

-- STATS maxD --

min ESS = 8.84374650001385

max BMK = 0.350519335293446

max MCSE = 16.2716632093964

all stationary: FALSE

burn: 1020

-- STATS 2D --

min ESS = 15.047898914986

max BMK = 0.386240089552838

max MCSE = 12.372469542534

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 1

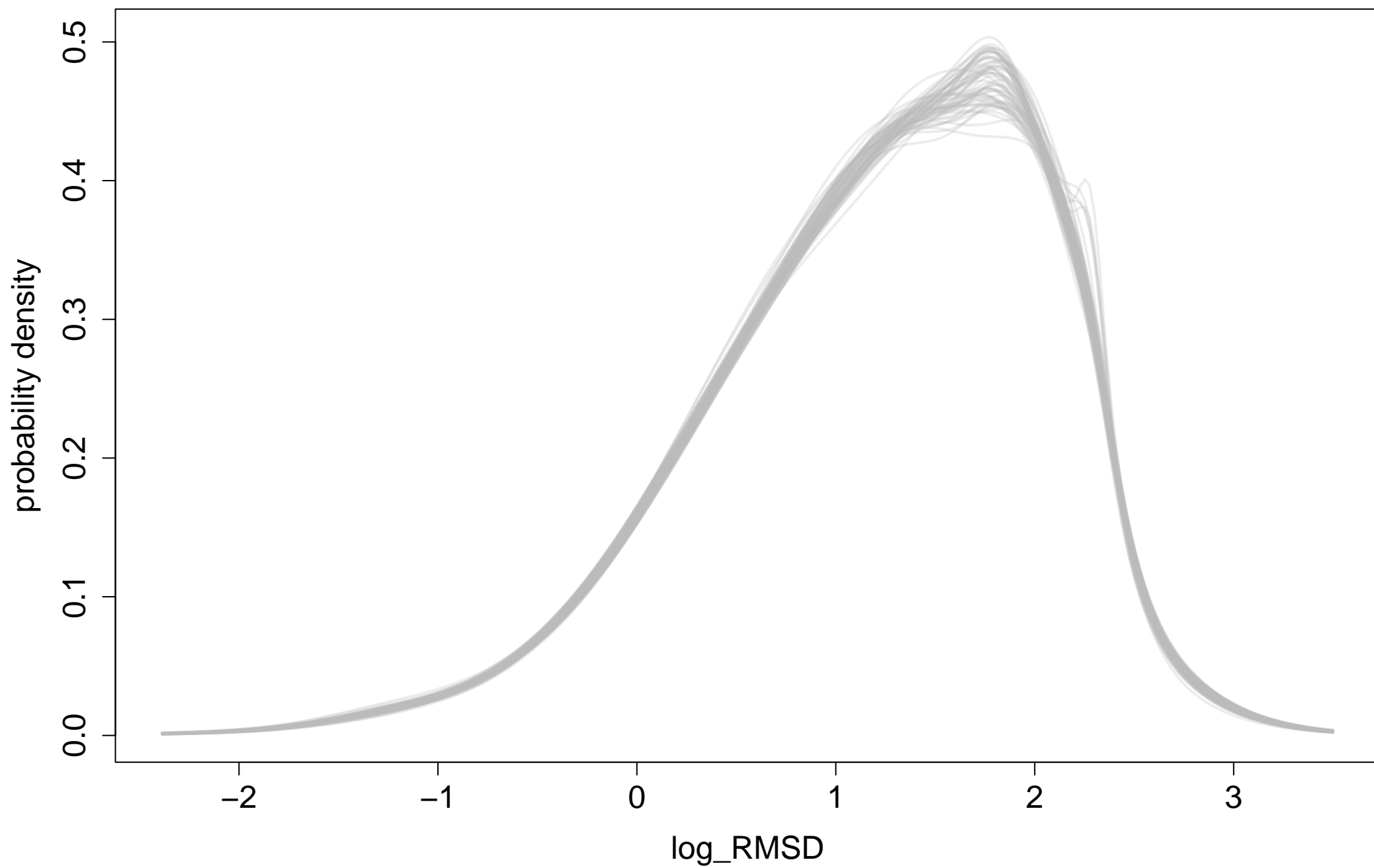
max MCSE = NaN

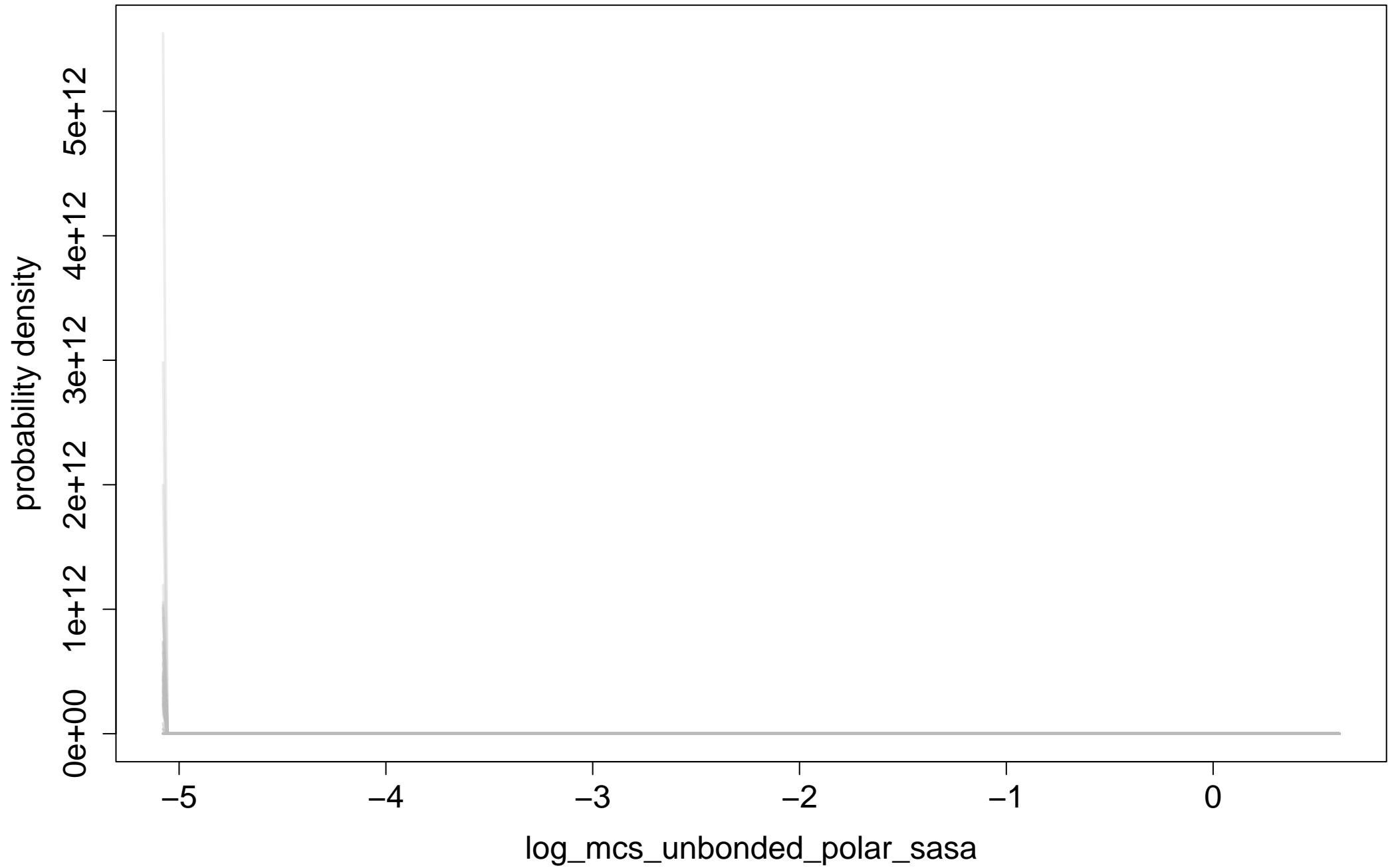
all stationary: FALSE

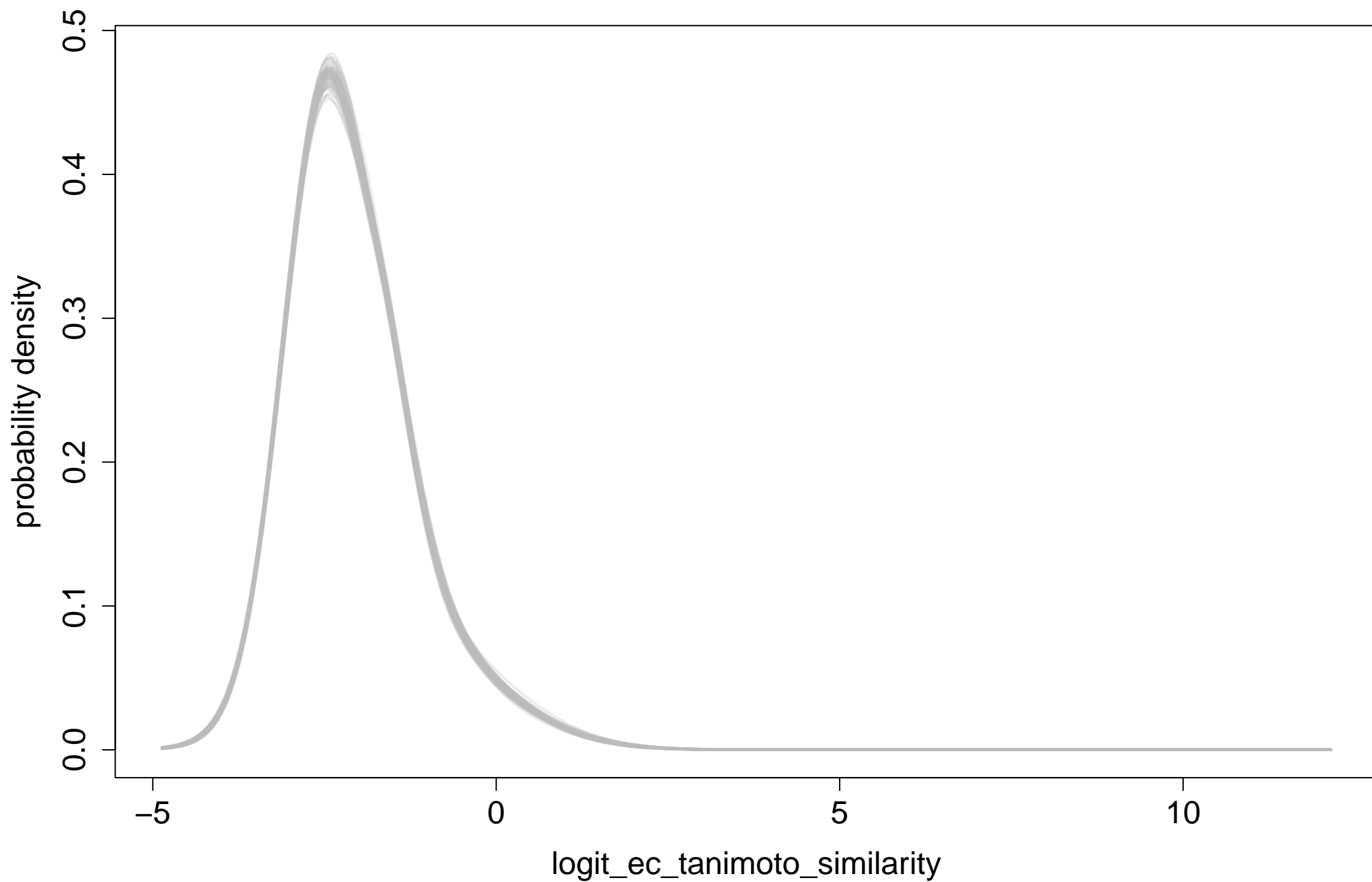
burn: 1020

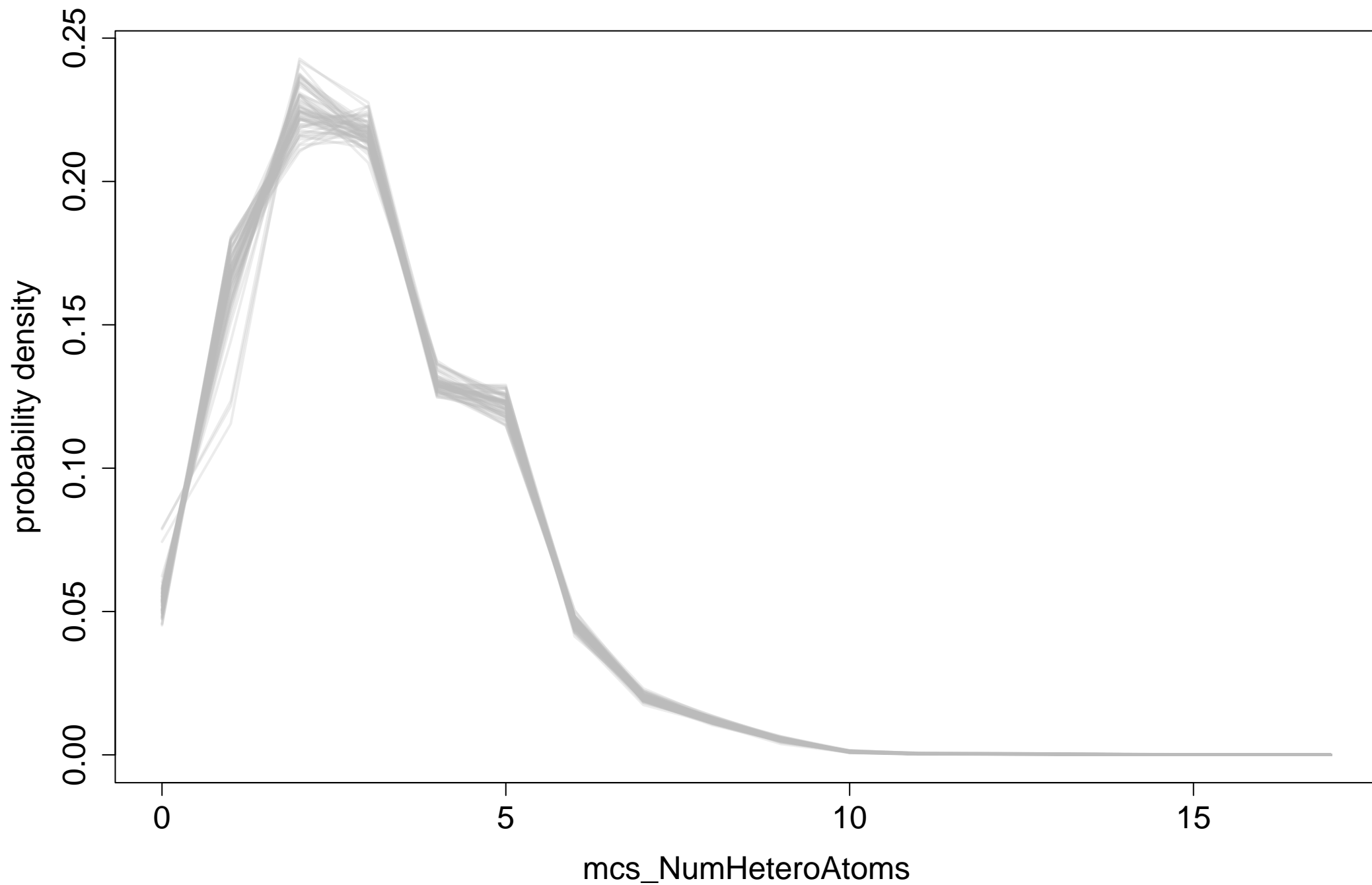
Occupied clusters: 47 of 64

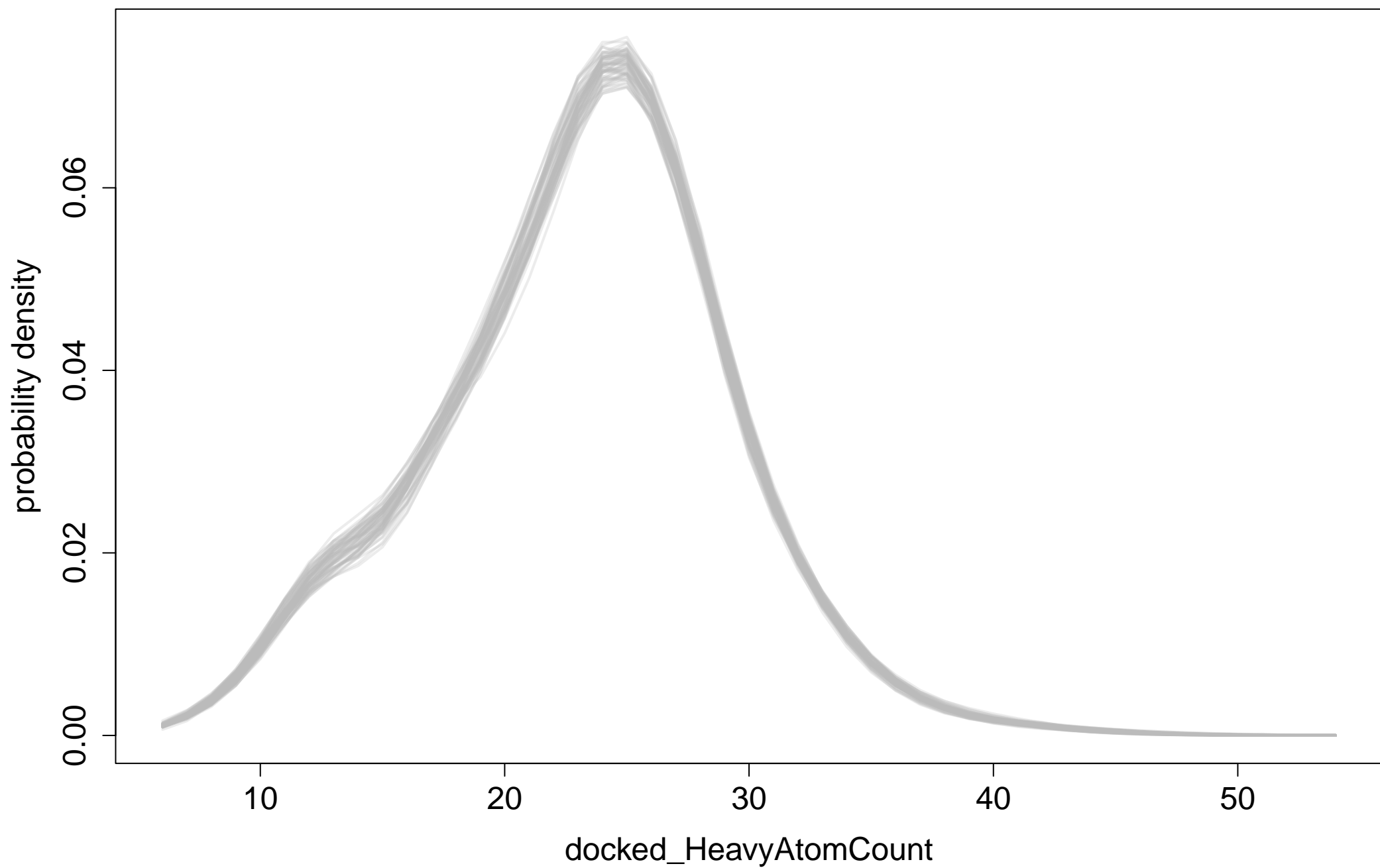
LL: -72900 +- 4100

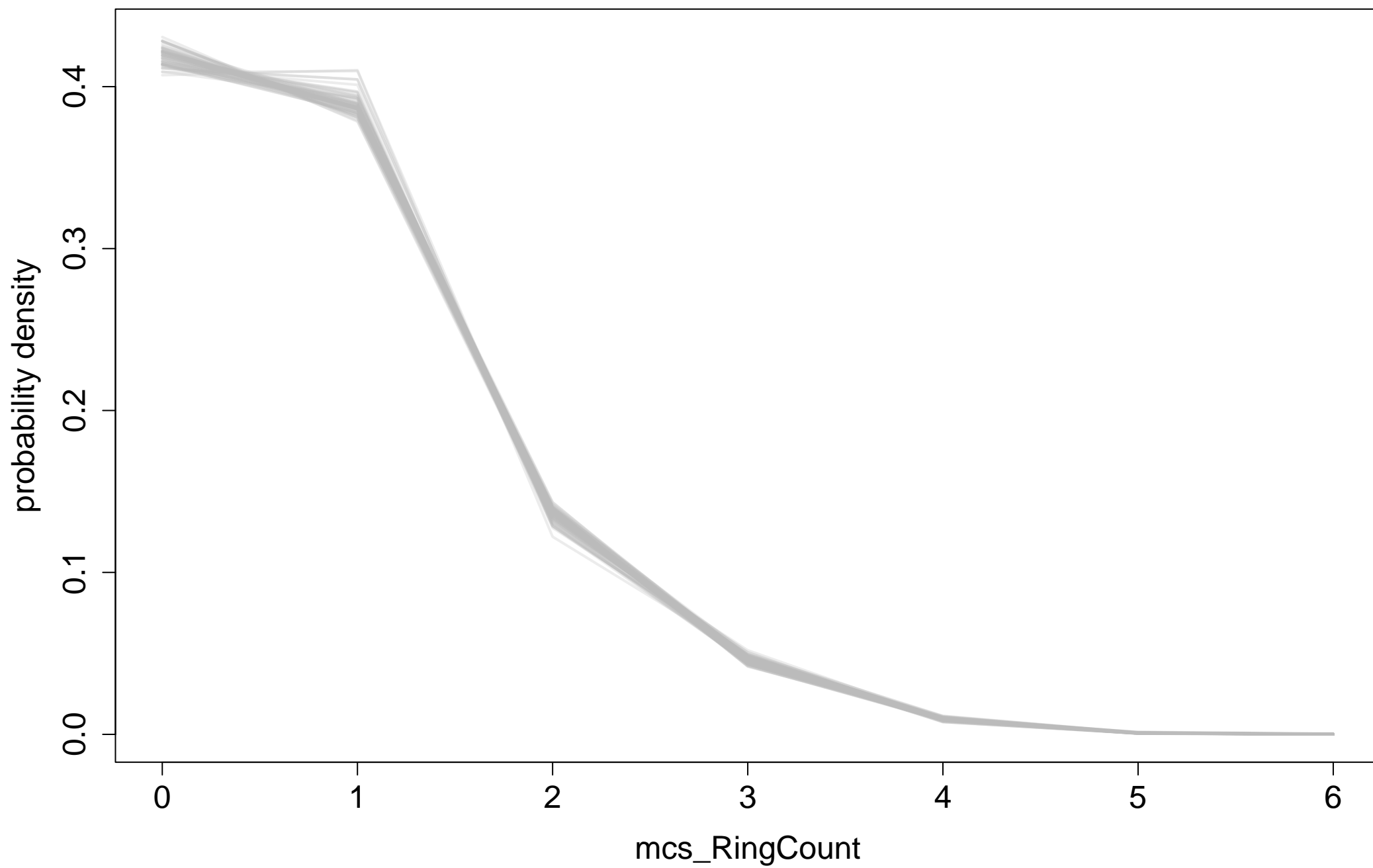


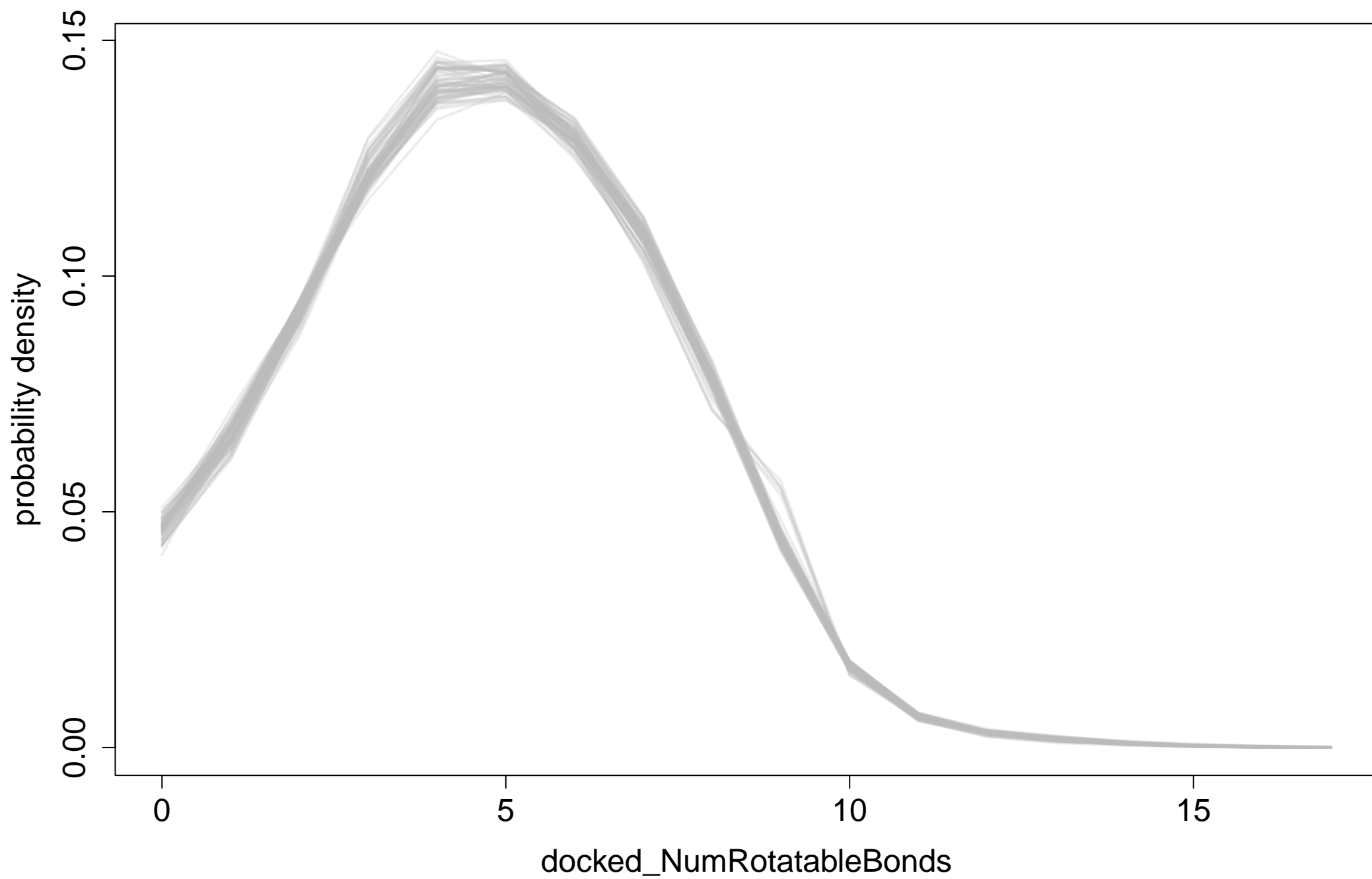


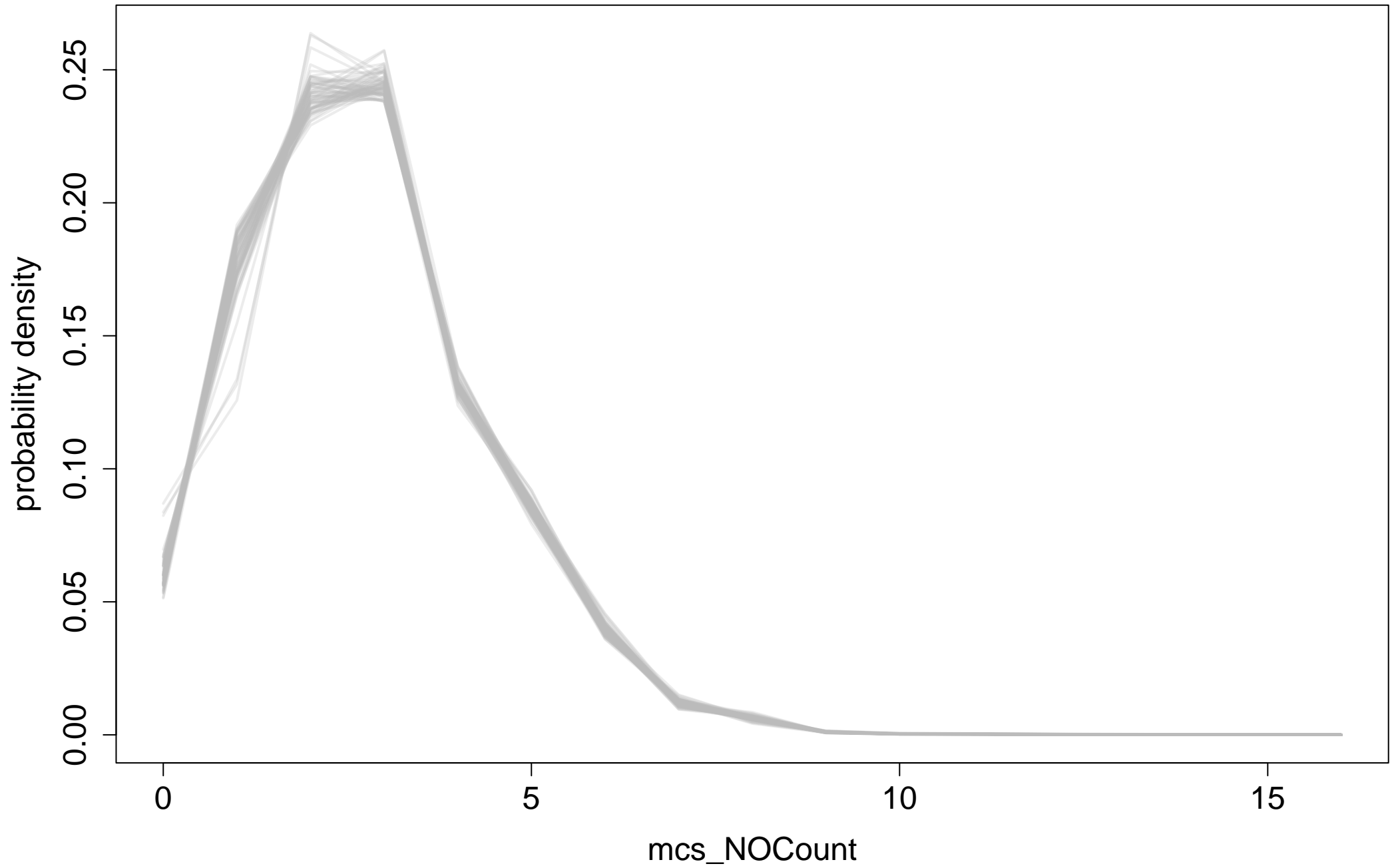


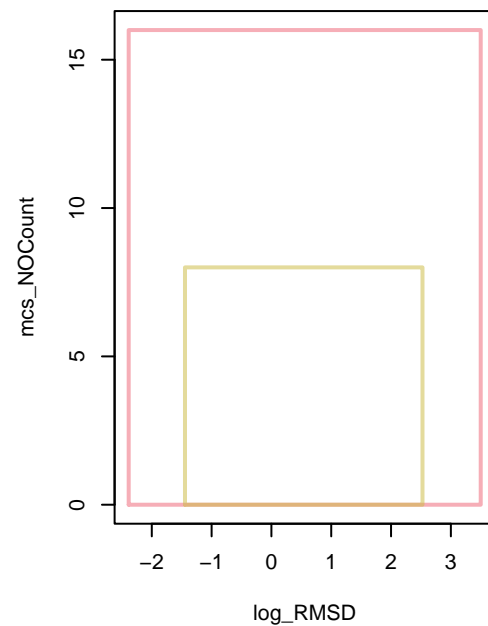
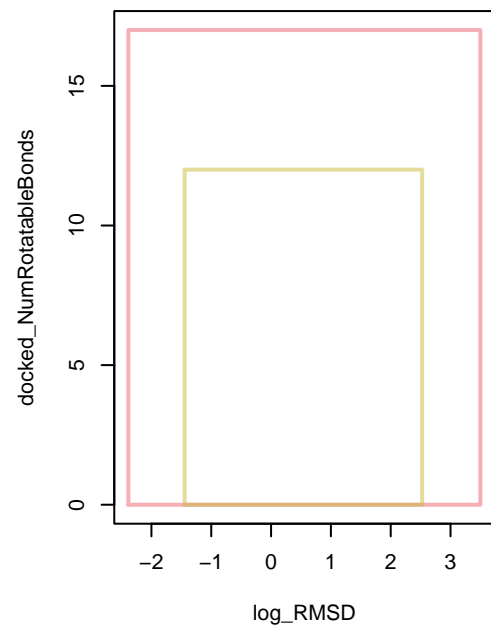
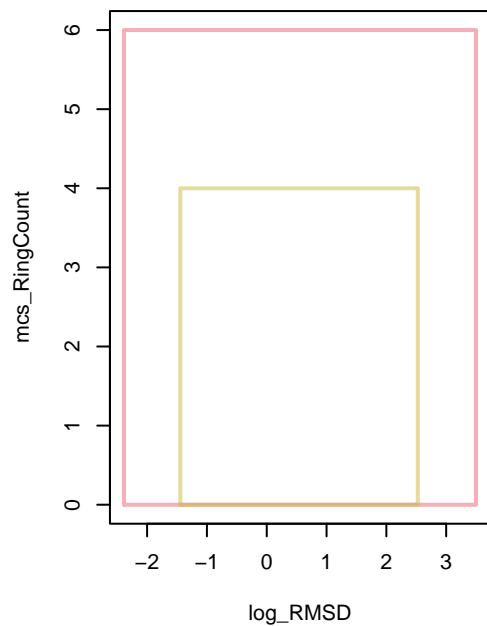
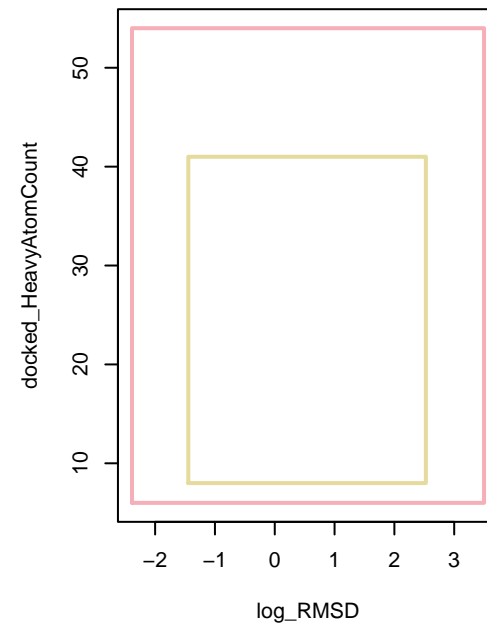
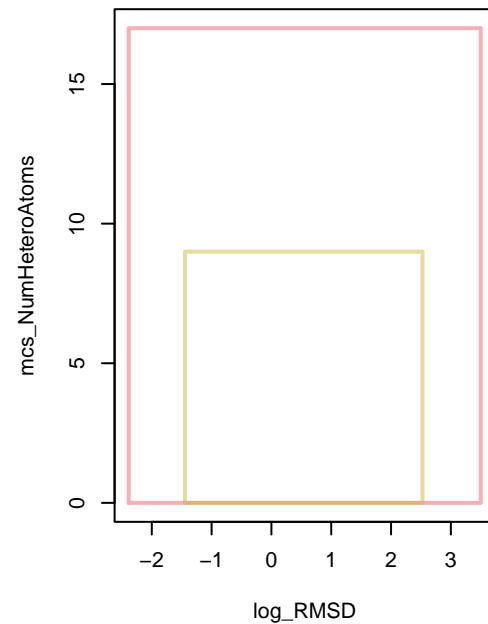
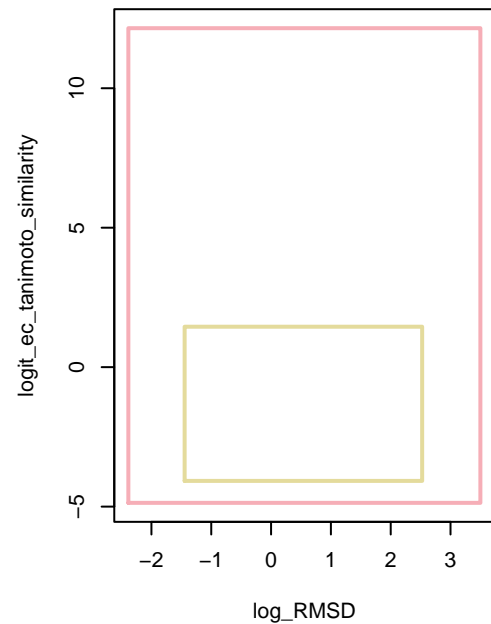
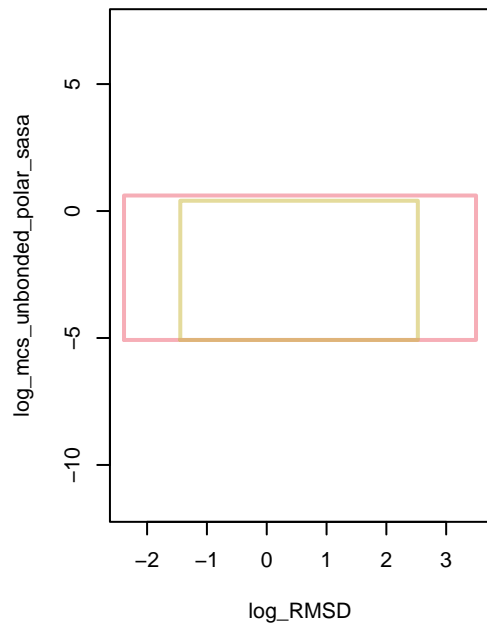




