

-- STATS maxD --

min ESS = 7.27451663851487

max BMK = 0.602333375823862

max MCSE = 16.4178985748371

all stationary: FALSE

burn: 714

-- STATS 2D --

min ESS = 10.0327124421252

max BMK = 0.347566252369673

max MCSE = 16.2586467062423

all stationary: FALSE

burn: 102

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.454813986359933

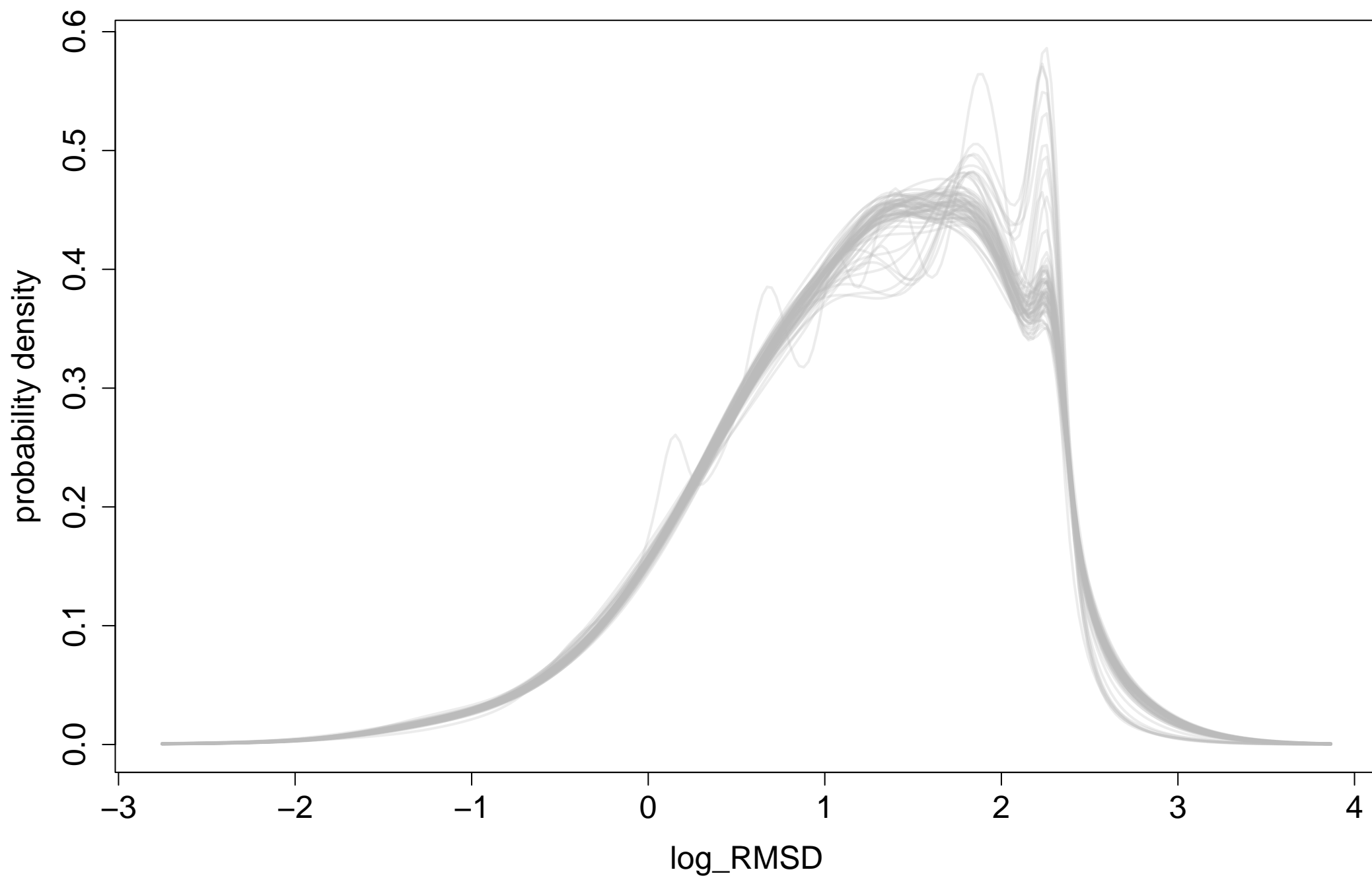
max MCSE = NaN

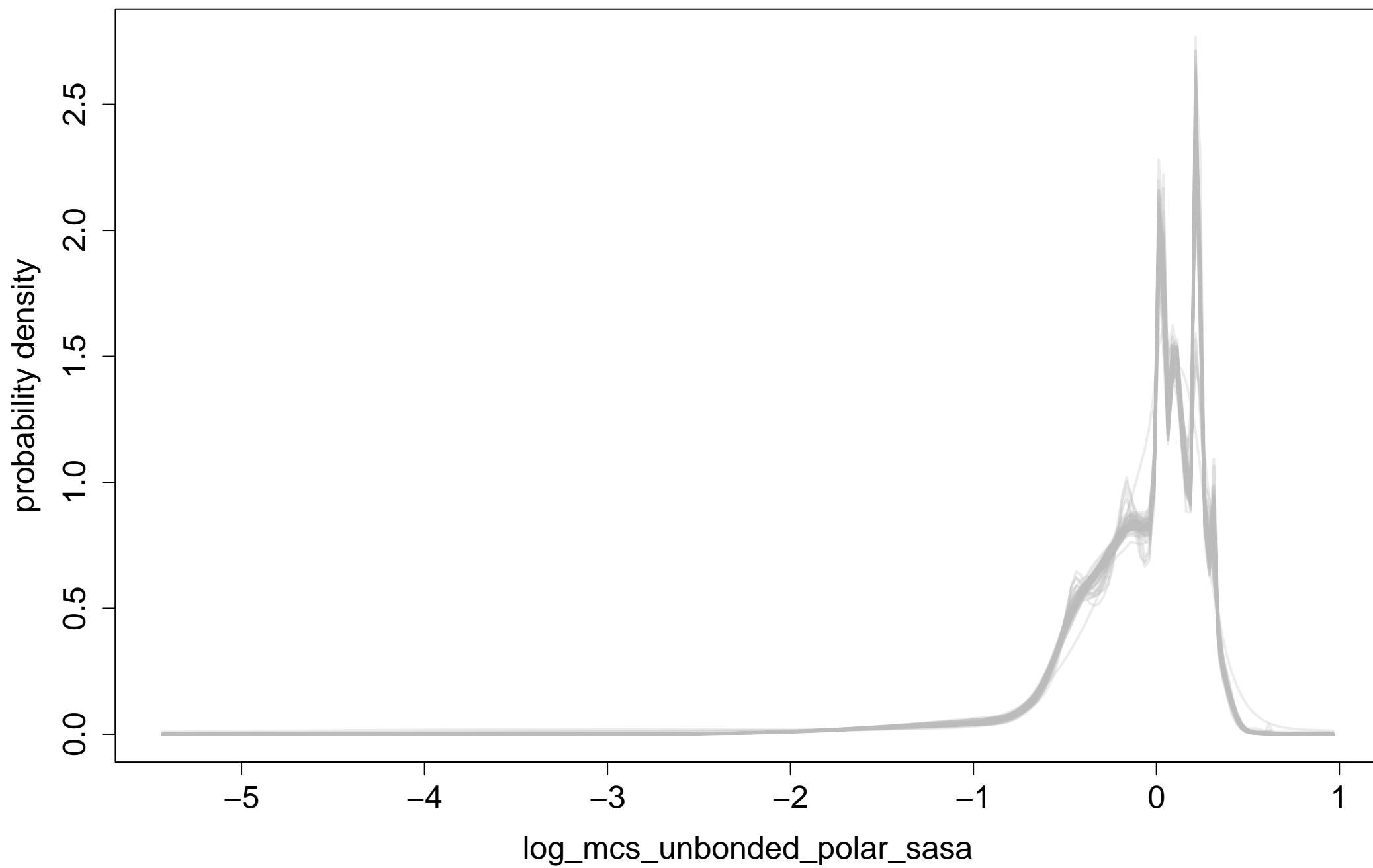
all stationary: FALSE

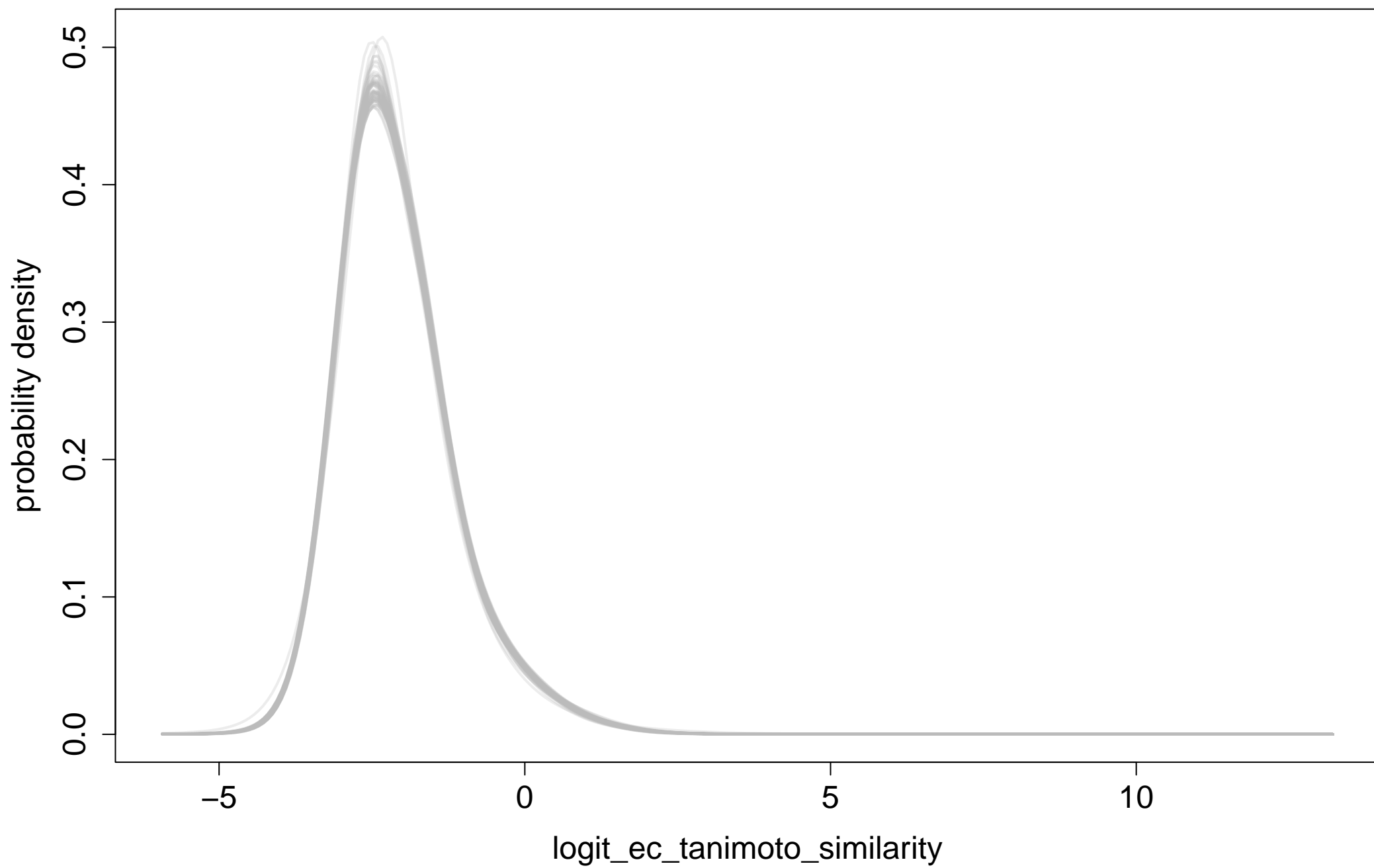
burn: 1020

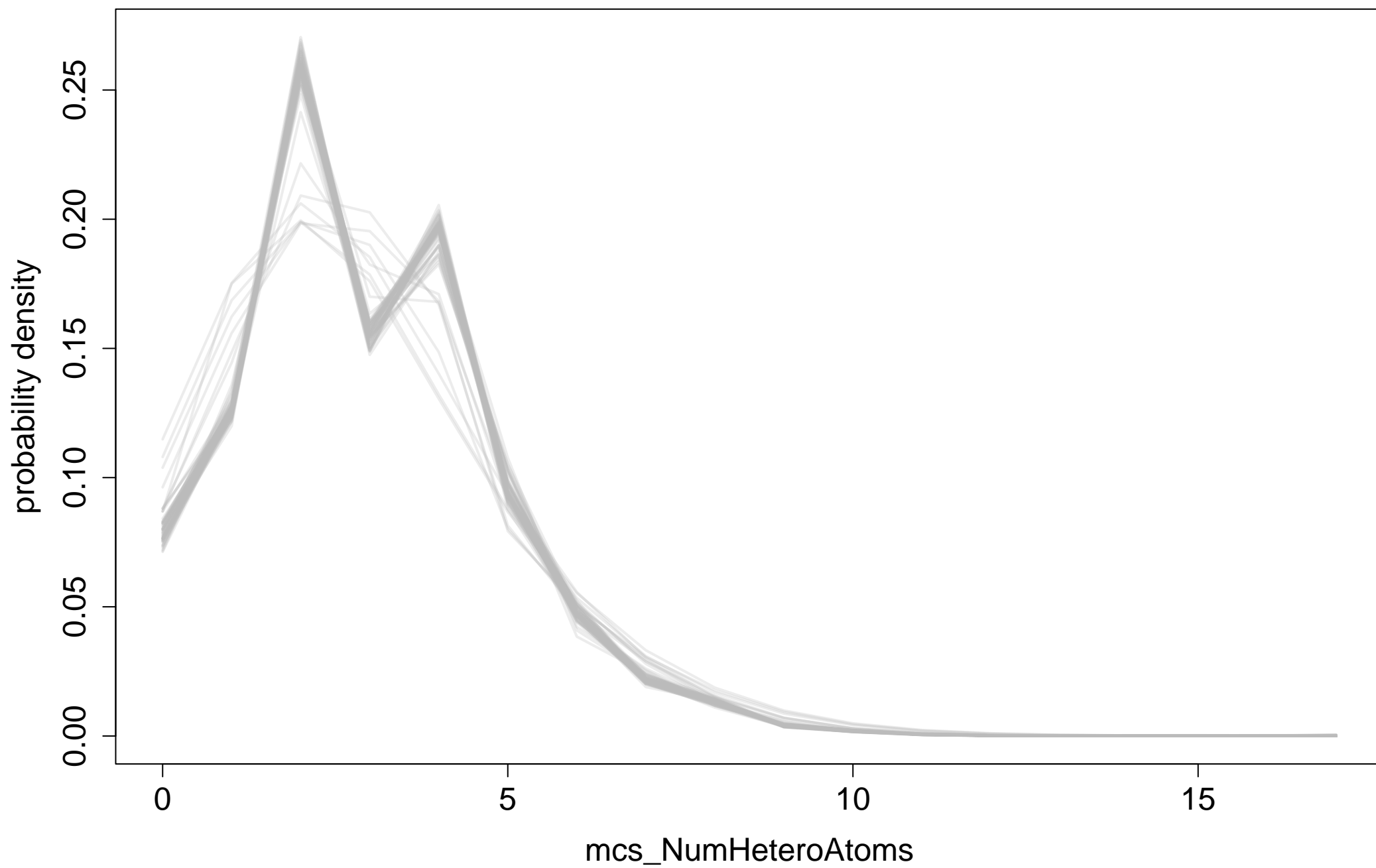
Occupied clusters: 60 of 64

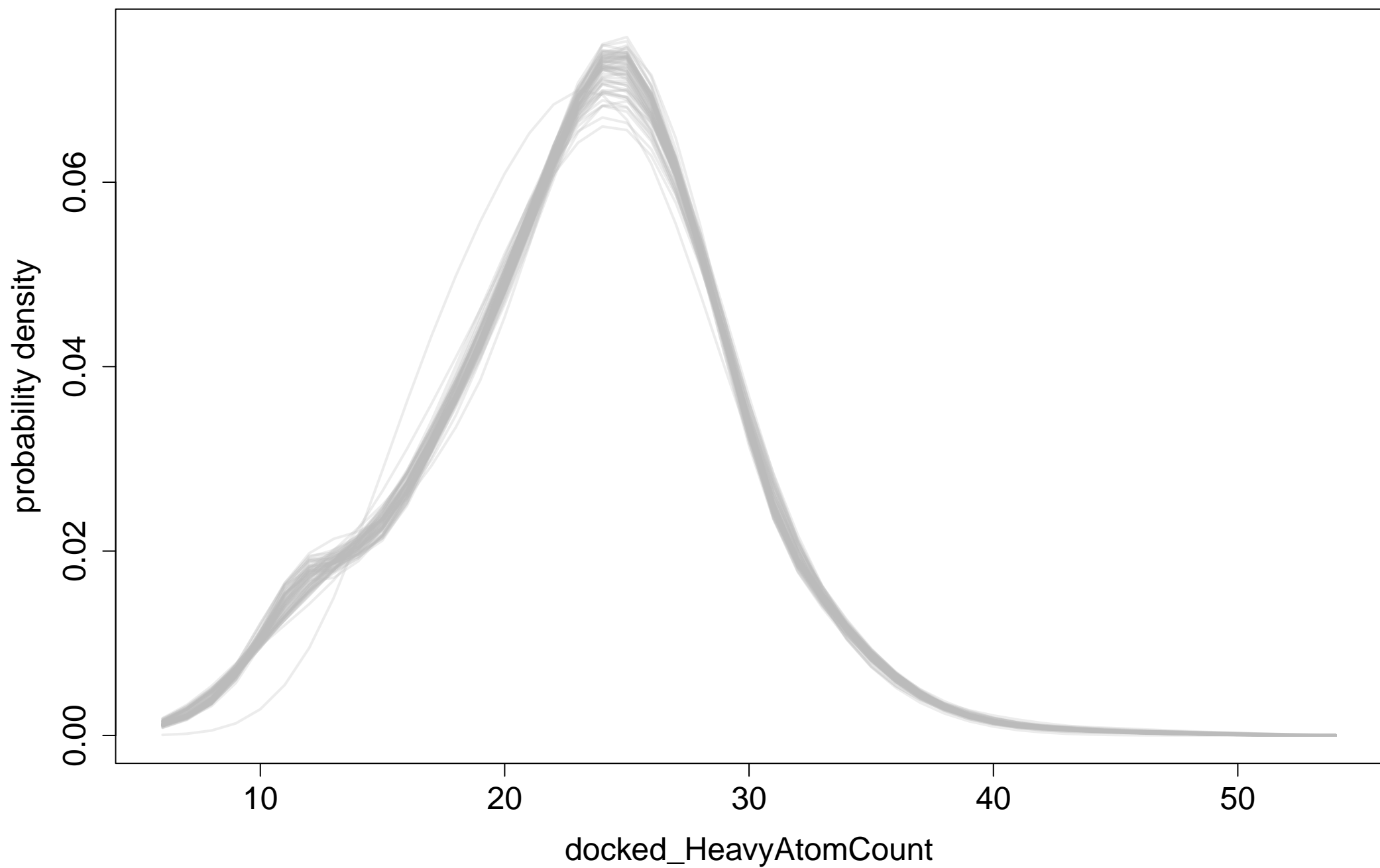
LL: -73800 +- 4470

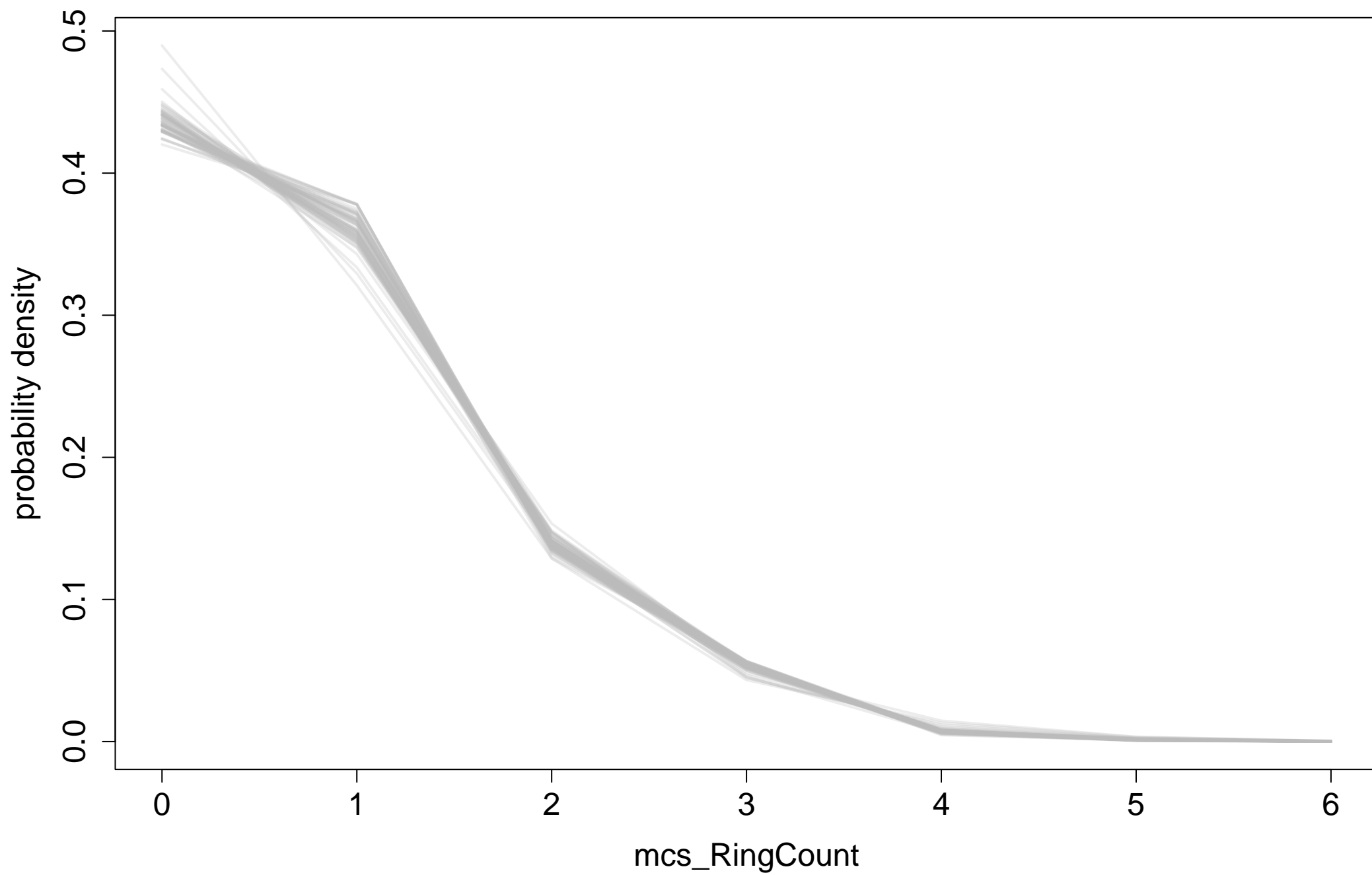


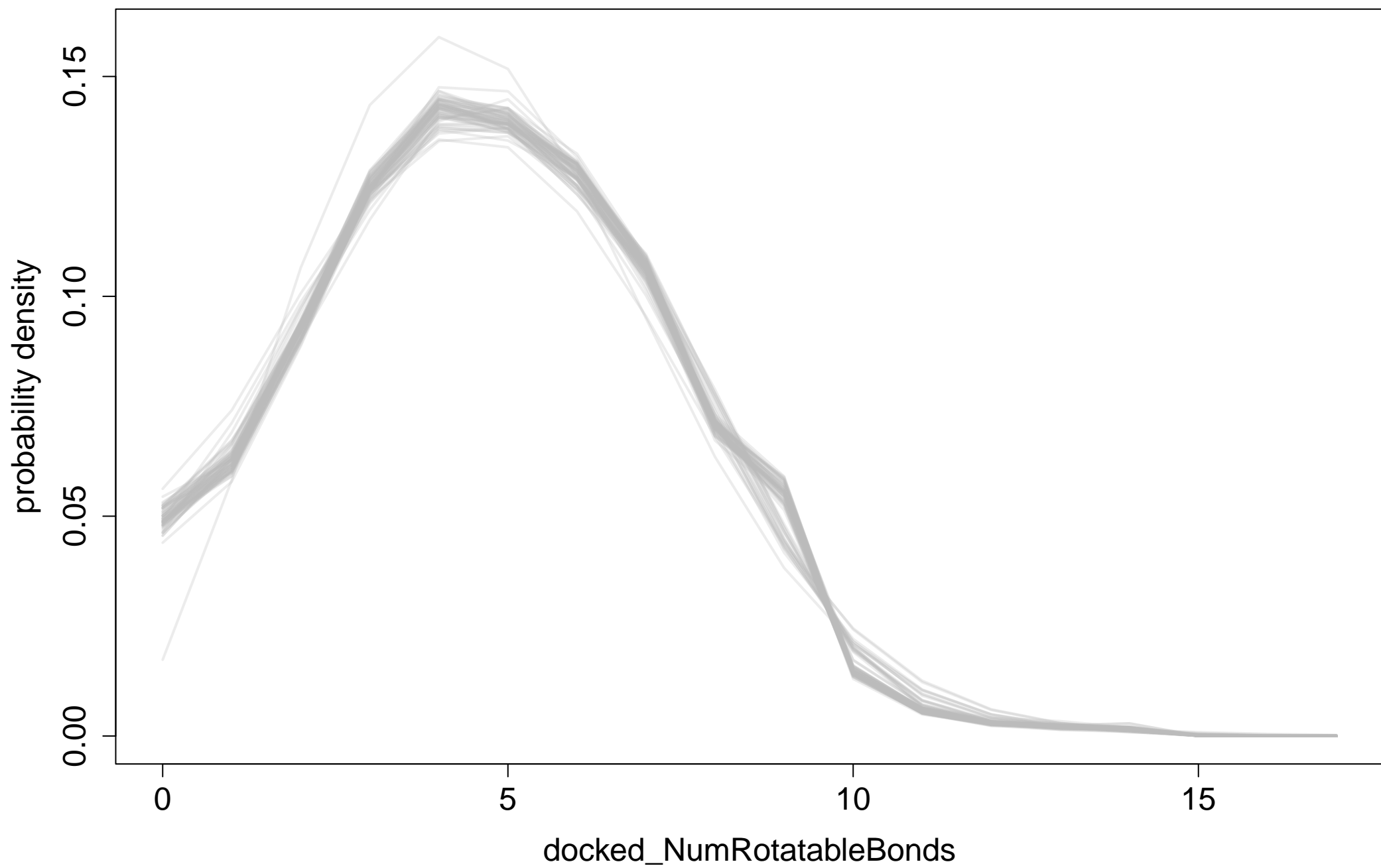


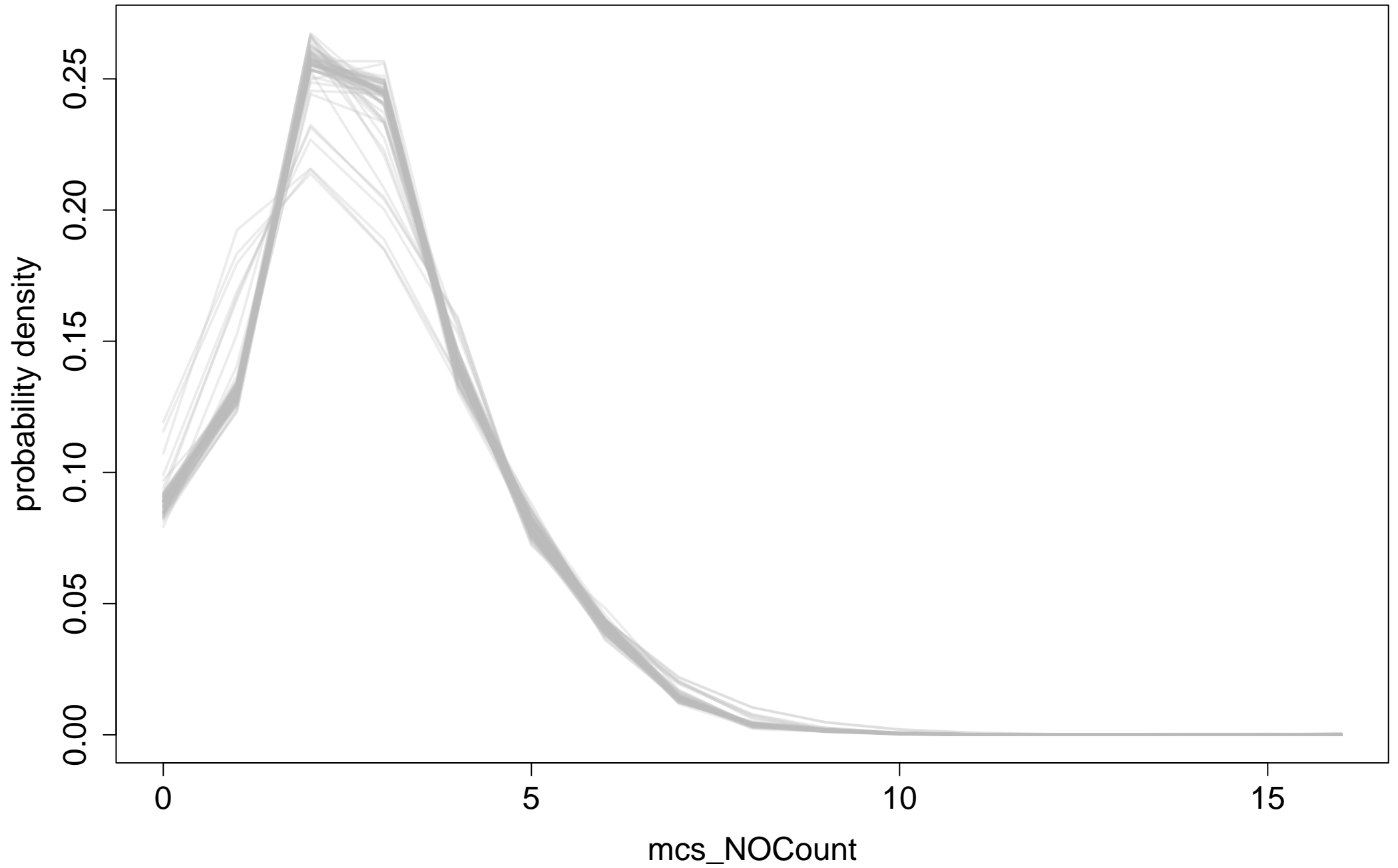


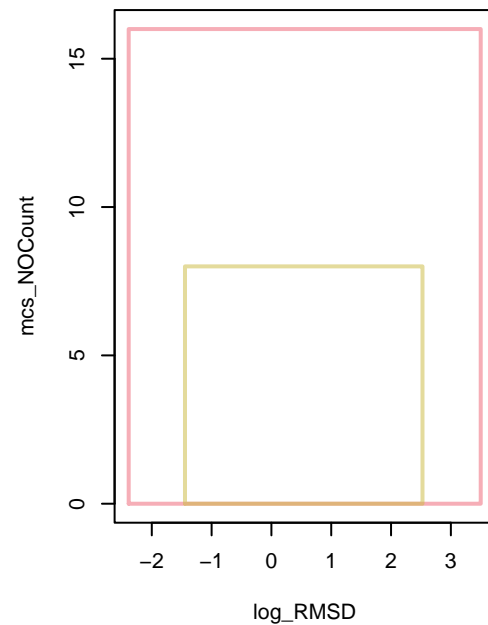
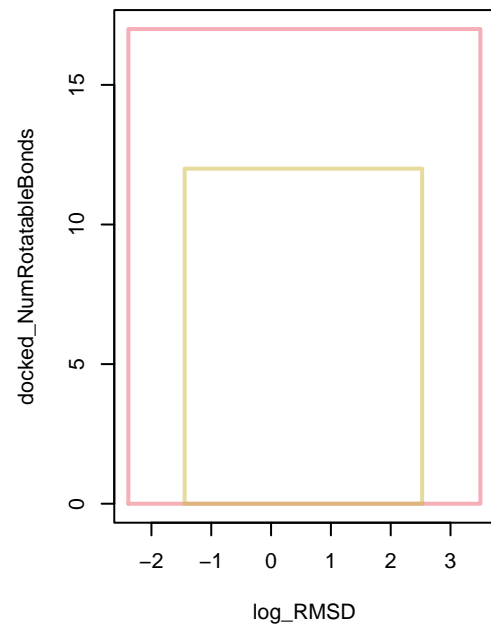
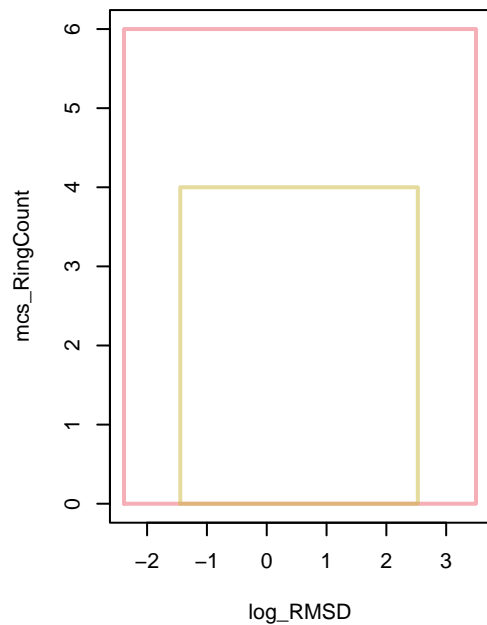
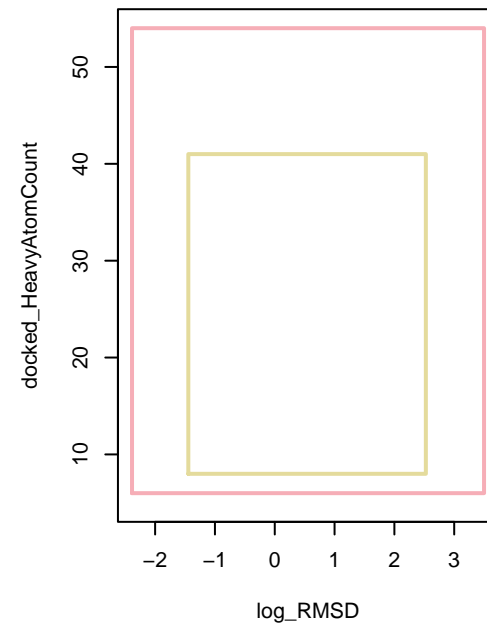
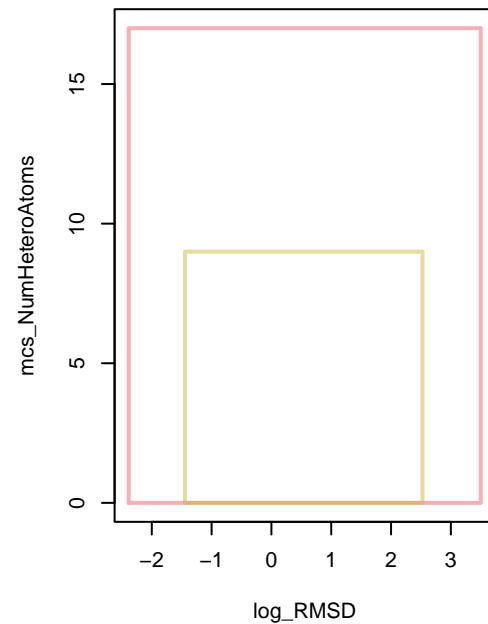
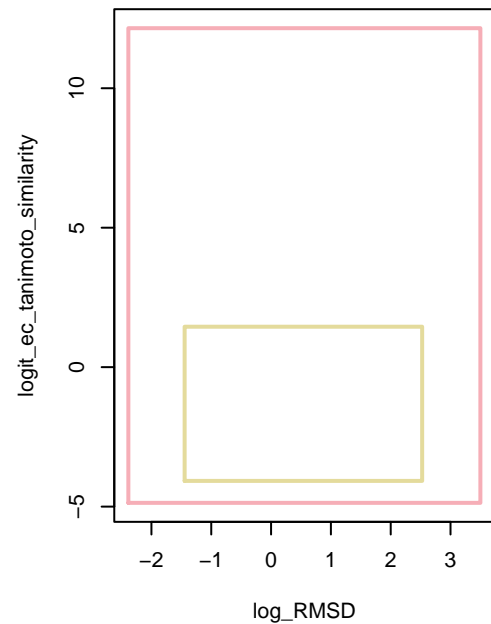
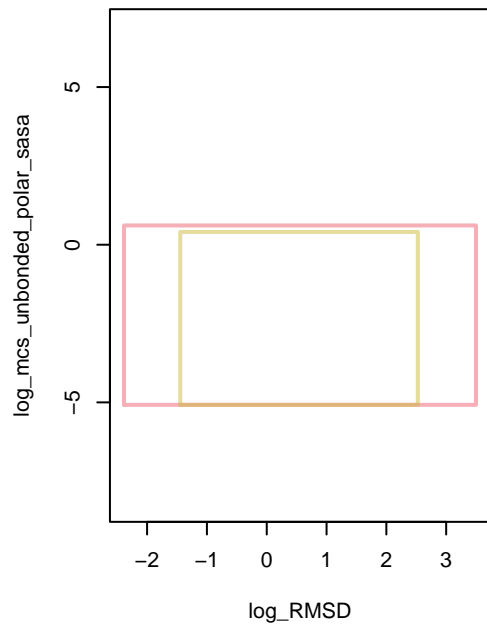




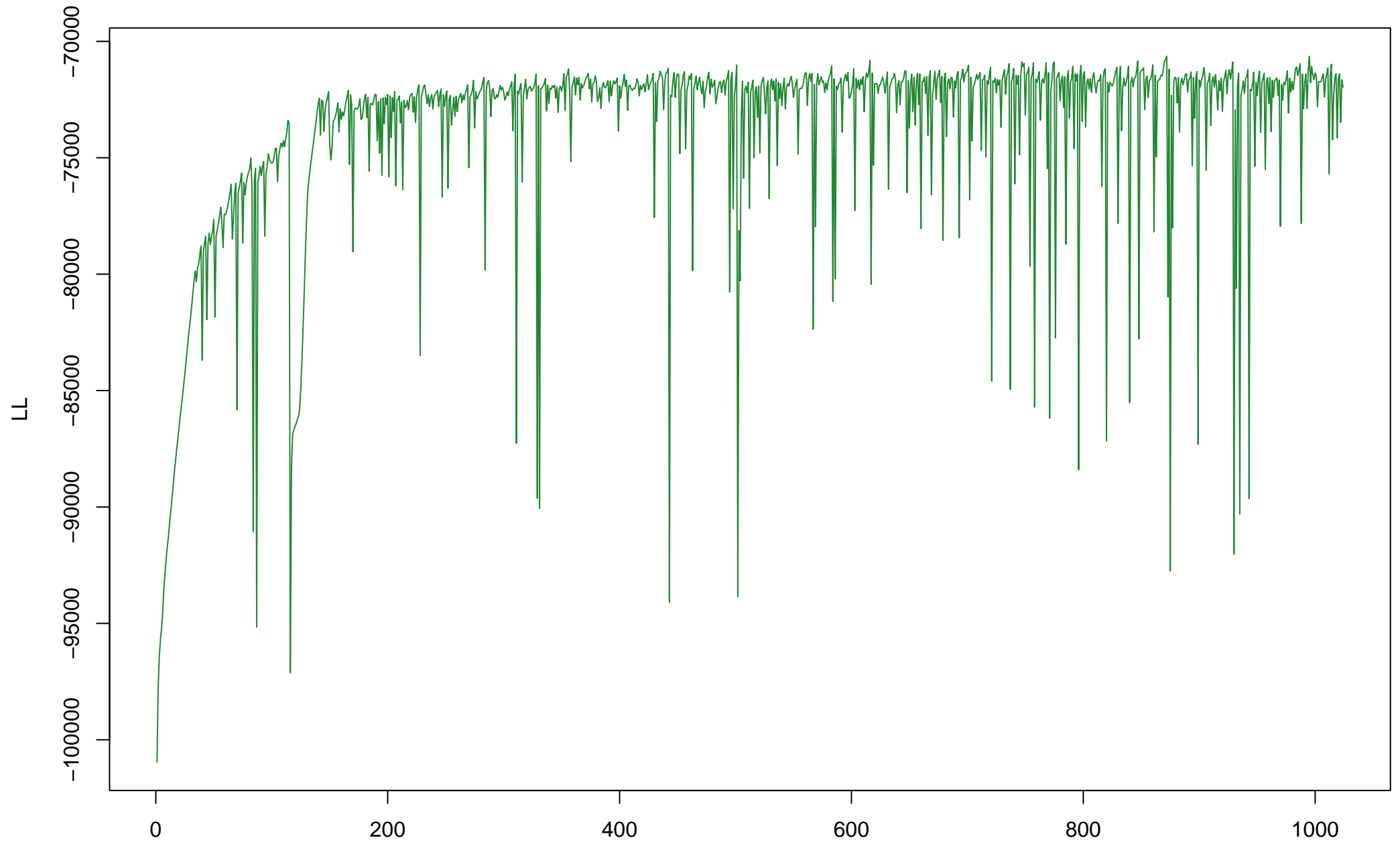




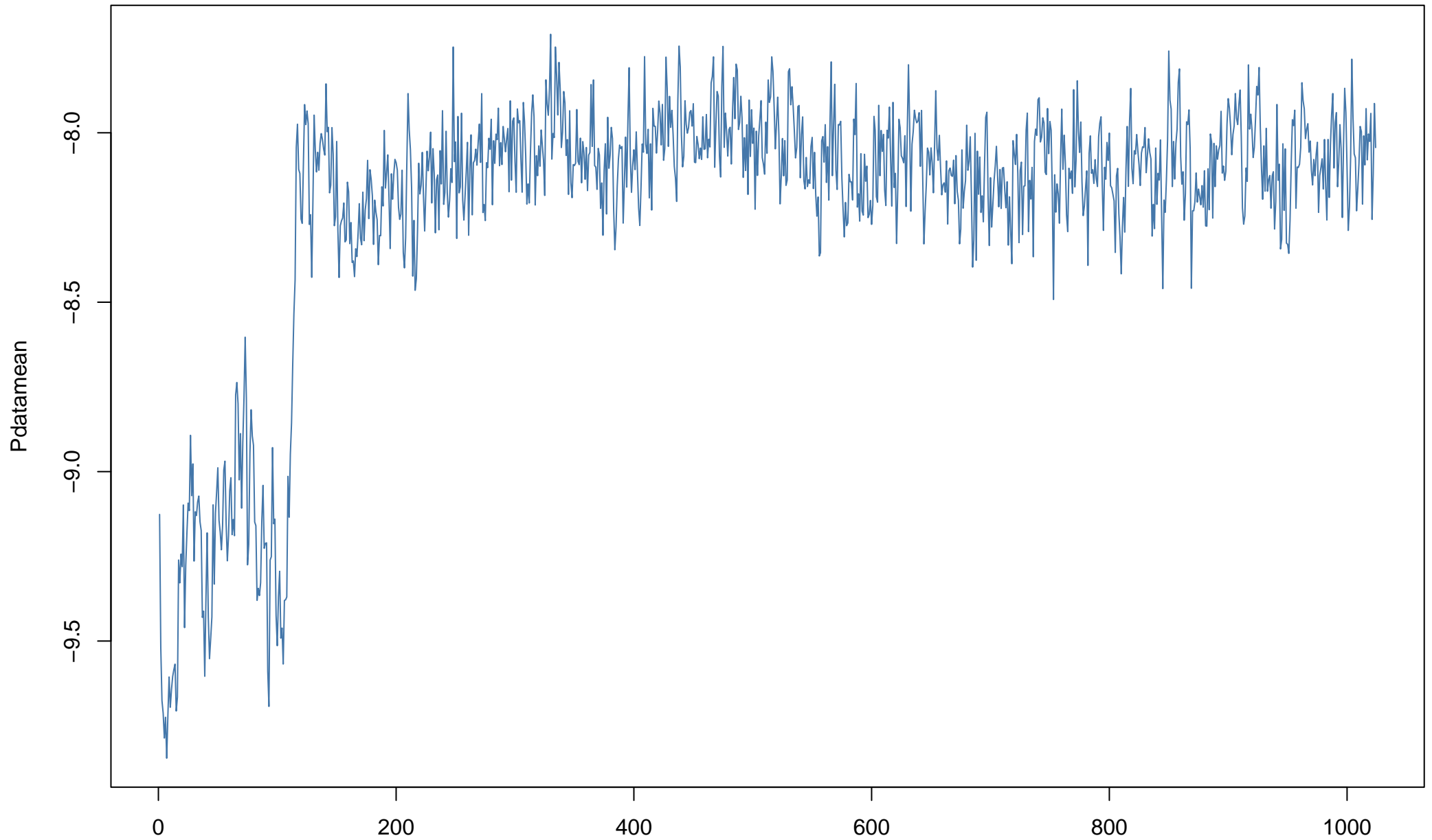




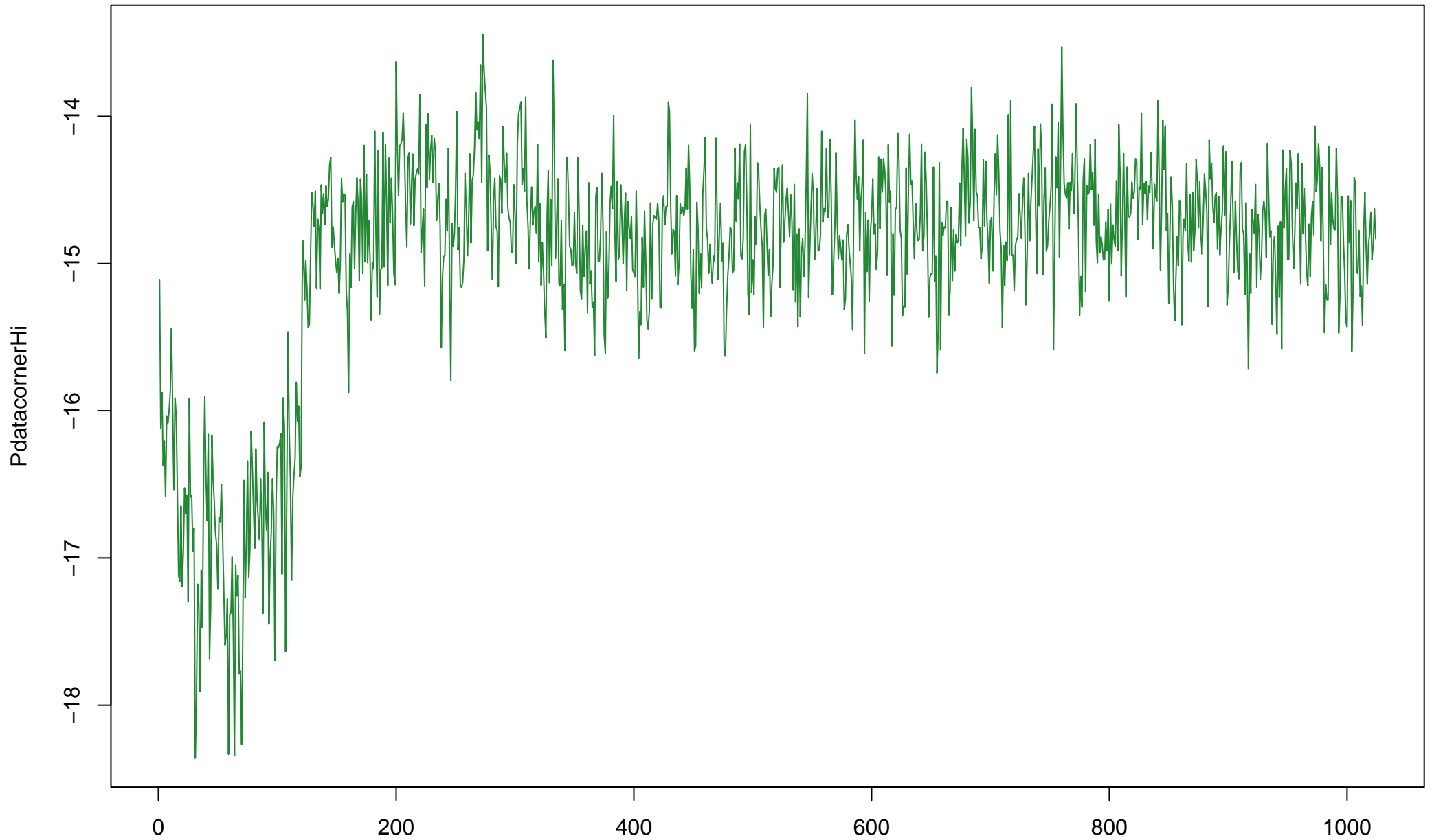
LL



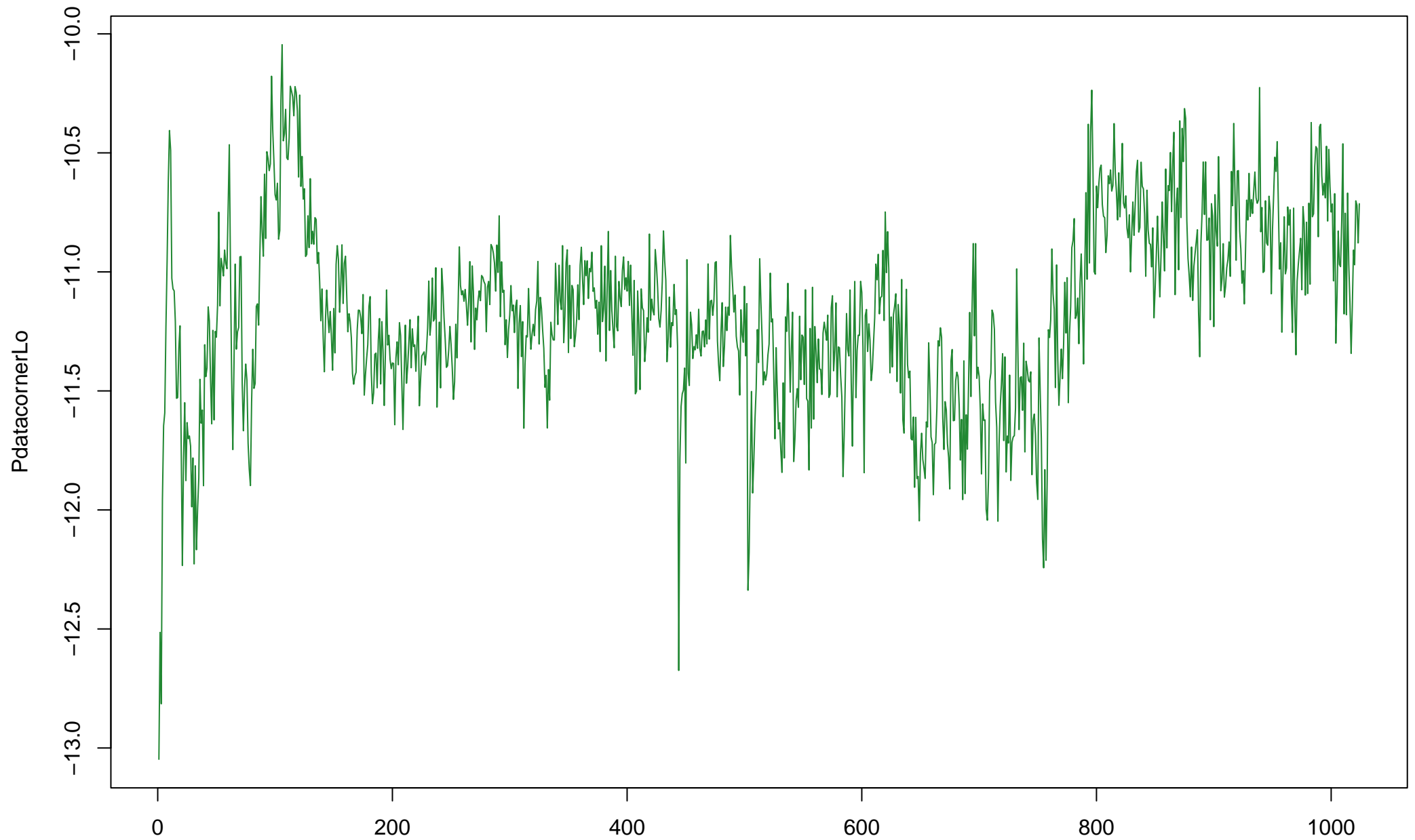
Pdatamean
ESS = 9.72 | BMK = 0.343 | MCSE(6.27) = 15.5 | stat: FALSE | burn: 102



