

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.842240618398604

max MCSE = 17.7688618829735

all stationary: FALSE

burn: 1020

-- STATS 2D --

min ESS = 10.2186846313861

max BMK = 0.536484986611595

max MCSE = 15.1954994503418

all stationary: FALSE

burn: 102

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.579711019013251

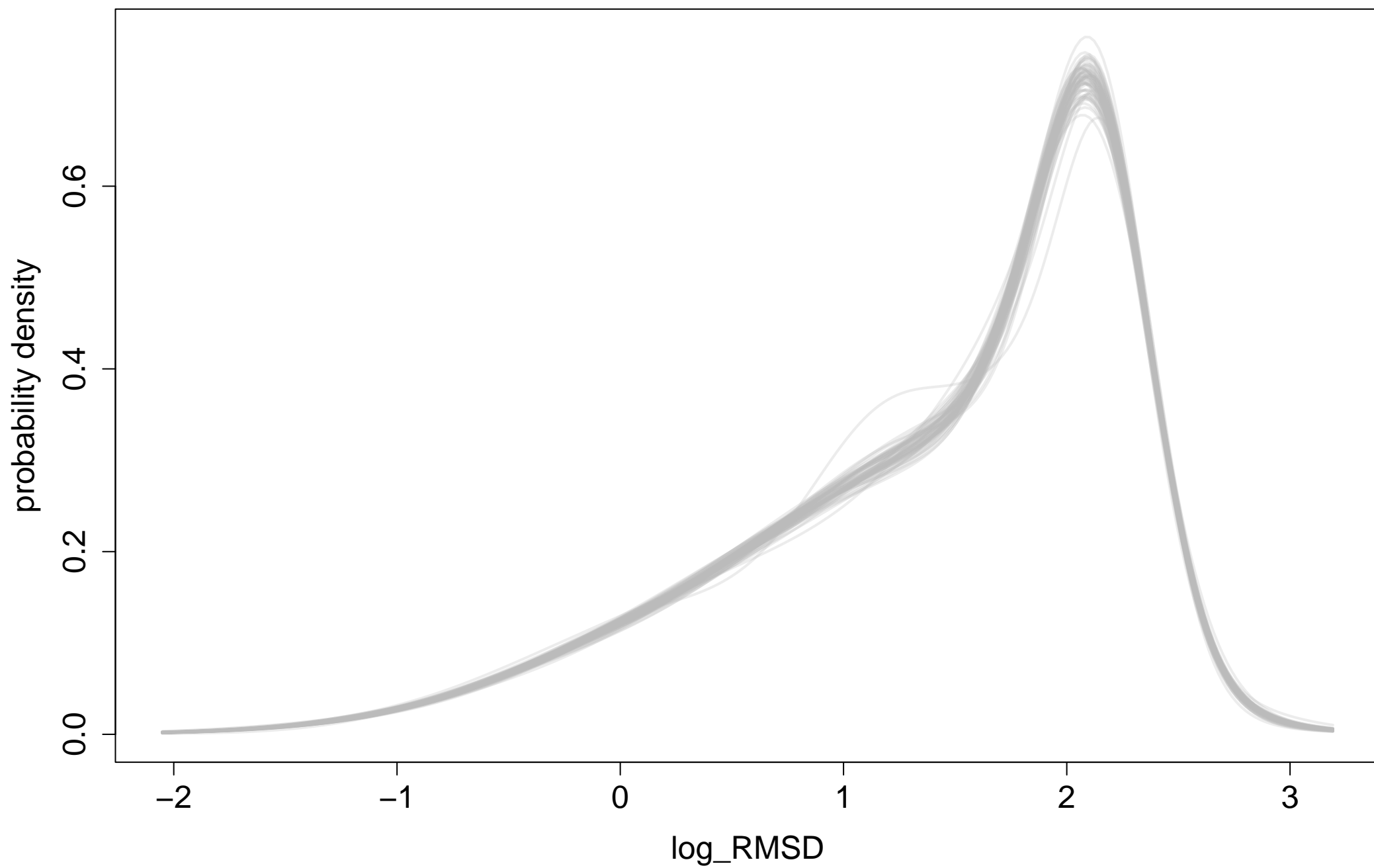
max MCSE = NaN

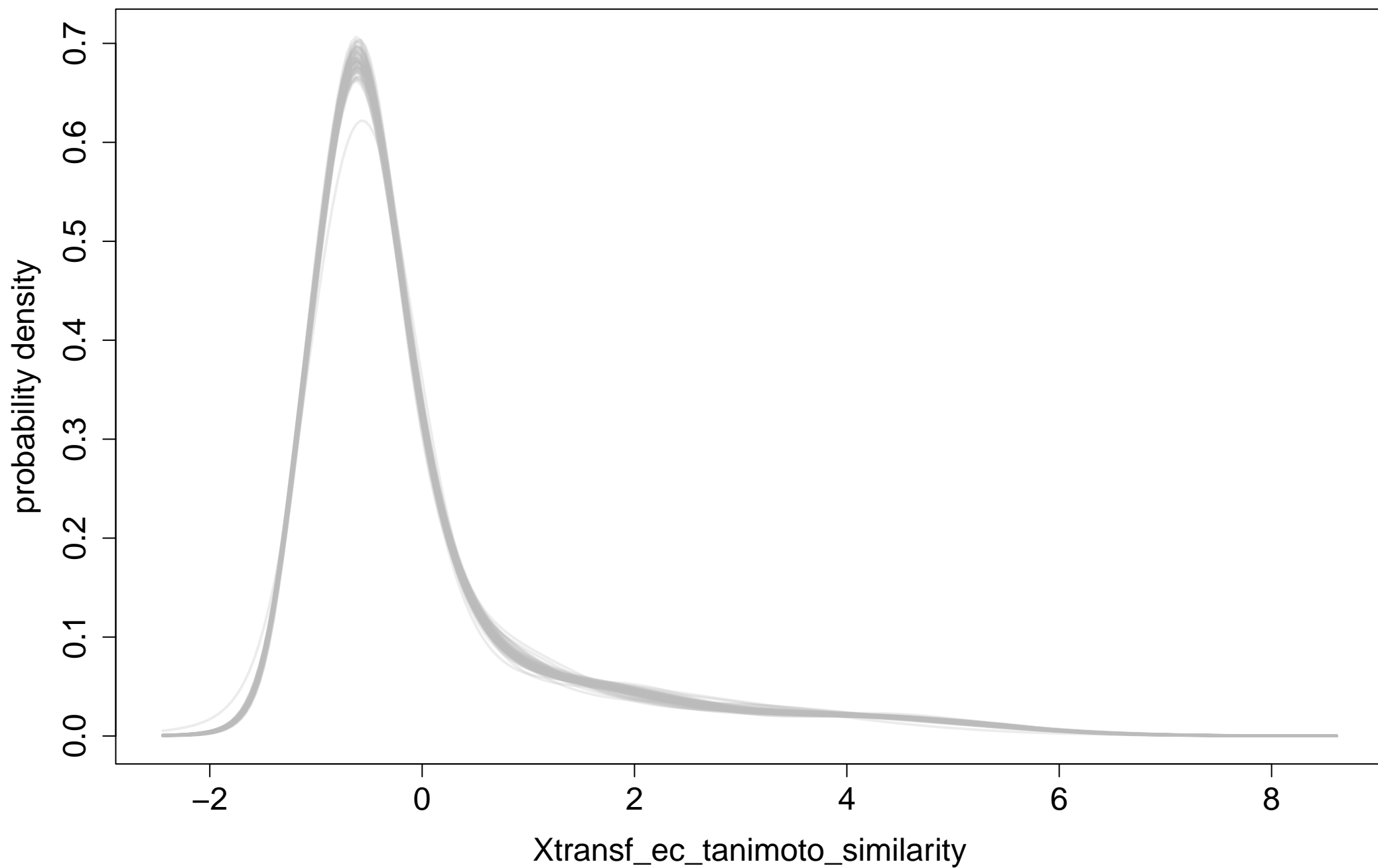
all stationary: FALSE

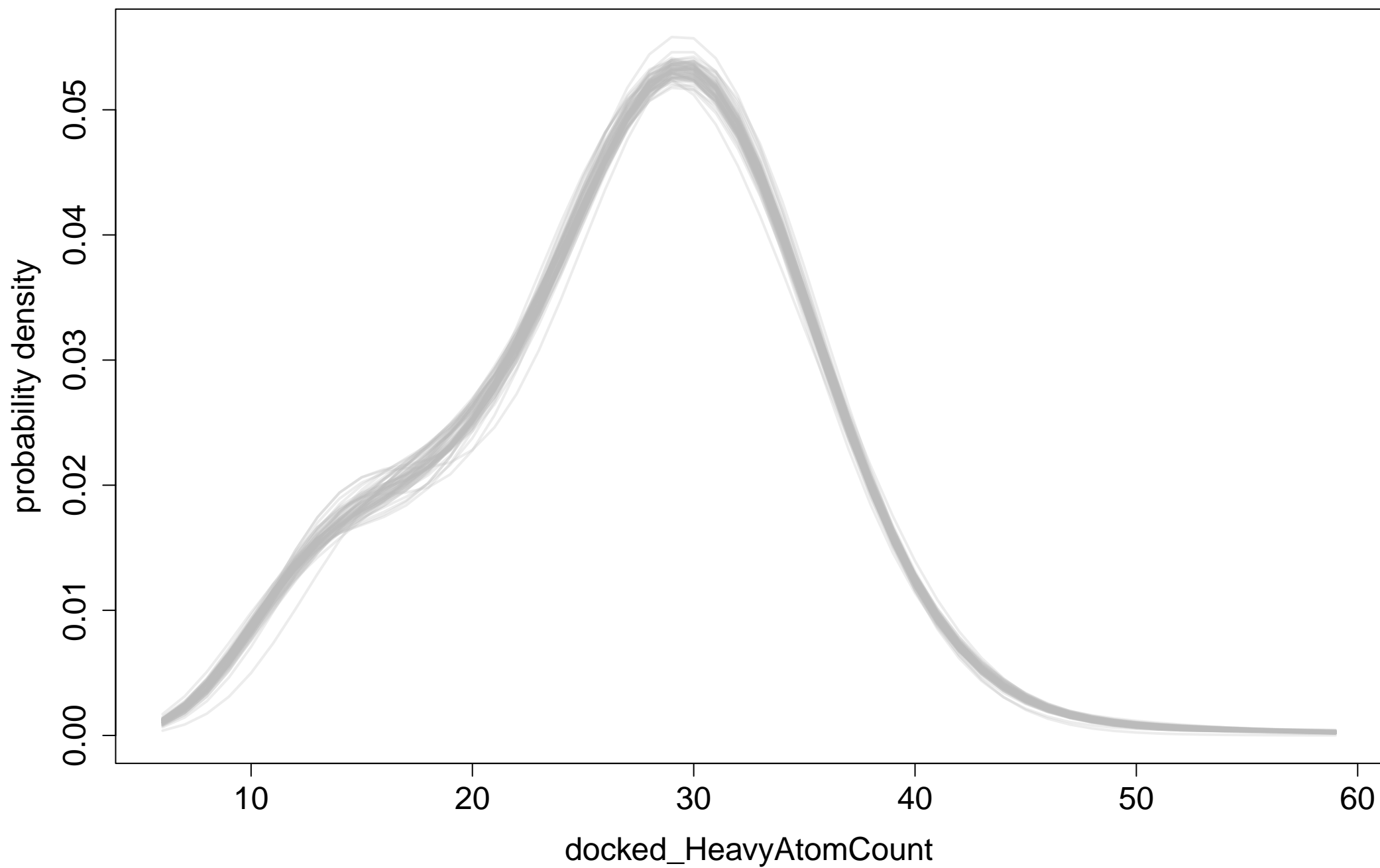
burn: 816

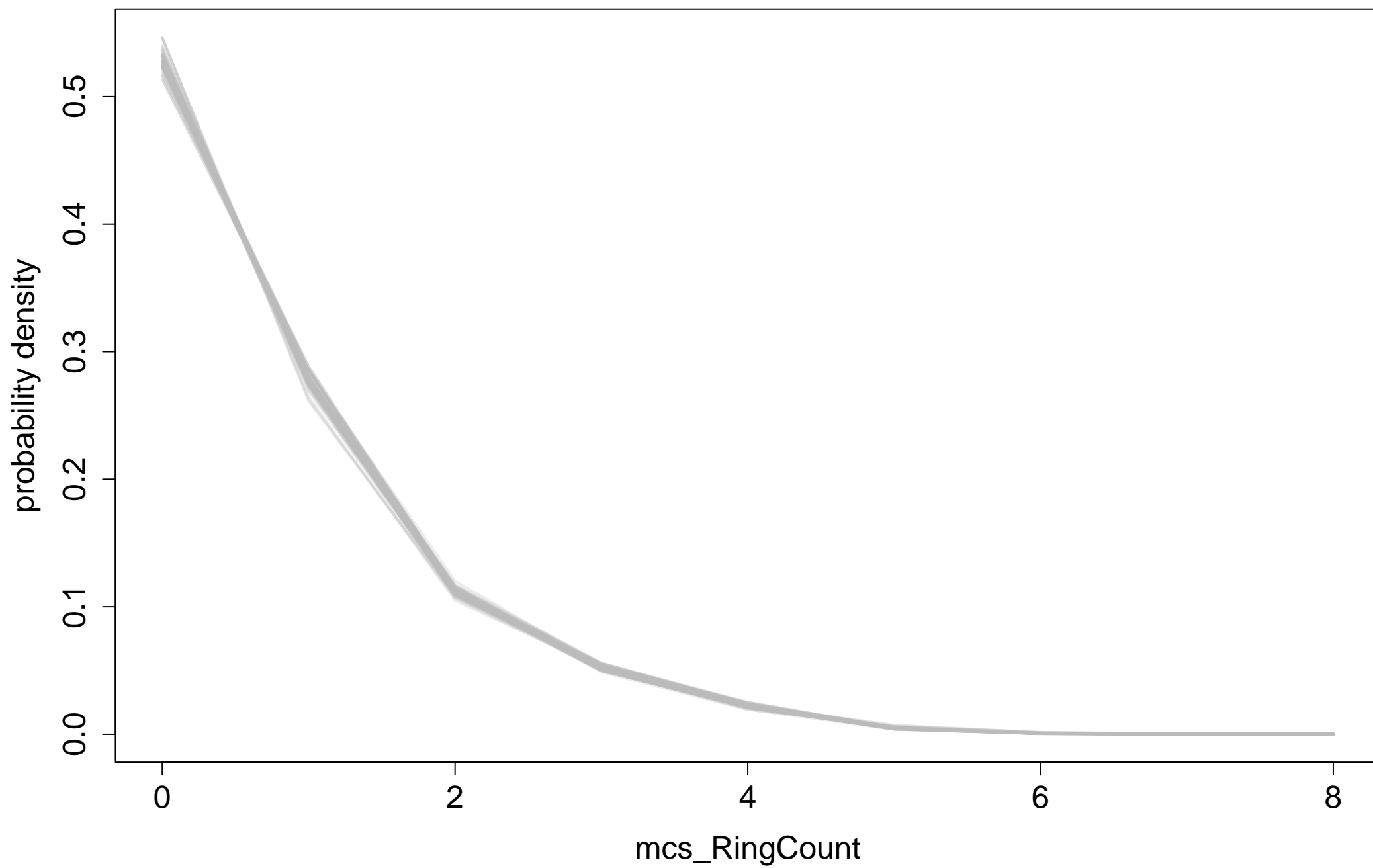
Occupied clusters: 39 of 64

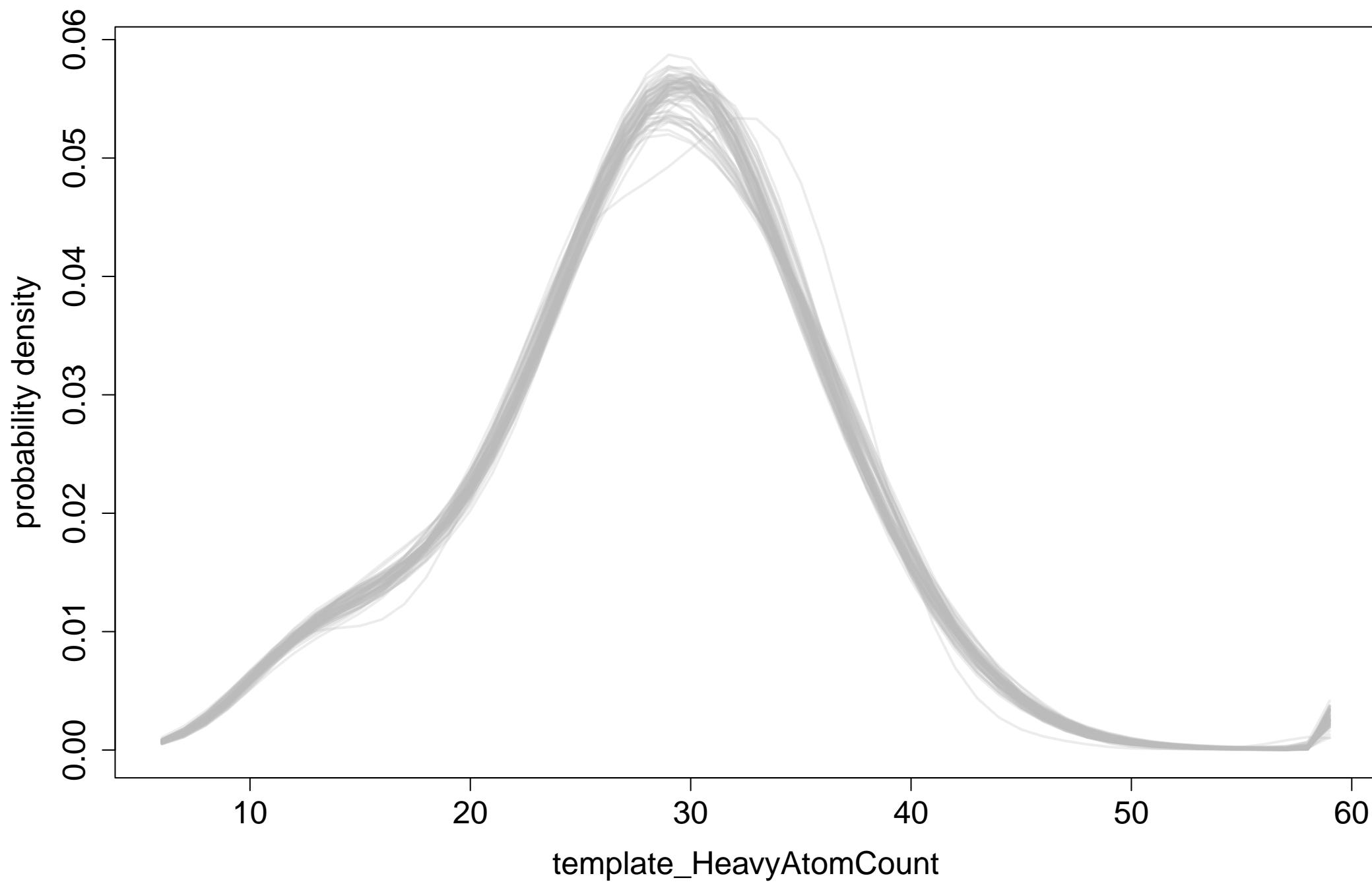
LL: -115000 +- 1510

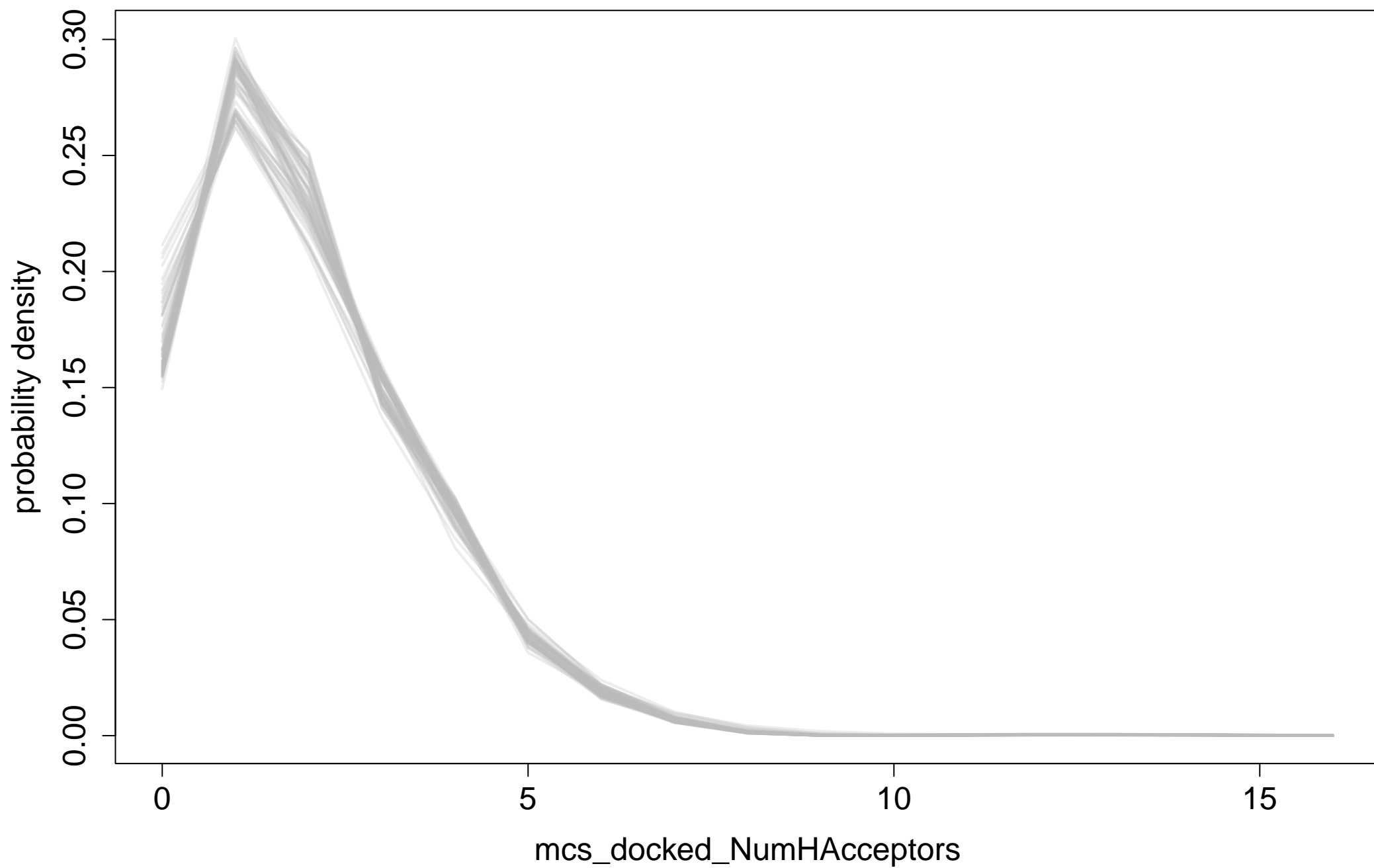


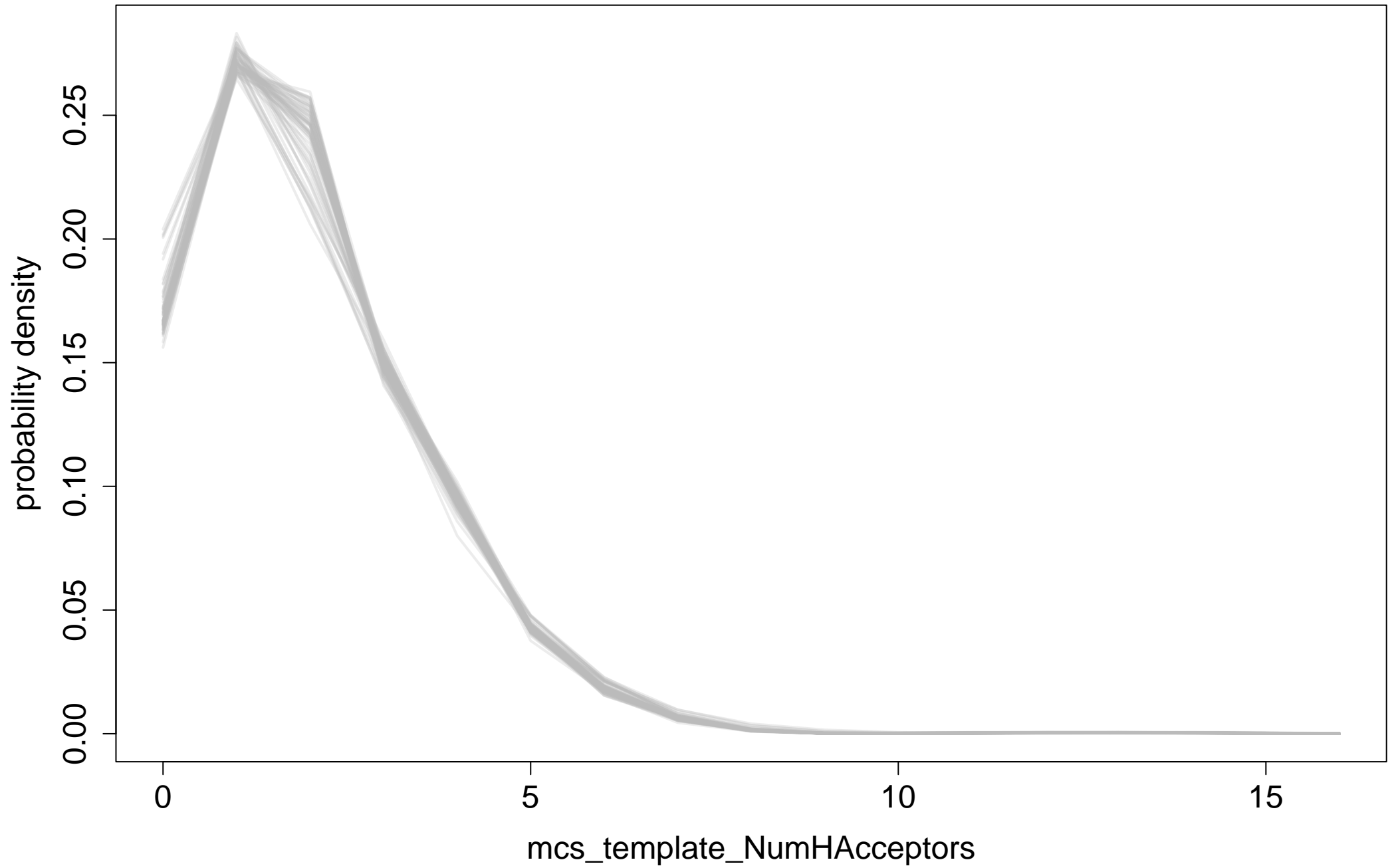


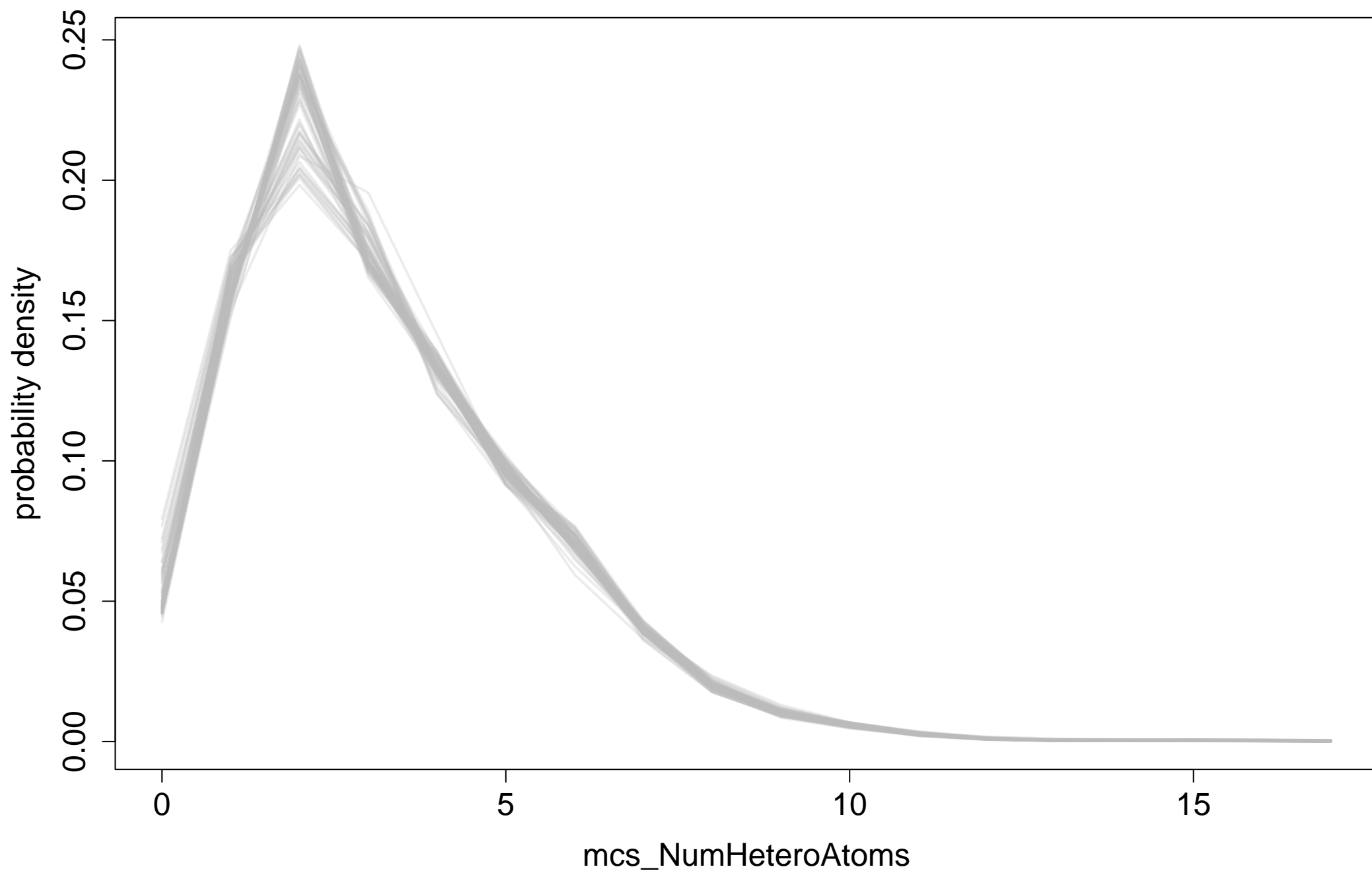


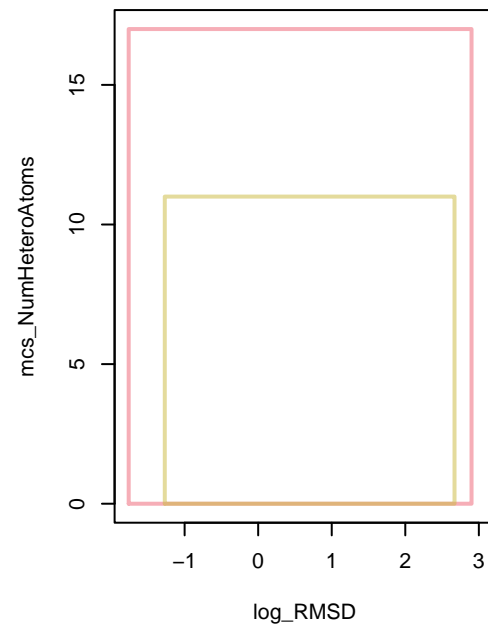
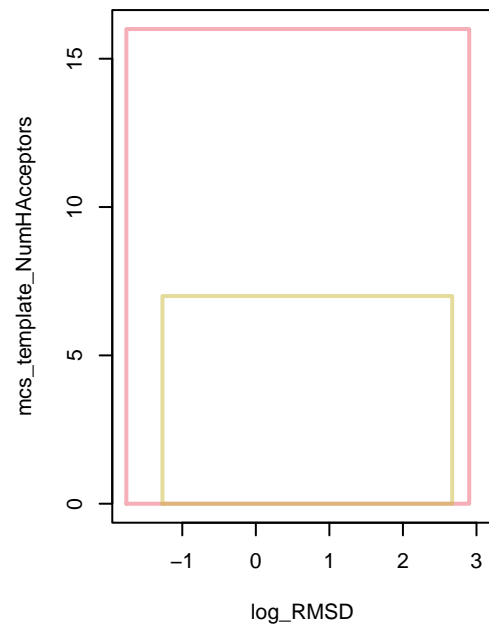
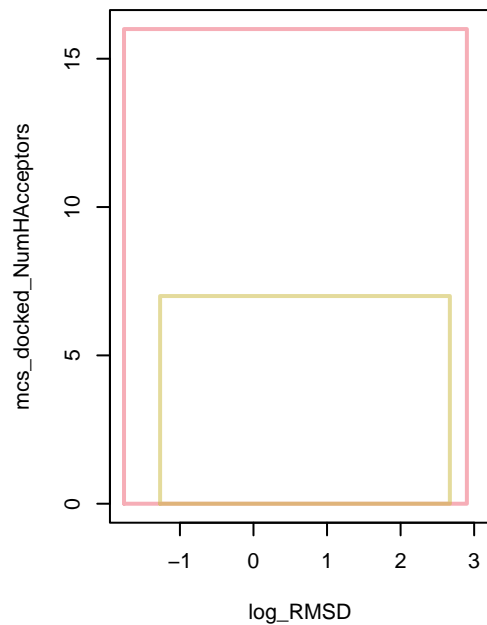
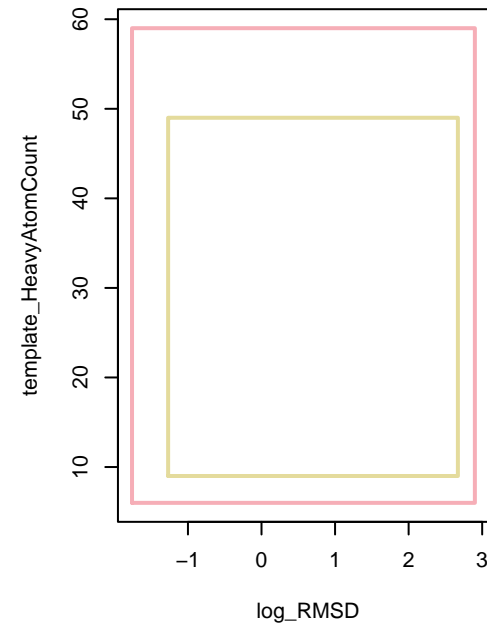
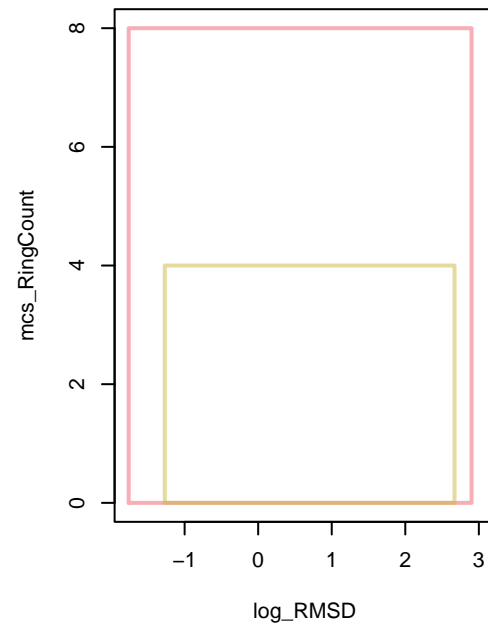
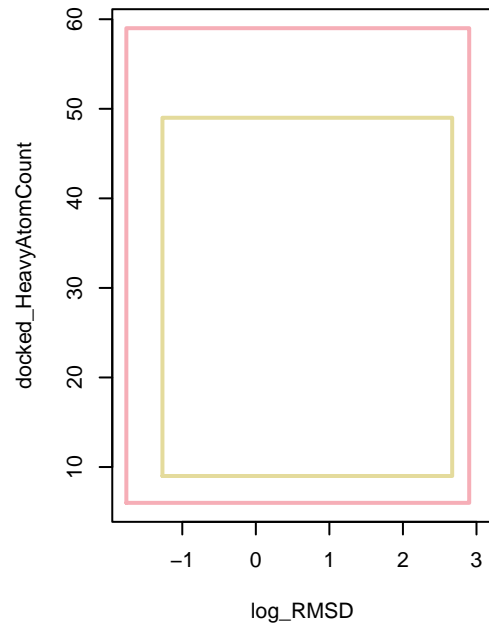
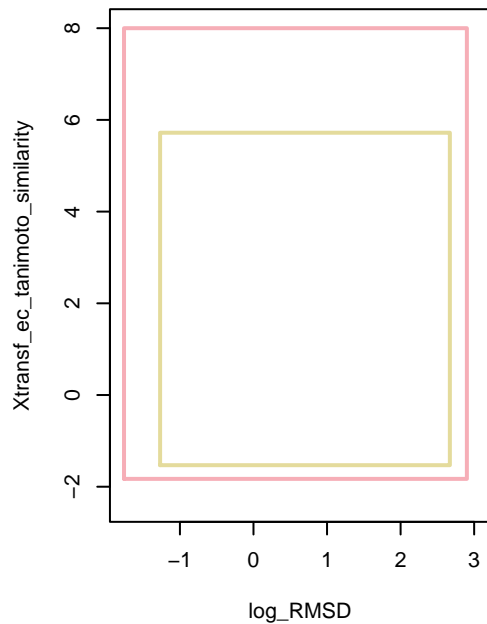




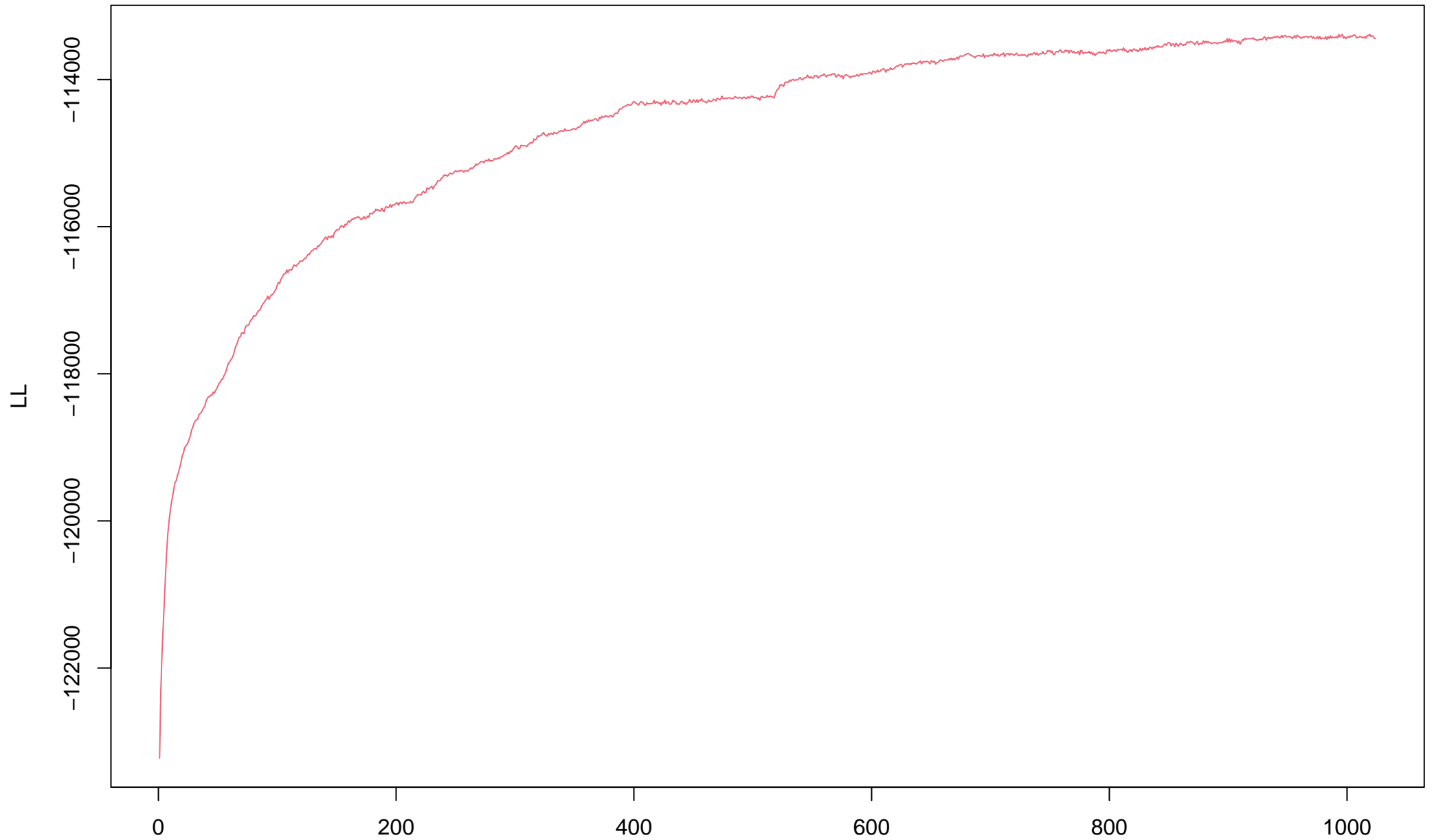




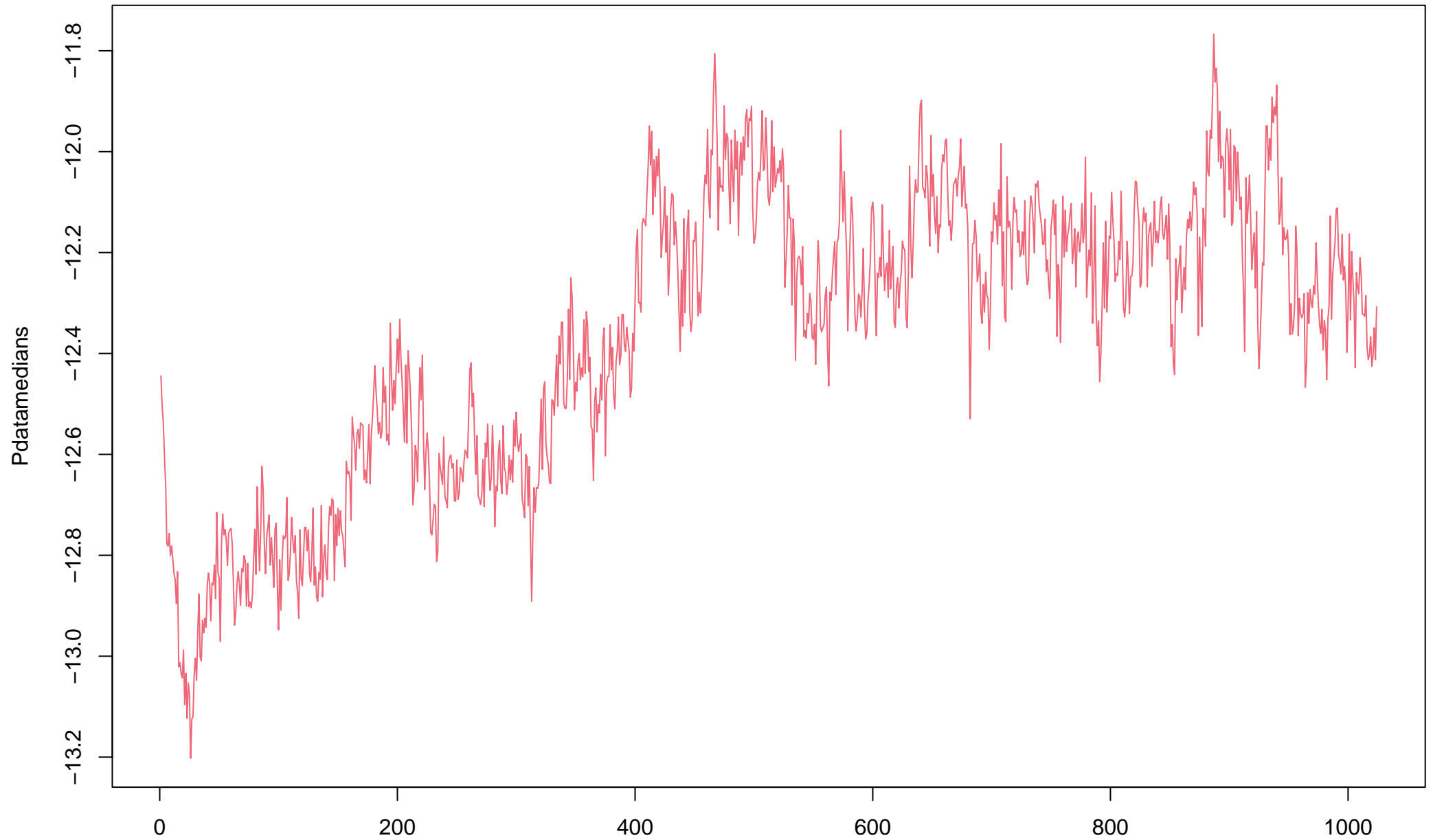




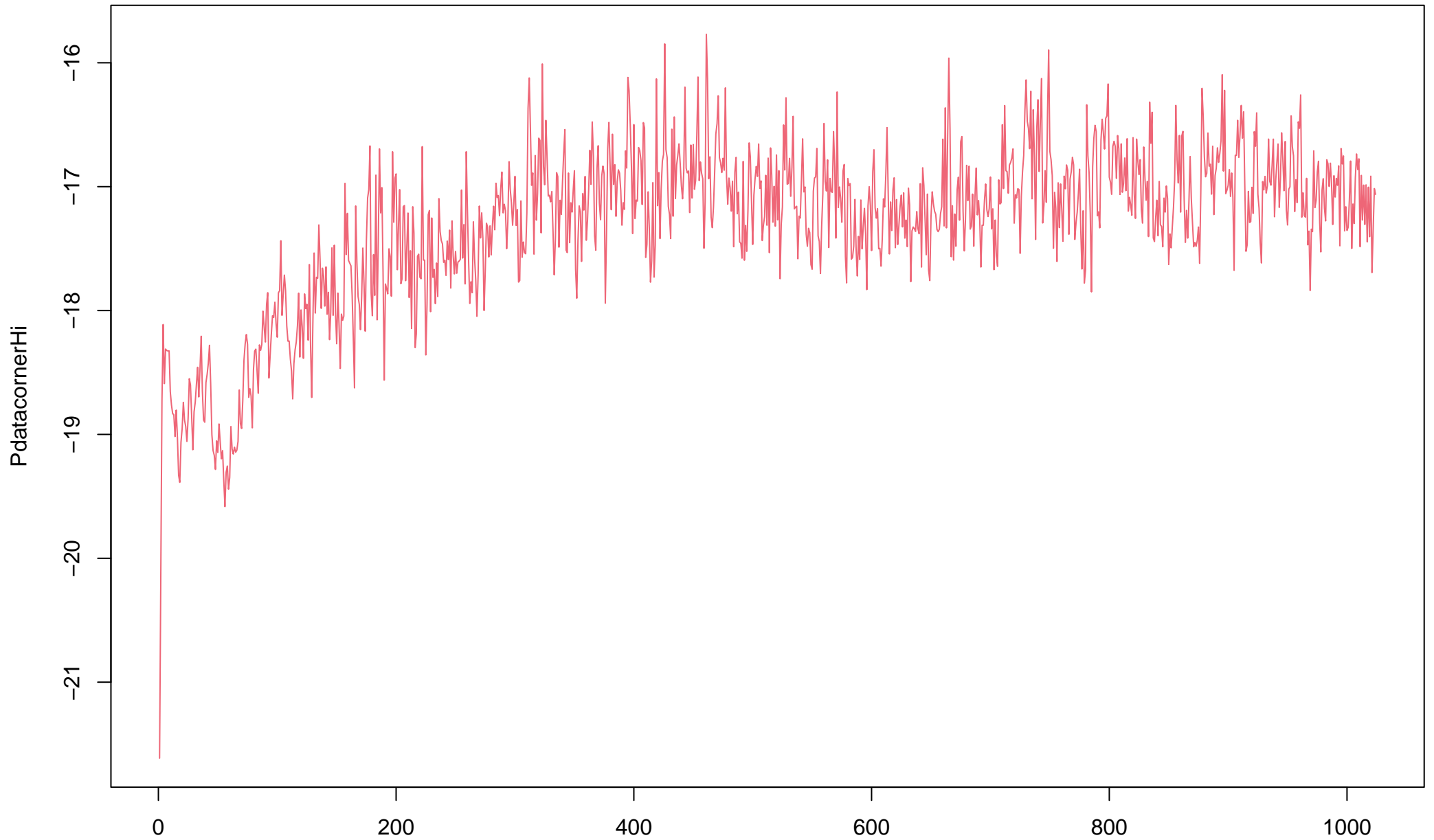
LL
ESS = 7.31 | BMK = 0.842 | MCSE(6.27) = 17.8 | stat: FALSE | burn: 1020



