

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 1

max MCSE = 15.4719471051888

all stationary: FALSE

burn: 1020

min percent.: 0.48828125

-- STATS 2D --

min ESS = 611.117138843453

max BMK = 0.0776231817356117

max MCSE = 4.13672158678551

all stationary: FALSE

burn: 0

min percent.: 0.87890625

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 1

max MCSE = NaN

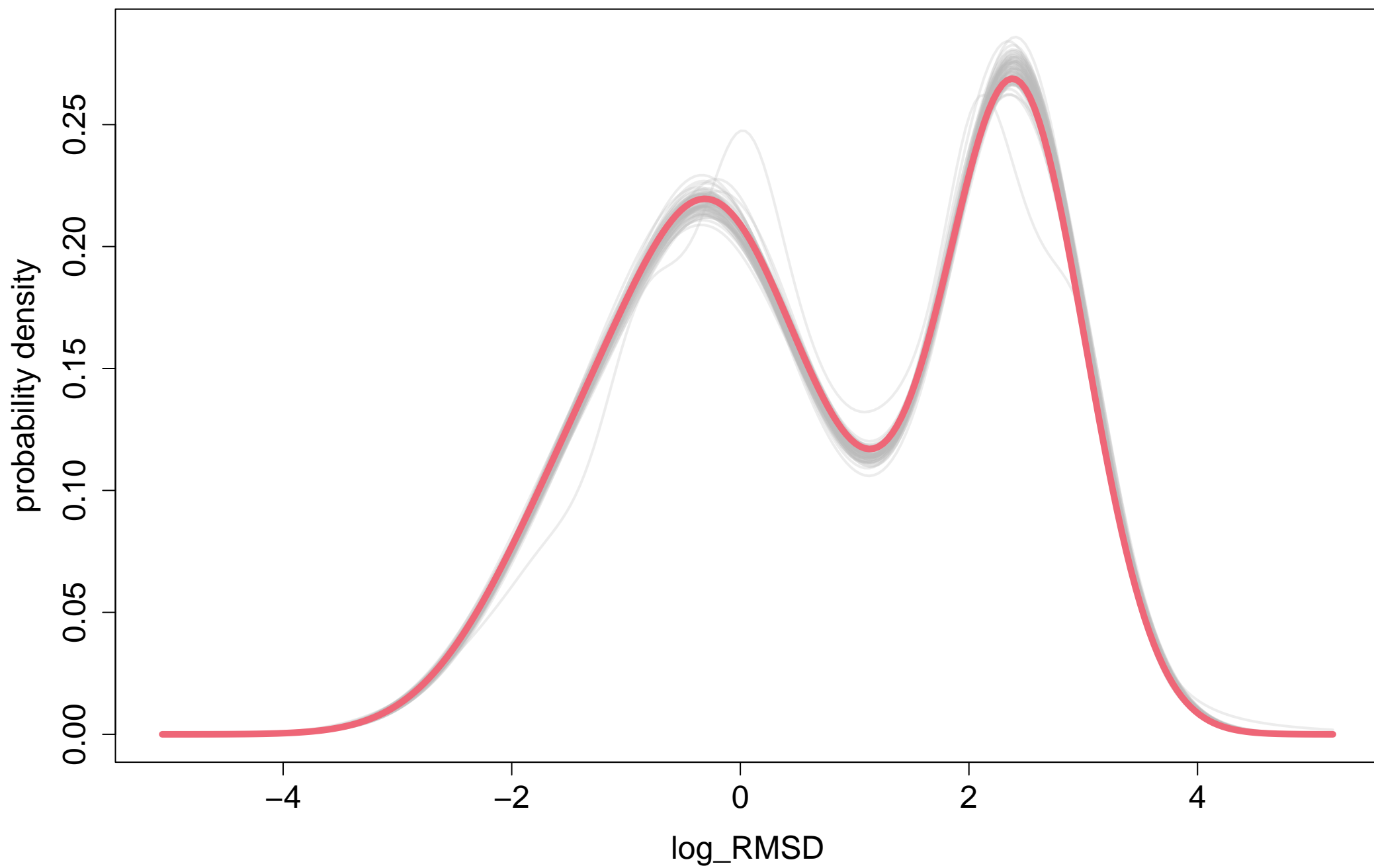
all stationary: FALSE

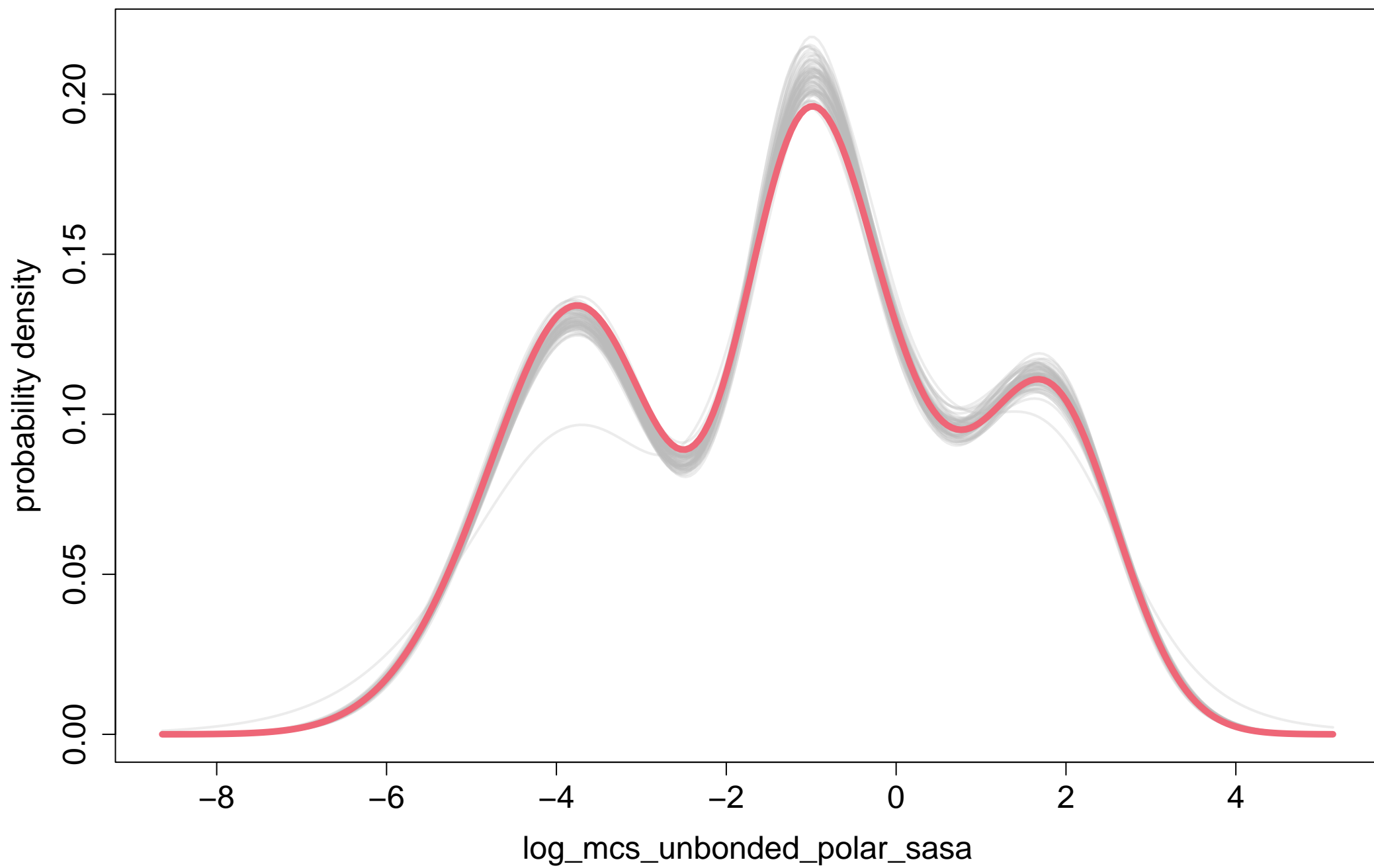
burn: 1020

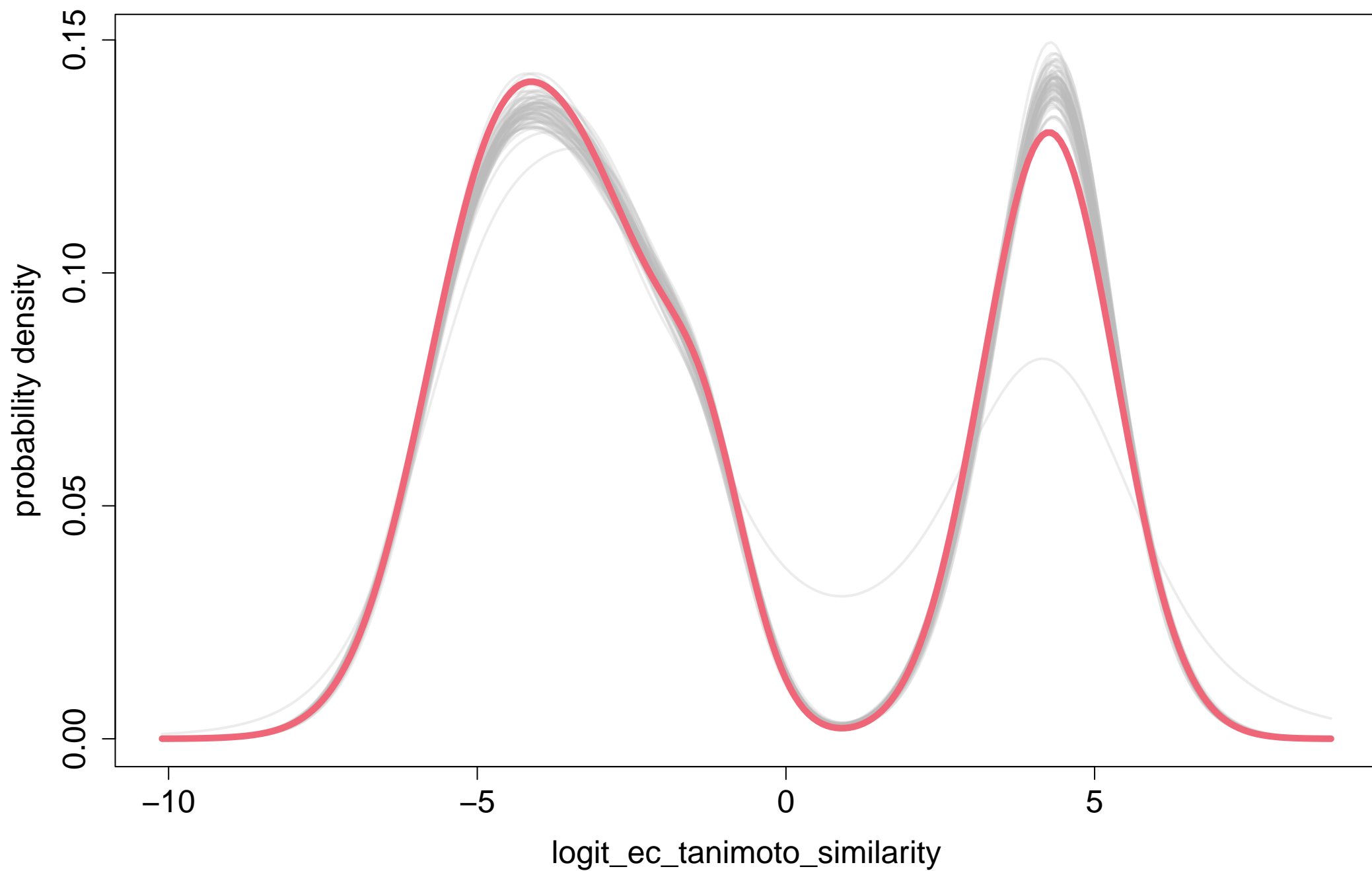
min percent.: 0

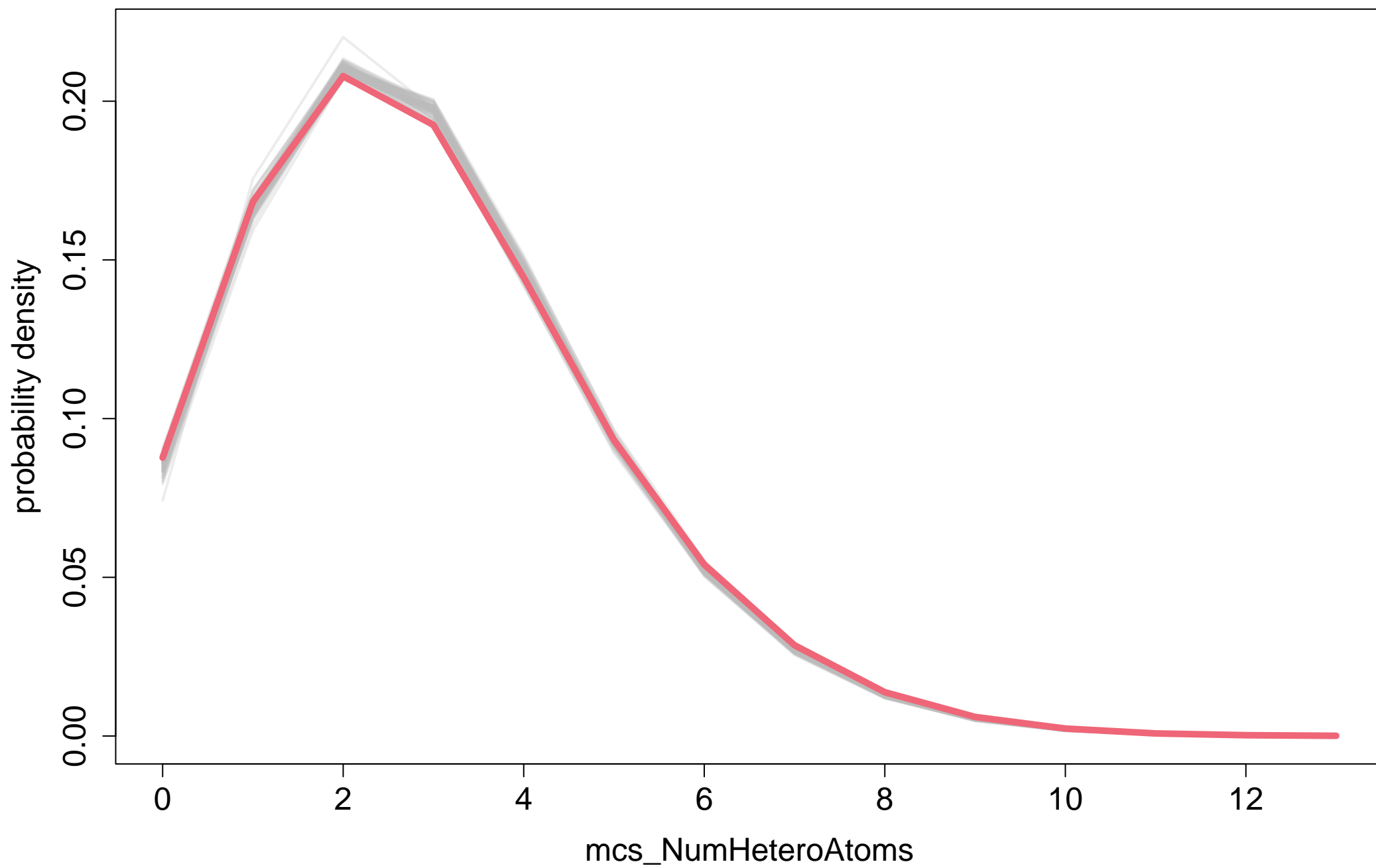
Occupied clusters: 12 of 64

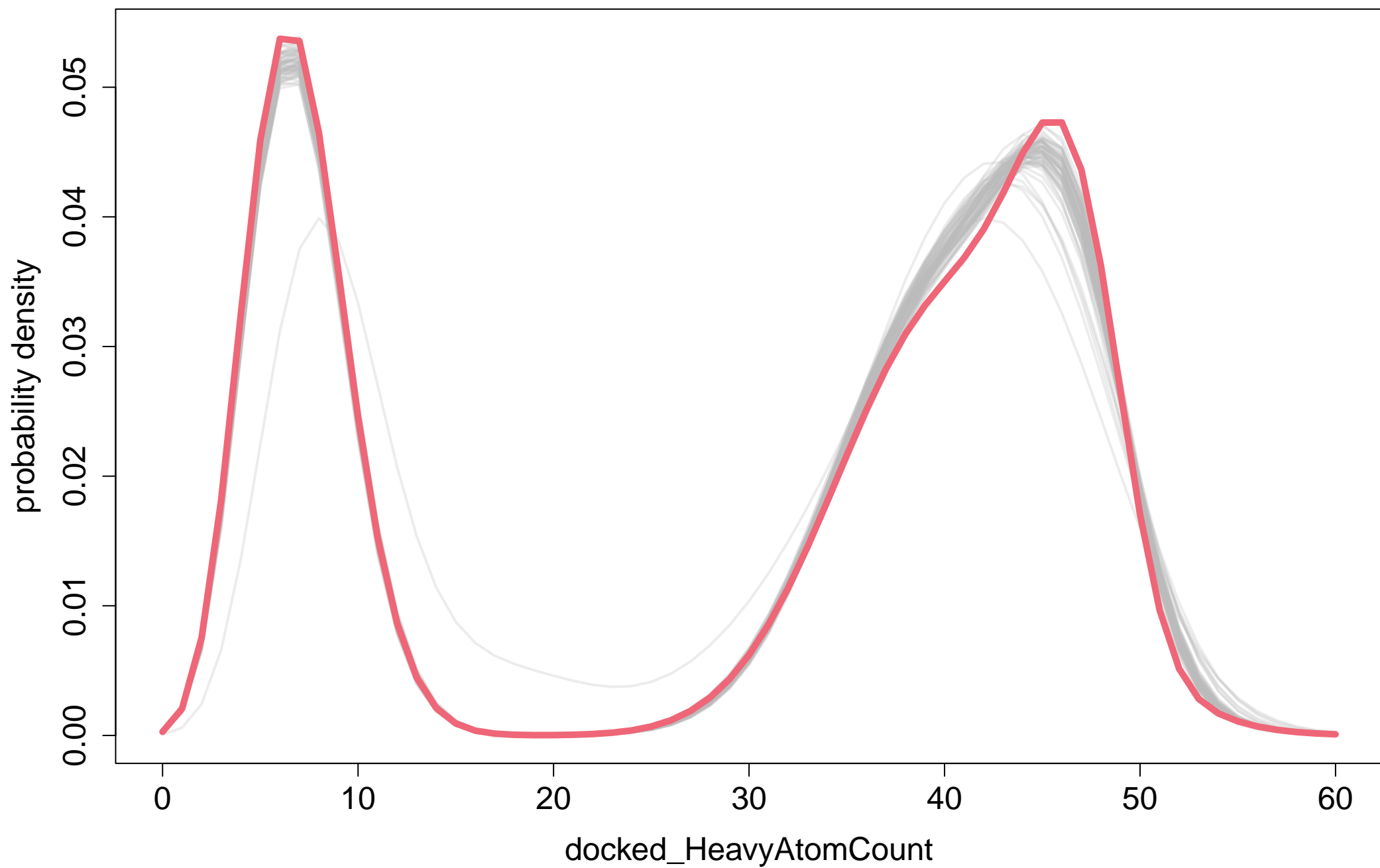
LL: -125000 +- 253

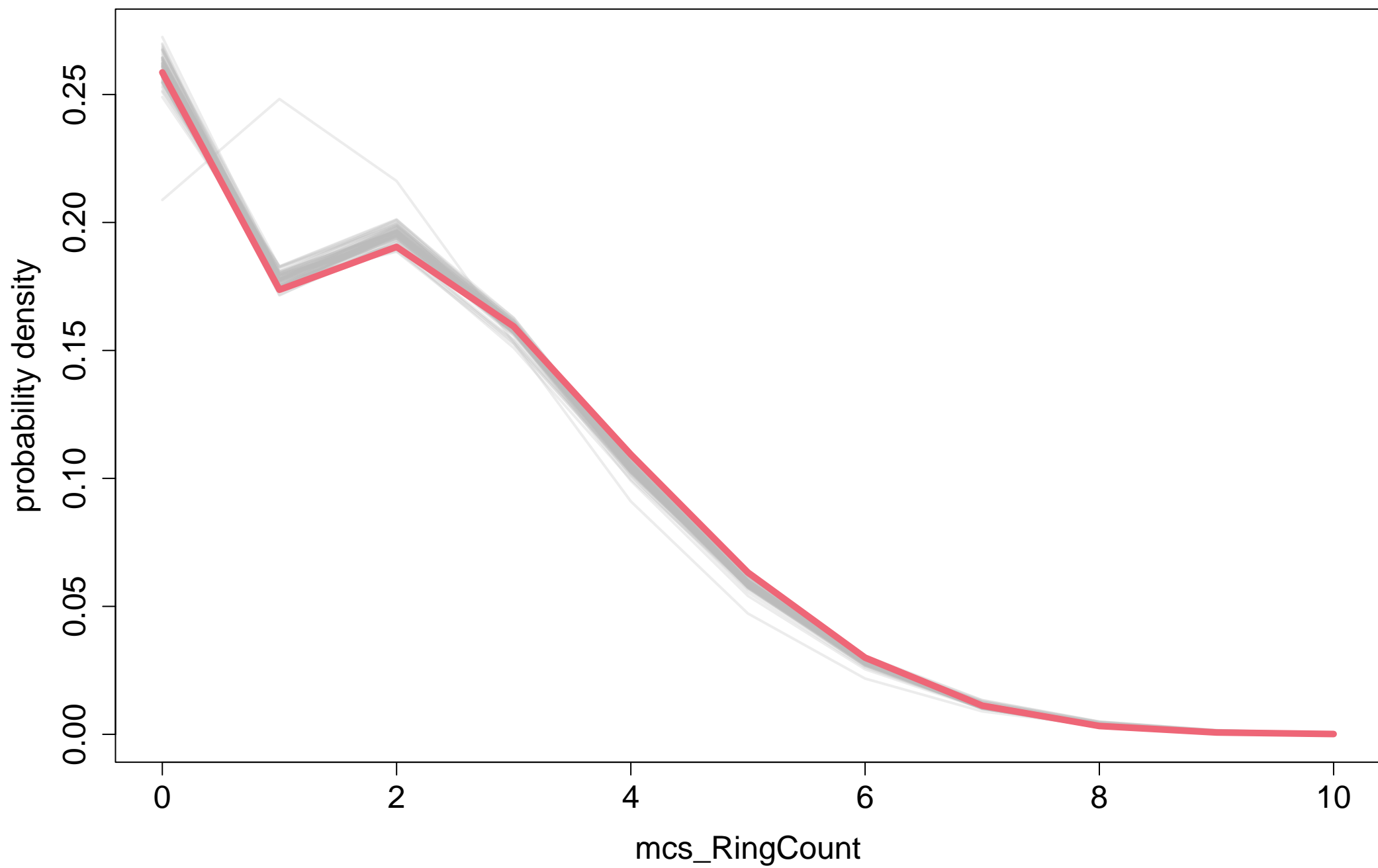


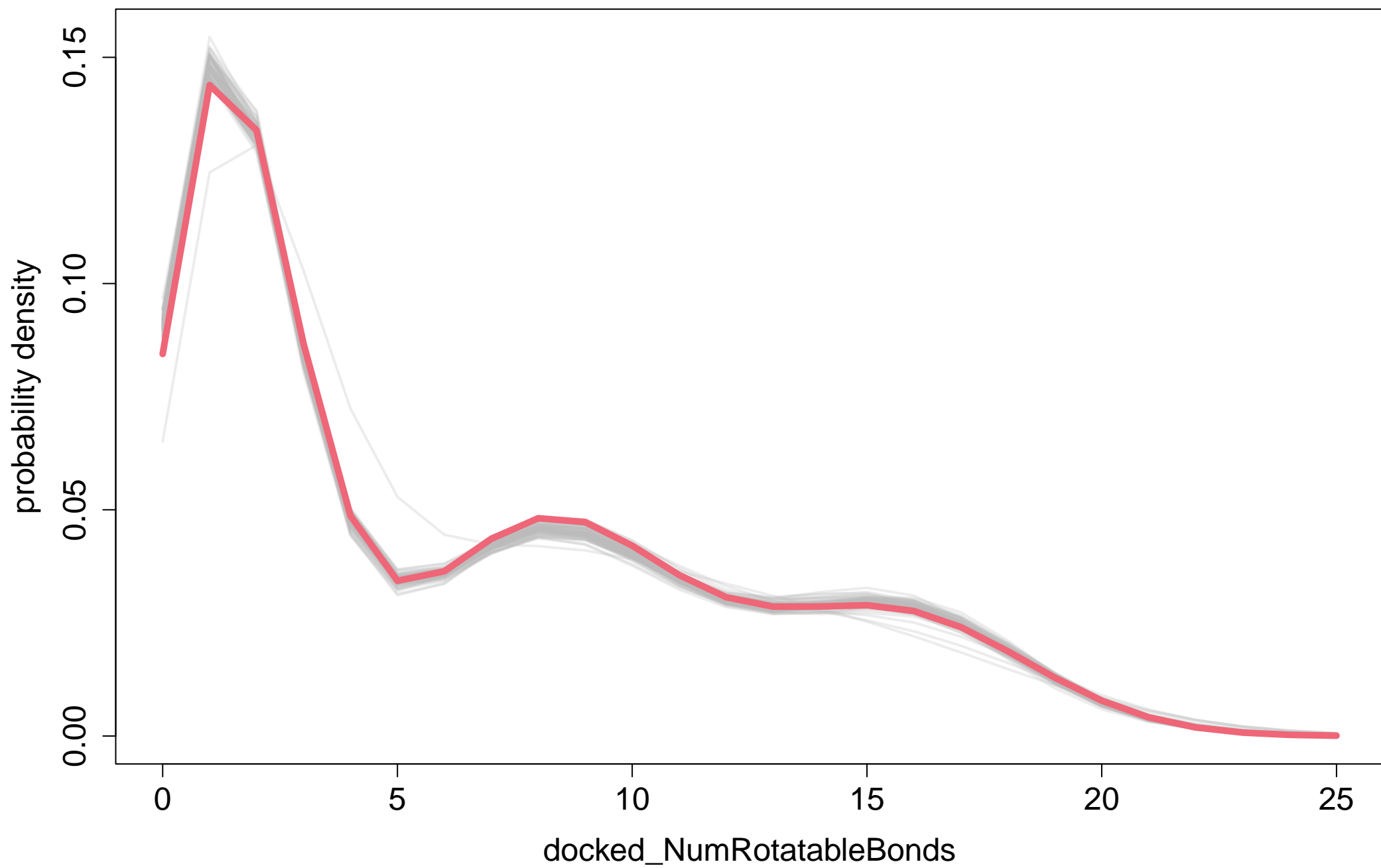


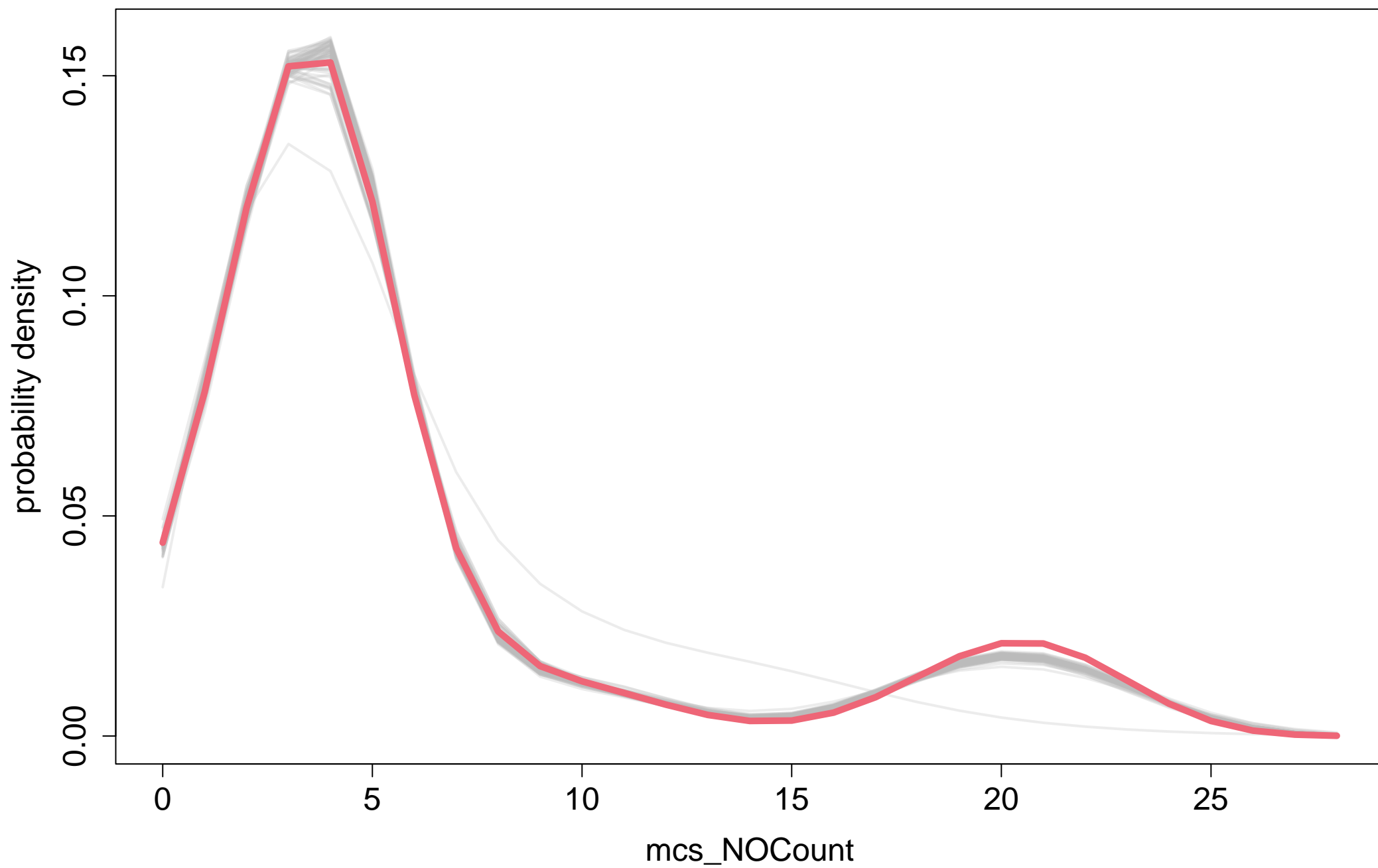


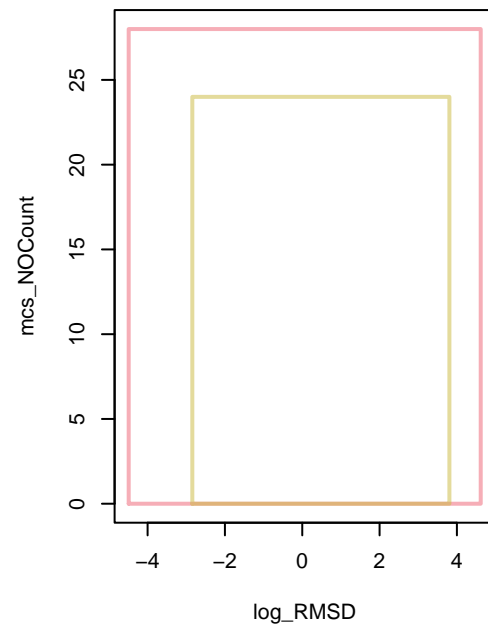
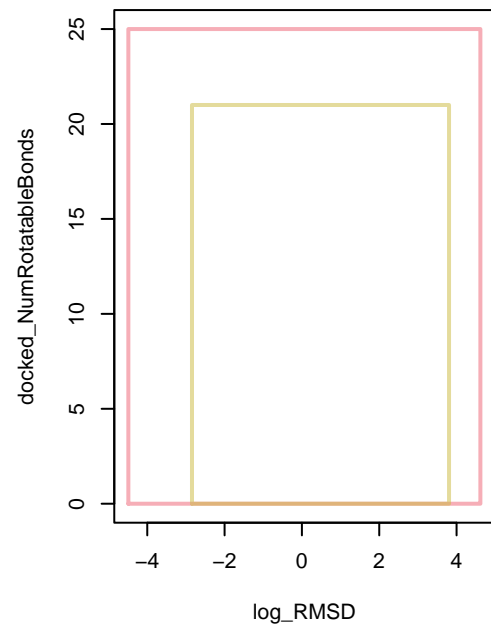
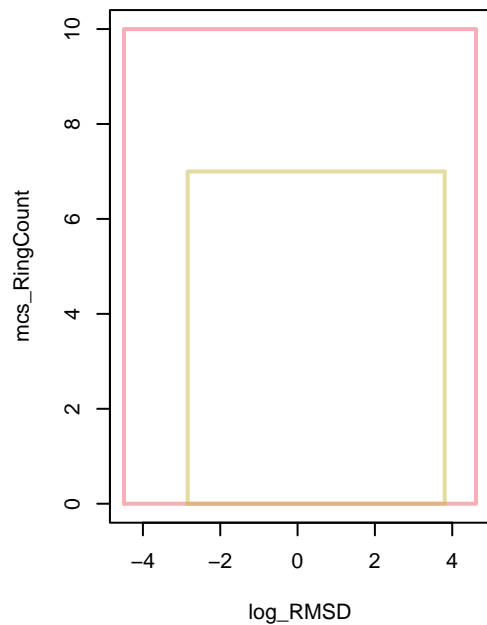
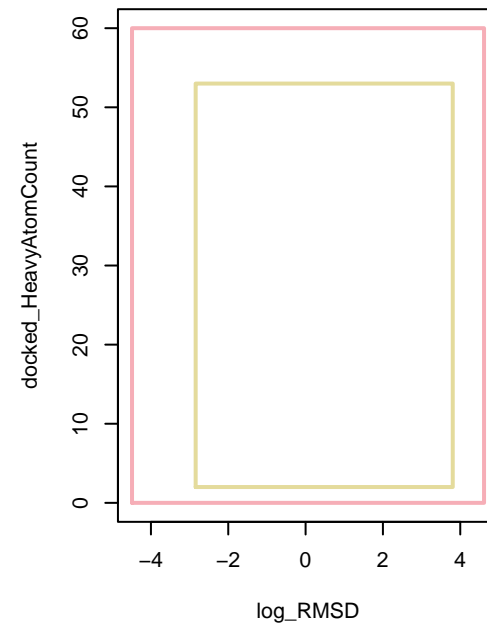
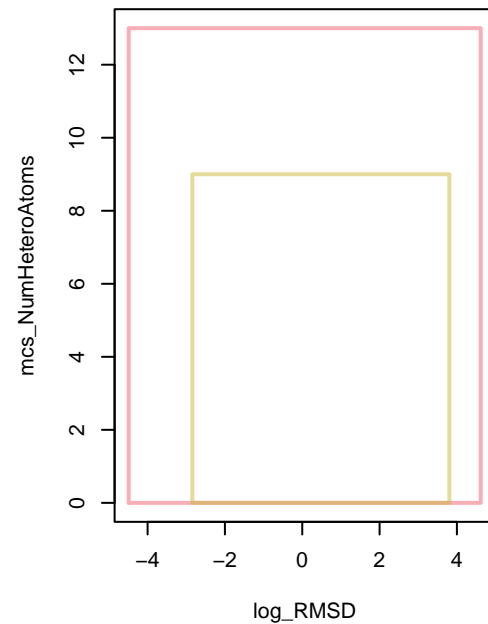
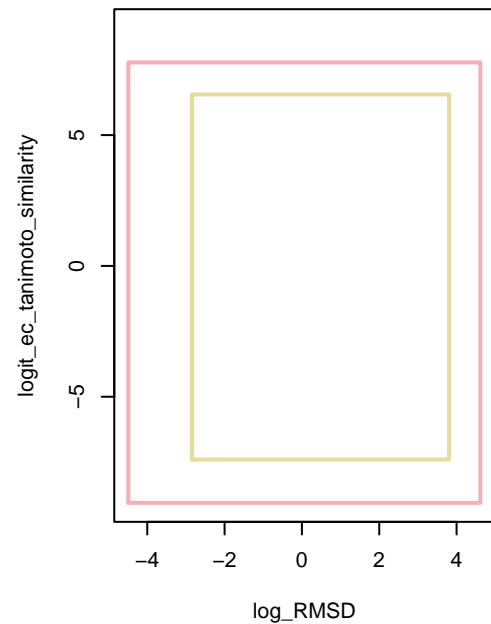
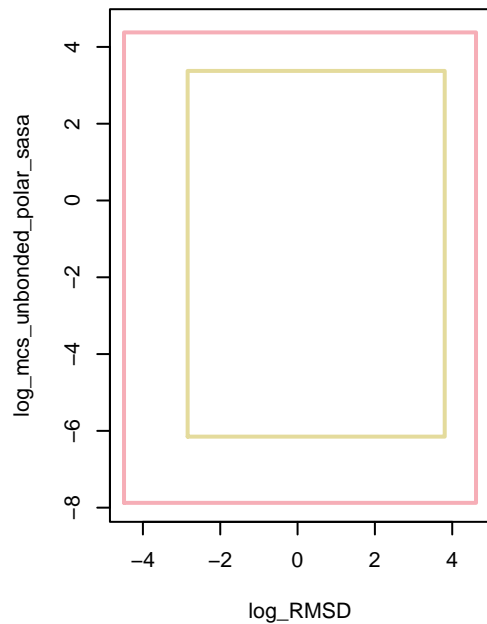




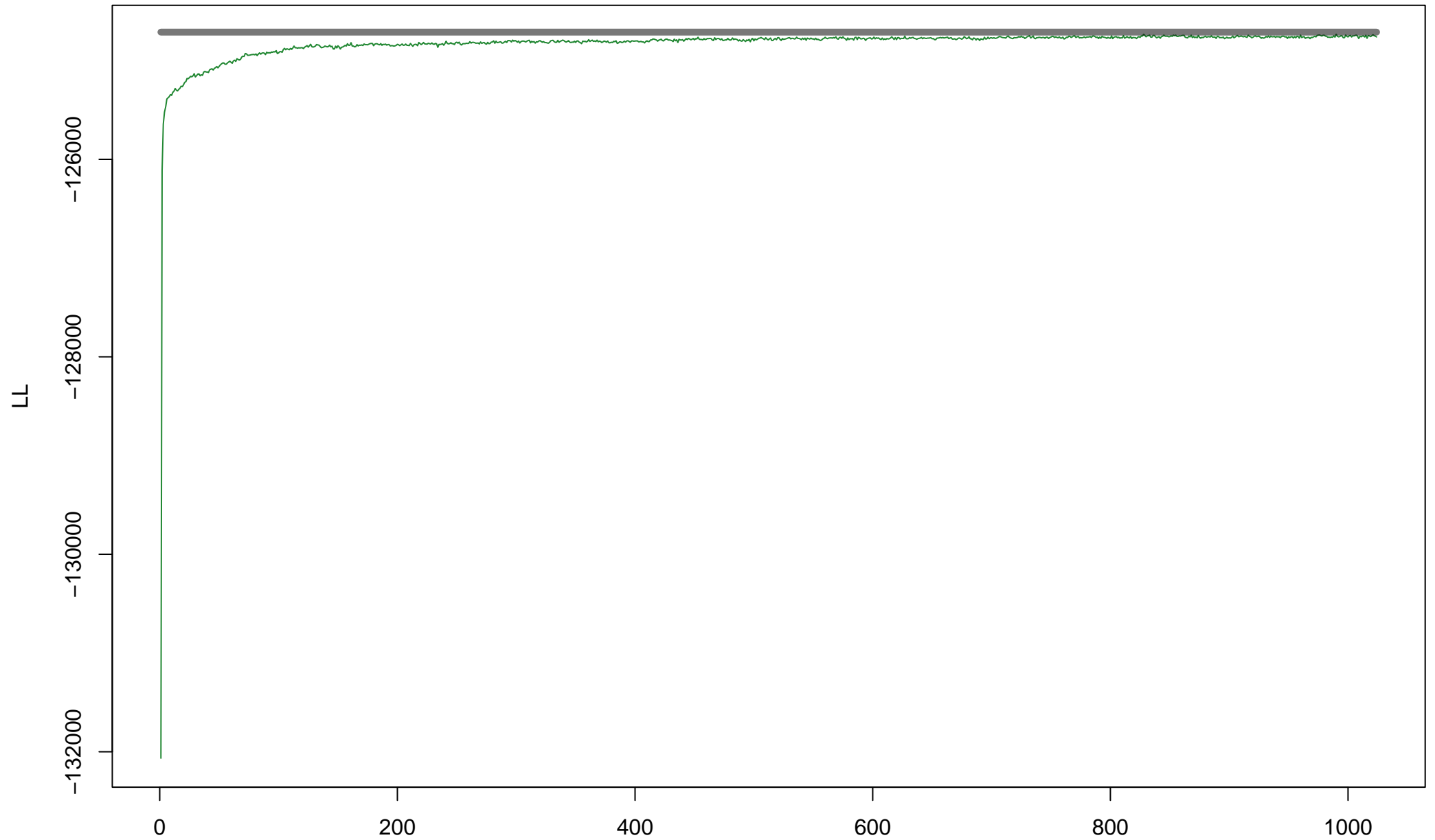






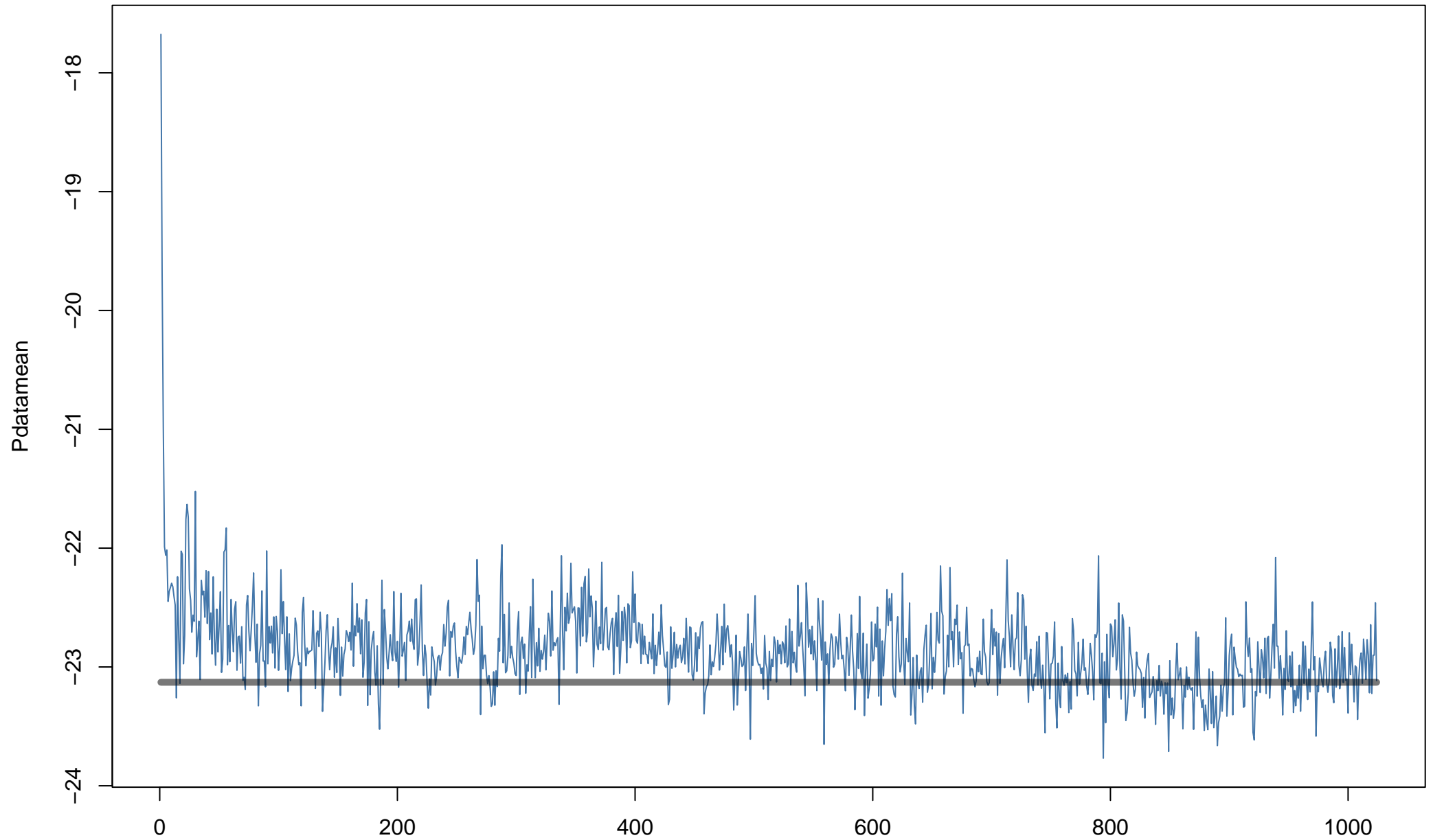


LL



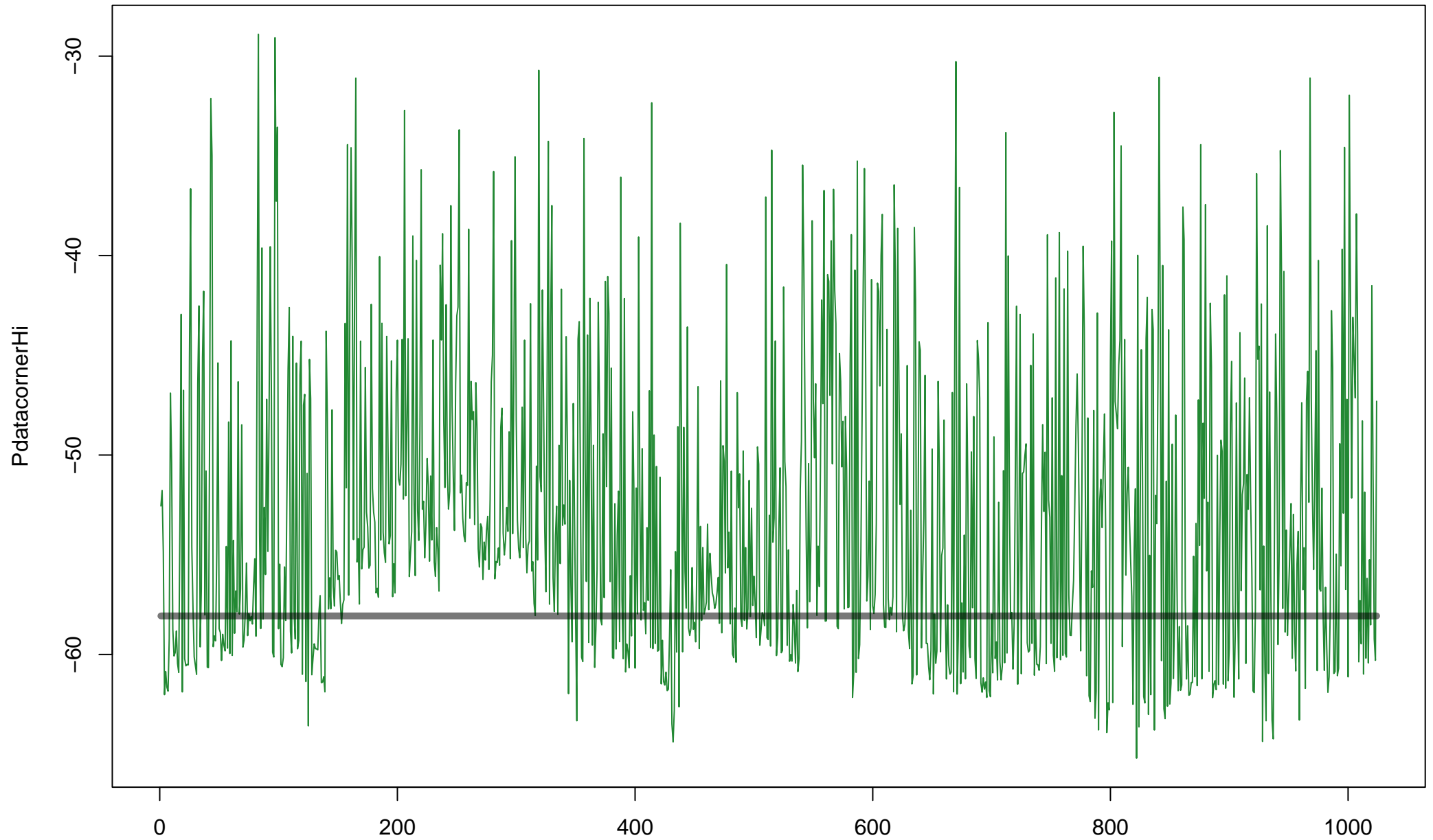
Pdatamean

ESS = 2.22e-16 | BMK = 0.327 | MCSE(6.27) = 4.01 | stat: TRUE | burn: 0 | percentile: 19.5



