

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.841670128985856

max MCSE = 17.8664713733702

all stationary: FALSE

burn: 1020

-- STATS 2D --

min ESS = 3.89438586311009

max BMK = 0.540539141820317

max MCSE = 16.2444754407565

all stationary: FALSE

burn: 102

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.56666349730653

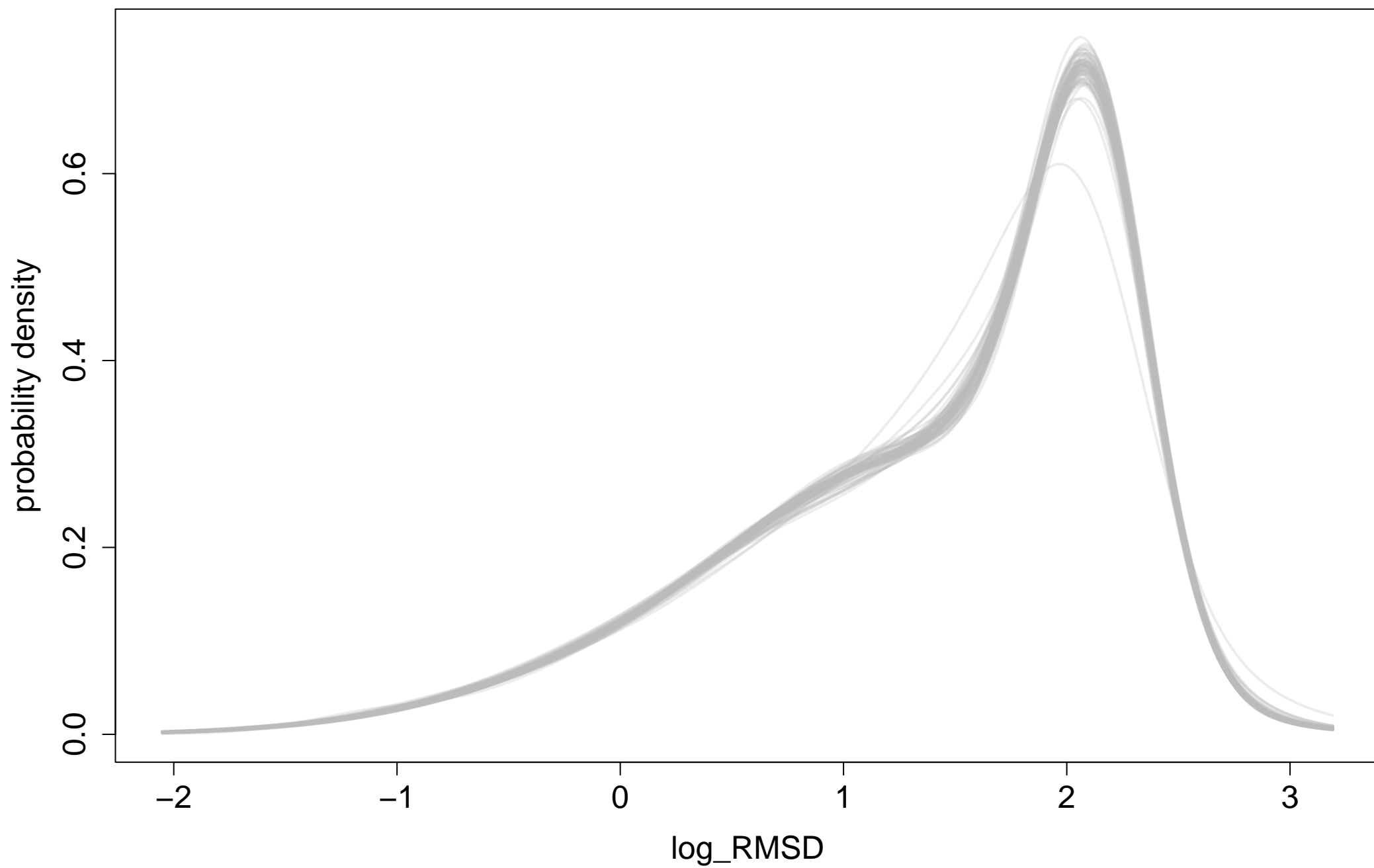
max MCSE = NaN

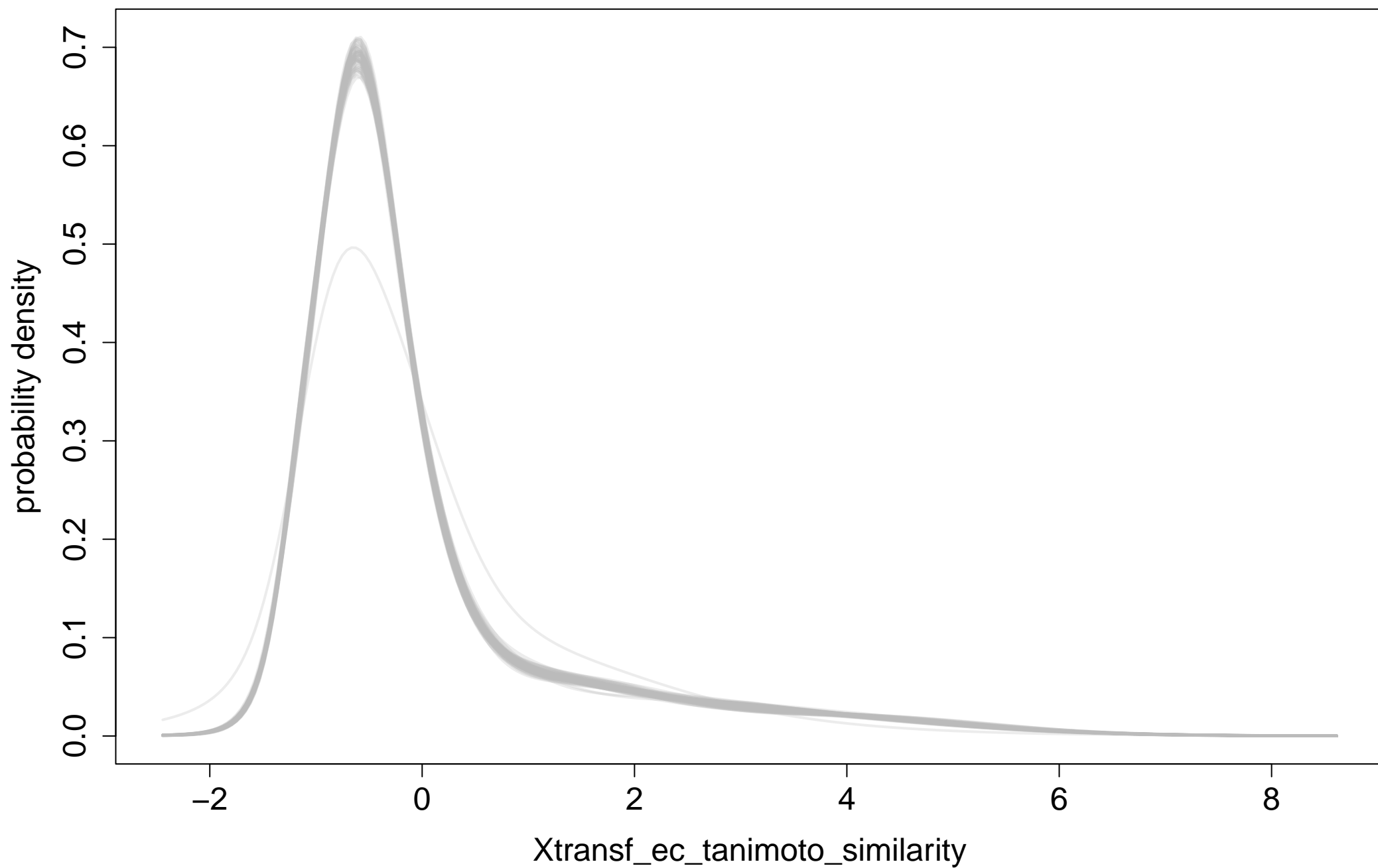
all stationary: FALSE

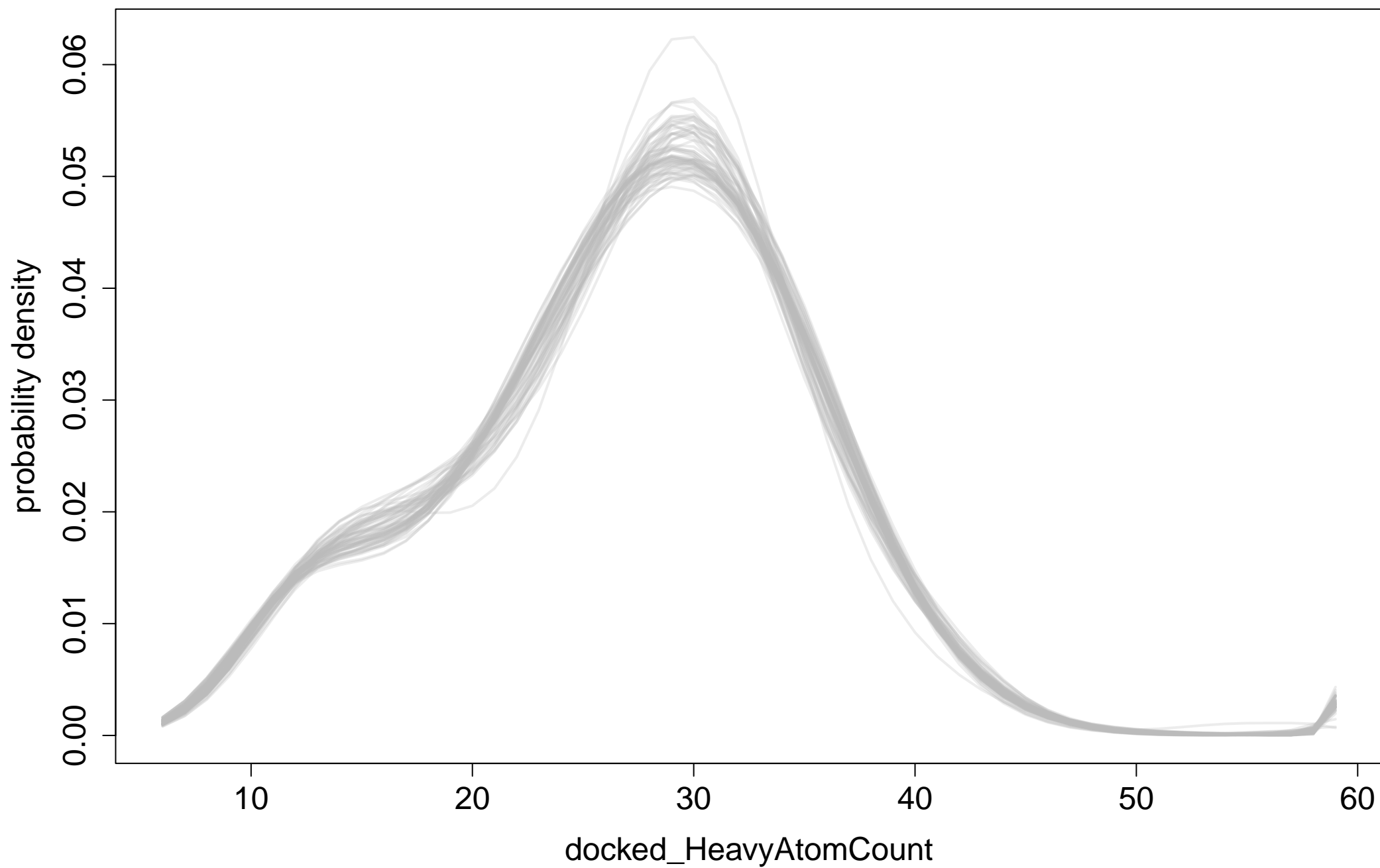
burn: 714

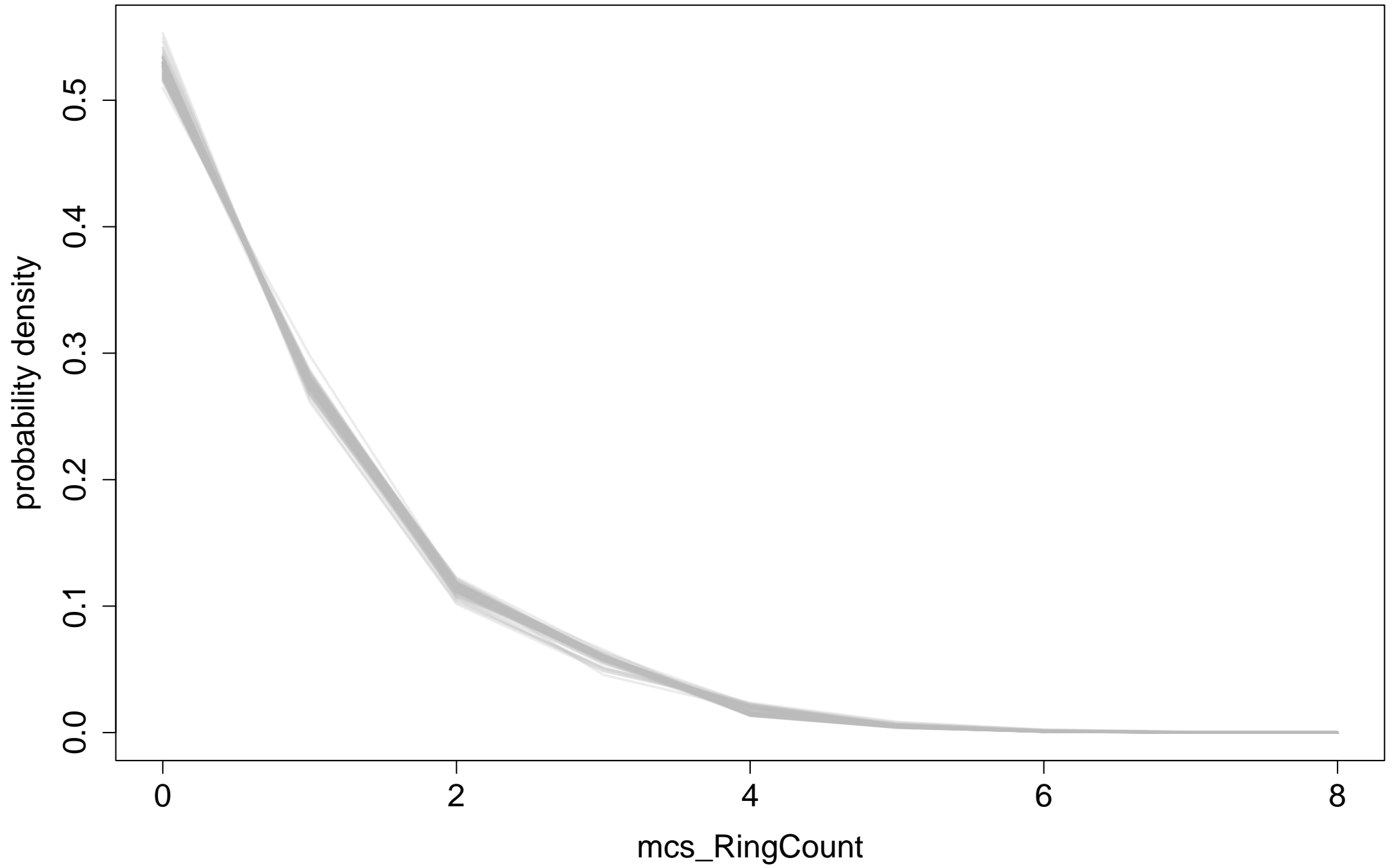
Occupied clusters: 35 of 91

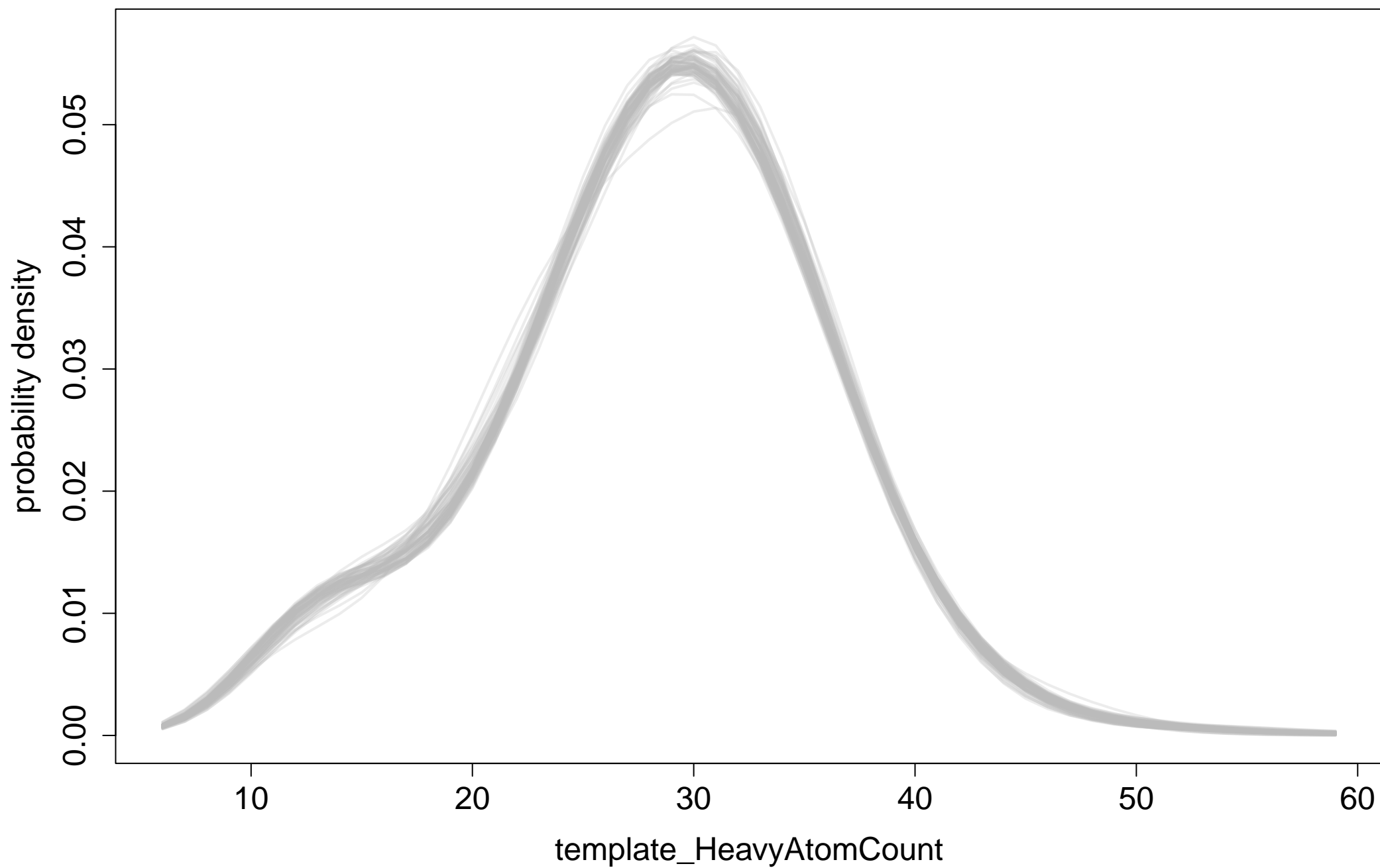
LL: -115000 +- 1890

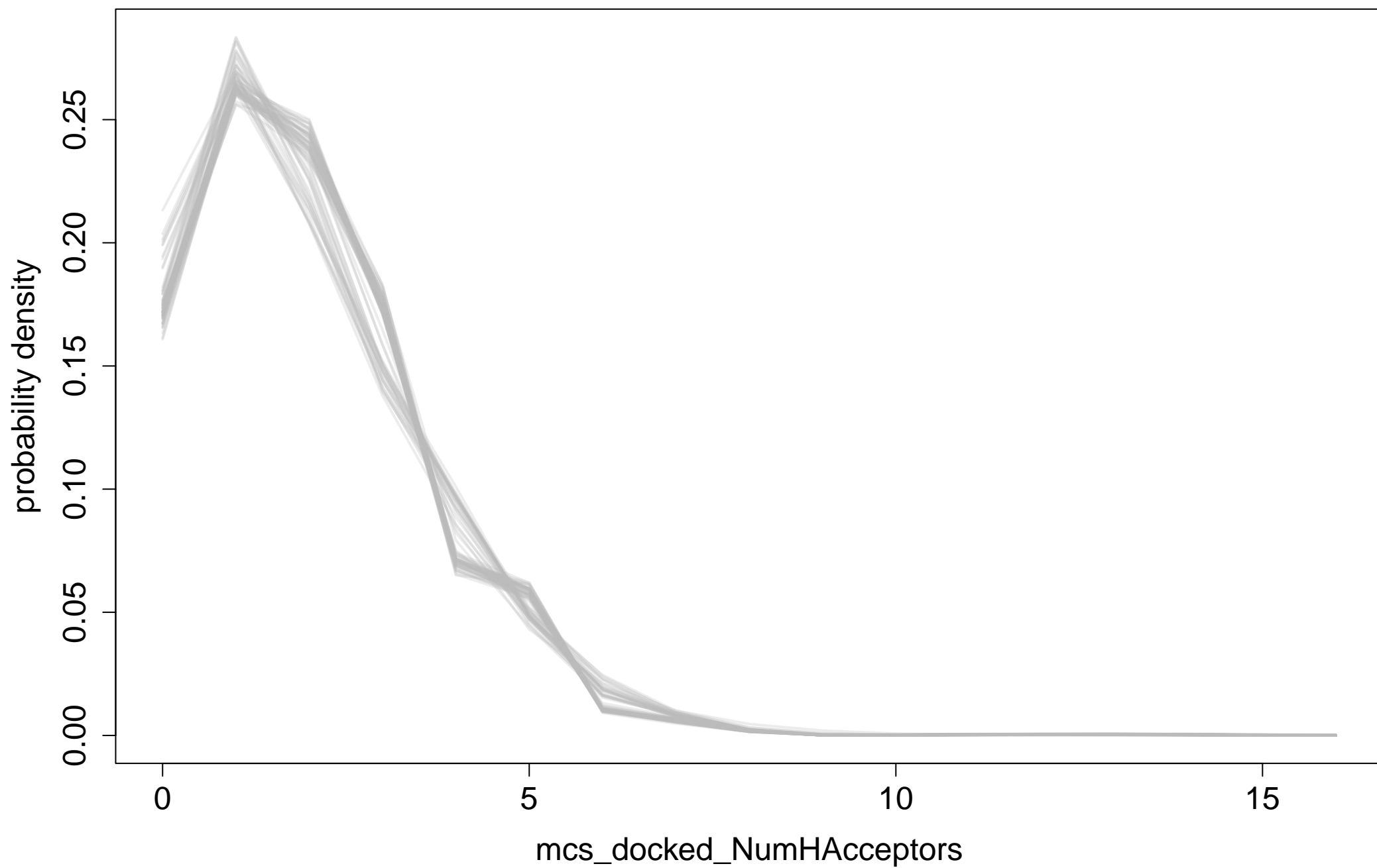


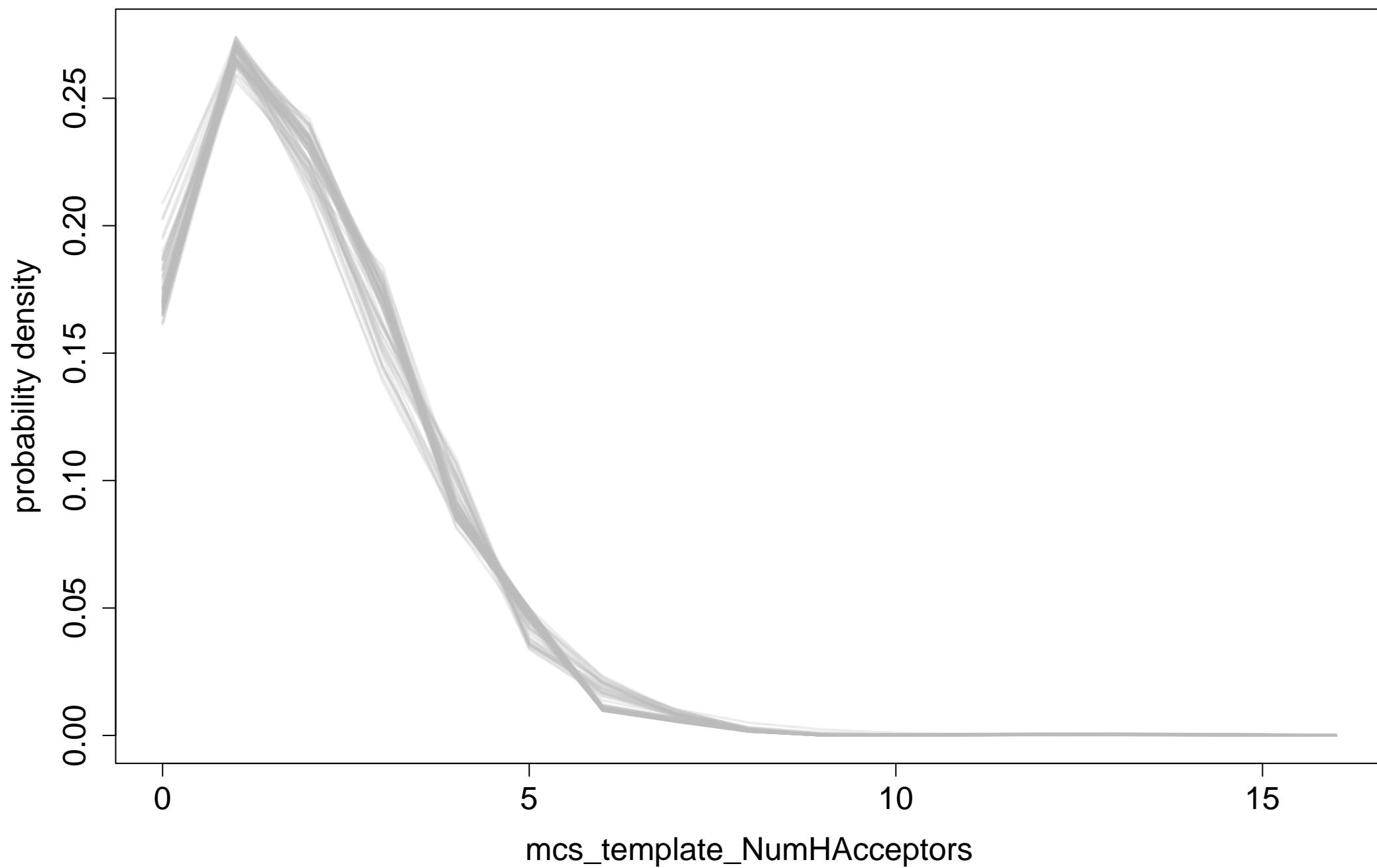


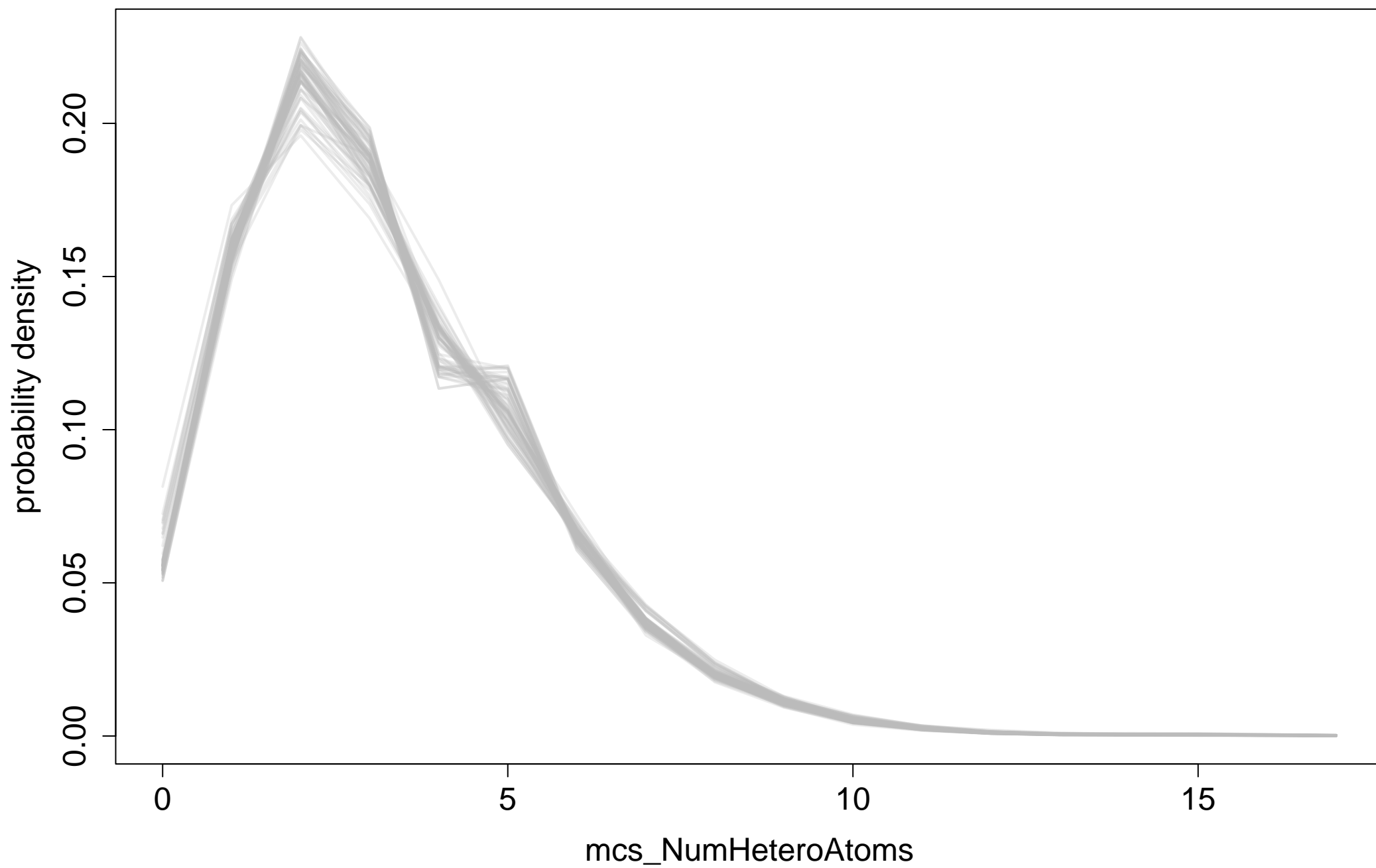


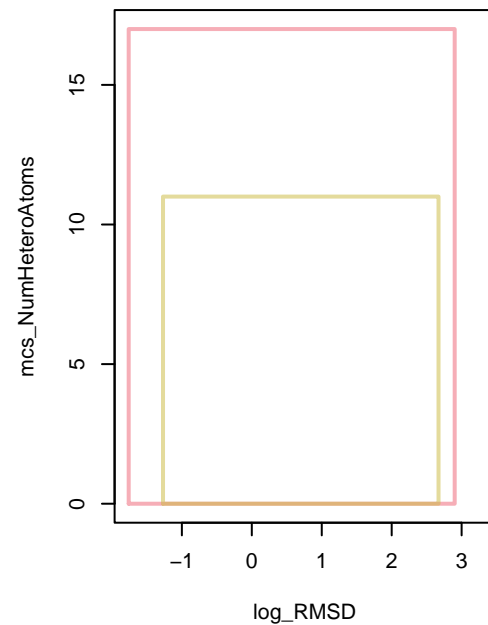
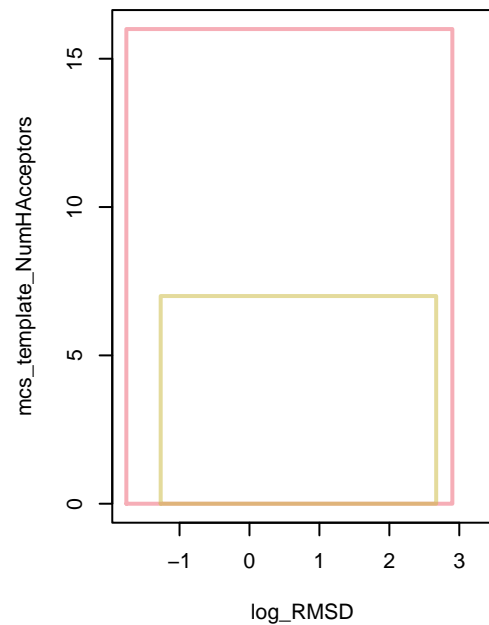
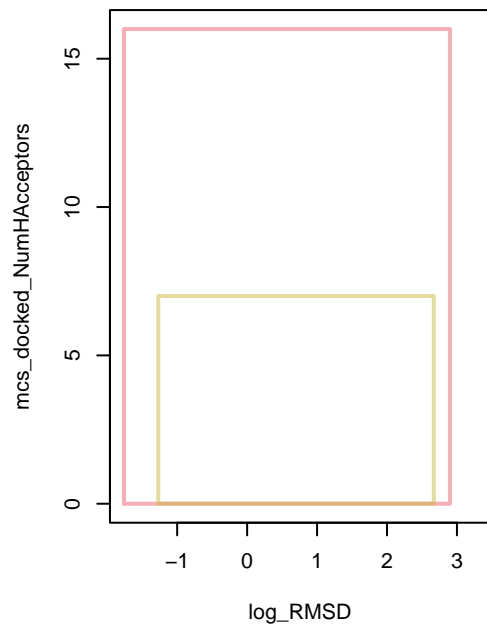
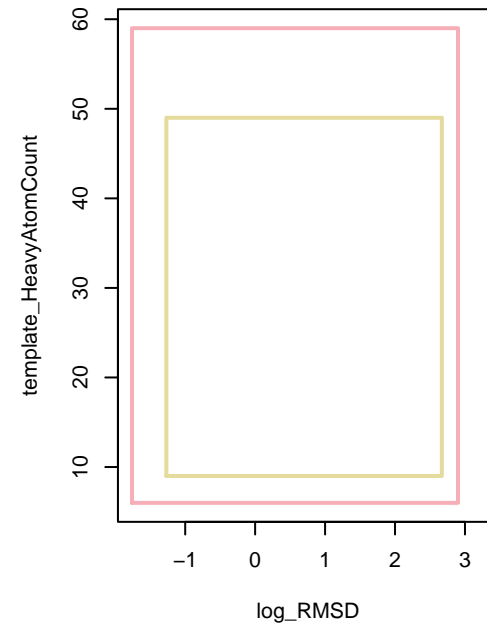
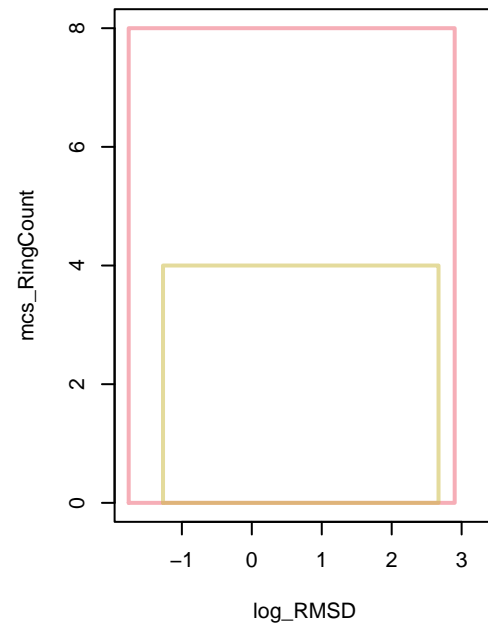
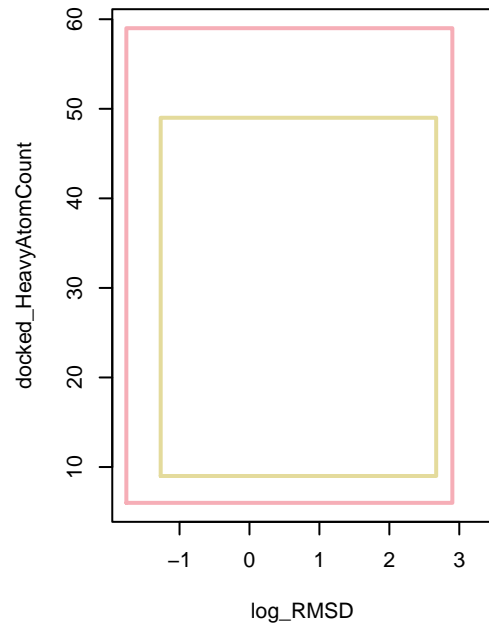
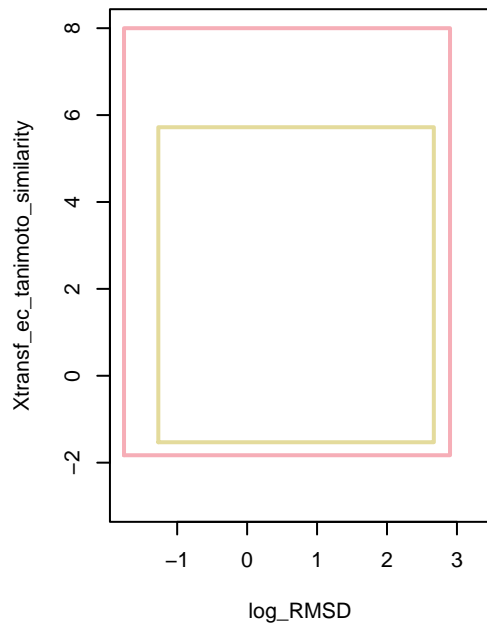




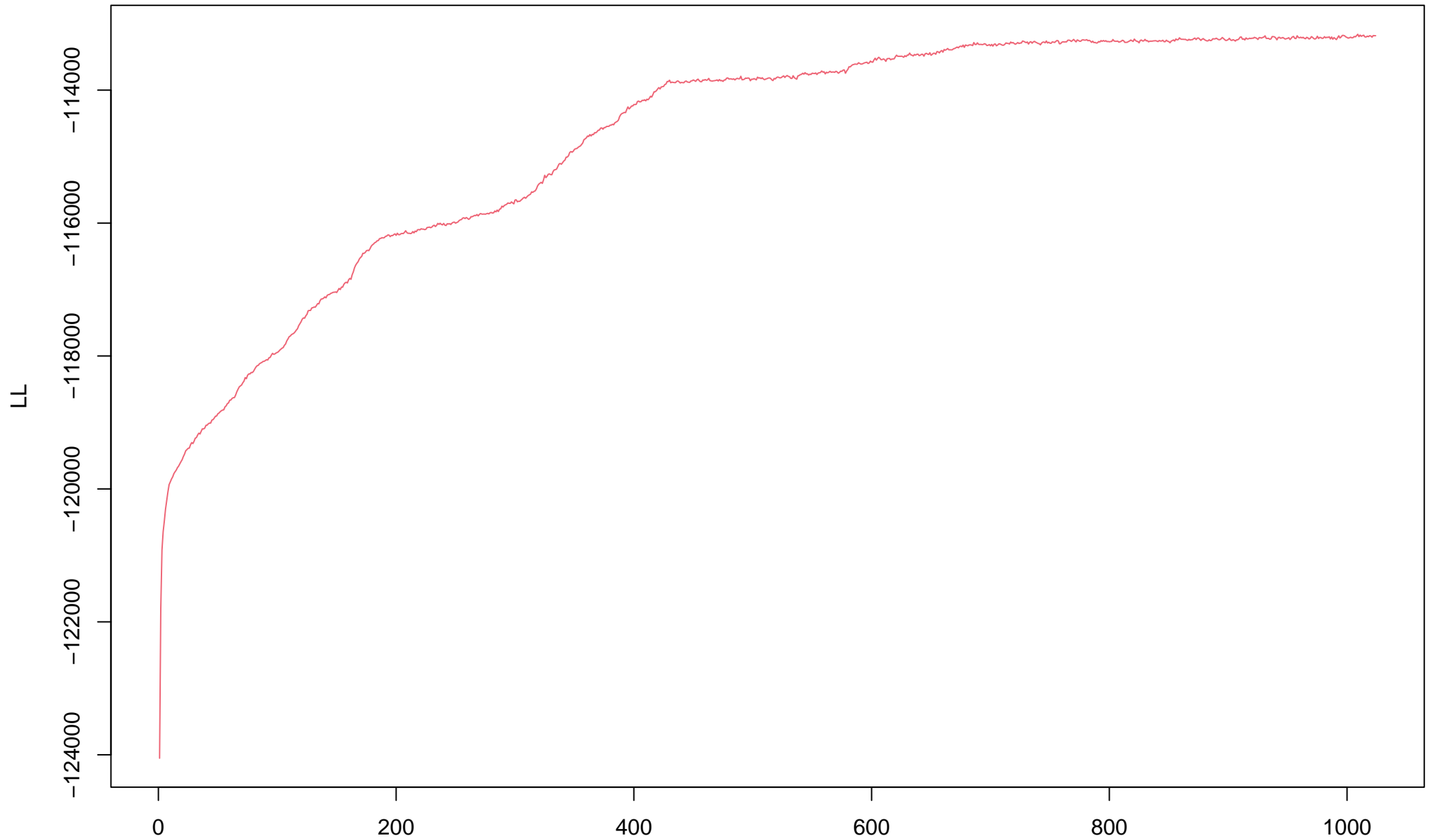




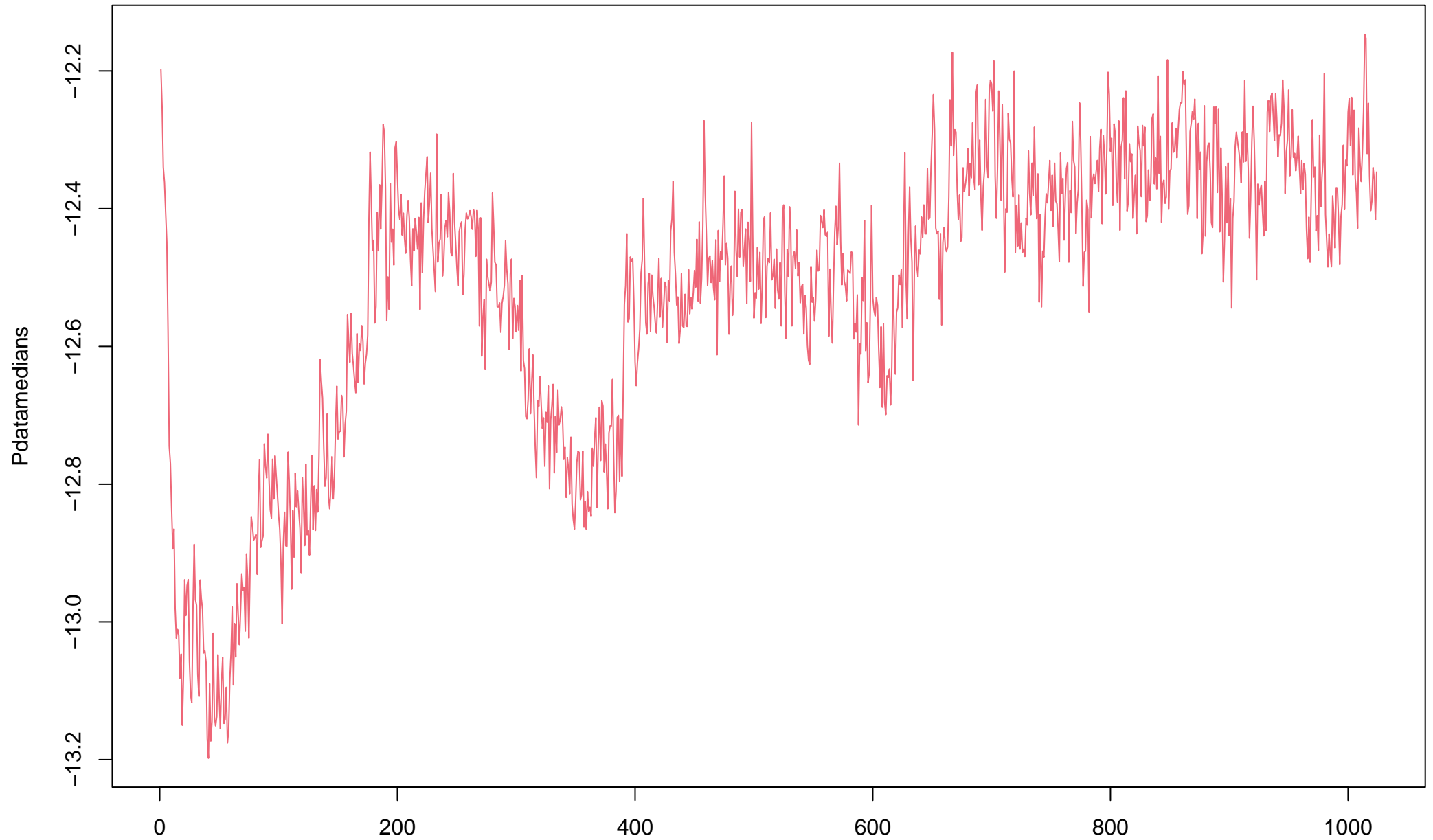




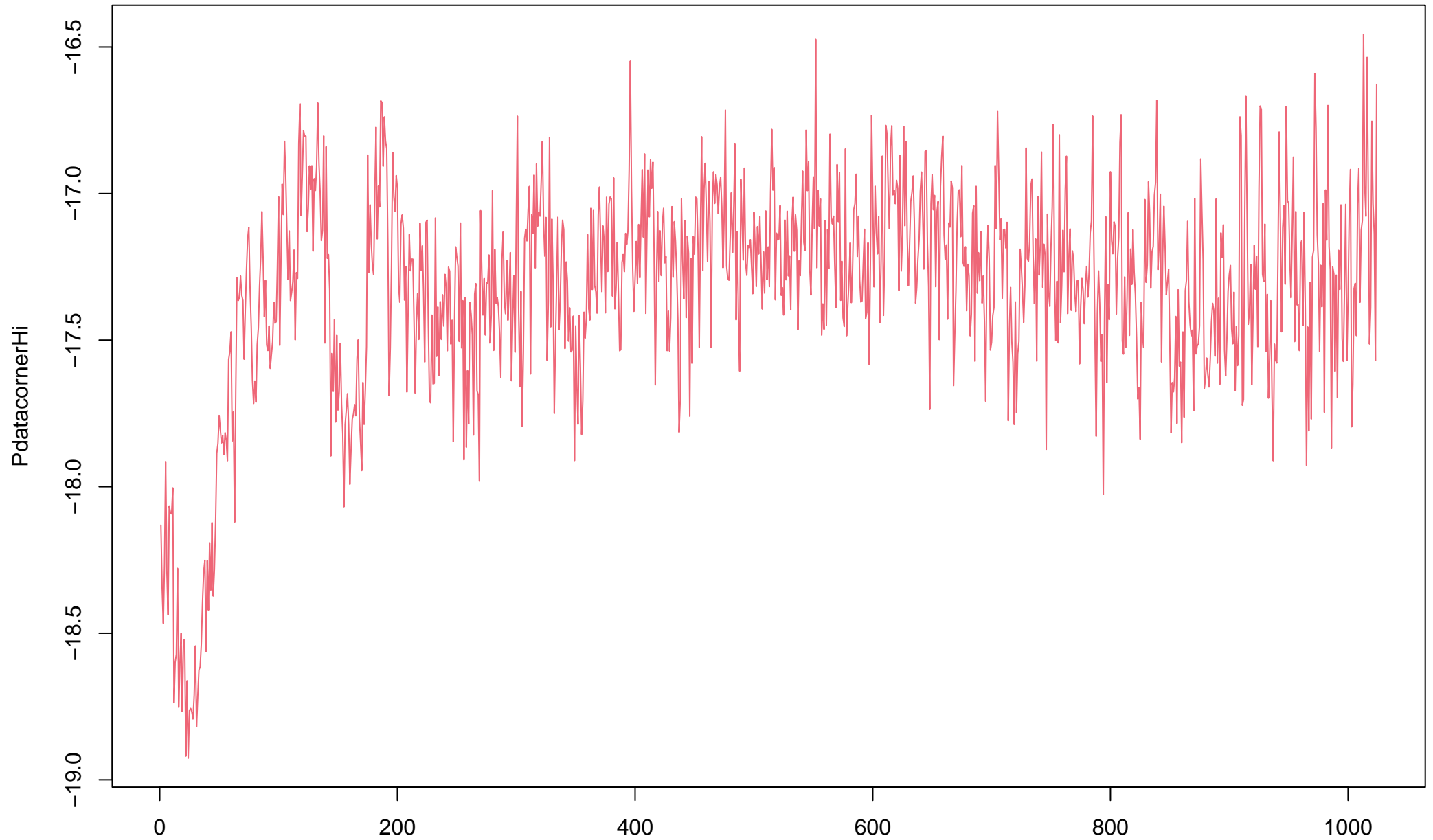
LL
ESS = 3.26 | BMK = 0.842 | MCSE(6.27) = 17.9 | stat: FALSE | burn: 1020



