

-- STATS maxD --

min ESS = 1.72542782773578

max BMK = 0.880561425958531

max MCSE = 17.2315225497648

all stationary: FALSE

burn: 1020

-- STATS 2D --

min ESS = 6.47641515616928

max BMK = 0.553670000126266

max MCSE = 15.5803748602898

all stationary: FALSE

burn: 204

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 1

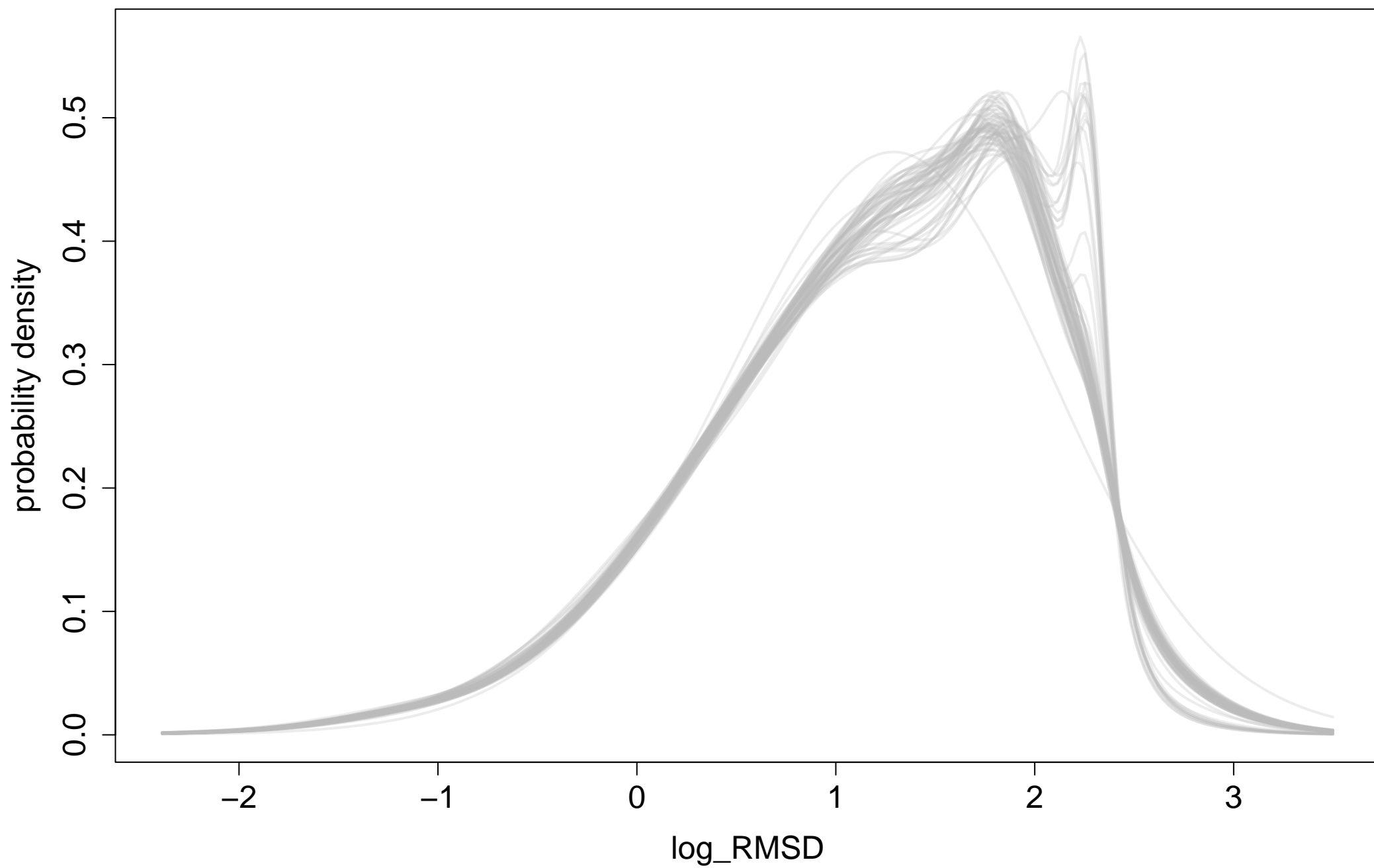
max MCSE = NaN

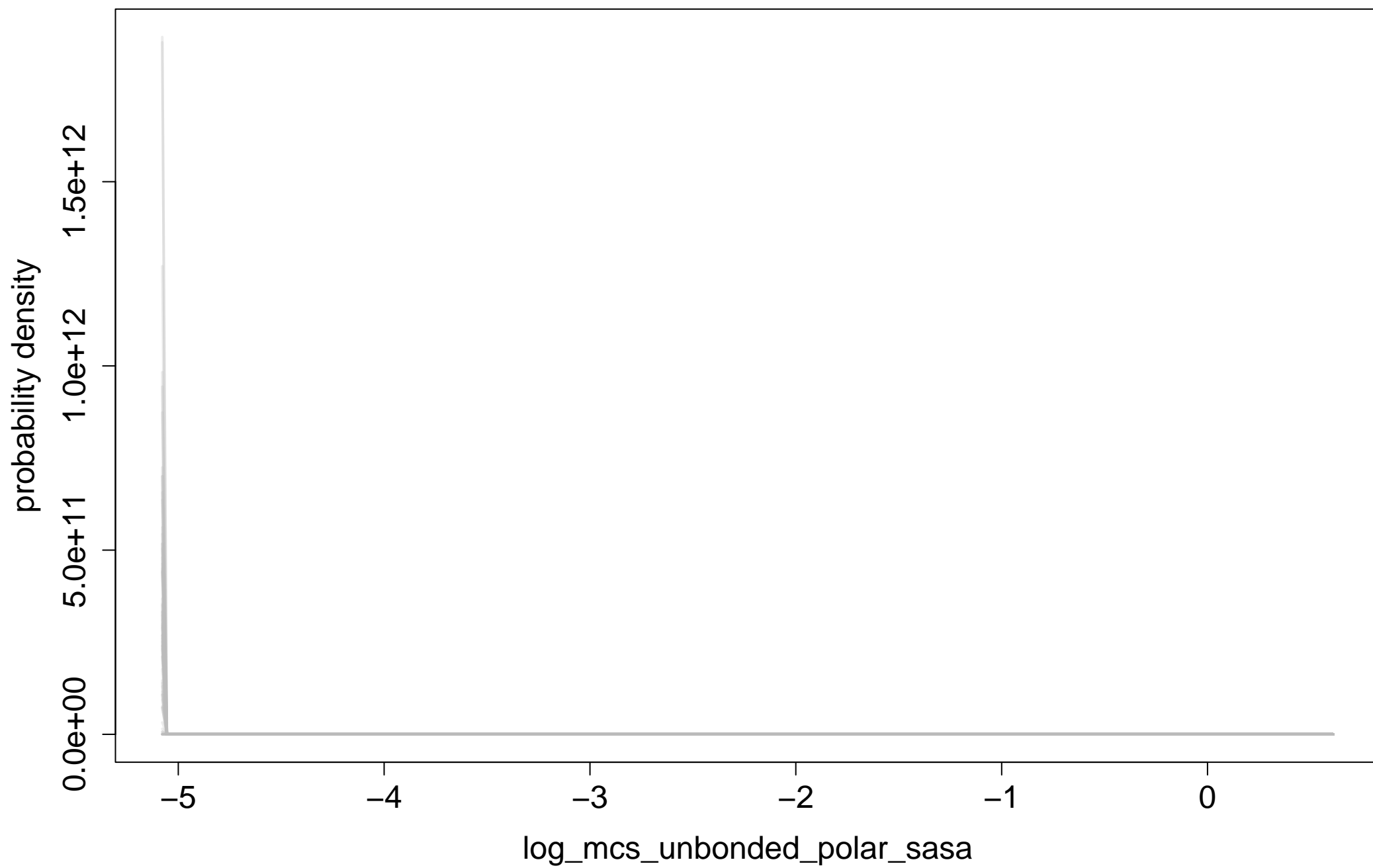
all stationary: FALSE

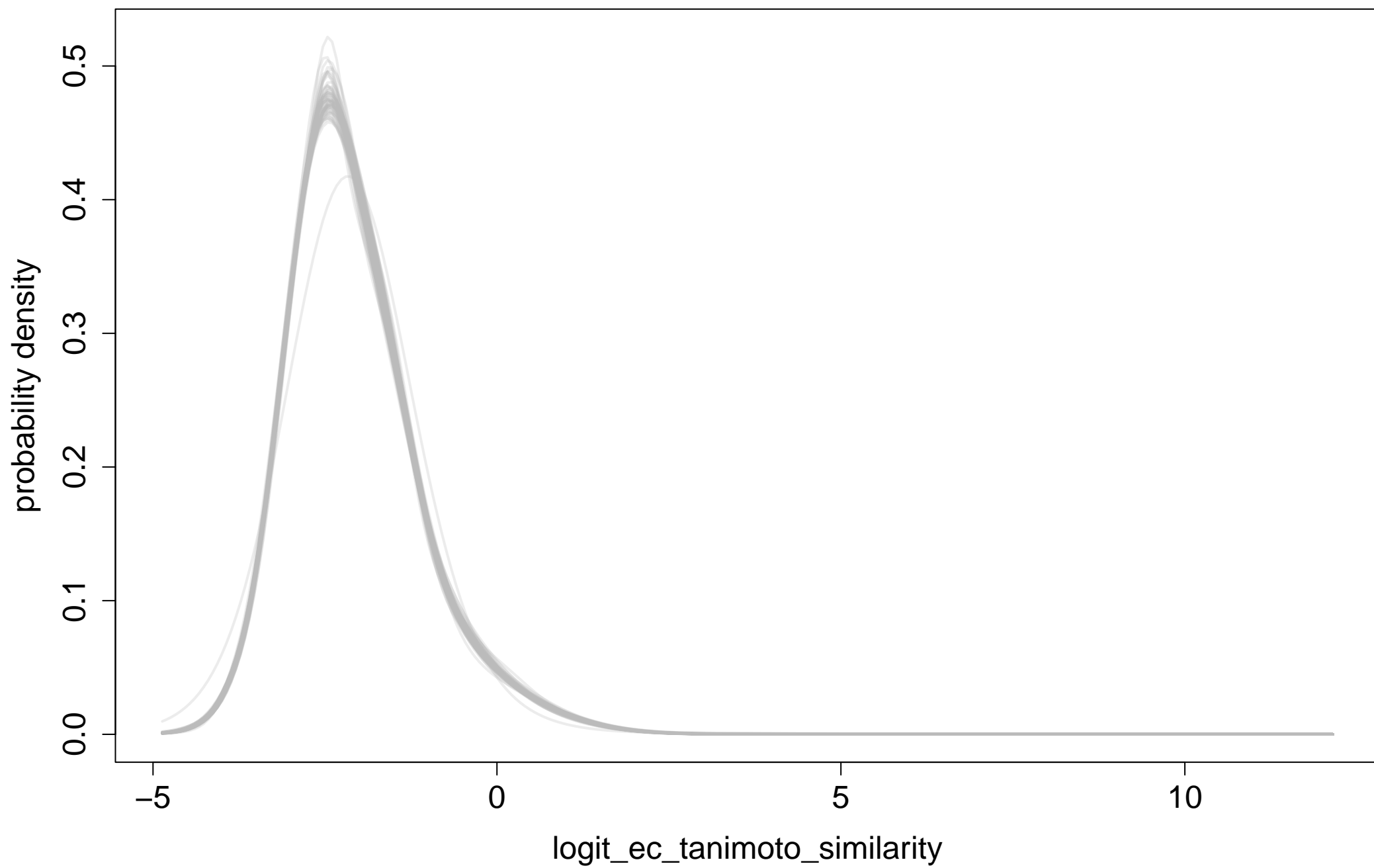
burn: 816

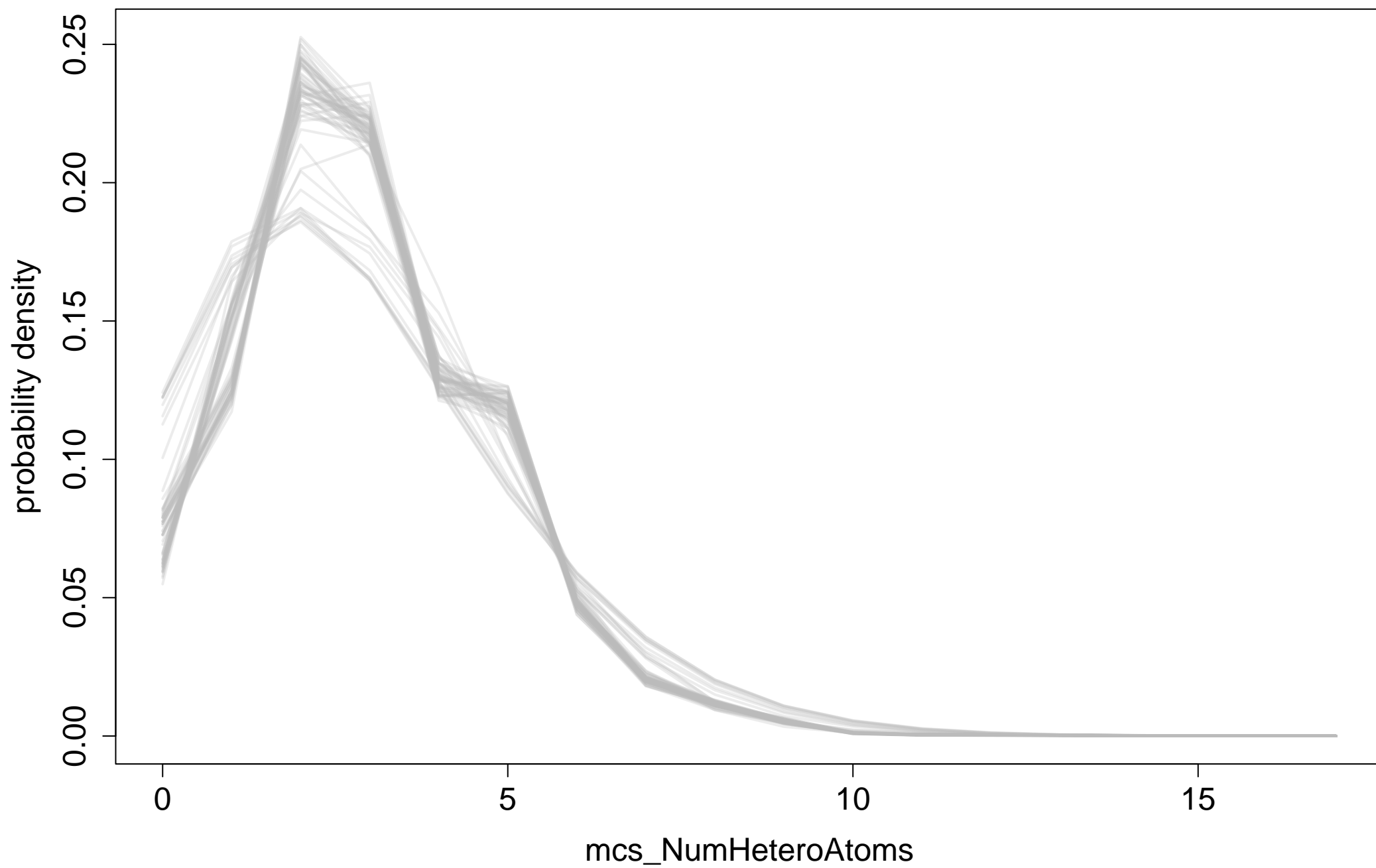
Occupied clusters: 55 of 64

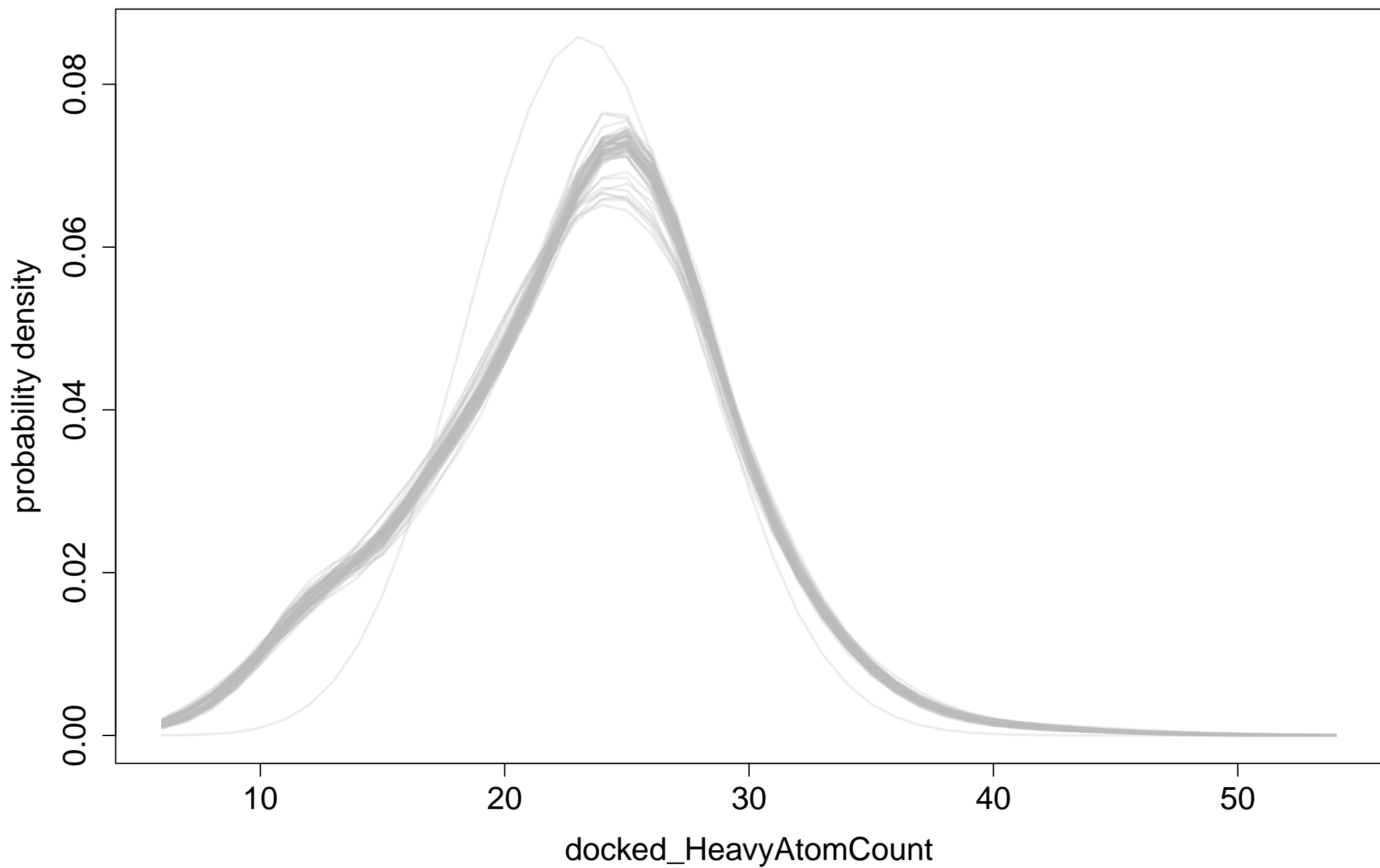
LL: -74600 +- 5280

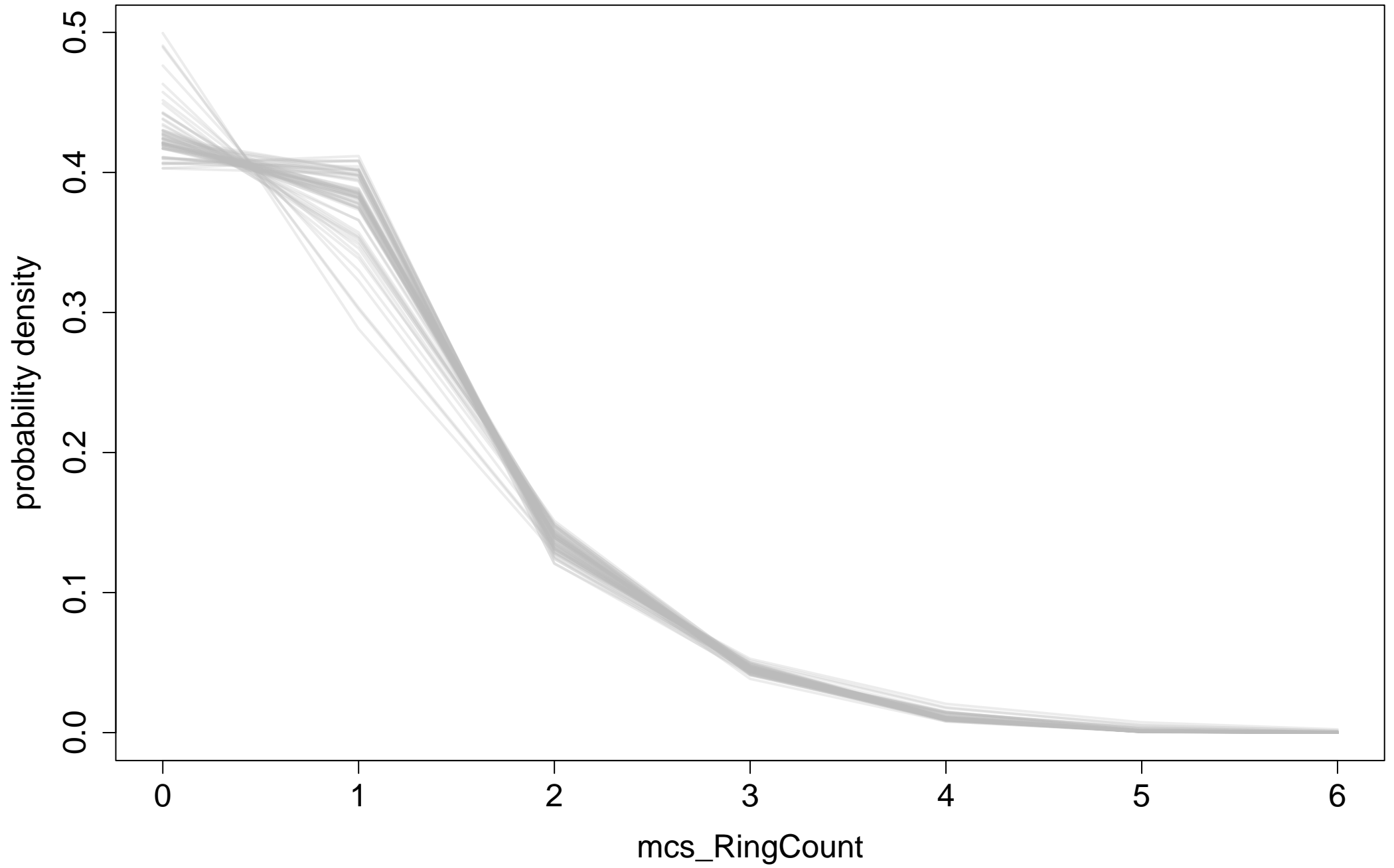


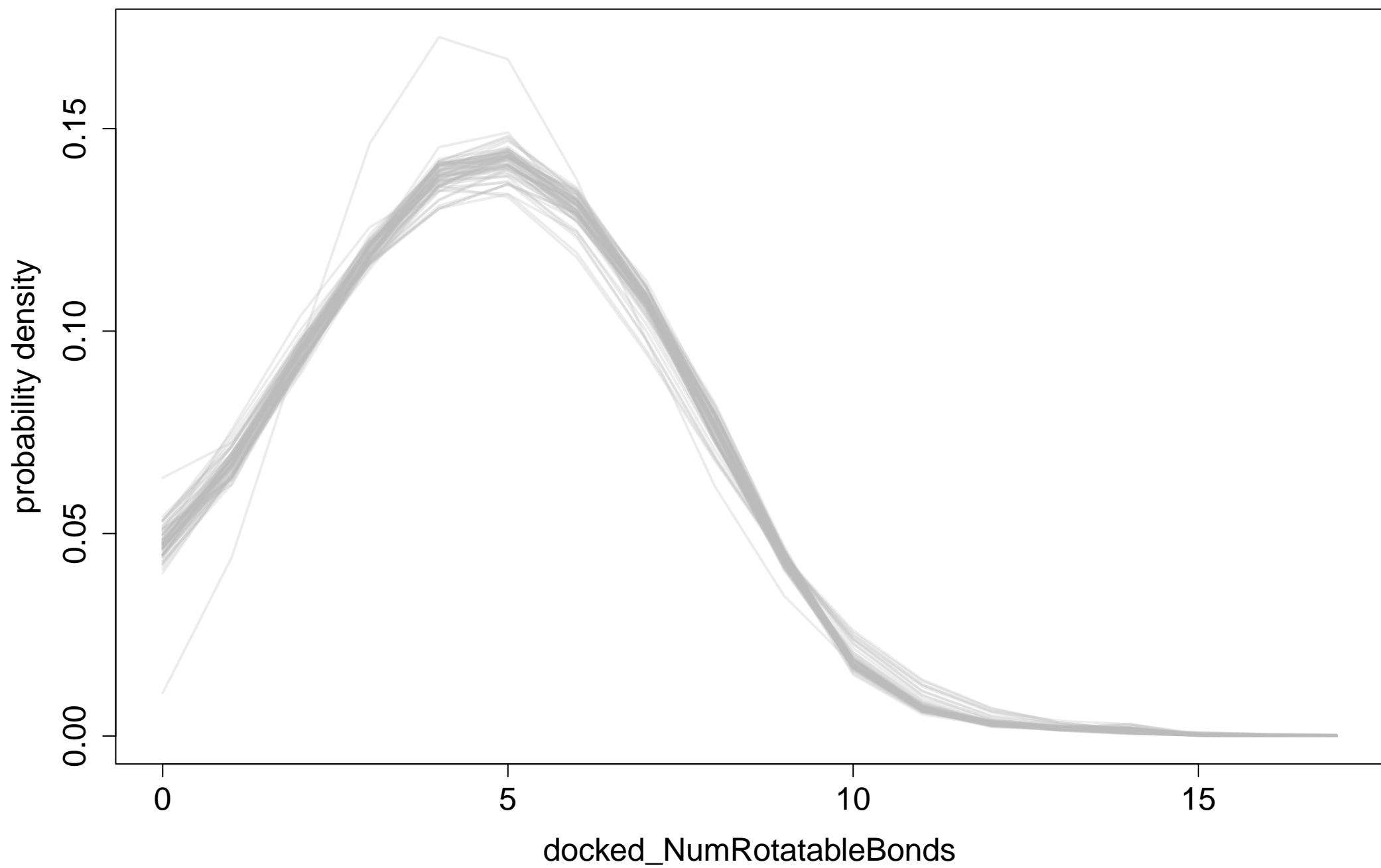


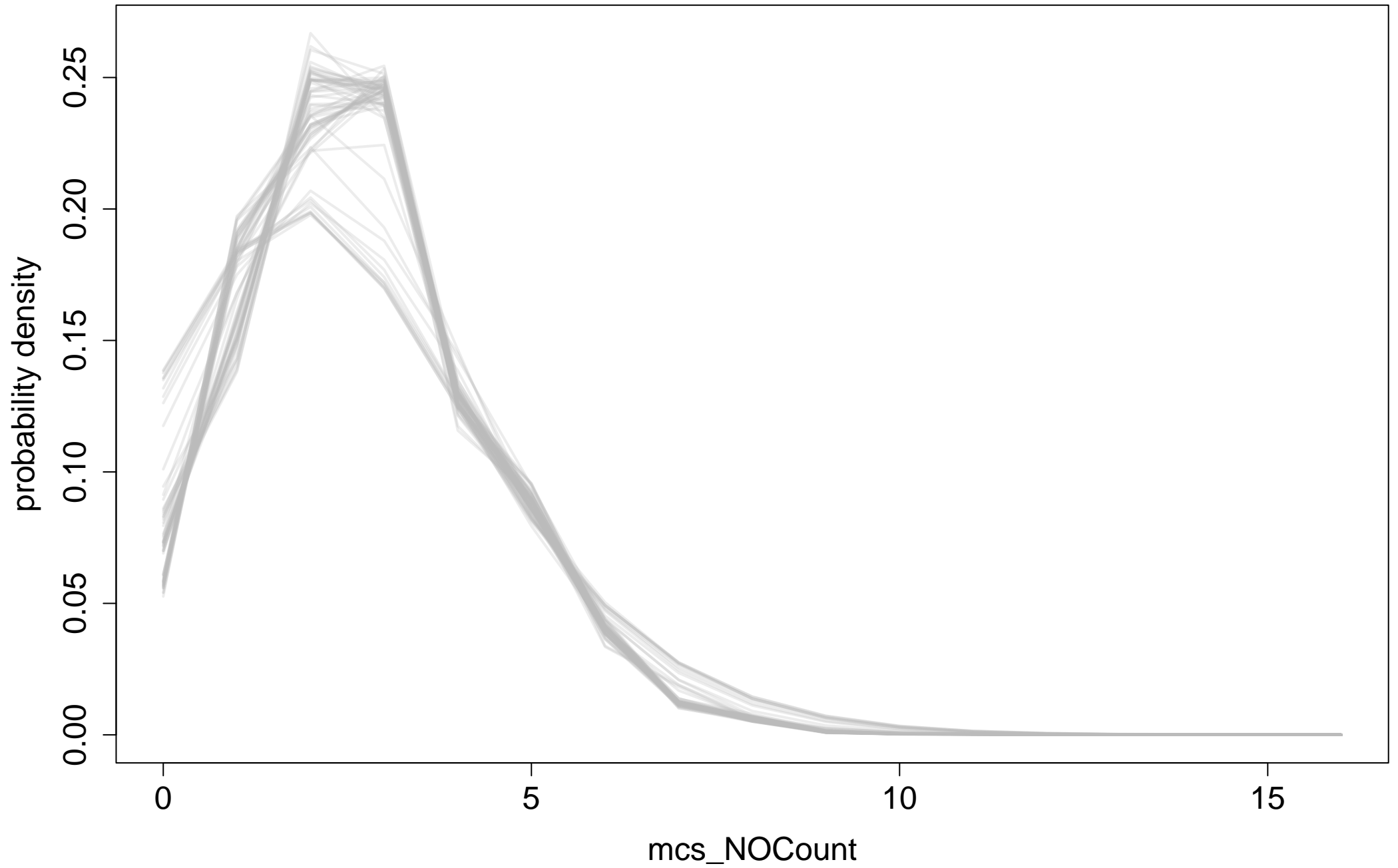


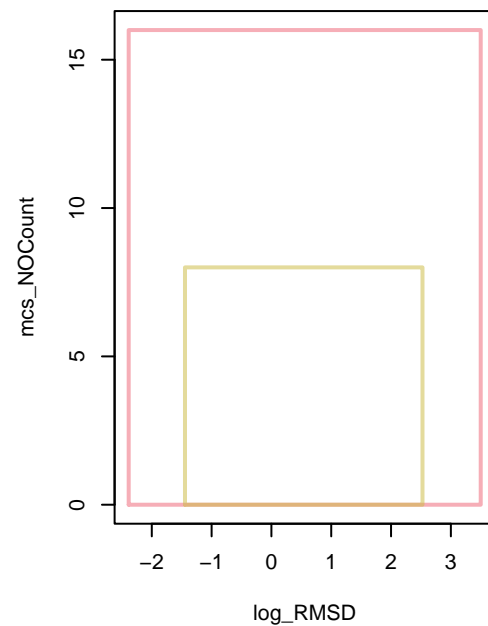
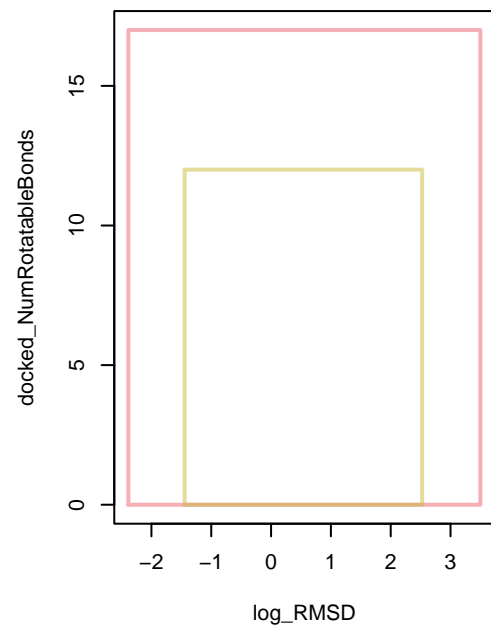
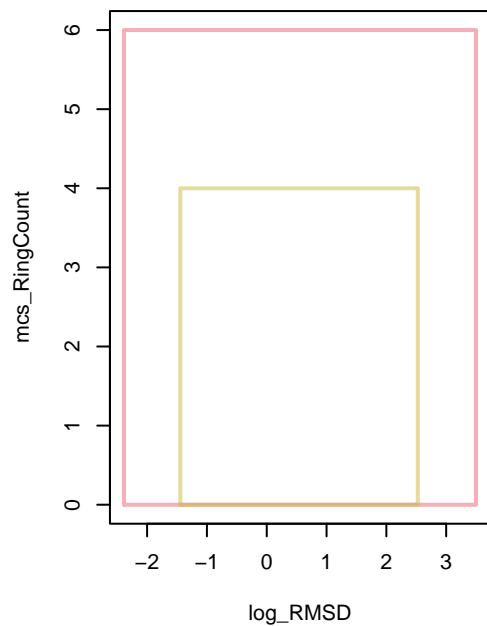
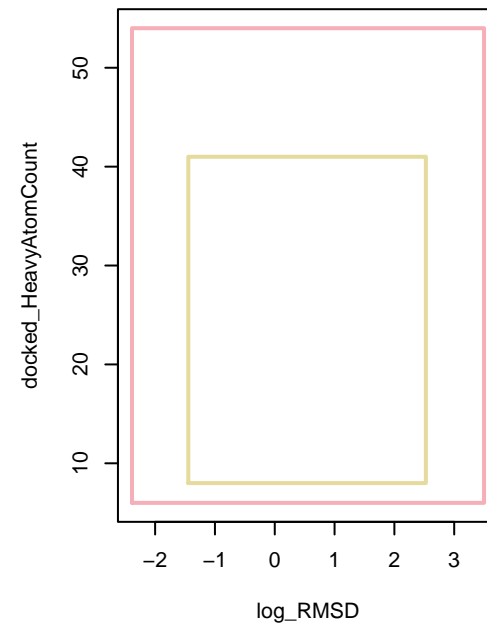
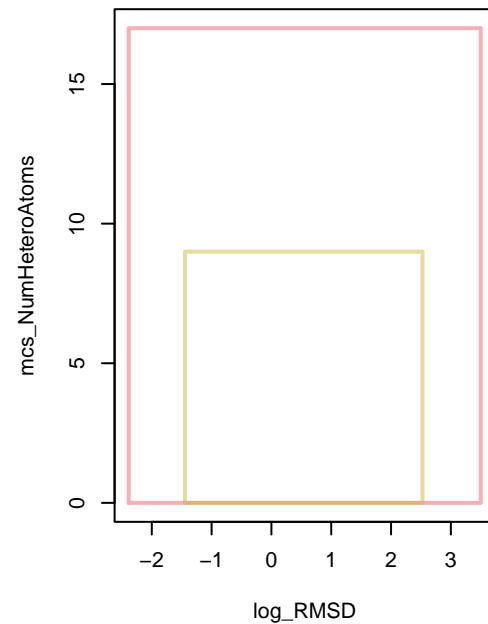
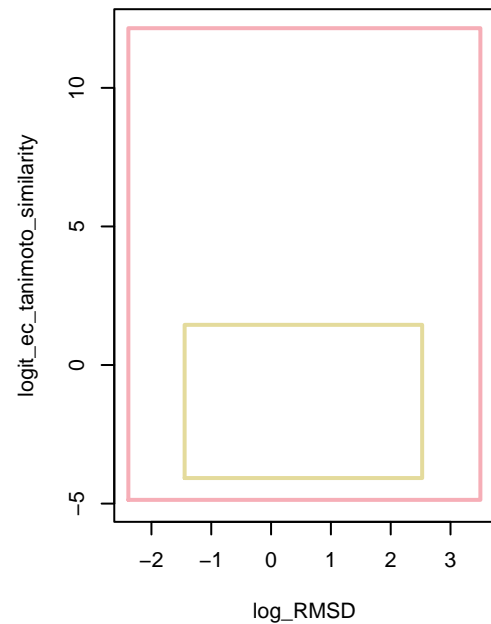
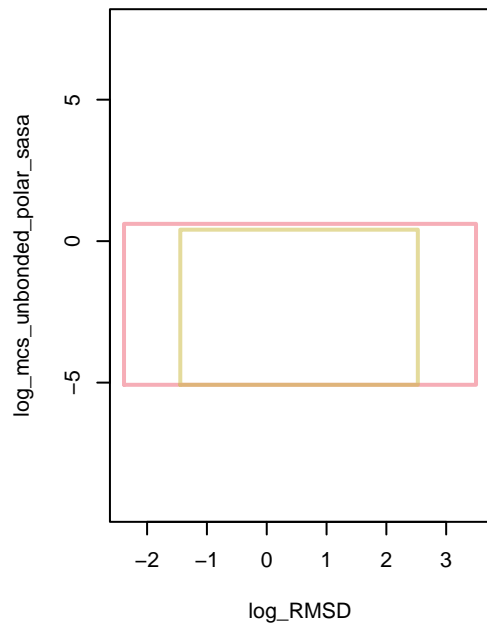