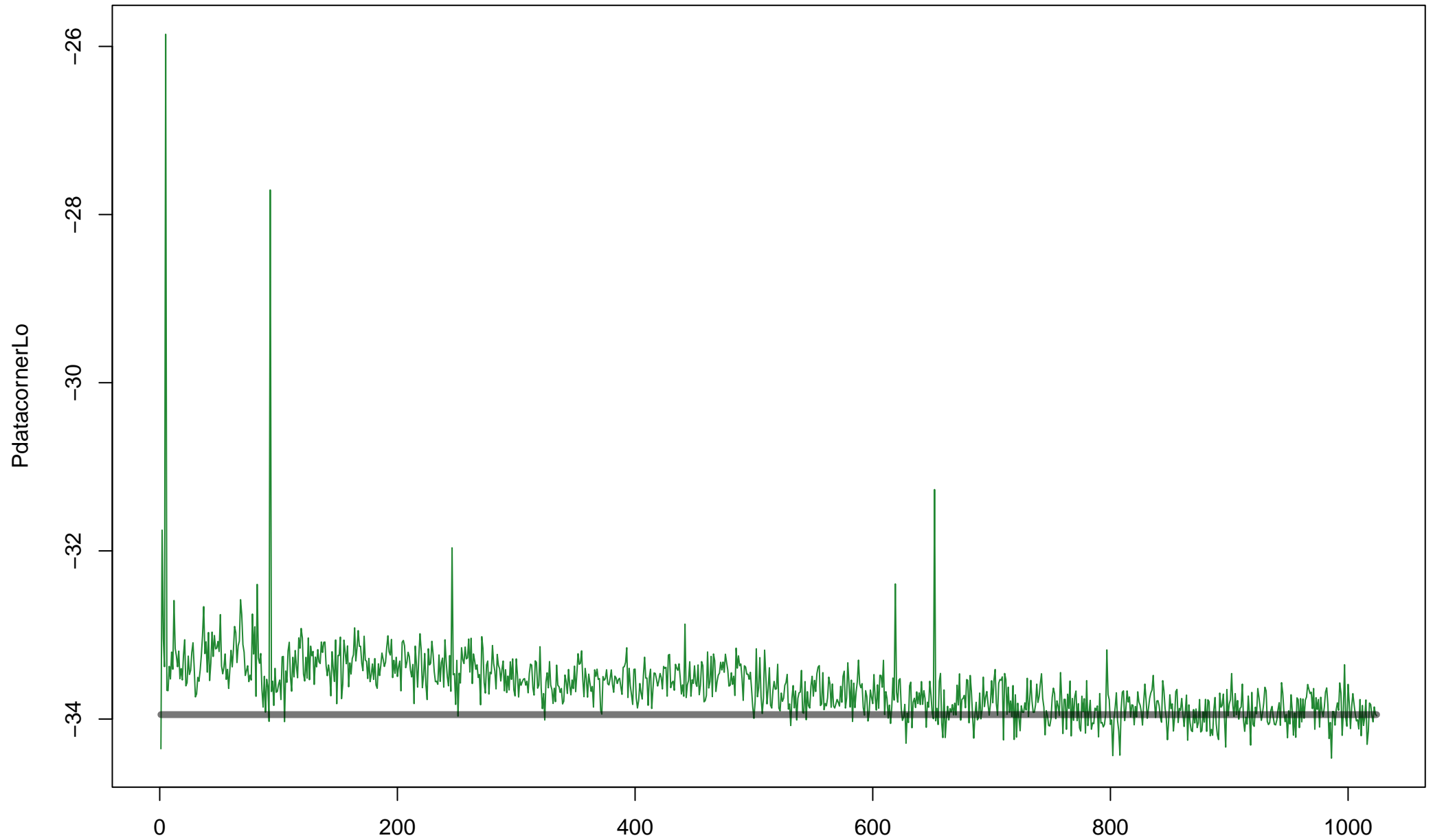
PdatacornerHi

ESS = $2.22\text{e-}16$ | BMK = 1 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 1020 | percentile: 32.1



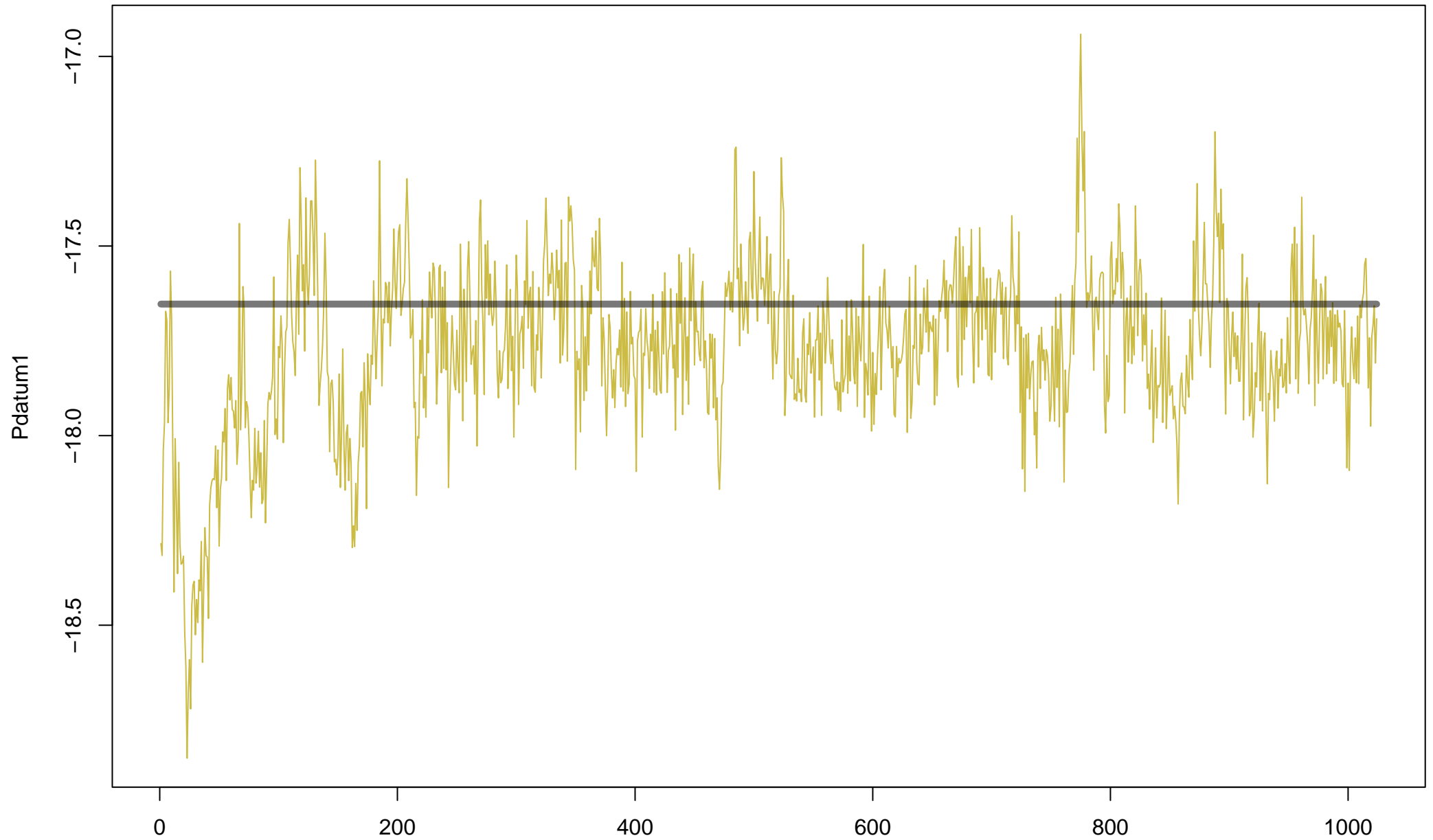
PdatacornerLo

ESS = 2.22e-16 | BMK = 1 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 102 | percentile: 15.9



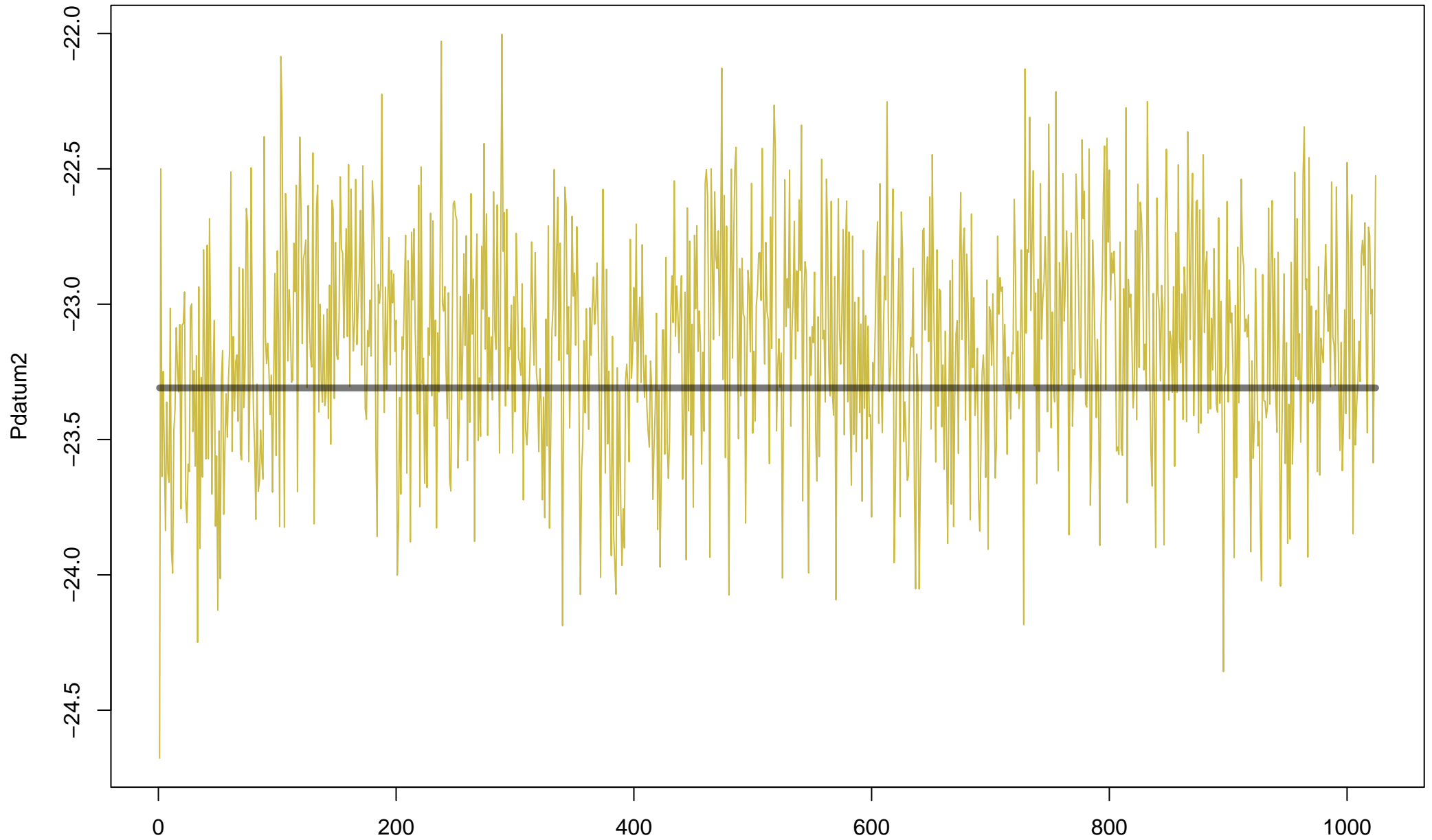
Pdatum1

ESS = 2.22e-16 | BMK = 0.236 | MCSE(6.27) = 10.9 | stat: FALSE | burn: 0 | percentile: 70.6



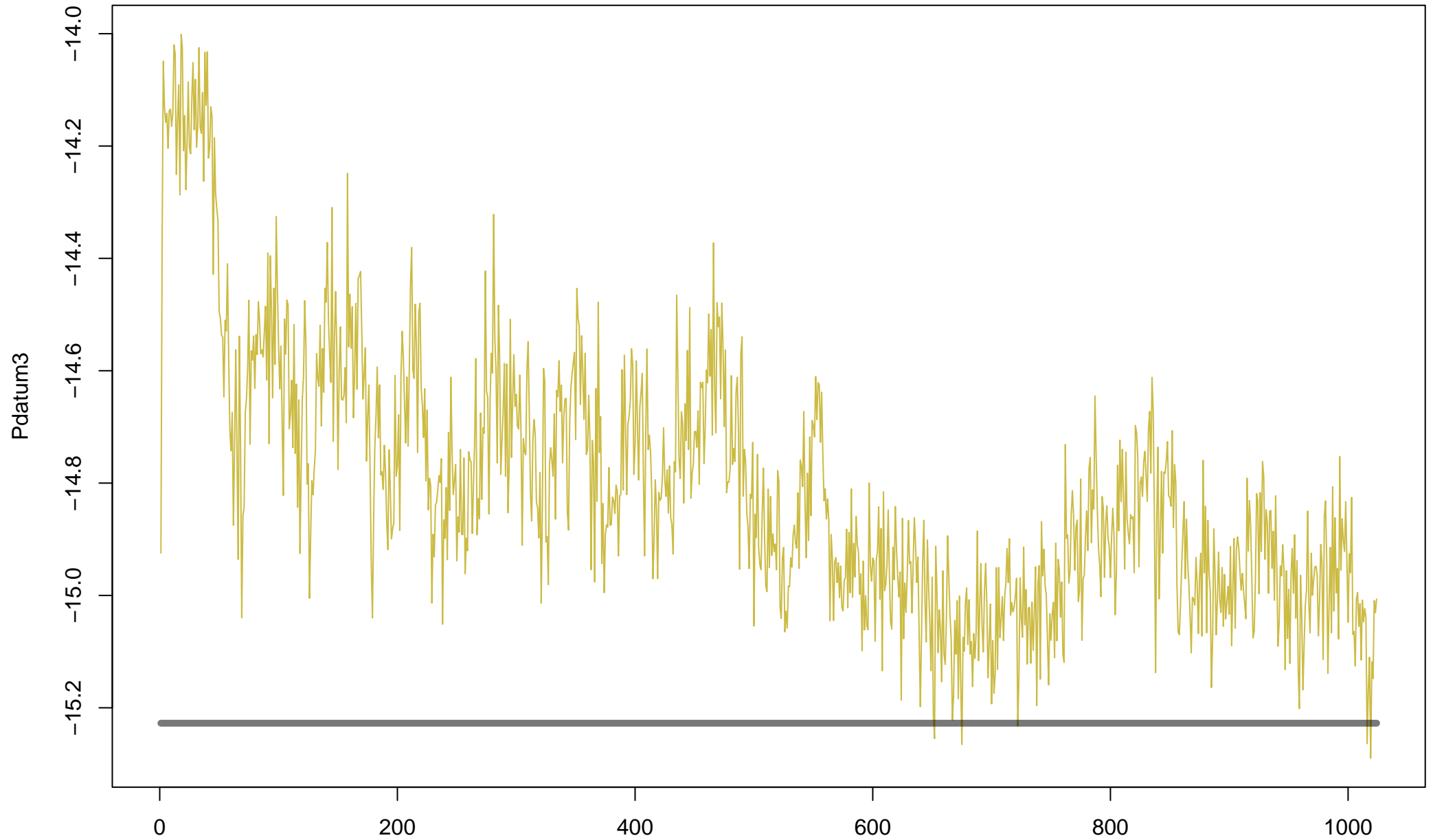
Pdatum2

ESS = 2.22e-16 | BMK = 0.0722 | MCSE(6.27) = 5.21 | stat: TRUE | burn: 0 | percentile: 32.8



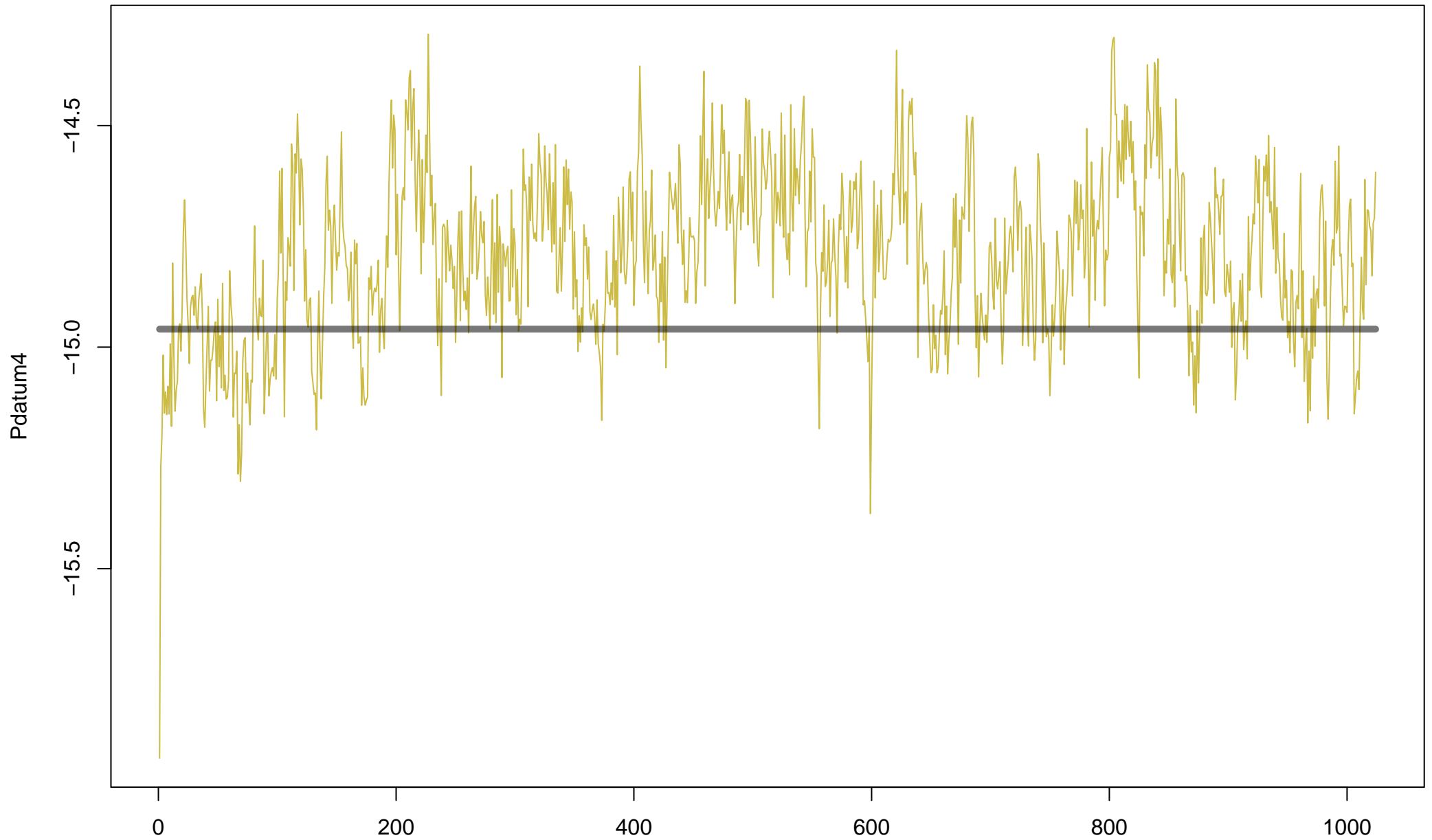
Pdatum3

ESS = 10.4 | BMK = 0.611 | MCSE(6.27) = 15.5 | stat: FALSE | burn: 0 | percentile: 0.488



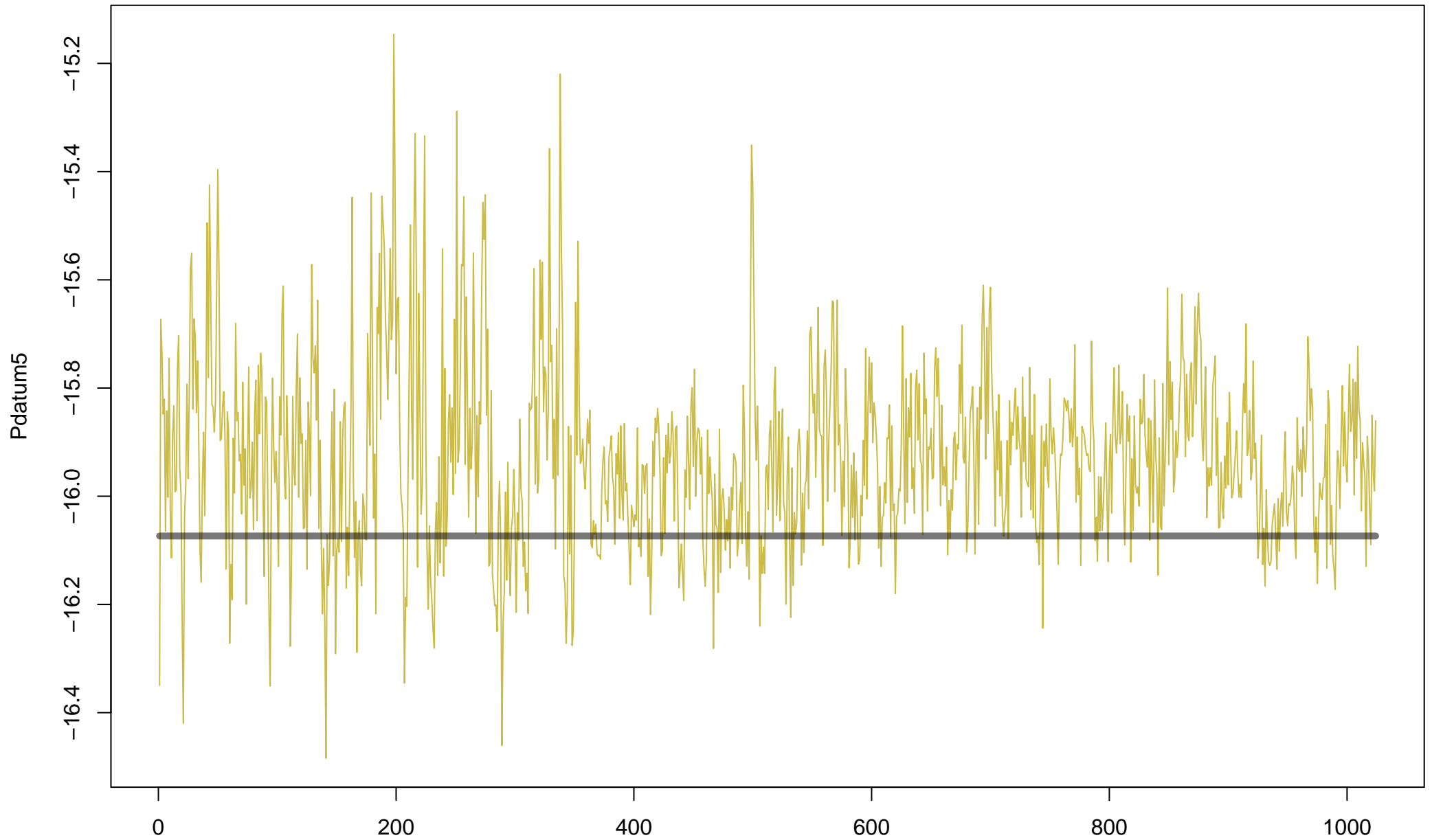
Pdatum4

ESS = 78.5 | BMK = 0.088 | MCSE(6.27) = 11.3 | stat: FALSE | burn: 0 | percentile: 17.8



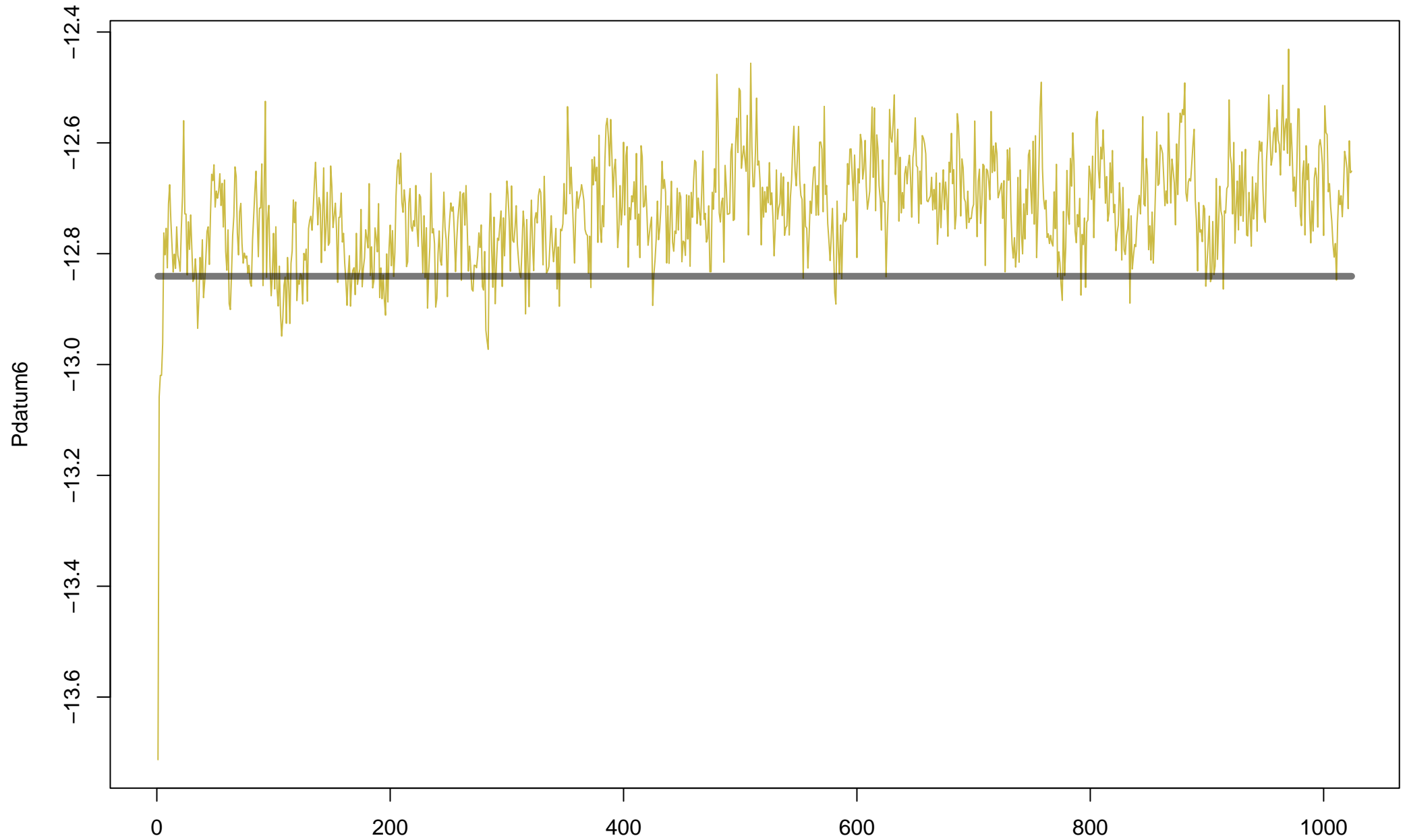
Pdatum5

ESS = 275 | BMK = 0.258 | MCSE(6.27) = 6.51 | stat: TRUE | burn: 0 | percentile: 17.6



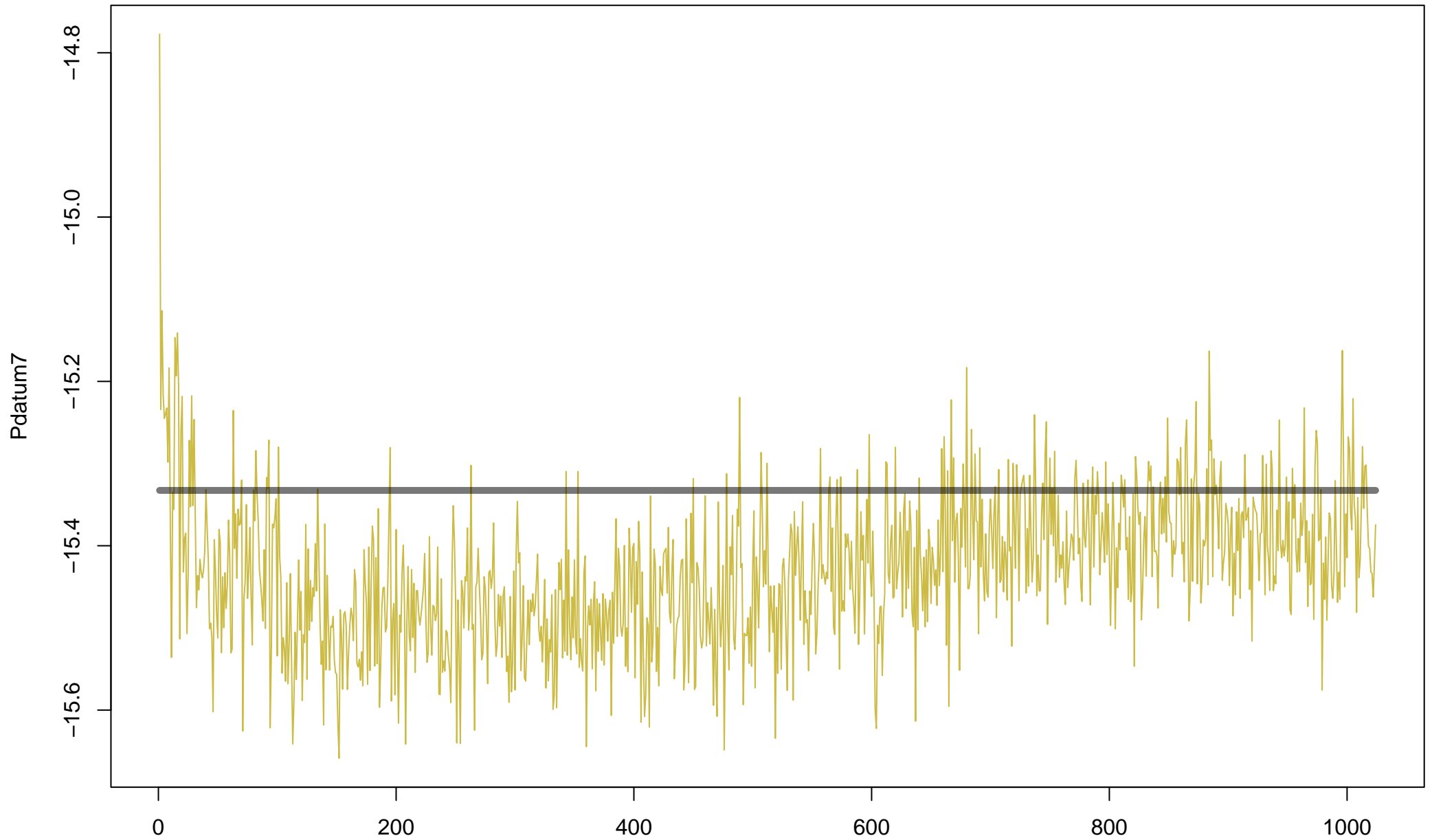
Pdatum6

ESS = 106 | BMK = 0.285 | MCSE(6.27) = 10.2 | stat: FALSE | burn: 0 | percentile: 8.89



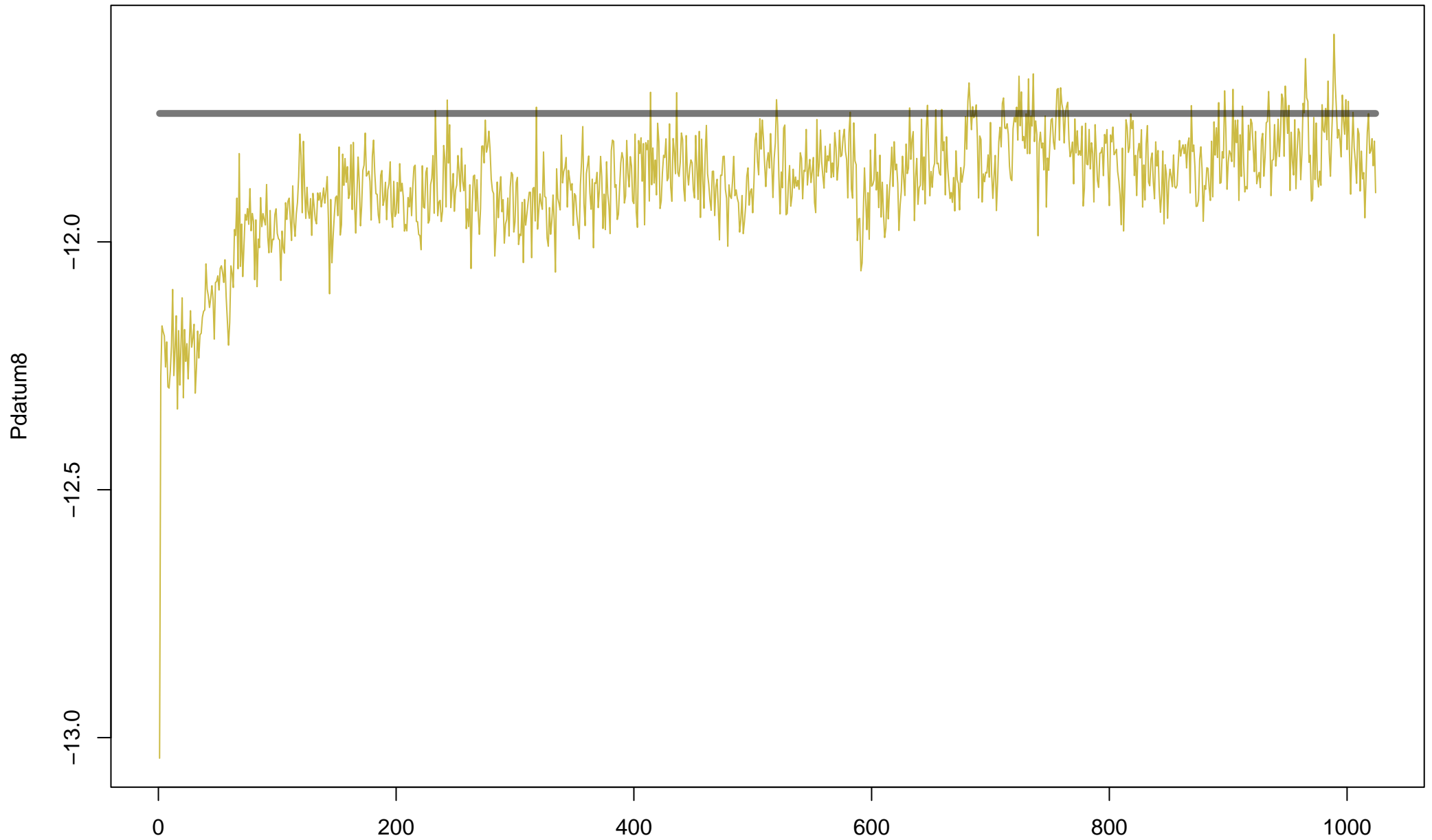
Pdatum7

ESS = 37.9 | BMK = 0.333 | MCSE(6.27) = 10.5 | stat: TRUE | burn: 0 | percentile: 86.7

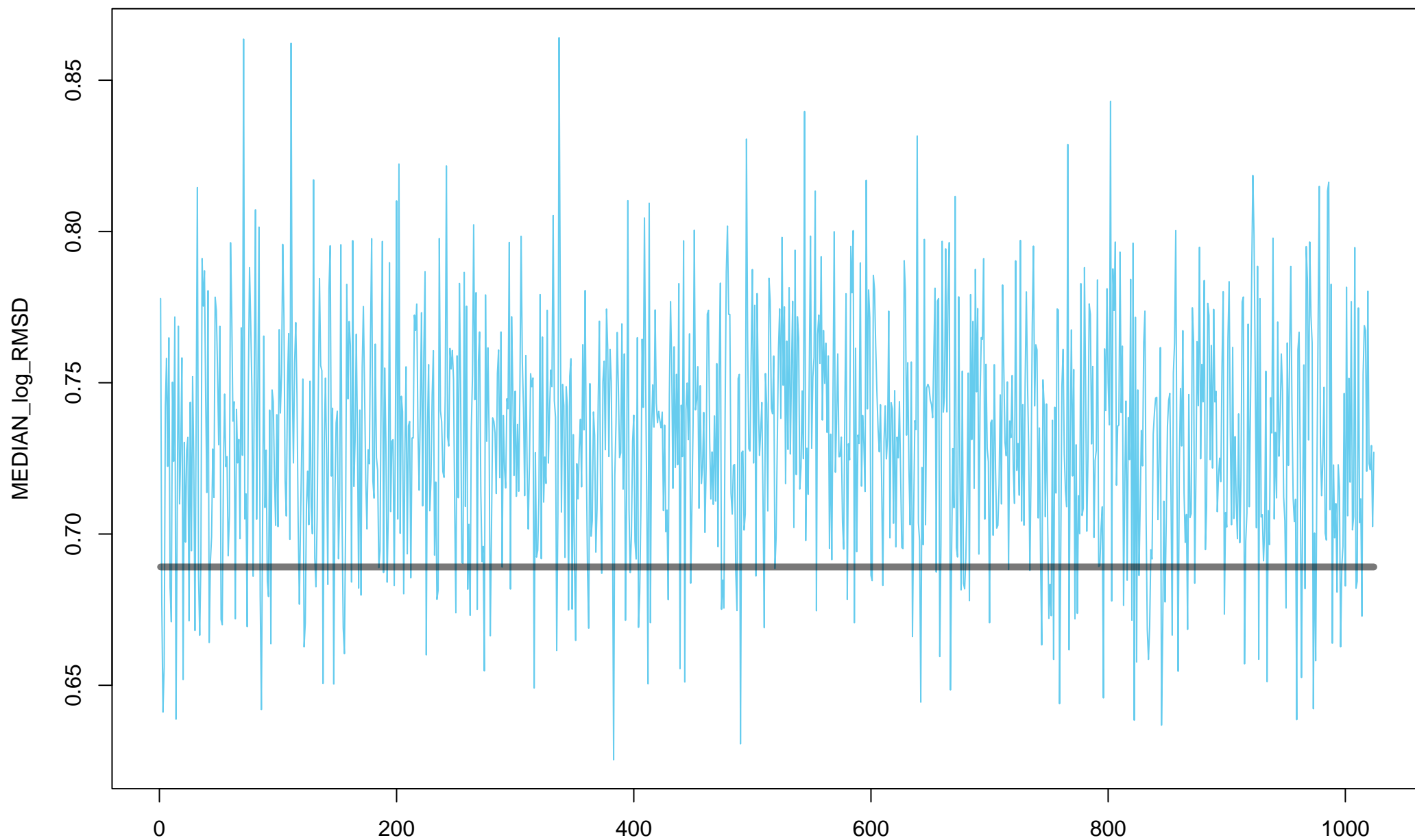


Pdatum8

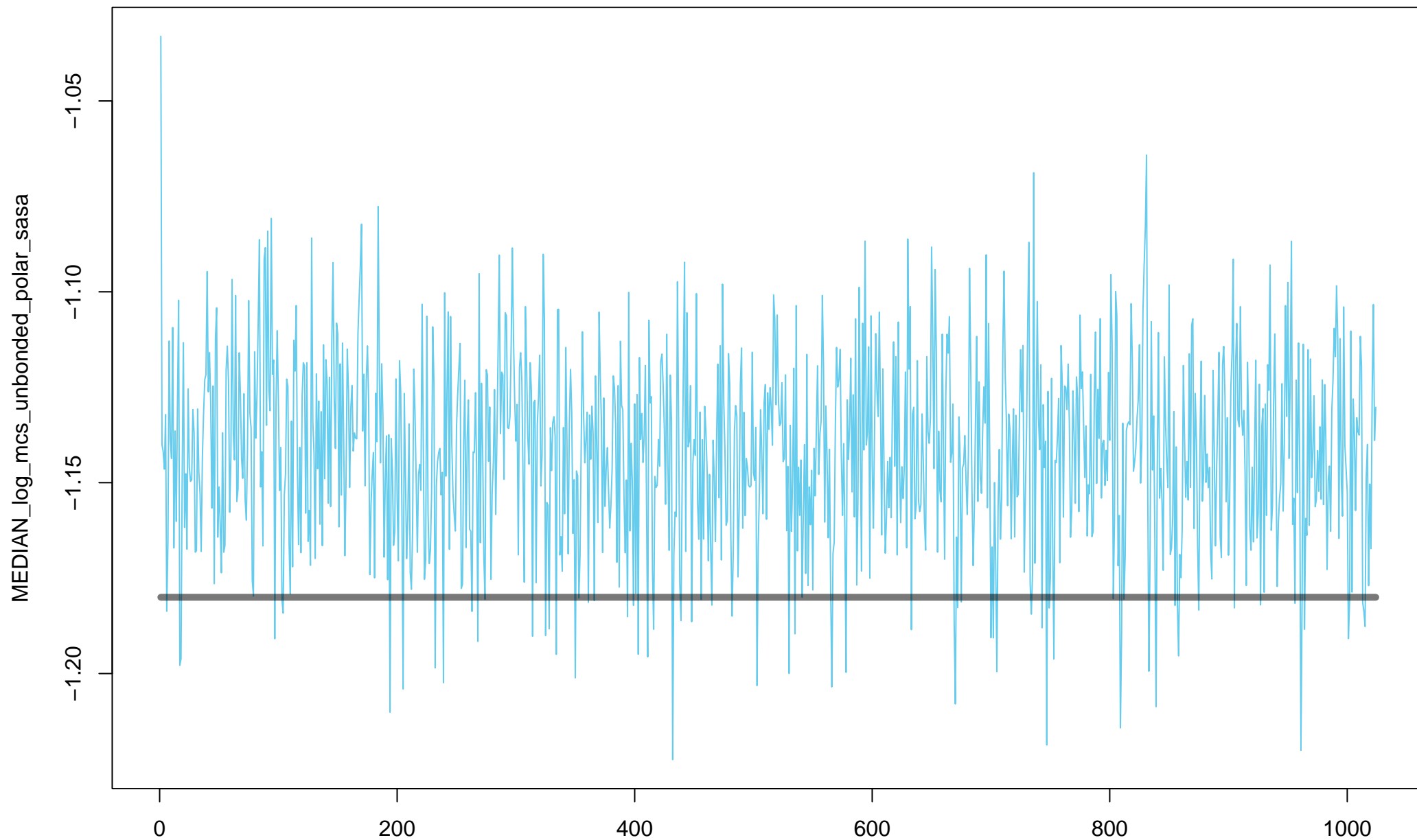
ESS = 14.8 | BMK = 0.414 | MCSE(6.27) = 14.3 | stat: FALSE | burn: 102 | percentile: 94.4



MEDIAN_log_RMSD
ESS = 1020 | BMK = 0.064 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0 | percentile: 13.8