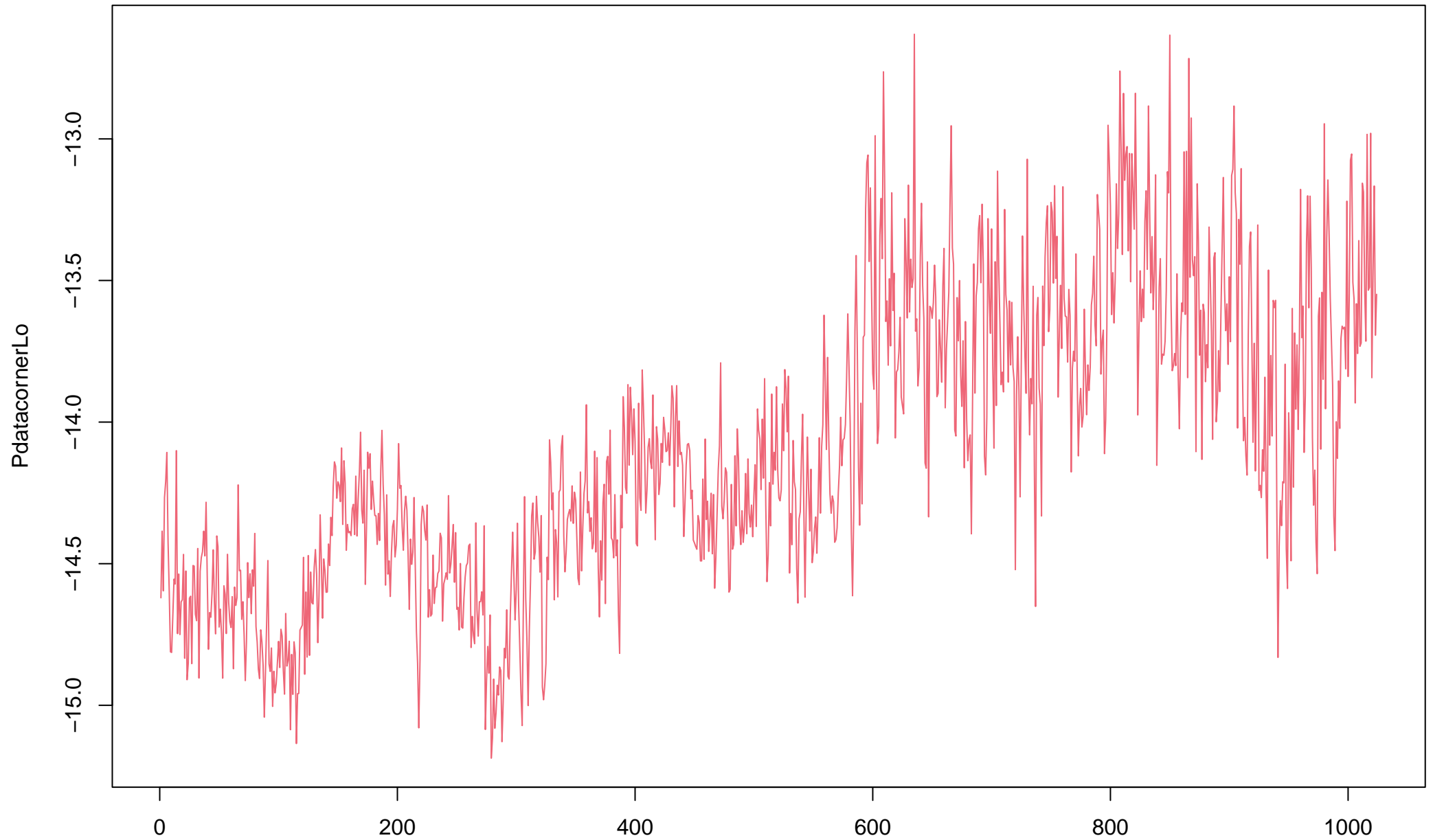
Pdatamedians
ESS = 5.75 | BMK = 0.538 | MCSE(6.27) = 16.2 | stat: FALSE | burn: 408



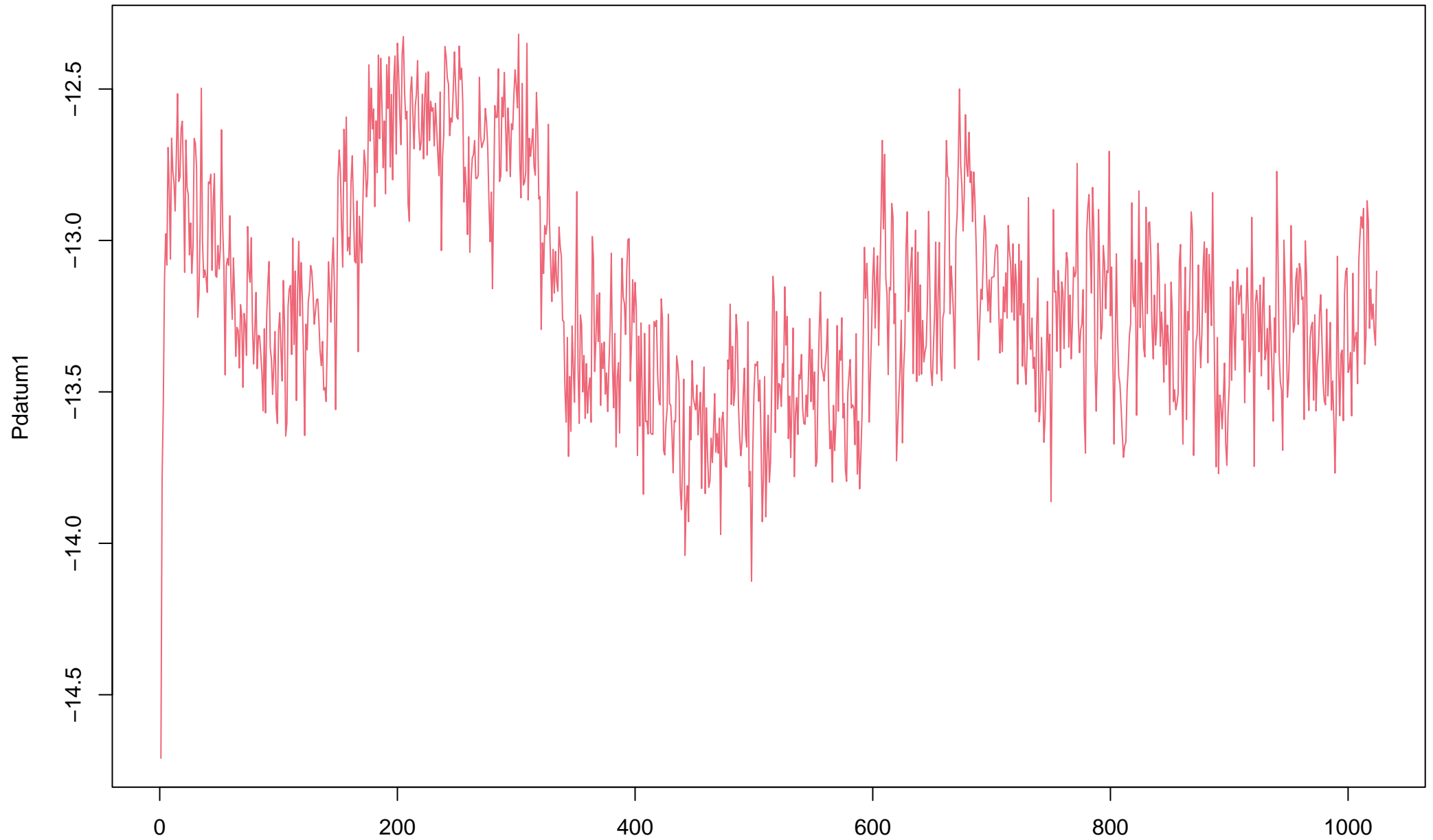
PdatacornerHi
ESS = 2.22e-16 | BMK = 0.2 | MCSE(6.27) = 10.7 | stat: FALSE | burn: 0



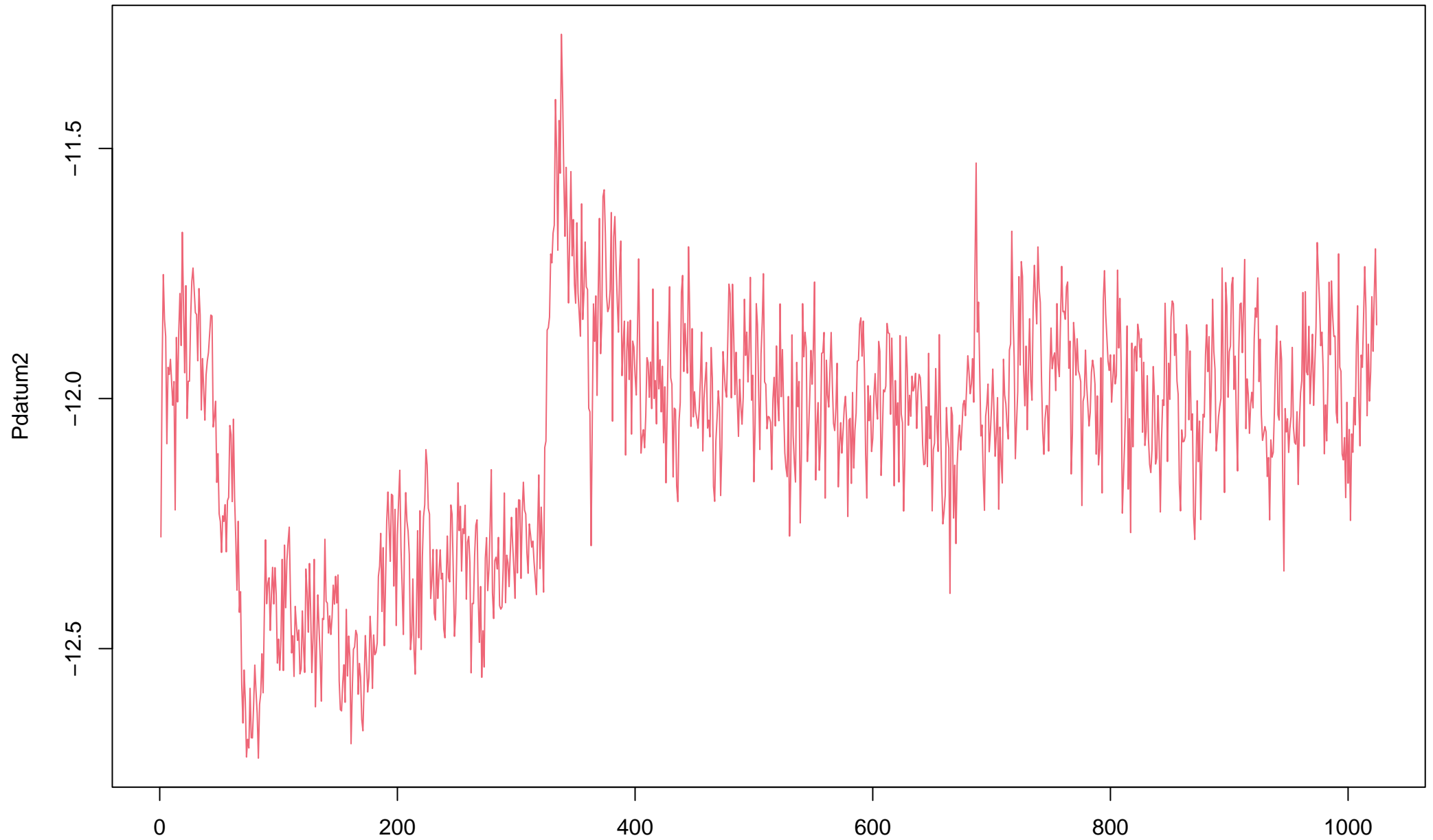
PdatacornerLo
ESS = 8.8 | BMK = 0.678 | MCSE(6.27) = 14 | stat: FALSE | burn: 0



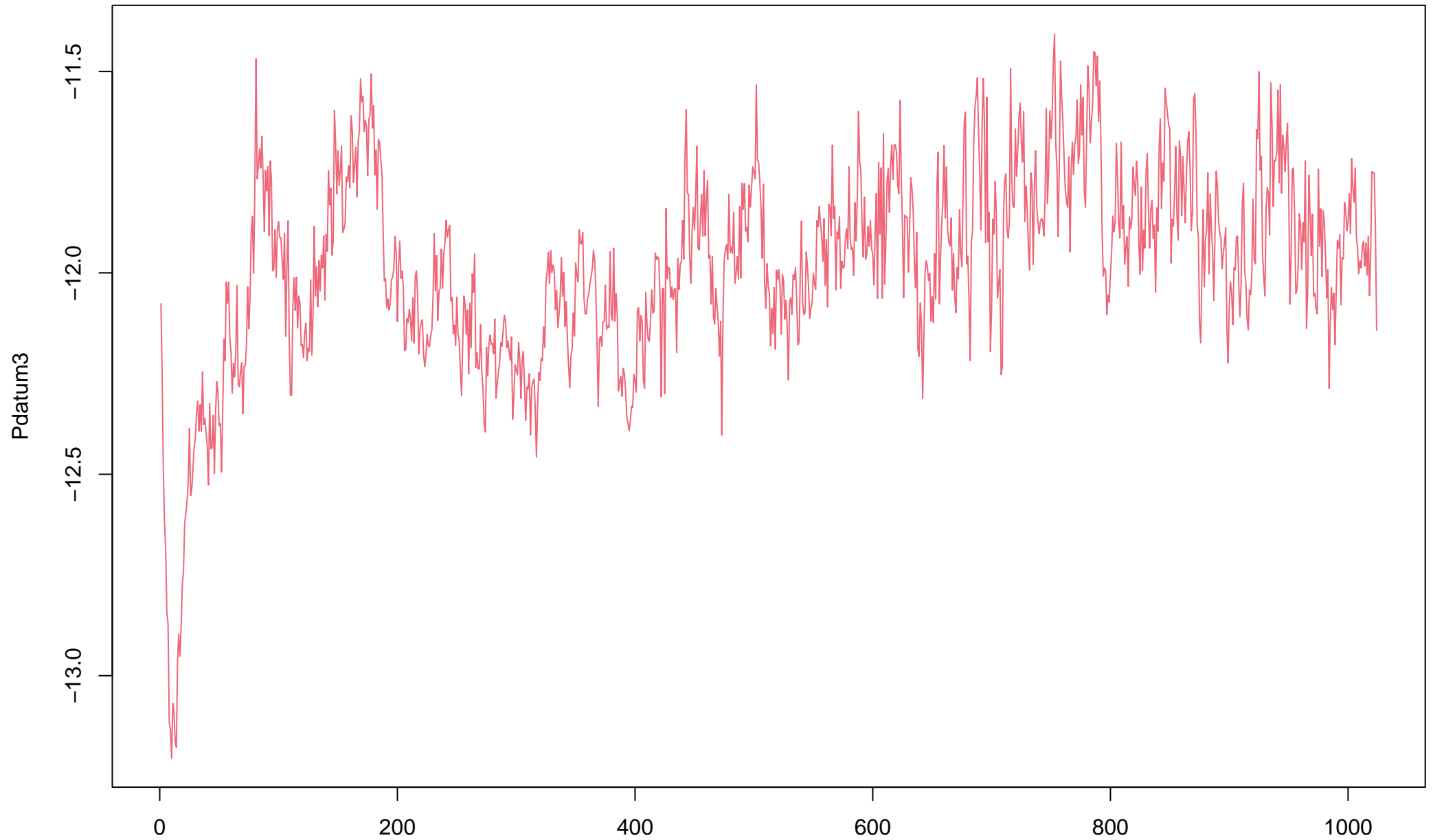
Pdatum1
ESS = 9.18 | BMK = 0.33 | MCSE(6.27) = 14.9 | stat: FALSE | burn: 408



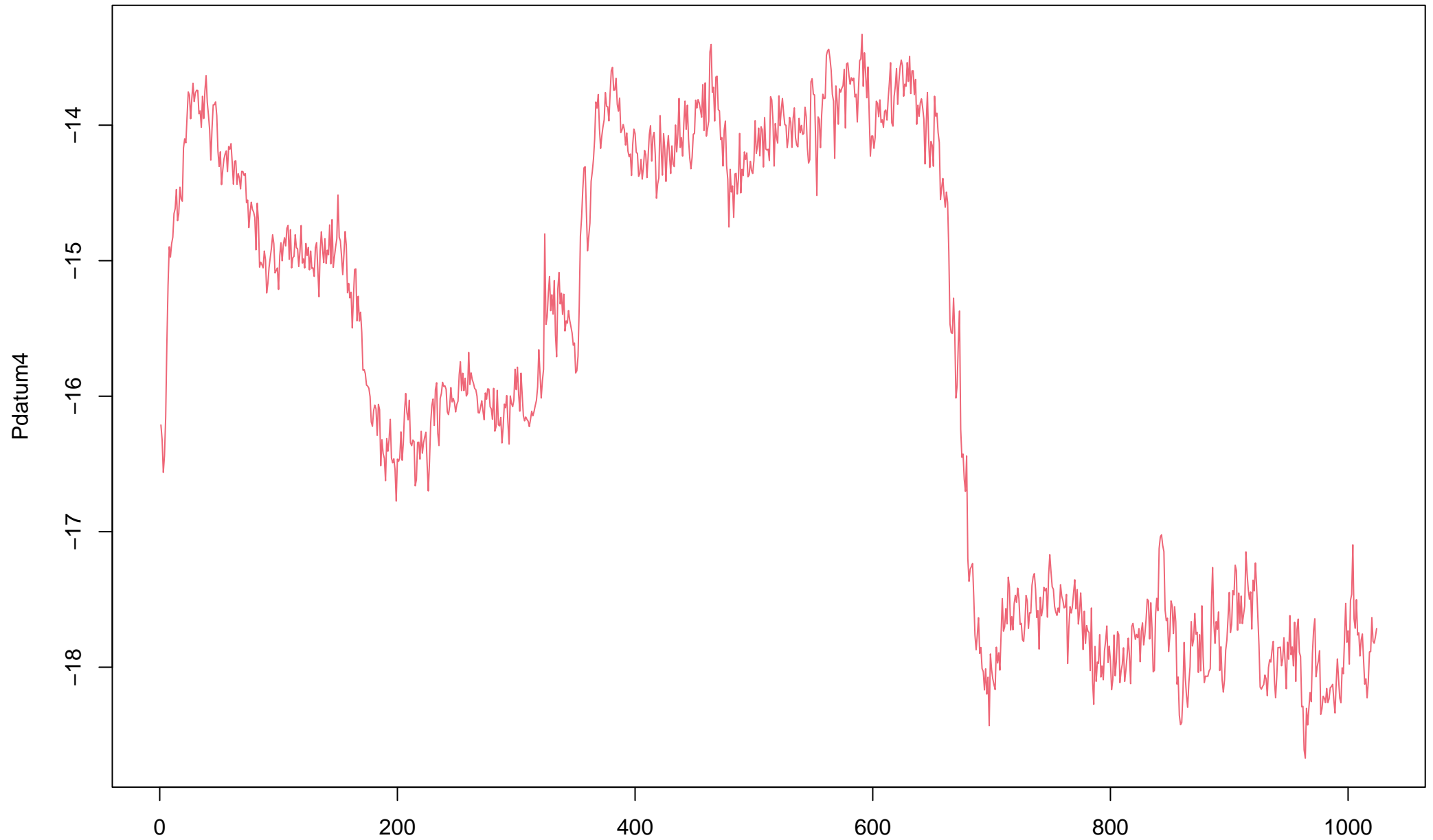
Pdatum2
ESS = 15.3 | BMK = 0.466 | MCSE(6.27) = 14.8 | stat: FALSE | burn: 306



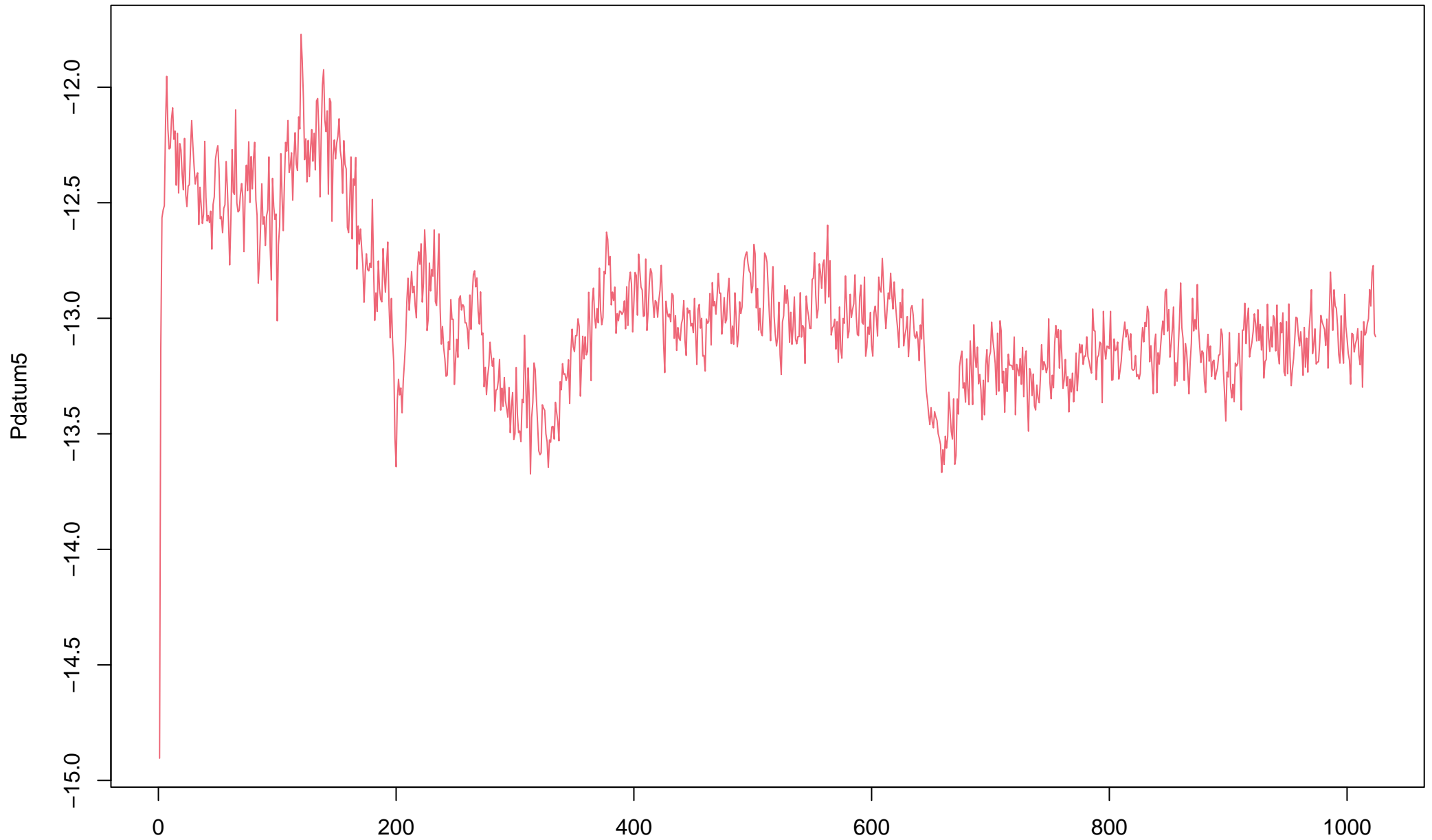
Pdatum3
ESS = 31.7 | BMK = 0.37 | MCSE(6.27) = 13.9 | stat: TRUE | burn: 204



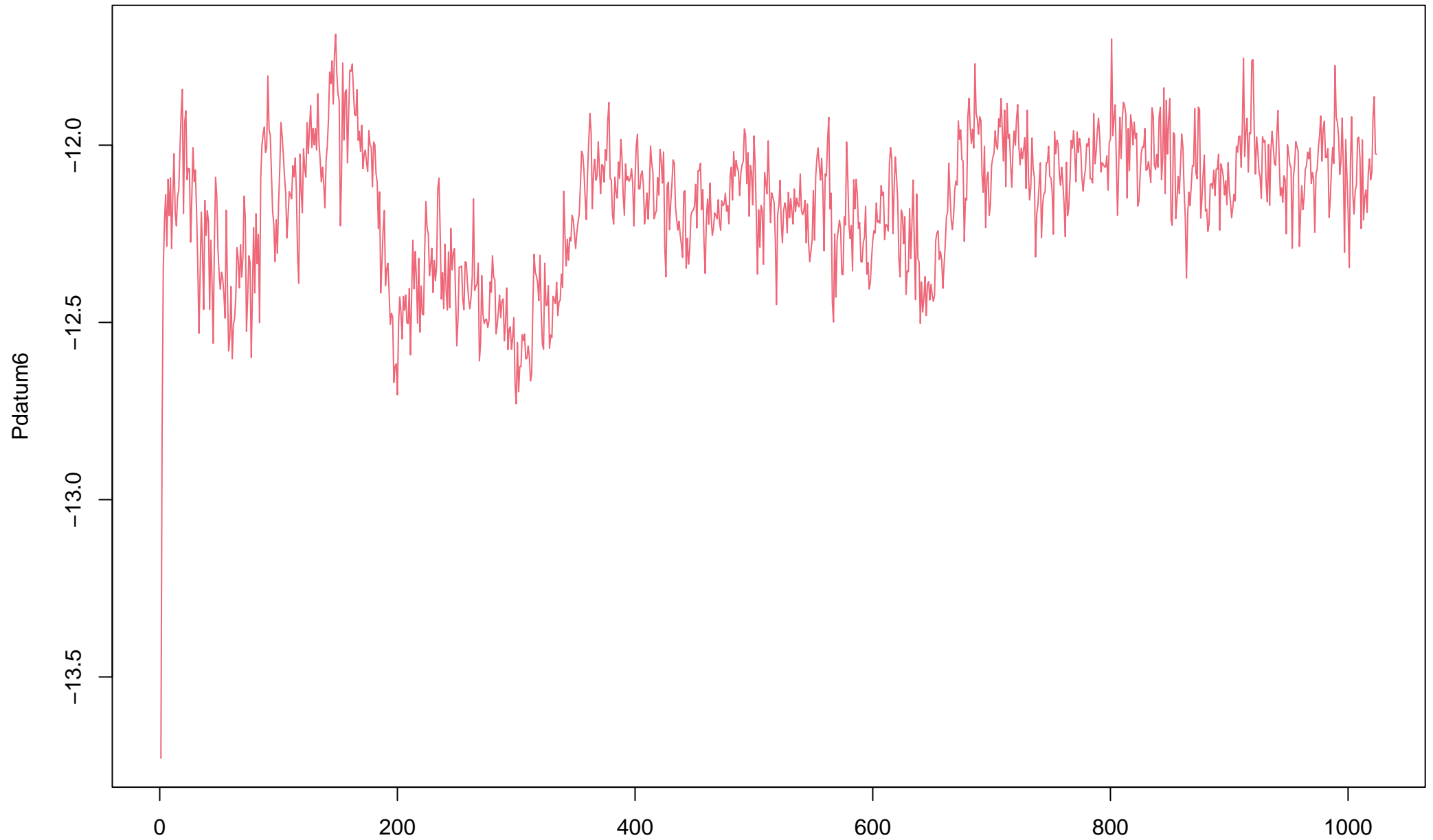
Pdatum4
ESS = 4.36 | BMK = 0.298 | MCSE(6.27) = 16.8 | stat: FALSE | burn: 714



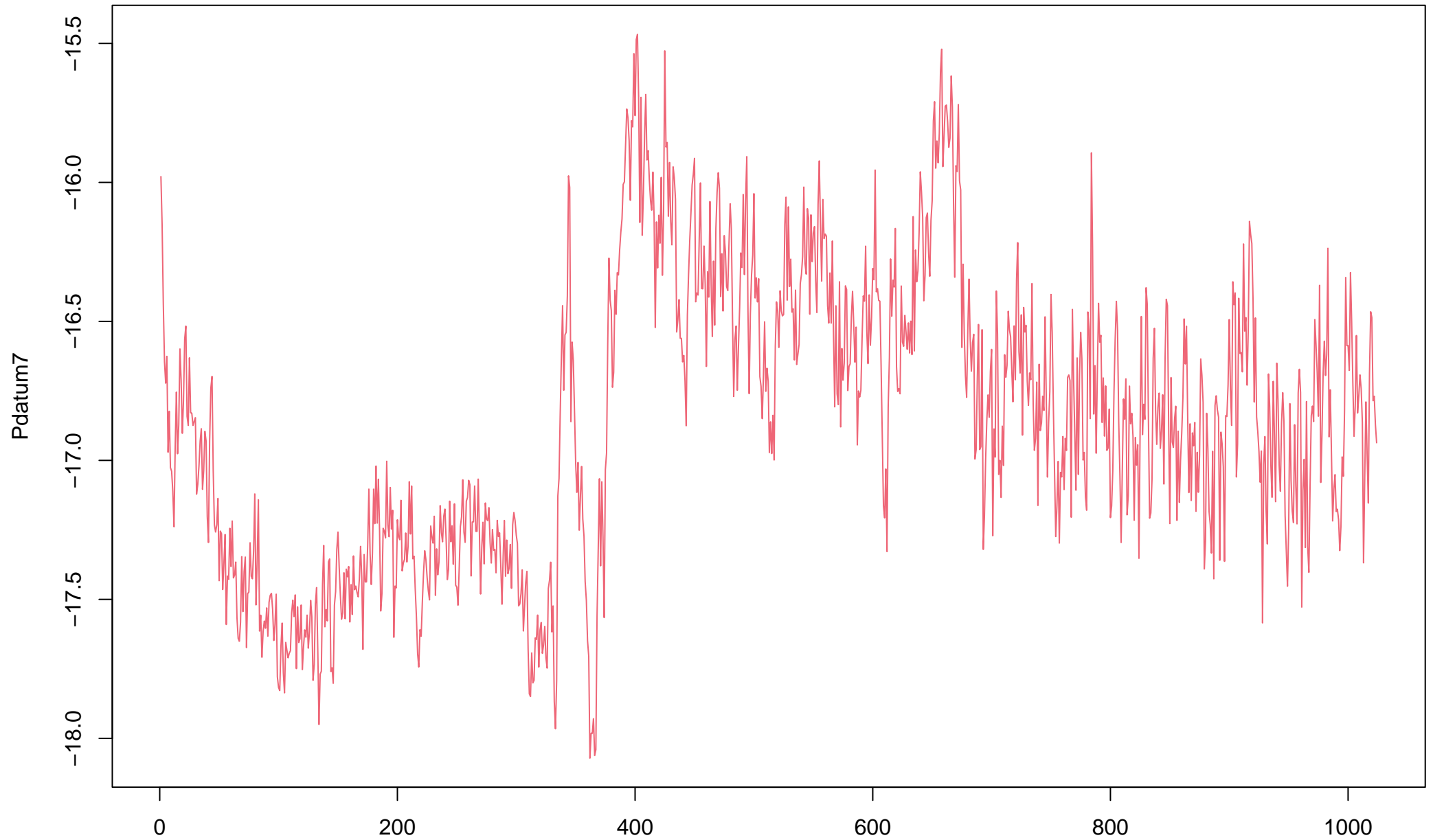
Pdatum5
ESS = 6.54 | BMK = 0.485 | MCSE(6.27) = 16 | stat: FALSE | burn: 612



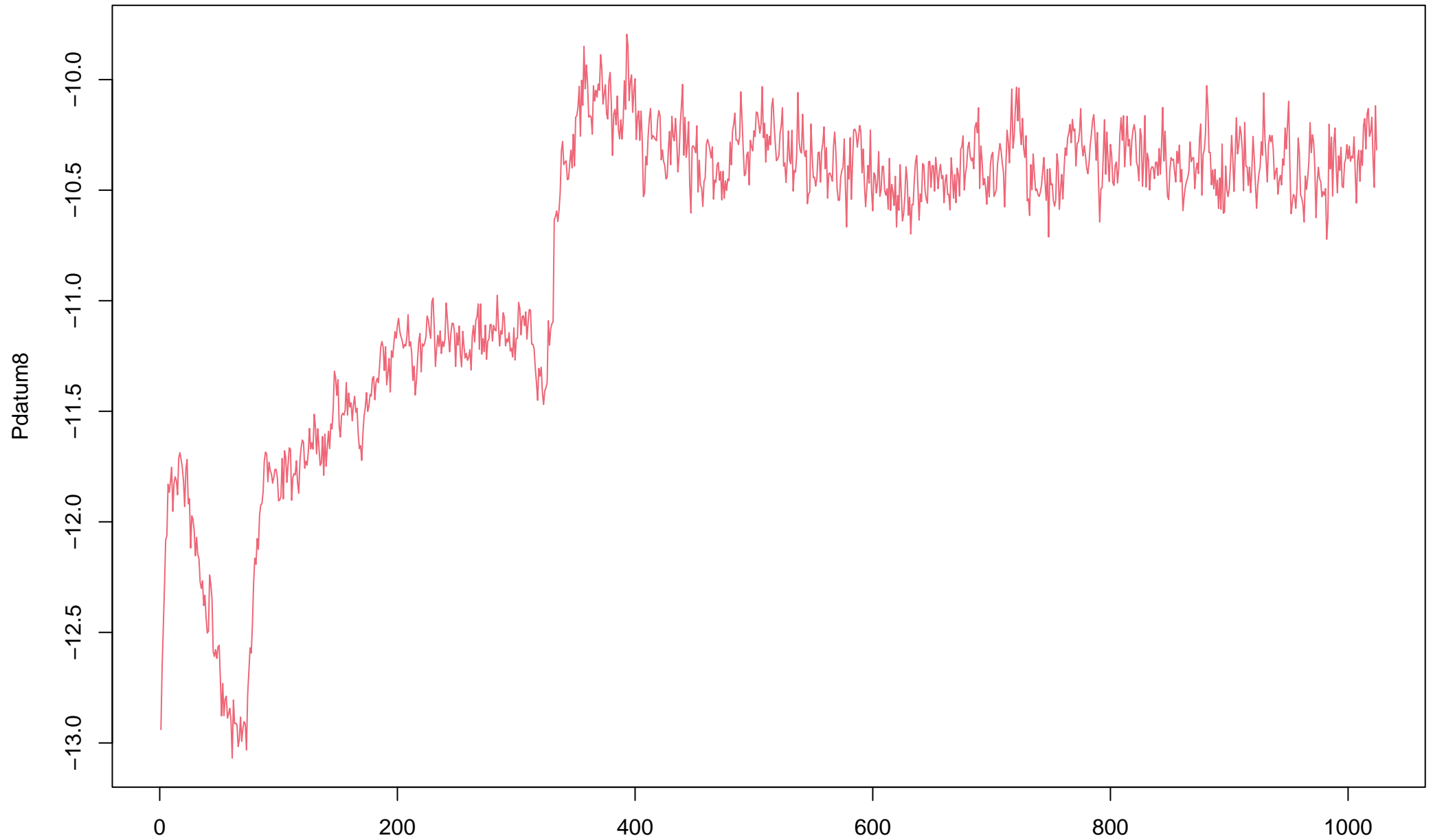
Pdatum6
ESS = 19.5 | BMK = 0.292 | MCSE(6.27) = 13.8 | stat: FALSE | burn: 204



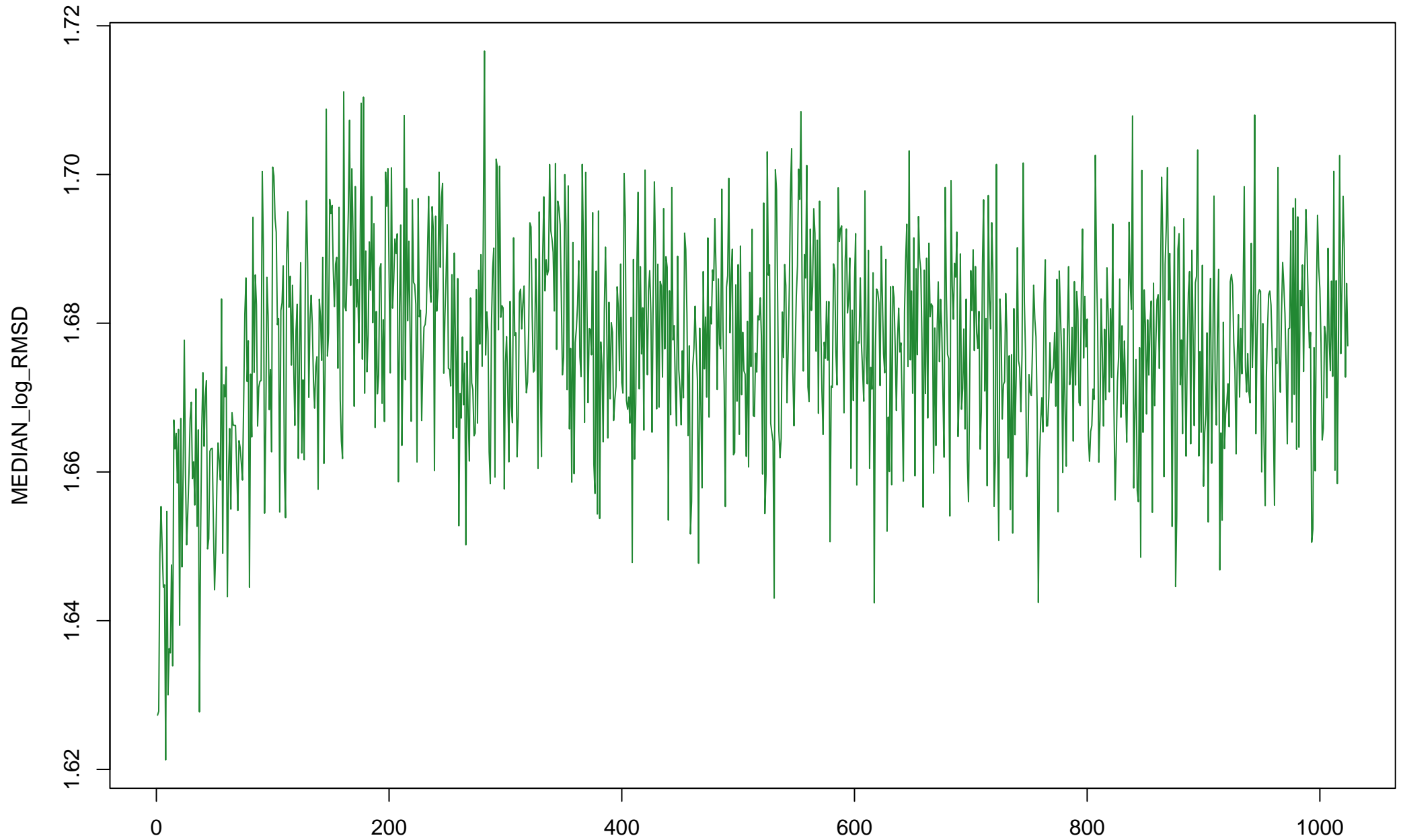
Pdatum7
ESS = 16.1 | BMK = 0.376 | MCSE(6.27) = 15.3 | stat: TRUE | burn: 306



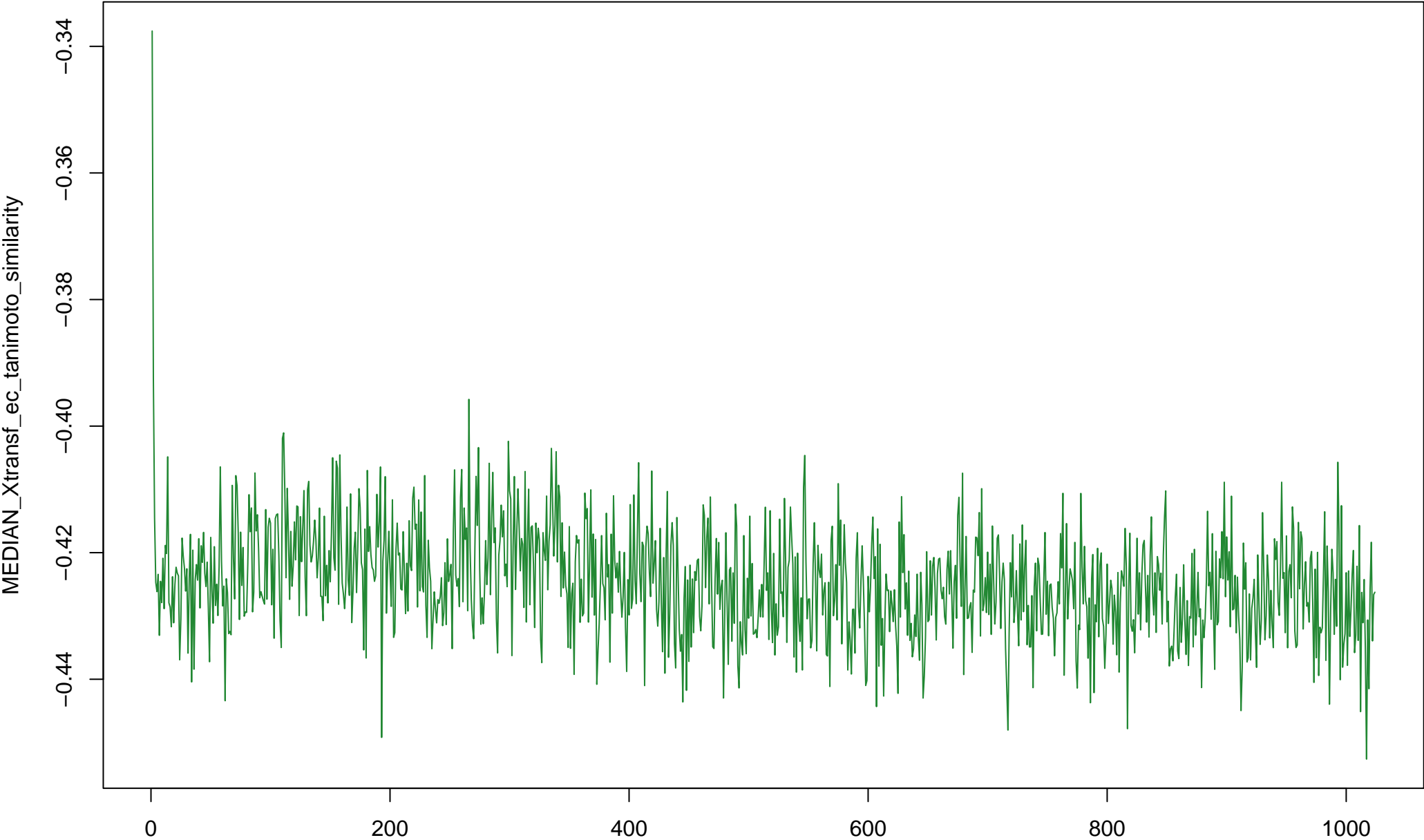
Pdatum8
ESS = 4.83 | BMK = 0.664 | MCSE(6.27) = 17.1 | stat: FALSE | burn: 306



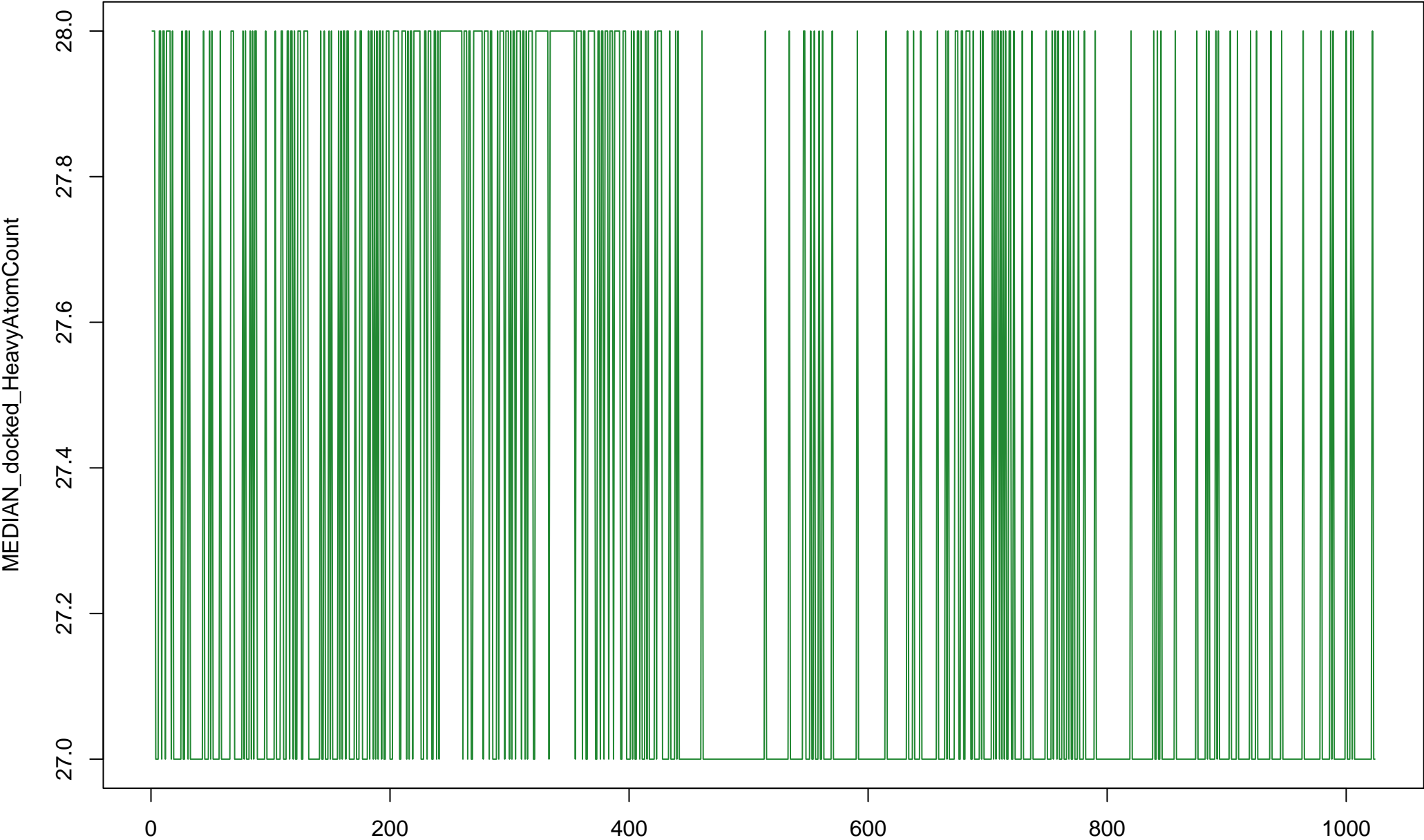
MEDIAN_log_RMSD
ESS = 79.1 | BMK = 0.106 | MCSE(6.27) = 8.77 | stat: FALSE | burn: 0



