

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 1

max MCSE = 5.46555931570576

all stationary: FALSE

burn: 1020

max percent.: 0

-- STATS 2D --

min ESS = 653.287763076683

max BMK = 0.069872784258695

max MCSE = 3.76283137009102

all stationary: FALSE

burn: 0

max percent.: 3.90625

-- STATS 1D --

min ESS = 130.882588867567

max BMK = 0.0960516557550705

max MCSE = 6.45344438869197

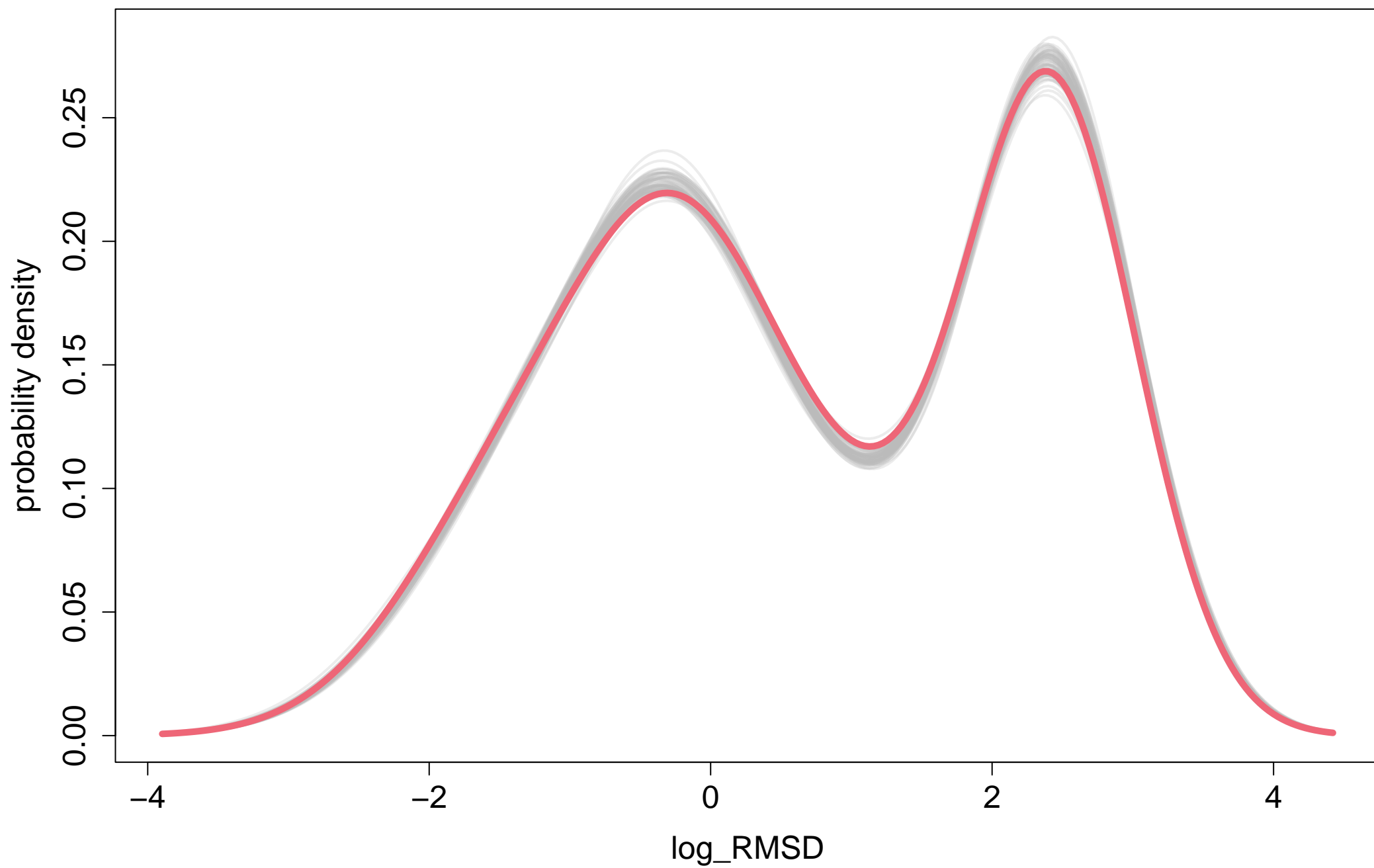
all stationary: FALSE

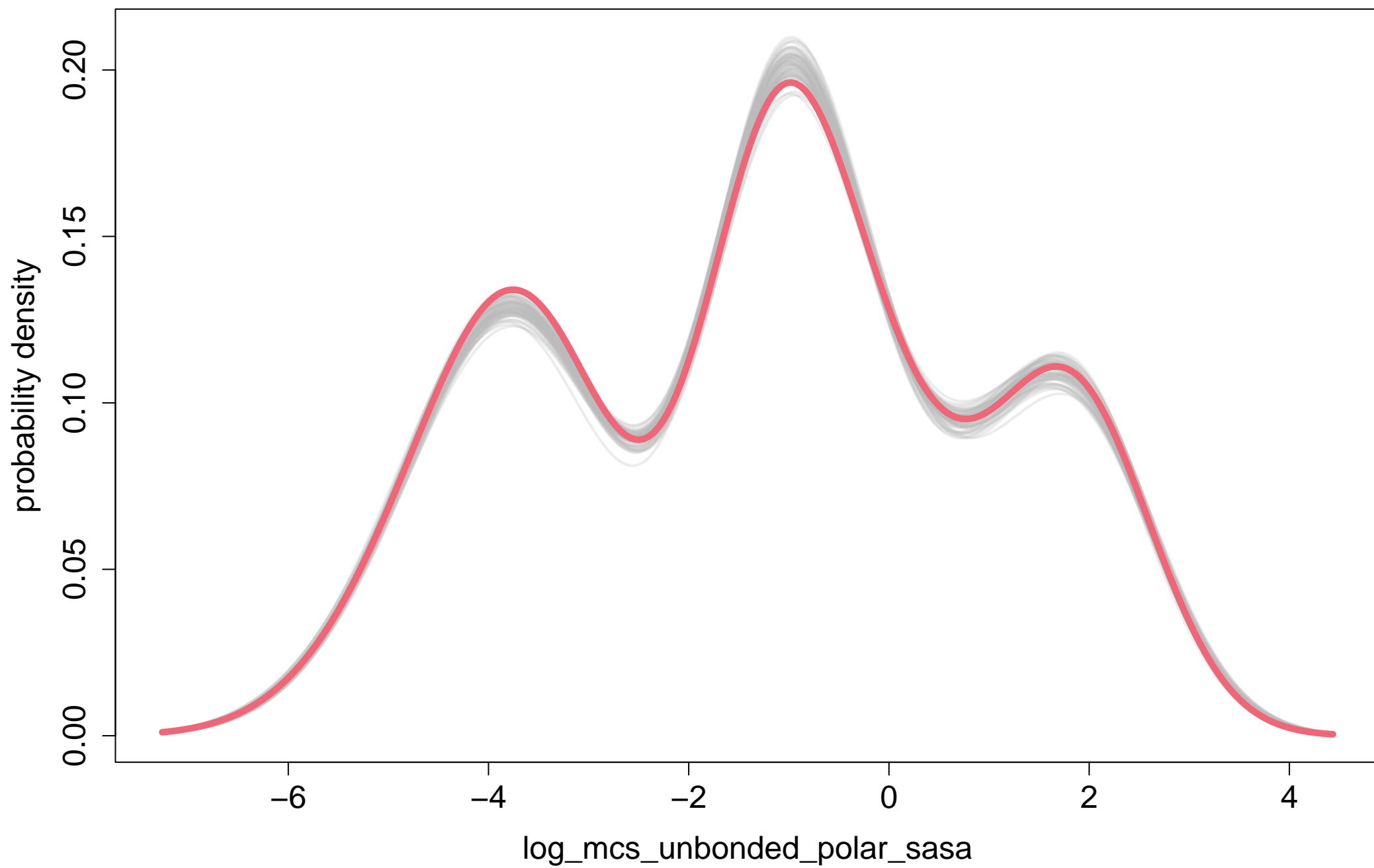
burn: 0

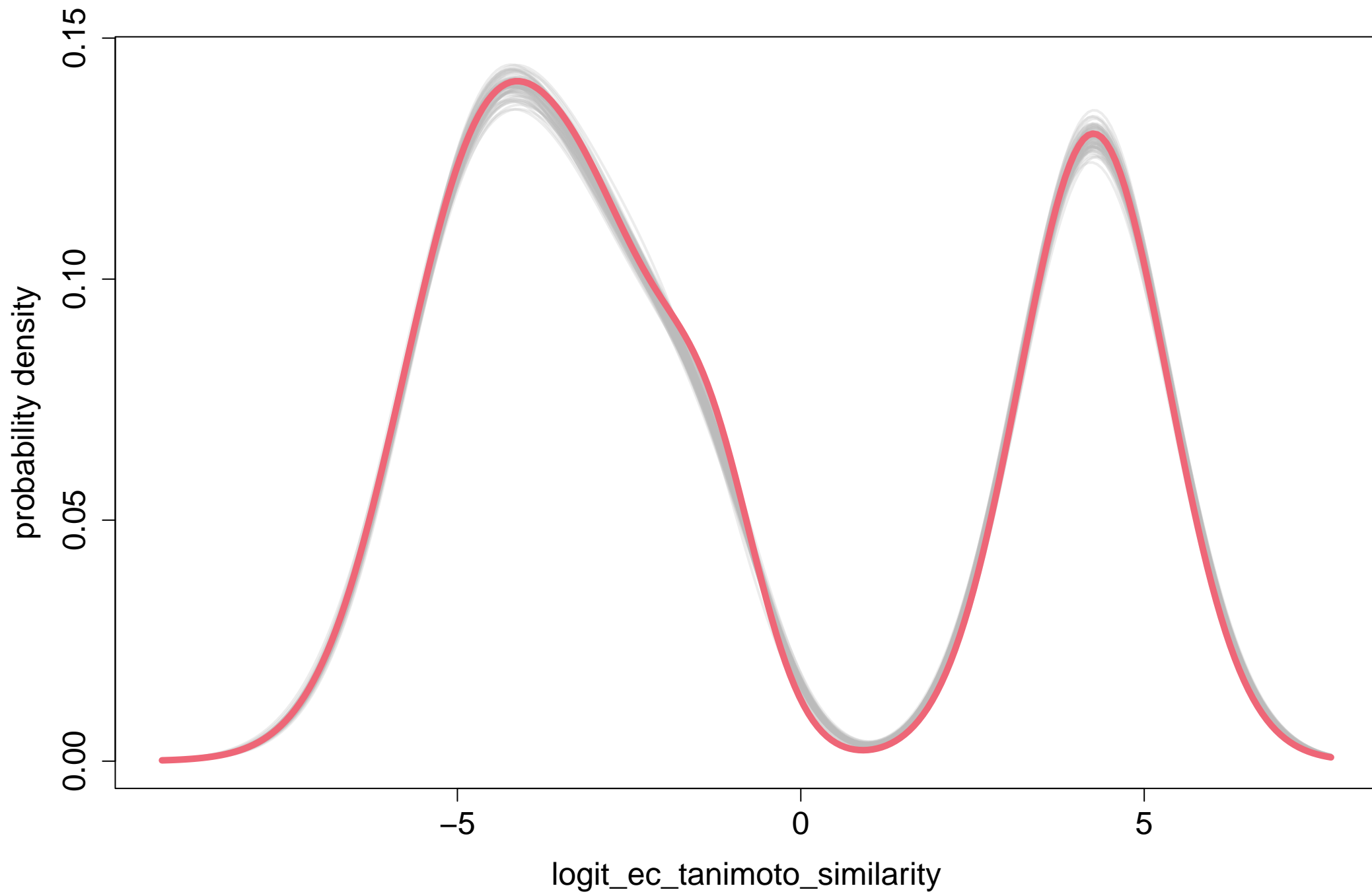
max percent.: 5.56640625

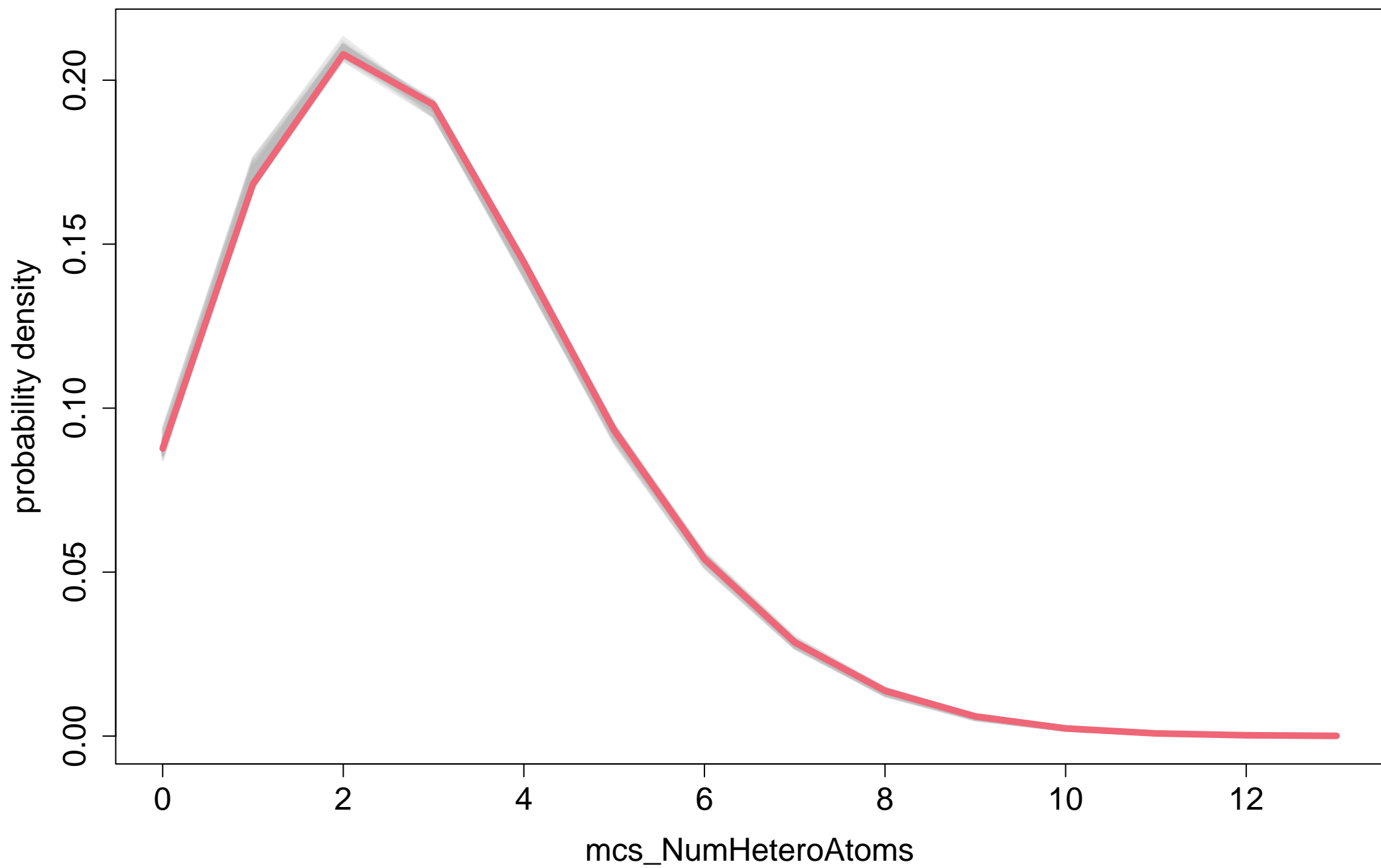
Occupied clusters: 9 of 64

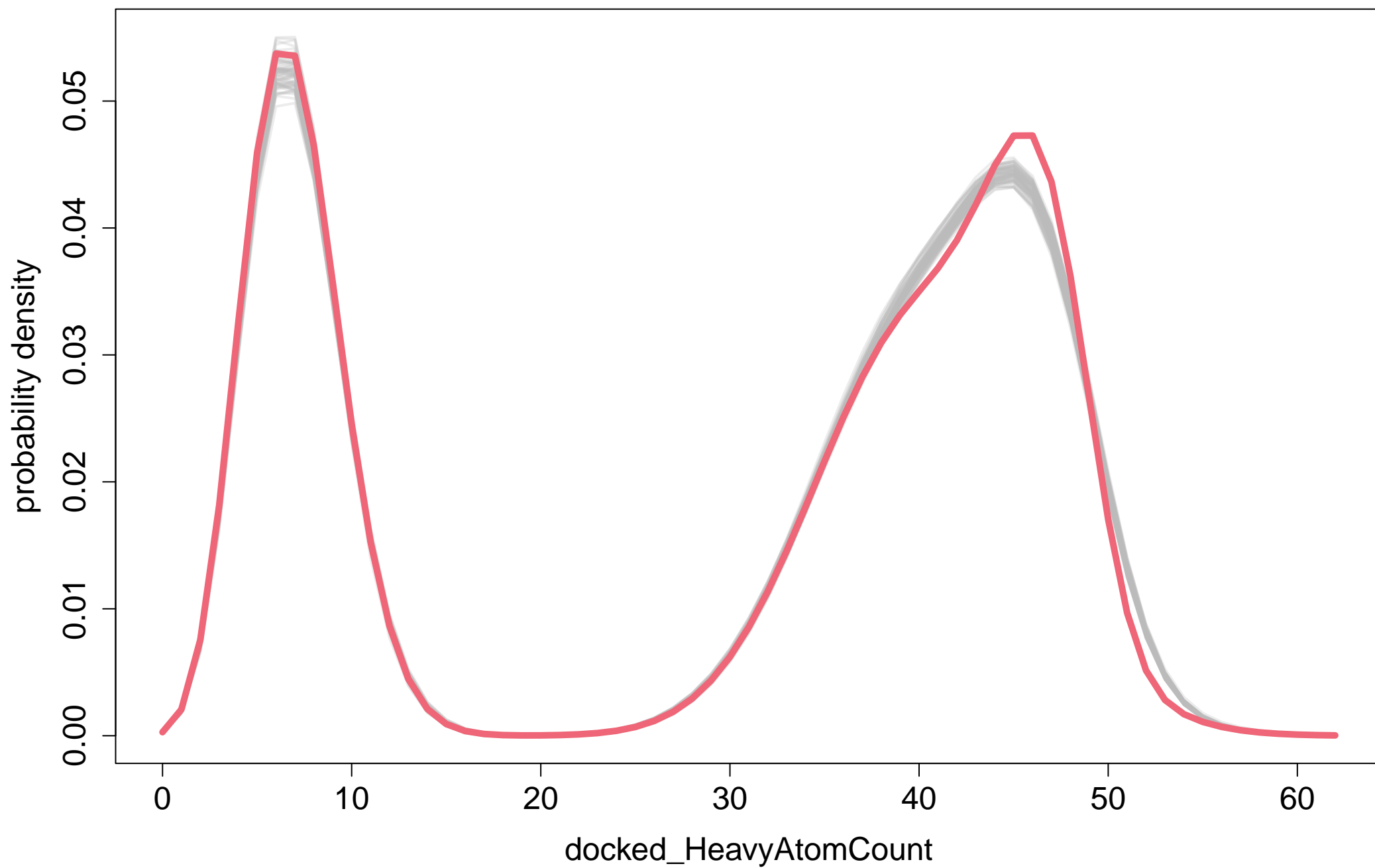
LL: -125000 +- 13.8

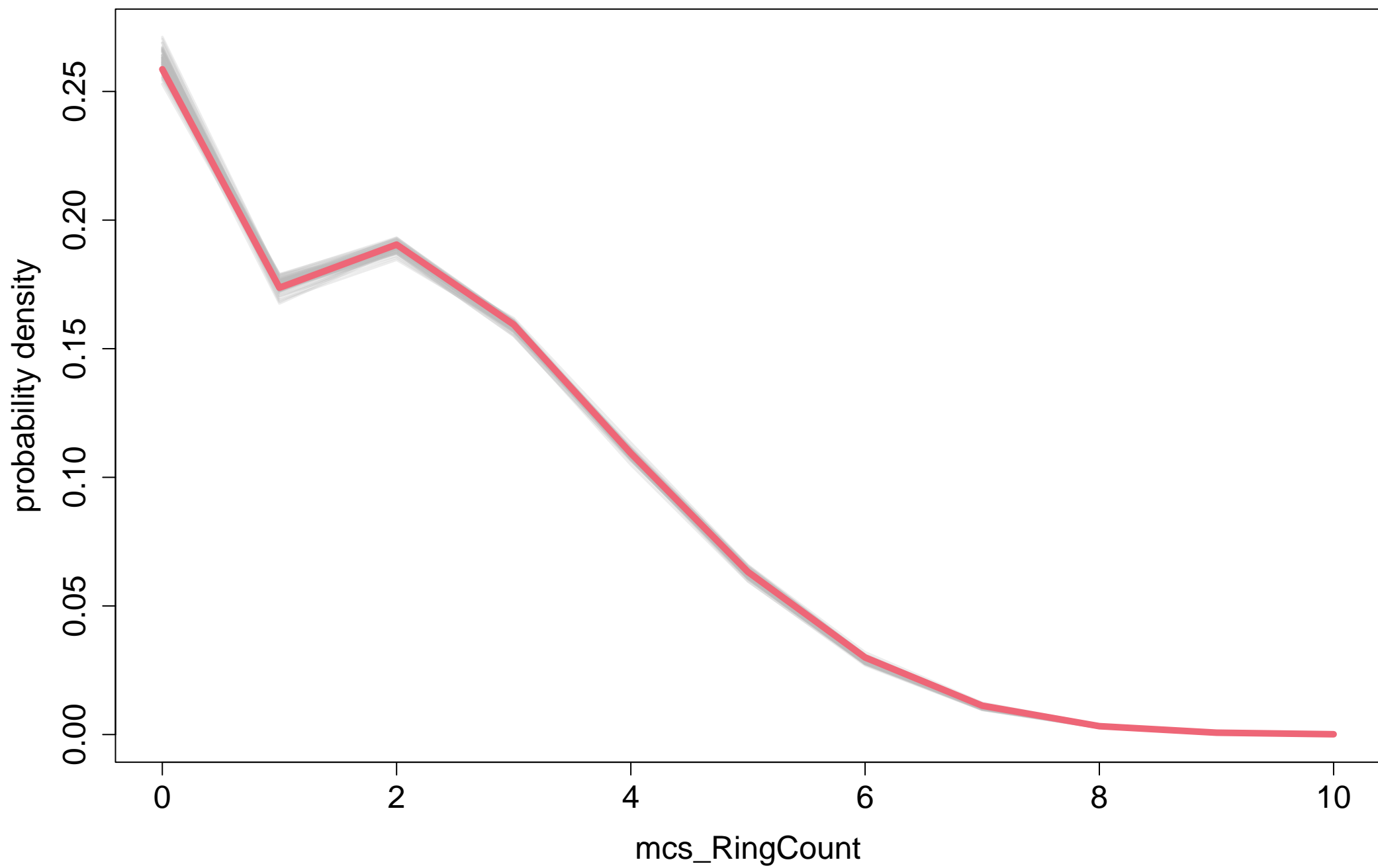


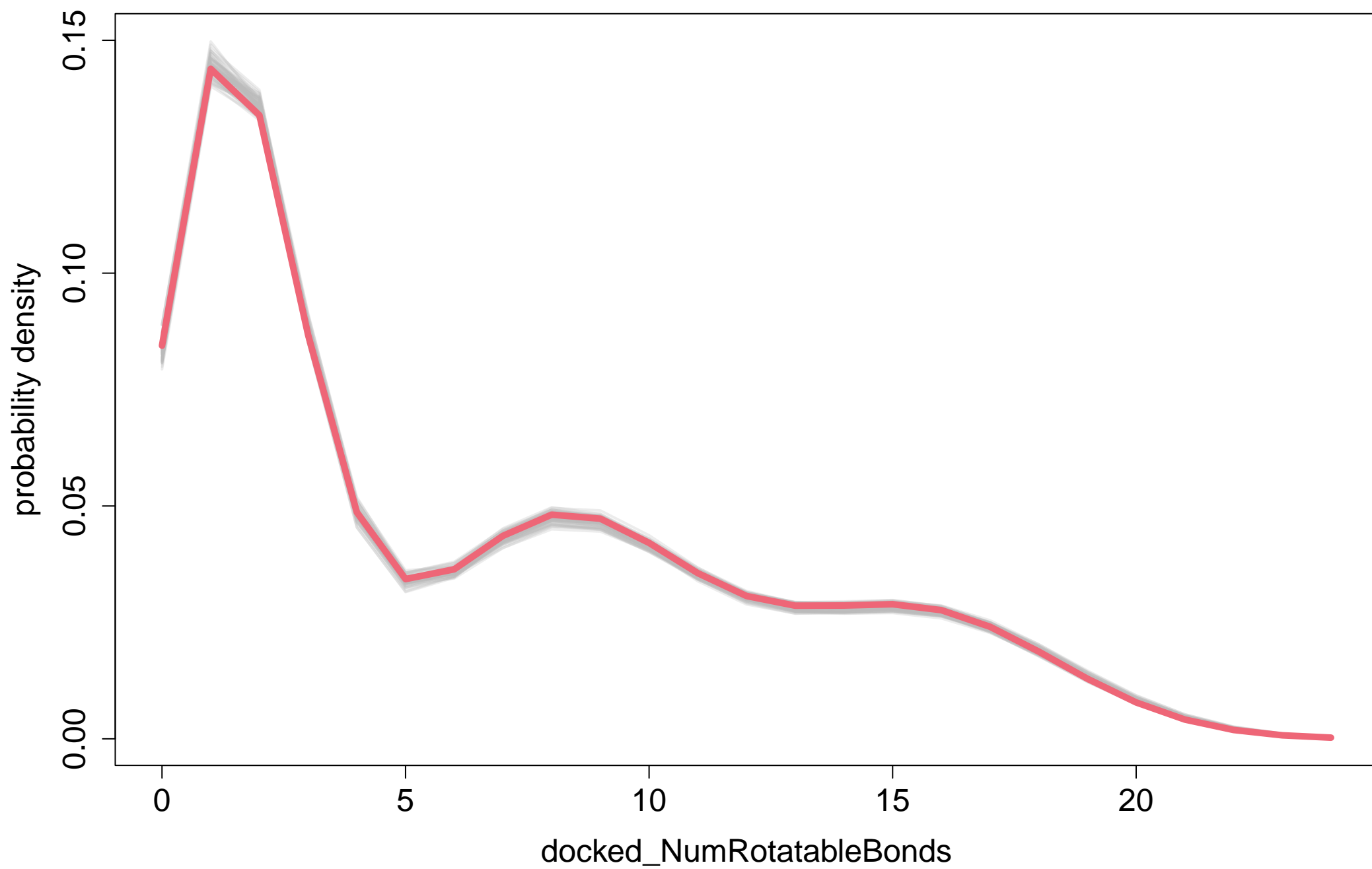


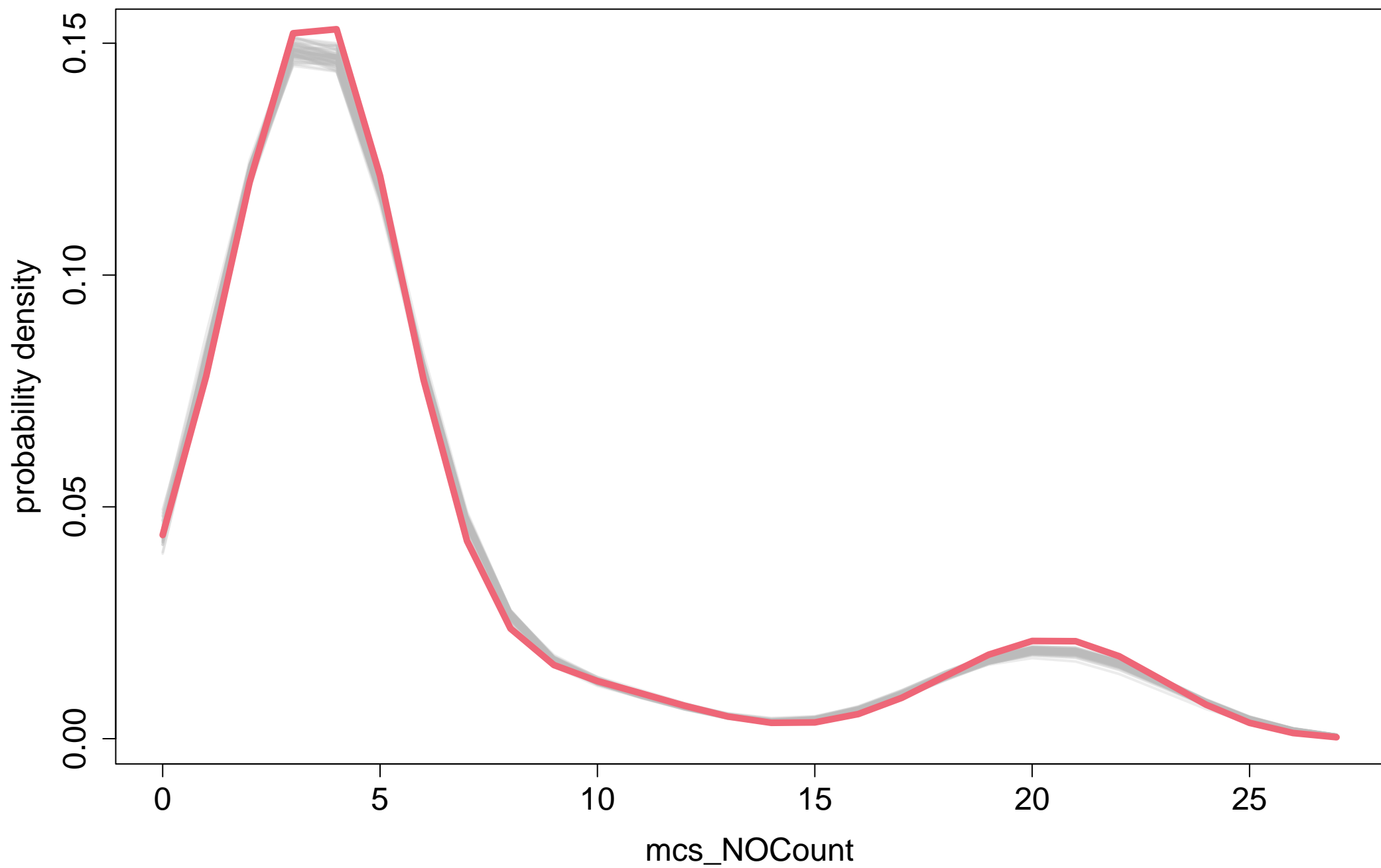


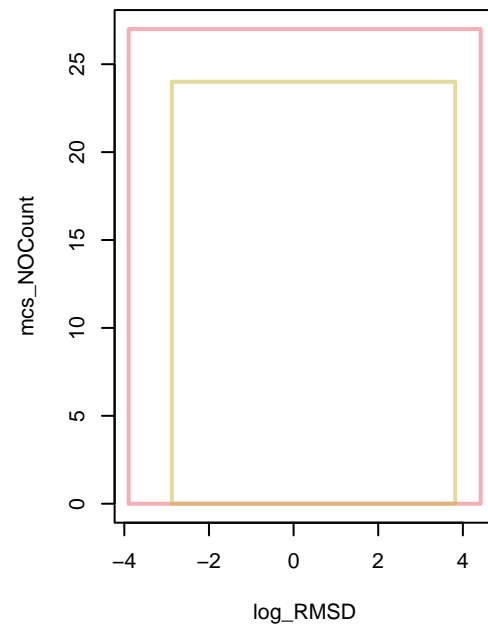
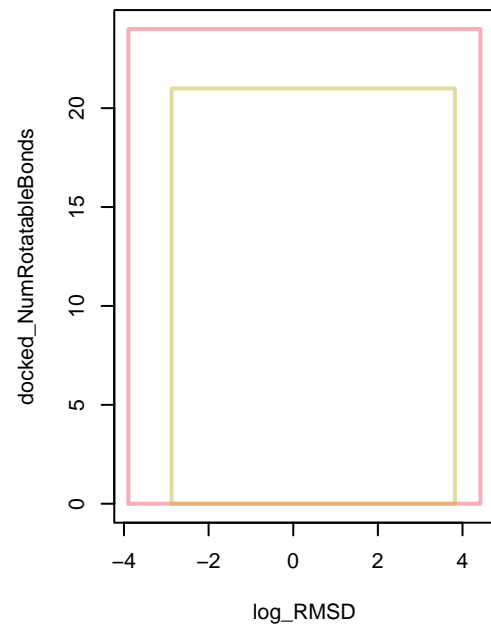
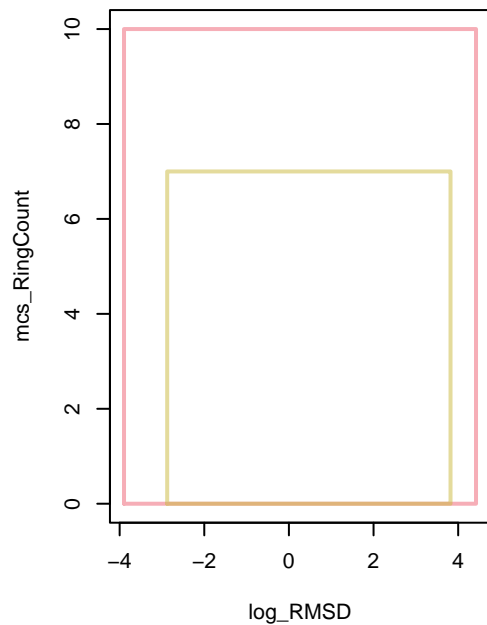
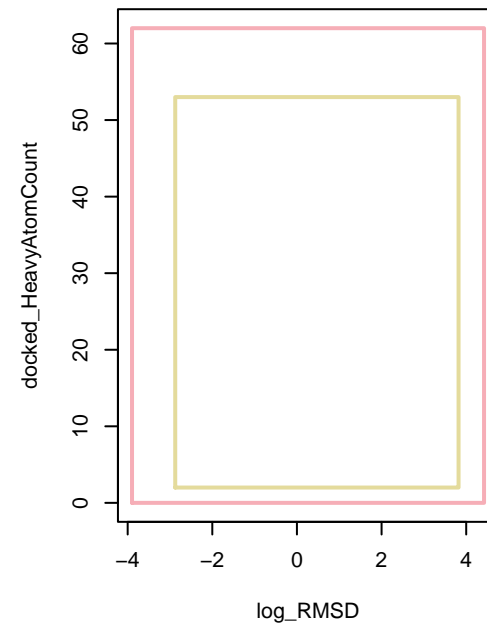
