

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 1

max MCSE = 11.2328734850634

all stationary: FALSE

burn: 1020

min percent.: 1.3671875

-- STATS 2D --

min ESS = 693.910264905334

max BMK = 0.0814494399162979

max MCSE = 4.02585765941912

all stationary: FALSE

burn: 0

min percent.: 1.5625

-- STATS 1D --

min ESS = 41.9155726876132

max BMK = 1

max MCSE = 9.77269637877877

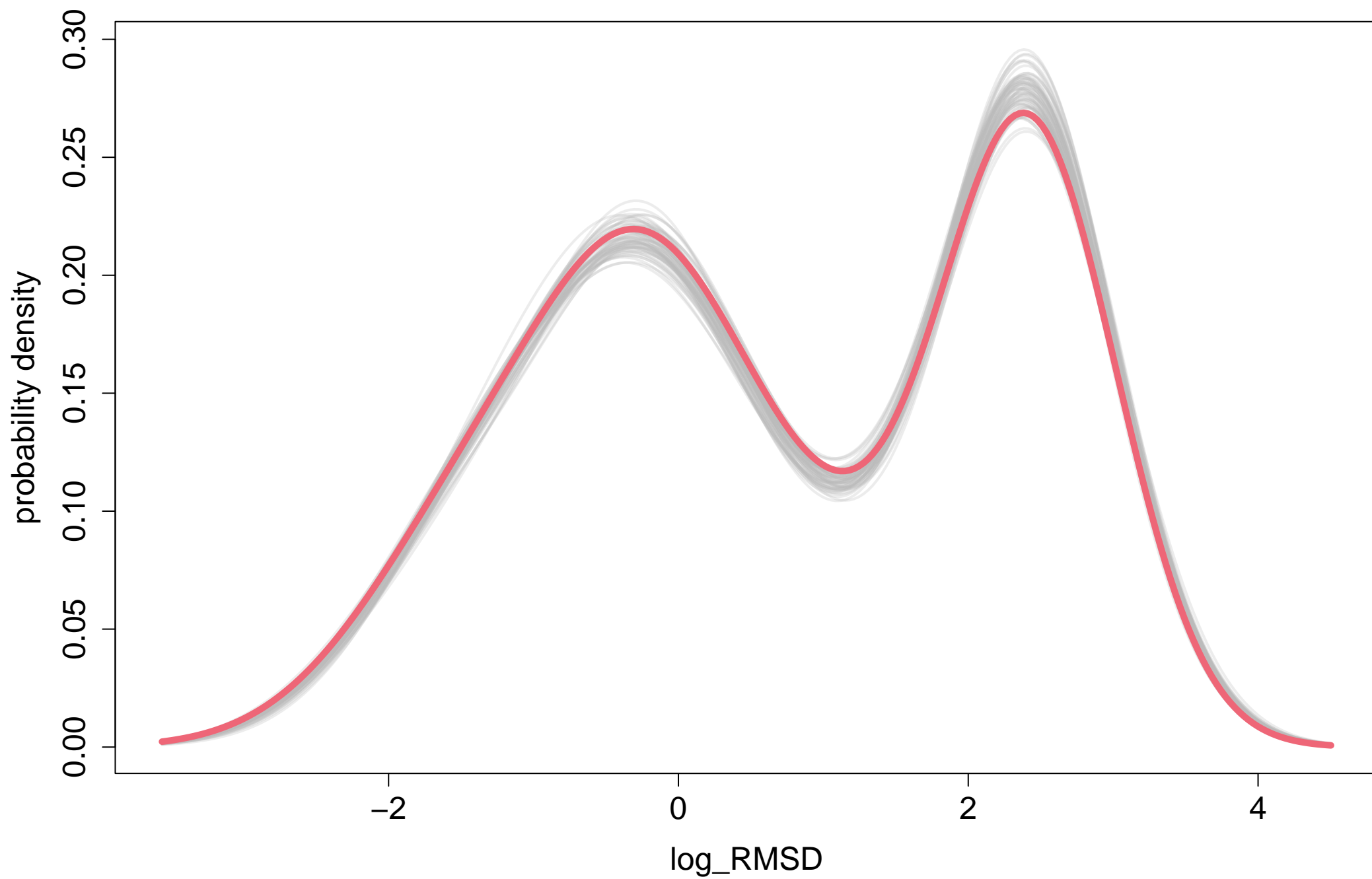
all stationary: FALSE

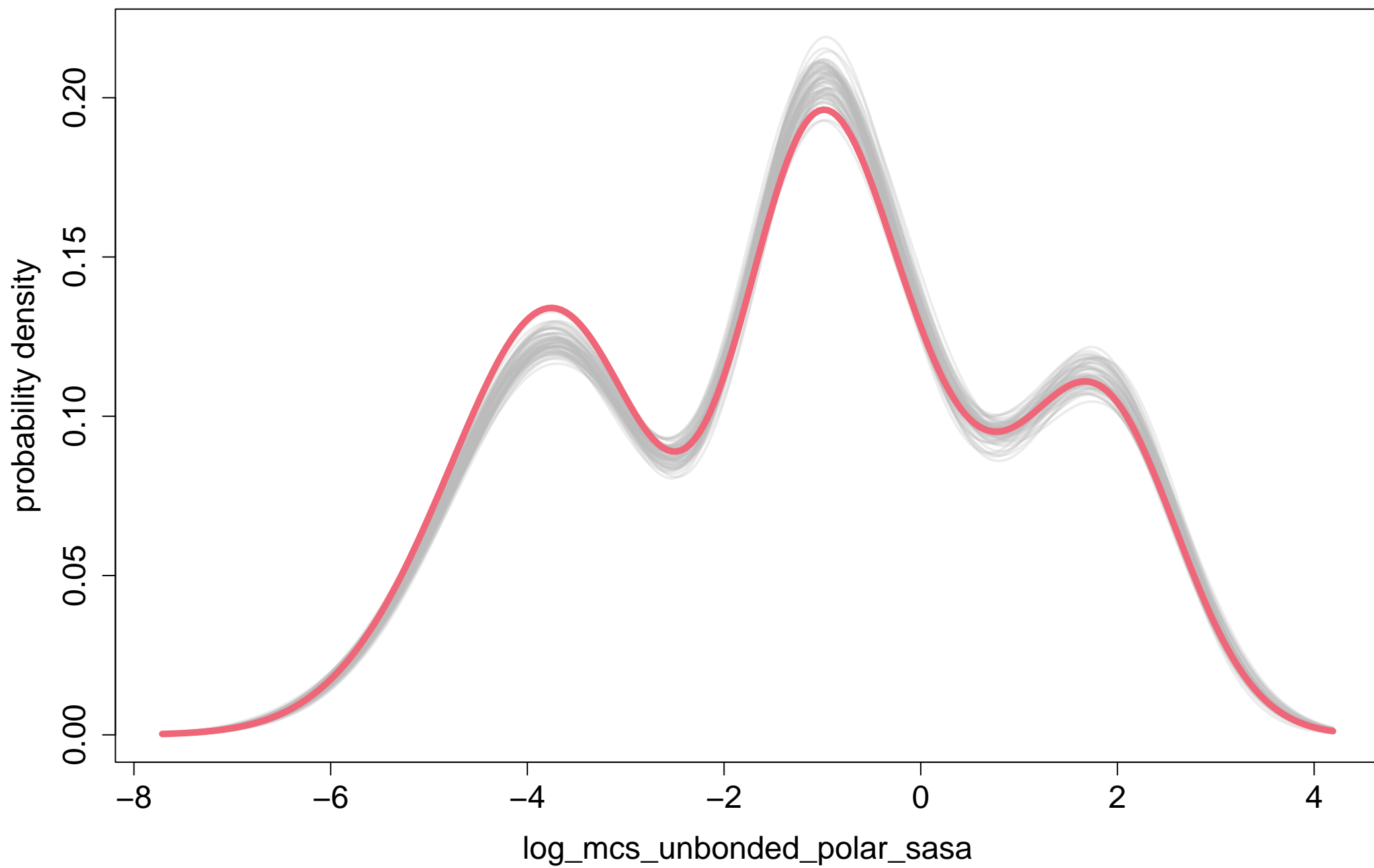
burn: 1020

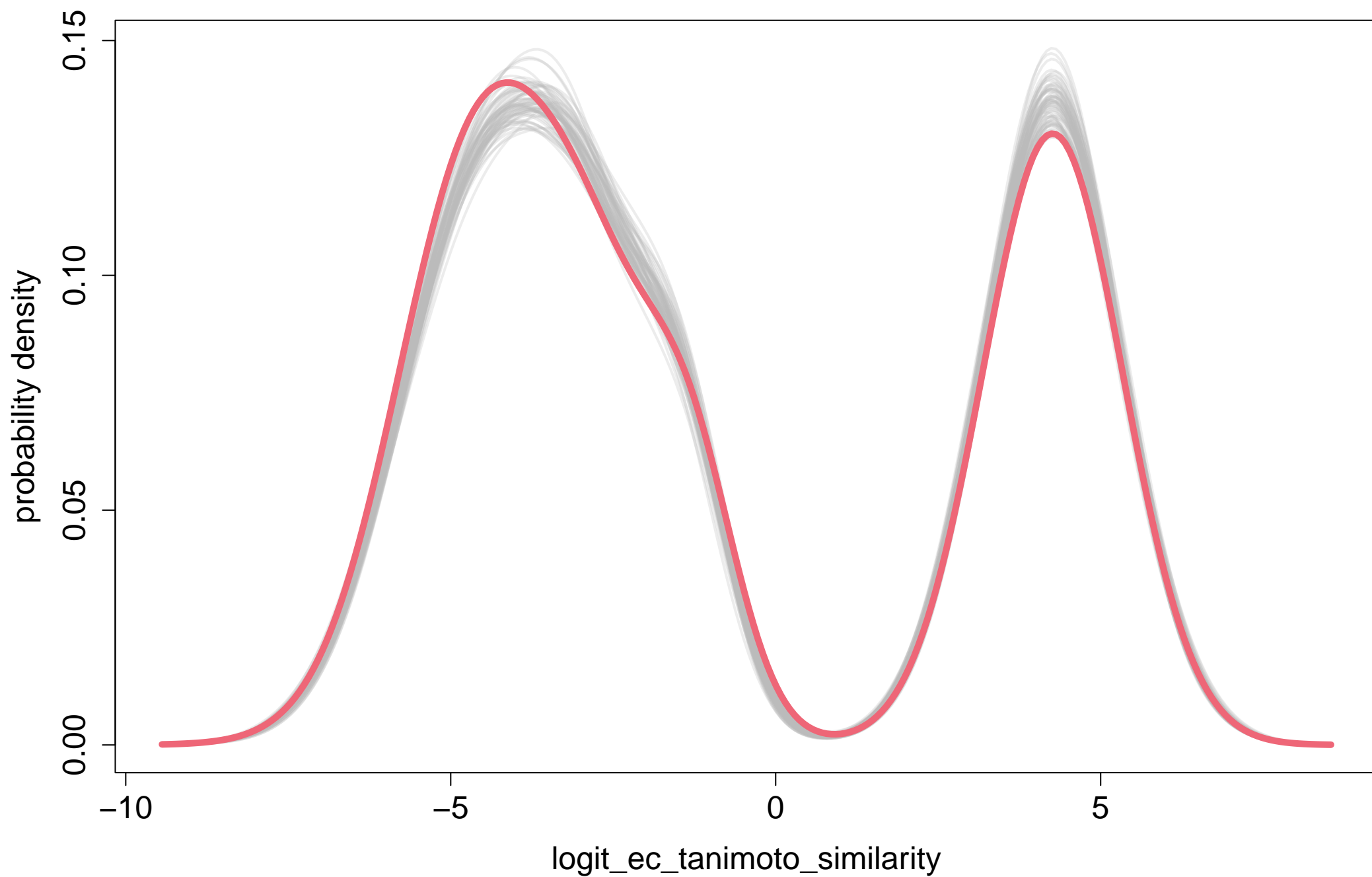
min percent.: 0.5859375

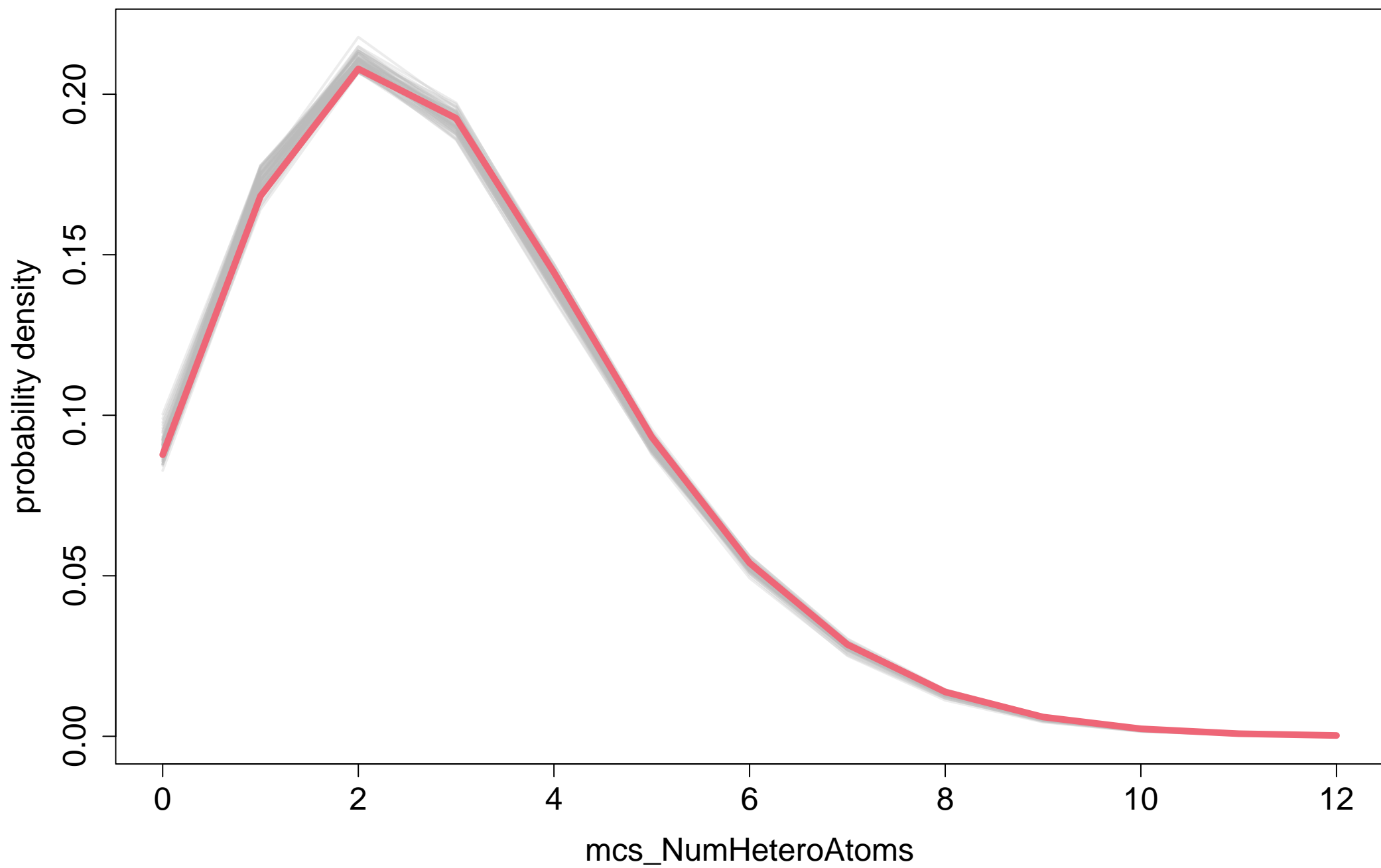
Occupied clusters: 9 of 64

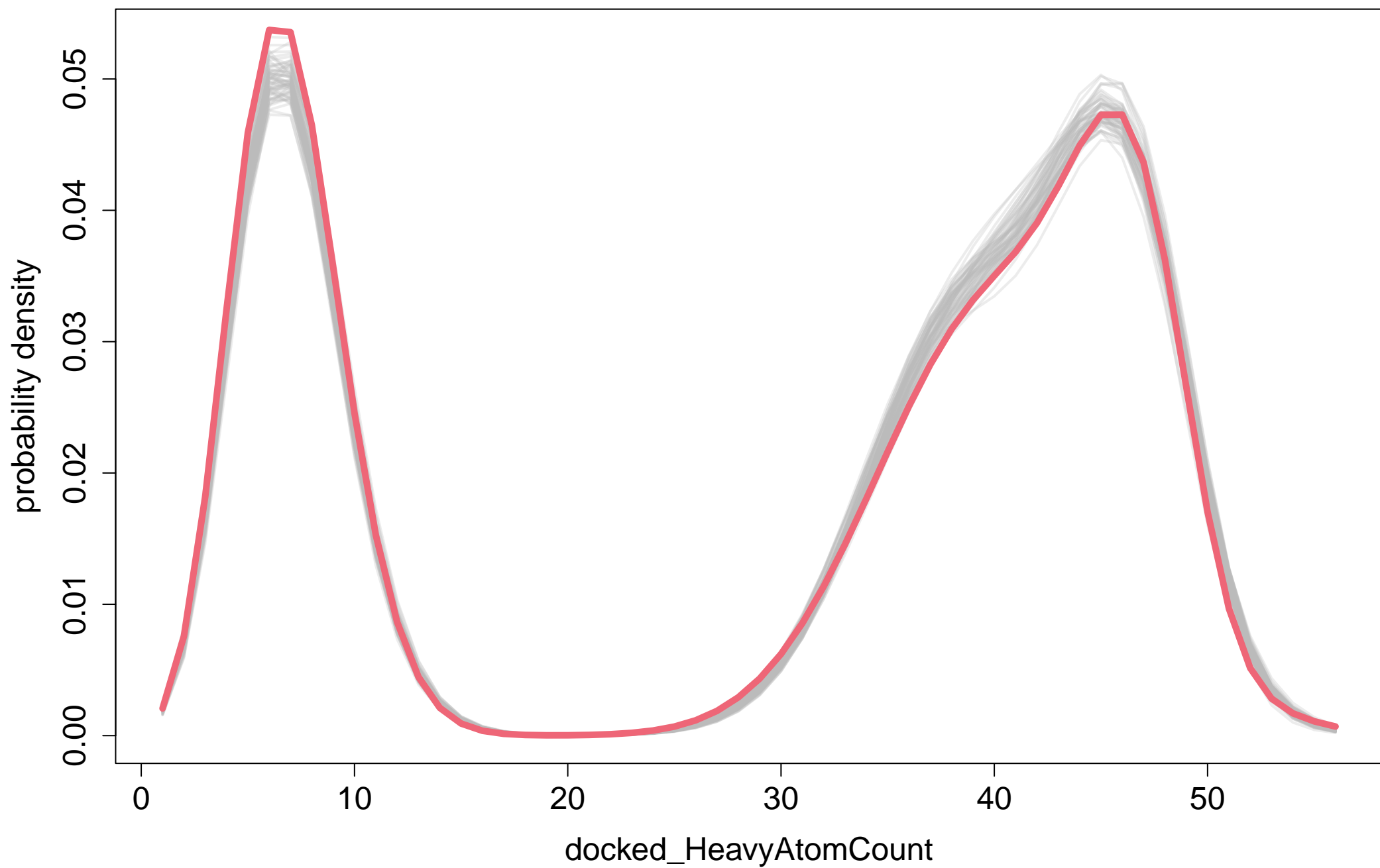
LL: -62400 +- 8.29

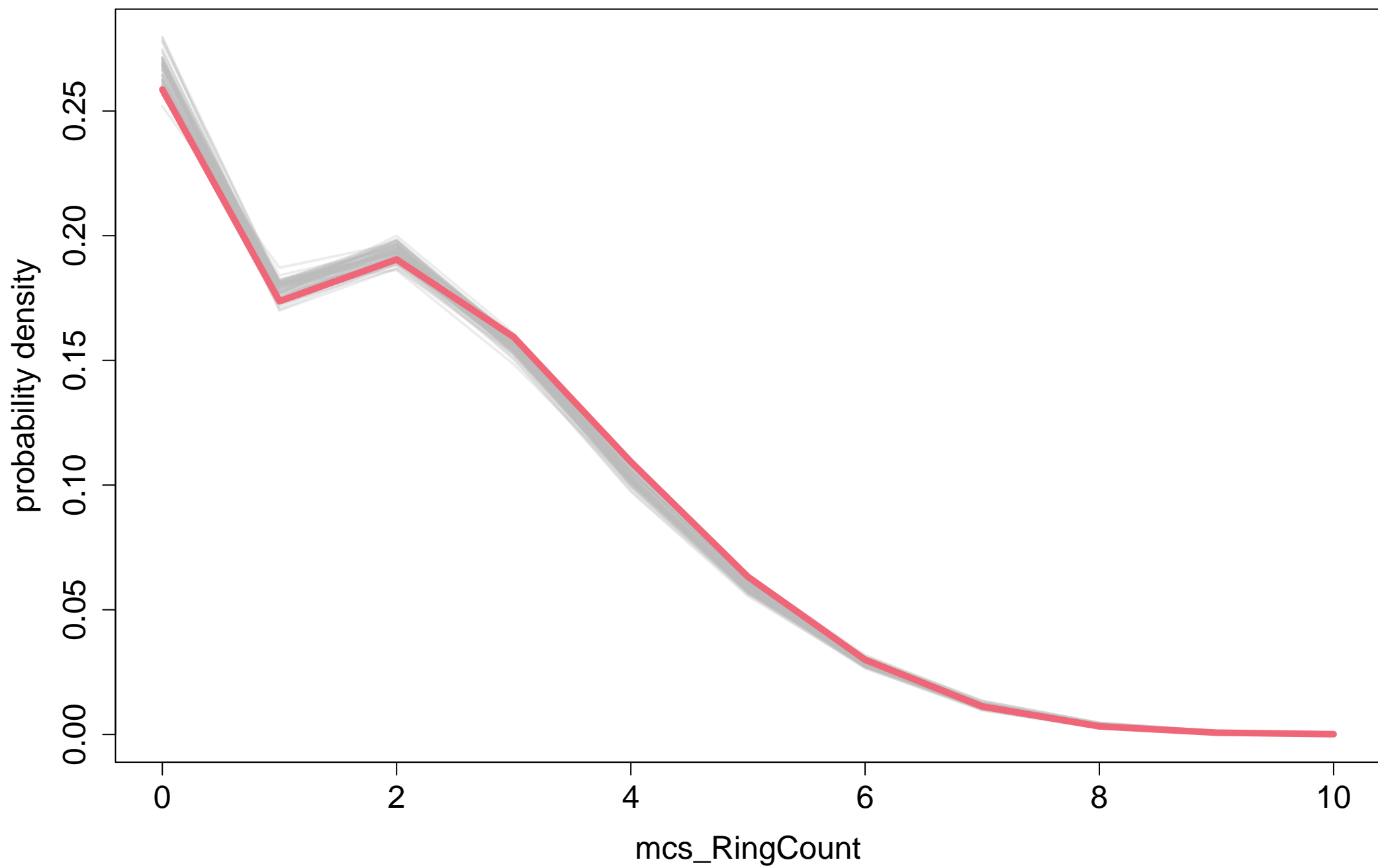


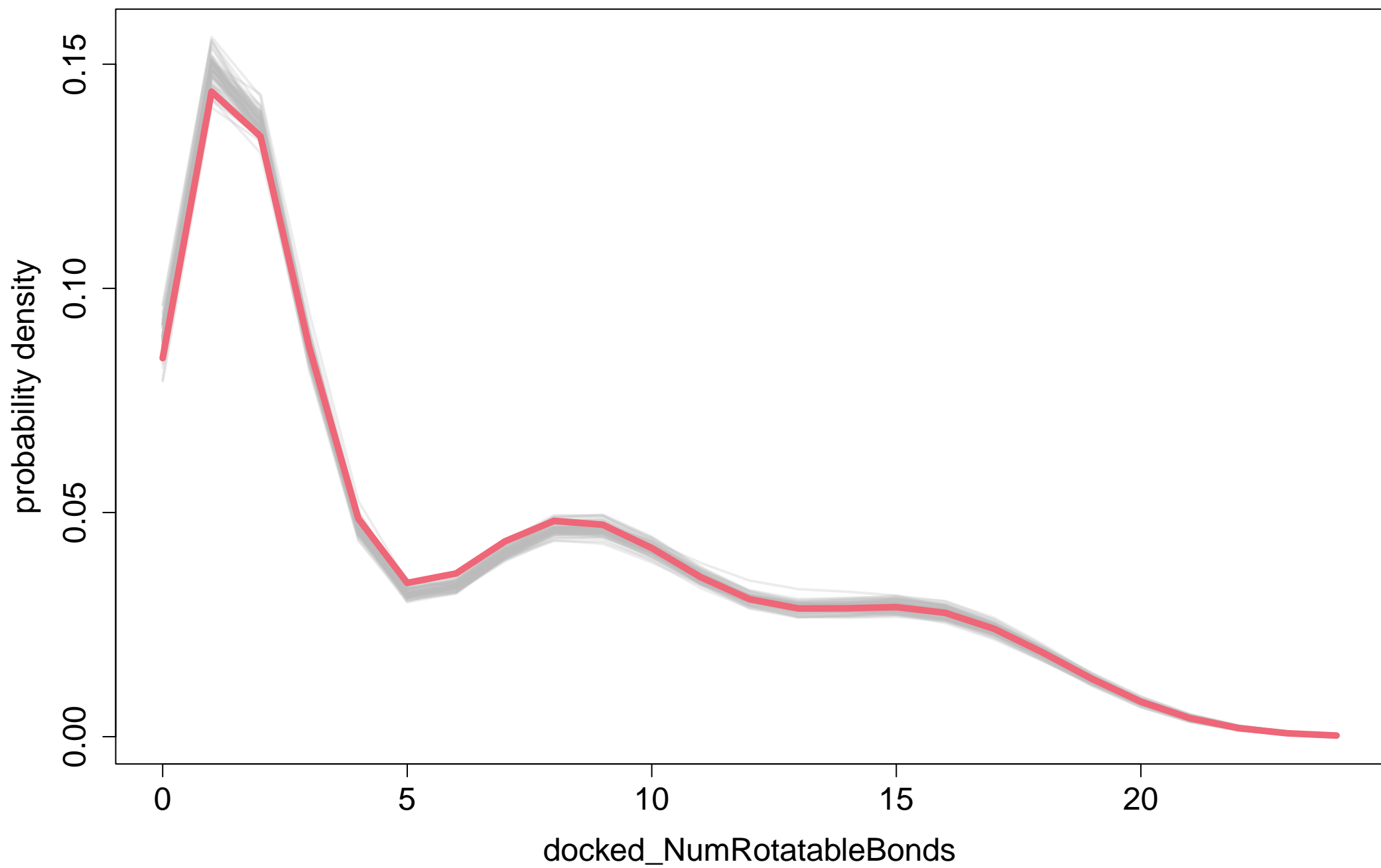


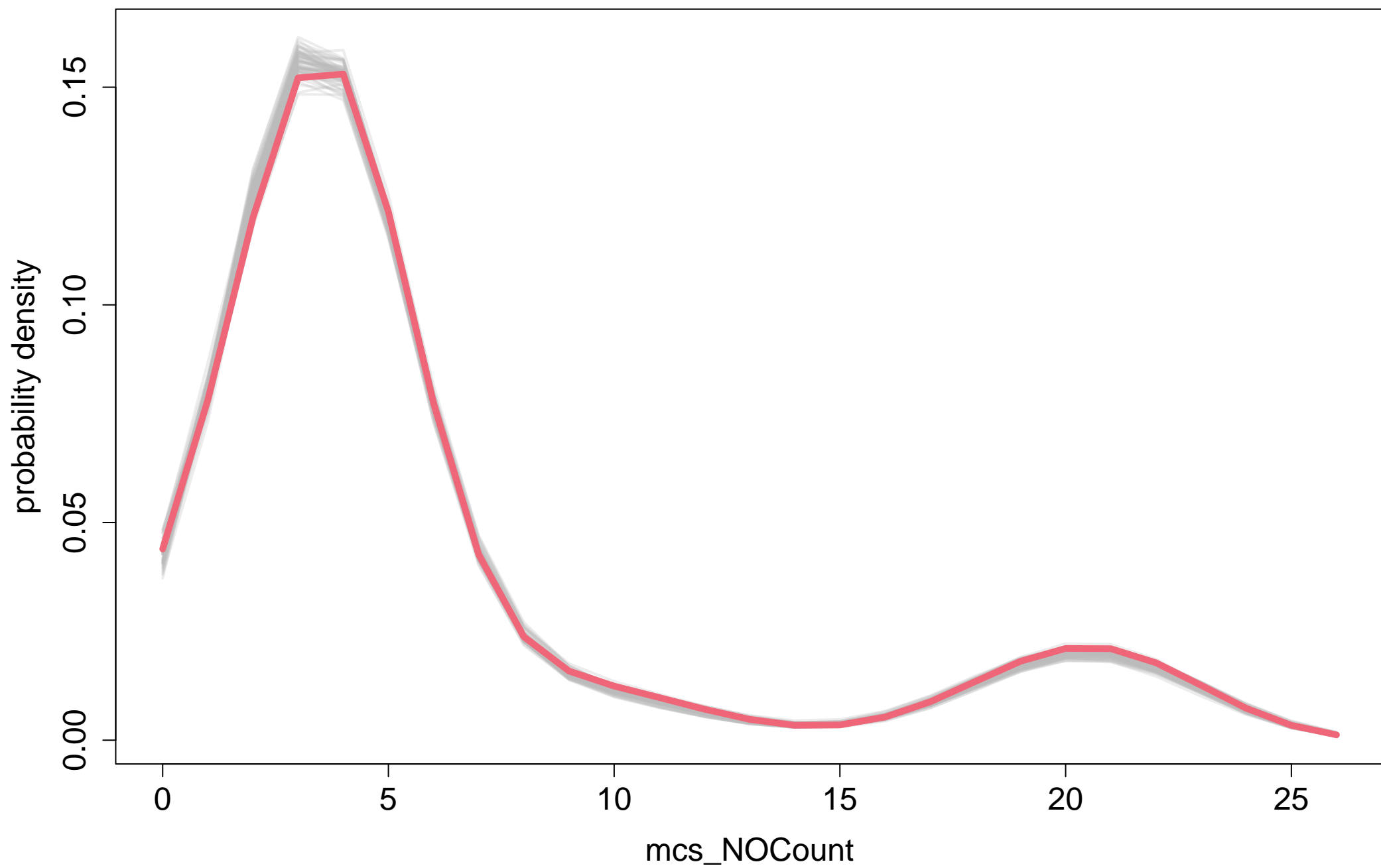


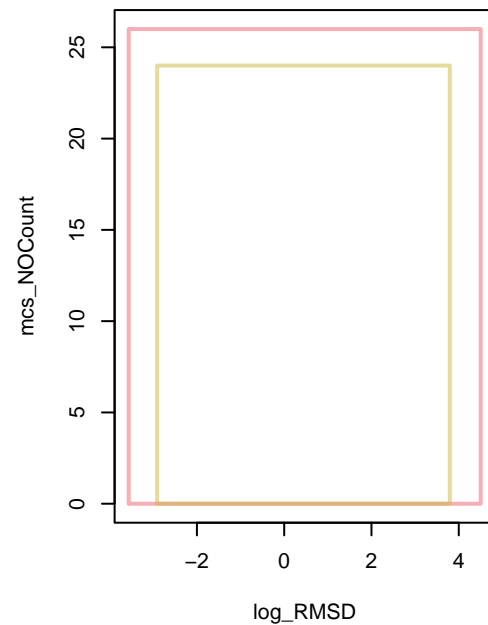
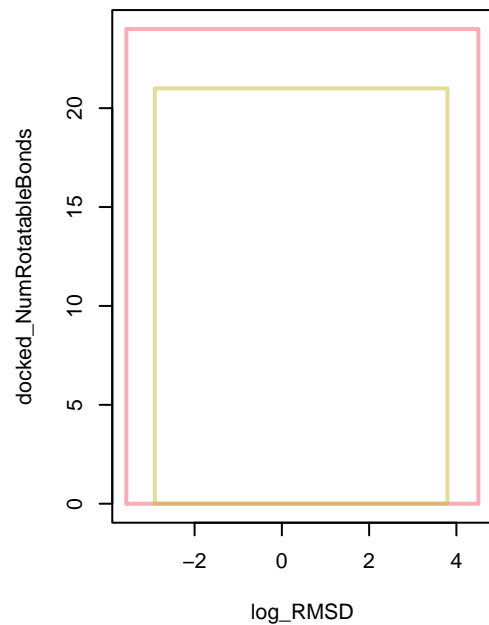
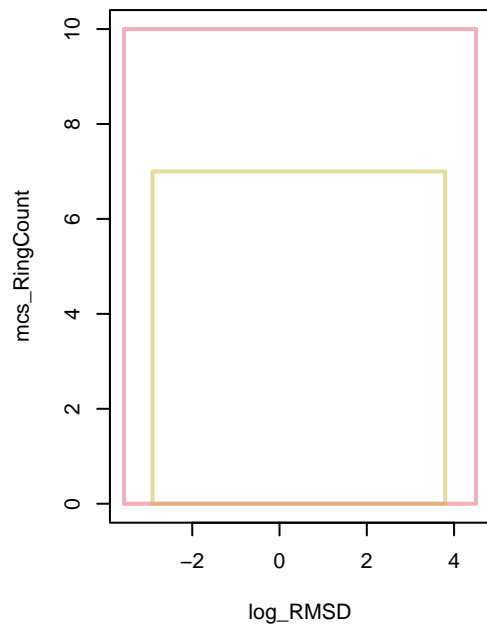
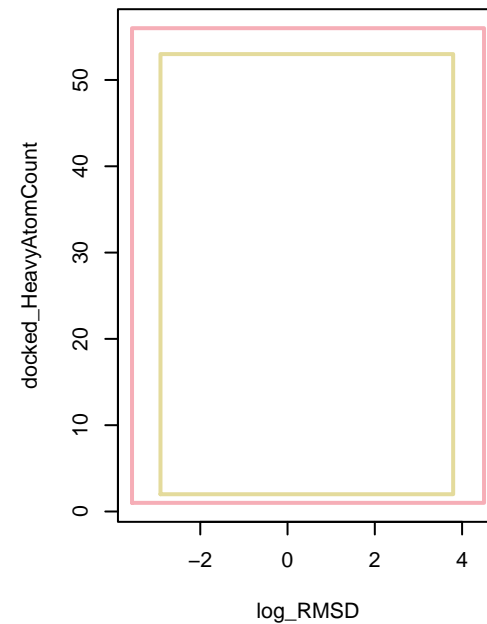