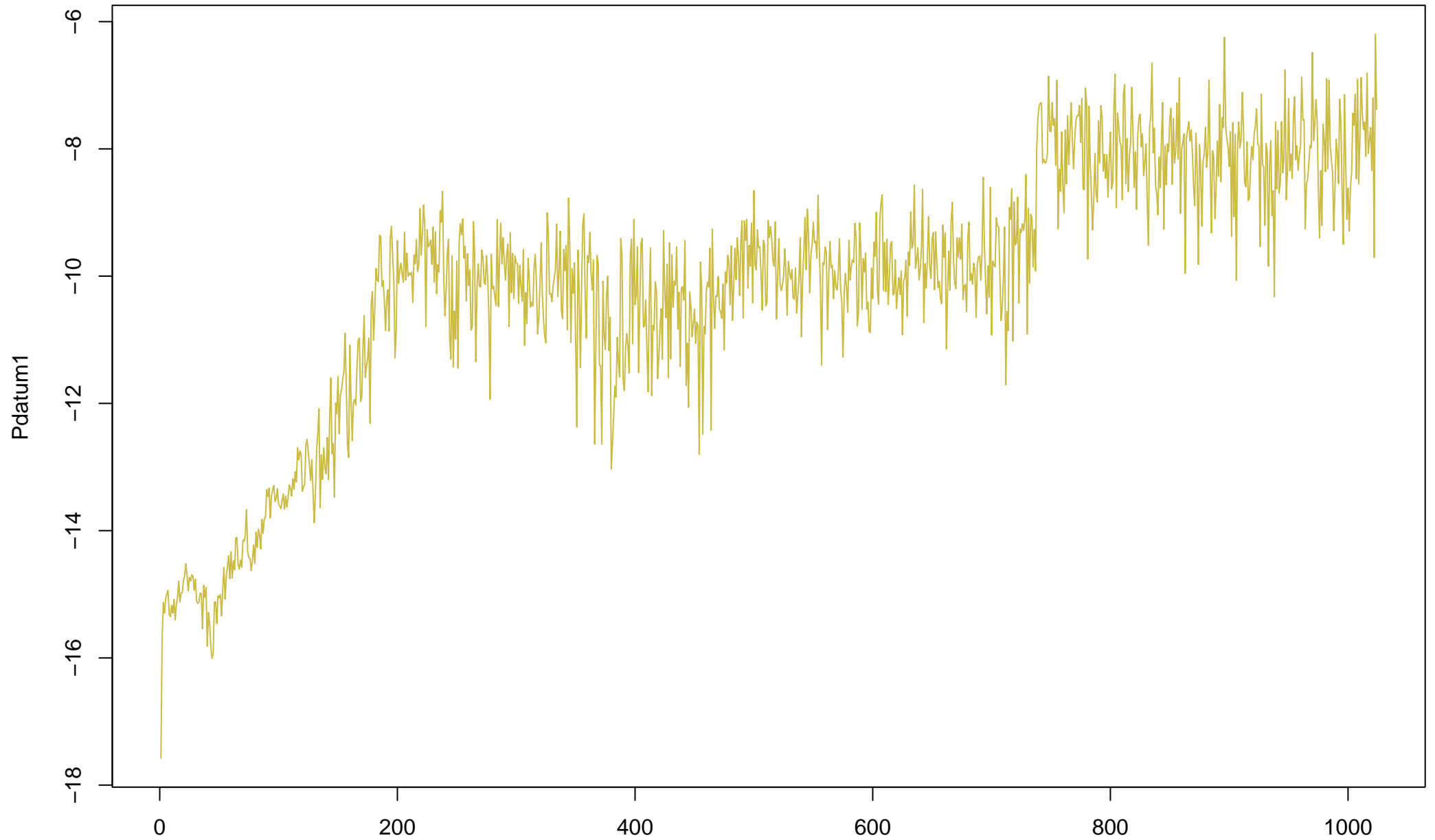
PdatacornerHi
ESS = 29.3 | BMK = 0.289 | MCSE(6.27) = 11.9 | stat: FALSE | burn: 102



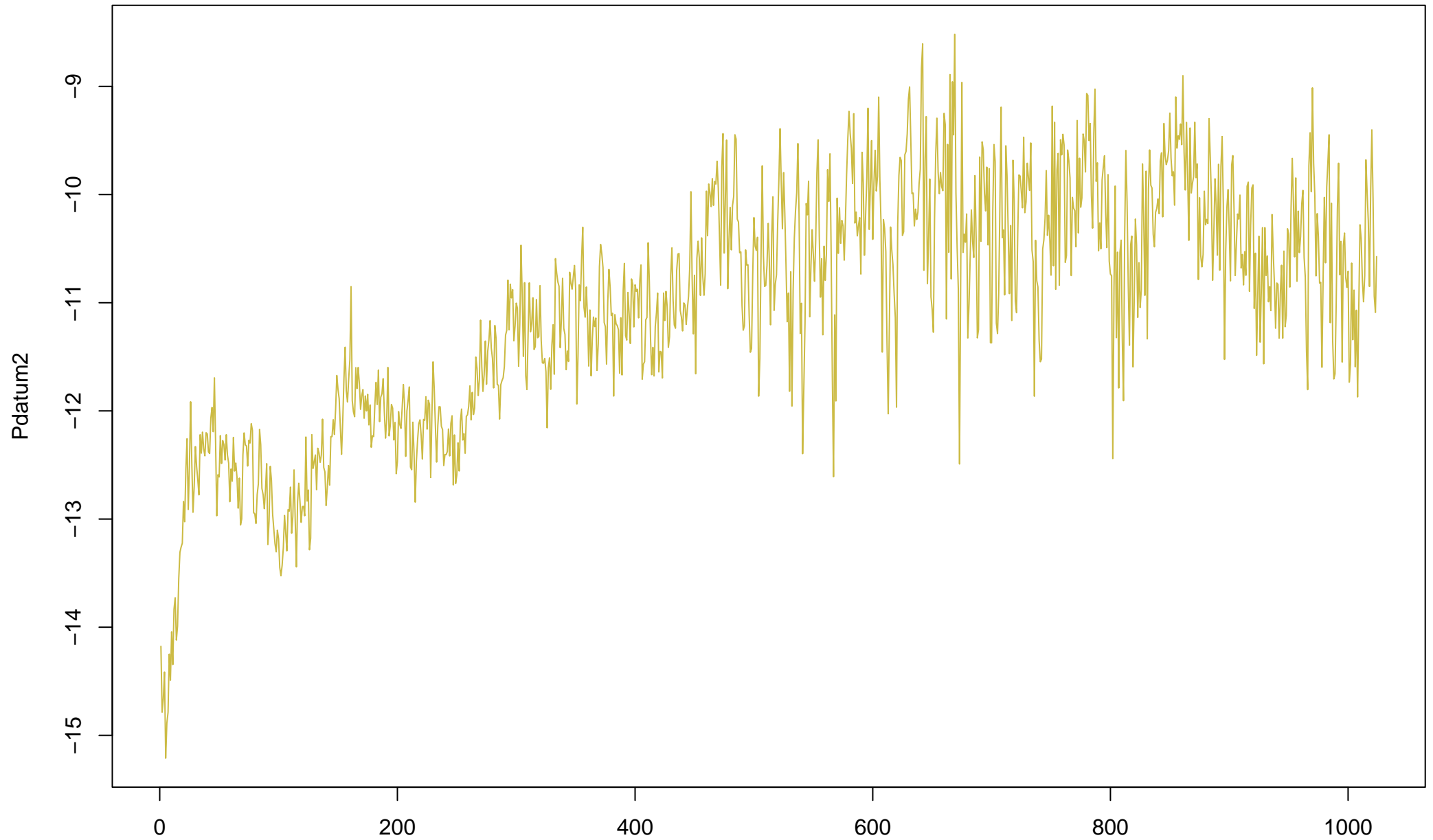
PdatacornerLo
ESS = 19.1 | BMK = 0.251 | MCSE(6.27) = 13.8 | stat: TRUE | burn: 0



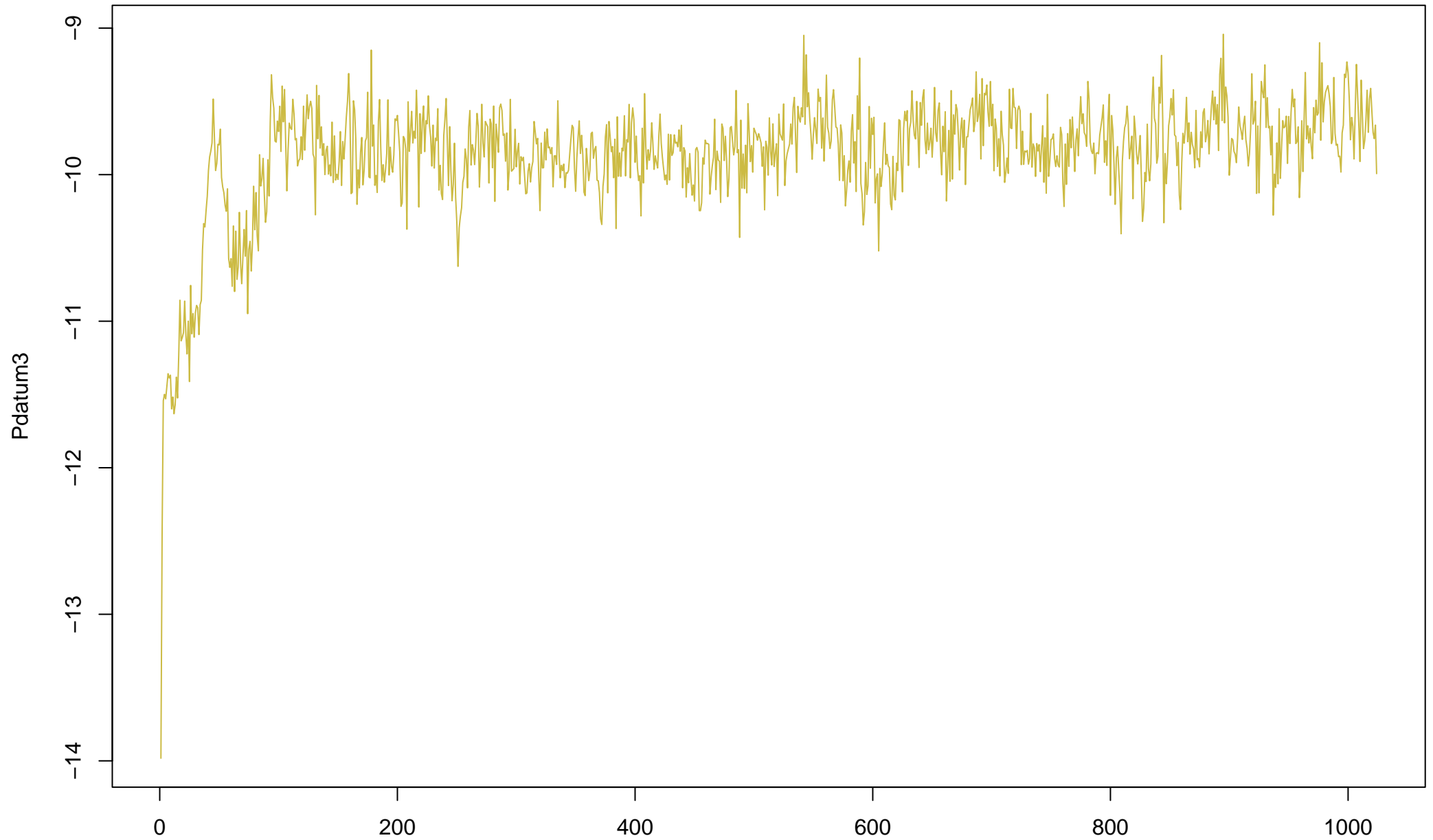
Pdatum1
ESS = 7.27 | BMK = 0.602 | MCSE(6.27) = 13.2 | stat: FALSE | burn: 714



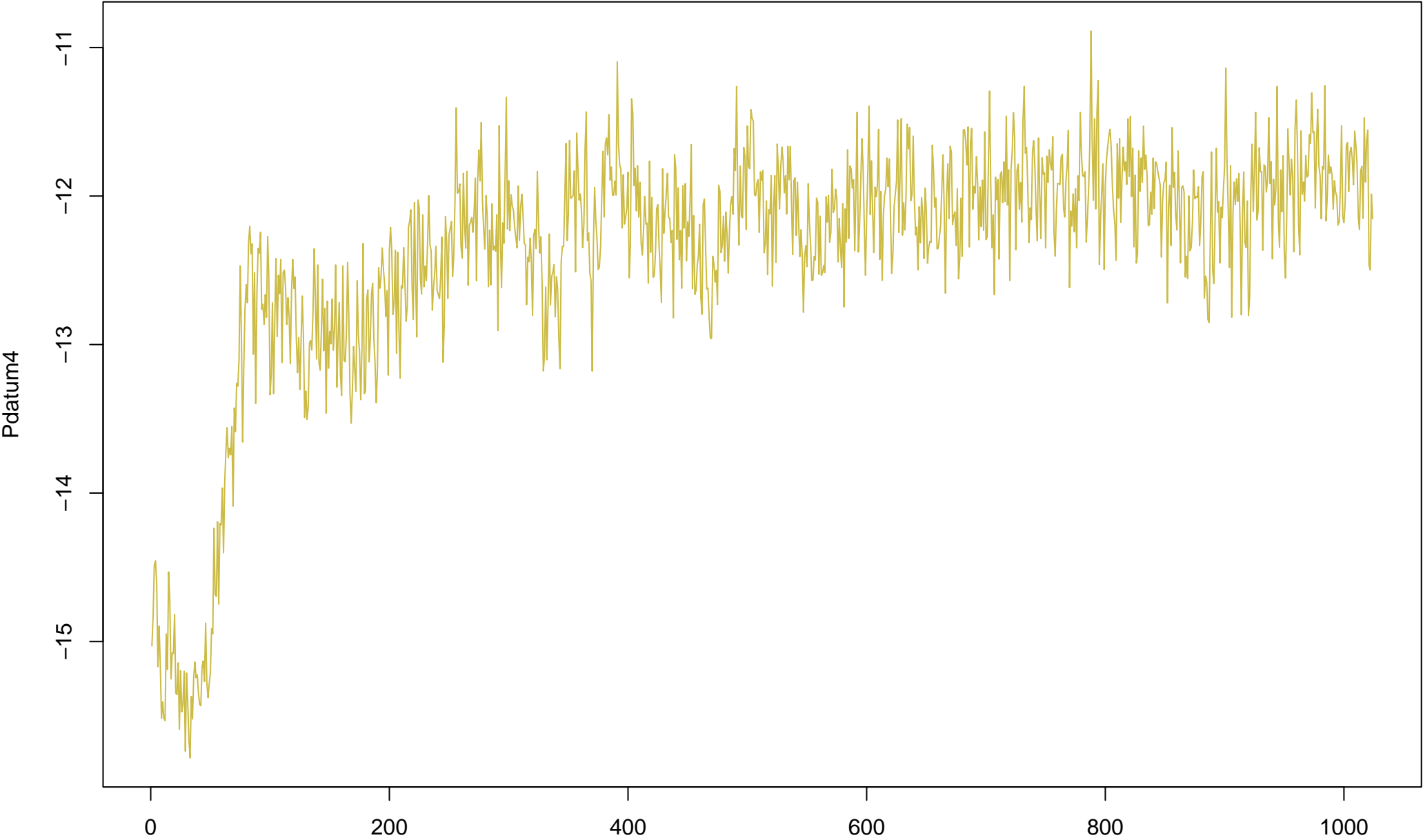
Pdatum2
ESS = 11 | BMK = 0.544 | MCSE(6.27) = 12.9 | stat: FALSE | burn: 0



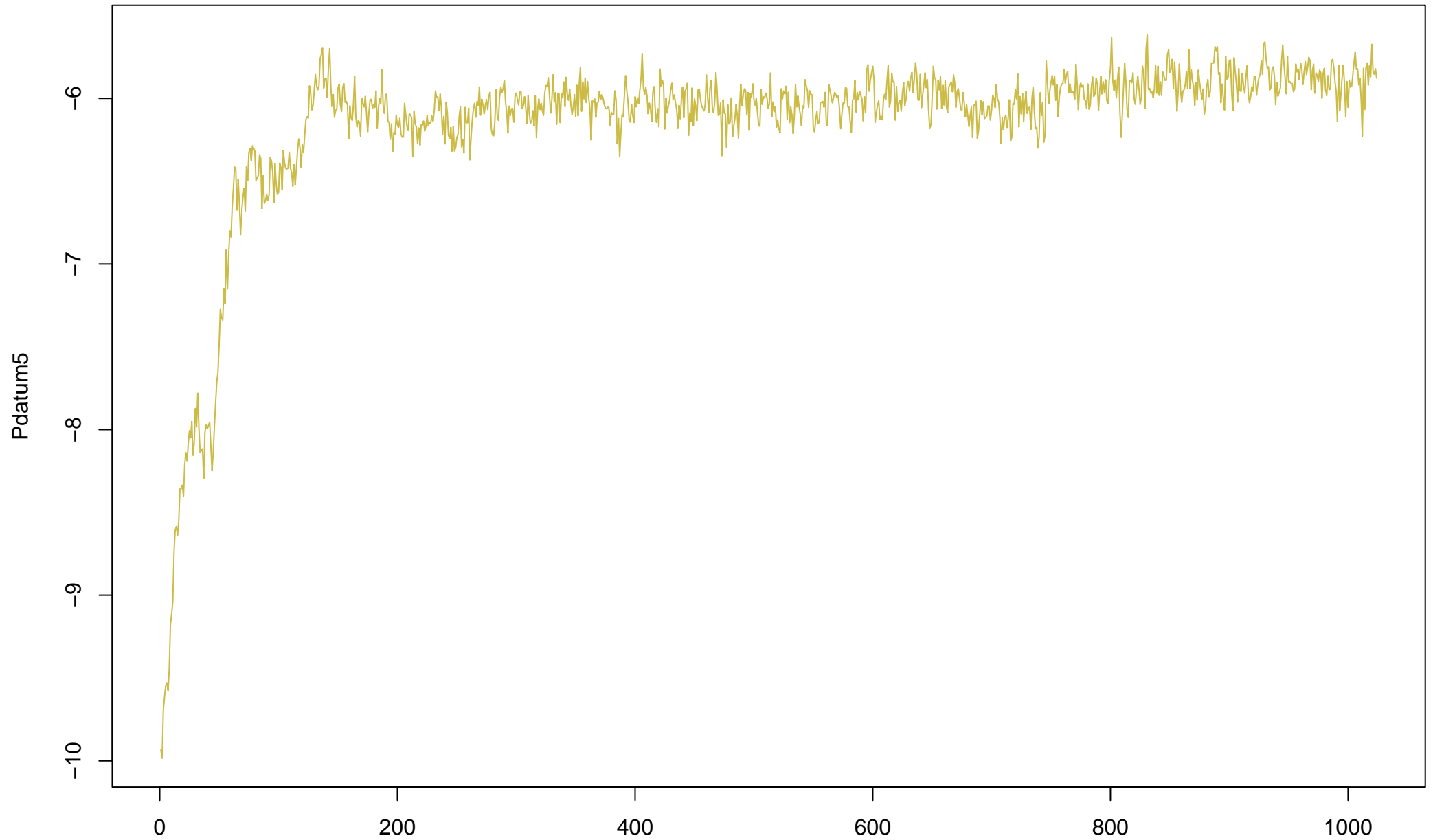
Pdatum3
ESS = 57.1 | BMK = 0.287 | MCSE(6.27) = 11.7 | stat: FALSE | burn: 102



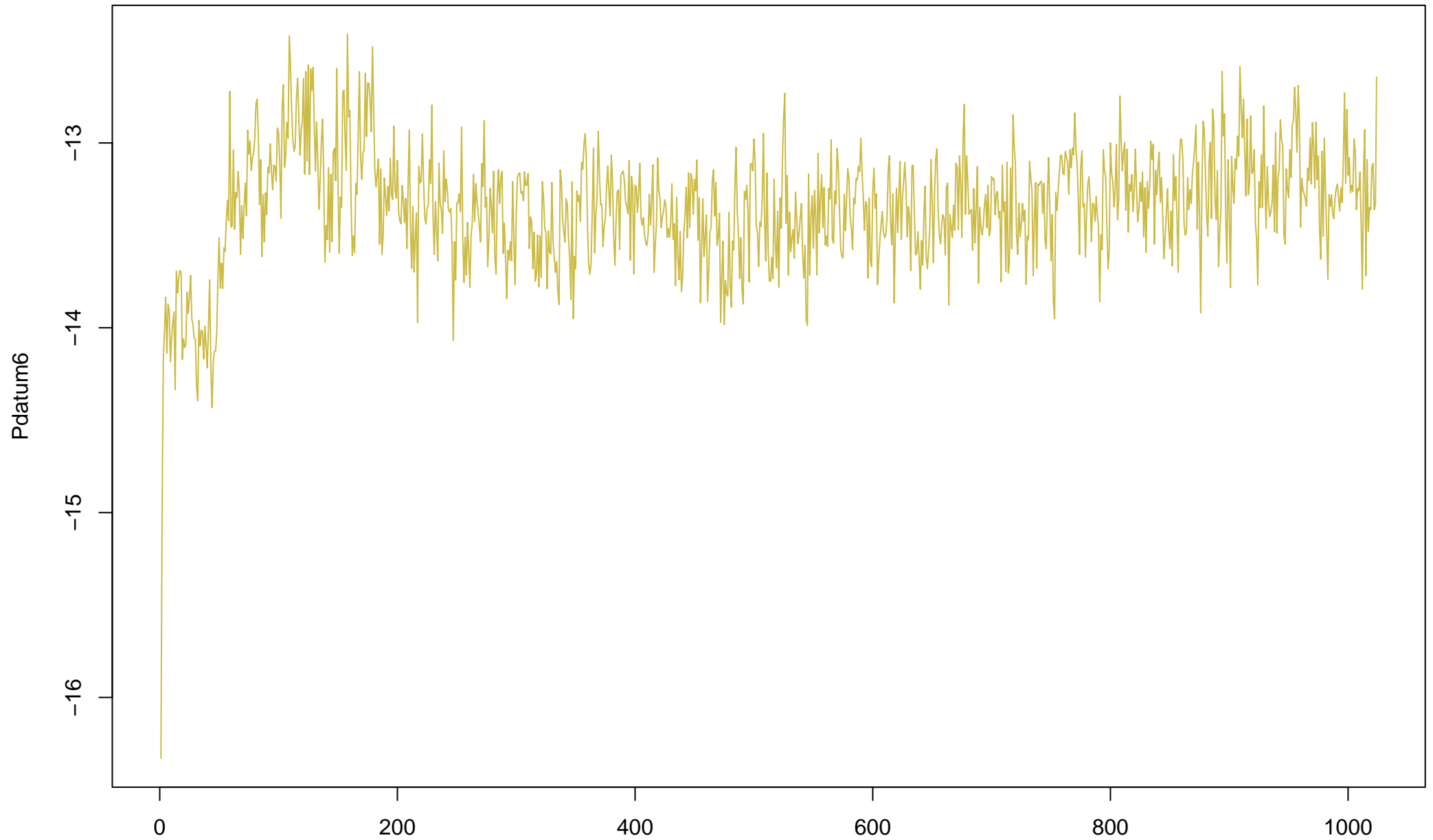
Pdatum4
ESS = 18.1 | BMK = 0.419 | MCSE(6.27) = 13.4 | stat: FALSE | burn: 204



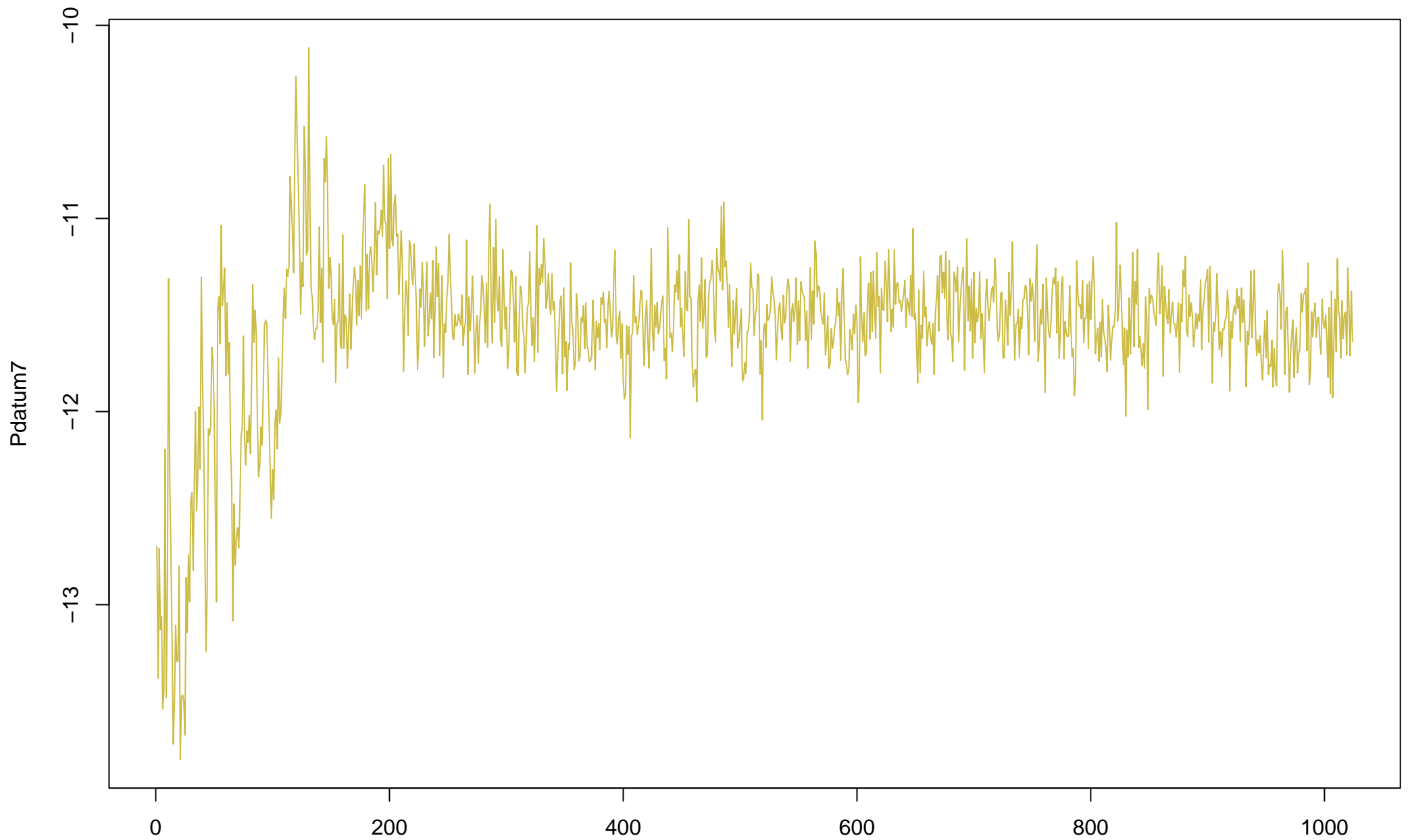
Pdatum5
ESS = 10.2 | BMK = 0.425 | MCSE(6.27) = 16.4 | stat: FALSE | burn: 102



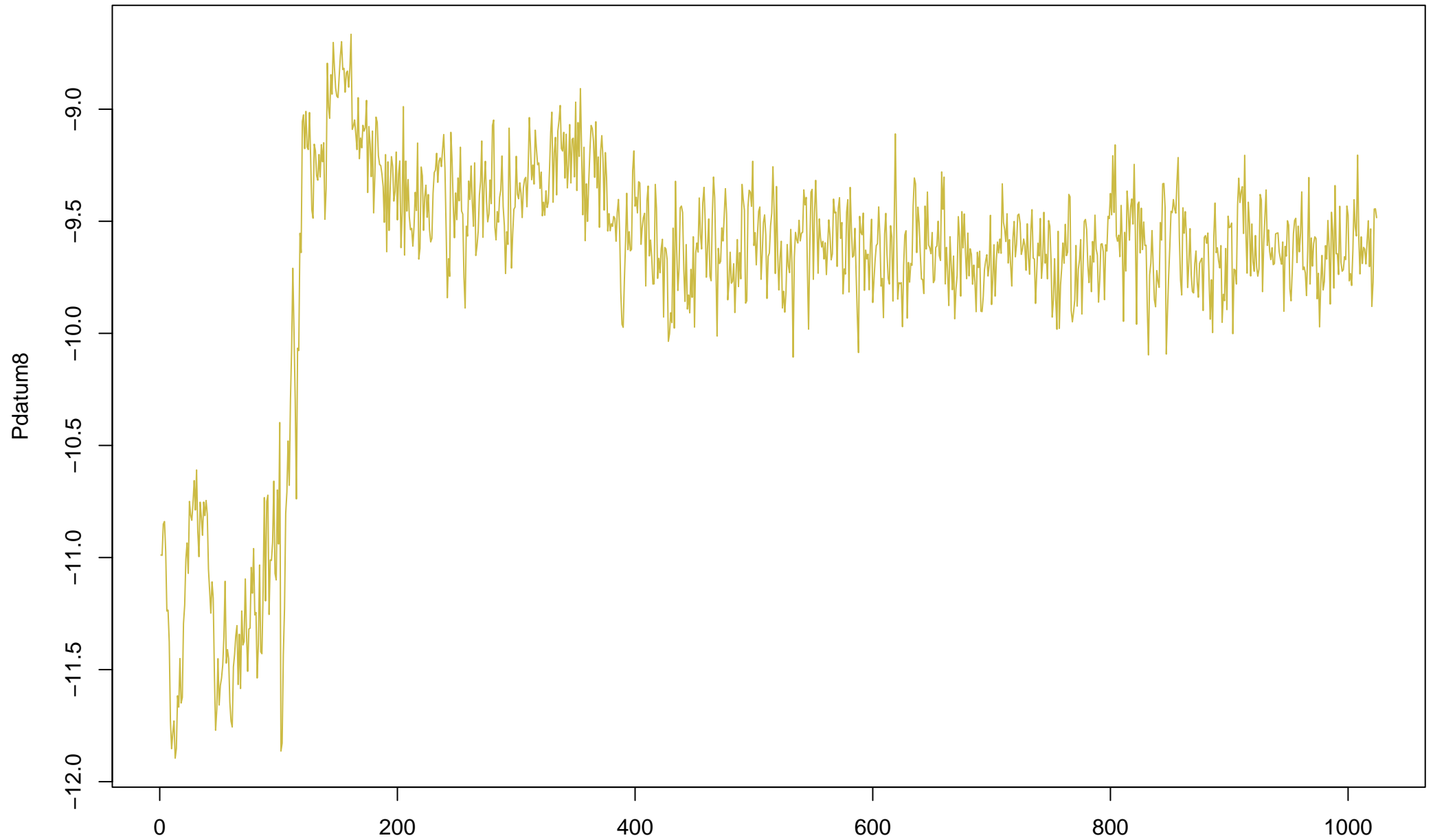
Pdatum6
ESS = 68 | BMK = 0.182 | MCSE(6.27) = 10.8 | stat: FALSE | burn: 0



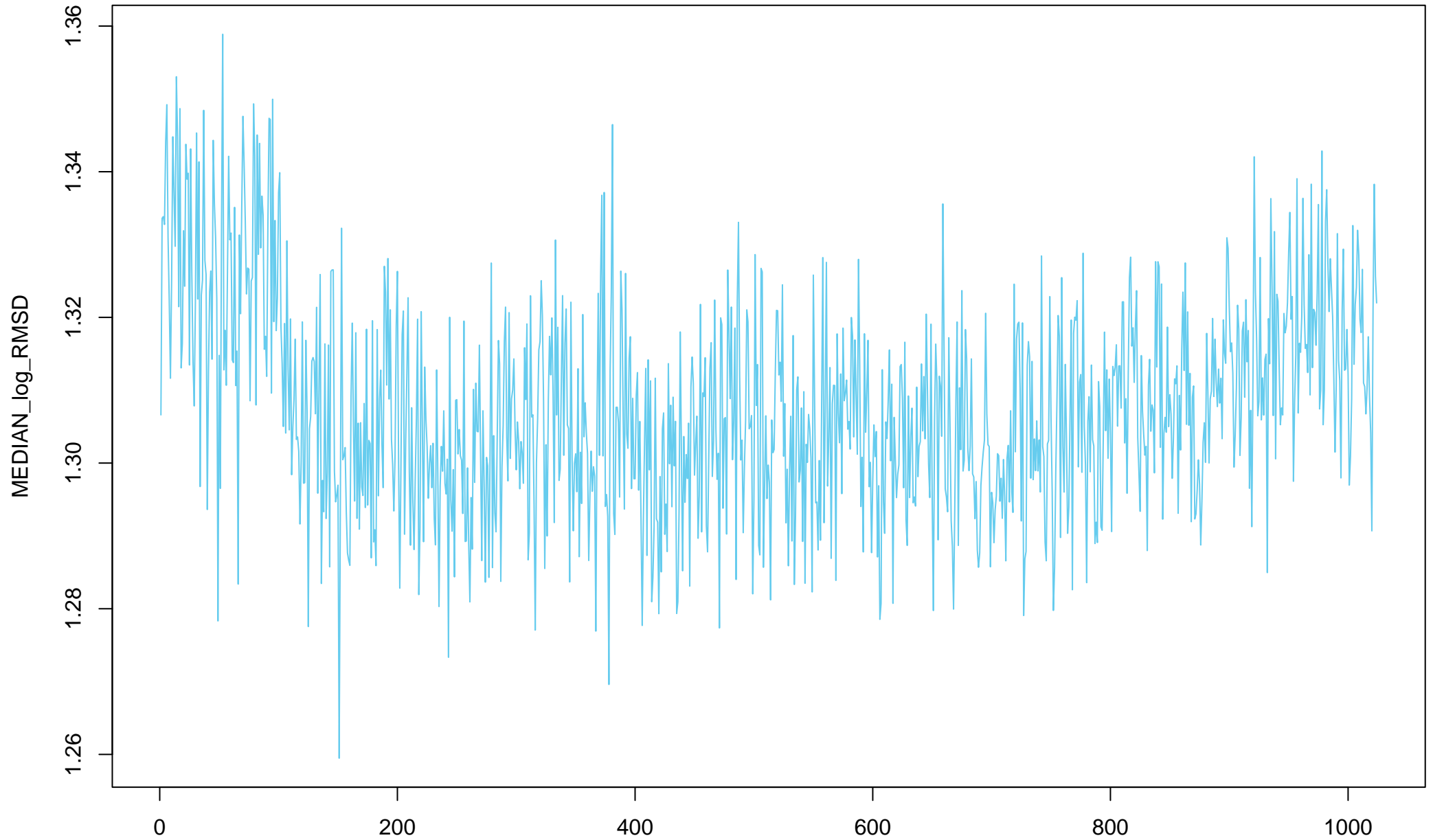
Pdatum7
ESS = 37.4 | BMK = 0.324 | MCSE(6.27) = 10.8 | stat: FALSE | burn: 102



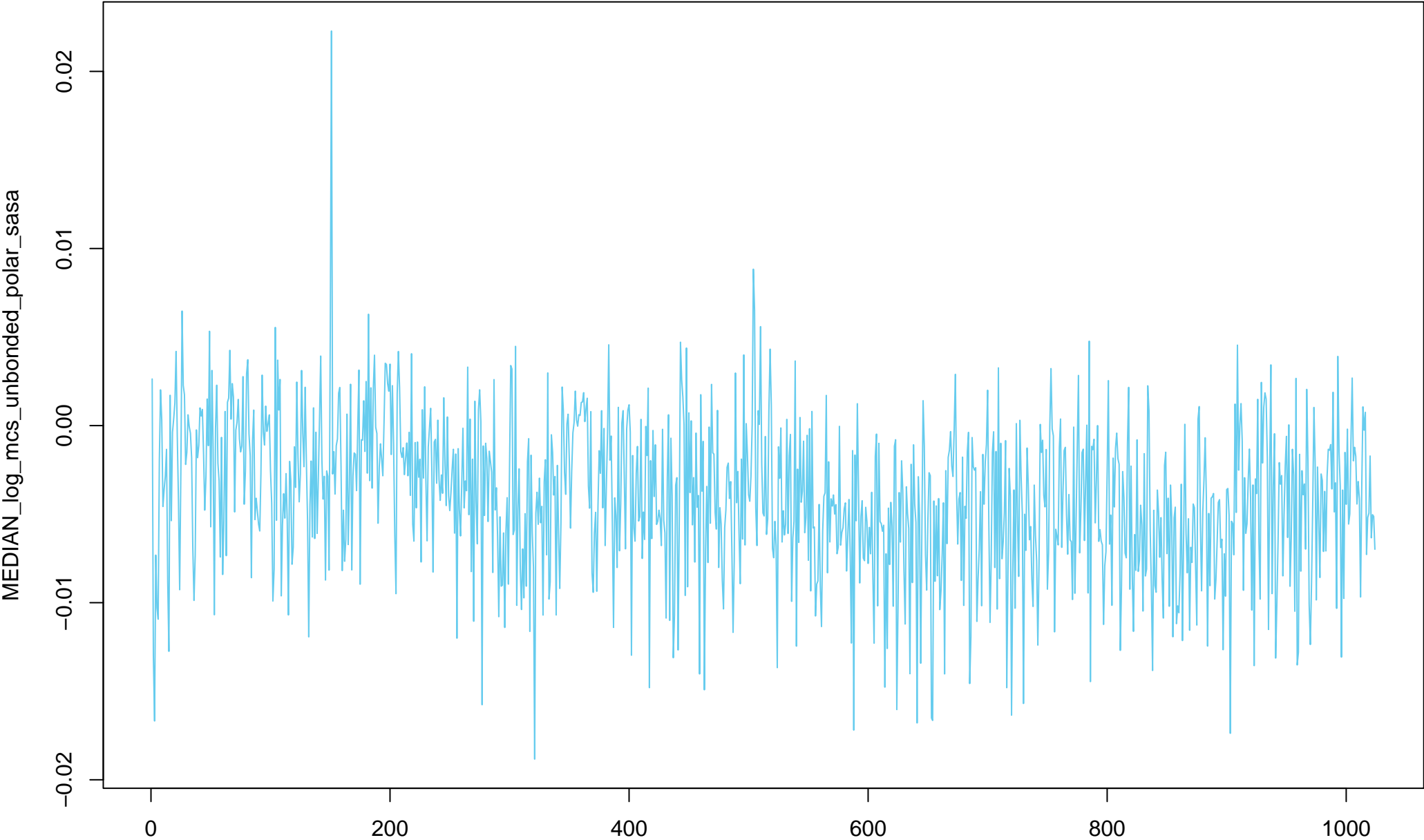
Pdatum8
ESS = 9.33 | BMK = 0.5 | MCSE(6.27) = 15.3 | stat: FALSE | burn: 408



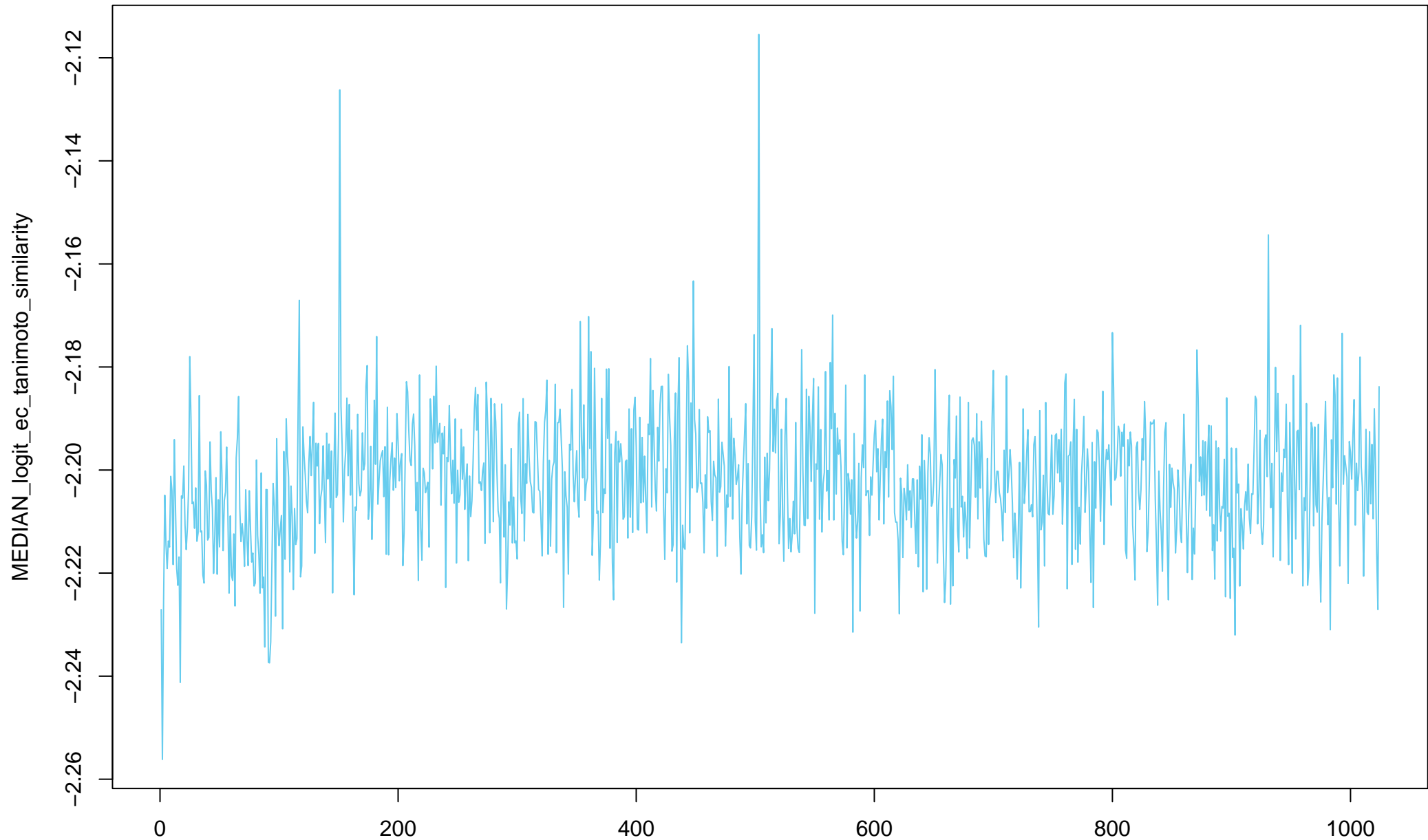
MEDIAN_log_RMSD
ESS = 28.3 | BMK = 0.154 | MCSE(6.27) = 10.1 | stat: FALSE | burn: 102



