

-- STATS maxD --

min ESS = 2.14276880755097

max BMK = 0.837984447972417

max MCSE = 13.5308605857961

all stationary: FALSE

burn: 2040

-- STATS 2D --

min ESS = 9.61743128892225

max BMK = 0.489632224954422

max MCSE = 12.2361203665701

all stationary: FALSE

burn: 1632

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 1

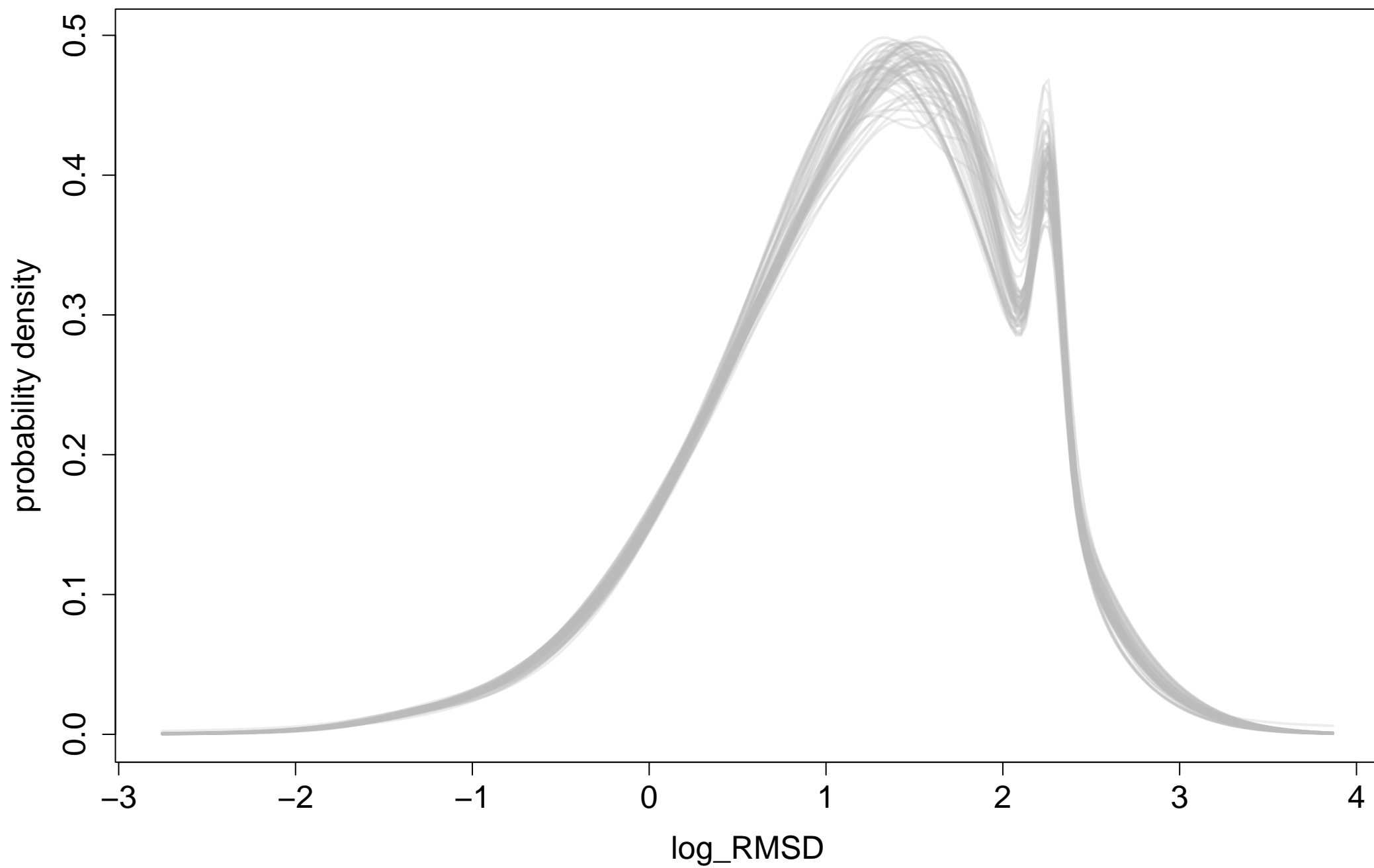
max MCSE = NaN

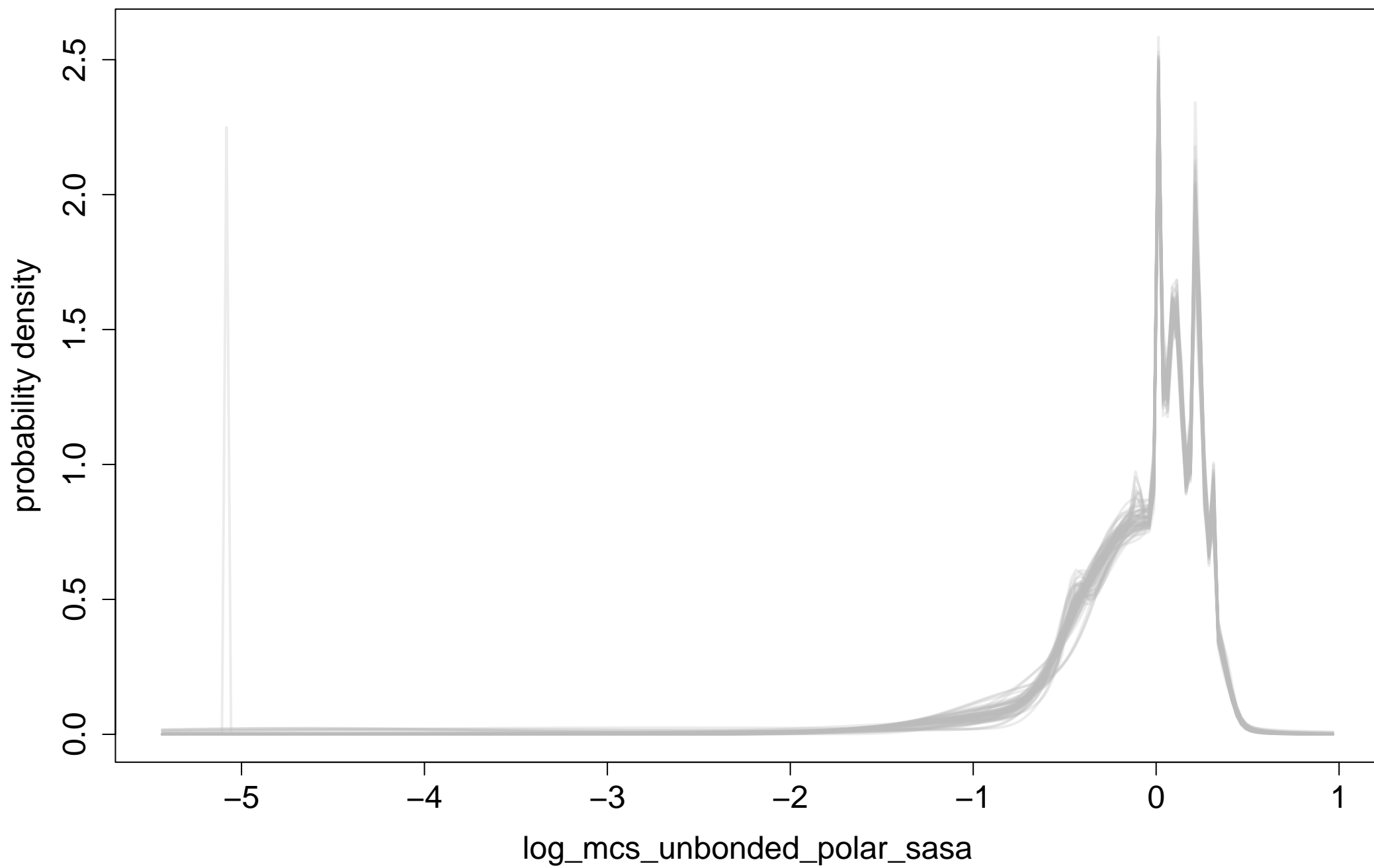
all stationary: FALSE

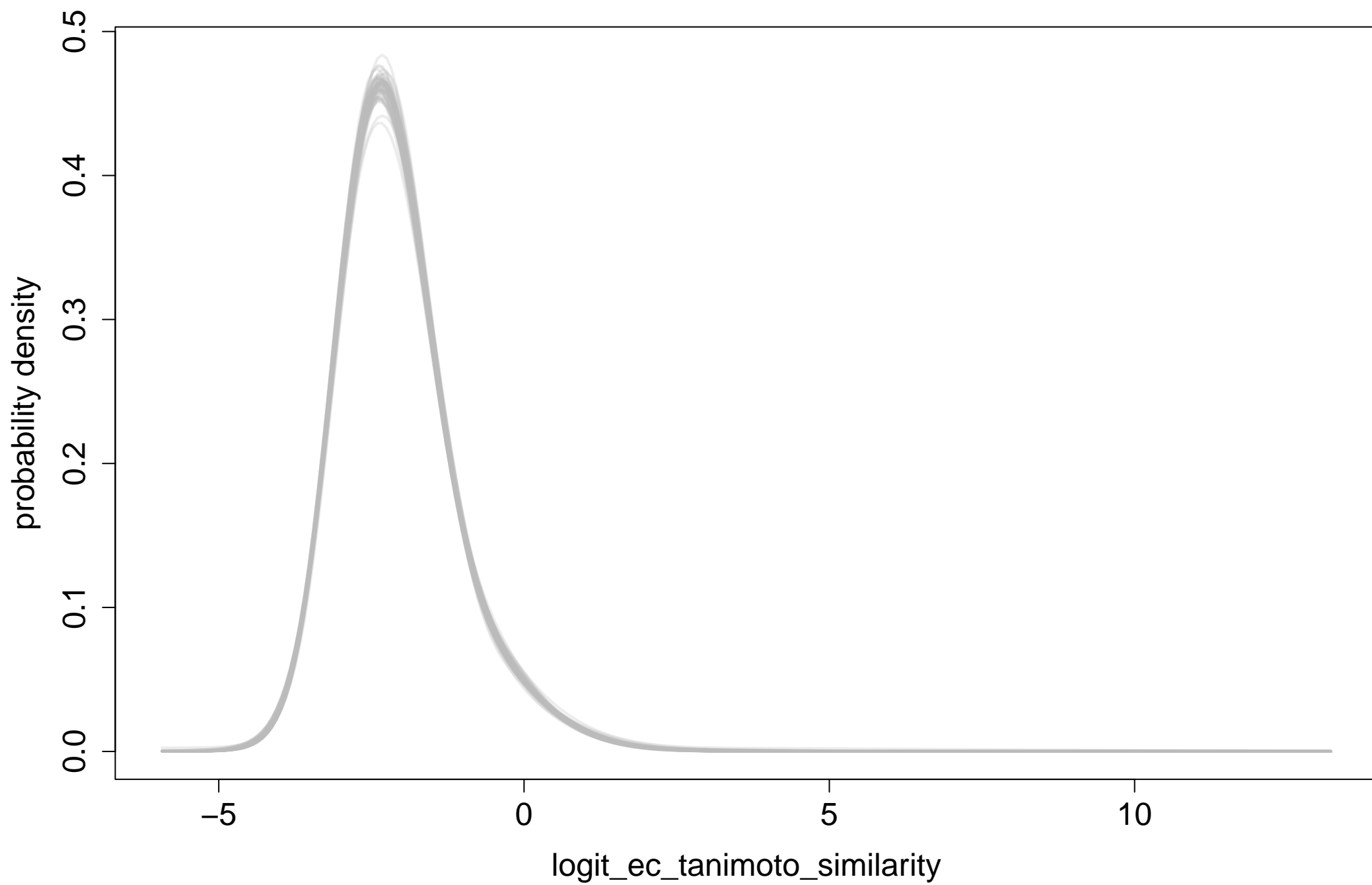
burn: 1632

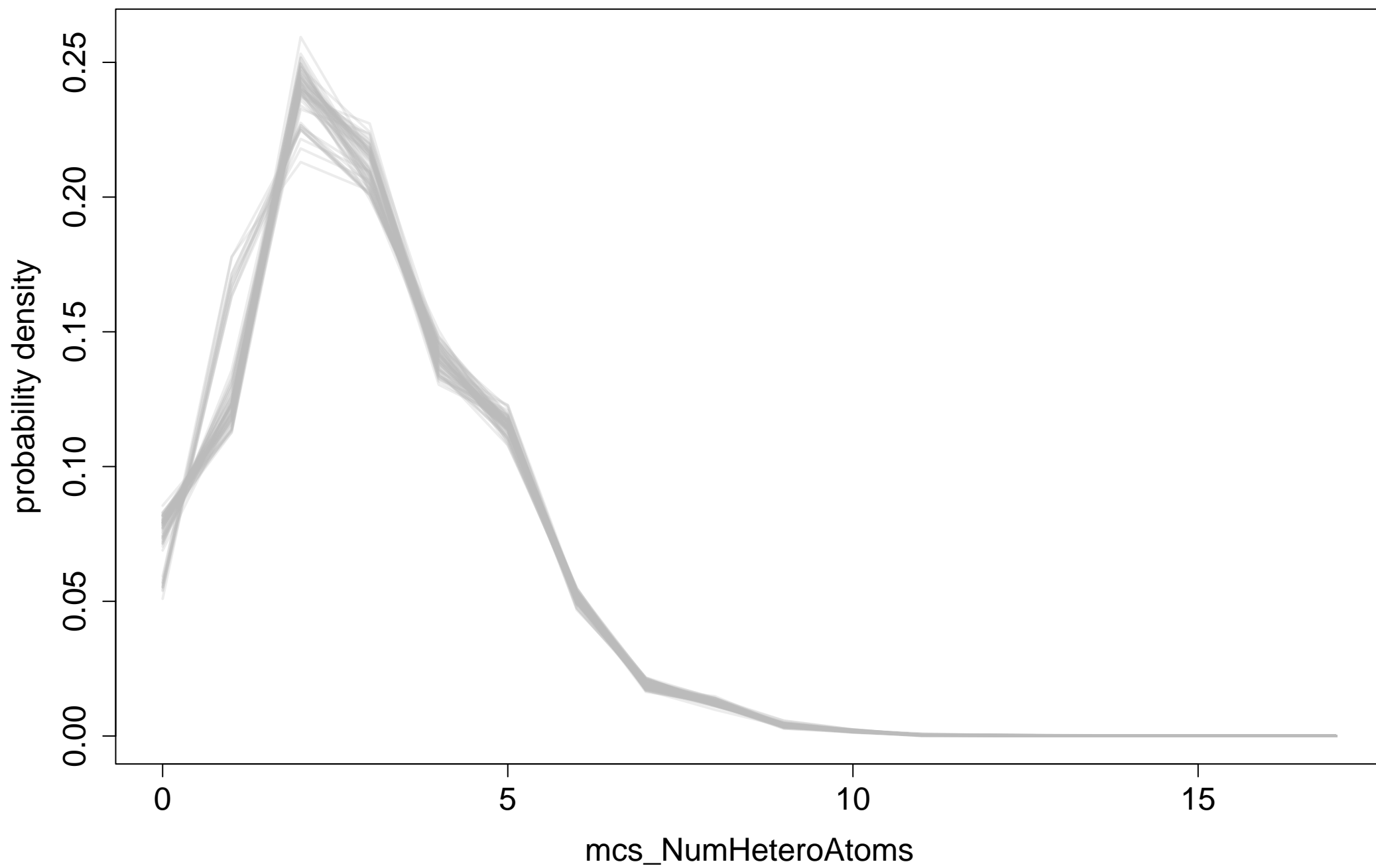
Occupied clusters: 32 of 64

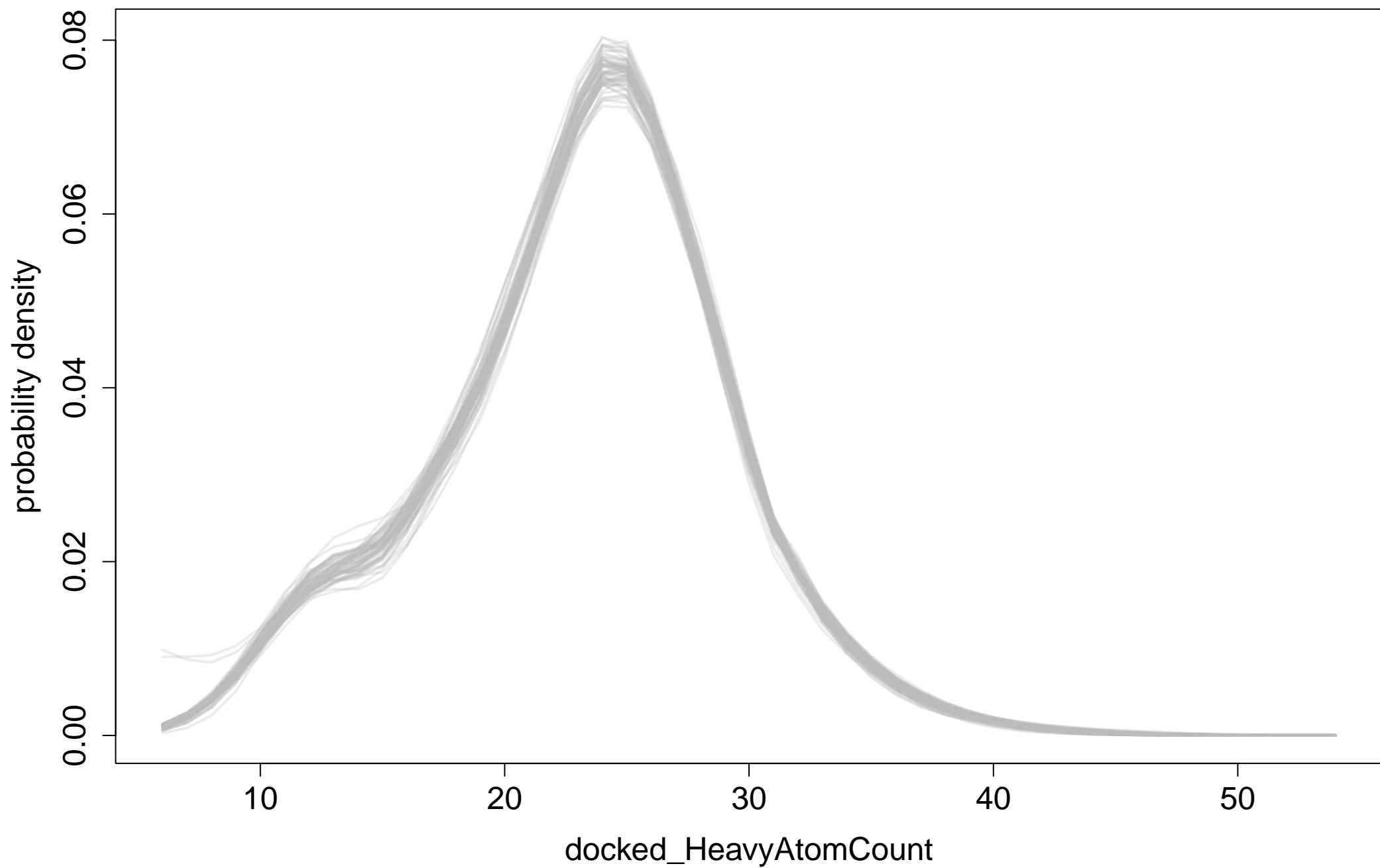
LL: -76100 +- 5550

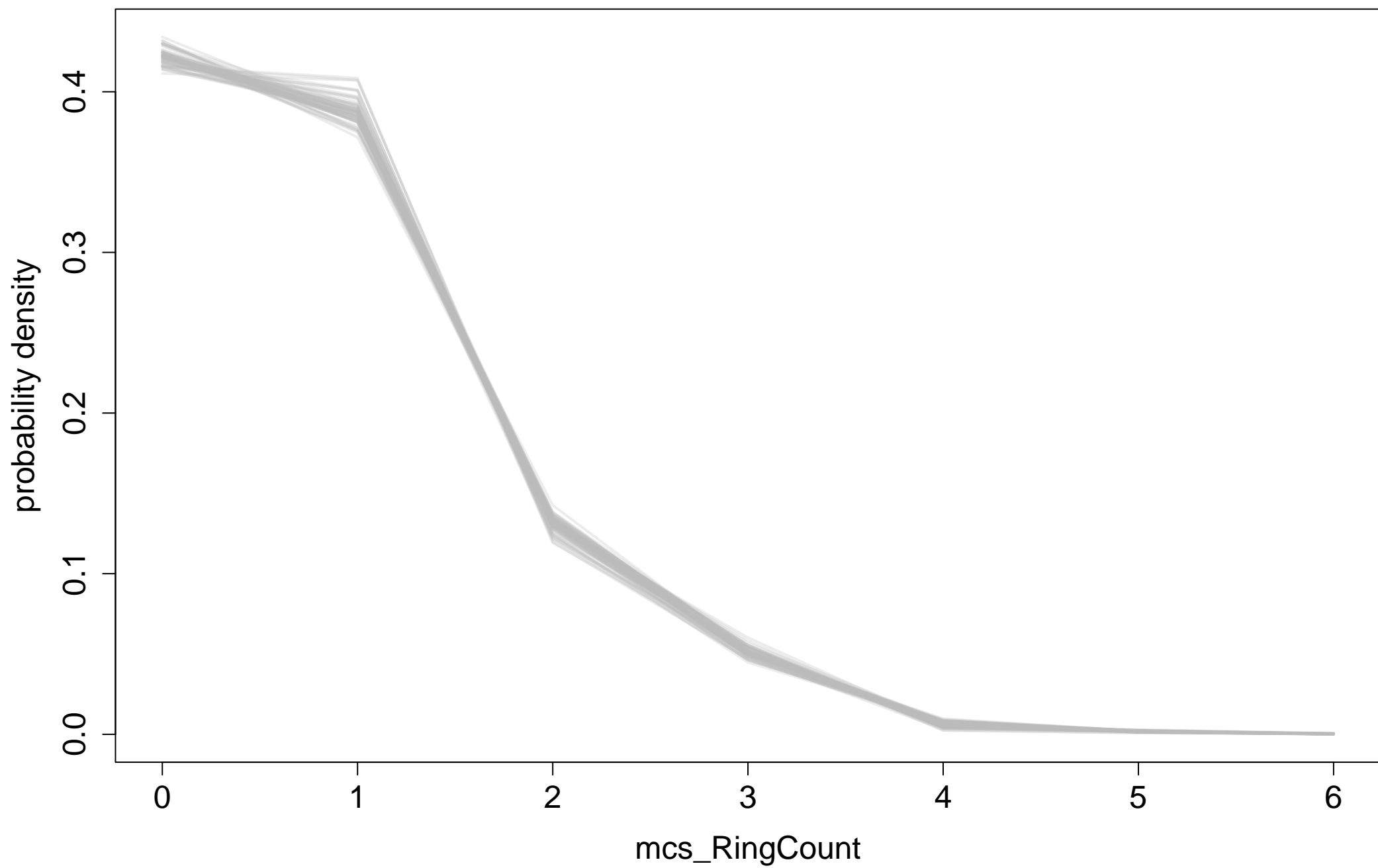


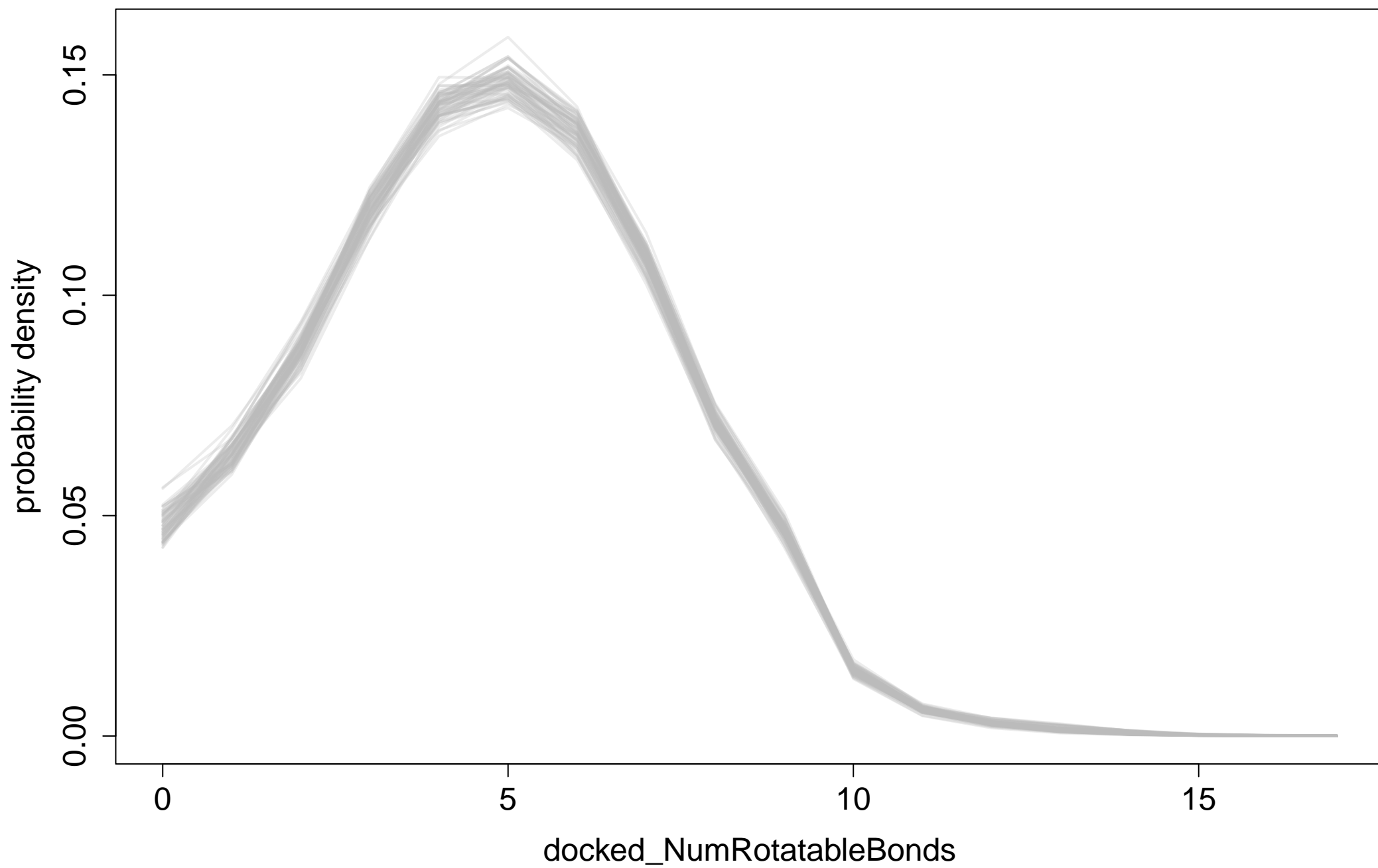


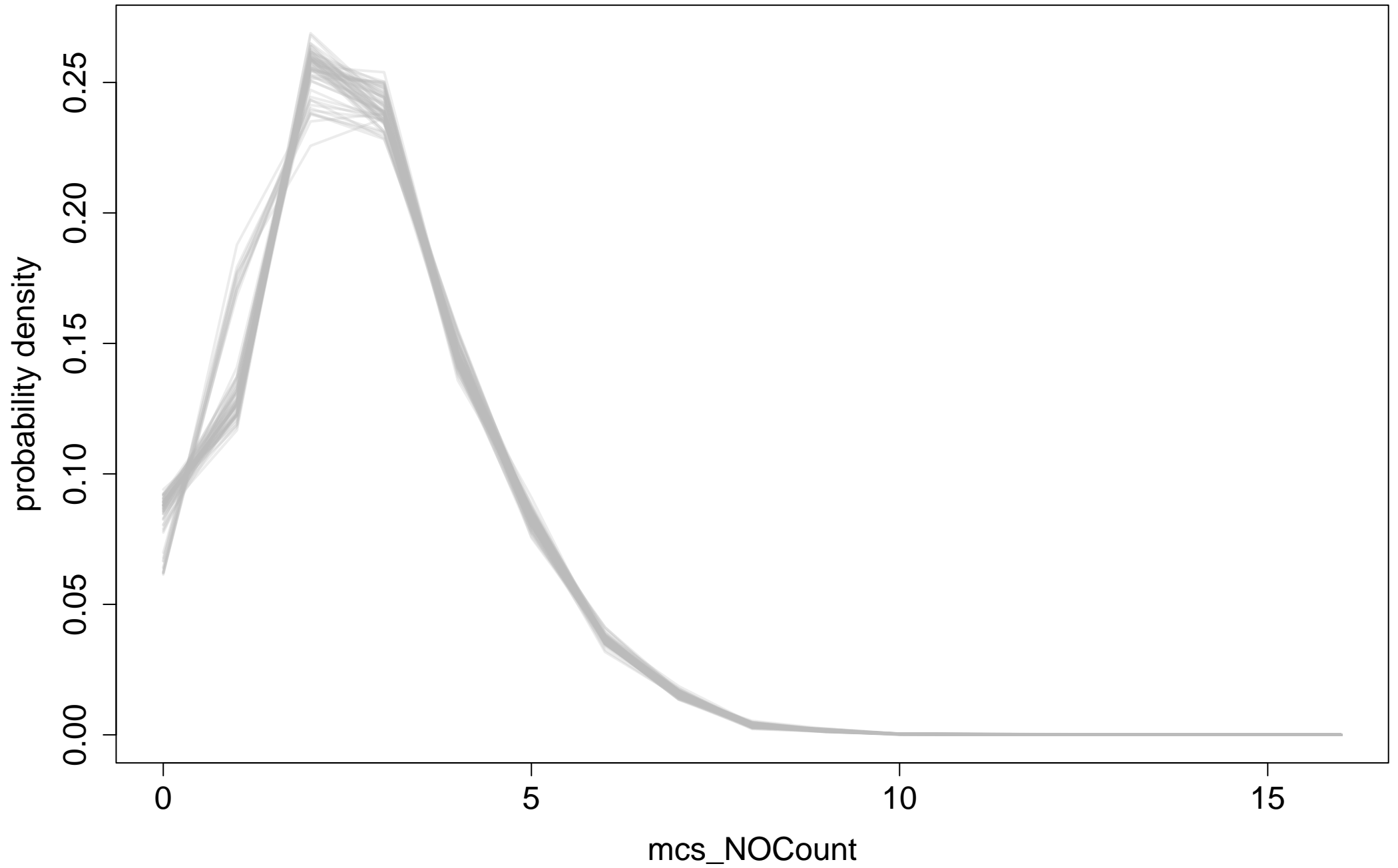


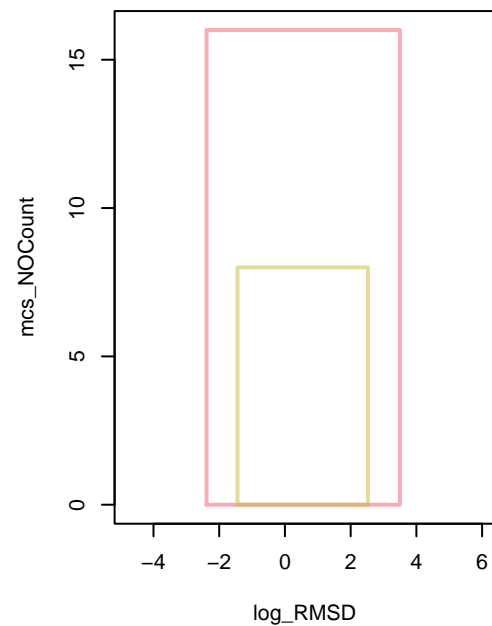
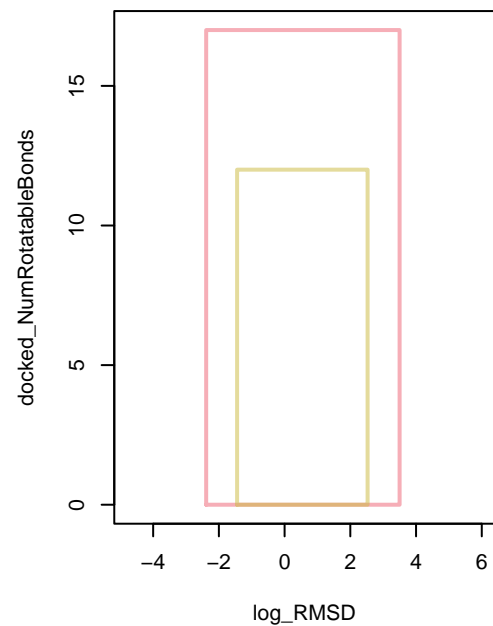
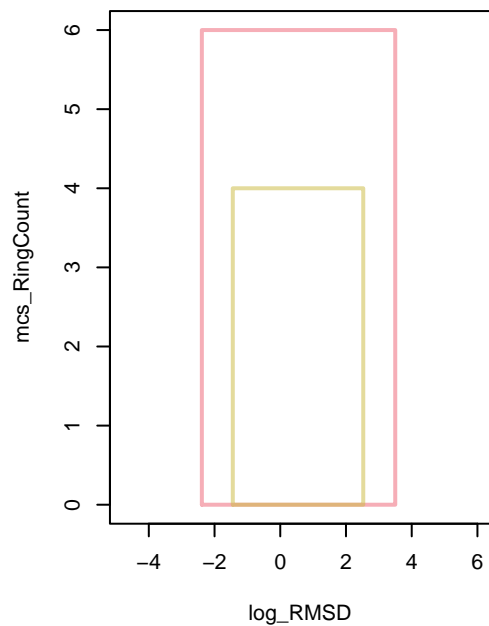
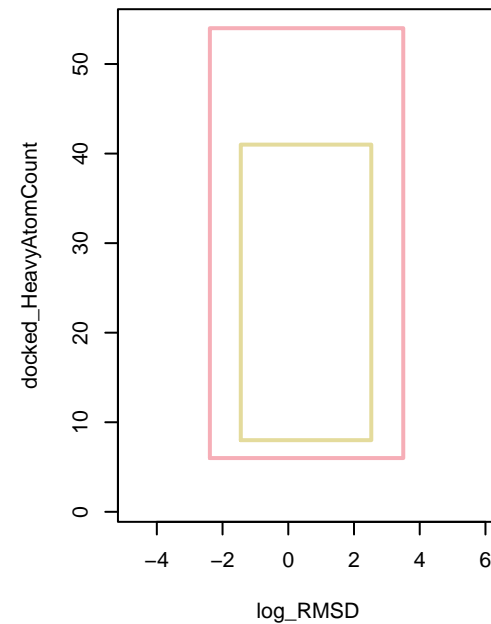
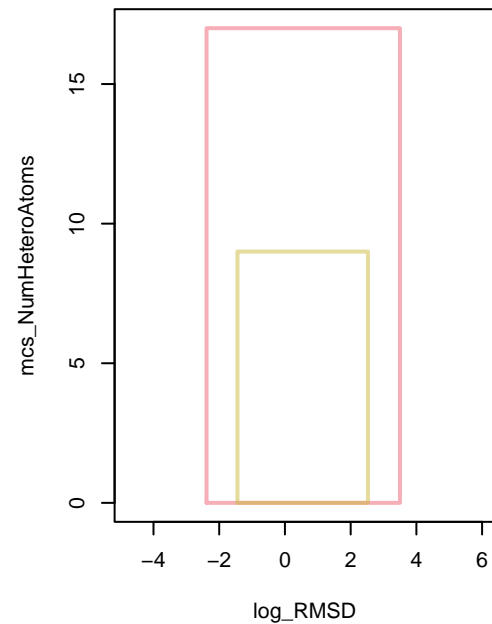
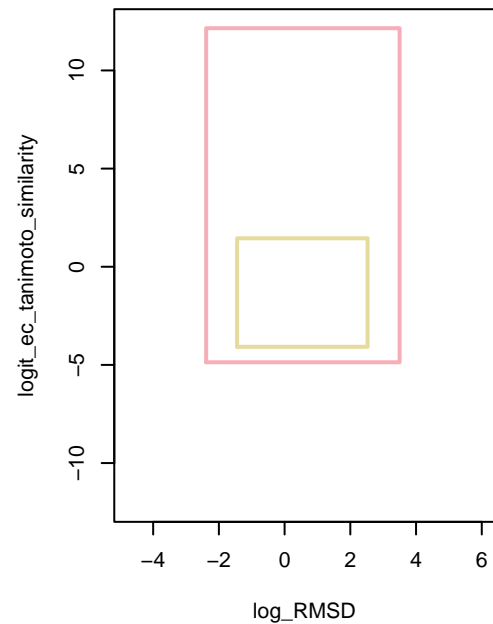
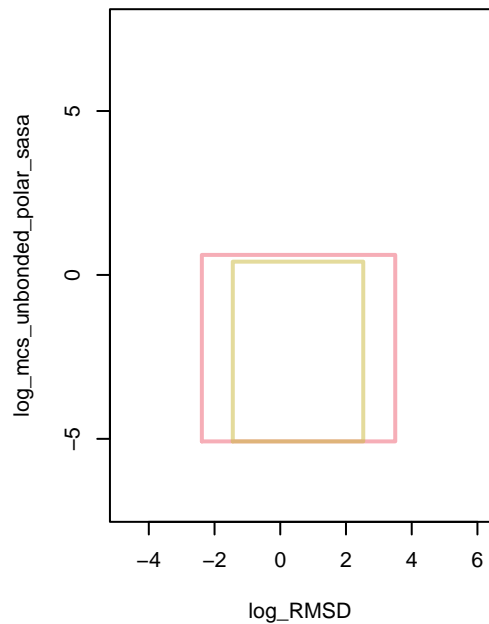




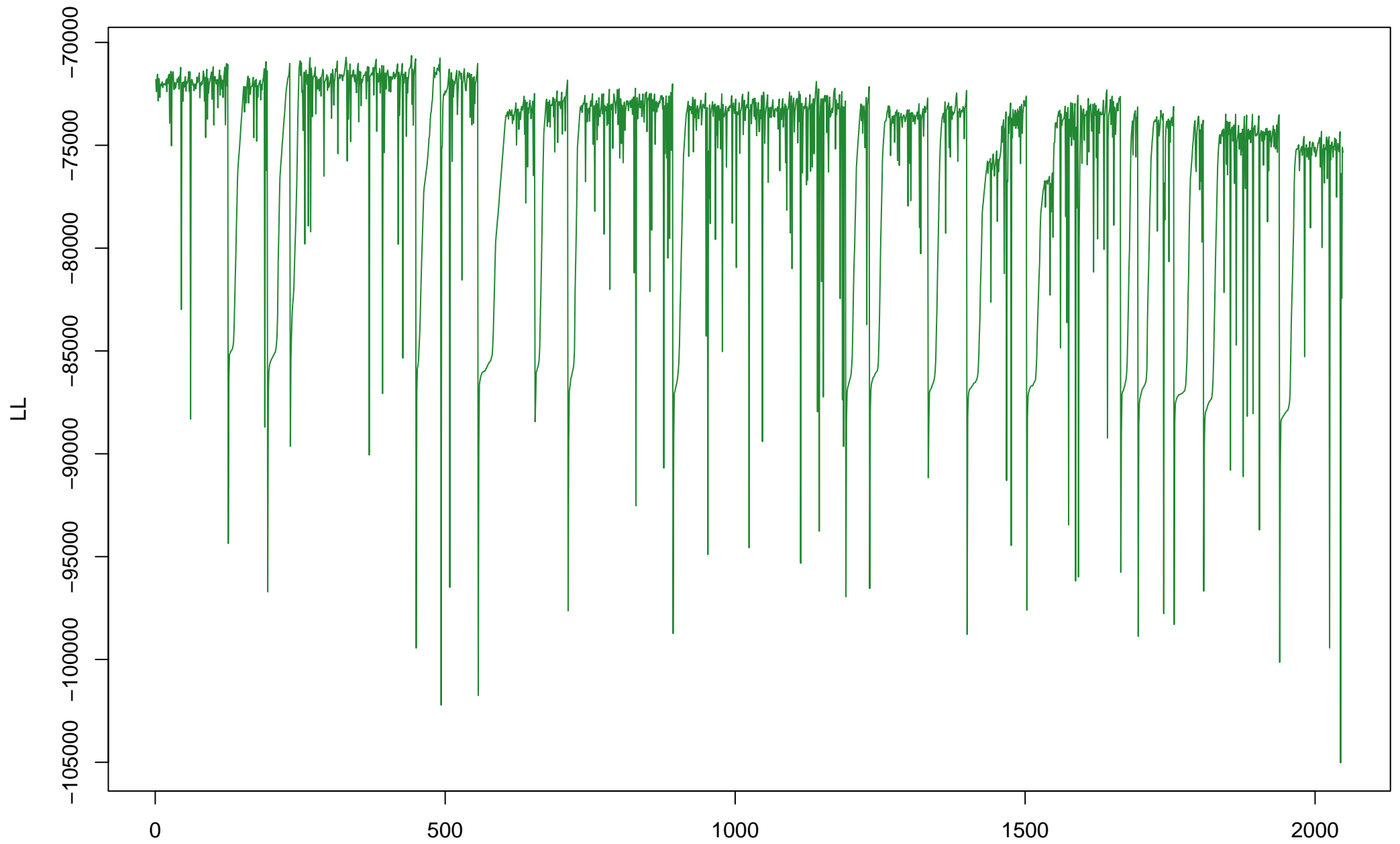




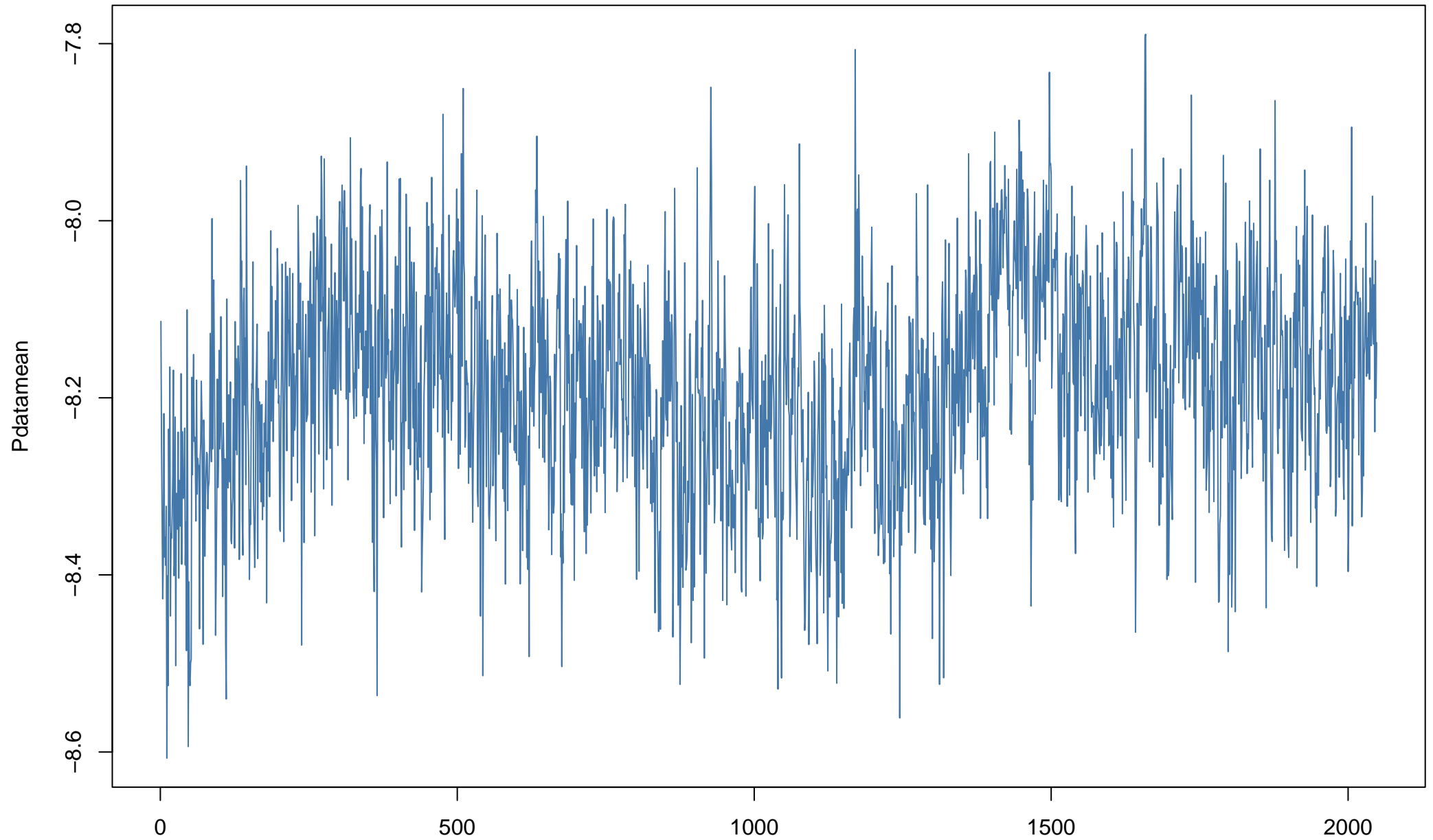




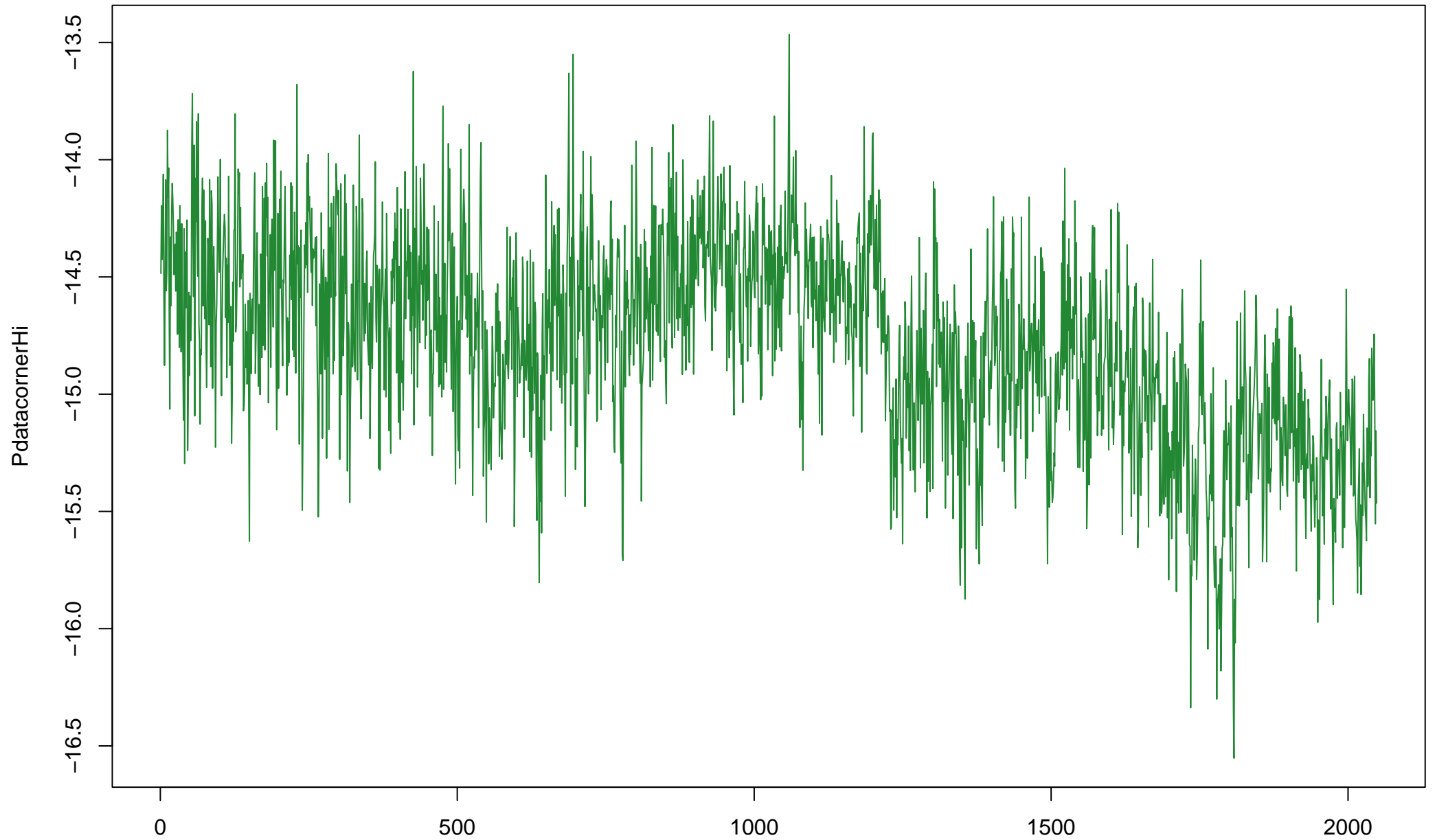
LL



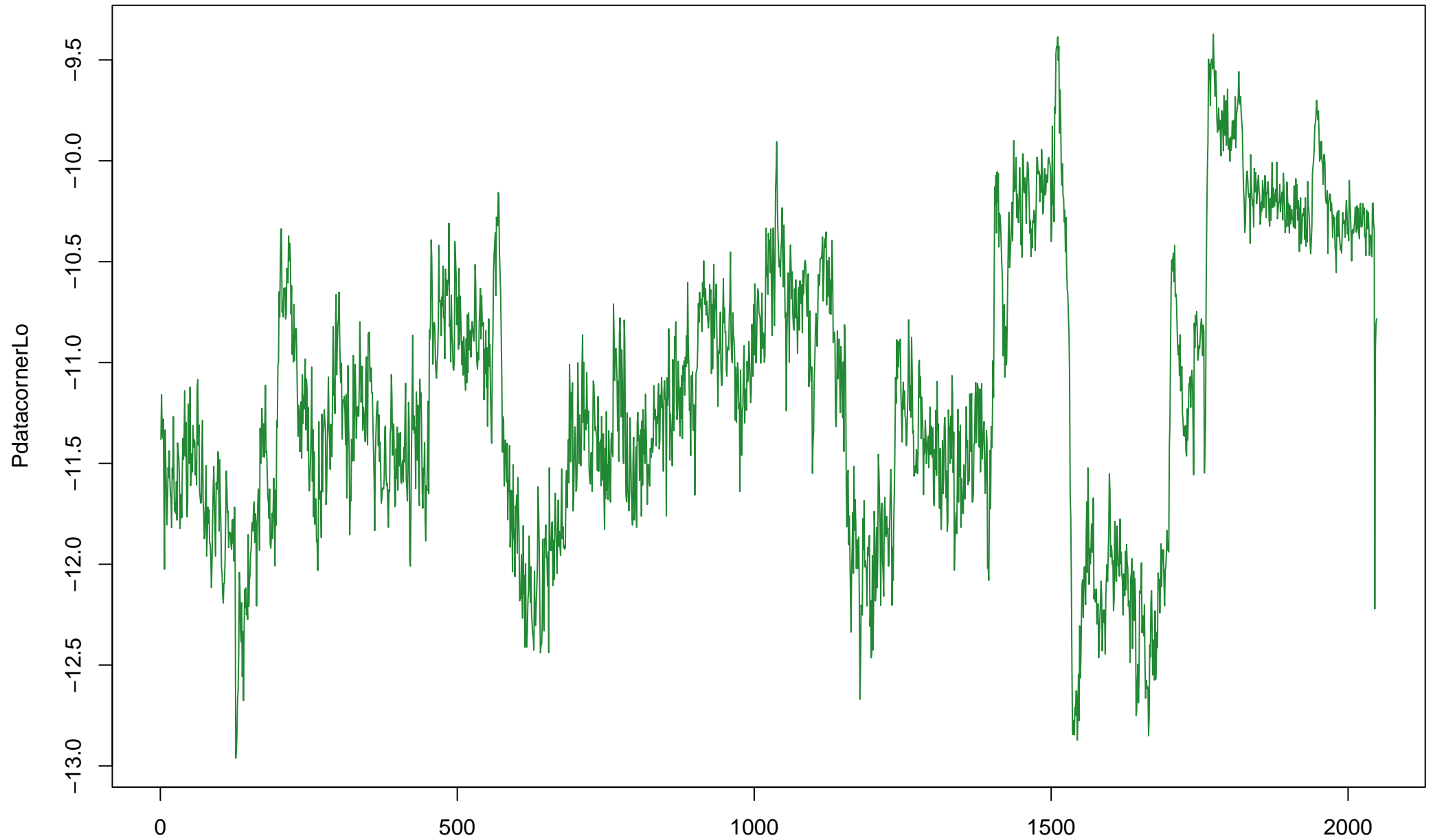
Pdatamean
ESS = 112 | BMK = 0.0893 | MCSE(6.27) = 7.26 | stat: FALSE | burn: 0