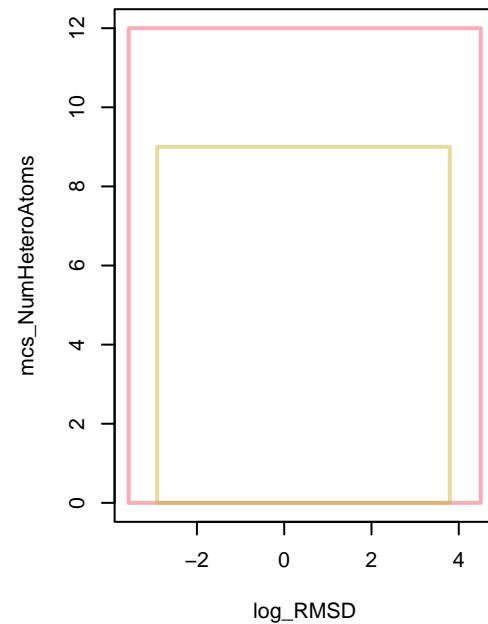
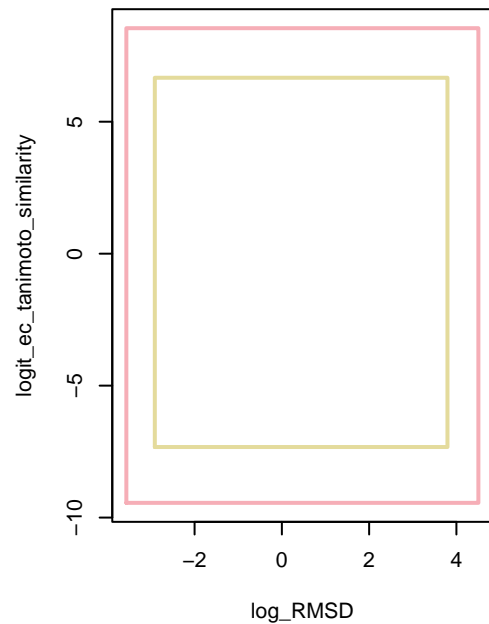
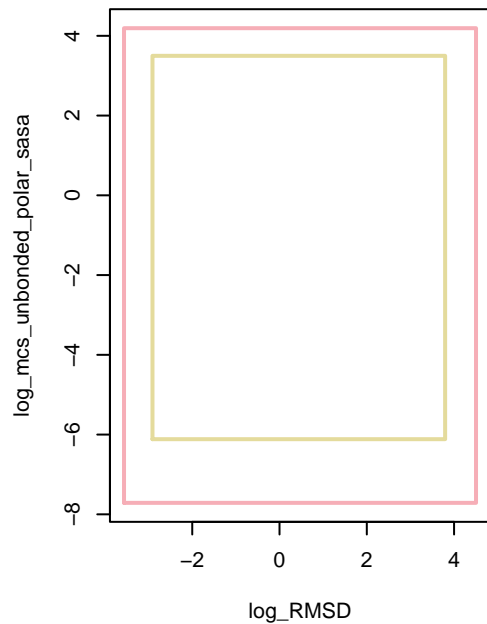




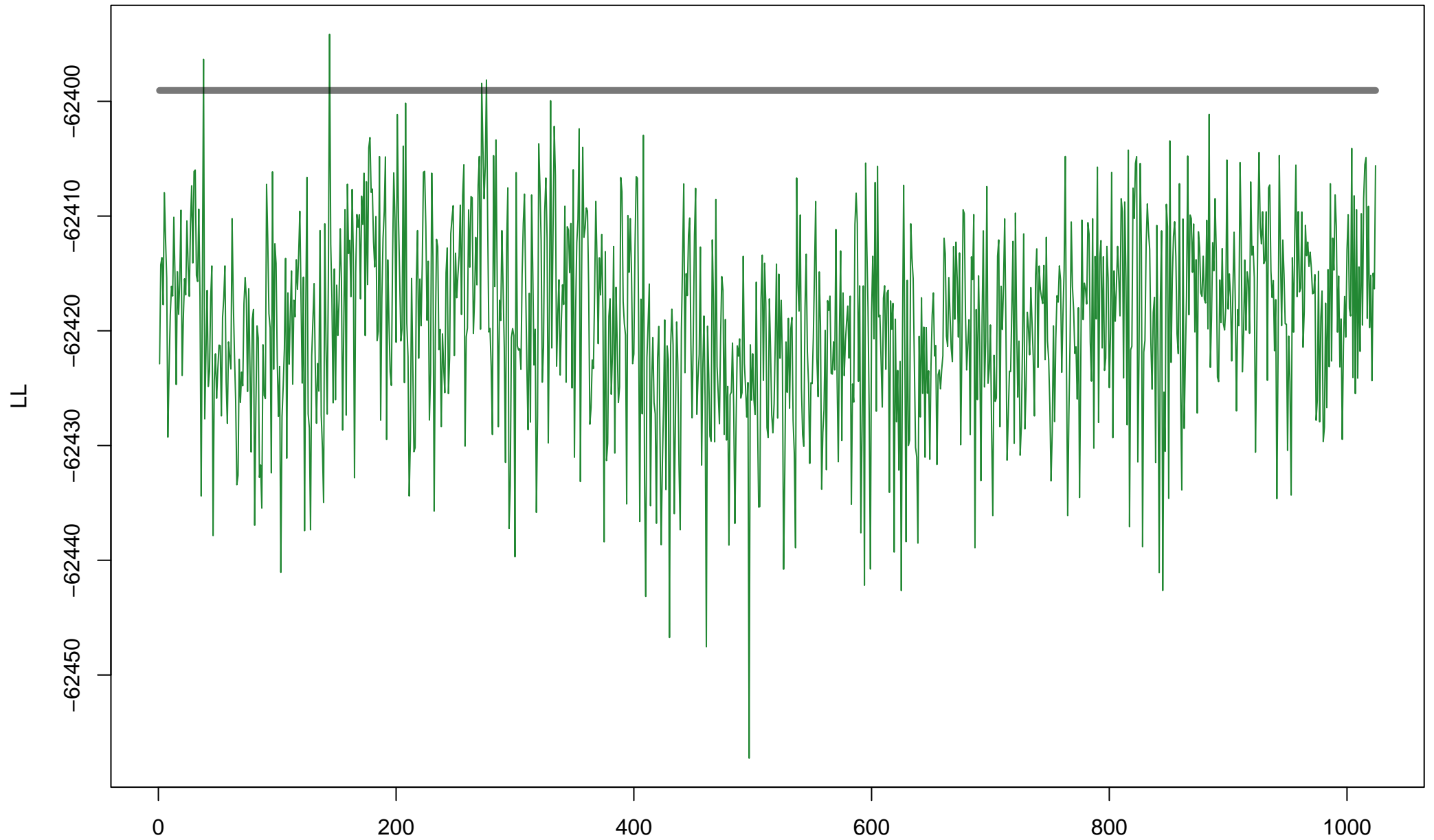






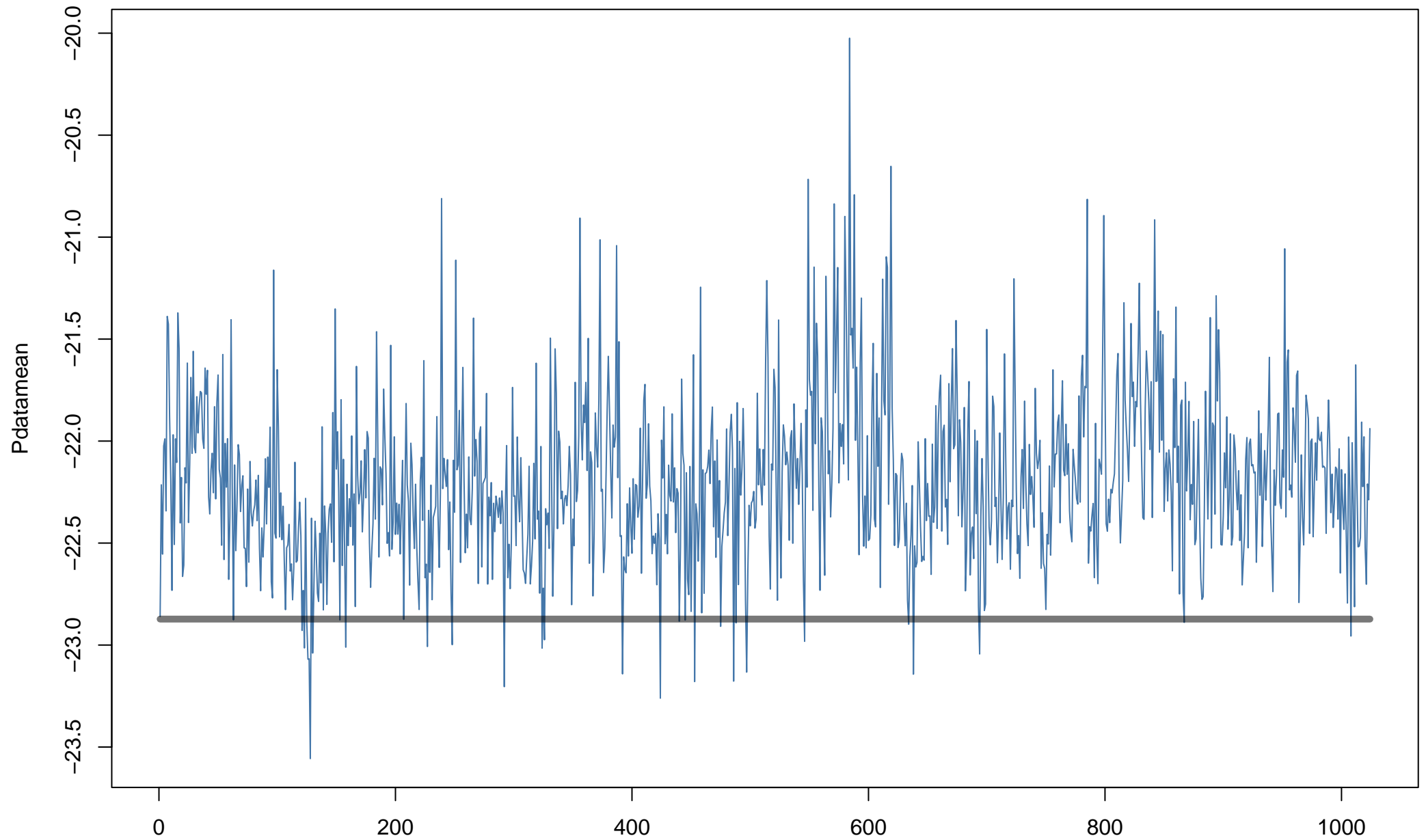


LL



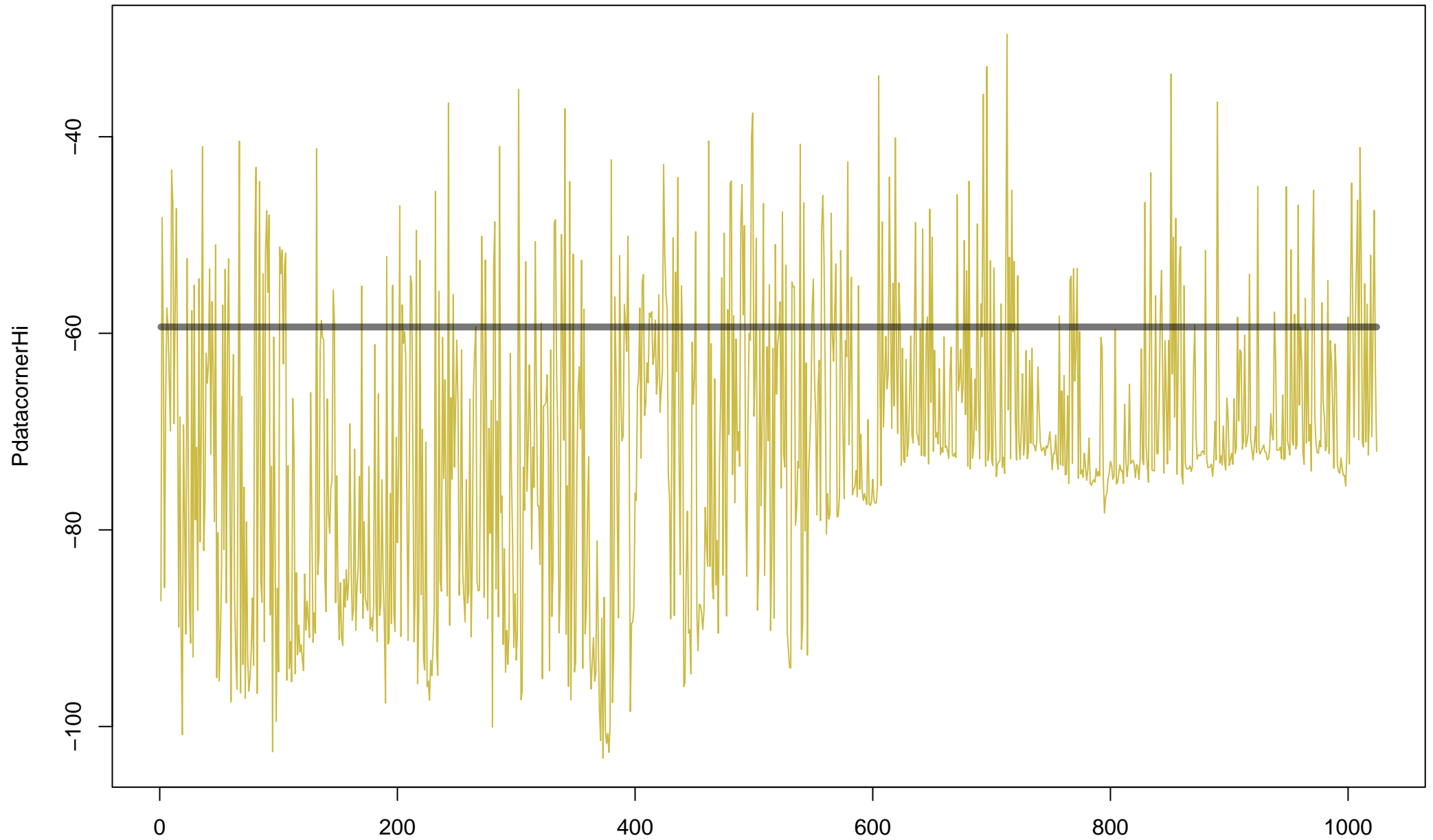
Pdatamean

ESS = 2.22e-16 | BMK = 0.157 | MCSE(6.27) = 6.34 | stat: TRUE | burn: 0 | percentile: 3.03



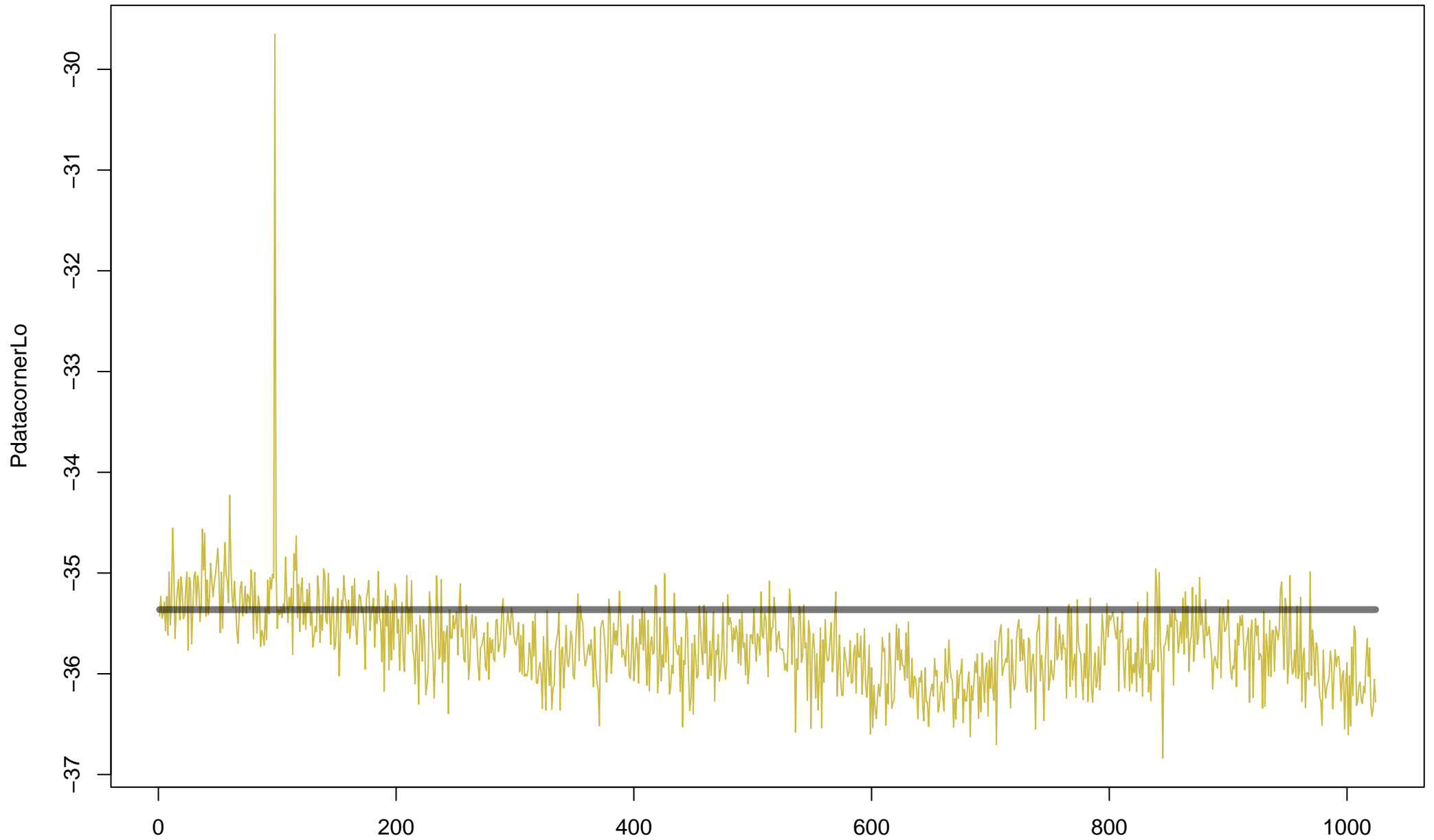
PdatacornerHi

ESS = 2.22e-16 | BMK = 1 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 1020 | percentile: 80.3



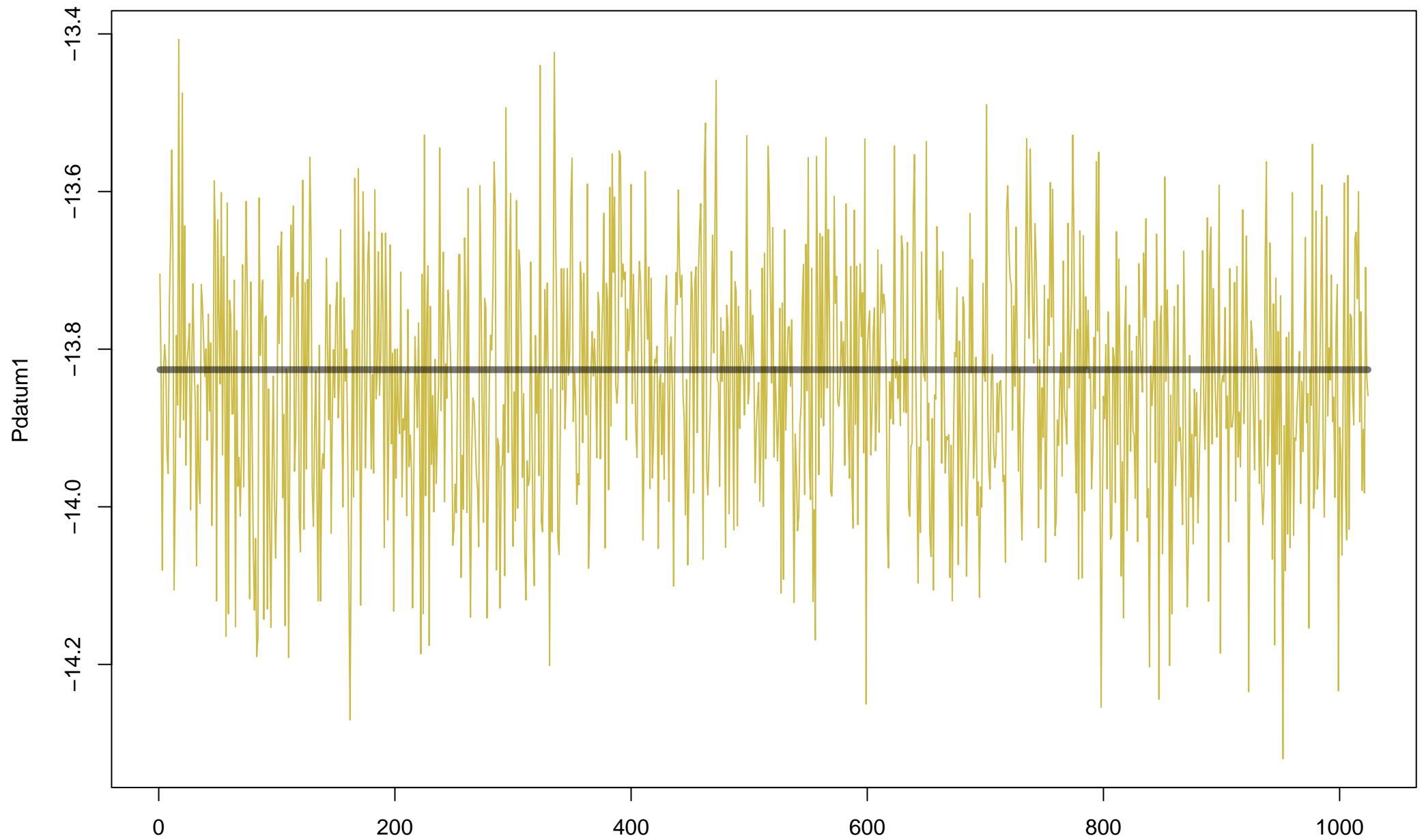
PdatacornerLo

ESS = 2.22e-16 | BMK = 0.381 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 102 | percentile: 82



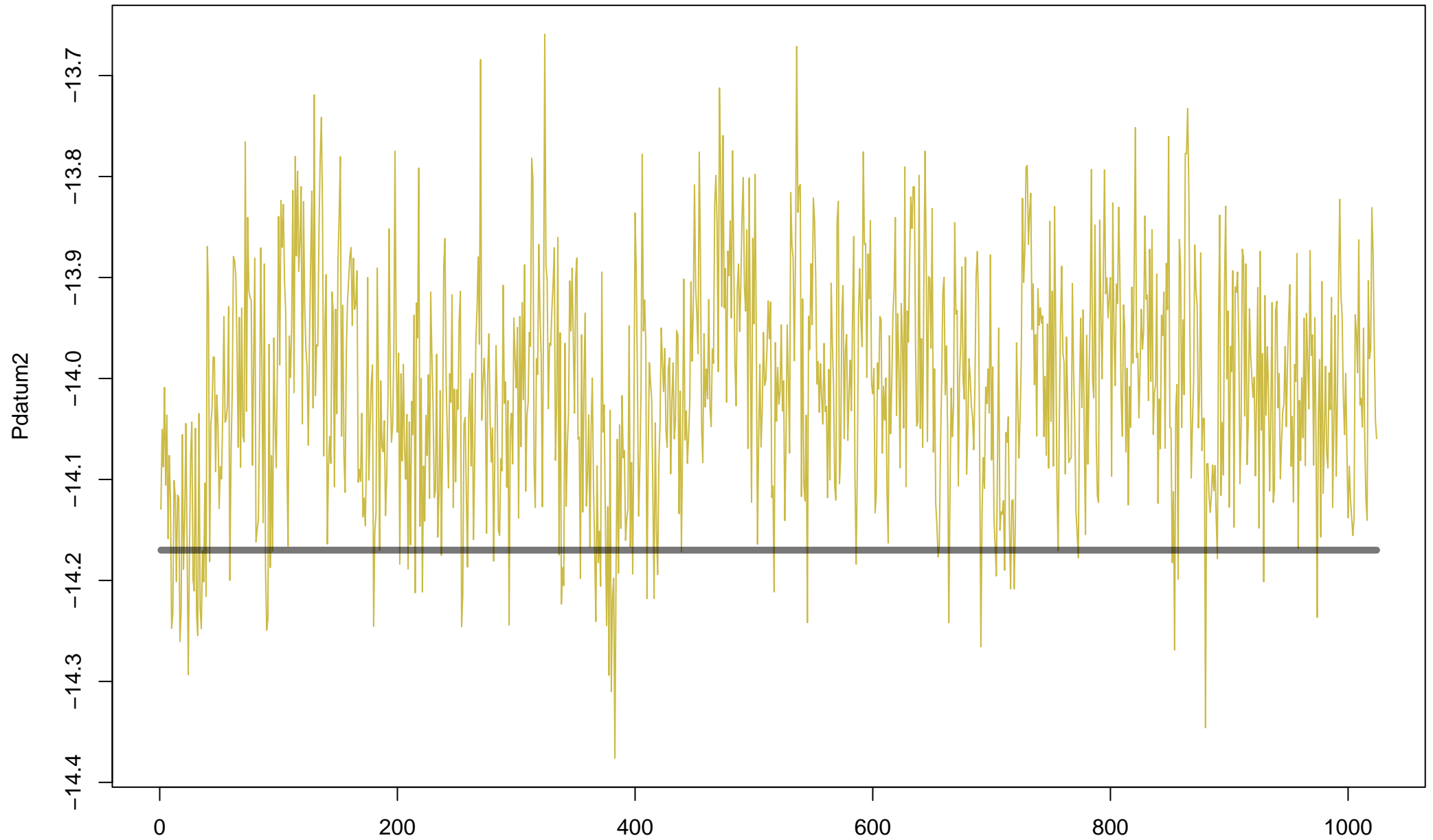
Pdatum1

ESS = 1020 | BMK = 0.0697 | MCSE(6.27) = 3.79 | stat: TRUE | burn: 0 | percentile: 55.9



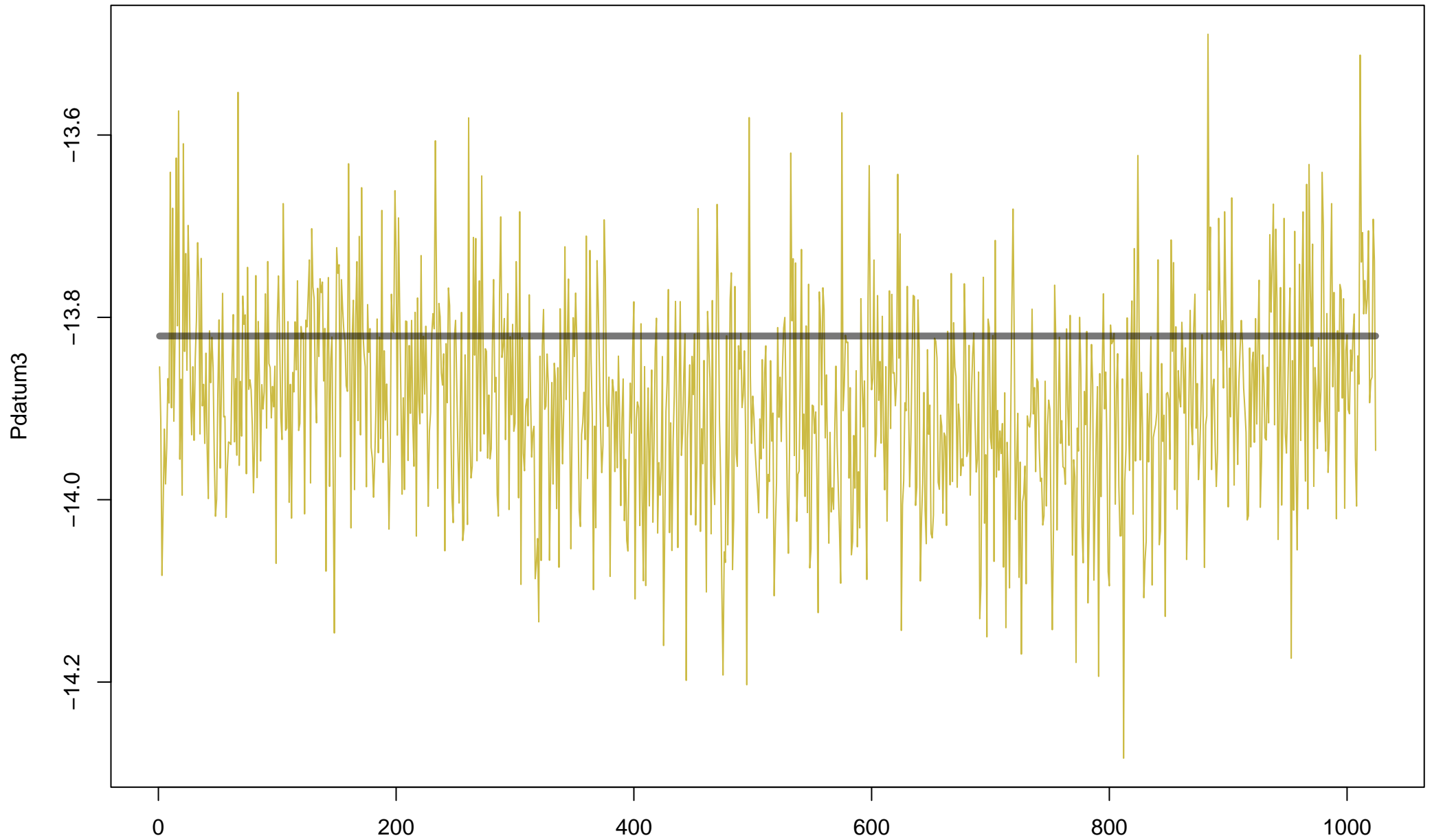
Pdatum2

ESS = 184 | BMK = 0.11 | MCSE(6.27) = 7.44 | stat: FALSE | burn: 0 | percentile: 7.42