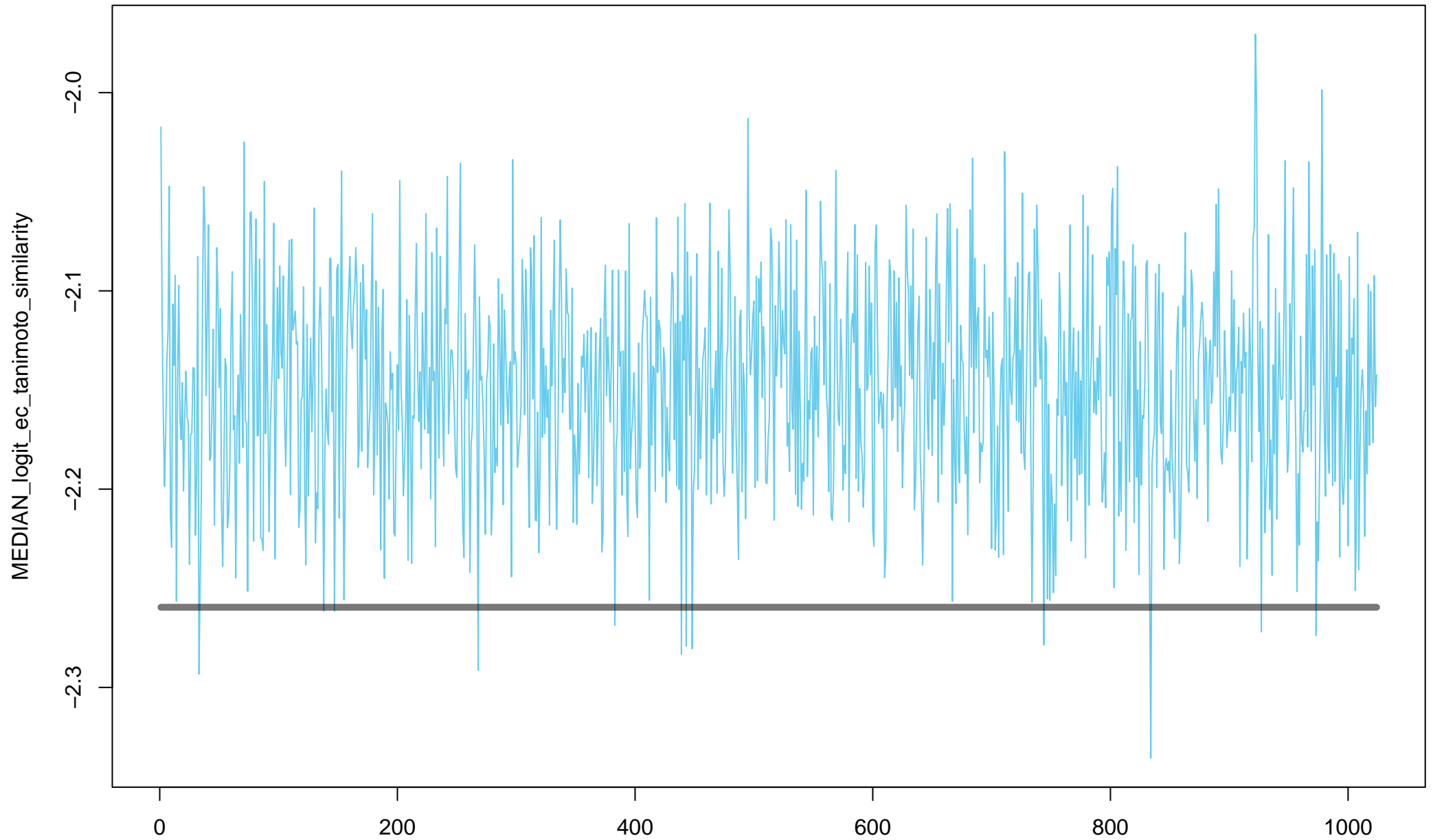


MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 866 | BMK = 0.048 | MCSE(6.27) = 3.79 | stat: TRUE | burn: 0 | percentile: 6.93



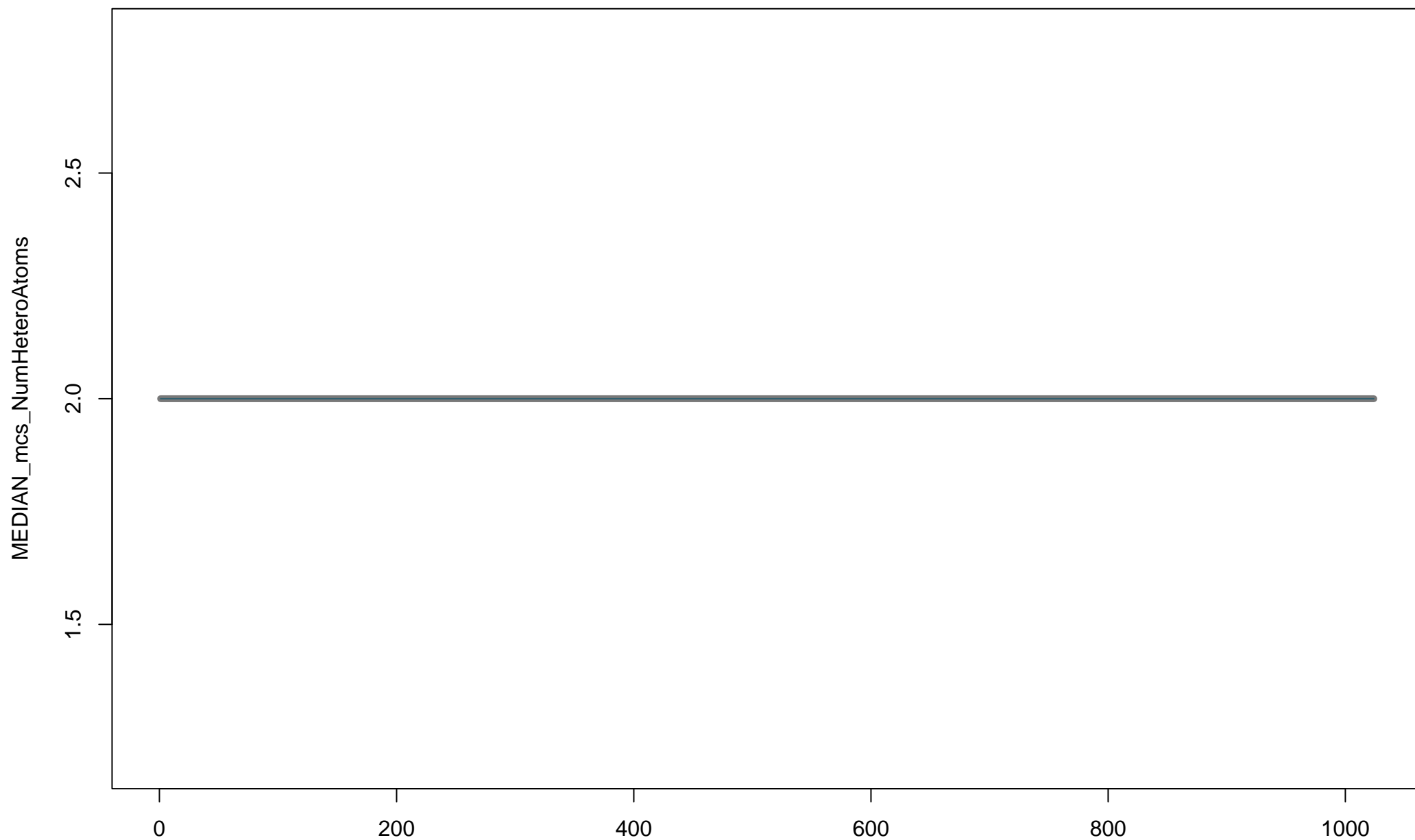
MEDIAN_logit_ec_tanimoto_similarity

ESS = 1020 | BMK = 0.0513 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0 | percentile: 1.17

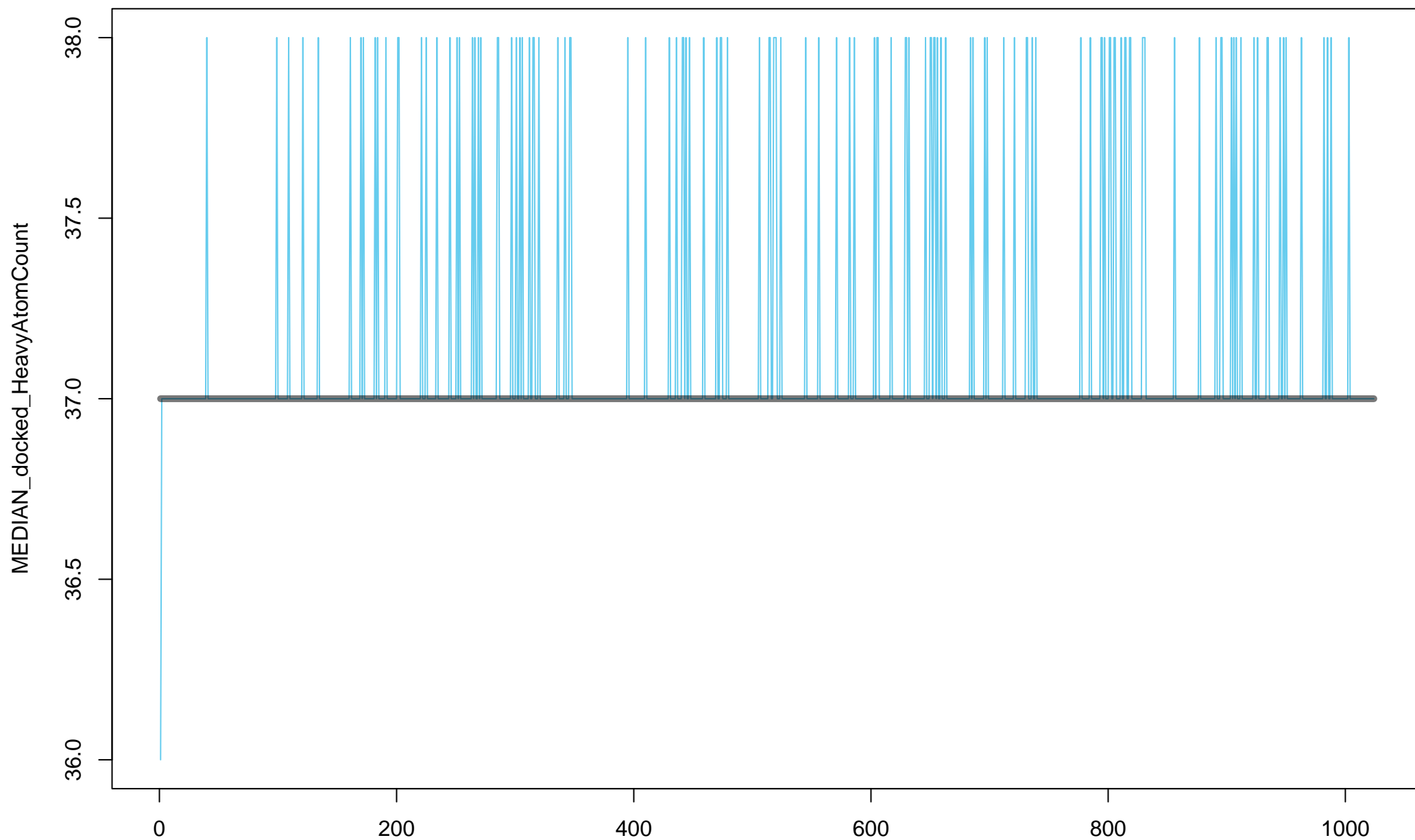


MEDIAN_mcs_NumHeteroAtoms

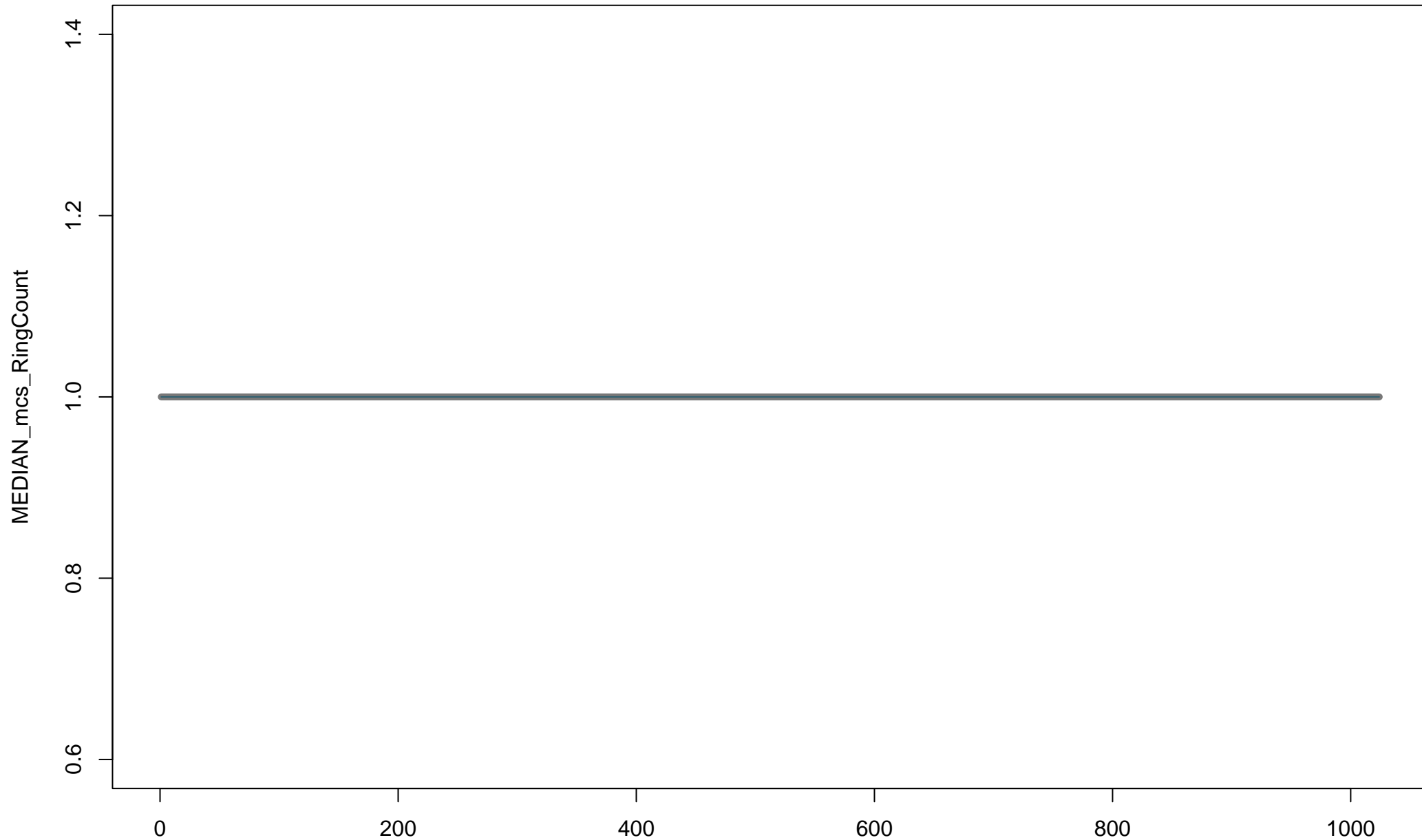
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100



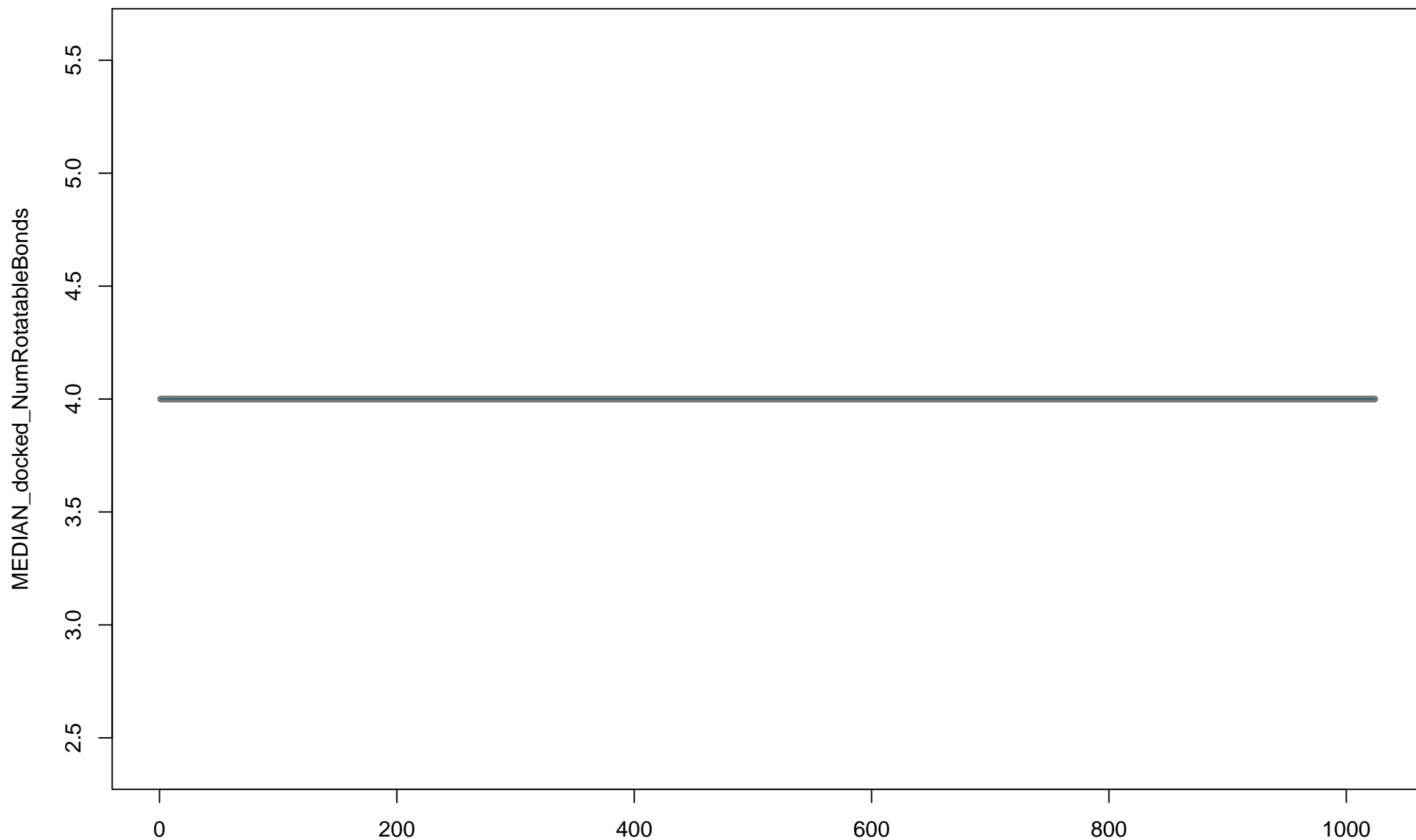
MEDIAN_docked_HeavyAtomCount
ESS = 711 | BMK = 0.0829 | MCSE(6.27) = 4.66 | stat: FALSE | burn: 0 | percentile: 87.8



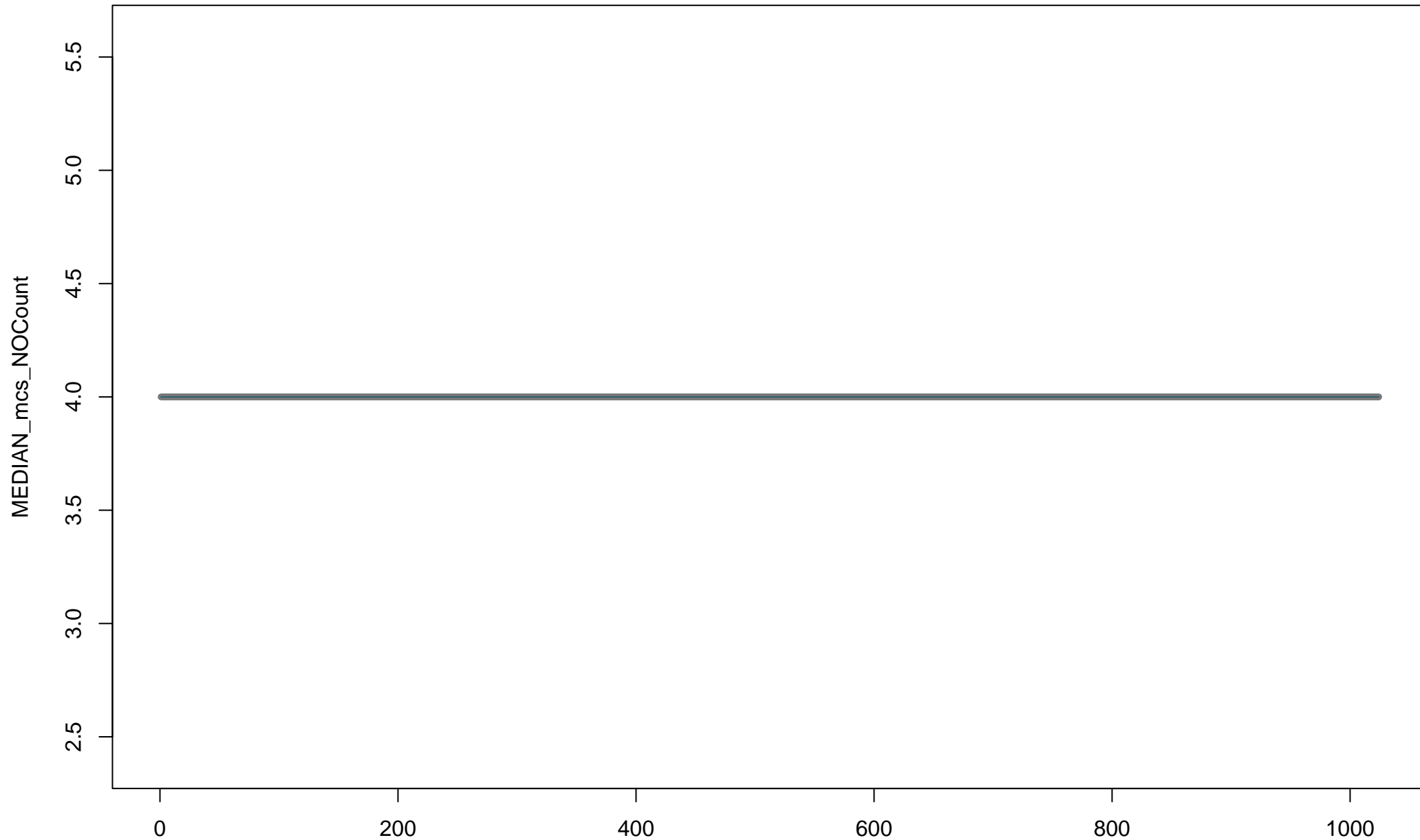
MEDIAN_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100



MEDIAN_docked_NumRotatableBonds
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100

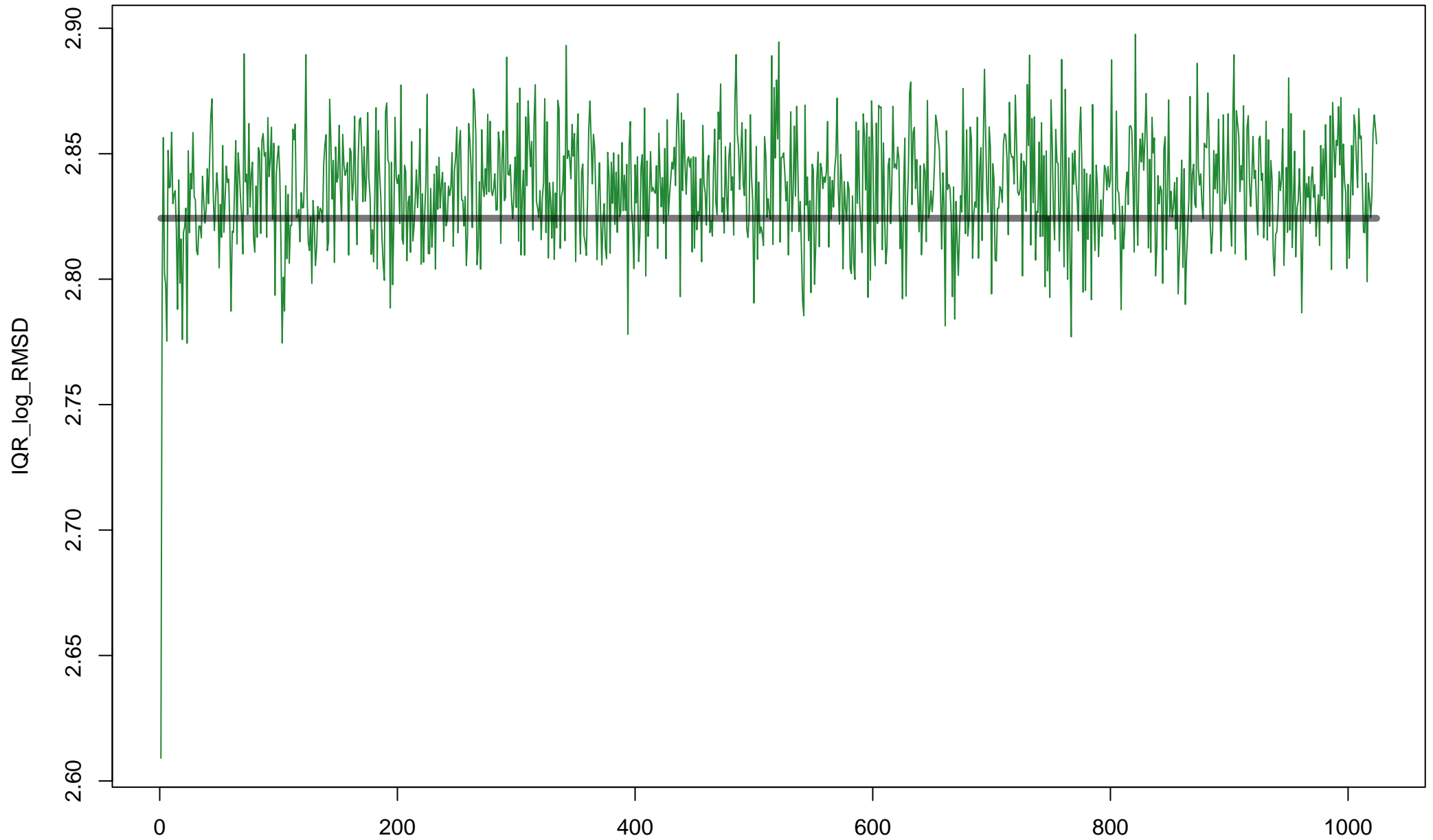


MEDIAN_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100



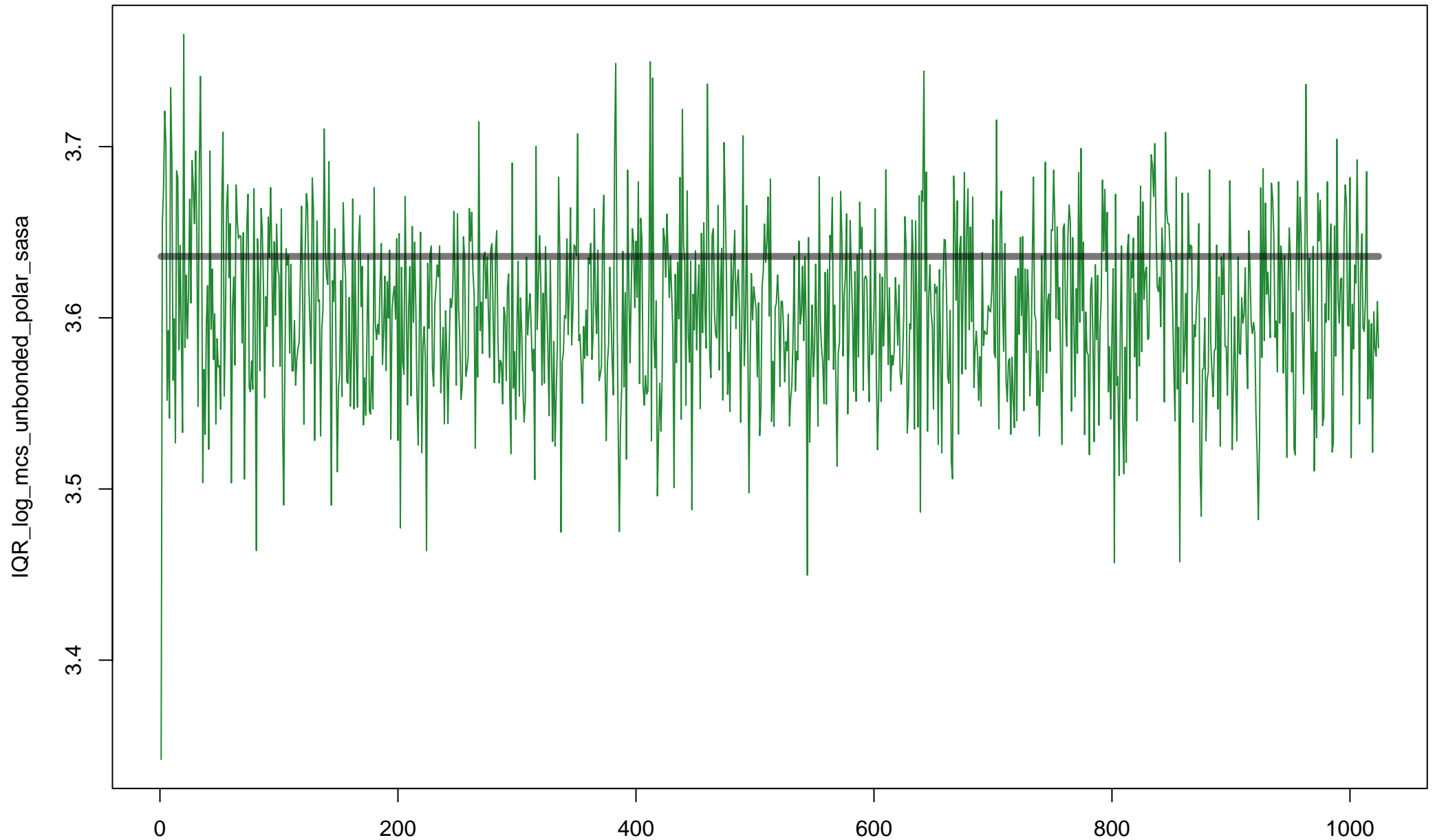
IQR_log_RMSD

ESS = 640 | BMK = 0.0669 | MCSE(6.27) = 4.64 | stat: TRUE | burn: 0 | percentile: 28.5



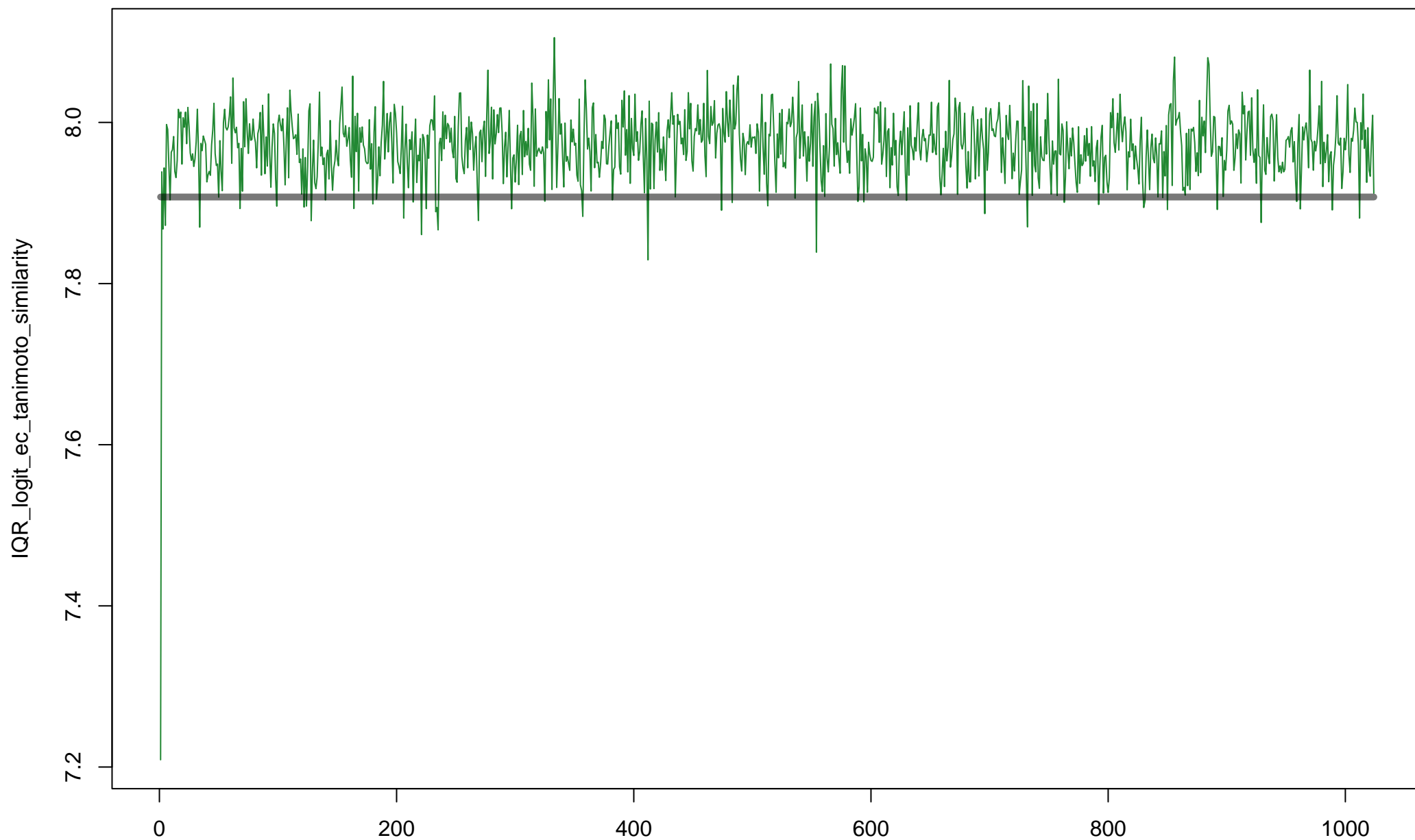
IQR_log_mcs_unbonded_polar_sasa

ESS = 1020 | BMK = 0.0675 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | percentile: 73.4

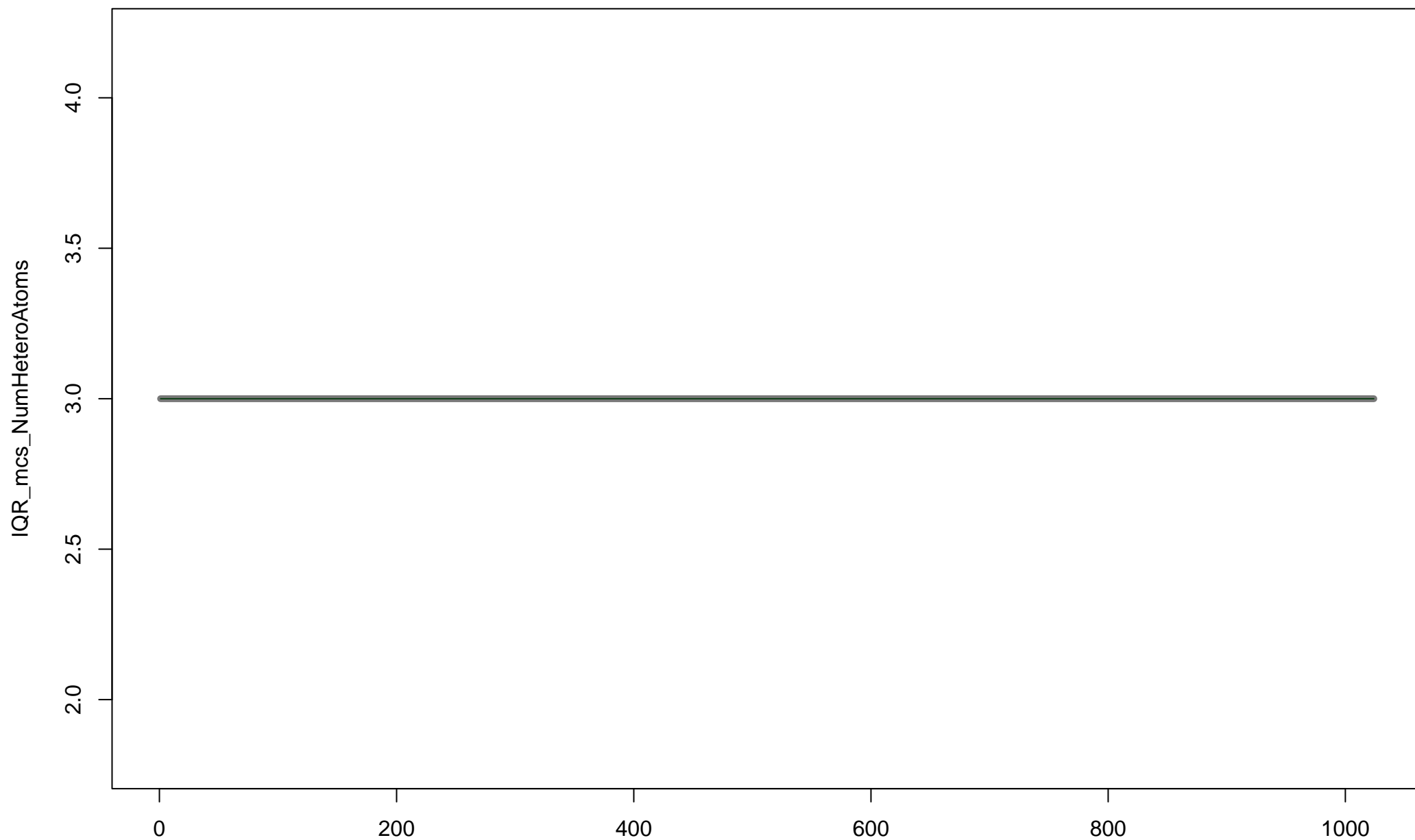


IQR_logit_ec_tanimoto_similarity

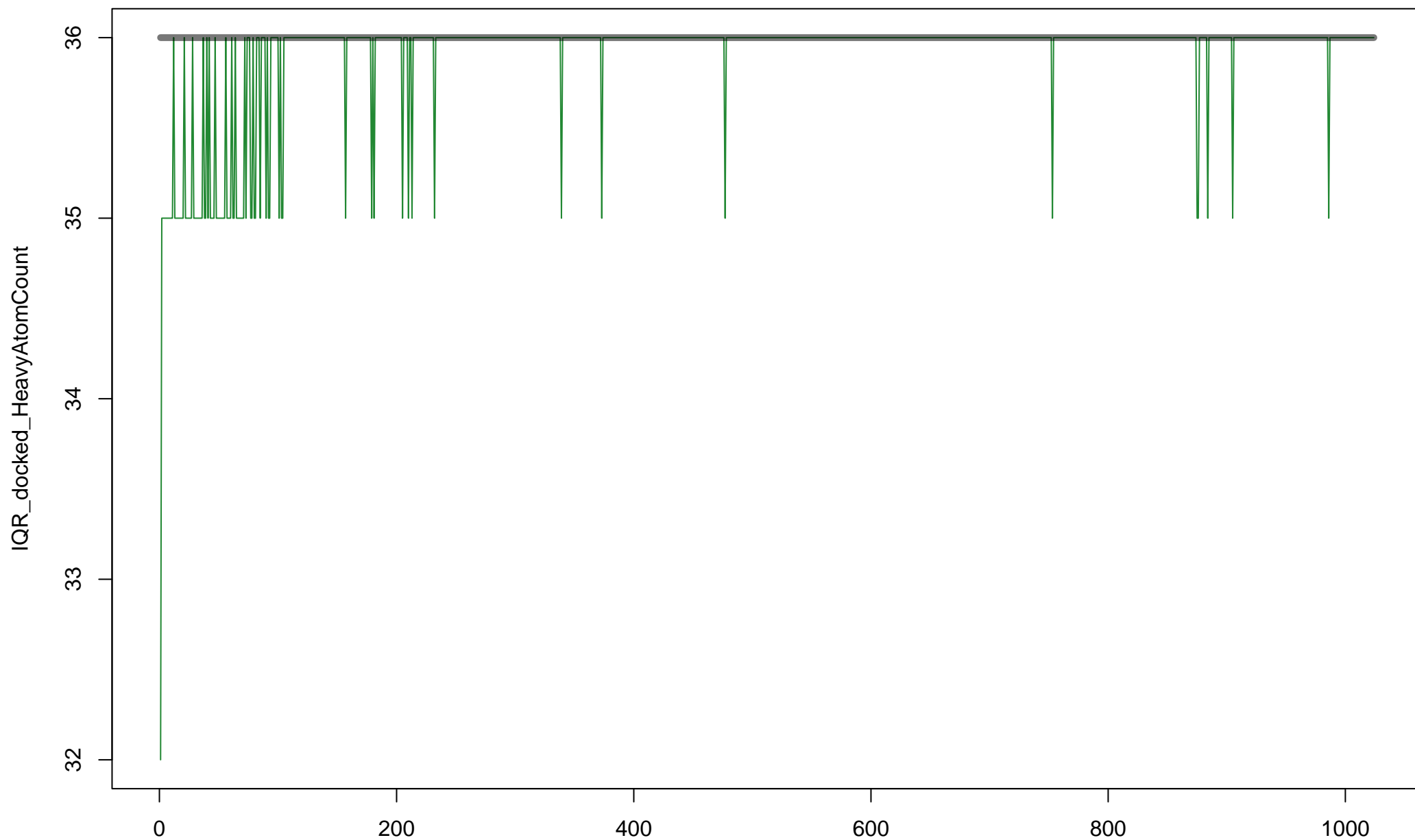
ESS = 709 | BMK = 0.0669 | MCSE(6.27) = 3.39 | stat: TRUE | burn: 0 | percentile: 4.88



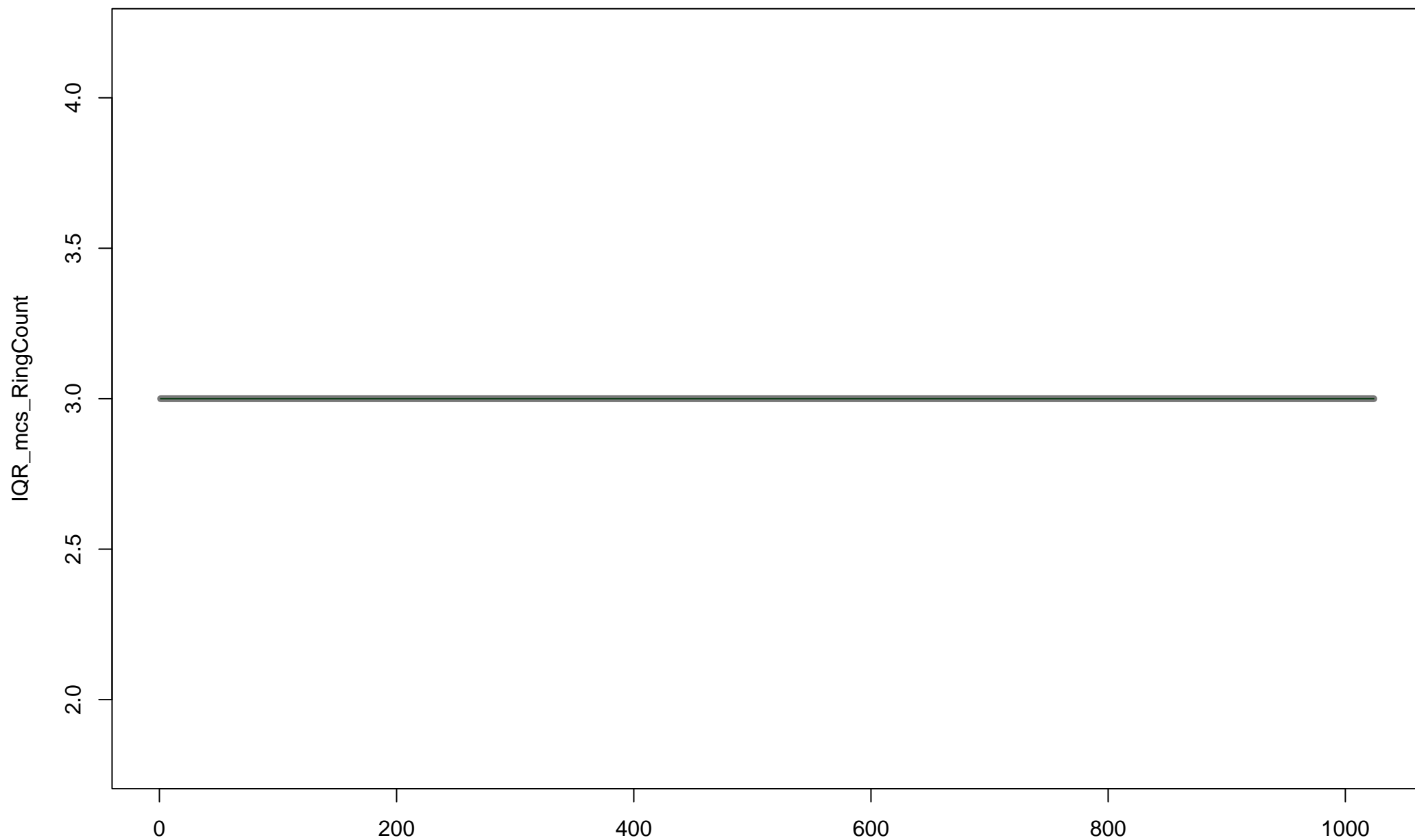
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100



IQR_docked_HeavyAtomCount
ESS = 12.7 | BMK = 0.443 | MCSE(6.27) = 13.3 | stat: FALSE | burn: 102 | percentile: 100