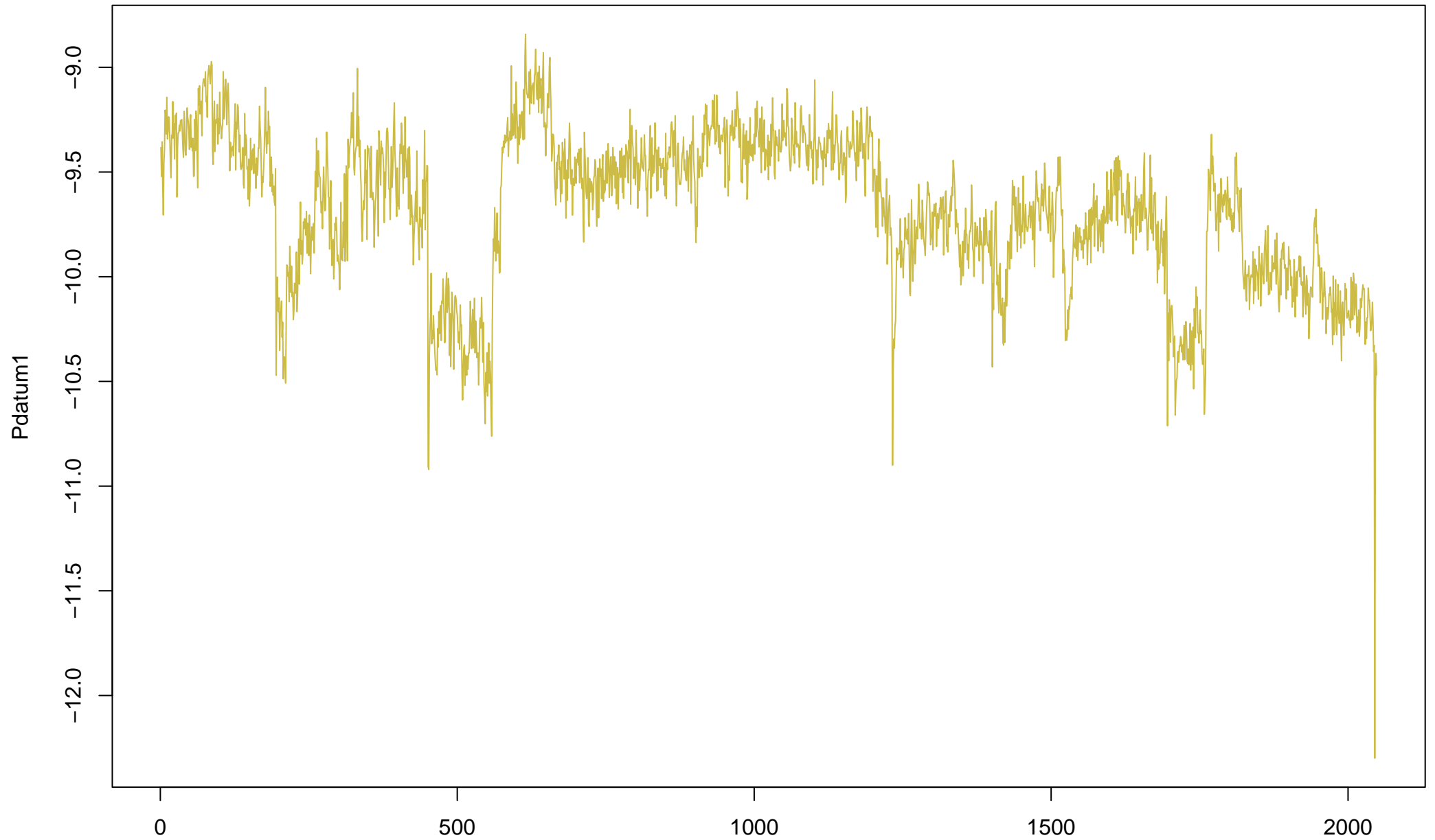
PdatacornerHi
ESS = 26.2 | BMK = 0.33 | MCSE(6.27) = 9.32 | stat: FALSE | burn: 0



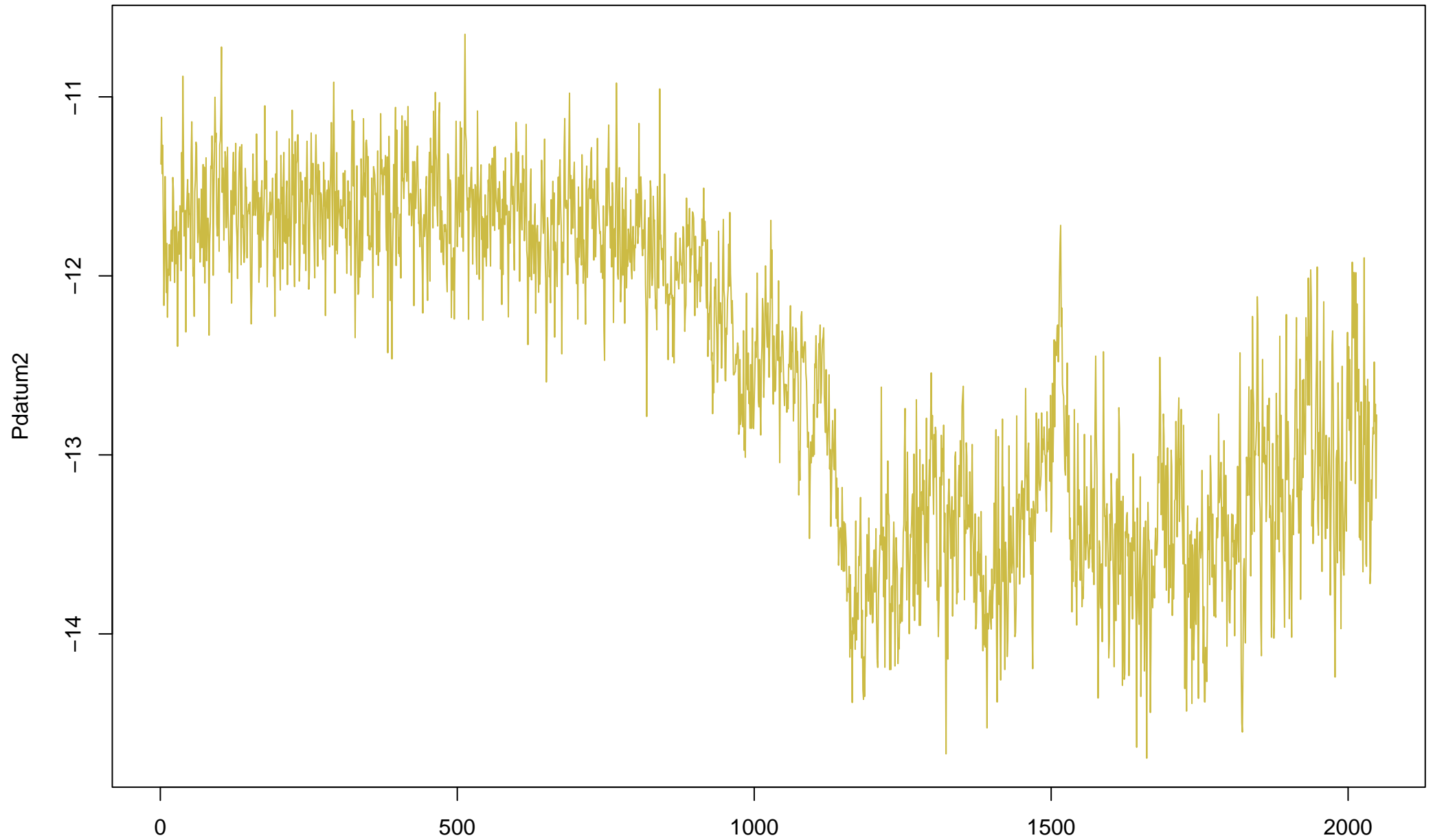
PdatacornerLo
ESS = 18.8 | BMK = 0.437 | MCSE(6.27) = 13.5 | stat: FALSE | burn: 2040



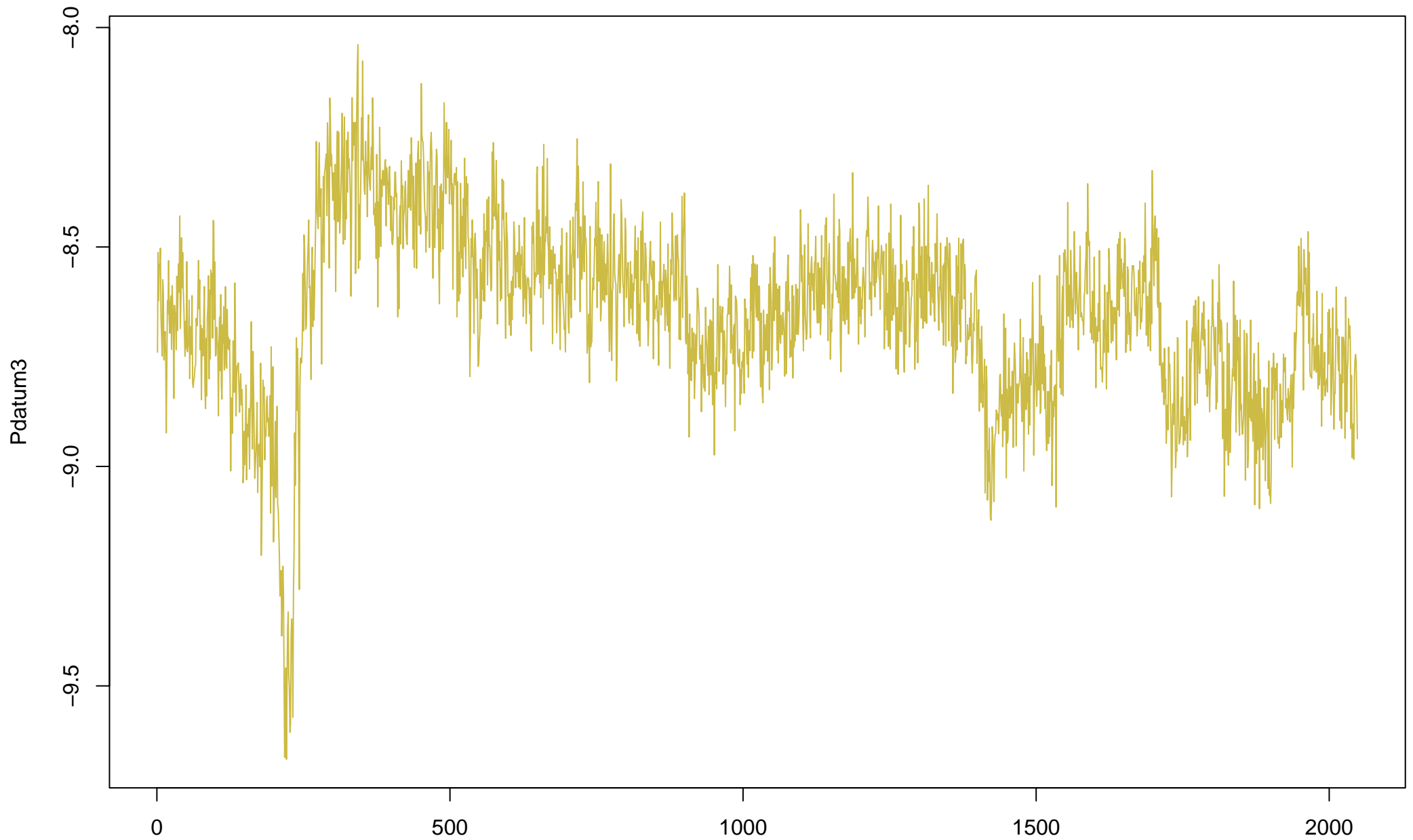
Pdatum1
ESS = 15.7 | BMK = 0.337 | MCSE(6.27) = 12.9 | stat: FALSE | burn: 2040



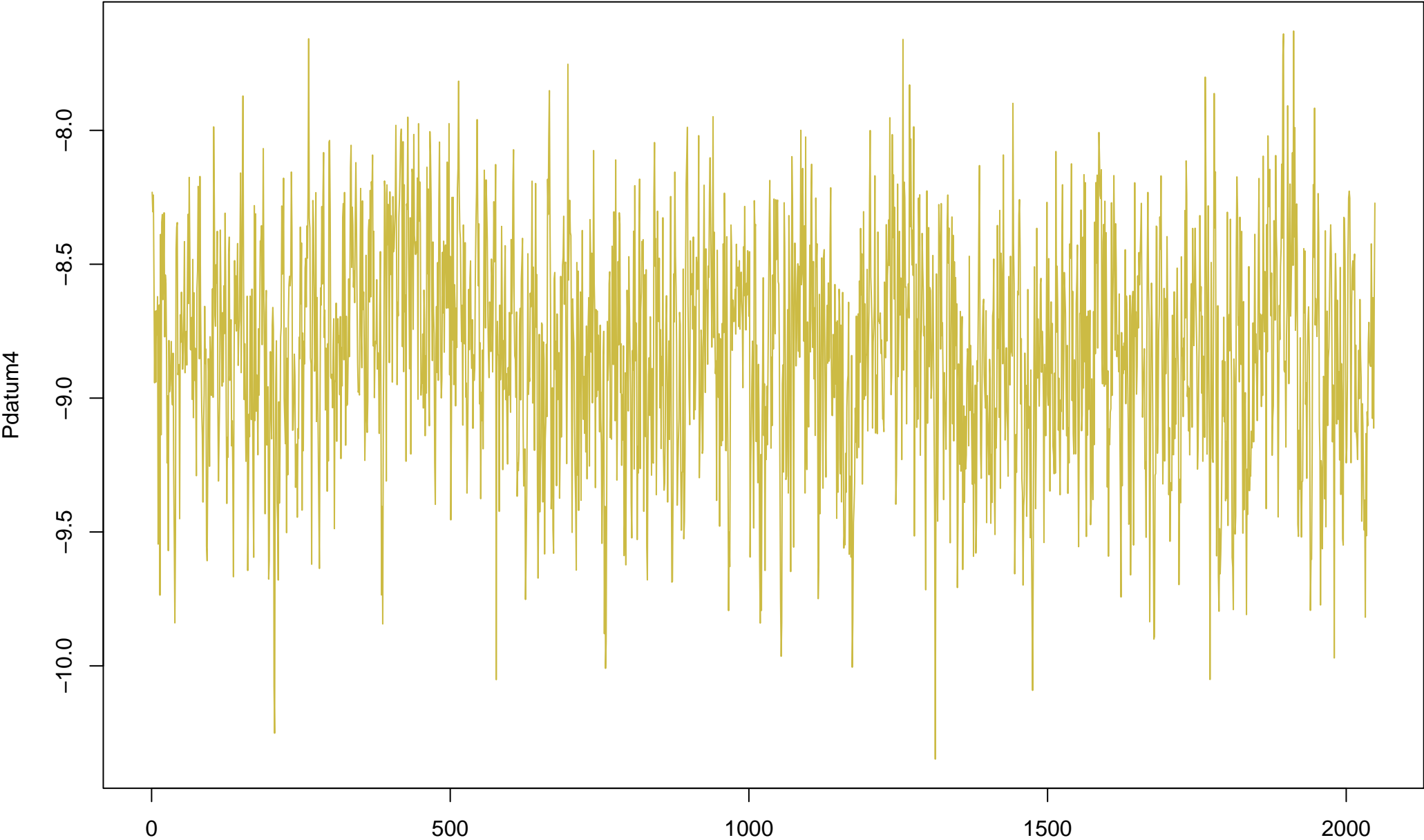
Pdatum2
ESS = 2.14 | BMK = 0.838 | MCSE(6.27) = 13.4 | stat: FALSE | burn: 1020



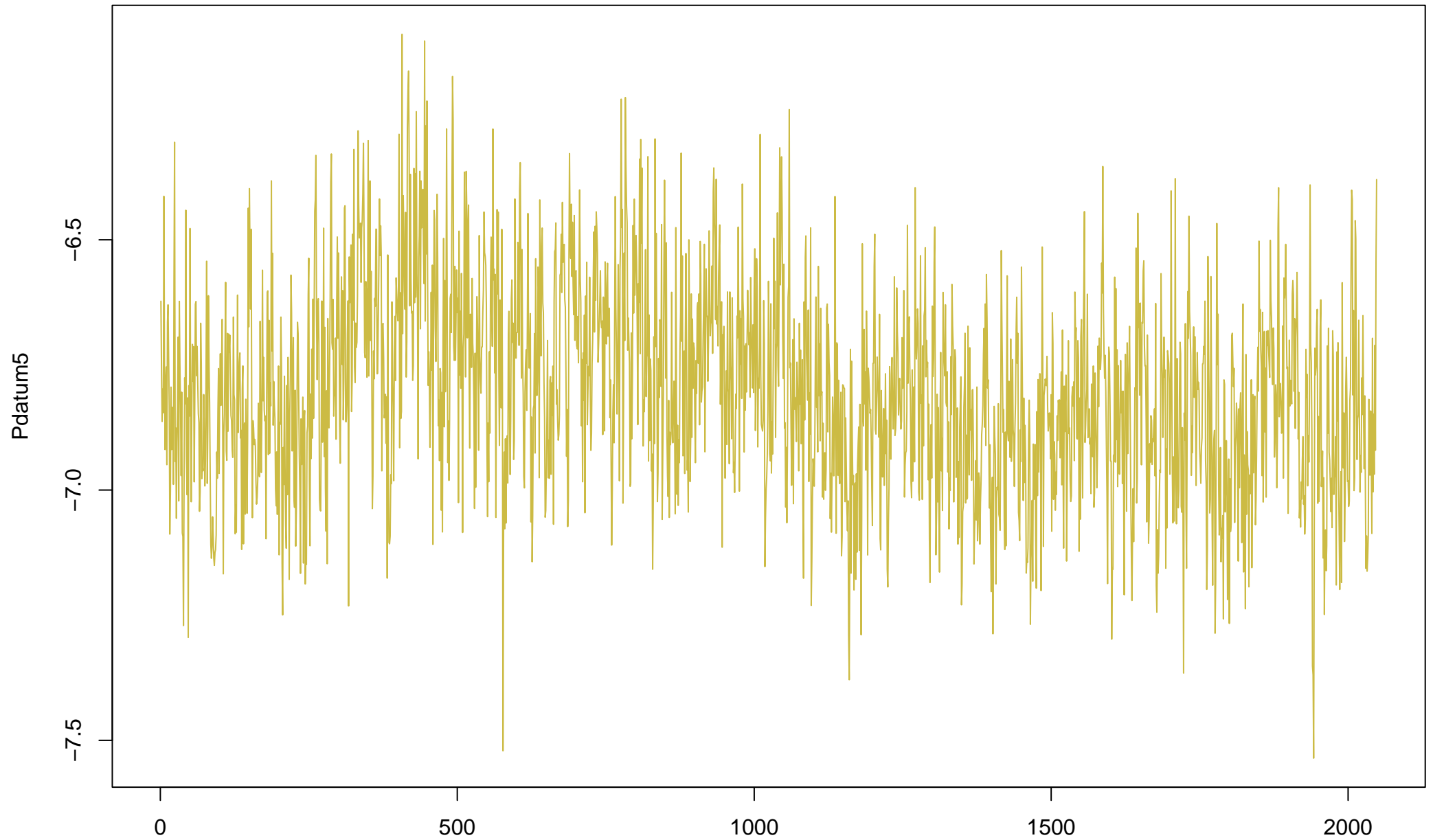
Pdatum3
ESS = 15.2 | BMK = 0.334 | MCSE(6.27) = 12.3 | stat: FALSE | burn: 204



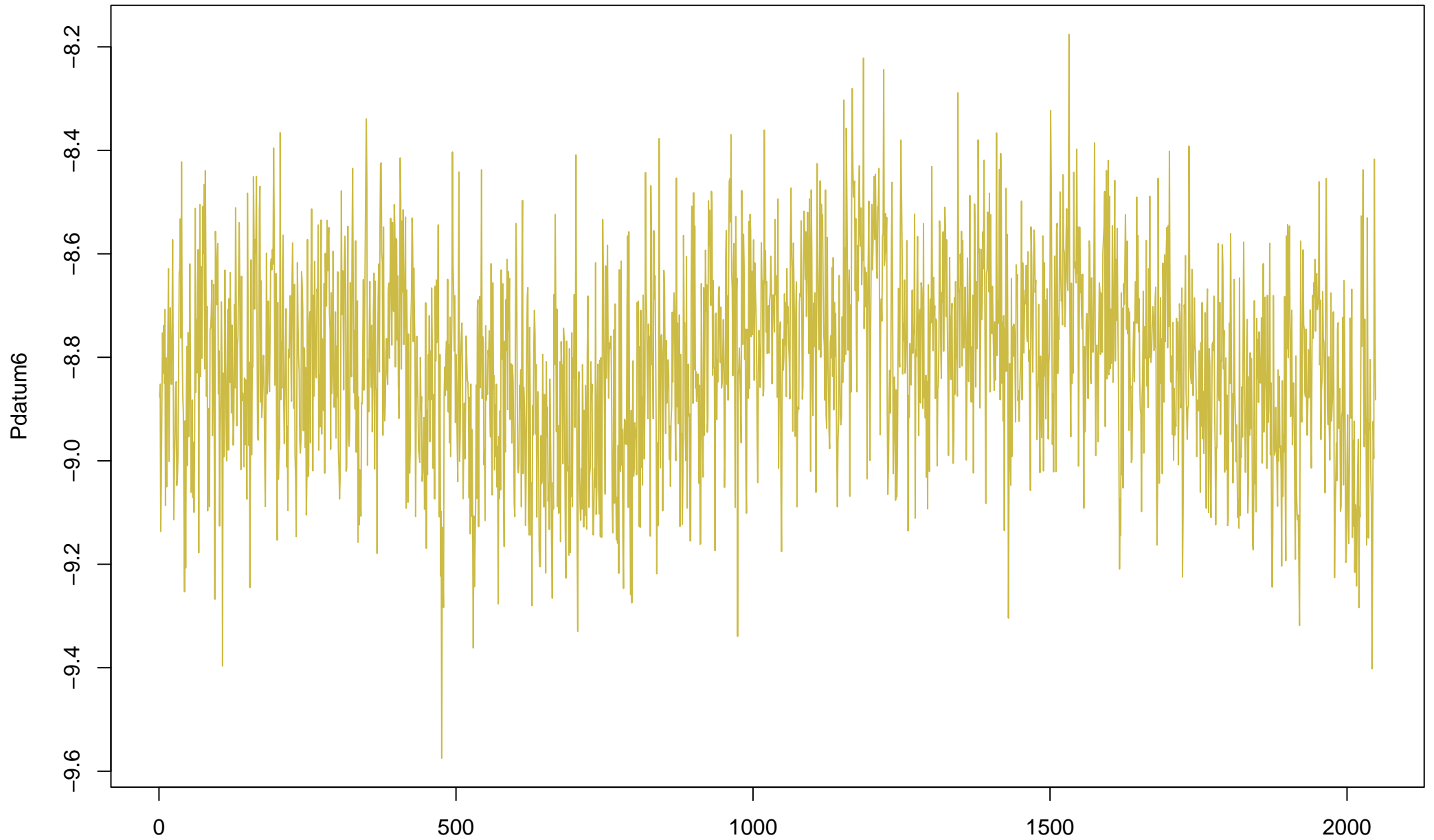
Pdatum4
ESS = 695 | BMK = 0.0639 | MCSE(6.27) = 4.58 | stat: TRUE | burn: 0



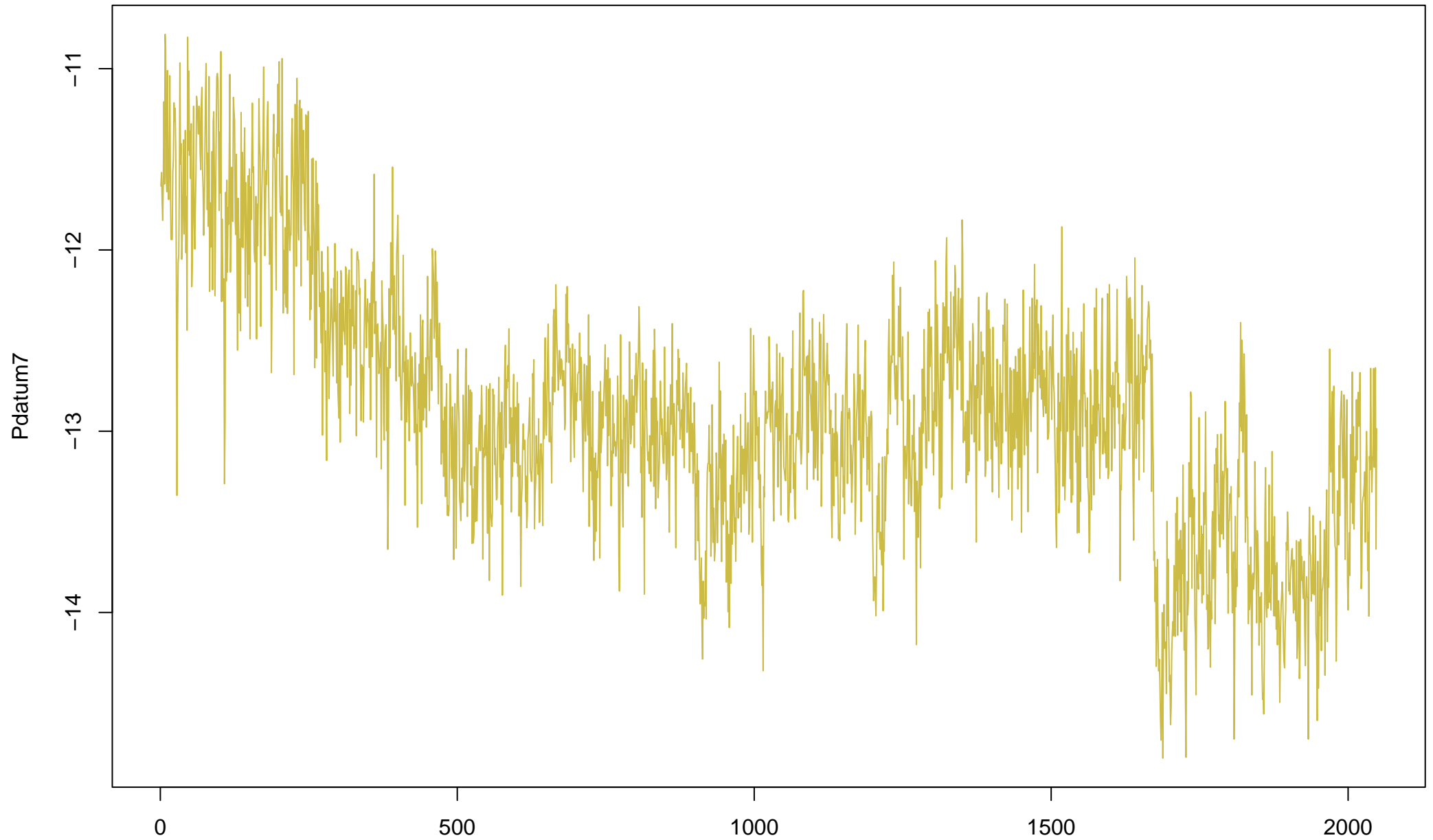
Pdatum5
ESS = 140 | BMK = 0.227 | MCSE(6.27) = 7.36 | stat: TRUE | burn: 0



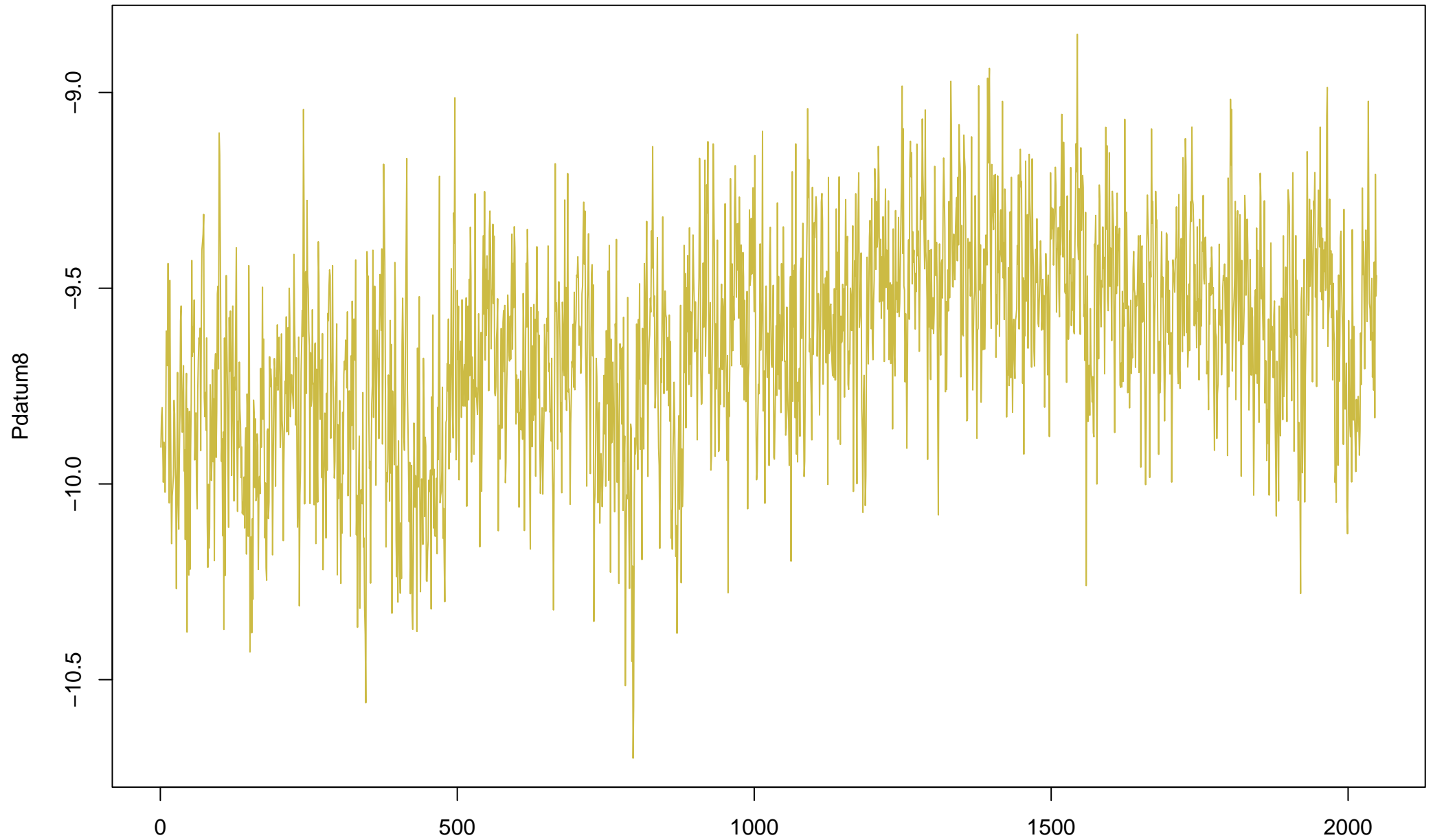
Pdatum6
ESS = 120 | BMK = 0.112 | MCSE(6.27) = 6.26 | stat: TRUE | burn: 0



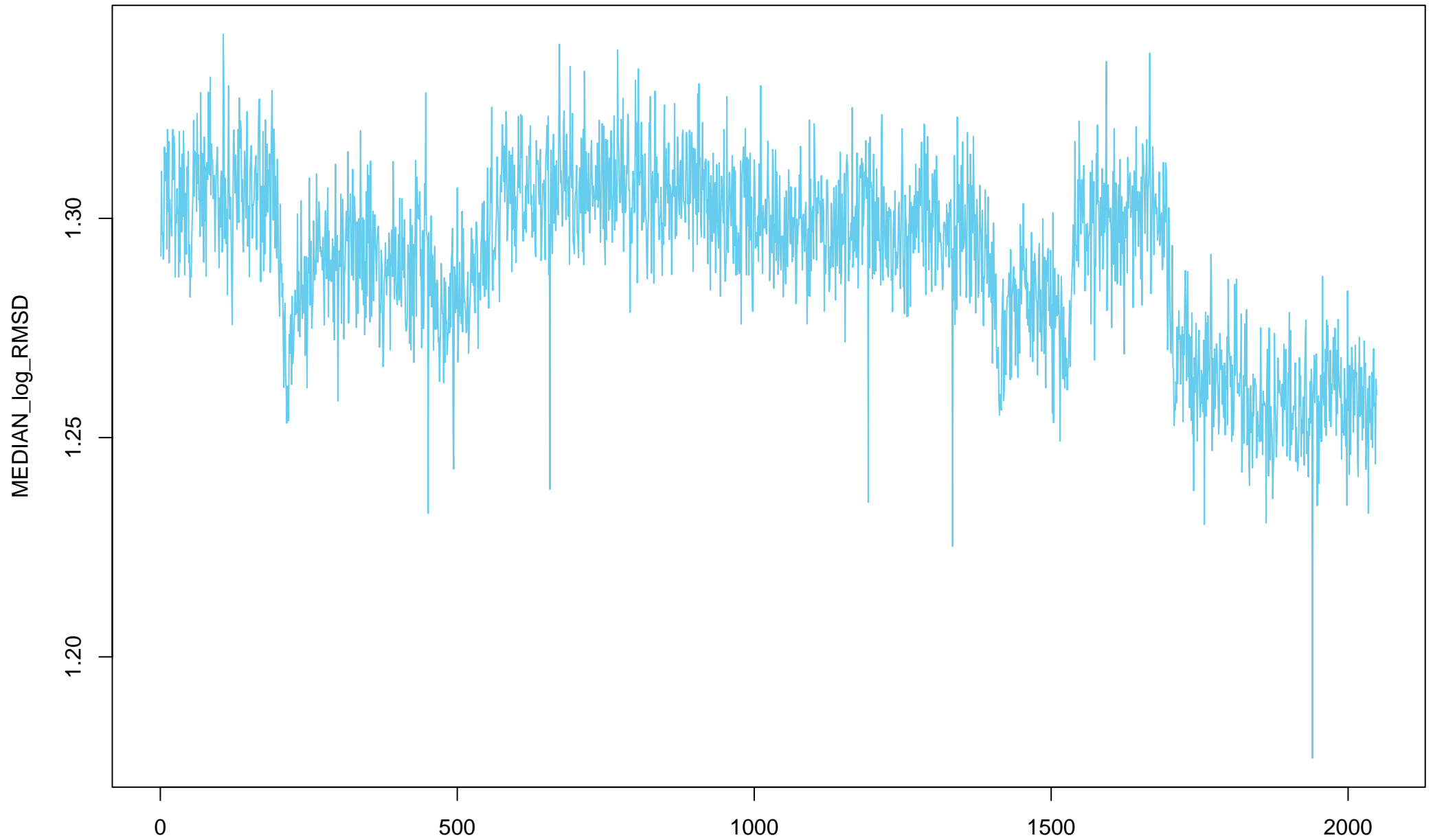
Pdatum7
ESS = 7.43 | BMK = 0.359 | MCSE(6.27) = 12.7 | stat: FALSE | burn: 408



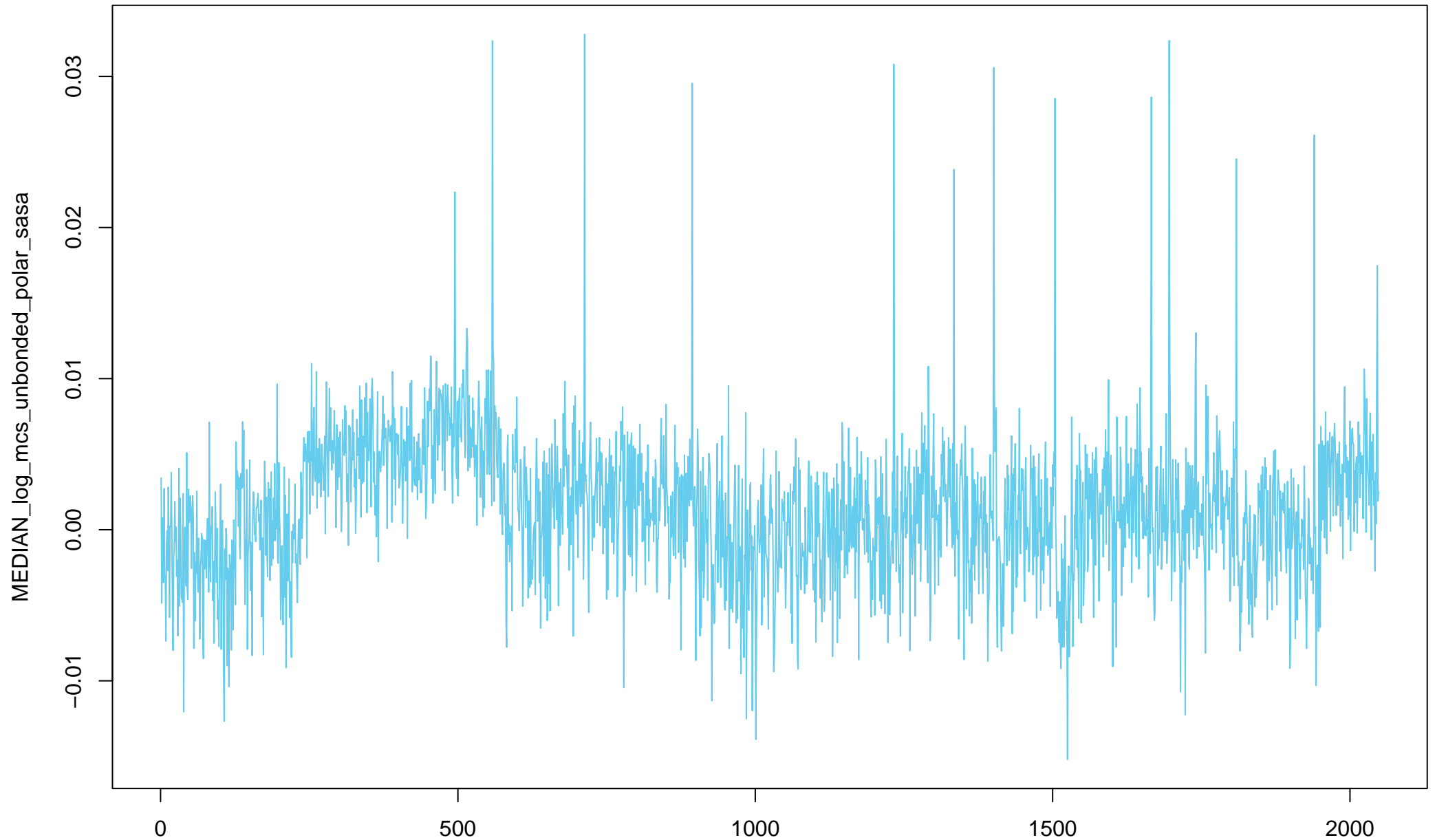
Pdatum8
ESS = 79.7 | BMK = 0.338 | MCSE(6.27) = 8.45 | stat: FALSE | burn: 0



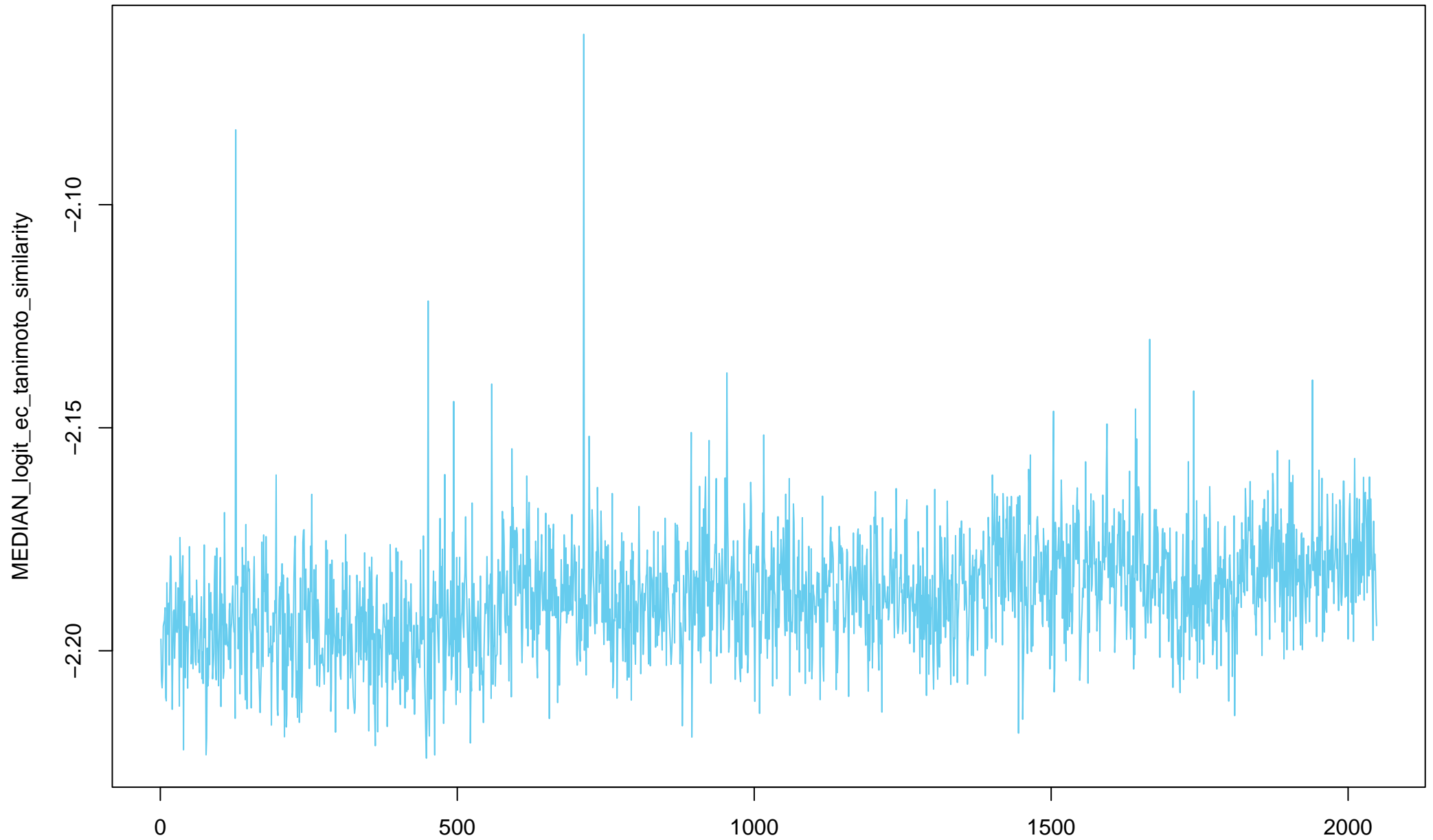
MEDIAN_log_RMSD
ESS = 11.3 | BMK = 0.332 | MCSE(6.27) = 11.9 | stat: FALSE | burn: 0