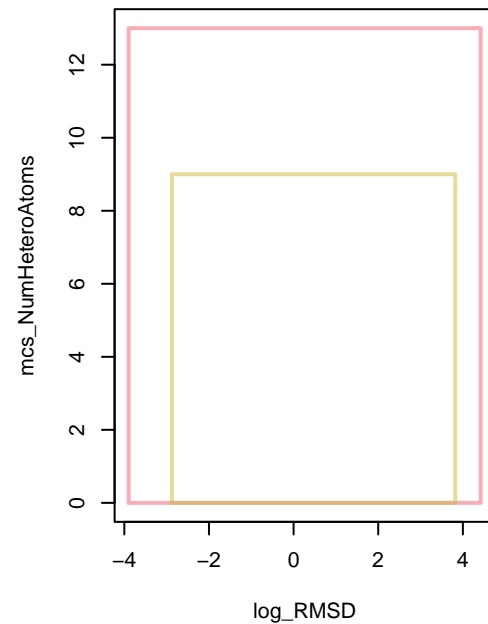
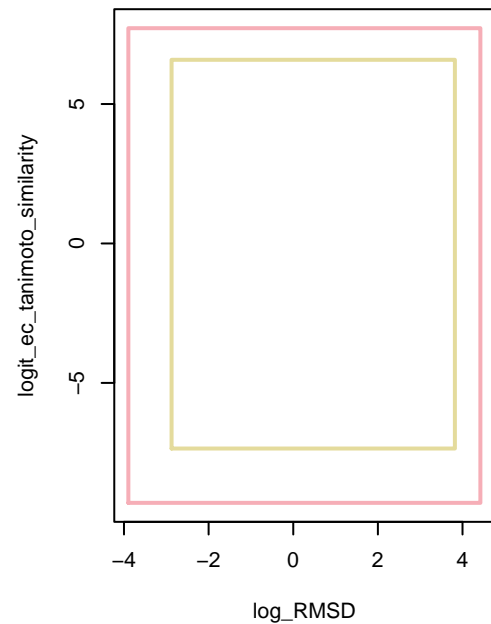
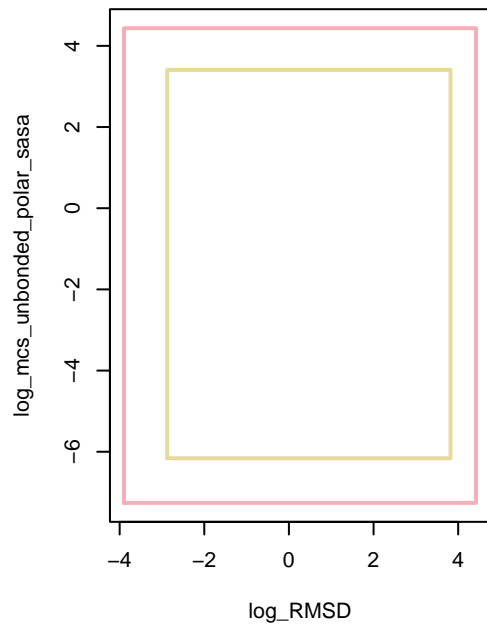




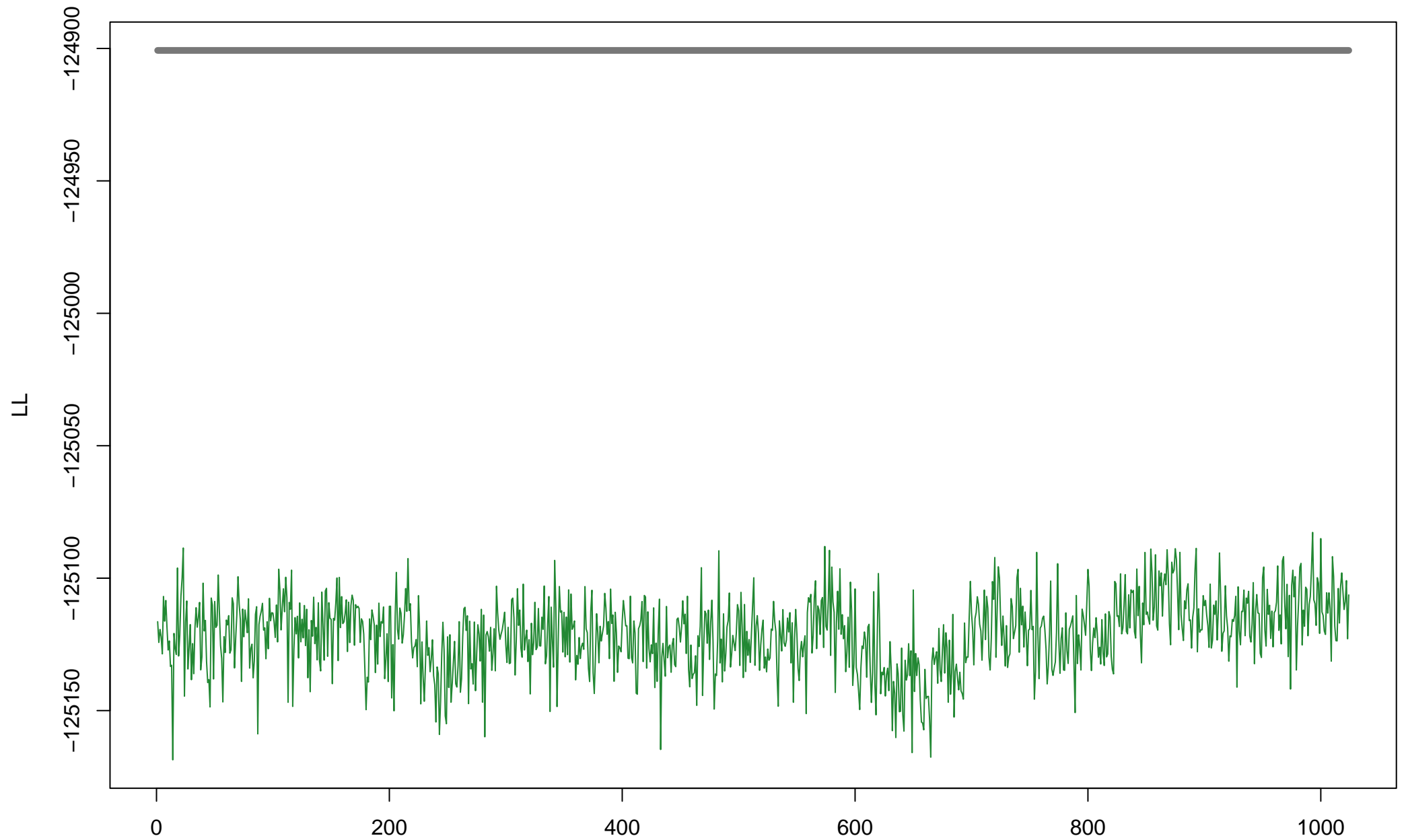






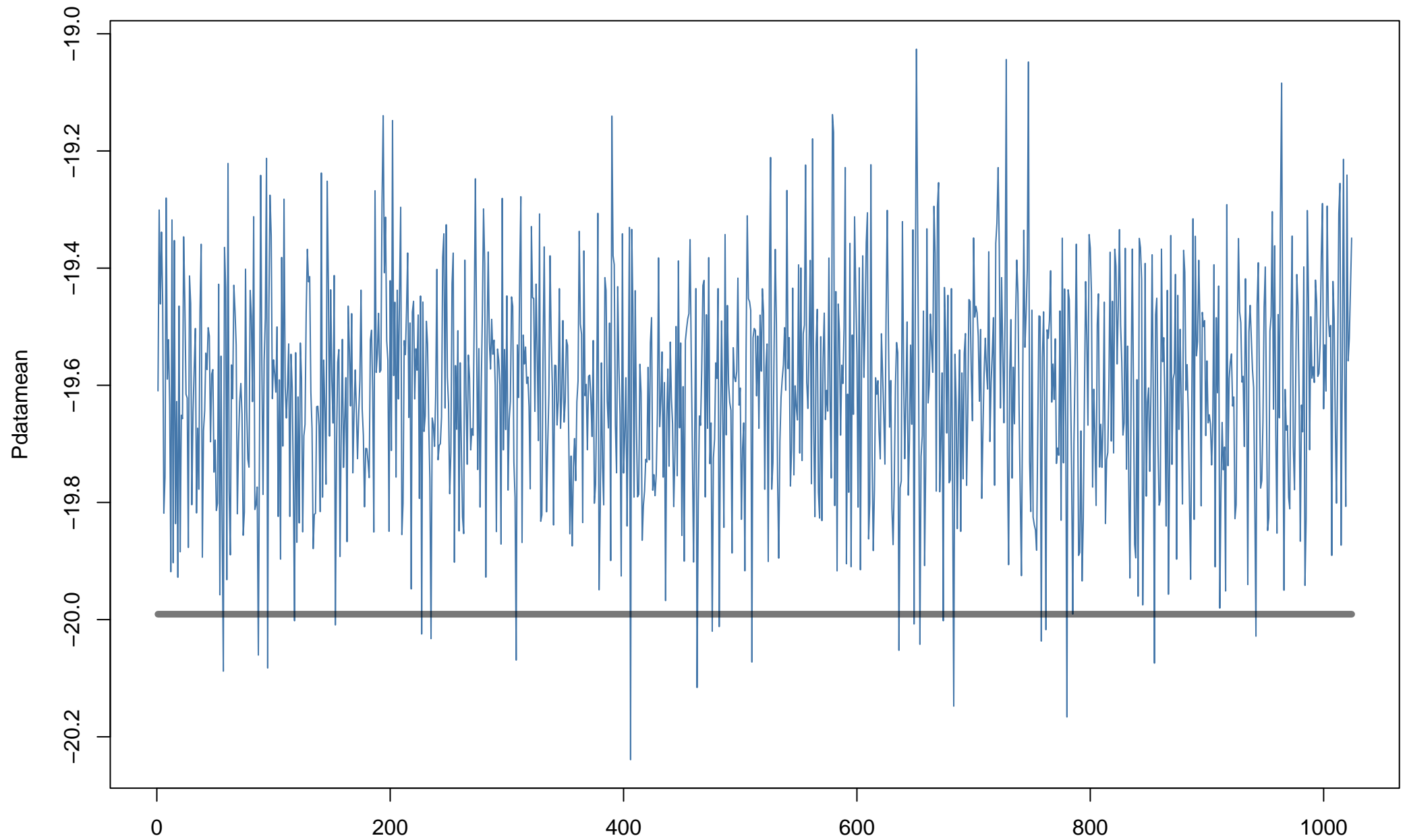


LL



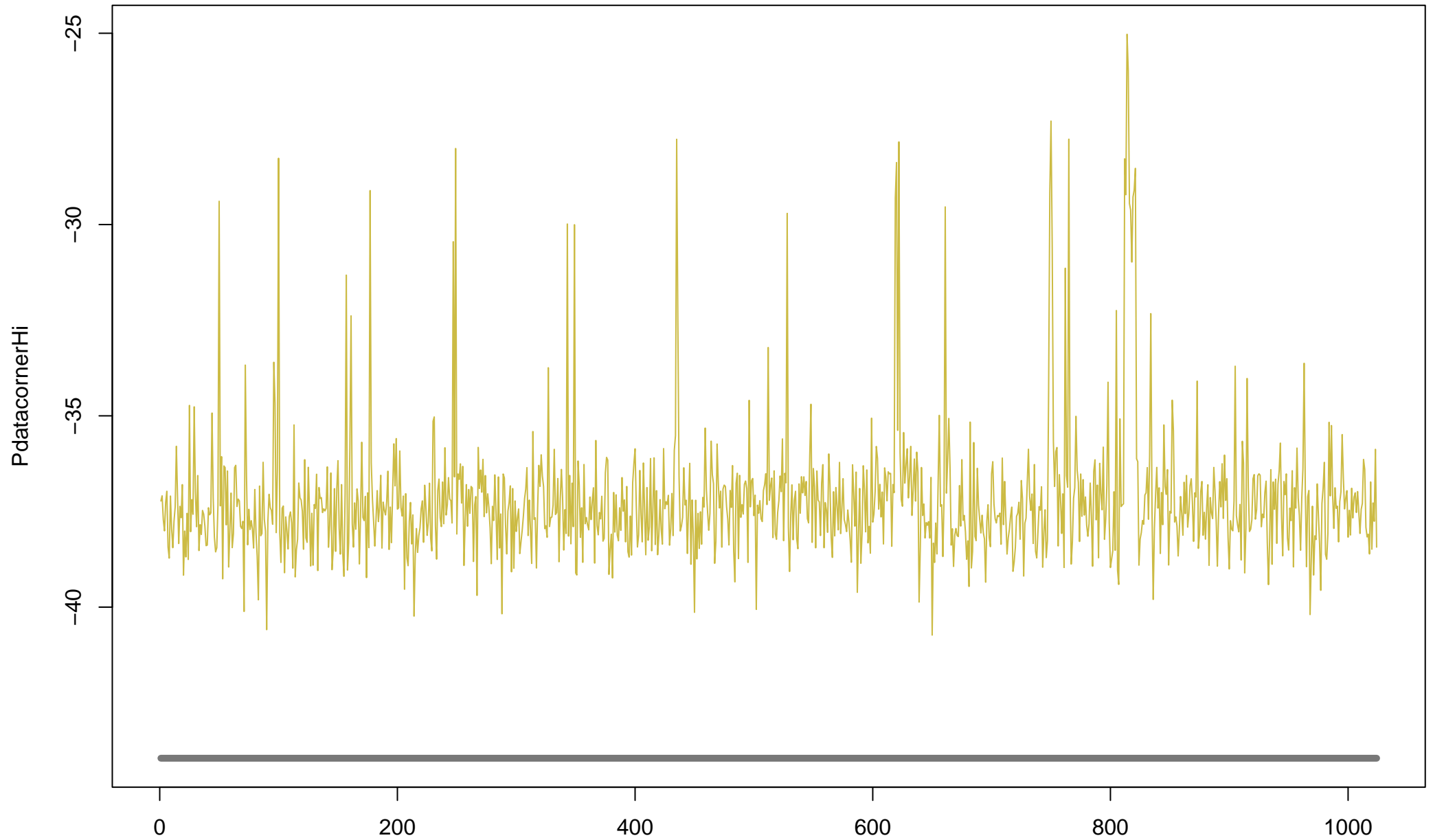
Pdatamean

ESS = 2.22e-16 | BMK = 0.0659 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0 | percentile: 2.25



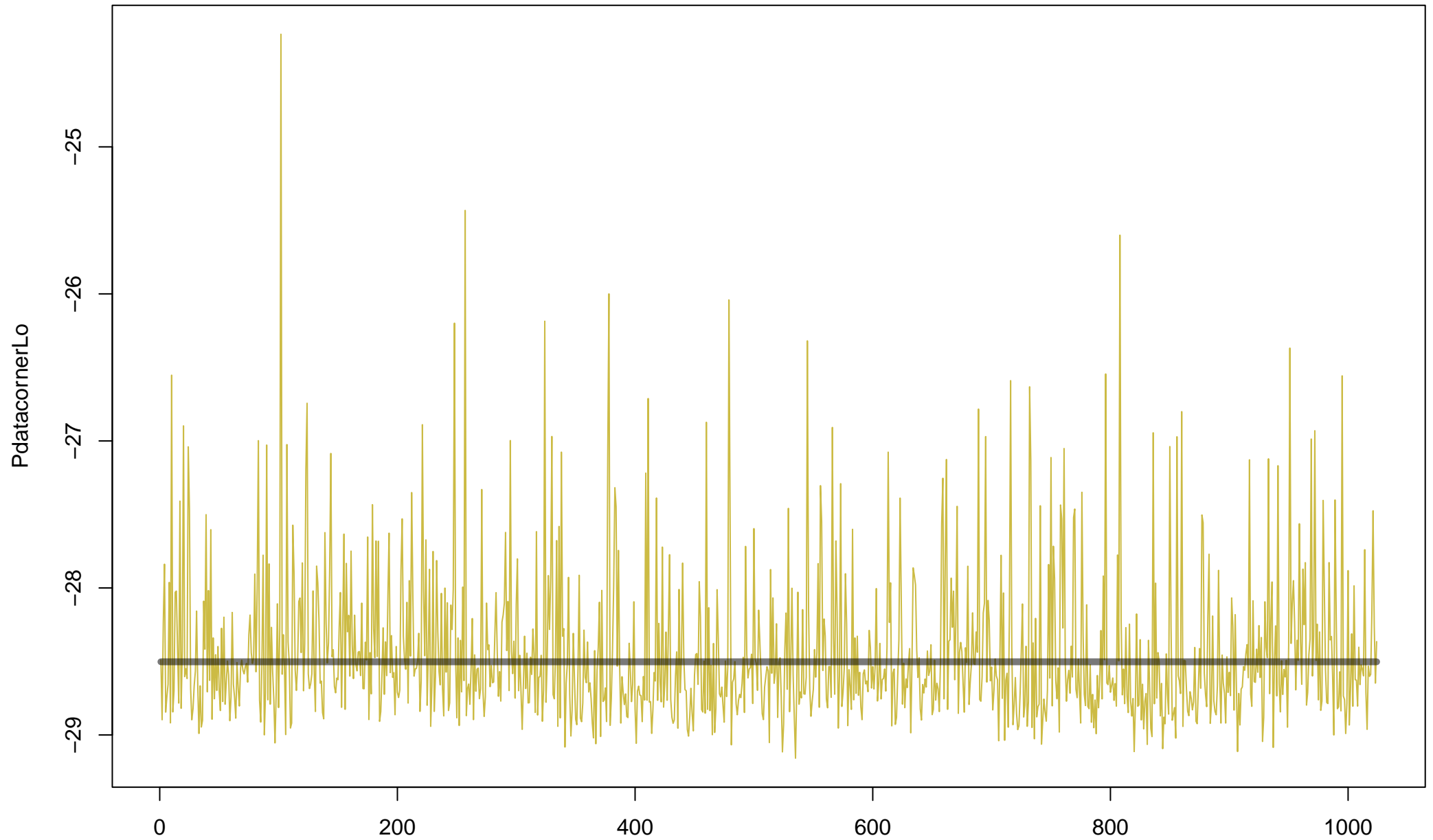
PdatacornerHi

ESS = 2.22e-16 | BMK = 1 | MCSE(6.27) = 4.39 | stat: TRUE | burn: 1020 | percentile: 0



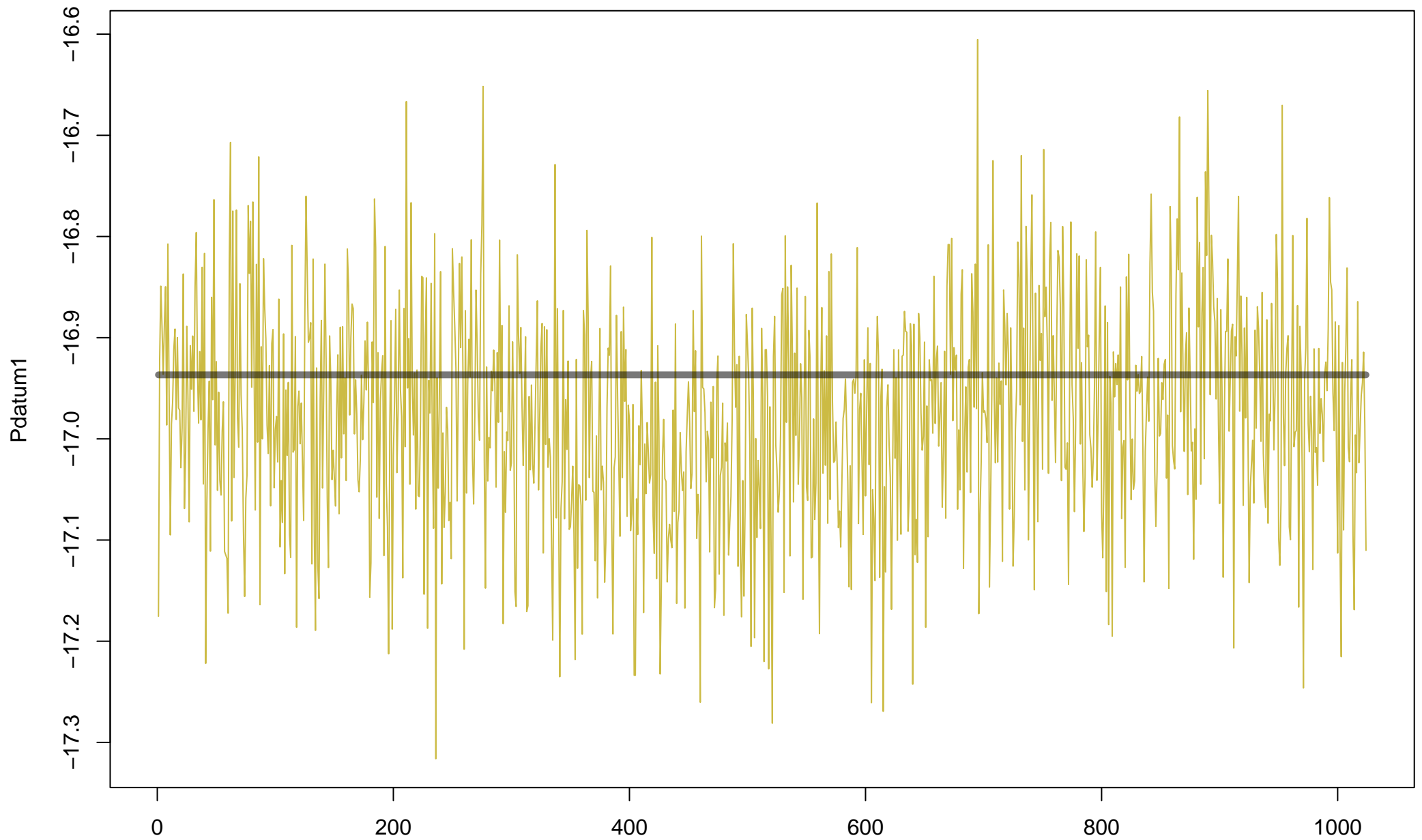
PdatacornerLo

ESS = 2.22e-16 | BMK = 0.137 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | percentile: 59.6



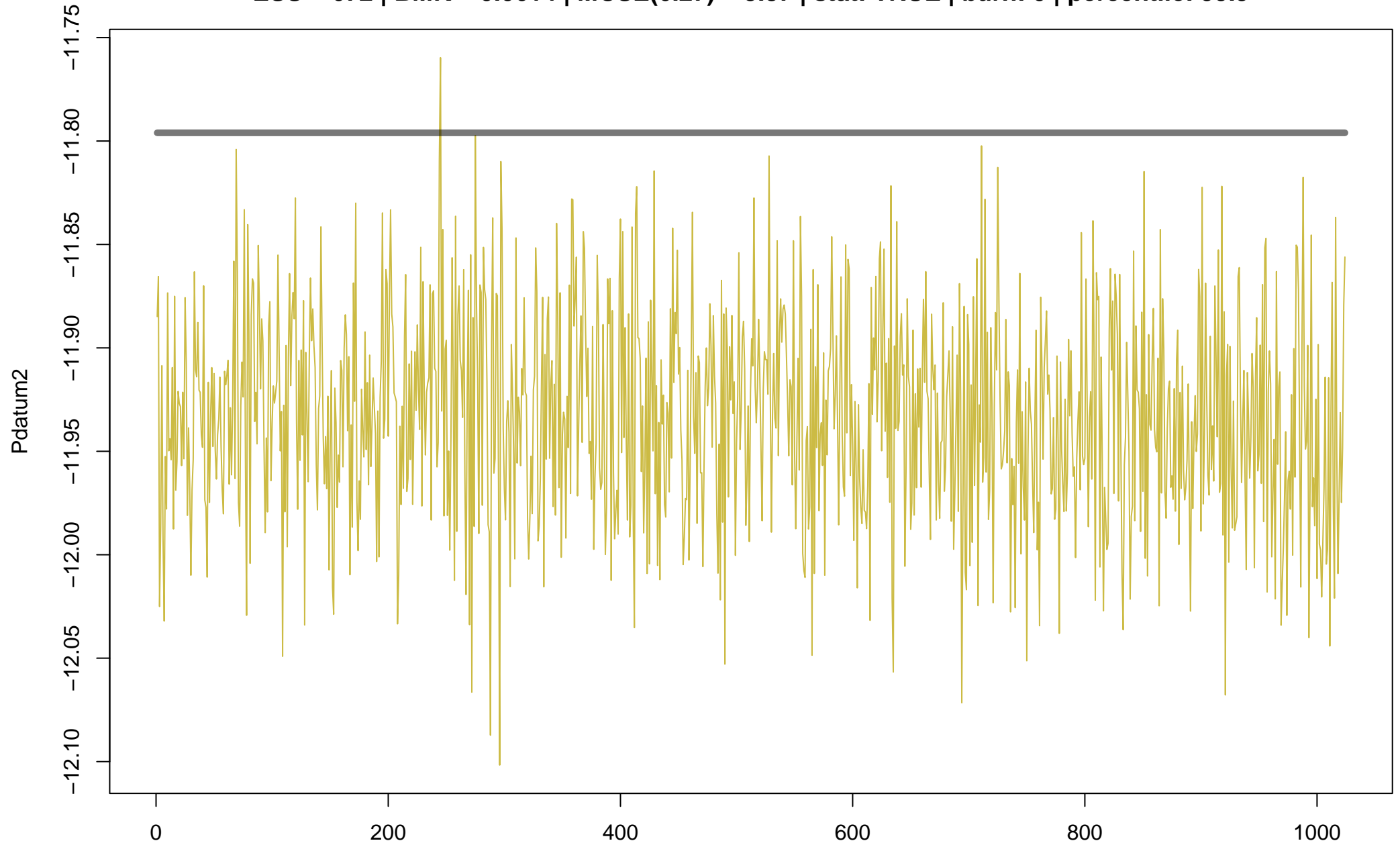
Pdatum1

ESS = 2.22e-16 | BMK = 0.0791 | MCSE(6.27) = 5.47 | stat: TRUE | burn: 0 | percentile: 64.6



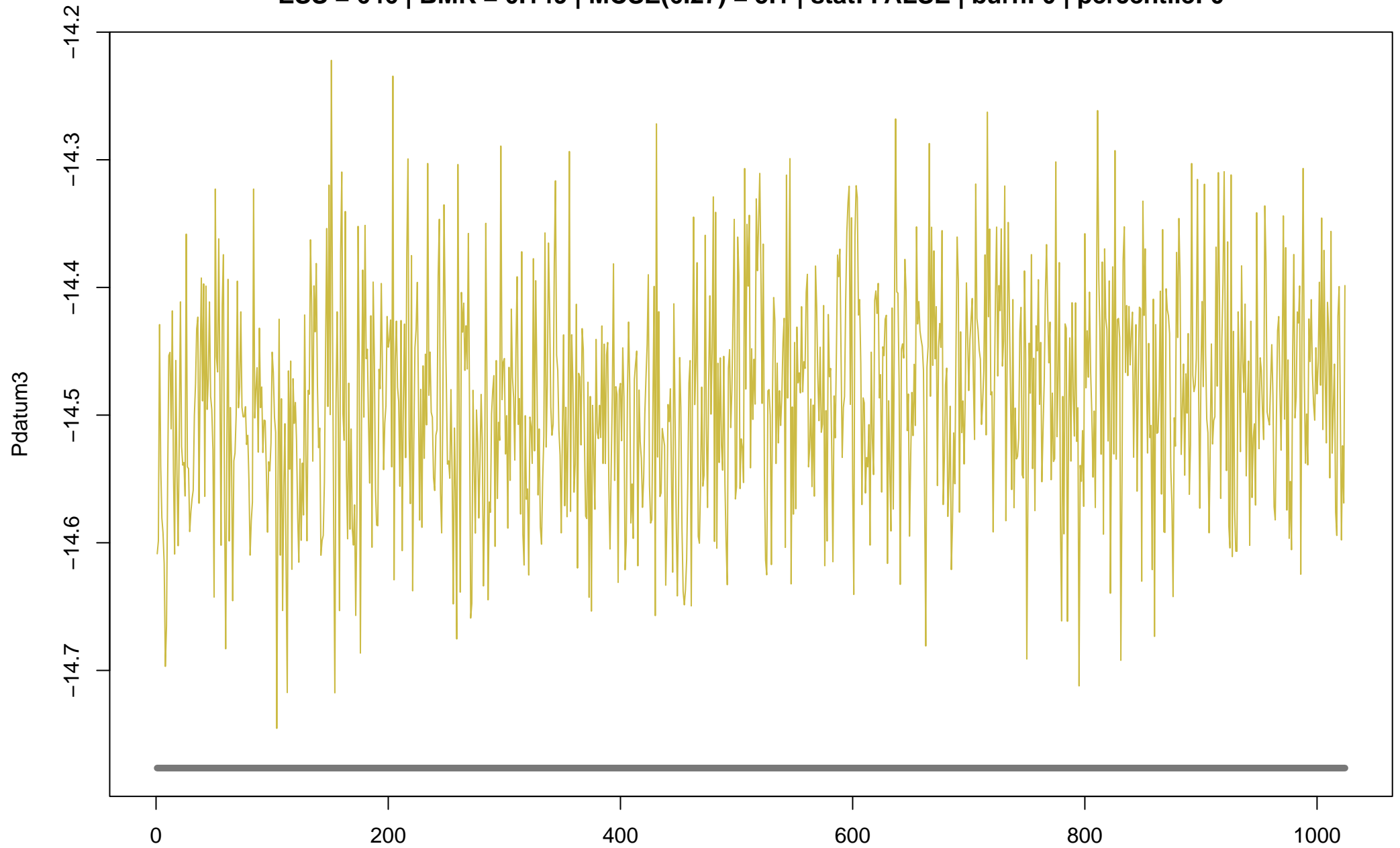
Pdatum2

ESS = 672 | BMK = 0.0614 | MCSE(6.27) = 3.87 | stat: TRUE | burn: 0 | percentile: 99.9