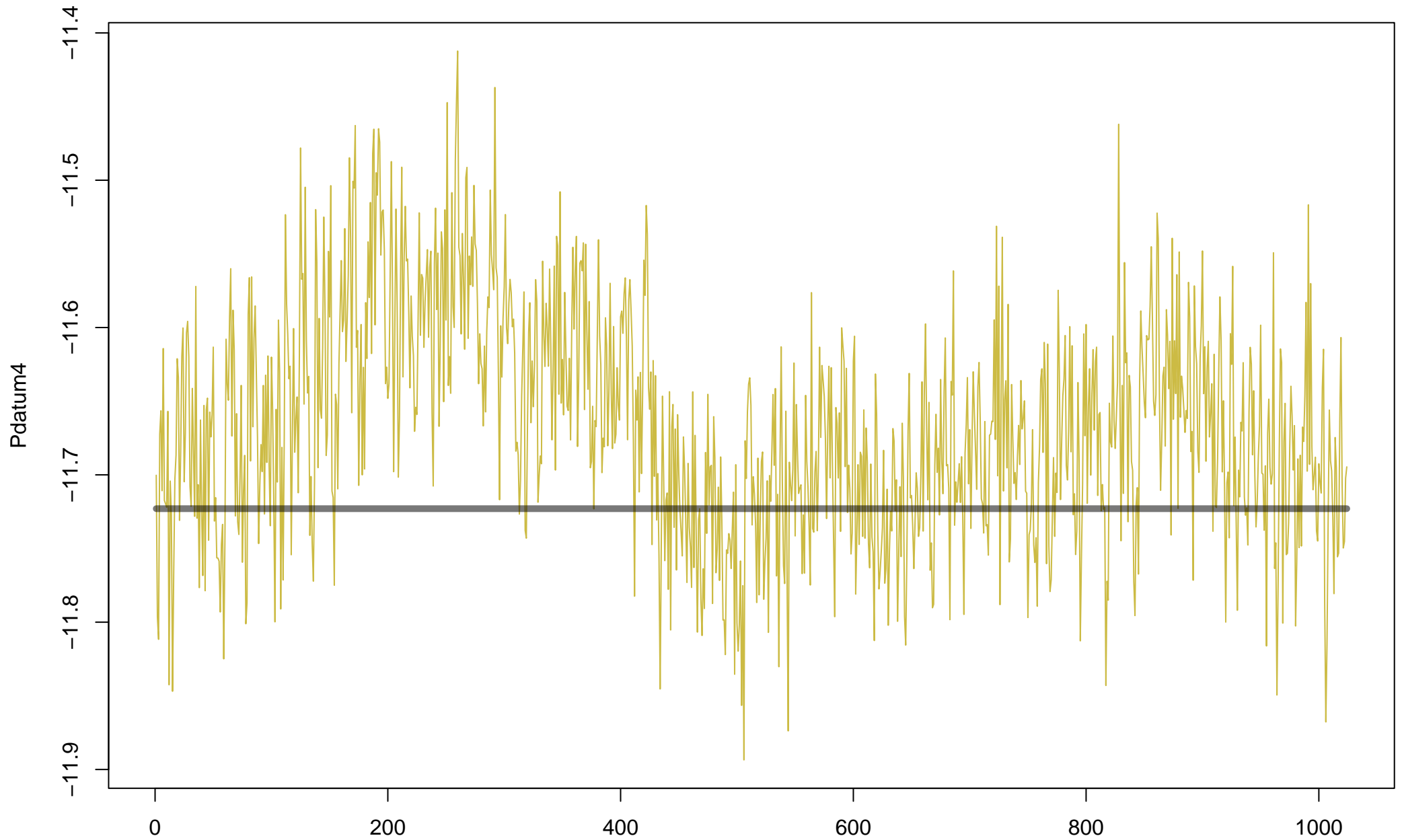
Pdatum3

ESS = 172 | BMK = 0.0684 | MCSE(6.27) = 5.68 | stat: FALSE | burn: 0 | percentile: 75.1



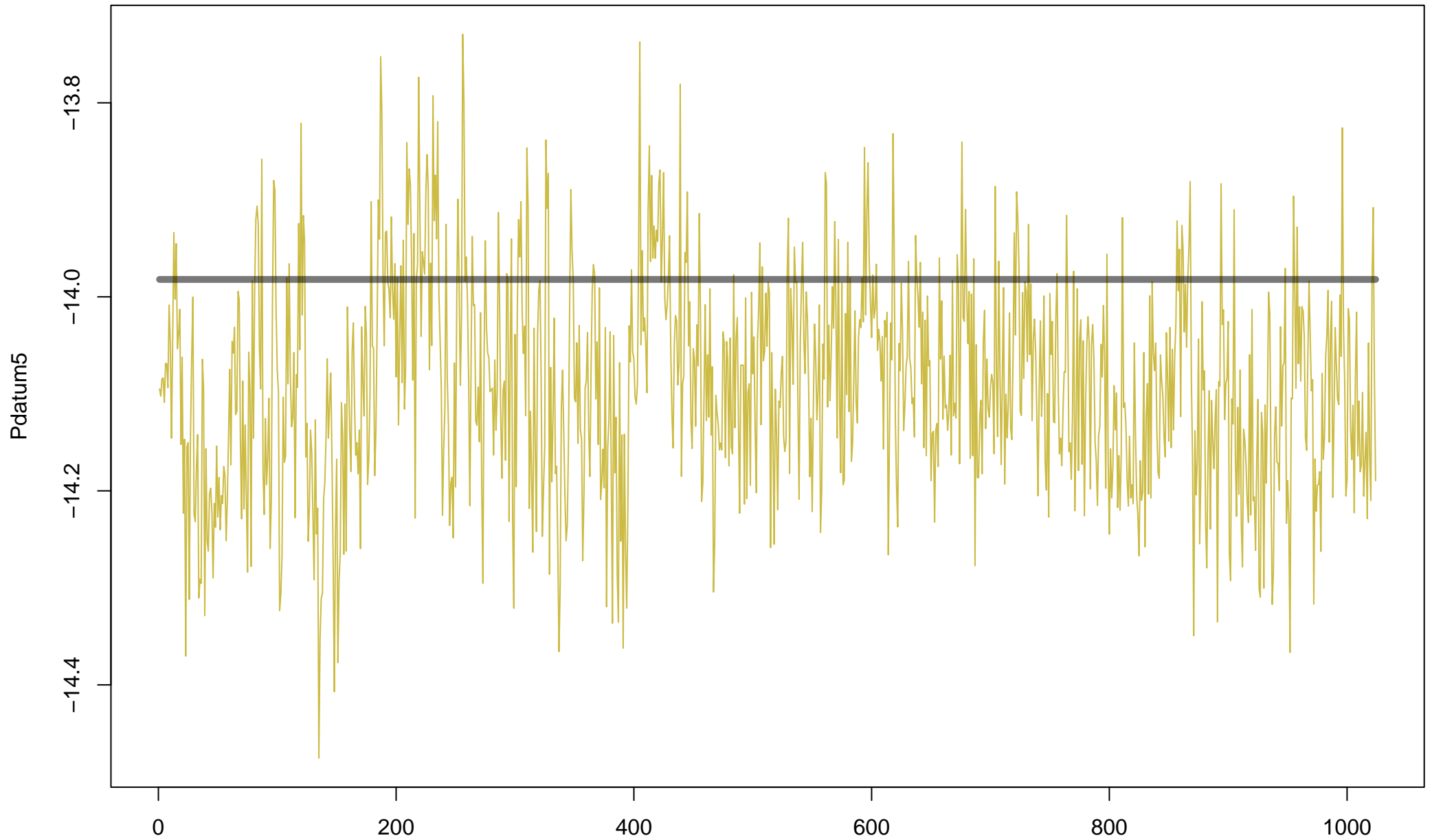
Pdatum4

ESS = 10.1 | BMK = 0.255 | MCSE(6.27) = 11.2 | stat: TRUE | burn: 0 | percentile: 23.5



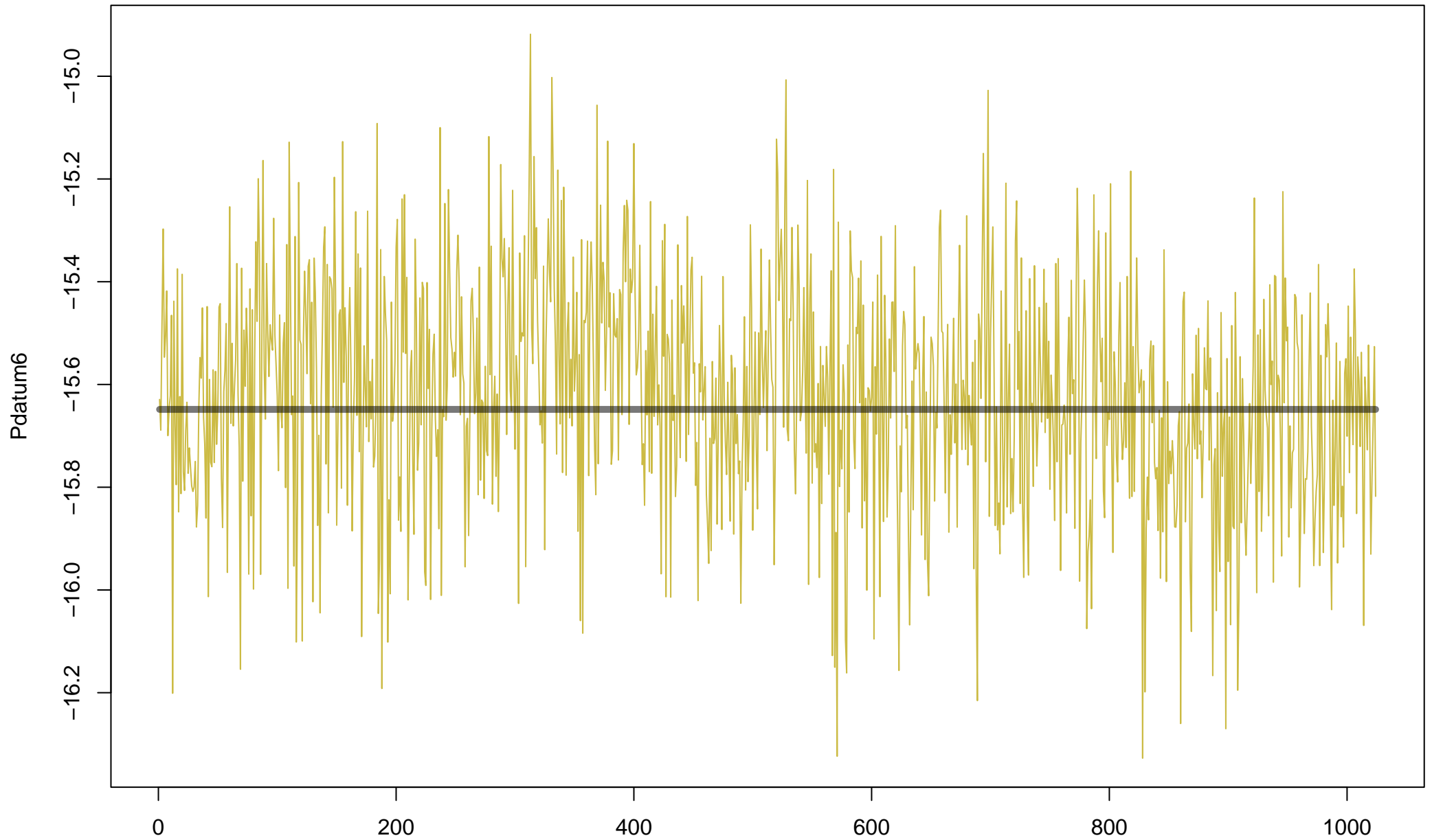
Pdatum5

ESS = 157 | BMK = 0.134 | MCSE(6.27) = 7.76 | stat: TRUE | burn: 0 | percentile: 85.2



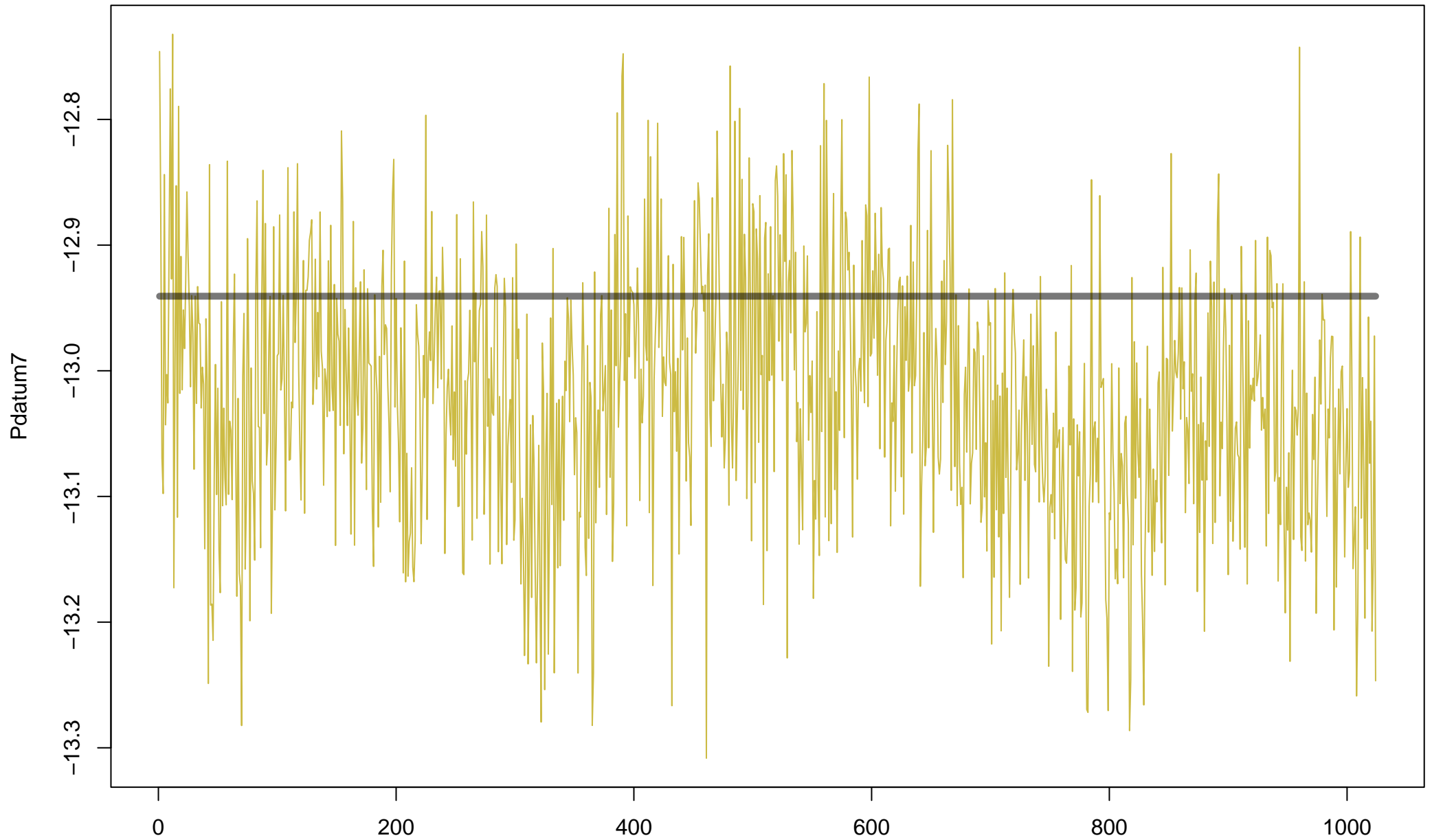
Pdatum6

ESS = 101 | BMK = 0.118 | MCSE(6.27) = 6.01 | stat: TRUE | burn: 0 | percentile: 45



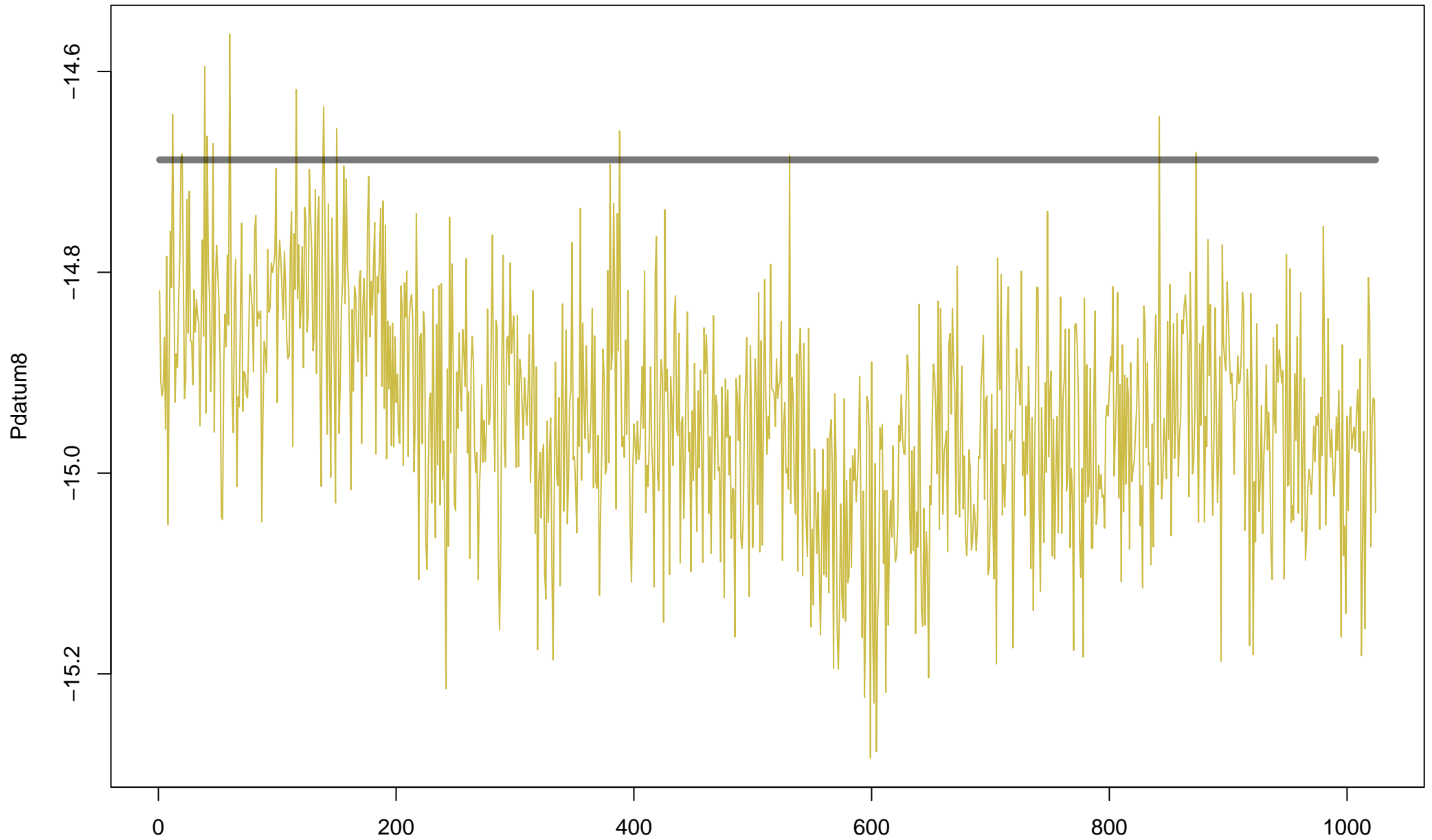
Pdatum7

ESS = 123 | BMK = 0.0922 | MCSE(6.27) = 7.71 | stat: TRUE | burn: 0 | percentile: 78.5

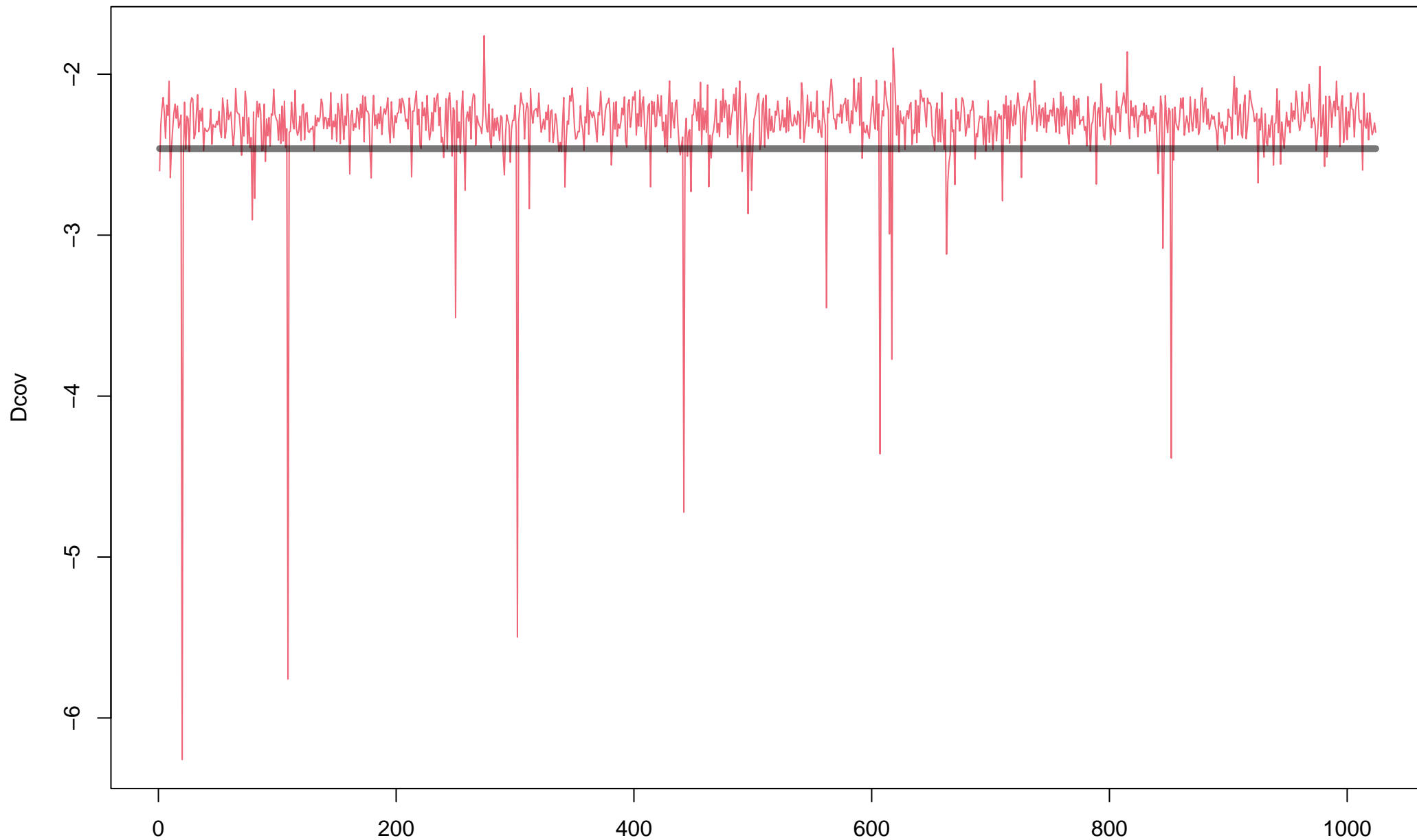


Pdatum8

ESS = 22.7 | BMK = 0.247 | MCSE(6.27) = 10.3 | stat: FALSE | burn: 0 | percentile: 98.6

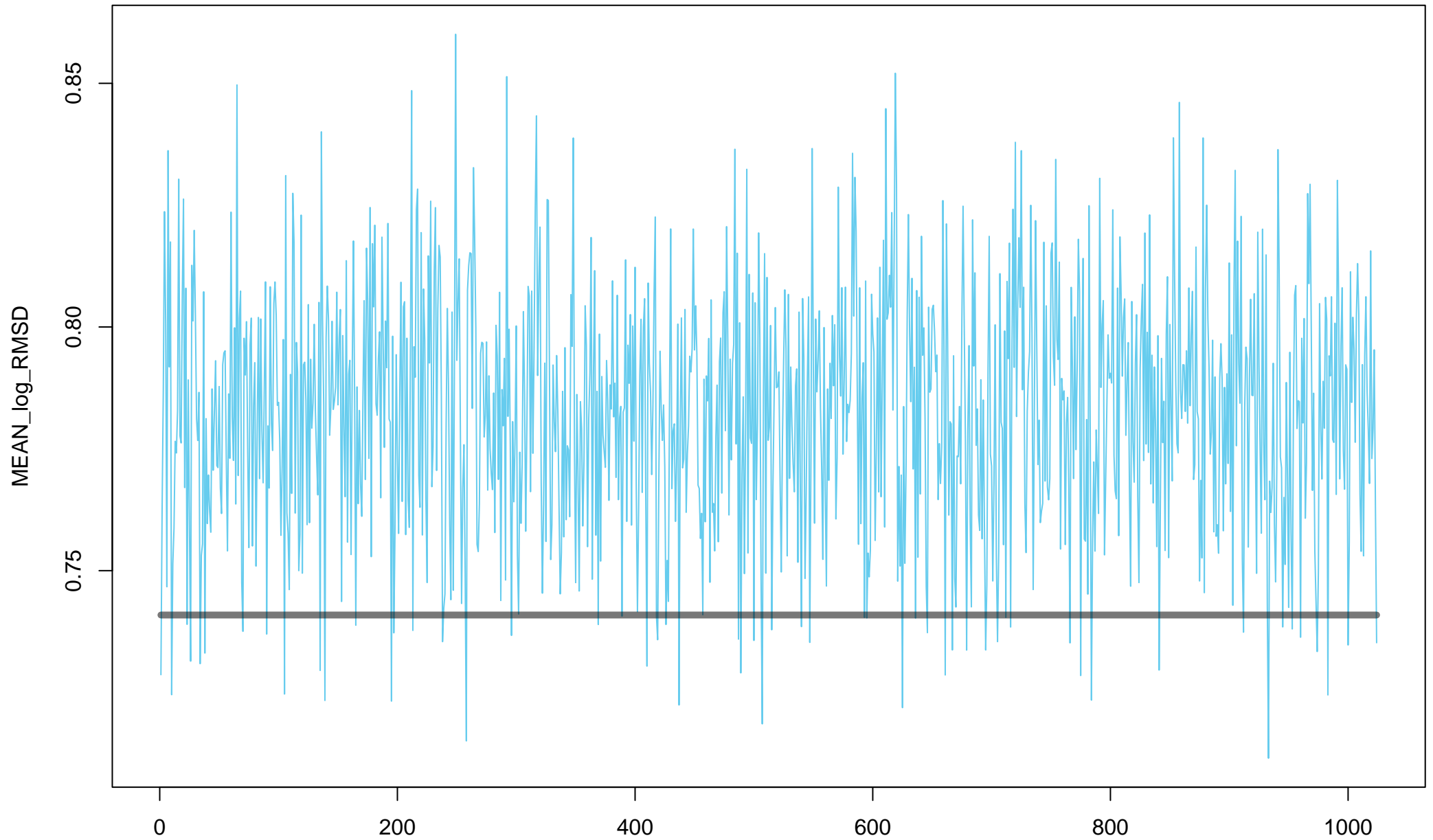


Dcov
ESS = 1020 | BMK = 0.127 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0 | percentile: 92

