

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 1

max MCSE = 14.2445576411731

all stationary: FALSE

burn: 1020

min percent.: 1.171875

-- STATS 2D --

min ESS = 11.8059808810312

max BMK = 0.326861657808357

max MCSE = 9.95589336922989

all stationary: FALSE

burn: 0

min percent.: 1.7578125

-- STATS 1D --

min ESS = 13.3691278952772

max BMK = 1

max MCSE = 12.9781124280532

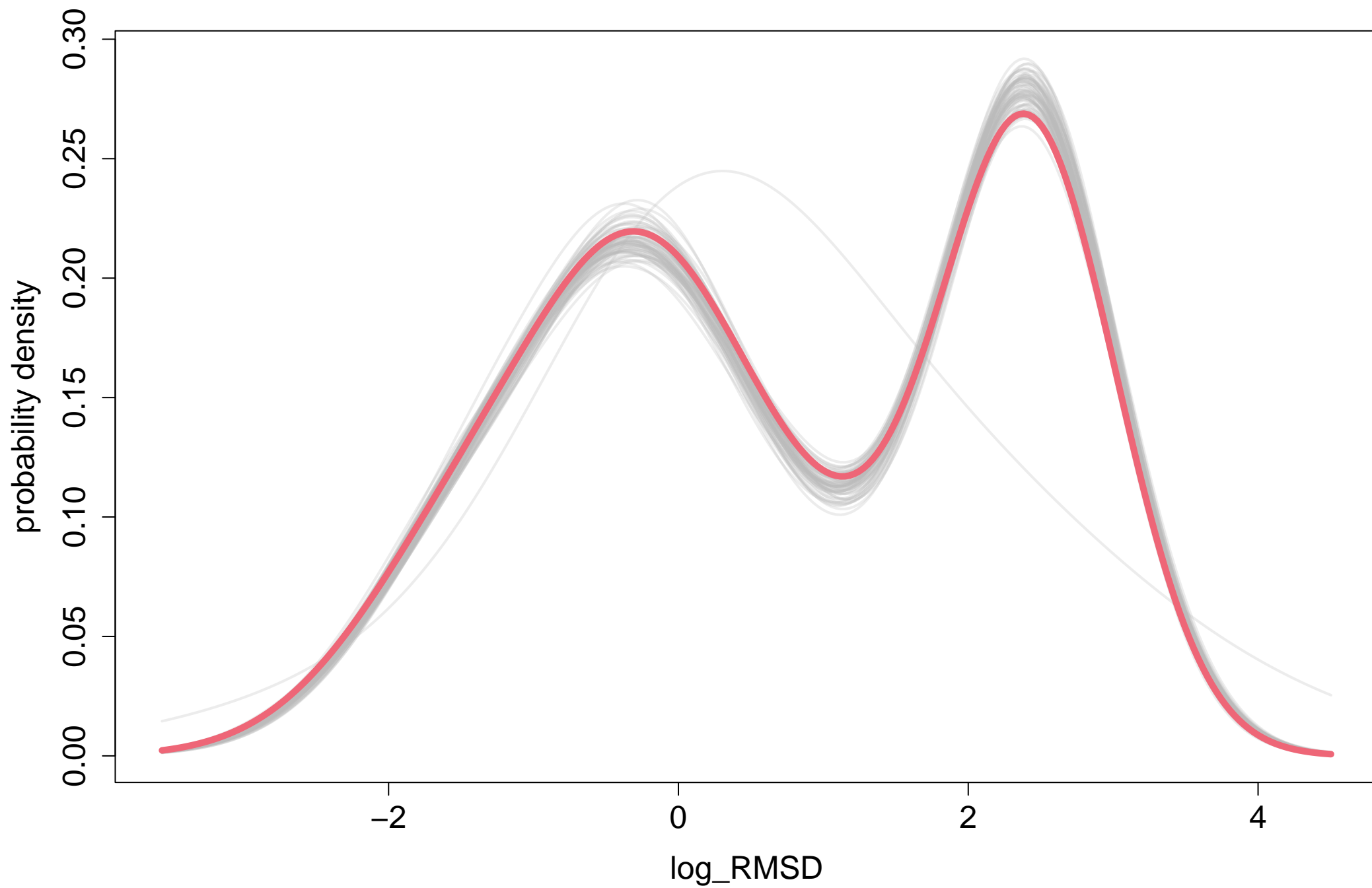
all stationary: FALSE

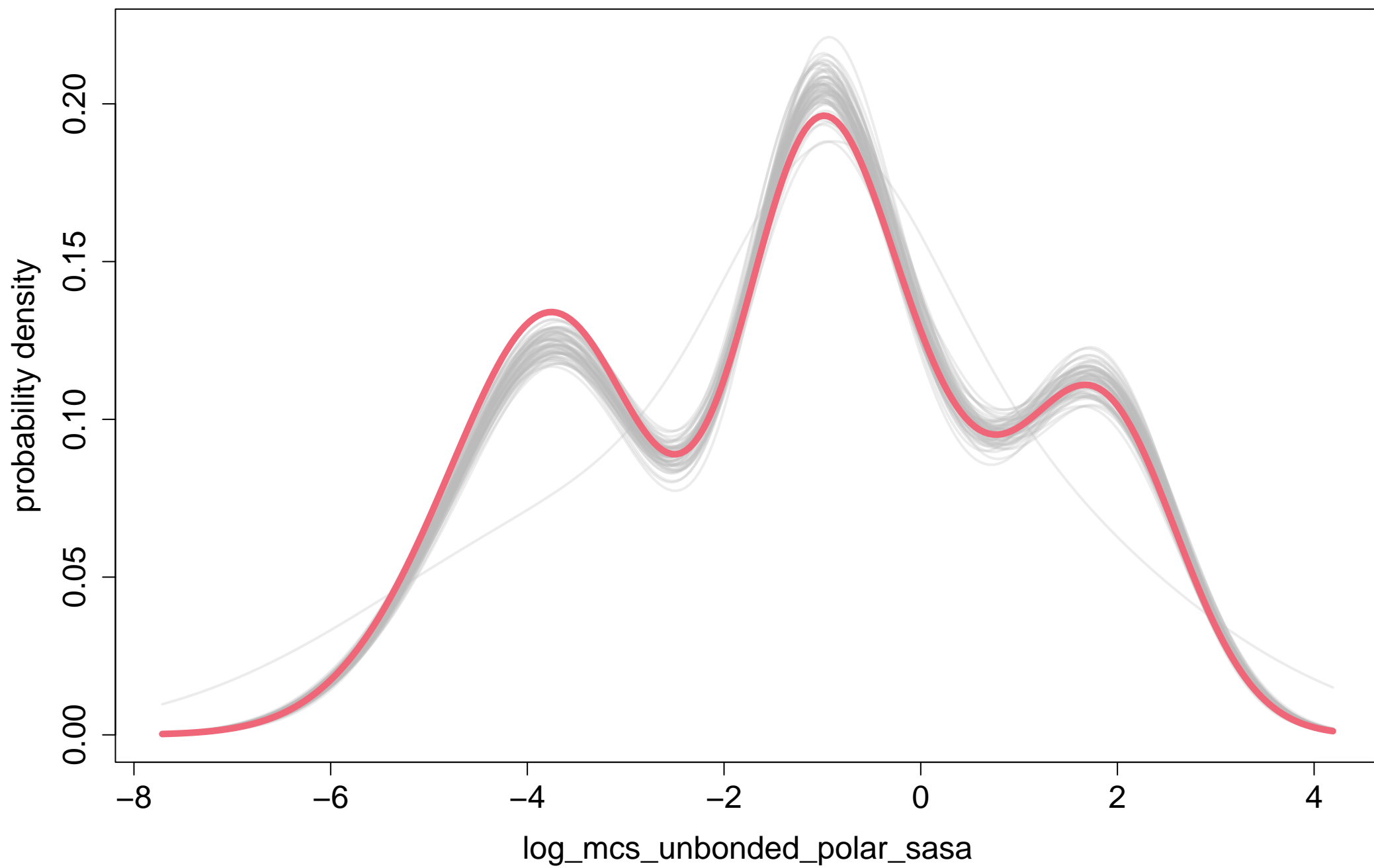
burn: 1020

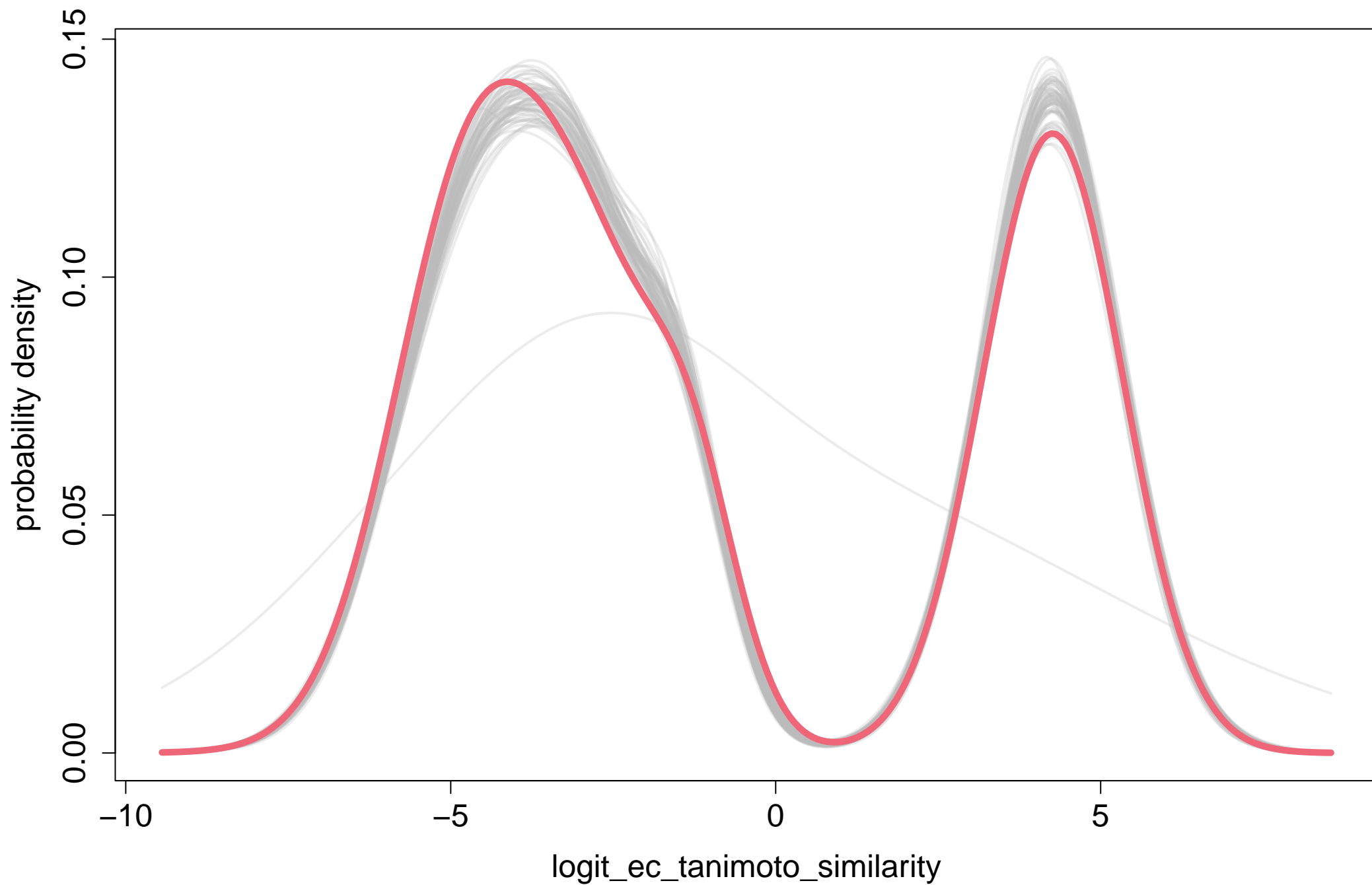
min percent.: 0.29296875

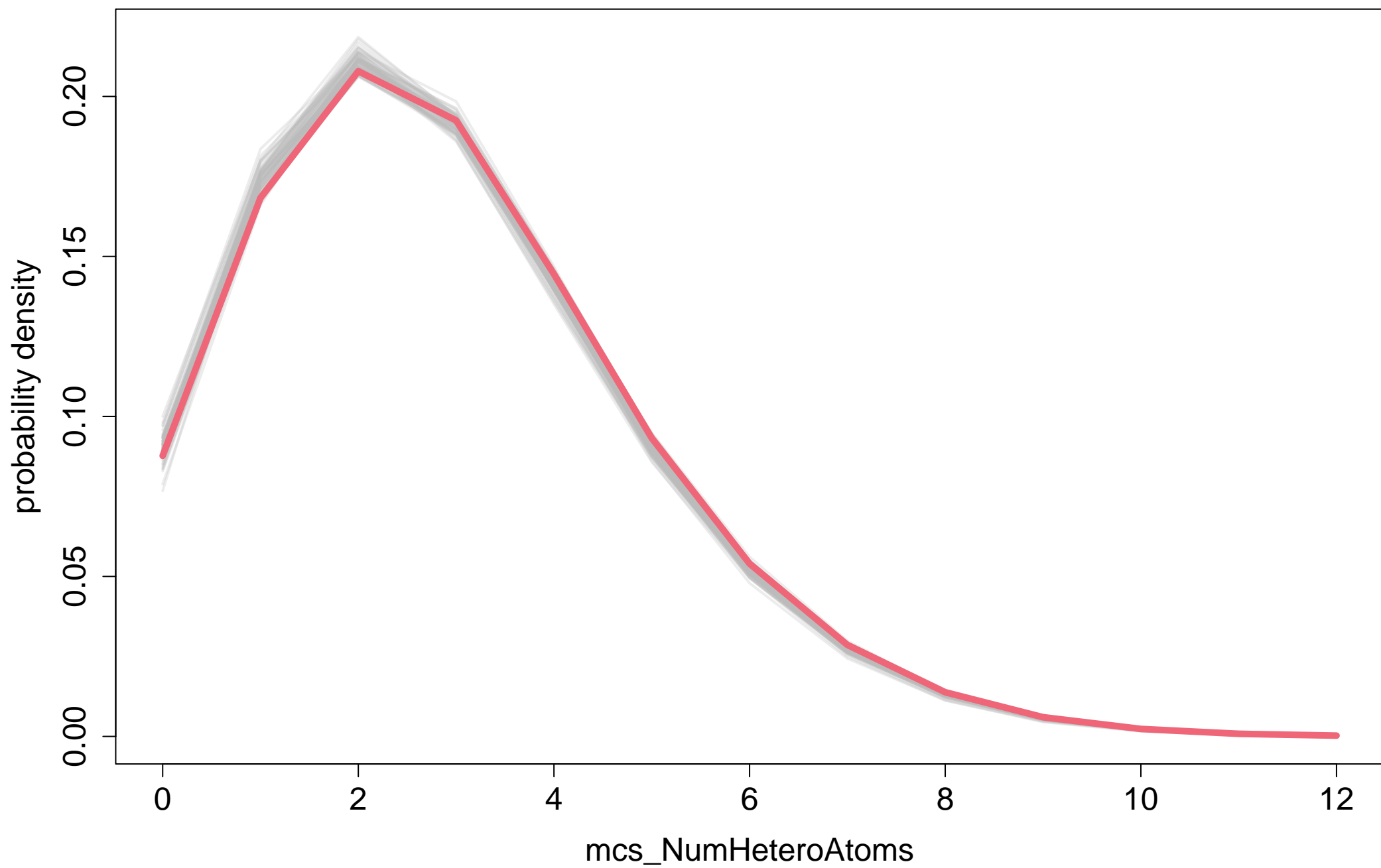
Occupied clusters: 10 of 64

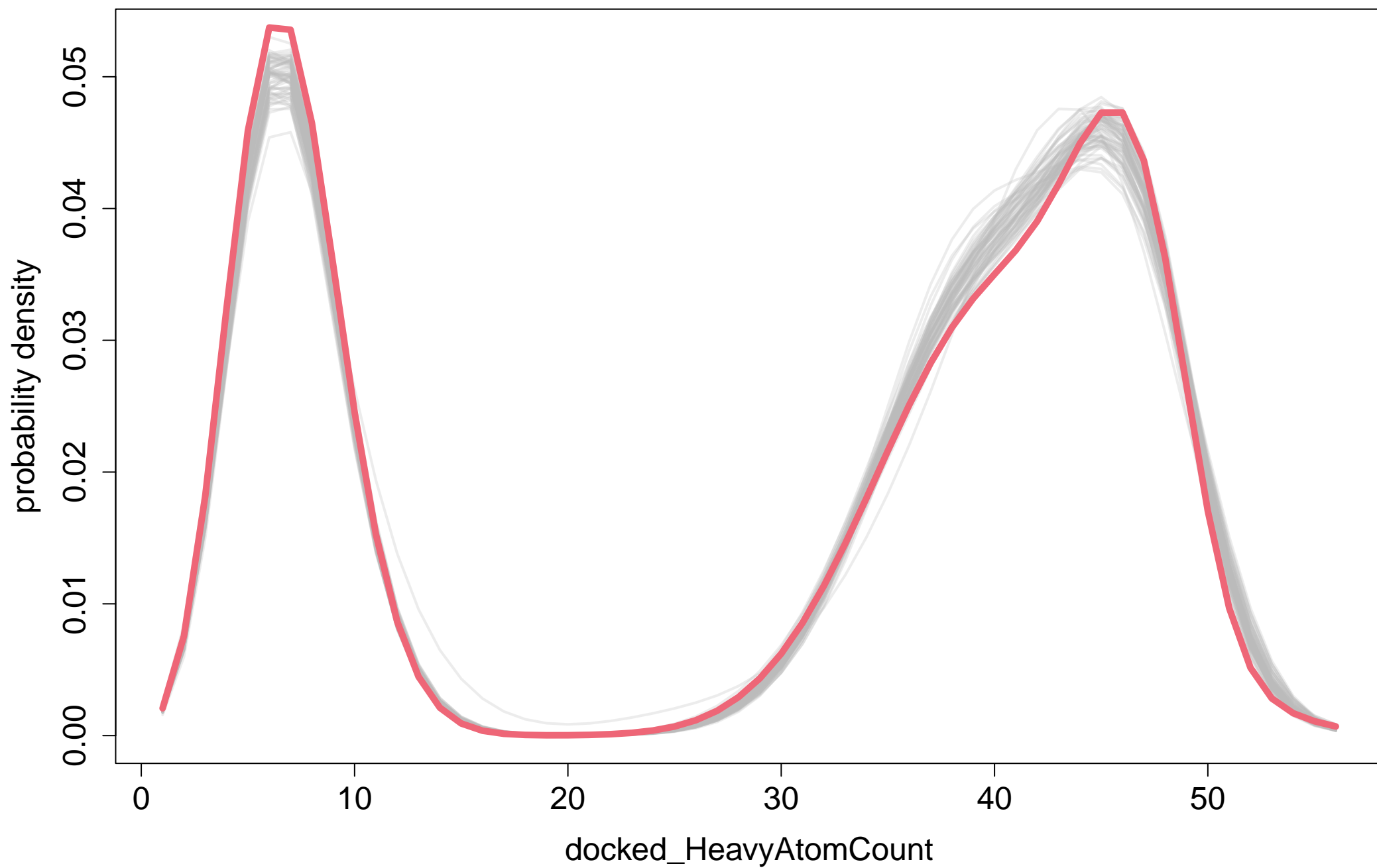
LL: -62500 +- 309

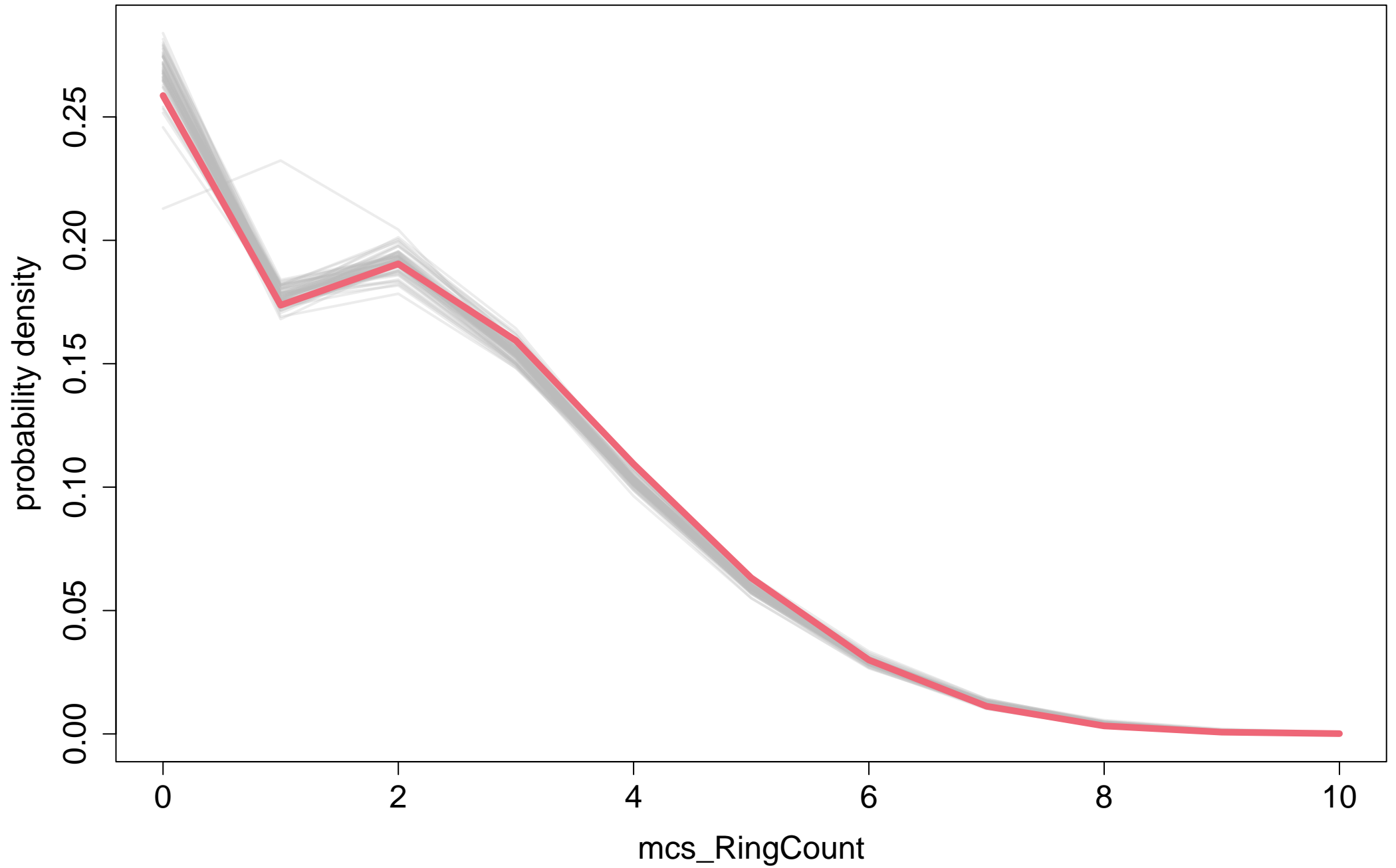


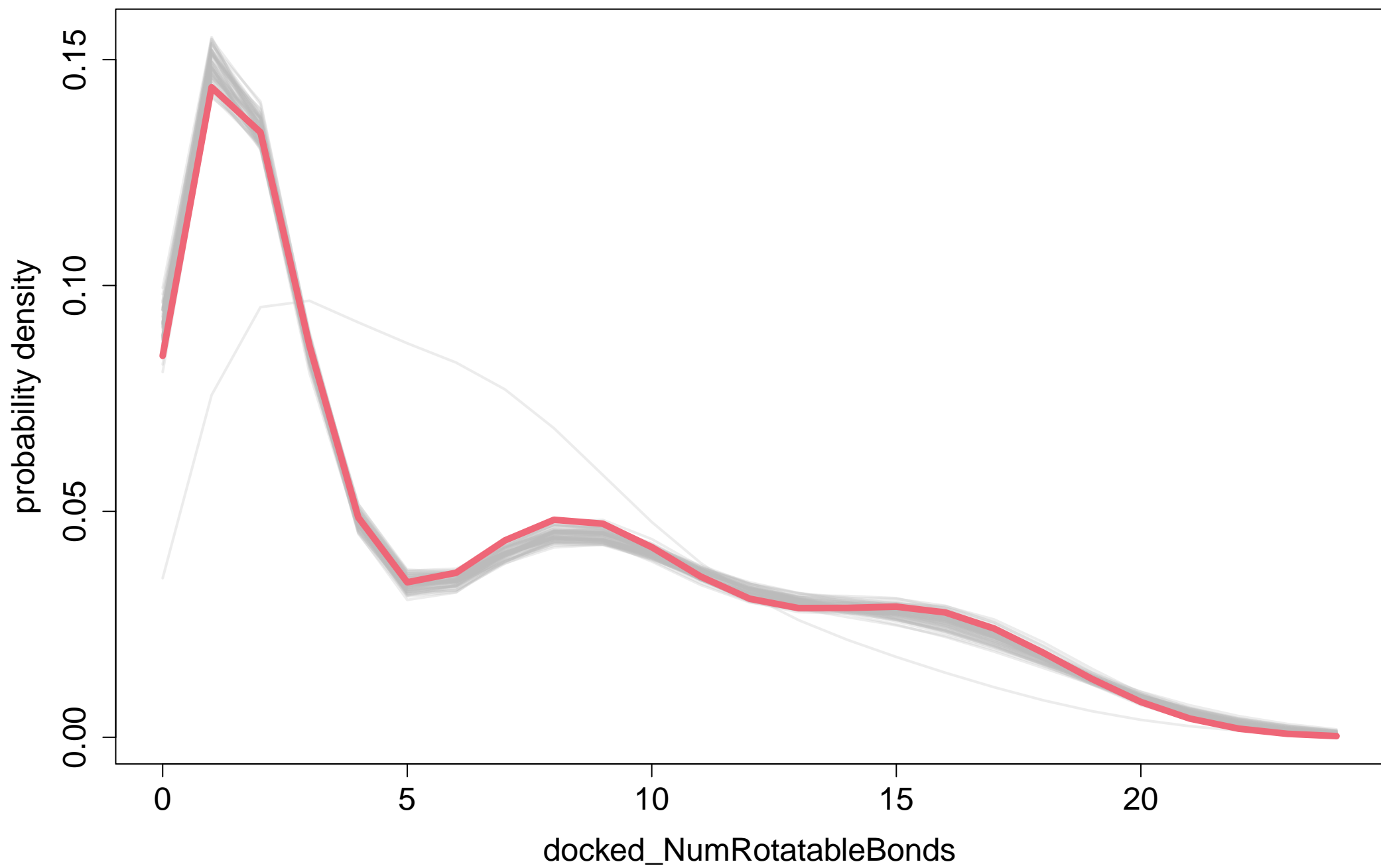


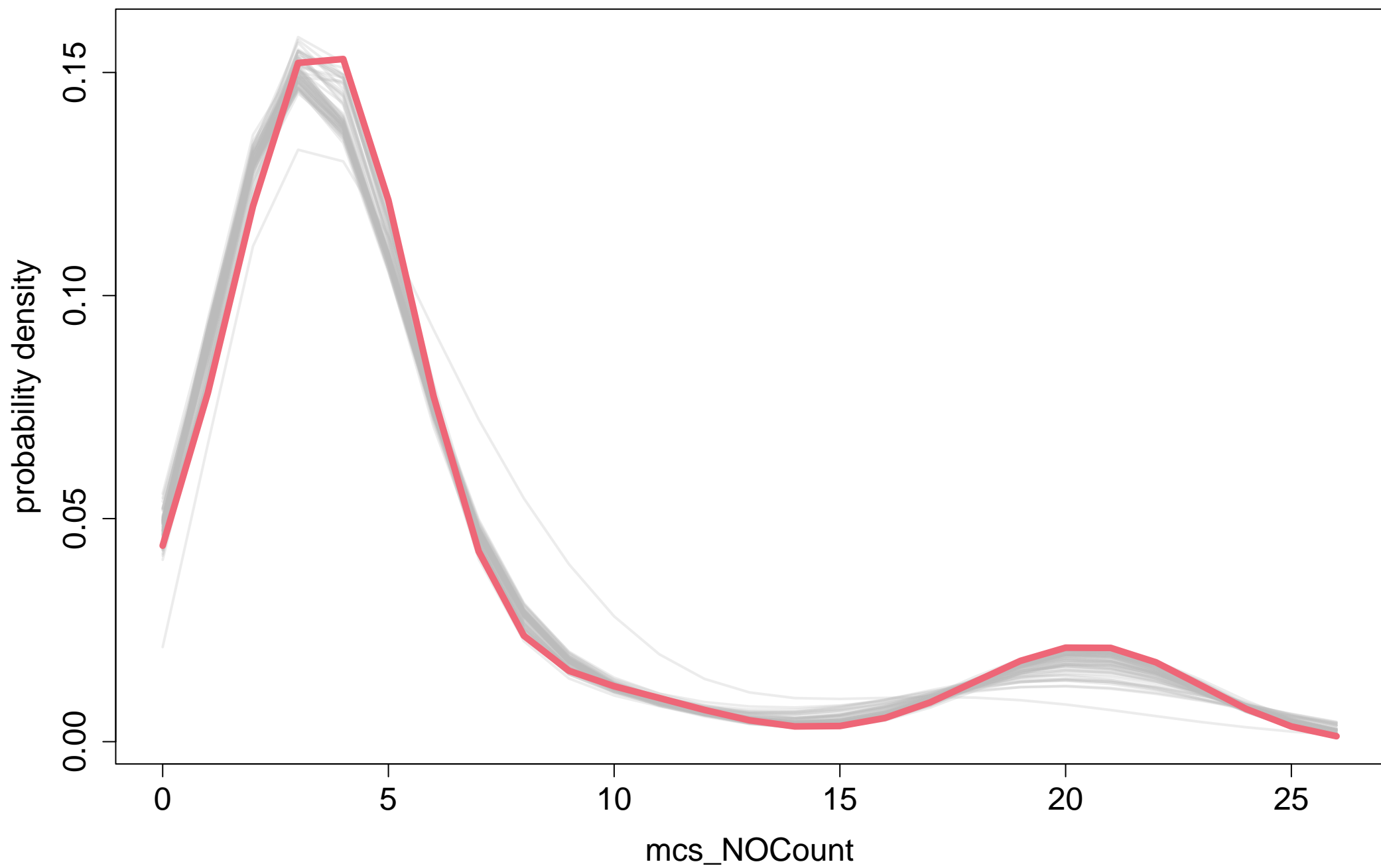


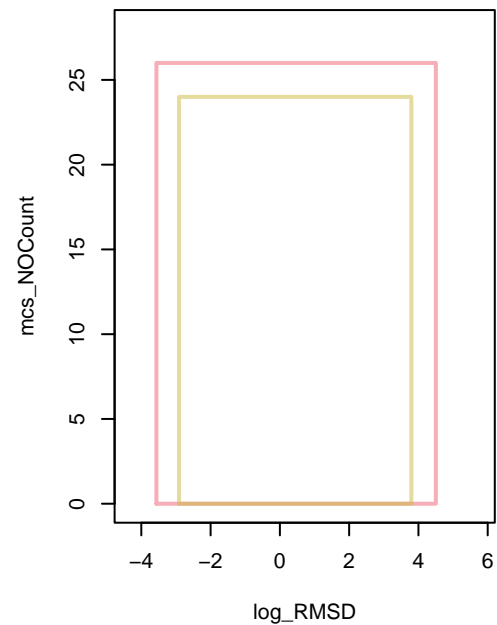
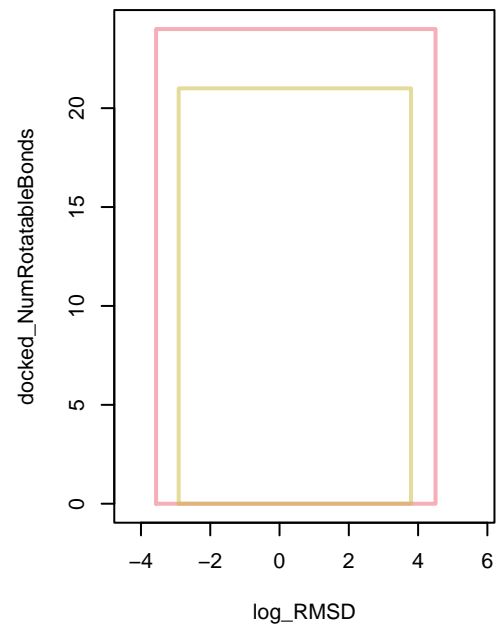
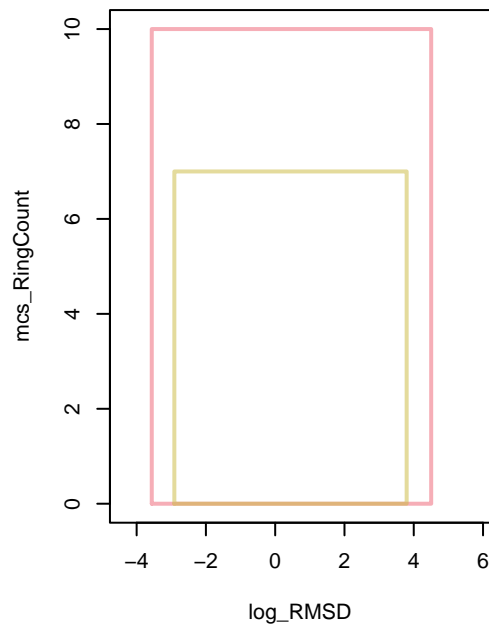
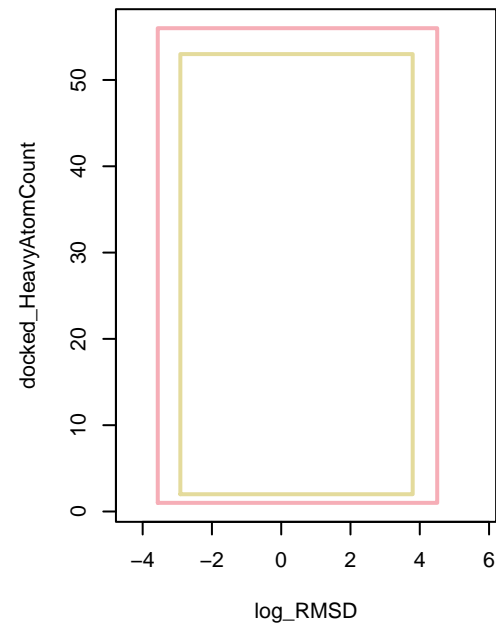
