

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.931894023232706

max MCSE = 17.7650666195848

all stationary: FALSE

burn: 1020

-- STATS 2D --

min ESS = 9.92197848642884

max BMK = 0.458038739549057

max MCSE = 14.6172331298776

all stationary: FALSE

burn: 204

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.524517028214303

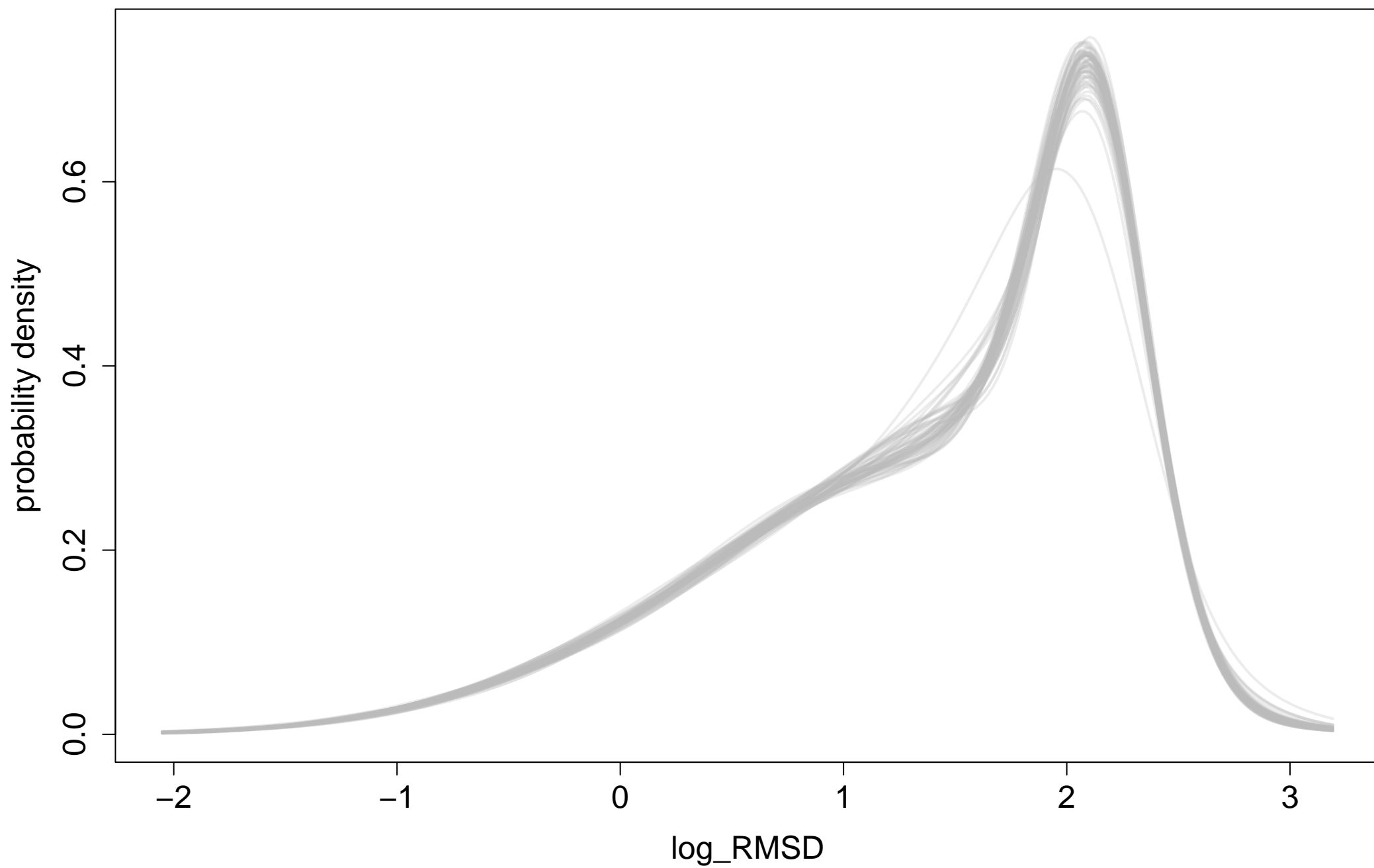
max MCSE = NaN

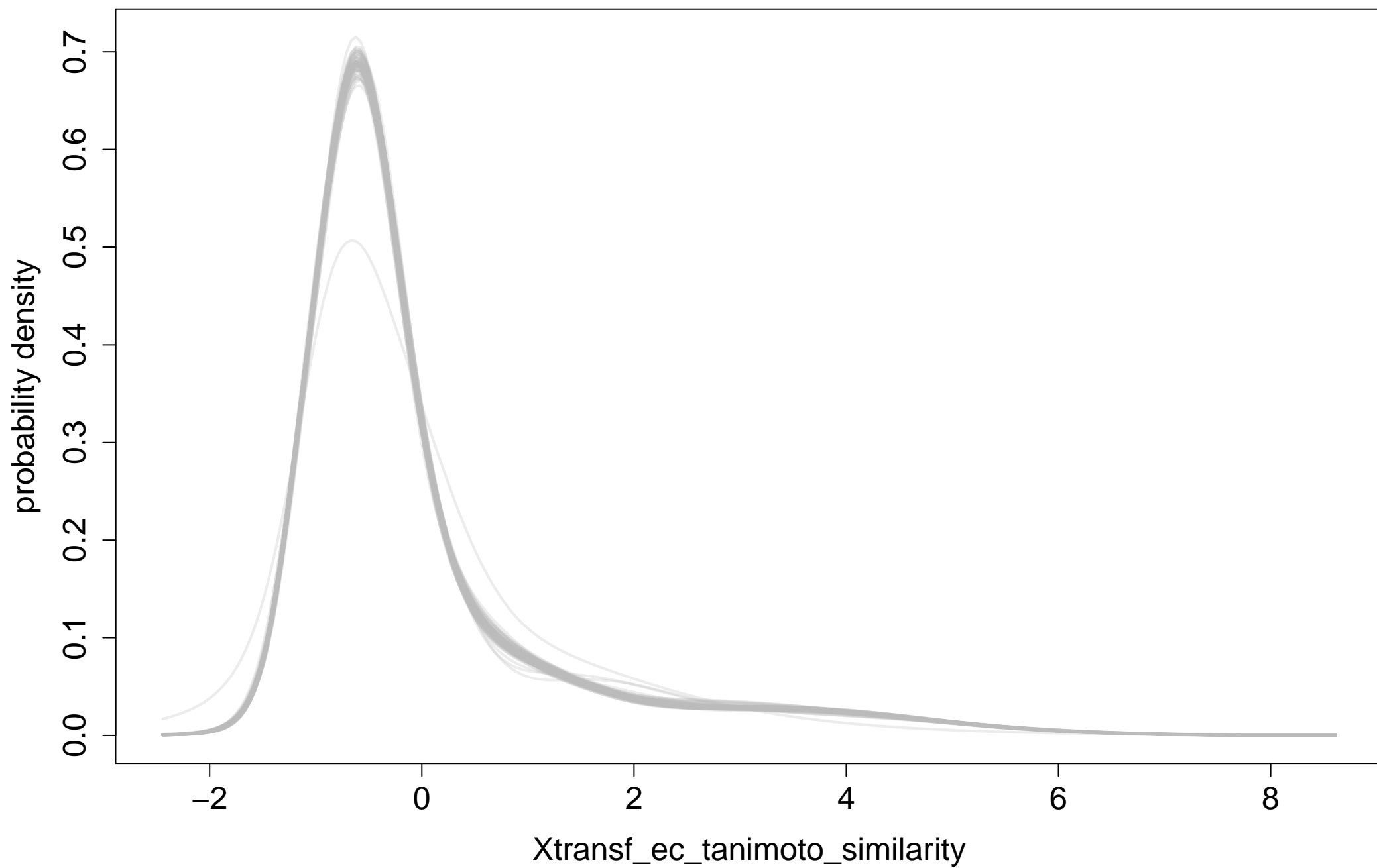
all stationary: FALSE

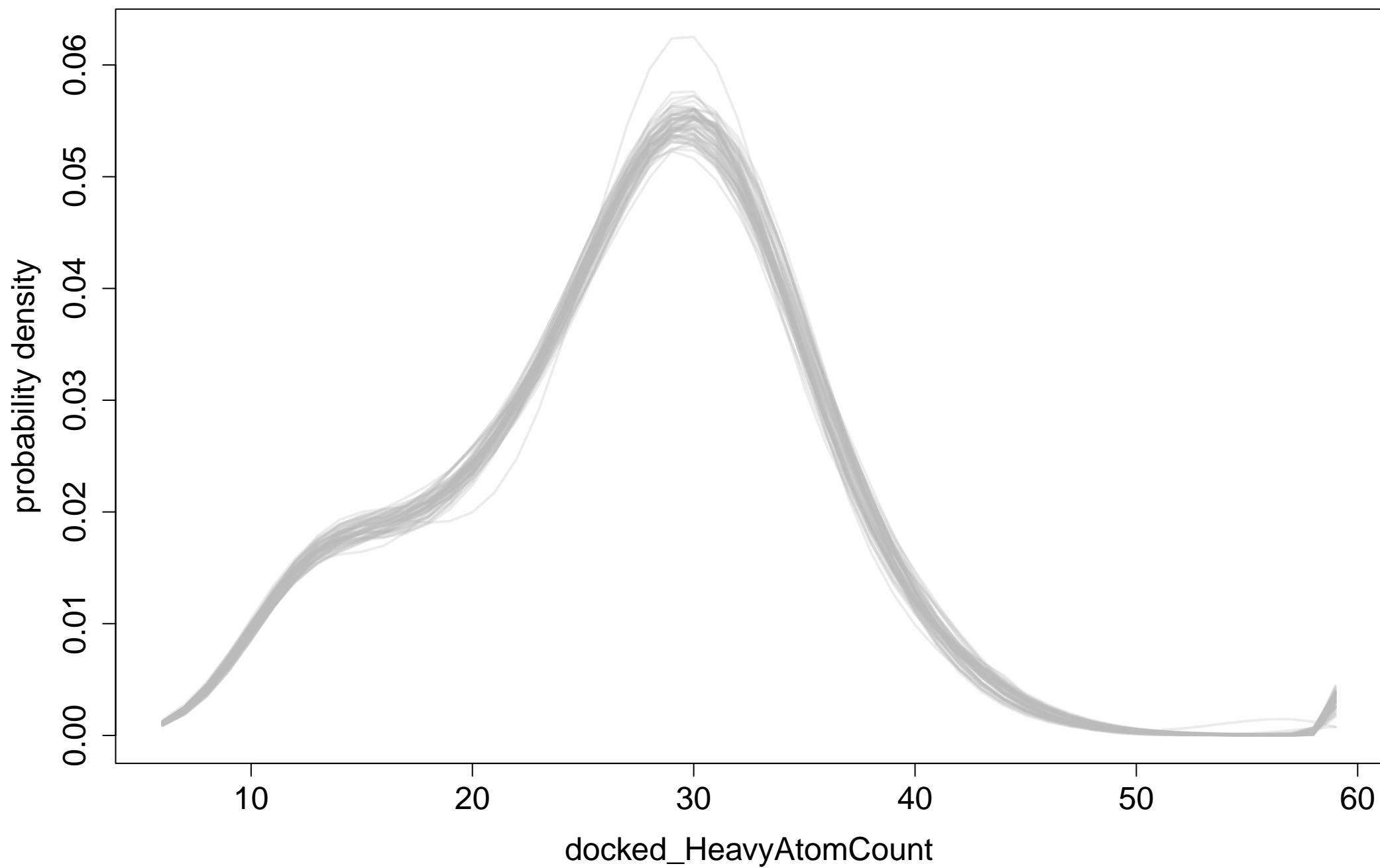
burn: 102

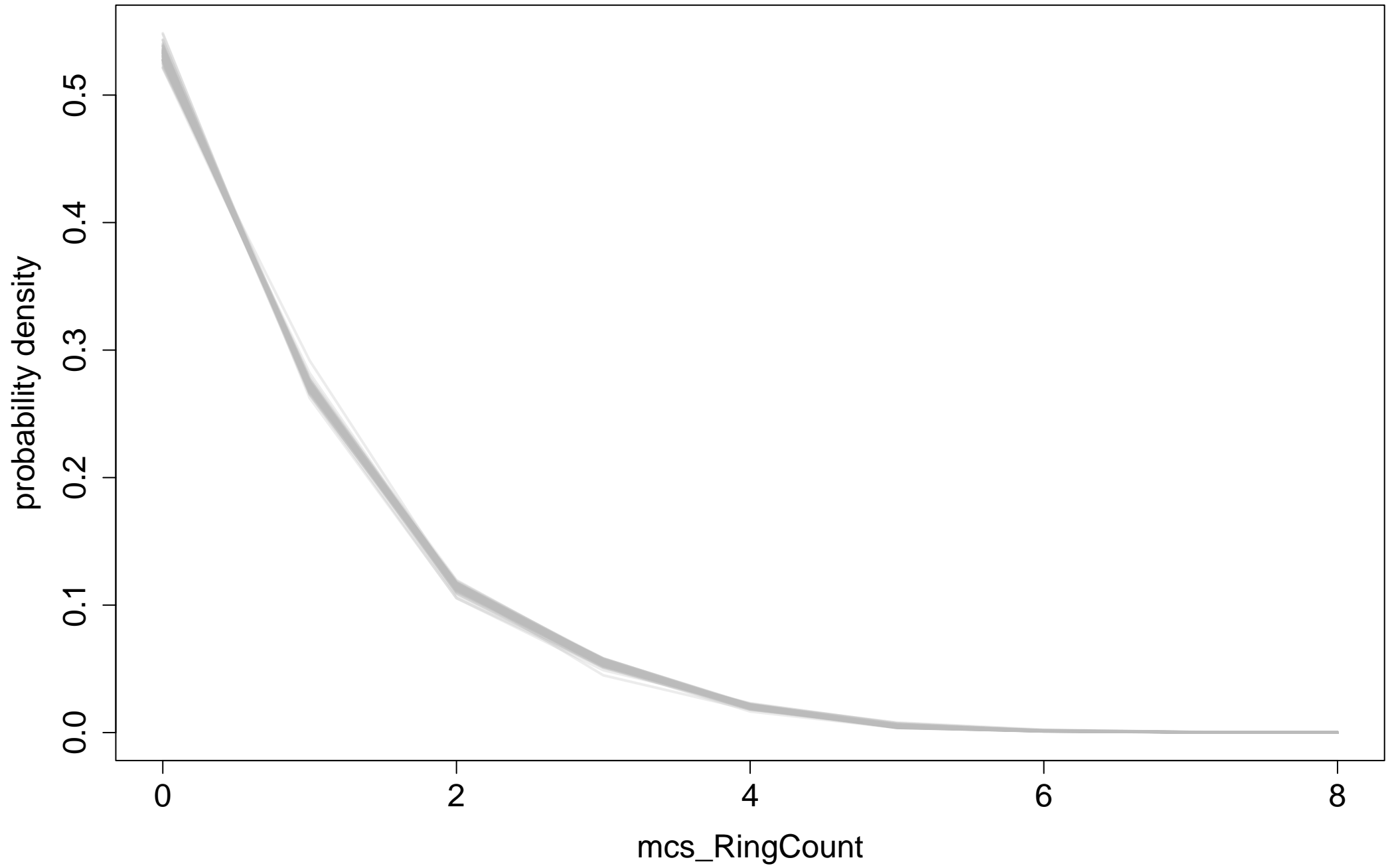
Occupied clusters: 32 of 91

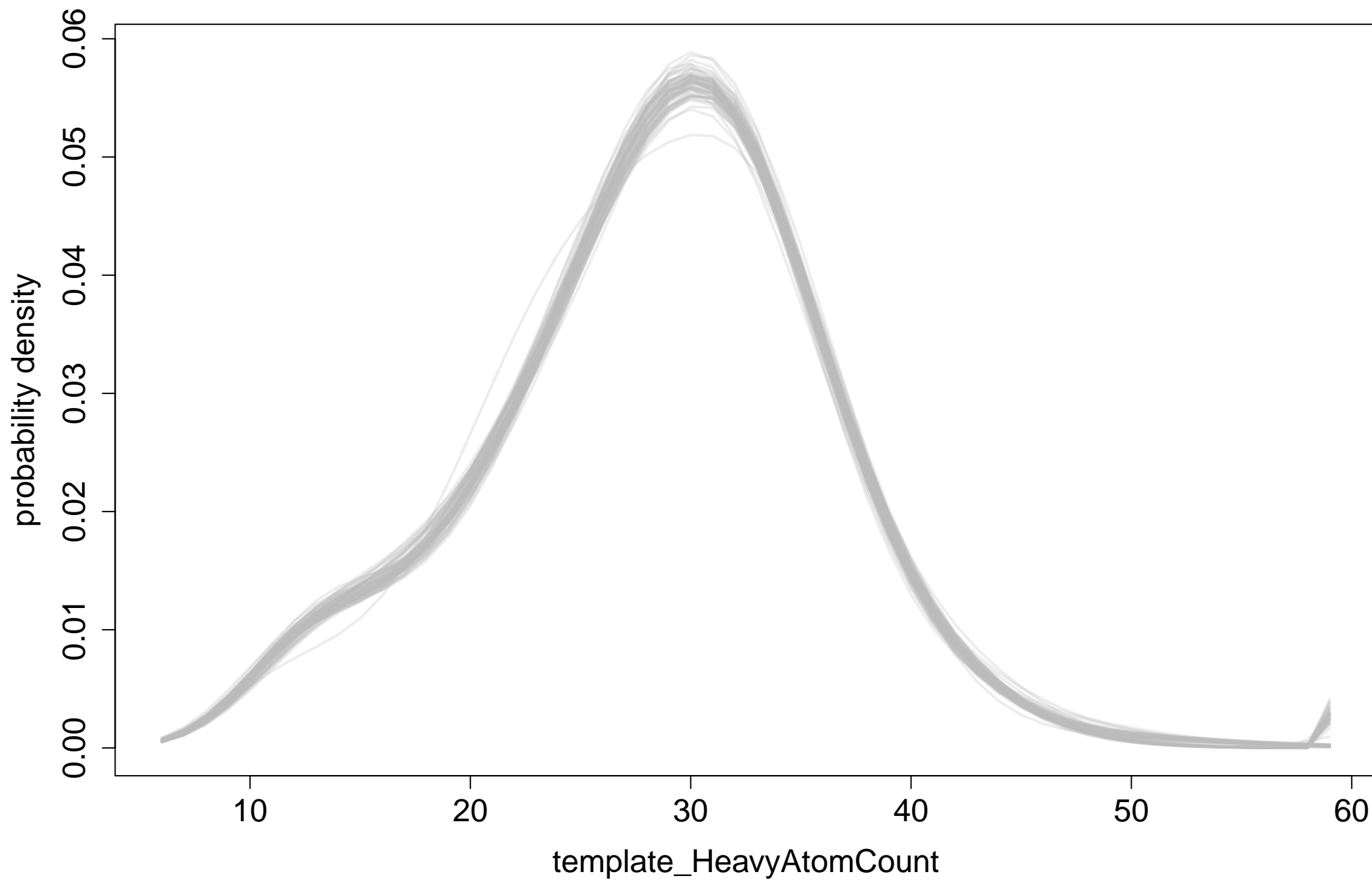
LL: -116000 +- 1230

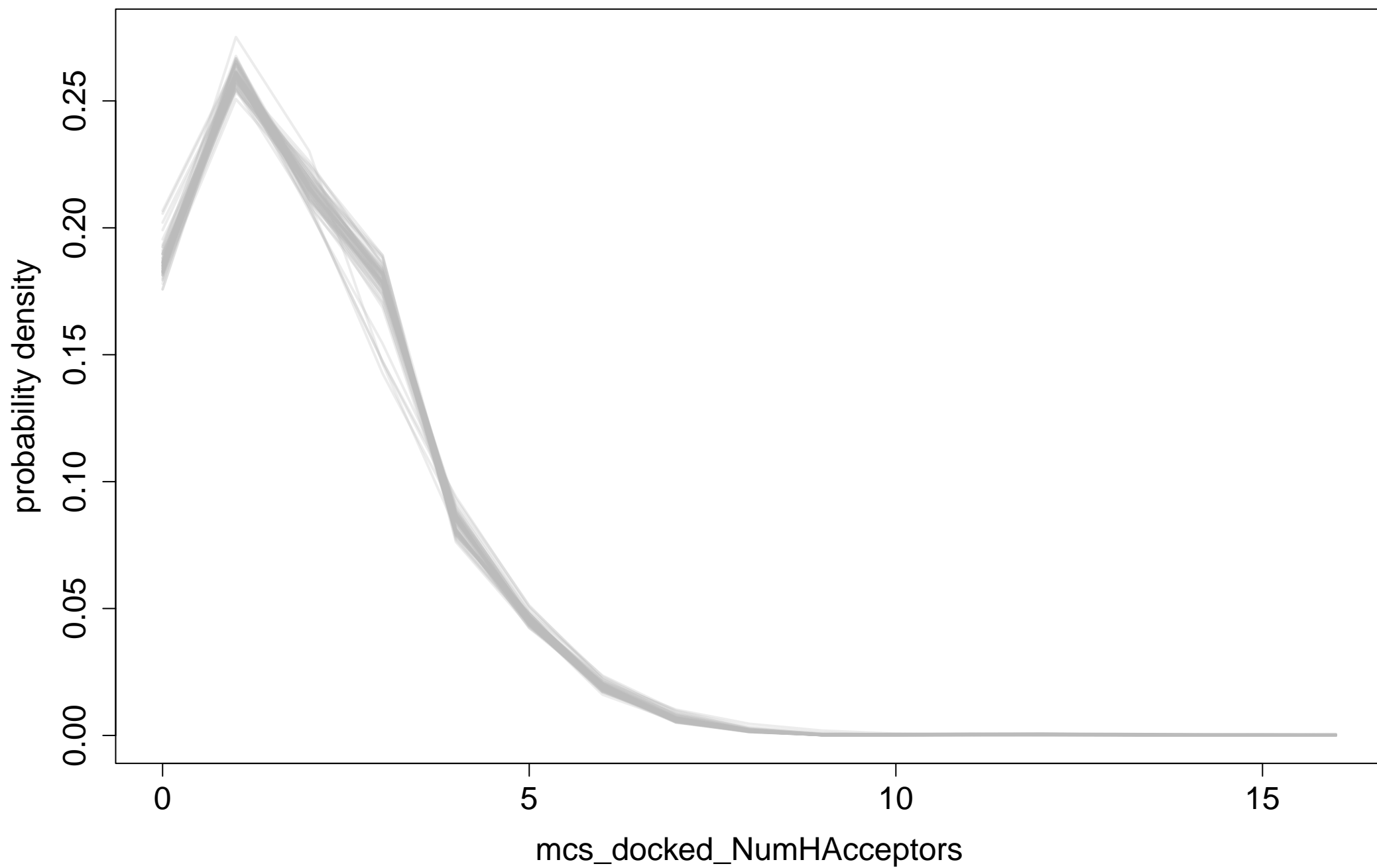