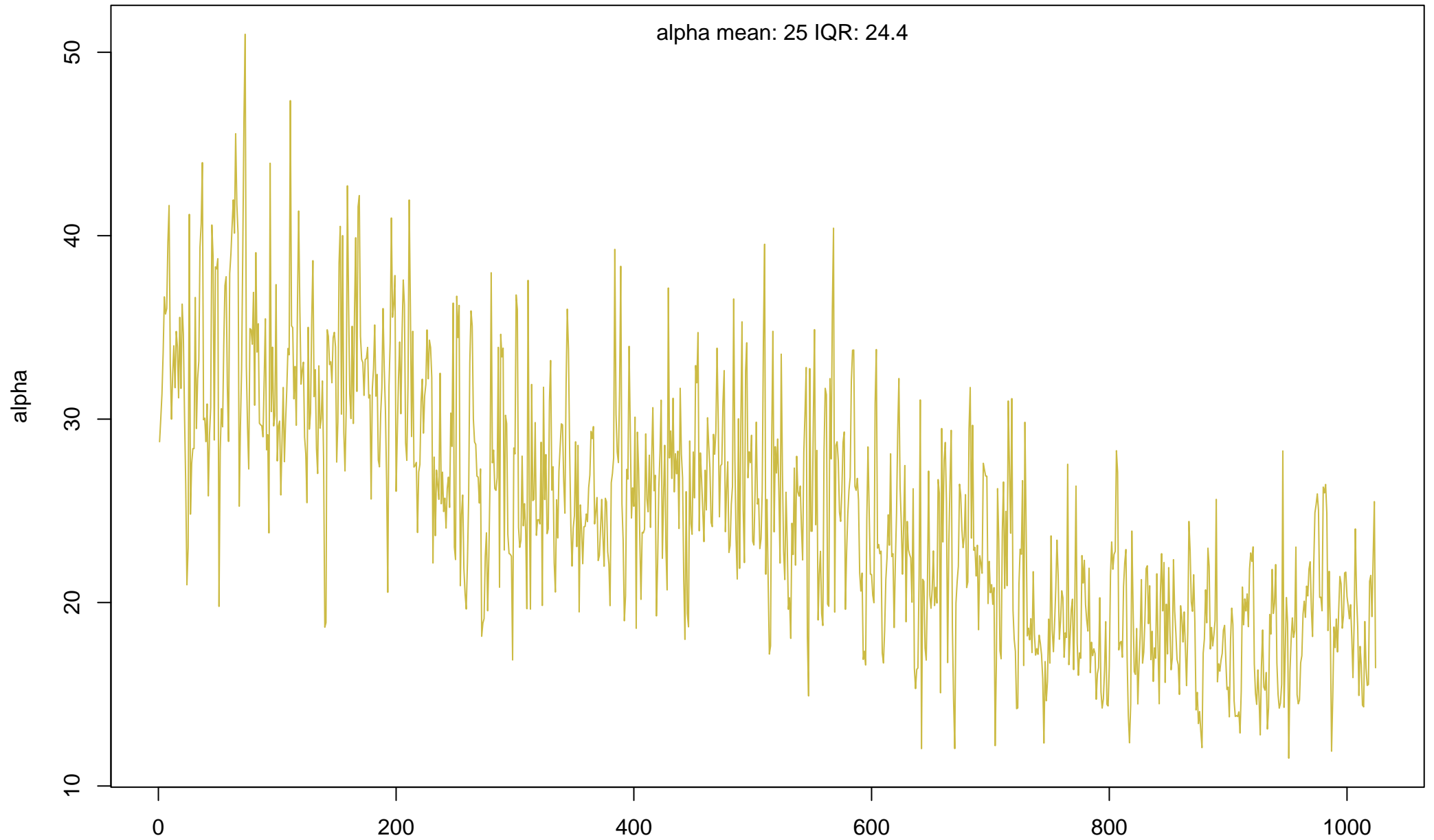




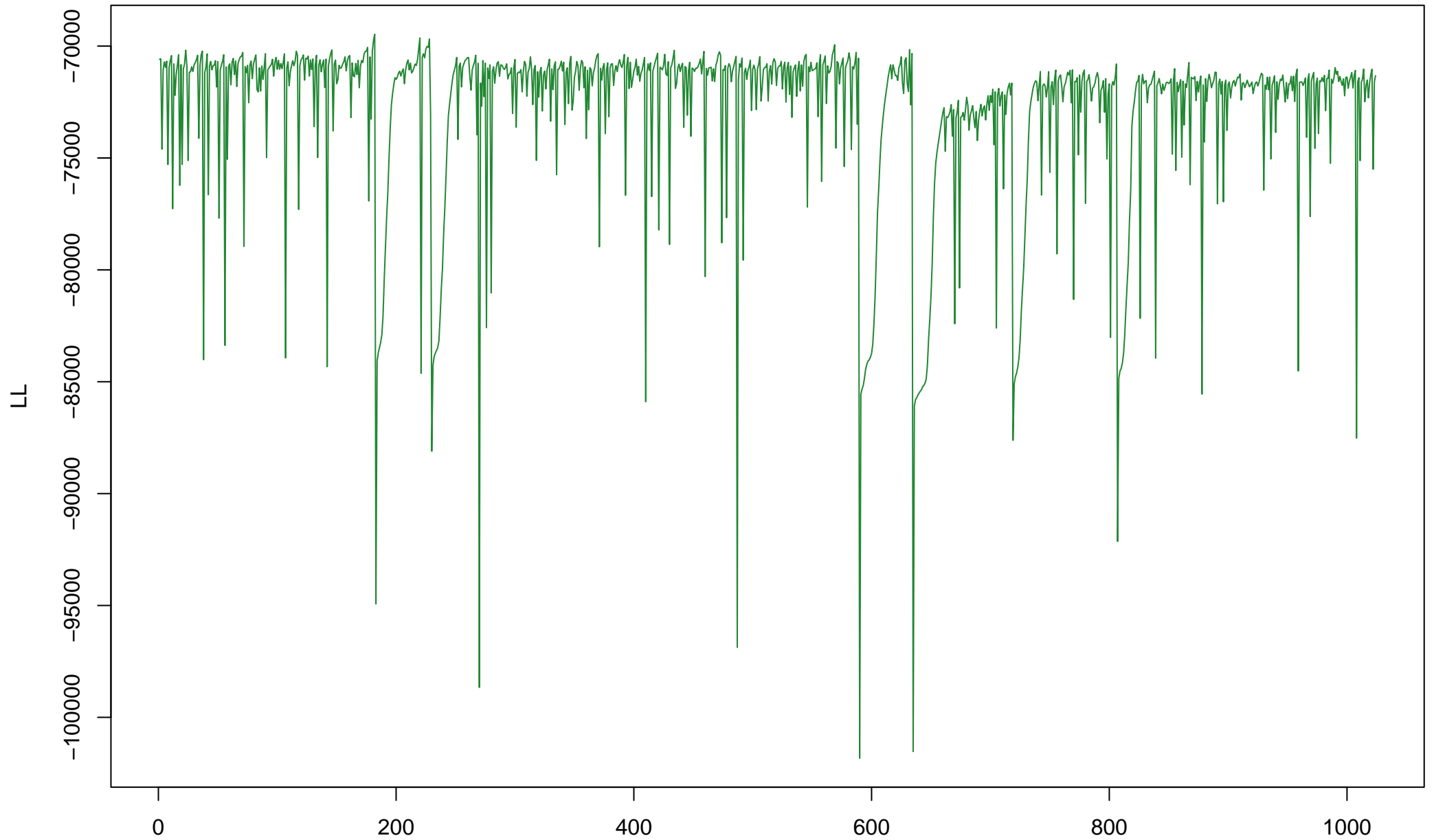




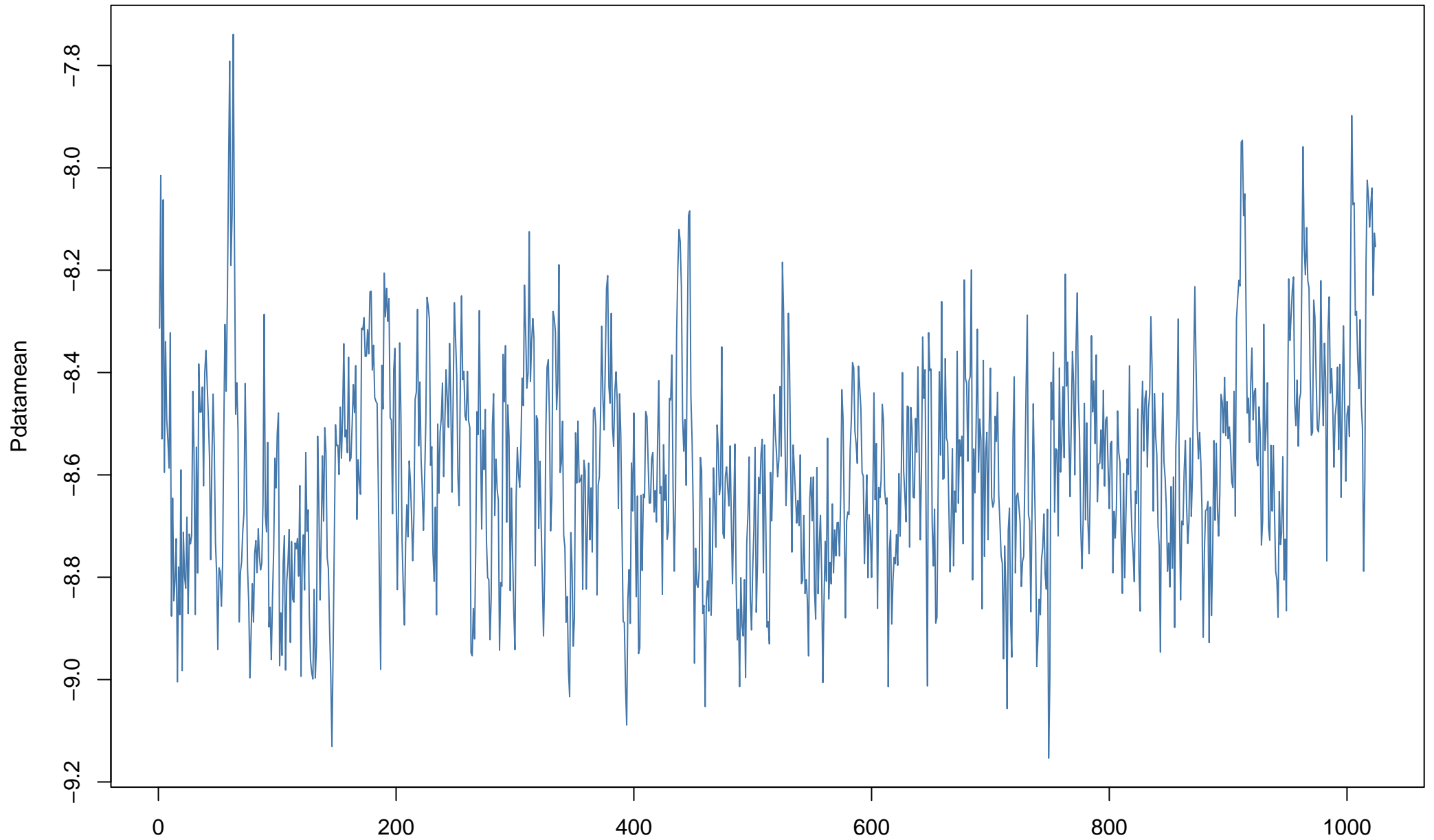
alpha



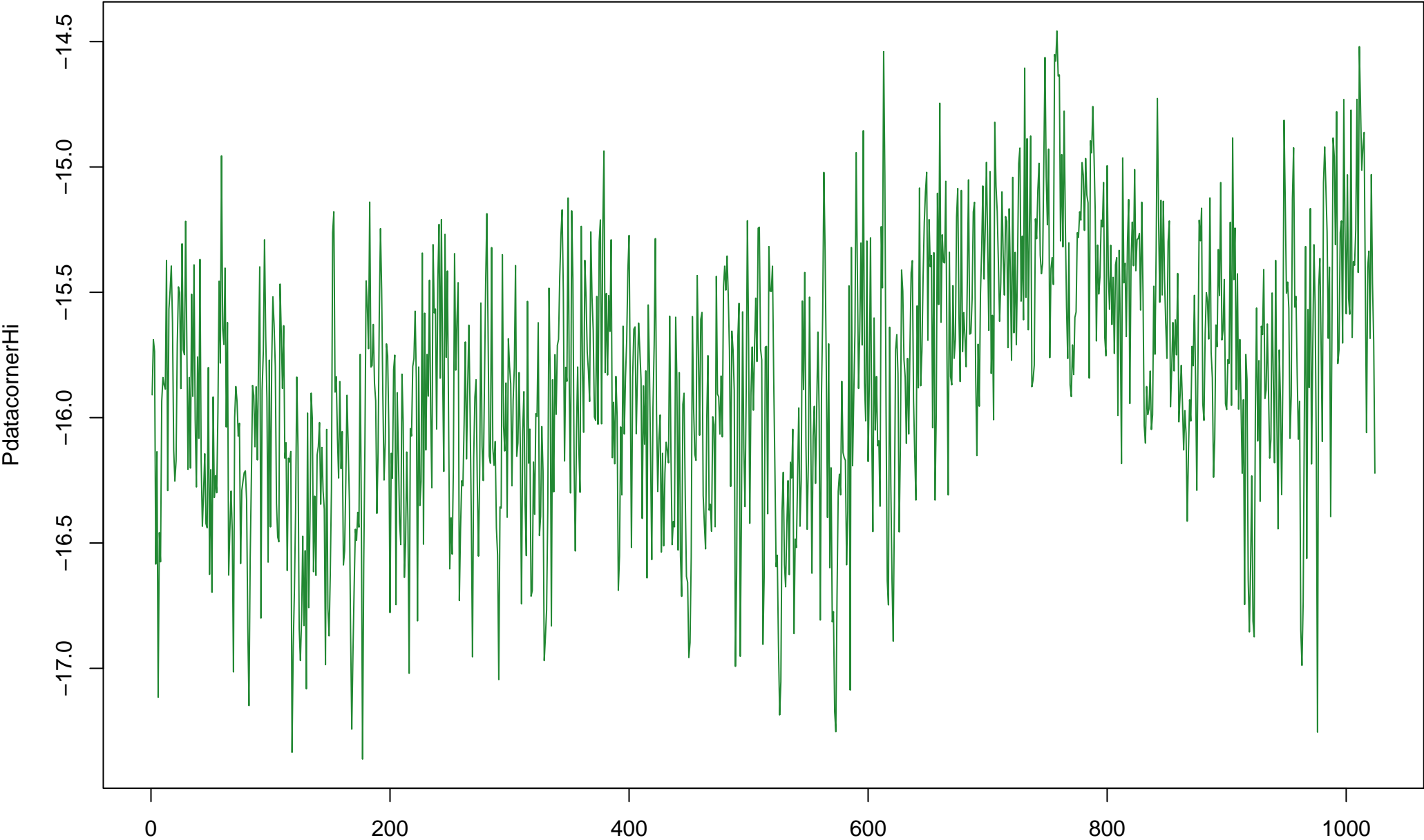
LL



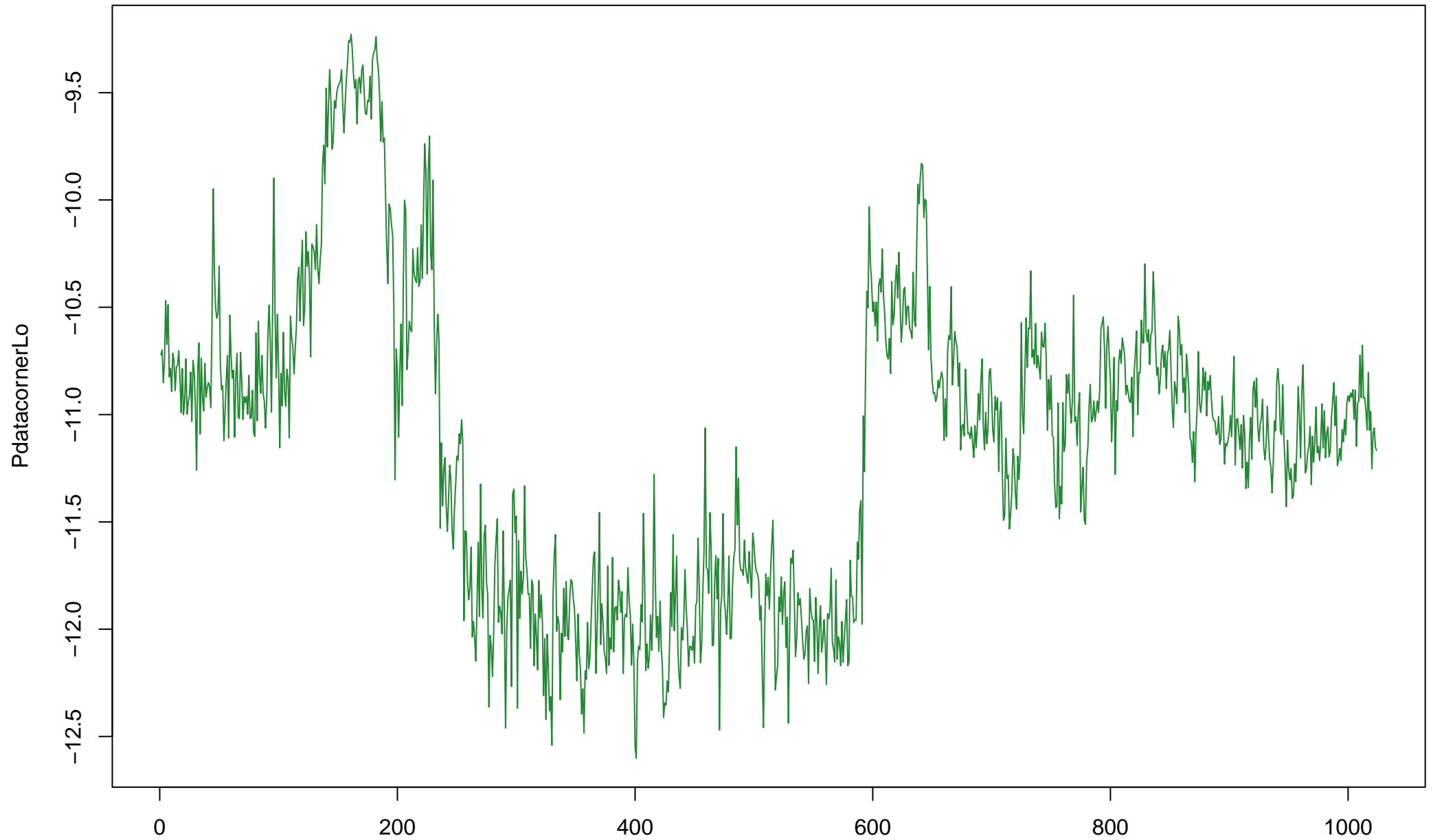
Pdatamean
ESS = 138 | BMK = 0.123 | MCSE(6.27) = 9.38 | stat: TRUE | burn: 0



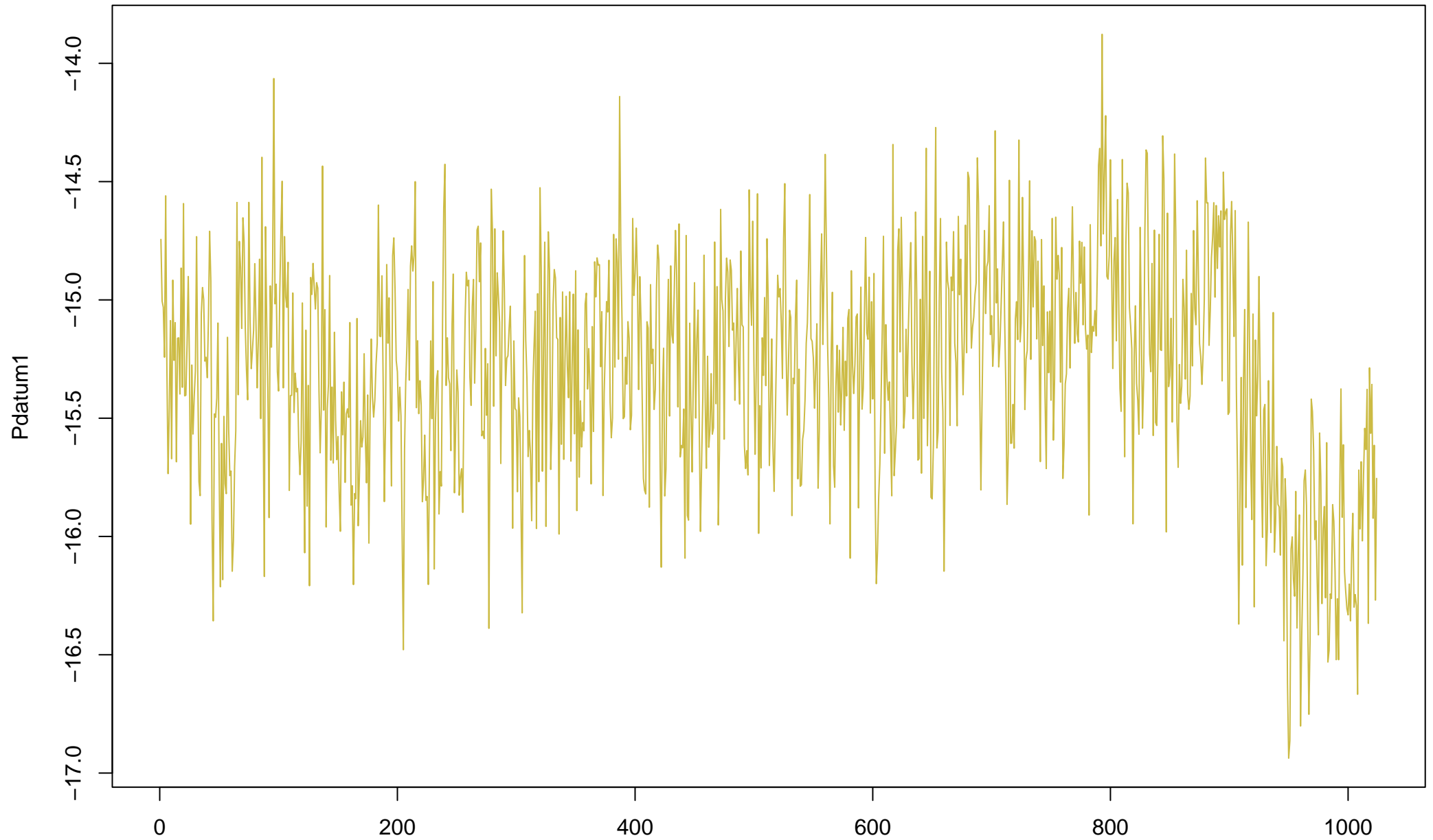
PdatacornerHi
ESS = 54.2 | BMK = 0.308 | MCSE(6.27) = 10.7 | stat: FALSE | burn: 0



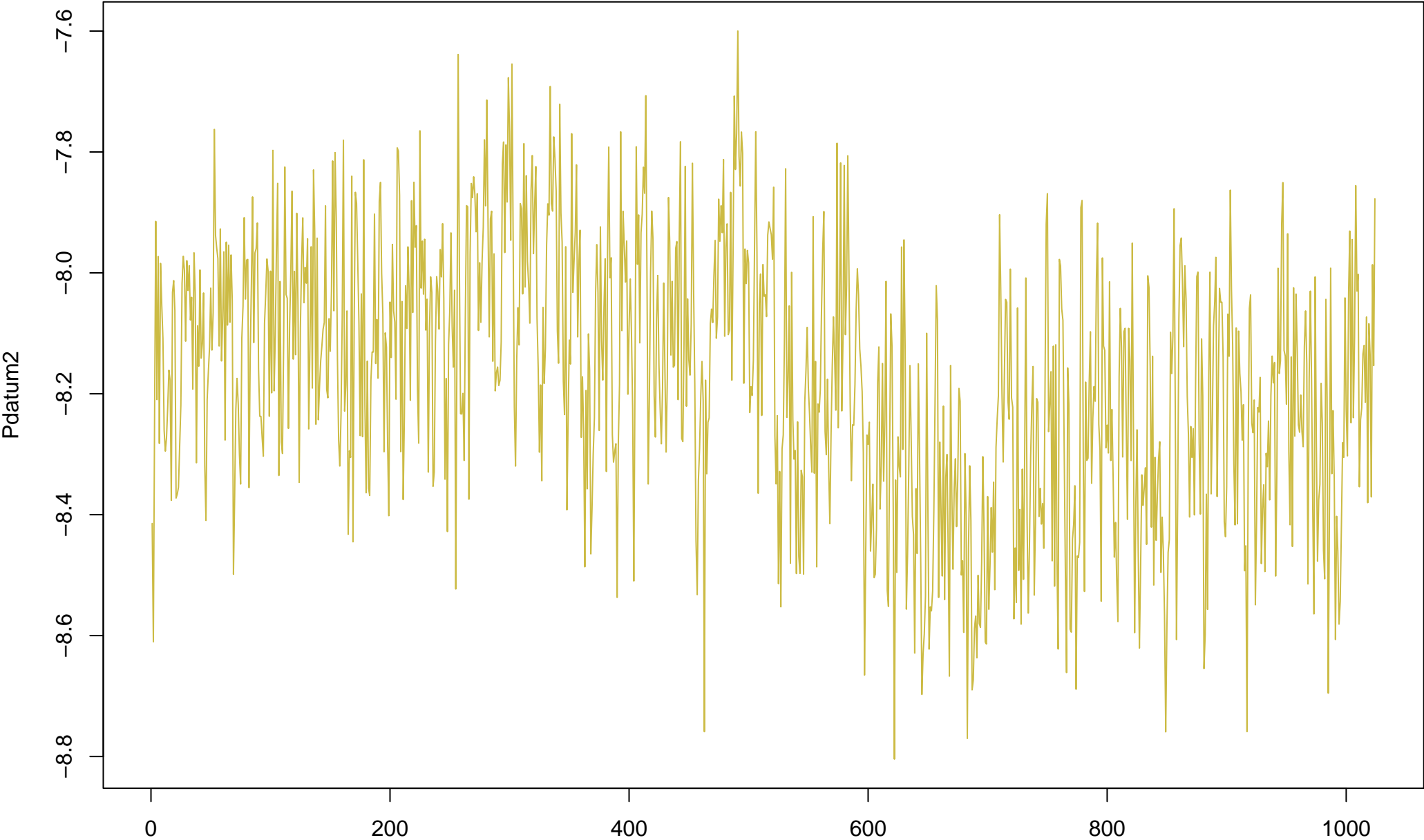
PdatacornerLo
ESS = 9.81 | BMK = 0.35 | MCSE(6.27) = 16.3 | stat: FALSE | burn: 612



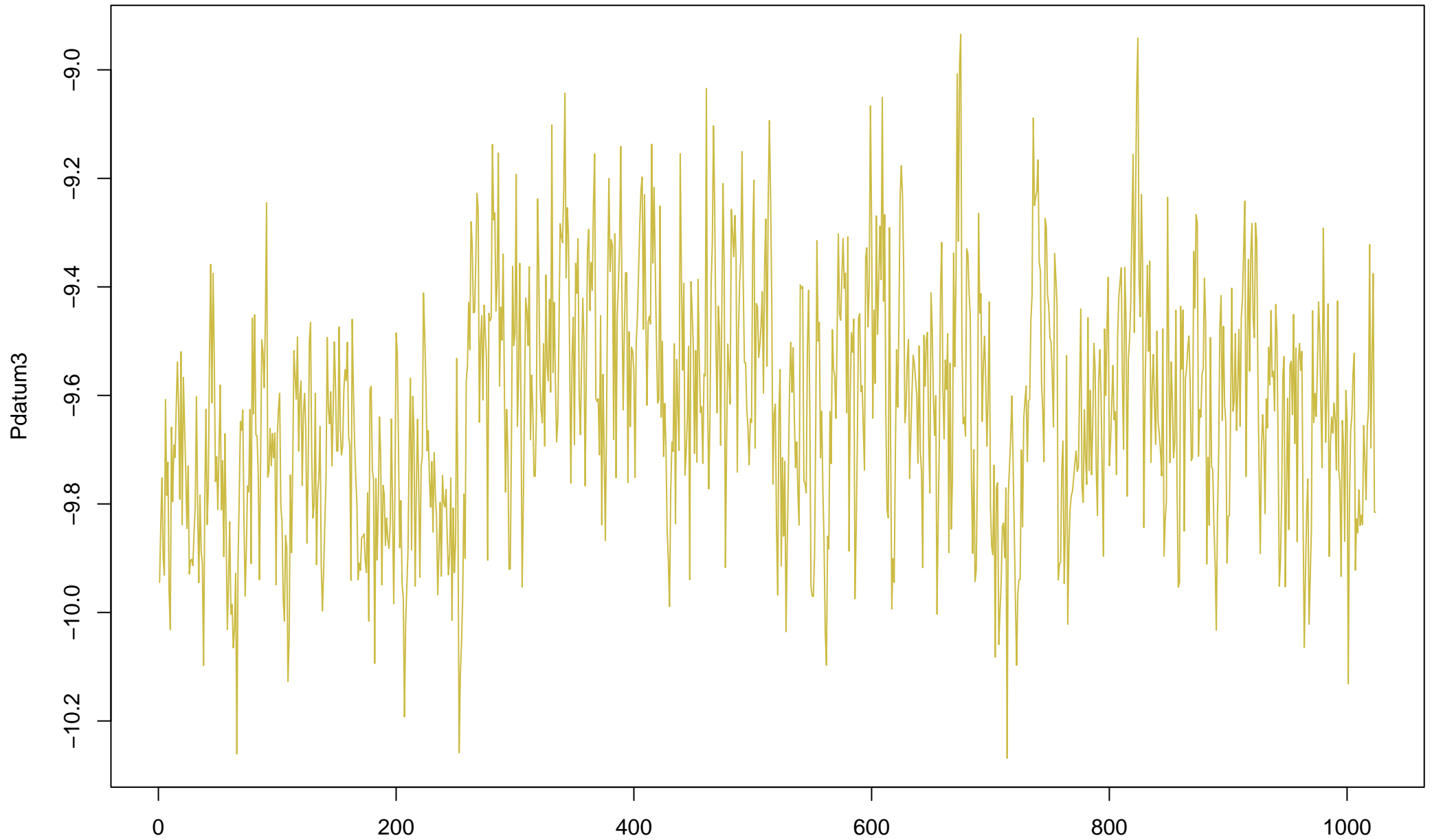
Pdatum1
ESS = 87.1 | BMK = 0.146 | MCSE(6.27) = 9.01 | stat: TRUE | burn: 1020



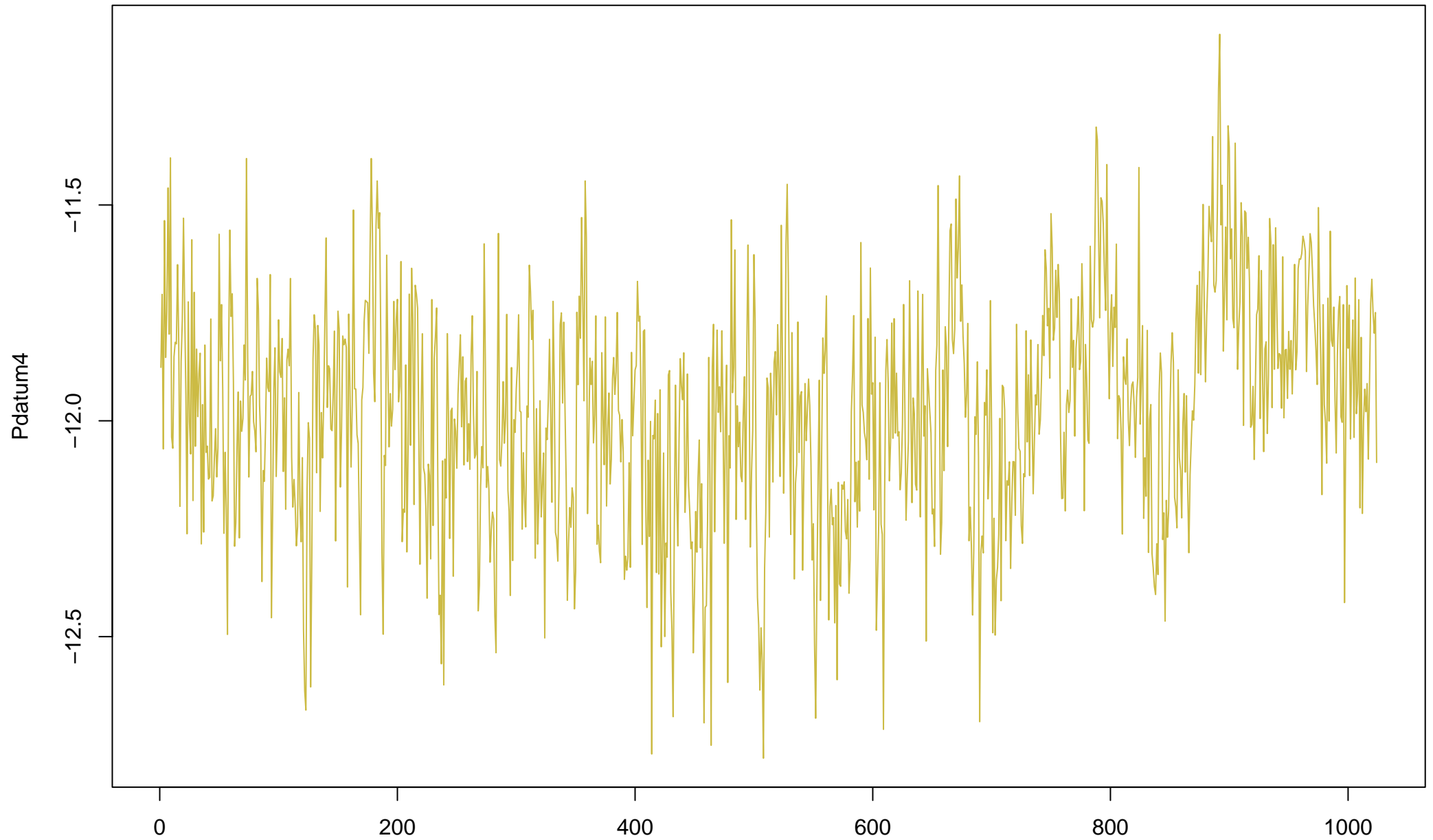
Pdatum2
ESS = 33.8 | BMK = 0.351 | MCSE(6.27) = 9.89 | stat: FALSE | burn: 0



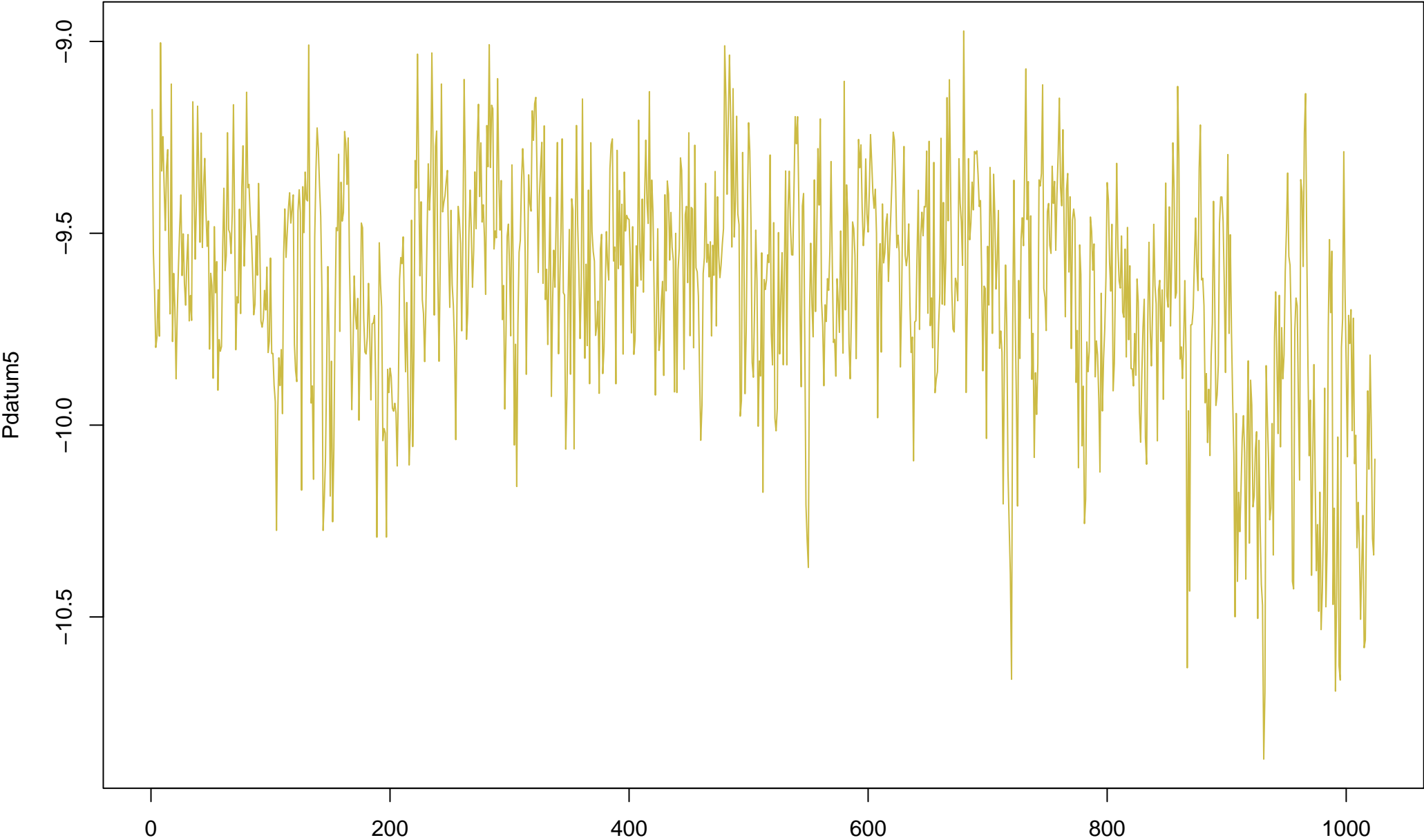
Pdatum3
ESS = 112 | BMK = 0.0693 | MCSE(6.27) = 9.16 | stat: FALSE | burn: 0



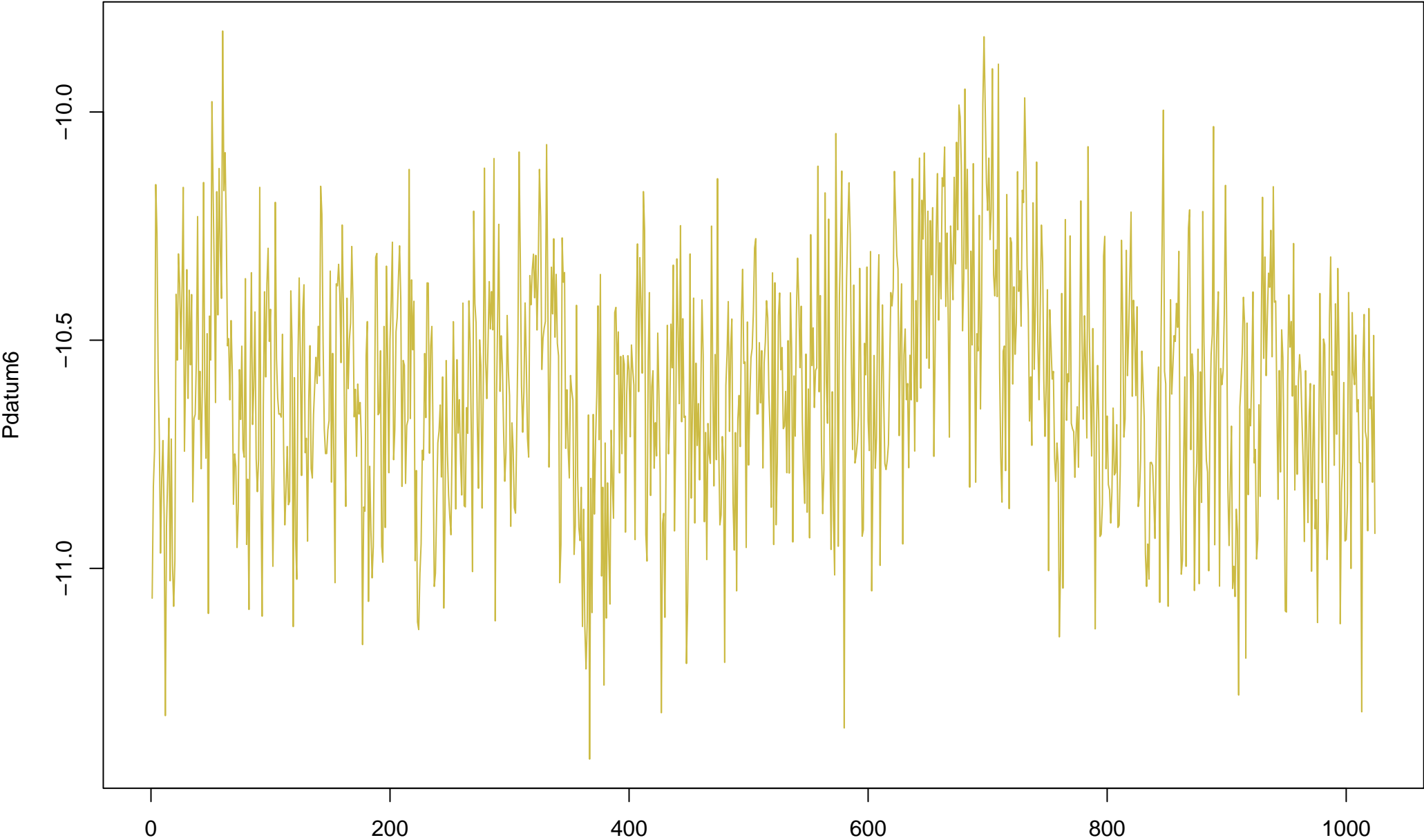
Pdatum4
ESS = 82.8 | BMK = 0.134 | MCSE(6.27) = 9.48 | stat: TRUE | burn: 0



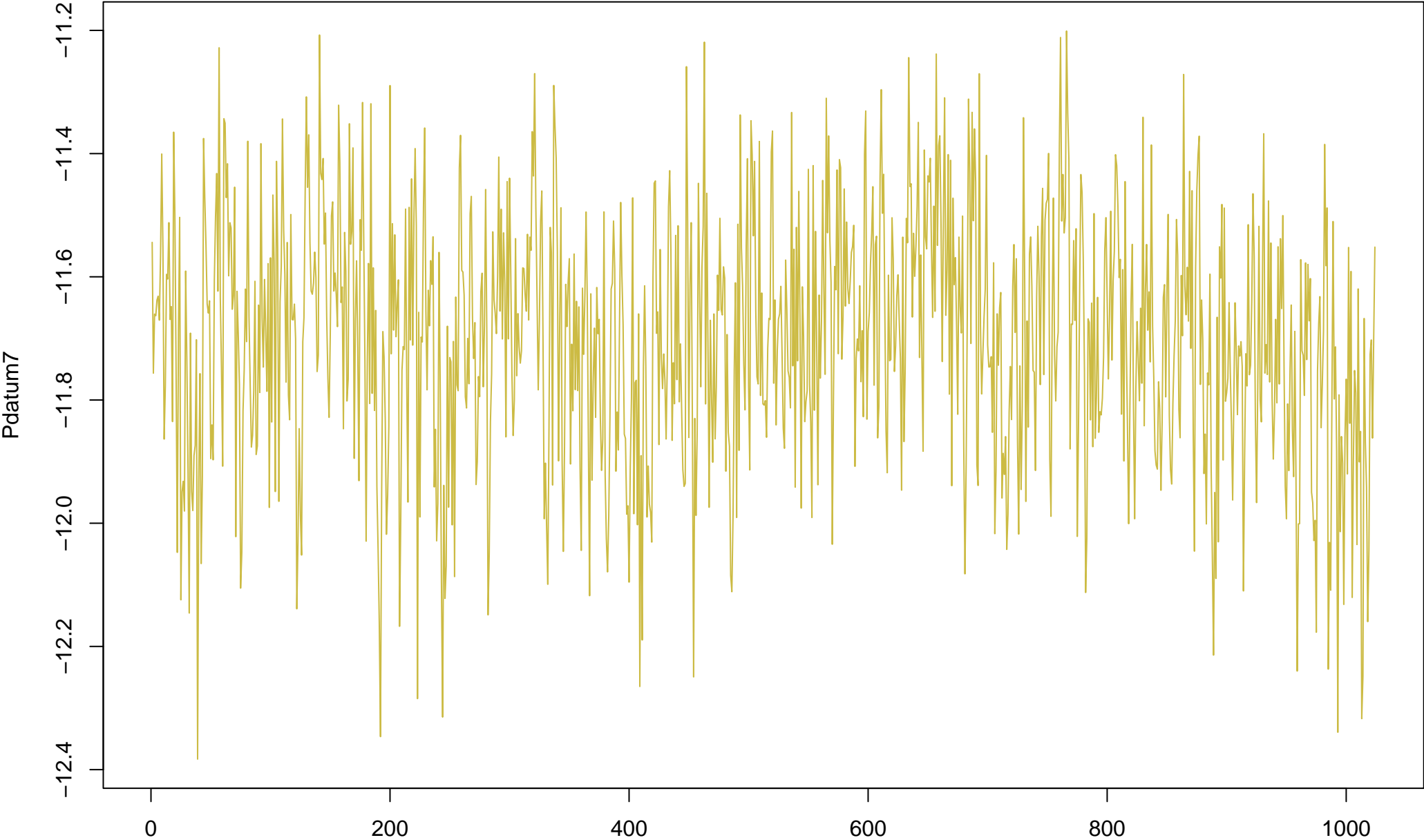
Pdatum5
ESS = 134 | BMK = 0.187 | MCSE(6.27) = 8.93 | stat: FALSE | burn: 0



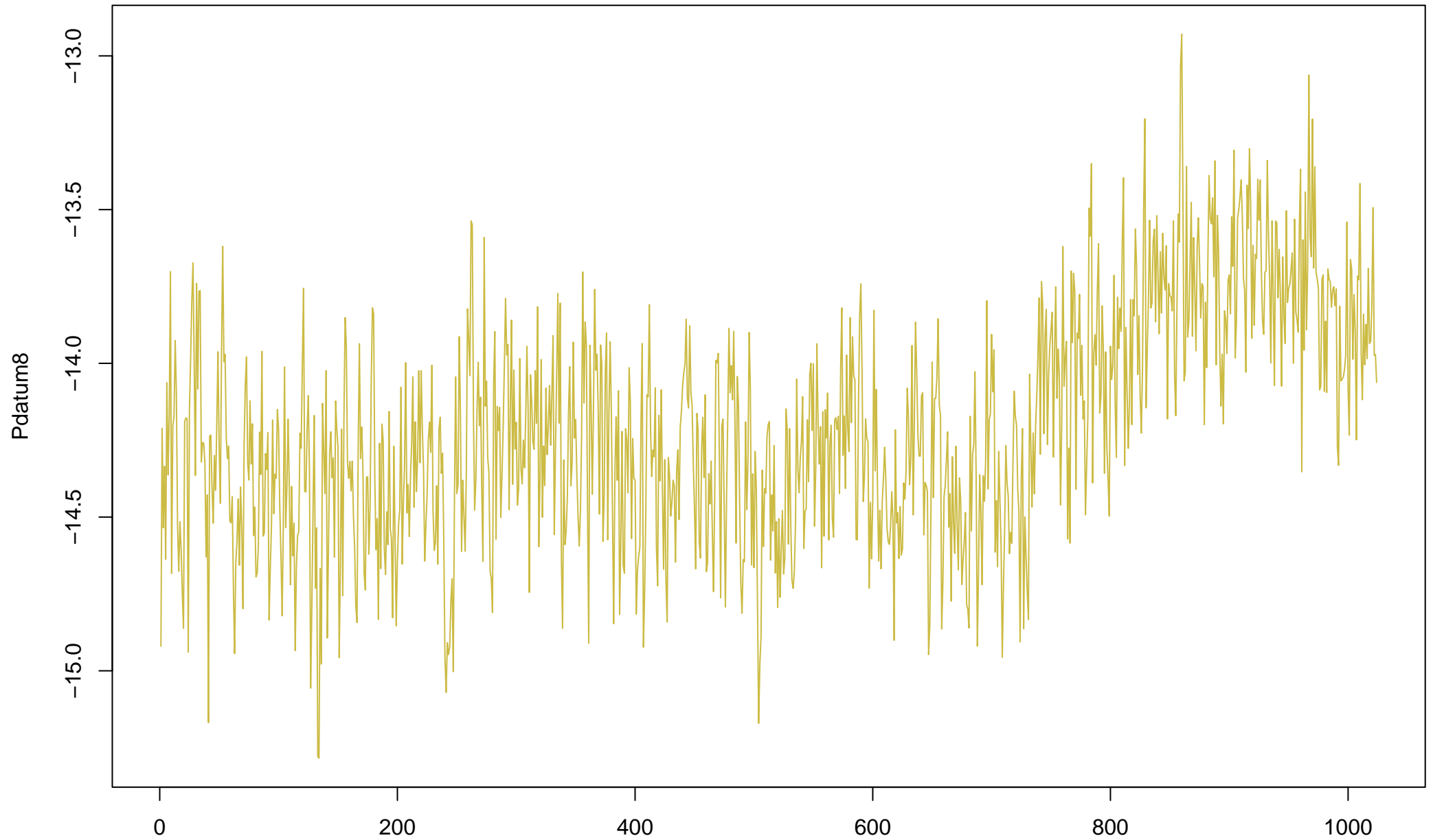
Pdatum6
ESS = 158 | BMK = 0.0999 | MCSE(6.27) = 8.51 | stat: TRUE | burn: 0



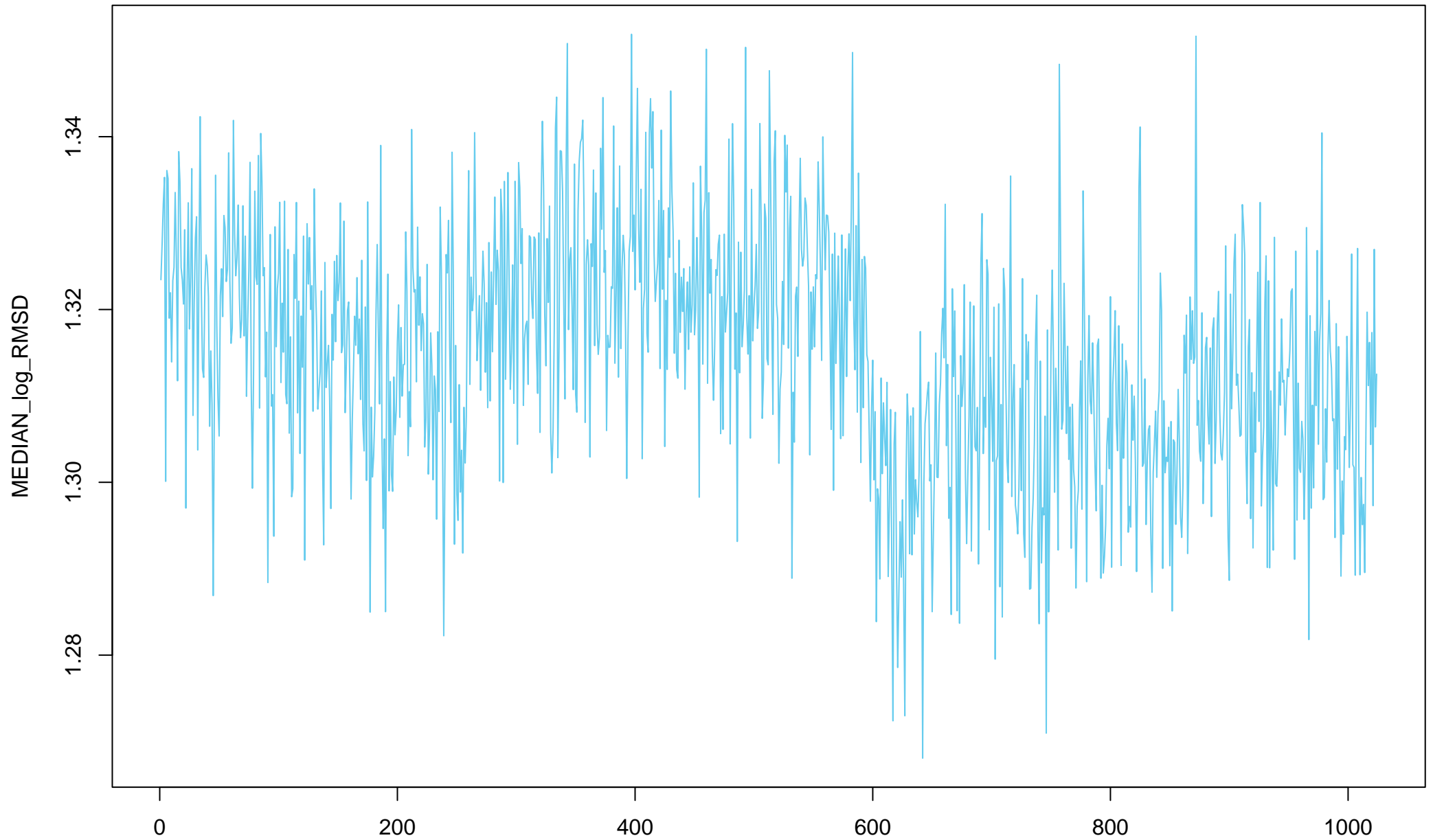
Pdatum7
ESS = 286 | BMK = 0.0493 | MCSE(6.27) = 6.45 | stat: TRUE | burn: 0



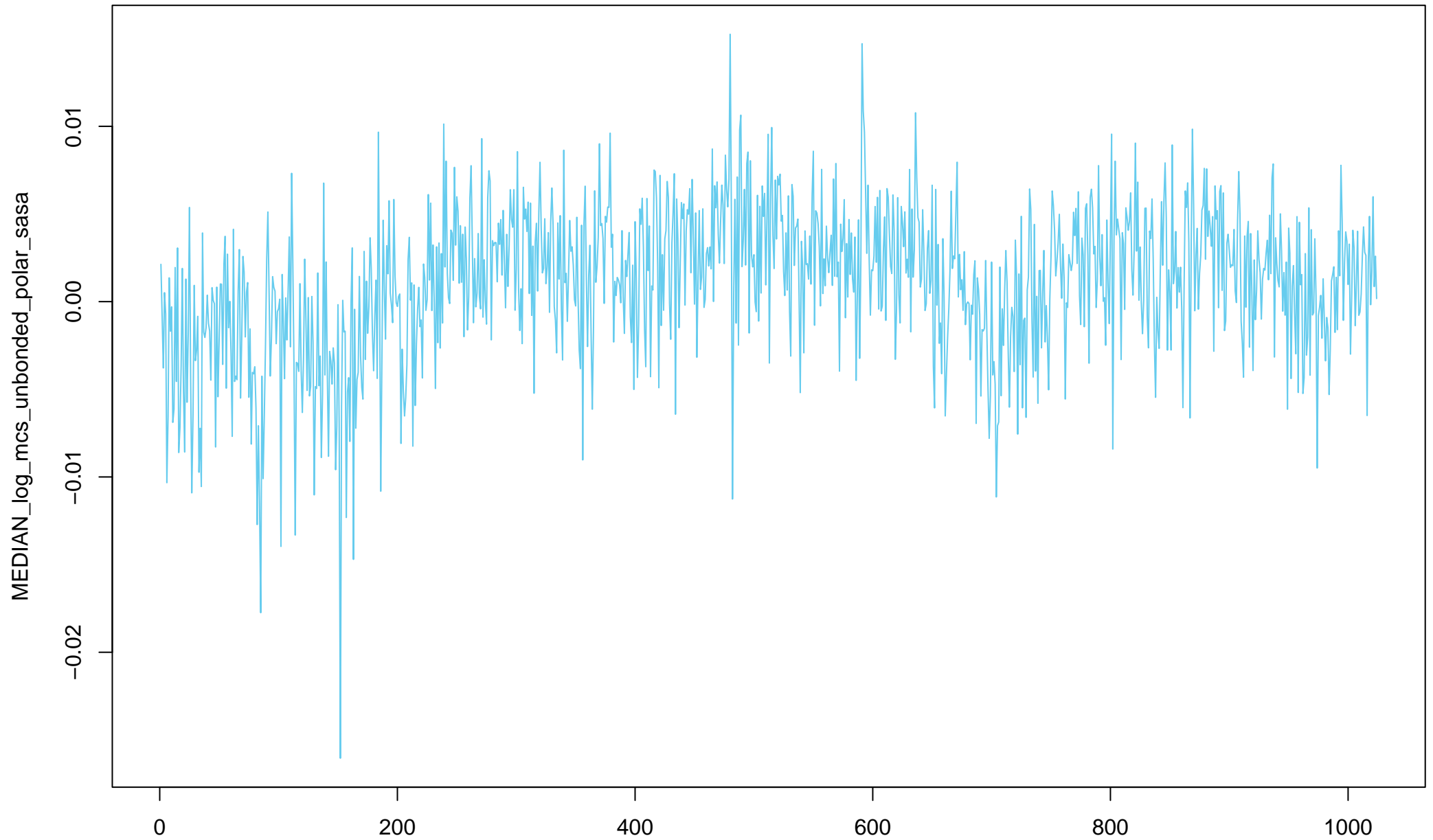
Pdatum8
ESS = 8.84 | BMK = 0.321 | MCSE(6.27) = 13 | stat: FALSE | burn: 0