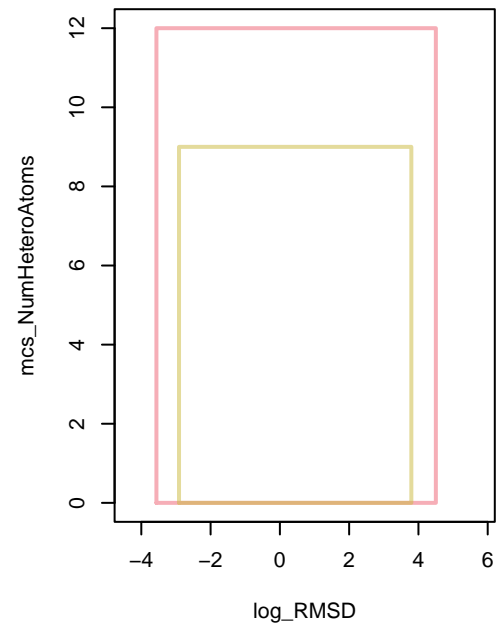
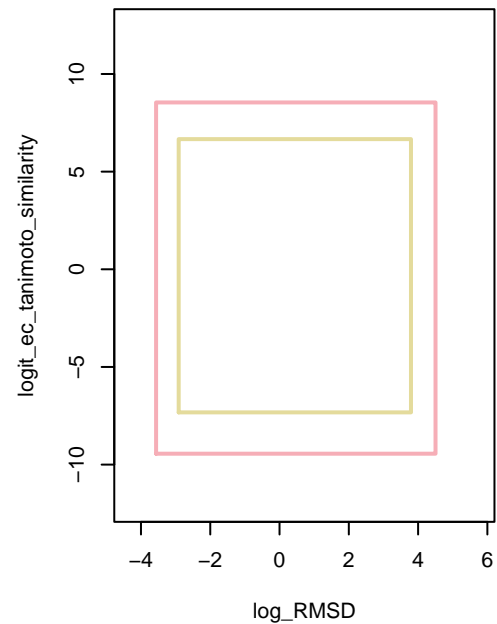
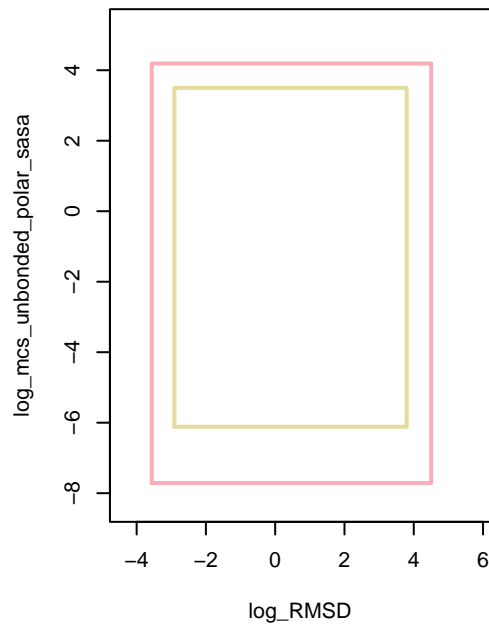




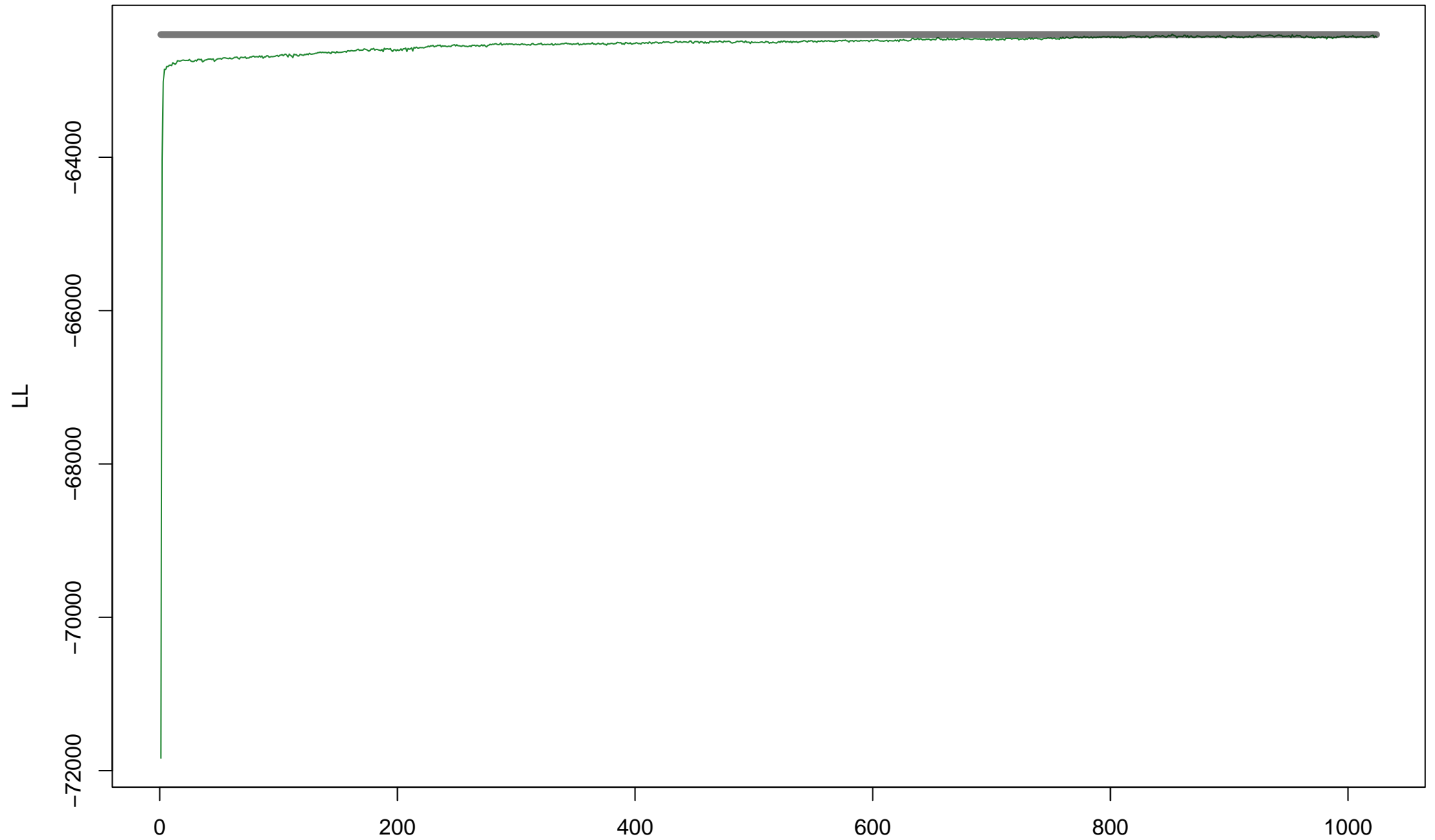






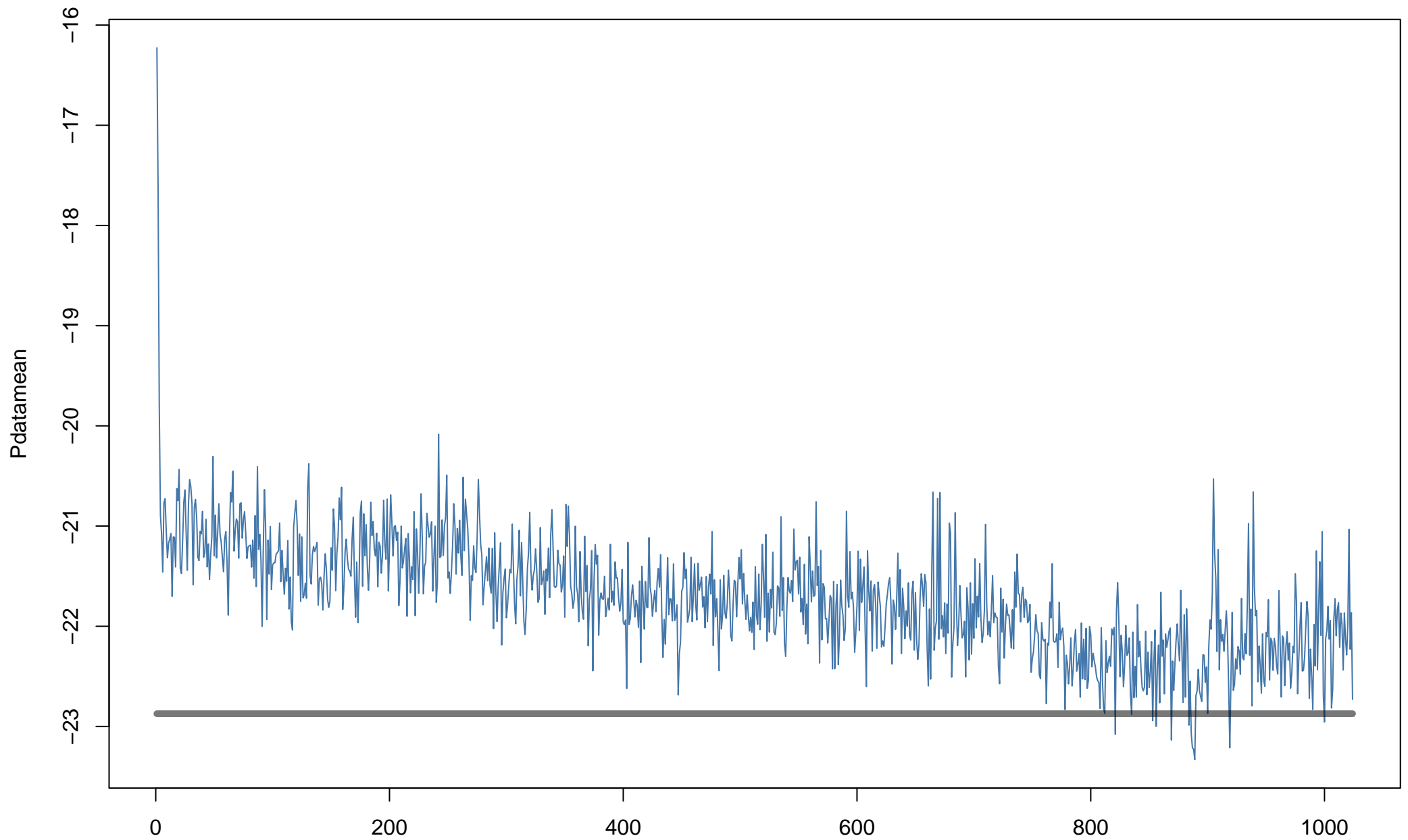


LL



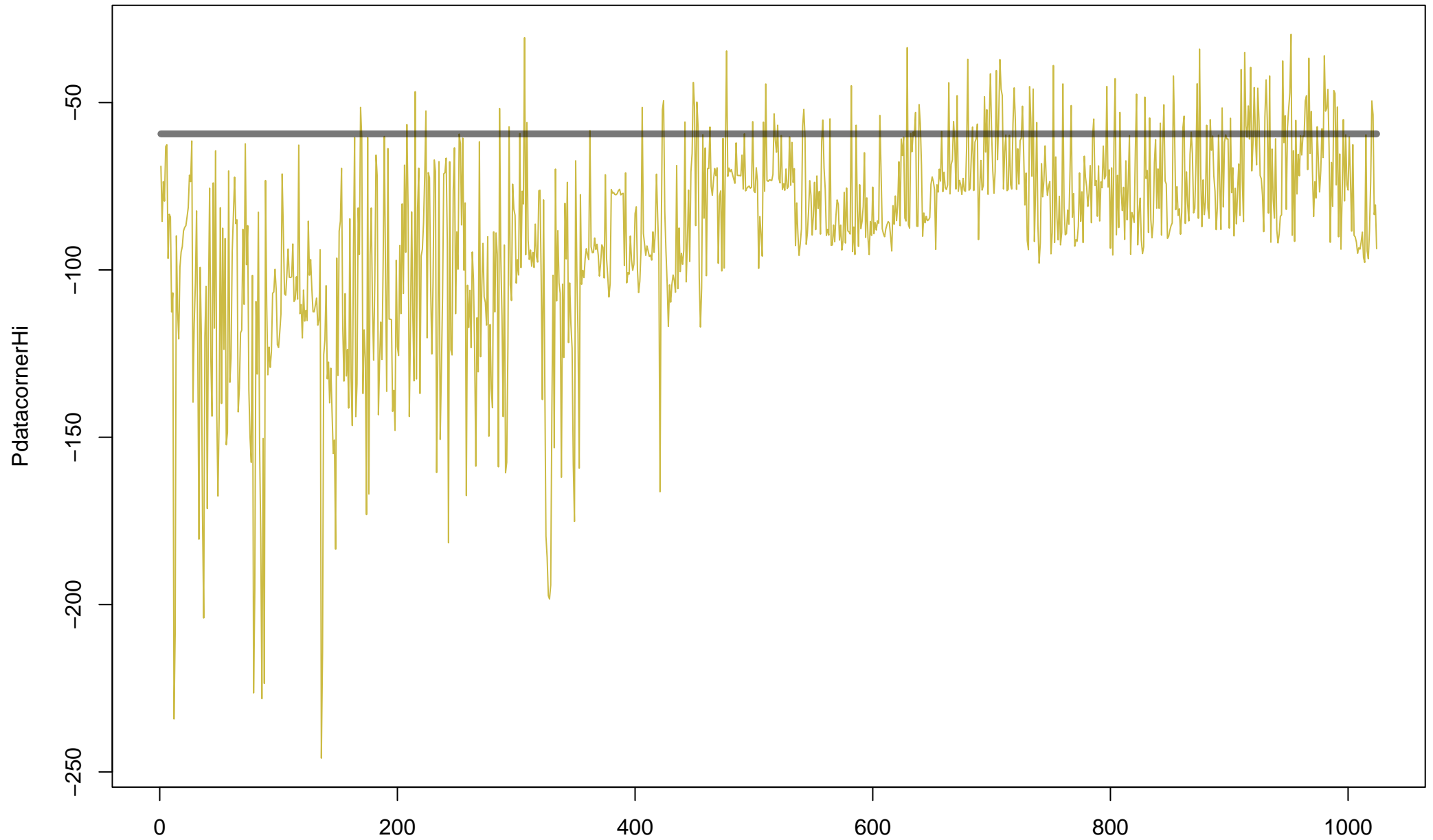
Pdatamean

ESS = 2.22e-16 | BMK = 0.6 | MCSE(6.27) = 4.29 | stat: TRUE | burn: 0 | percentile: 1.17



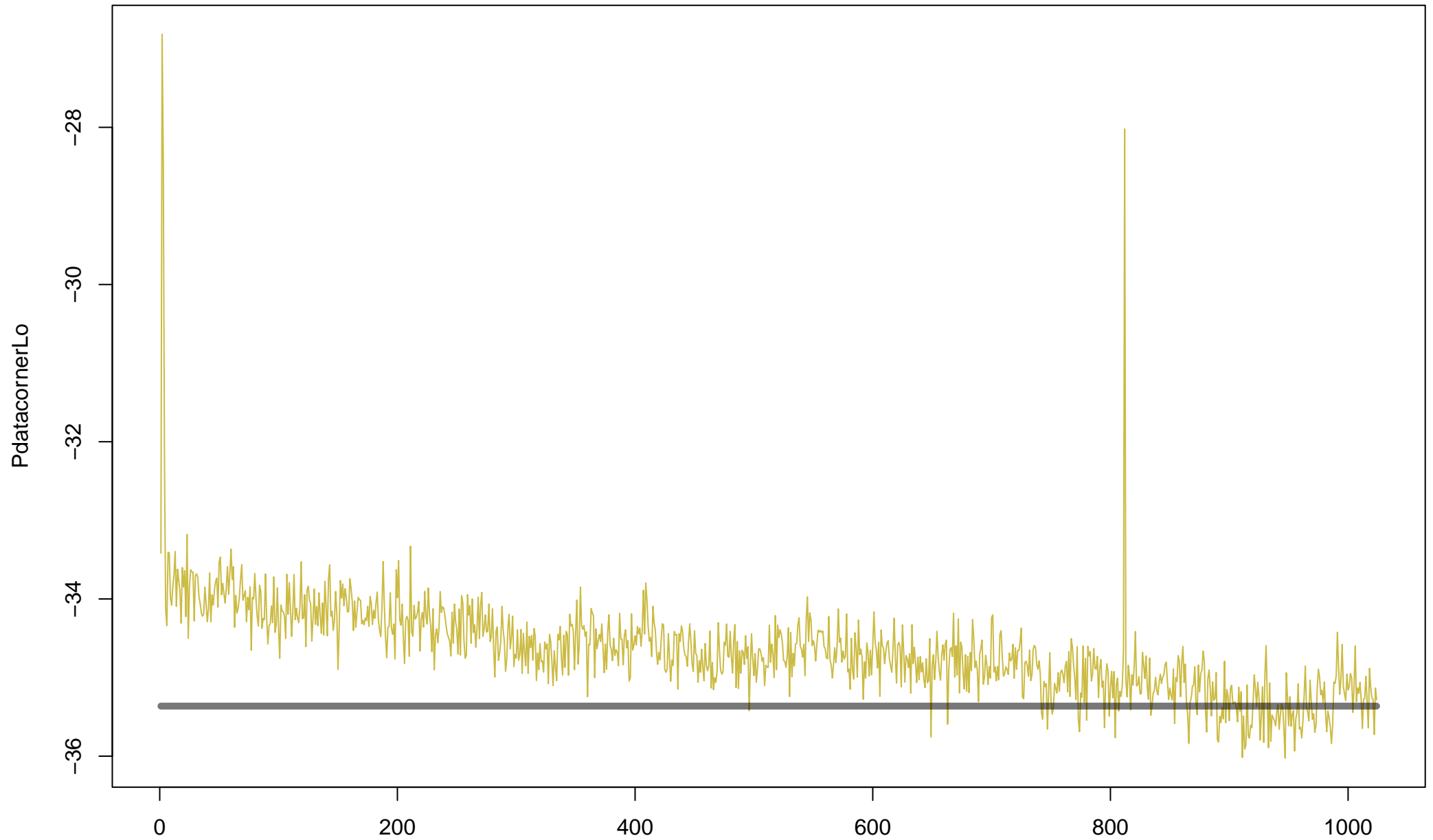
PdatacornerHi

ESS = $2.22\text{e-}16$ | BMK = 1 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 1020 | percentile: 88.1

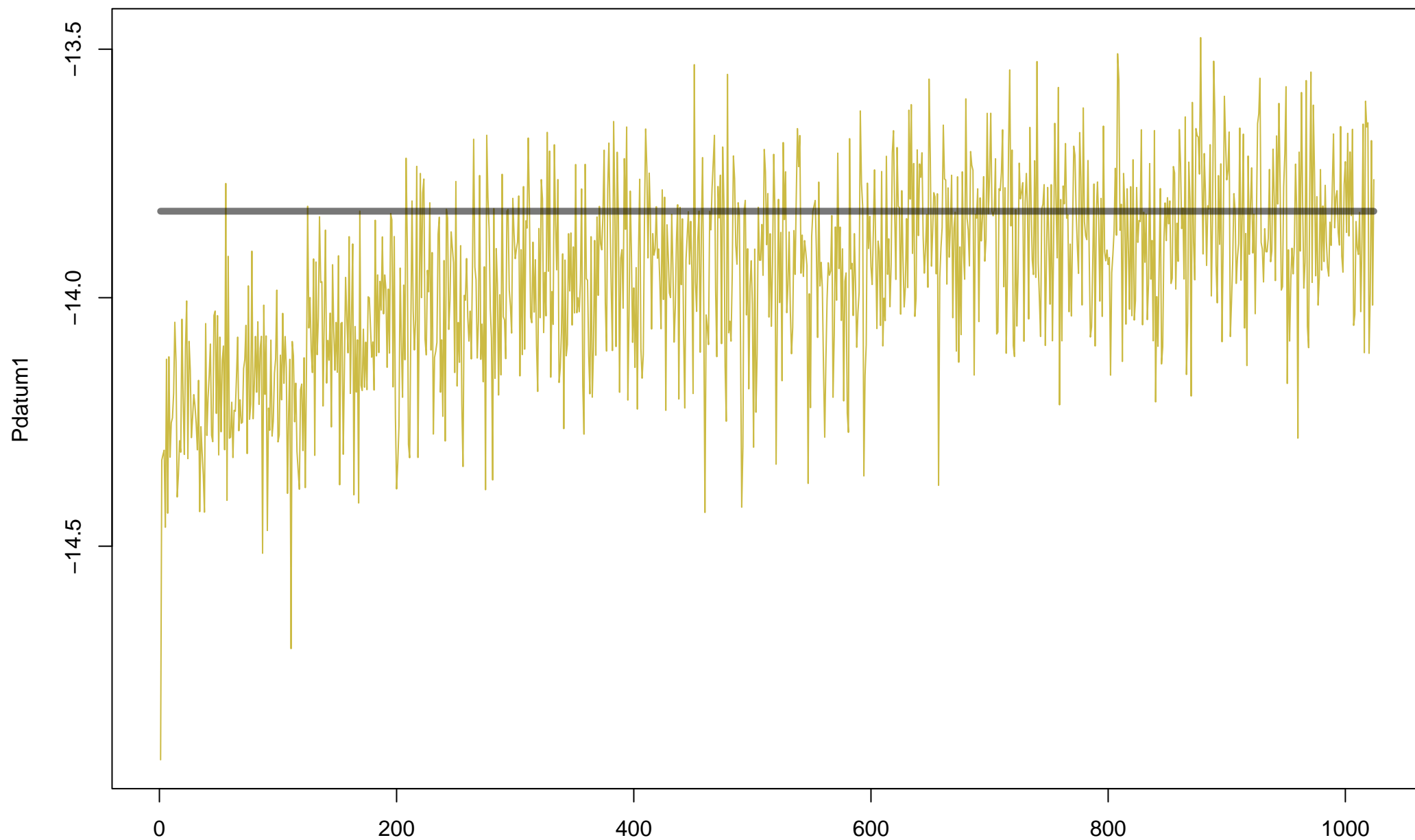


PdatacornerLo

ESS = 2.22e-16 | BMK = 1 | MCSE(6.27) = 3.65 | stat: TRUE | burn: 816 | percentile: 8.69

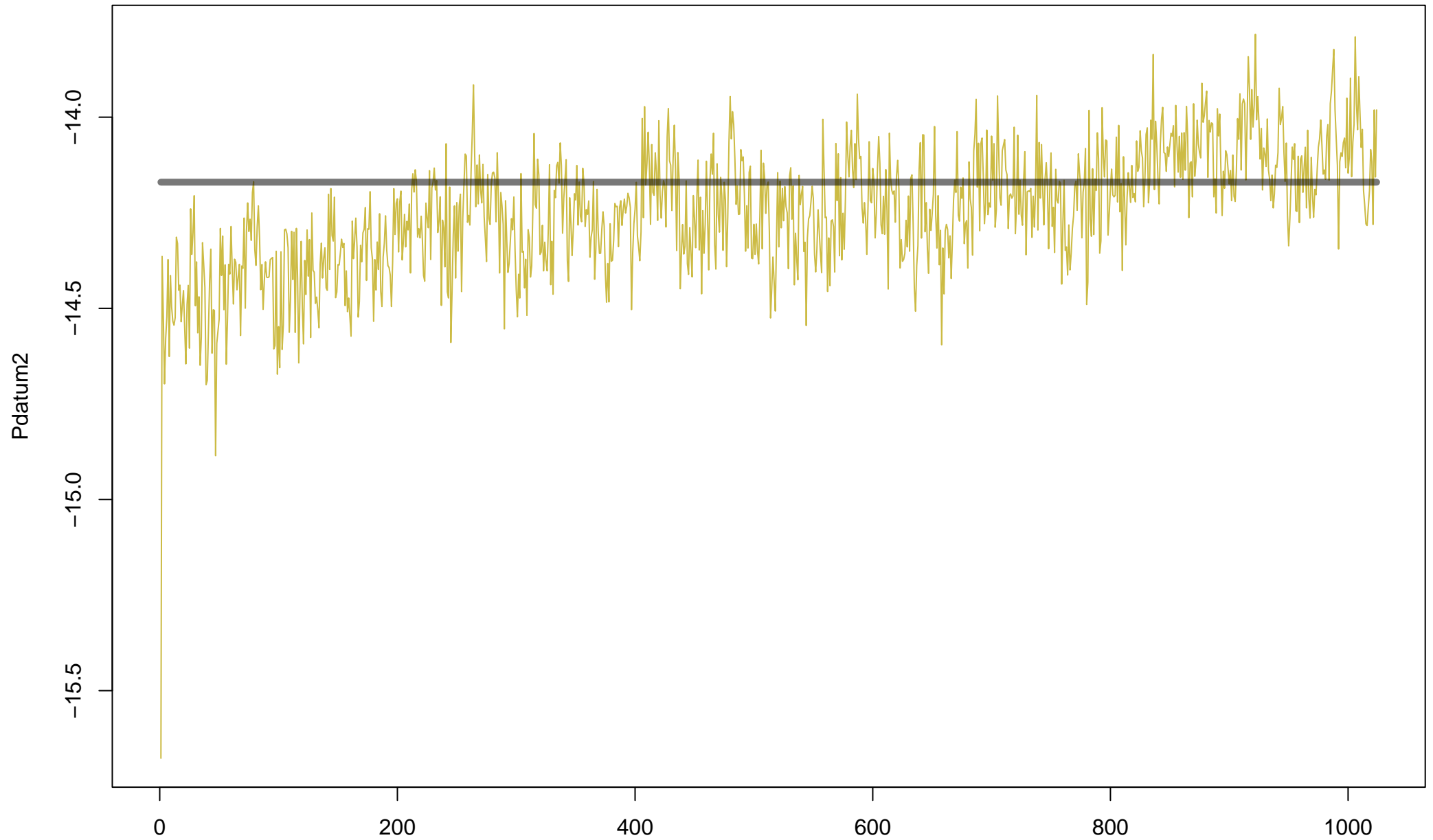


Pdatum1
ESS = 18.7 | BMK = 0.331 | MCSE(6.27) = 10.6 | stat: FALSE | burn: 0 | percentile: 73.6



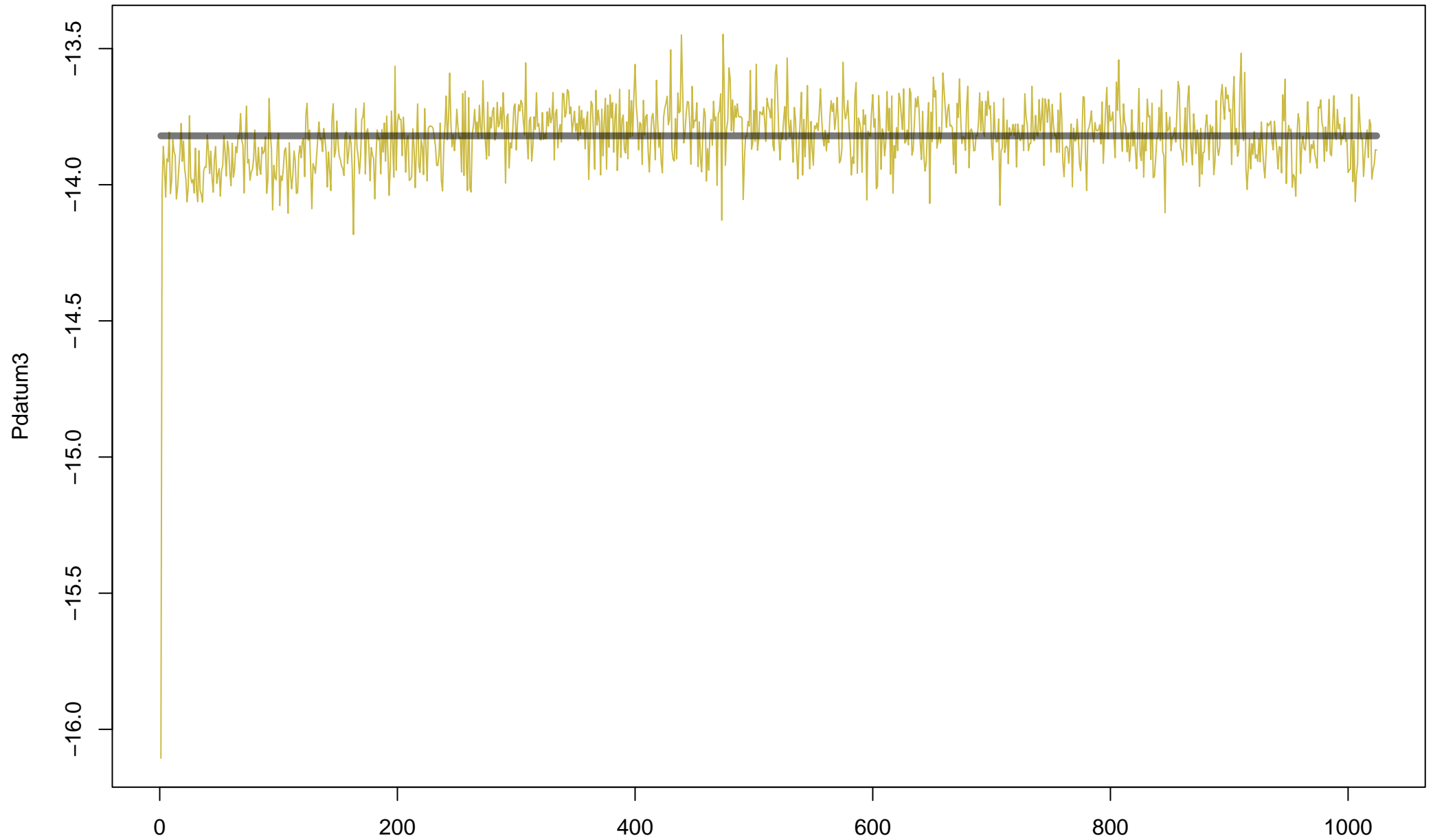
Pdatum2

ESS = 24.7 | BMK = 0.349 | MCSE(6.27) = 12.7 | stat: FALSE | burn: 0 | percentile: 66.9