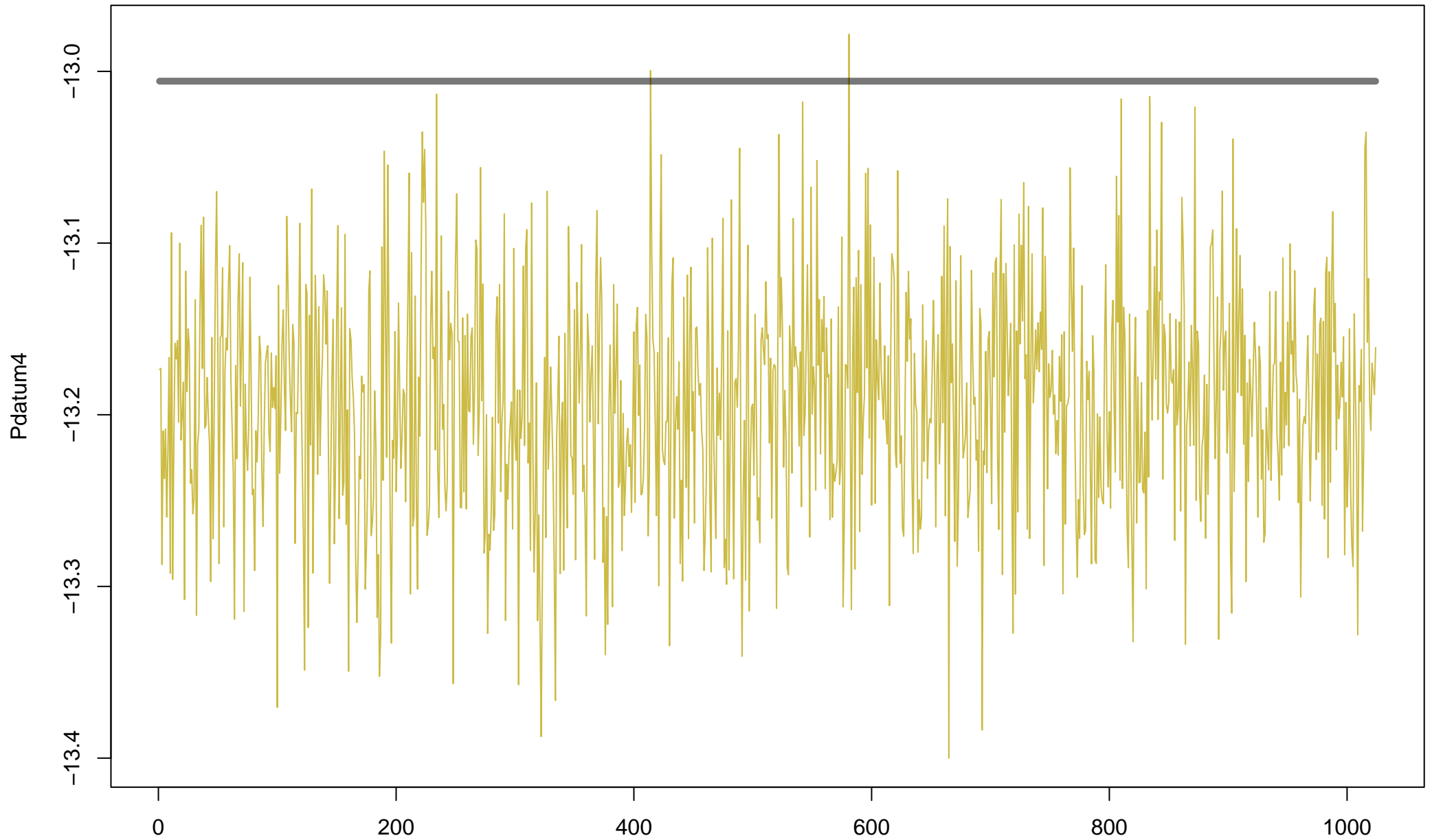
Pdatum3

ESS = 646 | BMK = 0.149 | MCSE(6.27) = 5.1 | stat: FALSE | burn: 0 | percentile: 0



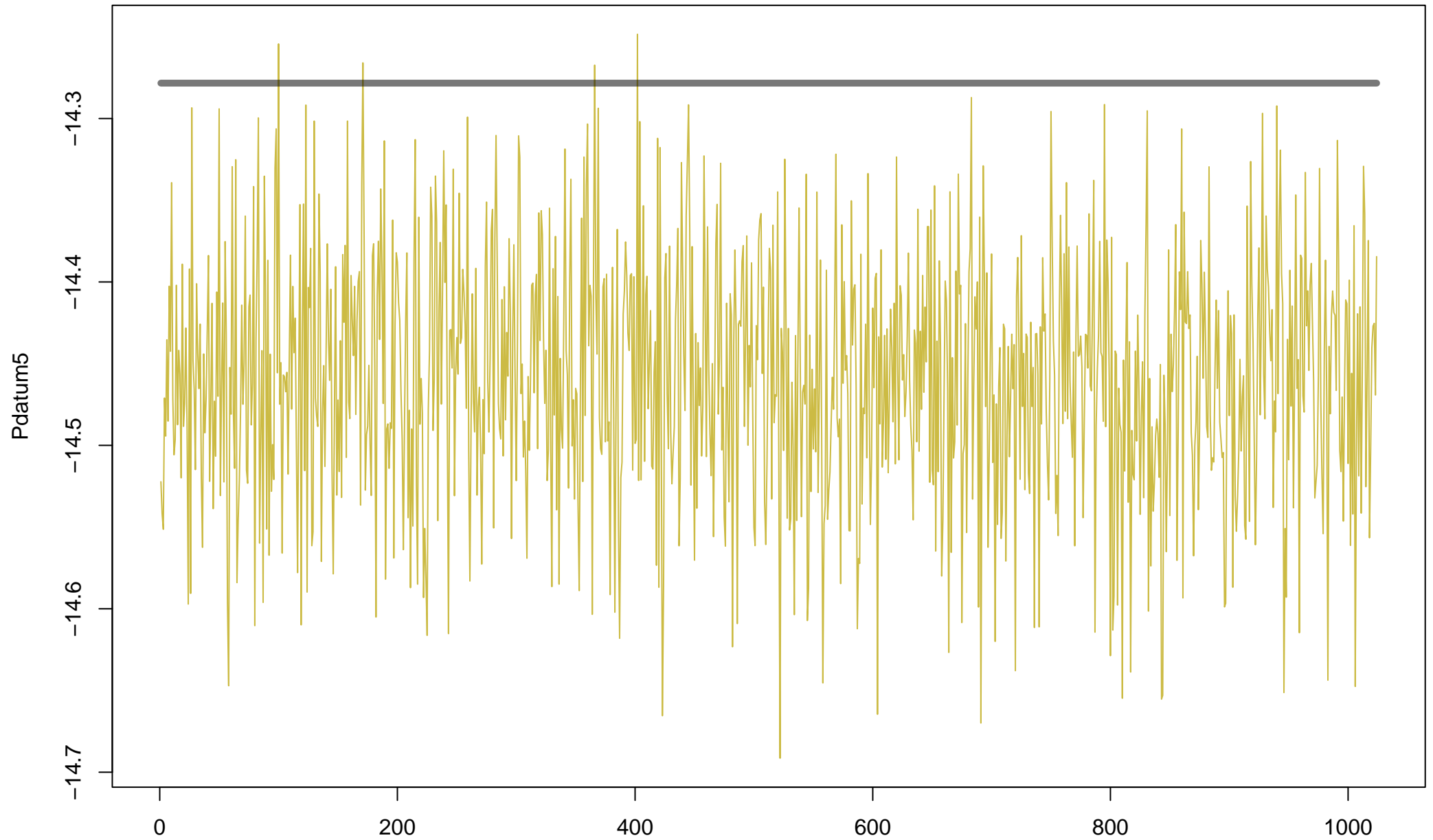
Pdatum4

ESS = 1020 | BMK = 0.0916 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 0 | percentile: 99.8



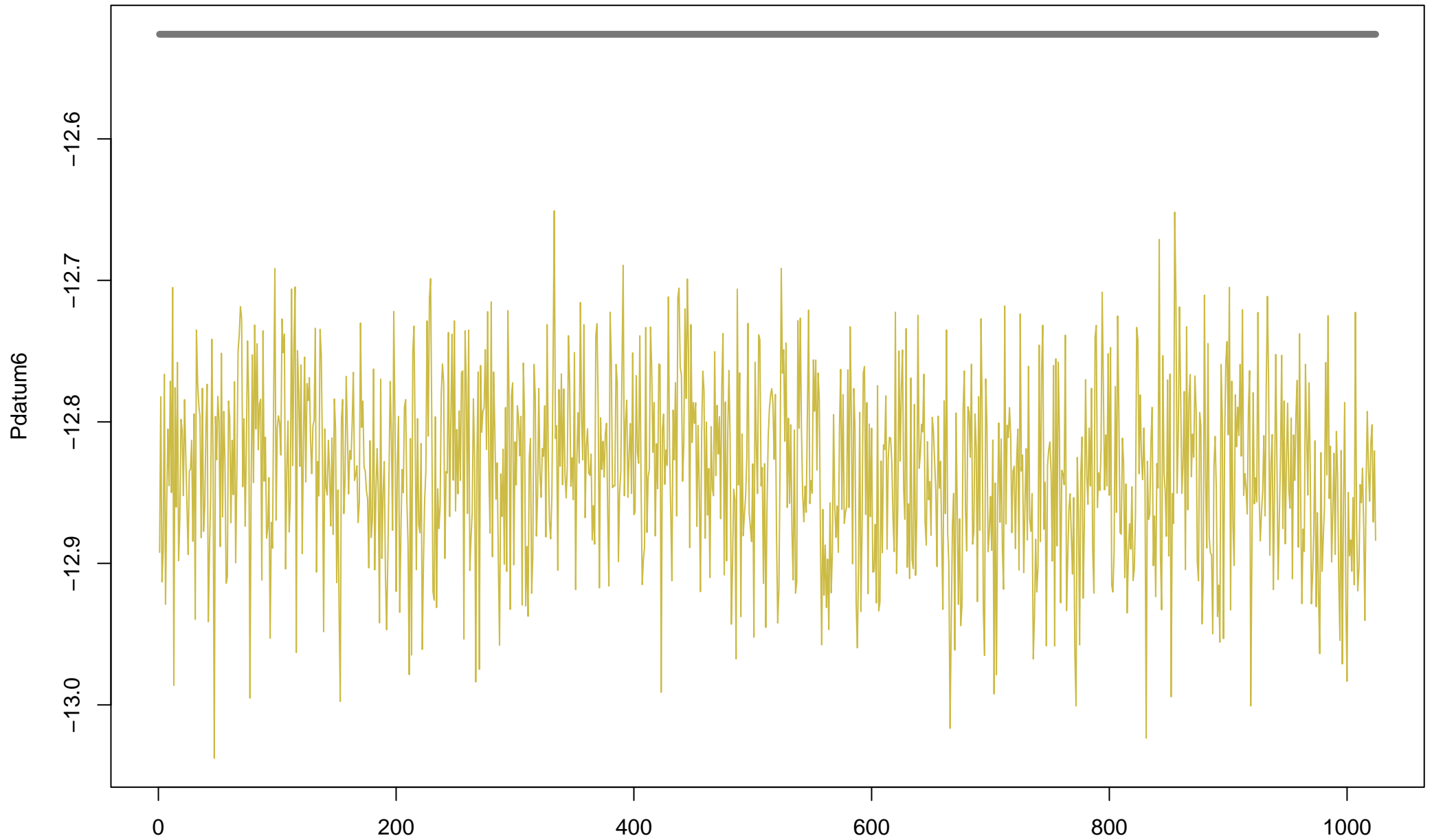
Pdatum5

ESS = 1020 | BMK = 0.0855 | MCSE(6.27) = 3.29 | stat: TRUE | burn: 0 | percentile: 99.6



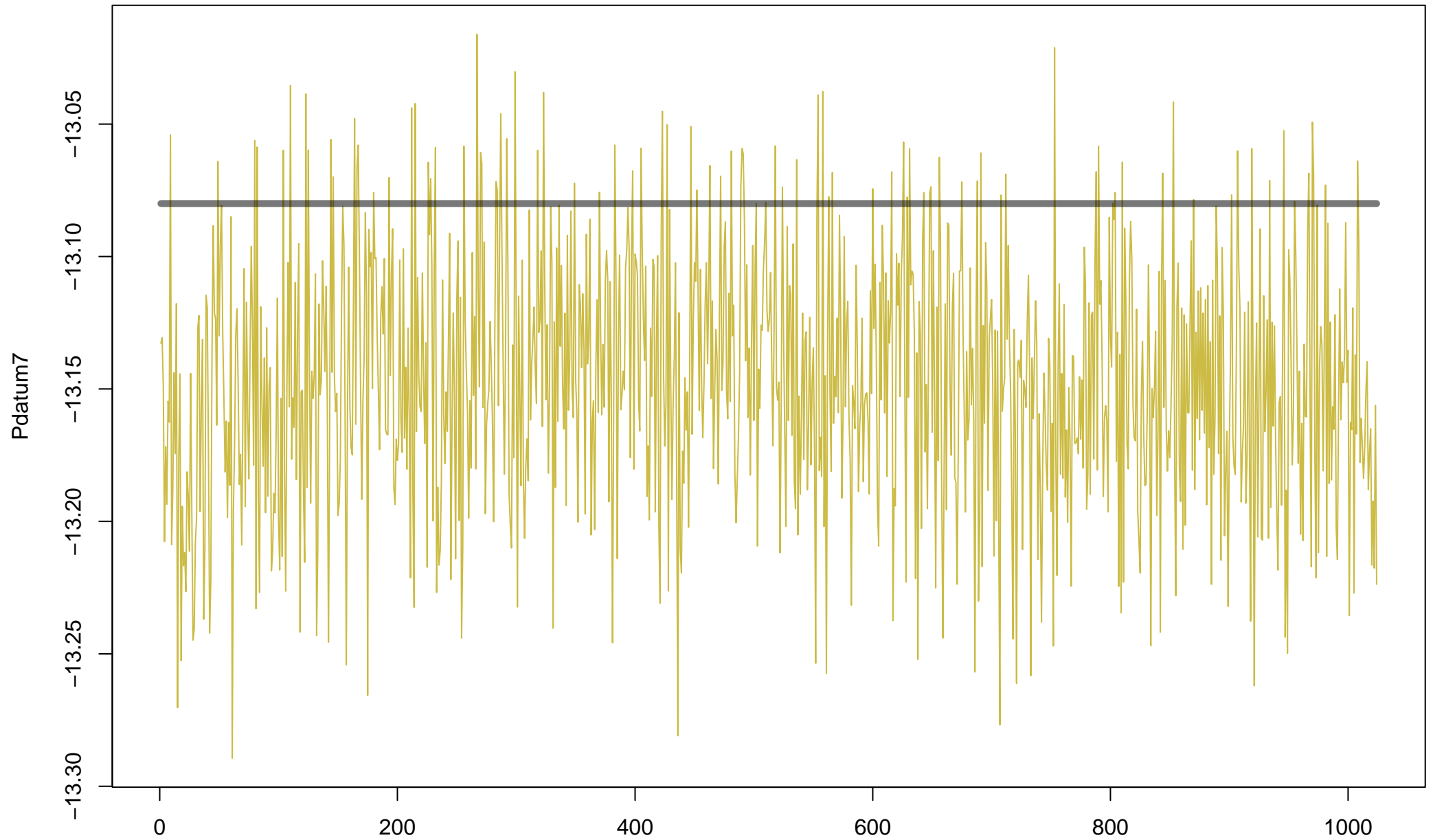
Pdatum6

ESS = 775 | BMK = 0.103 | MCSE(6.27) = 4.54 | stat: FALSE | burn: 0 | percentile: 100



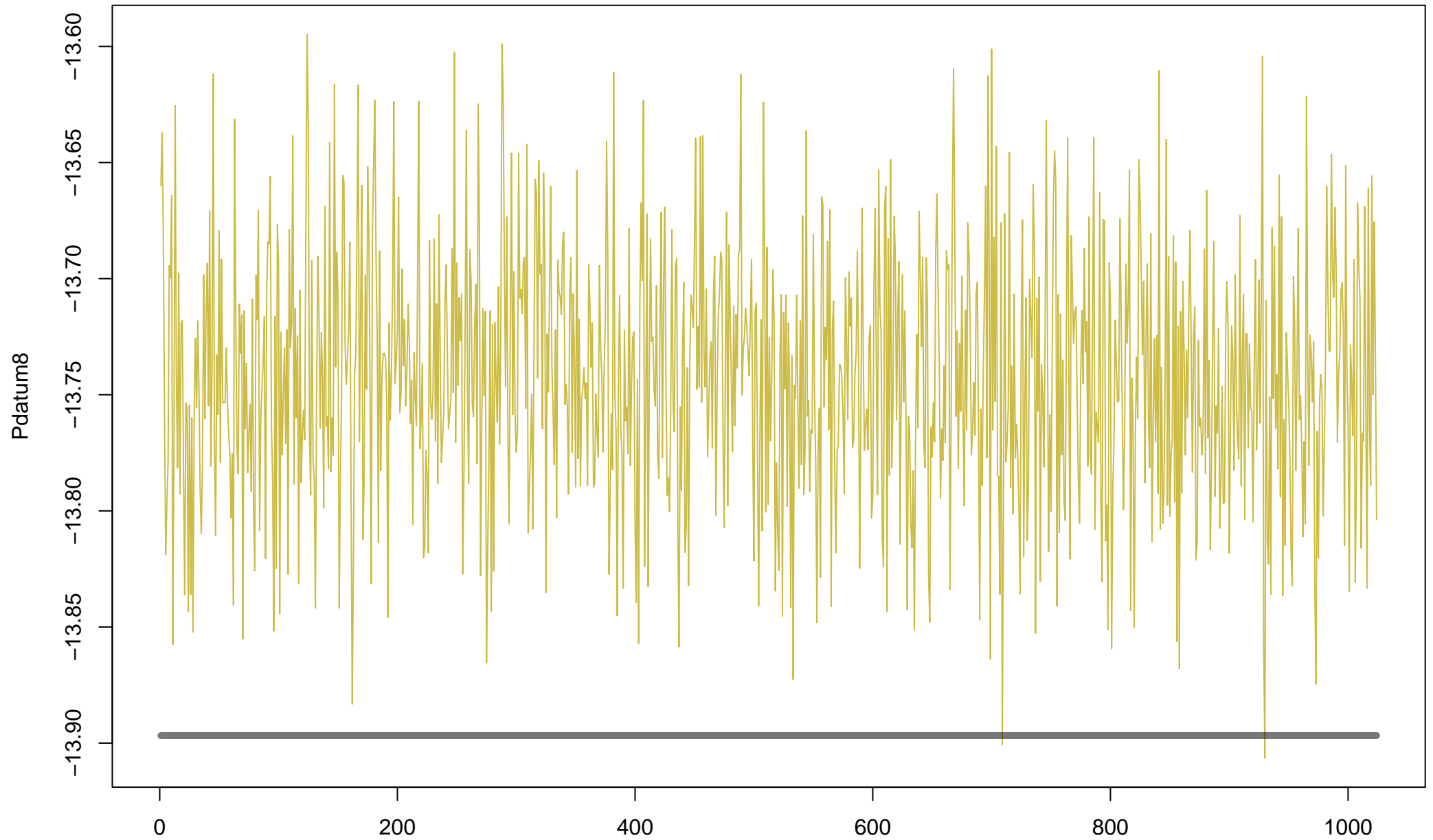
Pdatum7

ESS = 696 | BMK = 0.0599 | MCSE(6.27) = 4.51 | stat: FALSE | burn: 0 | percentile: 91.4



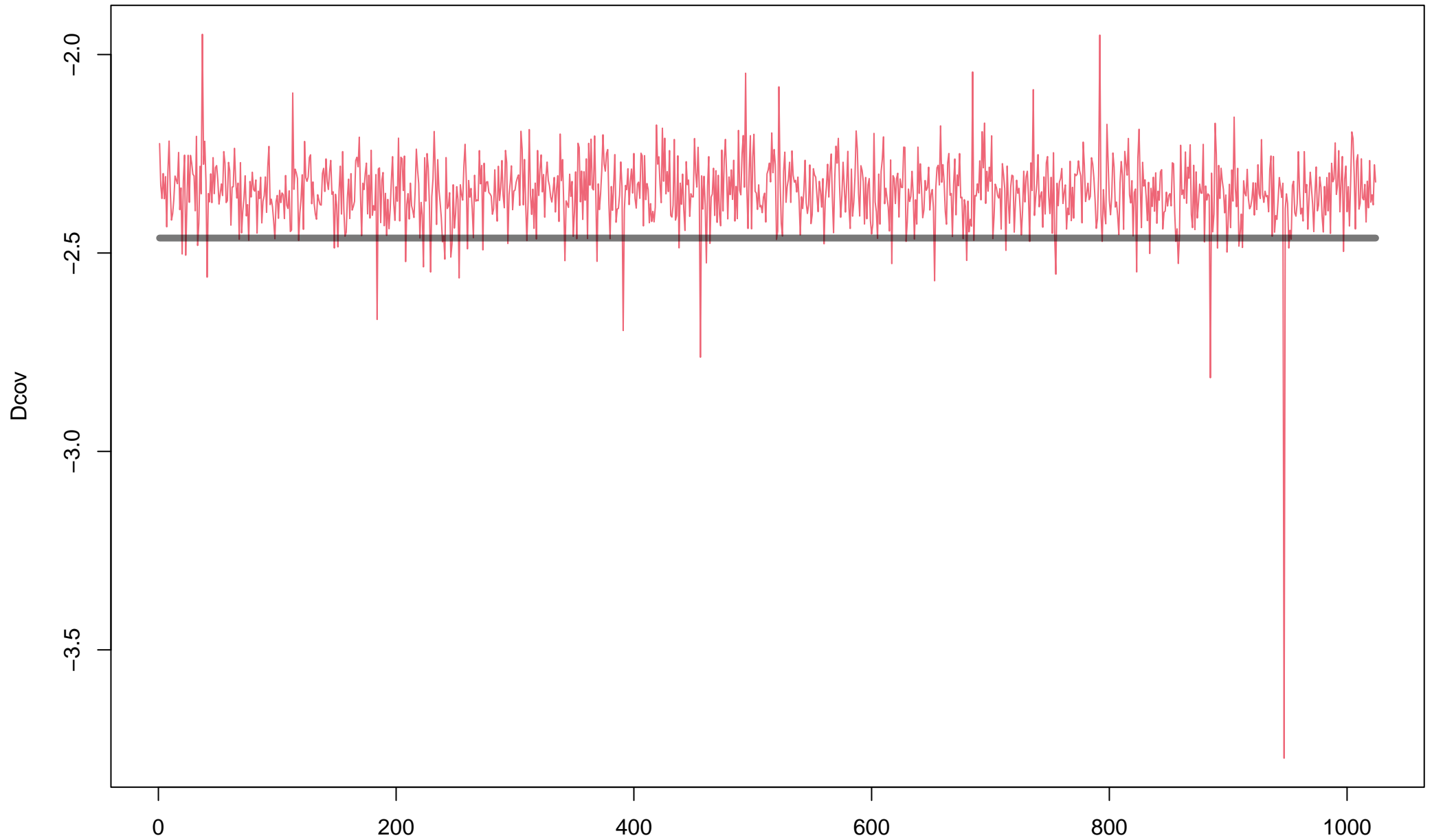
Pdatum8

ESS = 1020 | BMK = 0.0687 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 0 | percentile: 0.195



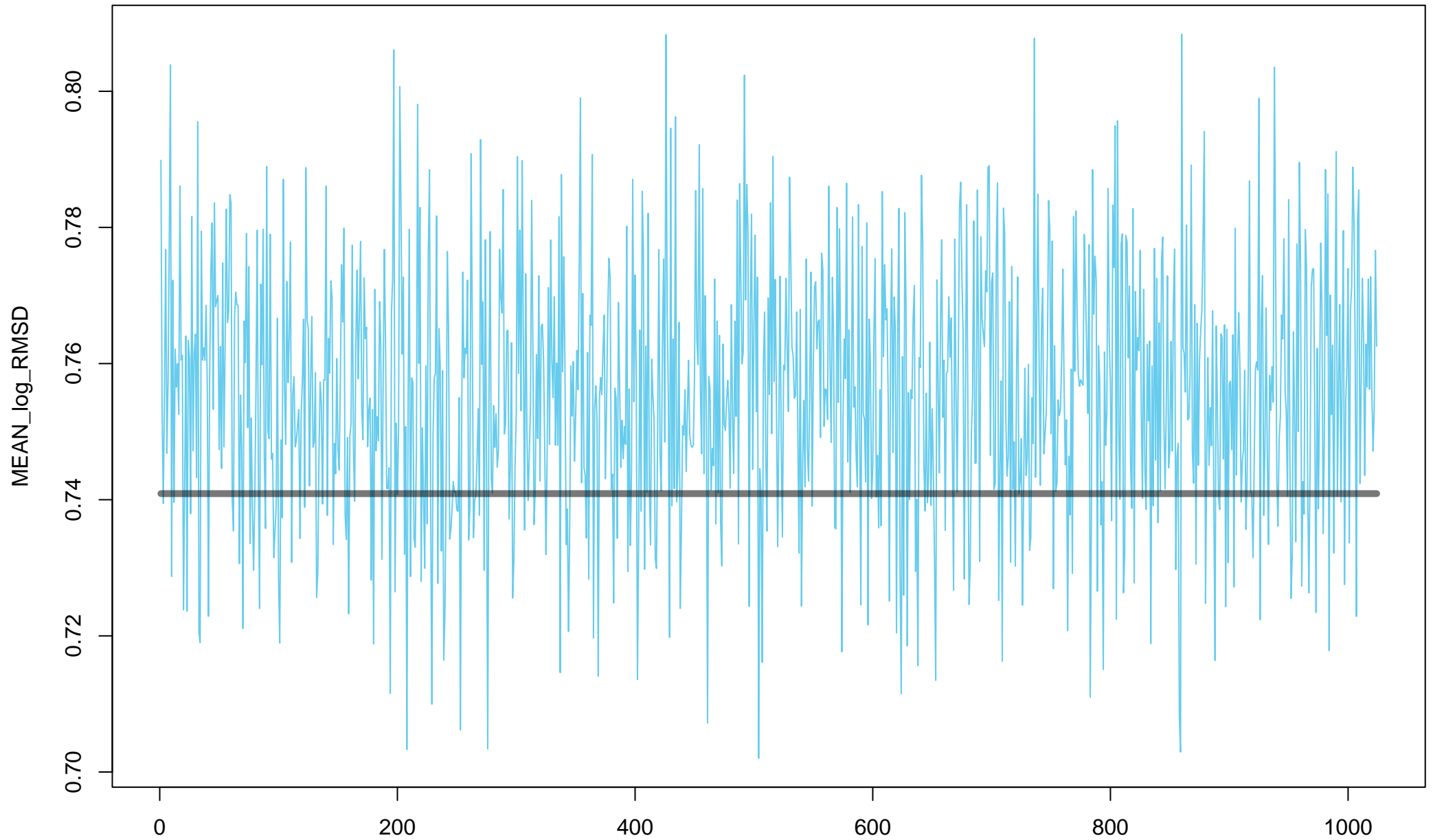
Dcov

ESS = 1020 | BMK = 0.0841 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0 | percentile: 93.8

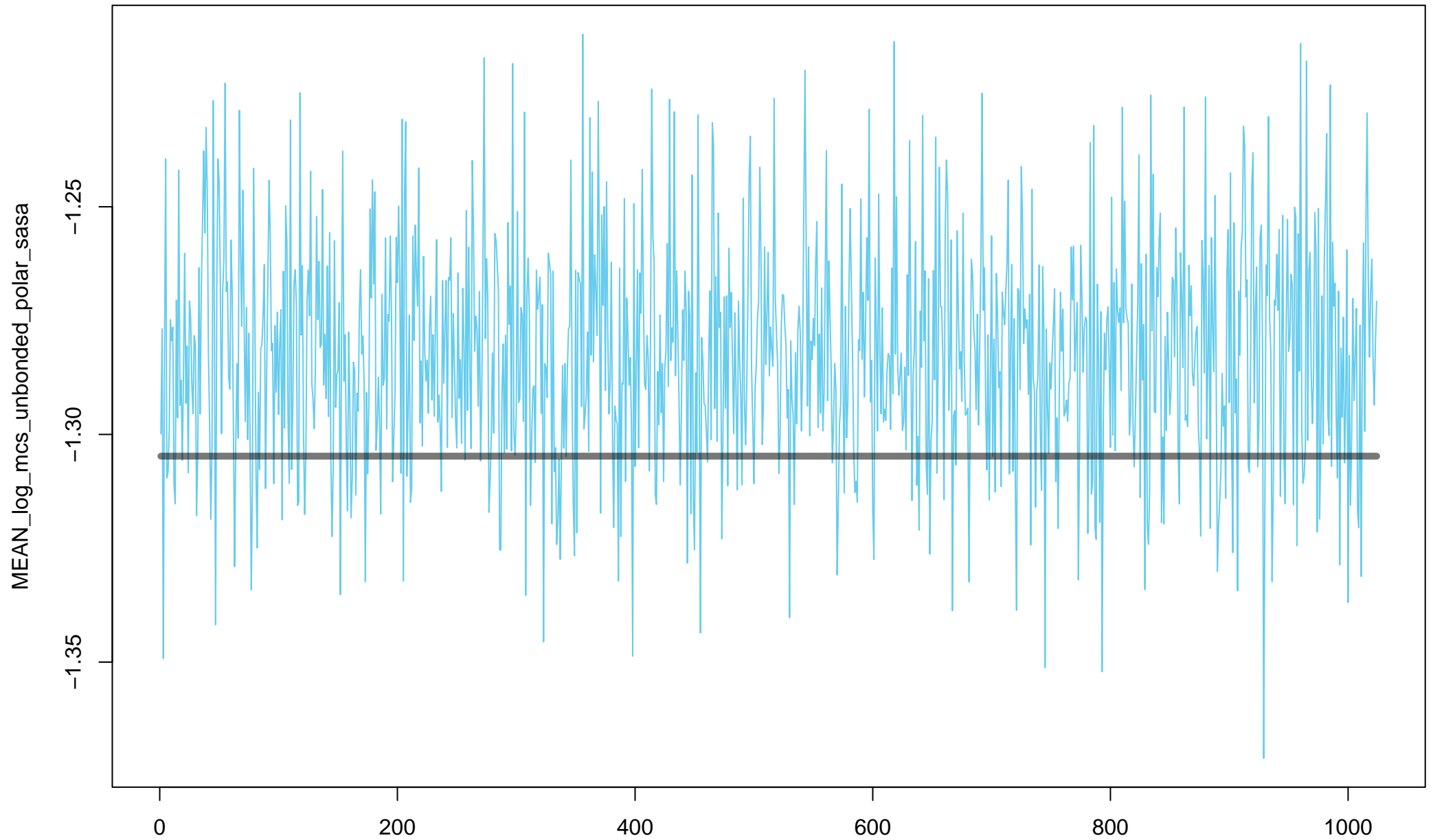


MEAN_log_RMSD

ESS = 1020 | BMK = 0.0529 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0 | percentile: 20.9