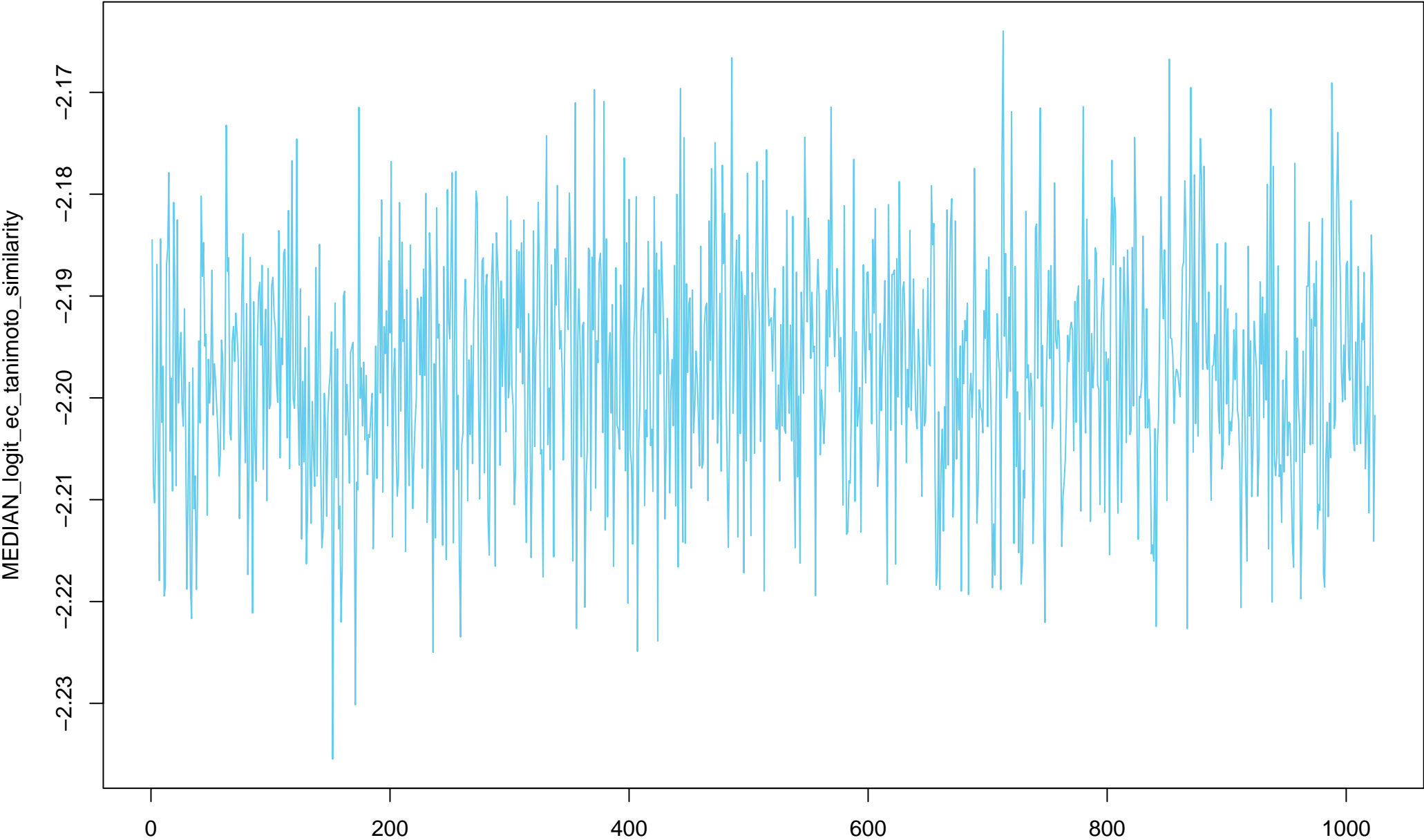
MEDIAN_log_RMSD
ESS = 22.9 | BMK = 0.298 | MCSE(6.27) = 10.1 | stat: FALSE | burn: 0



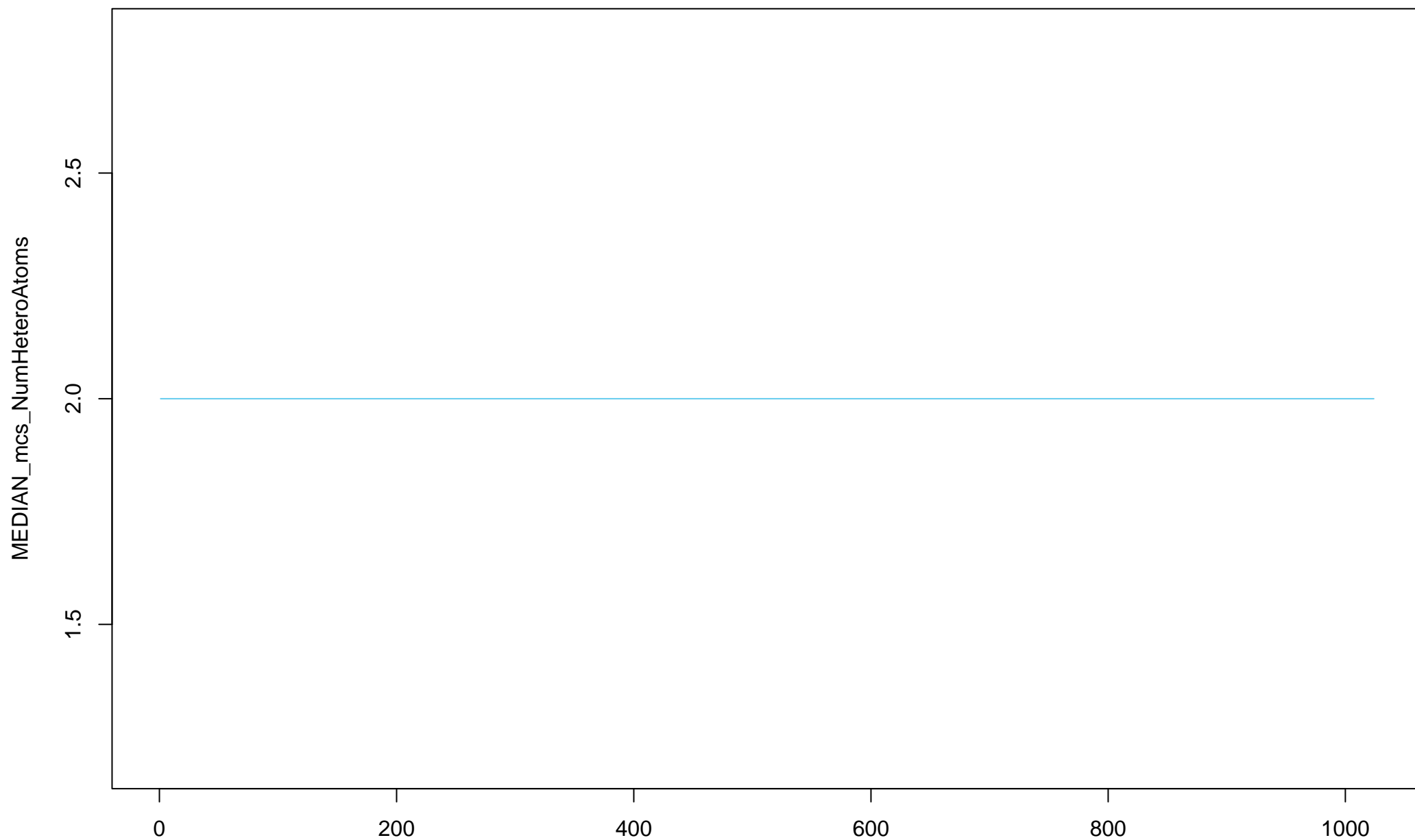
MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 47.4 | BMK = 0.144 | MCSE(6.27) = 9.7 | stat: FALSE | burn: 0



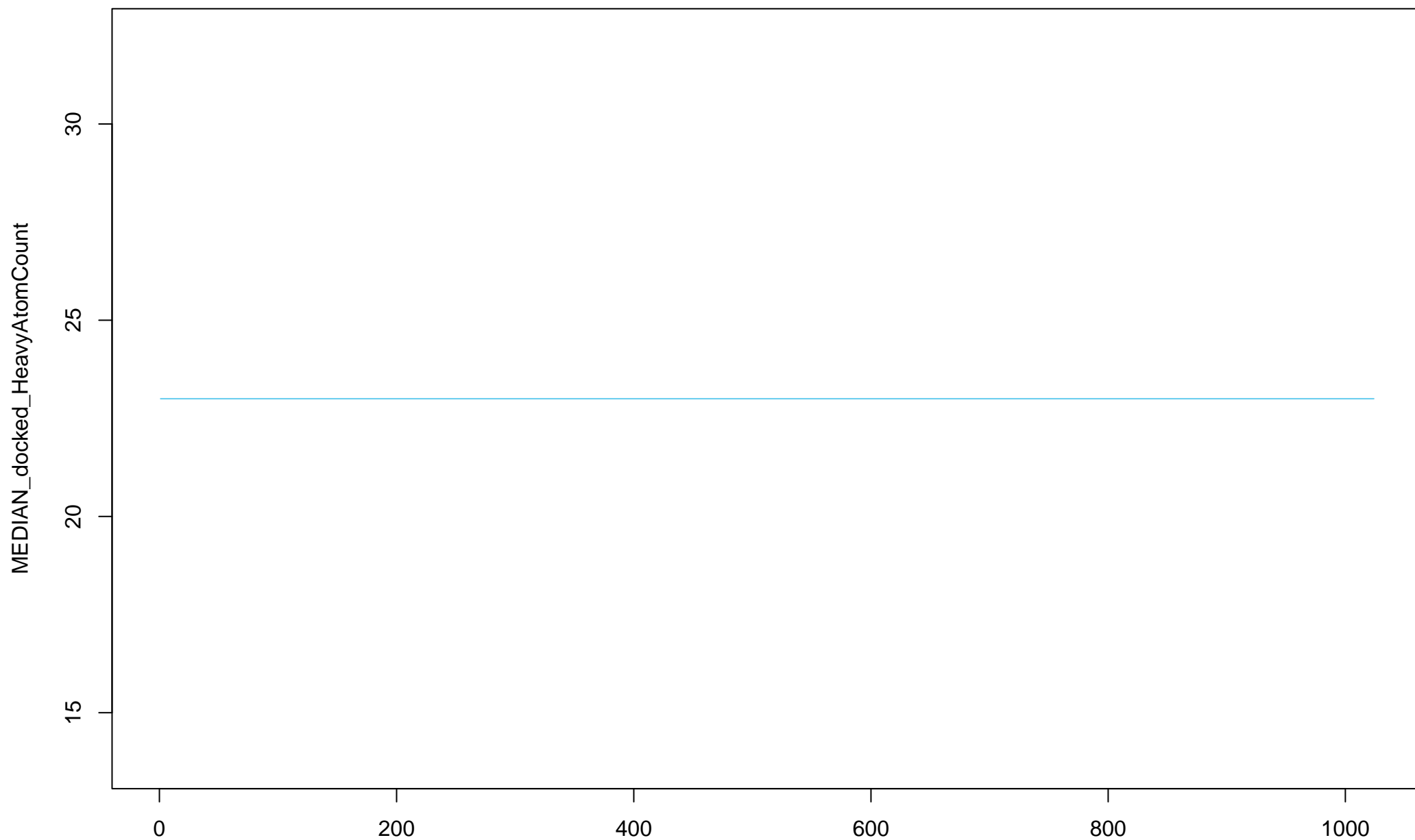
MEDIAN_logit_ec_tanimoto_similarity
ESS = 909 | BMK = 0.0681 | MCSE(6.27) = 4.01 | stat: TRUE | burn: 0



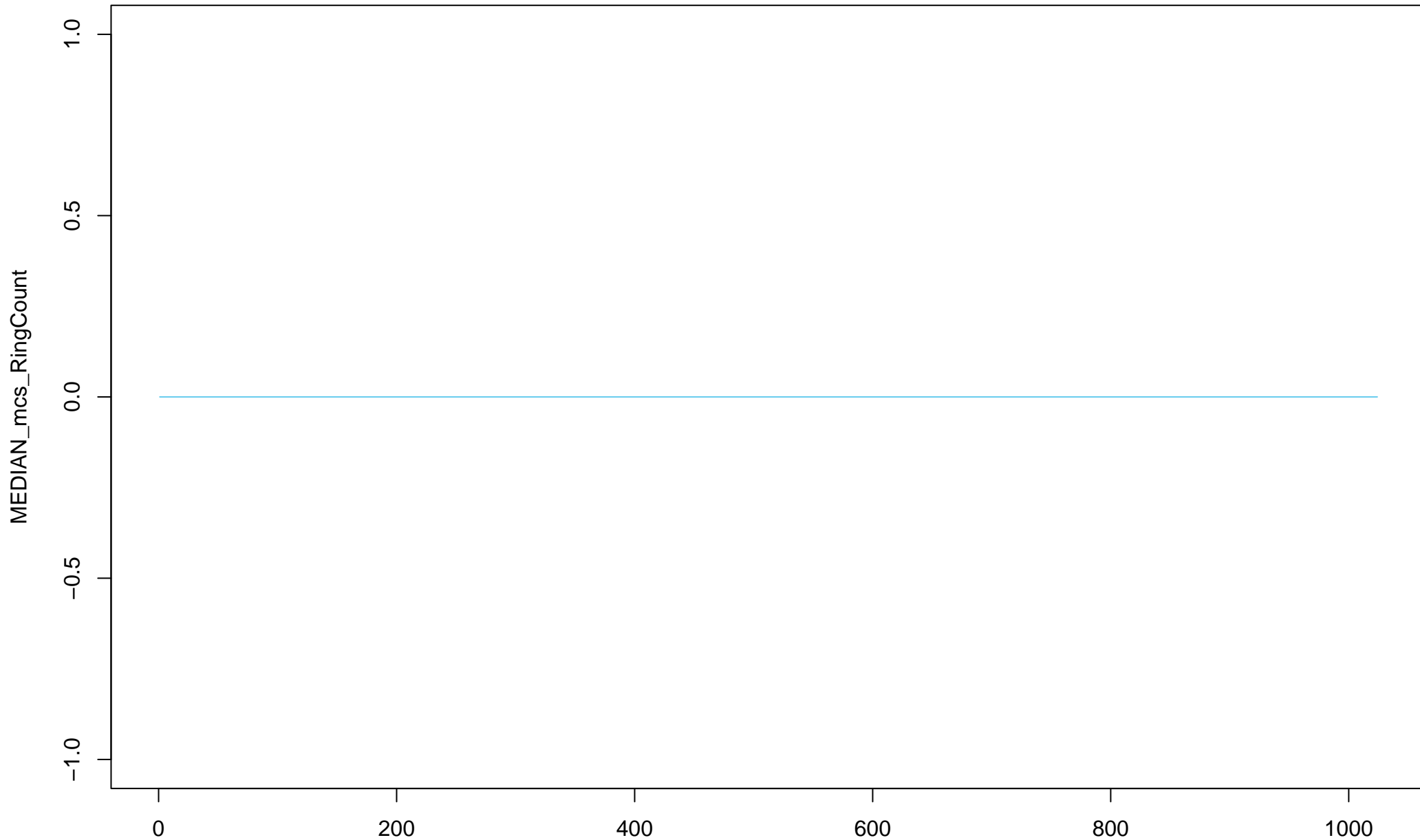
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



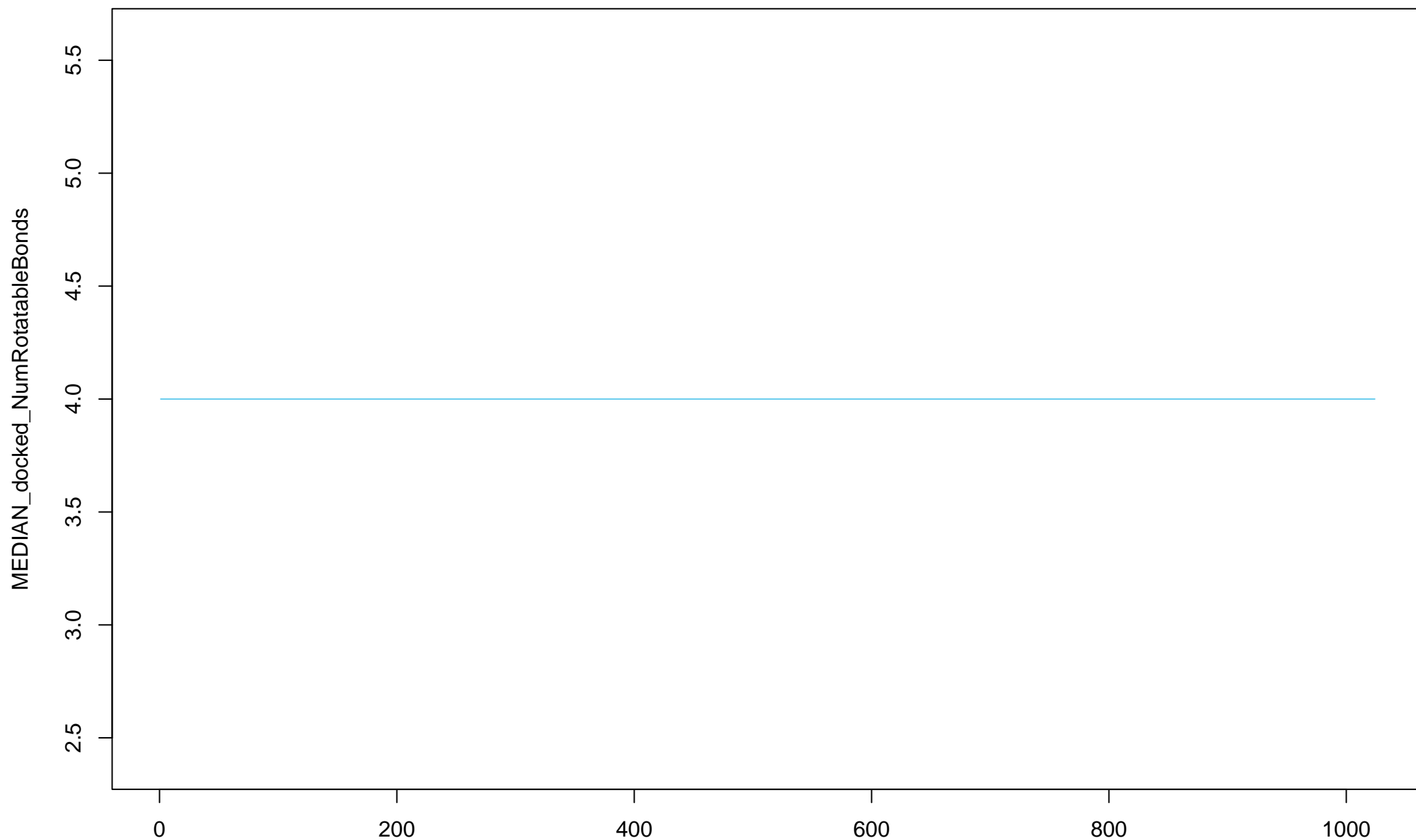
MEDIAN_docked_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



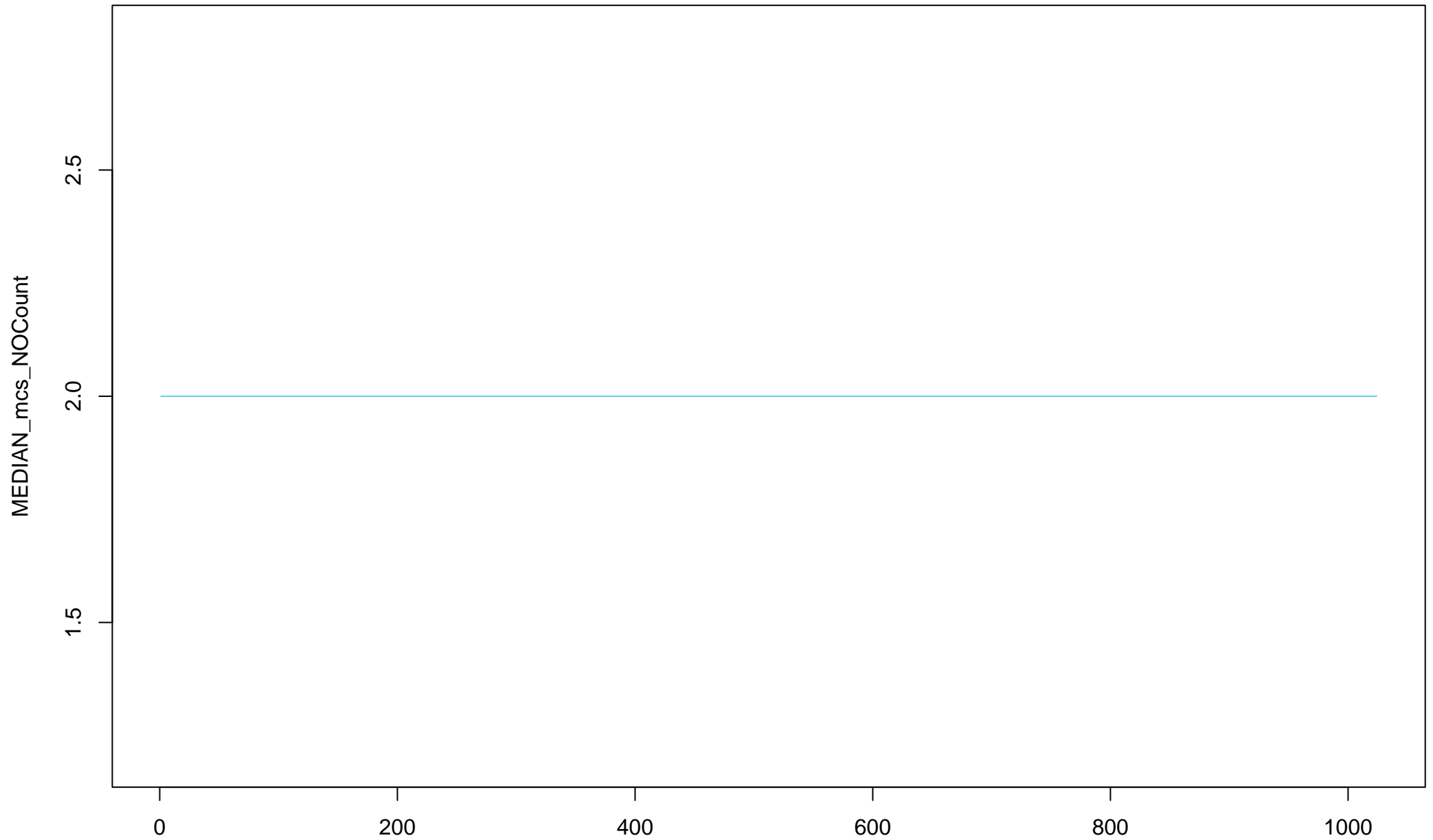
MEDIAN_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



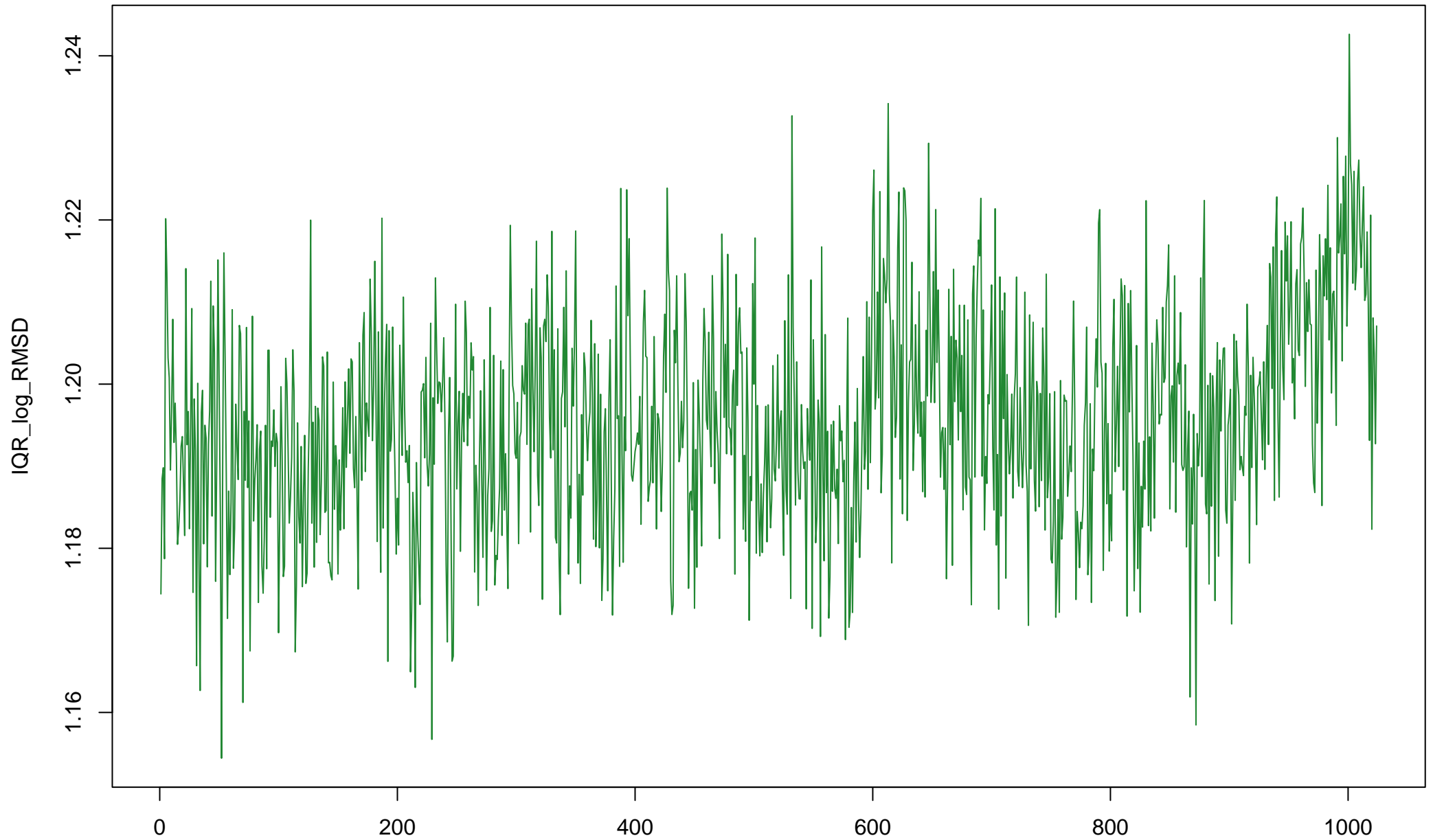
MEDIAN_docked_NumRotatableBonds
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



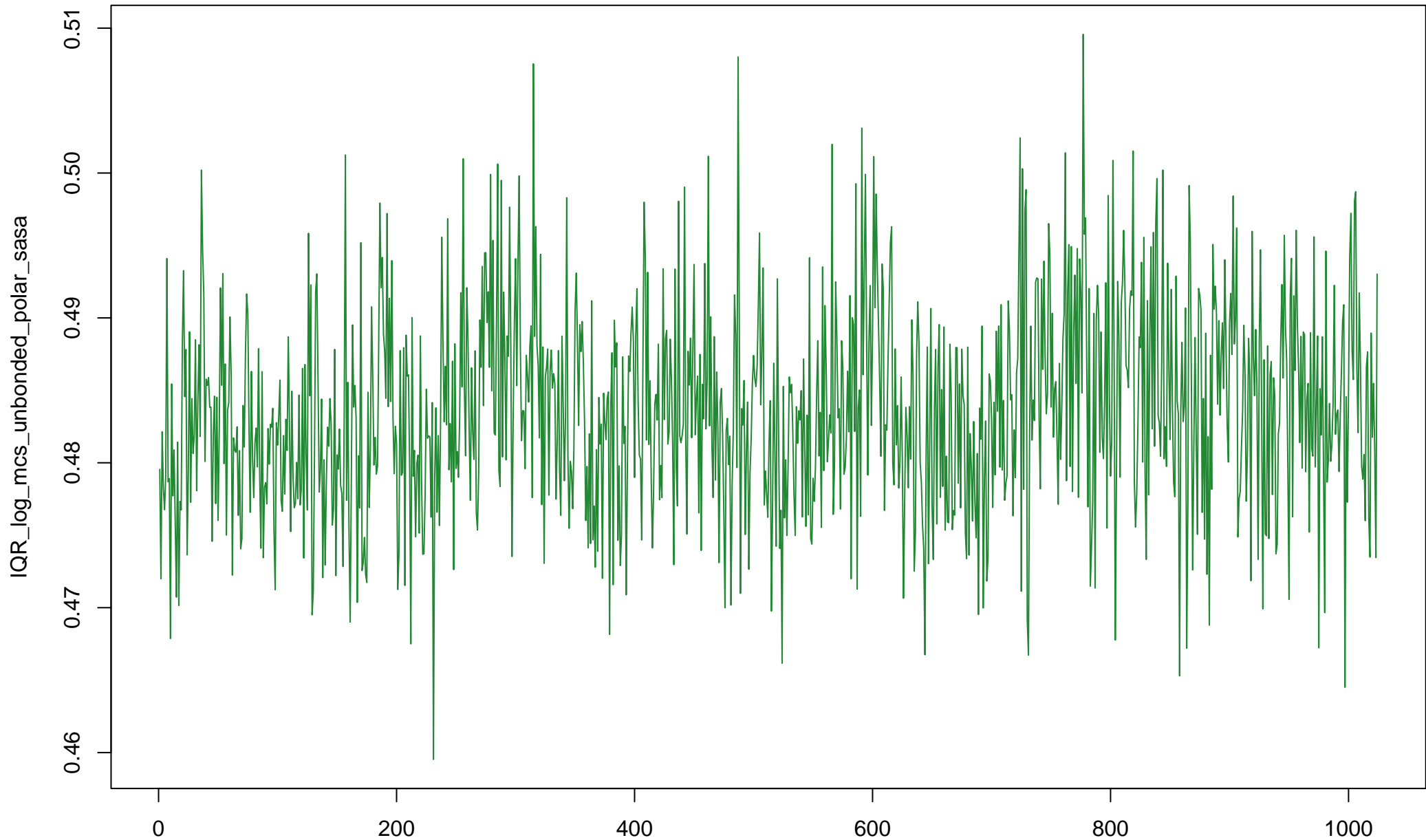
MEDIAN_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



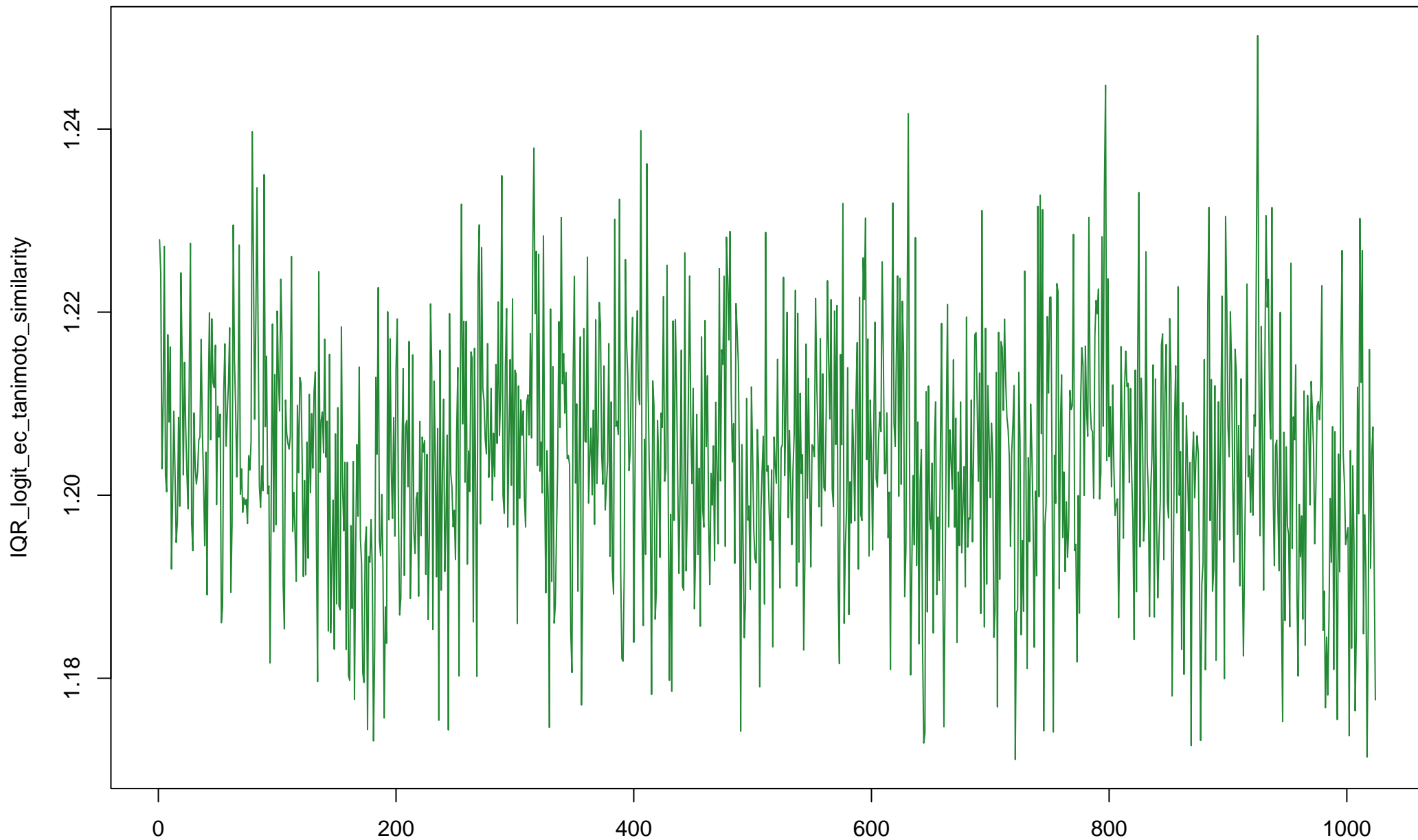
IQR_log_RMSD
ESS = 59.6 | BMK = 0.16 | MCSE(6.27) = 8.06 | stat: FALSE | burn: 0



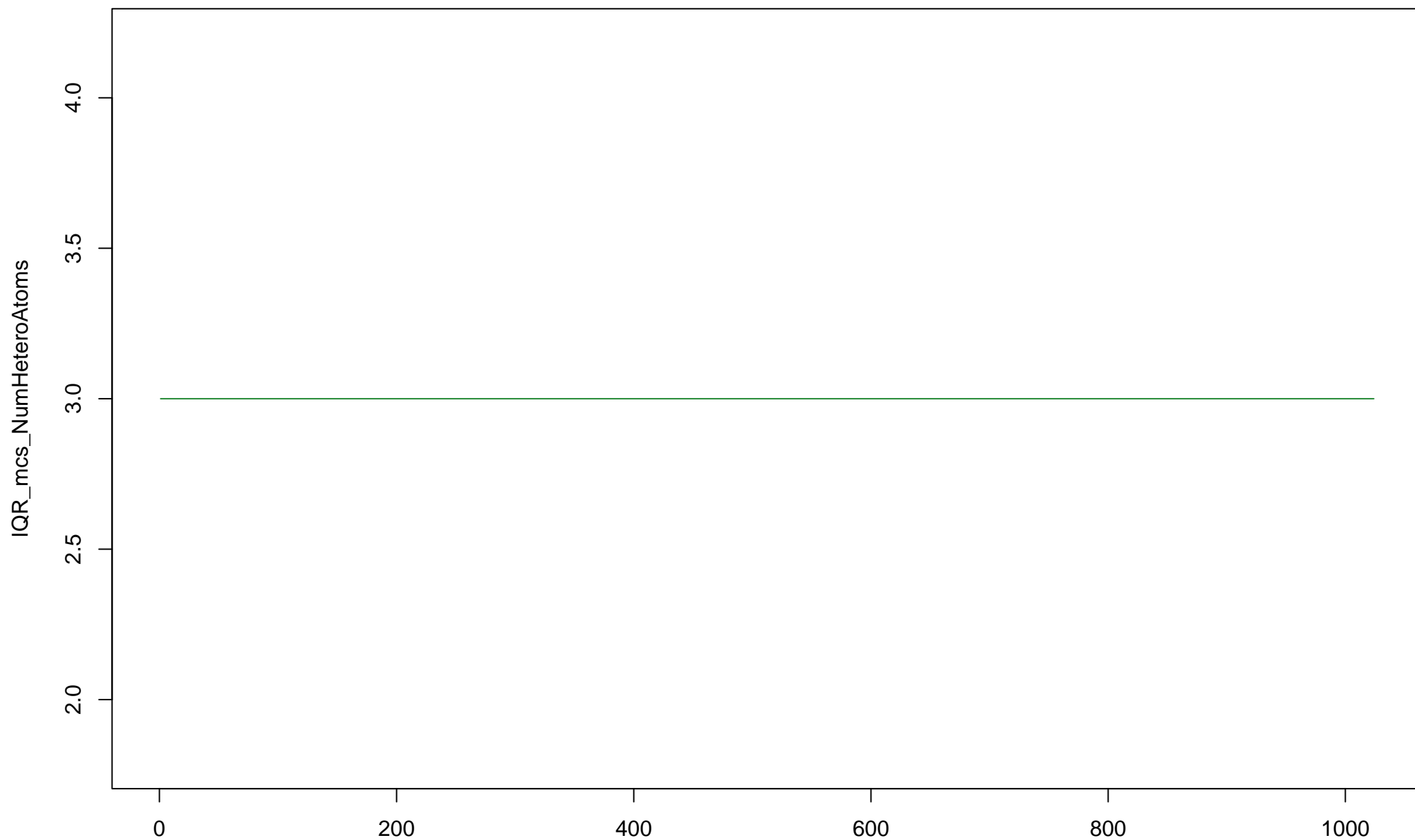
IQR_log_mcs_unbonded_polar_sasa
ESS = 276 | BMK = 0.0994 | MCSE(6.27) = 5.69 | stat: FALSE | burn: 0



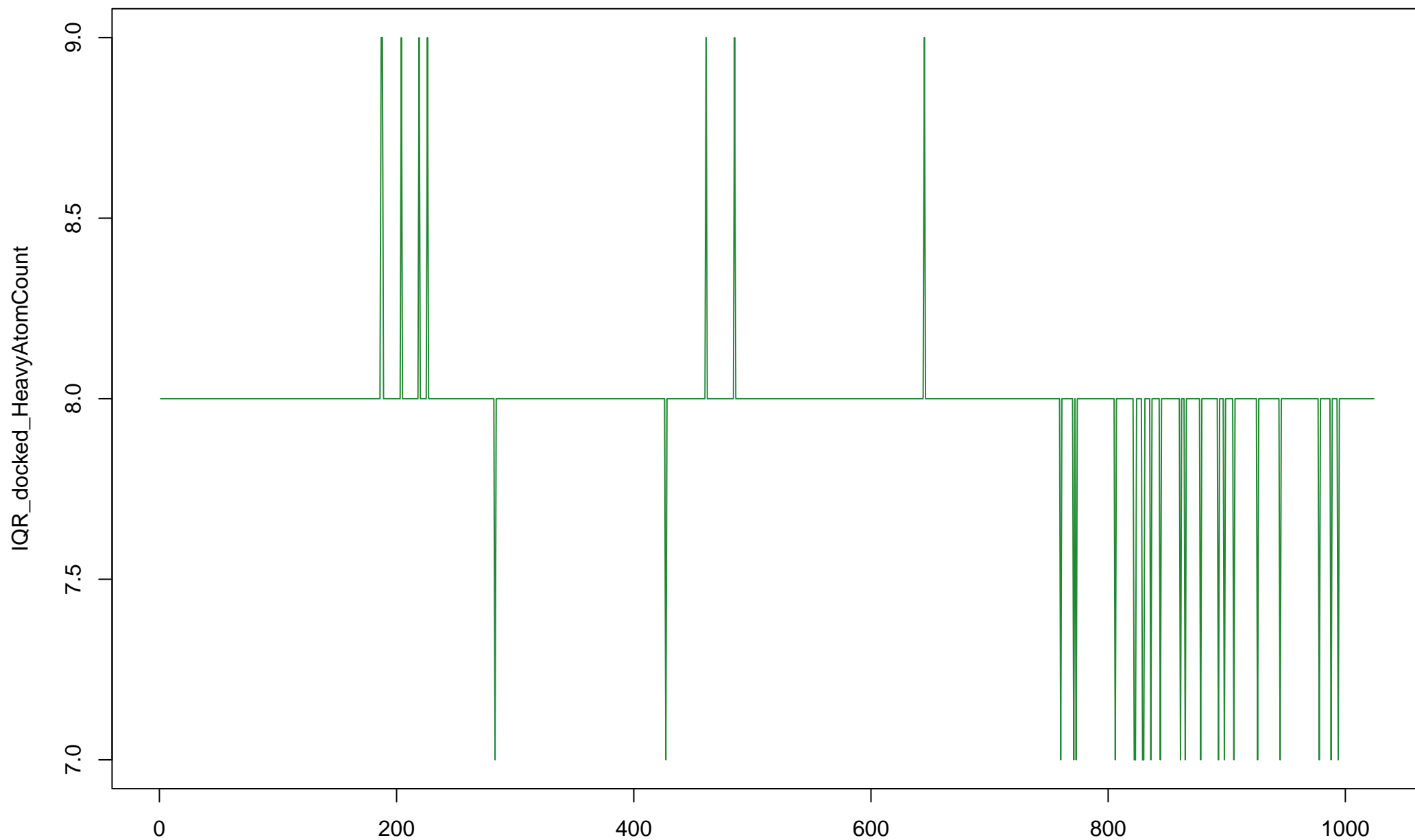
IQR_logit_ec_tanimoto_similarity
ESS = 368 | BMK = 0.0449 | MCSE(6.27) = 5.36 | stat: FALSE | burn: 0



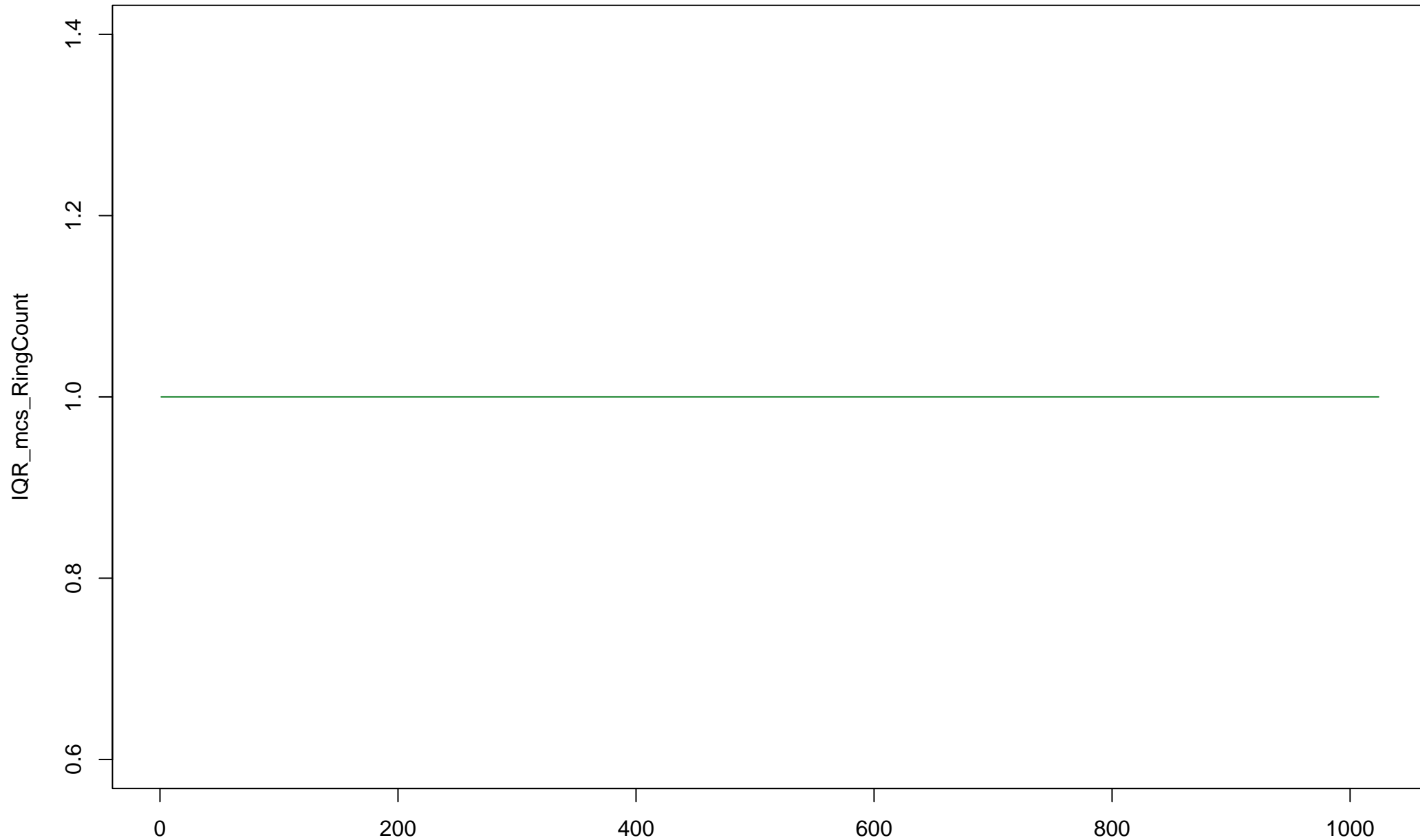
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