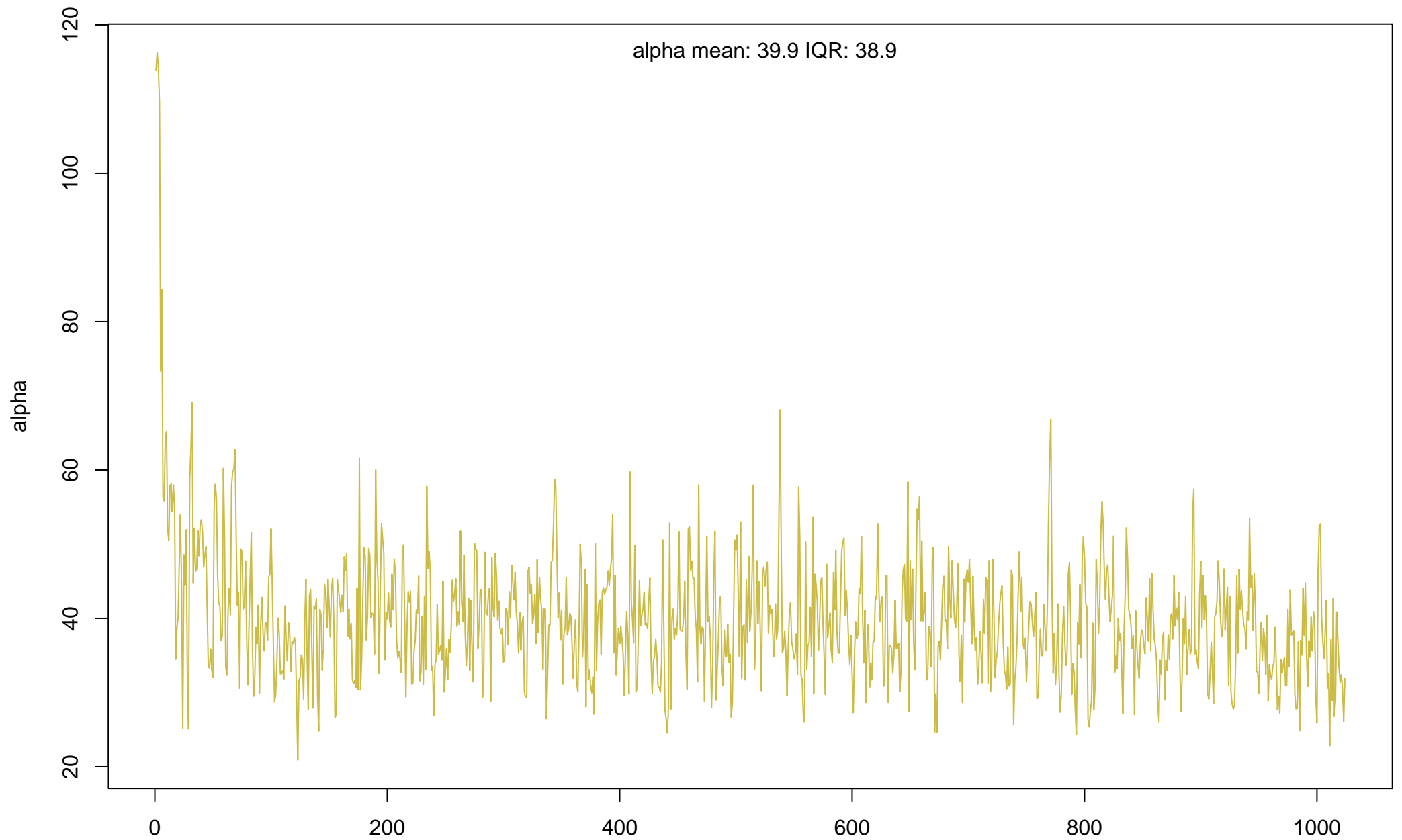




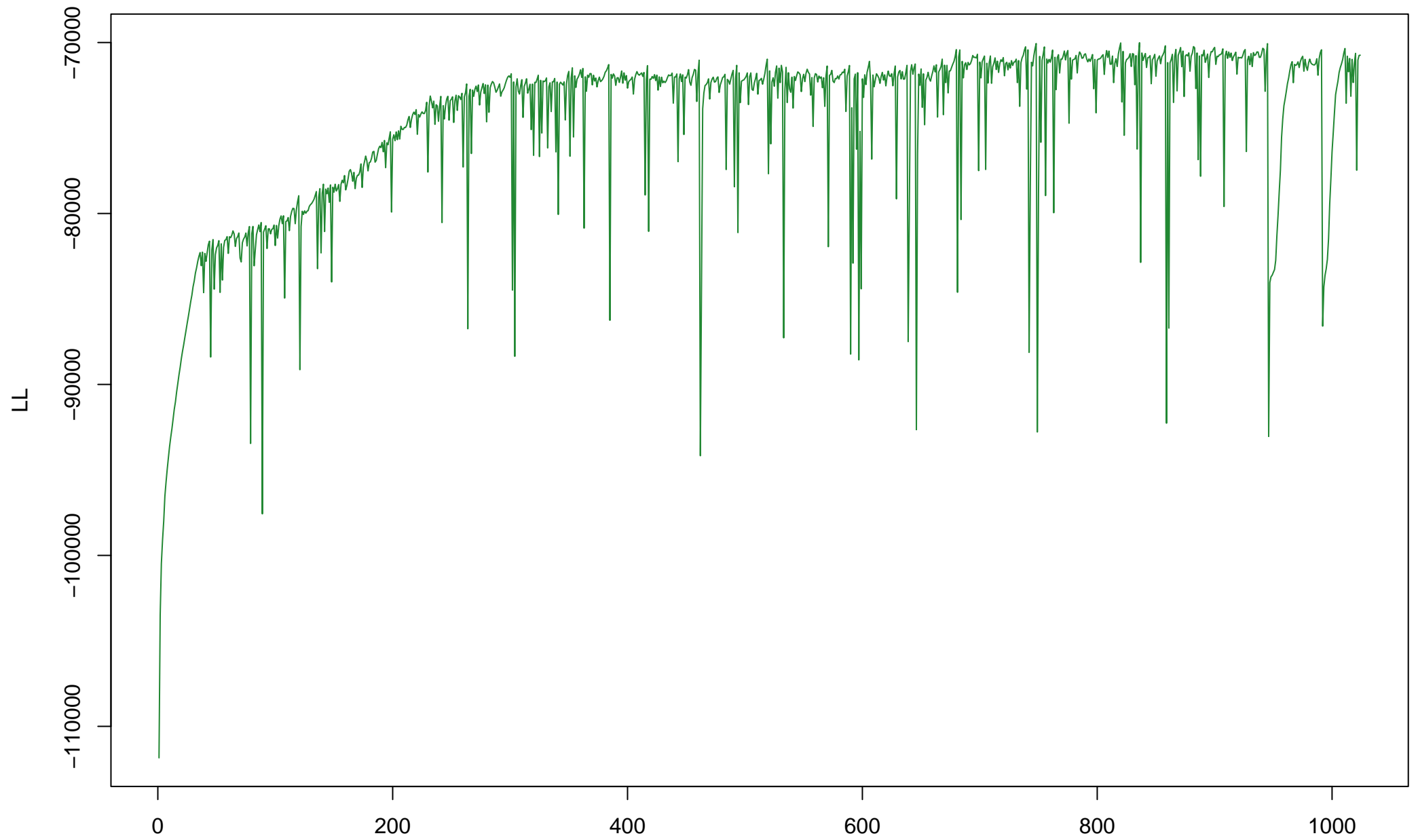




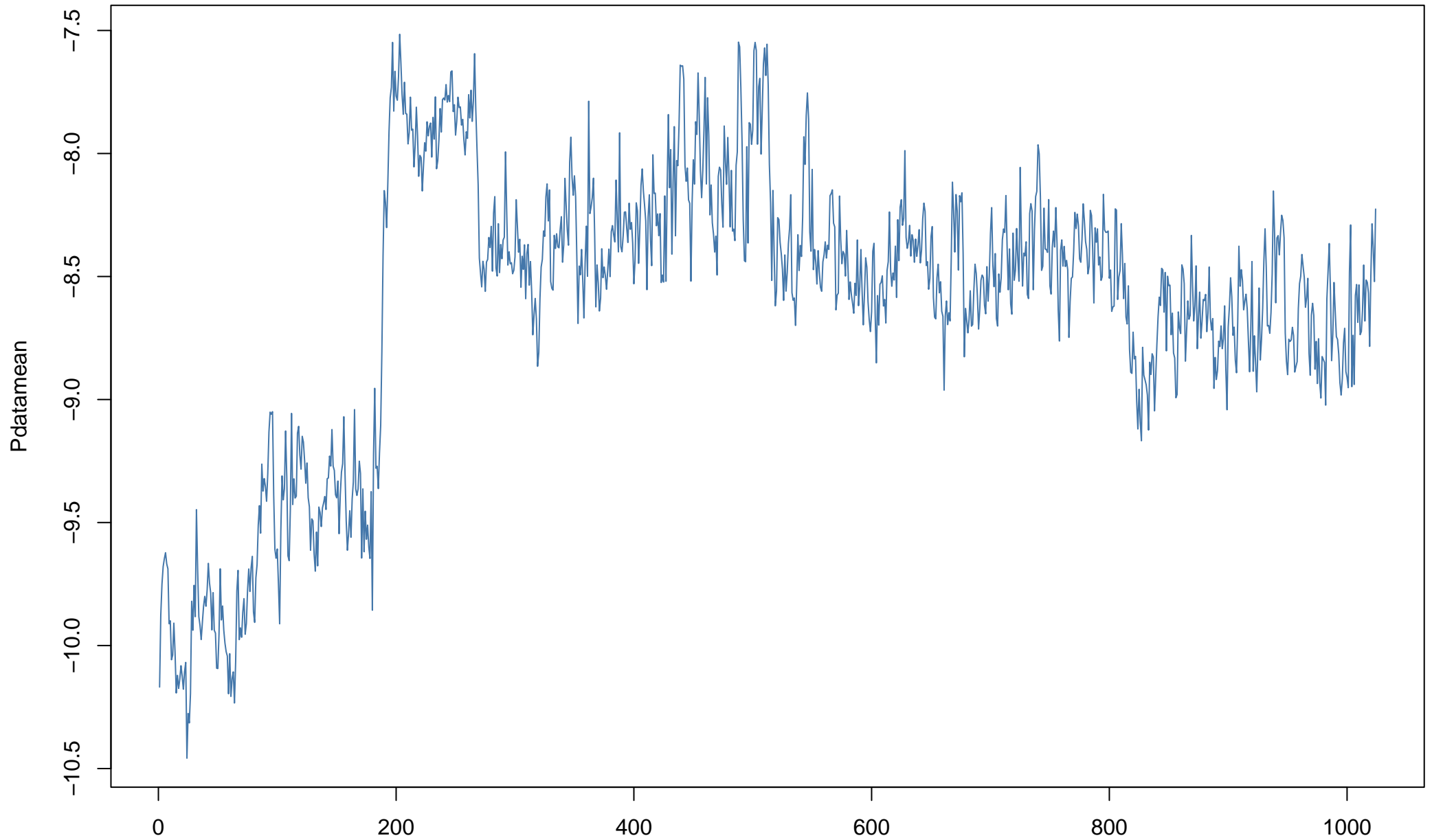
alpha



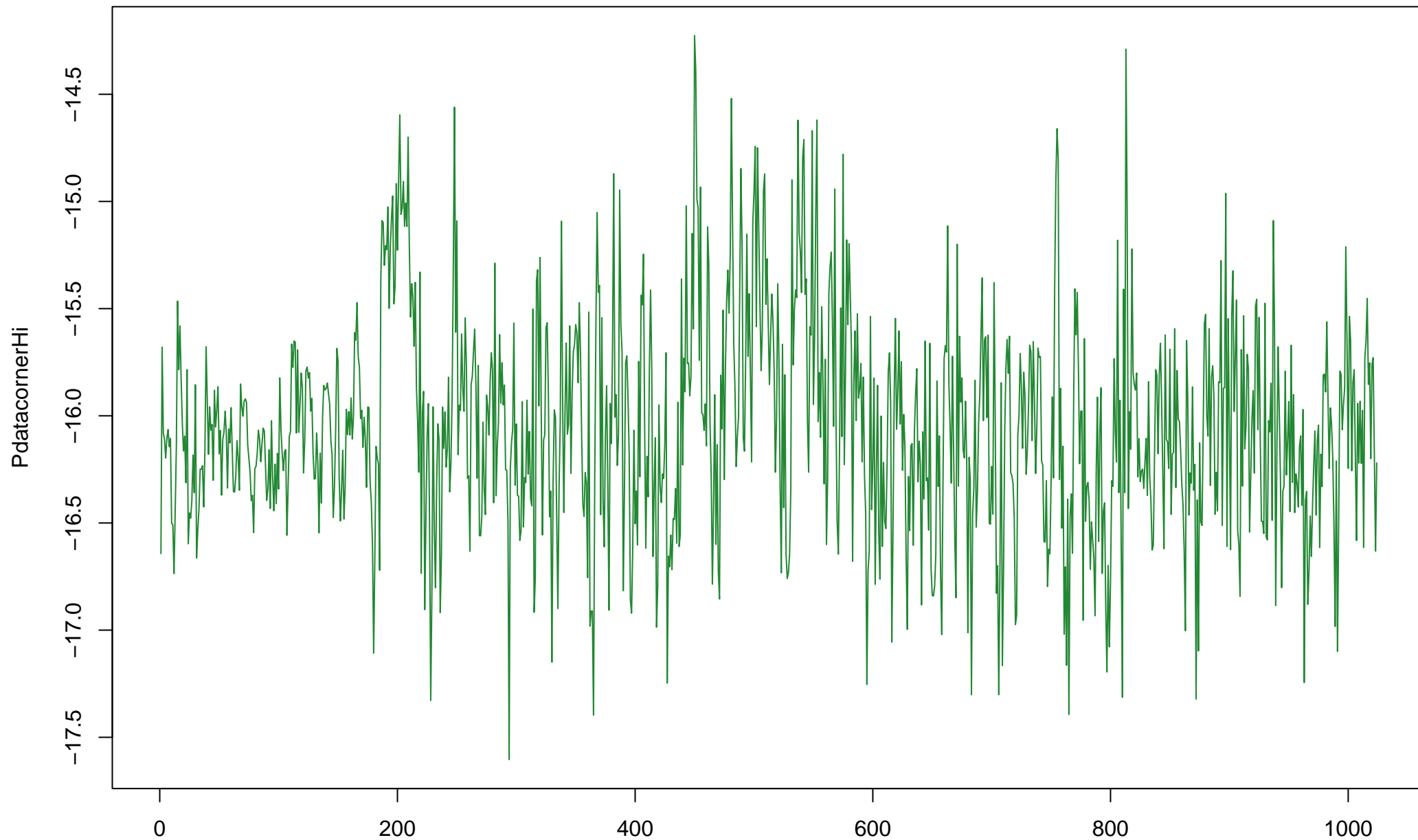
LL



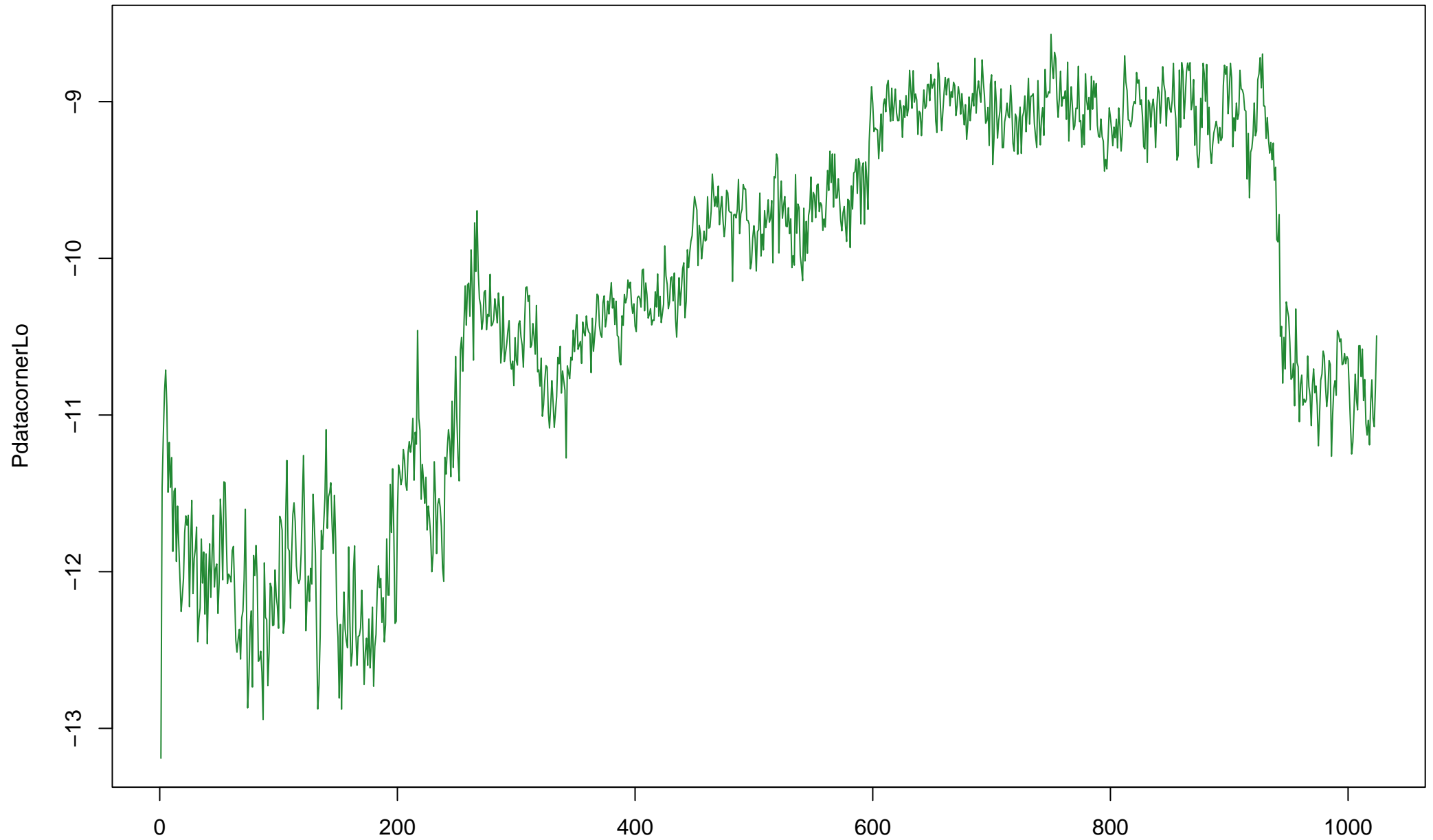
Pdatamean
ESS = 9.31 | BMK = 0.521 | MCSE(6.27) = 15.9 | stat: FALSE | burn: 816



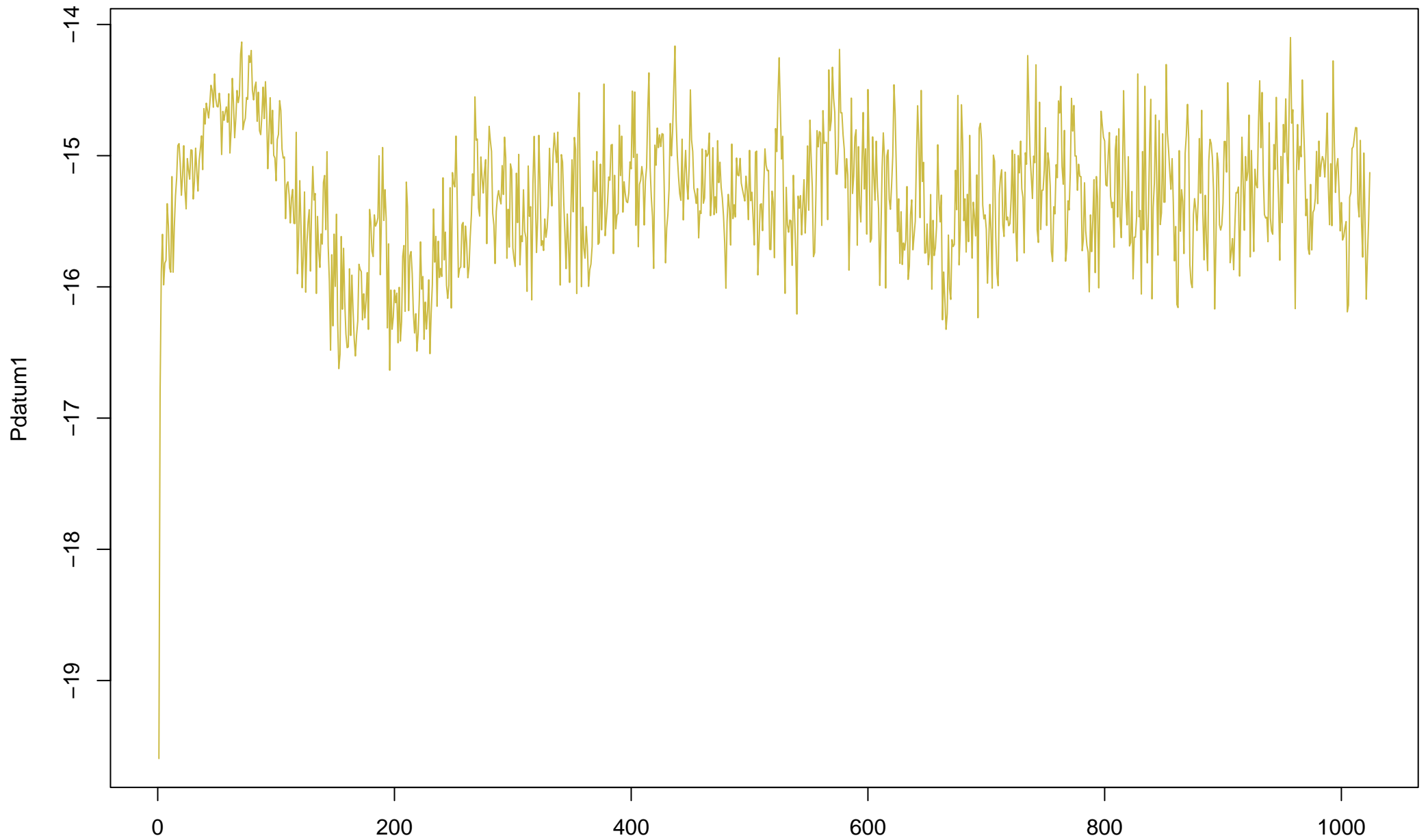
PdatacornerHi
ESS = 109 | BMK = 0.127 | MCSE(6.27) = 8.1 | stat: FALSE | burn: 0



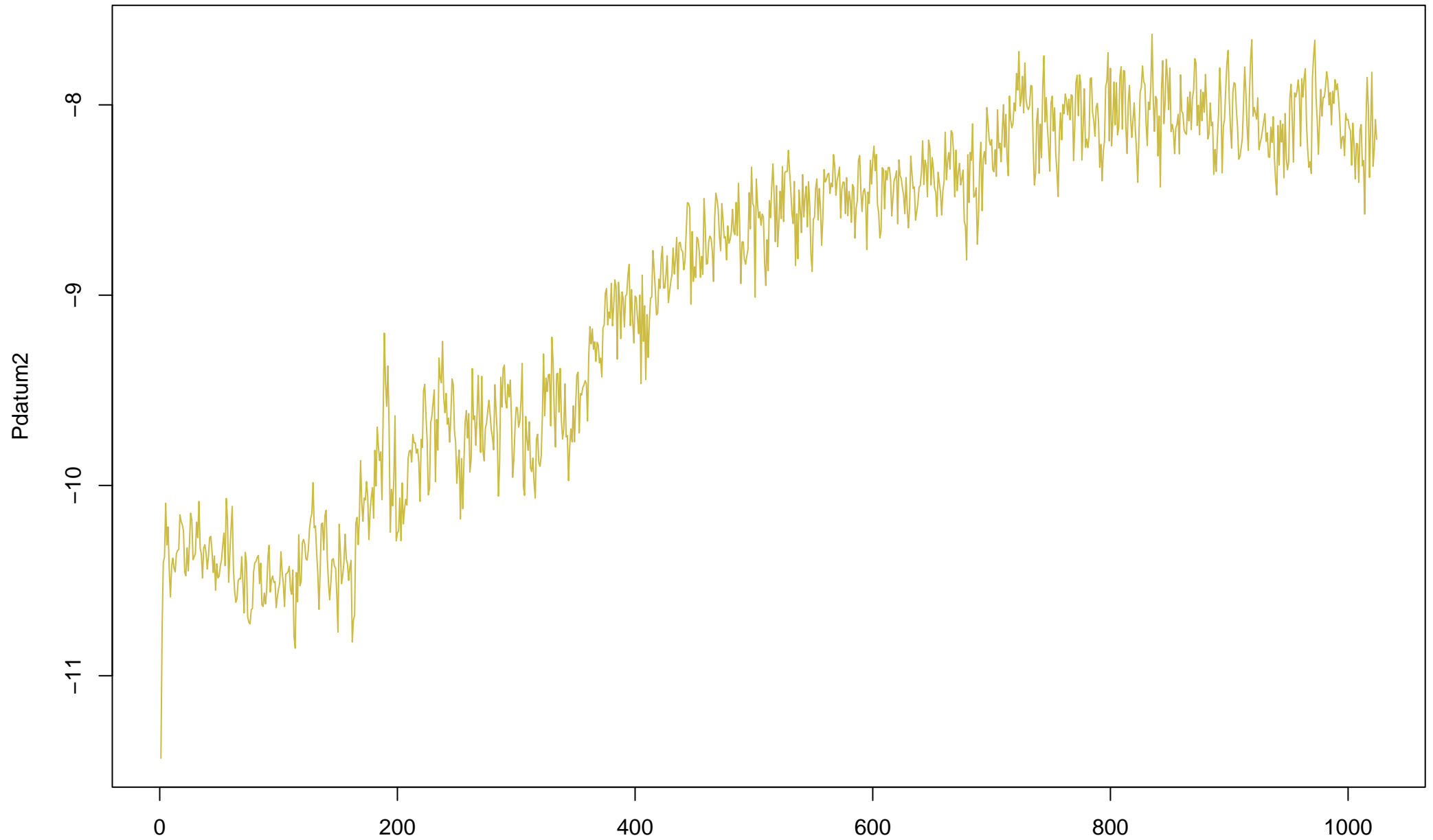
PdatacornerLo
ESS = 2.05 | BMK = 0.681 | MCSE(6.27) = 17.2 | stat: FALSE | burn: 1020



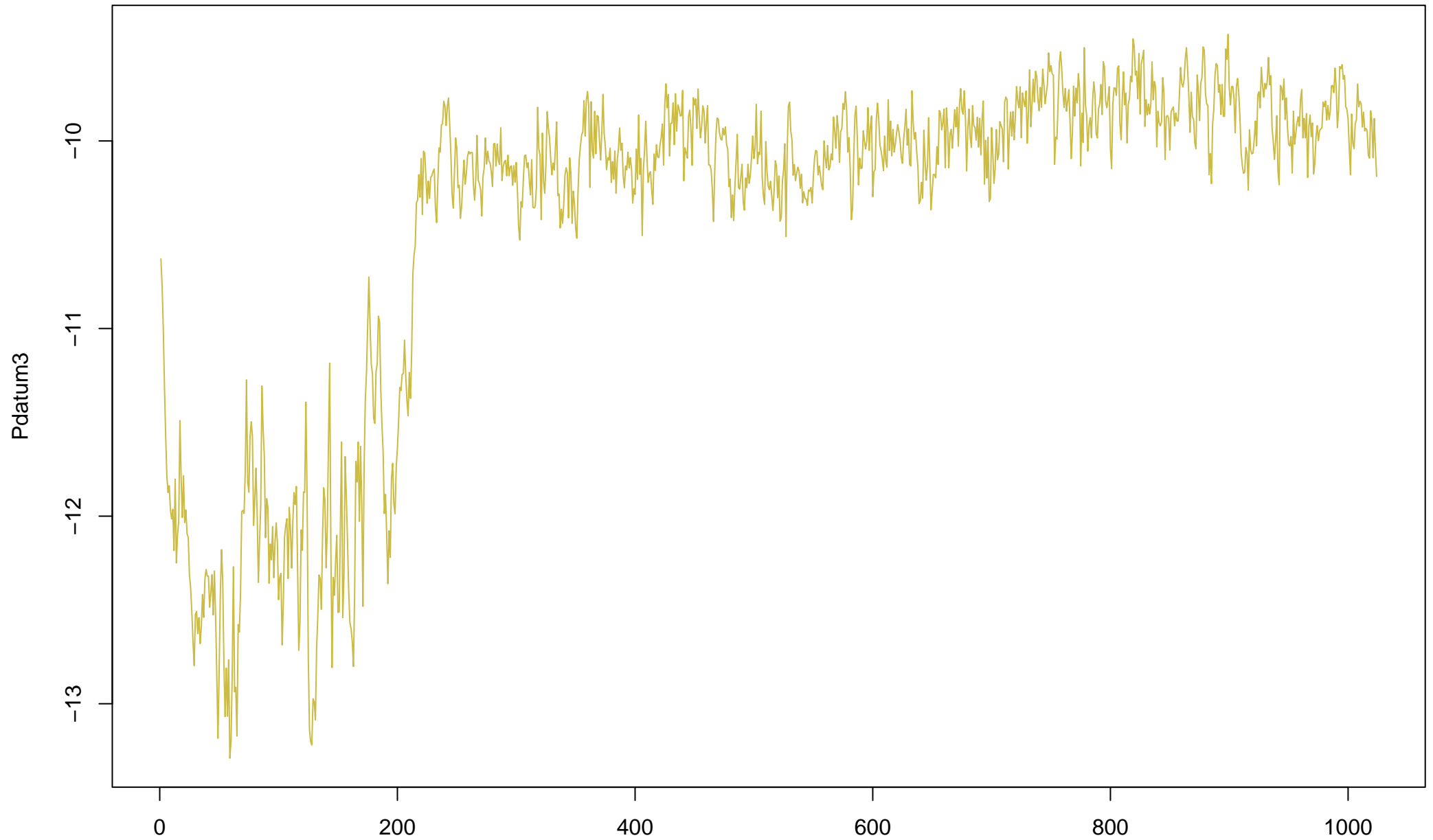
Pdatum1
ESS = 33 | BMK = 0.113 | MCSE(6.27) = 10.5 | stat: FALSE | burn: 102



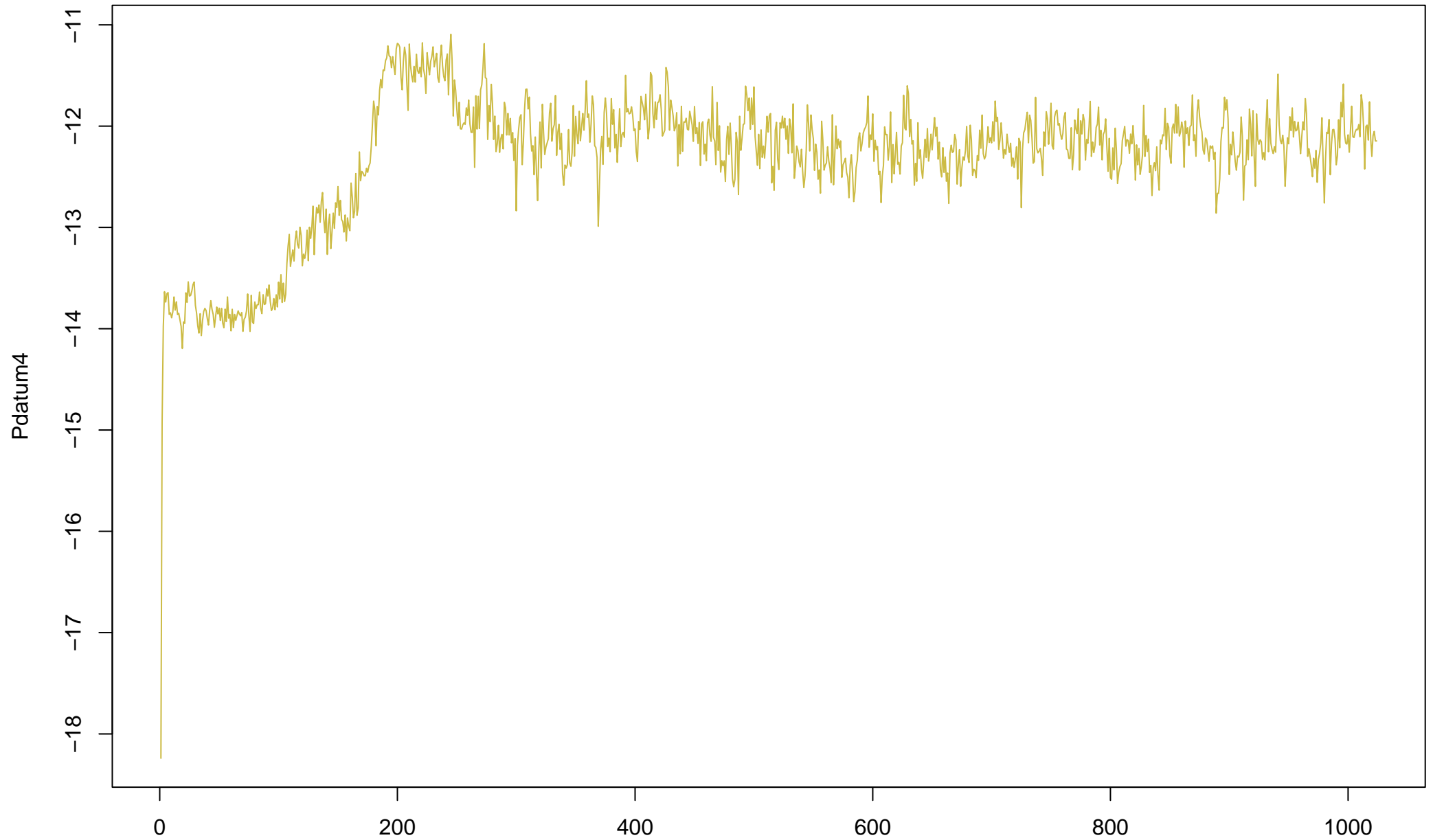
Pdatum2
ESS = 1.73 | BMK = 0.881 | MCSE(6.27) = 17.2 | stat: FALSE | burn: 714



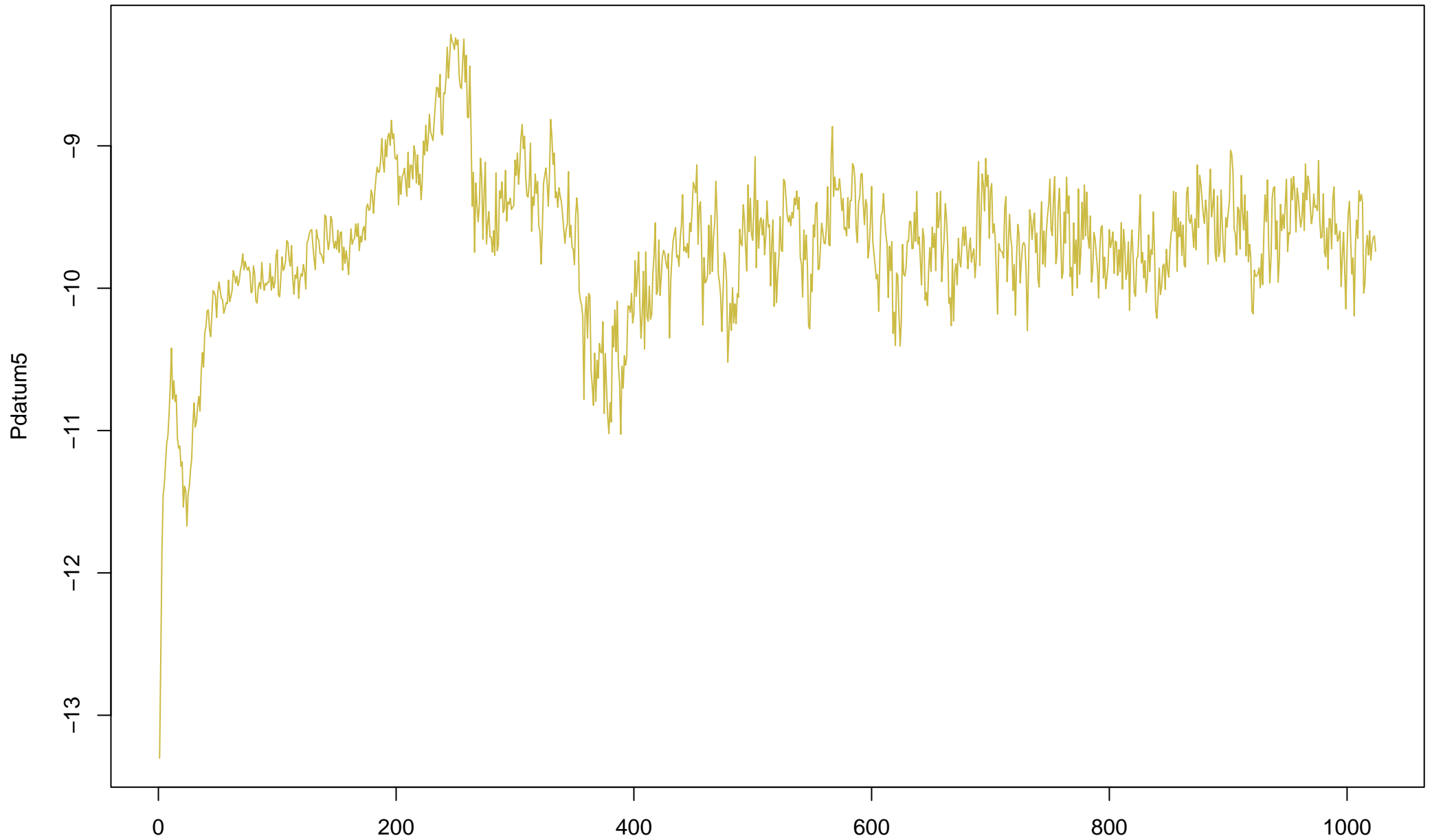
Pdatum3
ESS = 4.2 | BMK = 0.523 | MCSE(6.27) = 16.7 | stat: FALSE | burn: 204



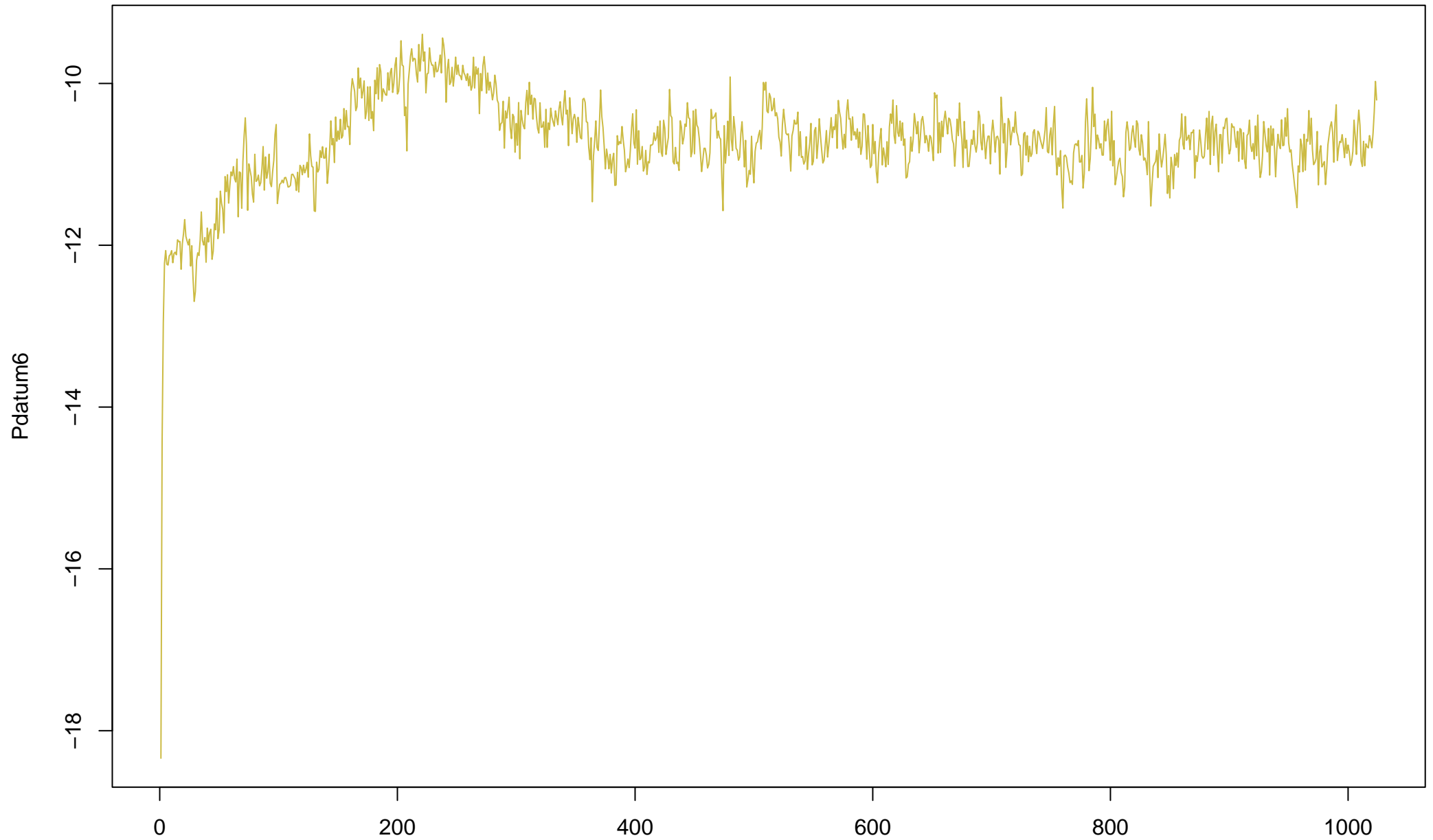
Pdatum4
ESS = 9.74 | BMK = 0.485 | MCSE(6.27) = 15.2 | stat: FALSE | burn: 204



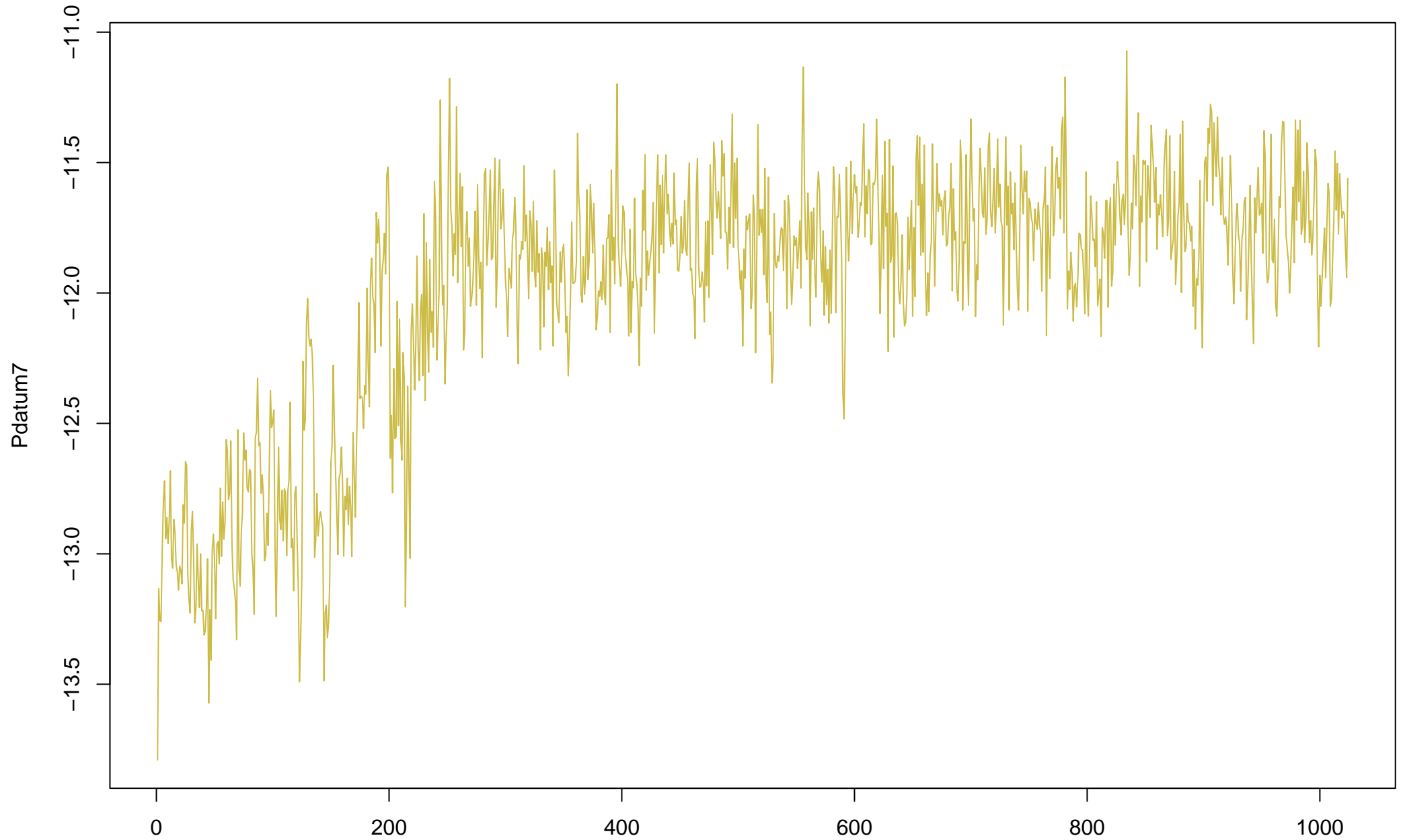
Pdatum5
ESS = 15.1 | BMK = 0.352 | MCSE(6.27) = 15 | stat: FALSE | burn: 306



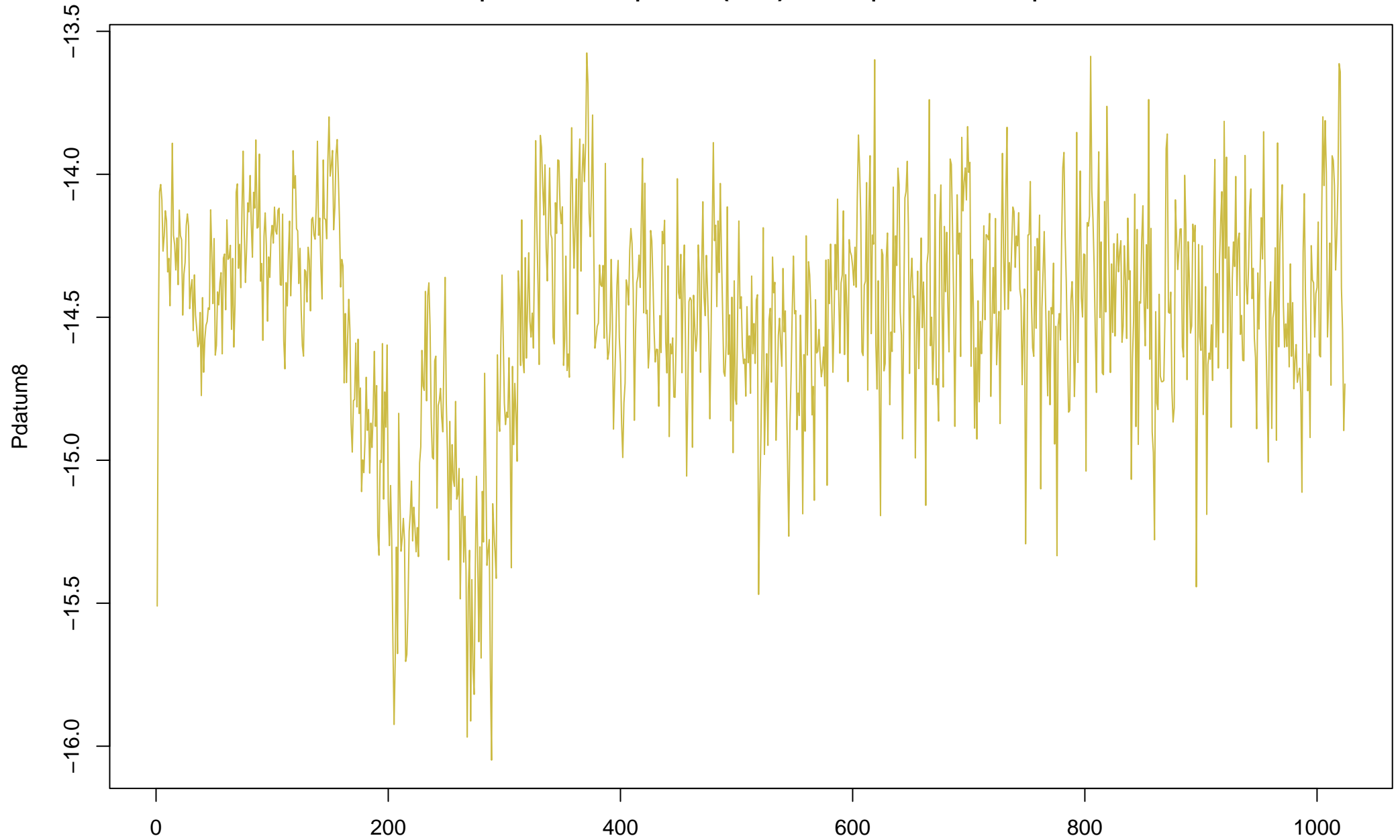
Pdatum6
ESS = 5.53 | BMK = 0.414 | MCSE(6.27) = 15.3 | stat: FALSE | burn: 306



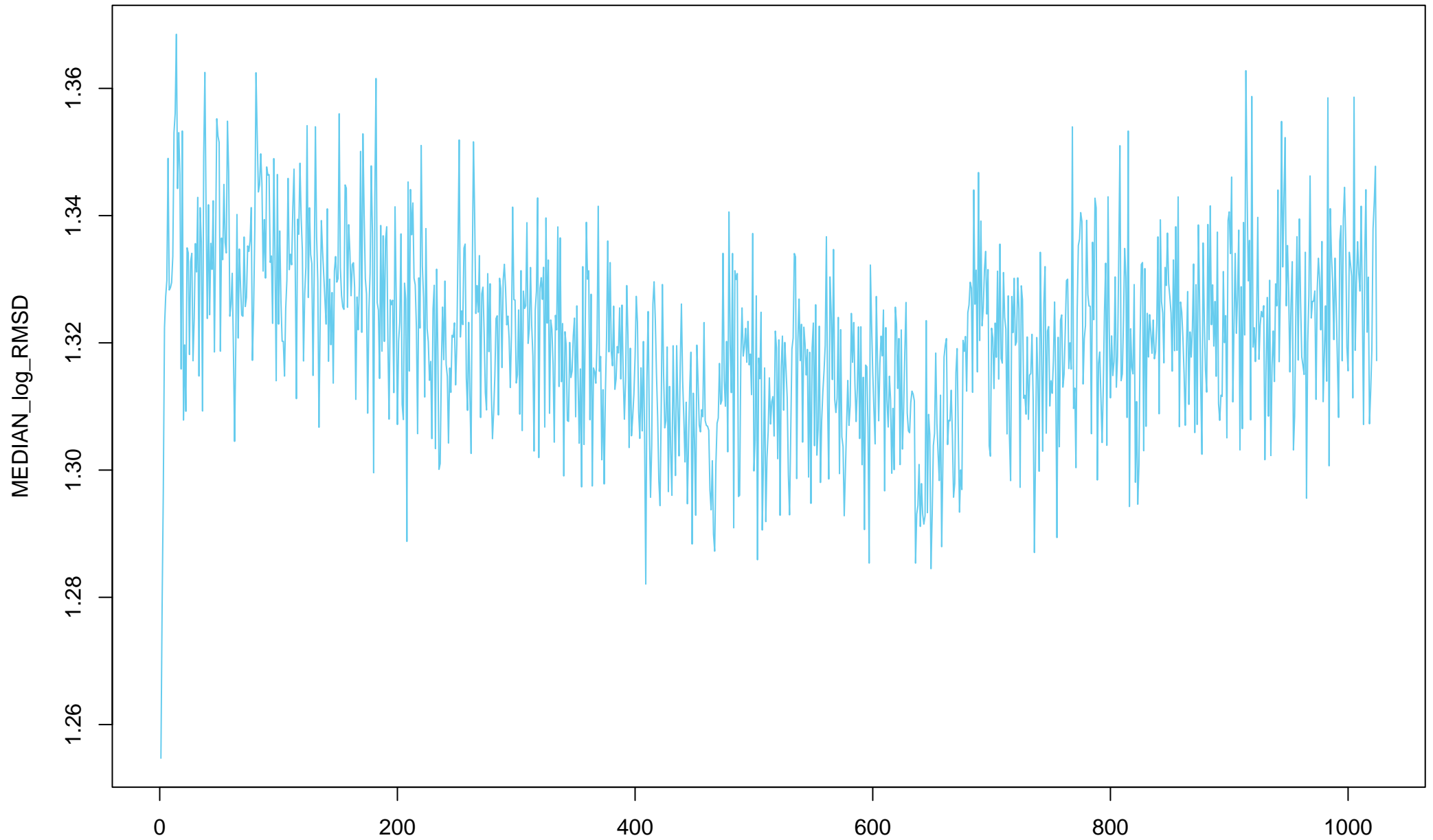
Pdatum7
ESS = 11.1 | BMK = 0.455 | MCSE(6.27) = 14.3 | stat: FALSE | burn: 0



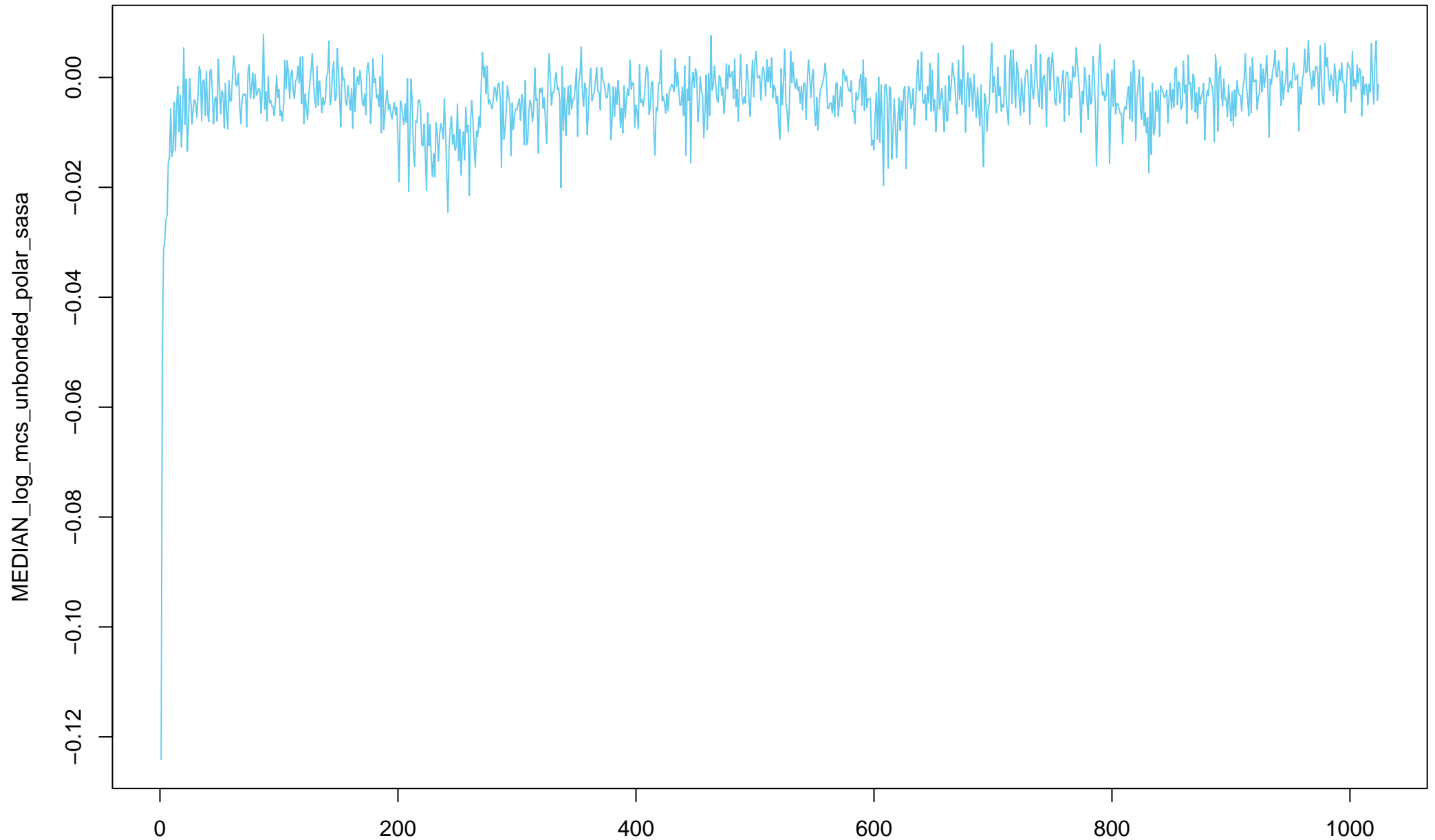
Pdatum8
ESS = 37.1 | BMK = 0.15 | MCSE(6.27) = 11.2 | stat: FALSE | burn: 306