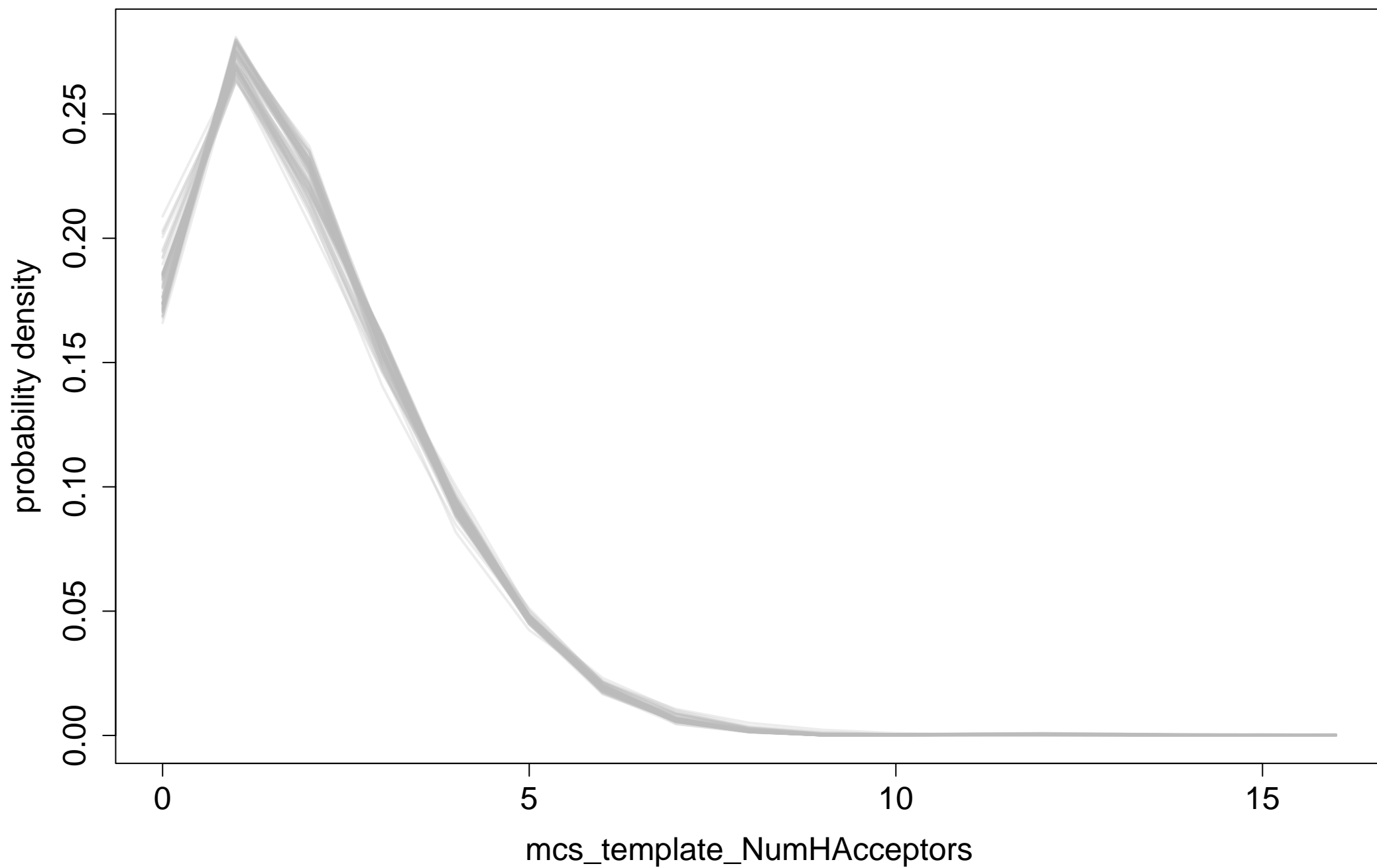


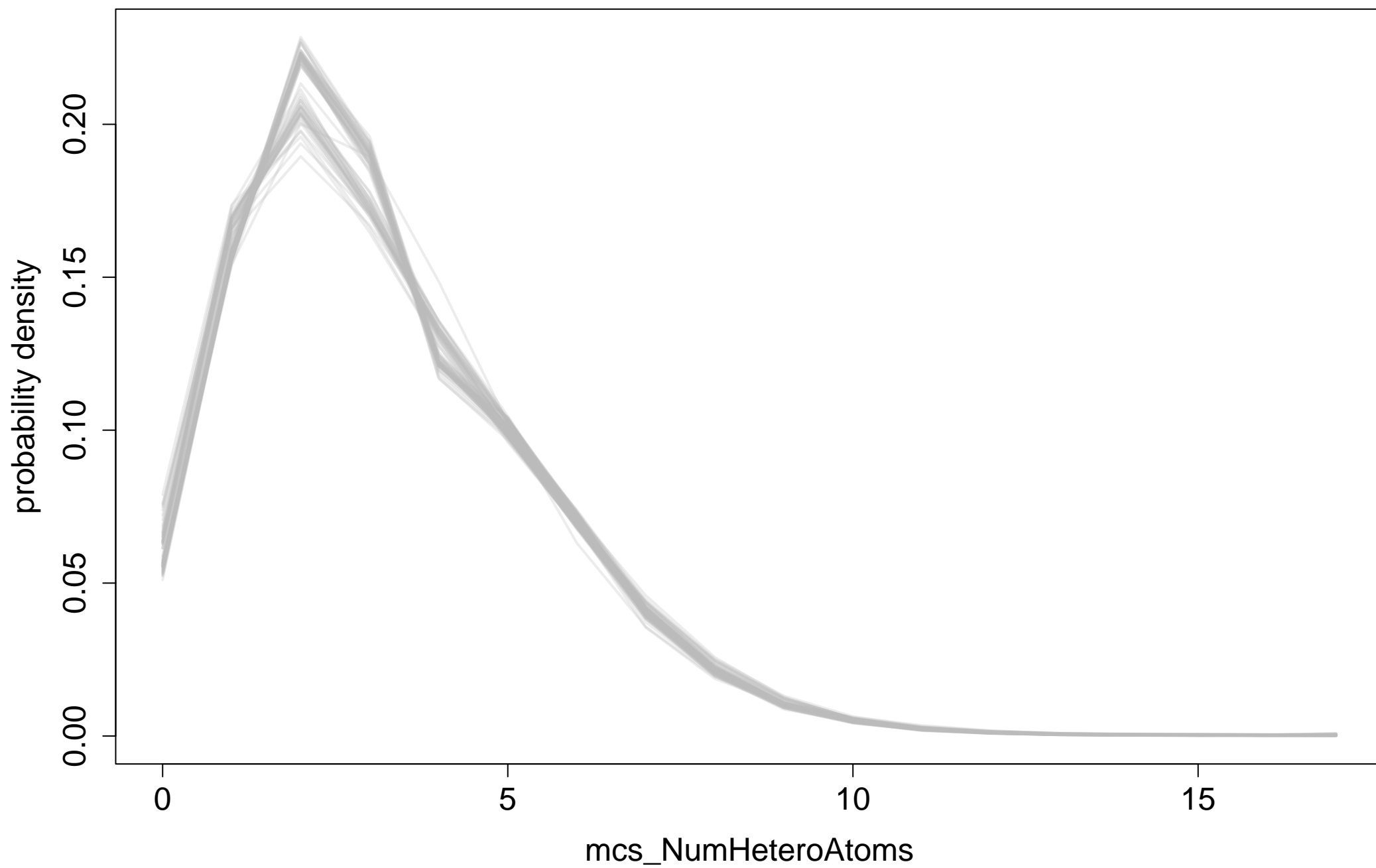


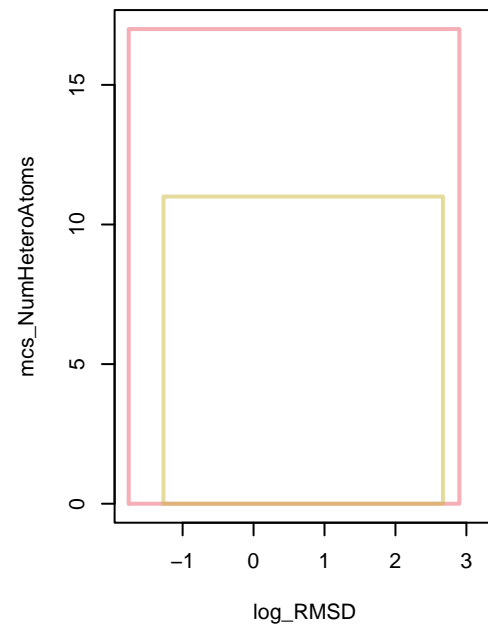
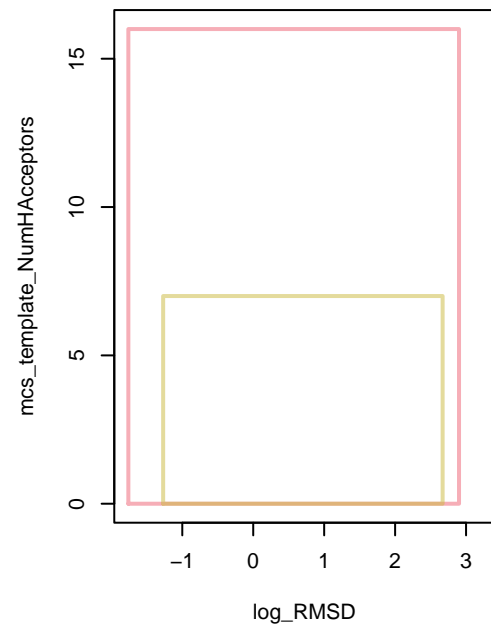
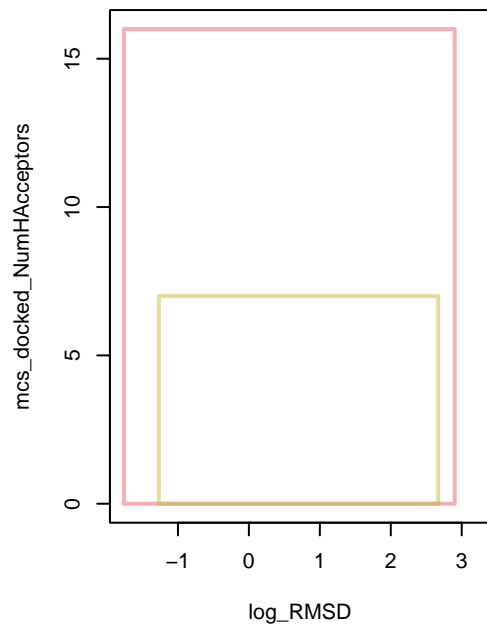
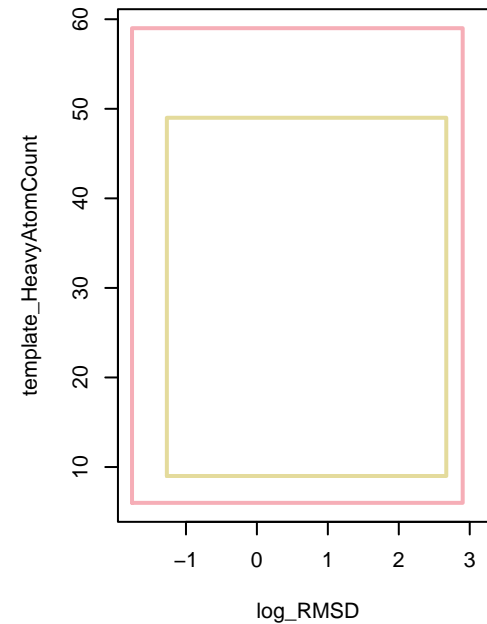
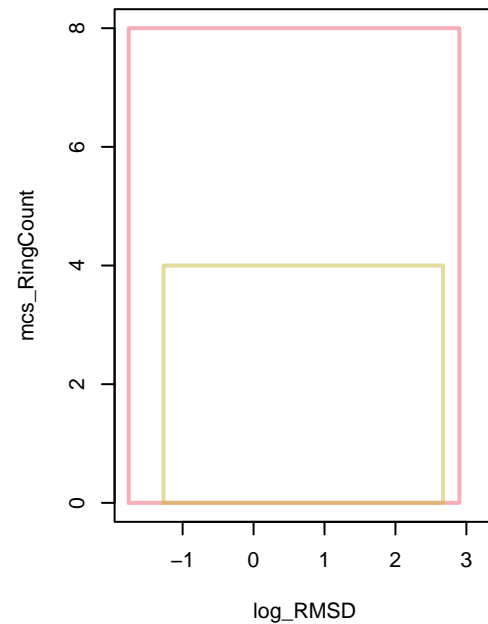
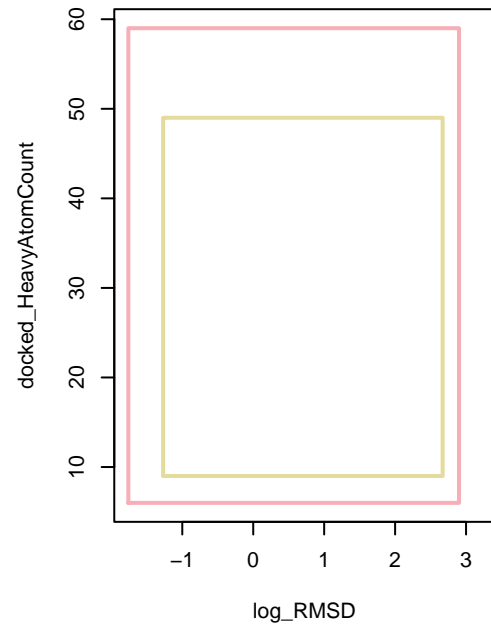
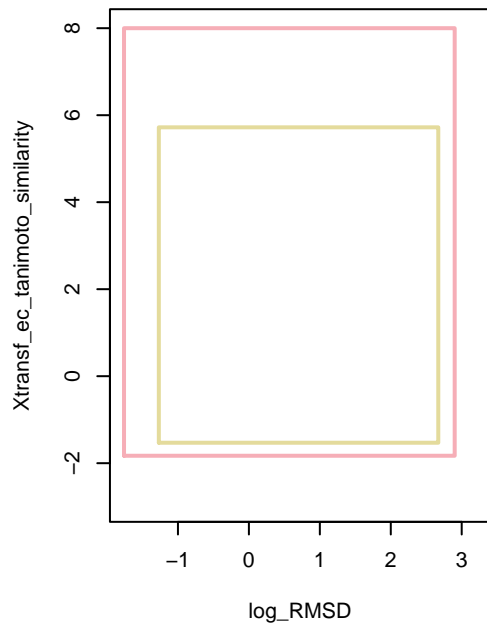




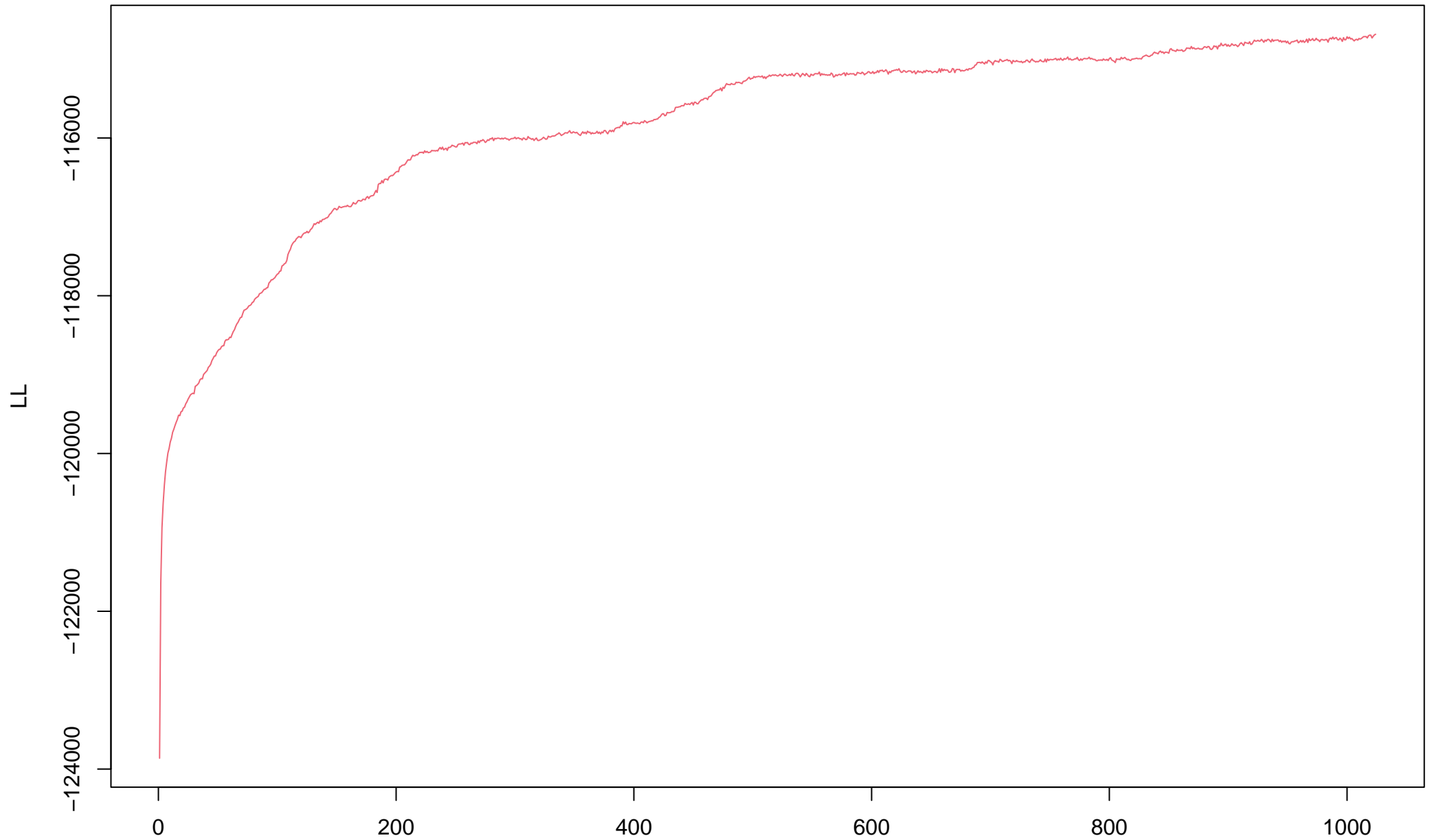




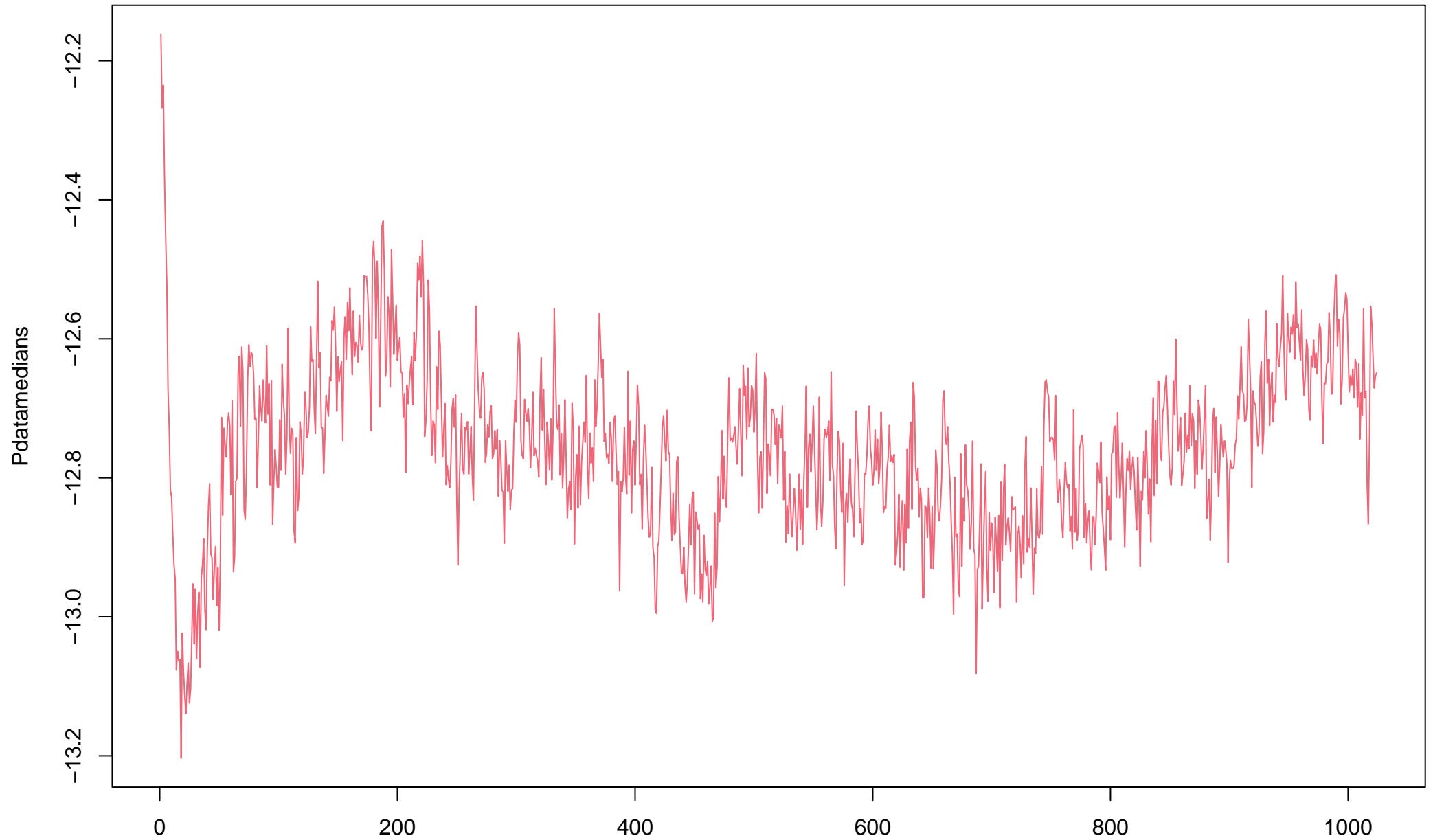




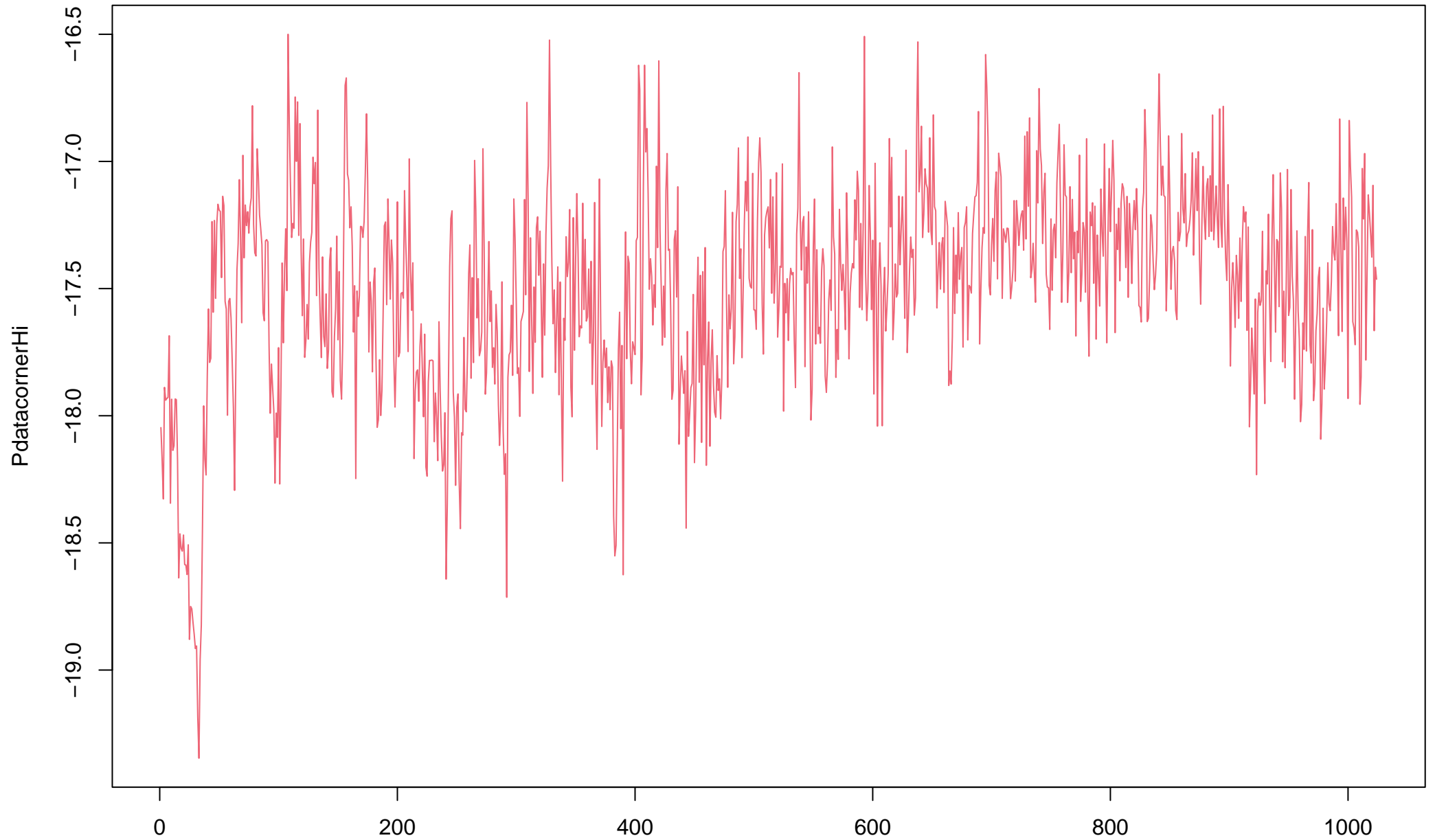
LL
ESS = 5.02 | BMK = 0.88 | MCSE(6.27) = 17.8 | stat: FALSE | burn: 1020



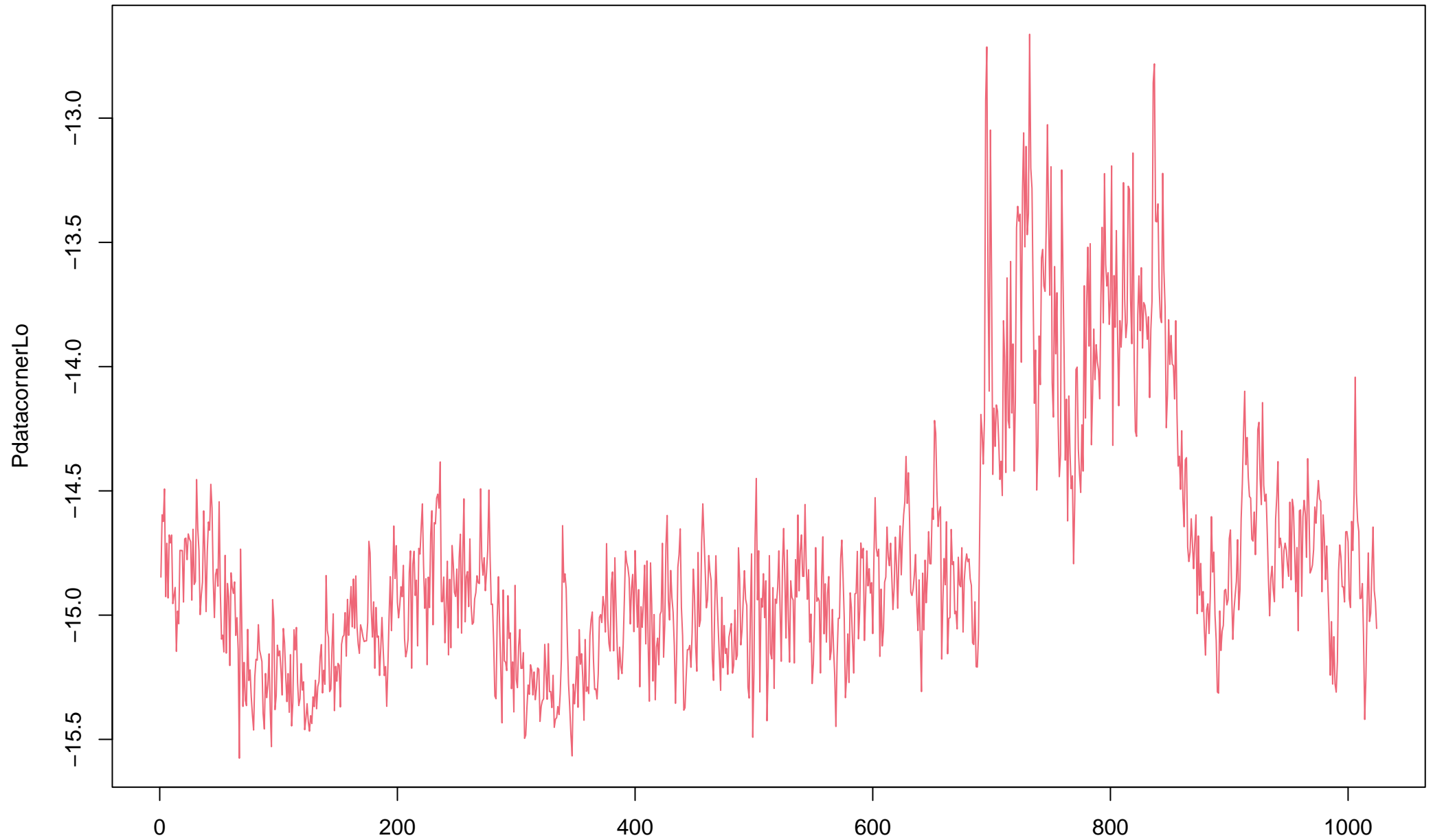
Pdatamedians
ESS = 32.9 | BMK = 0.187 | MCSE(6.27) = 12.4 | stat: TRUE | burn: 1020