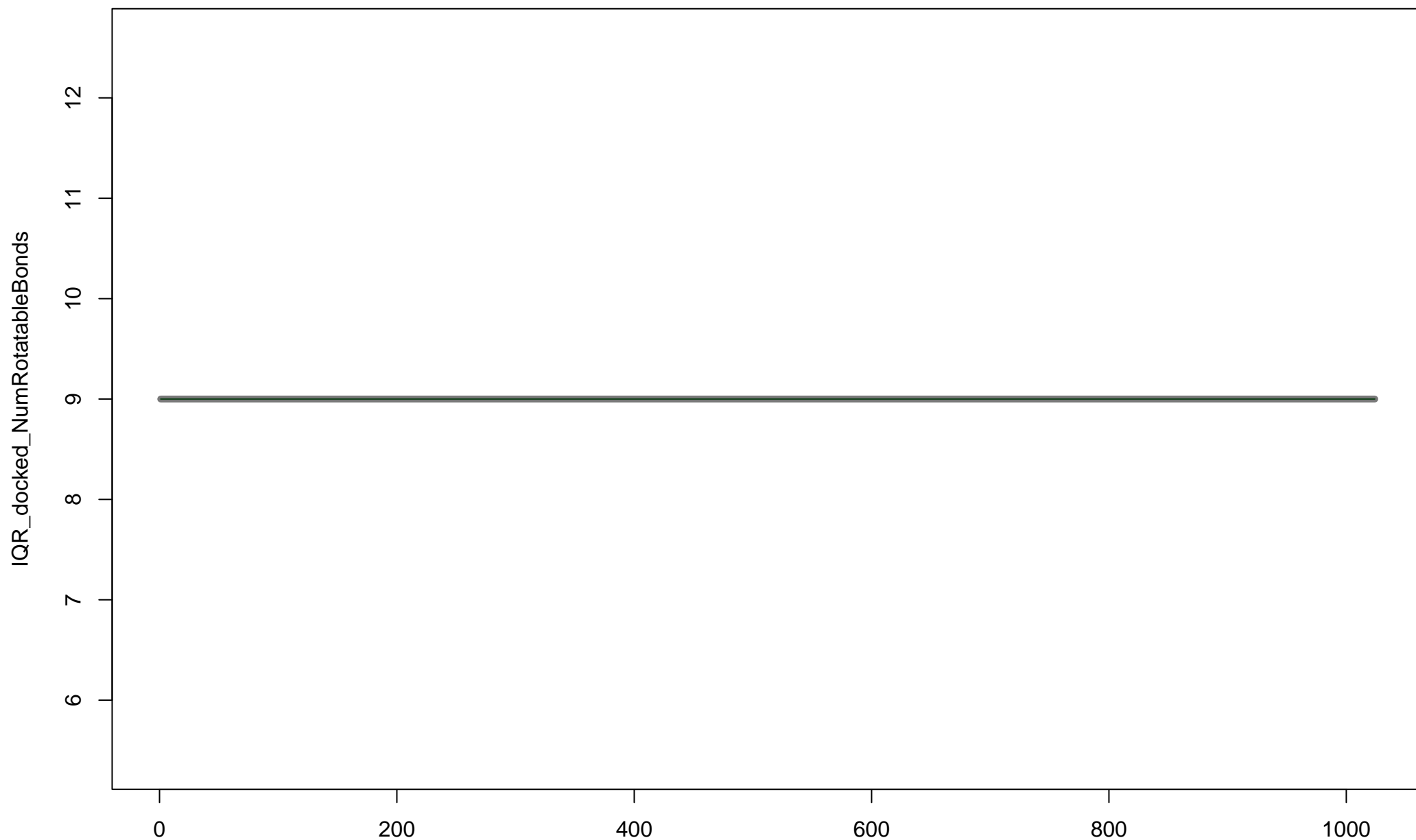


IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100

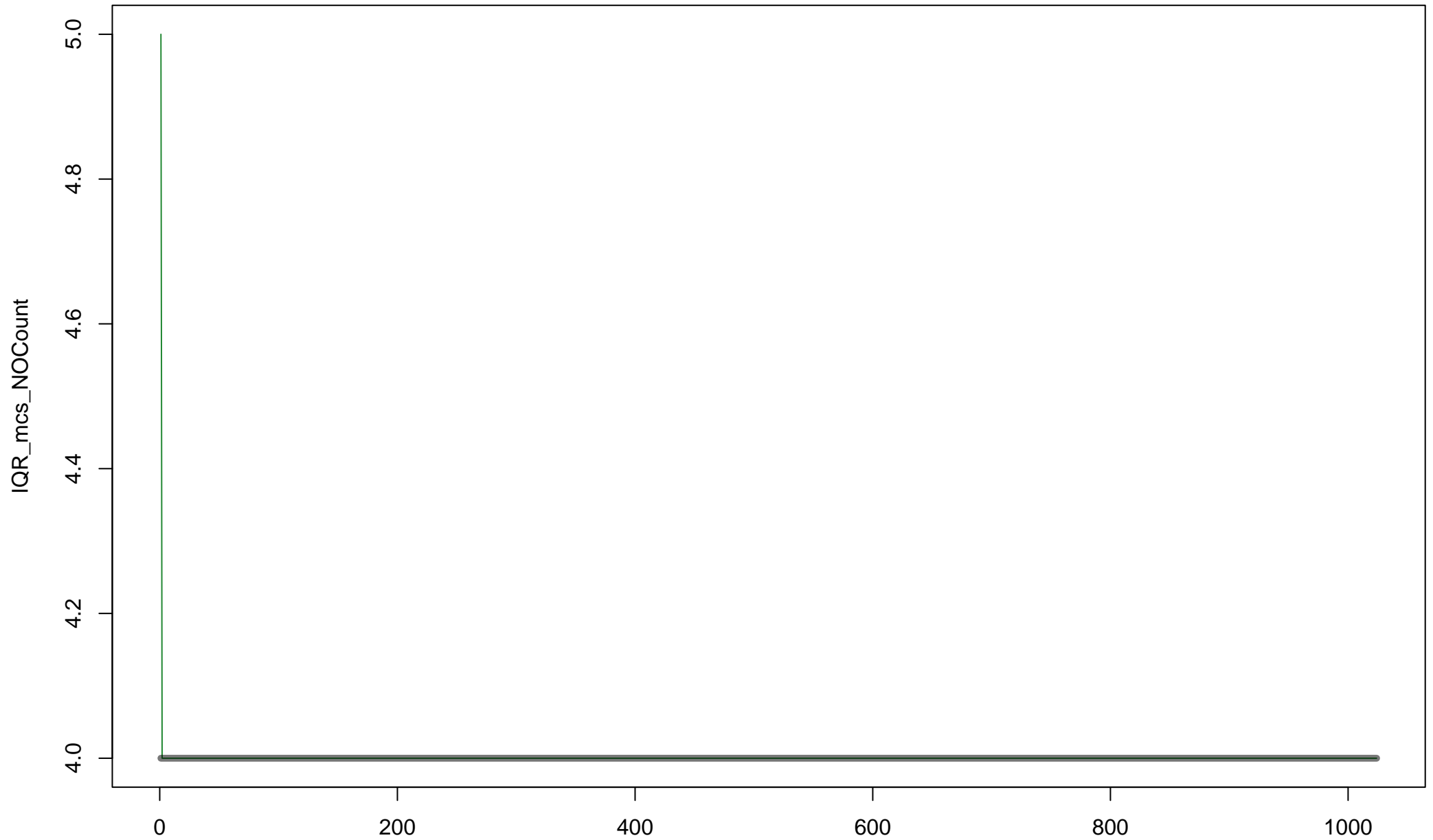


IQR_docked_NumRotatableBonds

ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100

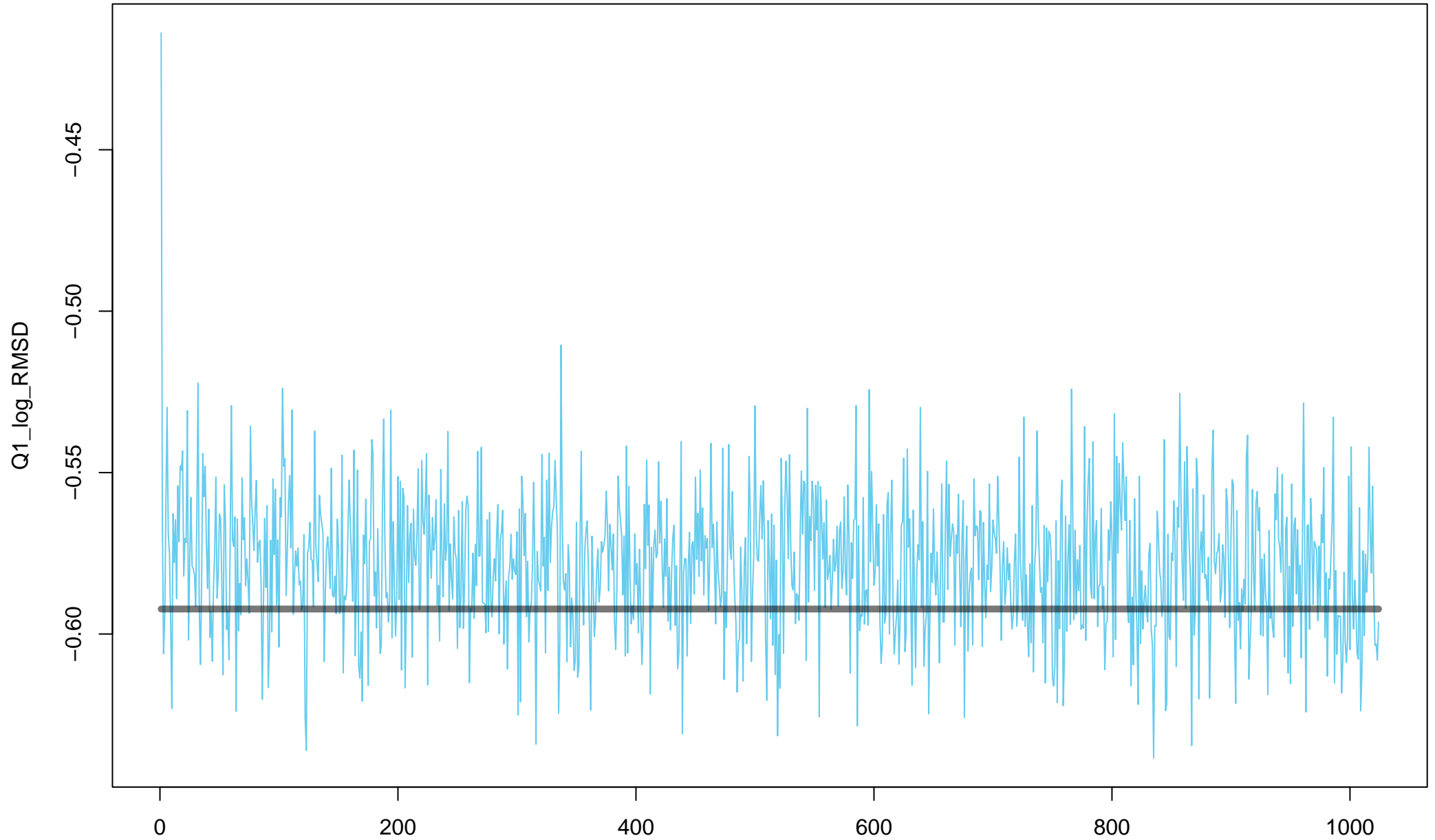


IQR_mcs_NOCCount
ESS = 1020 | BMK = 0.594 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102 | percentile: 99.9

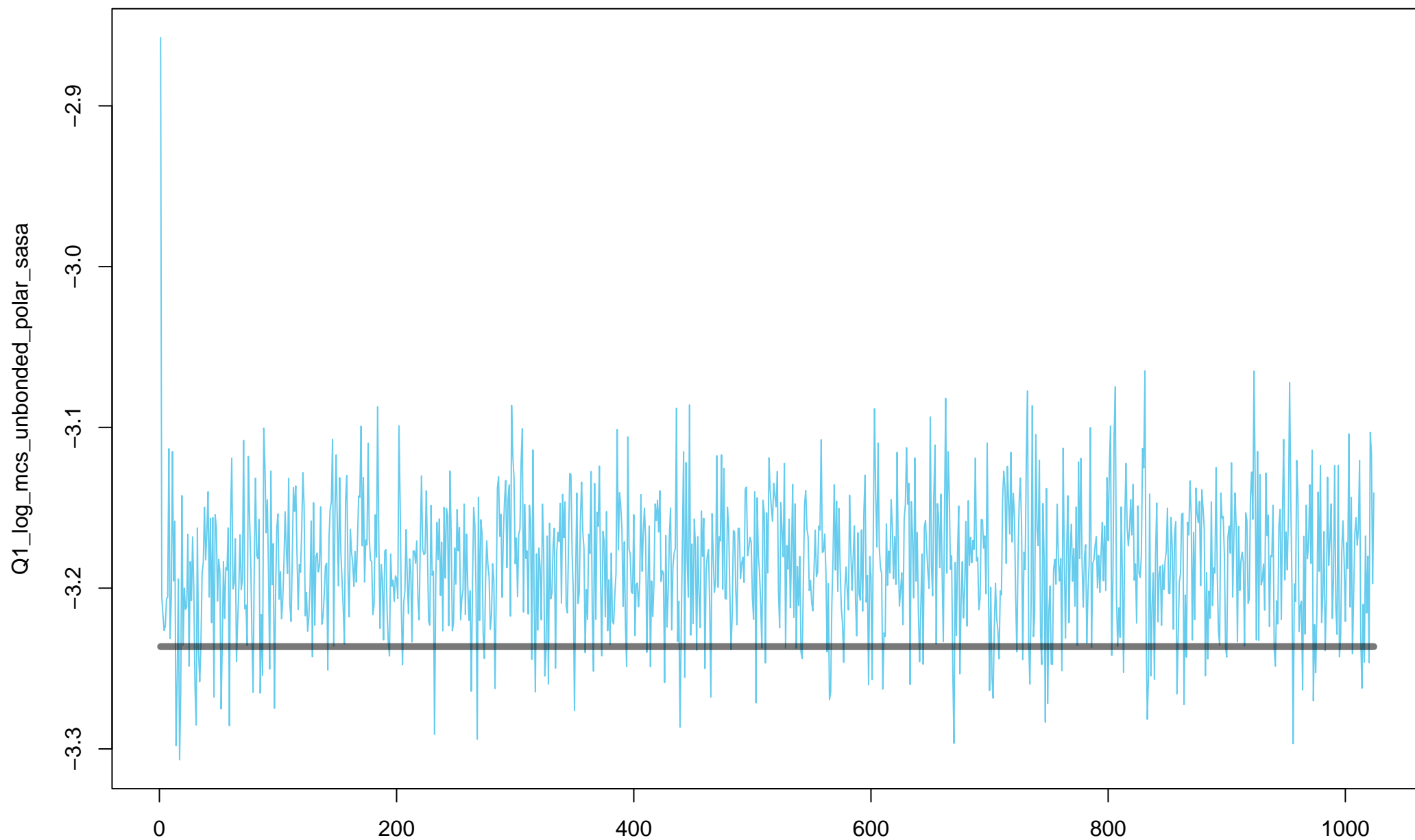


Q1_log_RMSD

ESS = 1020 | BMK = 0.0703 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0 | percentile: 26.4

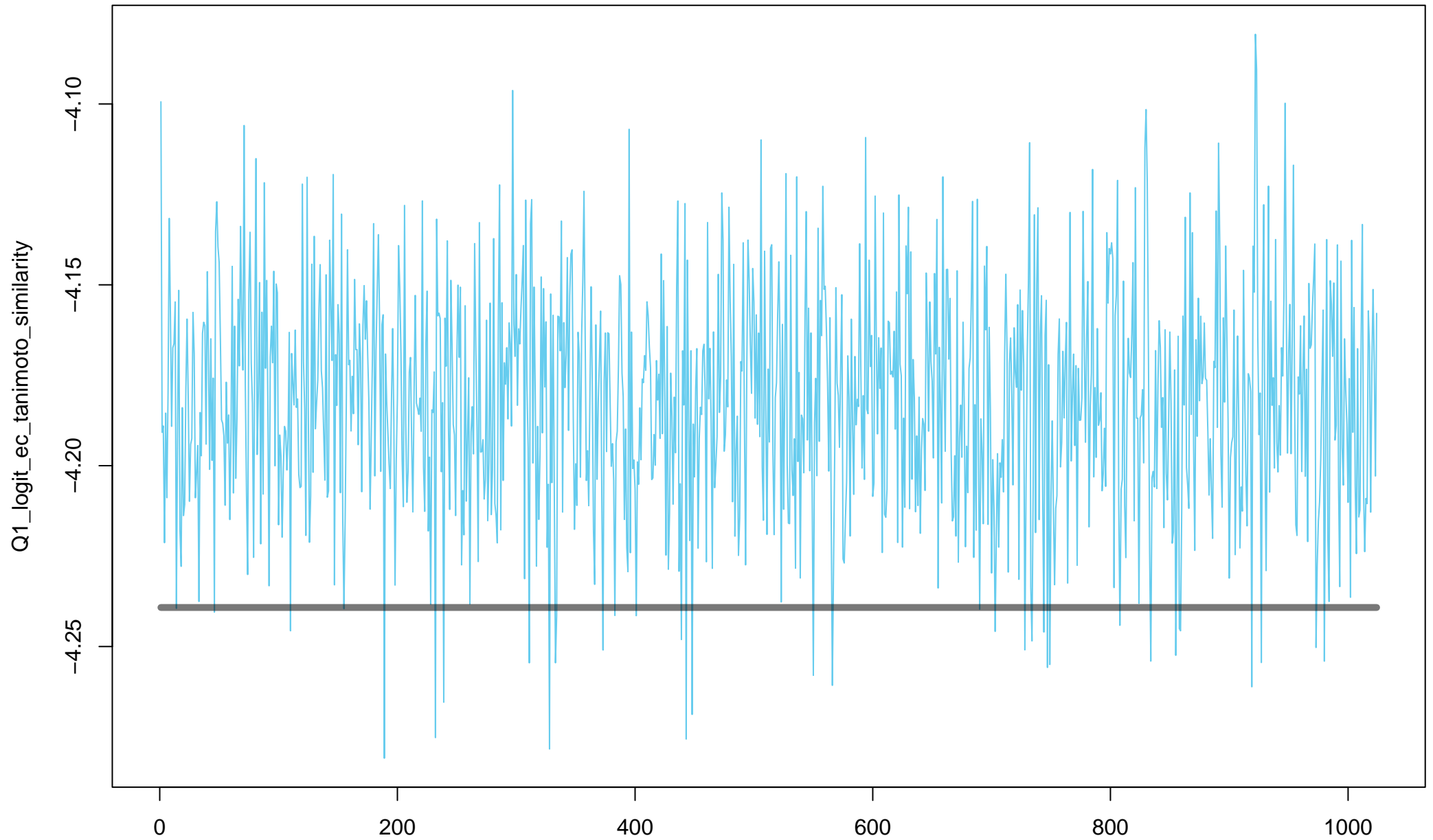


Q1_log_mcs_unbonded_polar_sasa
ESS = 919 | BMK = 0.0748 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 0 | percentile: 10.4

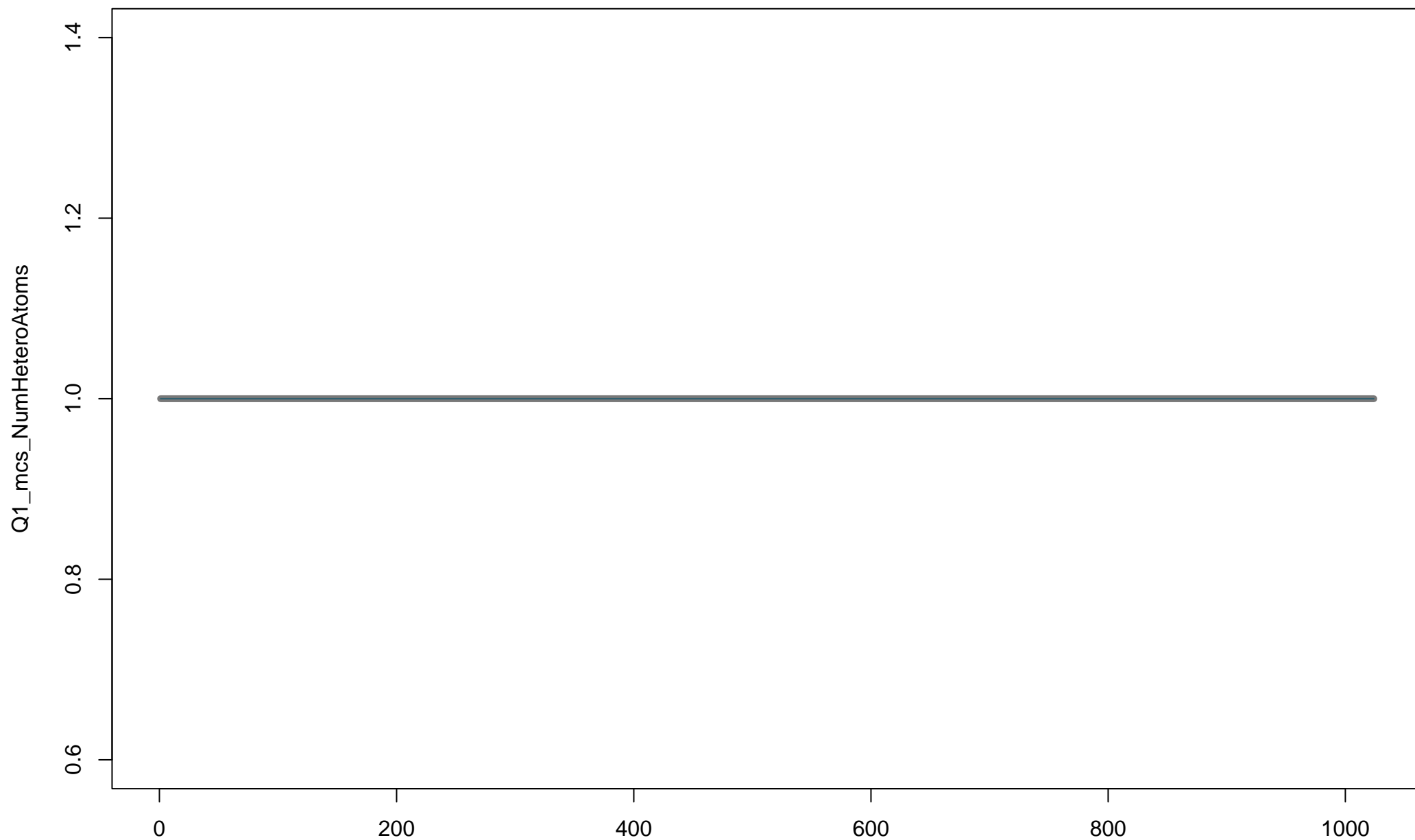


Q1_logit_ec_tanimoto_similarity

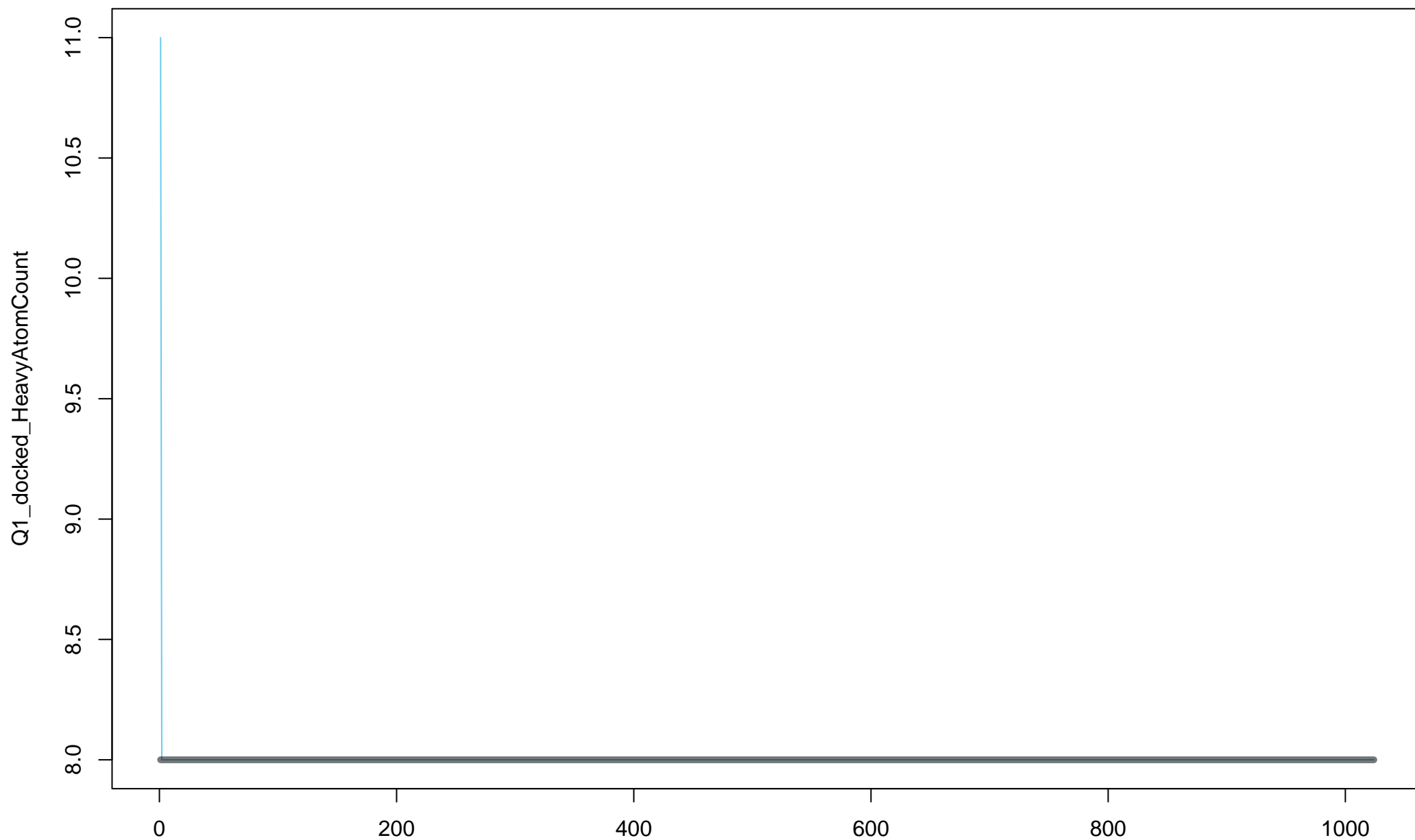
ESS = 1020 | BMK = 0.0613 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | percentile: 3.42



Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100

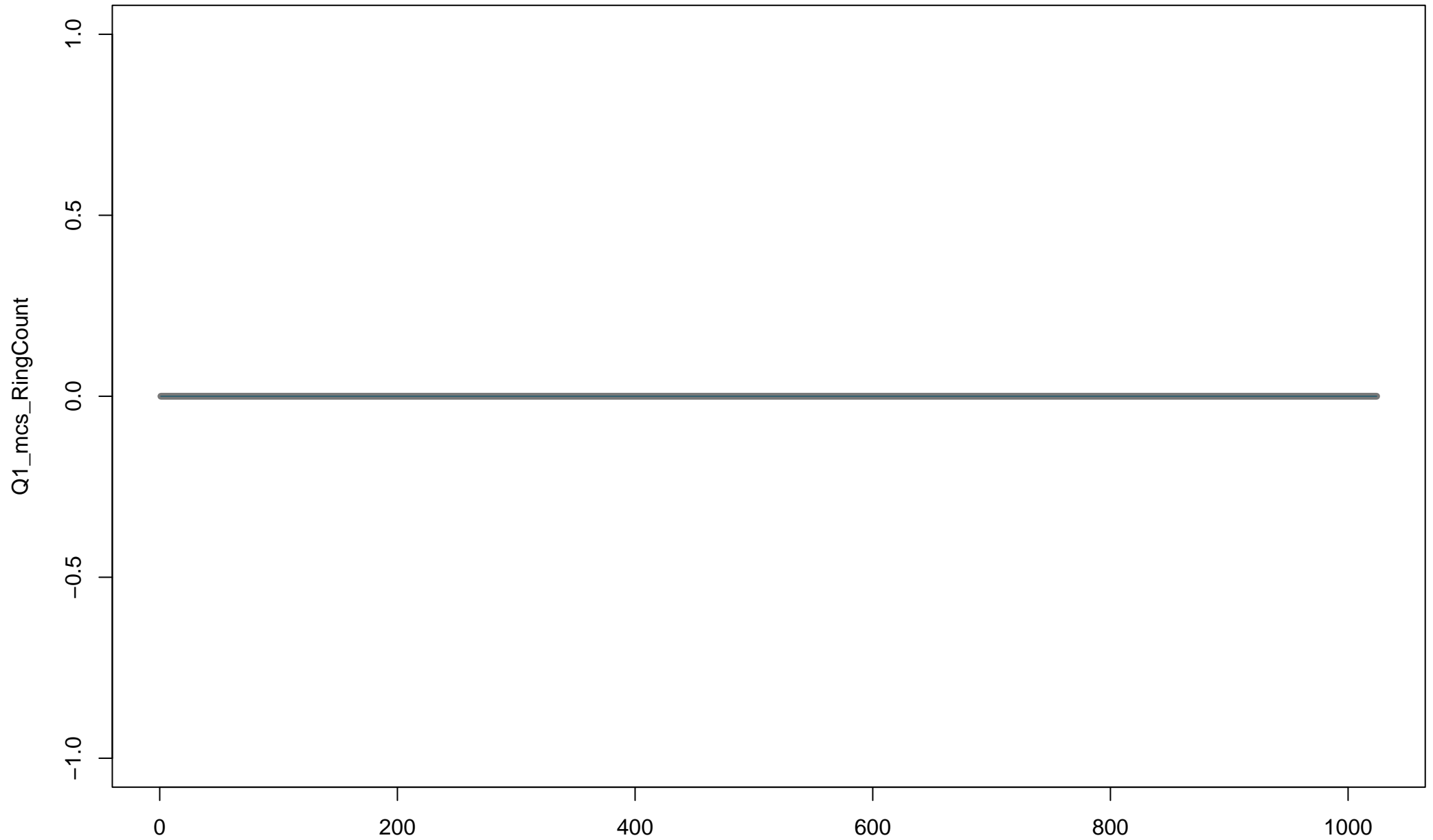


Q1_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.619 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102 | percentile: 99.9



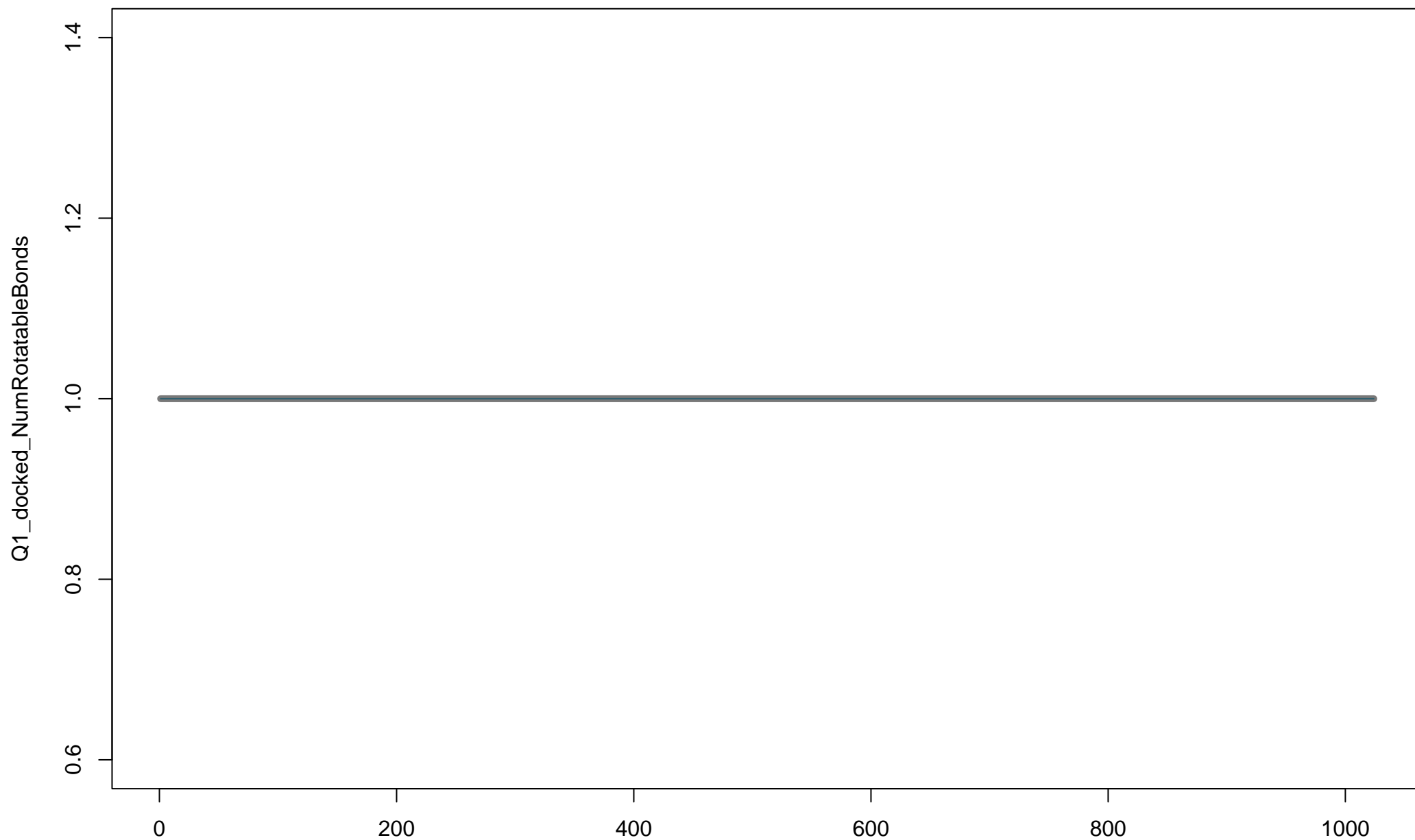
Q1_mcs_RingCount

ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100



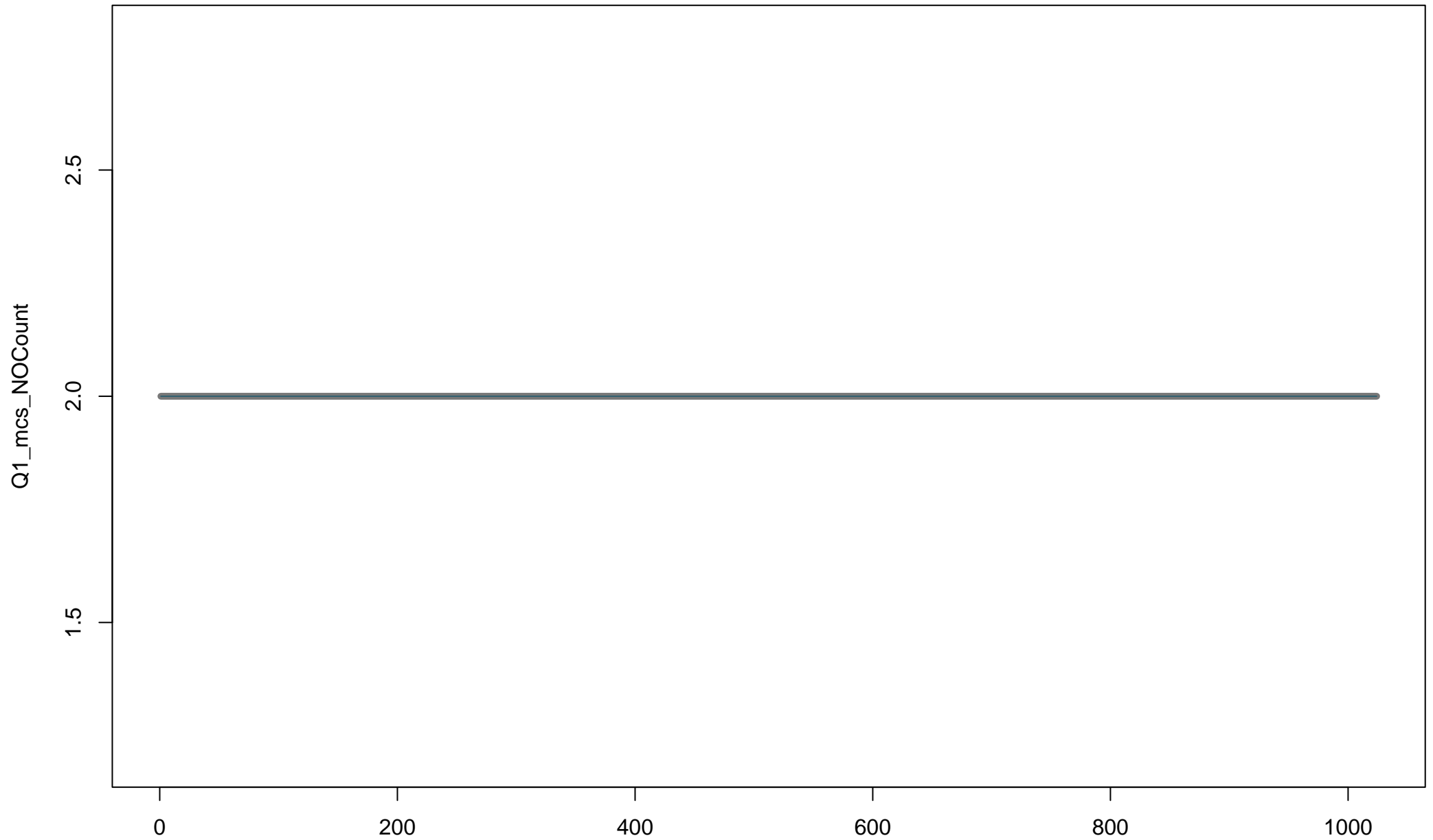
Q1_docked_NumRotatableBonds

ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100



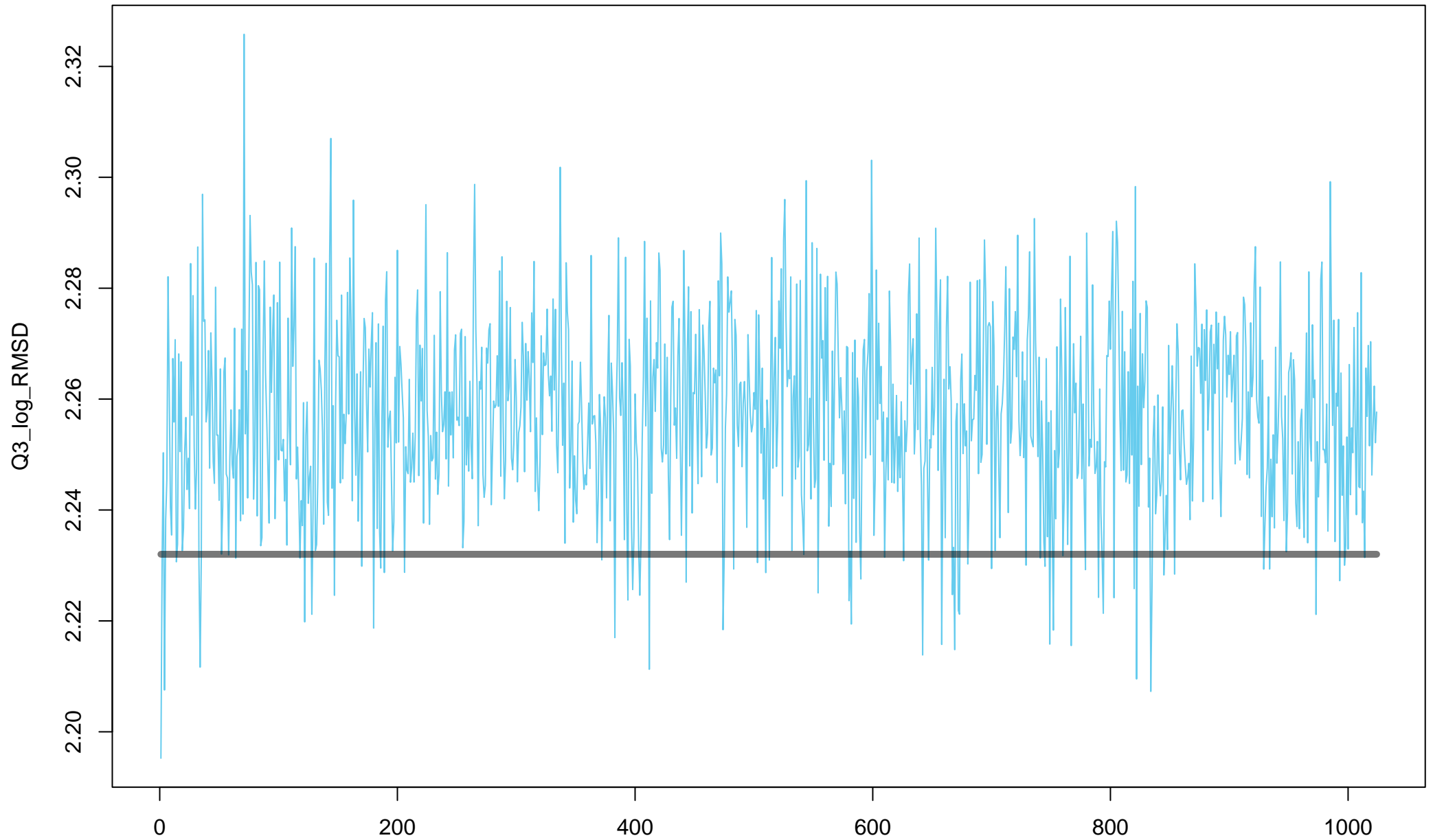
Q1_mcs_NOCount

ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100

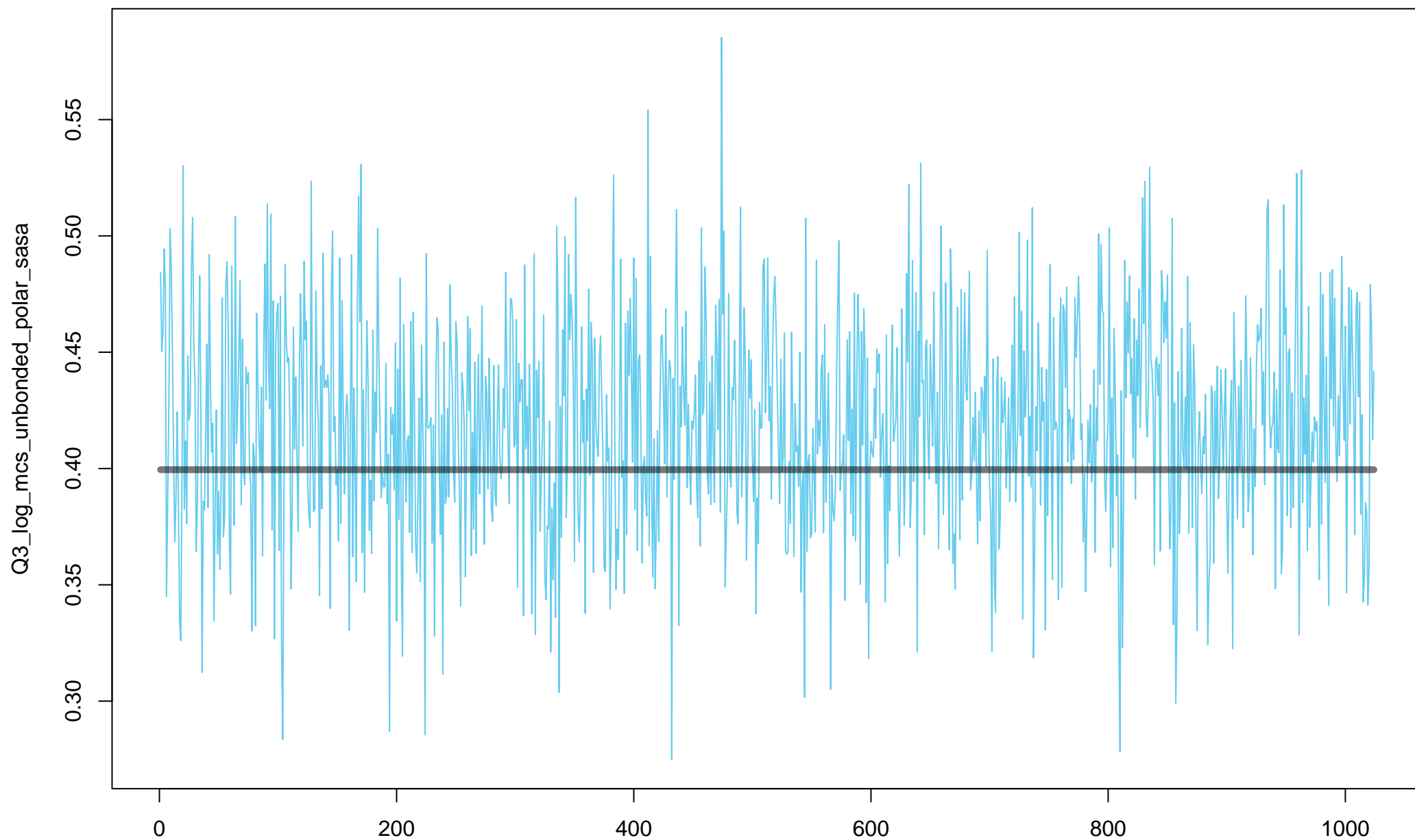


Q3_log_RMSD

ESS = 713 | BMK = 0.0437 | MCSE(6.27) = 4.7 | stat: TRUE | burn: 0 | percentile: 6.93

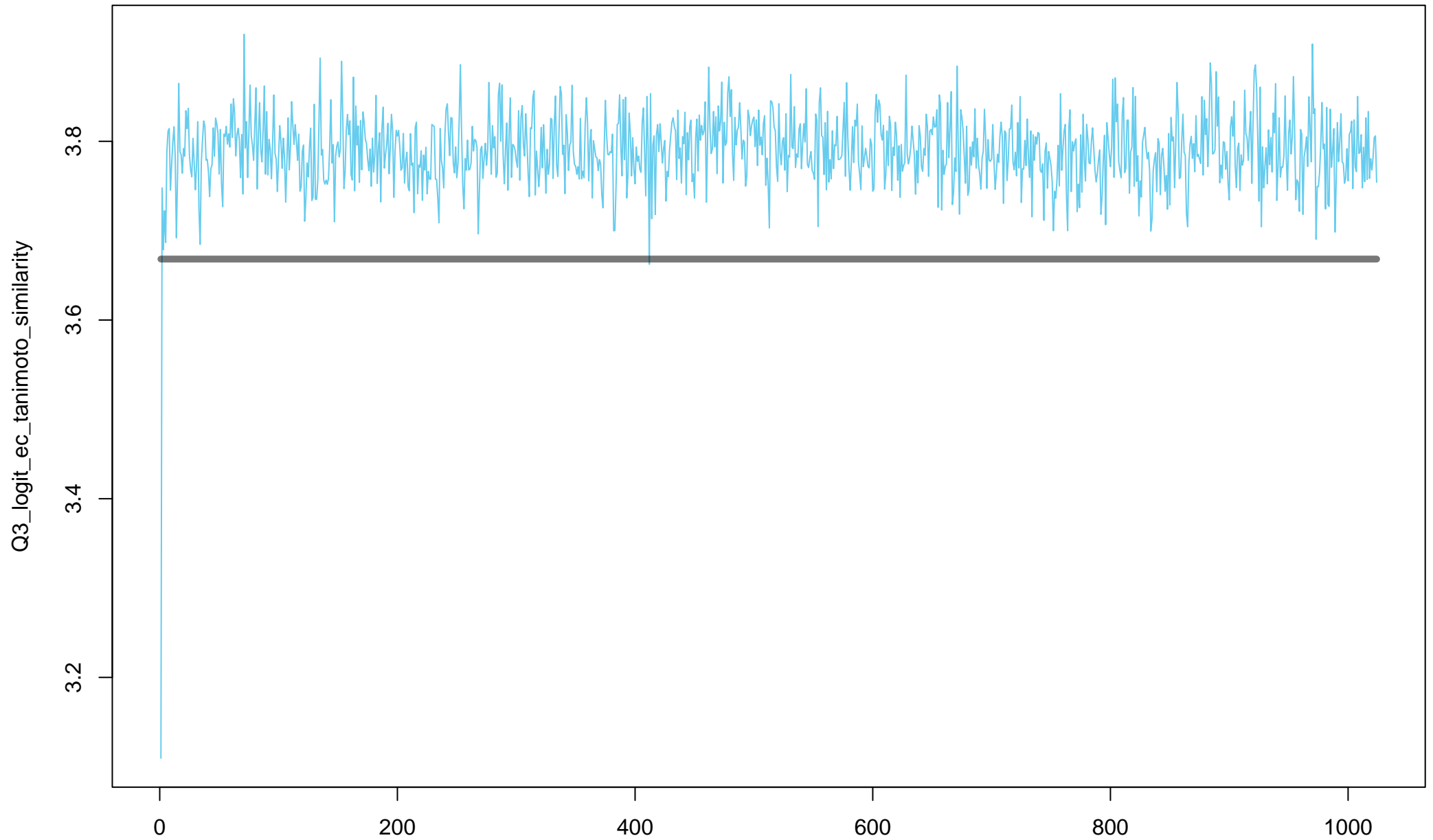


Q3_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0503 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0 | percentile: 33.9