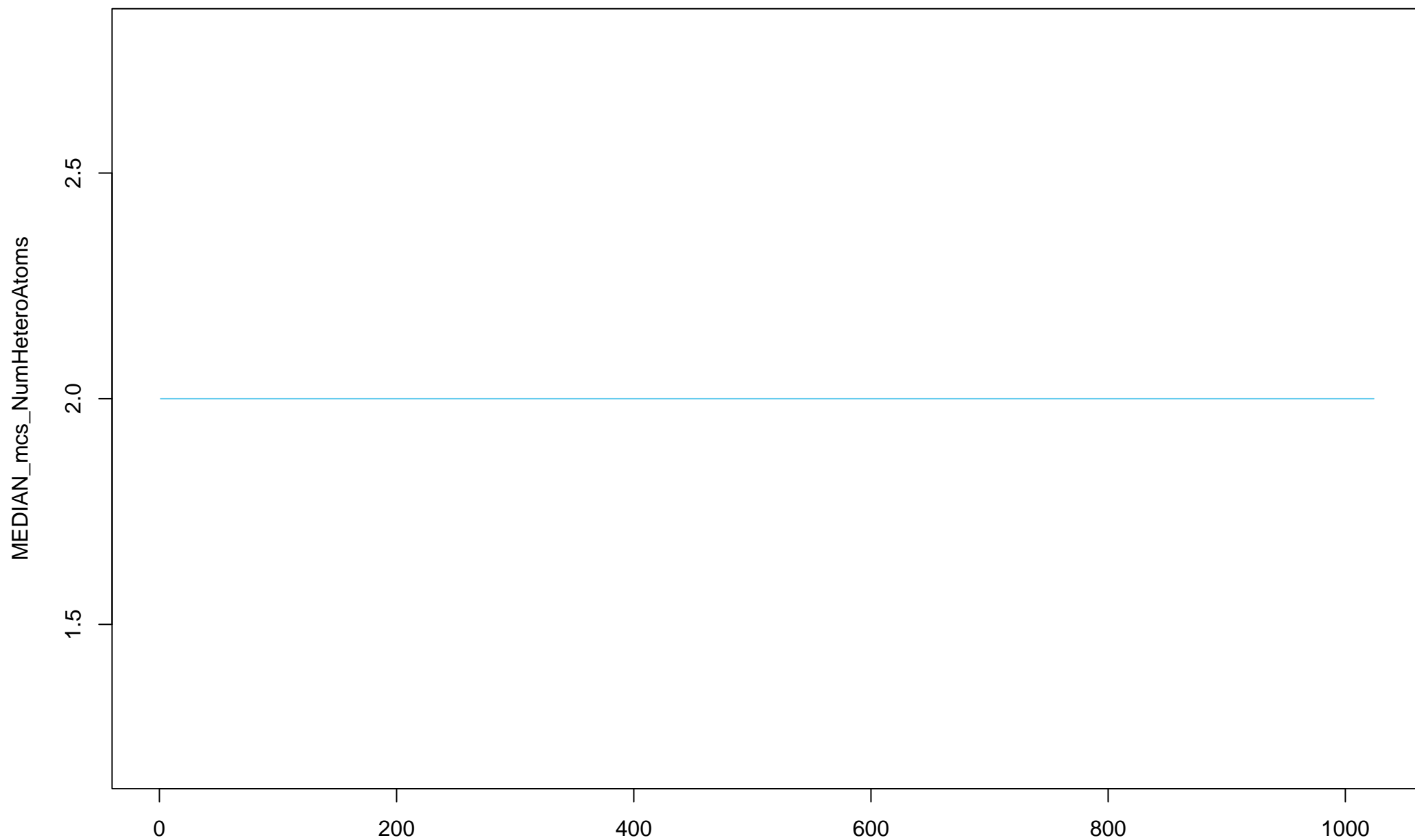
MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 232 | BMK = 0.188 | MCSE(6.27) = 6.42 | stat: FALSE | burn: 0



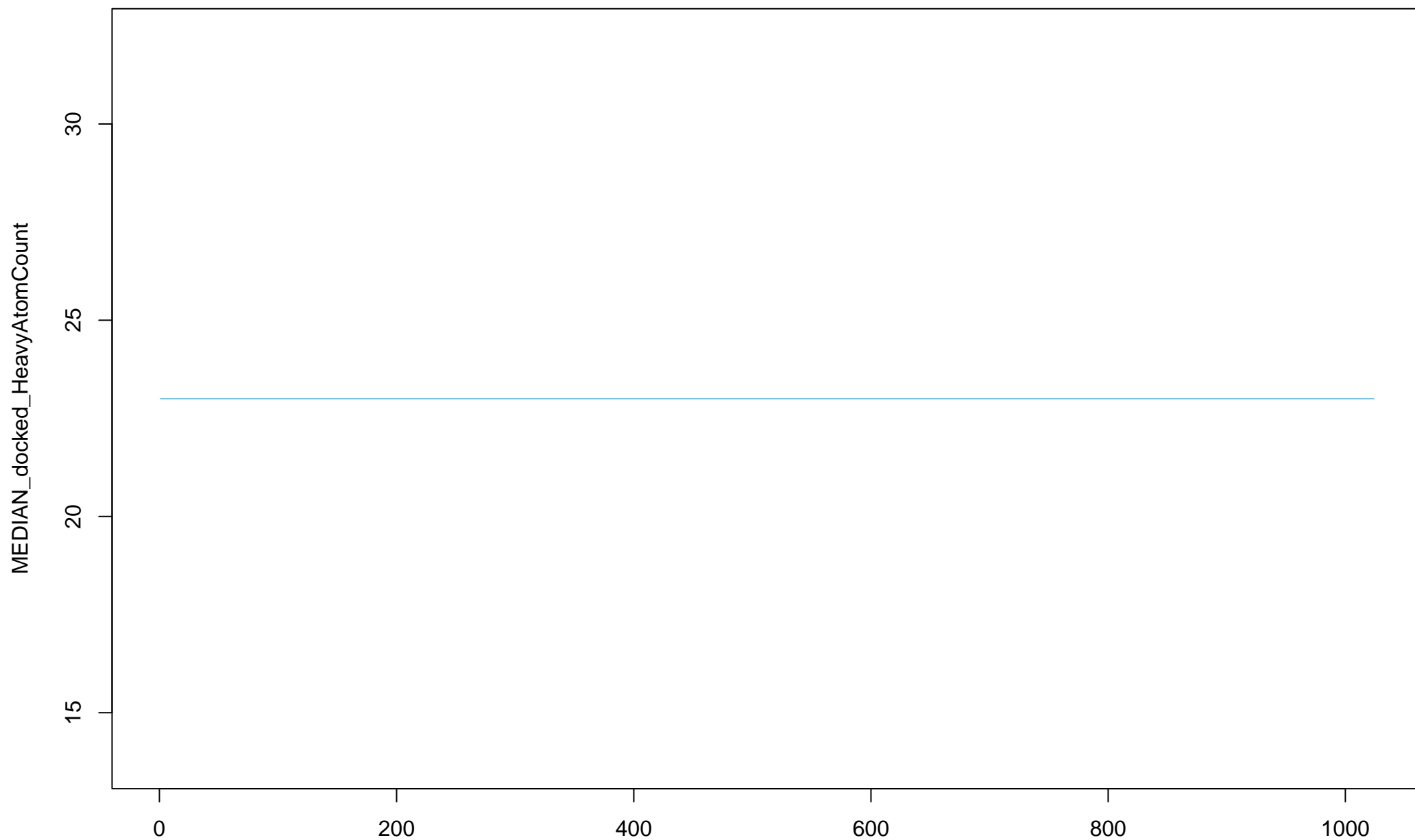
MEDIAN_logit_ec_tanimoto_similarity
ESS = 284 | BMK = 0.0784 | MCSE(6.27) = 5.62 | stat: FALSE | burn: 0



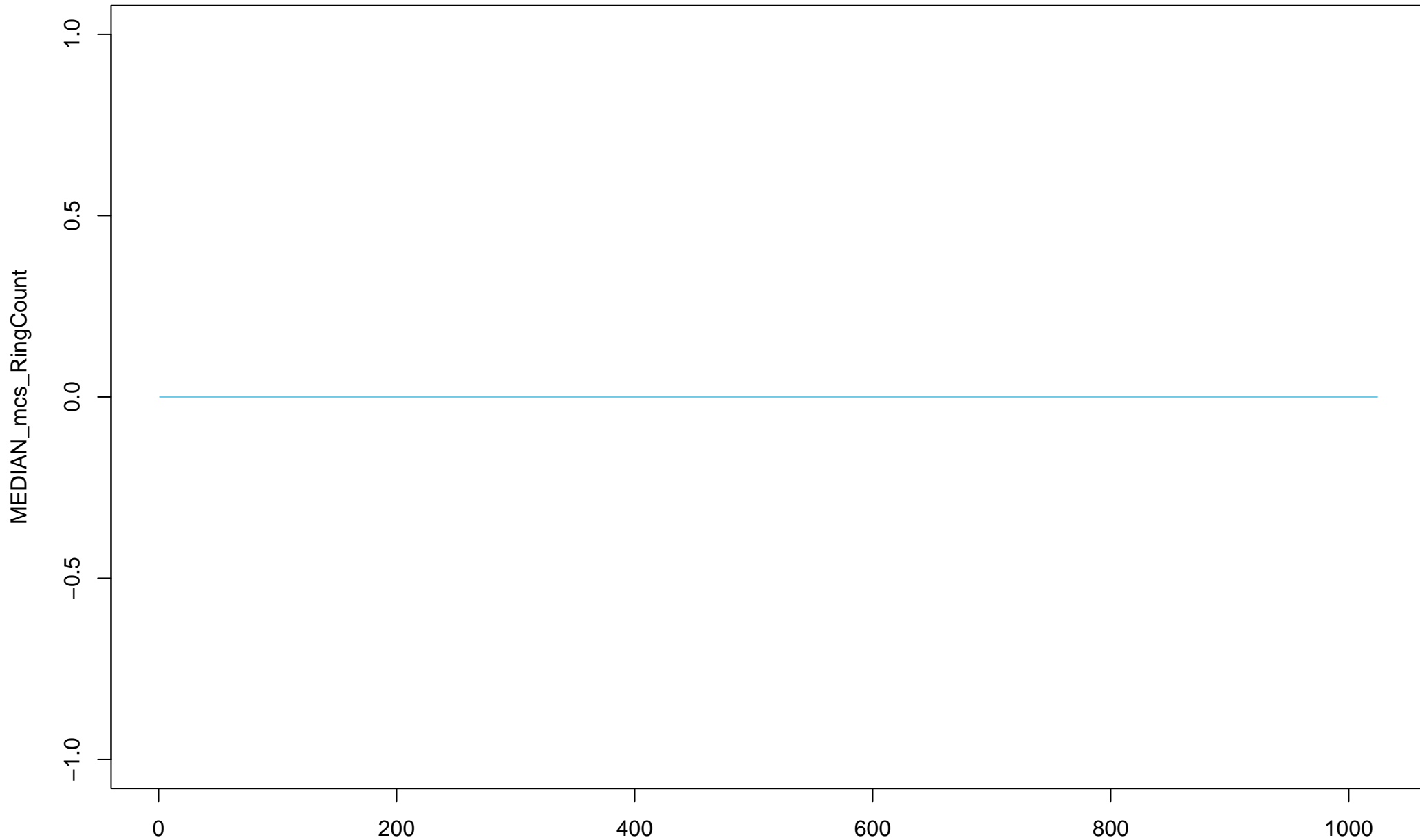
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



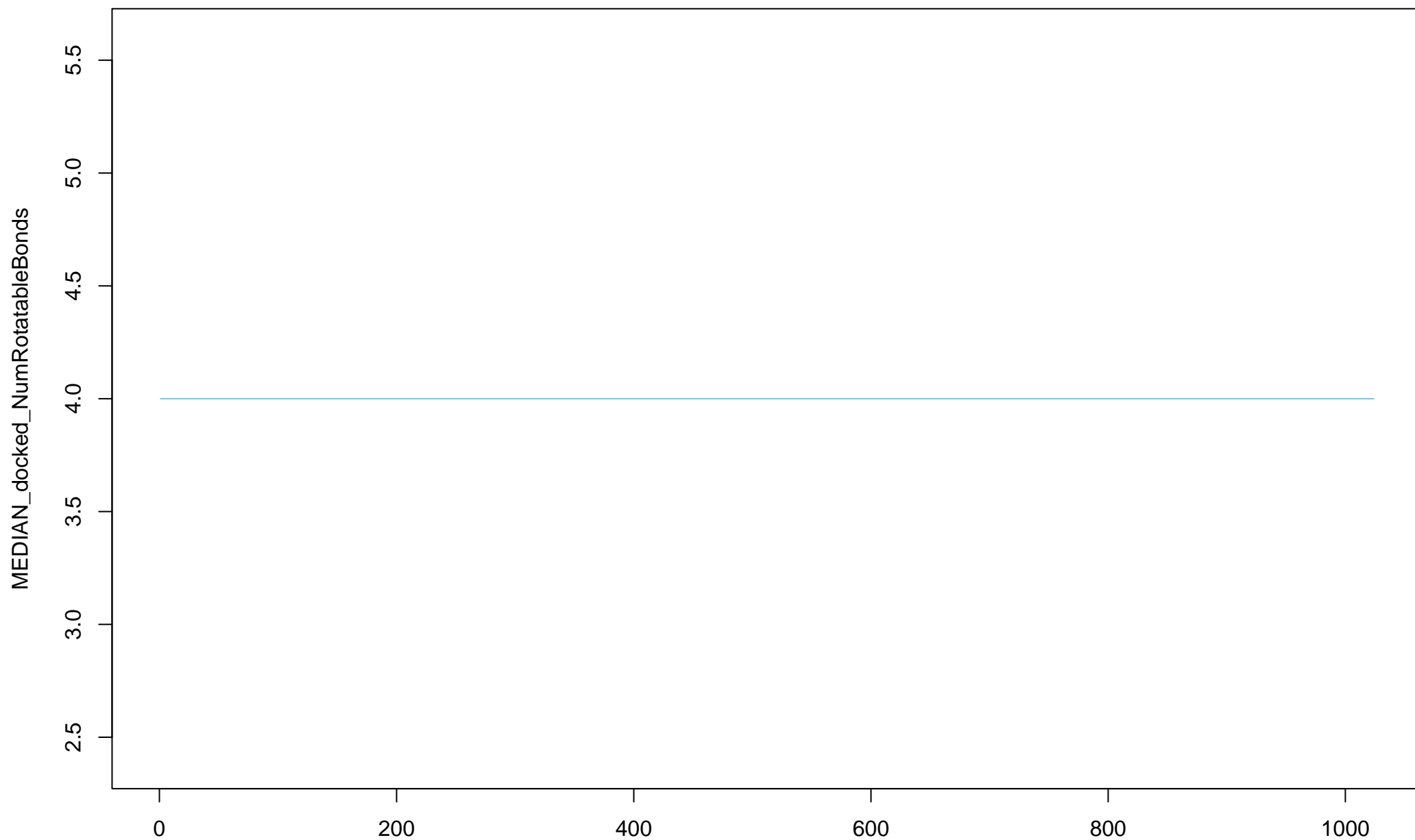
MEDIAN_docked_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



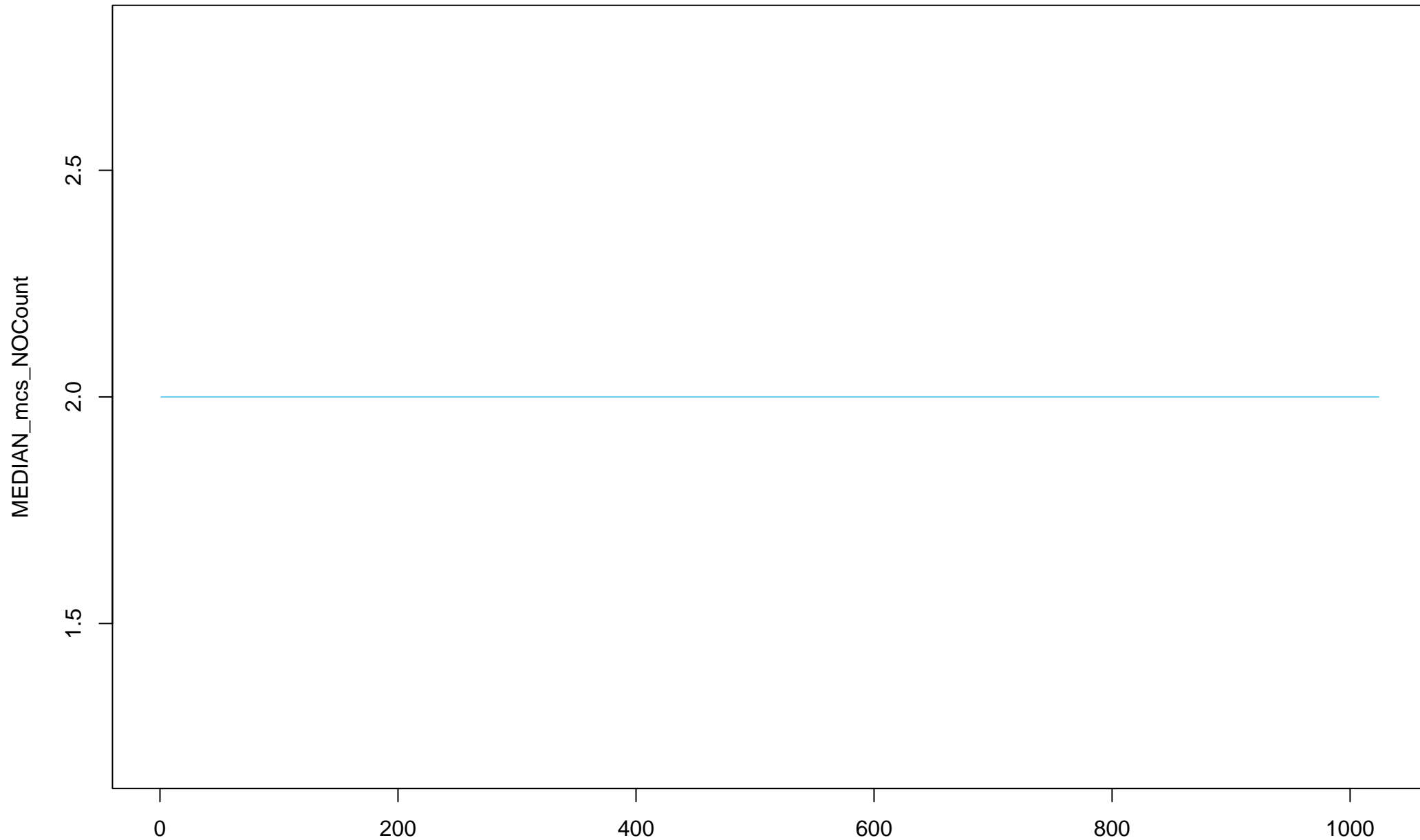
MEDIAN_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



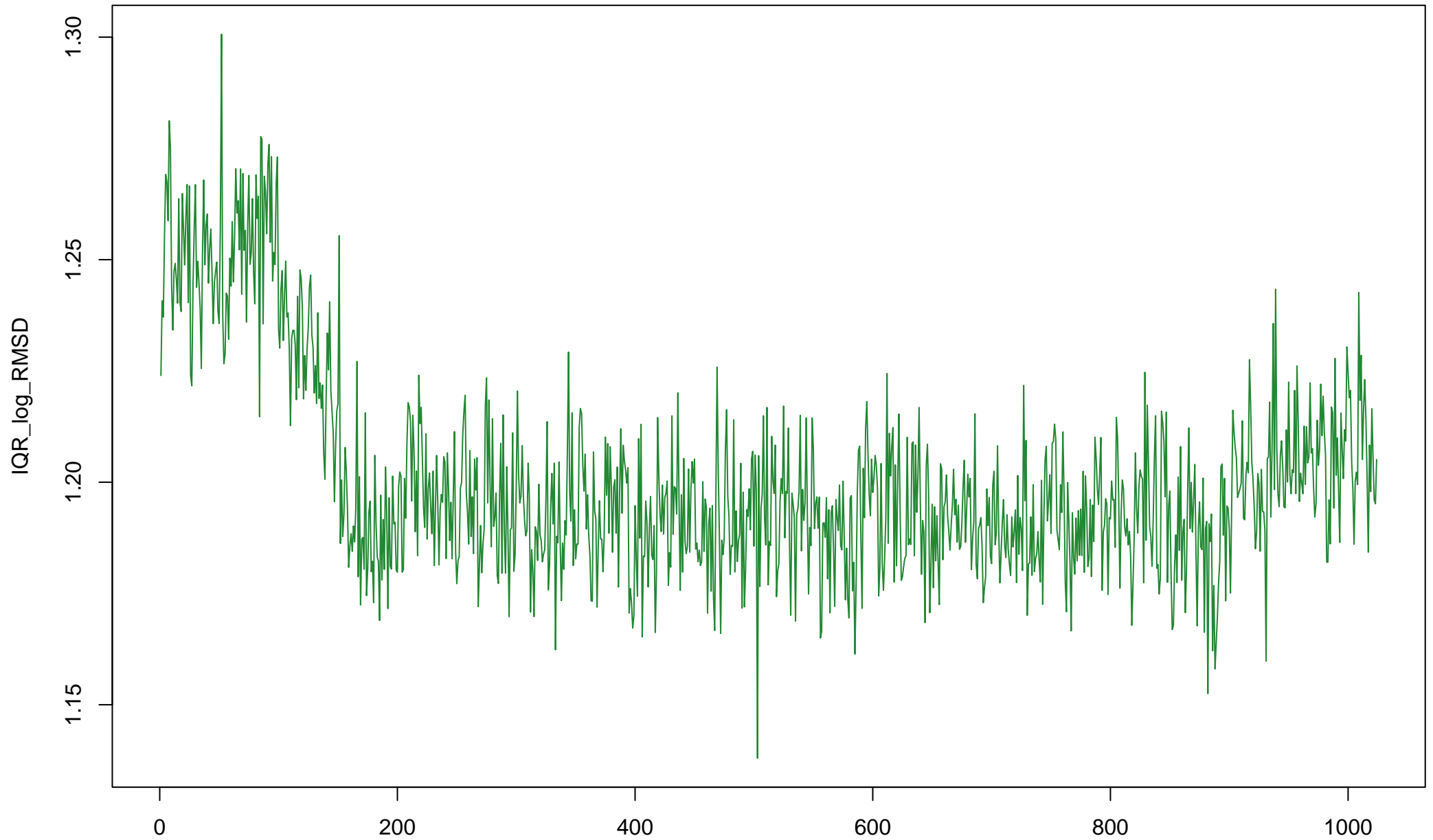
MEDIAN_docked_NumRotatableBonds
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



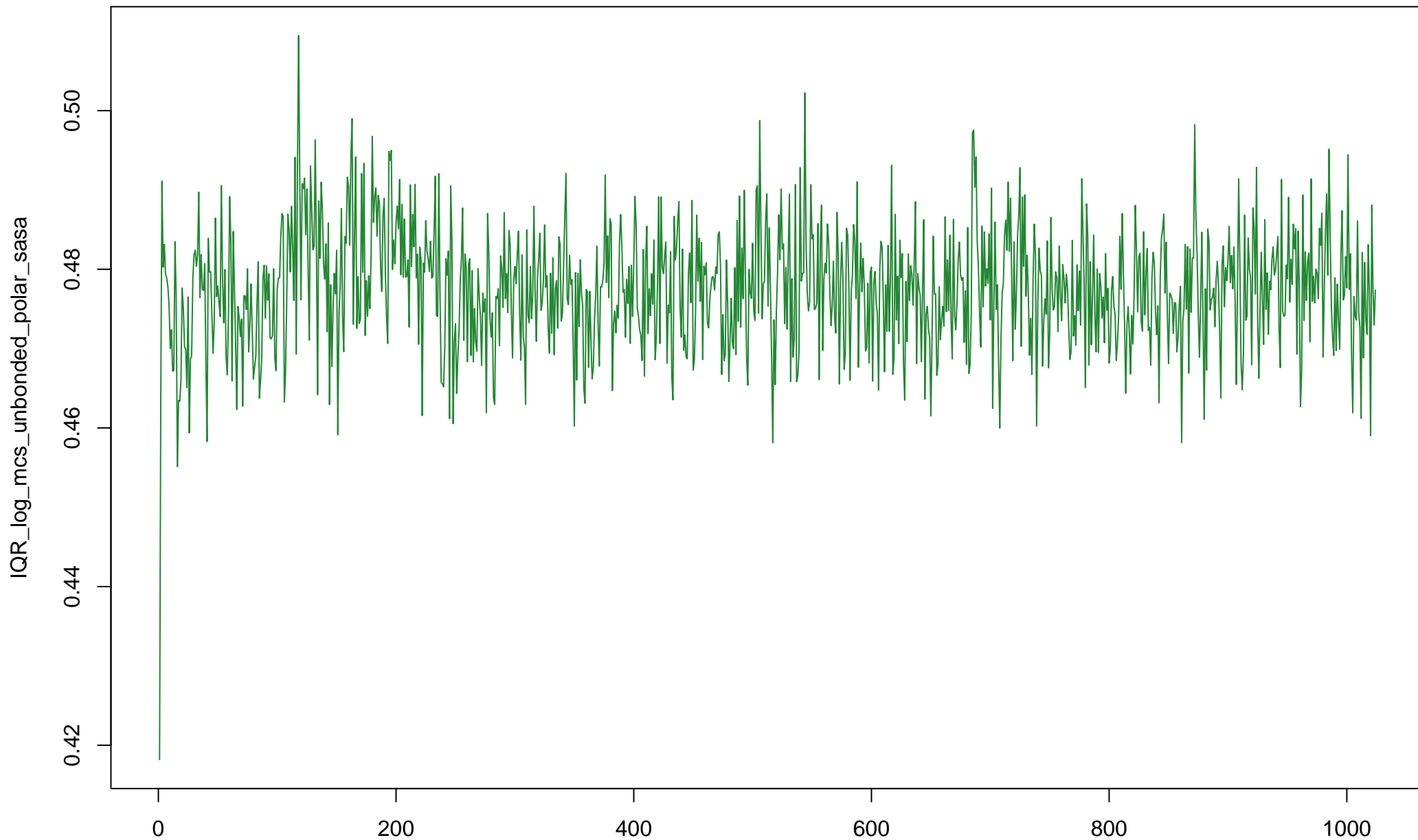
MEDIAN_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



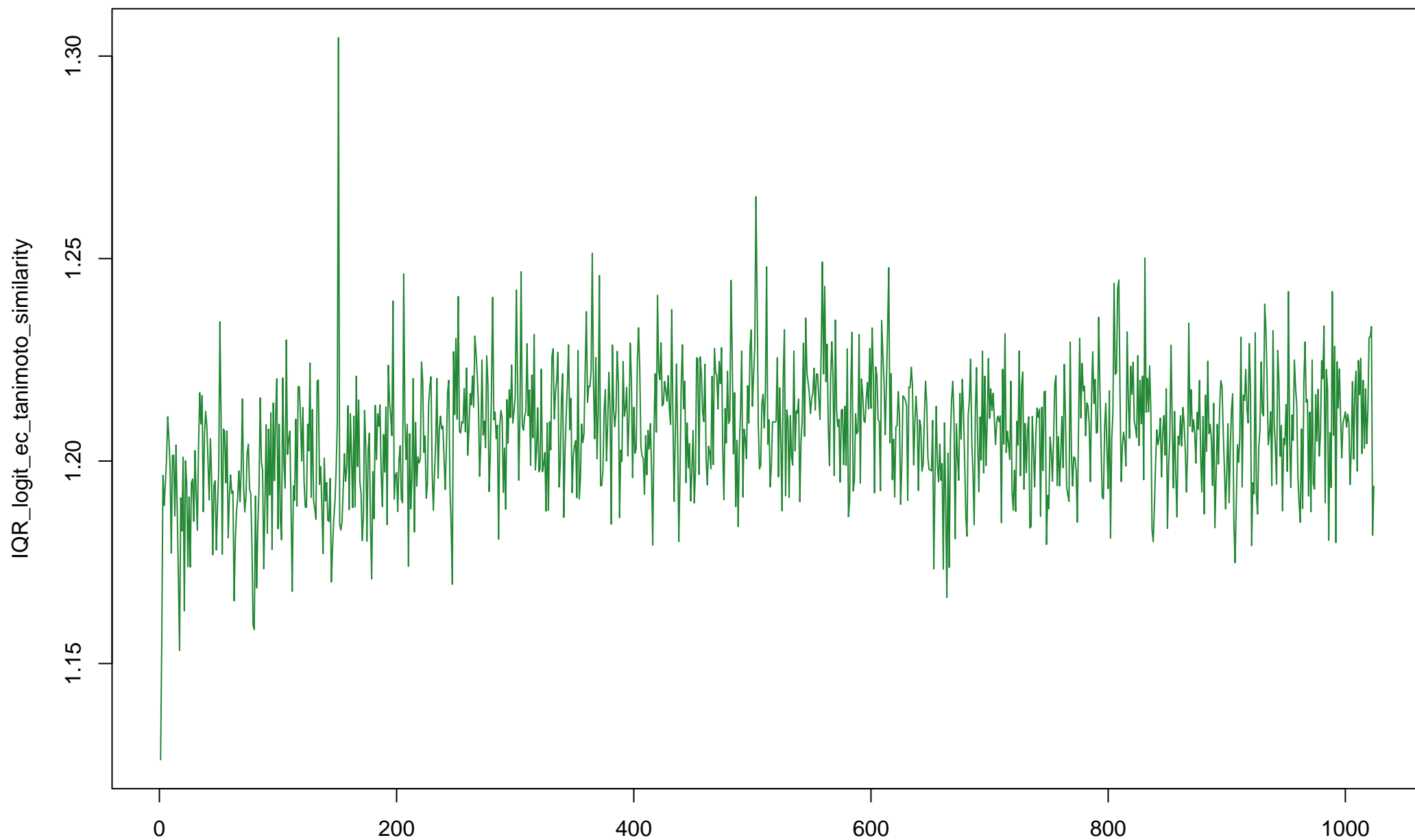
IQR_log_RMSD
ESS = 9.72 | BMK = 0.318 | MCSE(6.27) = 14.9 | stat: FALSE | burn: 102



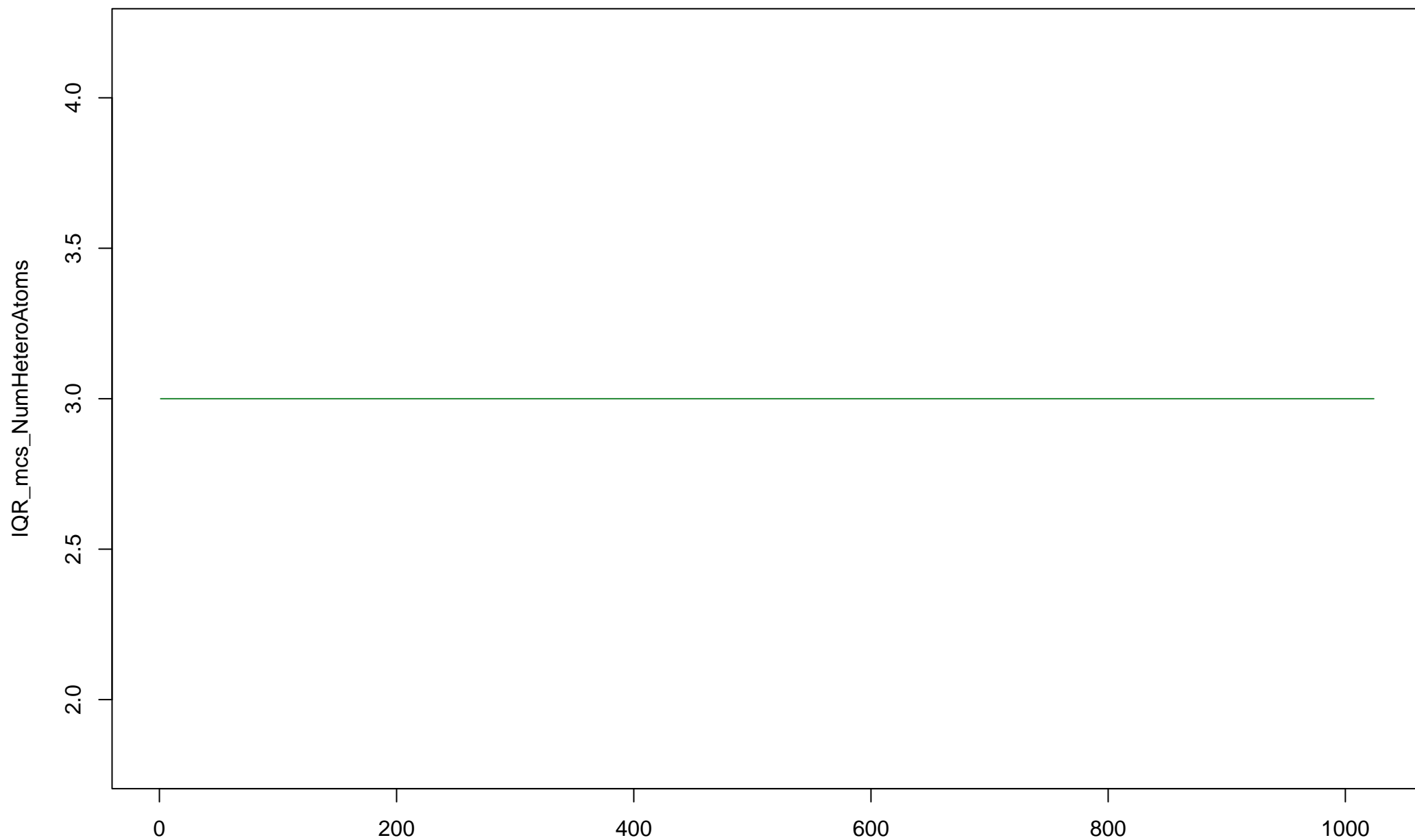
IQR_log_mcs_unbonded_polar_sasa
ESS = 446 | BMK = 0.0718 | MCSE(6.27) = 5.73 | stat: FALSE | burn: 0



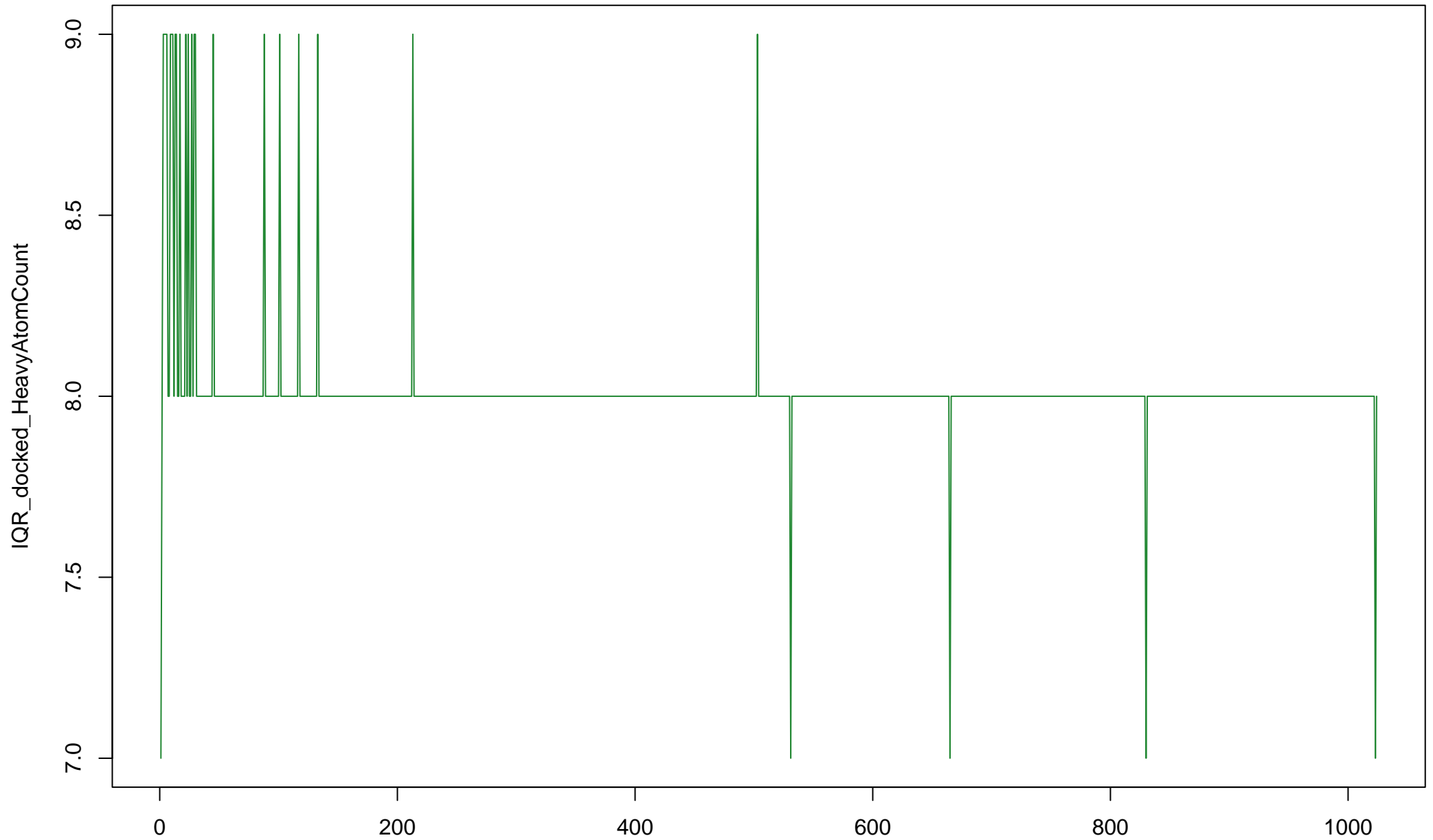
IQR_logit_ec_tanimoto_similarity
ESS = 95 | BMK = 0.125 | MCSE(6.27) = 7.95 | stat: FALSE | burn: 0



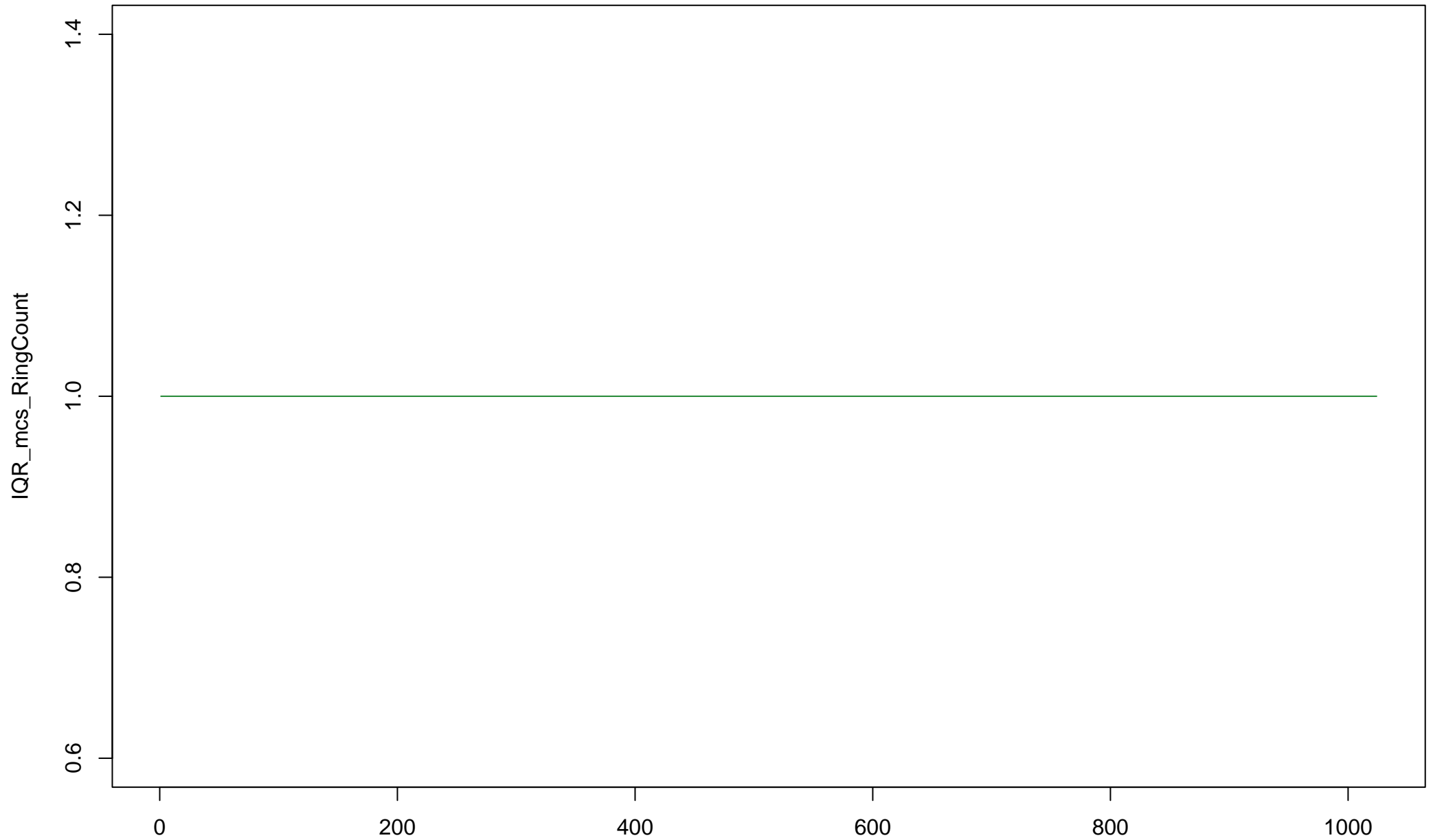
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



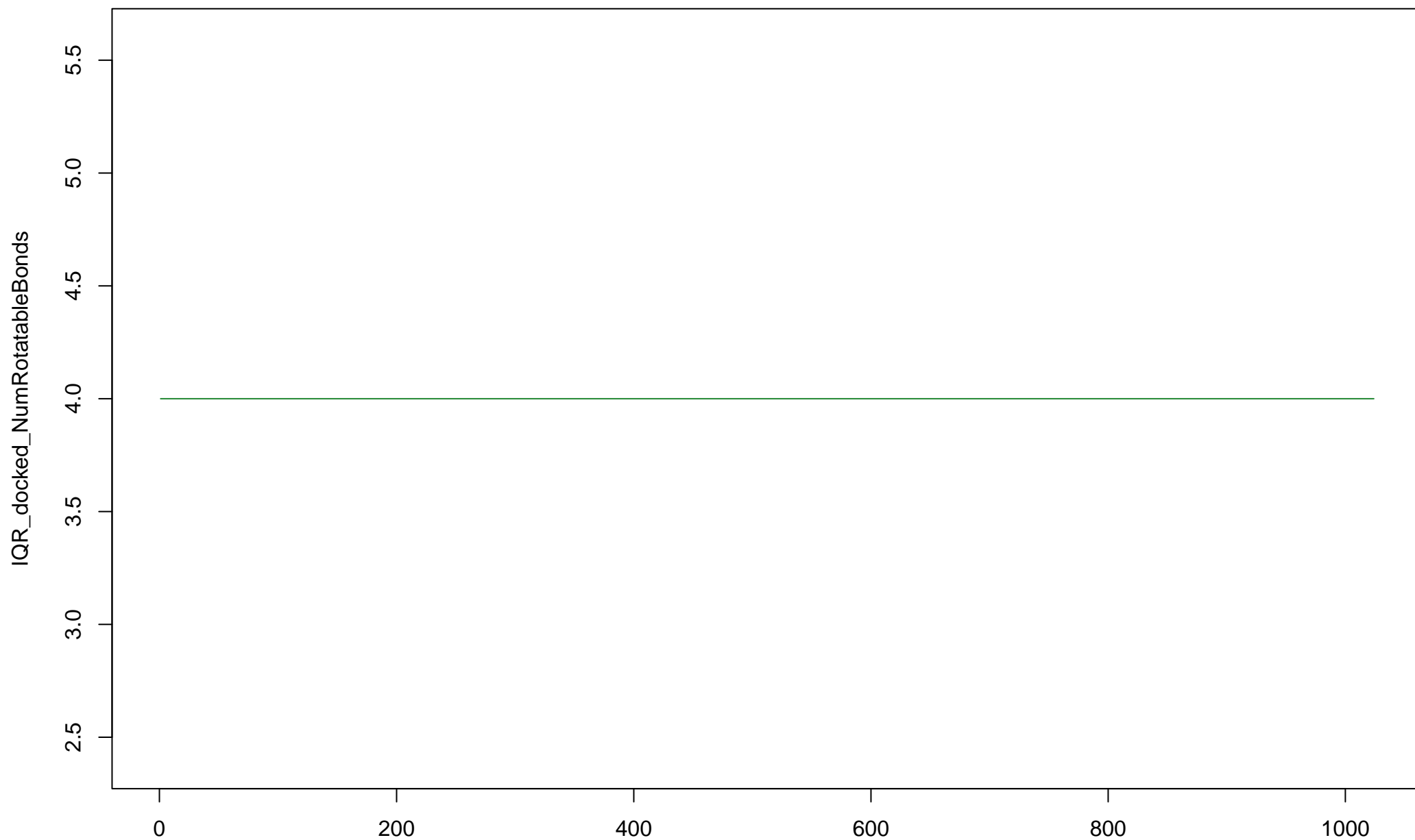
IQR_docked_HeavyAtomCount
ESS = 74.7 | BMK = 0.399 | MCSE(6.27) = 8.68 | stat: FALSE | burn: 1020