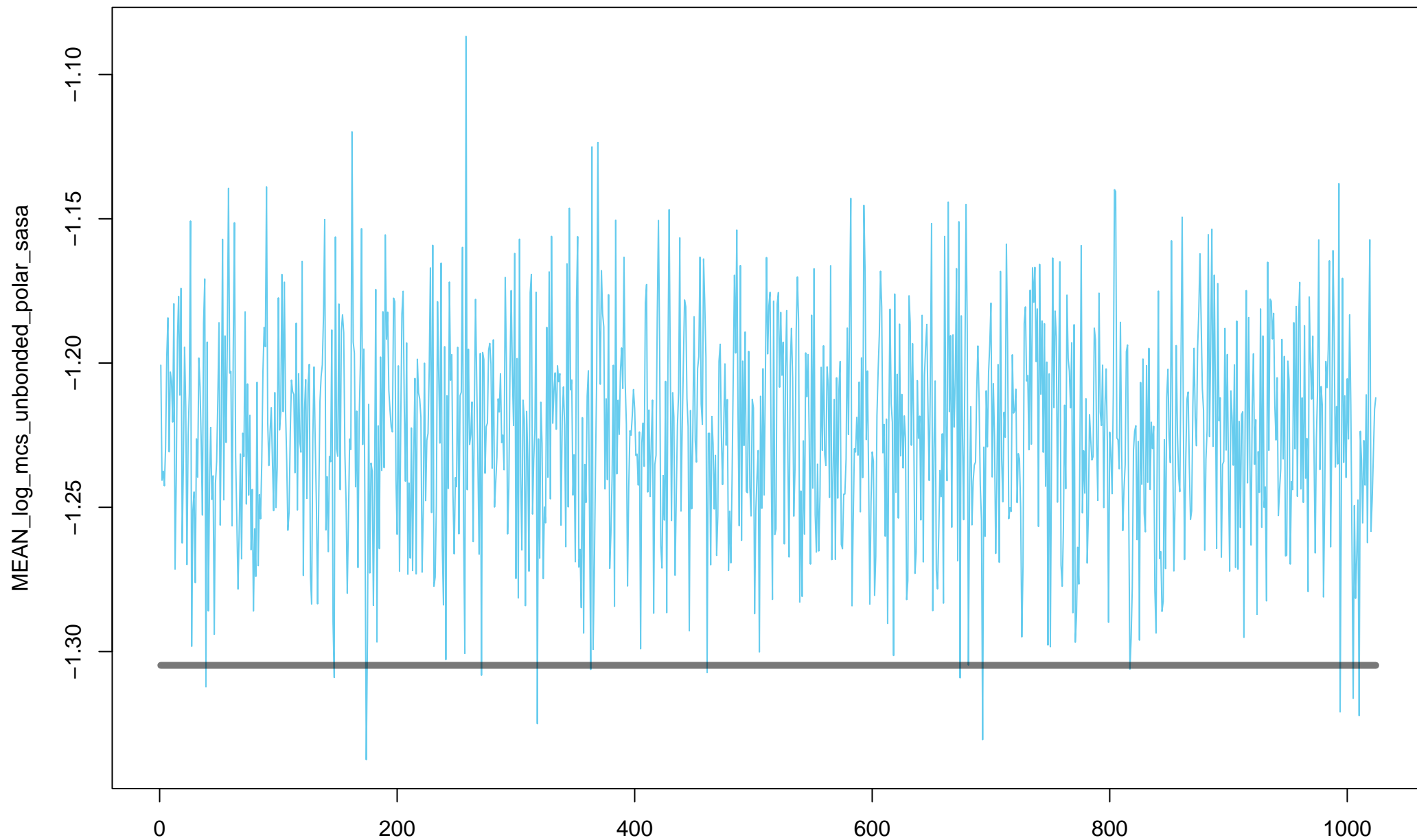


MEAN_log_RMSD

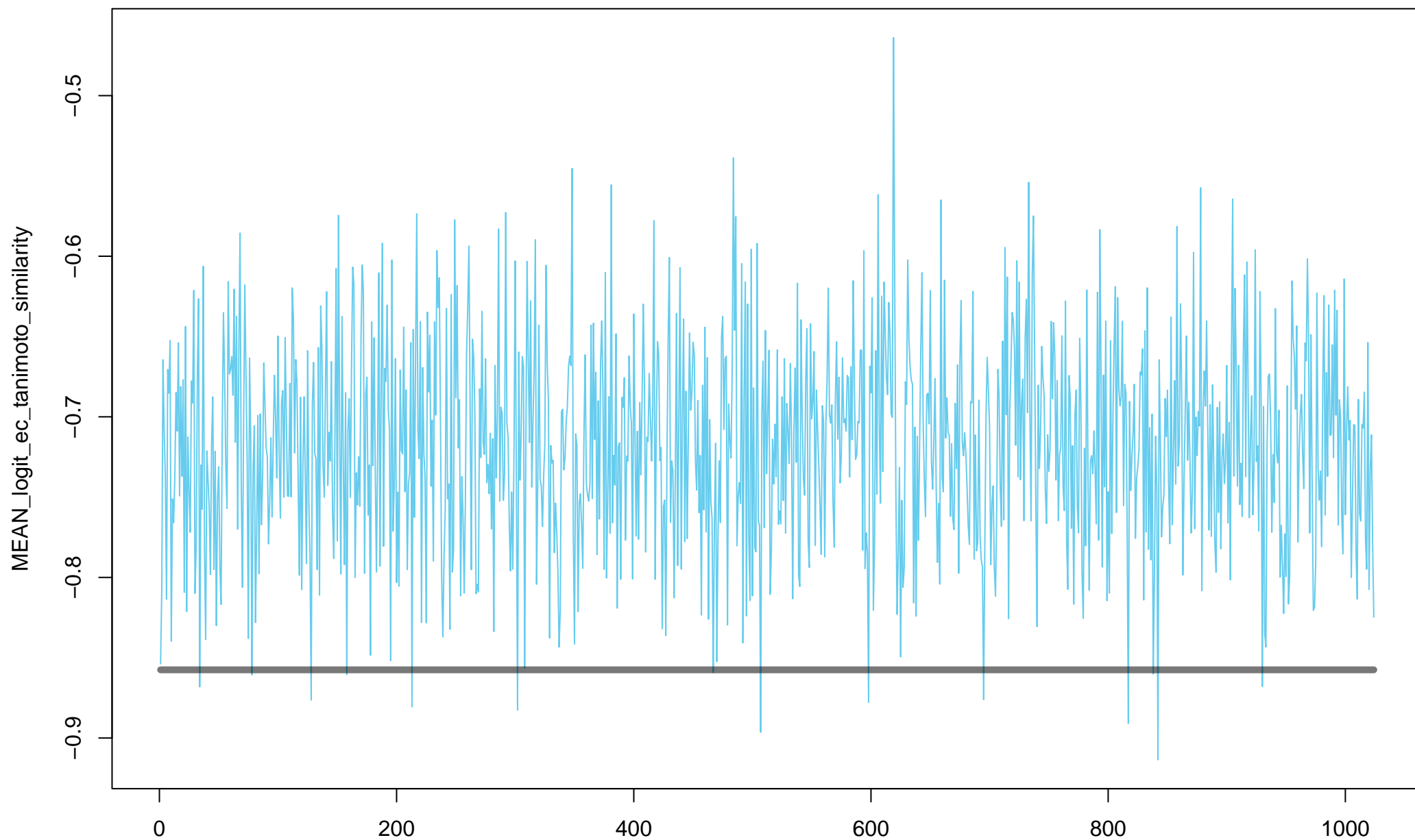
ESS = 1020 | BMK = 0.0305 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | percentile: 5.57



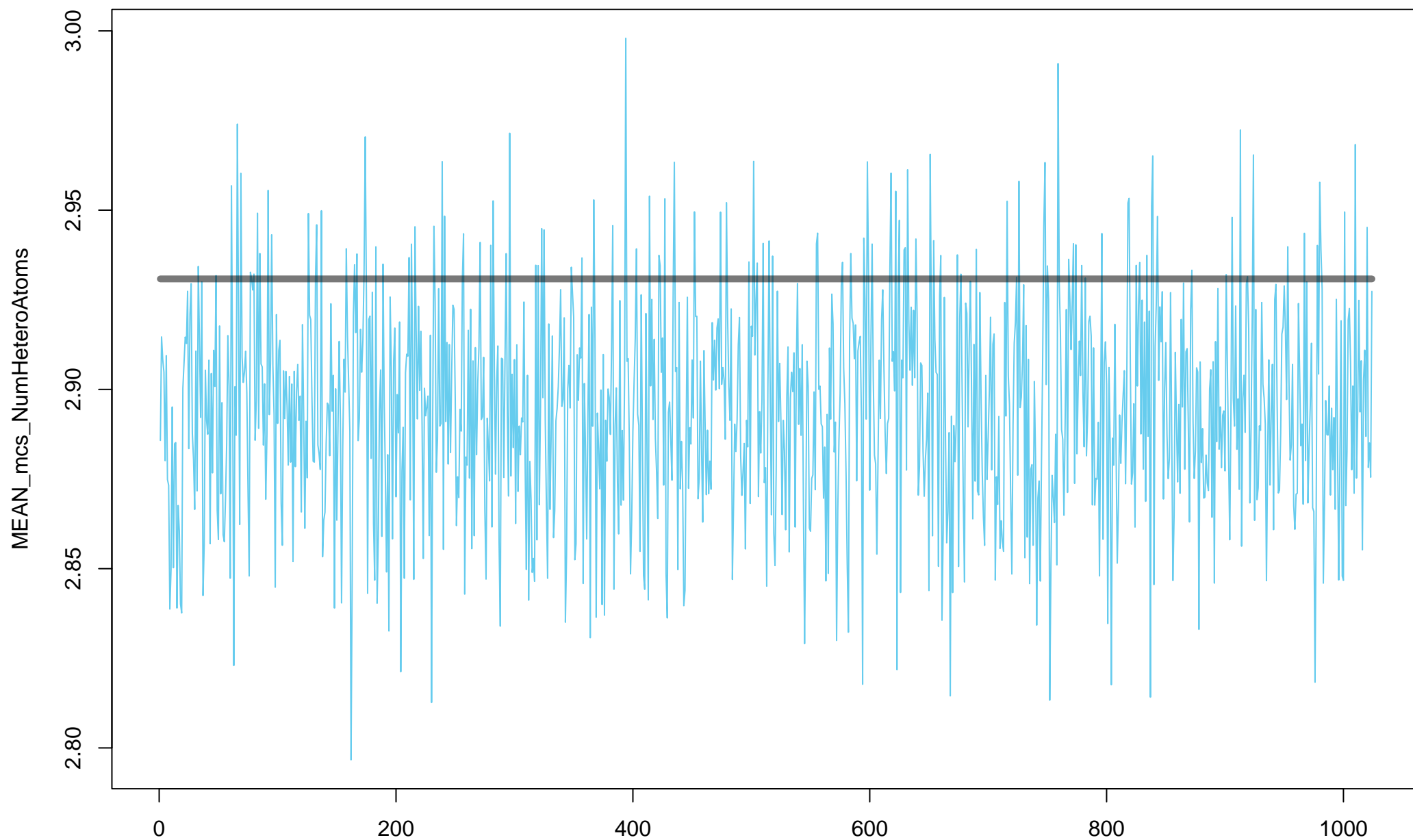
MEAN_log_mcs_unbonded_polar_sasa
ESS = 858 | BMK = 0.0484 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0 | percentile: 1.27



MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.075 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | percentile: 1.37

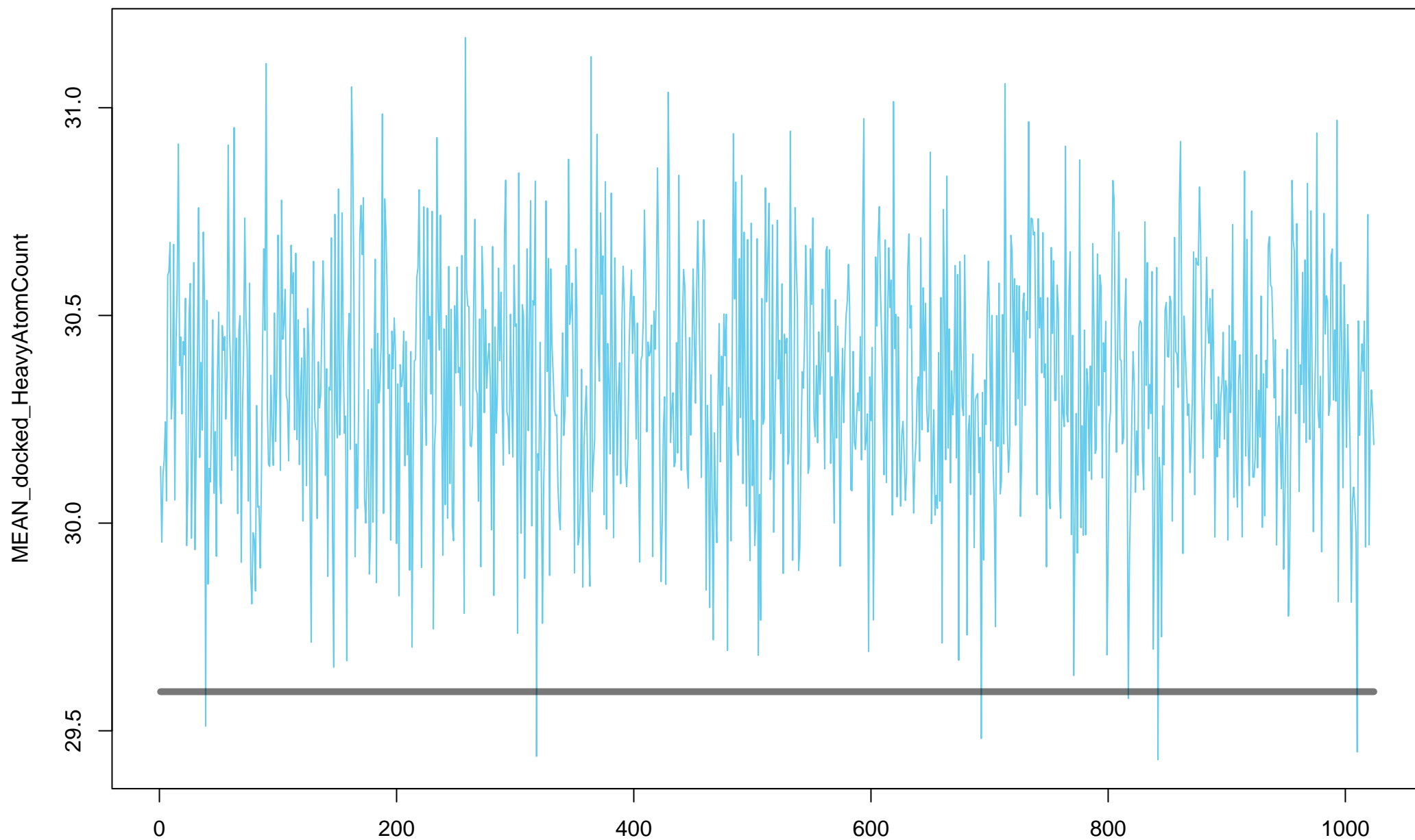


MEAN_mcs_NumHeteroAtoms
ESS = 874 | BMK = 0.06 | MCSE(6.27) = 3.4 | stat: TRUE | burn: 0 | percentile: 88.7

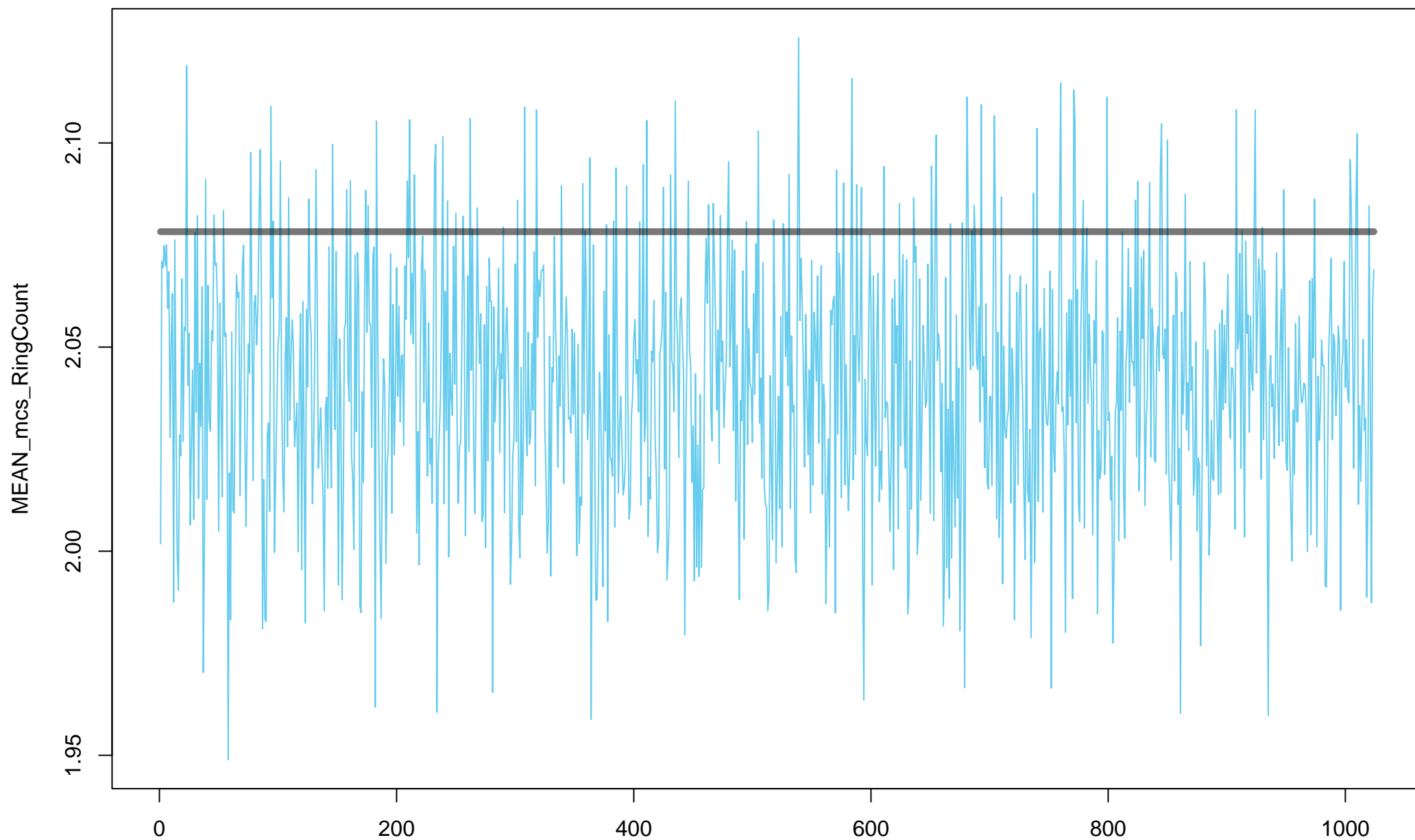


MEAN_docked_HeavyAtomCount

ESS = 1020 | BMK = 0.068 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0 | percentile: 0.586

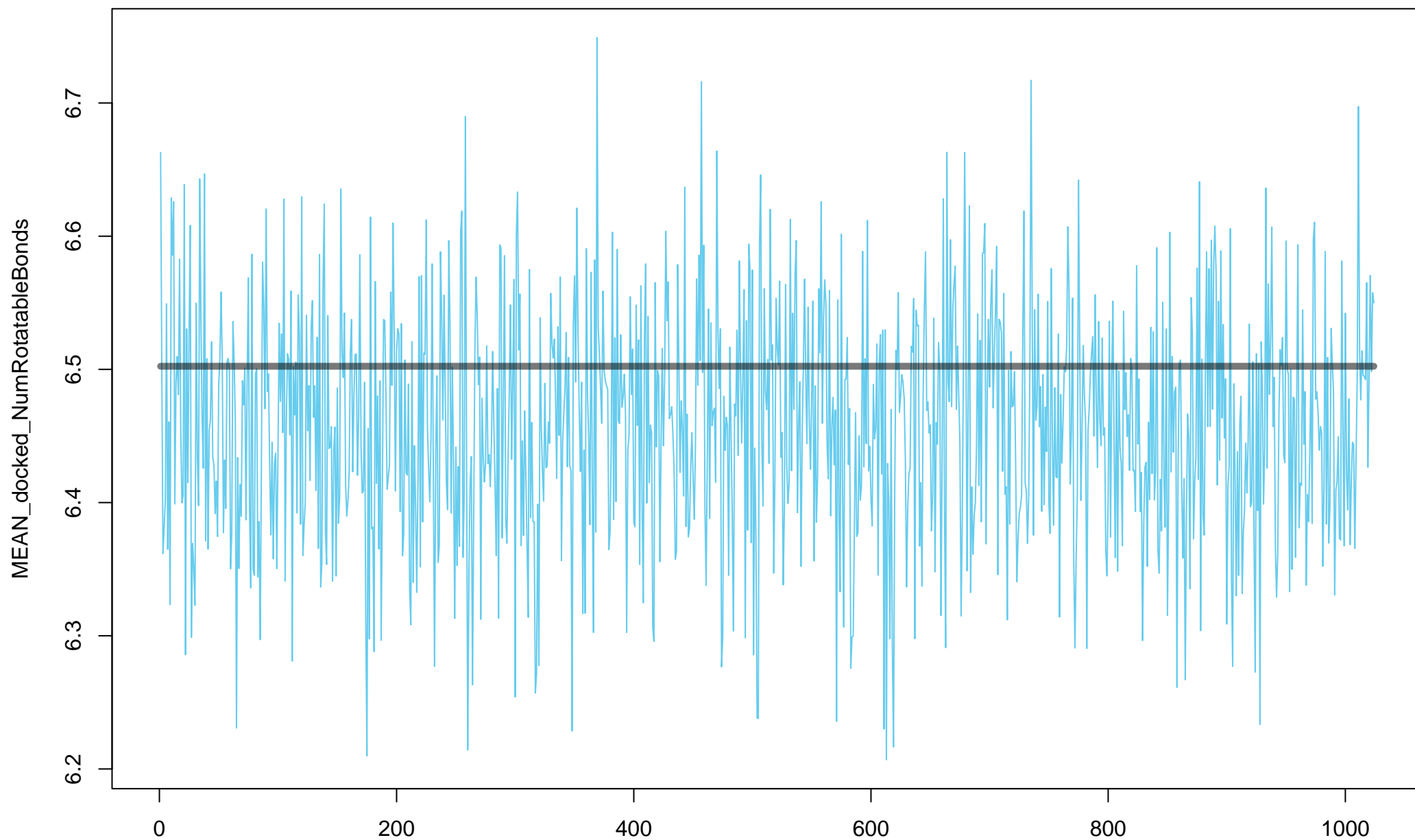


MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0362 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0 | percentile: 89.6



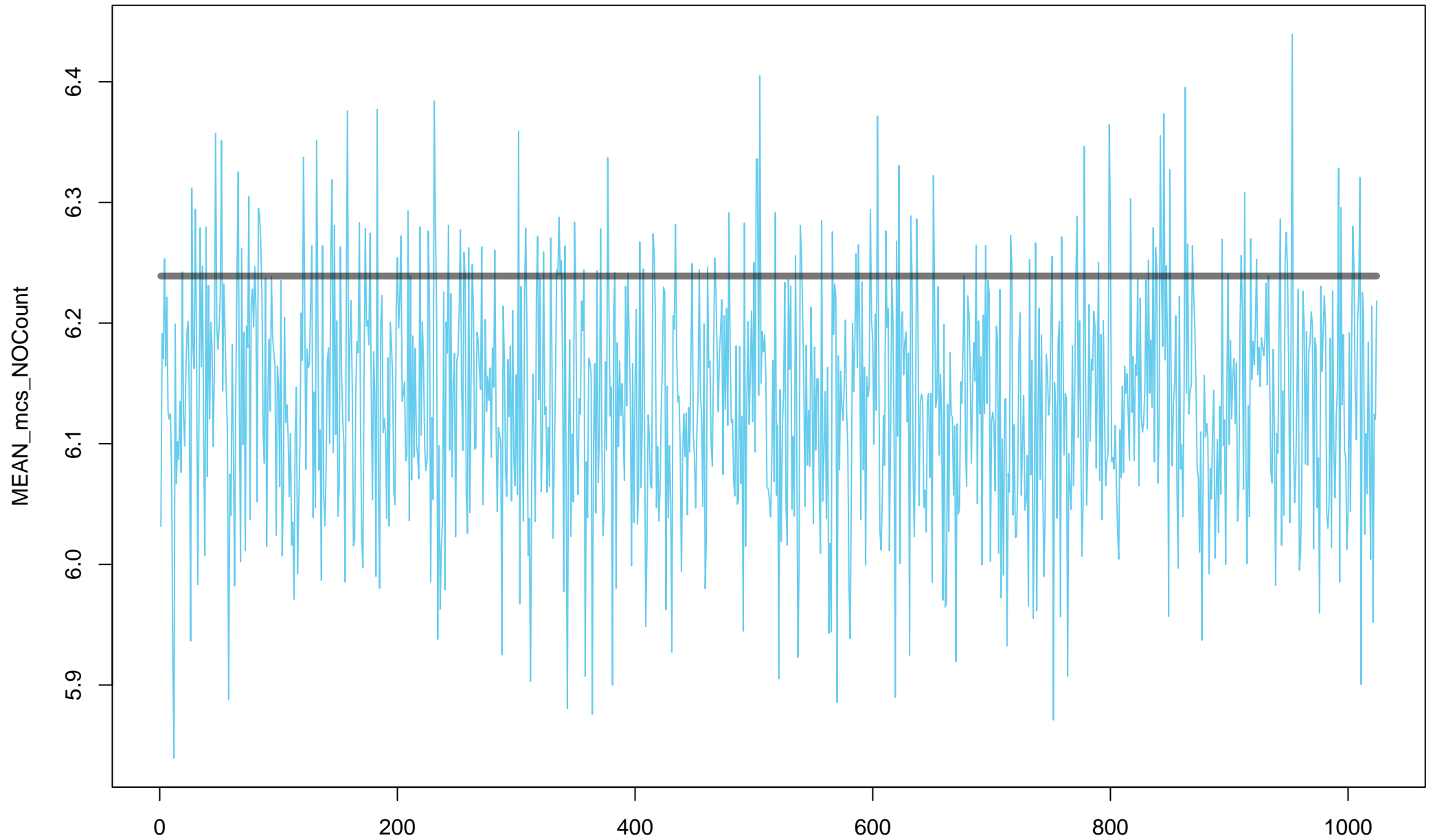
MEAN_docked_NumRotatableBonds

ESS = 1020 | BMK = 0.0387 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | percentile: 69.3



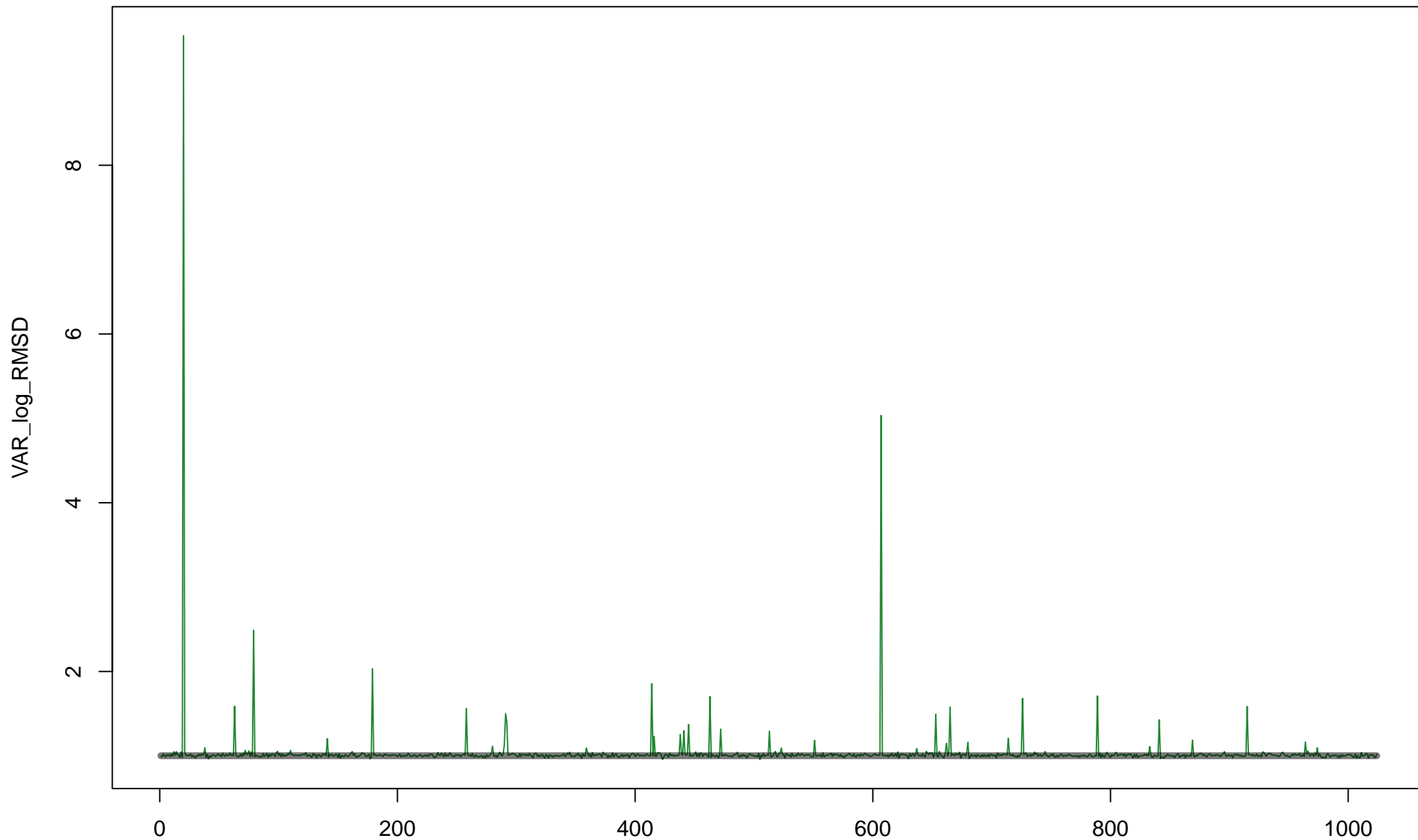
MEAN_mcs_NOCount

ESS = 1020 | BMK = 0.0409 | MCSE(6.27) = 3.58 | stat: TRUE | burn: 0 | percentile: 86.5