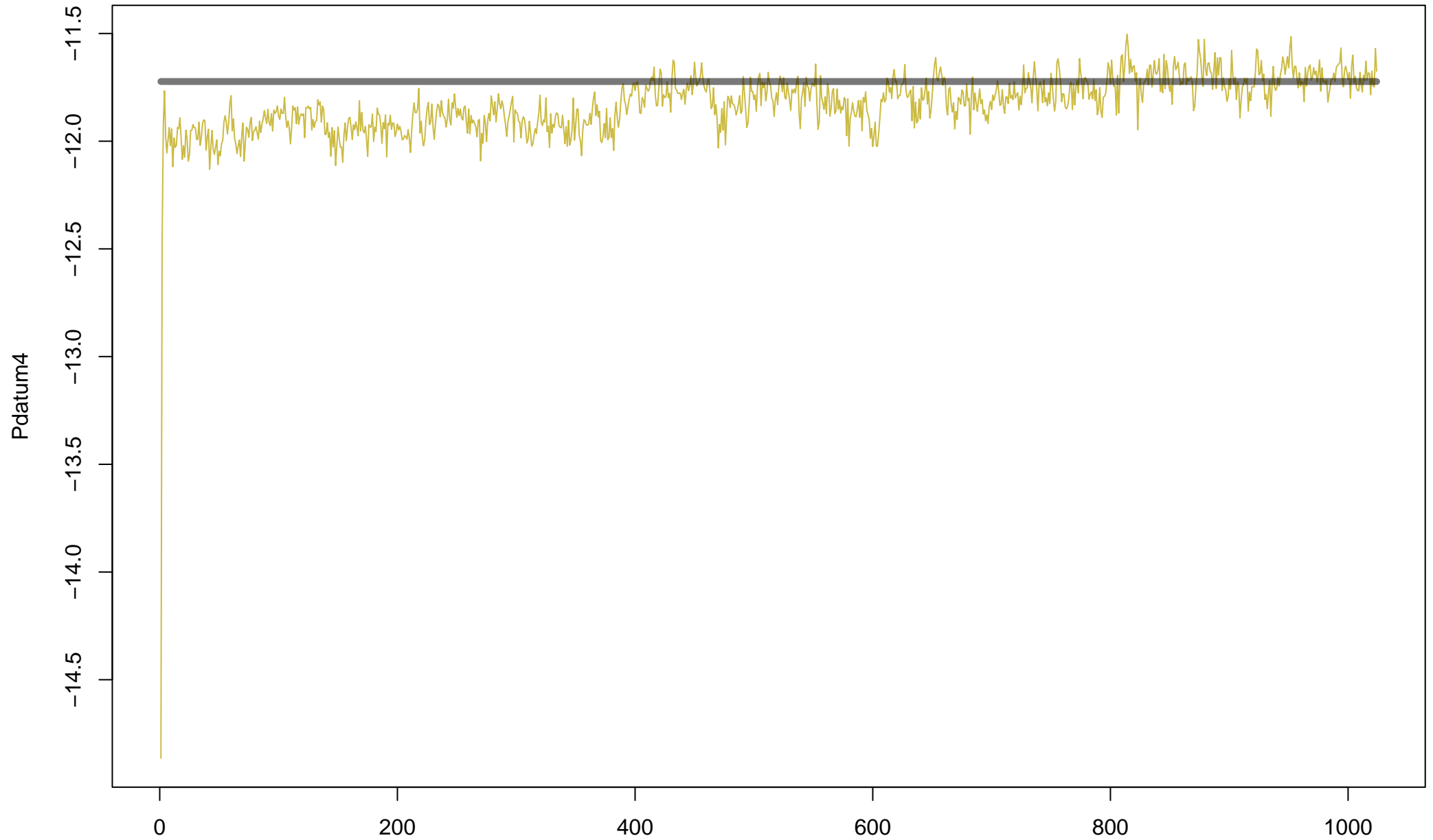
Pdatum3

ESS = 39.2 | BMK = 0.128 | MCSE(6.27) = 7.95 | stat: FALSE | burn: 0 | percentile: 49.7



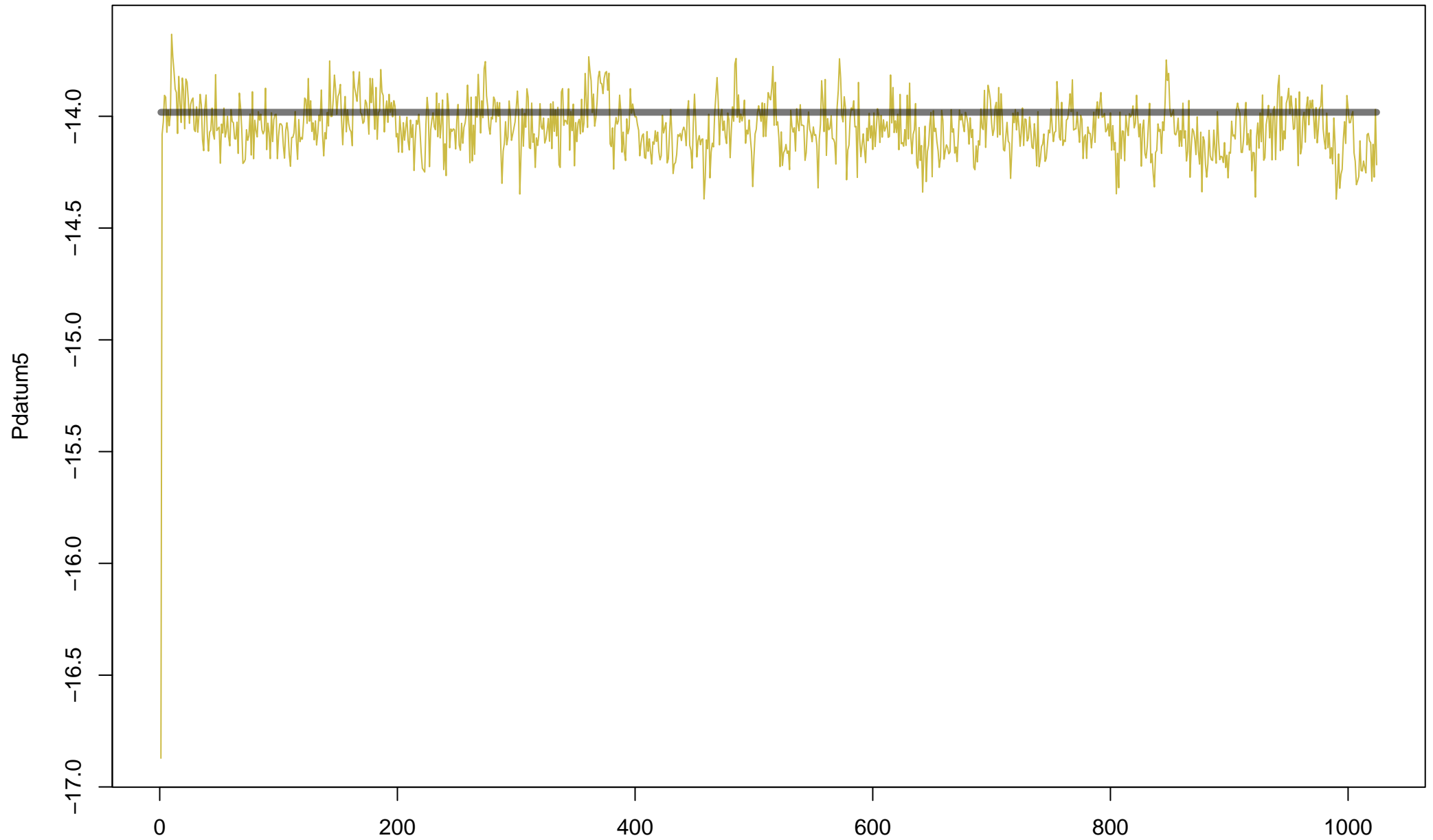
Pdatum4

ESS = 6.77 | BMK = 0.488 | MCSE(6.27) = 14.2 | stat: FALSE | burn: 0 | percentile: 79.6



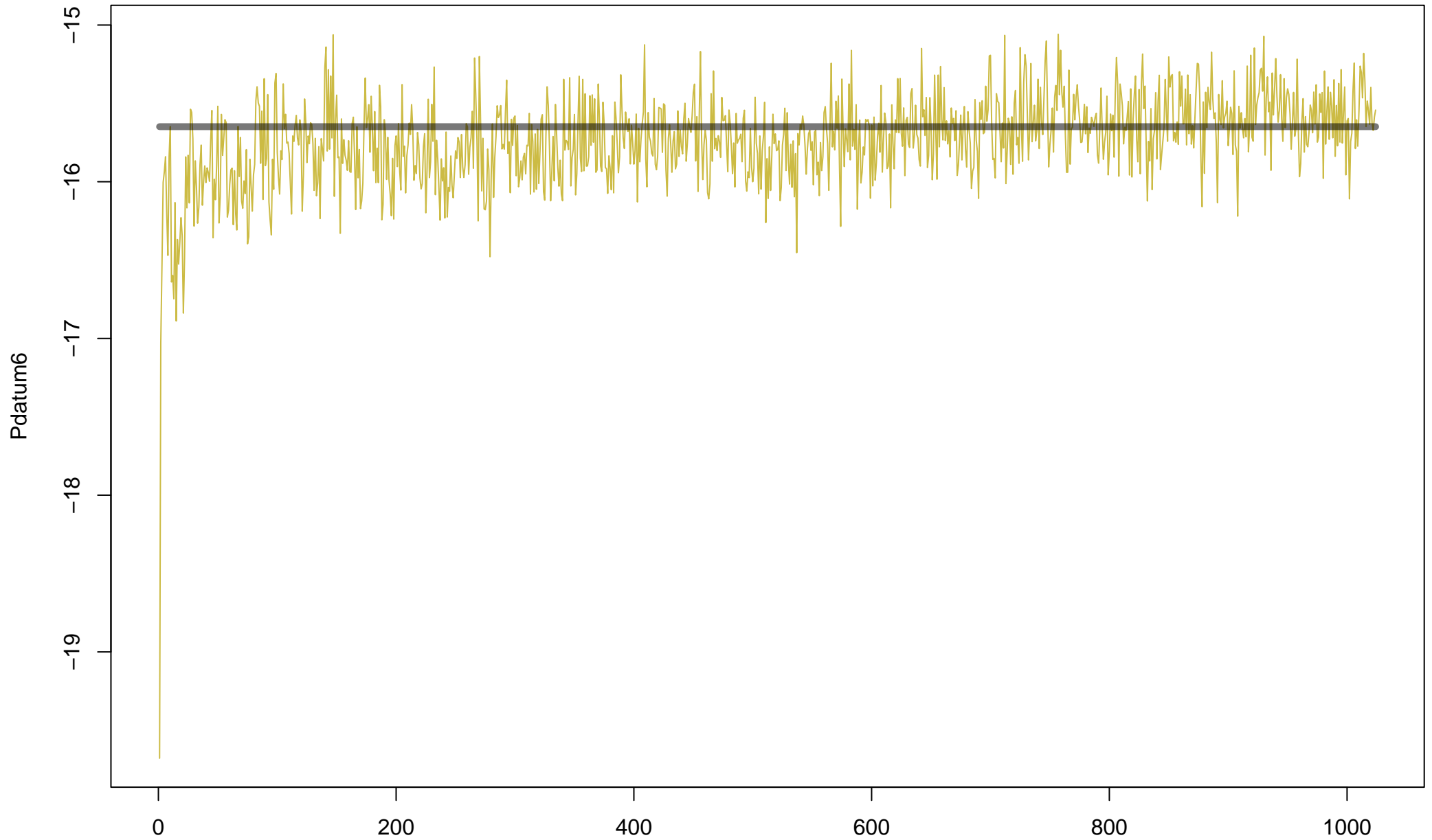
Pdatum5

ESS = 197 | BMK = 0.14 | MCSE(6.27) = 7.31 | stat: FALSE | burn: 0 | percentile: 75.3



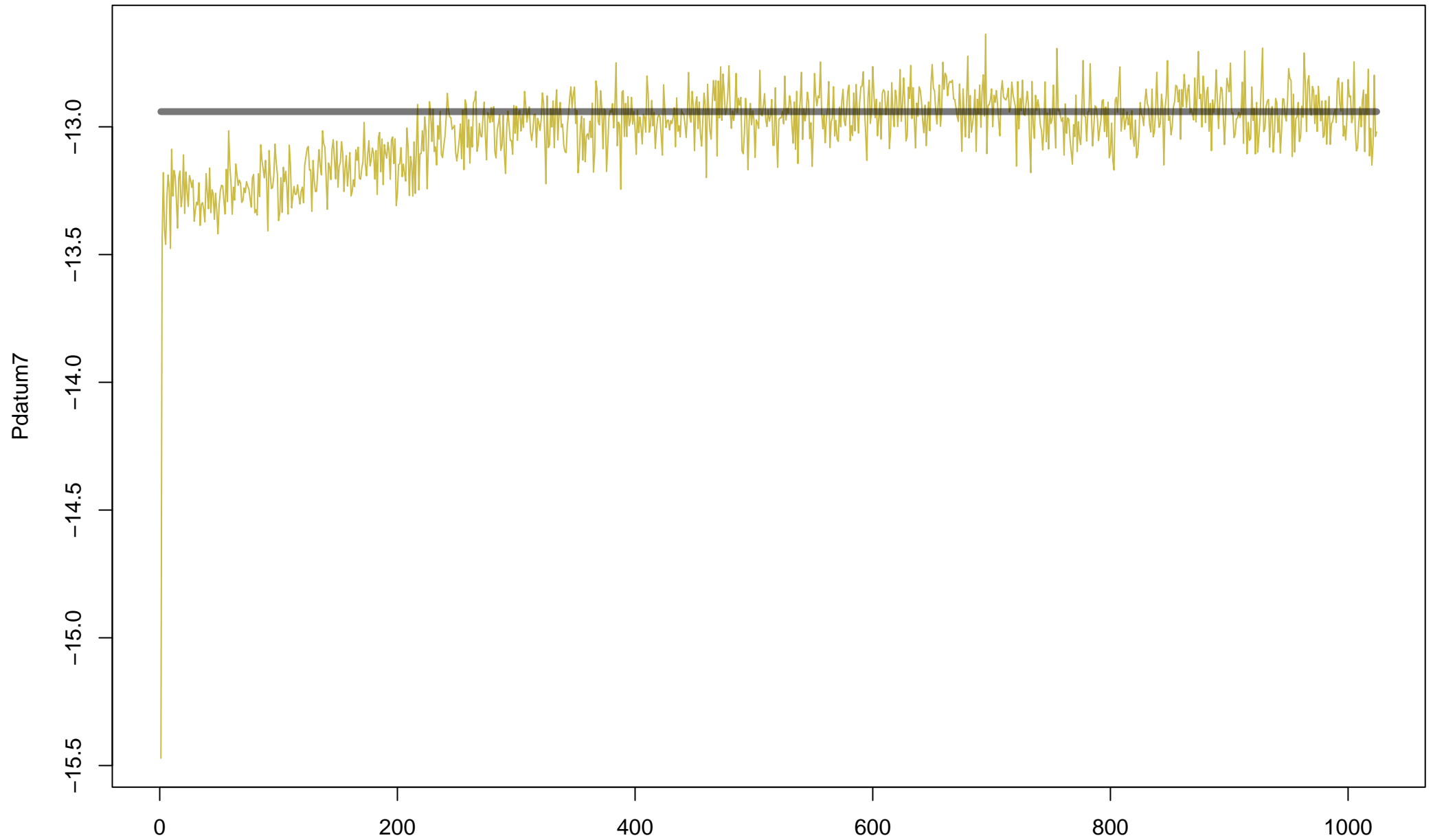
Pdatum6

ESS = 57.1 | BMK = 0.26 | MCSE(6.27) = 8.77 | stat: FALSE | burn: 0 | percentile: 62



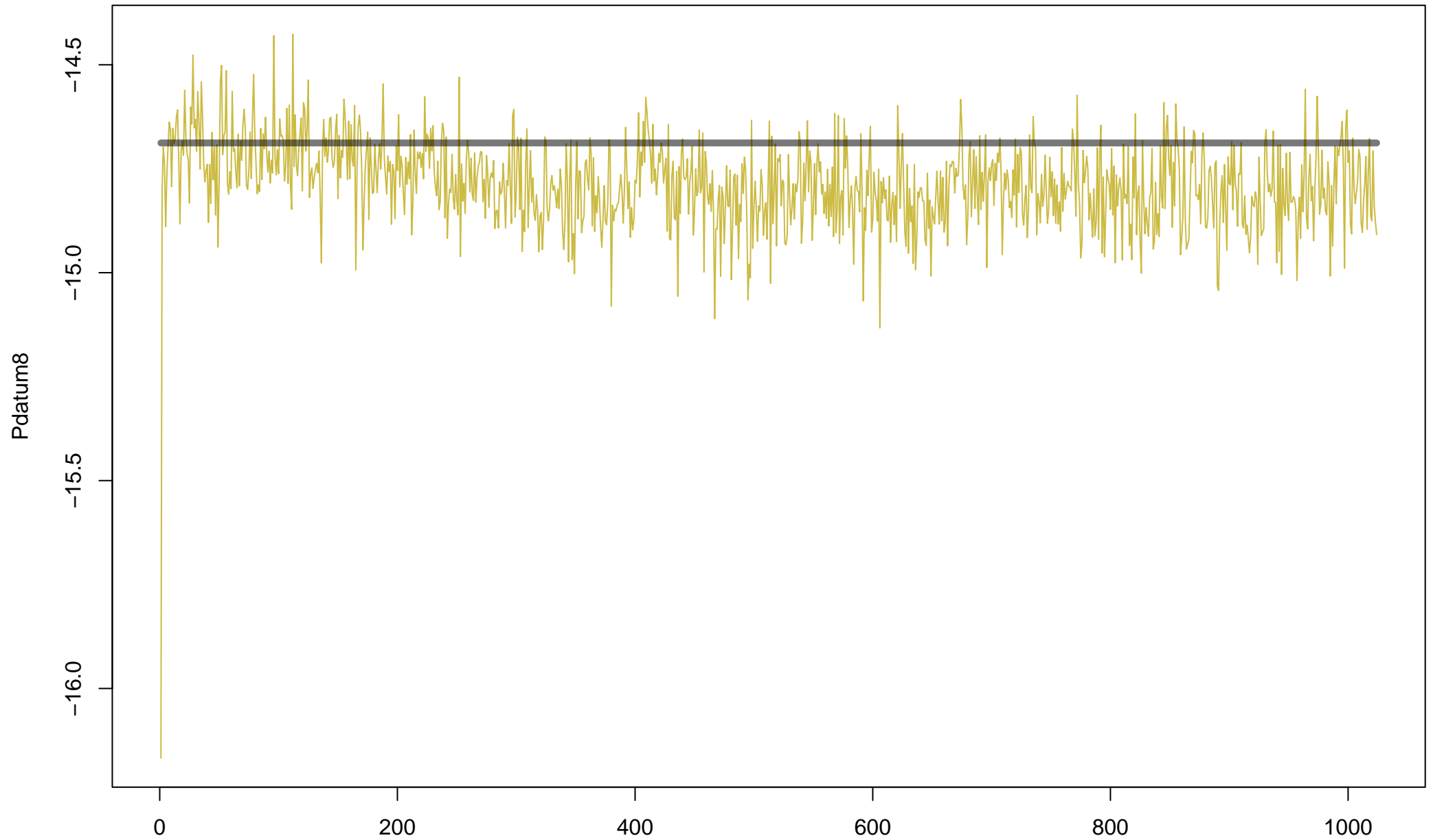
Pdatum7

ESS = 8.94 | BMK = 0.42 | MCSE(6.27) = 13.4 | stat: FALSE | burn: 0 | percentile: 65.9



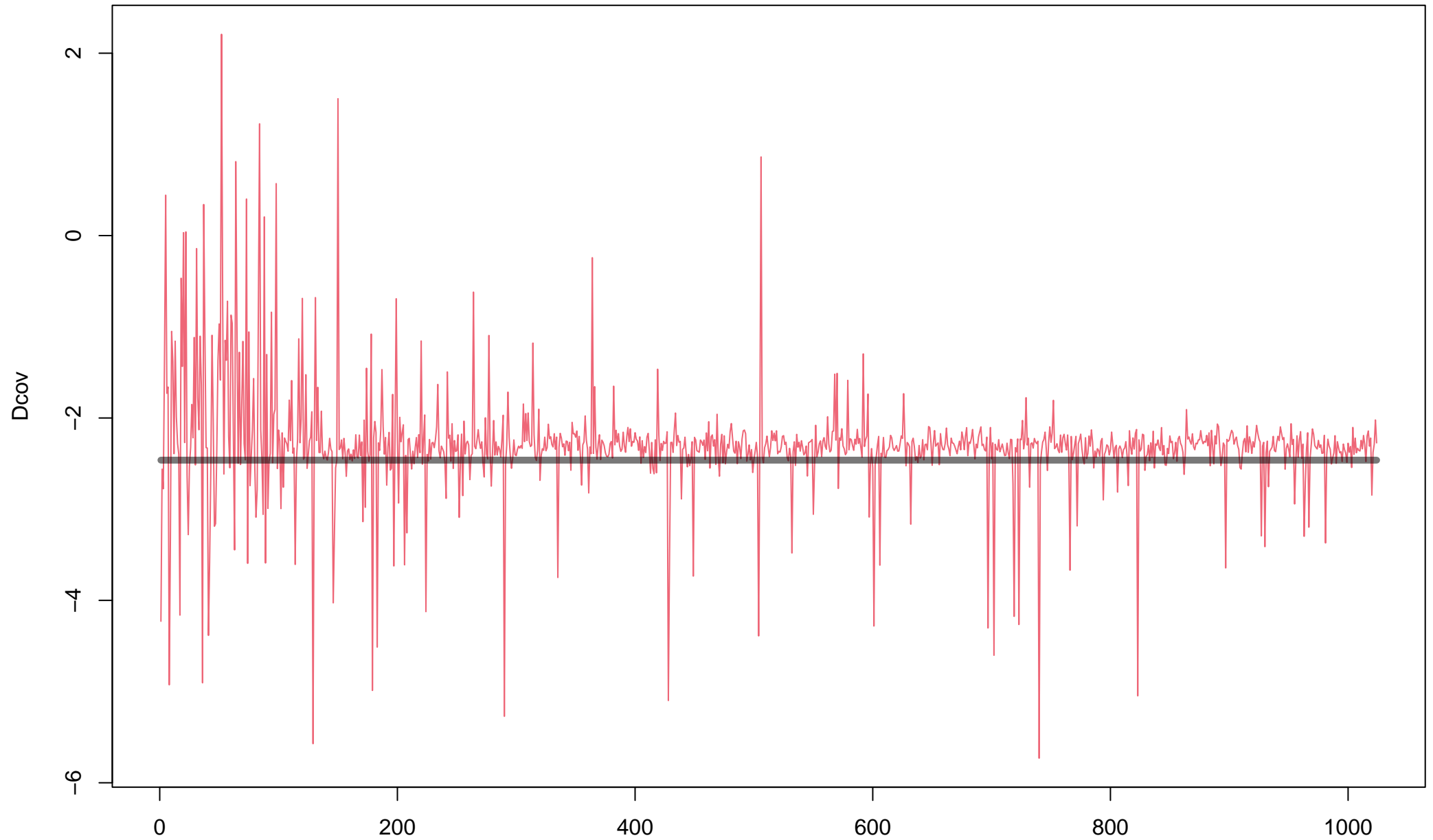
Pdatum8

ESS = 134 | BMK = 0.168 | MCSE(6.27) = 7.39 | stat: FALSE | burn: 0 | percentile: 84.2



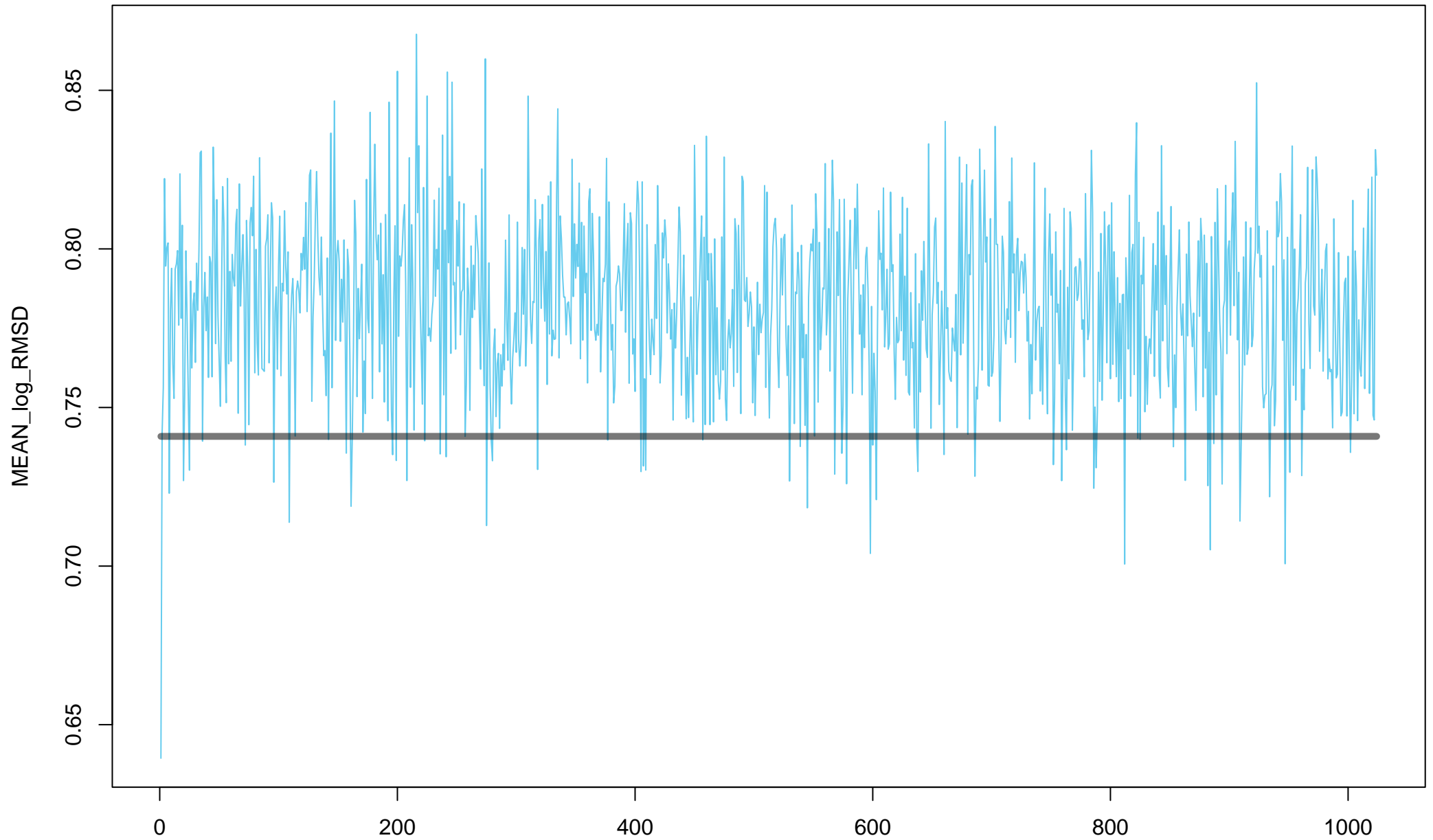
Dcov

ESS = 1020 | BMK = 0.508 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 102 | percentile: 81



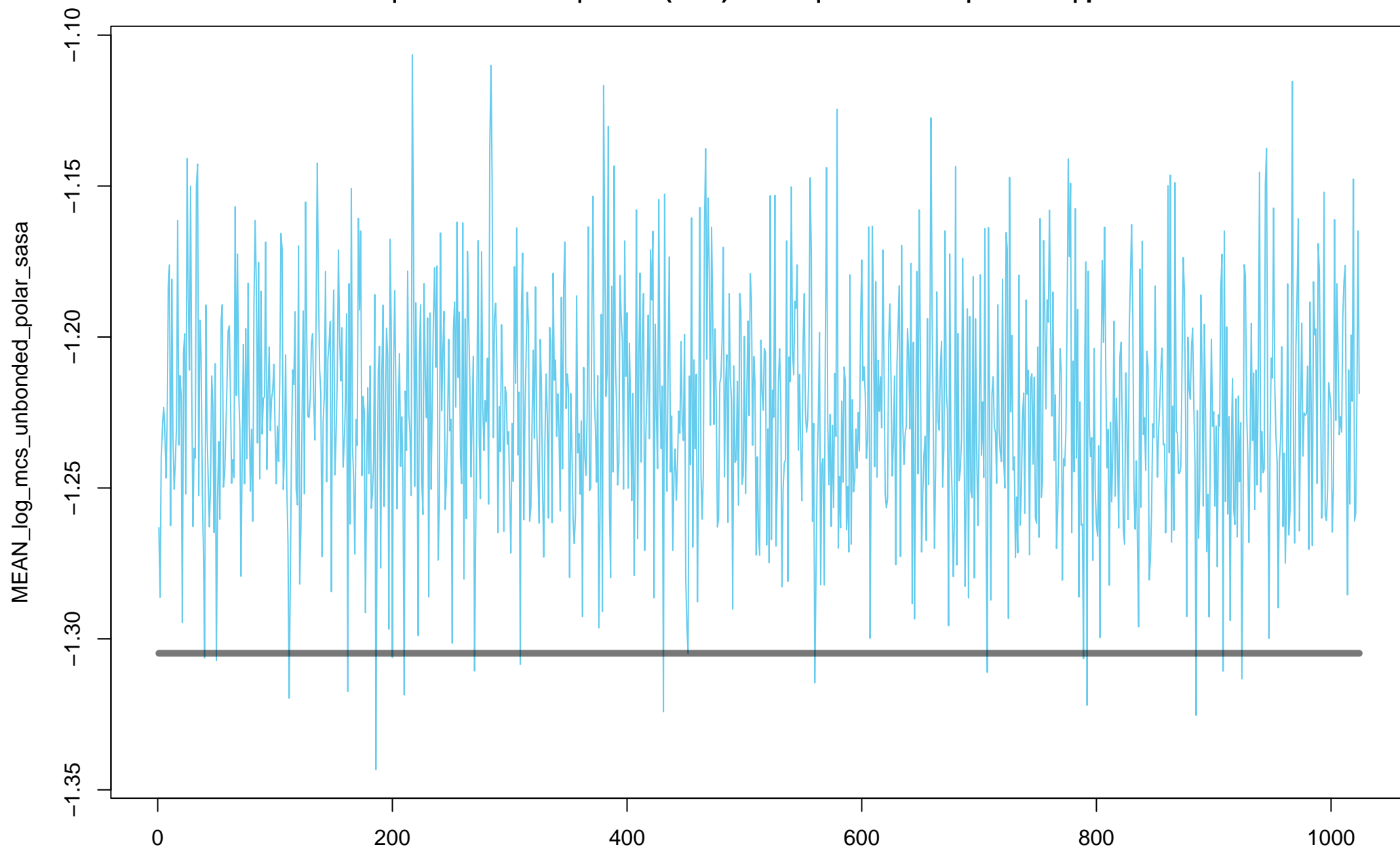
MEAN_log_RMSD

ESS = 1020 | BMK = 0.0808 | MCSE(6.27) = 3.54 | stat: TRUE | burn: 0 | percentile: 6.05