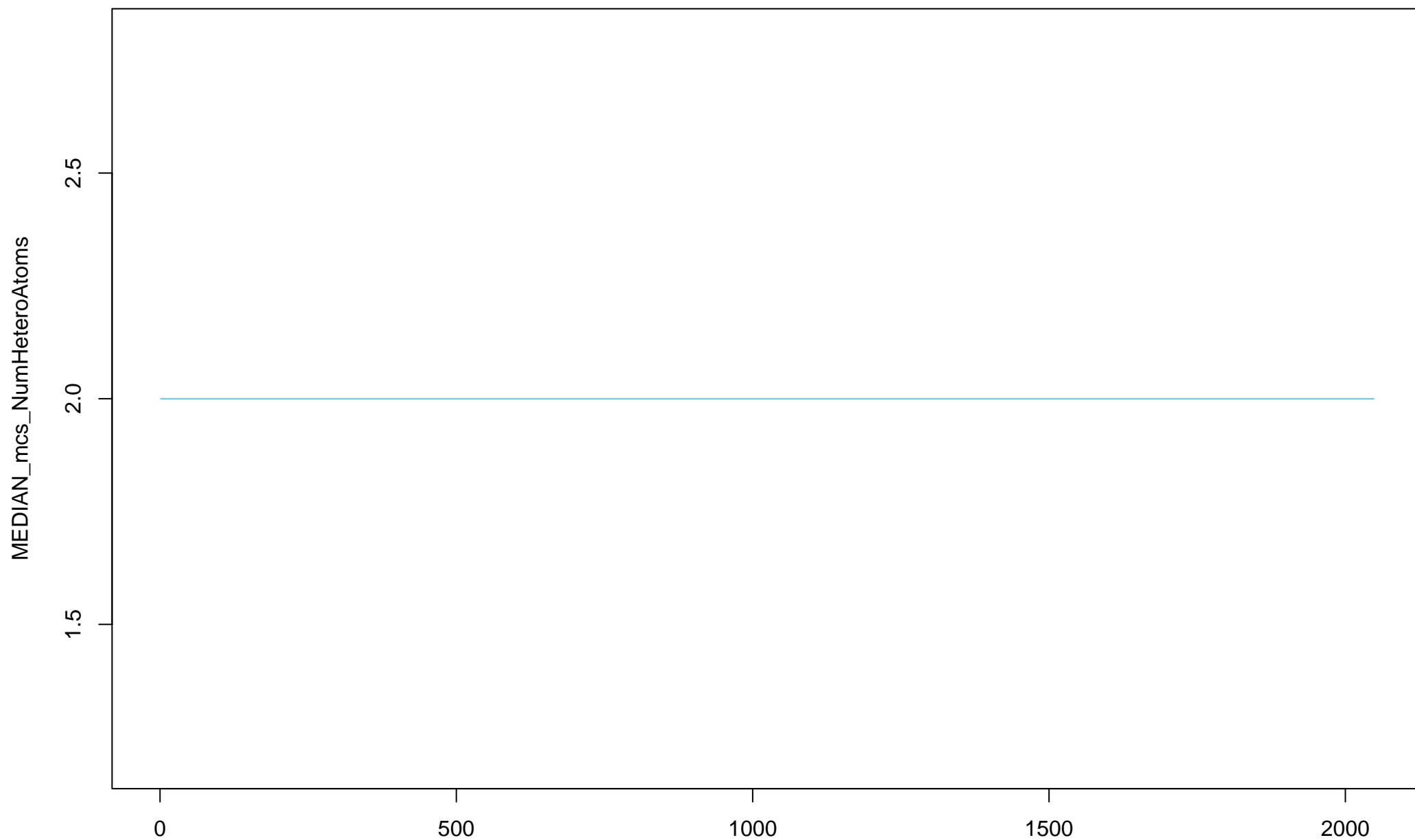
MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 60.2 | BMK = 0.159 | MCSE(6.27) = 7.56 | stat: FALSE | burn: 0



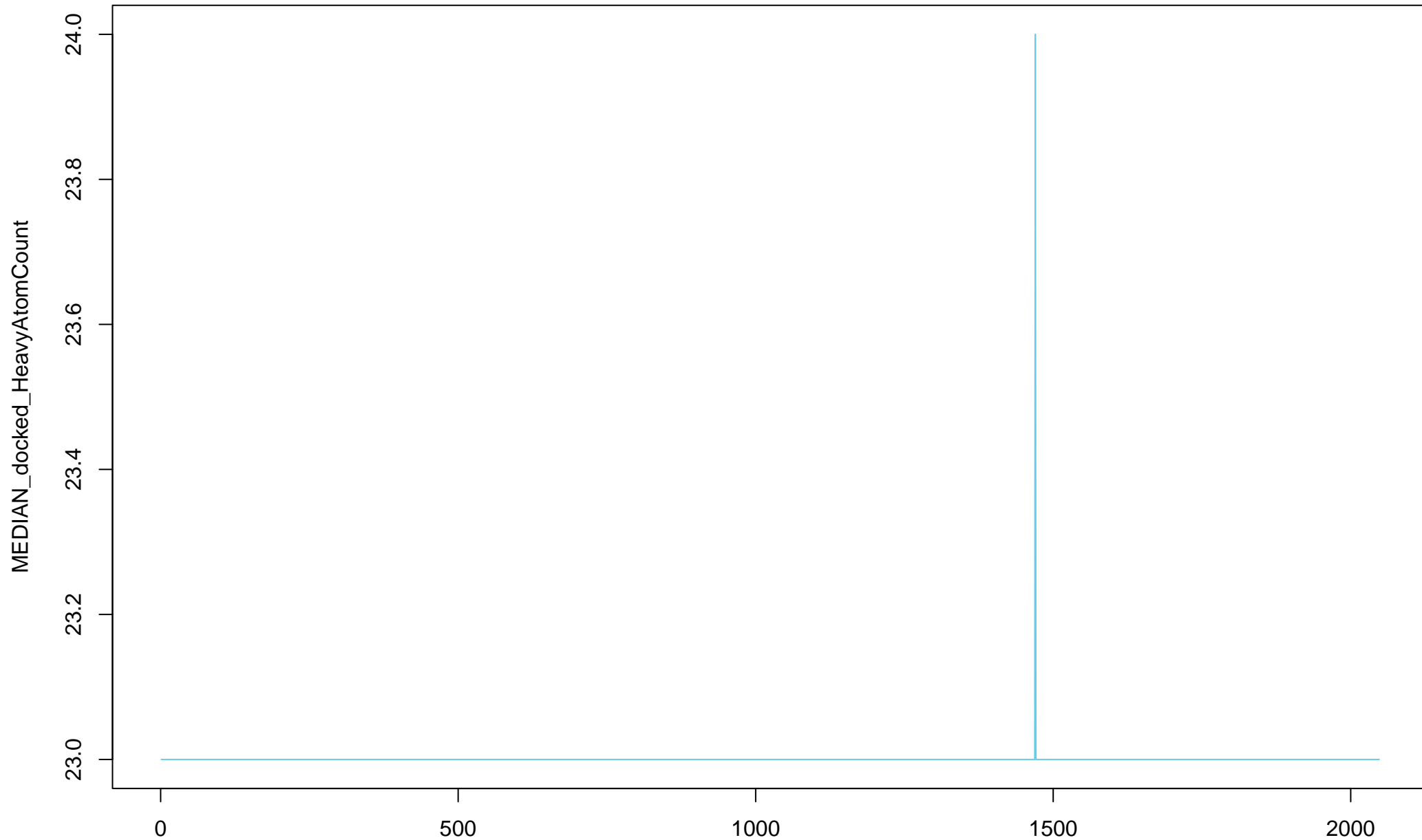
MEDIAN_logit_ec_tanimoto_similarity
ESS = 69.1 | BMK = 0.245 | MCSE(6.27) = 6.39 | stat: FALSE | burn: 0



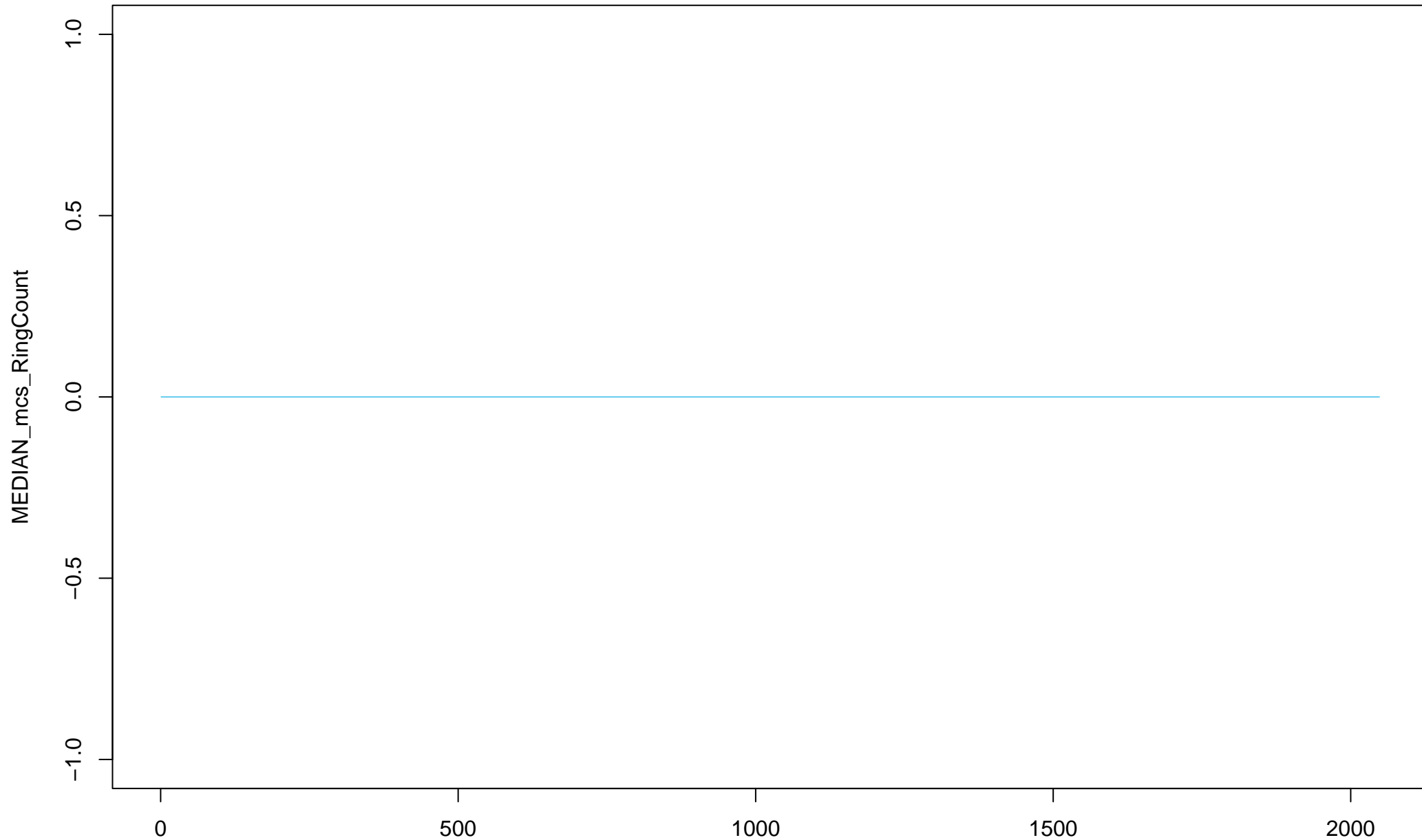
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



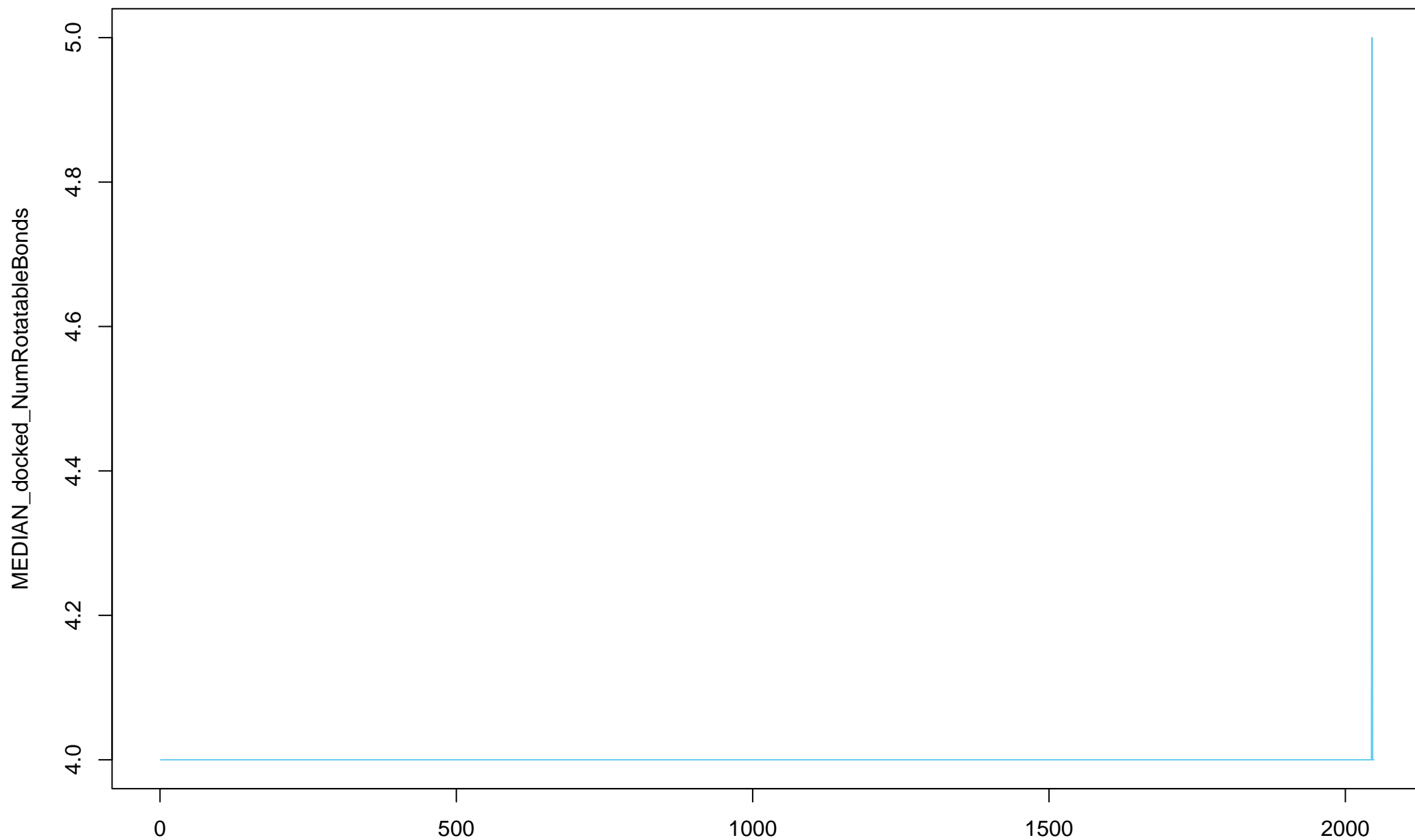
MEDIAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.524 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 1632



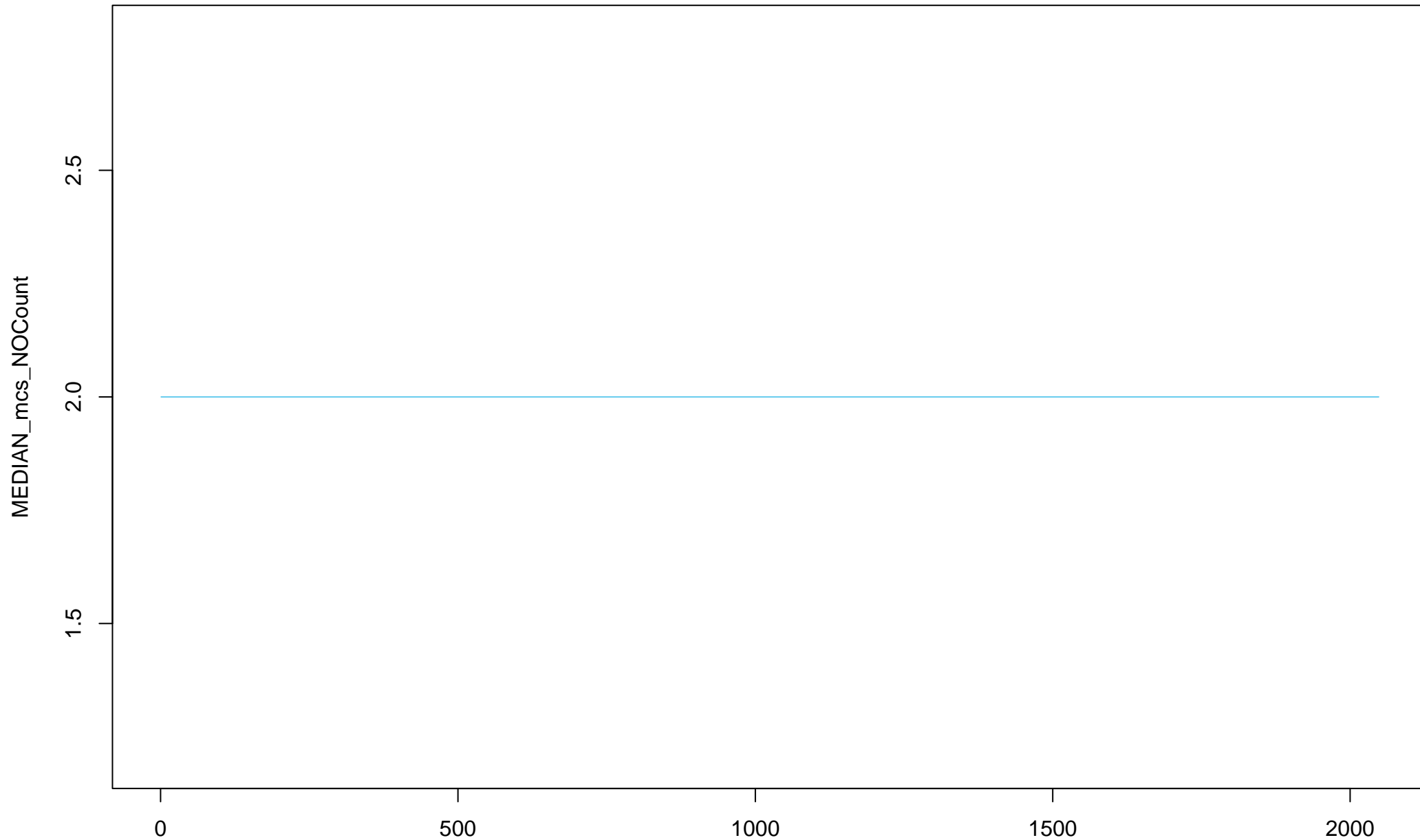
MEDIAN_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



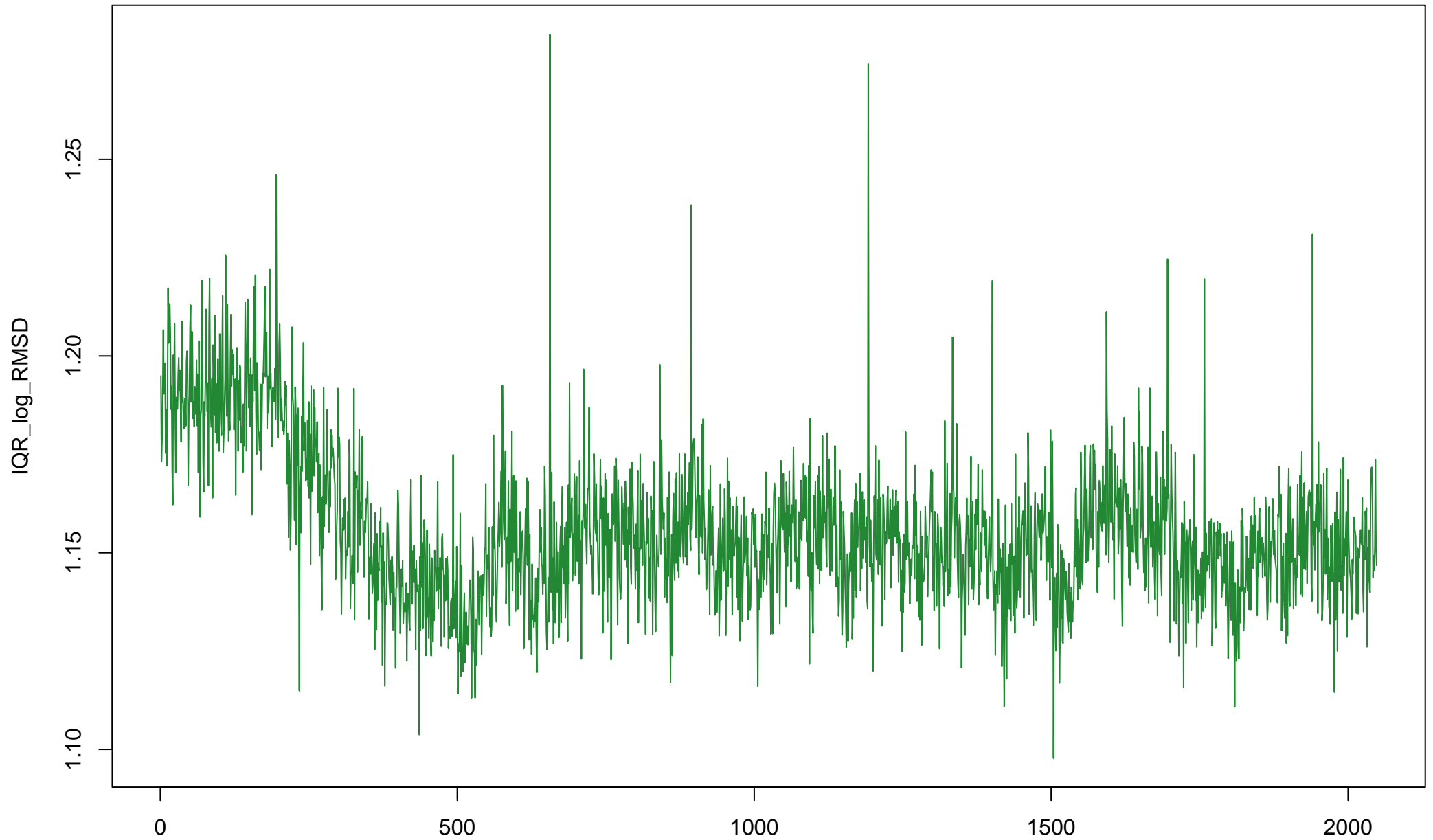
MEDIAN_docked_NumRotatableBonds
ESS = 2050 | BMK = 0.617 | MCSE(6.27) = 0 | stat: FALSE | burn: 0



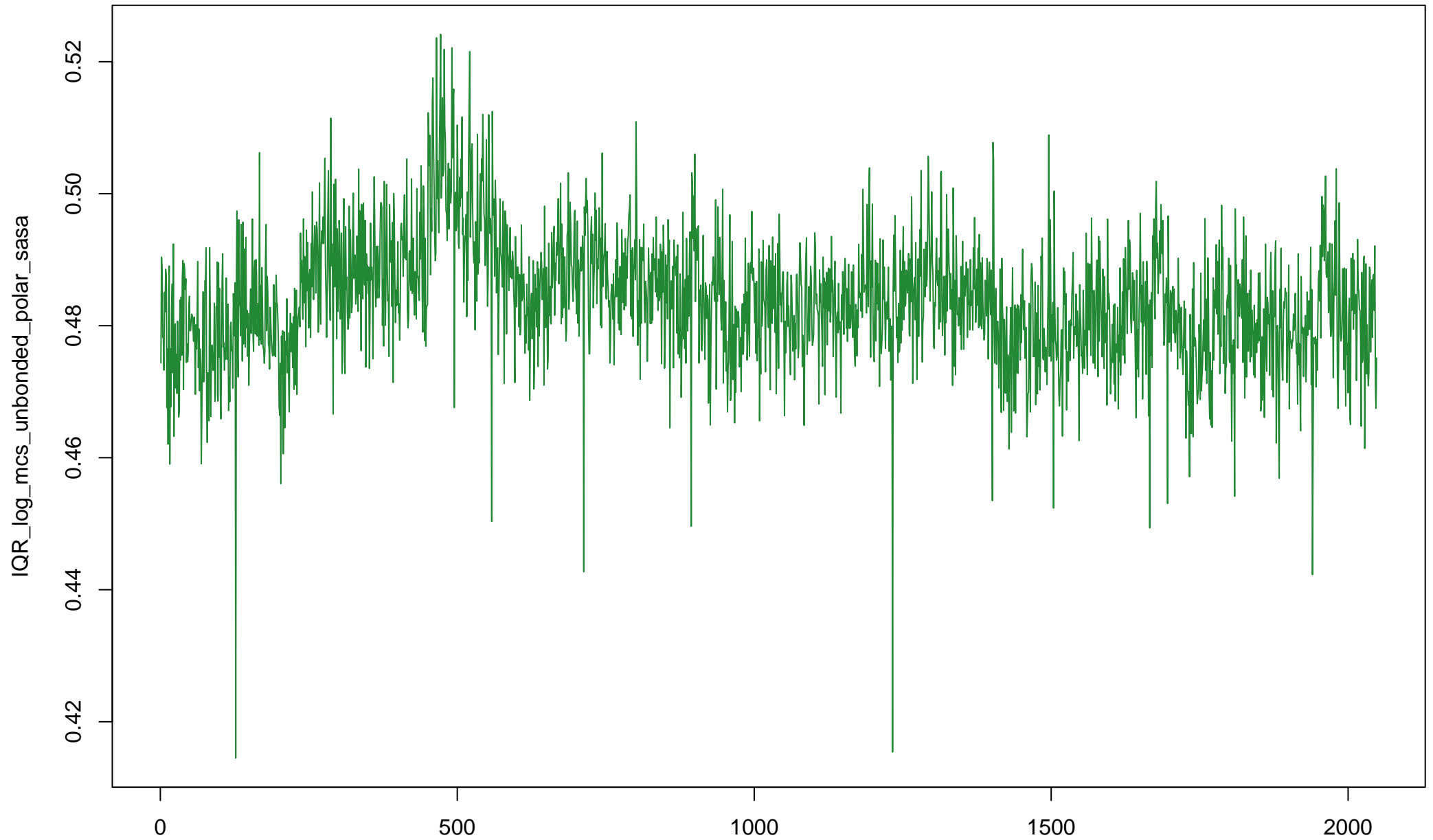
MEDIAN_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



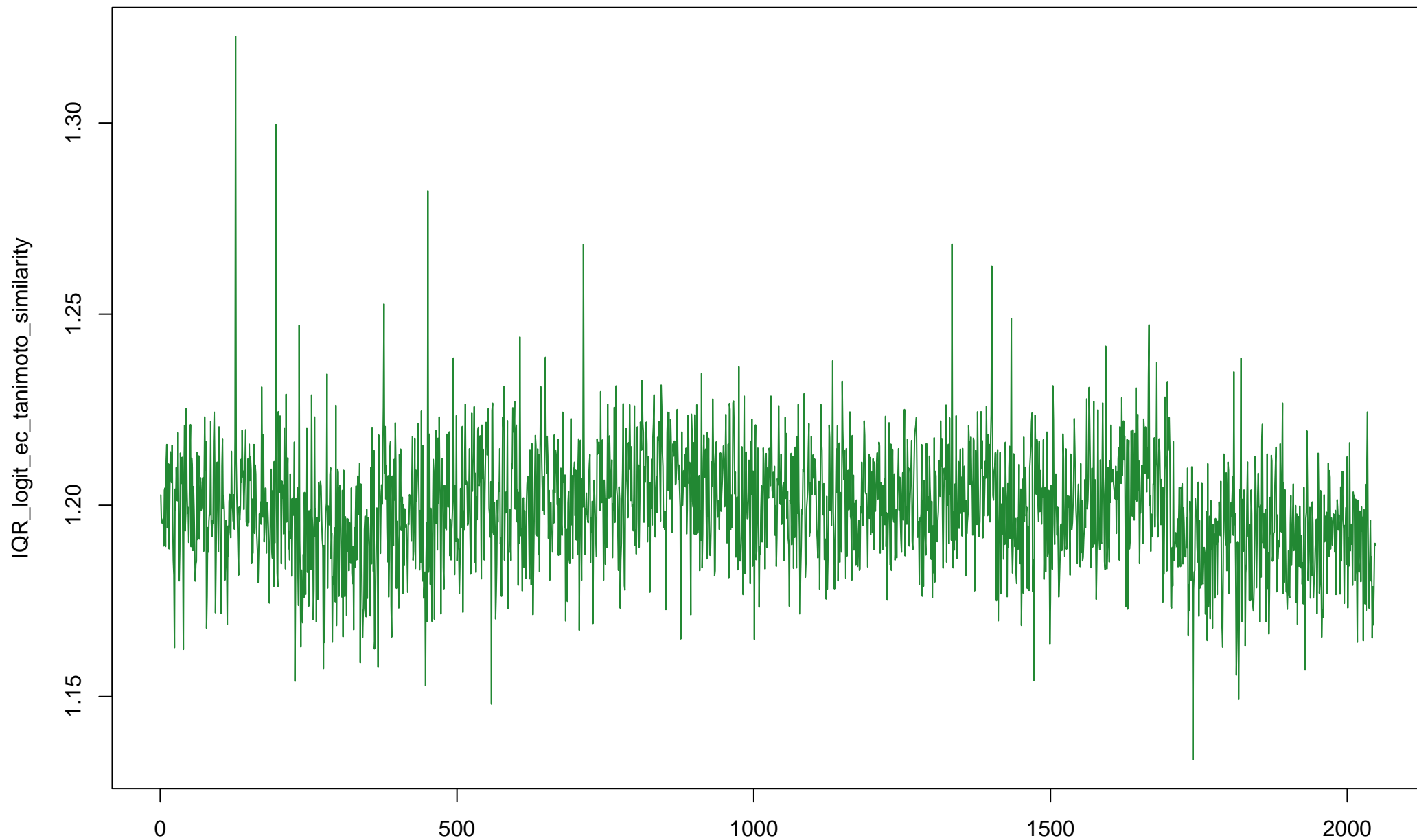
IQR_log_RMSD
ESS = 15.1 | BMK = 0.27 | MCSE(6.27) = 10.7 | stat: FALSE | burn: 204



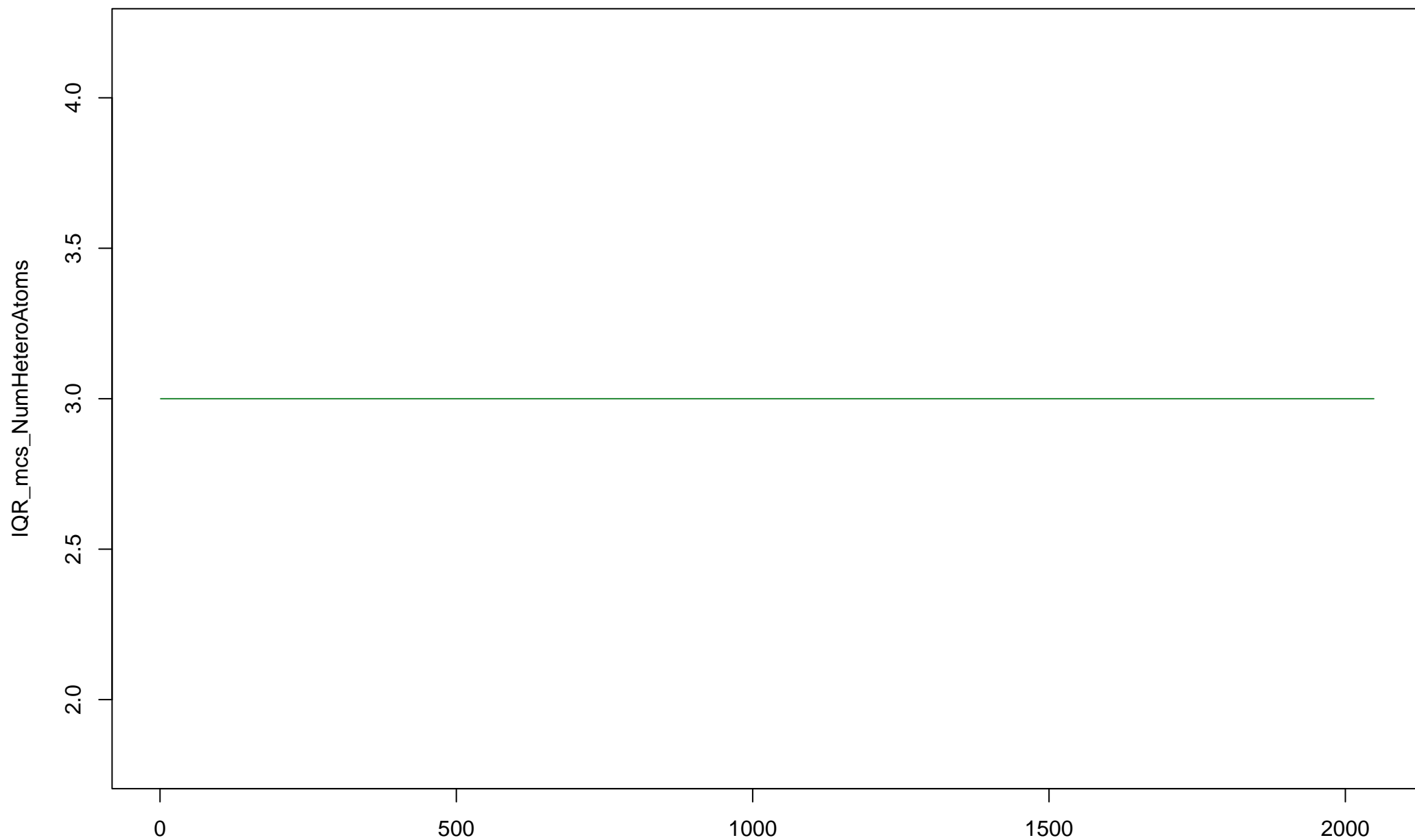
IQR_log_mcs_unbonded_polar_sasa
ESS = 66.2 | BMK = 0.202 | MCSE(6.27) = 8.37 | stat: FALSE | burn: 0



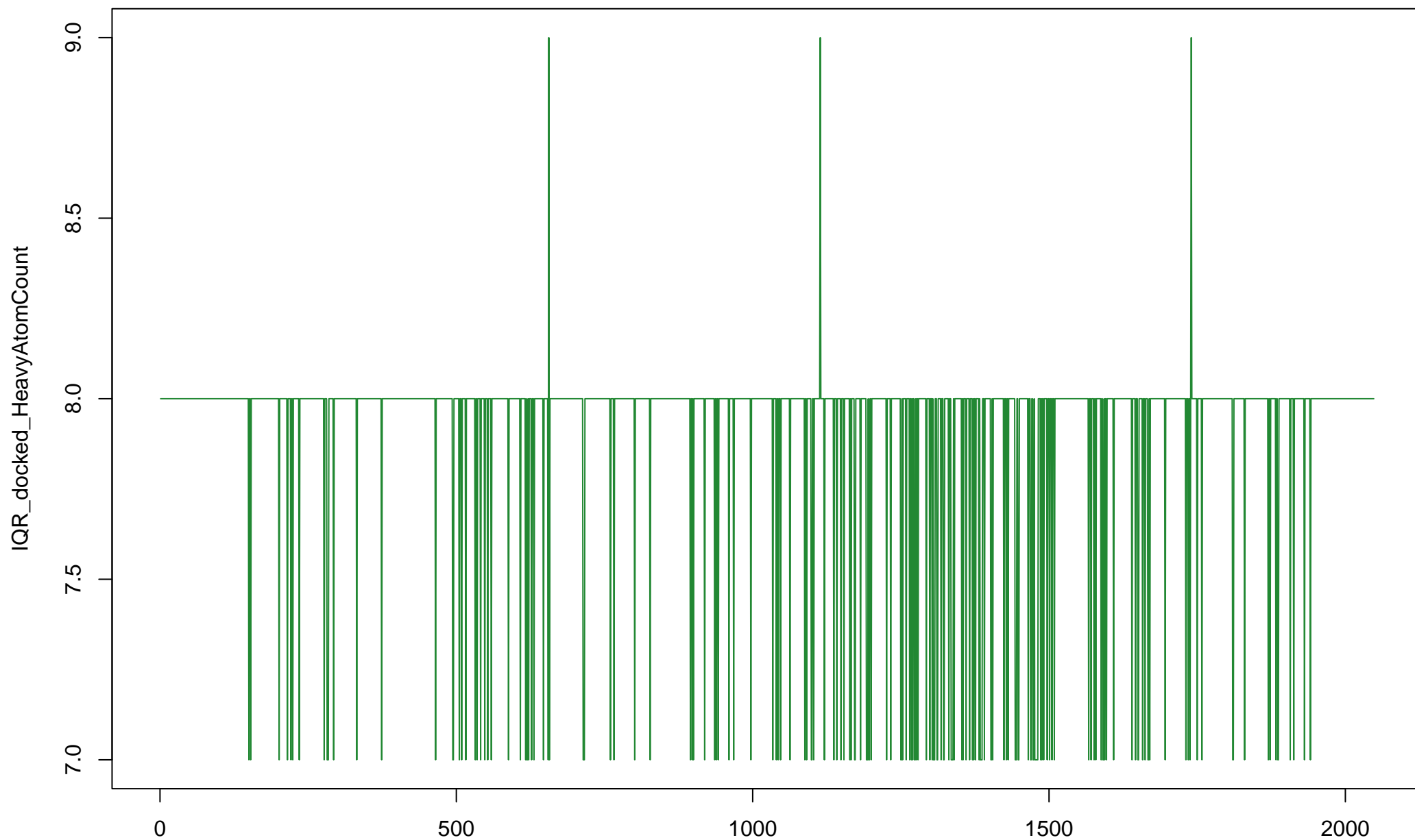
IQR_logit_ec_tanimoto_similarity
ESS = 148 | BMK = 0.0714 | MCSE(6.27) = 5 | stat: TRUE | burn: 0



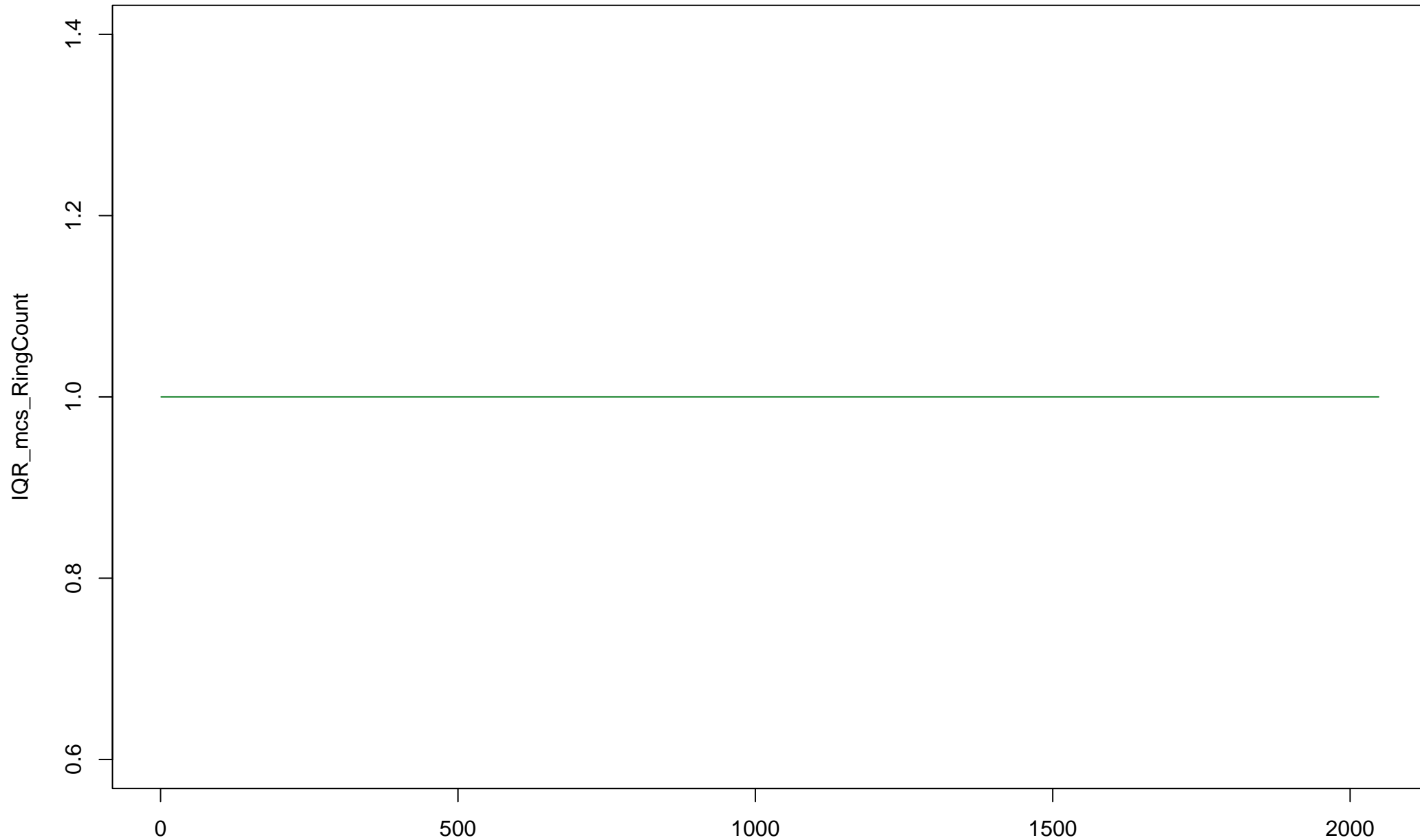
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



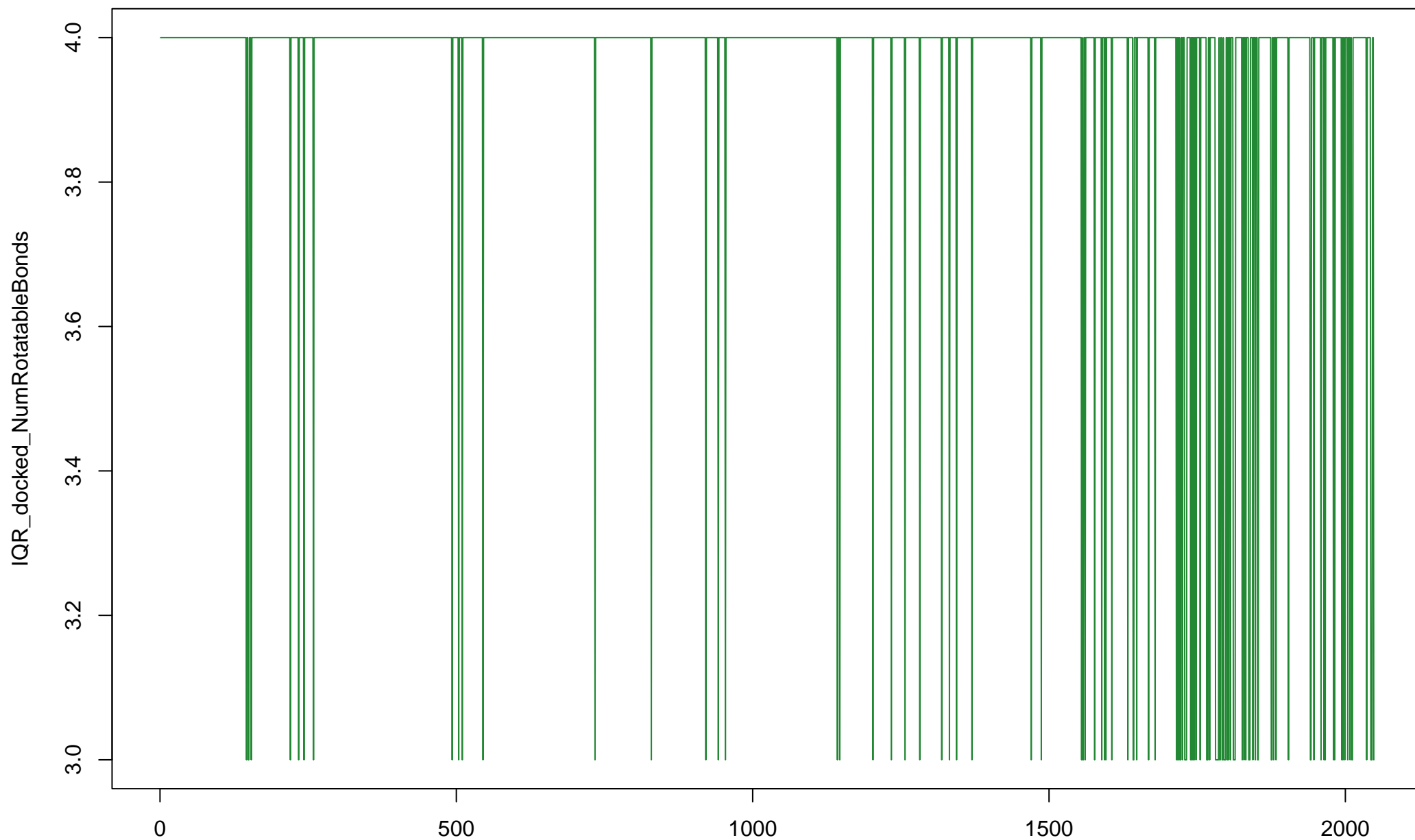
IQR_docked_HeavyAtomCount
ESS = 405 | BMK = 0.21 | MCSE(6.27) = 4.17 | stat: FALSE | burn: 0