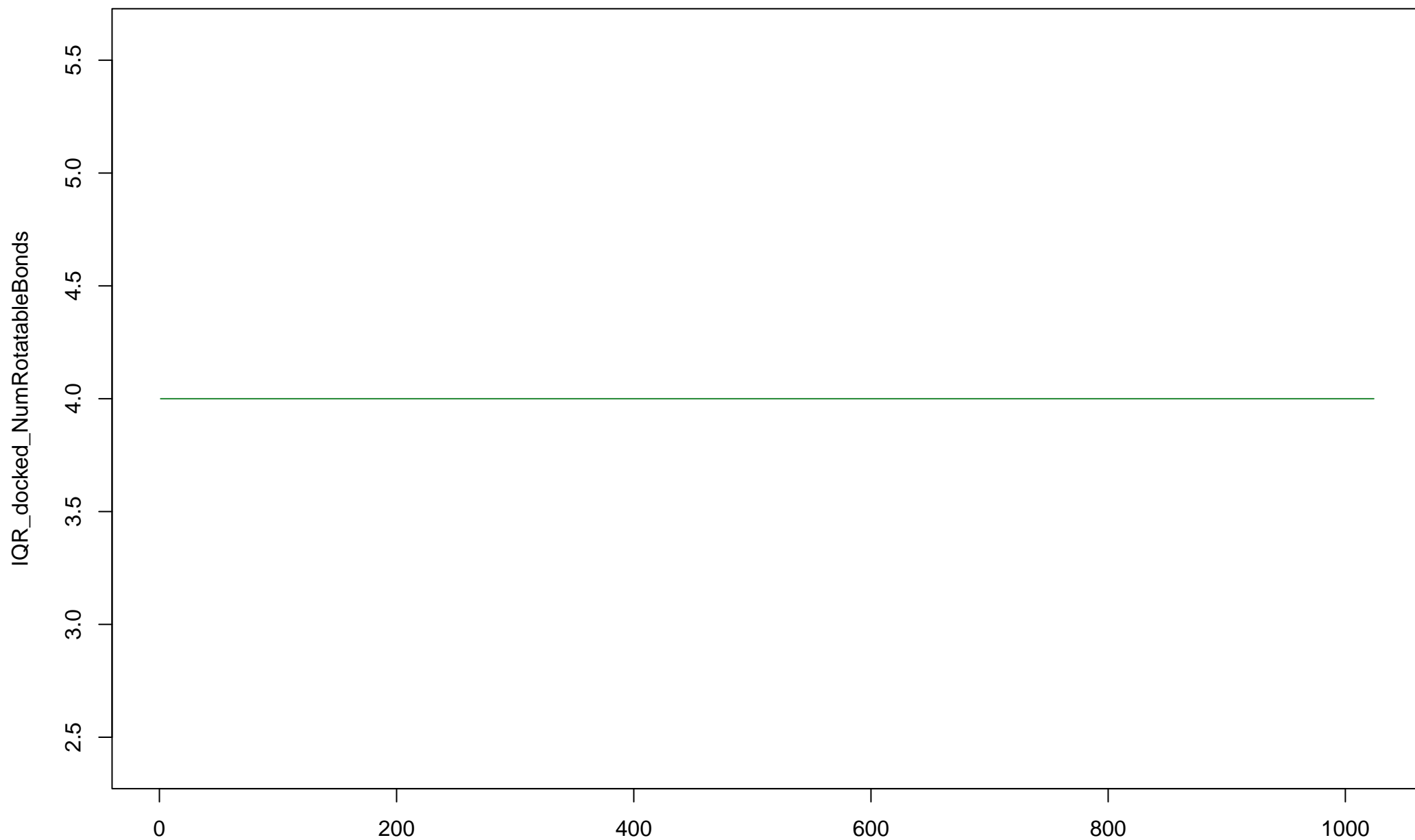
IQR_docked_HeavyAtomCount
ESS = 211 | BMK = 0.222 | MCSE(6.27) = 4.78 | stat: FALSE | burn: 612



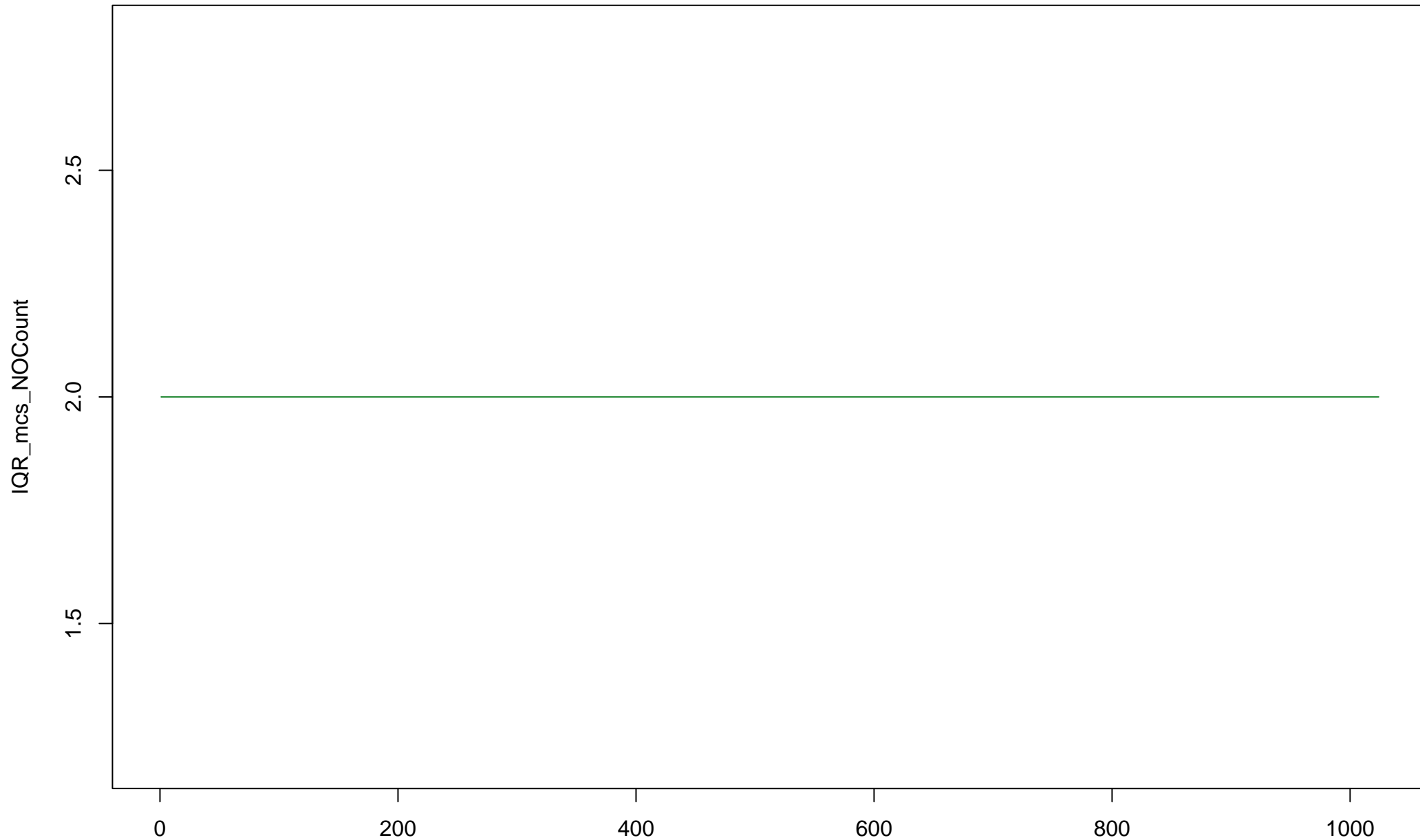
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



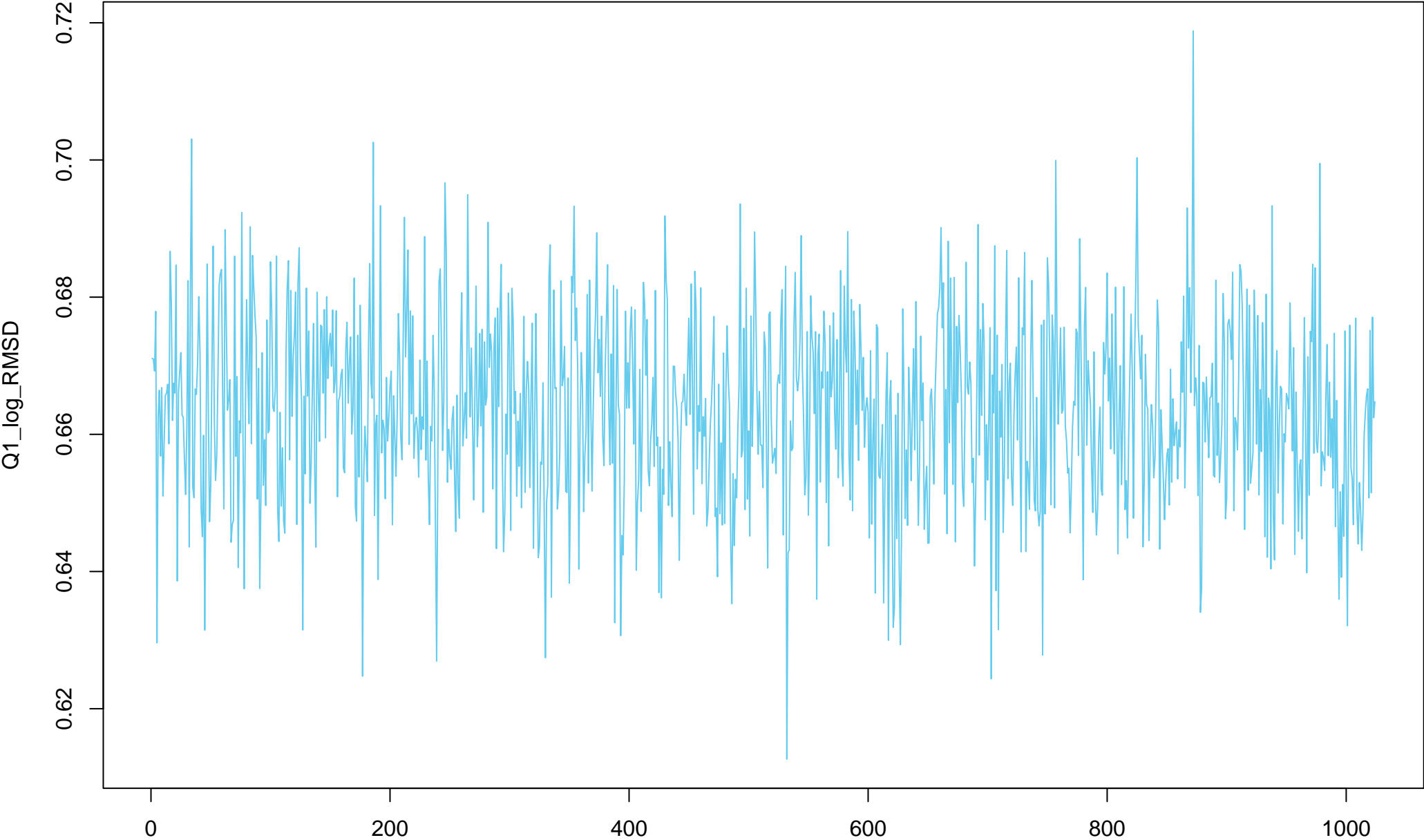
IQR_docked_NumRotatableBonds
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



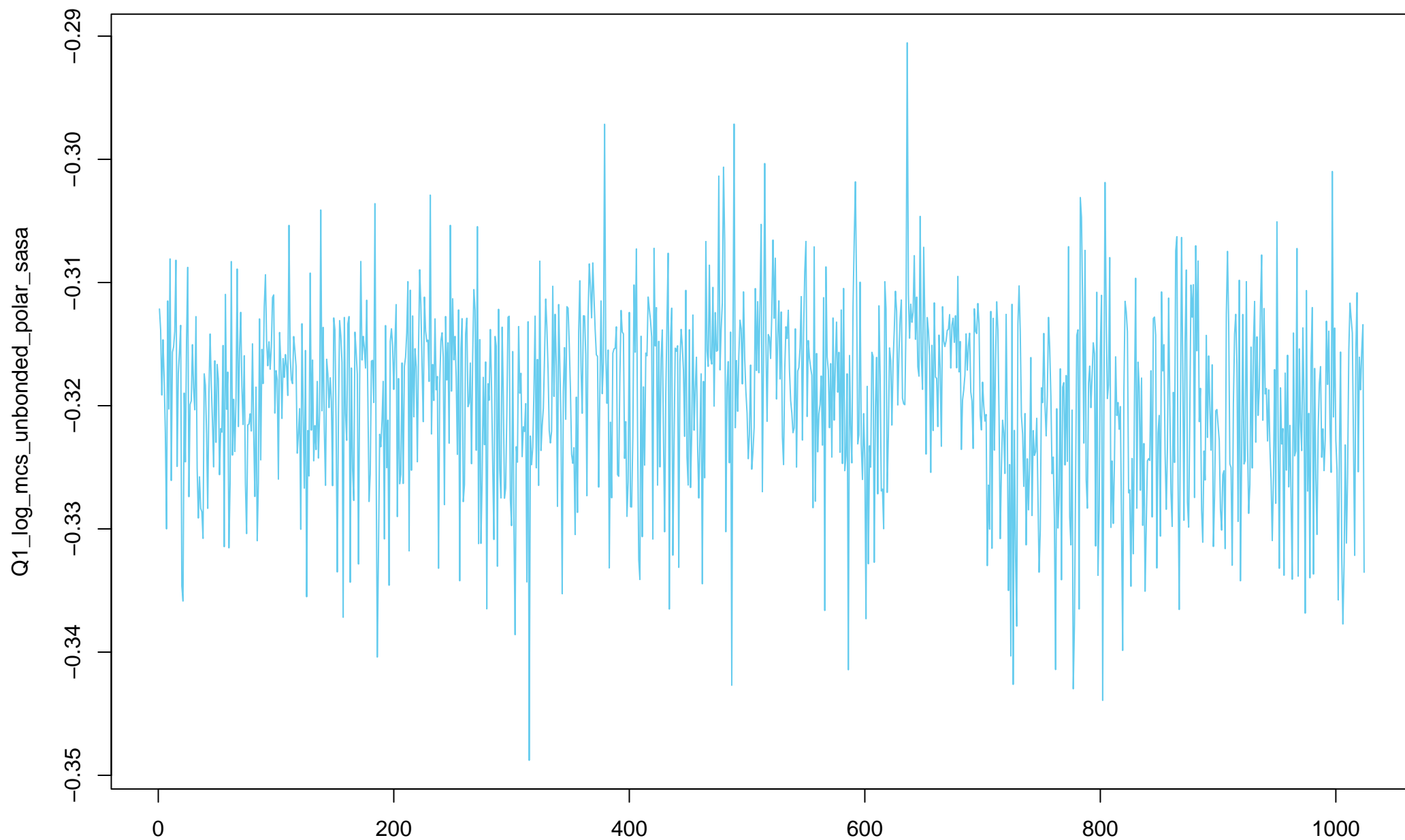
IQR_mcs_NOCOUNT
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



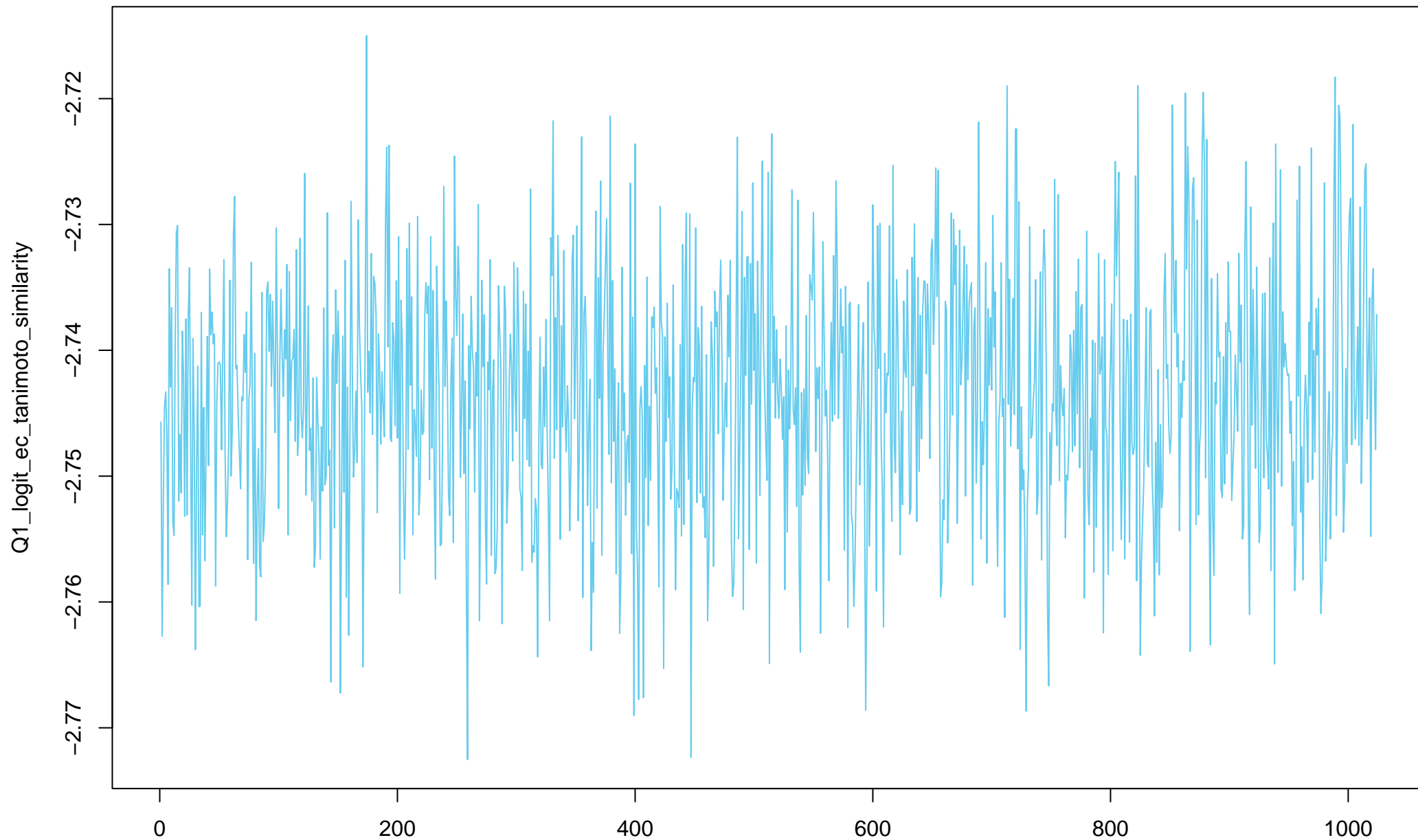
Q1_log_RMSD
ESS = 871 | BMK = 0.0621 | MCSE(6.27) = 3.83 | stat: TRUE | burn: 0



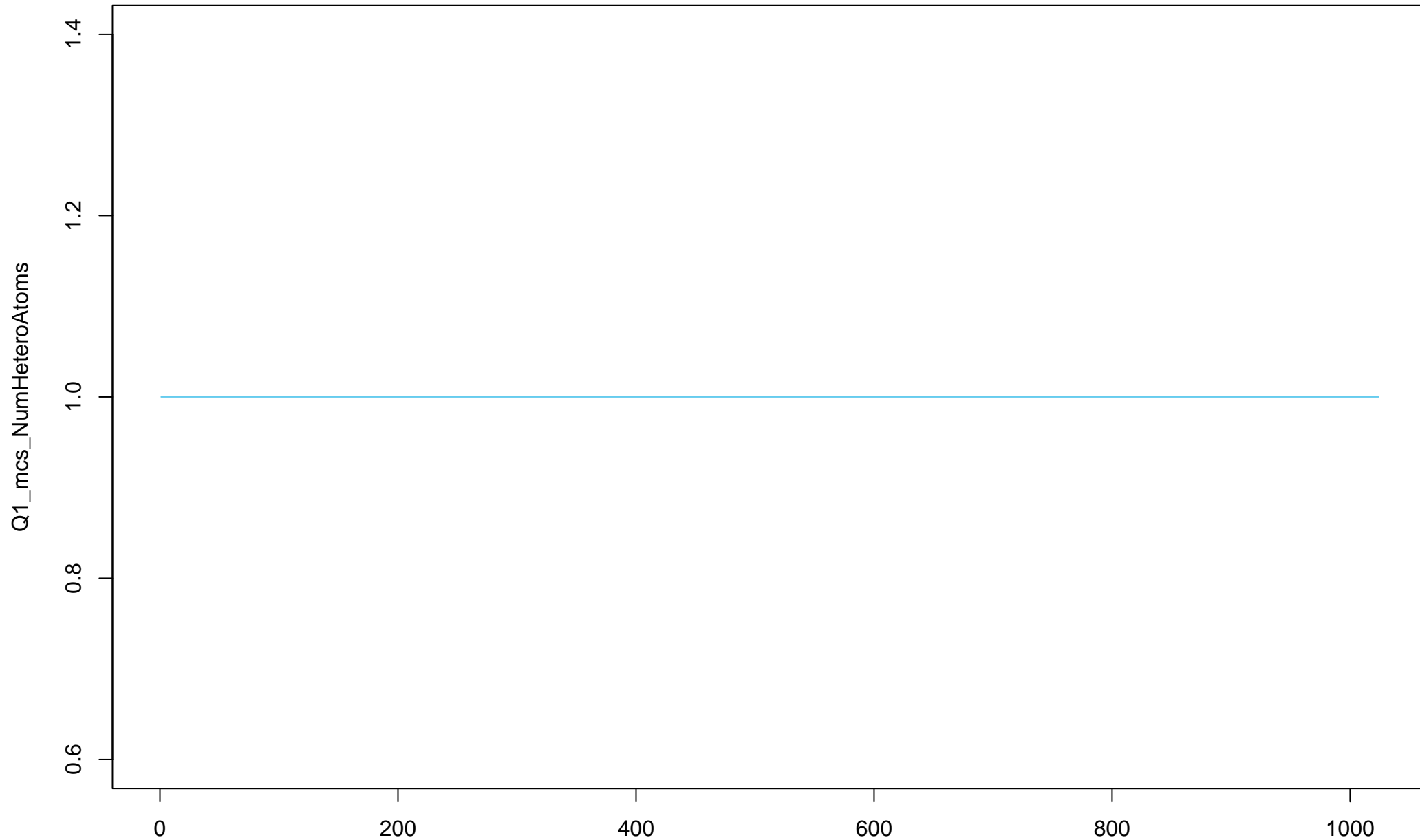
Q1_log_mcs_unbonded_polar_sasa
ESS = 273 | BMK = 0.0823 | MCSE(6.27) = 5.2 | stat: TRUE | burn: 0



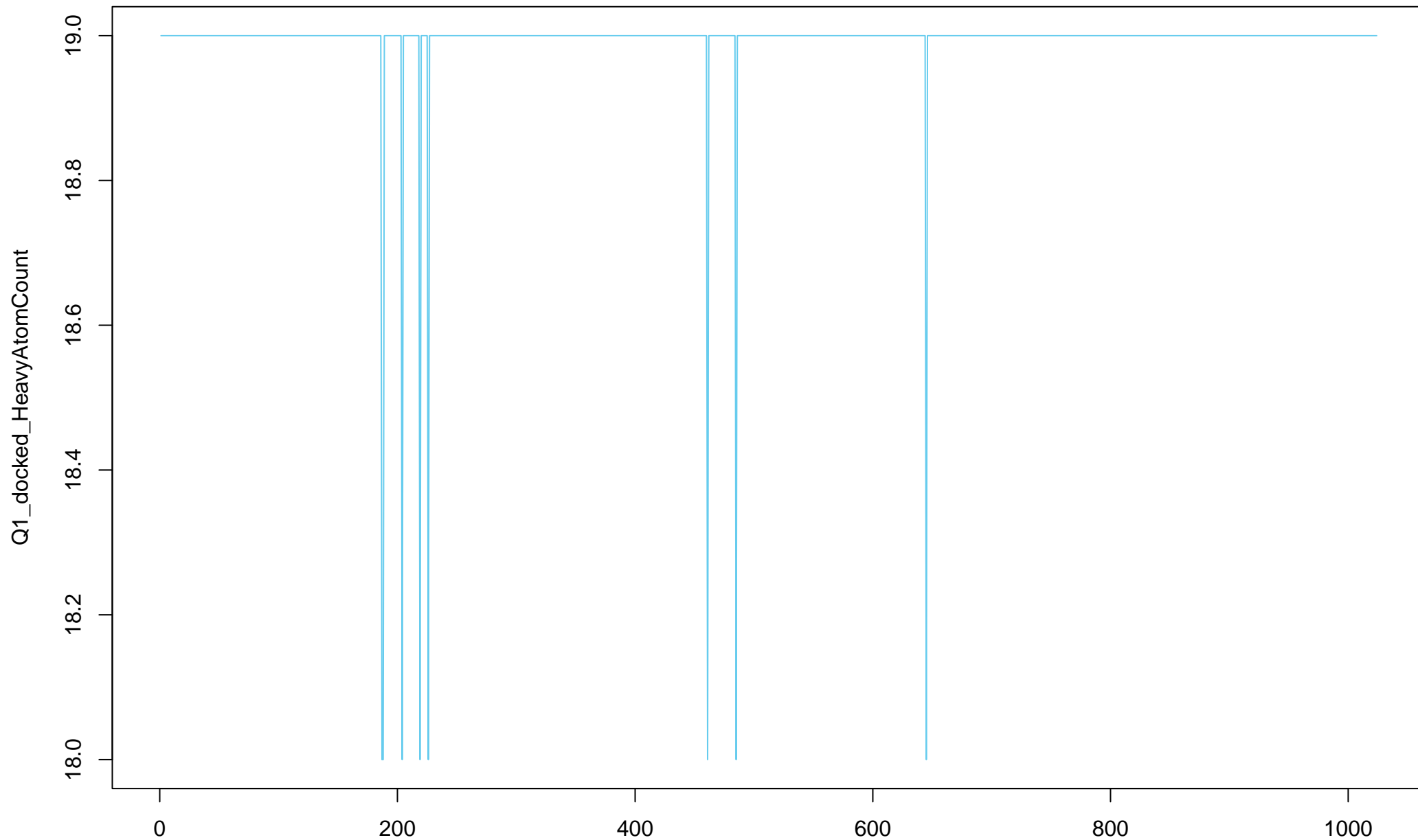
Q1_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0695 | MCSE(6.27) = 3.64 | stat: TRUE | burn: 0



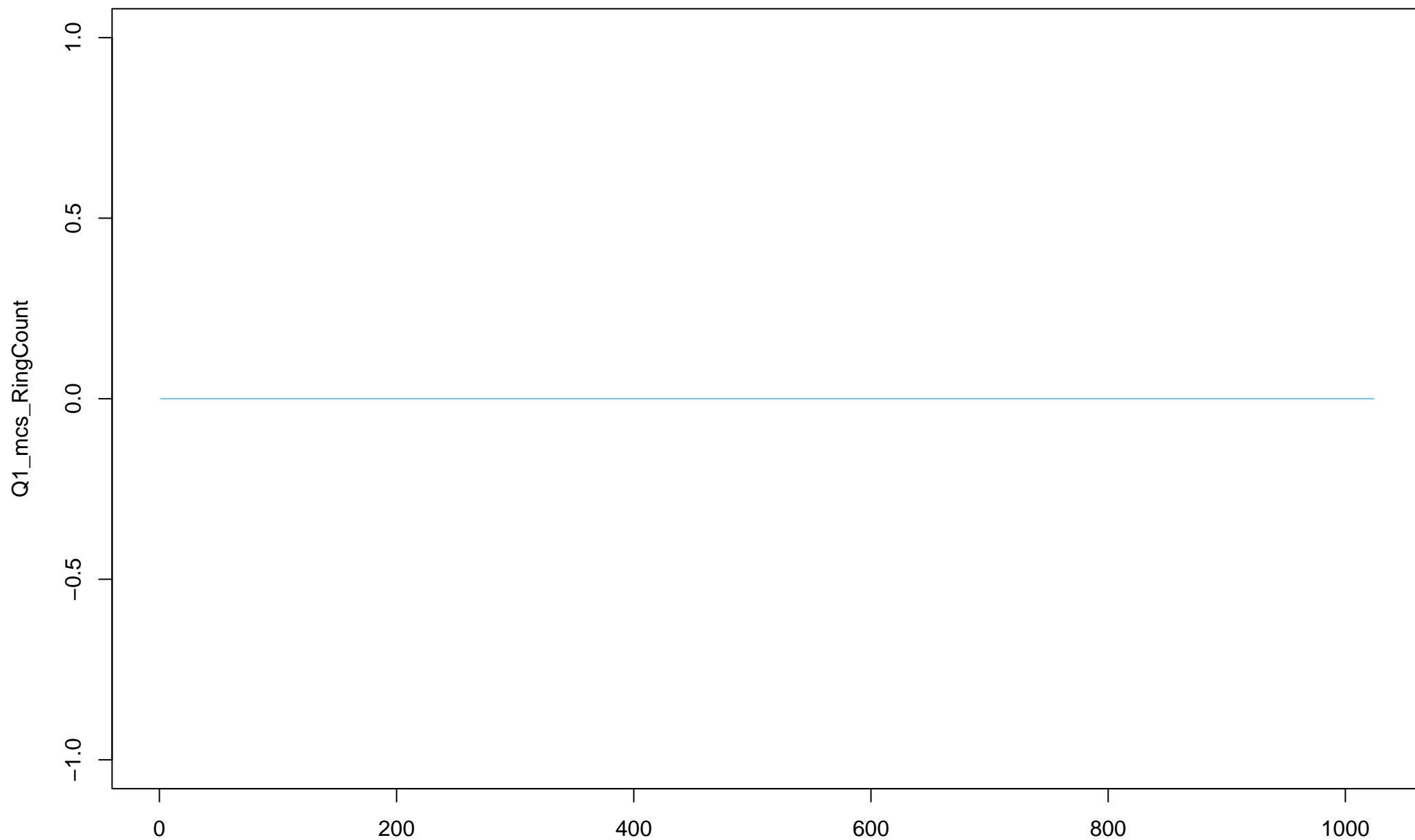
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



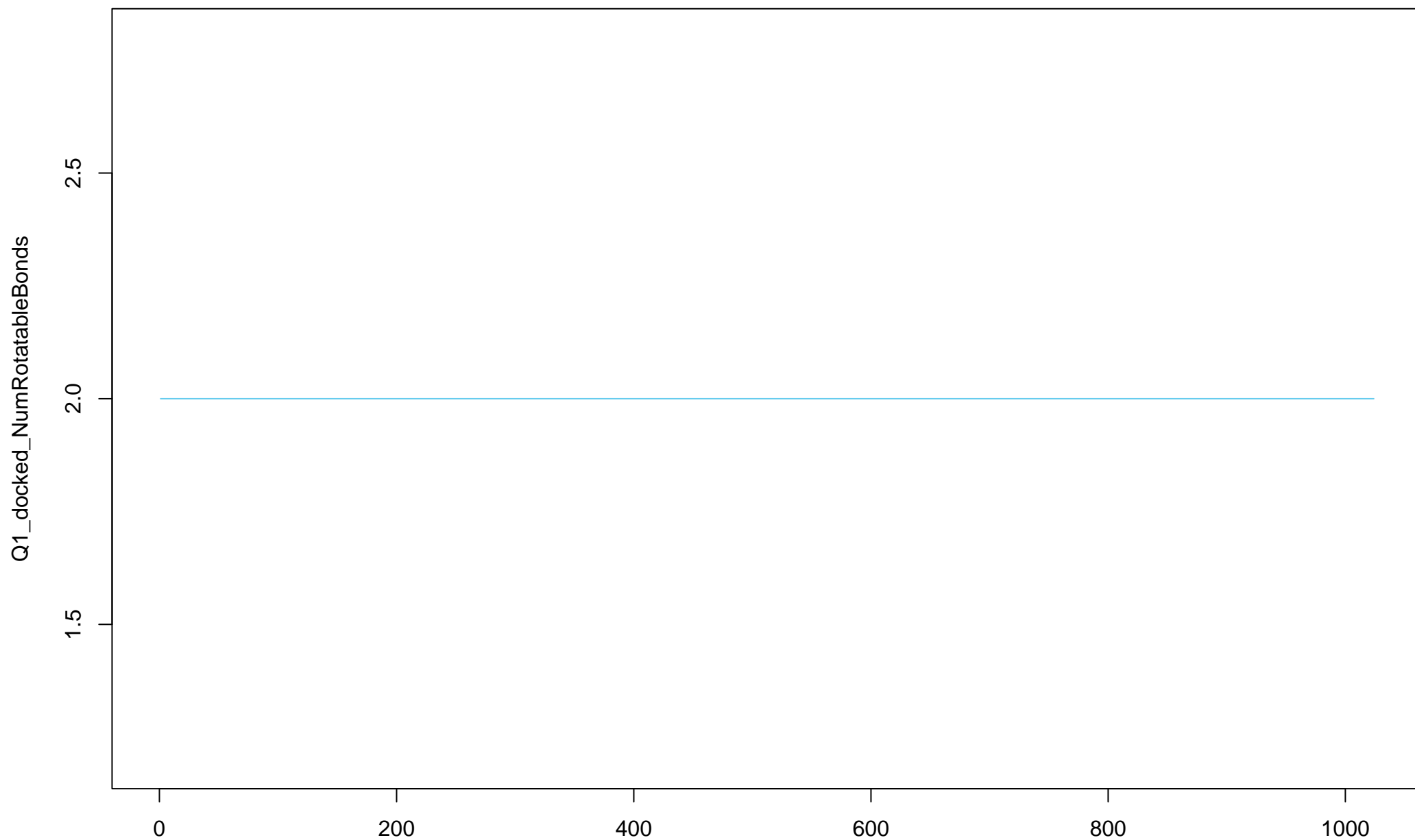
Q1_docked_HeavyAtomCount
ESS = 317 | BMK = 0.309 | MCSE(6.27) = 3.56 | stat: TRUE | burn: 0



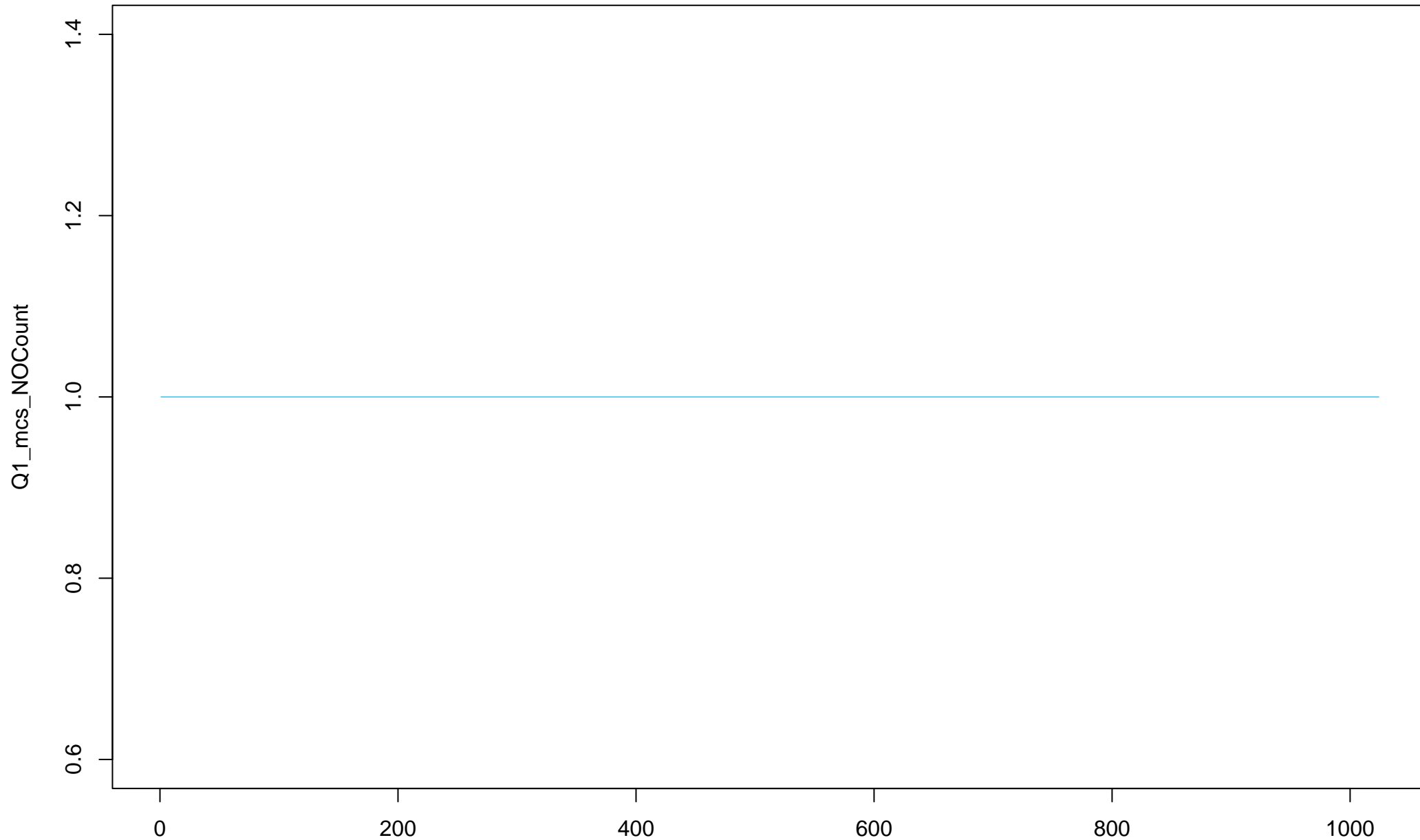
Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



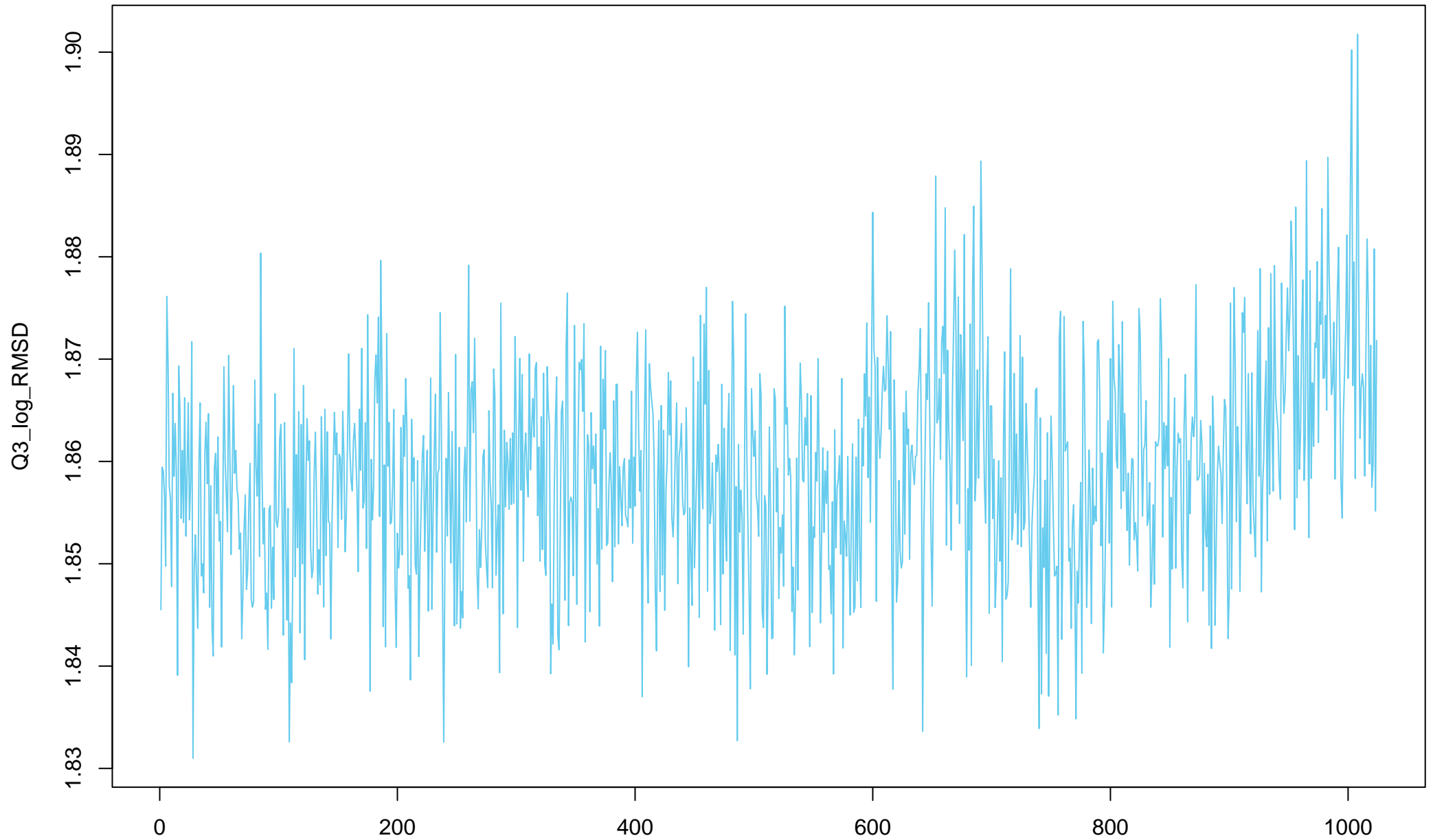
Q1_docked_NumRotatableBonds
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



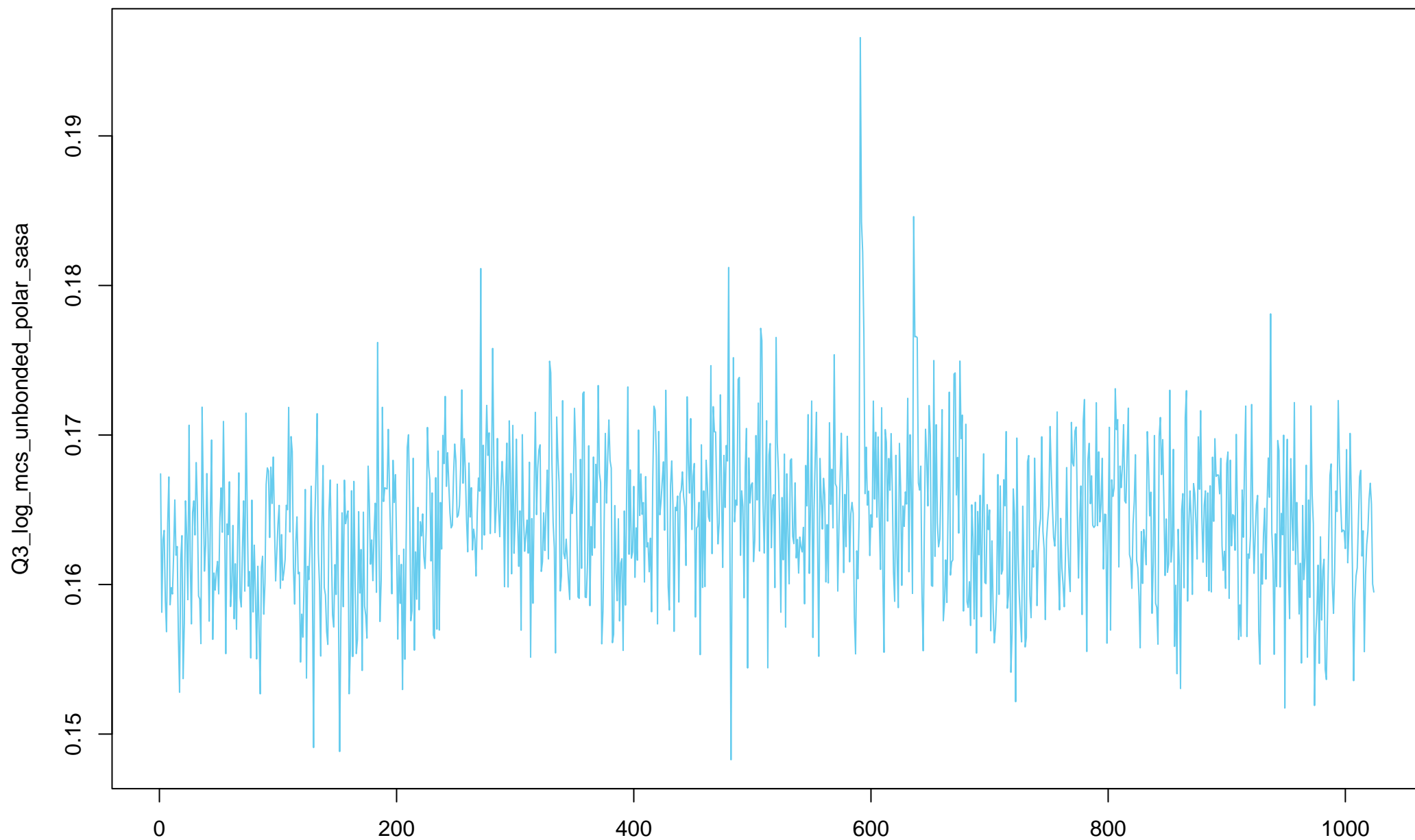
Q1_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



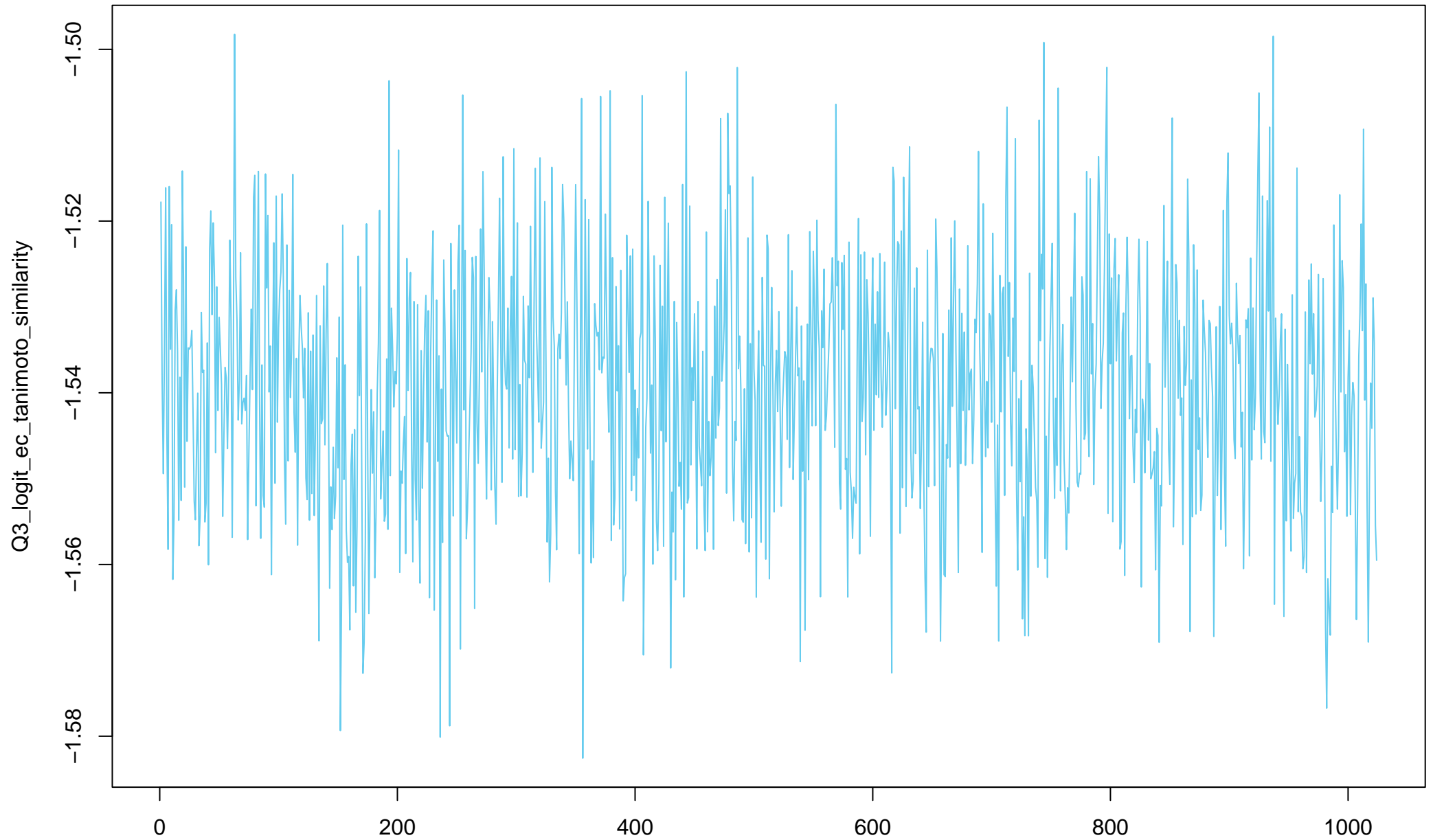
Q3_log_RMSD
ESS = 79 | BMK = 0.167 | MCSE(6.27) = 7.74 | stat: FALSE | burn: 0