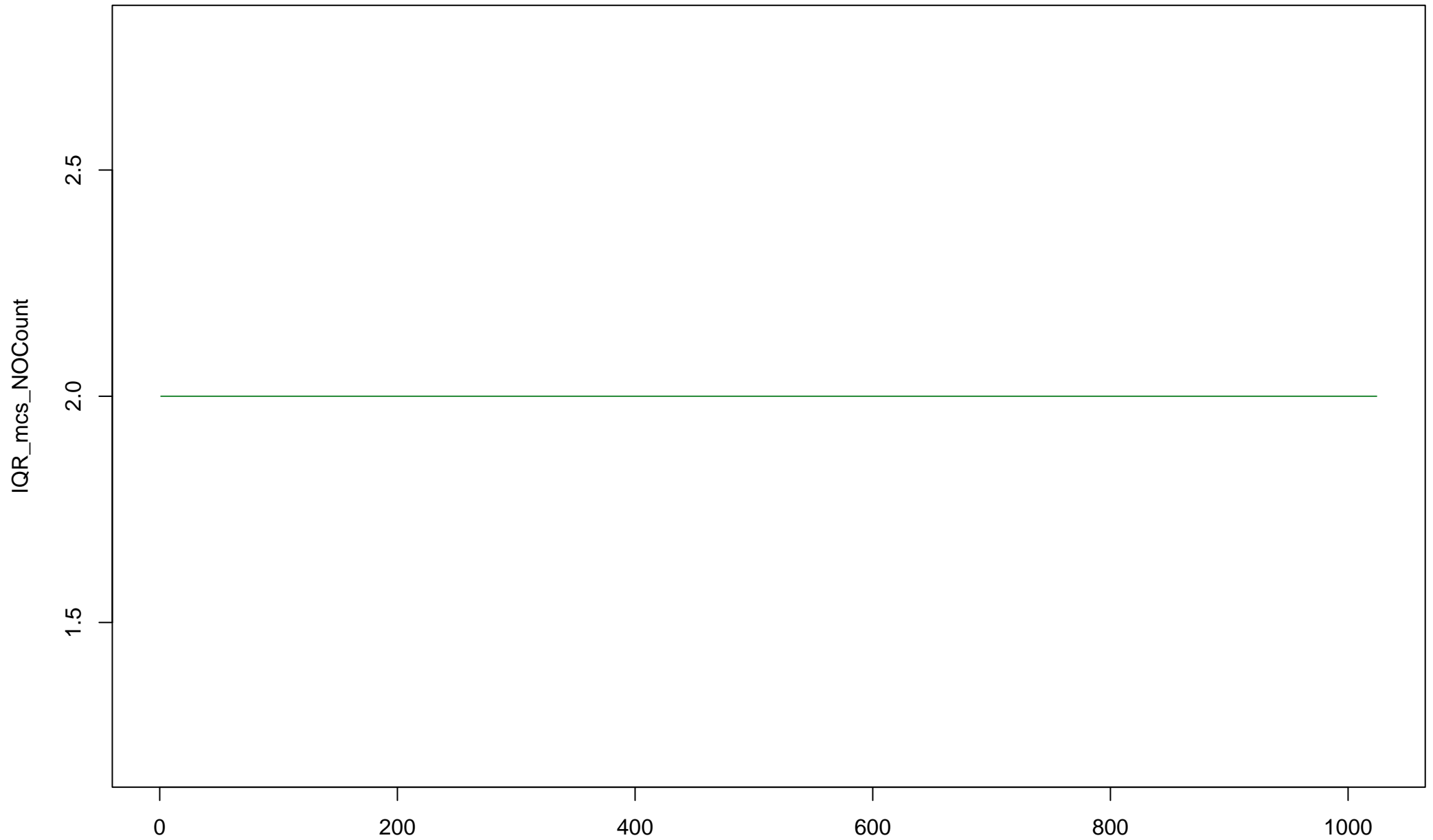
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



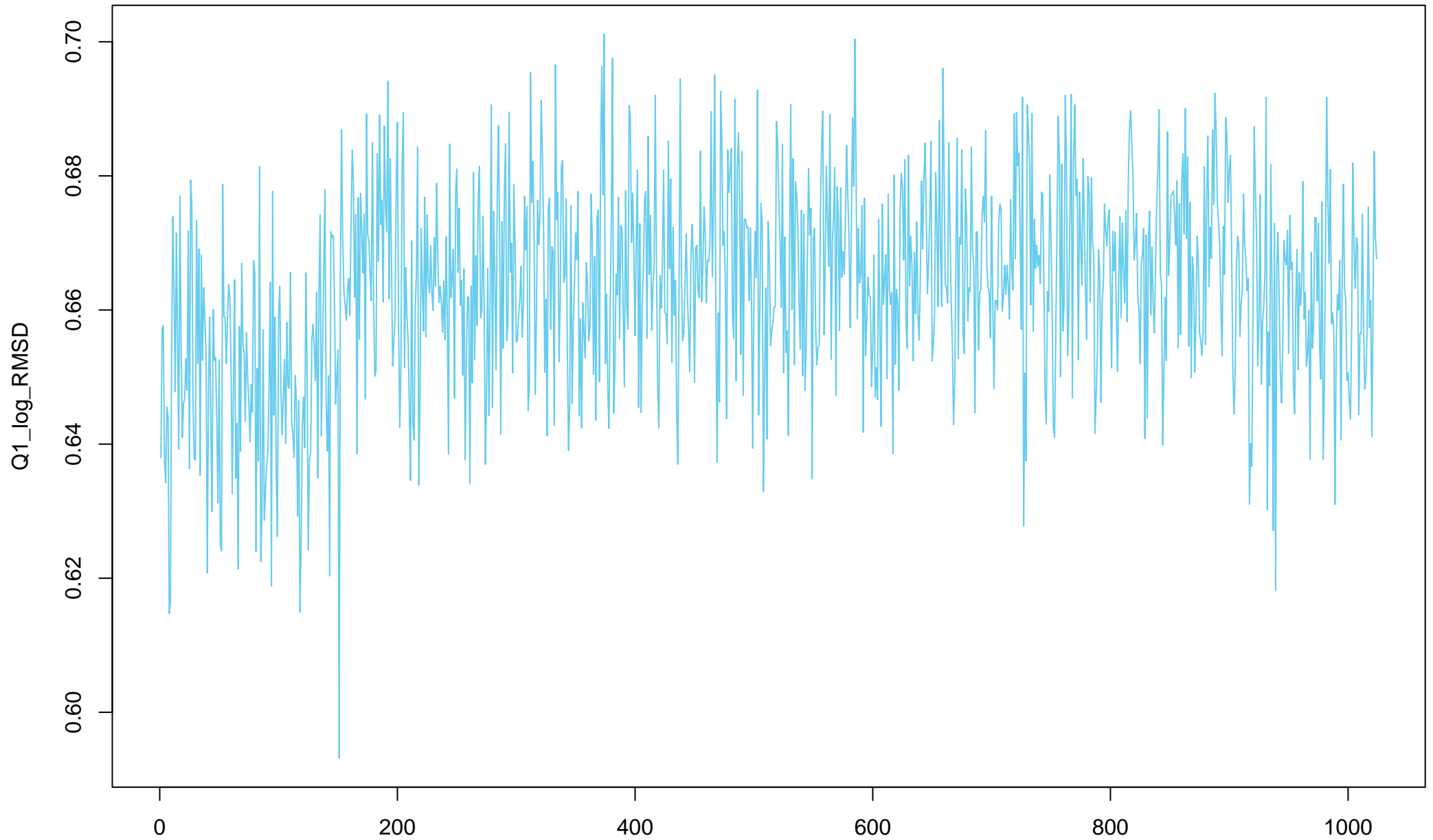
IQR_docked_NumRotatableBonds
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



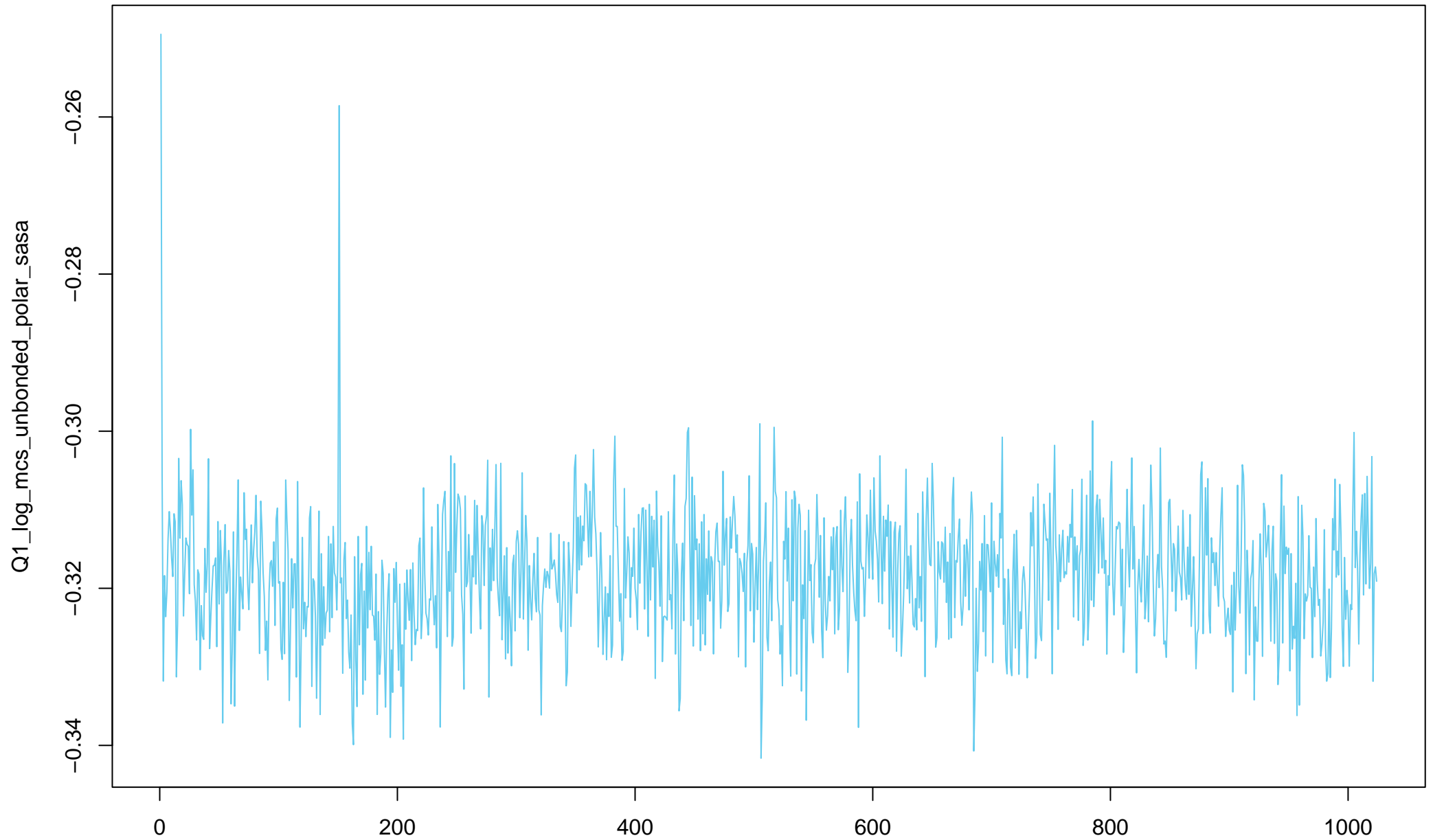
IQR_mcs_NOCOUNT
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



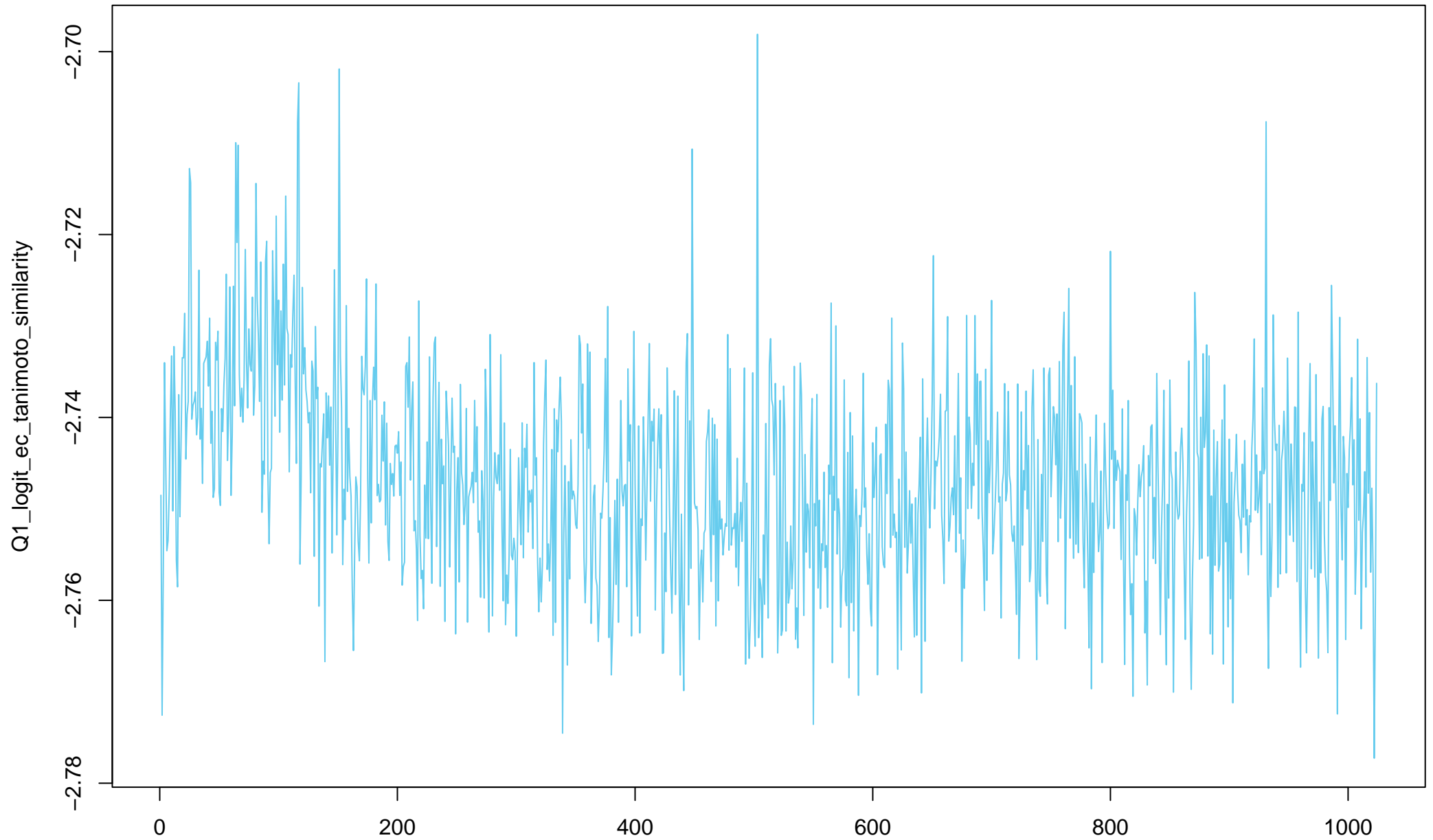
Q1_log_RMSD
ESS = 69.3 | BMK = 0.154 | MCSE(6.27) = 7.91 | stat: FALSE | burn: 0



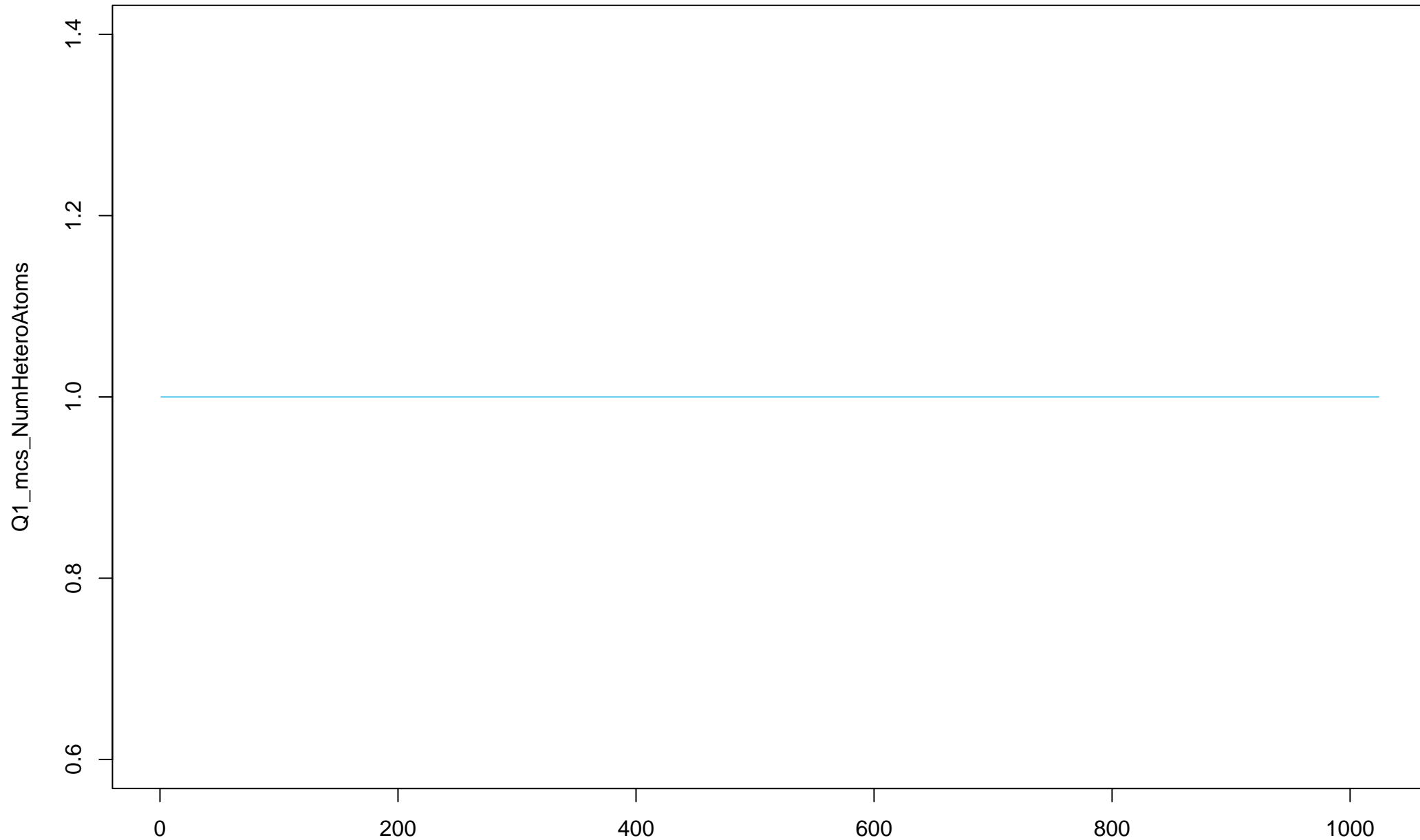
Q1_log_mcs_unbonded_polar_sasa
ESS = 565 | BMK = 0.0719 | MCSE(6.27) = 4.83 | stat: TRUE | burn: 0



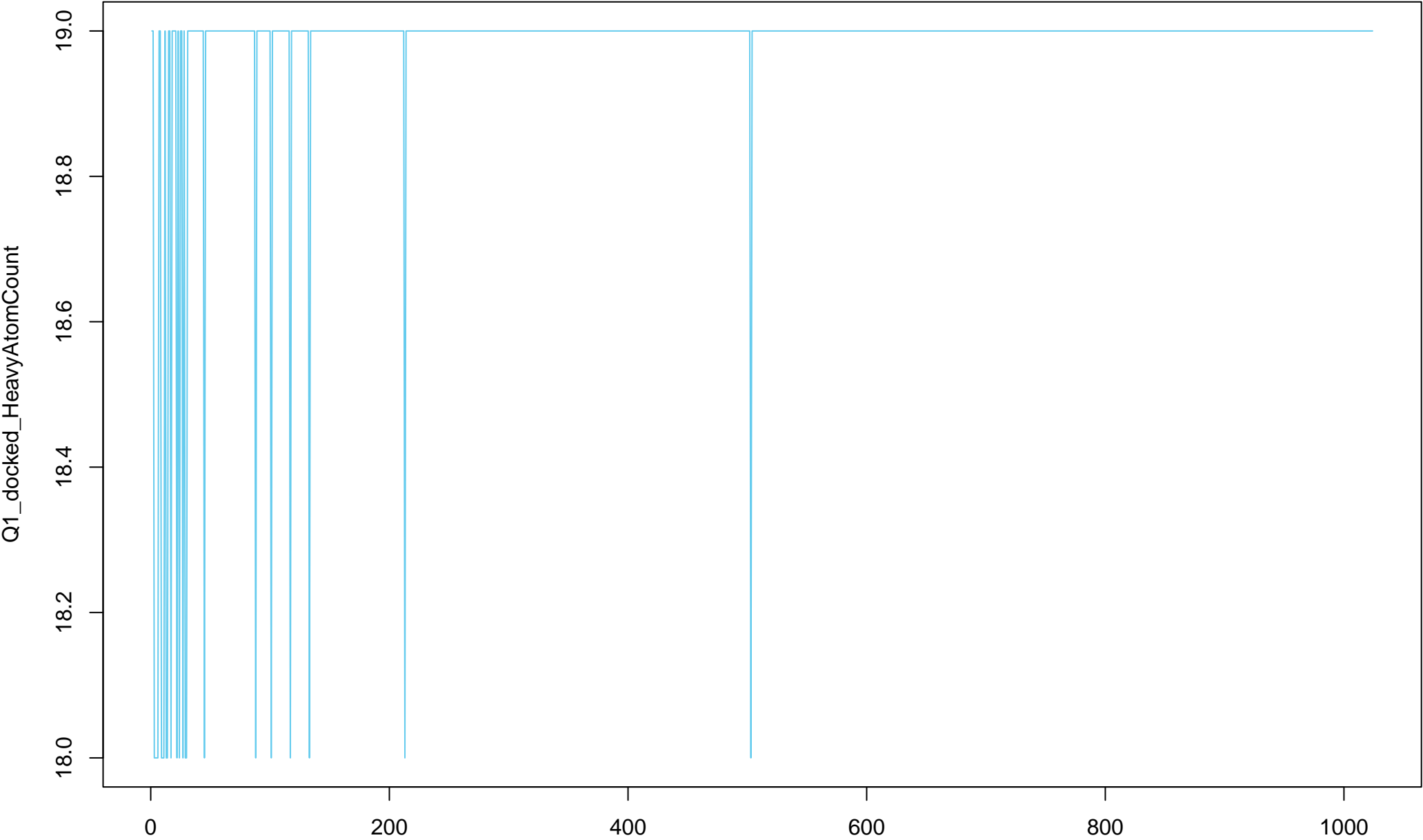
Q1_logit_ec_tanimoto_similarity
ESS = 43.3 | BMK = 0.137 | MCSE(6.27) = 7.79 | stat: FALSE | burn: 0



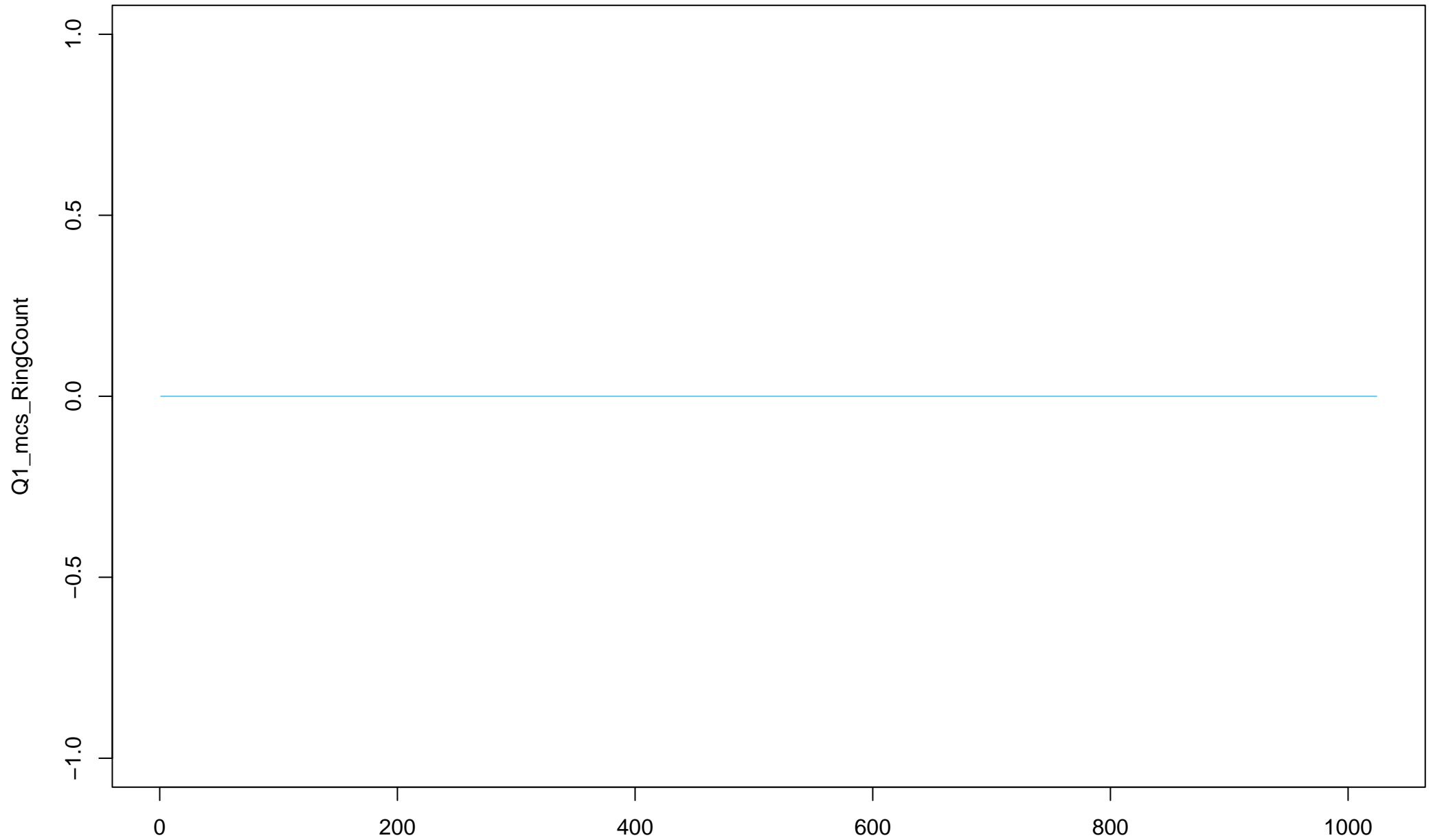
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



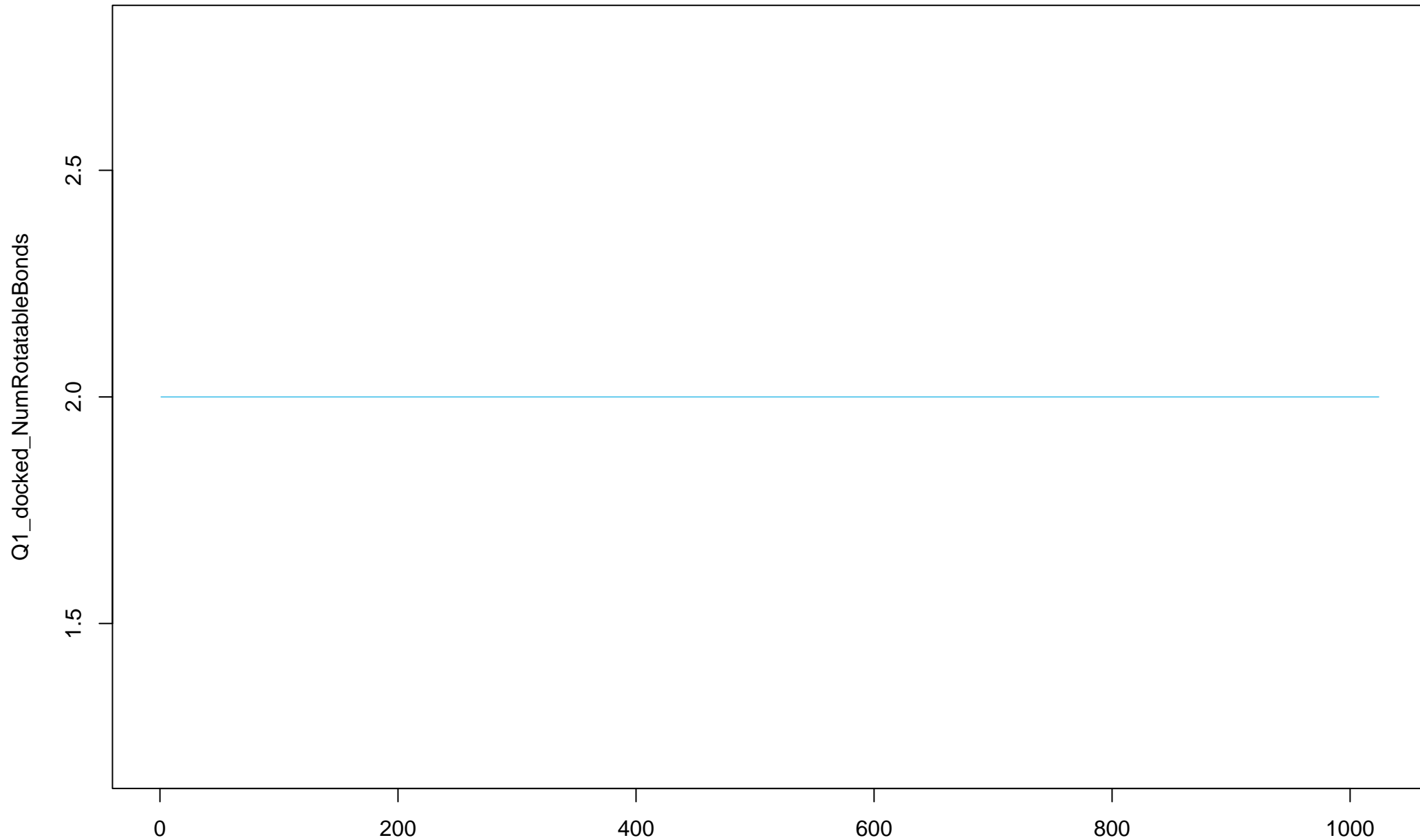
Q1_docked_HeavyAtomCount
ESS = 69.6 | BMK = 0.455 | MCSE(6.27) = 10.1 | stat: FALSE | burn: 0



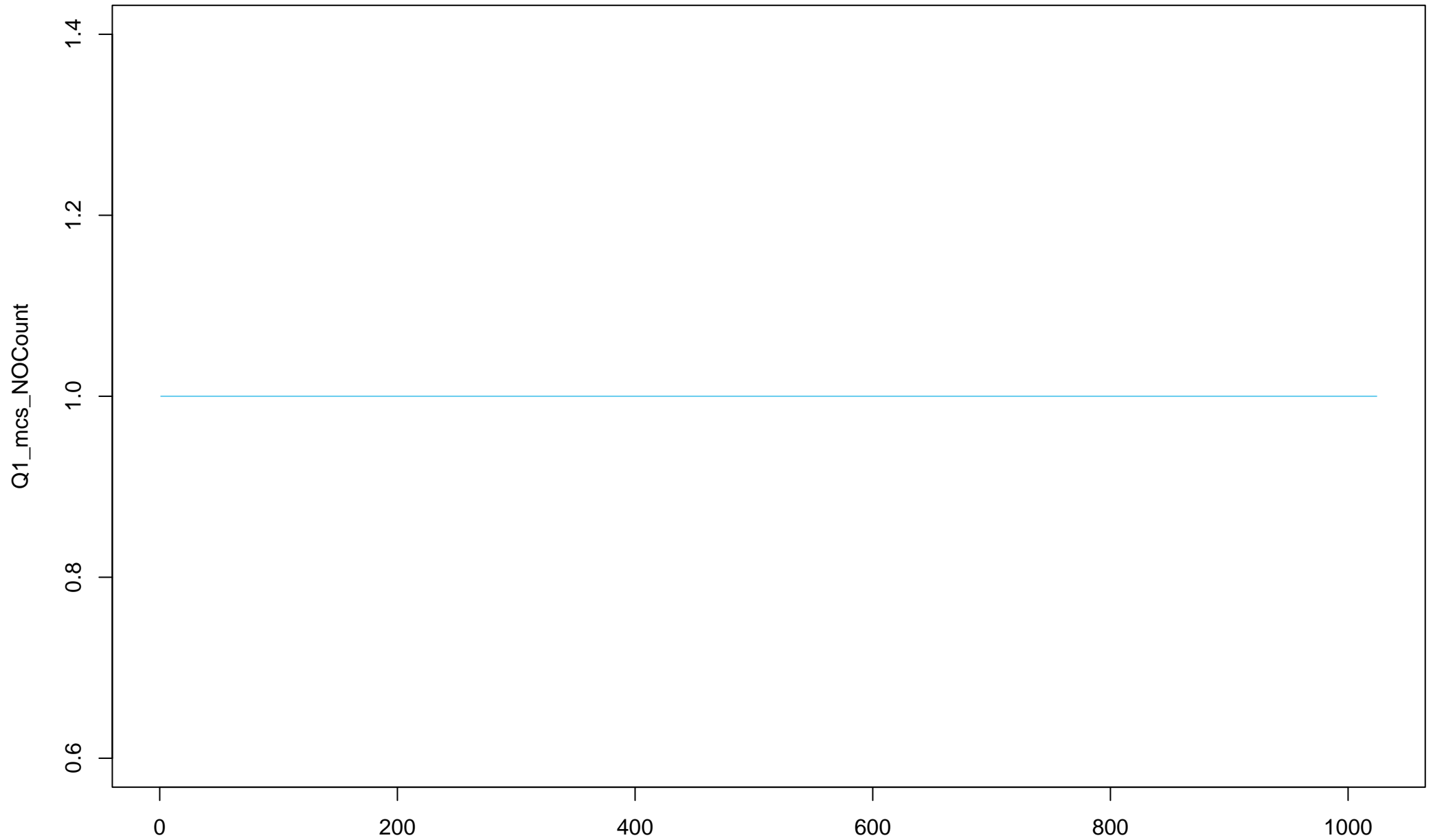
Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



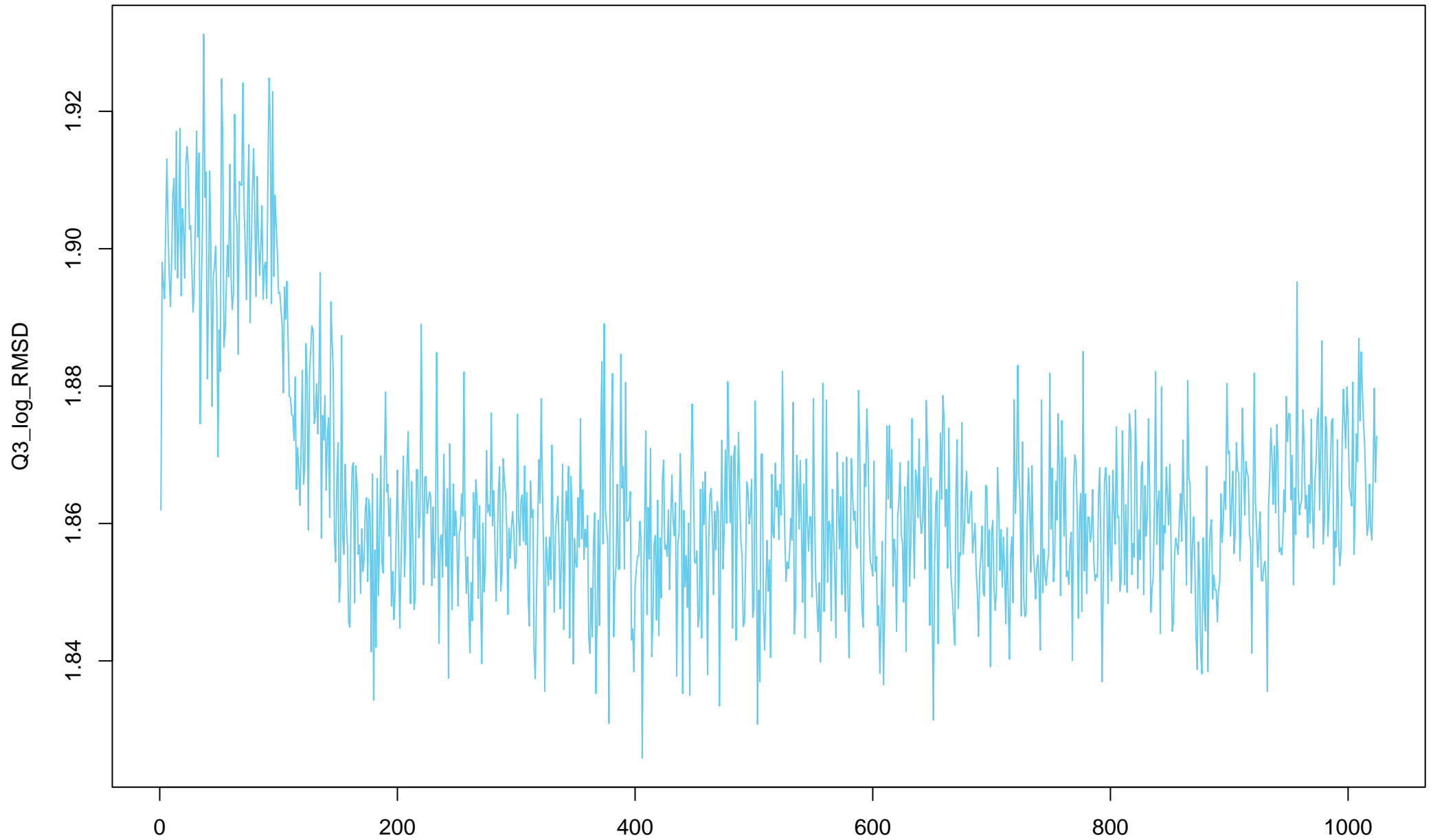
Q1_docked_NumRotatableBonds
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



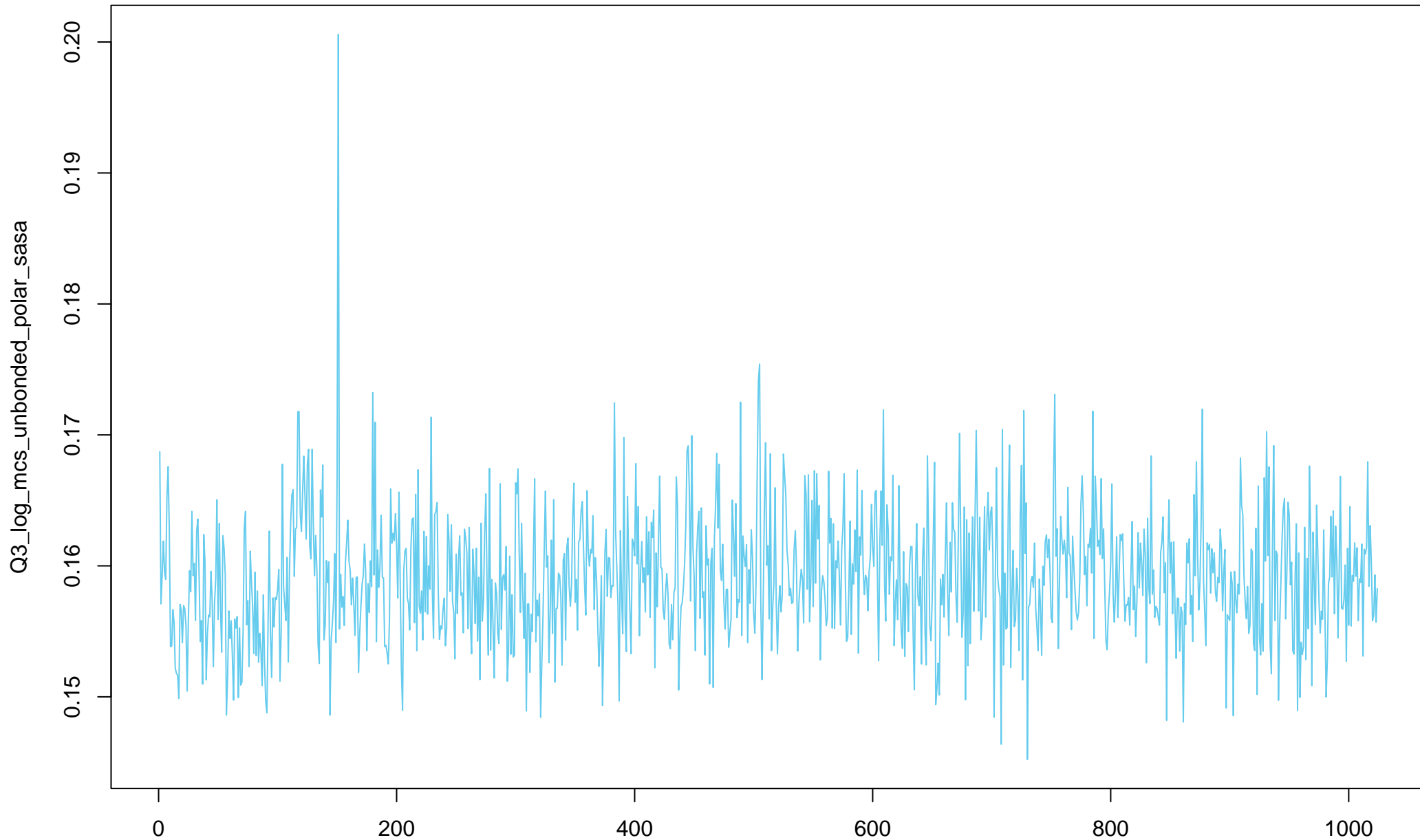
Q1_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



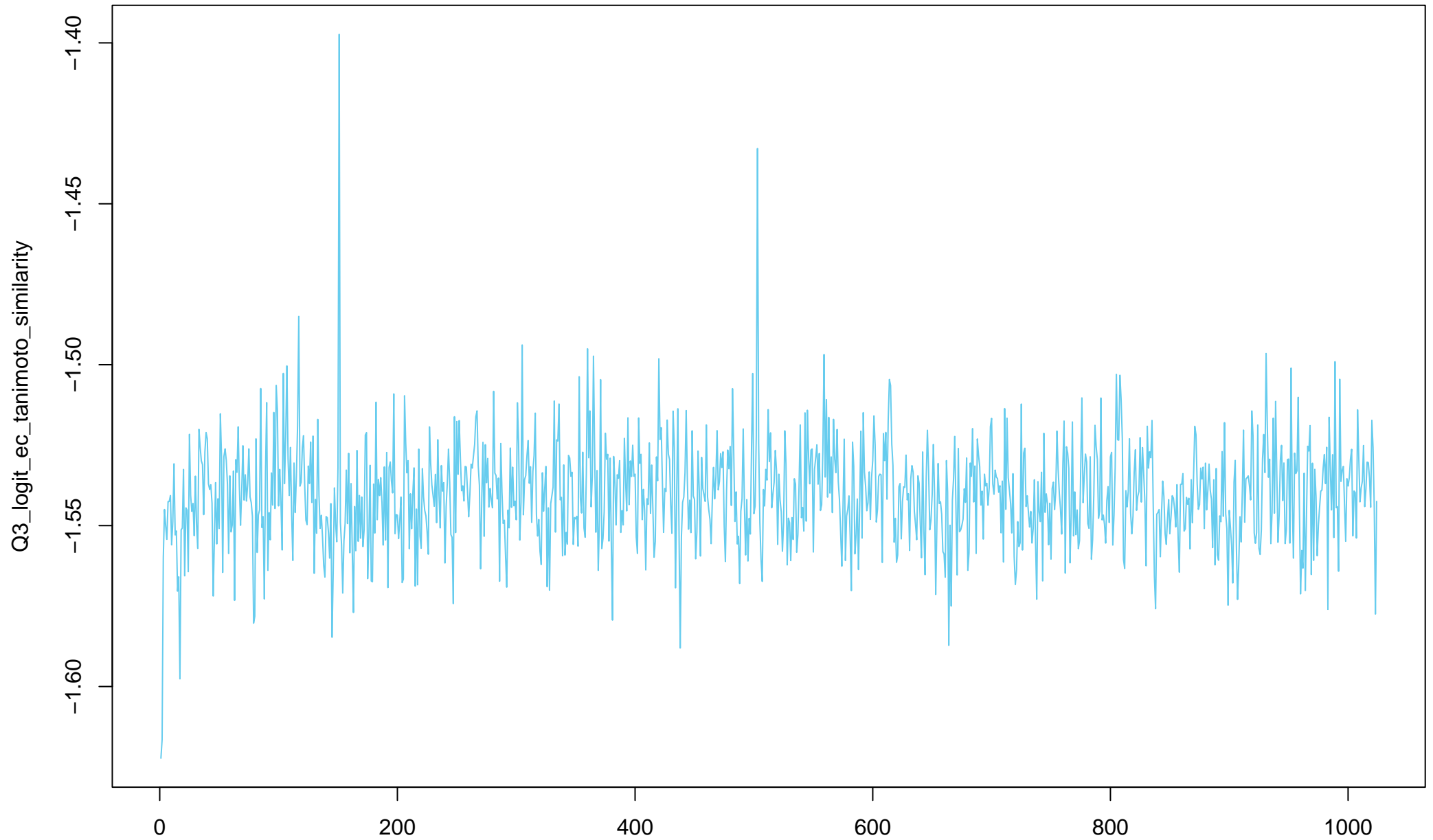
Q3_log_RMSD
ESS = 10.6 | BMK = 0.308 | MCSE(6.27) = 14.1 | stat: FALSE | burn: 102