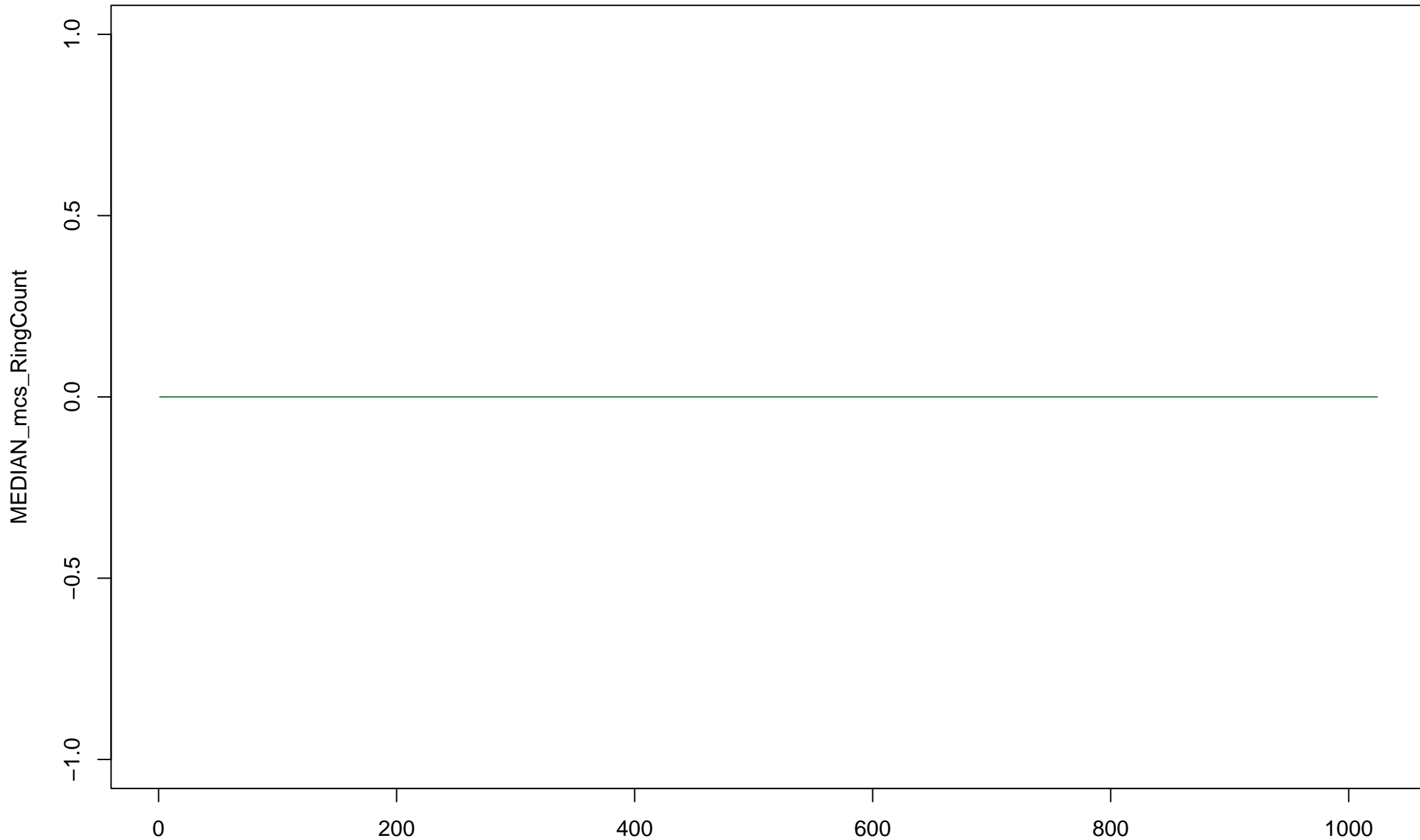
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 134 | BMK = 0.196 | MCSE(6.27) = 6.56 | stat: FALSE | burn: 0



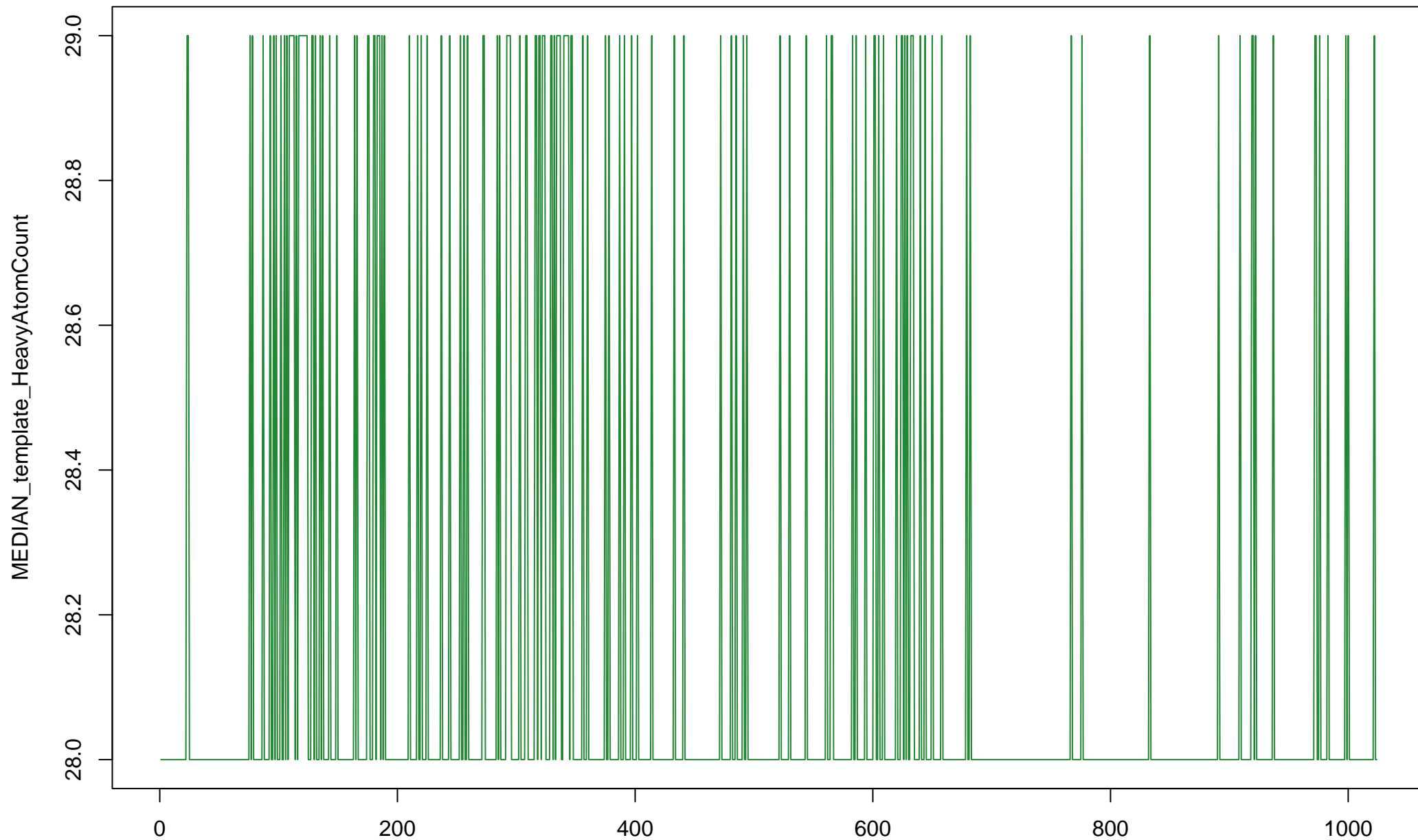
MEDIAN_docked_HeavyAtomCount
ESS = 20.1 | BMK = 0.205 | MCSE(6.27) = 9.92 | stat: FALSE | burn: 0



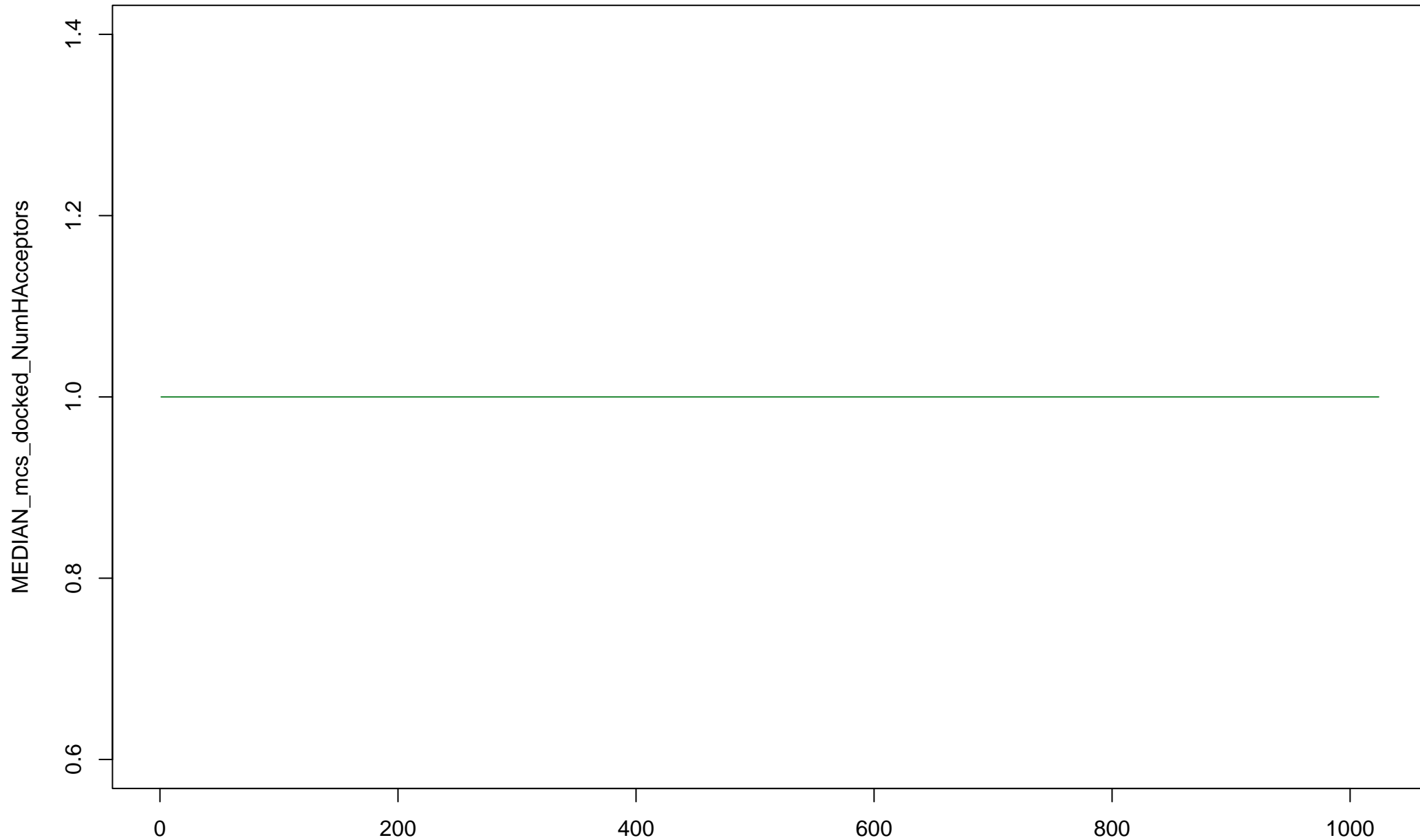
MEDIAN_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



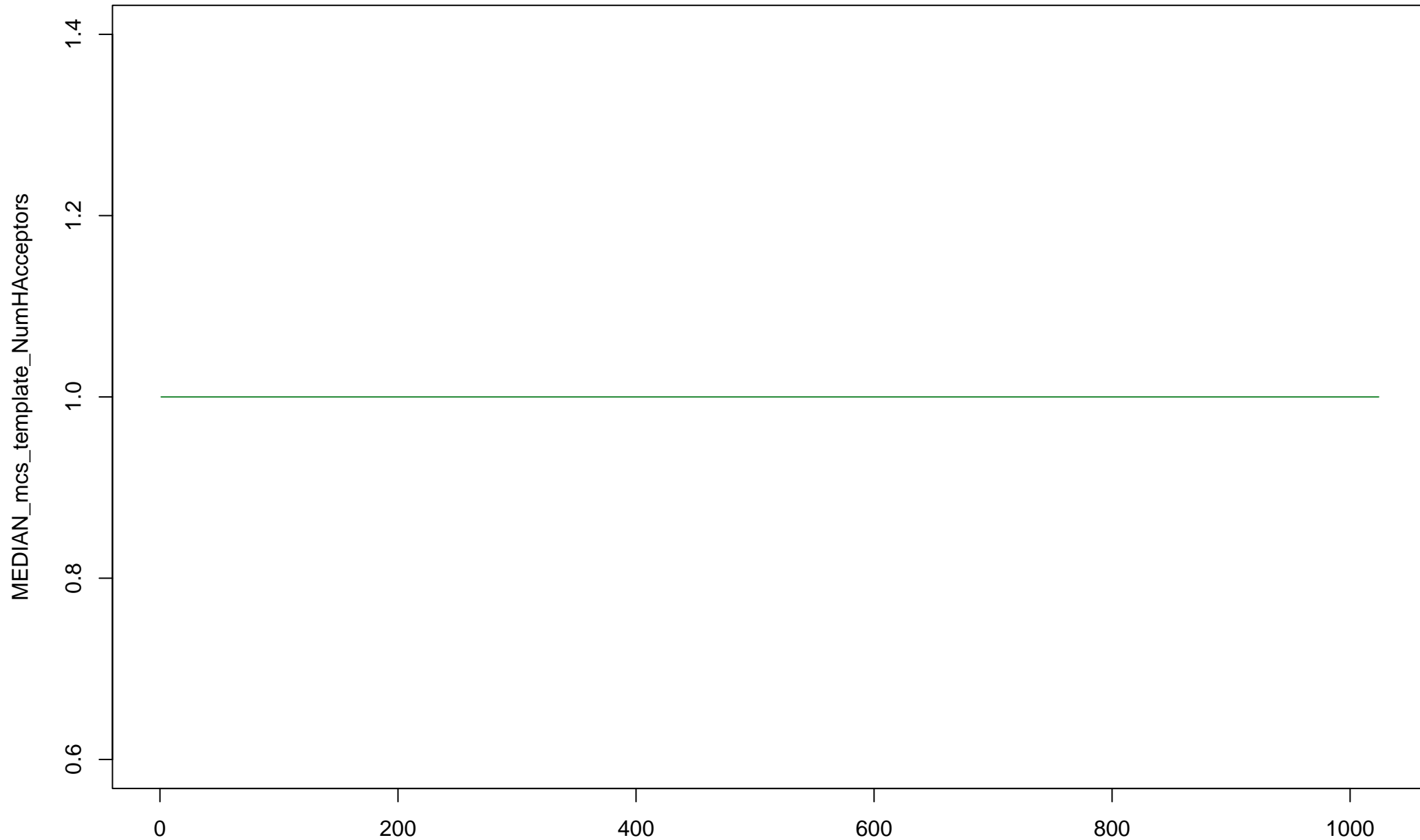
MEDIAN_template_HeavyAtomCount
ESS = 164 | BMK = 0.148 | MCSE(6.27) = 7.31 | stat: TRUE | burn: 0



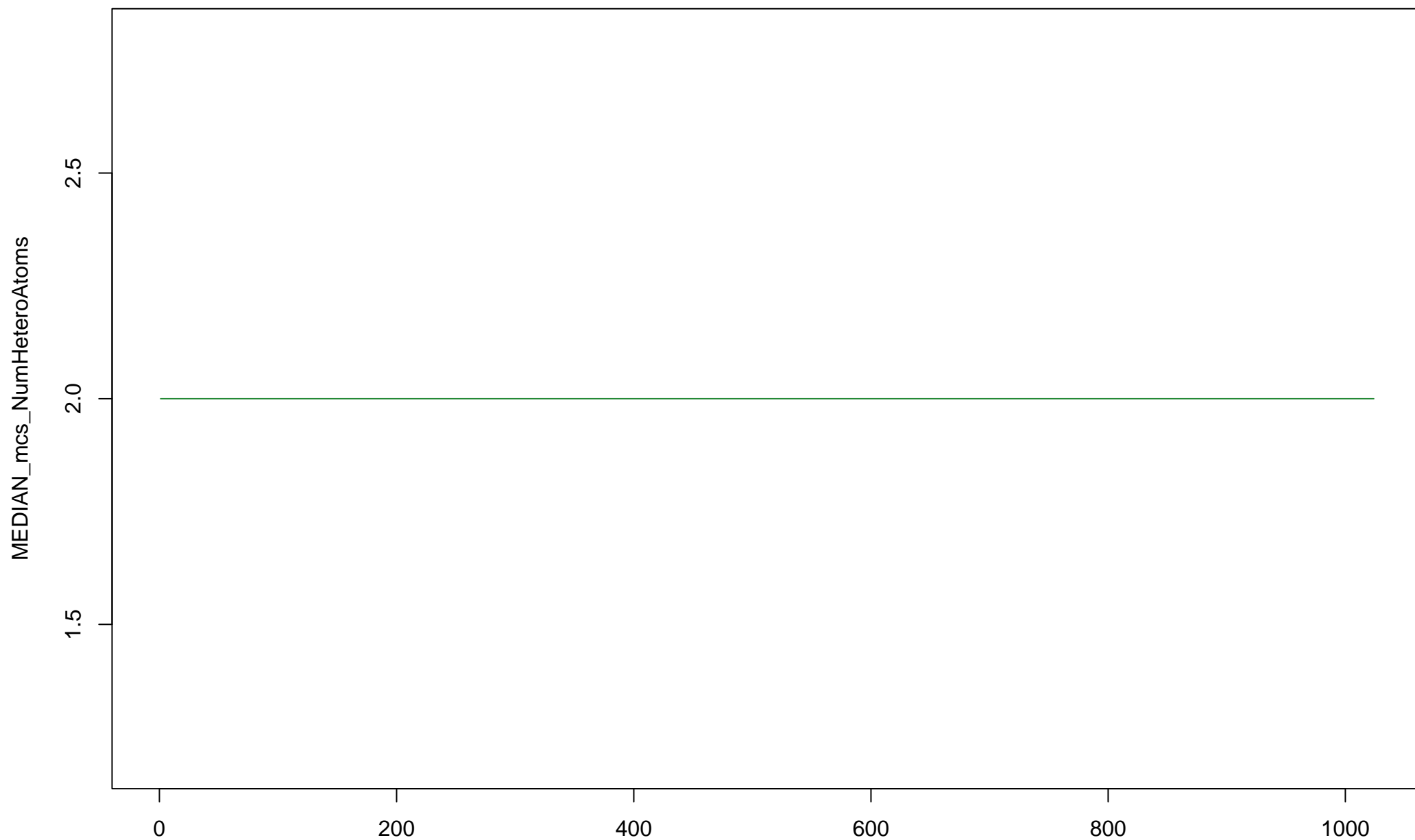
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



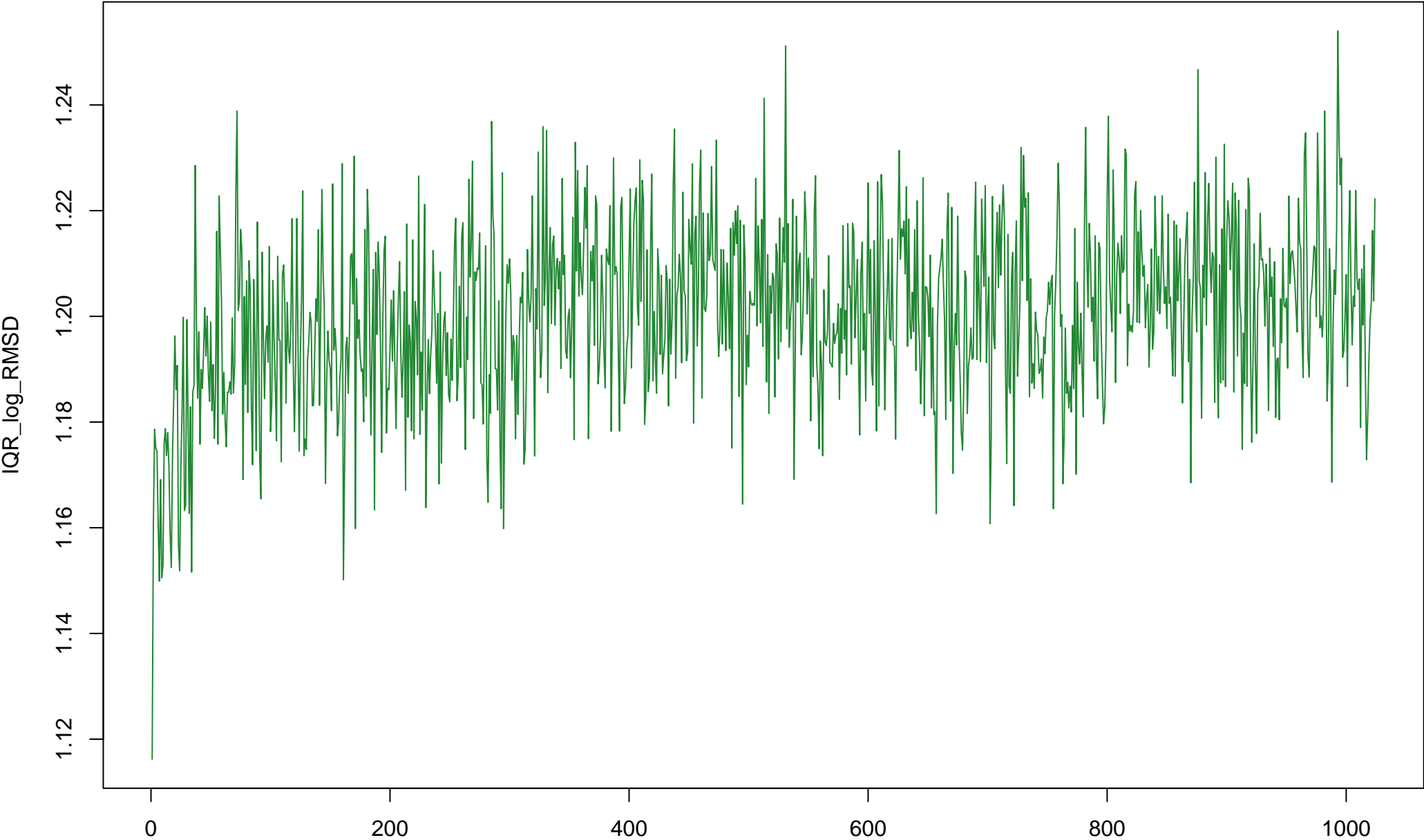
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



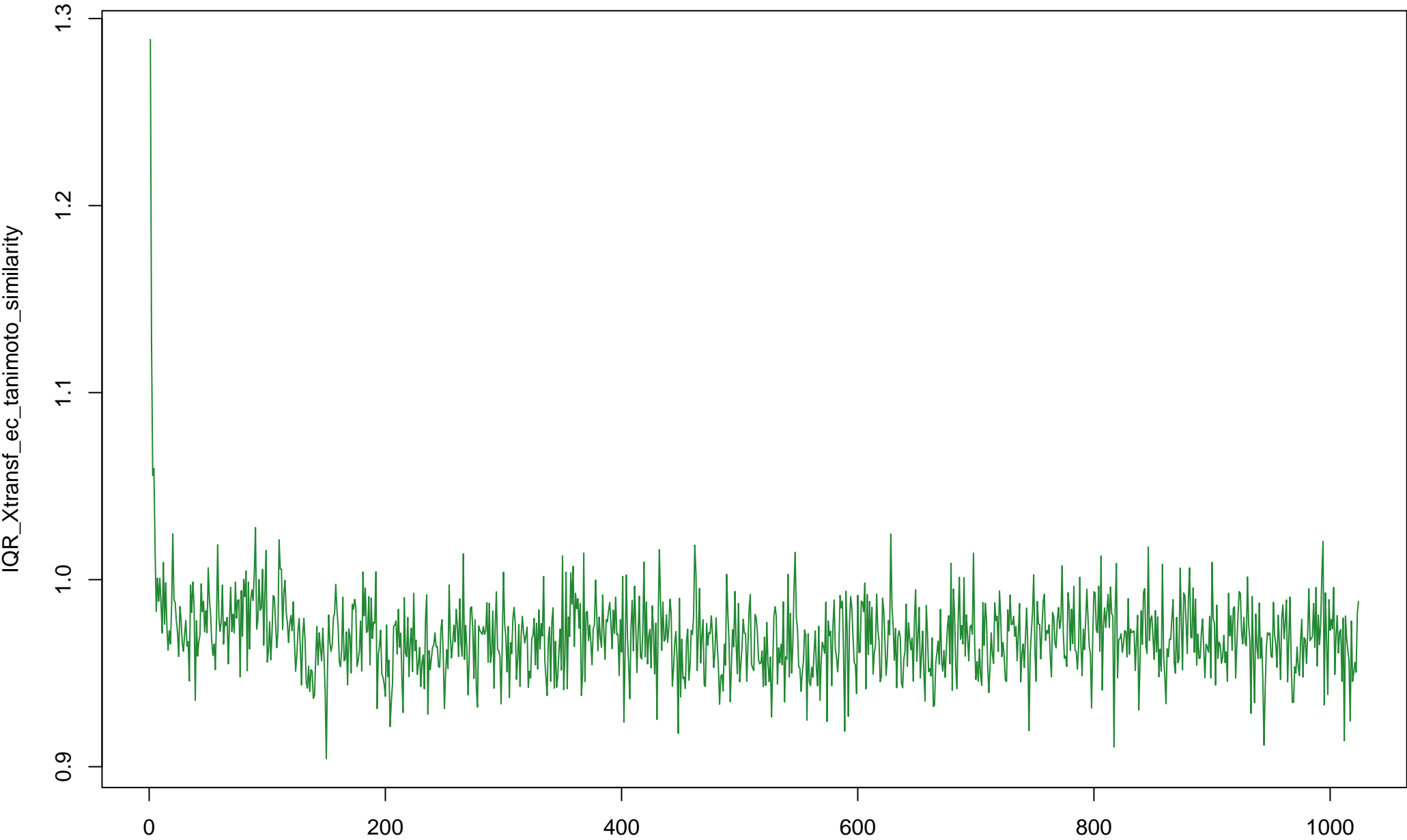
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



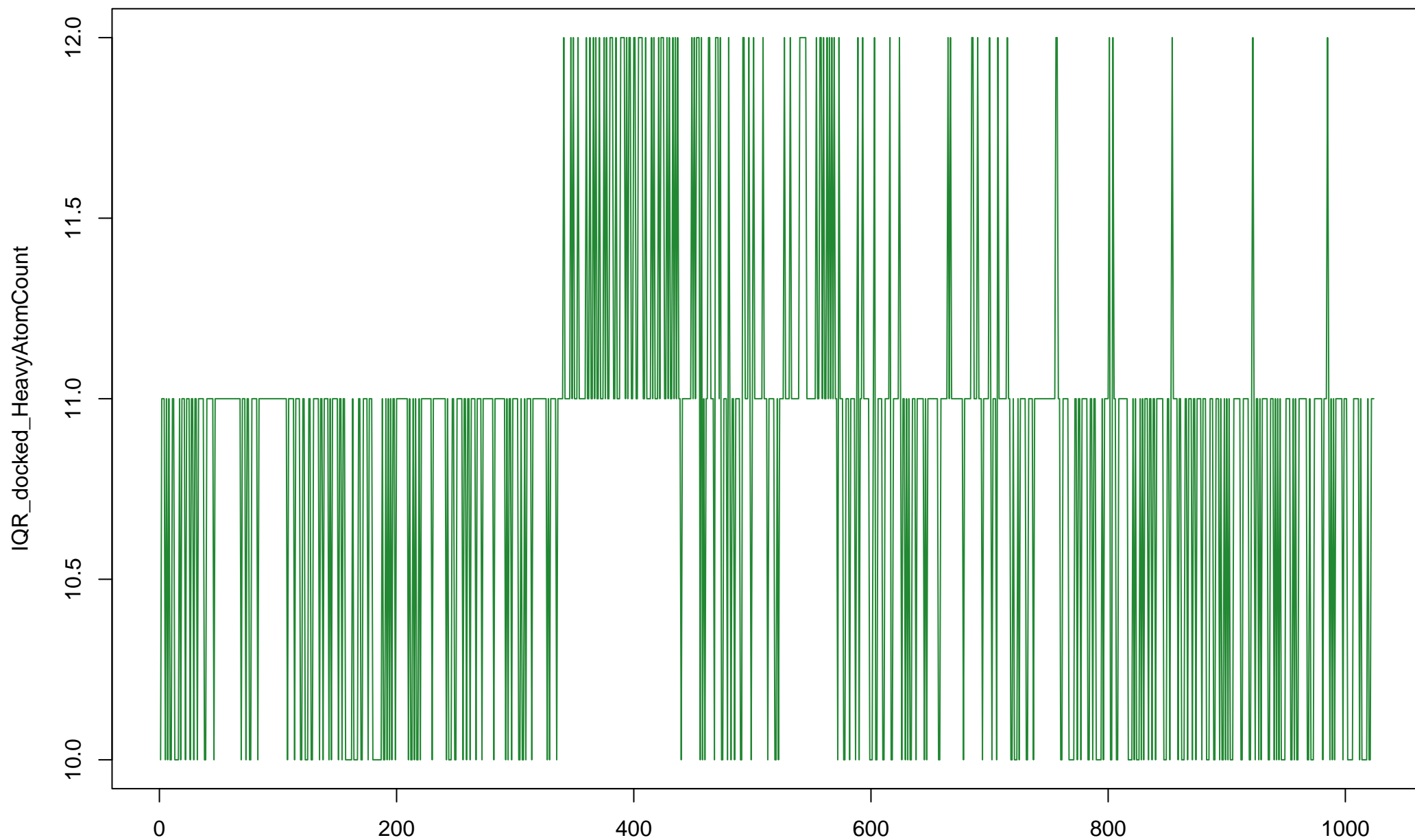
IQR_log_RMSD
ESS = 72.3 | BMK = 0.148 | MCSE(6.27) = 8.06 | stat: FALSE | burn: 0



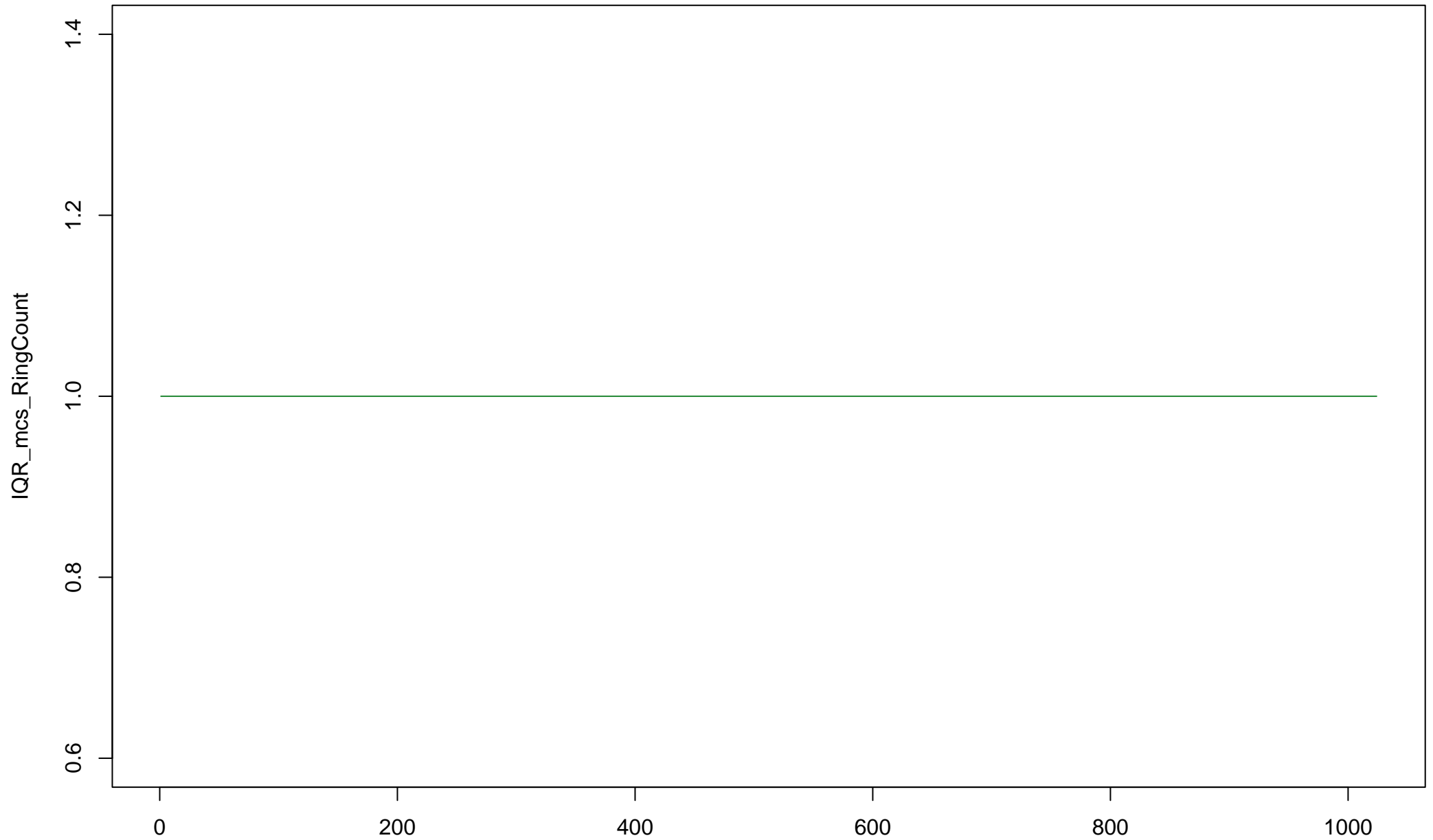
IQR_Xtransf_ec_tanimoto_similarity
ESS = 291 | BMK = 0.0879 | MCSE(6.27) = 6.6 | stat: FALSE | burn: 0



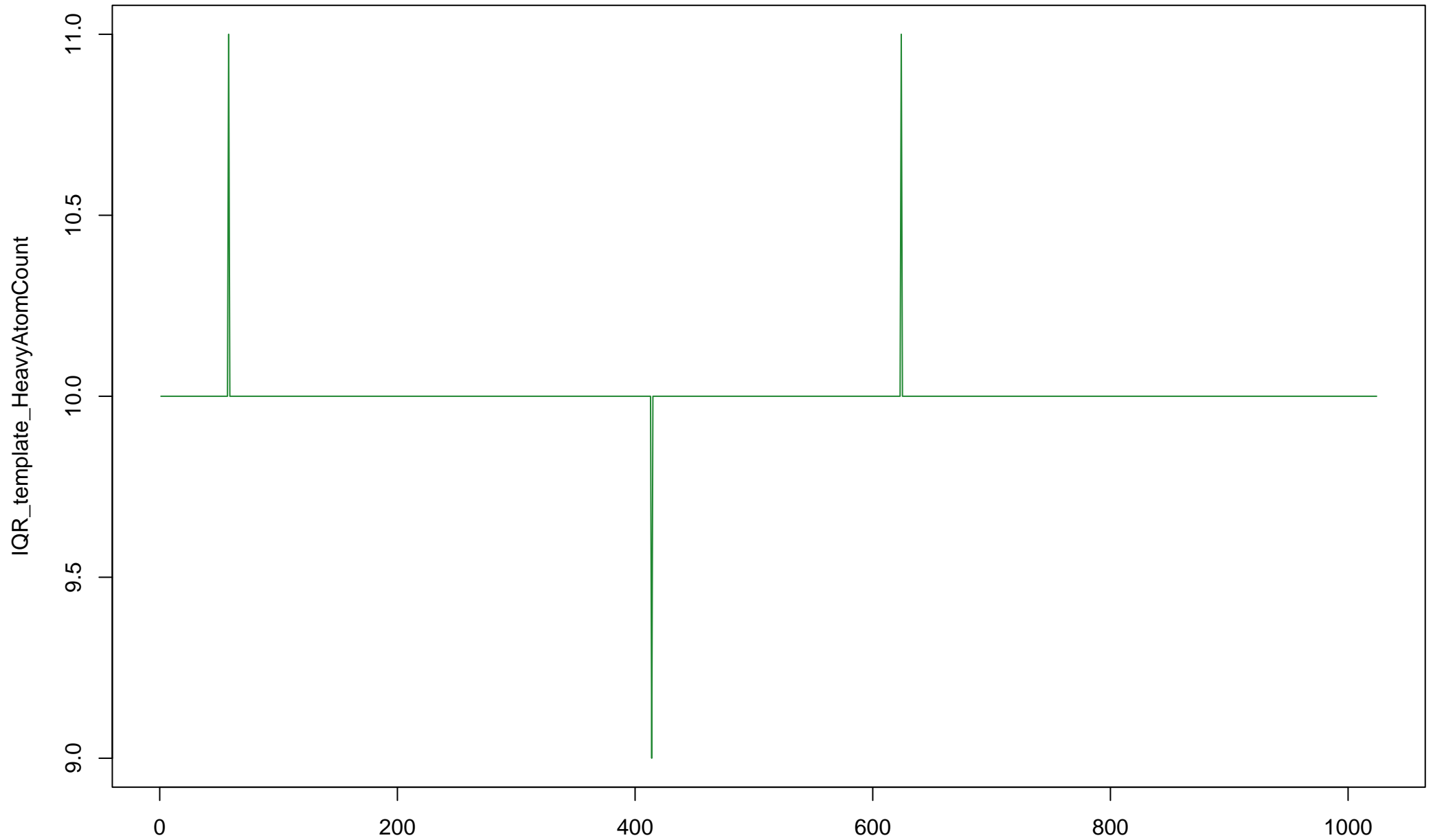
IQR_docked_HeavyAtomCount
ESS = 45.6 | BMK = 0.0518 | MCSE(6.27) = 8.28 | stat: TRUE | burn: 0



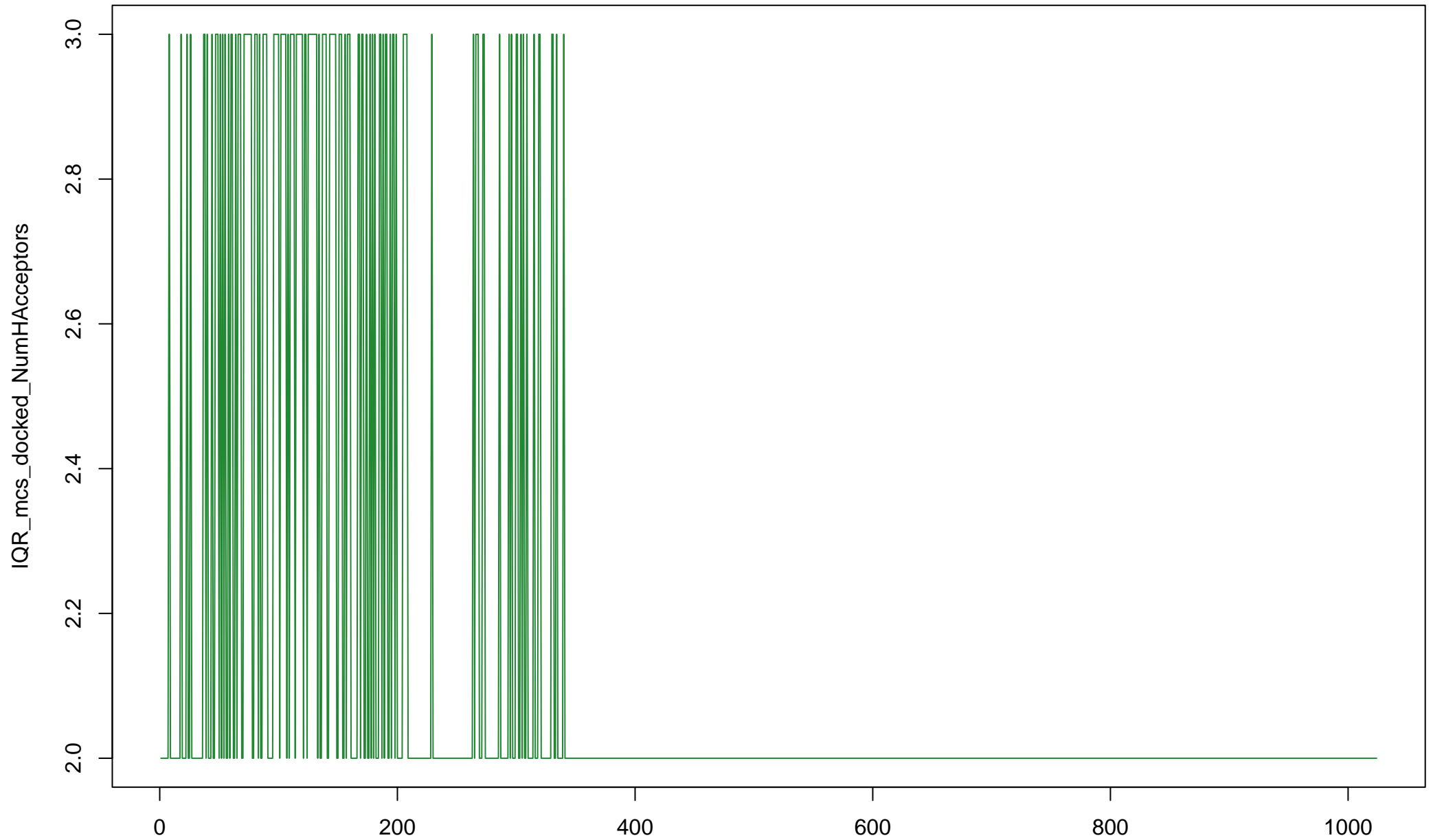
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



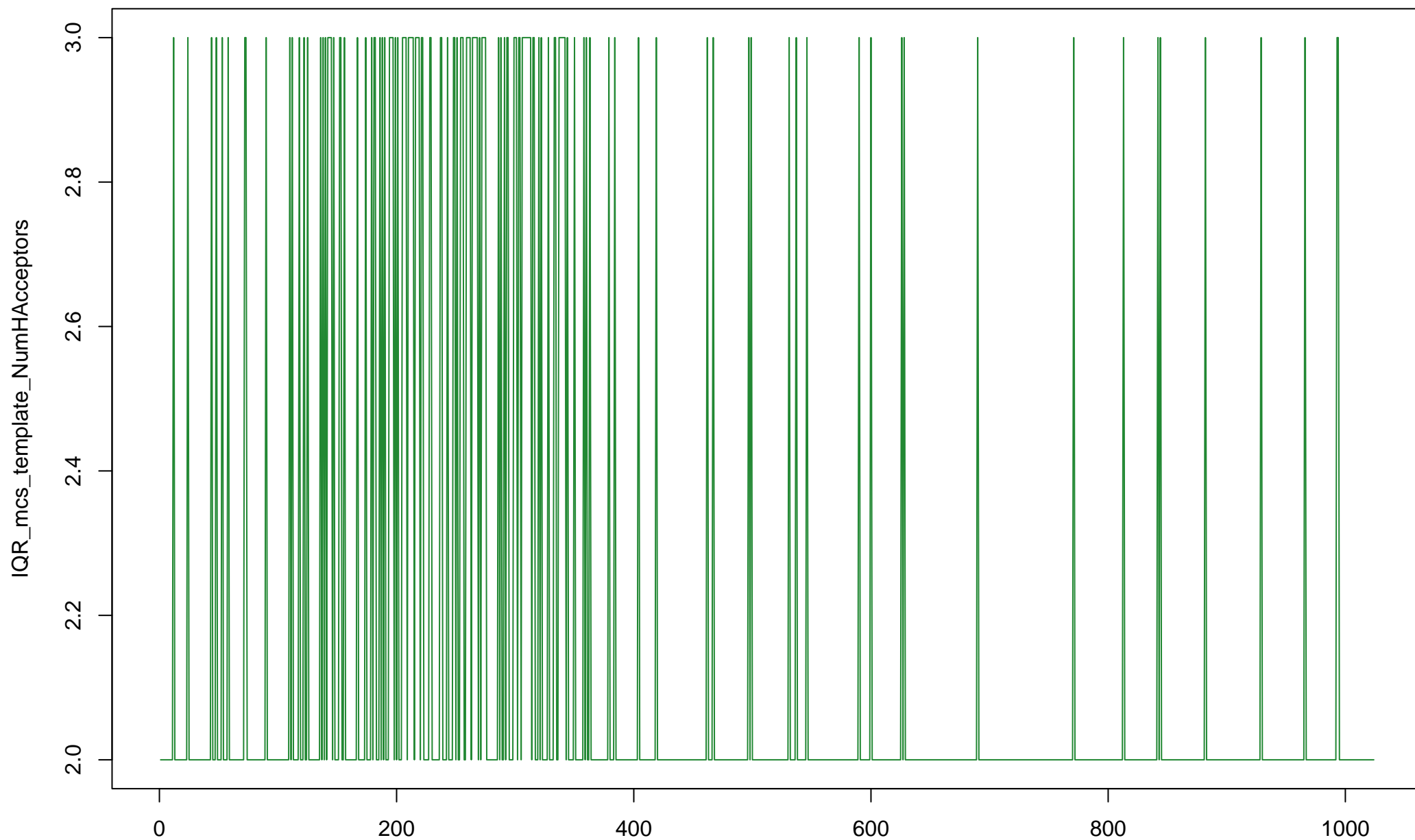
IQR_template_HeavyAtomCount
ESS = 1020 | BMK = 0.166 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 714



