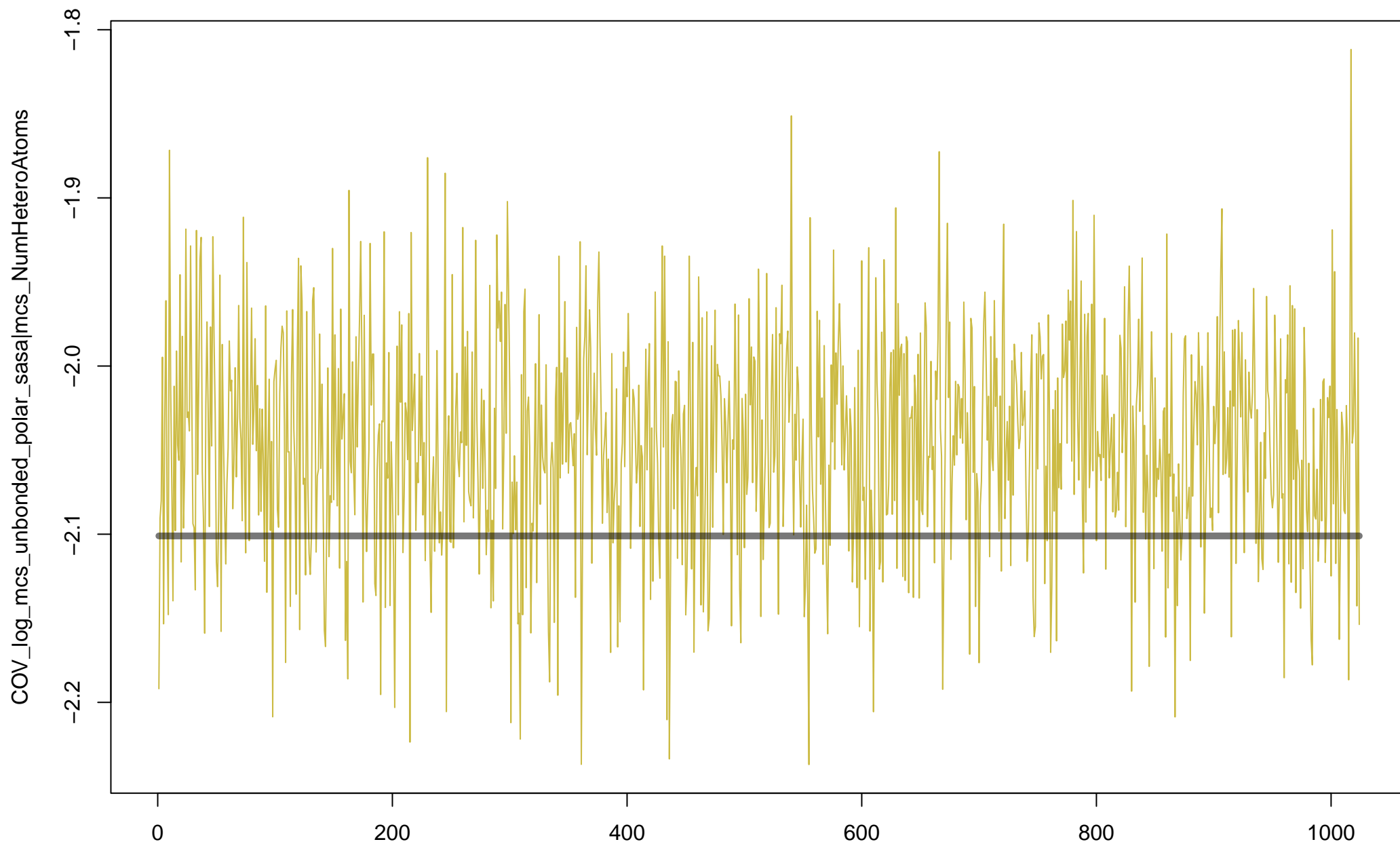
ESS = 1020 | BMK = 0.0451 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0 | percentile: 97.6



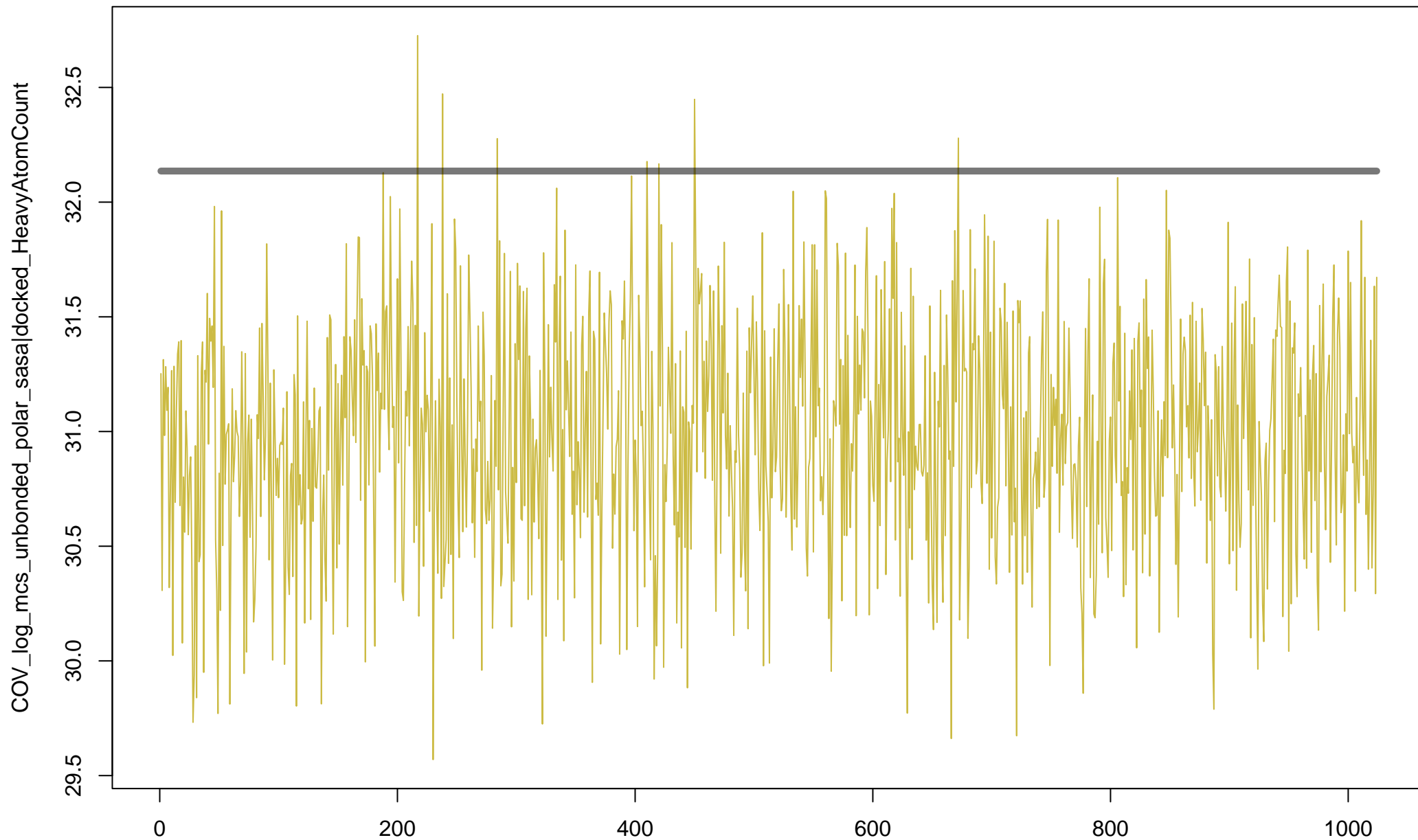
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0763 | MCSE(6.27) = 3.36 | stat: FALSE | burn: 0 | percentile: 97.6