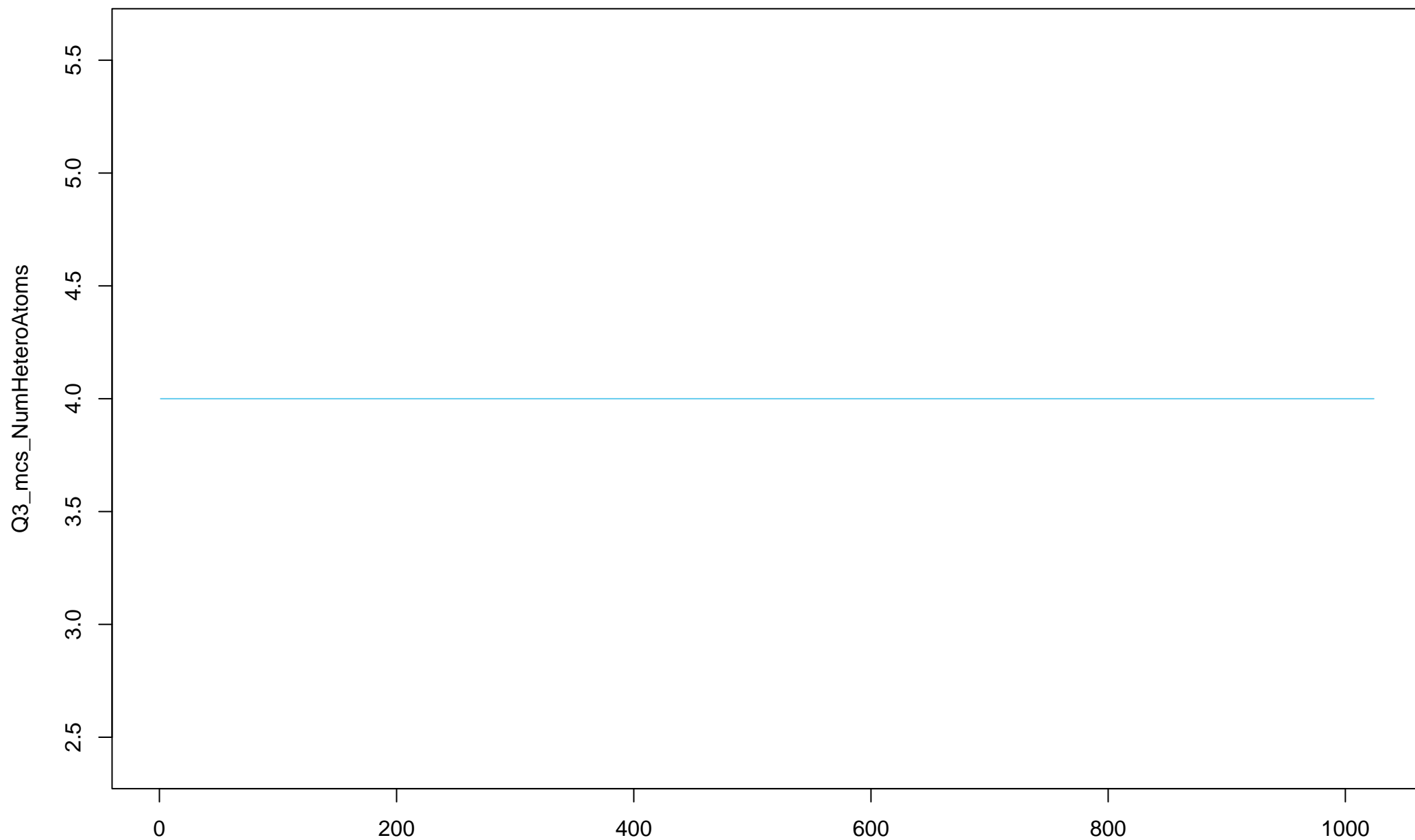
Q3_log_mcs_unbonded_polar_sasa
ESS = 247 | BMK = 0.0611 | MCSE(6.27) = 6.25 | stat: FALSE | burn: 0



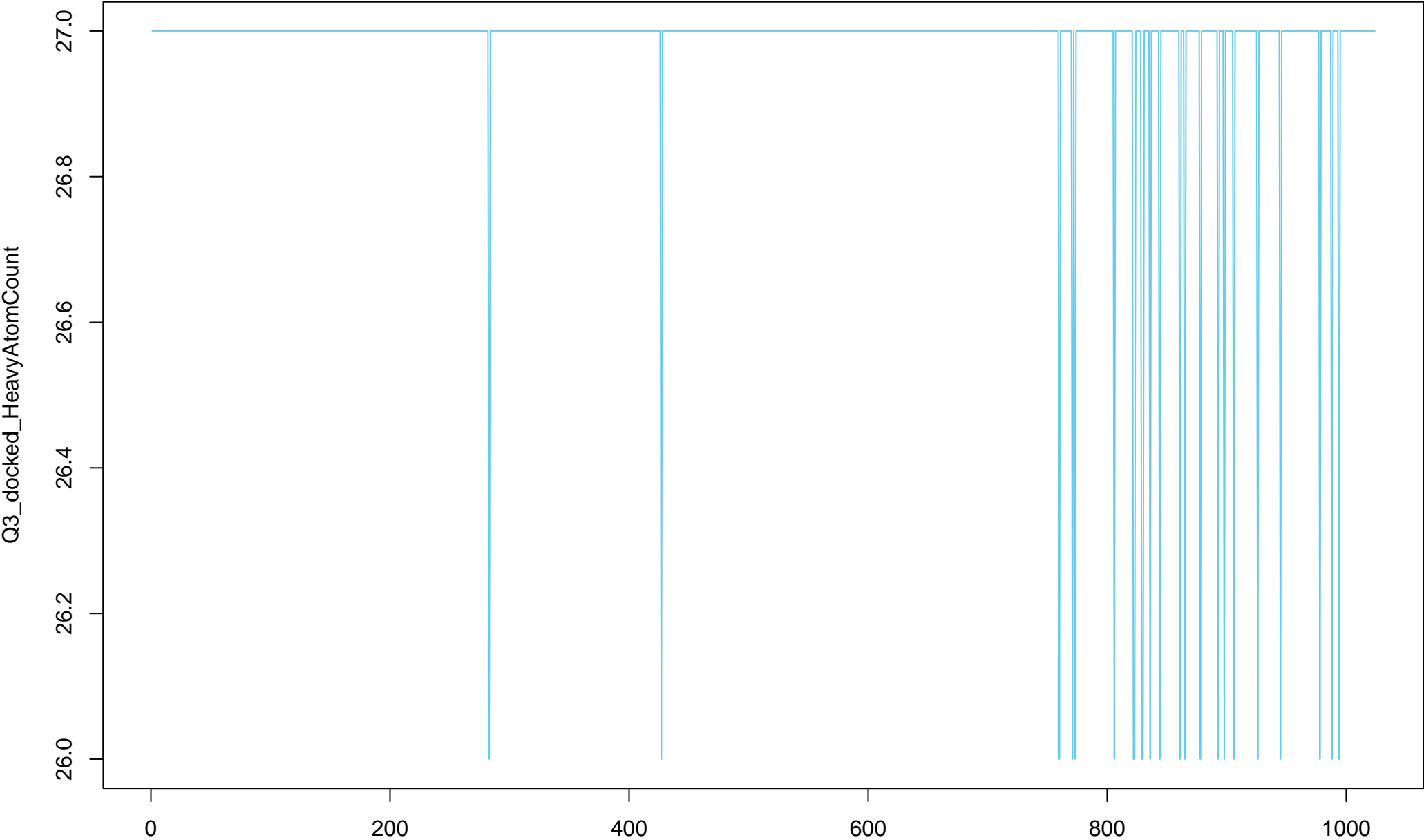
Q3_logit_ec_tanimoto_similarity
ESS = 930 | BMK = 0.0588 | MCSE(6.27) = 4.23 | stat: TRUE | burn: 0



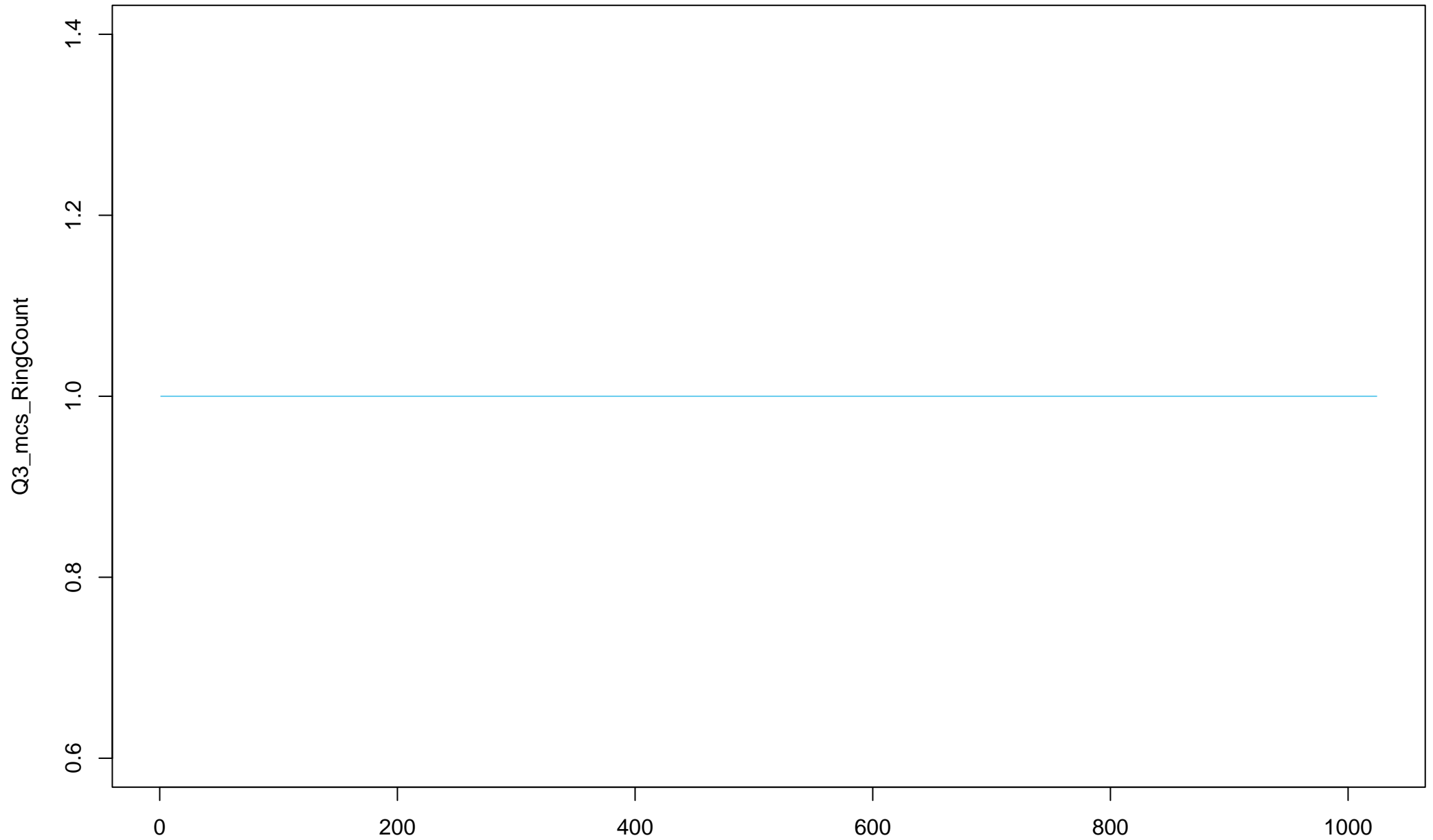
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



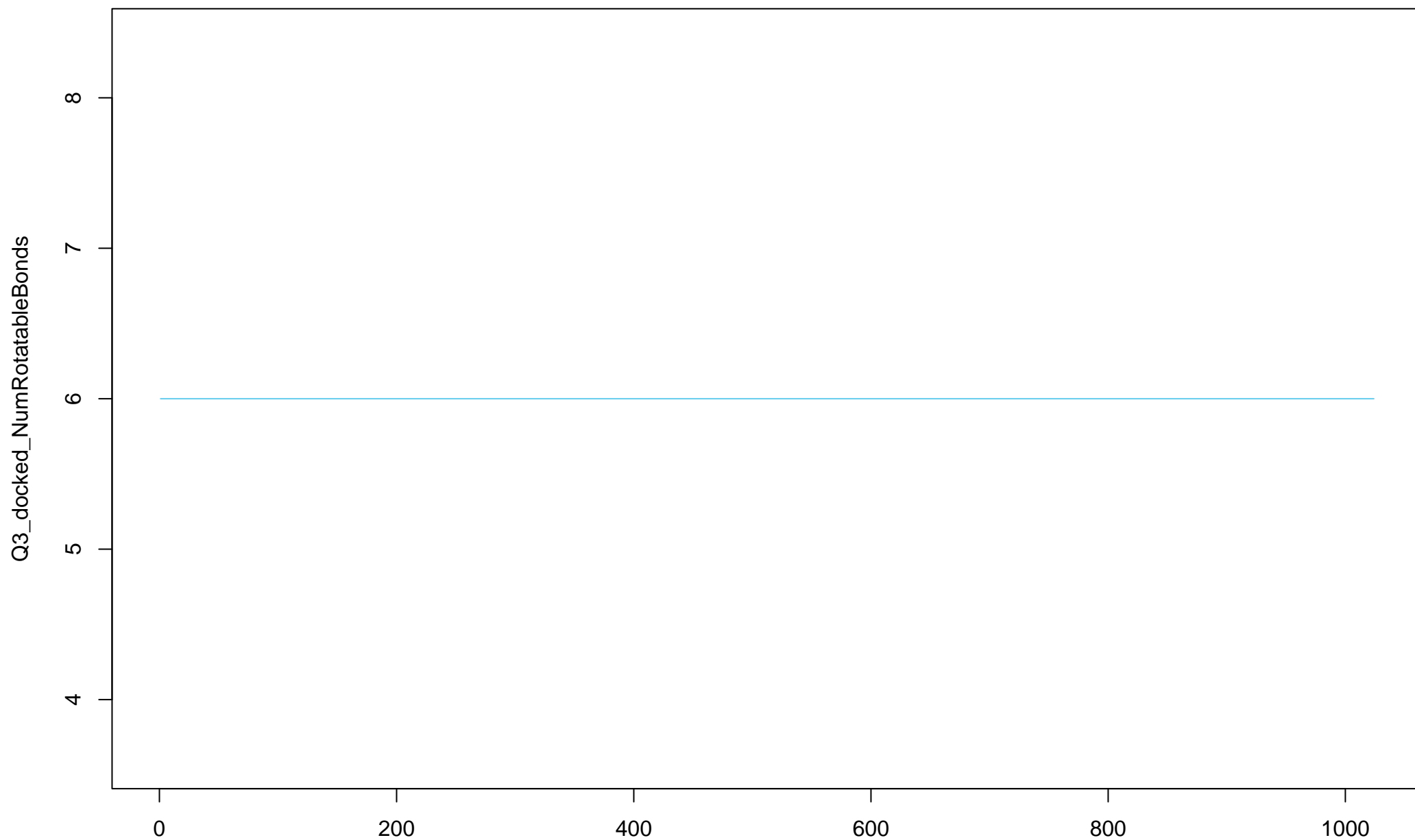
Q3_docked_HeavyAtomCount
ESS = 229 | BMK = 0.357 | MCSE(6.27) = 4.66 | stat: FALSE | burn: 0



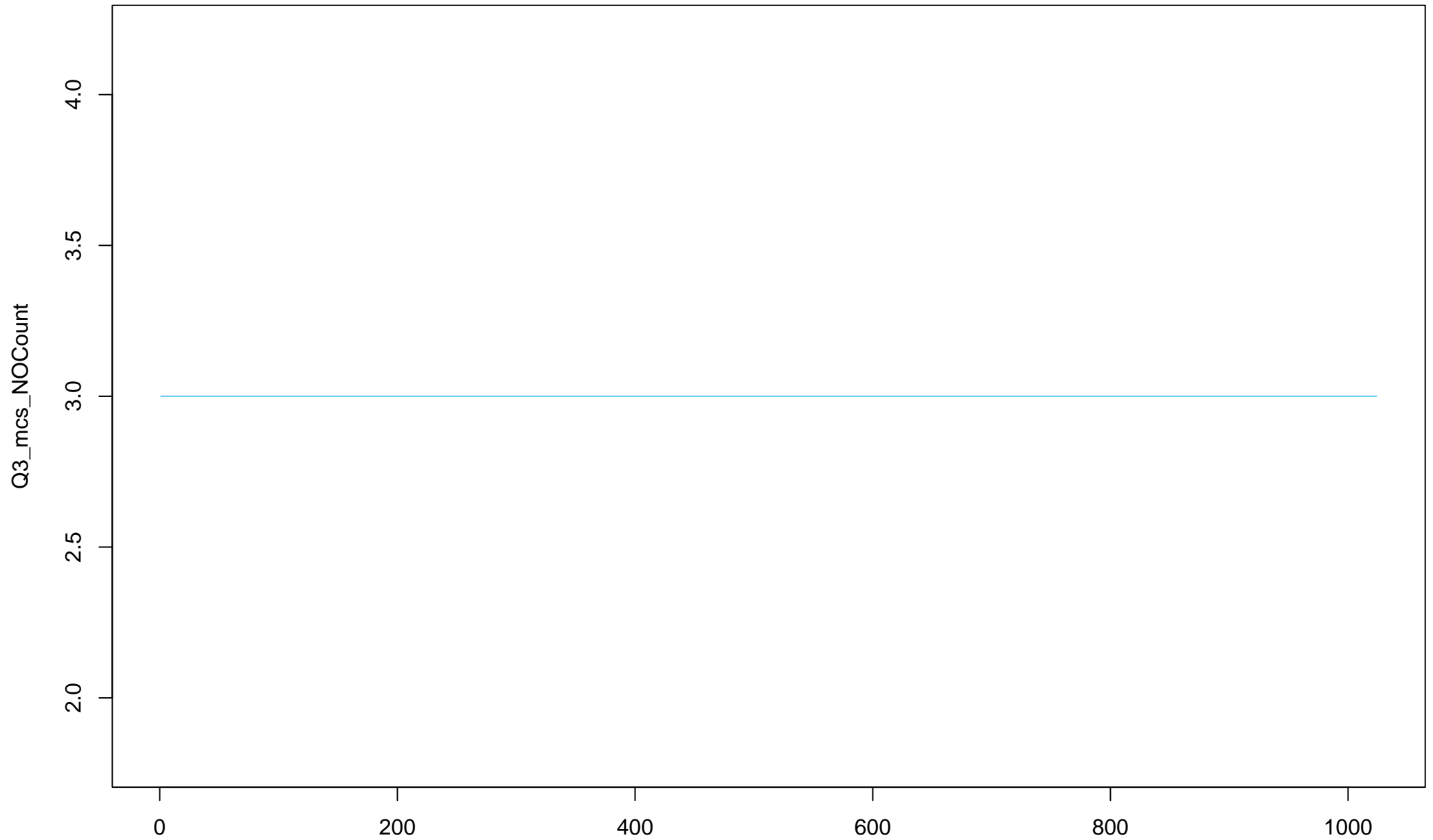
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



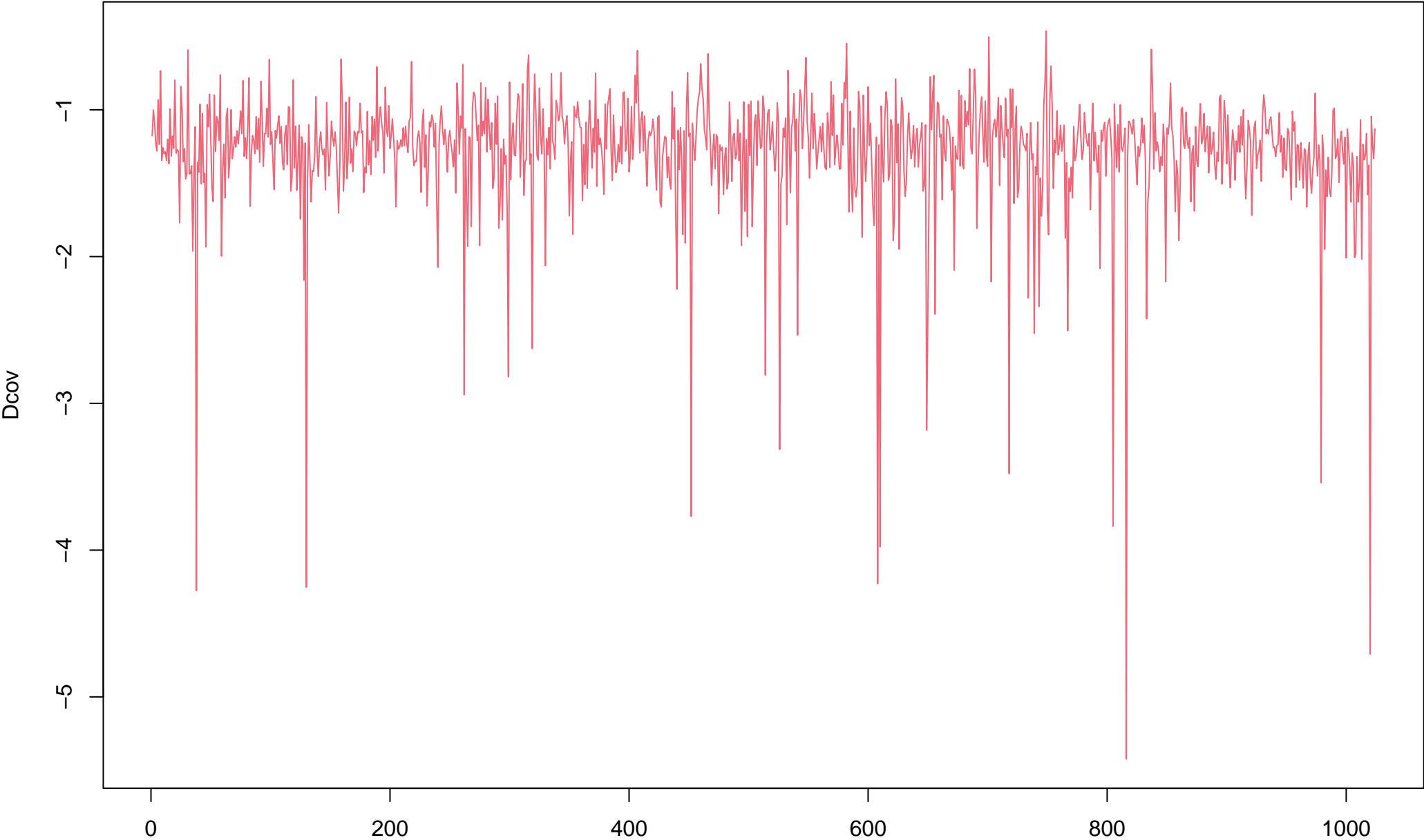
Q3_docked_NumRotatableBonds
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



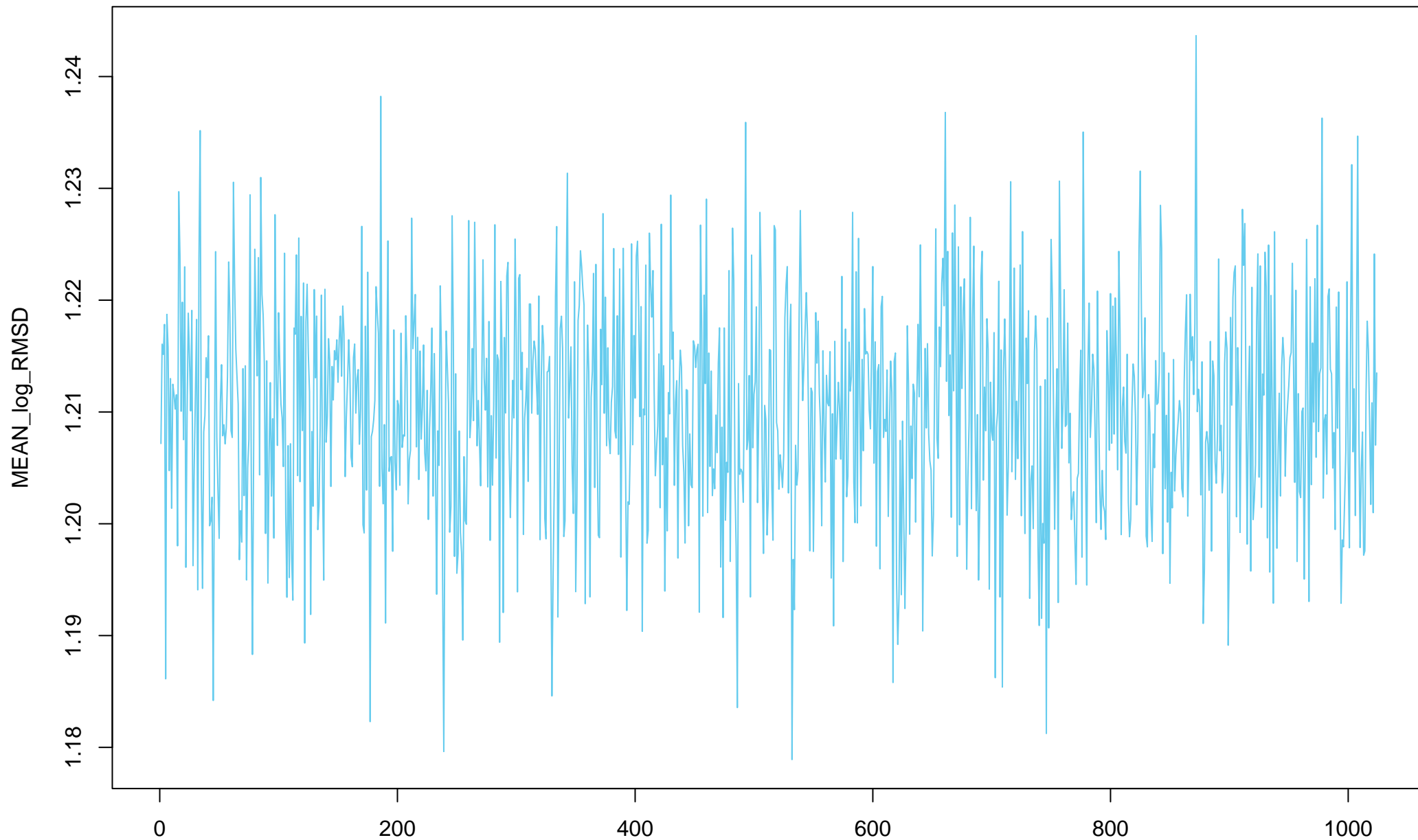
Q3_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



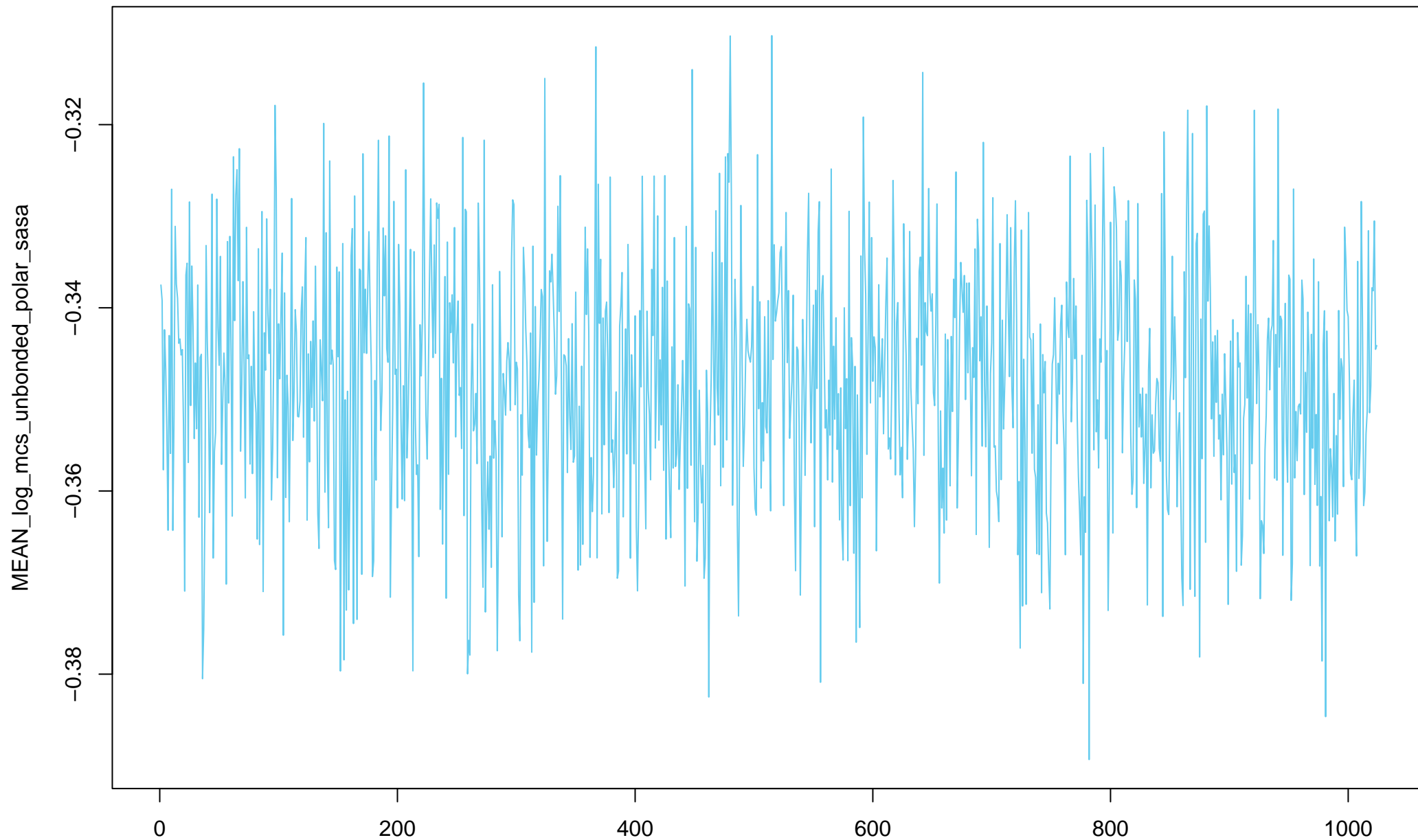
Dcov
ESS = 909 | BMK = 0.0854 | MCSE(6.27) = 3.88 | stat: TRUE | burn: 0



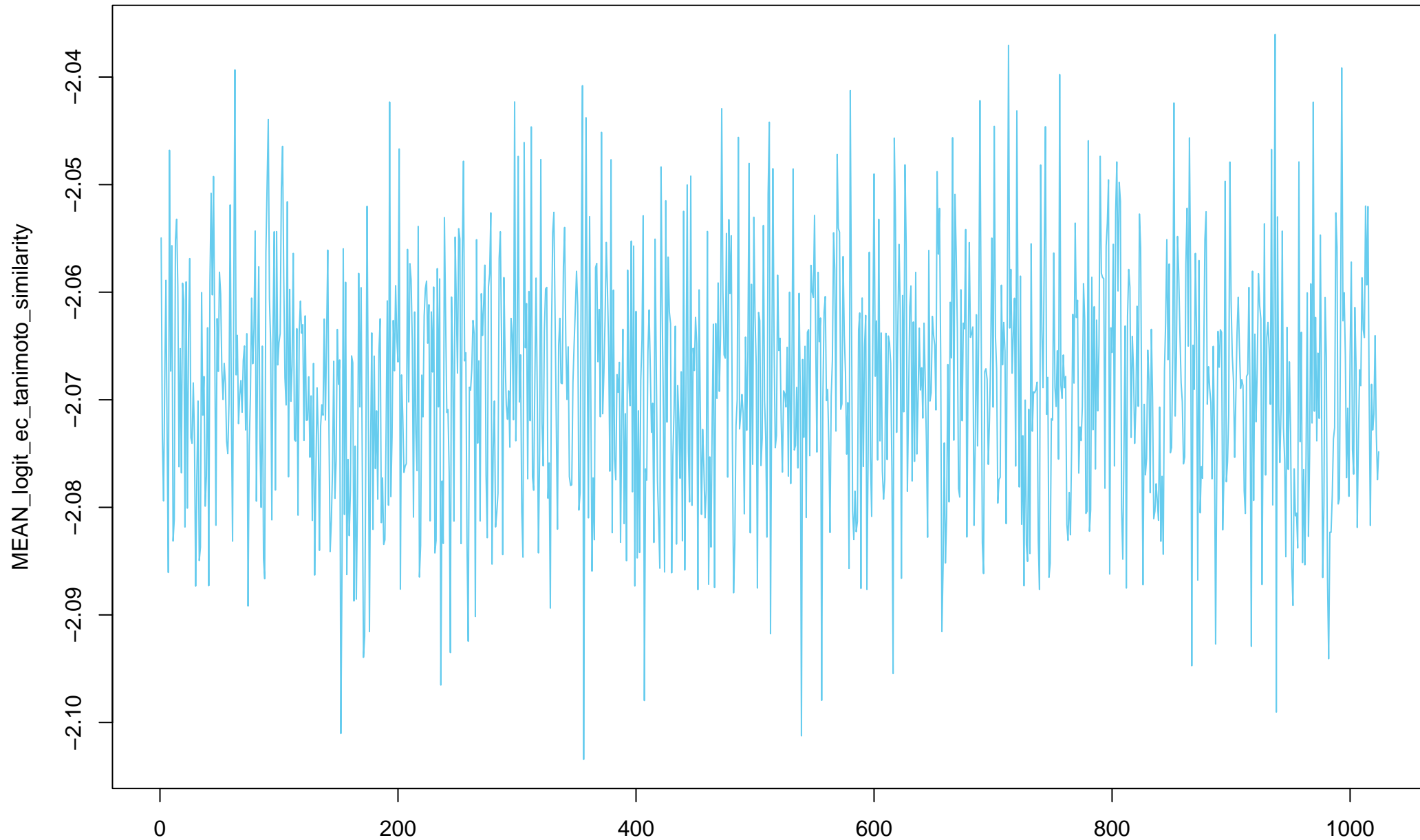
MEAN_log_RMSD
ESS = 1020 | BMK = 0.0325 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0



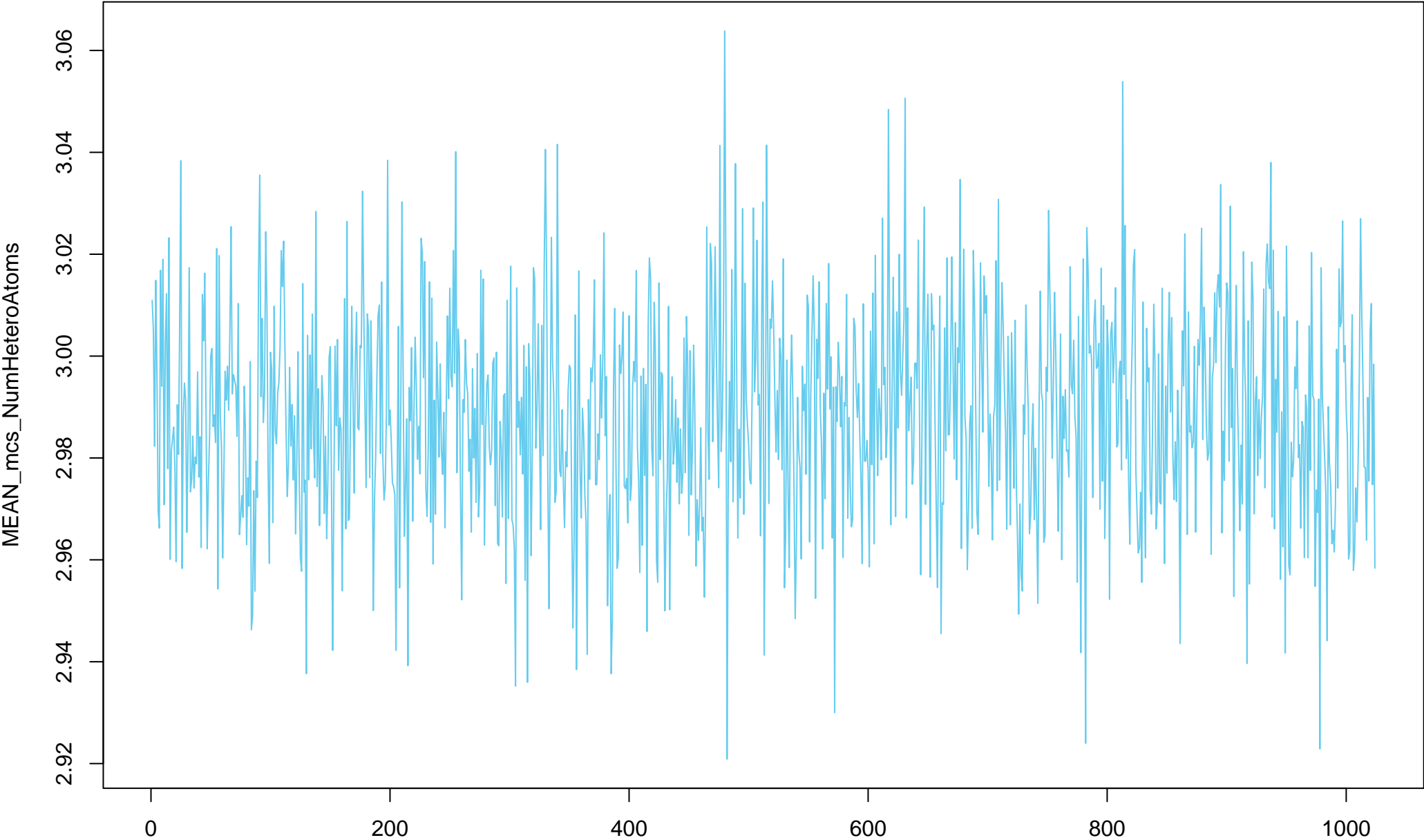
MEAN_log_mcs_unbonded_polar_sasa
ESS = 680 | BMK = 0.048 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0



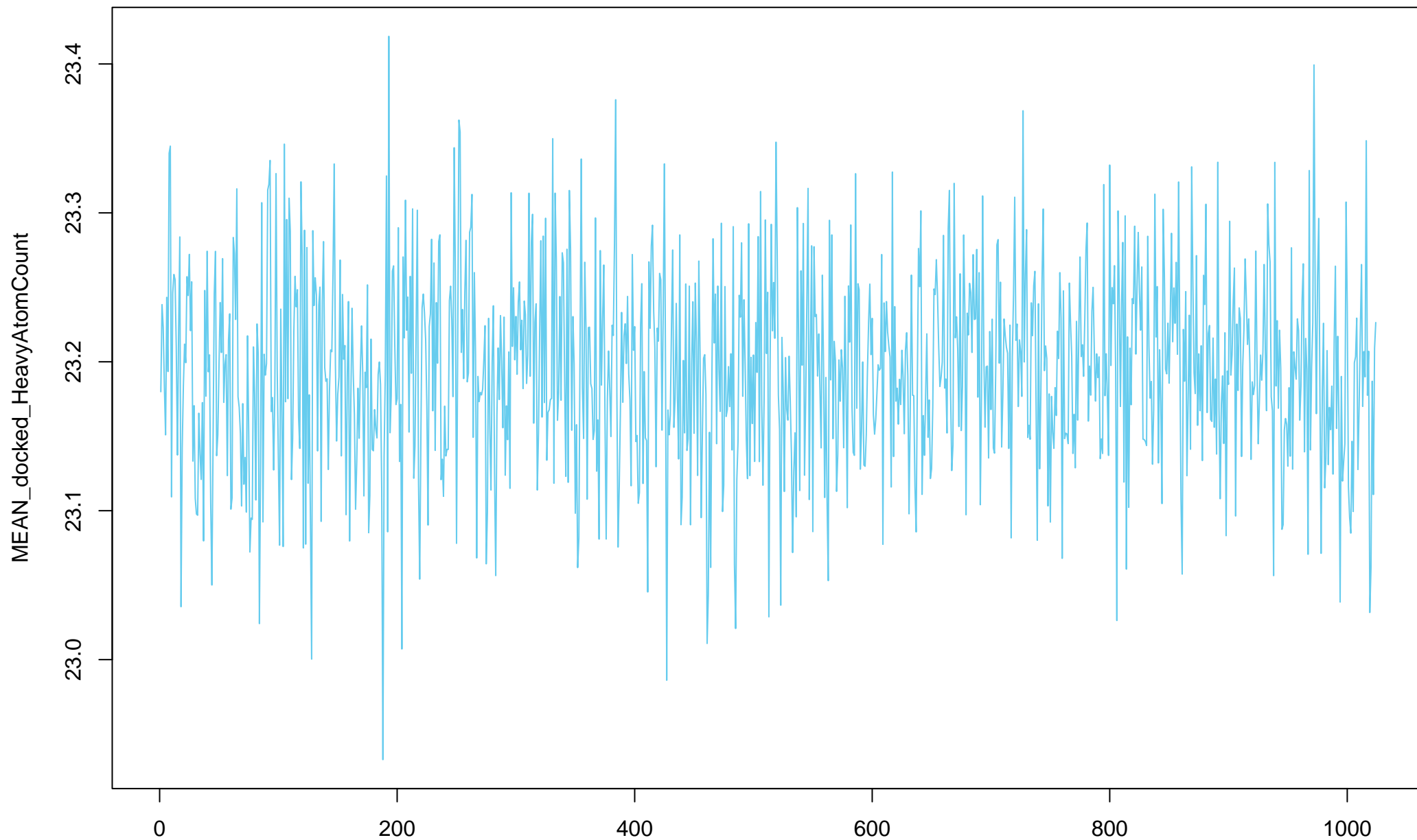
MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0409 | MCSE(6.27) = 3.42 | stat: TRUE | burn: 0



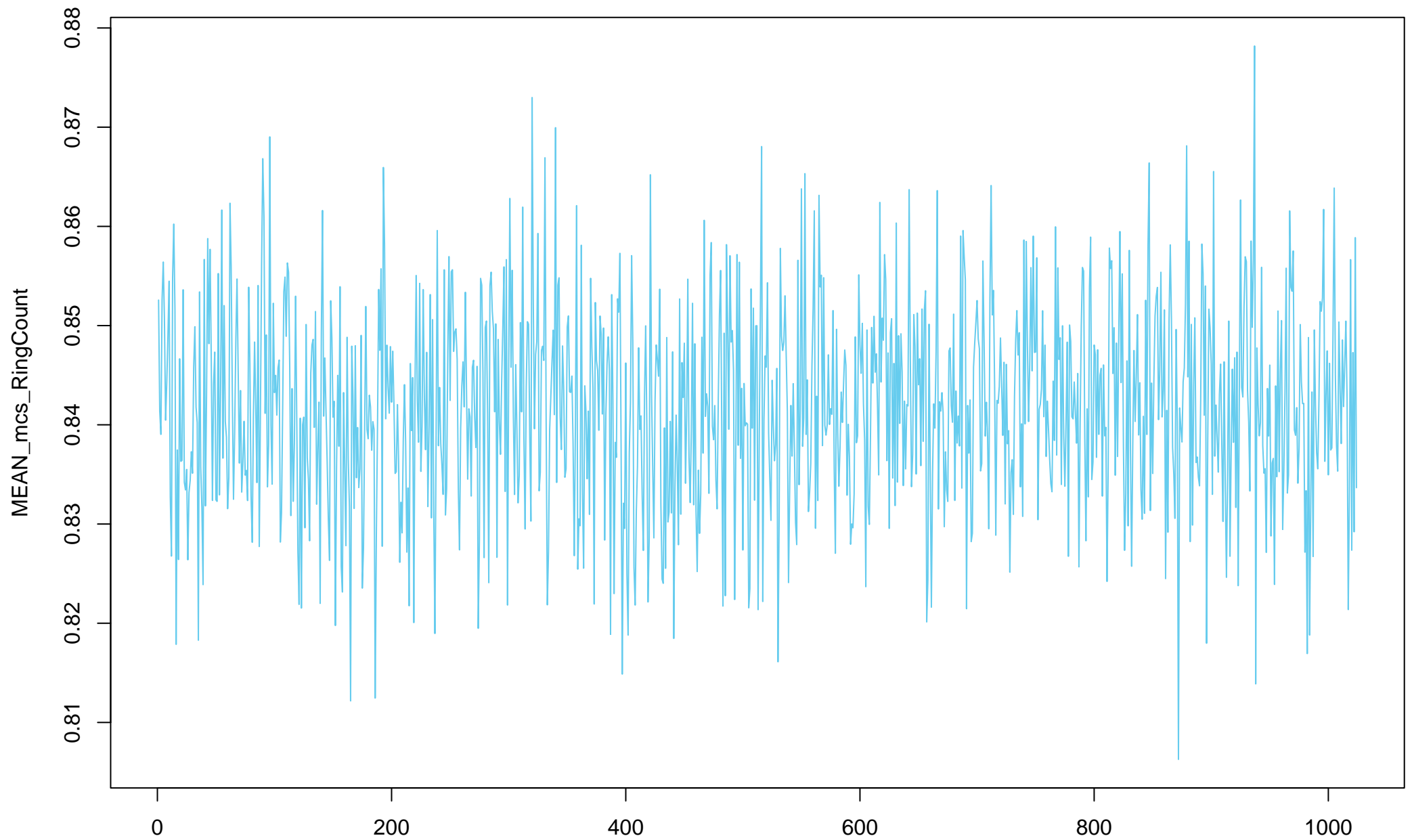
MEAN_mcs_NumHeteroAtoms
ESS = 920 | BMK = 0.0742 | MCSE(6.27) = 3.62 | stat: TRUE | burn: 0