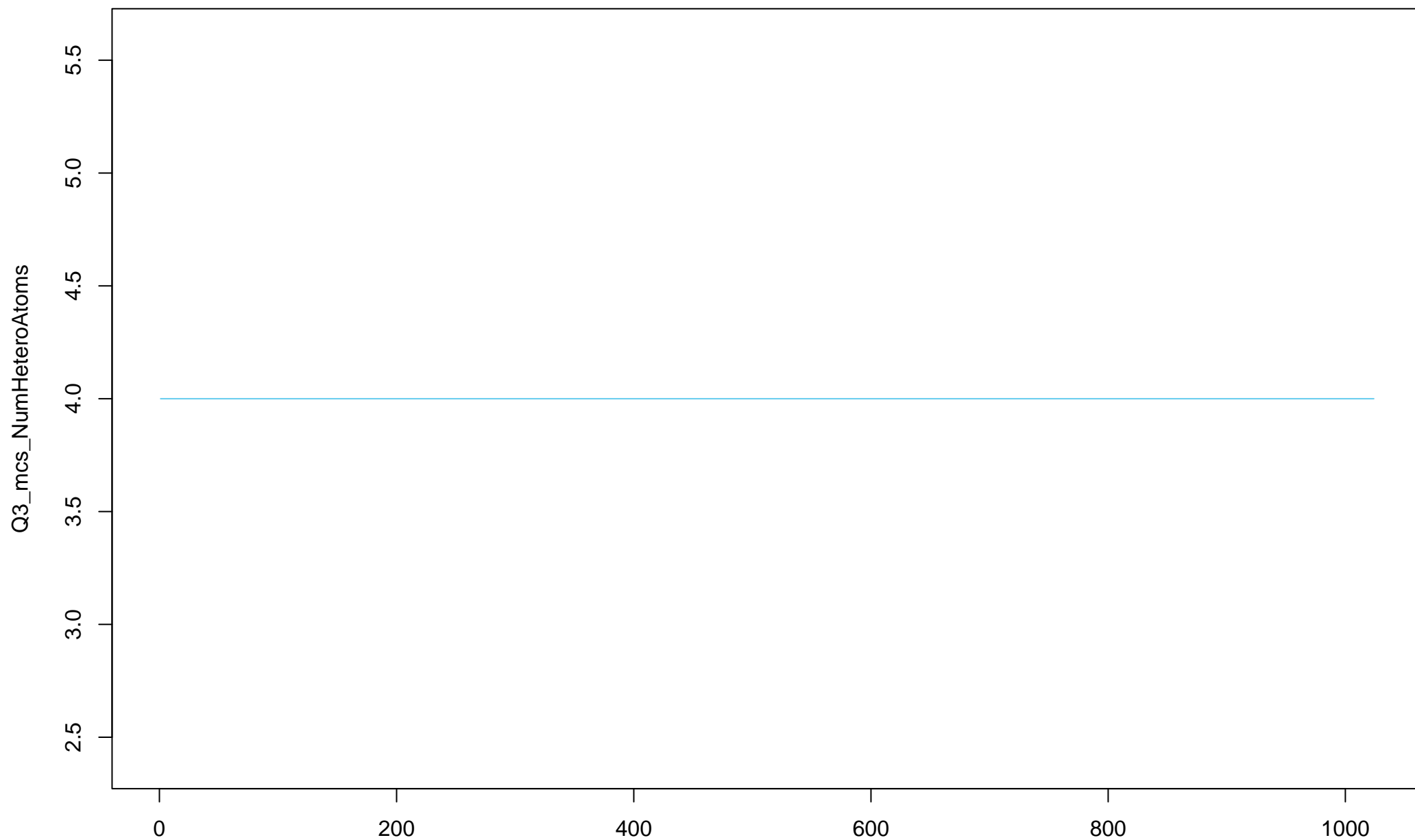
Q3_log_mcs_unbonded_polar_sasa
ESS = 537 | BMK = 0.0777 | MCSE(6.27) = 4.79 | stat: FALSE | burn: 0



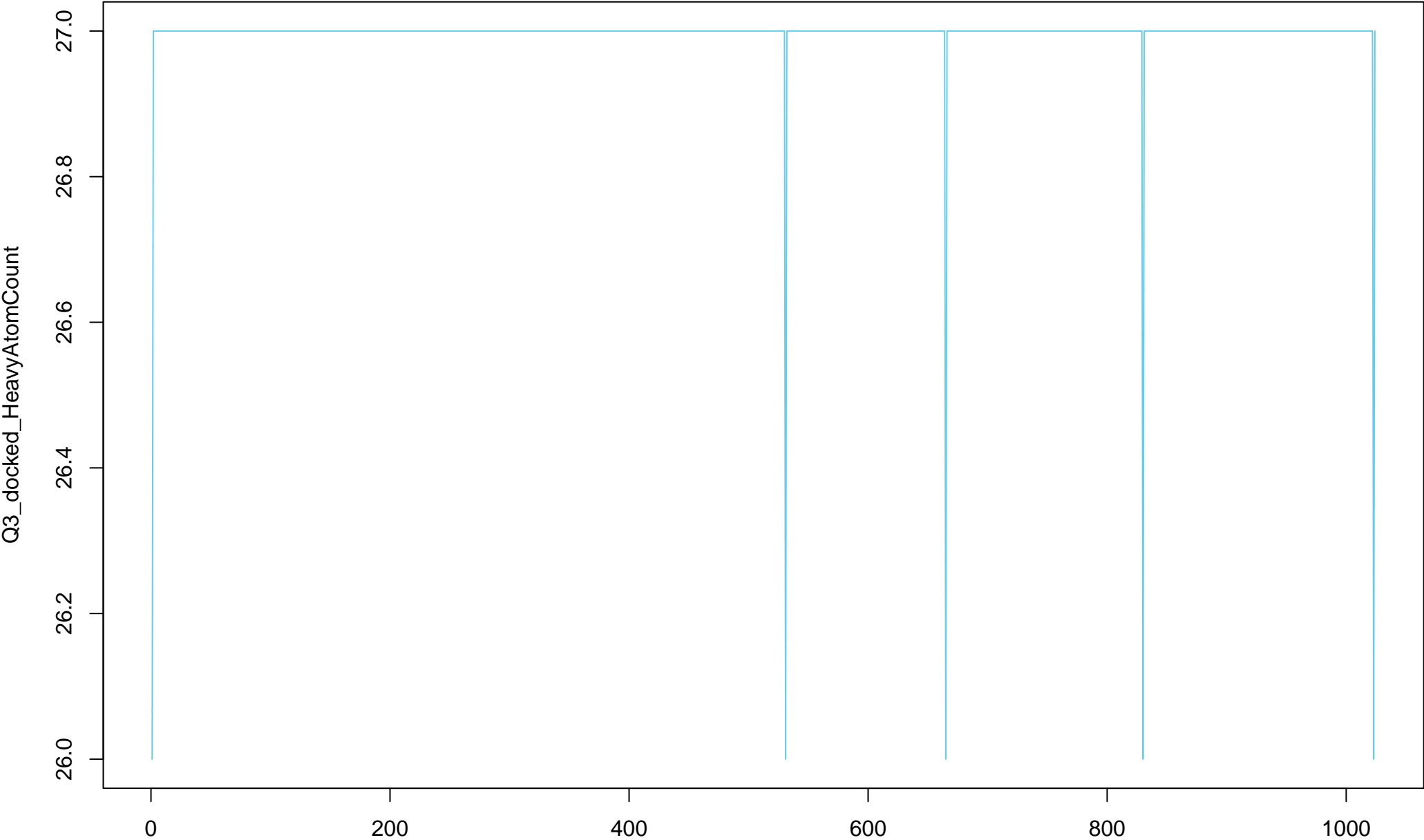
Q3_logit_ec_tanimoto_similarity
ESS = 754 | BMK = 0.0771 | MCSE(6.27) = 4.92 | stat: TRUE | burn: 0



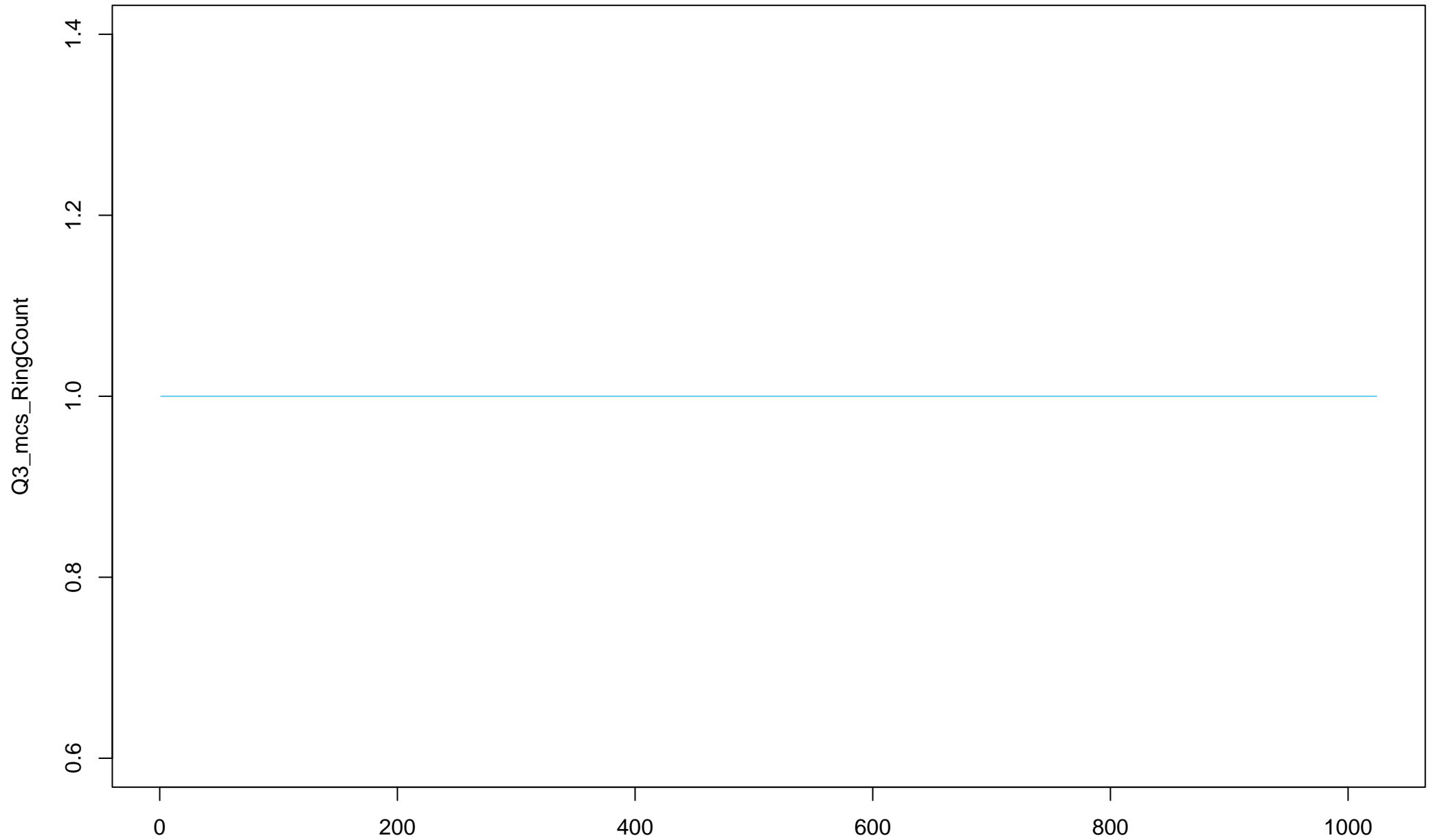
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



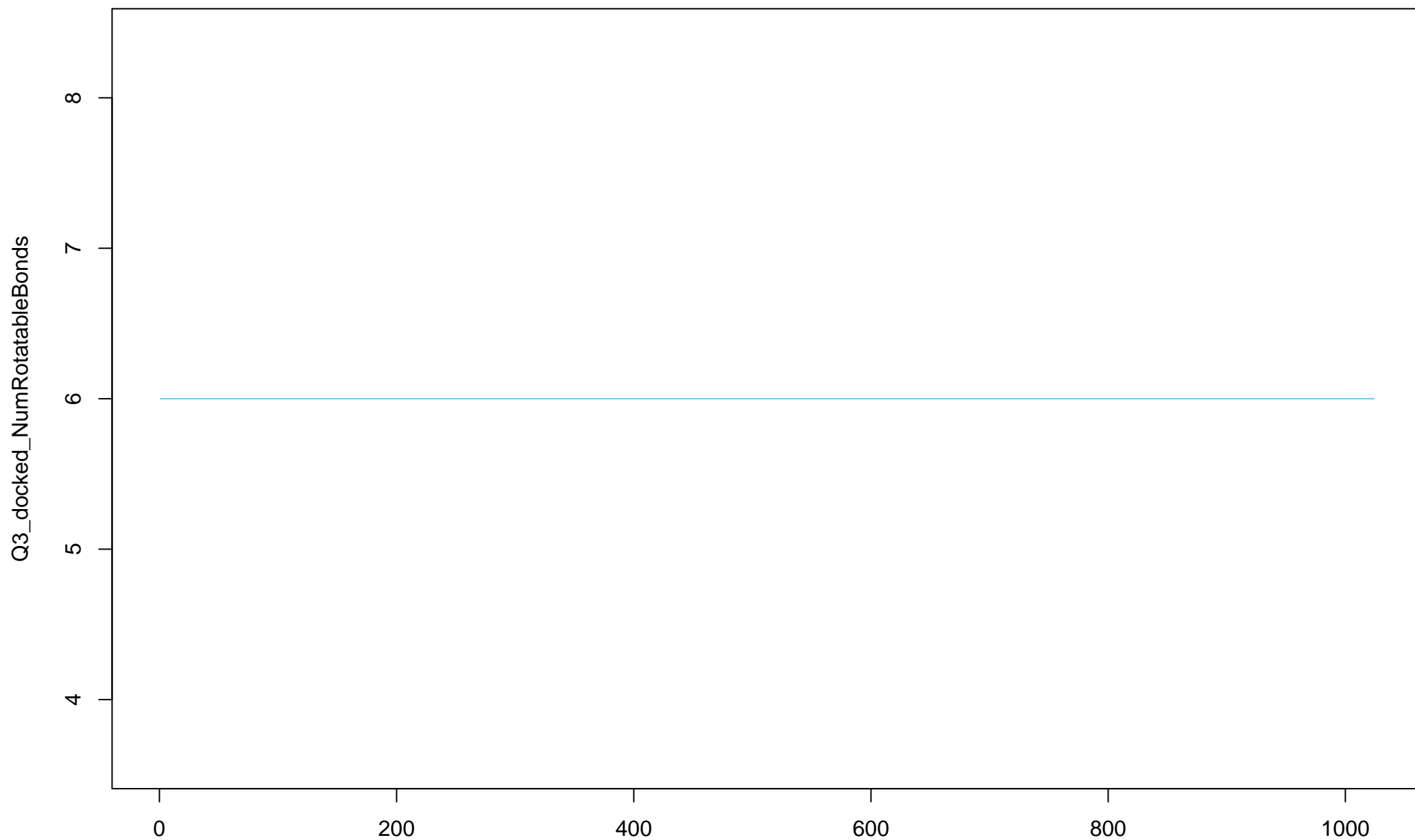
Q3_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.232 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0



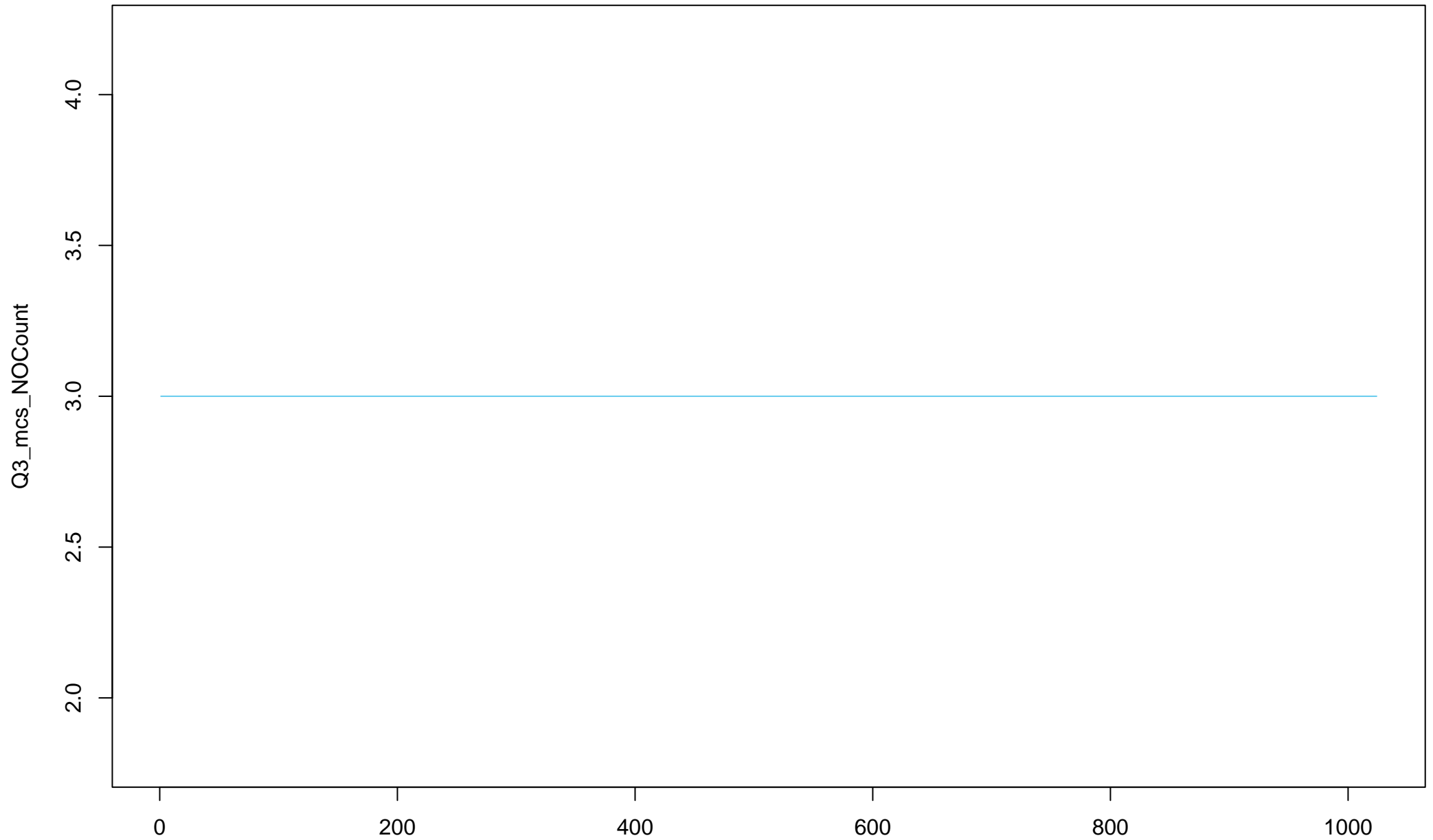
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



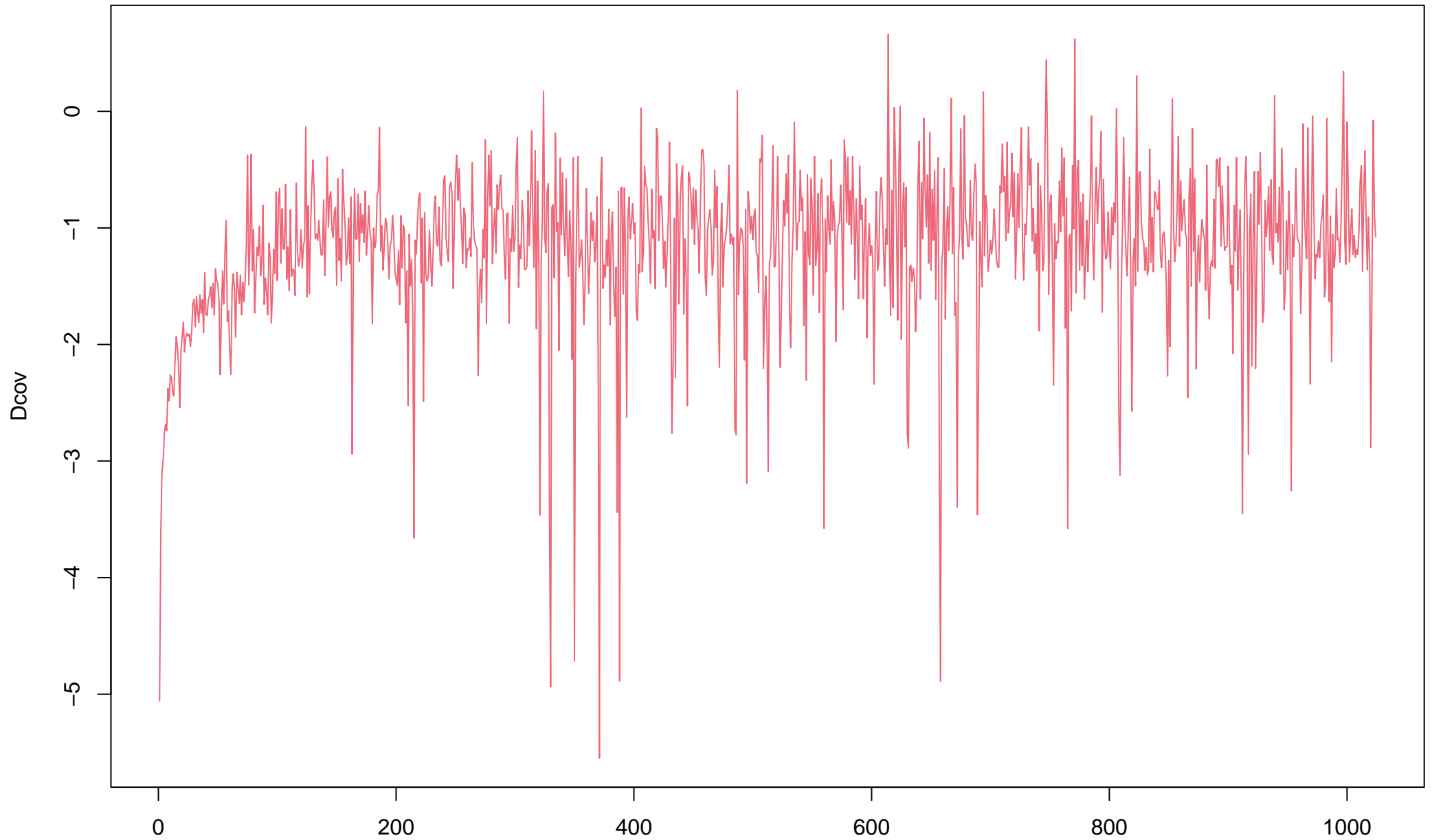
Q3_docked_NumRotatableBonds
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



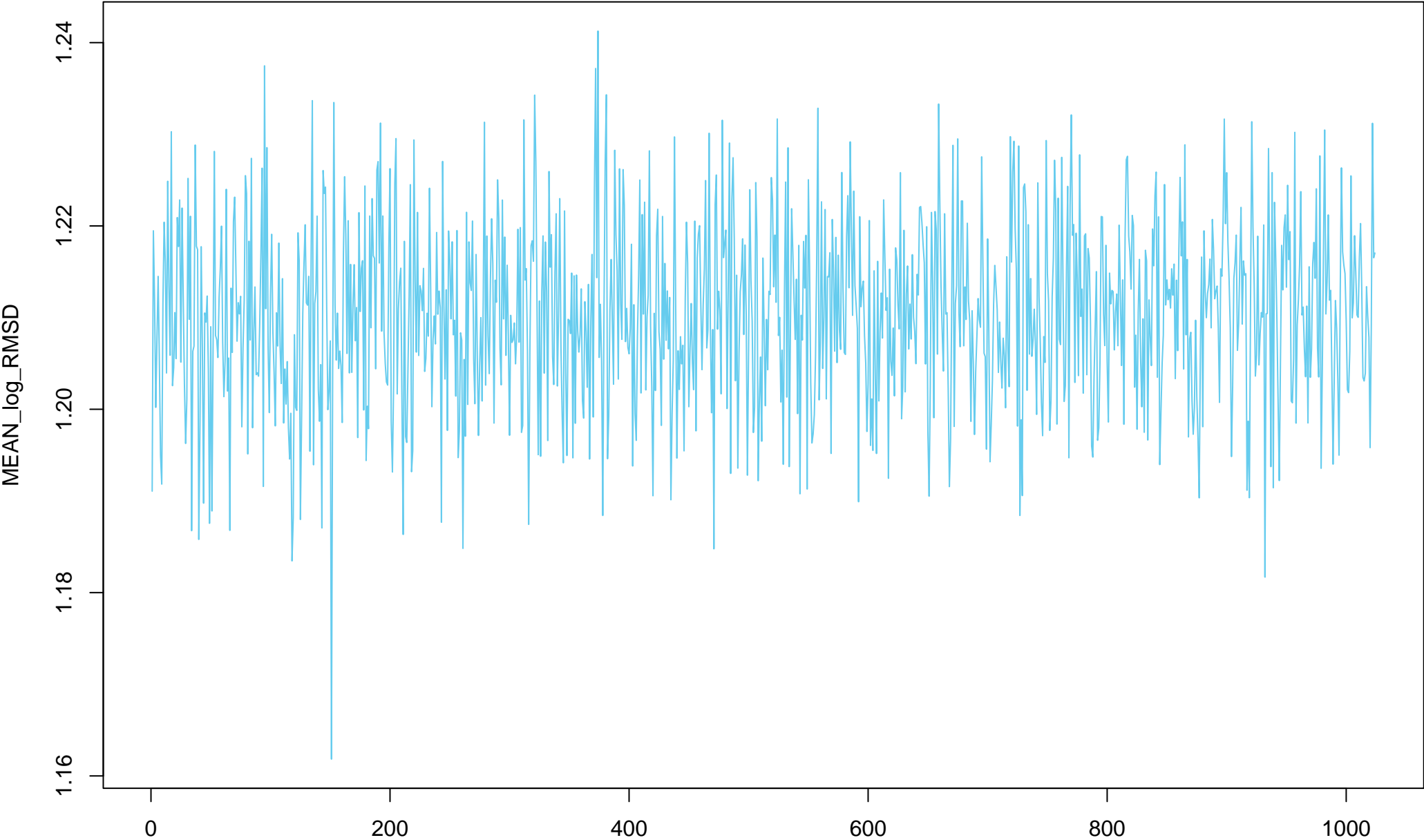
Q3_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



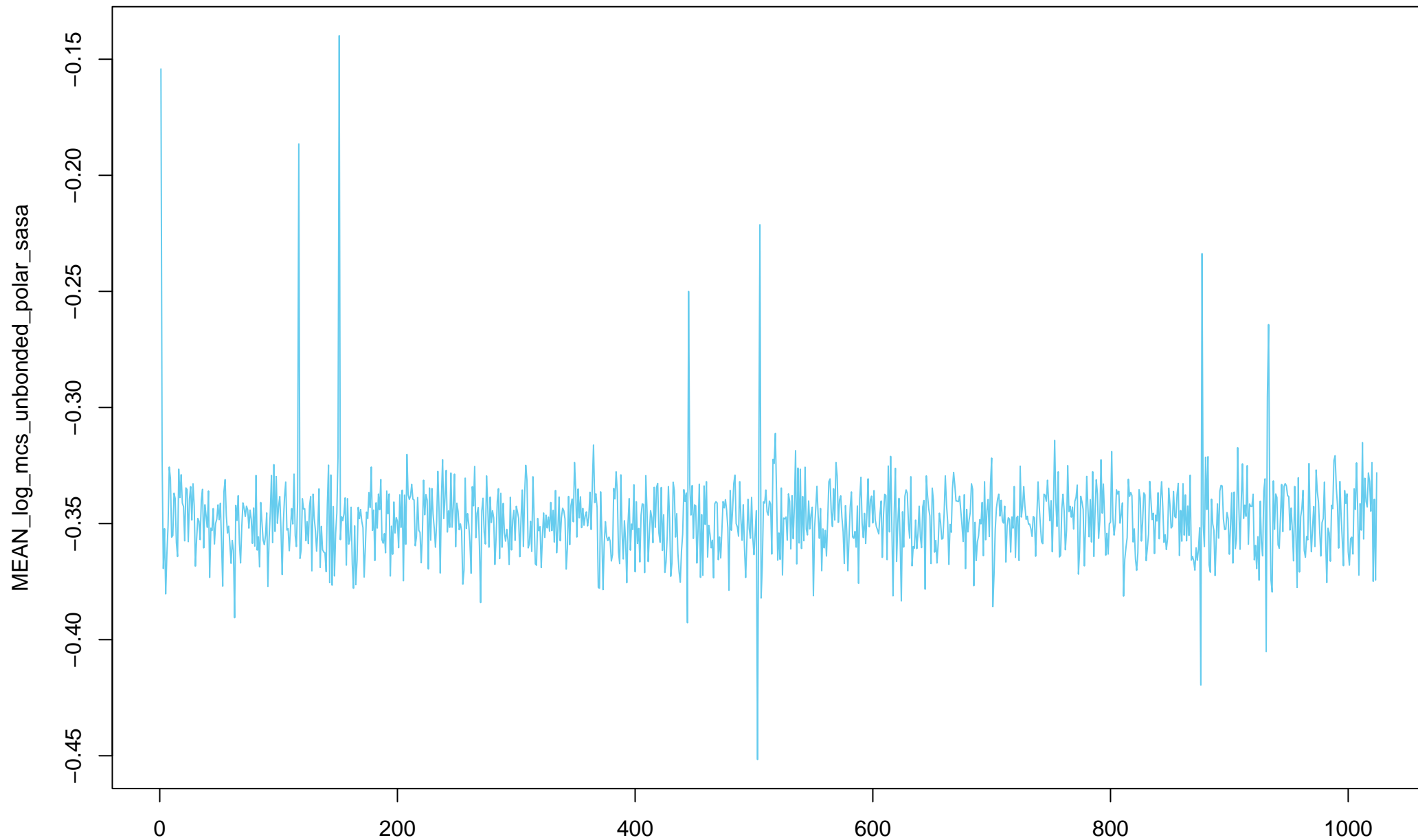
Dcov
ESS = 318 | BMK = 0.152 | MCSE(6.27) = 5.03 | stat: FALSE | burn: 102



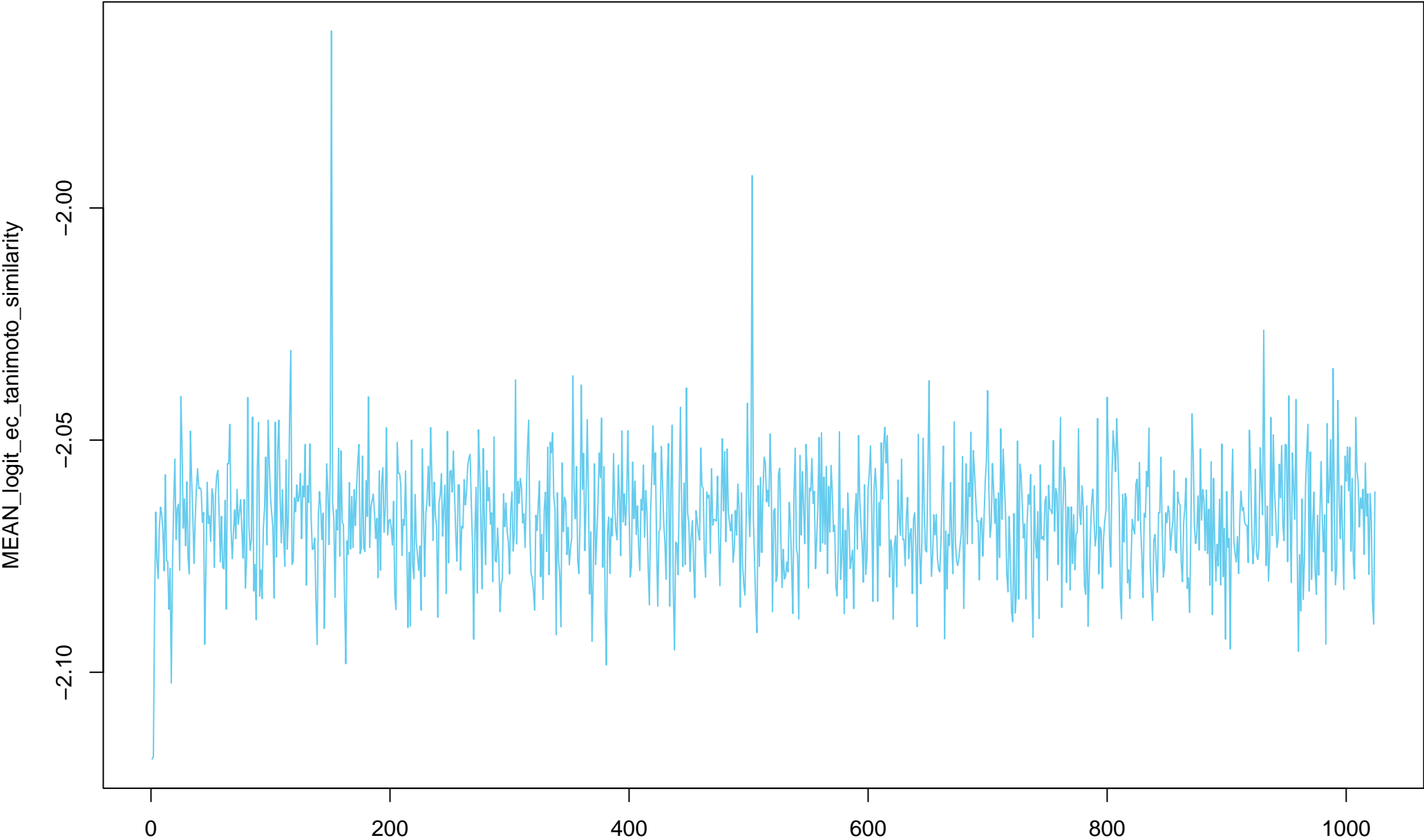
MEAN_log_RMSD
ESS = 918 | BMK = 0.0873 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0



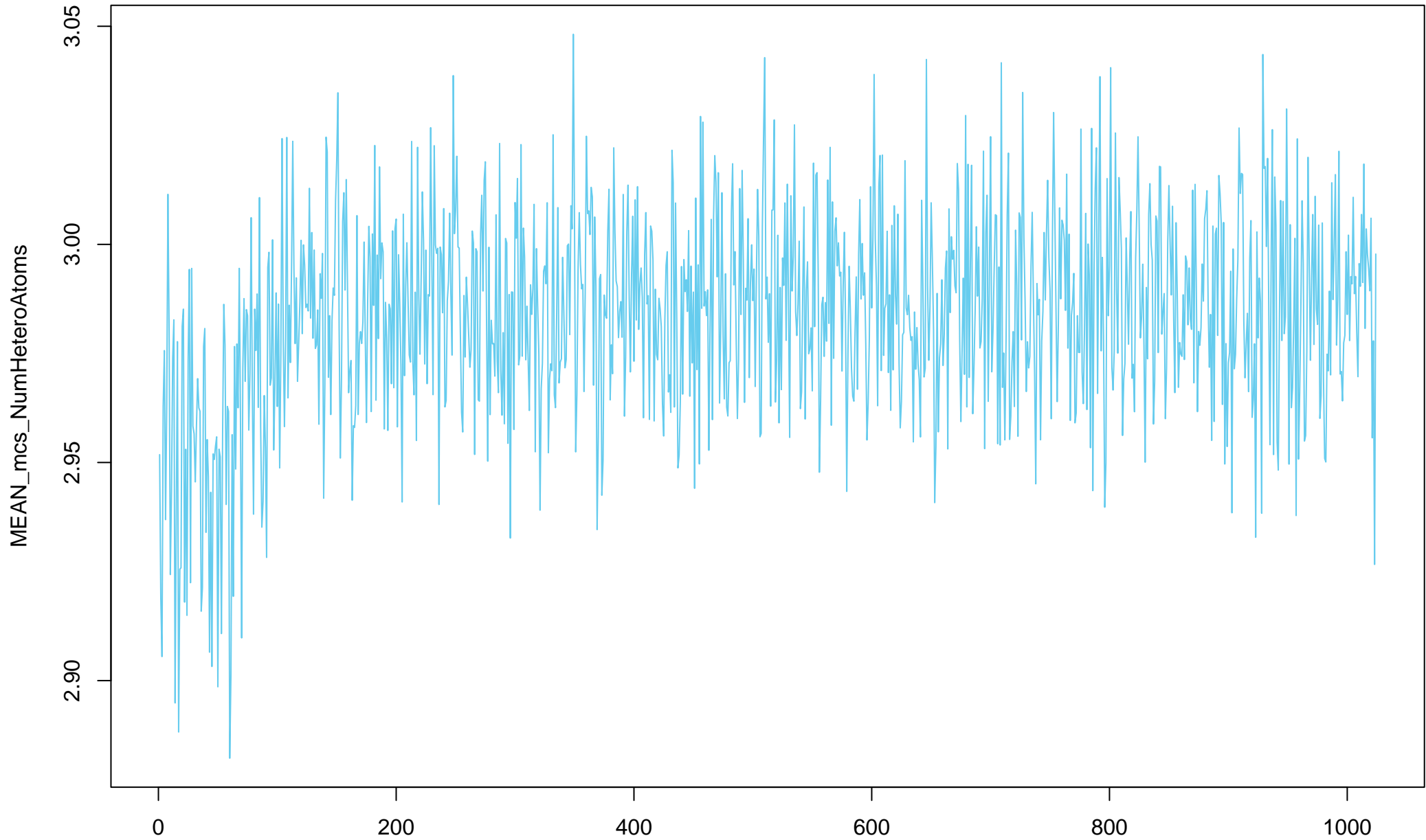
MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.117 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0



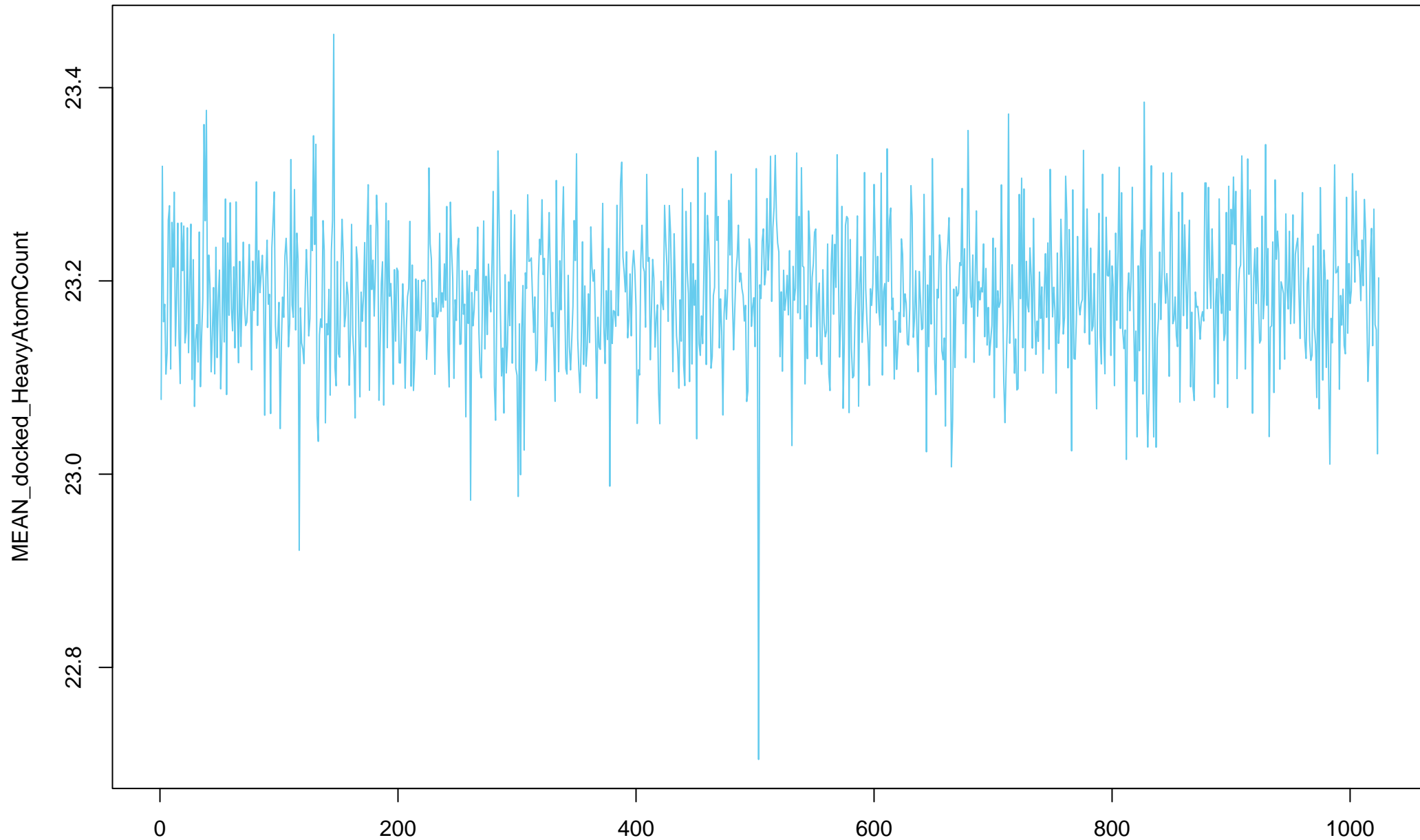
MEAN_logit_ec_tanimoto_similarity
ESS = 843 | BMK = 0.0735 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0



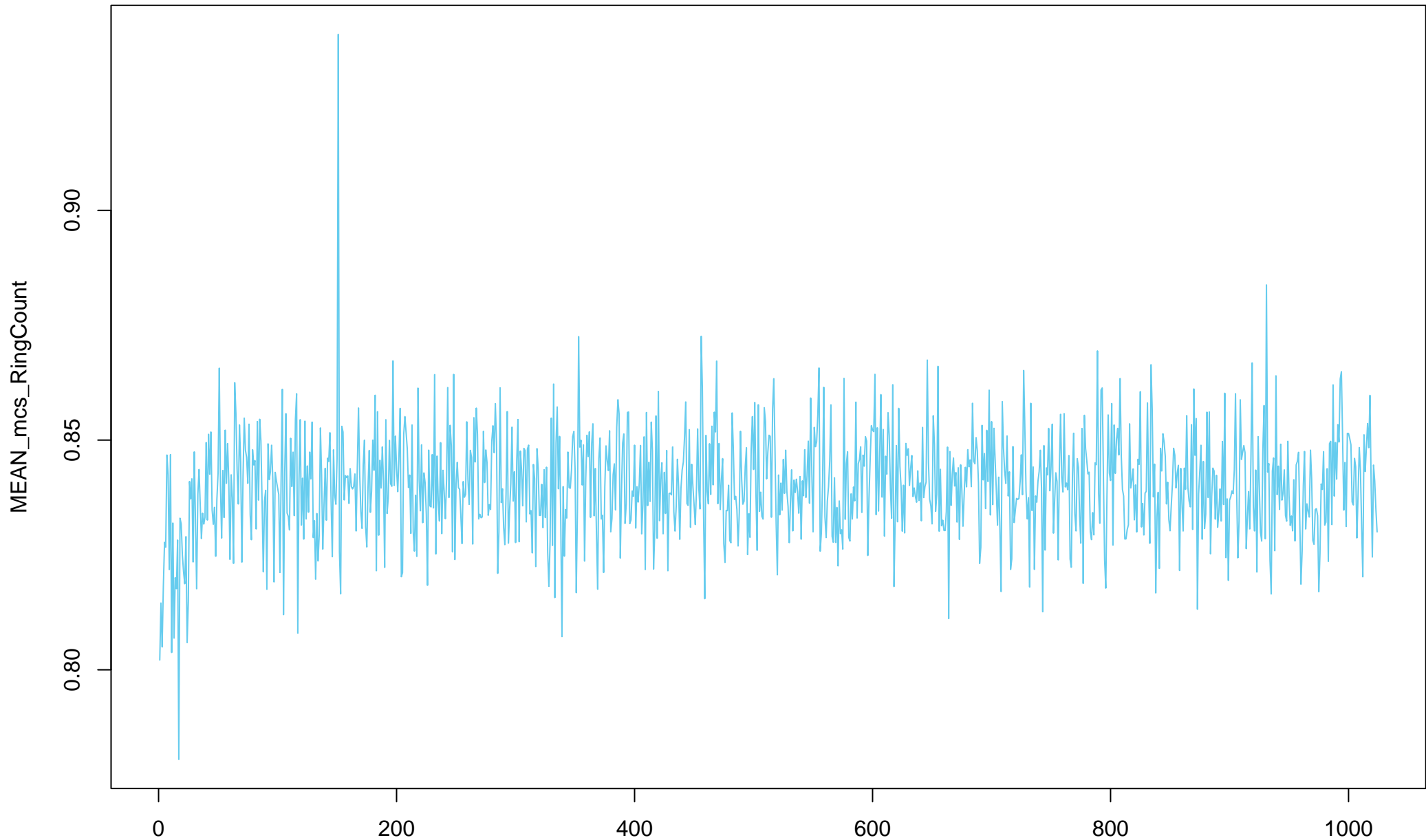
MEAN_mcs_NumHeteroAtoms
ESS = 62.5 | BMK = 0.142 | MCSE(6.27) = 7.76 | stat: FALSE | burn: 0