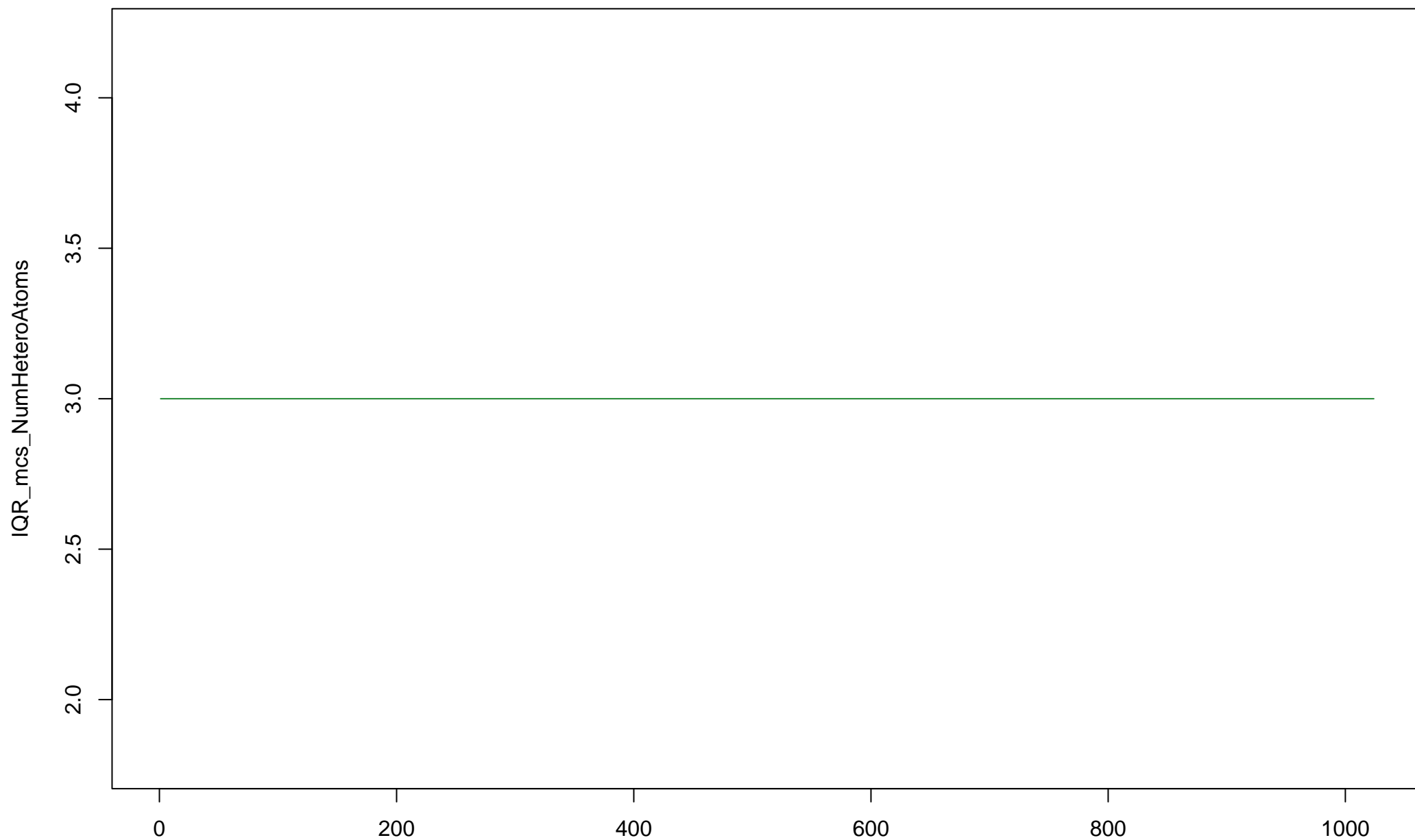
IQR_mcs_docked_NumHAcceptors
ESS = 5.43 | BMK = 0.506 | MCSE(6.27) = 12.1 | stat: FALSE | burn: 0



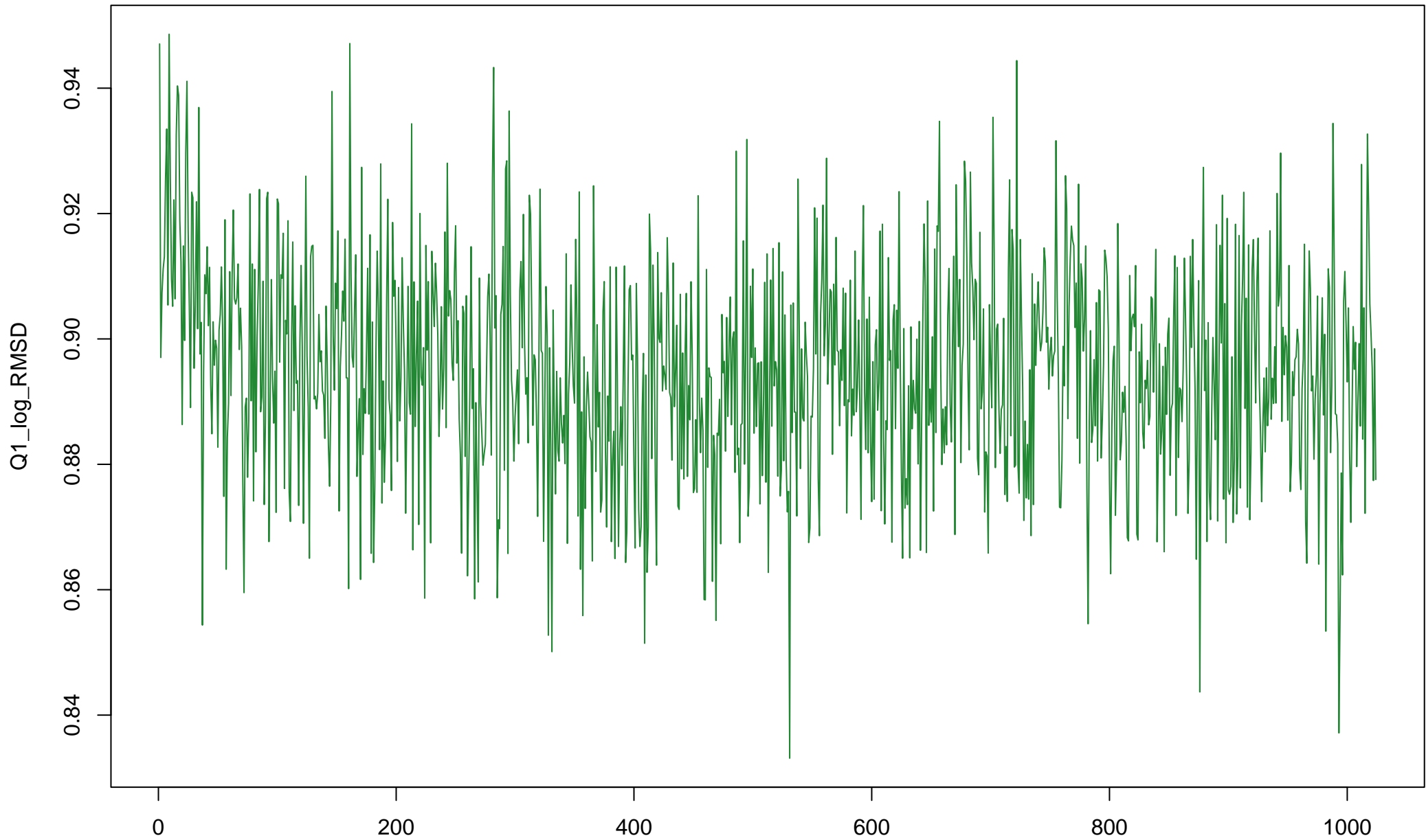
IQR_mcs_template_NumHAcceptors
ESS = 73.4 | BMK = 0.318 | MCSE(6.27) = 9.18 | stat: TRUE | burn: 0



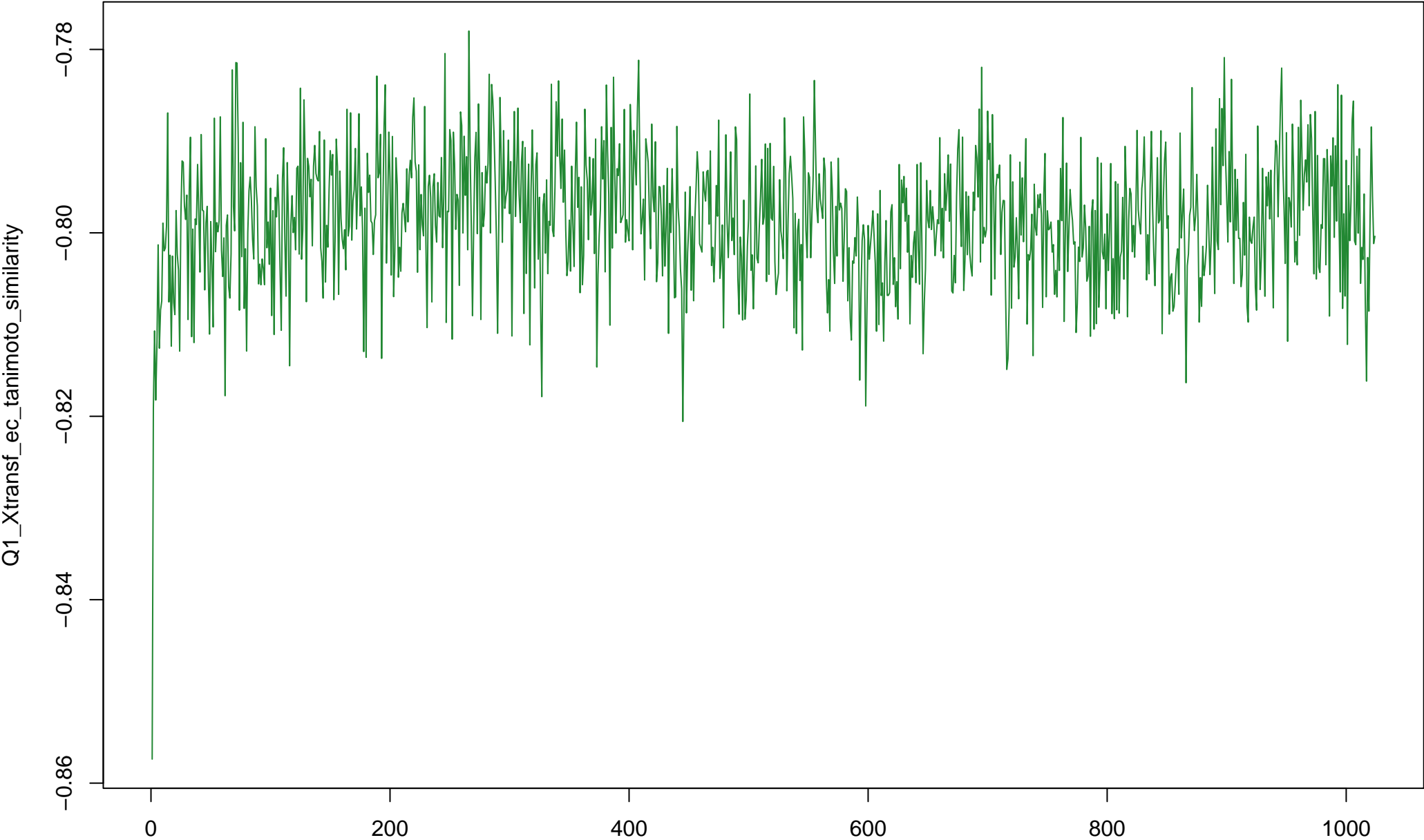
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



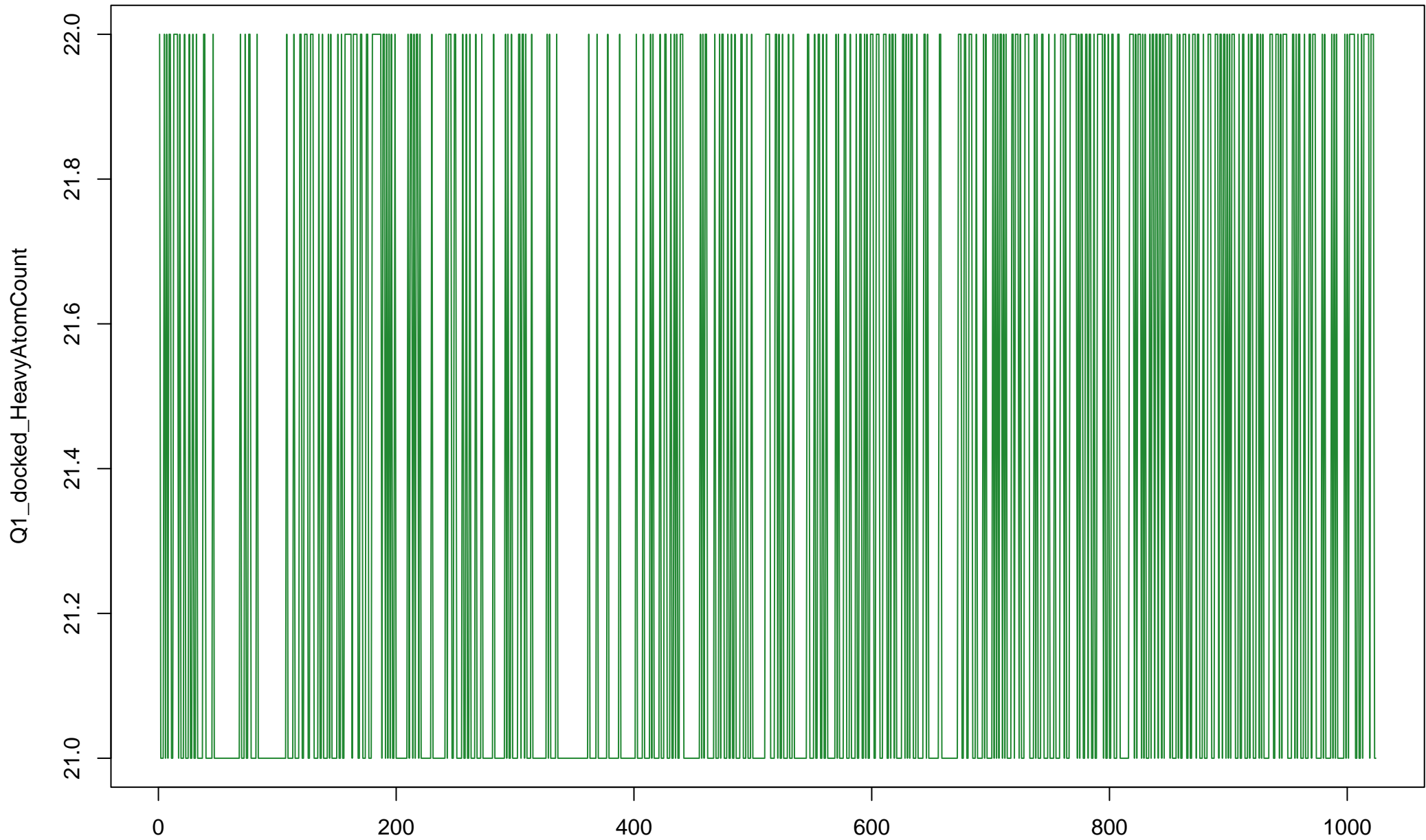
Q1_log_RMSD
ESS = 390 | BMK = 0.0821 | MCSE(6.27) = 5.85 | stat: FALSE | burn: 0



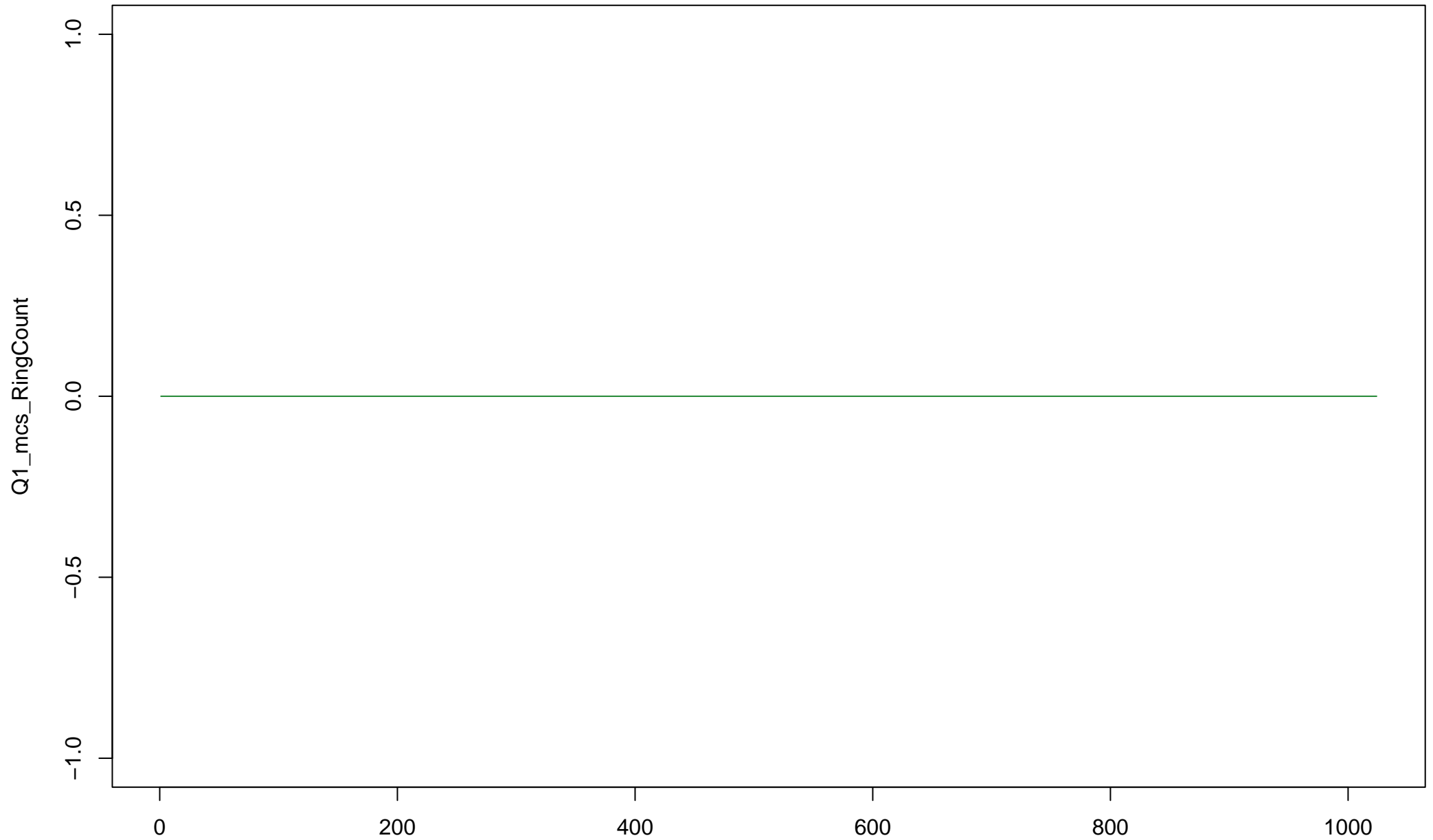
Q1_Xtransf_ec_tanimoto_similarity
ESS = 385 | BMK = 0.0943 | MCSE(6.27) = 6.04 | stat: TRUE | burn: 0



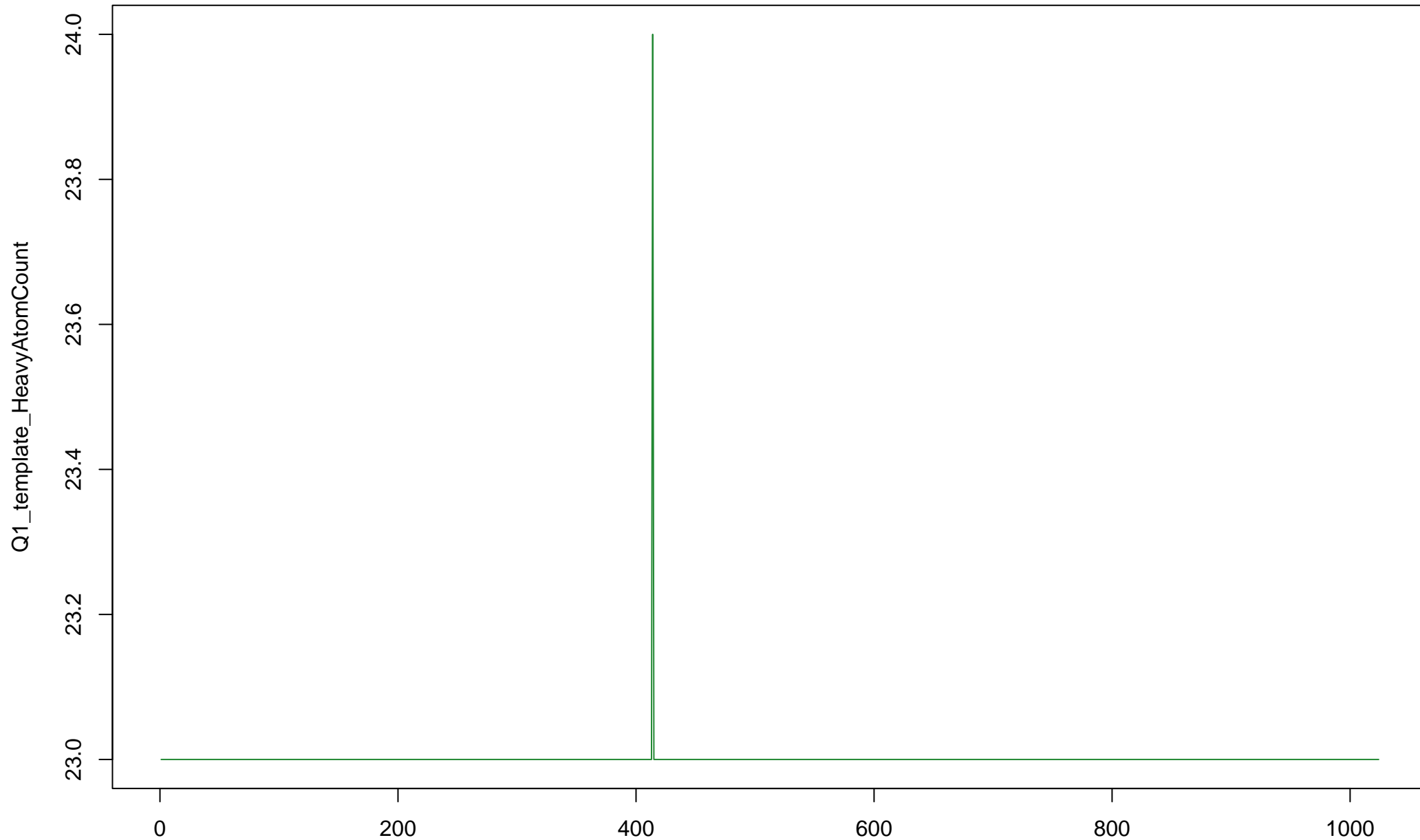
Q1_docked_HeavyAtomCount
ESS = 289 | BMK = 0.0982 | MCSE(6.27) = 5.82 | stat: FALSE | burn: 0



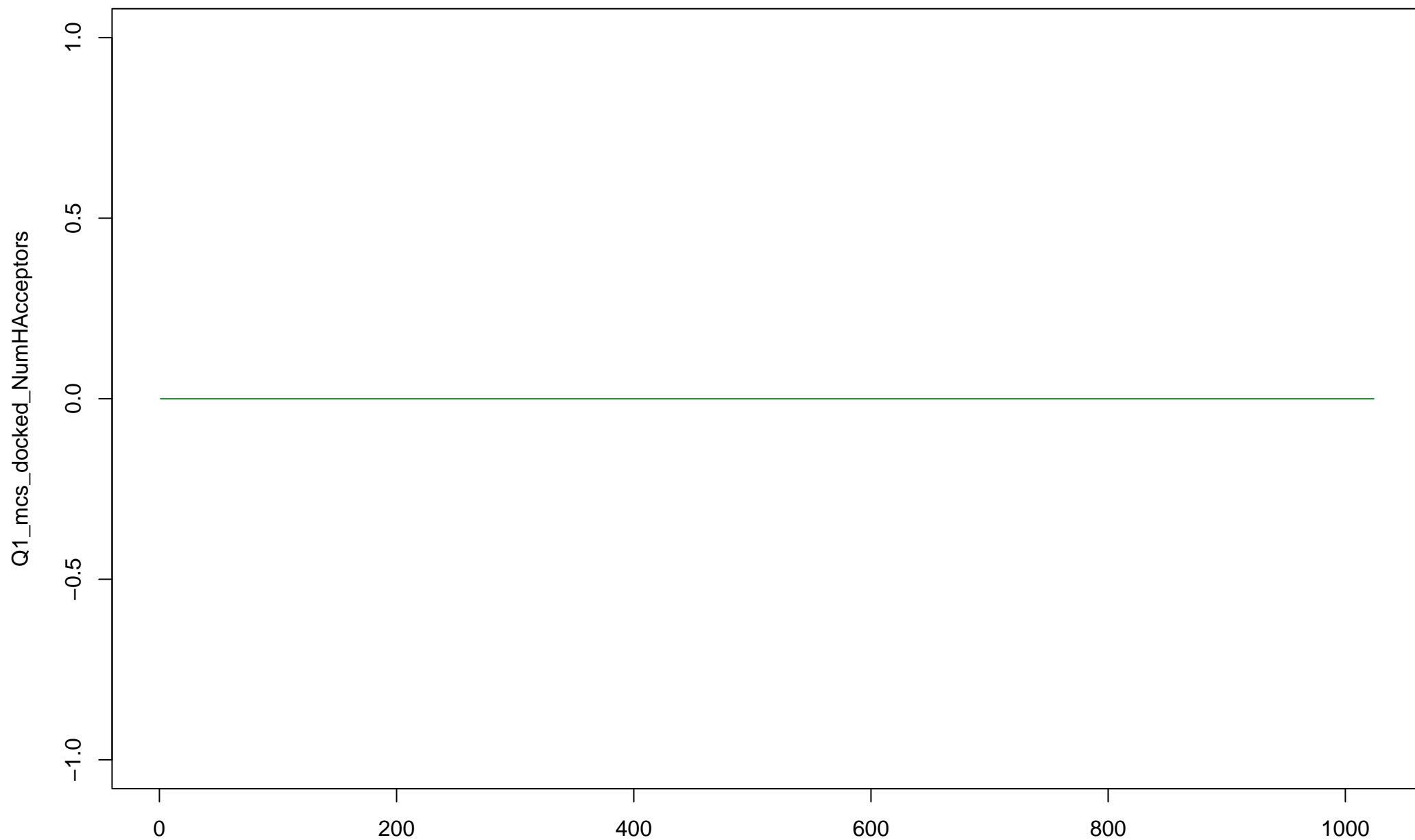
Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



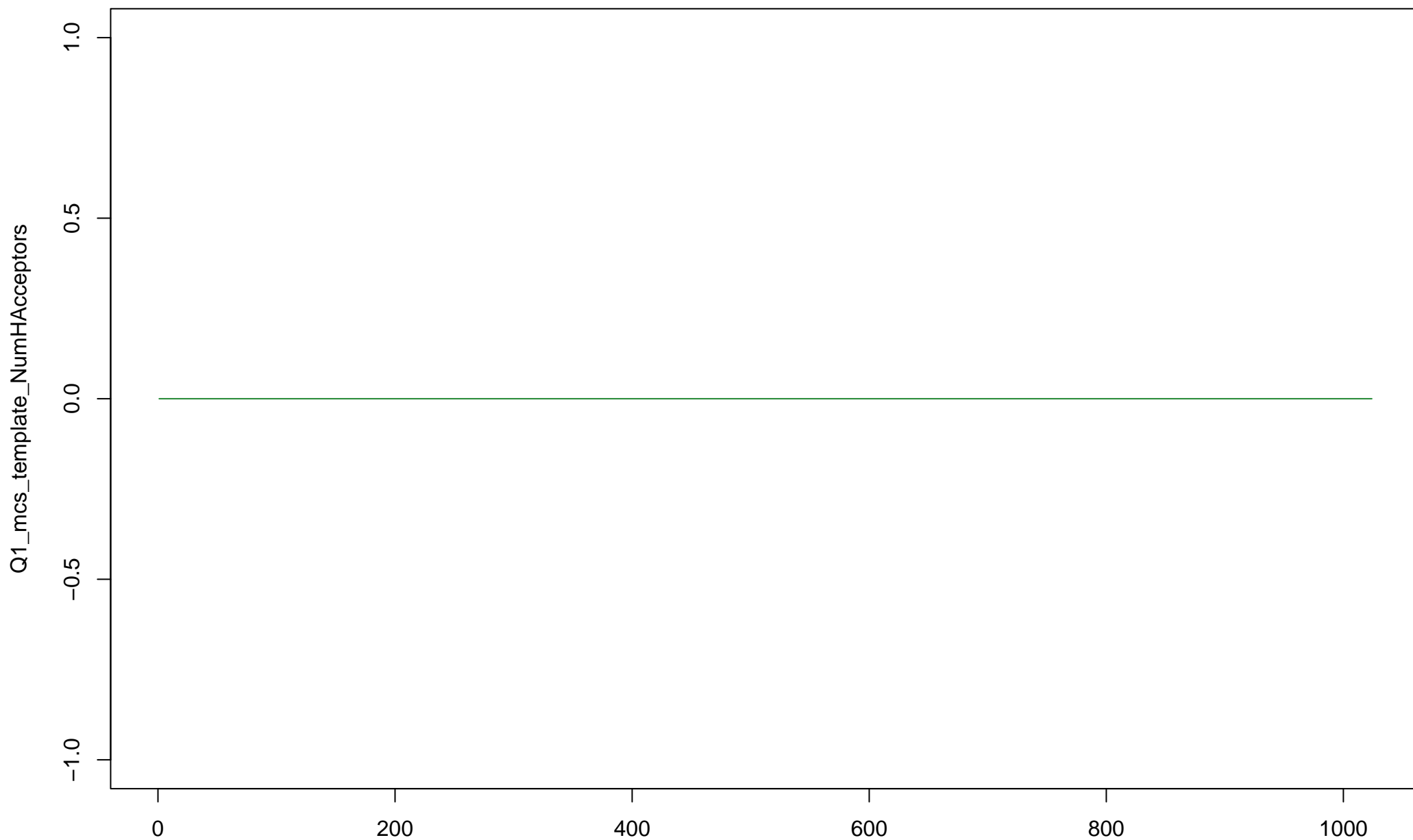
Q1_template_HeavyAtomCount
ESS = 1020 | BMK = 0.516 | MCSE(6.27) = 3.12 | stat: FALSE | burn: 0



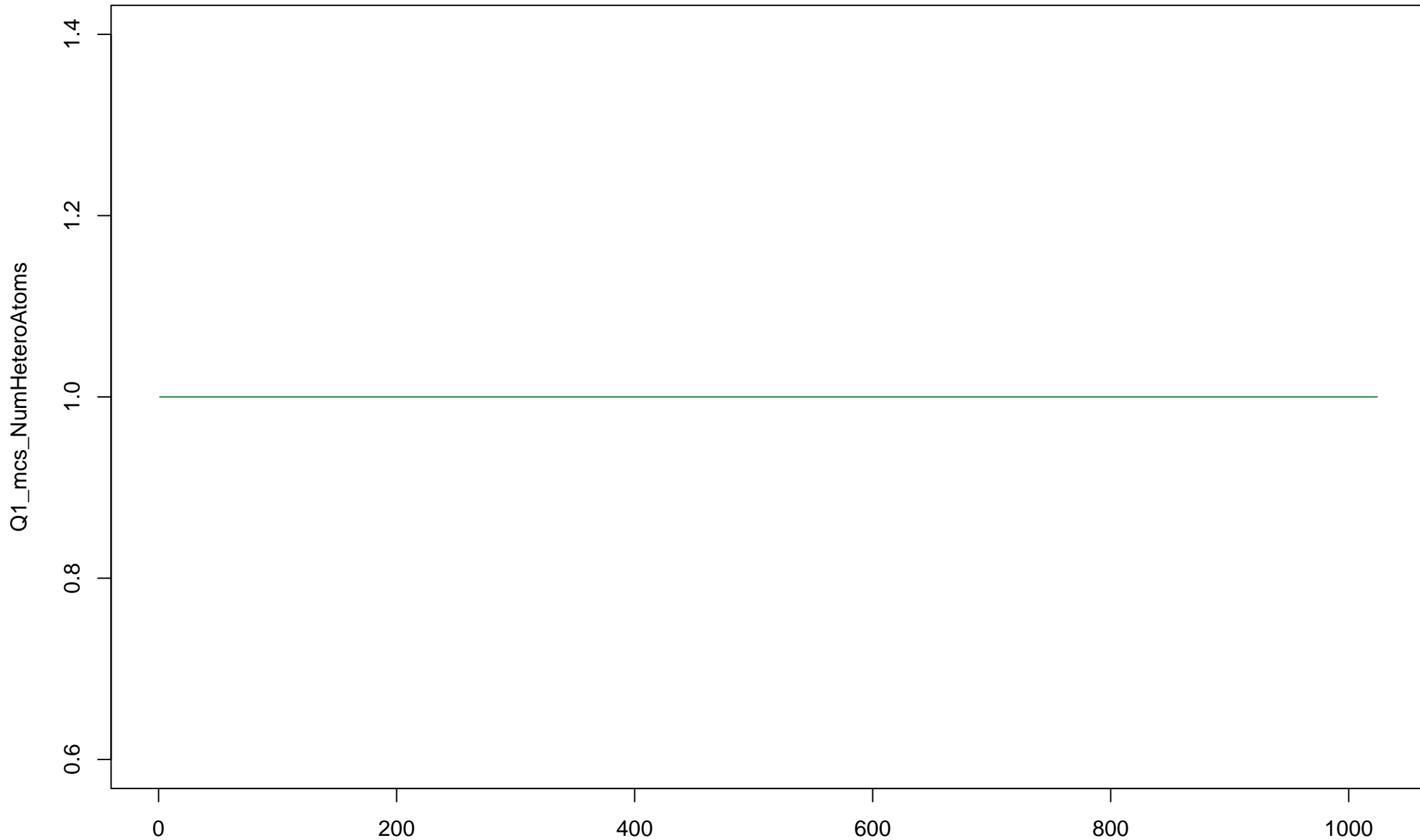
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



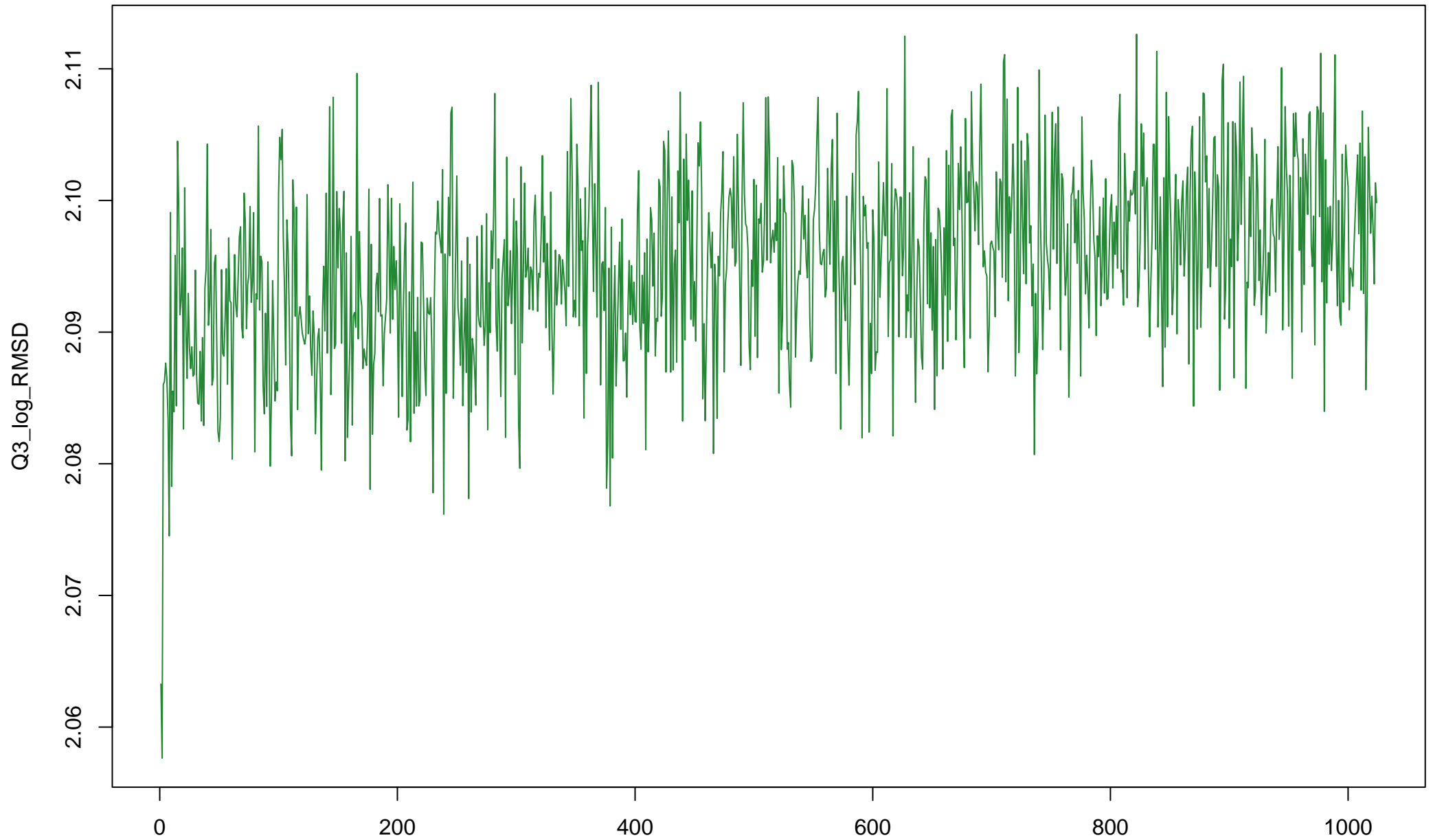
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



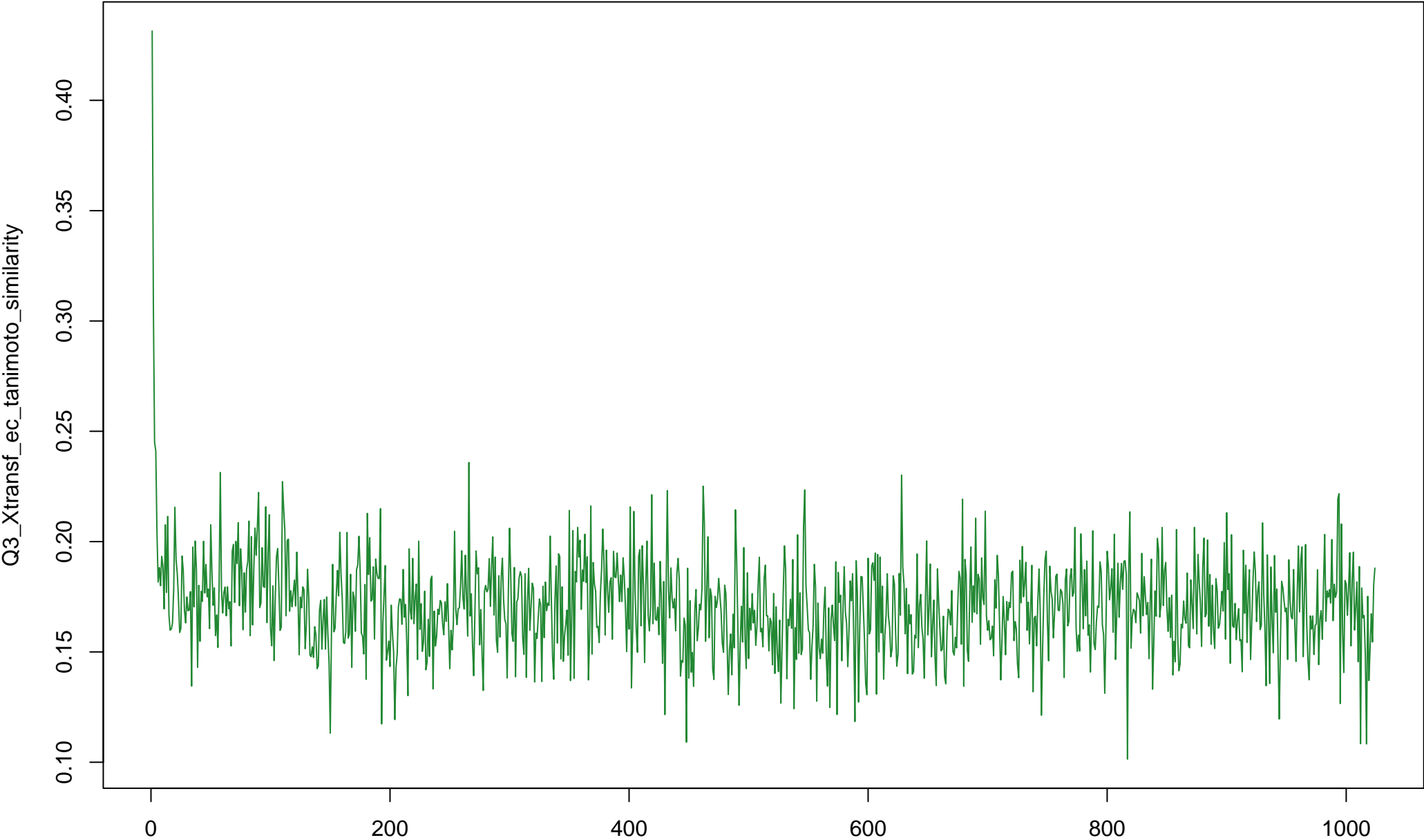
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



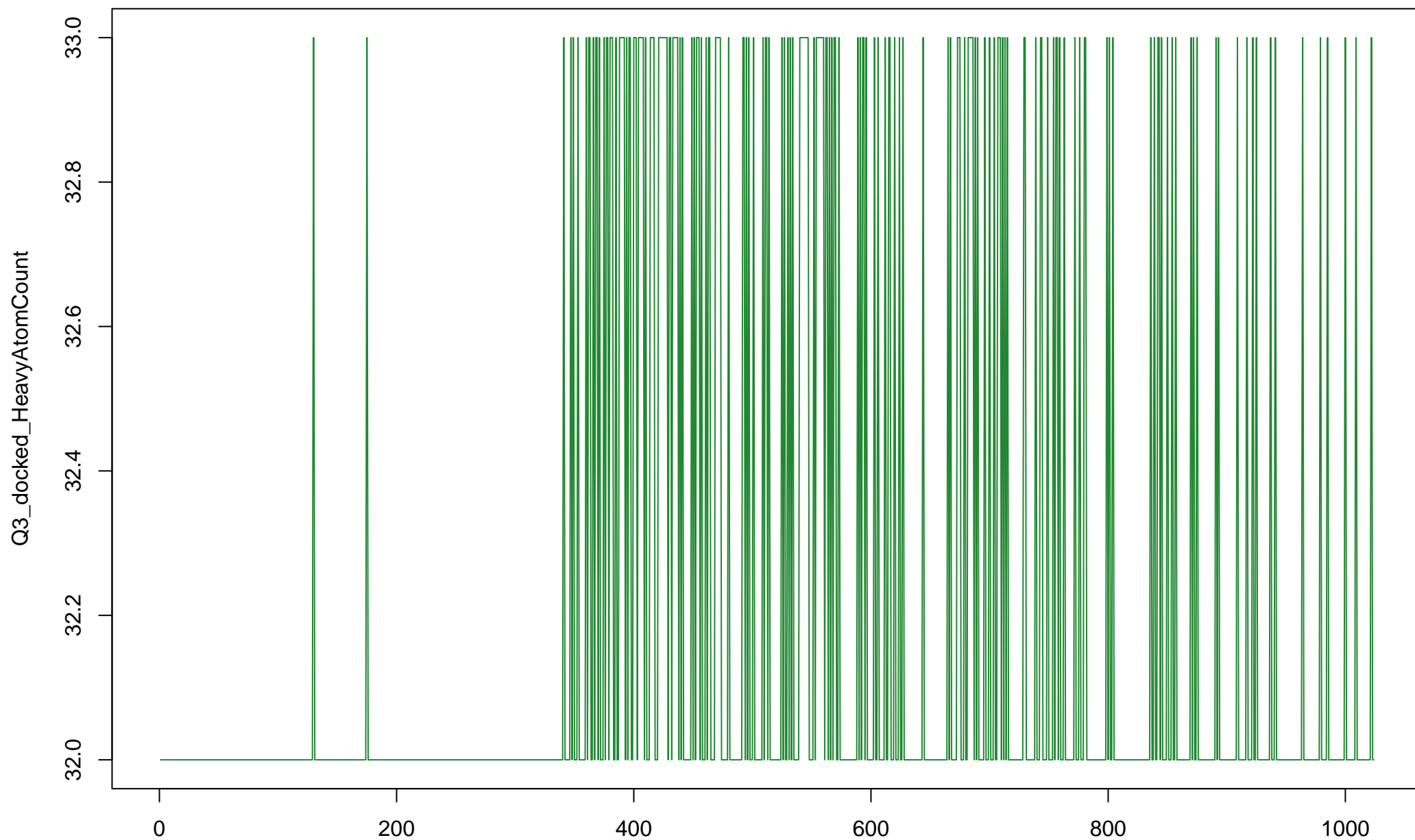
Q3_log_RMSD
ESS = 84.8 | BMK = 0.244 | MCSE(6.27) = 7.85 | stat: FALSE | burn: 0