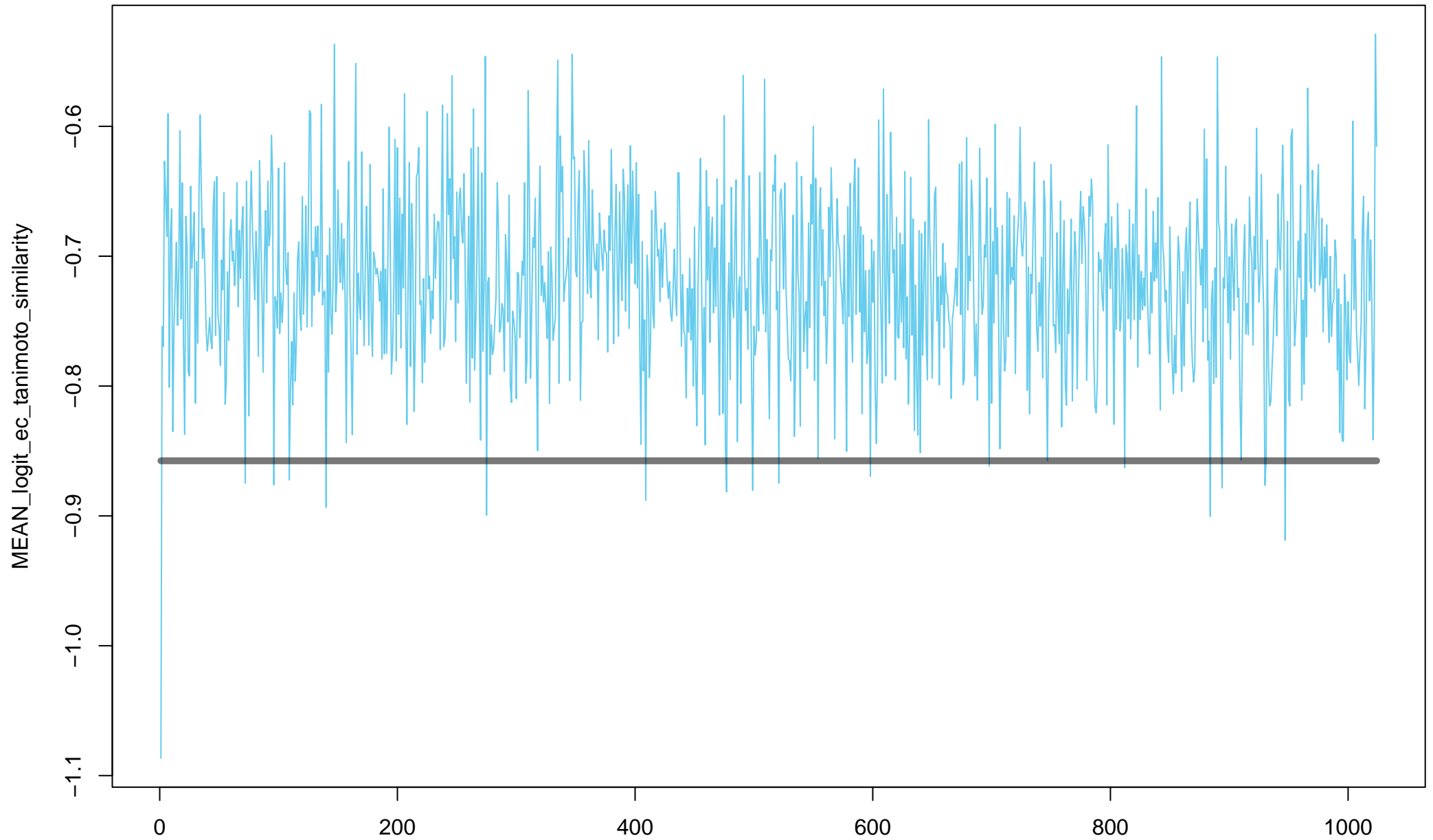
MEAN_log_mcs_unbonded_polar_sasa

ESS = 1020 | BMK = 0.0602 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0 | percentile: 1.66



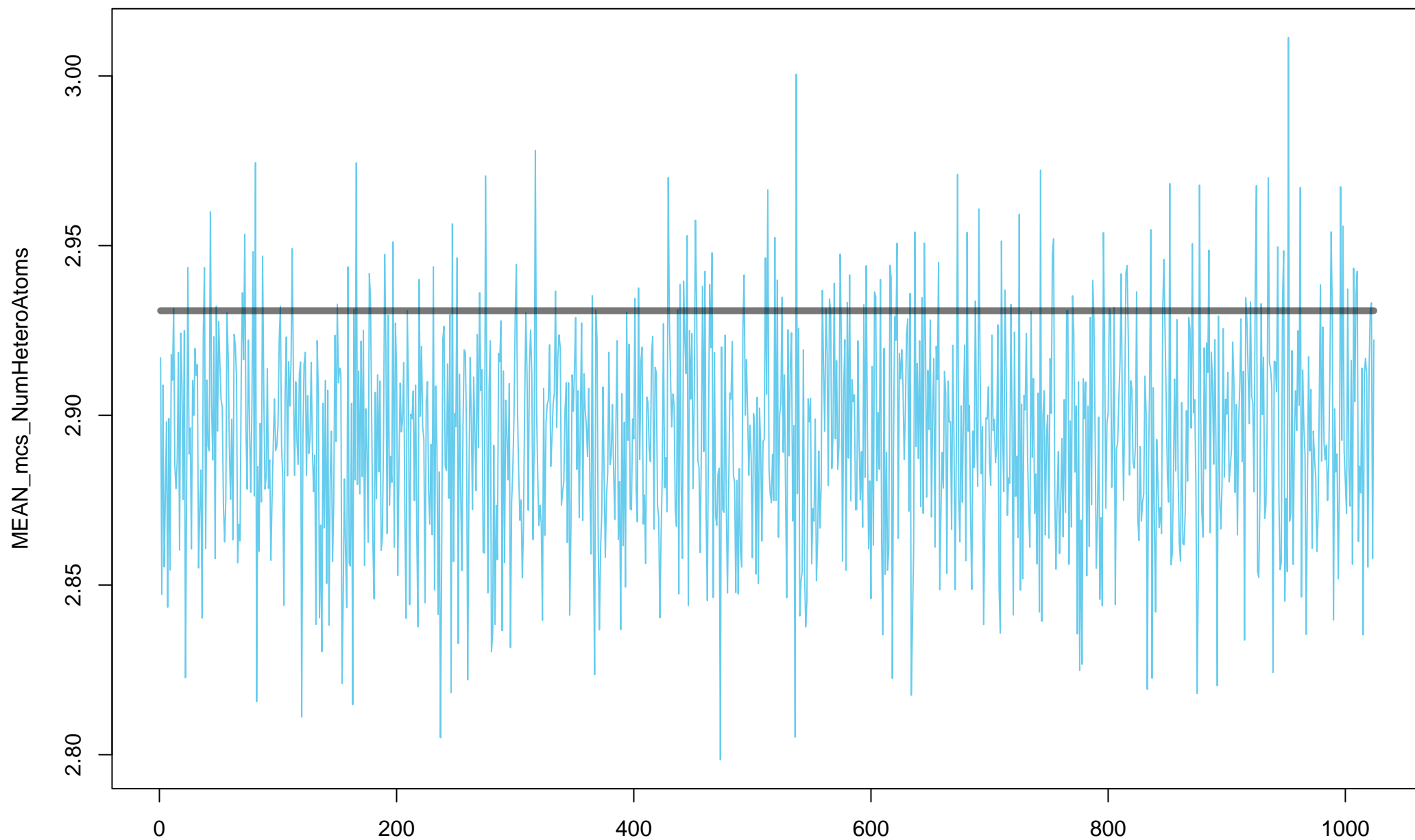
MEAN_logit_ec_tanimoto_similarity

ESS = 1020 | BMK = 0.0749 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | percentile: 1.66



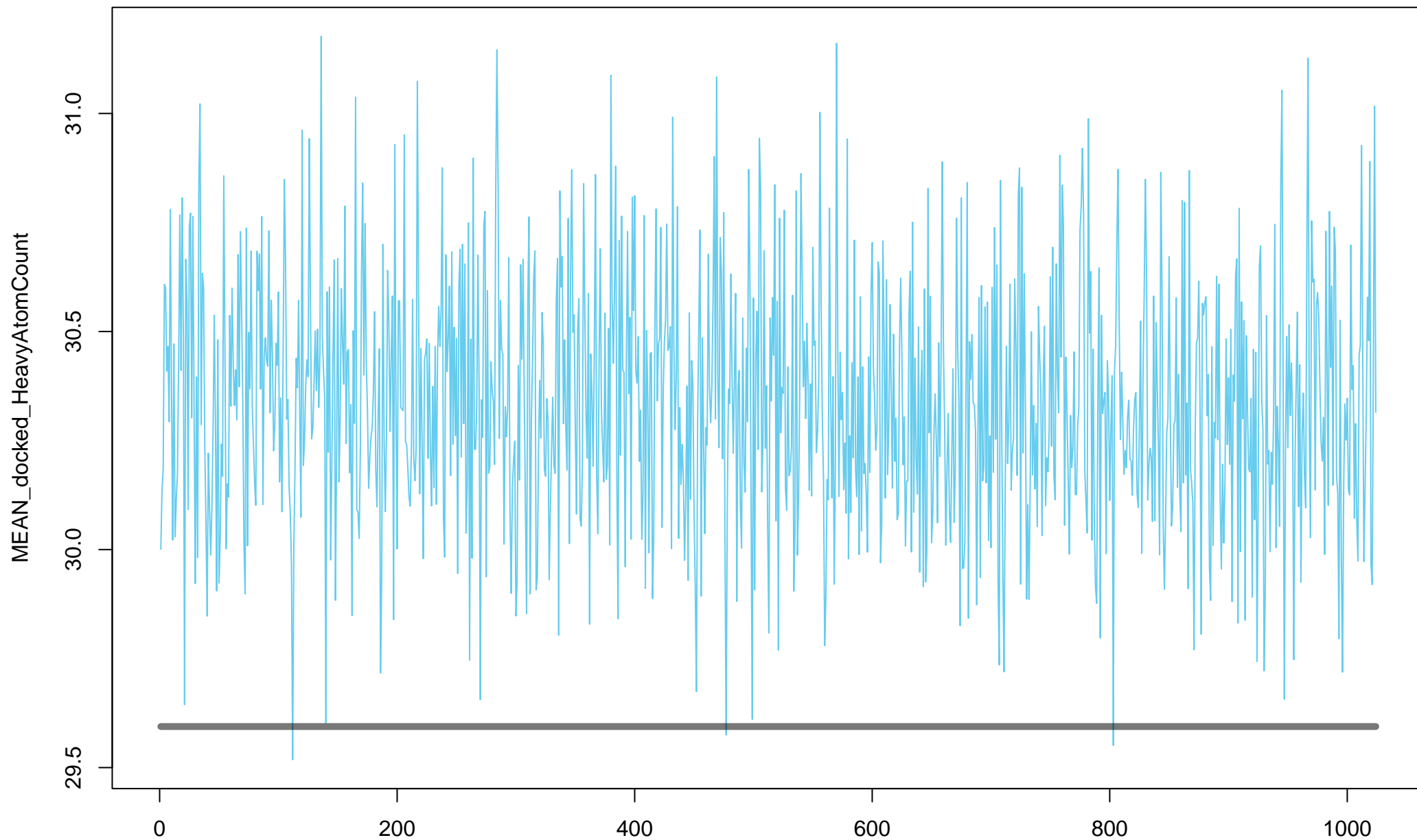
MEAN_mcs_NumHeteroAtoms

ESS = 1020 | BMK = 0.0658 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0 | percentile: 88.3



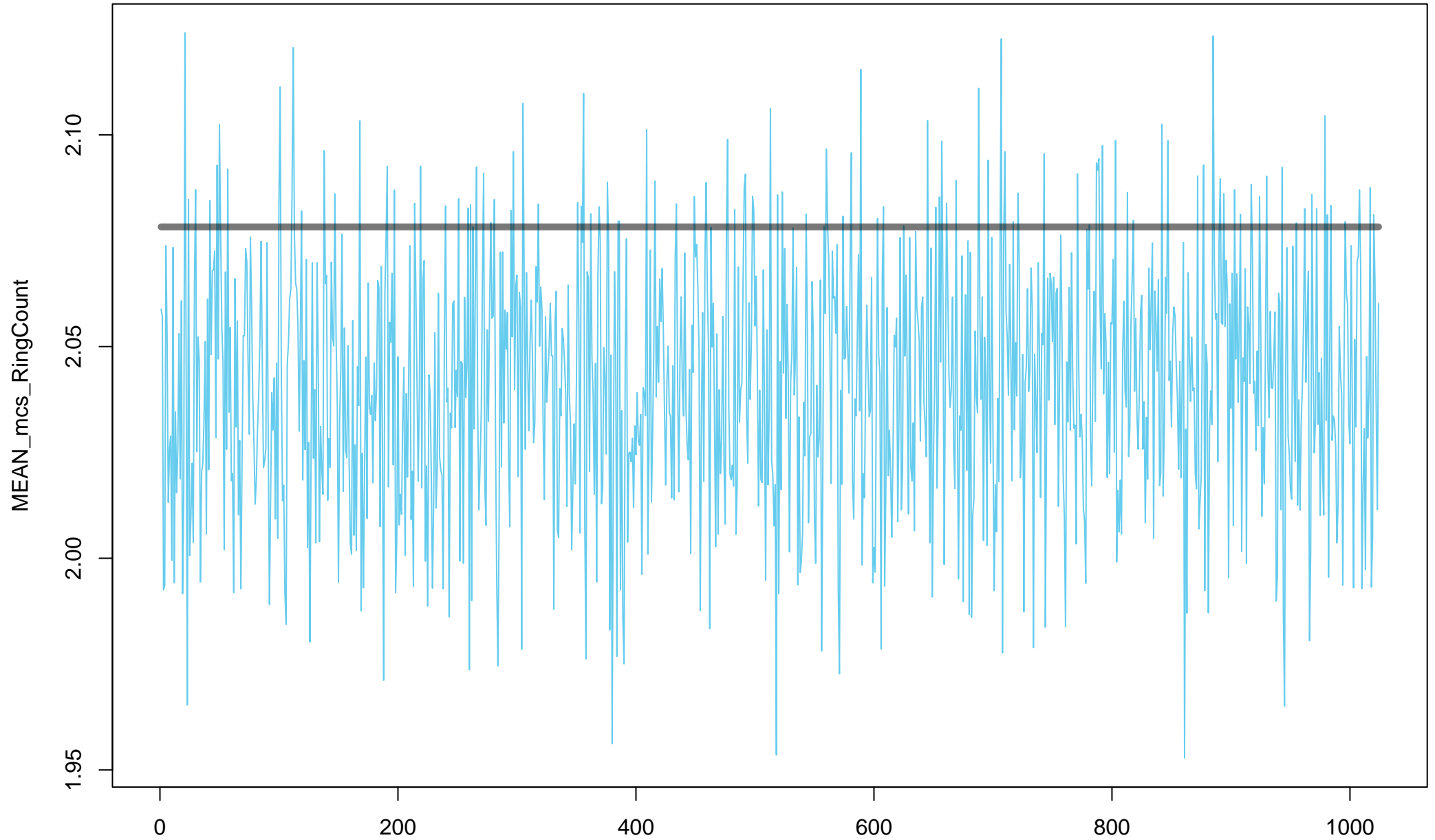
MEAN_docked_HeavyAtomCount

ESS = 1020 | BMK = 0.0693 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | percentile: 0.293



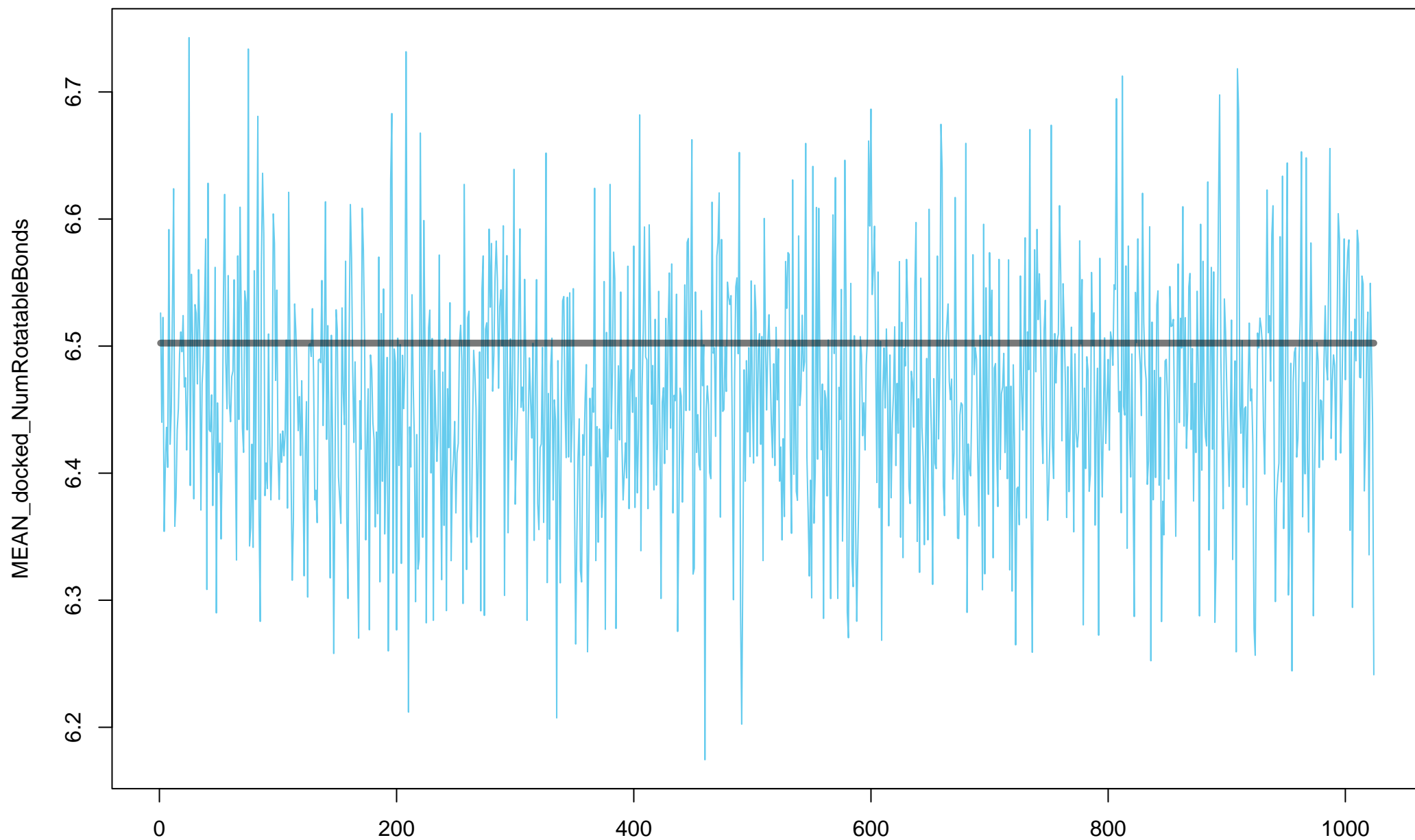
MEAN_mcs_RingCount

ESS = 1020 | BMK = 0.0395 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0 | percentile: 89.4



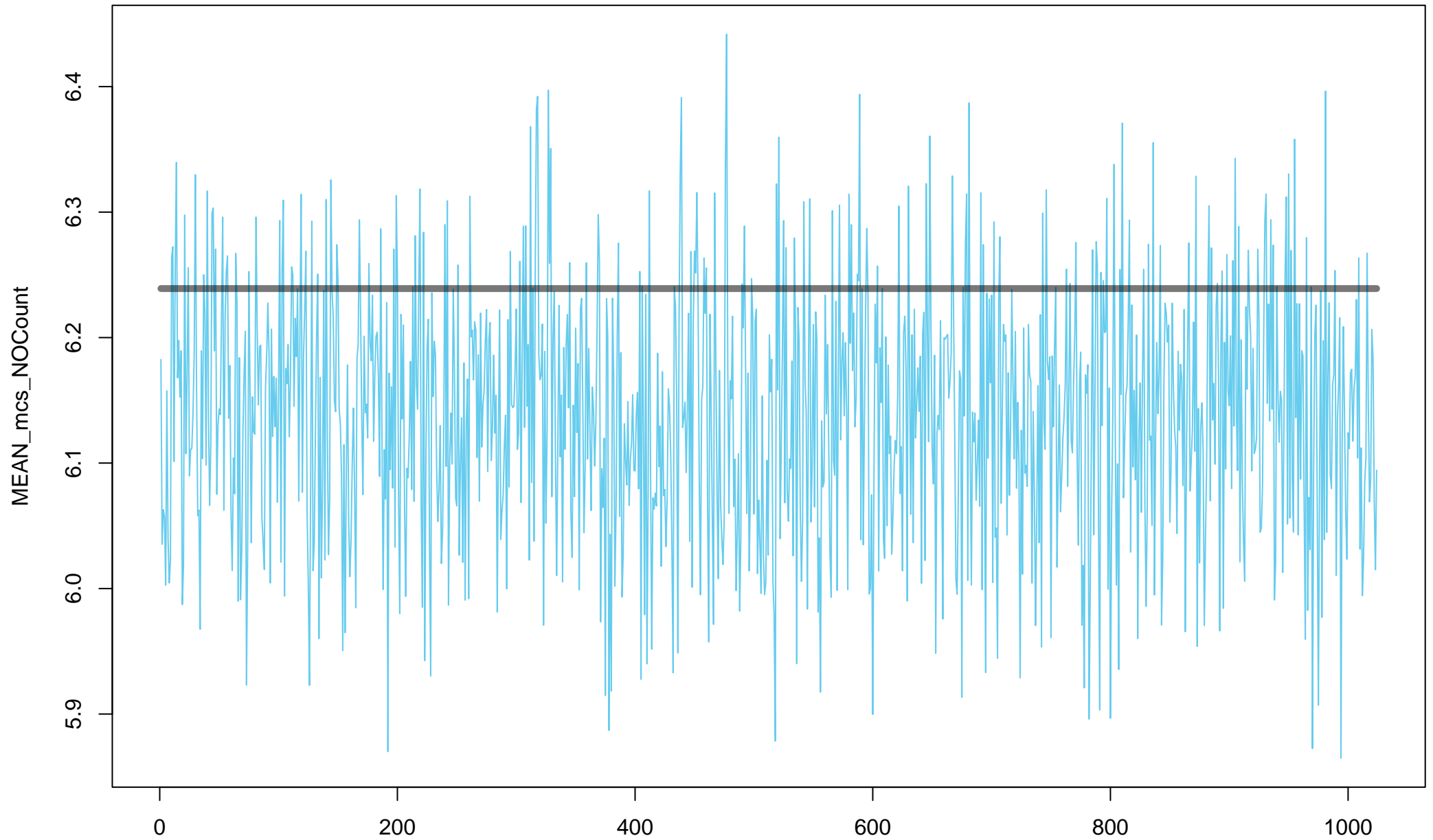
MEAN_docked_NumRotatableBonds

ESS = 1020 | BMK = 0.0589 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 0 | percentile: 68.8

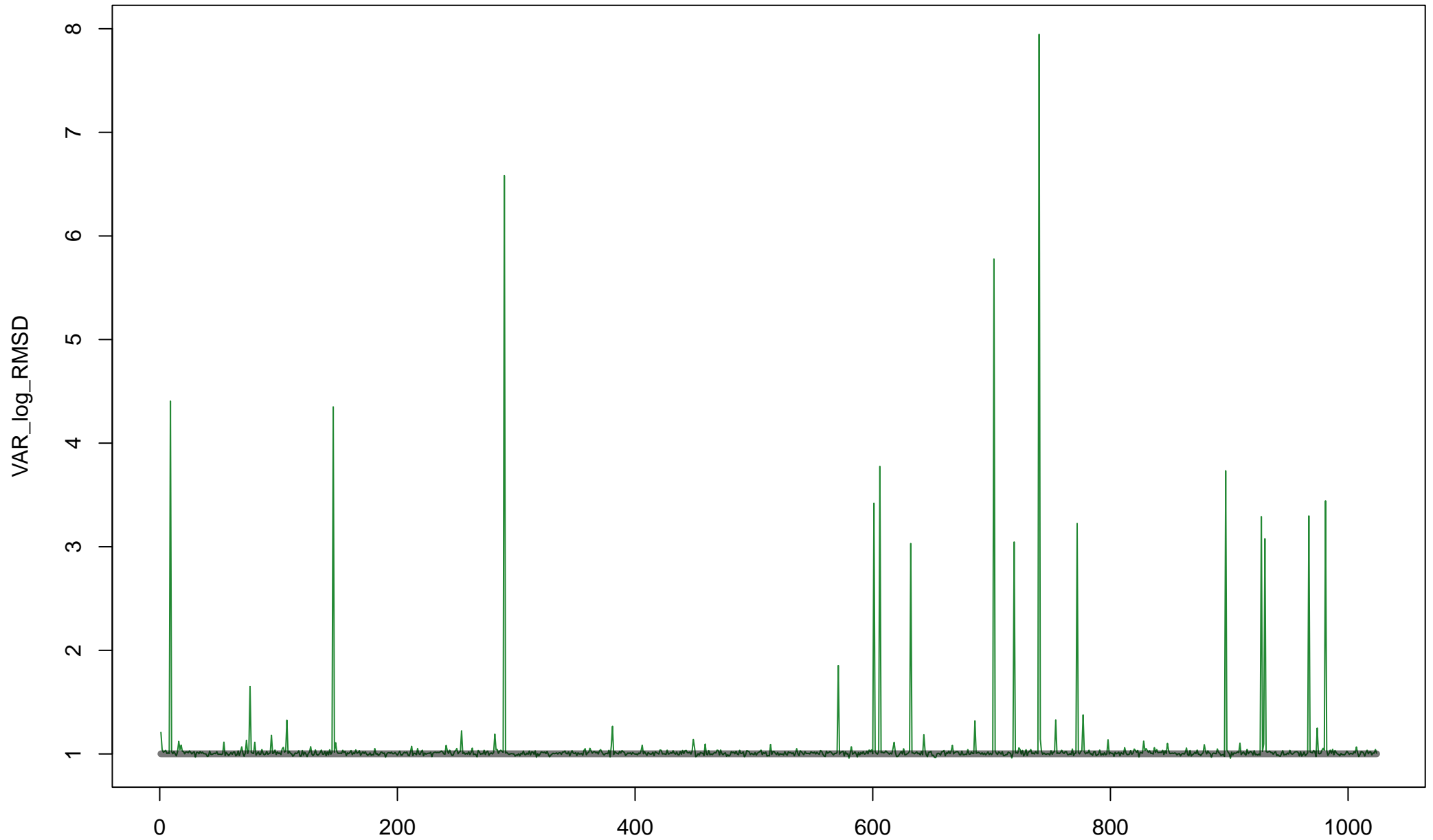


MEAN_mcs_NOCount

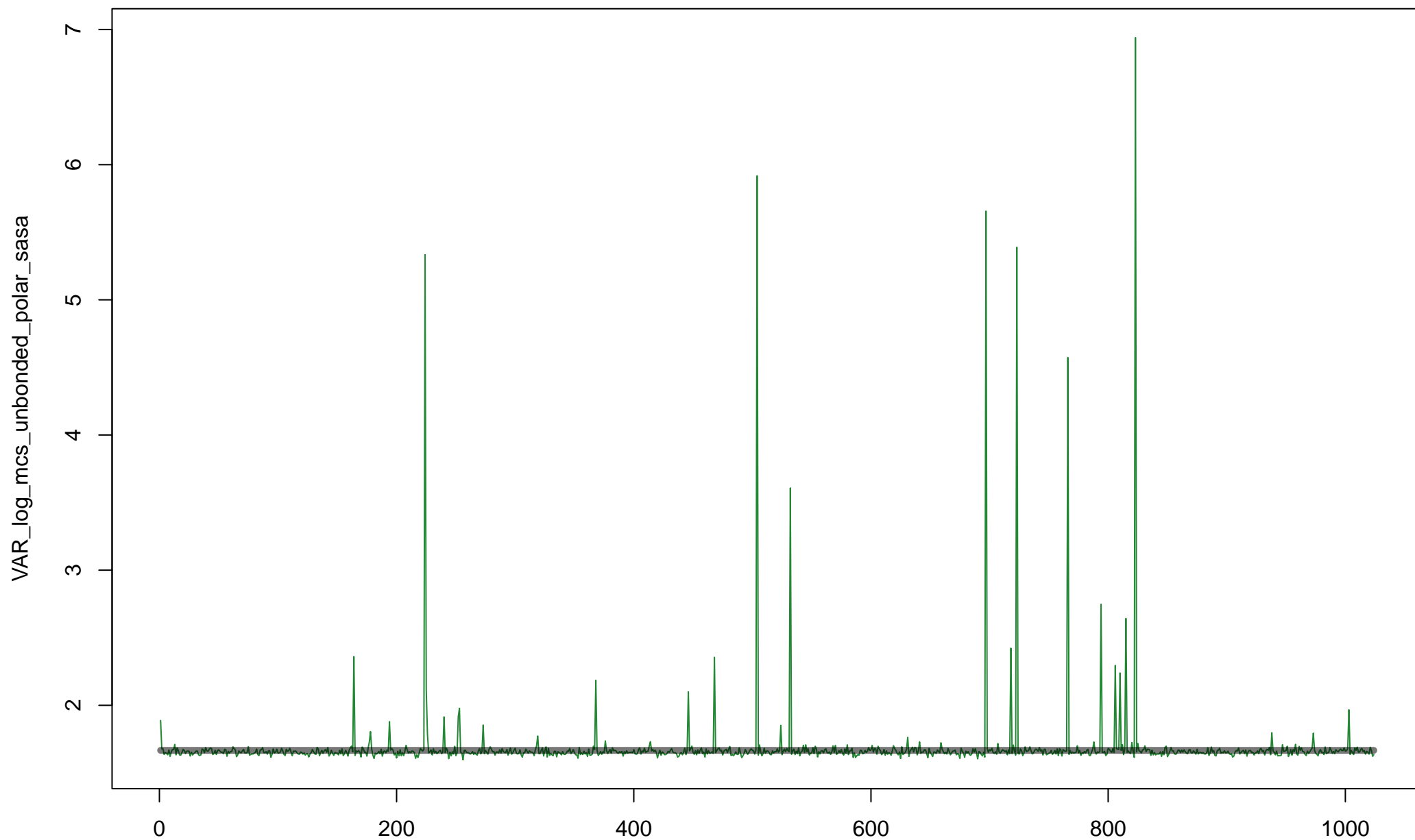
ESS = 1020 | BMK = 0.0345 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0 | percentile: 84.6