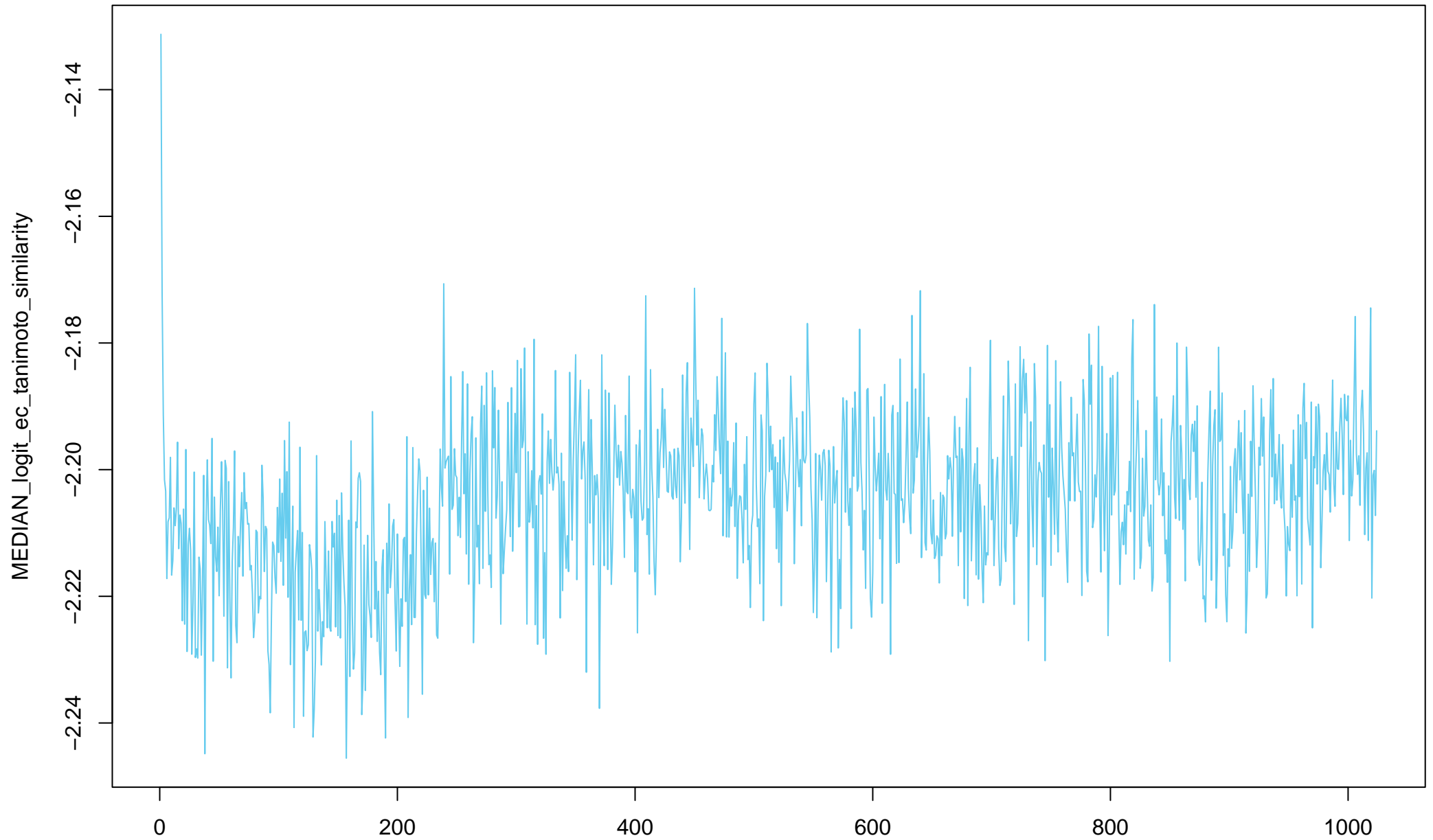
MEDIAN_log_RMSD
ESS = 29.9 | BMK = 0.113 | MCSE(6.27) = 9.77 | stat: FALSE | burn: 0



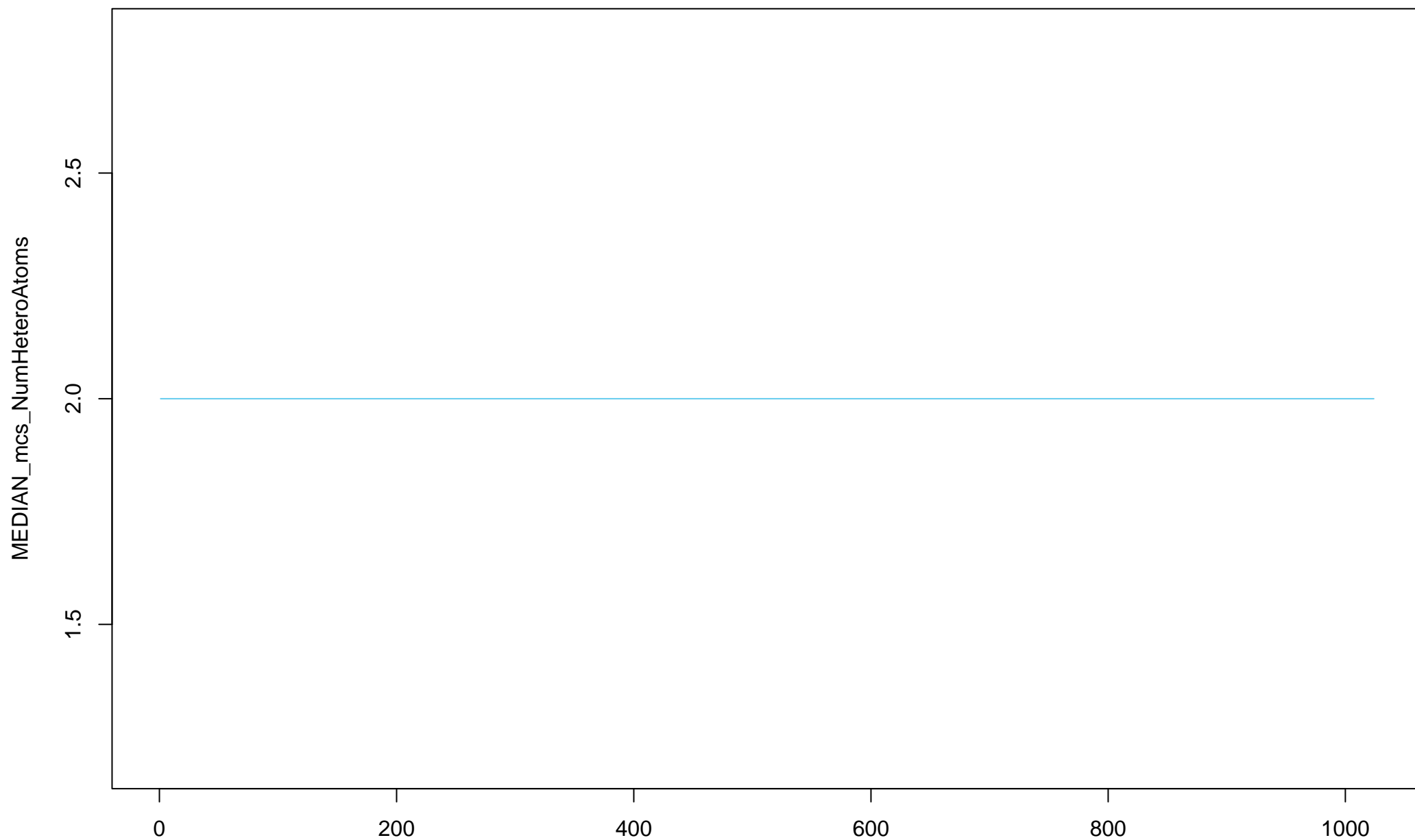
MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 166 | BMK = 0.147 | MCSE(6.27) = 8.56 | stat: TRUE | burn: 0



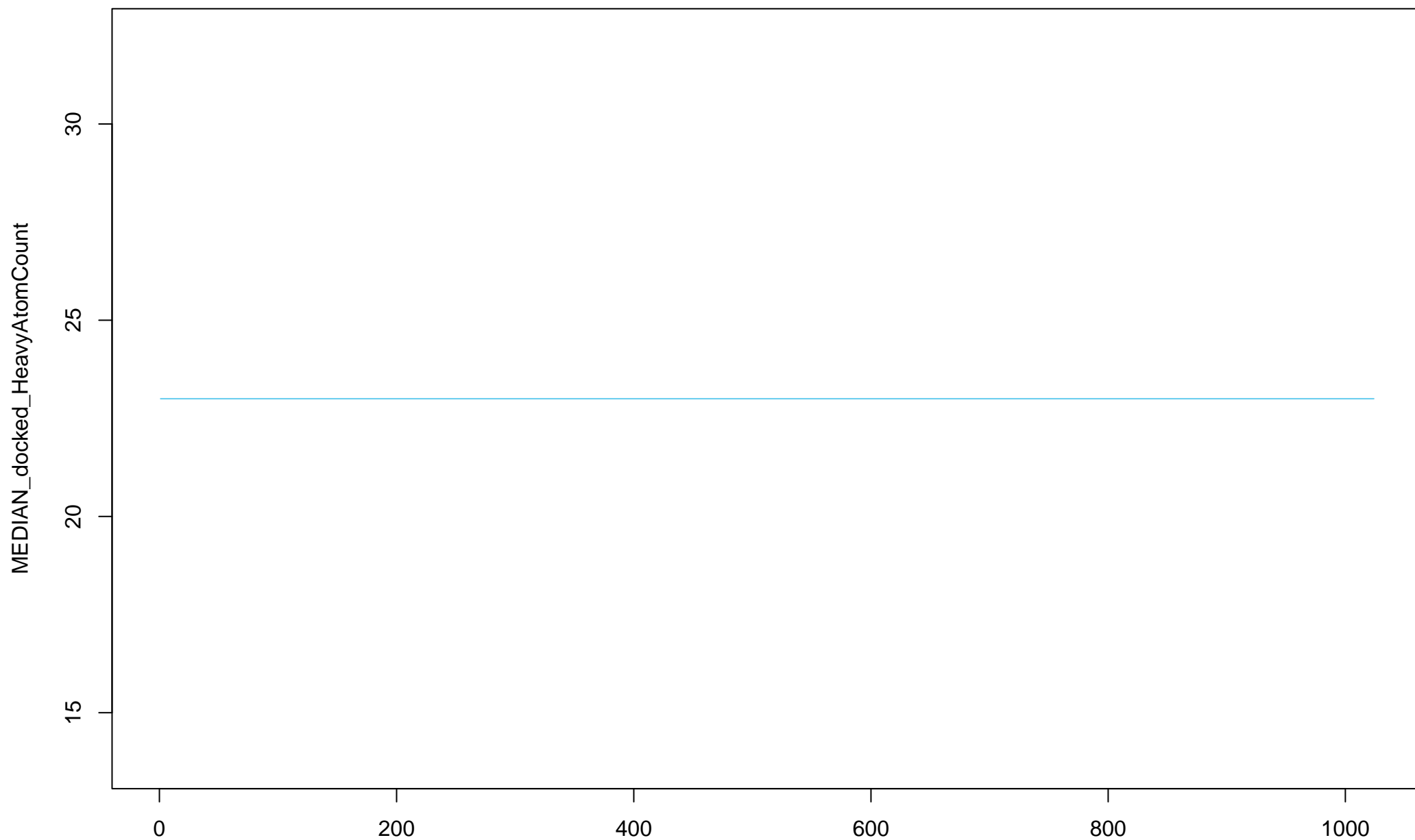
MEDIAN_logit_ec_tanimoto_similarity
ESS = 38.7 | BMK = 0.2 | MCSE(6.27) = 8.45 | stat: FALSE | burn: 0



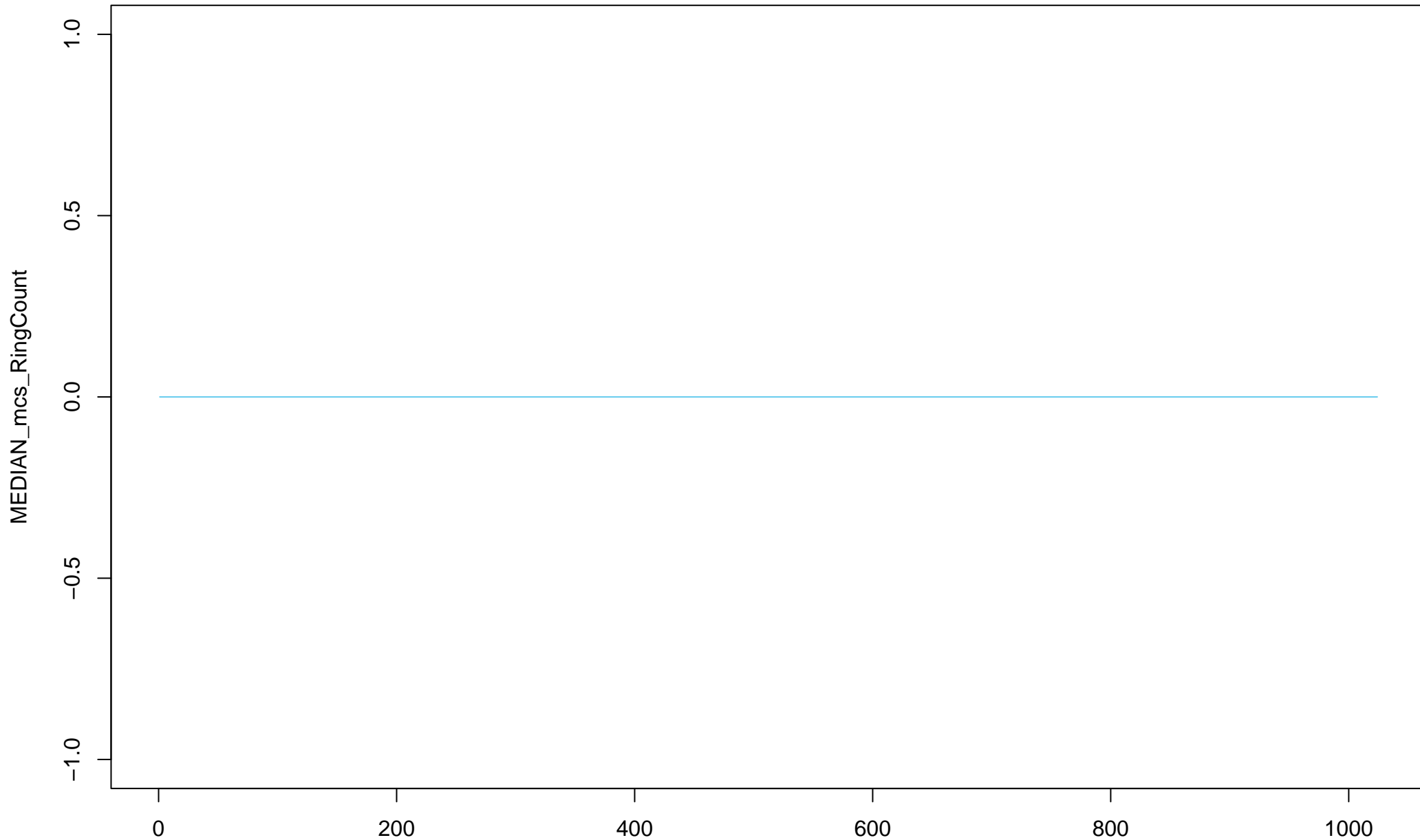
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



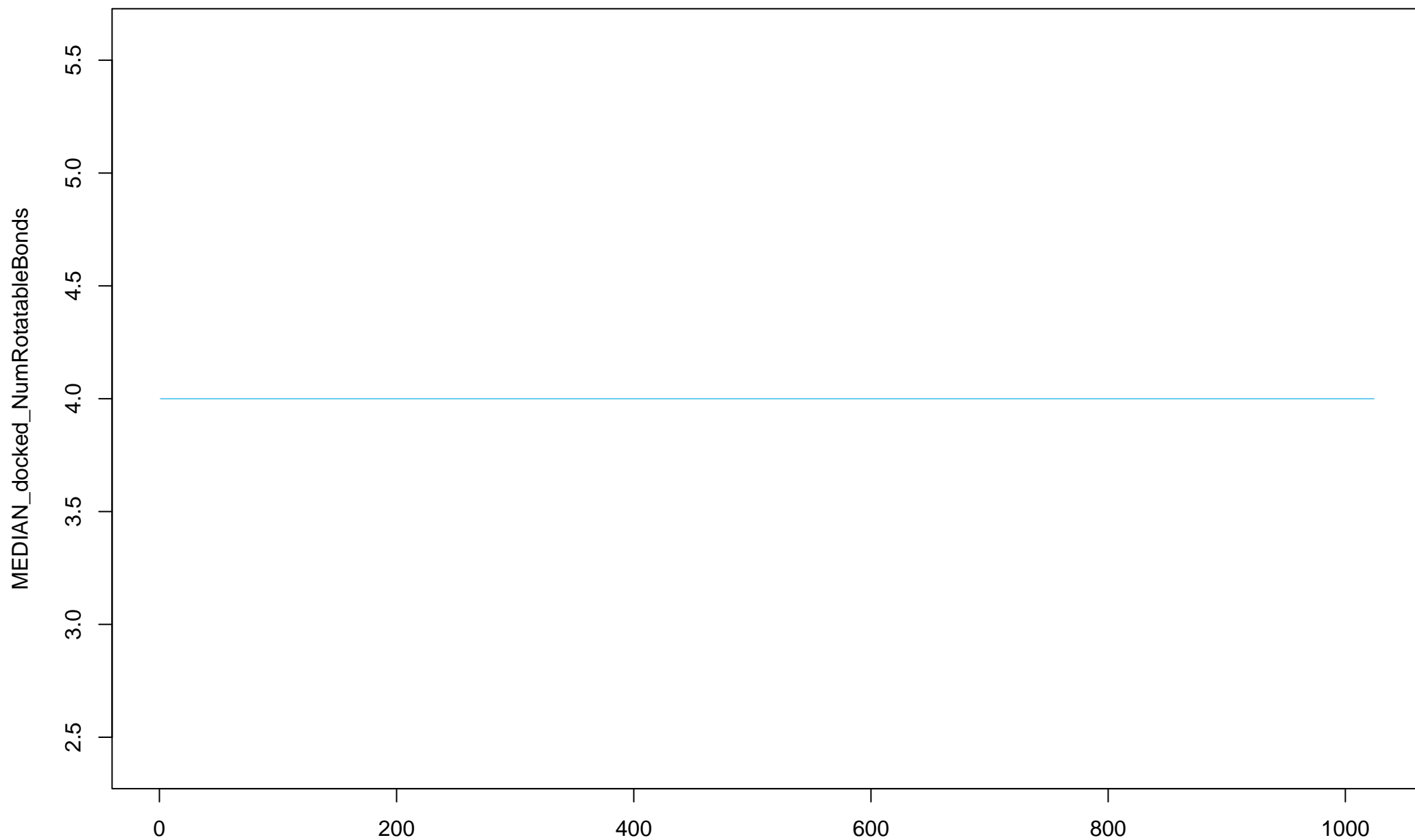
MEDIAN_docked_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



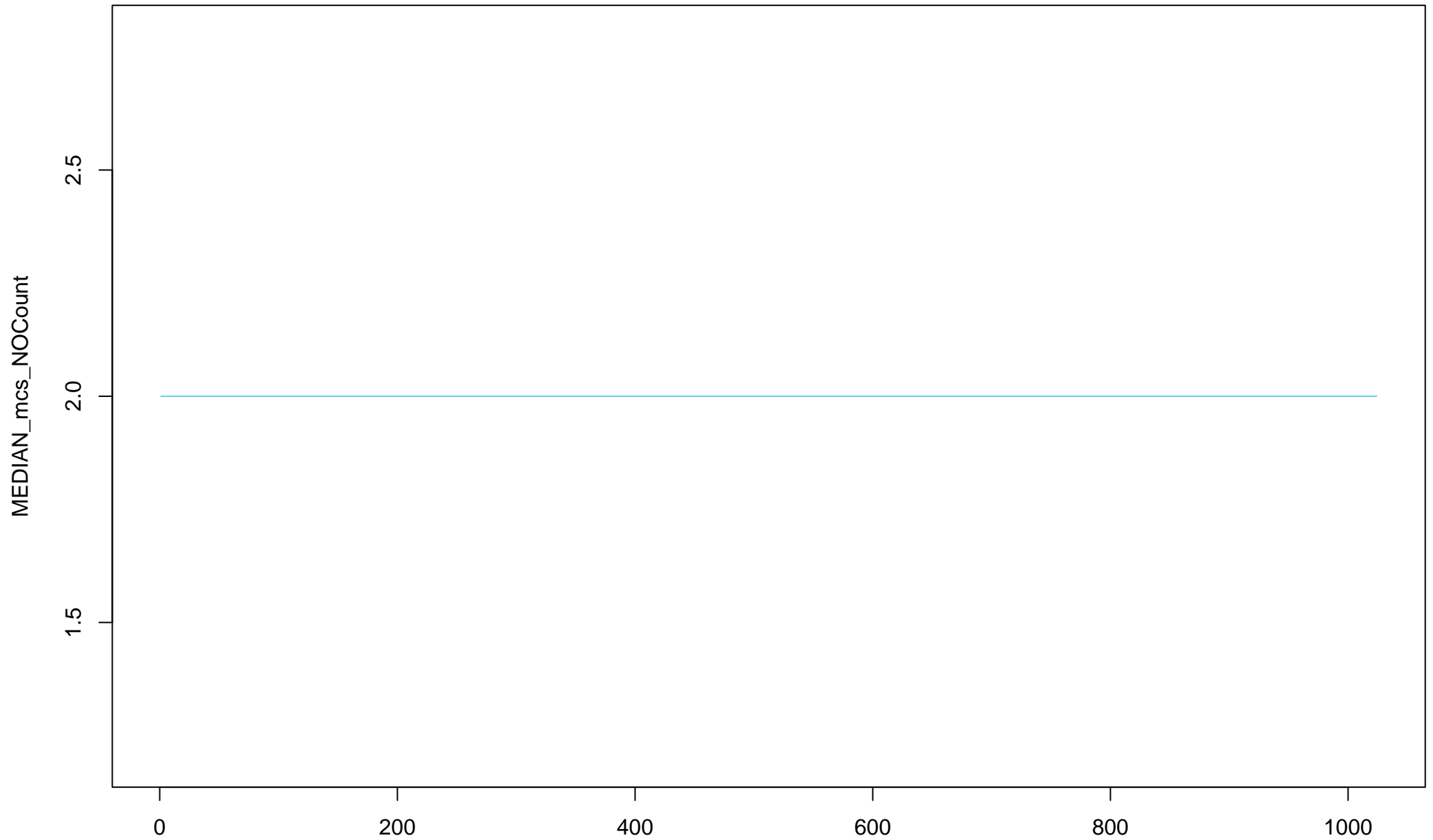
MEDIAN_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



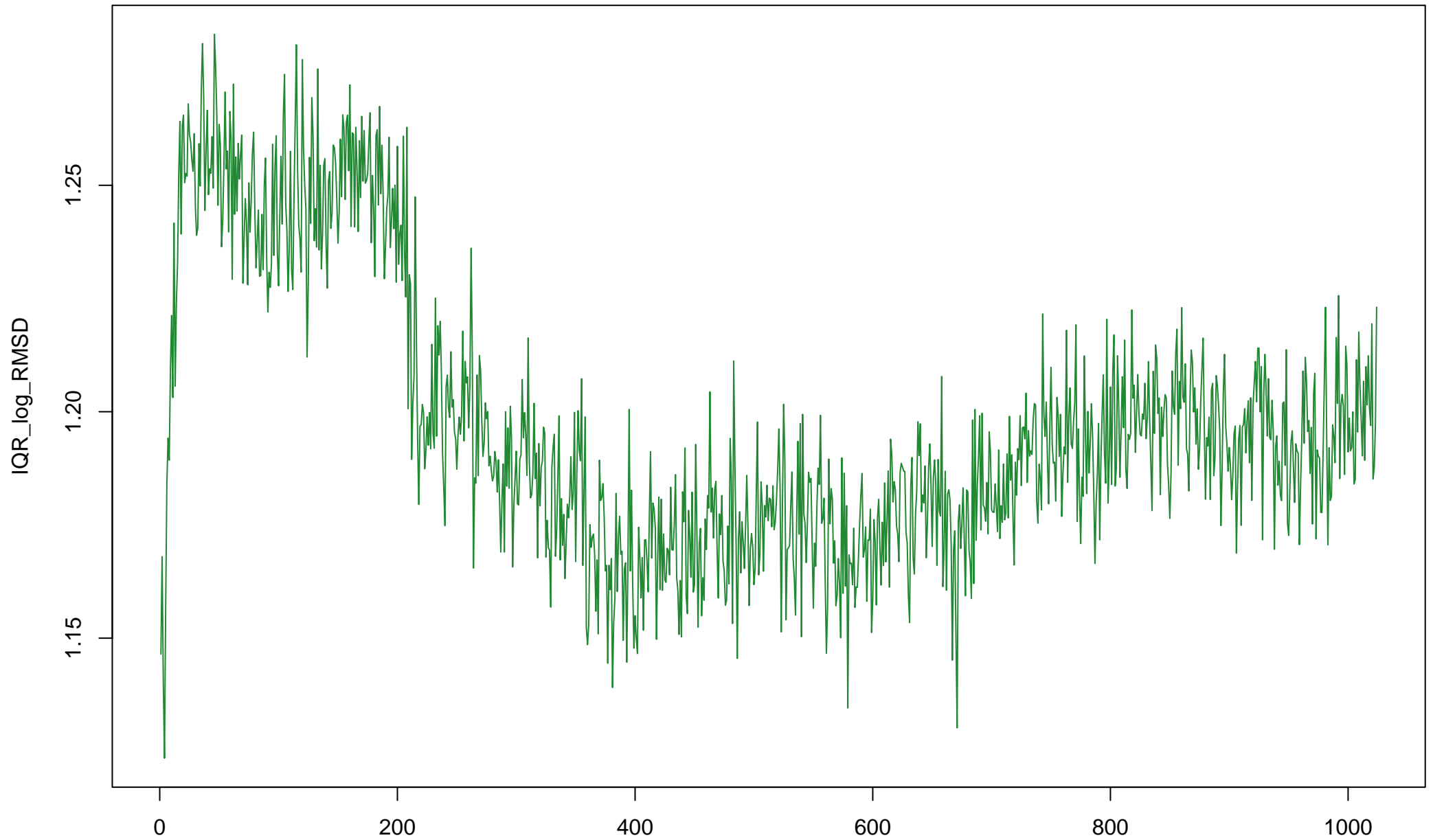
MEDIAN_docked_NumRotatableBonds
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



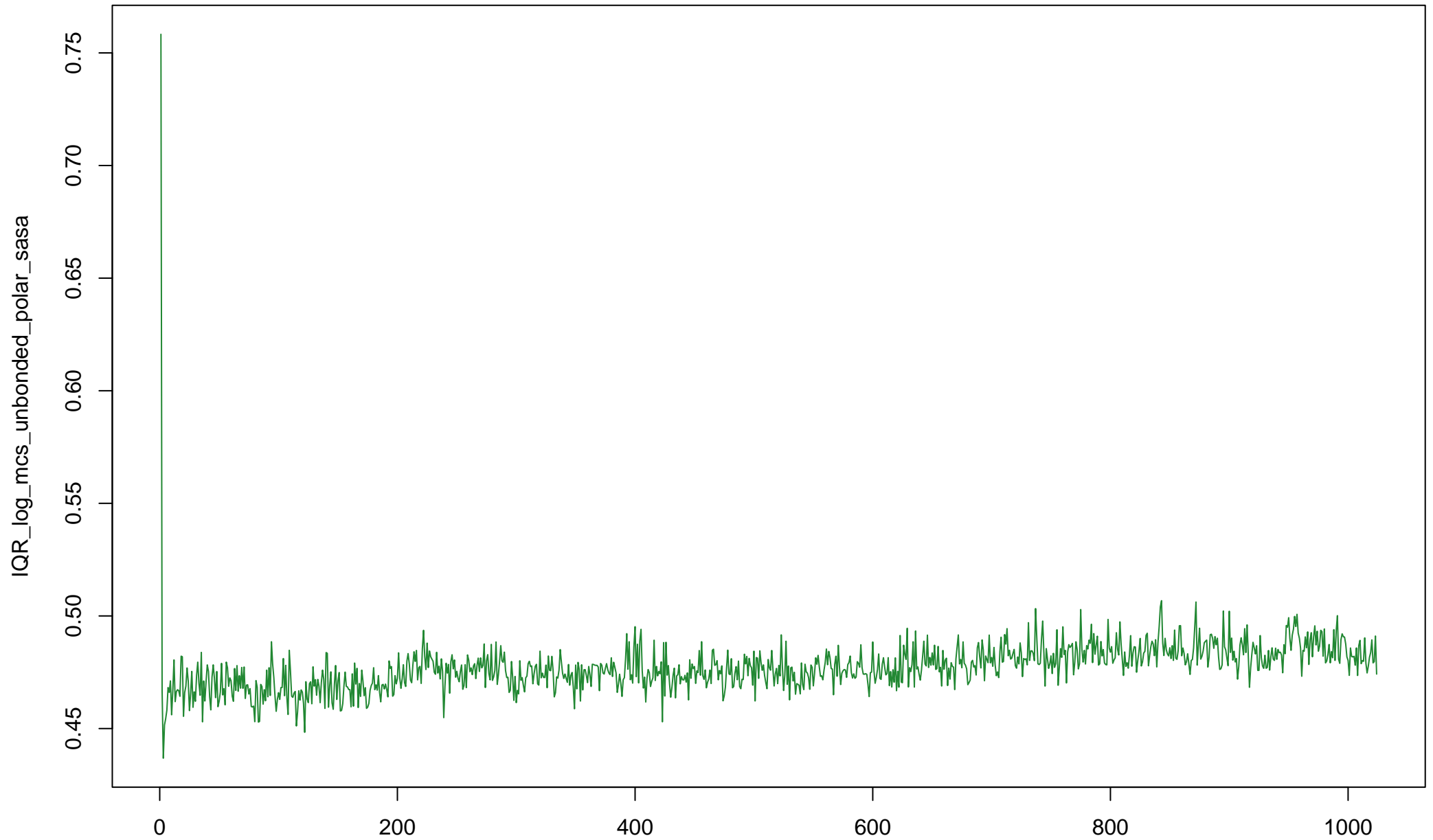
MEDIAN_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



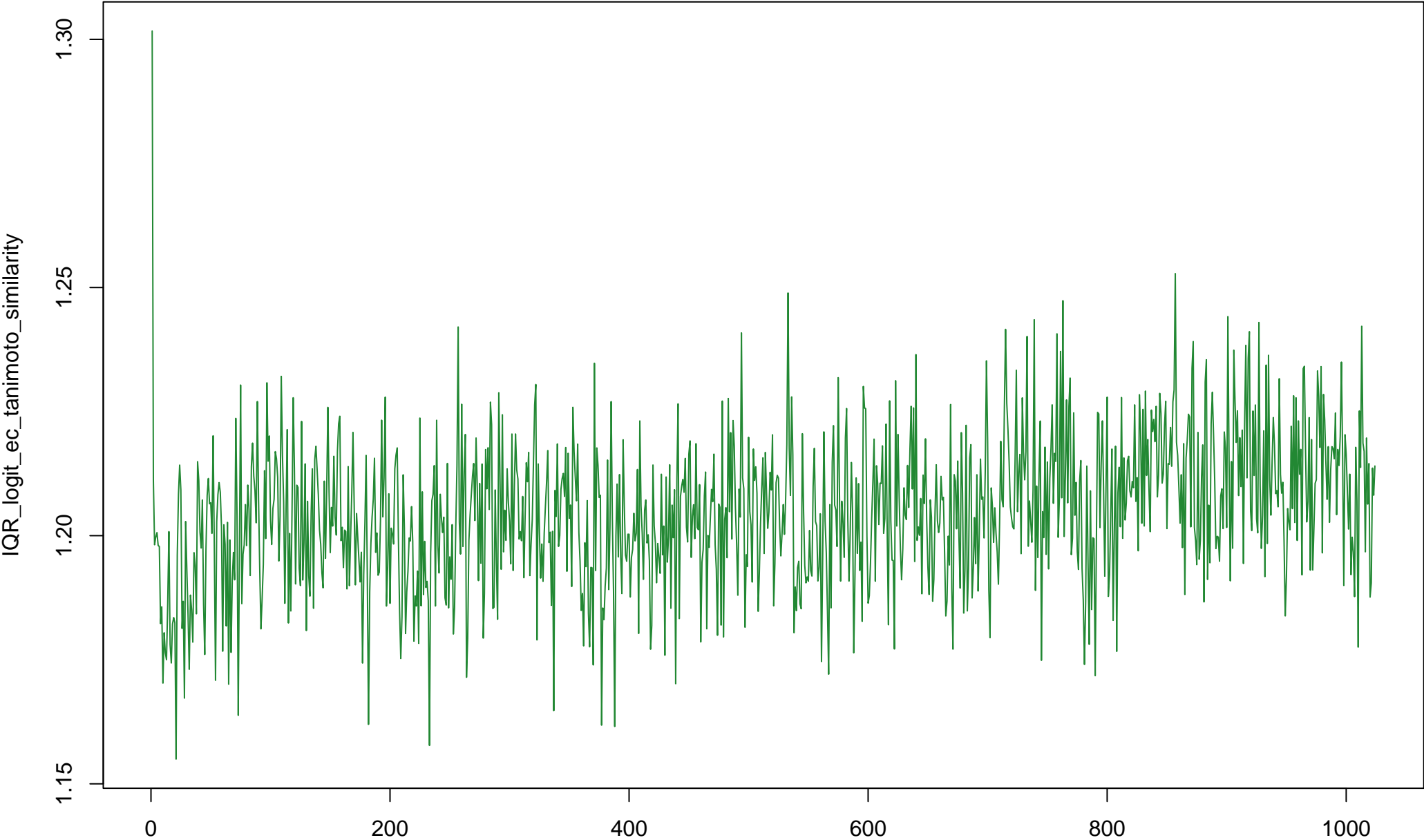
IQR_log_RMSD
ESS = 4.27 | BMK = 0.465 | MCSE(6.27) = 15.8 | stat: FALSE | burn: 204



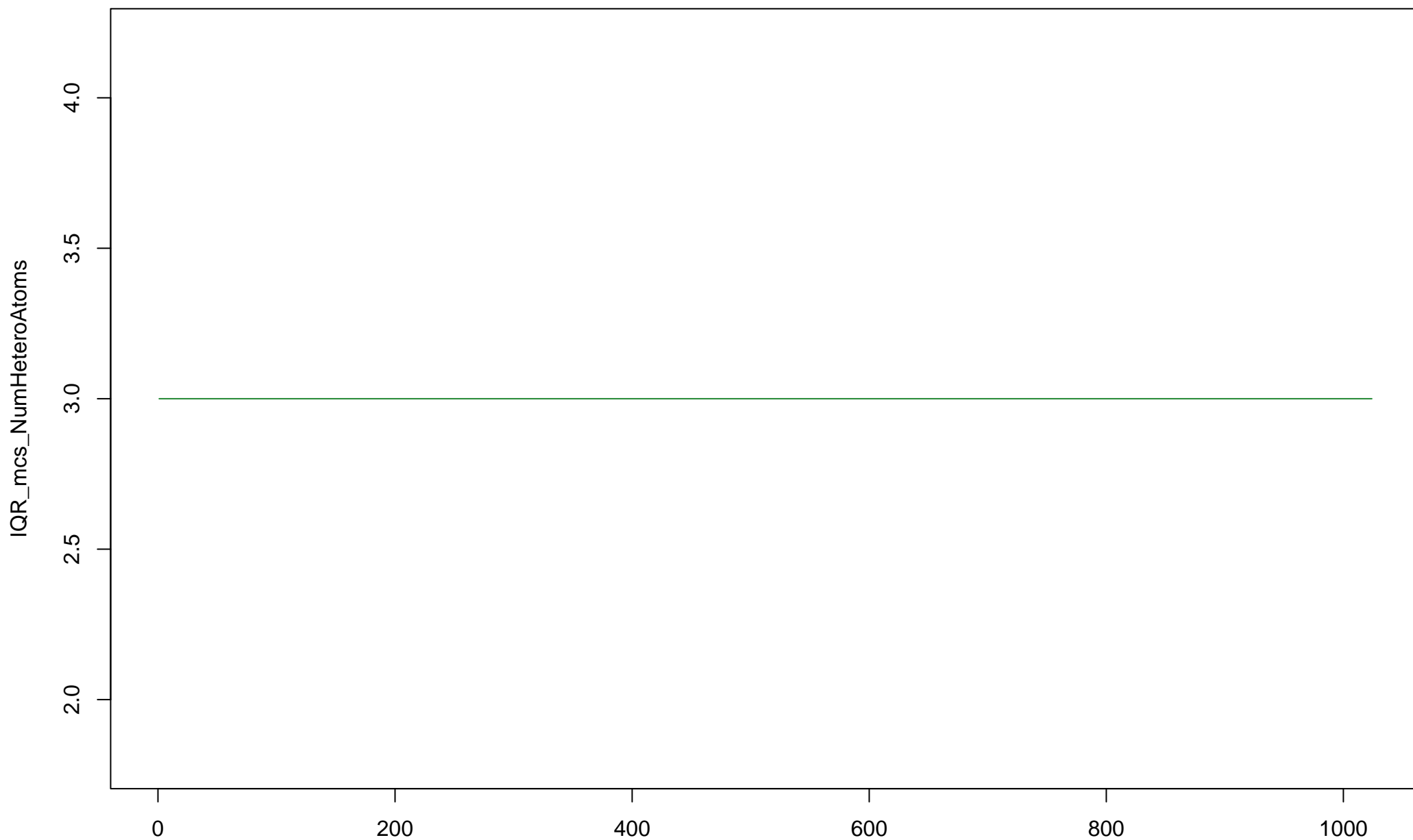
IQR_log_mcs_unbonded_polar_sasa
ESS = 36.6 | BMK = 0.423 | MCSE(6.27) = 8.4 | stat: FALSE | burn: 0



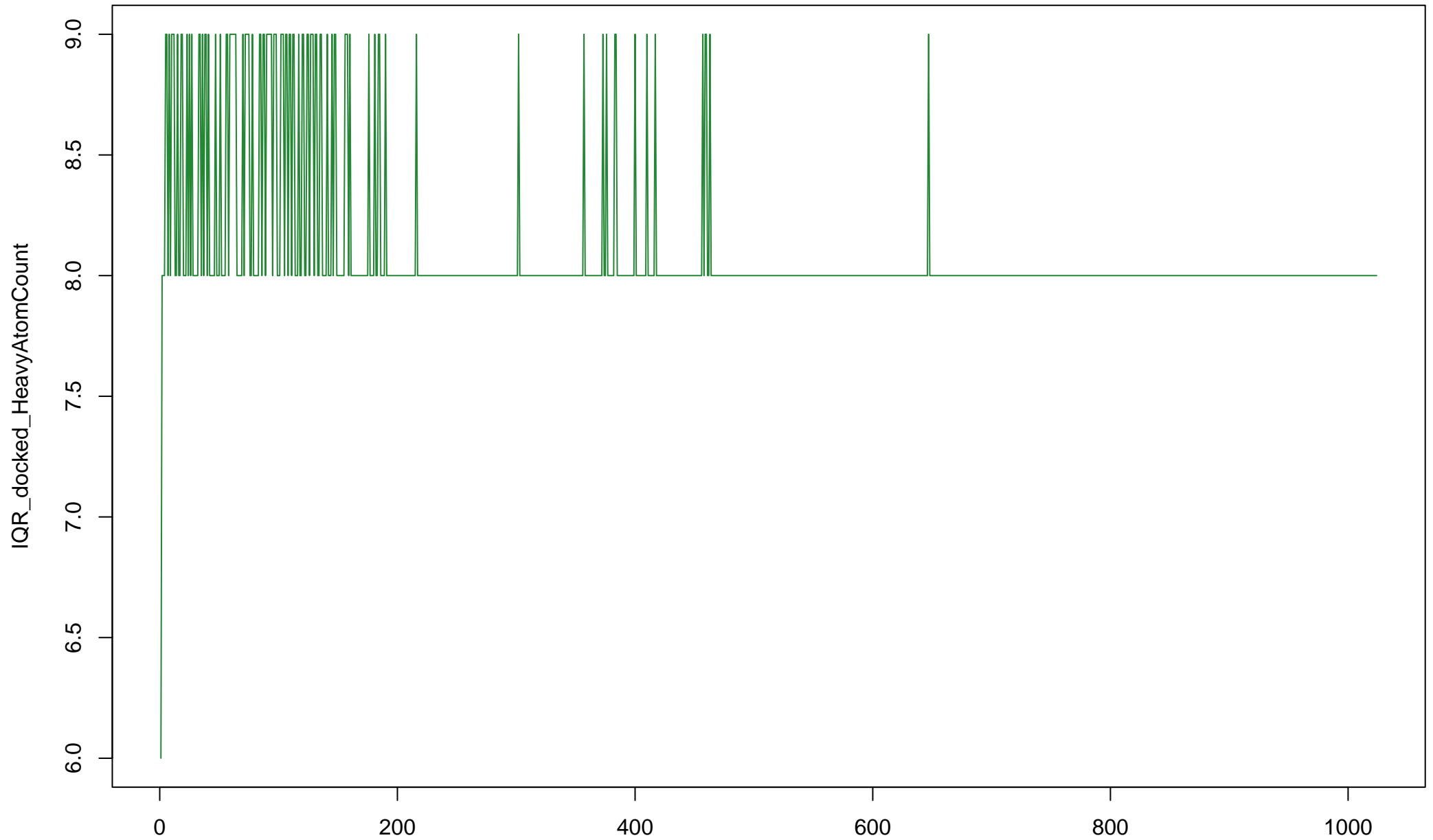
IQR_logit_ec_tanimoto_similarity
ESS = 136 | BMK = 0.197 | MCSE(6.27) = 7.12 | stat: FALSE | burn: 0



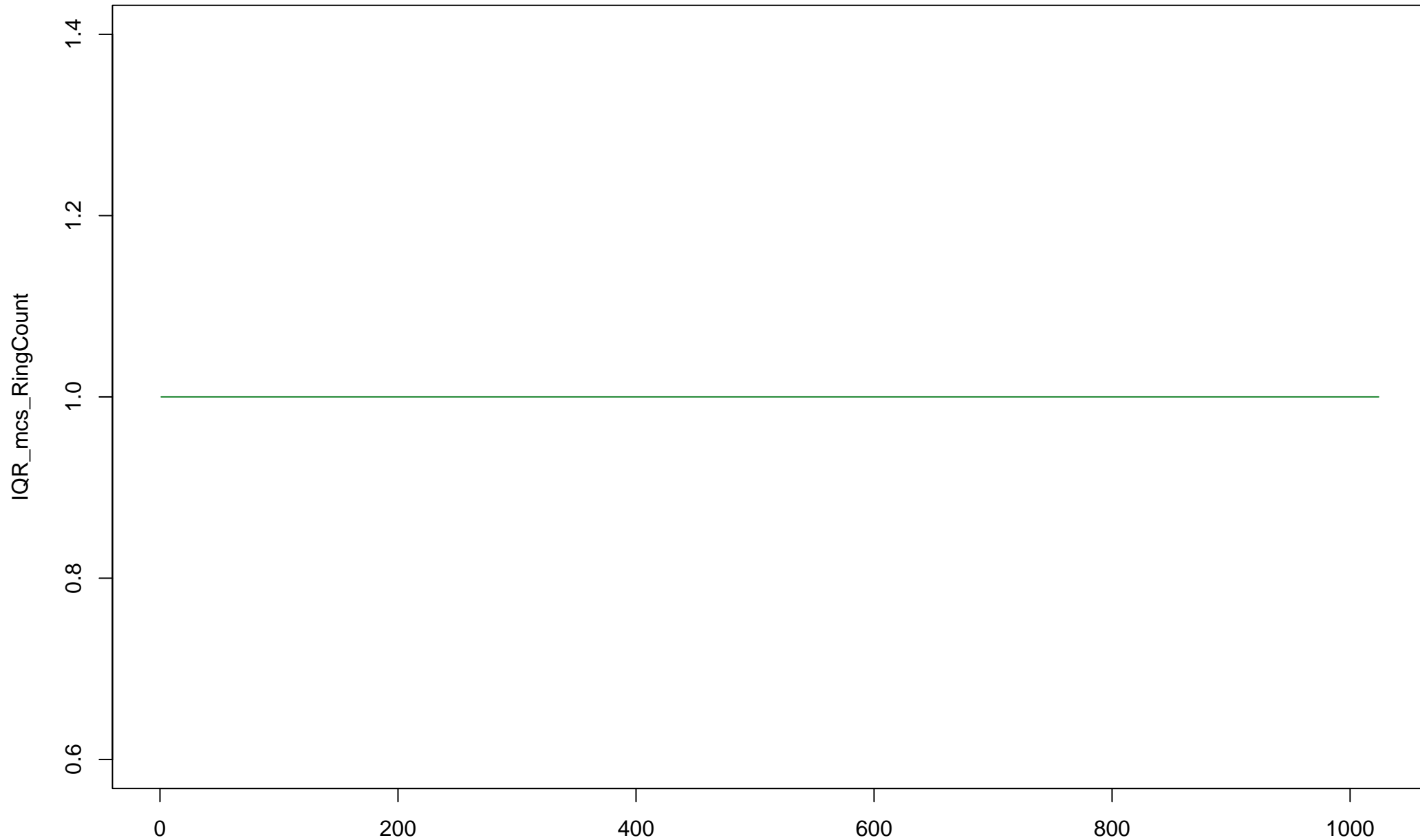
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