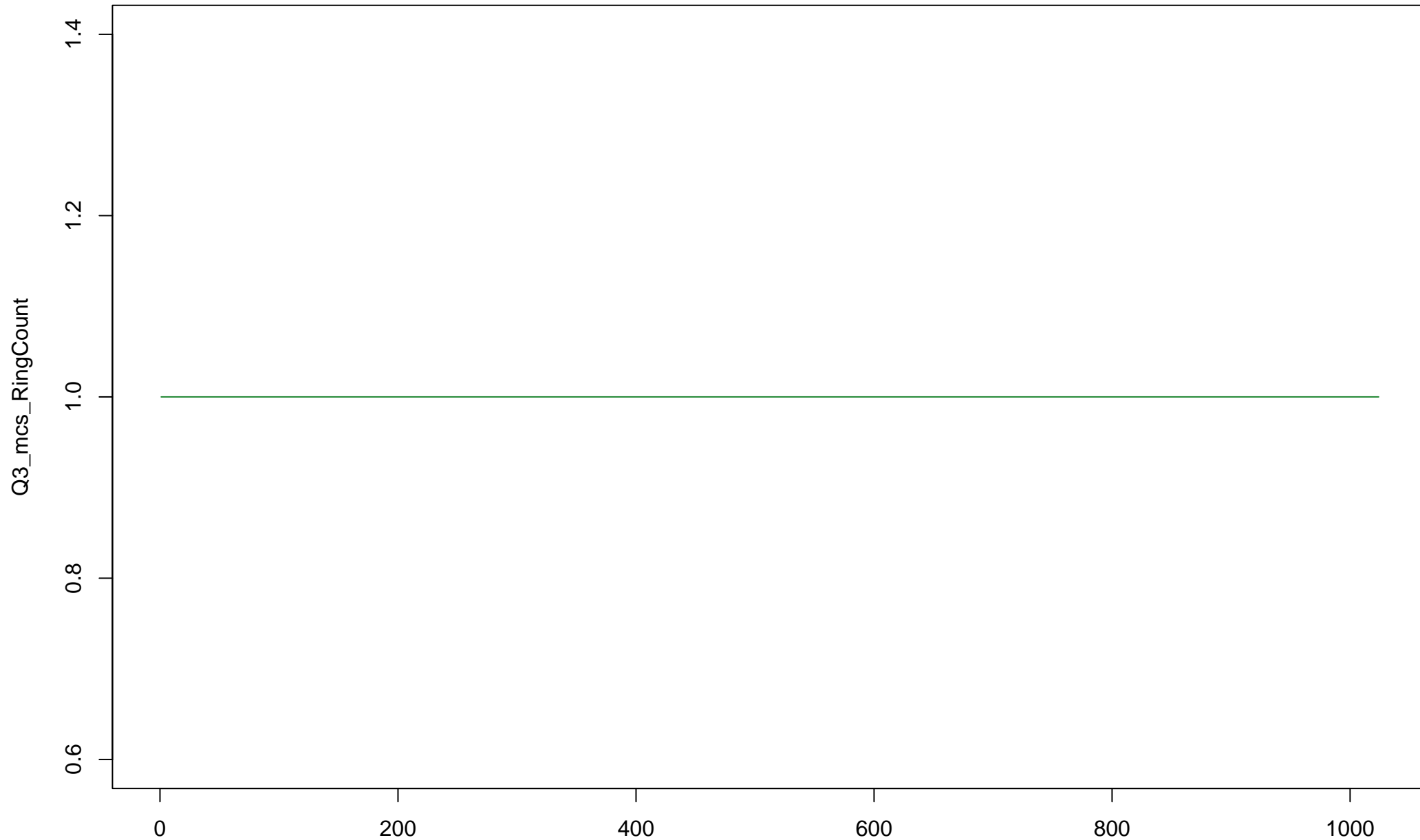
Q3_Xtransf_ec_tanimoto_similarity
ESS = 386 | BMK = 0.0932 | MCSE(6.27) = 5.9 | stat: FALSE | burn: 0



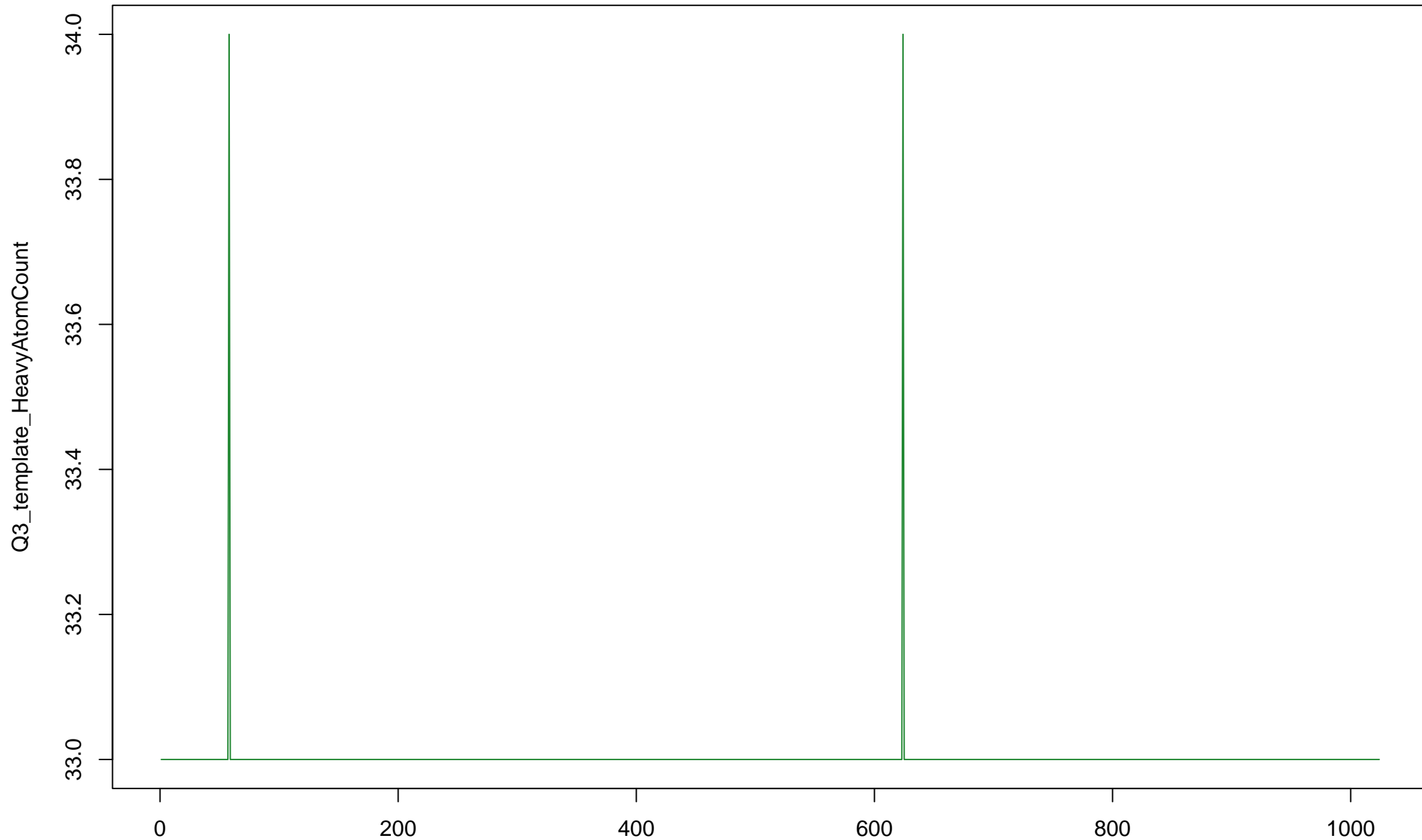
Q3_docked_HeavyAtomCount
ESS = 46.8 | BMK = 0.0522 | MCSE(6.27) = 8.78 | stat: FALSE | burn: 0



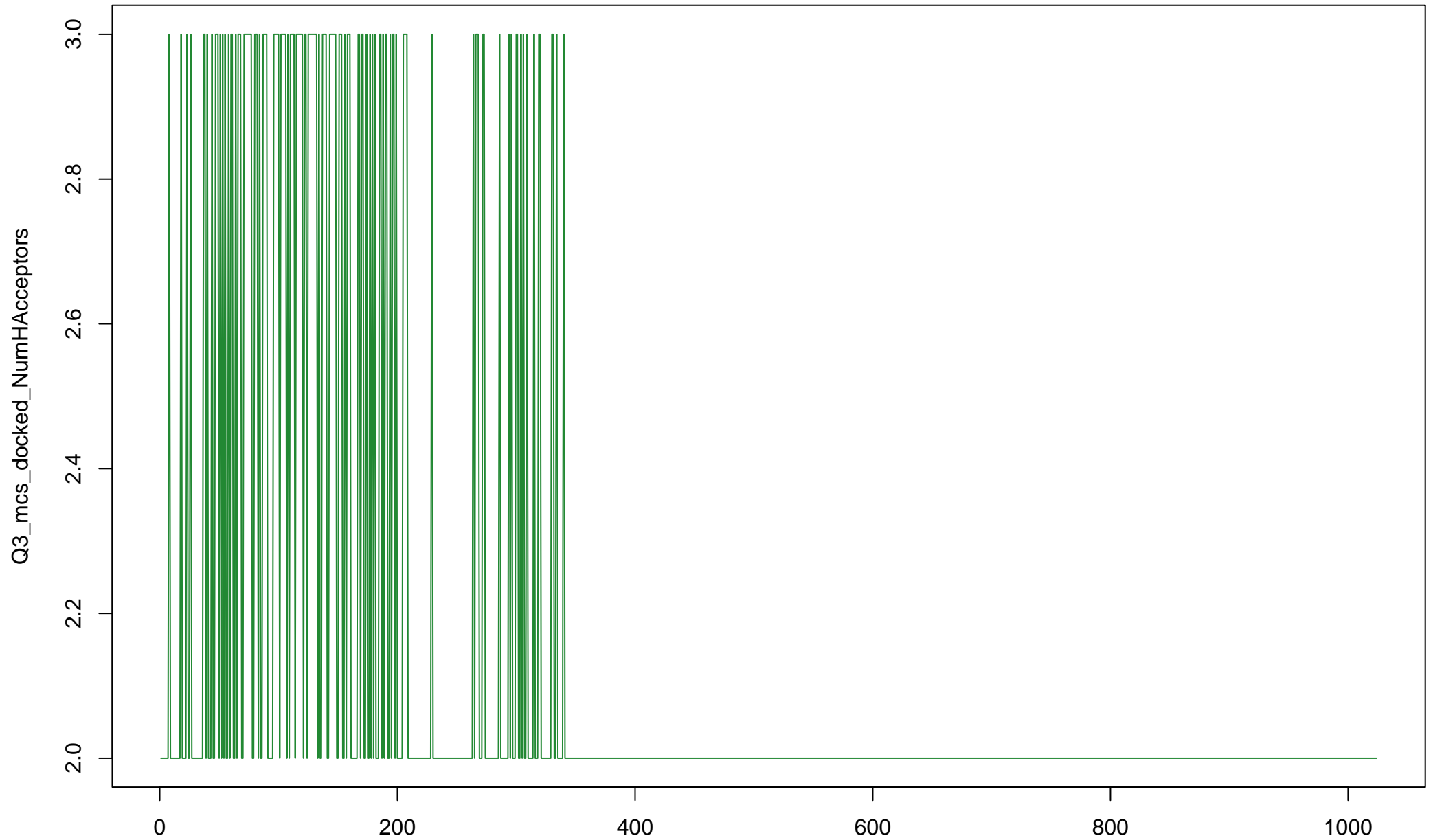
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



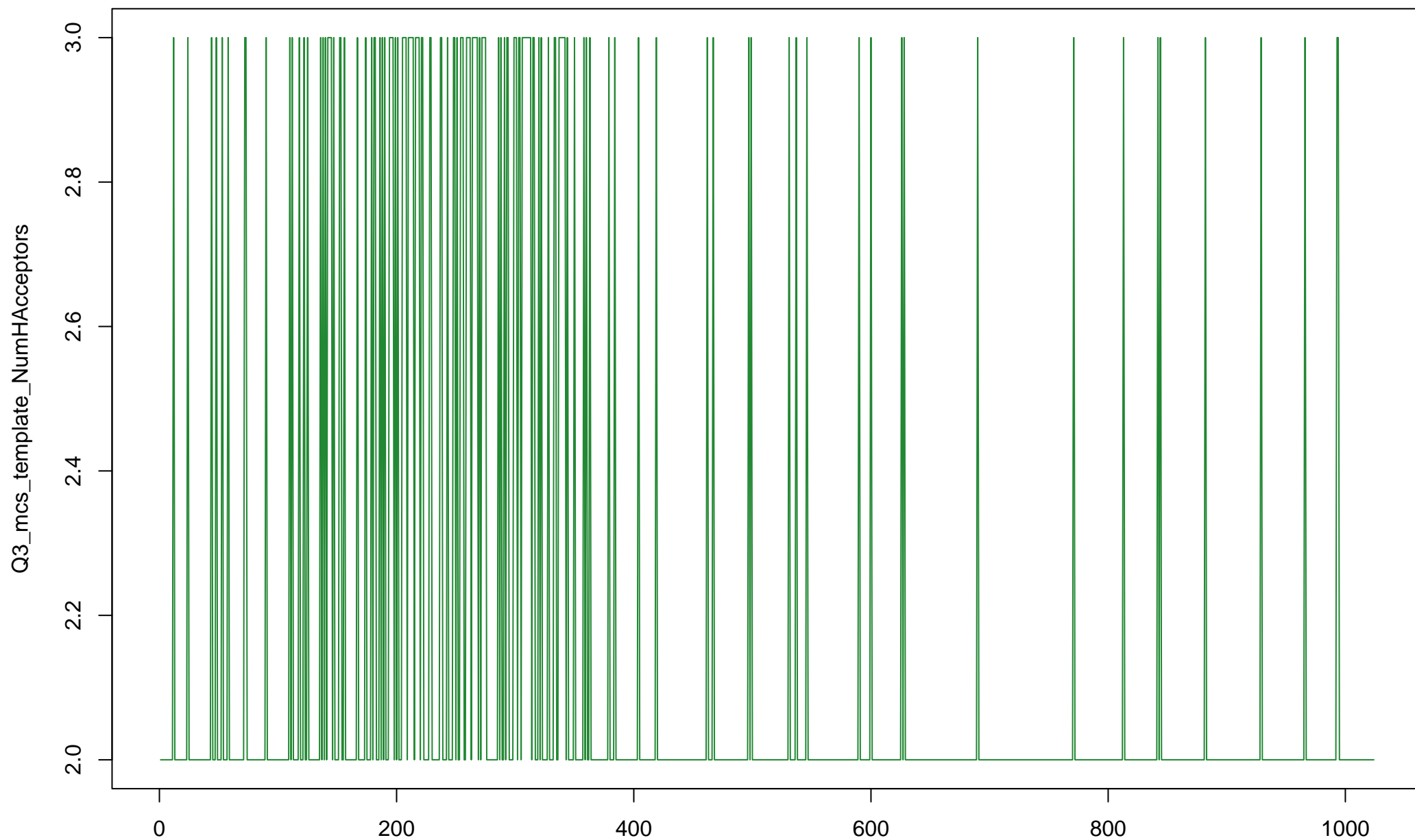
Q3_template_HeavyAtomCount
ESS = 1020 | BMK = 0 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0



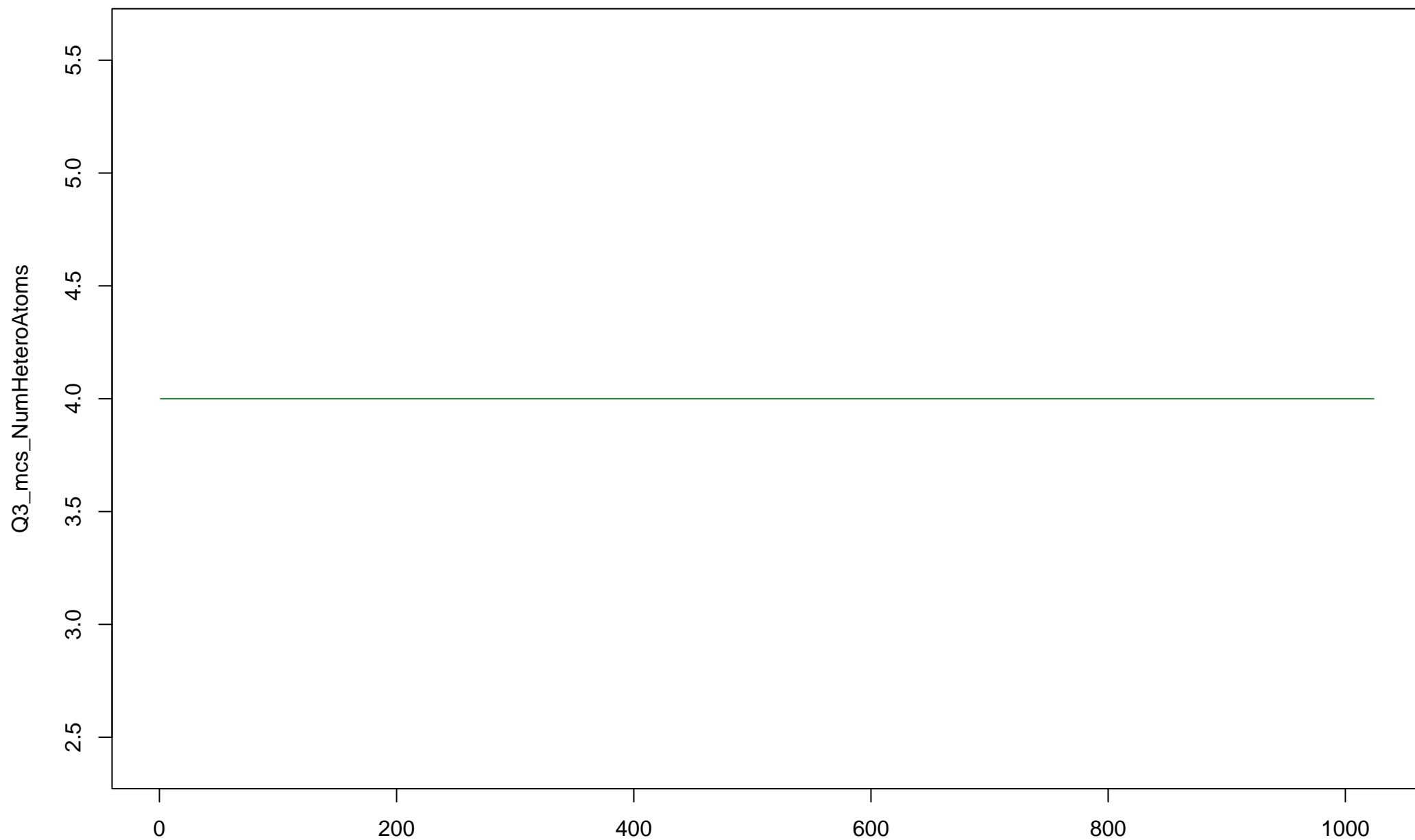
Q3_mcs_docked_NumHAcceptors
ESS = 5.43 | BMK = 0.506 | MCSE(6.27) = 12.1 | stat: FALSE | burn: 0



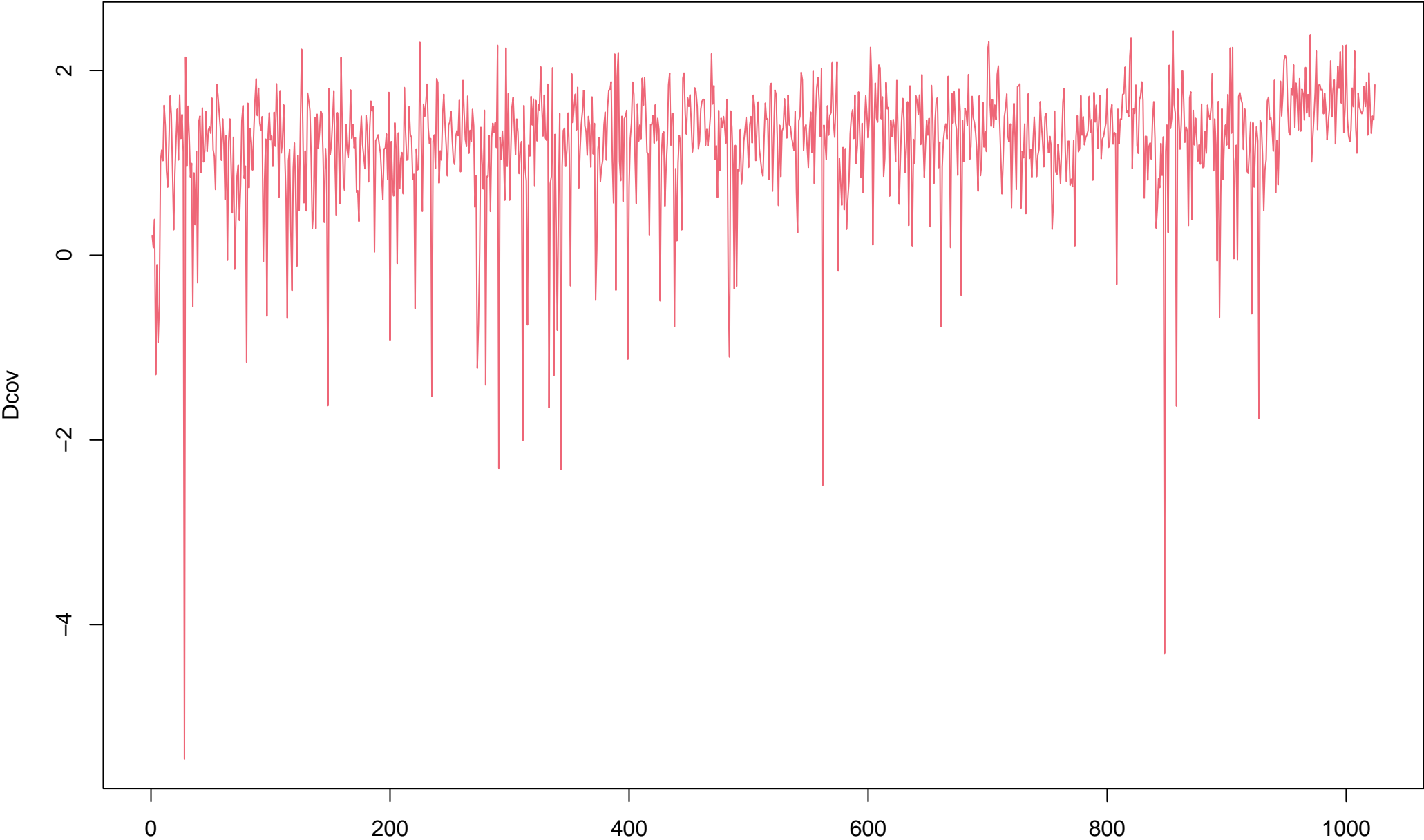
Q3_mcs_template_NumHAcceptors
ESS = 73.4 | BMK = 0.318 | MCSE(6.27) = 9.18 | stat: TRUE | burn: 0



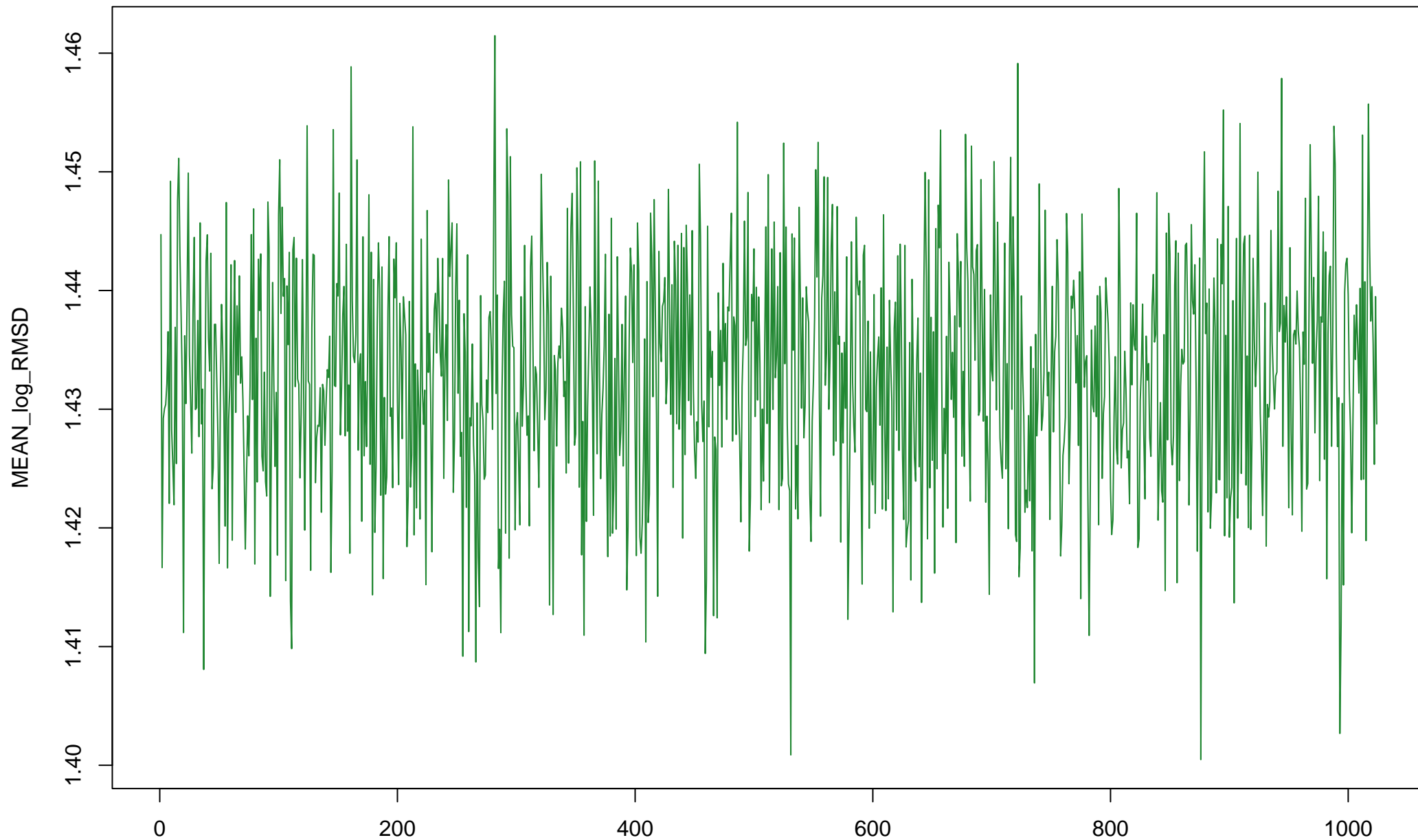
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



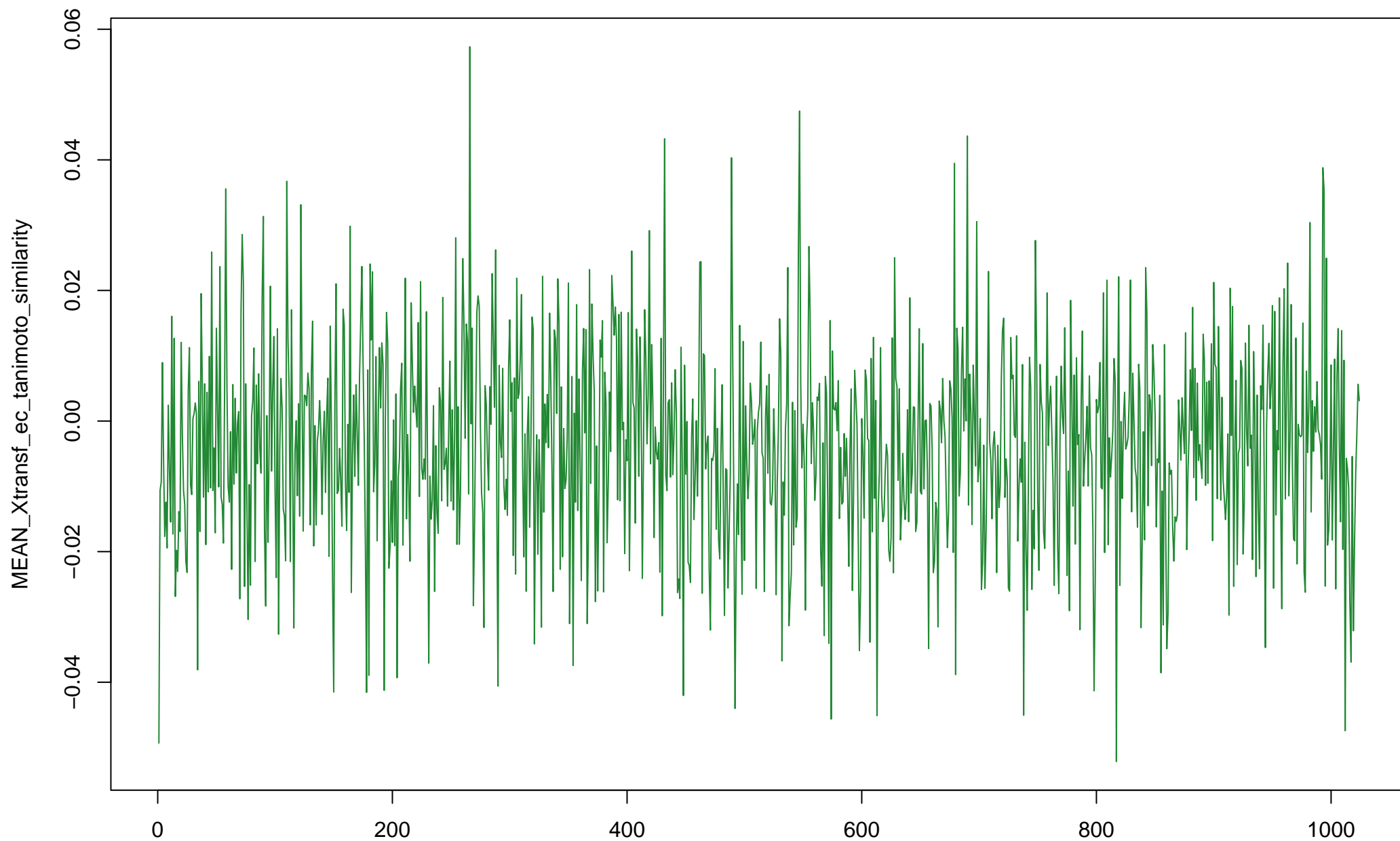
Dcov
ESS = 239 | BMK = 0.165 | MCSE(6.27) = 5.82 | stat: FALSE | burn: 0



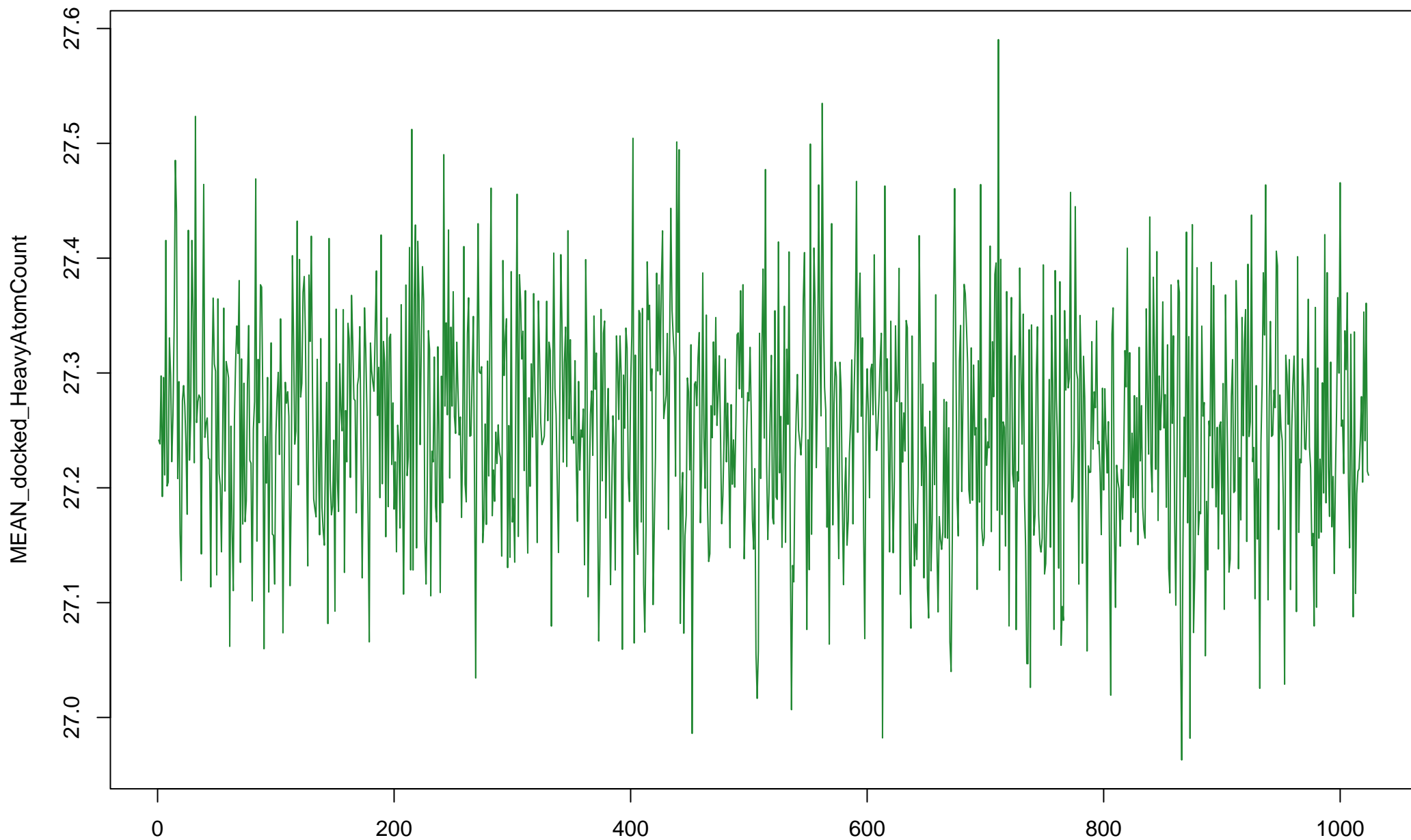
MEAN_log_RMSD
ESS = 1020 | BMK = 0.0712 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0



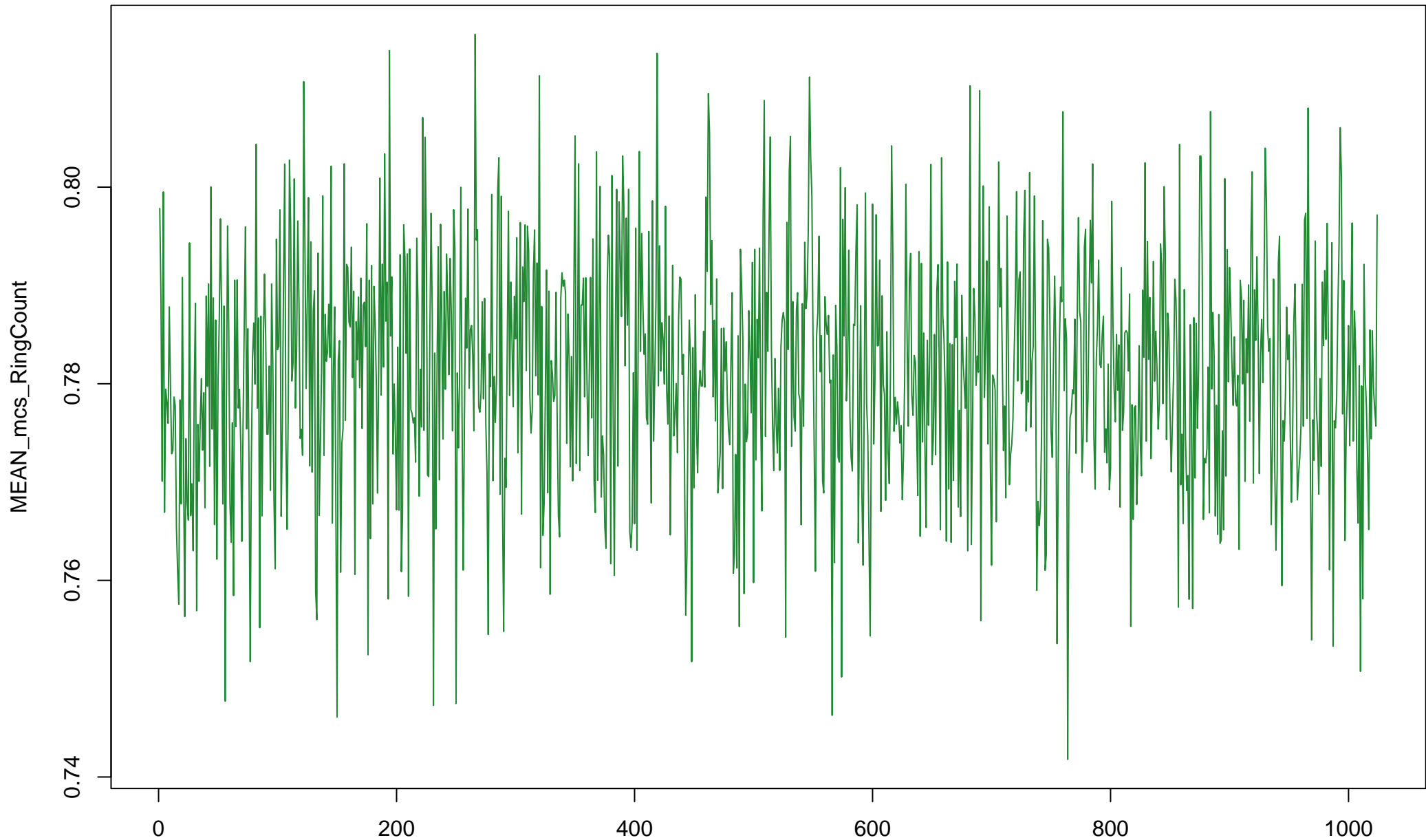
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0641 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0



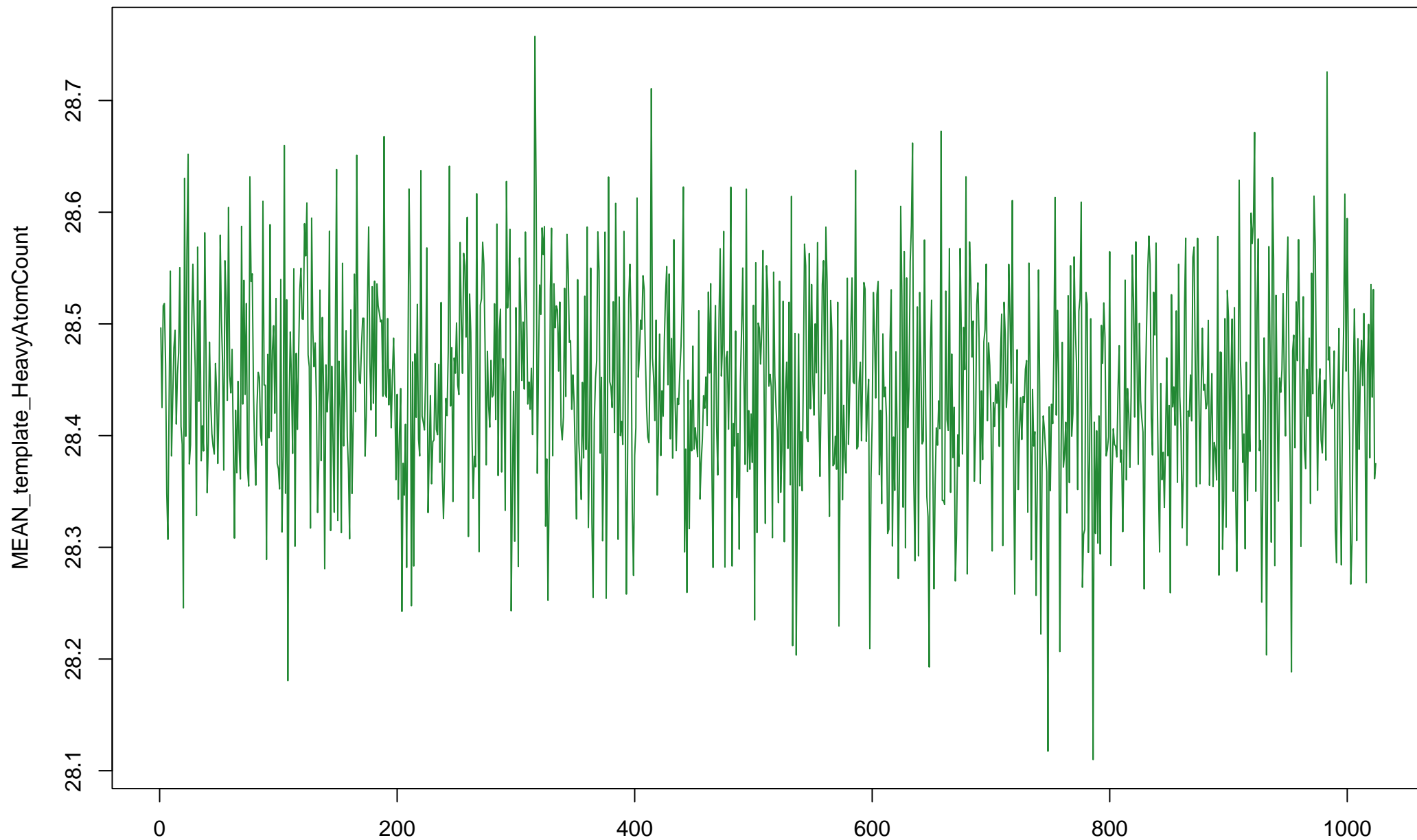
MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0787 | MCSE(6.27) = 3.75 | stat: TRUE | burn: 0



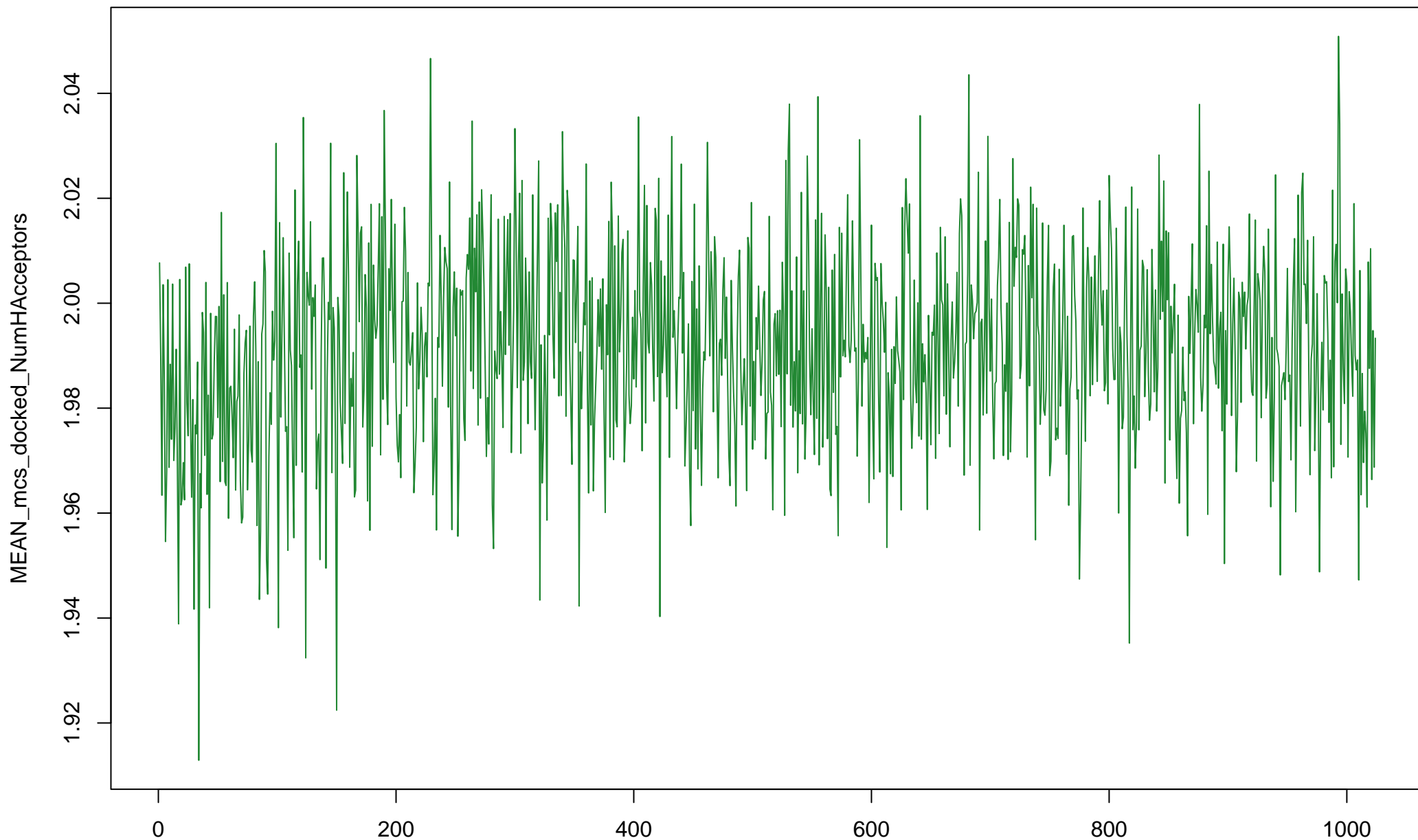
MEAN_mcs_RingCount
ESS = 888 | BMK = 0.0613 | MCSE(6.27) = 3.33 | stat: FALSE | burn: 0