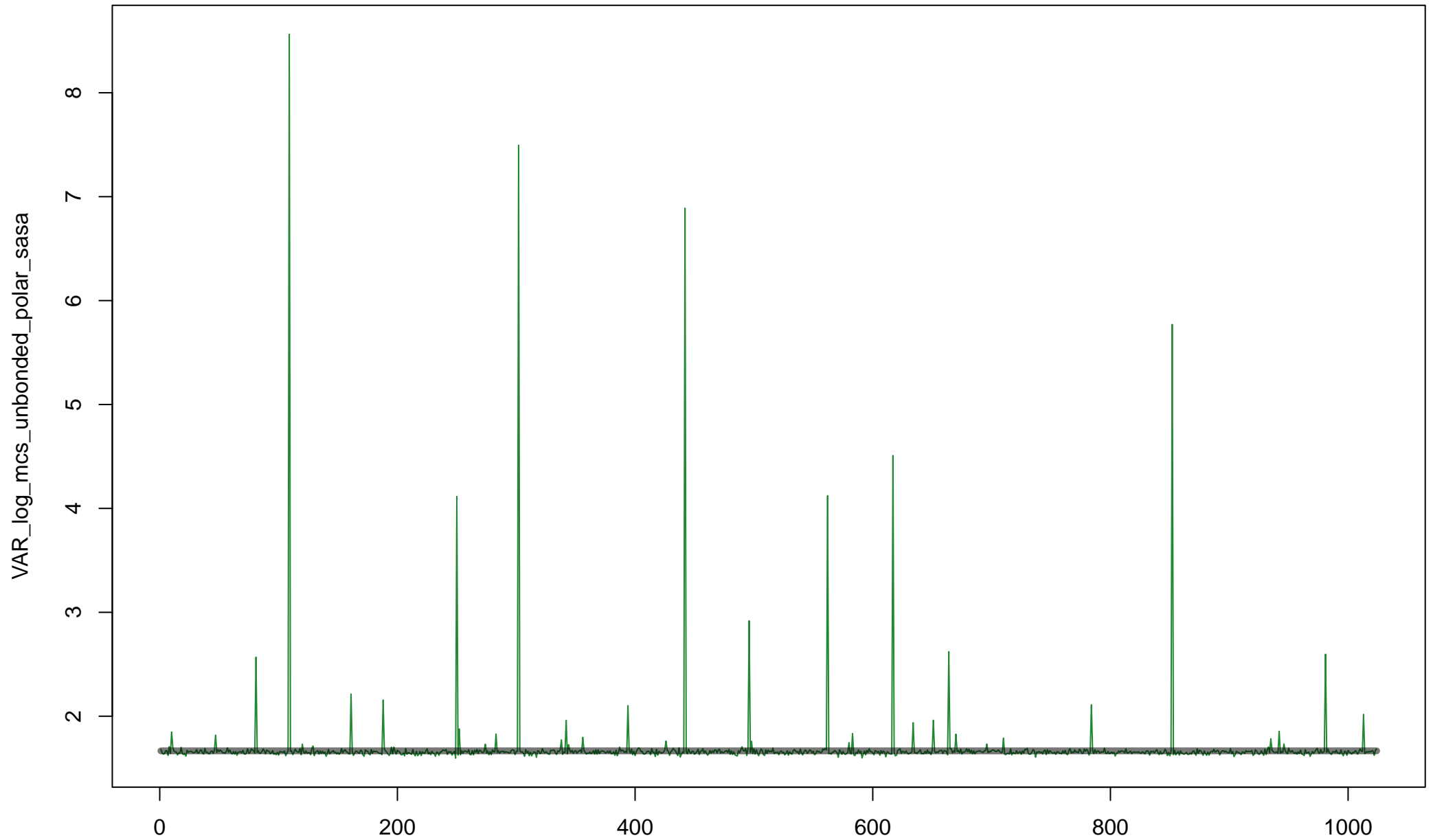


VAR_log_RMSD

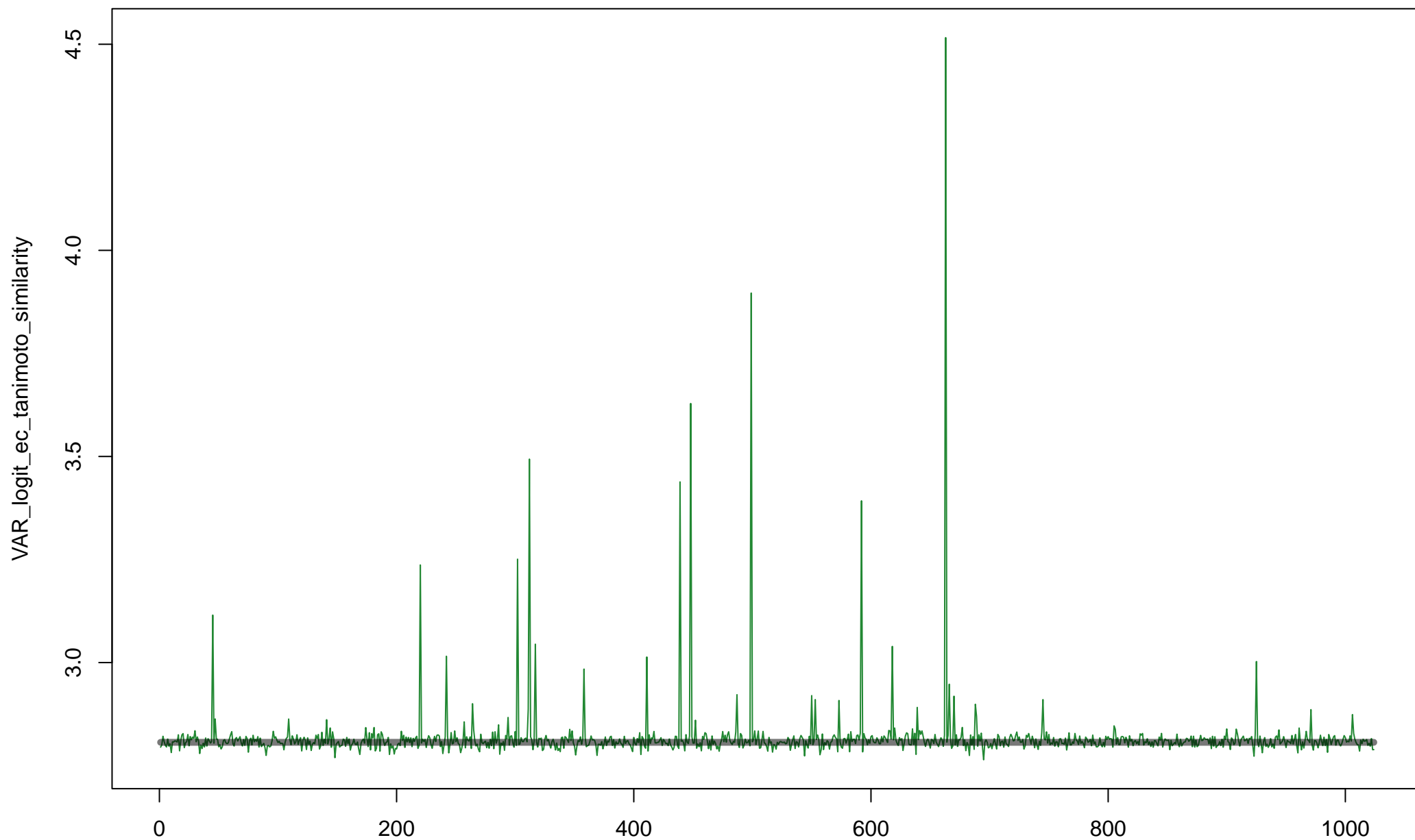
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 612 | percentile: 38



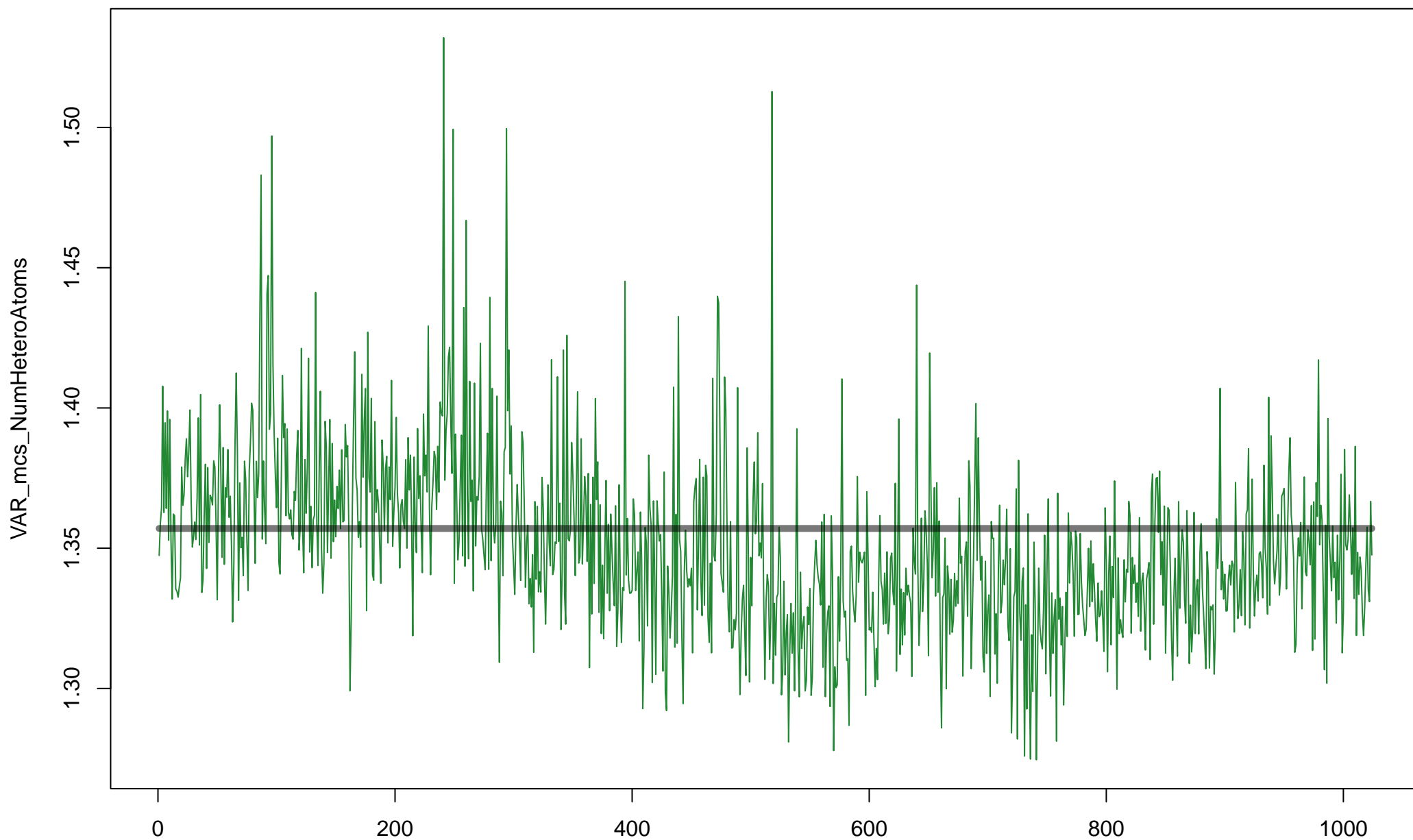
VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 1020 | percentile: 74.6



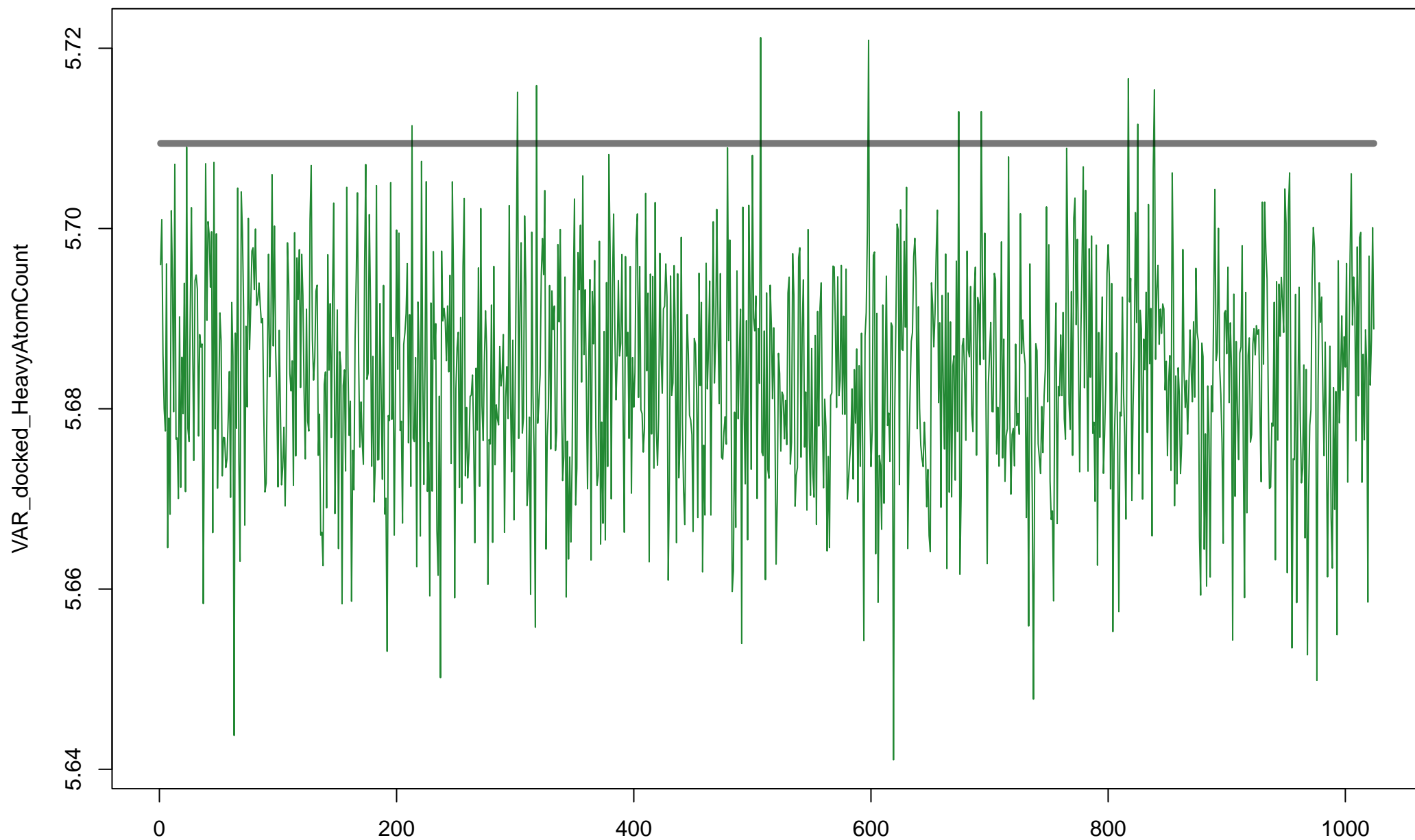
VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.146 | MCSE(6.27) = 3.28 | stat: TRUE | burn: 0 | percentile: 43.8



VAR_mcs_NumHeteroAtoms
ESS = 41.9 | BMK = 0.333 | MCSE(6.27) = 9.77 | stat: FALSE | burn: 0 | percentile: 62.7

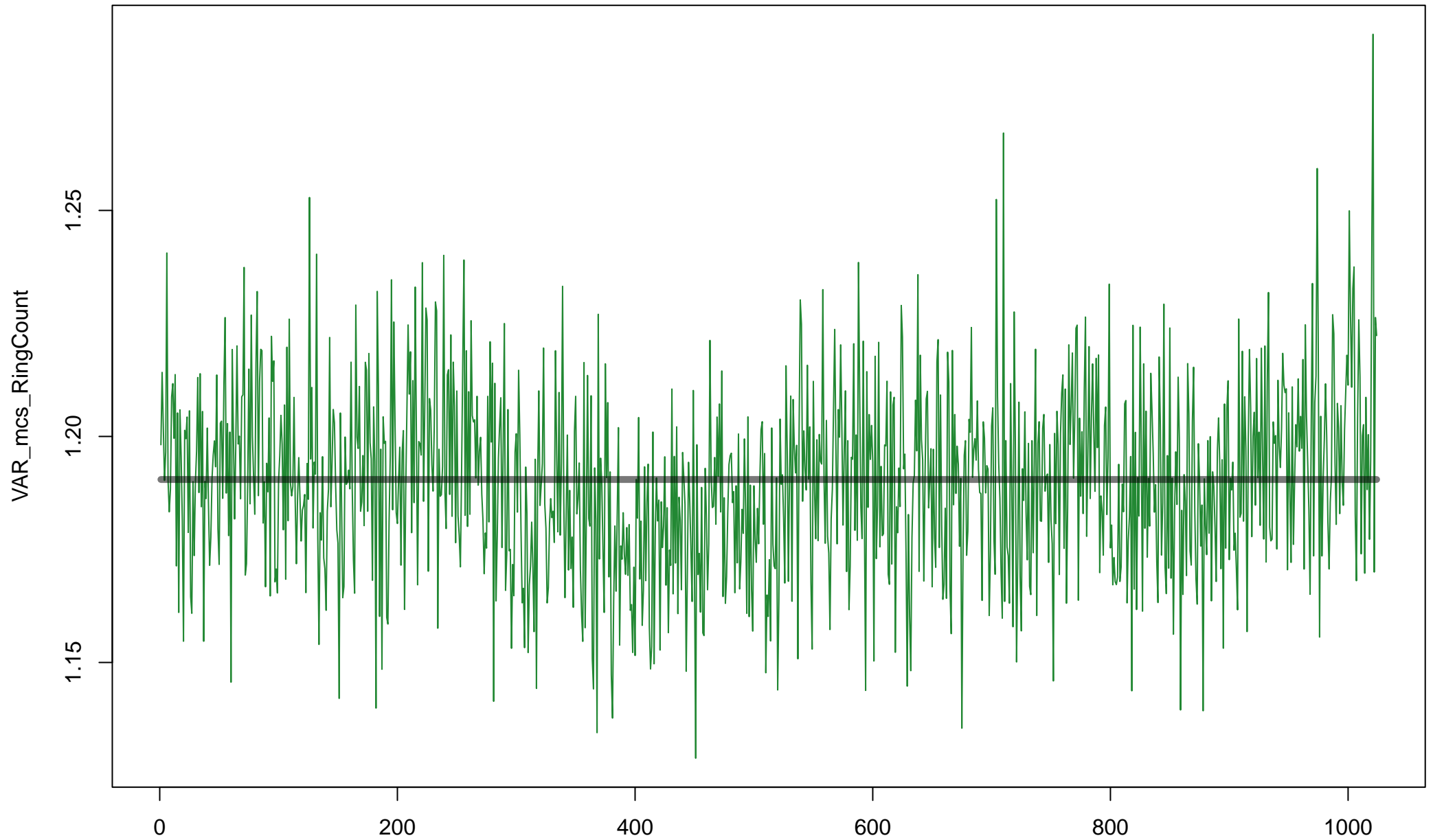


VAR_docked_HeavyAtomCount
ESS = 901 | BMK = 0.057 | MCSE(6.27) = 3.32 | stat: TRUE | burn: 0 | percentile: 99



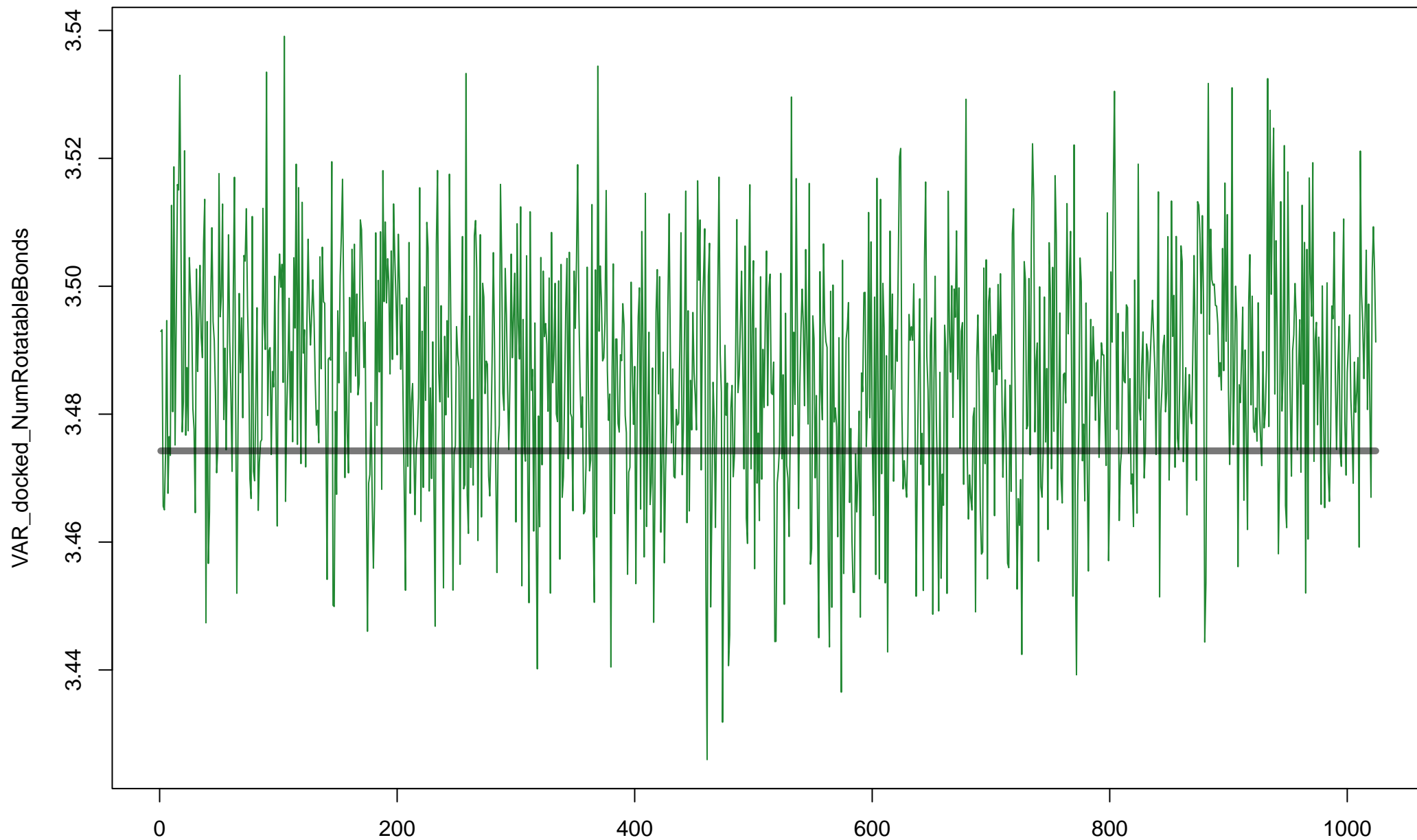
VAR_mcs_RingCount

ESS = 104 | BMK = 0.0873 | MCSE(6.27) = 6.37 | stat: TRUE | burn: 0 | percentile: 51.4



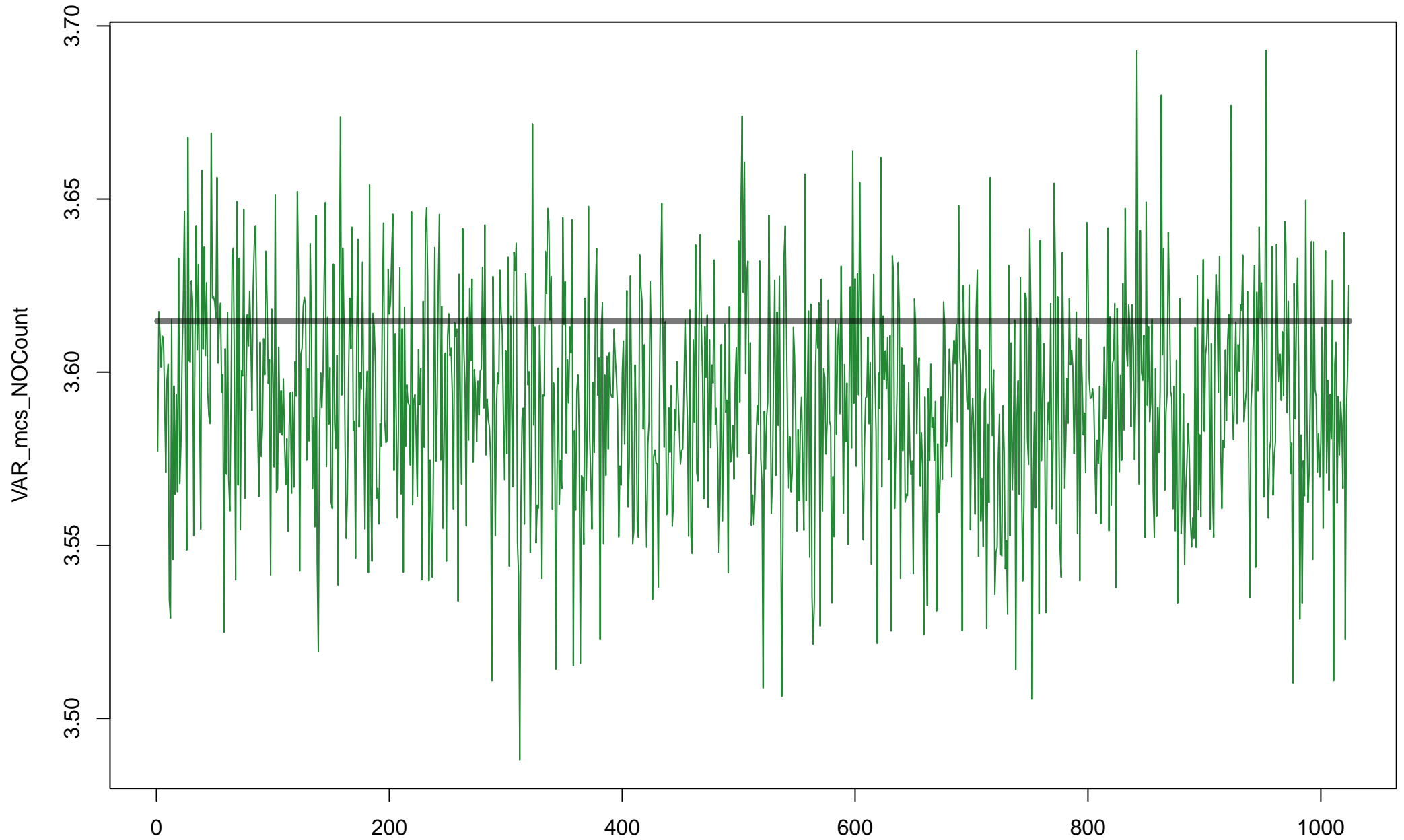
VAR_docked_NumRotatableBonds

ESS = 761 | BMK = 0.0555 | MCSE(6.27) = 3.69 | stat: TRUE | burn: 0 | percentile: 26.4

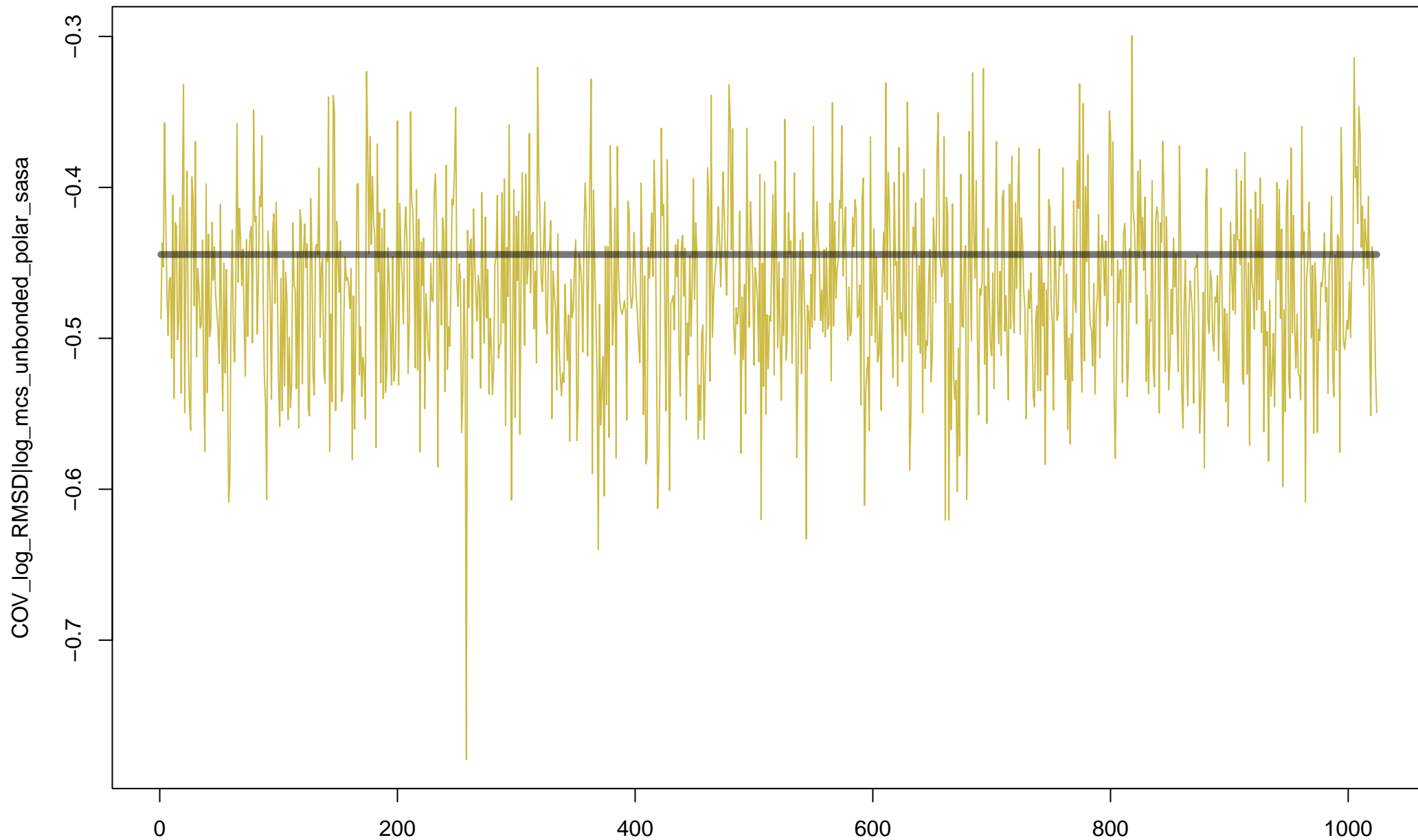


VAR_mcs_NOCount

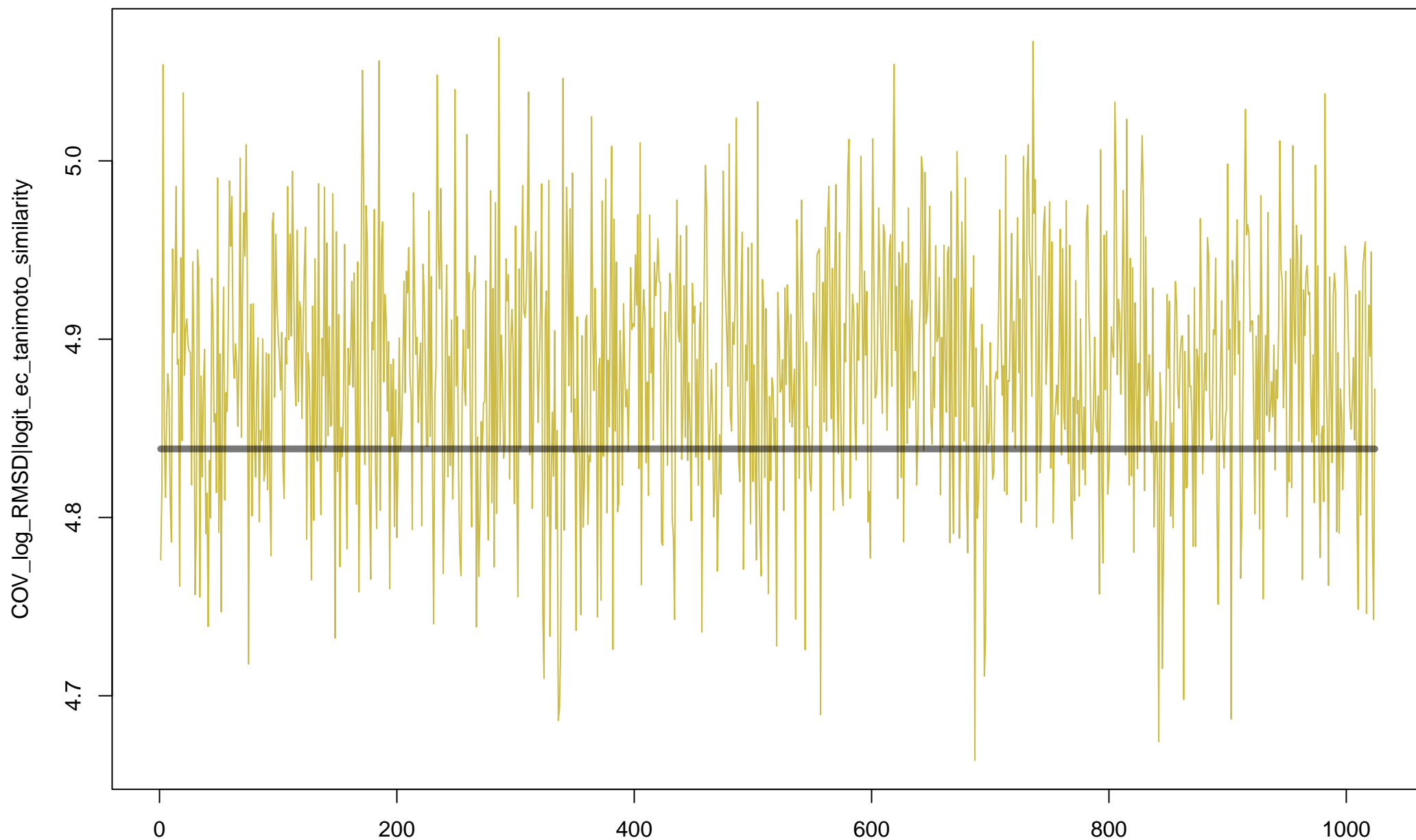
ESS = 856 | BMK = 0.0682 | MCSE(6.27) = 4.17 | stat: FALSE | burn: 0 | percentile: 76.9