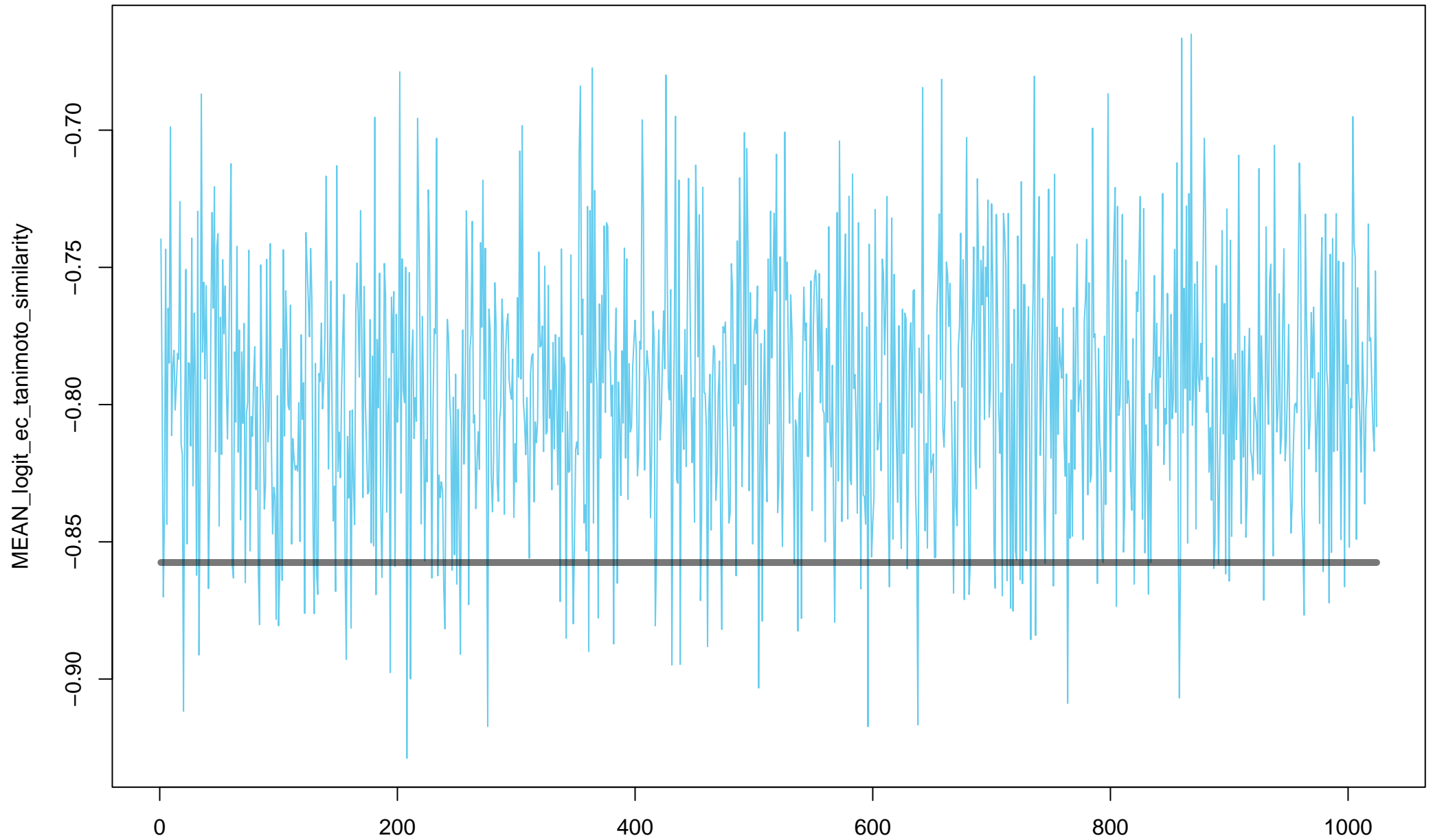


MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0354 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0 | percentile: 17



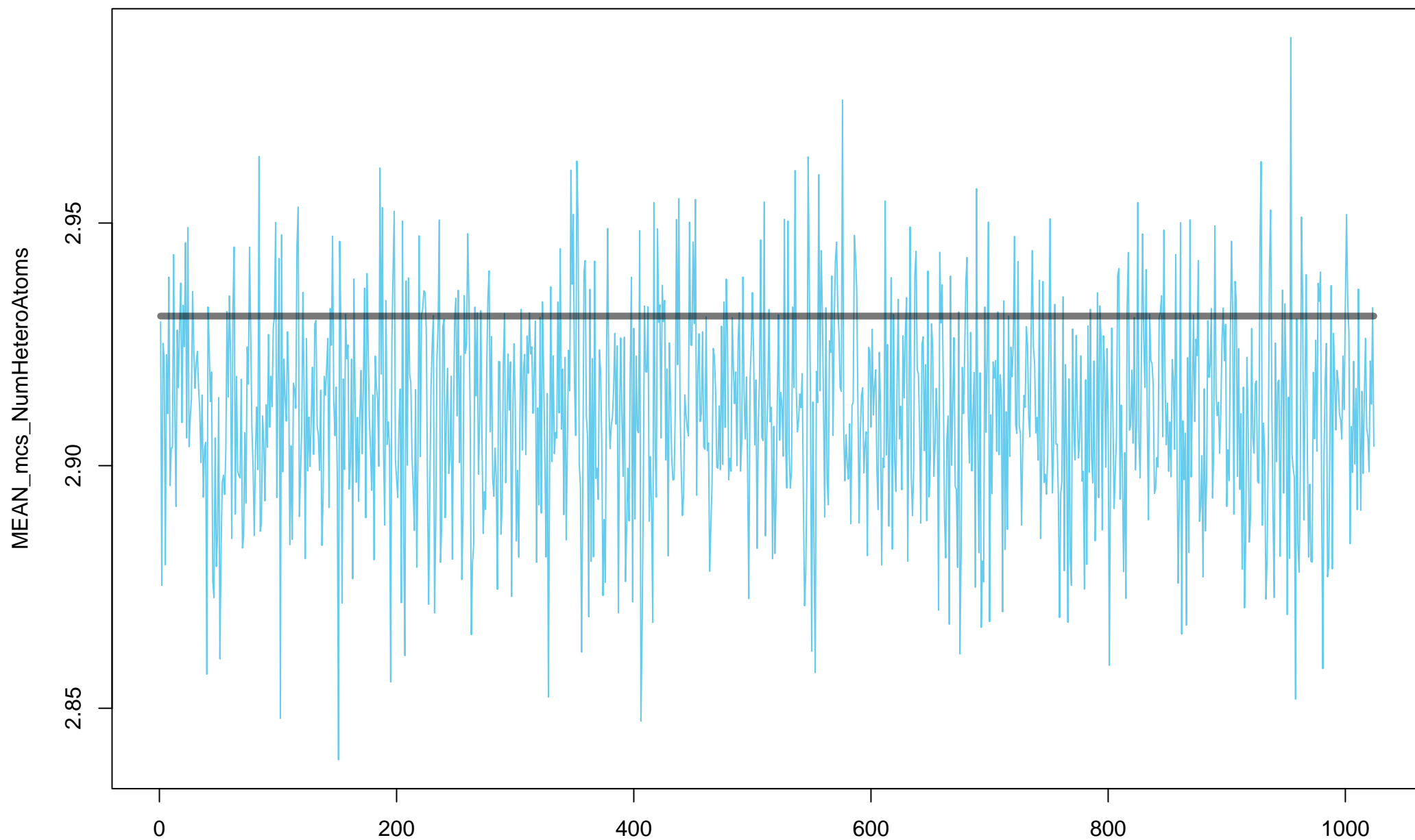
MEAN_logit_ec_tanimoto_similarity

ESS = 1020 | BMK = 0.0682 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 0 | percentile: 9.18



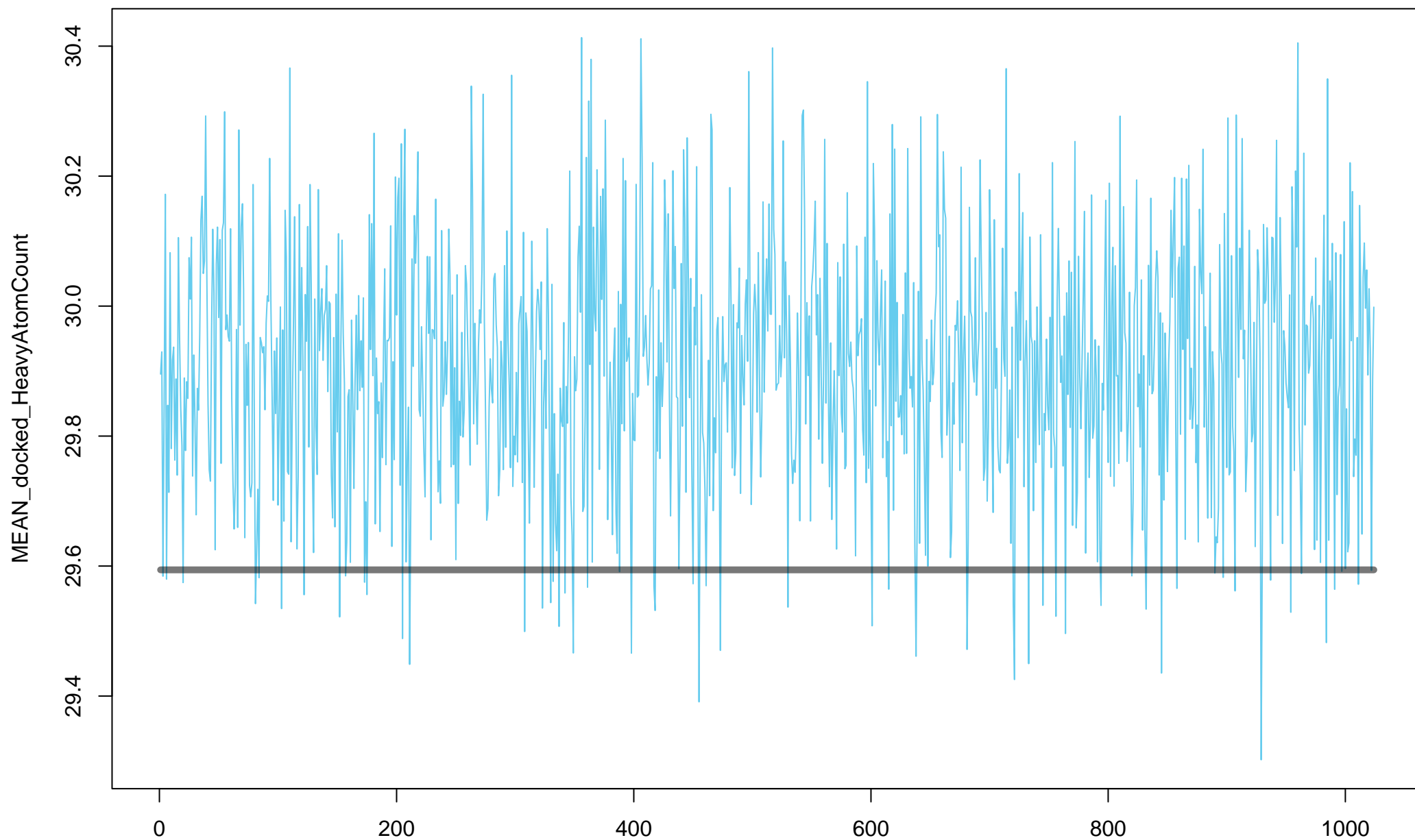
MEAN_mcs_NumHeteroAtoms

ESS = 1020 | BMK = 0.0502 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0 | percentile: 82

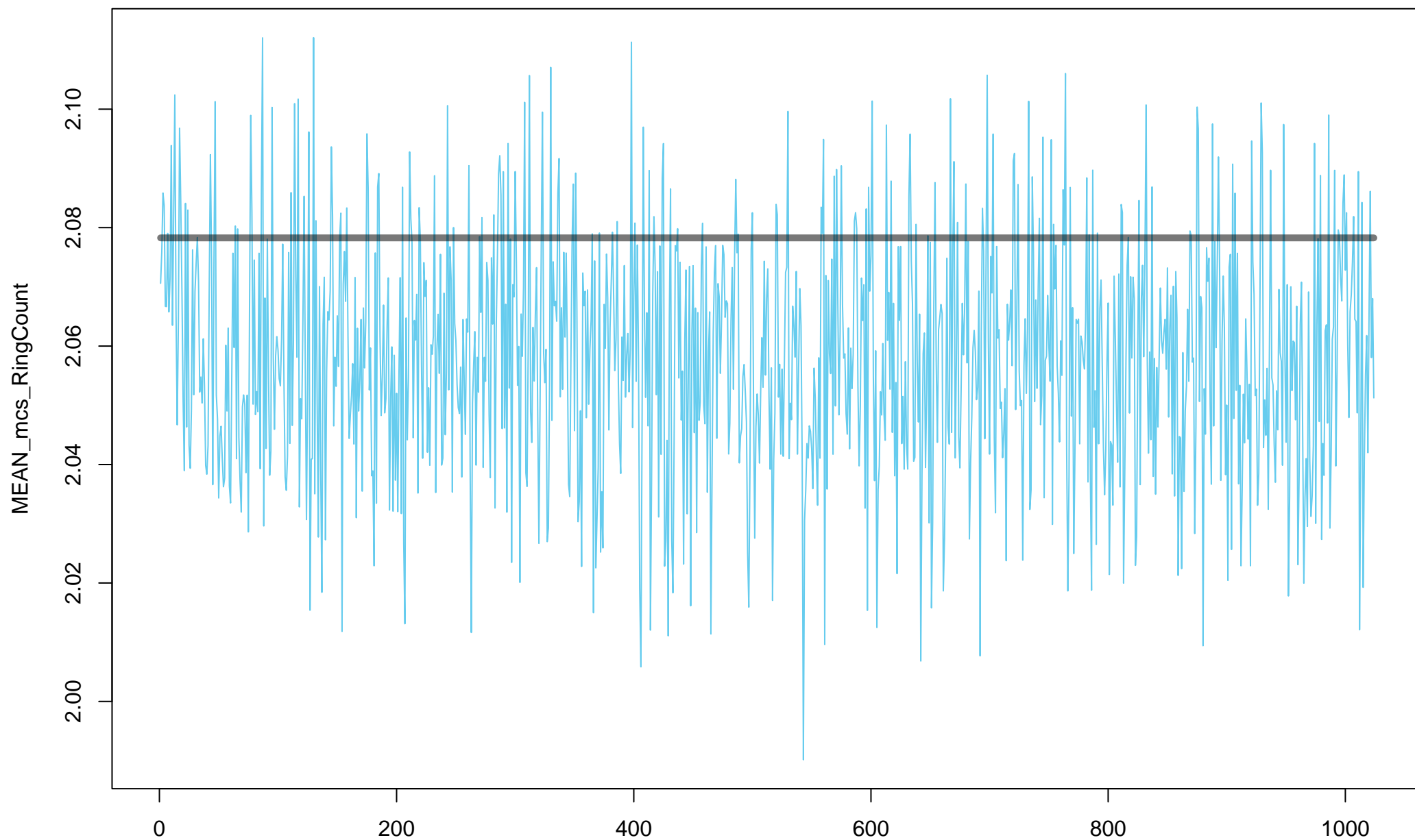


MEAN_docked_HeavyAtomCount

ESS = 1020 | BMK = 0.0252 | MCSE(6.27) = 3.44 | stat: TRUE | burn: 0 | percentile: 5.57

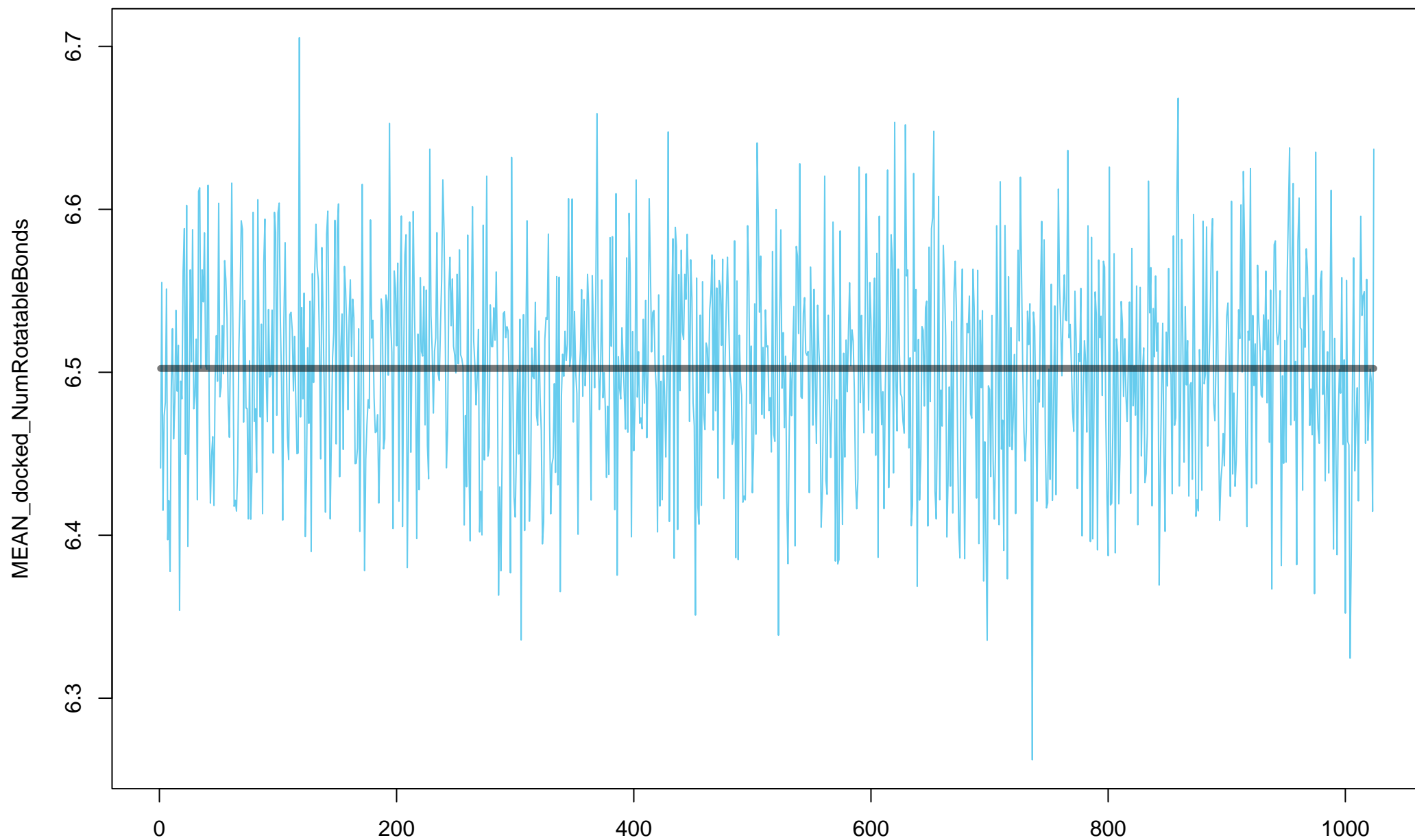


MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0452 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0 | percentile: 85



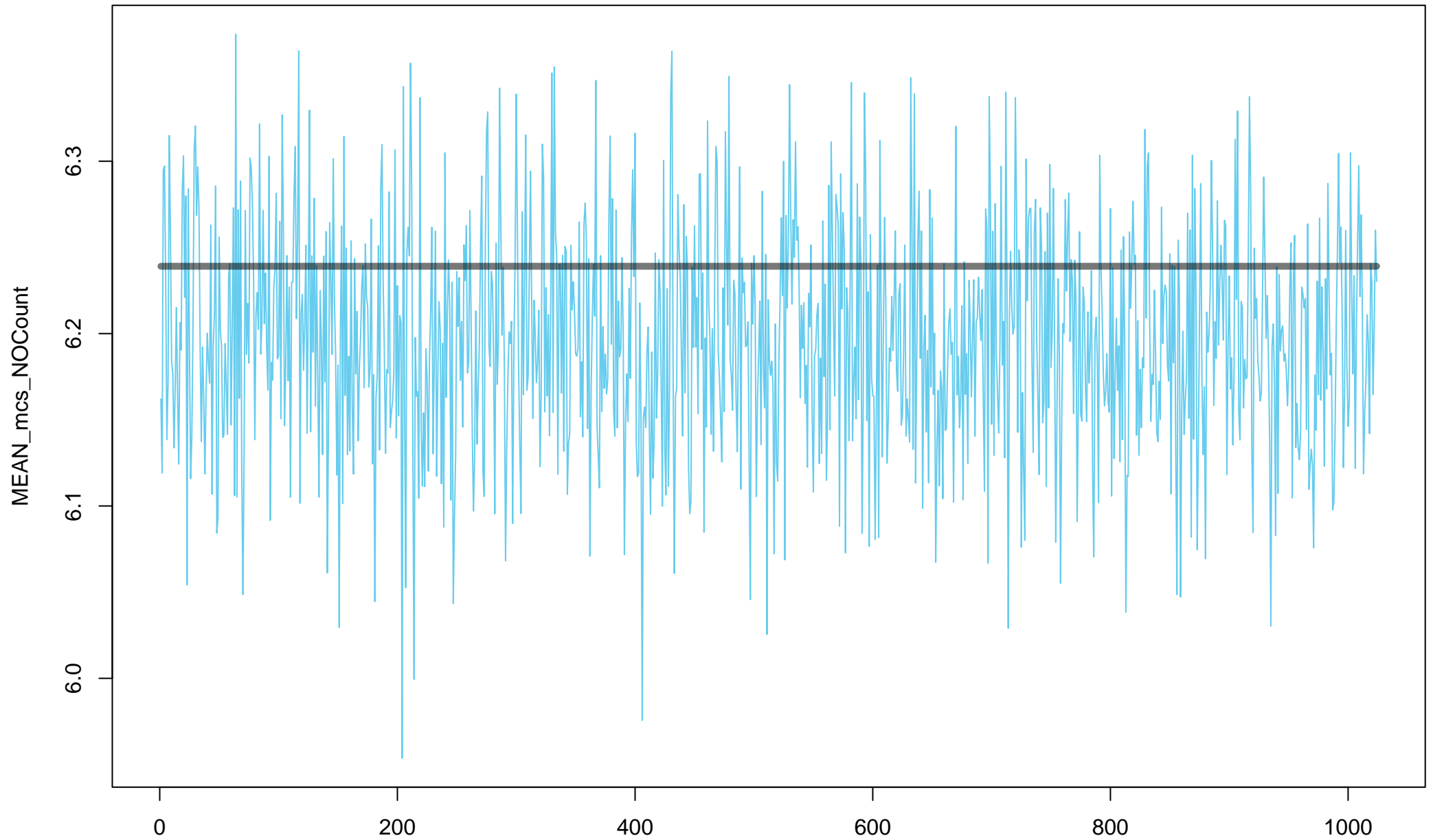
MEAN_docked_NumRotatableBonds

ESS = 1020 | BMK = 0.0534 | MCSE(6.27) = 3.42 | stat: TRUE | burn: 0 | percentile: 48.9



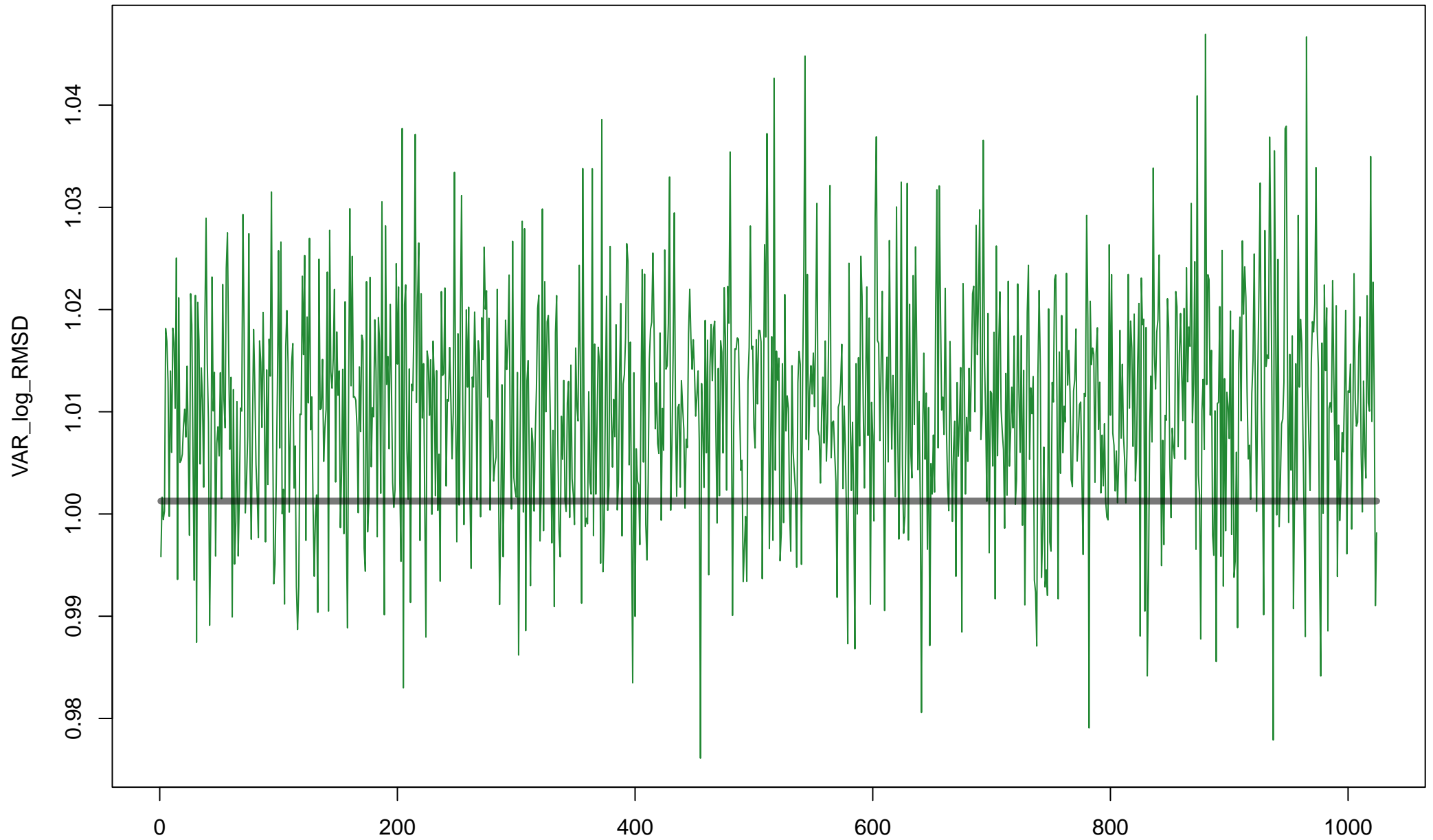
MEAN_mcs_NOCount

ESS = 1020 | BMK = 0.0635 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0 | percentile: 74.1



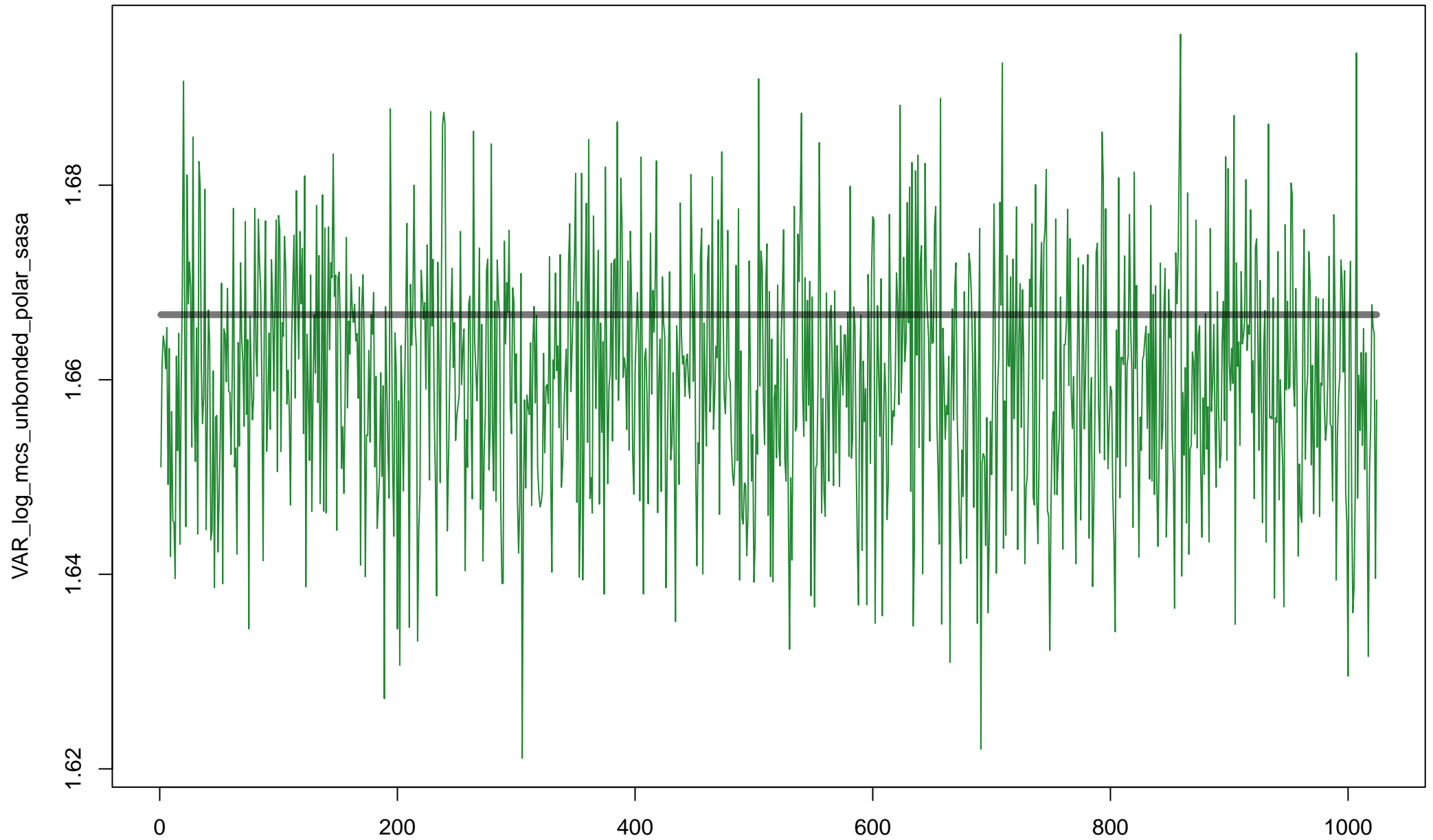
VAR_log_RMSD

ESS = 1020 | BMK = 0.0735 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0 | percentile: 19.4