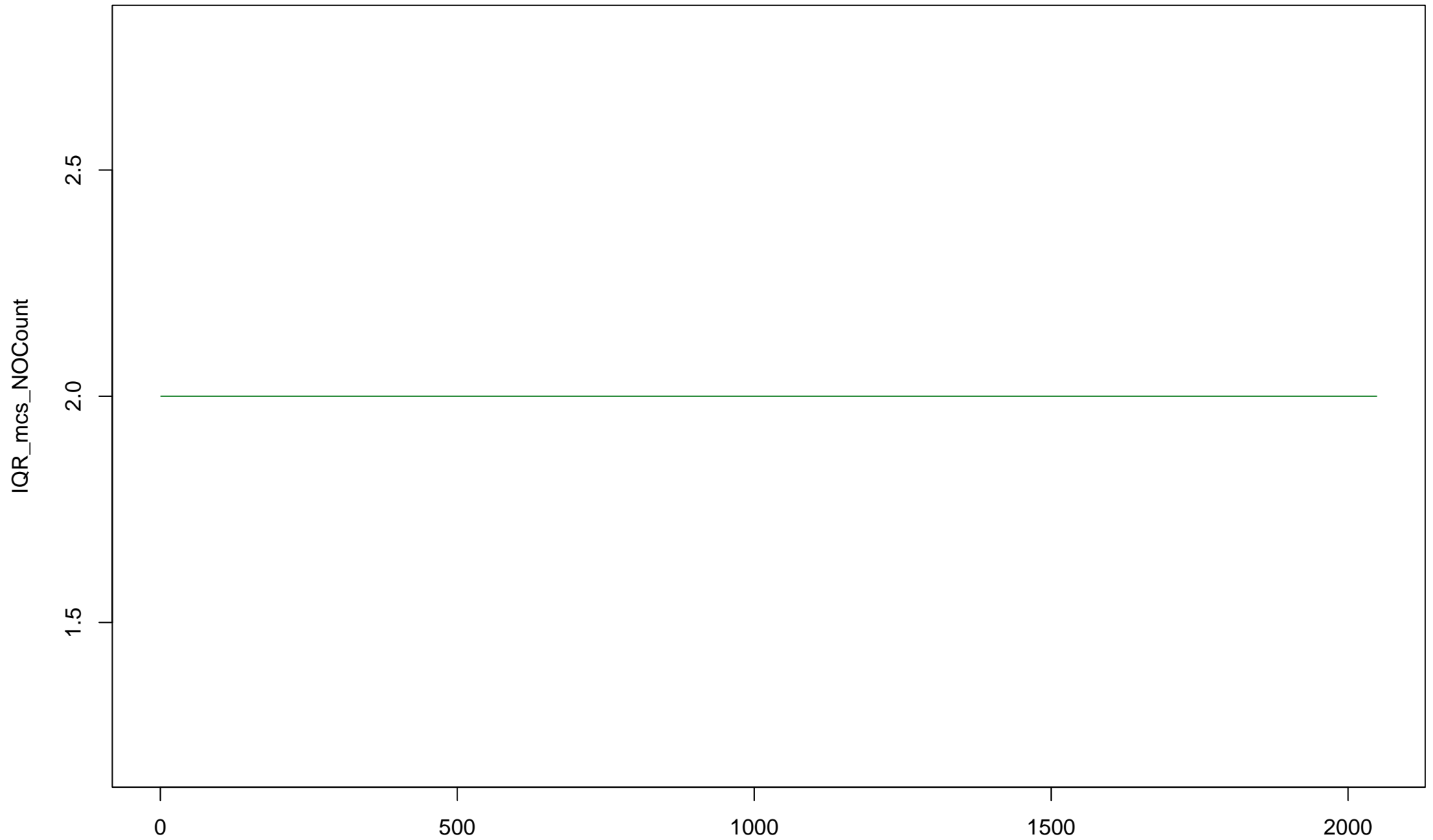
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



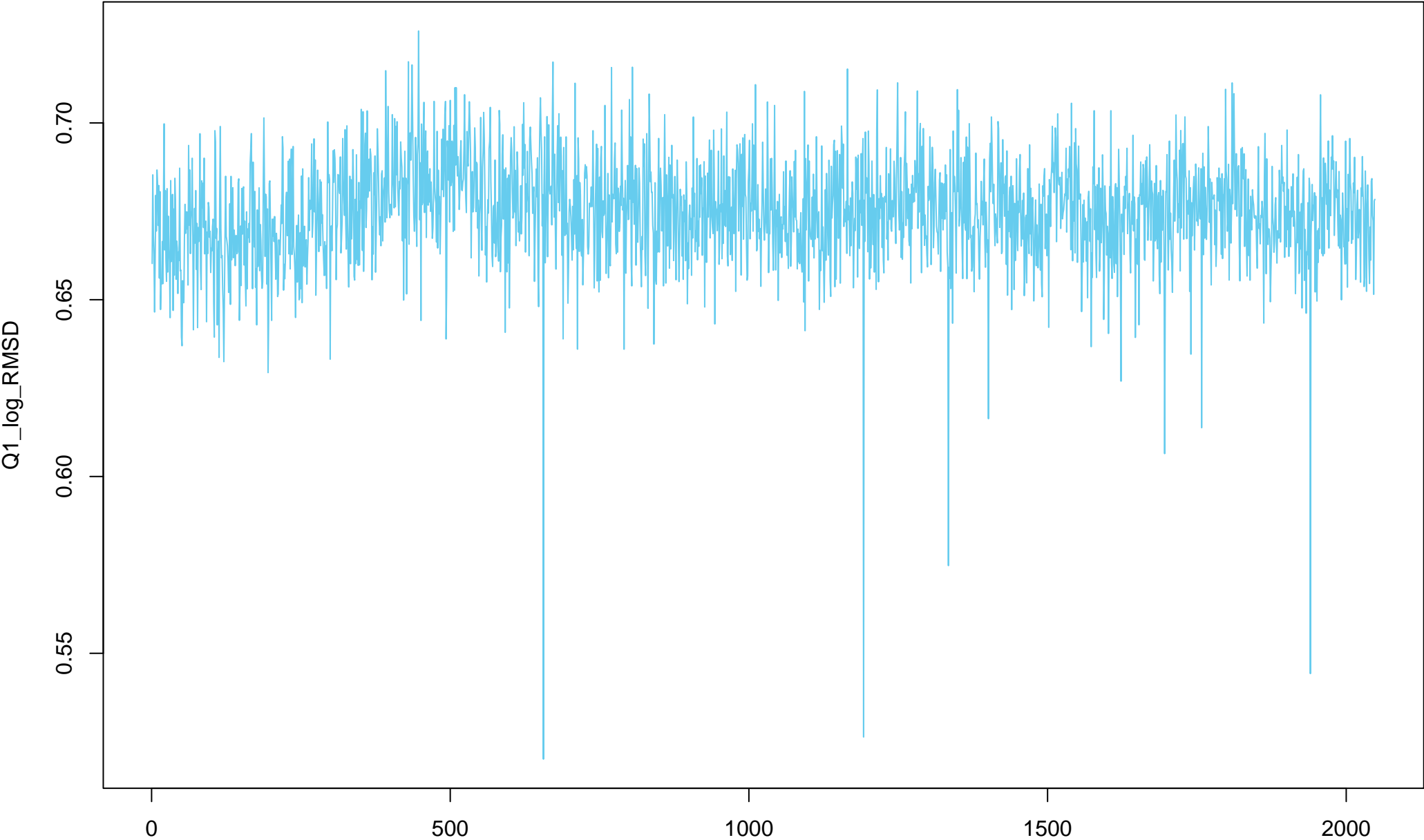
IQR_docked_NumRotatableBonds
ESS = 131 | BMK = 0.29 | MCSE(6.27) = 5.85 | stat: FALSE | burn: 0



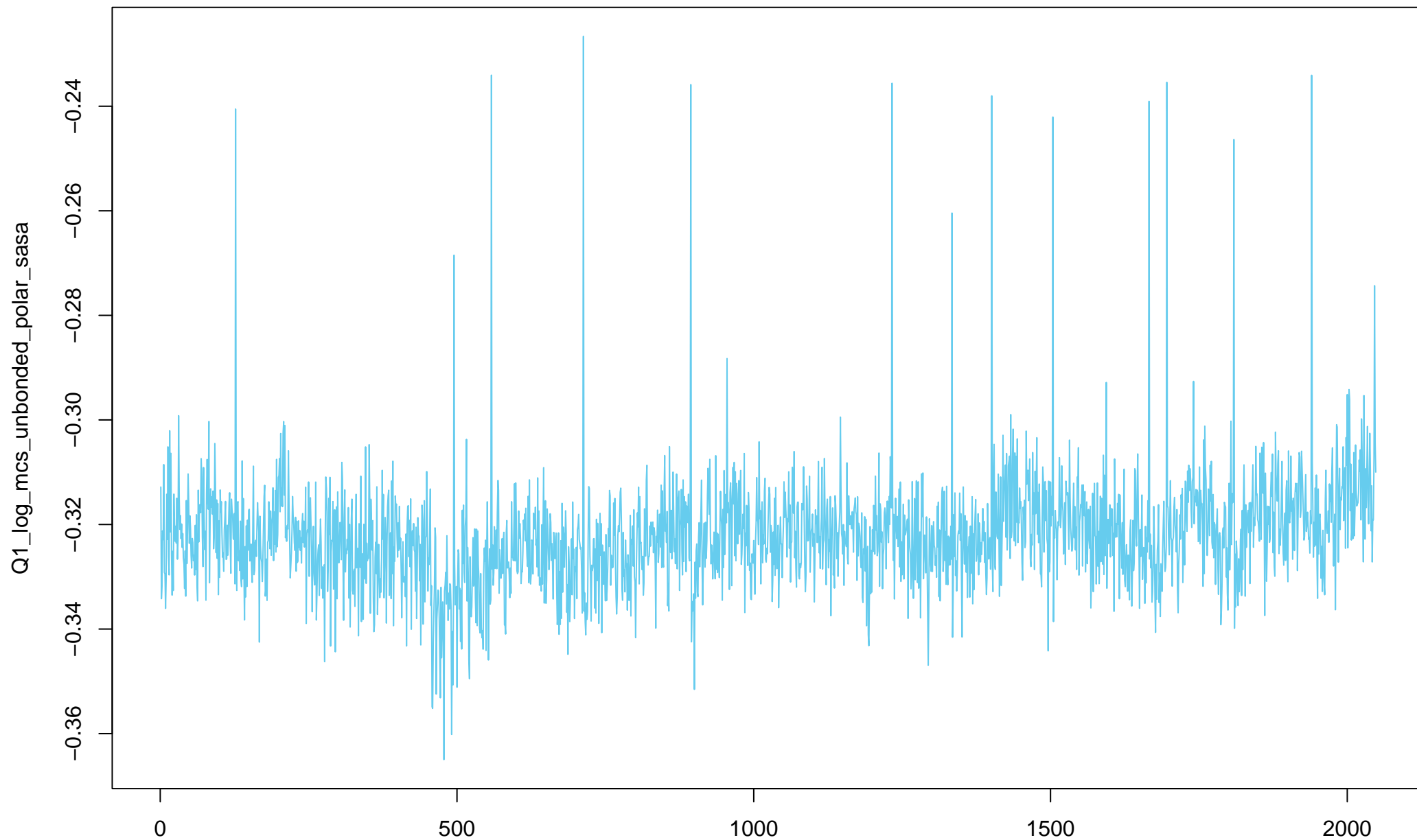
IQR_mcs_NOCOUNT
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



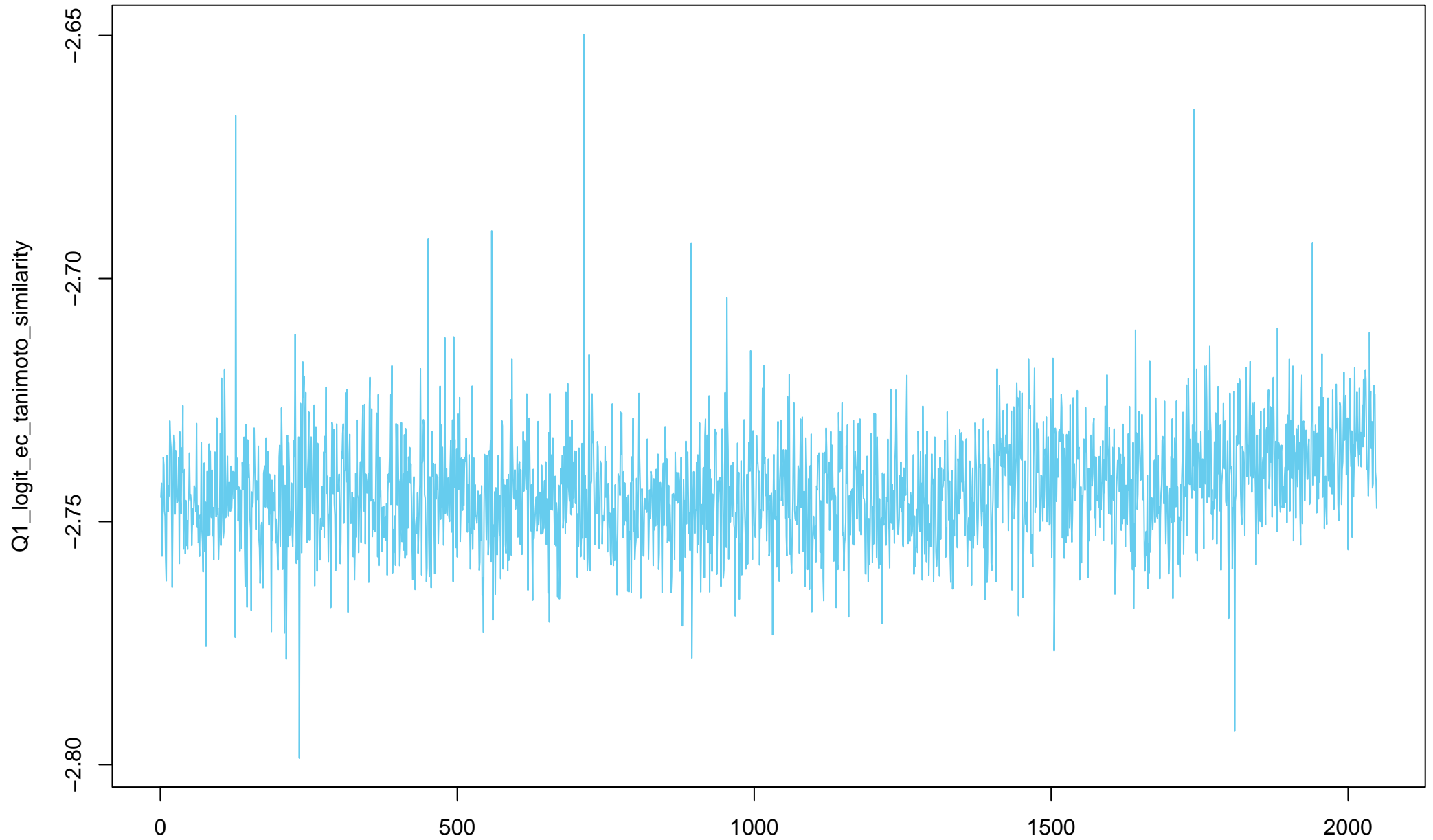
Q1_log_RMSD
ESS = 329 | BMK = 0.107 | MCSE(6.27) = 4.45 | stat: FALSE | burn: 0



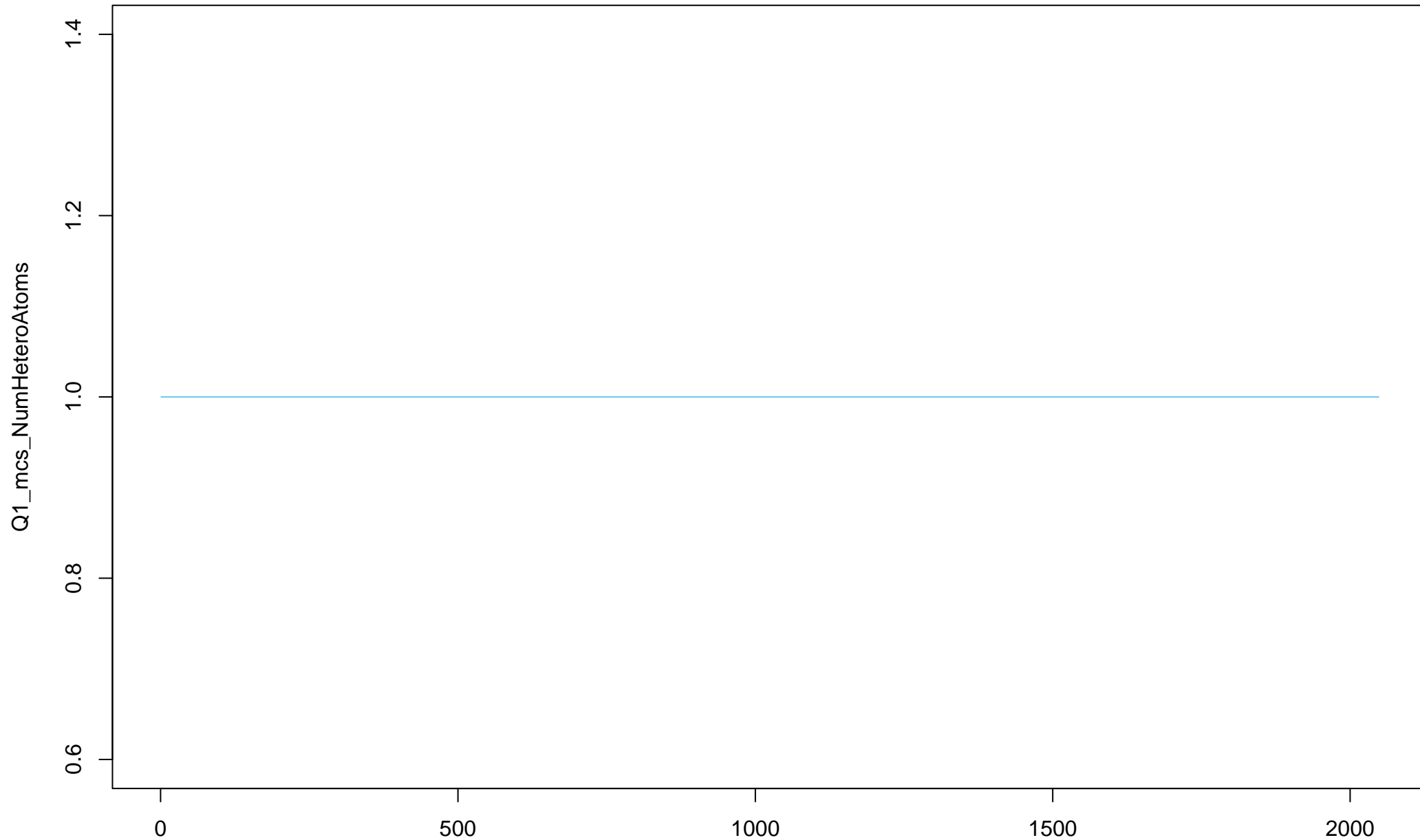
Q1_log_mcs_unbonded_polar_sasa
ESS = 115 | BMK = 0.185 | MCSE(6.27) = 5.55 | stat: TRUE | burn: 0



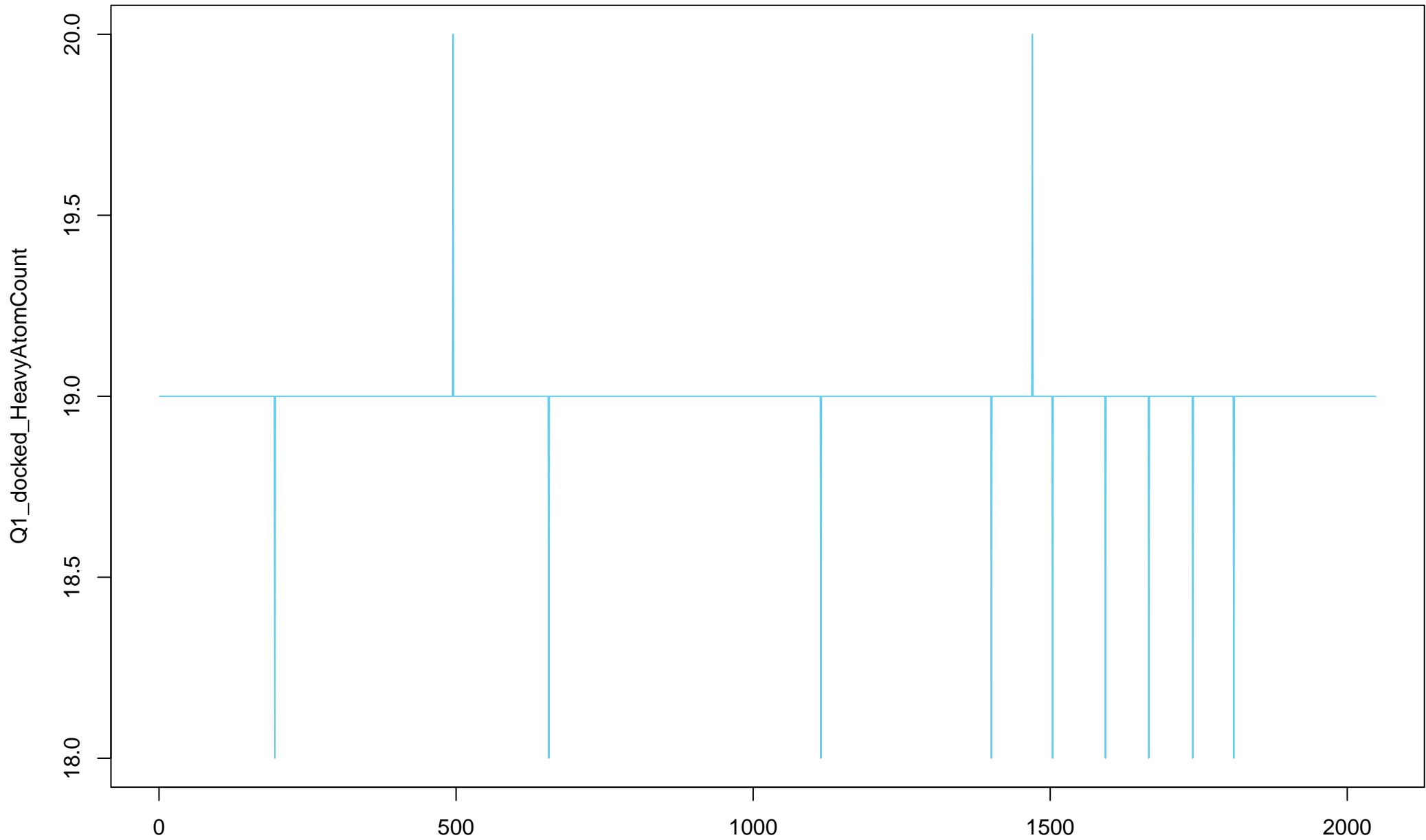
Q1_logit_ec_tanimoto_similarity
ESS = 221 | BMK = 0.13 | MCSE(6.27) = 4.47 | stat: FALSE | burn: 0



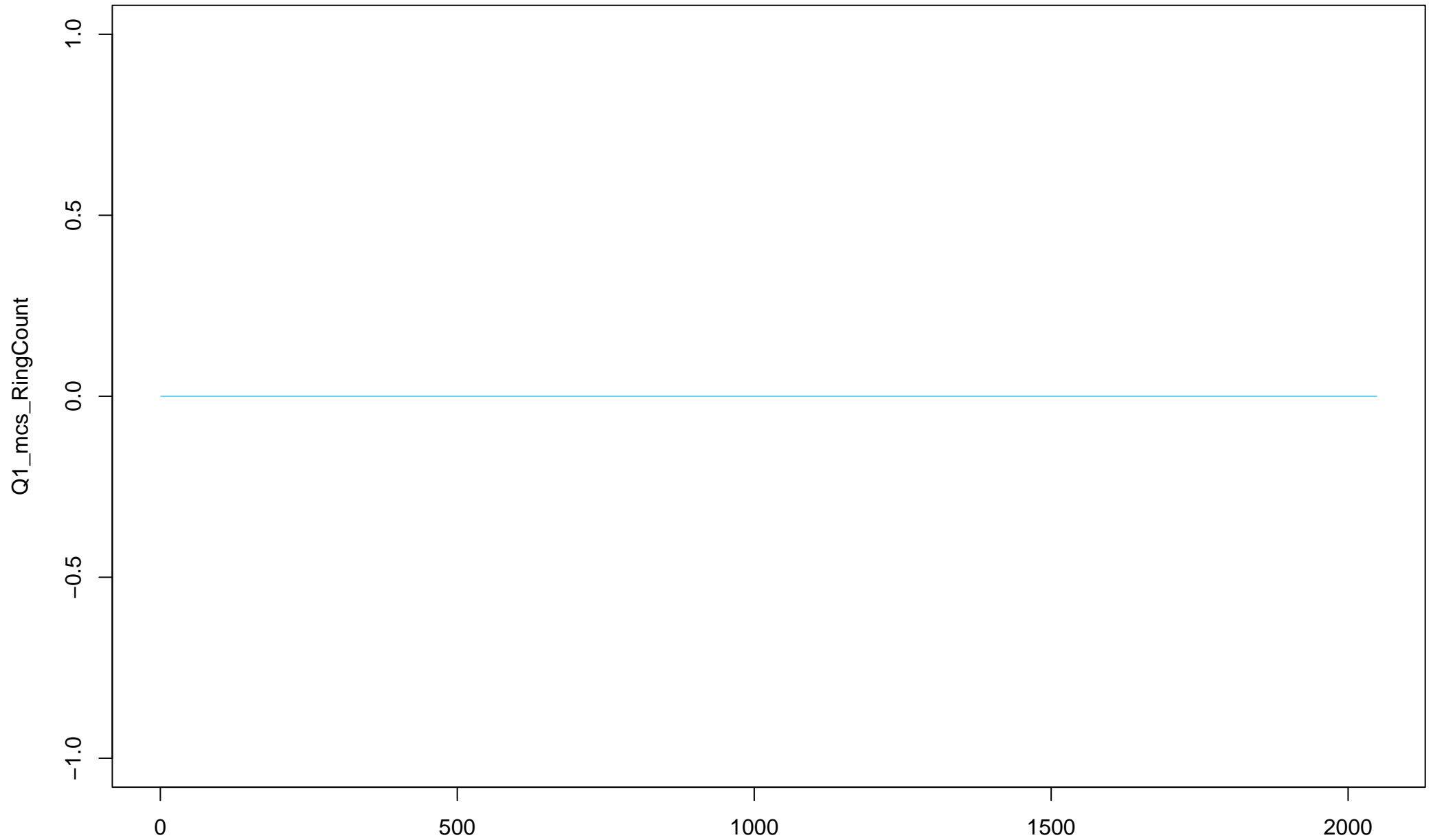
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



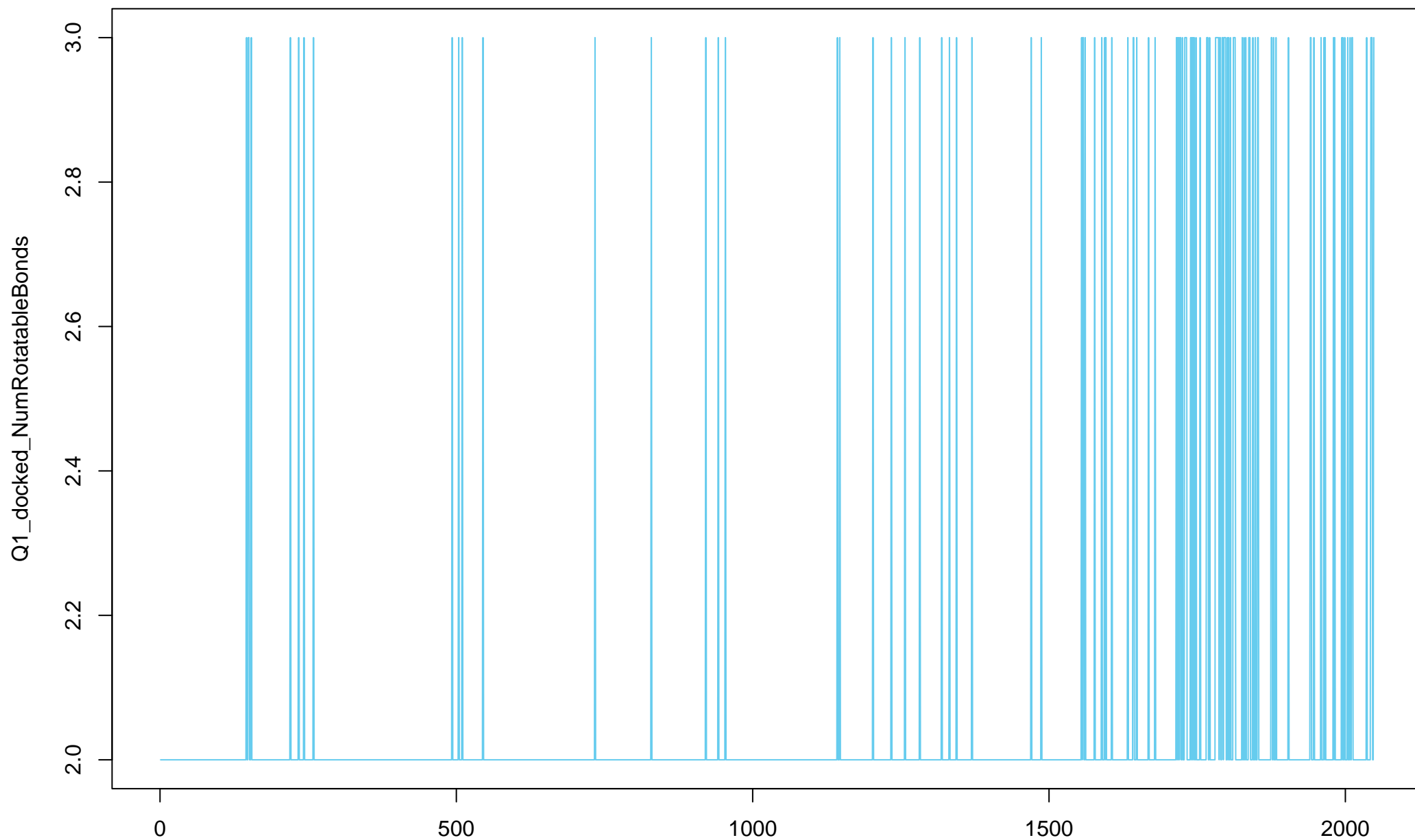
Q1_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.235 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 1020



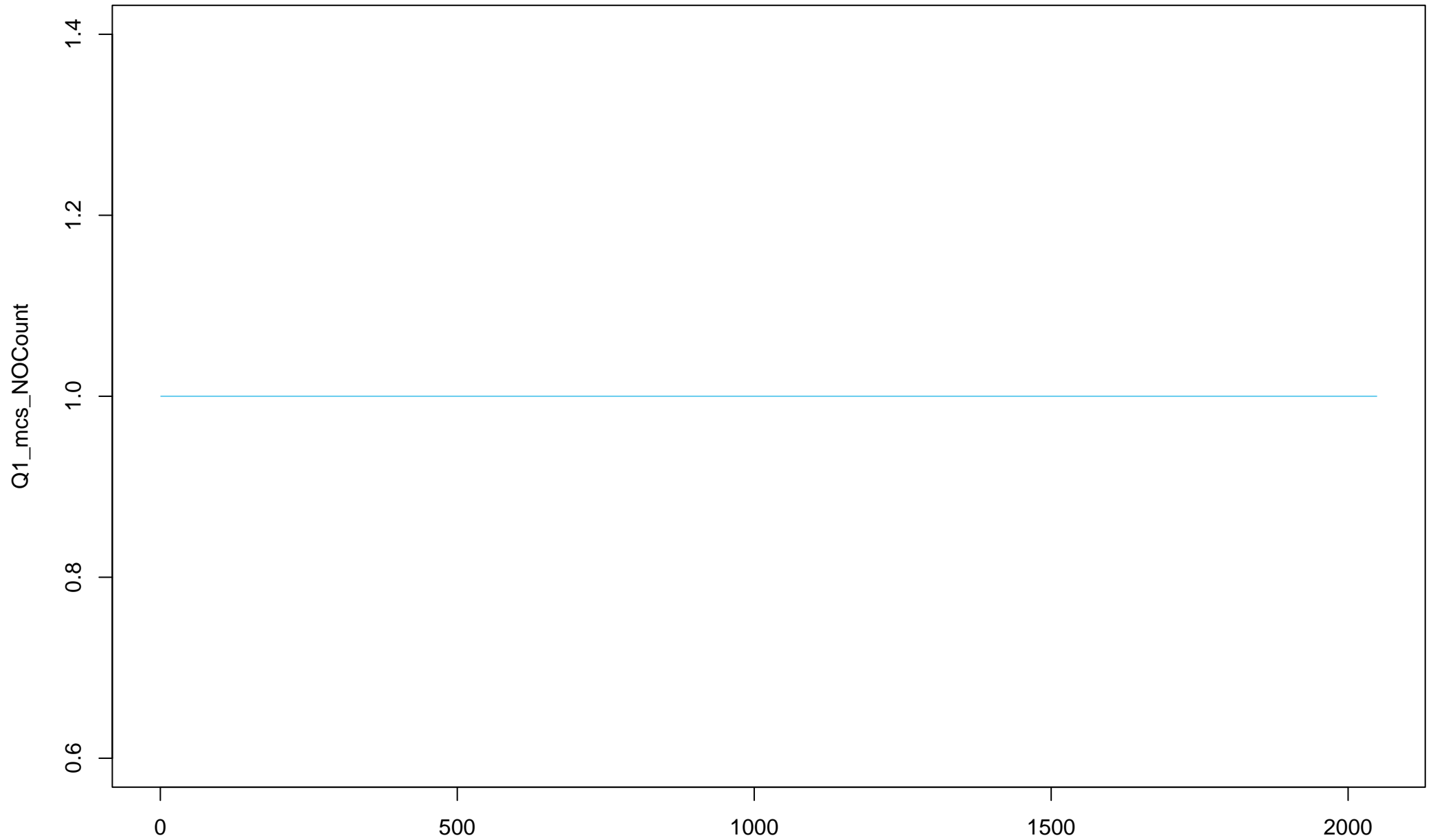
Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



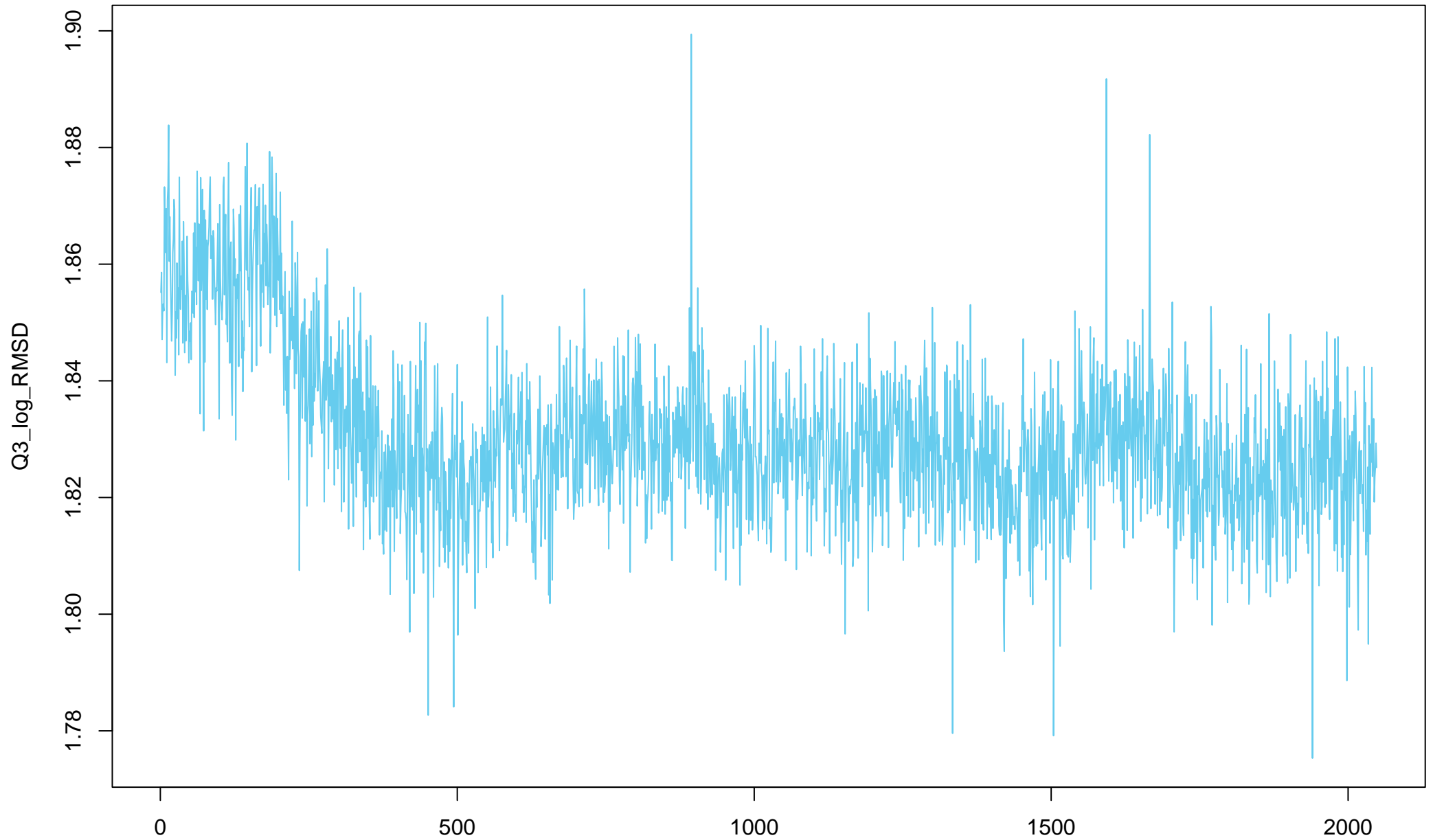
Q1_docked_NumRotatableBonds
ESS = 131 | BMK = 0.29 | MCSE(6.27) = 5.85 | stat: FALSE | burn: 0



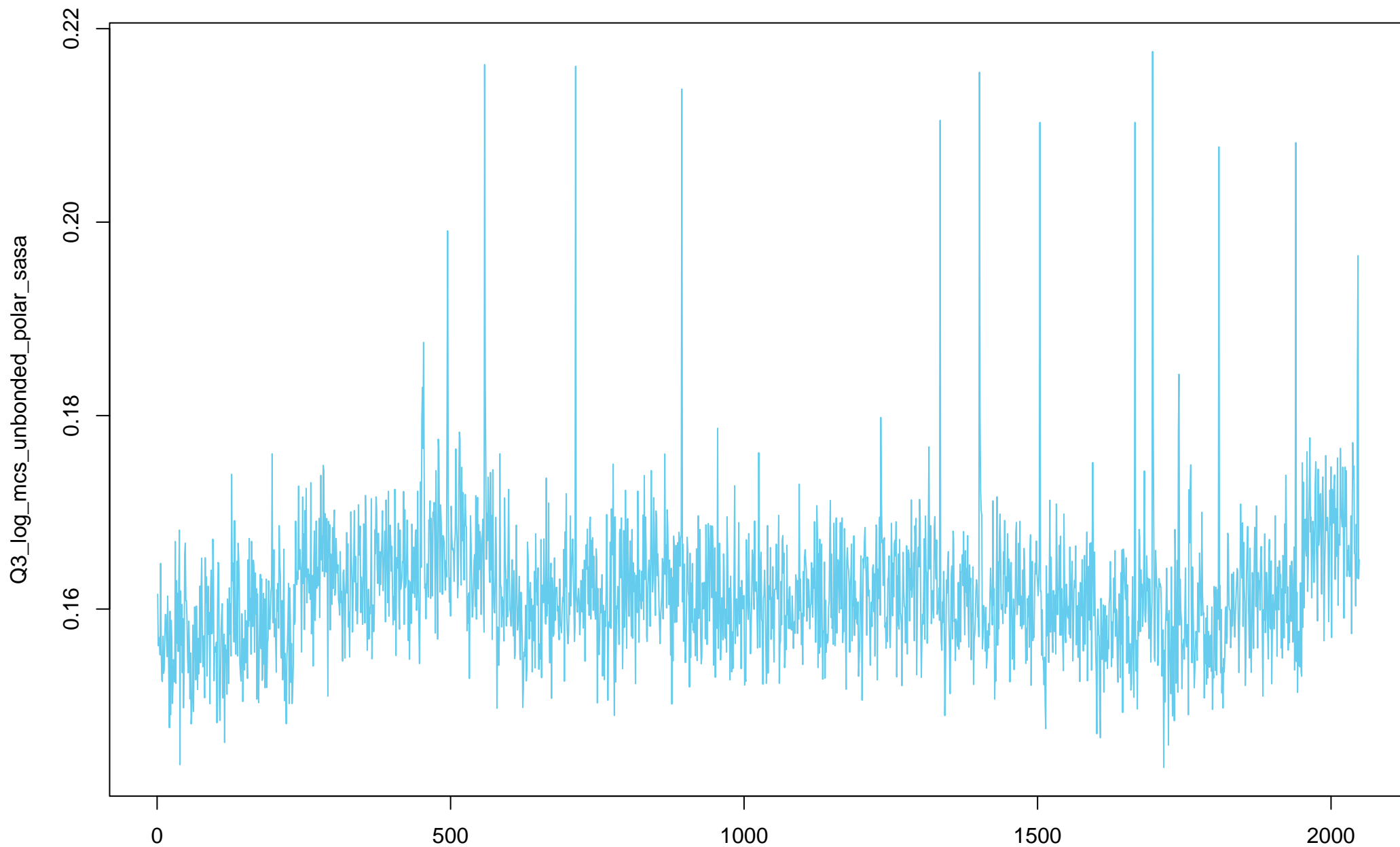
Q1_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



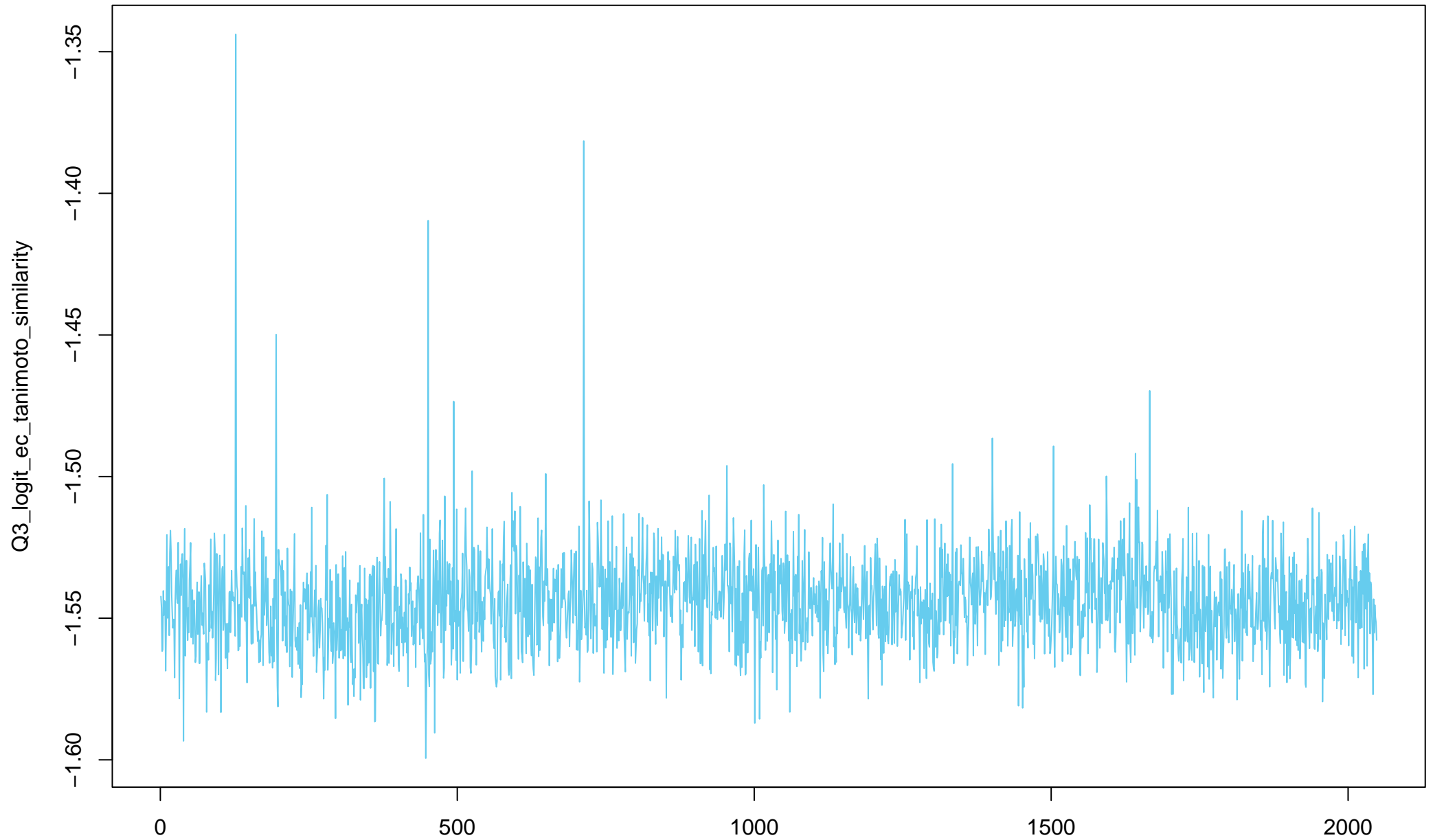
Q3_log_RMSD
ESS = 11.8 | BMK = 0.298 | MCSE(6.27) = 10.6 | stat: FALSE | burn: 204