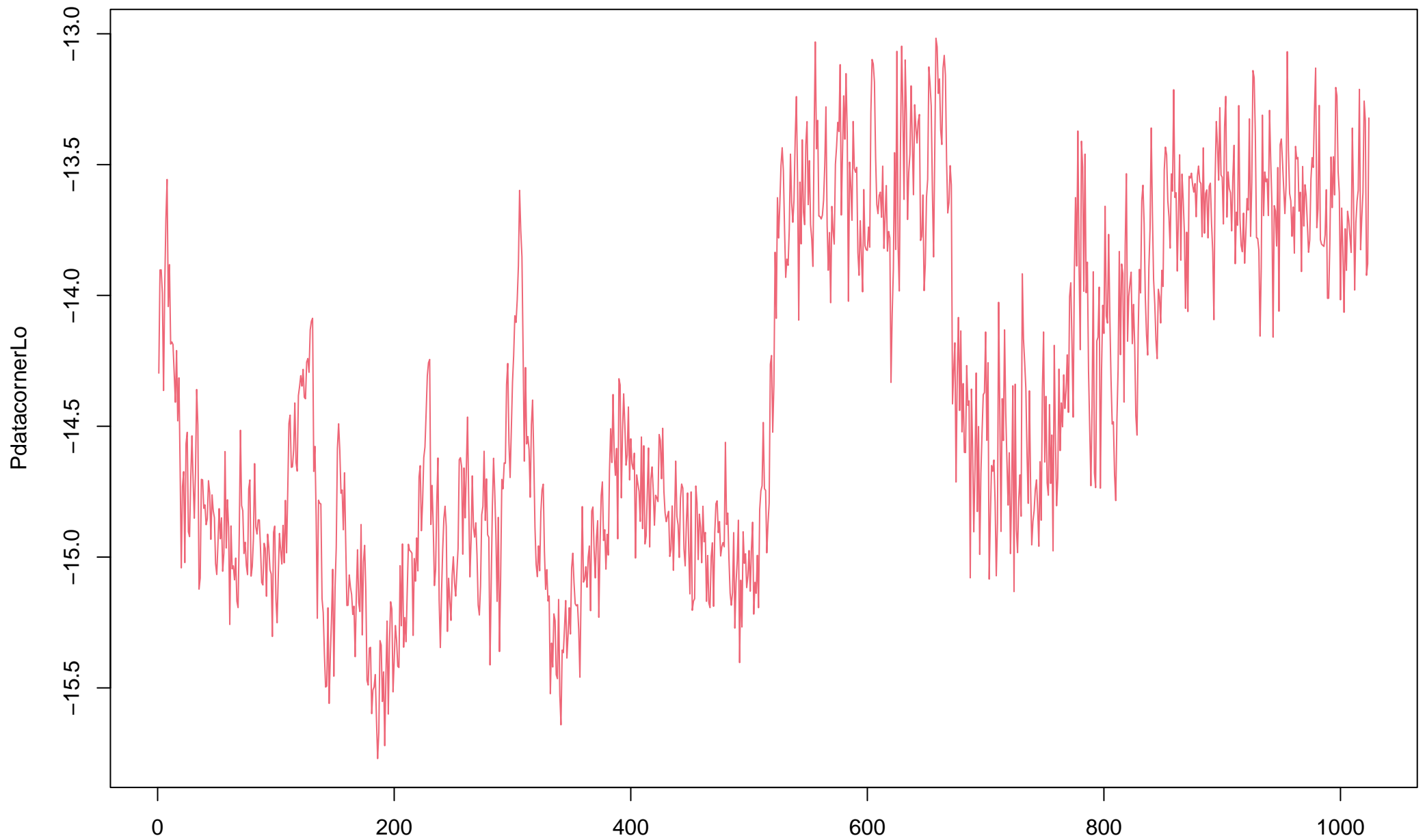
Pdatamedians
ESS = 5.06 | BMK = 0.636 | MCSE(6.27) = 16.3 | stat: FALSE | burn: 408



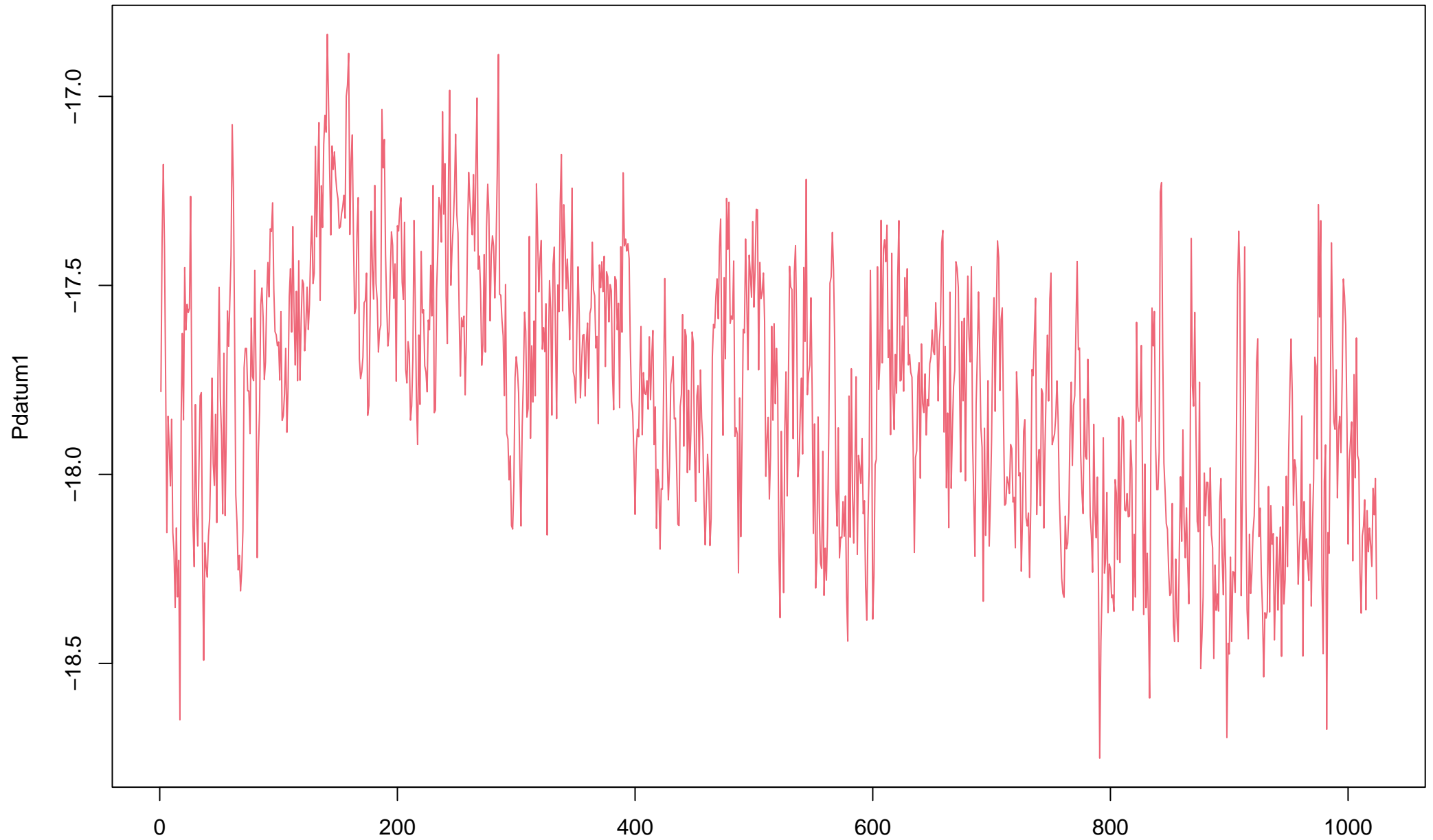
PdatacornerHi
ESS = 15 | BMK = 0.384 | MCSE(6.27) = 12.1 | stat: FALSE | burn: 102



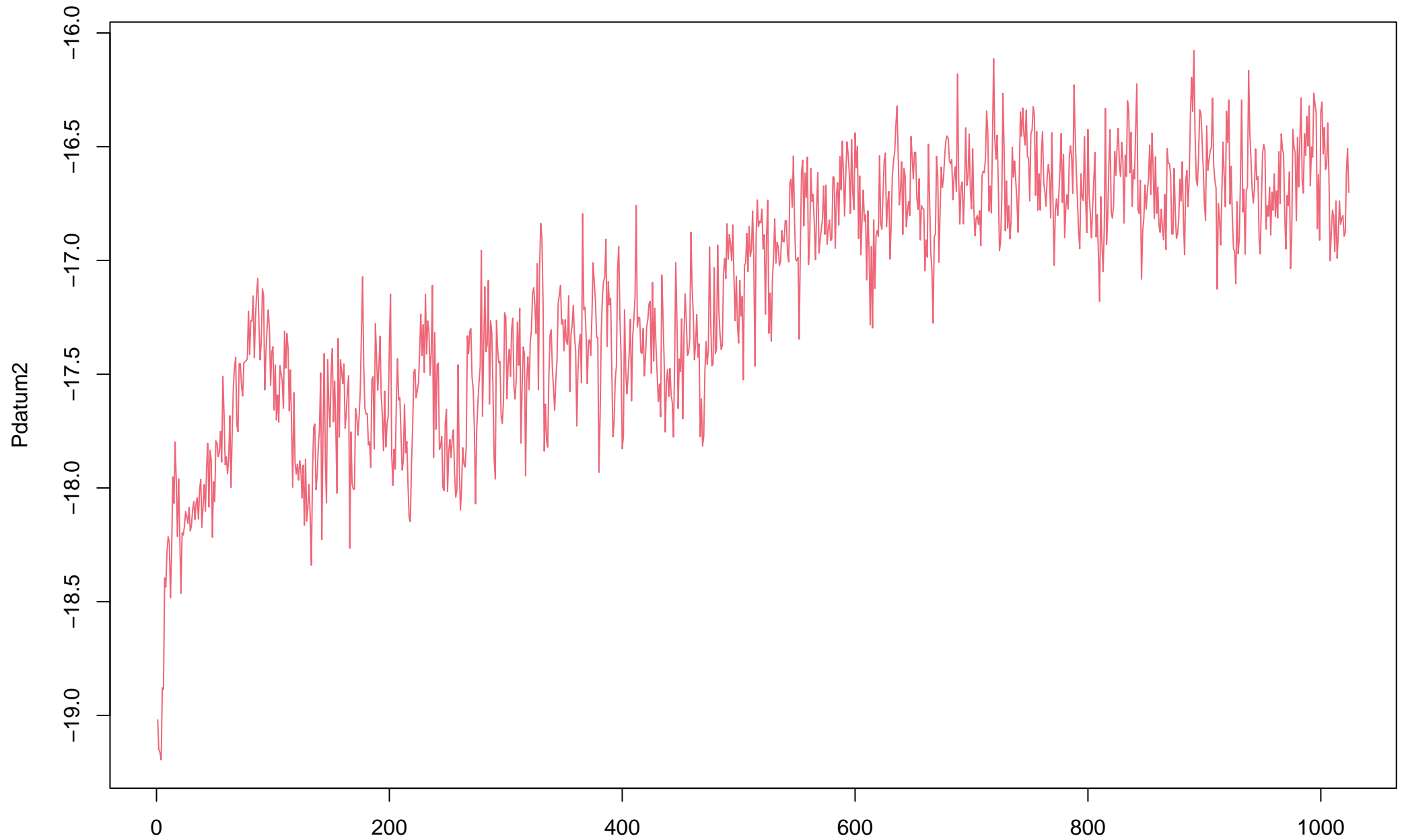
PdatacornerLo
ESS = 6.08 | BMK = 0.667 | MCSE(6.27) = 15.9 | stat: FALSE | burn: 816



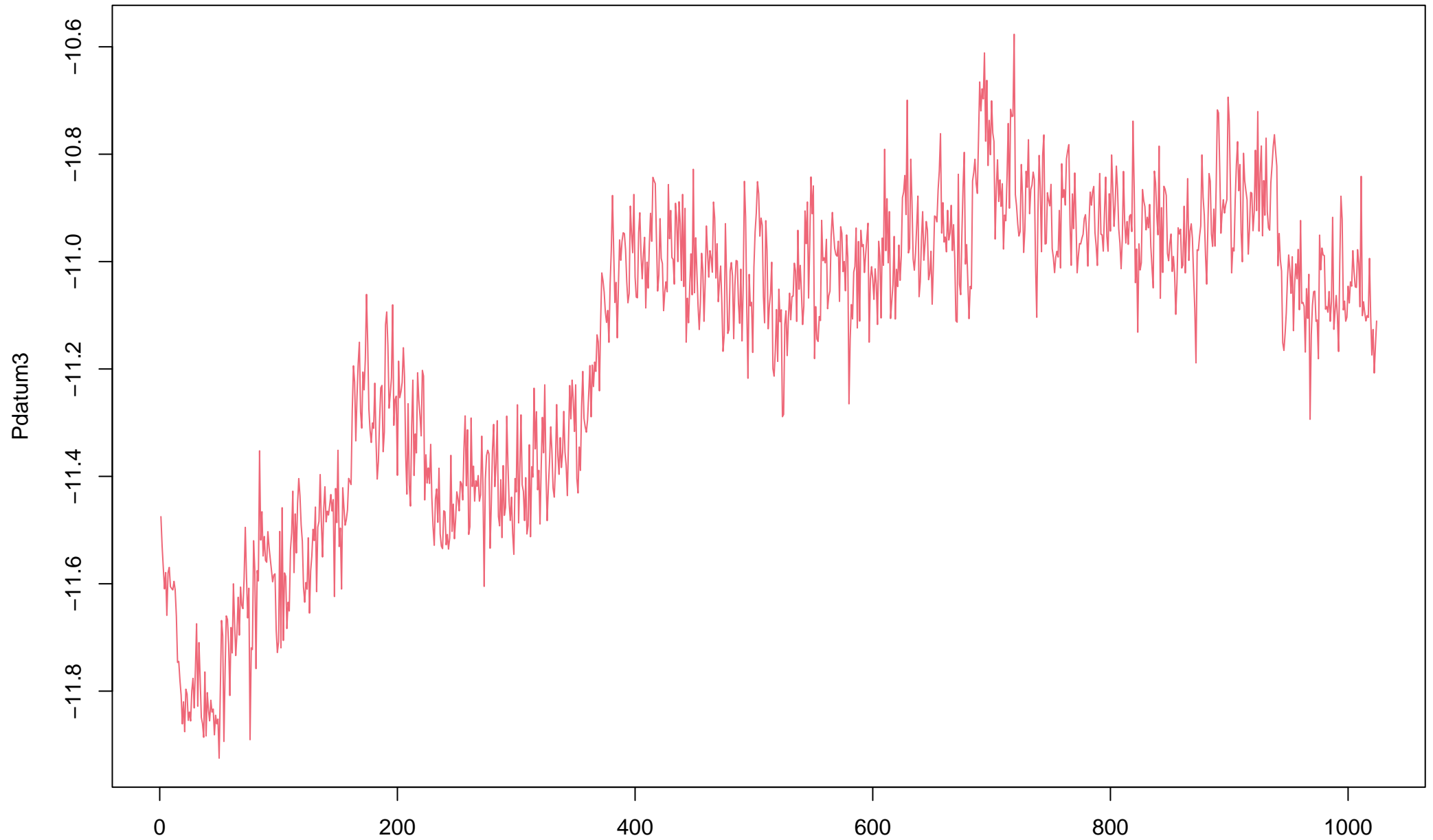
Pdatum1
ESS = 2.22e-16 | BMK = 0.371 | MCSE(6.27) = 12.5 | stat: TRUE | burn: 0



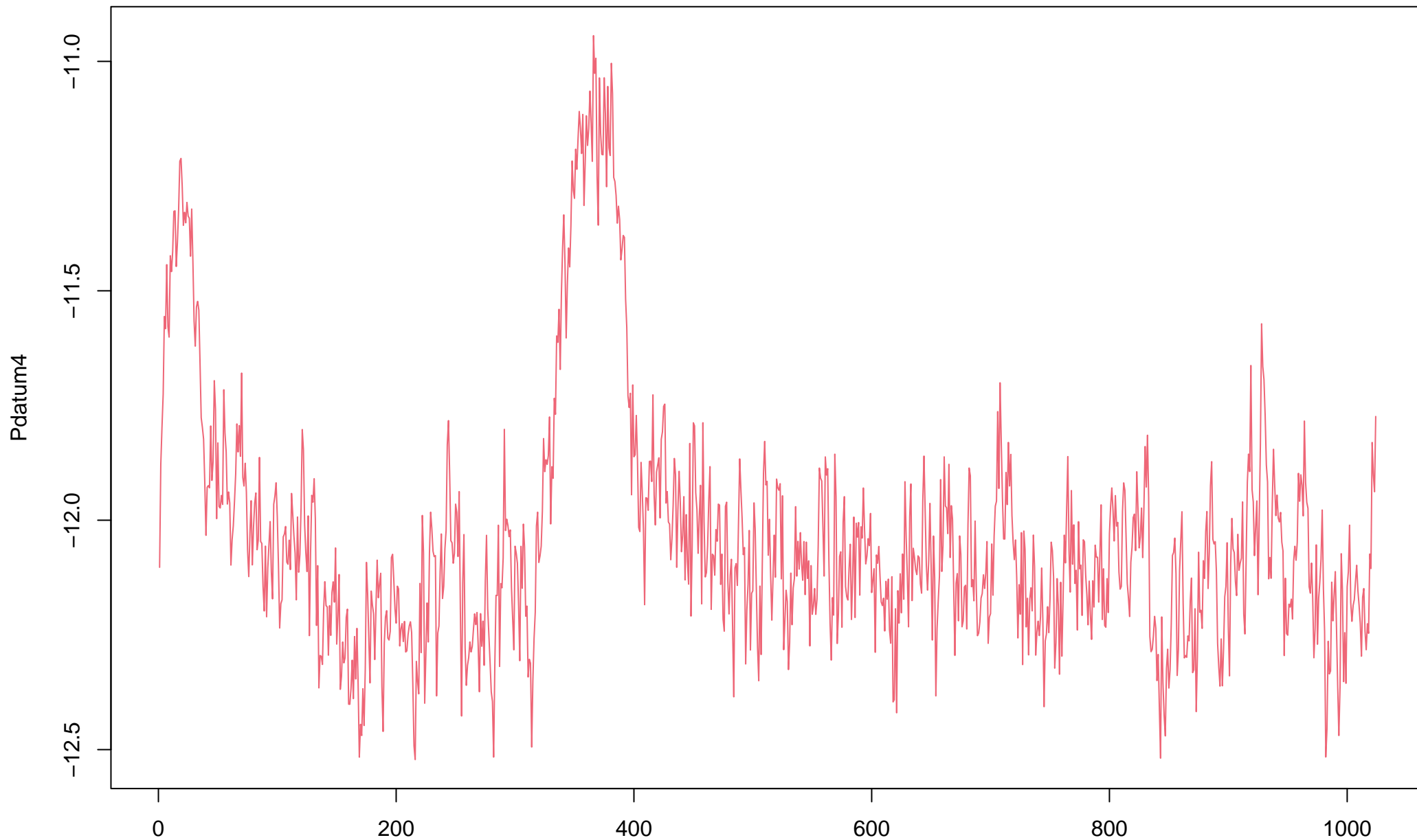
Pdatum2
ESS = 2.22e-16 | BMK = 0.841 | MCSE(6.27) = 15.9 | stat: FALSE | burn: 510



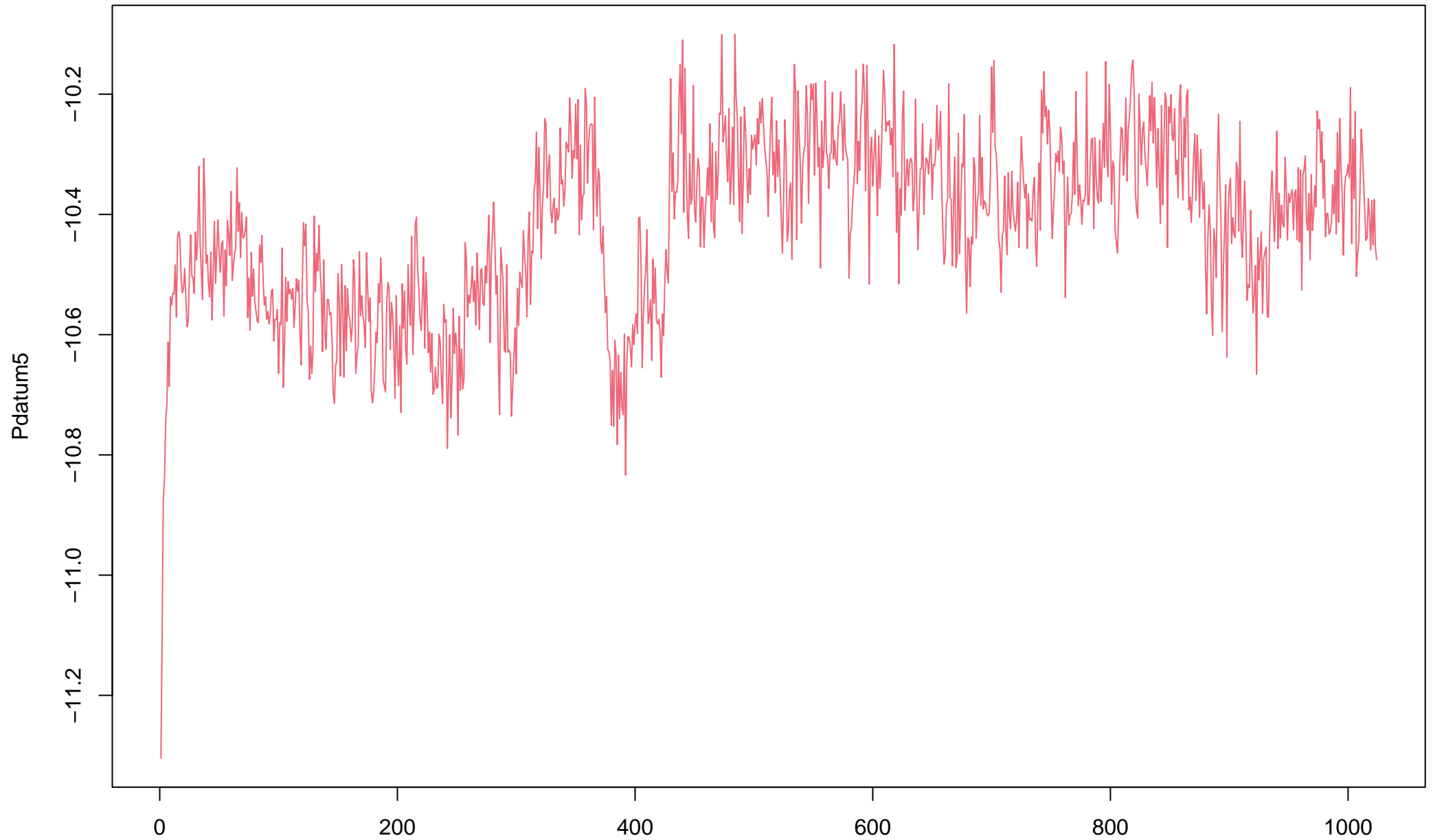
Pdatum3
ESS = 4.05 | BMK = 0.64 | MCSE(6.27) = 16.8 | stat: FALSE | burn: 408



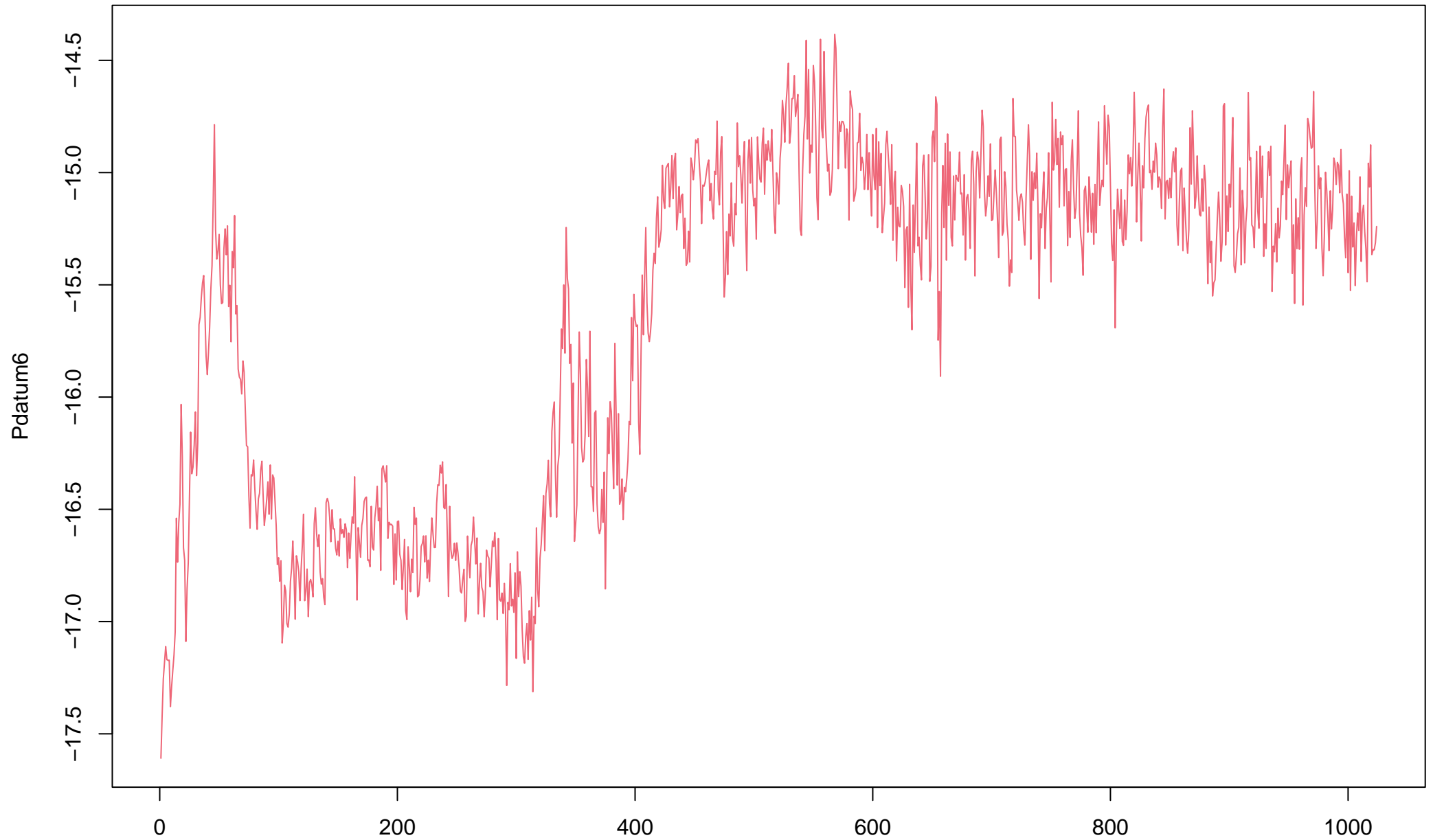
Pdatum4
ESS = 16.9 | BMK = 0.329 | MCSE(6.27) = 16 | stat: FALSE | burn: 408



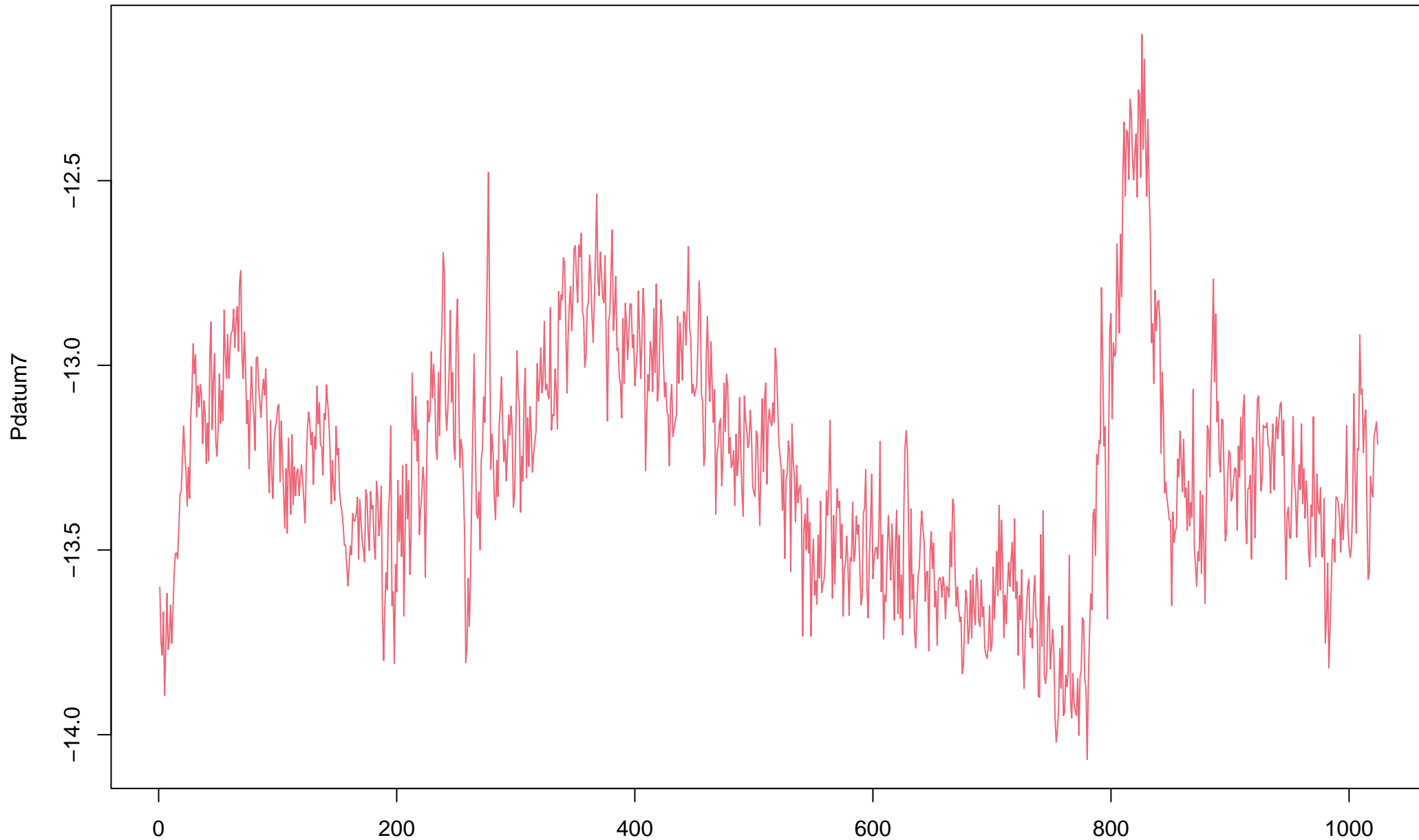
Pdatum5
ESS = 20.1 | BMK = 0.444 | MCSE(6.27) = 13.8 | stat: FALSE | burn: 0



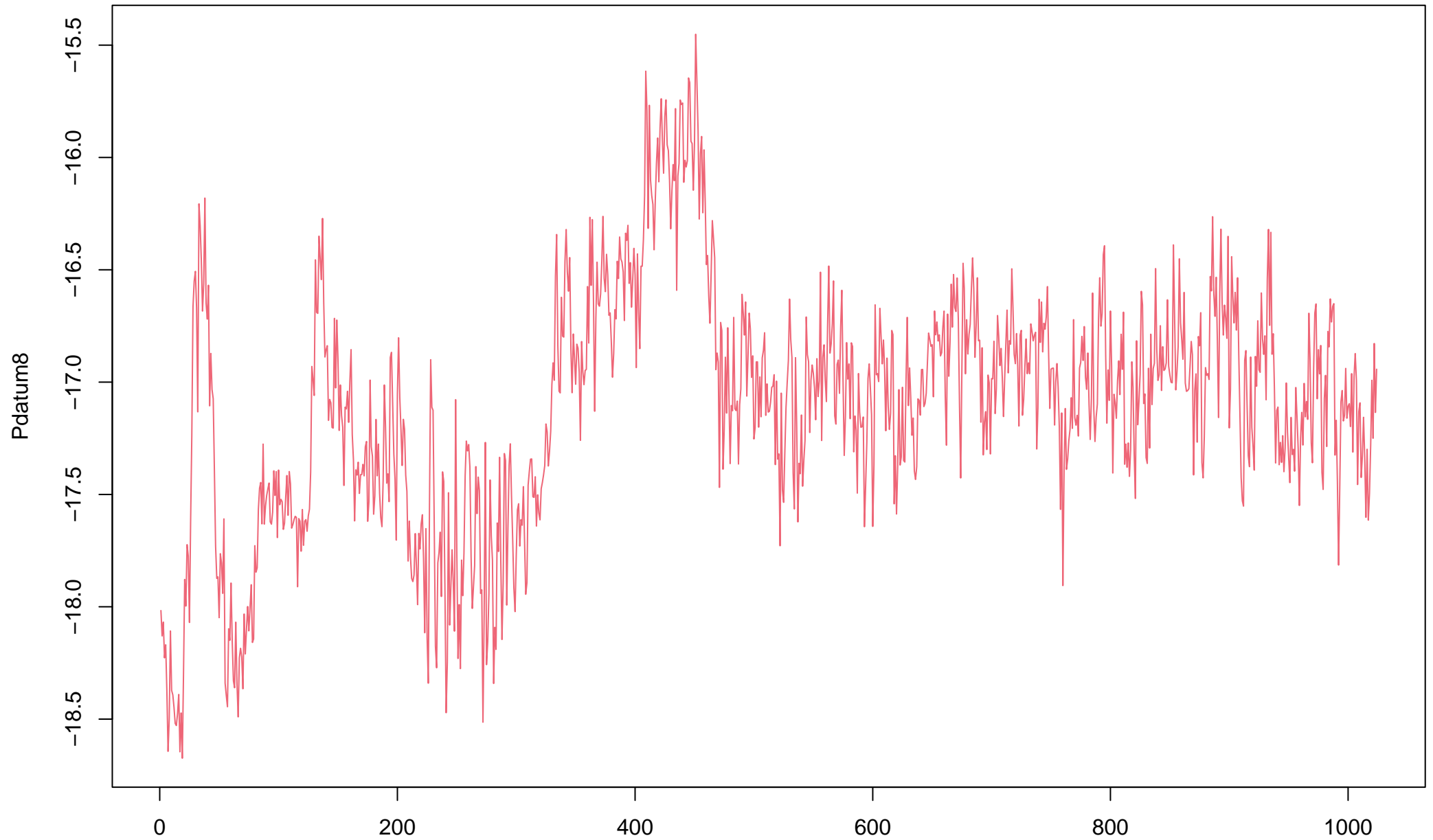
Pdatum6
ESS = 3.52 | BMK = 0.671 | MCSE(6.27) = 16.5 | stat: FALSE | burn: 408



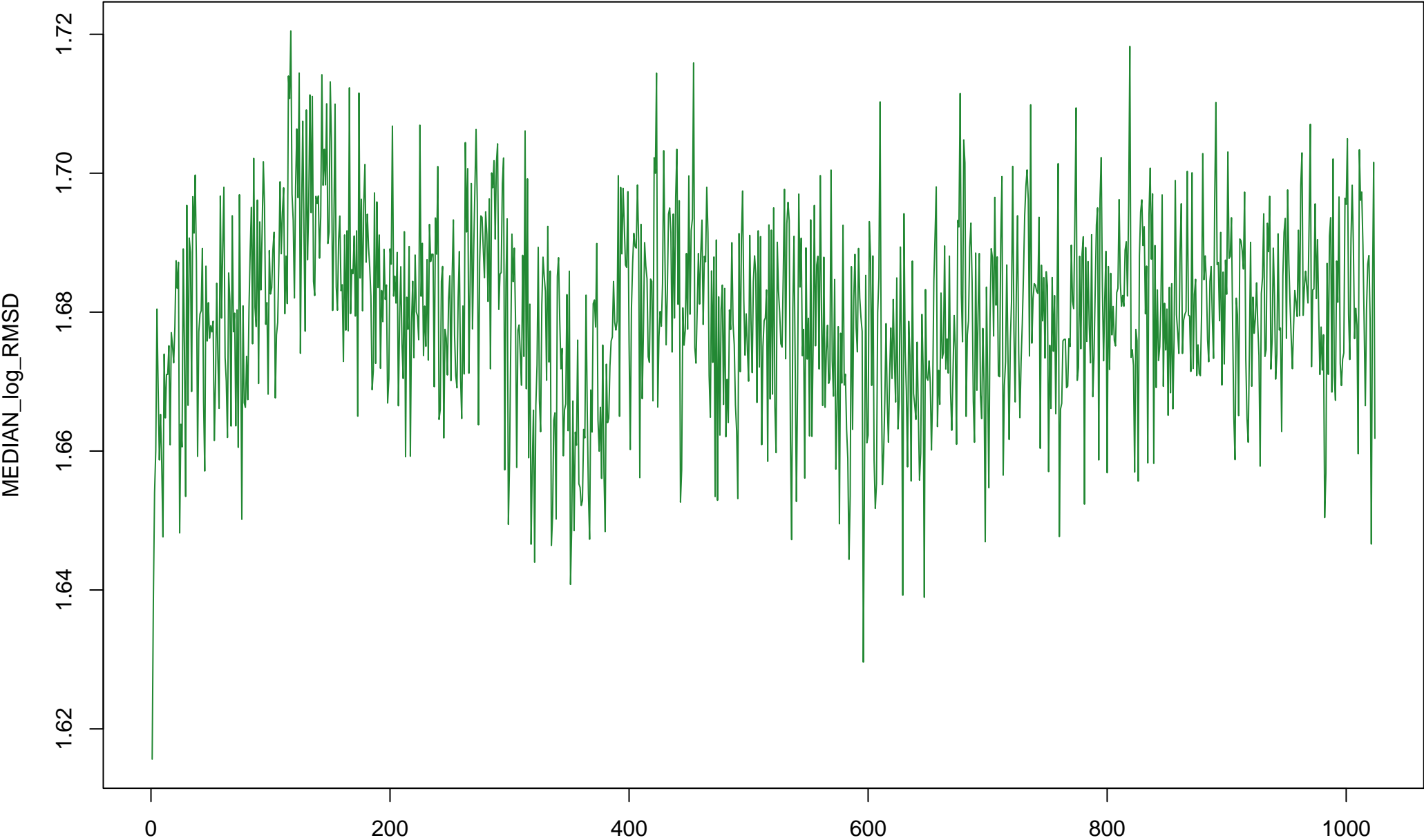
Pdatum7
ESS = 21.6 | BMK = 0.393 | MCSE(6.27) = 15.2 | stat: FALSE | burn: 510



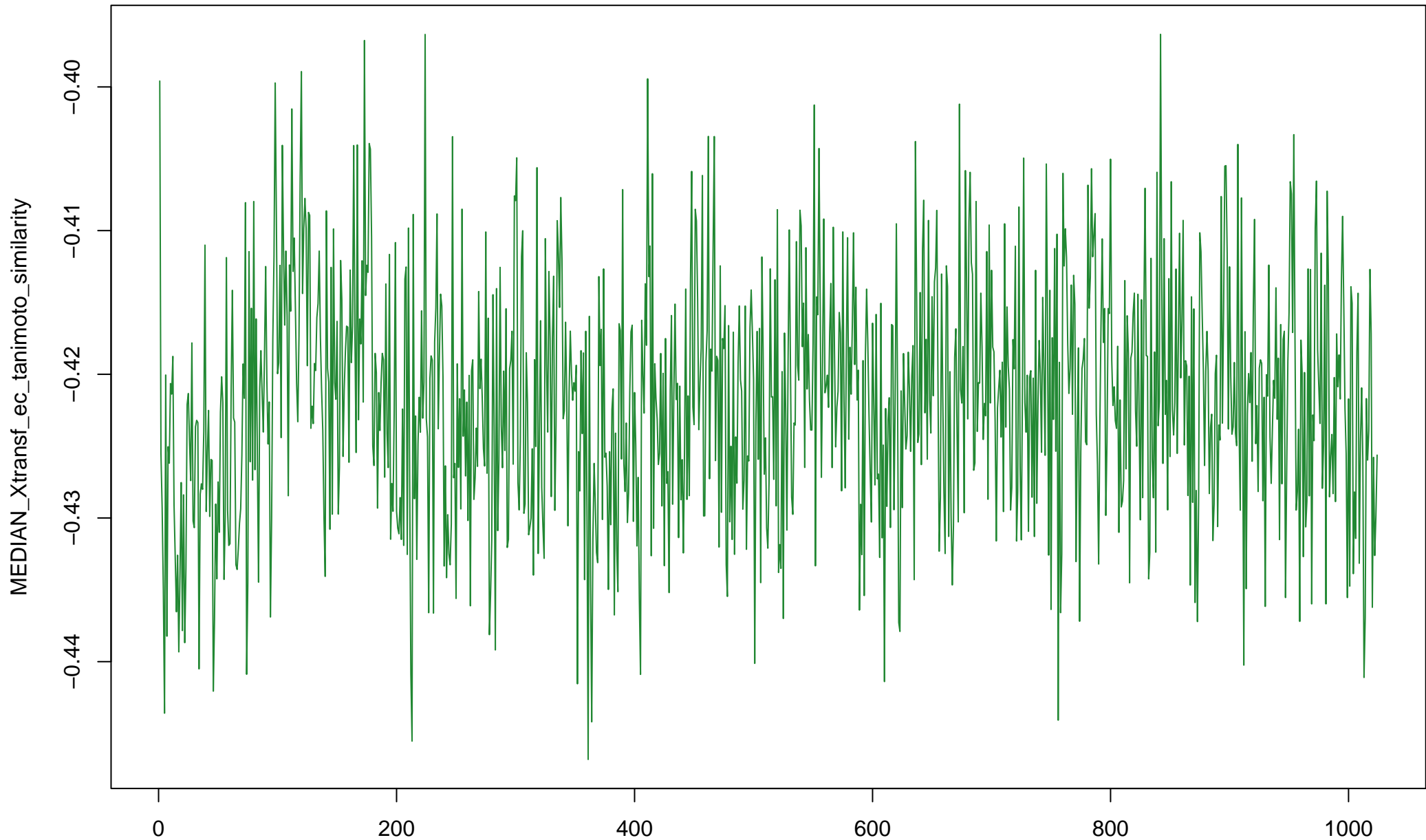
Pdatum8
ESS = 16.8 | BMK = 0.428 | MCSE(6.27) = 14.5 | stat: FALSE | burn: 510



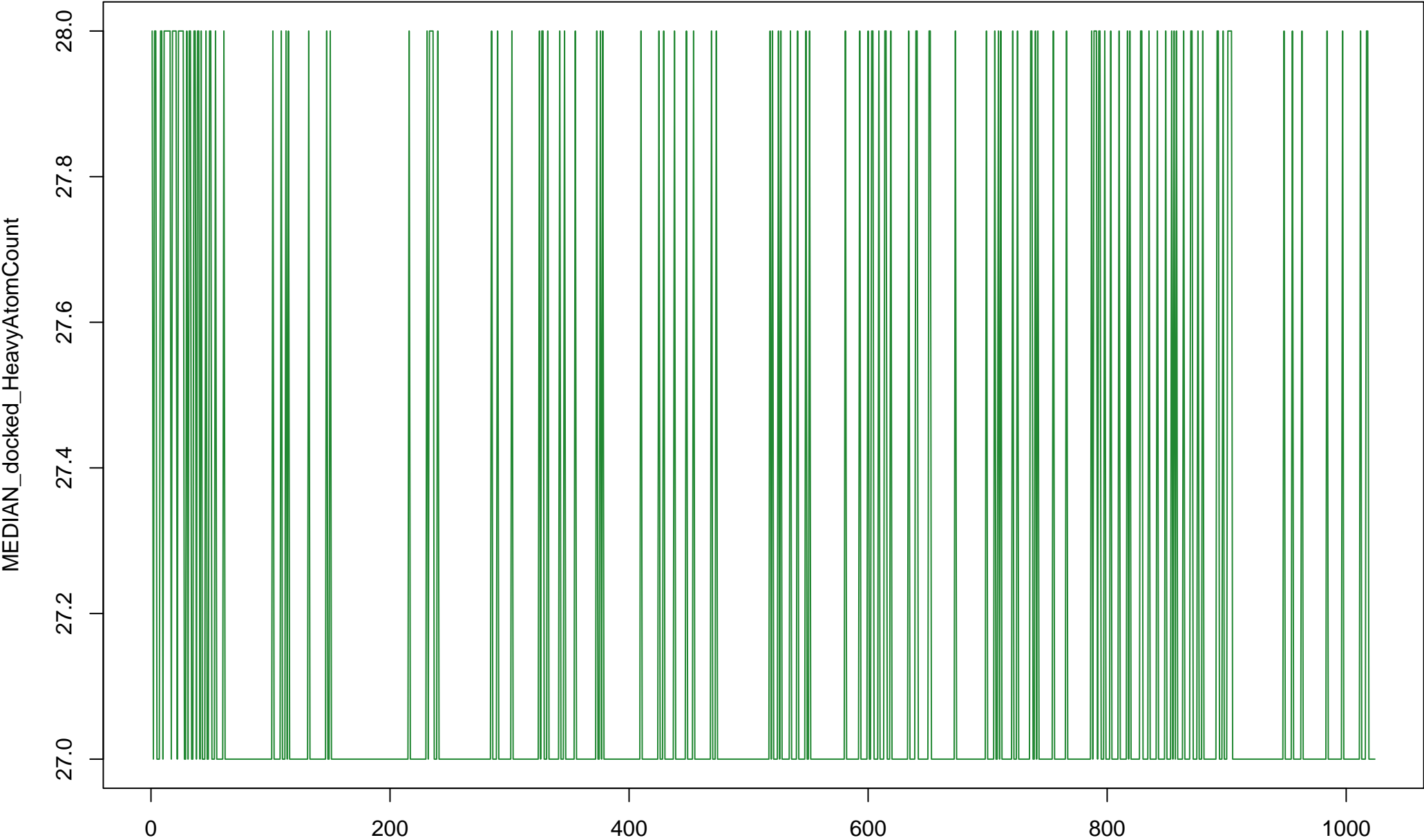
MEDIAN_log_RMSD
ESS = 115 | BMK = 0.0941 | MCSE(6.27) = 8.12 | stat: TRUE | burn: 0