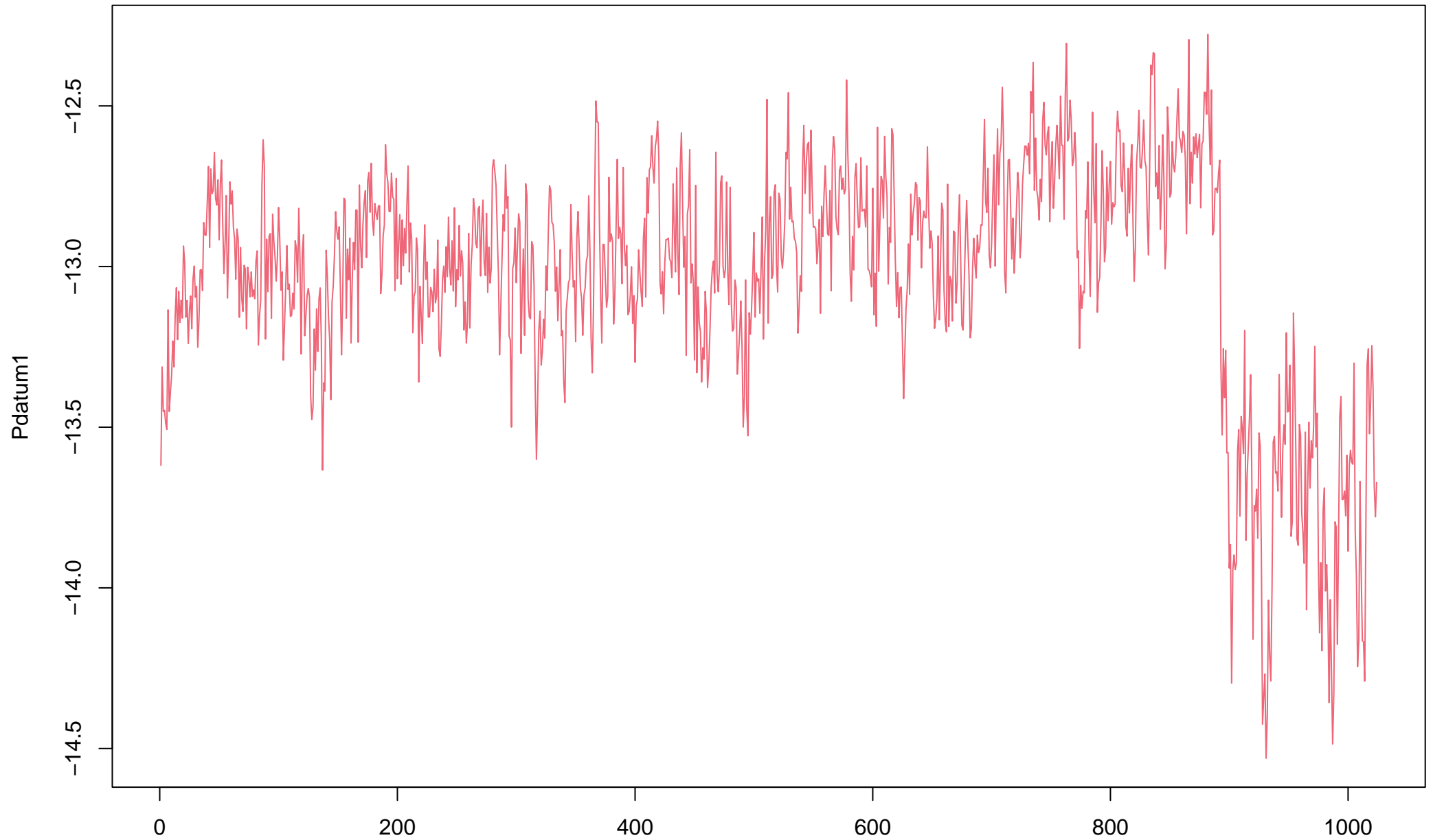
PdatacornerHi
ESS = 2.22e-16 | BMK = 0.294 | MCSE(6.27) = 9.53 | stat: FALSE | burn: 0



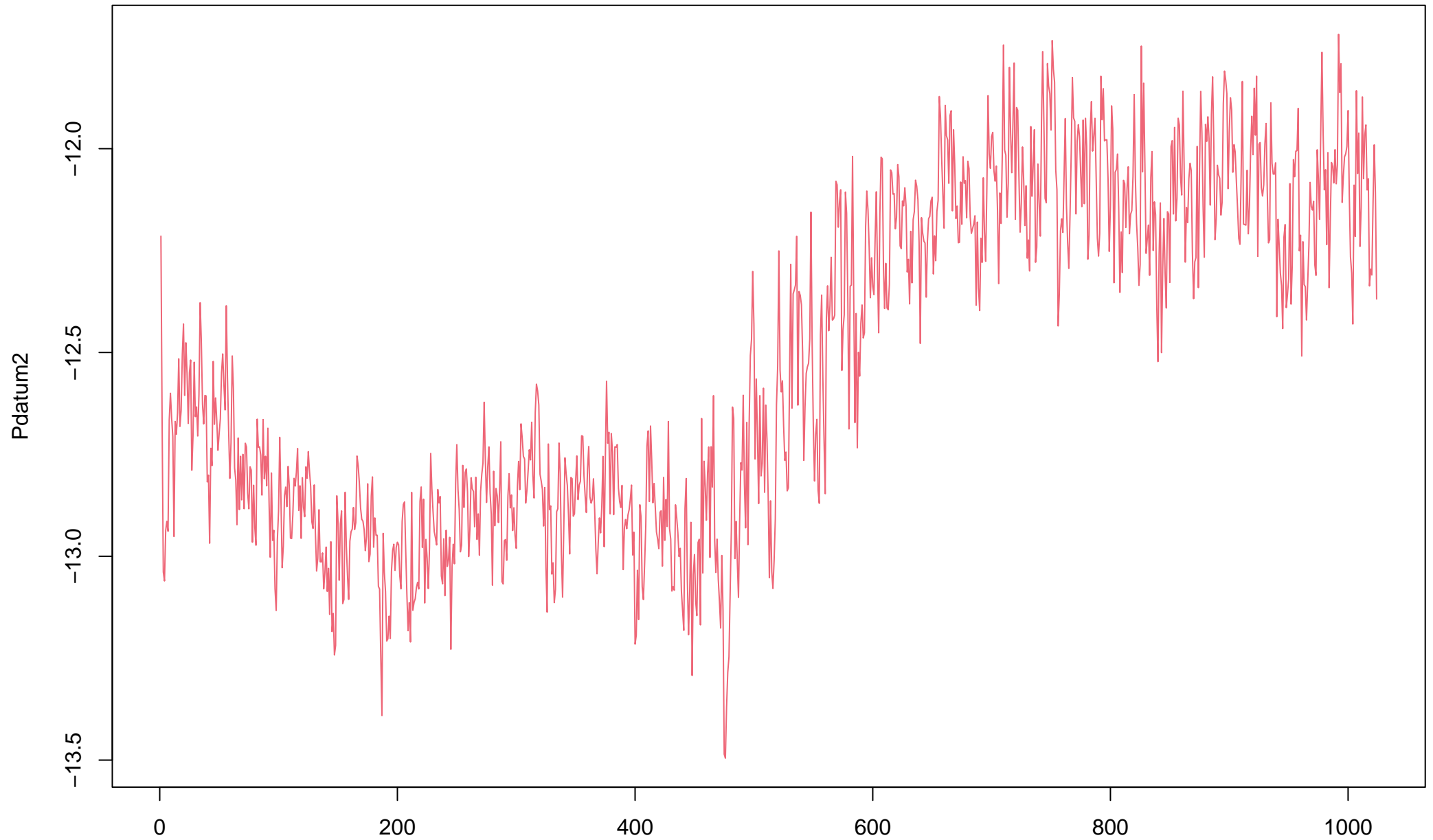
PdatacornerLo
ESS = 8.47 | BMK = 0.491 | MCSE(6.27) = 13.8 | stat: FALSE | burn: 714



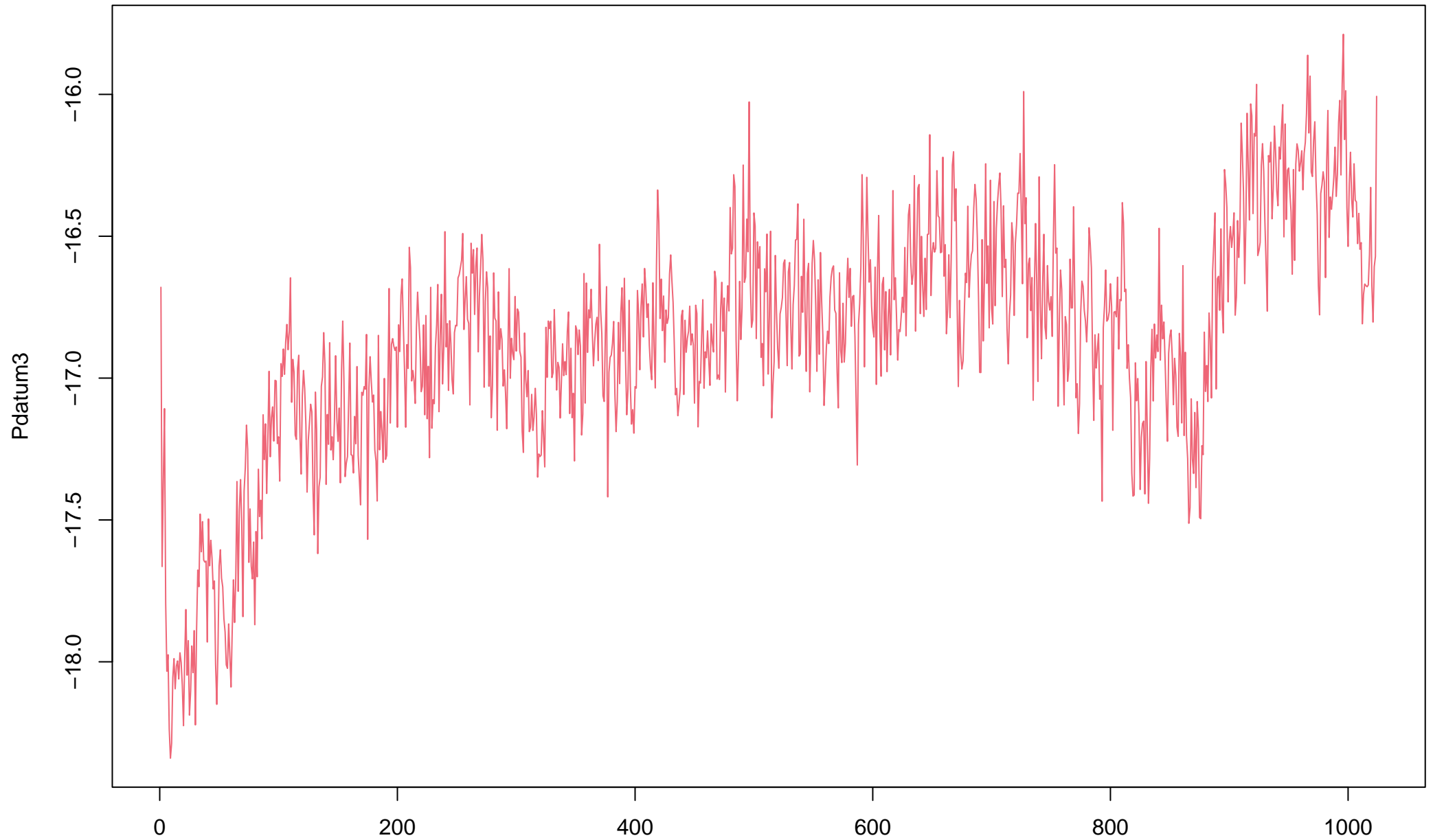
Pdatum1
ESS = 20.7 | BMK = 0.386 | MCSE(6.27) = 14.4 | stat: TRUE | burn: 1020



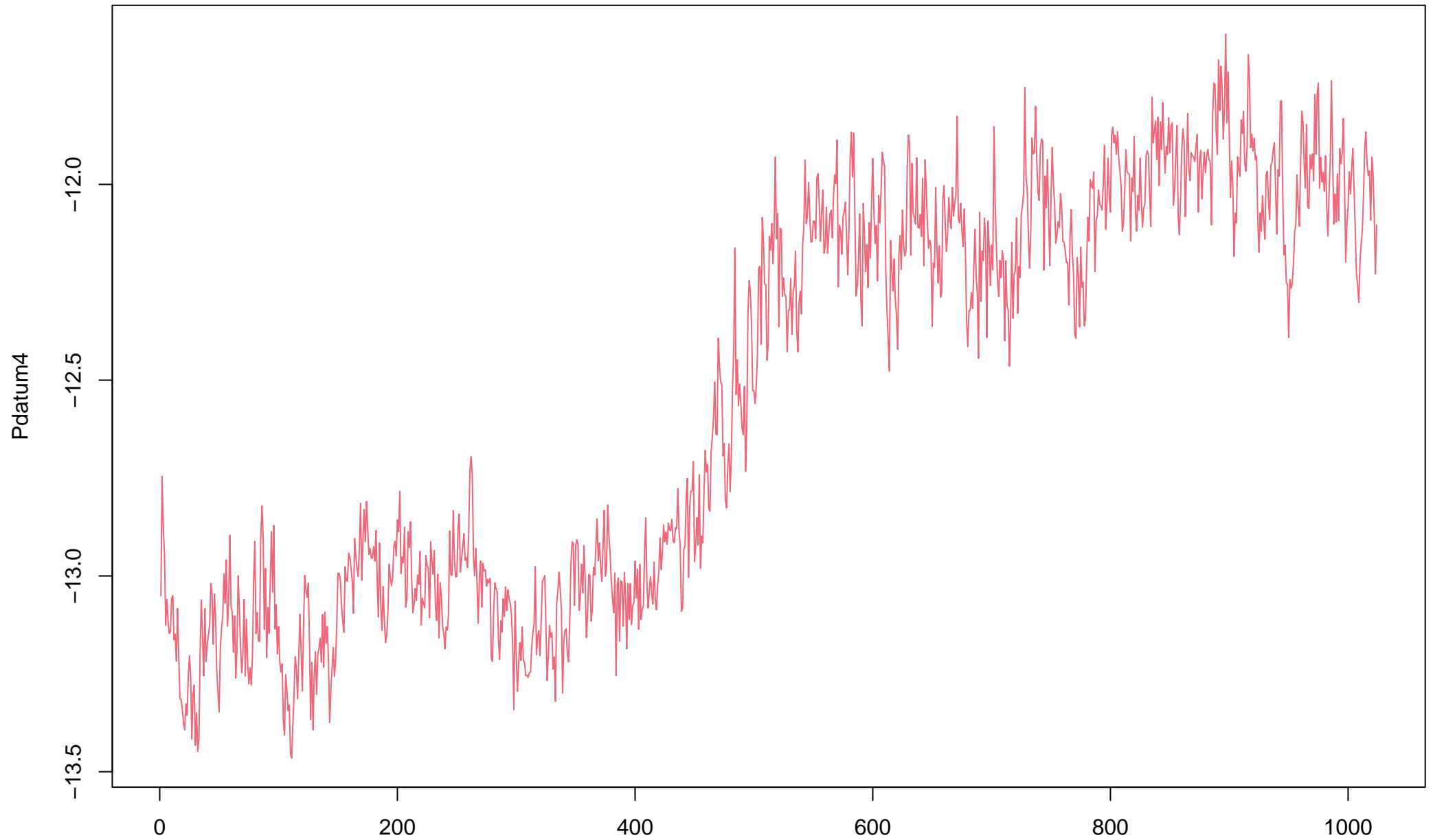
Pdatum2
ESS = 1.74 | BMK = 0.825 | MCSE(6.27) = 16.4 | stat: FALSE | burn: 612



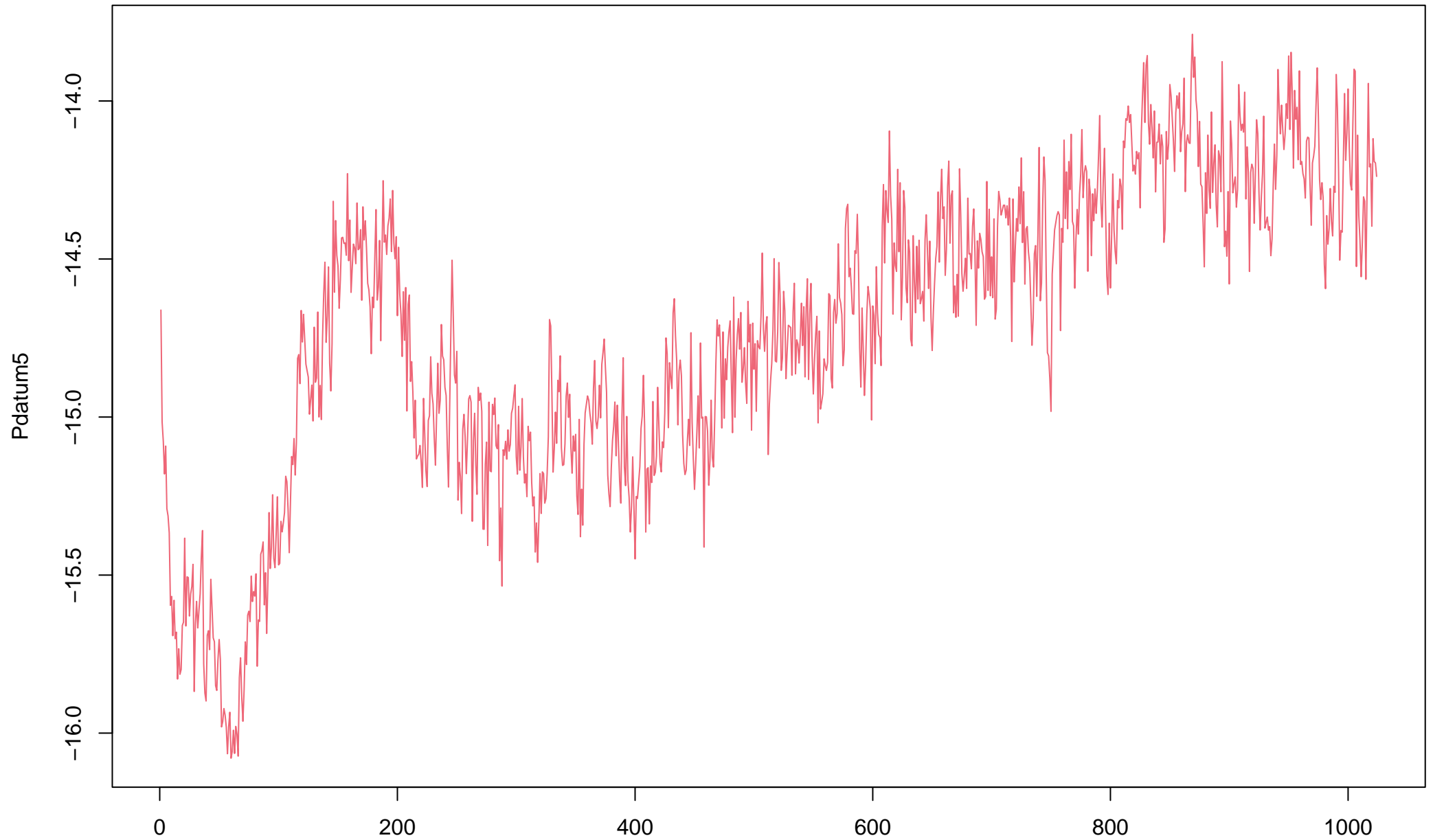
Pdatum3
ESS = 8.86 | BMK = 0.409 | MCSE(6.27) = 14.7 | stat: FALSE | burn: 1020



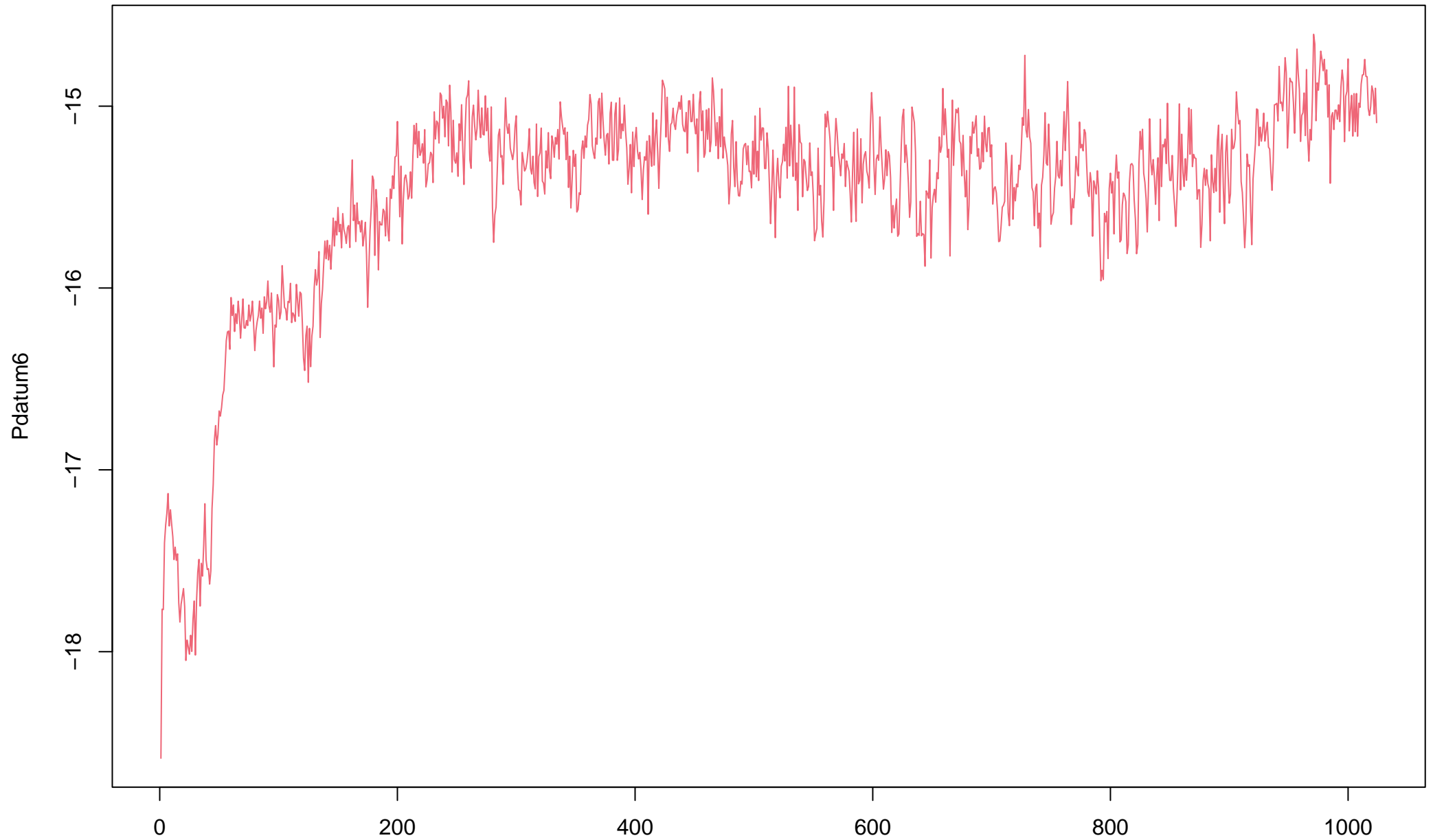
Pdatum4
ESS = 3.39 | BMK = 0.932 | MCSE(6.27) = 17.2 | stat: FALSE | burn: 510



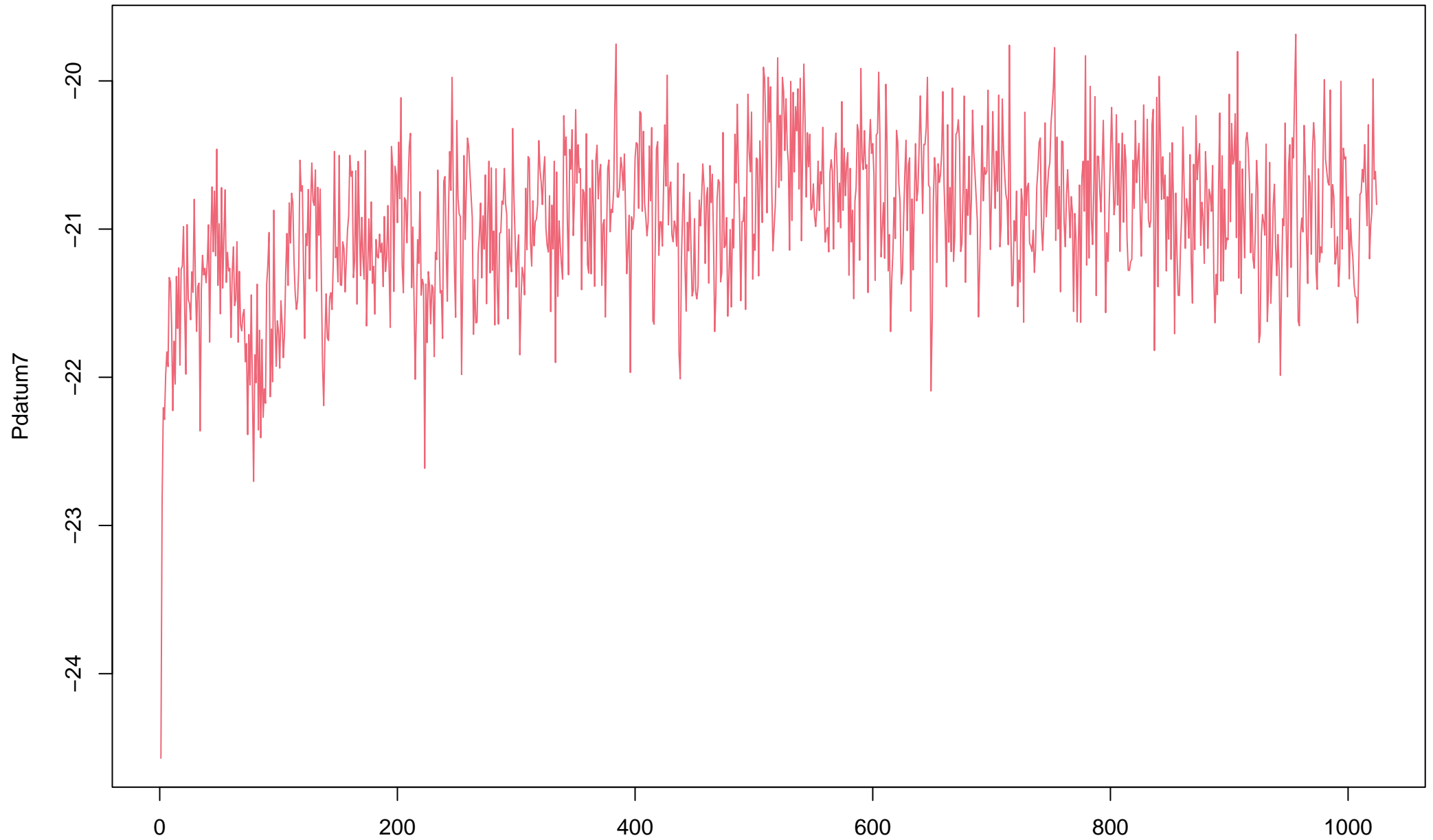
Pdatum5
ESS = 3.85 | BMK = 0.673 | MCSE(6.27) = 16.3 | stat: FALSE | burn: 204