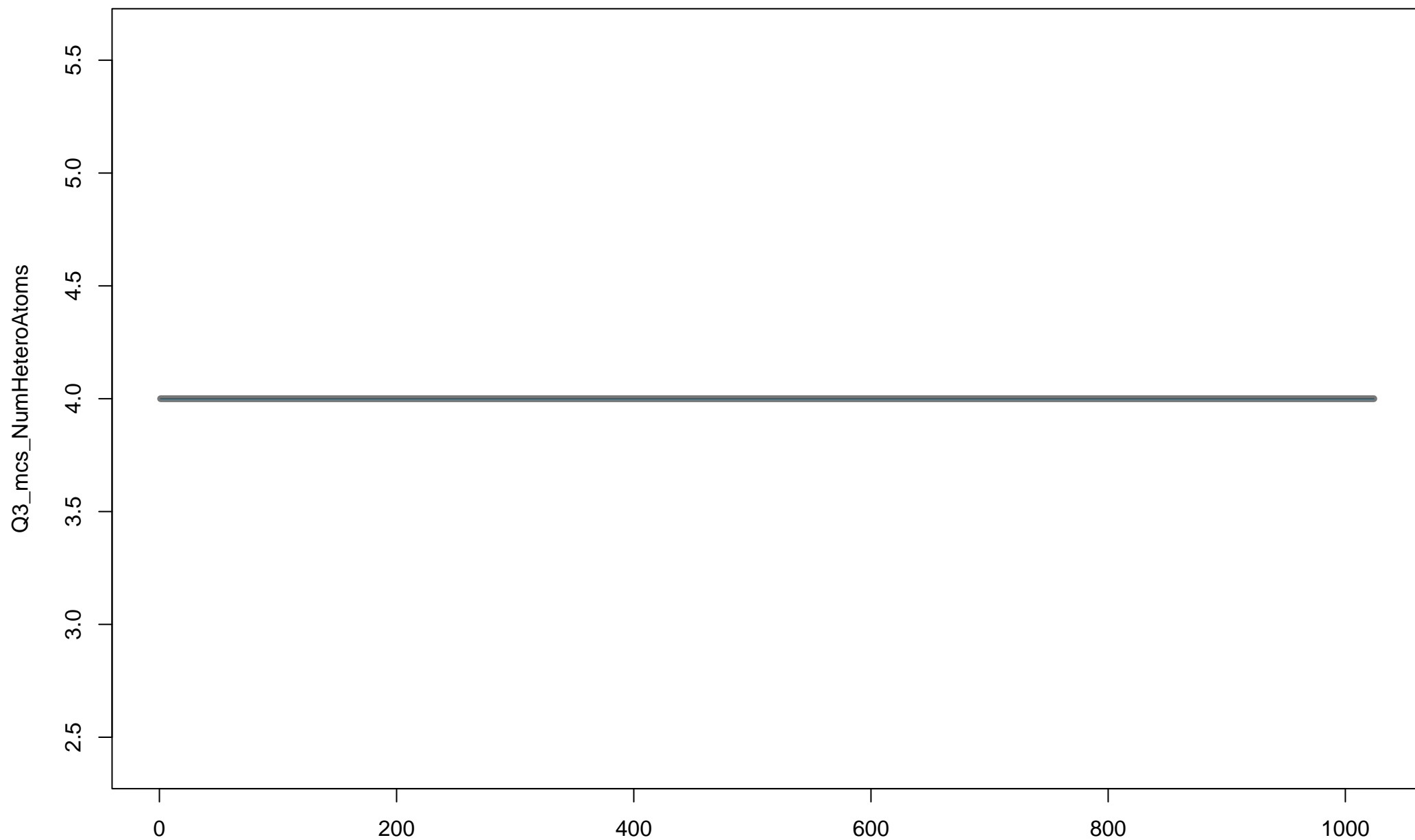
Q3_logit_ec_tanimoto_similarity

ESS = 889 | BMK = 0.0661 | MCSE(6.27) = 4.19 | stat: TRUE | burn: 0 | percentile: 0.195

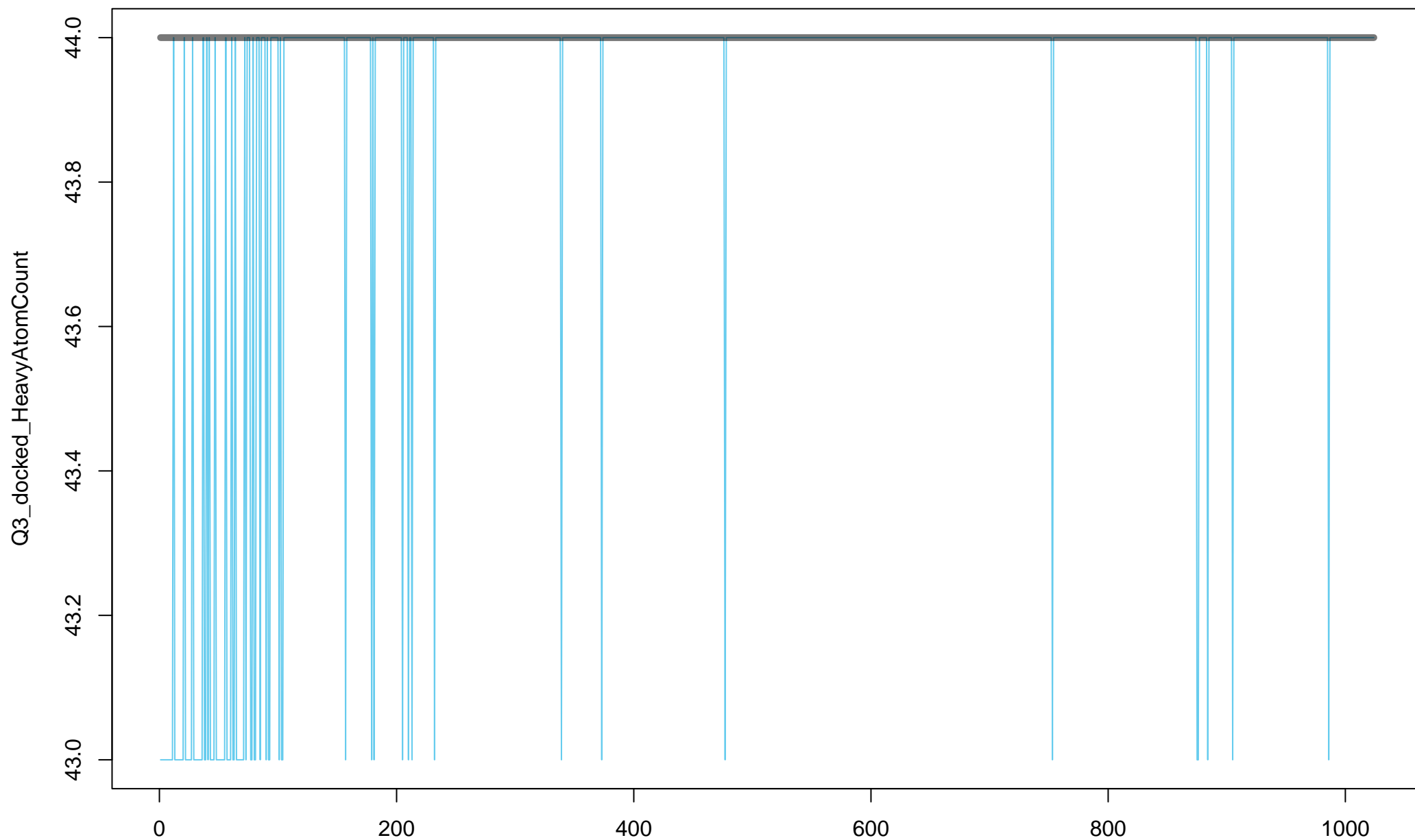


Q3_mcs_NumHeteroAtoms

ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100

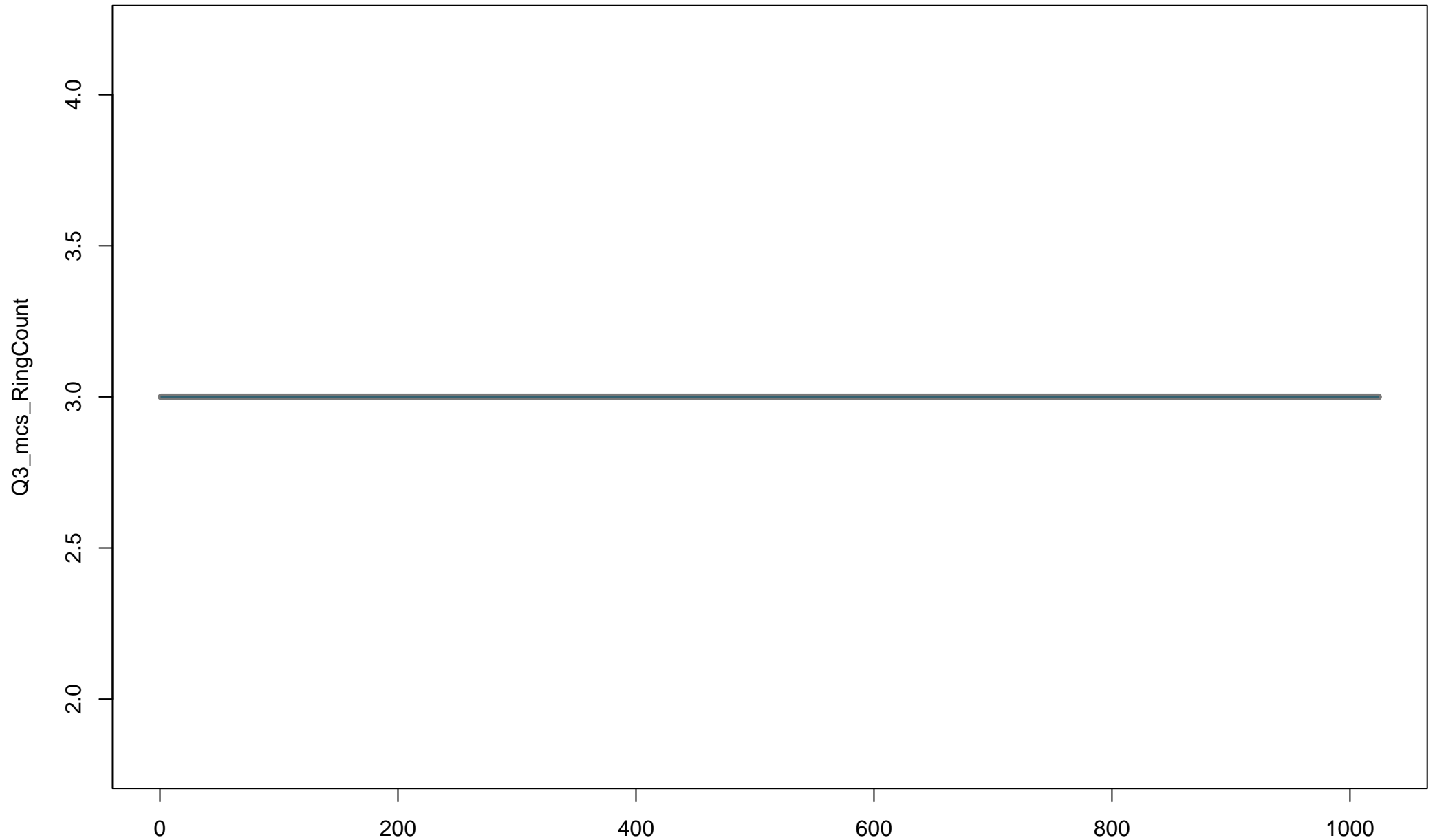


Q3_docked_HeavyAtomCount
ESS = 9.78 | BMK = 0.39 | MCSE(6.27) = 13.7 | stat: FALSE | burn: 714 | percentile: 100



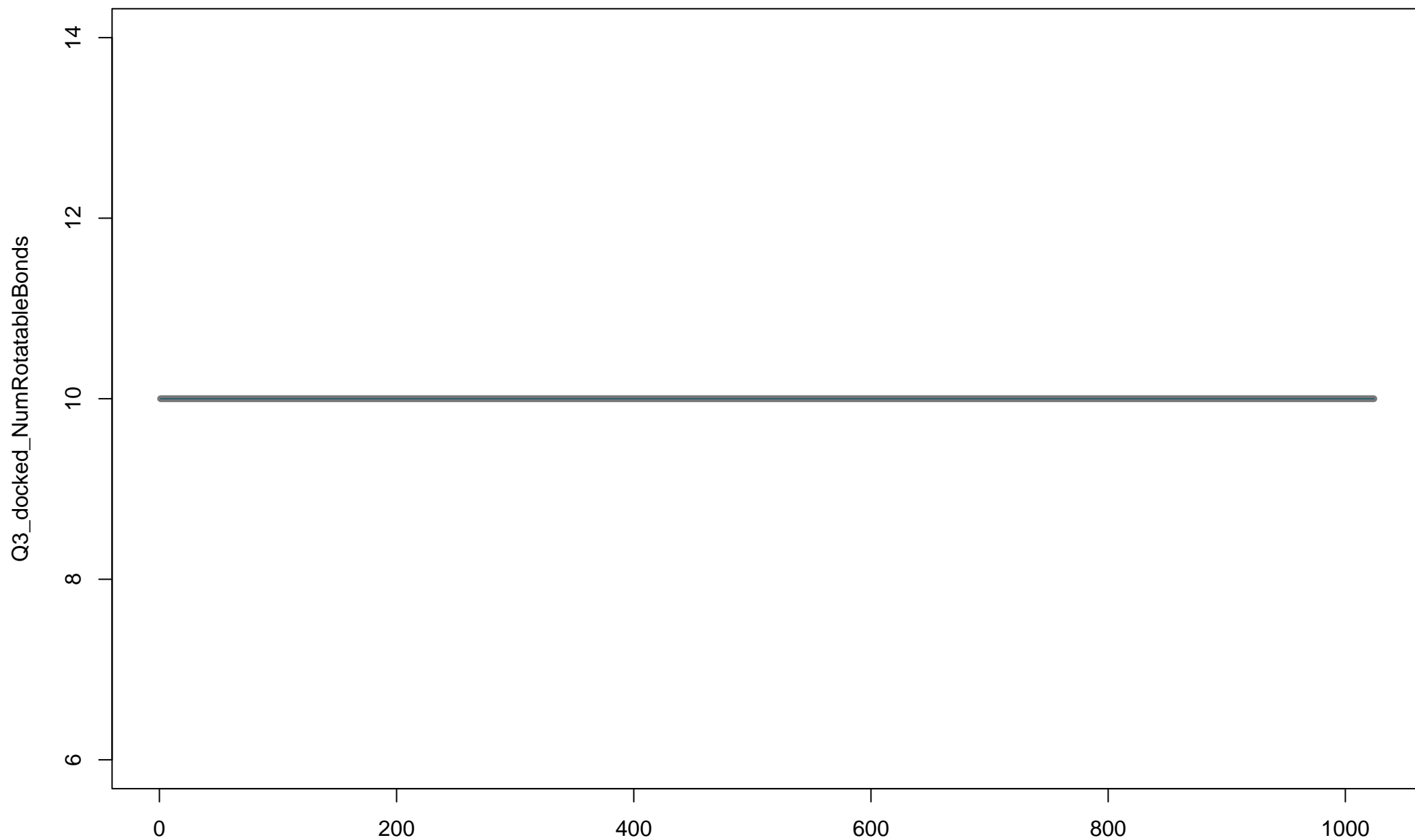
Q3_mcs_RingCount

ESS = $2.22\text{e-}16$ | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100



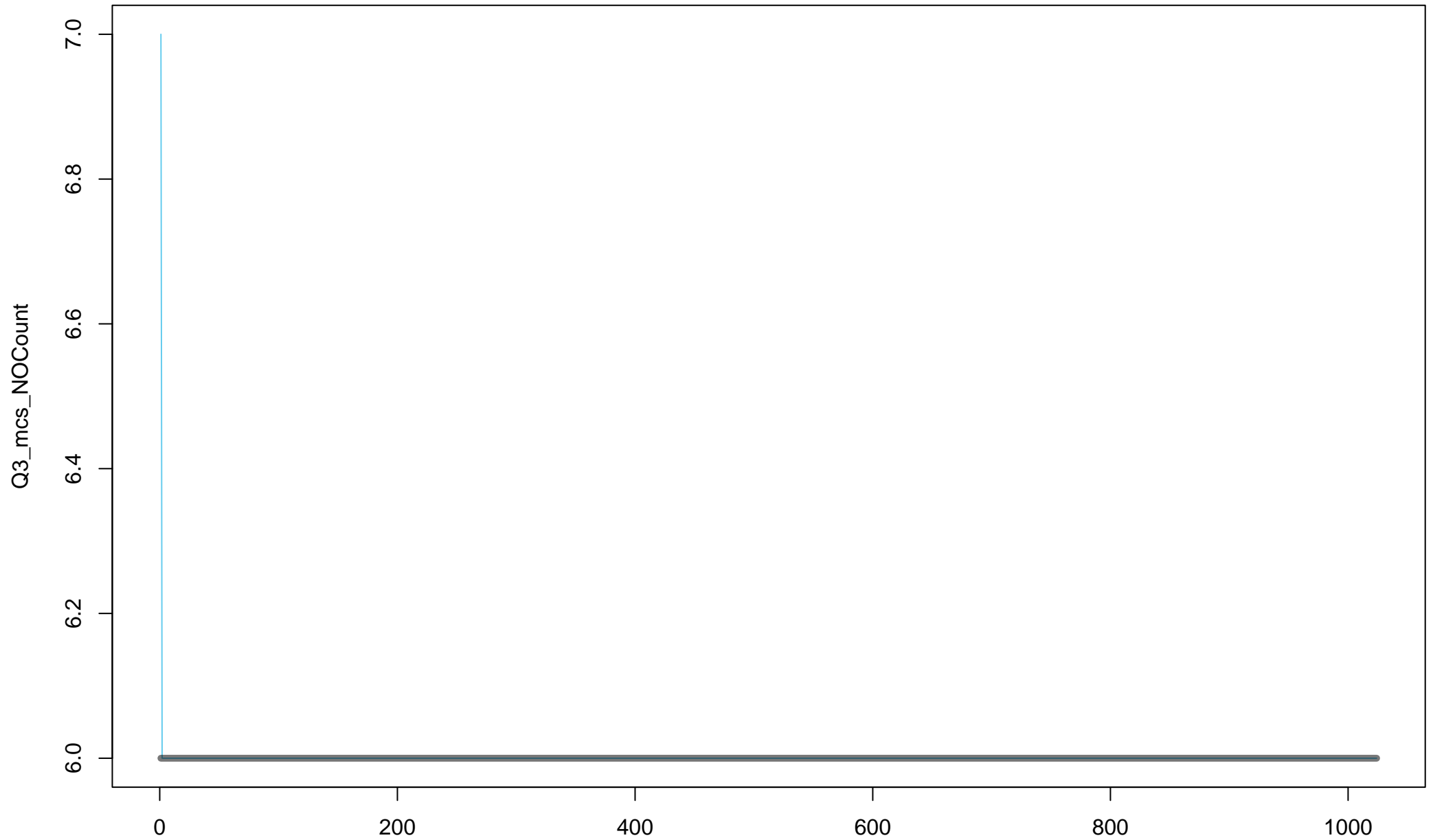
Q3_docked_NumRotatableBonds

ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100



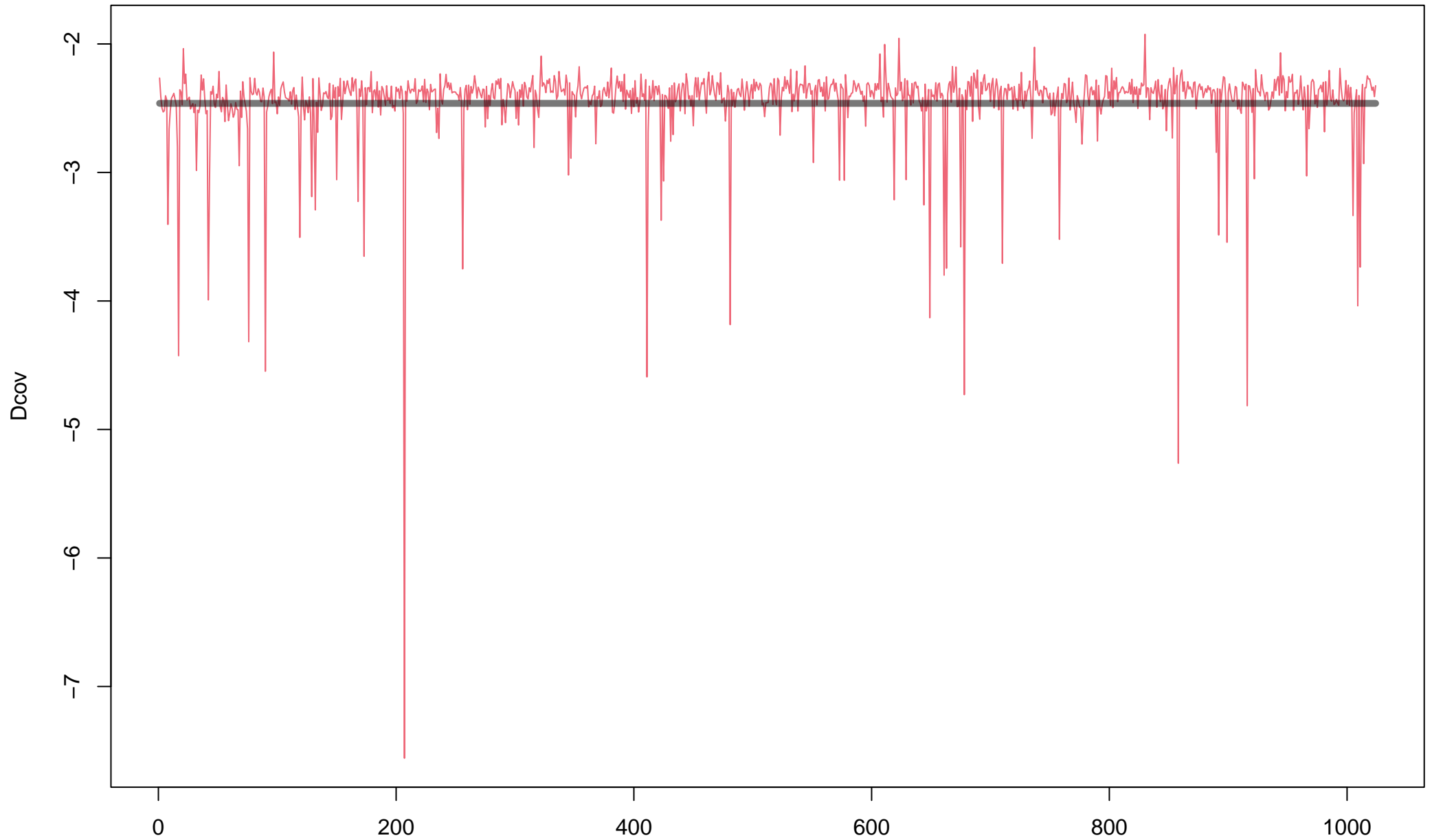
Q3_mcs_NOCount

ESS = 1020 | BMK = 0.567 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102 | percentile: 99.9



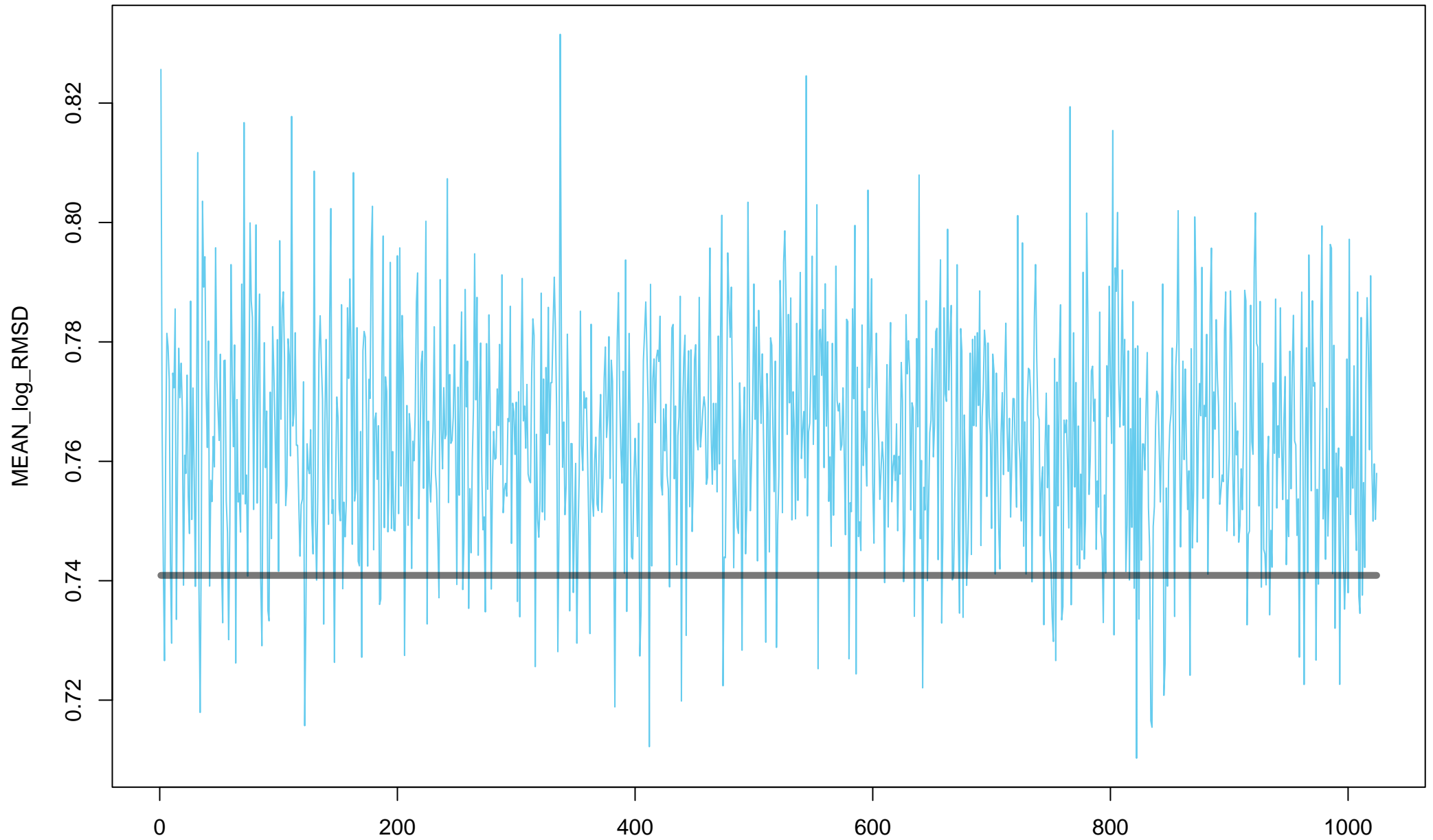
Dcov

ESS = 726 | BMK = 0.11 | MCSE(6.27) = 3.86 | stat: FALSE | burn: 0 | percentile: 76.5

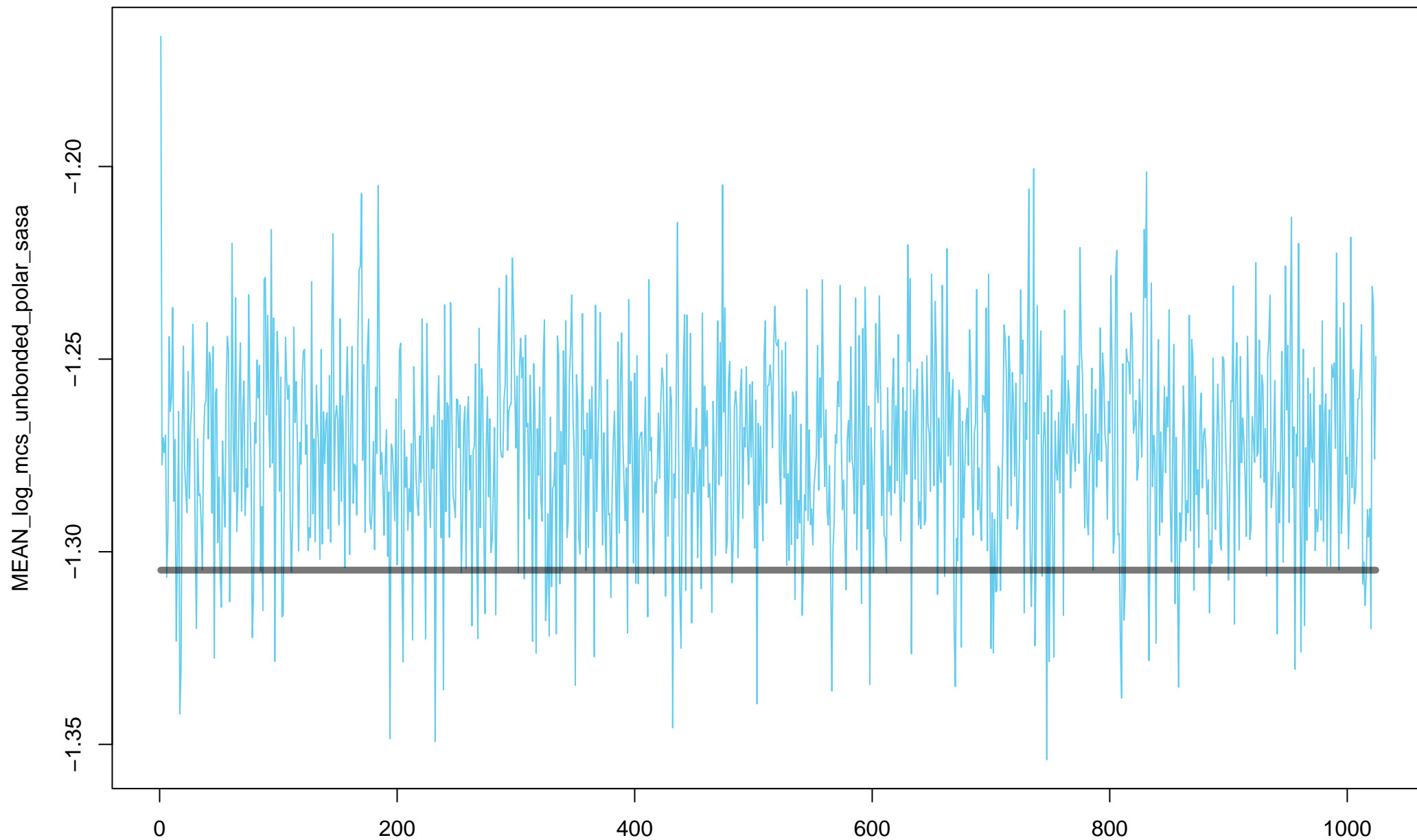


MEAN_log_RMSD

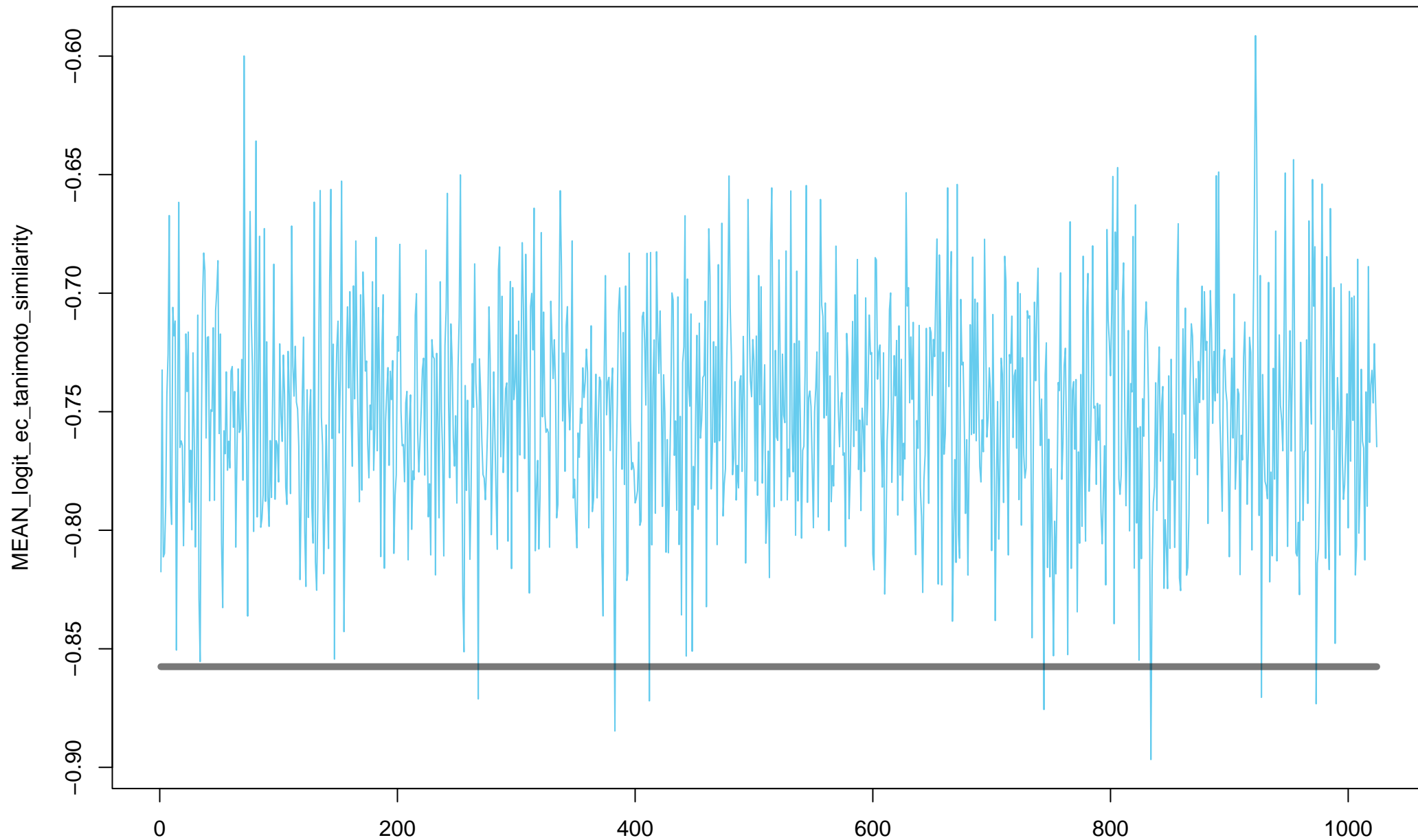
ESS = 1020 | BMK = 0.0346 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0 | percentile: 10.1



MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0477 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0 | percentile: 10.7

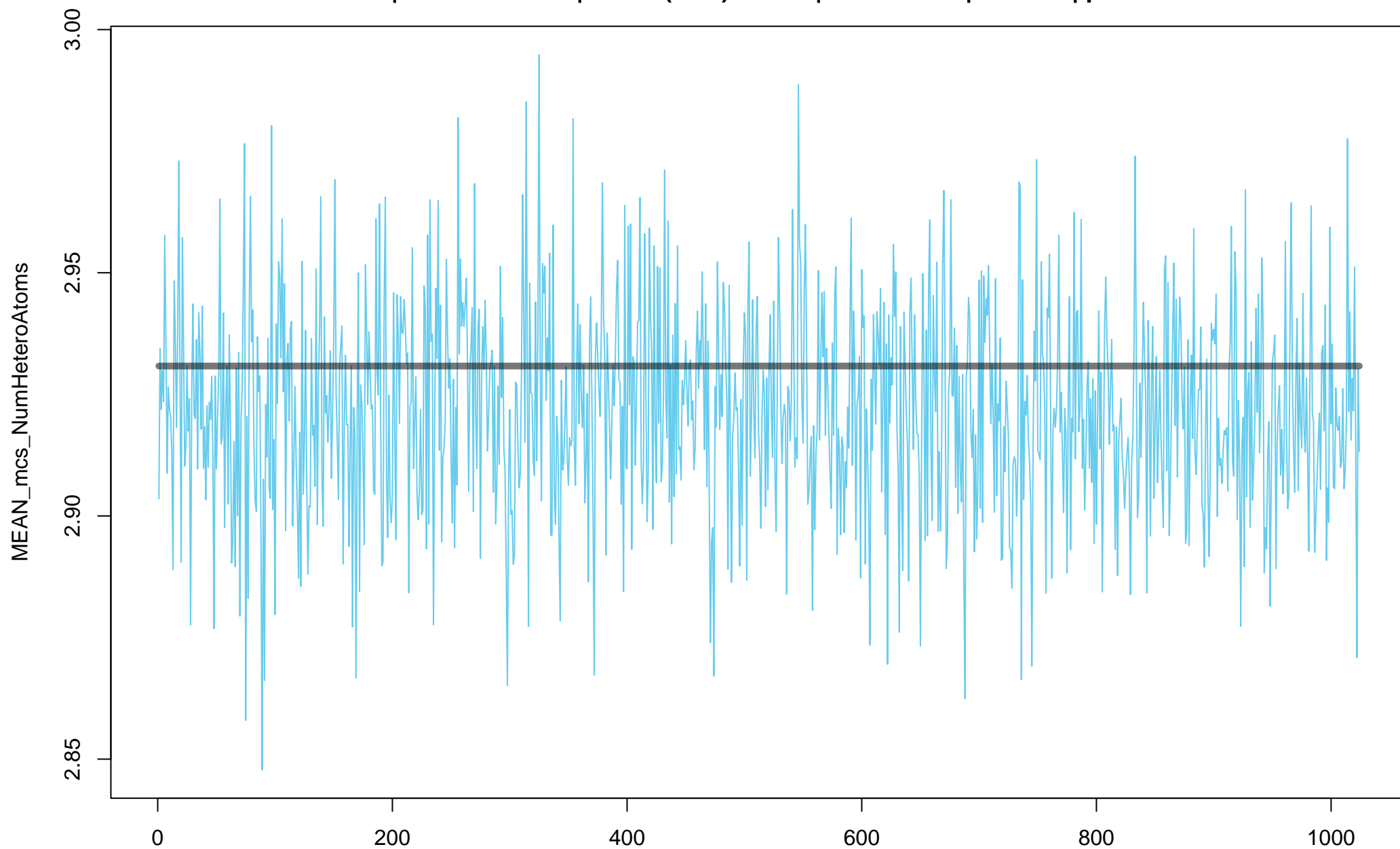


MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0409 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0 | percentile: 0.684



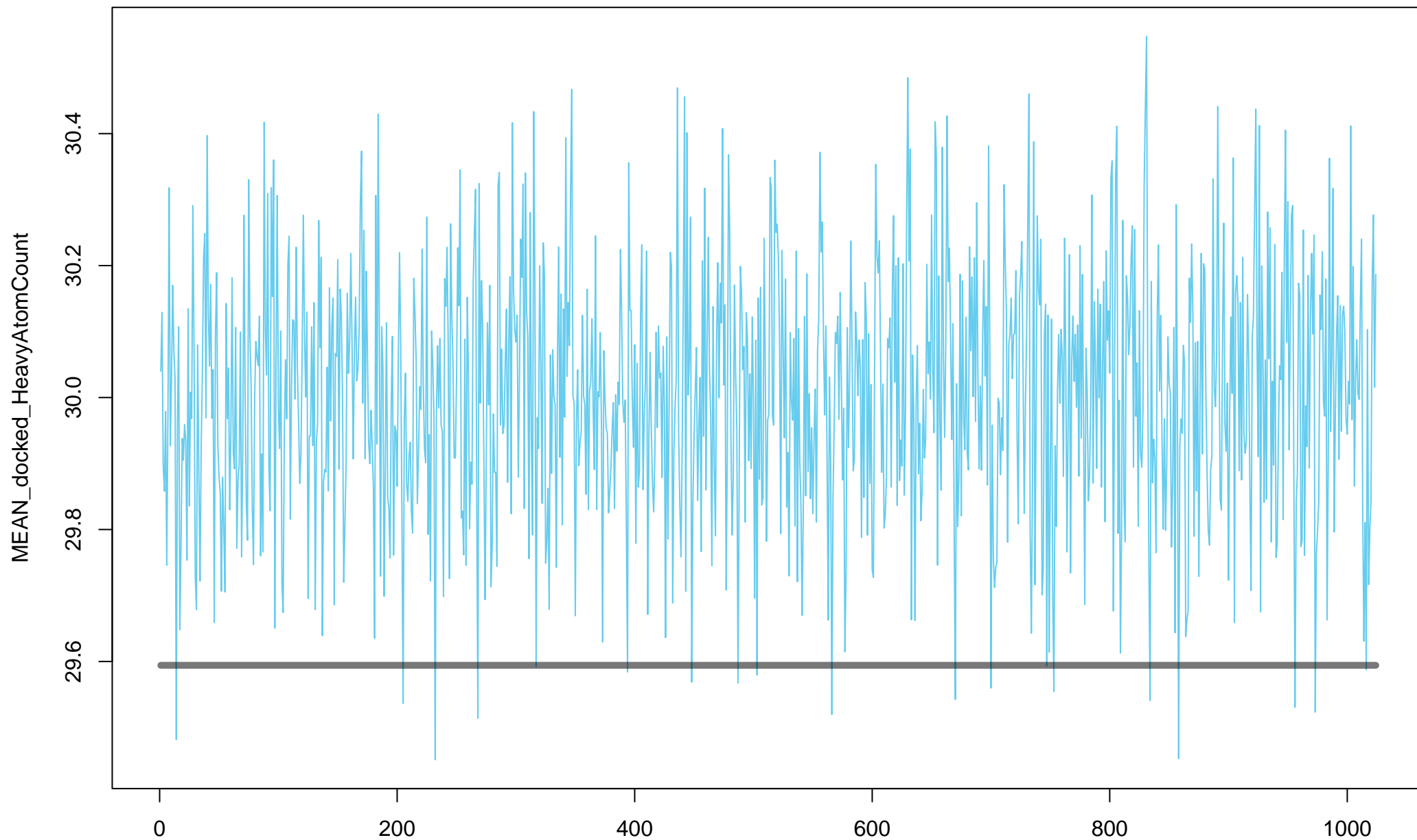
MEAN_mcs_NumHeteroAtoms

ESS = 1020 | BMK = 0.0688 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0 | percentile: 67.3



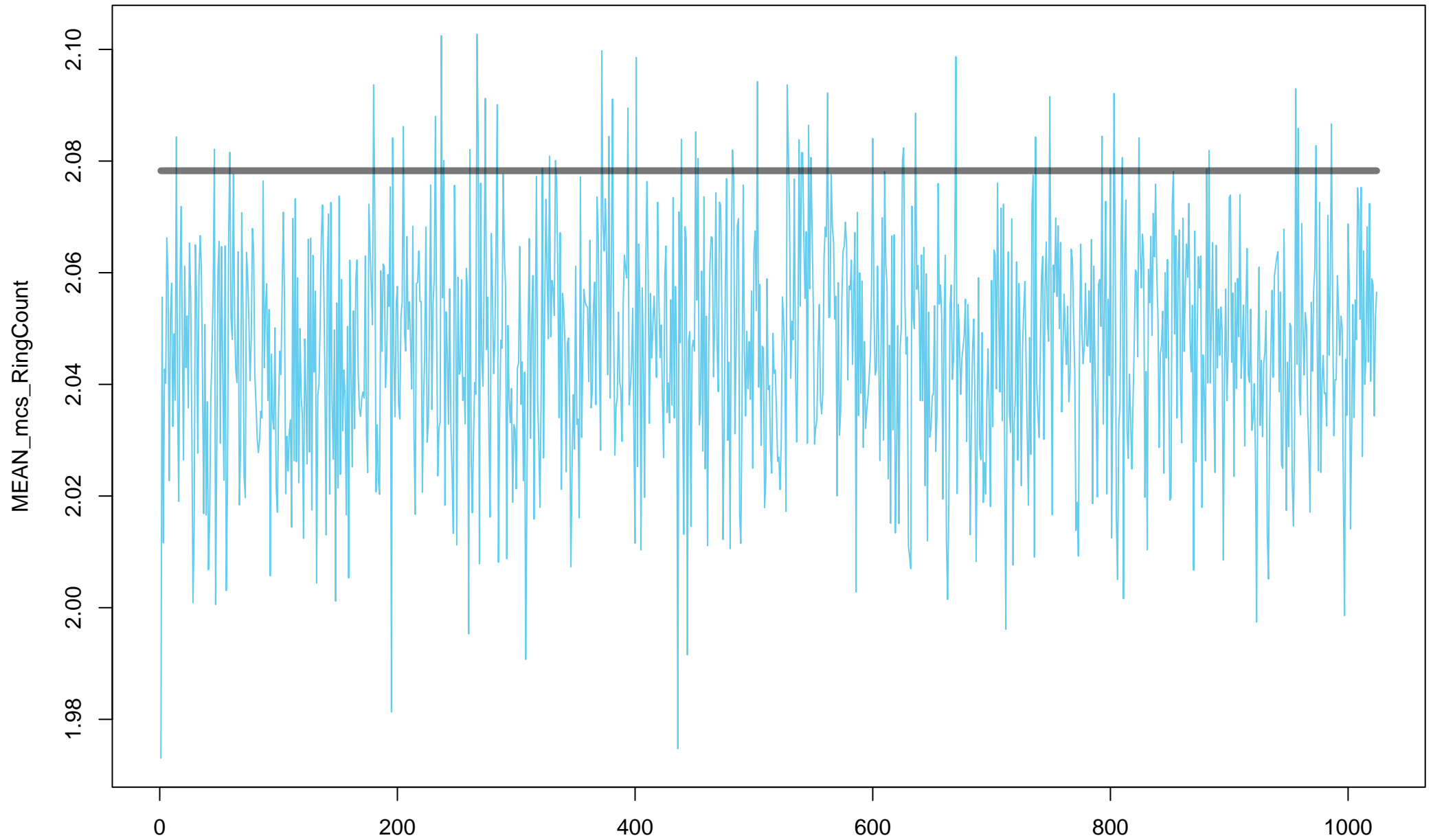
MEAN_docked_HeavyAtomCount

ESS = 920 | BMK = 0.0568 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0 | percentile: 1.86