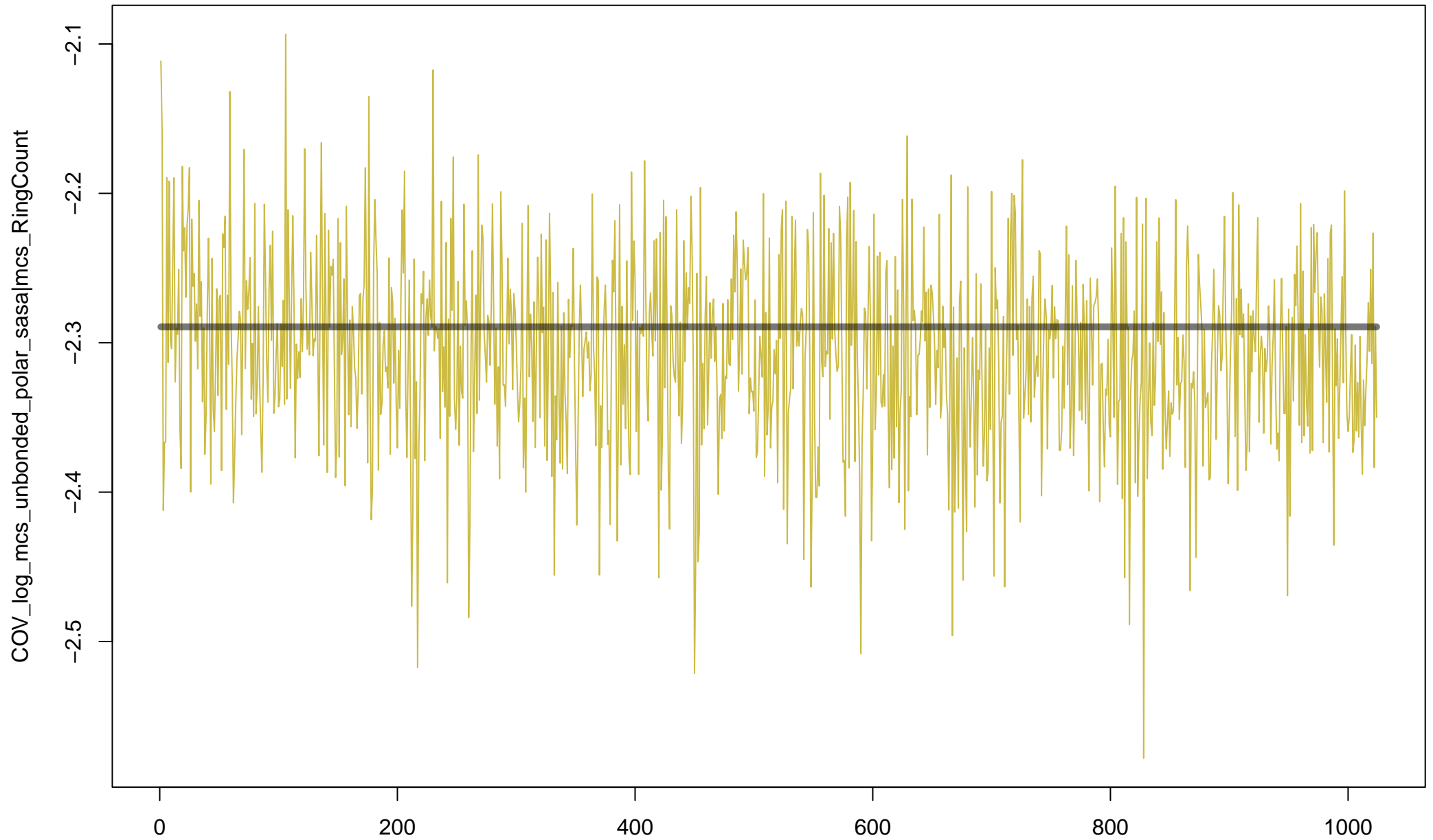
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0626 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0 | percentile: 18.7



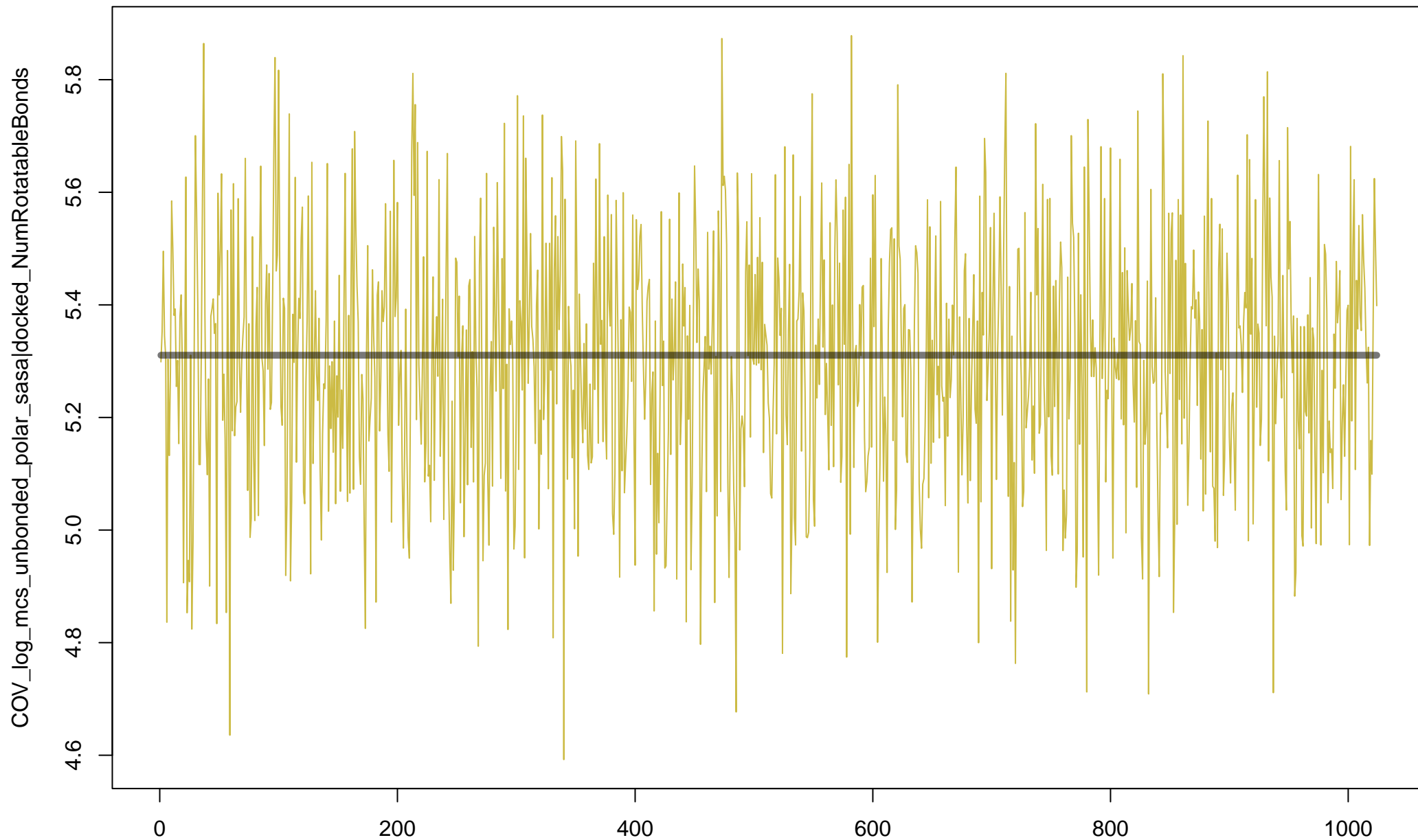
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0721 | MCSE(6.27) = 3.64 | stat: FALSE | burn: 0 | percentile: 99.3



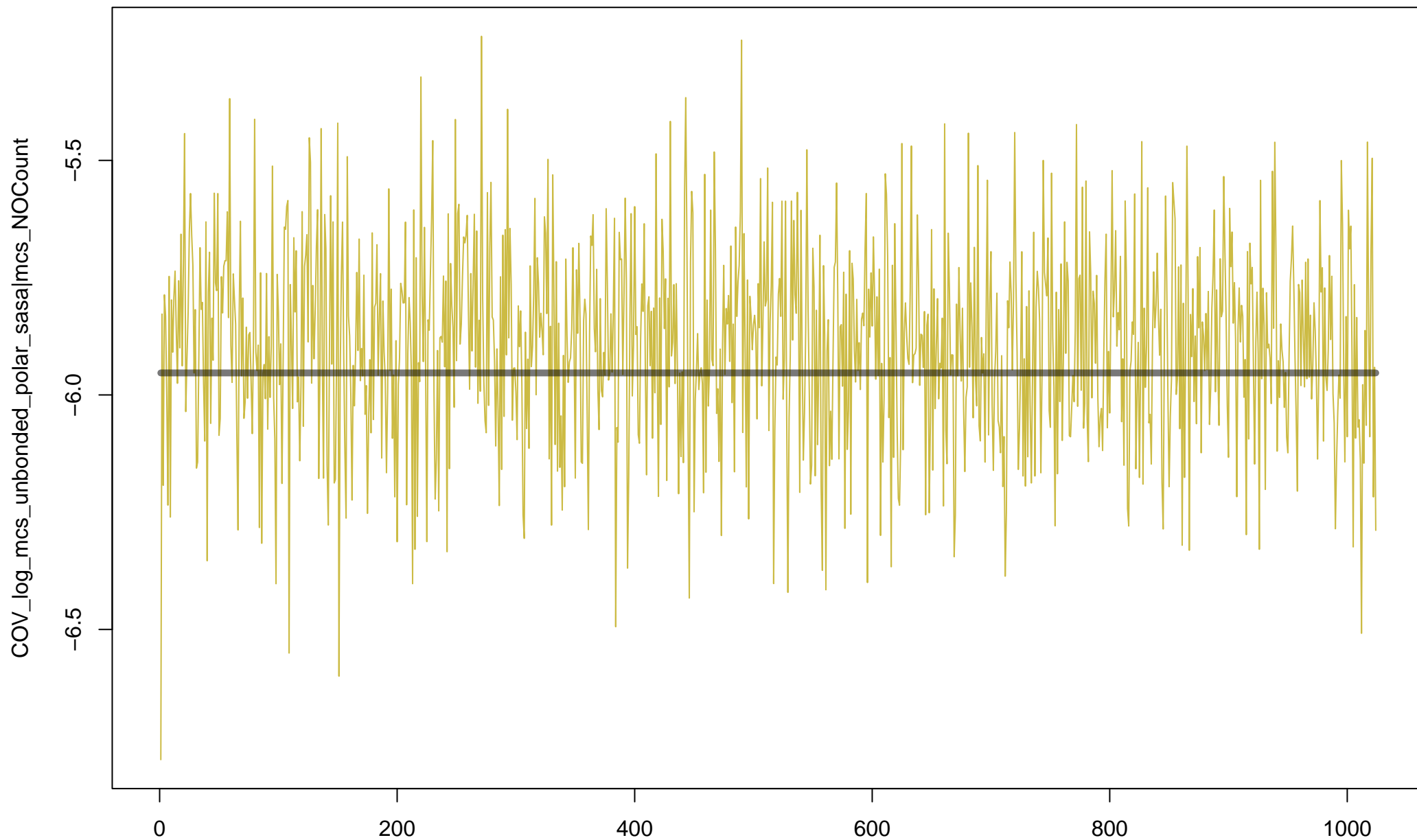
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0952 | MCSE(6.27) = 3.71 | stat: FALSE | burn: 0 | percentile: 61.4