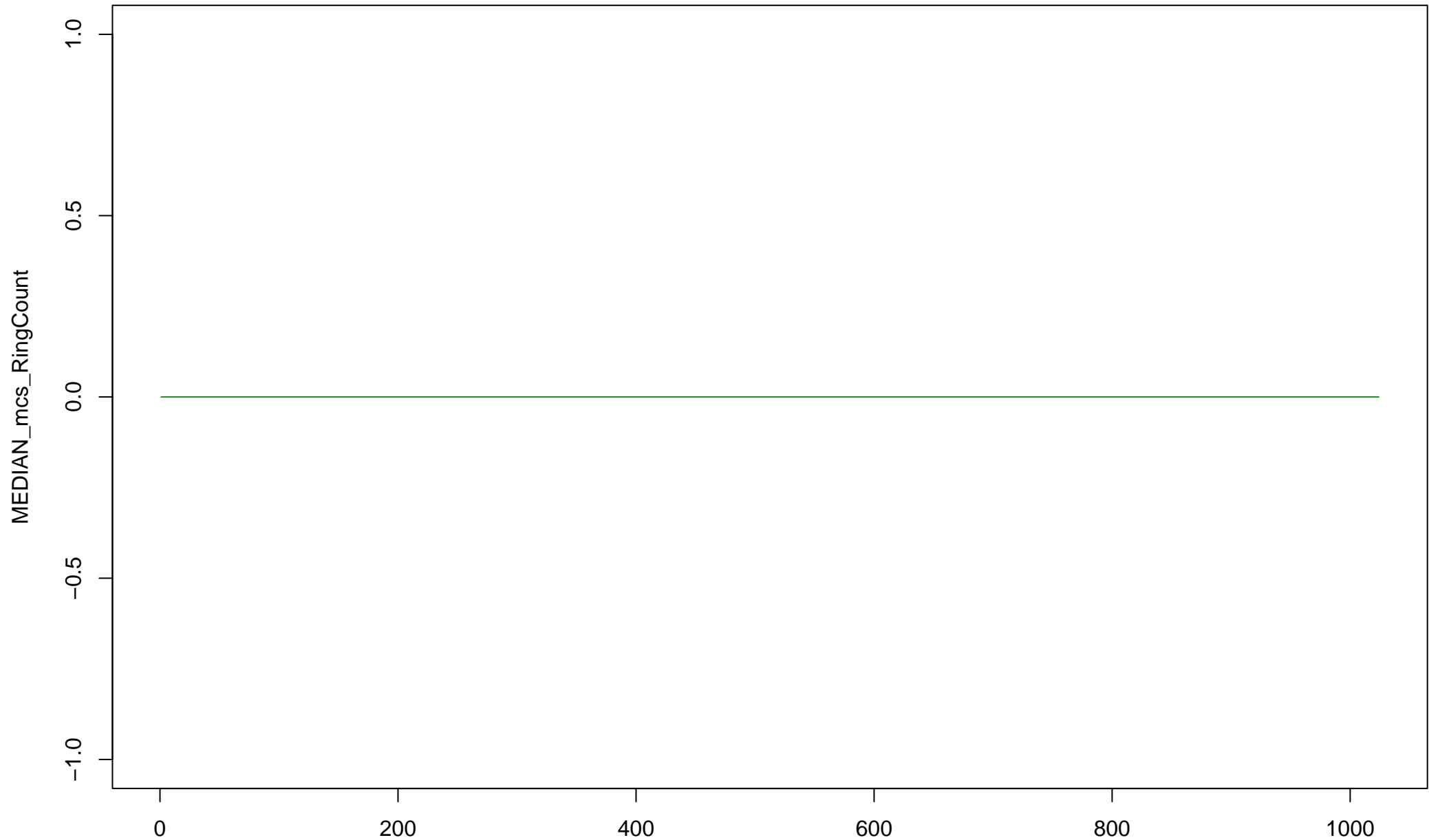
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 277 | BMK = 0.0859 | MCSE(6.27) = 6.33 | stat: FALSE | burn: 0



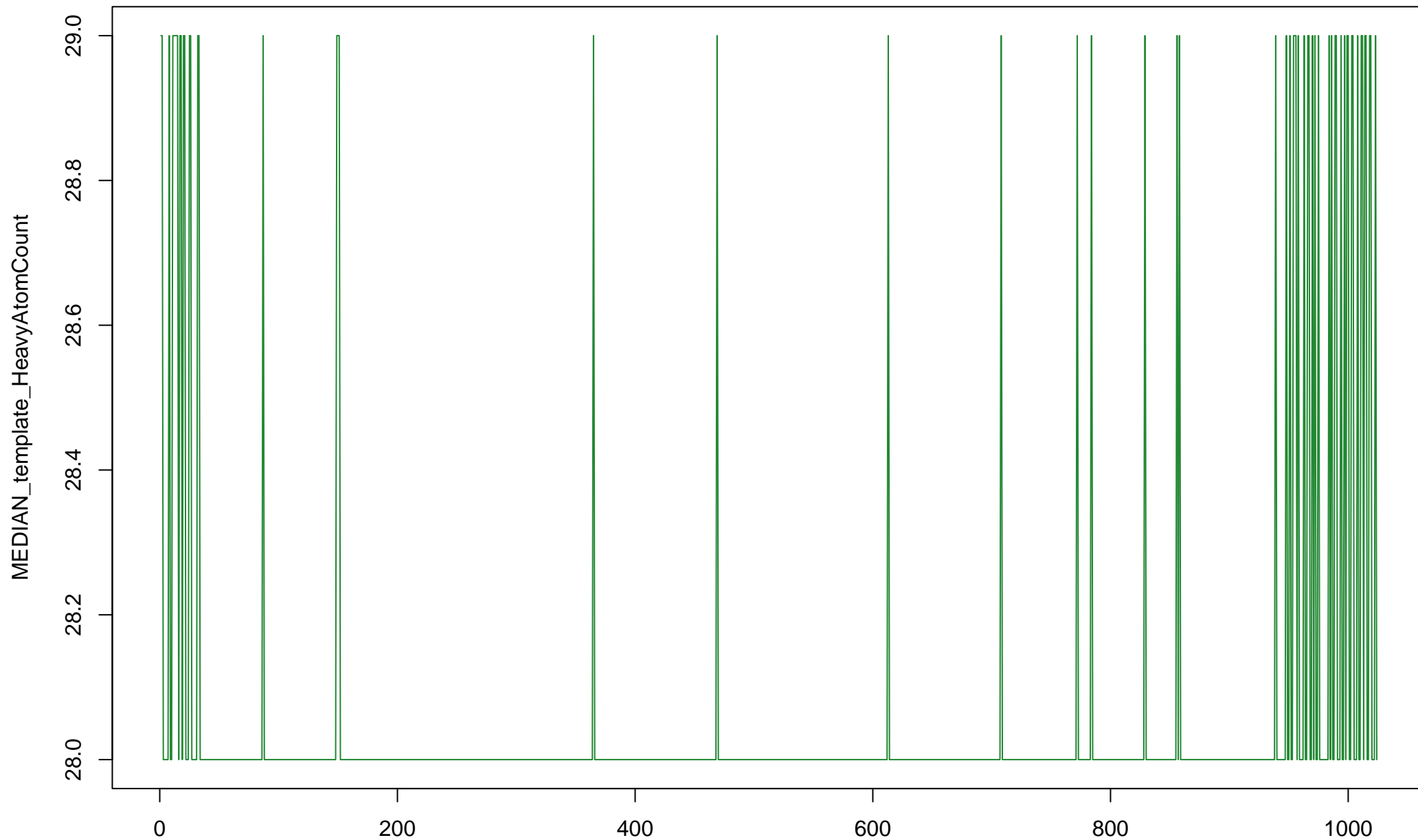
MEDIAN_docked_HeavyAtomCount
ESS = 141 | BMK = 0.0152 | MCSE(6.27) = 6.5 | stat: FALSE | burn: 0



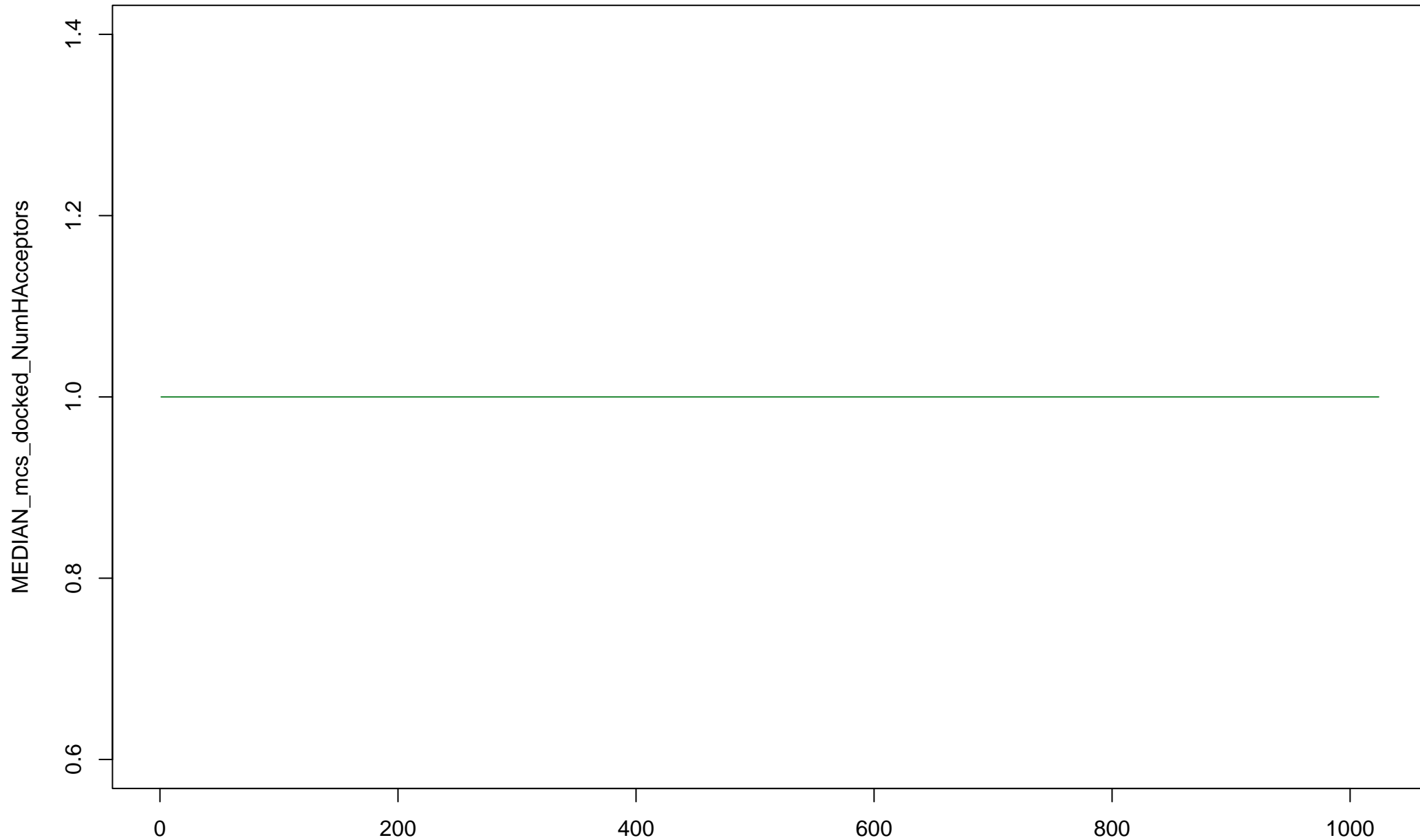
MEDIAN_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



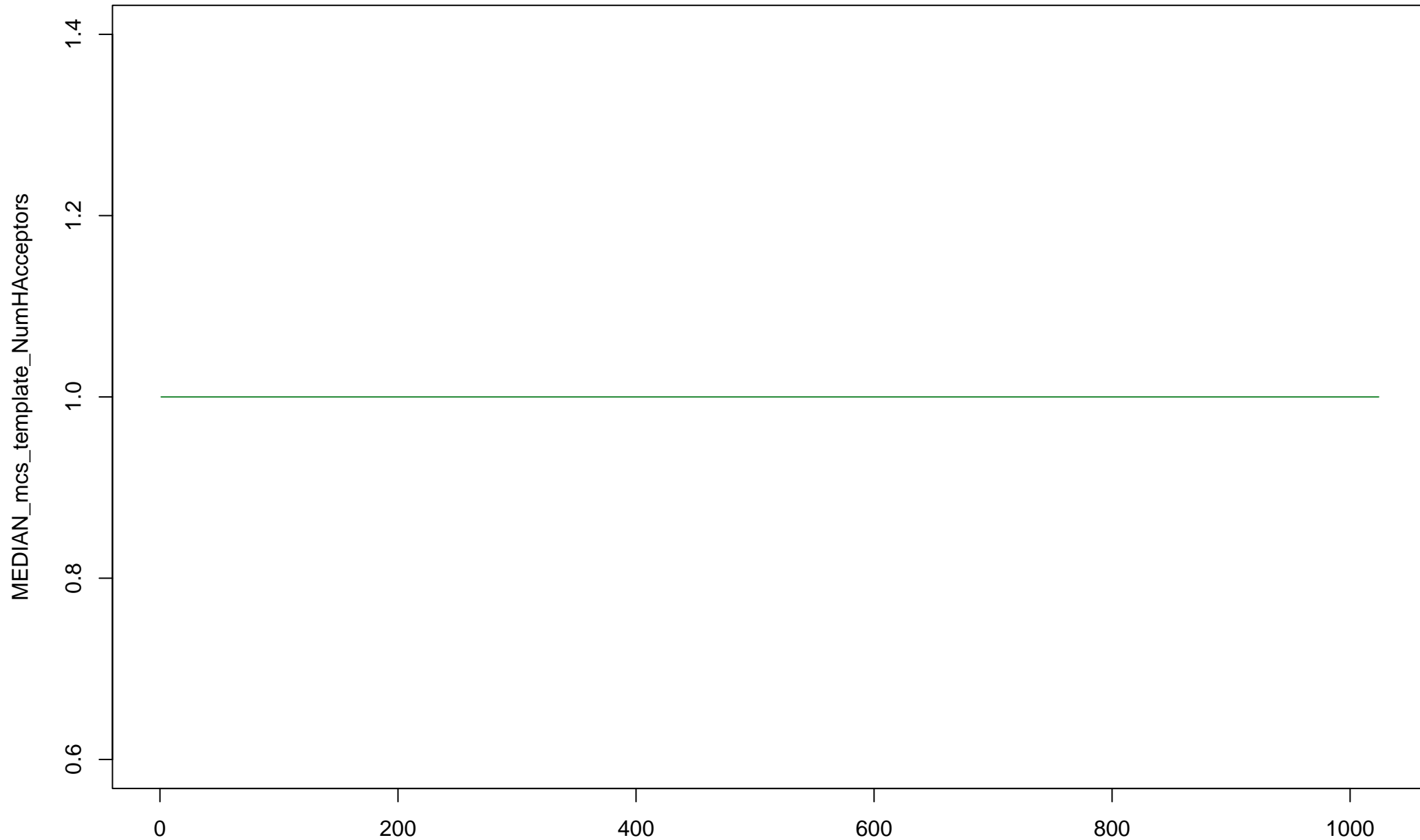
MEDIAN_template_HeavyAtomCount
ESS = 73.7 | BMK = 0.0962 | MCSE(6.27) = 9.27 | stat: TRUE | burn: 0



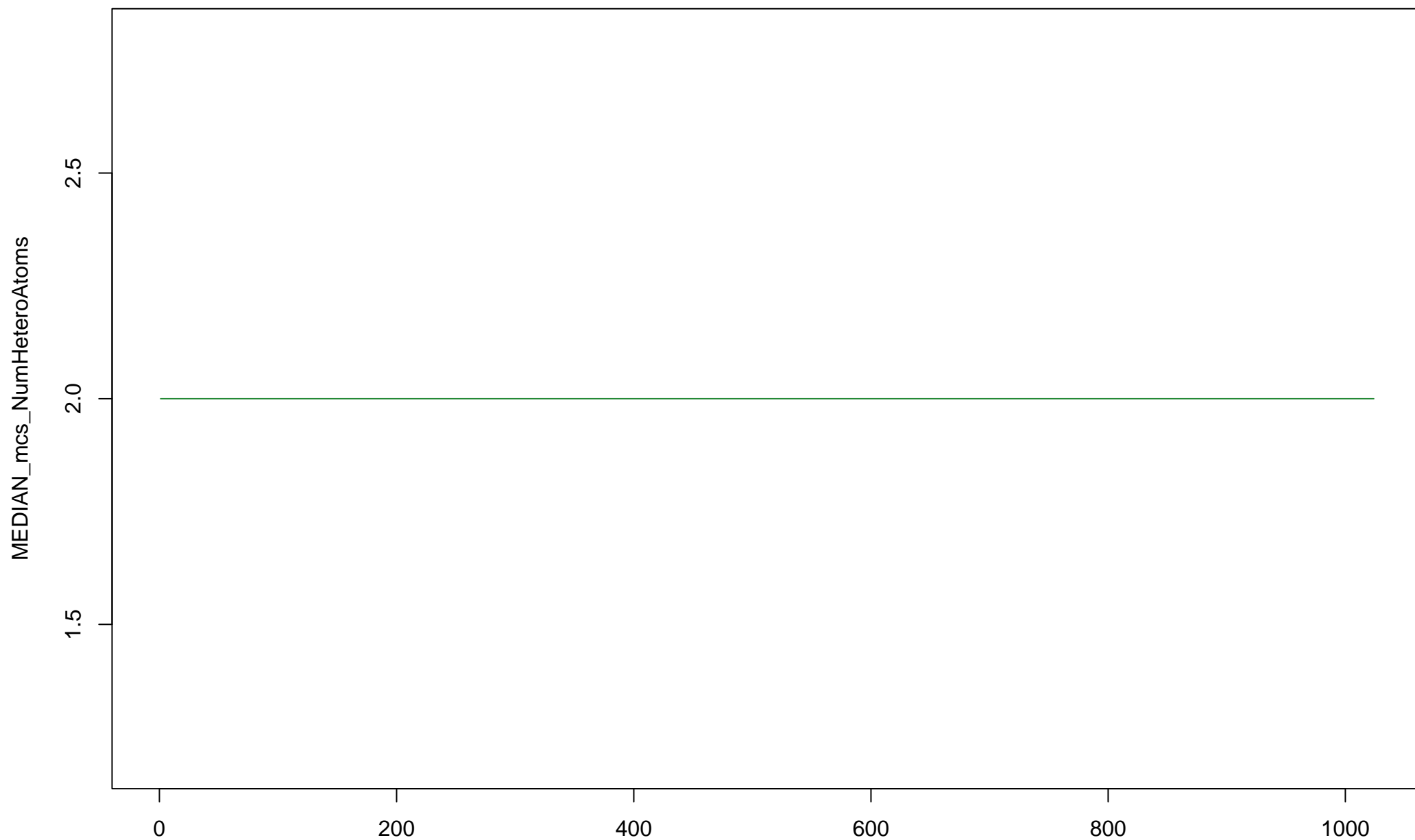
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



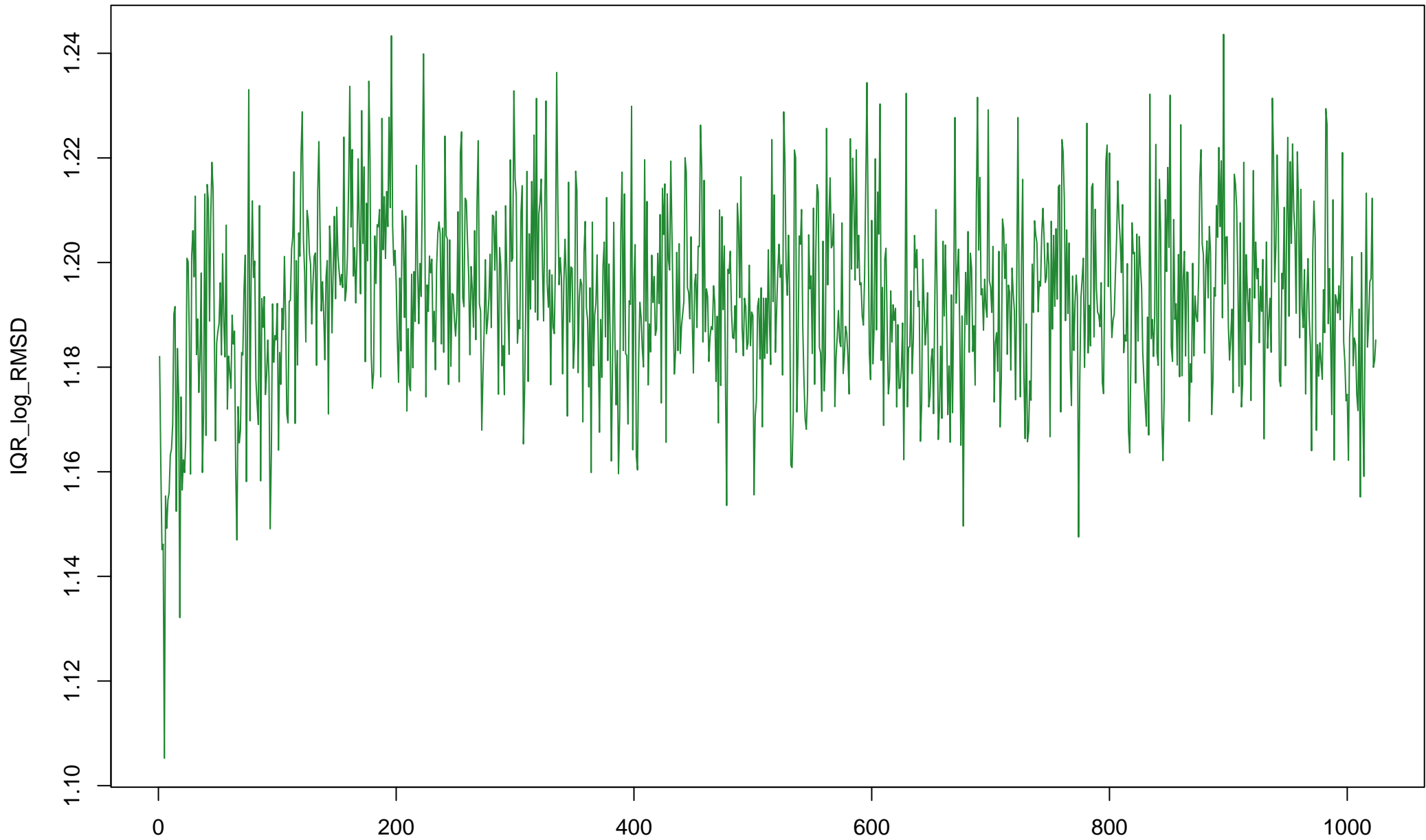
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



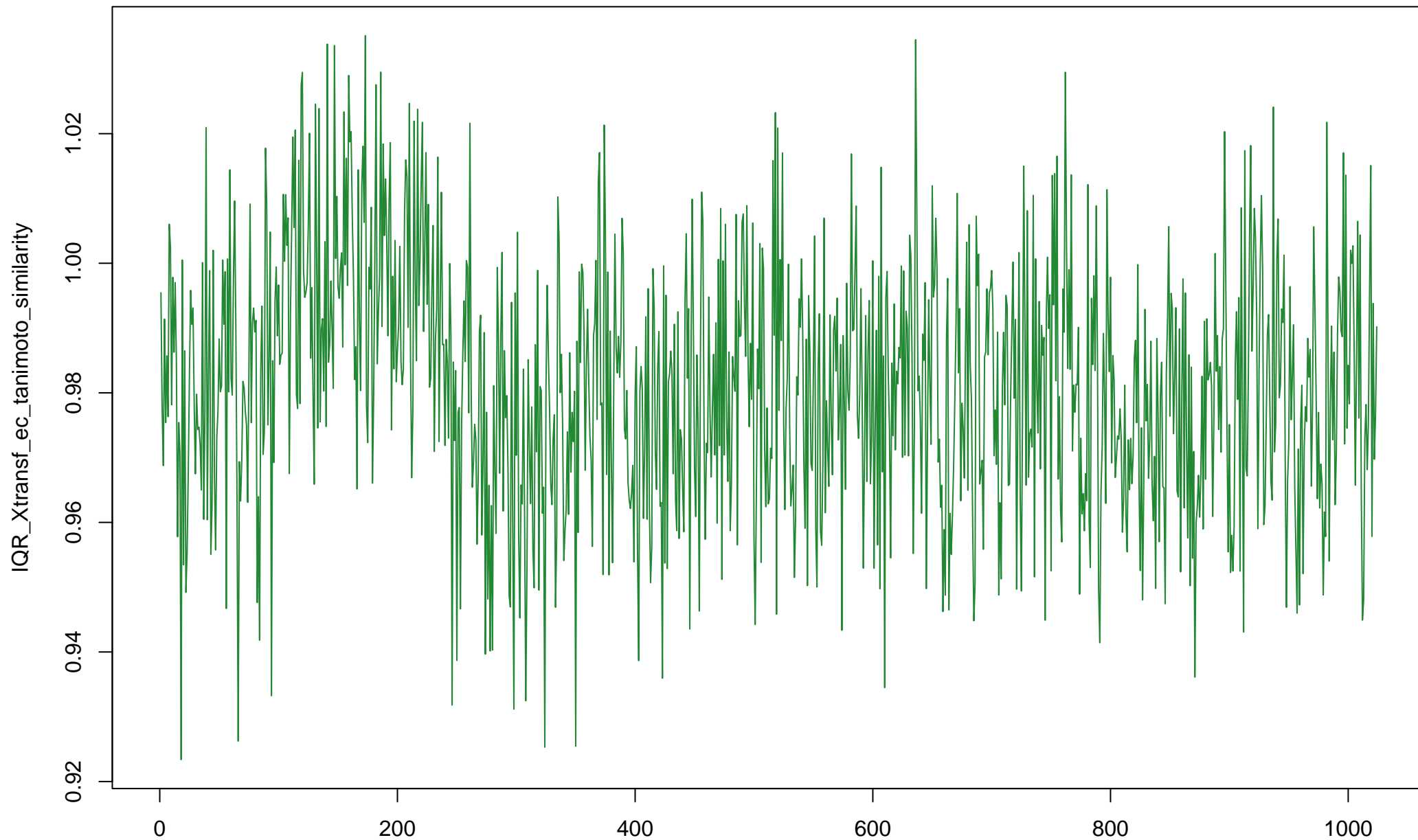
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



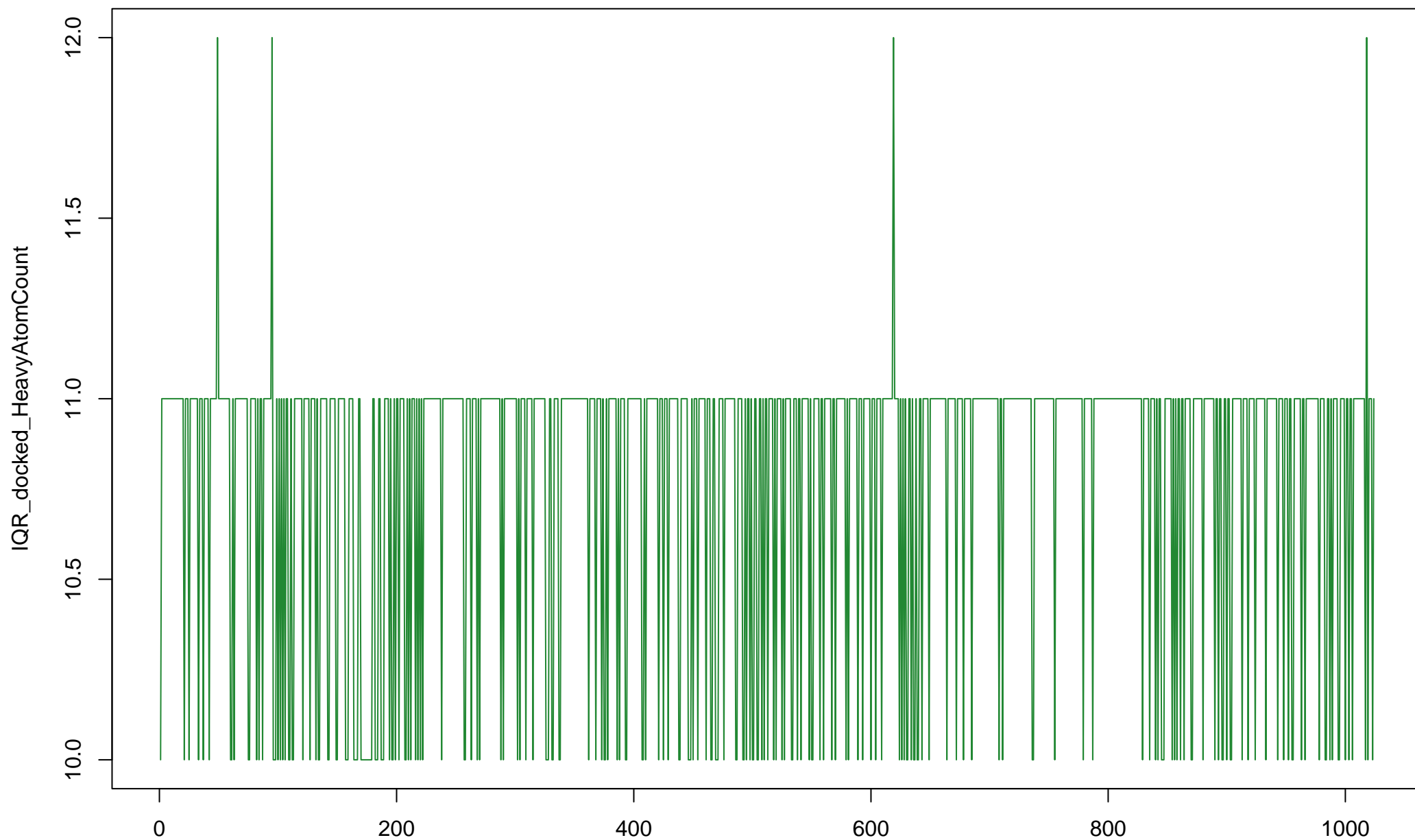
IQR_log_RMSD
ESS = 166 | BMK = 0.0828 | MCSE(6.27) = 7.05 | stat: FALSE | burn: 0



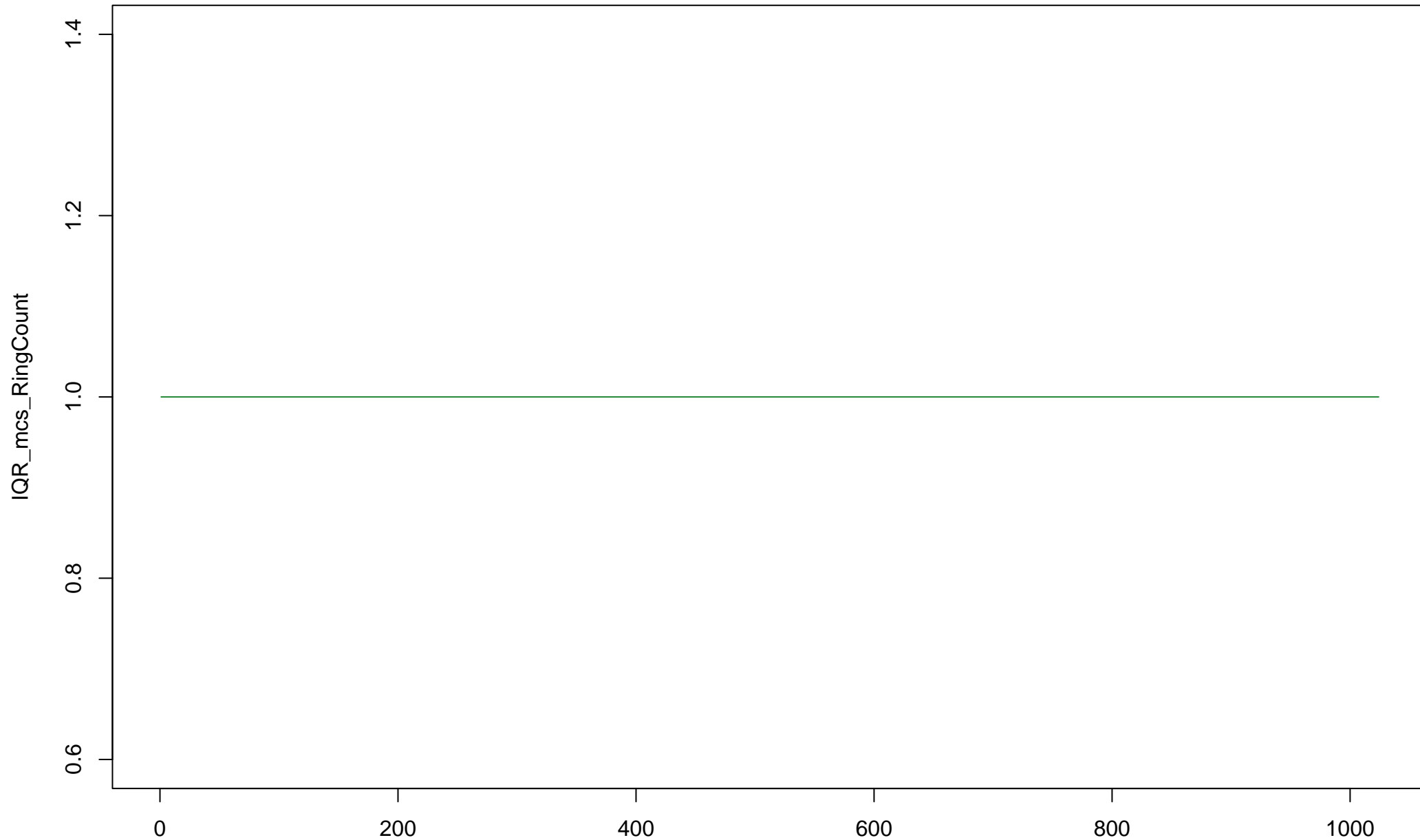
IQR_Xtransf_ec_tanimoto_similarity
ESS = 110 | BMK = 0.108 | MCSE(6.27) = 7.34 | stat: TRUE | burn: 0



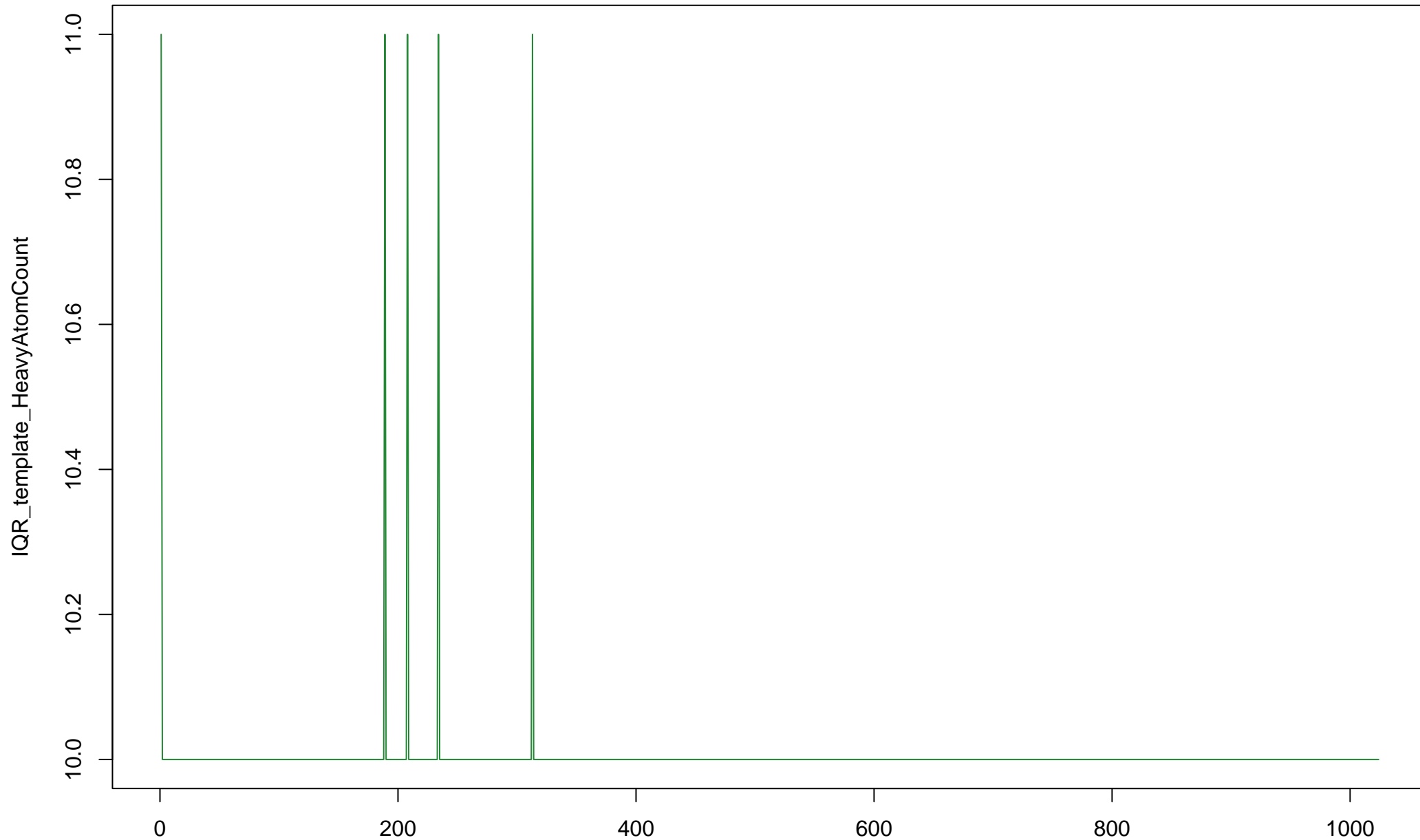
IQR_docked_HeavyAtomCount
ESS = 331 | BMK = 0.0781 | MCSE(6.27) = 5.3 | stat: TRUE | burn: 0



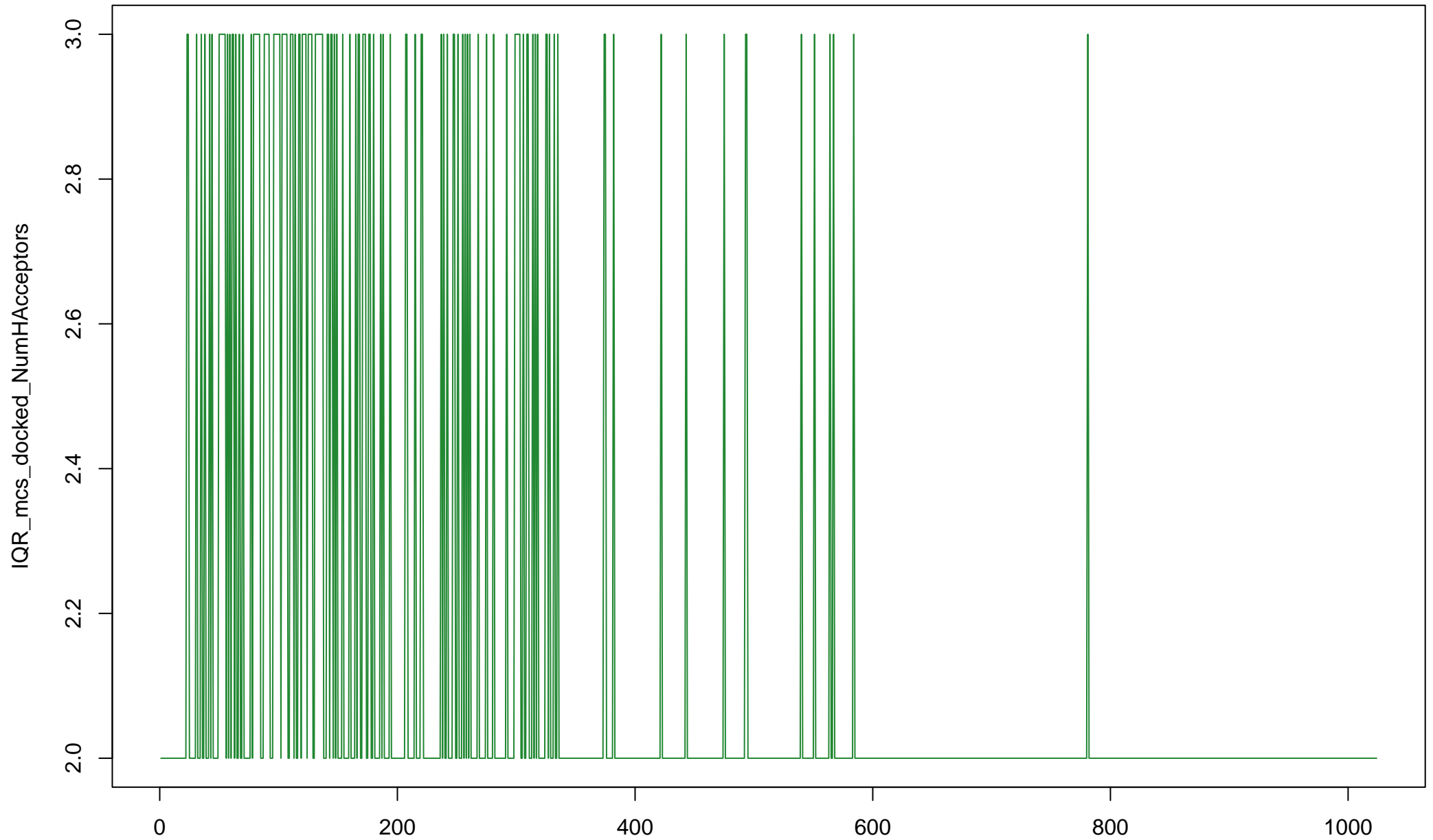
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



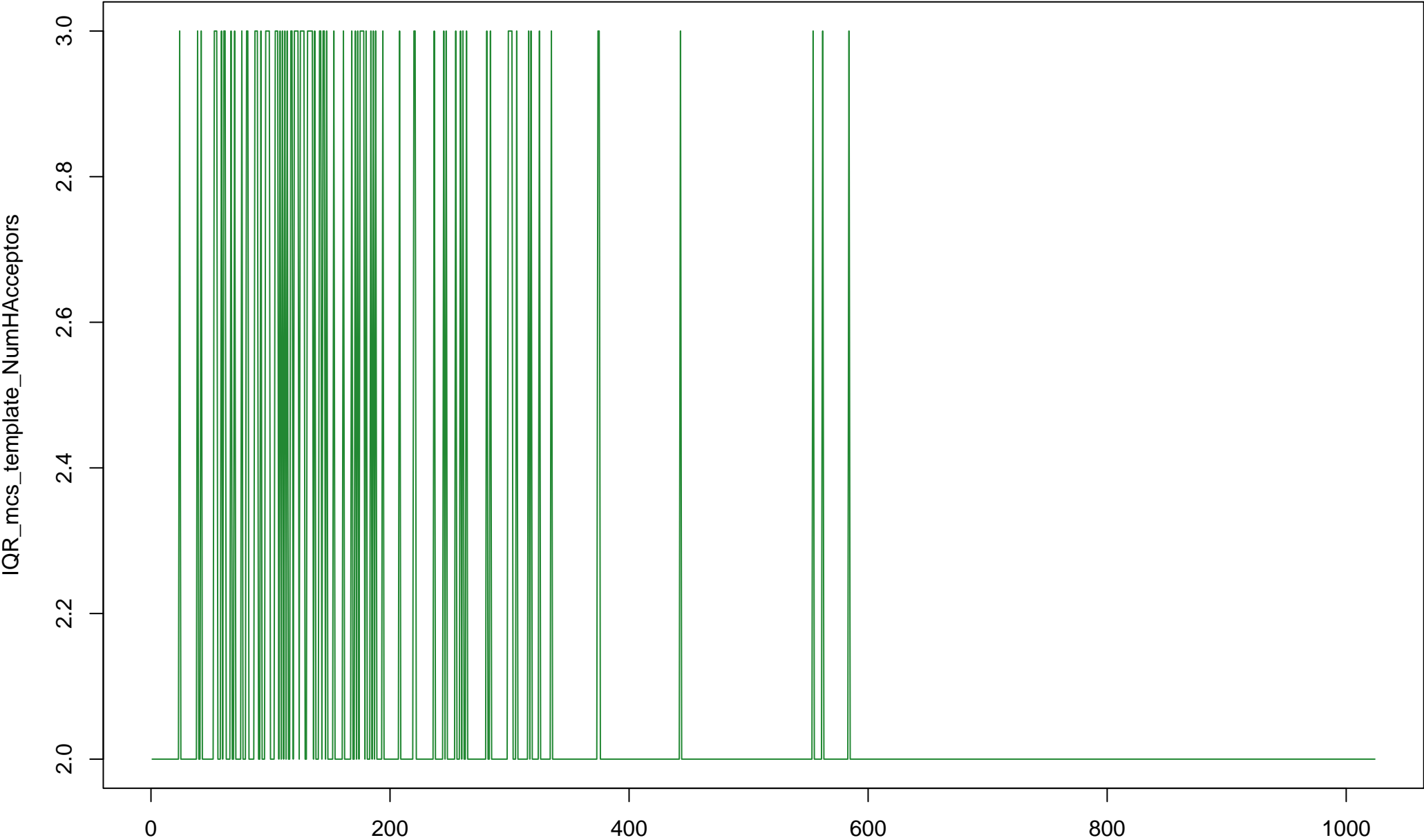
IQR_template_HeavyAtomCount
ESS = 530 | BMK = 0.505 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 408