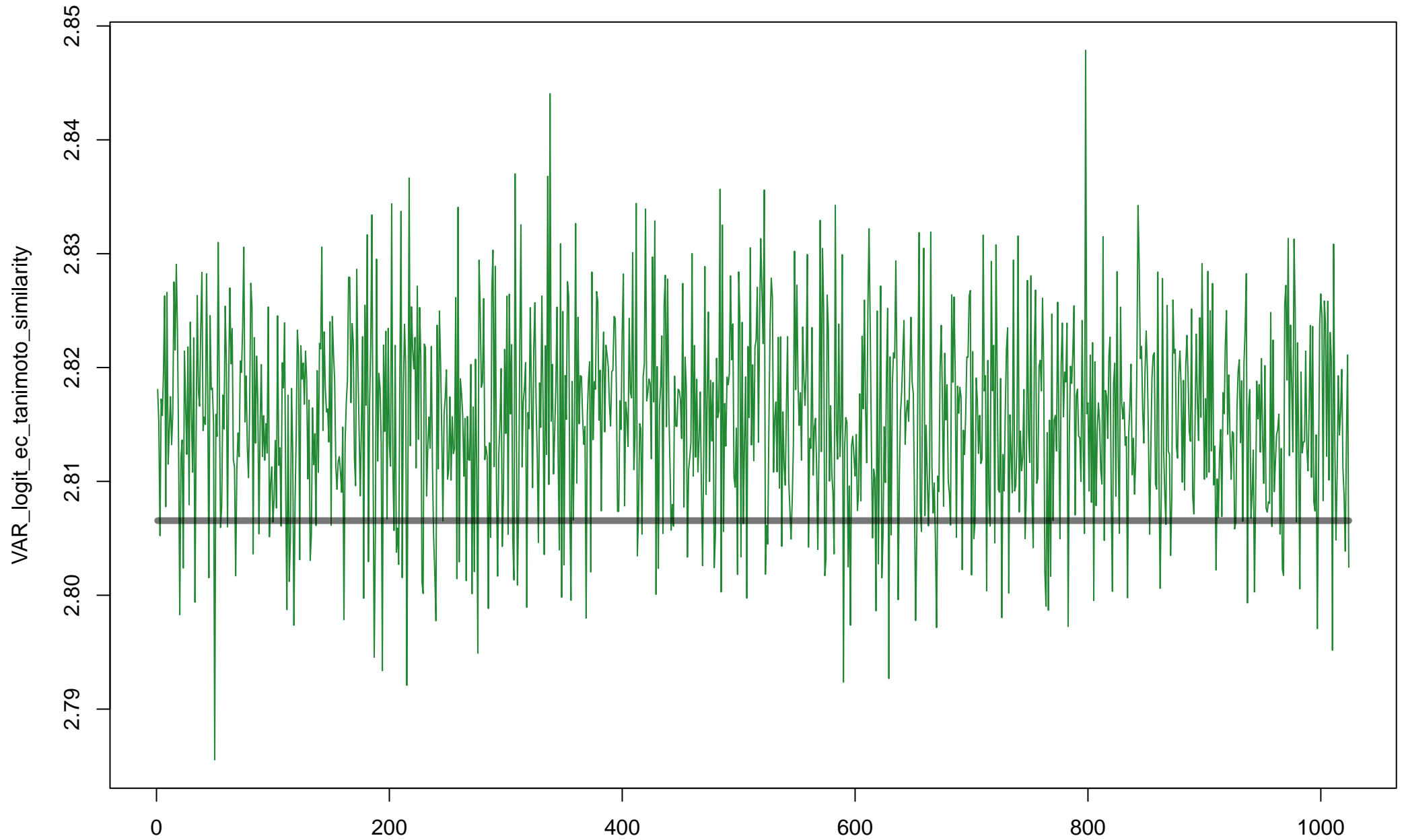
VAR_log_mcs_unbonded_polar_sasa

ESS = 1020 | BMK = 0.0525 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0 | percentile: 70.6

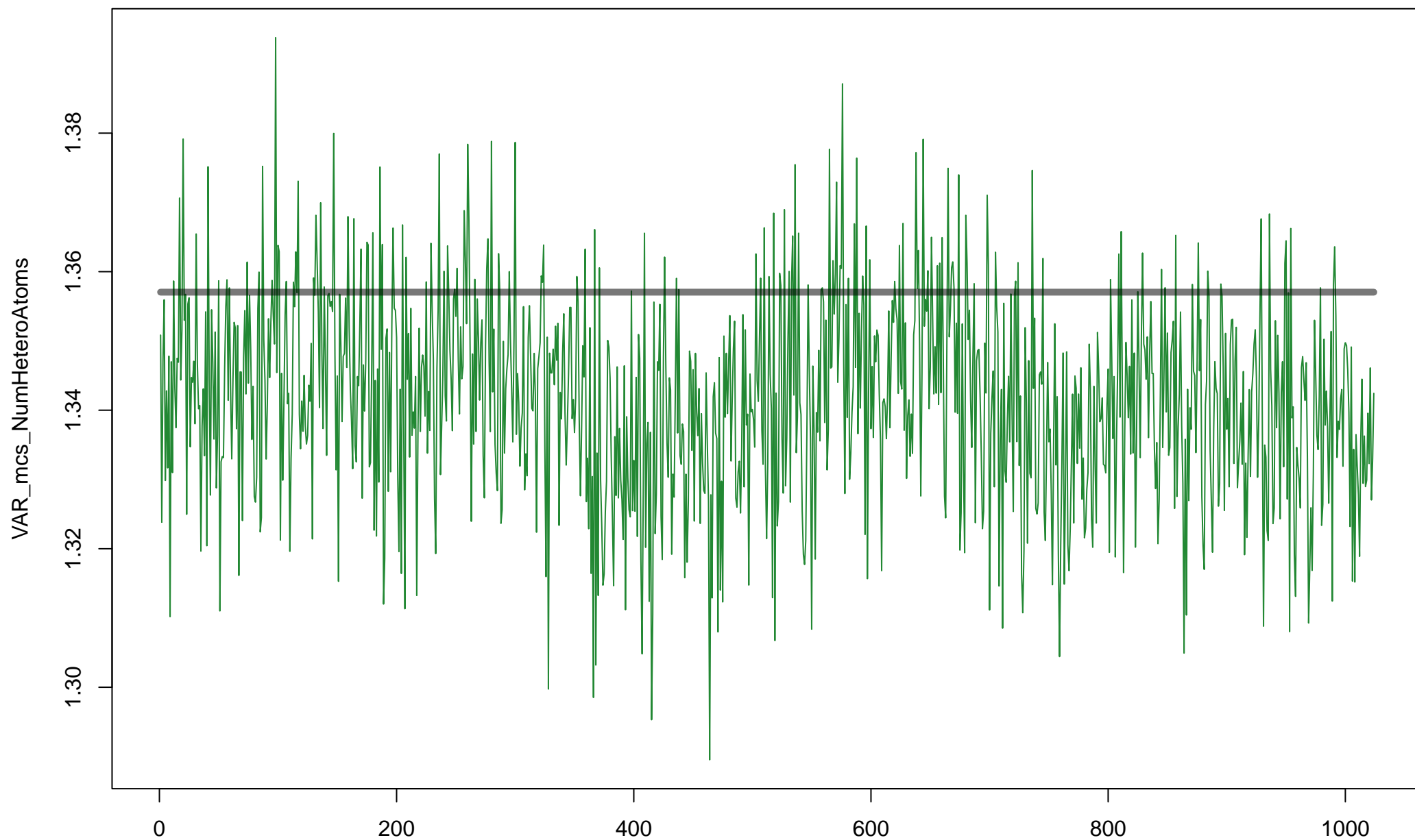


VAR_logit_ec_tanimoto_similarity

ESS = 1020 | BMK = 0.0741 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | percentile: 15

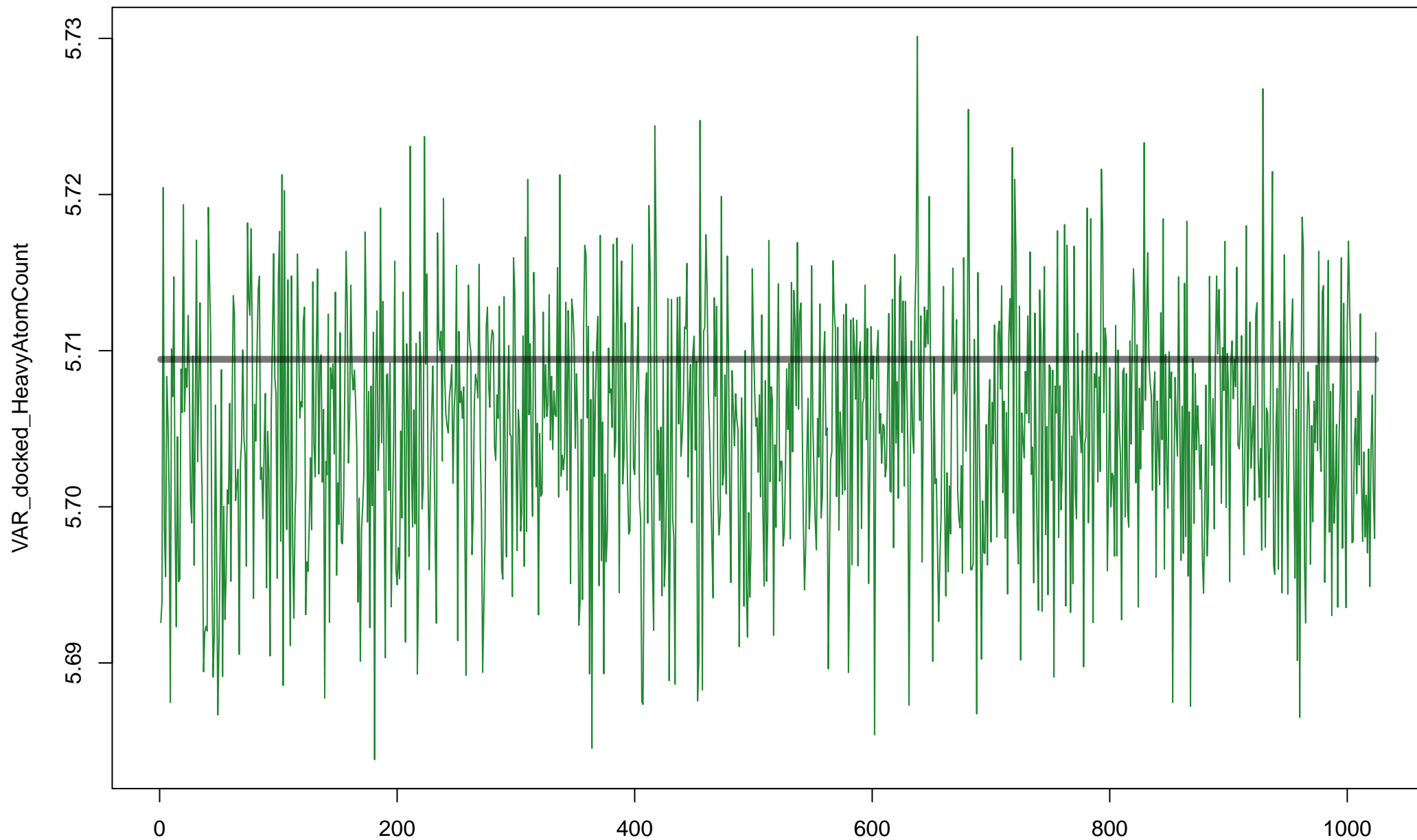


VAR_mcs_NumHeteroAtoms
ESS = 131 | BMK = 0.0566 | MCSE(6.27) = 6.45 | stat: FALSE | burn: 0 | percentile: 86.1

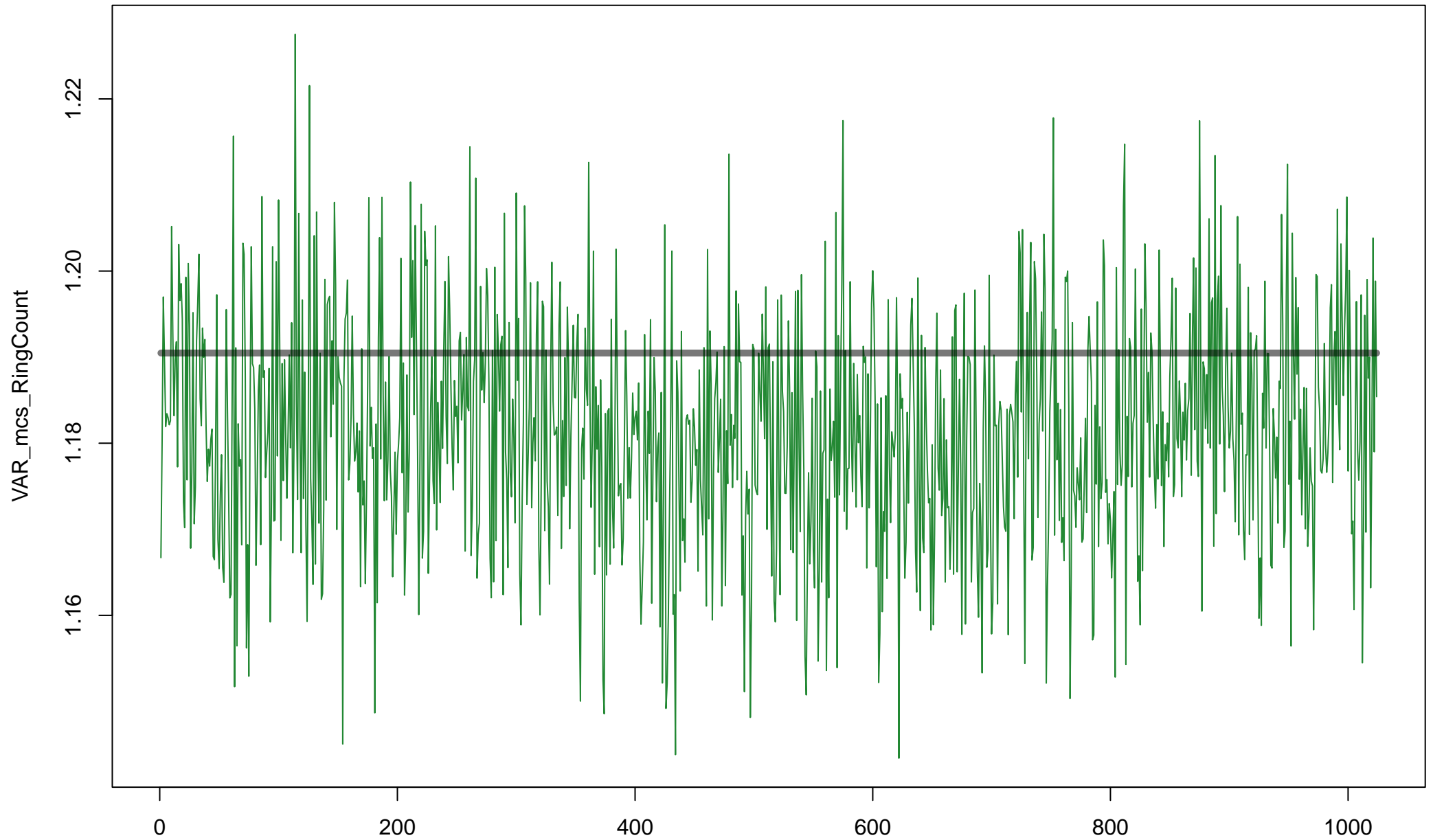


VAR_docked_HeavyAtomCount

ESS = 1020 | BMK = 0.0707 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0 | percentile: 72.7

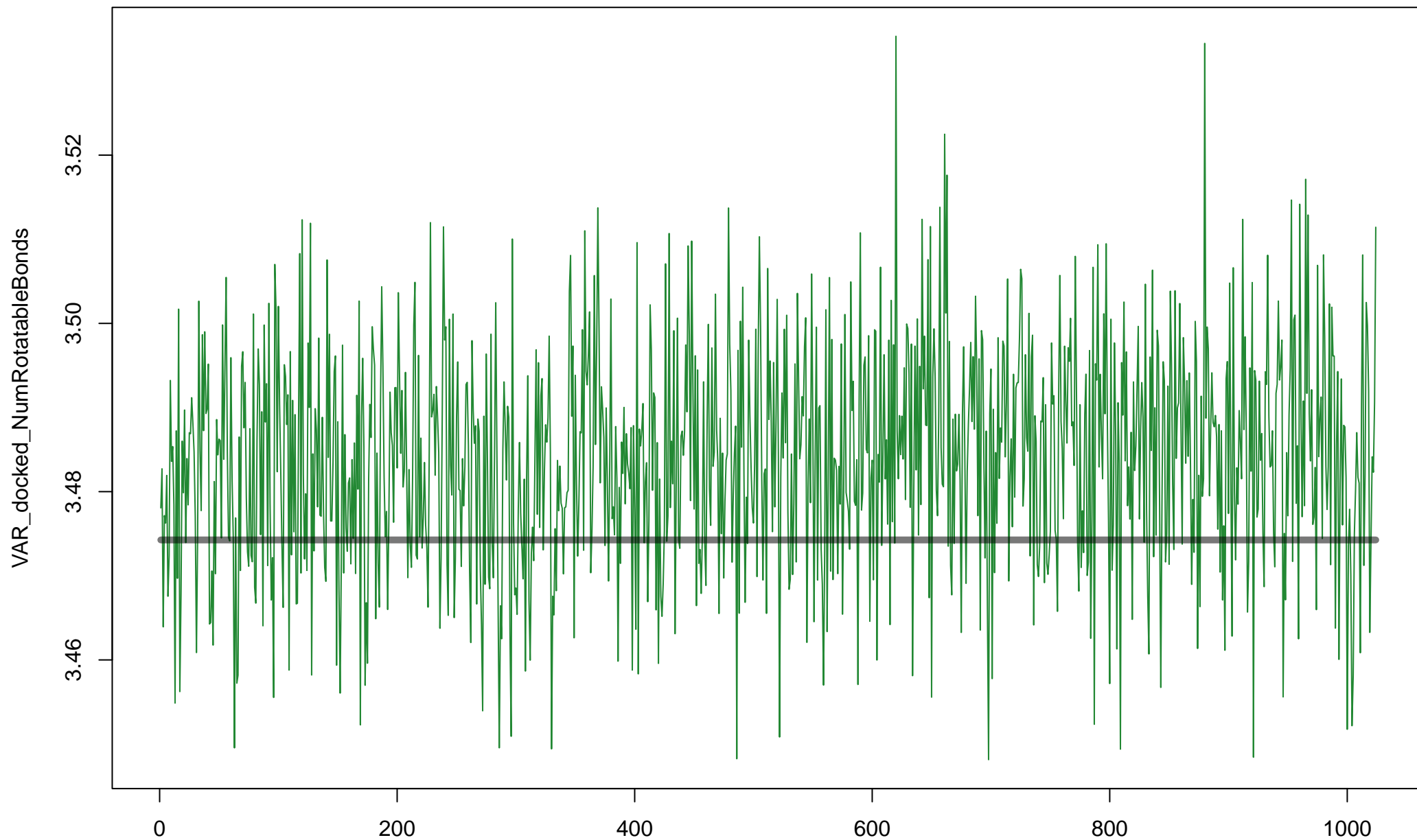


VAR_mcs_RingCount
ESS = 910 | BMK = 0.051 | MCSE(6.27) = 4.27 | stat: TRUE | burn: 0 | percentile: 75.8



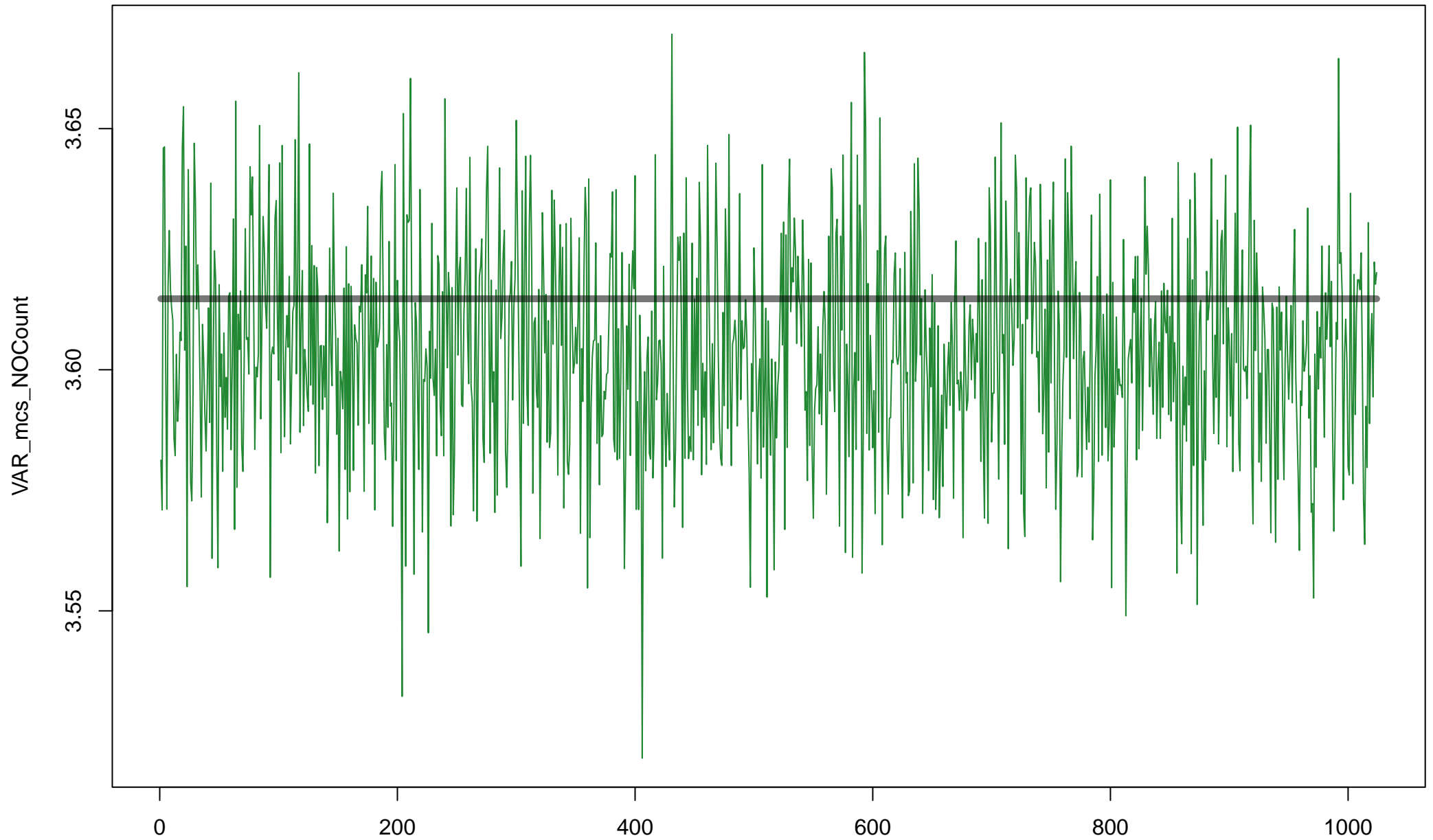
VAR_docked_NumRotatableBonds

ESS = 1020 | BMK = 0.0961 | MCSE(6.27) = 4.05 | stat: FALSE | burn: 0 | percentile: 24.2

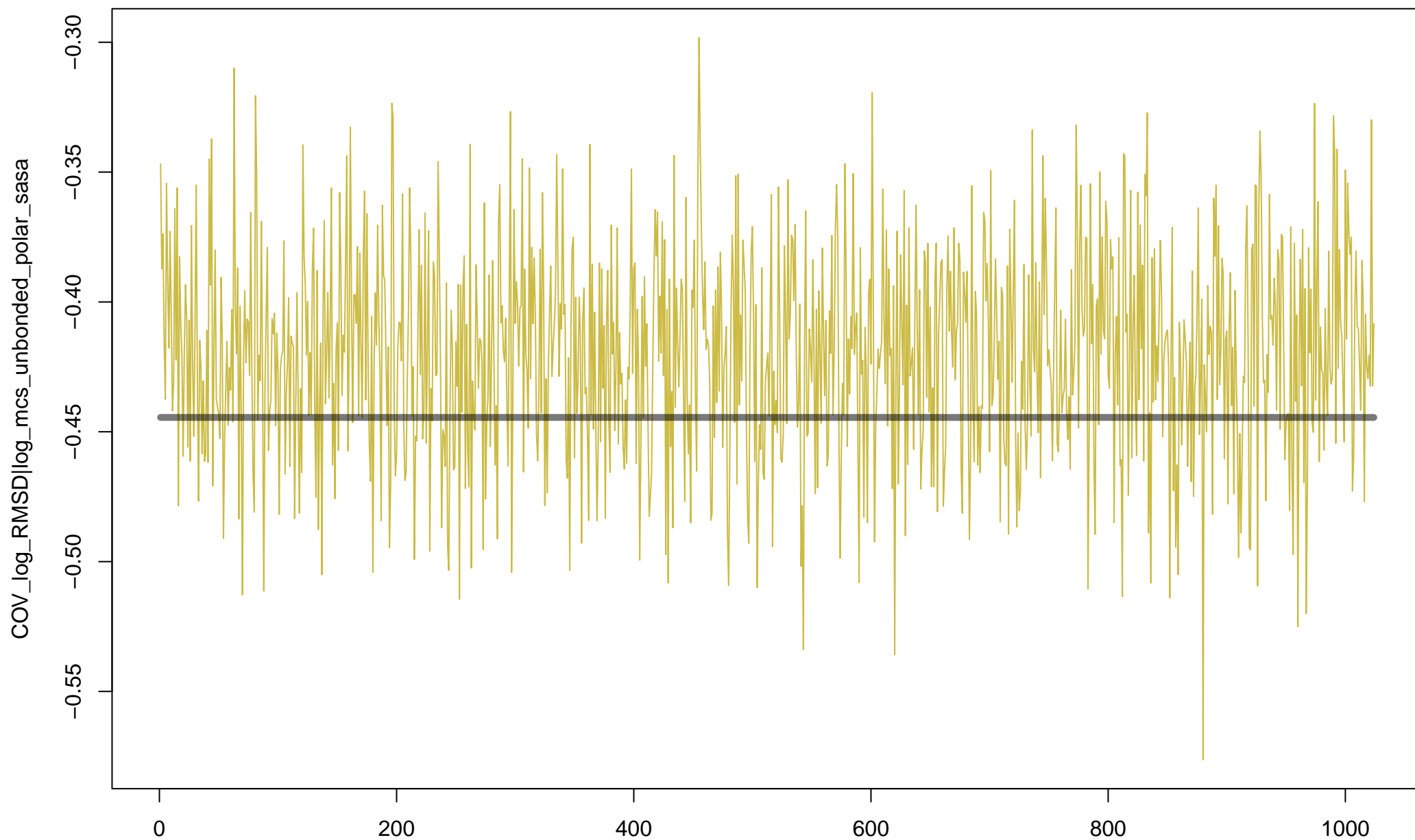


VAR_mcs_NOCount

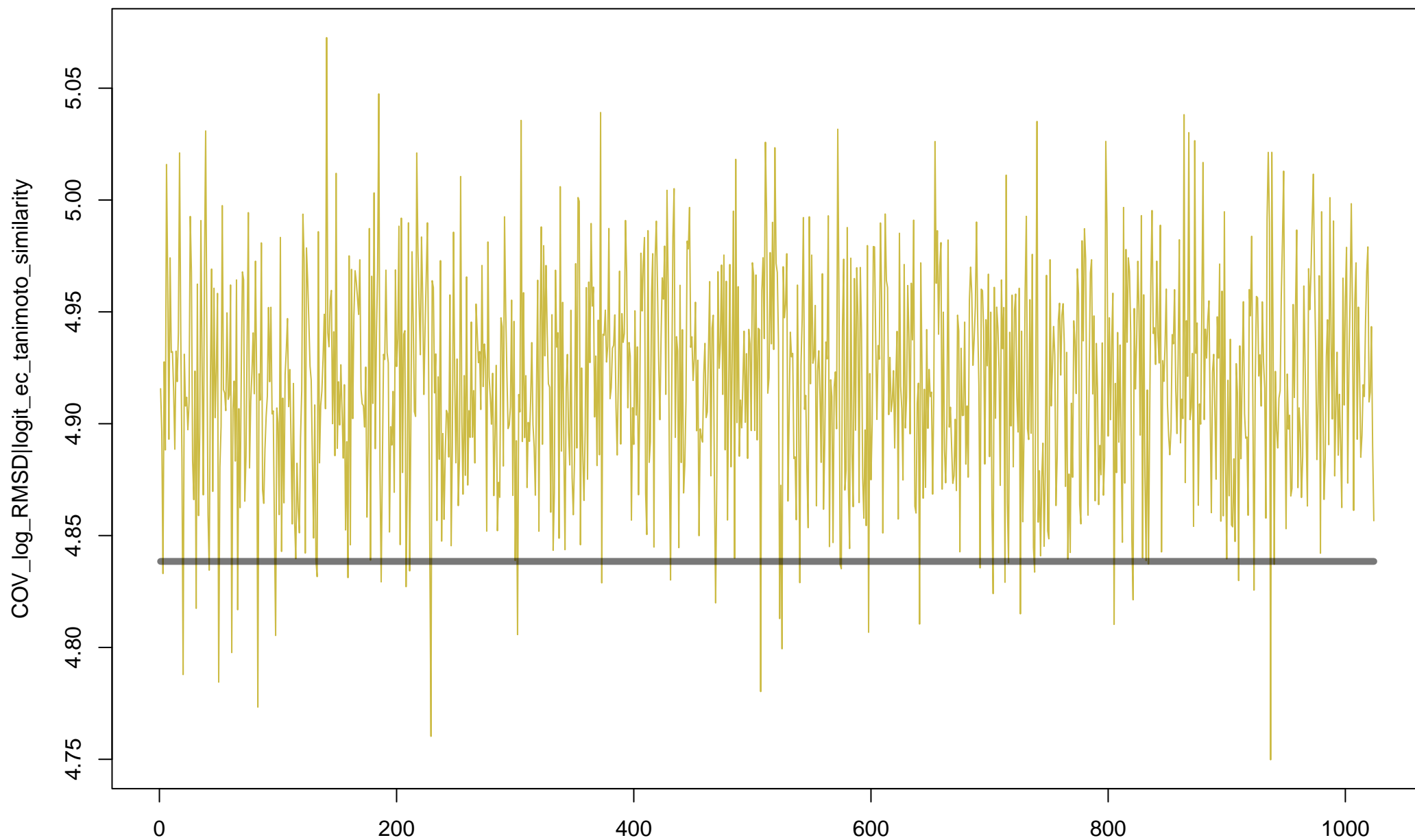
ESS = 1020 | BMK = 0.0539 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 0 | percentile: 69.5



COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0567 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | percentile: 26.9