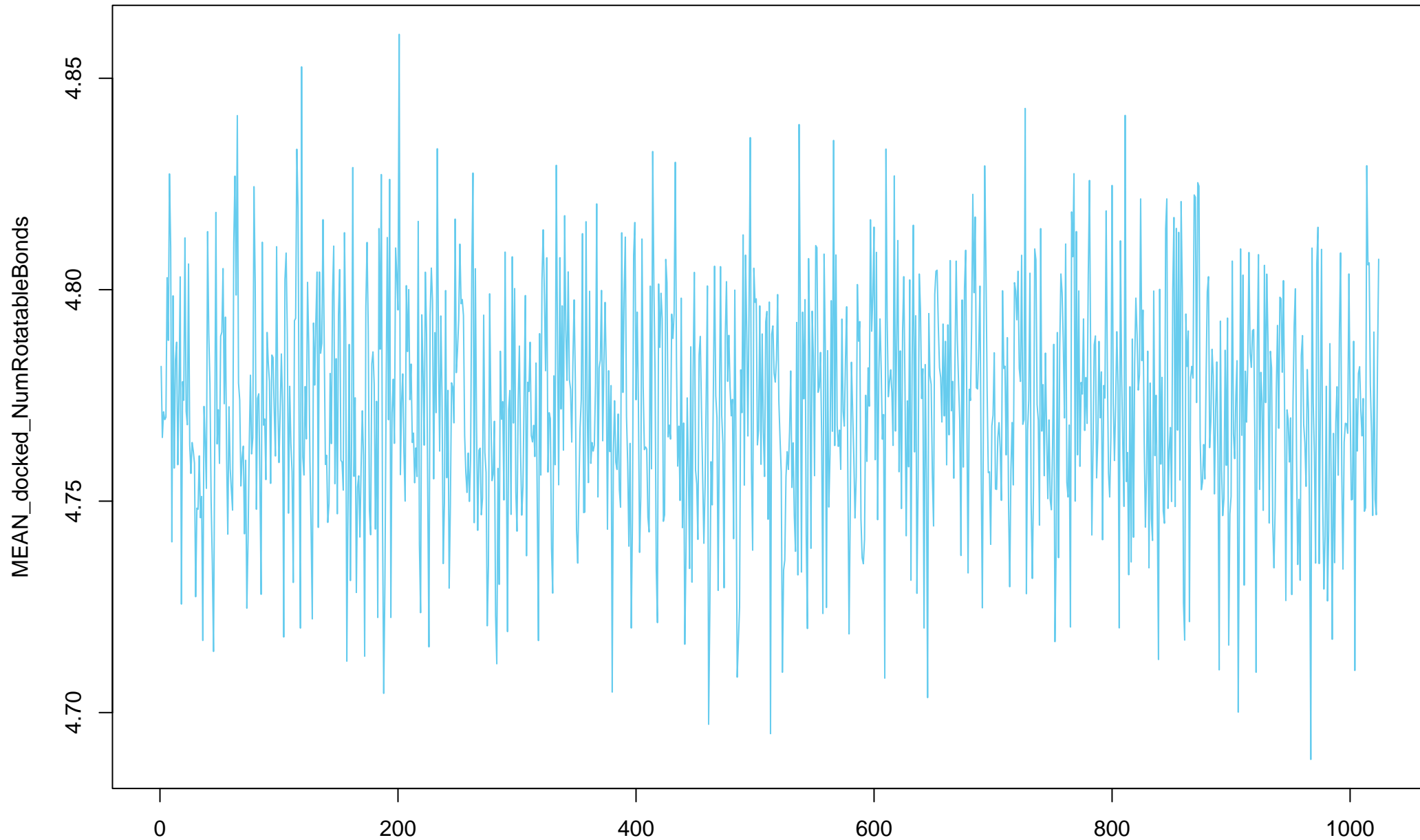
MEAN_docked_HeavyAtomCount
ESS = 927 | BMK = 0.083 | MCSE(6.27) = 3.35 | stat: TRUE | burn: 0



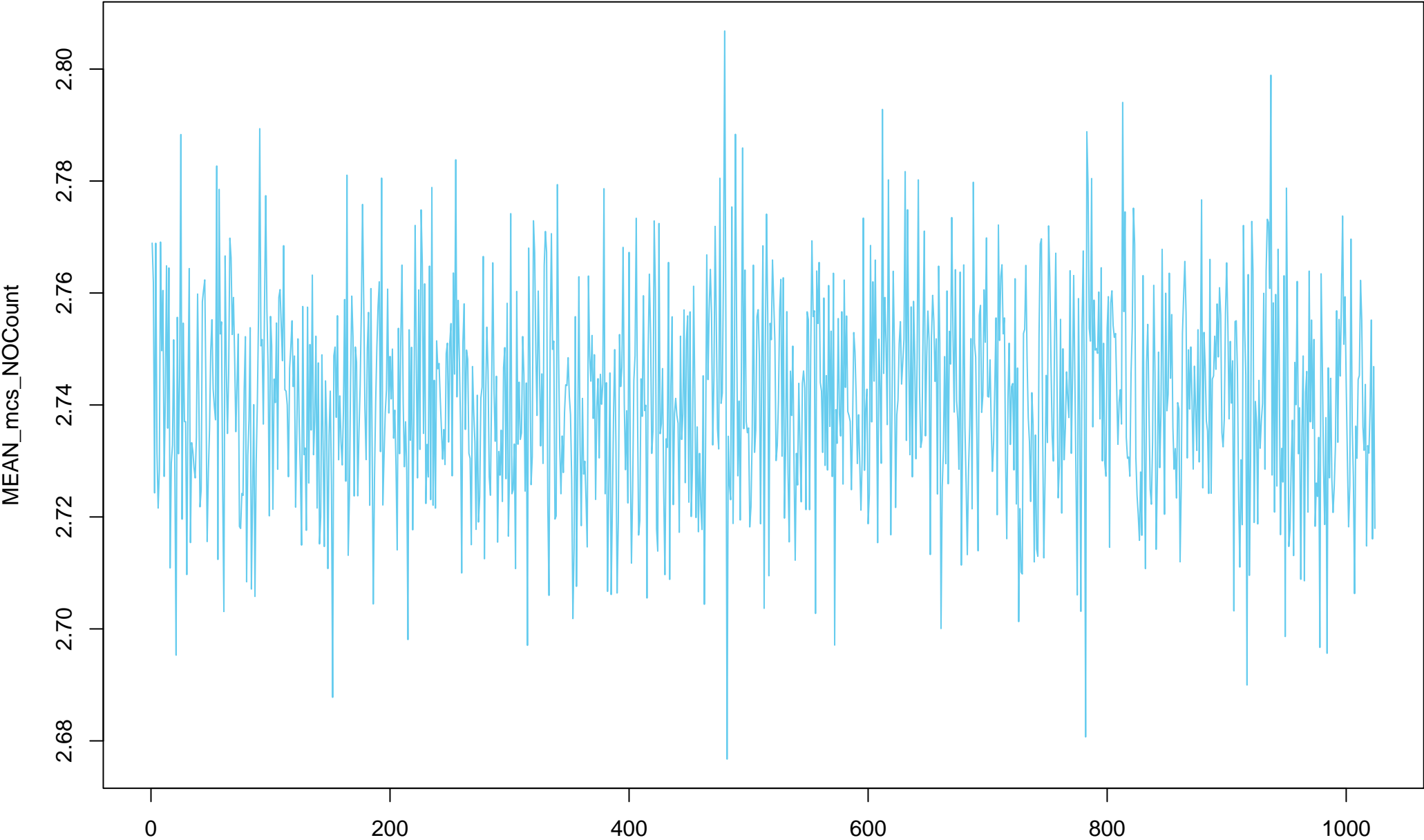
MEAN_mcs_RingCount
ESS = 912 | BMK = 0.0726 | MCSE(6.27) = 3.29 | stat: TRUE | burn: 0



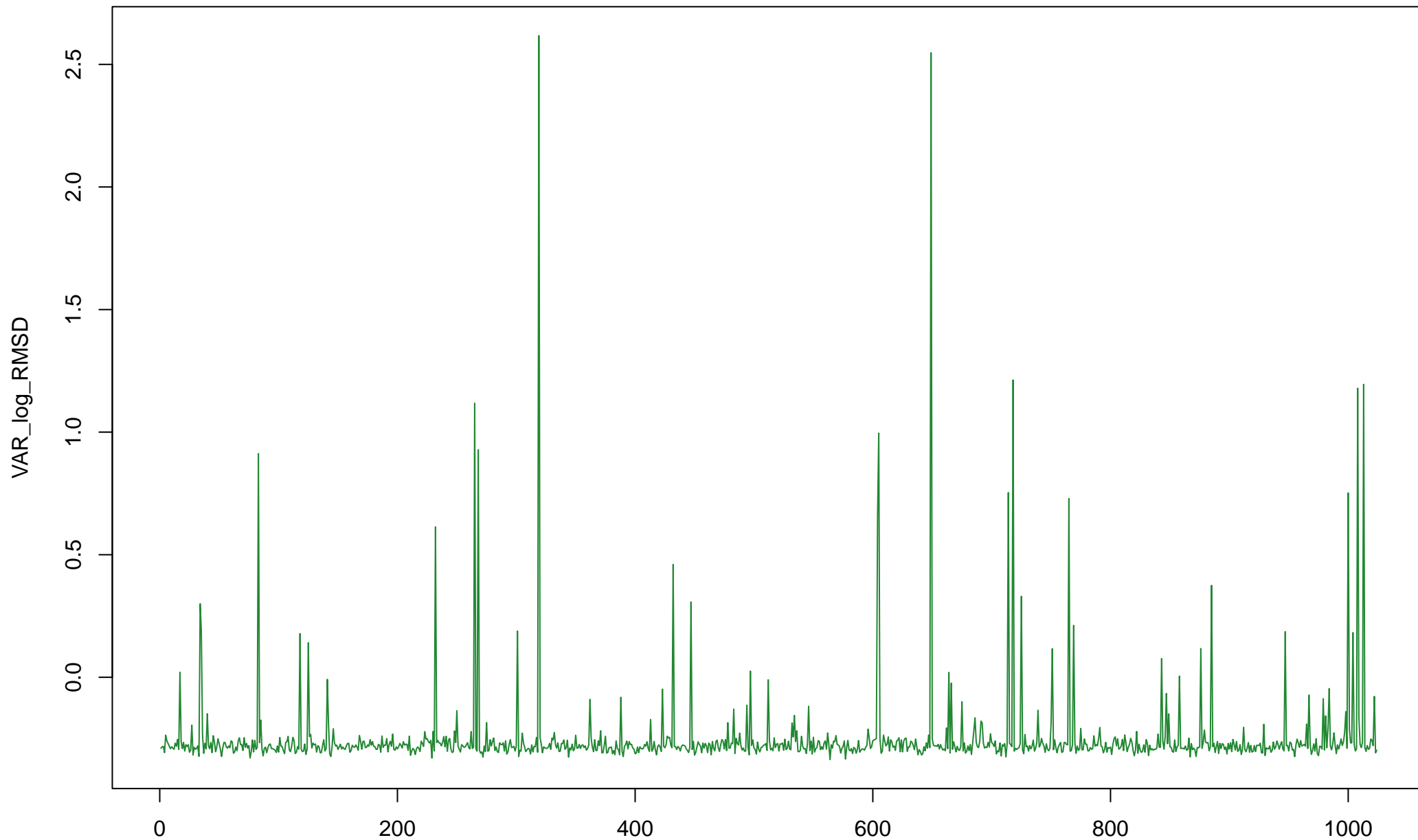
MEAN_docked_NumRotatableBonds
ESS = 882 | BMK = 0.0461 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0



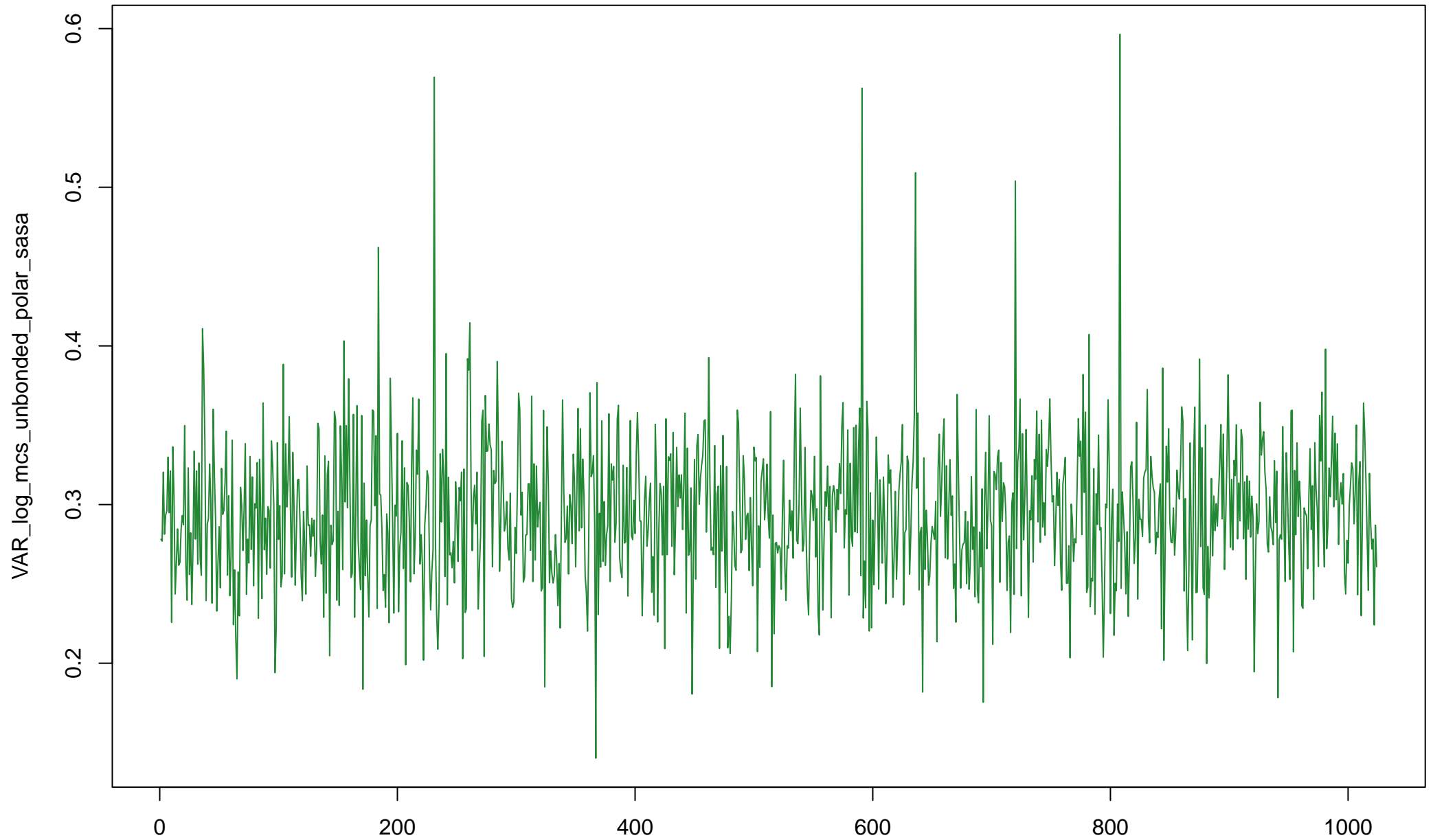
MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0508 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0



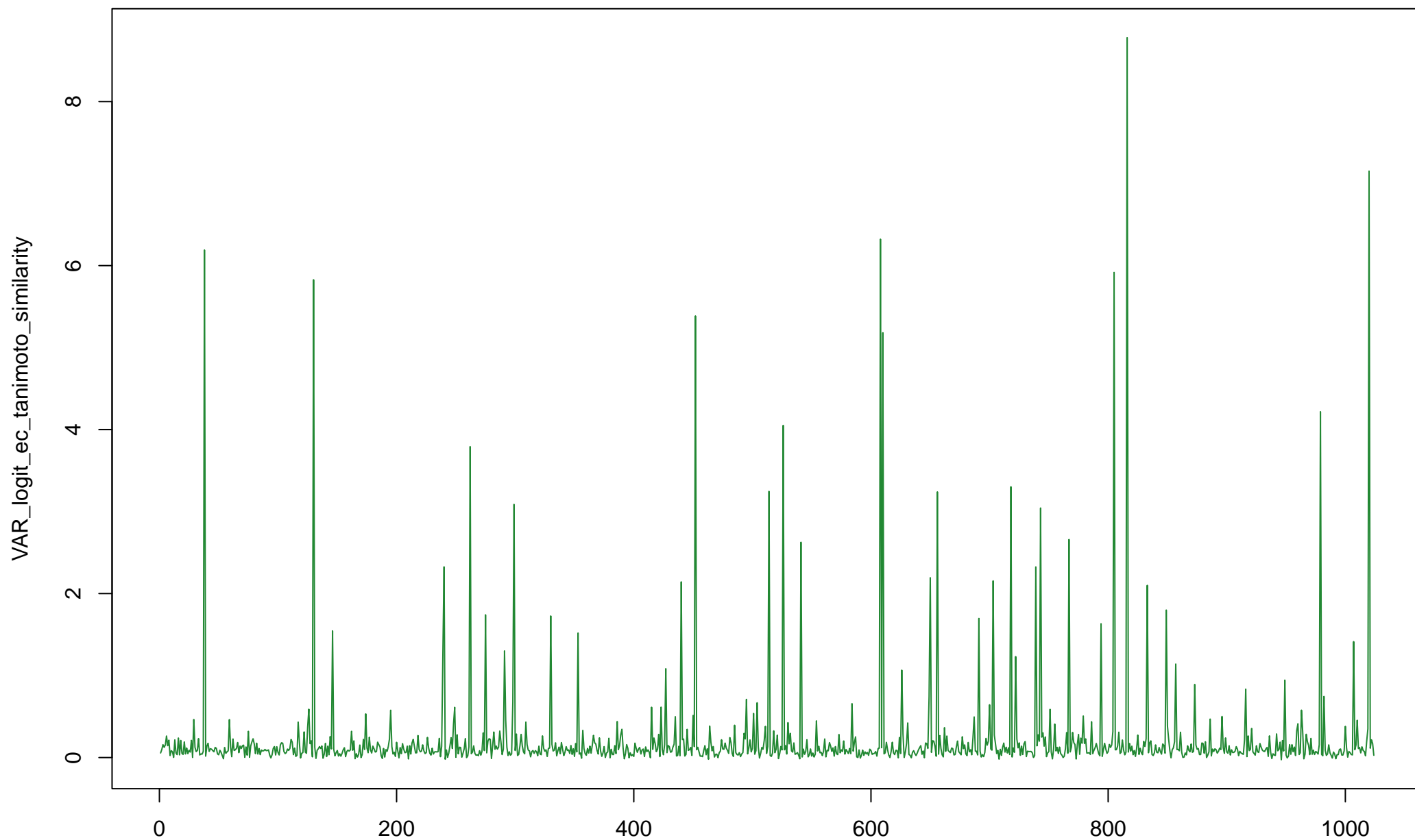
VAR_log_RMSD
ESS = 1020 | BMK = 0.235 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0



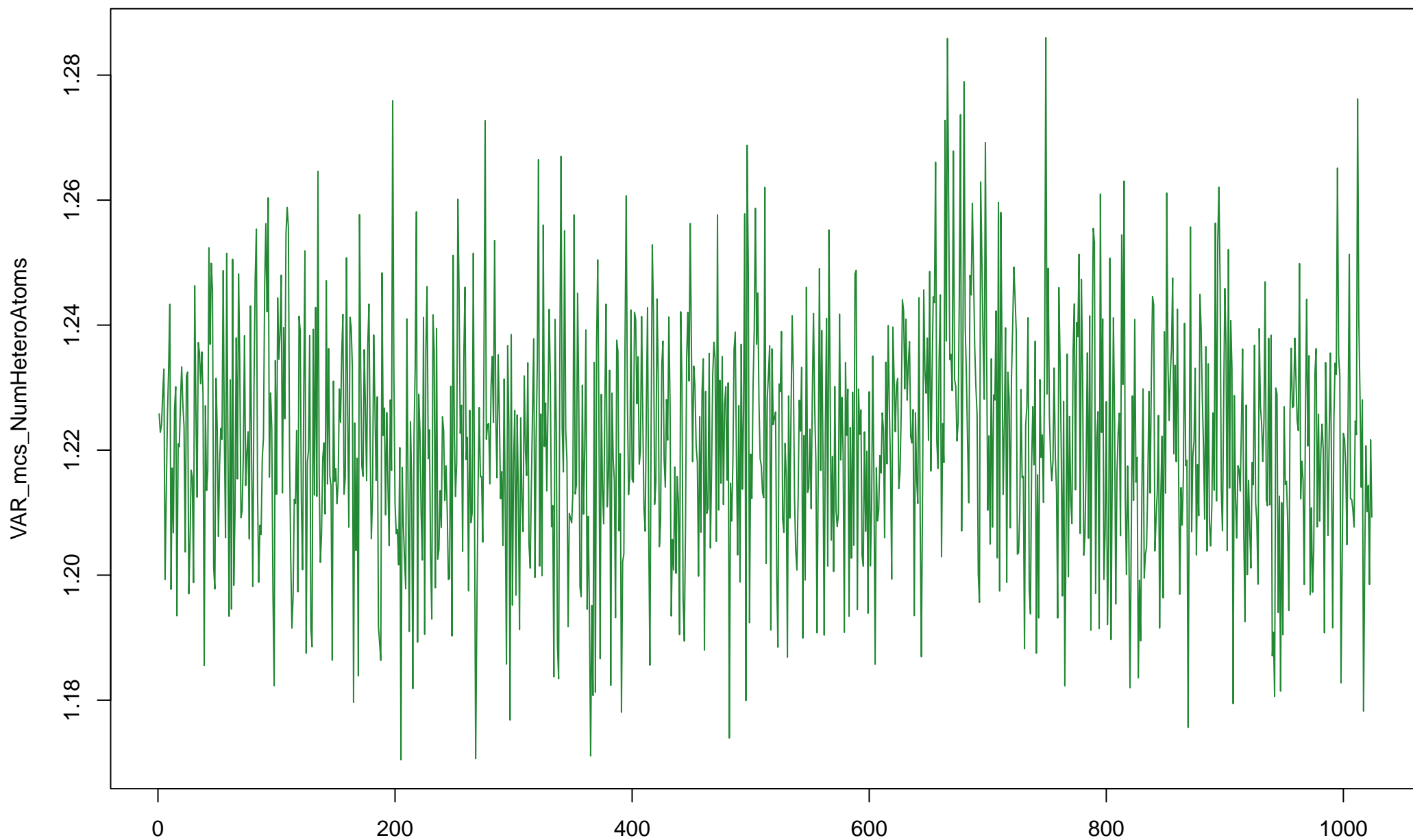
VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0809 | MCSE(6.27) = 2.75 | stat: FALSE | burn: 0



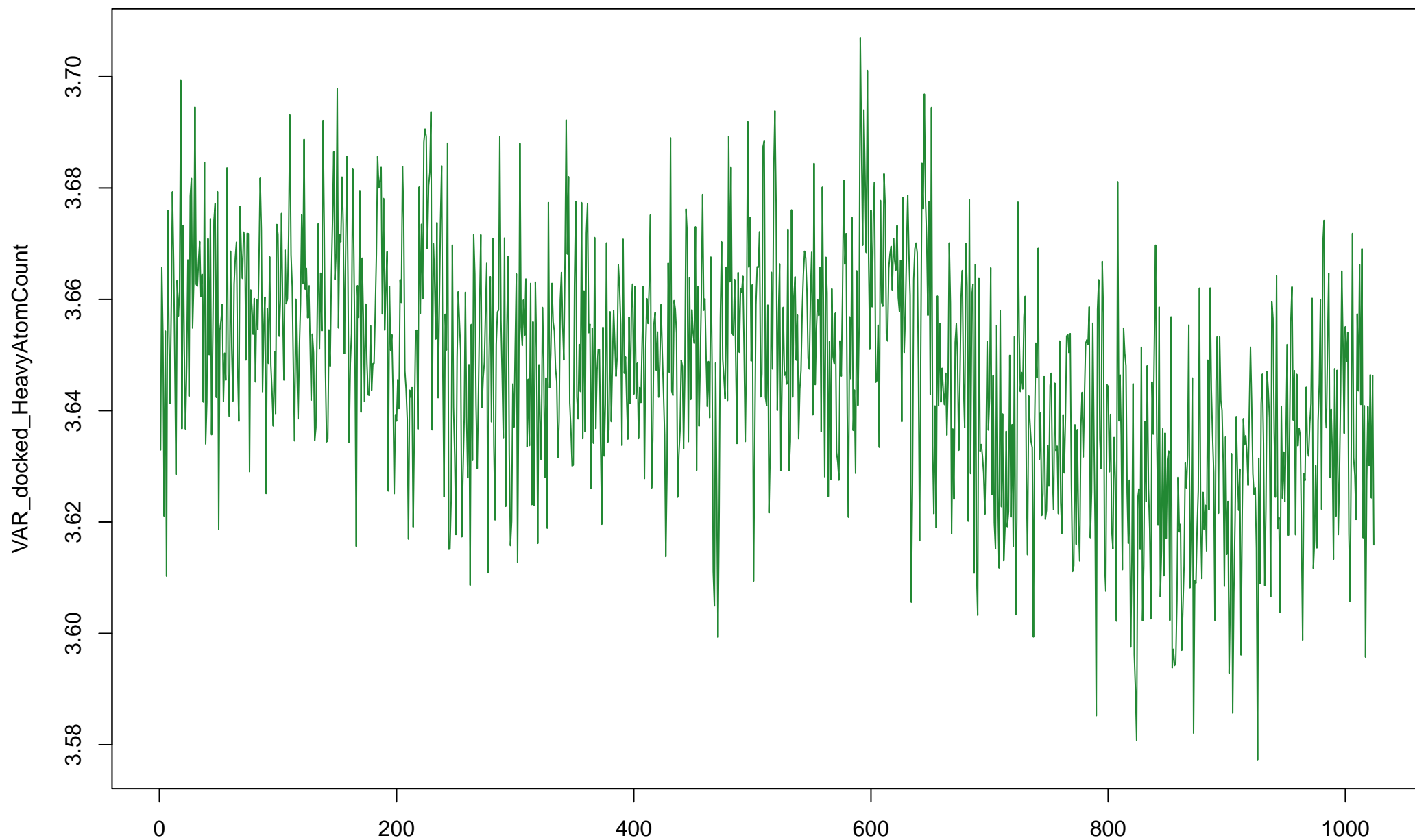
VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 1020



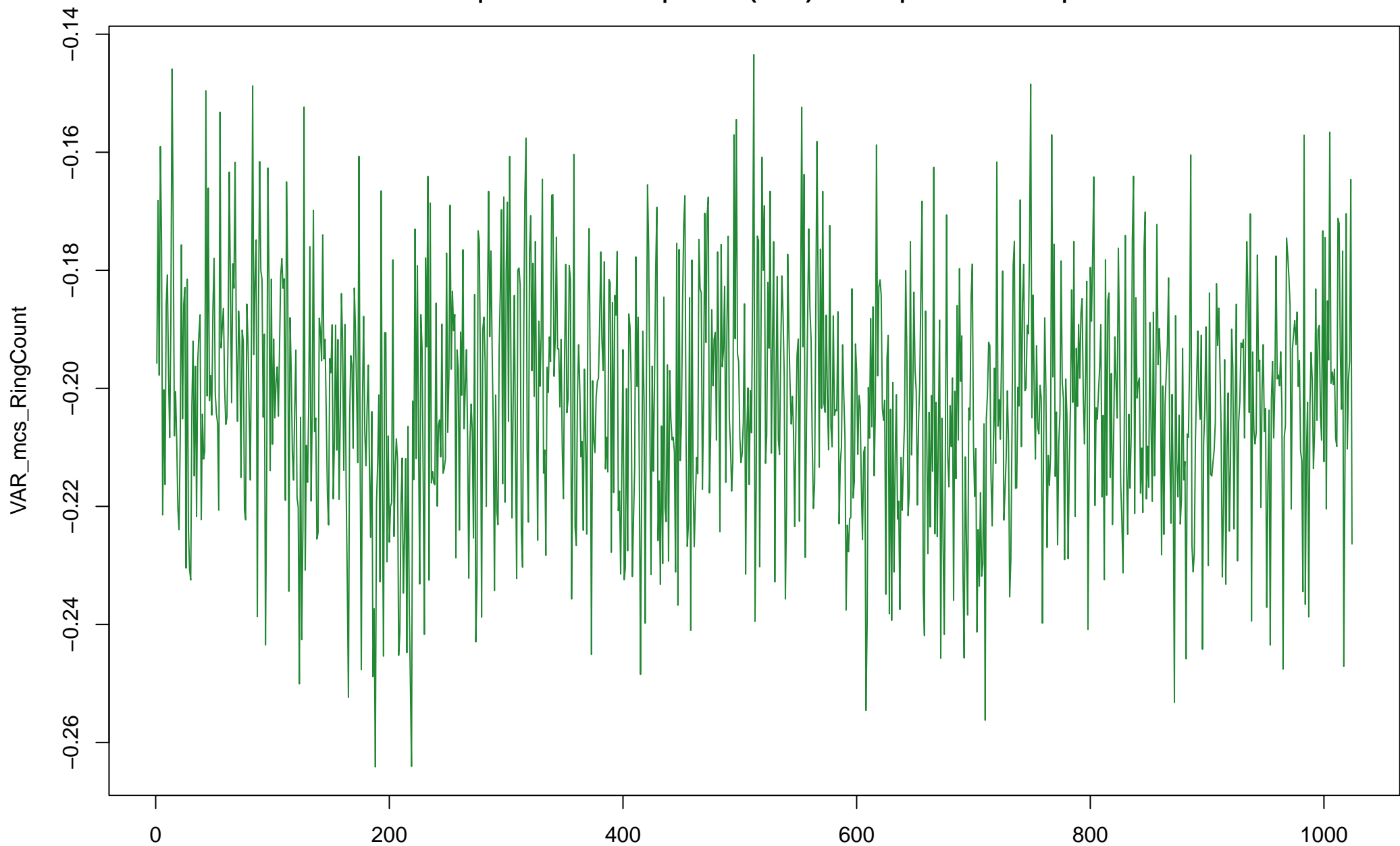
VAR_mcs_NumHeteroAtoms
ESS = 882 | BMK = 0.0457 | MCSE(6.27) = 4.3 | stat: TRUE | burn: 0



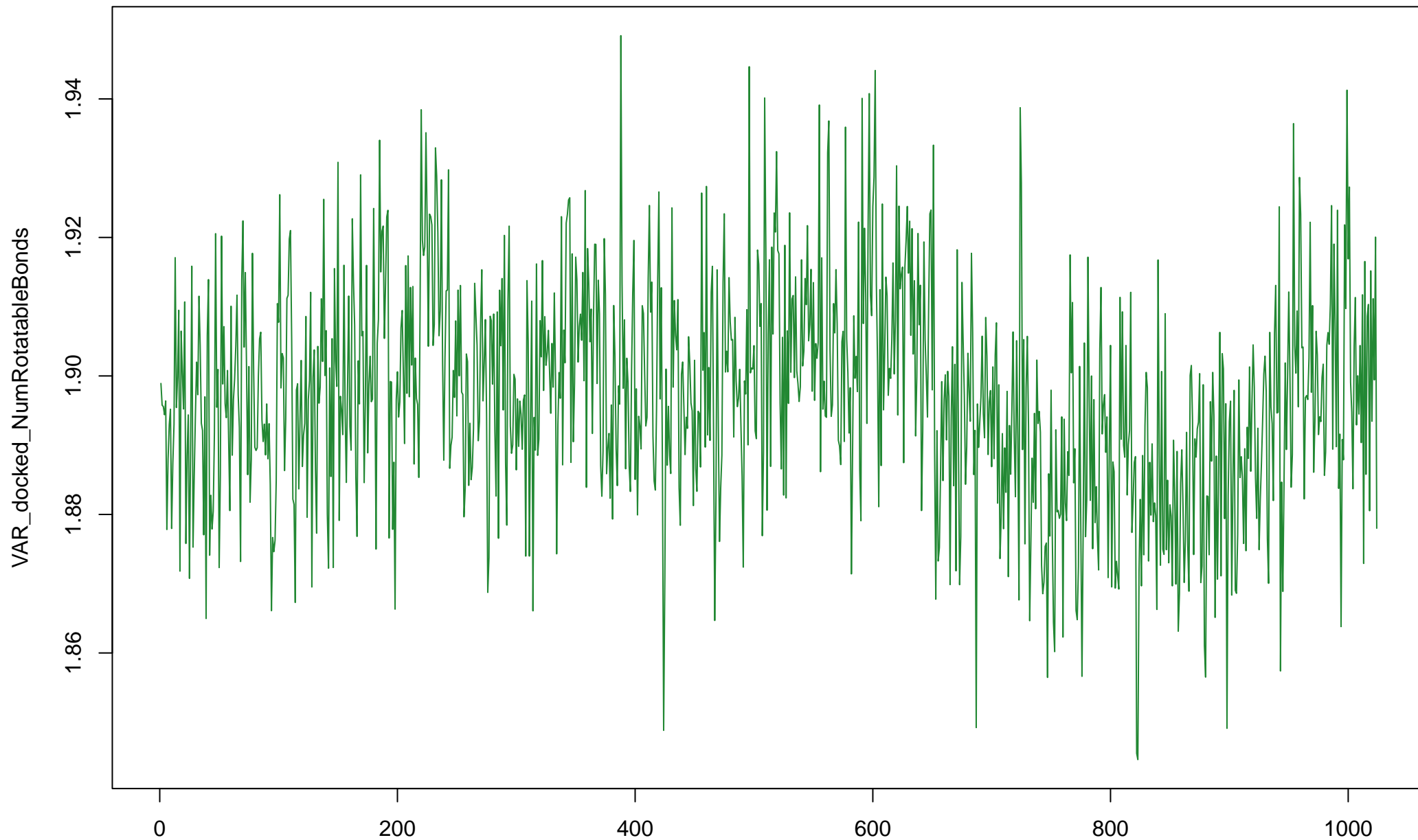
VAR_docked_HeavyAtomCount
ESS = 36.4 | BMK = 0.254 | MCSE(6.27) = 9.87 | stat: FALSE | burn: 0



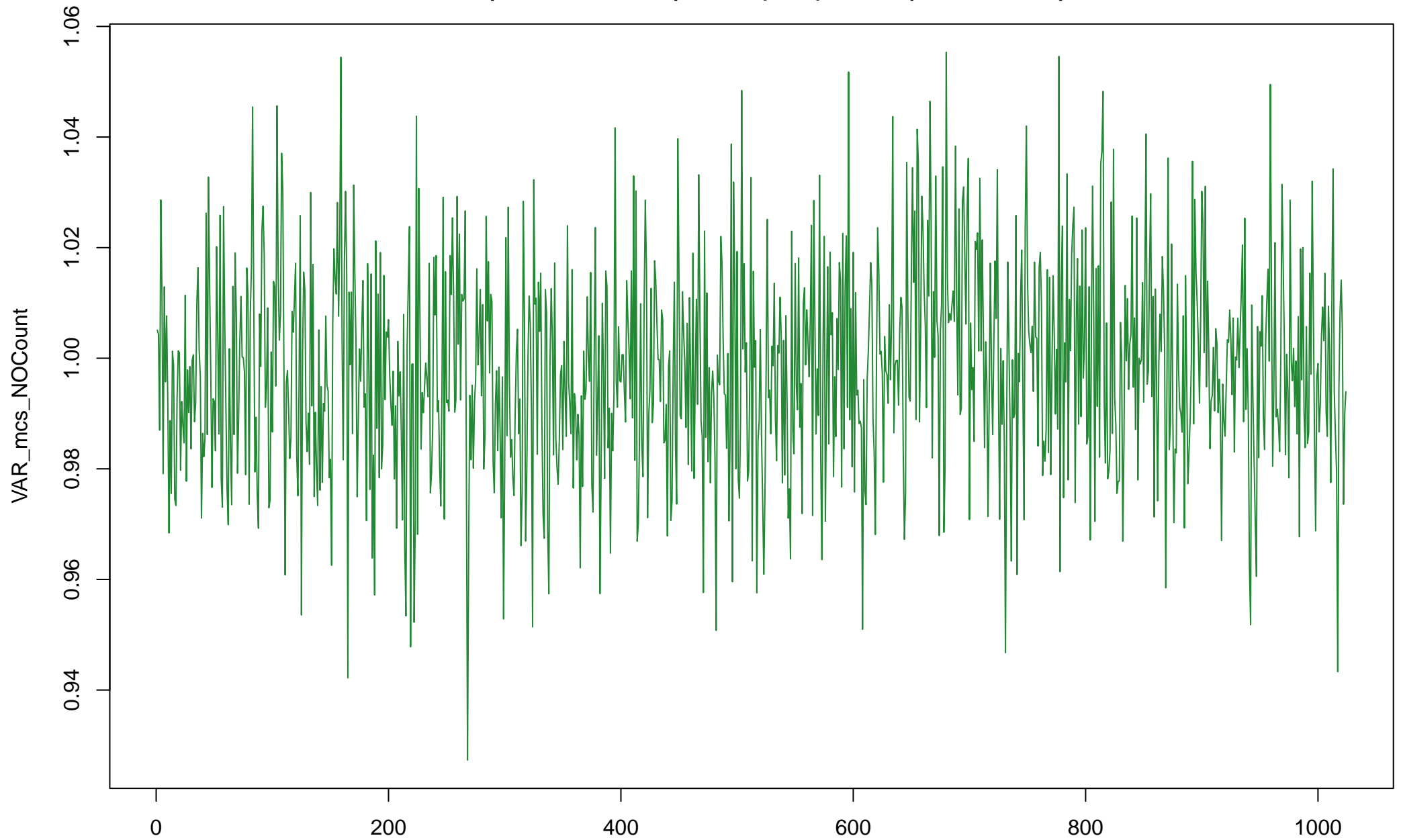
VAR_mcs_RingCount
ESS = 432 | BMK = 0.0739 | MCSE(6.27) = 5.07 | stat: FALSE | burn: 0



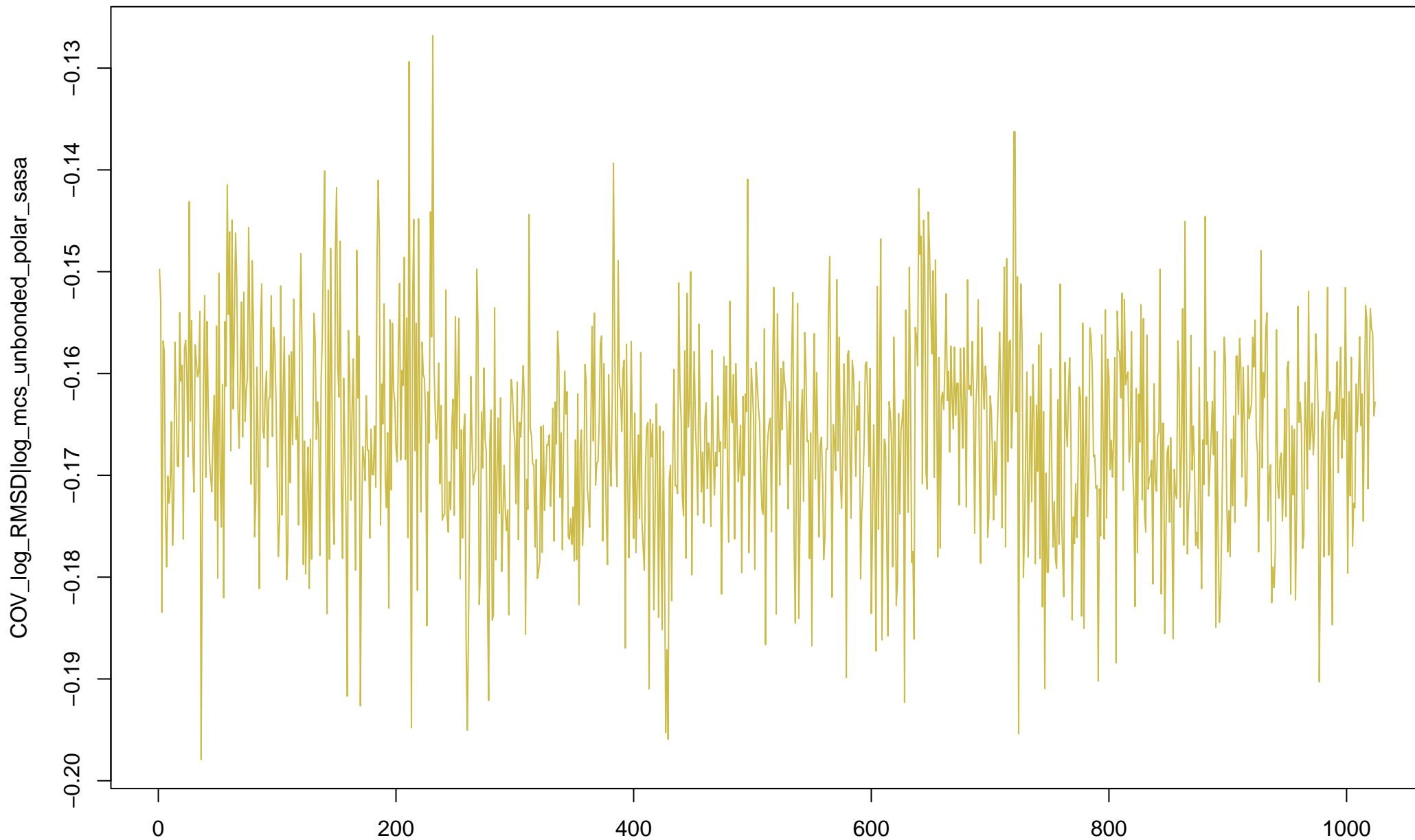
VAR_docked_NumRotatableBonds
ESS = 38.6 | BMK = 0.134 | MCSE(6.27) = 8.54 | stat: TRUE | burn: 0



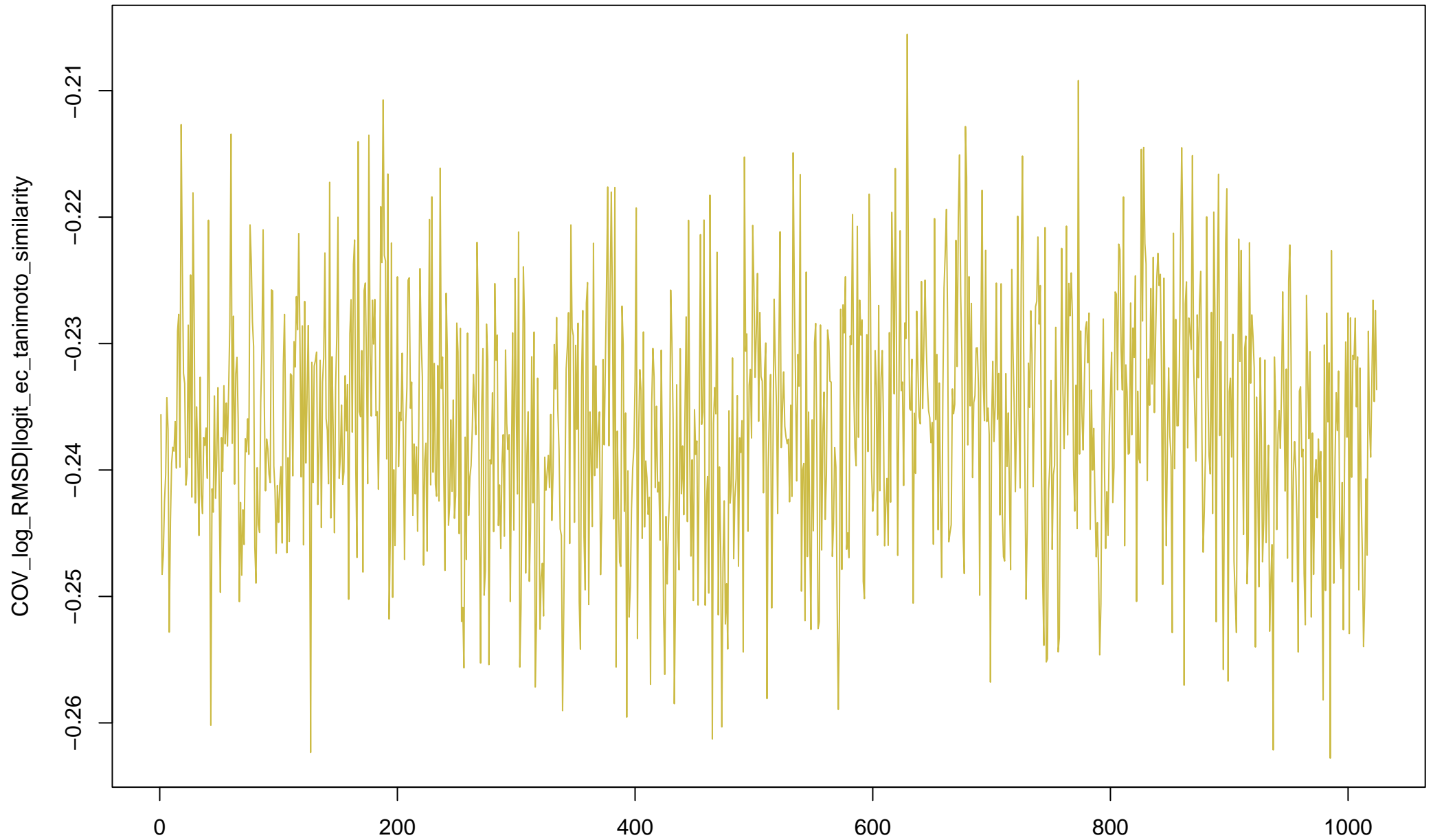
VAR_mcs_NOCount
ESS = 1020 | BMK = 0.0794 | MCSE(6.27) = 3.96 | stat: TRUE | burn: 0