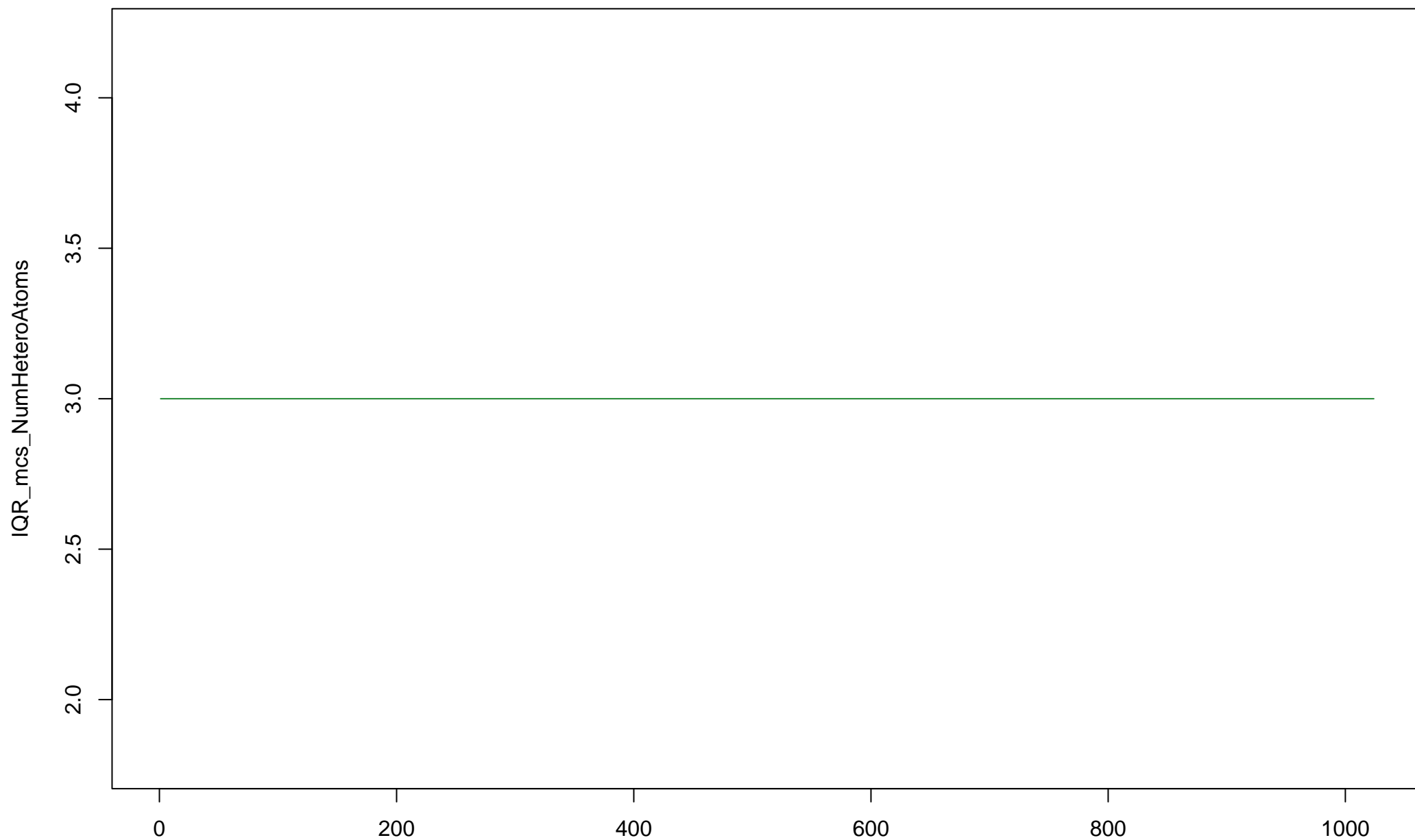
IQR_mcs_docked_NumHAcceptors
ESS = 15 | BMK = 0.434 | MCSE(6.27) = 10 | stat: FALSE | burn: 816



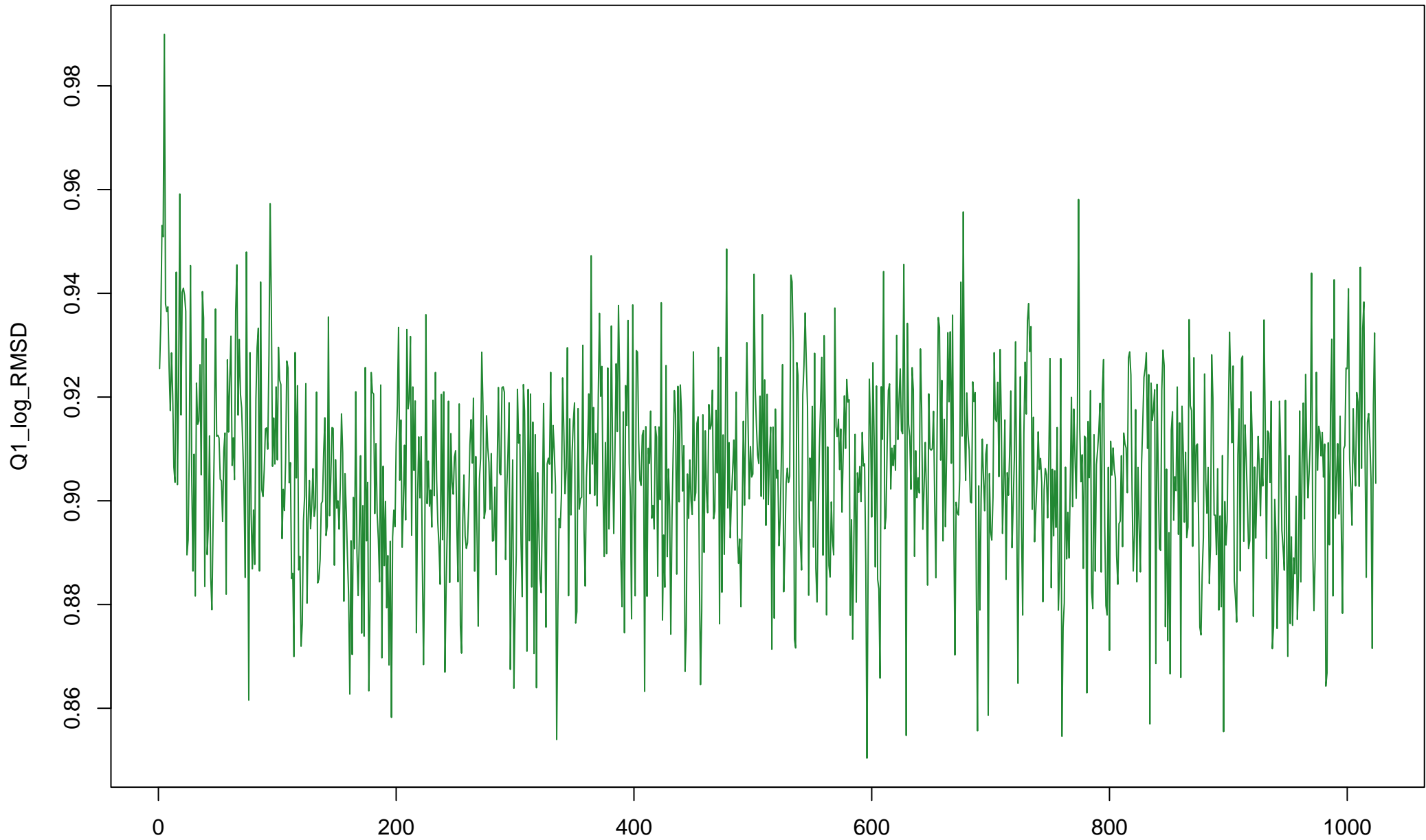
IQR_mcs_template_NumHAcceptors
ESS = 29.6 | BMK = 0.459 | MCSE(6.27) = 9.31 | stat: FALSE | burn: 0



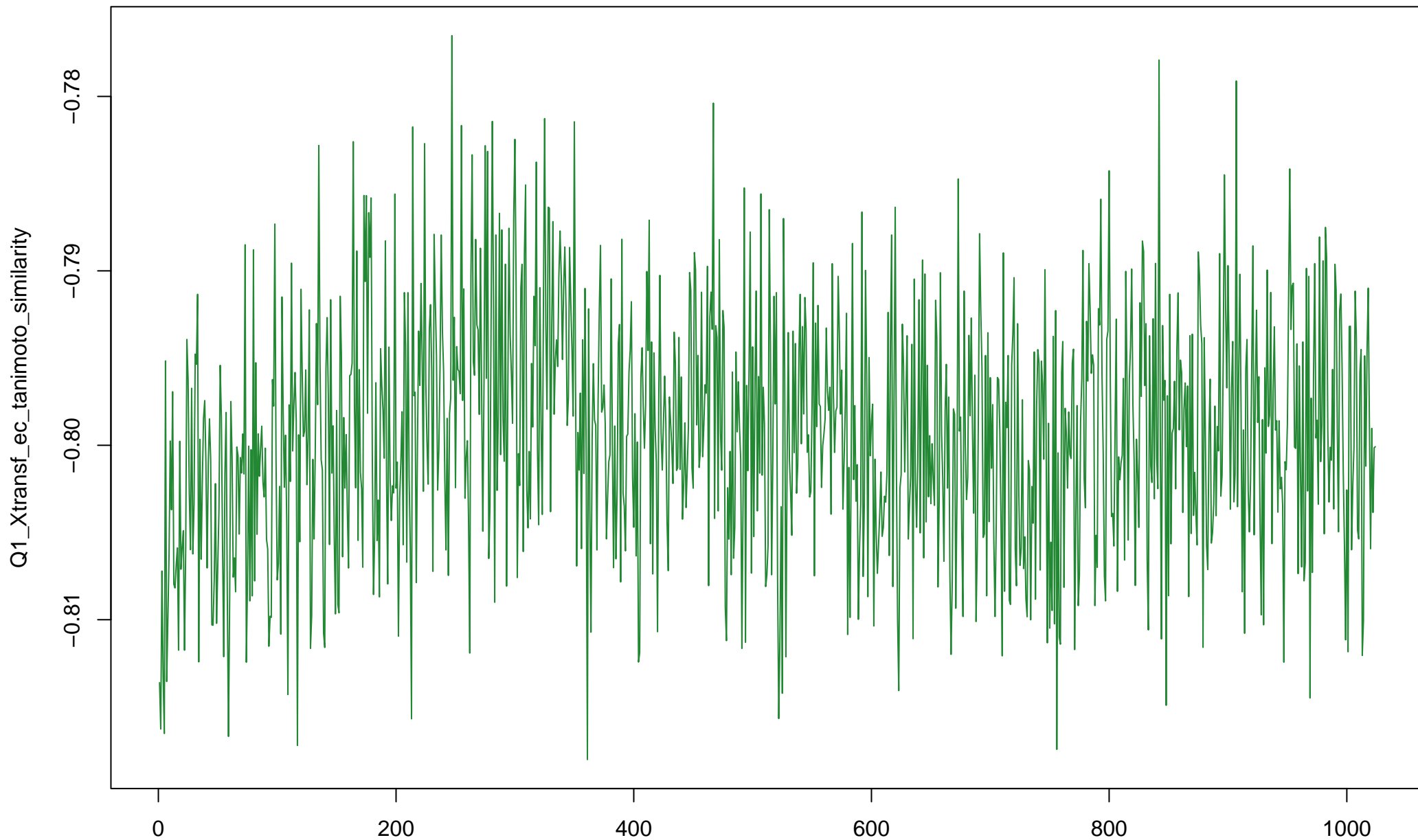
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



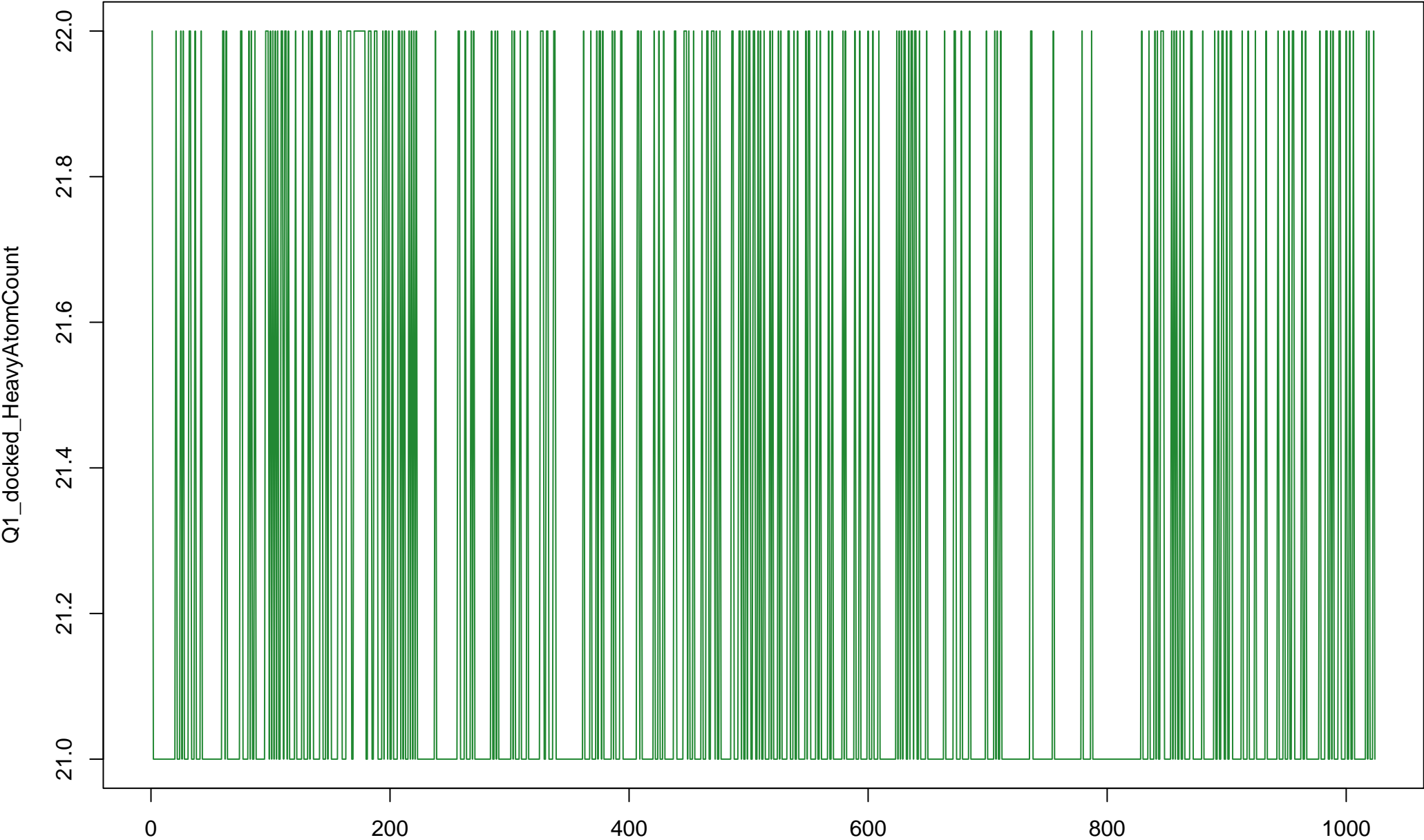
Q1_log_RMSD
ESS = 486 | BMK = 0.0537 | MCSE(6.27) = 5.75 | stat: FALSE | burn: 0



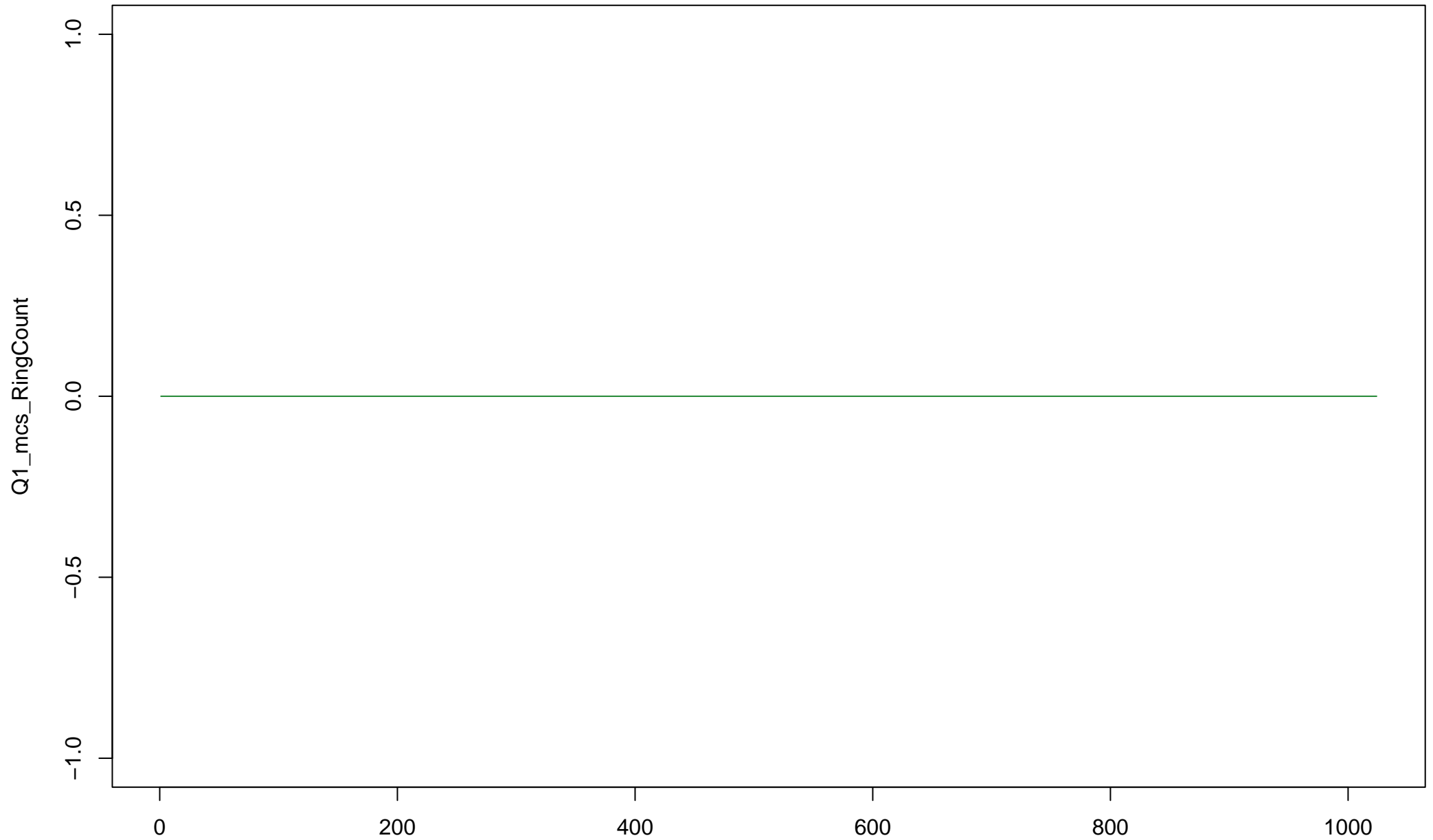
Q1_Xtransf_ec_tanimoto_similarity
ESS = 154 | BMK = 0.0801 | MCSE(6.27) = 6.18 | stat: FALSE | burn: 0



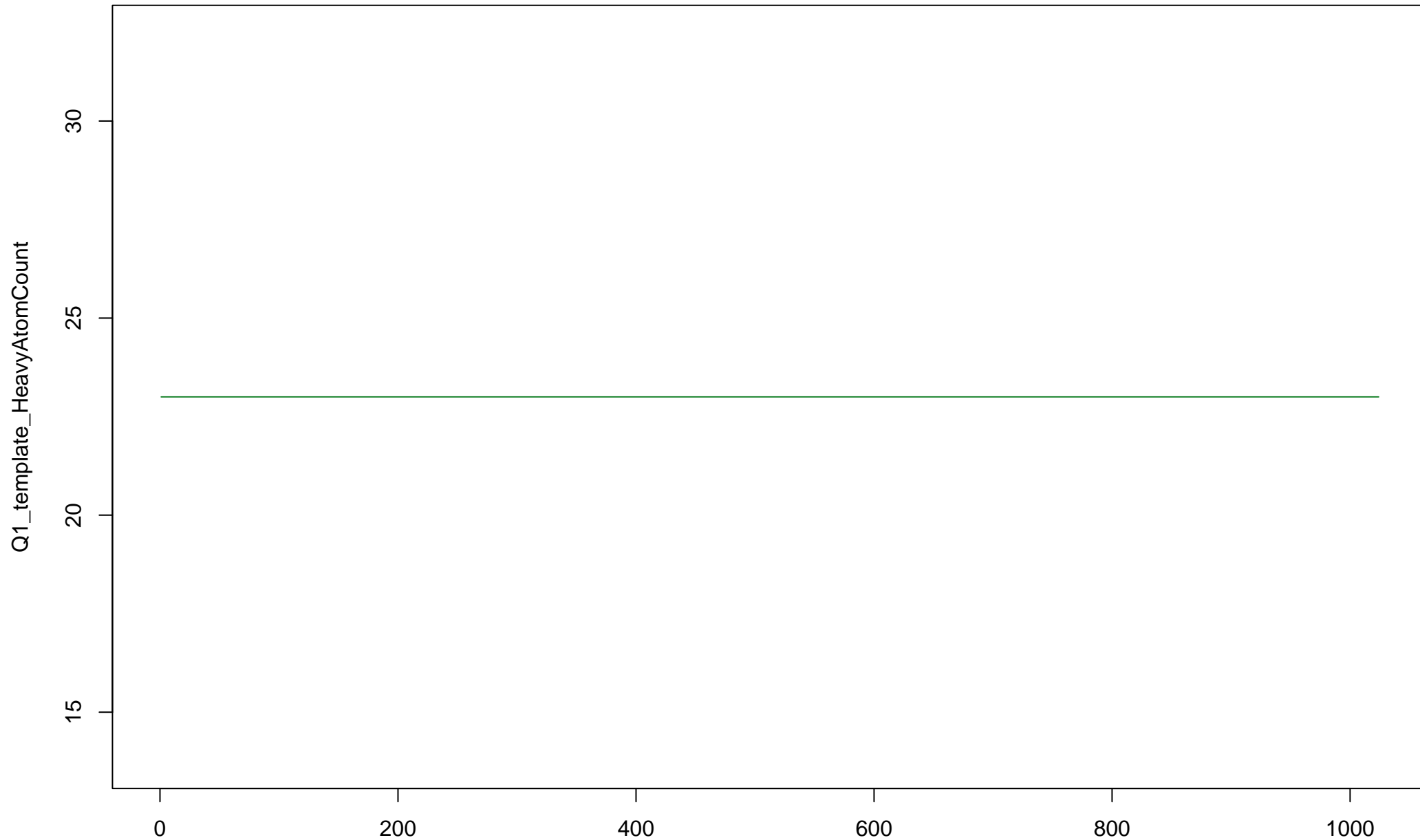
Q1_docked_HeavyAtomCount
ESS = 449 | BMK = 0.0674 | MCSE(6.27) = 5.24 | stat: TRUE | burn: 0



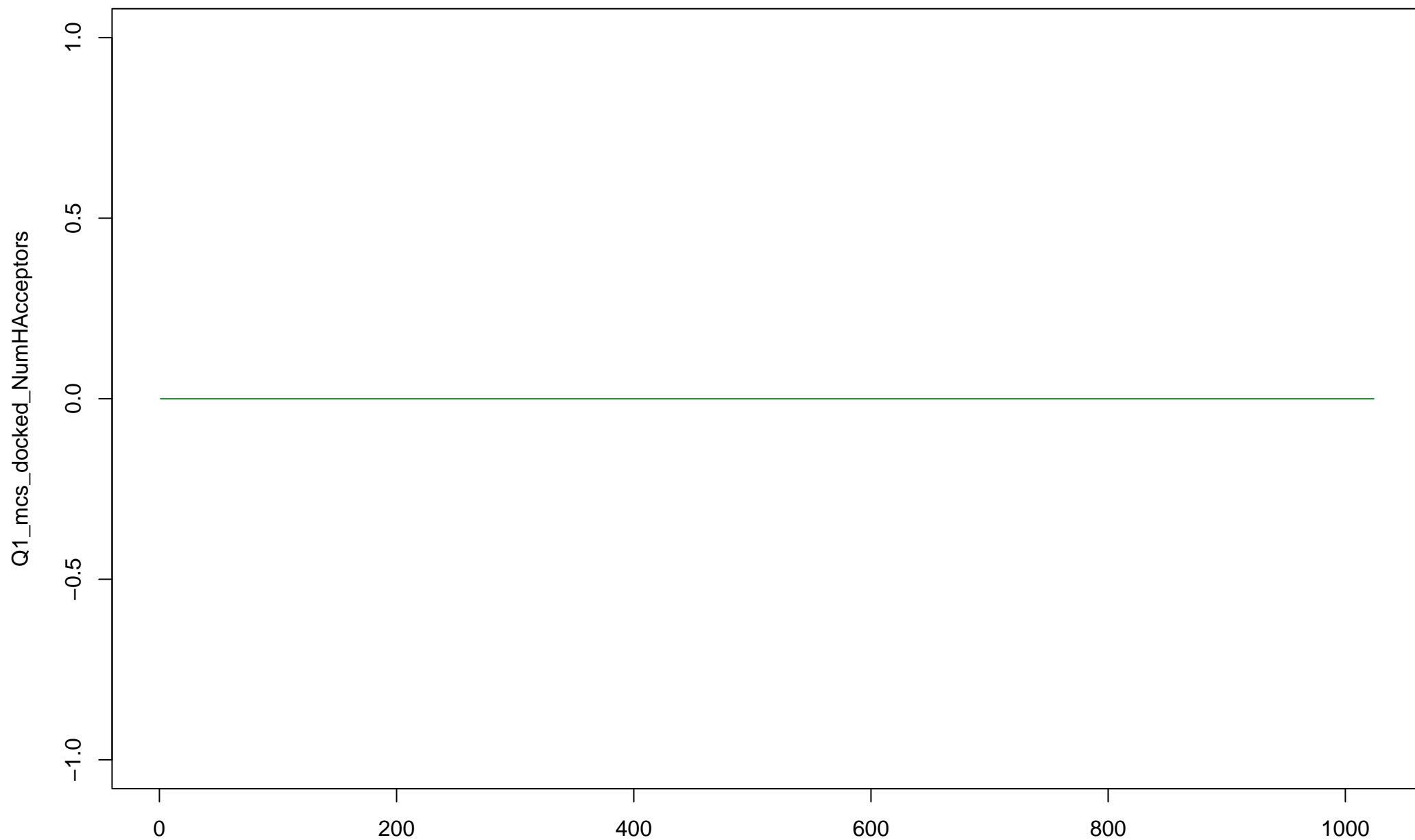
Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



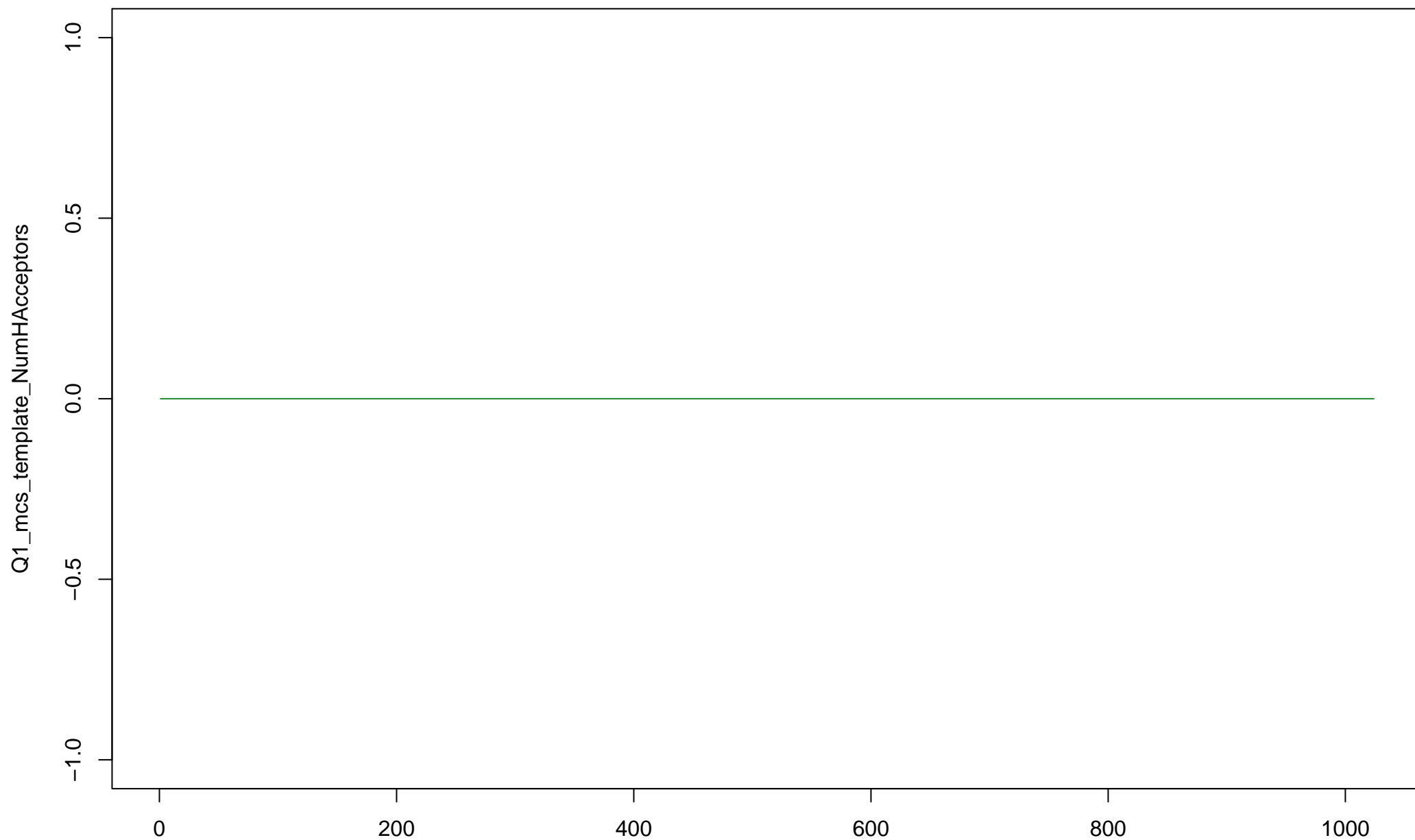
Q1_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



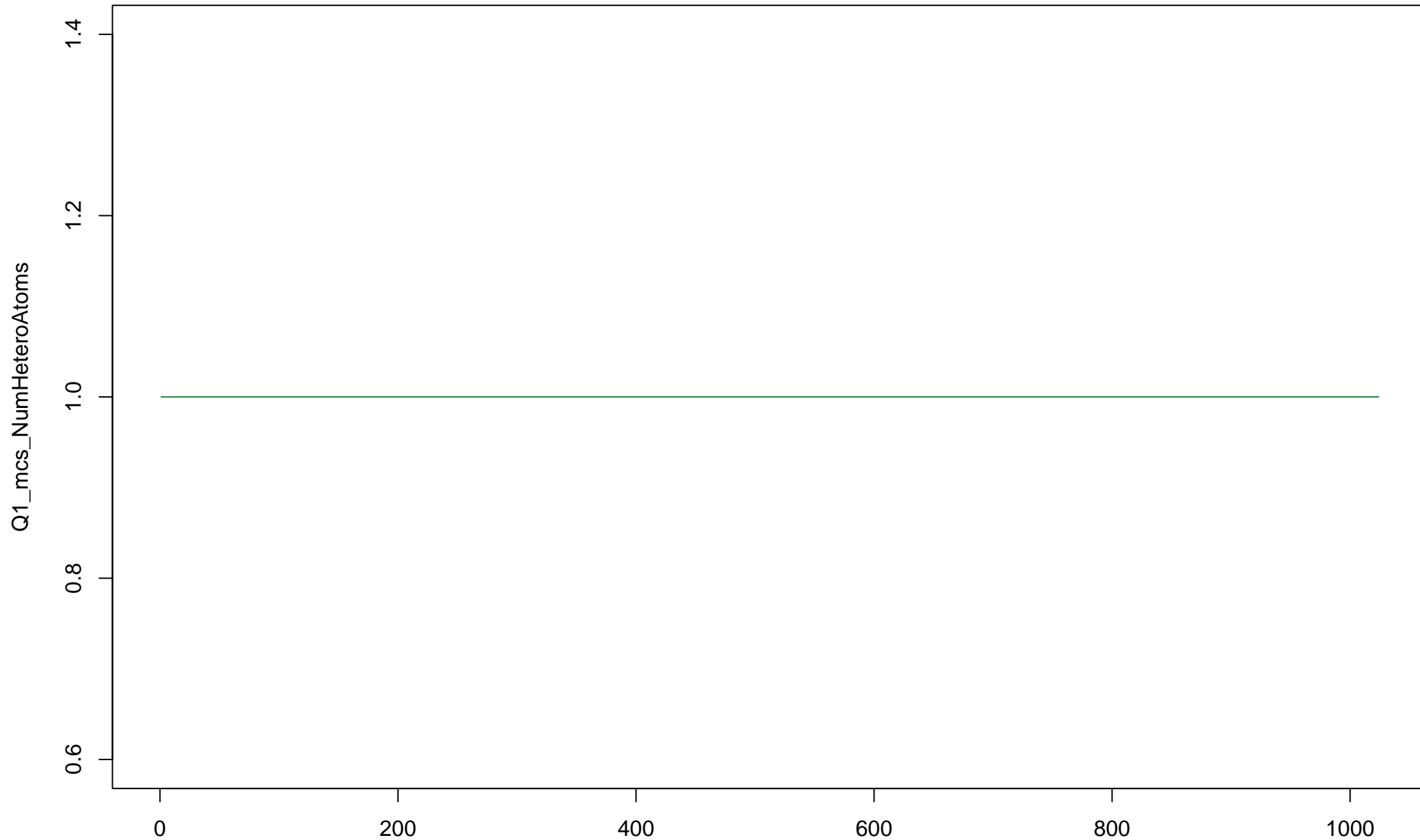
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



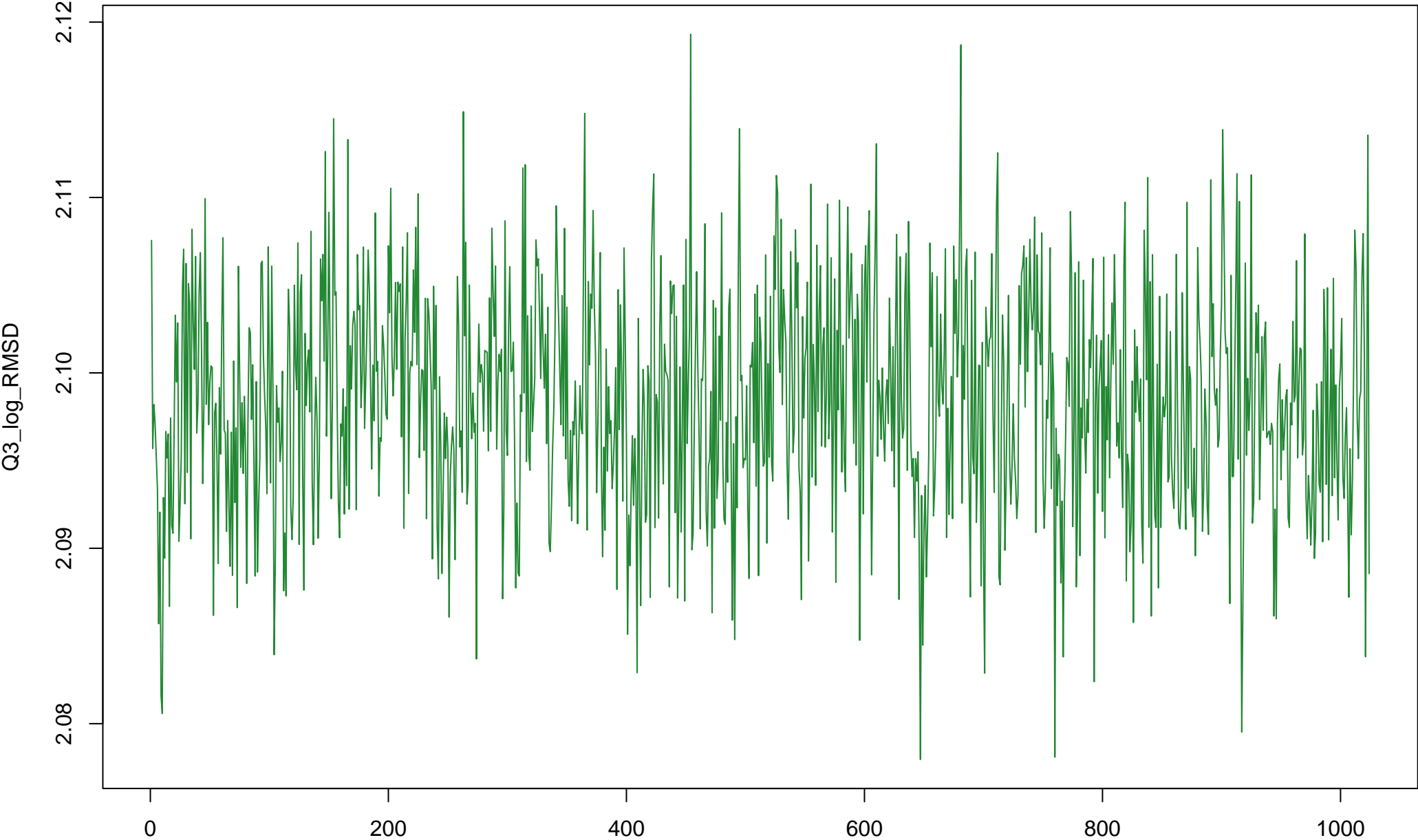
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



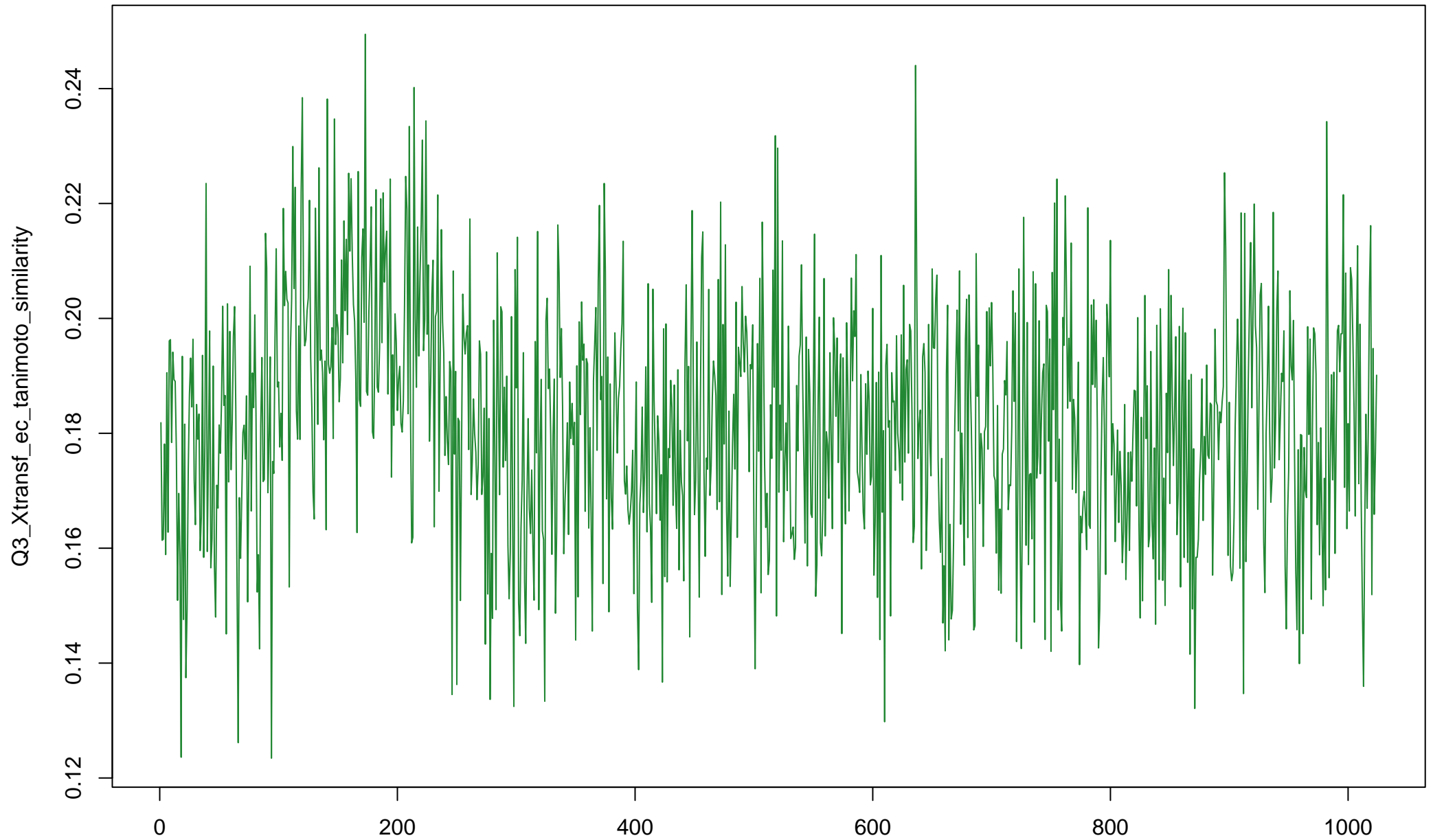
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



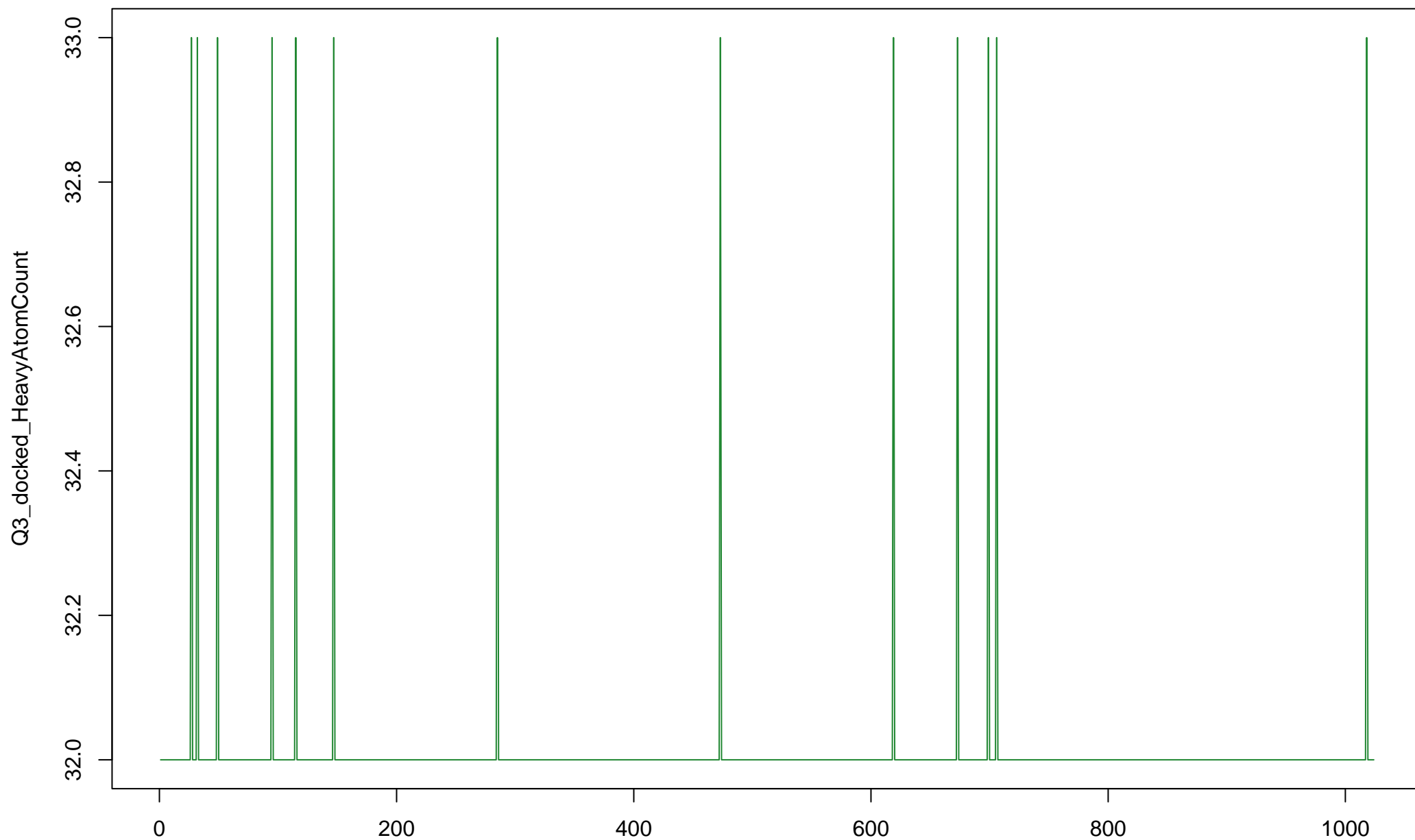
Q3_log_RMSD
ESS = 614 | BMK = 0.0461 | MCSE(6.27) = 4.51 | stat: TRUE | burn: 0