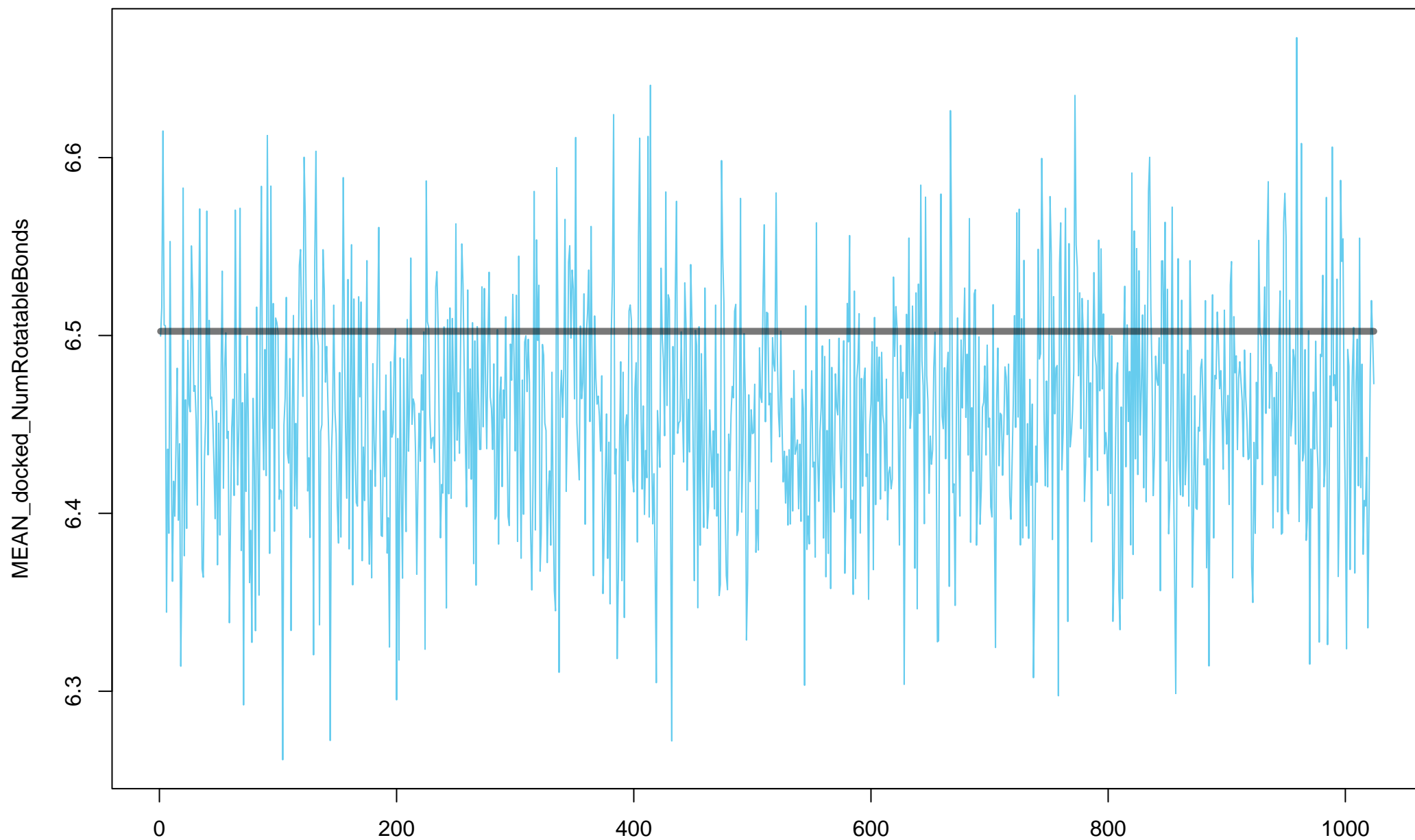
MEAN_mcs_RingCount

ESS = 1020 | BMK = 0.0615 | MCSE(6.27) = 3.49 | stat: TRUE | burn: 0 | percentile: 94.8



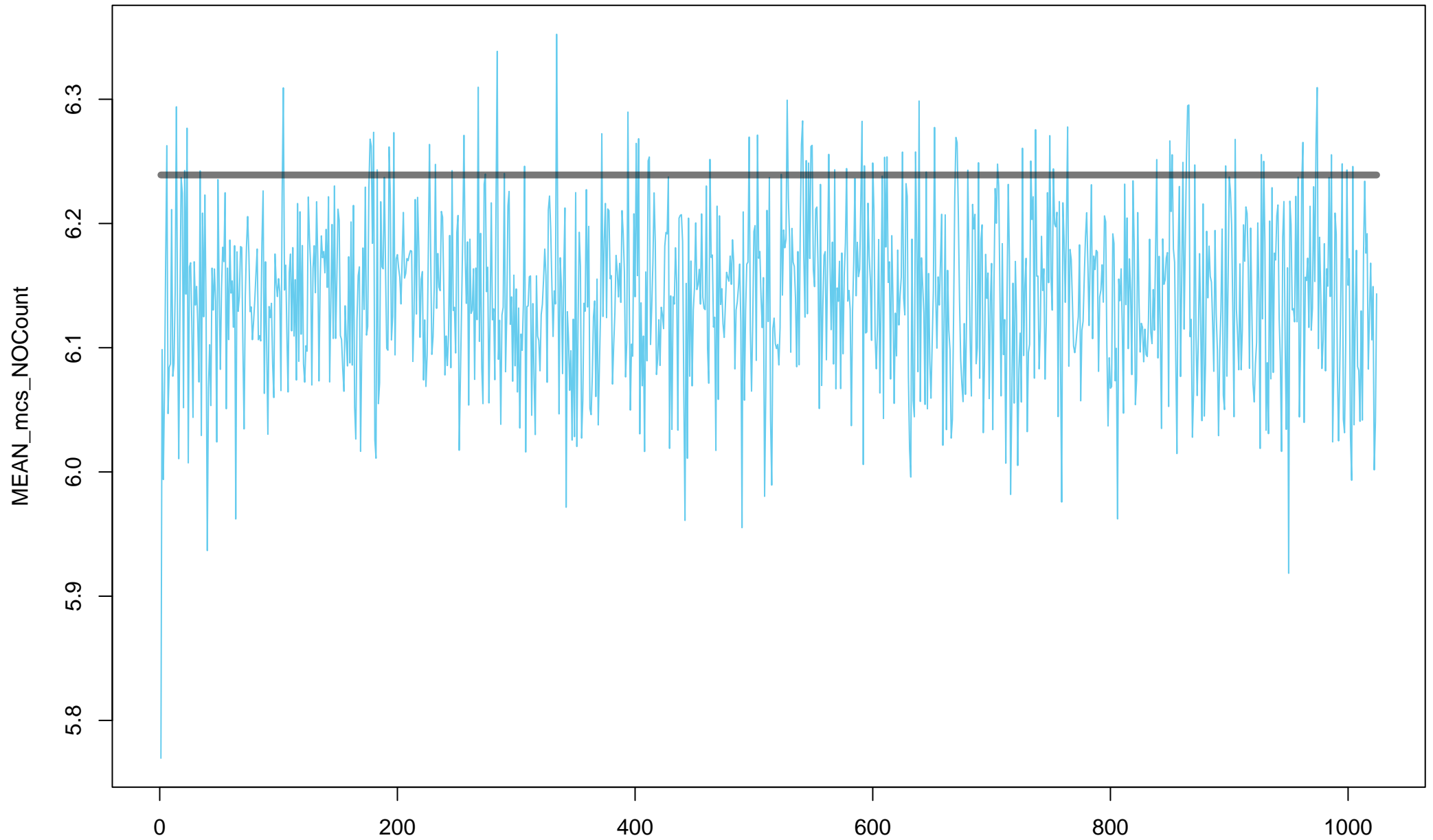
MEAN_docked_NumRotatableBonds

ESS = 1020 | BMK = 0.056 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | percentile: 78.4



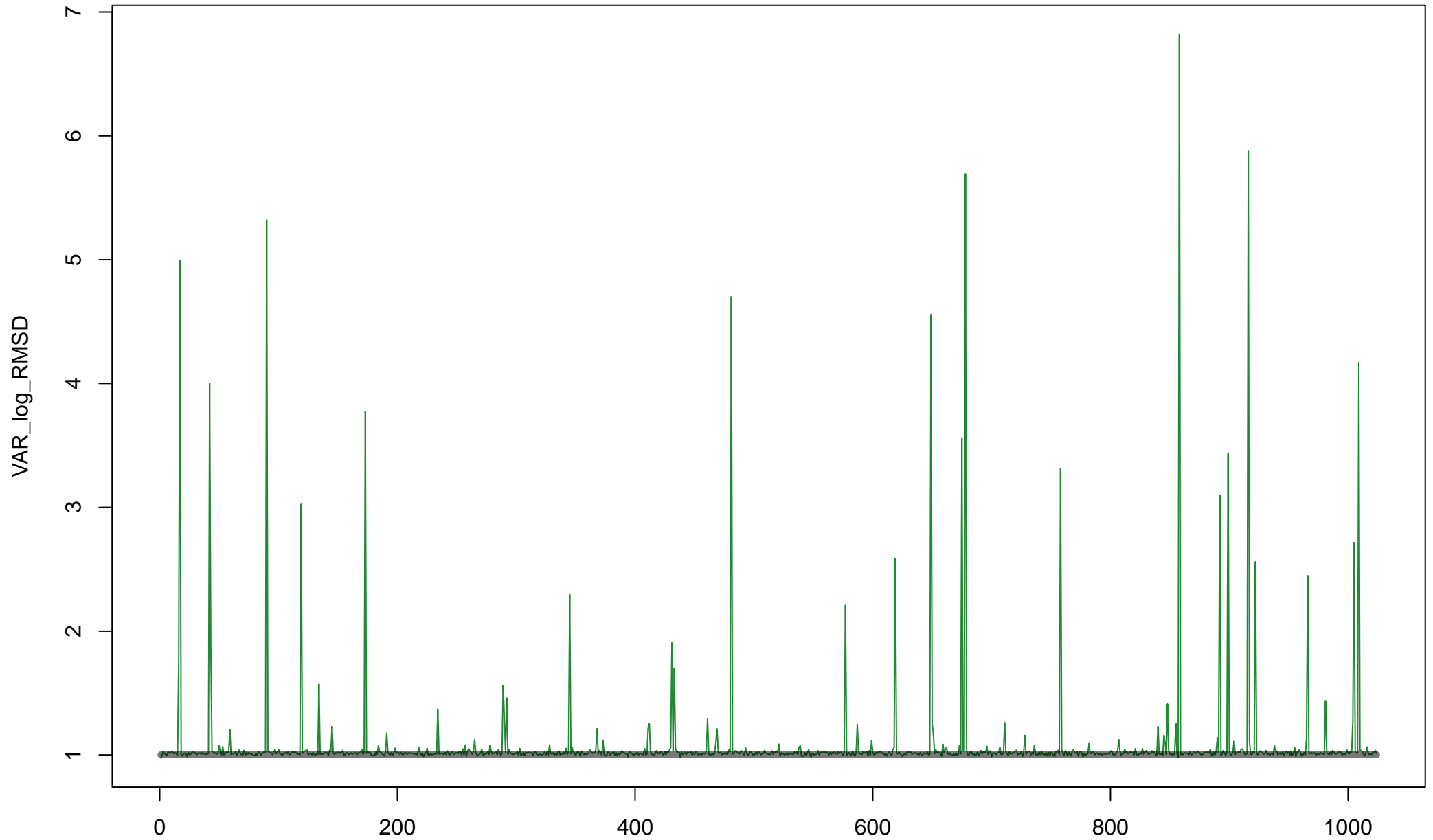
MEAN_mcs_NOCount

ESS = 1020 | BMK = 0.0829 | MCSE(6.27) = 3.34 | stat: FALSE | burn: 0 | percentile: 92

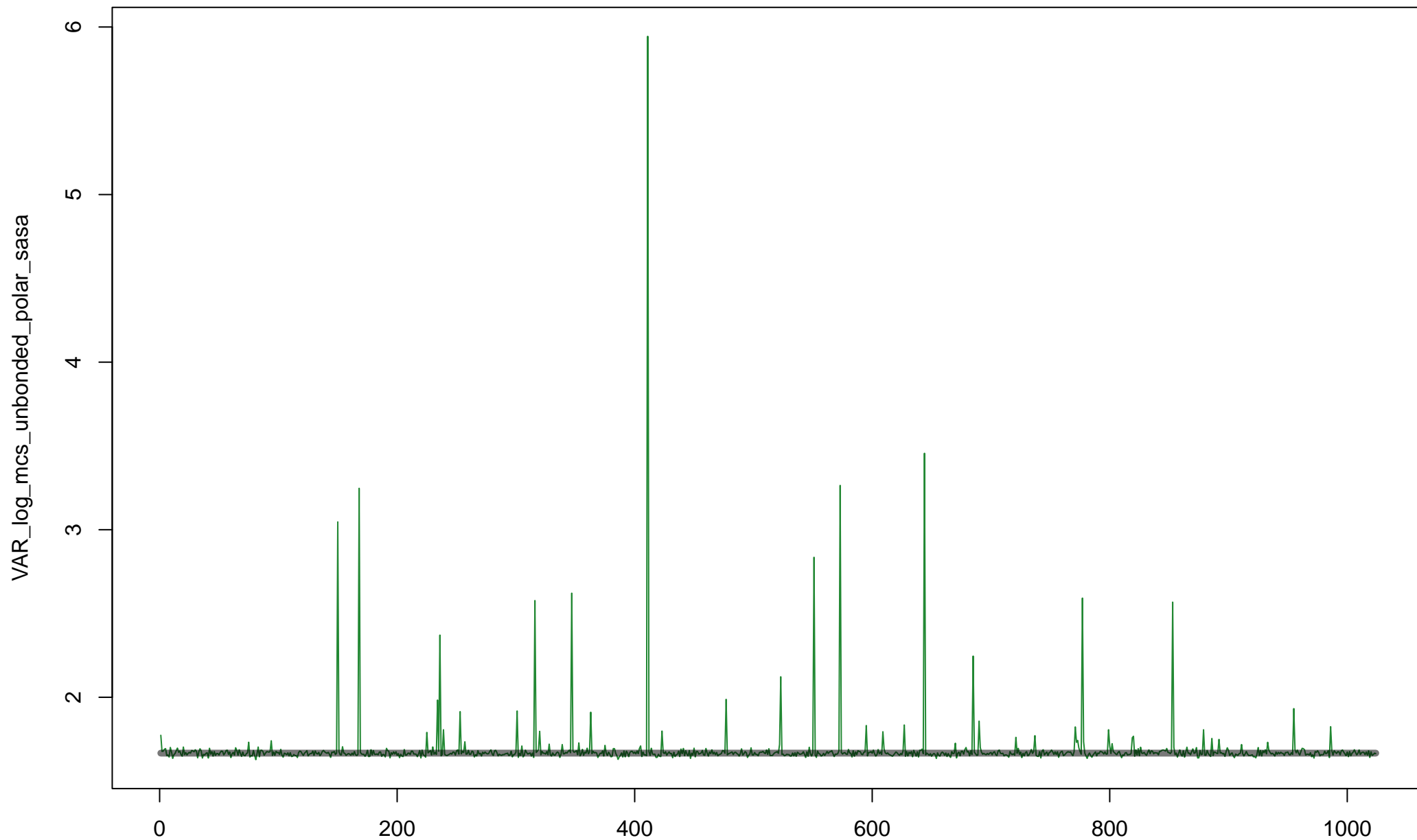


VAR_log_RMSD

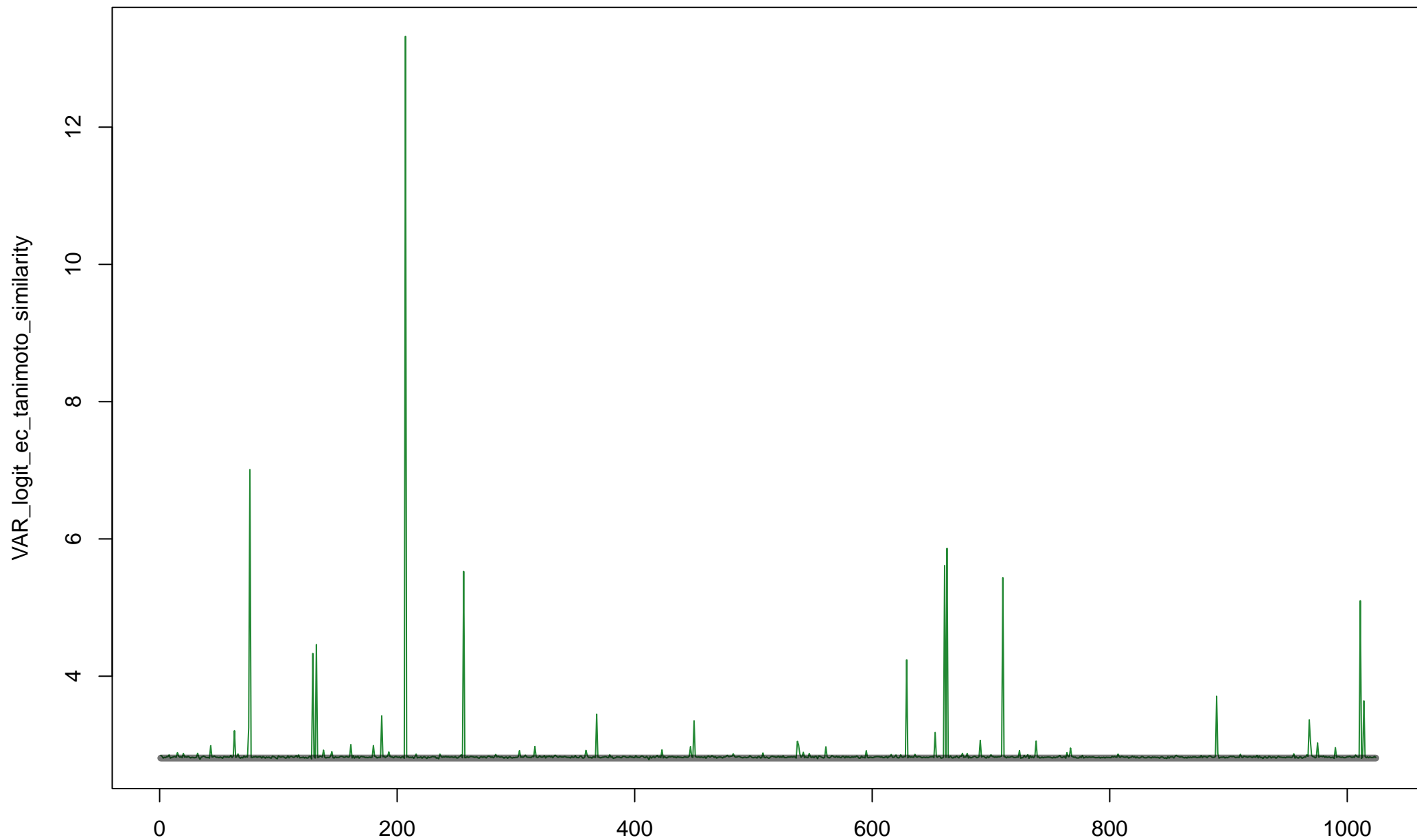
ESS = 1020 | BMK = 1 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 1020 | percentile: 15.4



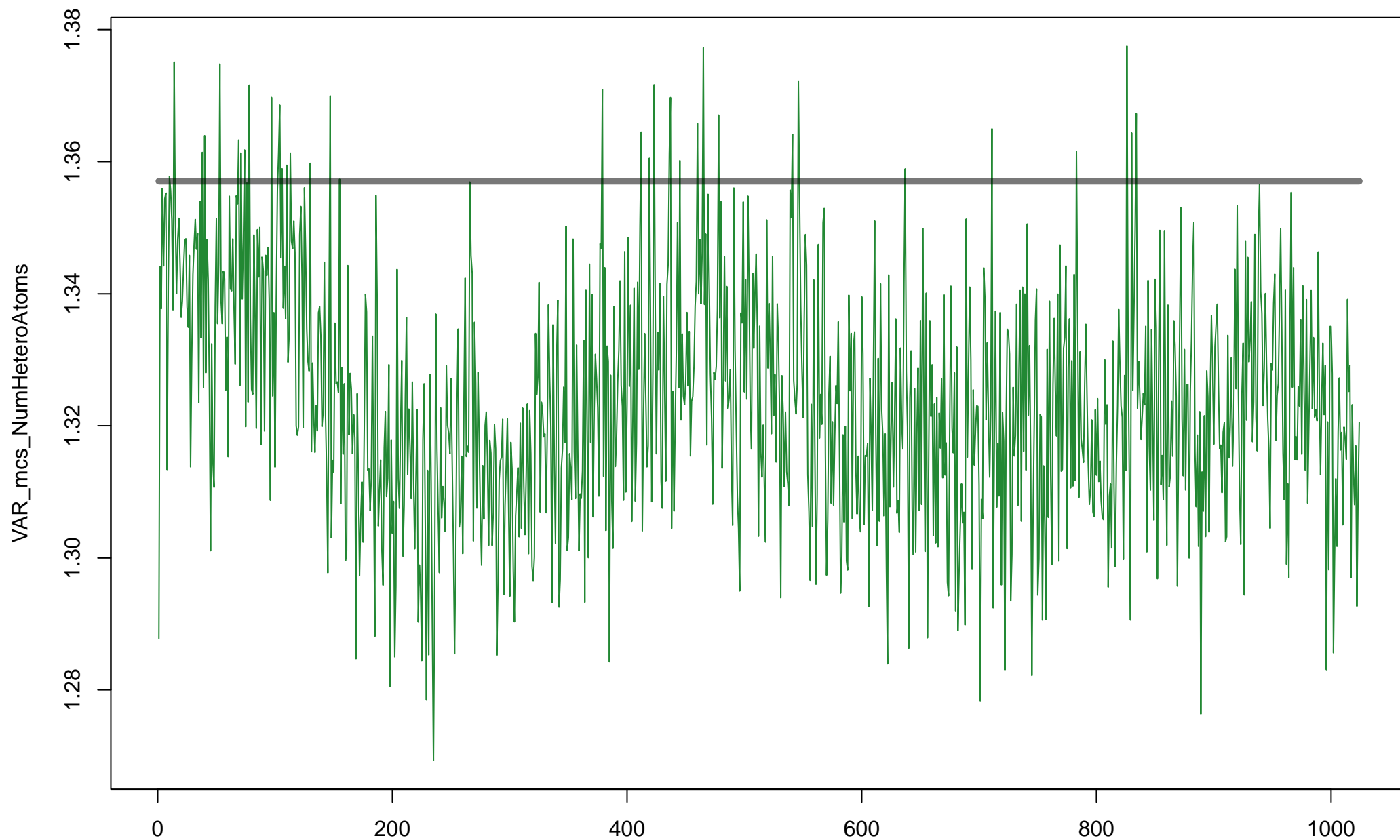
VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.344 | MCSE(6.27) = 3.08 | stat: FALSE | burn: 510 | percentile: 54.6



VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 714 | percentile: 5.18

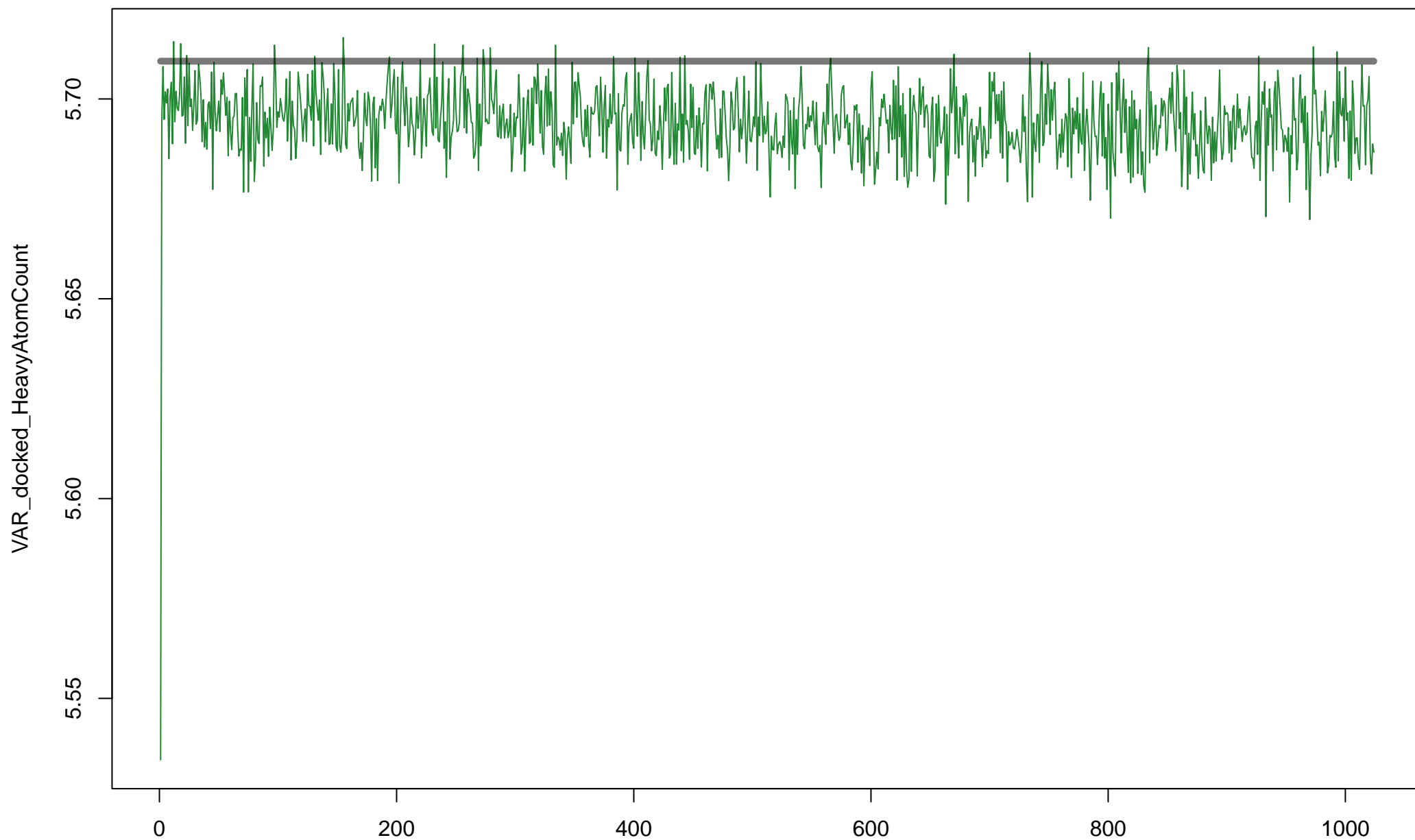


VAR_mcs_NumHeteroAtoms
ESS = 46.6 | BMK = 0.129 | MCSE(6.27) = 8.96 | stat: FALSE | burn: 0 | percentile: 96.5

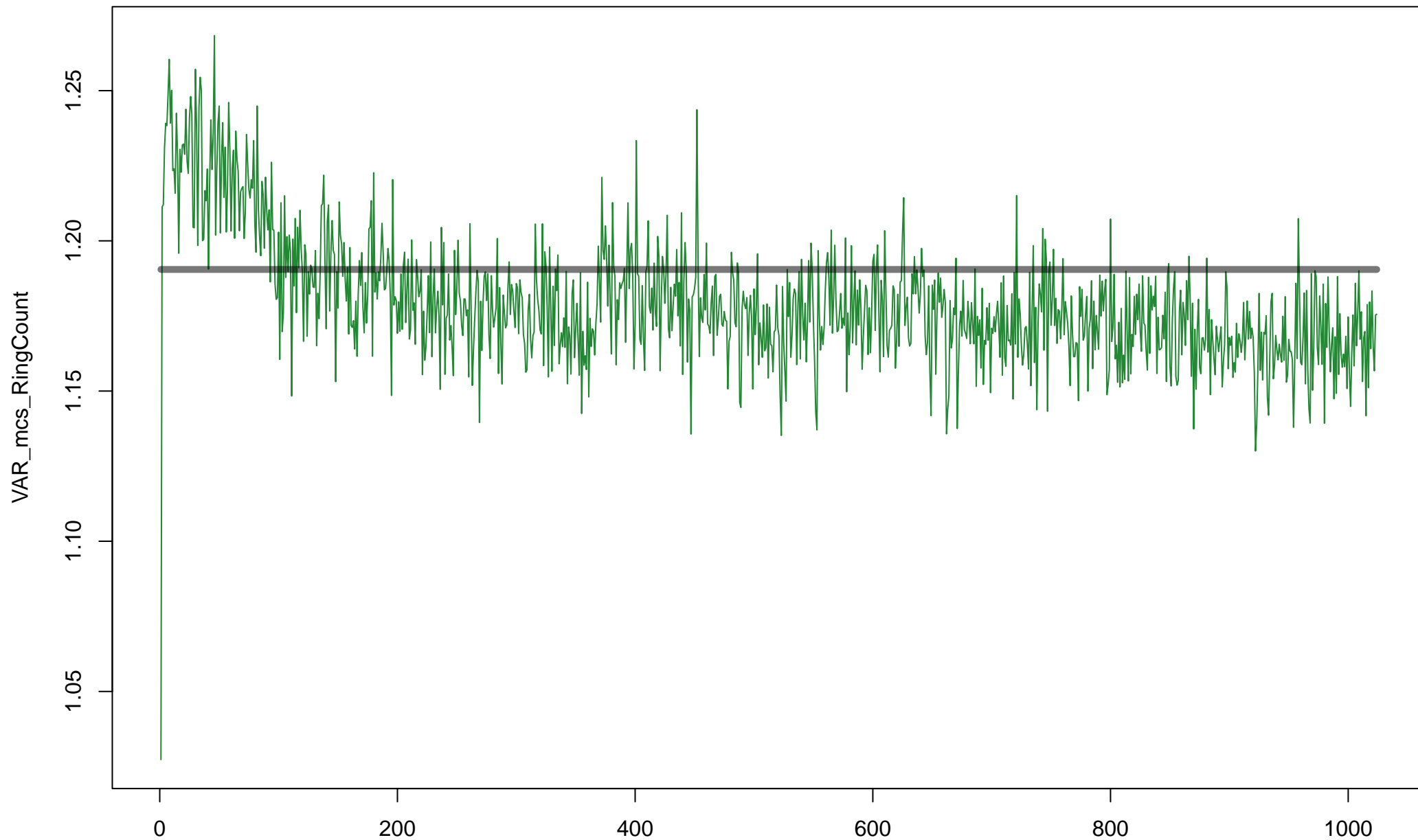


VAR_docked_HeavyAtomCount

ESS = 1020 | BMK = 0.143 | MCSE(6.27) = 3.82 | stat: TRUE | burn: 0 | percentile: 97.5

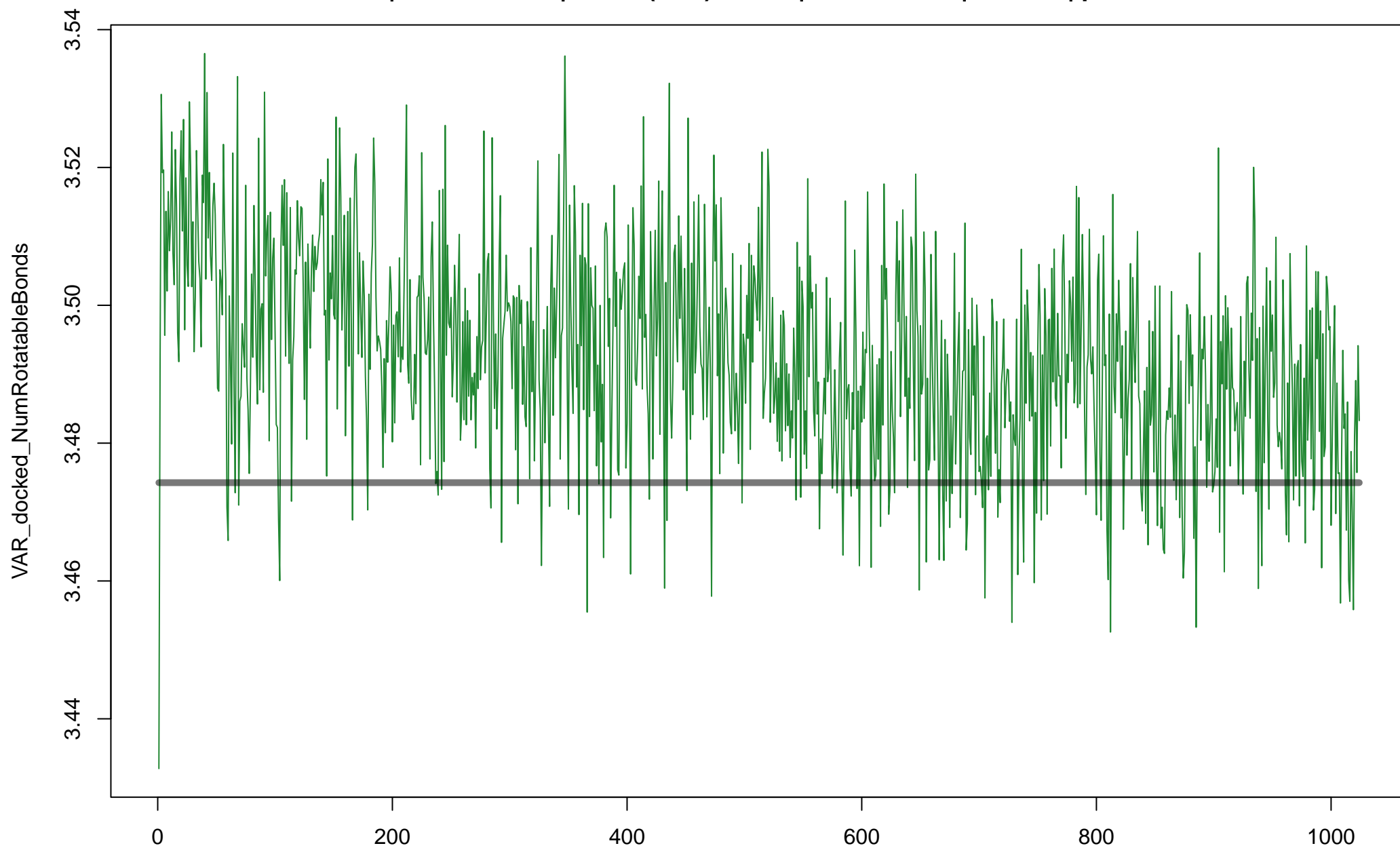


VAR_mcs_RingCount
ESS = 10.9 | BMK = 0.346 | MCSE(6.27) = 12.6 | stat: FALSE | burn: 102 | percentile: 77.9



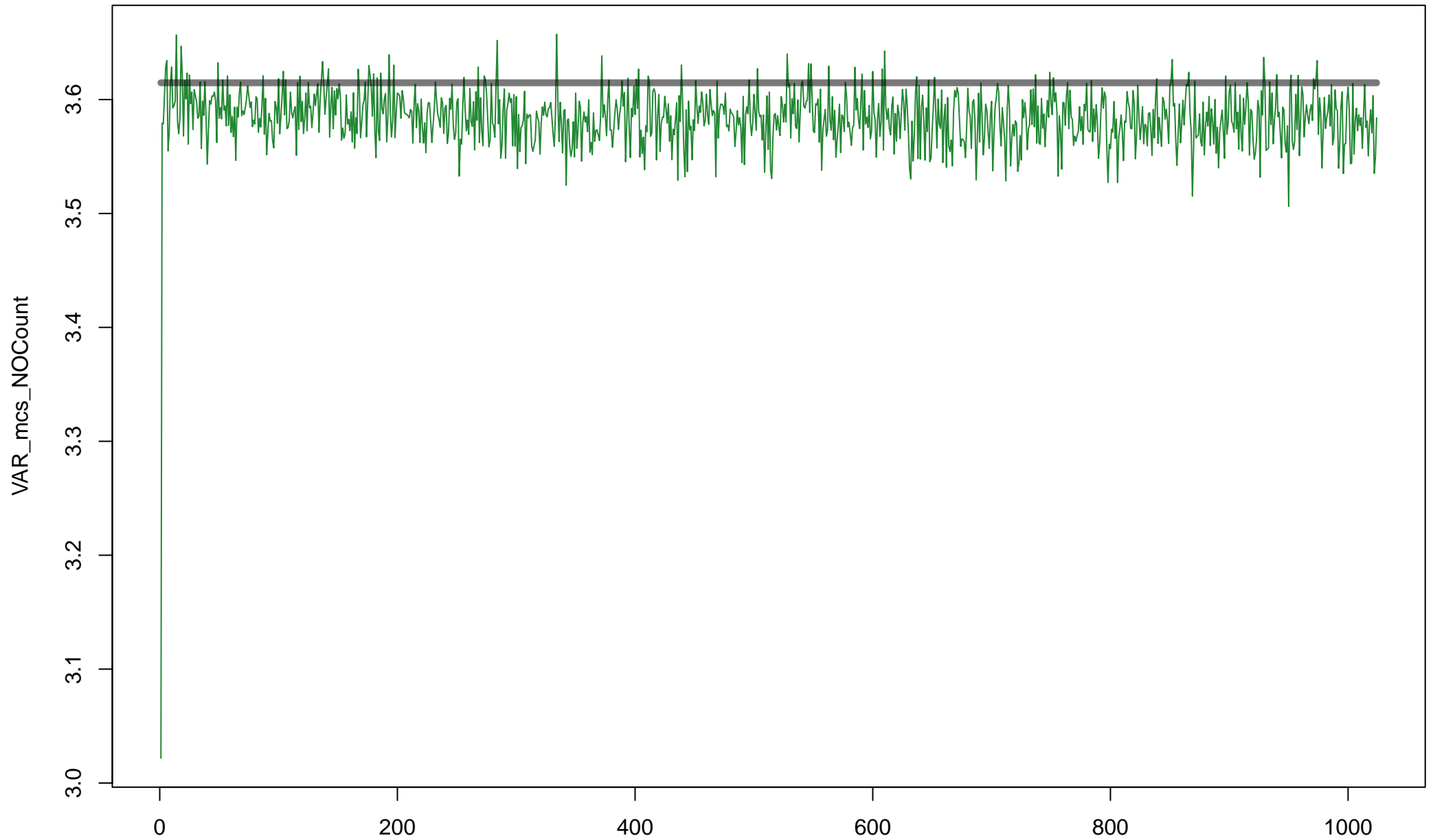
VAR_docked_NumRotatableBonds

ESS = 45.9 | BMK = 0.269 | MCSE(6.27) = 7.93 | stat: FALSE | burn: 0 | percentile: 11.8

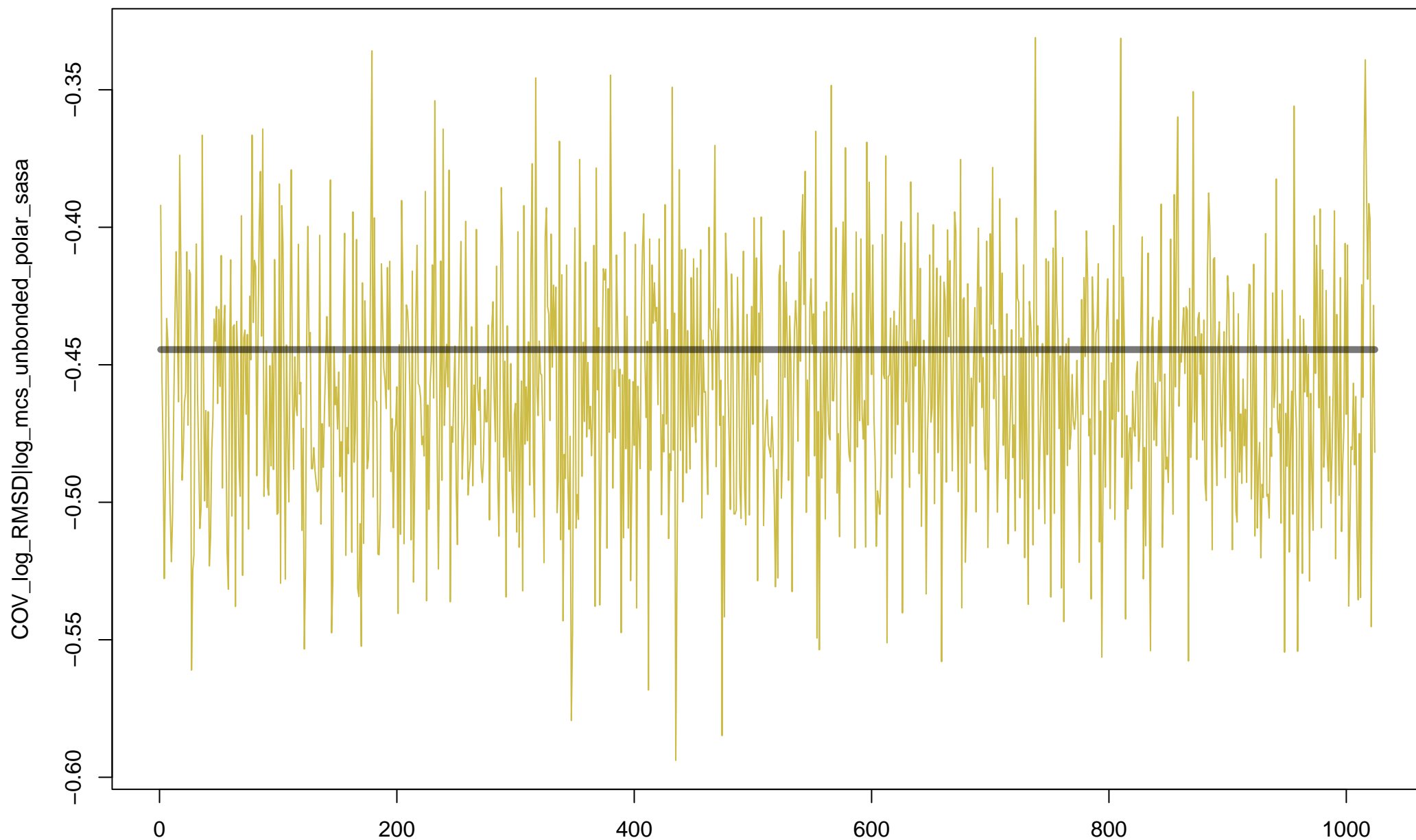


VAR_mcs_NOCount

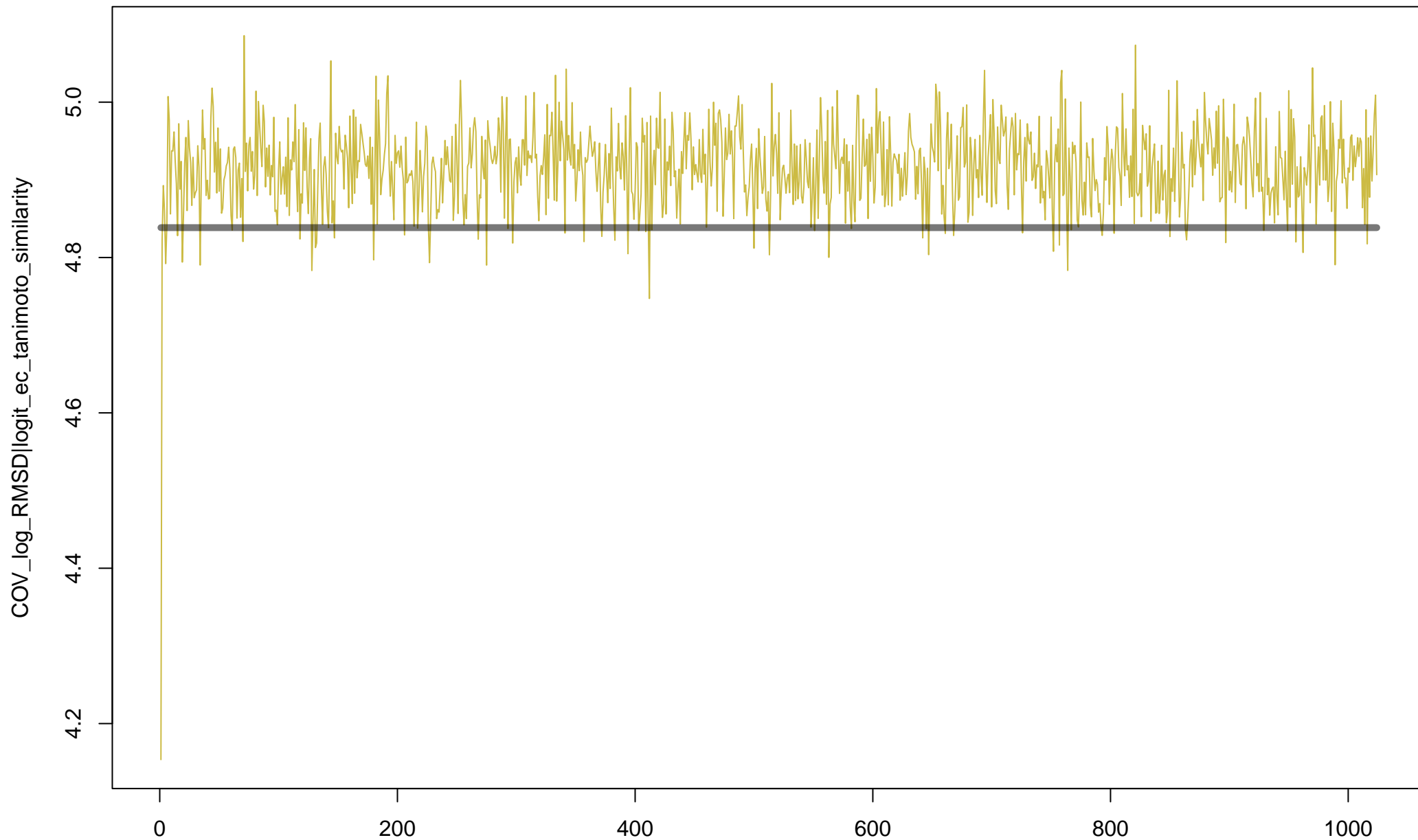
ESS = 933 | BMK = 0.0977 | MCSE(6.27) = 3.53 | stat: TRUE | burn: 0 | percentile: 91.4