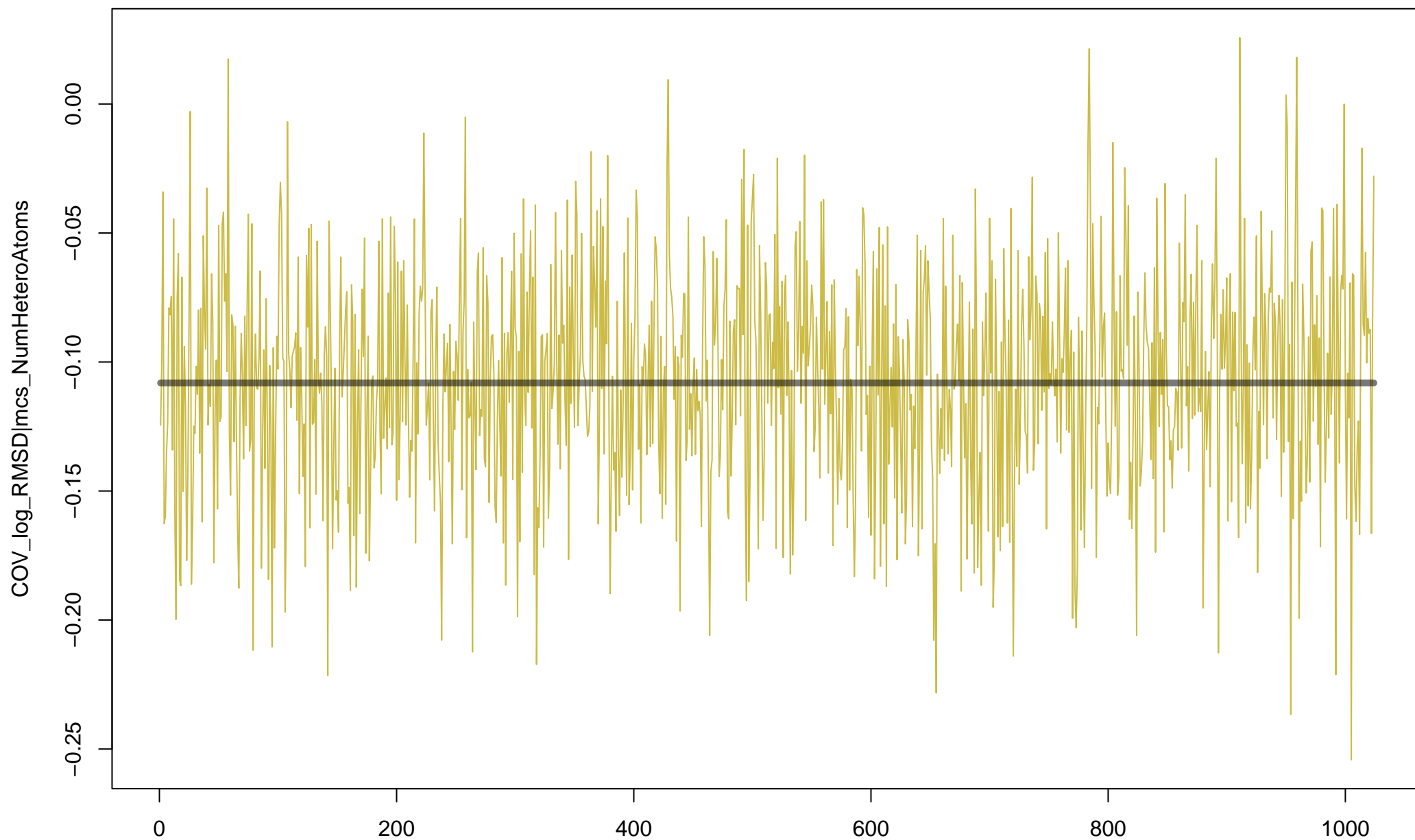
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 879 | BMK = 0.0548 | MCSE(6.27) = 3.7 | stat: TRUE | burn: 0 | percentile: 66.7



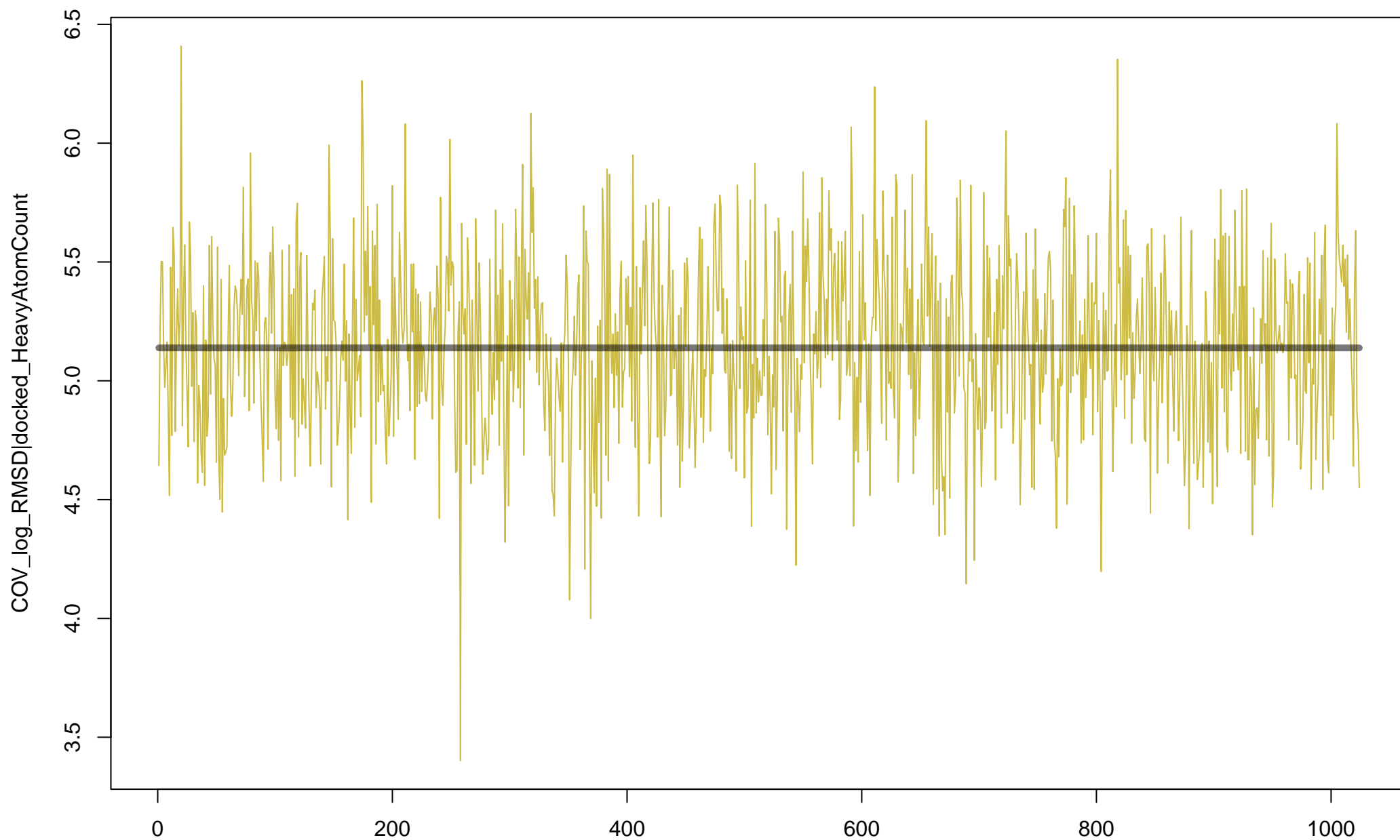
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 747 | BMK = 0.0692 | MCSE(6.27) = 4.03 | stat: TRUE | burn: 0 | percentile: 25.4



COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0432 | MCSE(6.27) = 3.4 | stat: TRUE | burn: 0 | percentile: 47.7

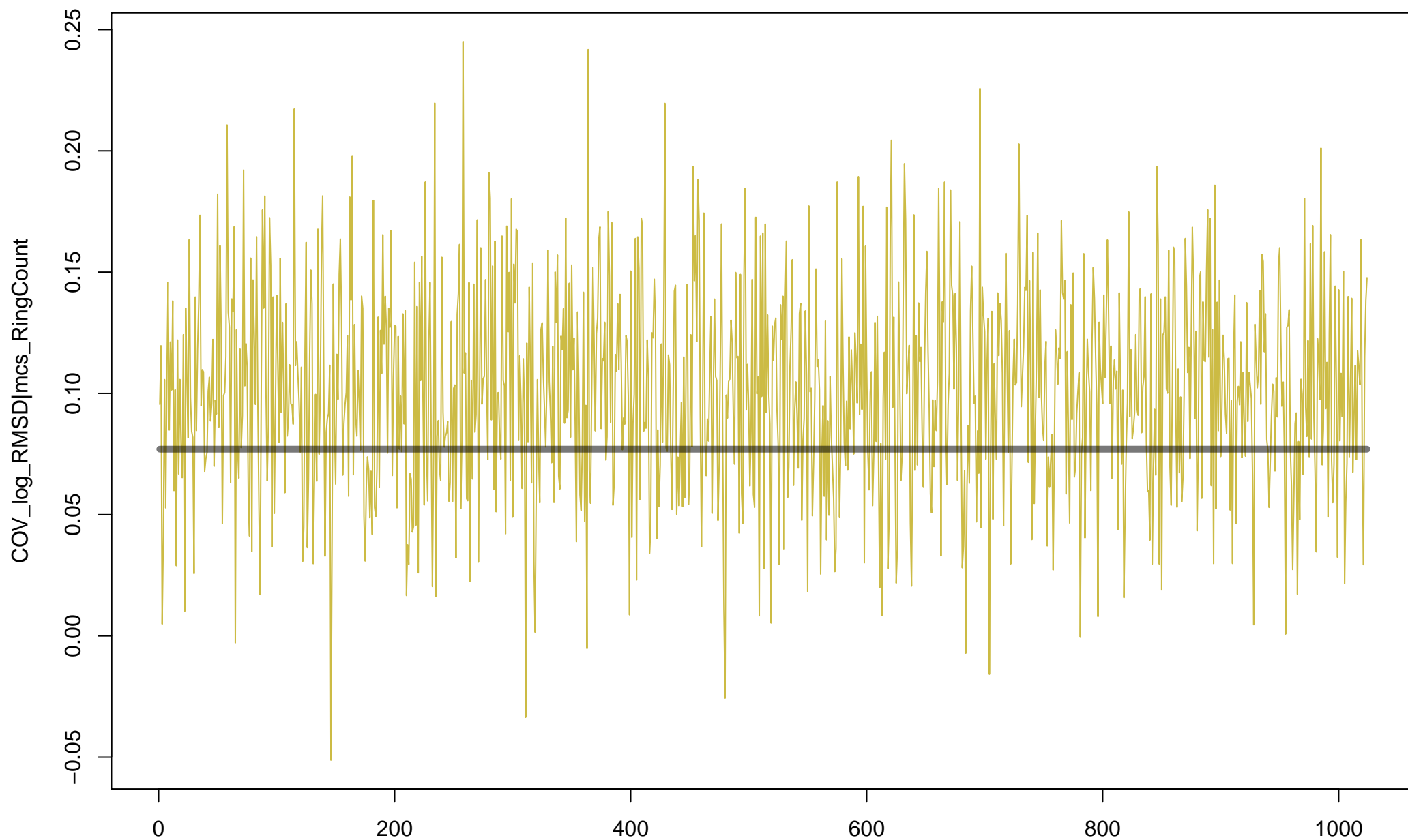


COV_log_RMSD|docked_HeavyAtomCount
ESS = 694 | BMK = 0.0518 | MCSE(6.27) = 3.83 | stat: TRUE | burn: 0 | percentile: 49.6

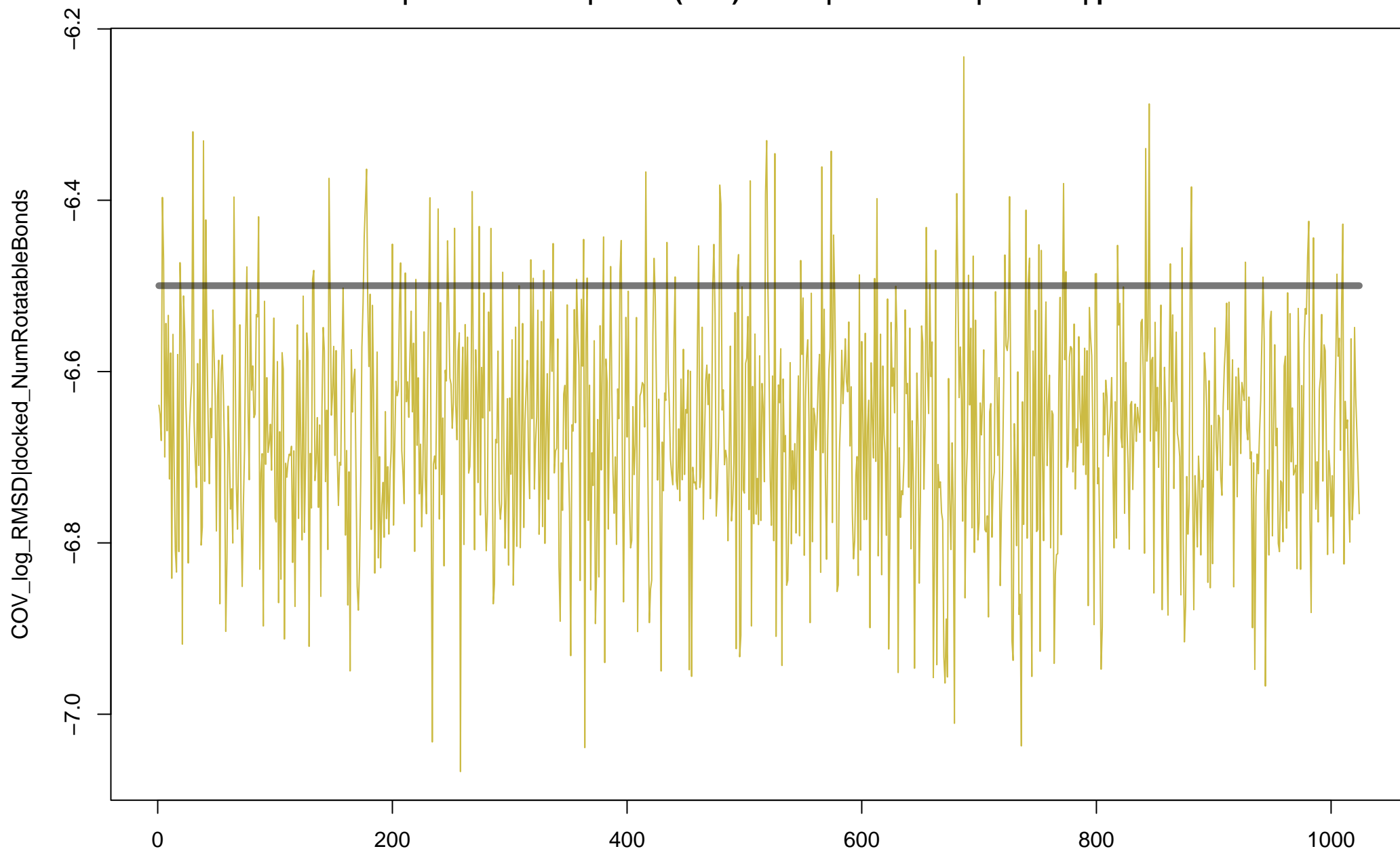


COV_log_RMSD|mcs_RingCount

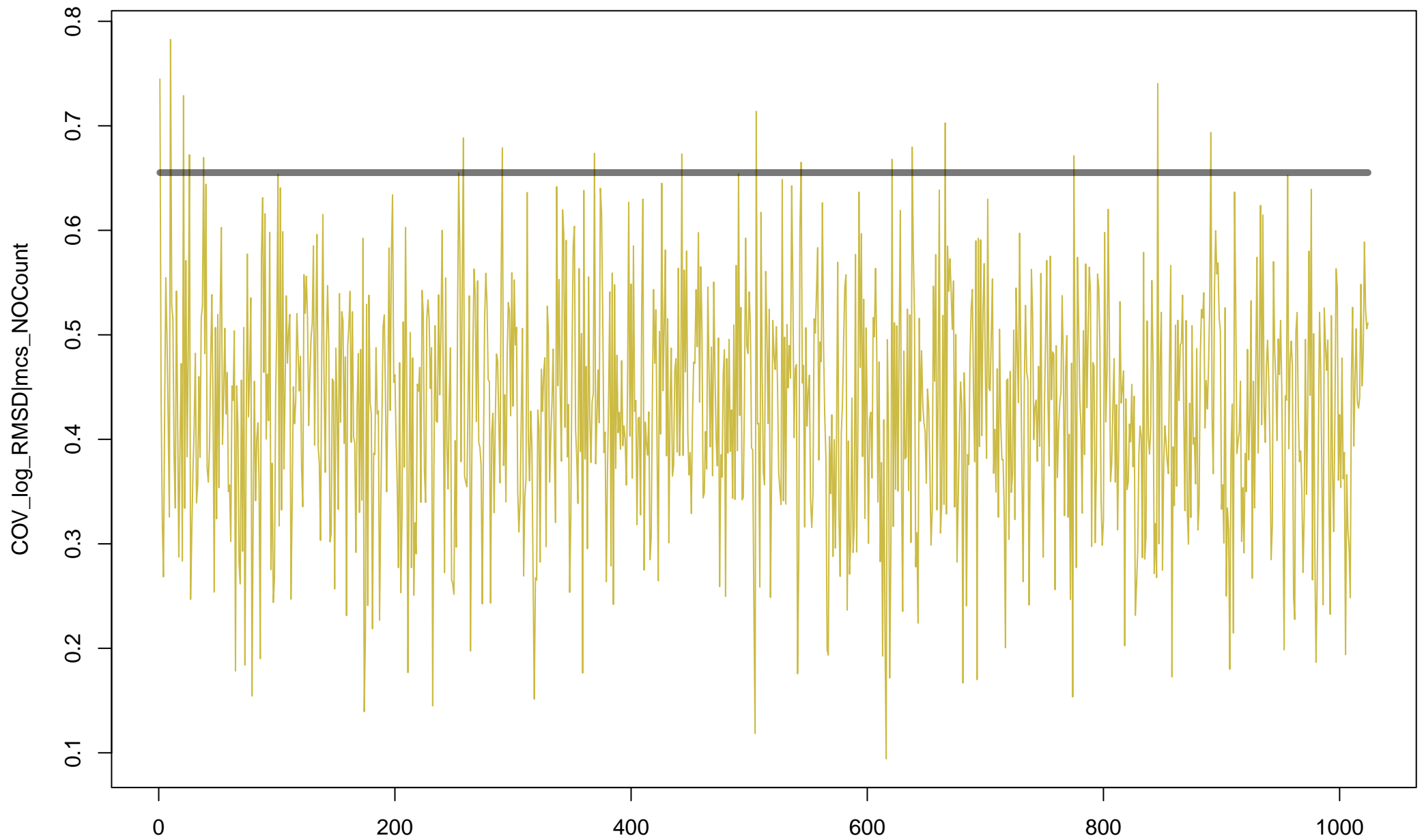
ESS = 1020 | BMK = 0.0596 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0 | percentile: 29.7



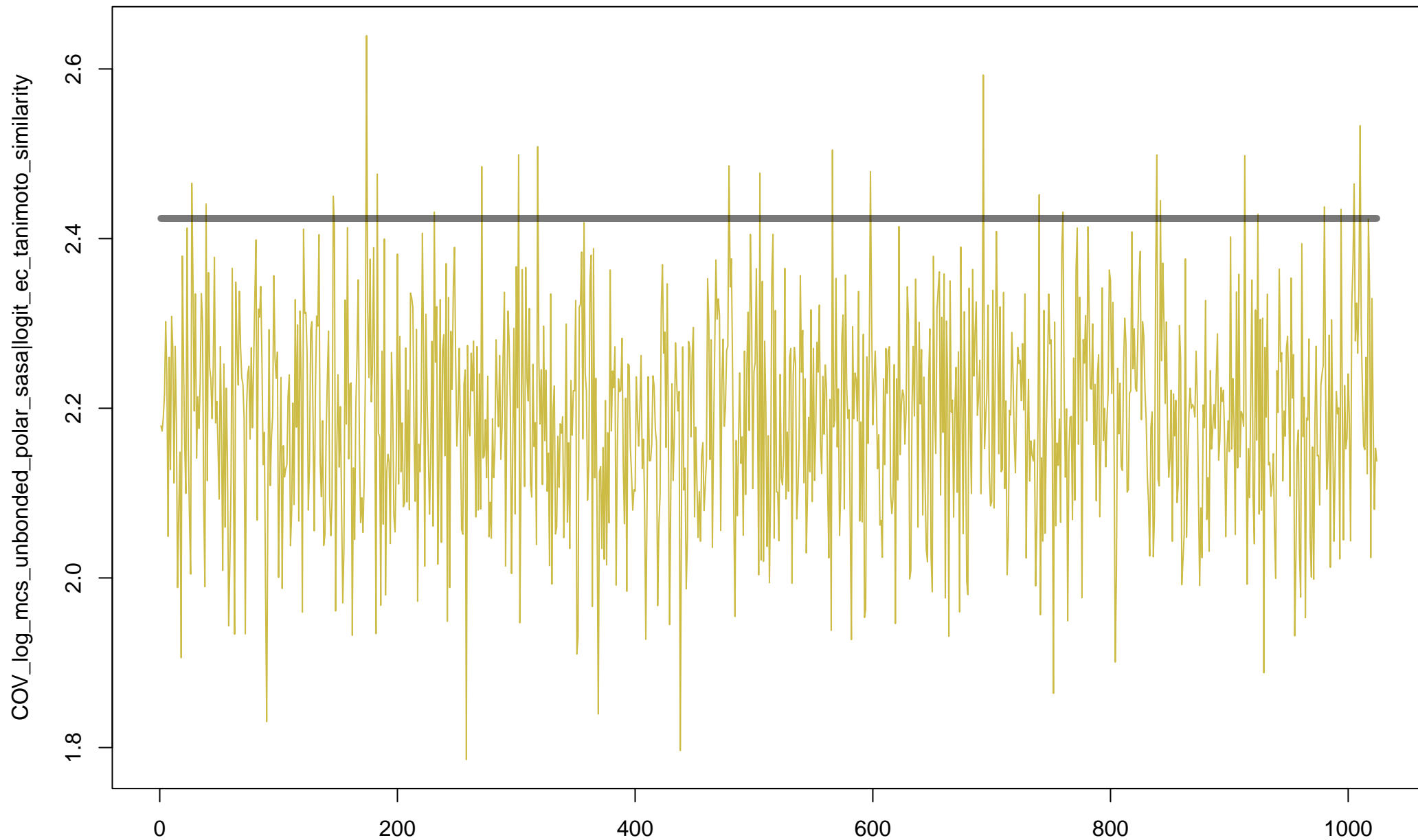
COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0543 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0 | percentile: 91



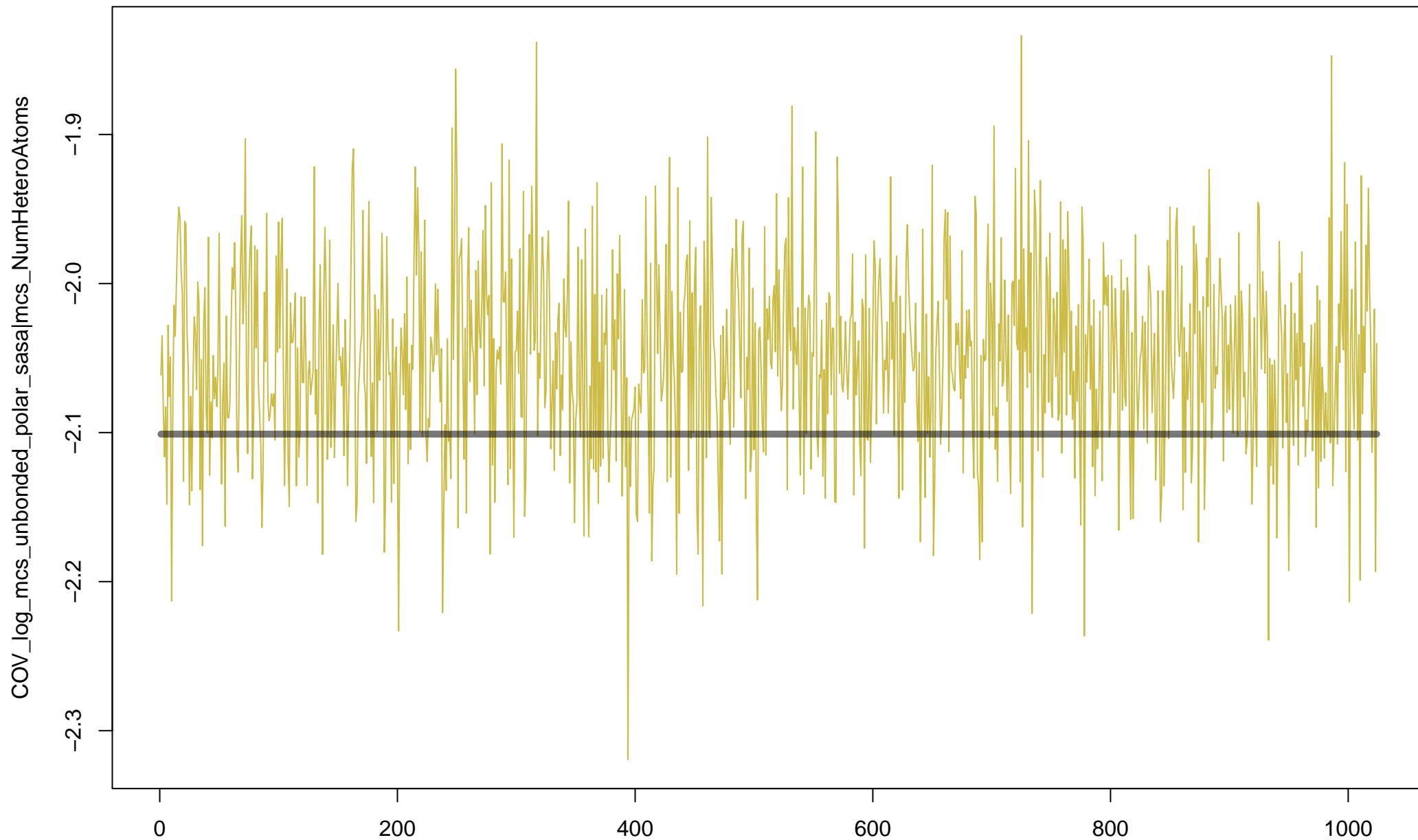
COV_log_RMSD|mcs_NOCount
ESS = 872 | BMK = 0.0529 | MCSE(6.27) = 3 | stat: TRUE | burn: 0 | percentile: 98.3



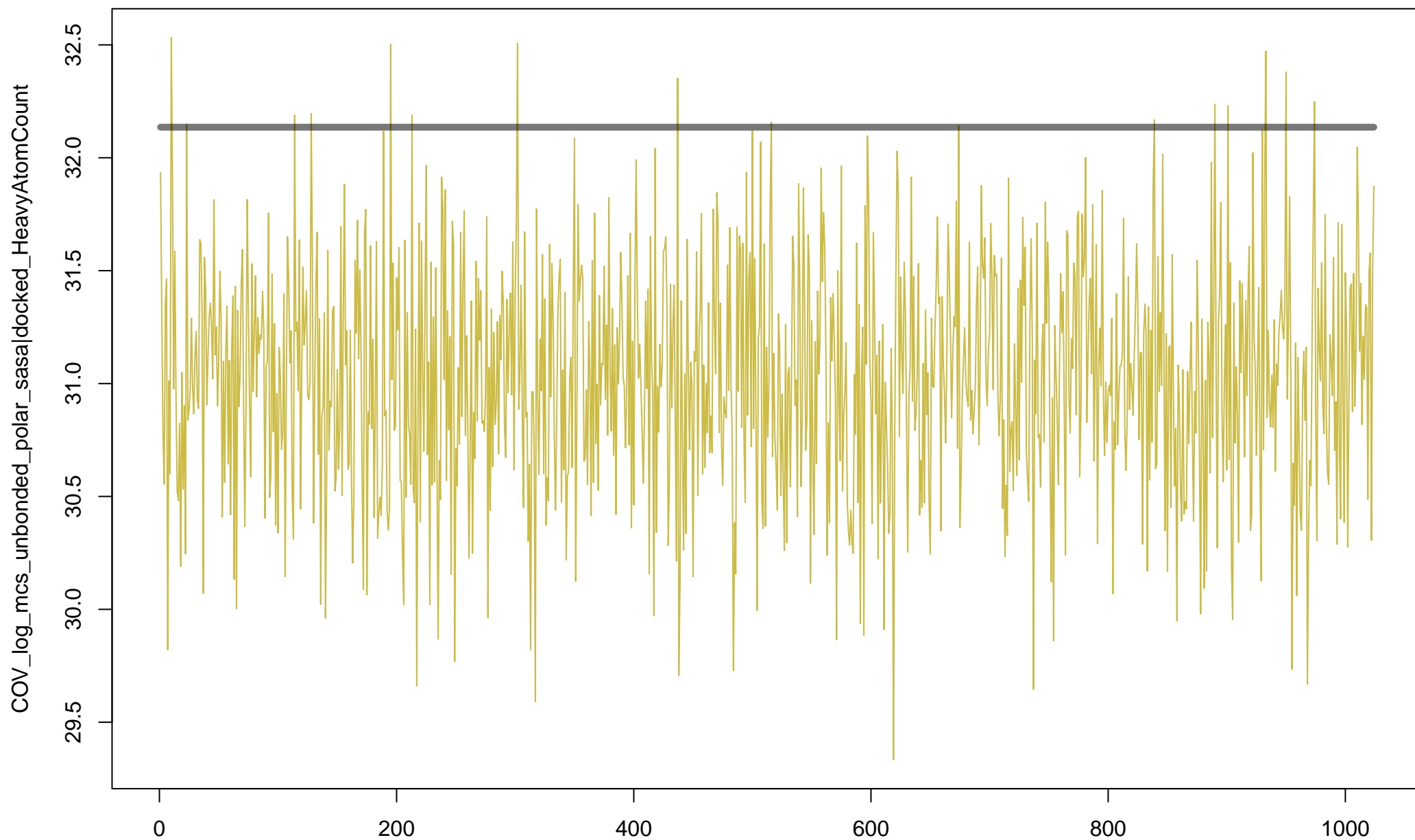
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.048 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0 | percentile: 97.7