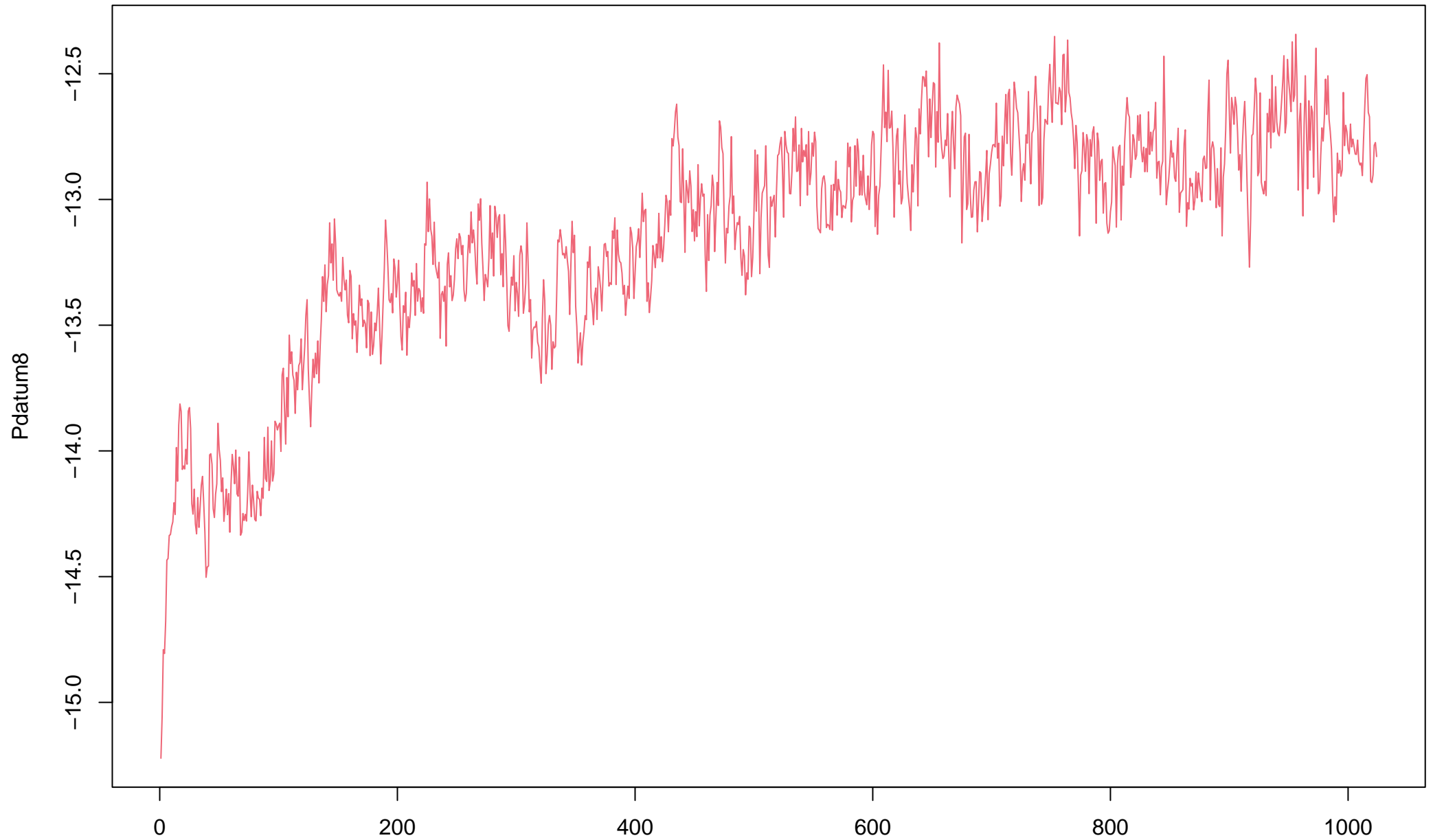
Pdatum6
ESS = 7.08 | BMK = 0.341 | MCSE(6.27) = 15.5 | stat: FALSE | burn: 1020



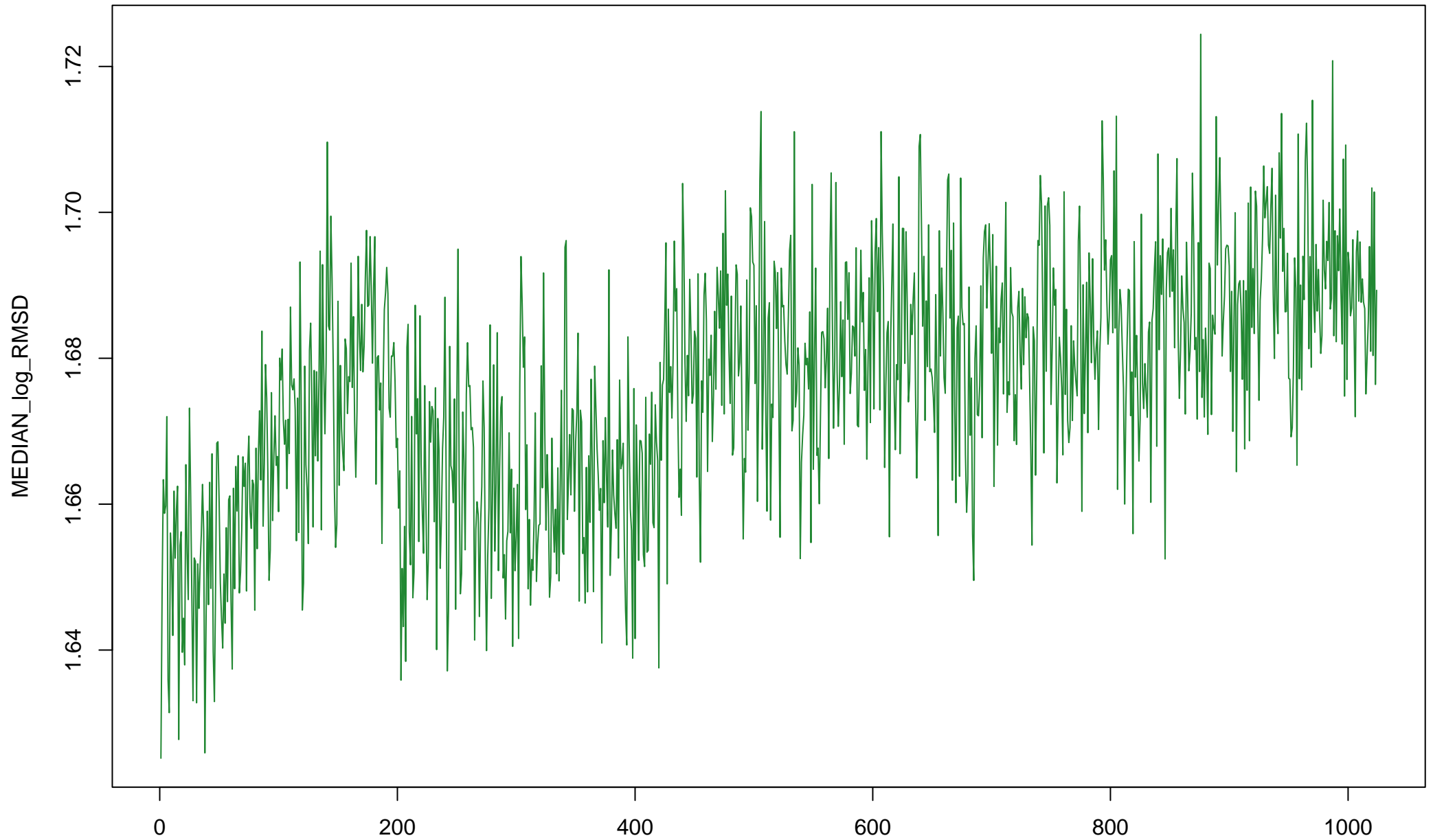
Pdatum7
ESS = 2.22e-16 | BMK = 0.234 | MCSE(6.27) = 8.65 | stat: TRUE | burn: 0



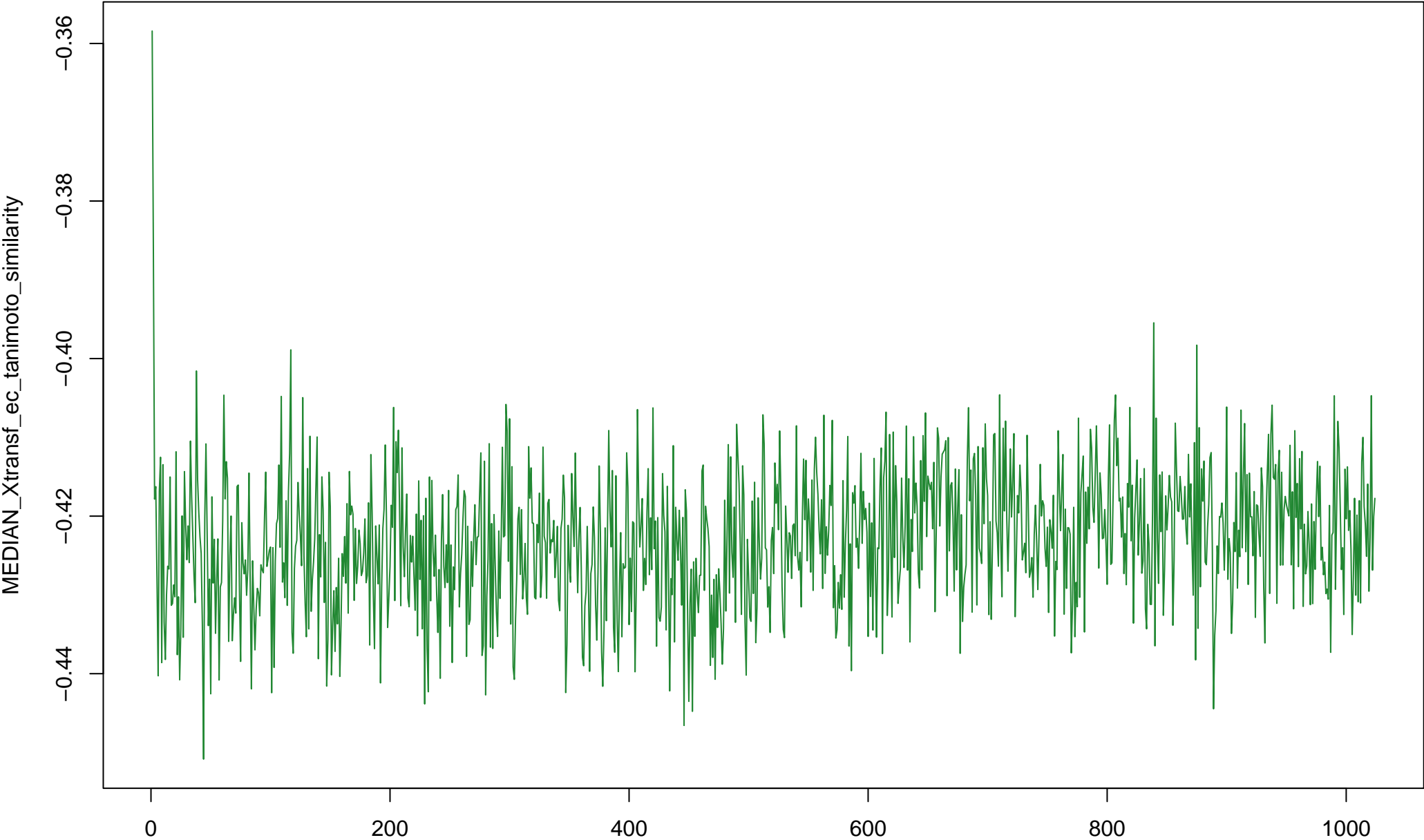
Pdatum8
ESS = 7.34 | BMK = 0.74 | MCSE(6.27) = 16.4 | stat: FALSE | burn: 408



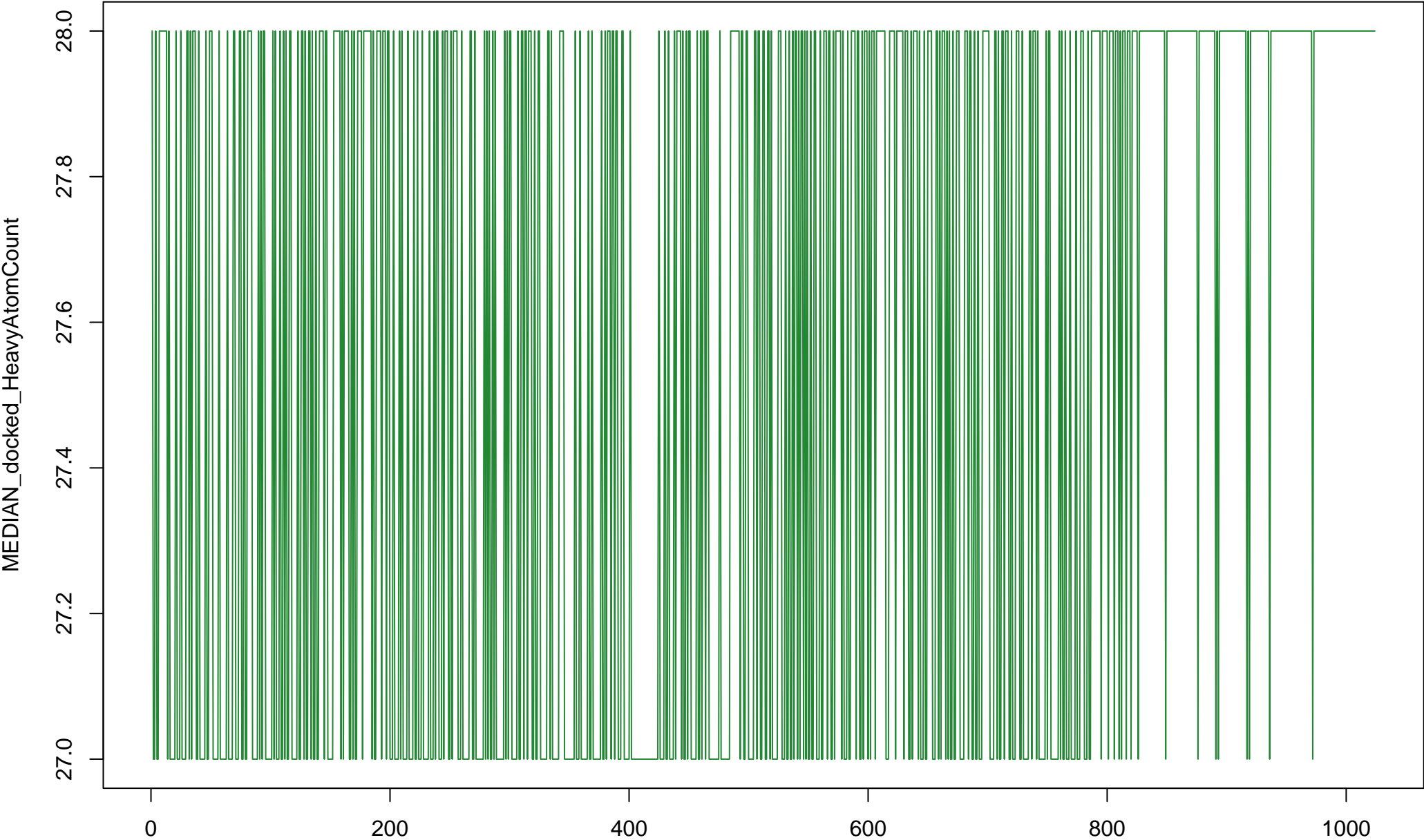
MEDIAN_log_RMSD
ESS = 18.5 | BMK = 0.429 | MCSE(6.27) = 12.5 | stat: FALSE | burn: 102



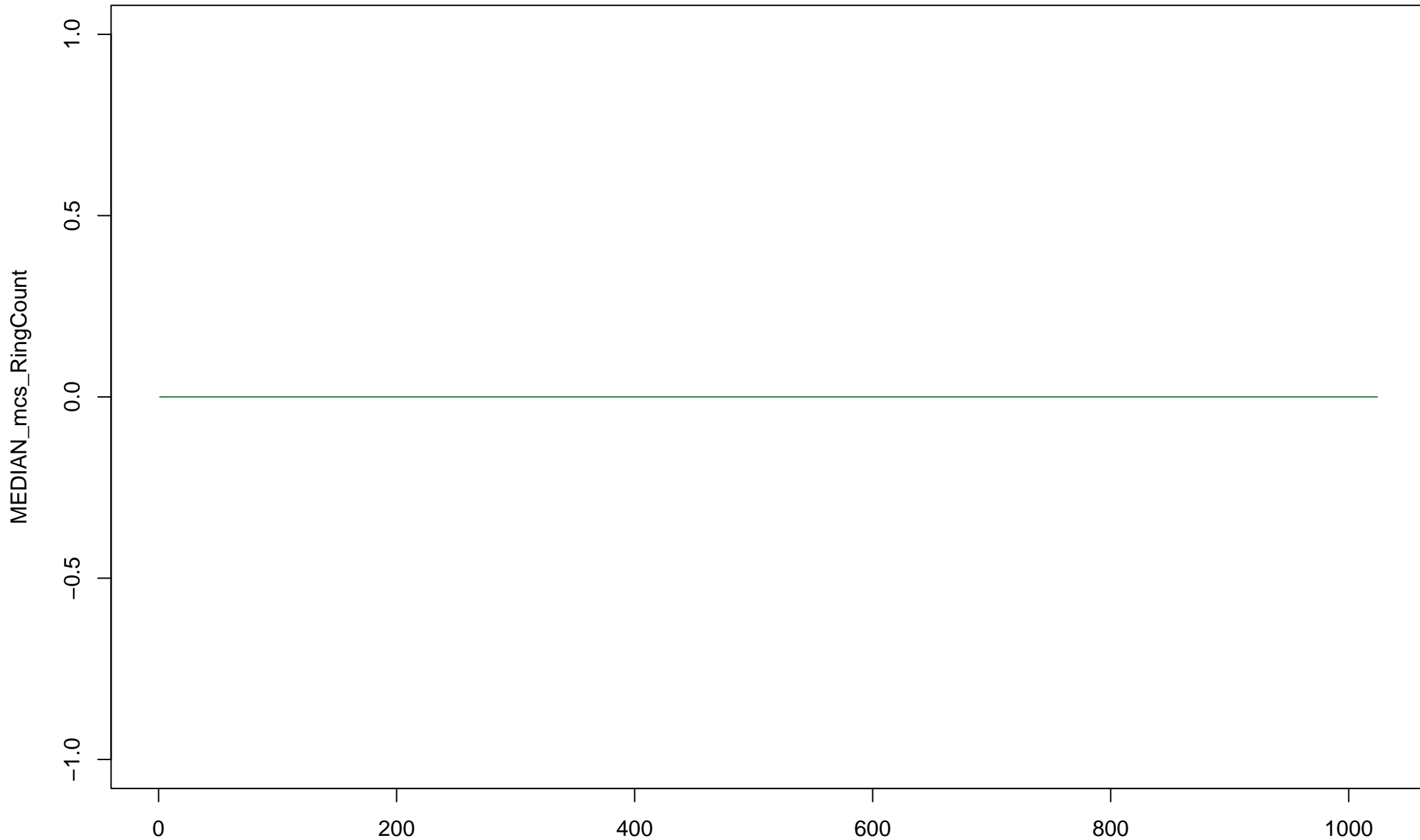
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 449 | BMK = 0.199 | MCSE(6.27) = 5.58 | stat: FALSE | burn: 0



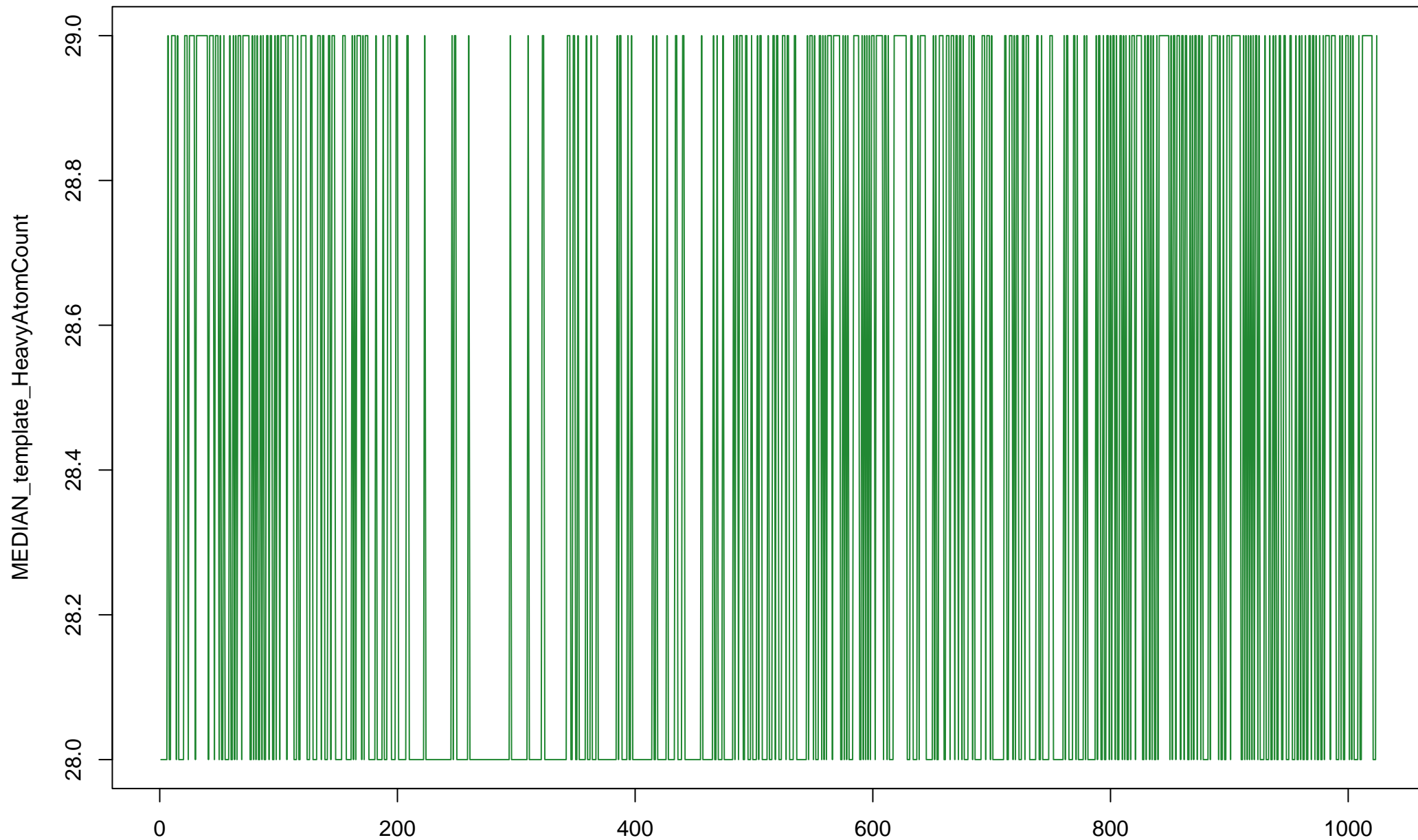
MEDIAN_docked_HeavyAtomCount
ESS = 27.2 | BMK = 0.164 | MCSE(6.27) = 8.68 | stat: FALSE | burn: 0



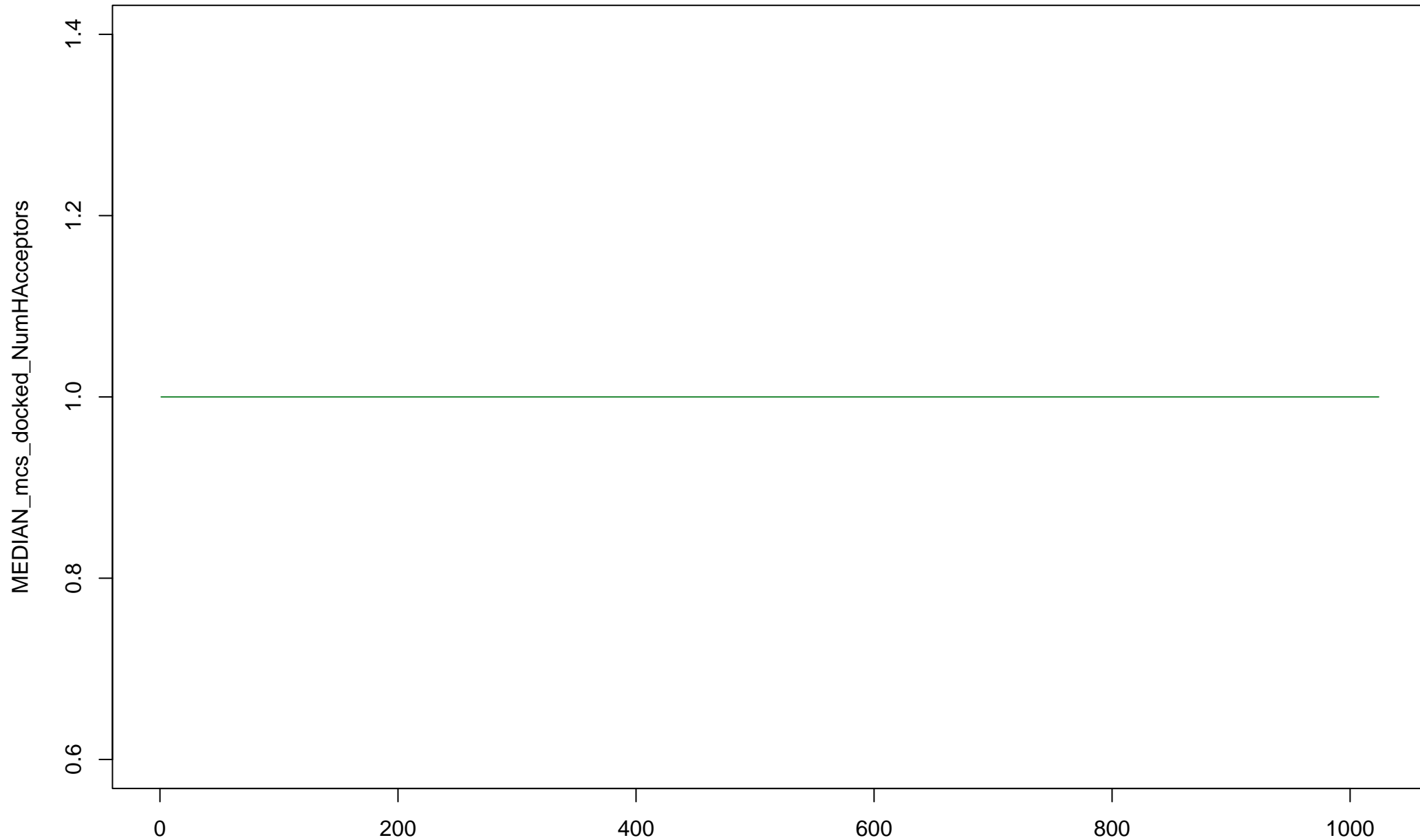
MEDIAN_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