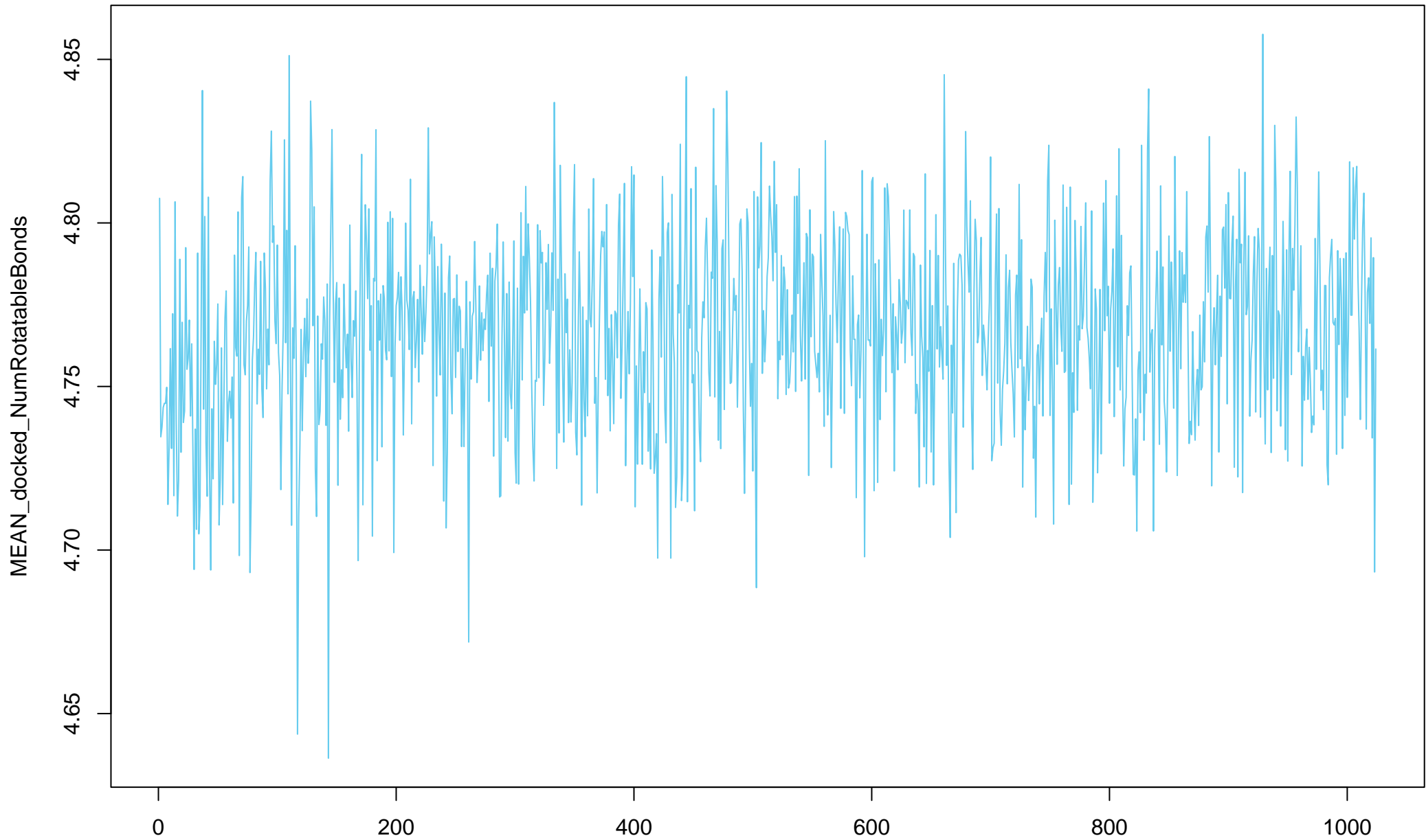
MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0766 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0



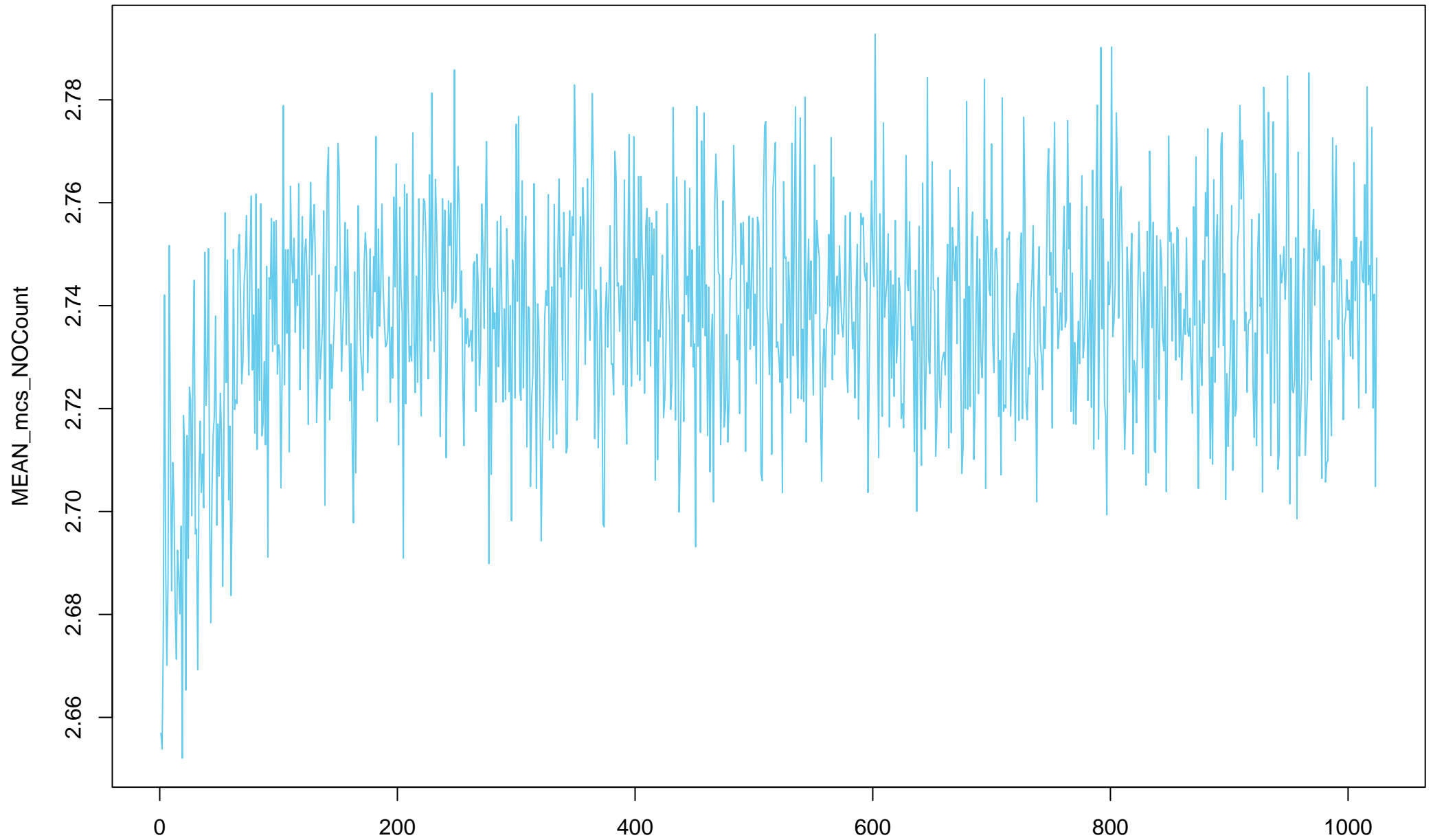
MEAN_mcs_RingCount
ESS = 379 | BMK = 0.0999 | MCSE(6.27) = 5.02 | stat: FALSE | burn: 0



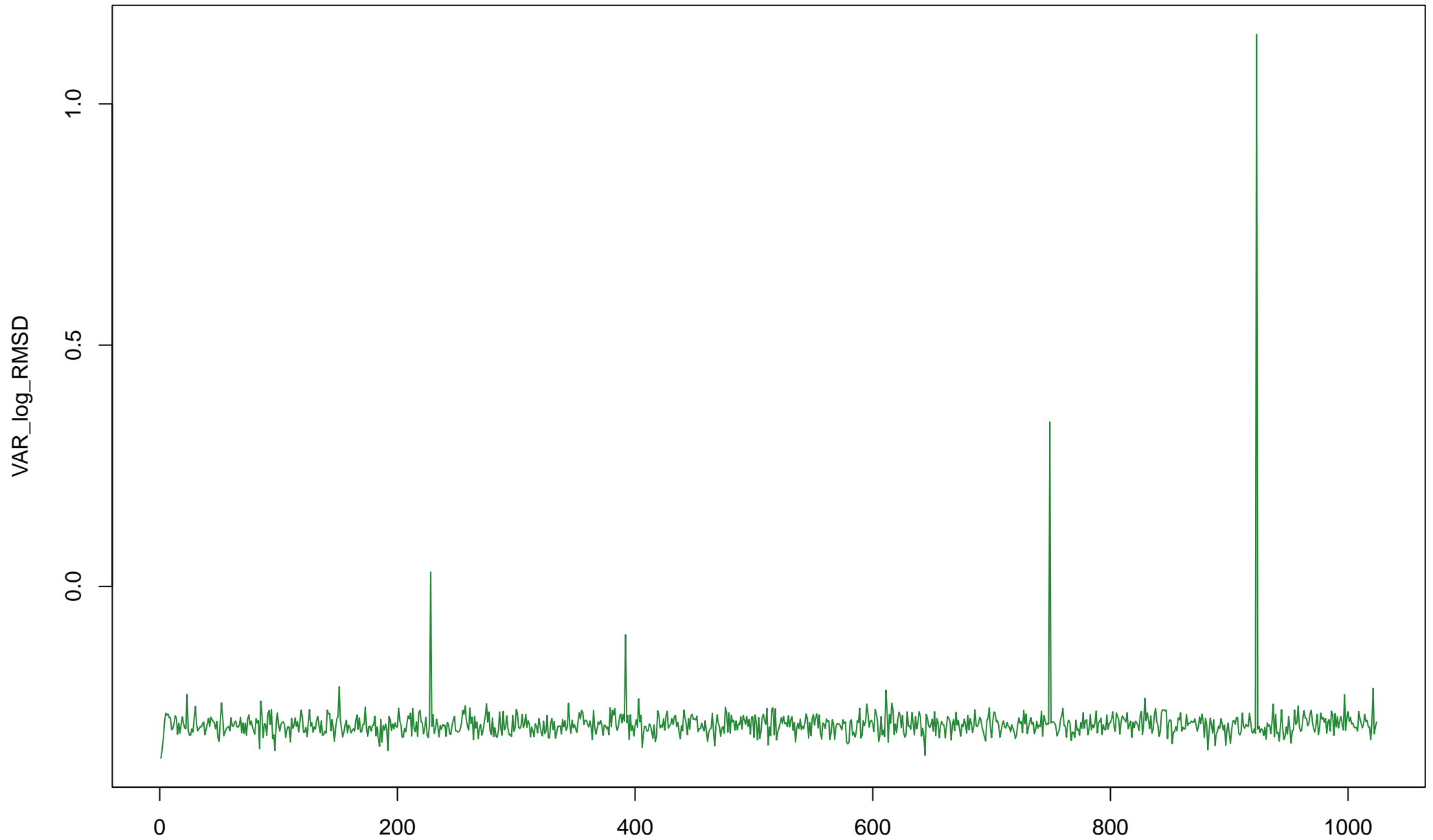
MEAN_docked_NumRotatableBonds
ESS = 906 | BMK = 0.0917 | MCSE(6.27) = 4.17 | stat: FALSE | burn: 0



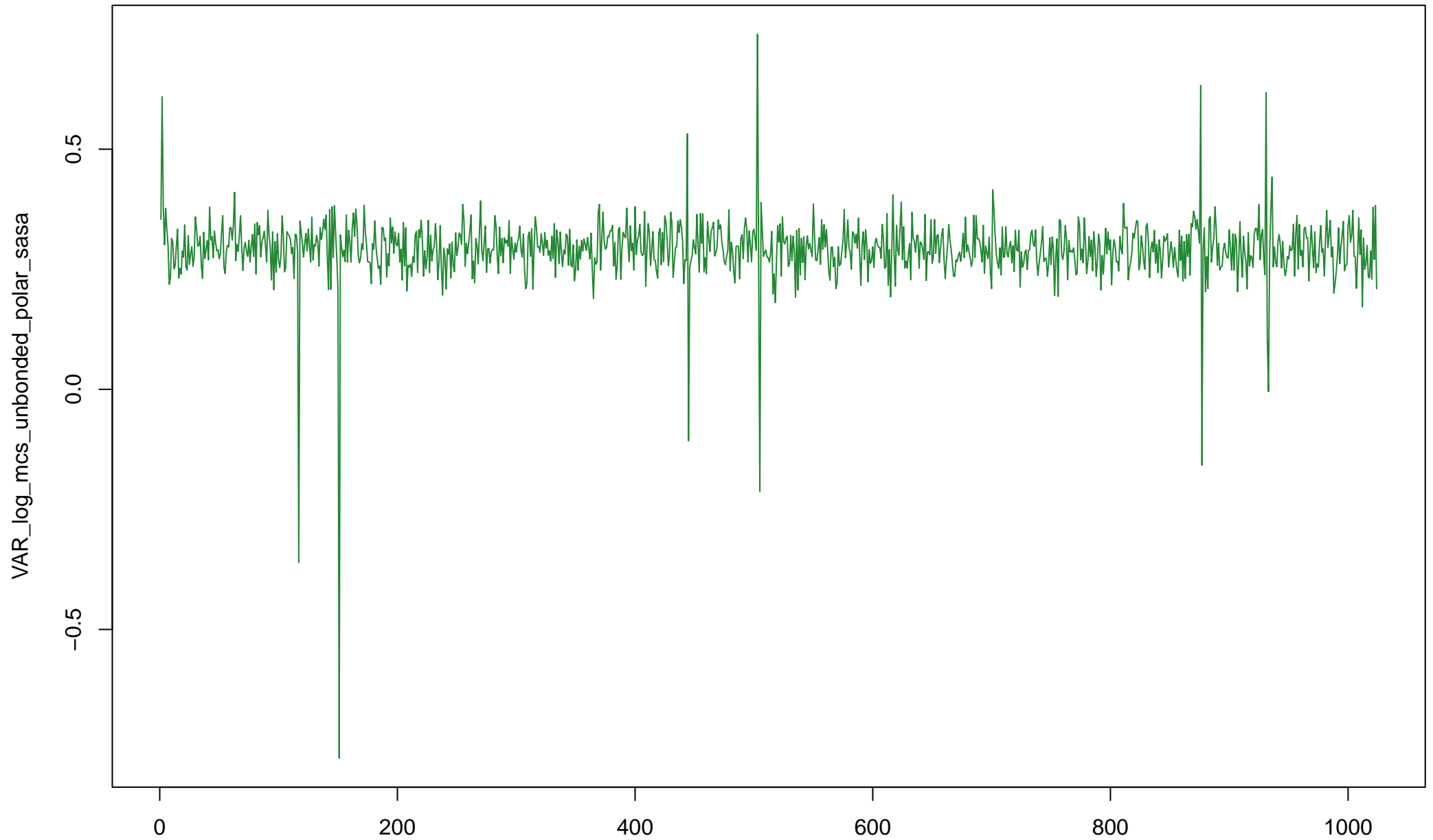
MEAN_mcs_NOCount
ESS = 101 | BMK = 0.15 | MCSE(6.27) = 7.68 | stat: FALSE | burn: 0



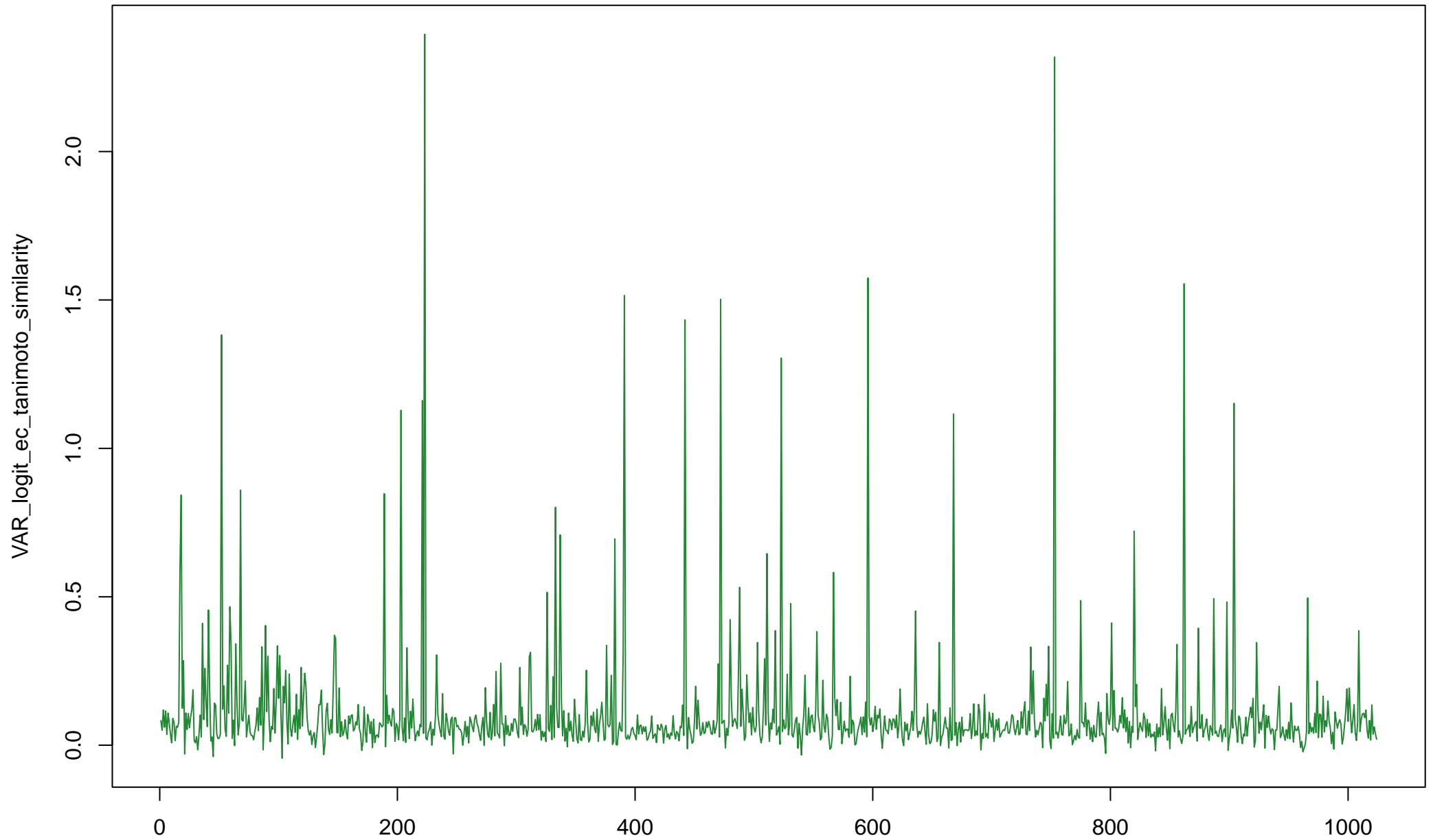
VAR_log_RMSD
ESS = 1020 | BMK = 0.0765 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0



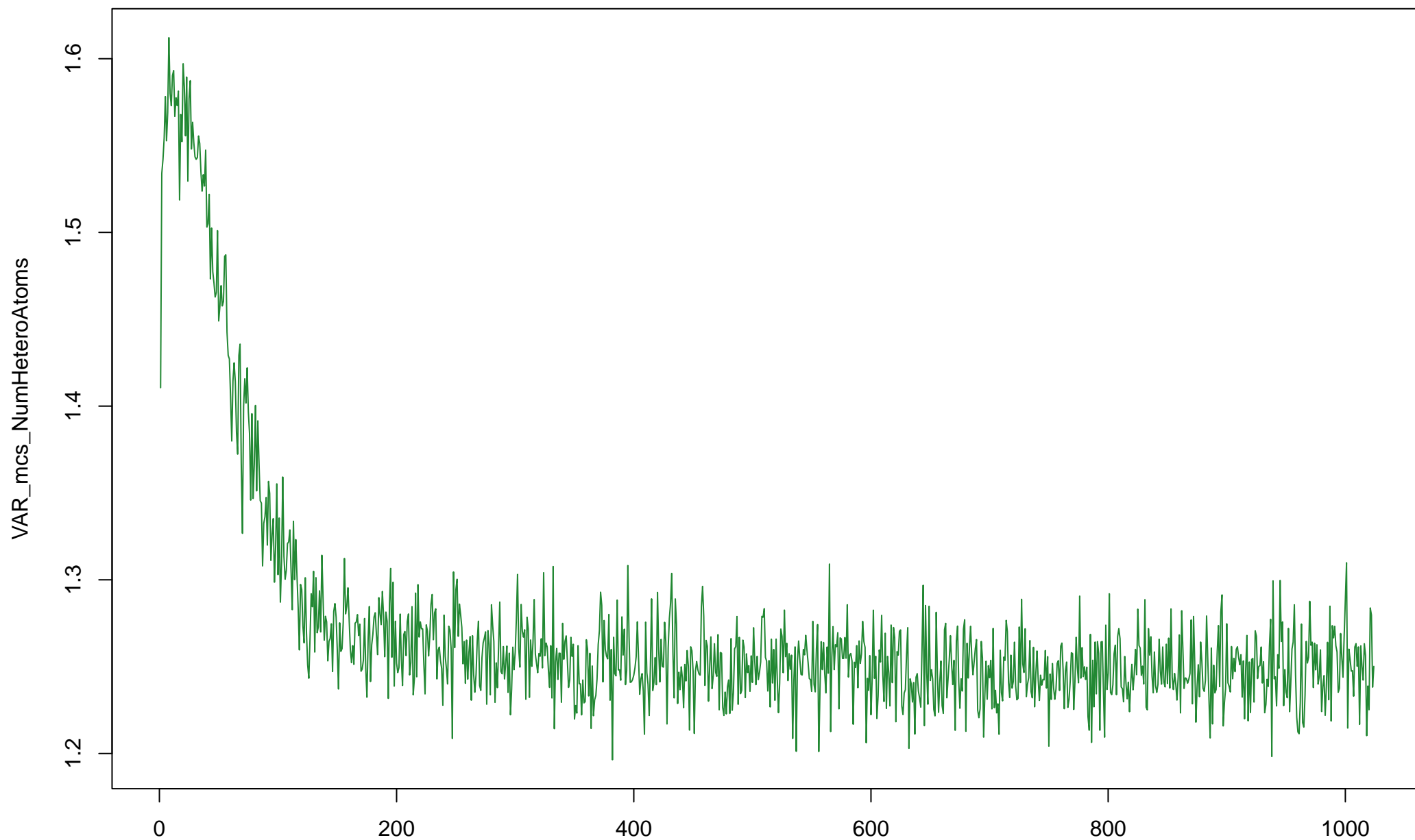
VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.111 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0



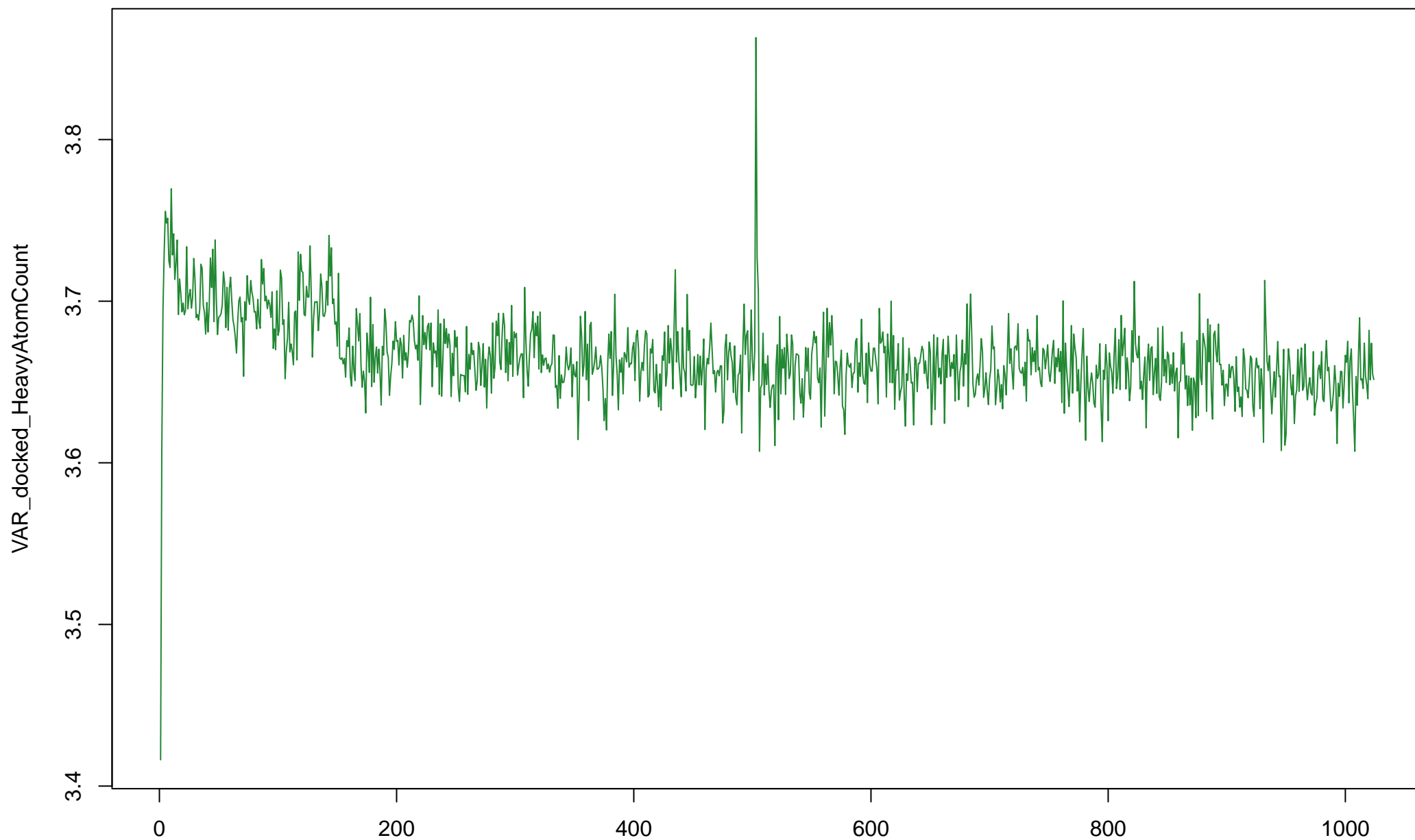
VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.176 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0



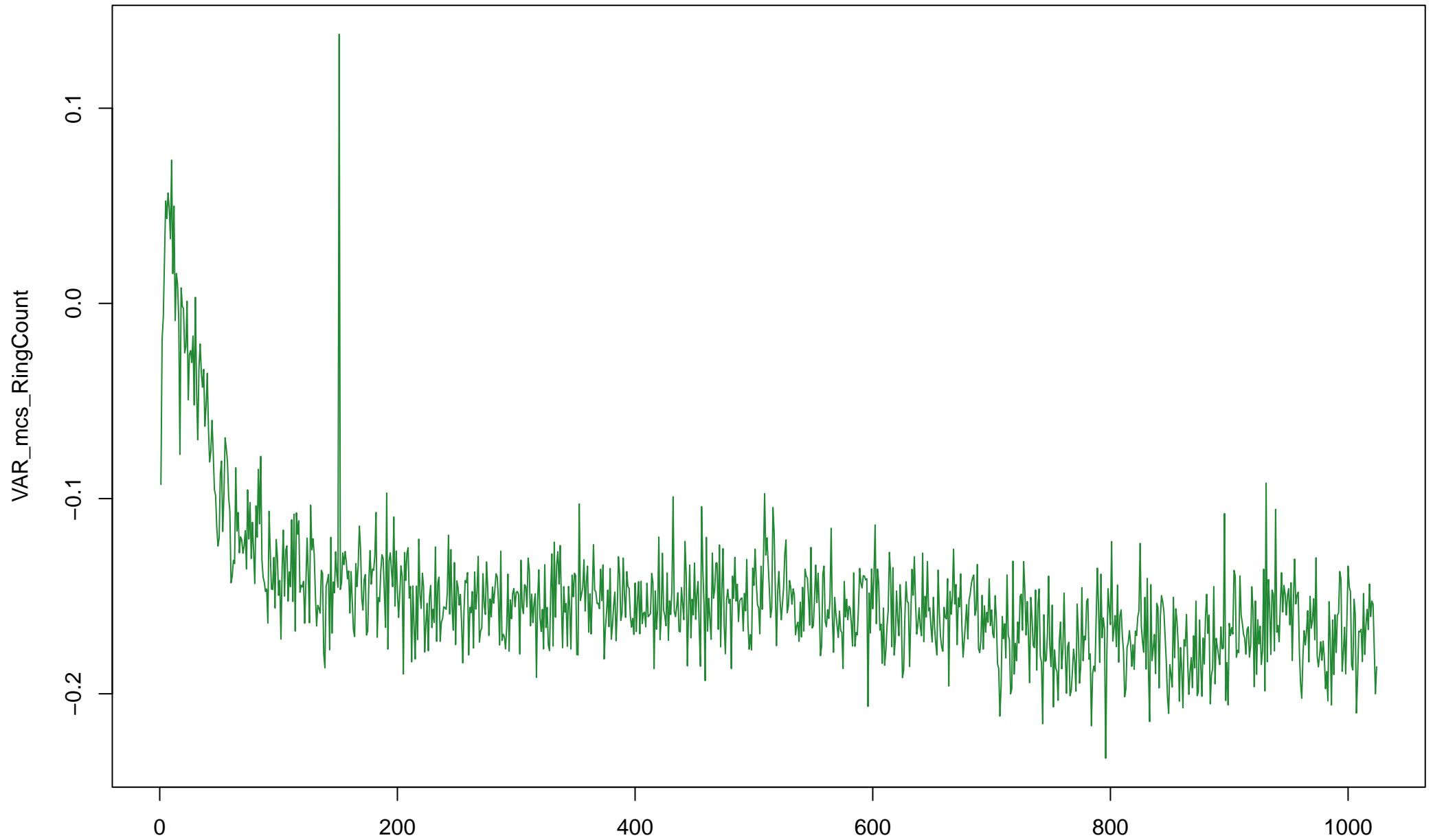
VAR_mcs_NumHeteroAtoms
ESS = 5.99 | BMK = 0.379 | MCSE(6.27) = 17.2 | stat: FALSE | burn: 102



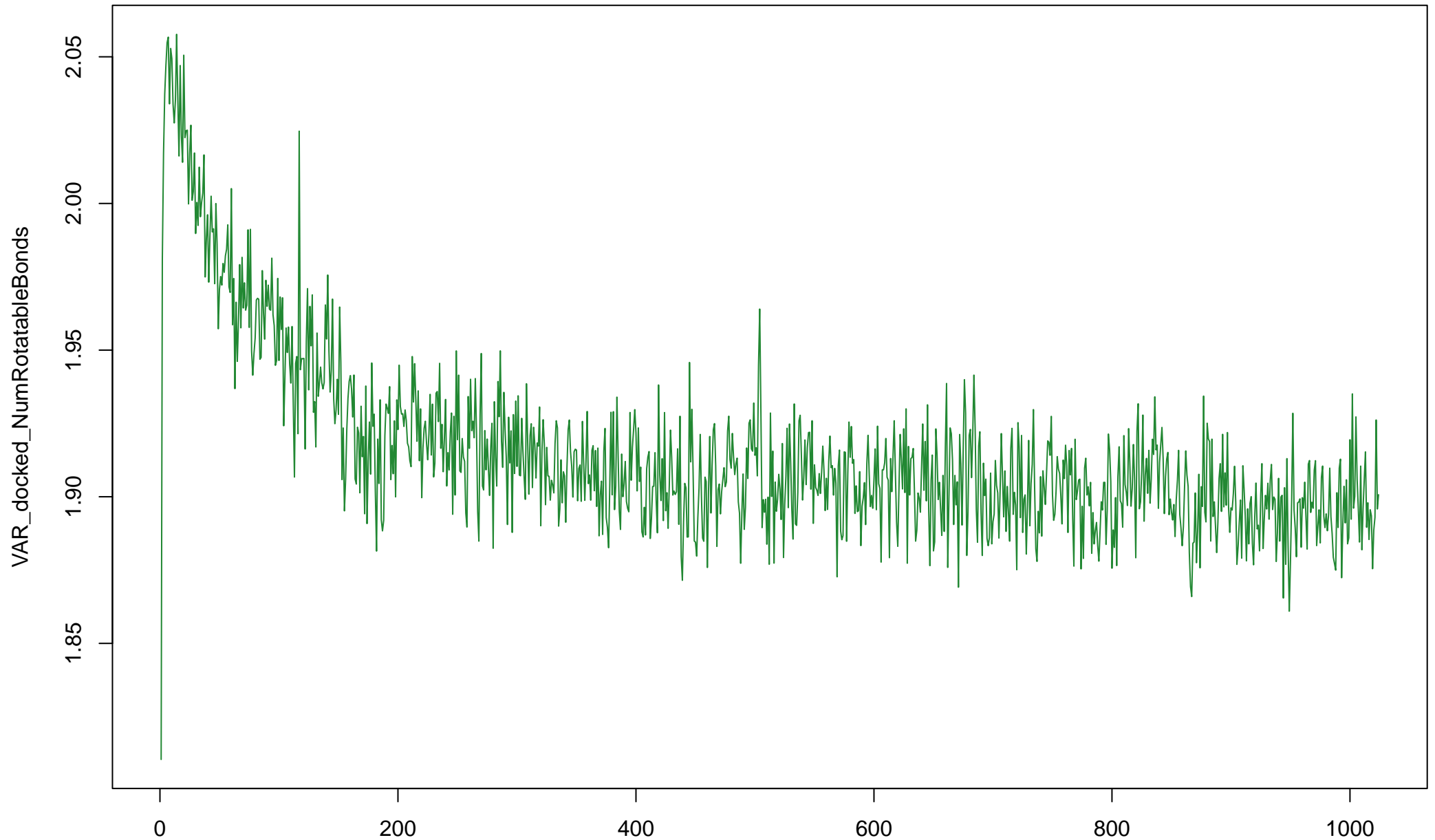
VAR_docked_HeavyAtomCount
ESS = 26.2 | BMK = 0.319 | MCSE(6.27) = 10.5 | stat: FALSE | burn: 0



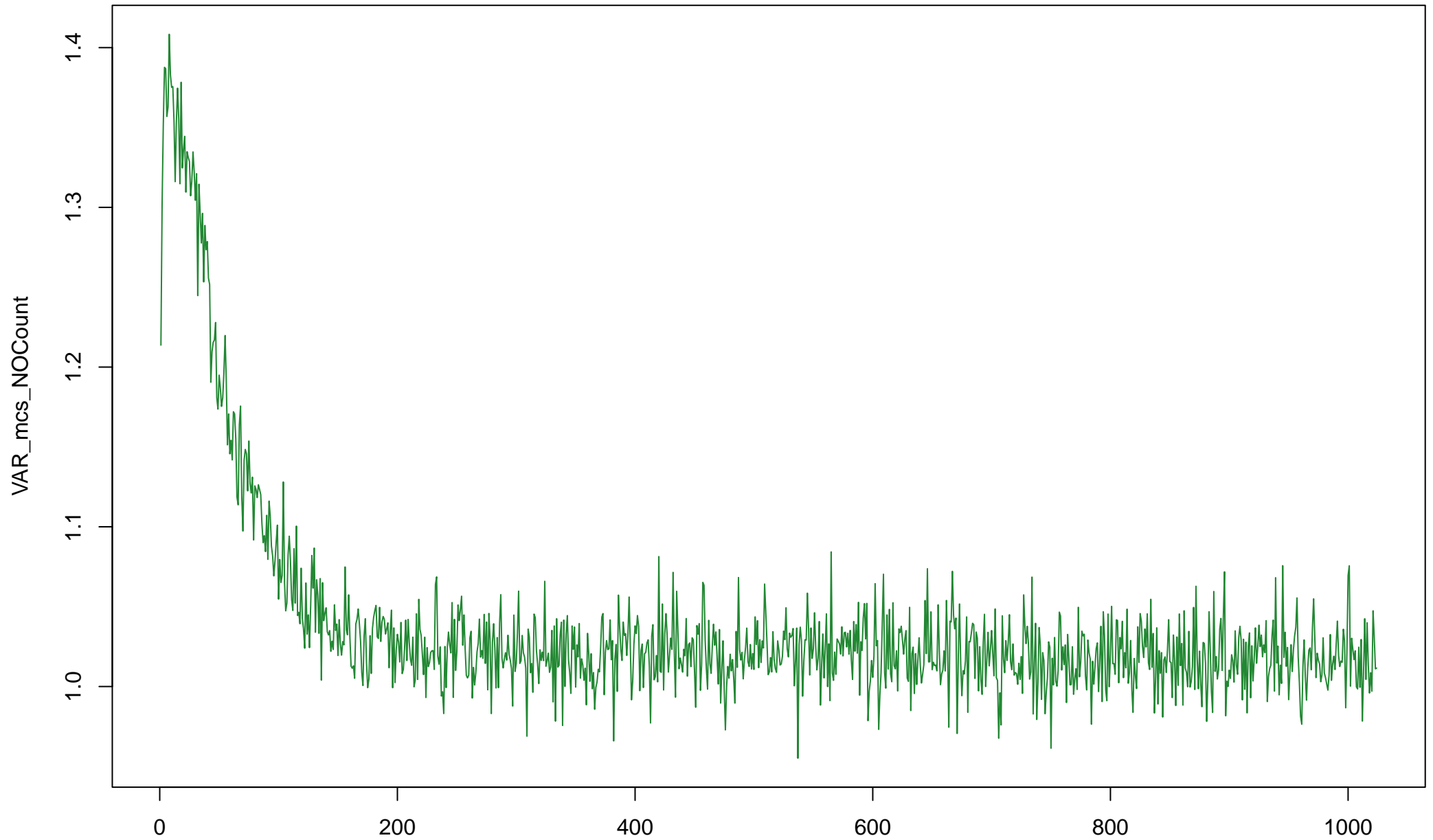
VAR_mcs_RingCount
ESS = 20.2 | BMK = 0.384 | MCSE(6.27) = 14.9 | stat: FALSE | burn: 102



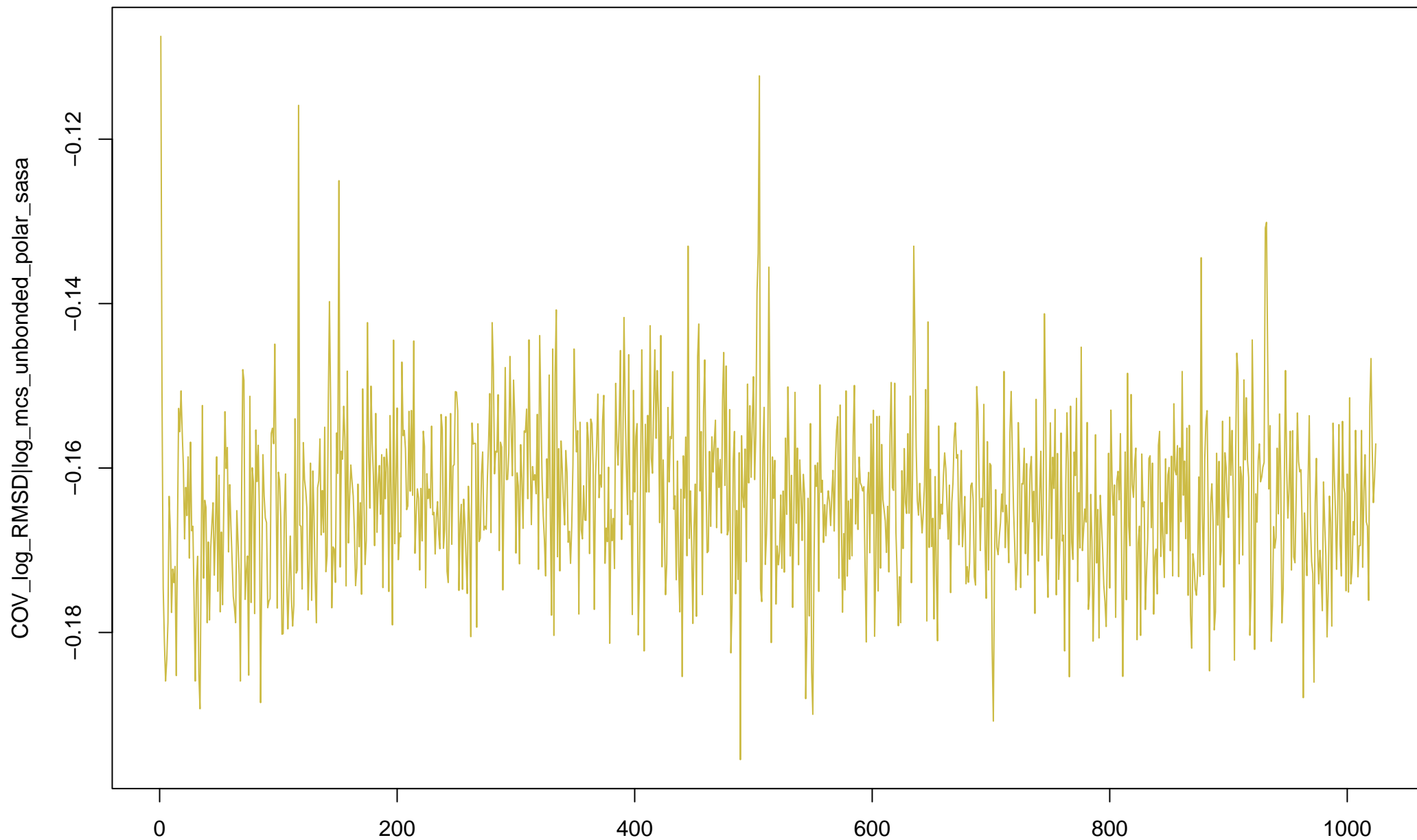
VAR_docked_NumRotatableBonds
ESS = 10.6 | BMK = 0.44 | MCSE(6.27) = 15.5 | stat: FALSE | burn: 102



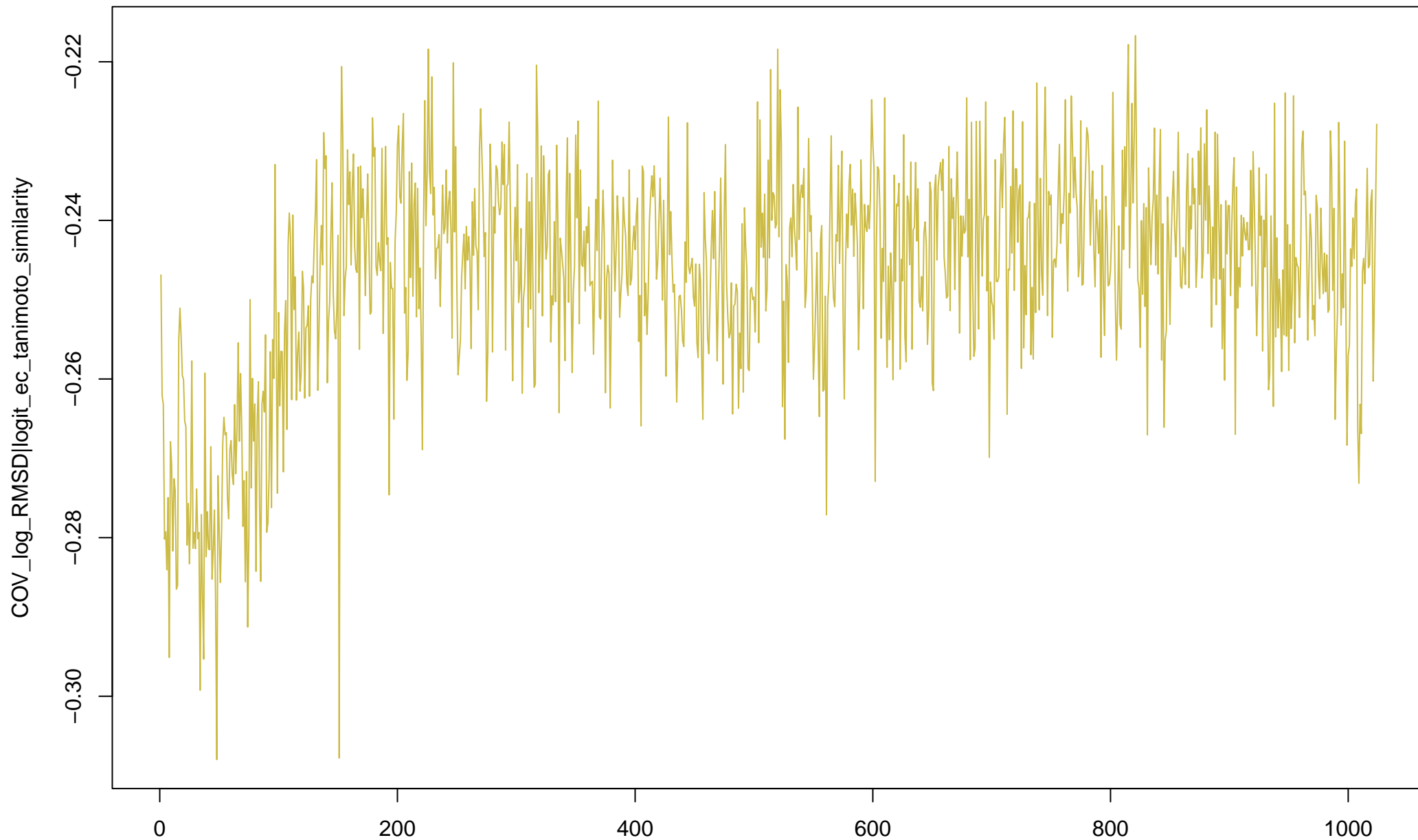
VAR_mcs_NOCount
ESS = 8.21 | BMK = 0.336 | MCSE(6.27) = 17.1 | stat: FALSE | burn: 102



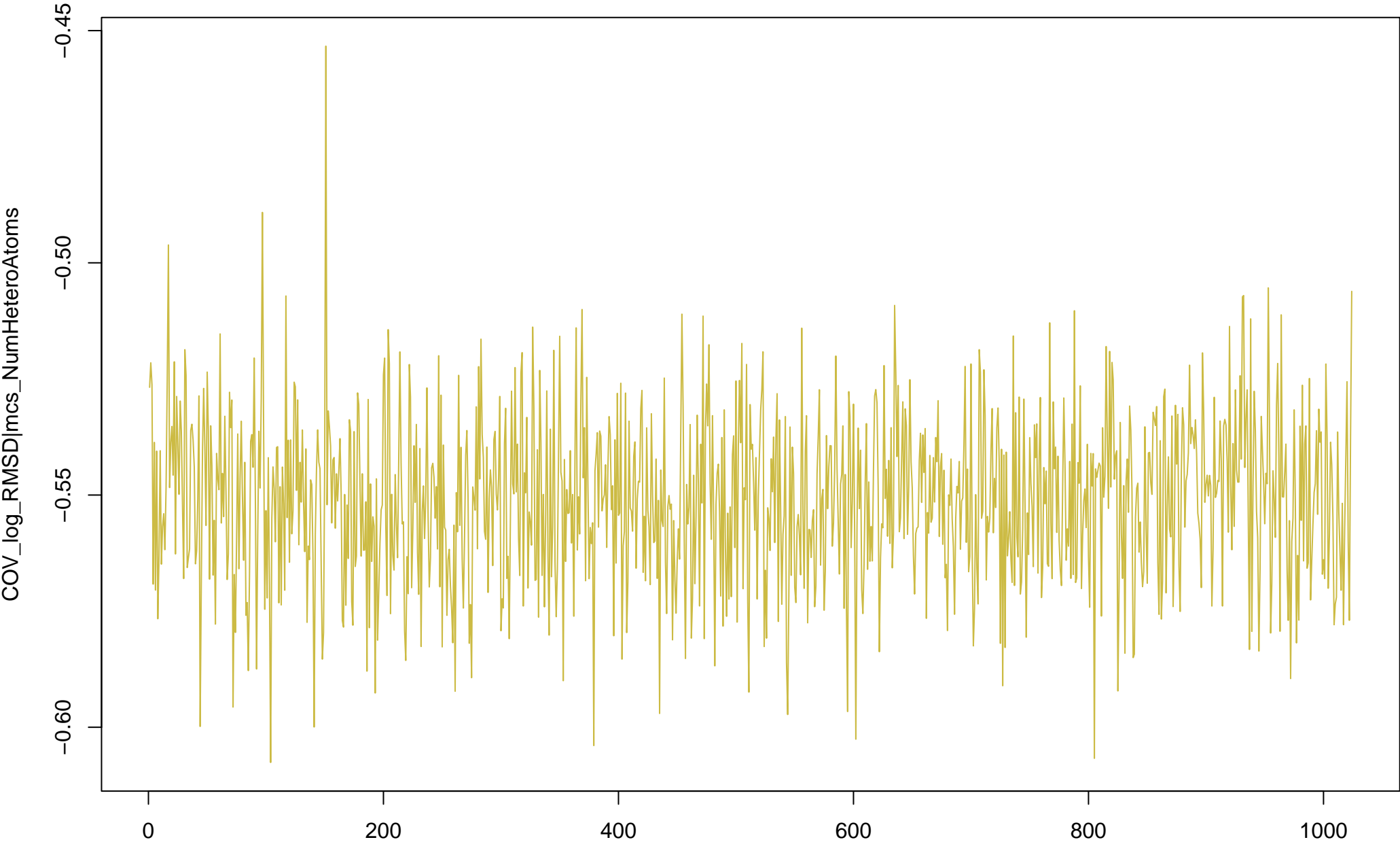
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 548 | BMK = 0.103 | MCSE(6.27) = 4.78 | stat: TRUE | burn: 0