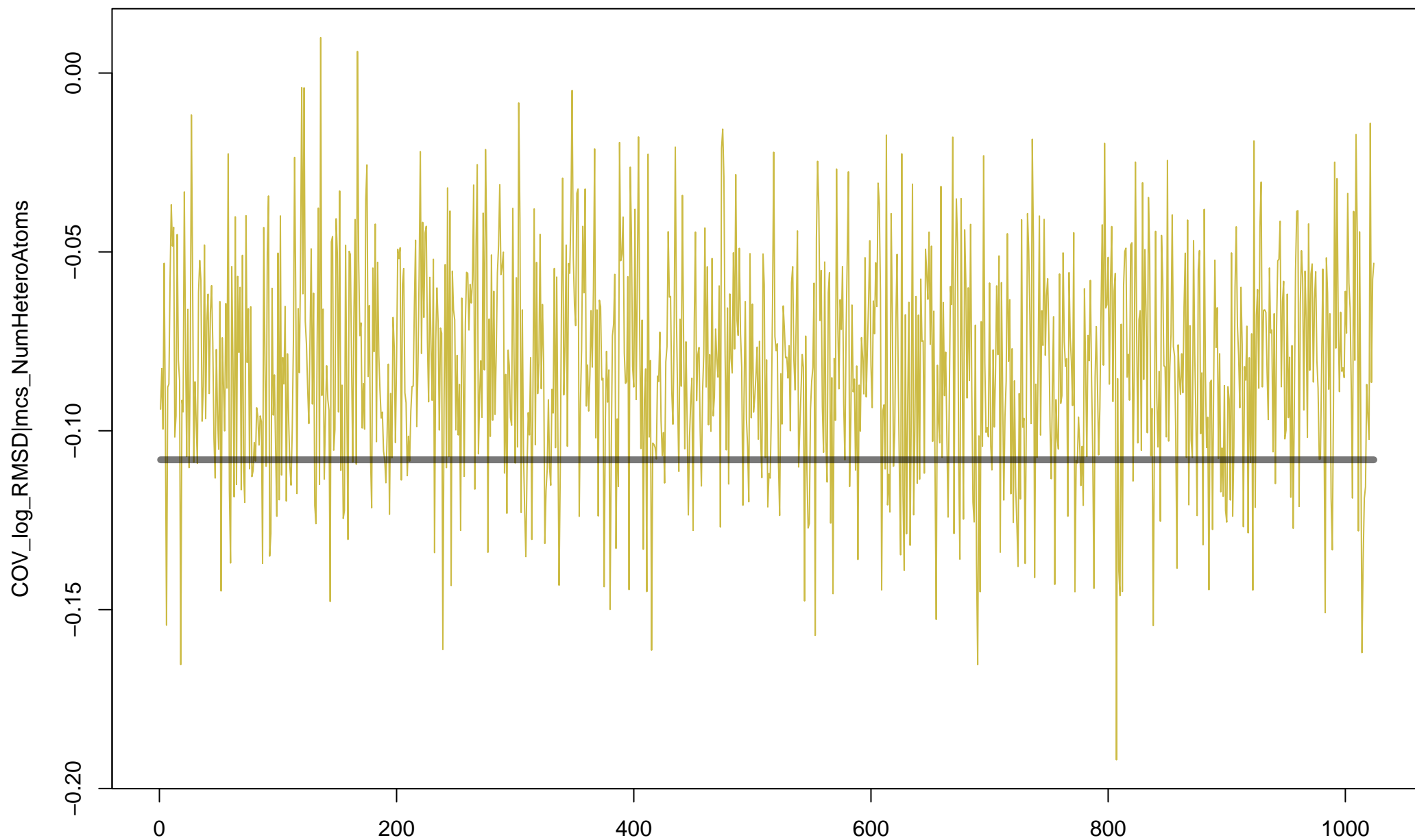
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0495 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0 | percentile: 63.6



COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 783 | BMK = 0.0635 | MCSE(6.27) = 4.14 | stat: TRUE | burn: 0 | percentile: 5.66

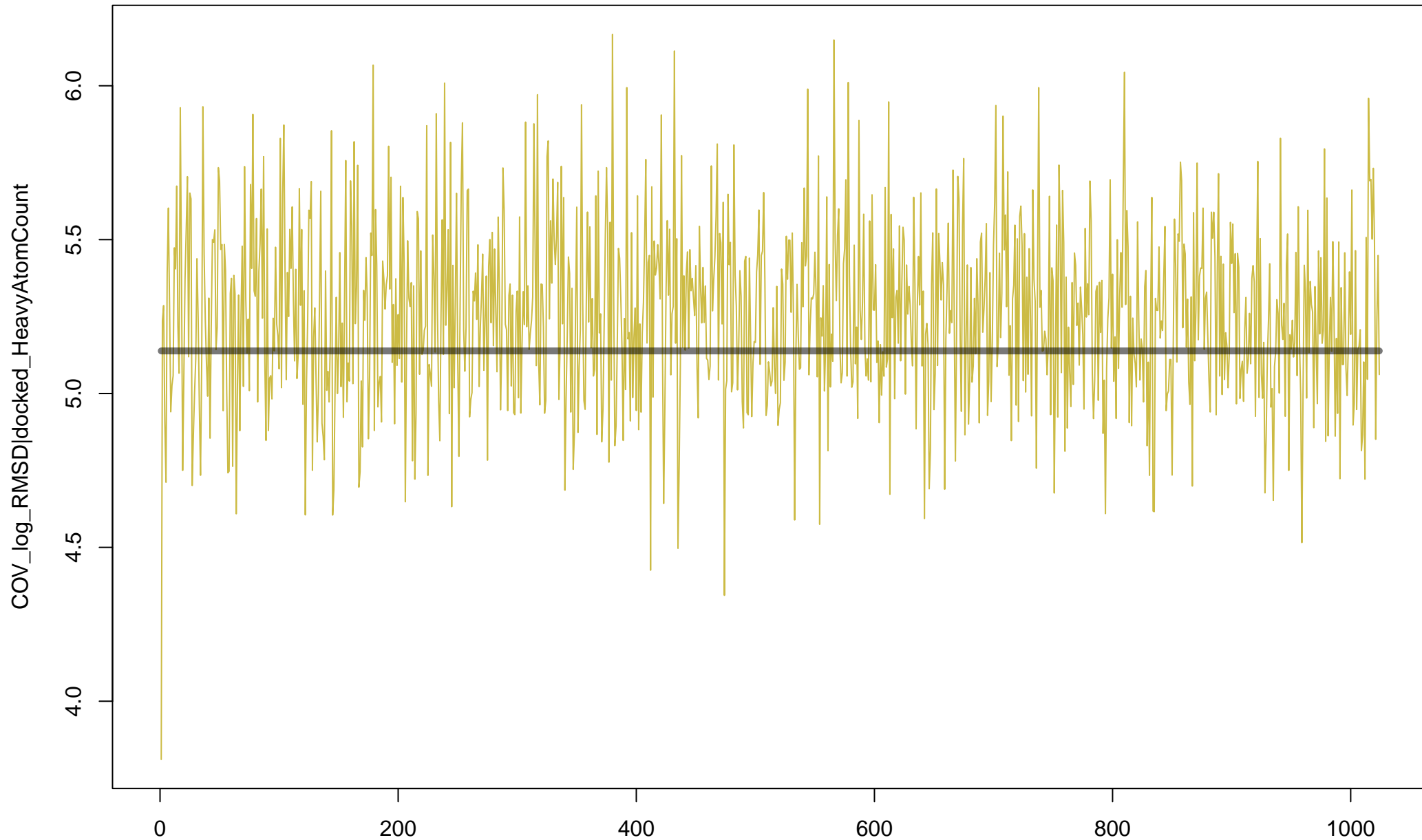


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 742 | BMK = 0.0686 | MCSE(6.27) = 2.9 | stat: TRUE | burn: 0 | percentile: 18.8

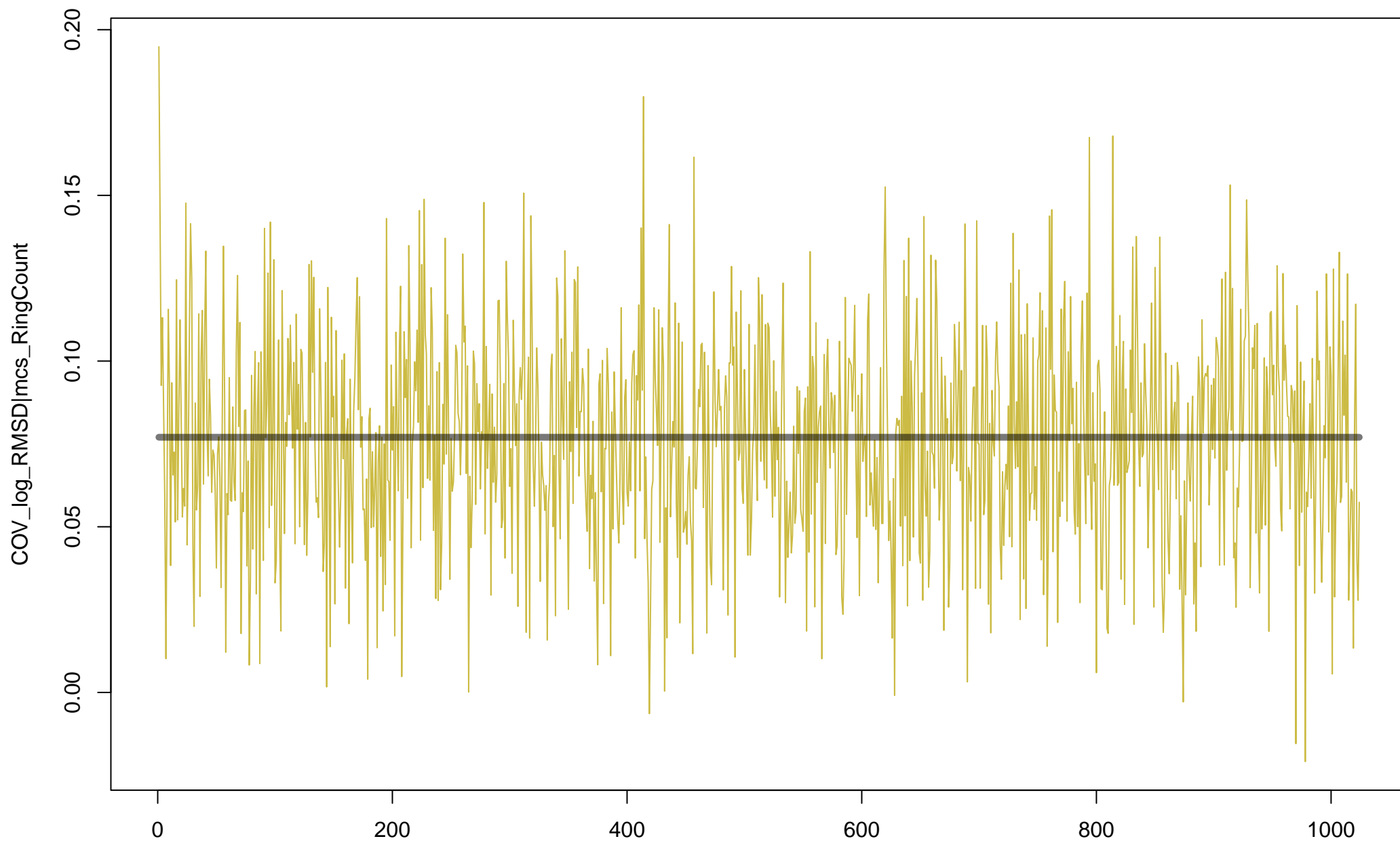


COV_log_RMSD|docked_HeavyAtomCount

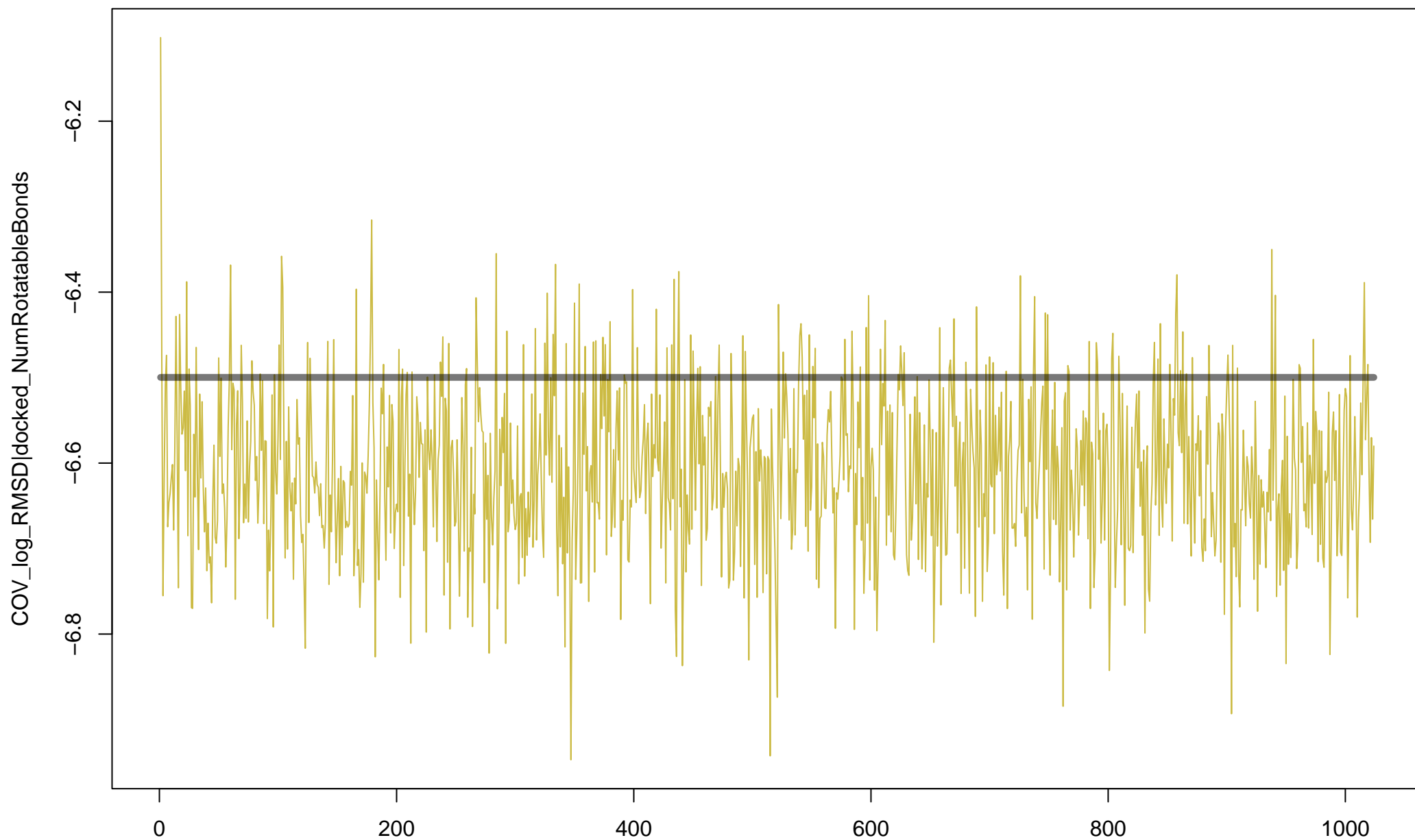
ESS = 1020 | BMK = 0.0776 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0 | percentile: 35.6



COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0454 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0 | percentile: 50.9

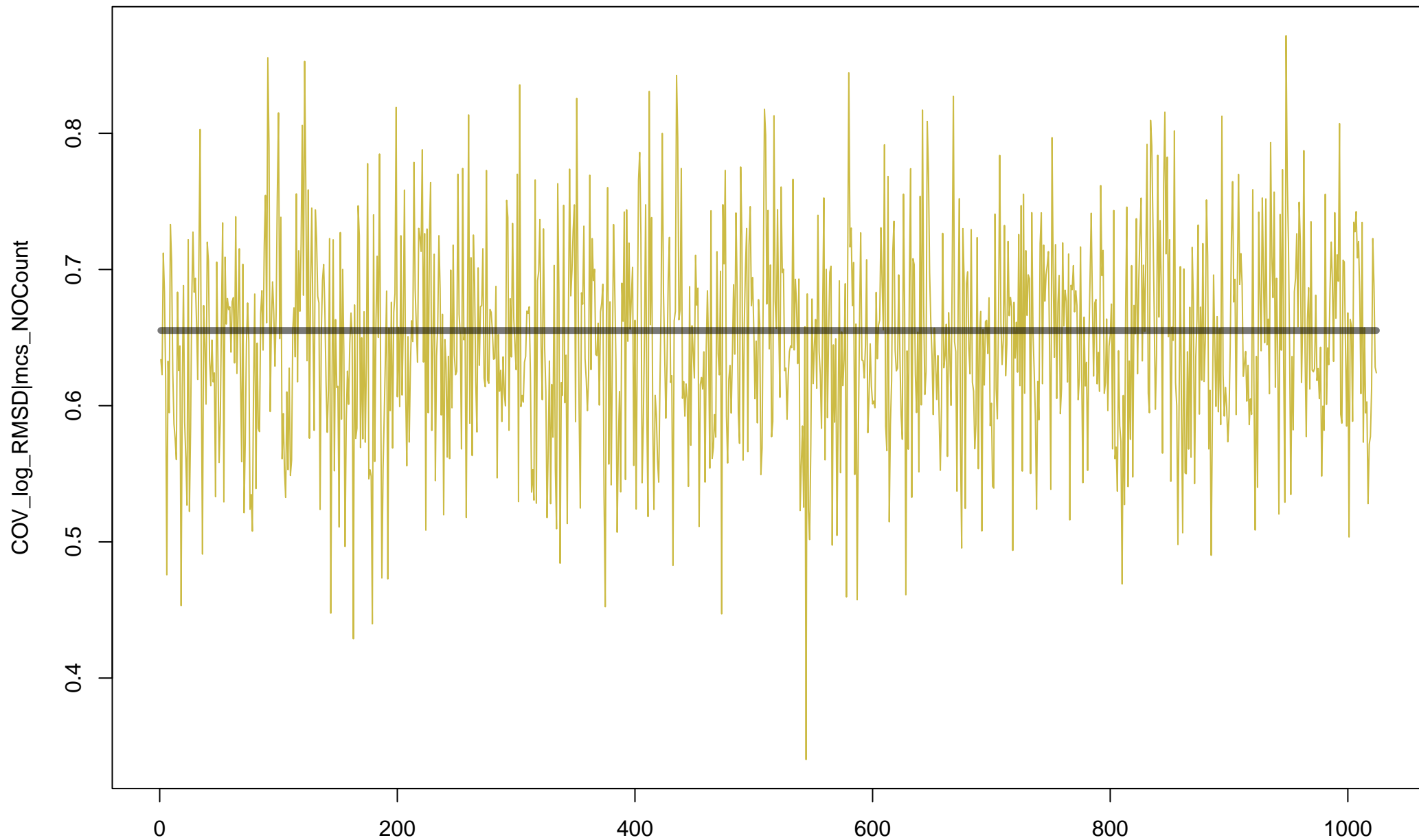


COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0594 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0 | percentile: 86.4

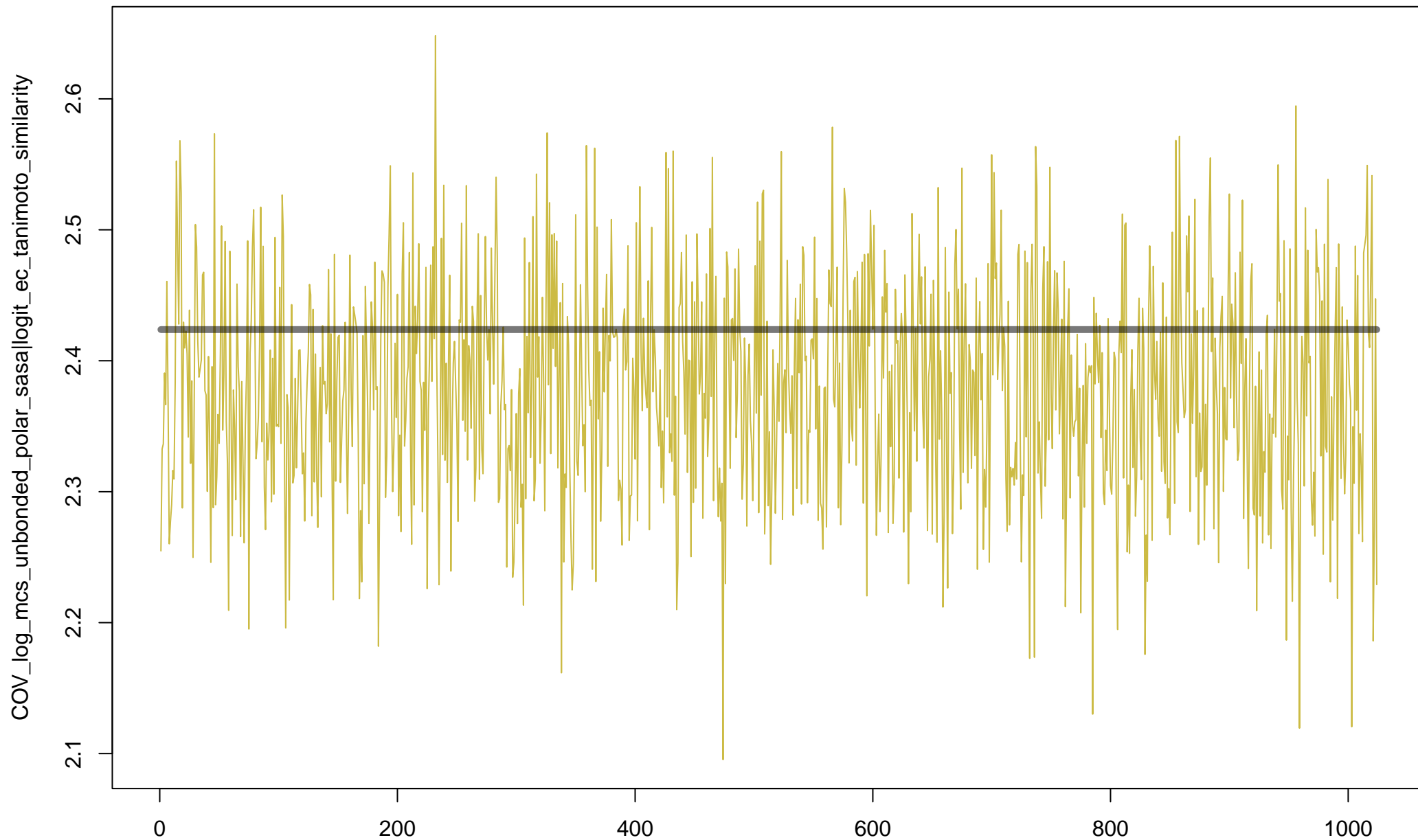


COV_log_RMSD|mcs_NOCount

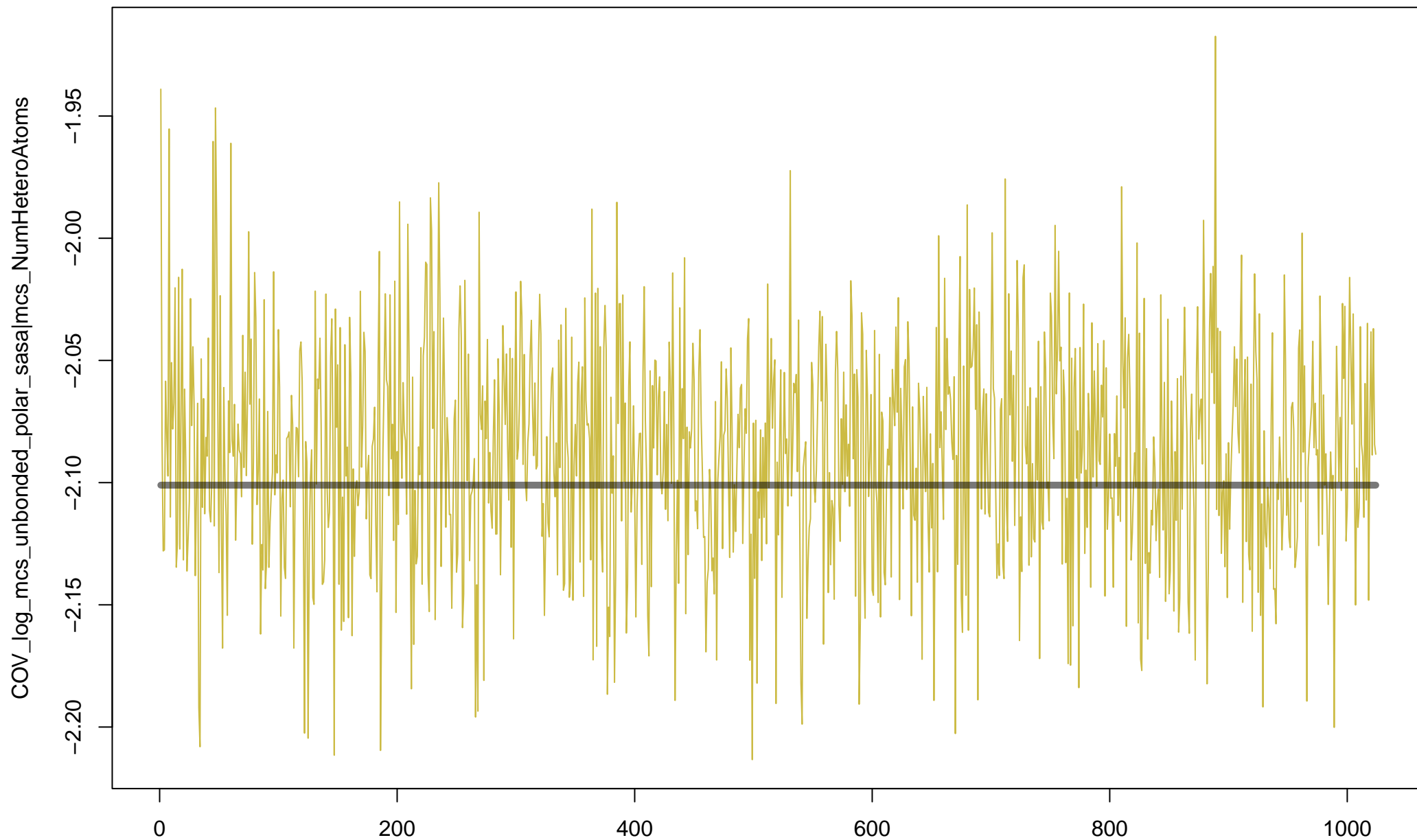
ESS = 611 | BMK = 0.0596 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0 | percentile: 54.3



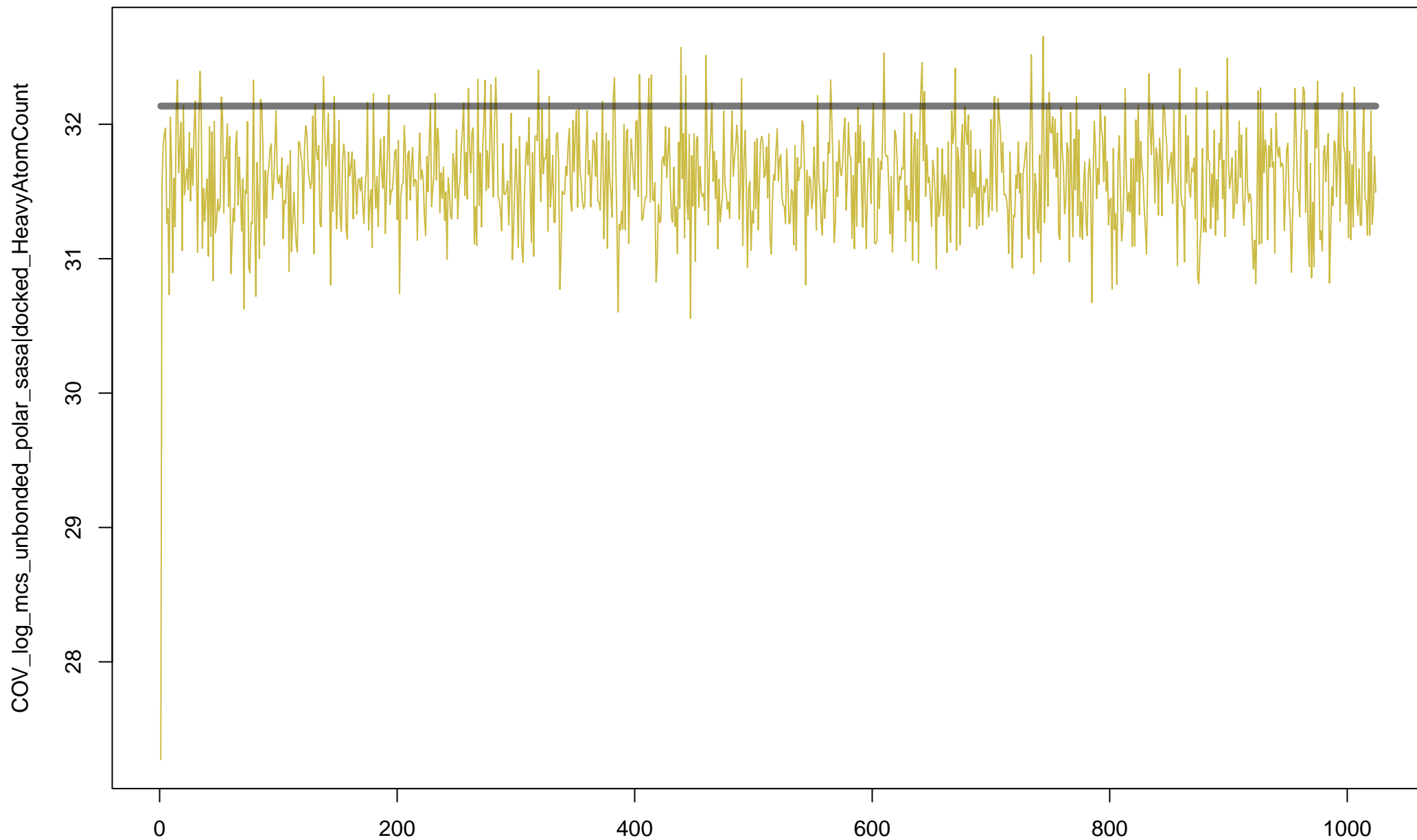
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0473 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | percentile: 70.2



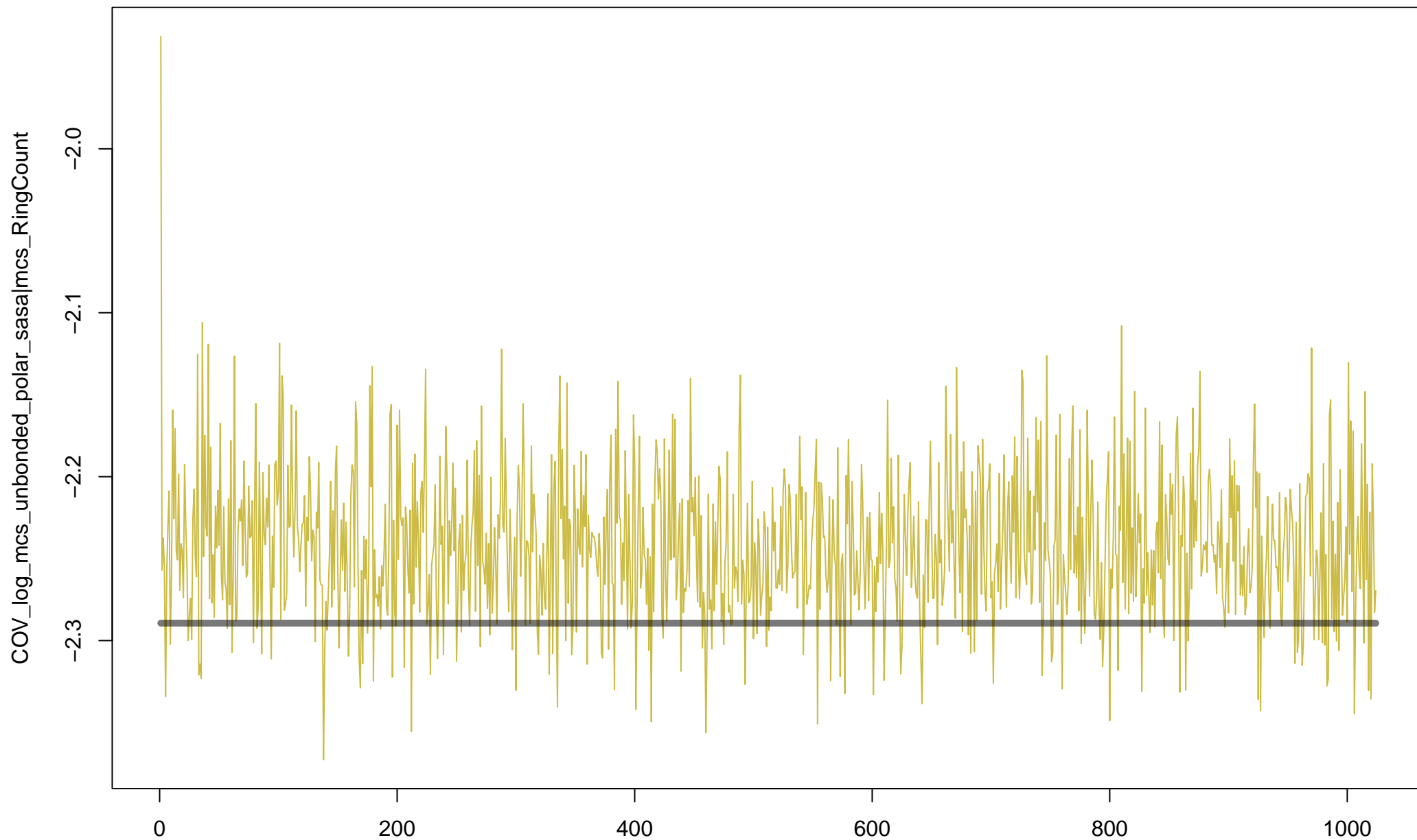
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0535 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | percentile: 37.8



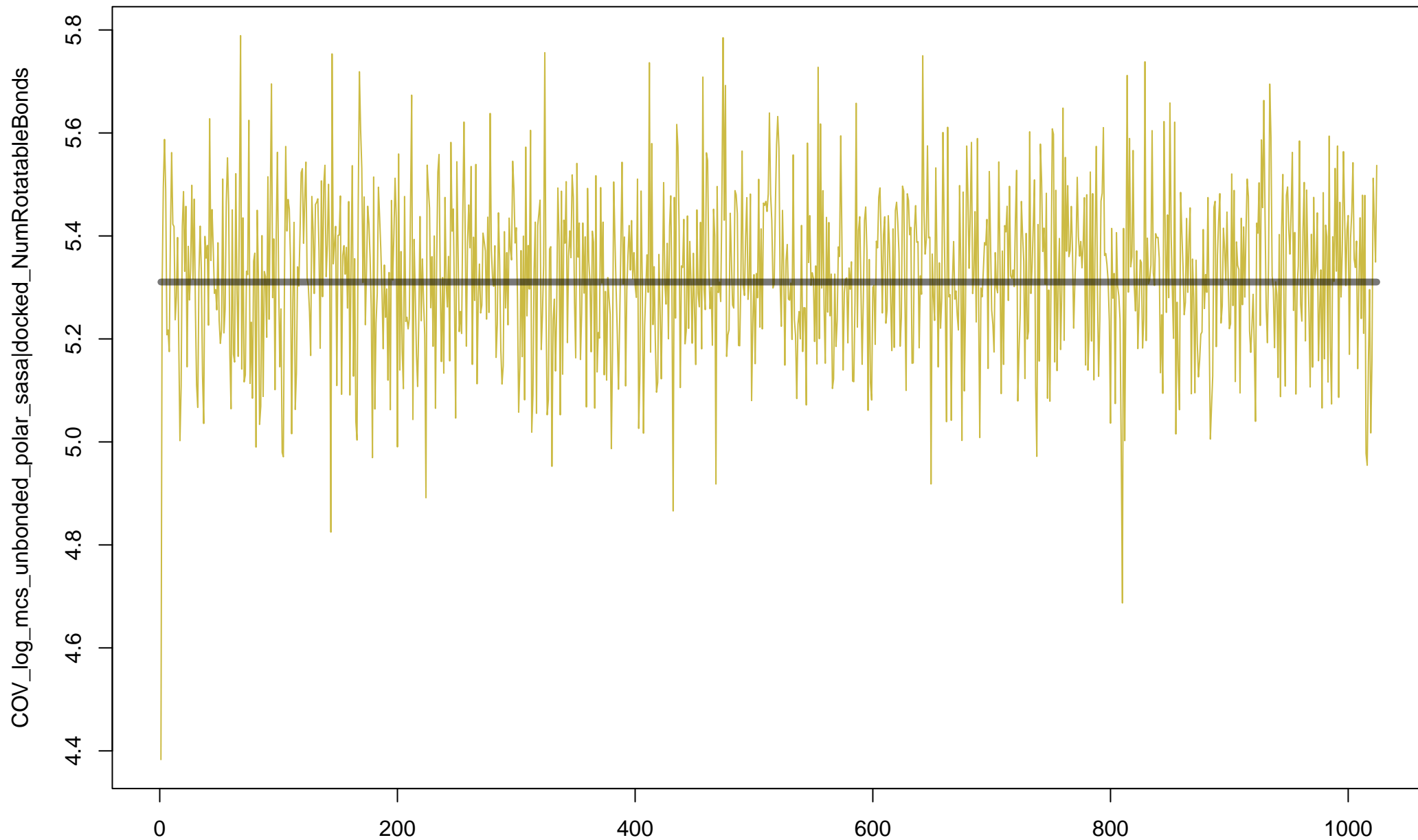
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0567 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0 | percentile: 93.2



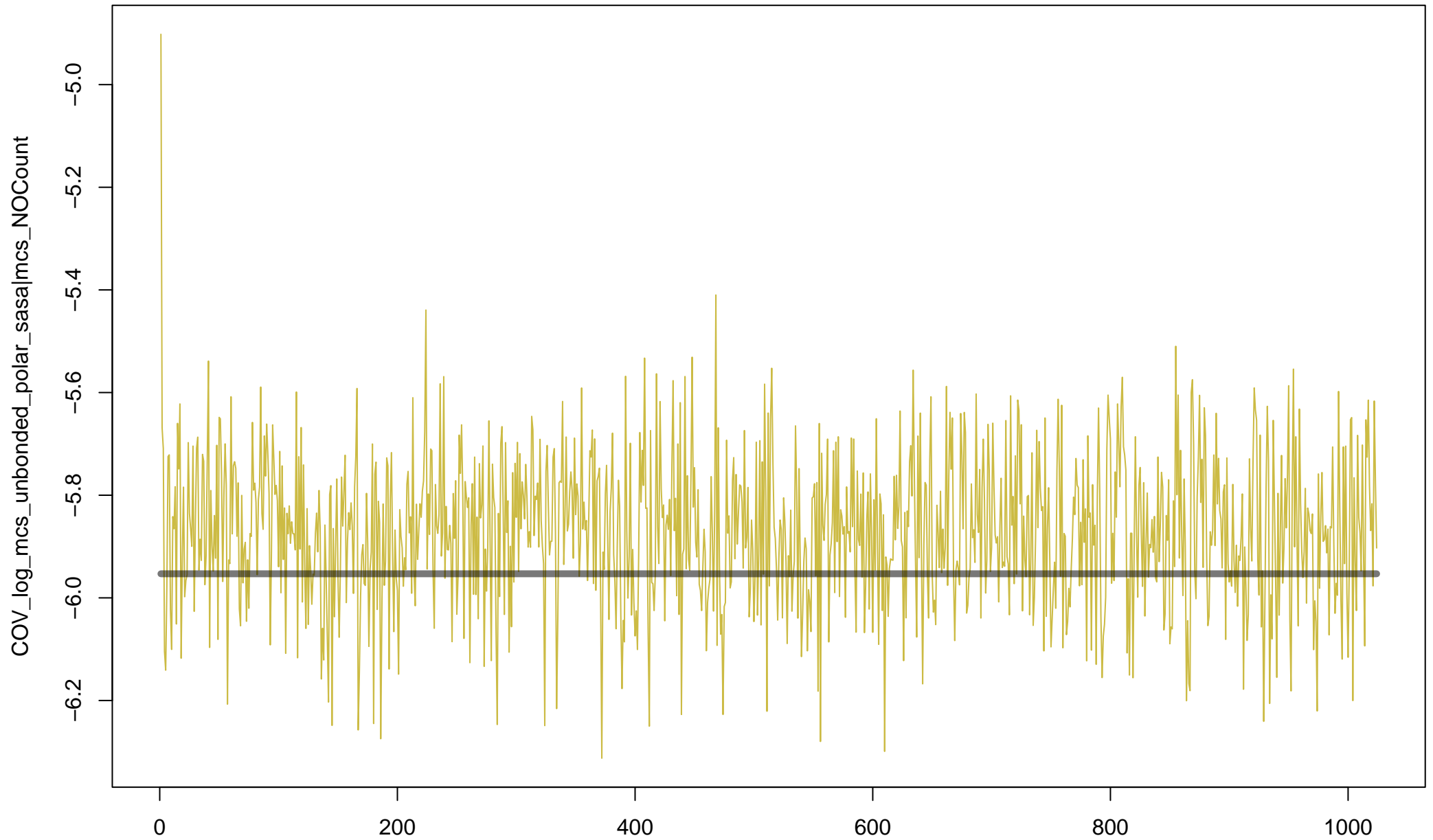
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0563 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0 | percentile: 13.6



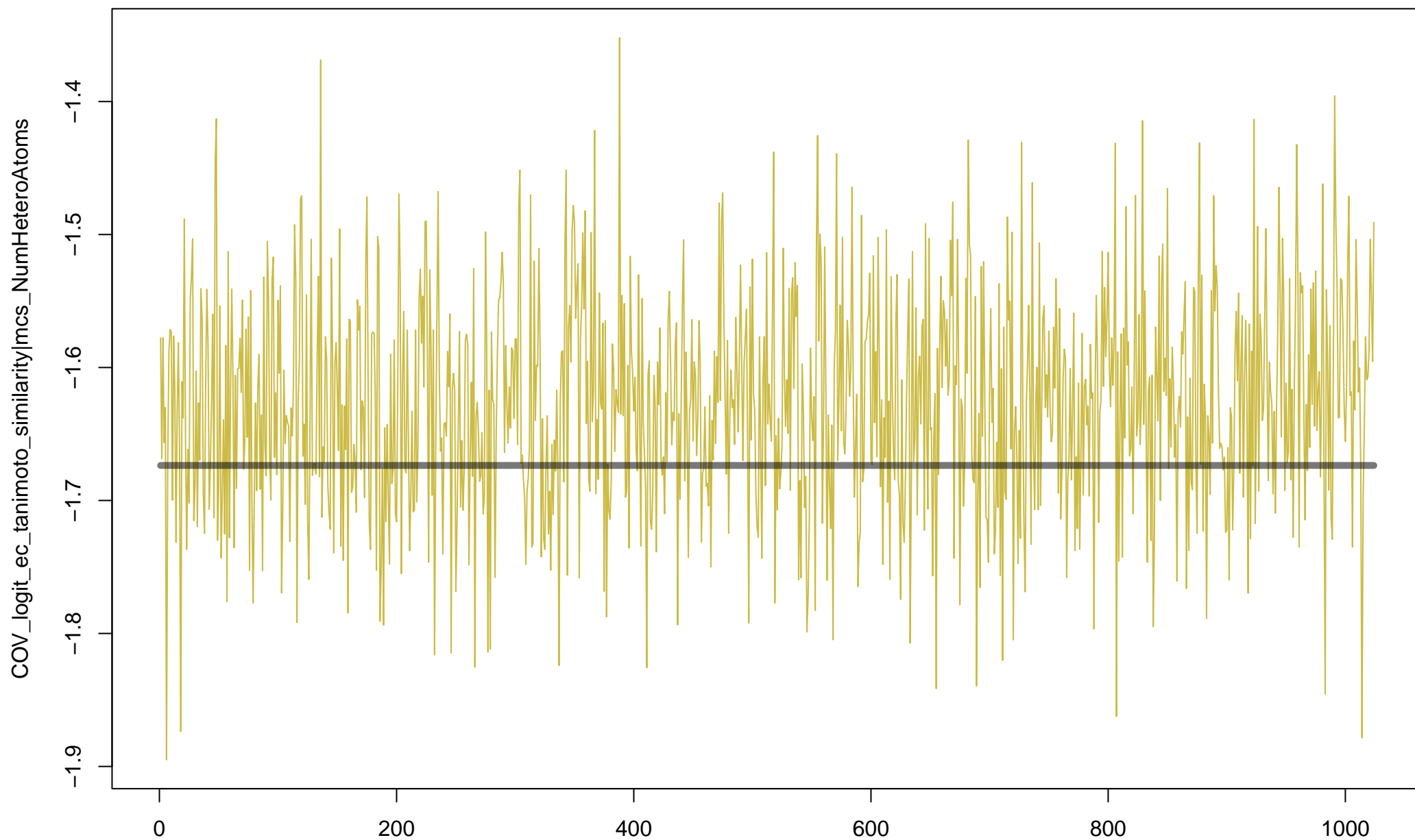
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0691 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0 | percentile: 45.5



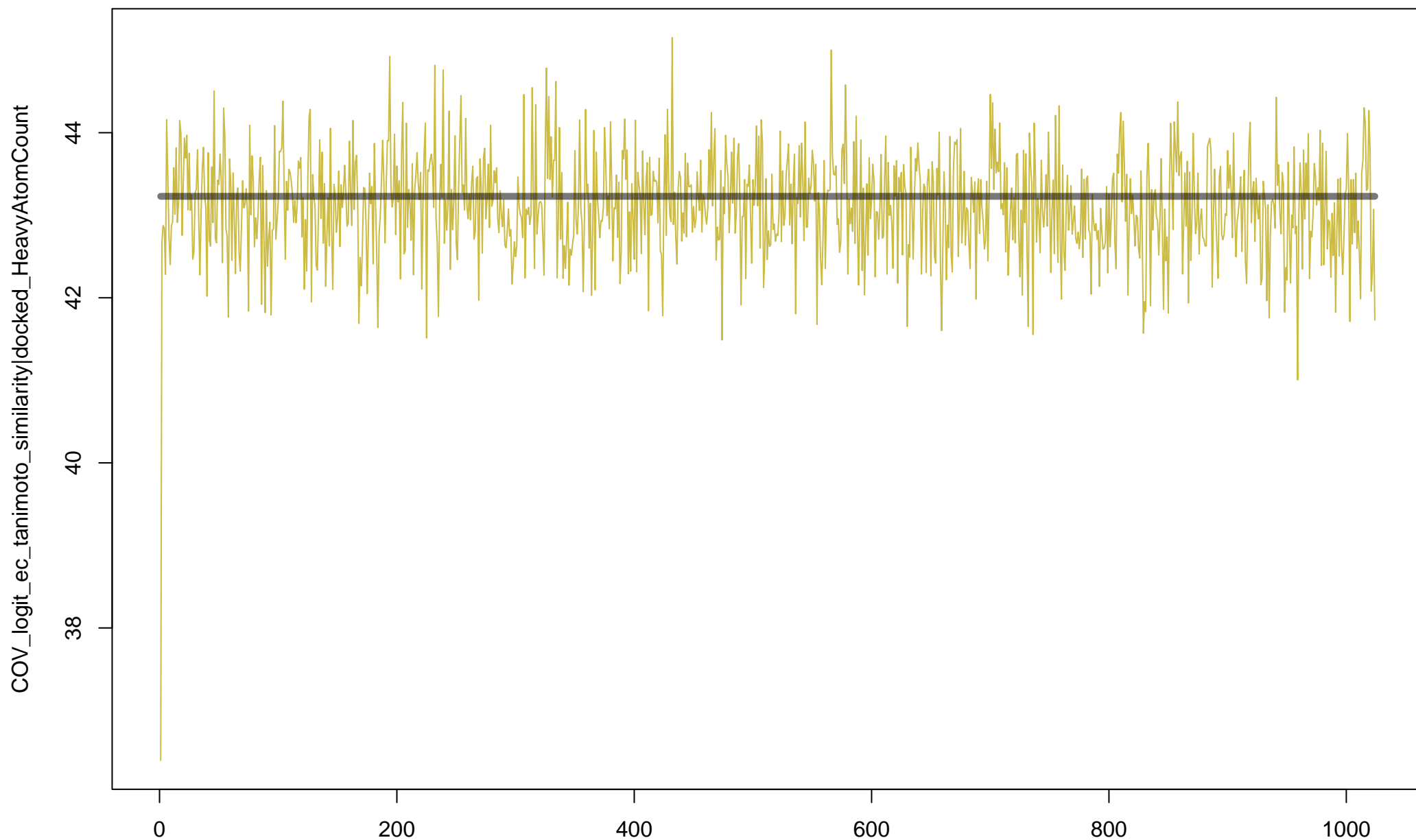
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0747 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0 | percentile: 28