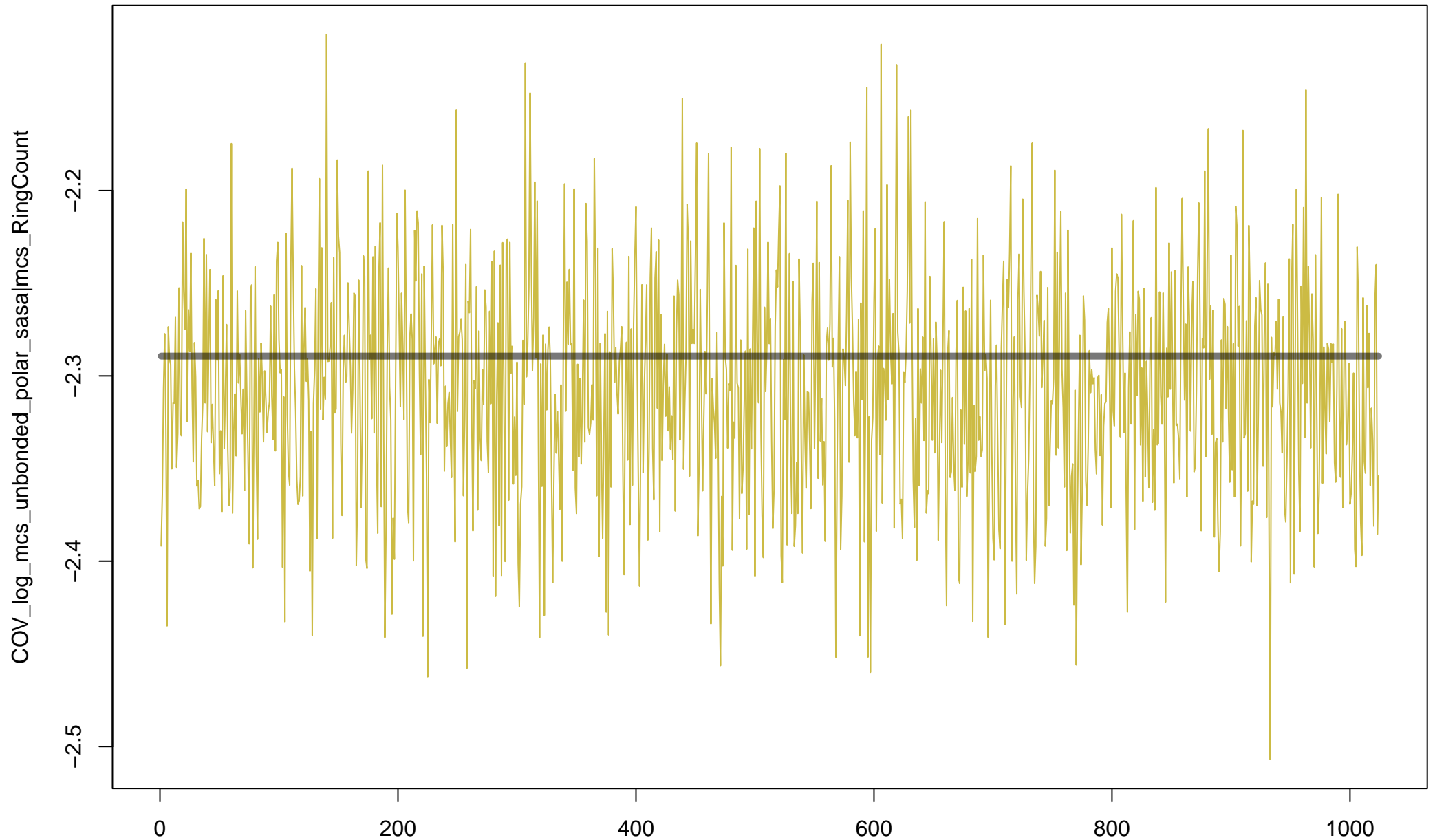
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0567 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0 | percentile: 21.3



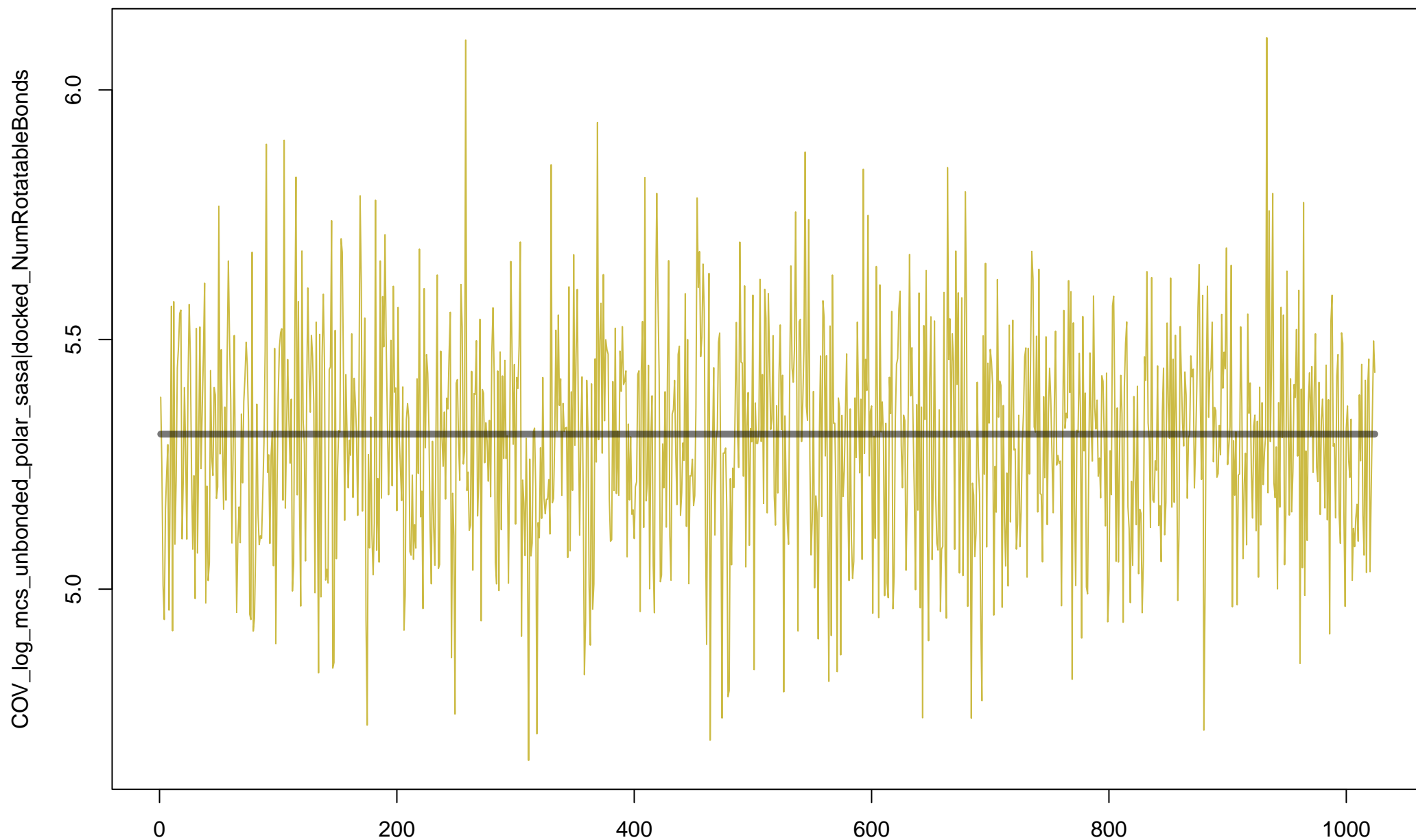
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0435 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | percentile: 98.4



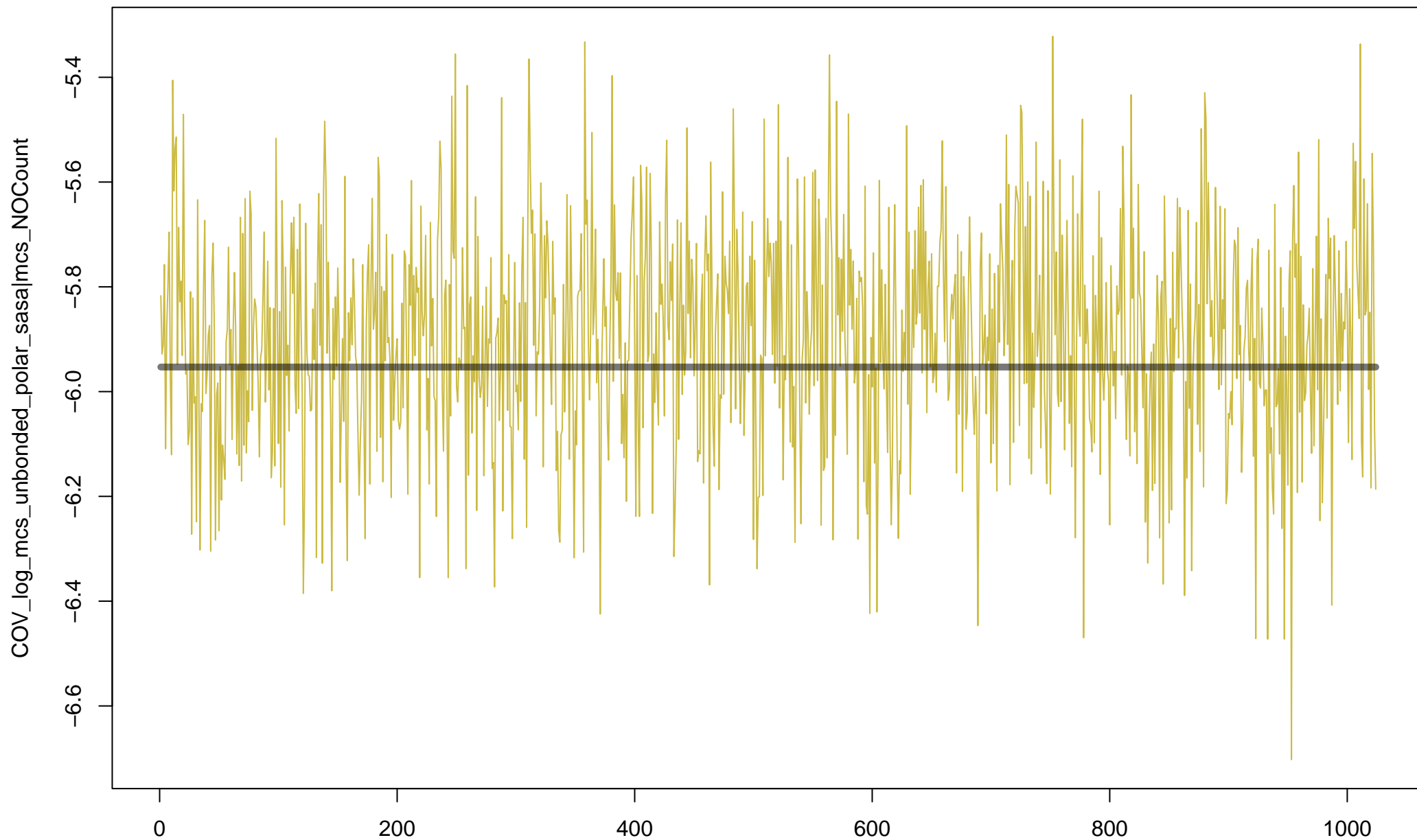
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0576 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0 | percentile: 60



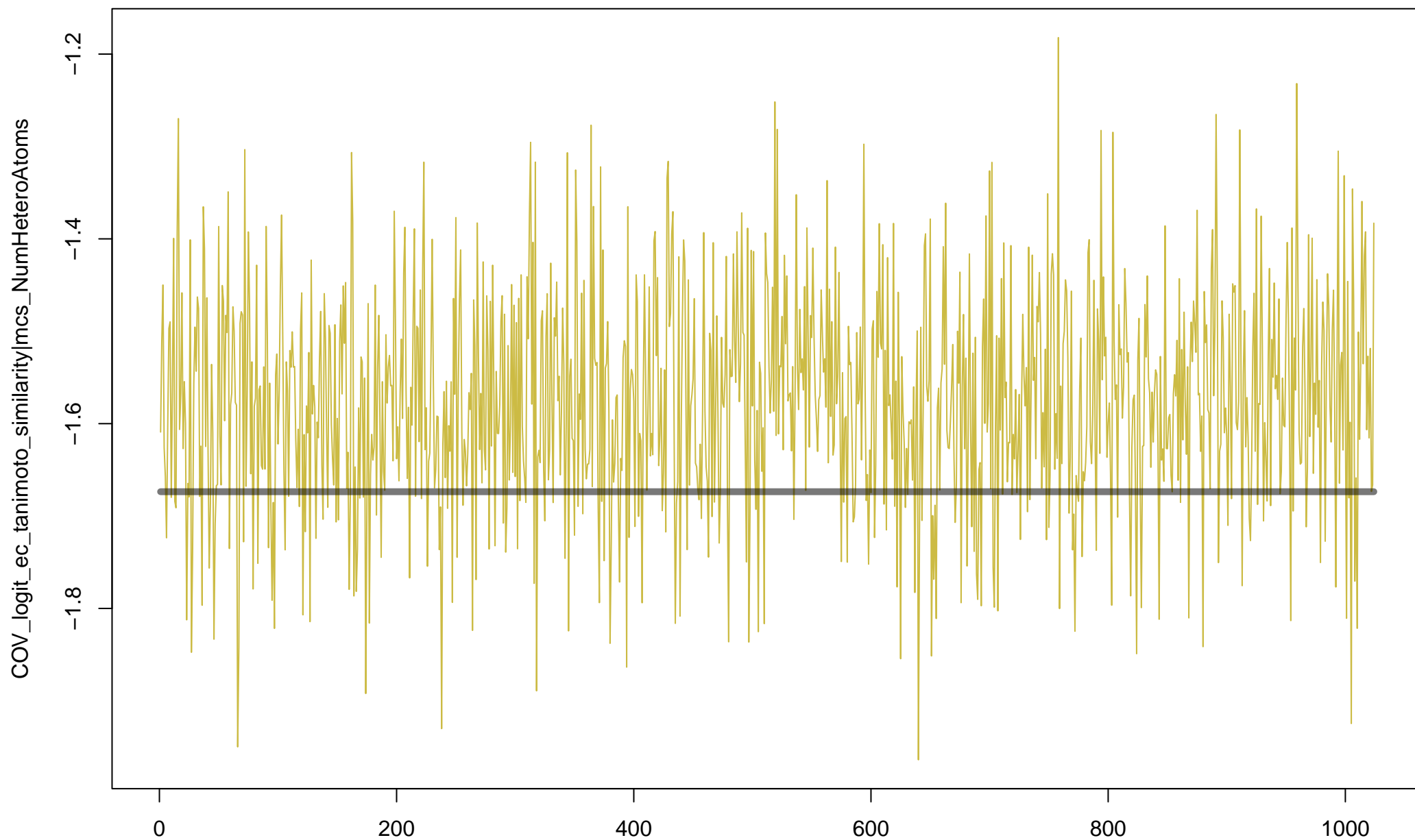
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0506 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | percentile: 51.2



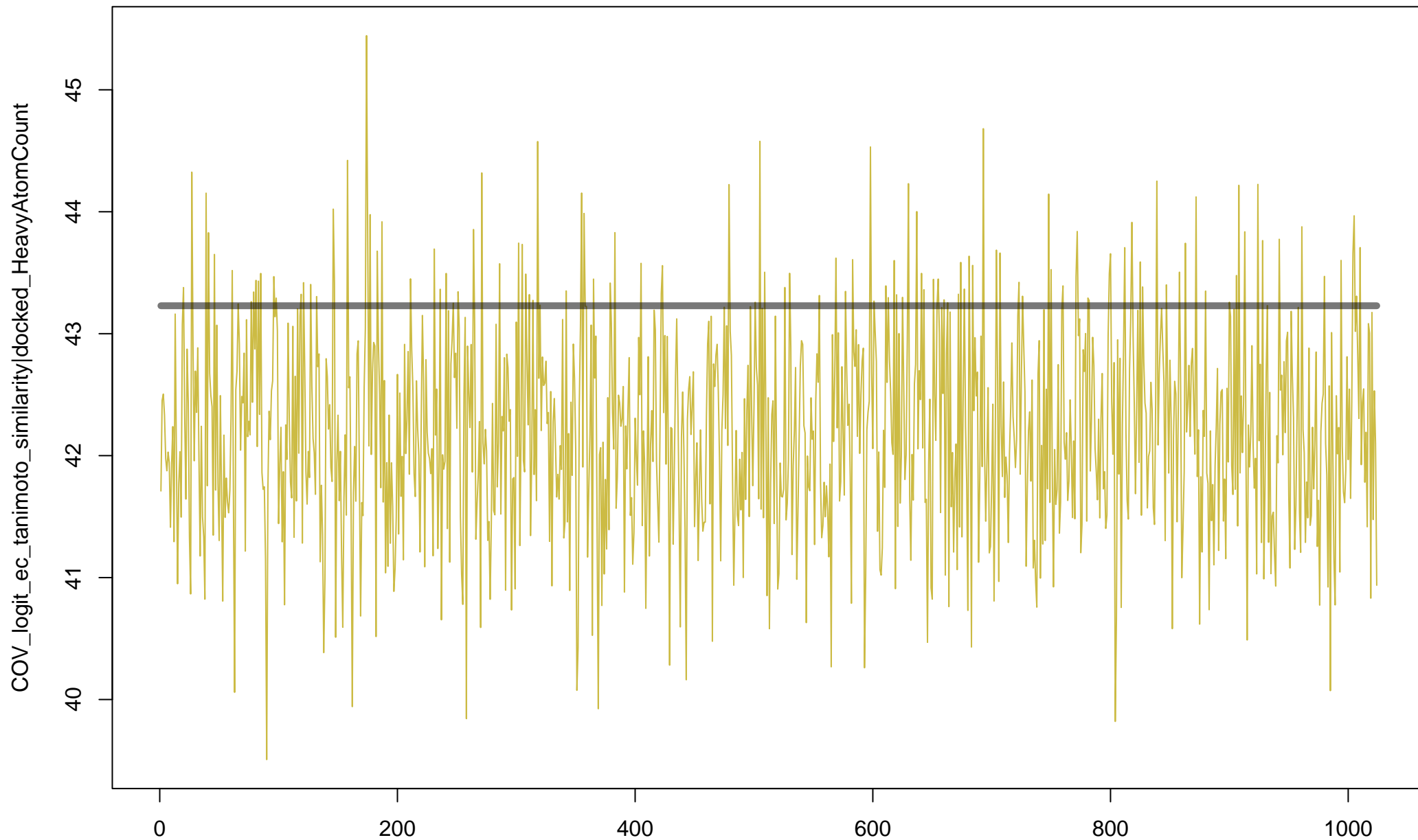
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 937 | BMK = 0.0605 | MCSE(6.27) = 3.61 | stat: TRUE | burn: 0 | percentile: 38.5



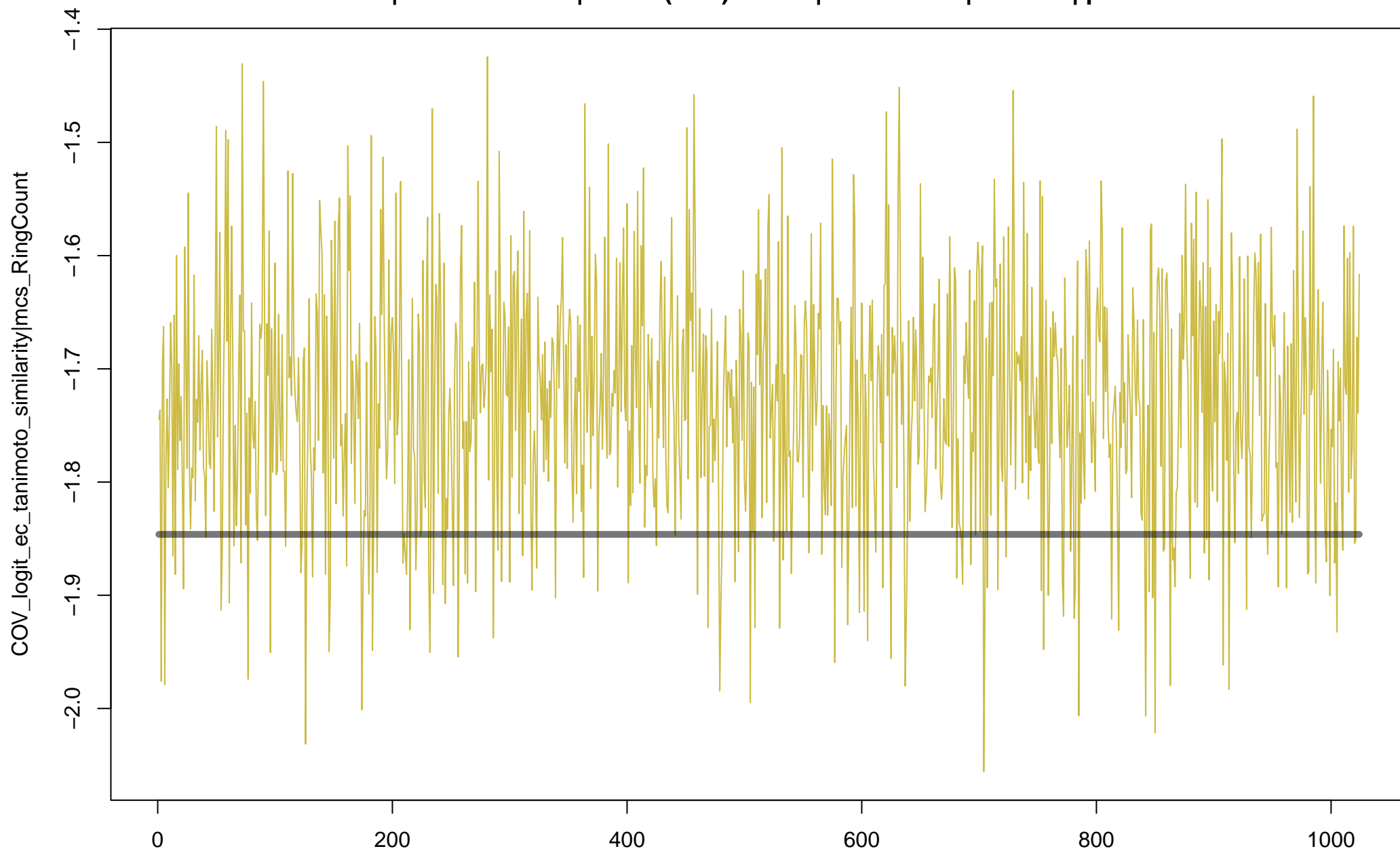
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0692 | MCSE(6.27) = 3.41 | stat: TRUE | burn: 0 | percentile: 19.2



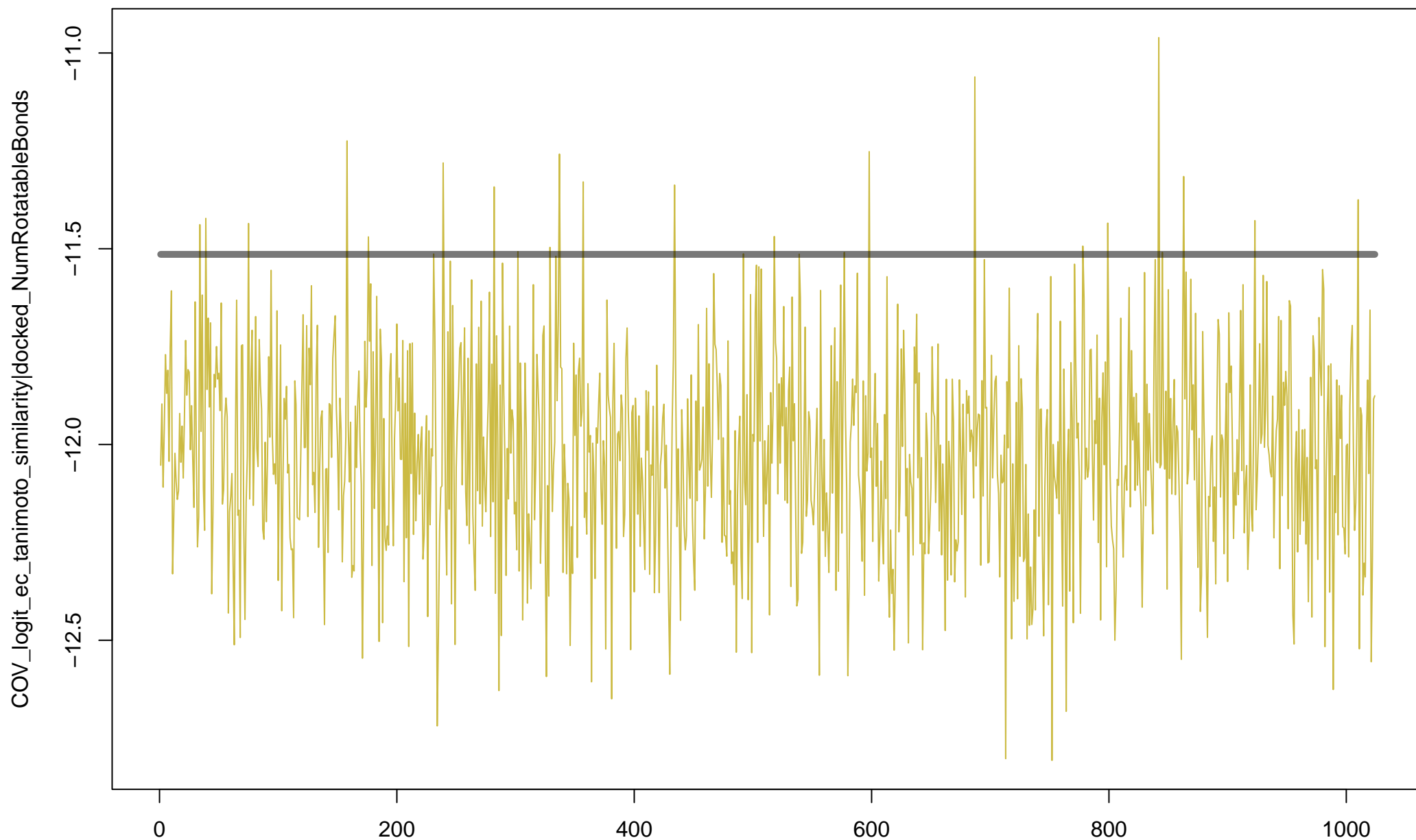
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 835 | BMK = 0.0431 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0 | percentile: 88.3



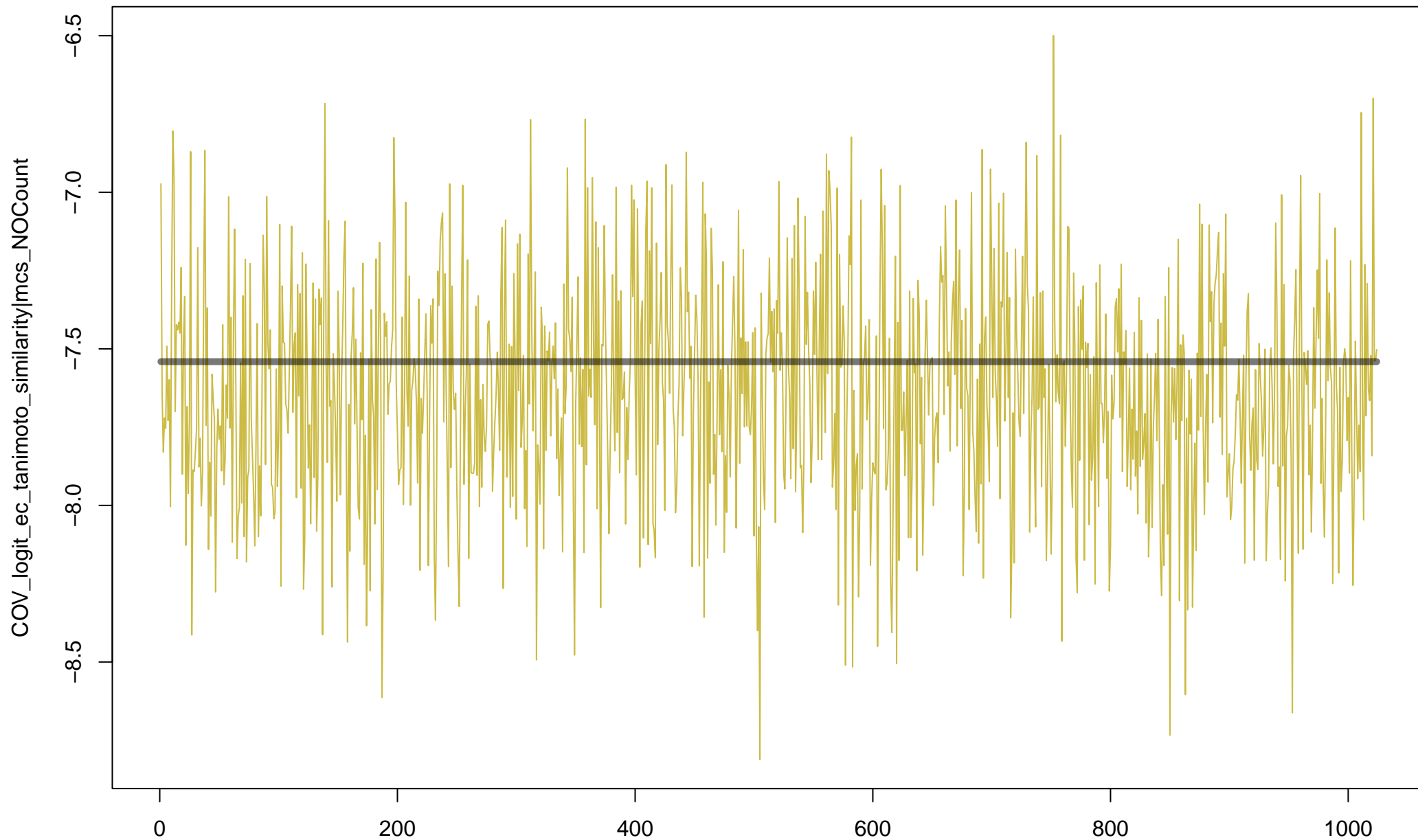
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0425 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0 | percentile: 13.3



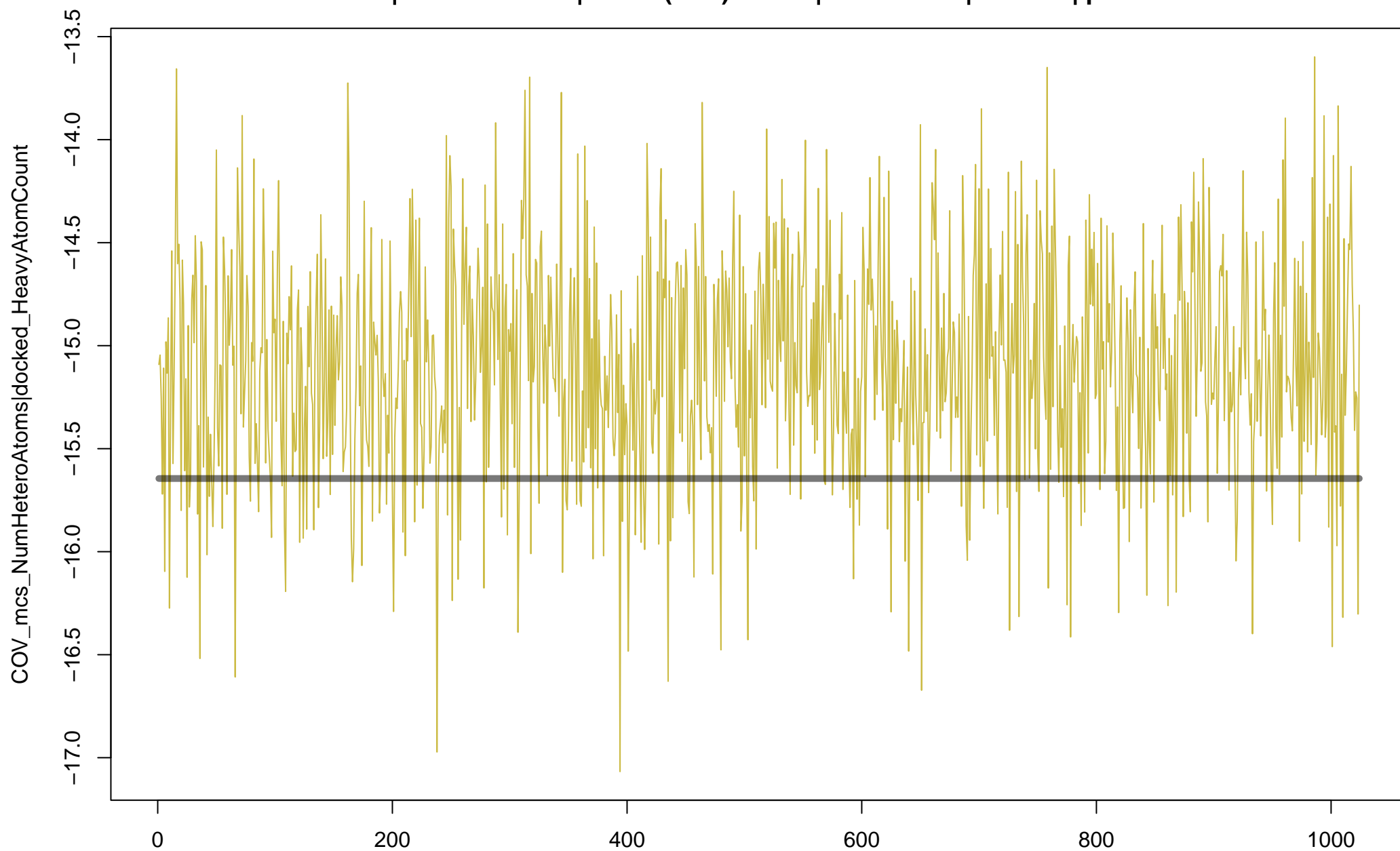
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0572 | MCSE(6.27) = 3.41 | stat: TRUE | burn: 0 | percentile: 97.5