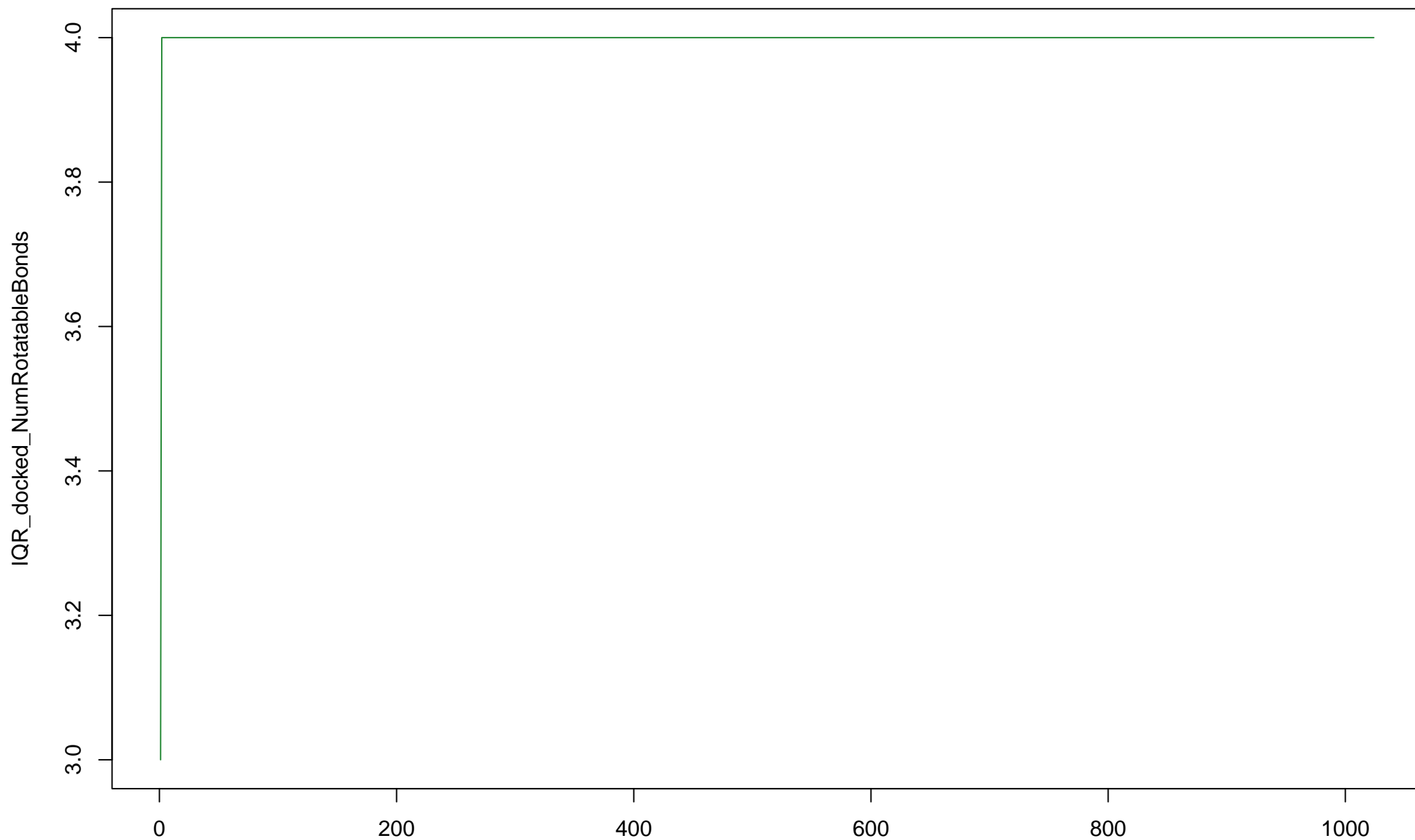
IQR_docked_HeavyAtomCount
ESS = 10.8 | BMK = 0.72 | MCSE(6.27) = 10.1 | stat: FALSE | burn: 714



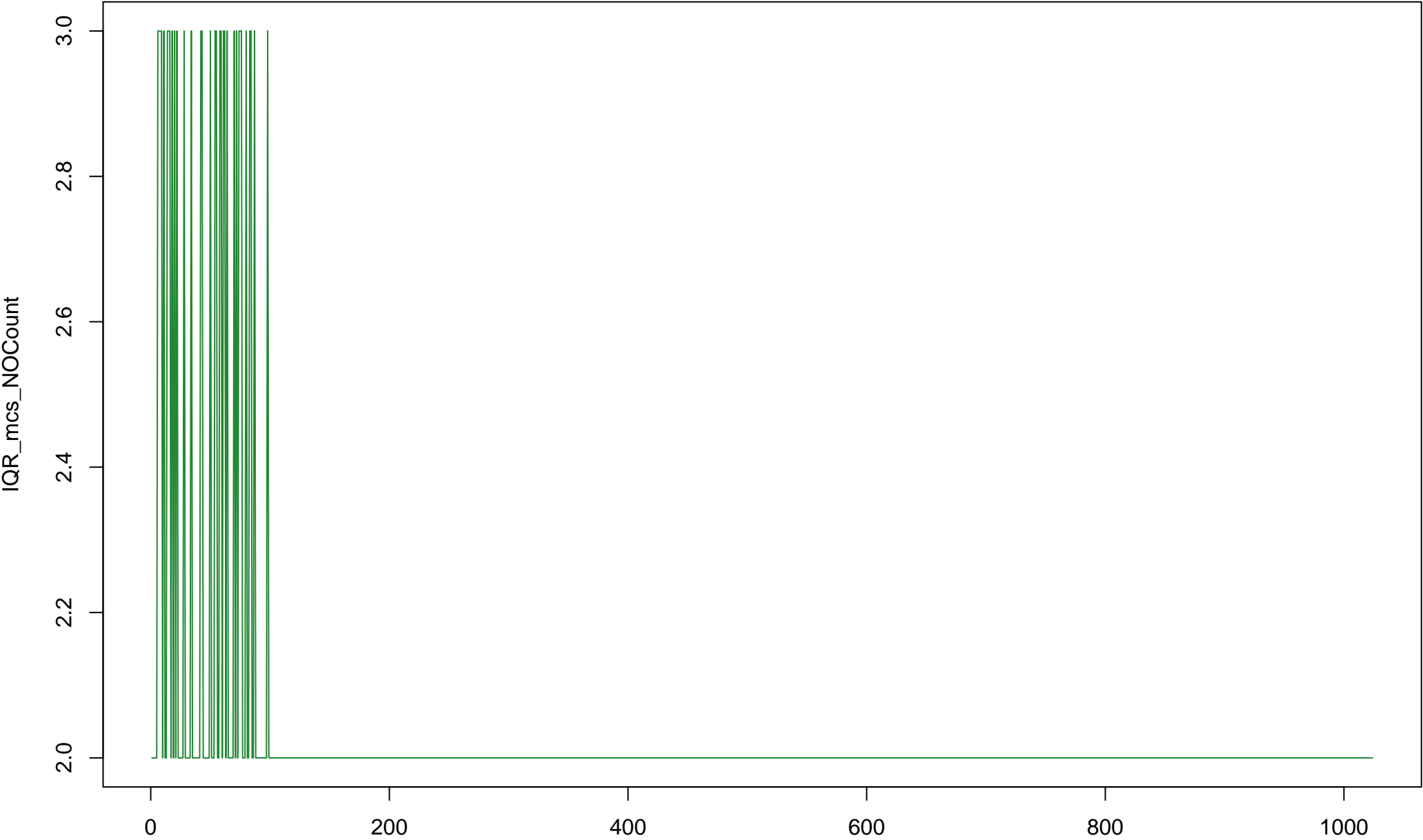
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



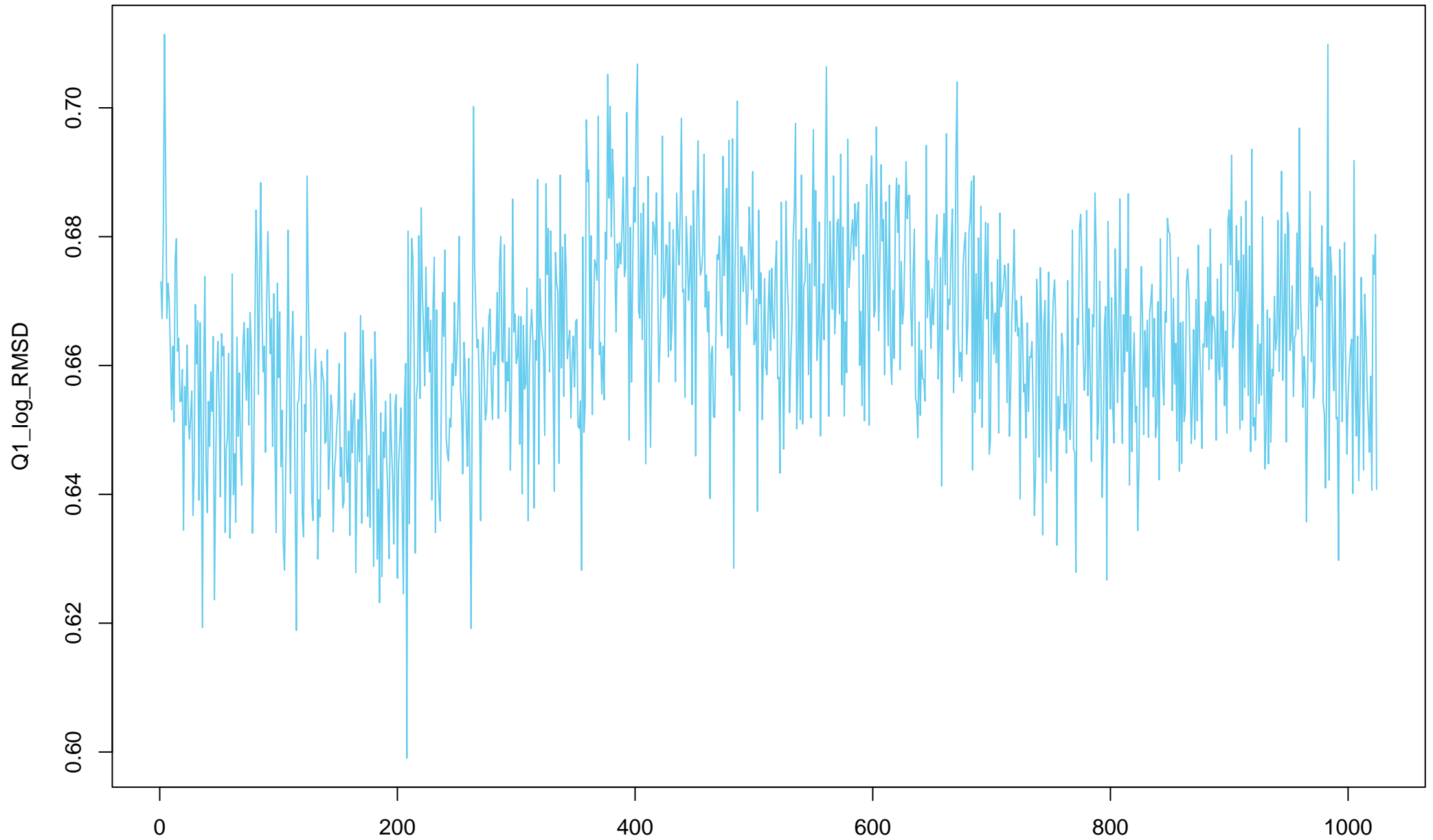
IQR_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.594 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102



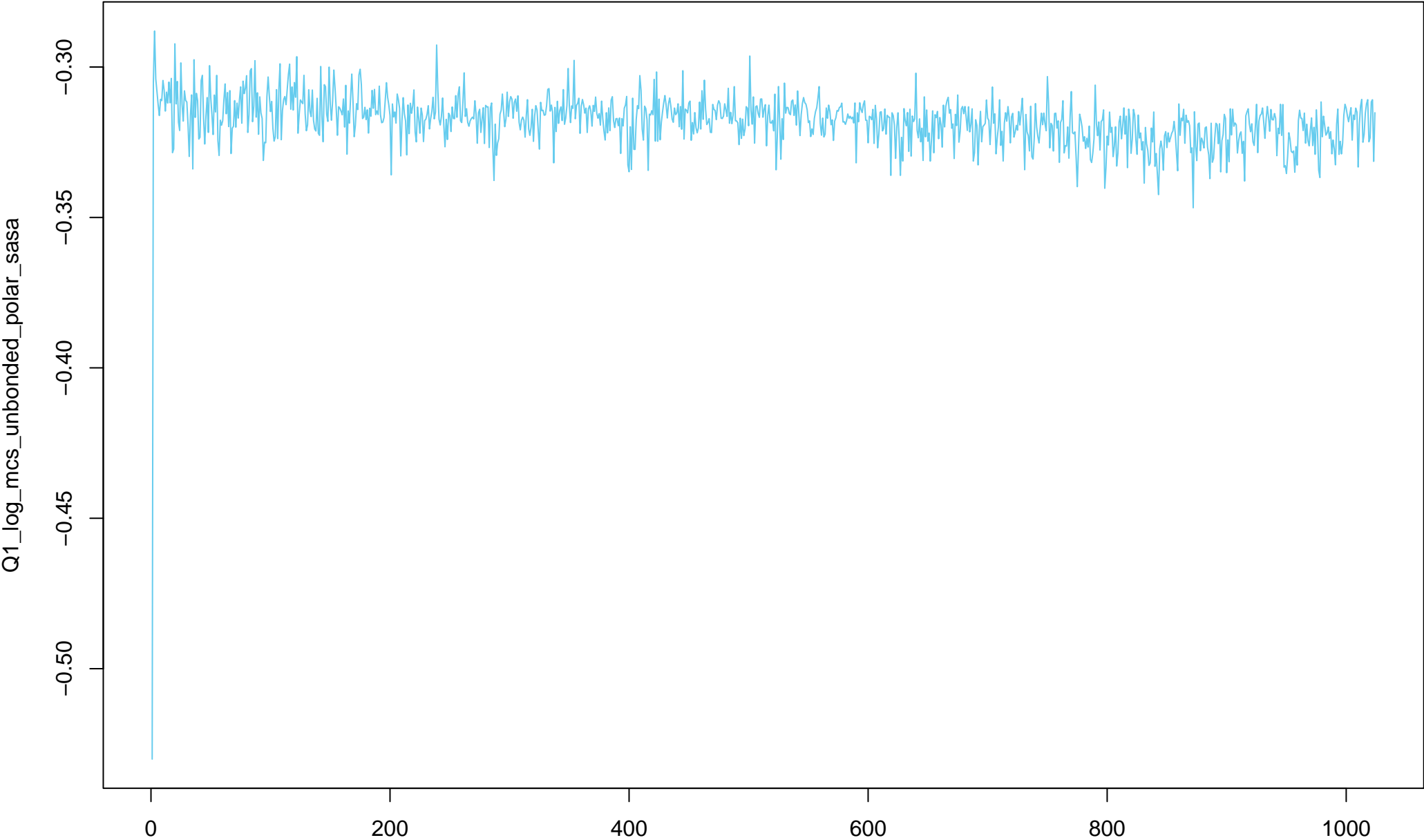
IQR_mcs_NOCCount
ESS = 32.5 | BMK = 0.471 | MCSE(6.27) = 9.93 | stat: FALSE | burn: 0



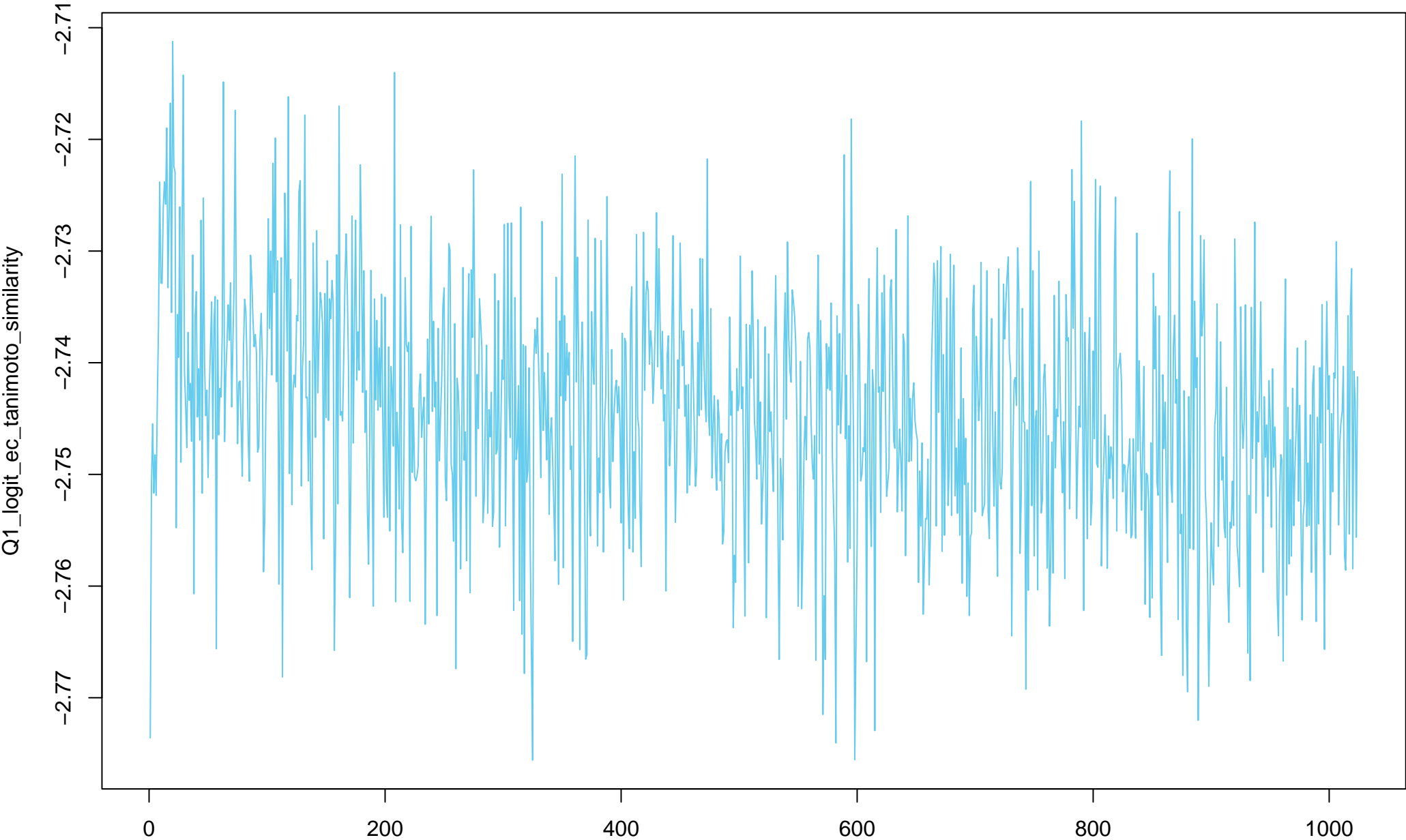
Q1_log_RMSD
ESS = 34.3 | BMK = 0.147 | MCSE(6.27) = 9.08 | stat: FALSE | burn: 0



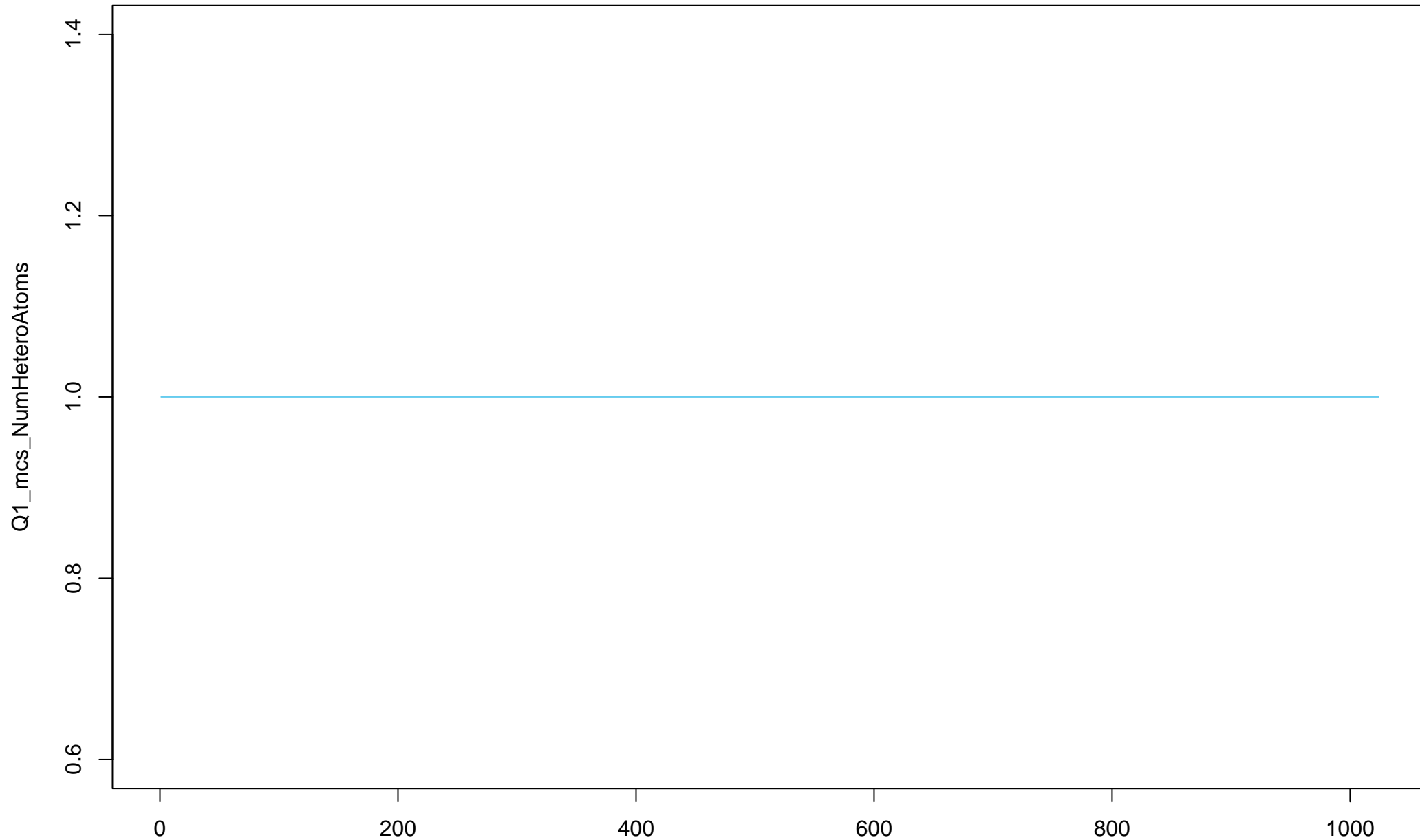
Q1_log_mcs_unbonded_polar_sasa
ESS = 202 | BMK = 0.292 | MCSE(6.27) = 6.18 | stat: FALSE | burn: 0



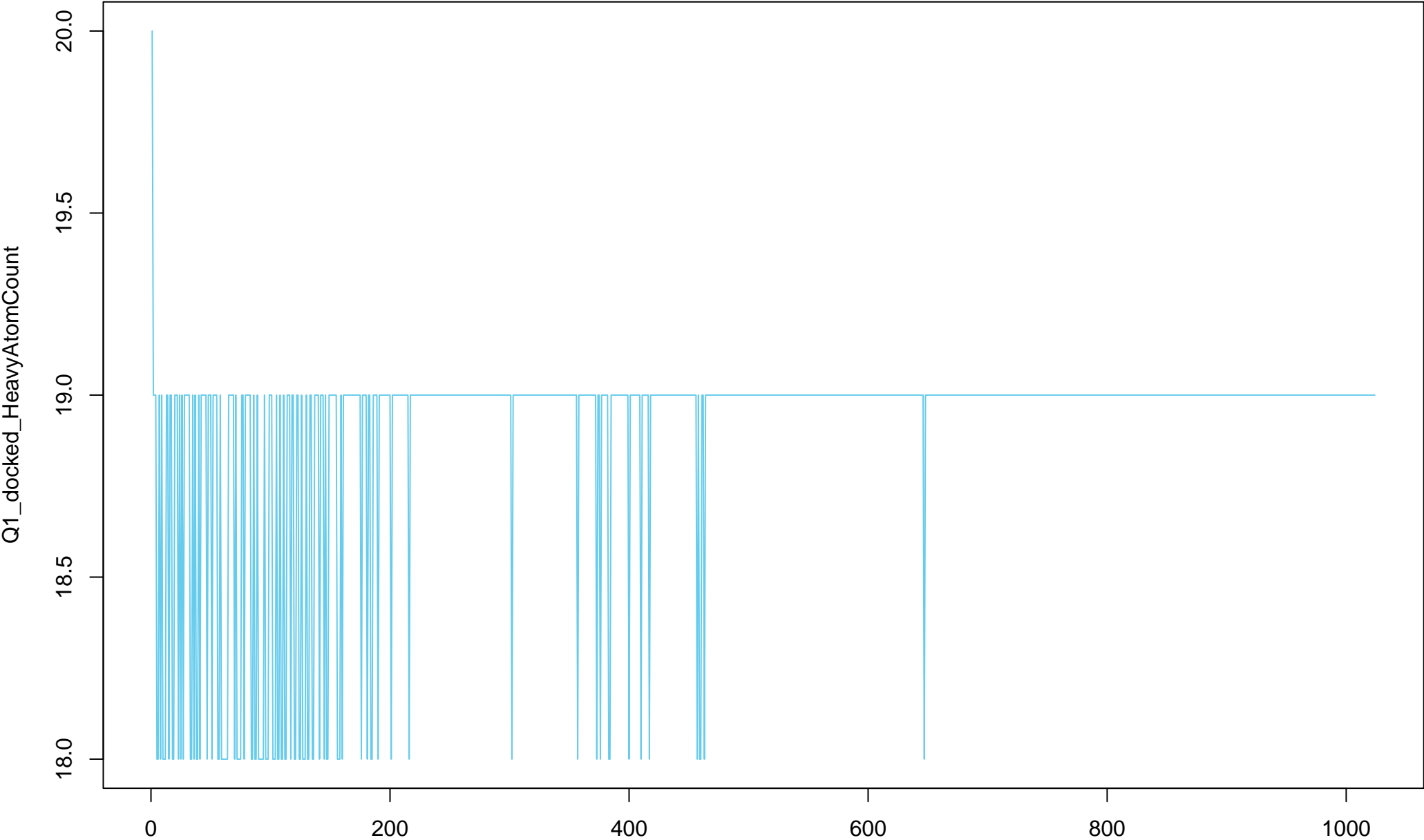
Q1_logit_ec_tanimoto_similarity
ESS = 454 | BMK = 0.155 | MCSE(6.27) = 5.78 | stat: FALSE | burn: 0



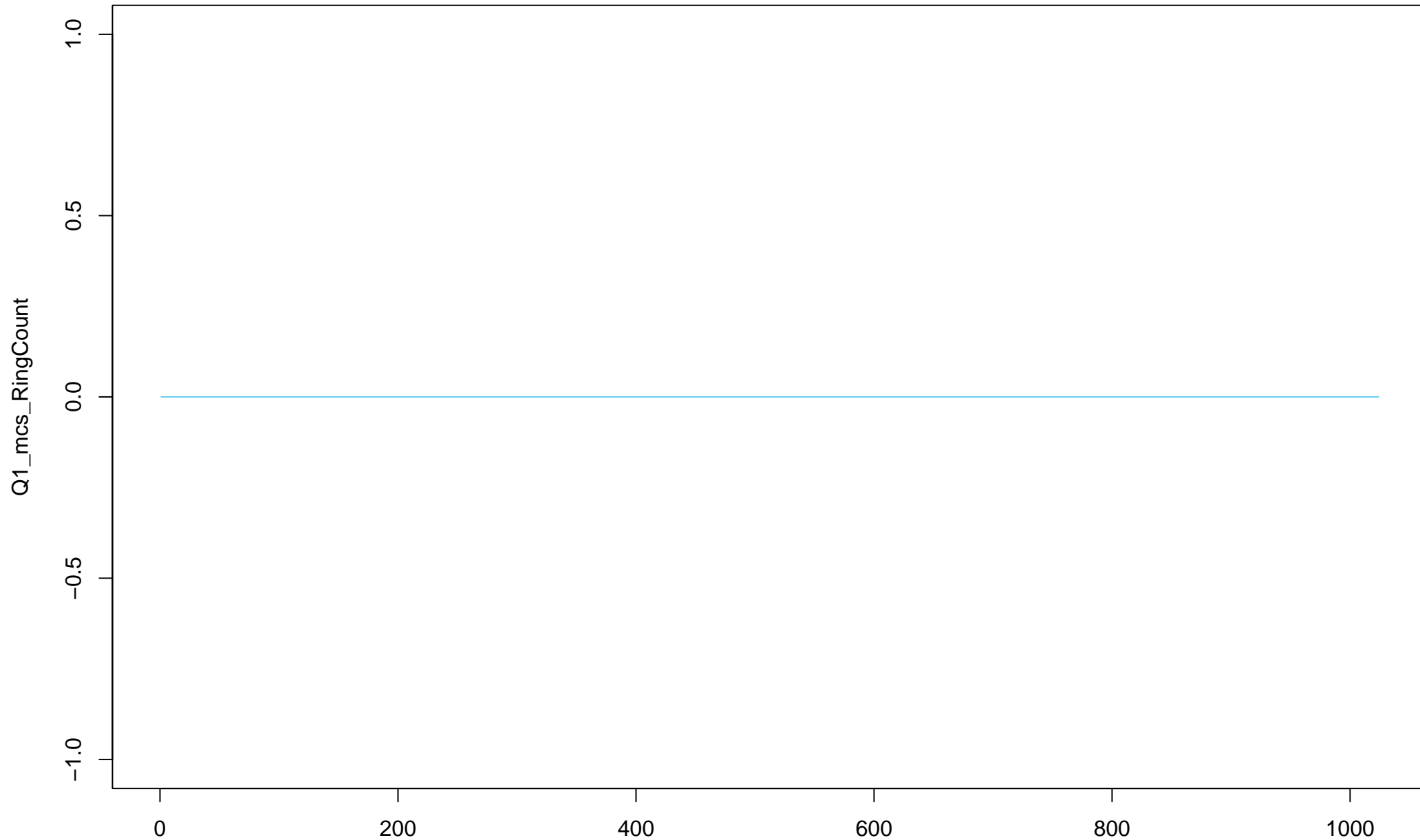
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



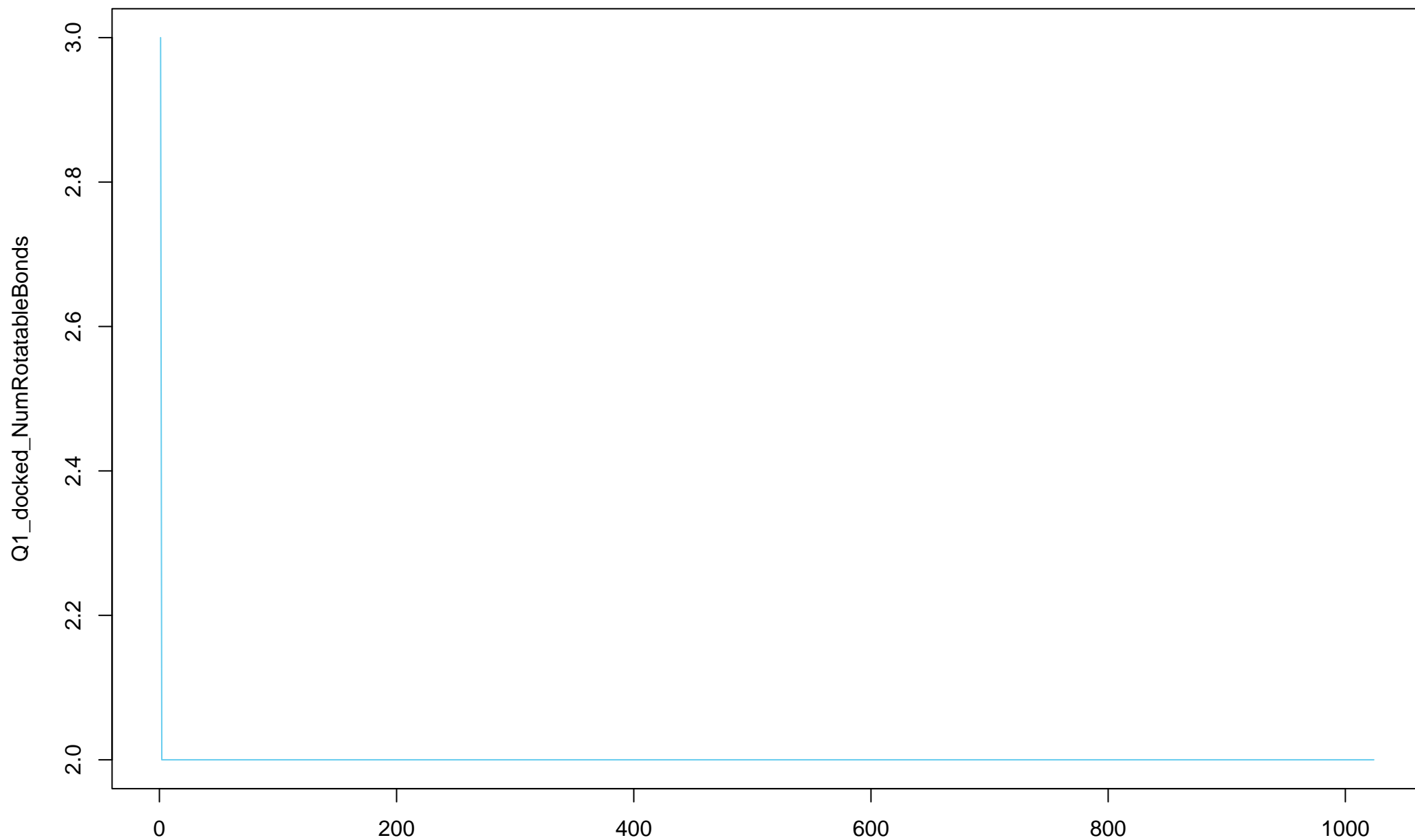
Q1_docked_HeavyAtomCount
ESS = 10.3 | BMK = 0.721 | MCSE(6.27) = 10.3 | stat: FALSE | burn: 0



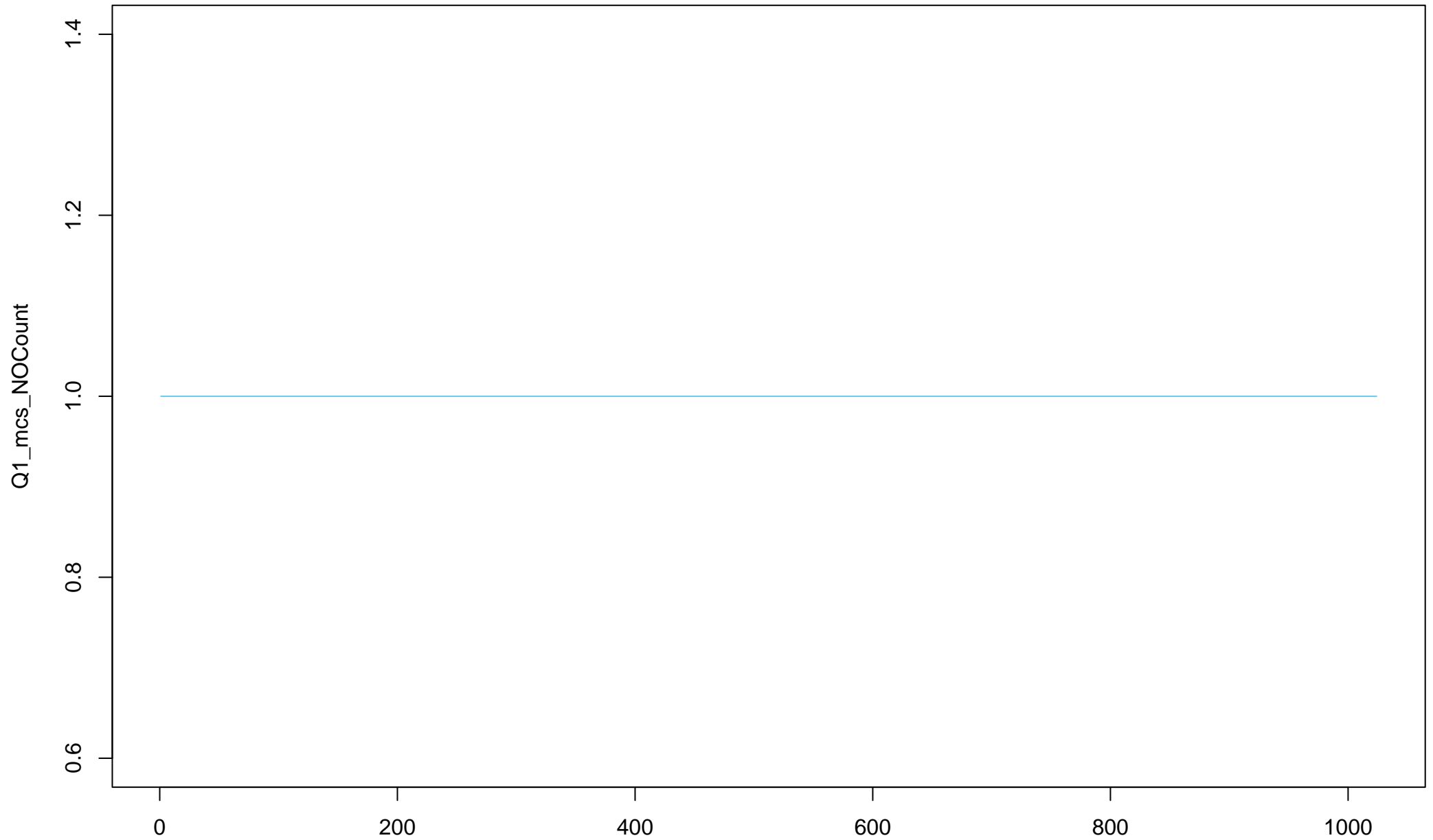
Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



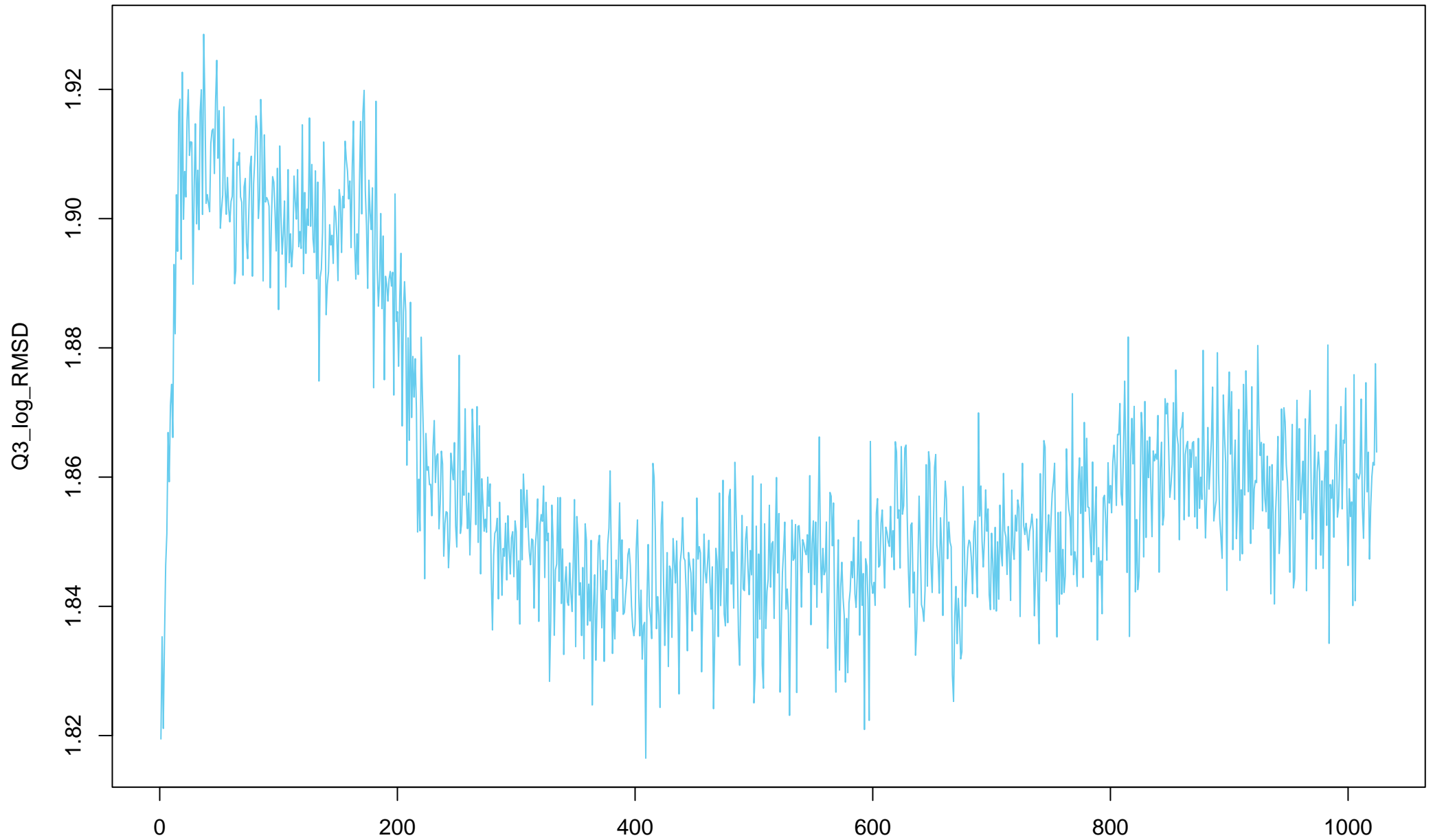
Q1_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.626 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102



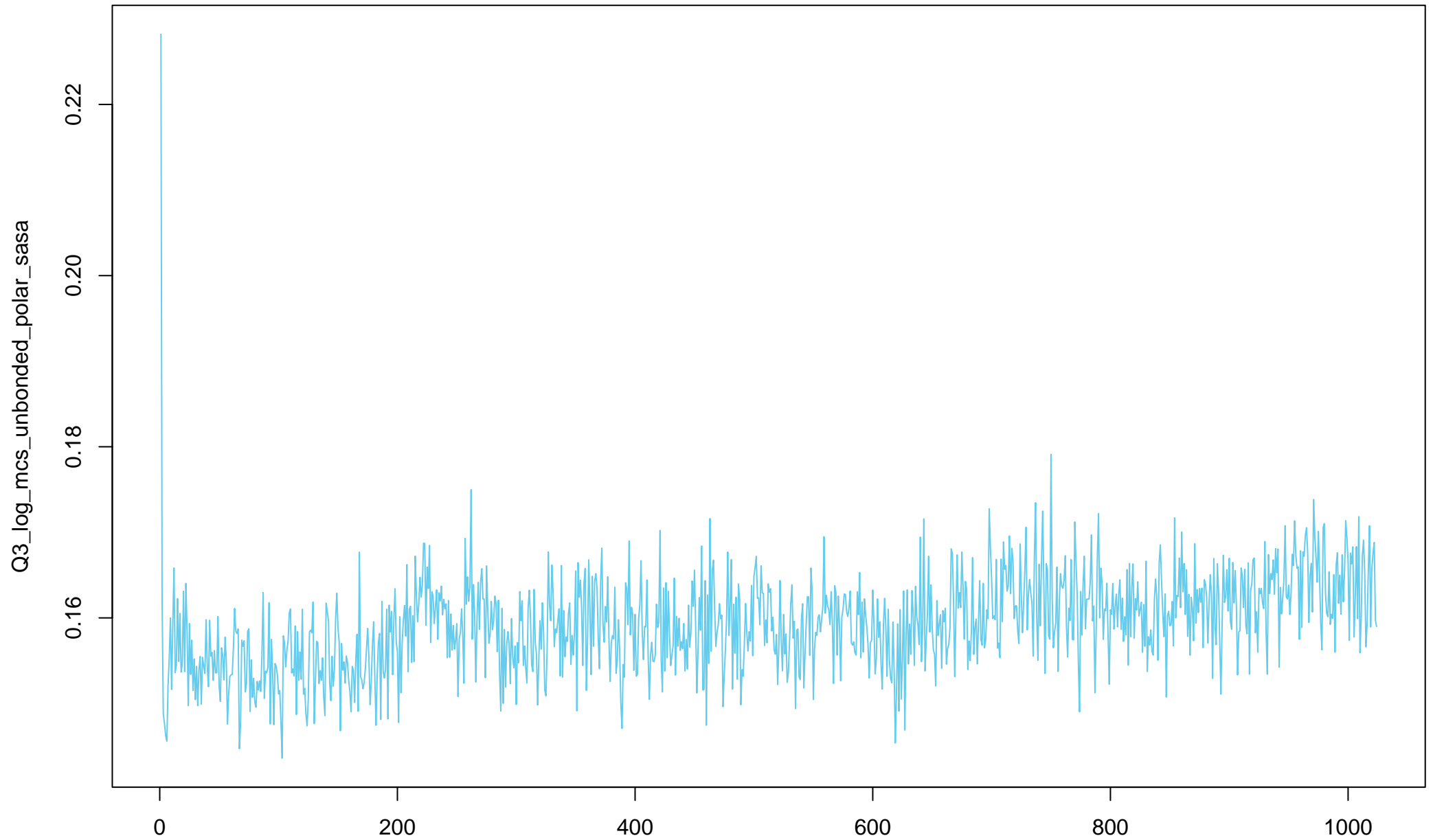
Q1_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



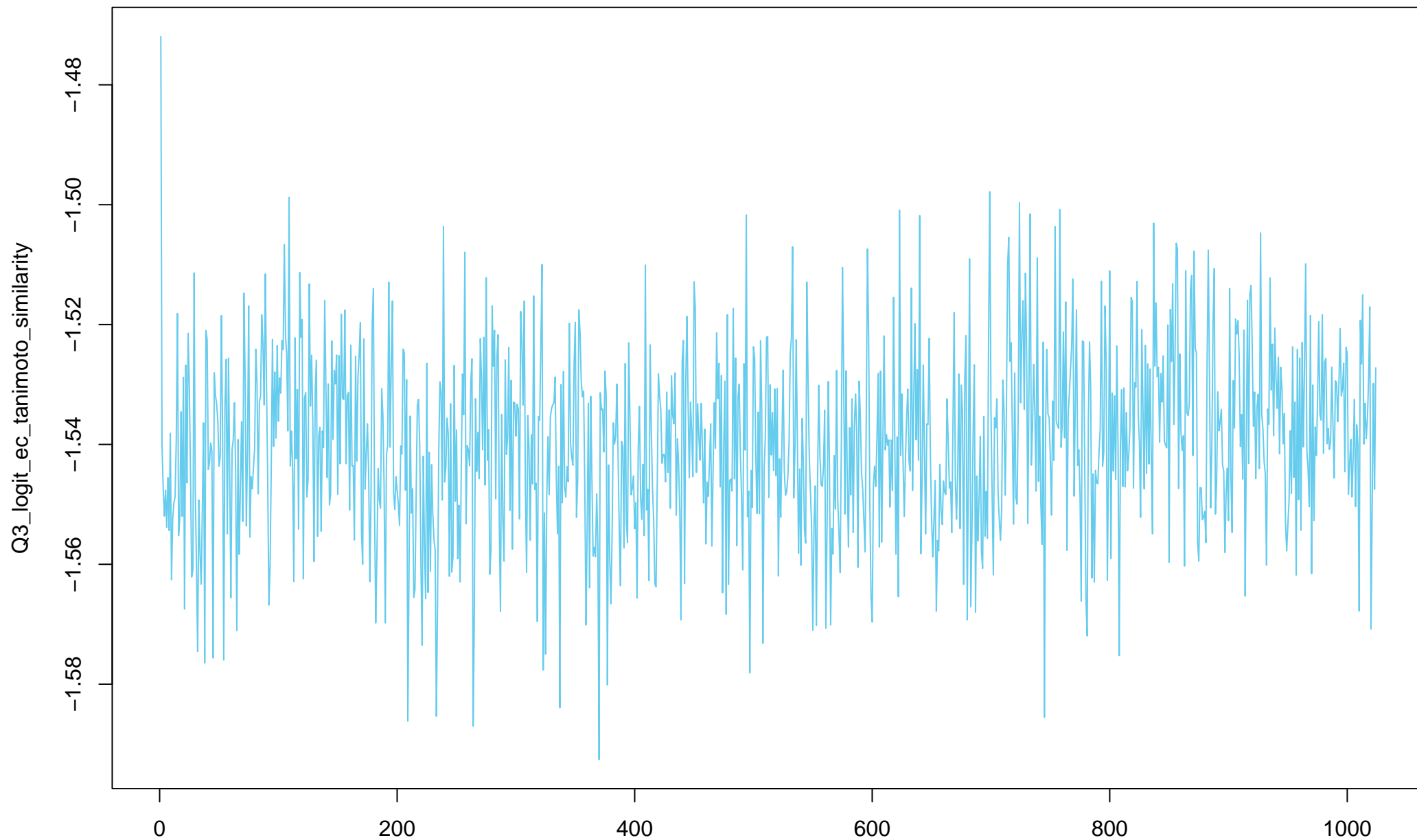
Q3_log_RMSD
ESS = 4.67 | BMK = 0.466 | MCSE(6.27) = 16 | stat: FALSE | burn: 204