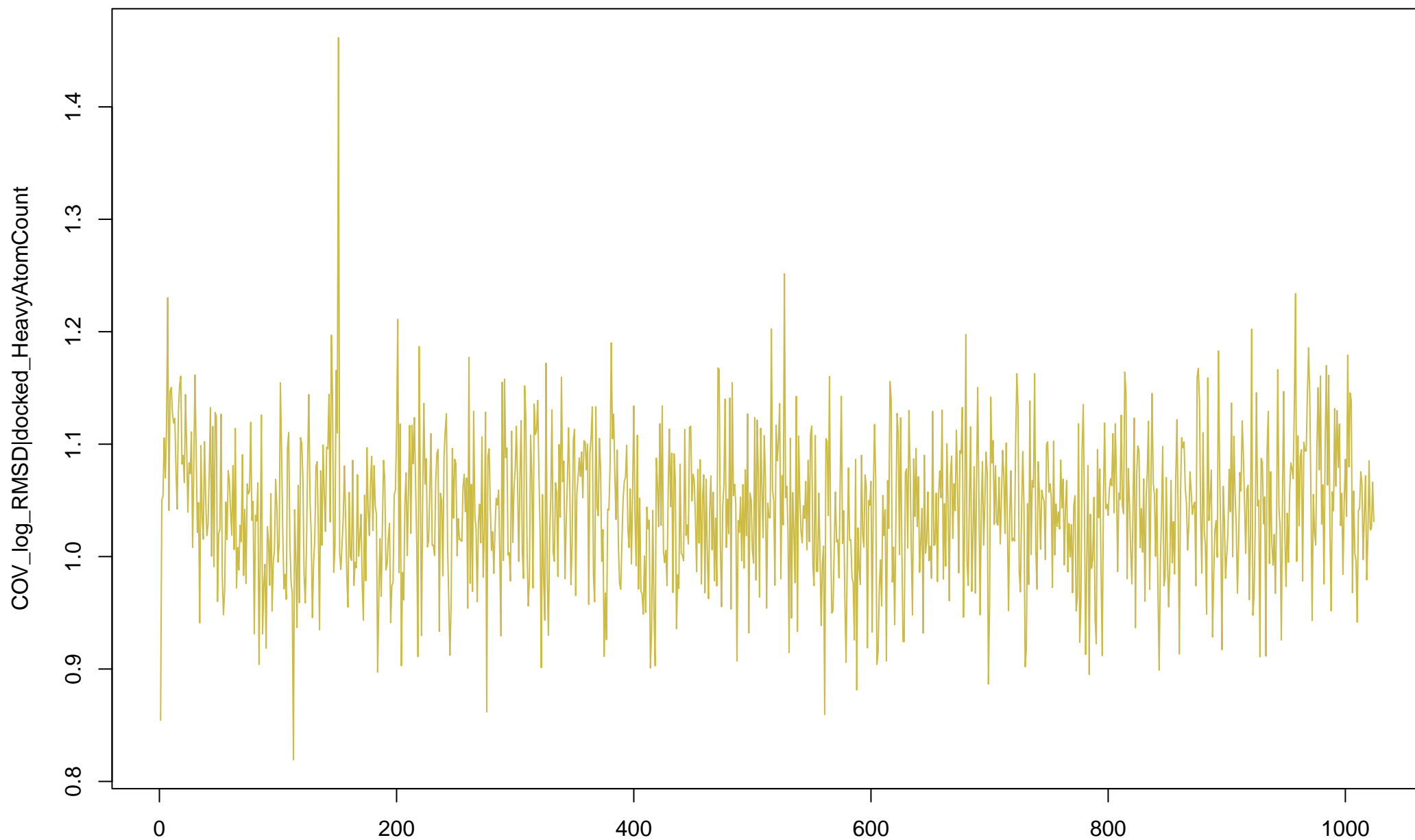
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 15.6 | BMK = 0.237 | MCSE(6.27) = 12.3 | stat: FALSE | burn: 102



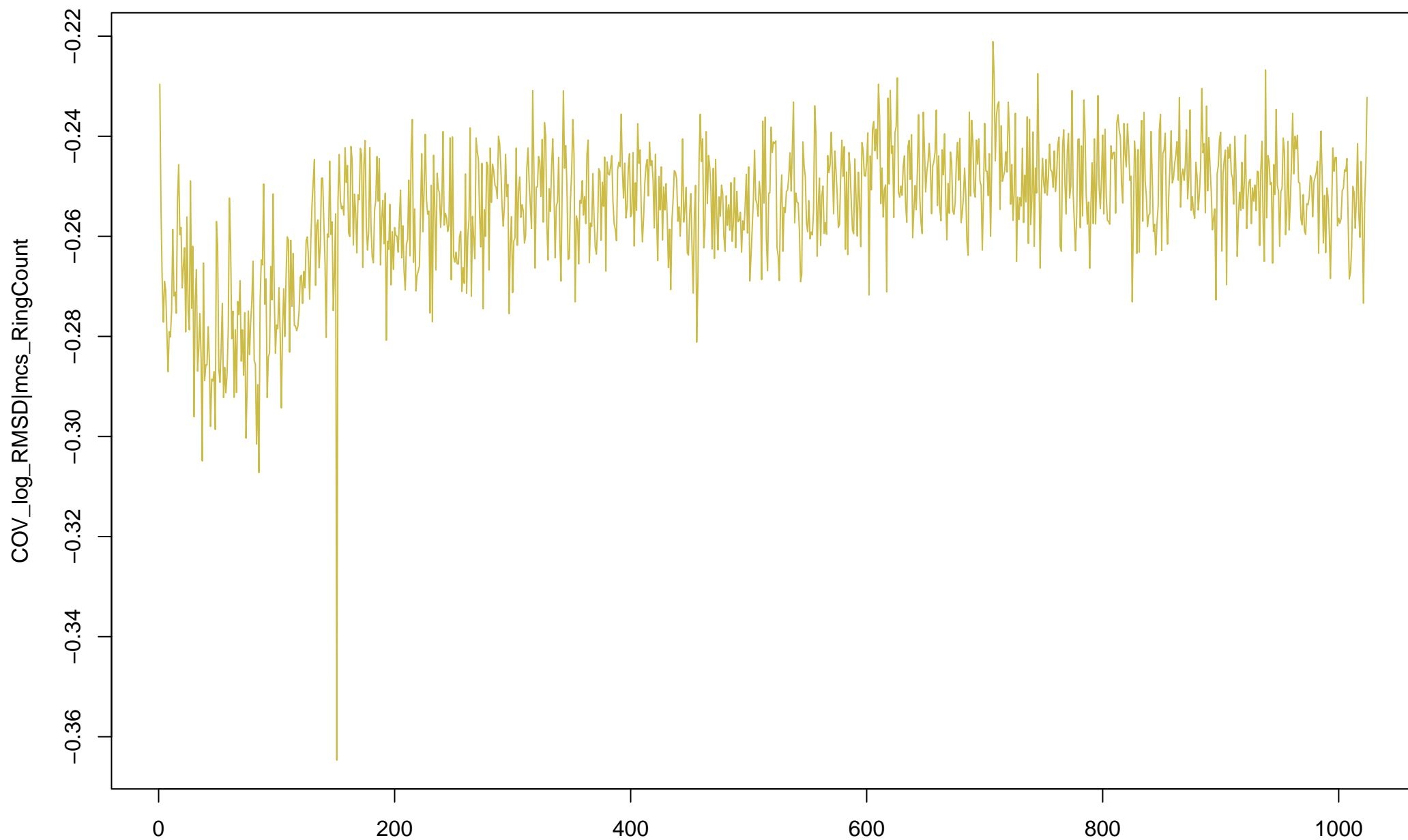
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 998 | BMK = 0.0644 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0



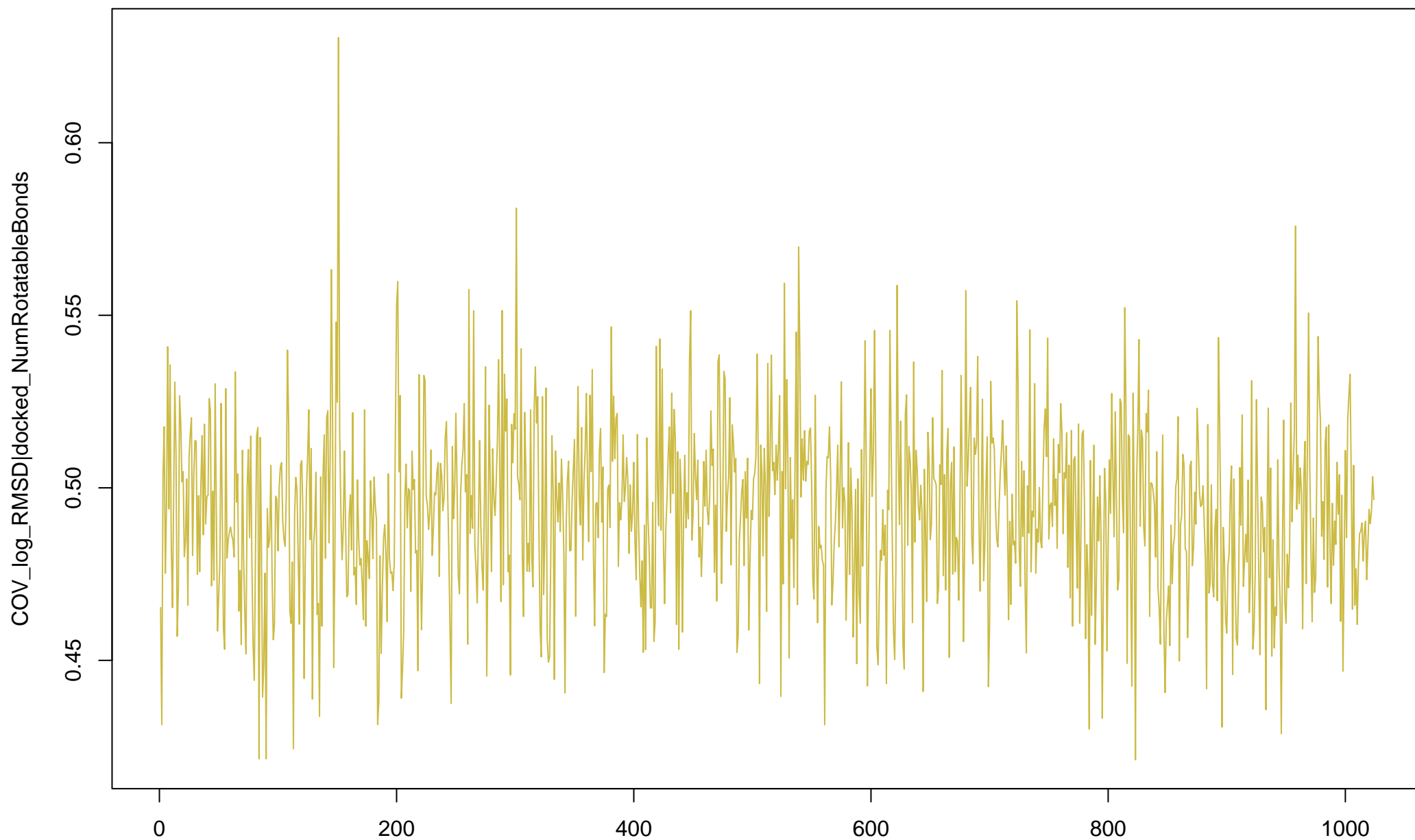
COV_log_RMSD|docked_HeavyAtomCount
ESS = 888 | BMK = 0.0631 | MCSE(6.27) = 4.81 | stat: TRUE | burn: 0



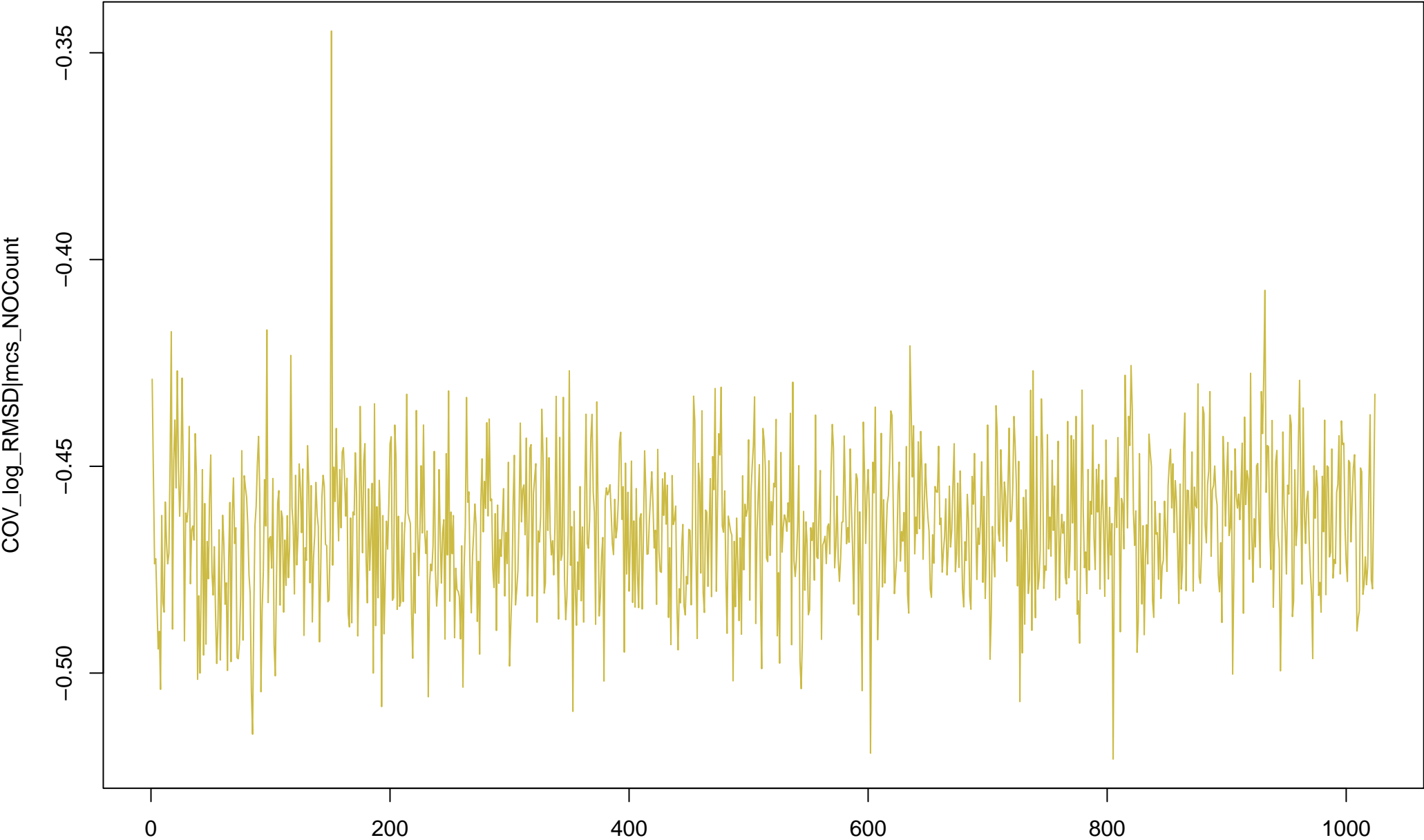
COV_log_RMSD|mcs_RingCount
ESS = 10.9 | BMK = 0.348 | MCSE(6.27) = 12.2 | stat: FALSE | burn: 0



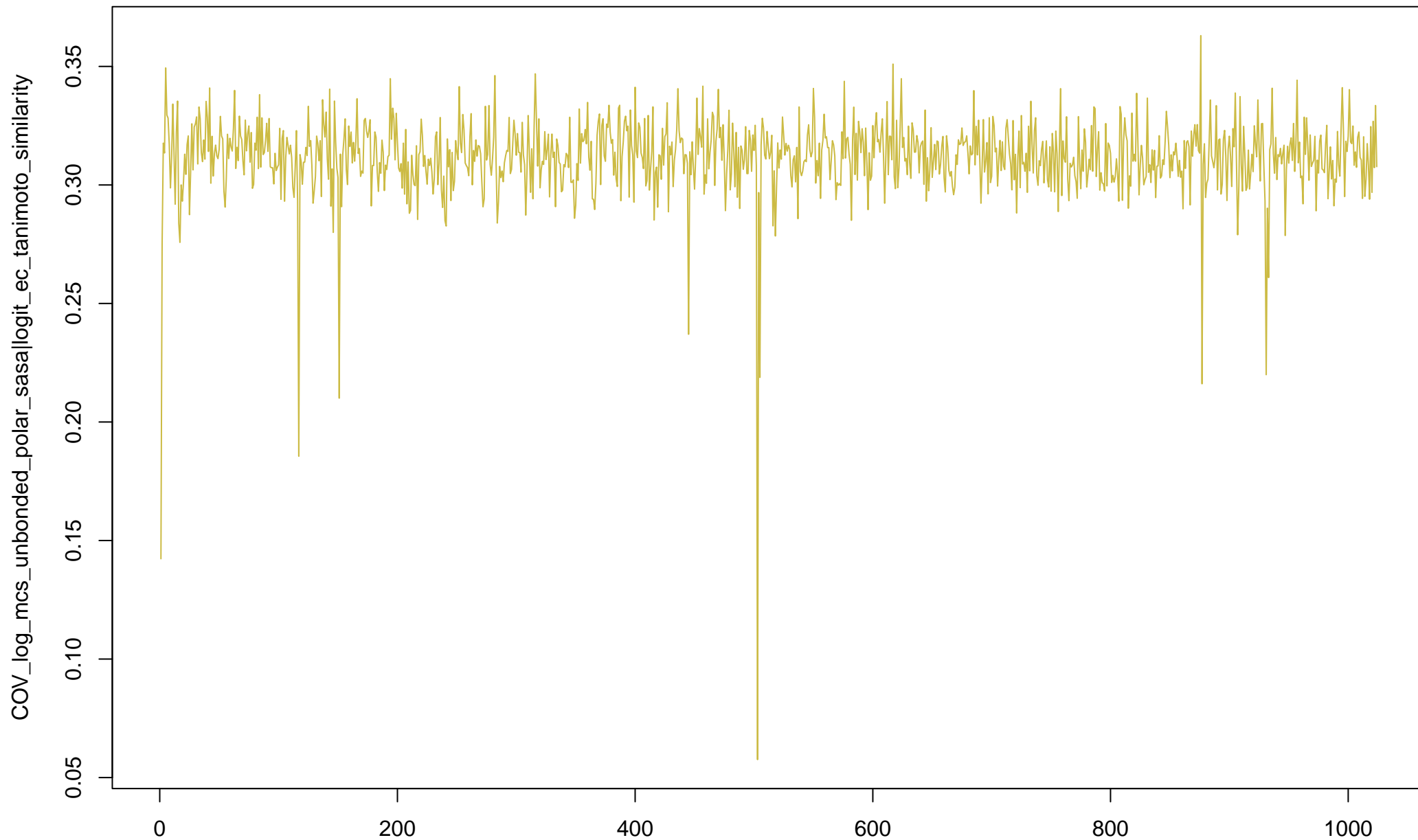
COV_log_RMSD|docked_NumRotatableBonds
ESS = 778 | BMK = 0.0393 | MCSE(6.27) = 4.84 | stat: TRUE | burn: 0



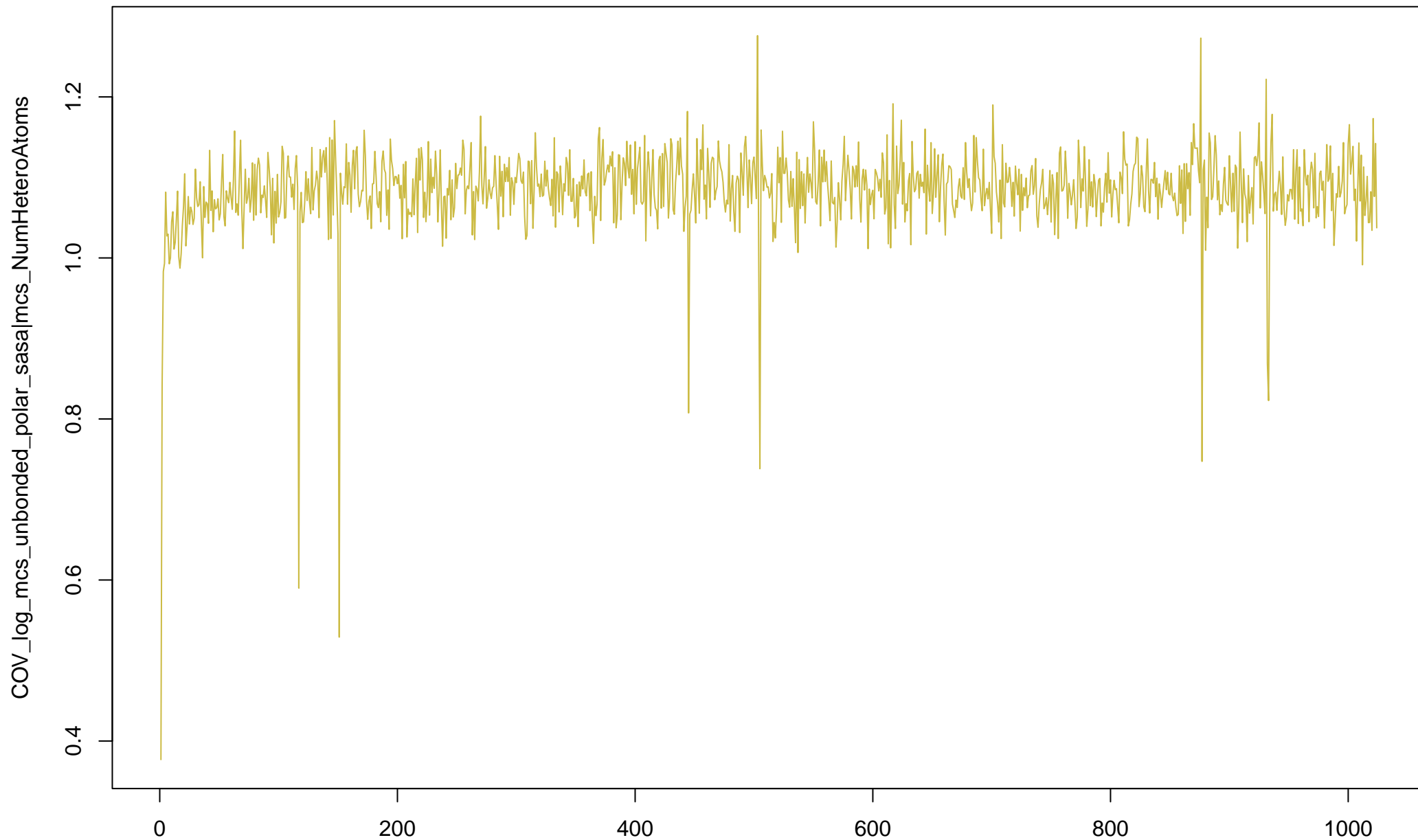
COV_log_RMSD|mcs_NOCount
ESS = 851 | BMK = 0.112 | MCSE(6.27) = 4.04 | stat: FALSE | burn: 0



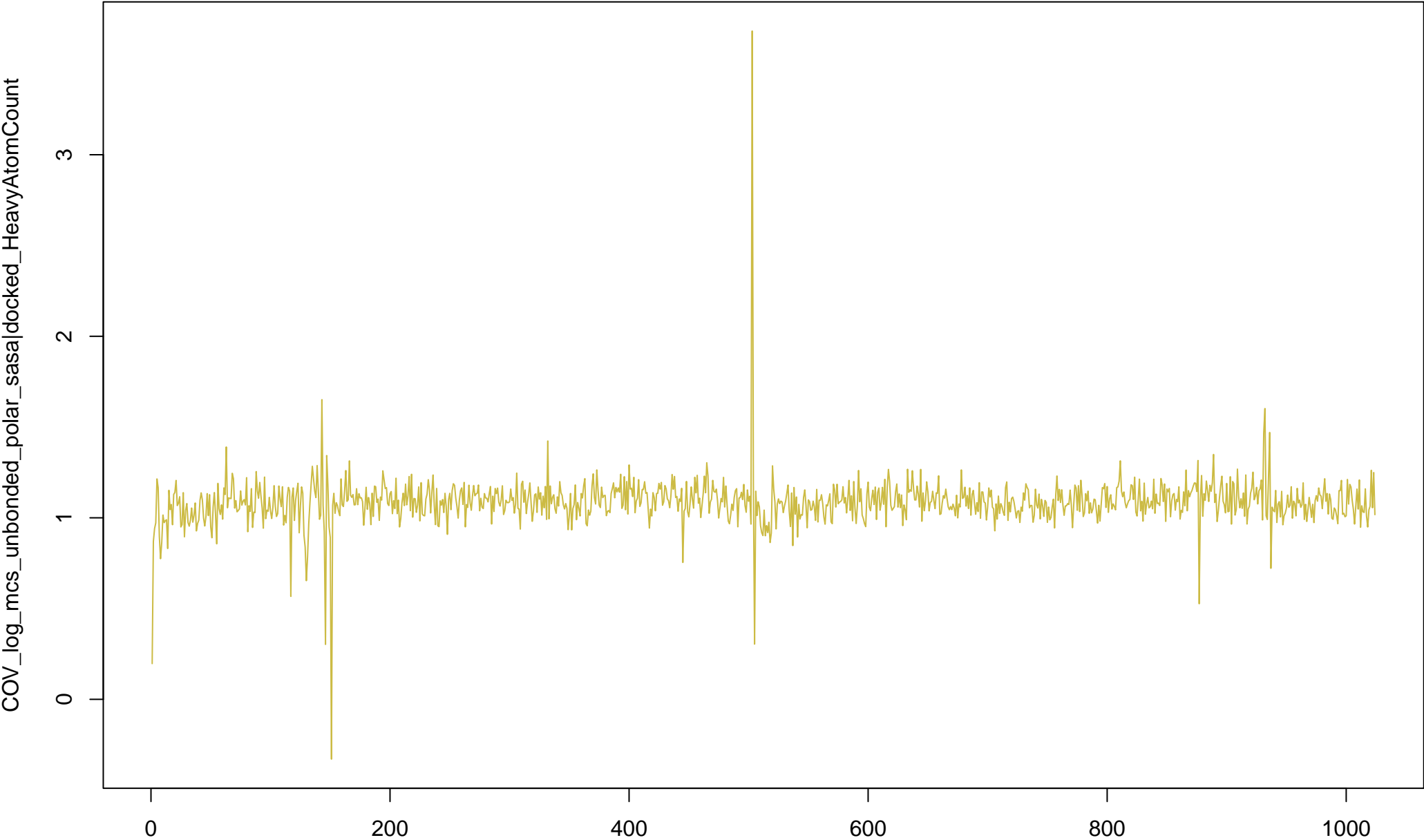
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 746 | BMK = 0.102 | MCSE(6.27) = 3.48 | stat: TRUE | burn: 0



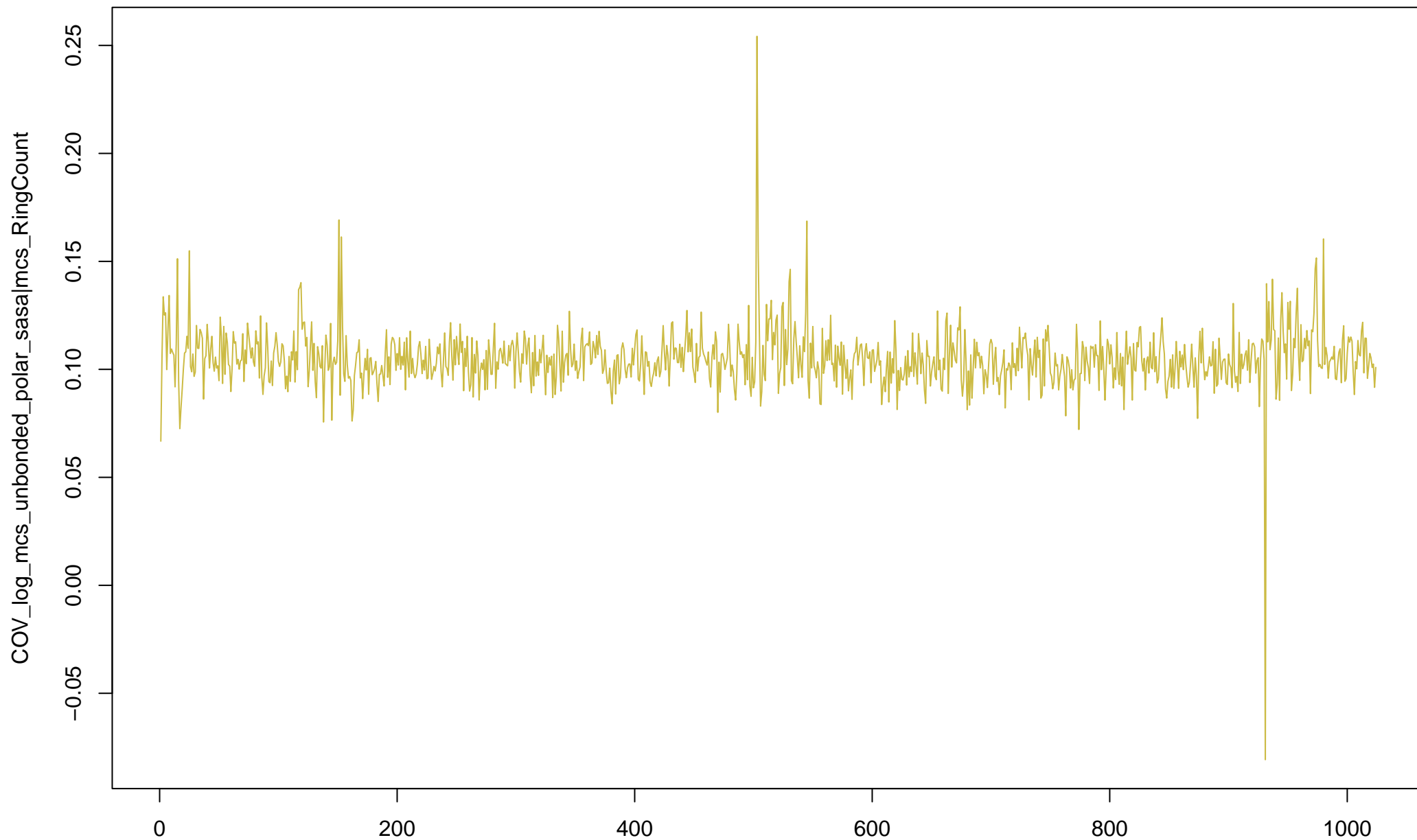
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 885 | BMK = 0.0937 | MCSE(6.27) = 4.95 | stat: FALSE | burn: 0



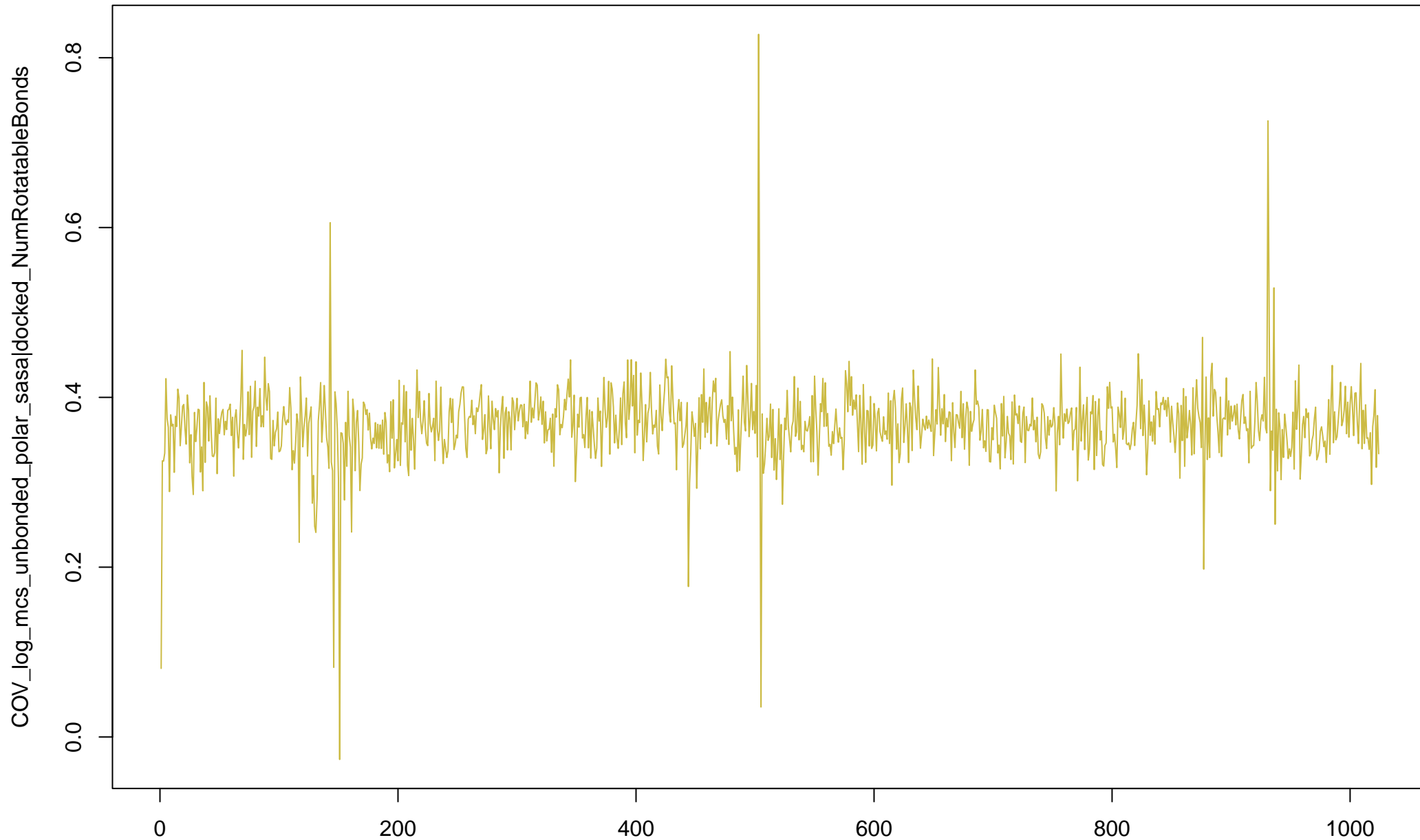
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 796 | BMK = 0.121 | MCSE(6.27) = 4.05 | stat: FALSE | burn: 0



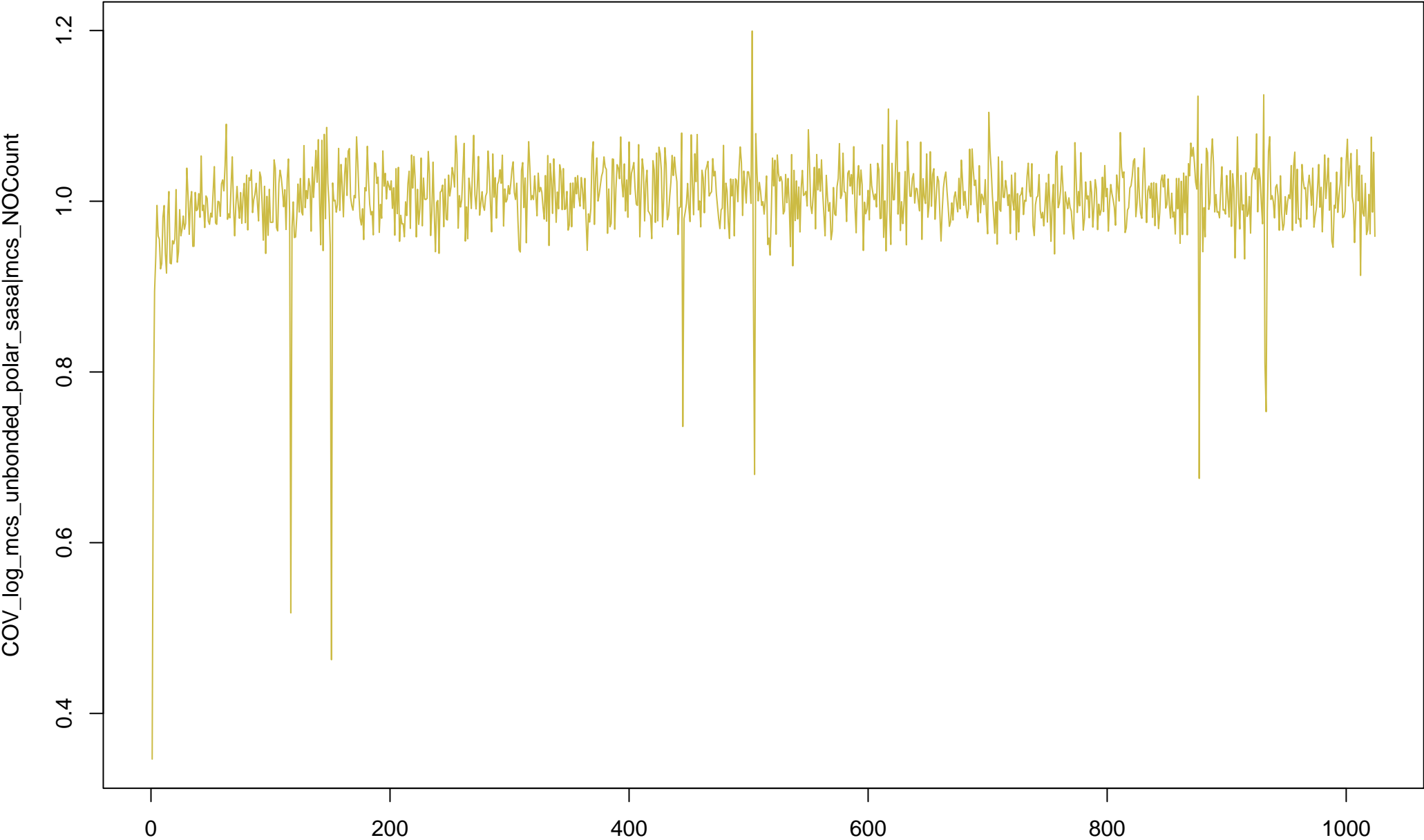
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 797 | BMK = 0.0759 | MCSE(6.27) = 4.06 | stat: TRUE | burn: 0



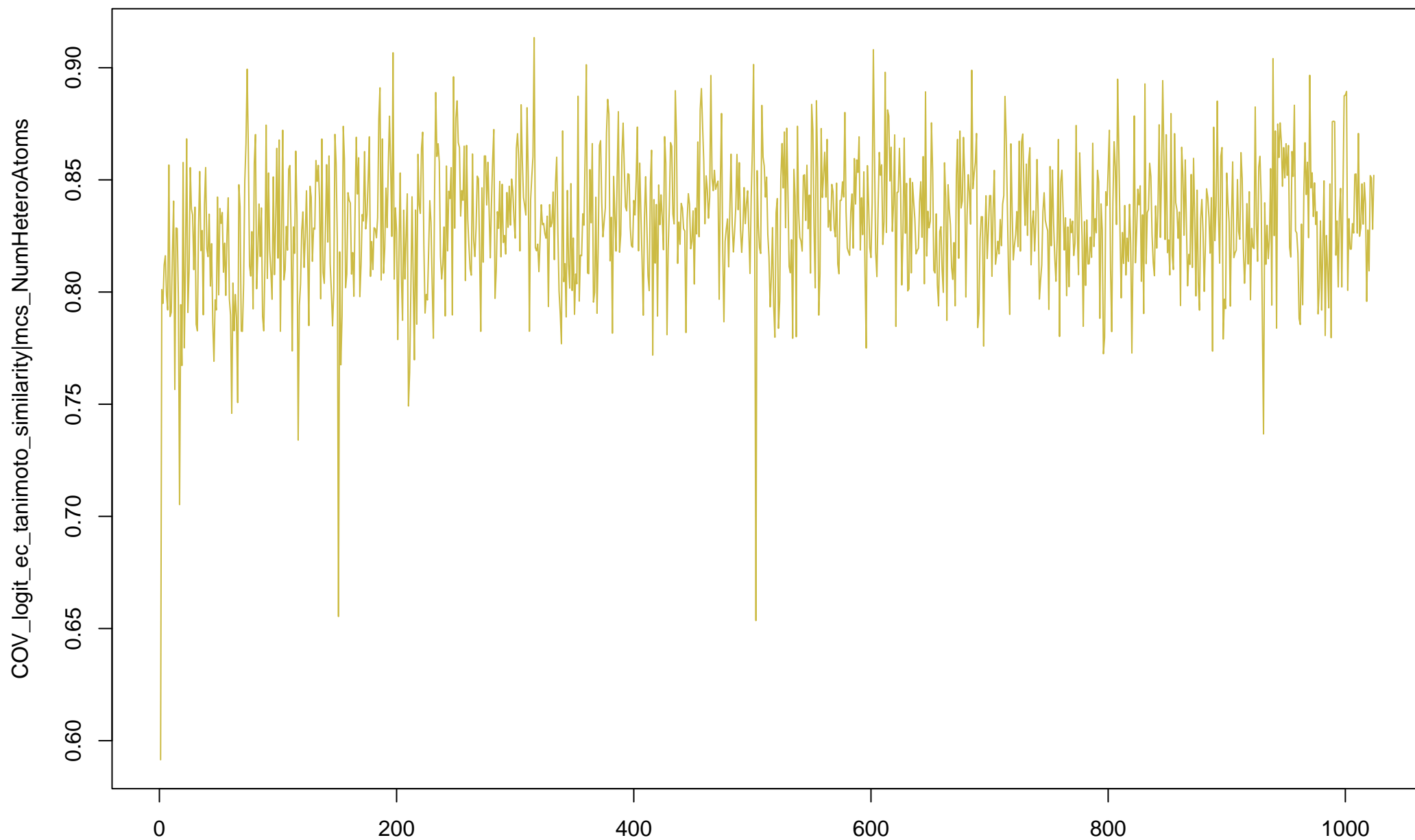
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 584 | BMK = 0.117 | MCSE(6.27) = 3.85 | stat: TRUE | burn: 0



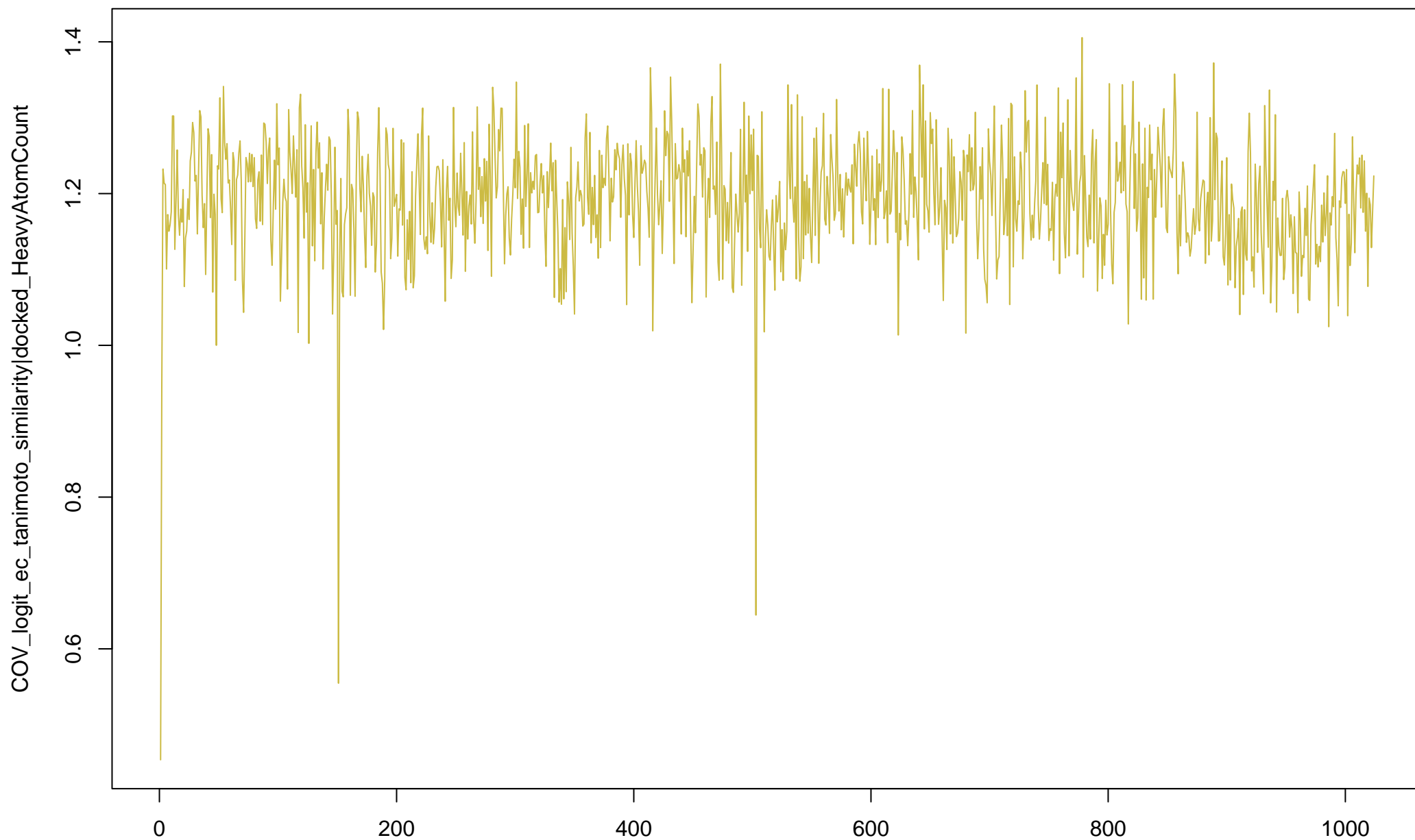
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 834 | BMK = 0.105 | MCSE(6.27) = 4.99 | stat: FALSE | burn: 0