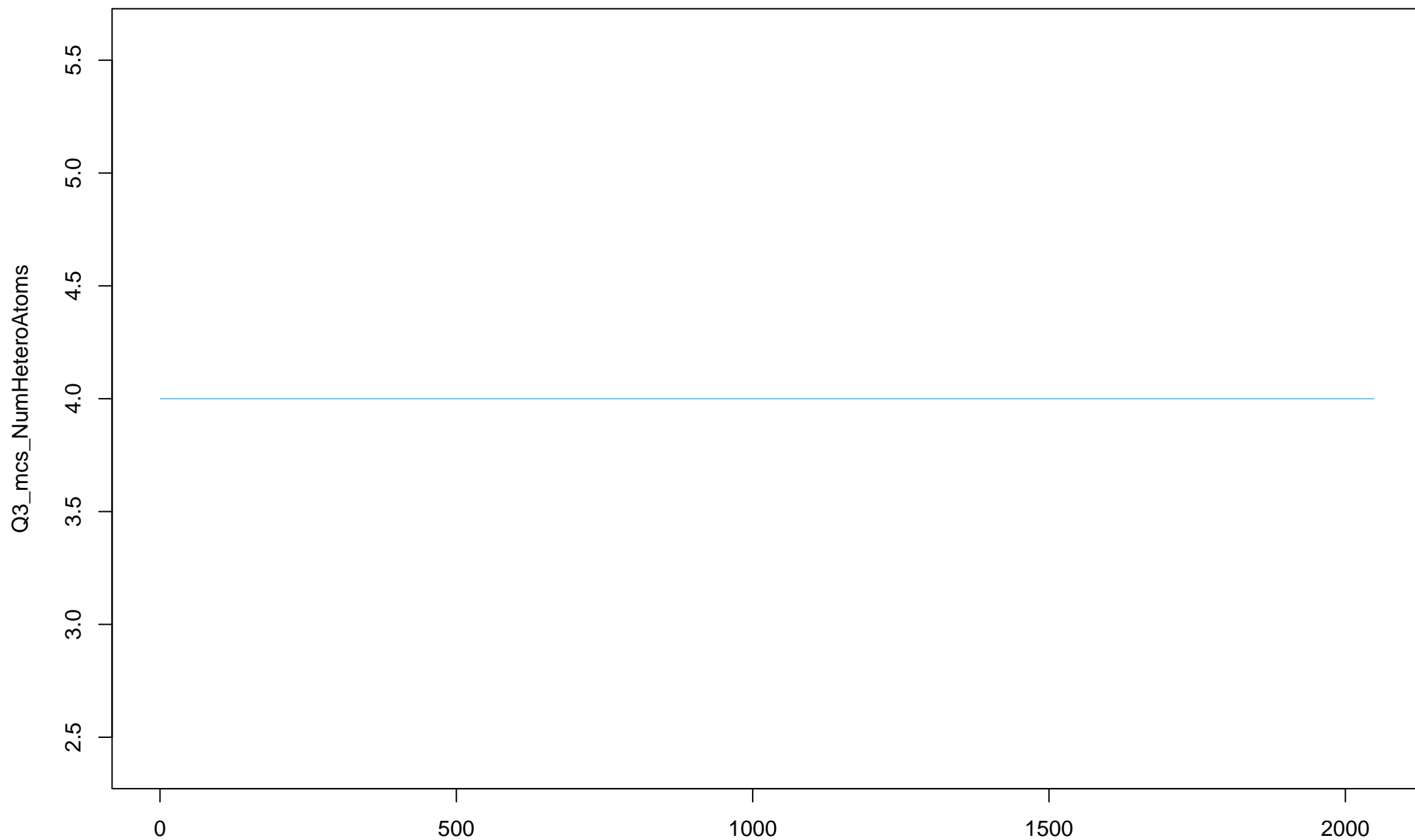
Q3_log_mcs_unbonded_polar_sasa
ESS = 165 | BMK = 0.0735 | MCSE(6.27) = 5.89 | stat: FALSE | burn: 0



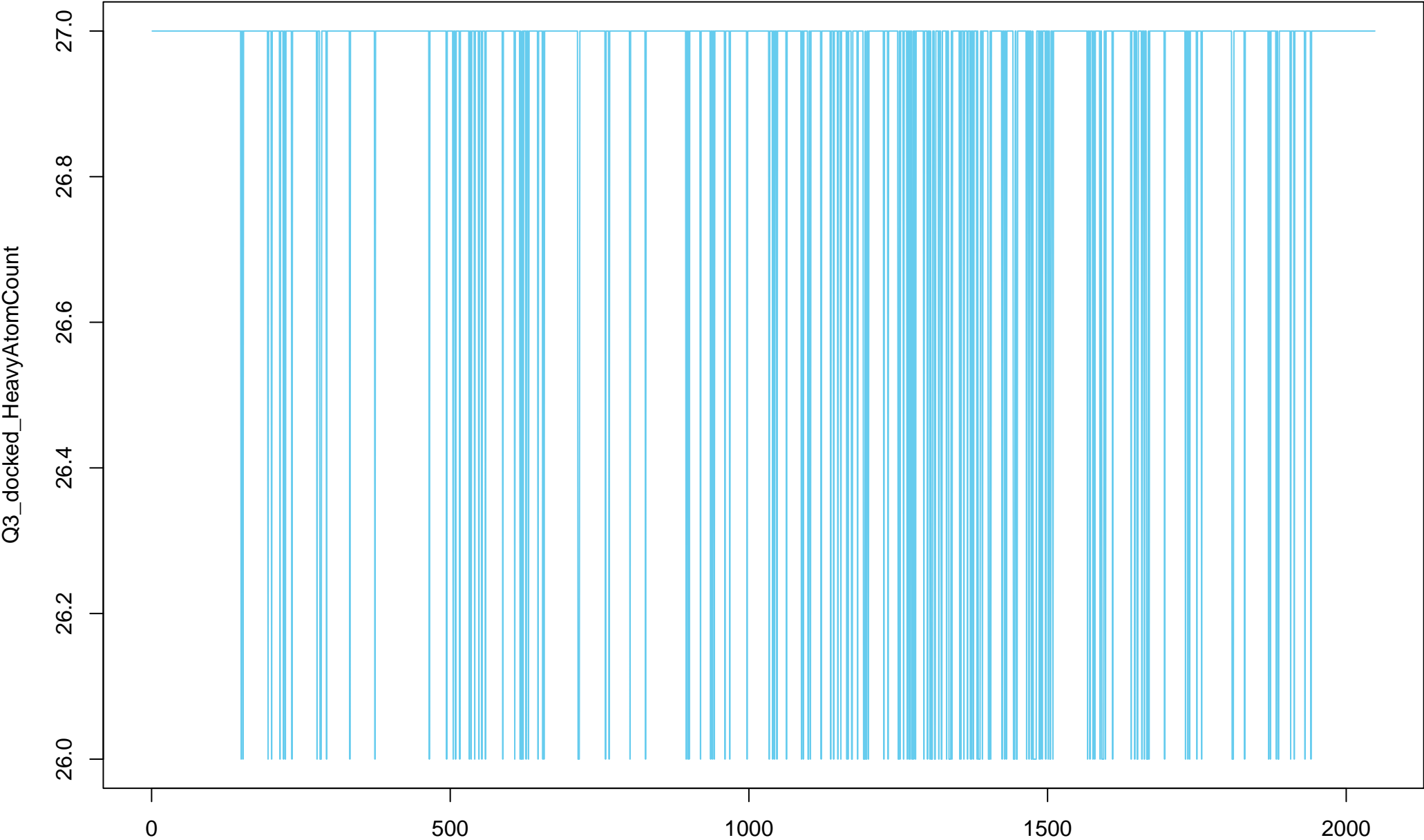
Q3_logit_ec_tanimoto_similarity
ESS = 589 | BMK = 0.0933 | MCSE(6.27) = 3.42 | stat: TRUE | burn: 0



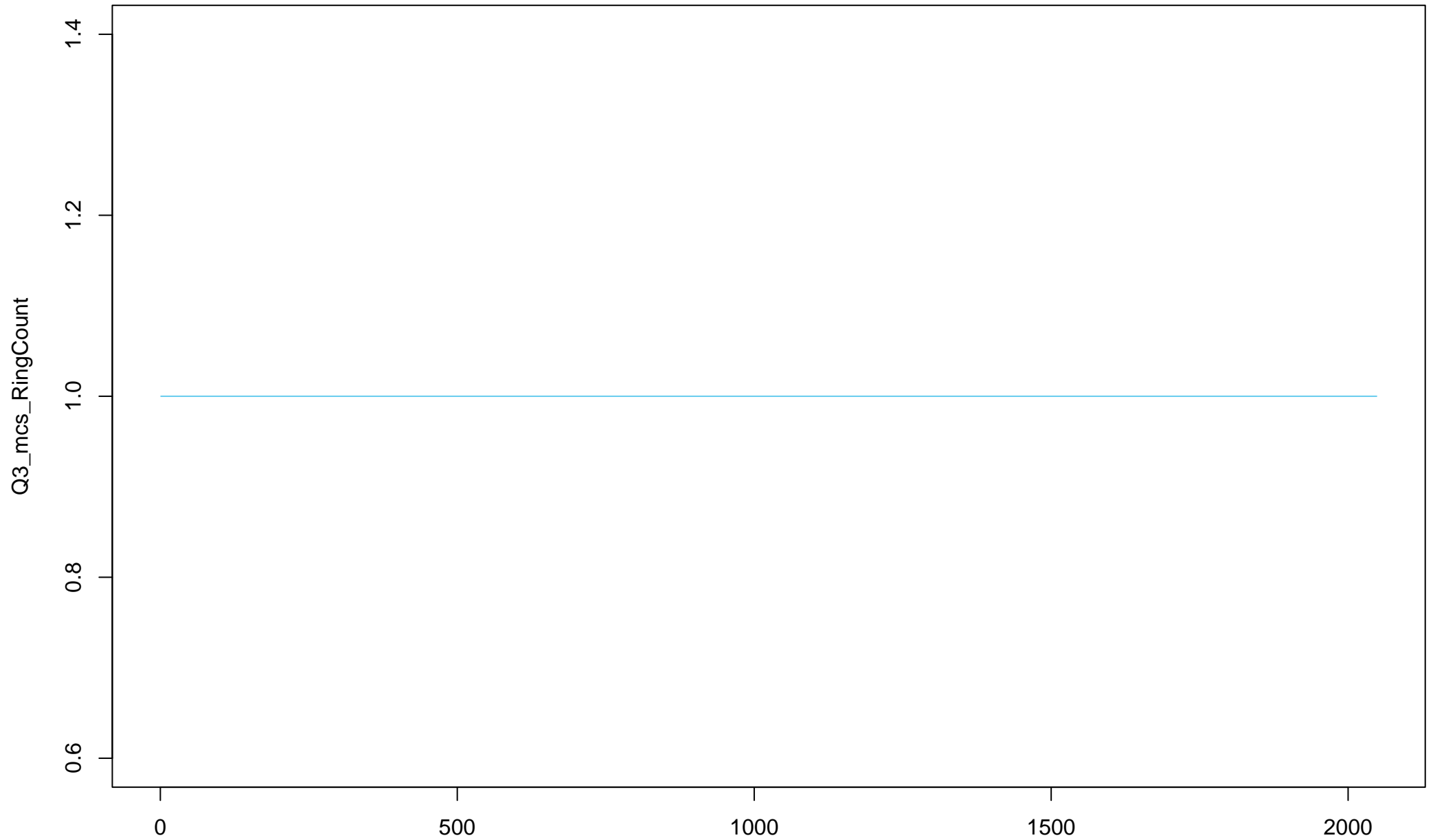
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



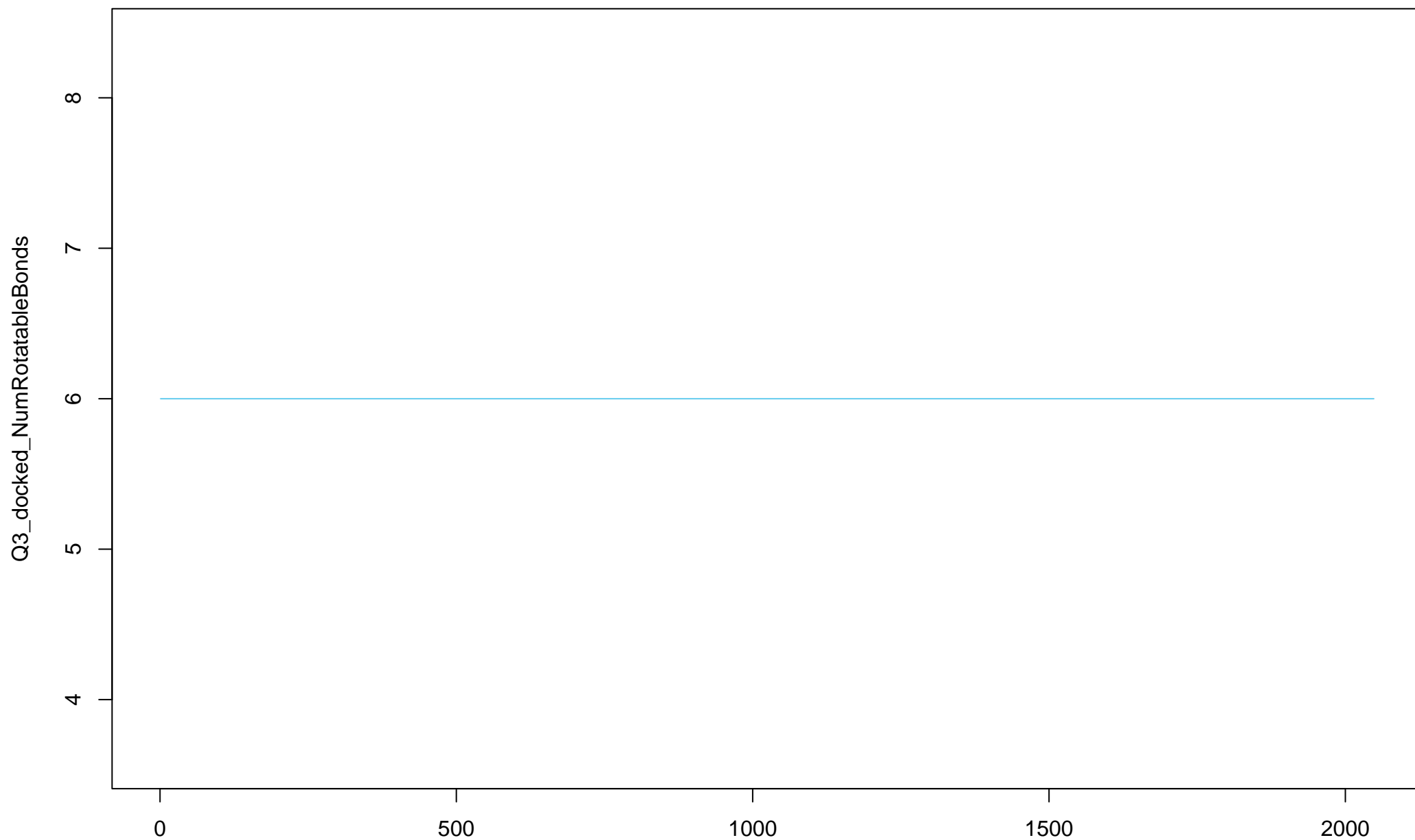
Q3_docked_HeavyAtomCount
ESS = 427 | BMK = 0.164 | MCSE(6.27) = 4.17 | stat: FALSE | burn: 0



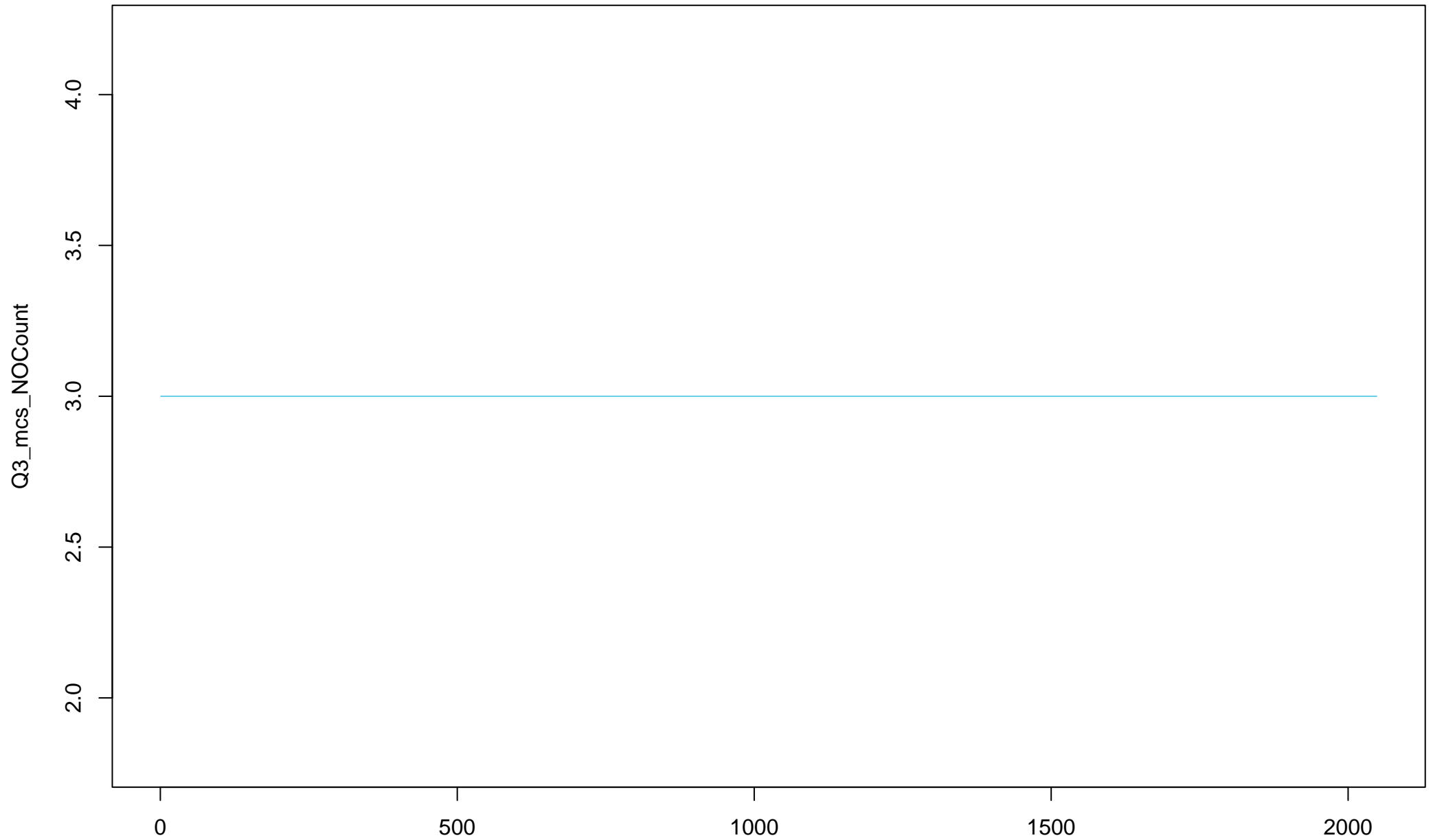
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



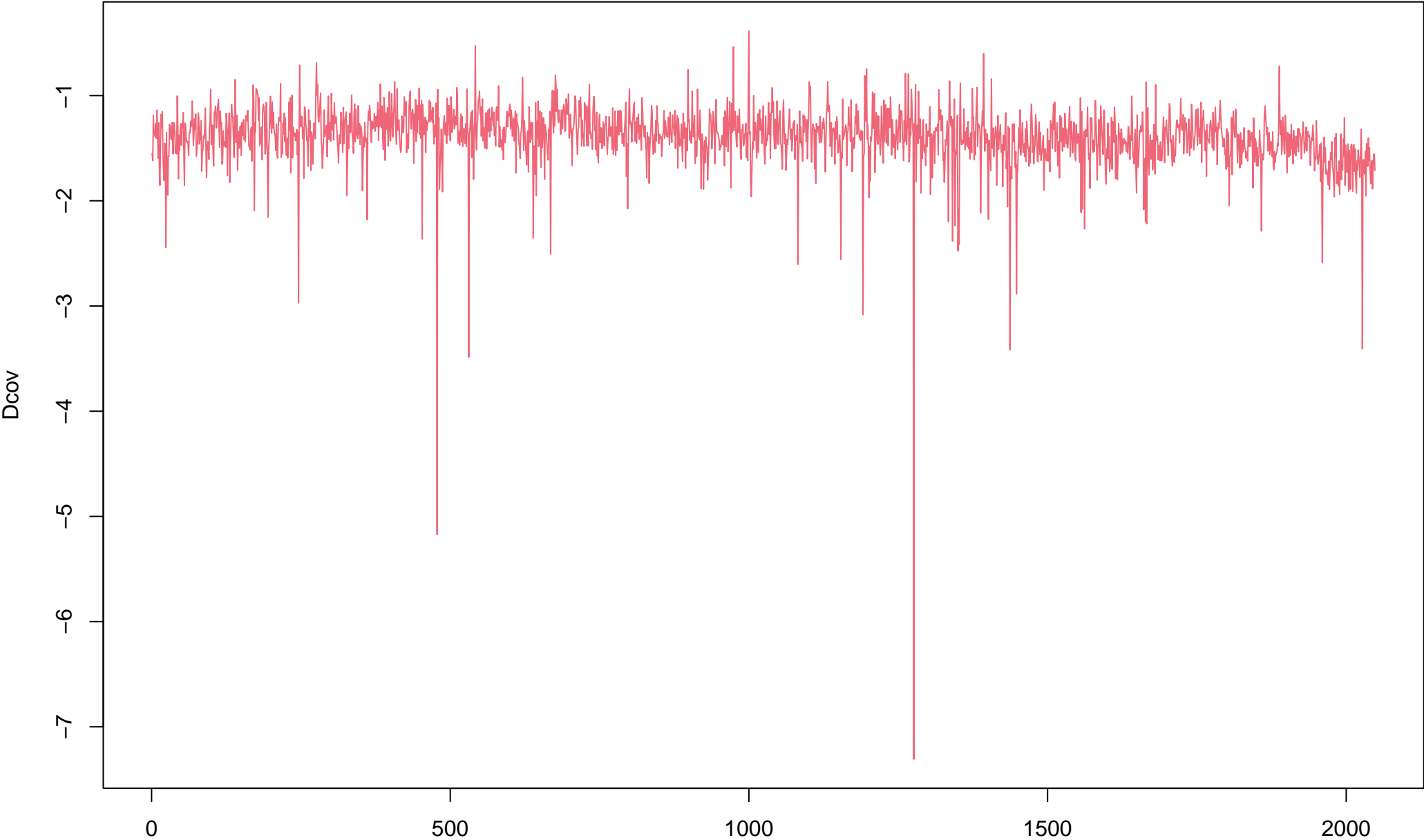
Q3_docked_NumRotatableBonds
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



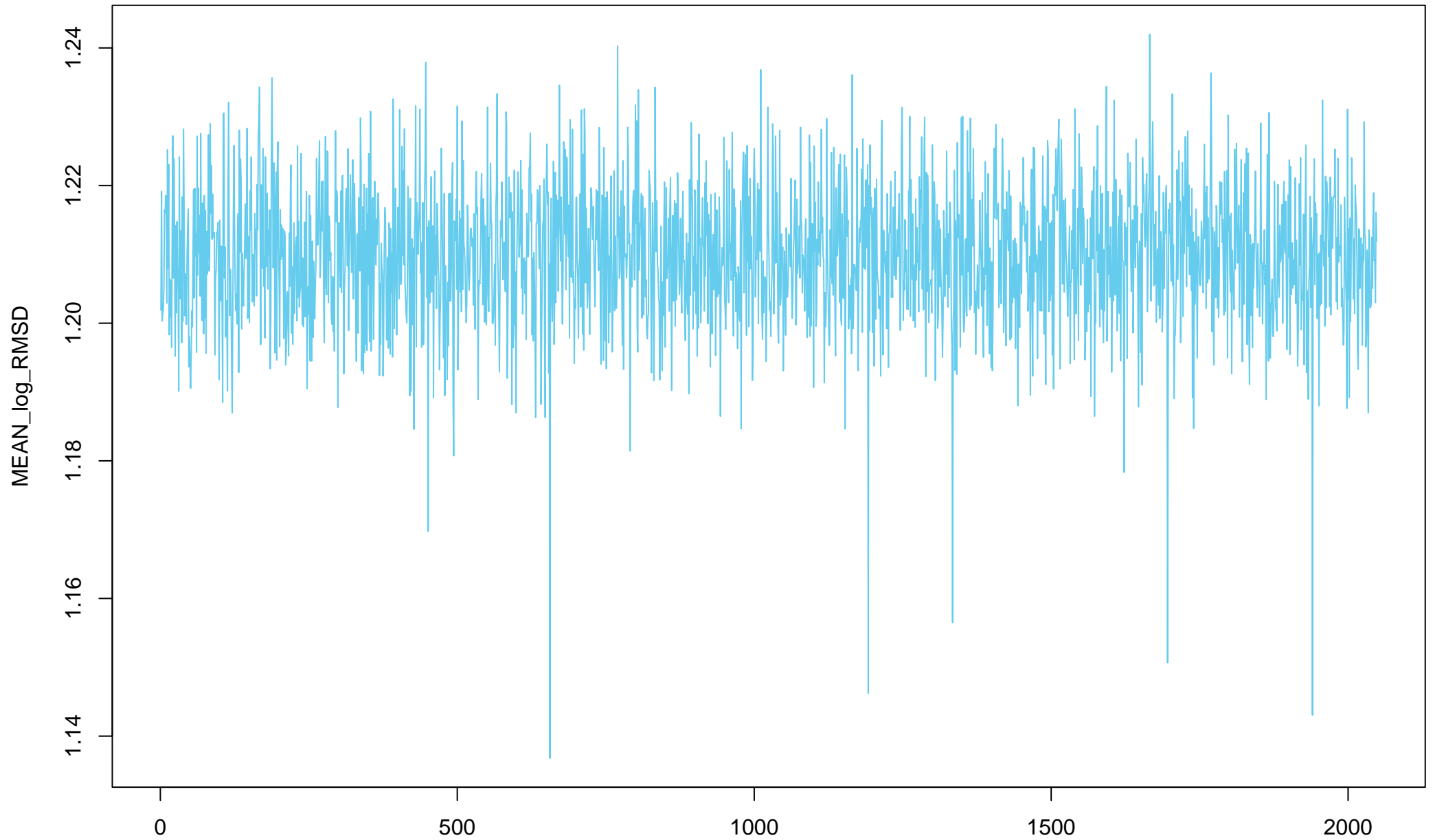
Q3_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



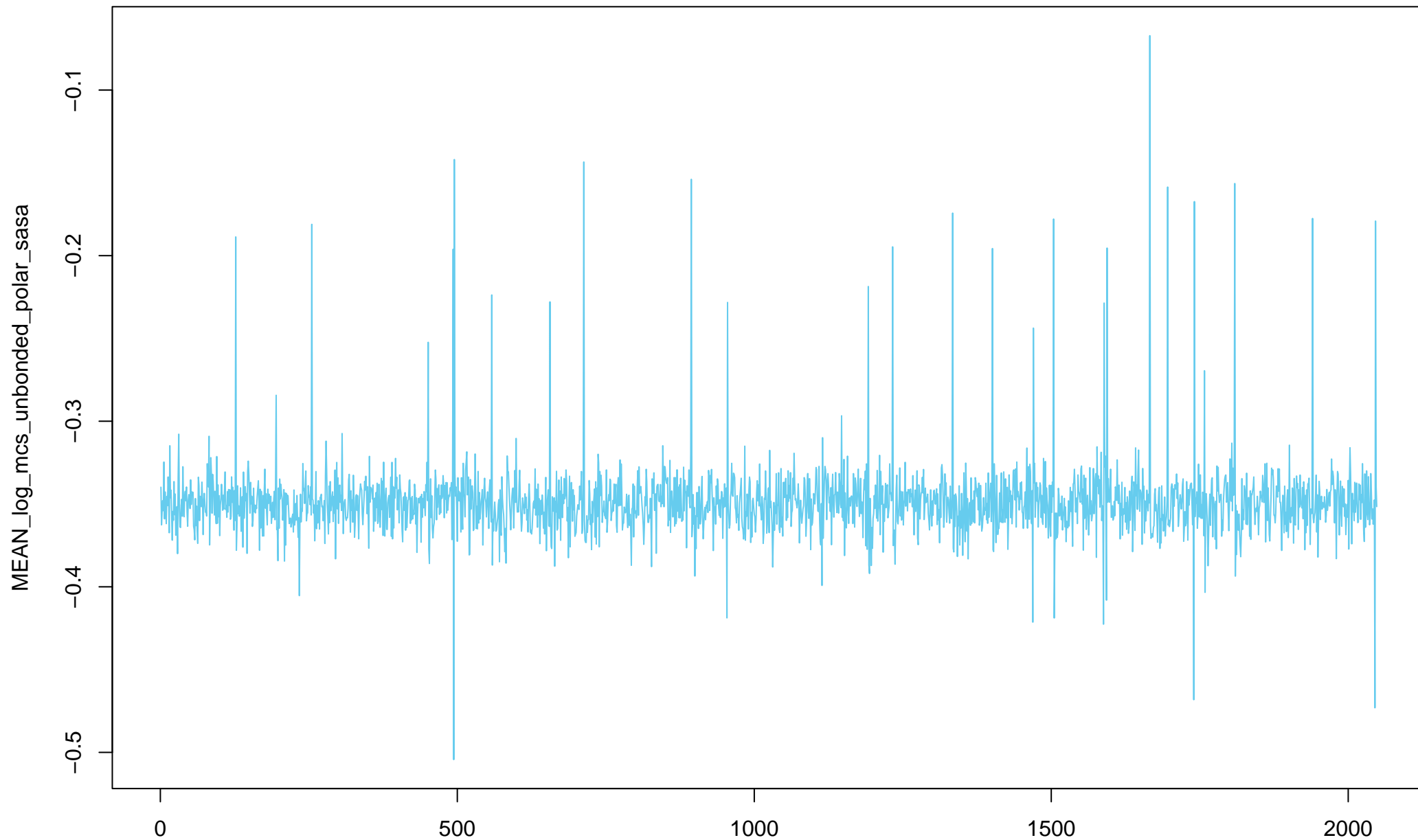
Dcov
ESS = 134 | BMK = 0.183 | MCSE(6.27) = 5.25 | stat: FALSE | burn: 0



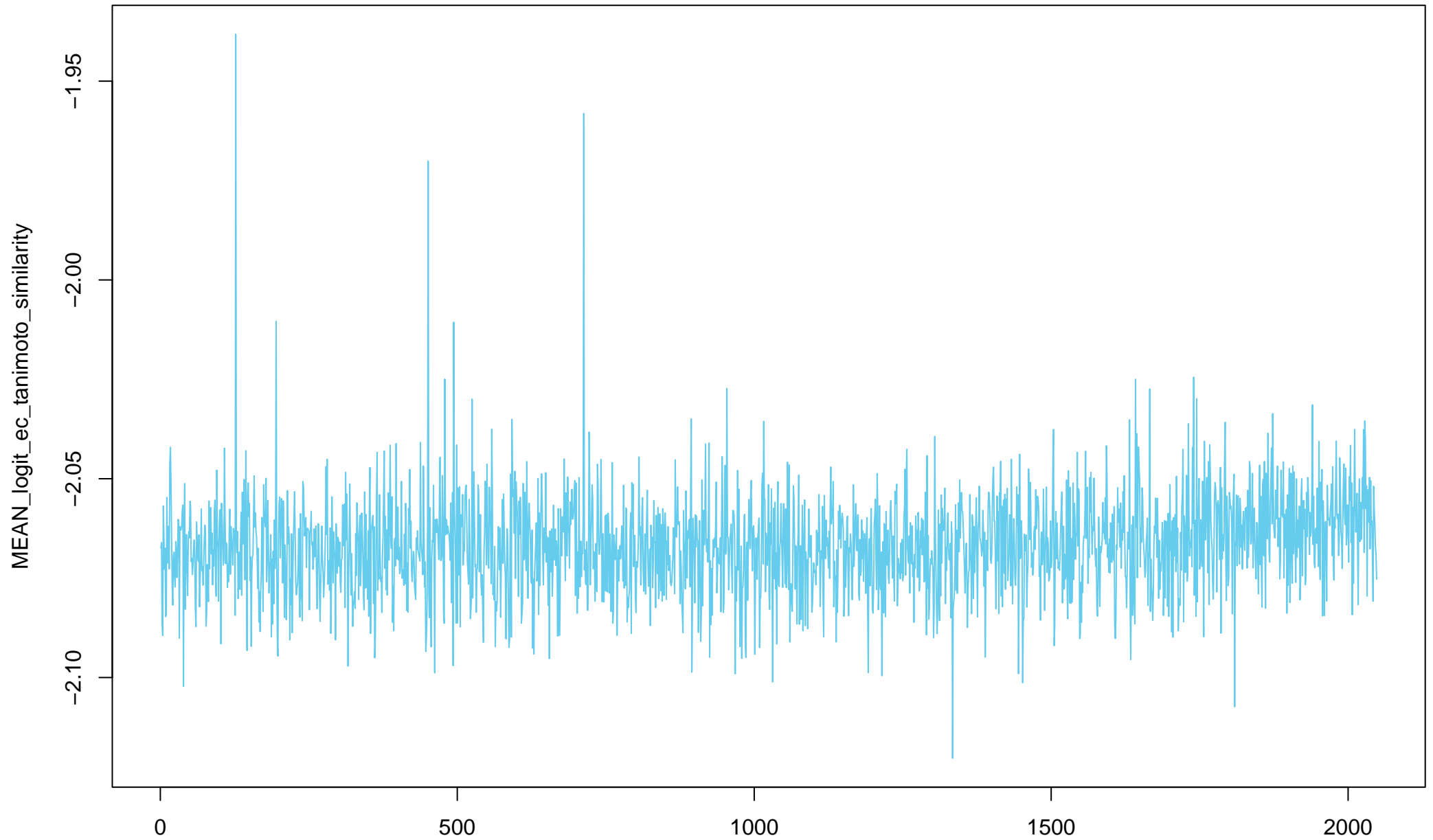
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0649 | MCSE(6.27) = 1.84 | stat: TRUE | burn: 0



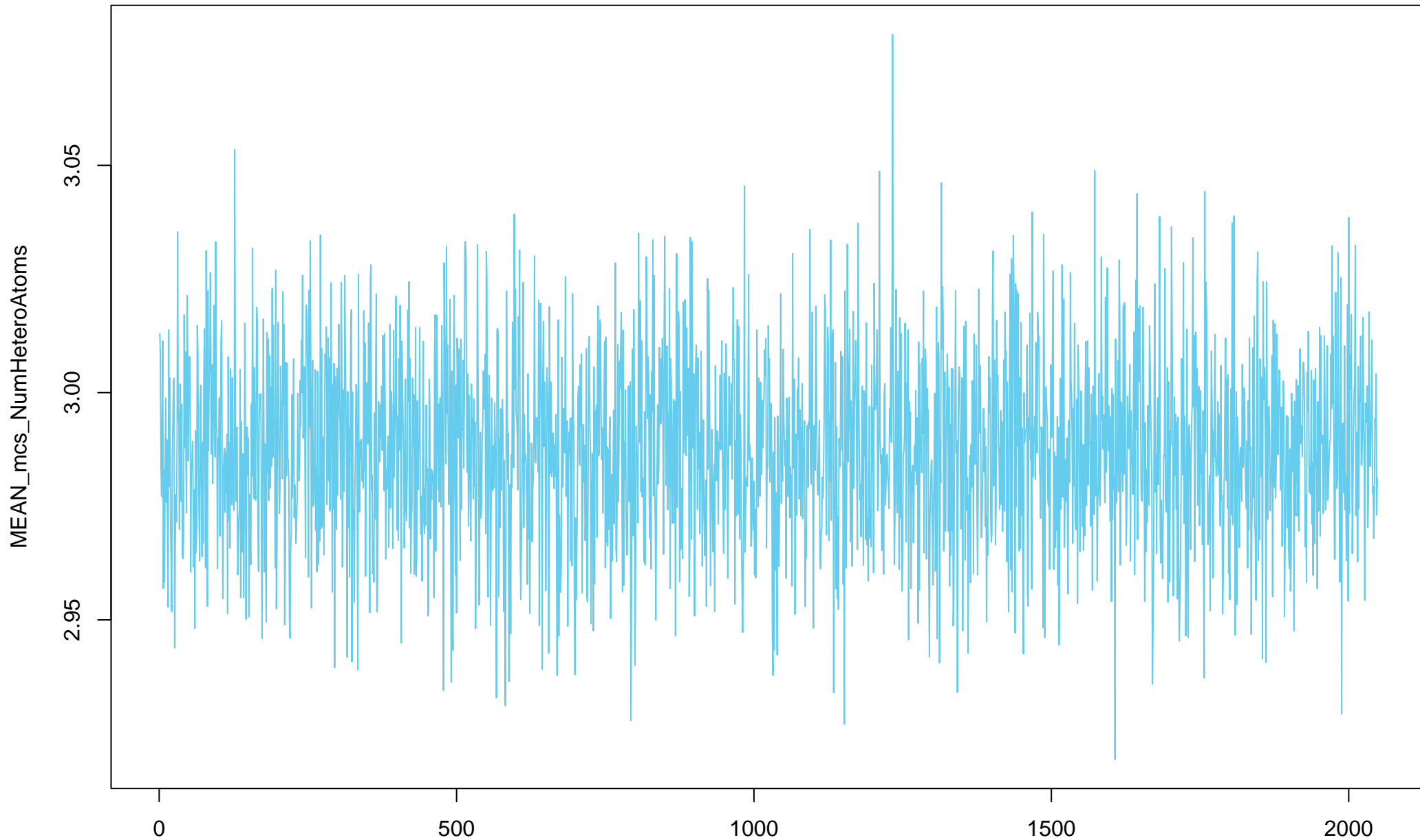
MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0919 | MCSE(6.27) = 1.41 | stat: TRUE | burn: 0



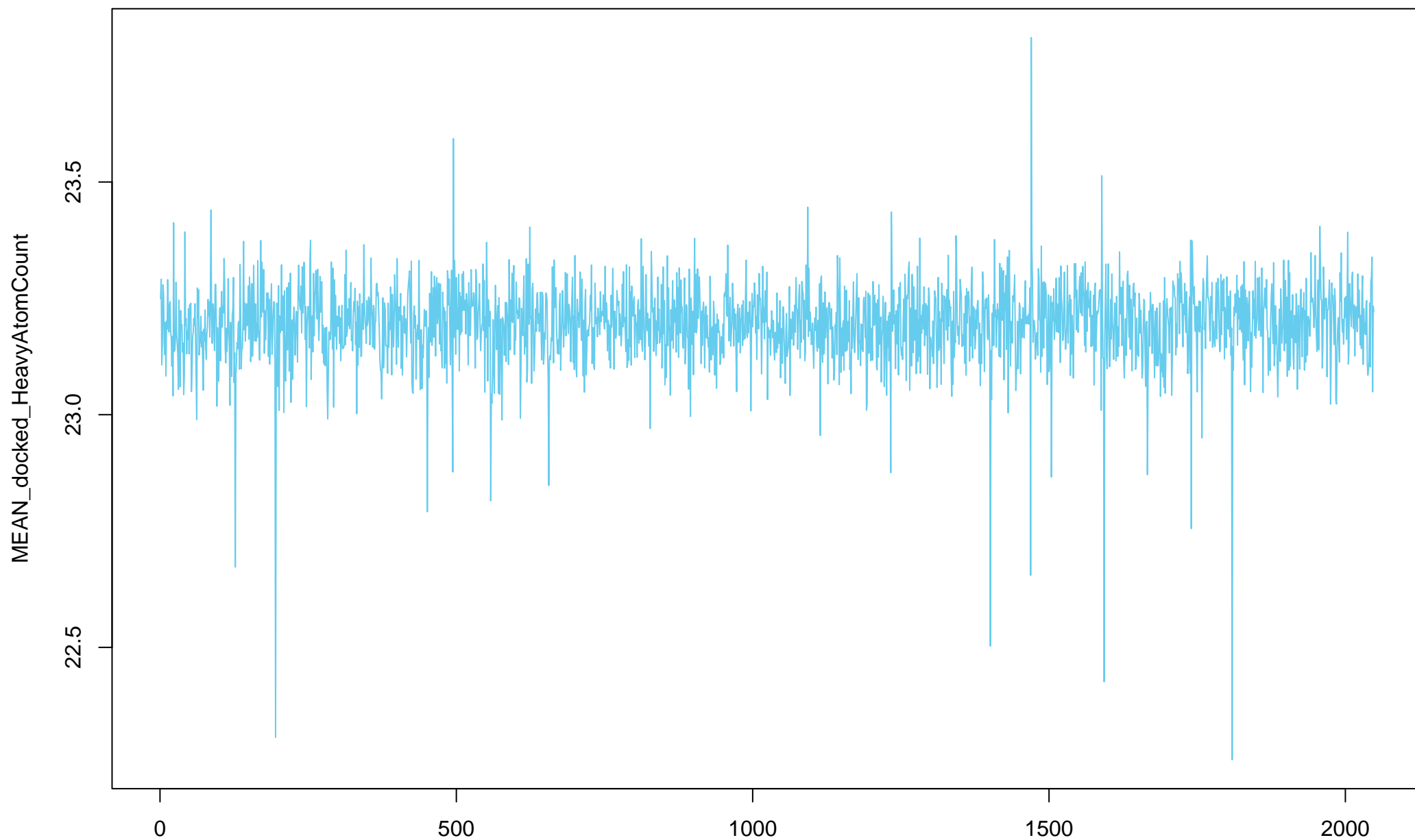
MEAN_logit_ec_tanimoto_similarity
ESS = 567 | BMK = 0.1 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0



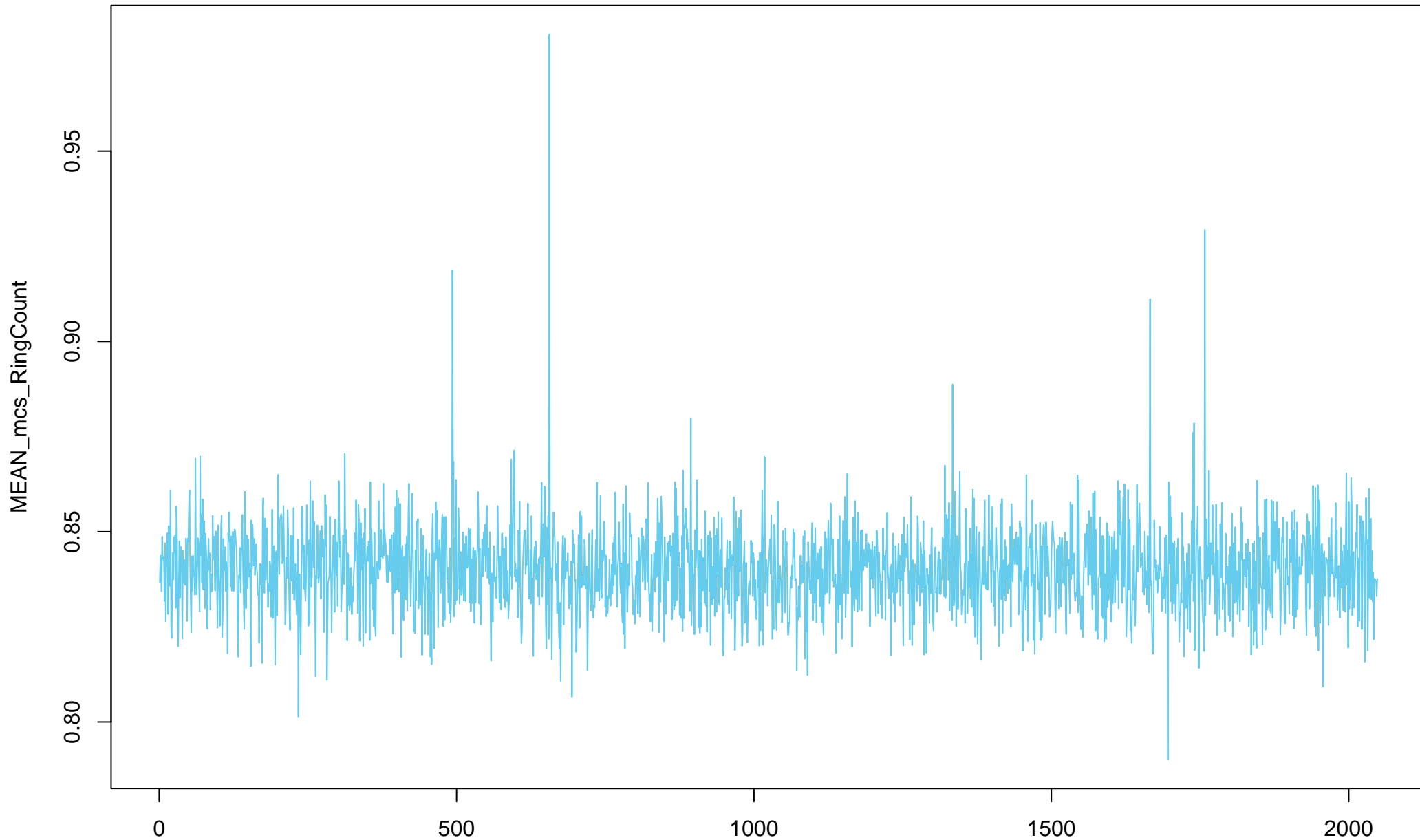
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0413 | MCSE(6.27) = 2.03 | stat: TRUE | burn: 0