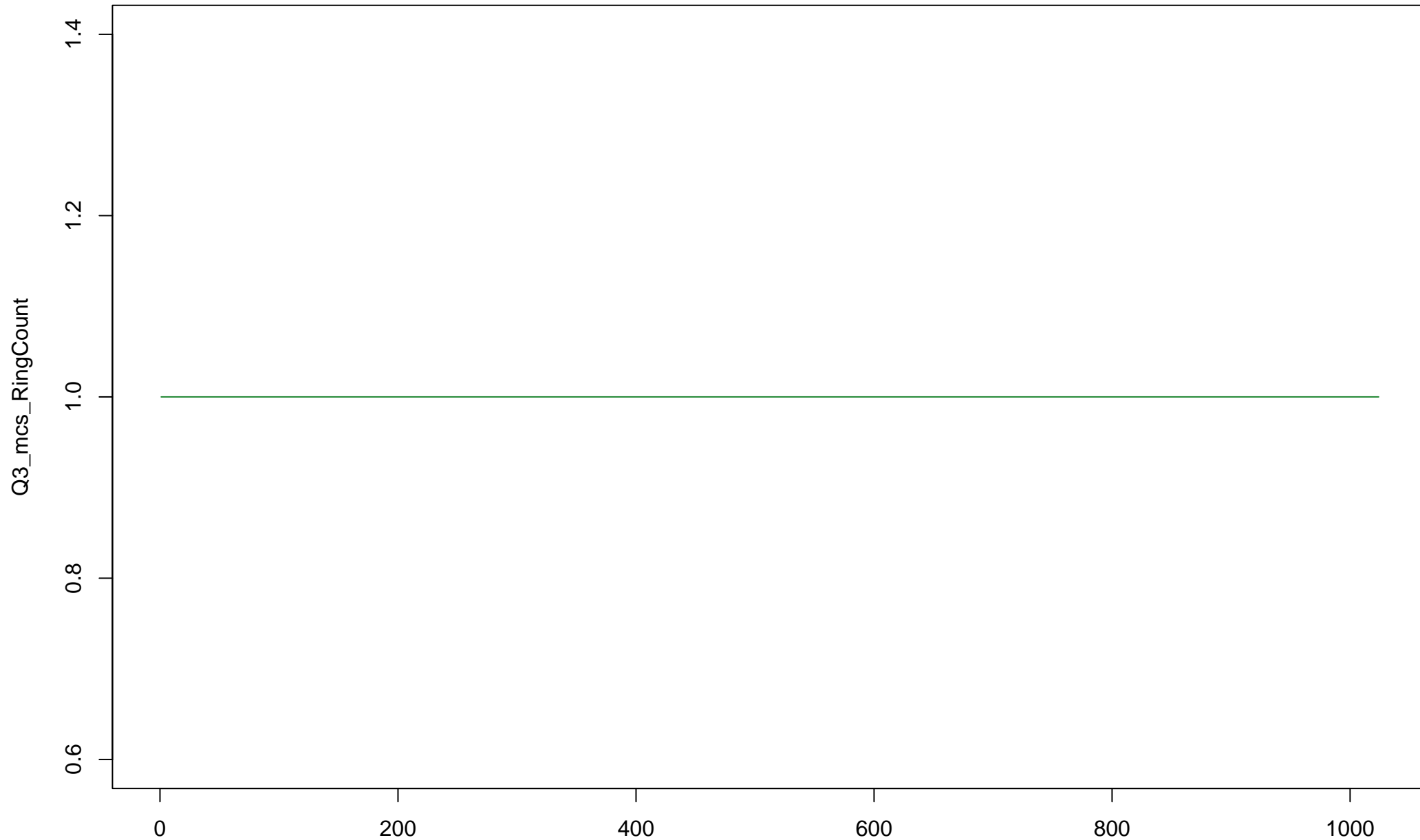
Q3_Xtransf_ec_tanimoto_similarity
ESS = 135 | BMK = 0.0919 | MCSE(6.27) = 6.75 | stat: TRUE | burn: 0



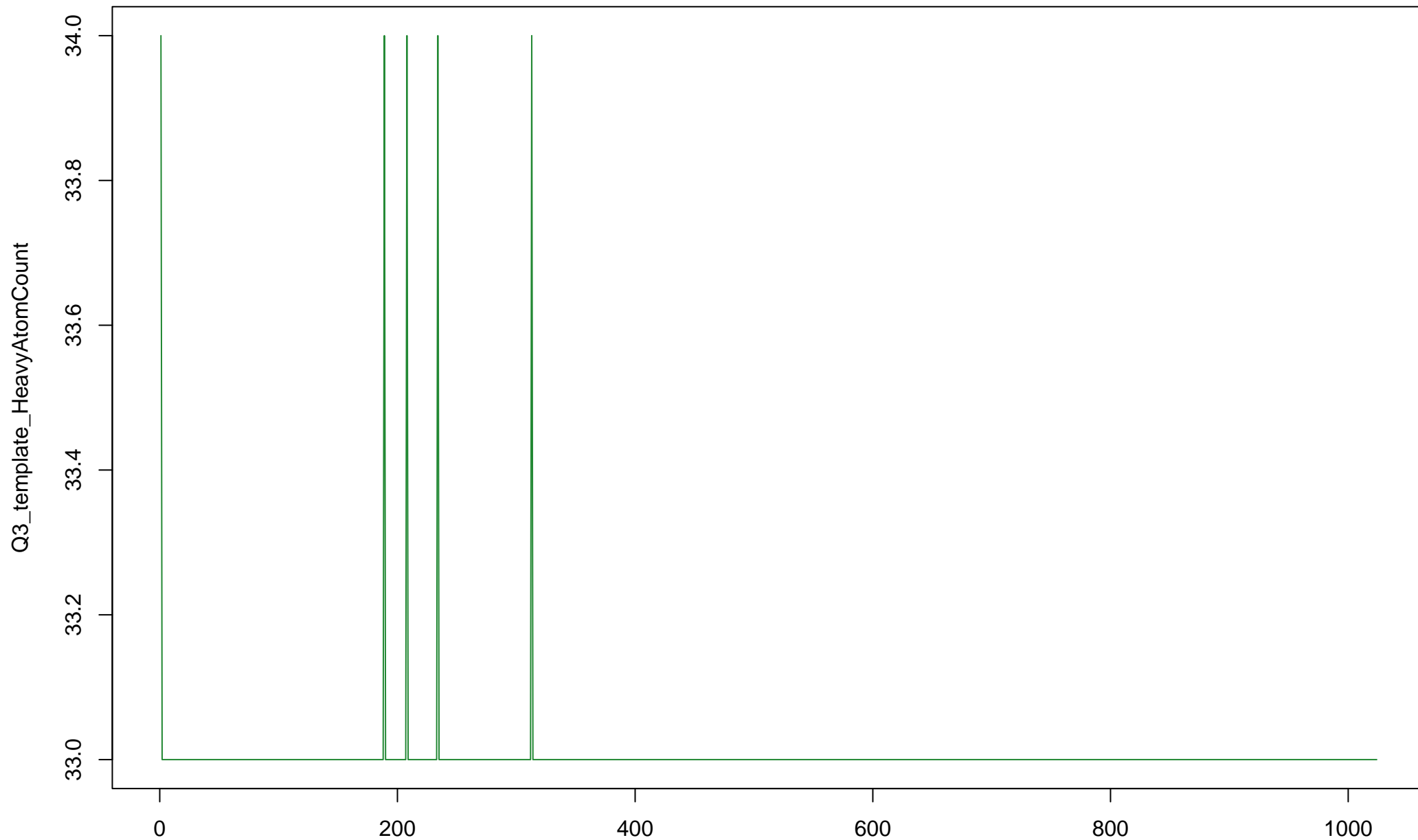
Q3_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0829 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0



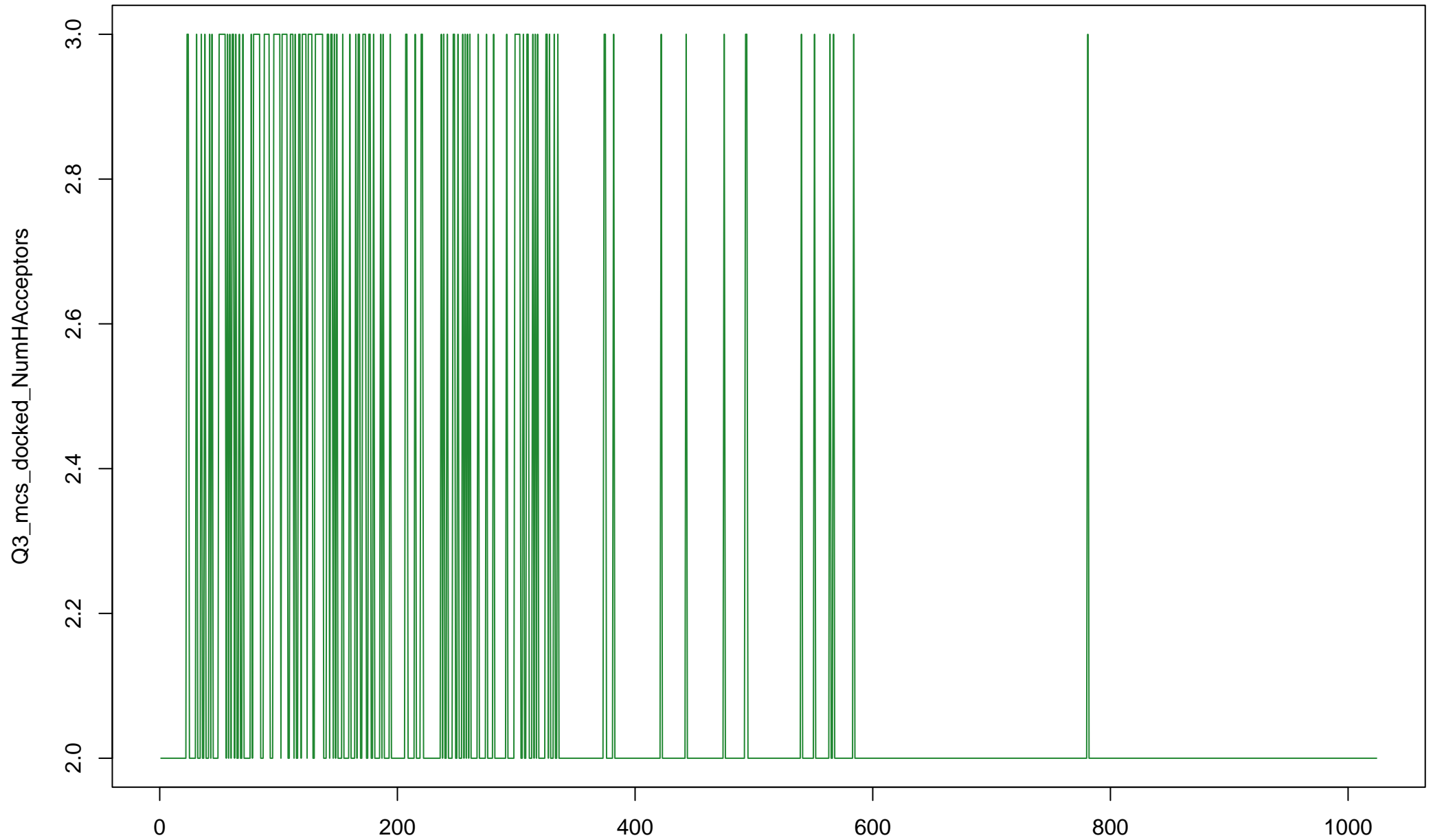
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



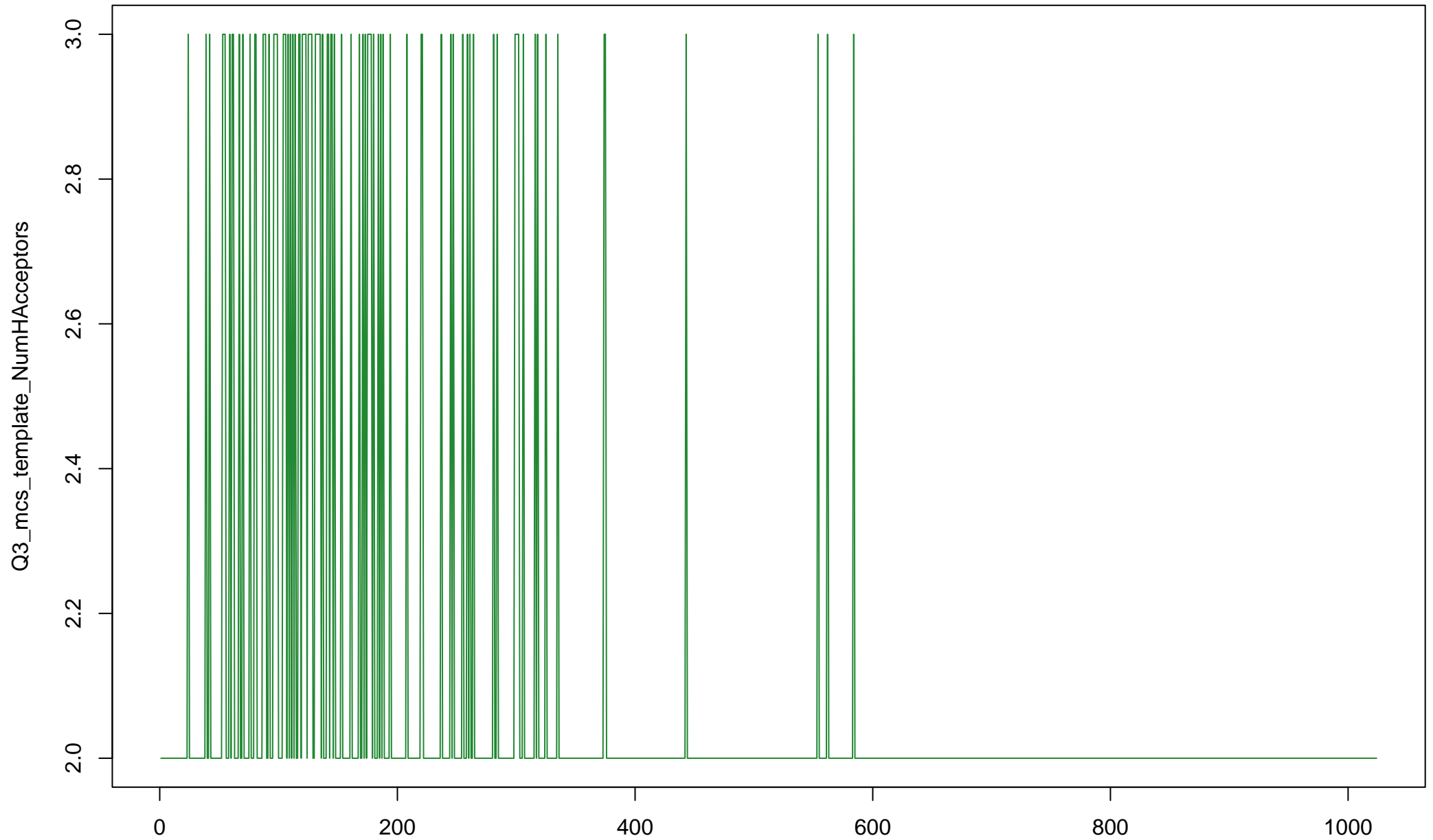
Q3_template_HeavyAtomCount
ESS = 530 | BMK = 0.488 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0



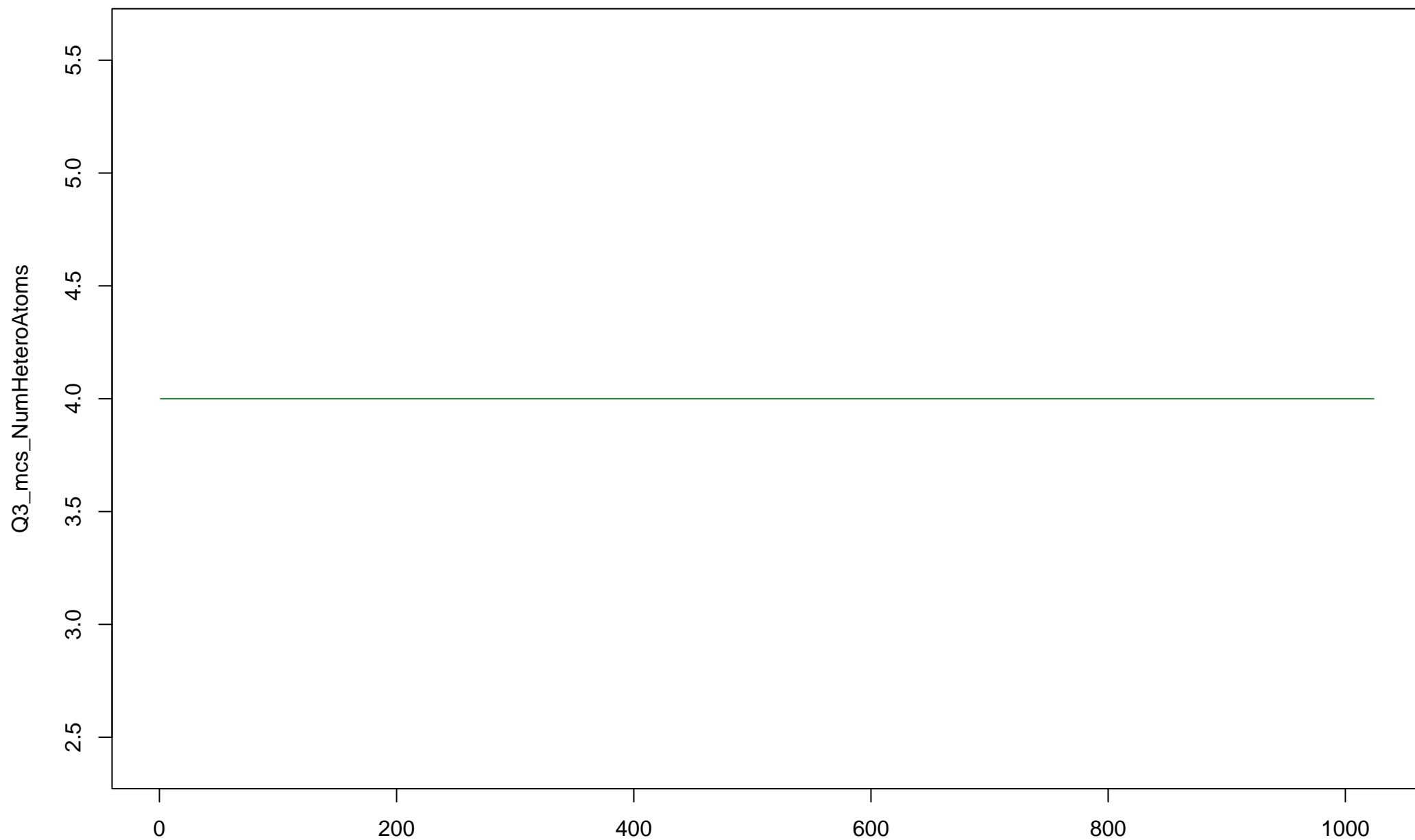
Q3_mcs_docked_NumHAcceptors
ESS = 15 | BMK = 0.434 | MCSE(6.27) = 10 | stat: FALSE | burn: 816



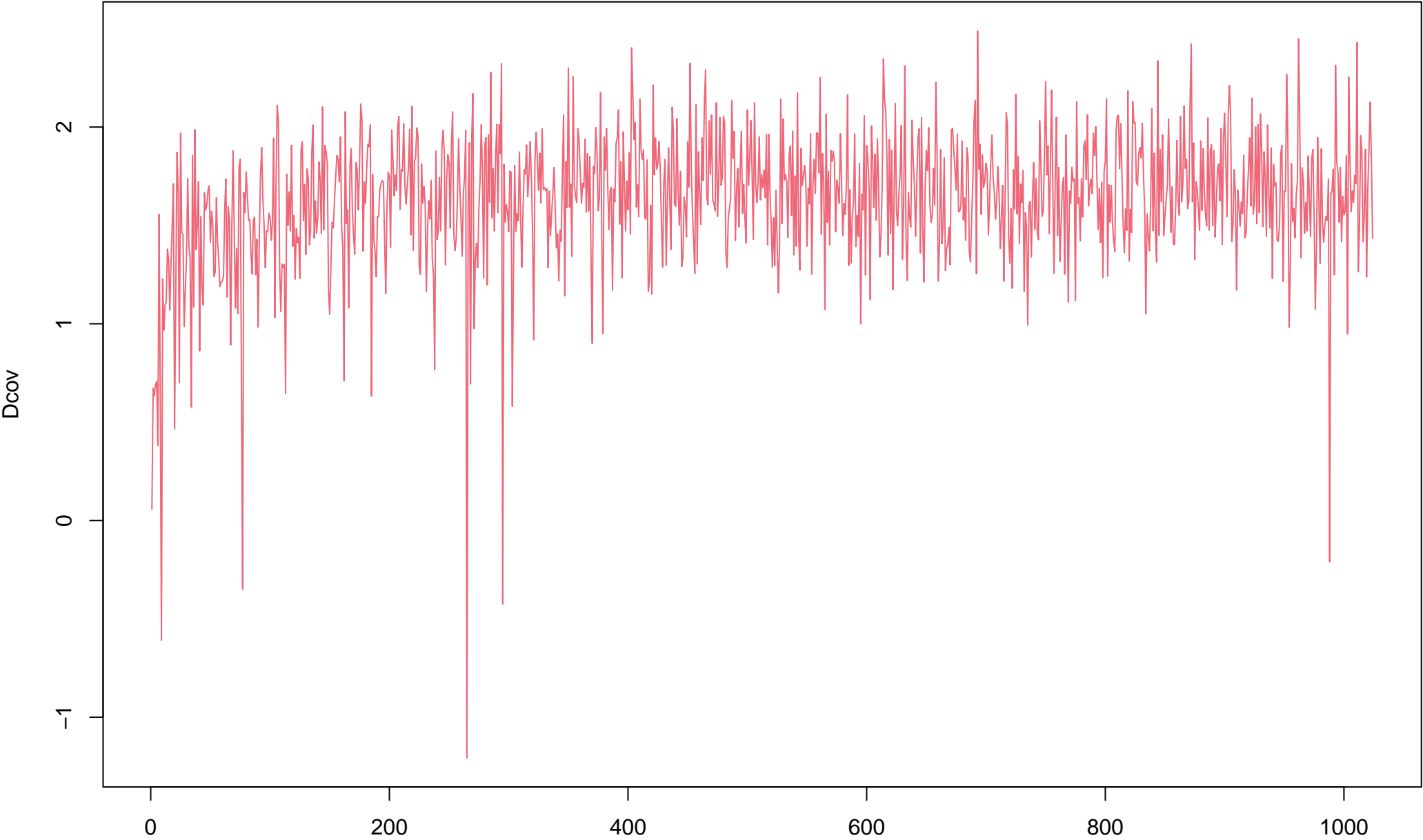
Q3_mcs_template_NumHAcceptors
ESS = 29.6 | BMK = 0.459 | MCSE(6.27) = 9.31 | stat: FALSE | burn: 0



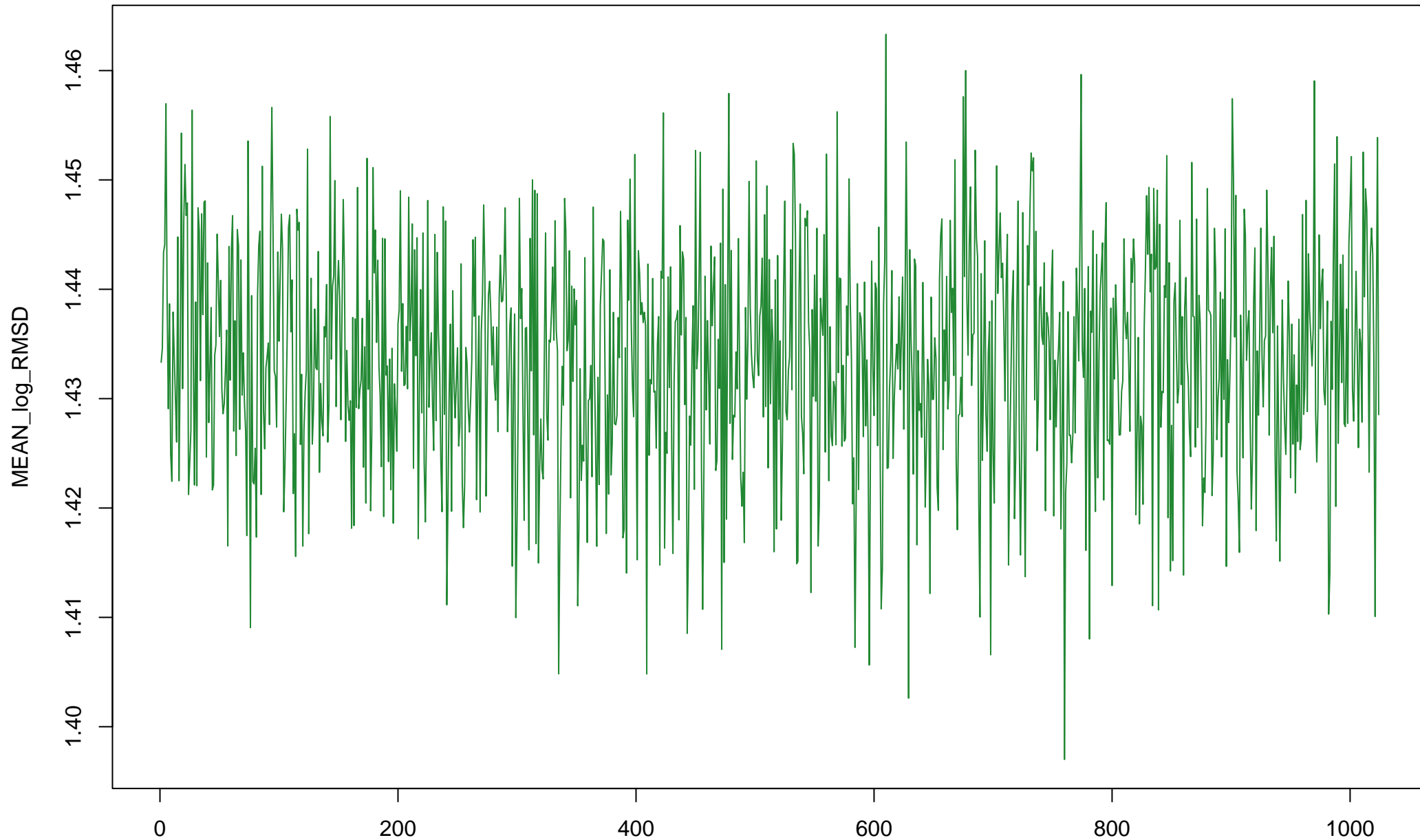
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



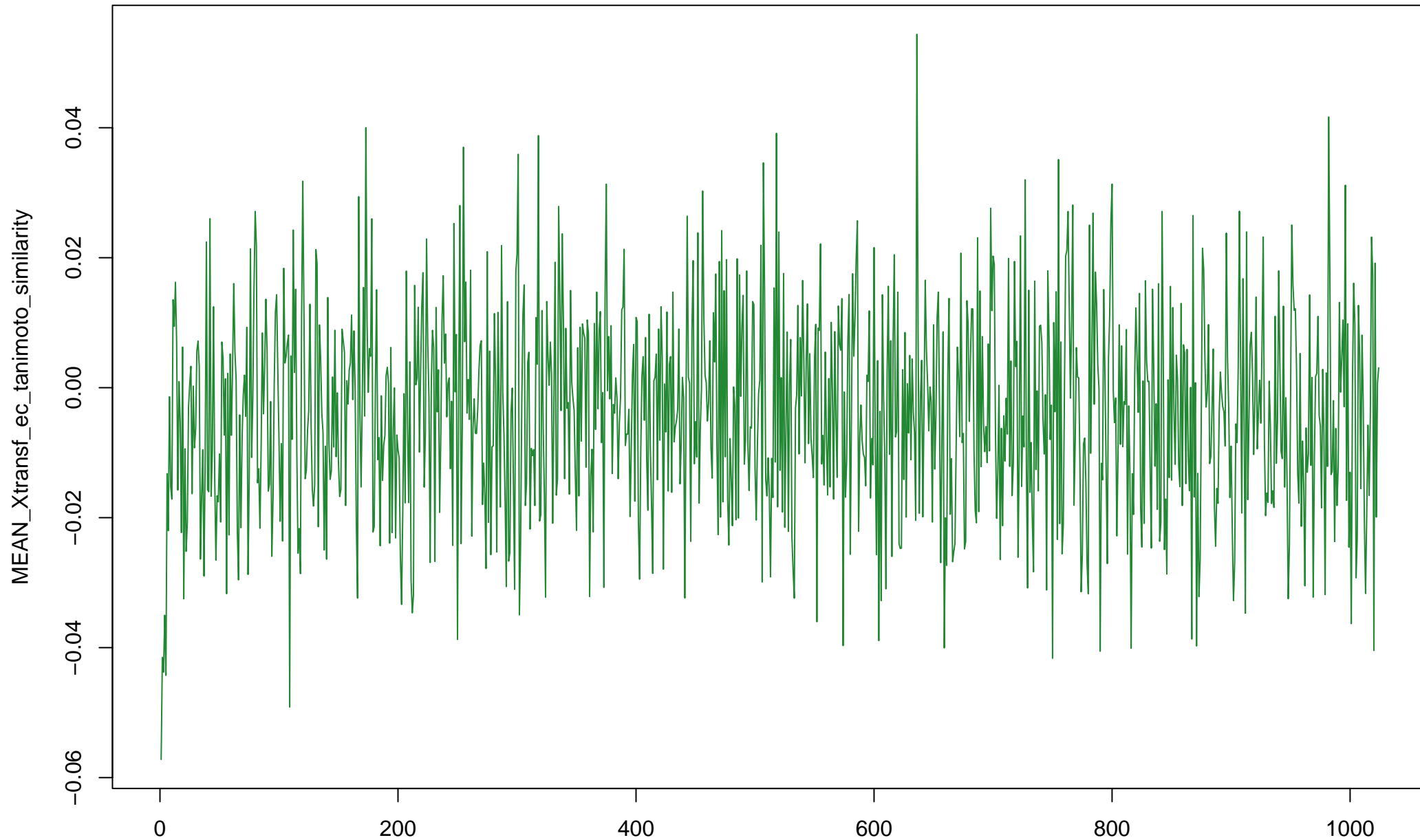
Dcov
ESS = 307 | BMK = 0.128 | MCSE(6.27) = 6.22 | stat: FALSE | burn: 0



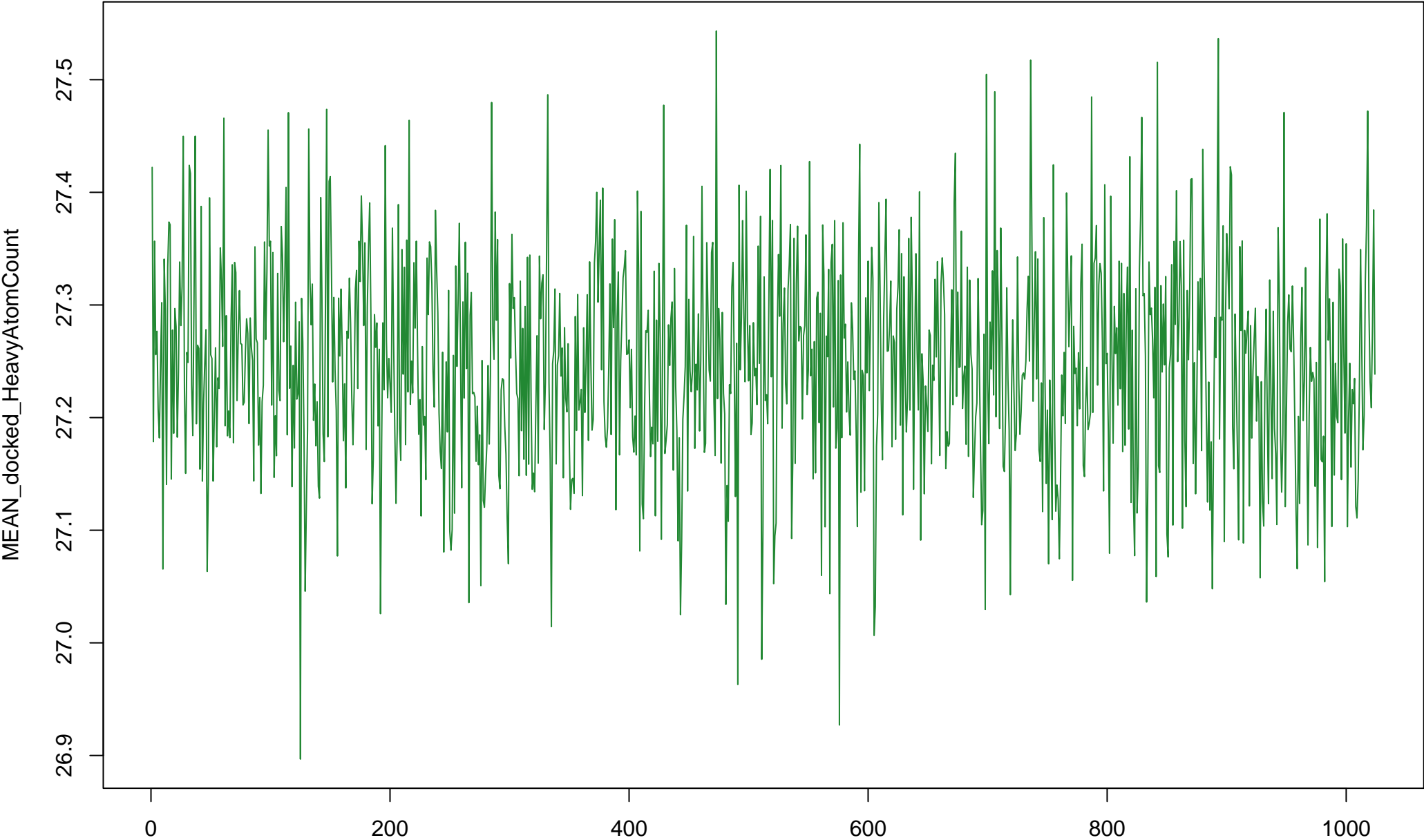
MEAN_log_RMSD
ESS = 1020 | BMK = 0.0518 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0



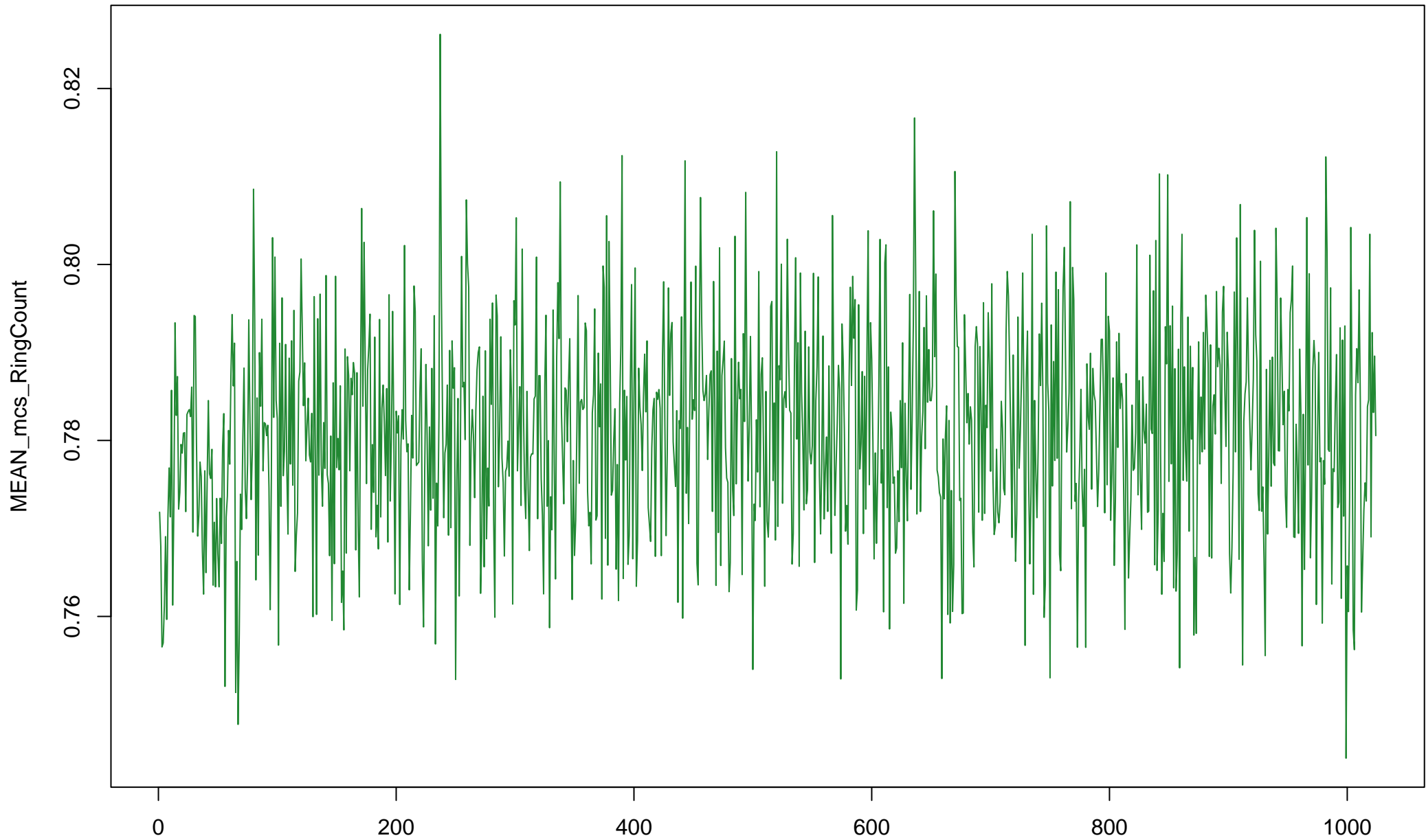
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0478 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0



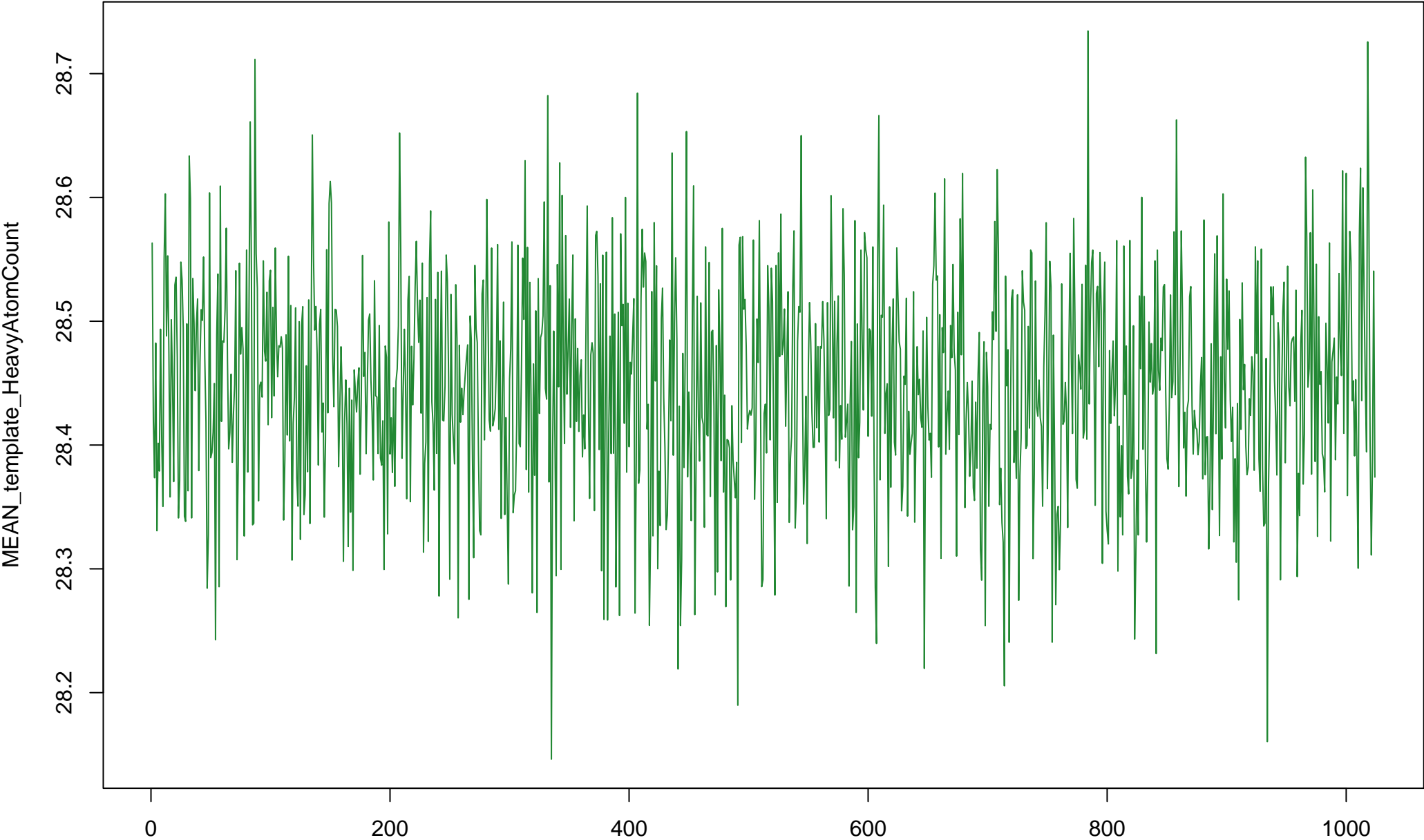
MEAN_docked_HeavyAtomCount
ESS = 843 | BMK = 0.0555 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0



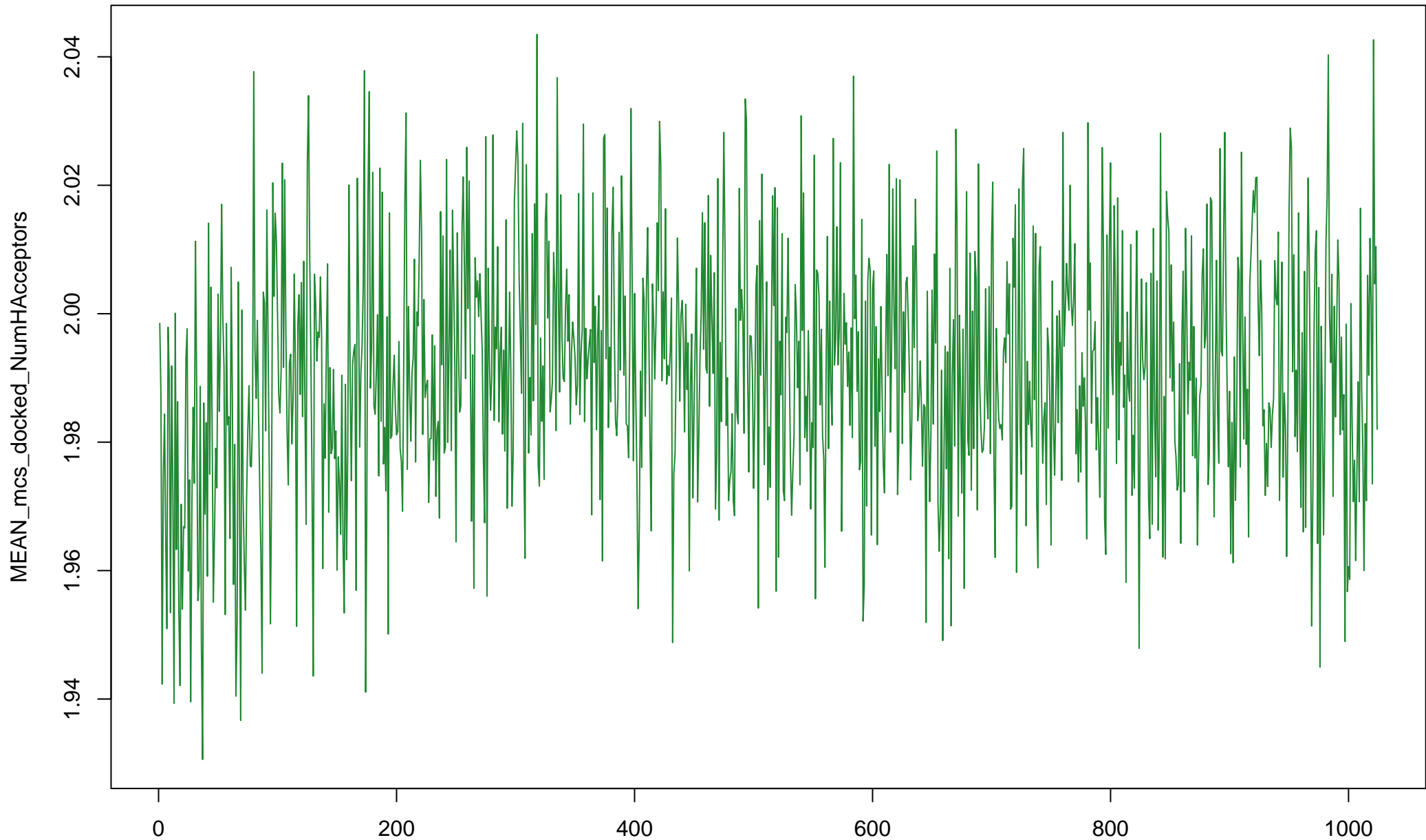
MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0645 | MCSE(6.27) = 3.2 | stat: FALSE | burn: 0