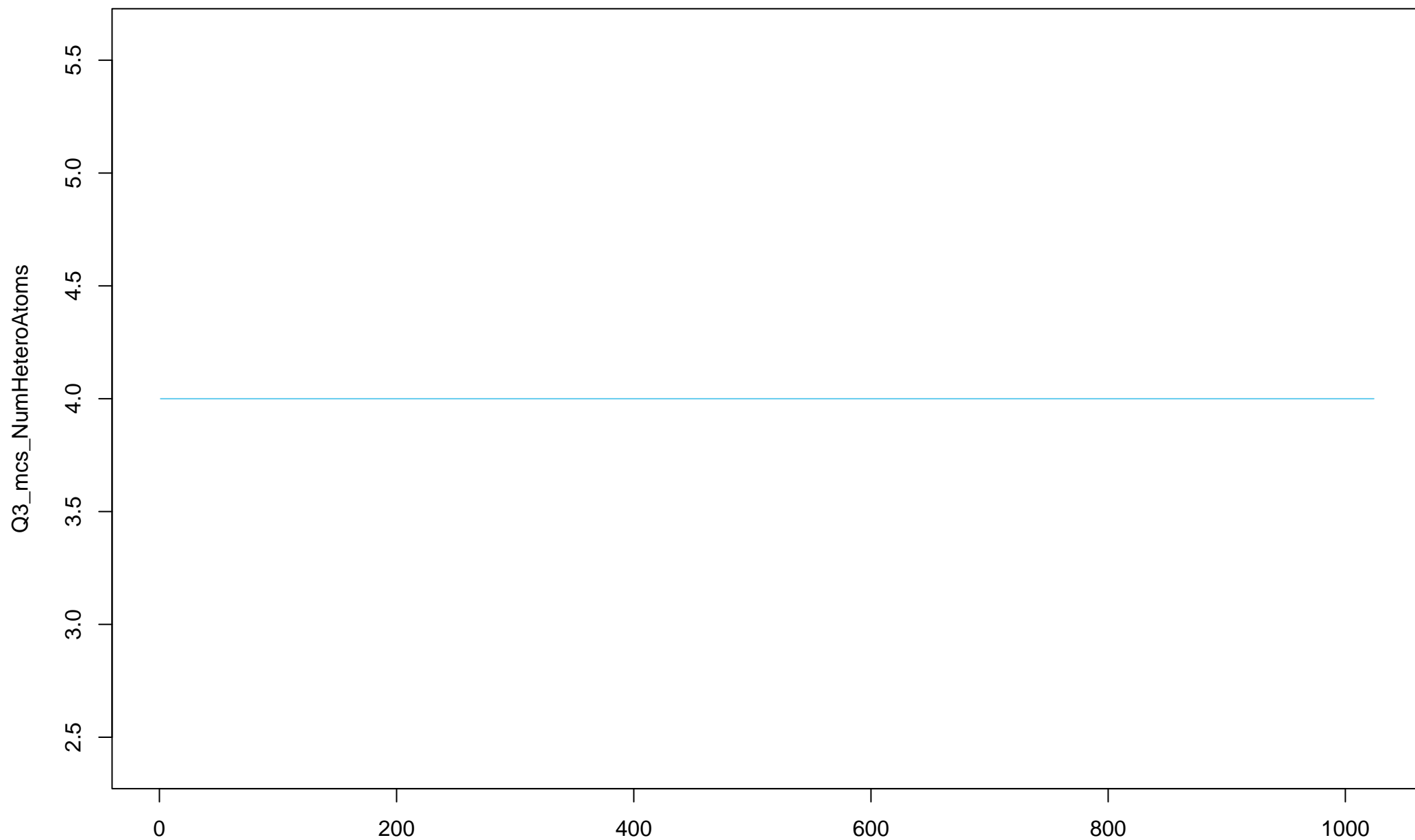
Q3_log_mcs_unbonded_polar_sasa
ESS = 45.3 | BMK = 0.261 | MCSE(6.27) = 9.1 | stat: FALSE | burn: 0



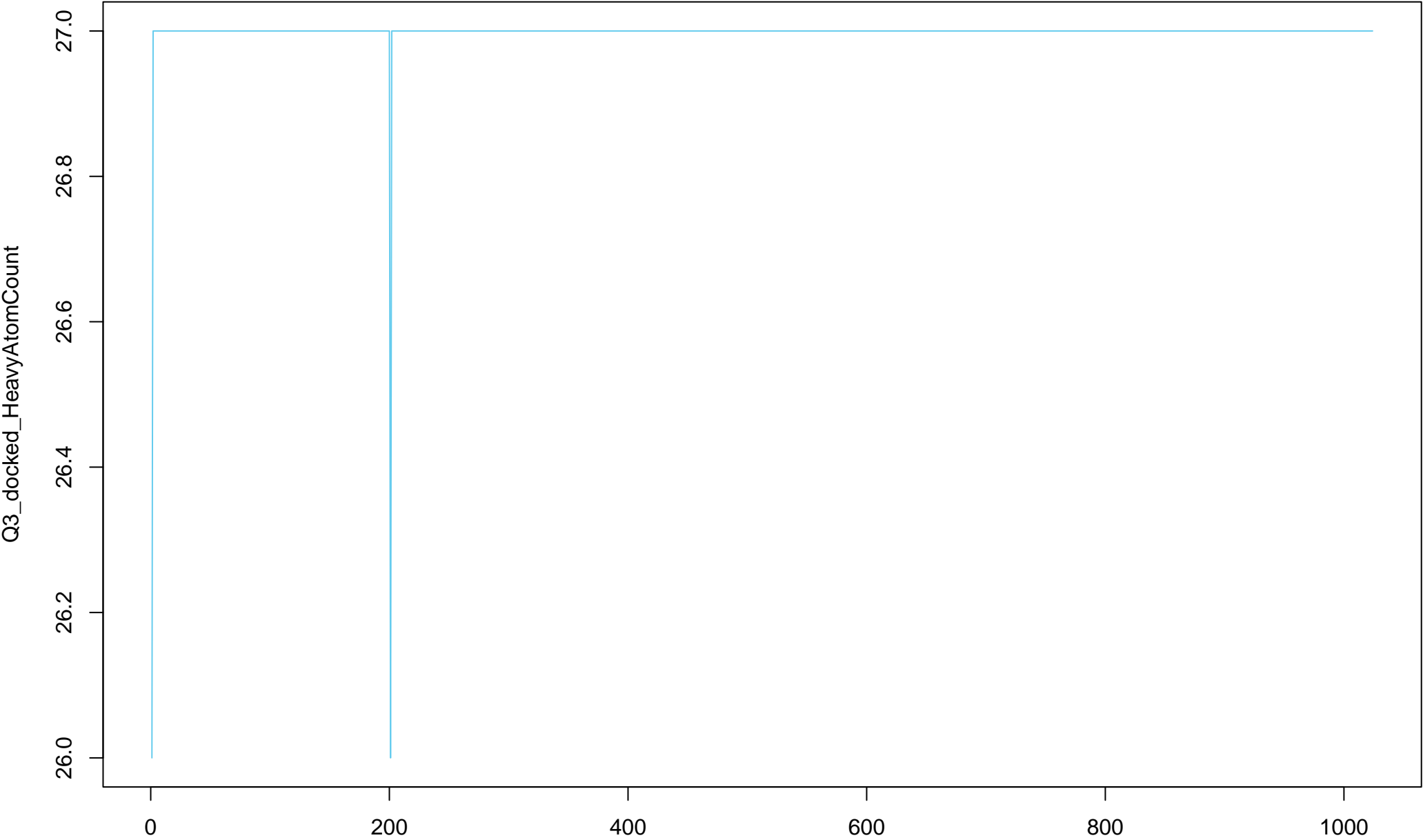
Q3_logit_ec_tanimoto_similarity
ESS = 203 | BMK = 0.098 | MCSE(6.27) = 5.15 | stat: TRUE | burn: 0



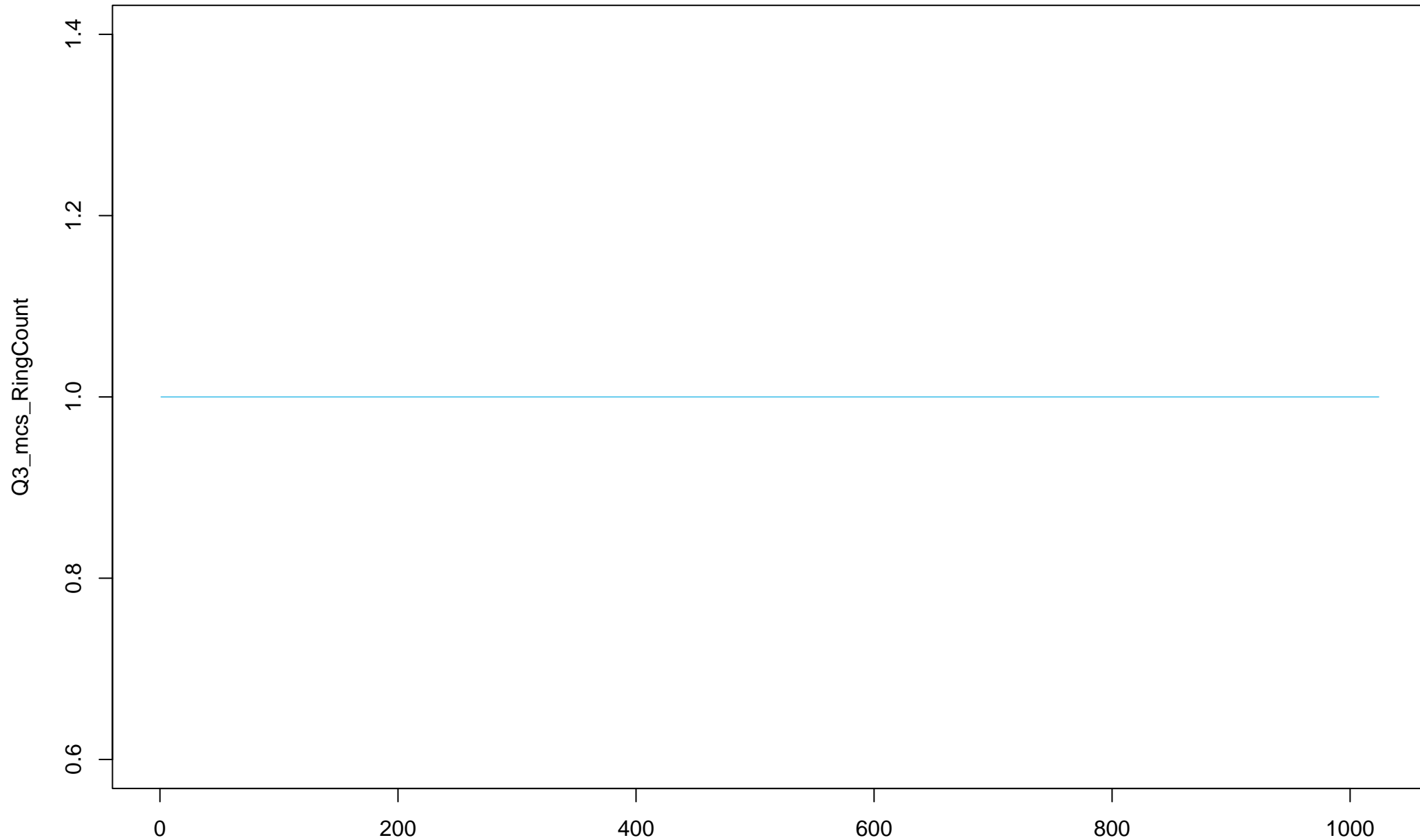
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



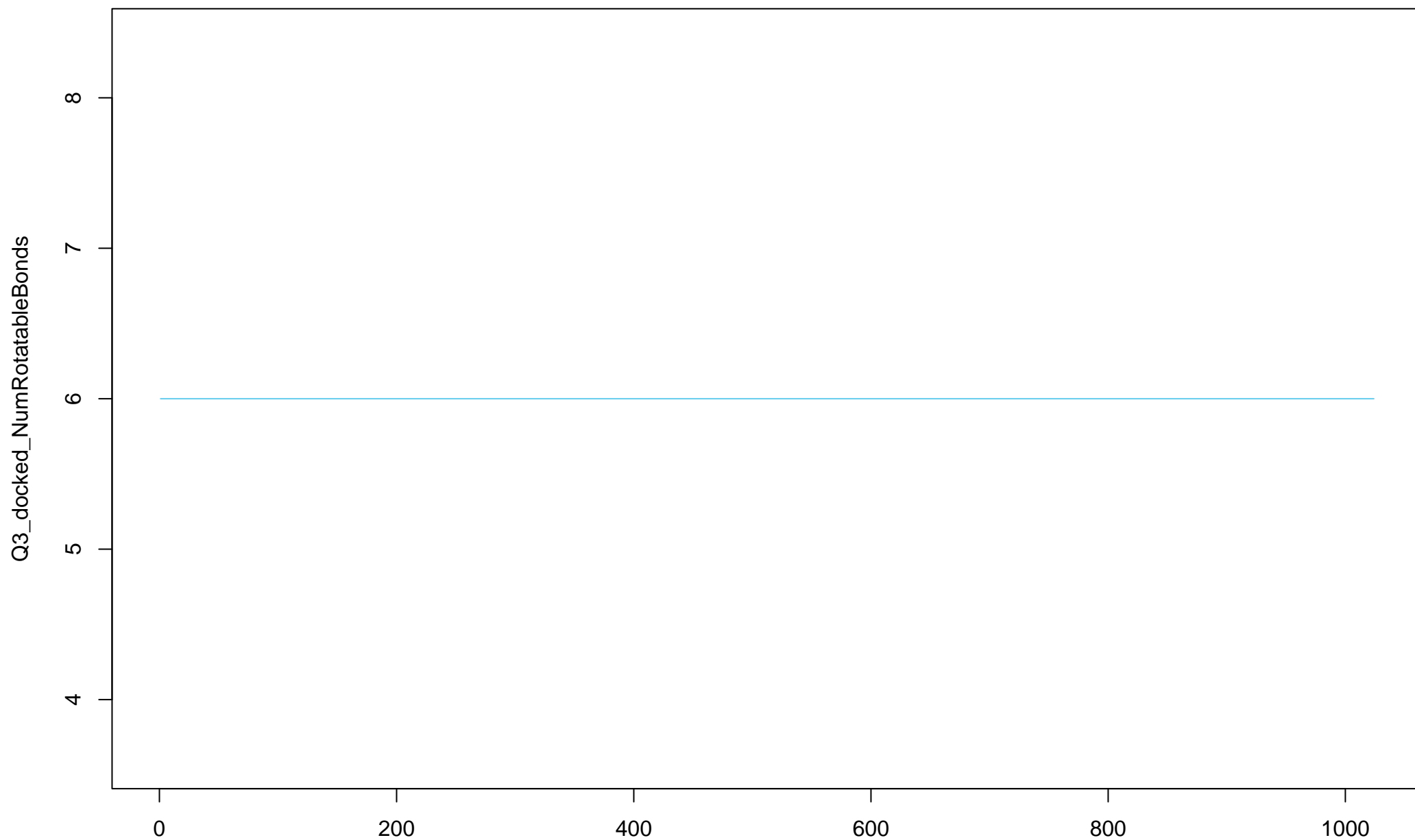
Q3_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.503 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0



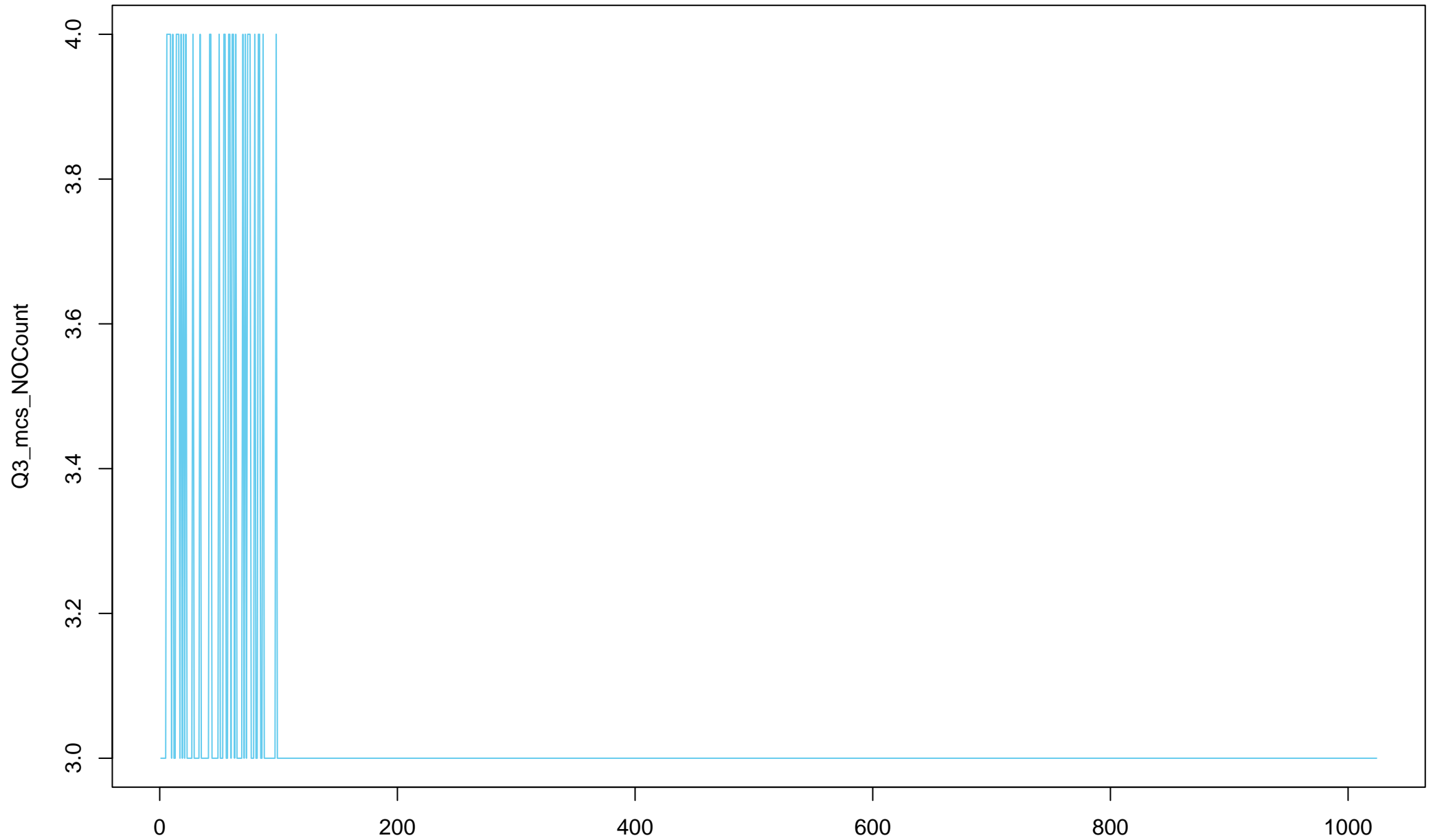
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



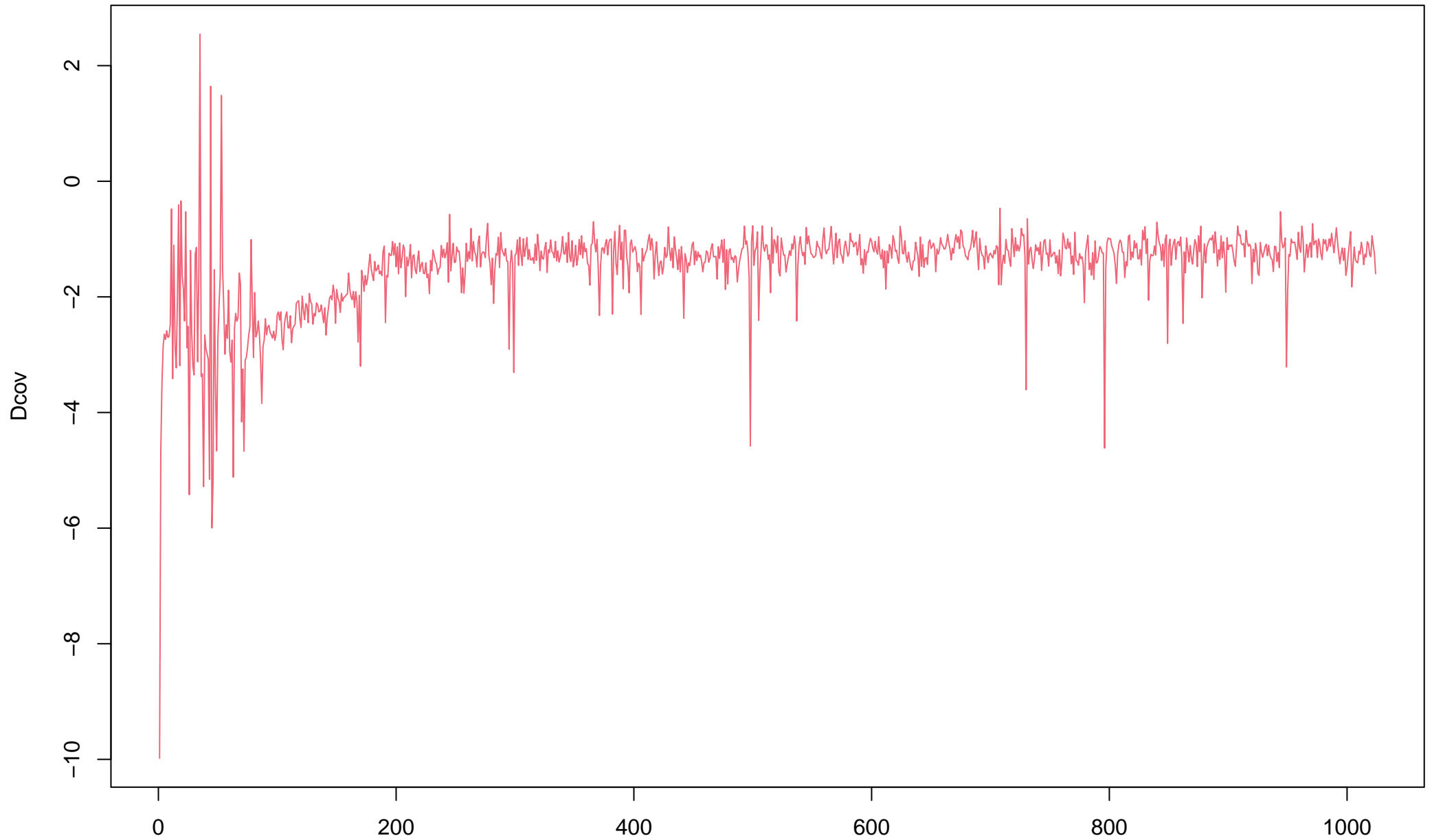
Q3_docked_NumRotatableBonds
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



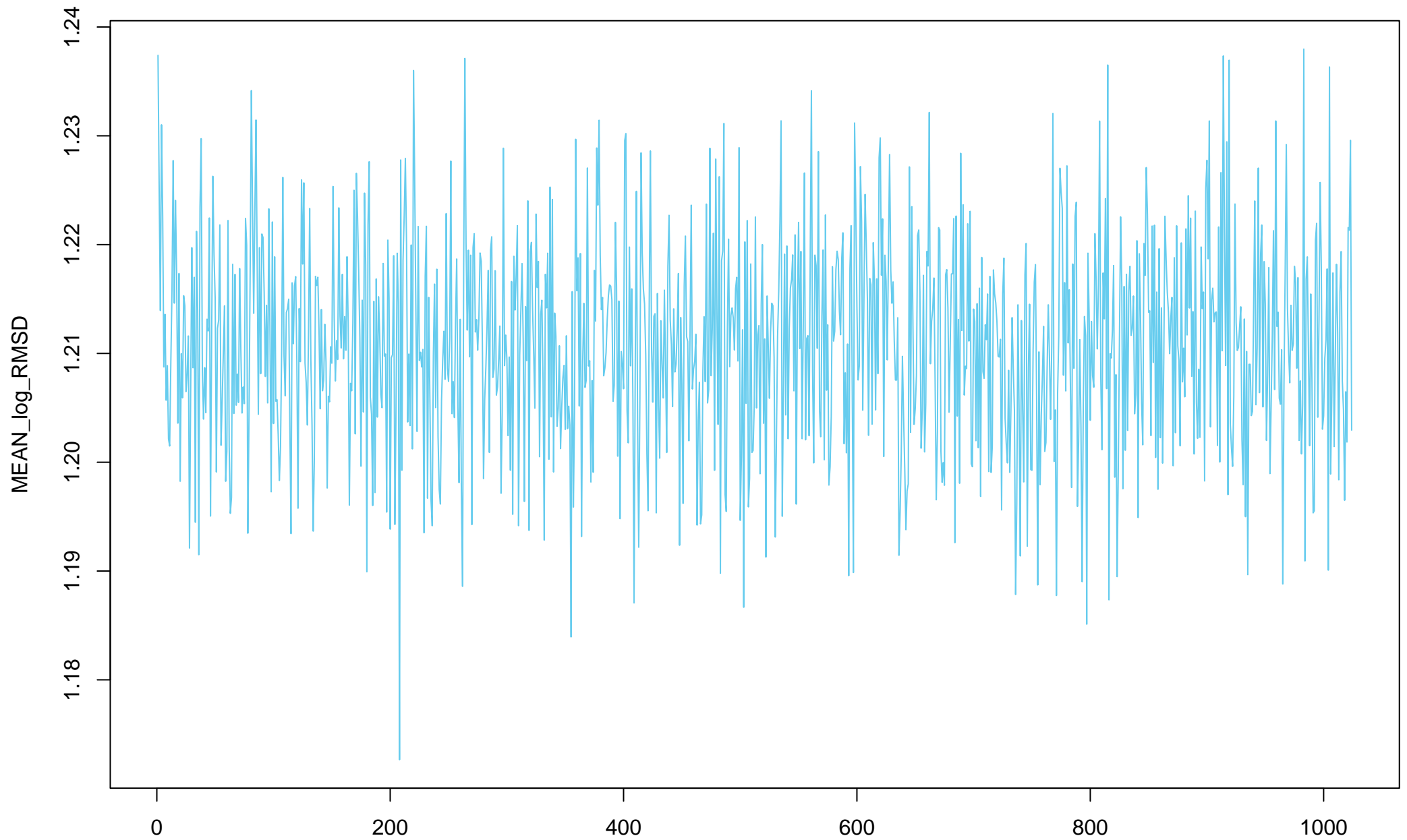
Q3_mcs_NOCount
ESS = 32.5 | BMK = 0.47 | MCSE(6.27) = 9.93 | stat: FALSE | burn: 0



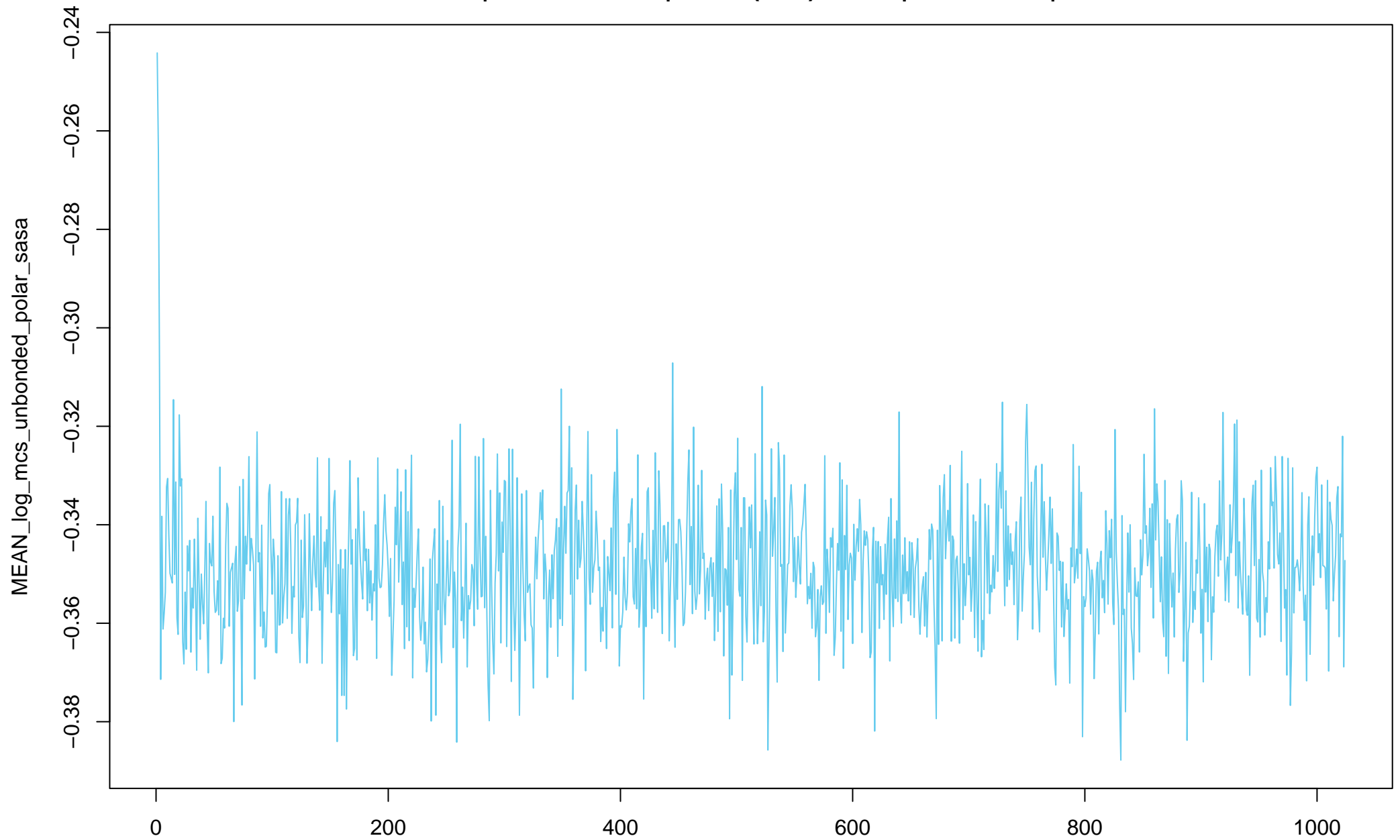
Dcov
ESS = 410 | BMK = 0.365 | MCSE(6.27) = 3.62 | stat: TRUE | burn: 204



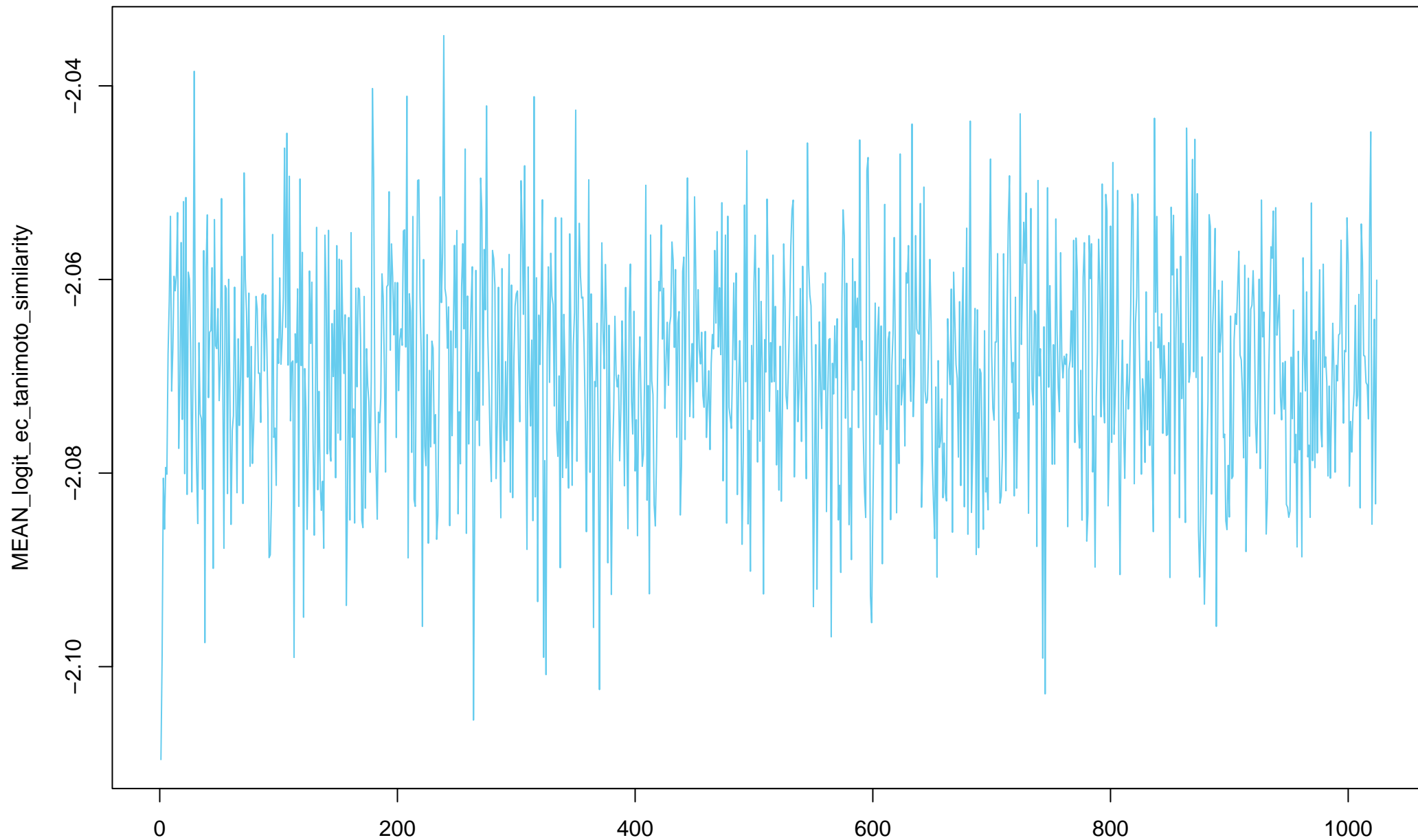
MEAN_log_RMSD
ESS = 1020 | BMK = 0.0684 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0



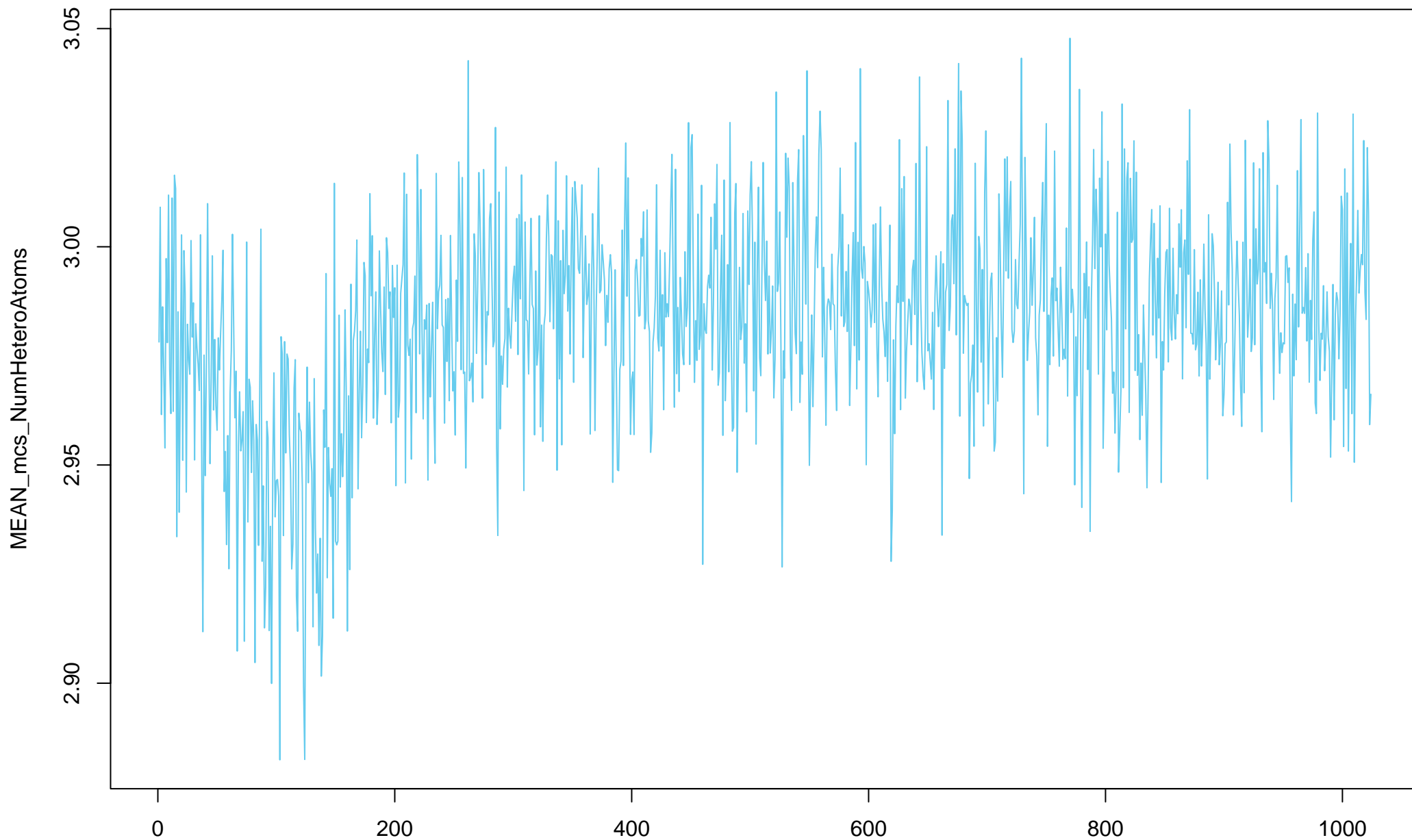
MEAN_log_mcs_unbonded_polar_sasa
ESS = 924 | BMK = 0.0726 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 0



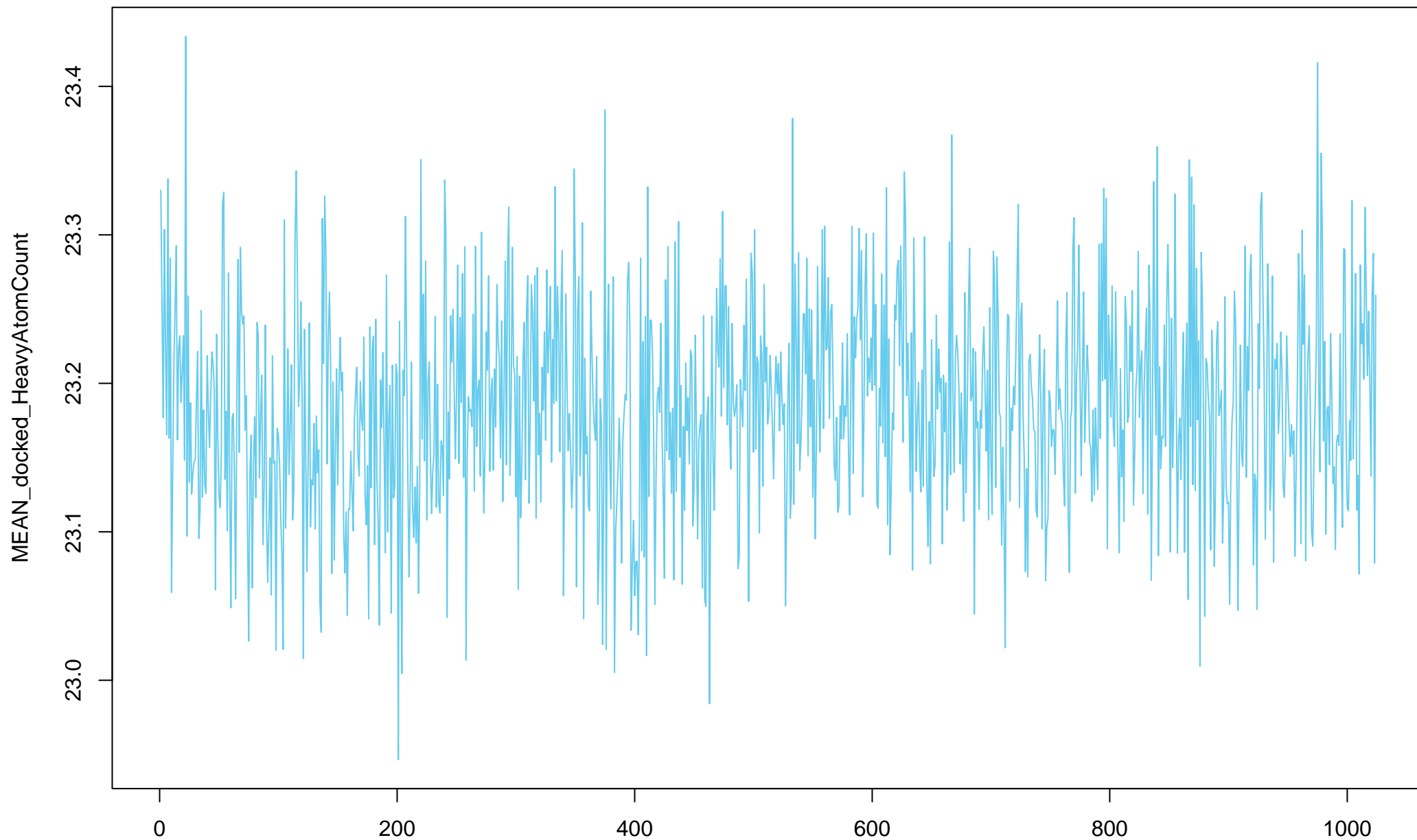
MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0645 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0



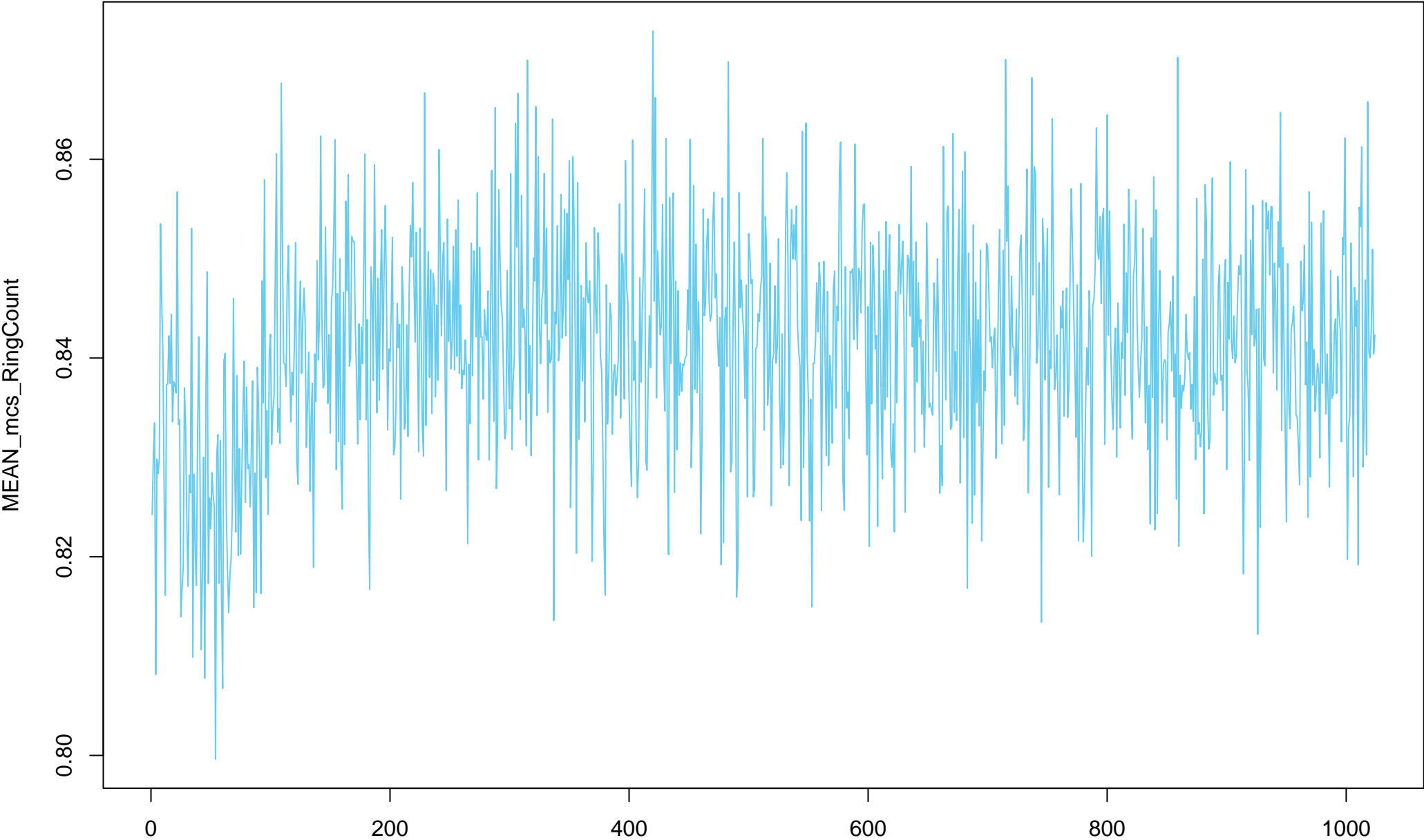
MEAN_mcs_NumHeteroAtoms
ESS = 18.3 | BMK = 0.211 | MCSE(6.27) = 9.24 | stat: FALSE | burn: 0