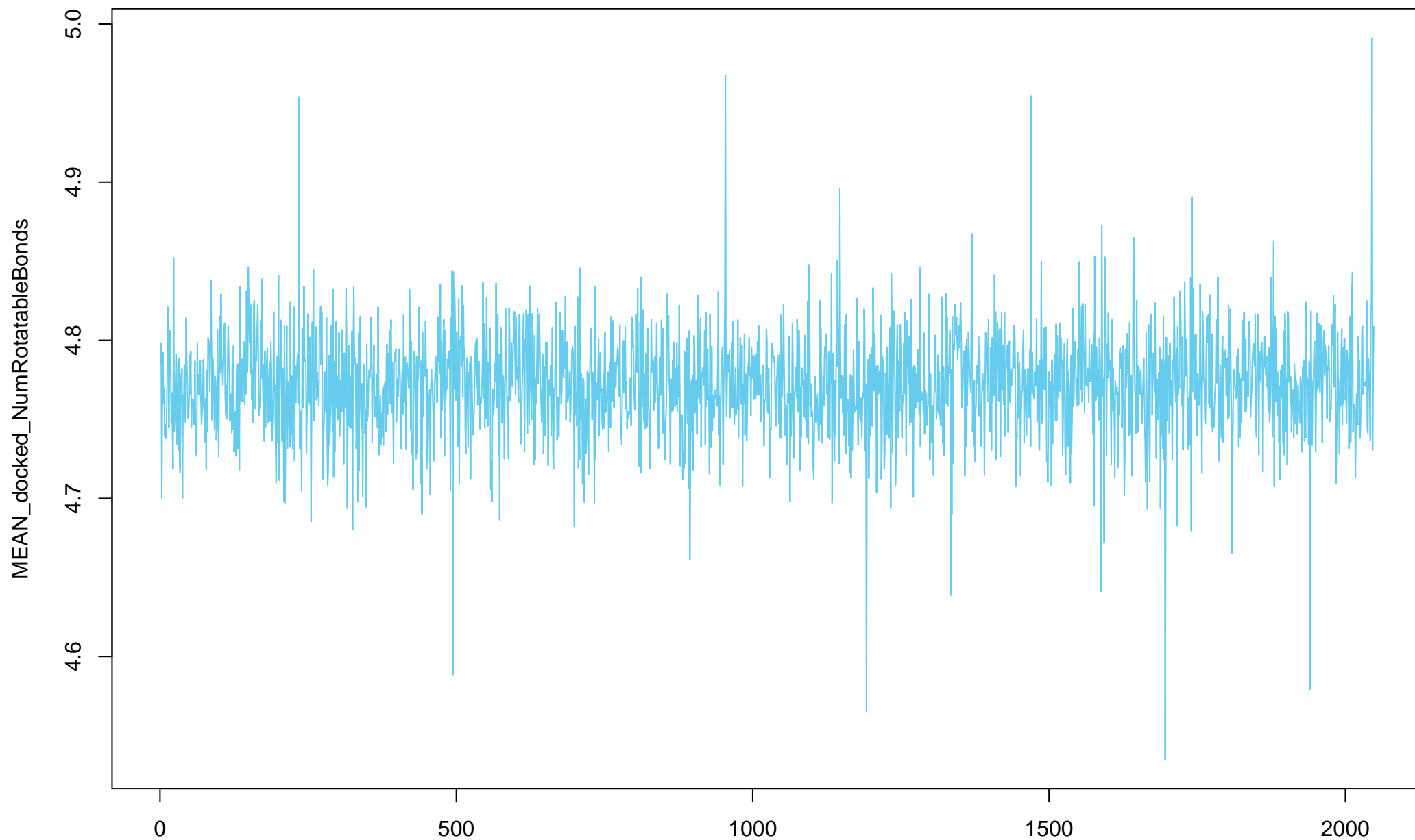
MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.081 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0



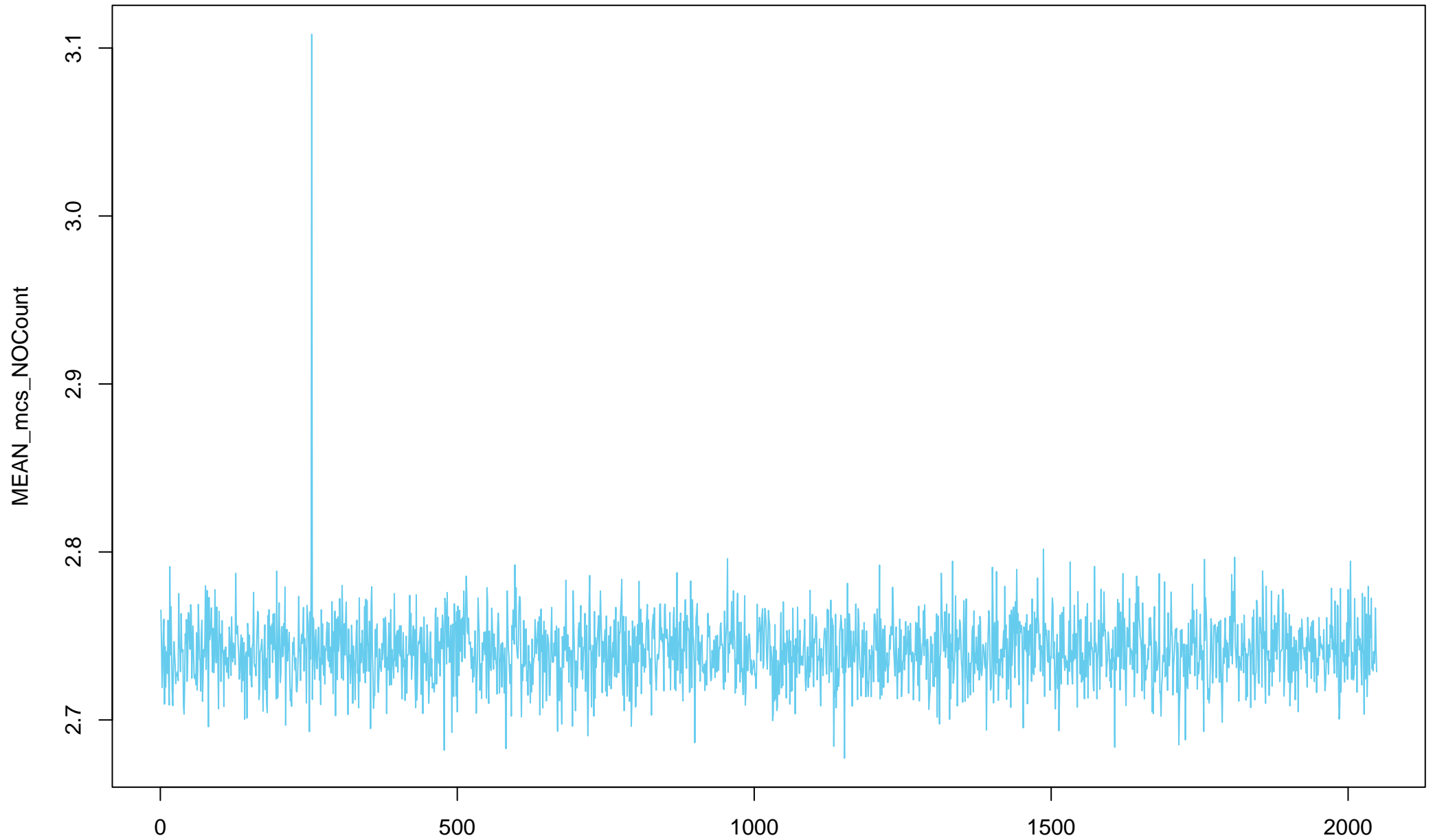
MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0636 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0



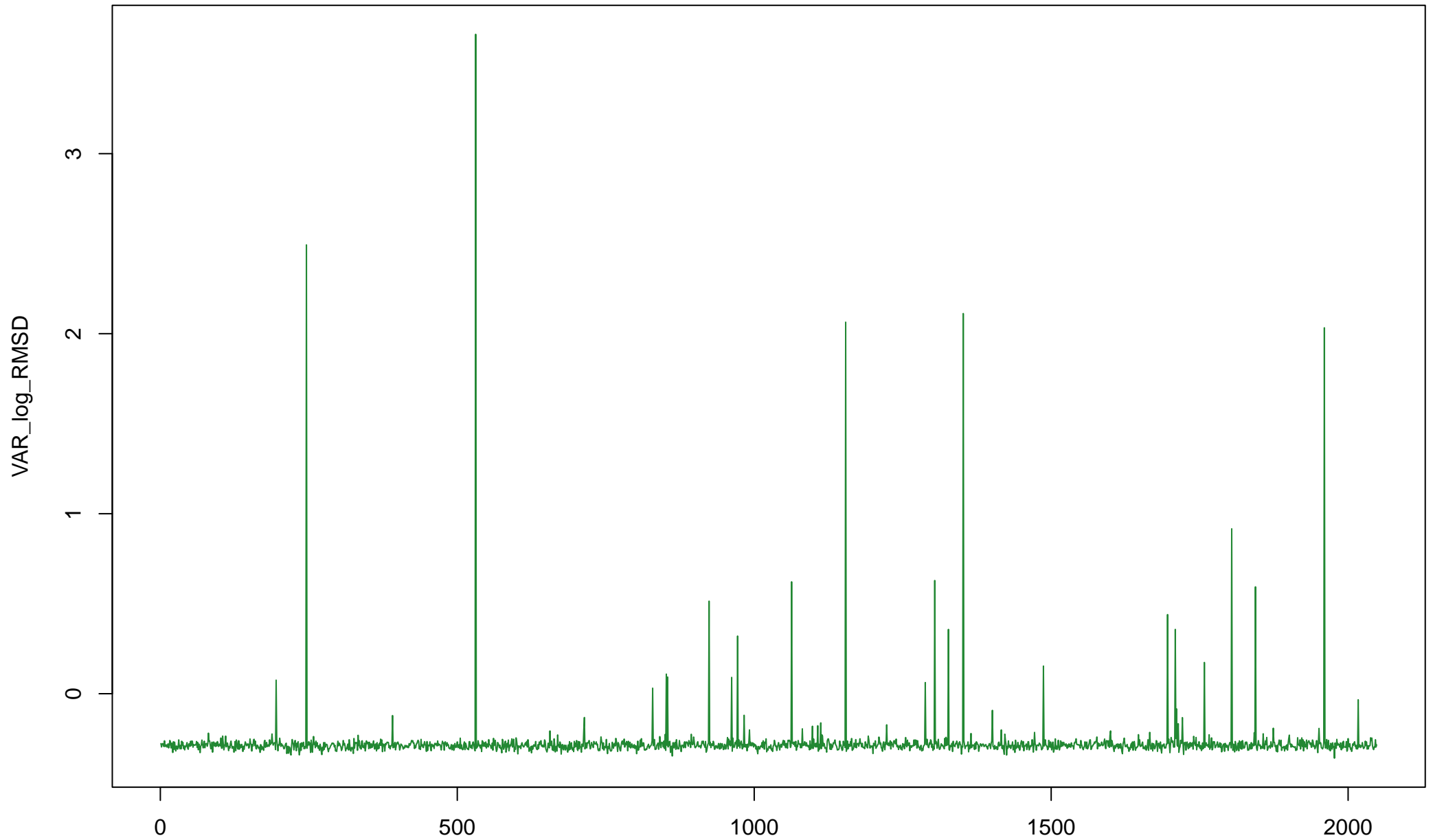
MEAN_docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0755 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0



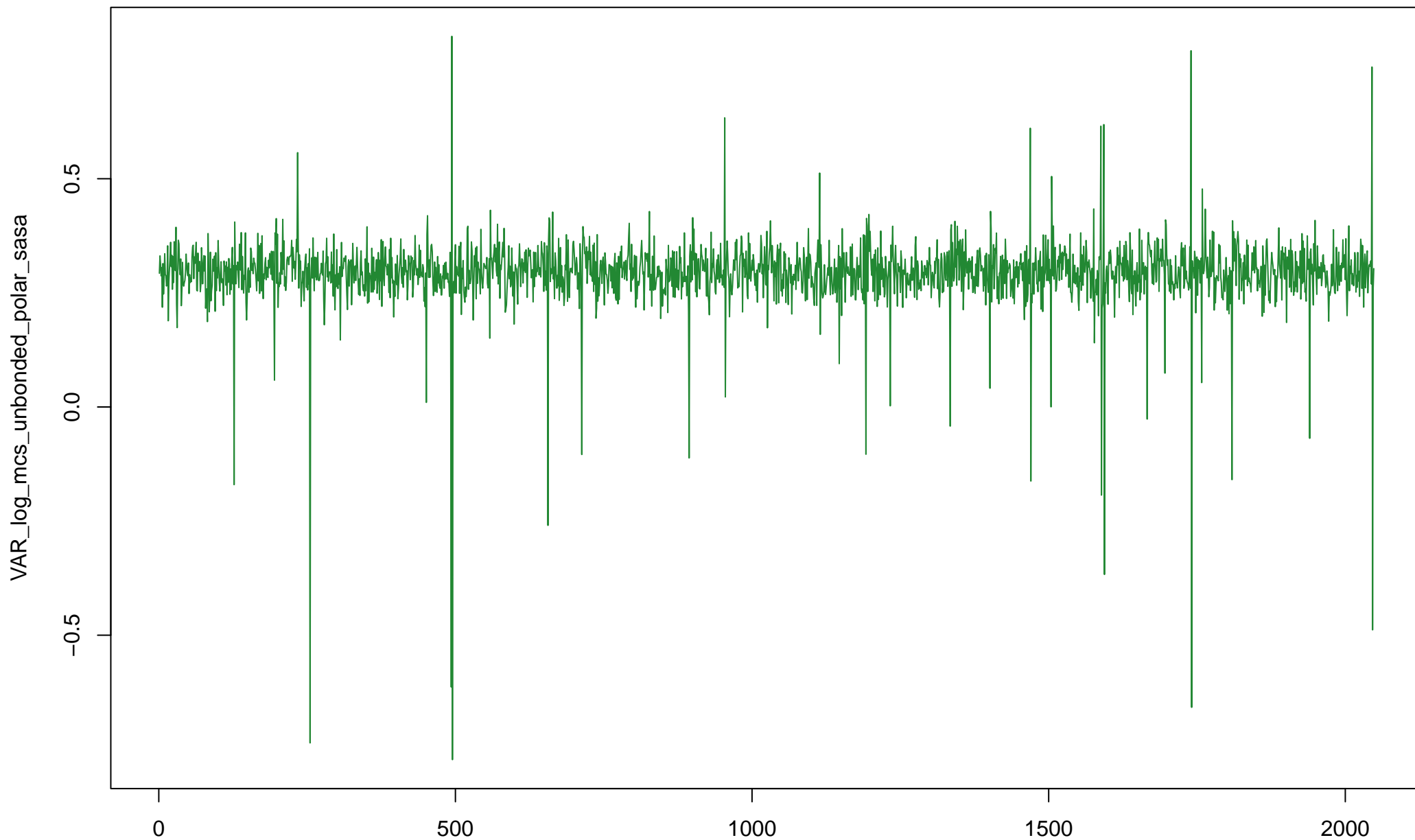
MEAN_mcs_NOCount
ESS = 2050 | BMK = 0.0431 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0



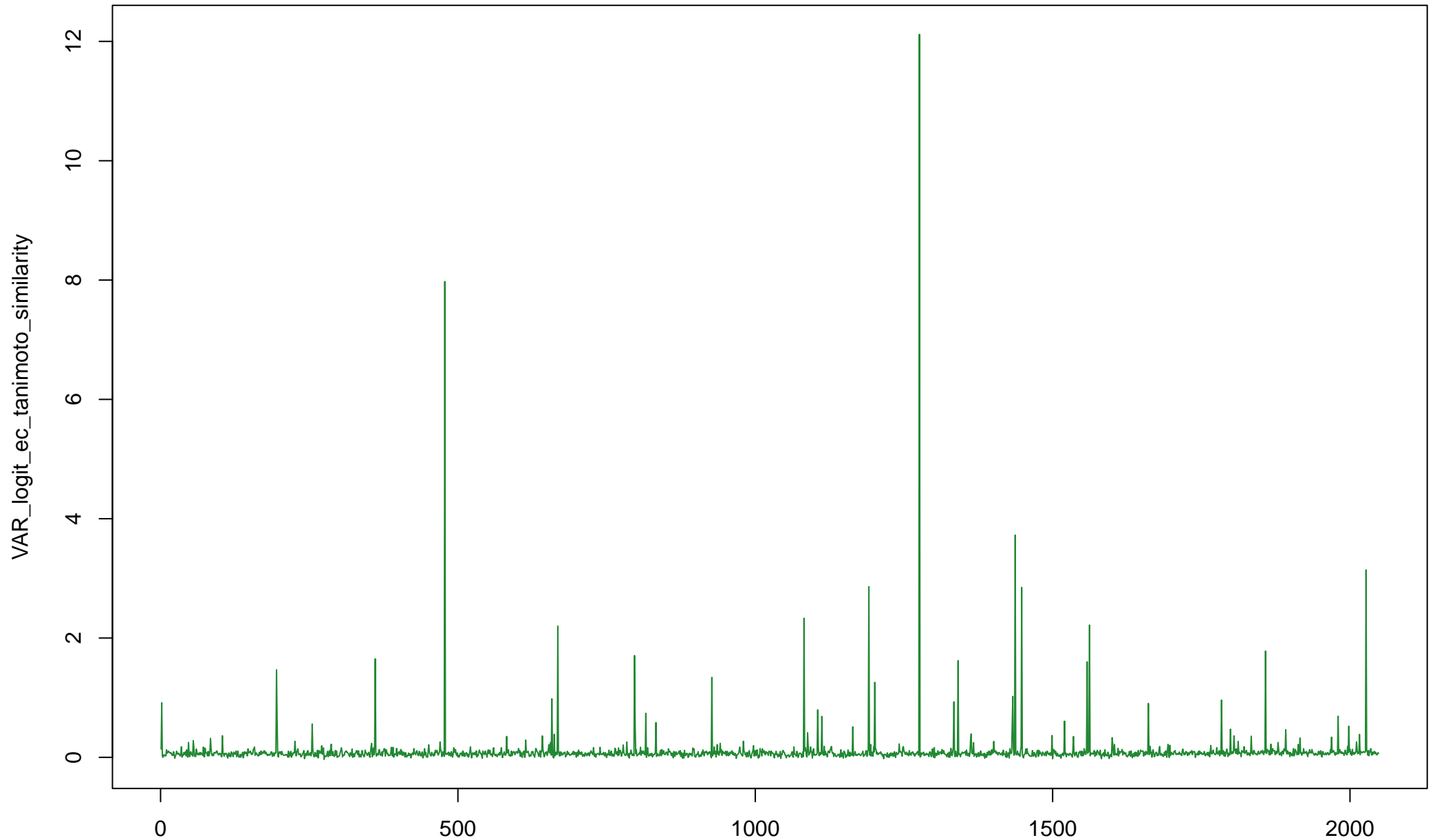
VAR_log_RMSD
ESS = 2050 | BMK = 0.207 | MCSE(6.27) = 2.14 | stat: FALSE | burn: 0



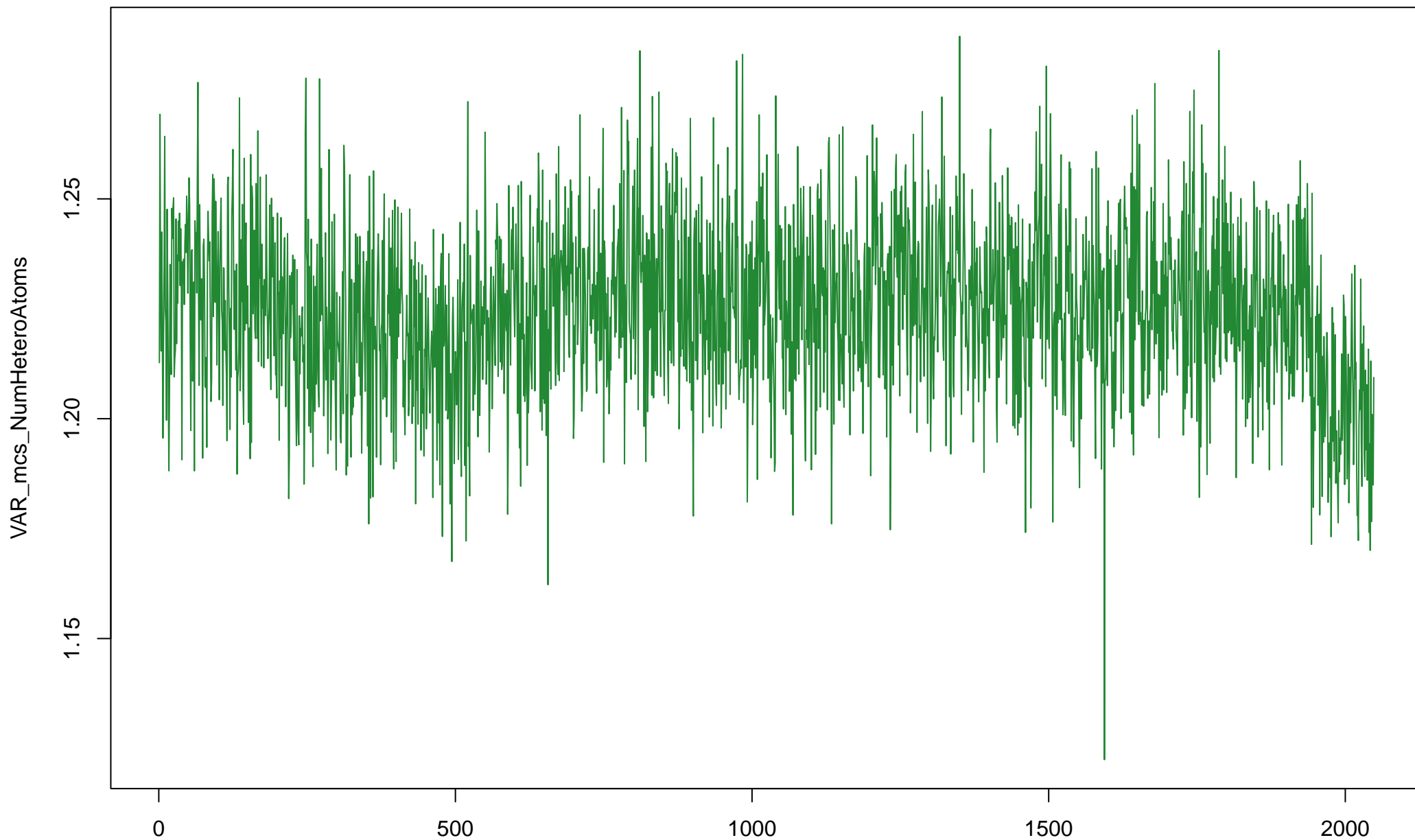
VAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0984 | MCSE(6.27) = 1.41 | stat: TRUE | burn: 0



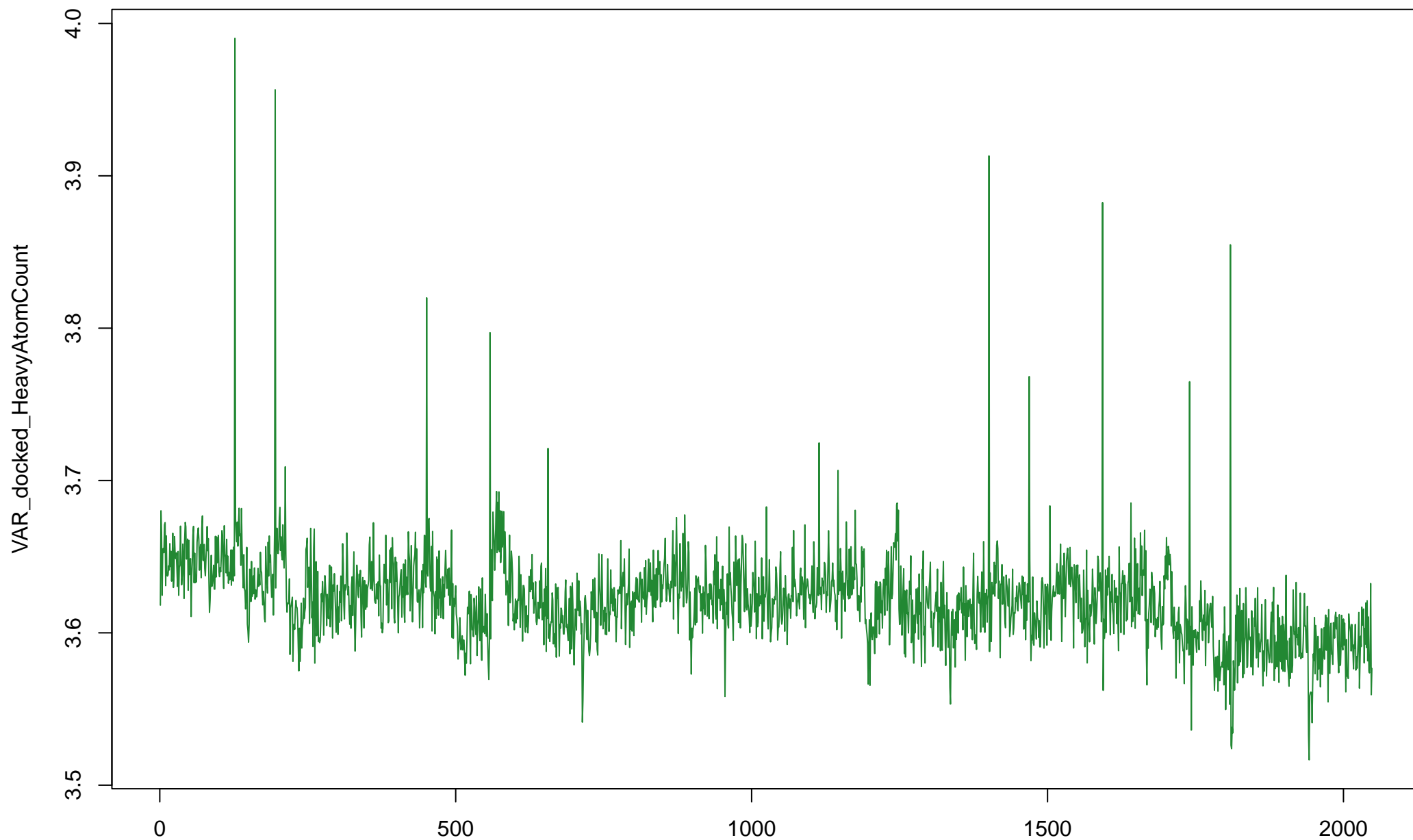
VAR_logit_ec_tanimoto_similarity
ESS = 2050 | BMK = 1 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 1428



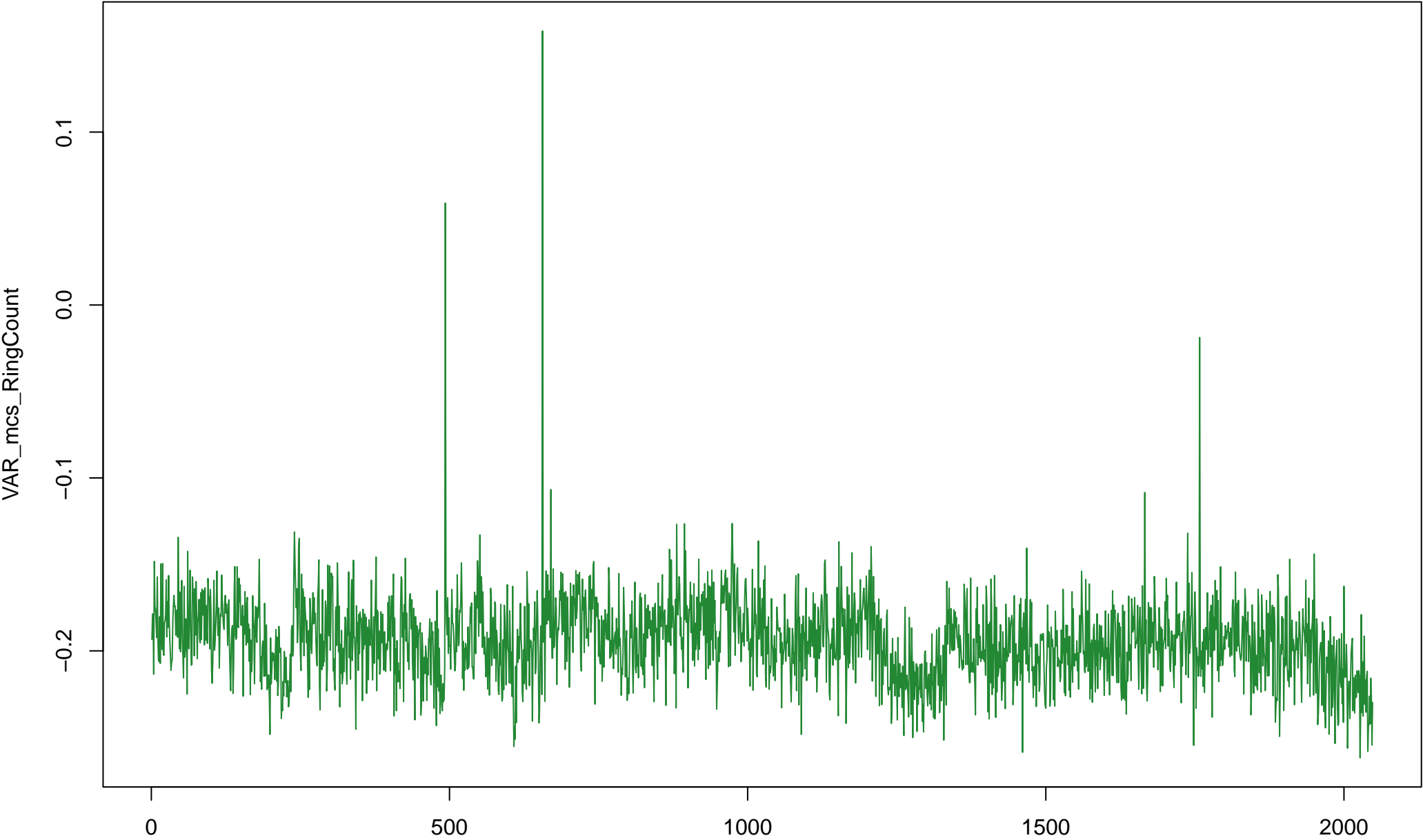
VAR_mcs_NumHeteroAtoms
ESS = 125 | BMK = 0.0424 | MCSE(6.27) = 4.74 | stat: FALSE | burn: 0



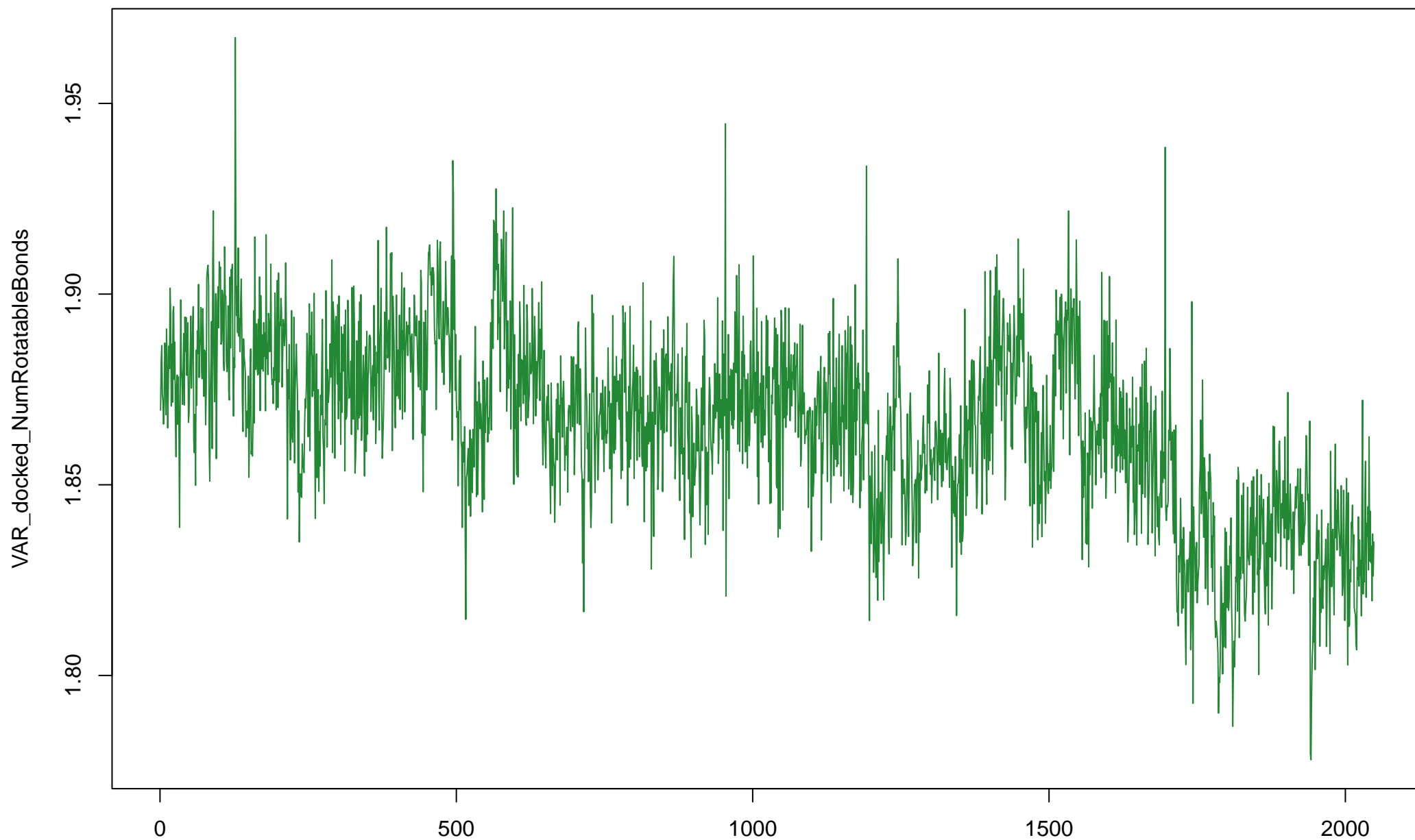
VAR_docked_HeavyAtomCount
ESS = 94.8 | BMK = 0.248 | MCSE(6.27) = 7.77 | stat: FALSE | burn: 0



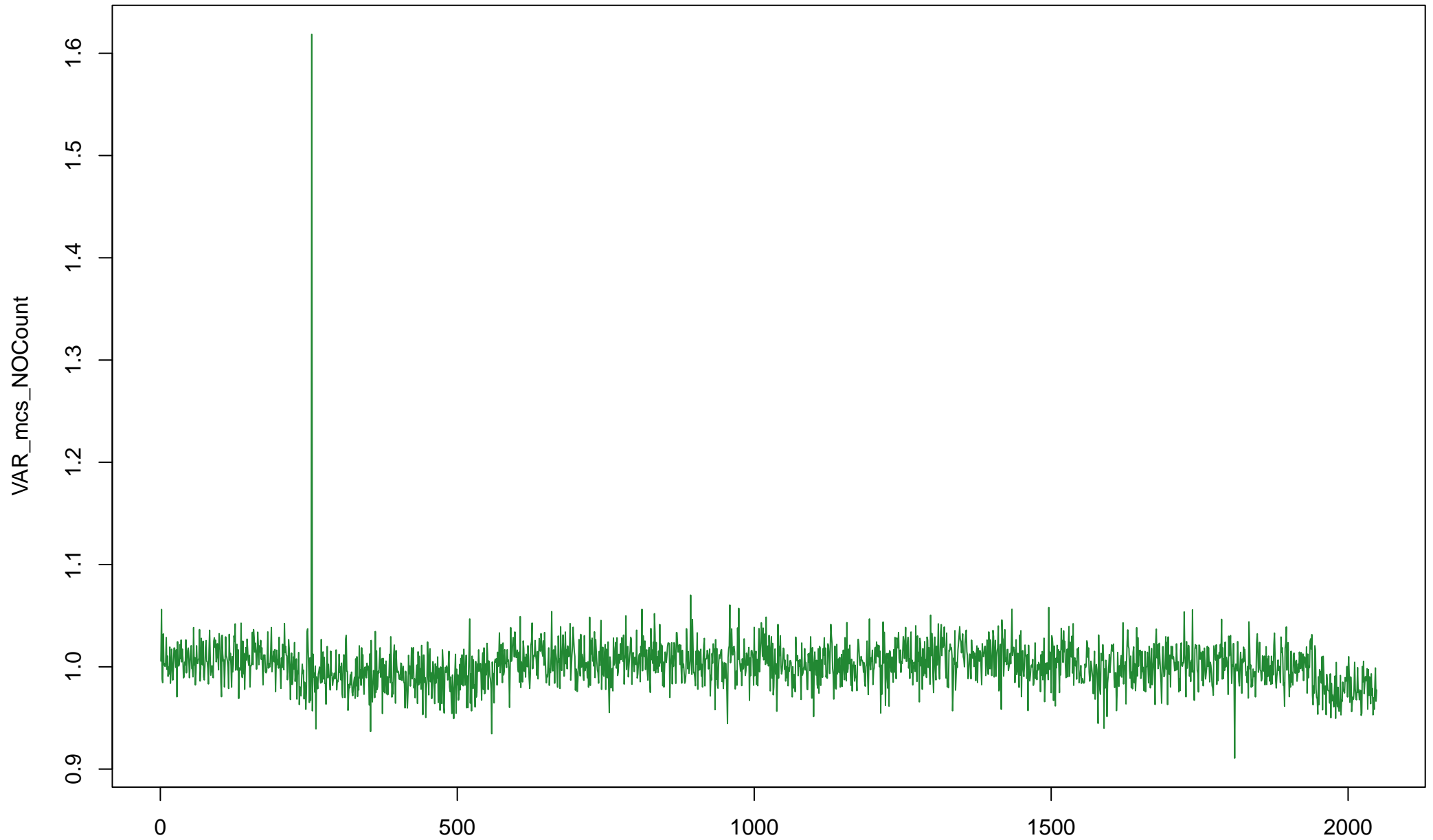
VAR_mcs_RingCount
ESS = 107 | BMK = 0.163 | MCSE(6.27) = 5.57 | stat: FALSE | burn: 0



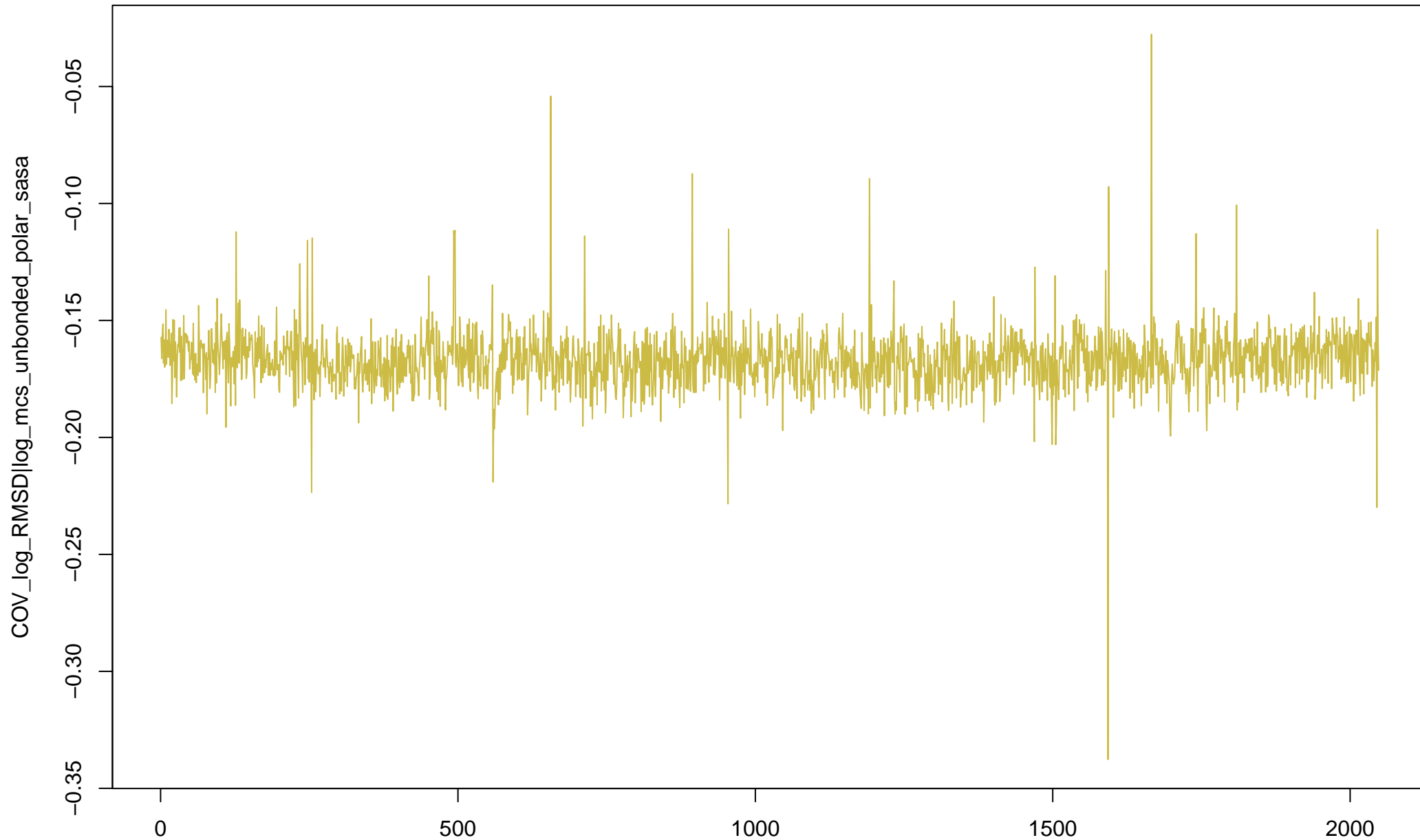
VAR_docked_NumRotatableBonds
ESS = 25.3 | BMK = 0.379 | MCSE(6.27) = 11 | stat: FALSE | burn: 1632



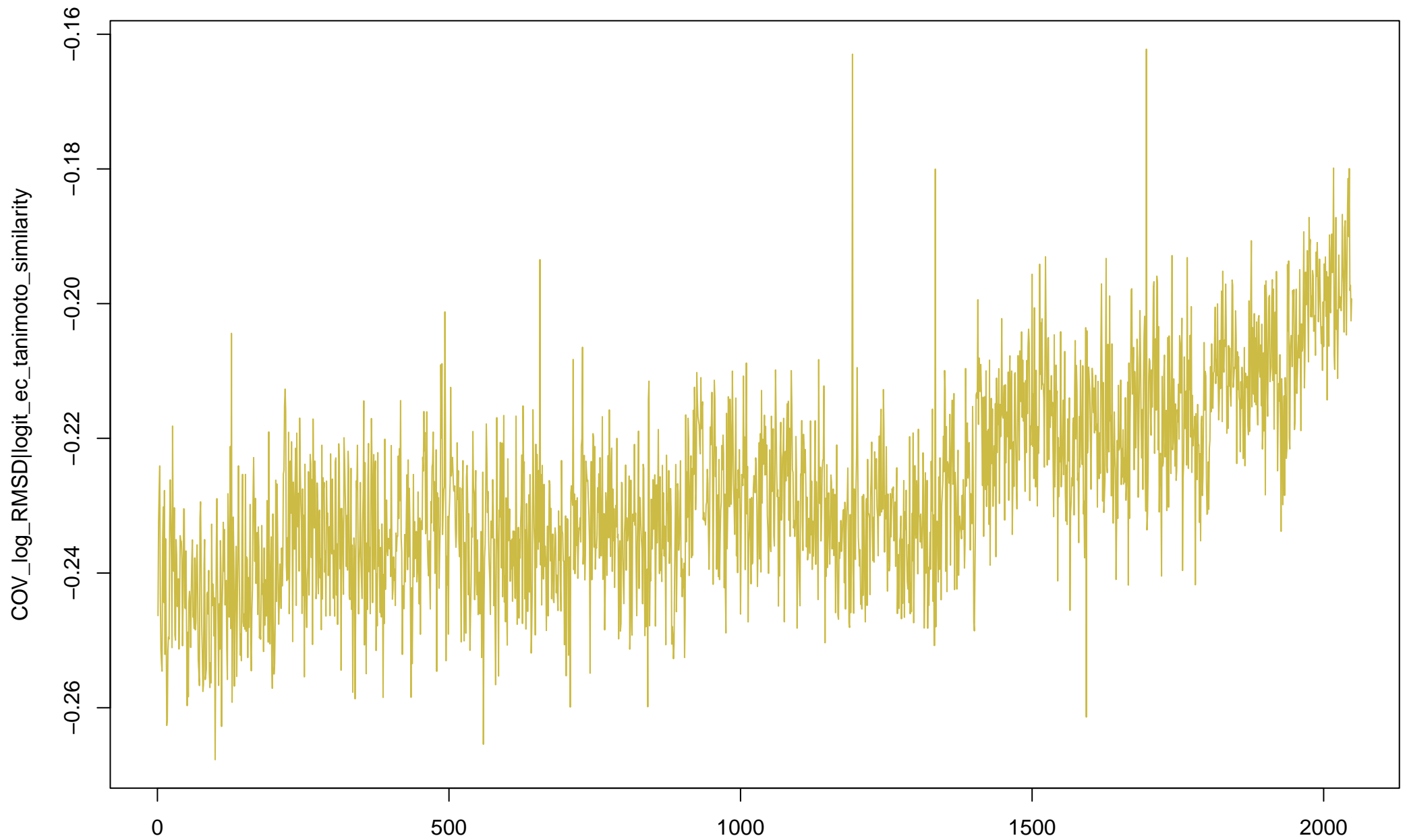
VAR_mcs_NOCount
ESS = 429 | BMK = 0.0474 | MCSE(6.27) = 4.31 | stat: FALSE | burn: 0



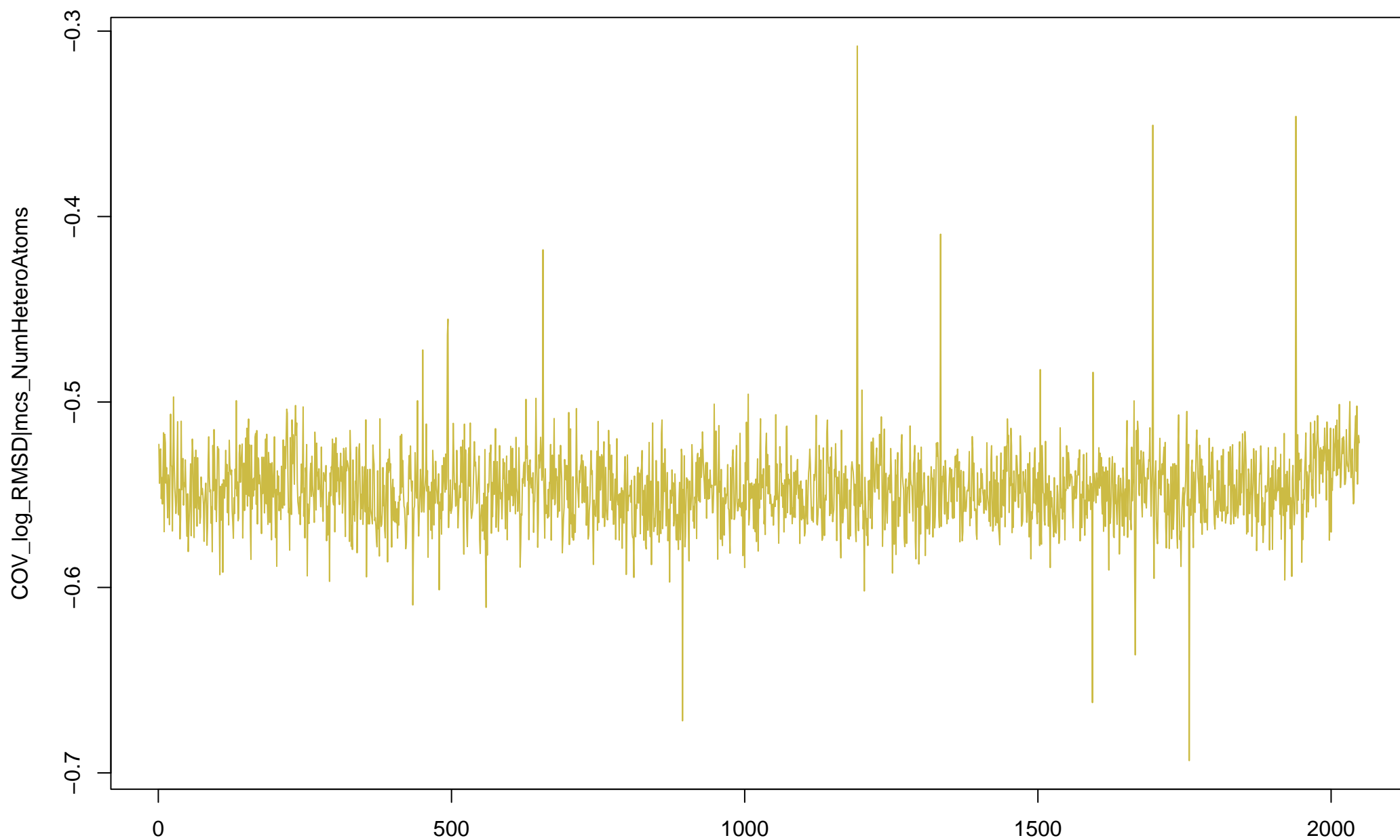
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1470 | BMK = 0.0816 | MCSE(6.27) = 2.9 | stat: FALSE | burn: 0