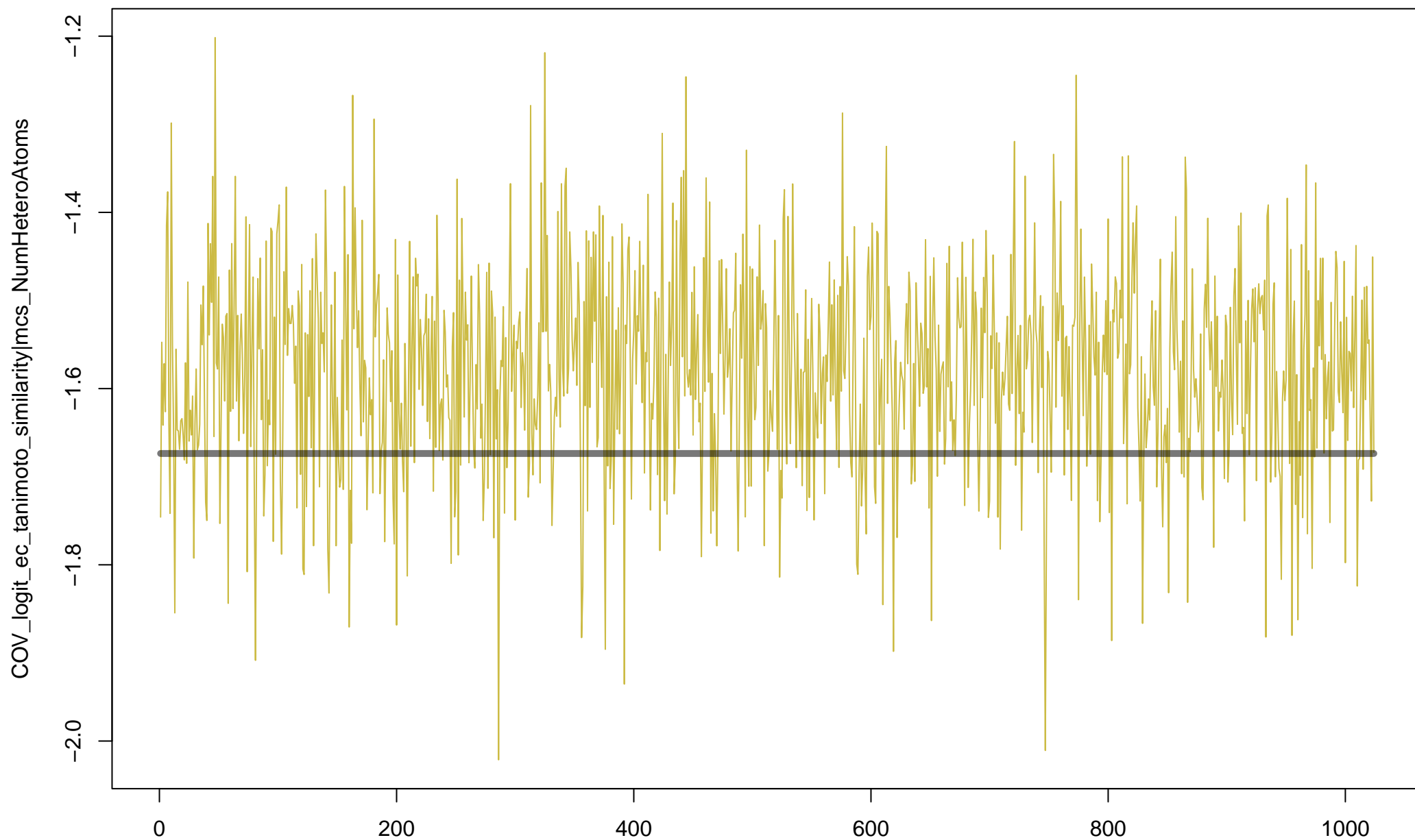
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0369 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0 | percentile: 51.9



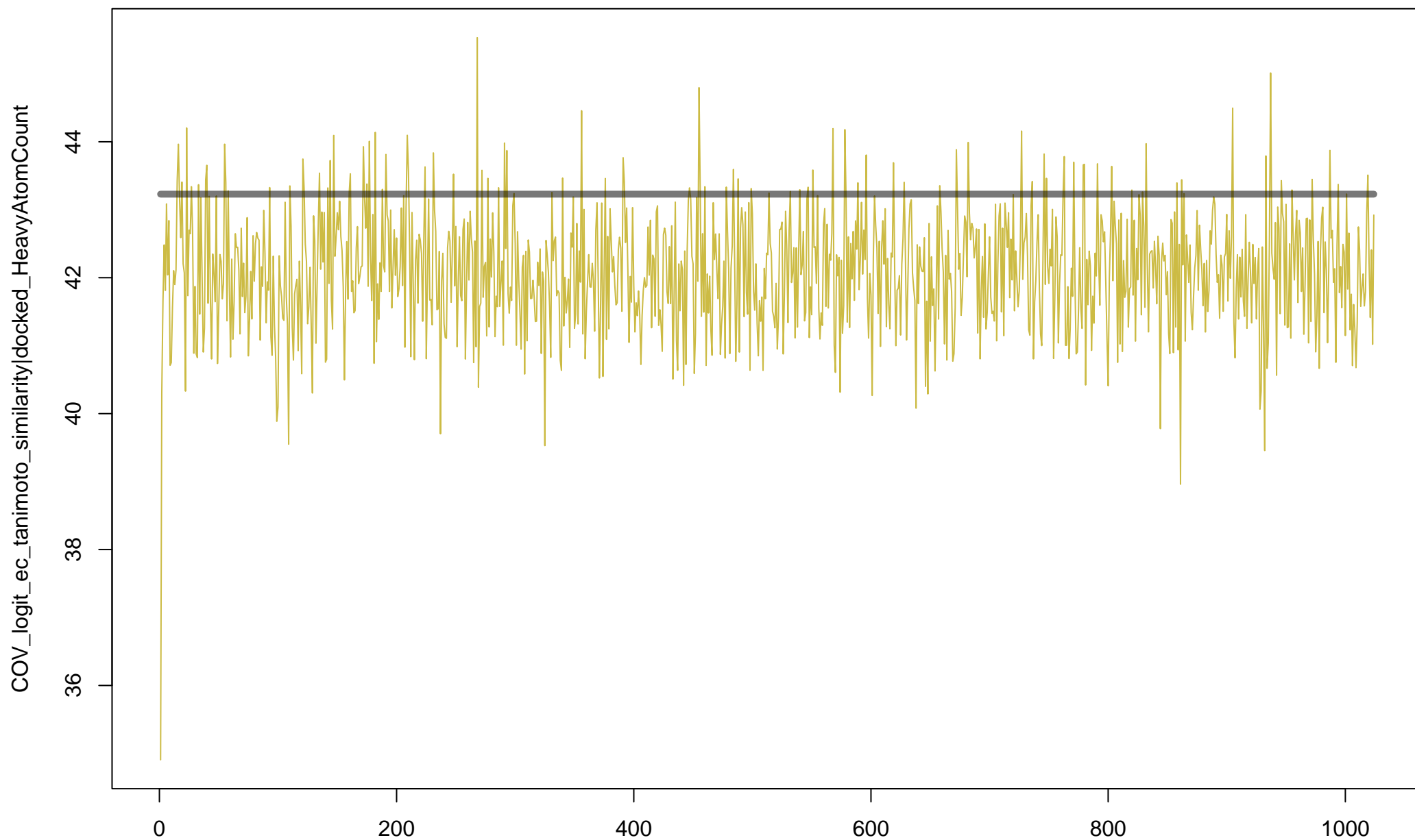
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0825 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0 | percentile: 36.2