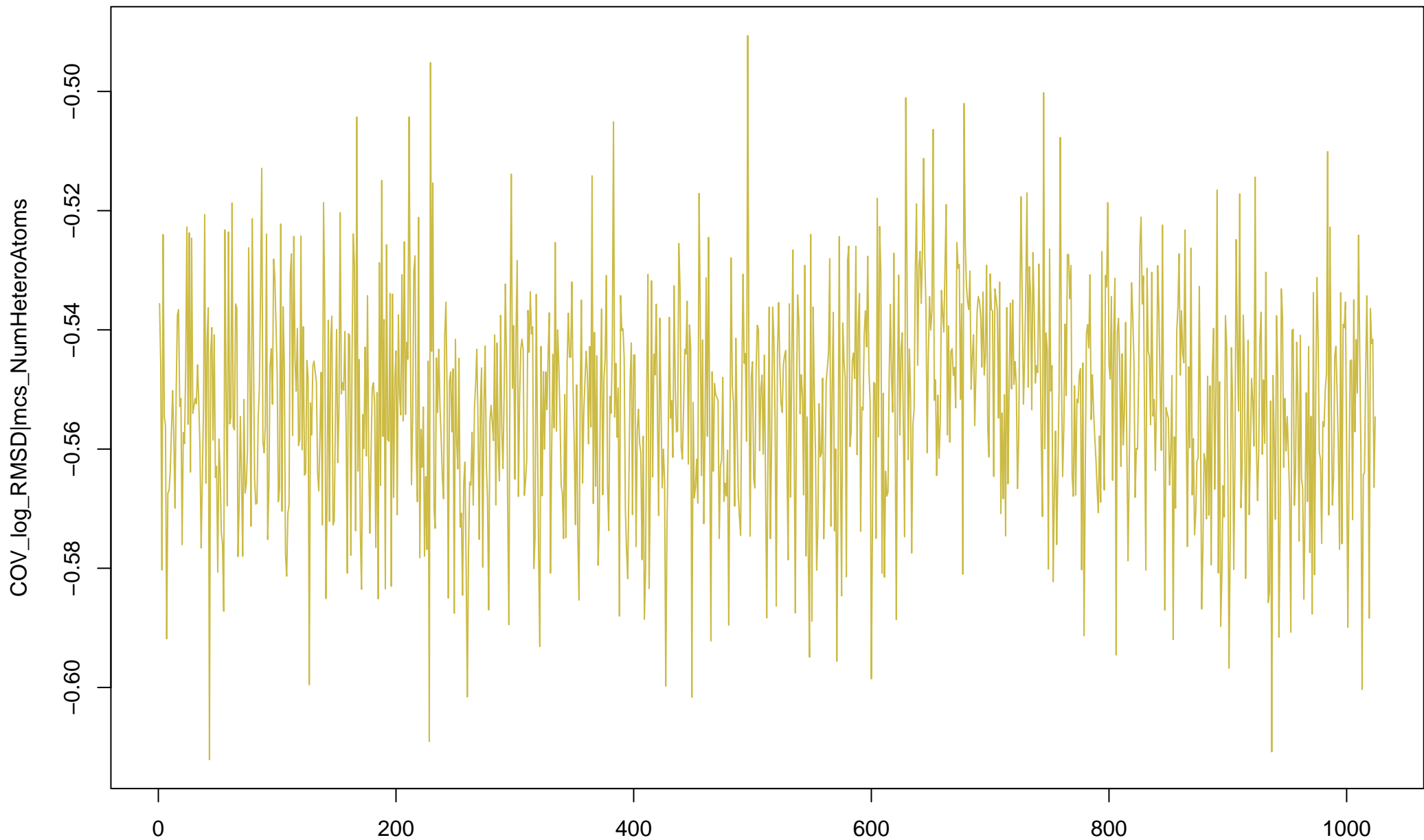
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 359 | BMK = 0.0669 | MCSE(6.27) = 5.25 | stat: FALSE | burn: 0



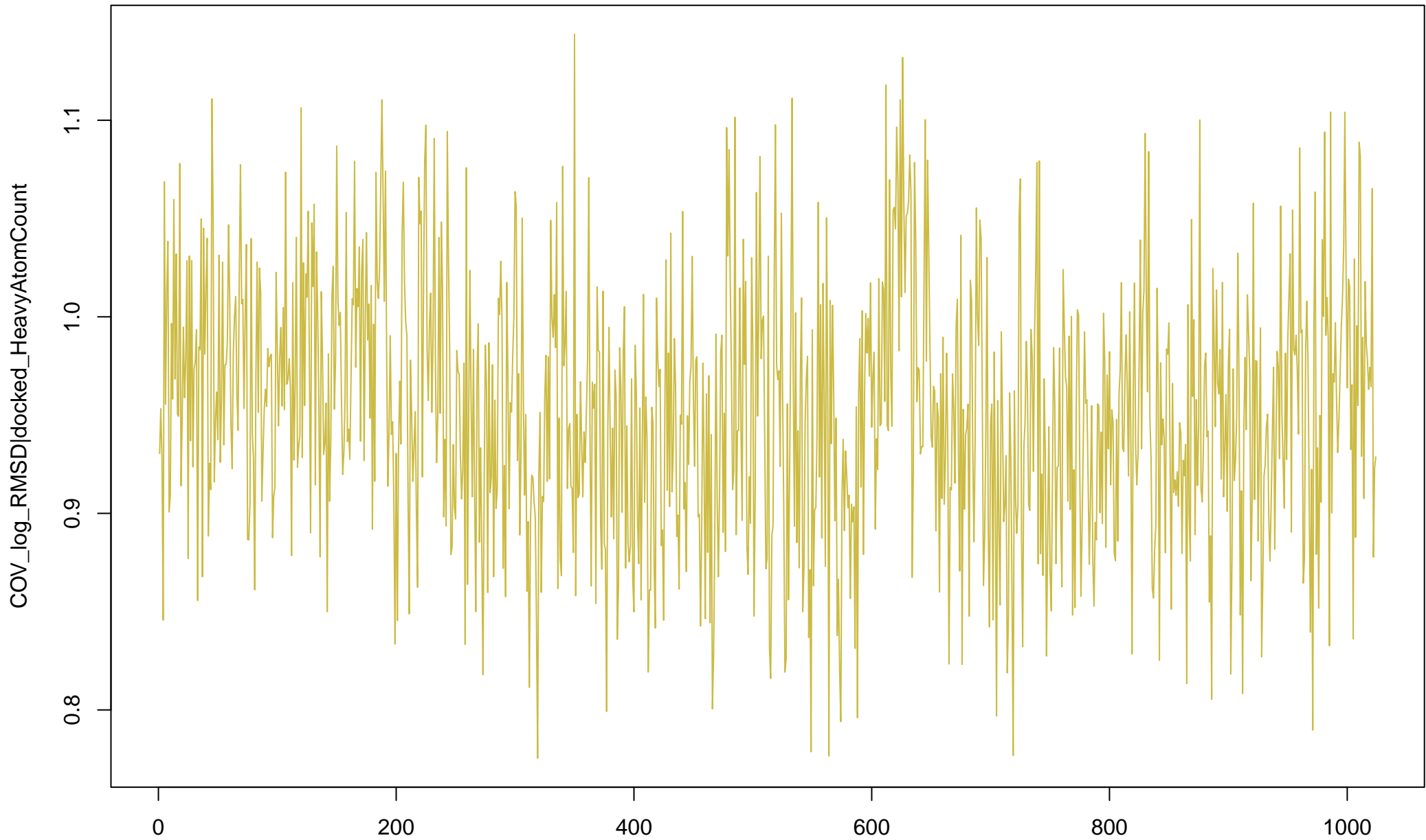
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 580 | BMK = 0.0842 | MCSE(6.27) = 5.31 | stat: TRUE | burn: 0



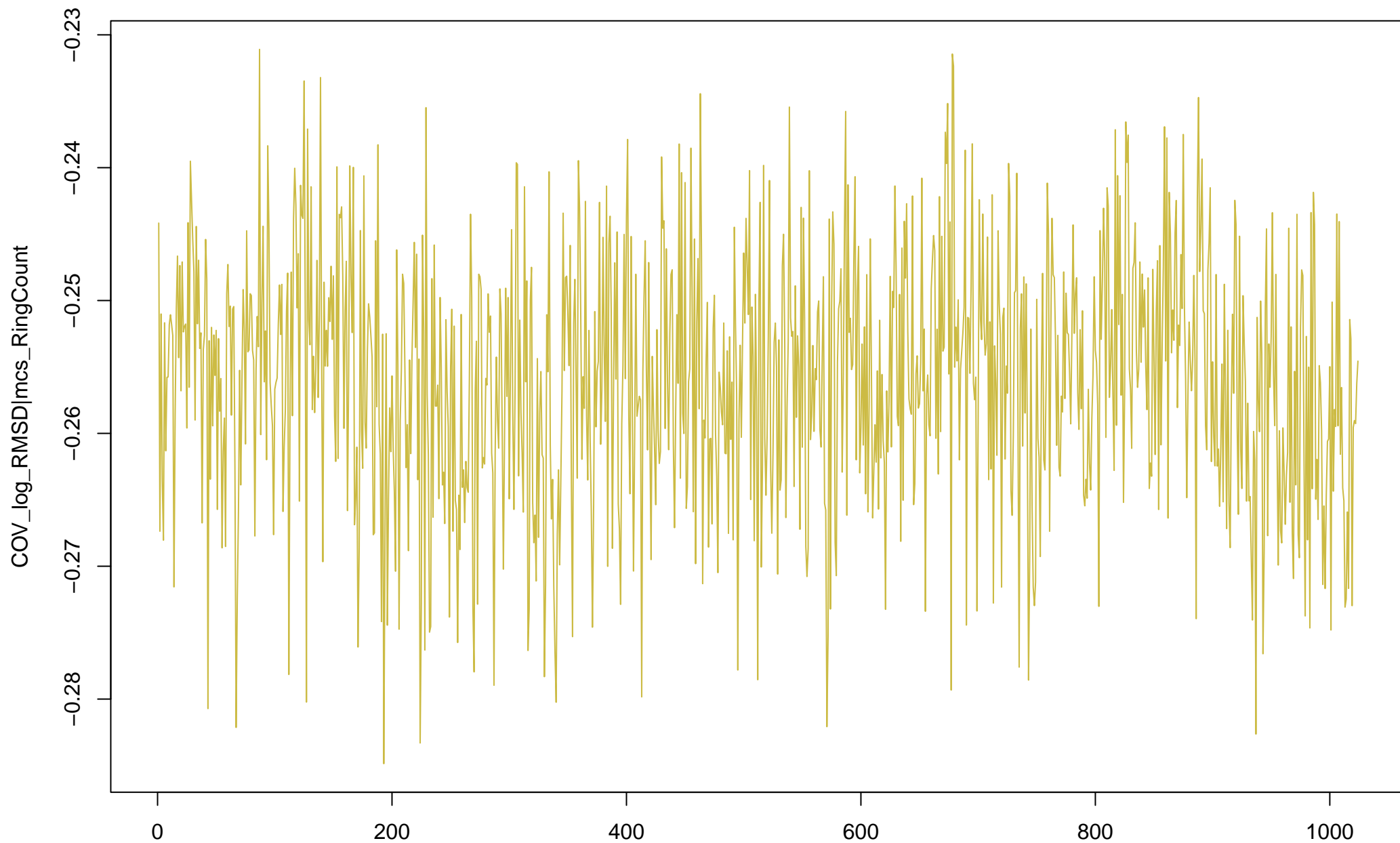
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 516 | BMK = 0.0881 | MCSE(6.27) = 5.01 | stat: TRUE | burn: 0



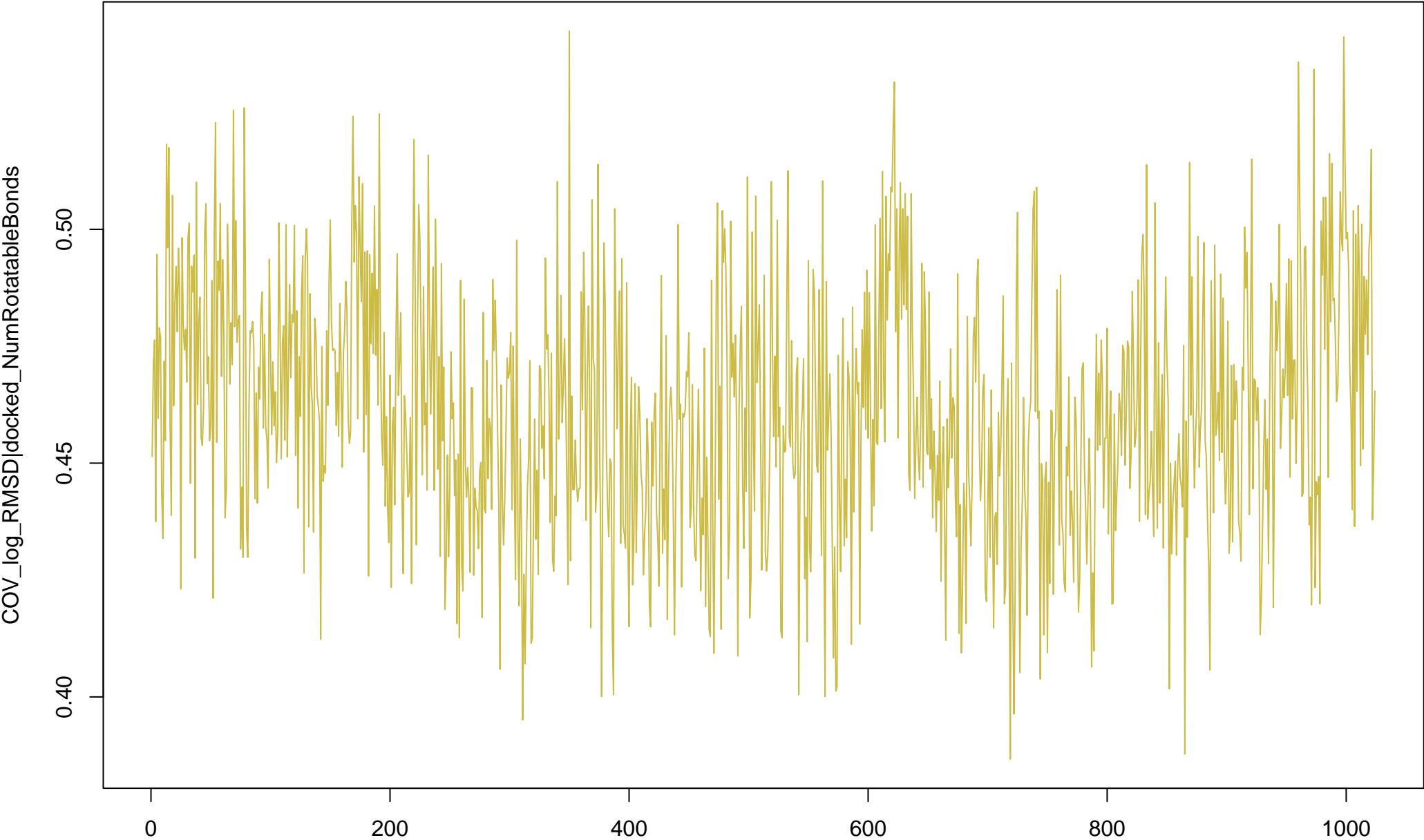
COV_log_RMSD|docked_HeavyAtomCount
ESS = 248 | BMK = 0.0686 | MCSE(6.27) = 6.58 | stat: FALSE | burn: 0



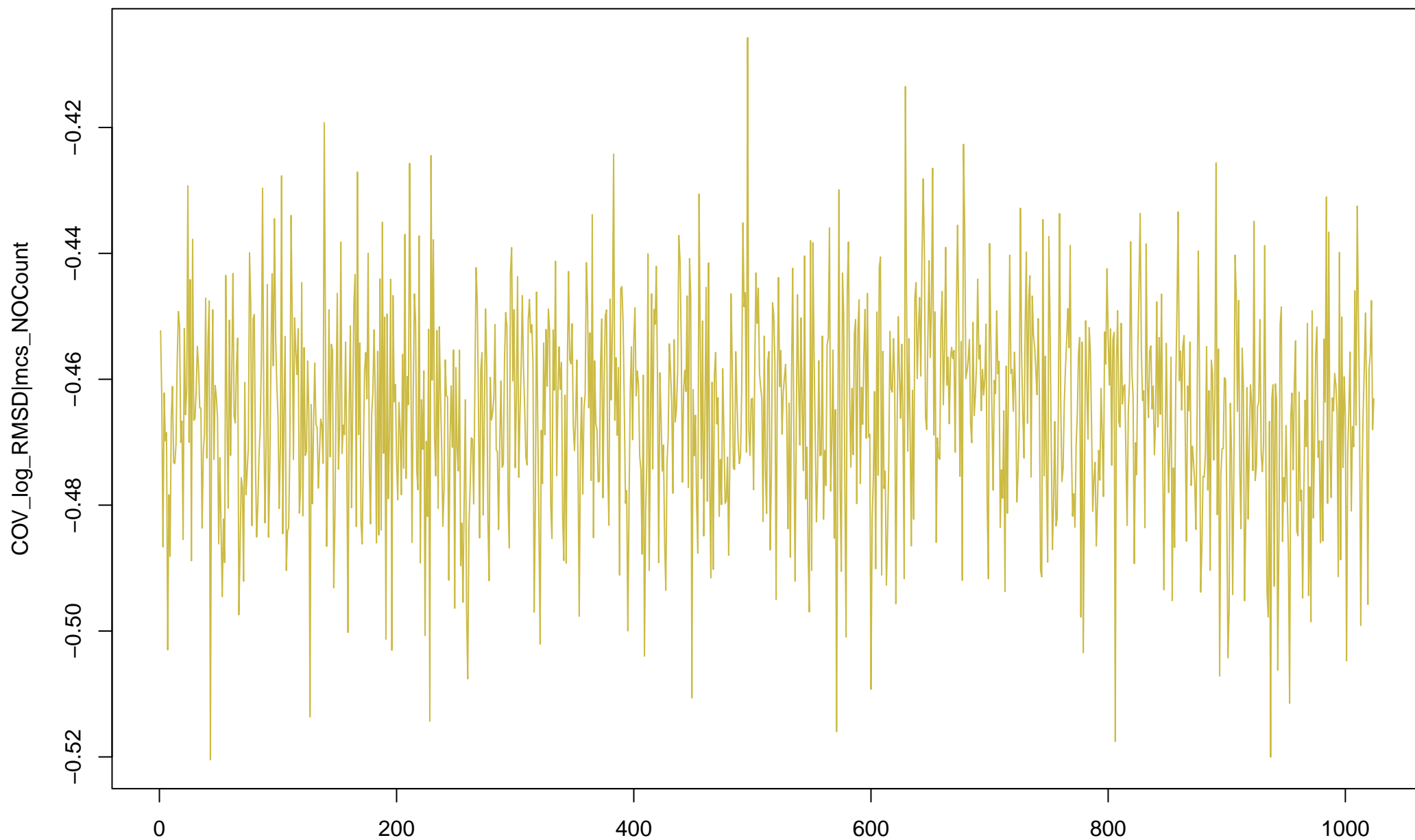
COV_log_RMSD|mcs_RingCount
ESS = 310 | BMK = 0.0482 | MCSE(6.27) = 5.39 | stat: TRUE | burn: 0



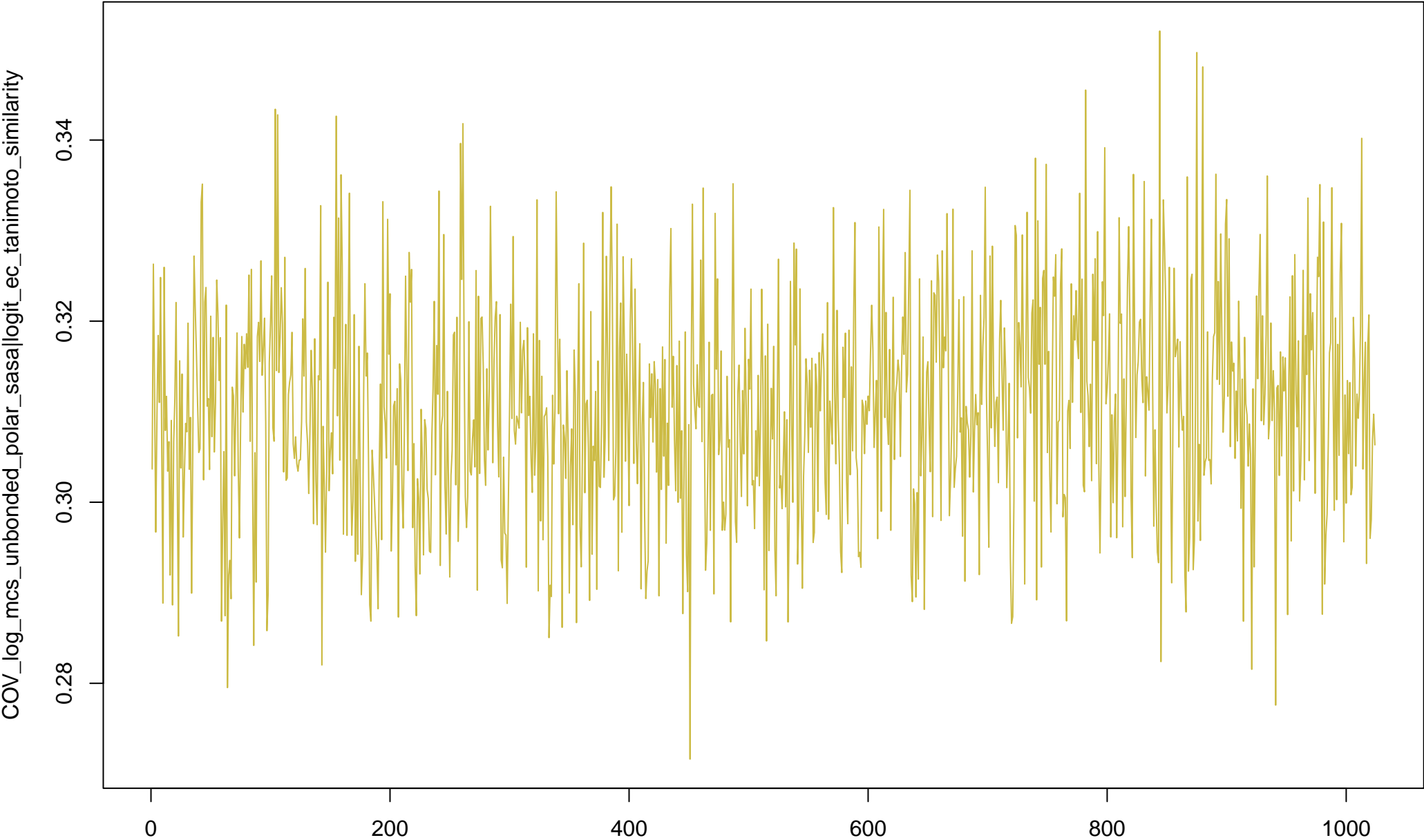
COV_log_RMSD|docked_NumRotatableBonds
ESS = 169 | BMK = 0.0652 | MCSE(6.27) = 7.7 | stat: FALSE | burn: 0



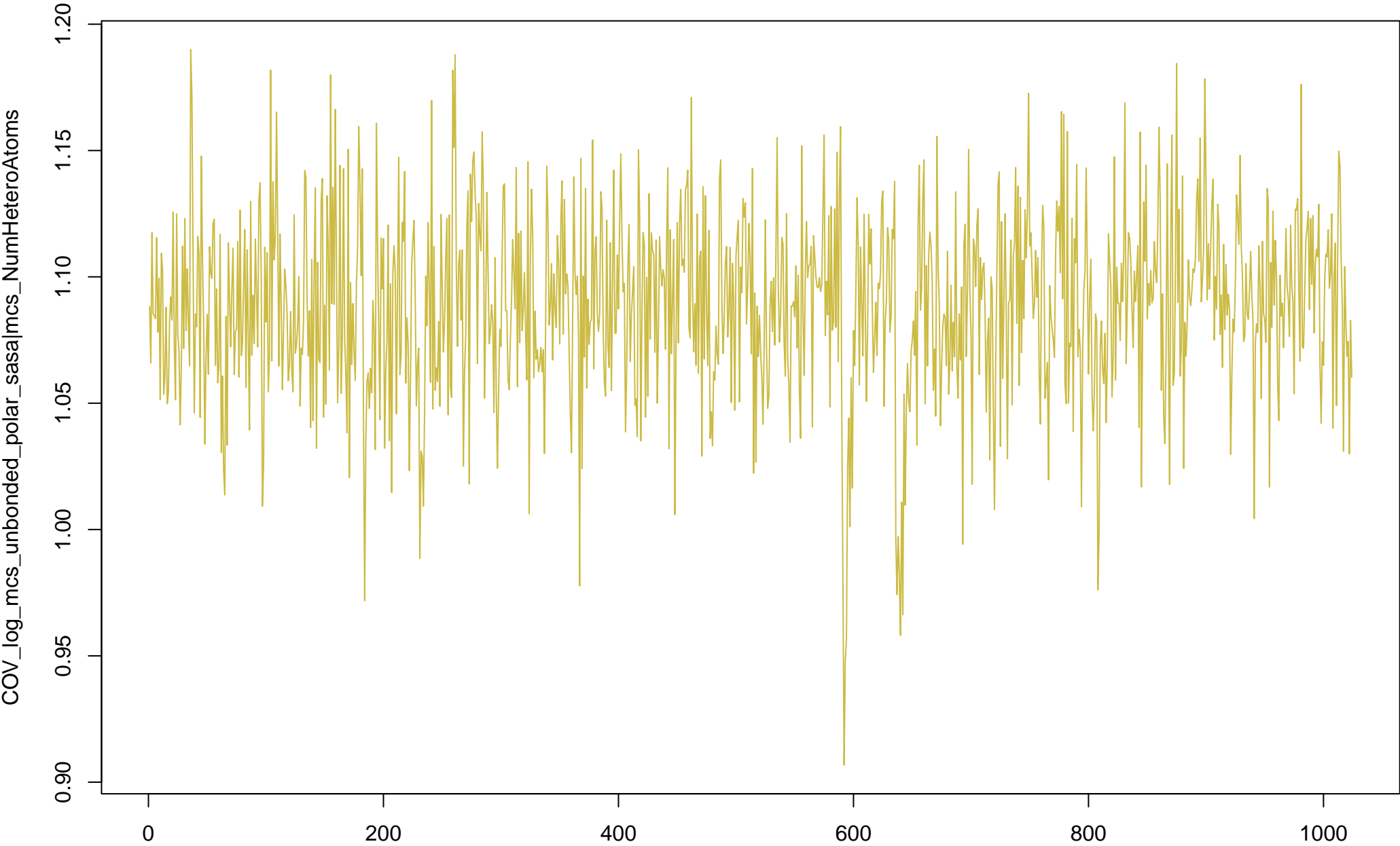
COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0481 | MCSE(6.27) = 4.19 | stat: TRUE | burn: 0



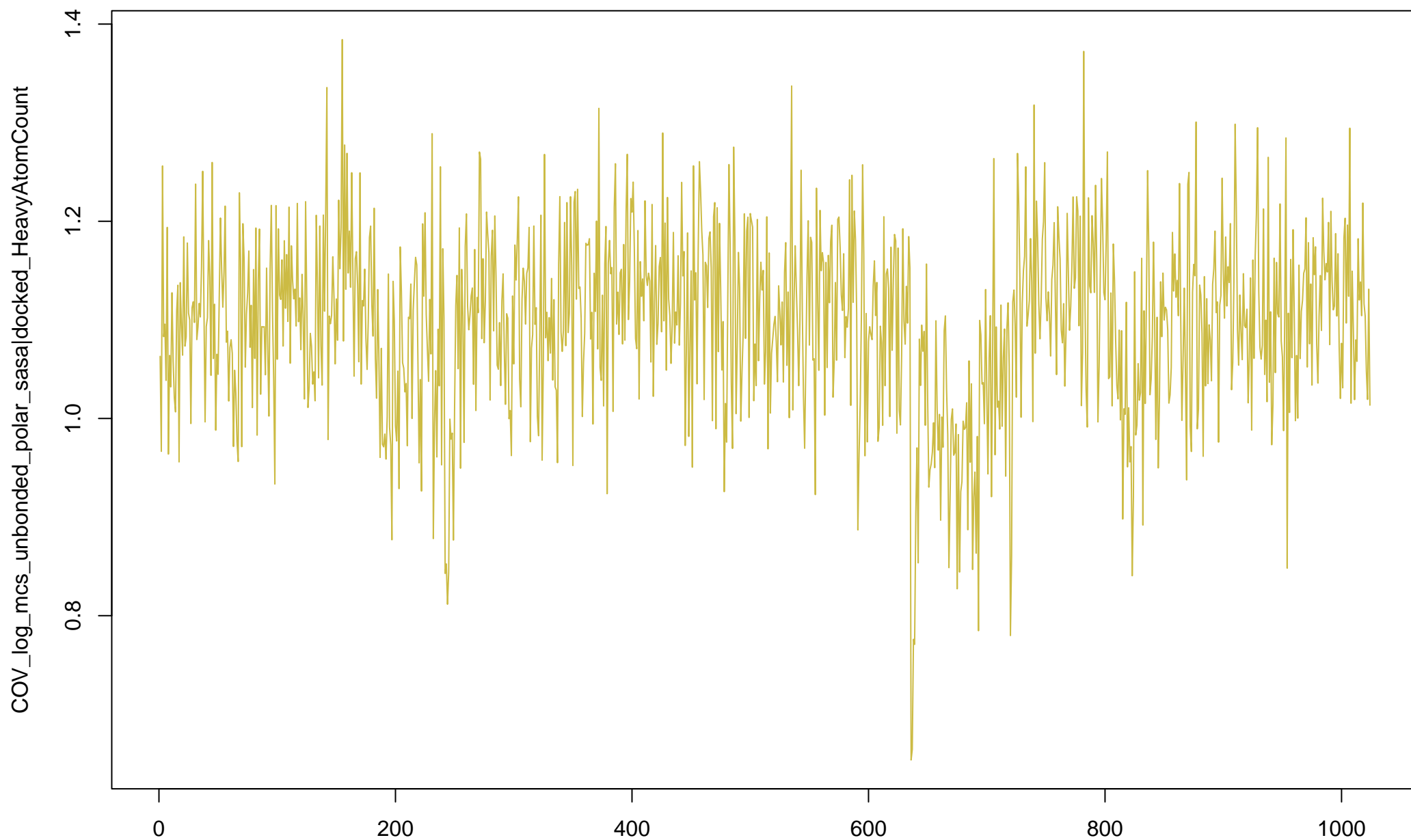
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 904 | BMK = 0.0883 | MCSE(6.27) = 3.76 | stat: TRUE | burn: 0



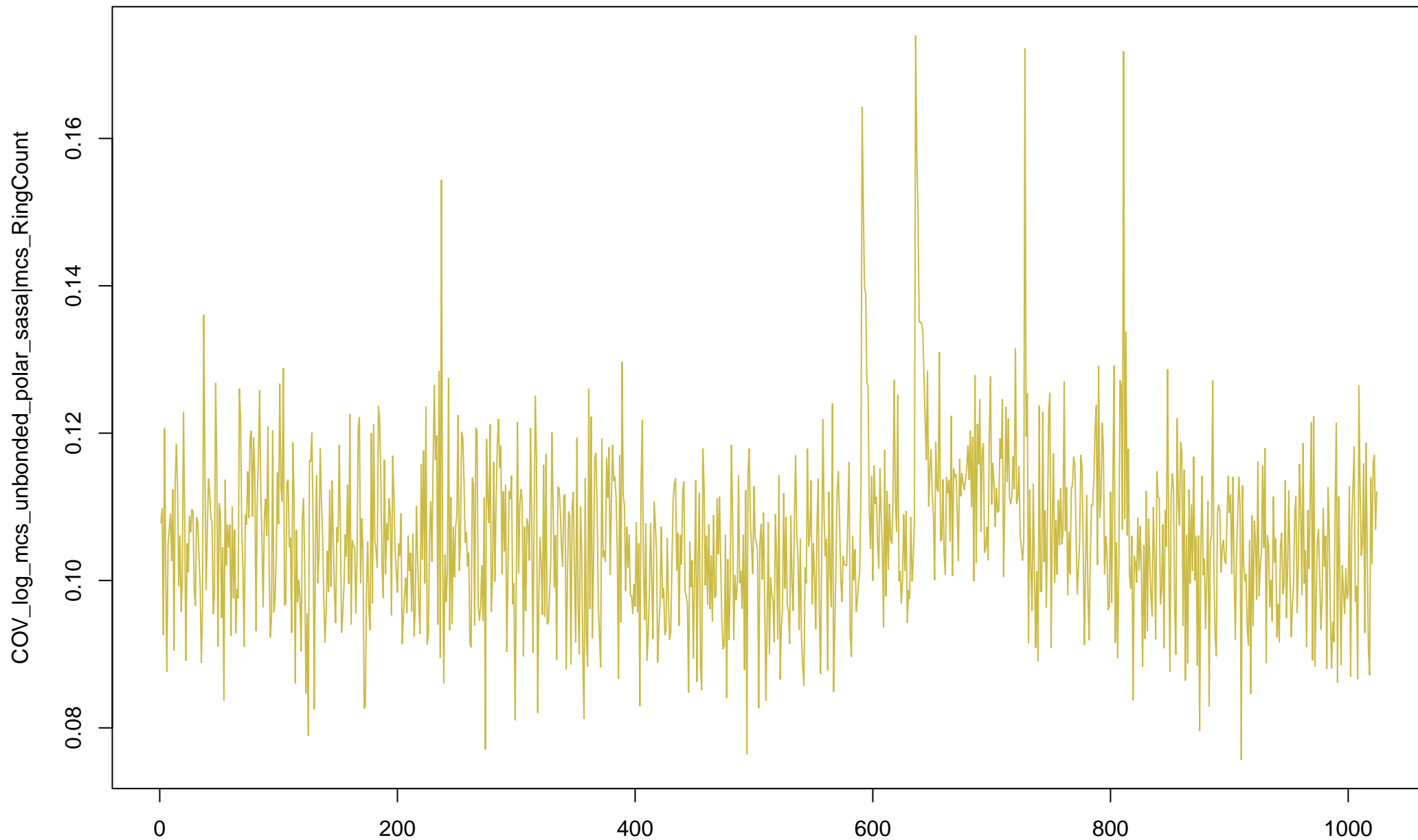
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 420 | BMK = 0.0897 | MCSE(6.27) = 4.07 | stat: TRUE | burn: 0



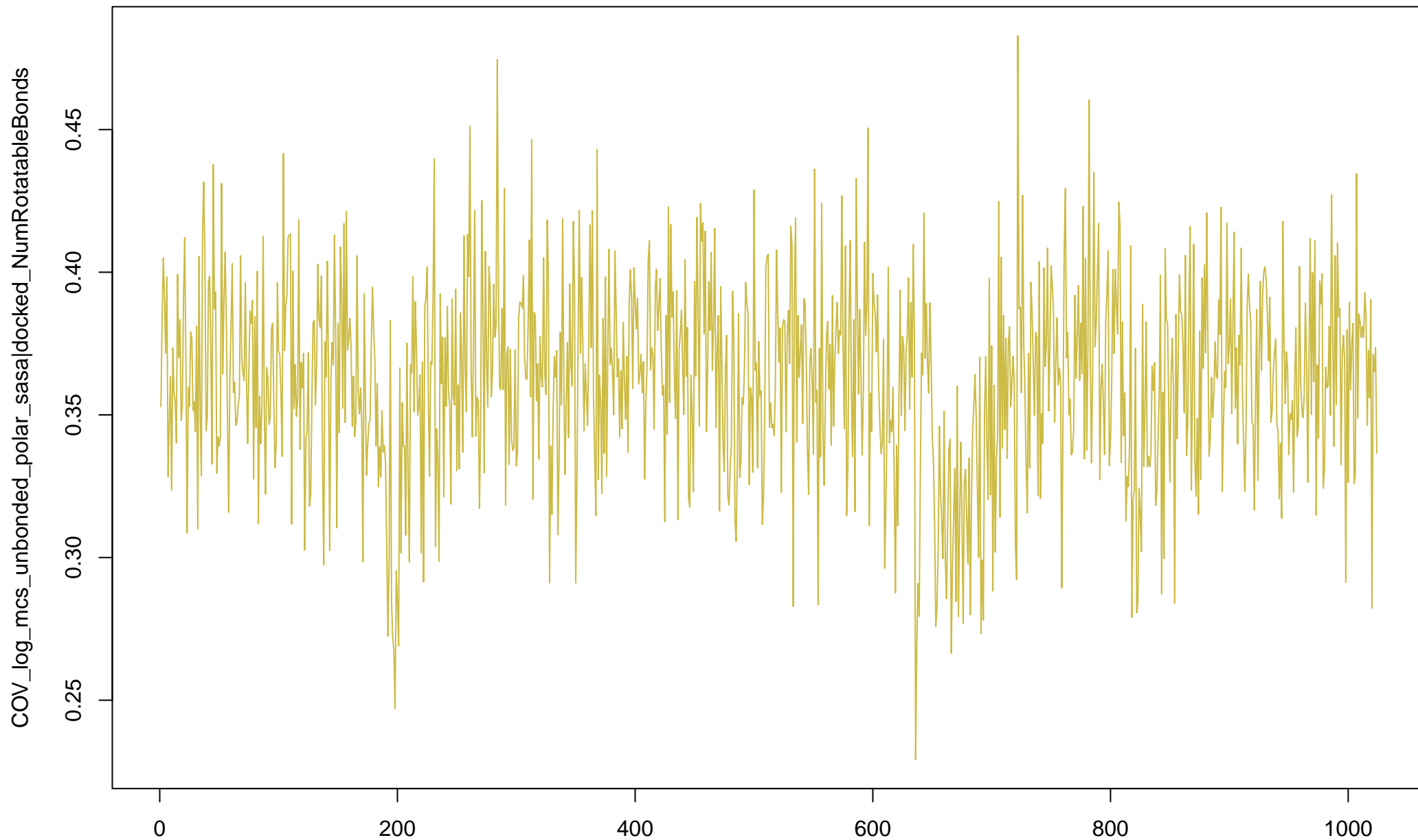
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 88.4 | BMK = 0.0921 | MCSE(6.27) = 7.67 | stat: TRUE | burn: 0



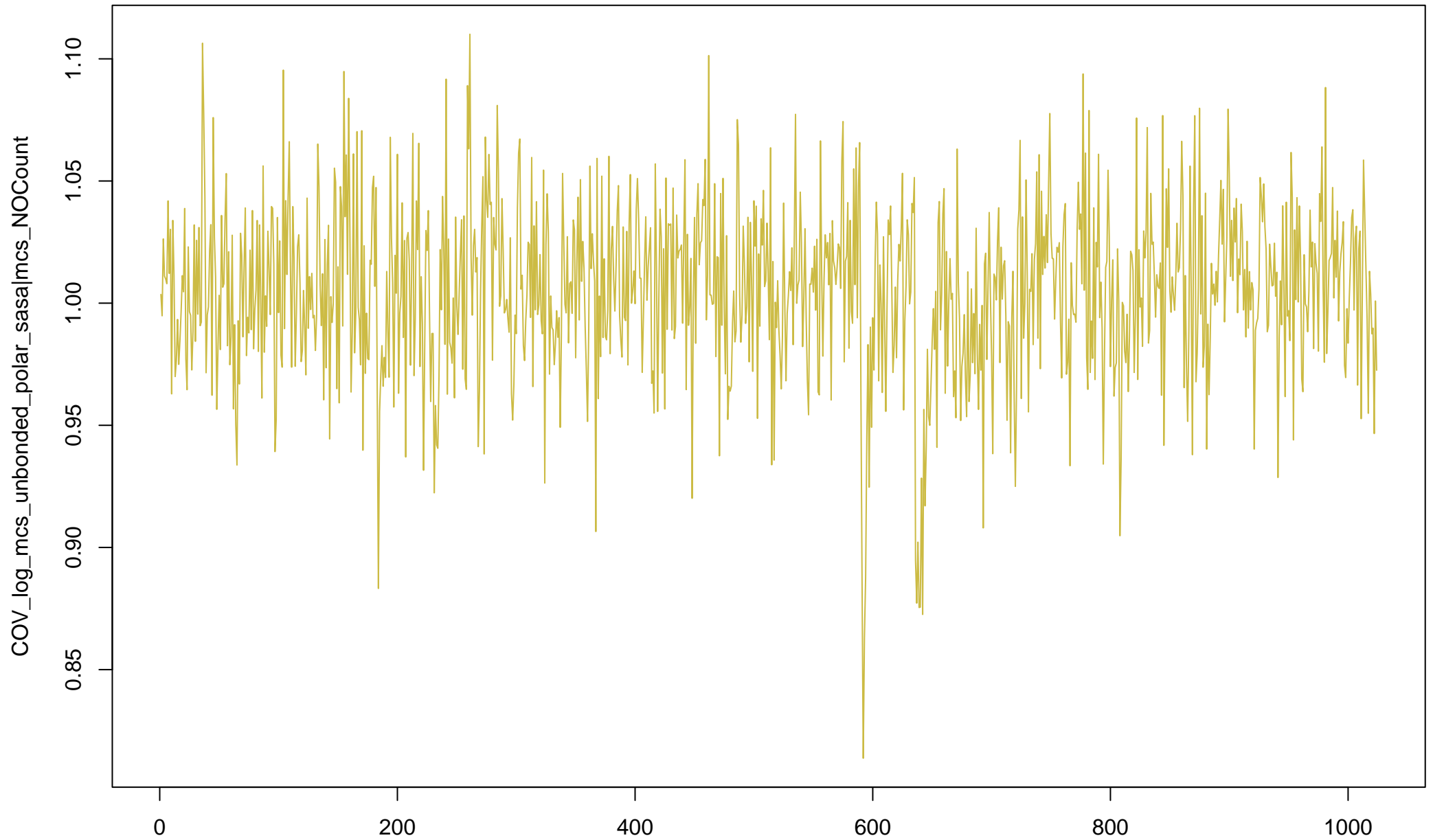
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 292 | BMK = 0.11 | MCSE(6.27) = 6.05 | stat: TRUE | burn: 0



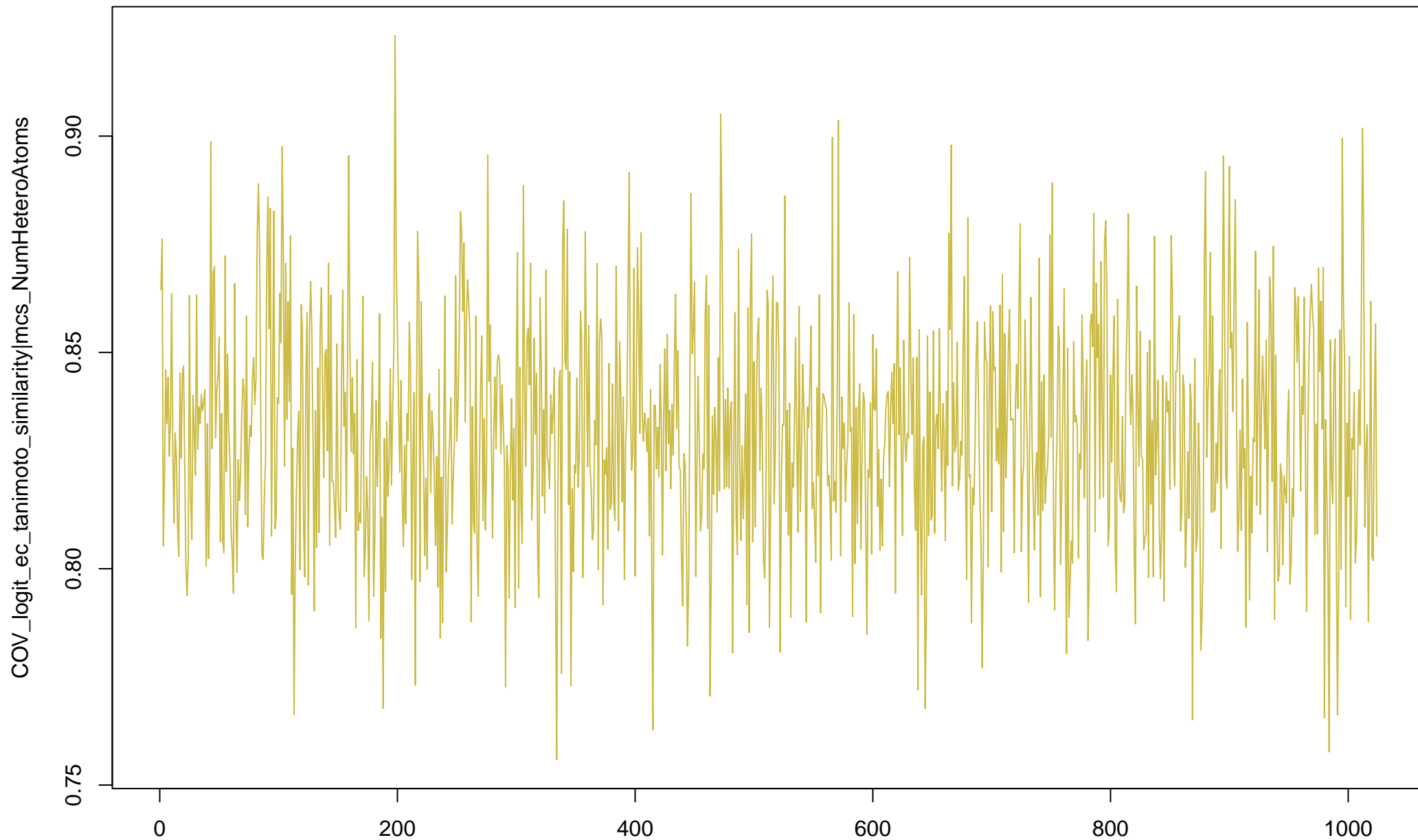
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 174 | BMK = 0.0784 | MCSE(6.27) = 6.6 | stat: TRUE | burn: 0



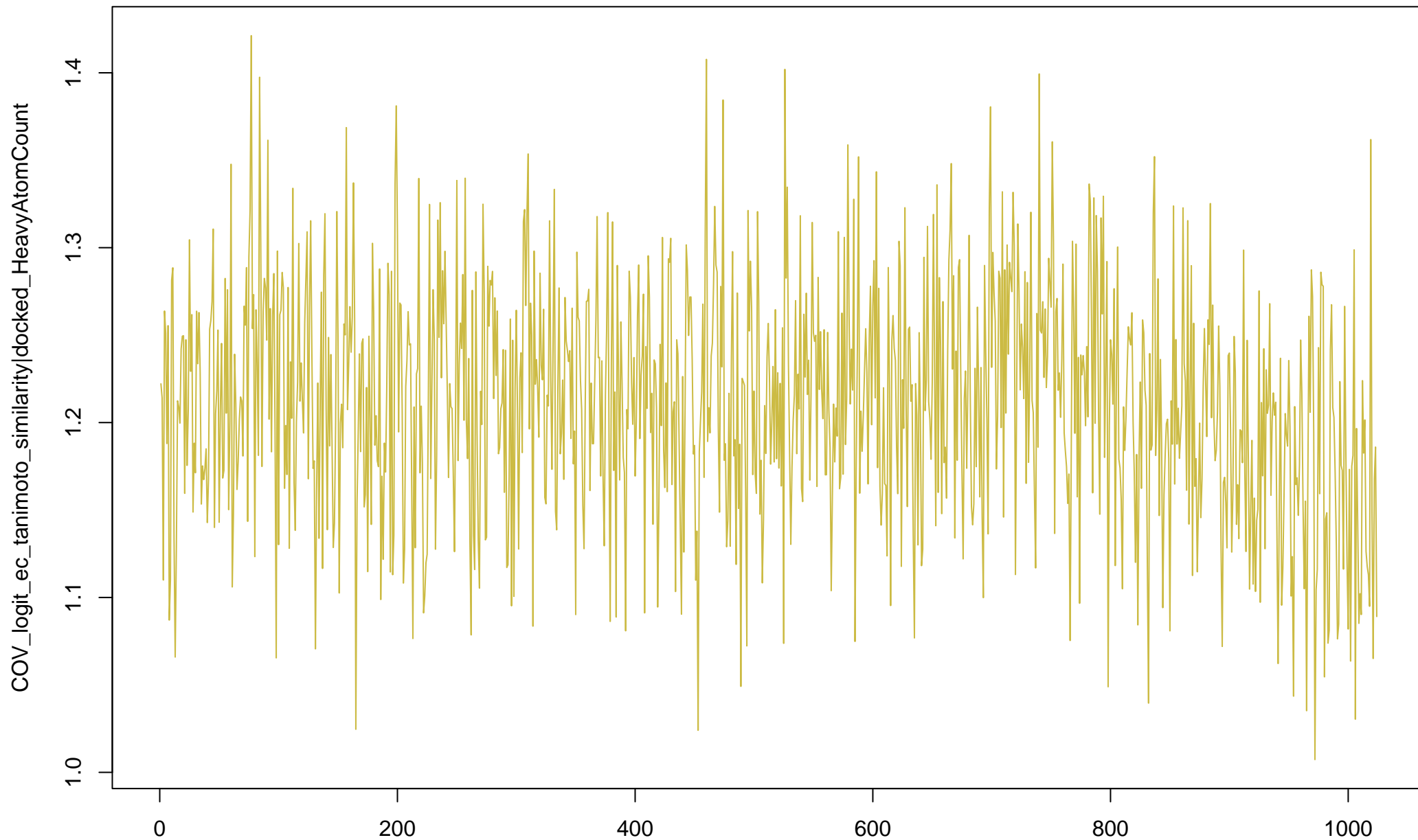
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 390 | BMK = 0.0945 | MCSE(6.27) = 4.71 | stat: TRUE | burn: 0