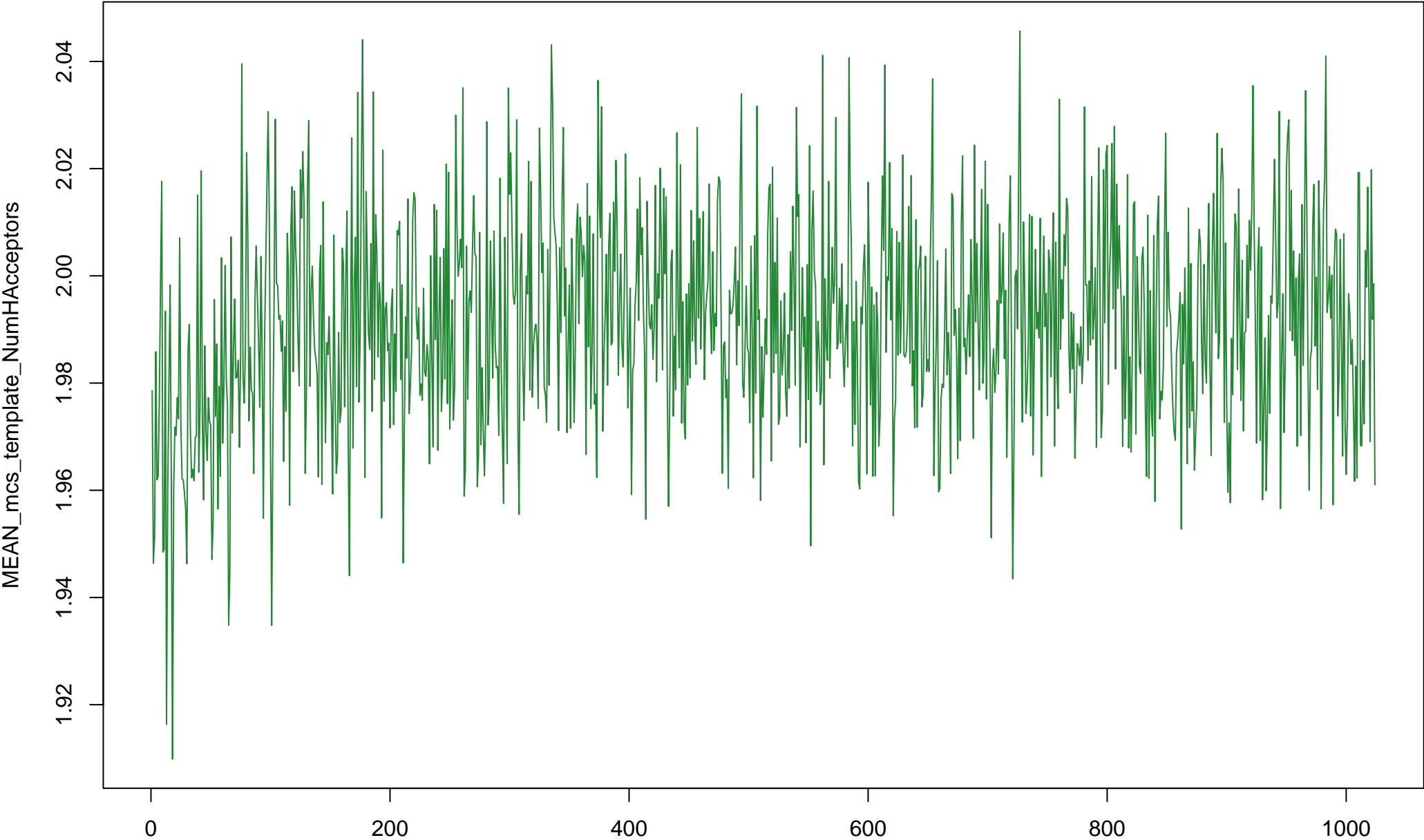
MEAN_template_HeavyAtomCount
ESS = 1020 | BMK = 0.0418 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0



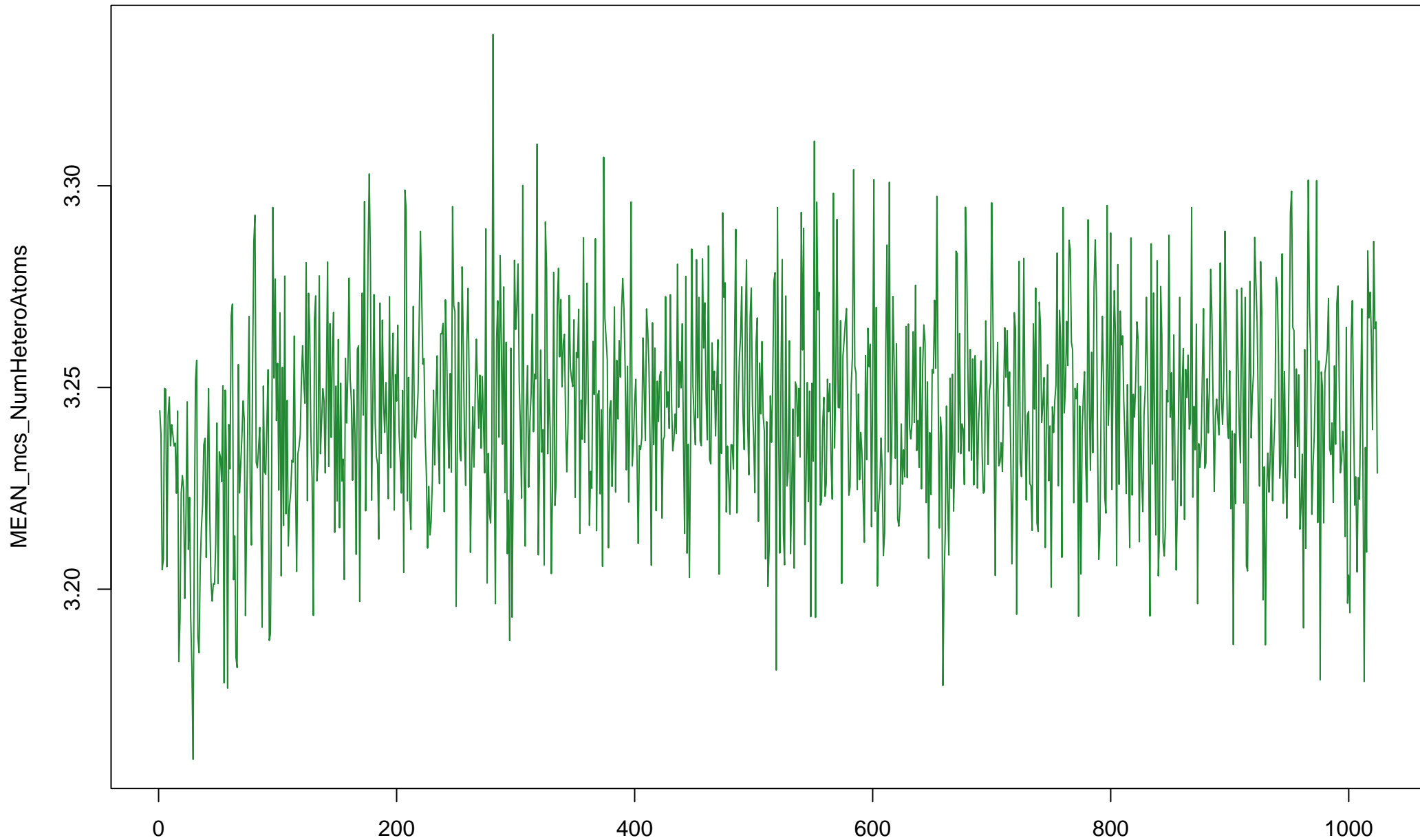
MEAN_mcs_docked_NumHAcceptors
ESS = 617 | BMK = 0.0851 | MCSE(6.27) = 5.29 | stat: FALSE | burn: 0



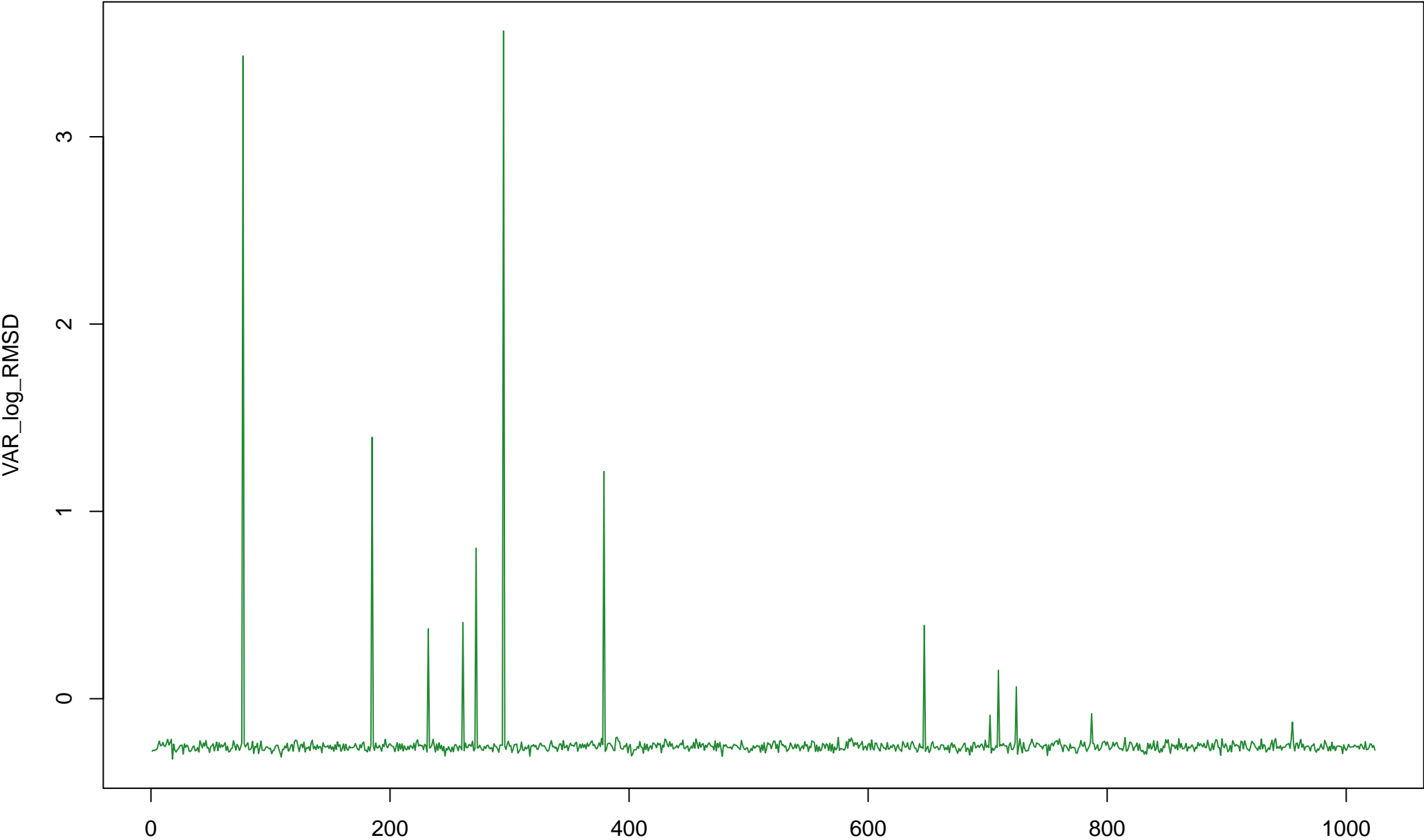
MEAN_mcs_template_NumHAcceptors
ESS = 190 | BMK = 0.078 | MCSE(6.27) = 5.63 | stat: FALSE | burn: 0



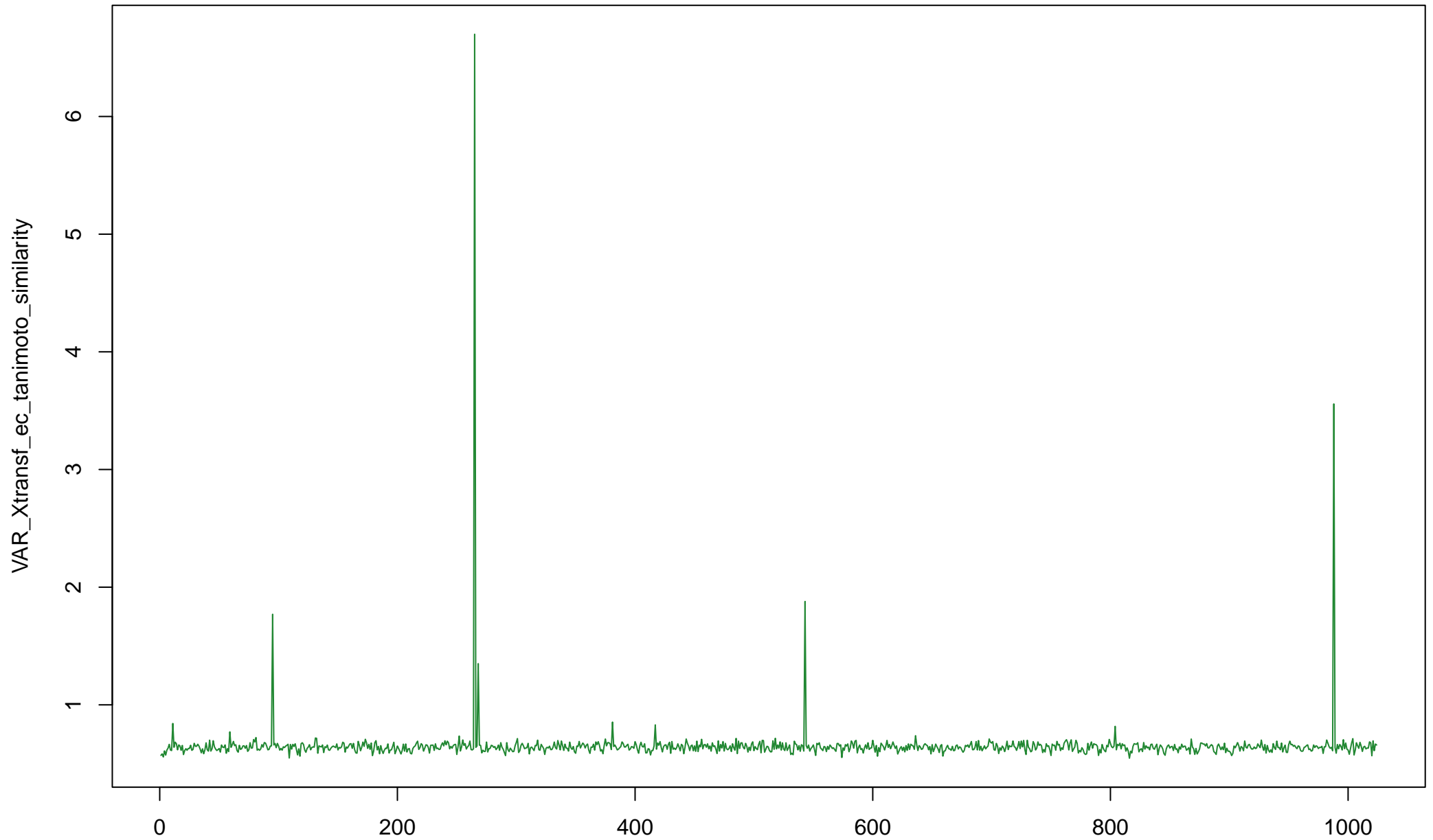
MEAN_mcs_NumHeteroAtoms
ESS = 794 | BMK = 0.0542 | MCSE(6.27) = 4.72 | stat: FALSE | burn: 0



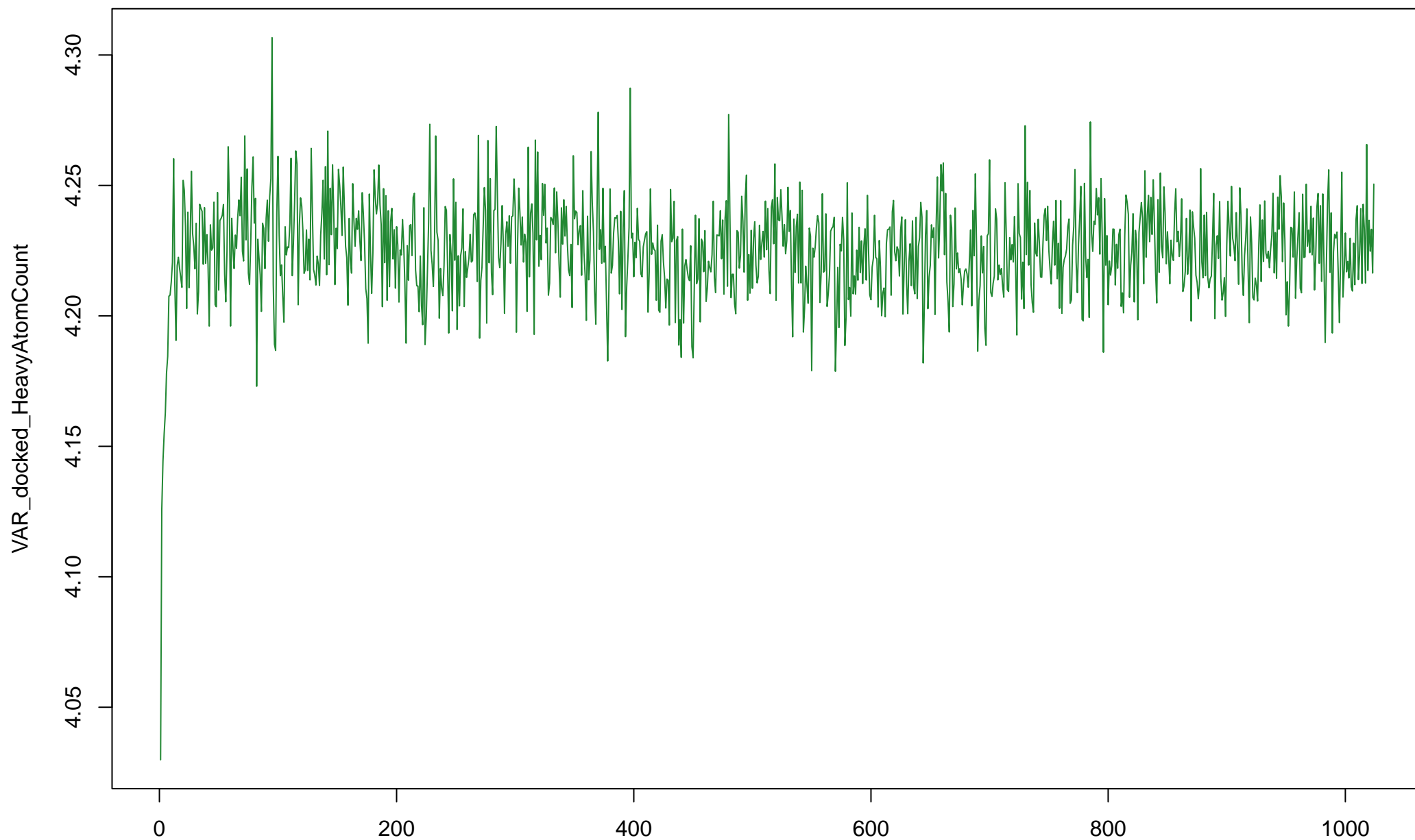
VAR_log_RMSD
ESS = 1020 | BMK = 0.268 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0



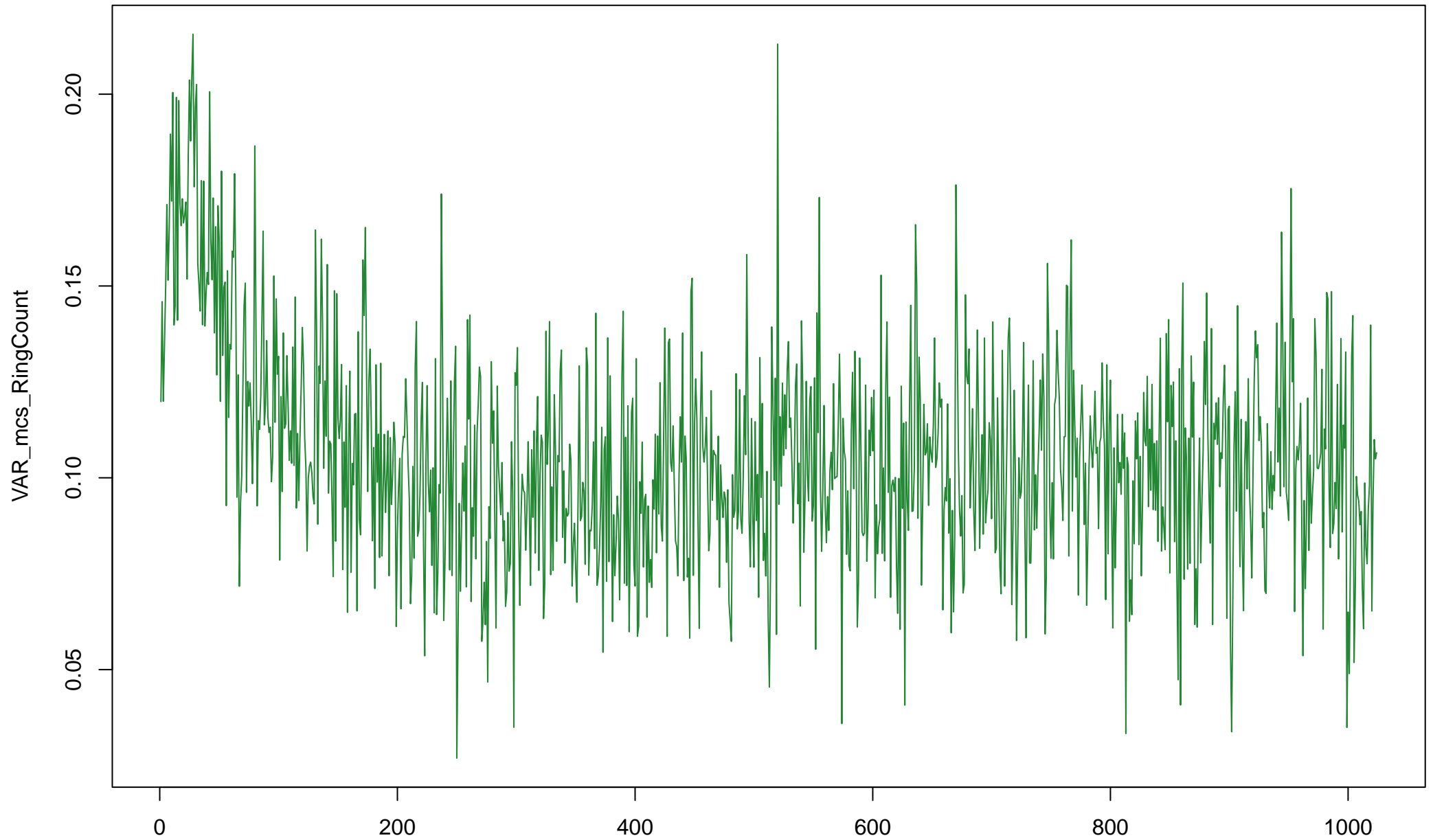
VAR_Xtransf_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.326 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 306



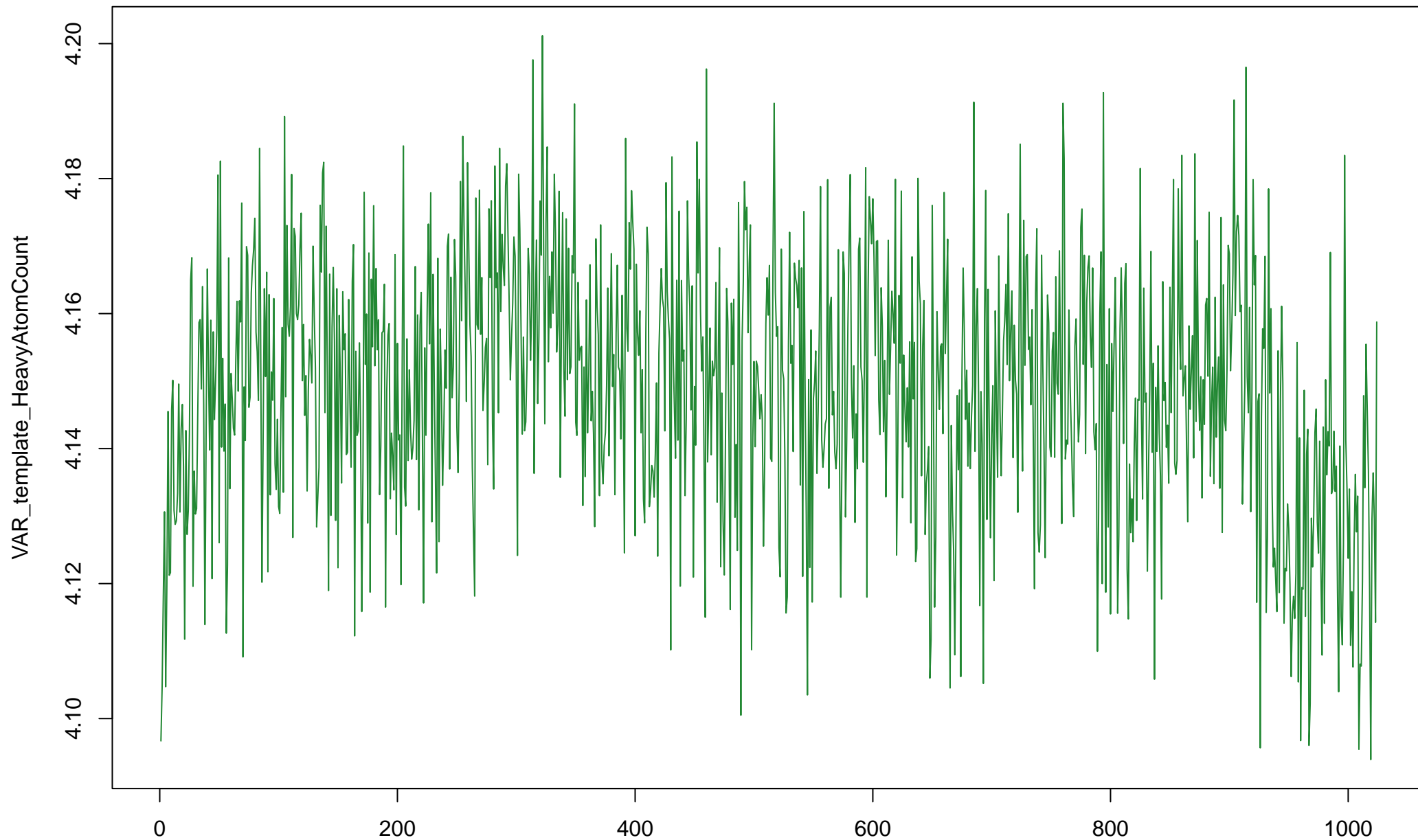
VAR_docked_HeavyAtomCount
ESS = 436 | BMK = 0.115 | MCSE(6.27) = 5.28 | stat: TRUE | burn: 0



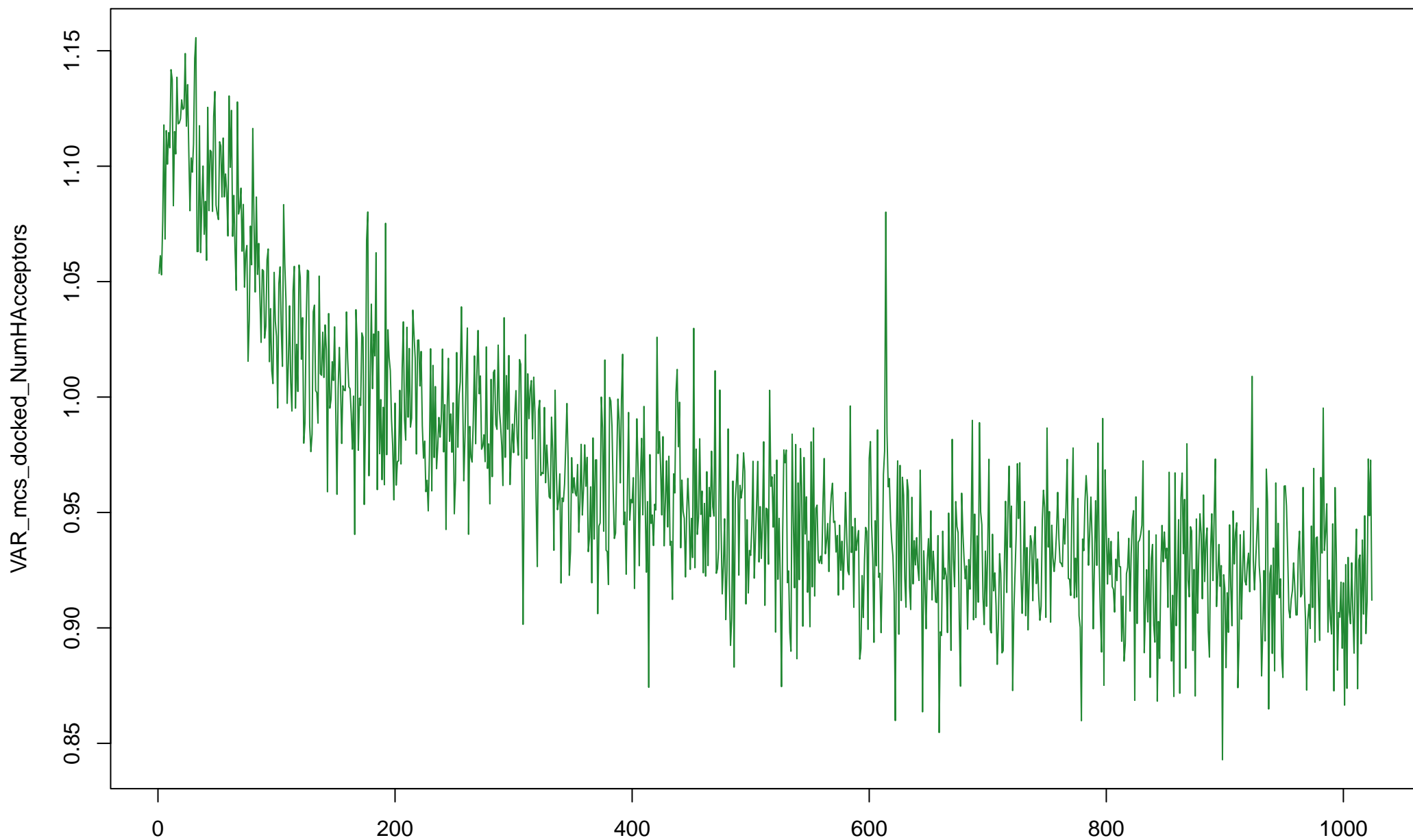
VAR_mcs_RingCount
ESS = 40.6 | BMK = 0.147 | MCSE(6.27) = 10.2 | stat: FALSE | burn: 0



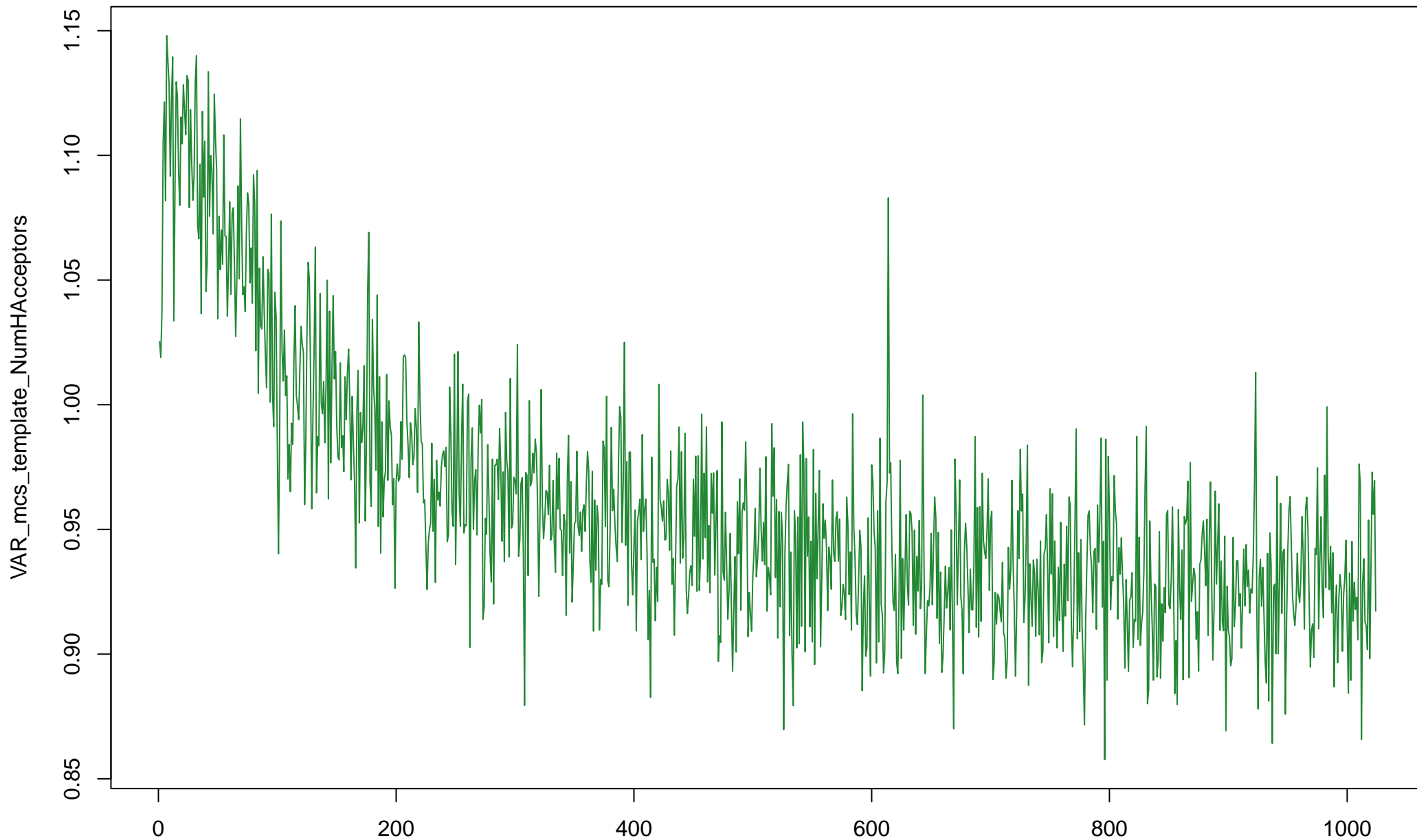
VAR_template_HeavyAtomCount
ESS = 84.2 | BMK = 0.114 | MCSE(6.27) = 7.91 | stat: TRUE | burn: 0



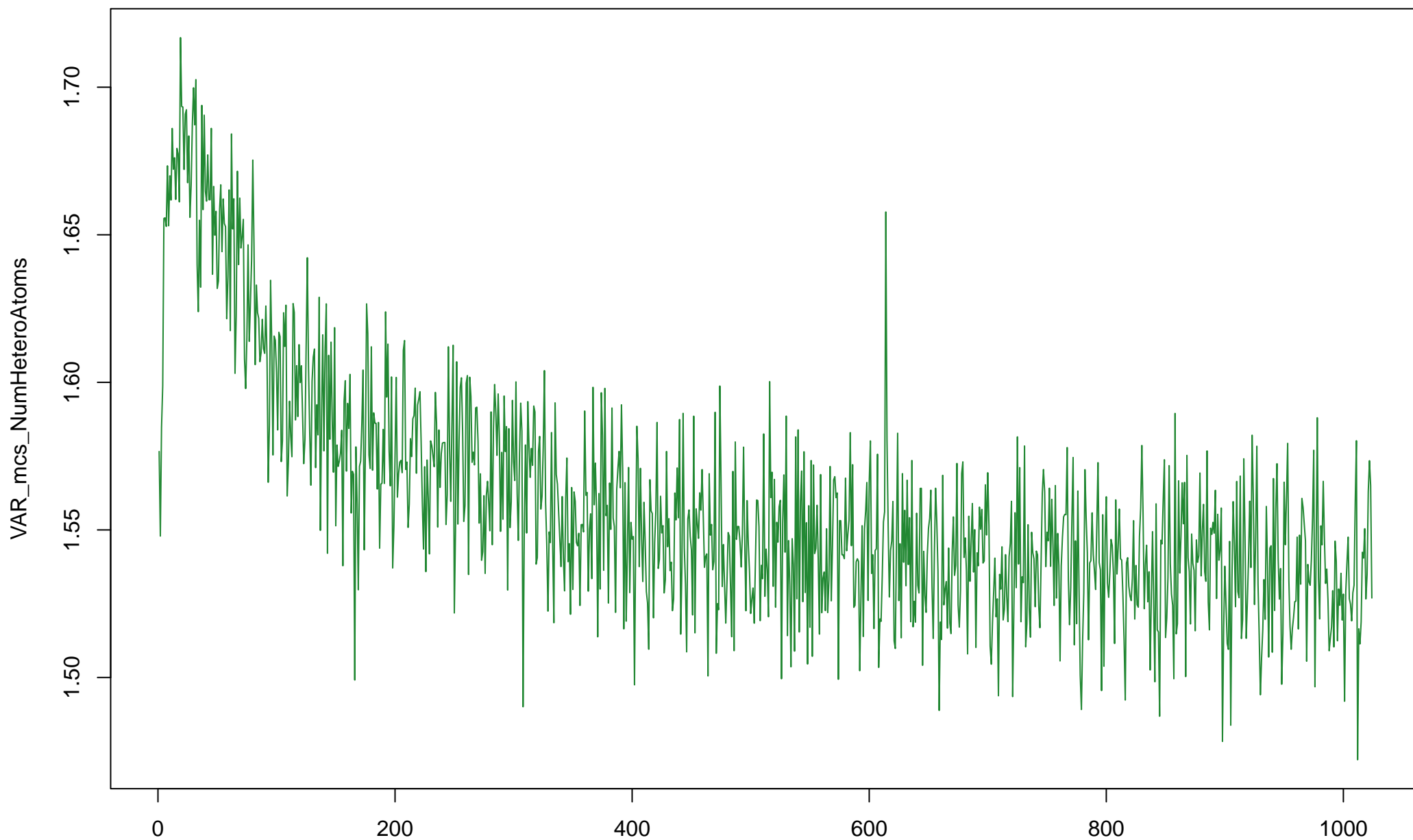
VAR_mcs_docked_NumHAcceptors
ESS = 4.71 | BMK = 0.58 | MCSE(6.27) = 16 | stat: FALSE | burn: 102



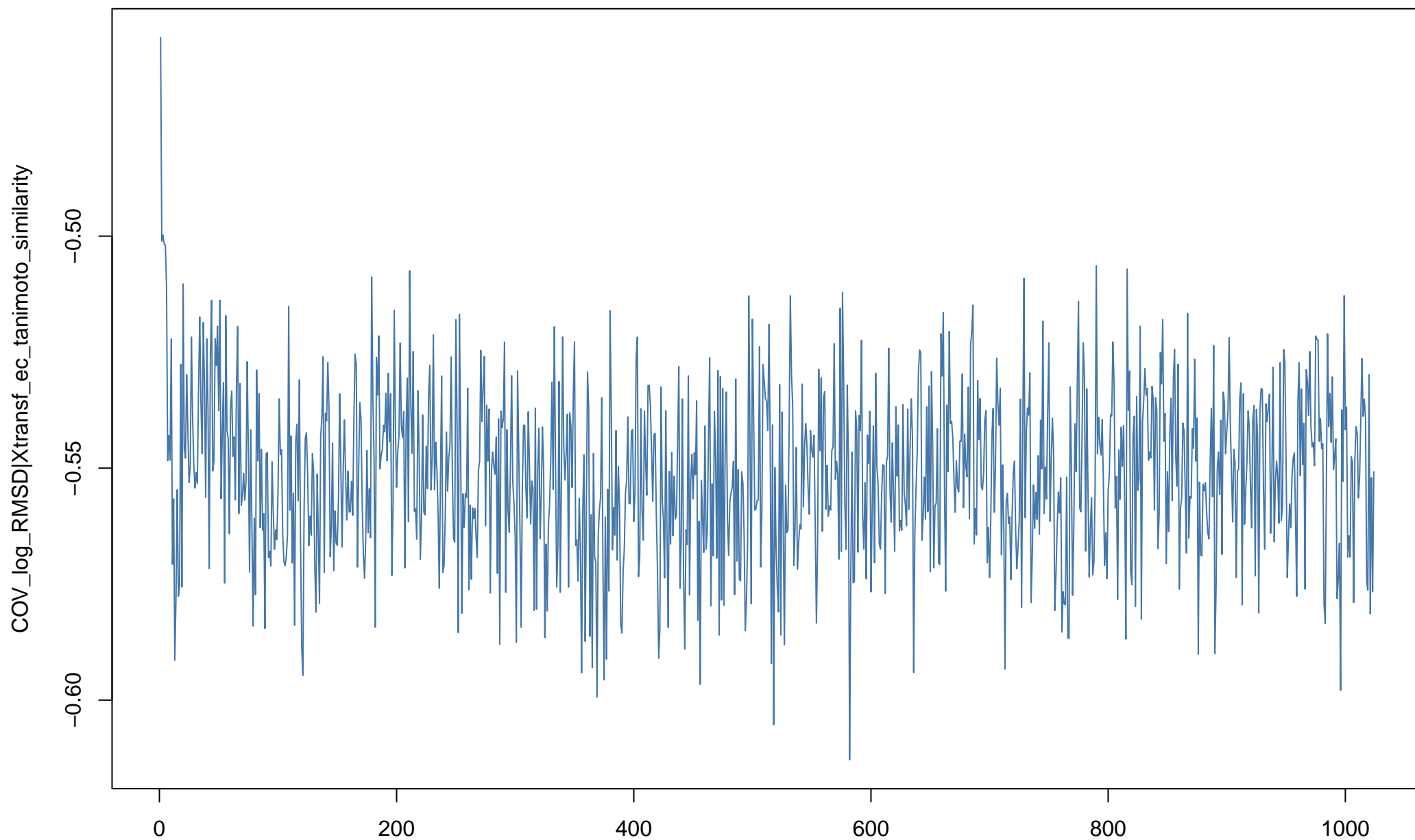
VAR_mcs_template_NumHAcceptors
ESS = 6.07 | BMK = 0.486 | MCSE(6.27) = 15.5 | stat: FALSE | burn: 102



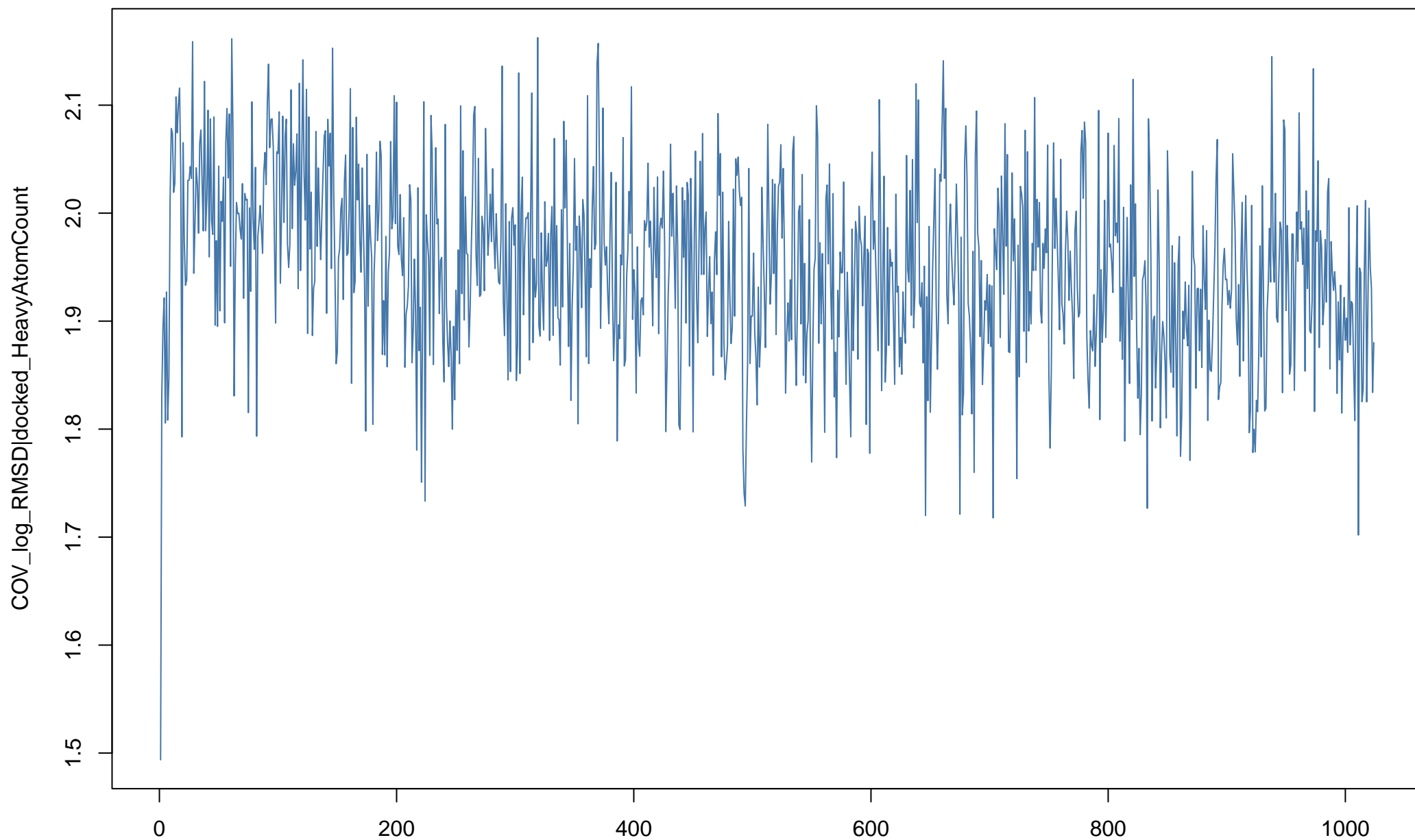
VAR_mcs_NumHeteroAtoms
ESS = 6.38 | BMK = 0.464 | MCSE(6.27) = 15.1 | stat: FALSE | burn: 102



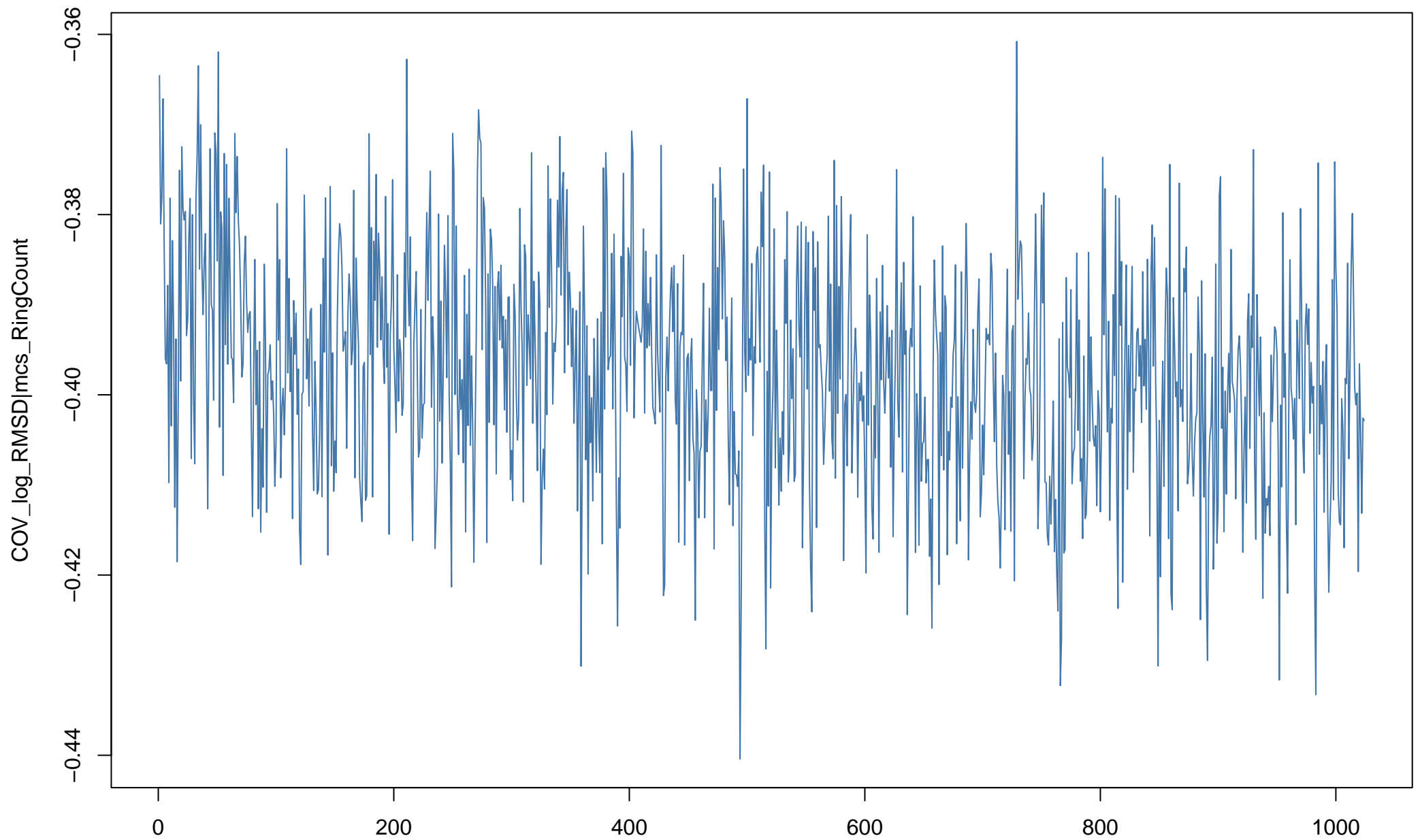
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 324 | BMK = 0.0741 | MCSE(6.27) = 5.43 | stat: TRUE | burn: 0