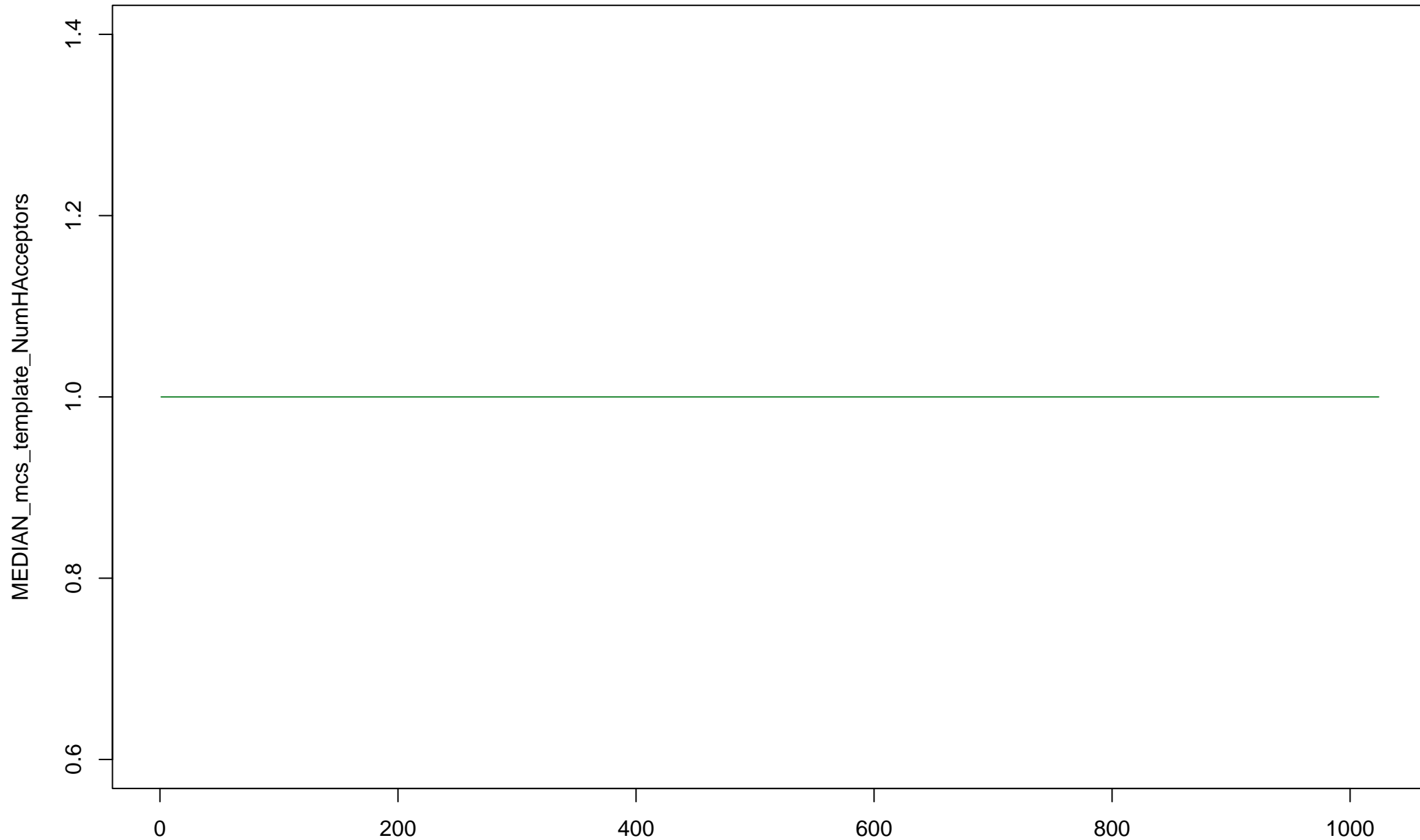
MEDIAN_template_HeavyAtomCount
ESS = 74.4 | BMK = 0.109 | MCSE(6.27) = 7.08 | stat: TRUE | burn: 0



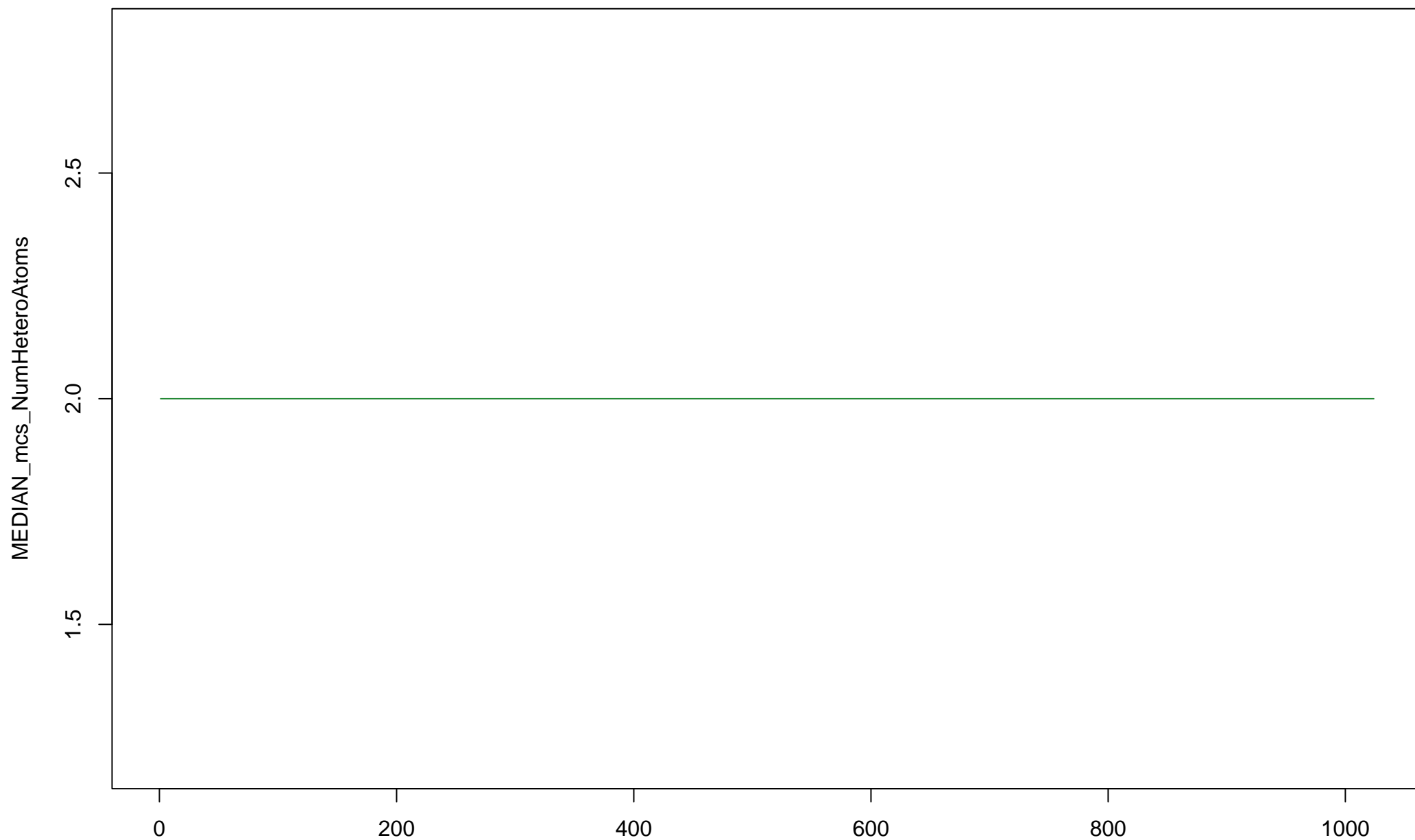
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



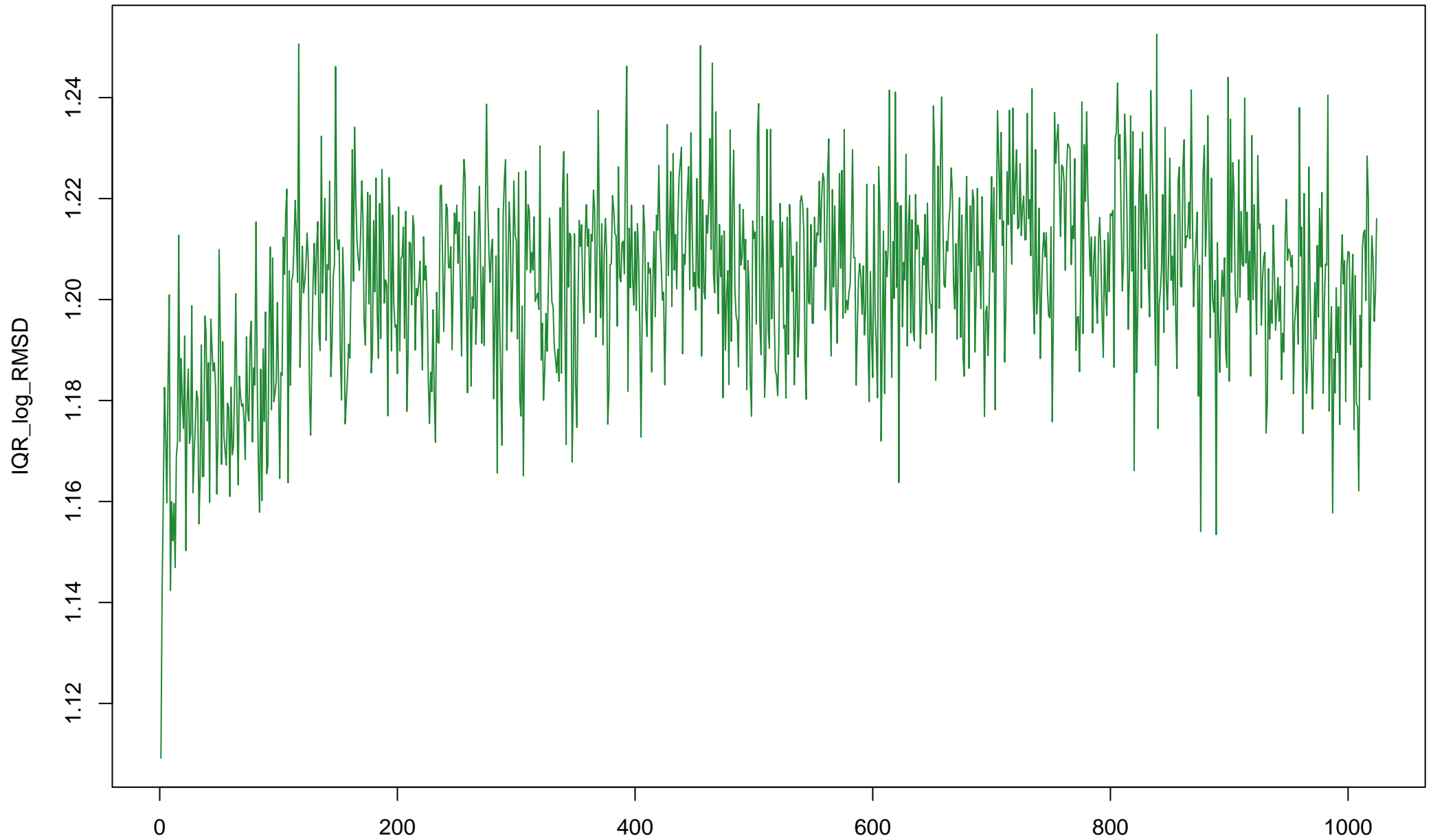
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



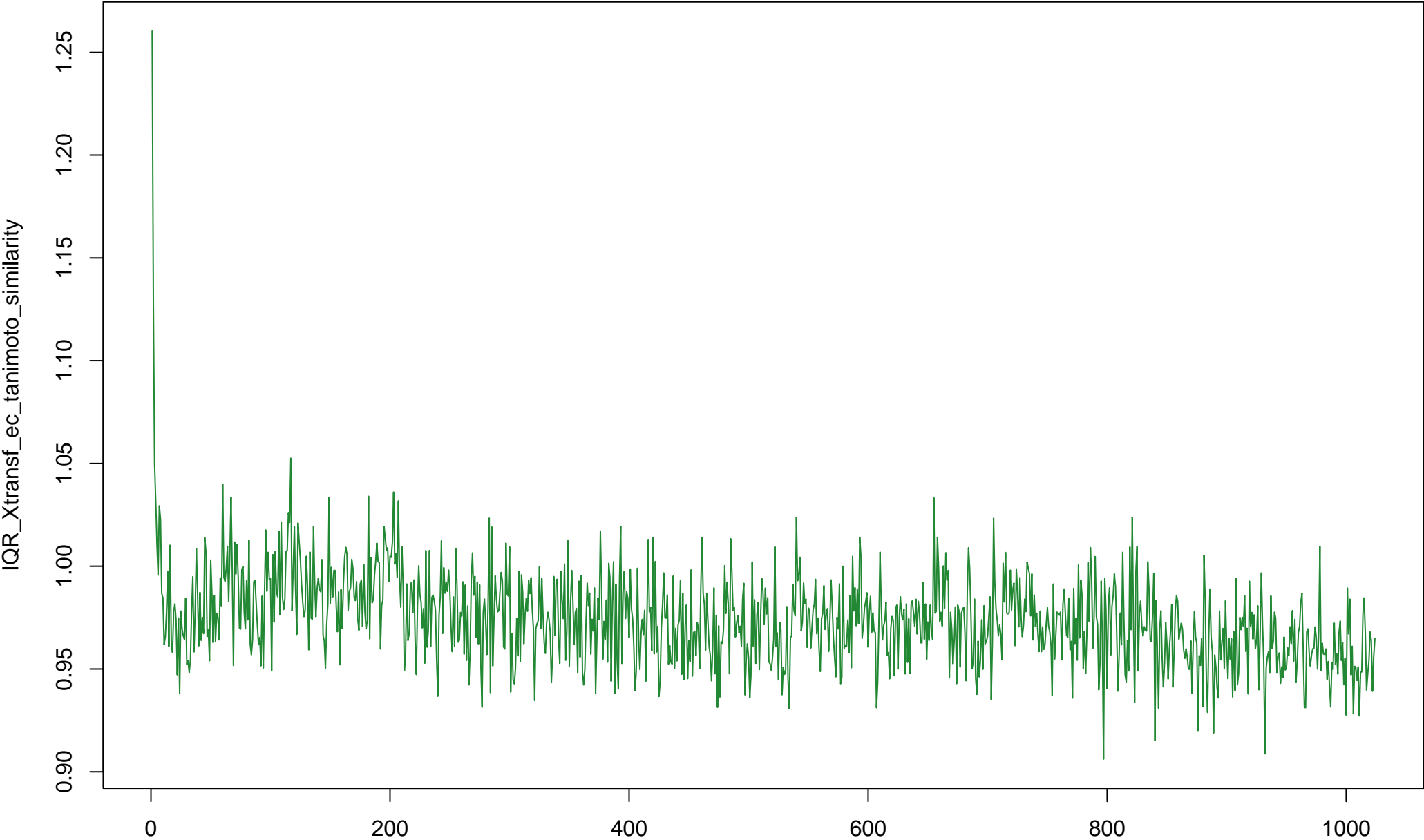
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



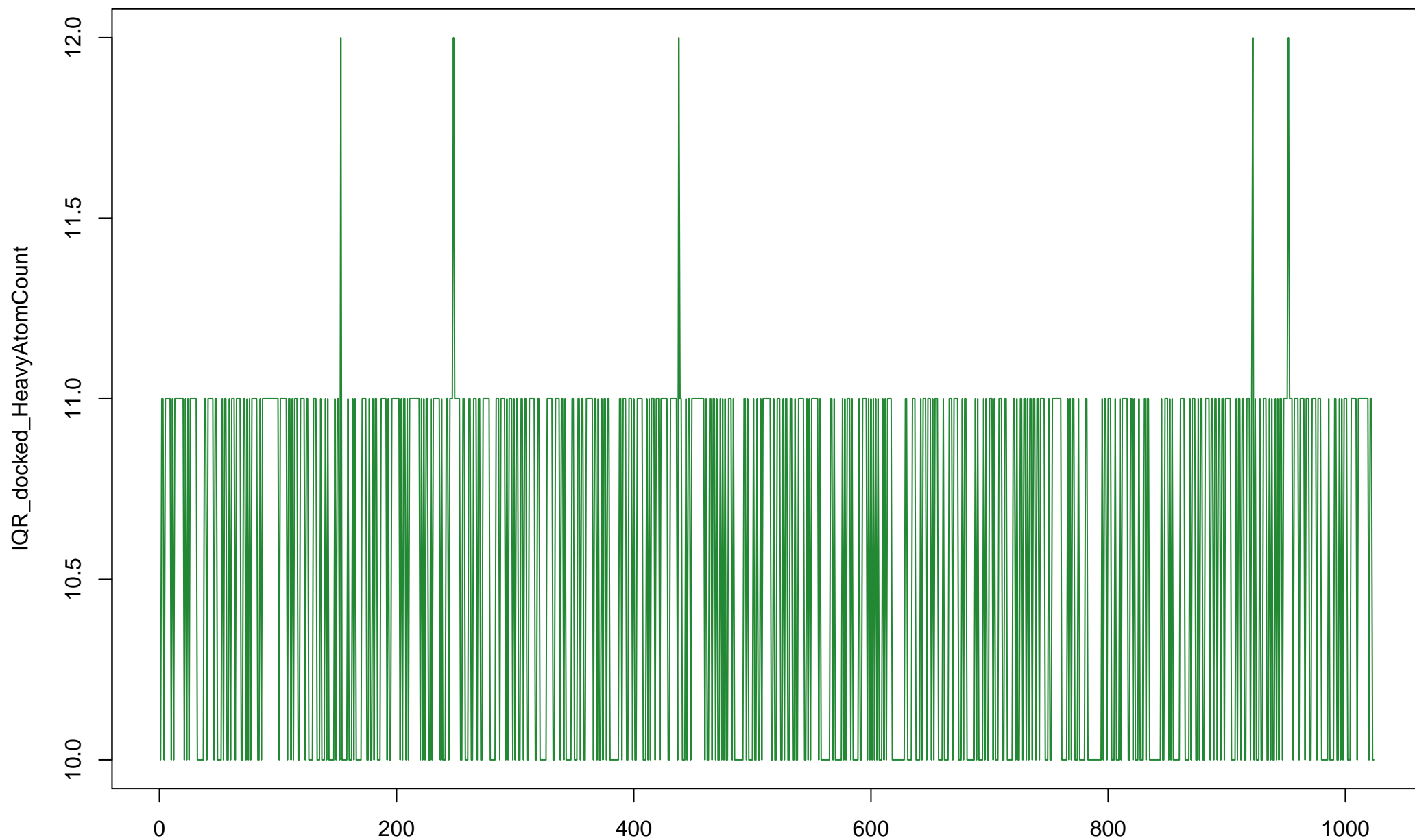
IQR_log_RMSD
ESS = 27.1 | BMK = 0.174 | MCSE(6.27) = 9.9 | stat: FALSE | burn: 102



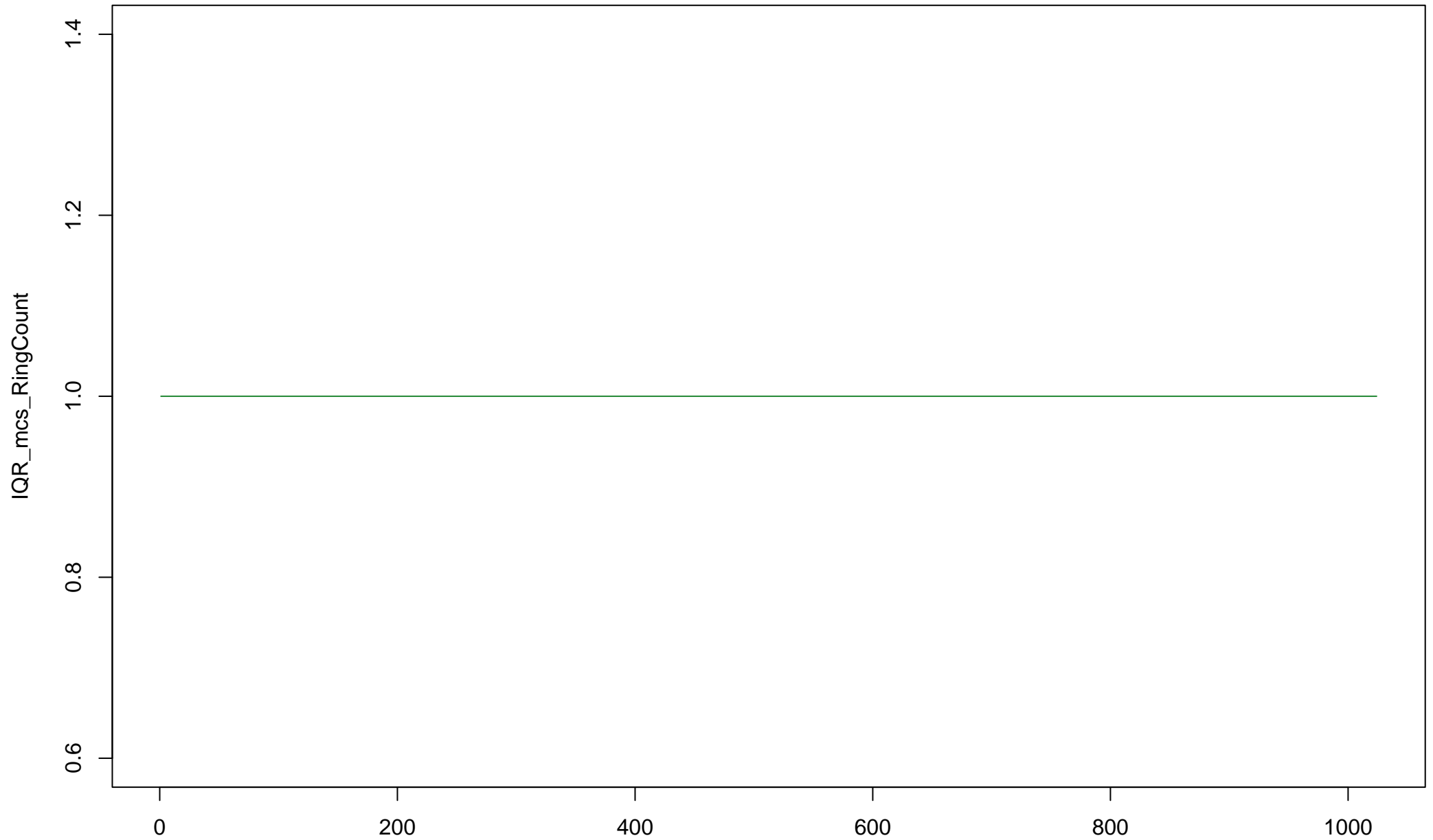
IQR_Xtransf_ec_tanimoto_similarity
ESS = 168 | BMK = 0.211 | MCSE(6.27) = 7.88 | stat: FALSE | burn: 0



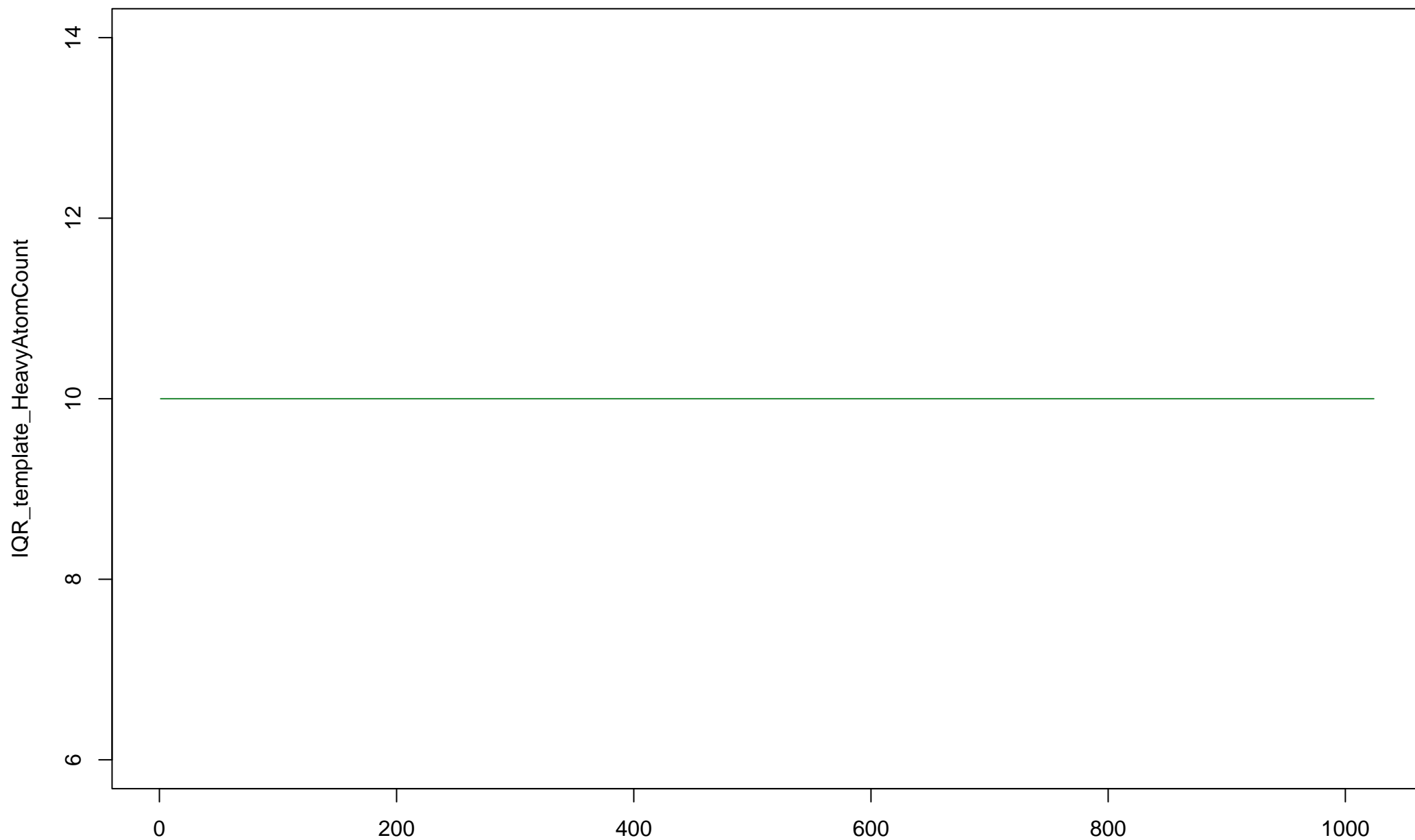
IQR_docked_HeavyAtomCount
ESS = 628 | BMK = 0.0594 | MCSE(6.27) = 4.56 | stat: FALSE | burn: 0