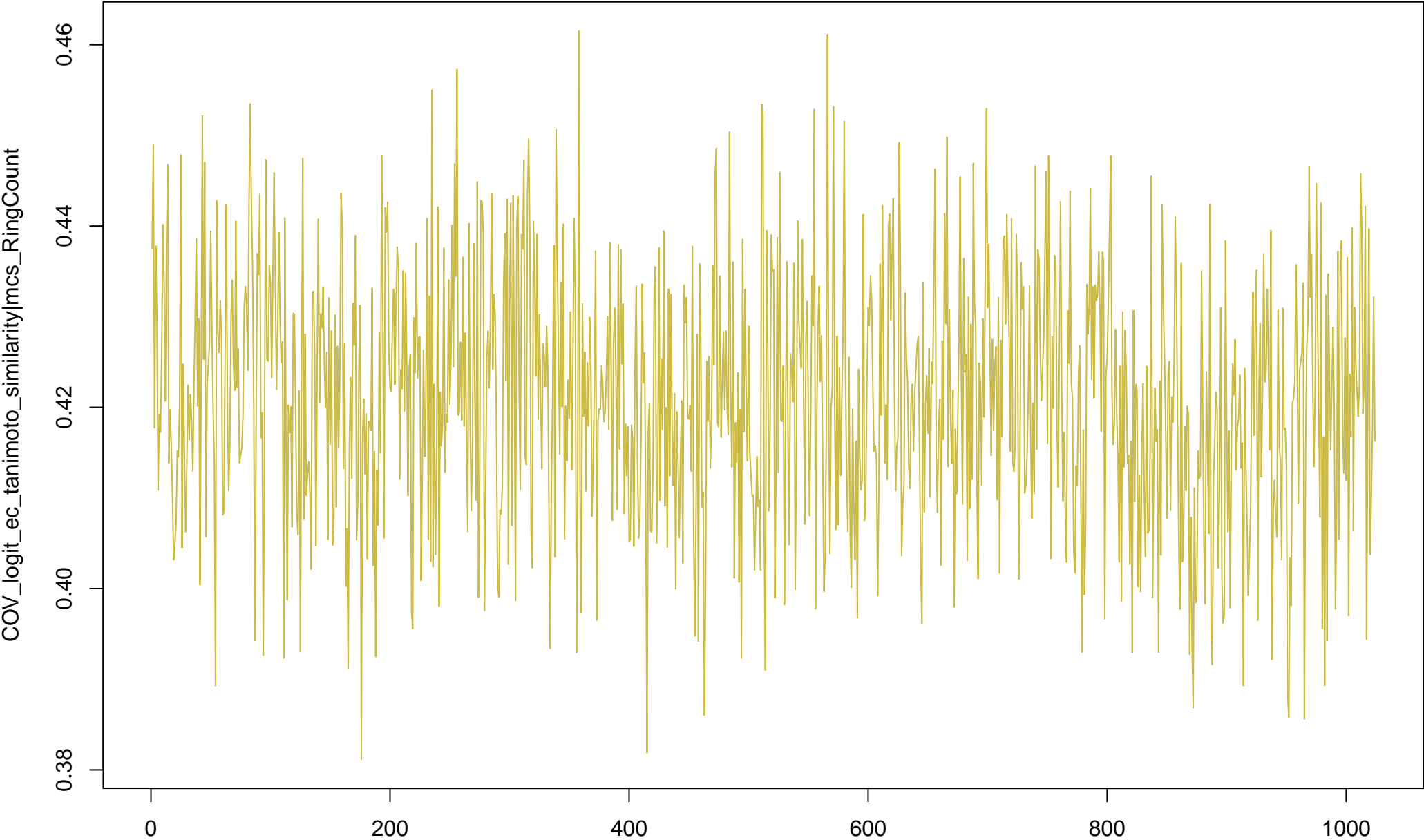
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 878 | BMK = 0.0378 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0



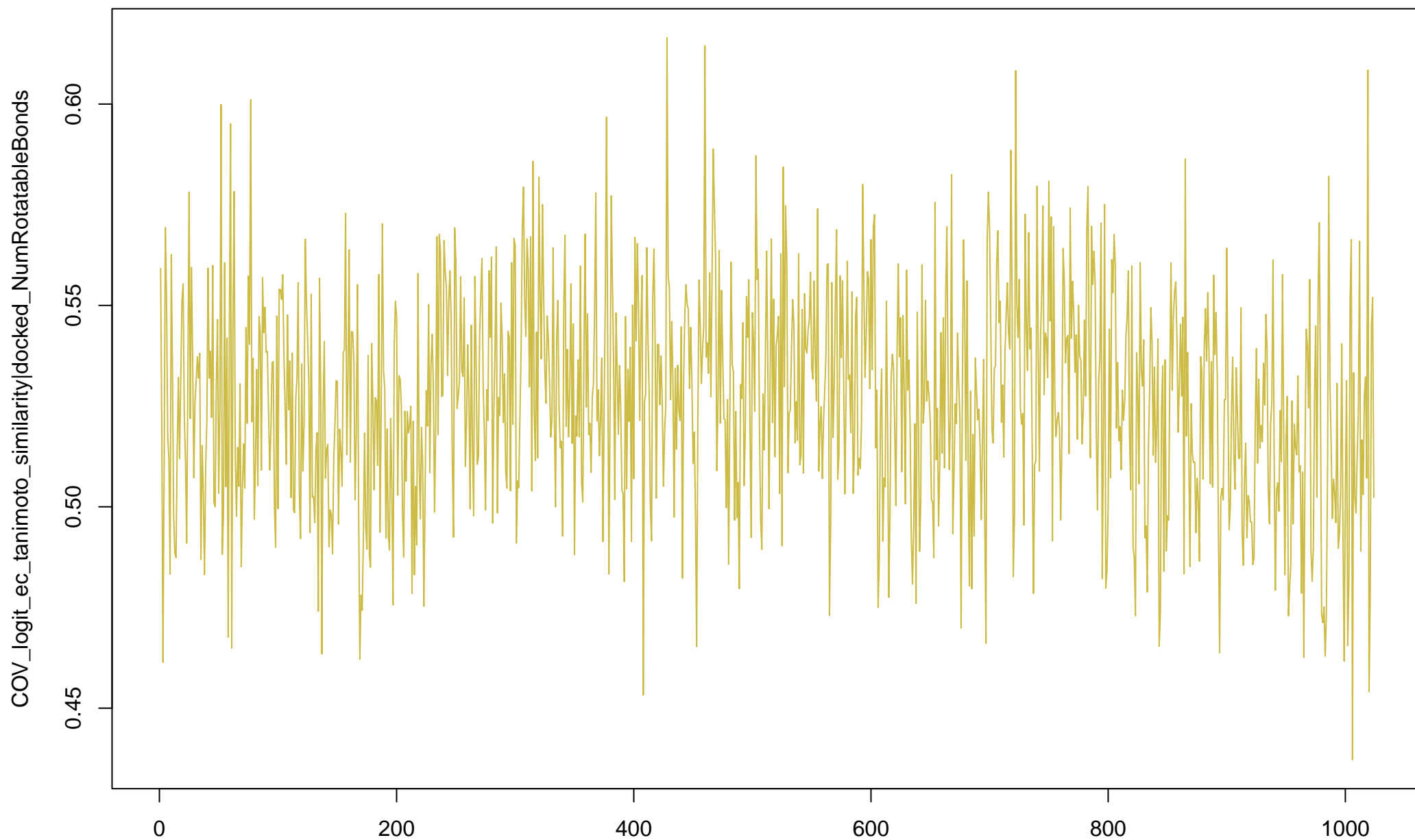
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 345 | BMK = 0.0629 | MCSE(6.27) = 5.49 | stat: TRUE | burn: 0



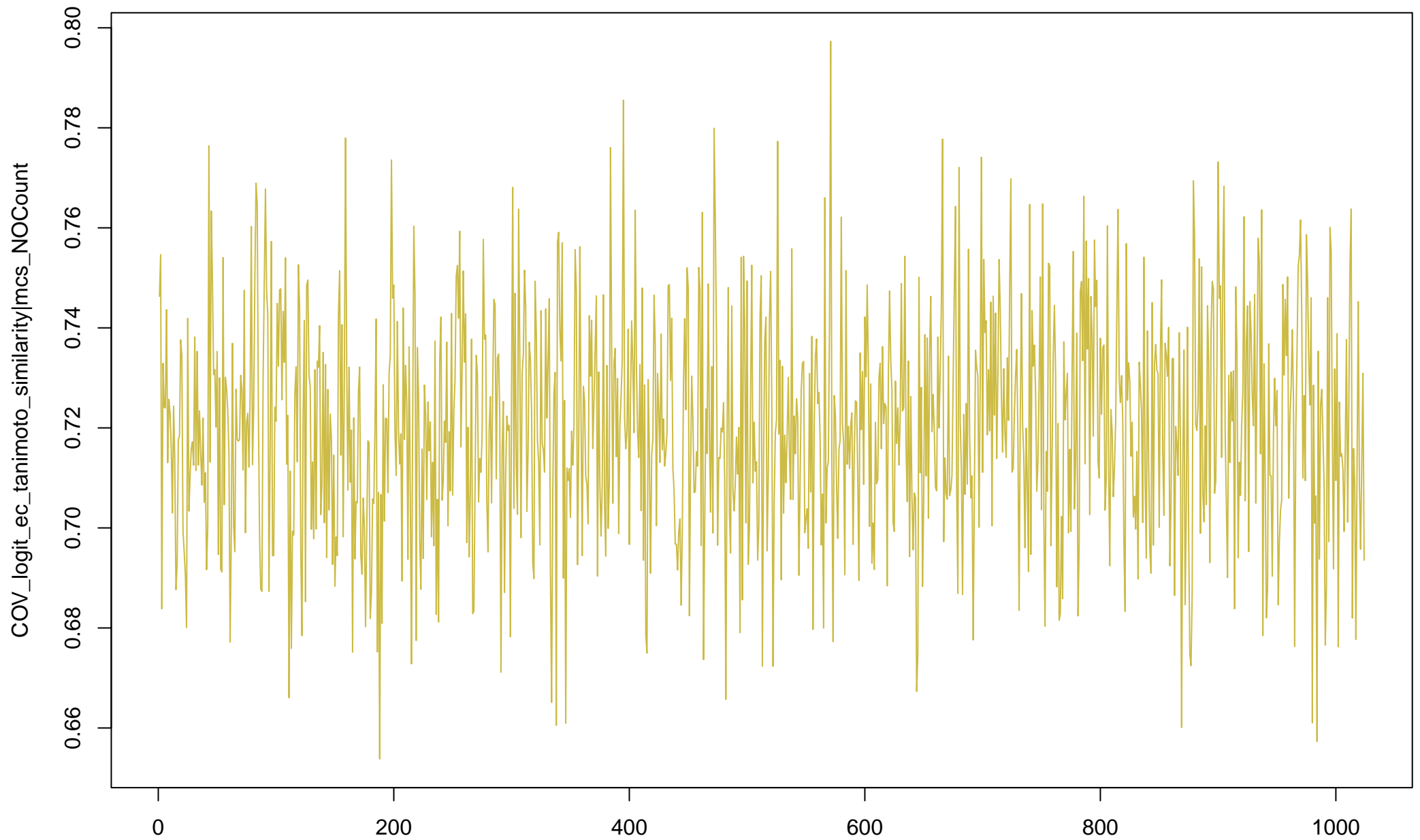
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 838 | BMK = 0.052 | MCSE(6.27) = 4.65 | stat: FALSE | burn: 0



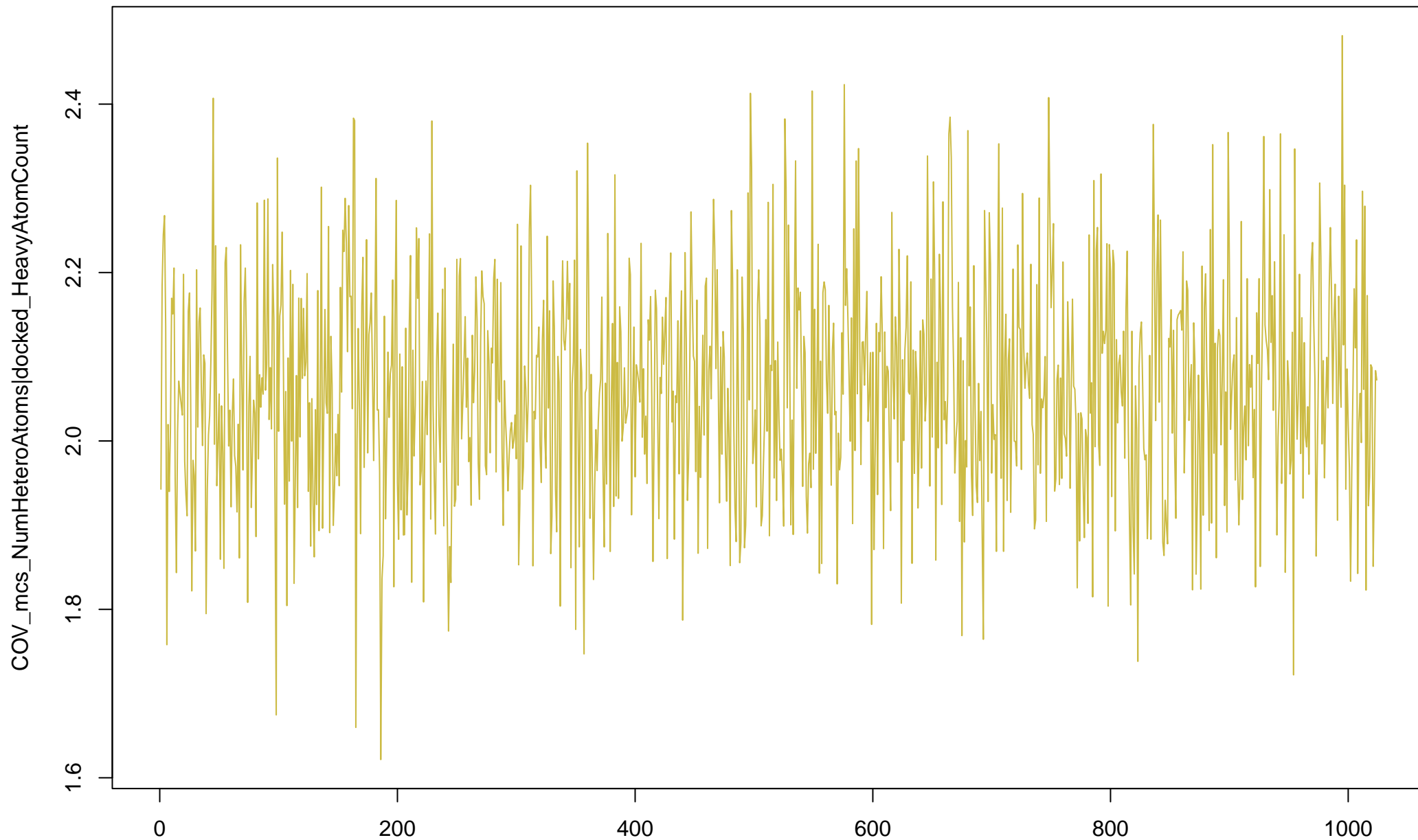
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 263 | BMK = 0.0611 | MCSE(6.27) = 5.77 | stat: TRUE | burn: 0



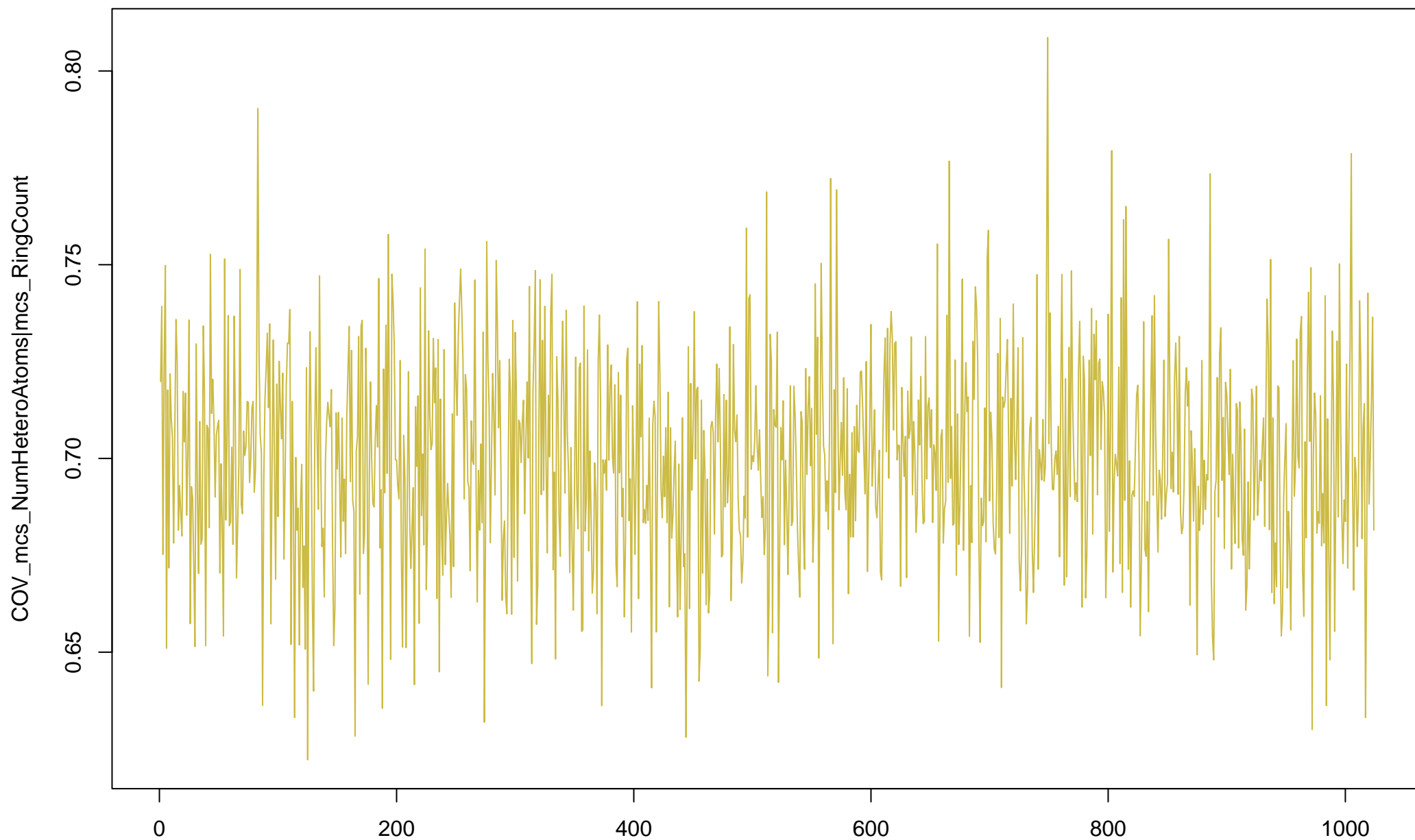
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 882 | BMK = 0.0389 | MCSE(6.27) = 3.39 | stat: TRUE | burn: 0



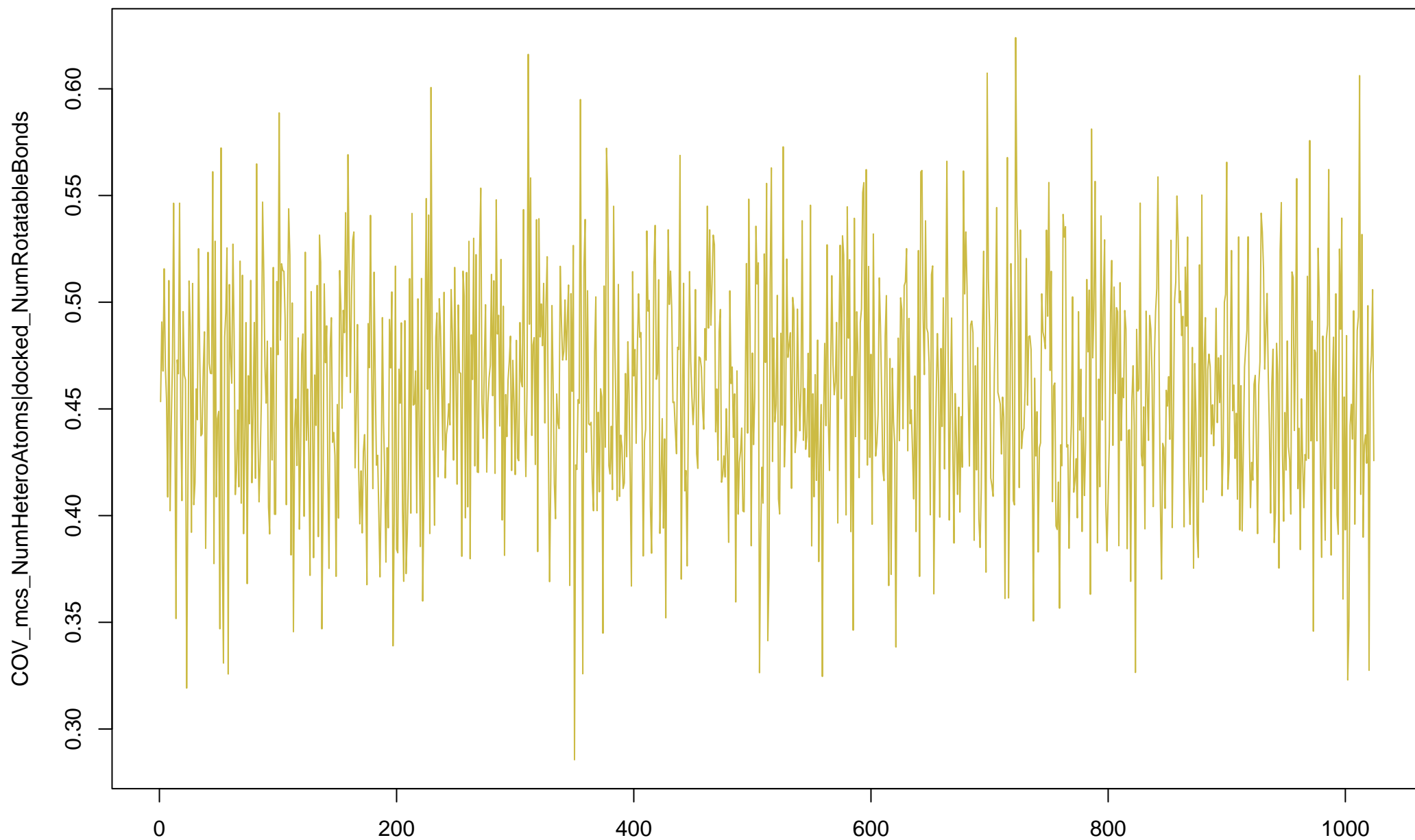
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0621 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0



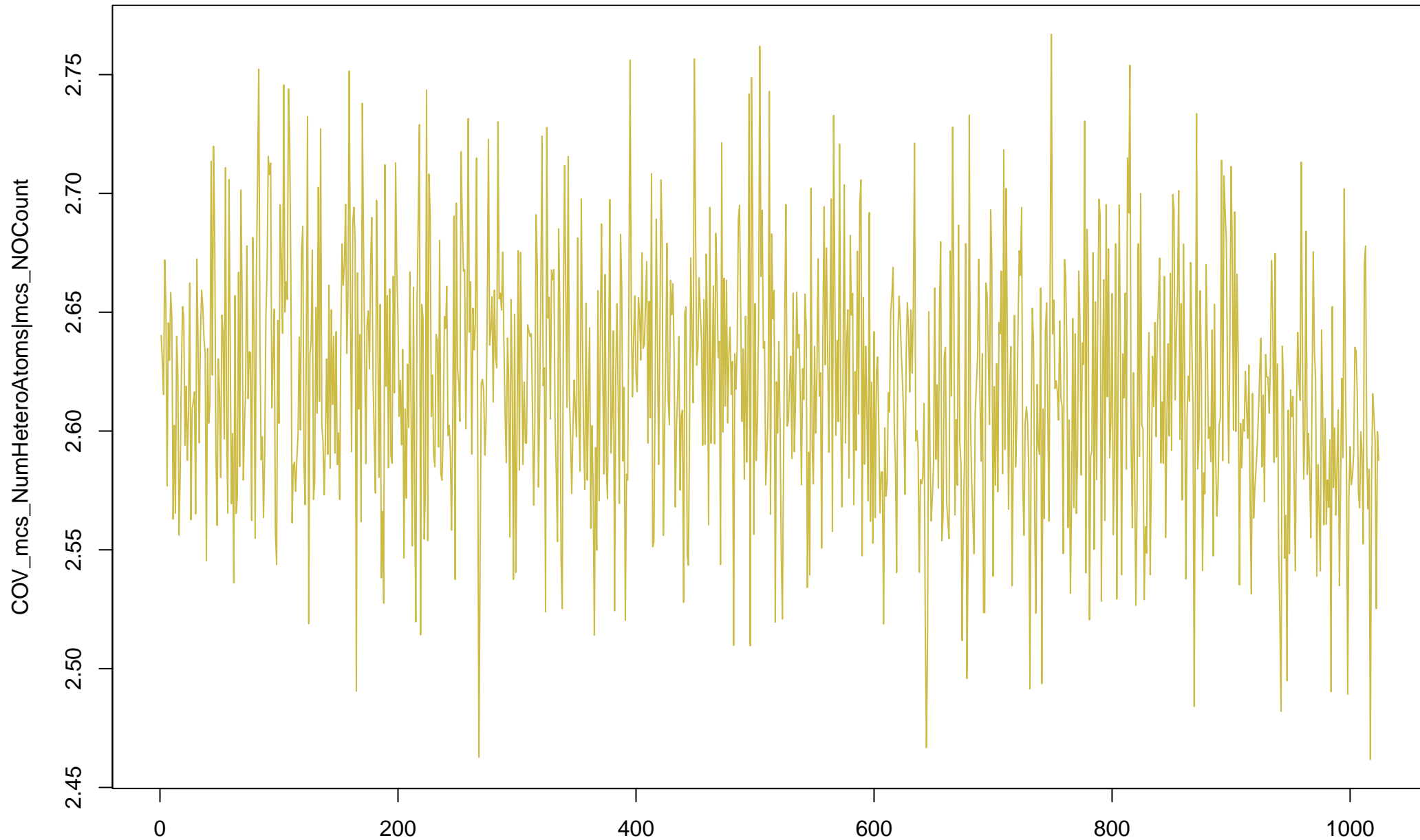
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0727 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0



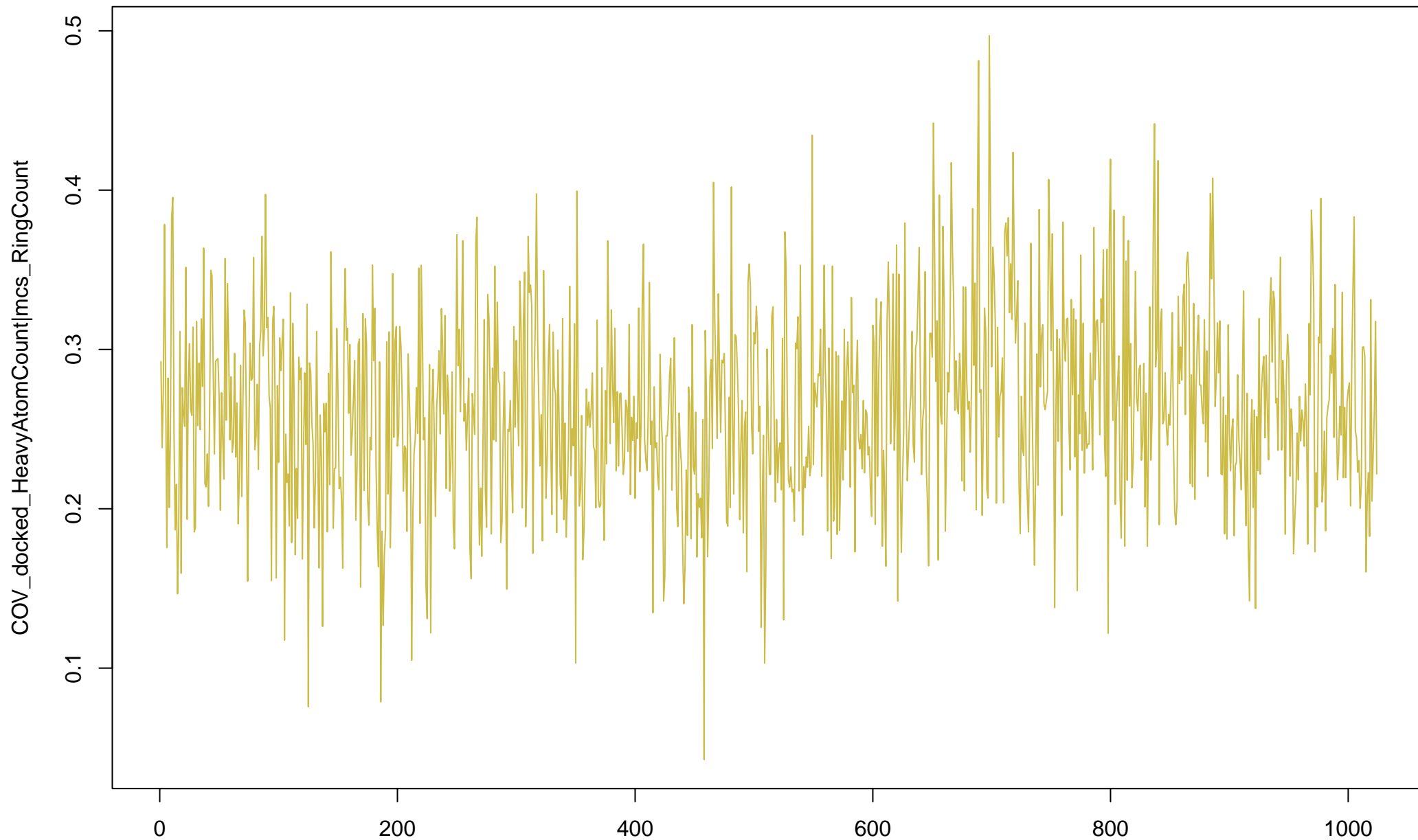
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0357 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0



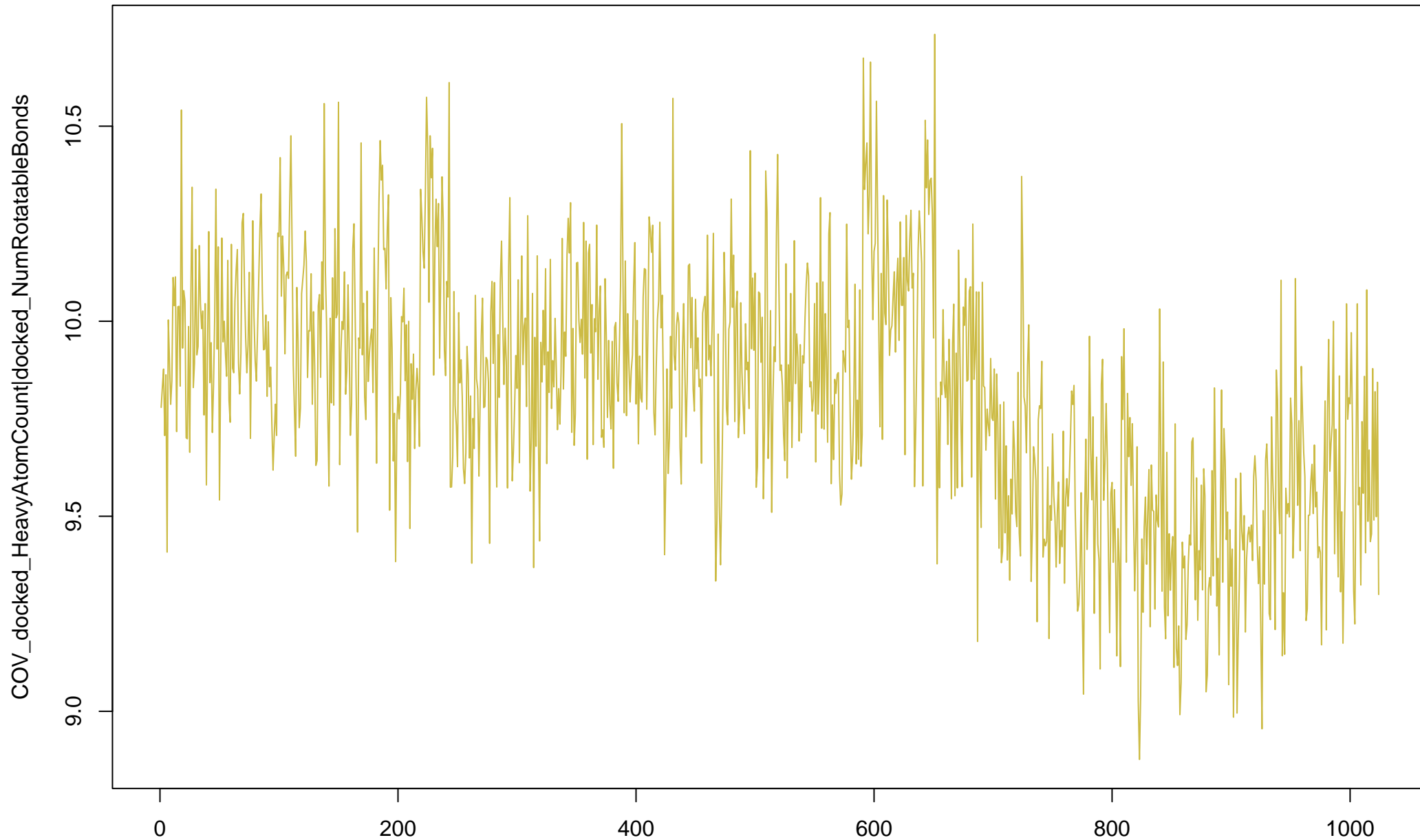
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 673 | BMK = 0.122 | MCSE(6.27) = 4.53 | stat: FALSE | burn: 0



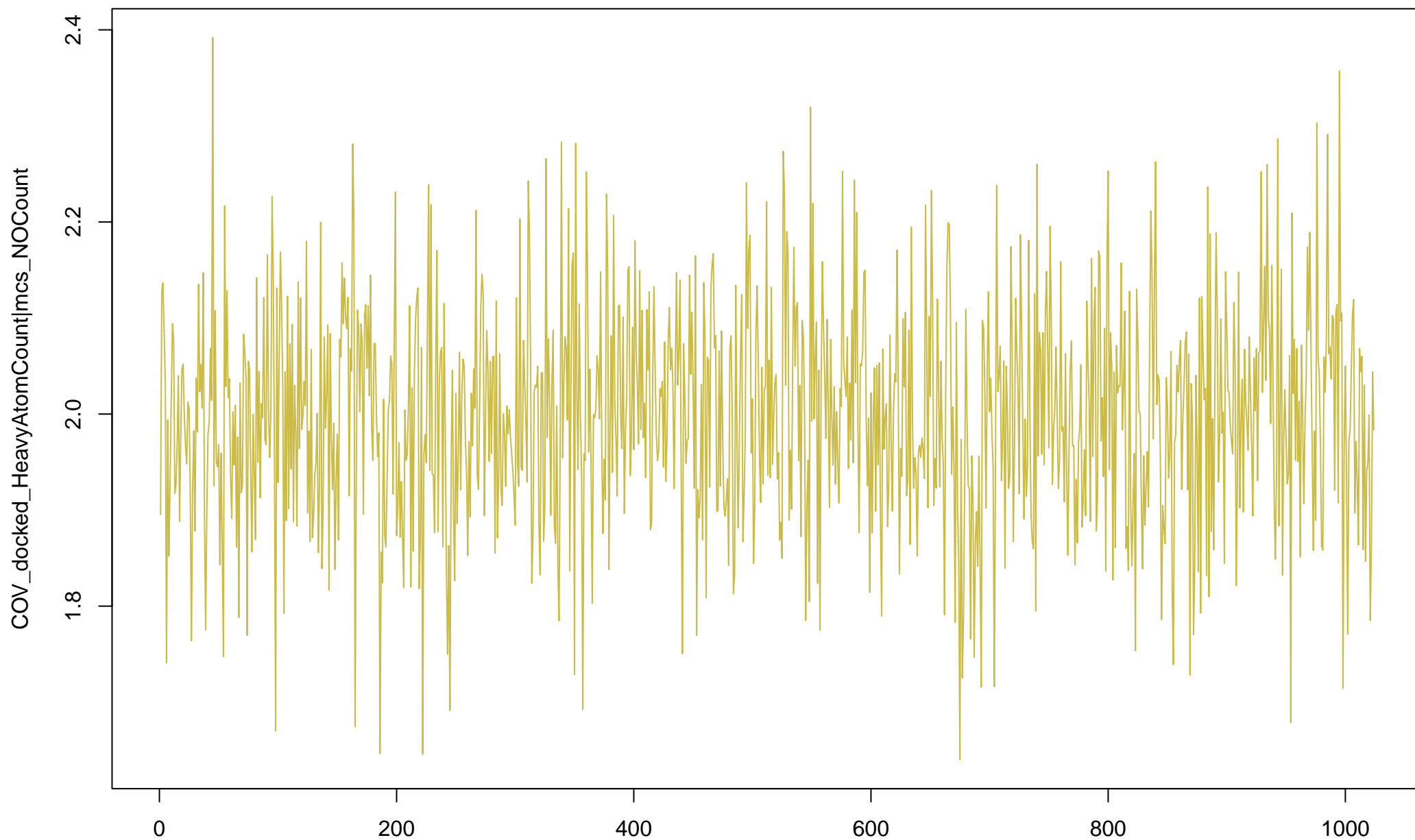
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 477 | BMK = 0.127 | MCSE(6.27) = 5.01 | stat: TRUE | burn: 0



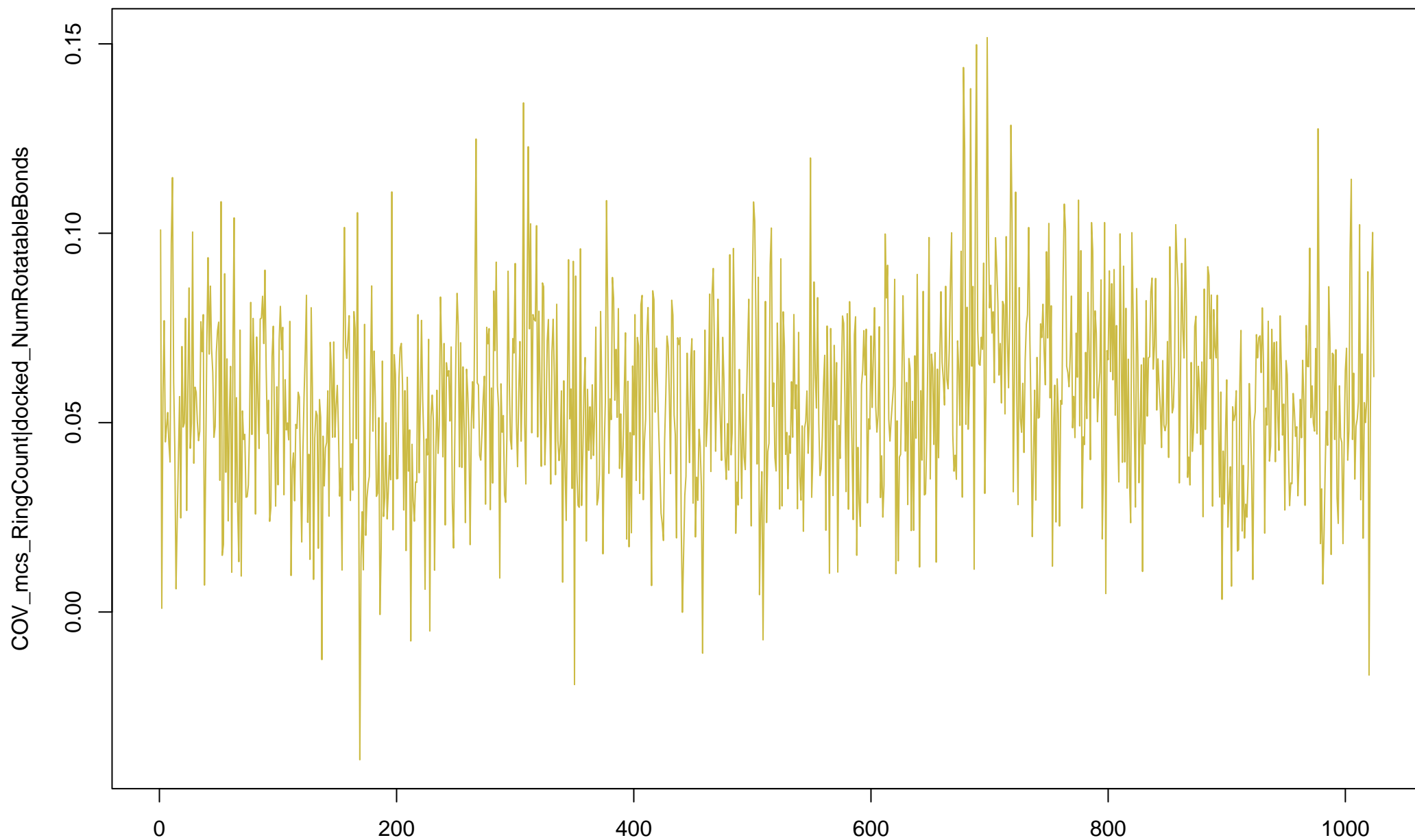
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 15 | BMK = 0.386 | MCSE(6.27) = 12.4 | stat: FALSE | burn: 0



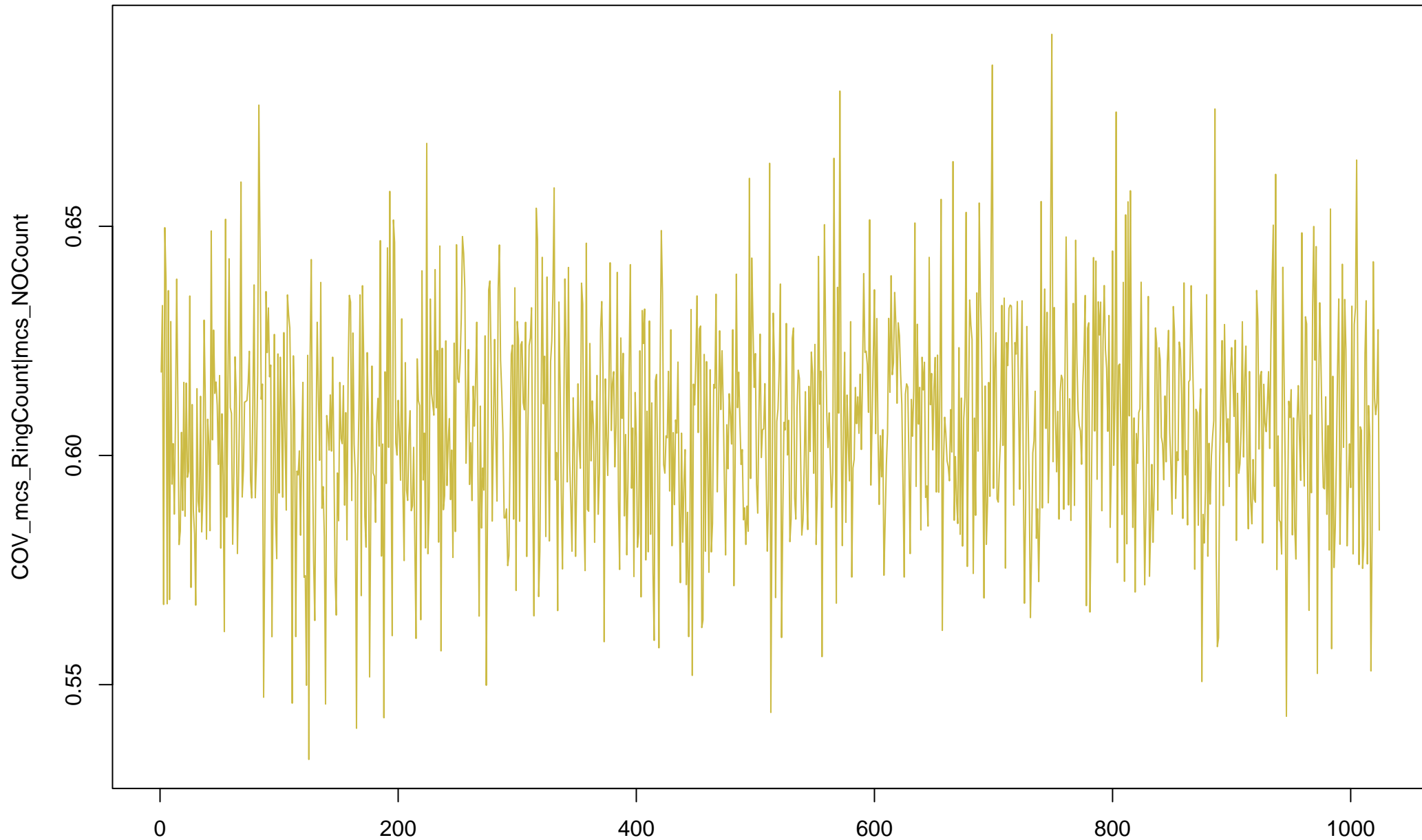
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 837 | BMK = 0.0433 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 177 | BMK = 0.105 | MCSE(6.27) = 5.57 | stat: TRUE | burn: 0



COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.0658 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 0



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.044 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0