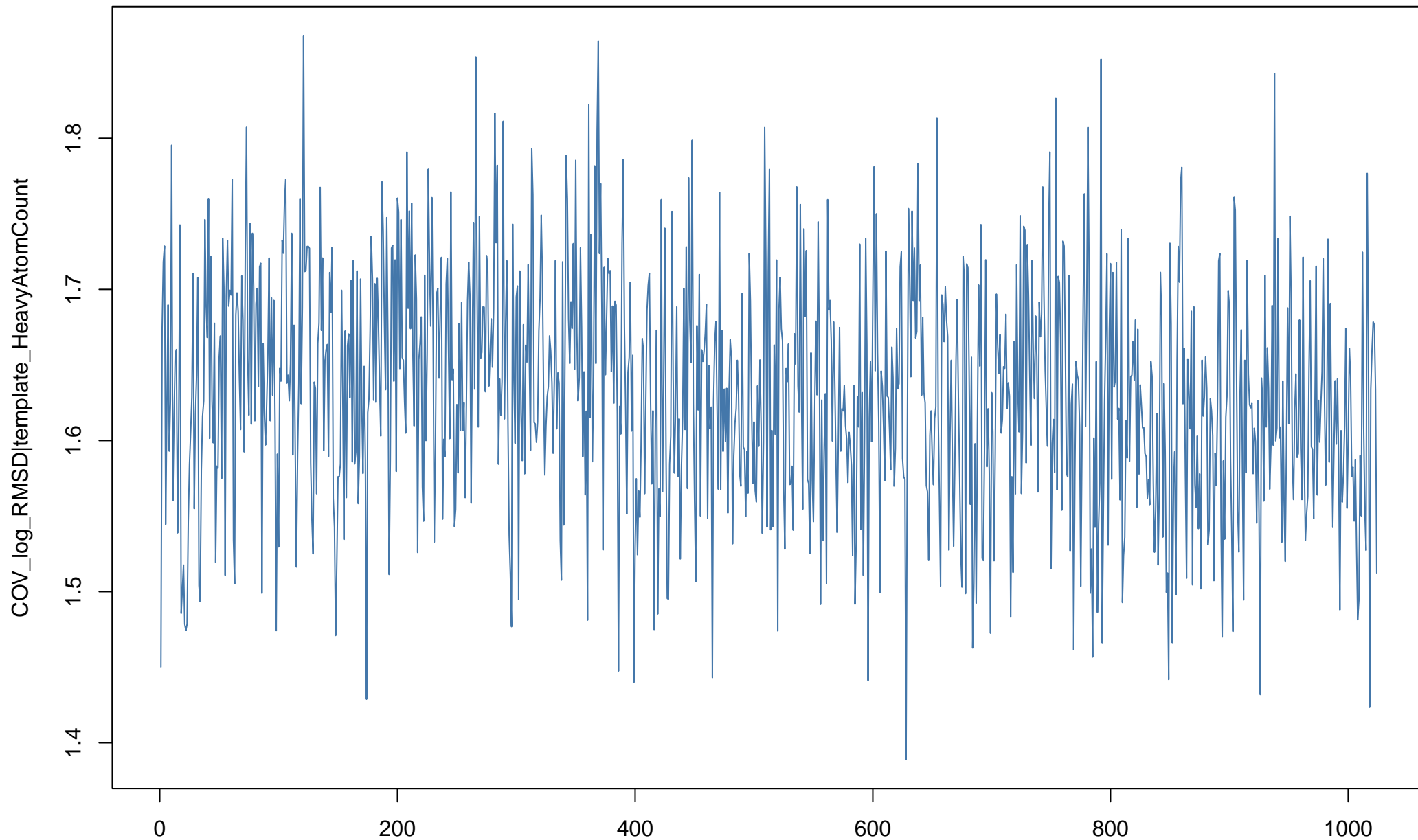
COV_log_RMSD|docked_HeavyAtomCount
ESS = 207 | BMK = 0.154 | MCSE(6.27) = 6.35 | stat: FALSE | burn: 0



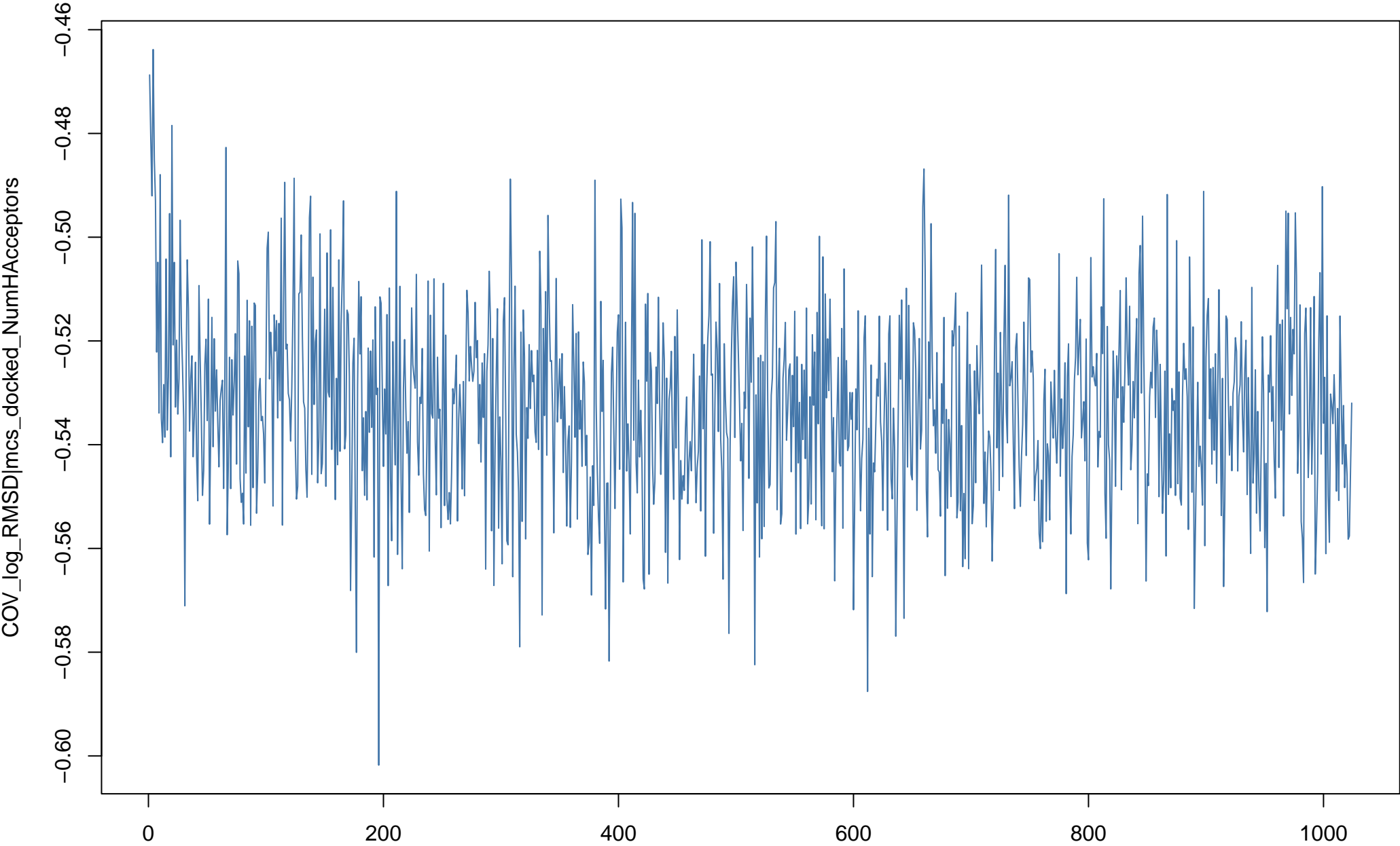
COV_log_RMSD|mcs_RingCount
ESS = 524 | BMK = 0.17 | MCSE(6.27) = 5.82 | stat: FALSE | burn: 0



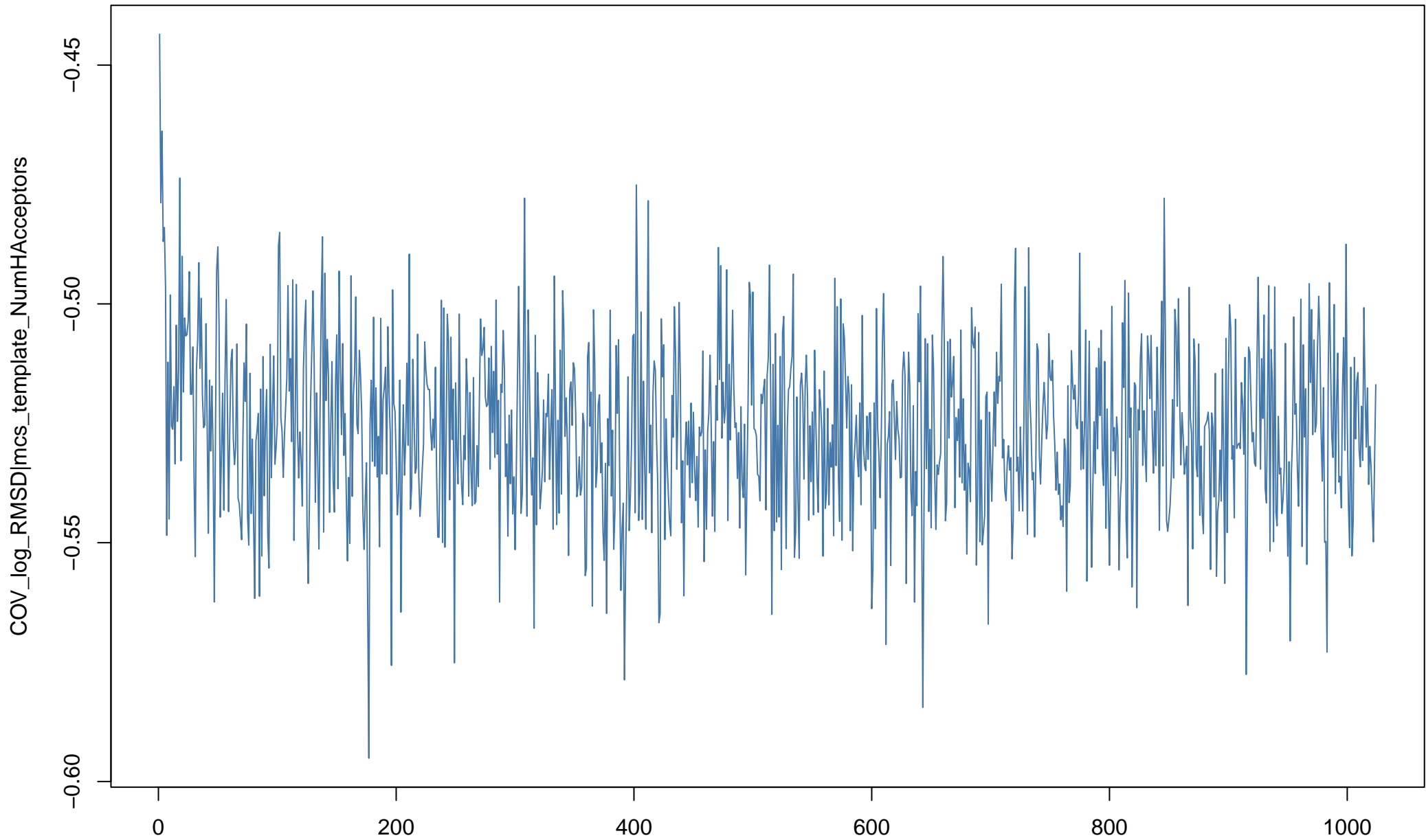
COV_log_RMSD|template_HeavyAtomCount
ESS = 553 | BMK = 0.112 | MCSE(6.27) = 5.38 | stat: TRUE | burn: 0



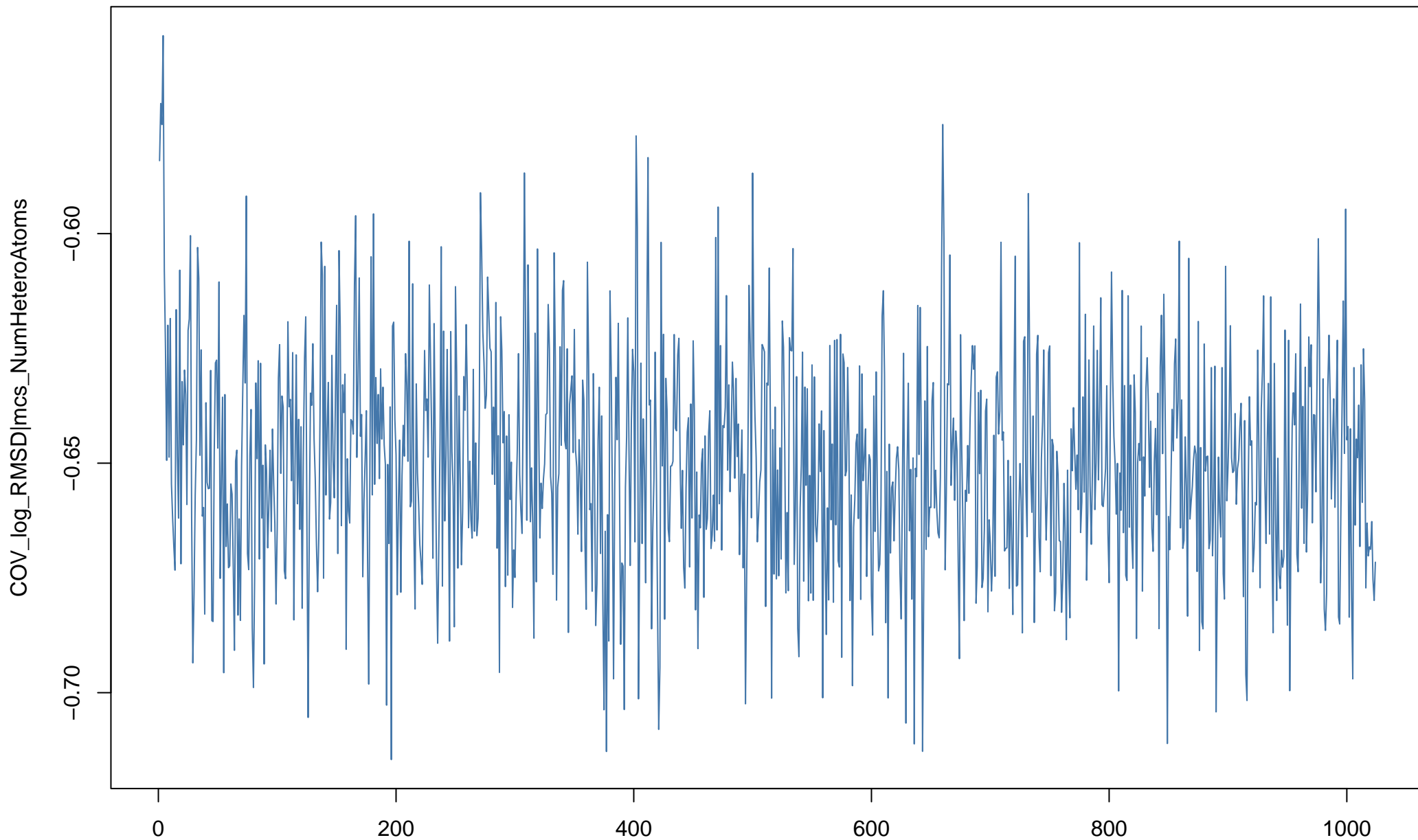
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 602 | BMK = 0.0803 | MCSE(6.27) = 4.9 | stat: FALSE | burn: 0



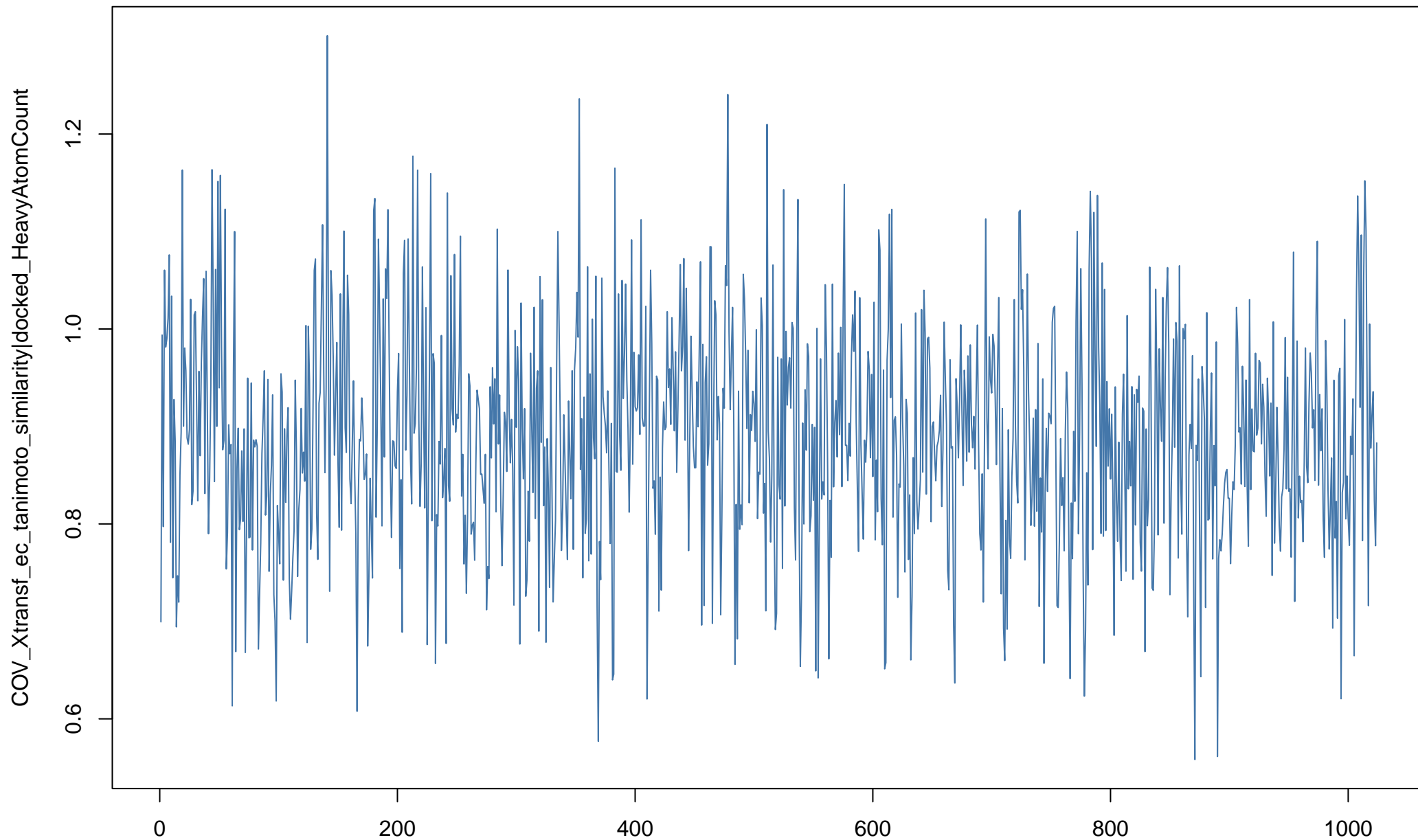
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 858 | BMK = 0.0733 | MCSE(6.27) = 4.38 | stat: FALSE | burn: 0



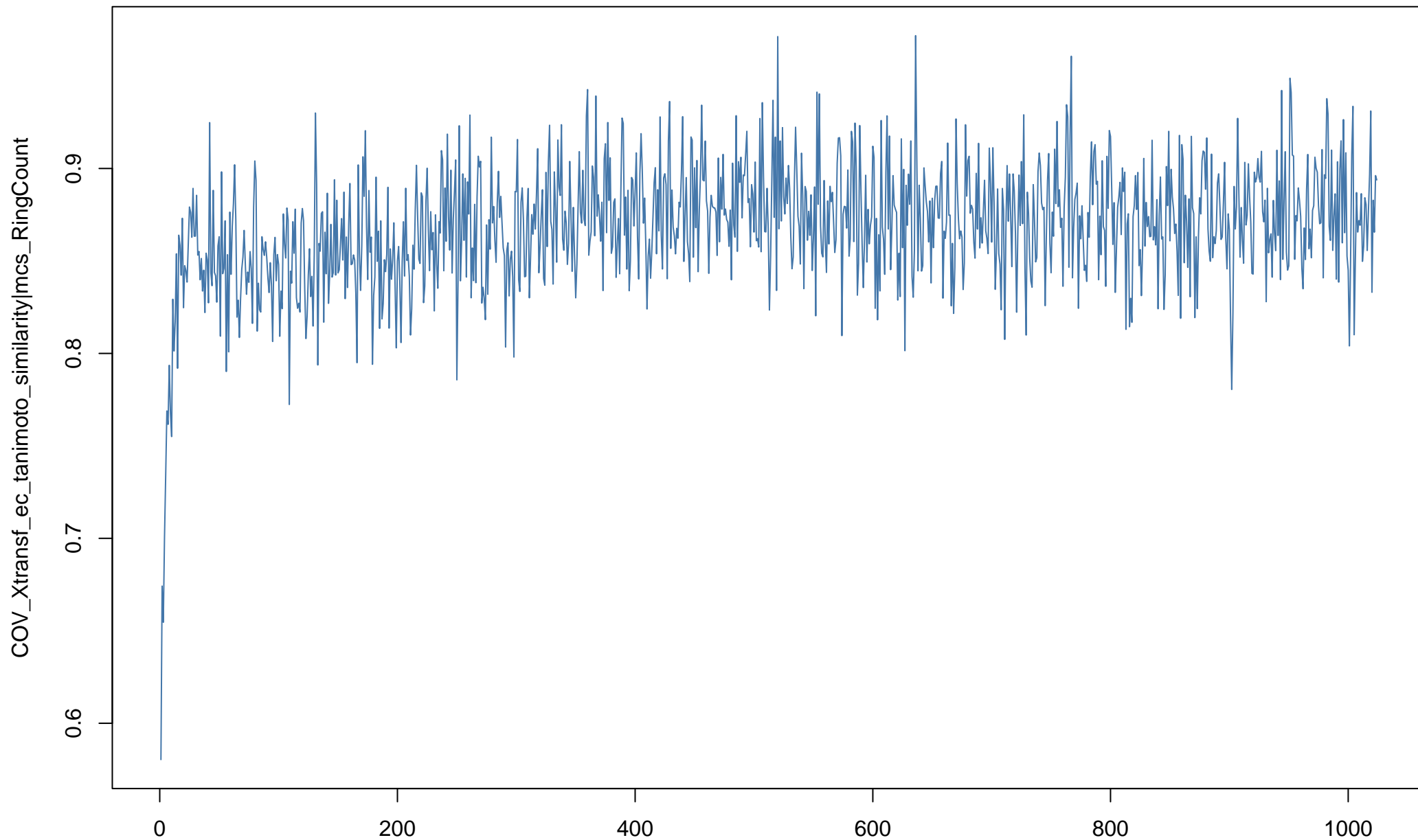
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 807 | BMK = 0.0873 | MCSE(6.27) = 4.26 | stat: TRUE | burn: 0



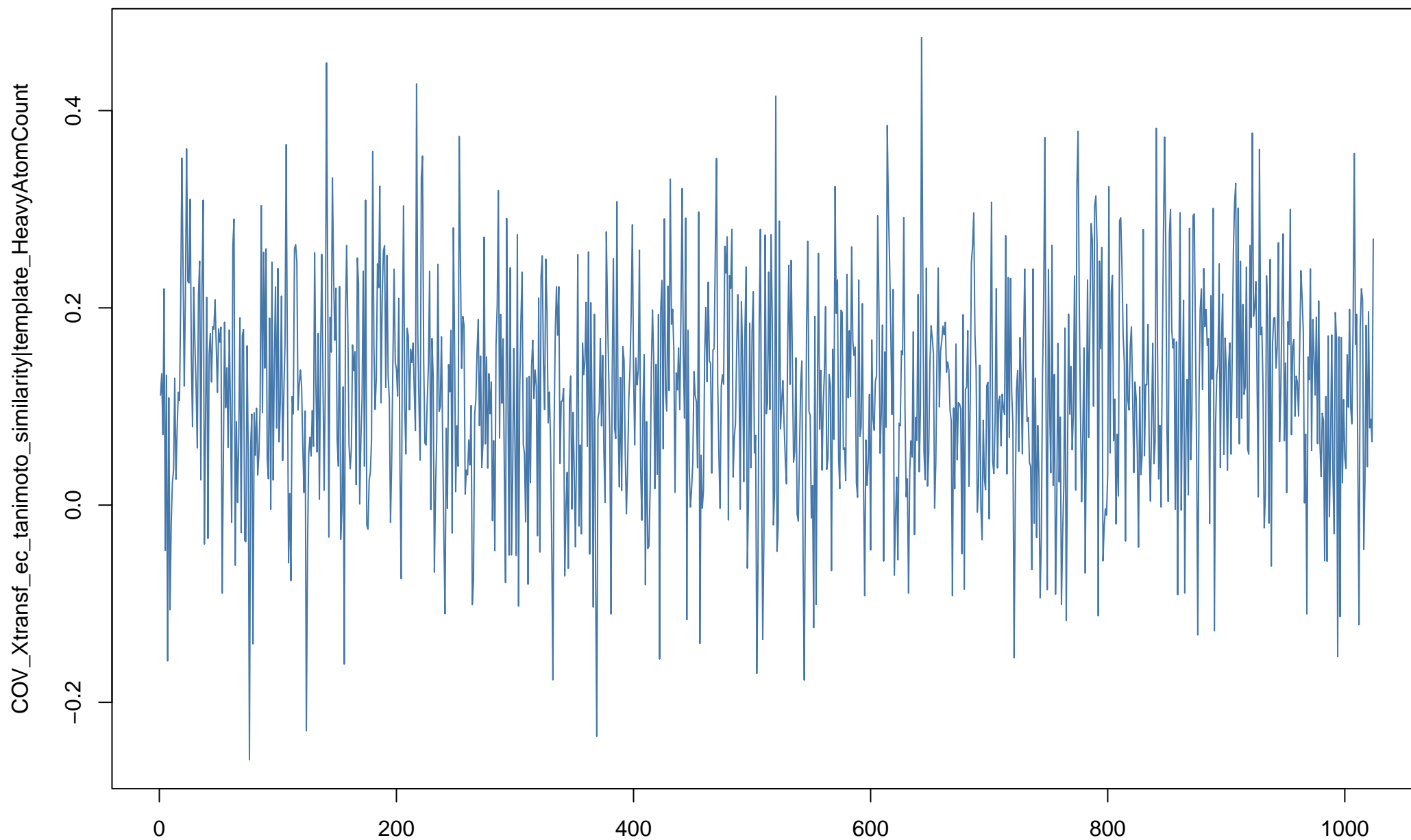
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 464 | BMK = 0.0794 | MCSE(6.27) = 4.91 | stat: TRUE | burn: 0



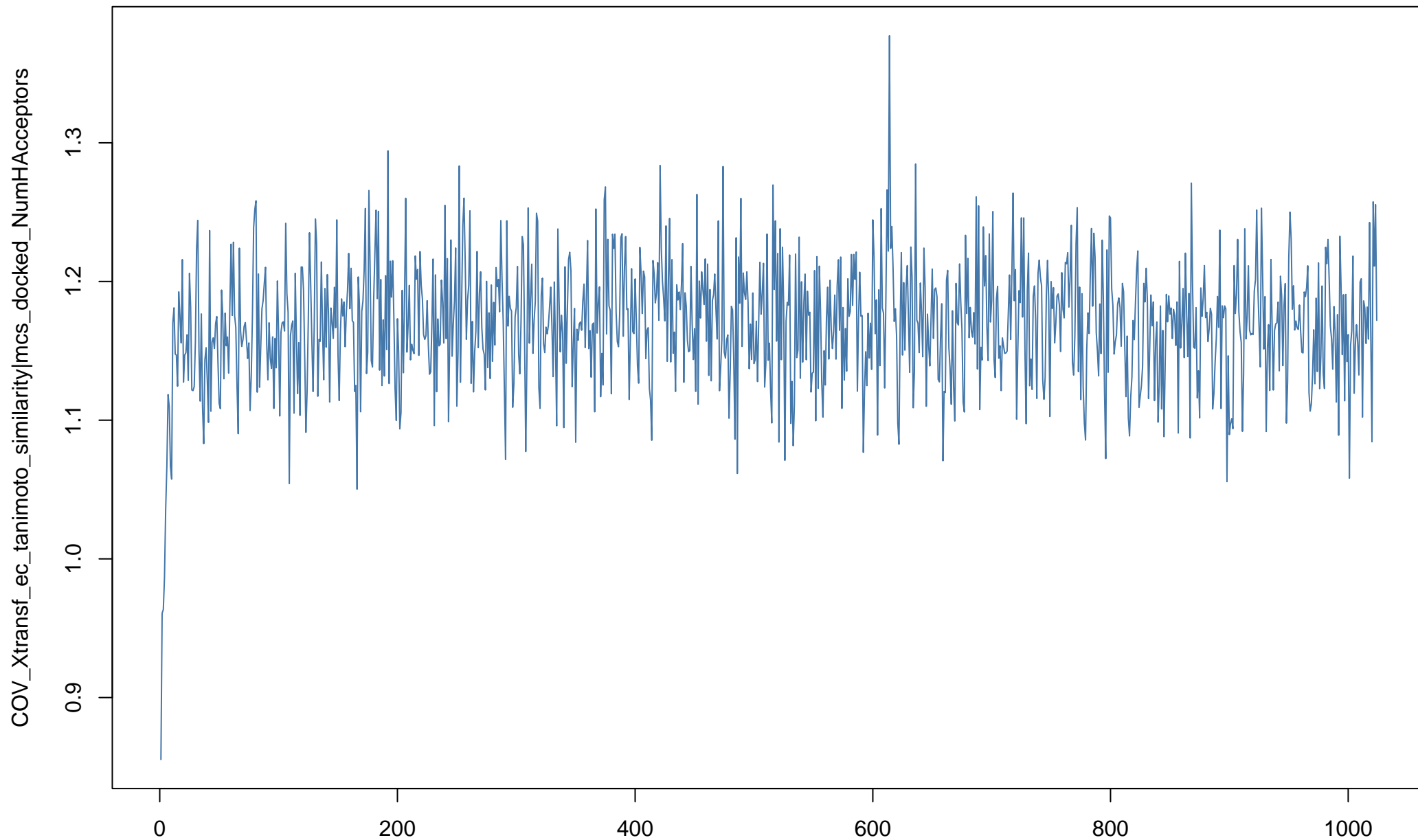
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 149 | BMK = 0.162 | MCSE(6.27) = 8.15 | stat: FALSE | burn: 0



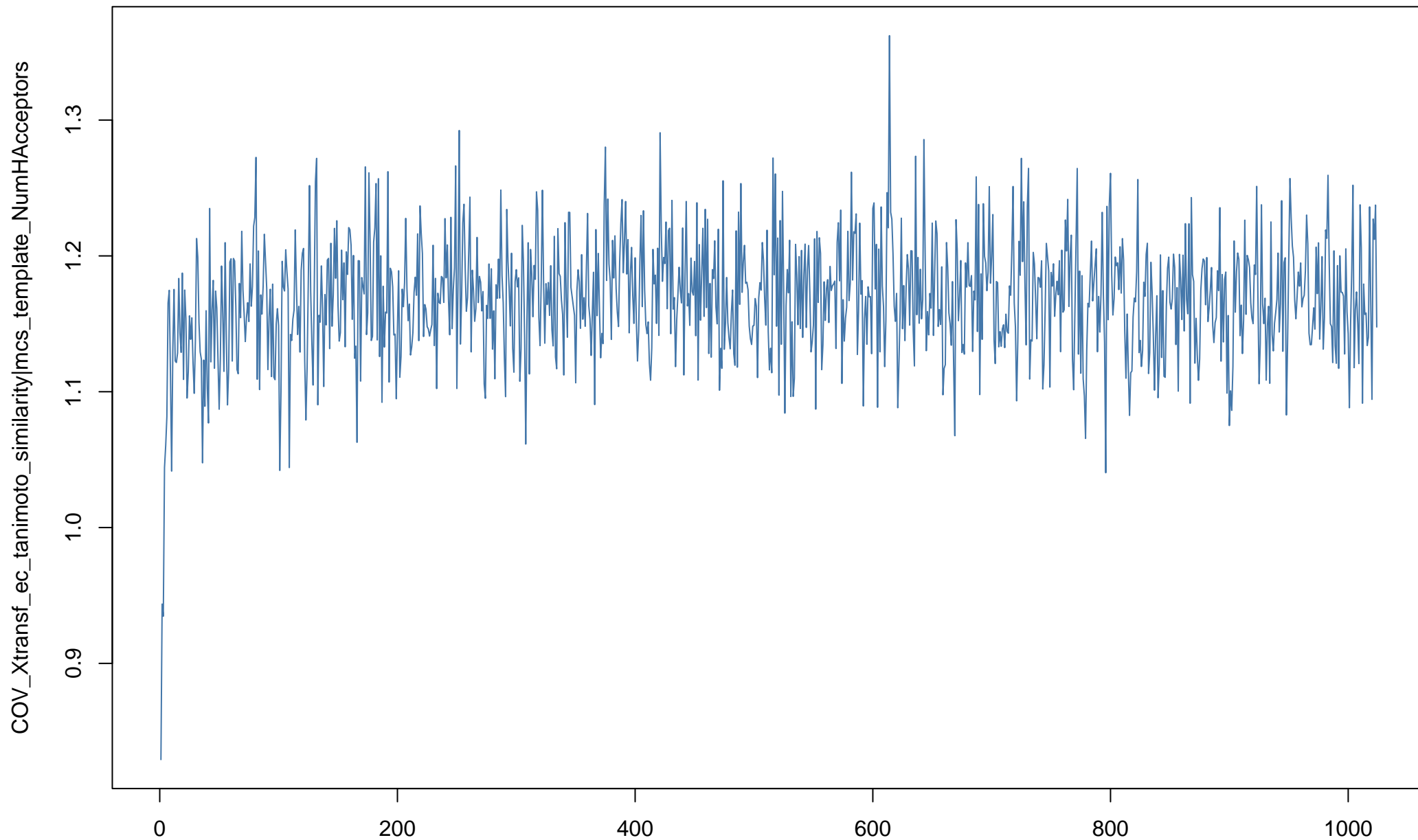
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 710 | BMK = 0.048 | MCSE(6.27) = 3.66 | stat: TRUE | burn: 0



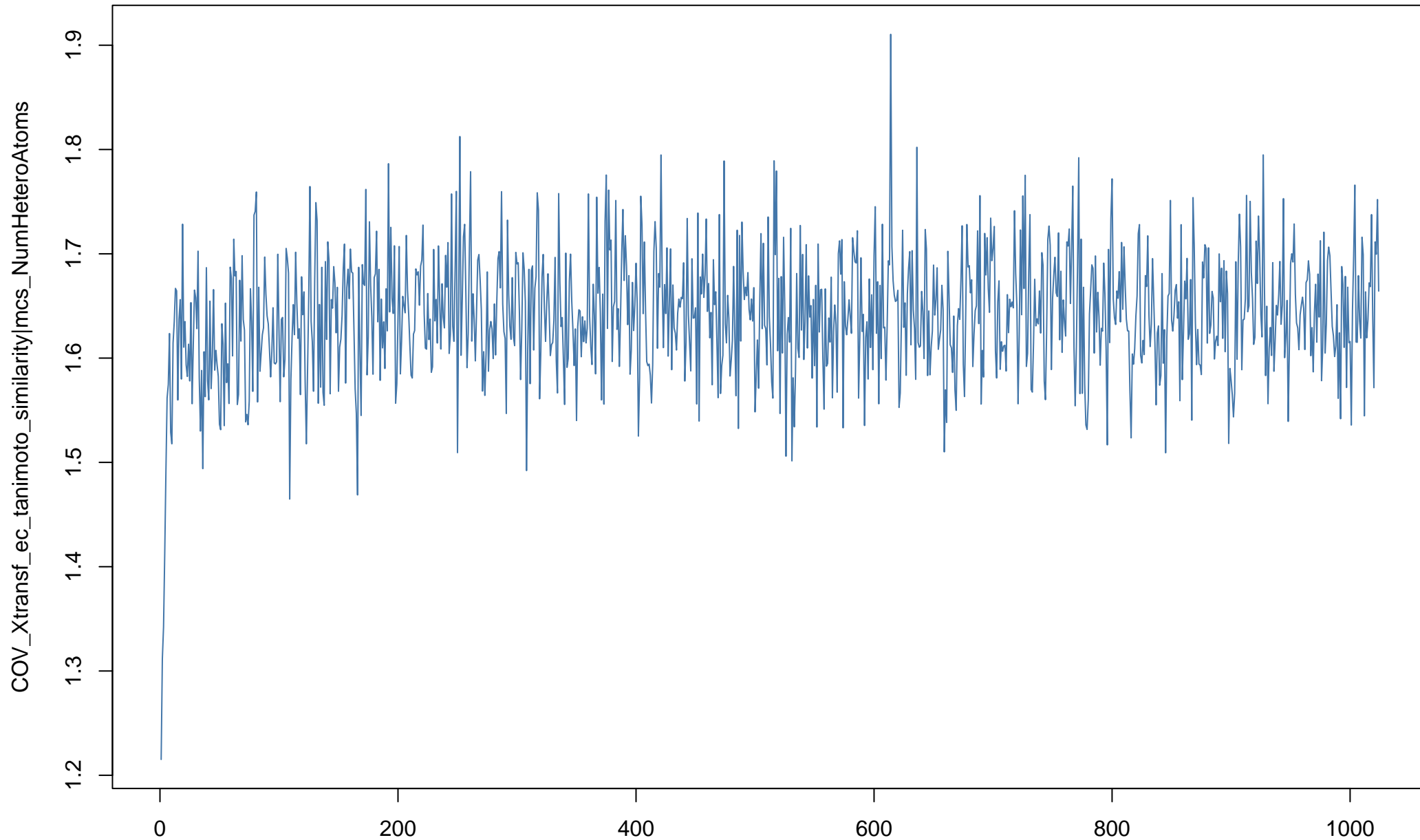
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 595 | BMK = 0.0887 | MCSE(6.27) = 4.69 | stat: FALSE | burn: 0



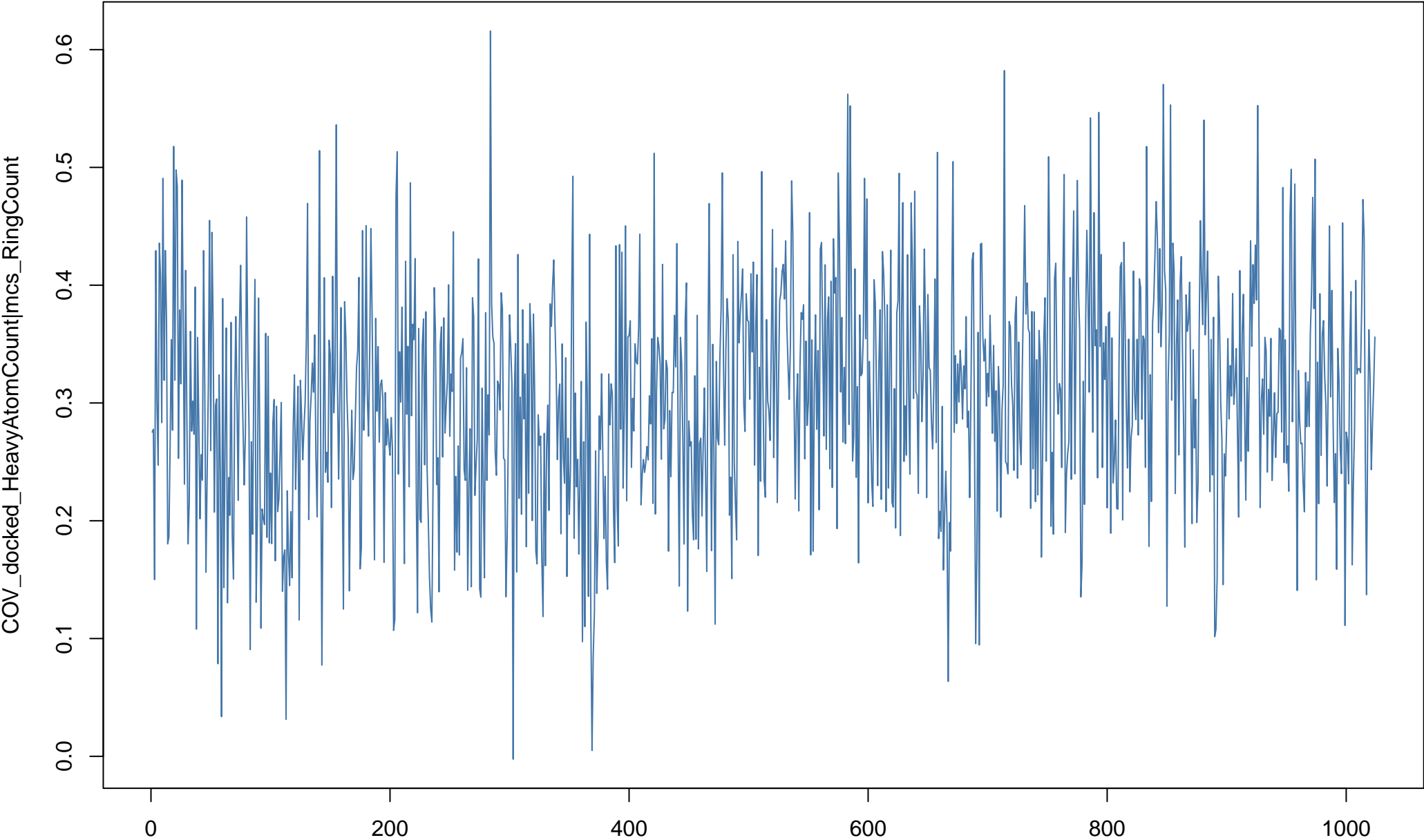
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 578 | BMK = 0.075 | MCSE(6.27) = 5.18 | stat: FALSE | burn: 0



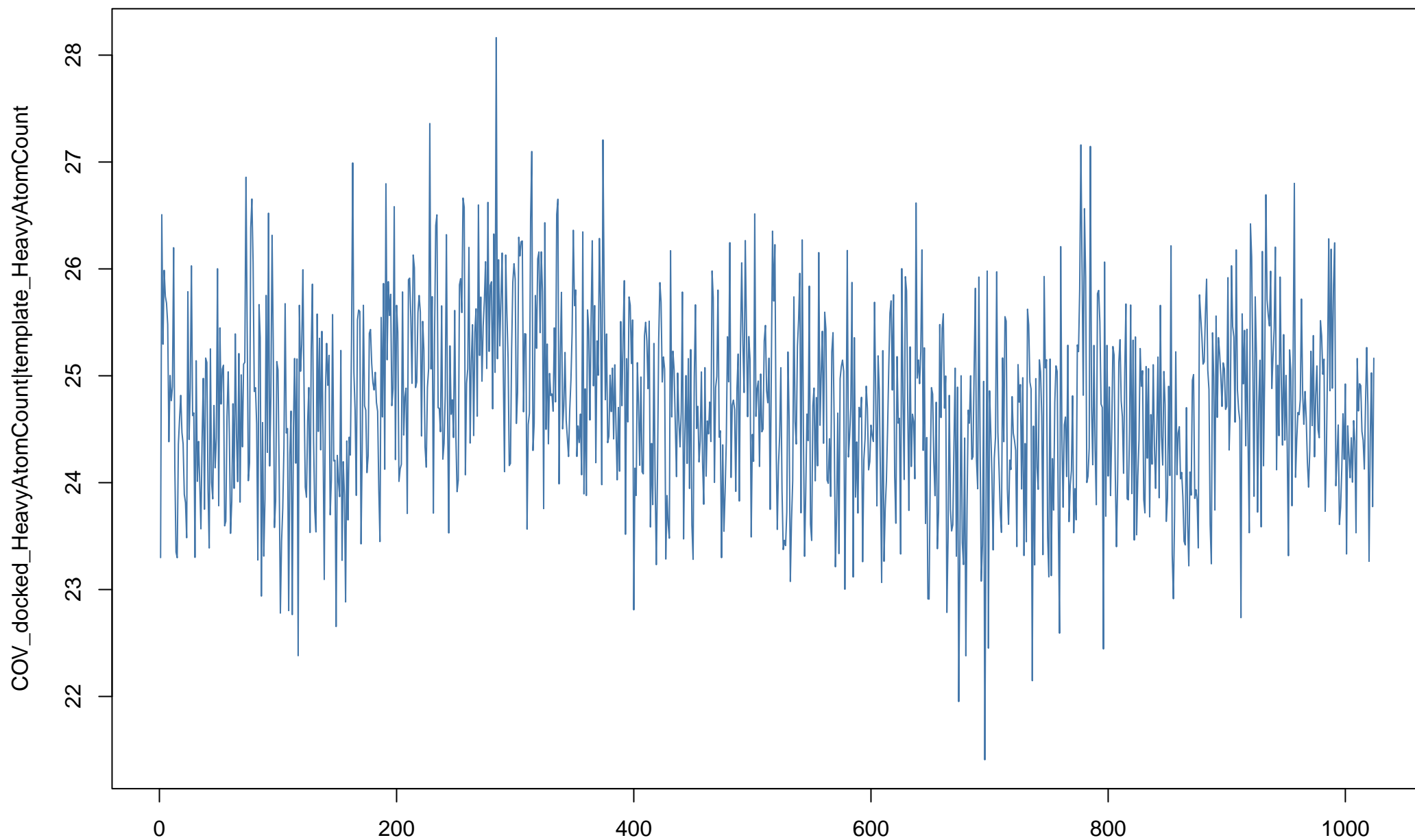
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 590 | BMK = 0.0873 | MCSE(6.27) = 5 | stat: FALSE | burn: 0