VAR_log_RMSD
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 816 | percentile: 34

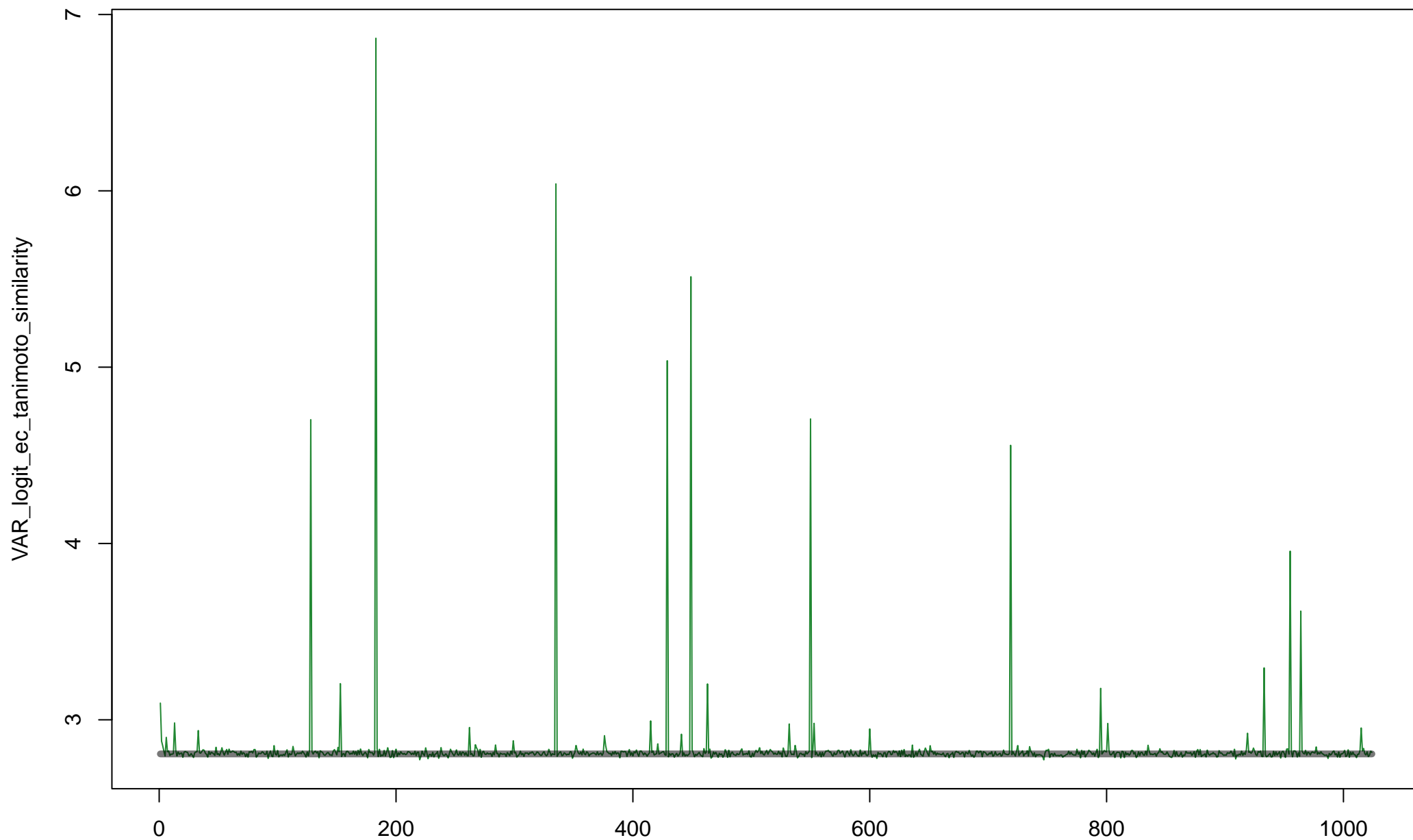


VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.515 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 1020 | percentile: 70.9

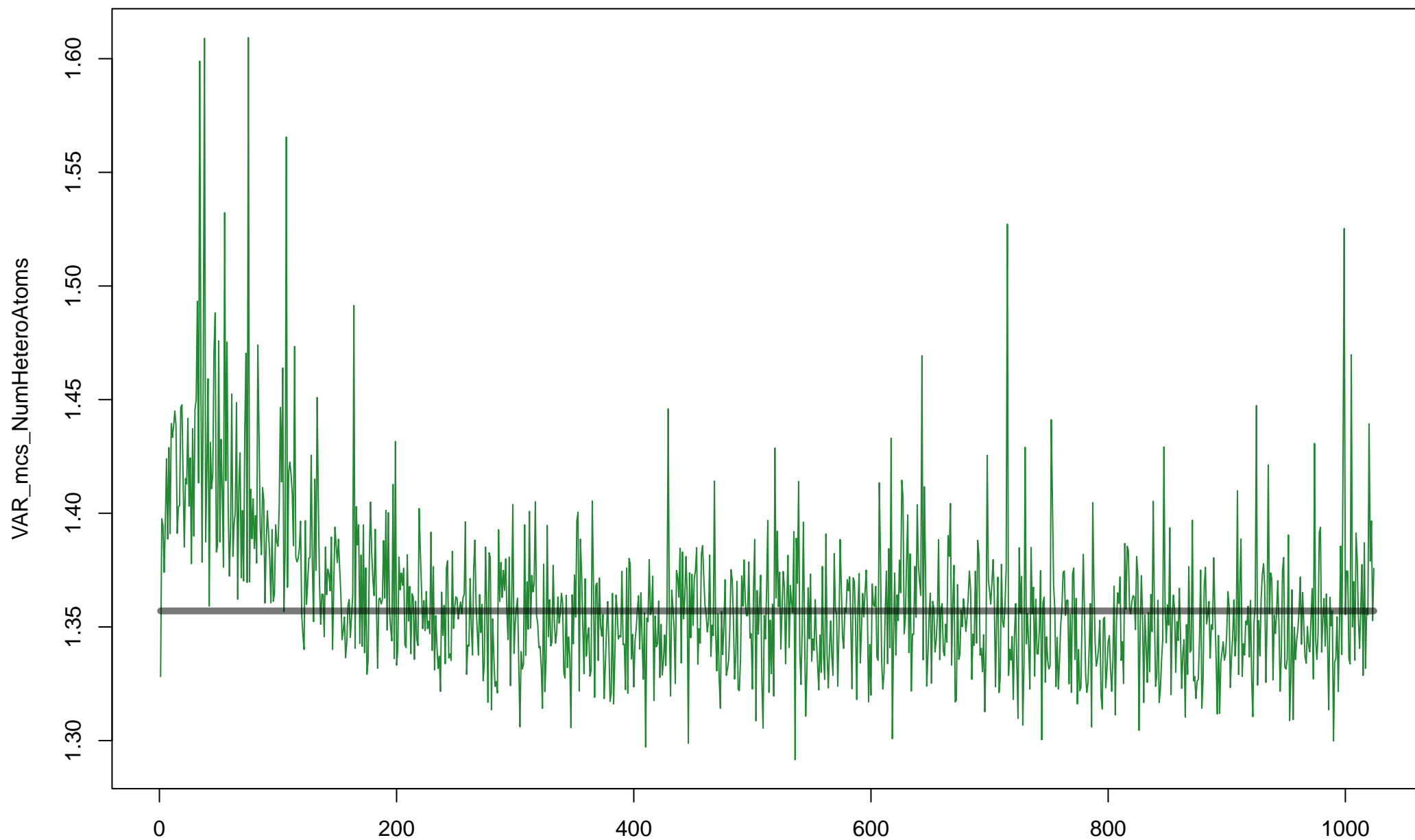


VAR_logit_ec_tanimoto_similarity

ESS = 1020 | BMK = 0.344 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 204 | percentile: 45.4

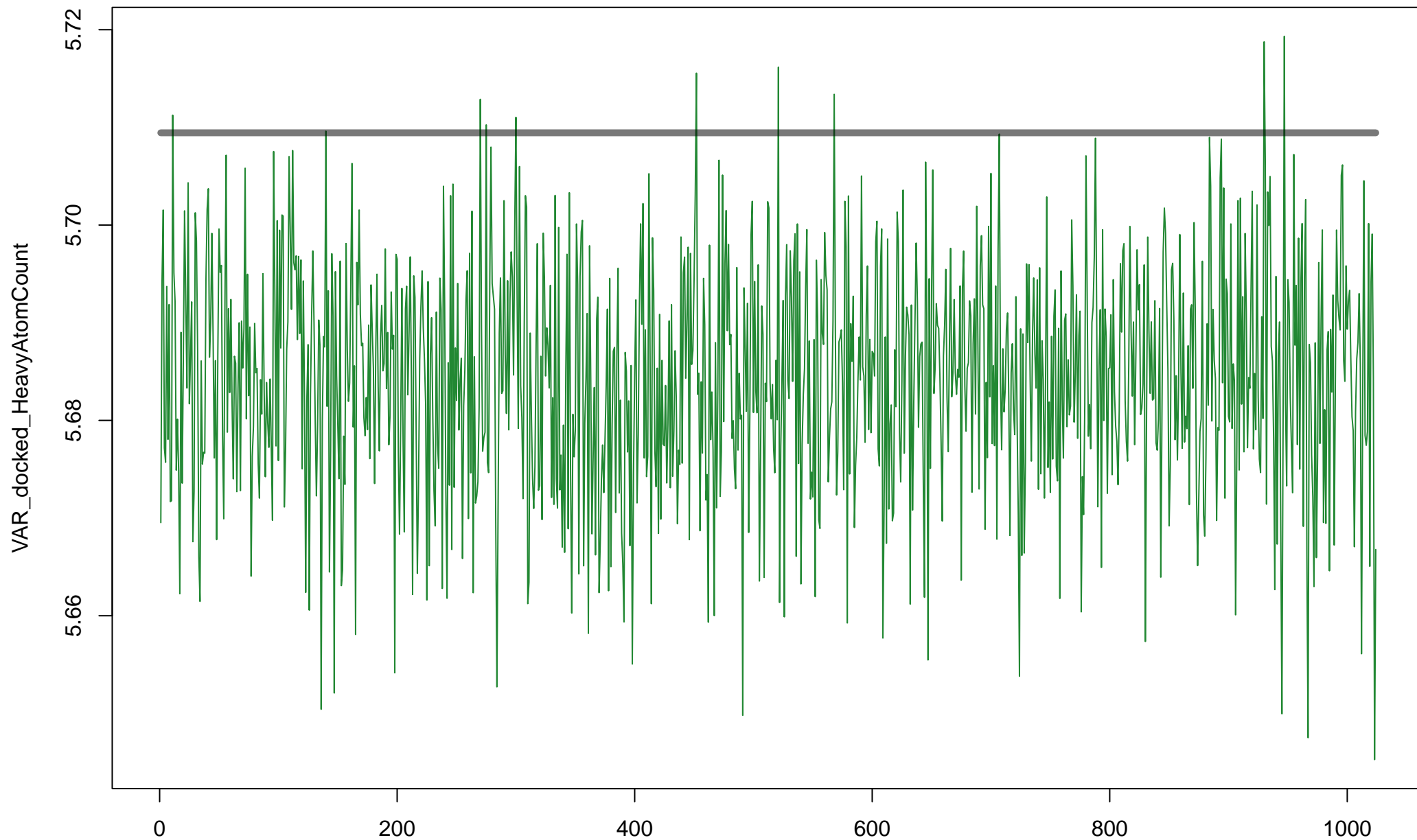


VAR_mcs_NumHeteroAtoms
ESS = 13.4 | BMK = 0.194 | MCSE(6.27) = 10.4 | stat: FALSE | burn: 0 | percentile: 50.3

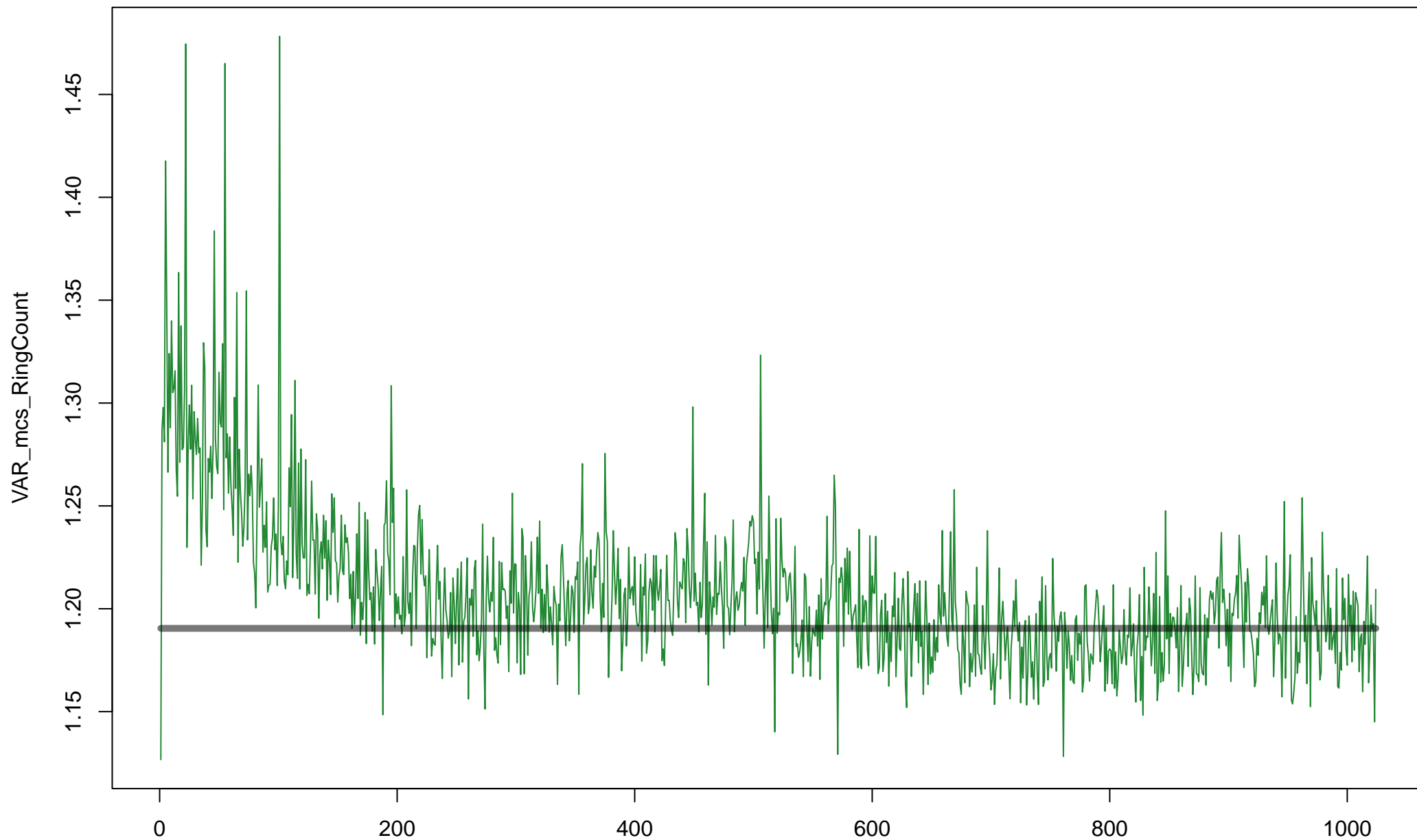


VAR_docked_HeavyAtomCount

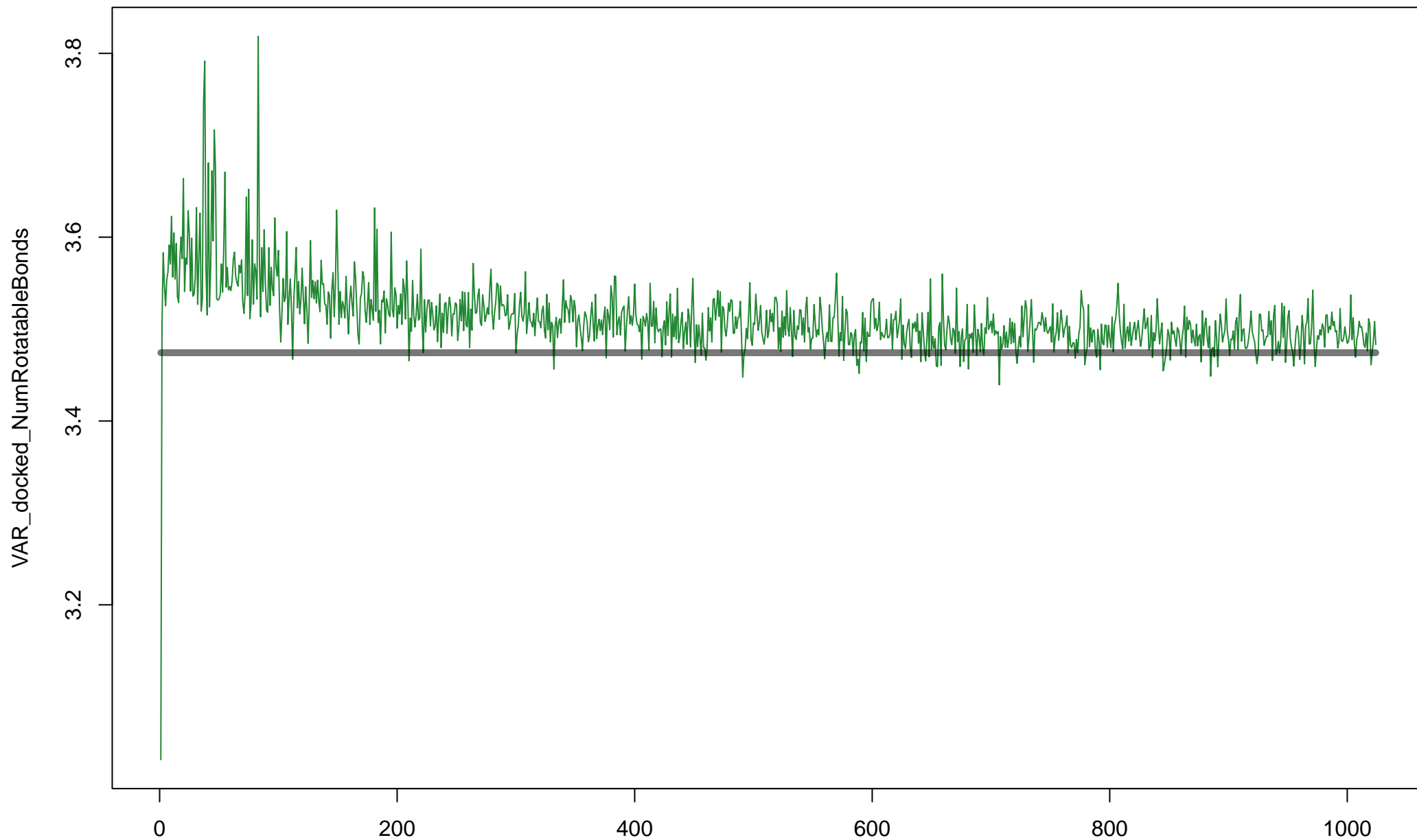
ESS = 1020 | BMK = 0.0532 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0 | percentile: 99



VAR_mcs_RingCount
ESS = 16.9 | BMK = 0.408 | MCSE(6.27) = 13 | stat: FALSE | burn: 0 | percentile: 32.6

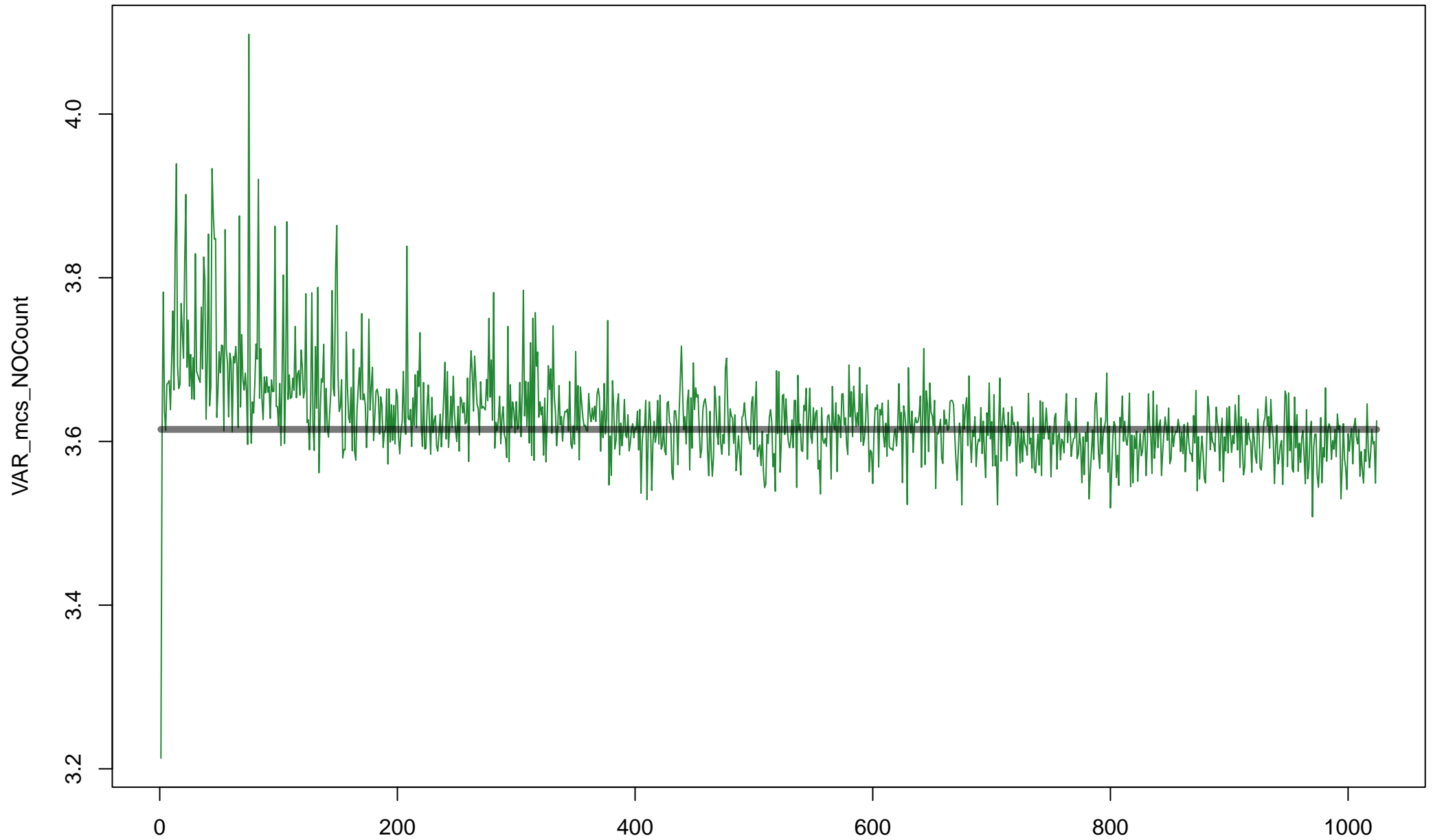


VAR_docked_NumRotatableBonds
ESS = 19.1 | BMK = 0.414 | MCSE(6.27) = 11 | stat: FALSE | burn: 0 | percentile: 7.13

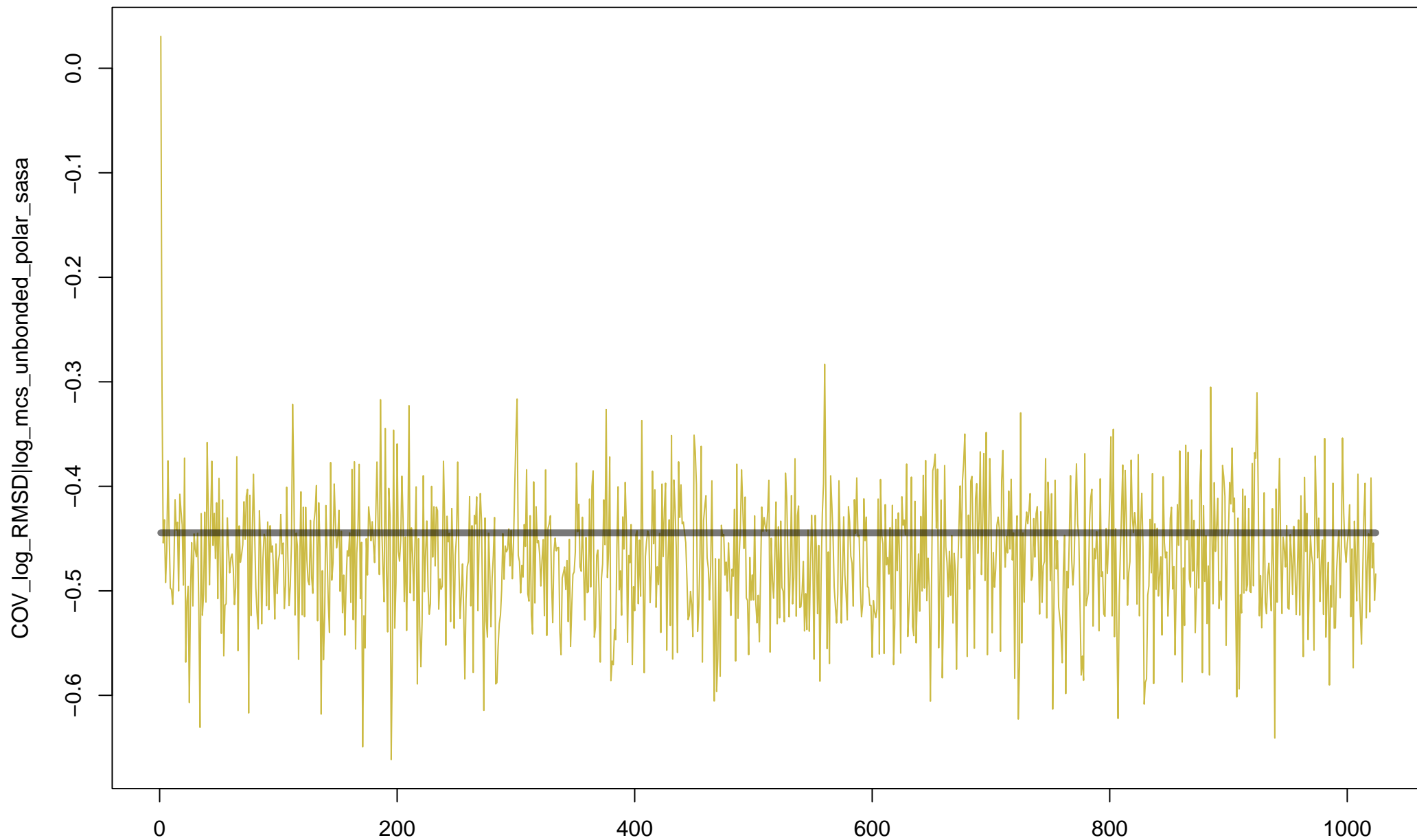


VAR_mcs_NOCount

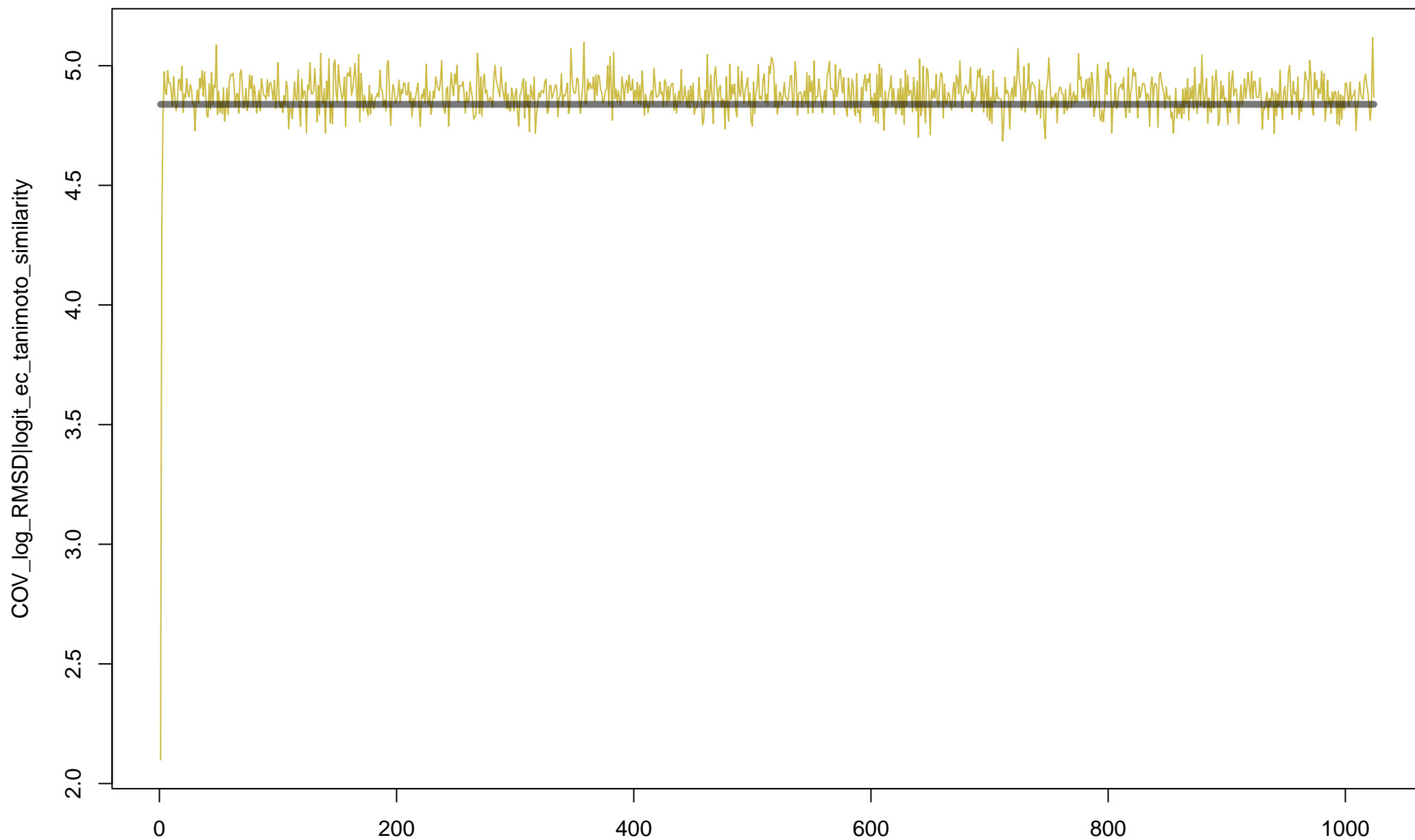
ESS = 14.4 | BMK = 0.349 | MCSE(6.27) = 10.1 | stat: FALSE | burn: 0 | percentile: 44.3



COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0696 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0 | percentile: 66.1