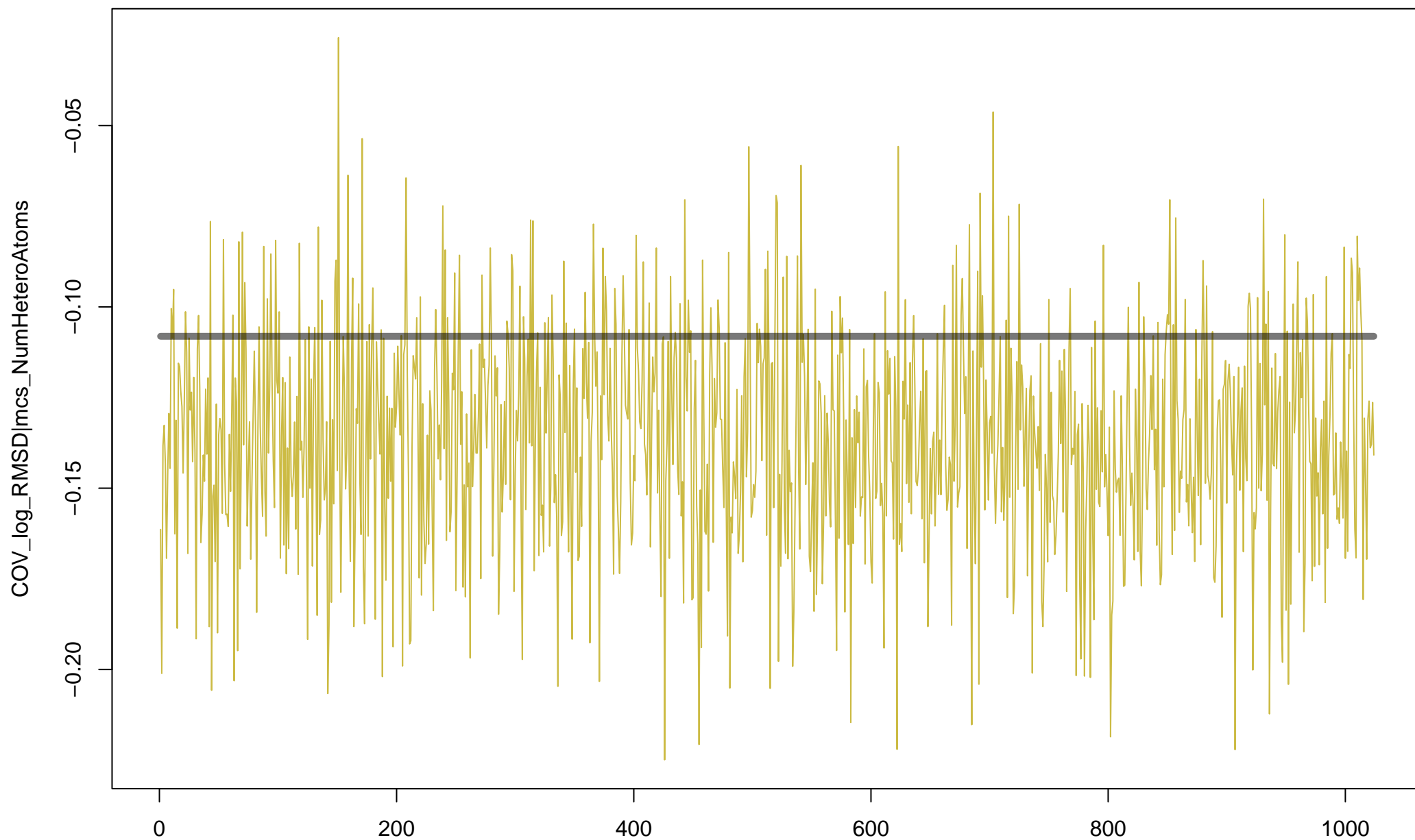


COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0571 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0 | percentile: 3.91

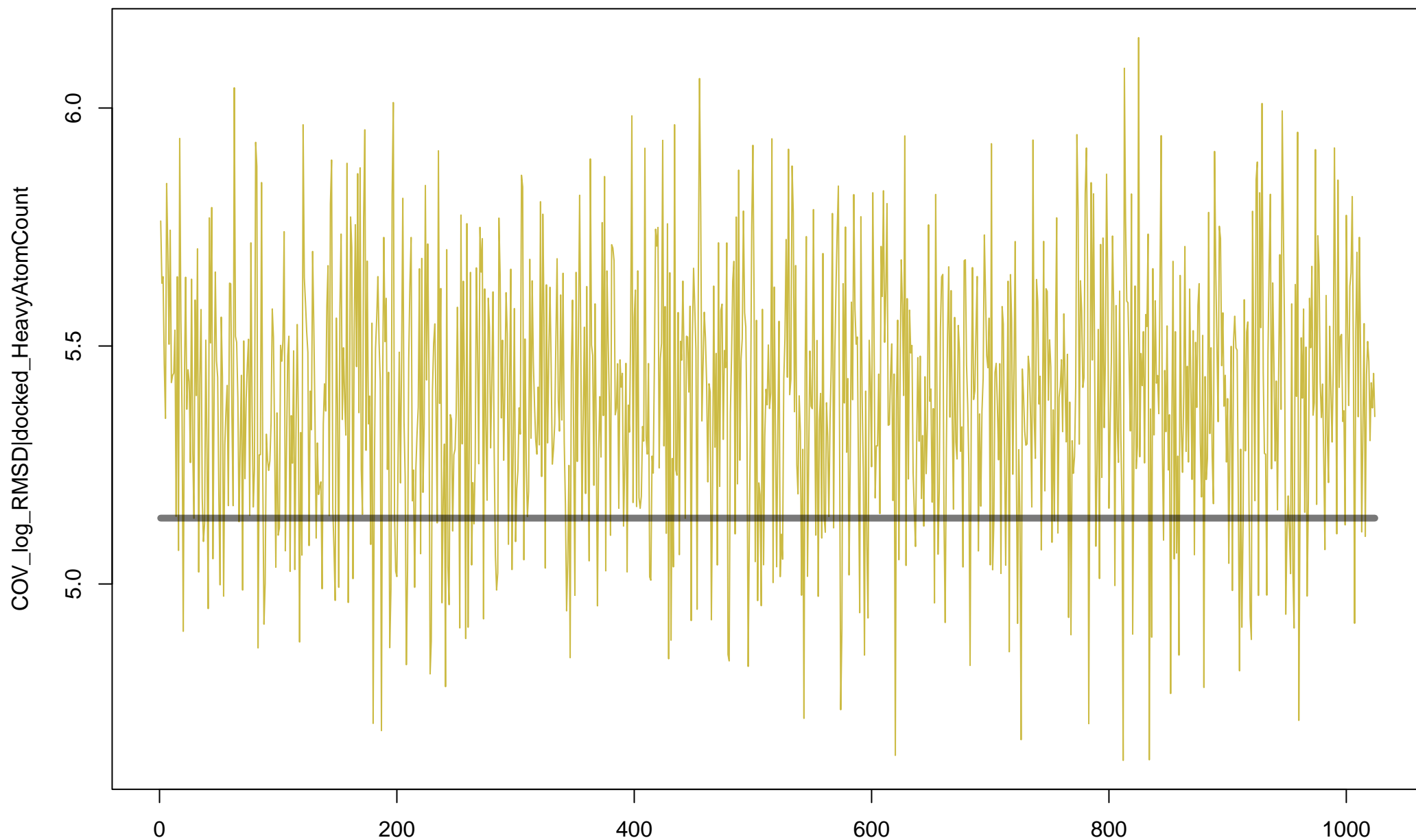


COV_log_RMSD|mcs_NumHeteroAtoms

ESS = 1020 | BMK = 0.0638 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0 | percentile: 83.9

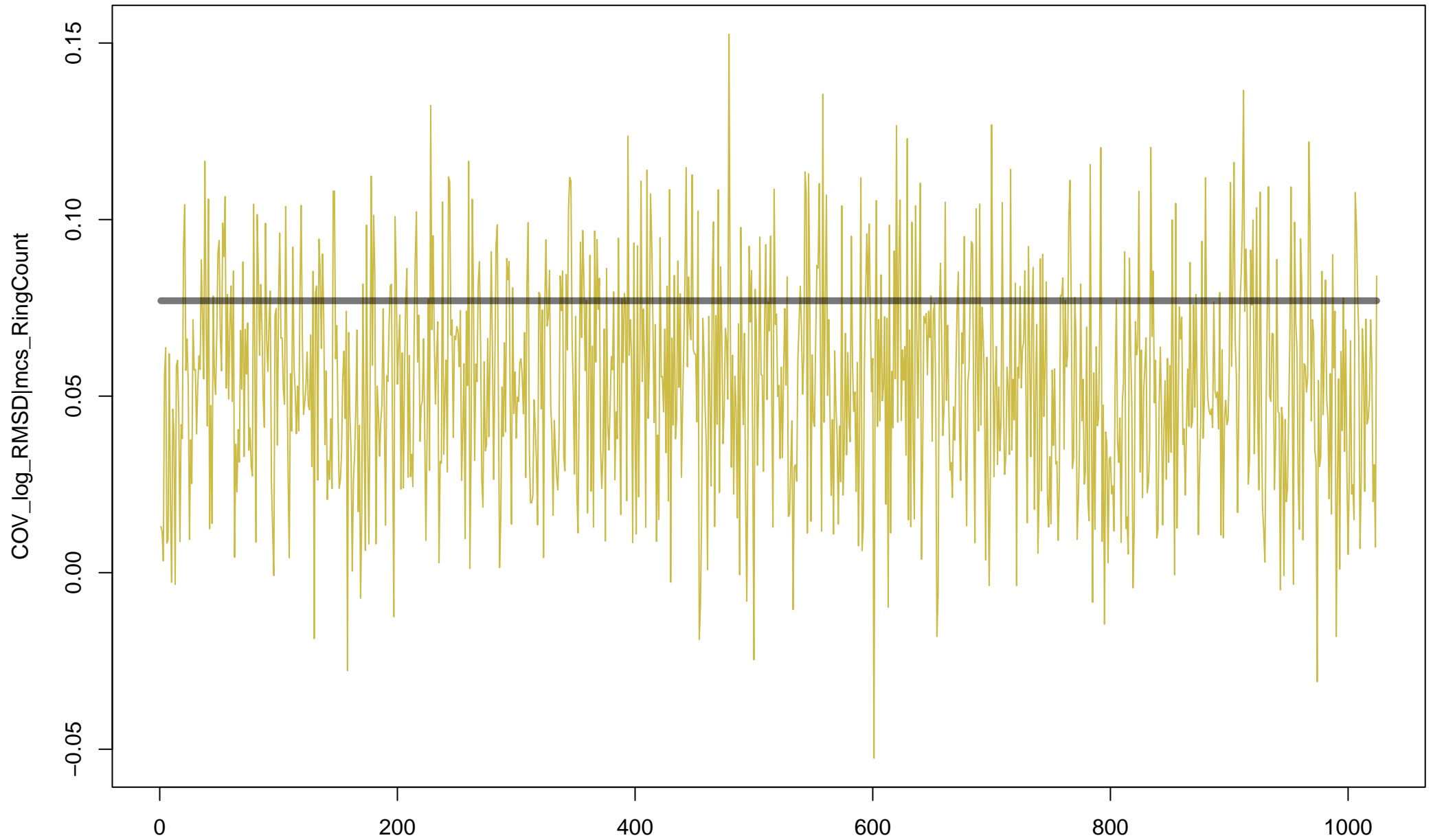


COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0554 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0 | percentile: 17.5

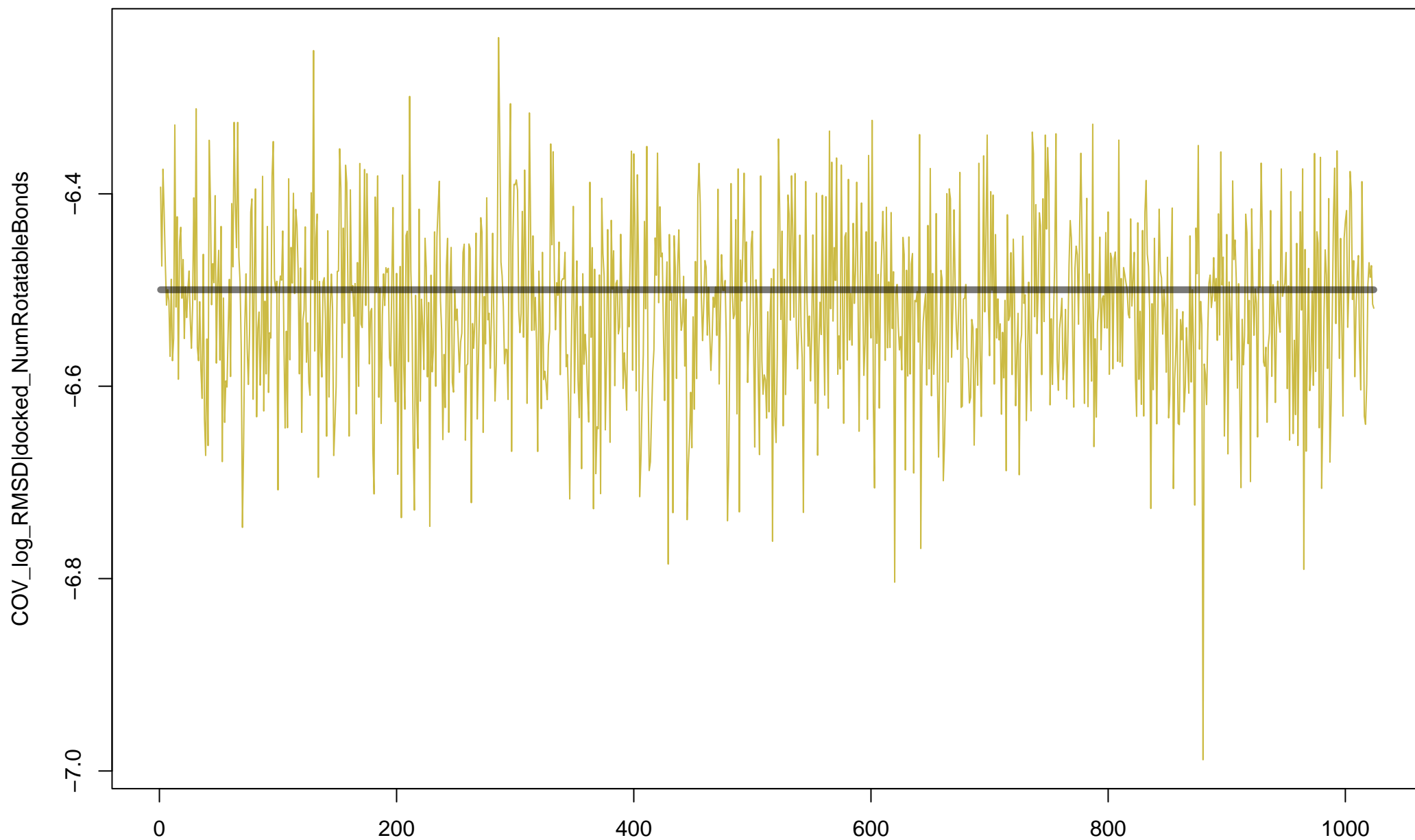


COV_log_RMSD|mcs_RingCount

ESS = 1020 | BMK = 0.0616 | MCSE(6.27) = 3.76 | stat: TRUE | burn: 0 | percentile: 78.2

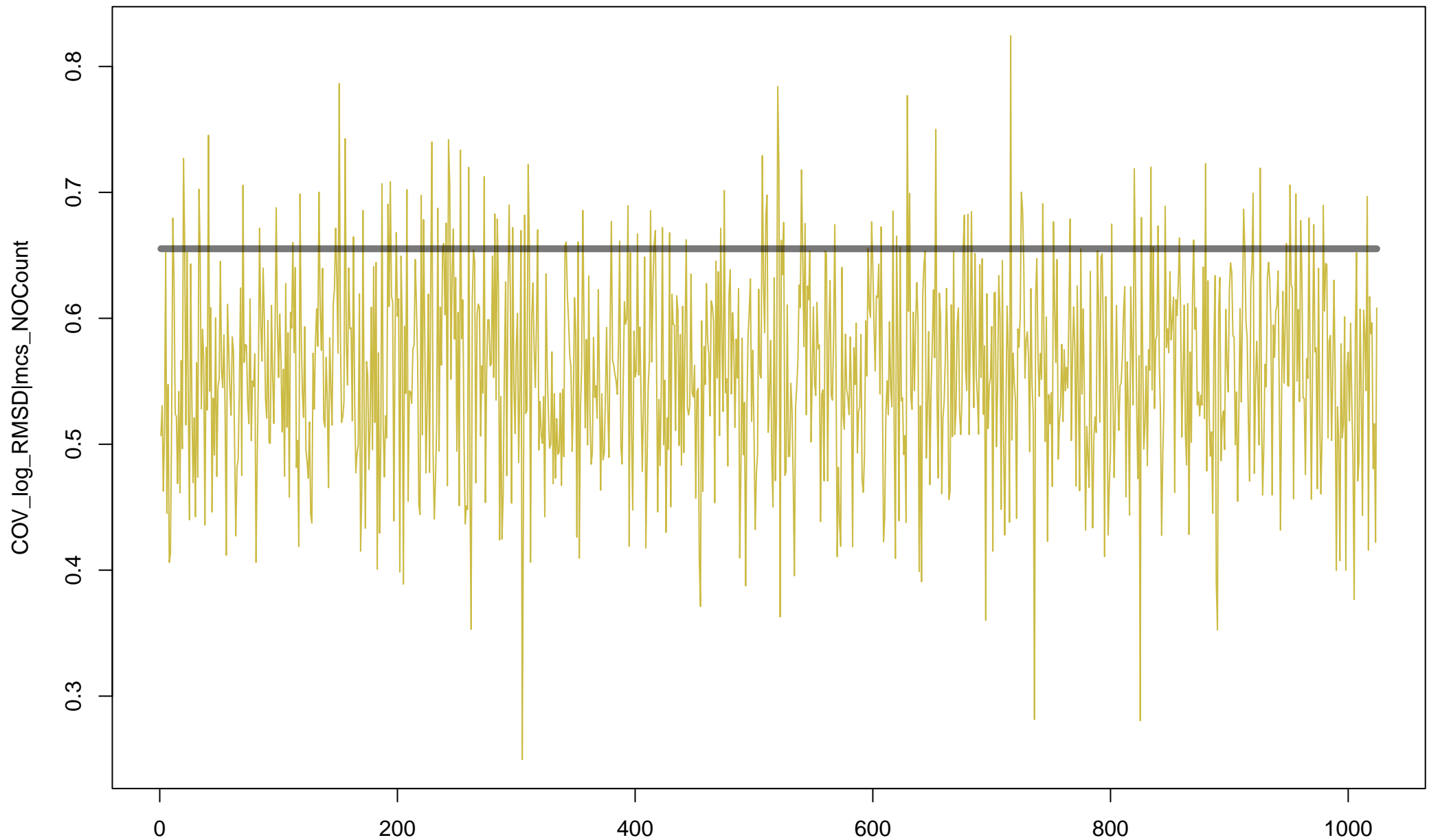


COV_log_RMSD|docked_NumRotatableBonds
ESS = 877 | BMK = 0.0655 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | percentile: 59.6

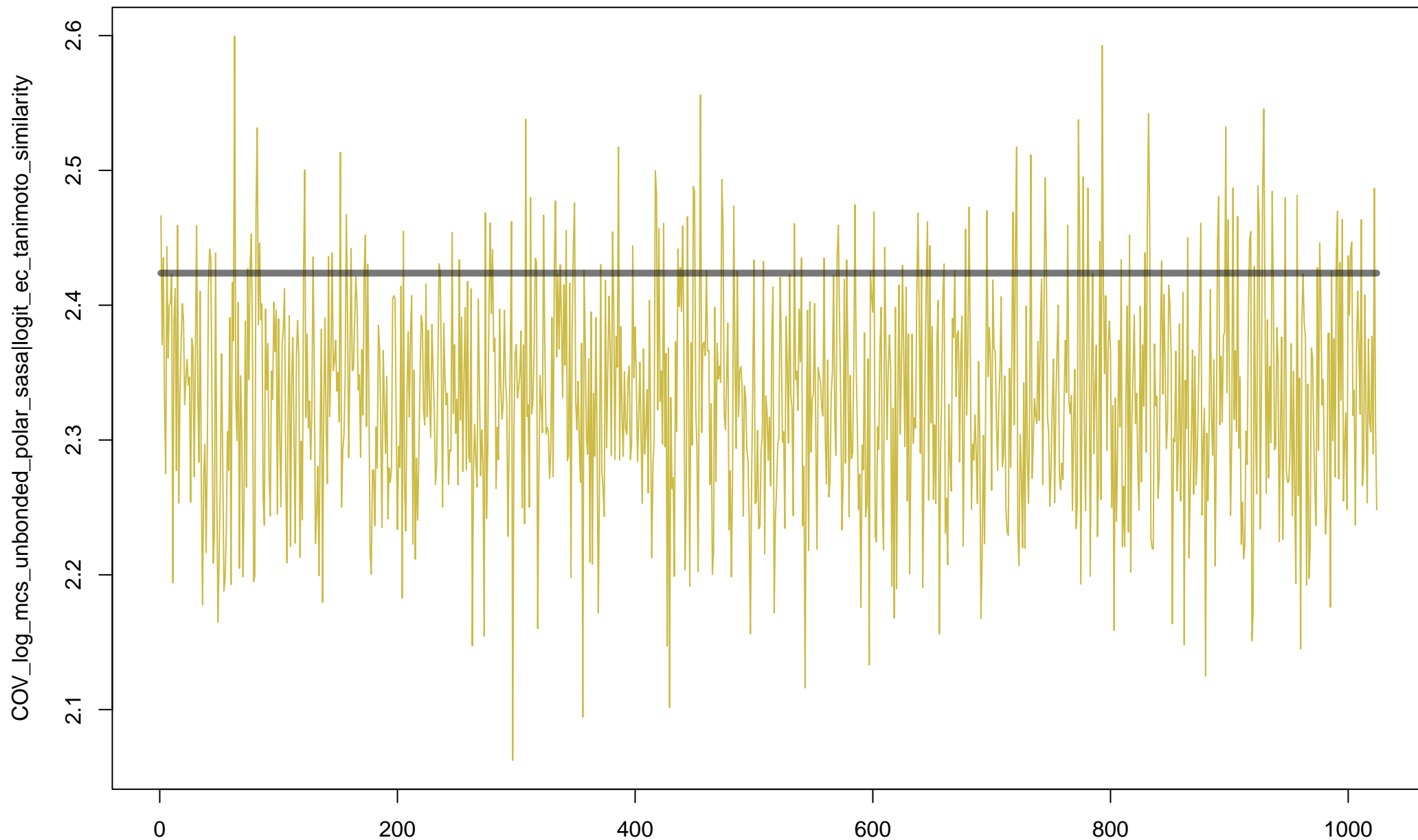


COV_log_RMSD|mcs_NOCount

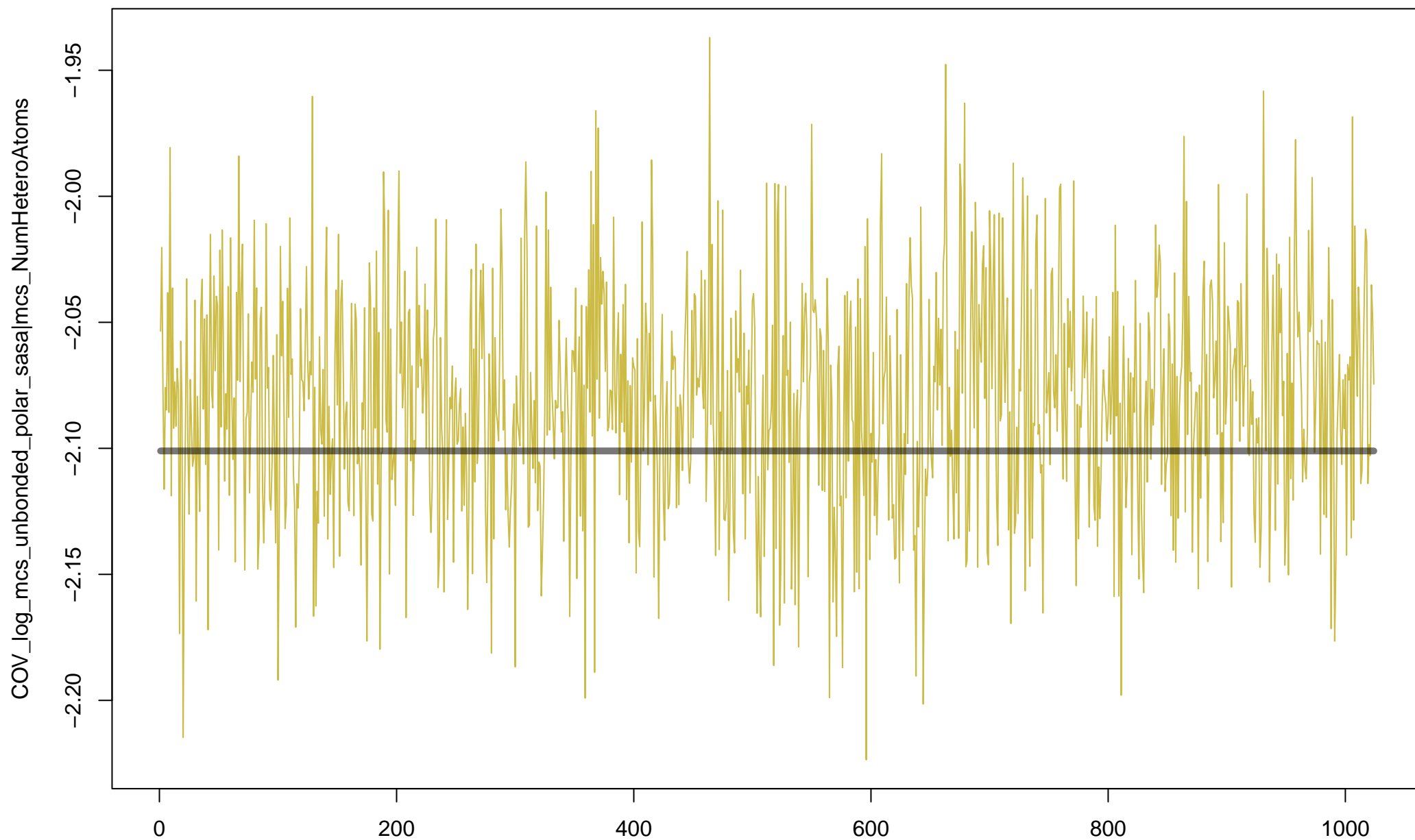
ESS = 1020 | BMK = 0.0578 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0 | percentile: 89.4



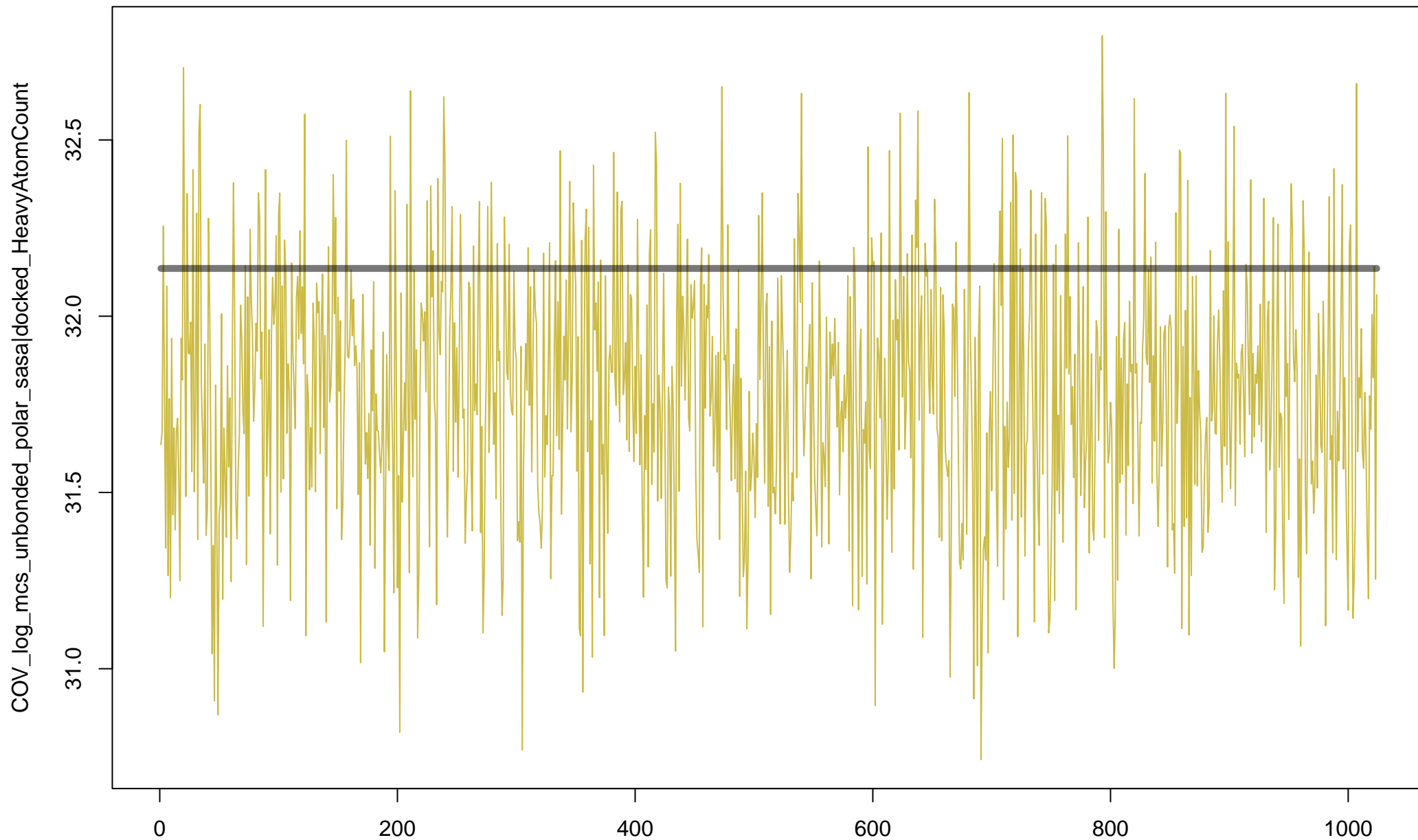
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0521 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | percentile: 86.6