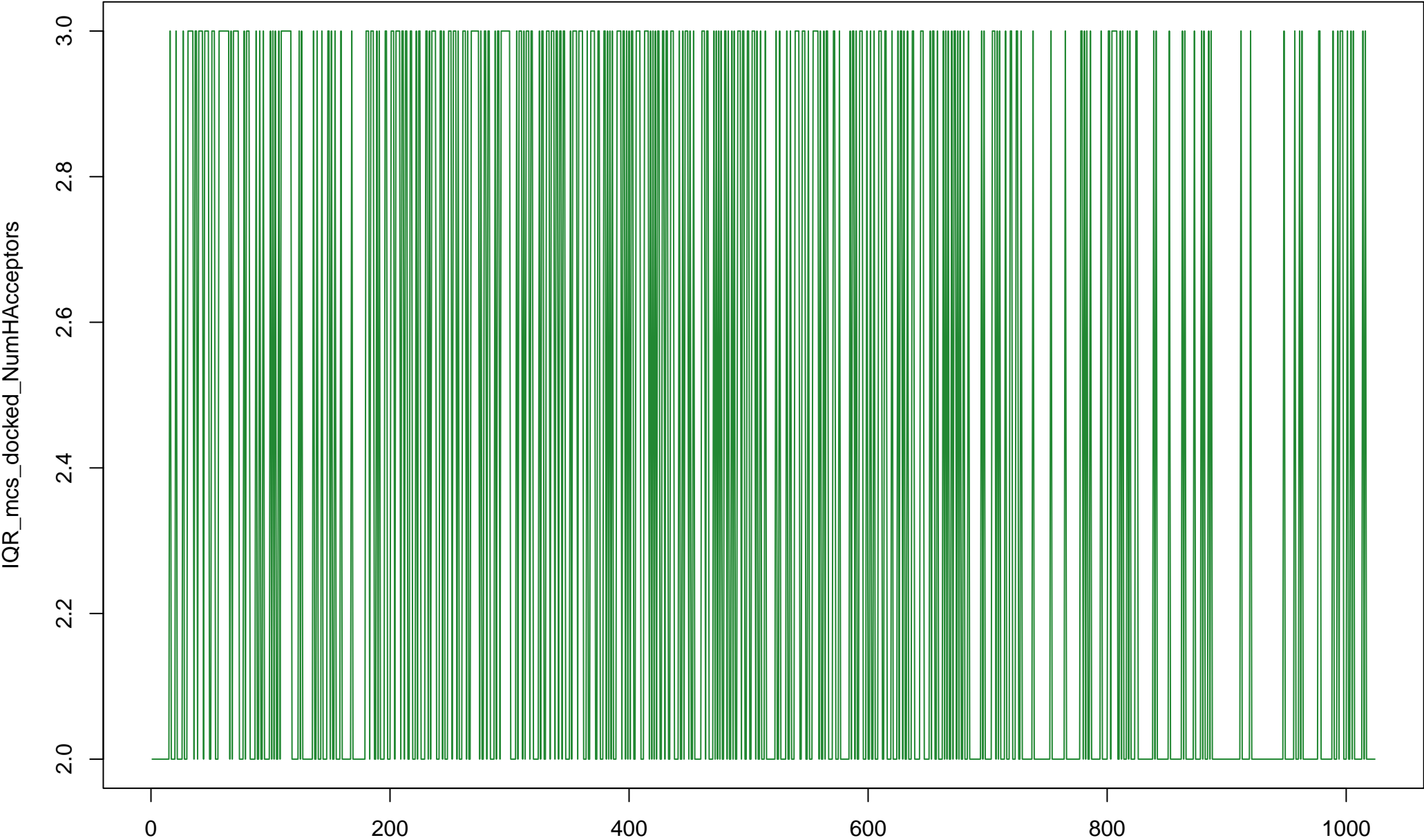
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



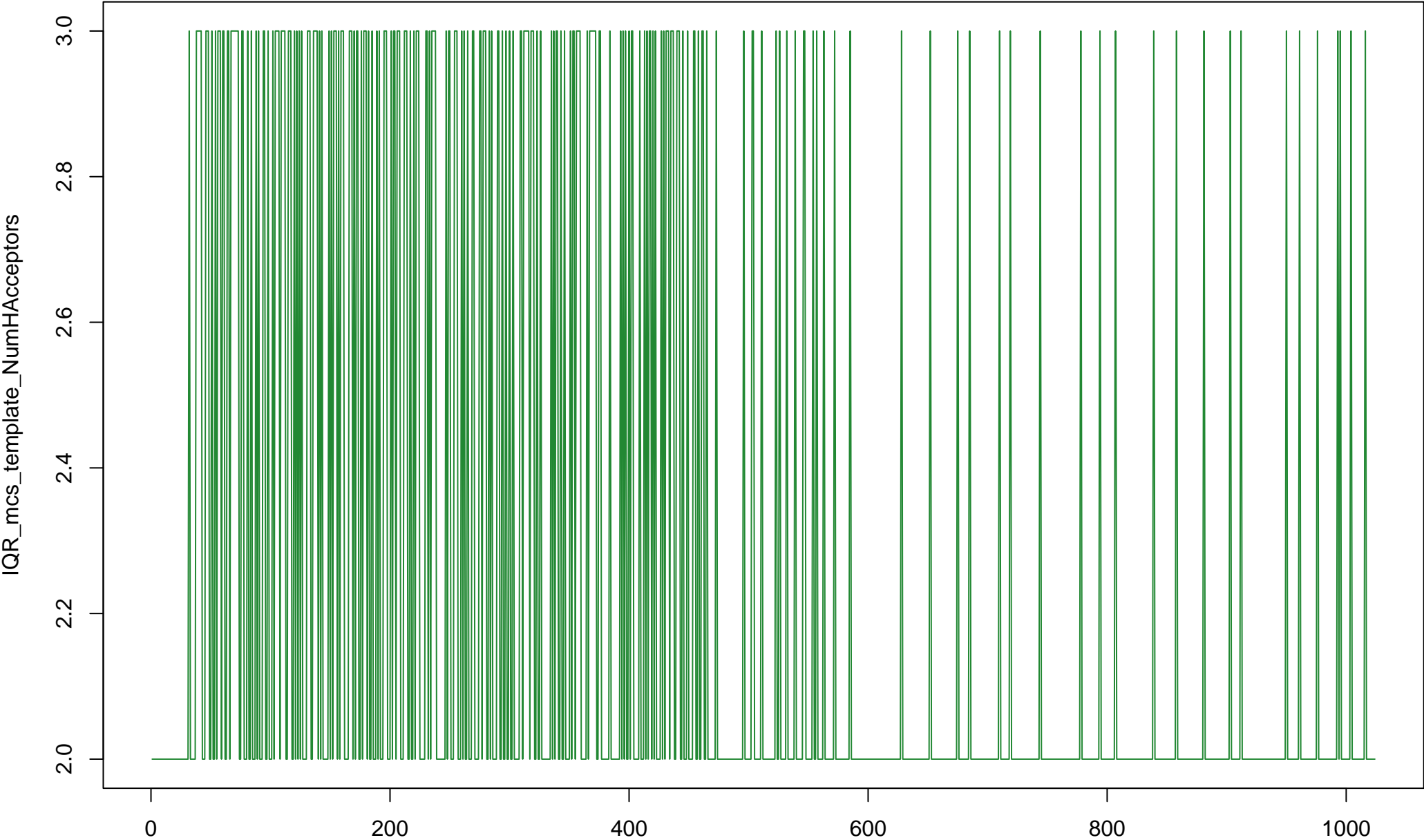
IQR_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



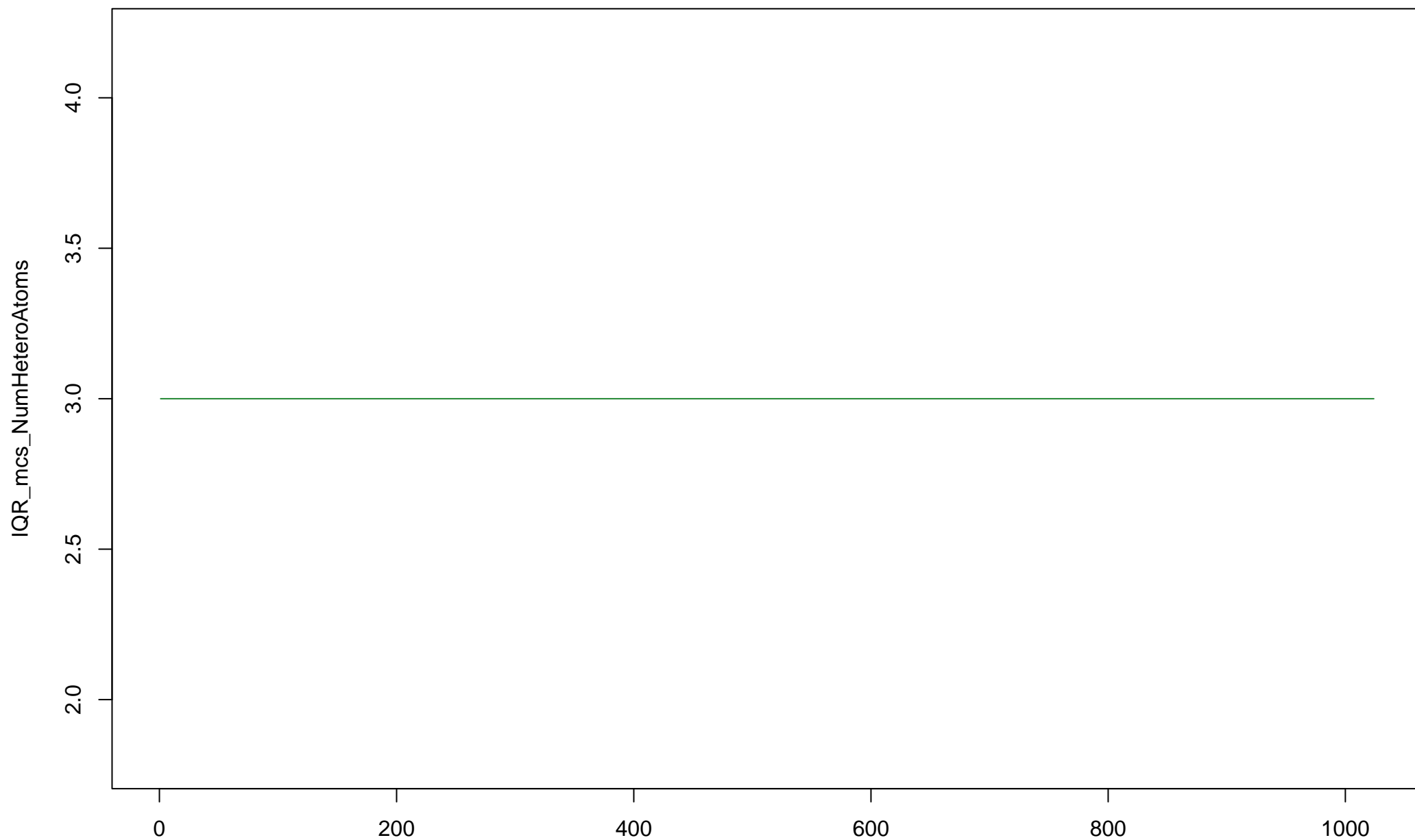
IQR_mcs_docked_NumHAcceptors
ESS = 175 | BMK = 0.329 | MCSE(6.27) = 6.68 | stat: FALSE | burn: 0



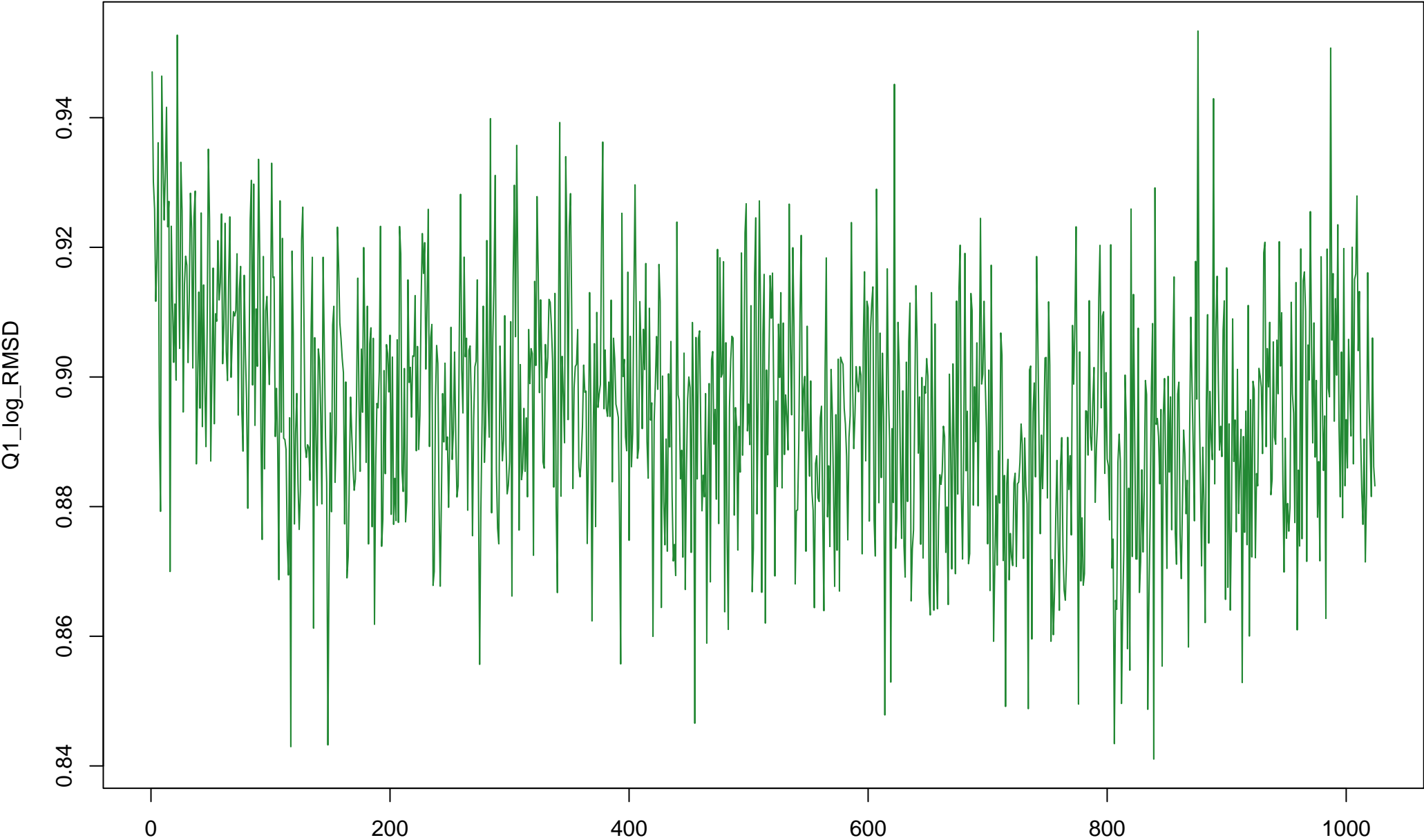
IQR_mcs_template_NumHAcceptors
ESS = 29.8 | BMK = 0.304 | MCSE(6.27) = 8.51 | stat: FALSE | burn: 0



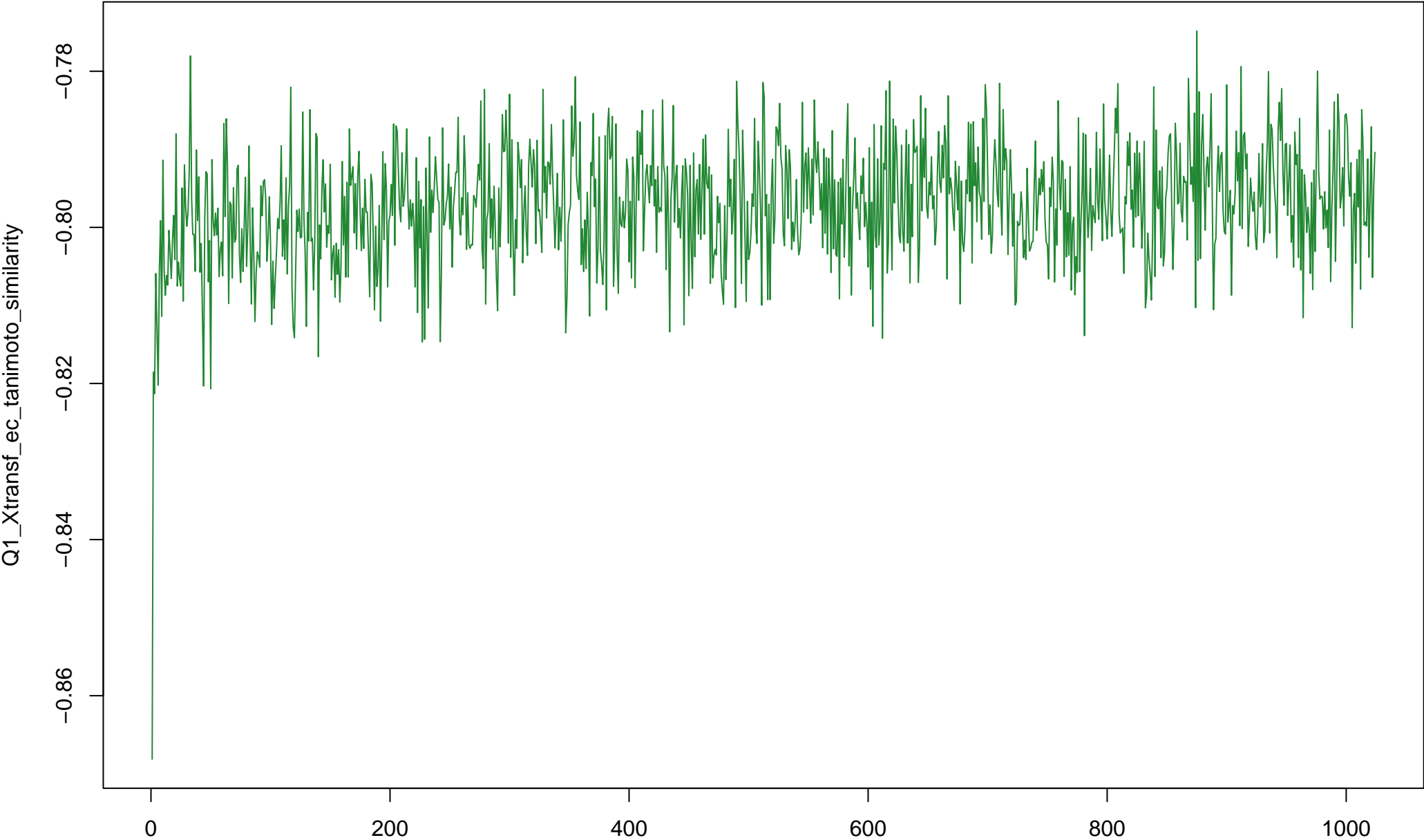
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



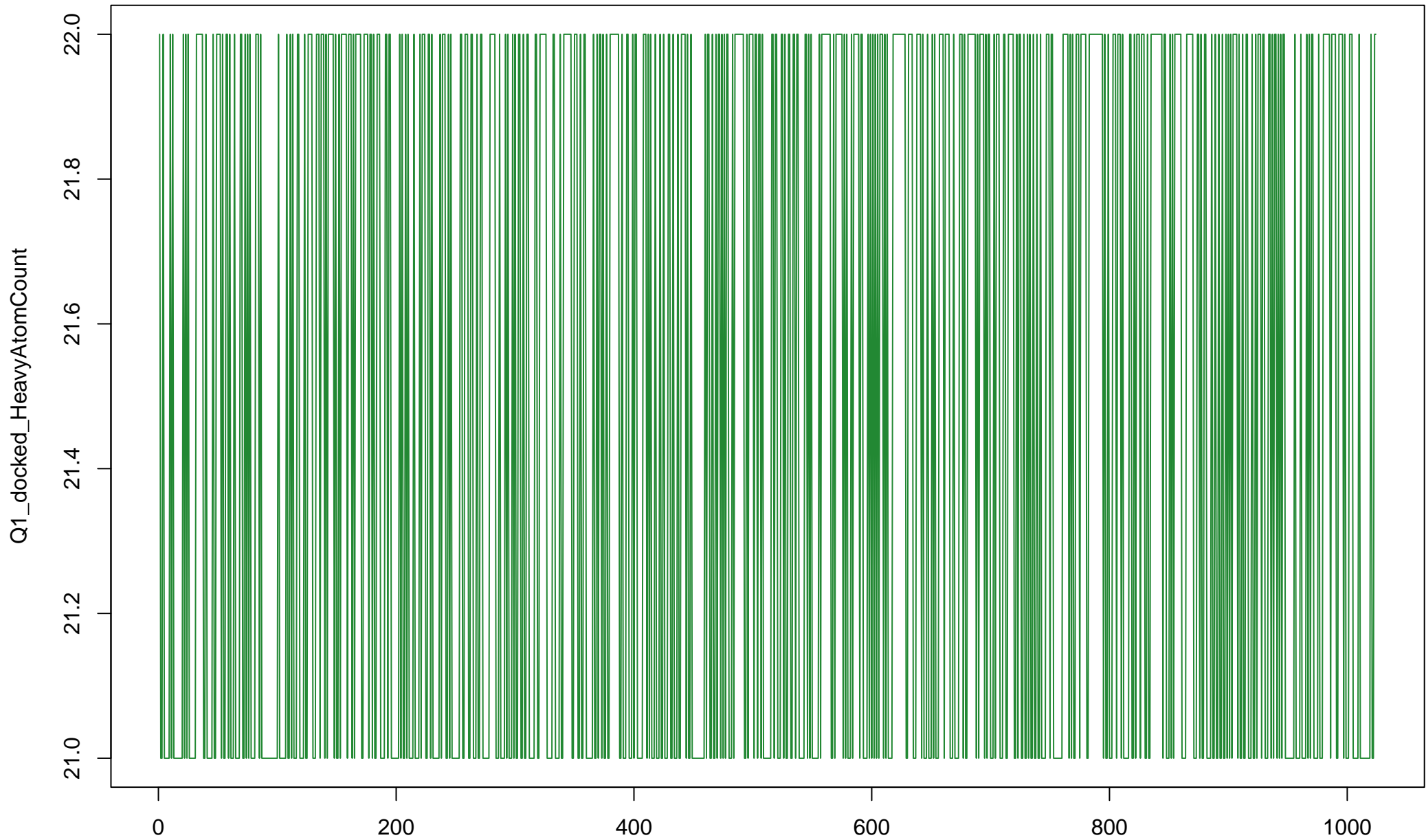
Q1_log_RMSD
ESS = 143 | BMK = 0.173 | MCSE(6.27) = 7.79 | stat: FALSE | burn: 0



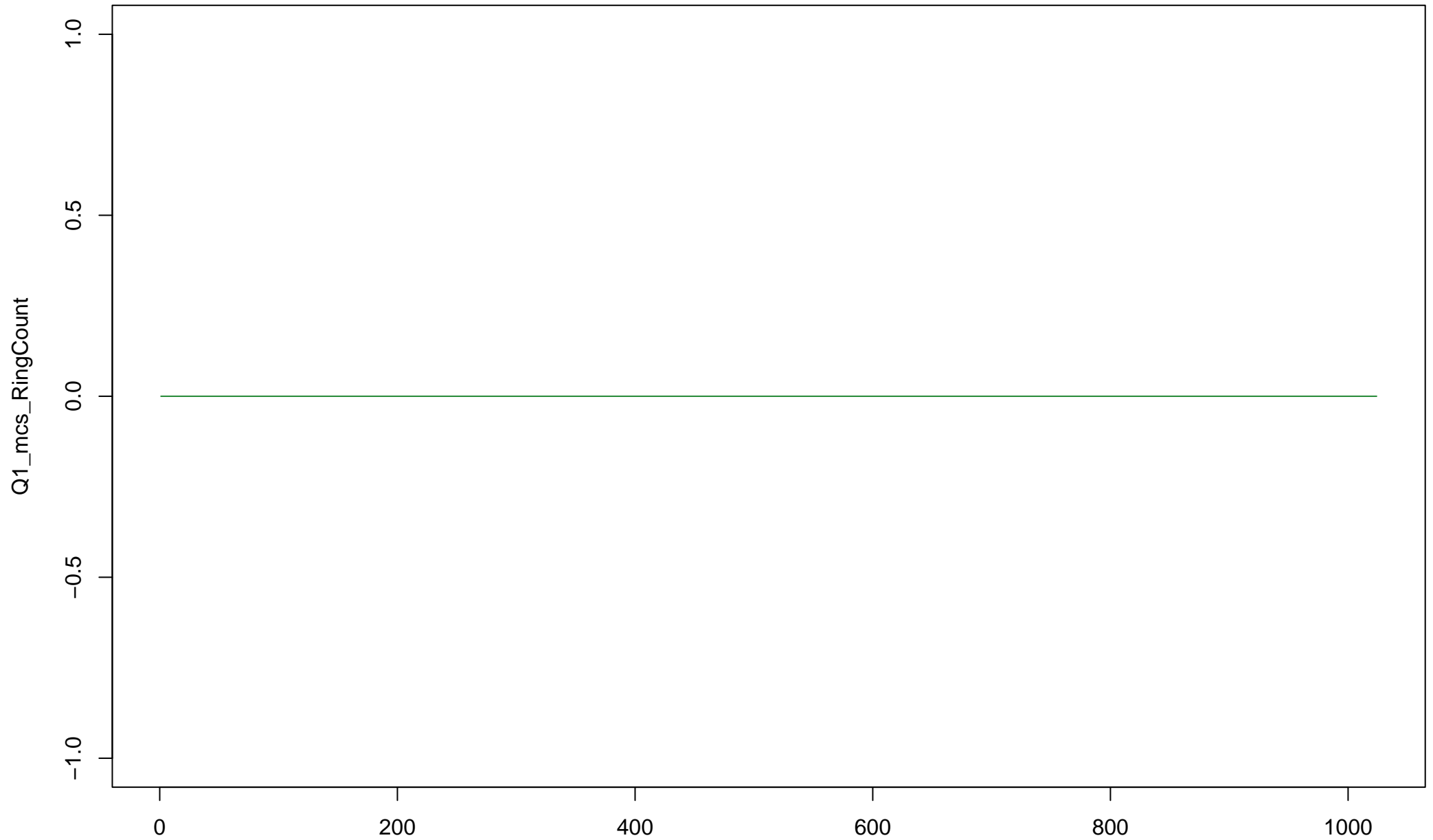
Q1_Xtransf_ec_tanimoto_similarity
ESS = 316 | BMK = 0.139 | MCSE(6.27) = 5.92 | stat: FALSE | burn: 0