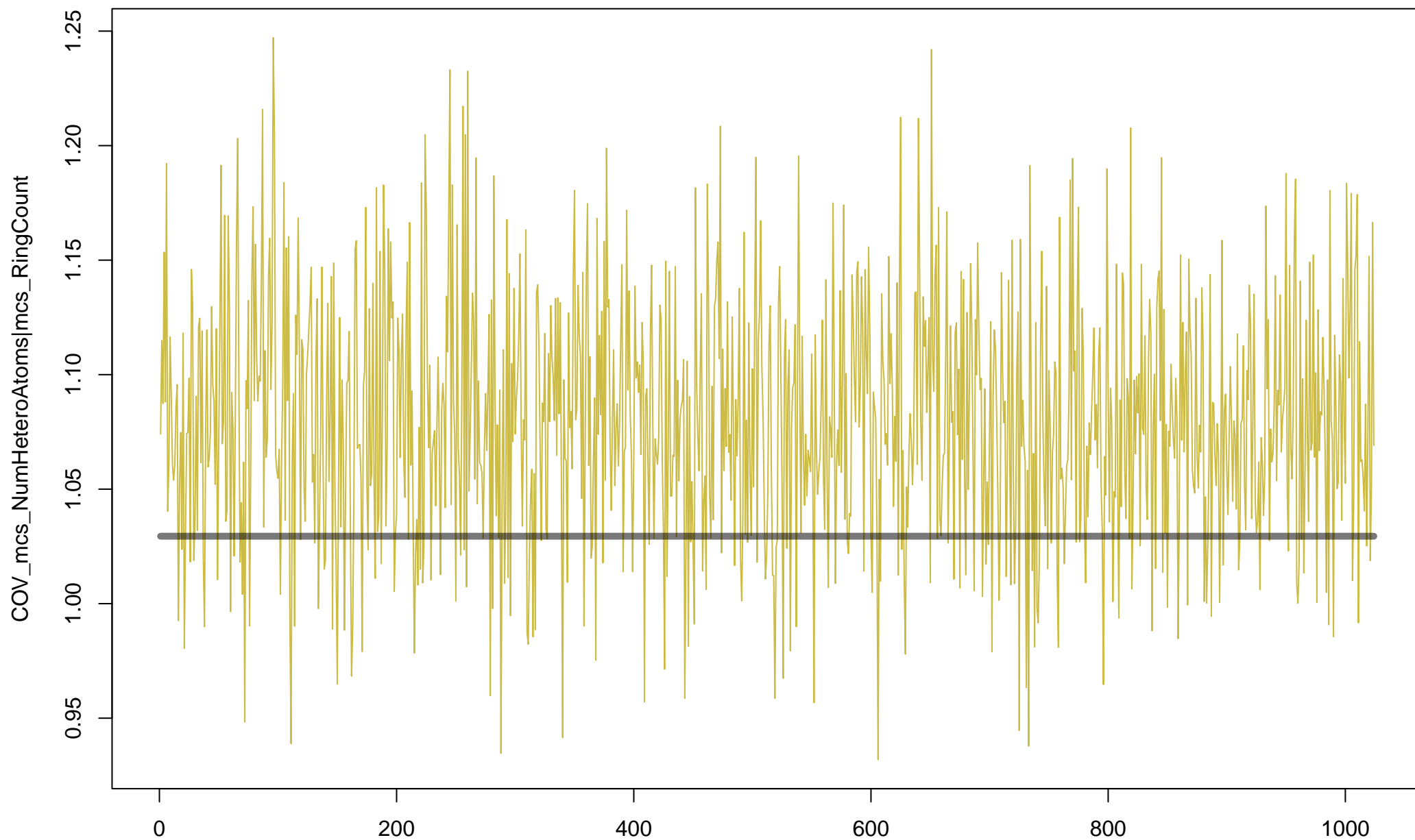
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0314 | MCSE(6.27) = 3.51 | stat: TRUE | burn: 0 | percentile: 61.6



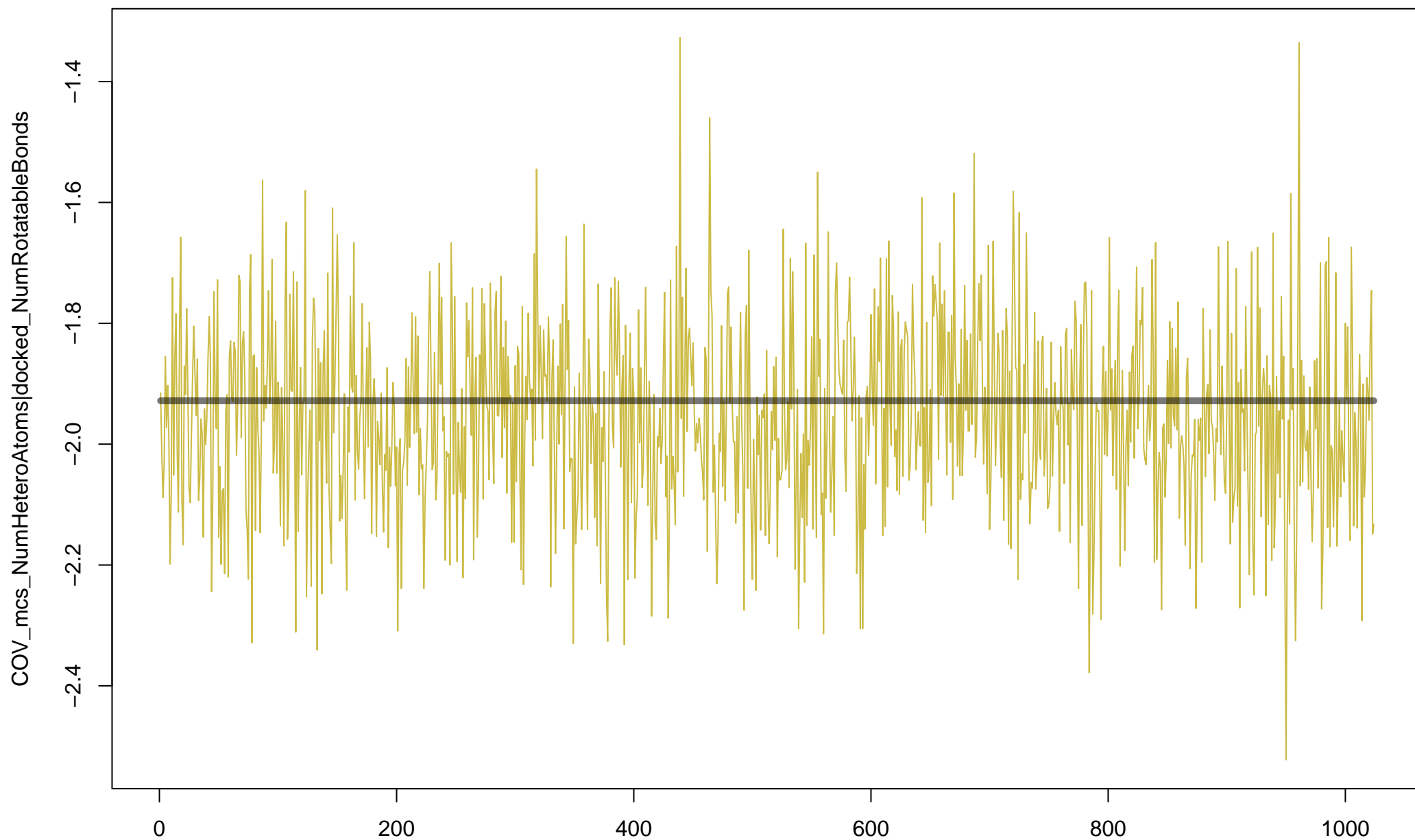
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0814 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0 | percentile: 14.9



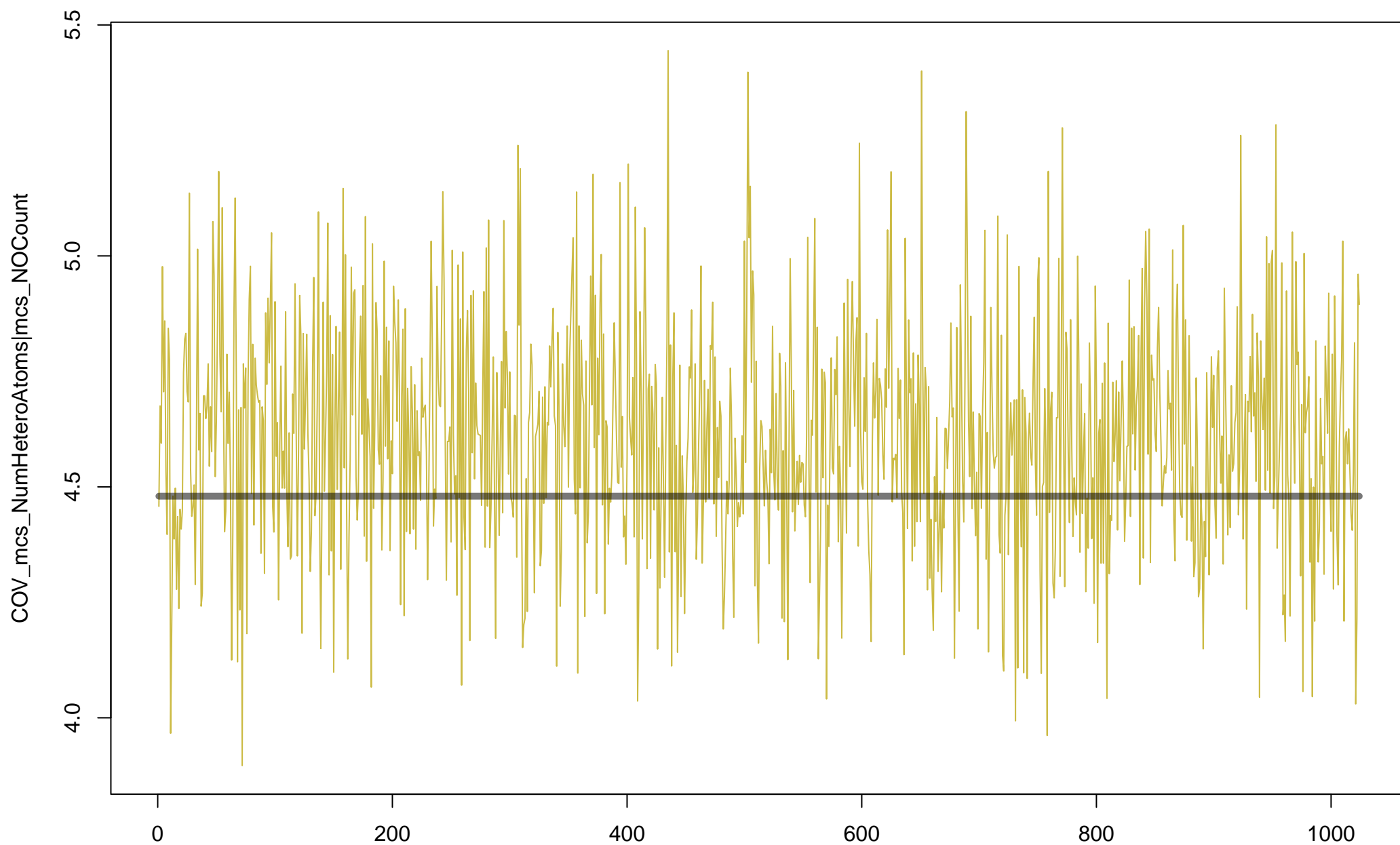
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0483 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0 | percentile: 17.9



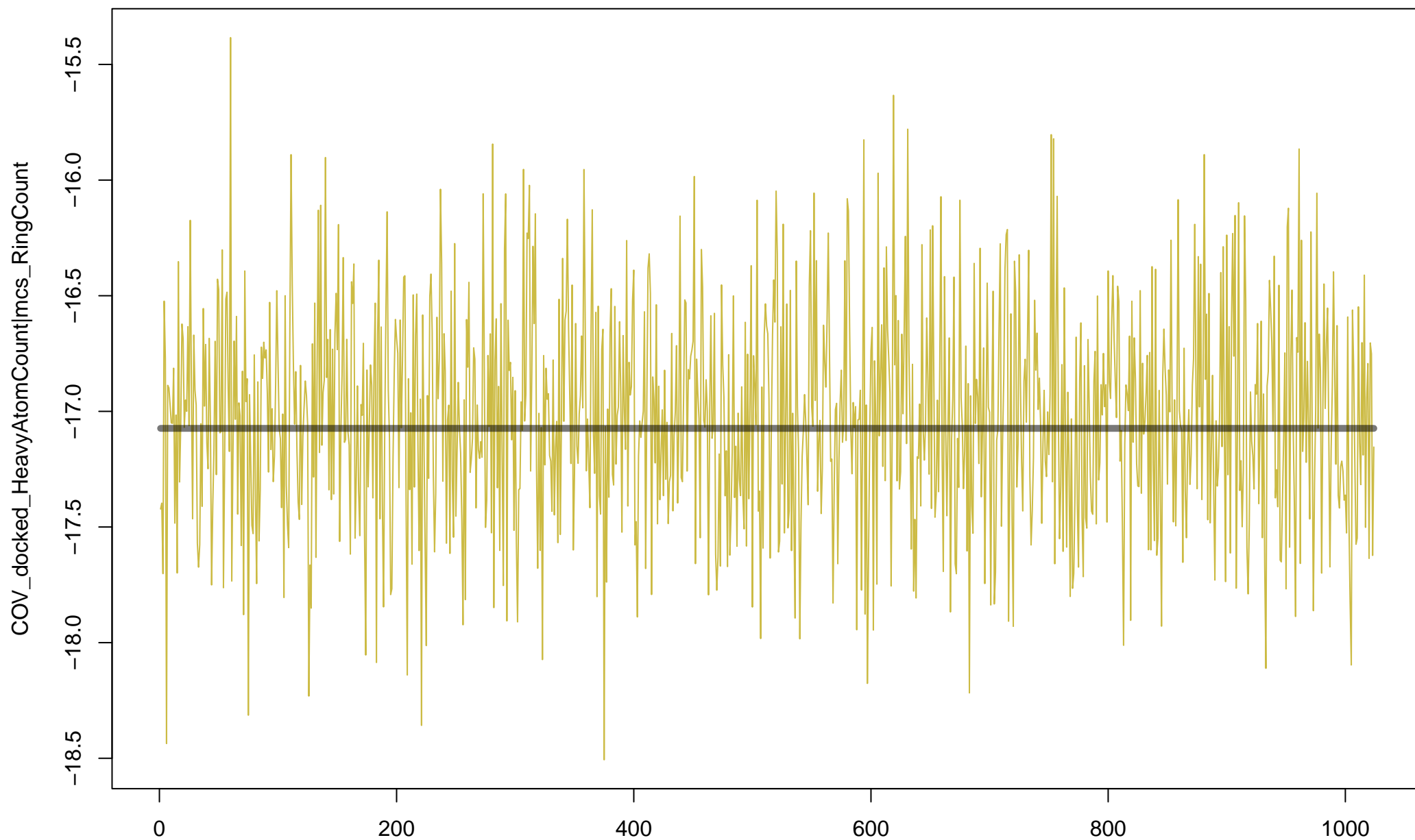
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0507 | MCSE(6.27) = 3.41 | stat: TRUE | burn: 0 | percentile: 58.7



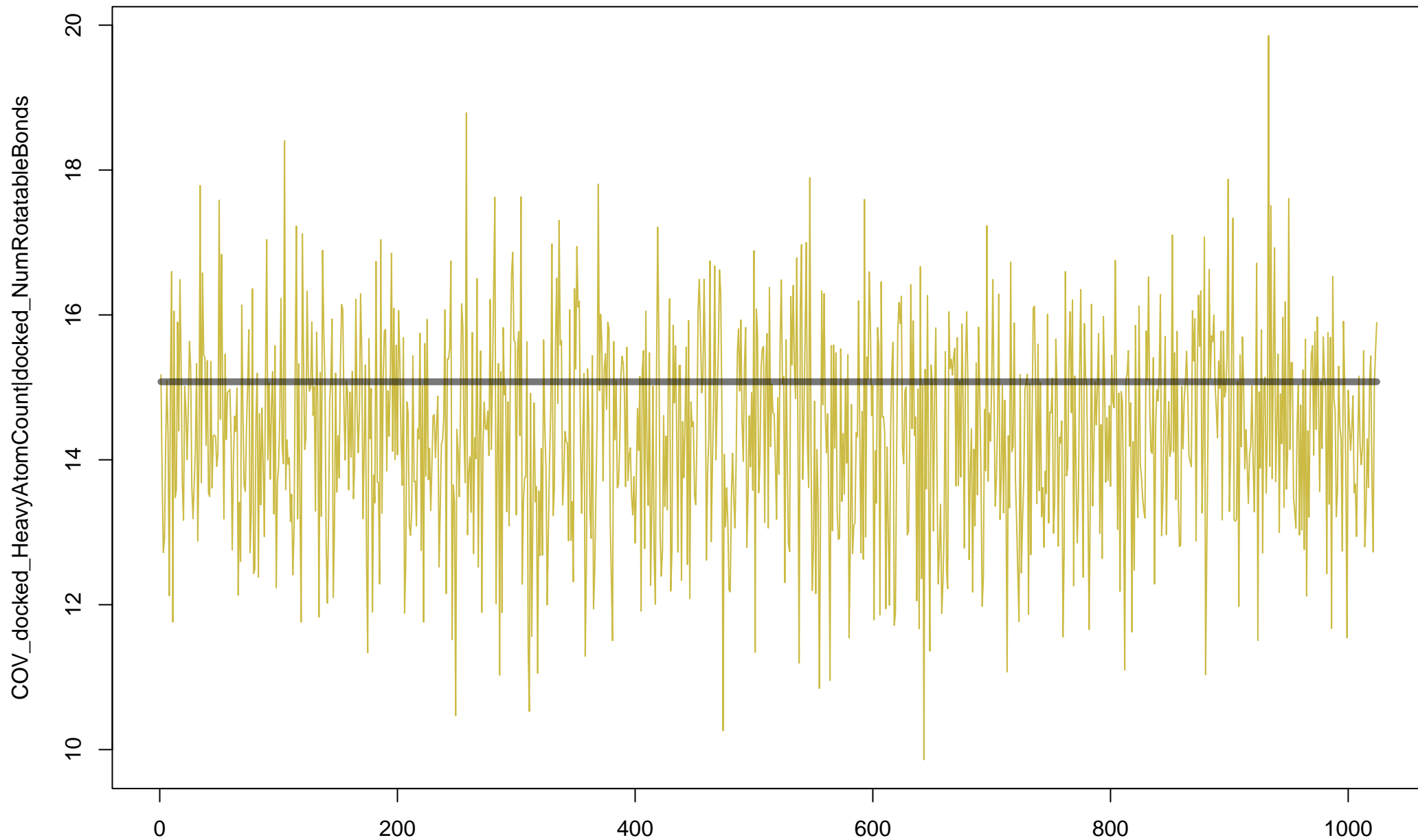
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0686 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | percentile: 29.9



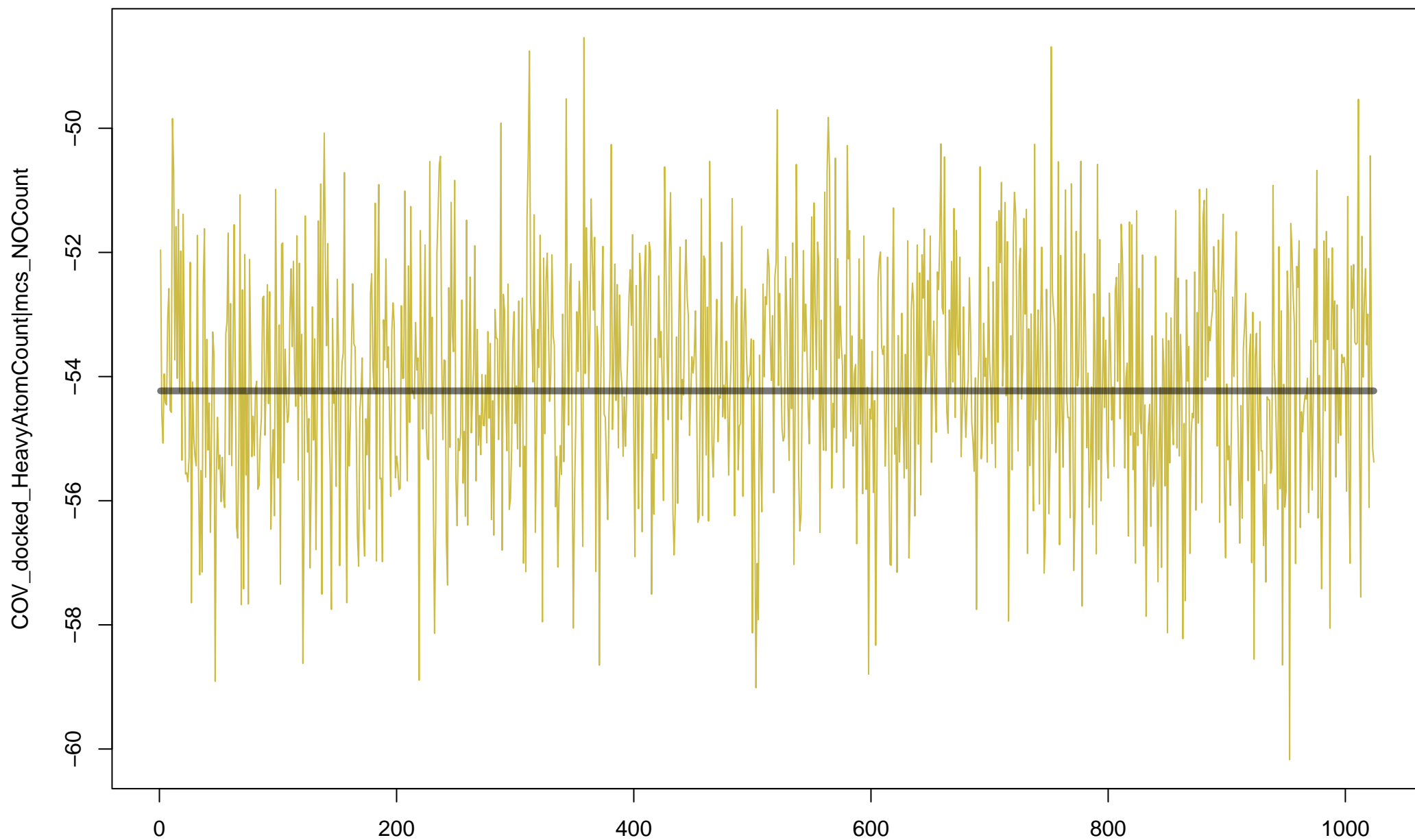
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0611 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0 | percentile: 44.4



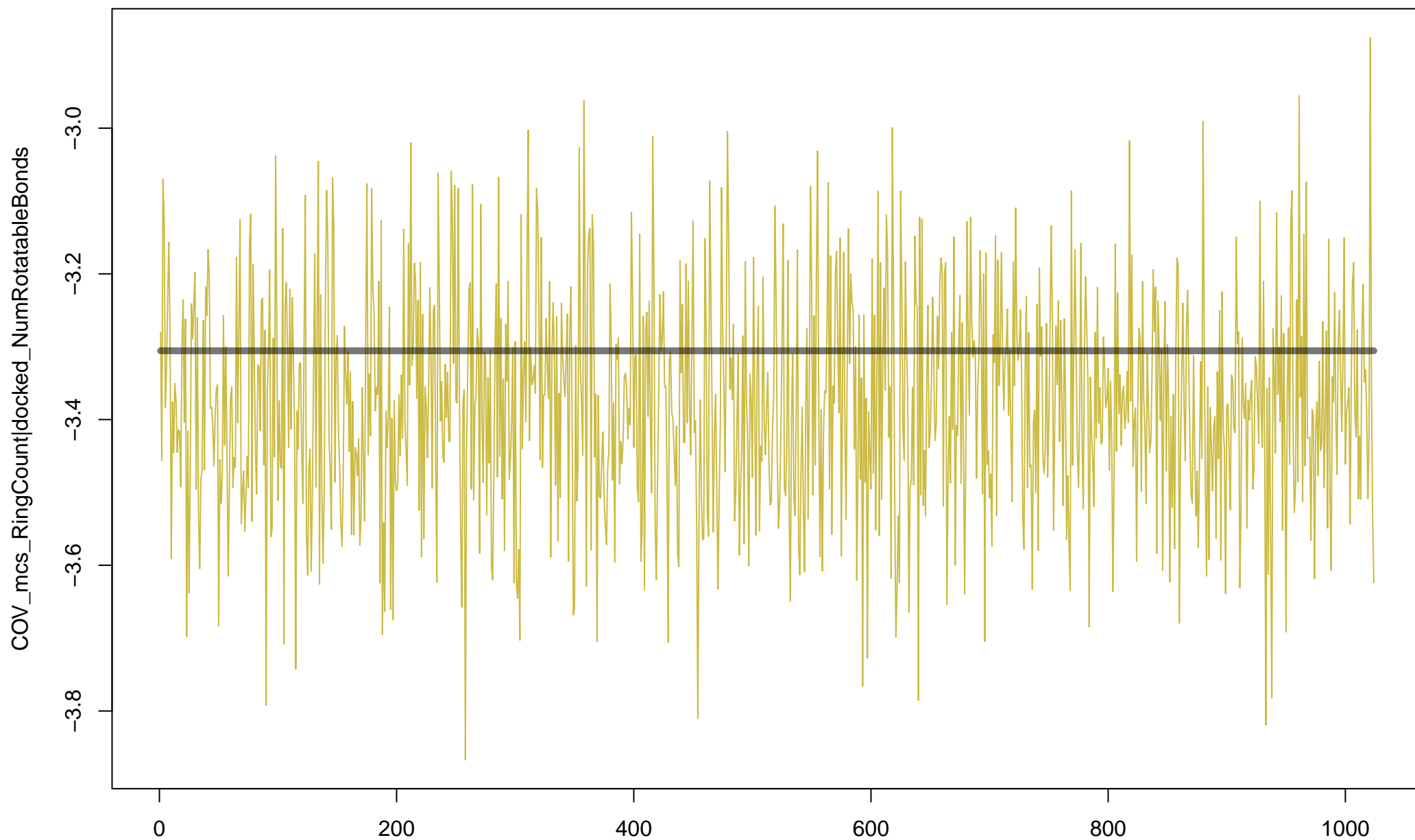
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0434 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0 | percentile: 68



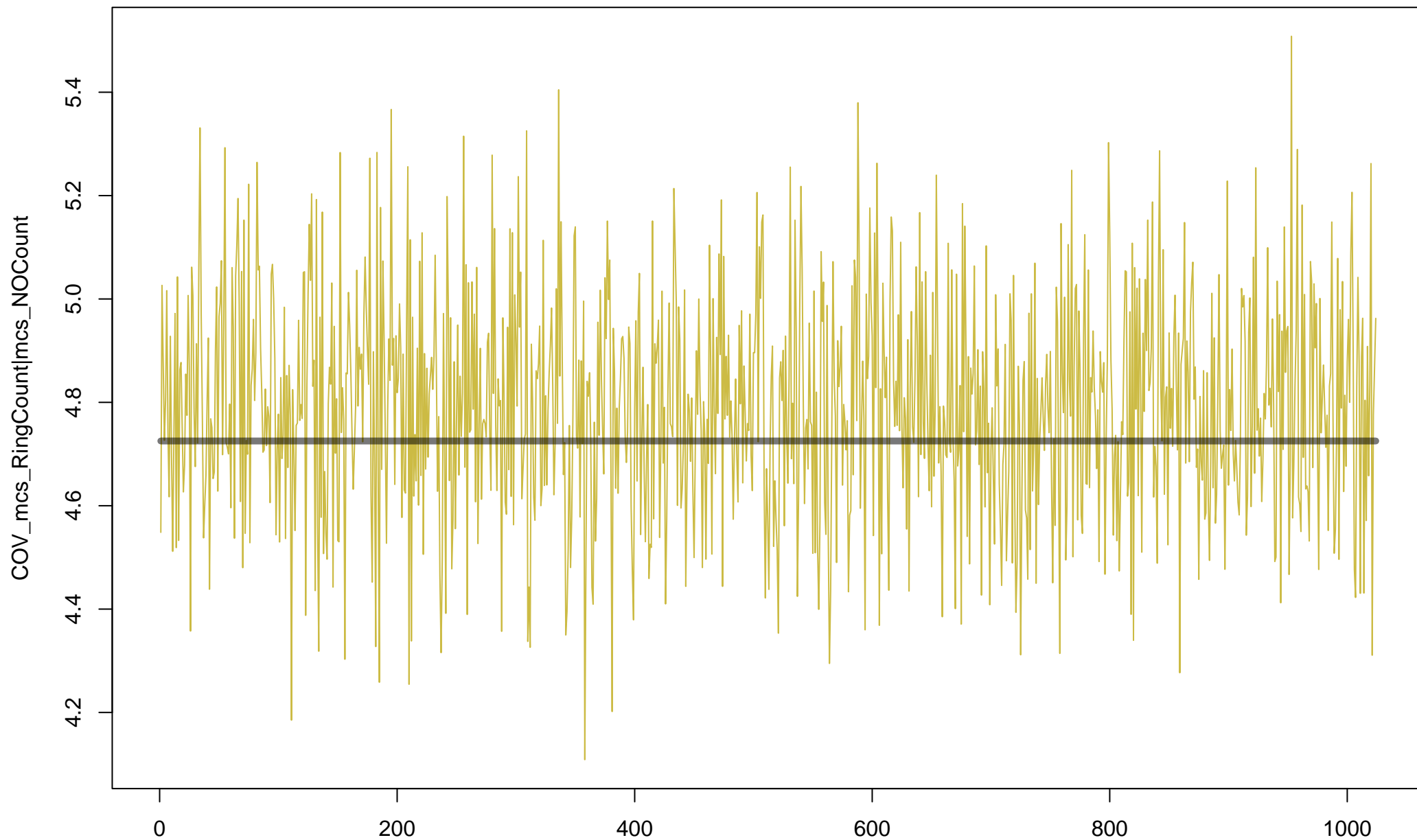
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0382 | MCSE(6.27) = 3.92 | stat: FALSE | burn: 0 | percentile: 46.5



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0479 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0 | percentile: 69



COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.0492 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | percentile: 37.6



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0573 | MCSE(6.27) = 2.97 | stat: FALSE | burn: 0 | percentile: 13.8