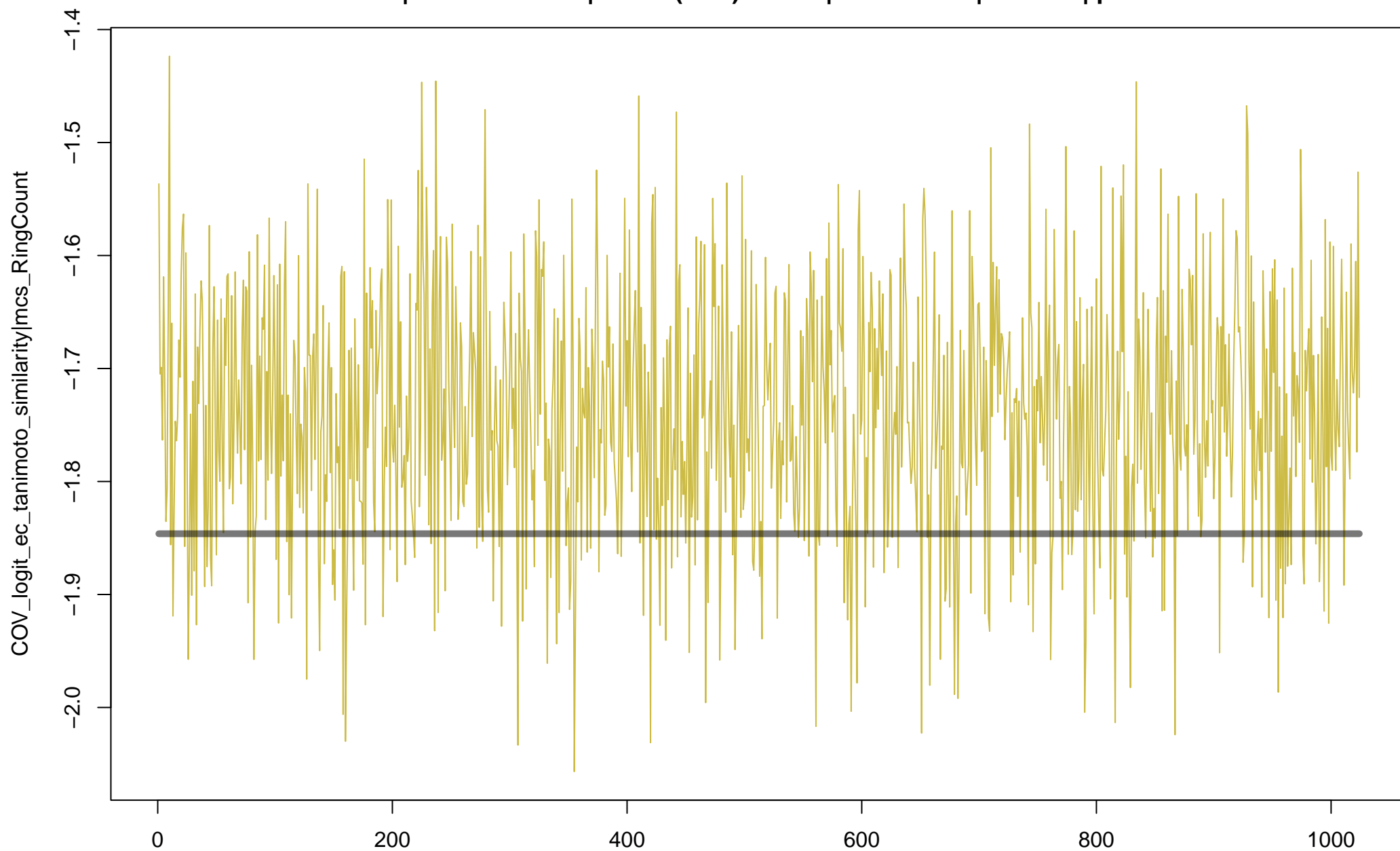
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0616 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0 | percentile: 19.7



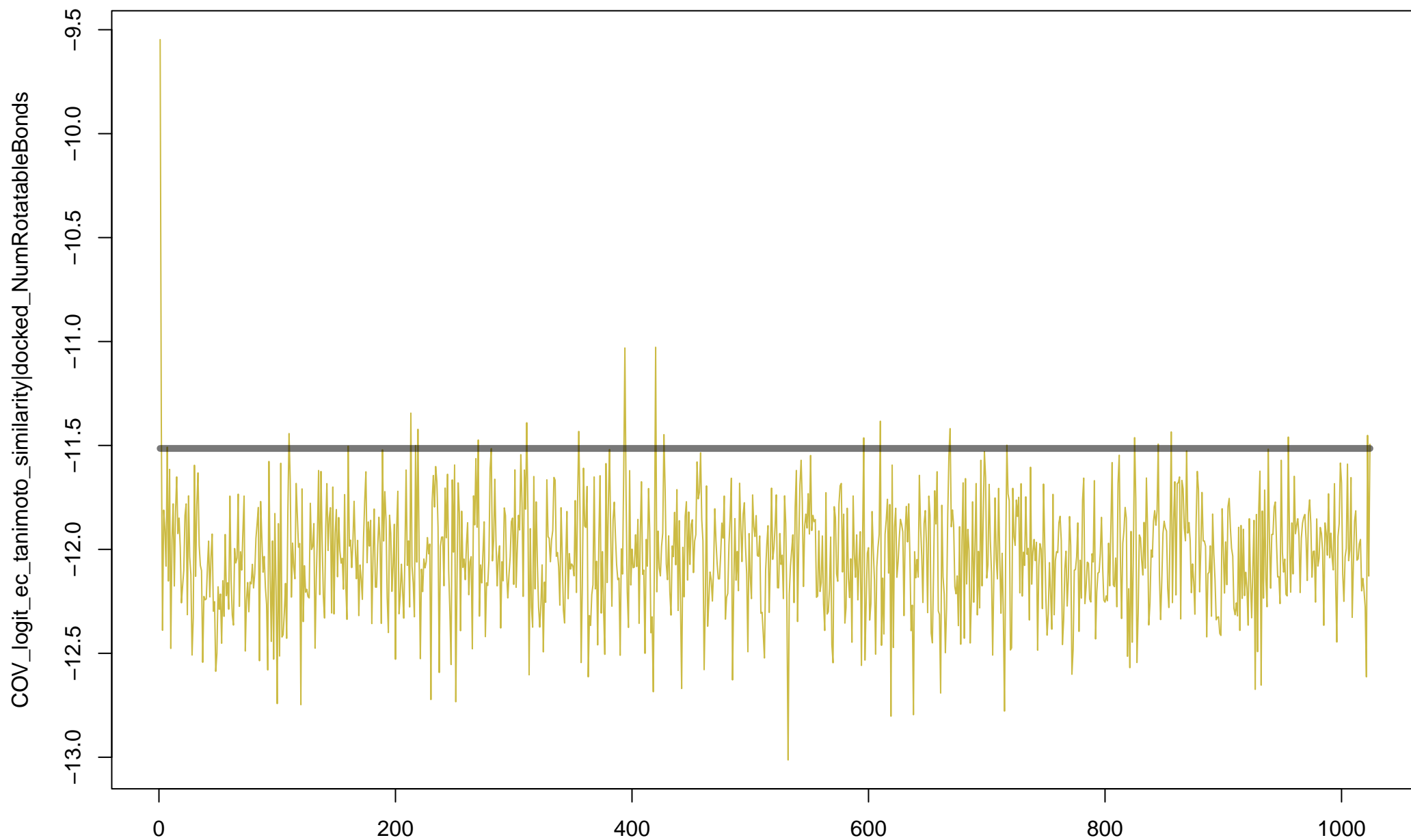
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0744 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | percentile: 90.9



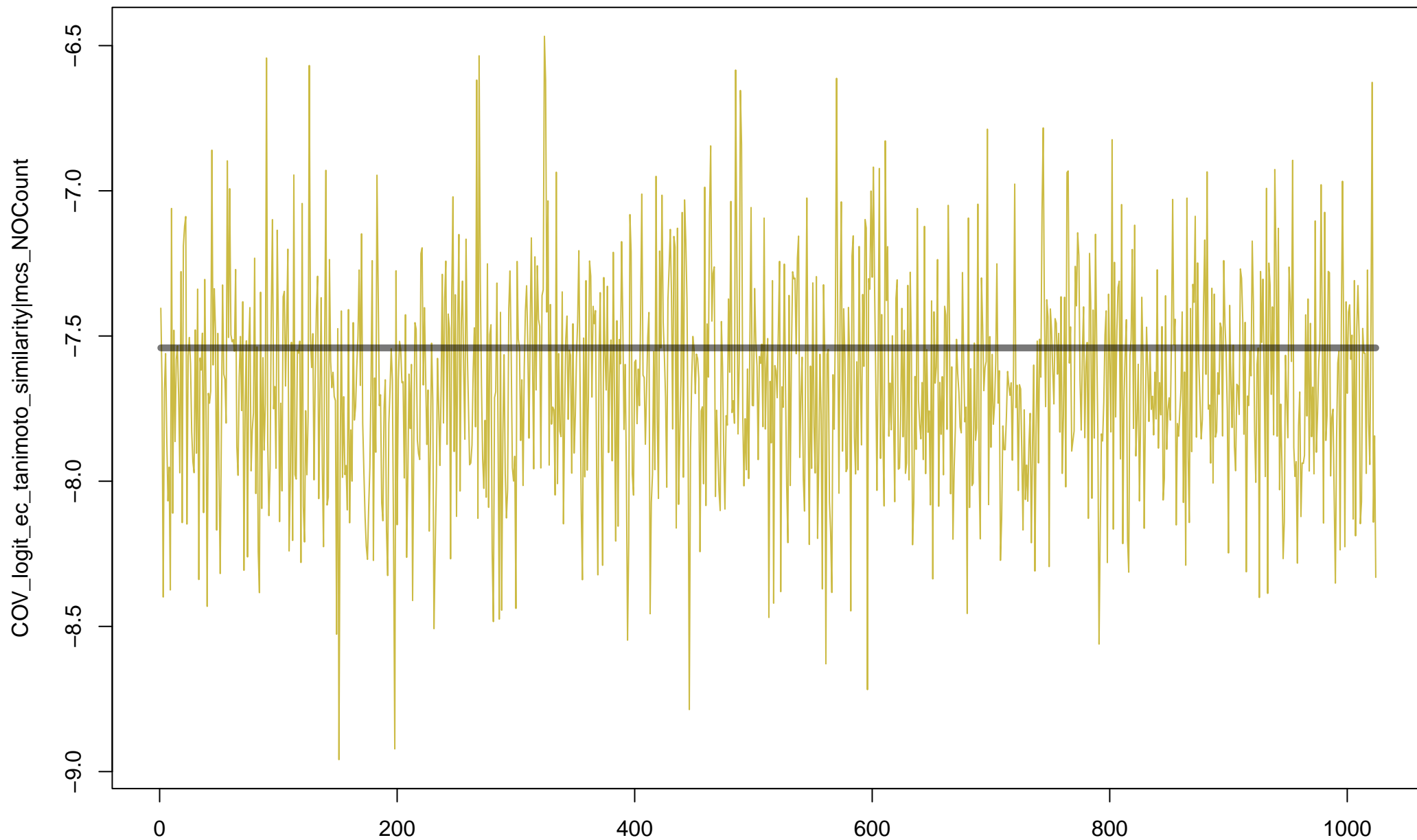
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0487 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0 | percentile: 17