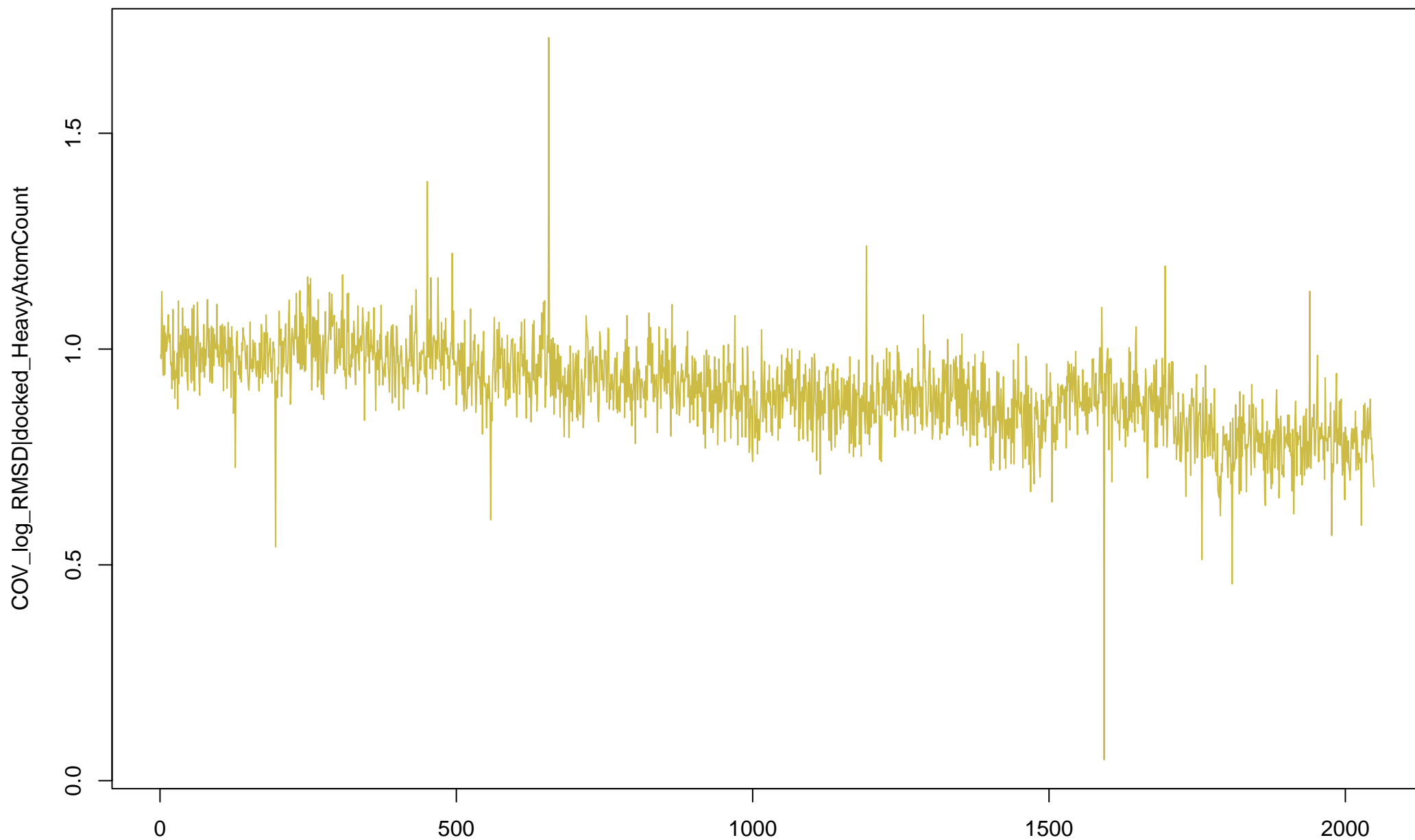
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 15.2 | BMK = 0.432 | MCSE(6.27) = 10.9 | stat: FALSE | burn: 0



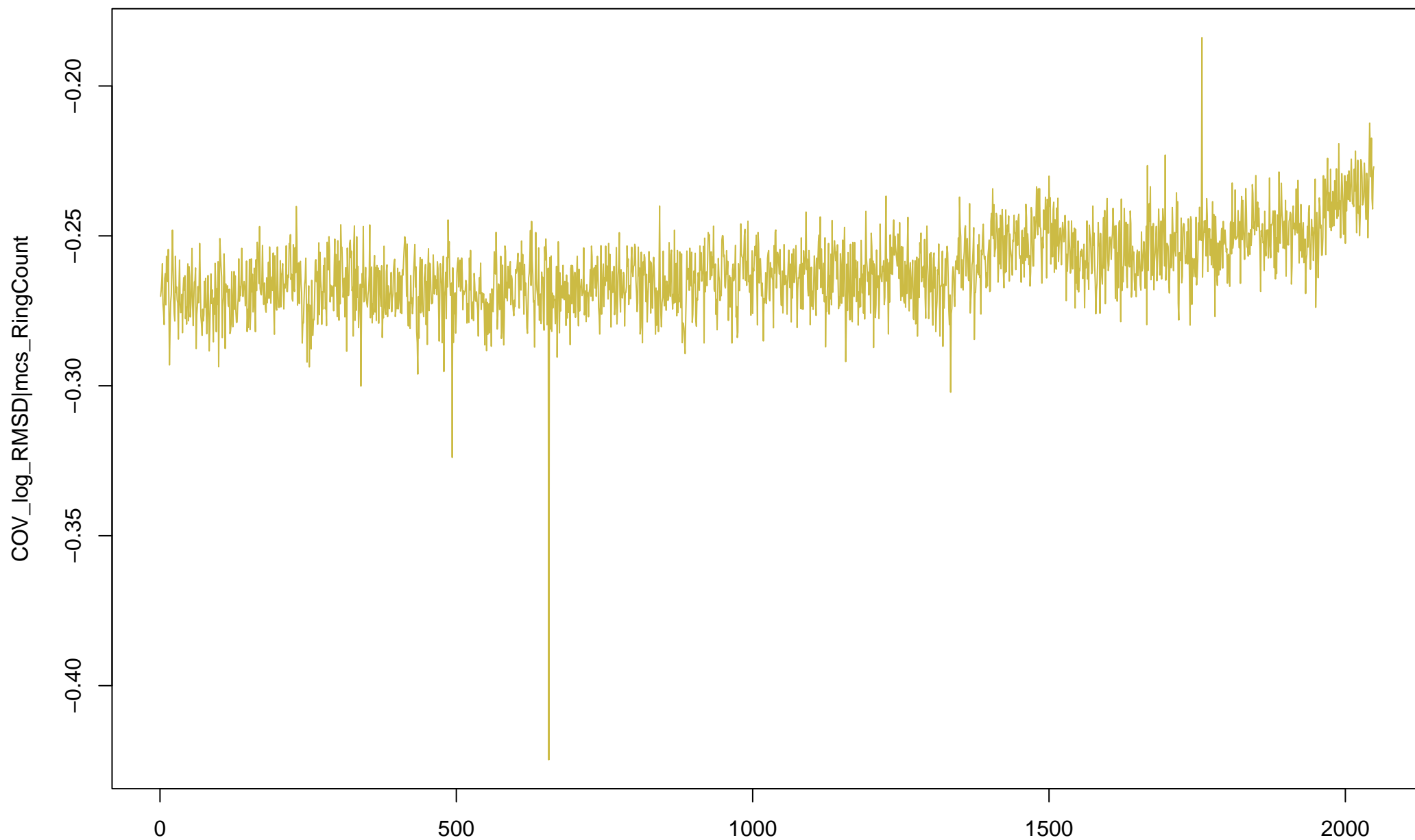
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1250 | BMK = 0.0811 | MCSE(6.27) = 3.32 | stat: TRUE | burn: 0



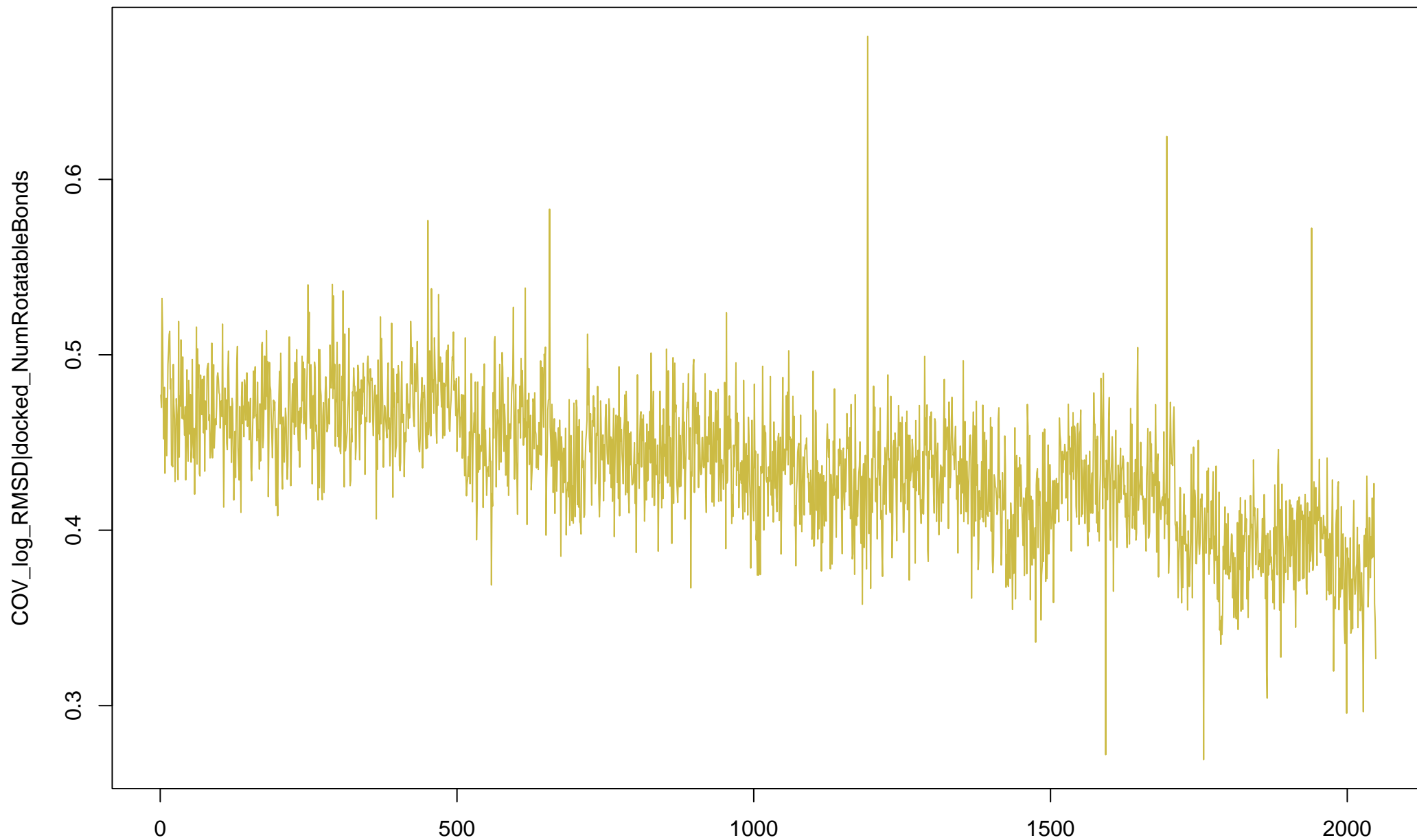
COV_log_RMSD|docked_HeavyAtomCount
ESS = 9.62 | BMK = 0.49 | MCSE(6.27) = 10.7 | stat: FALSE | burn: 0



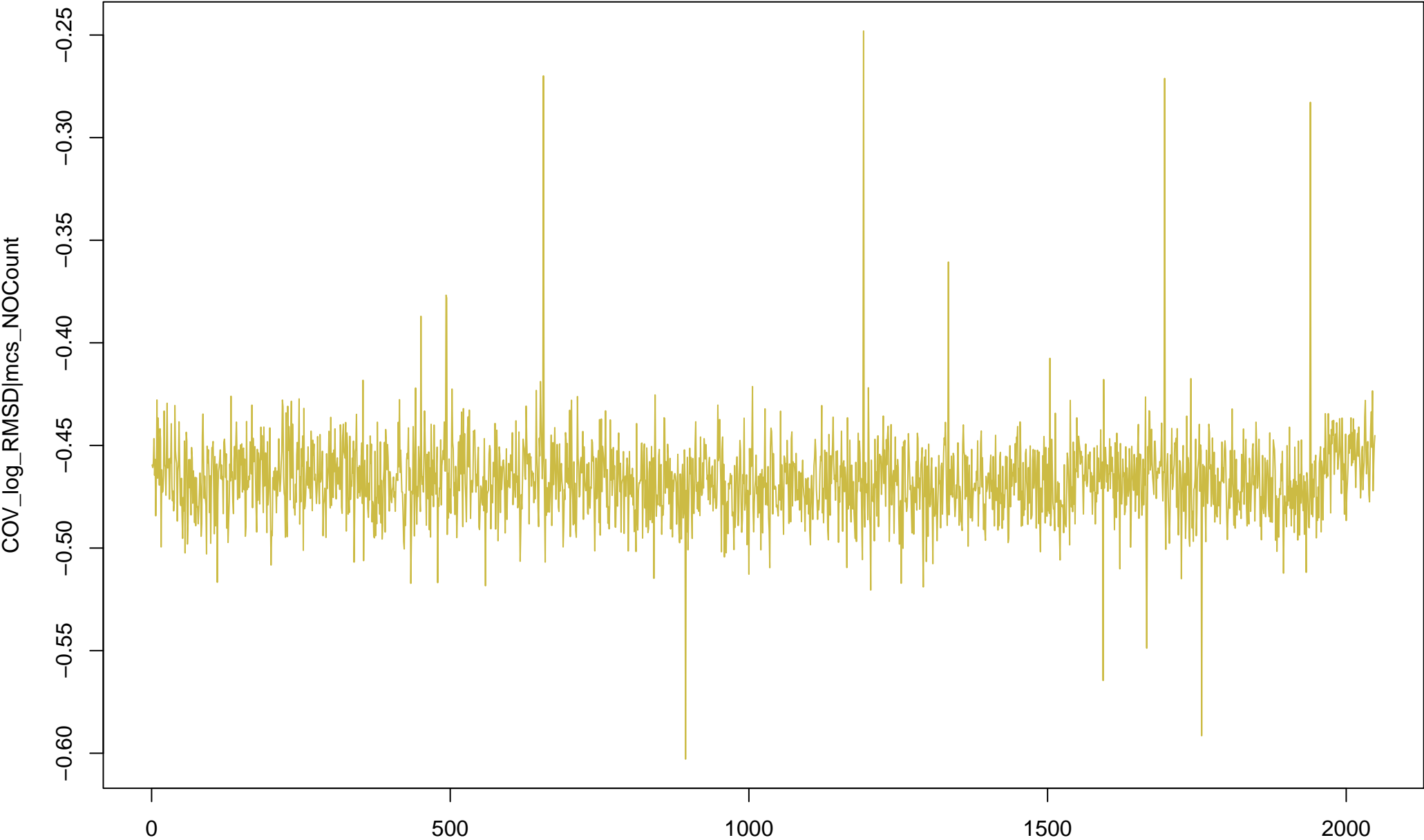
COV_log_RMSD|mcs_RingCount
ESS = 20 | BMK = 0.41 | MCSE(6.27) = 9.33 | stat: FALSE | burn: 0



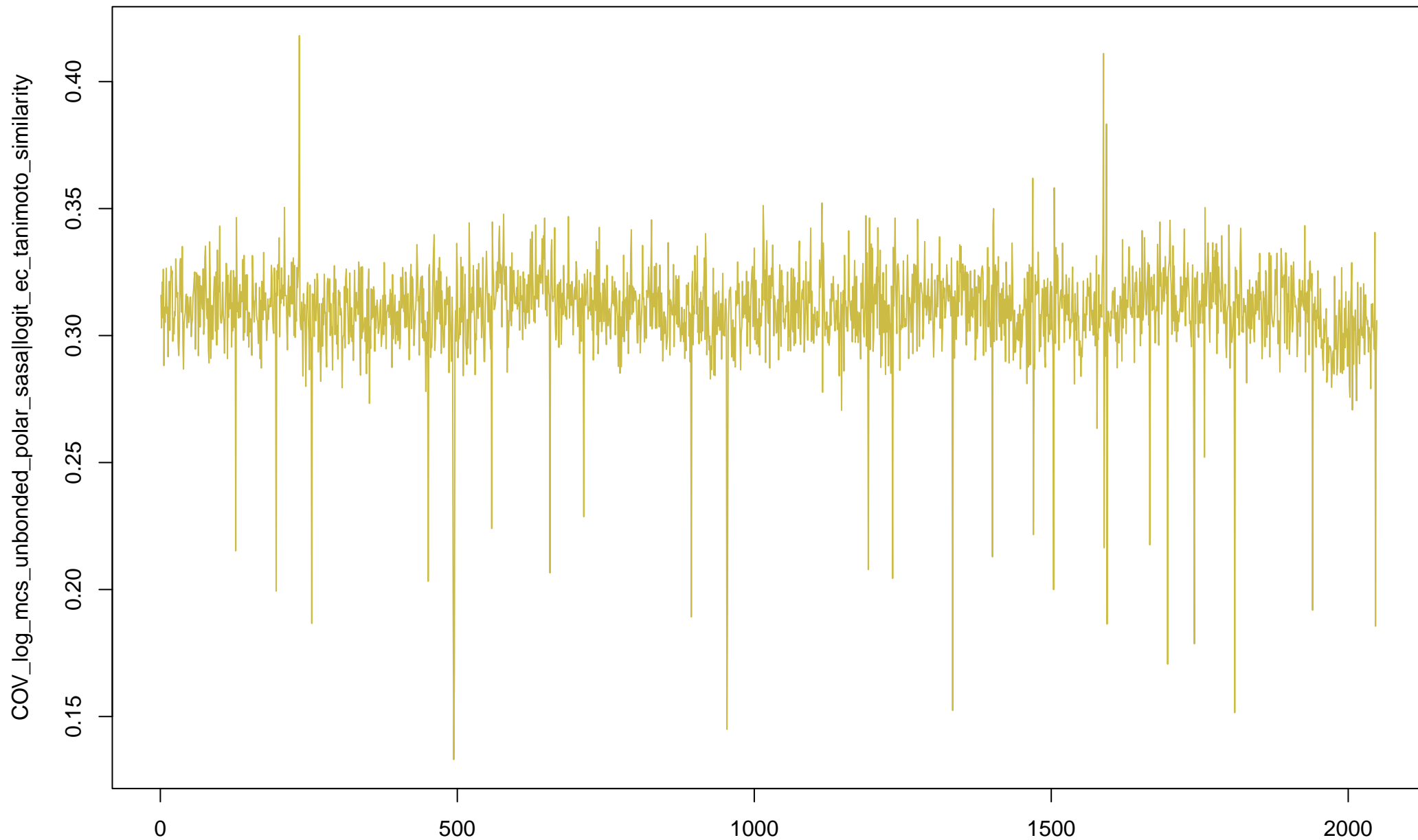
COV_log_RMSD|docked_NumRotatableBonds
ESS = 12.9 | BMK = 0.48 | MCSE(6.27) = 10.6 | stat: FALSE | burn: 0



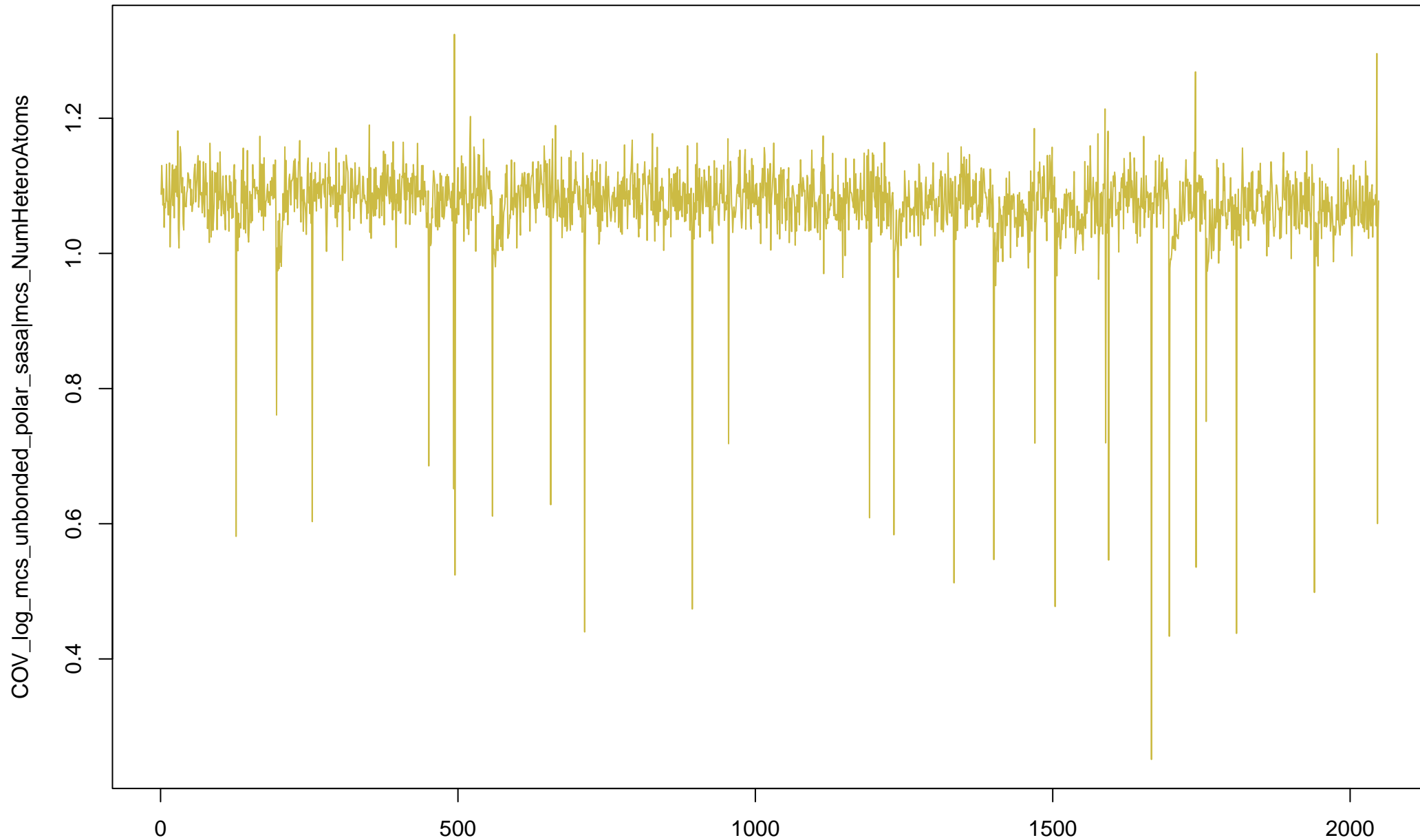
COV_log_RMSD|mcs_NOCount
ESS = 1380 | BMK = 0.0806 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0



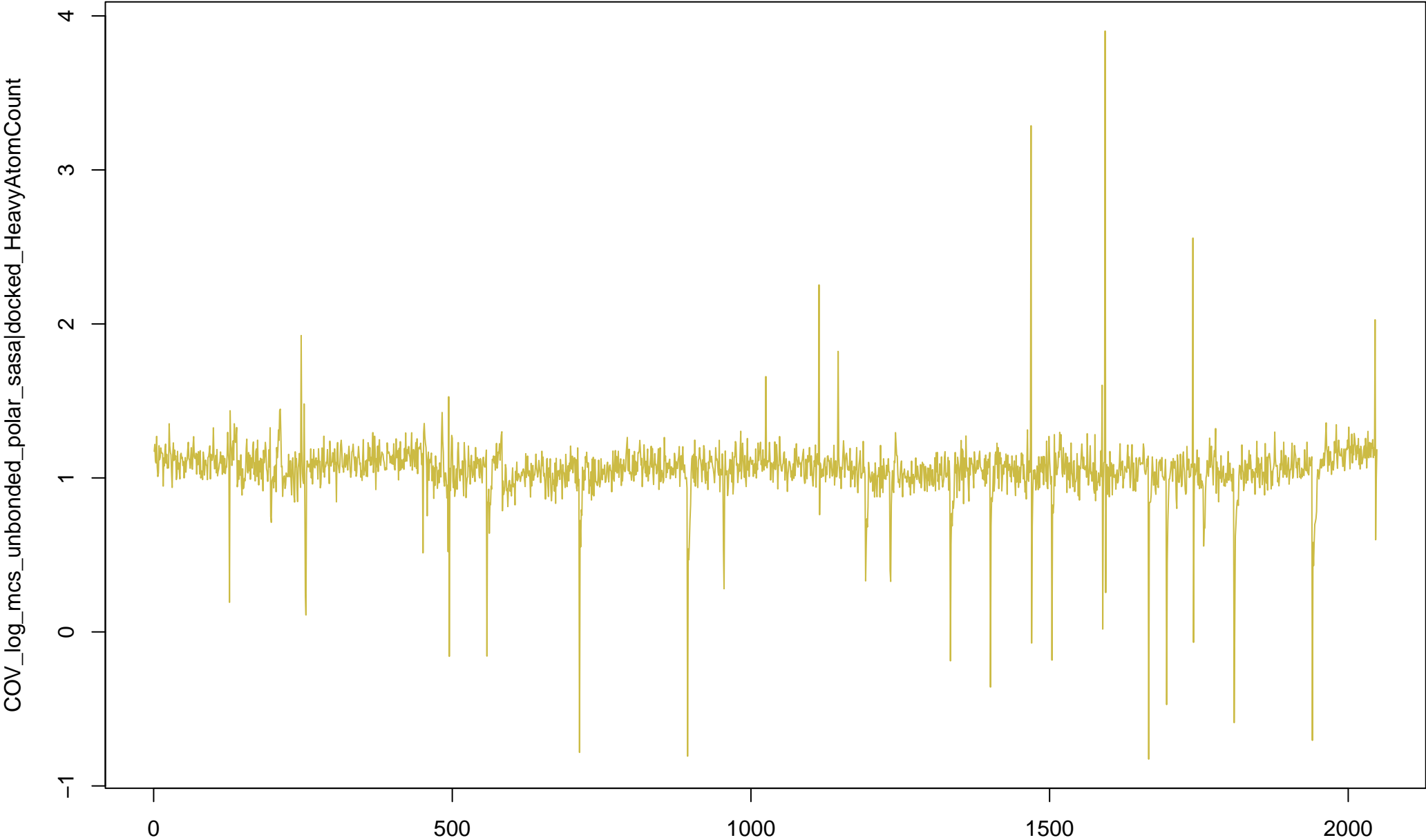
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1620 | BMK = 0.0838 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0



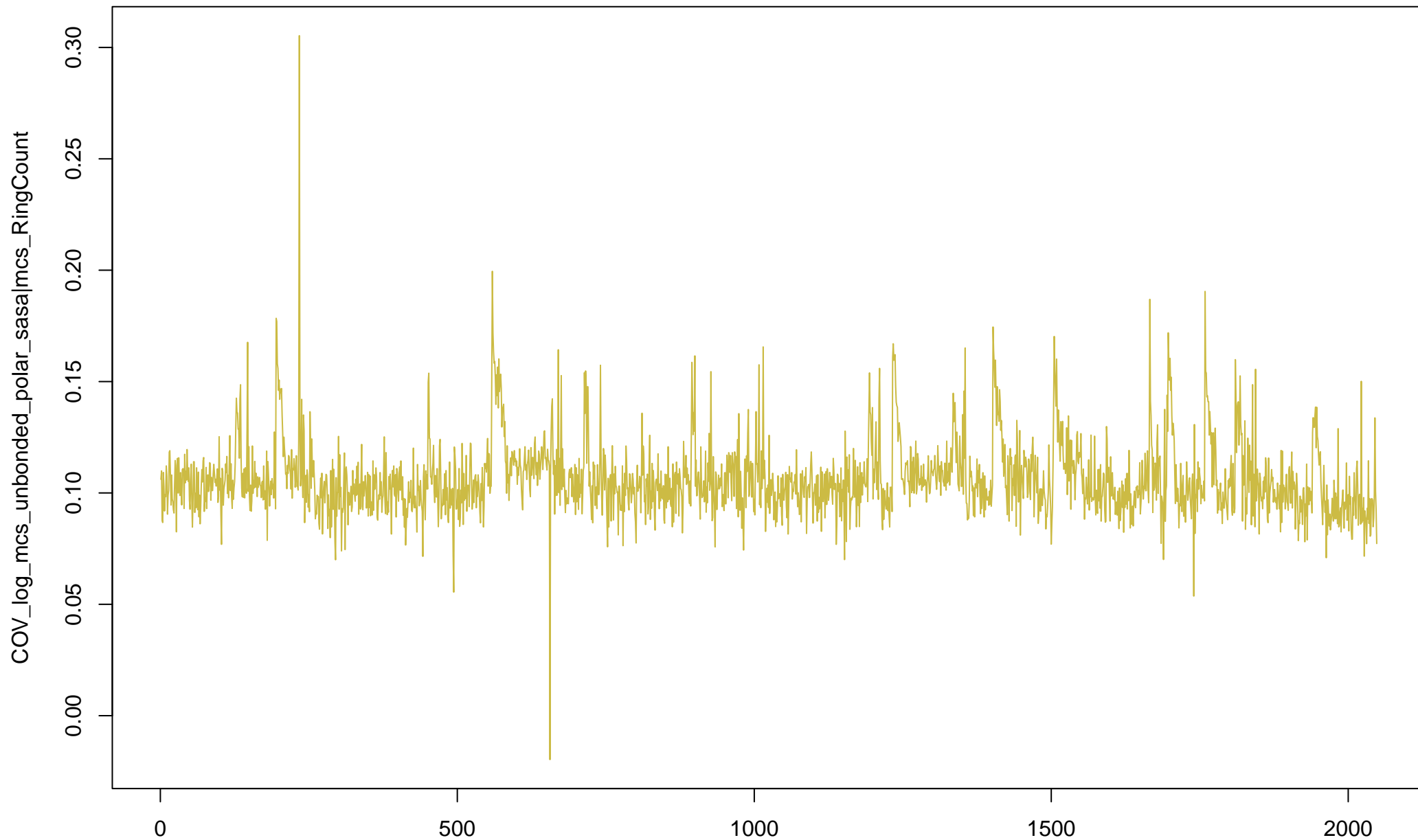
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1180 | BMK = 0.145 | MCSE(6.27) = 3.32 | stat: FALSE | burn: 0



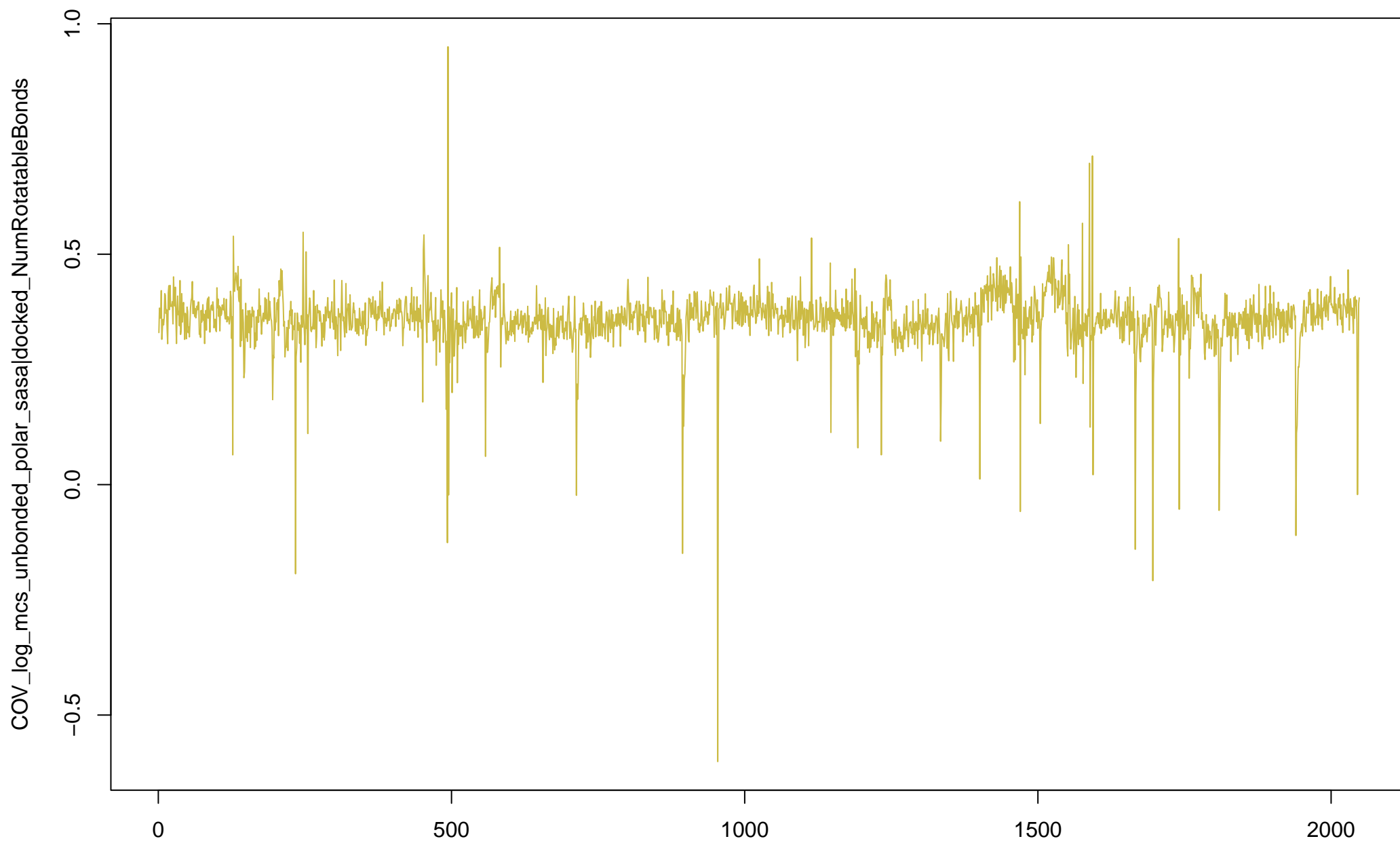
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 807 | BMK = 0.141 | MCSE(6.27) = 3.96 | stat: FALSE | burn: 0



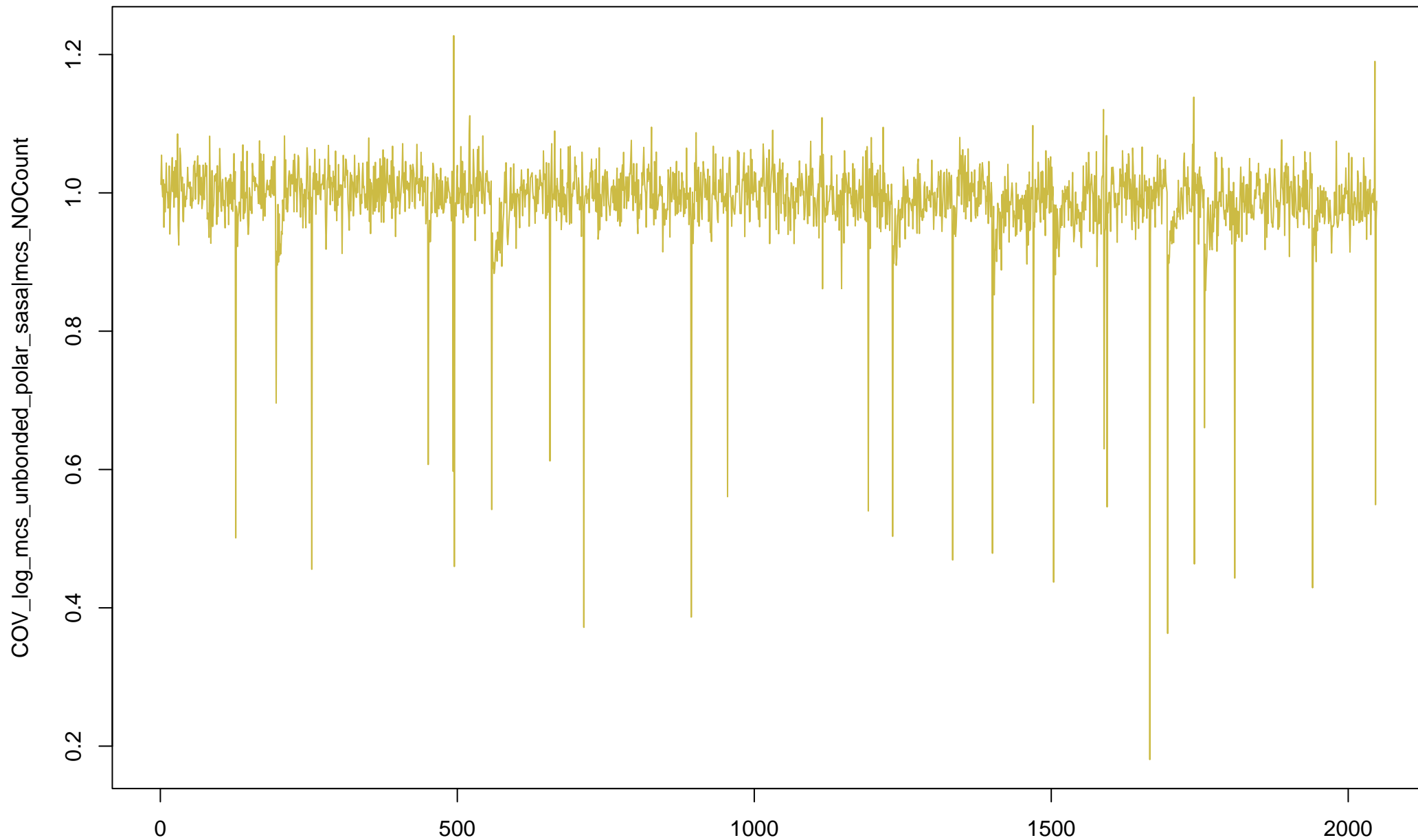
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 241 | BMK = 0.103 | MCSE(6.27) = 6.31 | stat: TRUE | burn: 0



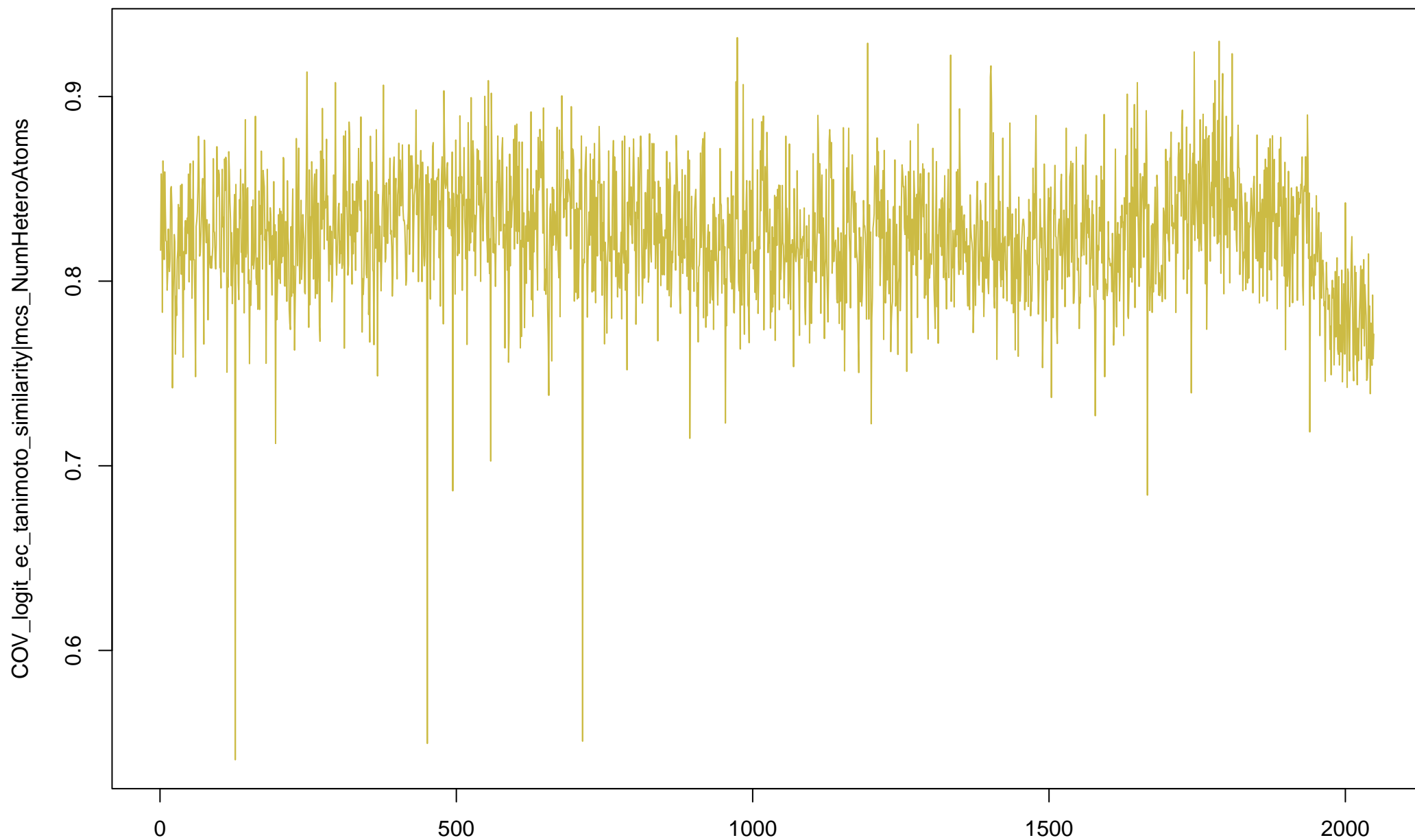
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 653 | BMK = 0.114 | MCSE(6.27) = 4.05 | stat: TRUE | burn: 0



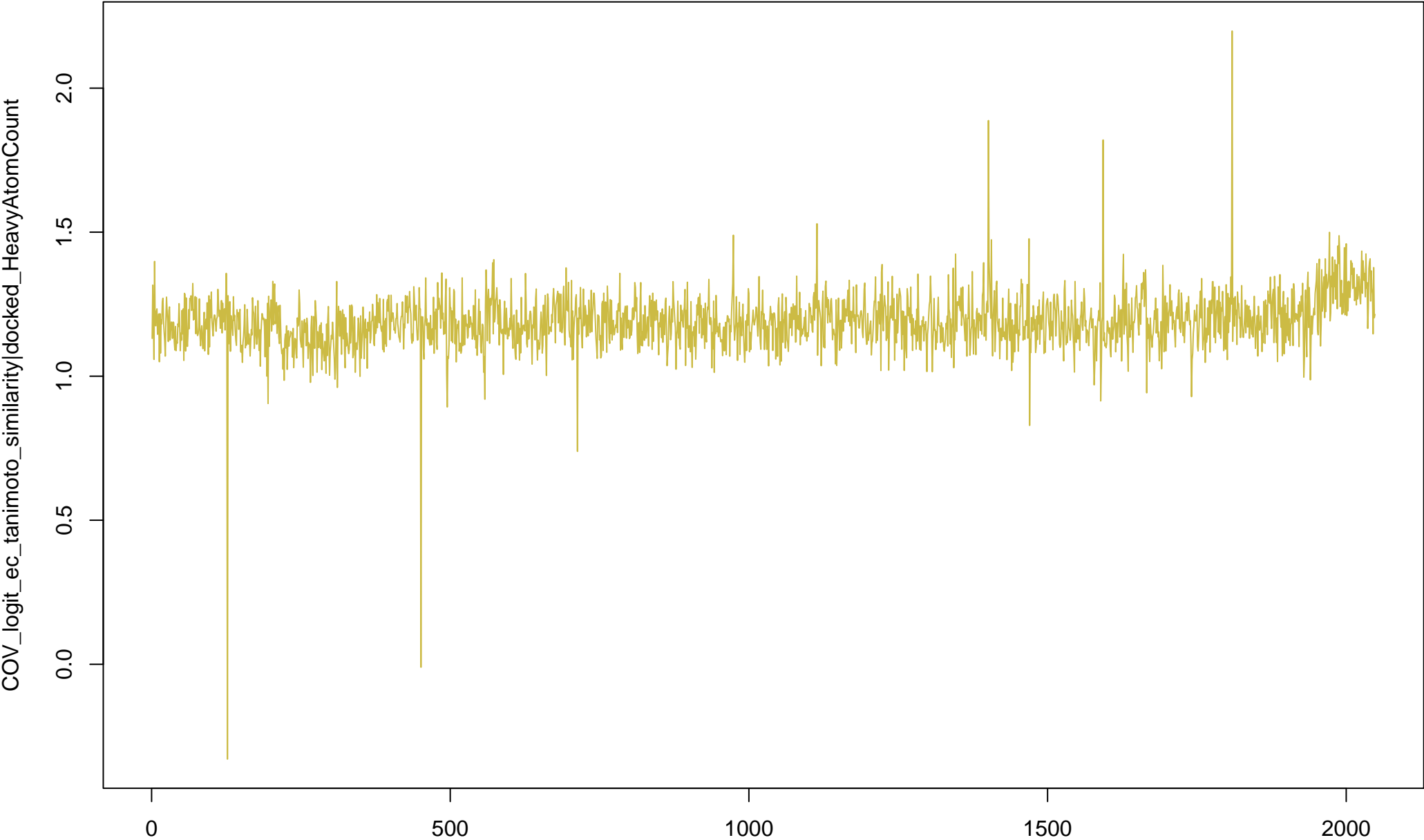
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1110 | BMK = 0.147 | MCSE(6.27) = 3.53 | stat: FALSE | burn: 0