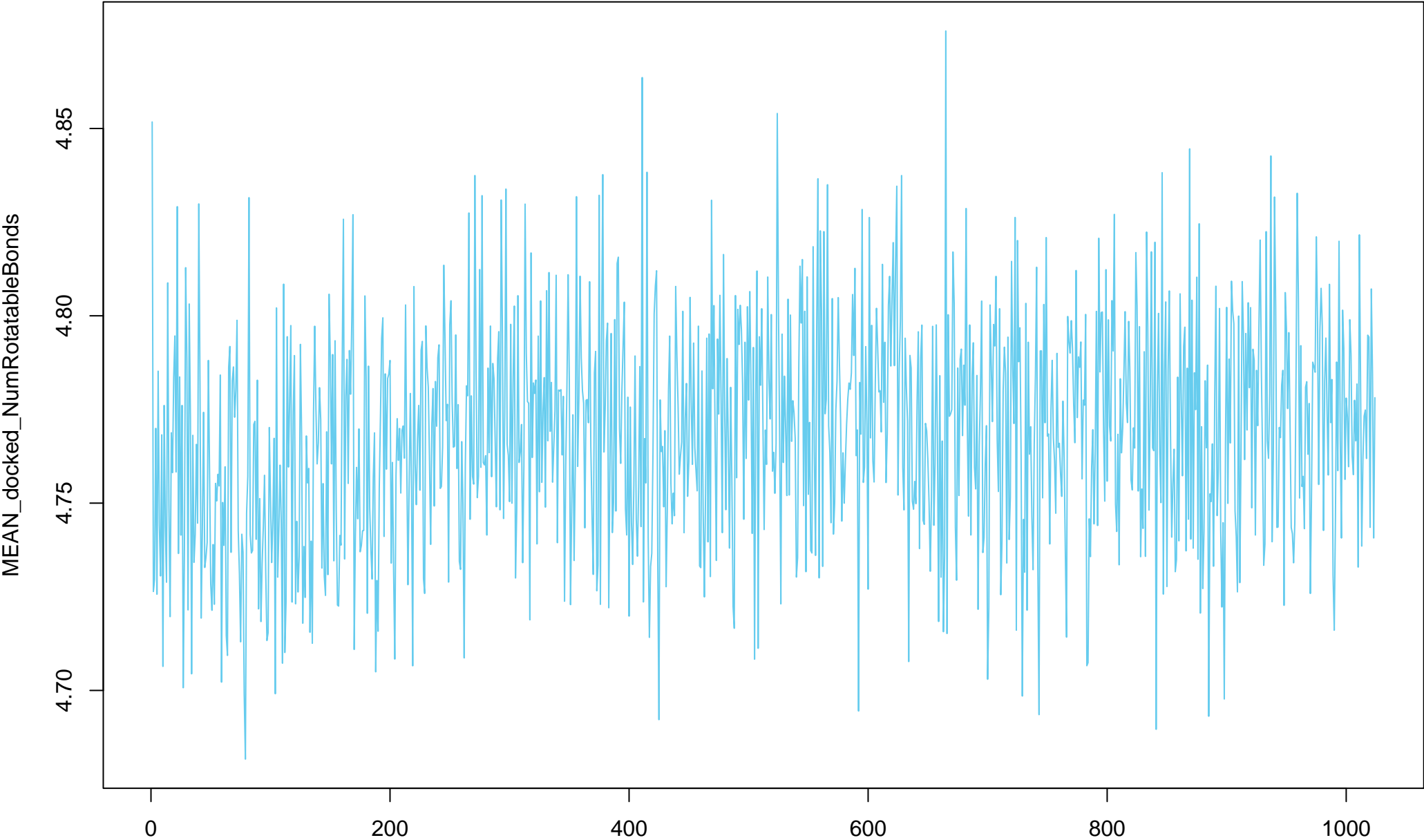
MEAN_docked_HeavyAtomCount
ESS = 684 | BMK = 0.102 | MCSE(6.27) = 4.15 | stat: TRUE | burn: 0



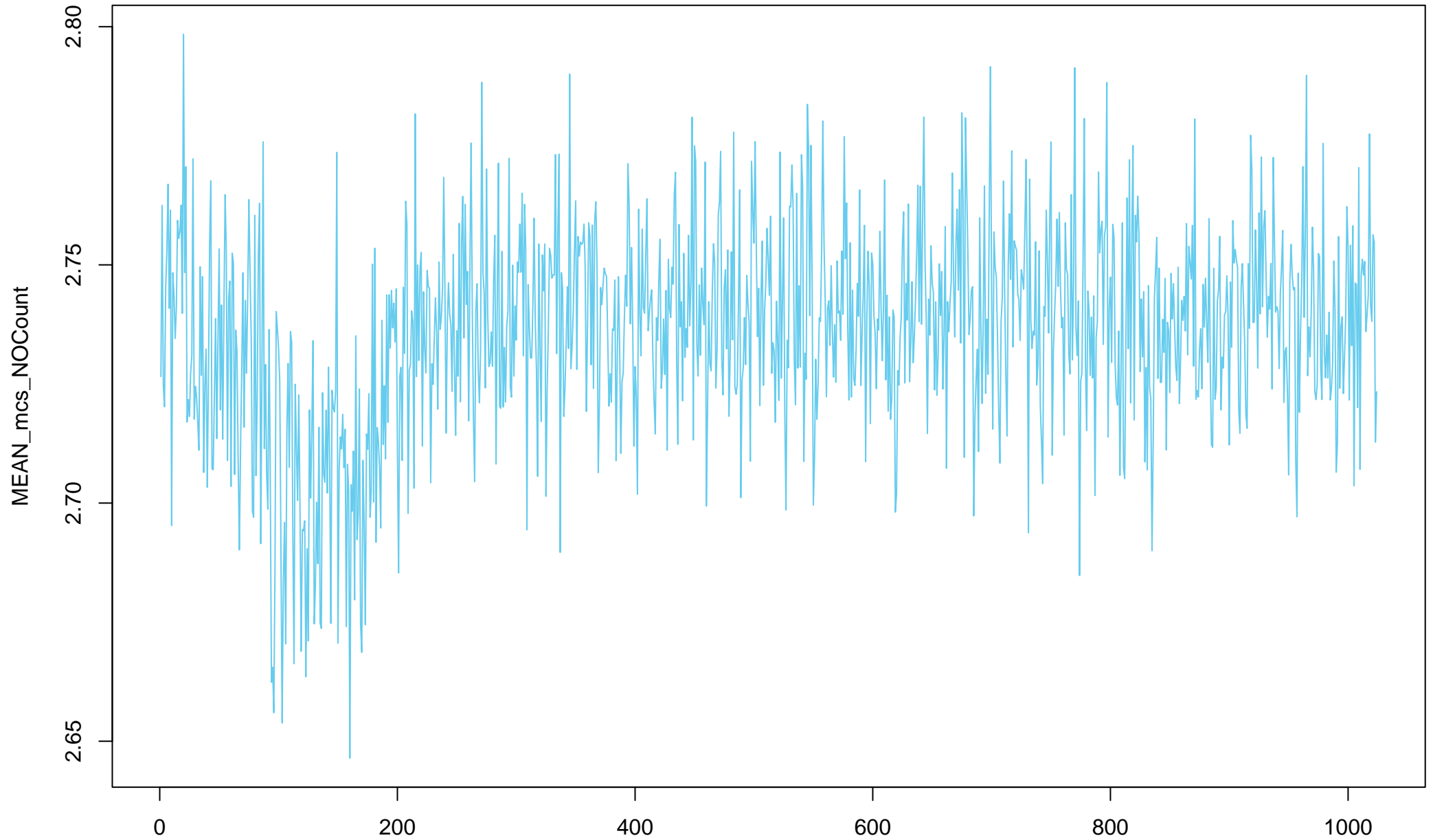
MEAN_mcs_RingCount
ESS = 115 | BMK = 0.102 | MCSE(6.27) = 6.91 | stat: FALSE | burn: 0



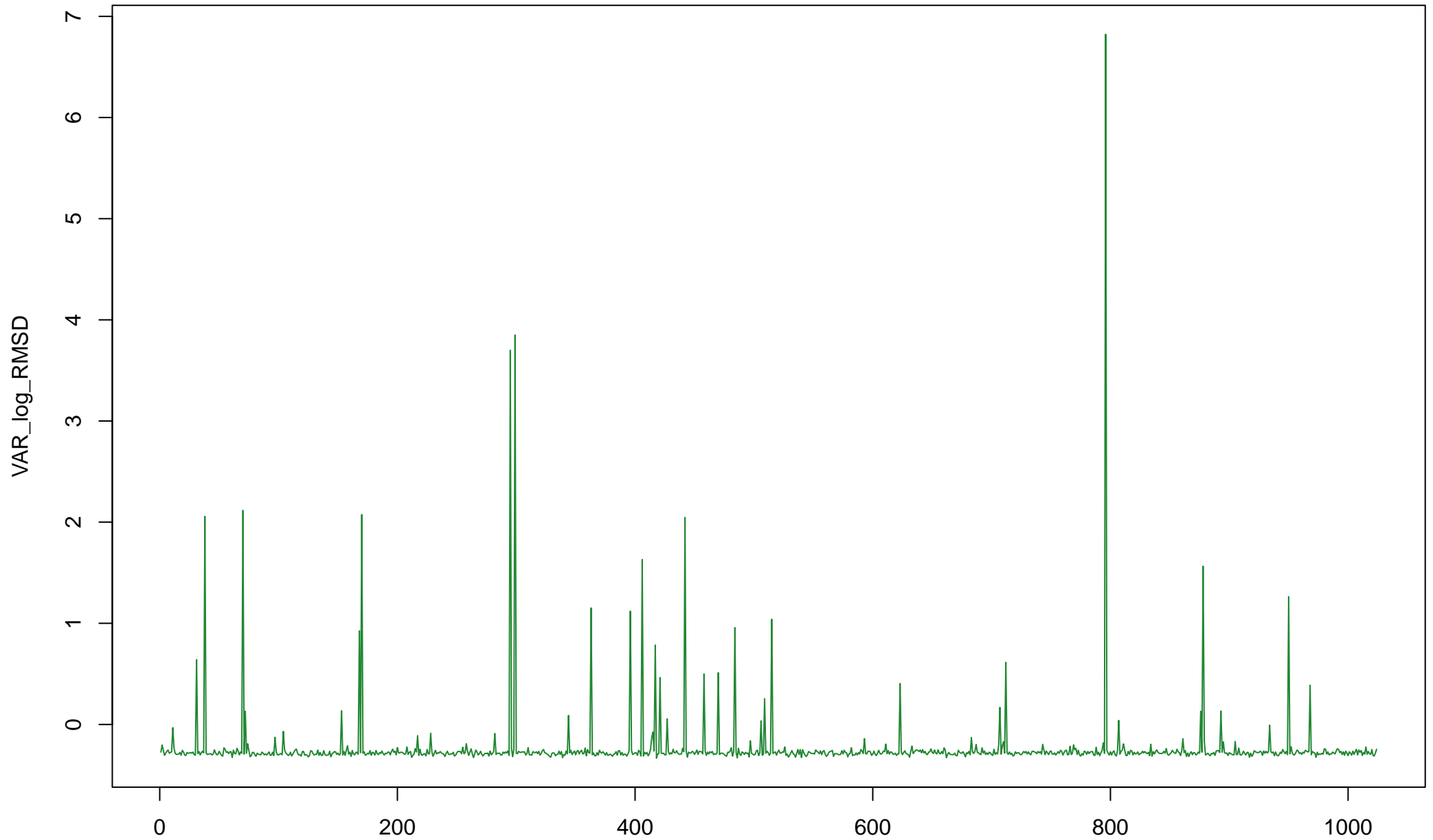
MEAN_docked_NumRotatableBonds
ESS = 230 | BMK = 0.108 | MCSE(6.27) = 4.84 | stat: FALSE | burn: 0



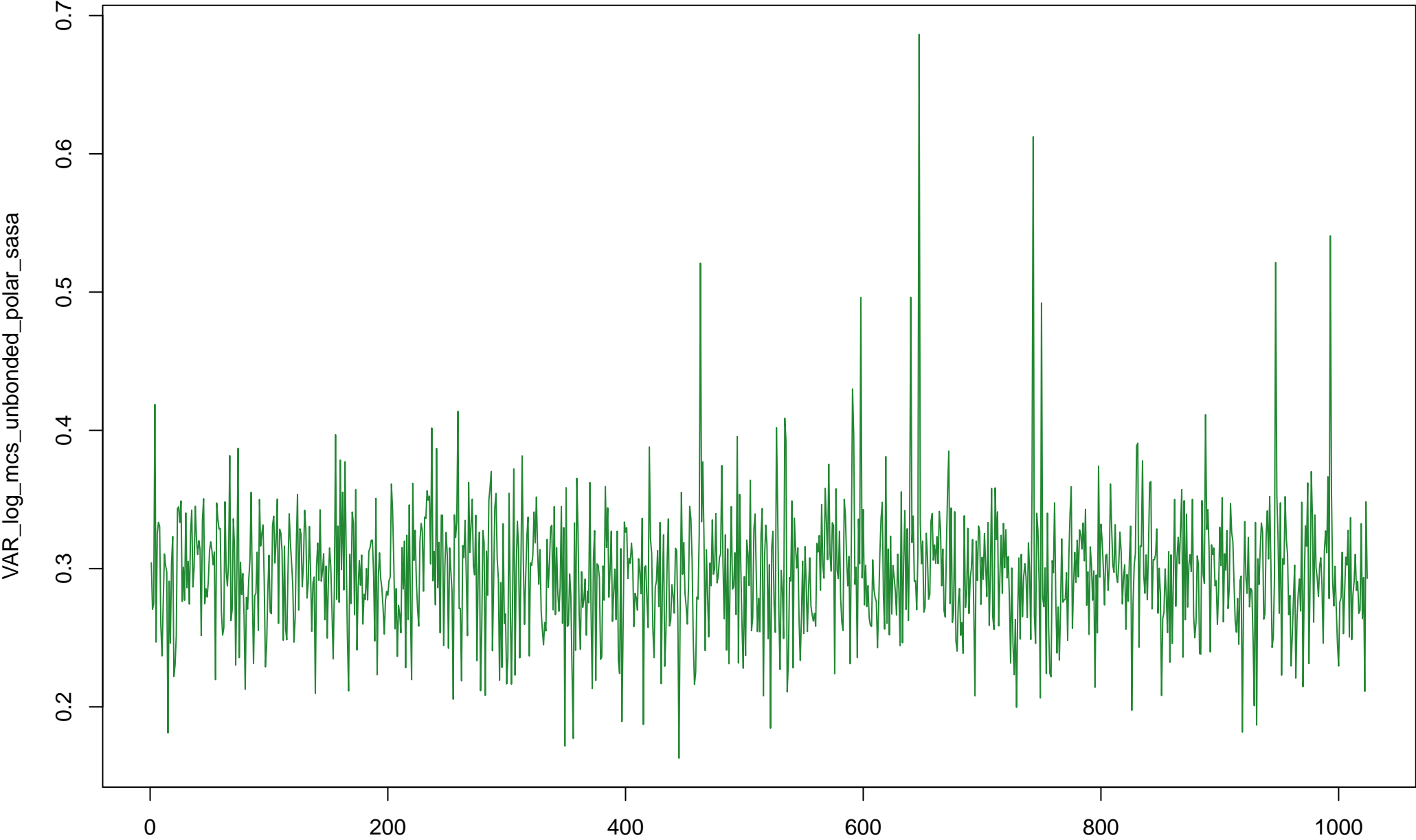
MEAN_mcs_NOCount
ESS = 62.8 | BMK = 0.187 | MCSE(6.27) = 8.89 | stat: FALSE | burn: 204



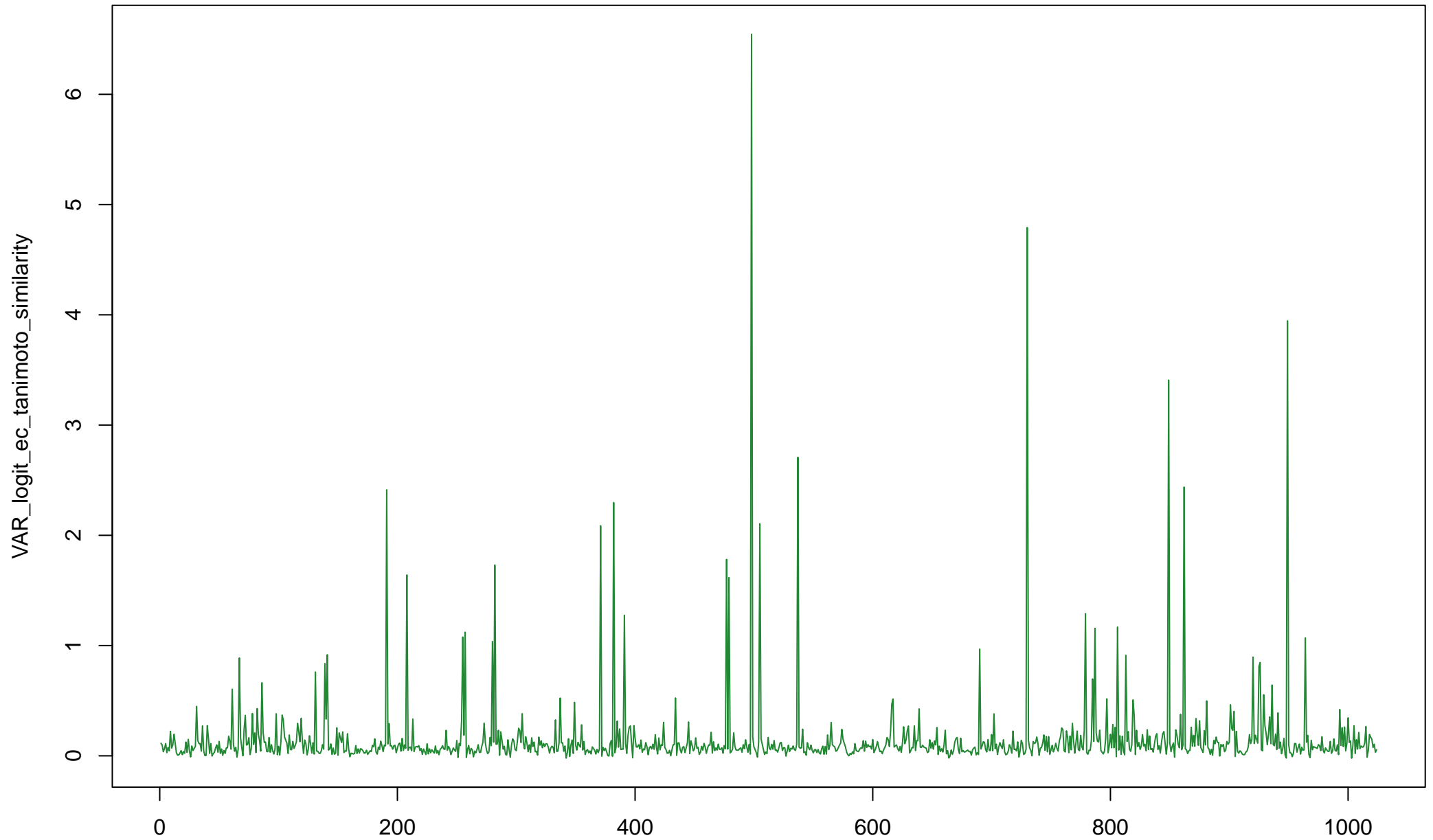
VAR_log_RMSD
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 816



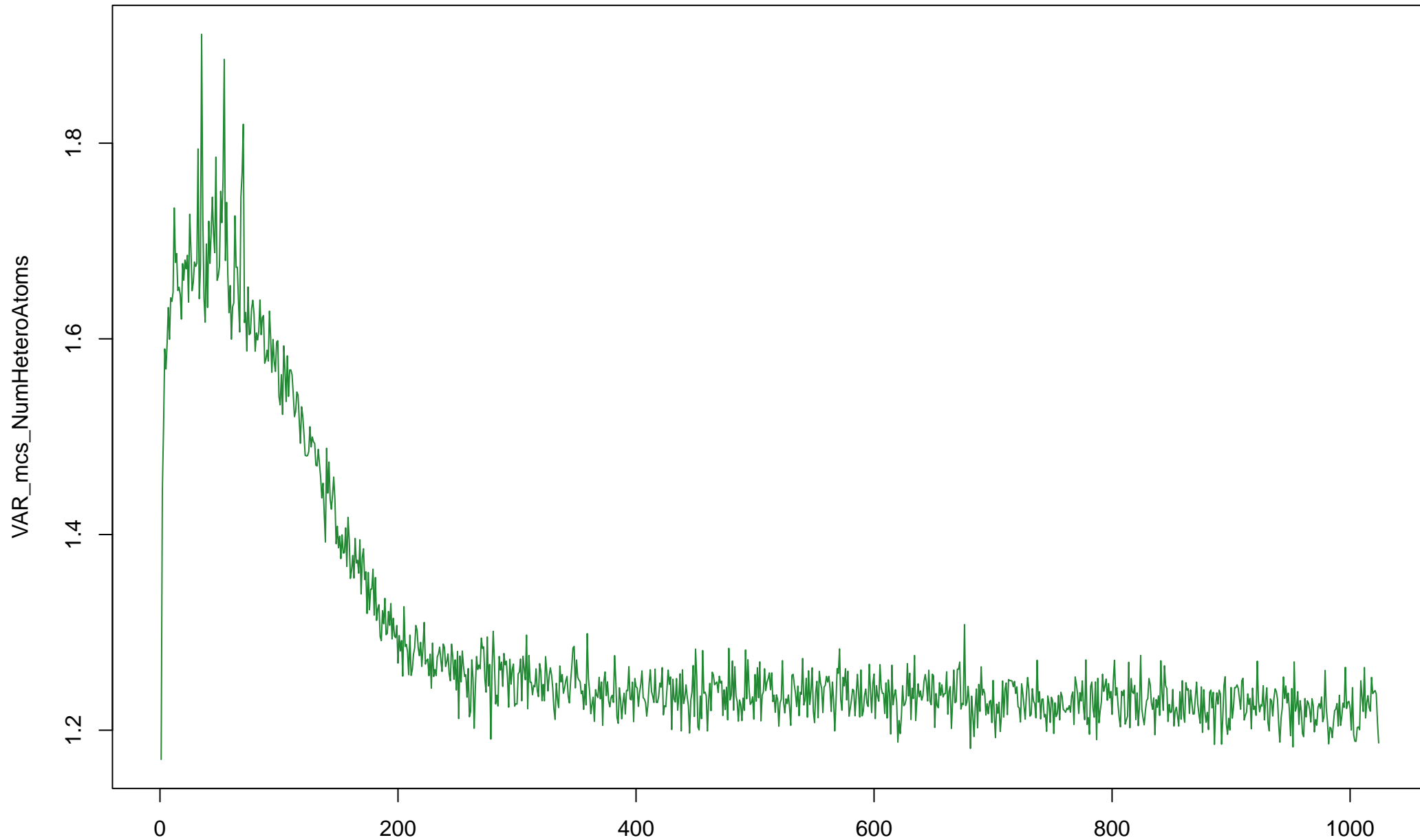
VAR_log_mcs_unbonded_polar_sasa
ESS = 843 | BMK = 0.0786 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0



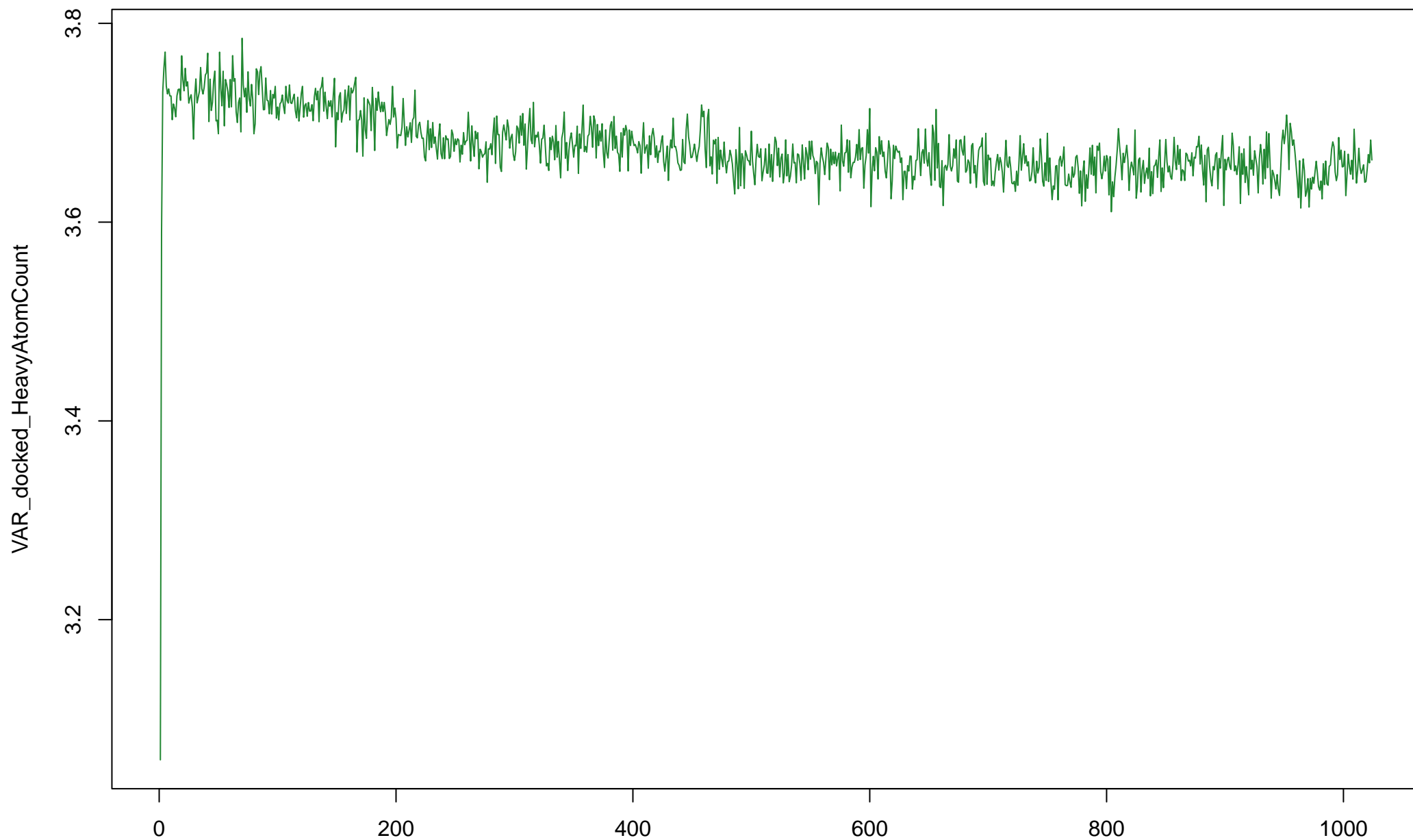
VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.628 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 510



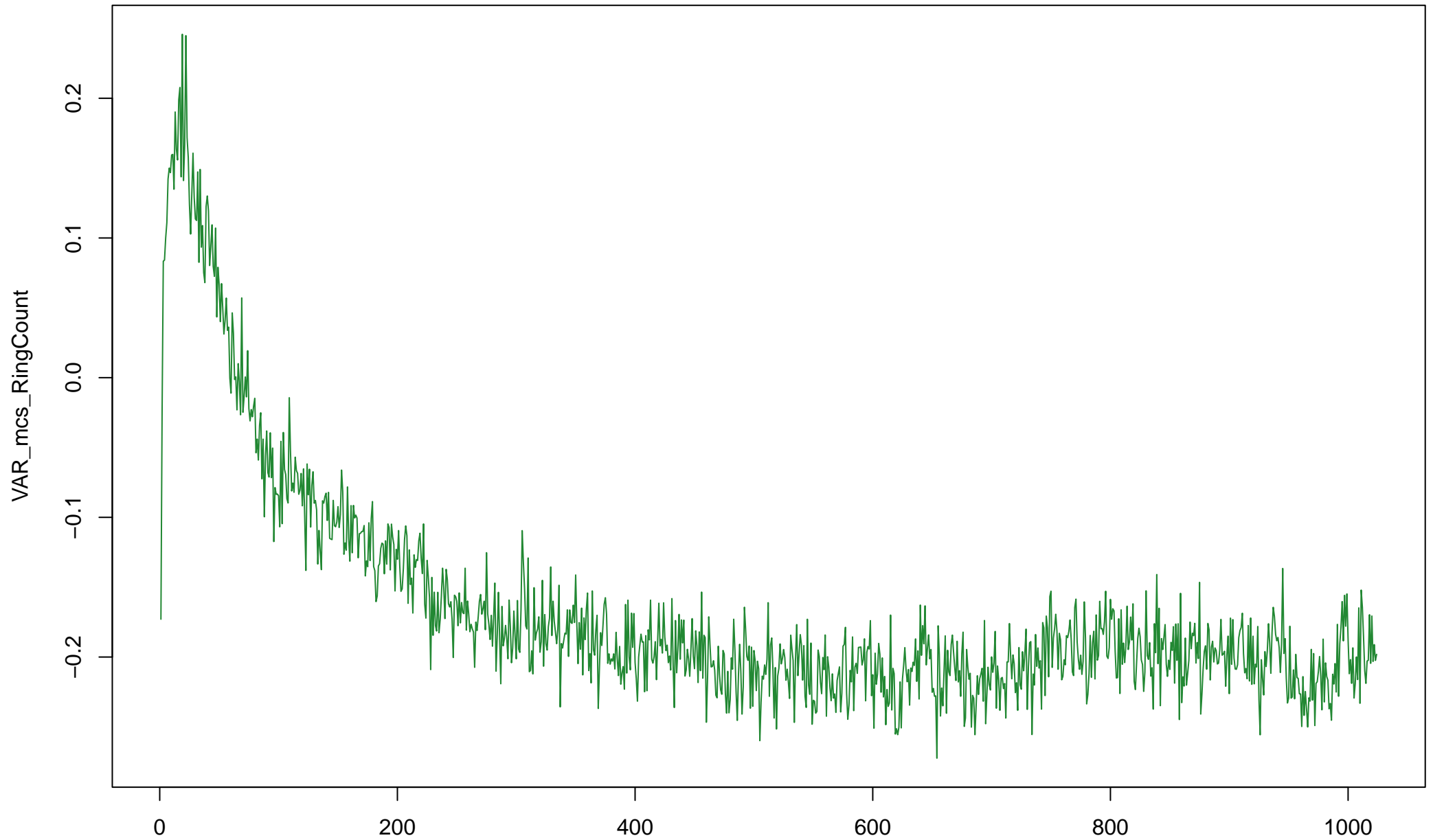
VAR_mcs_NumHeteroAtoms
ESS = 4.82 | BMK = 0.606 | MCSE(6.27) = 17.4 | stat: FALSE | burn: 204



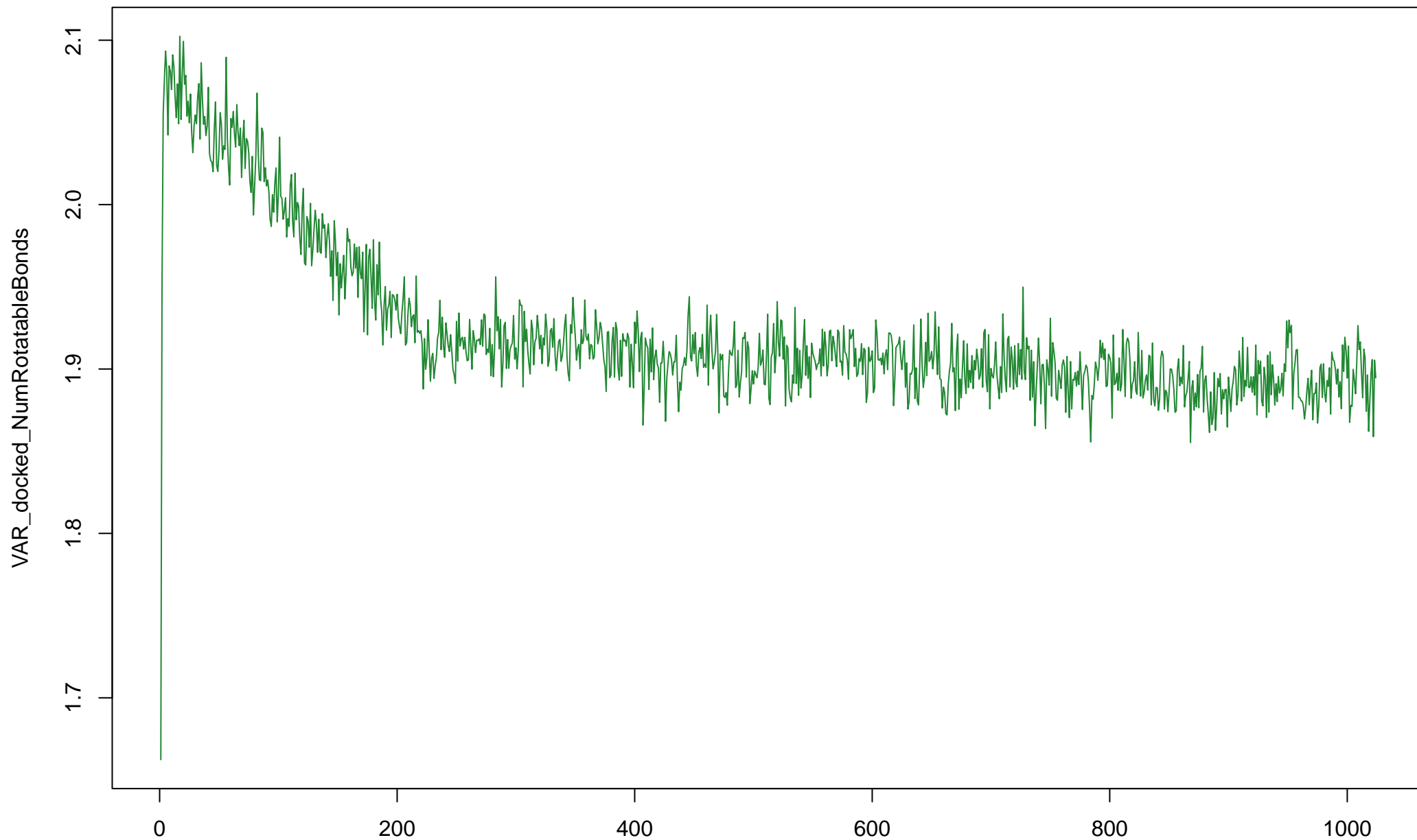
VAR_docked_HeavyAtomCount
ESS = 7.76 | BMK = 0.534 | MCSE(6.27) = 13 | stat: FALSE | burn: 204



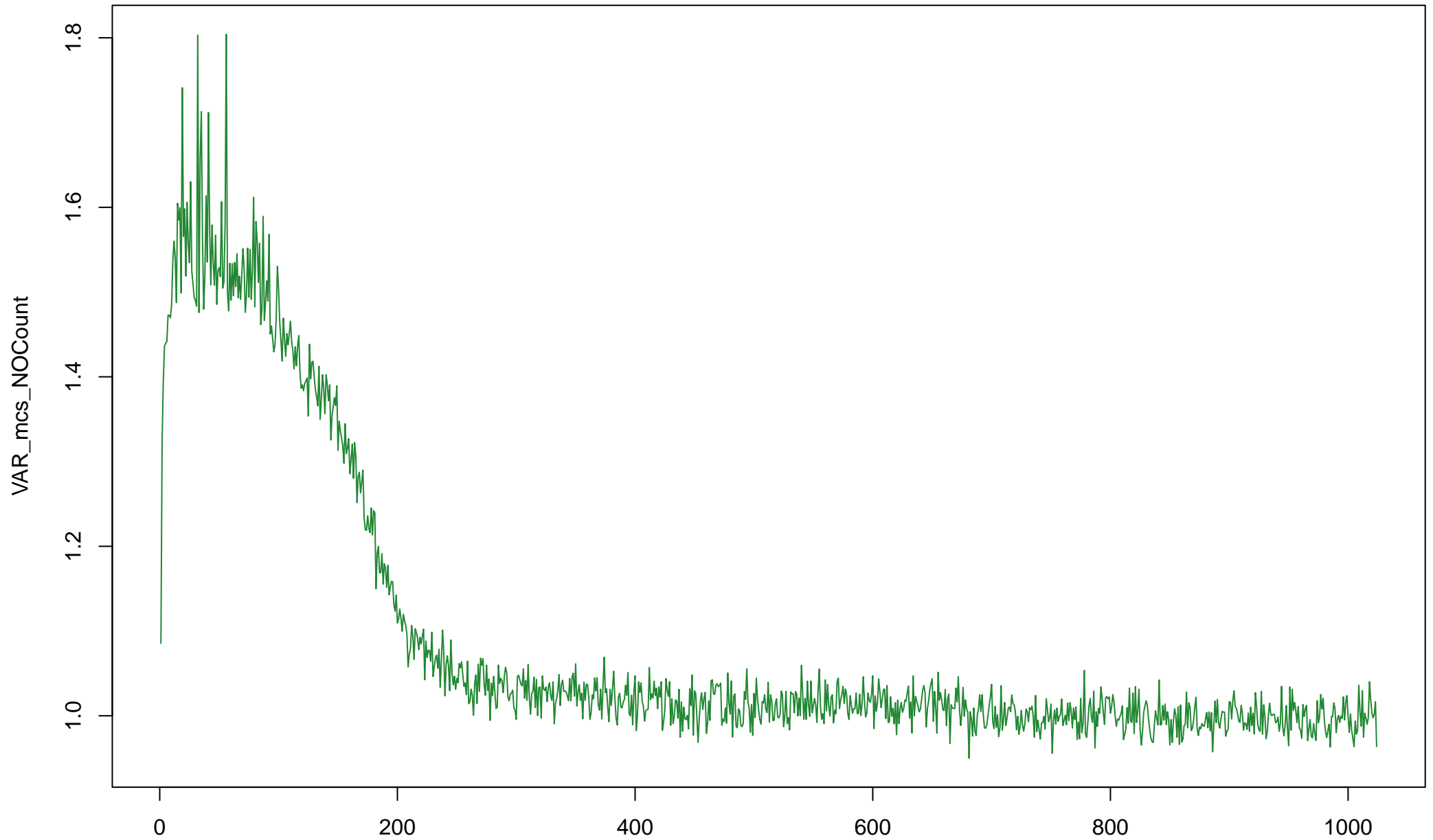
VAR_mcs_RingCount
ESS = 4.6 | BMK = 0.53 | MCSE(6.27) = 17.2 | stat: FALSE | burn: 204



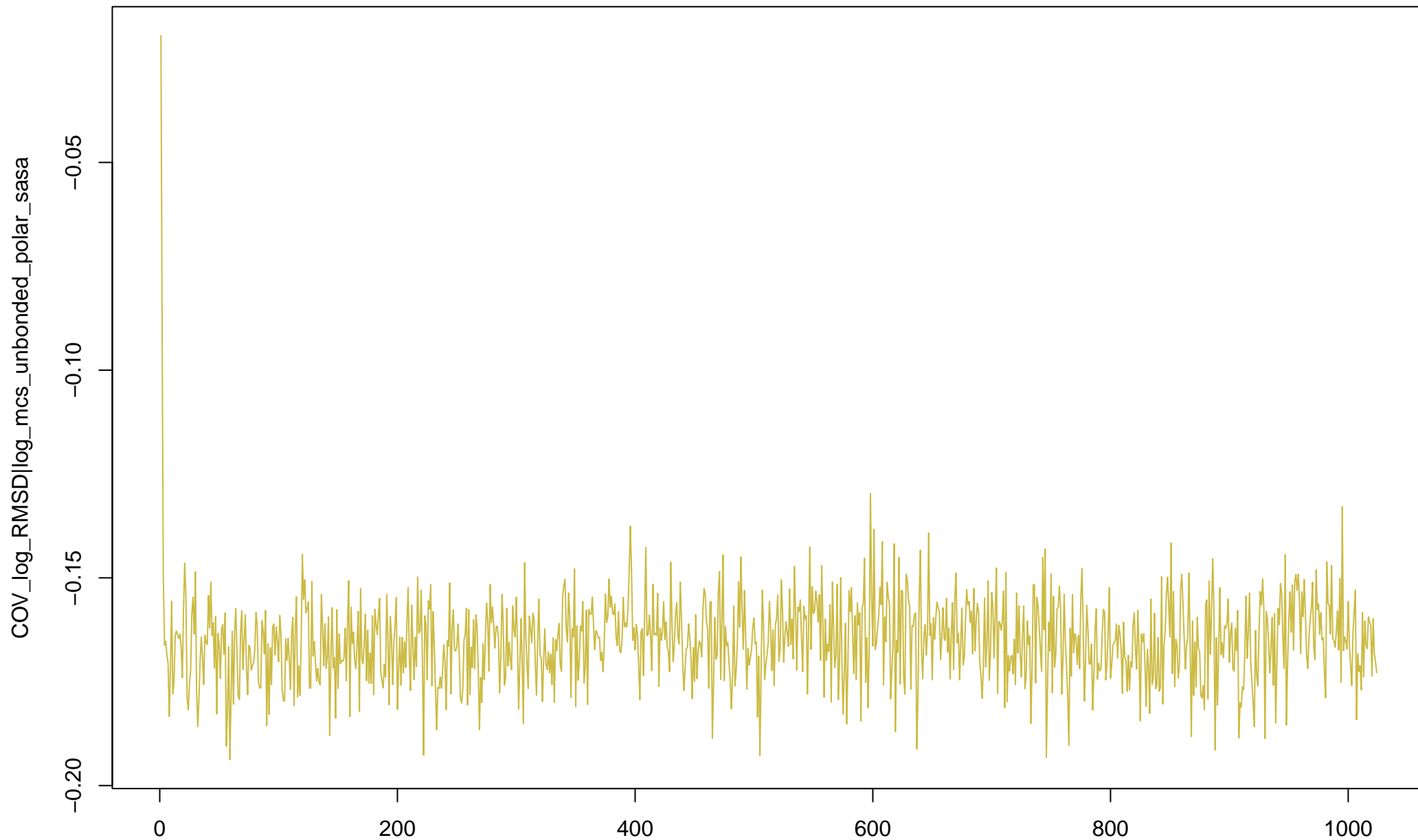
VAR_docked_NumRotatableBonds
ESS = 5.15 | BMK = 0.52 | MCSE(6.27) = 16.5 | stat: FALSE | burn: 204



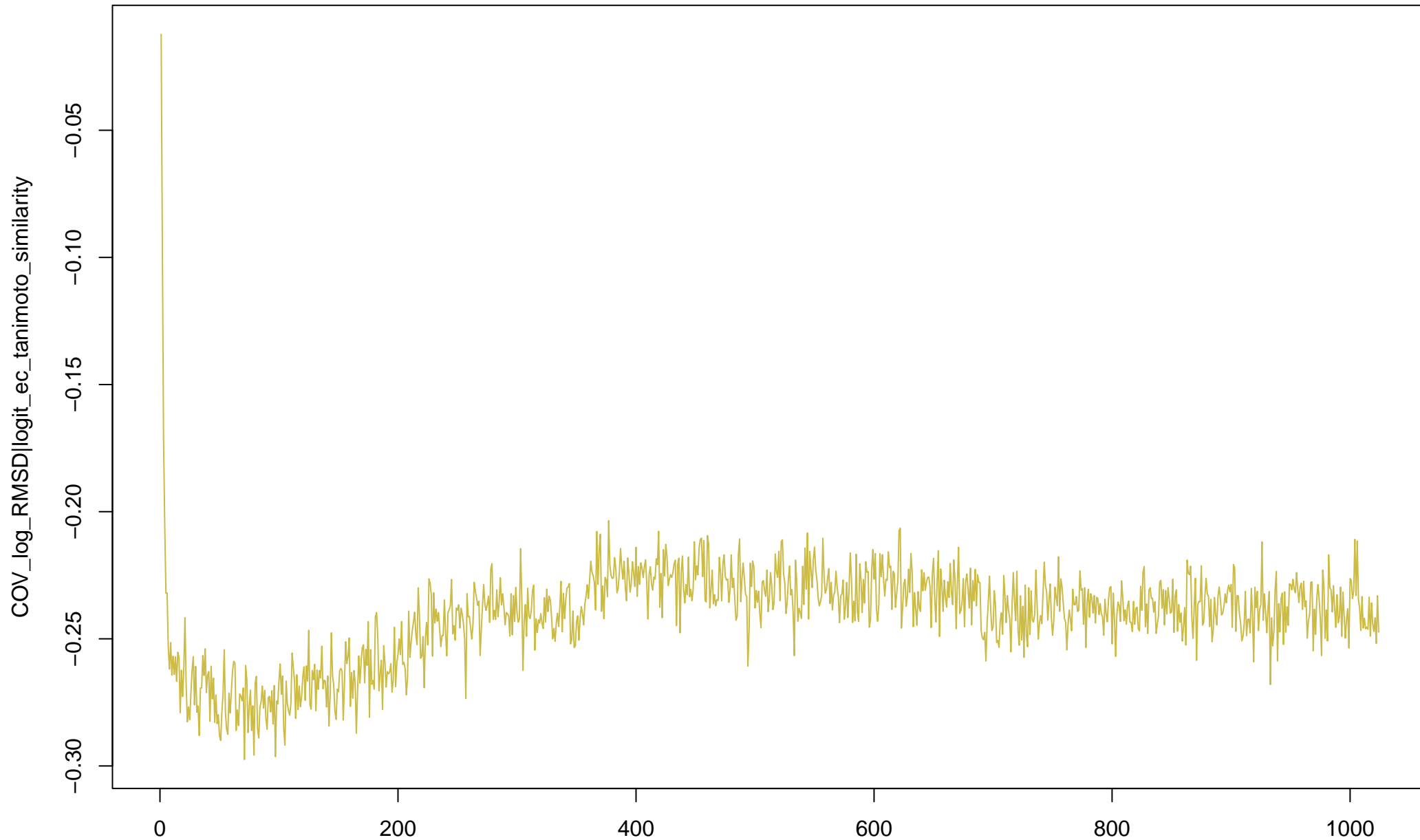
VAR_mcs_NOCount
ESS = 2.9 | BMK = 0.666 | MCSE(6.27) = 17.5 | stat: FALSE | burn: 204