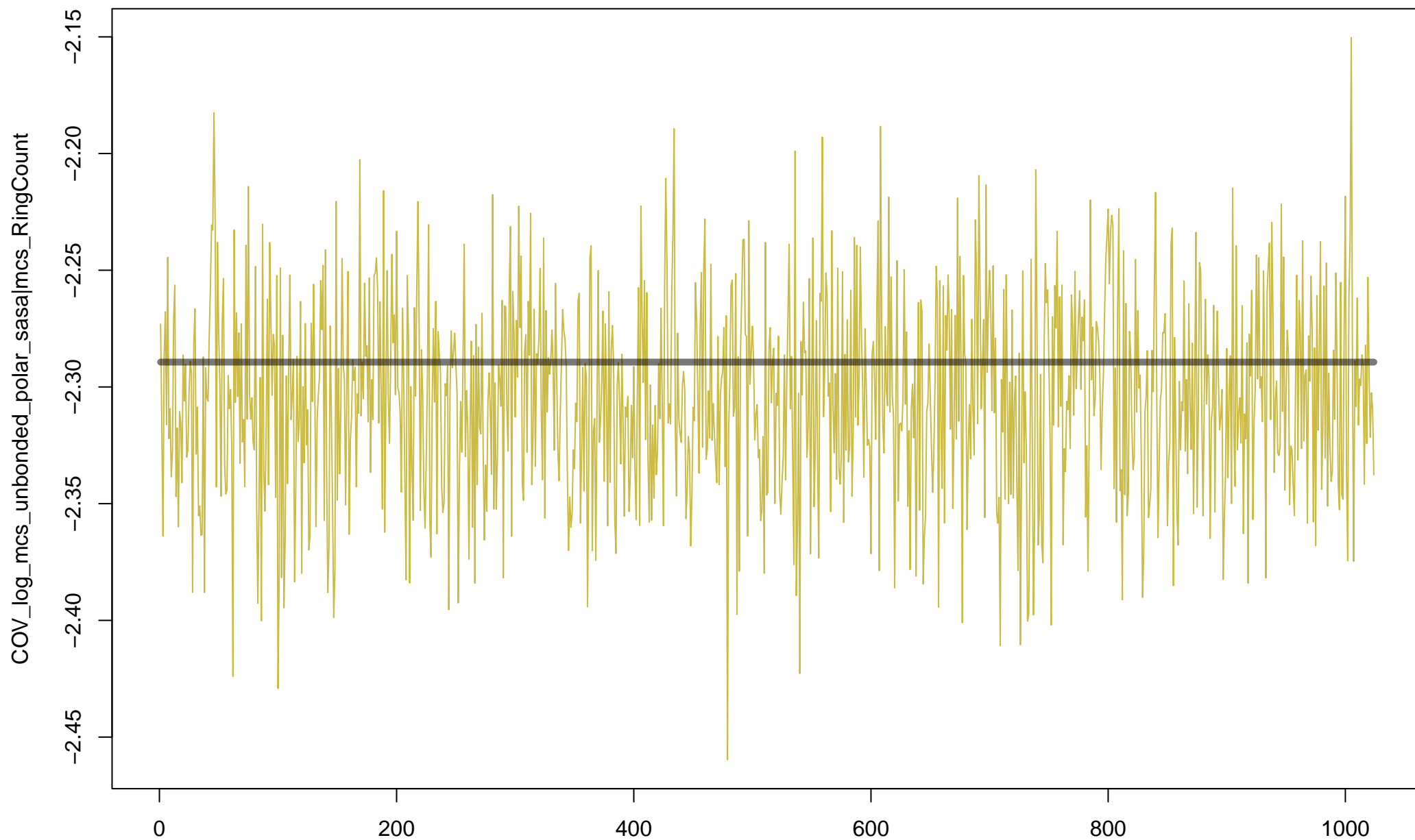
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 937 | BMK = 0.054 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0 | percentile: 31.9



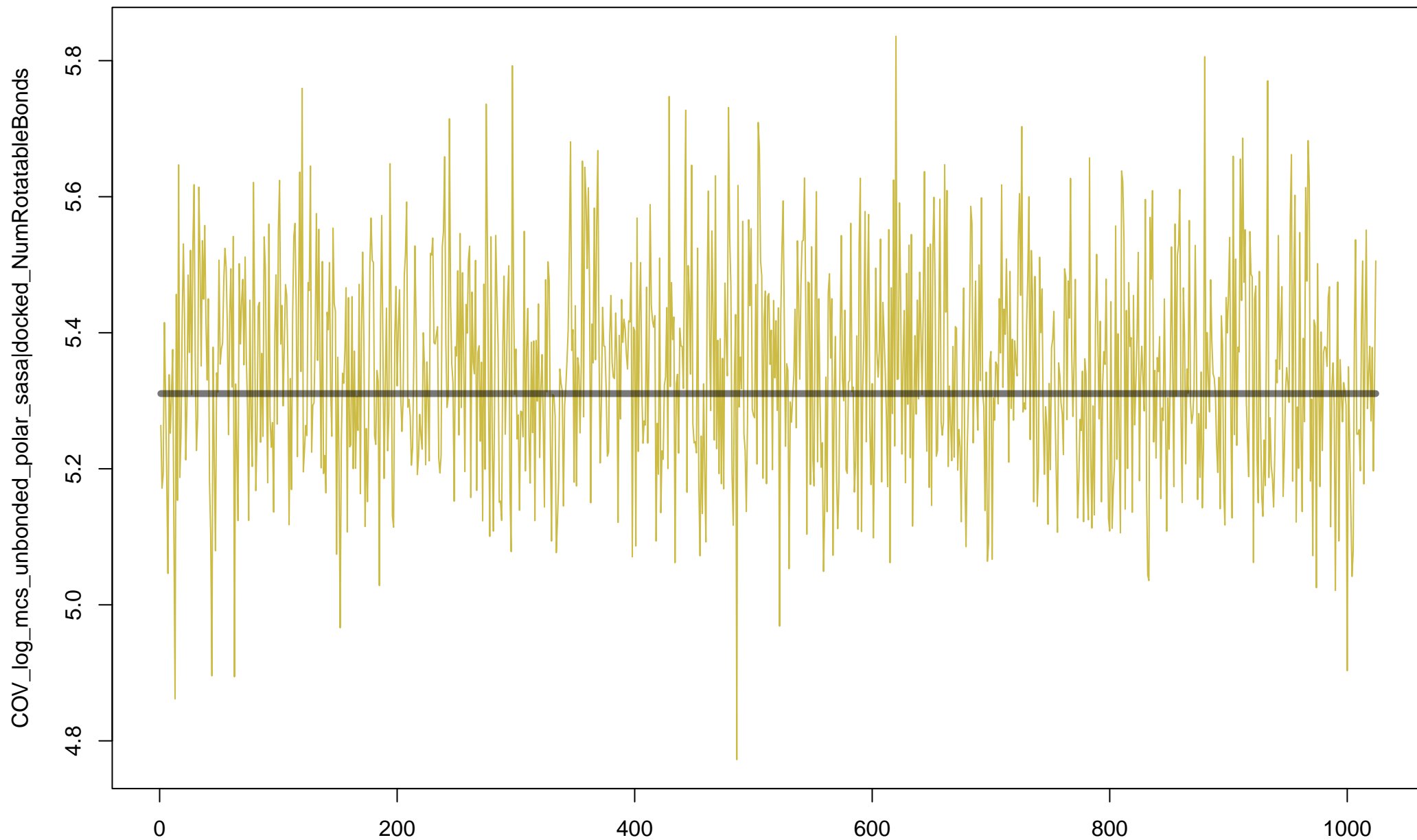
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.046 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0 | percentile: 85.1



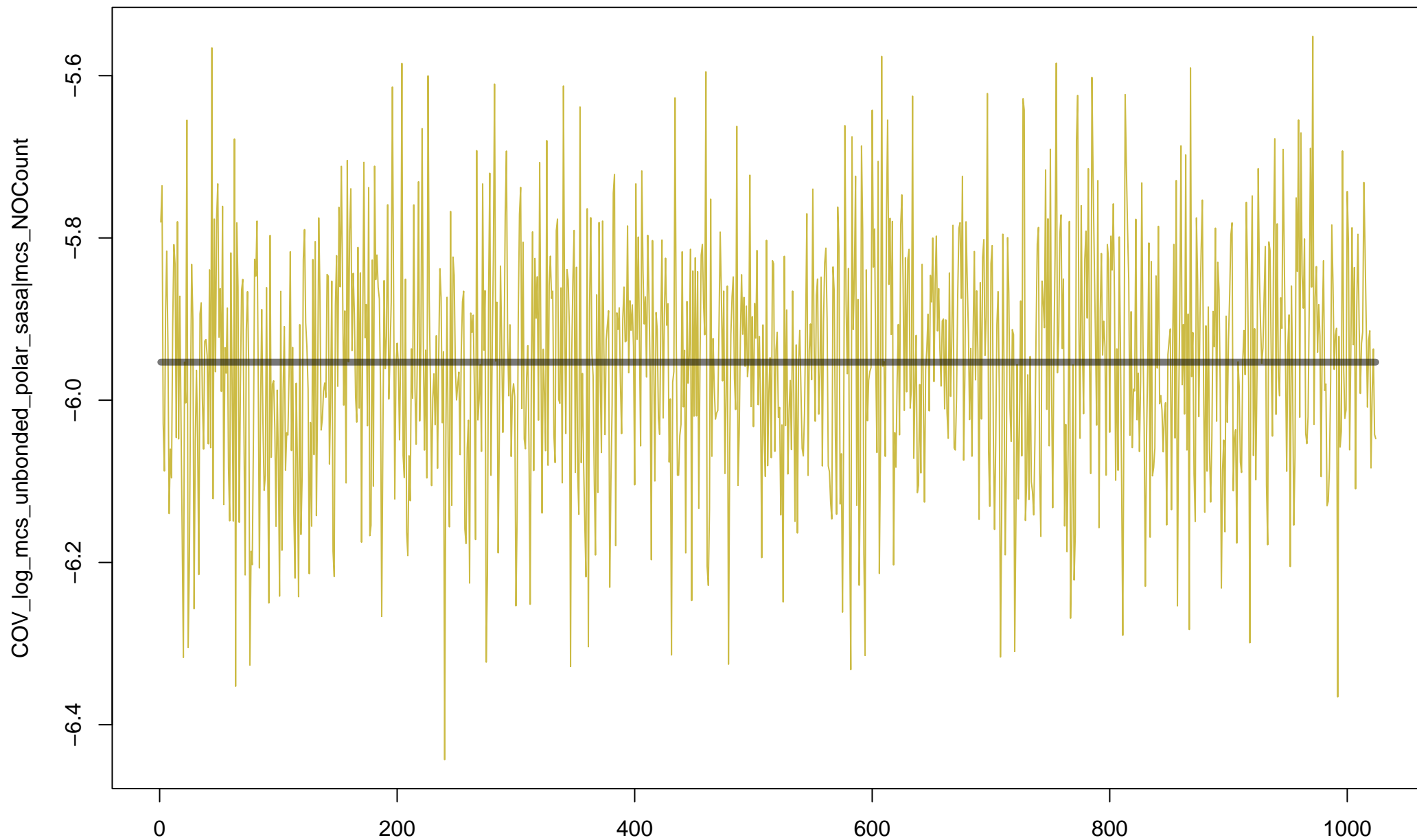
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0424 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0 | percentile: 64.8



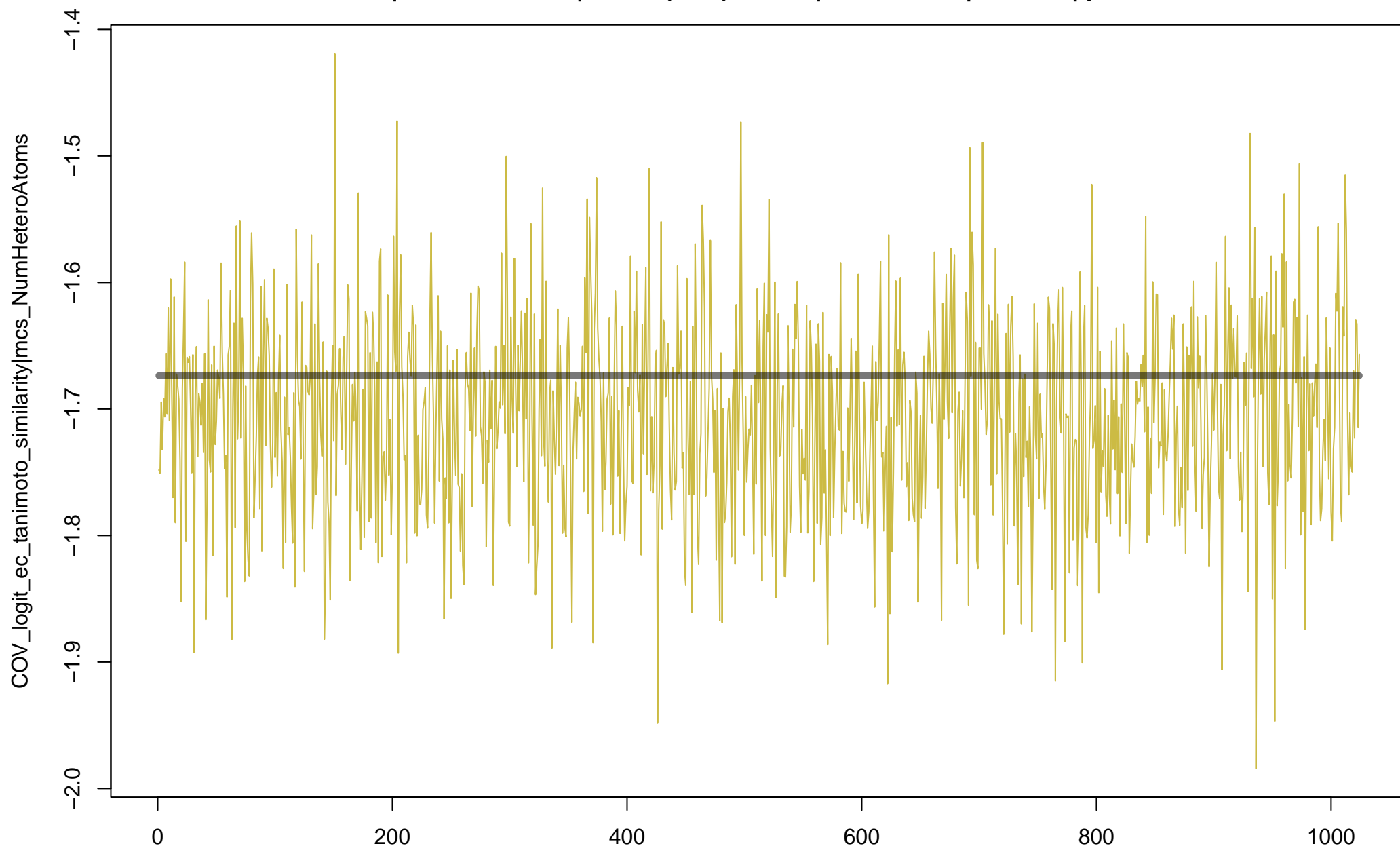
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0632 | MCSE(6.27) = 3.53 | stat: TRUE | burn: 0 | percentile: 42



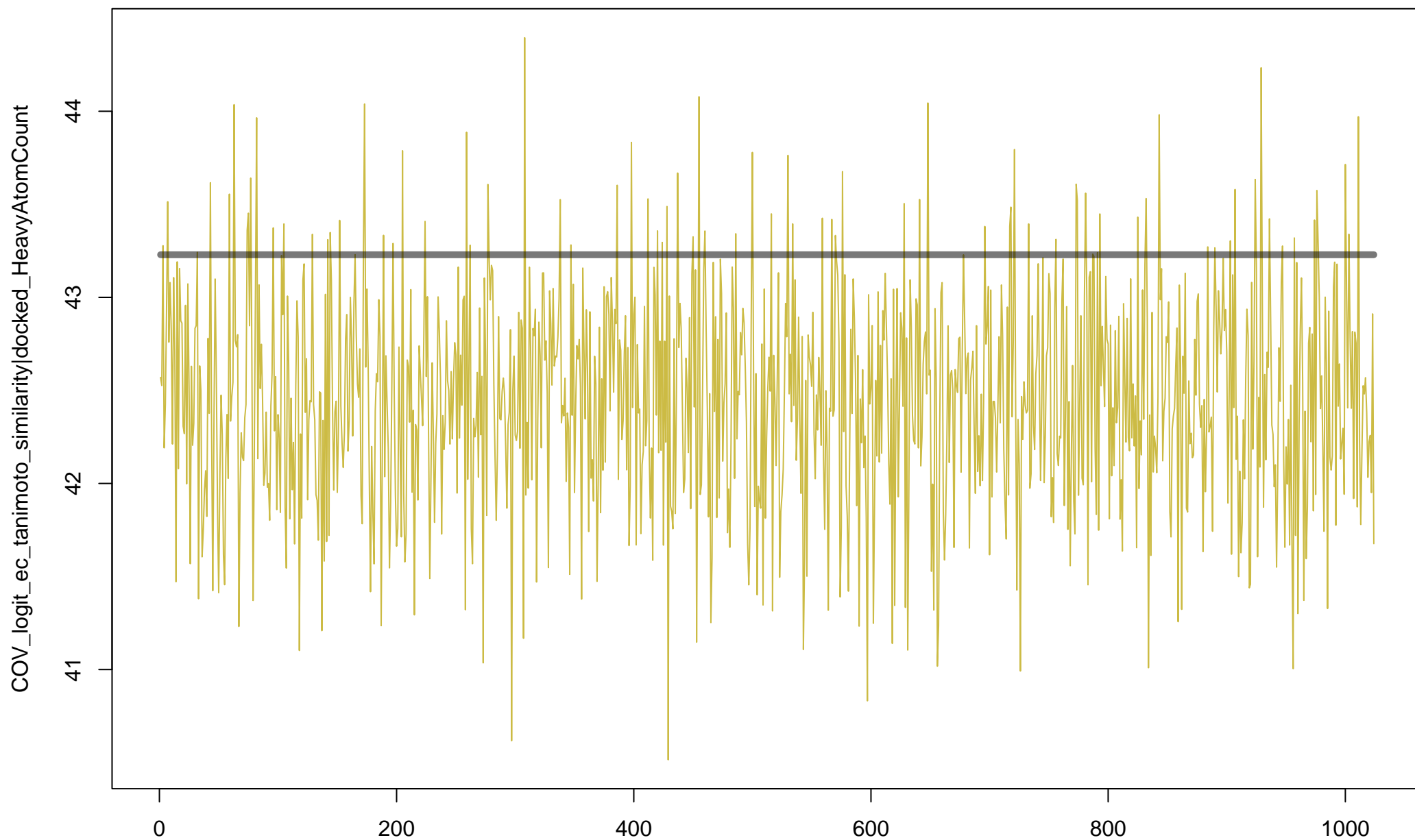
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0522 | MCSE(6.27) = 3.67 | stat: FALSE | burn: 0 | percentile: 49



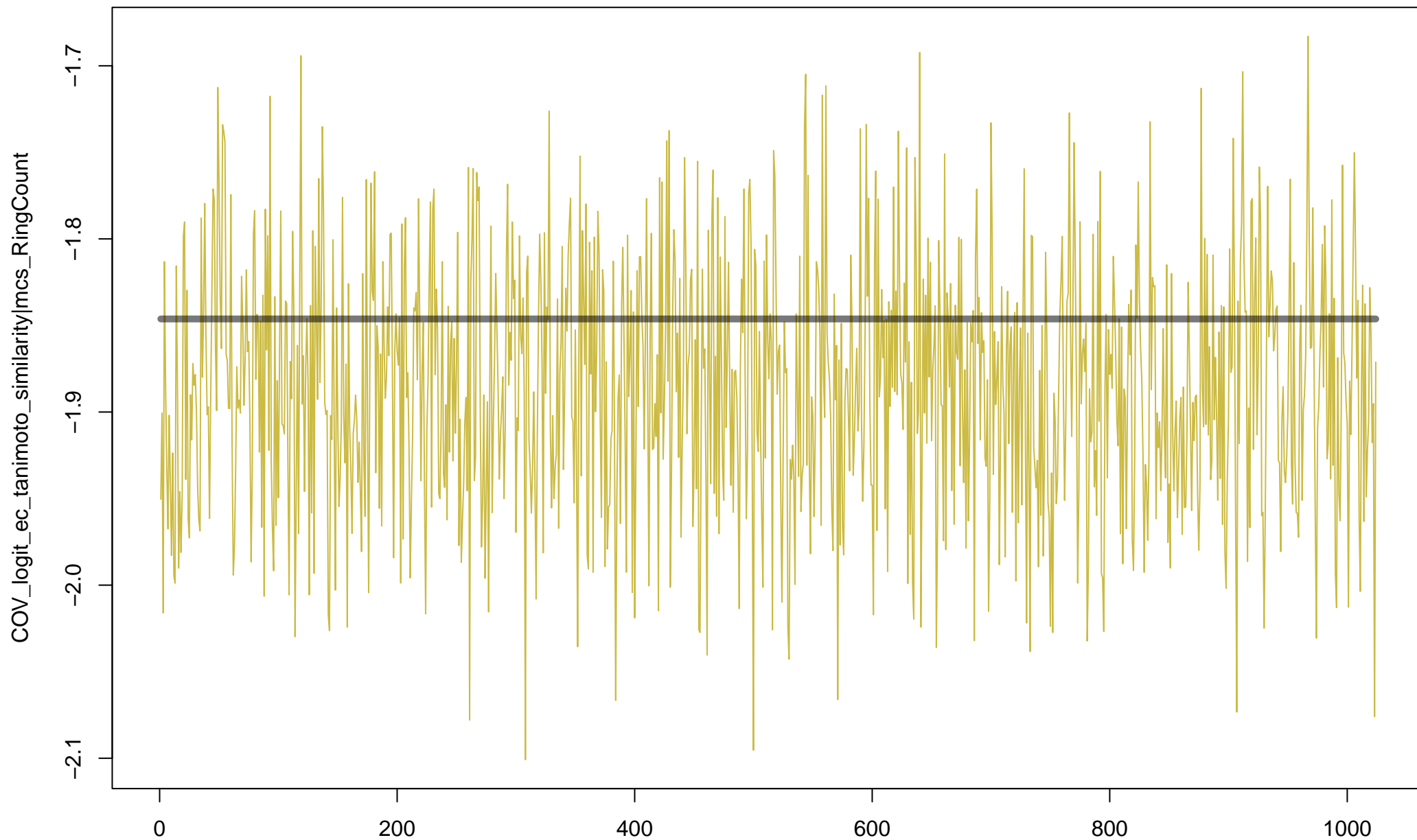
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0477 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 0 | percentile: 65.9



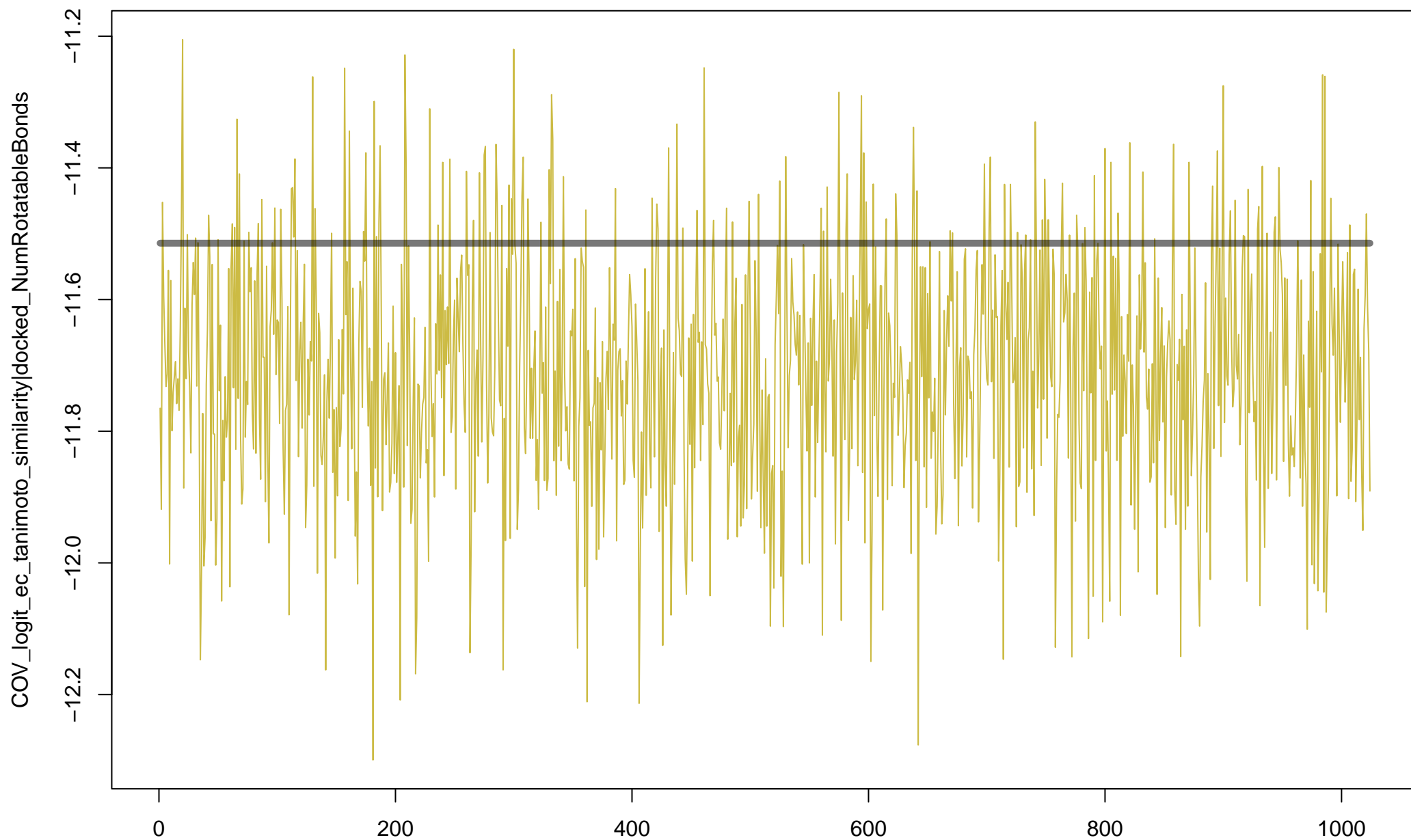
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0353 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | percentile: 92.3



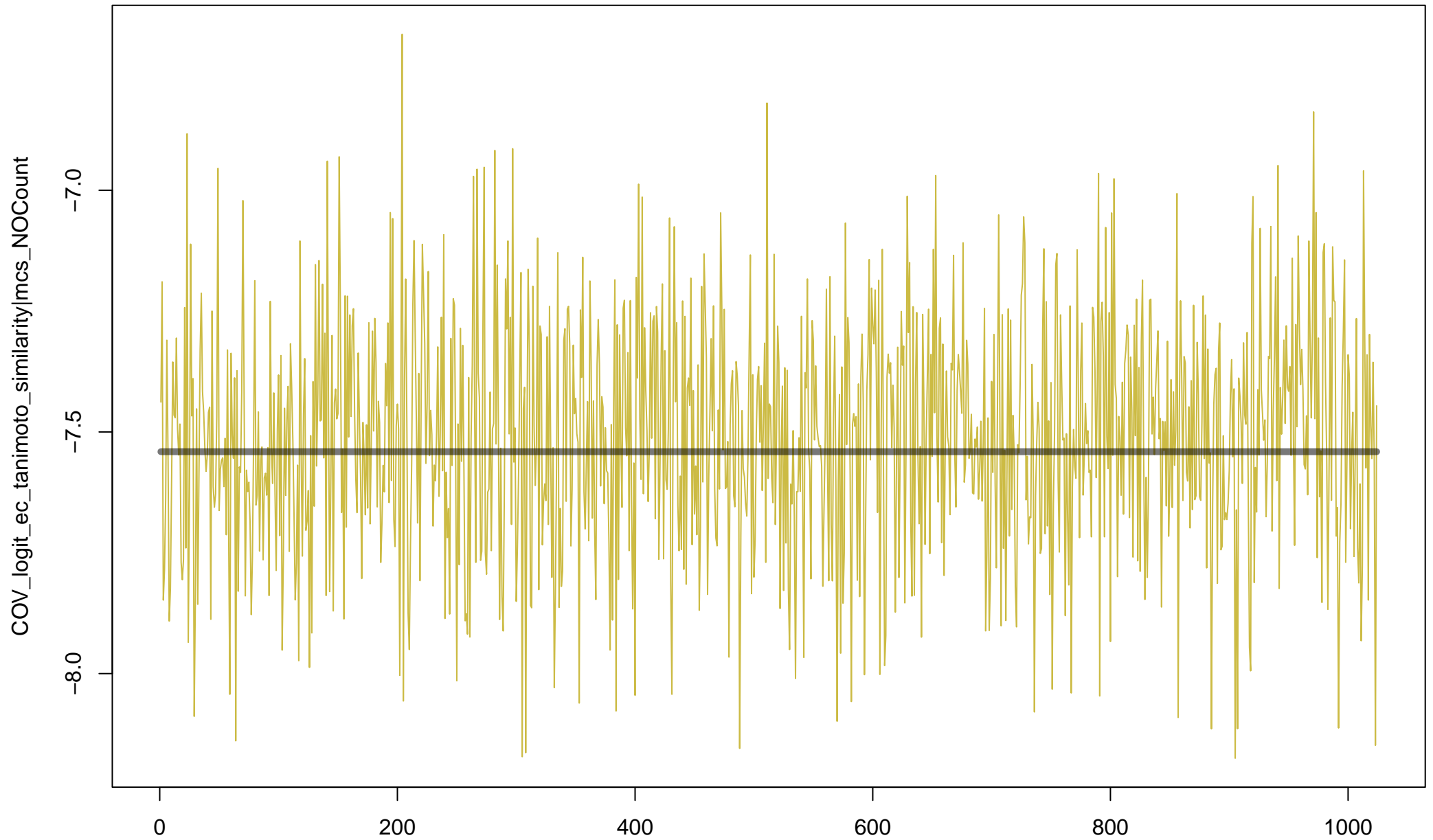
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 877 | BMK = 0.0642 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0 | percentile: 70.4



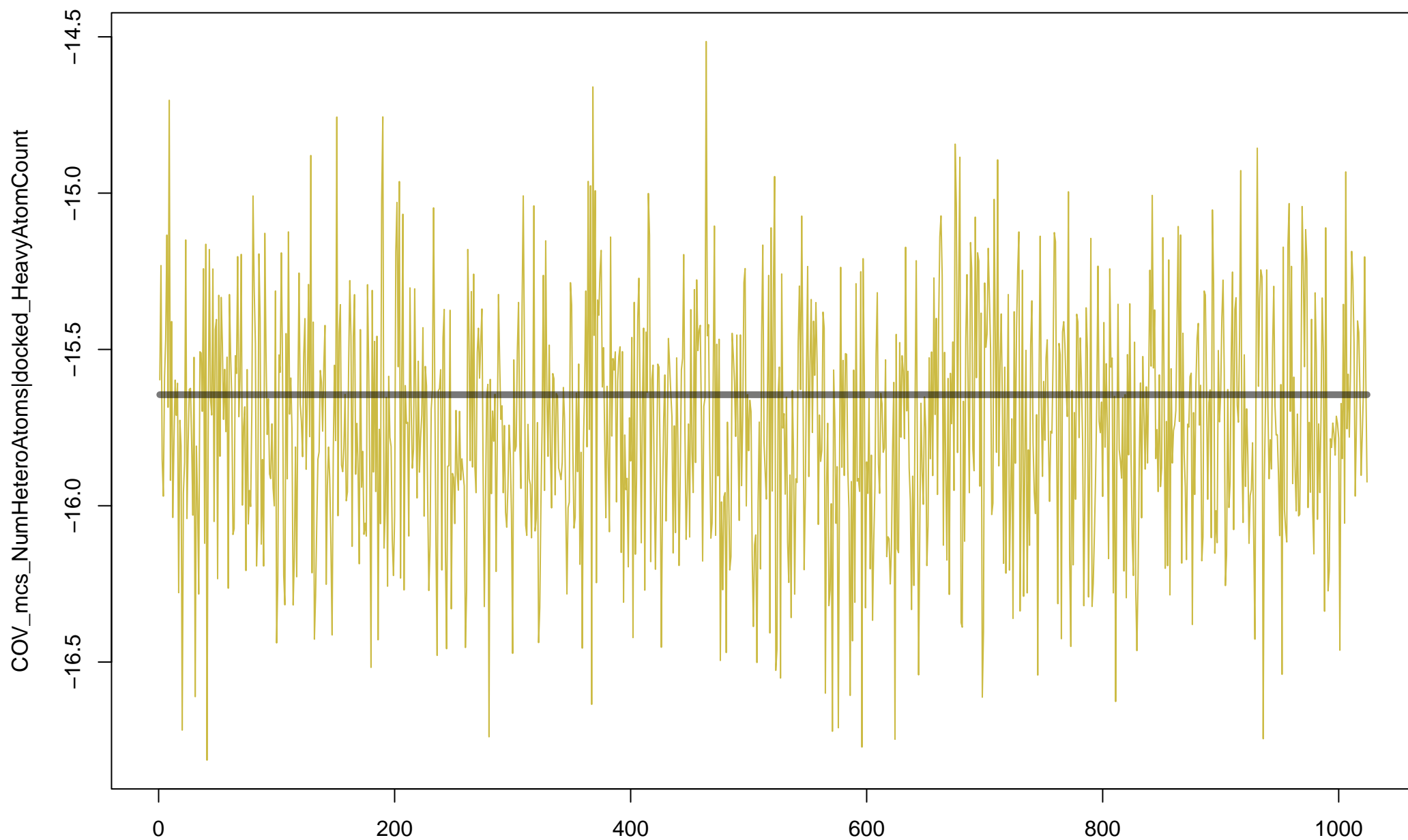
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0644 | MCSE(6.27) = 3.29 | stat: TRUE | burn: 0 | percentile: 86