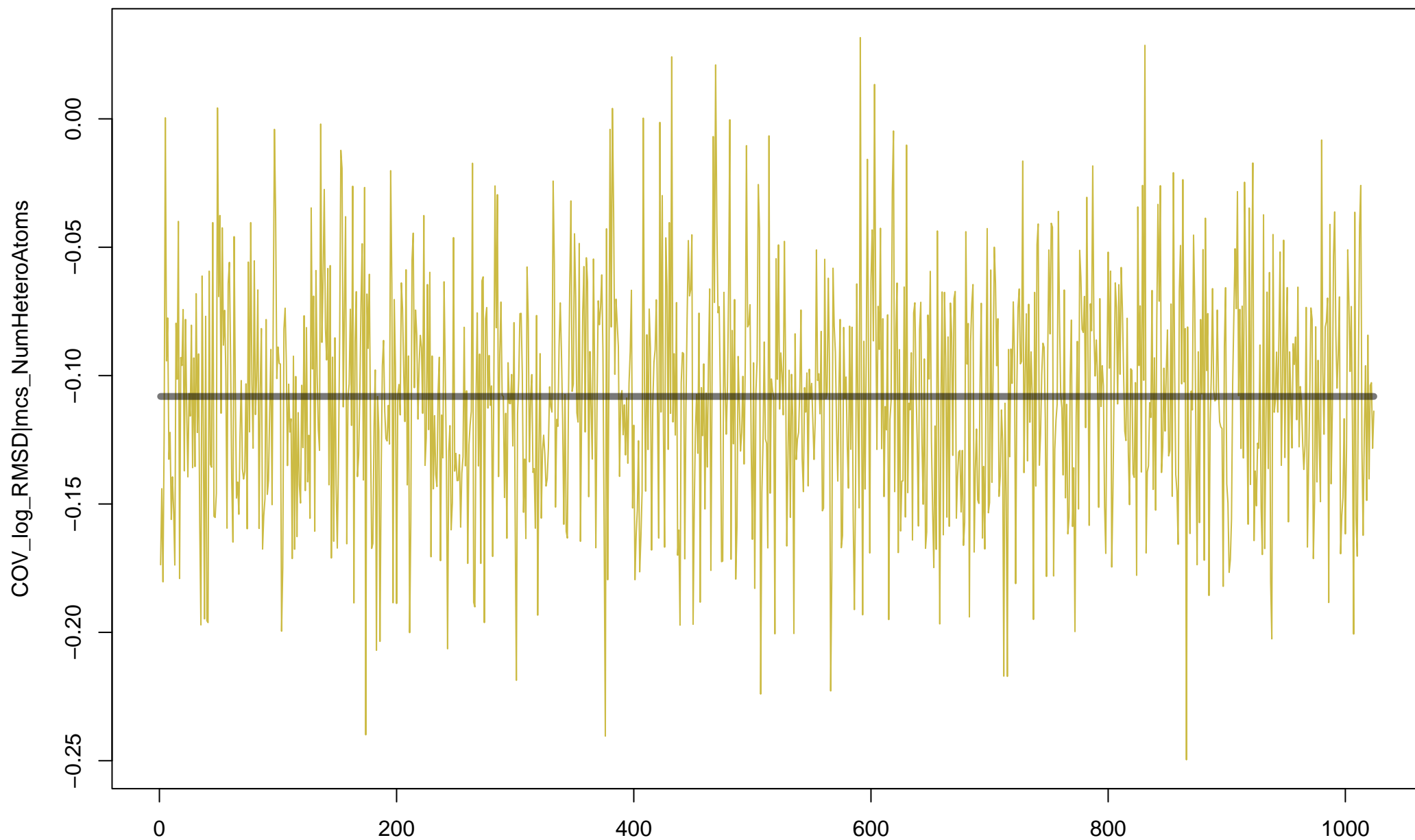


COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 804 | BMK = 0.0762 | MCSE(6.27) = 3.45 | stat: TRUE | burn: 0 | percentile: 26.1

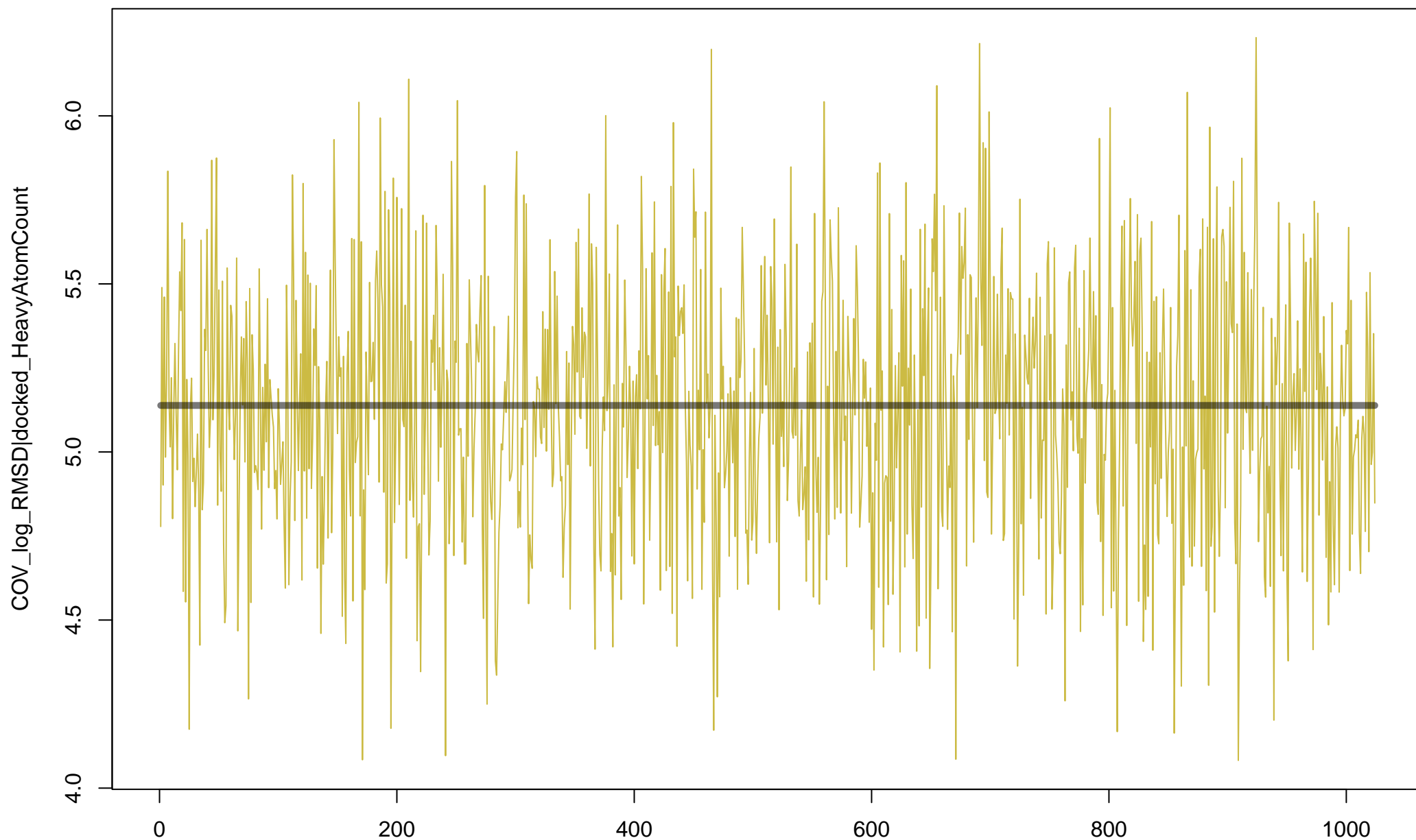


COV_log_RMSD|mcs_NumHeteroAtoms

ESS = 1020 | BMK = 0.0448 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0 | percentile: 49.5

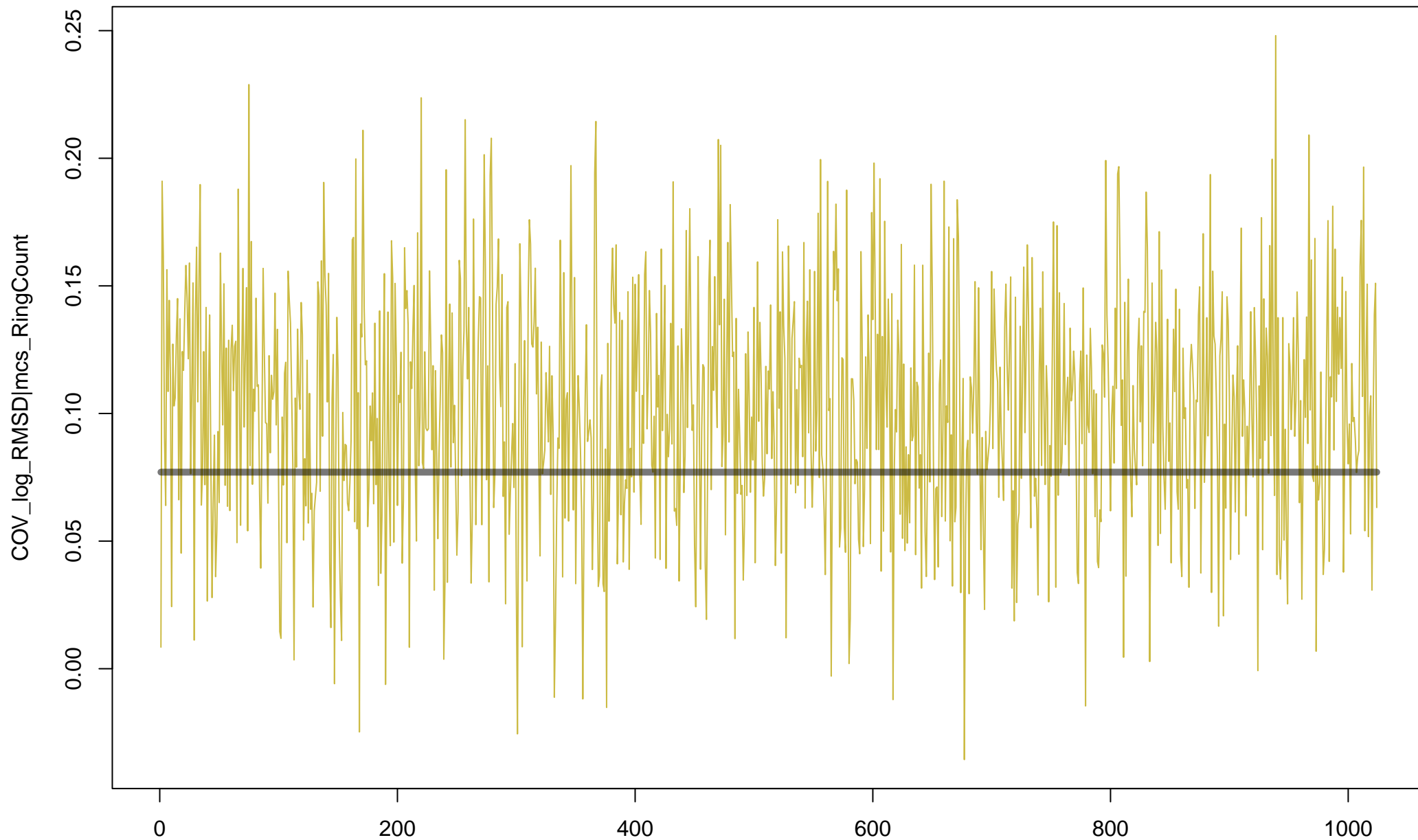


COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.056 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0 | percentile: 52.3

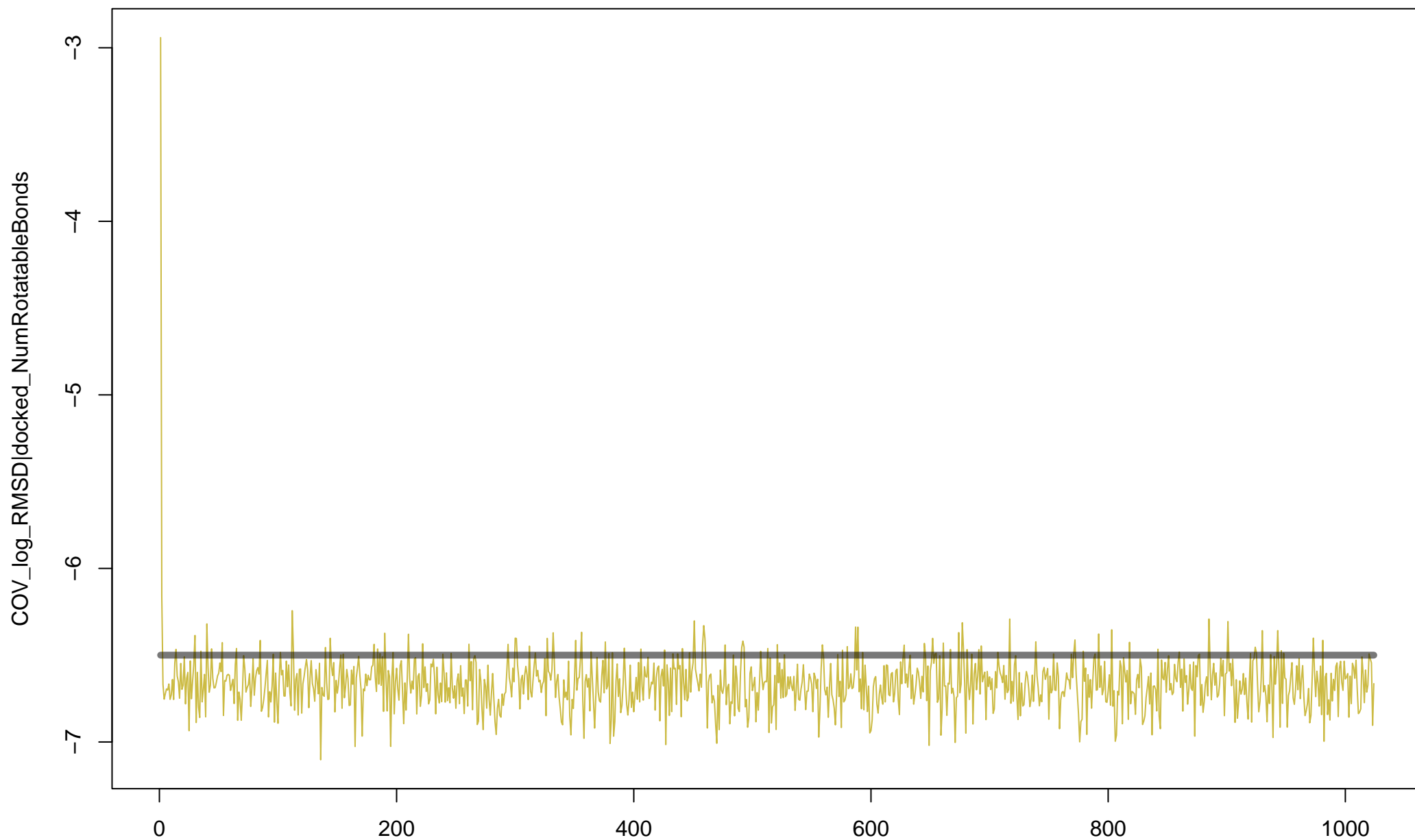


COV_log_RMSD|mcs_RingCount

ESS = 1020 | BMK = 0.0572 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | percentile: 30.2

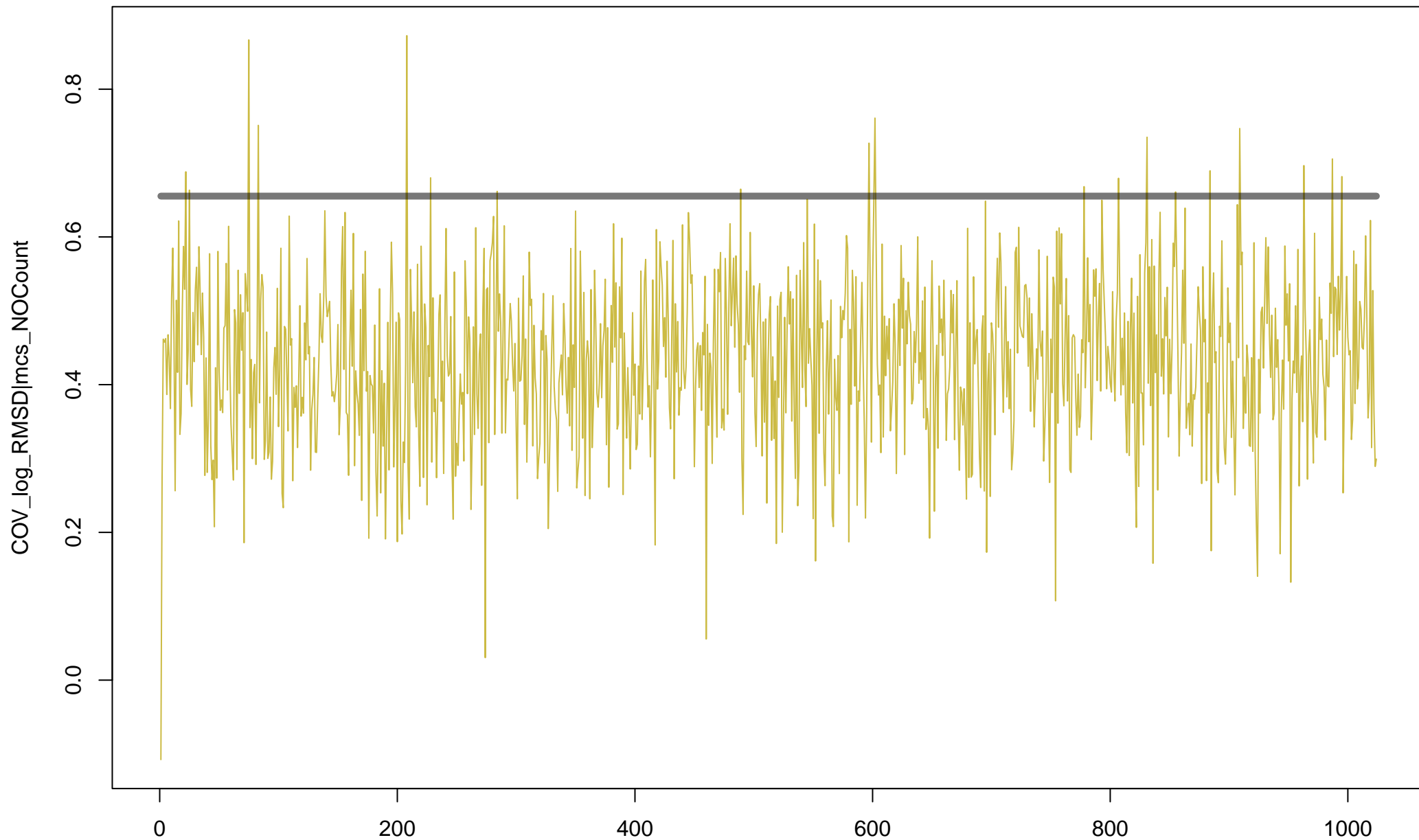


COV_log_RMSD|docked_NumRotatableBonds
ESS = 910 | BMK = 0.059 | MCSE(6.27) = 3.14 | stat: TRUE | burn: 0 | percentile: 89.3

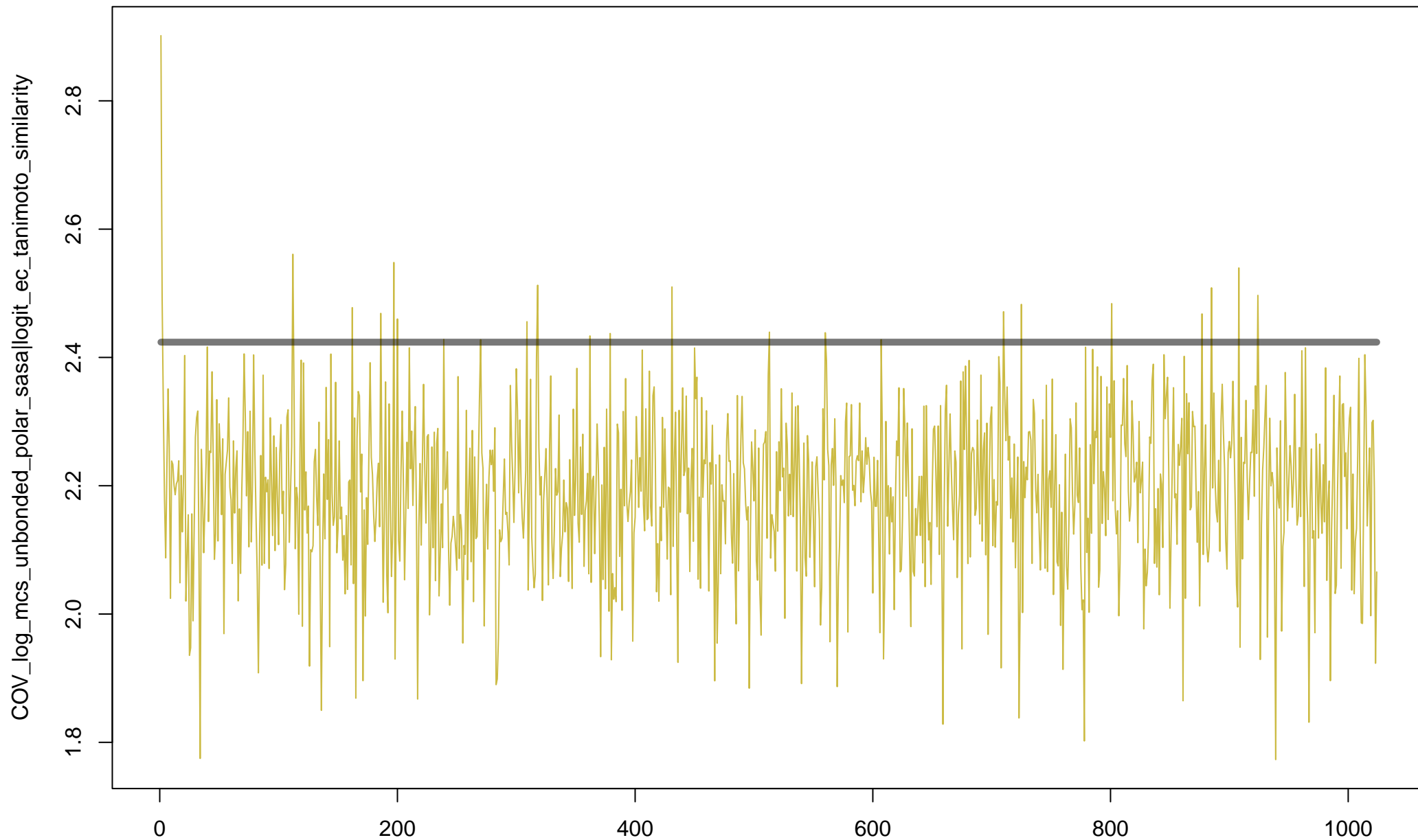


COV_log_RMSD|mcs_NOCount

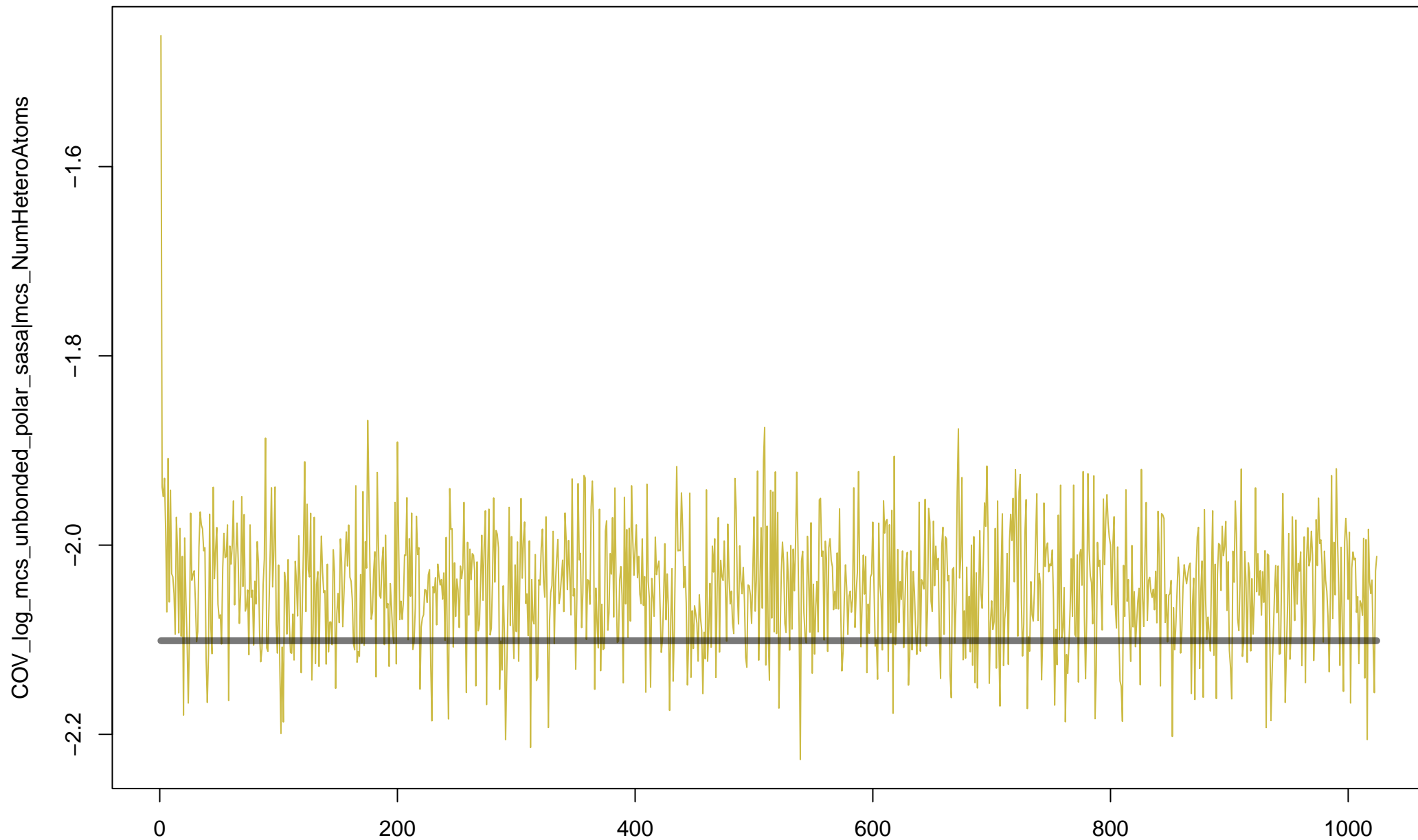
ESS = 1020 | BMK = 0.085 | MCSE(6.27) = 3.56 | stat: TRUE | burn: 0 | percentile: 98.1



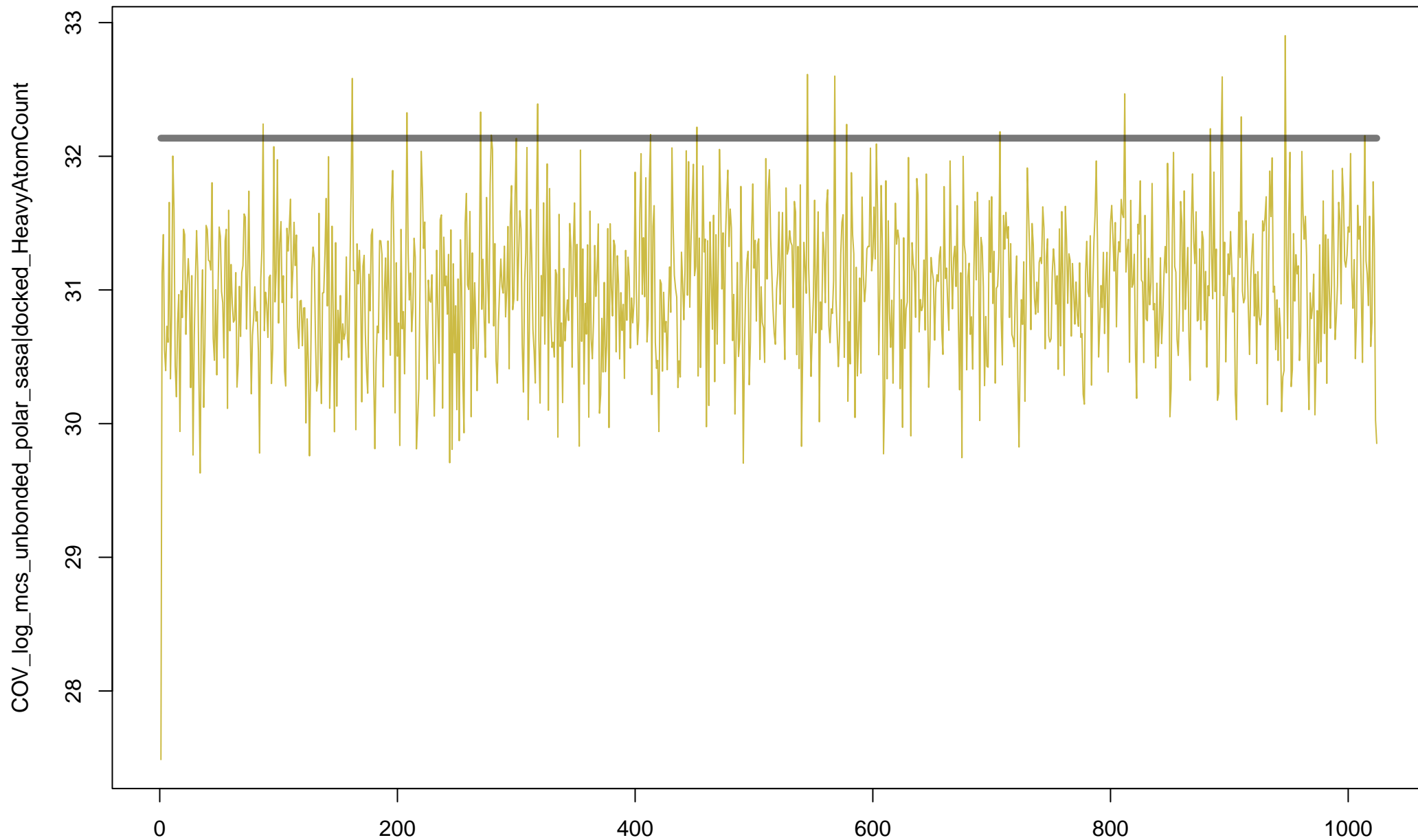
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0676 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0 | percentile: 97.7