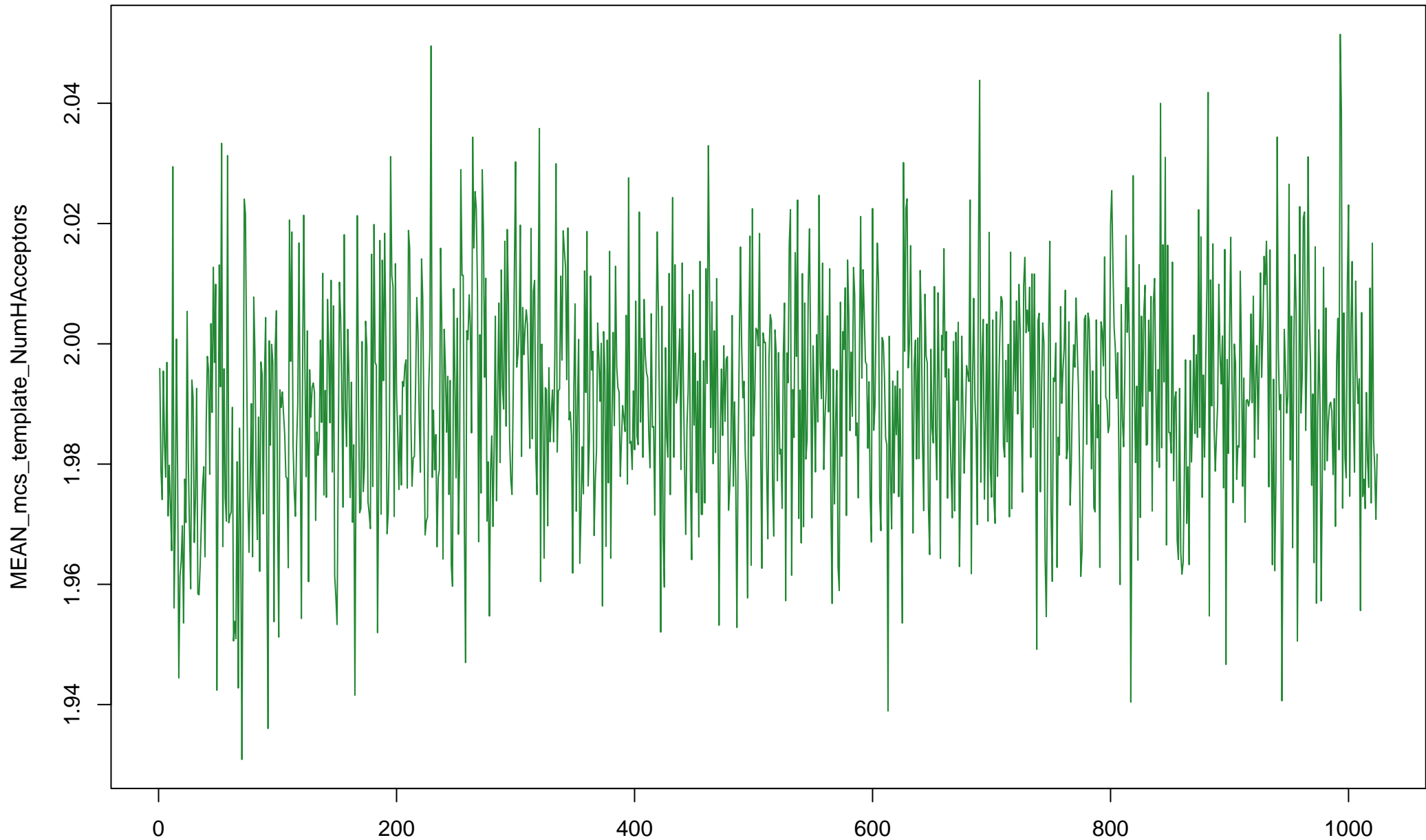
MEAN_template_HeavyAtomCount
ESS = 1020 | BMK = 0.0771 | MCSE(6.27) = 3.51 | stat: FALSE | burn: 0



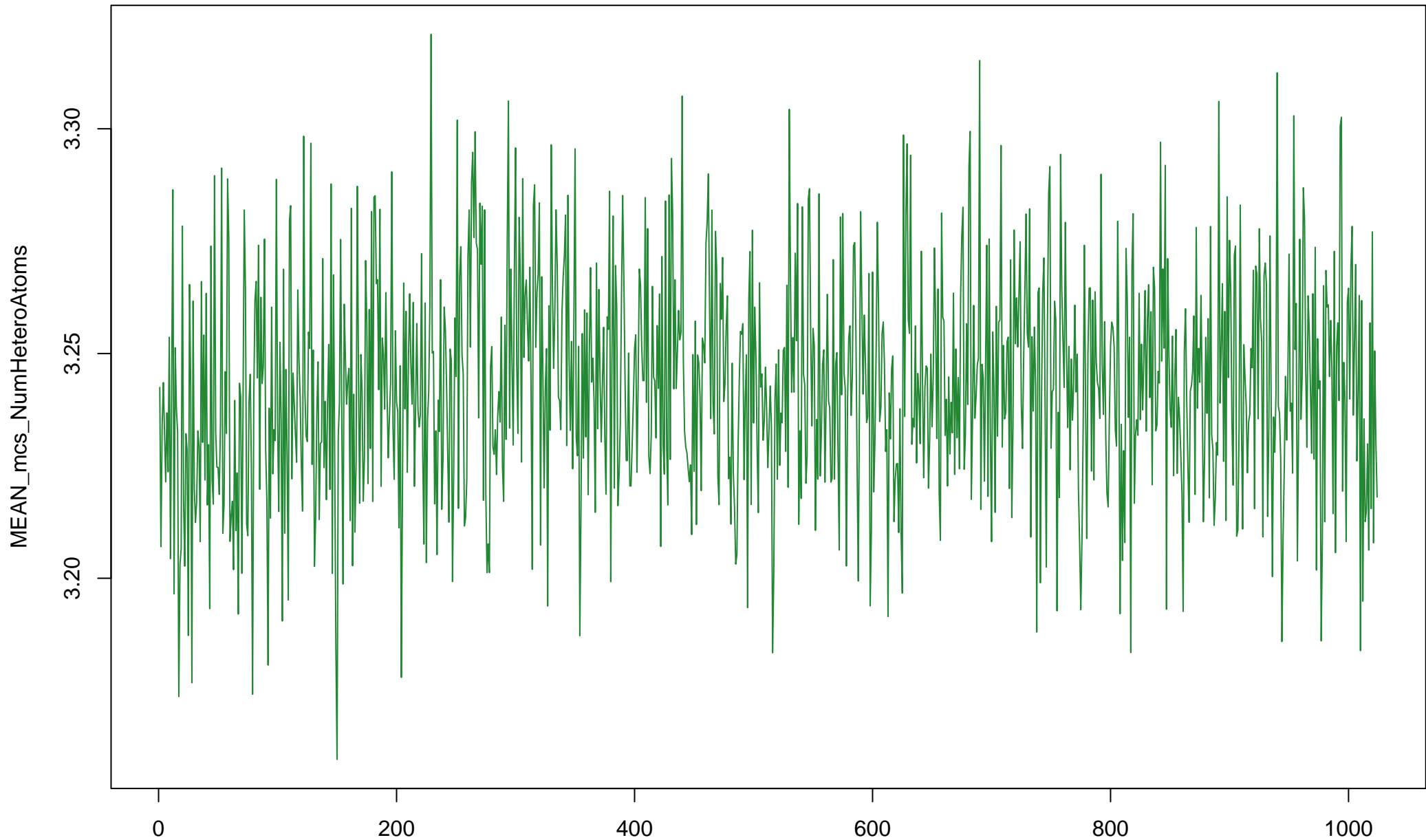
MEAN_mcs_docked_NumHAcceptors
ESS = 468 | BMK = 0.0847 | MCSE(6.27) = 4.61 | stat: FALSE | burn: 0



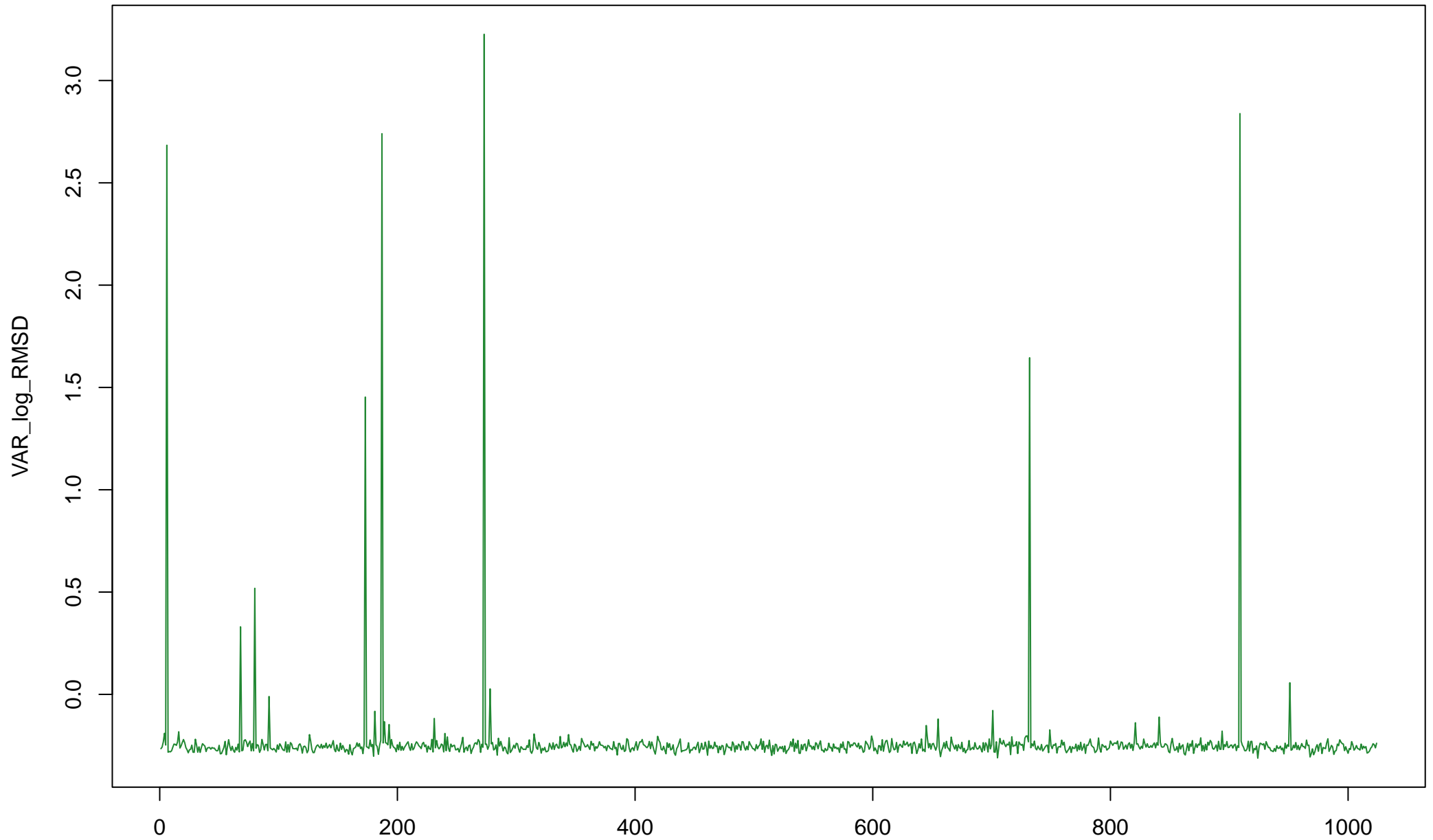
MEAN_mcs_template_NumHAcceptors
ESS = 501 | BMK = 0.0727 | MCSE(6.27) = 4.09 | stat: FALSE | burn: 0



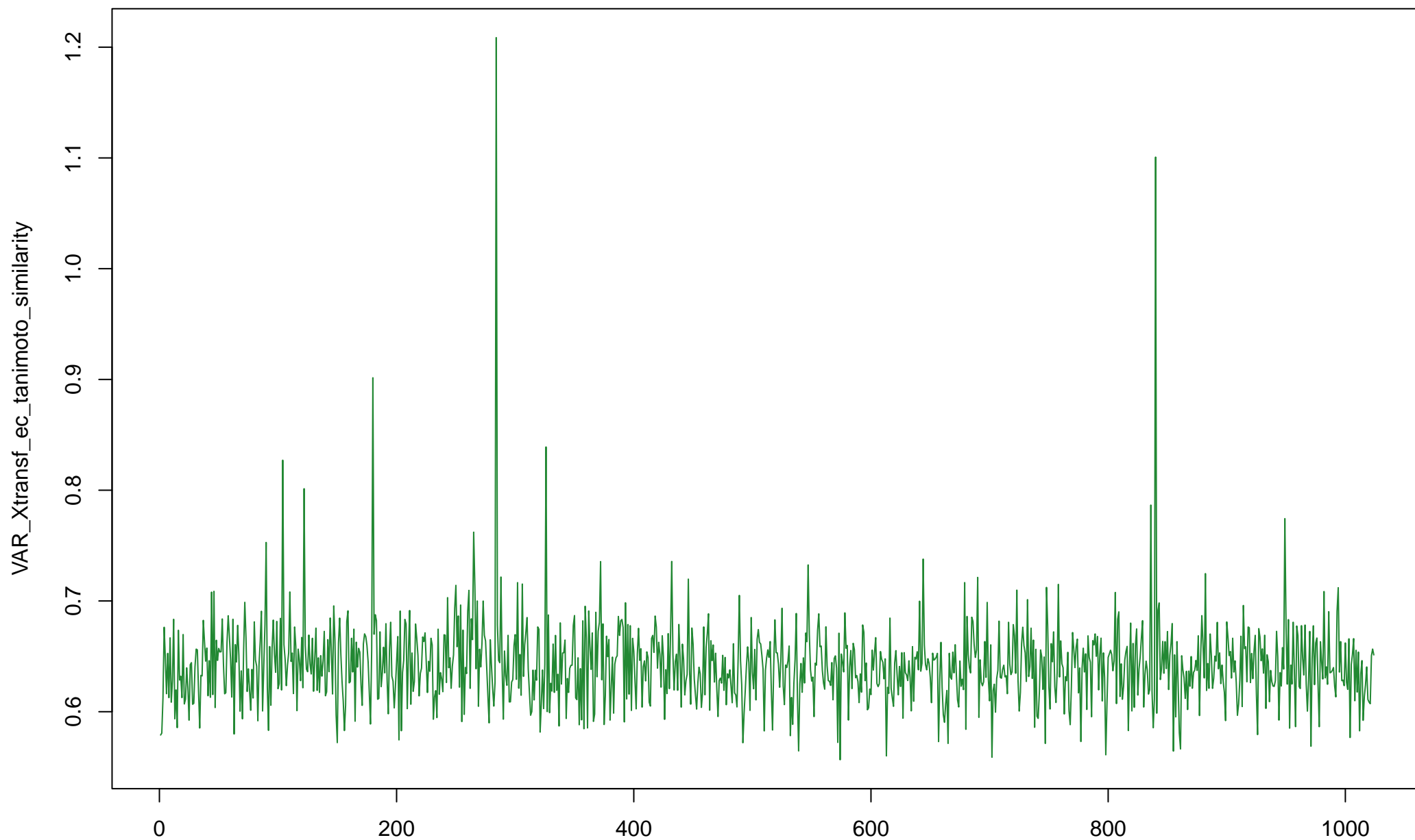
MEAN_mcs_NumHeteroAtoms
ESS = 561 | BMK = 0.0711 | MCSE(6.27) = 4.08 | stat: FALSE | burn: 0



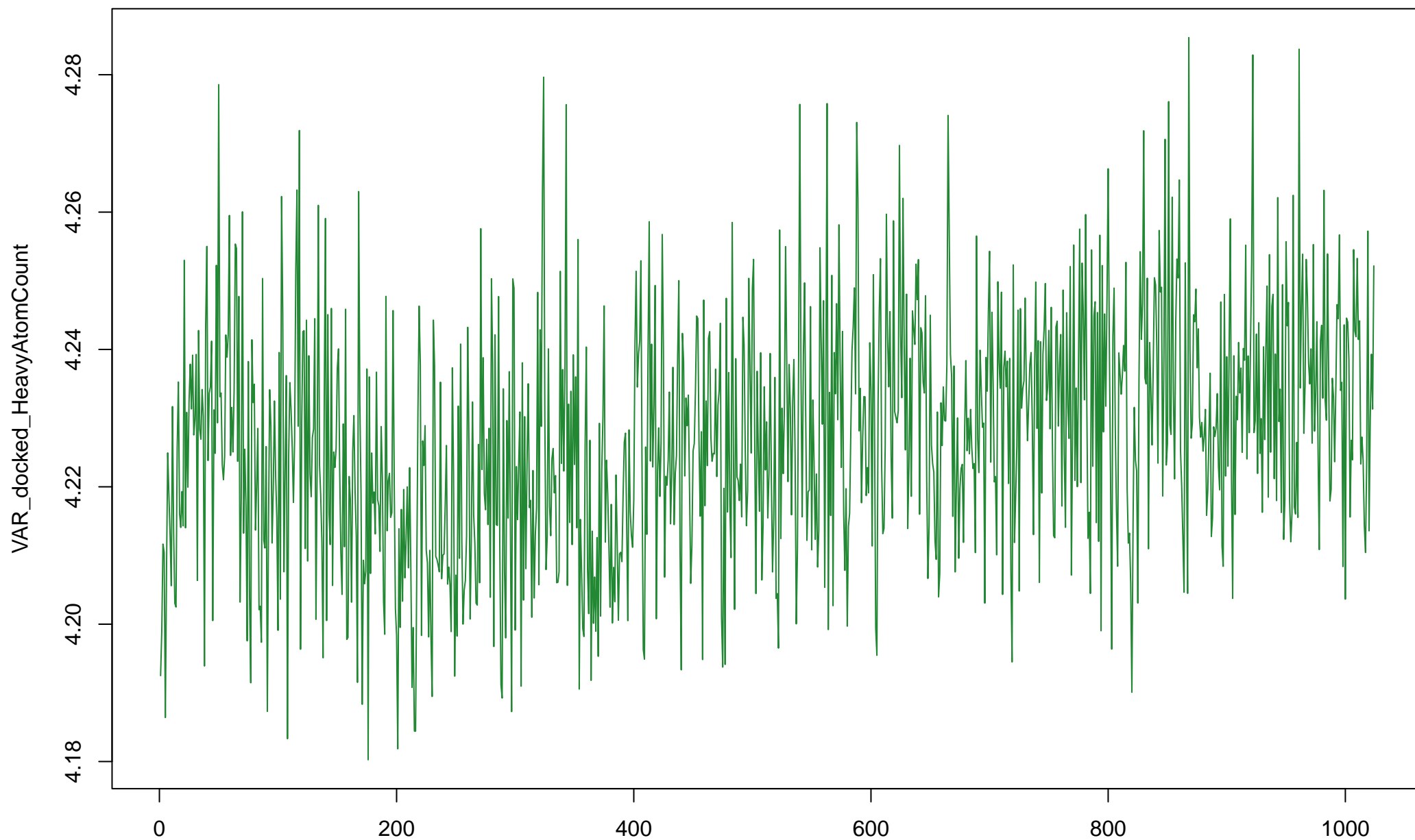
VAR_log_RMSD
ESS = 1020 | BMK = 0.2 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0



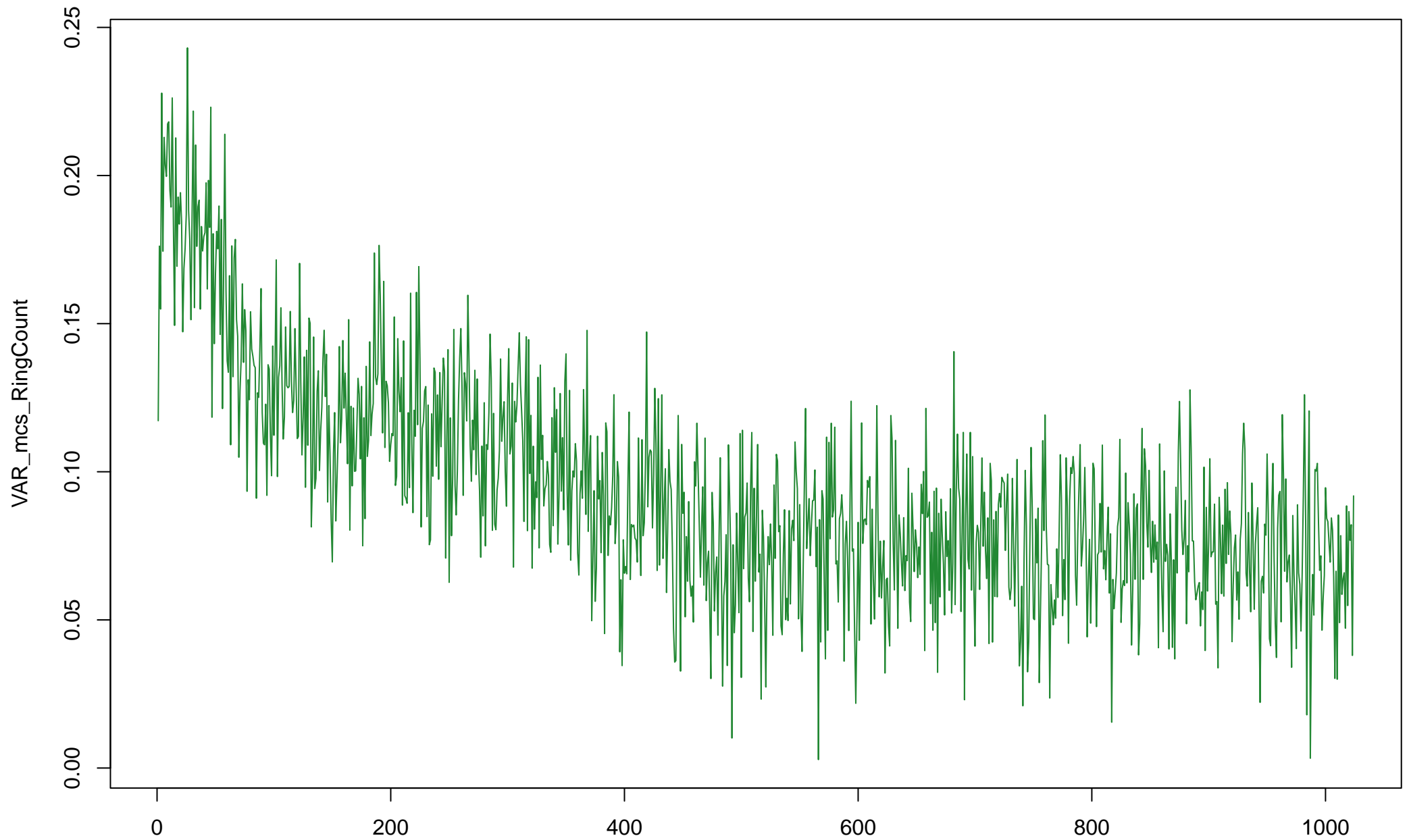
VAR_Xtransf_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.13 | MCSE(6.27) = 3.62 | stat: TRUE | burn: 0



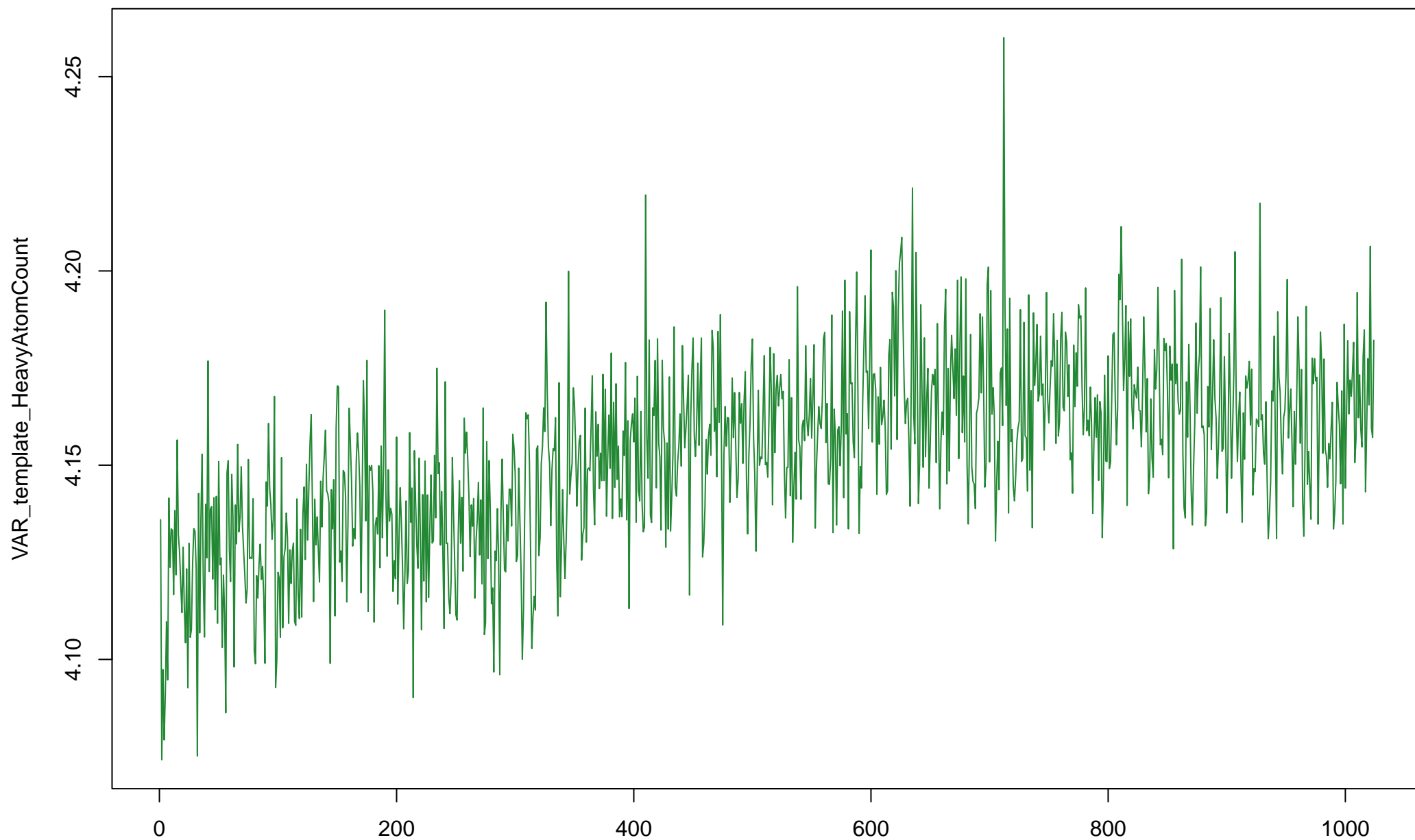
VAR_docked_HeavyAtomCount
ESS = 79.8 | BMK = 0.219 | MCSE(6.27) = 7.28 | stat: FALSE | burn: 0



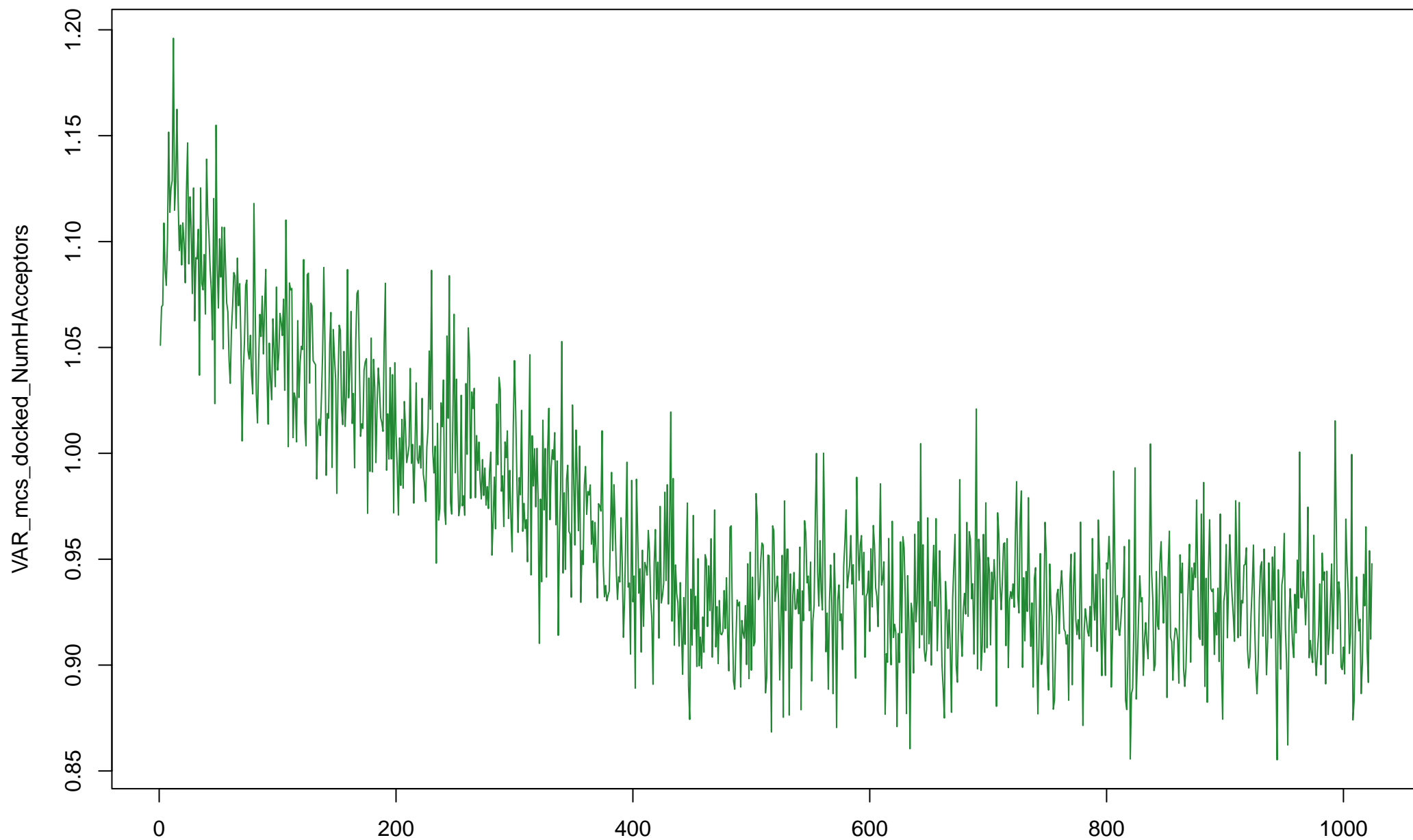
VAR_mcs_RingCount
ESS = 8.53 | BMK = 0.477 | MCSE(6.27) = 14.4 | stat: FALSE | burn: 0



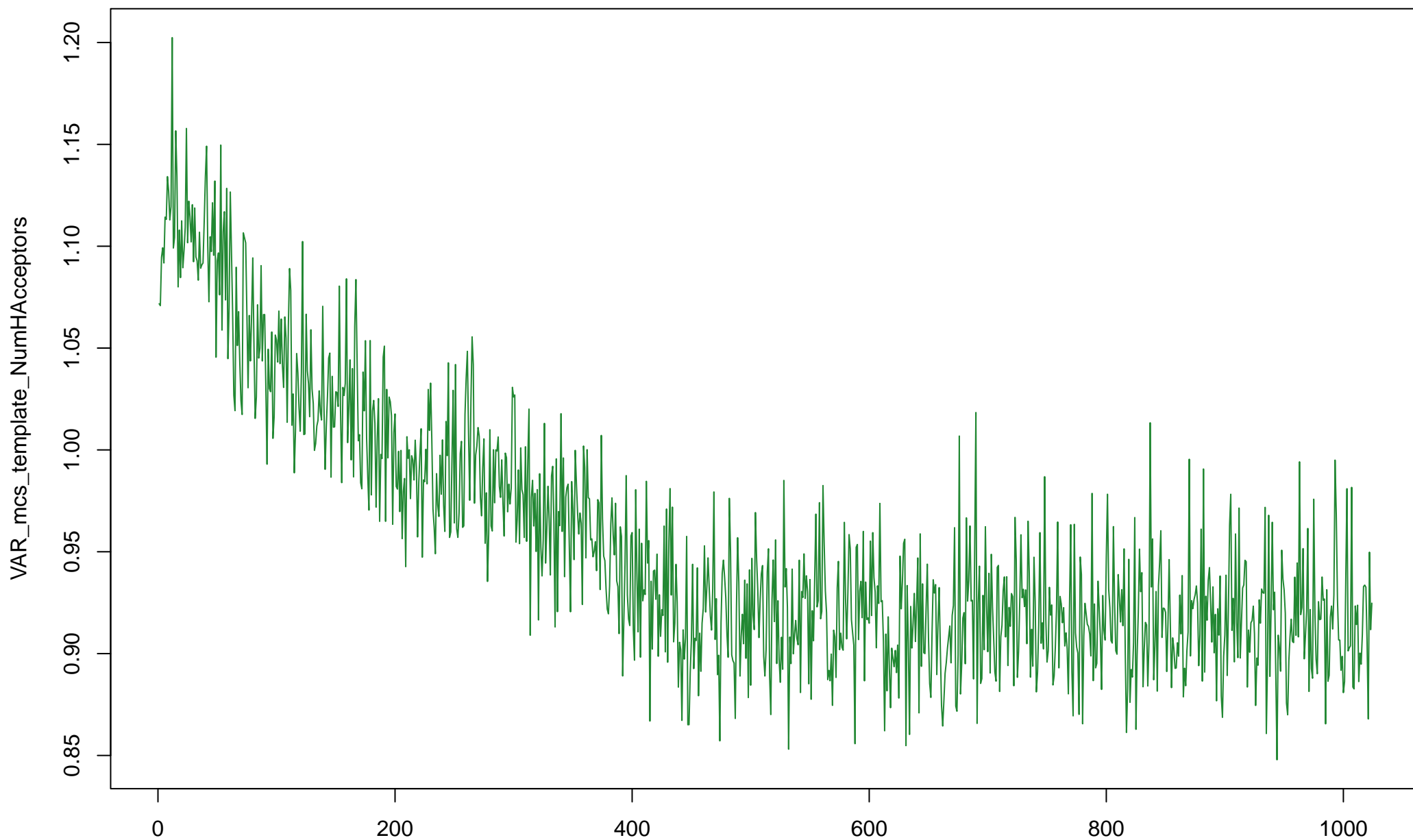
VAR_template_HeavyAtomCount
ESS = 9.44 | BMK = 0.462 | MCSE(6.27) = 12.1 | stat: FALSE | burn: 0



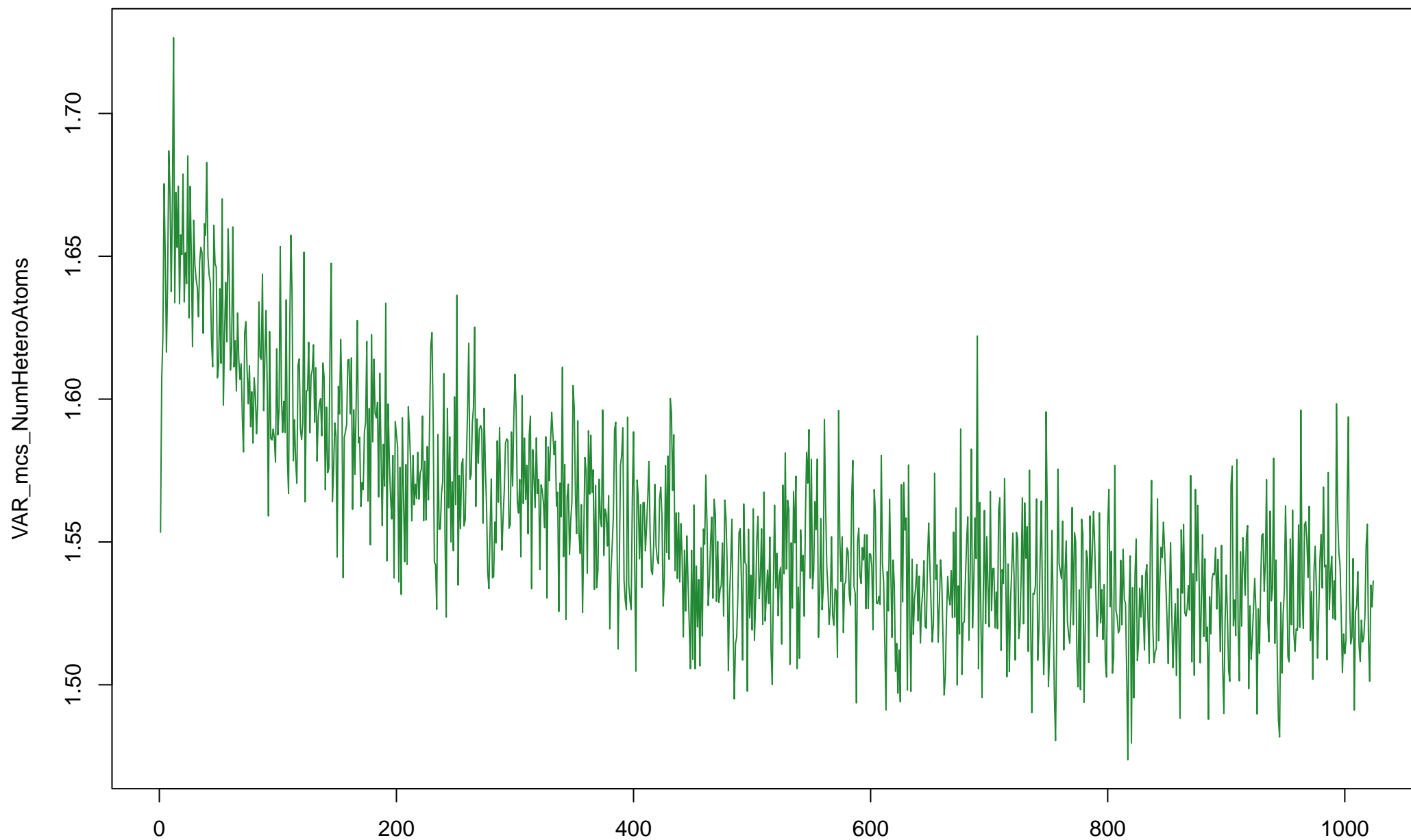
VAR_mcs_docked_NumHAcceptors
ESS = 4.51 | BMK = 0.565 | MCSE(6.27) = 16.1 | stat: FALSE | burn: 0



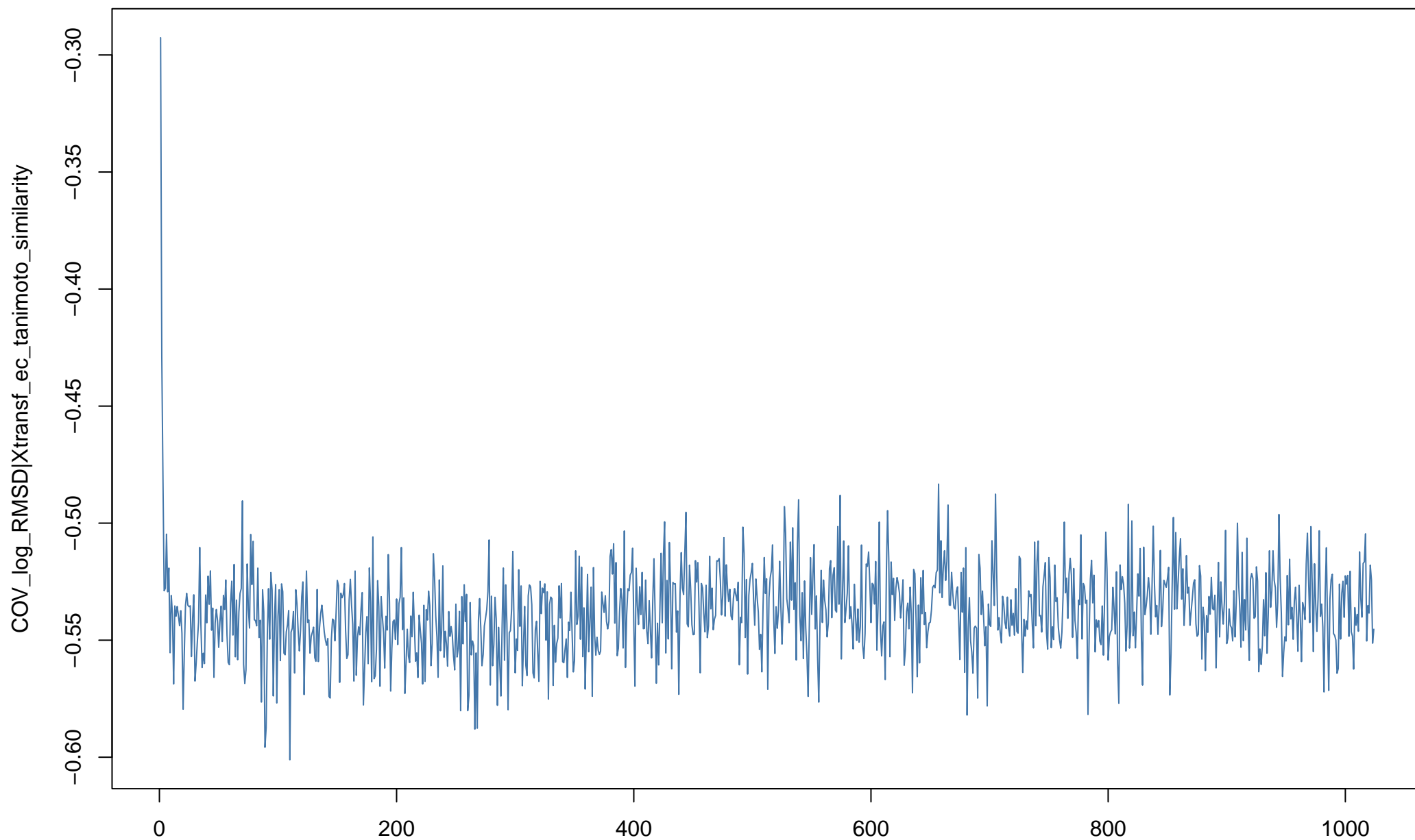
VAR_mcs_template_NumHAcceptors
ESS = 4.86 | BMK = 0.567 | MCSE(6.27) = 16.3 | stat: FALSE | burn: 102



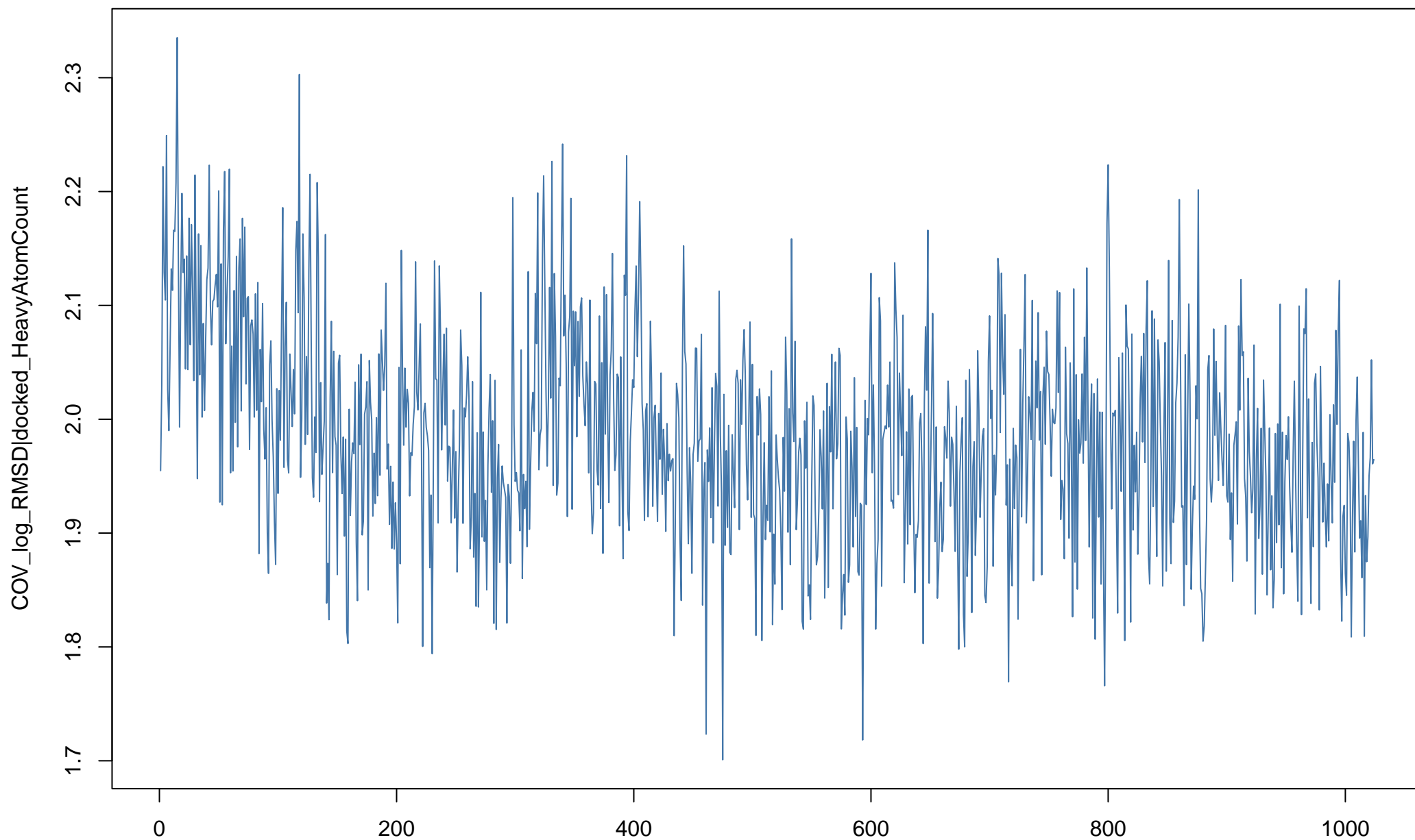
VAR_mcs_NumHeteroAtoms
ESS = 8.14 | BMK = 0.499 | MCSE(6.27) = 14.9 | stat: FALSE | burn: 0



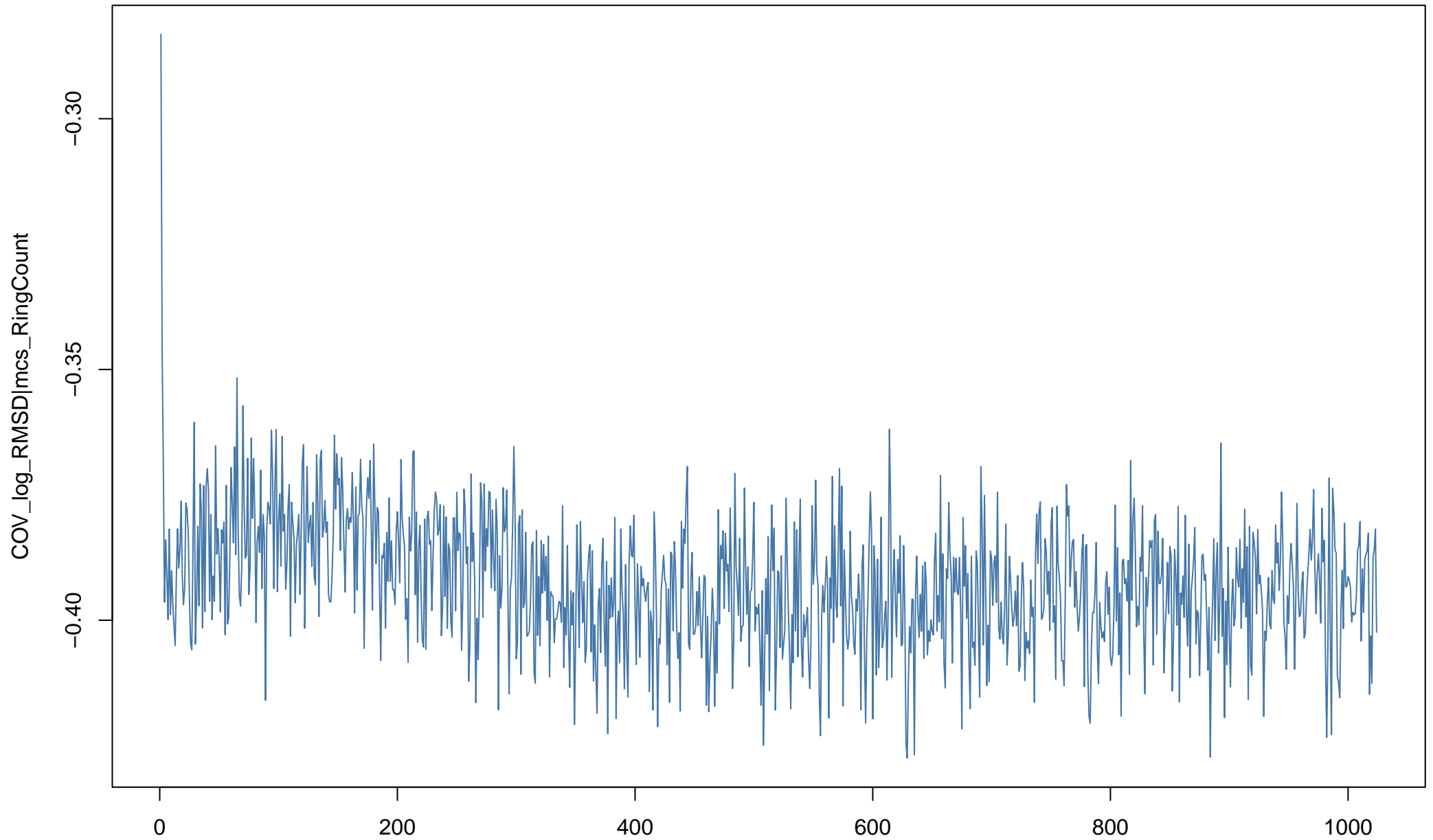
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 350 | BMK = 0.151 | MCSE(6.27) = 5.38 | stat: TRUE | burn: 0