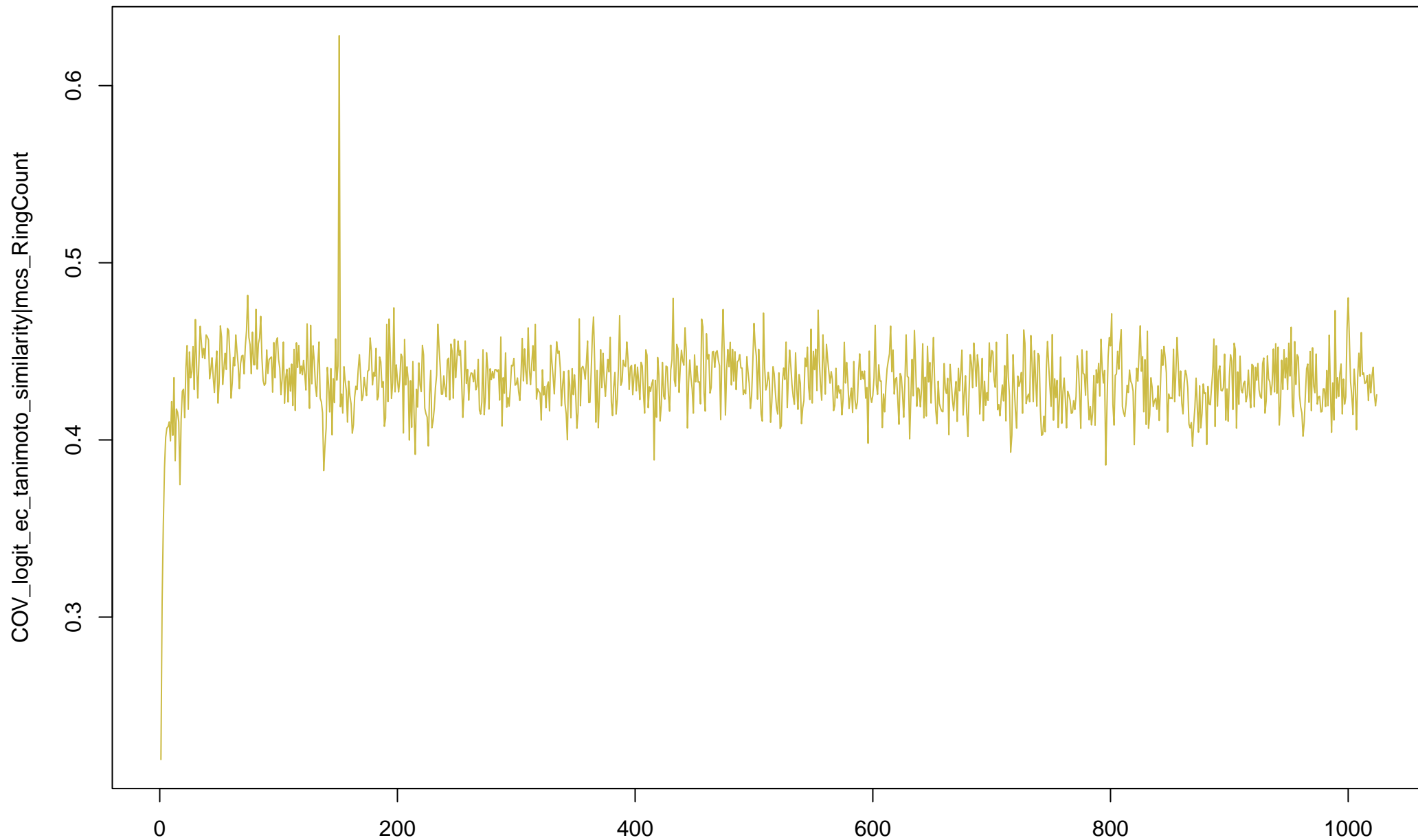
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 526 | BMK = 0.0915 | MCSE(6.27) = 5.23 | stat: FALSE | burn: 0



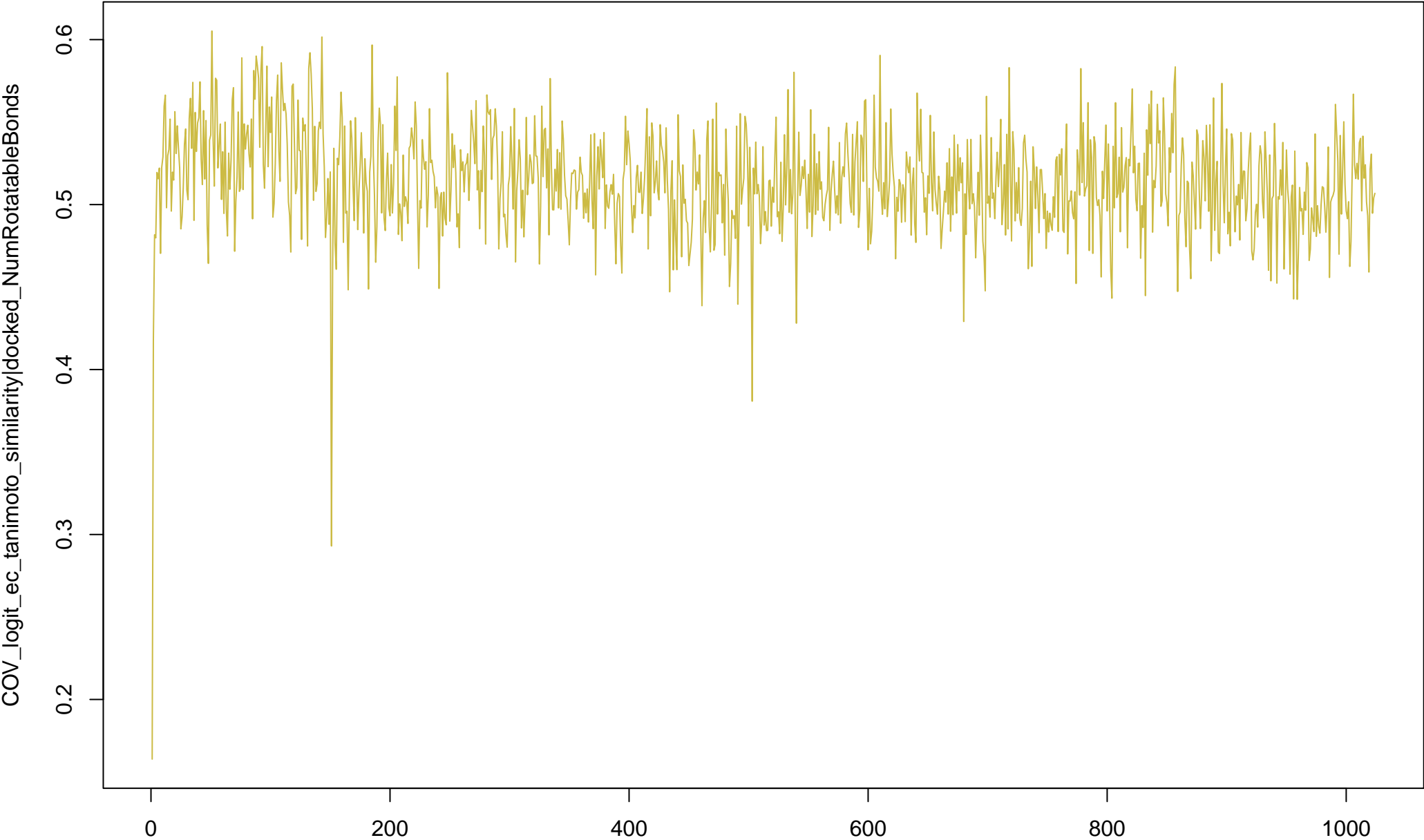
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 816 | BMK = 0.104 | MCSE(6.27) = 4.61 | stat: TRUE | burn: 0



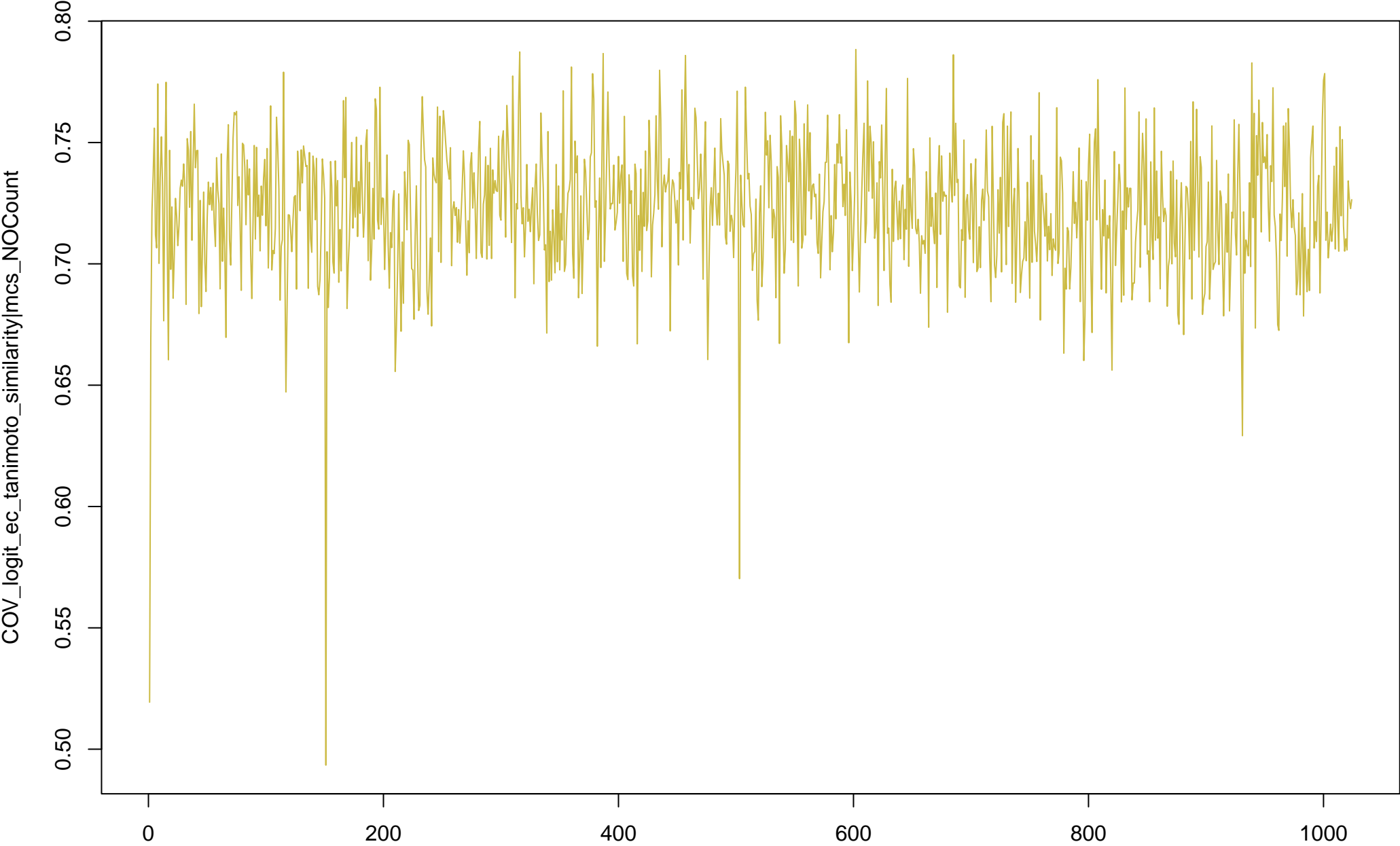
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 246 | BMK = 0.138 | MCSE(6.27) = 6.32 | stat: TRUE | burn: 0



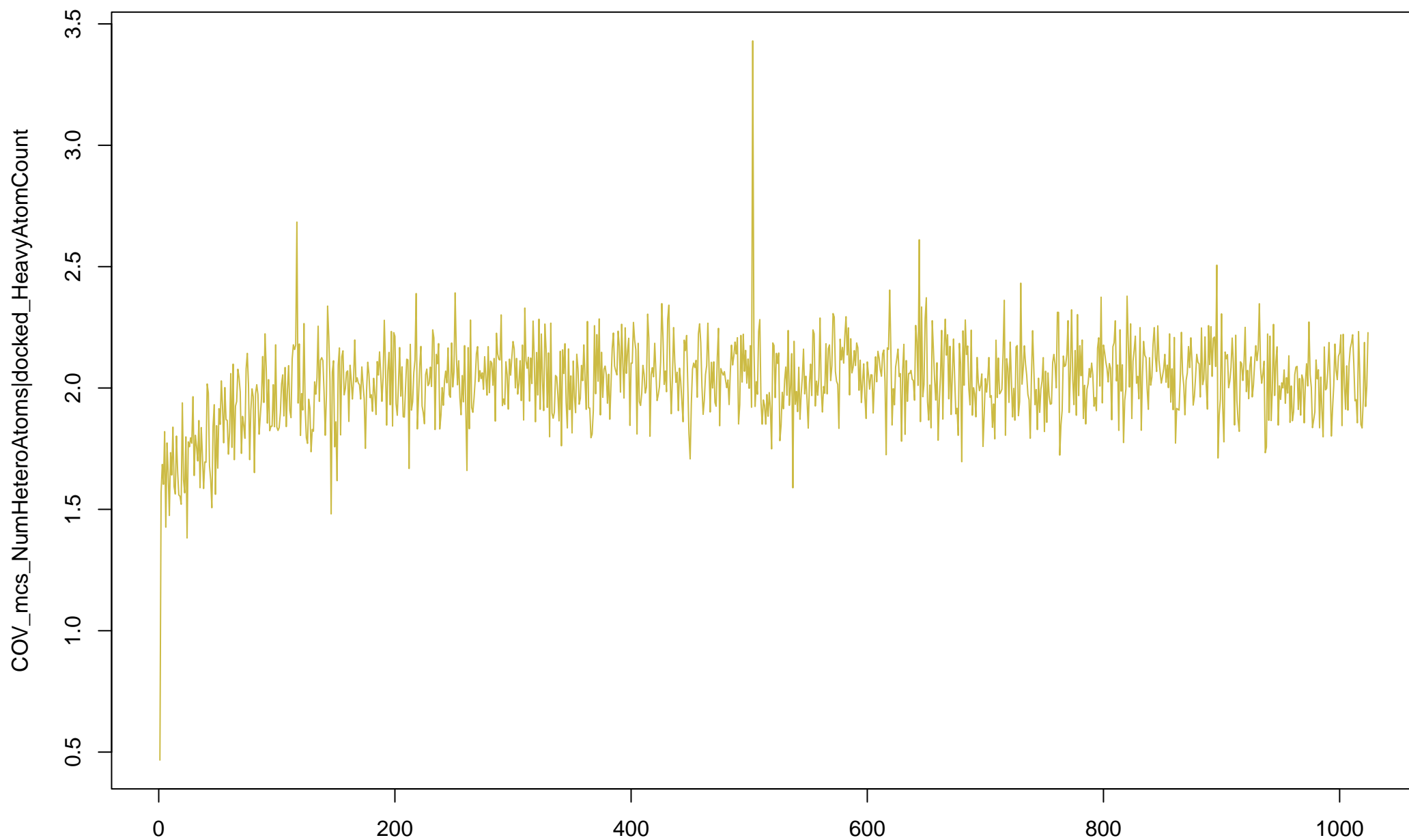
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 226 | BMK = 0.135 | MCSE(6.27) = 5.58 | stat: FALSE | burn: 0



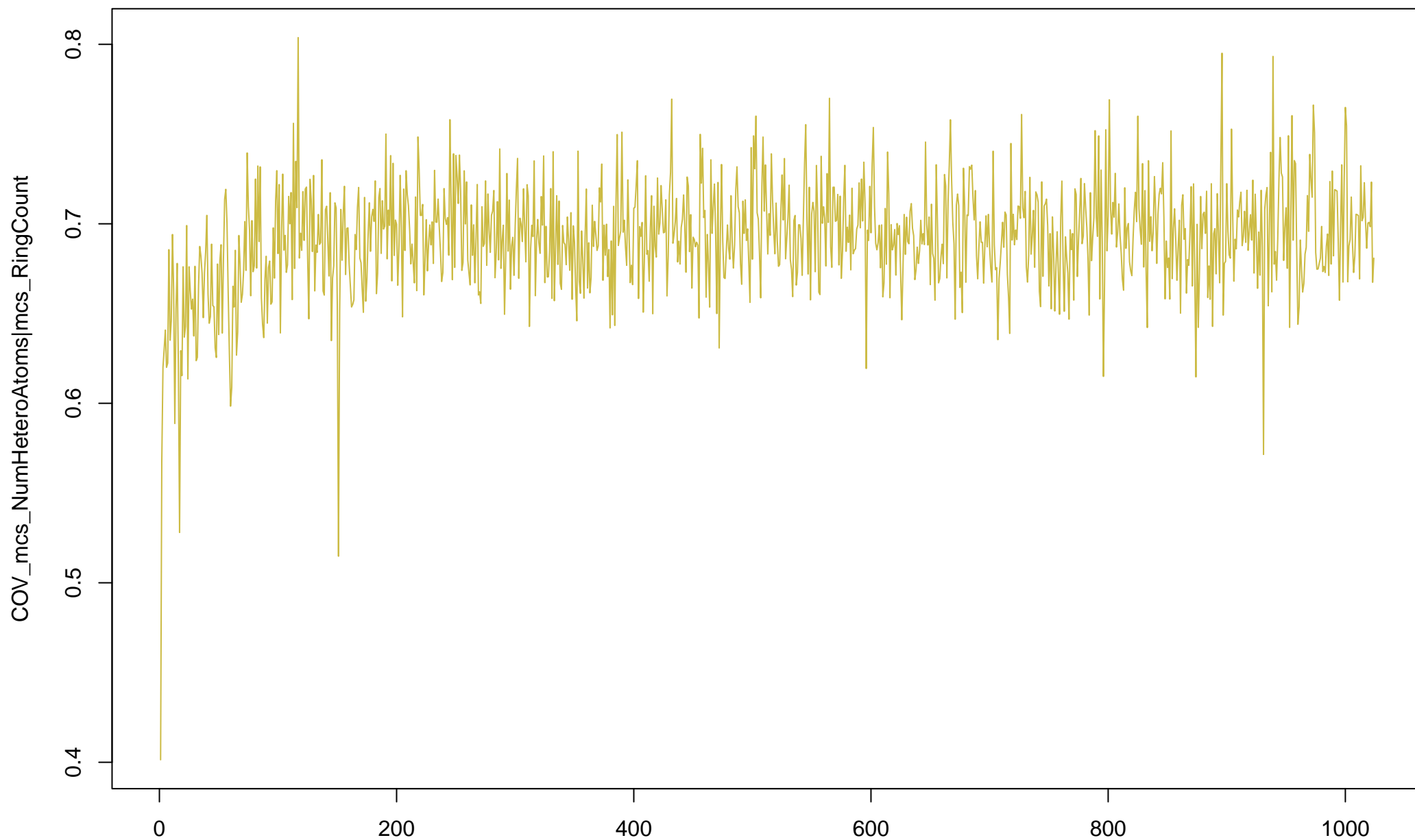
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 804 | BMK = 0.0946 | MCSE(6.27) = 3.74 | stat: TRUE | burn: 0



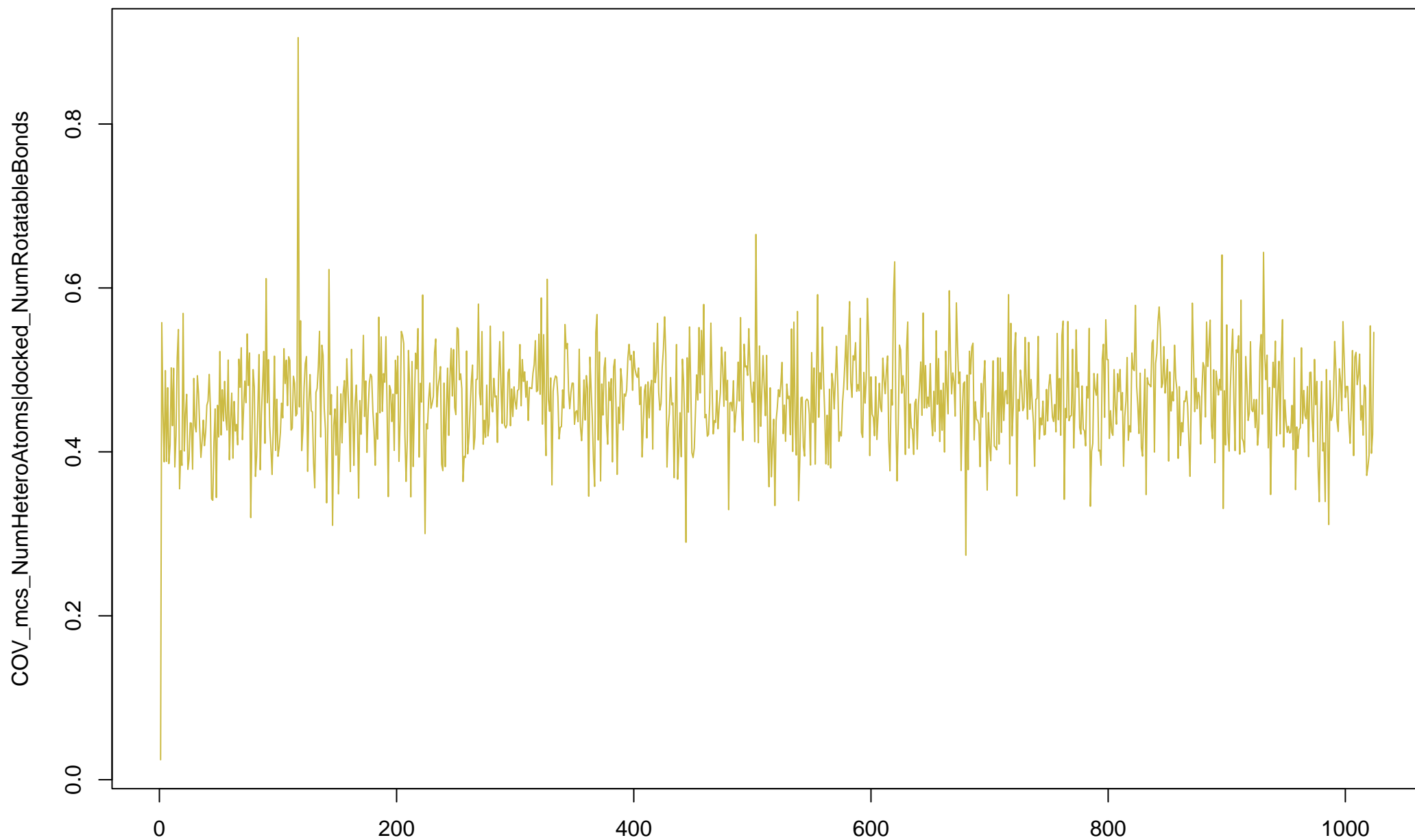
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 76.3 | BMK = 0.159 | MCSE(6.27) = 9.17 | stat: FALSE | burn: 0



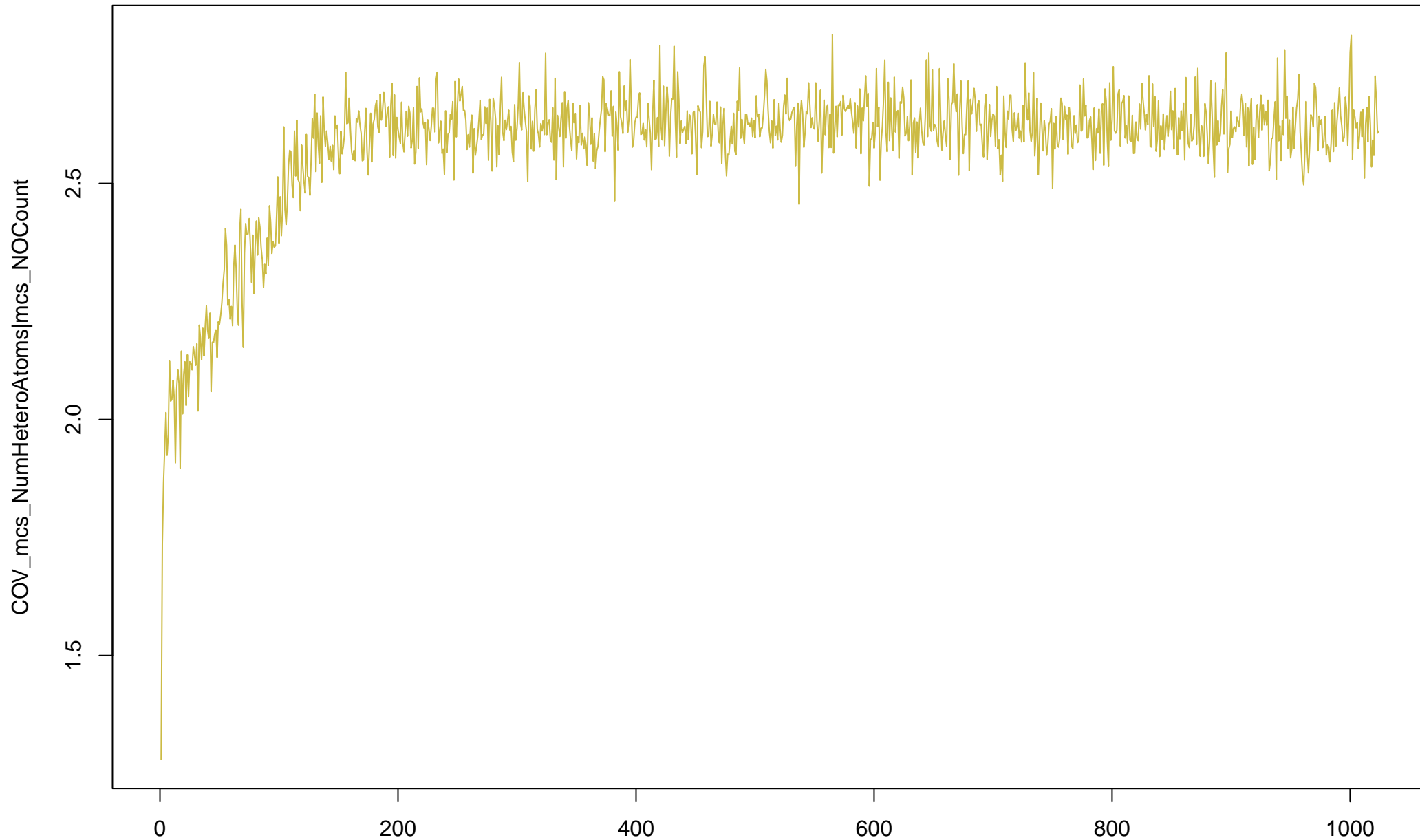
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 90.1 | BMK = 0.13 | MCSE(6.27) = 7.83 | stat: FALSE | burn: 0



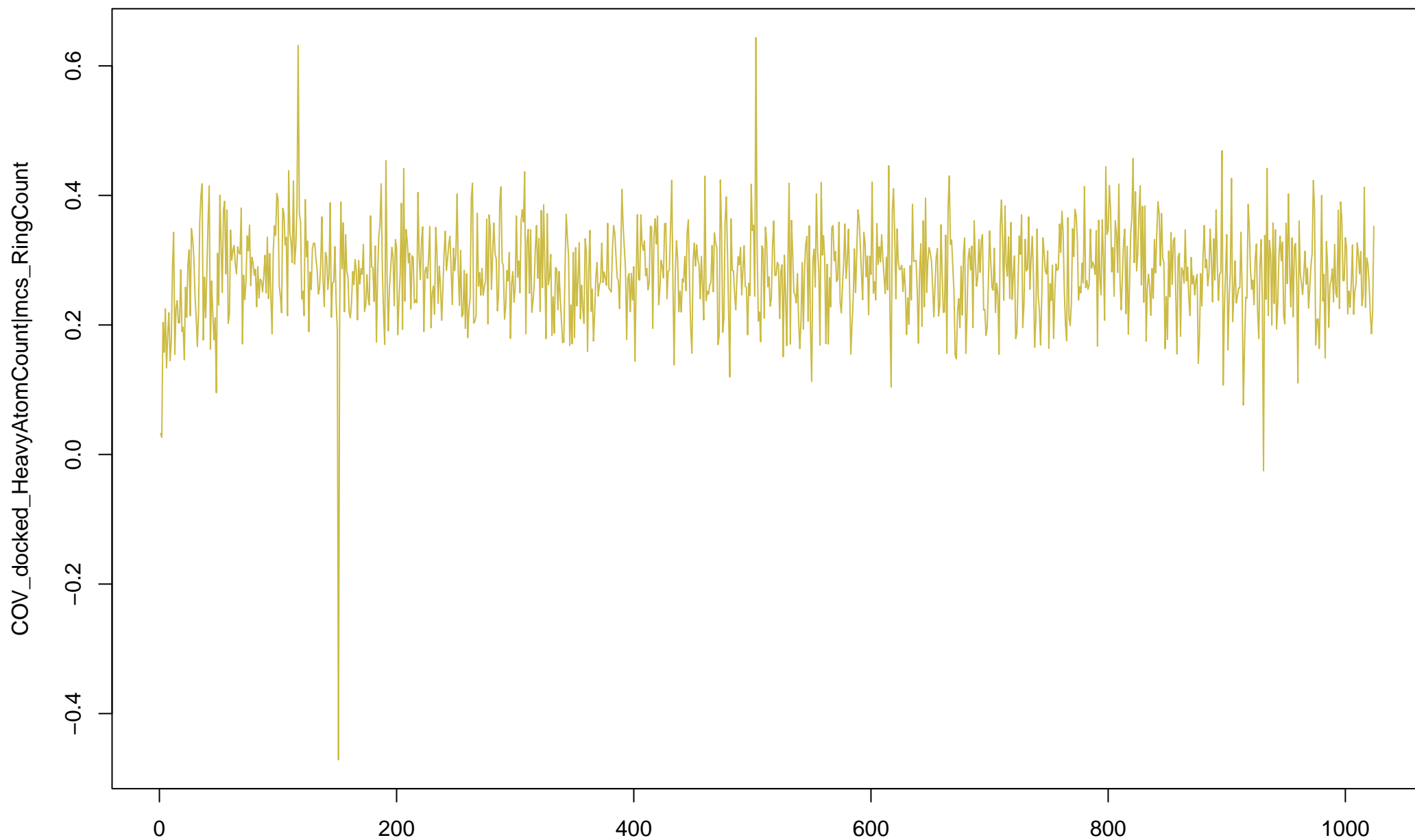
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0621 | MCSE(6.27) = 4.17 | stat: FALSE | burn: 0



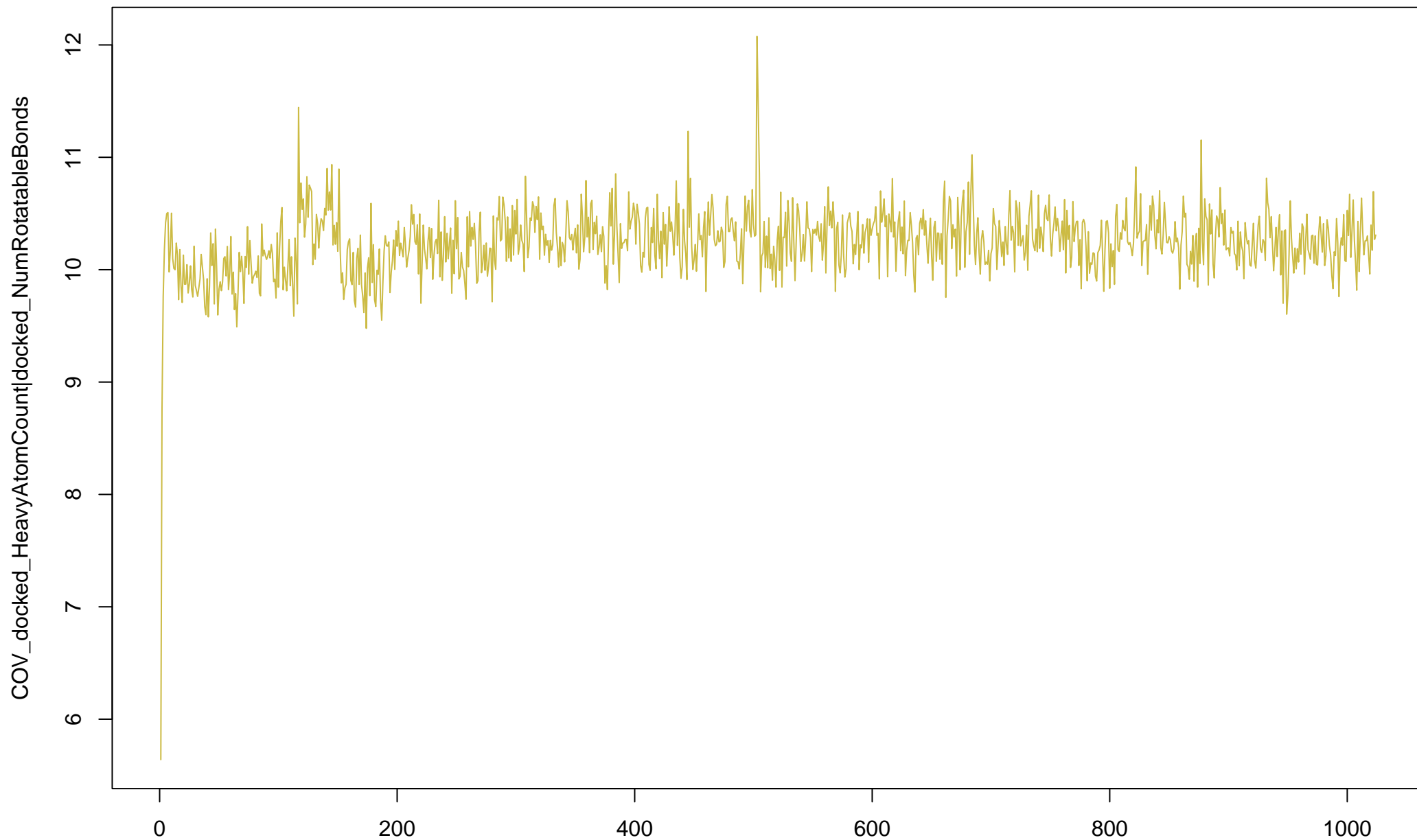
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 10 | BMK = 0.331 | MCSE(6.27) = 16.3 | stat: FALSE | burn: 102



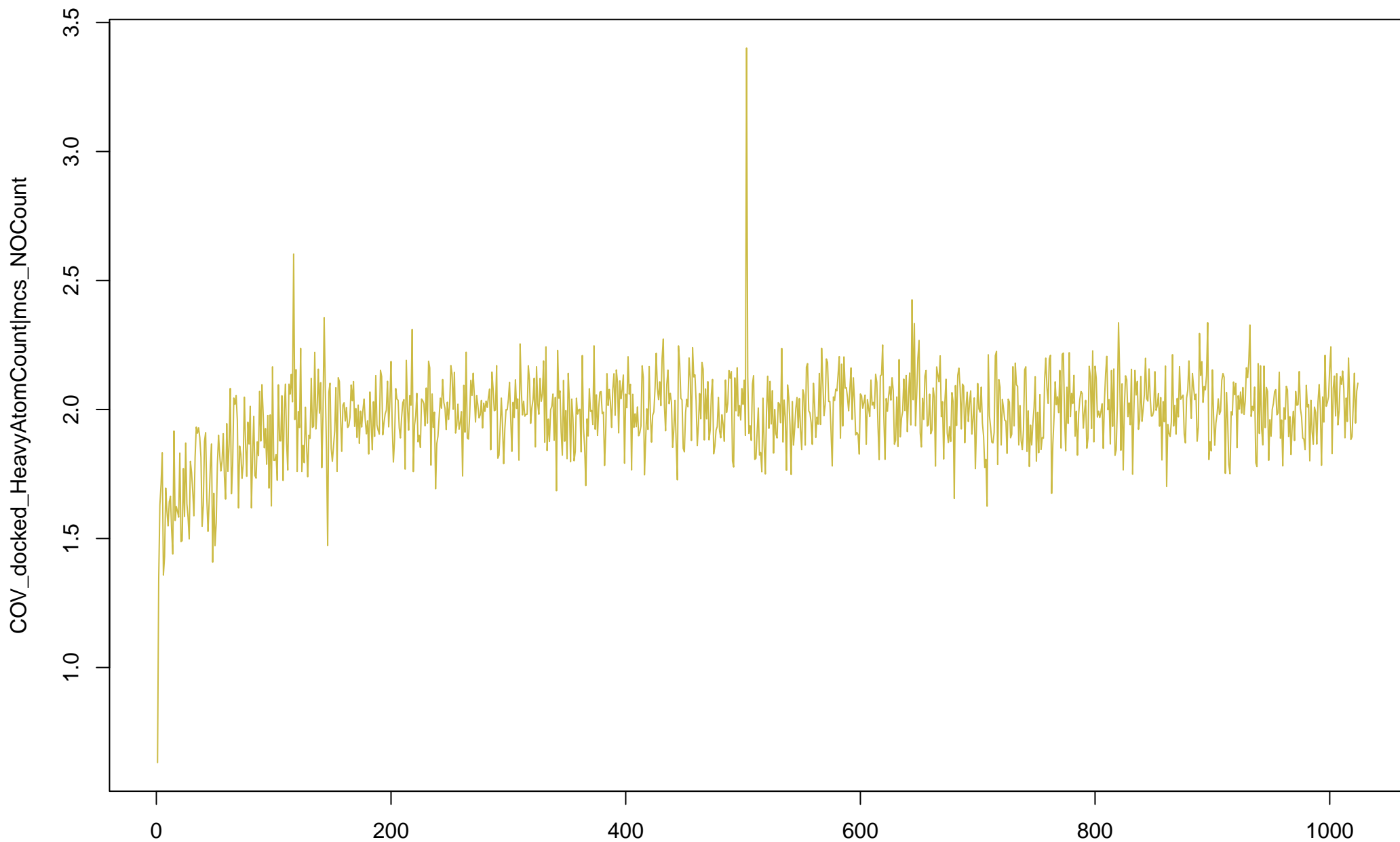
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 831 | BMK = 0.069 | MCSE(6.27) = 4.68 | stat: TRUE | burn: 0



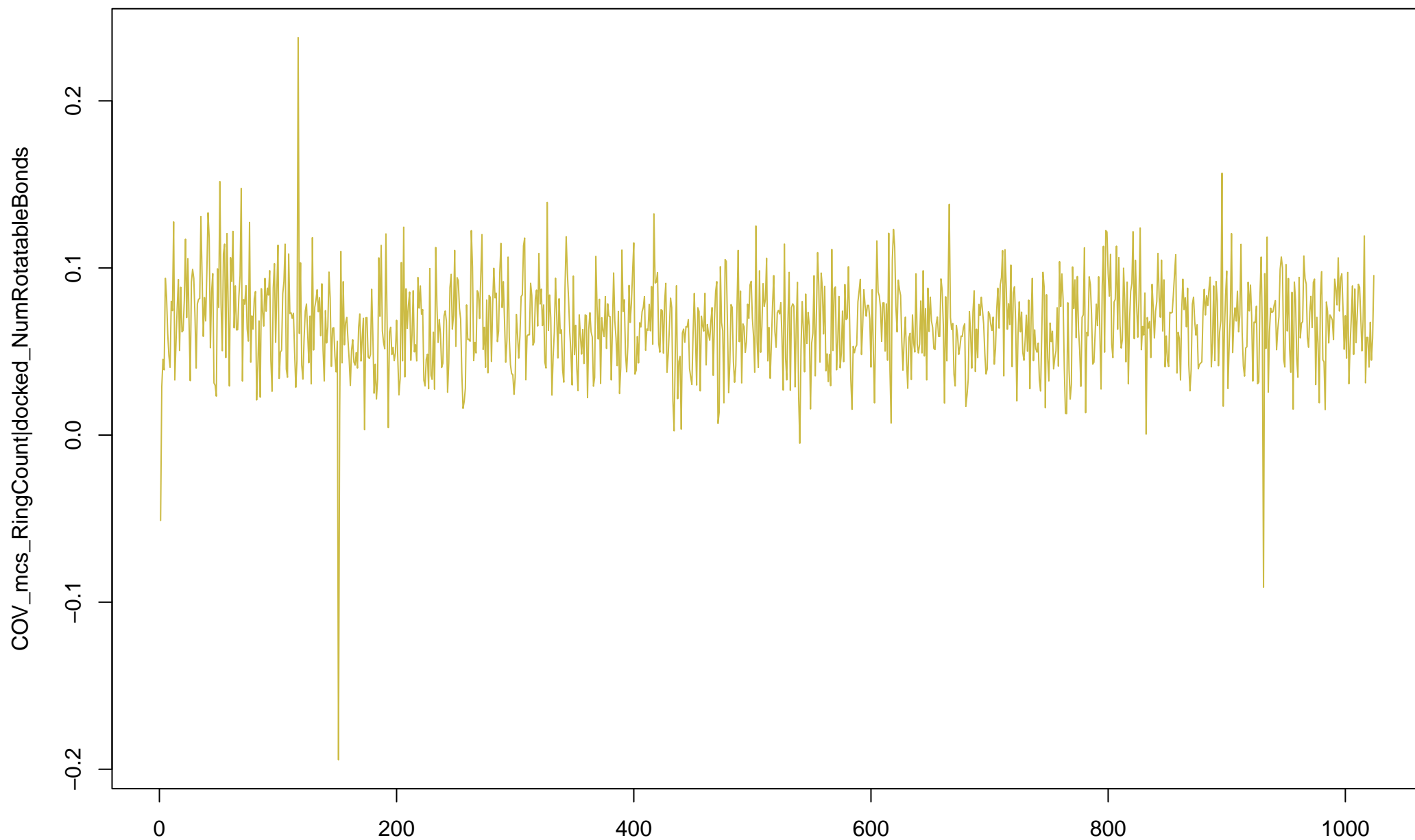
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 85.1 | BMK = 0.172 | MCSE(6.27) = 7.45 | stat: FALSE | burn: 0



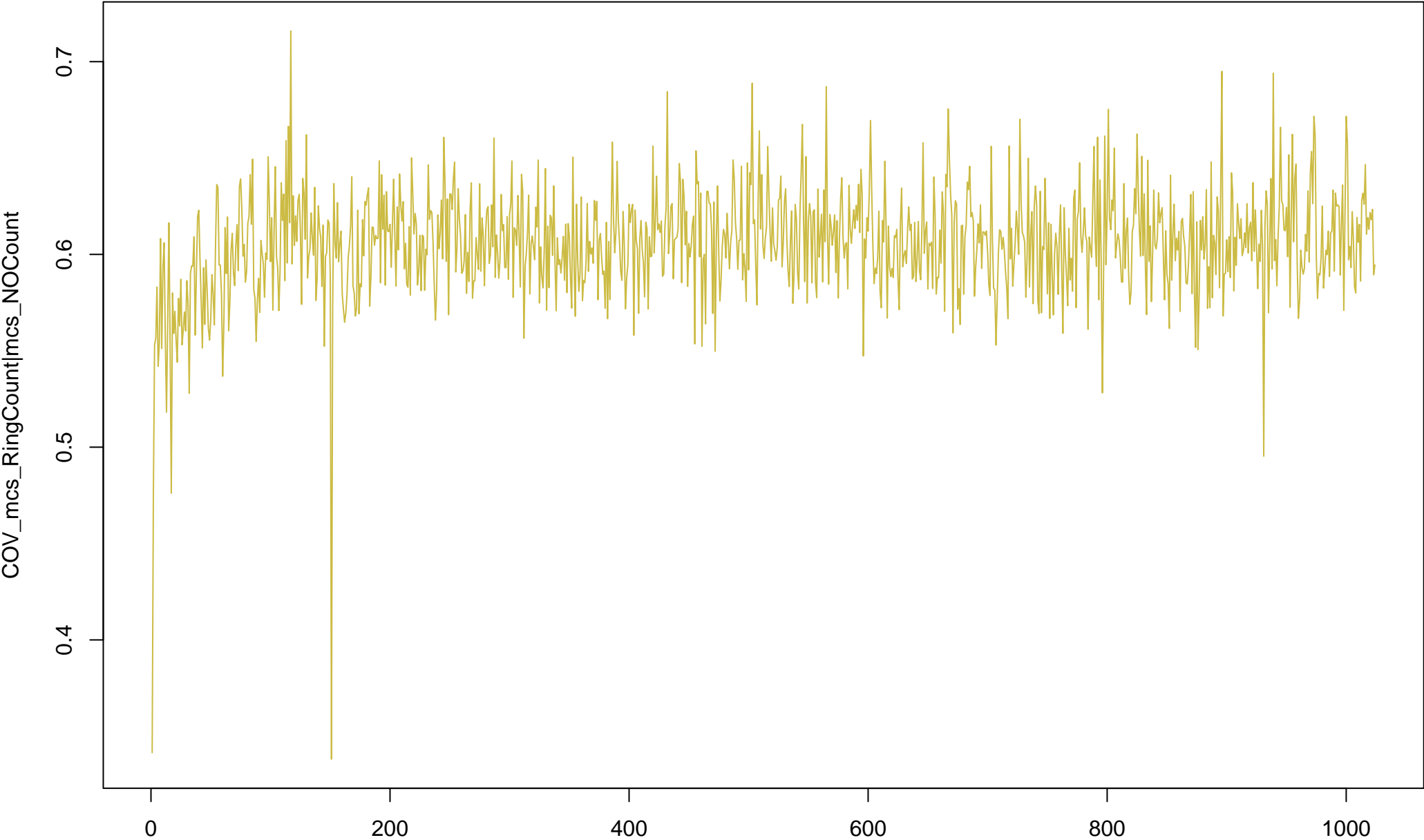
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 77.6 | BMK = 0.191 | MCSE(6.27) = 9.77 | stat: FALSE | burn: 0



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 871 | BMK = 0.077 | MCSE(6.27) = 3.85 | stat: TRUE | burn: 0



COV_mcs_RingCount|mcs_NOCount
ESS = 138 | BMK = 0.116 | MCSE(6.27) = 7.22 | stat: FALSE | burn: 0



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0689 | MCSE(6.27) = 3.83 | stat: TRUE | burn: 0