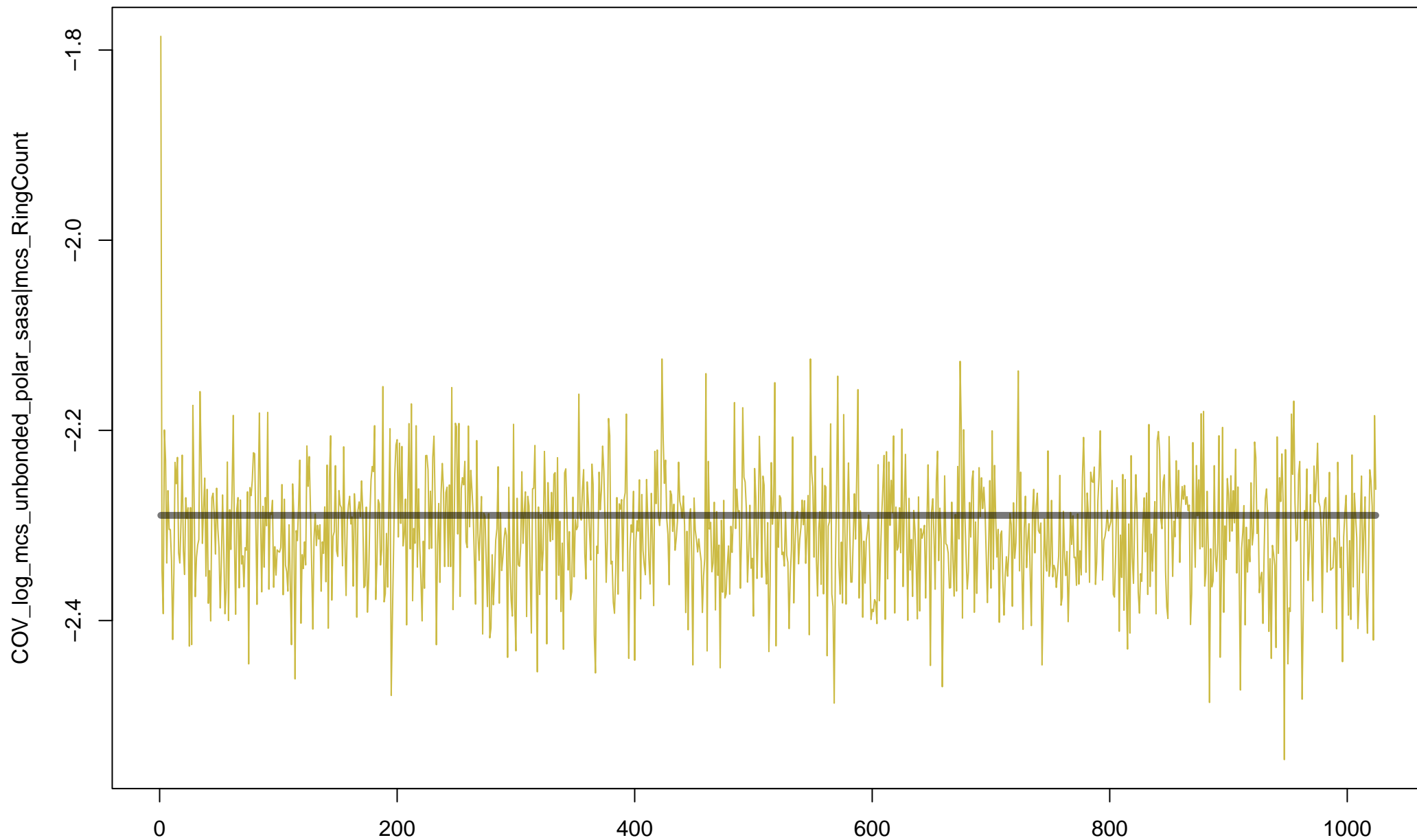
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0456 | MCSE(6.27) = 3 | stat: TRUE | burn: 0 | percentile: 19.3



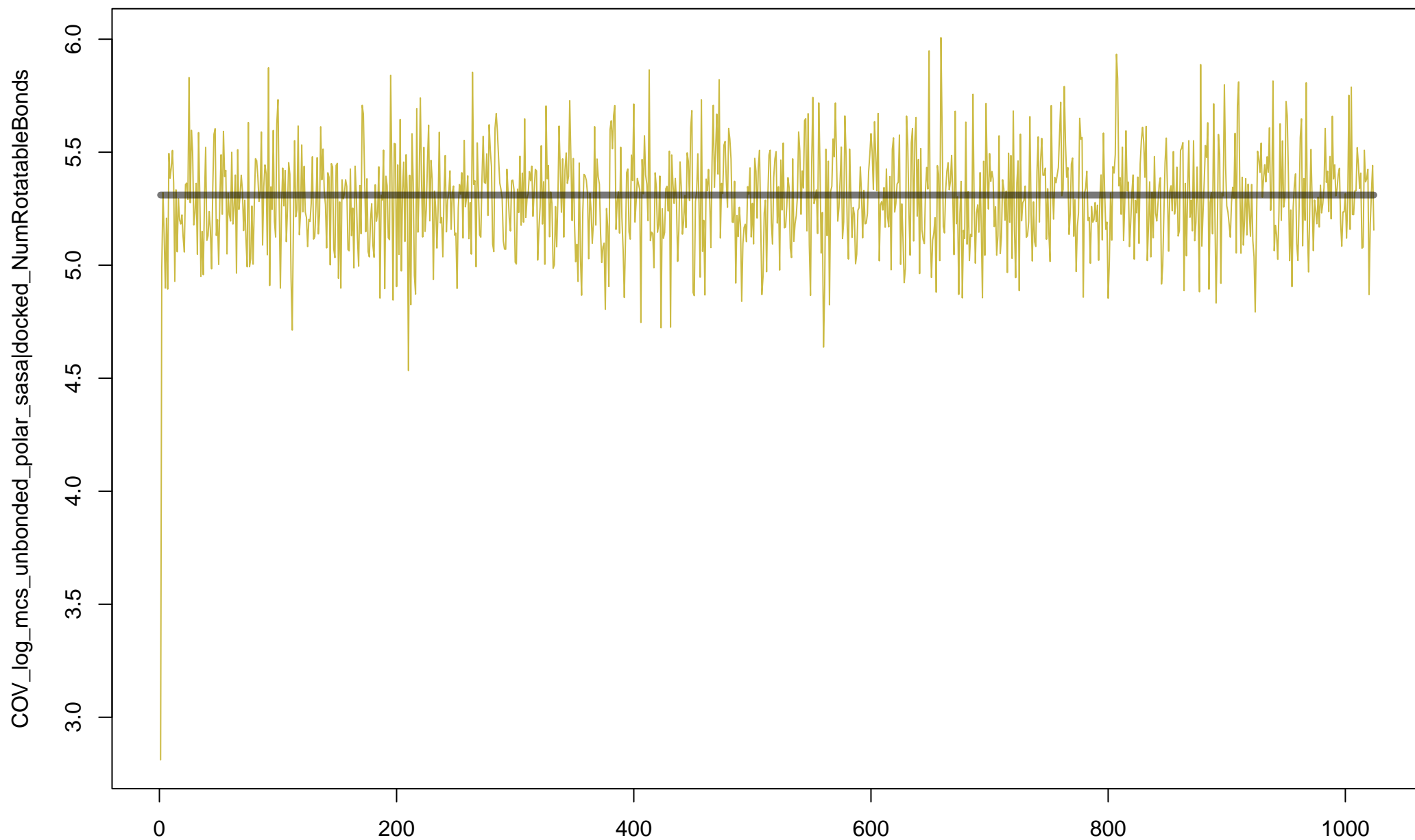
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 887 | BMK = 0.0911 | MCSE(6.27) = 3.83 | stat: FALSE | burn: 0 | percentile: 98.2



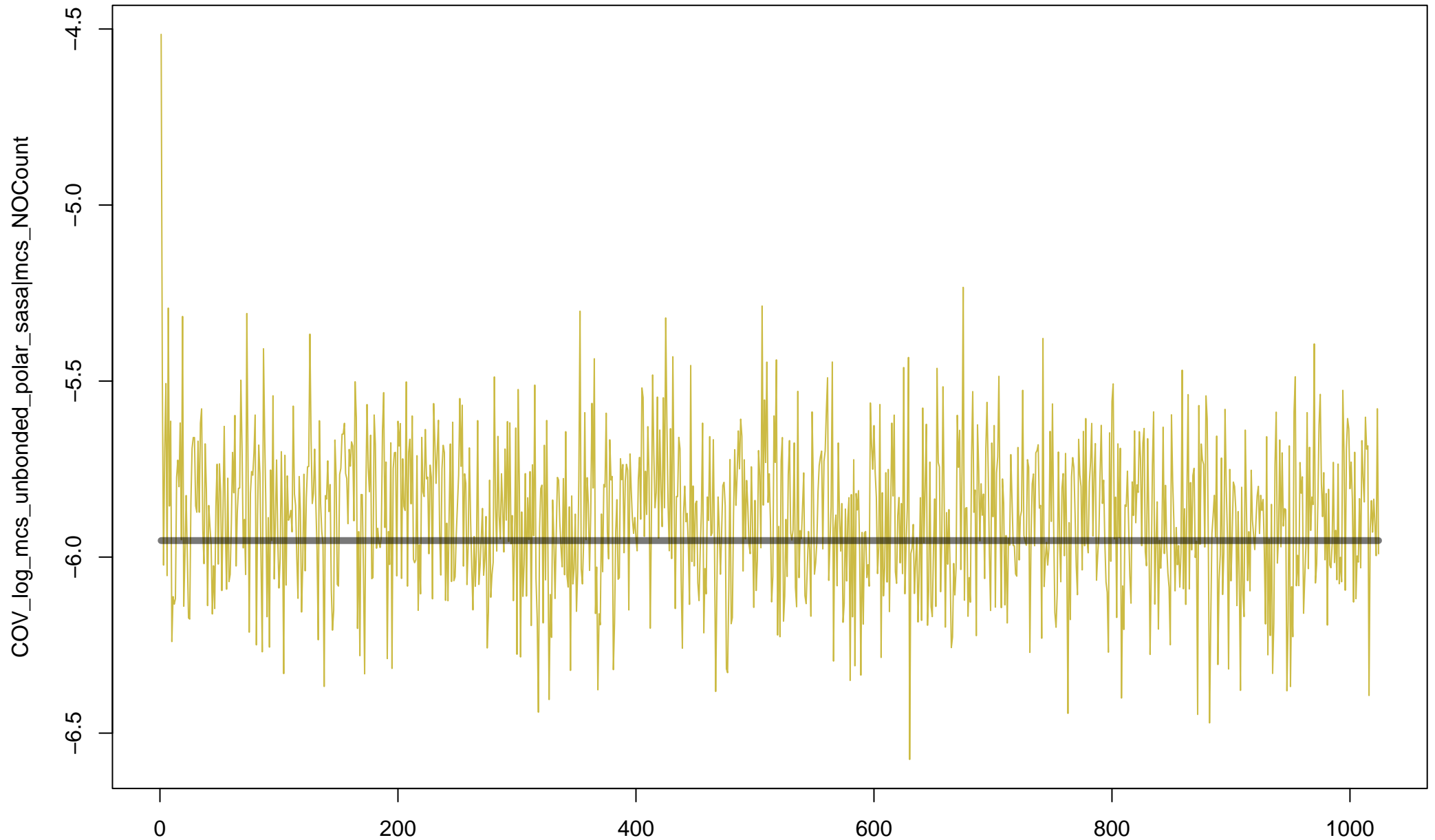
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0593 | MCSE(6.27) = 3.7 | stat: TRUE | burn: 0 | percentile: 60.8



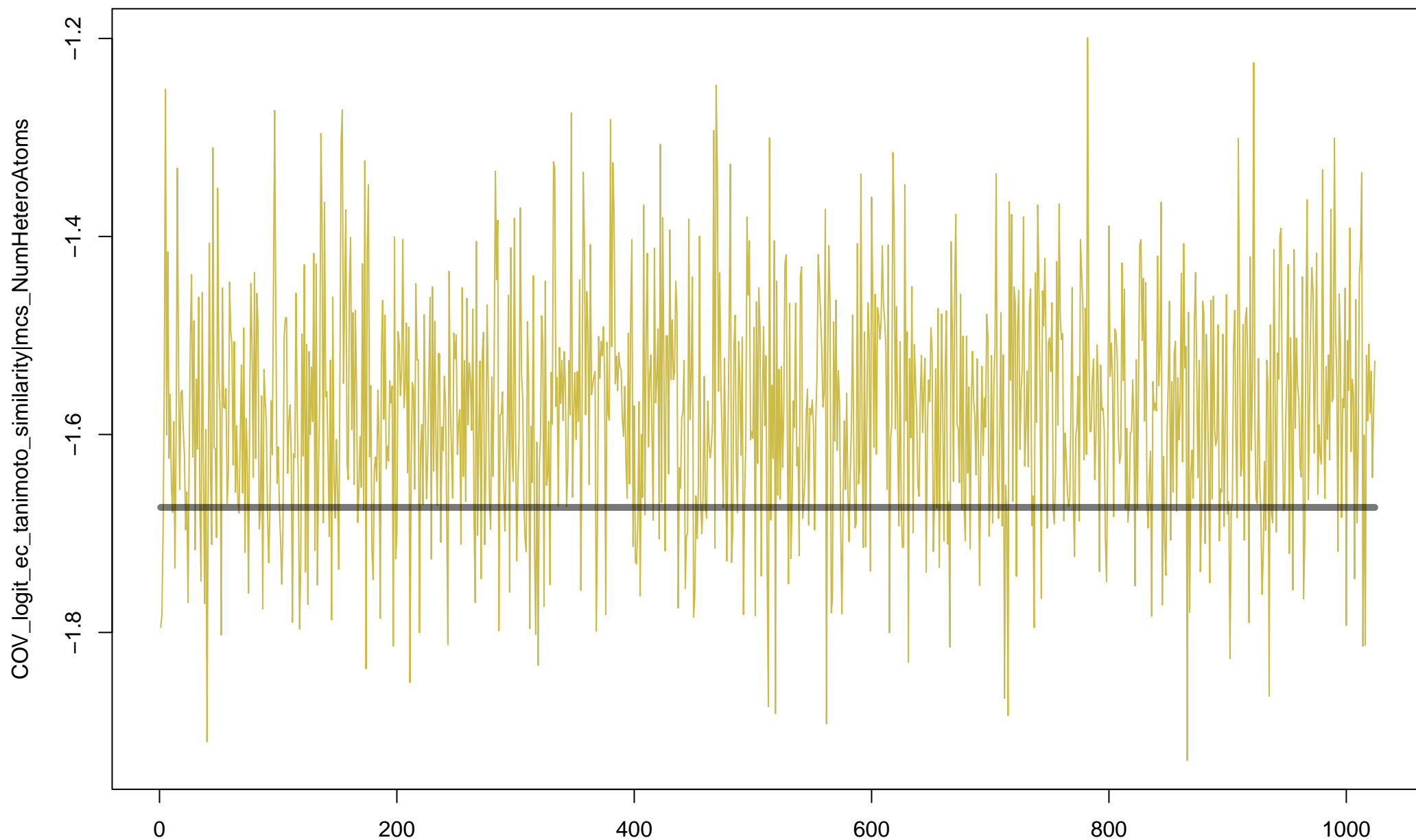
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 992 | BMK = 0.062 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0 | percentile: 52.3



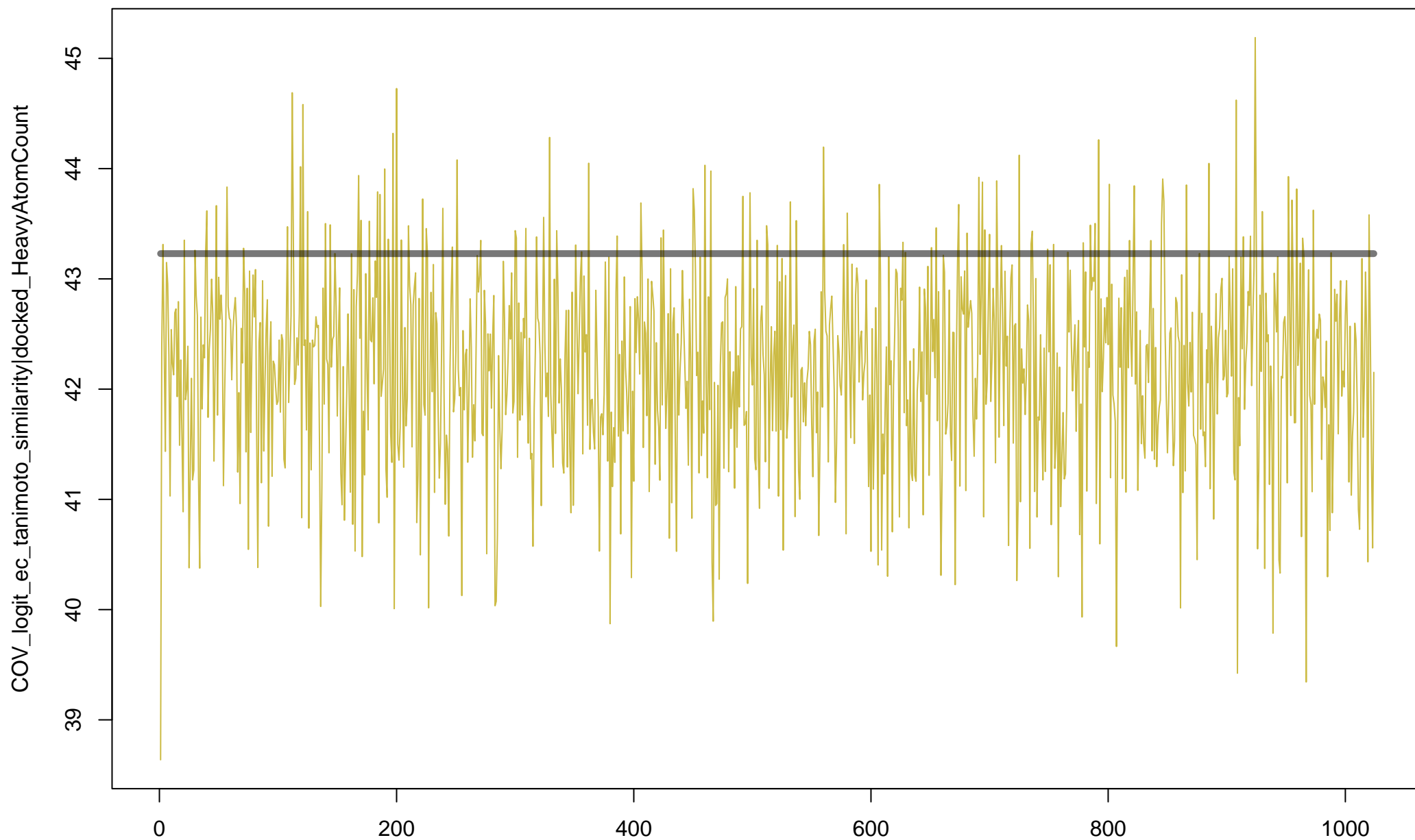
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0699 | MCSE(6.27) = 3.89 | stat: FALSE | burn: 0 | percentile: 38.3



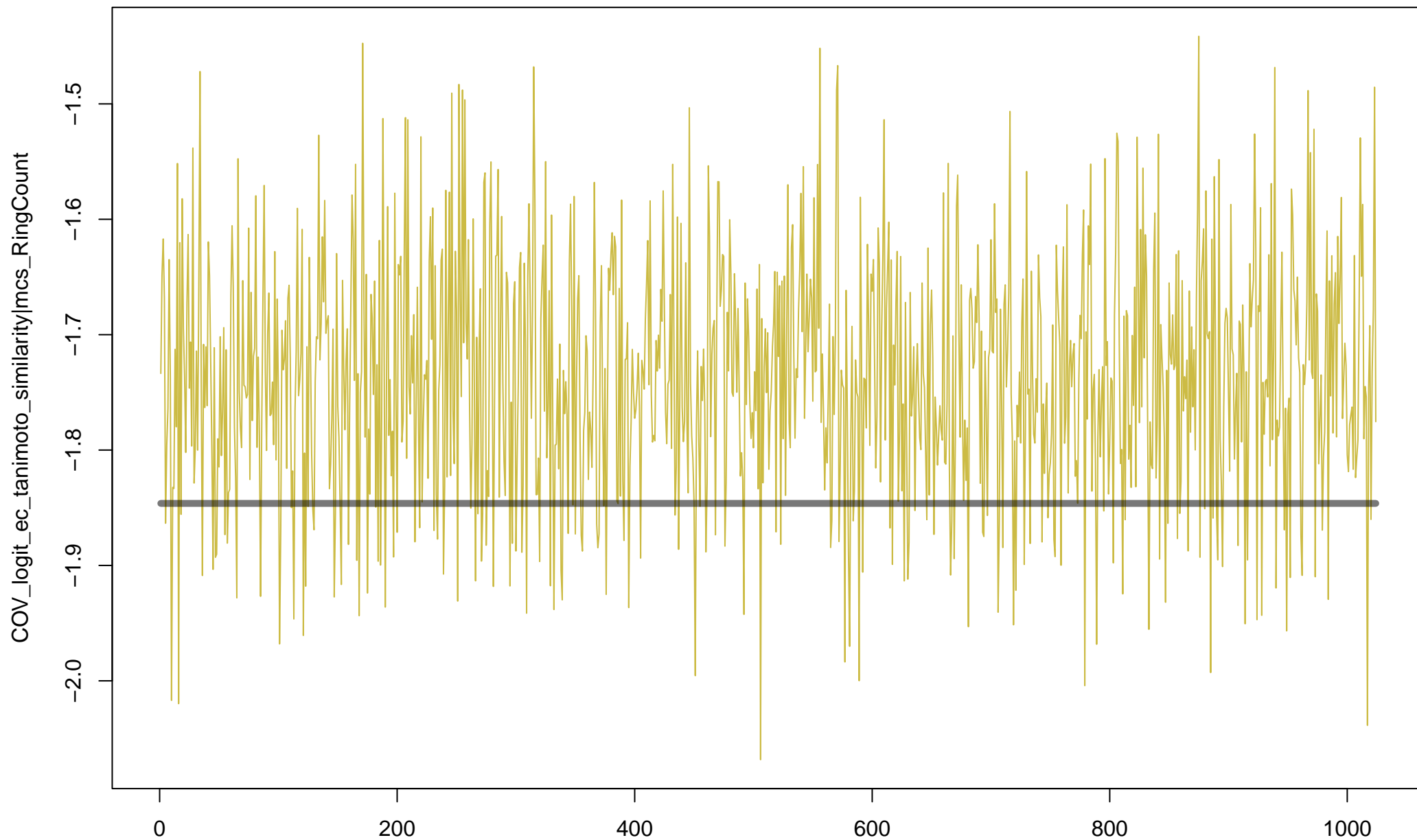
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0729 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0 | percentile: 20.5



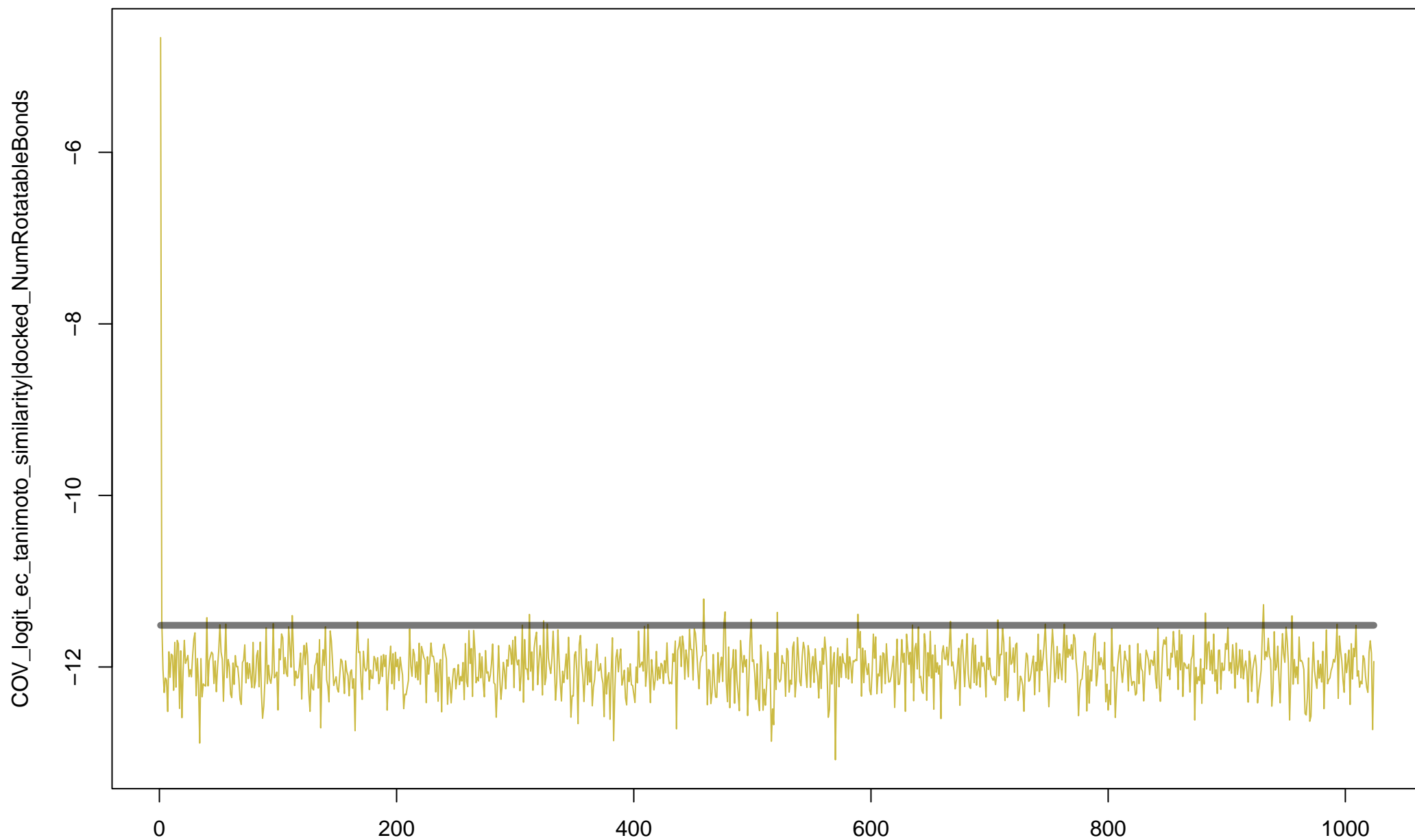
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0479 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | percentile: 89.4



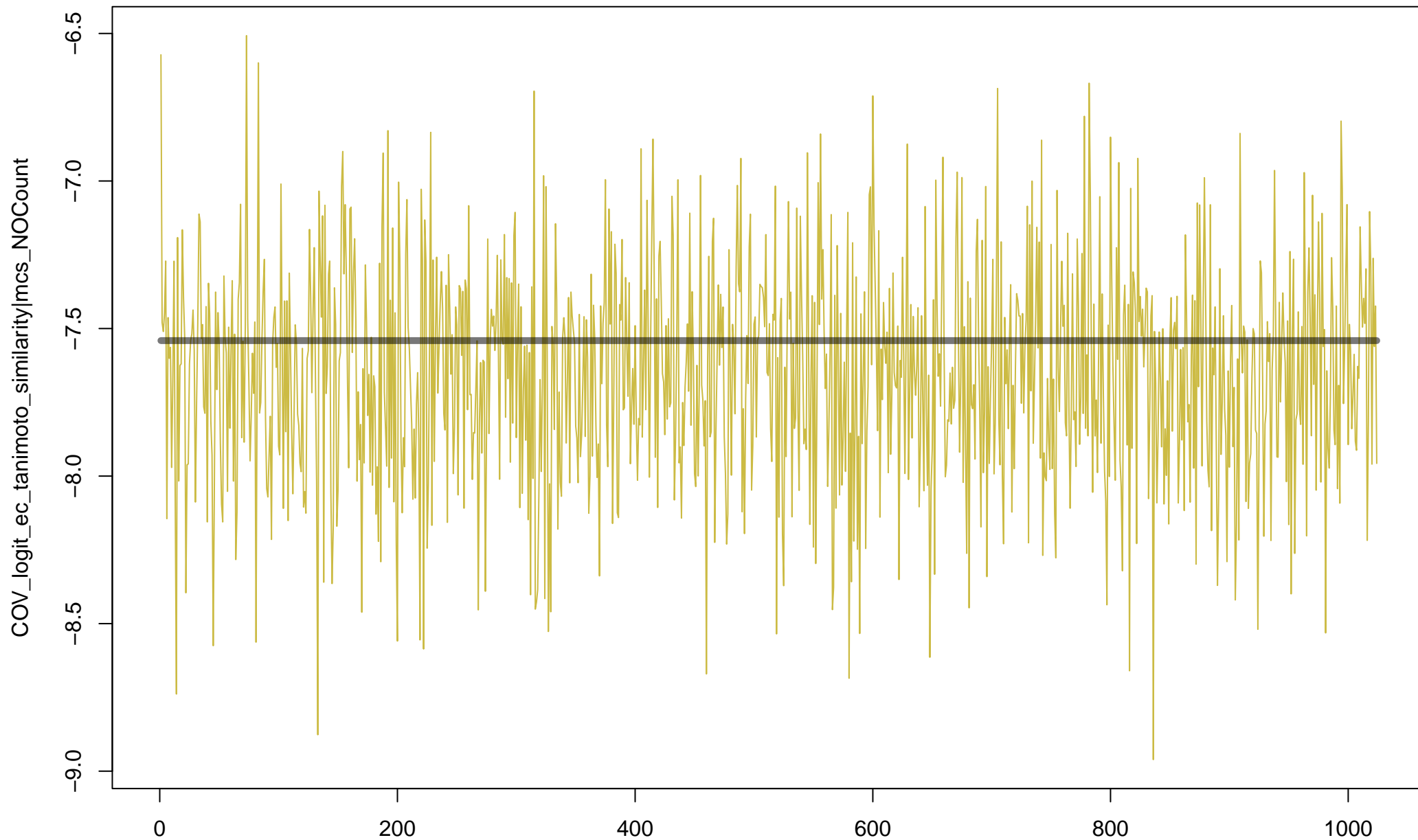
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0379 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0 | percentile: 15.1



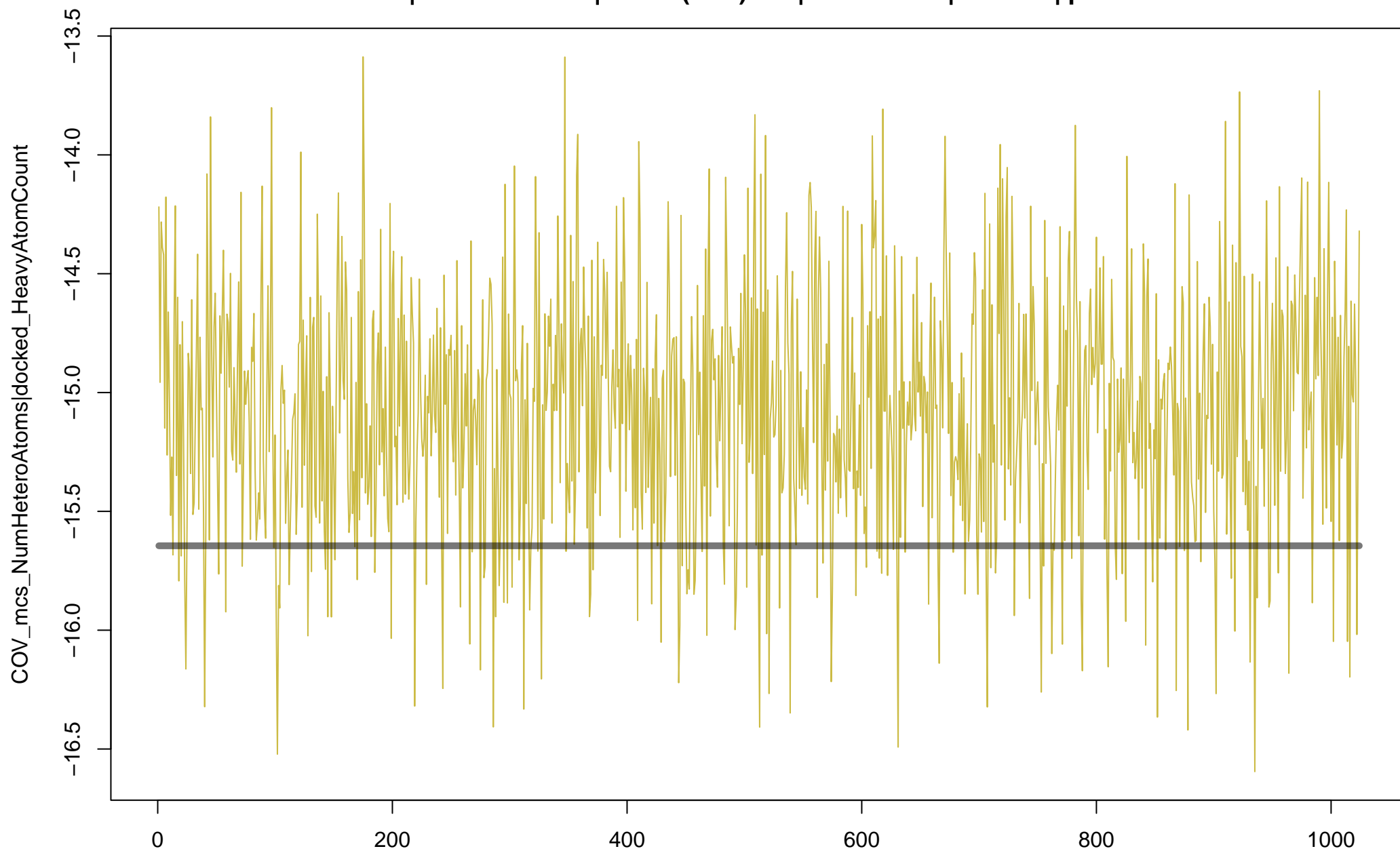
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0627 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0 | percentile: 97.3