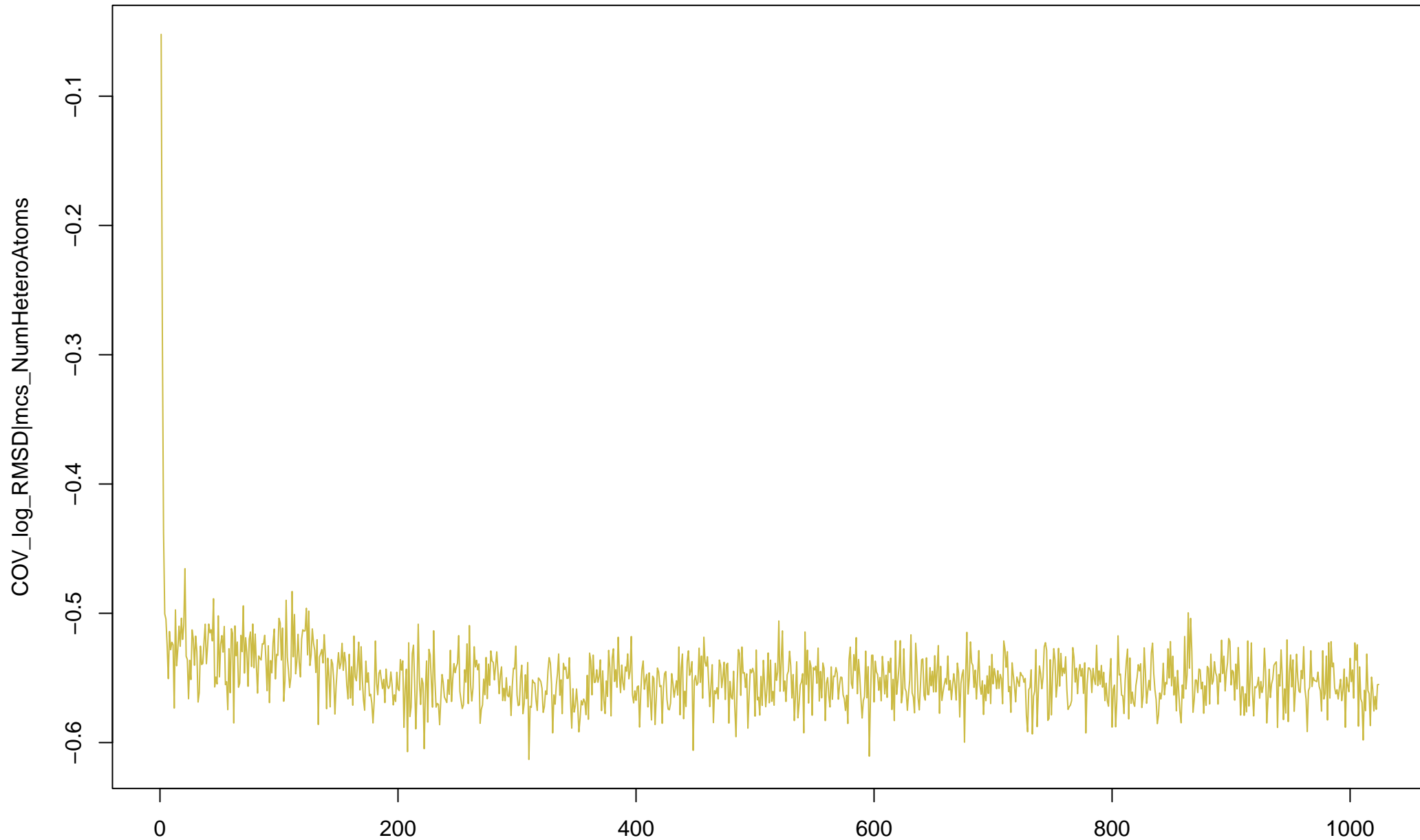
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 755 | BMK = 0.106 | MCSE(6.27) = 4.28 | stat: TRUE | burn: 0



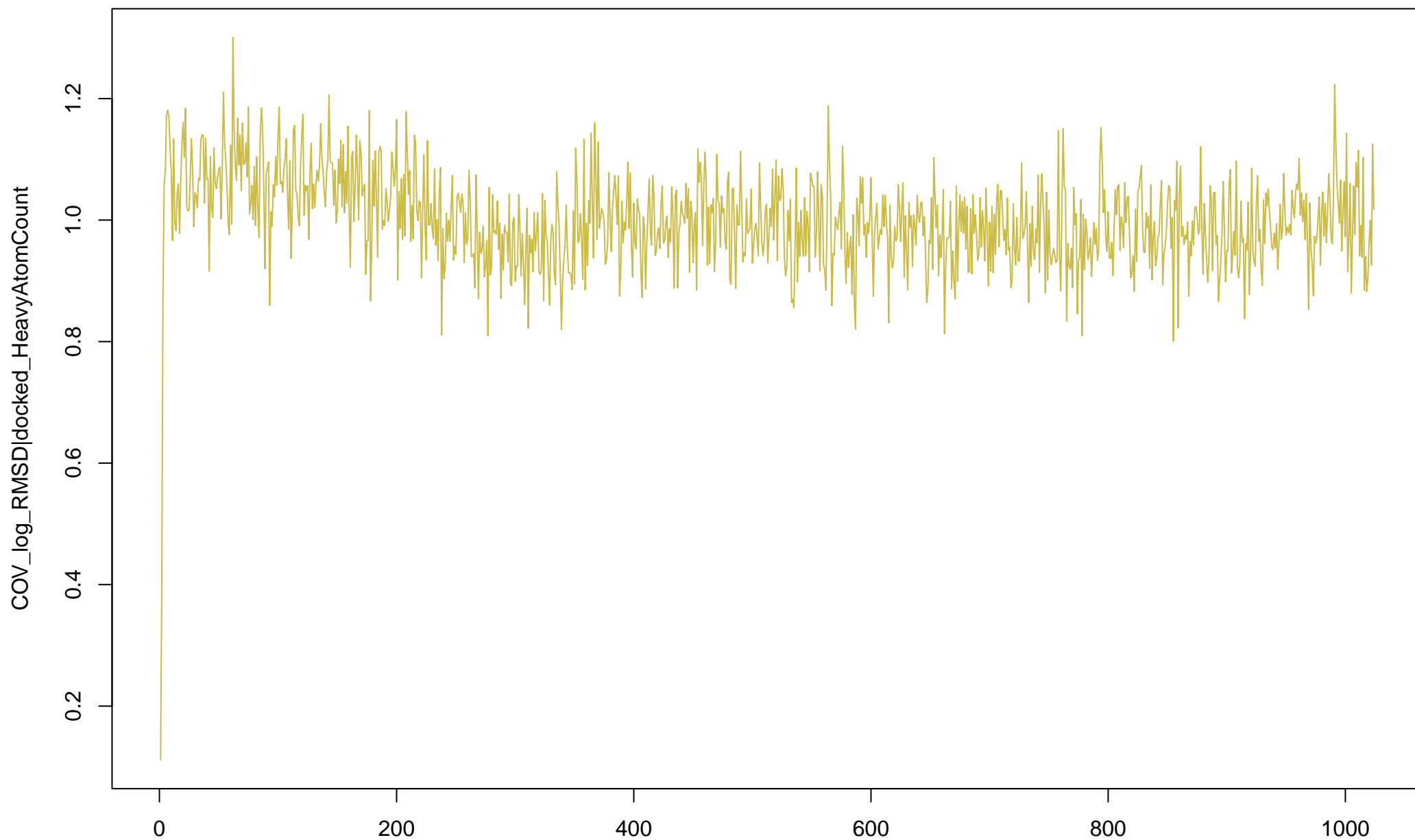
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 13.5 | BMK = 0.411 | MCSE(6.27) = 13 | stat: FALSE | burn: 204



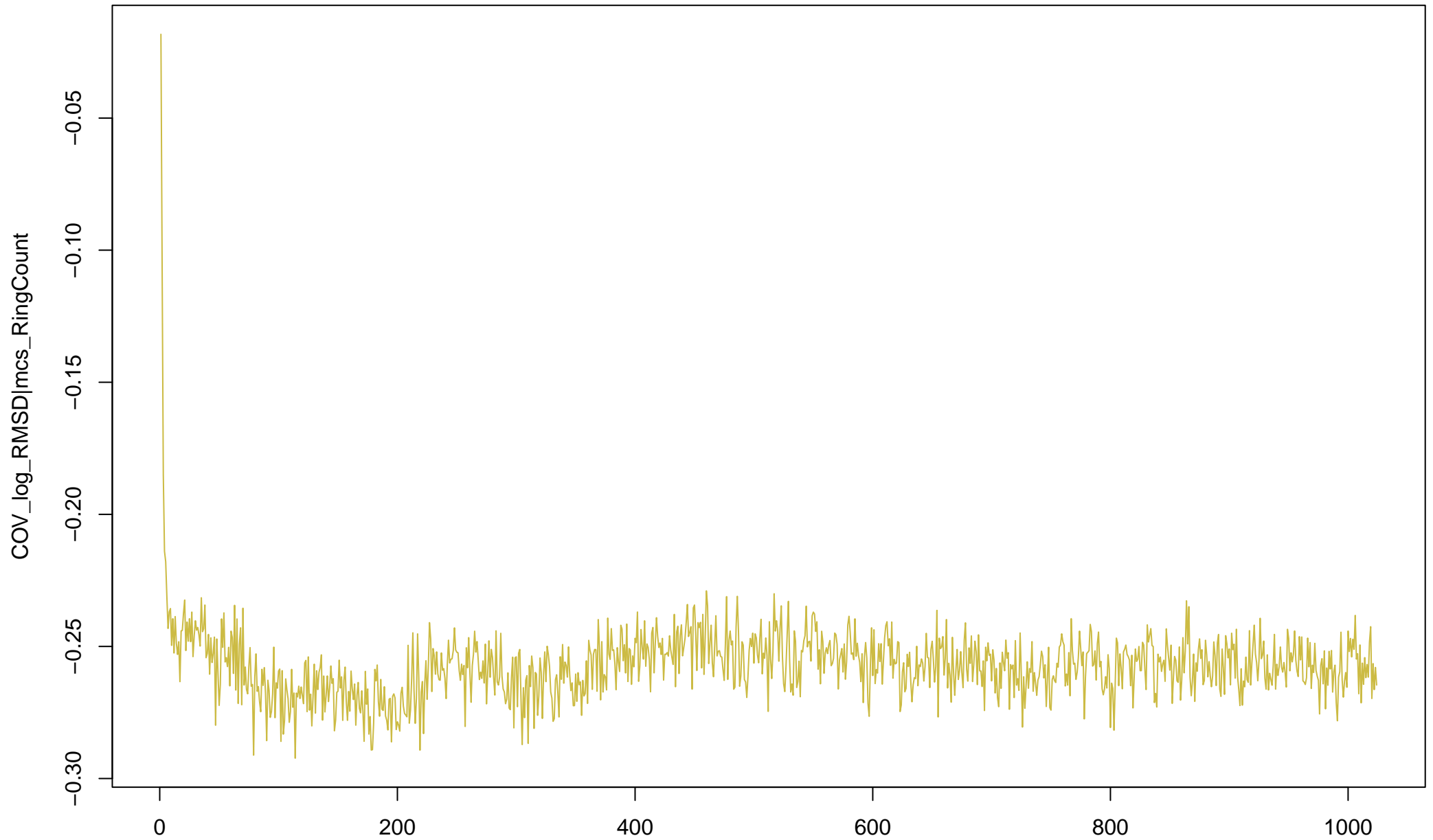
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 92.7 | BMK = 0.155 | MCSE(6.27) = 7.75 | stat: FALSE | burn: 0



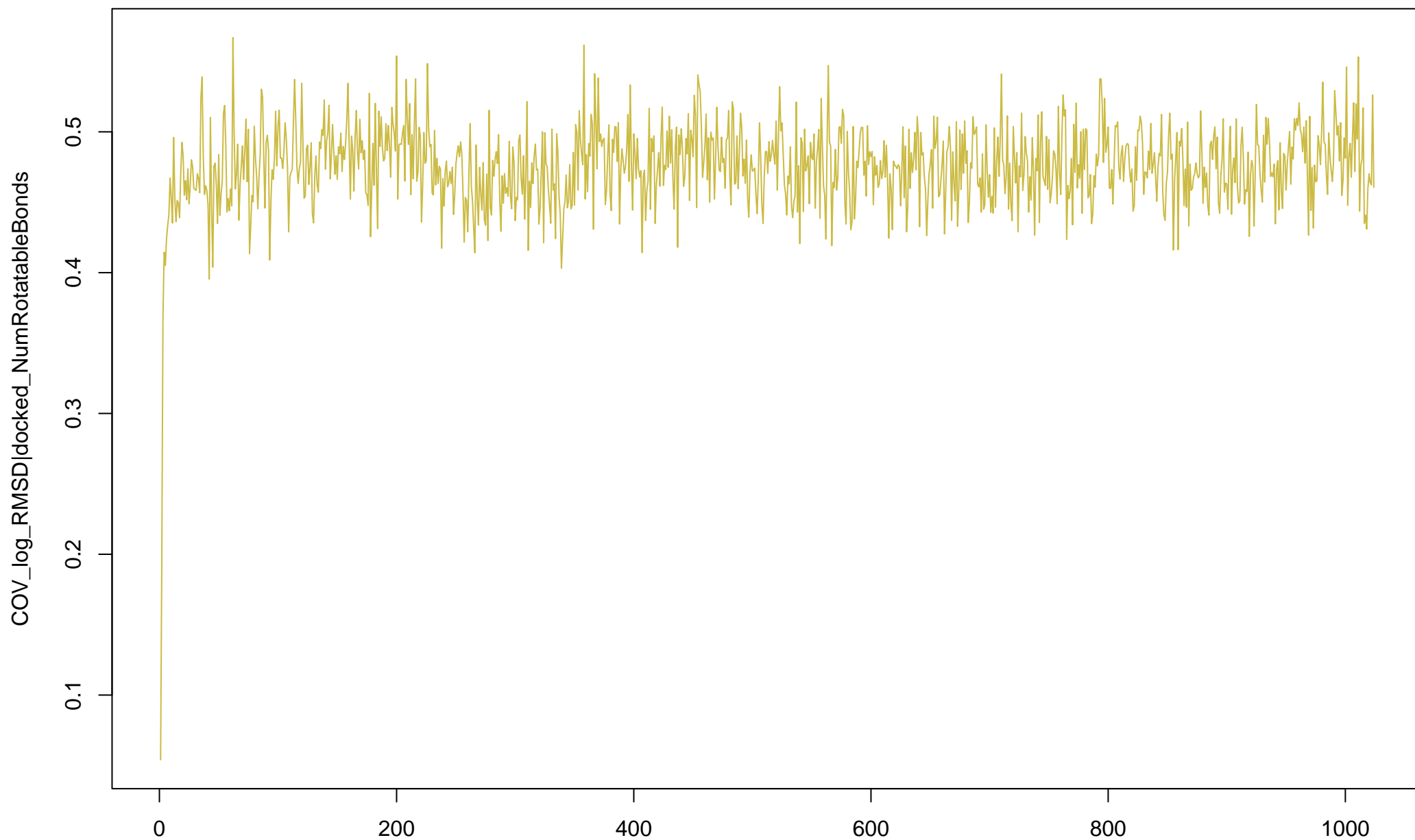
COV_log_RMSD|docked_HeavyAtomCount
ESS = 66.7 | BMK = 0.197 | MCSE(6.27) = 7.66 | stat: FALSE | burn: 0



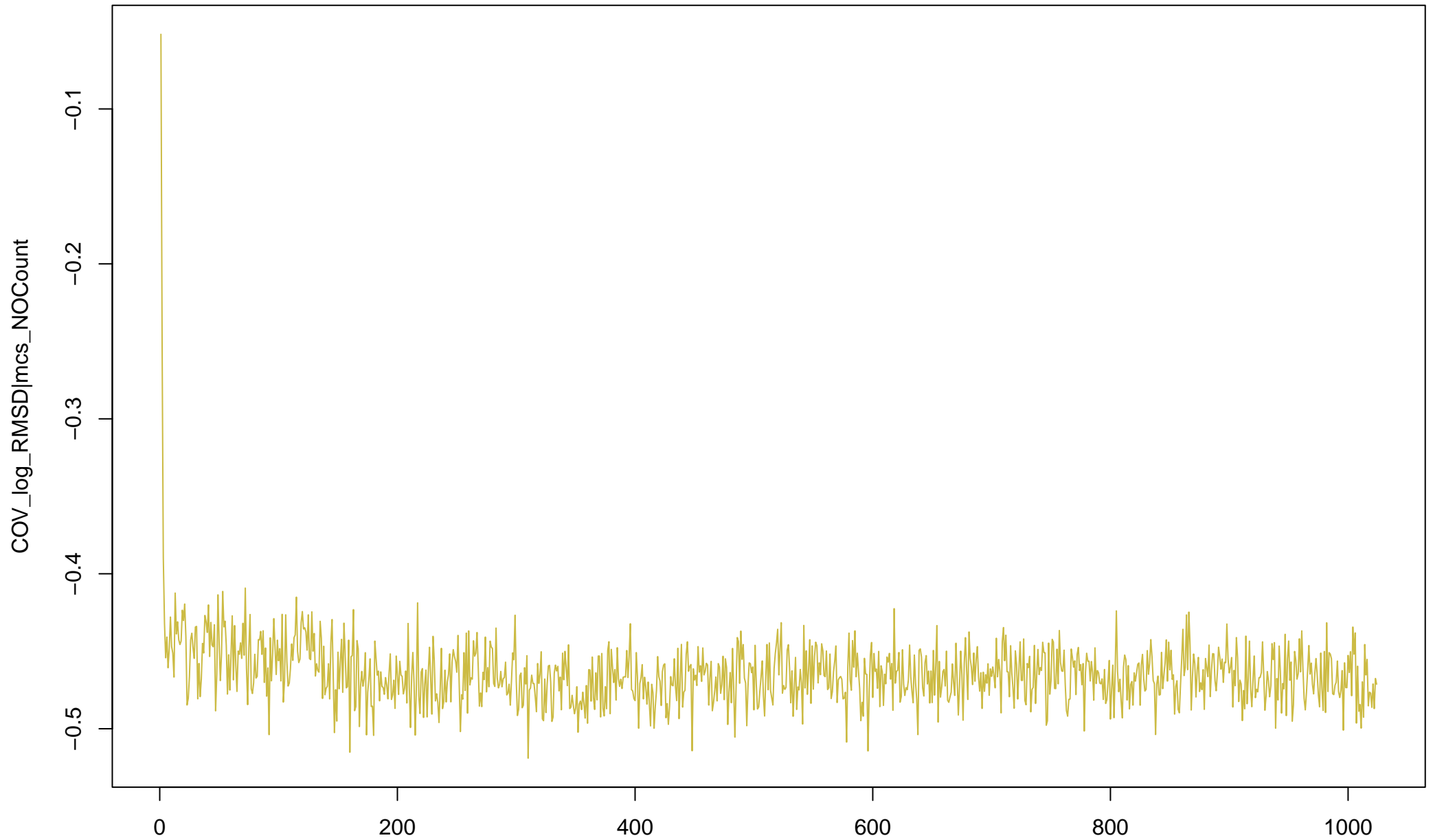
COV_log_RMSD|mcs_RingCount
ESS = 125 | BMK = 0.196 | MCSE(6.27) = 9.67 | stat: TRUE | burn: 102



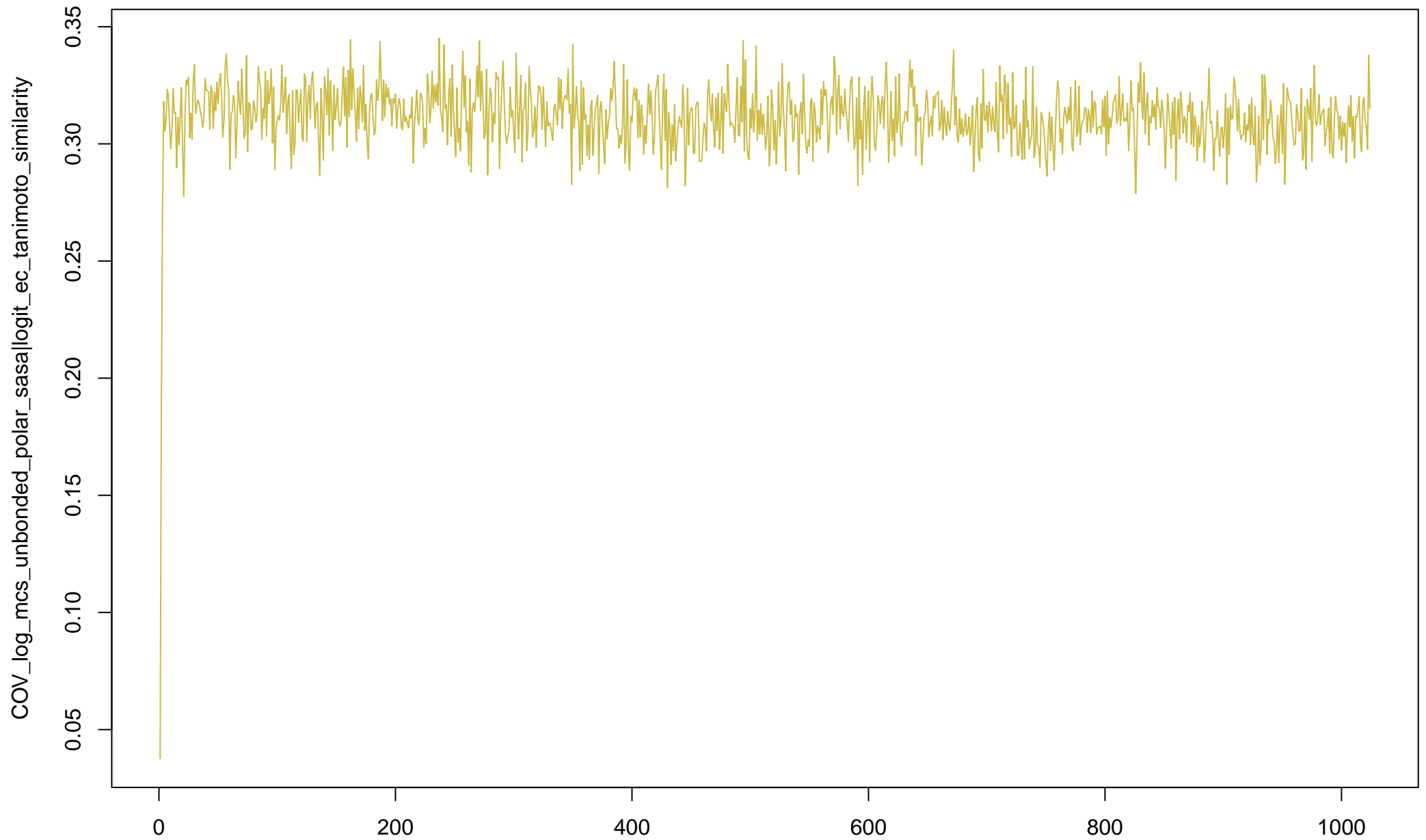
COV_log_RMSD|docked_NumRotatableBonds
ESS = 358 | BMK = 0.0926 | MCSE(6.27) = 6.37 | stat: TRUE | burn: 0



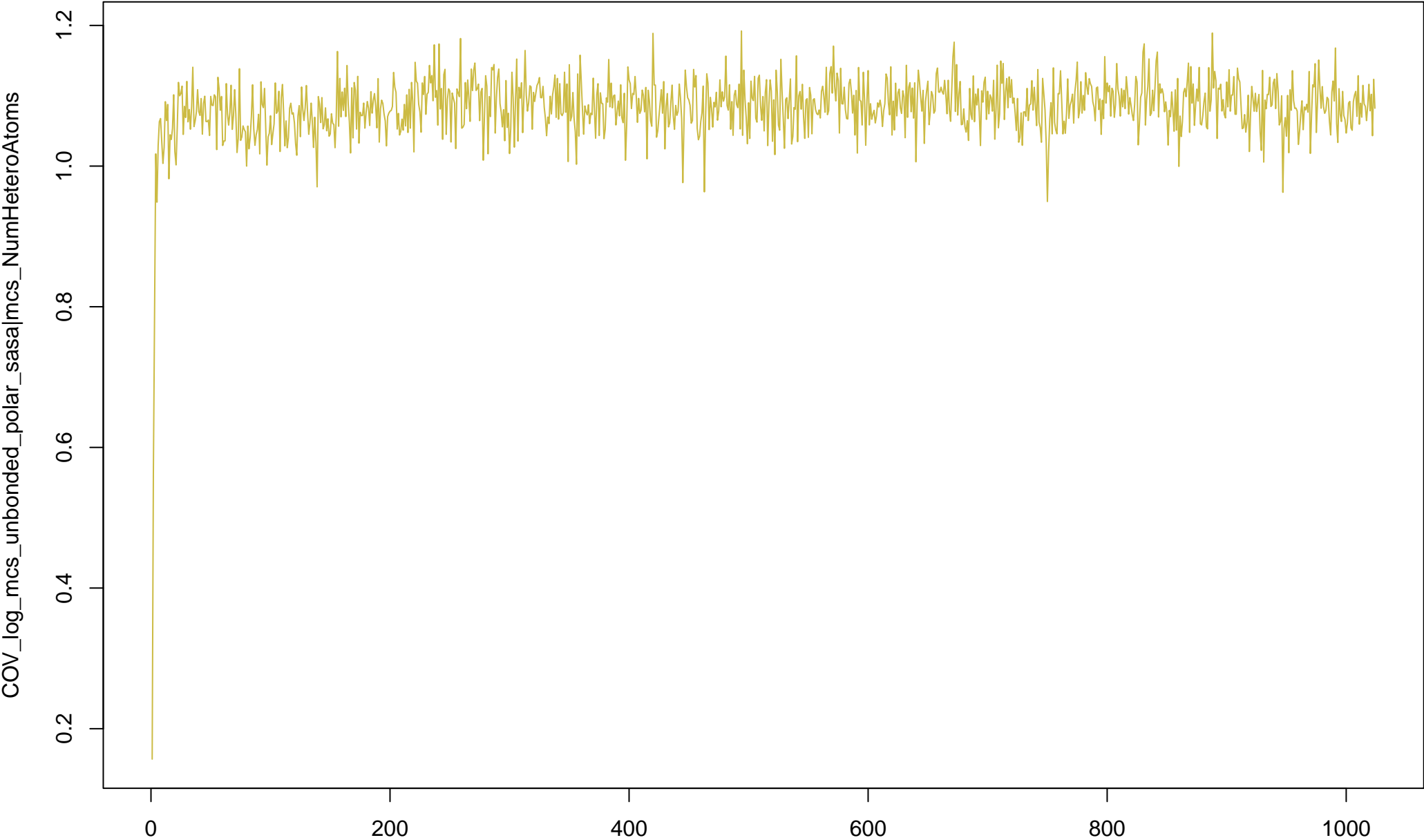
COV_log_RMSD|mcs_NOCount
ESS = 160 | BMK = 0.131 | MCSE(6.27) = 7.2 | stat: FALSE | burn: 0



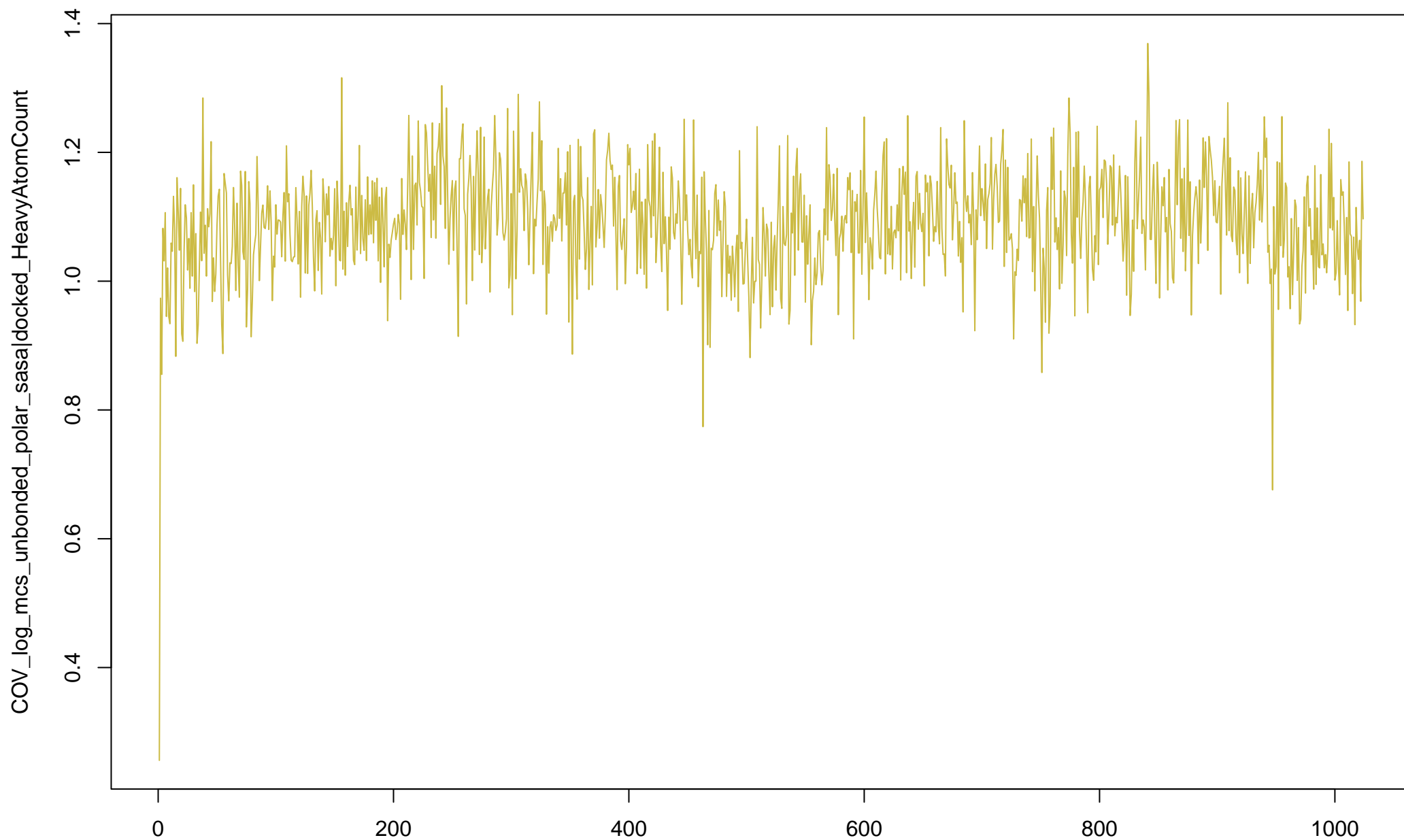
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 698 | BMK = 0.126 | MCSE(6.27) = 4.68 | stat: TRUE | burn: 0



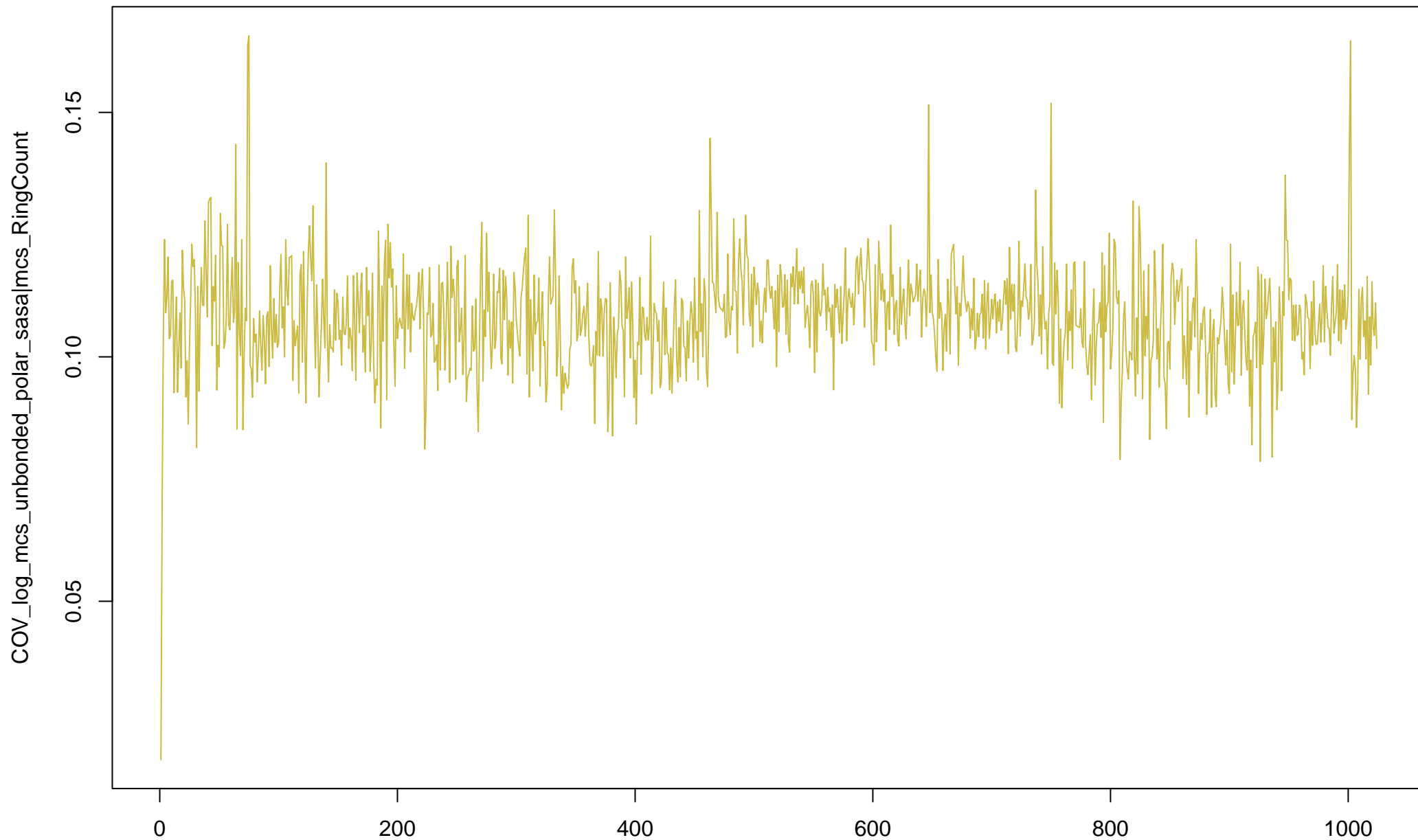
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 357 | BMK = 0.112 | MCSE(6.27) = 6.32 | stat: FALSE | burn: 0



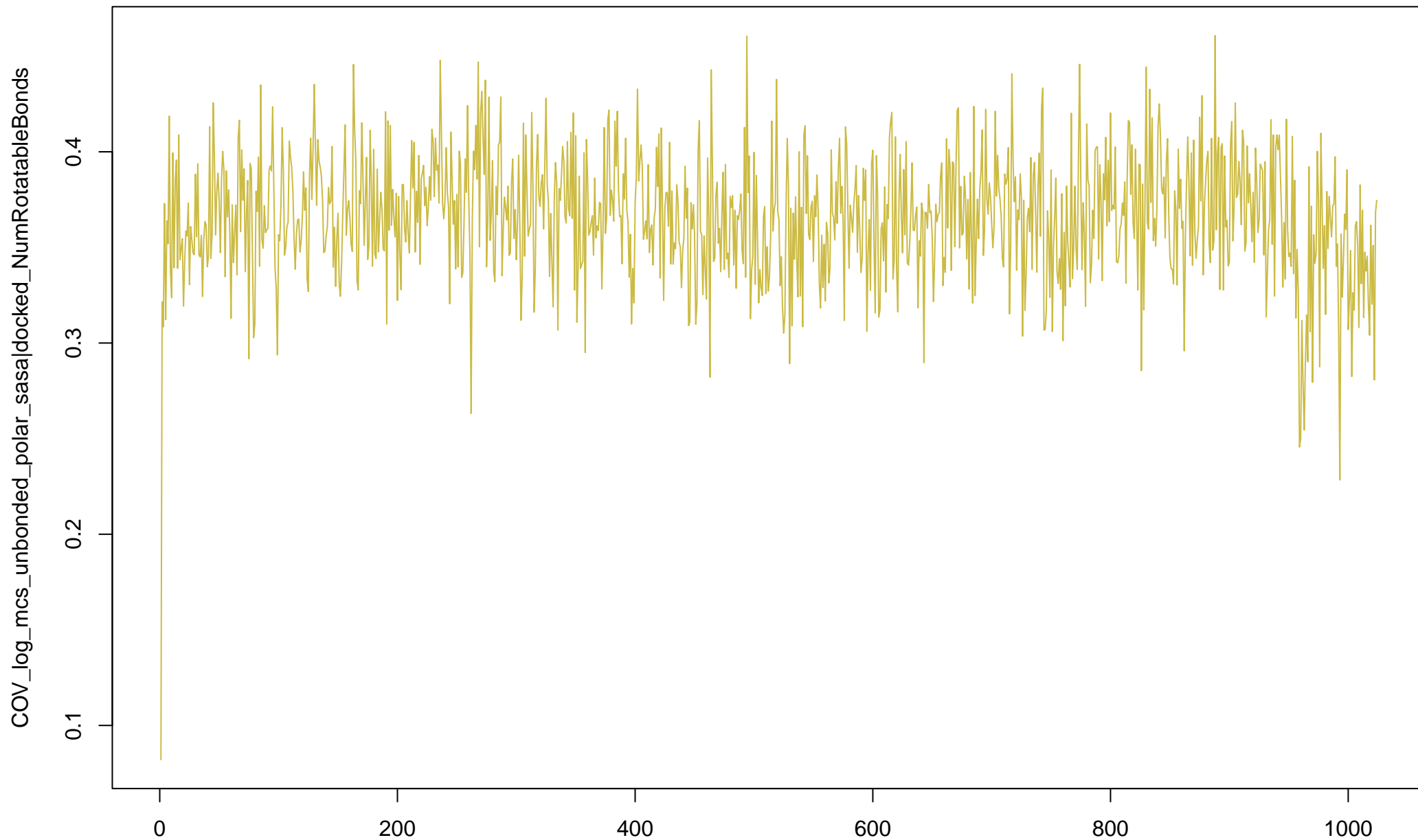
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 93.1 | BMK = 0.0719 | MCSE(6.27) = 6.11 | stat: FALSE | burn: 0



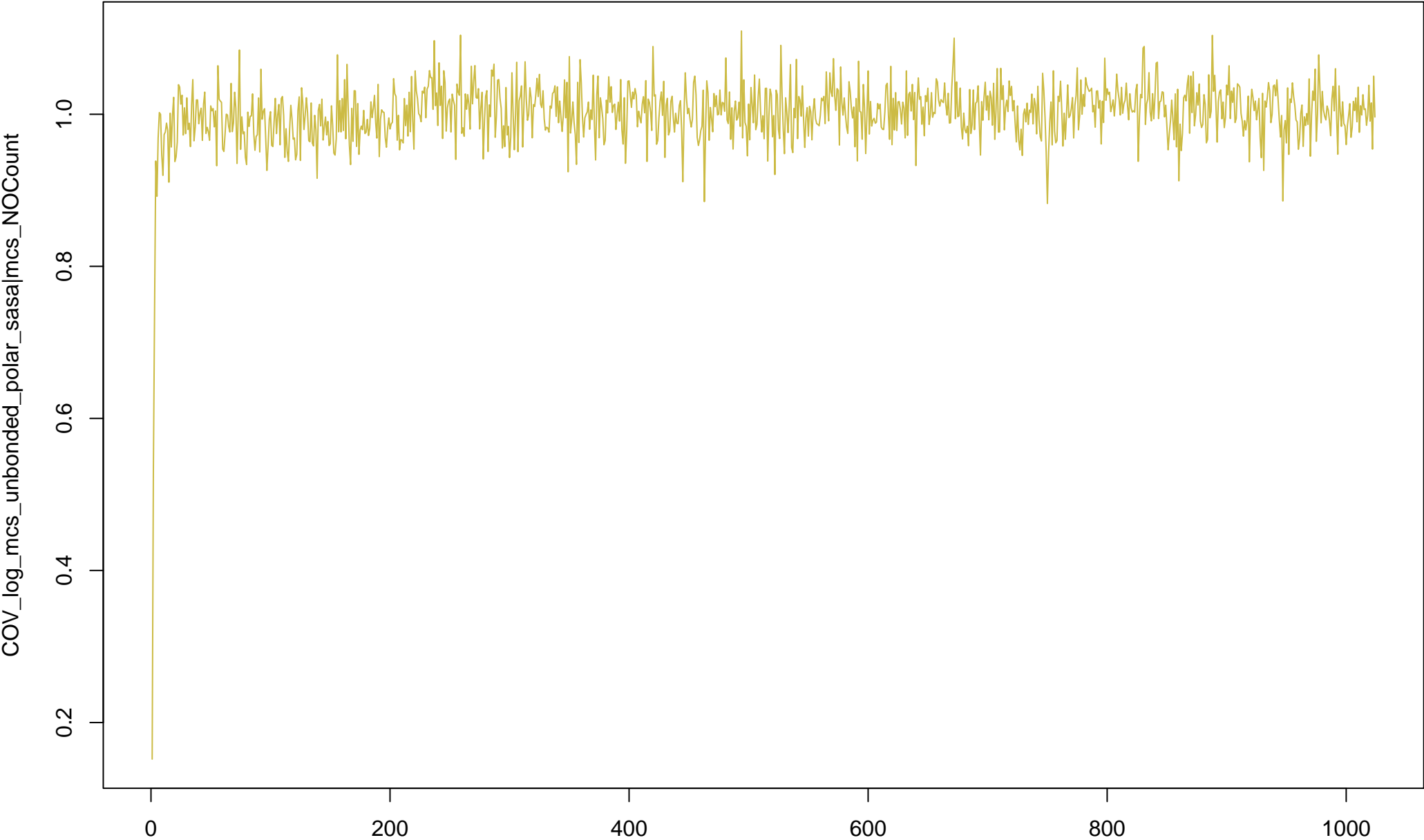
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 738 | BMK = 0.12 | MCSE(6.27) = 5.09 | stat: TRUE | burn: 0



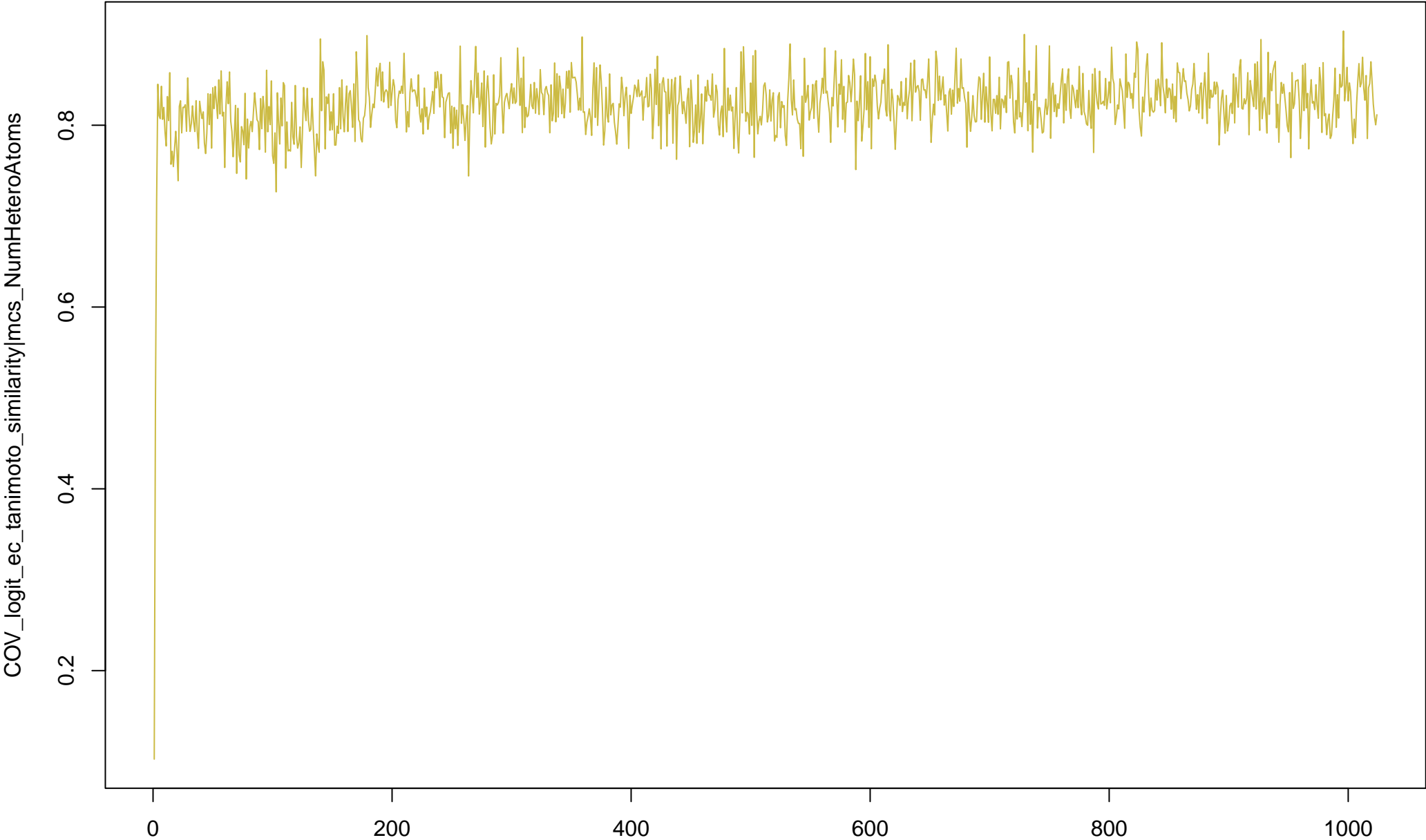
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 323 | BMK = 0.0859 | MCSE(6.27) = 5.51 | stat: TRUE | burn: 0



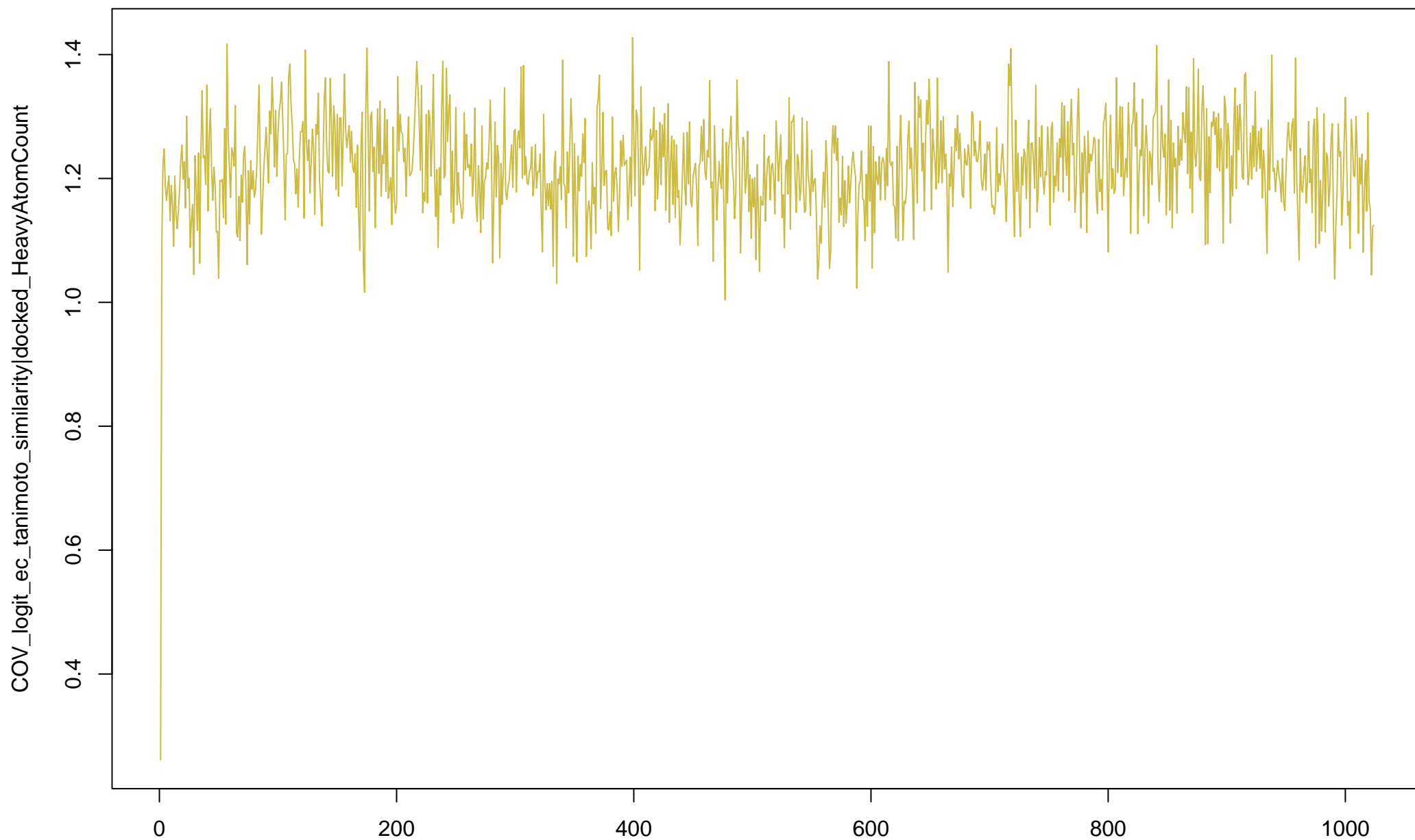
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 394 | BMK = 0.113 | MCSE(6.27) = 6.15 | stat: FALSE | burn: 0