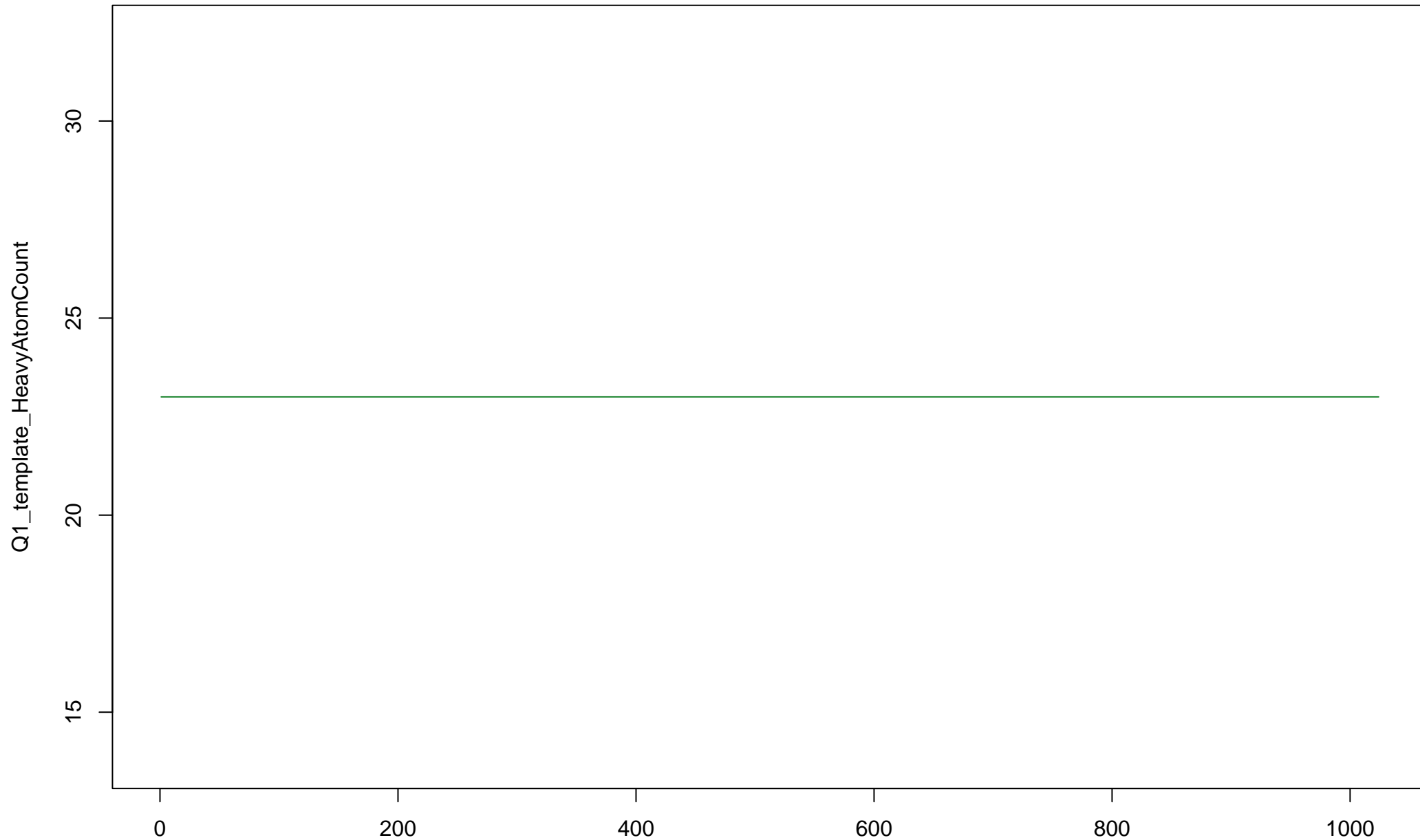
Q1_docked_HeavyAtomCount
ESS = 670 | BMK = 0.0443 | MCSE(6.27) = 4.34 | stat: FALSE | burn: 0



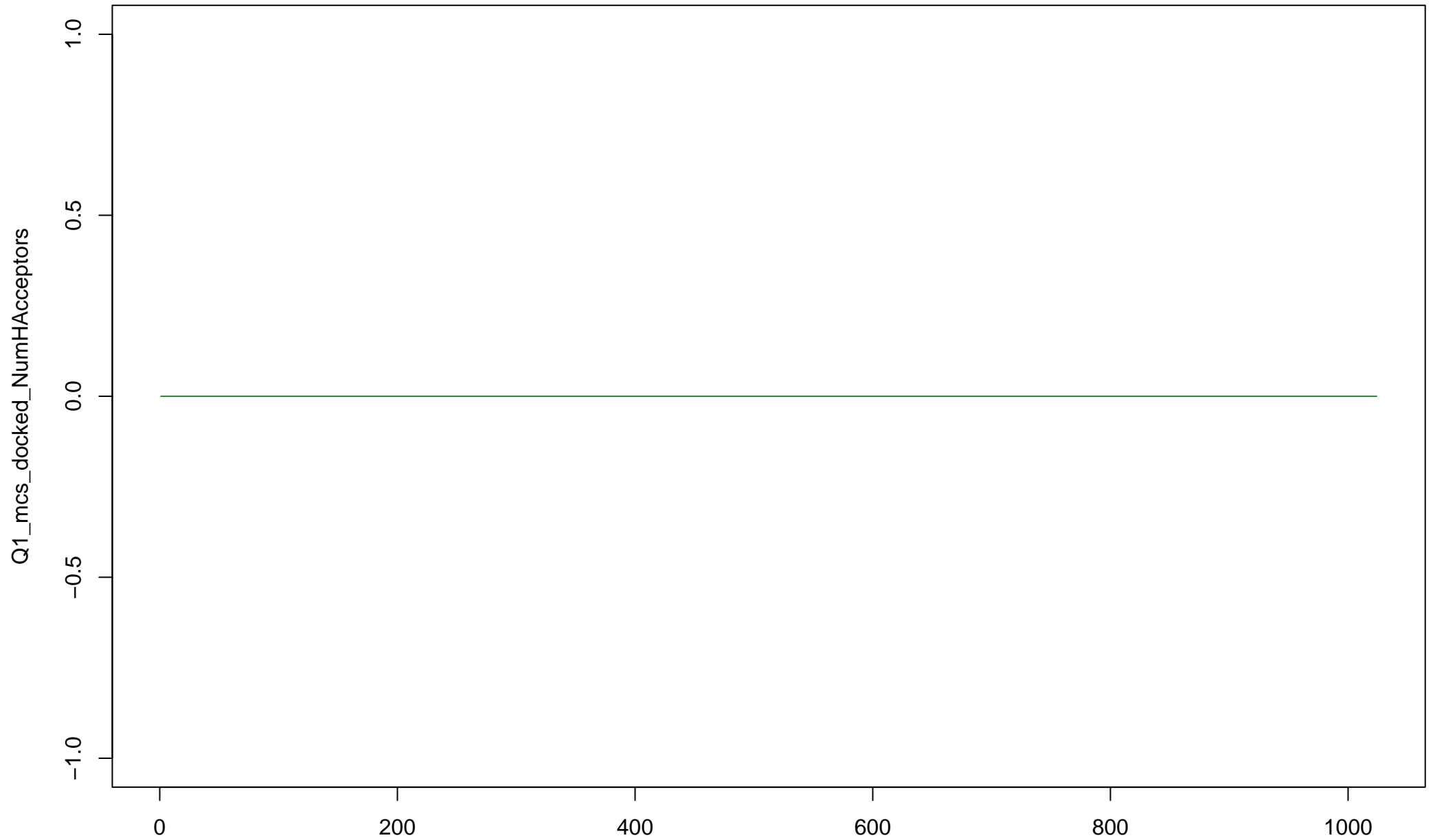
Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



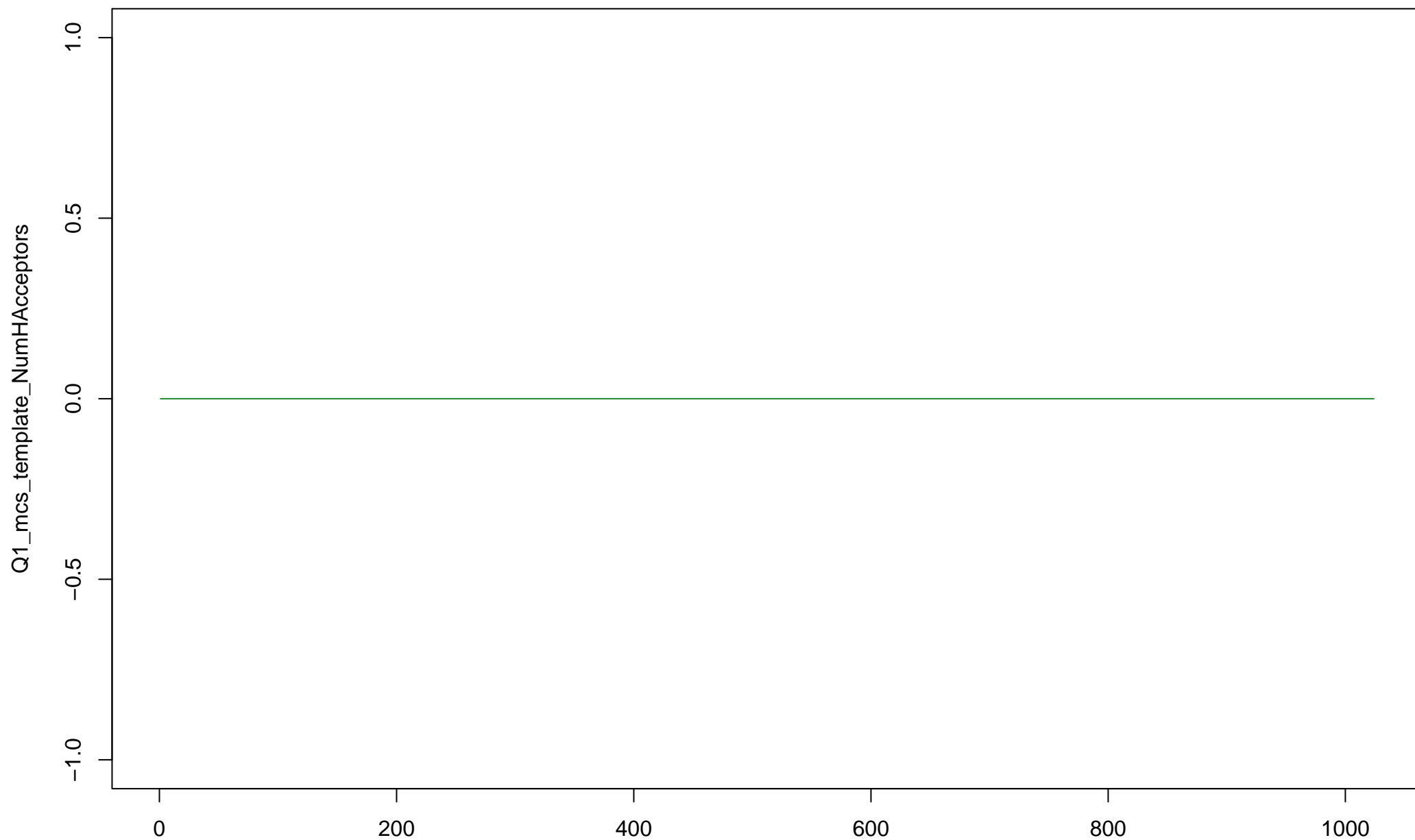
Q1_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



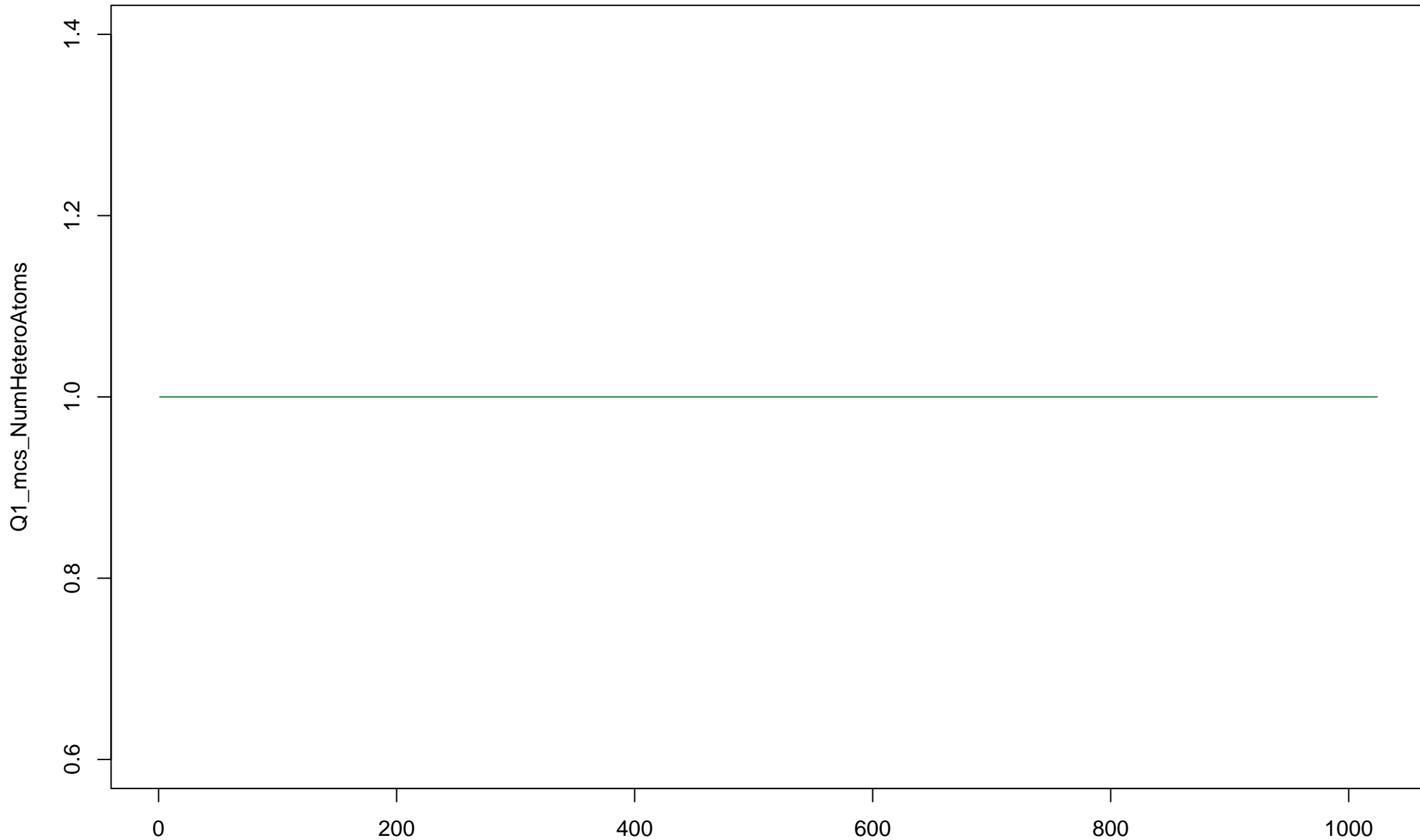
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



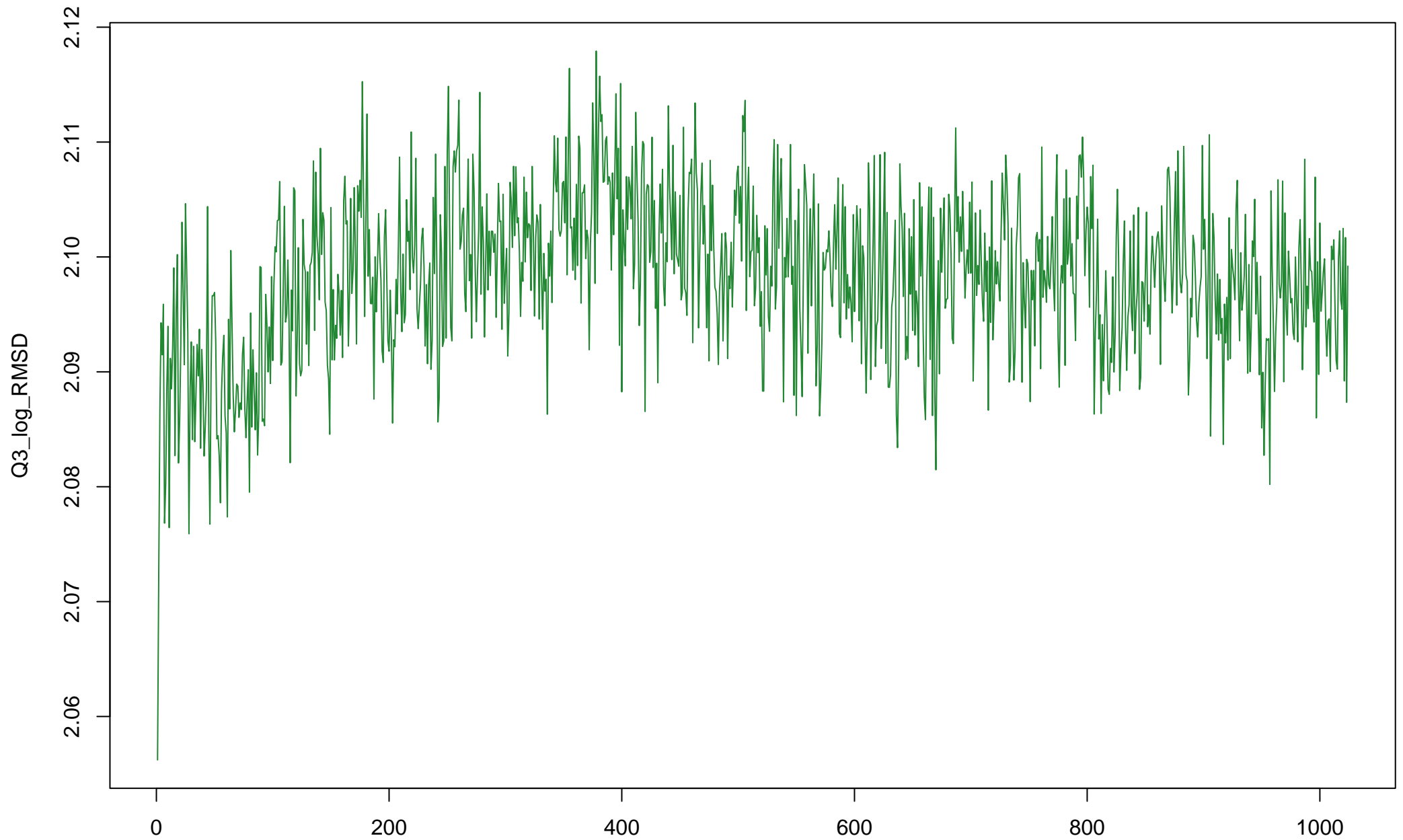
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



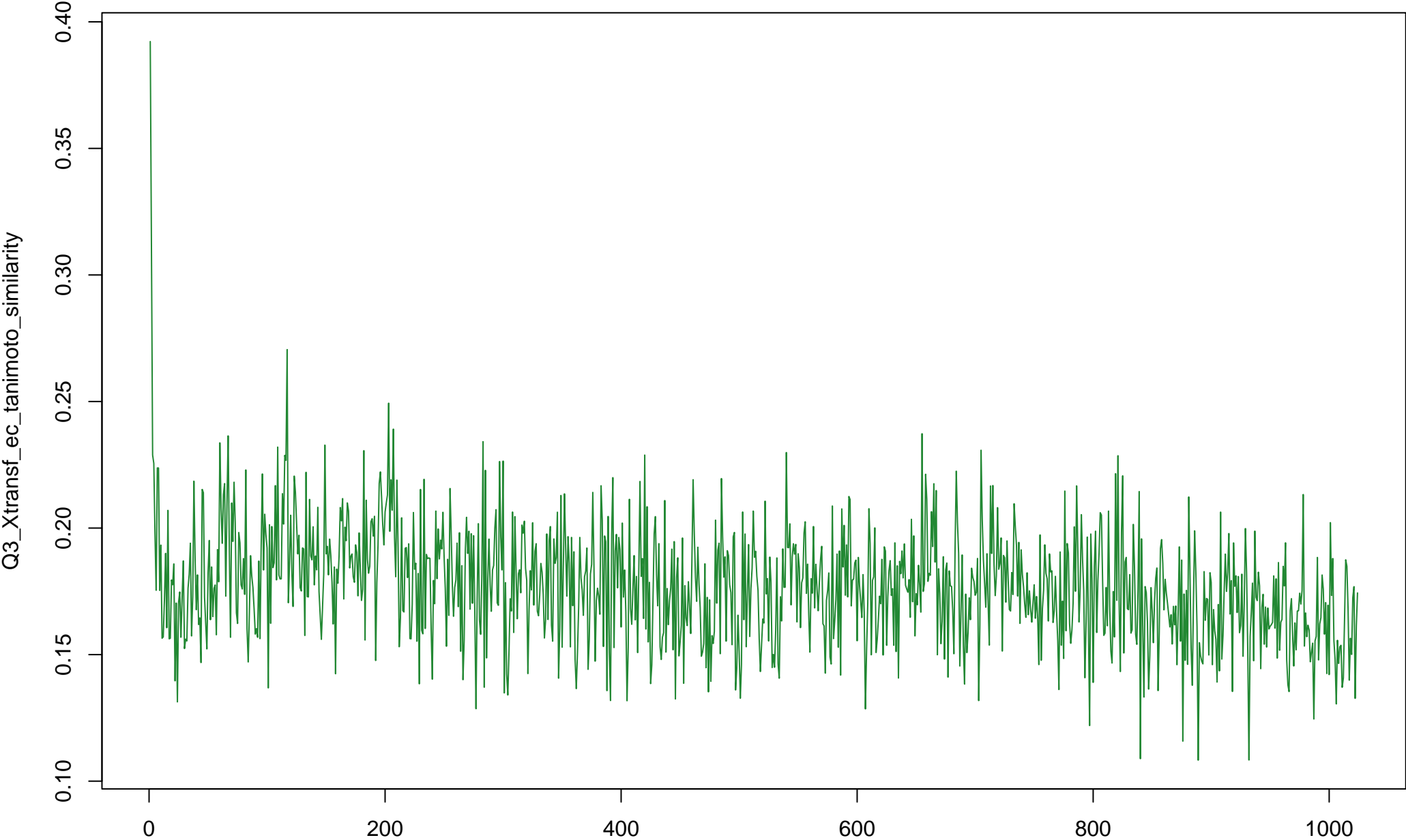
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



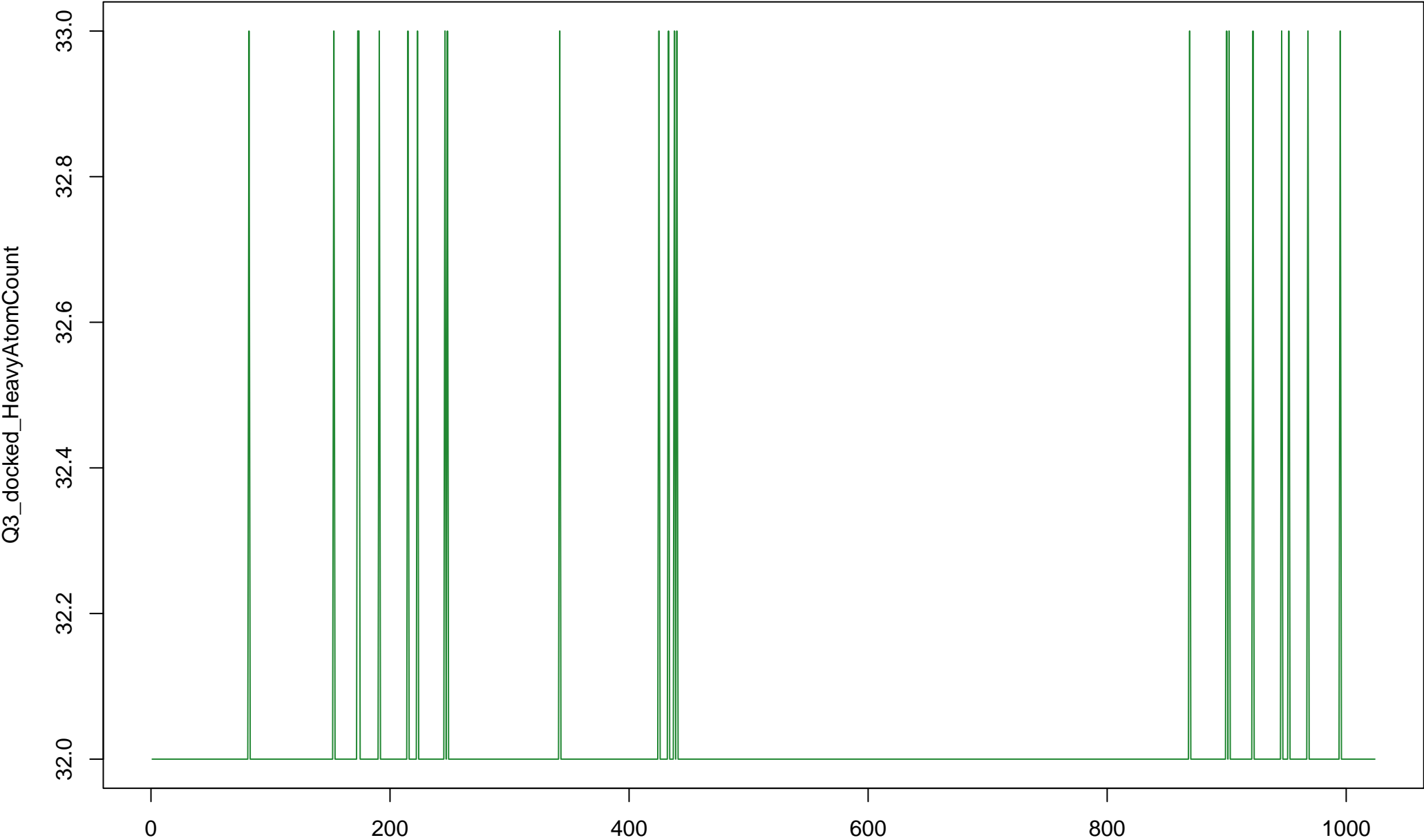
Q3_log_RMSD
ESS = 66.1 | BMK = 0.171 | MCSE(6.27) = 9.9 | stat: FALSE | burn: 0