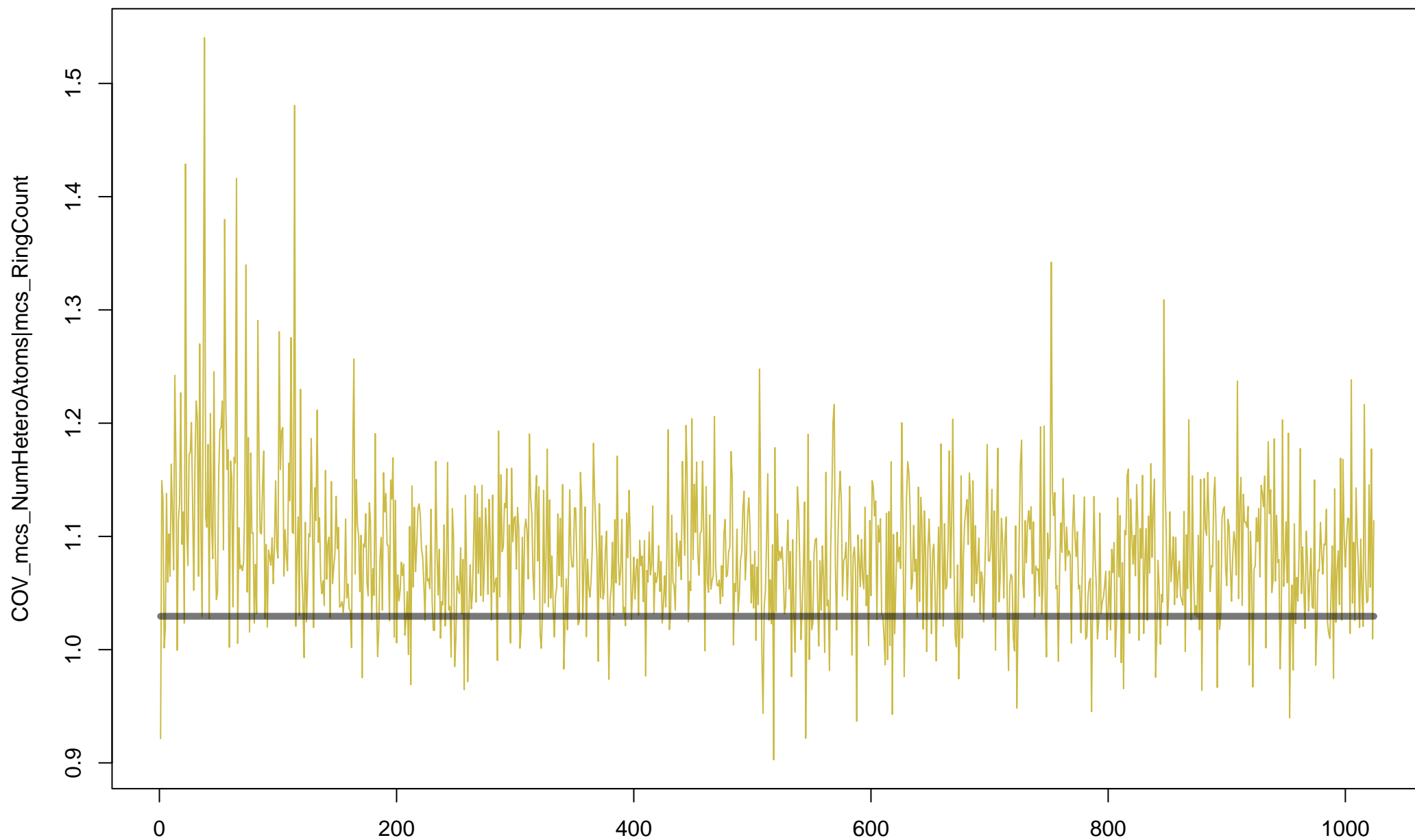
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0457 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0 | percentile: 60.2



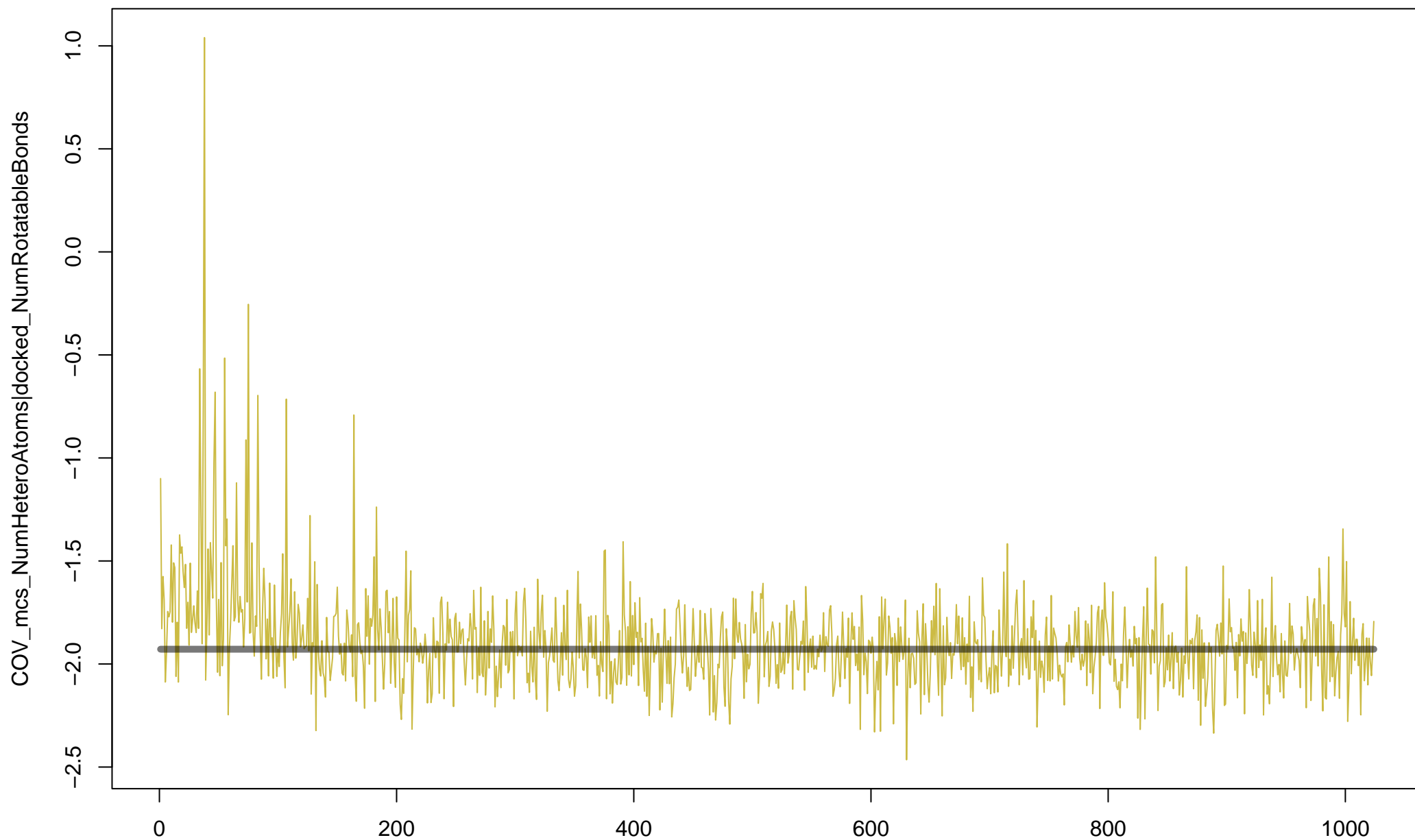
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0638 | MCSE(6.27) = 3 | stat: TRUE | burn: 0 | percentile: 13.5



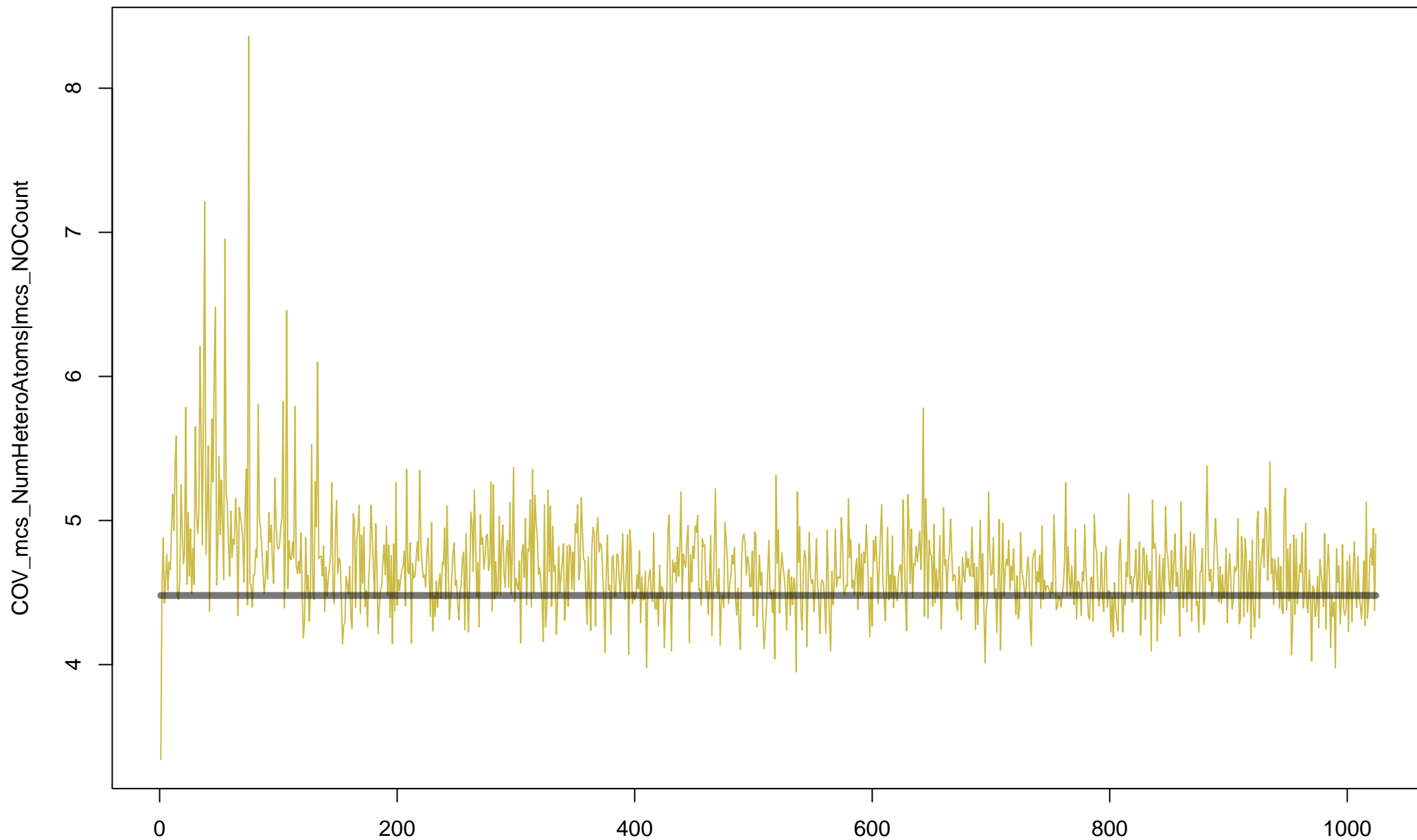
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 116 | BMK = 0.111 | MCSE(6.27) = 5.63 | stat: FALSE | burn: 0 | percentile: 16.3



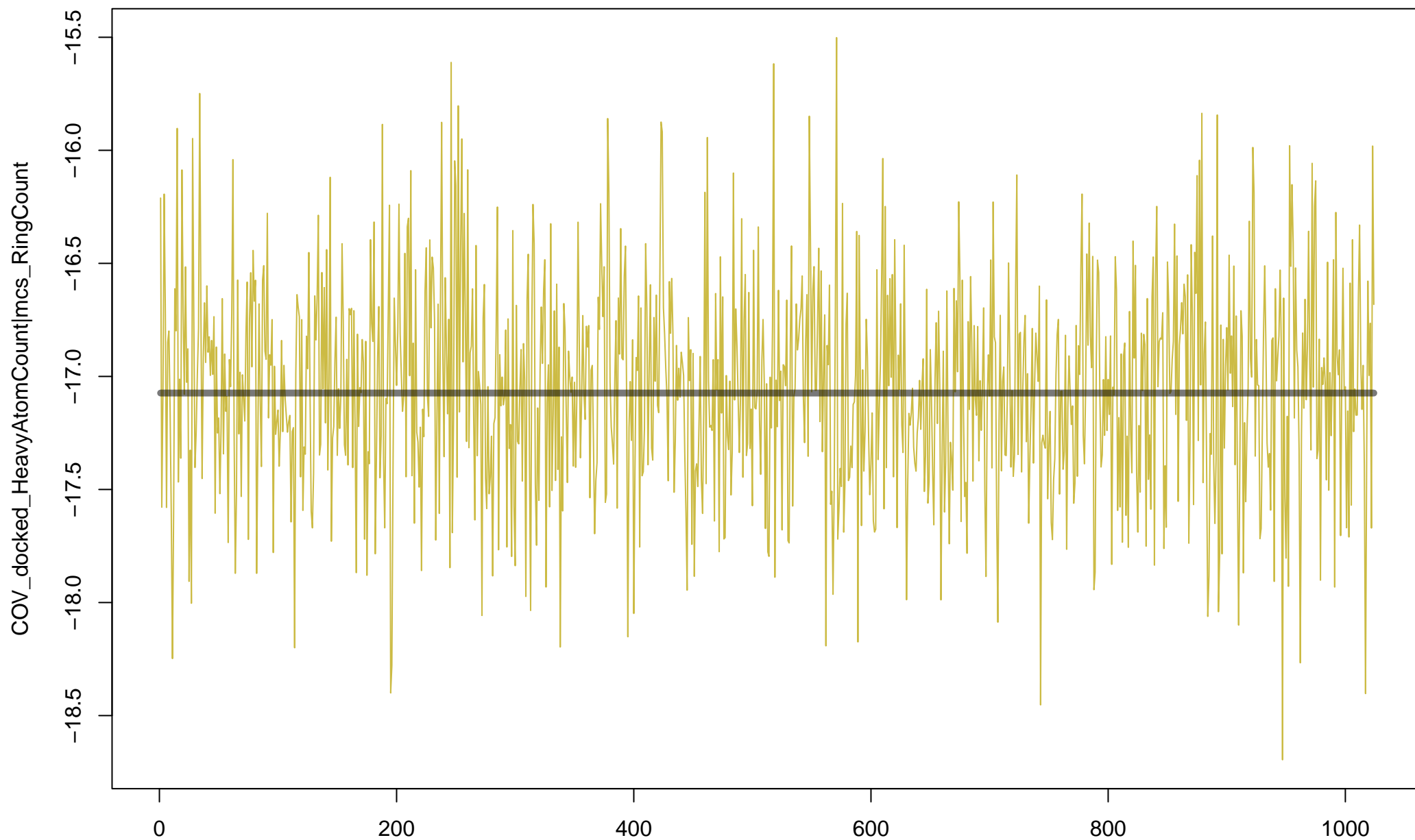
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 53 | BMK = 0.164 | MCSE(6.27) = 7.75 | stat: FALSE | burn: 0 | percentile: 46.4



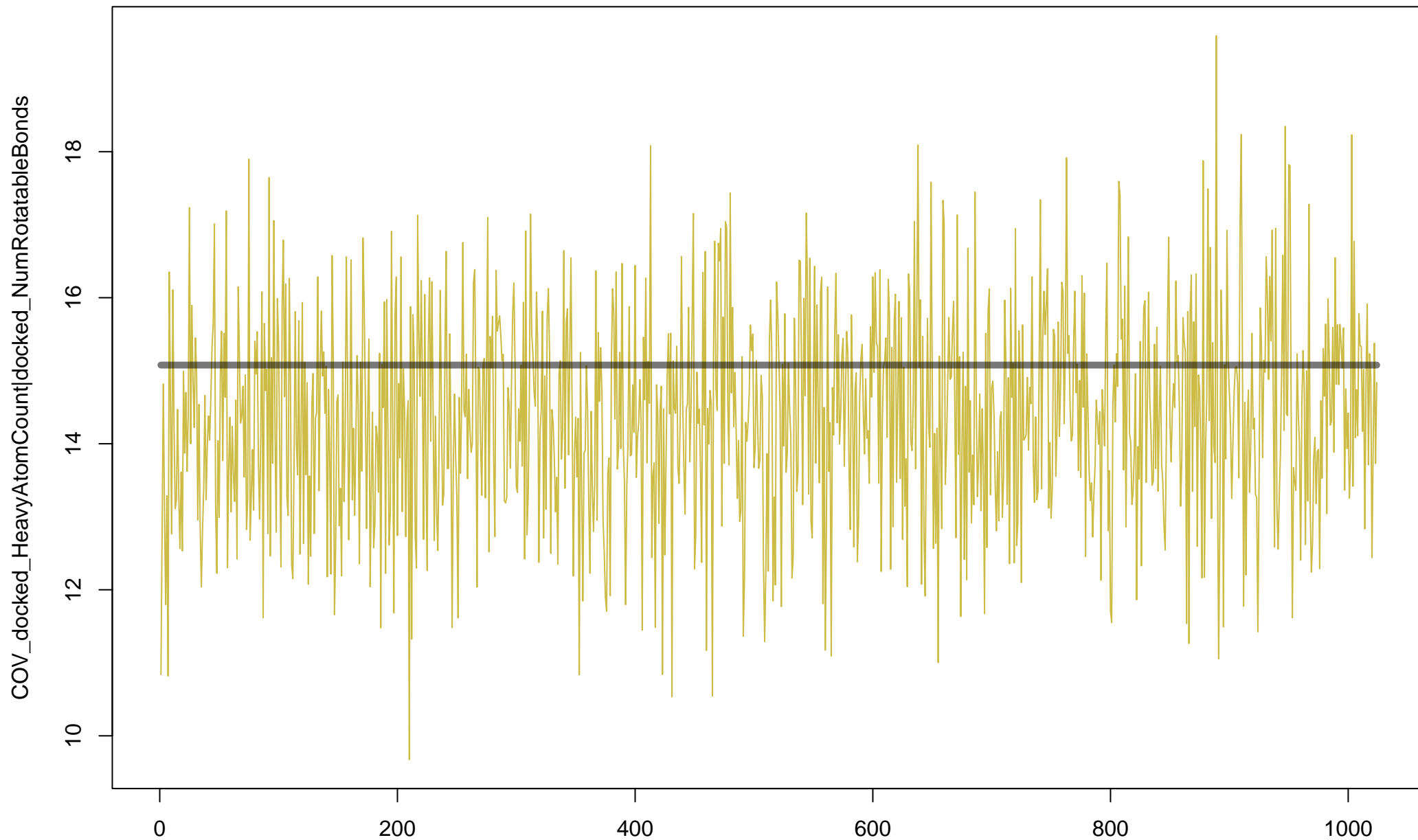
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 58.2 | BMK = 0.161 | MCSE(6.27) = 7.32 | stat: FALSE | burn: 0 | percentile: 26.4



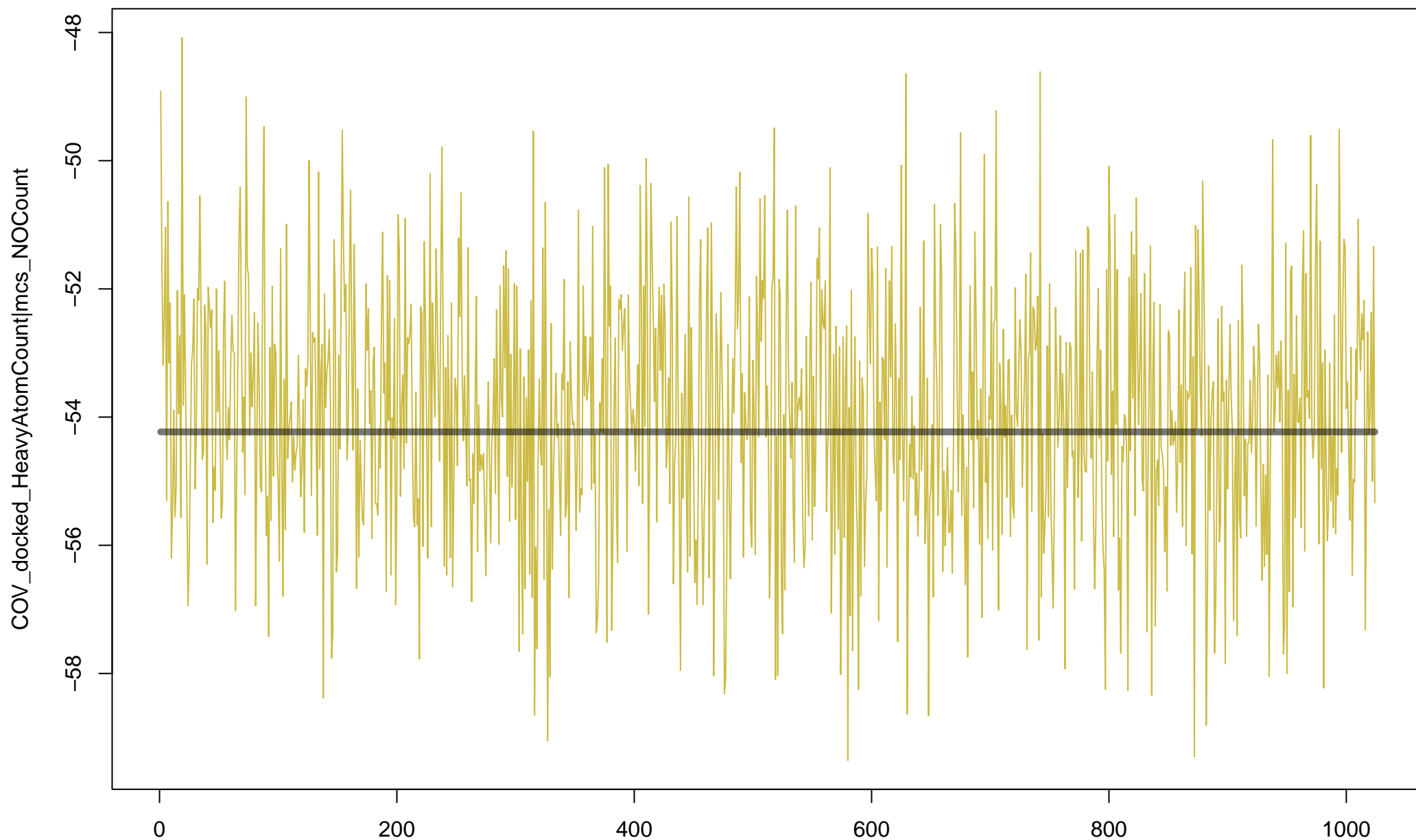
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0447 | MCSE(6.27) = 3.39 | stat: TRUE | burn: 0 | percentile: 47.2



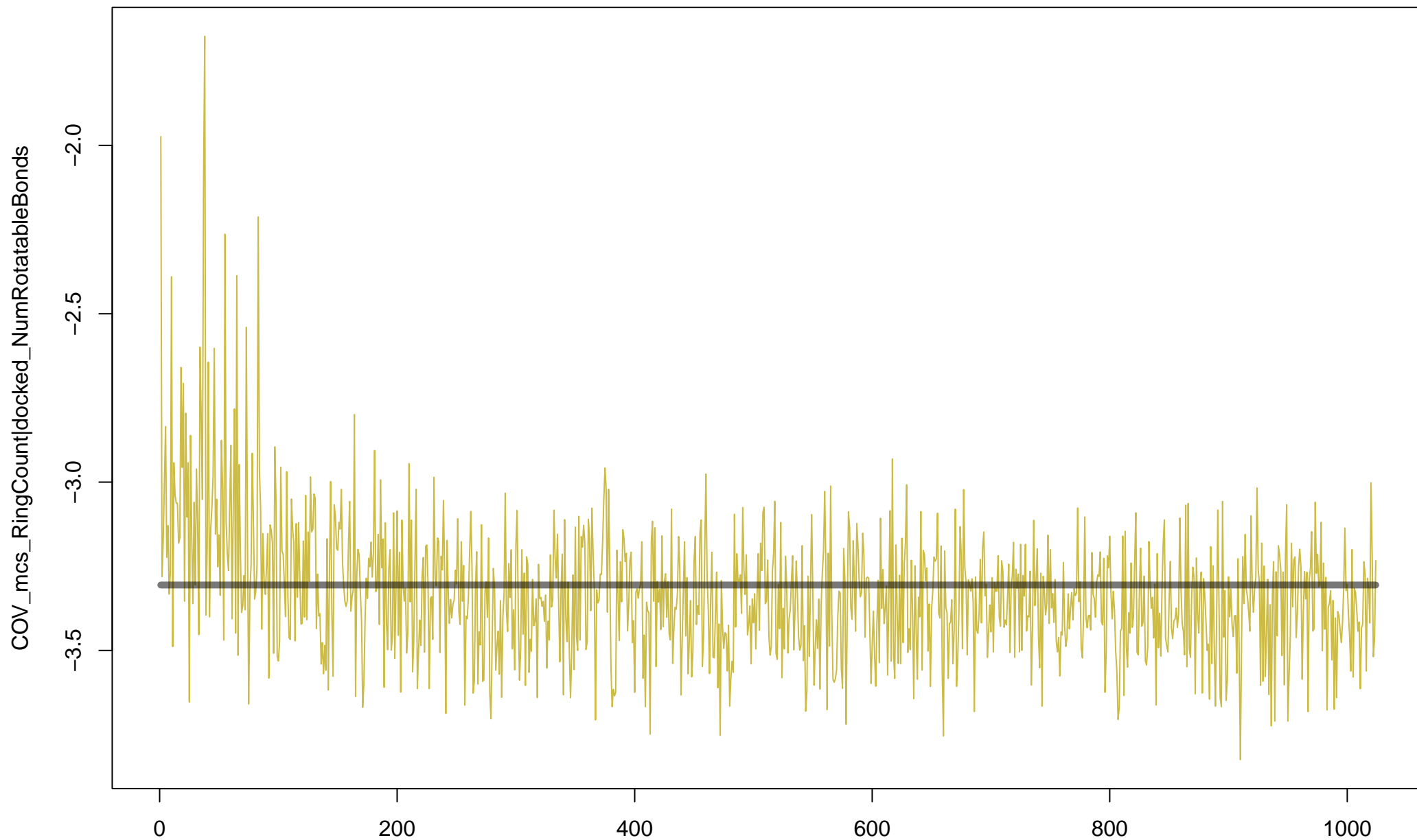
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 852 | BMK = 0.079 | MCSE(6.27) = 3.37 | stat: FALSE | burn: 0 | percentile: 69.2



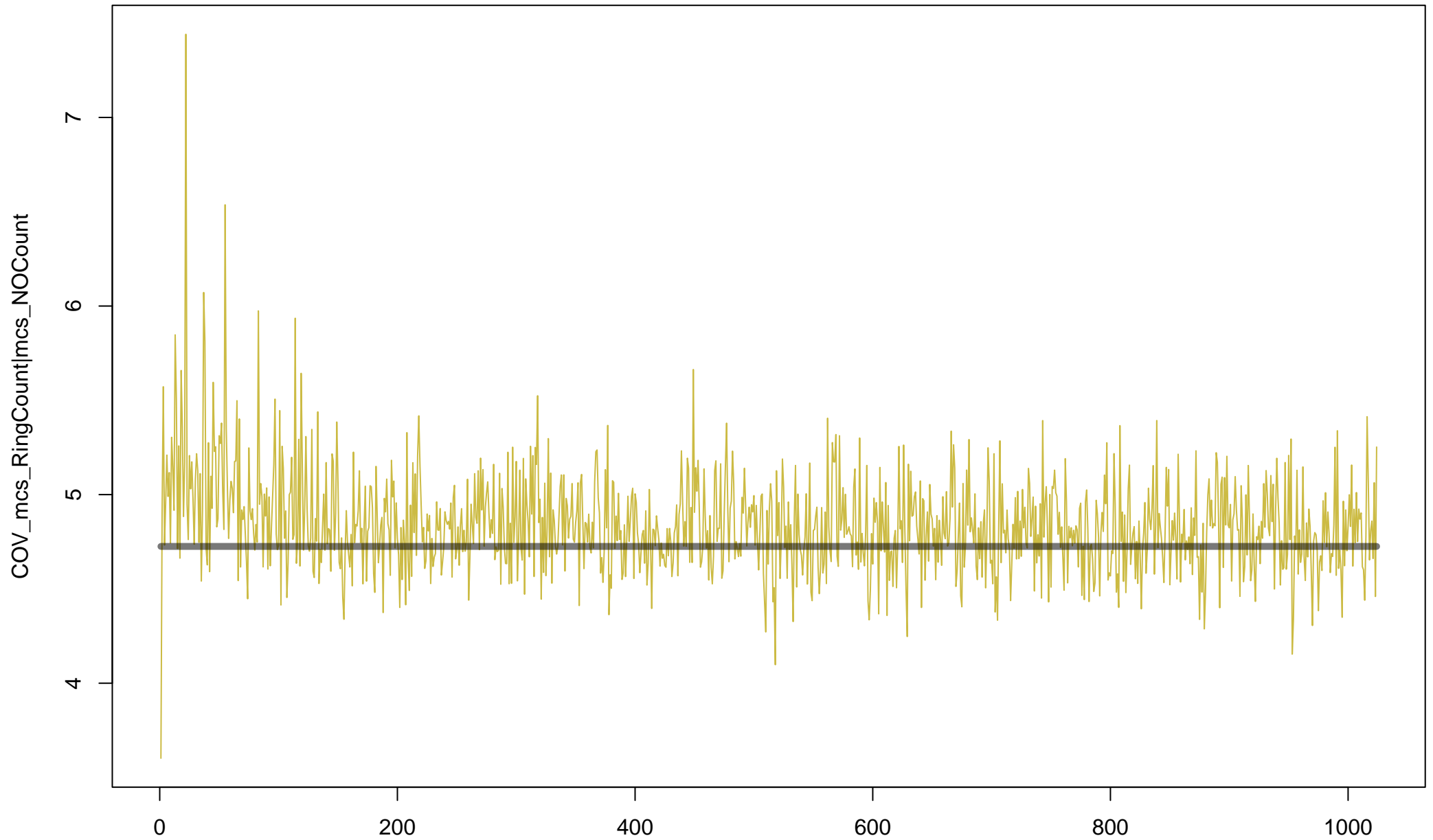
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0567 | MCSE(6.27) = 3.42 | stat: FALSE | burn: 0 | percentile: 44.7



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 40 | BMK = 0.197 | MCSE(6.27) = 8.08 | stat: FALSE | burn: 0 | percentile: 58.4



COV_mcs_RingCount|mcs_NOCount
ESS = 240 | BMK = 0.149 | MCSE(6.27) = 5.72 | stat: FALSE | burn: 0 | percentile: 33.1



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 11.8 | BMK = 0.327 | MCSE(6.27) = 9.96 | stat: FALSE | burn: 0 | percentile: 11.6