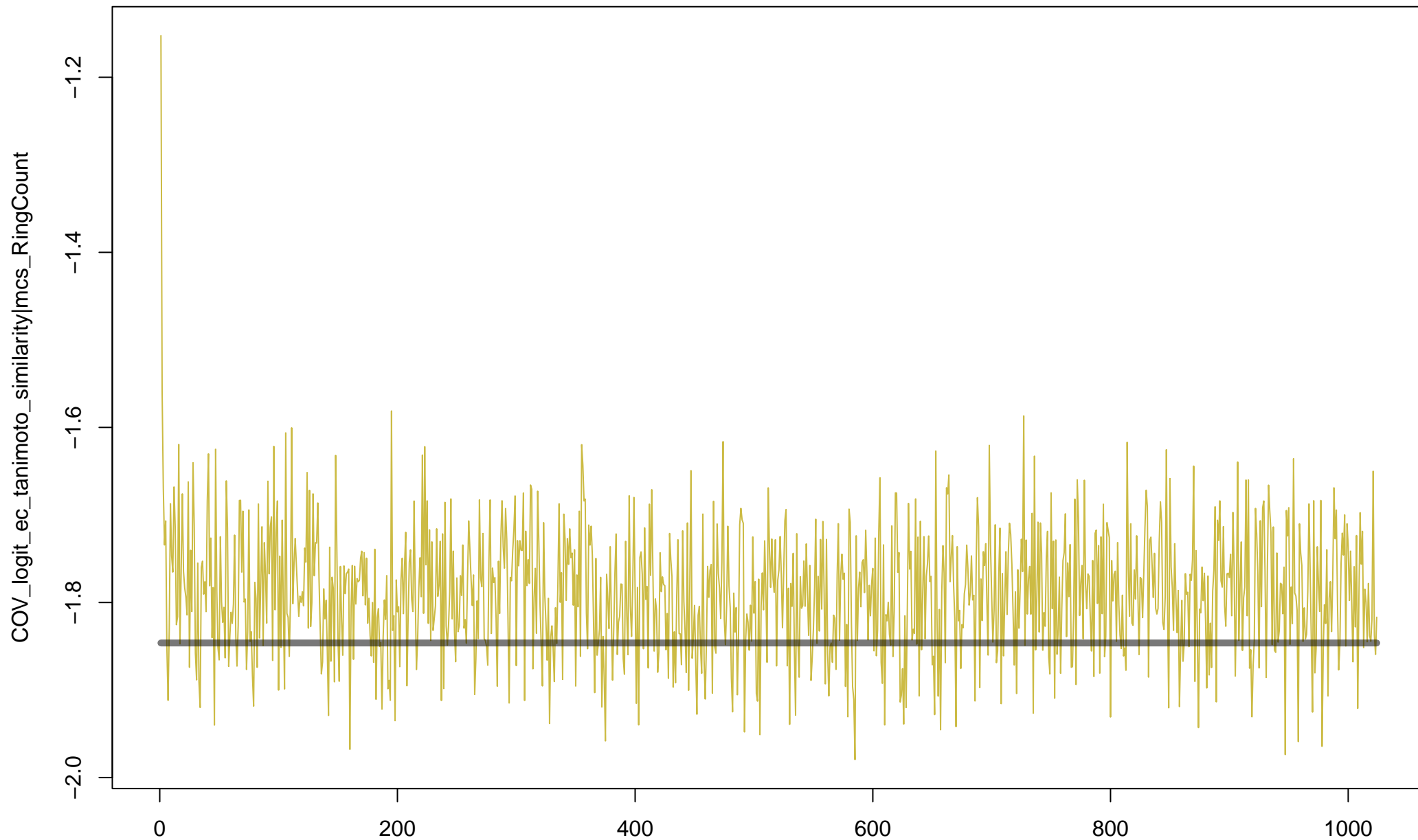
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0618 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0 | percentile: 28.8



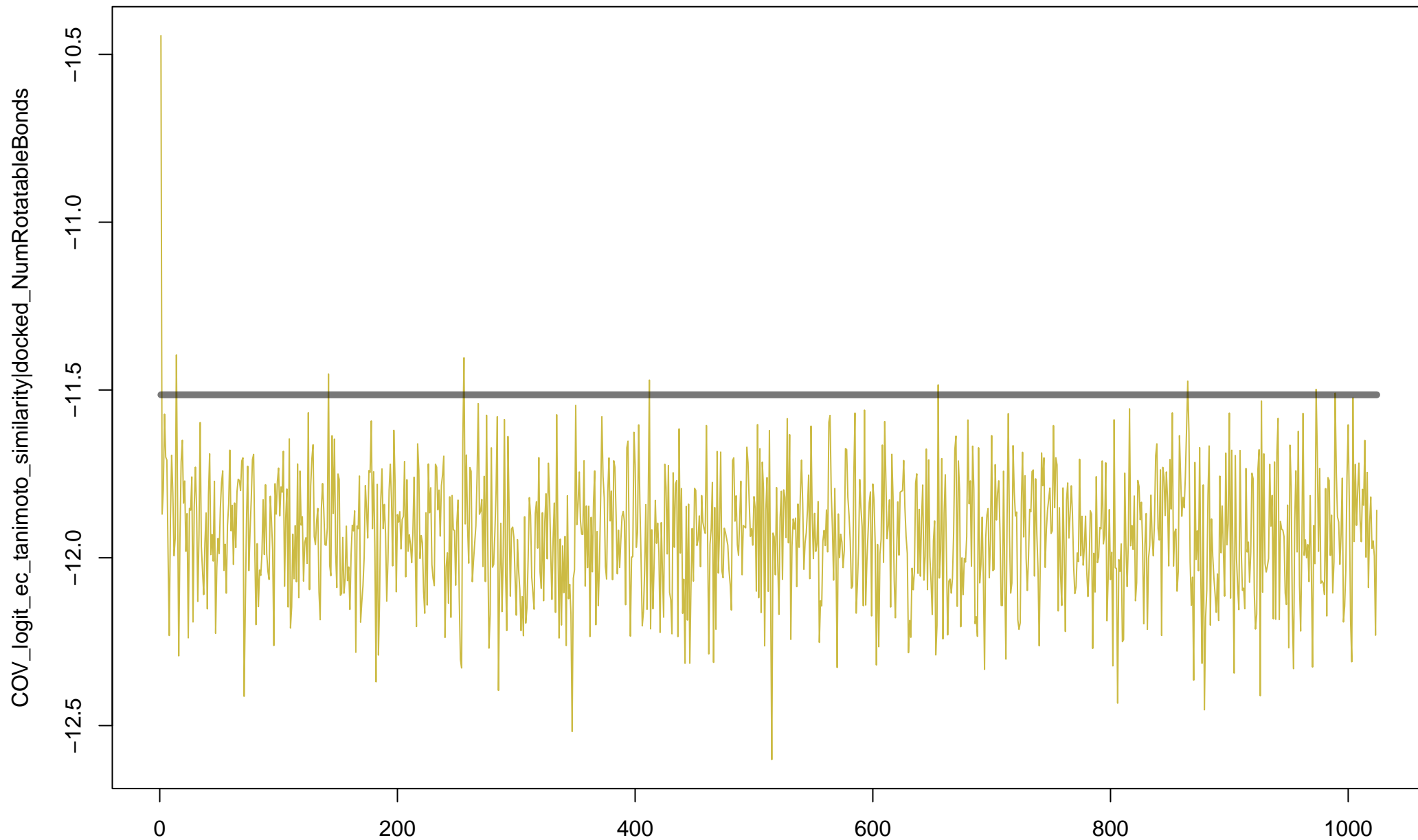
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0712 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 0 | percentile: 57



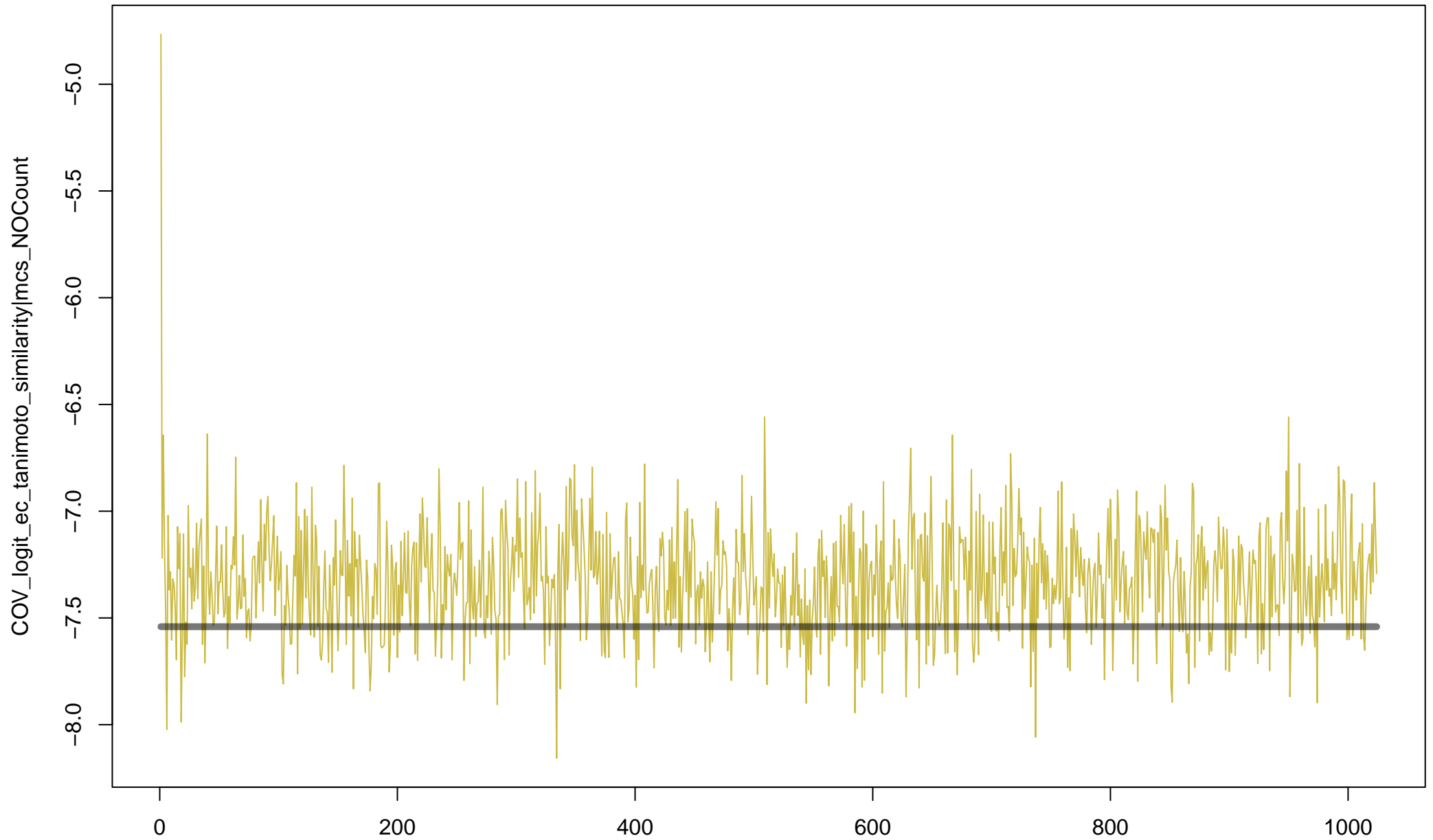
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0535 | MCSE(6.27) = 3.53 | stat: TRUE | burn: 0 | percentile: 22.6



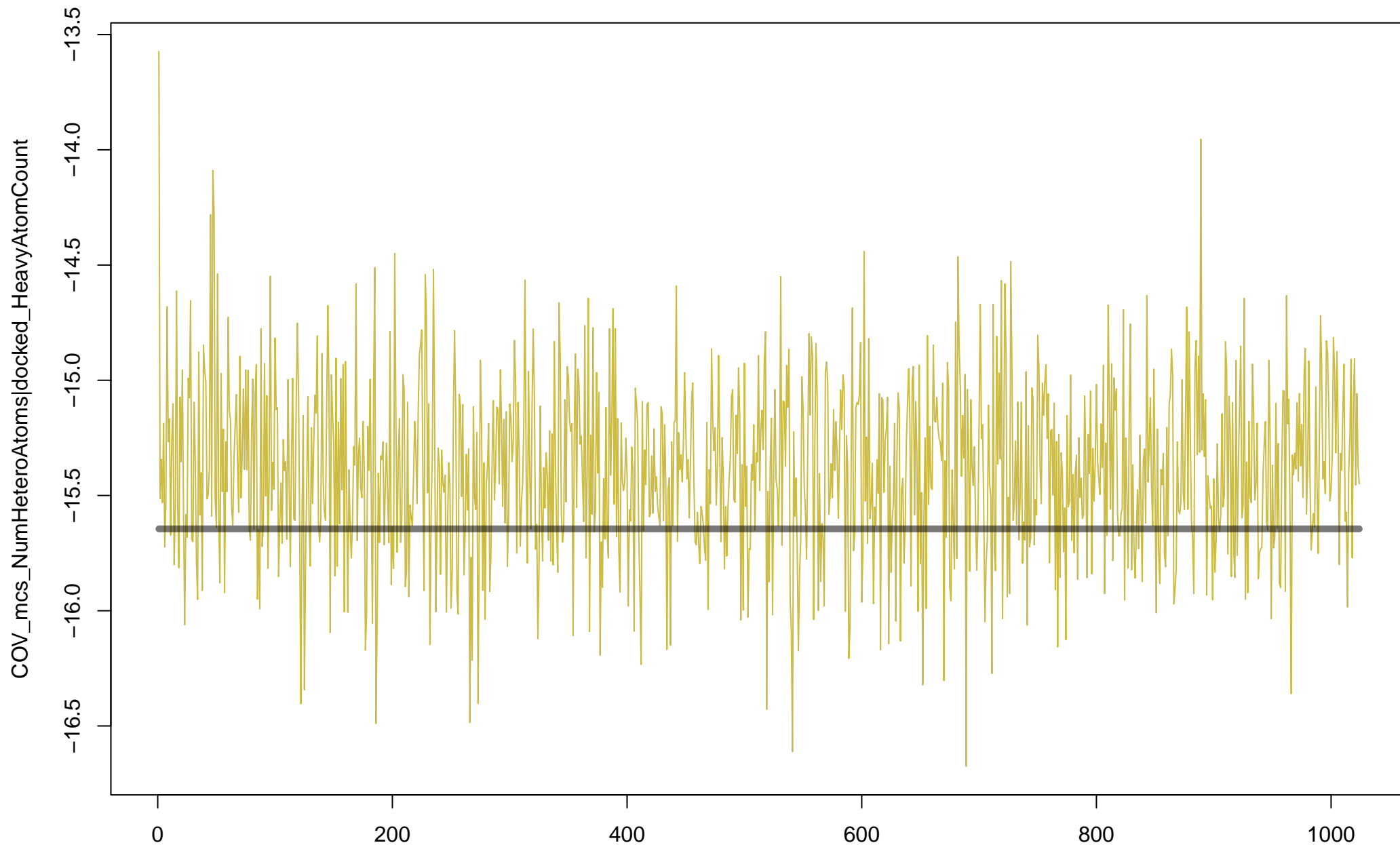
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0602 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0 | percentile: 99.1



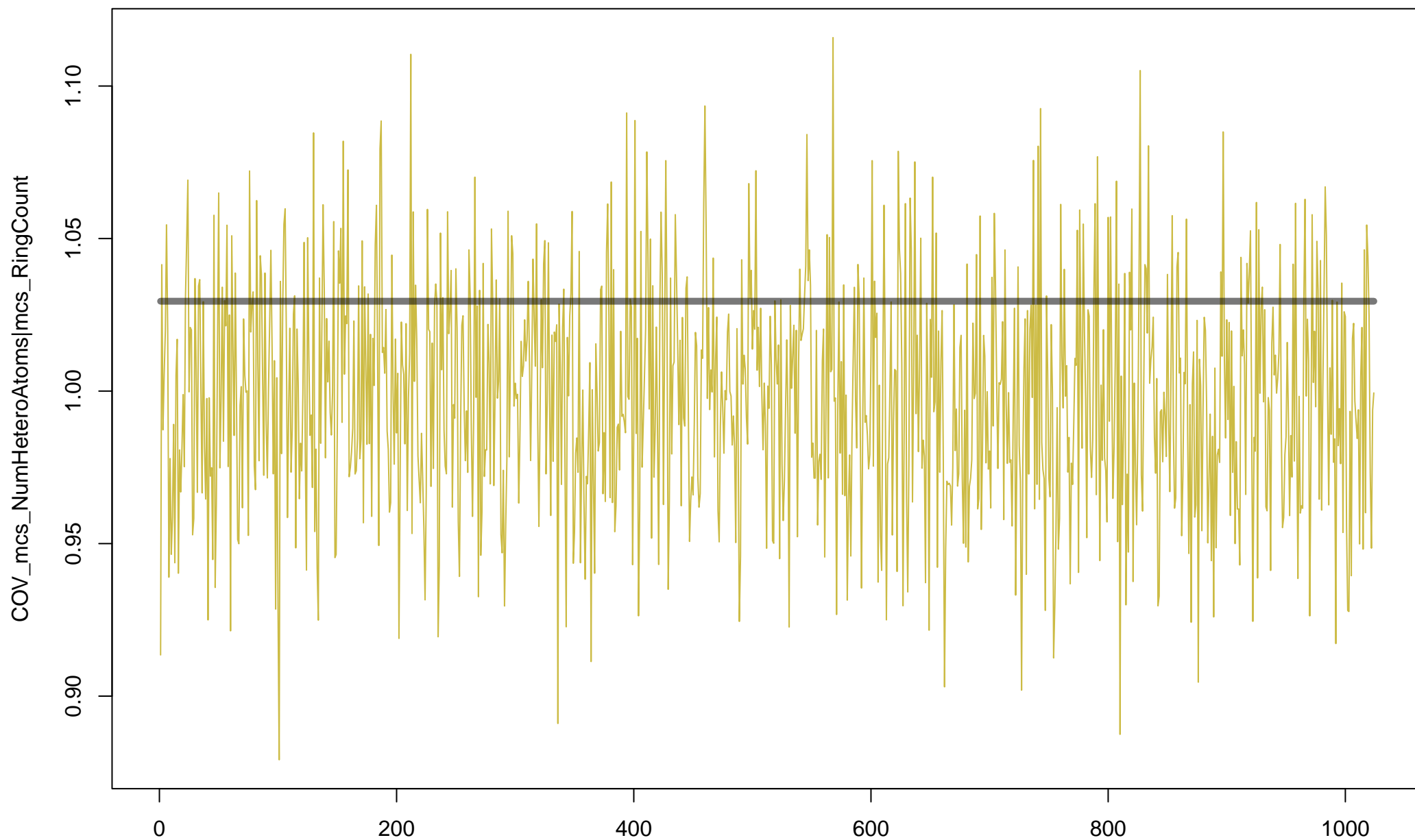
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0419 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | percentile: 19



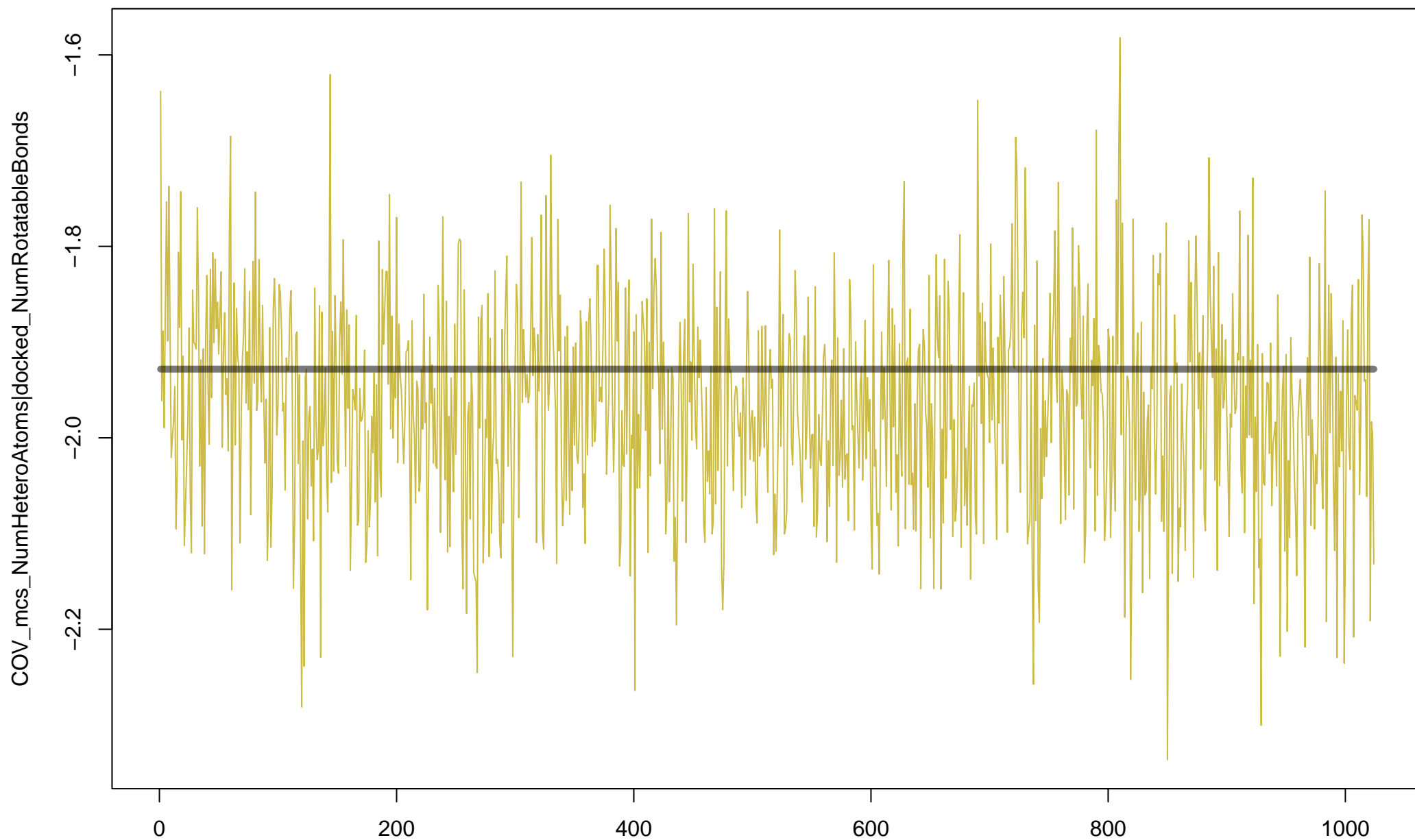
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0571 | MCSE(6.27) = 2.91 | stat: FALSE | burn: 0 | percentile: 24.7



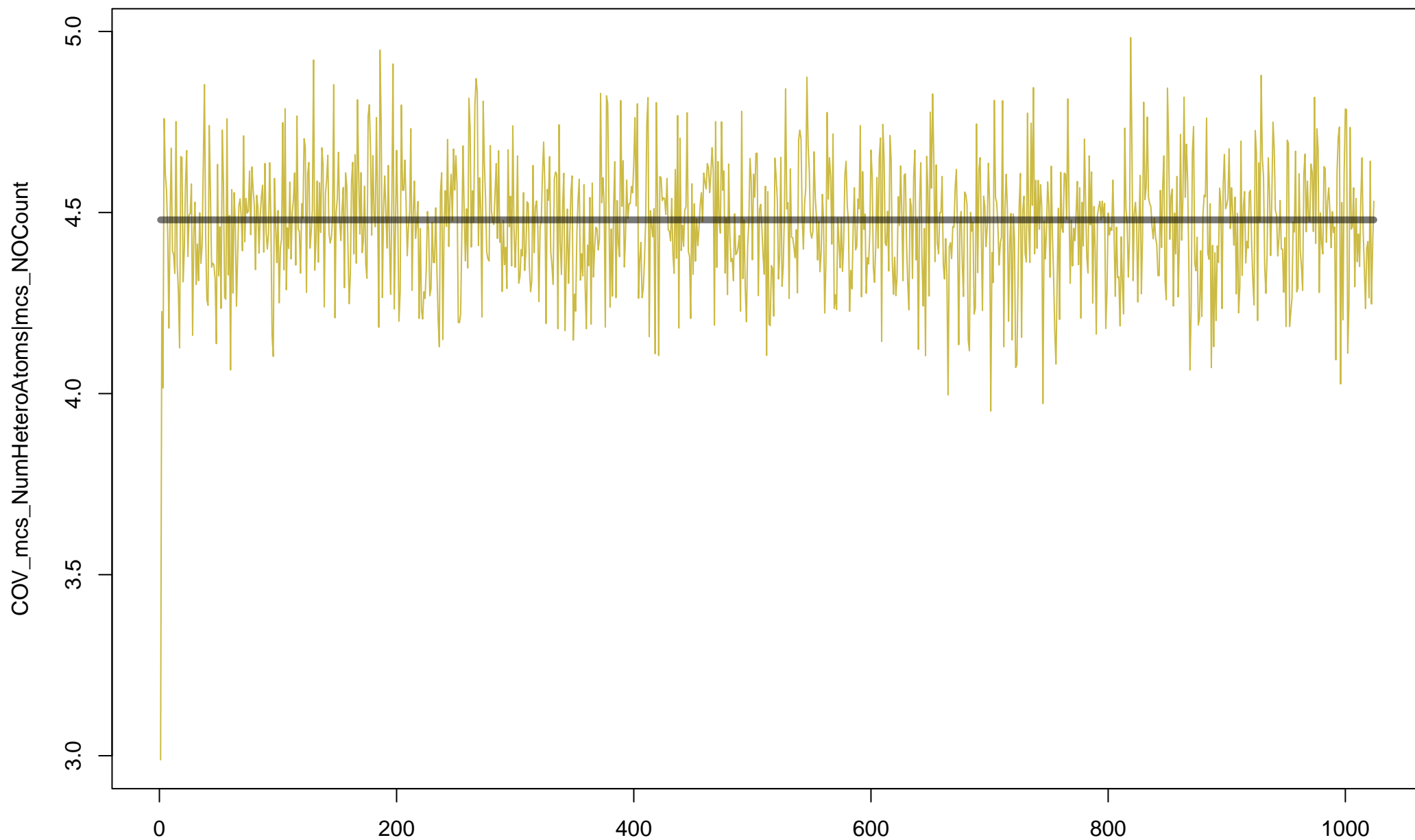
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0505 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | percentile: 80.2



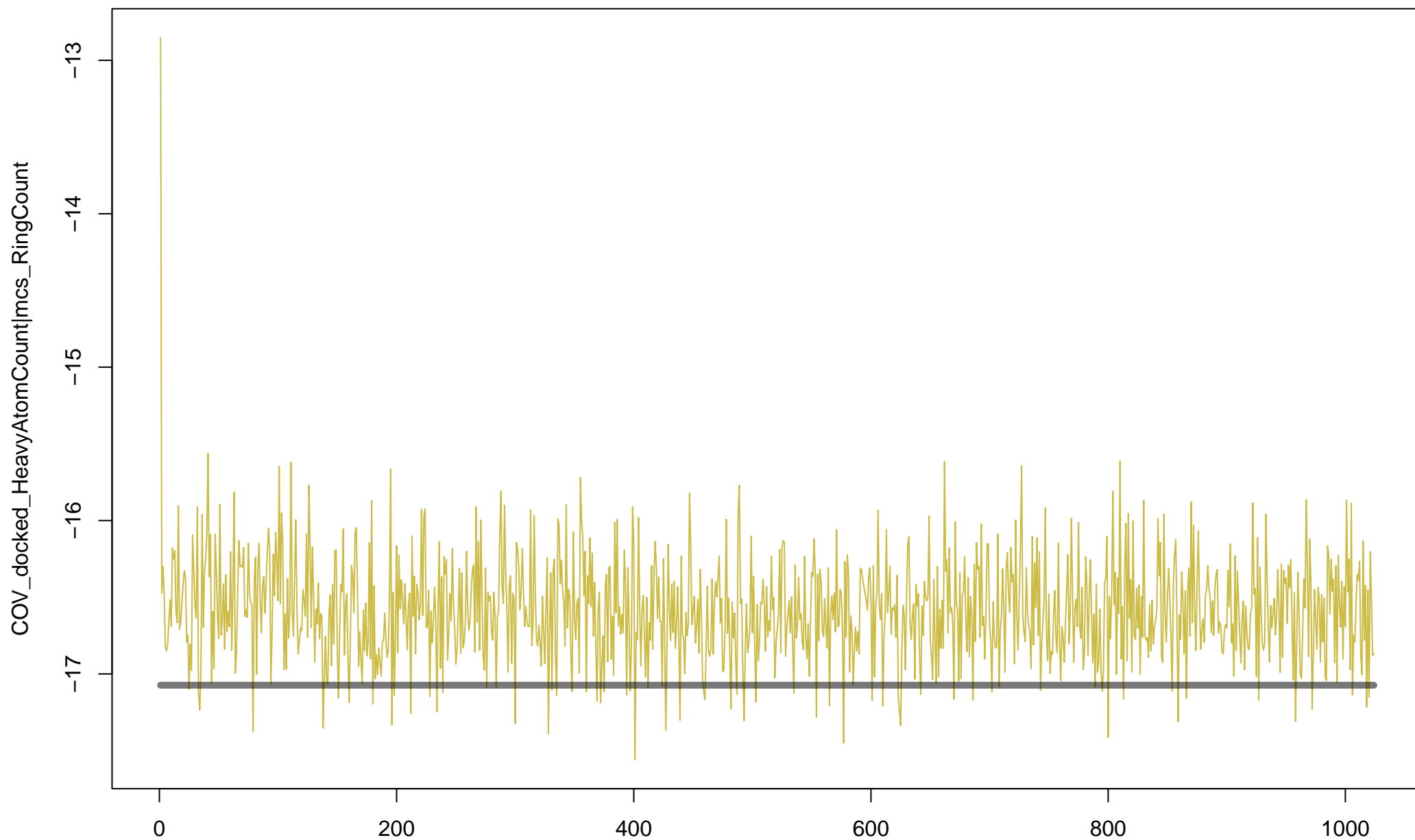
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 912 | BMK = 0.0601 | MCSE(6.27) = 3.95 | stat: FALSE | burn: 0 | percentile: 64.2



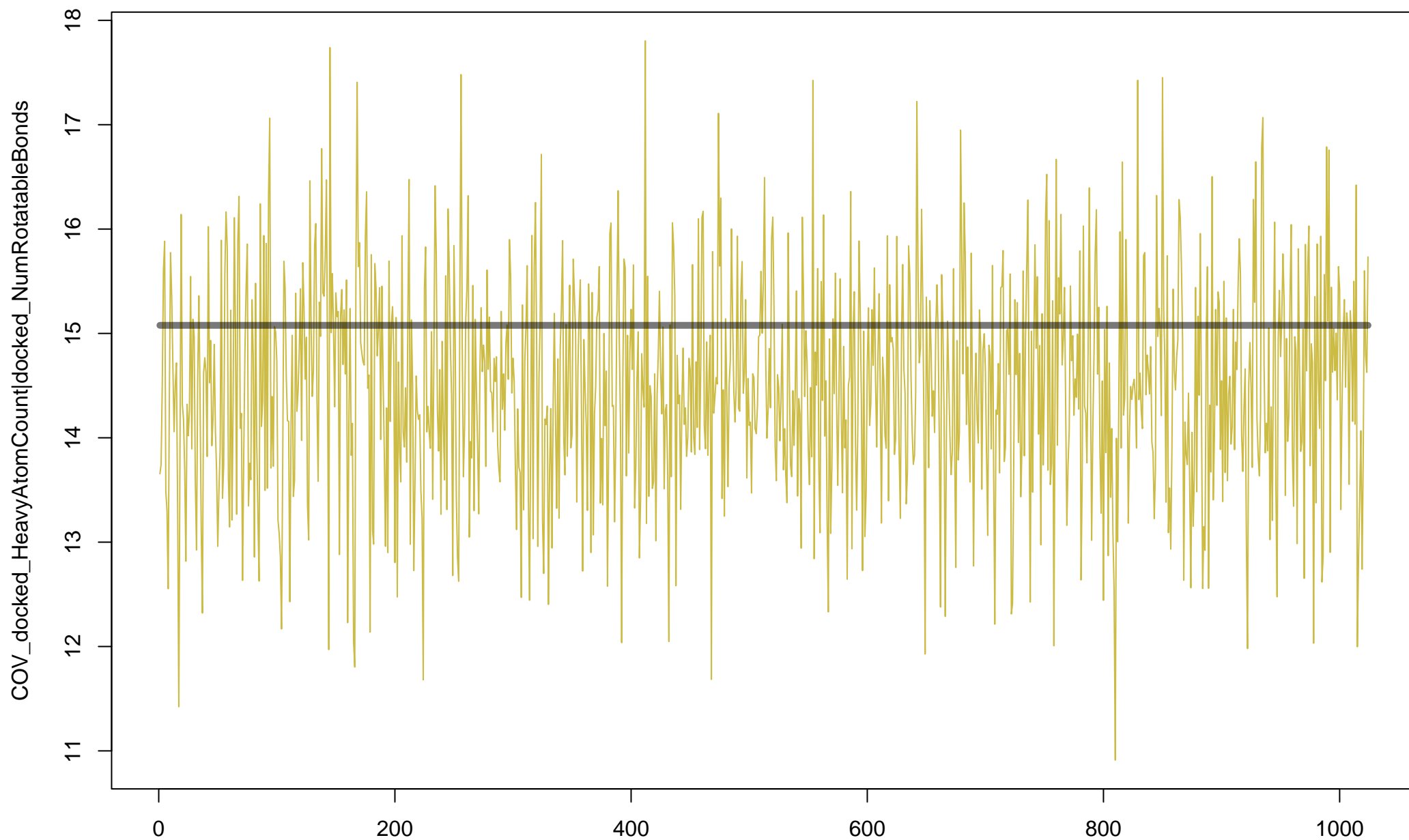
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0562 | MCSE(6.27) = 3.5 | stat: TRUE | burn: 0 | percentile: 52.9



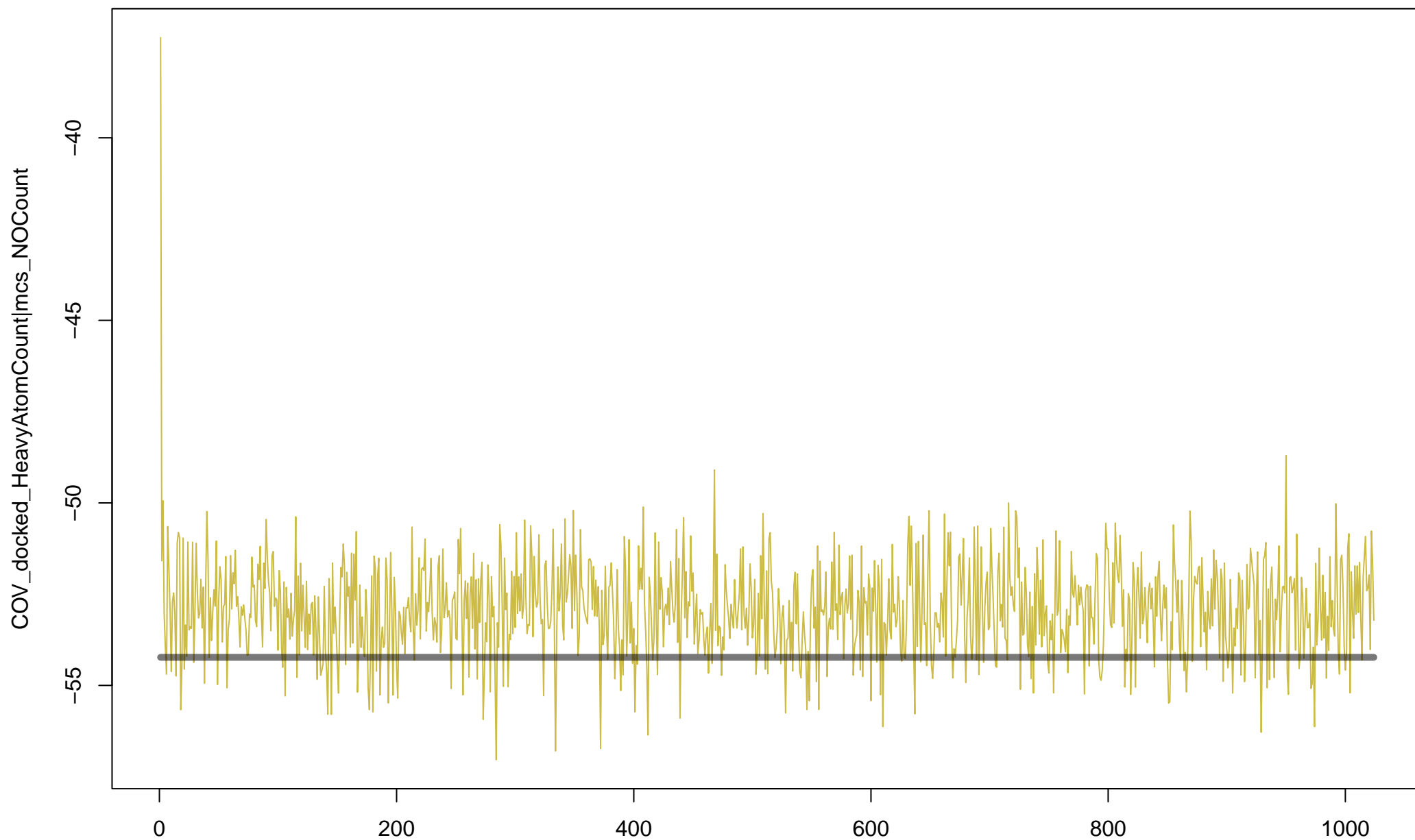
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0556 | MCSE(6.27) = 3.44 | stat: FALSE | burn: 0 | percentile: 6.45



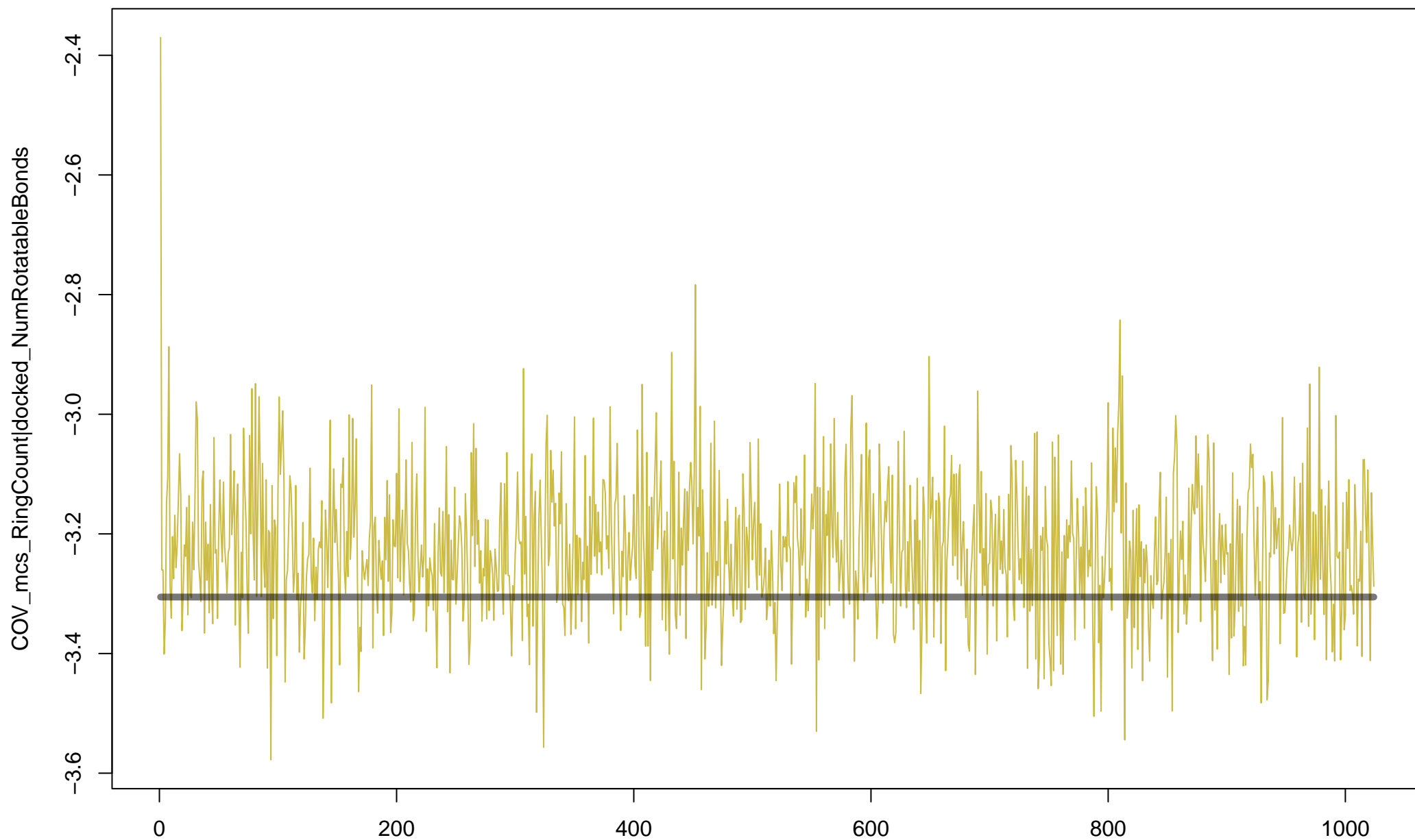
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0402 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | percentile: 72.2



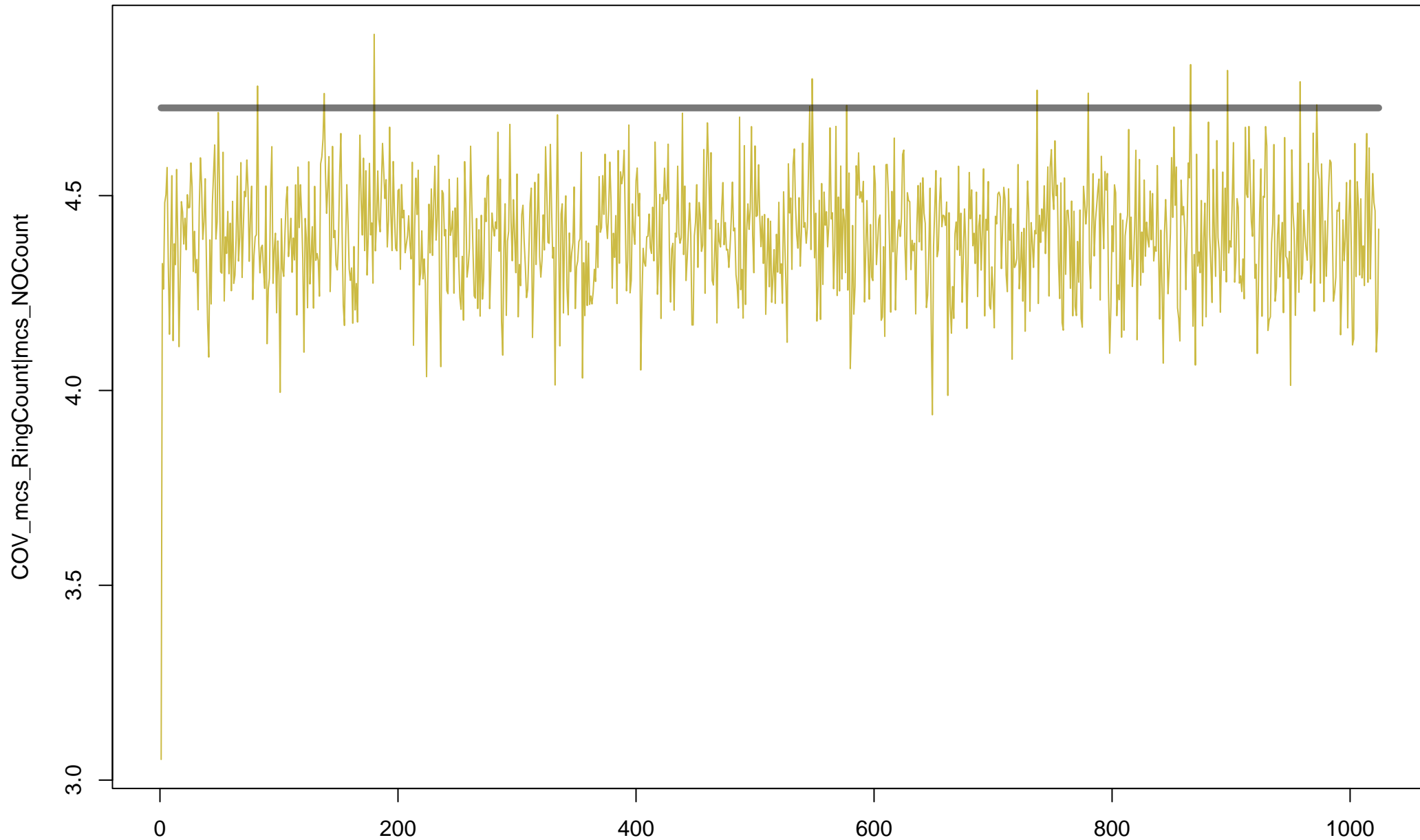
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0609 | MCSE(6.27) = 3.46 | stat: TRUE | burn: 0 | percentile: 15



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0698 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0 | percentile: 23.3



COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.0757 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0 | percentile: 98.8



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0486 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | percentile: 14.3