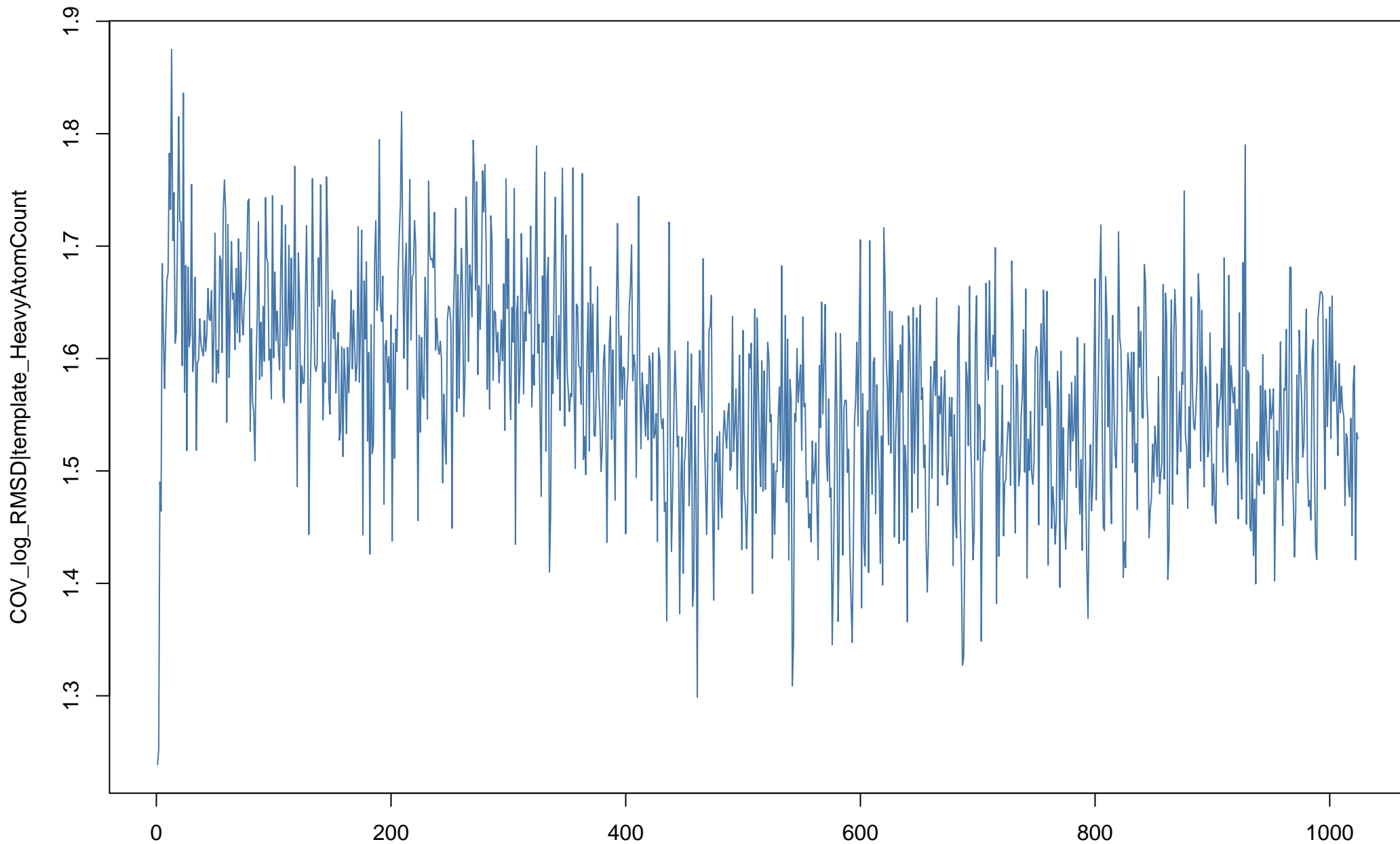
COV_log_RMSD|docked_HeavyAtomCount
ESS = 59.3 | BMK = 0.188 | MCSE(6.27) = 8.4 | stat: FALSE | burn: 0



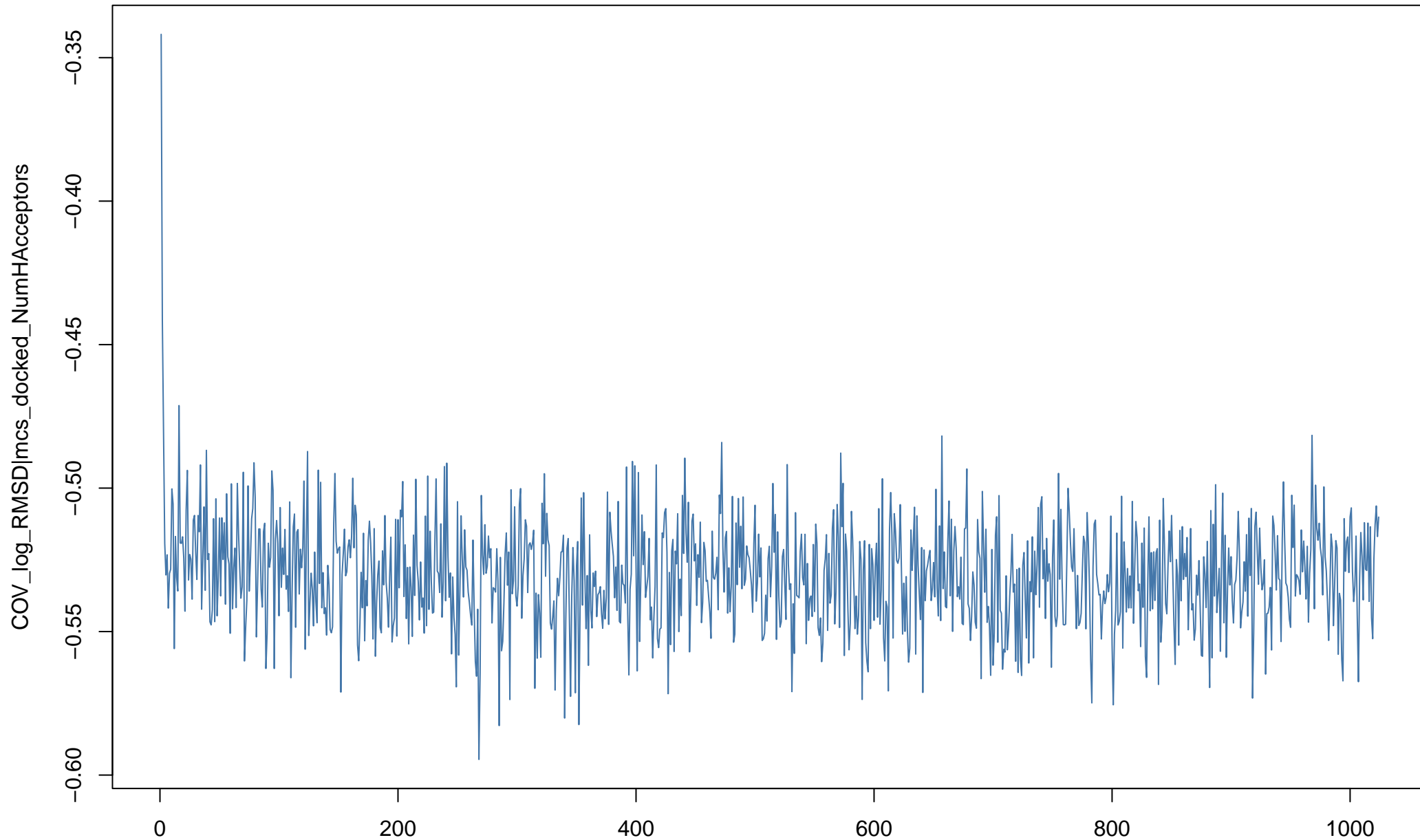
COV_log_RMSD|mcs_RingCount
ESS = 66.8 | BMK = 0.183 | MCSE(6.27) = 7.7 | stat: FALSE | burn: 0



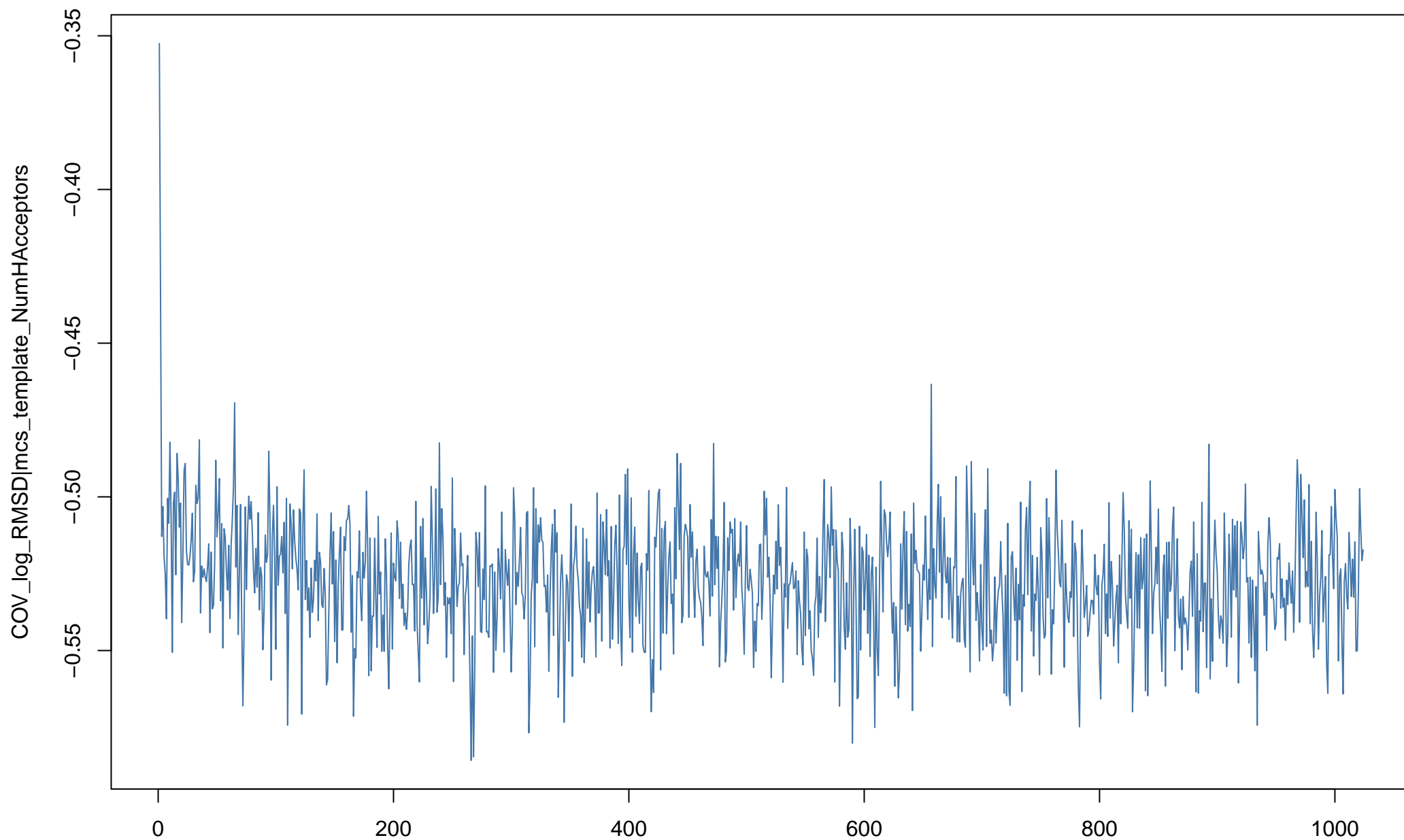
COV_log_RMSD|template_HeavyAtomCount
ESS = 26.4 | BMK = 0.297 | MCSE(6.27) = 9.45 | stat: FALSE | burn: 0



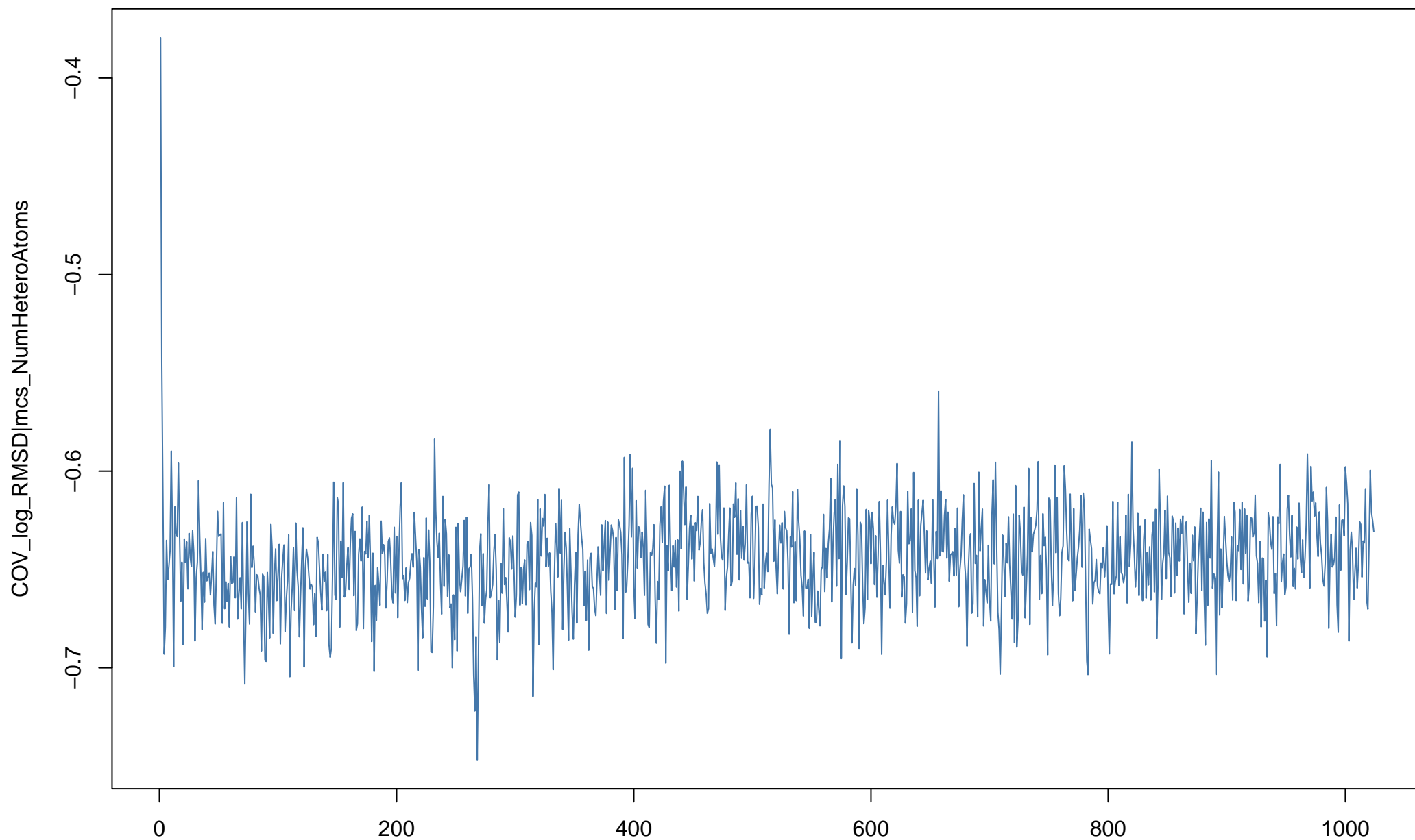
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 772 | BMK = 0.0966 | MCSE(6.27) = 4.67 | stat: FALSE | burn: 0



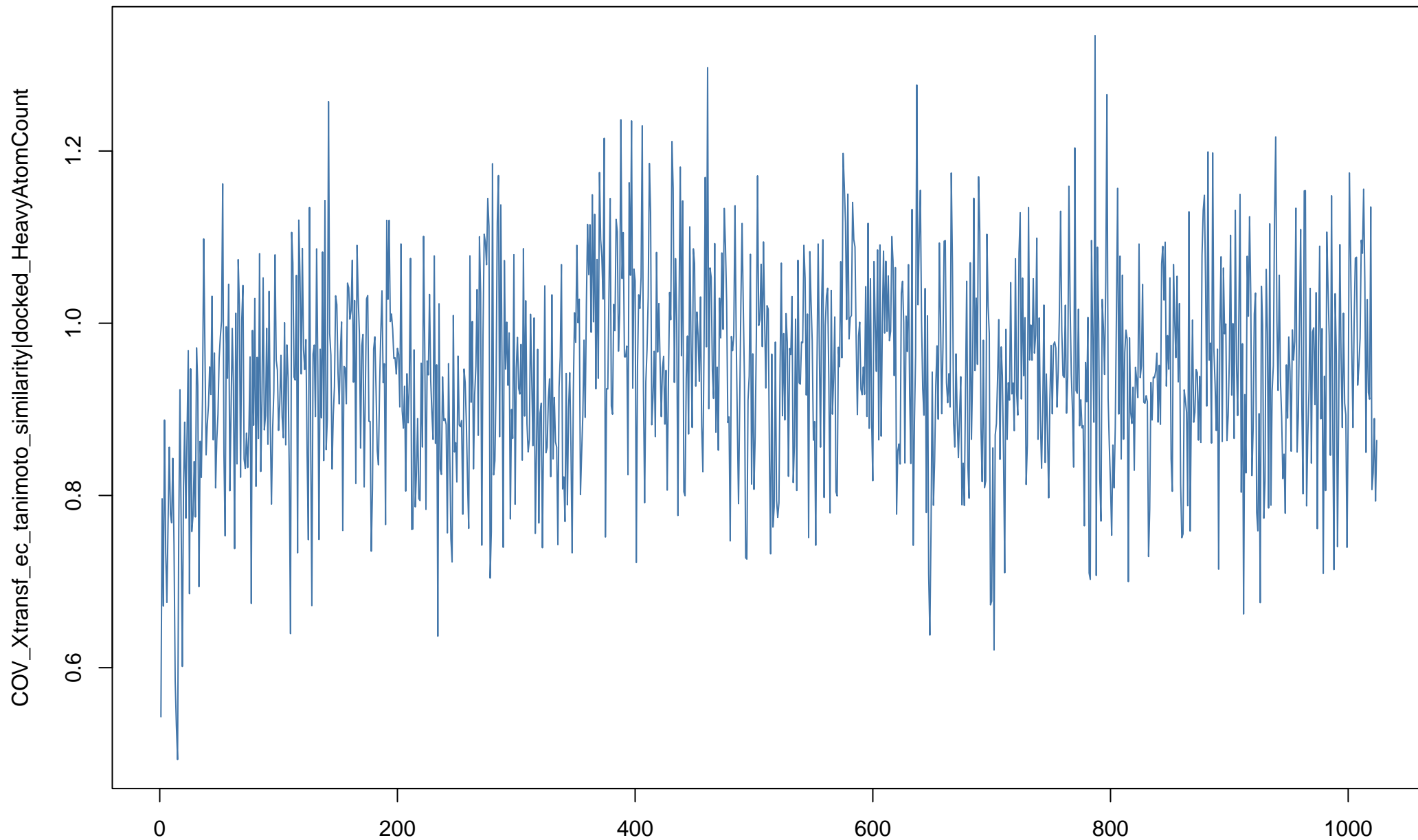
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 712 | BMK = 0.1 | MCSE(6.27) = 5.55 | stat: FALSE | burn: 0



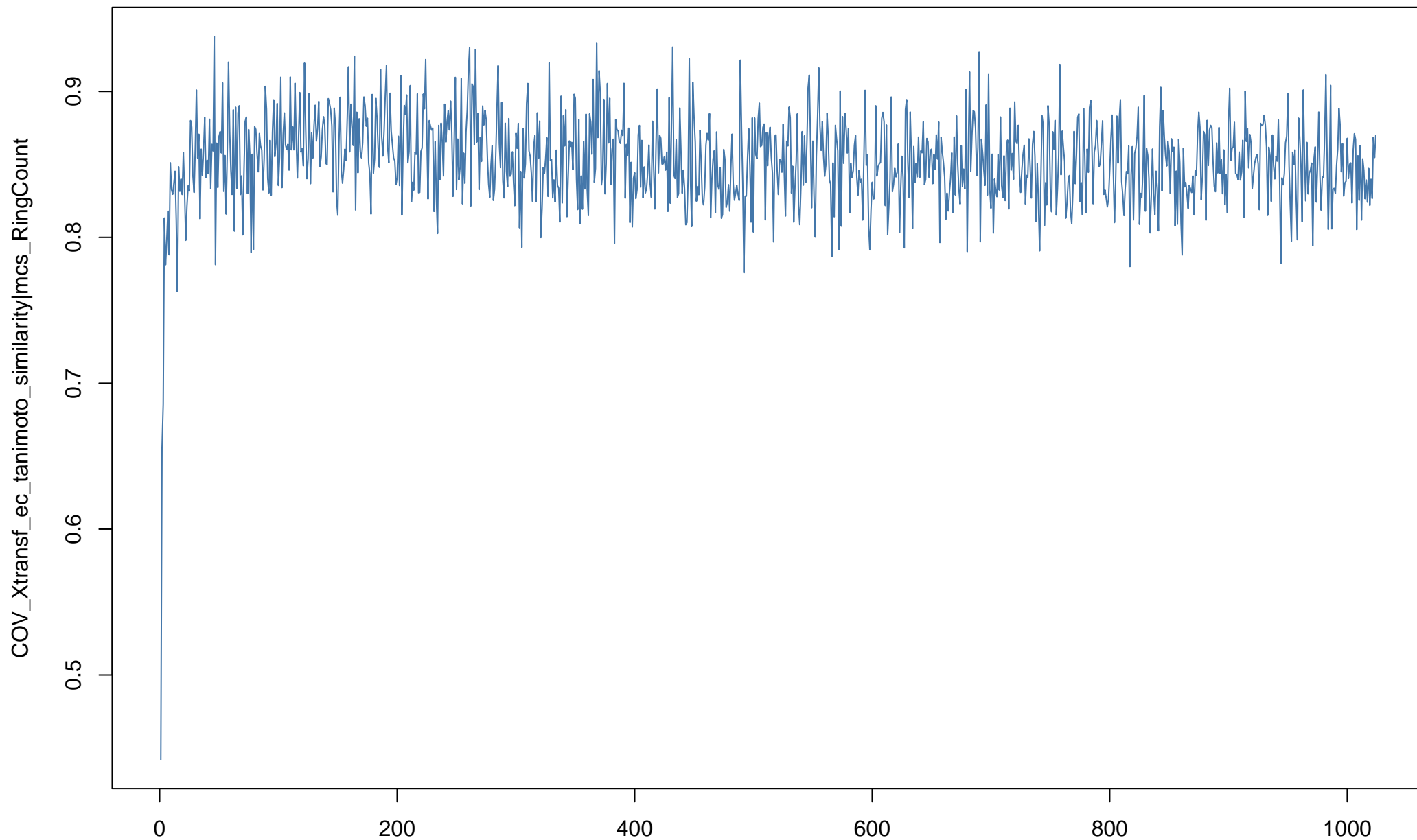
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 633 | BMK = 0.115 | MCSE(6.27) = 5.17 | stat: TRUE | burn: 0



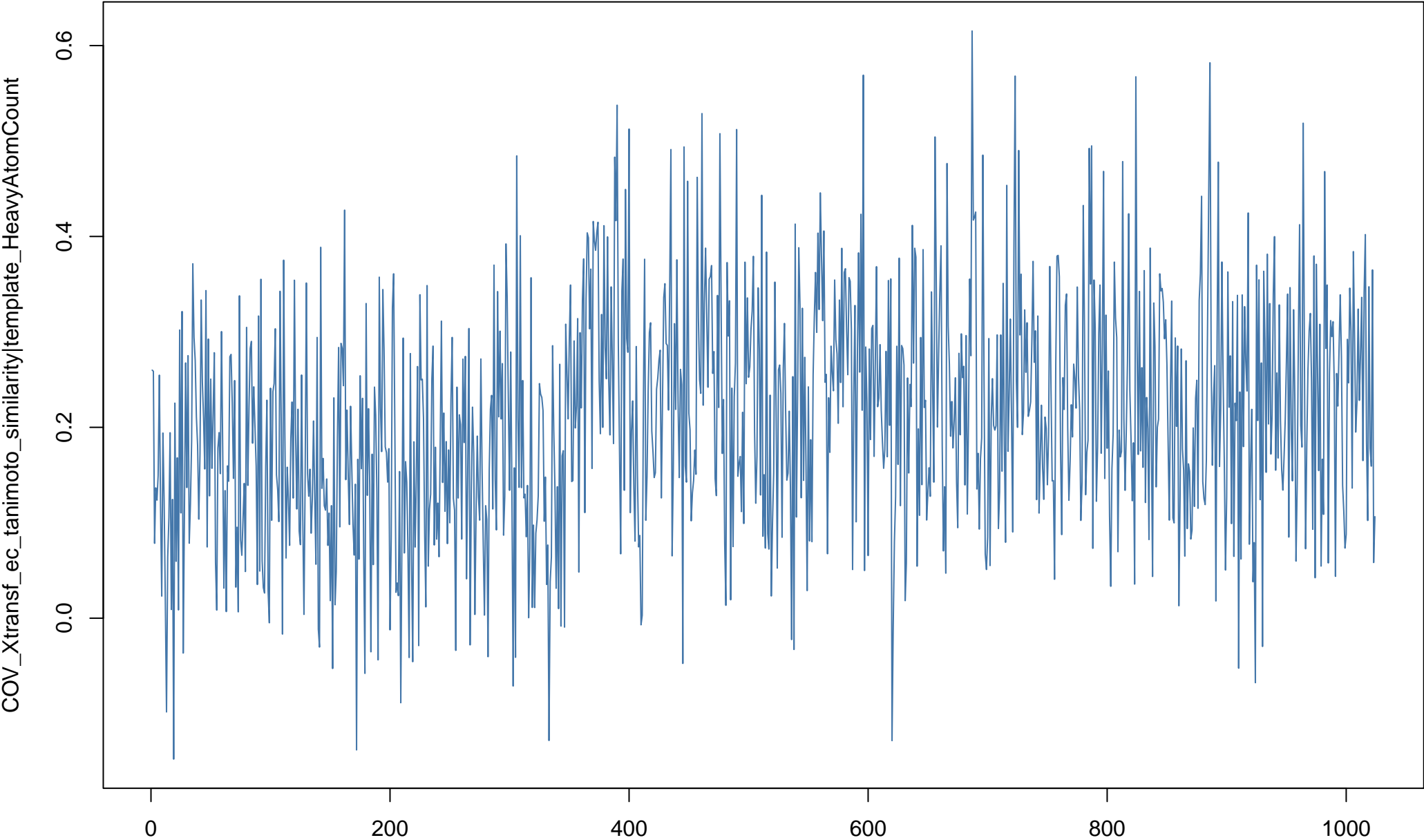
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 242 | BMK = 0.0608 | MCSE(6.27) = 6.52 | stat: FALSE | burn: 0



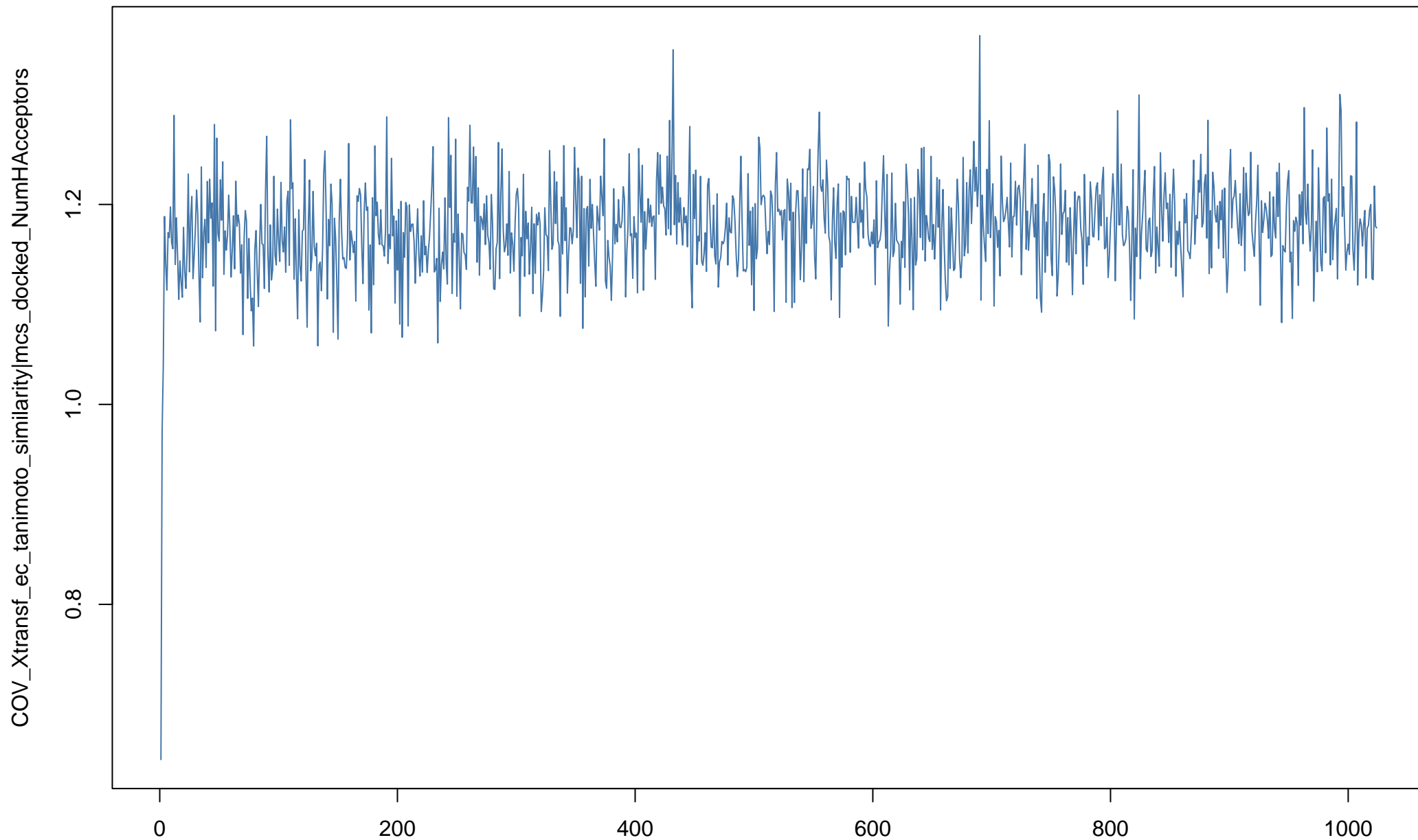
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 217 | BMK = 0.129 | MCSE(6.27) = 6.08 | stat: TRUE | burn: 0



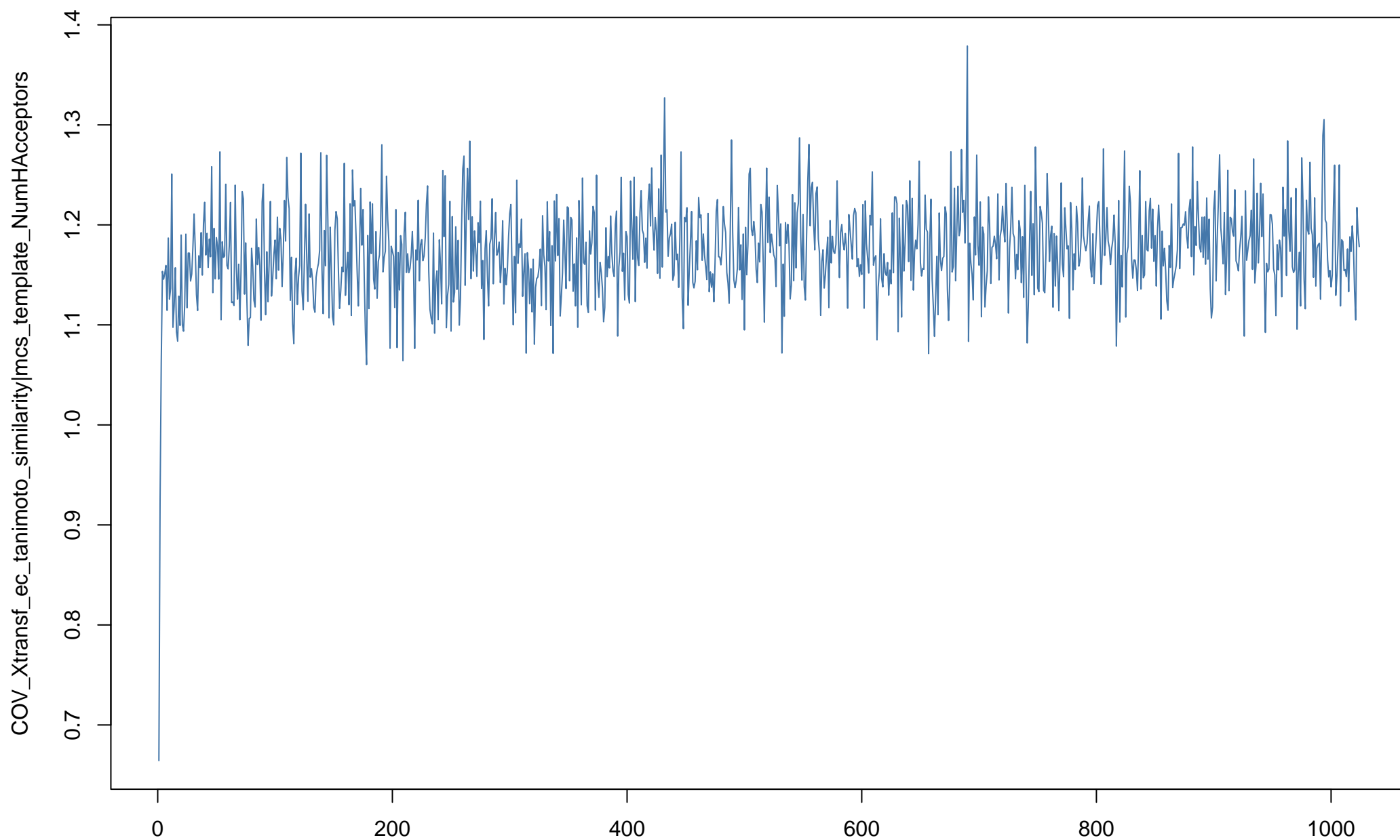
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 150 | BMK = 0.143 | MCSE(6.27) = 6.62 | stat: FALSE | burn: 0



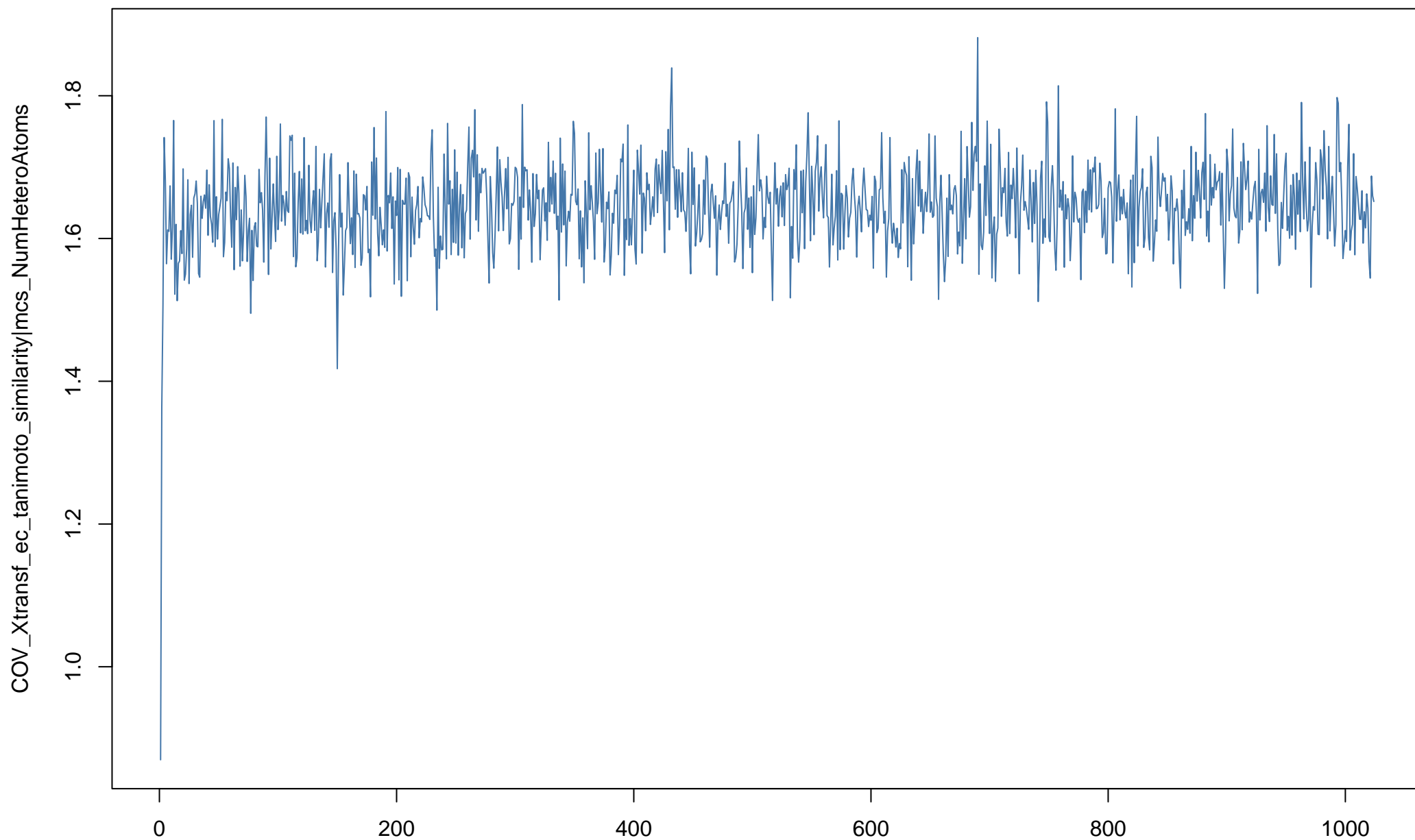
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 600 | BMK = 0.137 | MCSE(6.27) = 4.87 | stat: FALSE | burn: 0



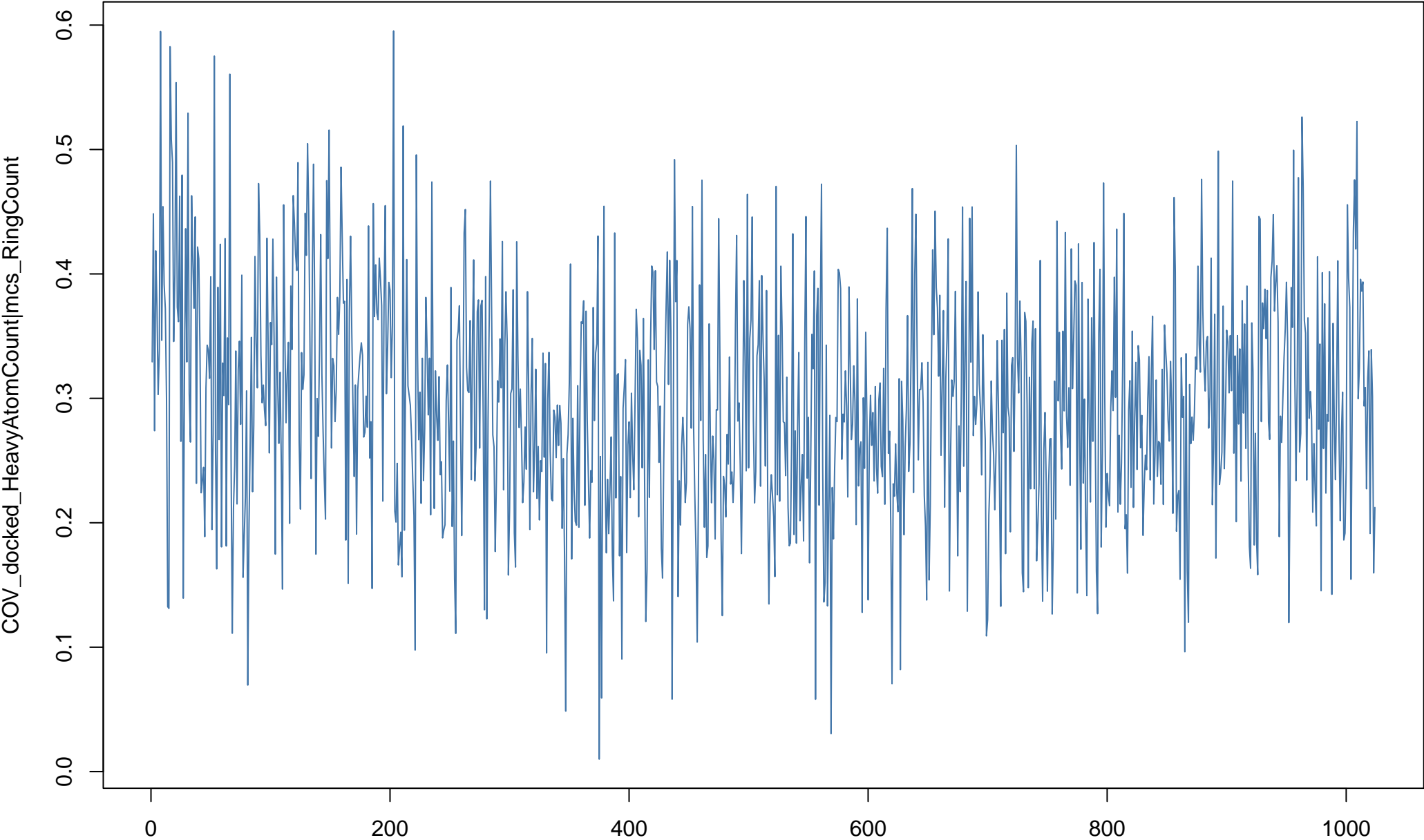
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 578 | BMK = 0.122 | MCSE(6.27) = 5.12 | stat: FALSE | burn: 0



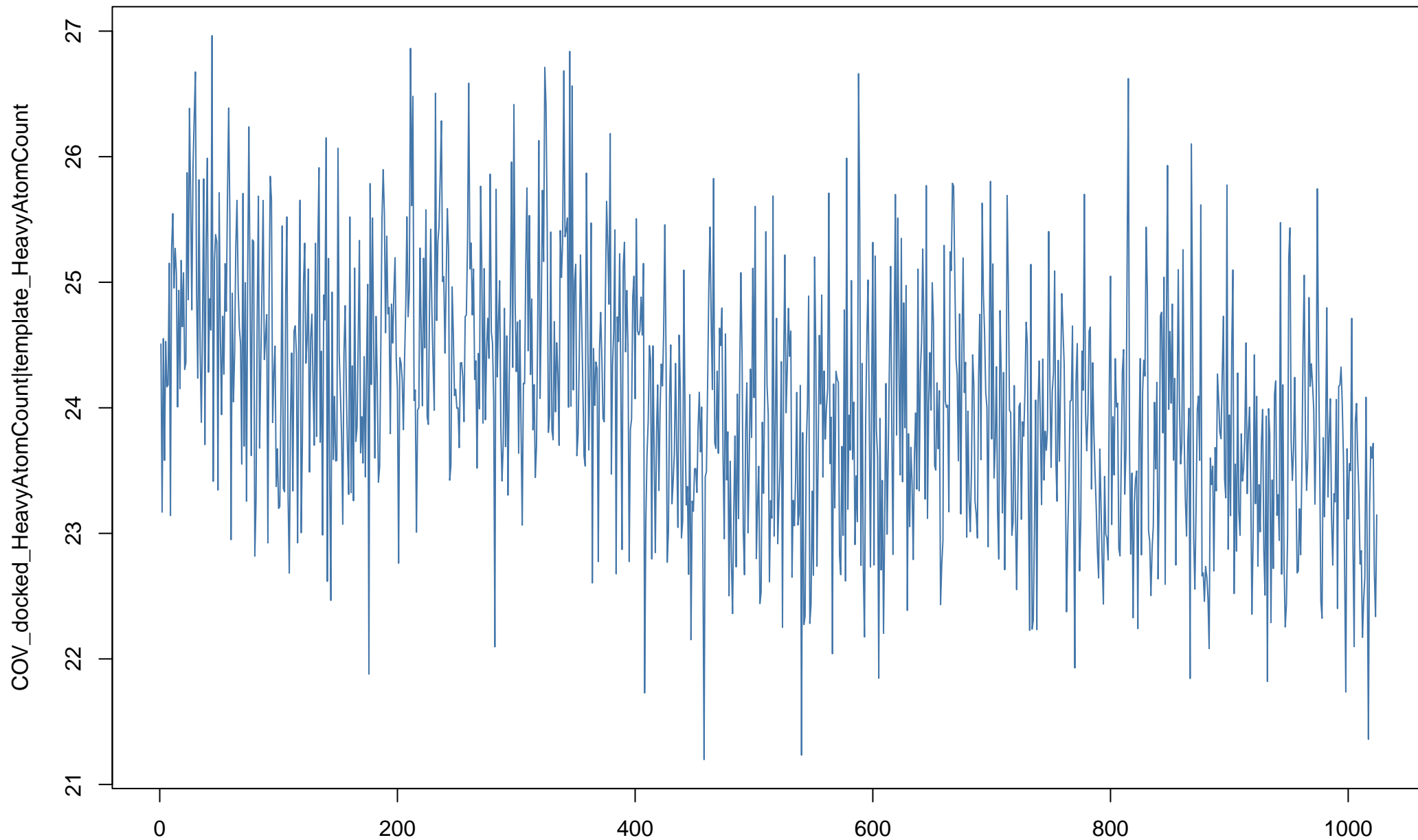
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 889 | BMK = 0.0852 | MCSE(6.27) = 4.49 | stat: FALSE | burn: 0