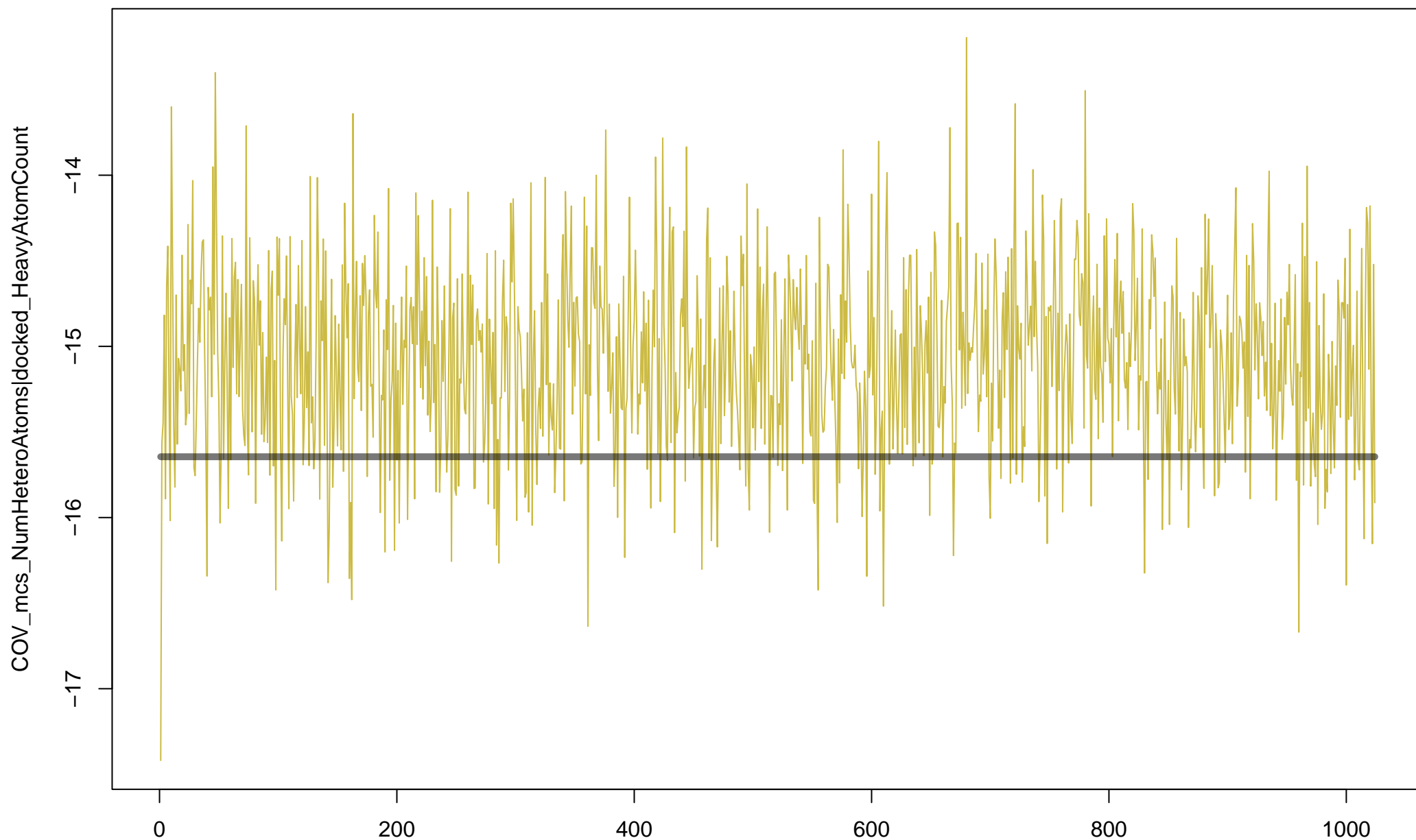
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 927 | BMK = 0.0703 | MCSE(6.27) = 3.55 | stat: TRUE | burn: 0 | percentile: 97.7



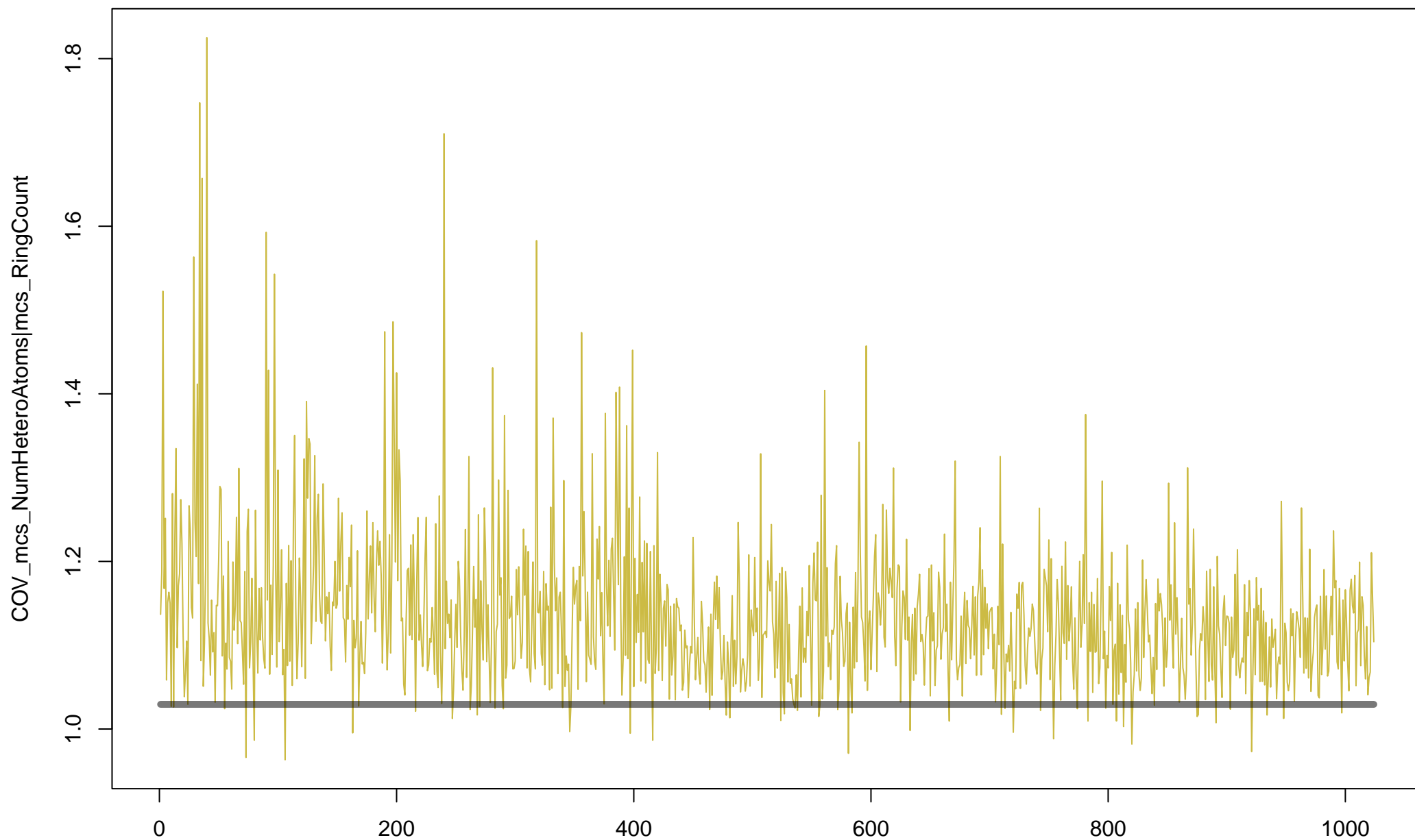
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0572 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0 | percentile: 64.6