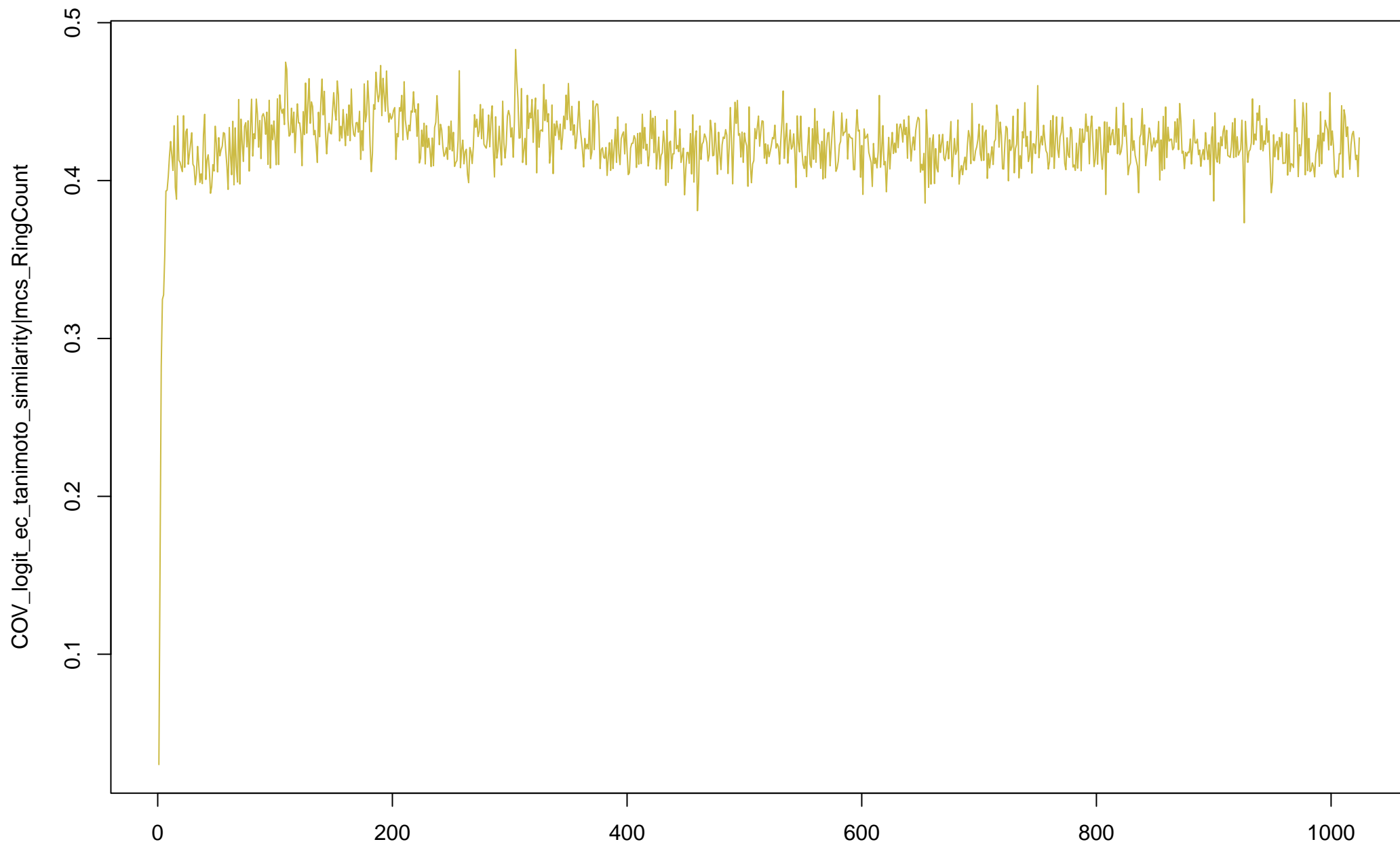
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 498 | BMK = 0.159 | MCSE(6.27) = 6.55 | stat: FALSE | burn: 0



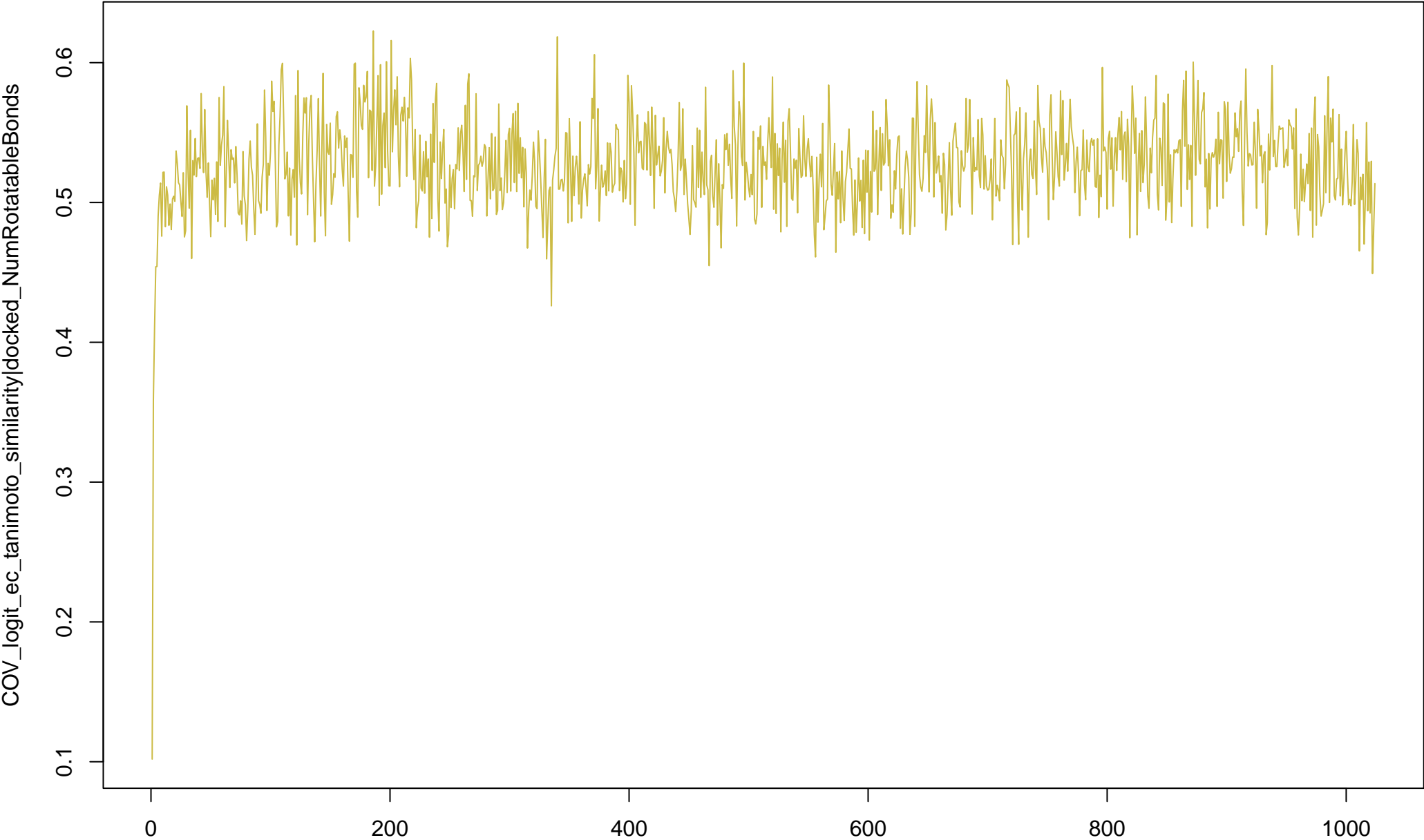
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 231 | BMK = 0.0569 | MCSE(6.27) = 5.82 | stat: TRUE | burn: 0



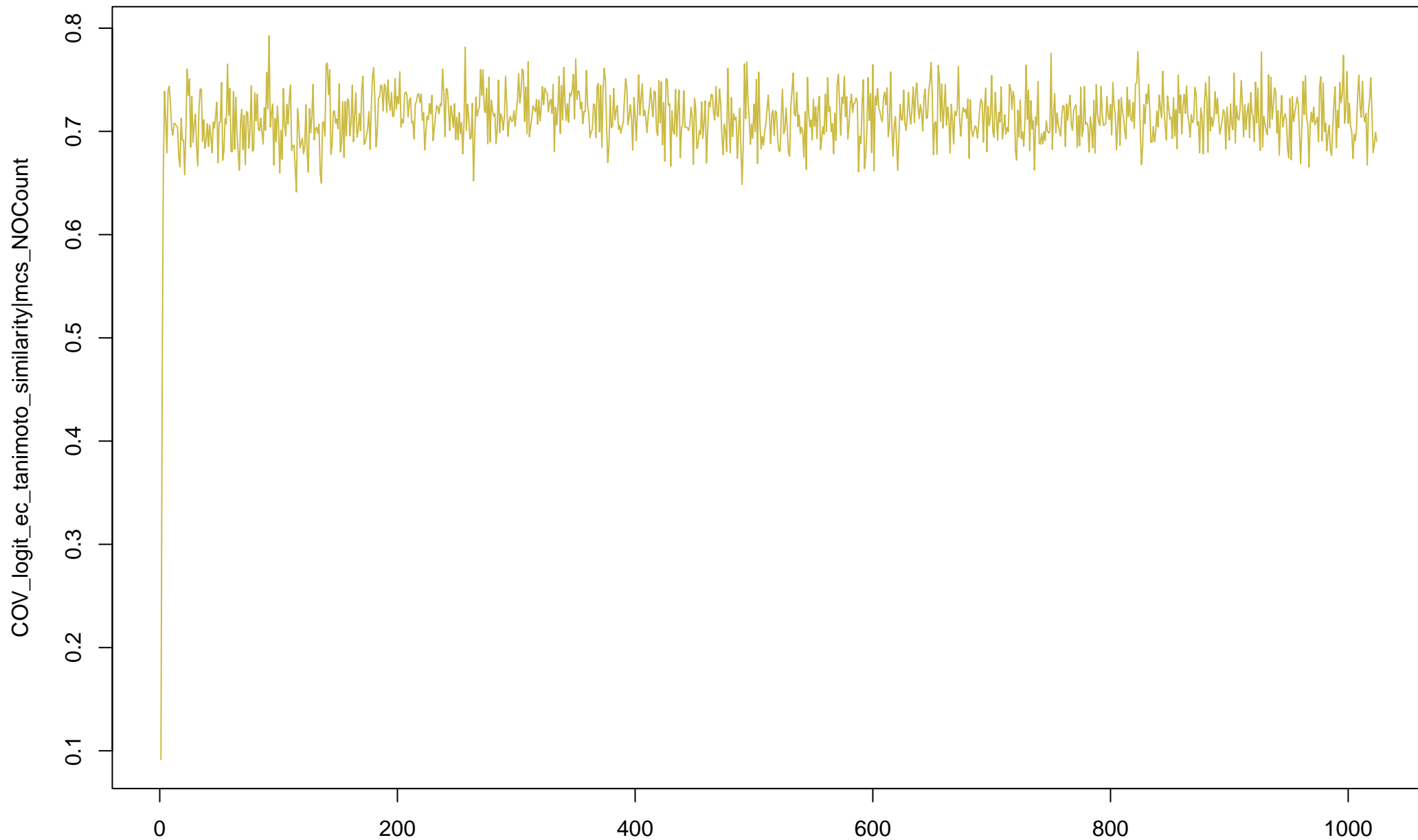
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 227 | BMK = 0.202 | MCSE(6.27) = 8.05 | stat: TRUE | burn: 0



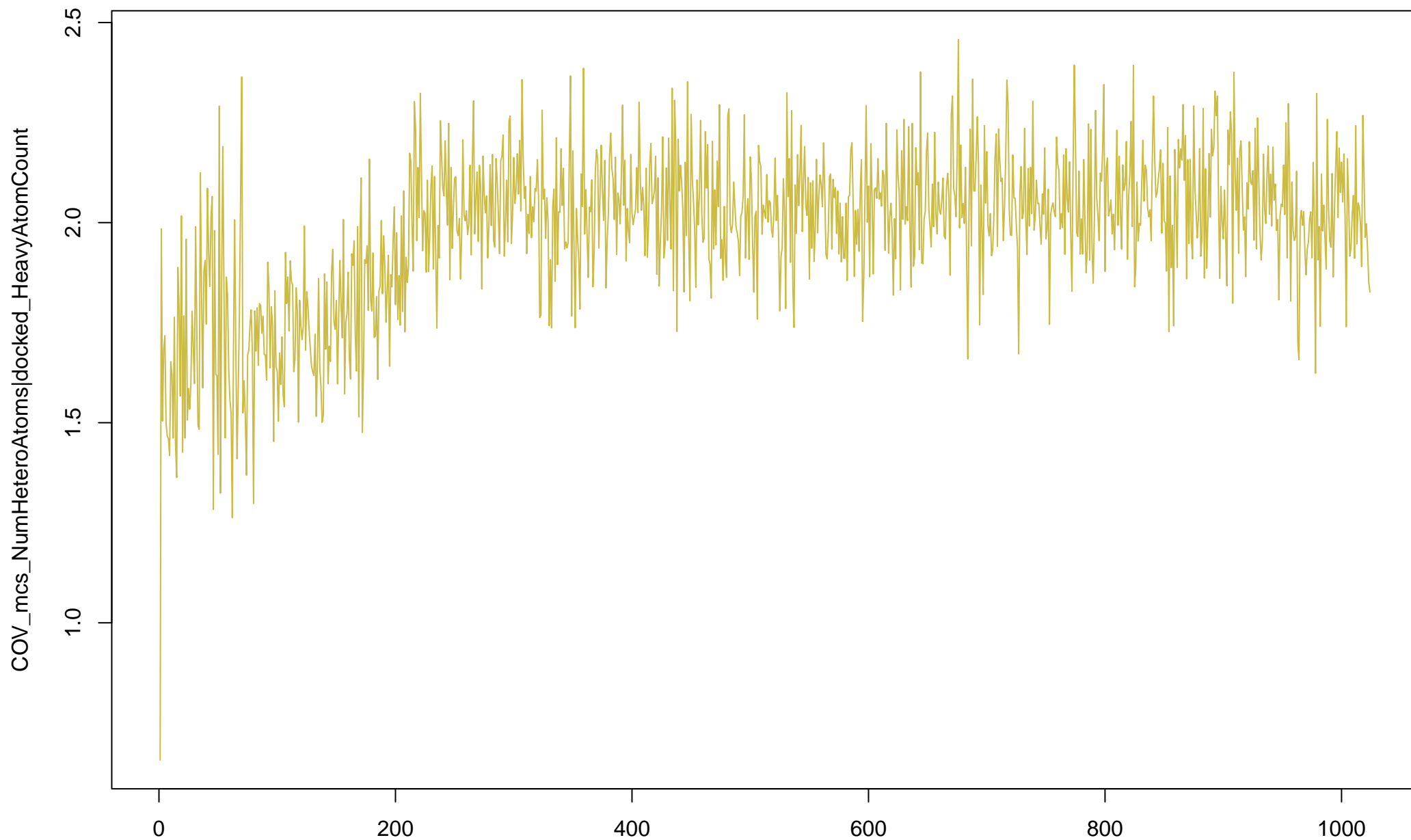
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 243 | BMK = 0.108 | MCSE(6.27) = 6.68 | stat: FALSE | burn: 0



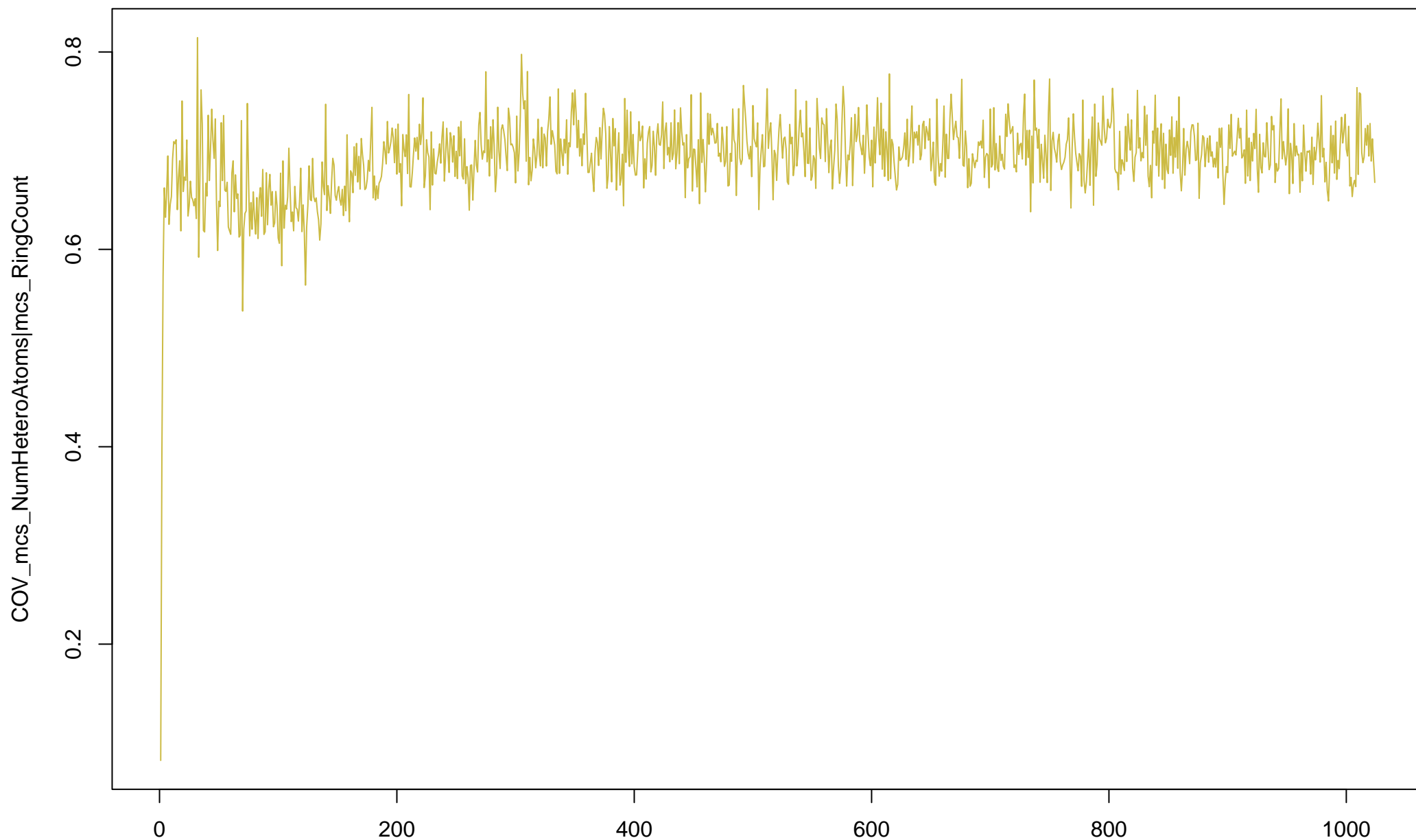
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 663 | BMK = 0.0845 | MCSE(6.27) = 4.96 | stat: TRUE | burn: 0



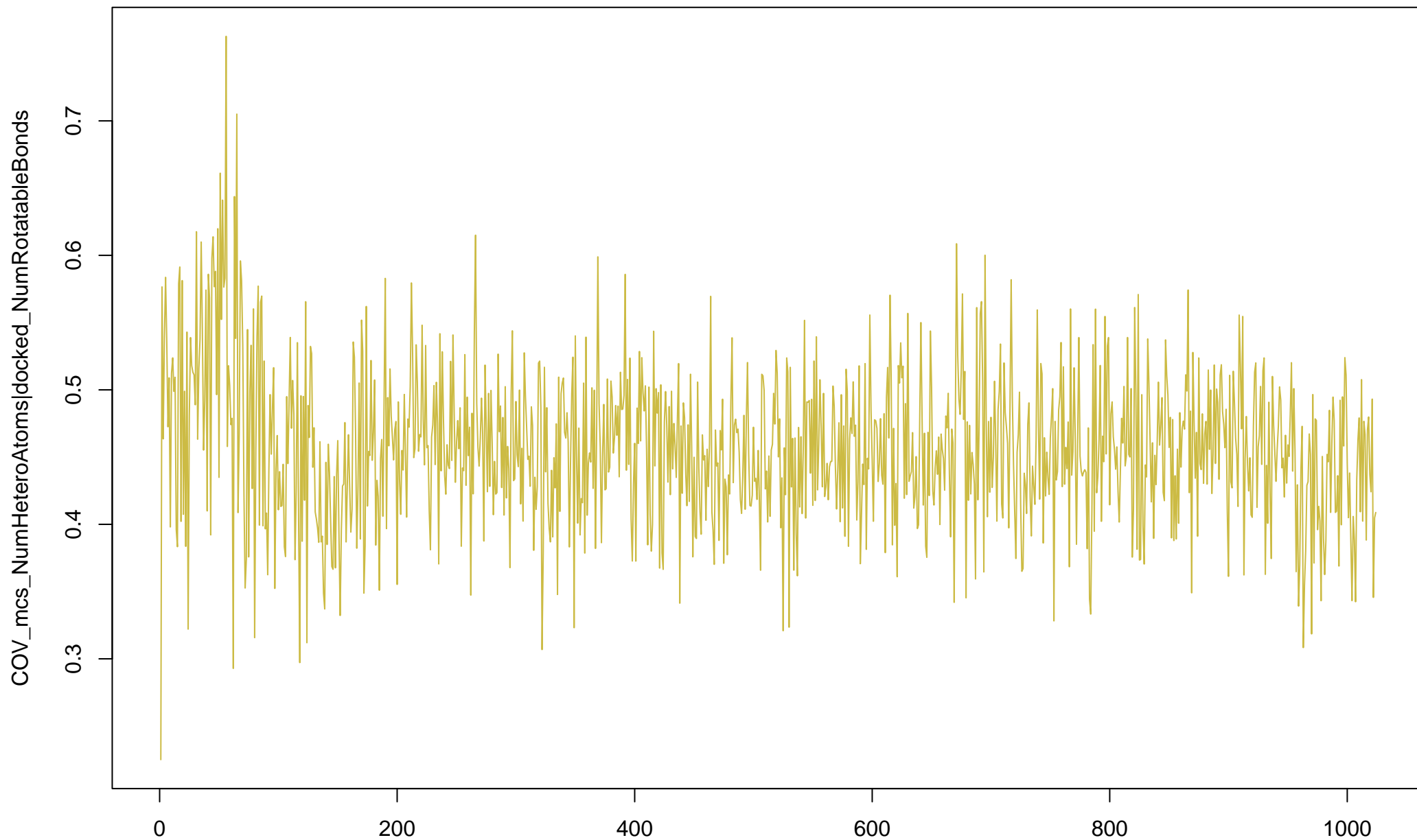
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 15.6 | BMK = 0.311 | MCSE(6.27) = 12 | stat: FALSE | burn: 204



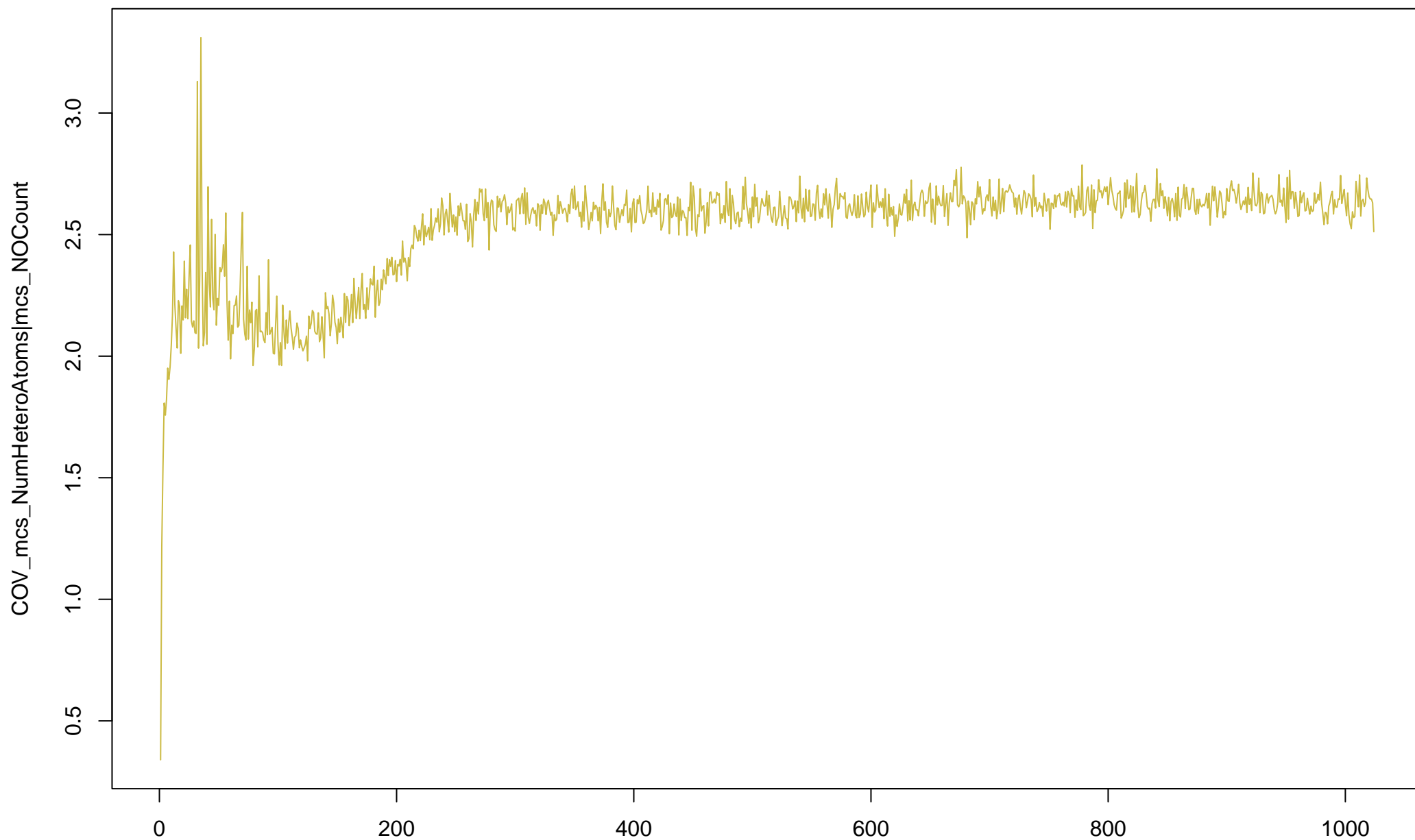
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 37.8 | BMK = 0.262 | MCSE(6.27) = 9.08 | stat: FALSE | burn: 0



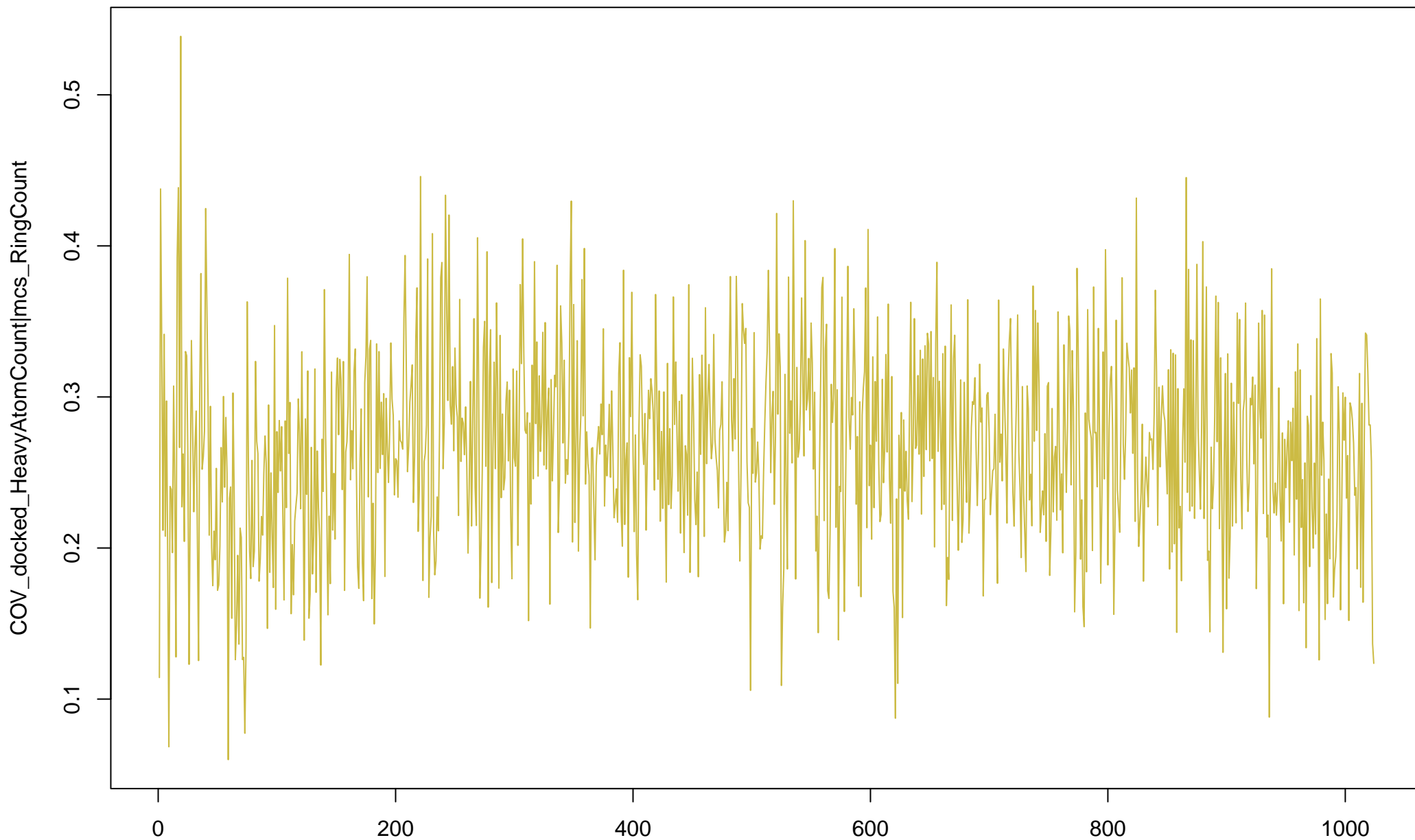
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 168 | BMK = 0.115 | MCSE(6.27) = 6.46 | stat: FALSE | burn: 0



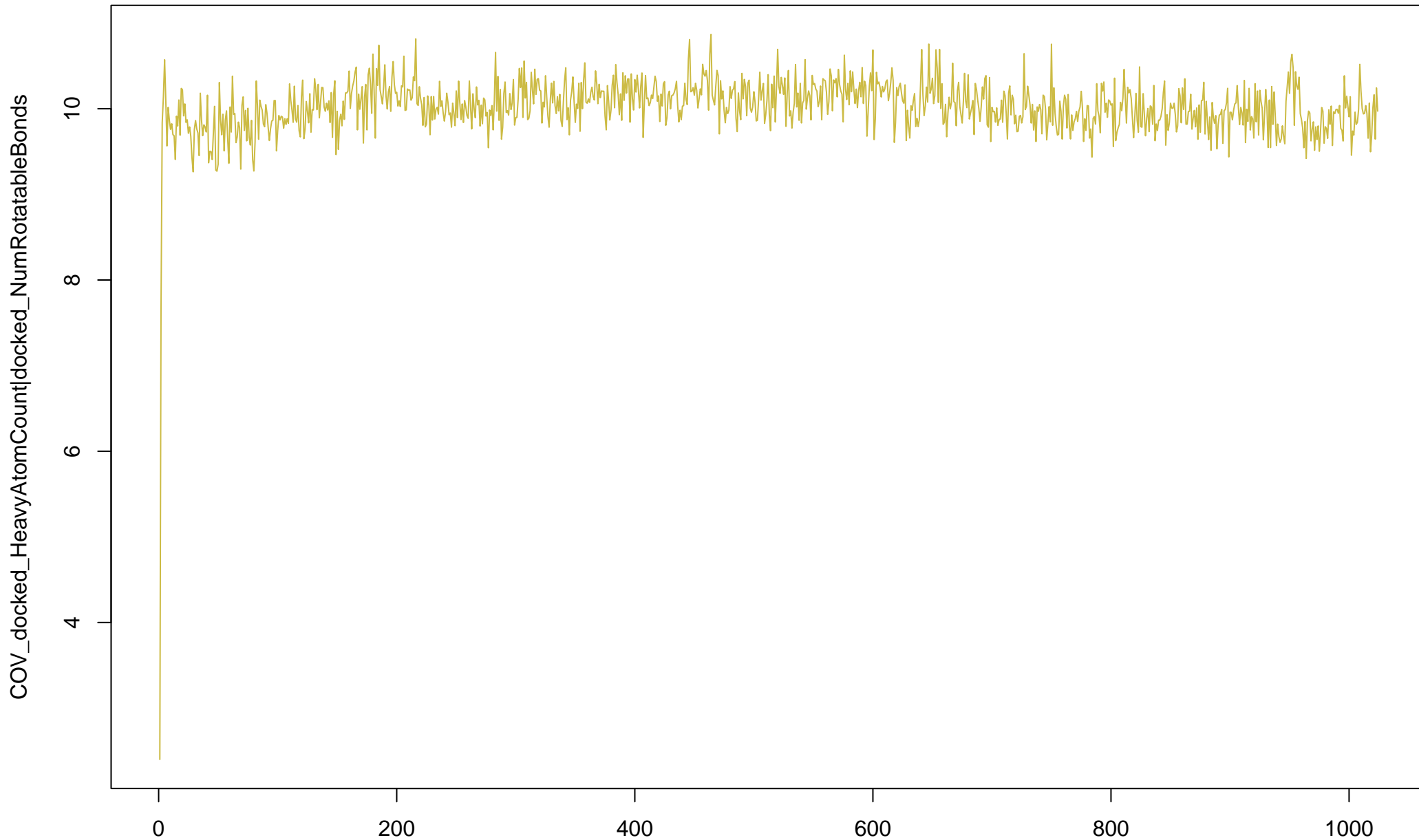
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 6.48 | BMK = 0.554 | MCSE(6.27) = 15.6 | stat: FALSE | burn: 204



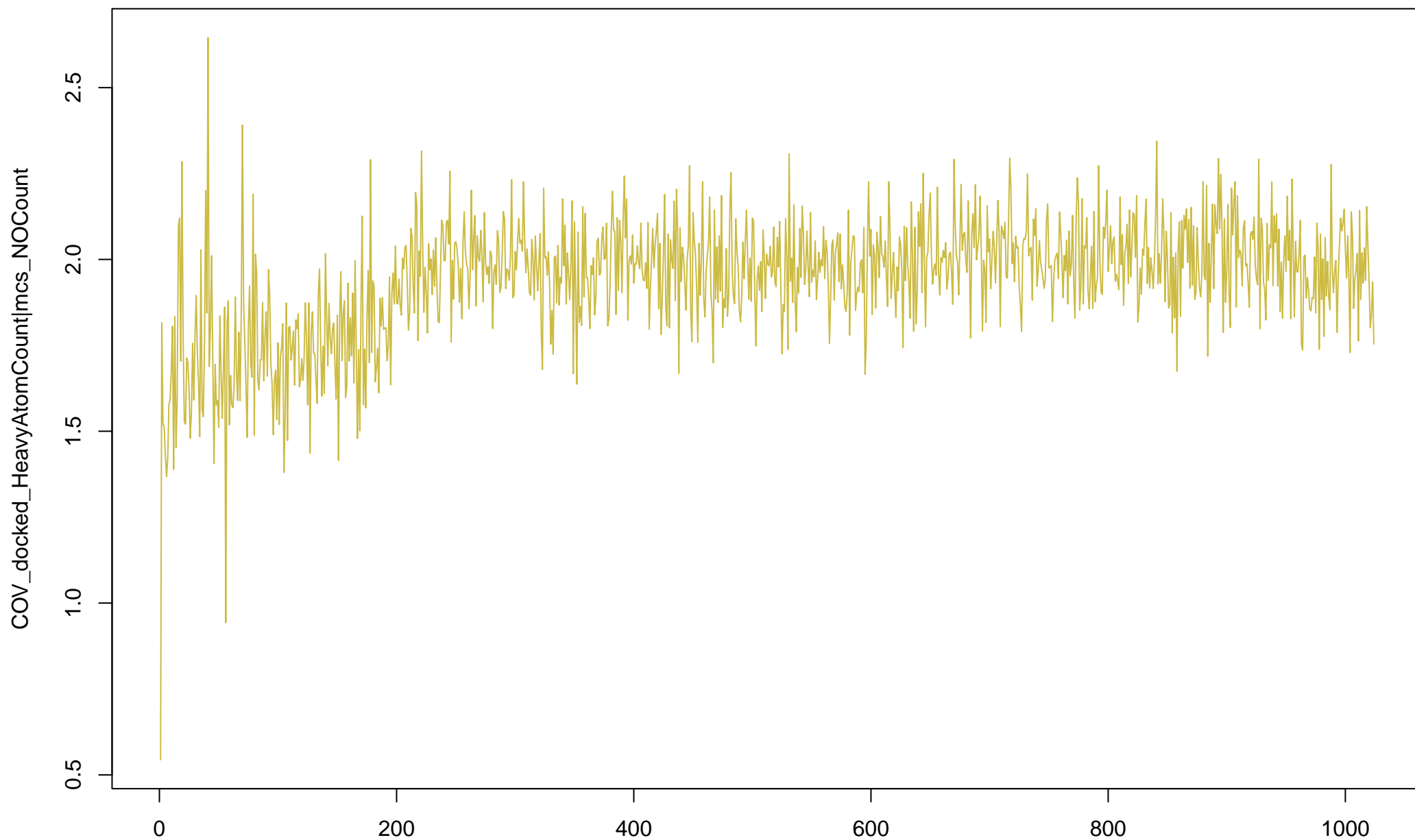
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 761 | BMK = 0.0528 | MCSE(6.27) = 4.86 | stat: FALSE | burn: 0



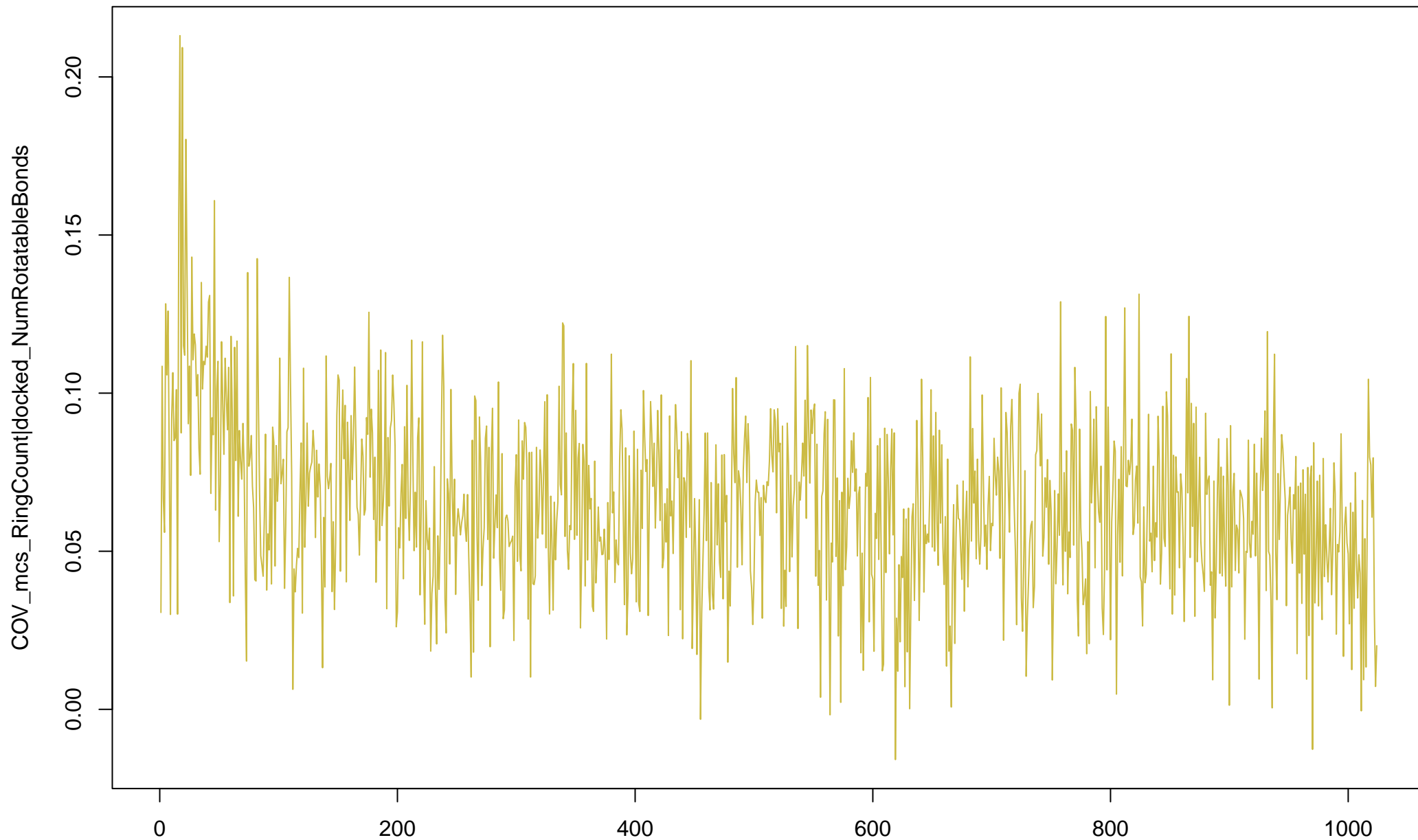
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 148 | BMK = 0.112 | MCSE(6.27) = 7.62 | stat: FALSE | burn: 0



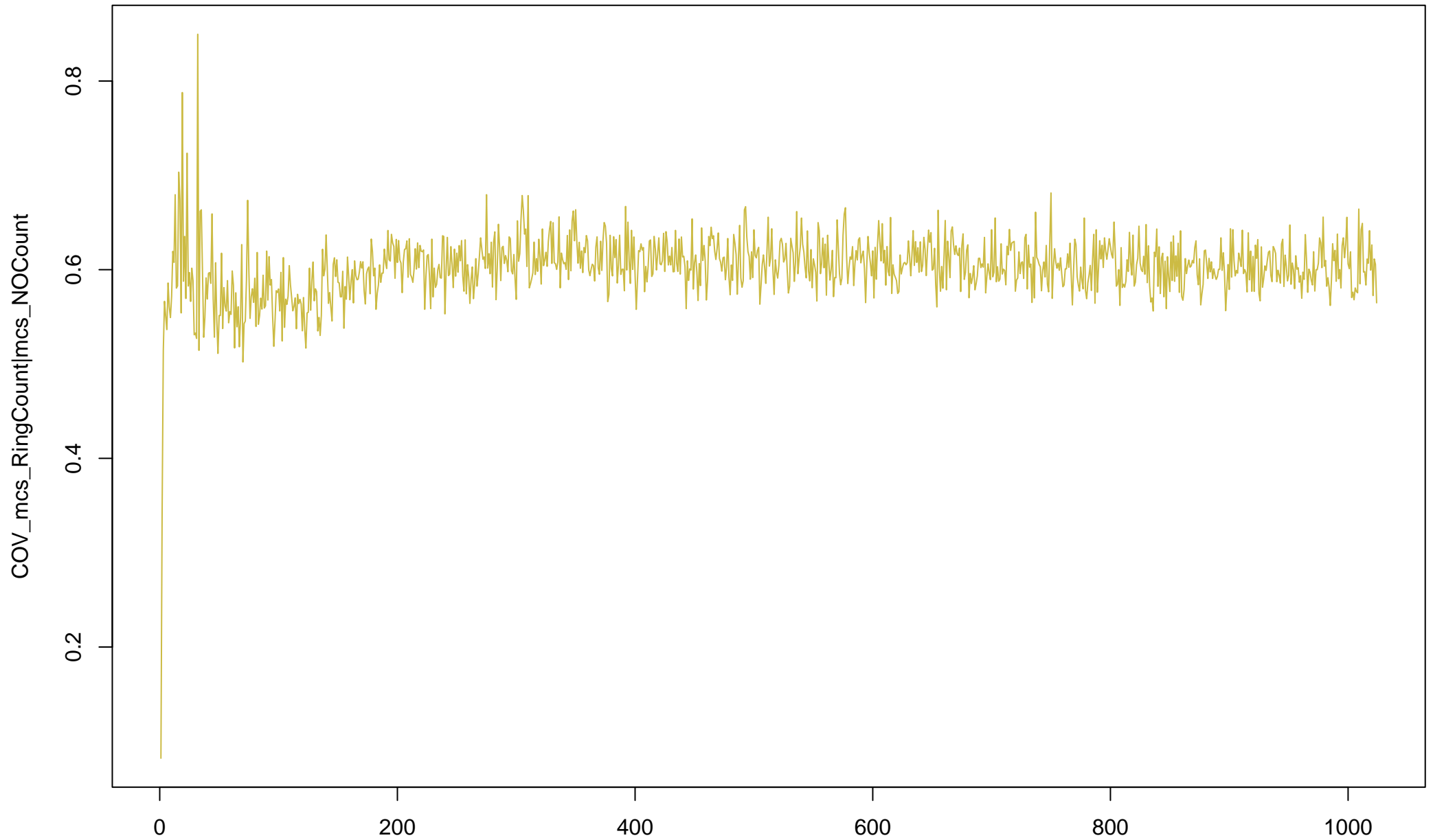
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 12.3 | BMK = 0.318 | MCSE(6.27) = 11.1 | stat: FALSE | burn: 204



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 110 | BMK = 0.148 | MCSE(6.27) = 7.63 | stat: FALSE | burn: 0



COV_mcs_RingCount|mcs_NOCount
ESS = 64.3 | BMK = 0.229 | MCSE(6.27) = 7.02 | stat: FALSE | burn: 0



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 63.5 | BMK = 0.161 | MCSE(6.27) = 7.62 | stat: FALSE | burn: 0