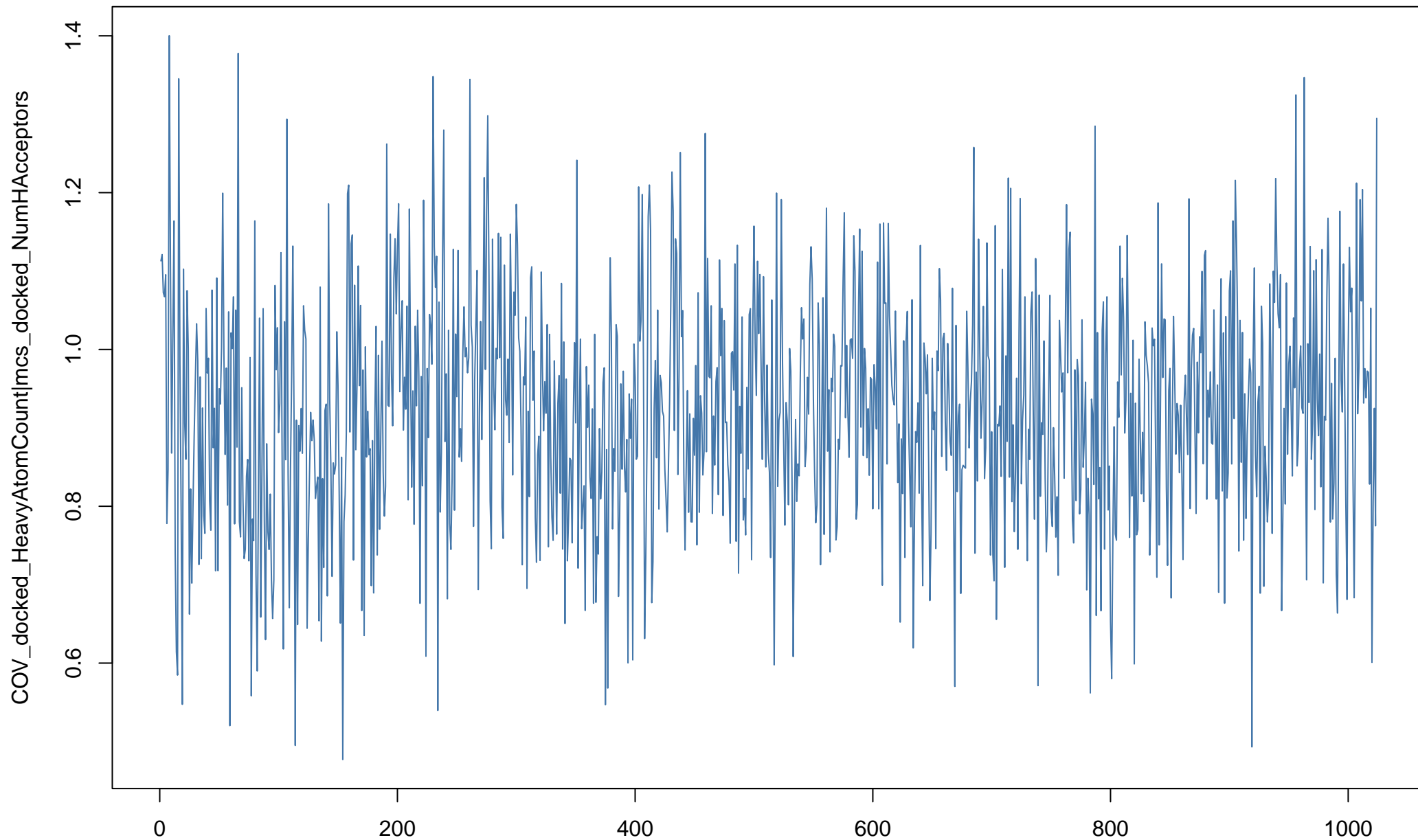
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 365 | BMK = 0.074 | MCSE(6.27) = 5.51 | stat: FALSE | burn: 0



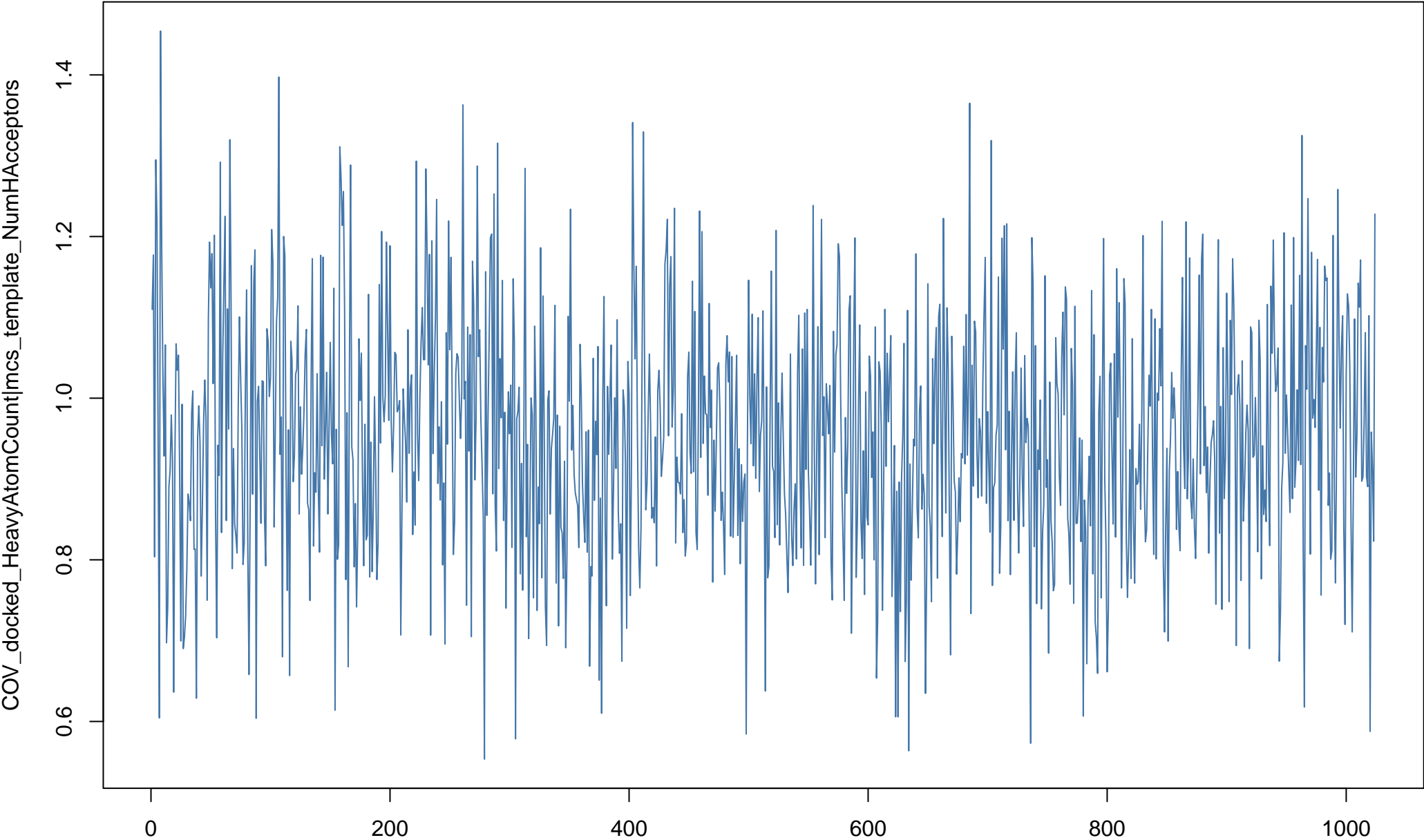
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 26.8 | BMK = 0.246 | MCSE(6.27) = 8.43 | stat: FALSE | burn: 0



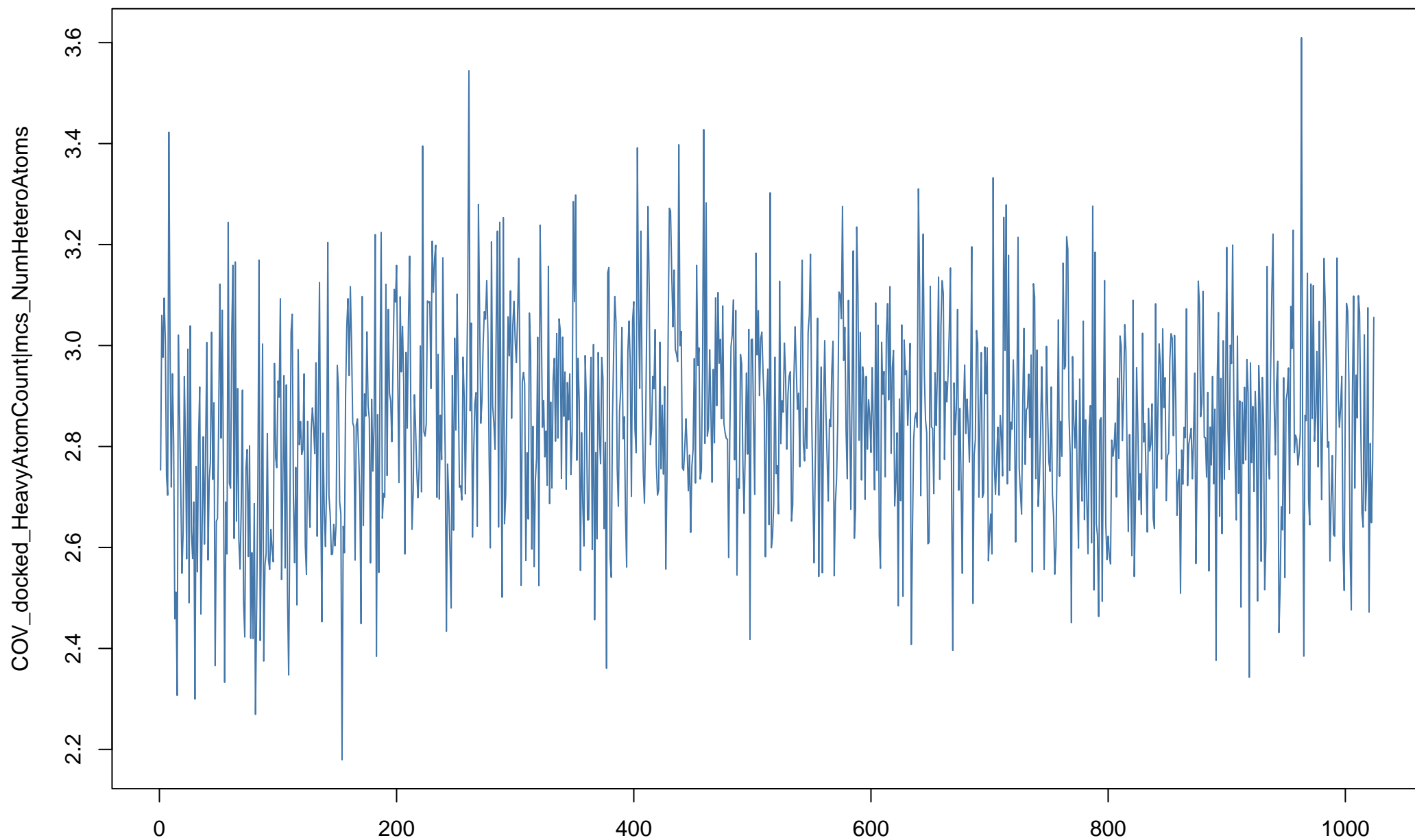
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 685 | BMK = 0.0617 | MCSE(6.27) = 4.46 | stat: TRUE | burn: 0



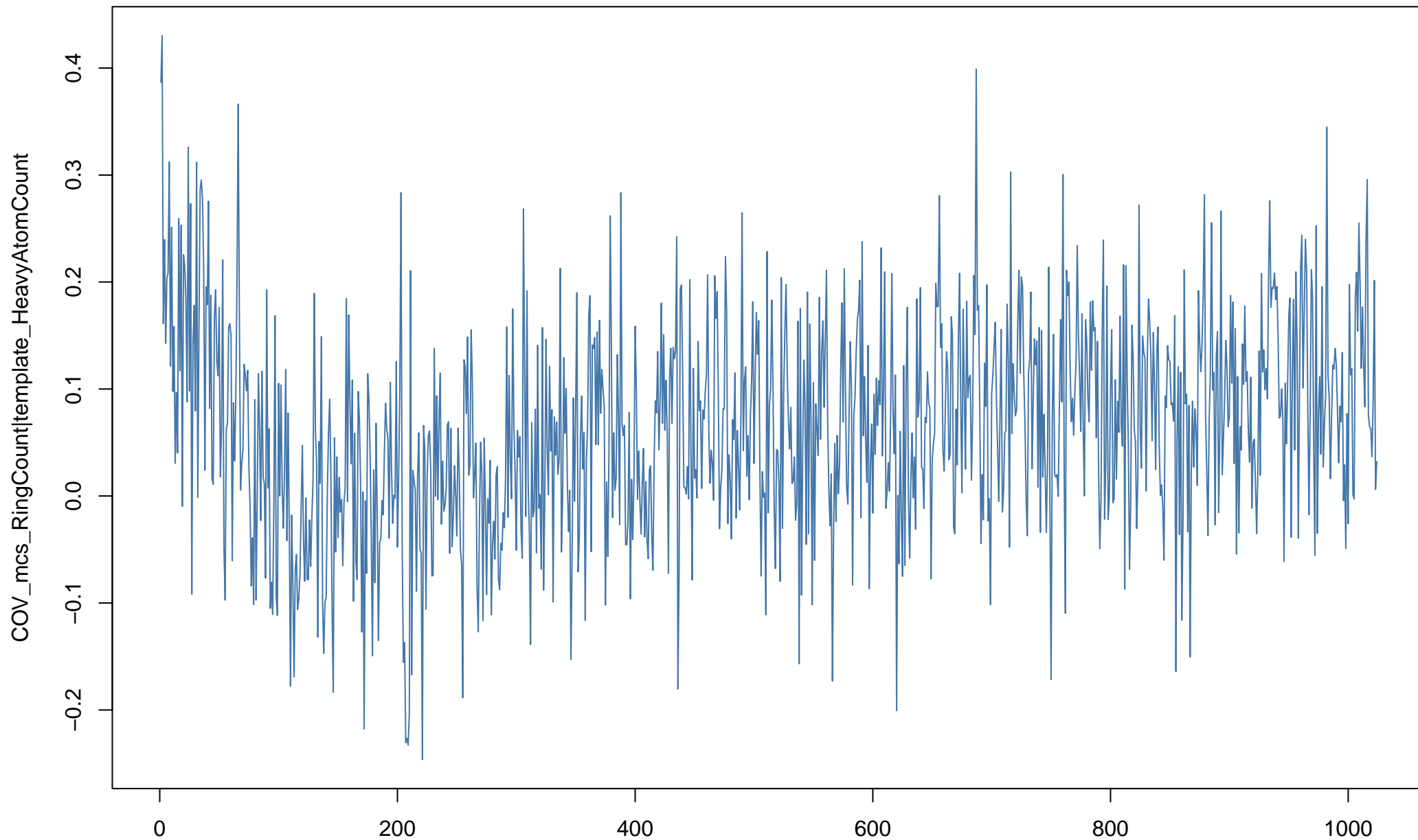
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 904 | BMK = 0.0749 | MCSE(6.27) = 4.02 | stat: TRUE | burn: 0



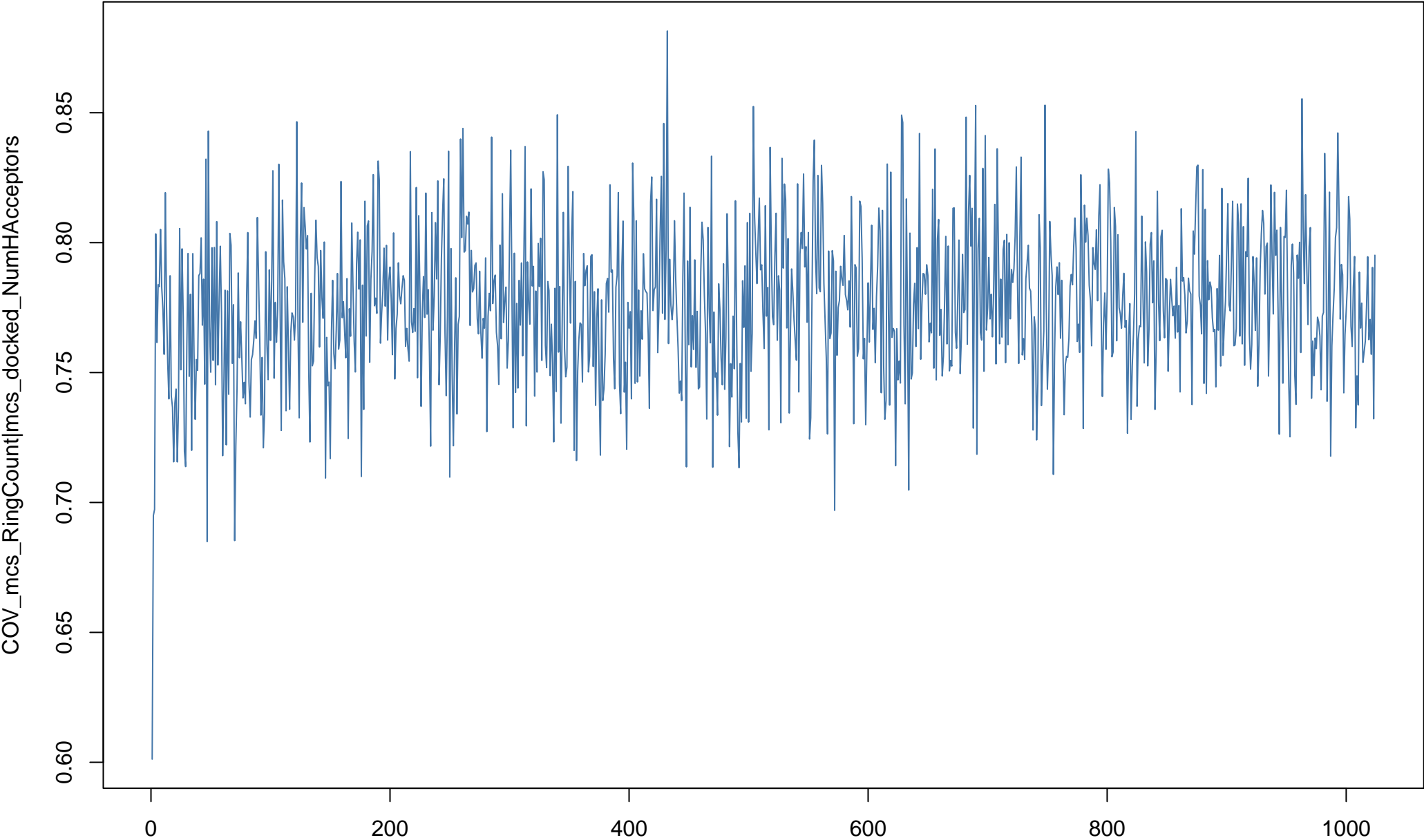
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 483 | BMK = 0.0962 | MCSE(6.27) = 5.56 | stat: FALSE | burn: 0



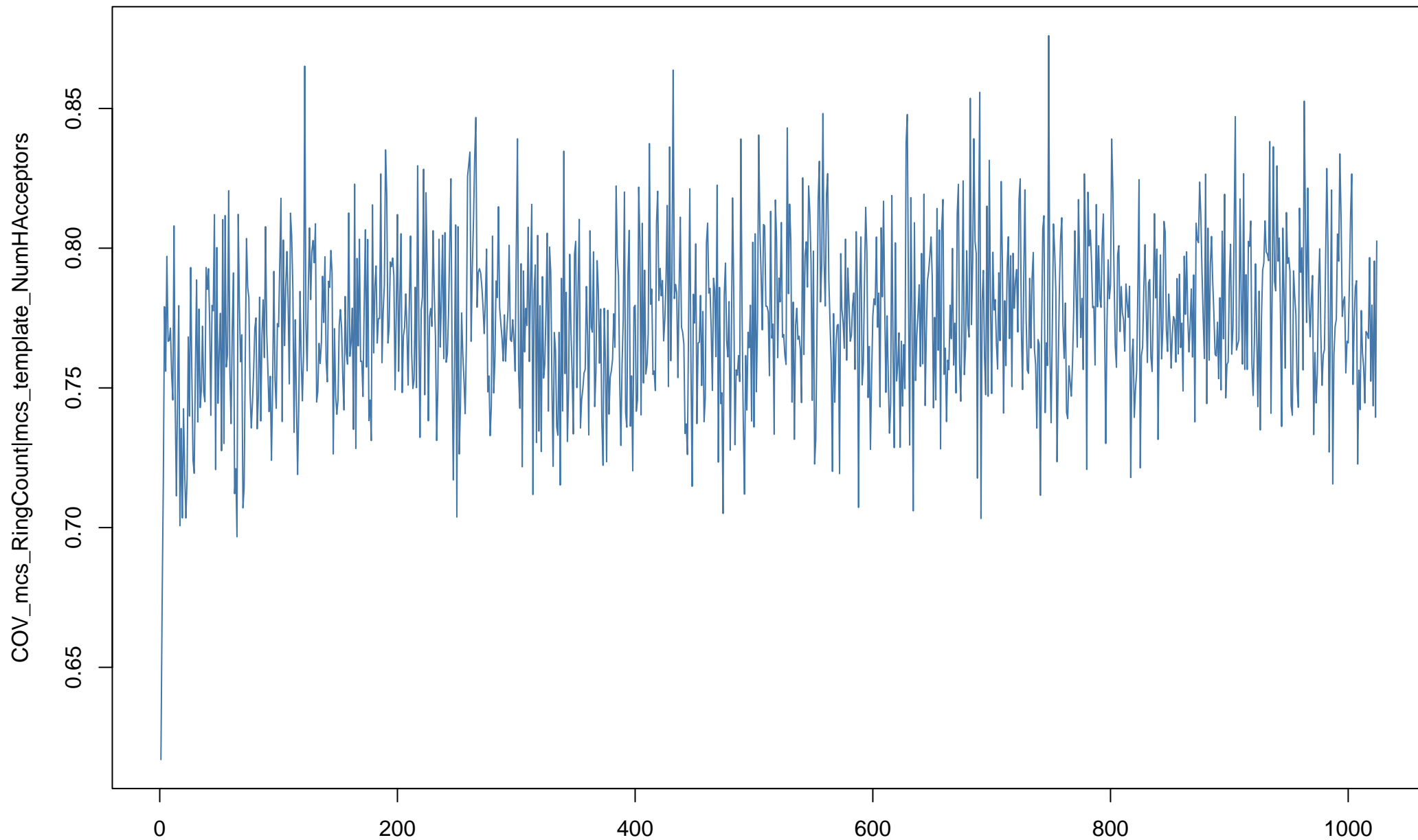
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 70.2 | BMK = 0.191 | MCSE(6.27) = 8.26 | stat: TRUE | burn: 0



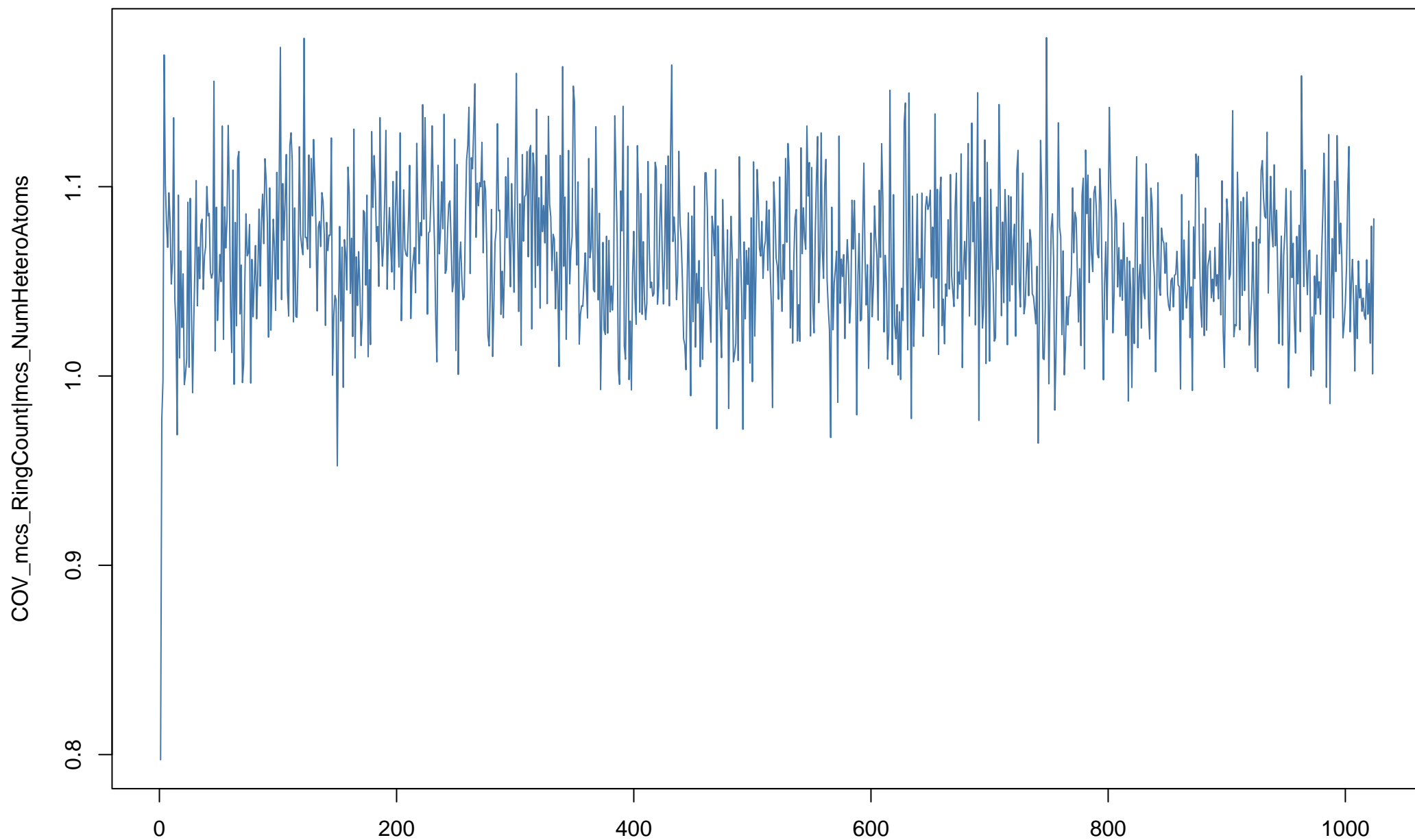
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 713 | BMK = 0.103 | MCSE(6.27) = 4.65 | stat: FALSE | burn: 0



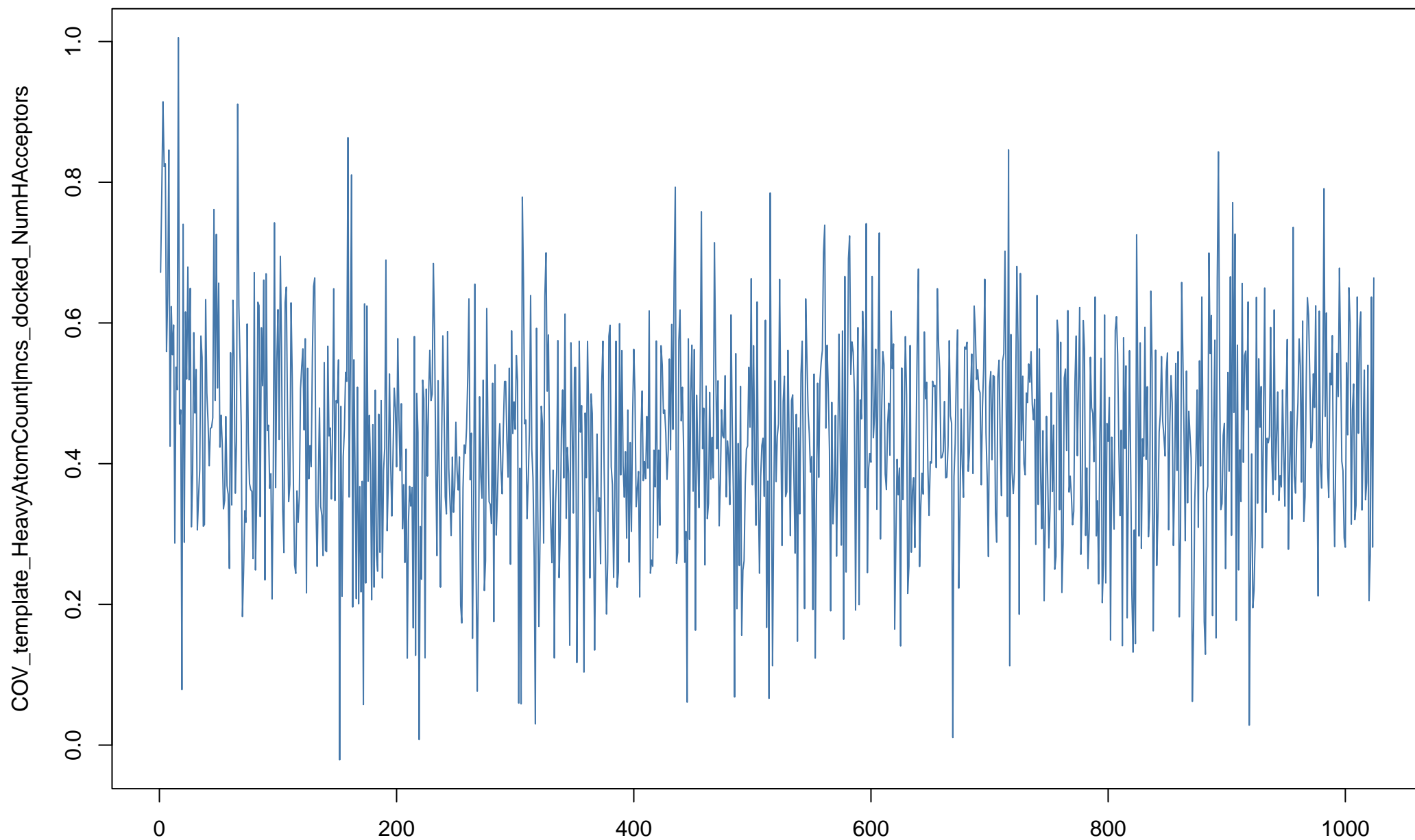
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 497 | BMK = 0.115 | MCSE(6.27) = 5.31 | stat: FALSE | burn: 0



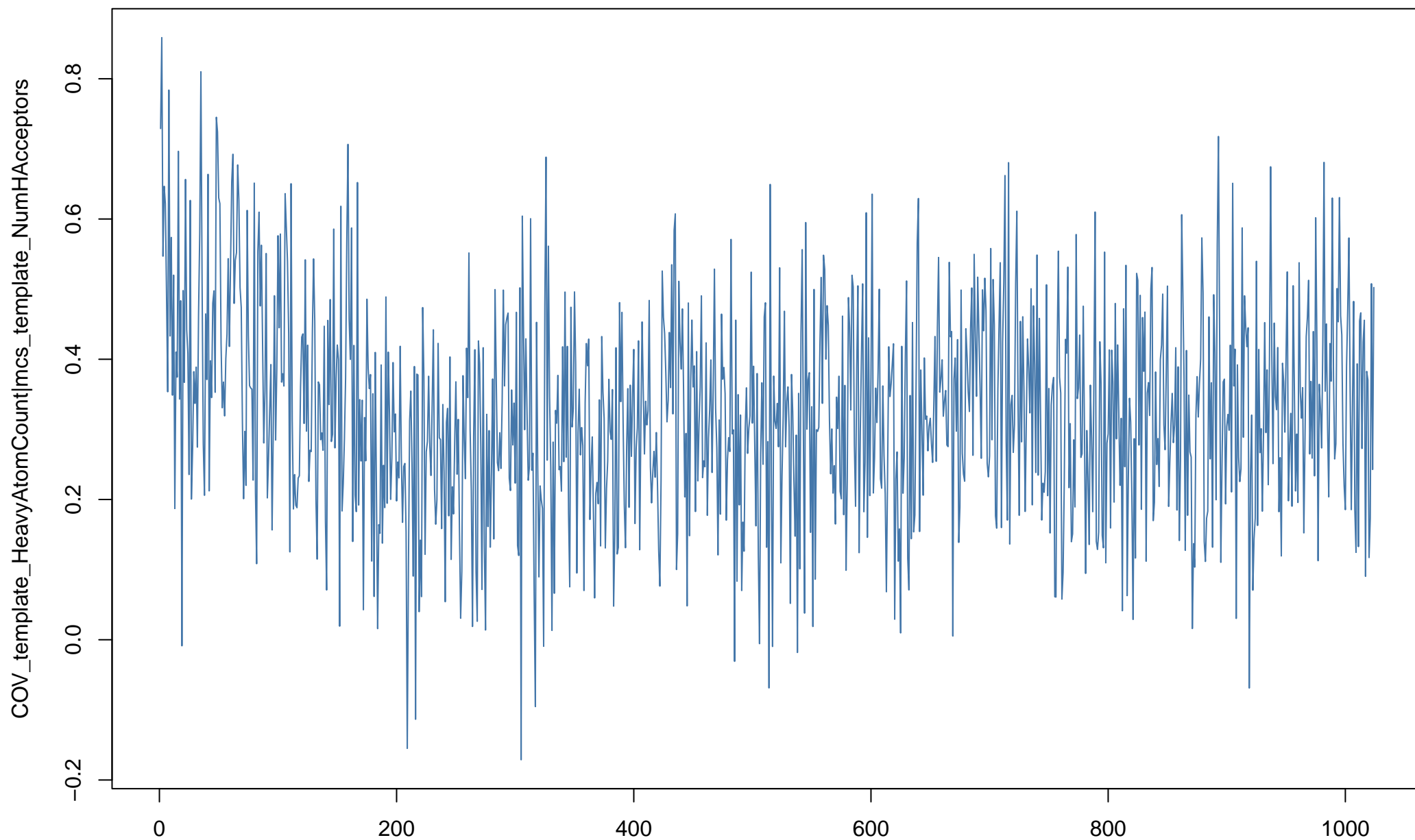
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 548 | BMK = 0.0874 | MCSE(6.27) = 4.8 | stat: TRUE | burn: 0



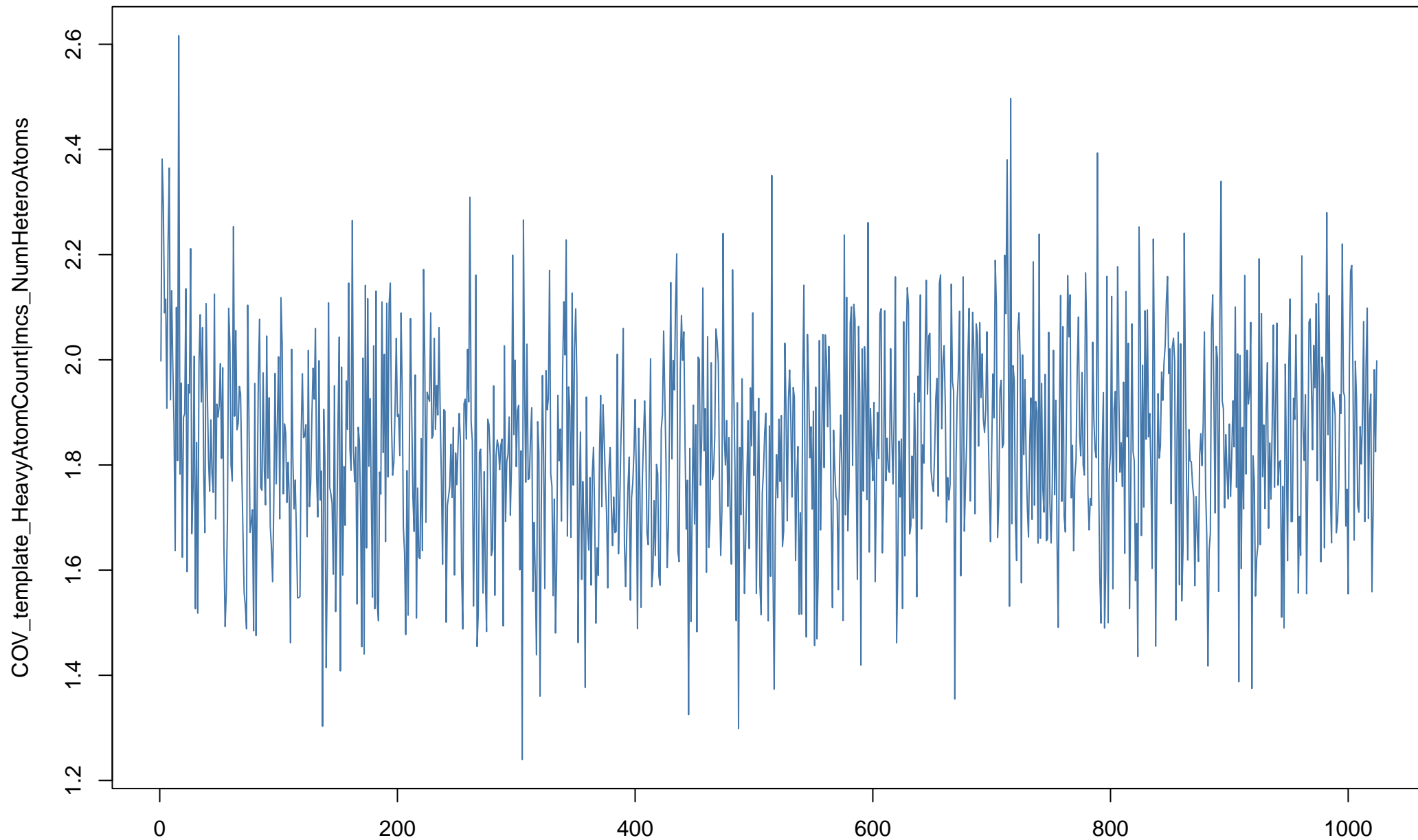
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 845 | BMK = 0.0755 | MCSE(6.27) = 4.68 | stat: FALSE | burn: 0



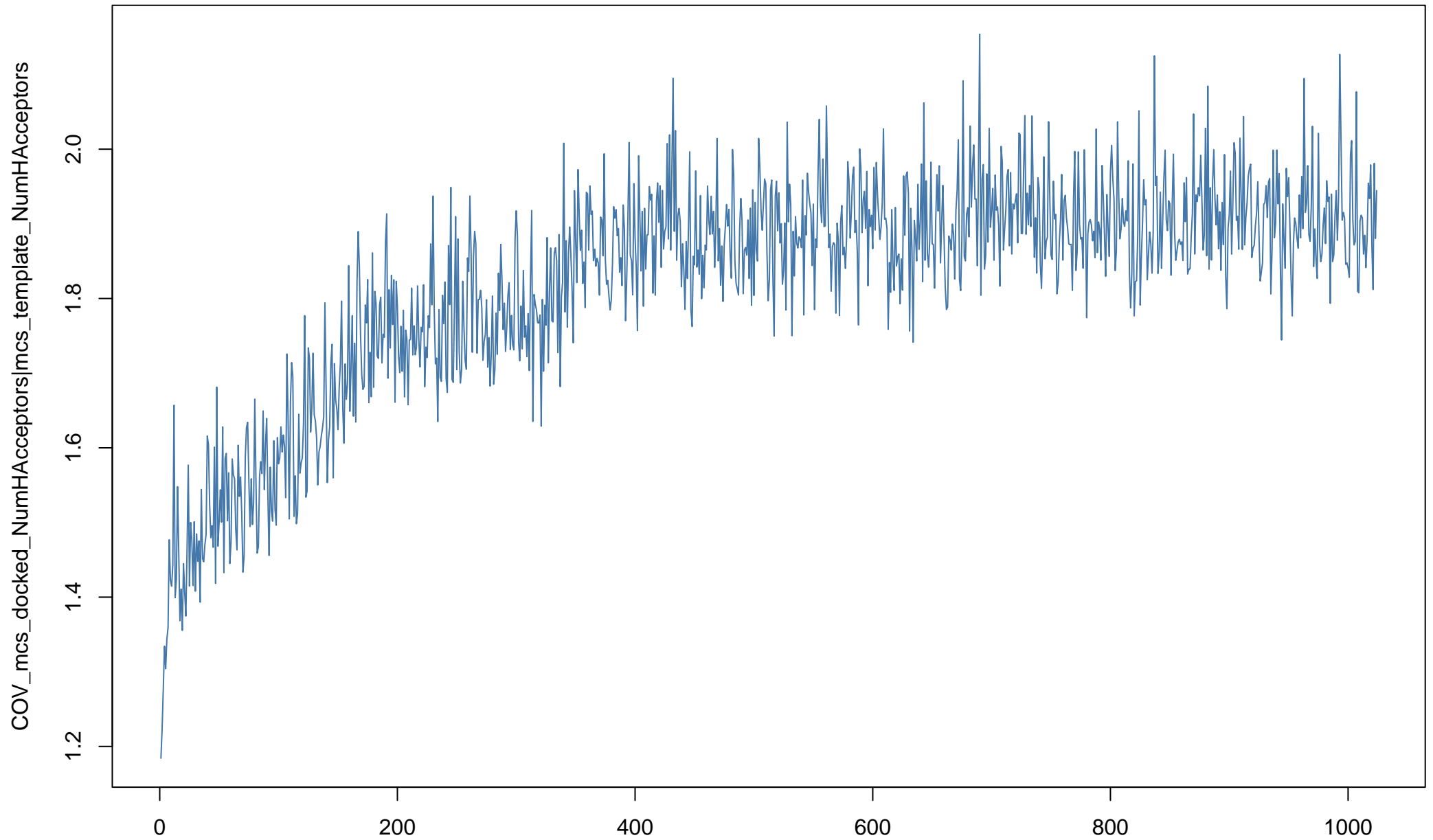
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 173 | BMK = 0.0757 | MCSE(6.27) = 6.31 | stat: FALSE | burn: 0



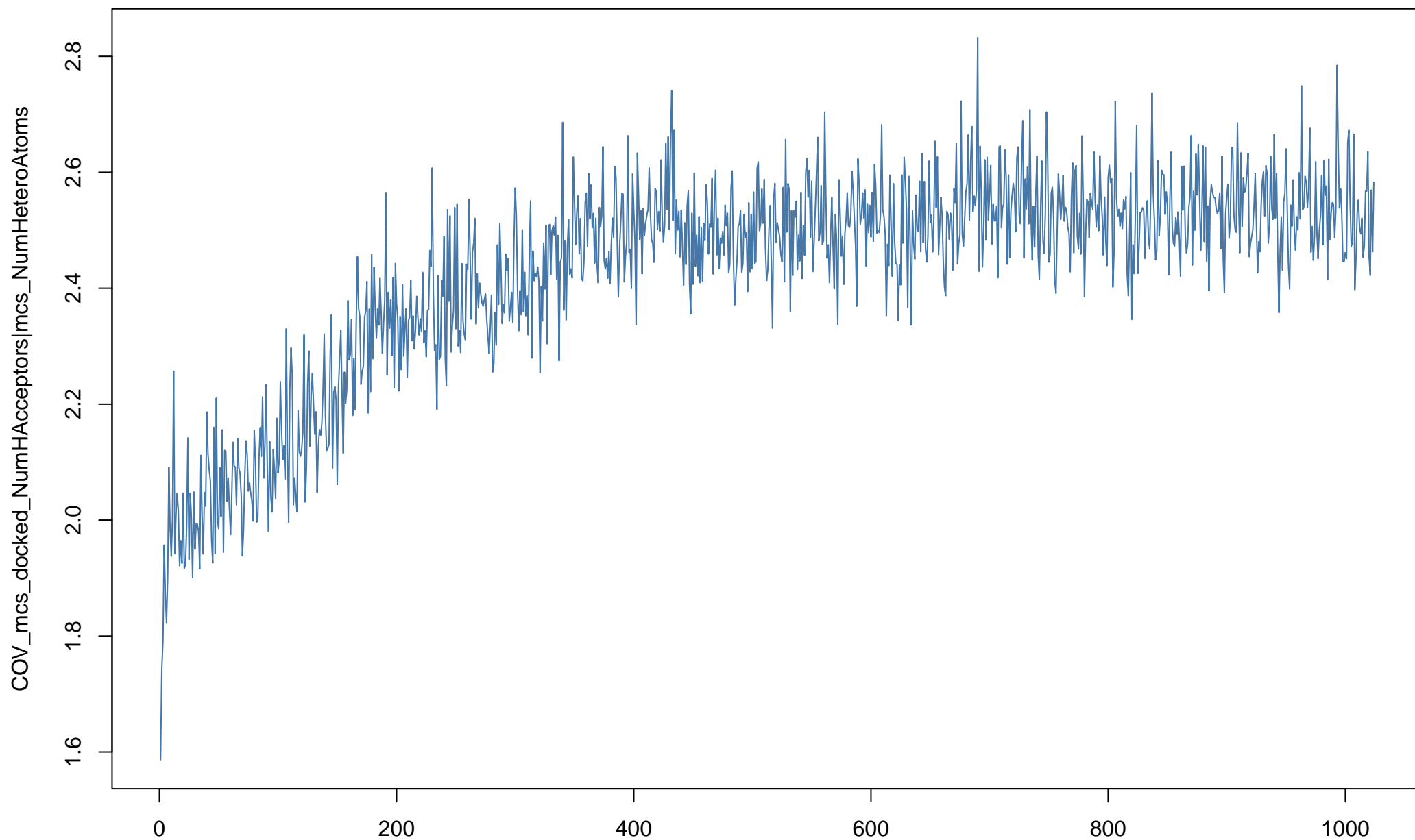
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 615 | BMK = 0.0921 | MCSE(6.27) = 4.72 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 4.82 | BMK = 0.541 | MCSE(6.27) = 16 | stat: FALSE | burn: 102



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 3.89 | BMK = 0.535 | MCSE(6.27) = 16.2 | stat: FALSE | burn: 102



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 4.03 | BMK = 0.53 | MCSE(6.27) = 16.1 | stat: FALSE | burn: 102