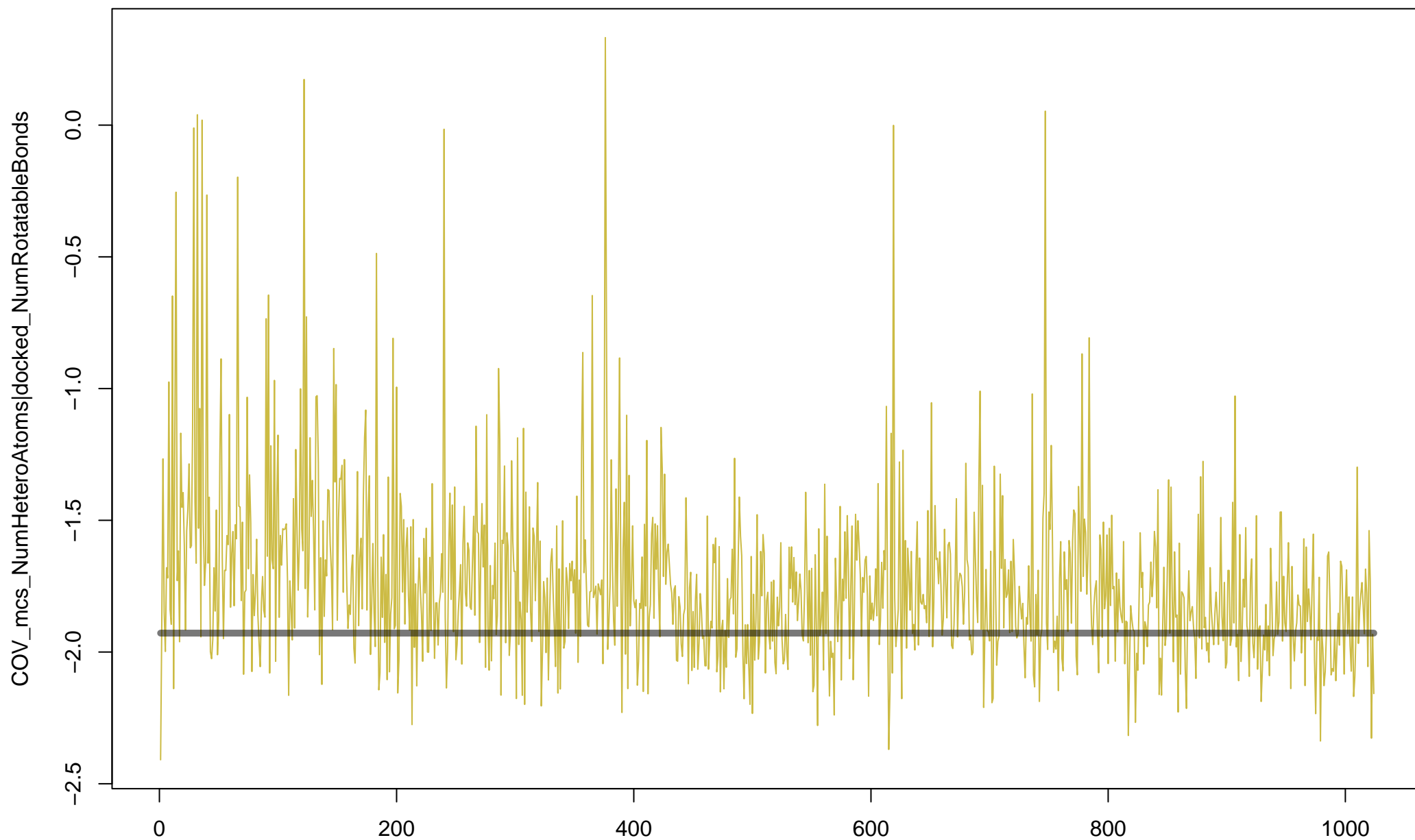
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0576 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 0 | percentile: 15.2



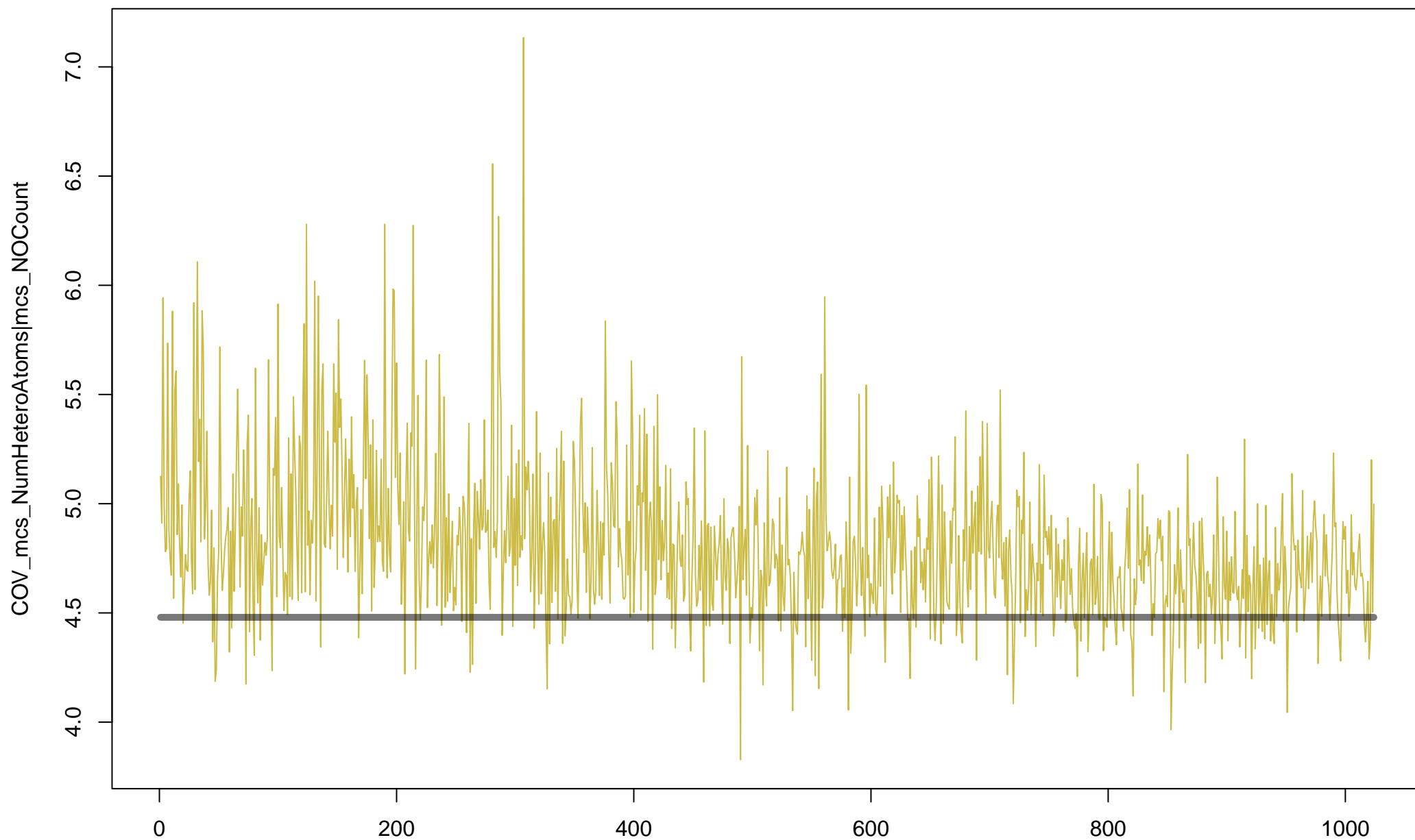
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 257 | BMK = 0.171 | MCSE(6.27) = 5.37 | stat: FALSE | burn: 0 | percentile: 5.57