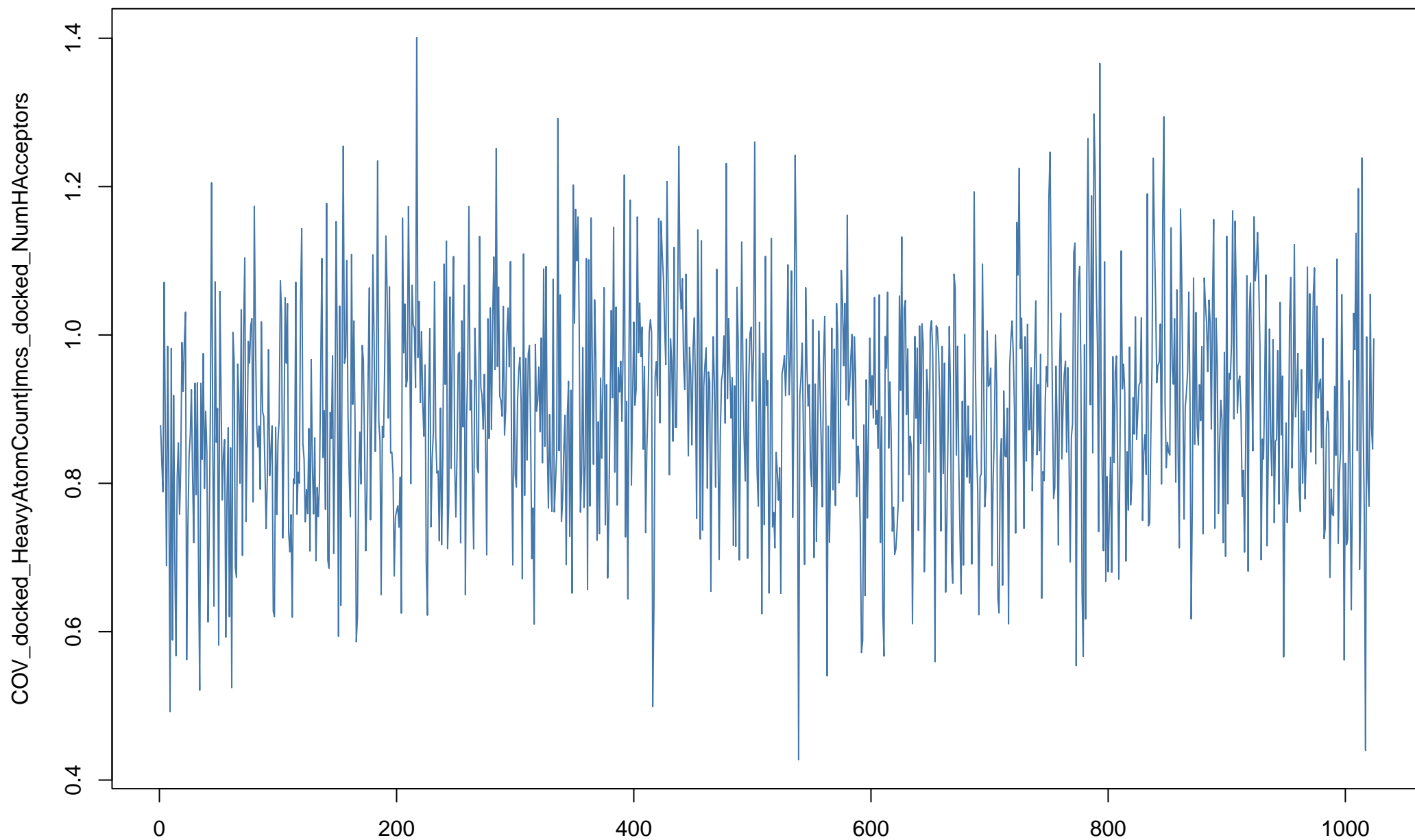
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 349 | BMK = 0.154 | MCSE(6.27) = 5.83 | stat: FALSE | burn: 0



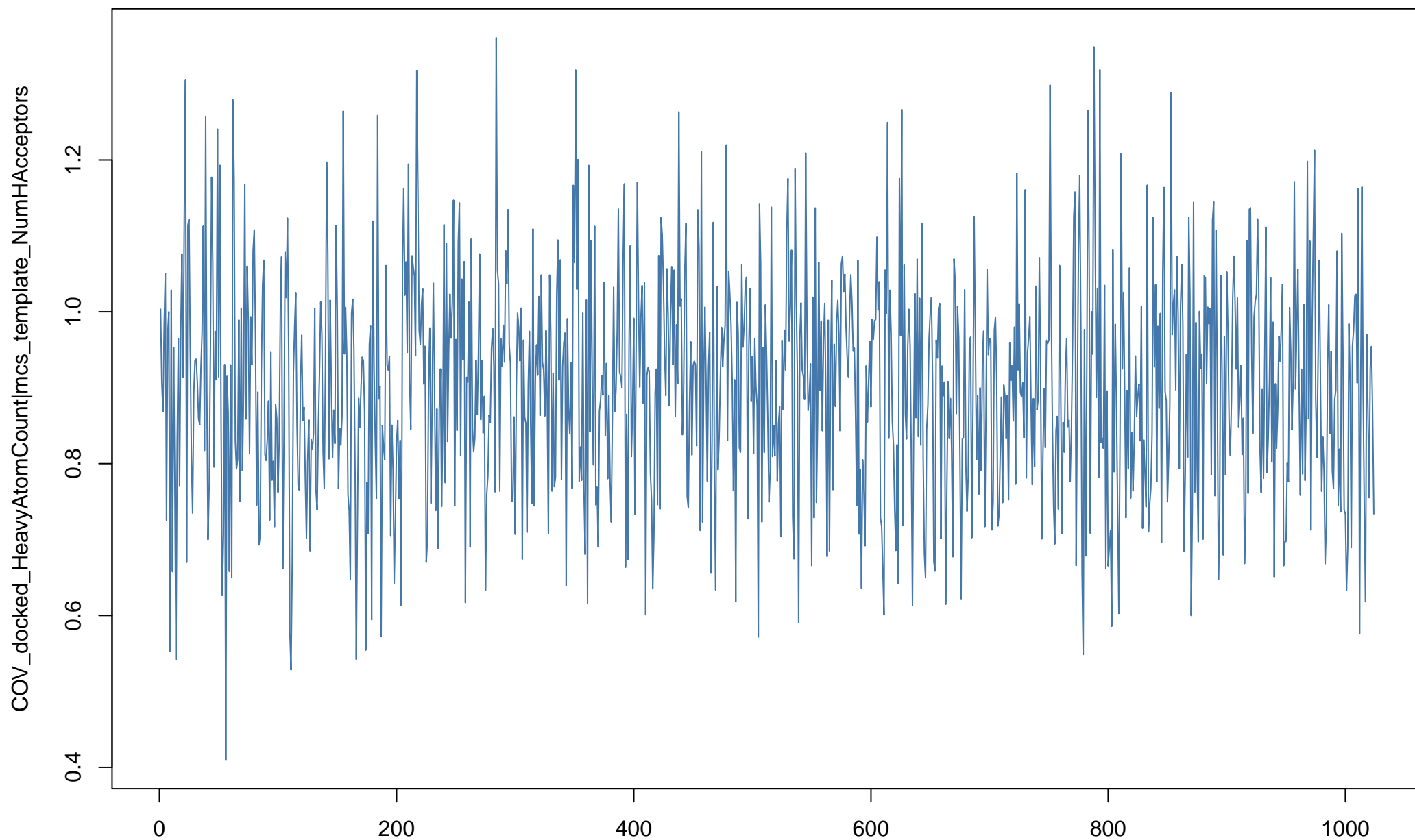
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 85 | BMK = 0.119 | MCSE(6.27) = 6.79 | stat: TRUE | burn: 0



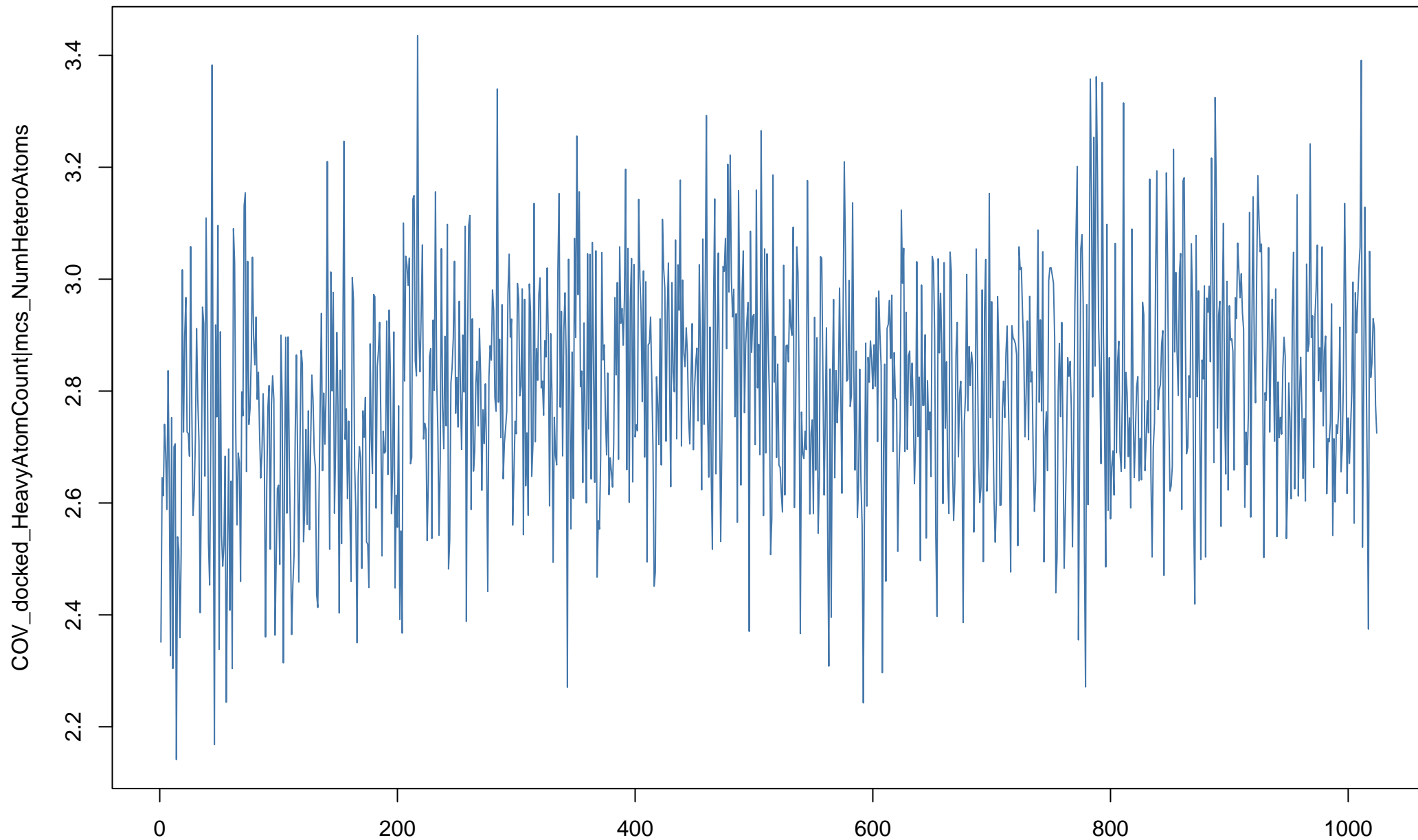
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 542 | BMK = 0.0246 | MCSE(6.27) = 4.49 | stat: FALSE | burn: 0



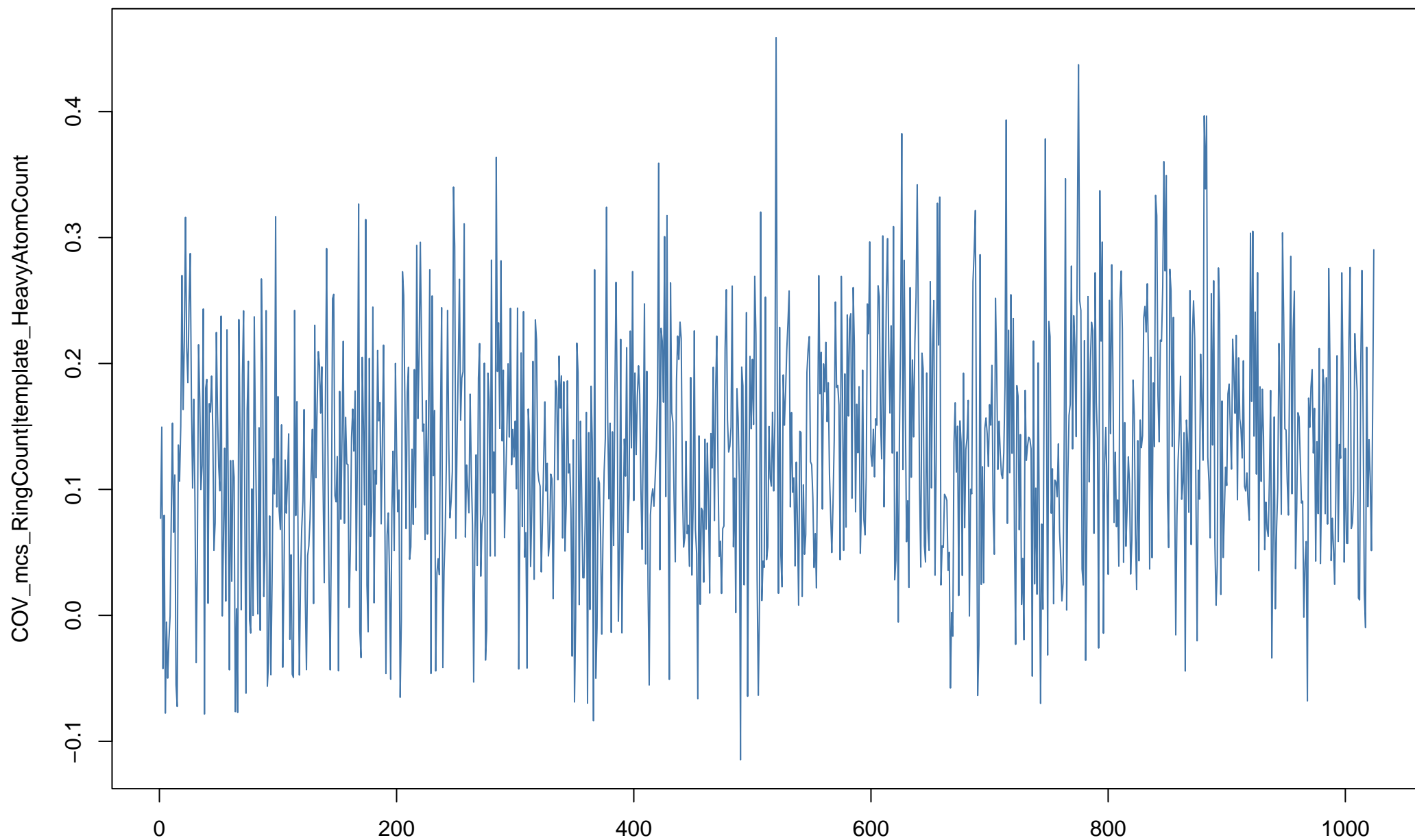
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 884 | BMK = 0.051 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0



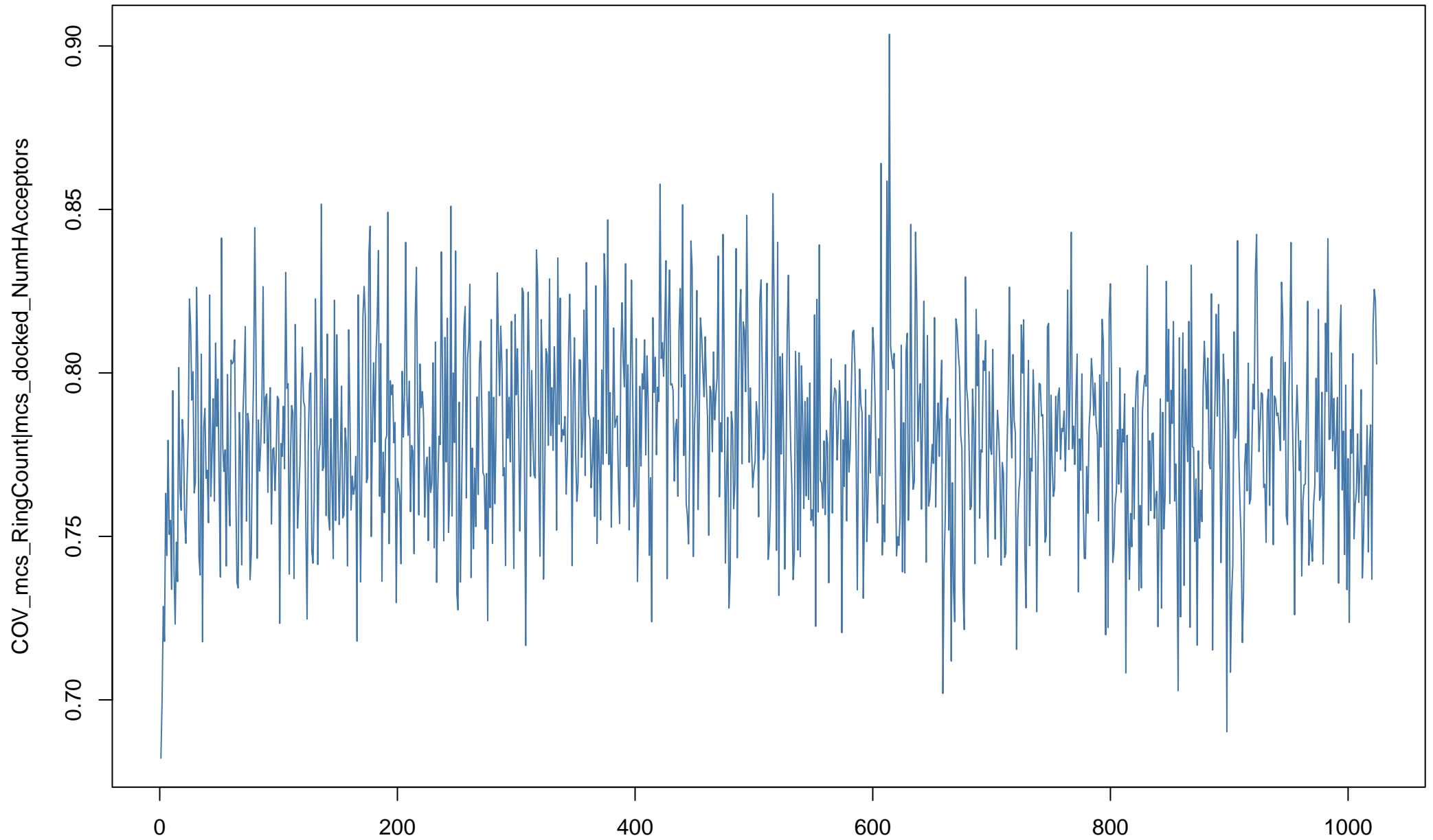
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 374 | BMK = 0.0717 | MCSE(6.27) = 5.58 | stat: FALSE | burn: 0



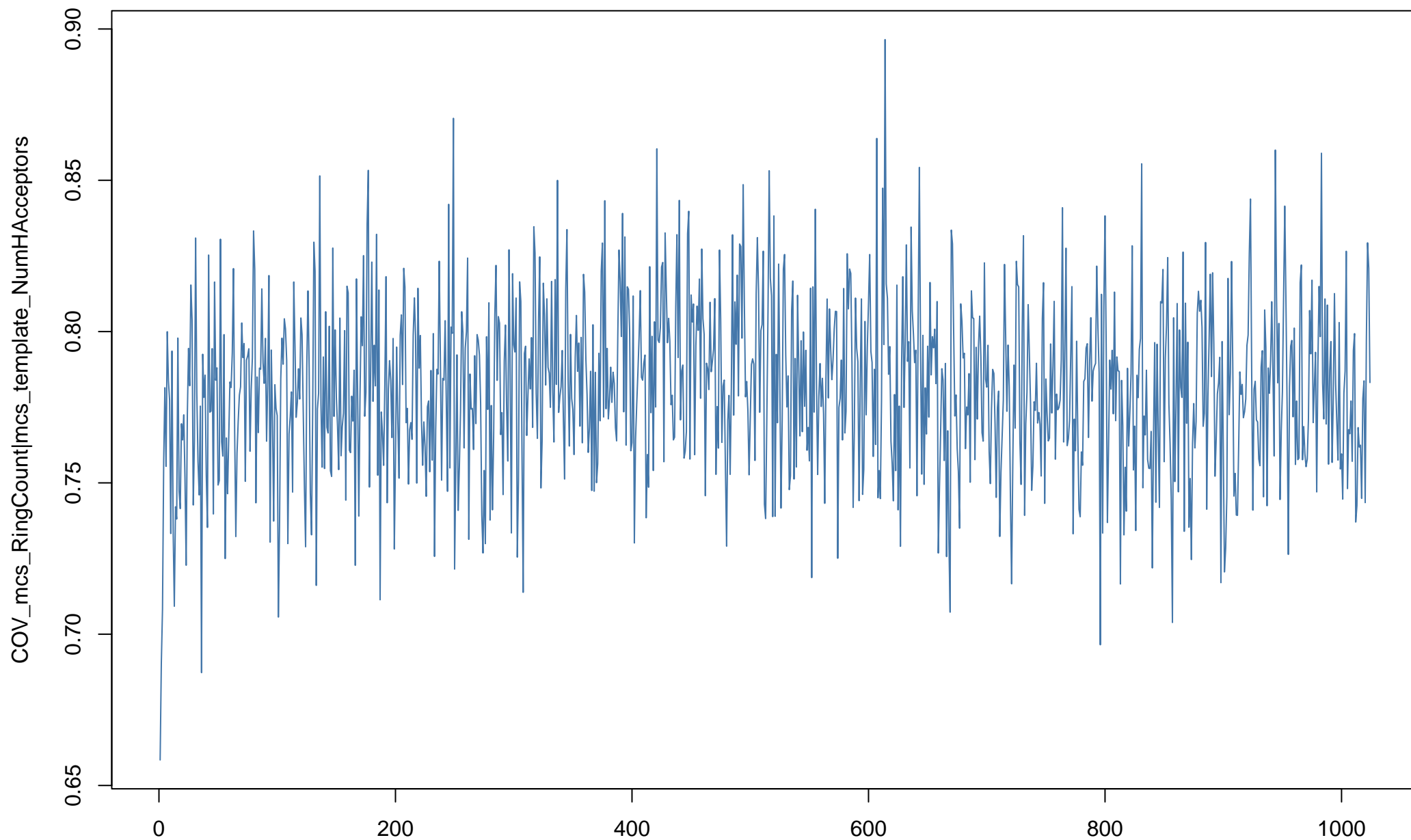
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 467 | BMK = 0.127 | MCSE(6.27) = 4.8 | stat: FALSE | burn: 0



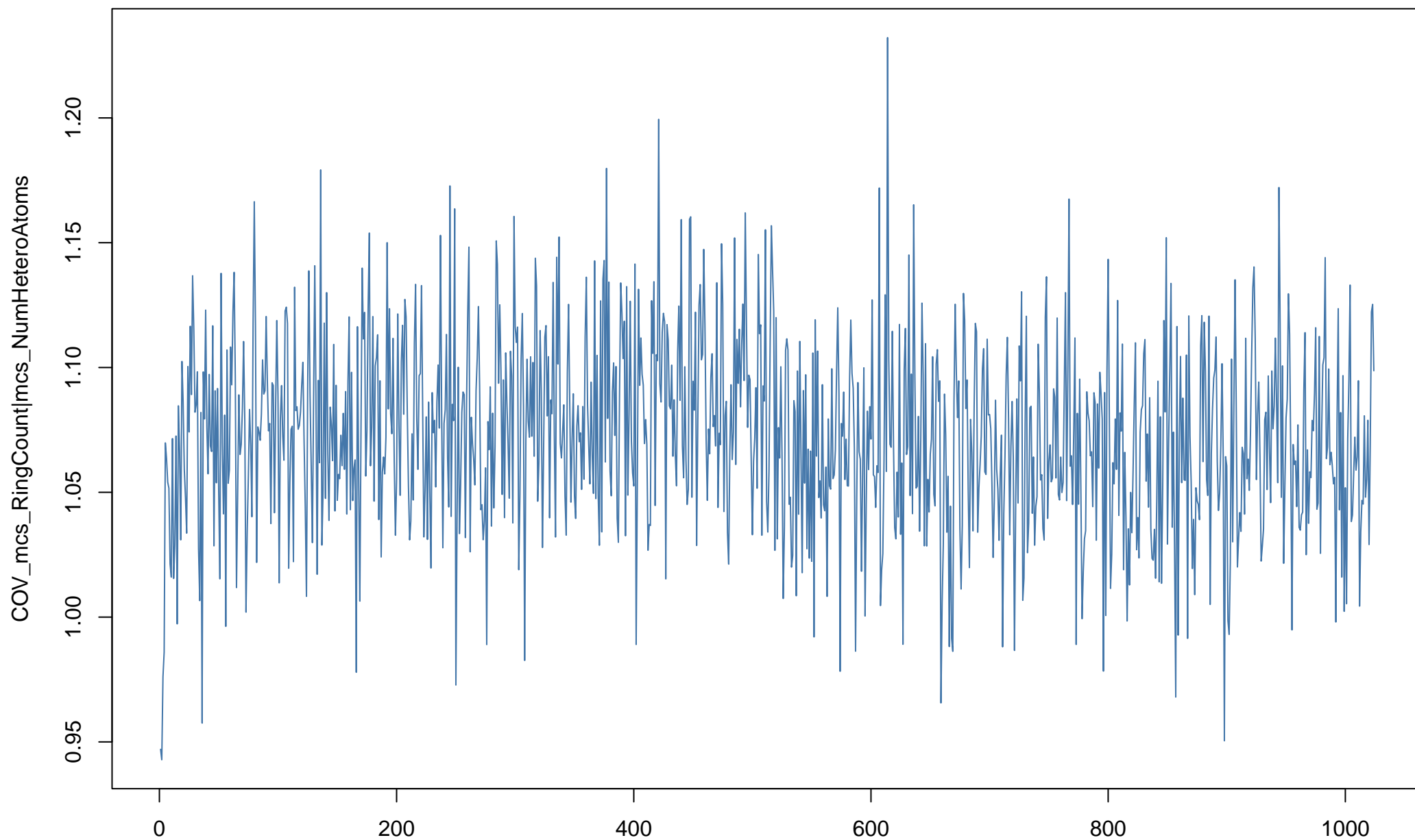
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 870 | BMK = 0.0807 | MCSE(6.27) = 4.15 | stat: TRUE | burn: 0



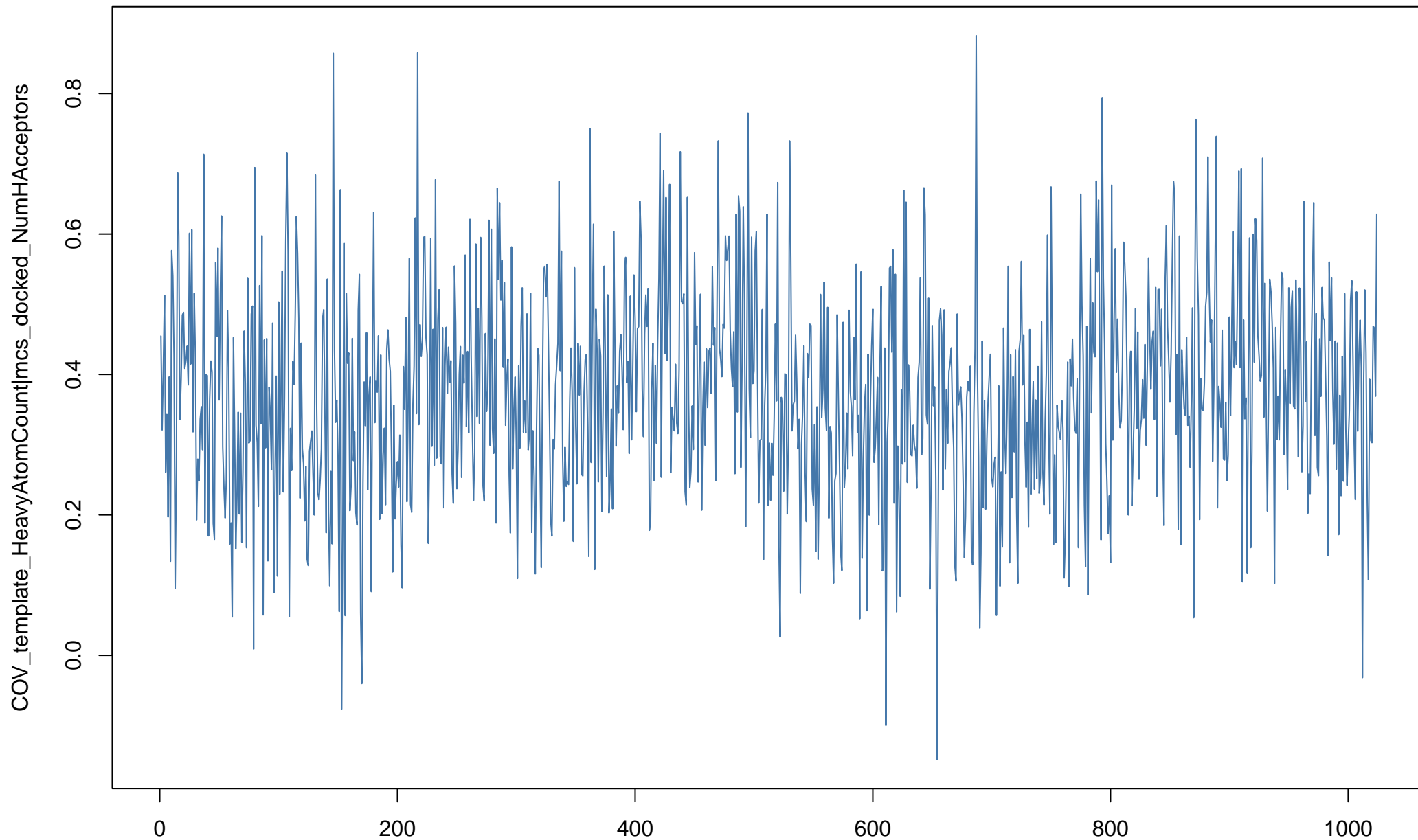
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 836 | BMK = 0.0545 | MCSE(6.27) = 4.27 | stat: FALSE | burn: 0



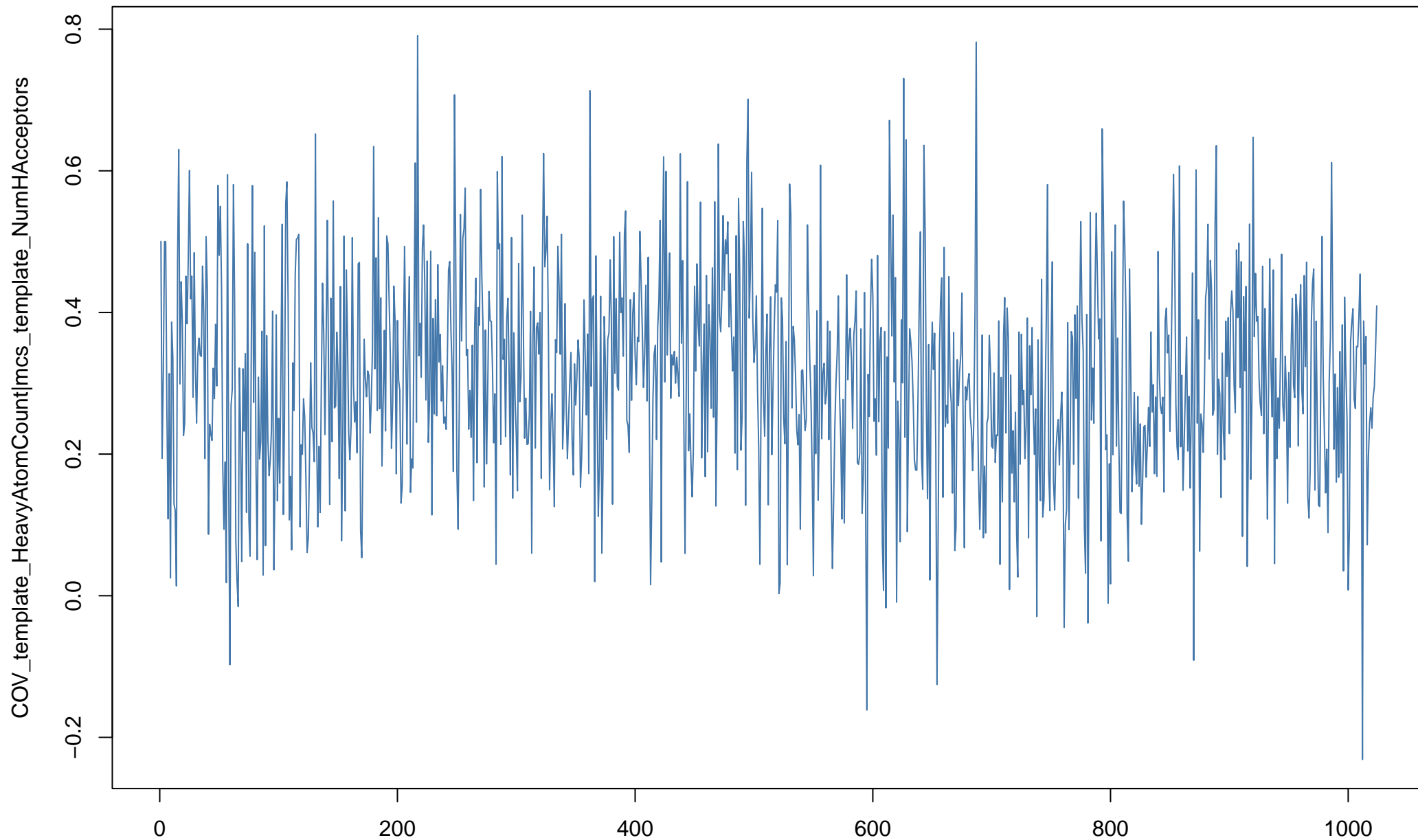
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 800 | BMK = 0.142 | MCSE(6.27) = 4.66 | stat: TRUE | burn: 0



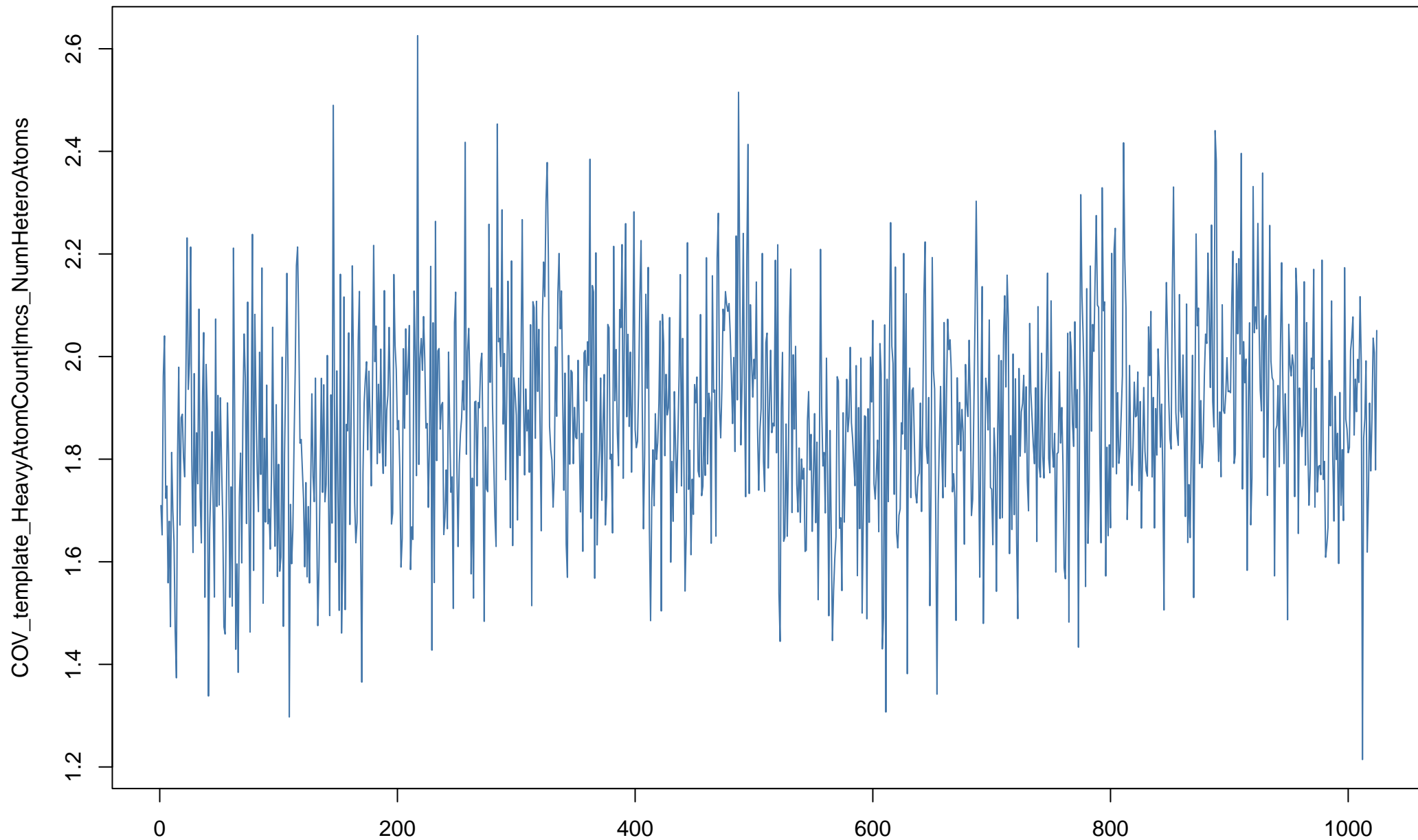
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 571 | BMK = 0.0635 | MCSE(6.27) = 4.92 | stat: TRUE | burn: 0



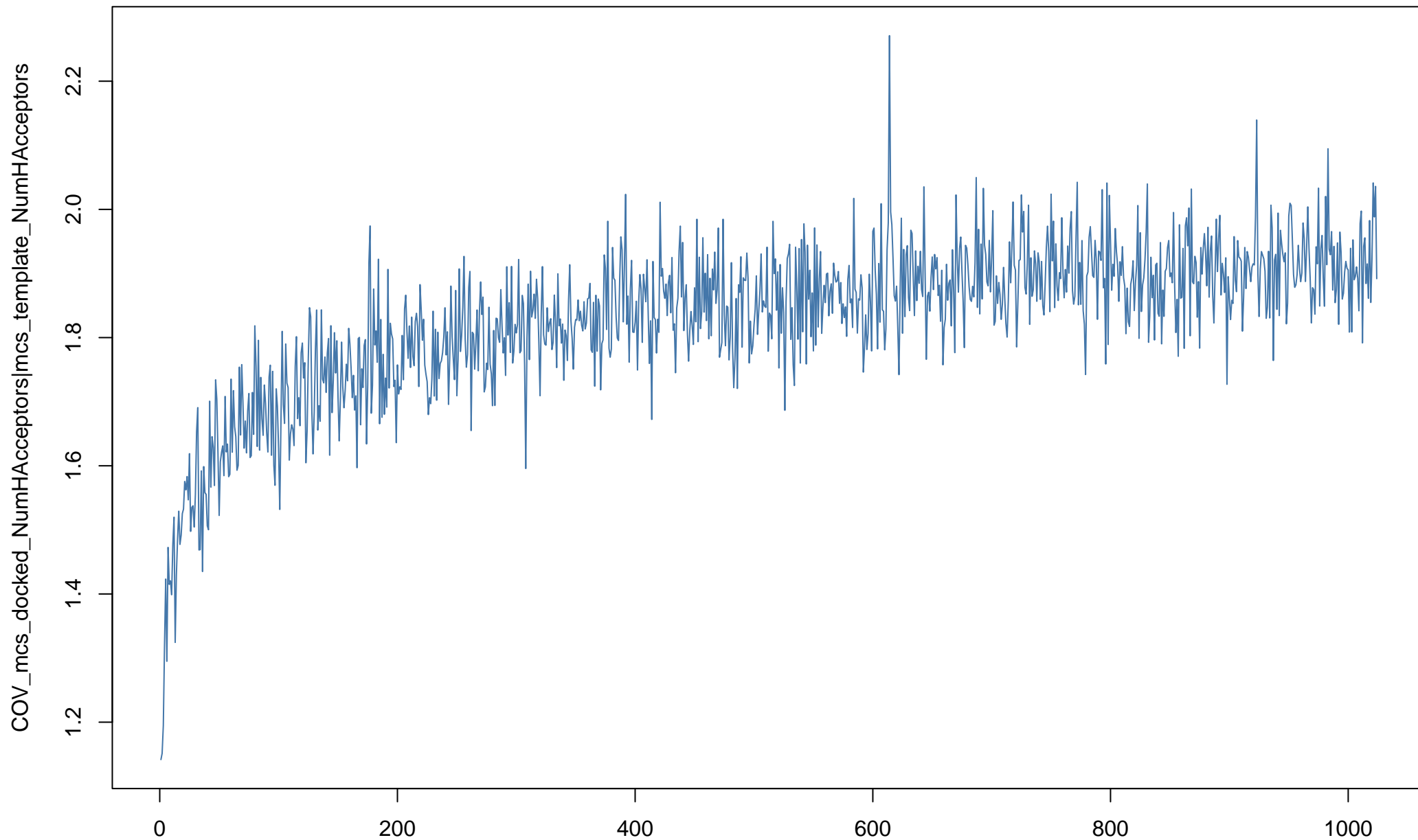
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 834 | BMK = 0.109 | MCSE(6.27) = 4.59 | stat: TRUE | burn: 0



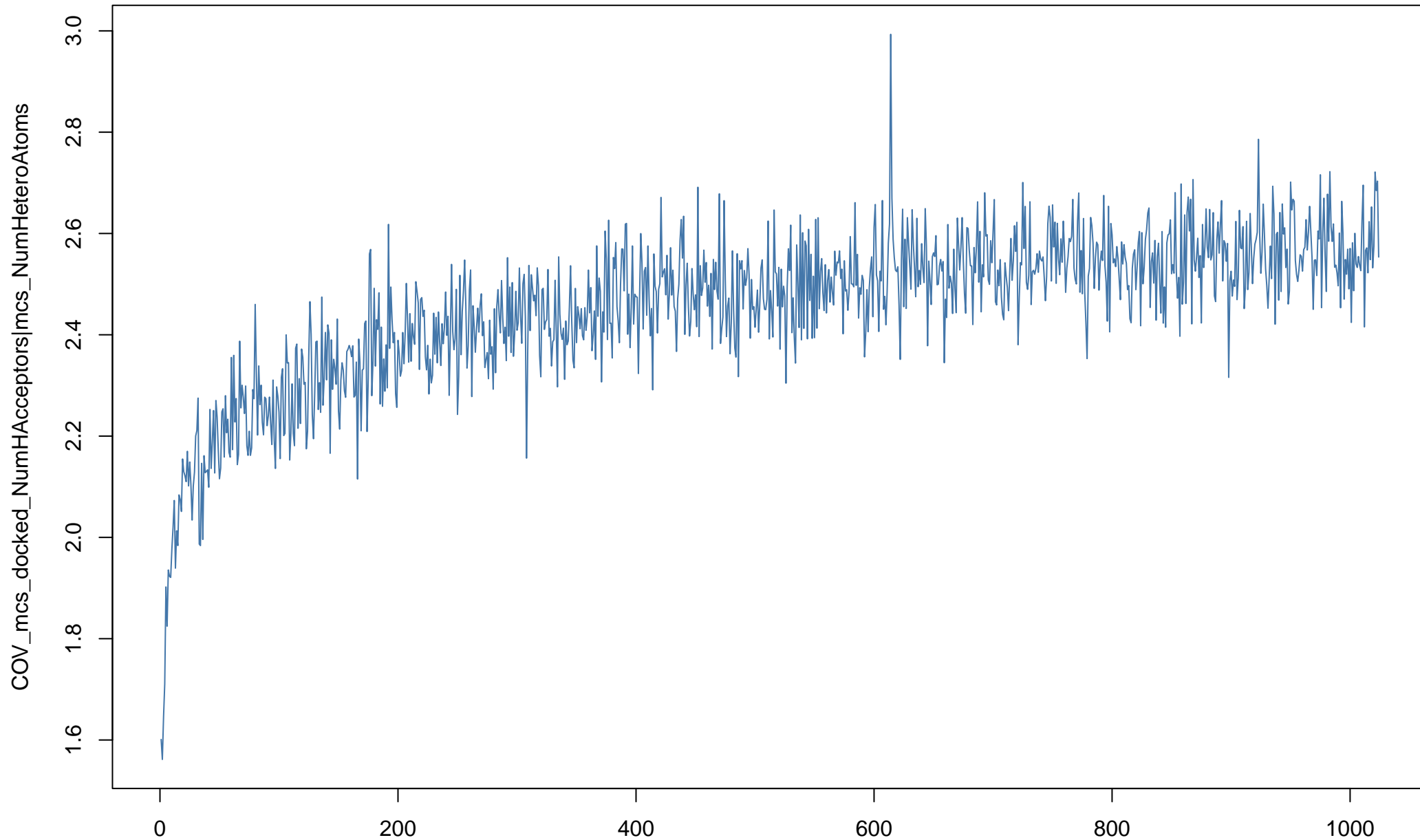
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 258 | BMK = 0.0642 | MCSE(6.27) = 5.69 | stat: FALSE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 10.5 | BMK = 0.506 | MCSE(6.27) = 14.9 | stat: FALSE | burn: 102



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 10.2 | BMK = 0.536 | MCSE(6.27) = 15.2 | stat: FALSE | burn: 102



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 10.2 | BMK = 0.519 | MCSE(6.27) = 15 | stat: FALSE | burn: 102