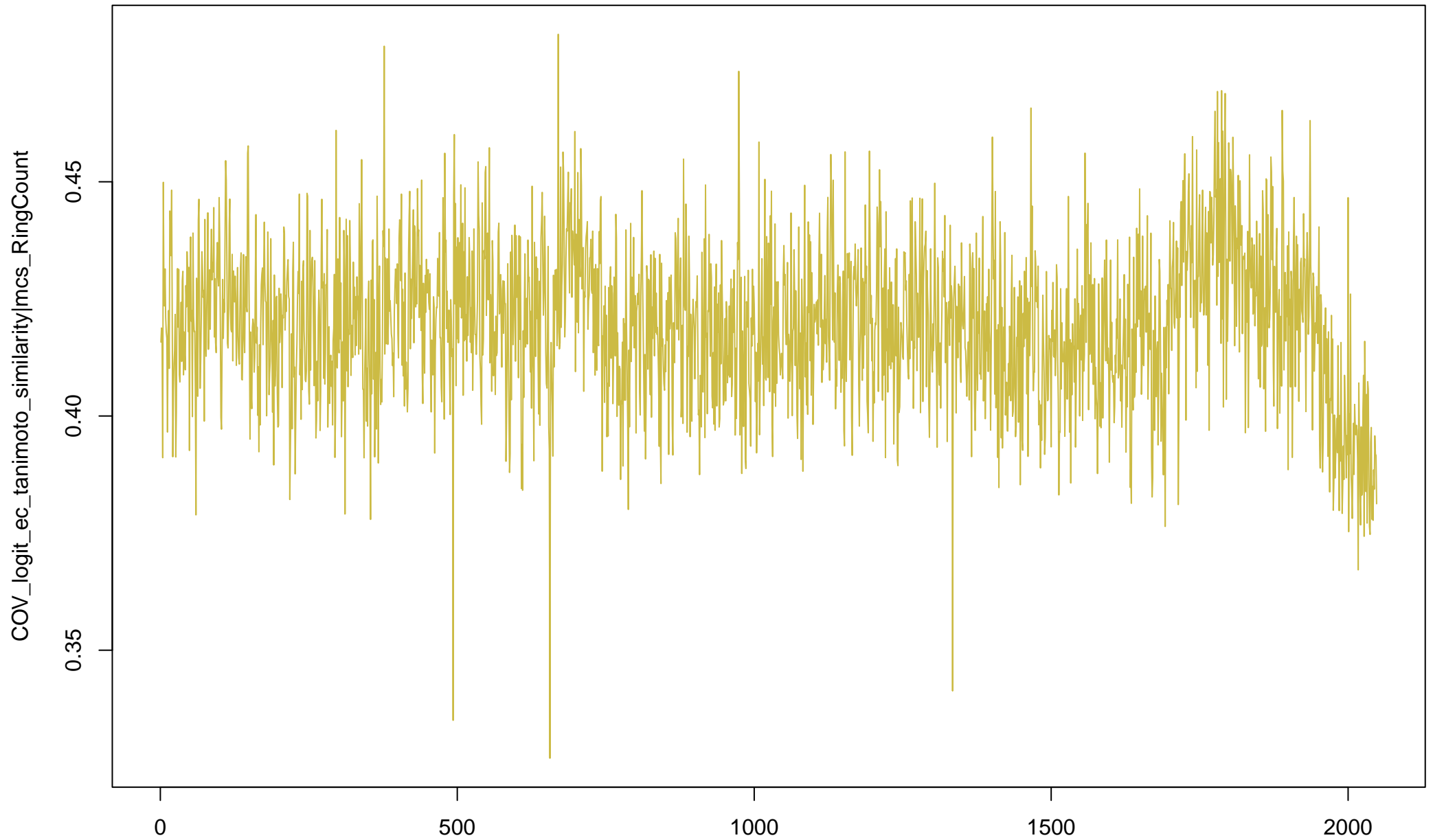
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 152 | BMK = 0.108 | MCSE(6.27) = 4.97 | stat: TRUE | burn: 0



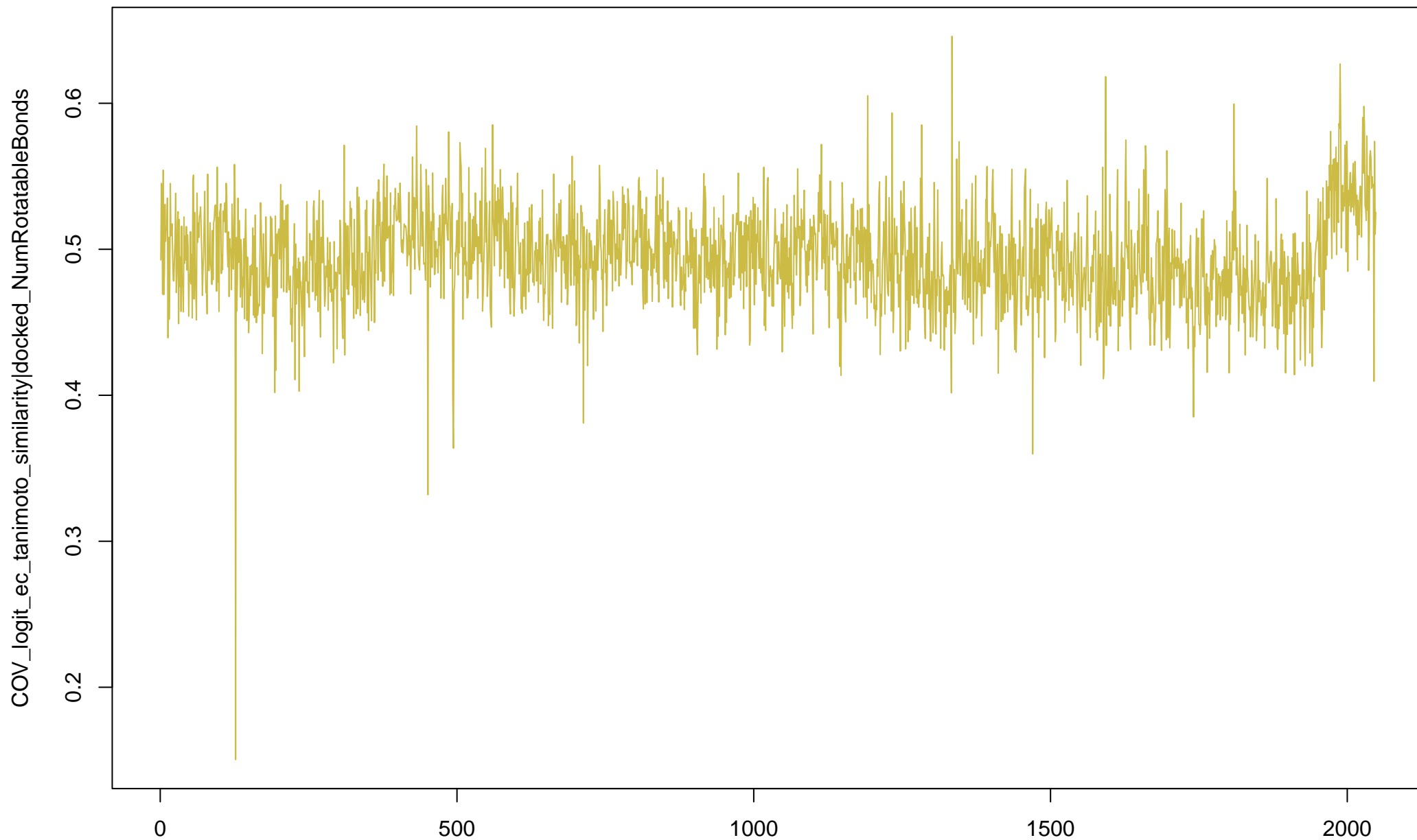
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 319 | BMK = 0.145 | MCSE(6.27) = 4.88 | stat: FALSE | burn: 0



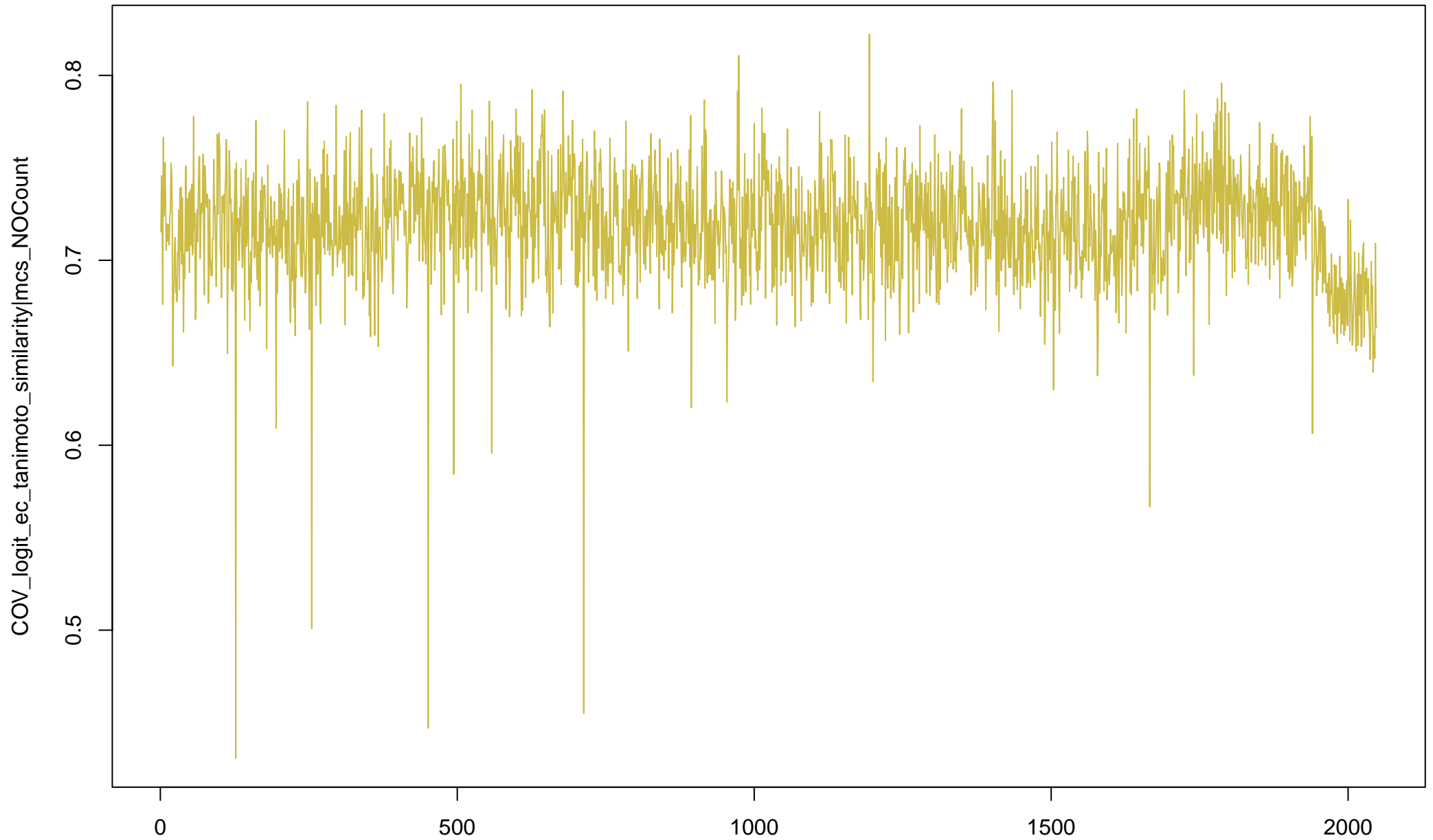
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 105 | BMK = 0.0972 | MCSE(6.27) = 6.23 | stat: TRUE | burn: 0



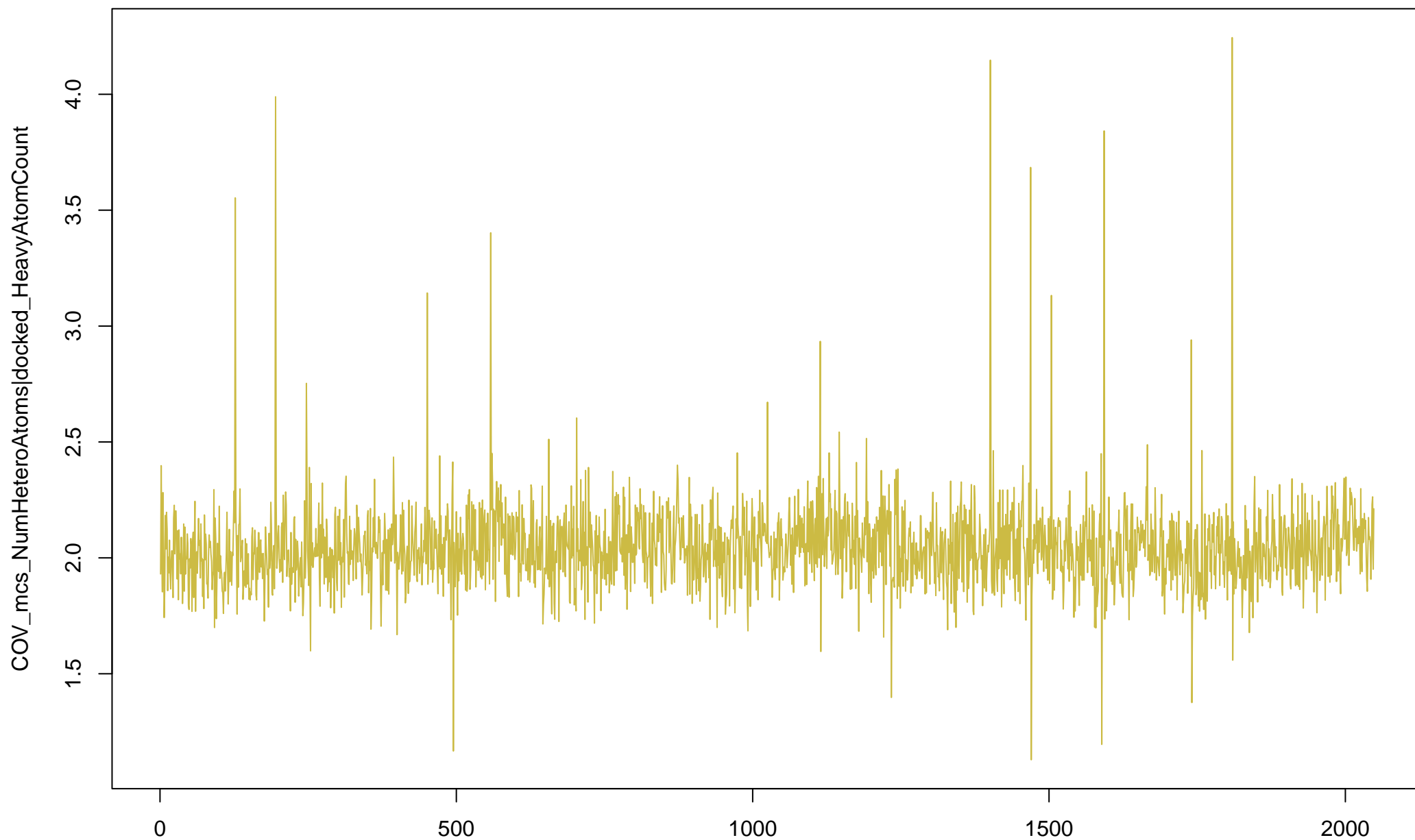
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 136 | BMK = 0.148 | MCSE(6.27) = 5.6 | stat: TRUE | burn: 0



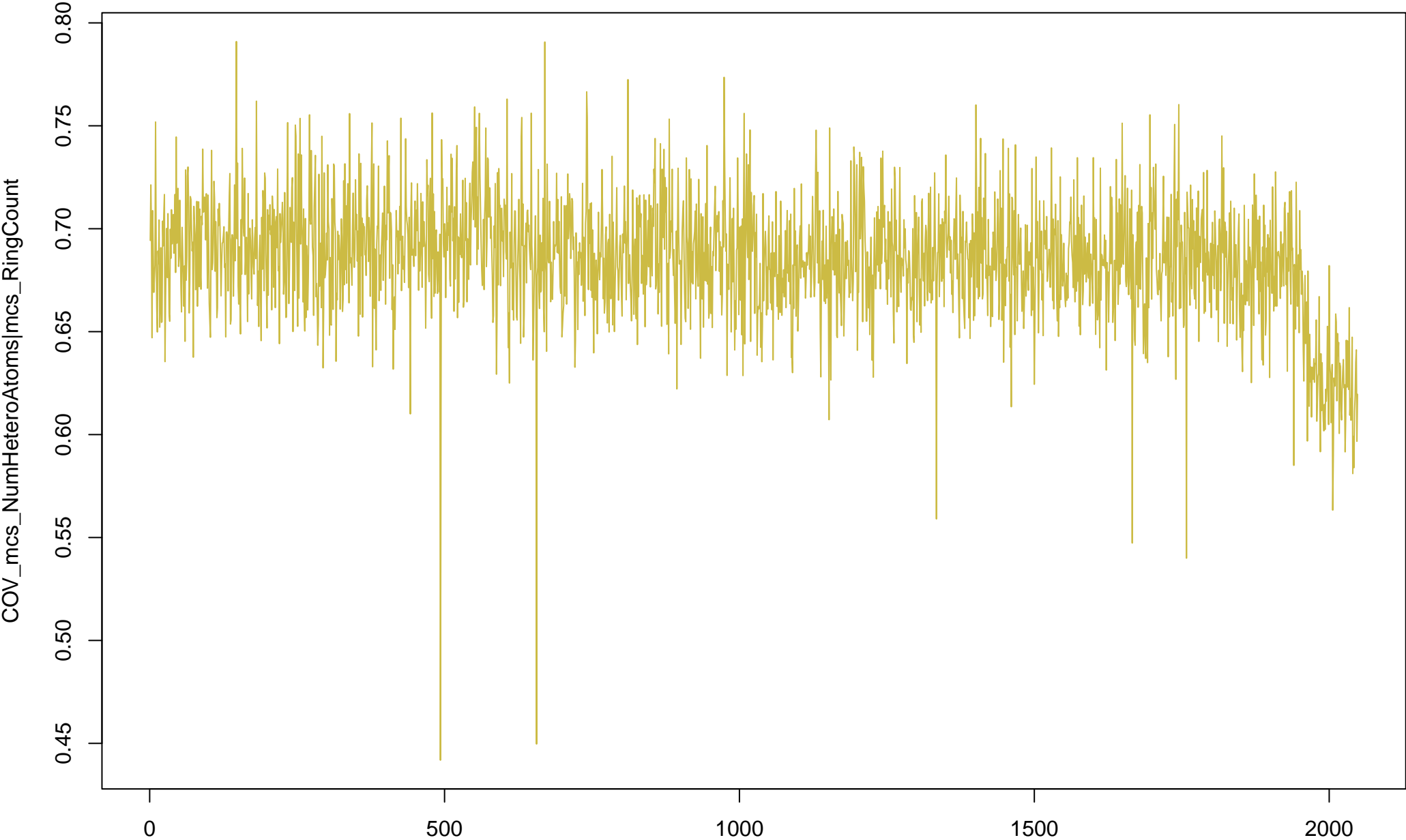
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 178 | BMK = 0.0958 | MCSE(6.27) = 4.68 | stat: TRUE | burn: 0



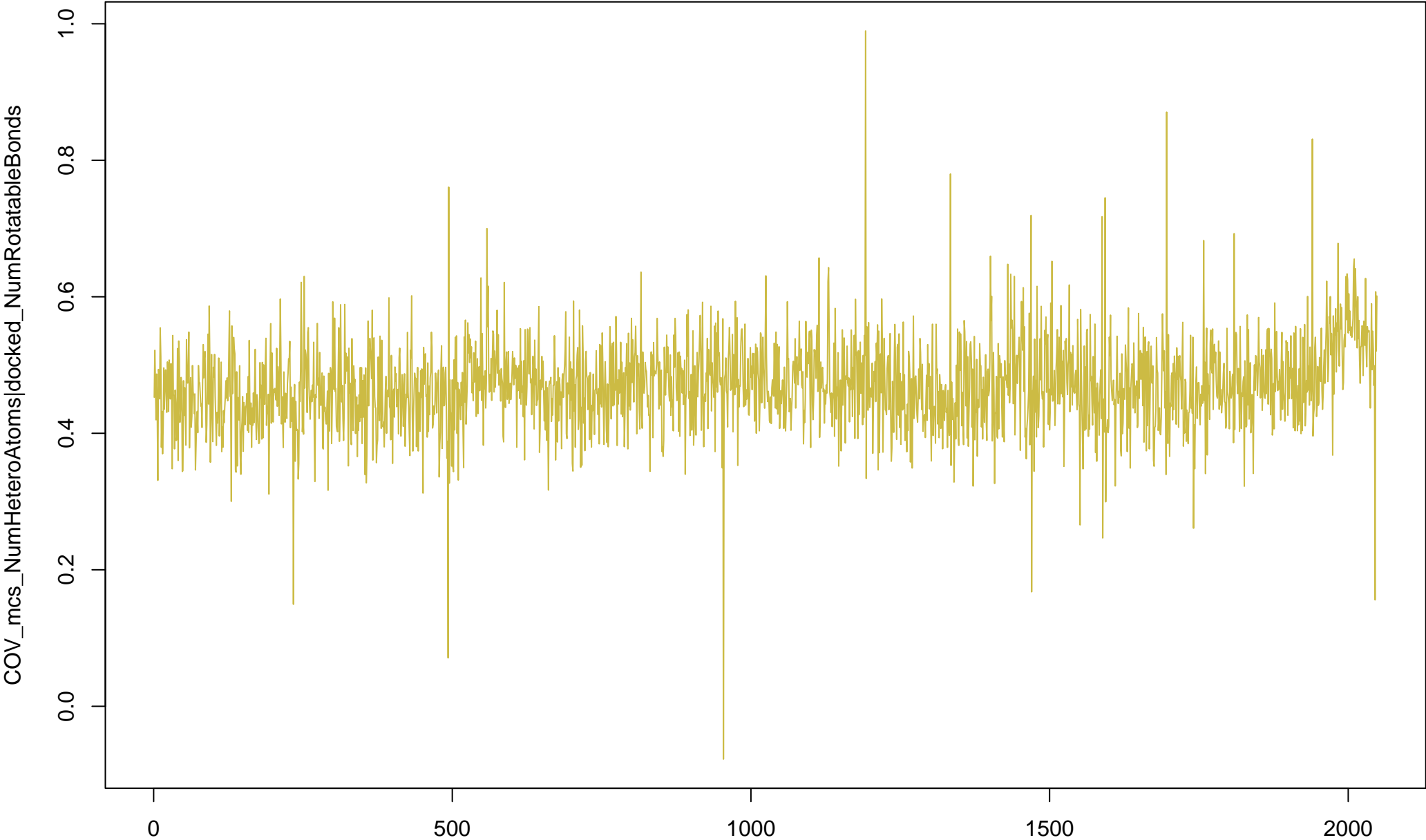
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0821 | MCSE(6.27) = 2.78 | stat: FALSE | burn: 0



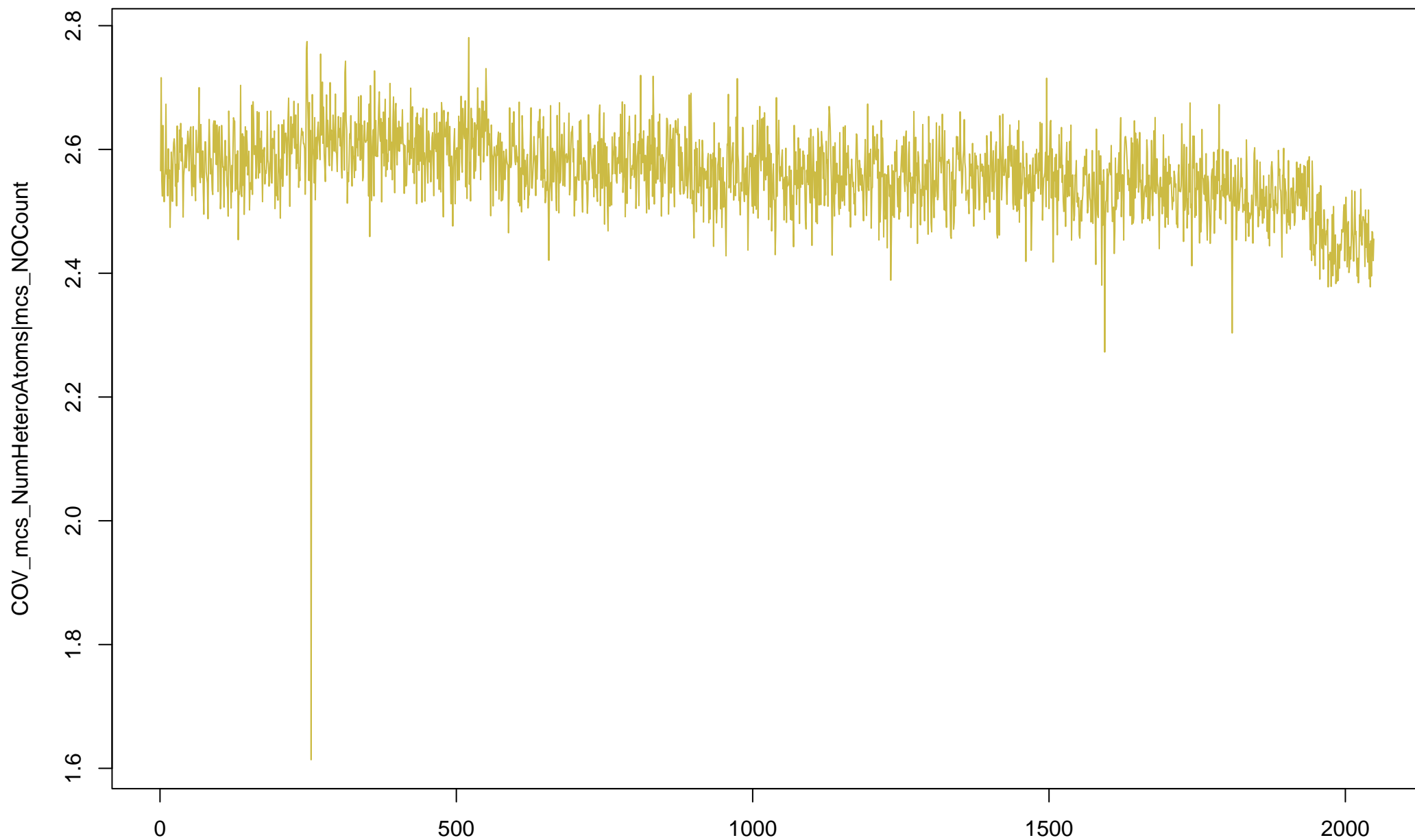
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 120 | BMK = 0.187 | MCSE(6.27) = 5.89 | stat: FALSE | burn: 0



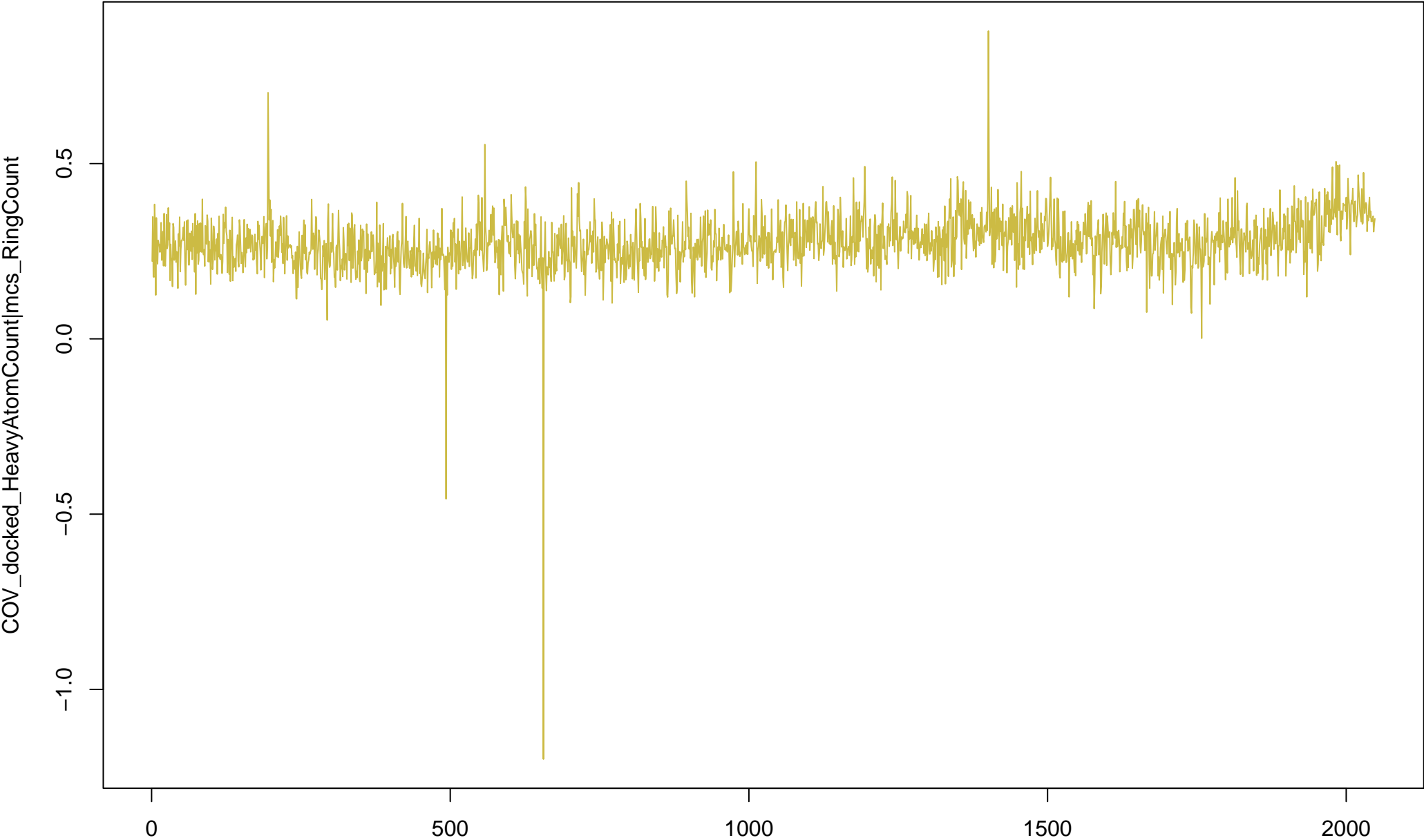
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 289 | BMK = 0.116 | MCSE(6.27) = 4.51 | stat: FALSE | burn: 0



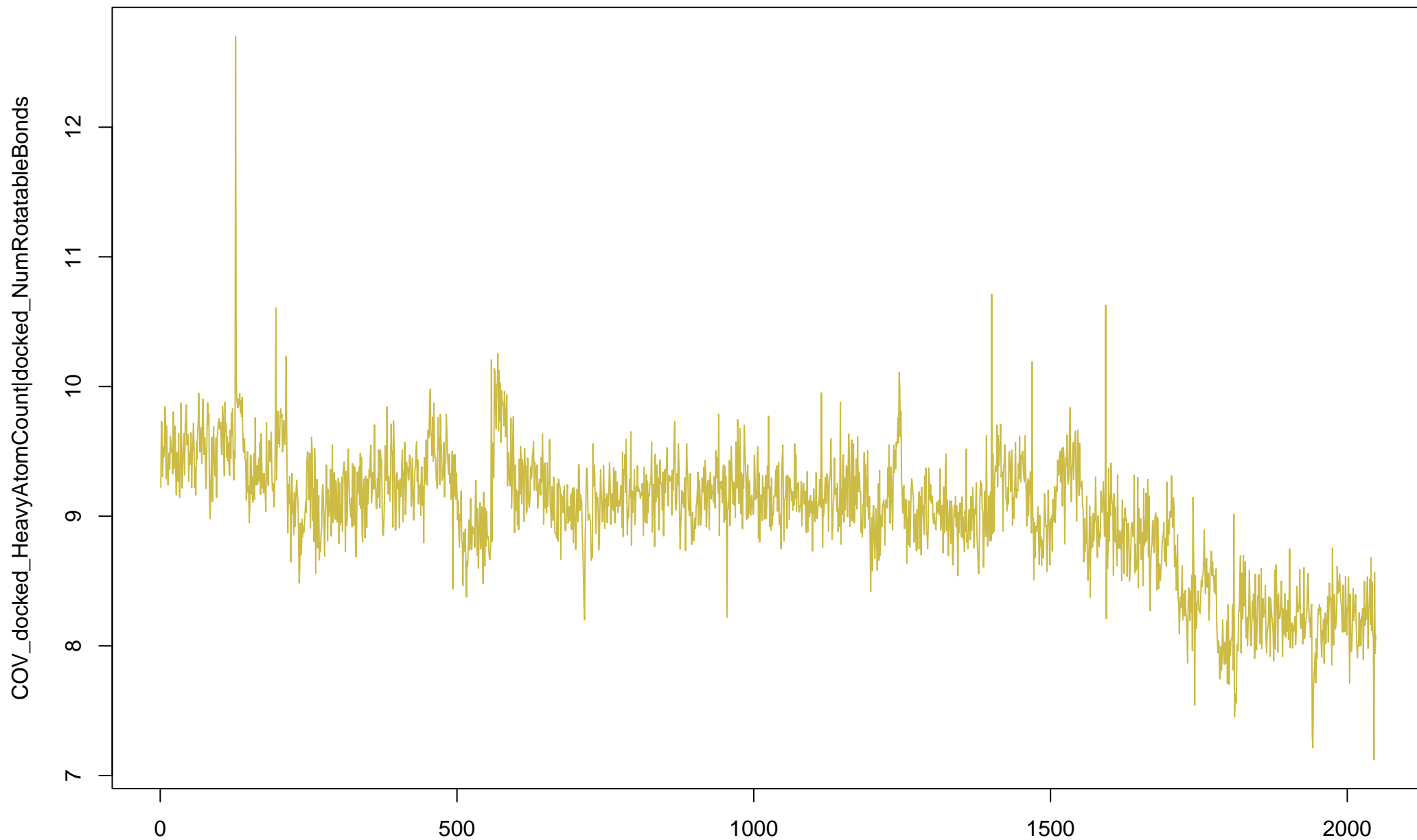
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 31 | BMK = 0.325 | MCSE(6.27) = 7.89 | stat: FALSE | burn: 0



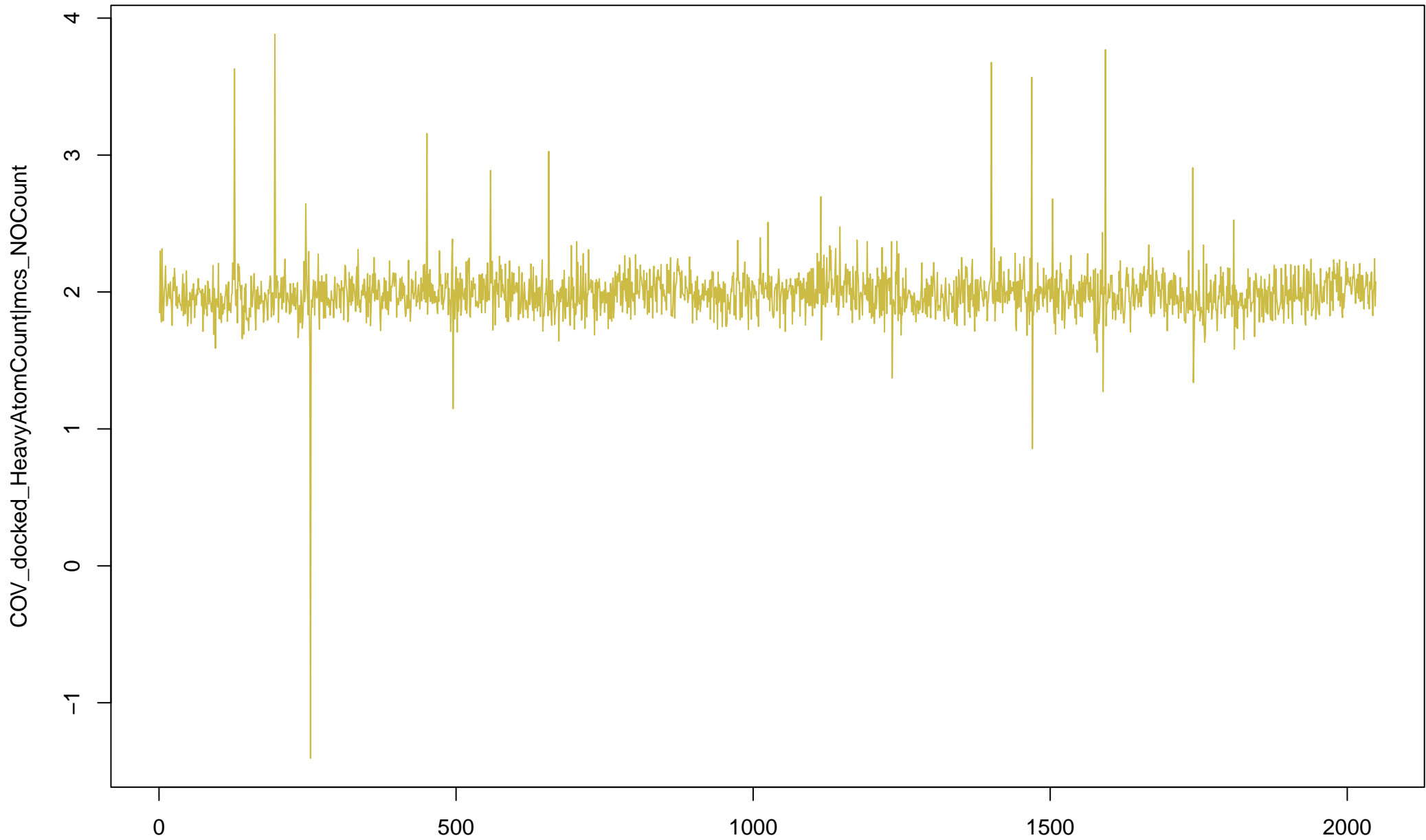
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 128 | BMK = 0.221 | MCSE(6.27) = 5.87 | stat: FALSE | burn: 0



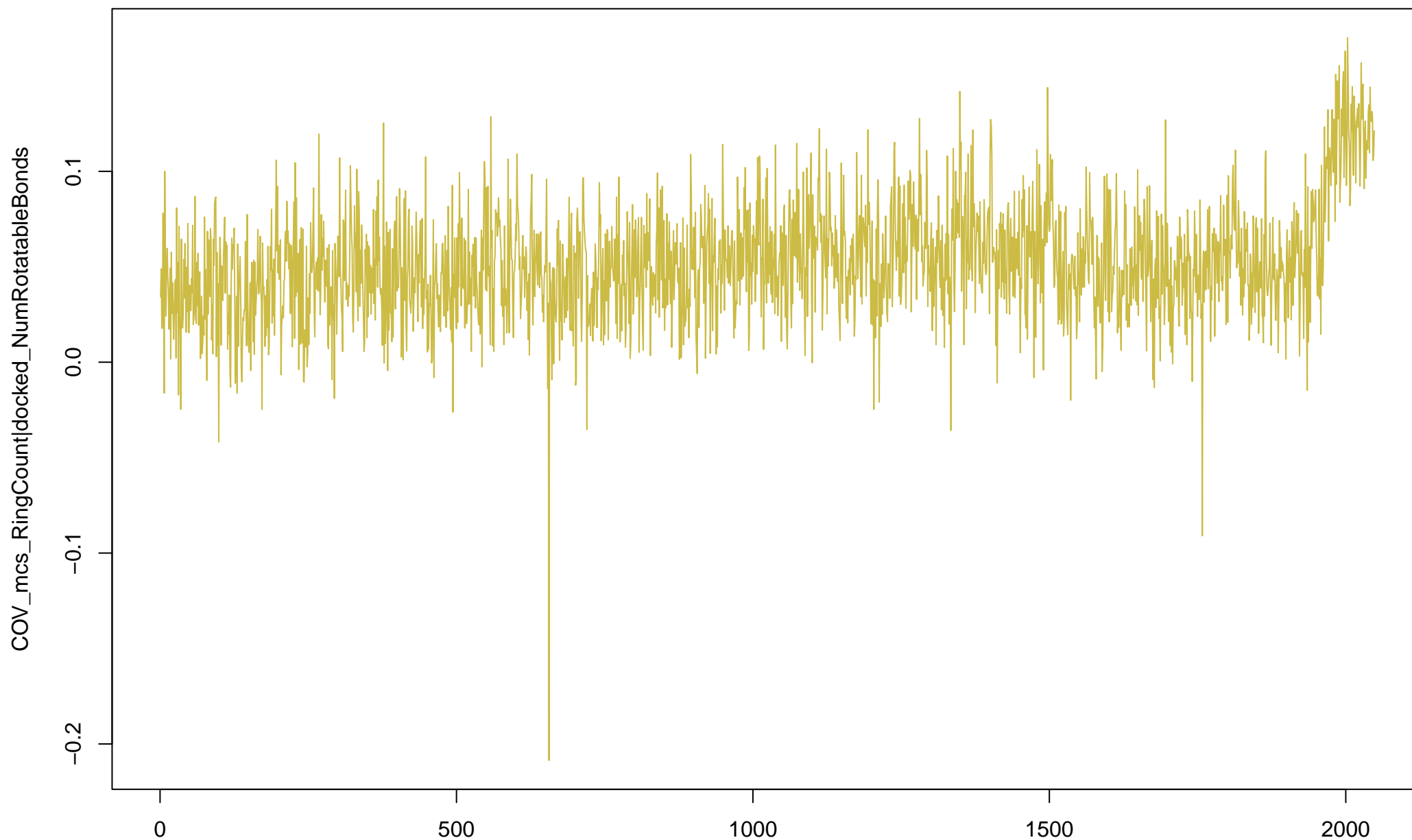
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 17.5 | BMK = 0.42 | MCSE(6.27) = 12.2 | stat: FALSE | burn: 1632



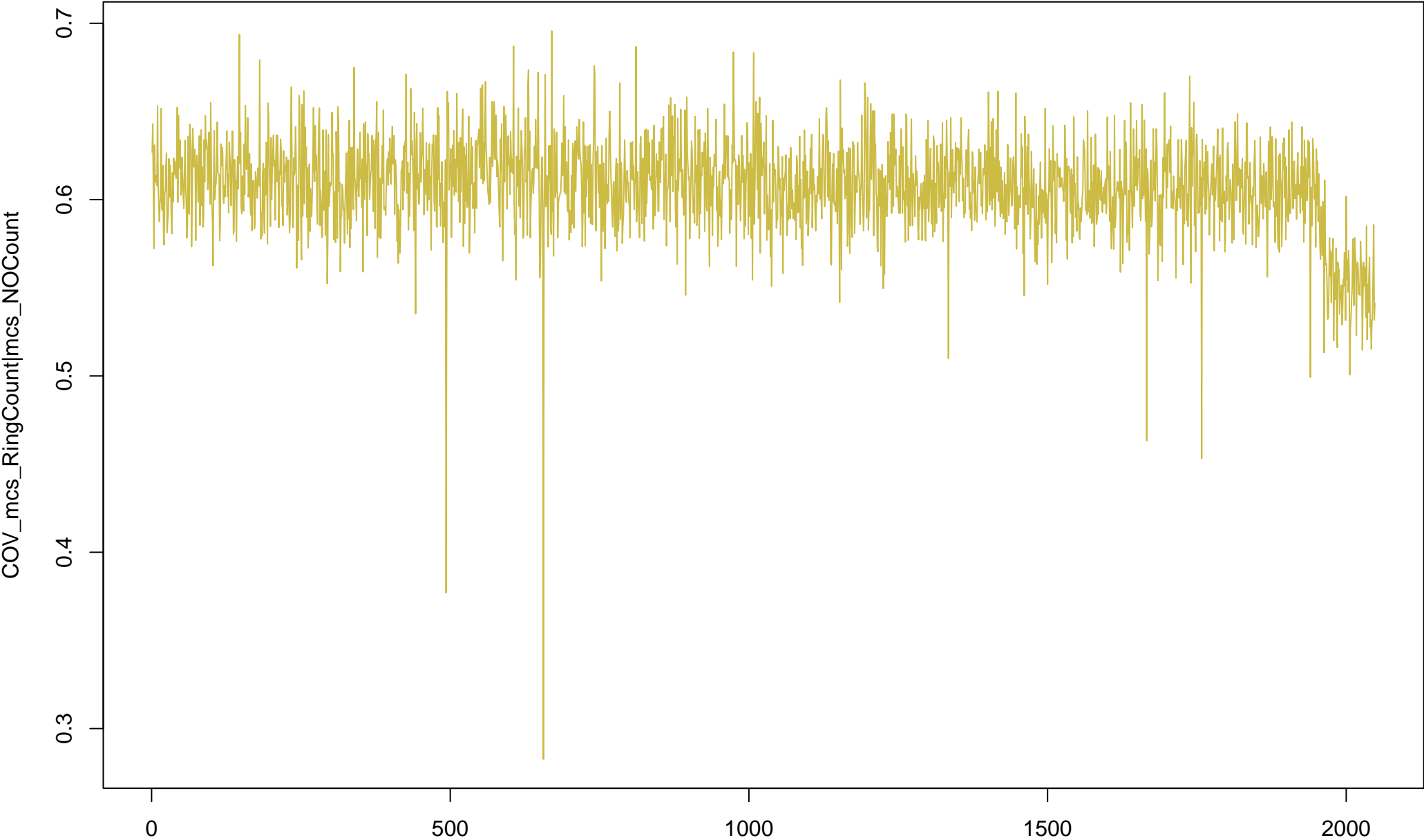
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 2050 | BMK = 0.0889 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 93.1 | BMK = 0.204 | MCSE(6.27) = 6.93 | stat: FALSE | burn: 0



COV_mcs_RingCount|mcs_NOCount
ESS = 103 | BMK = 0.187 | MCSE(6.27) = 5.74 | stat: FALSE | burn: 0



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 340 | BMK = 0.104 | MCSE(6.27) = 4.05 | stat: FALSE | burn: 0