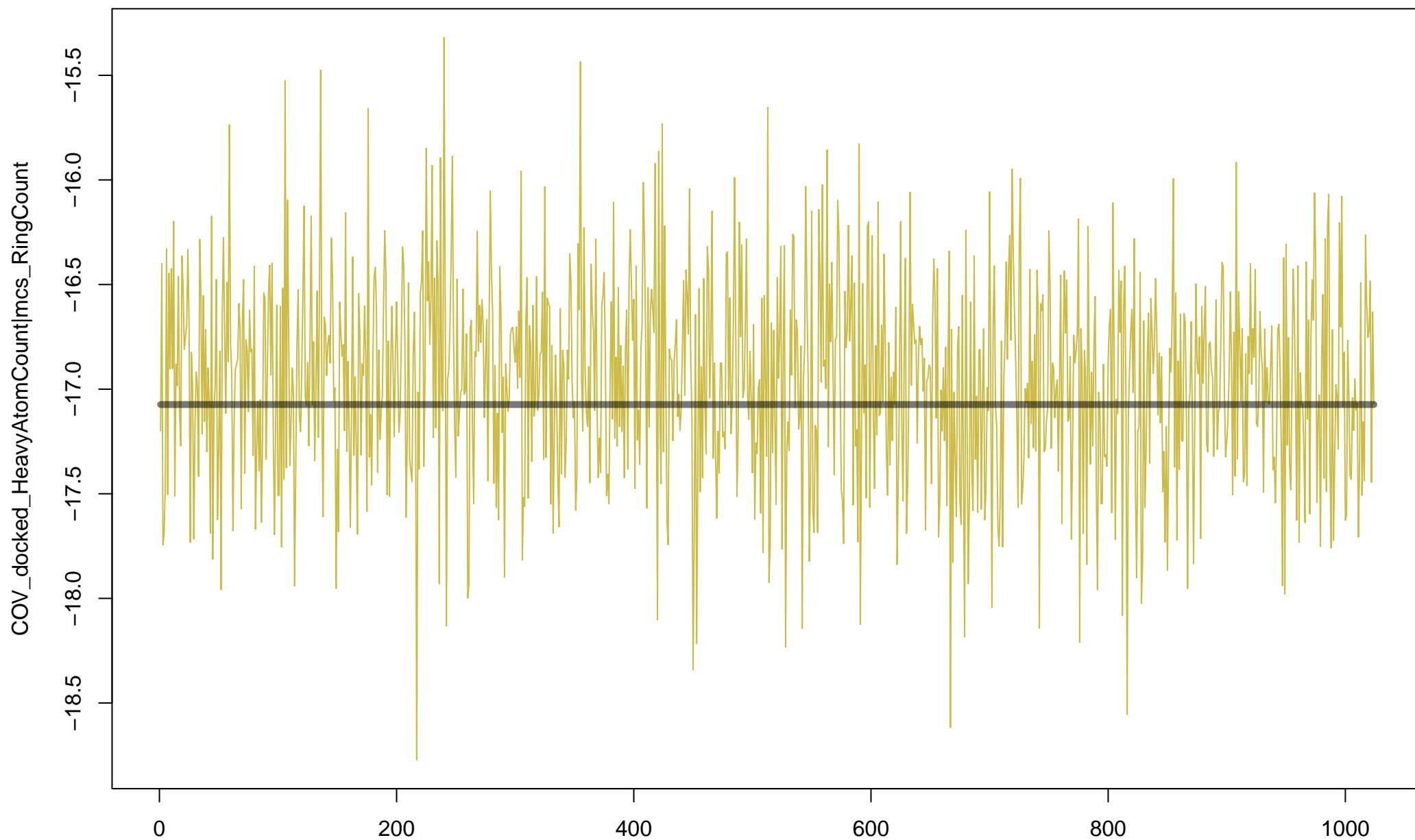
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 183 | BMK = 0.177 | MCSE(6.27) = 6.42 | stat: FALSE | burn: 0 | percentile: 27.7



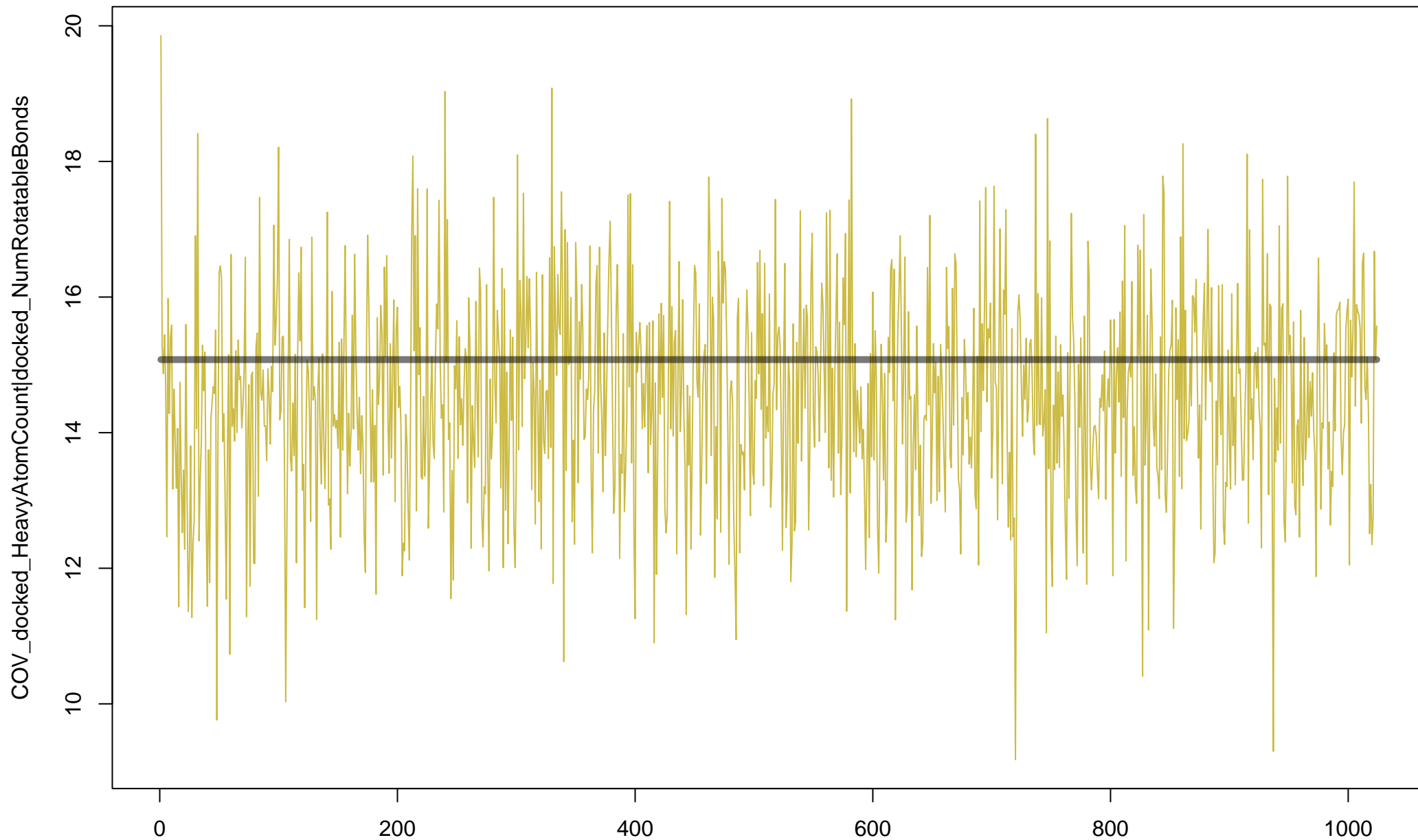
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 37.9 | BMK = 0.248 | MCSE(6.27) = 7.3 | stat: FALSE | burn: 0 | percentile: 14.3



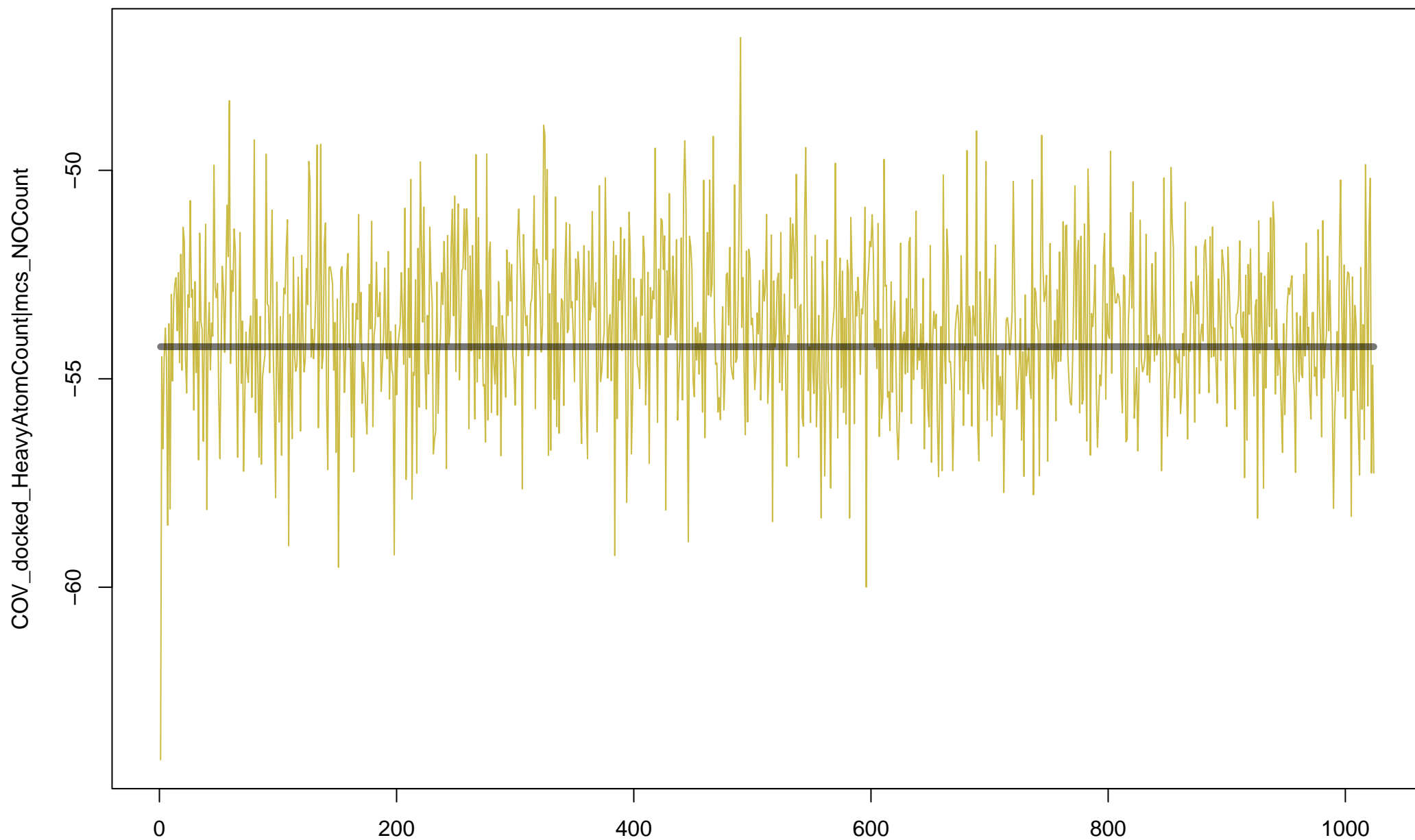
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.076 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0 | percentile: 39.7