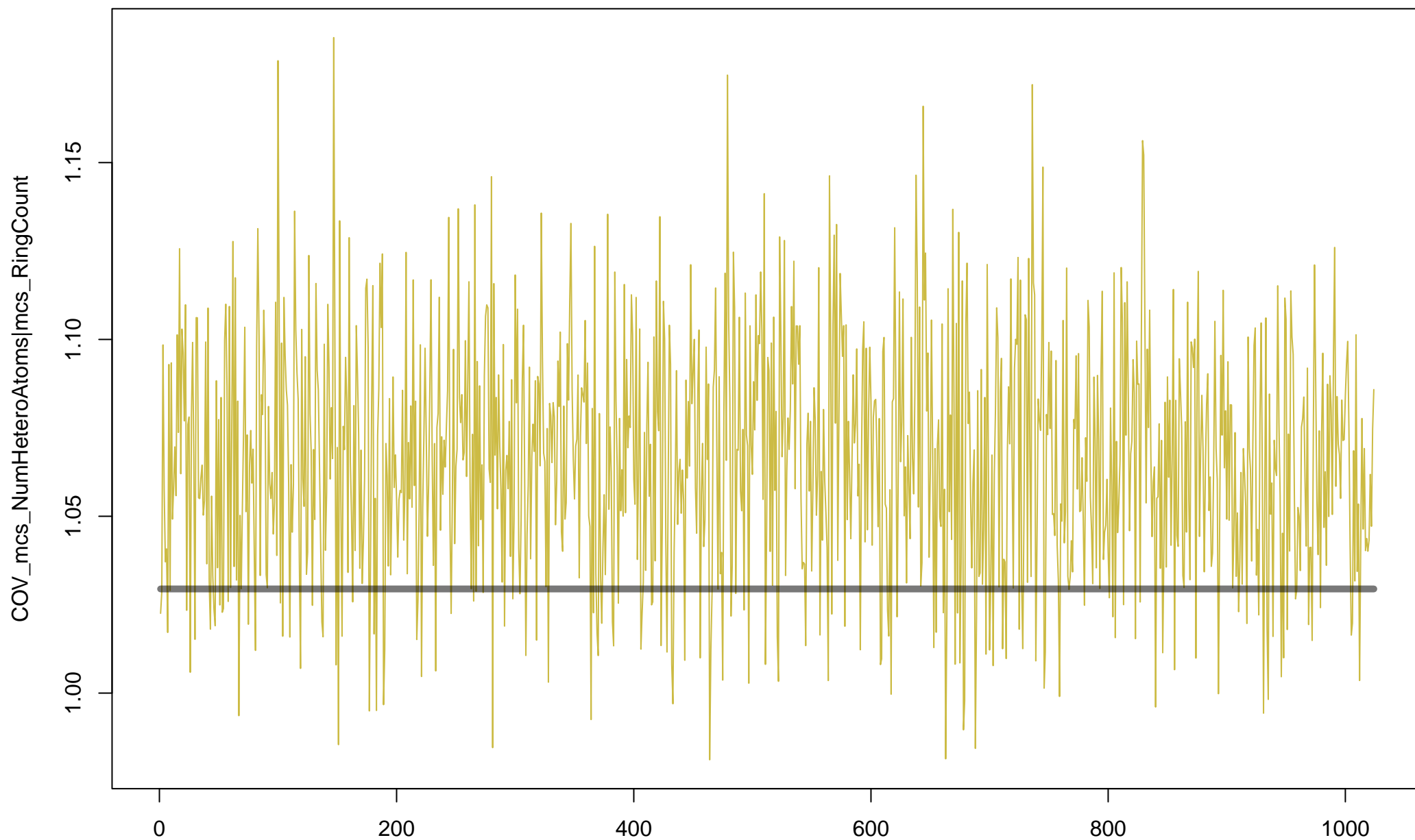
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0561 | MCSE(6.27) = 3.39 | stat: FALSE | burn: 0 | percentile: 44.7



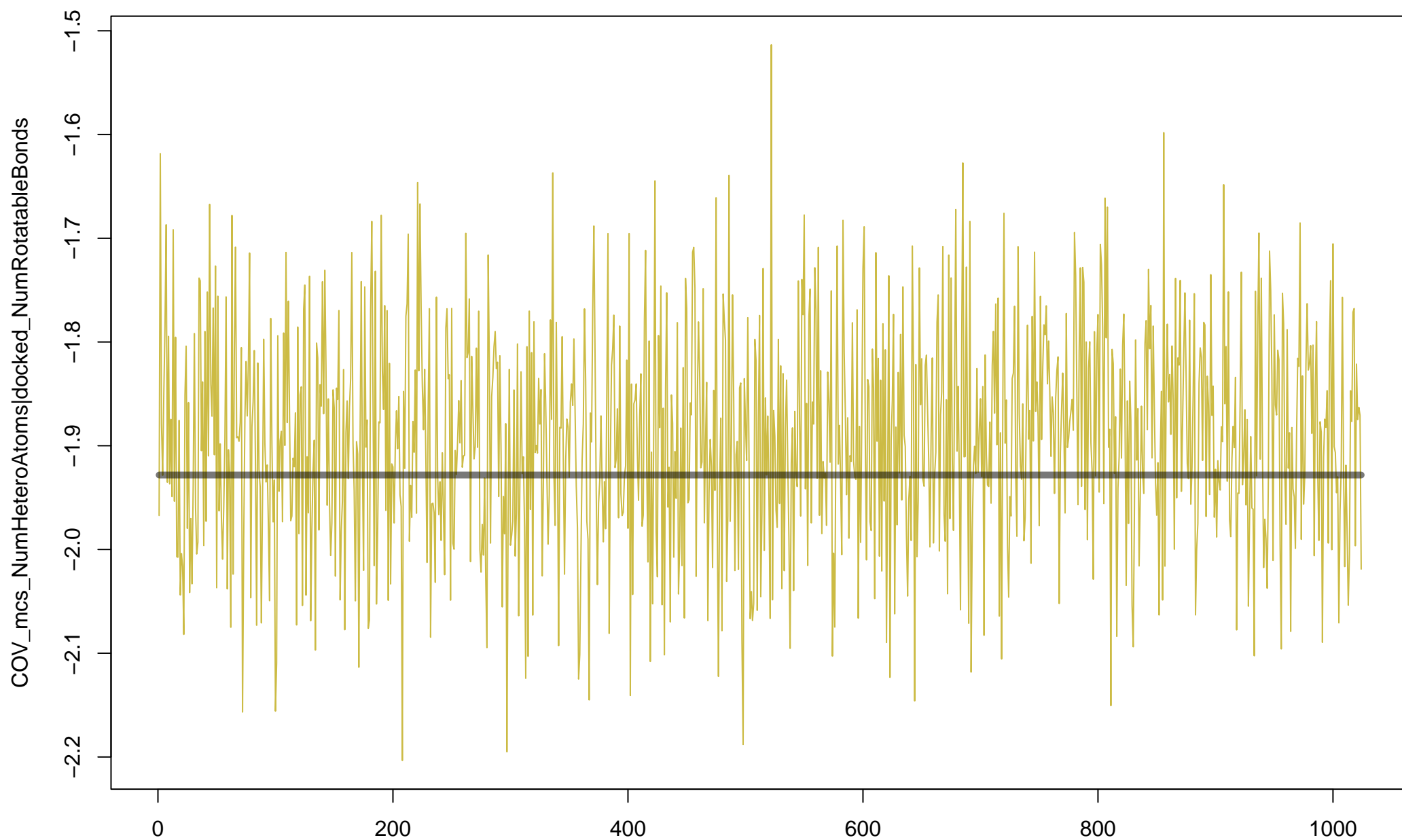
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0625 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | percentile: 60.3



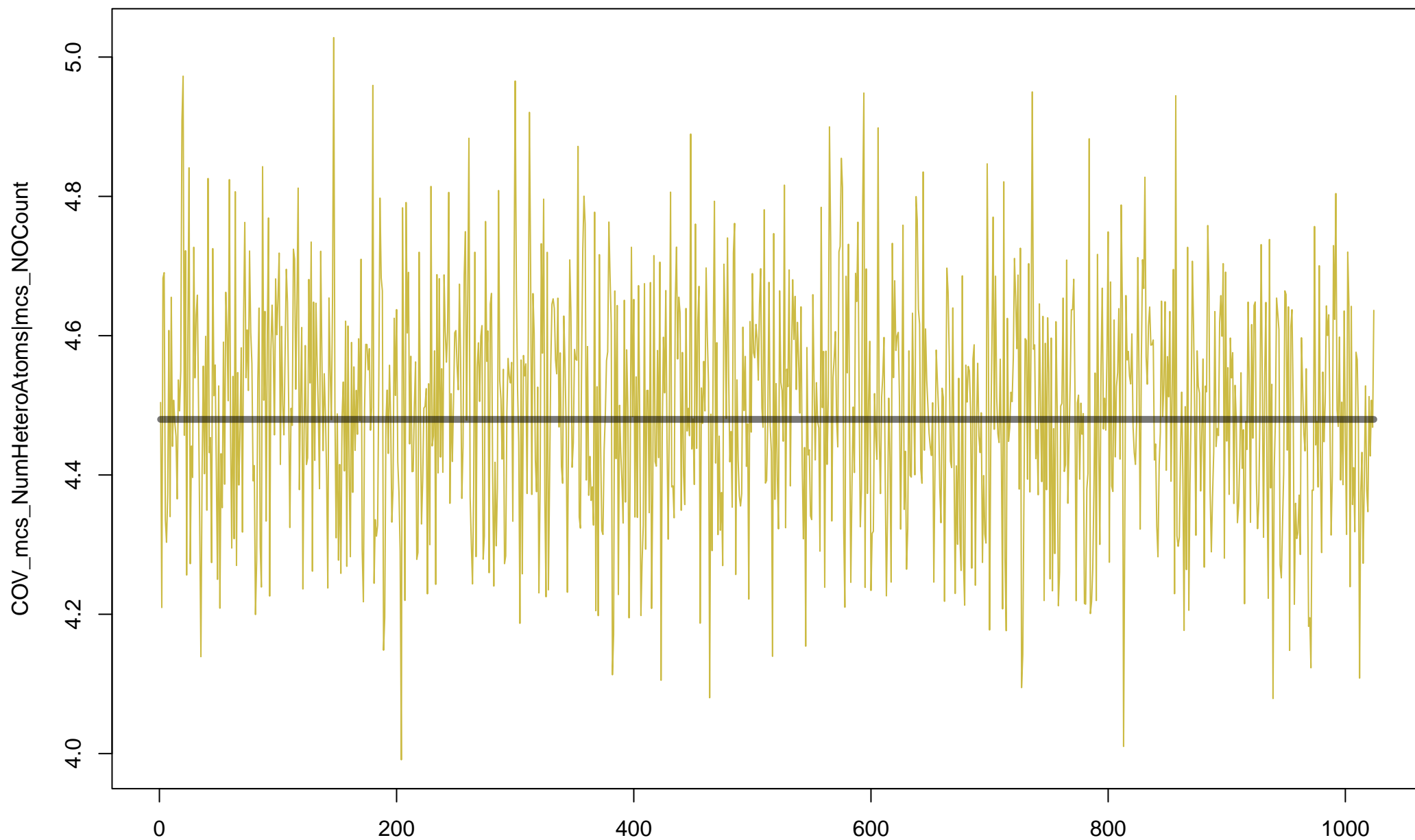
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0423 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | percentile: 14.1



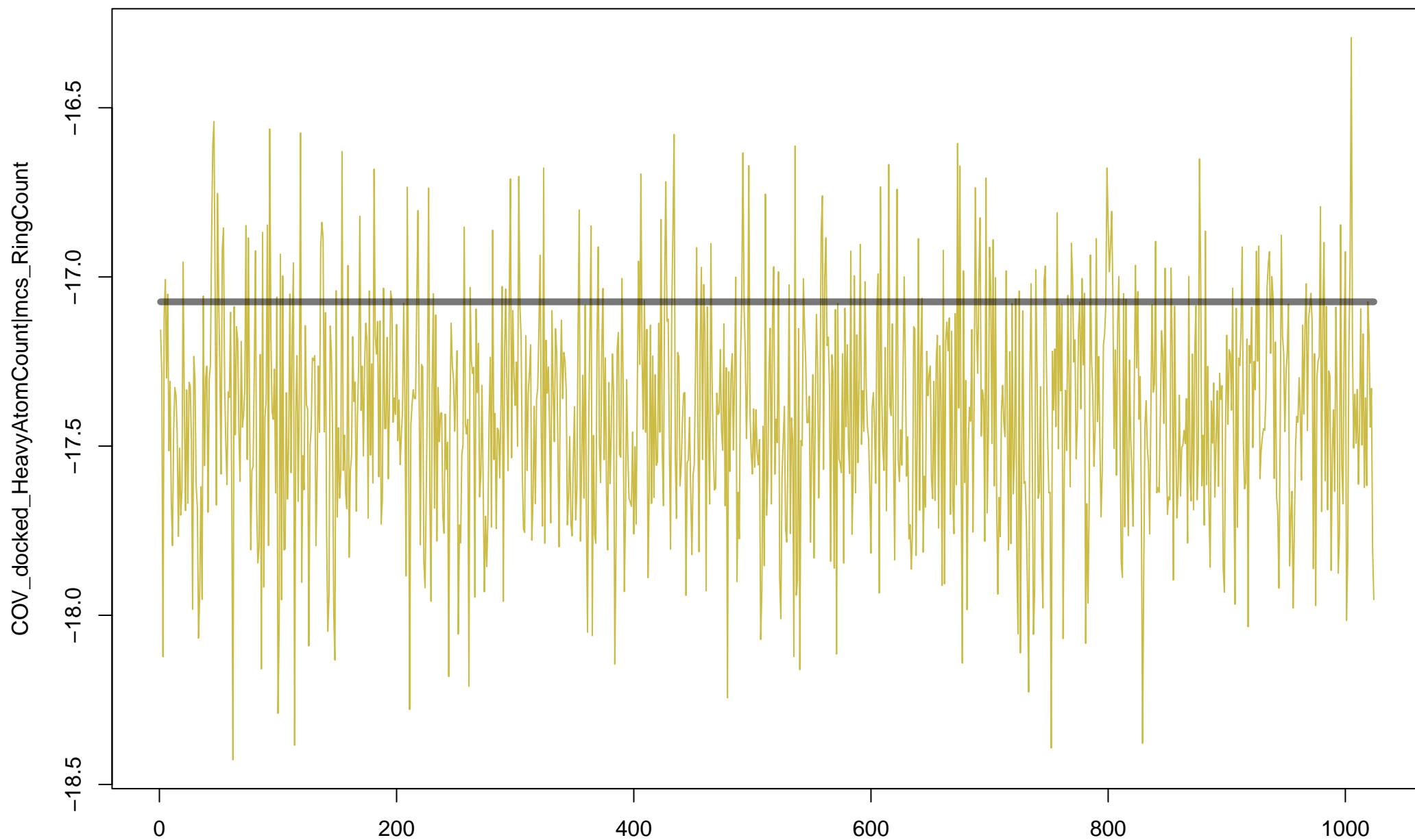
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0699 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0 | percentile: 37



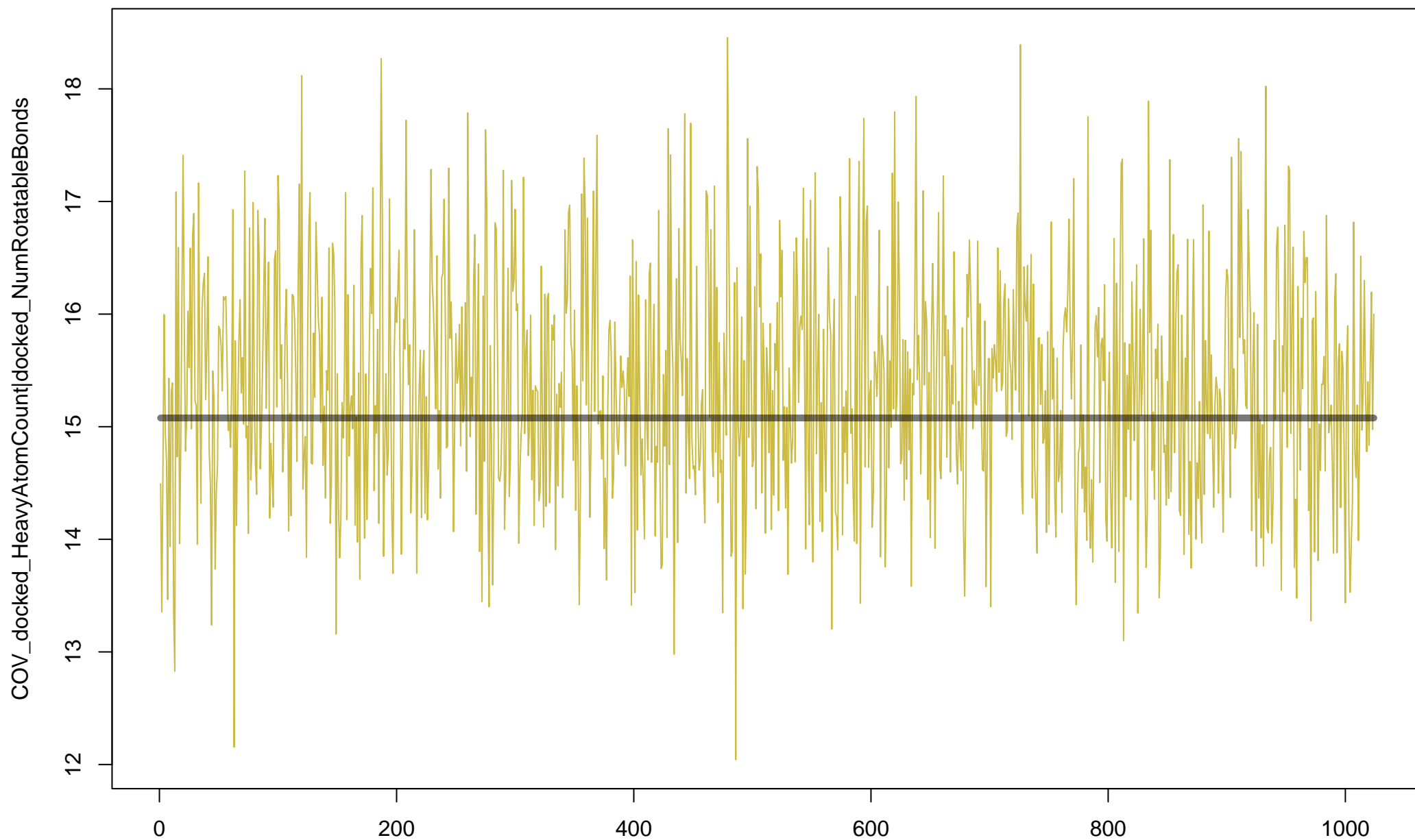
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0438 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0 | percentile: 46.3



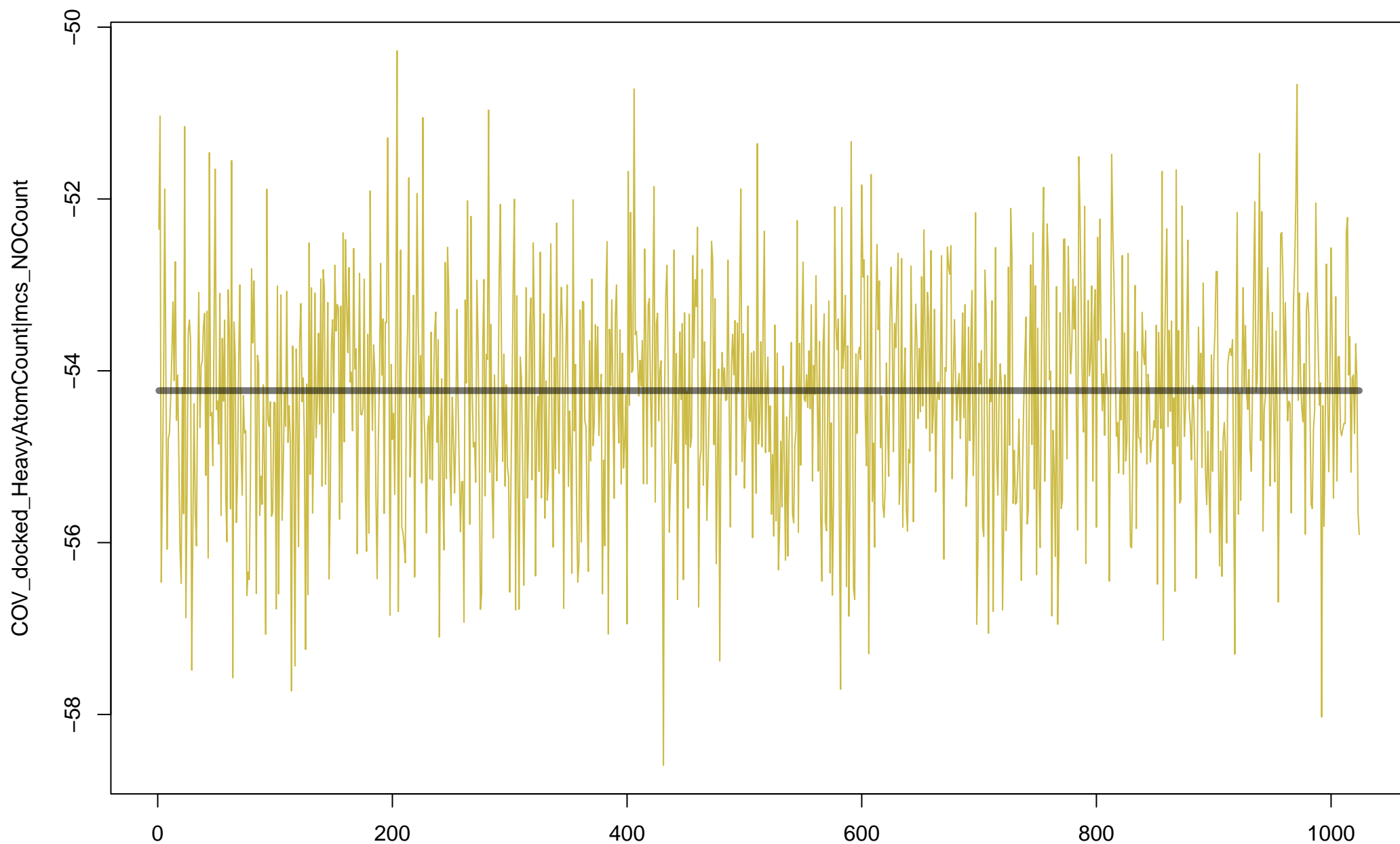
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0624 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | percentile: 84.8



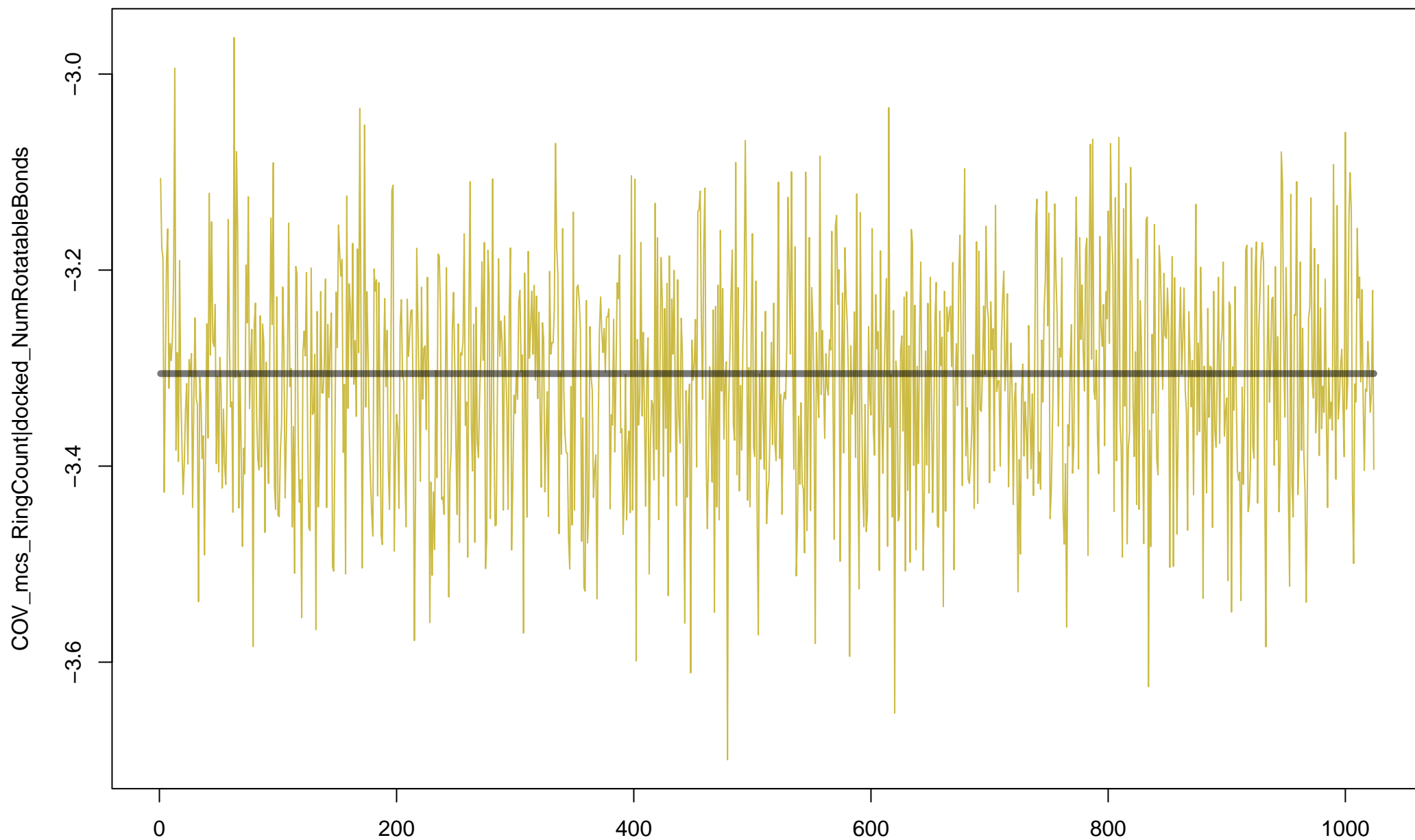
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0631 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | percentile: 40.5



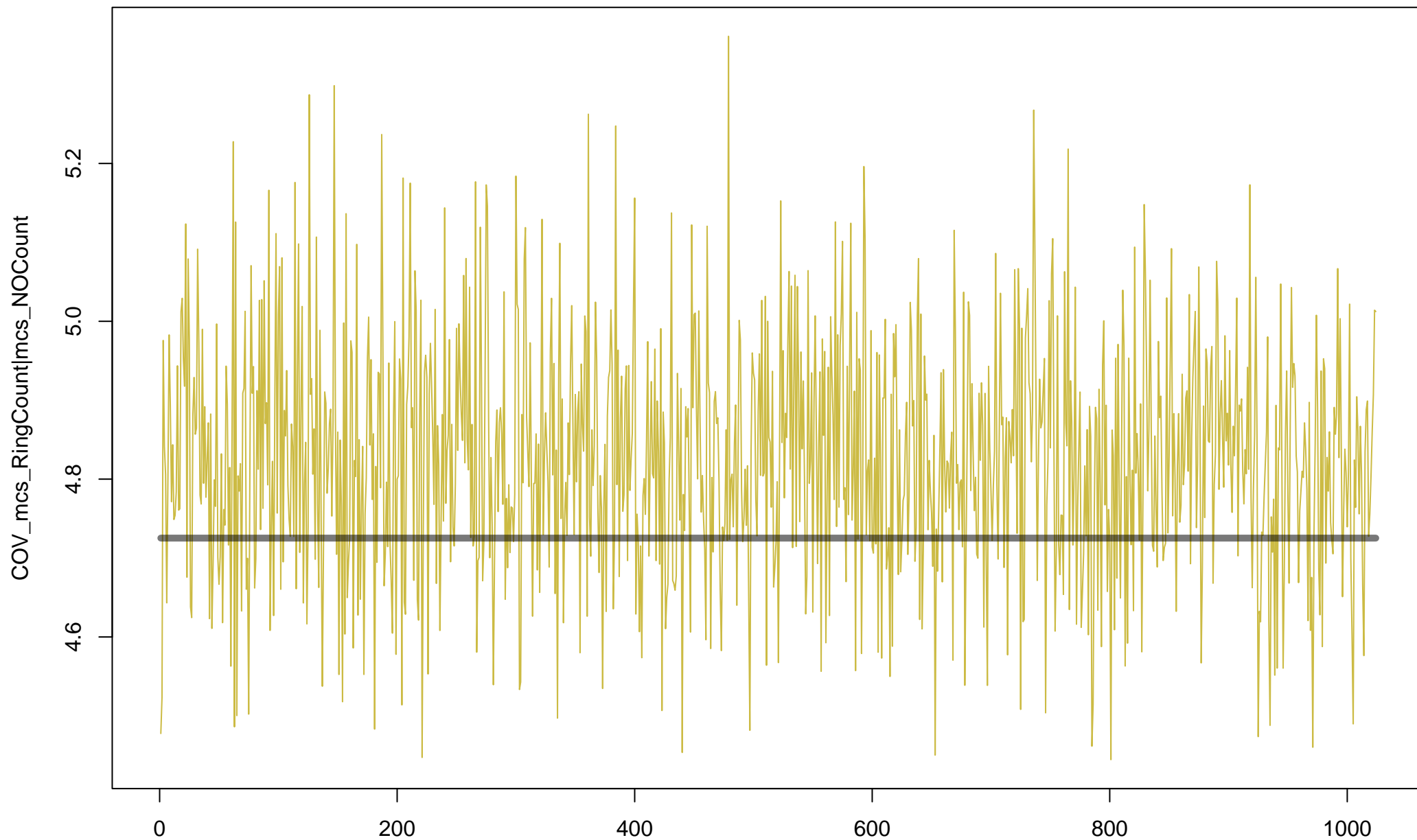
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 653 | BMK = 0.0622 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0 | percentile: 52.7



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0514 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | percentile: 53



COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.0655 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | percentile: 24.9



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0497 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0 | percentile: 38.3