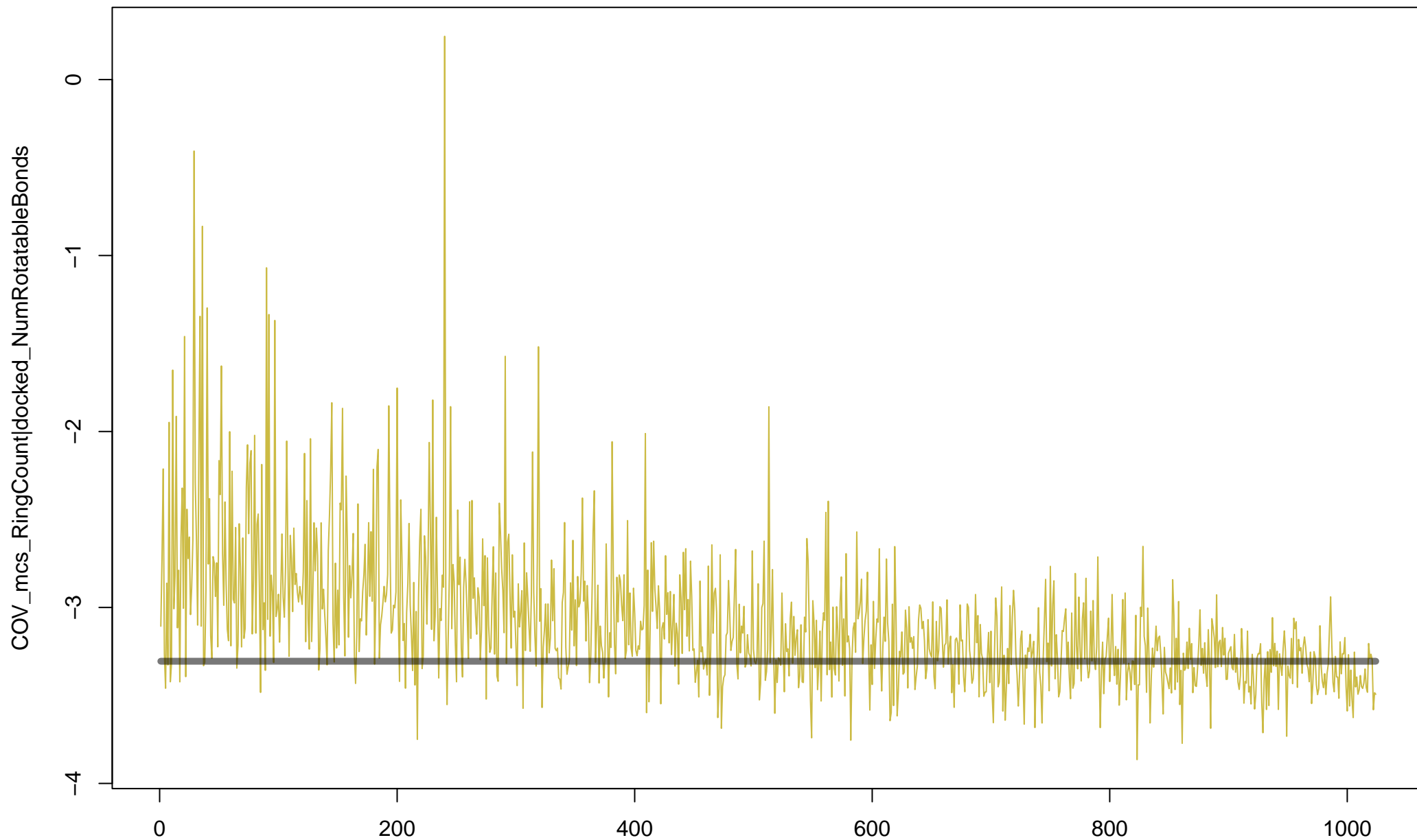
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.056 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0 | percentile: 64.7



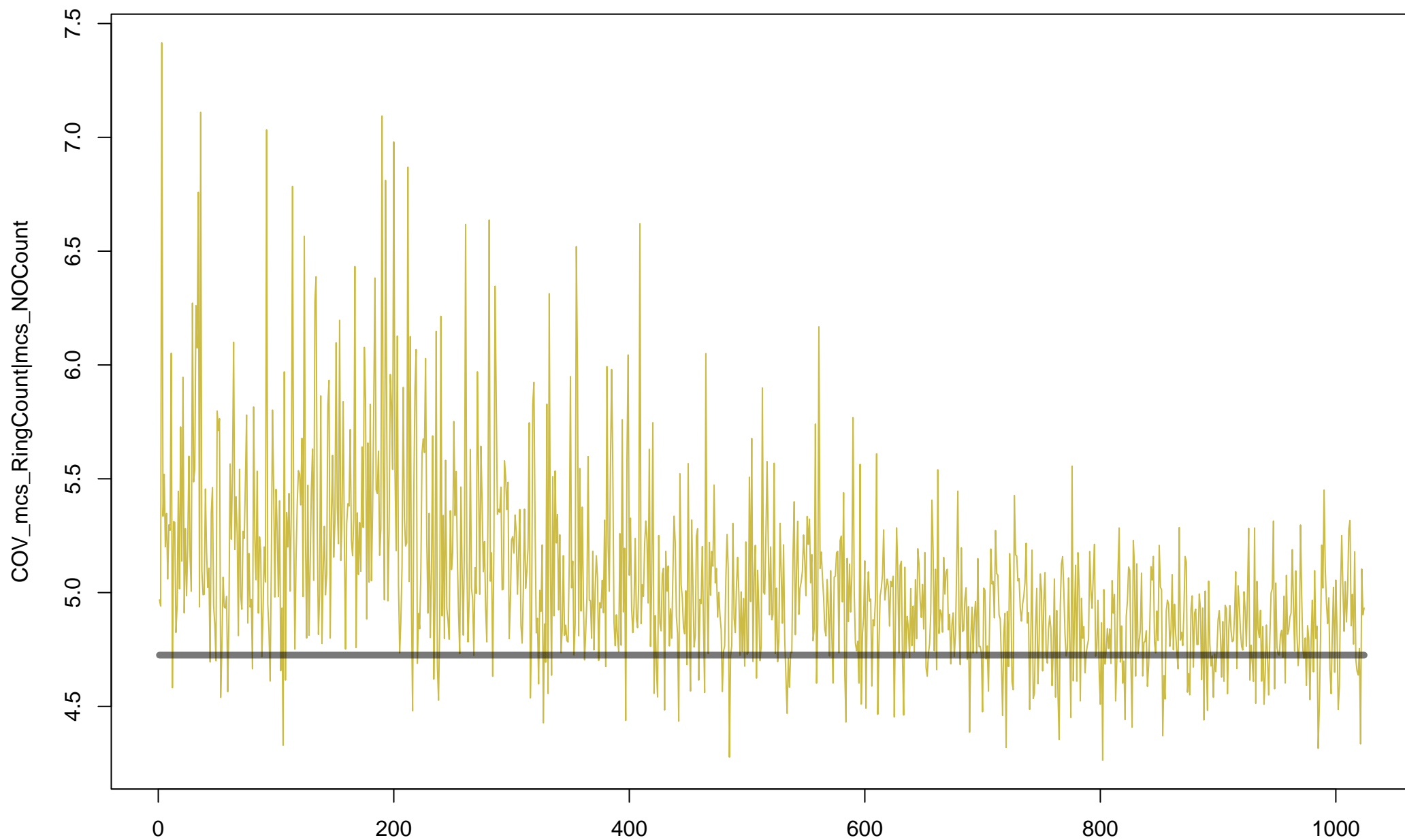
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0783 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0 | percentile: 41.1



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 15.8 | BMK = 0.379 | MCSE(6.27) = 9.71 | stat: FALSE | burn: 0 | percentile: 30



COV_mcs_RingCount|mcs_NOCount
ESS = 29.3 | BMK = 0.329 | MCSE(6.27) = 8.96 | stat: FALSE | burn: 0 | percentile: 16



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 4.37 | BMK = 0.483 | MCSE(6.27) = 11 | stat: FALSE | burn: 0 | percentile: 4.79