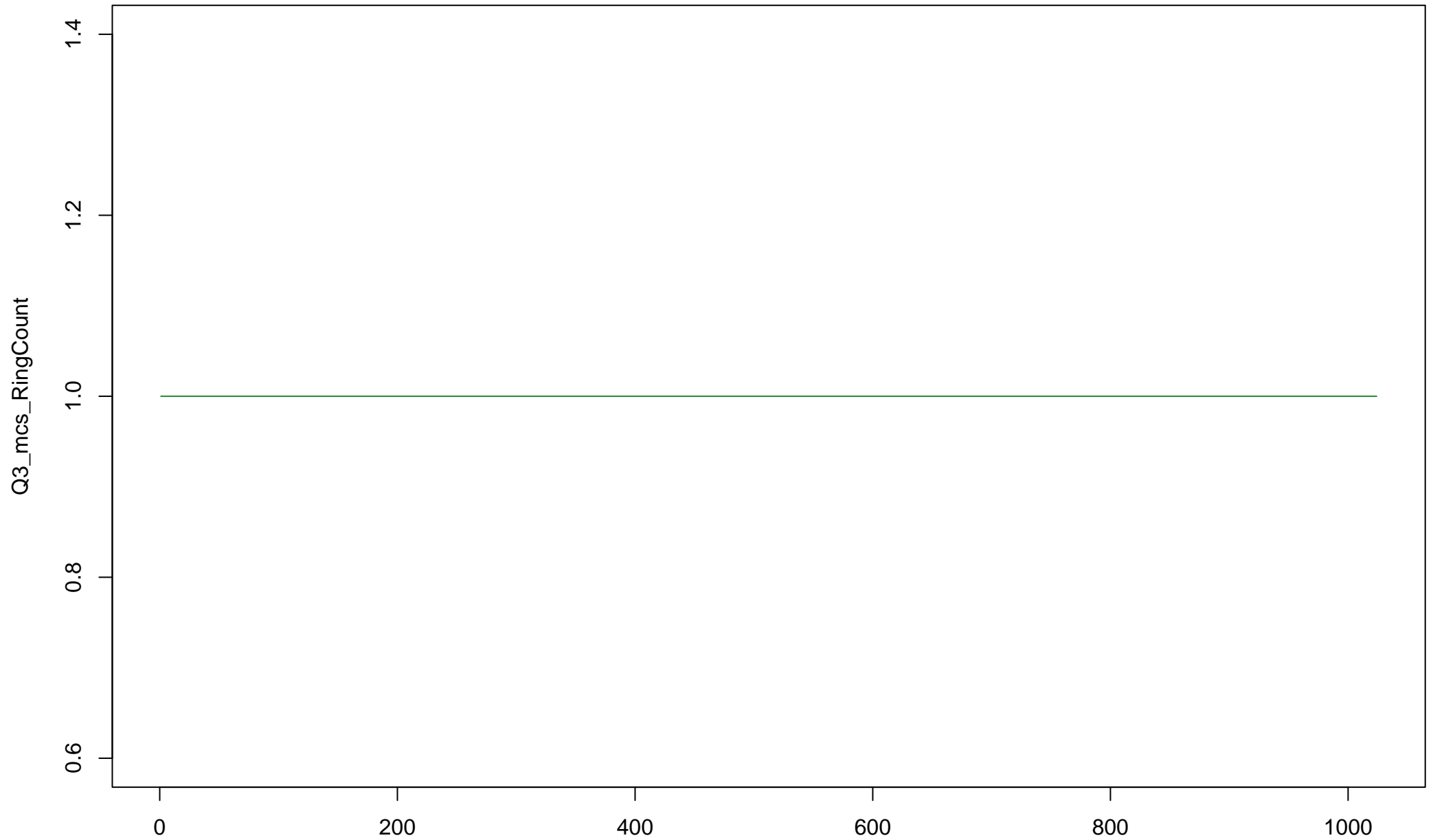
Q3_Xtransf_ec_tanimoto_similarity
ESS = 246 | BMK = 0.164 | MCSE(6.27) = 6.66 | stat: FALSE | burn: 0



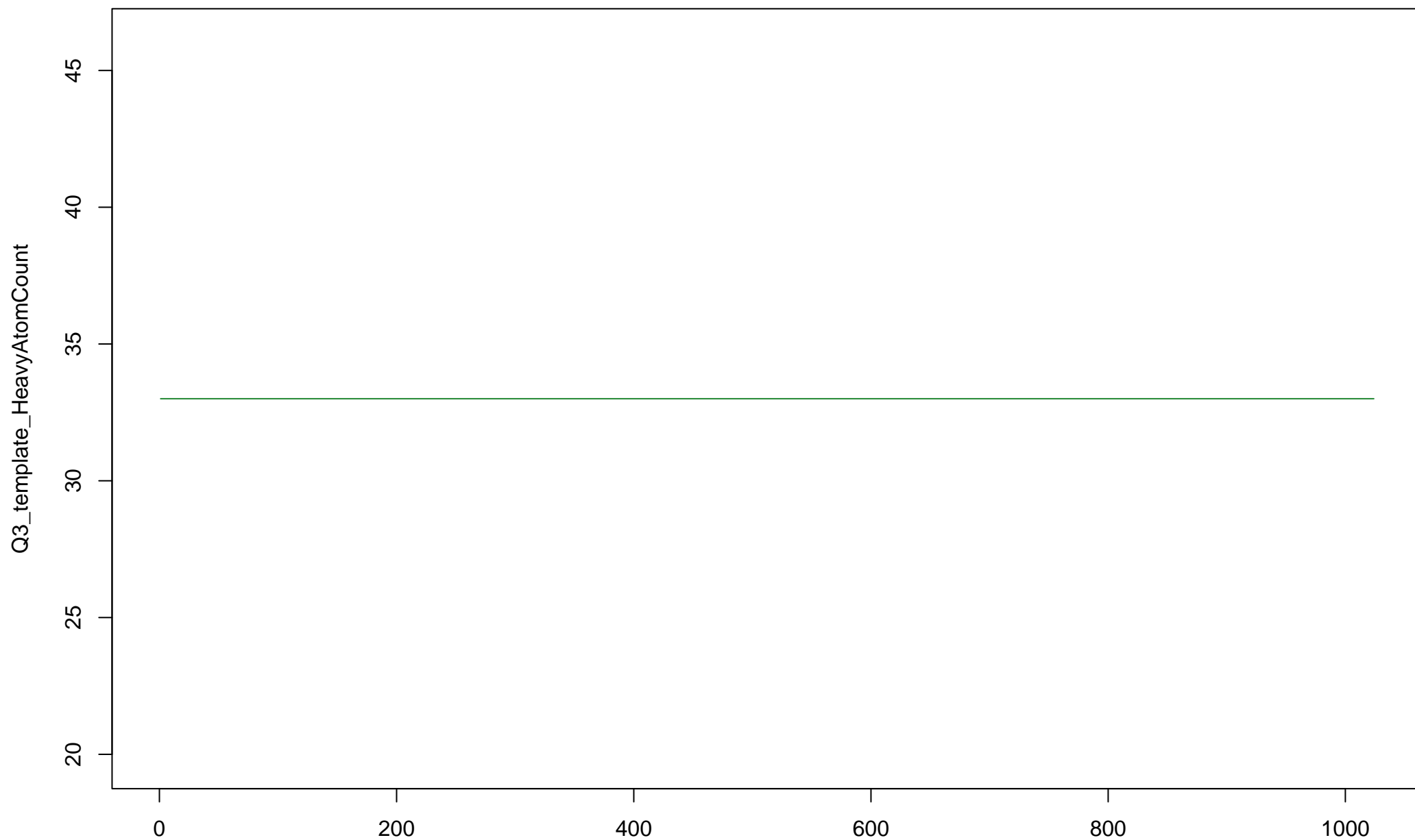
Q3_docked_HeavyAtomCount
ESS = 770 | BMK = 0.0984 | MCSE(6.27) = 4.15 | stat: TRUE | burn: 0



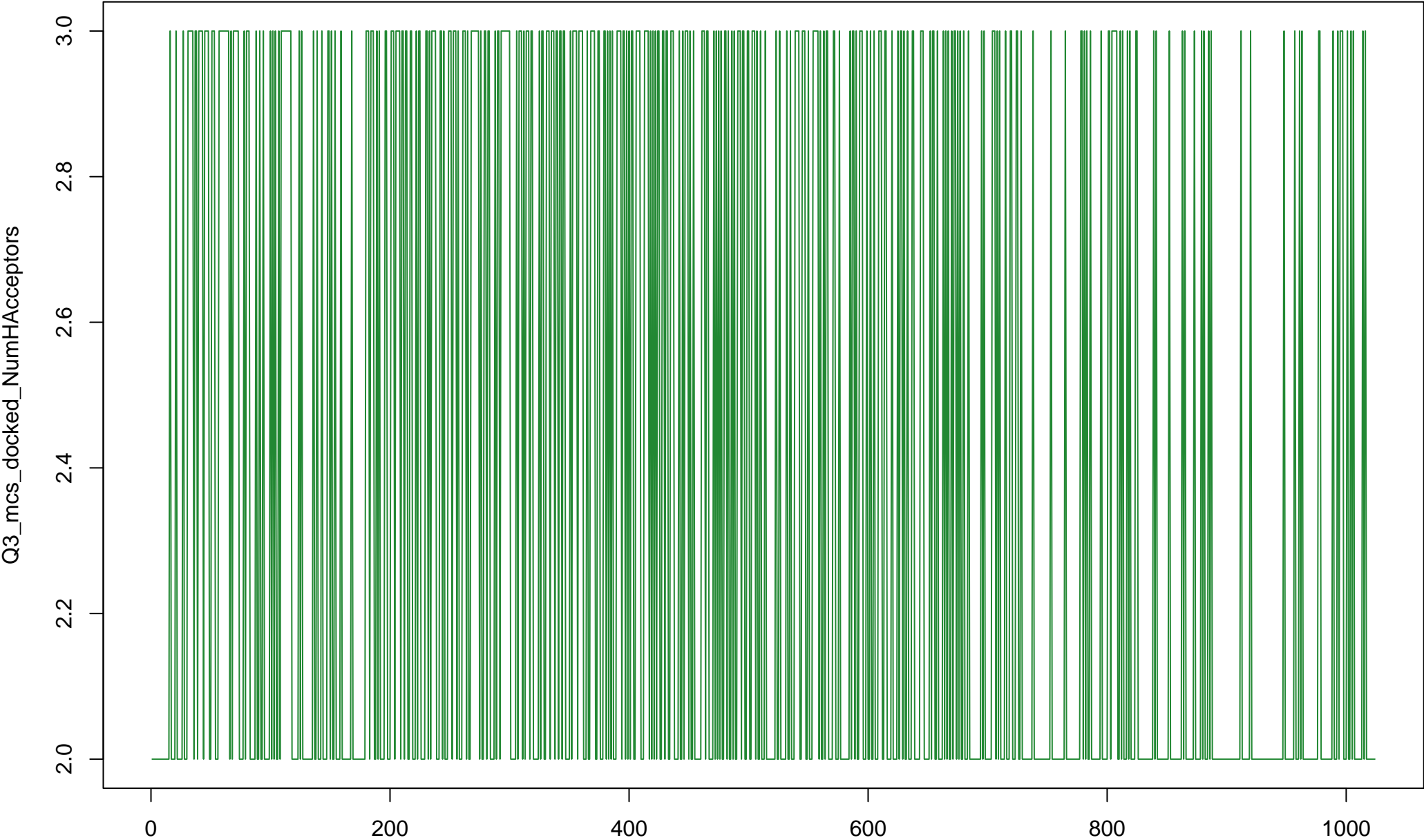
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



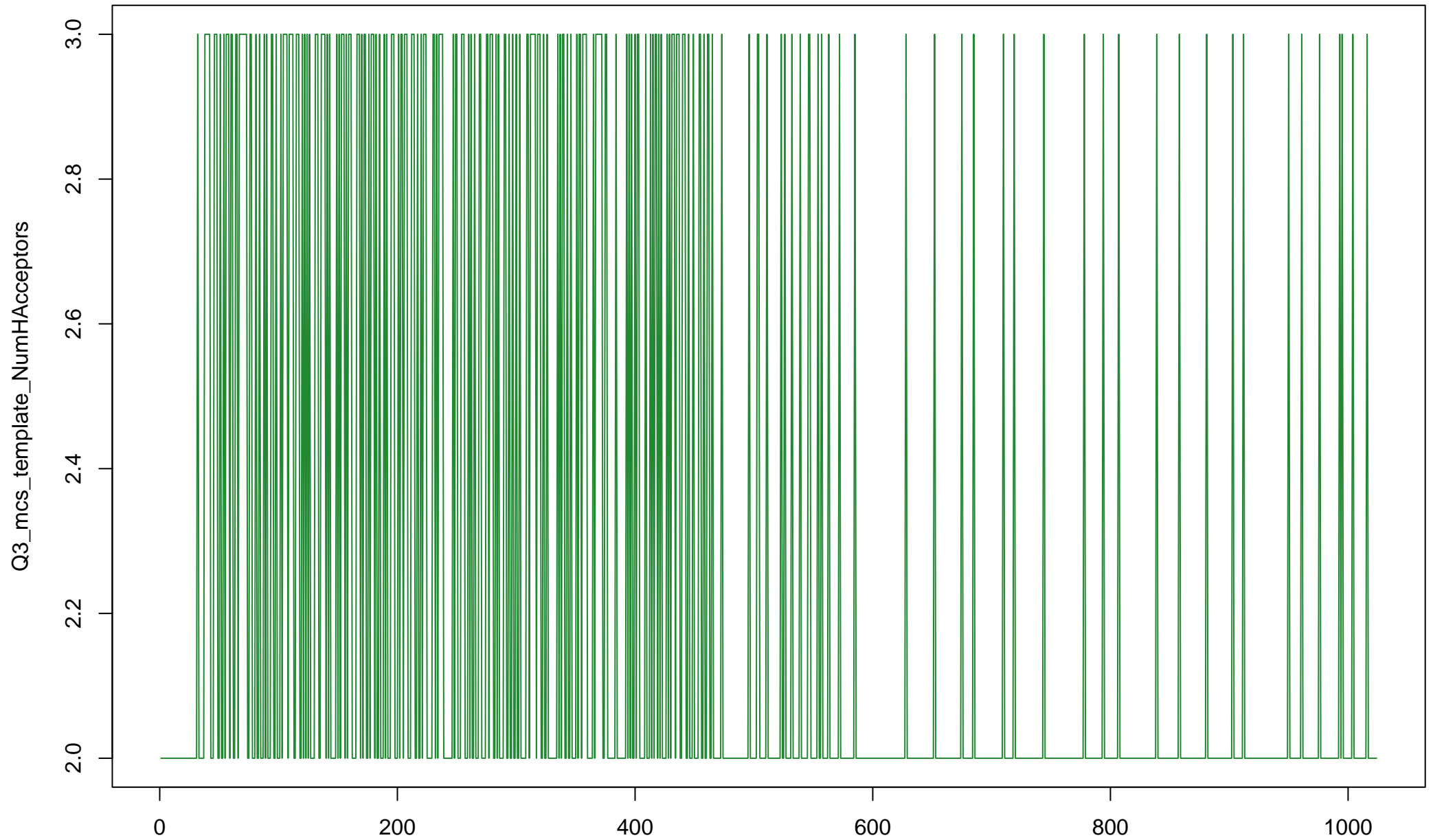
Q3_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



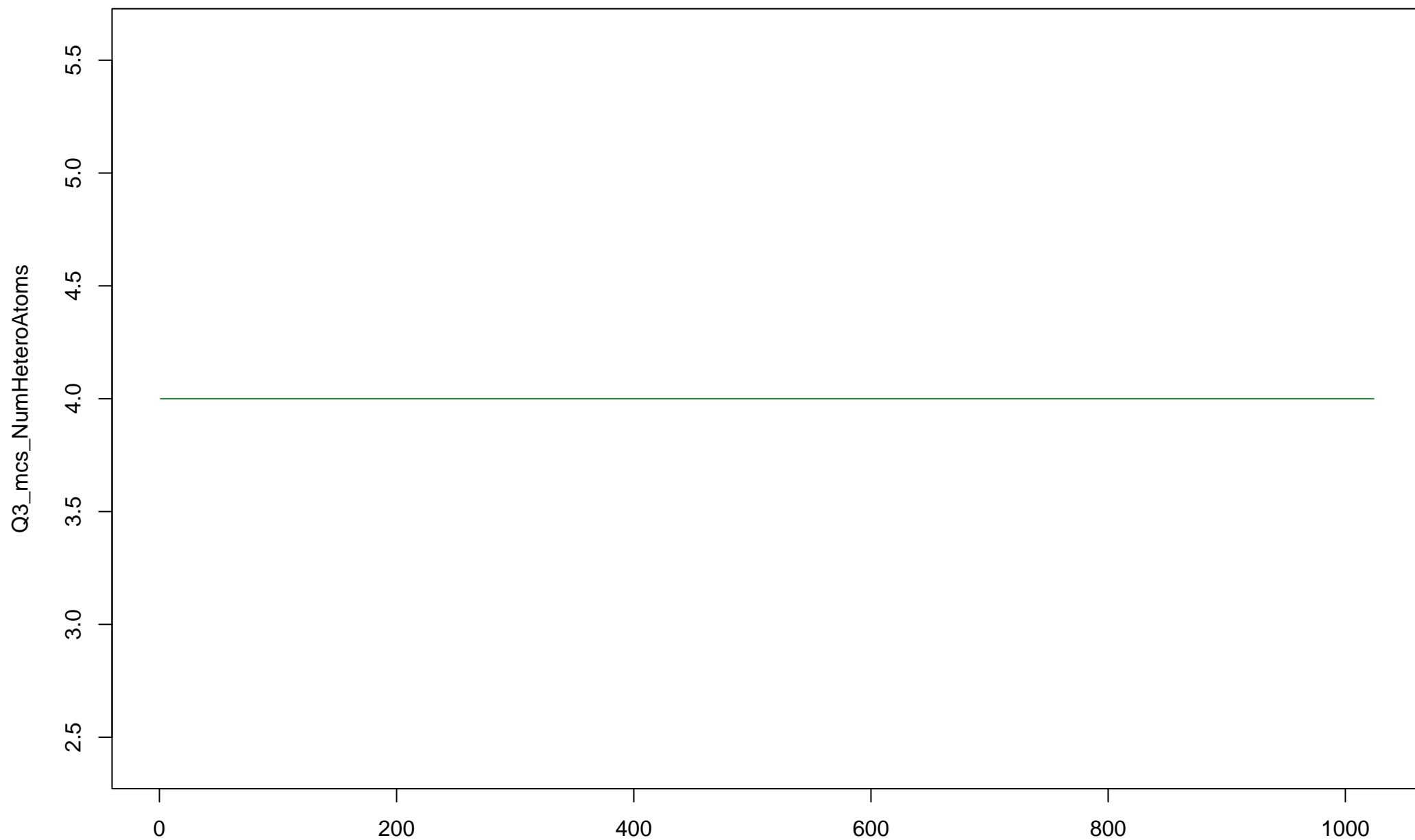
Q3_mcs_docked_NumHAcceptors
ESS = 175 | BMK = 0.329 | MCSE(6.27) = 6.68 | stat: FALSE | burn: 0



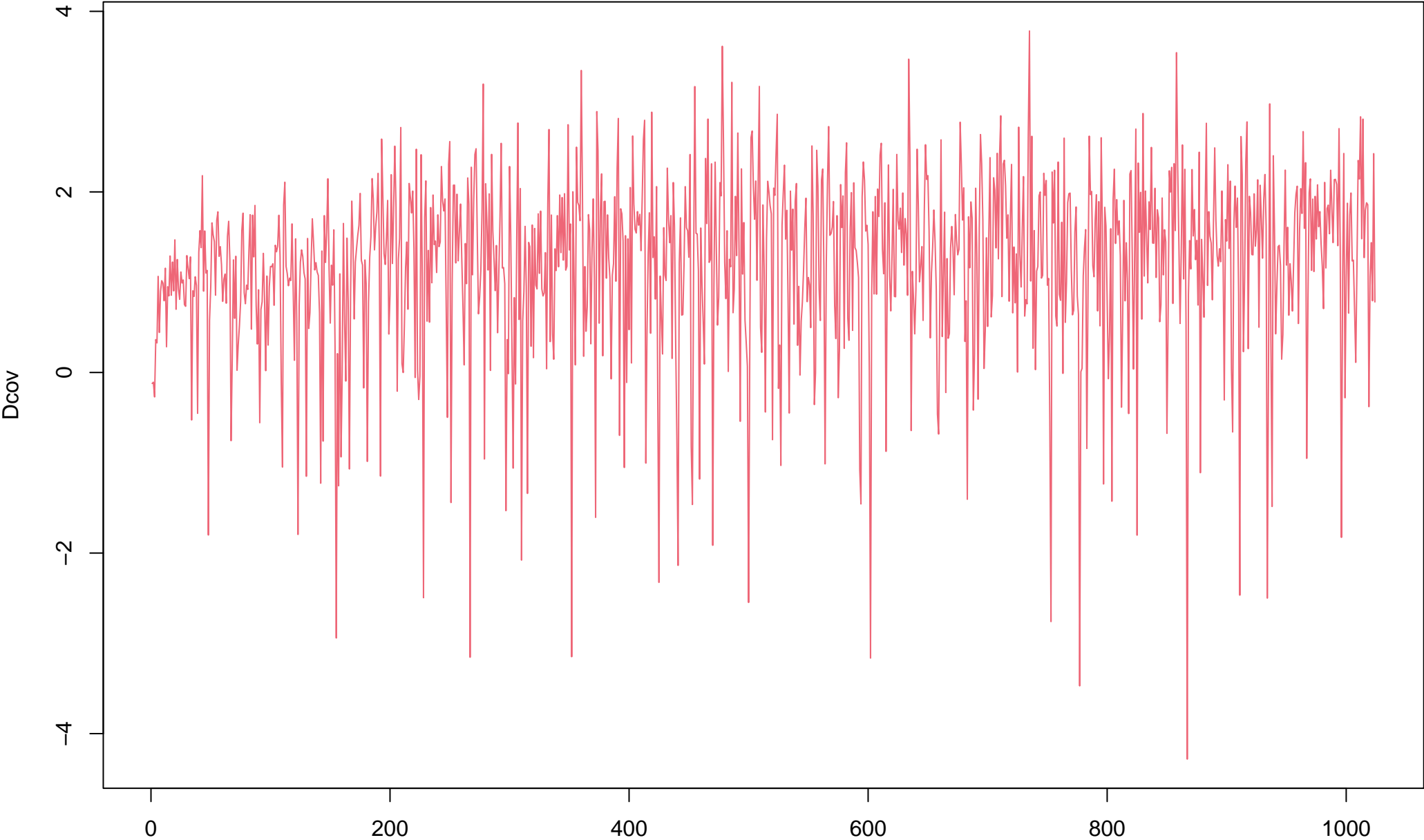
Q3_mcs_template_NumHAcceptors
ESS = 29.8 | BMK = 0.304 | MCSE(6.27) = 8.51 | stat: FALSE | burn: 0



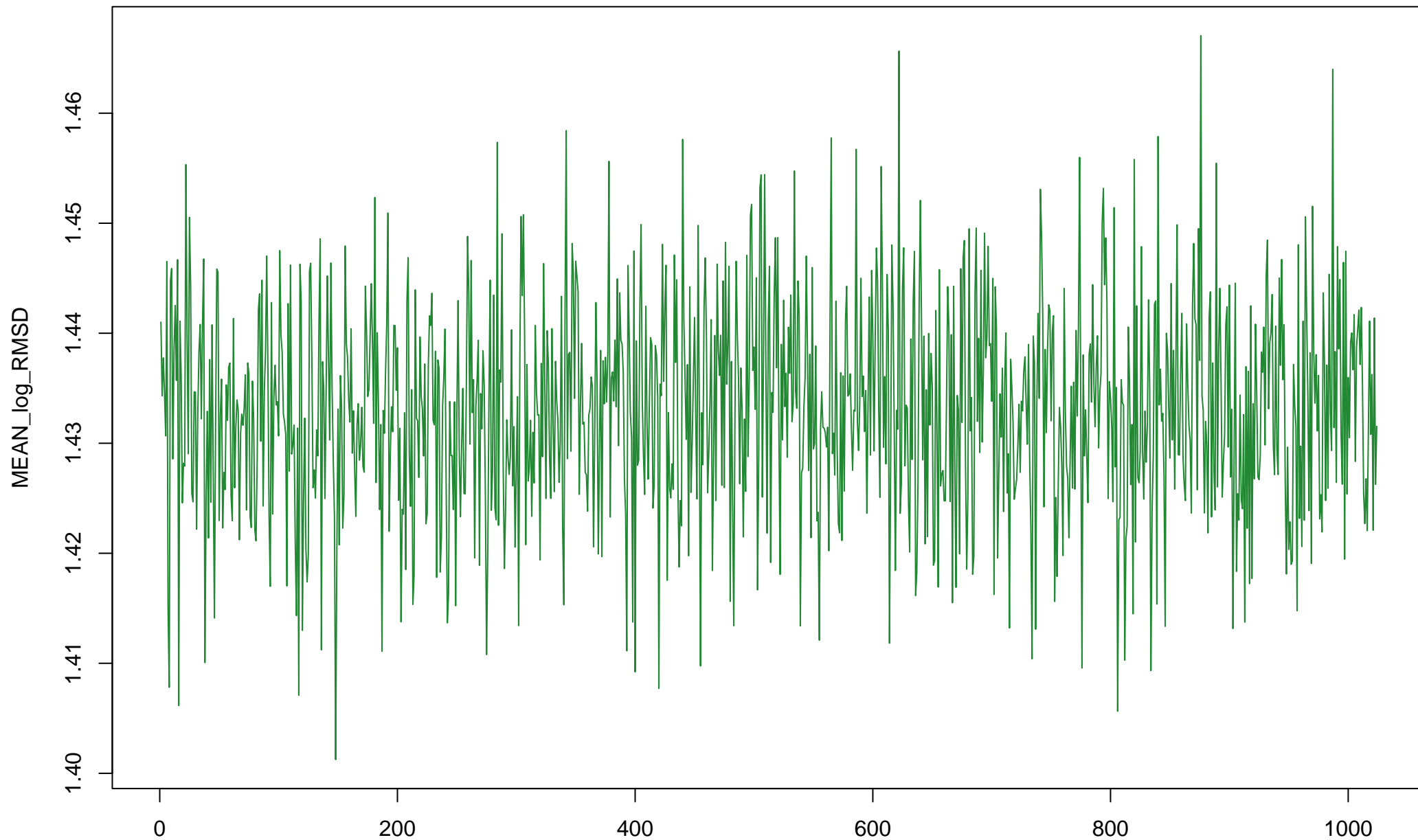
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



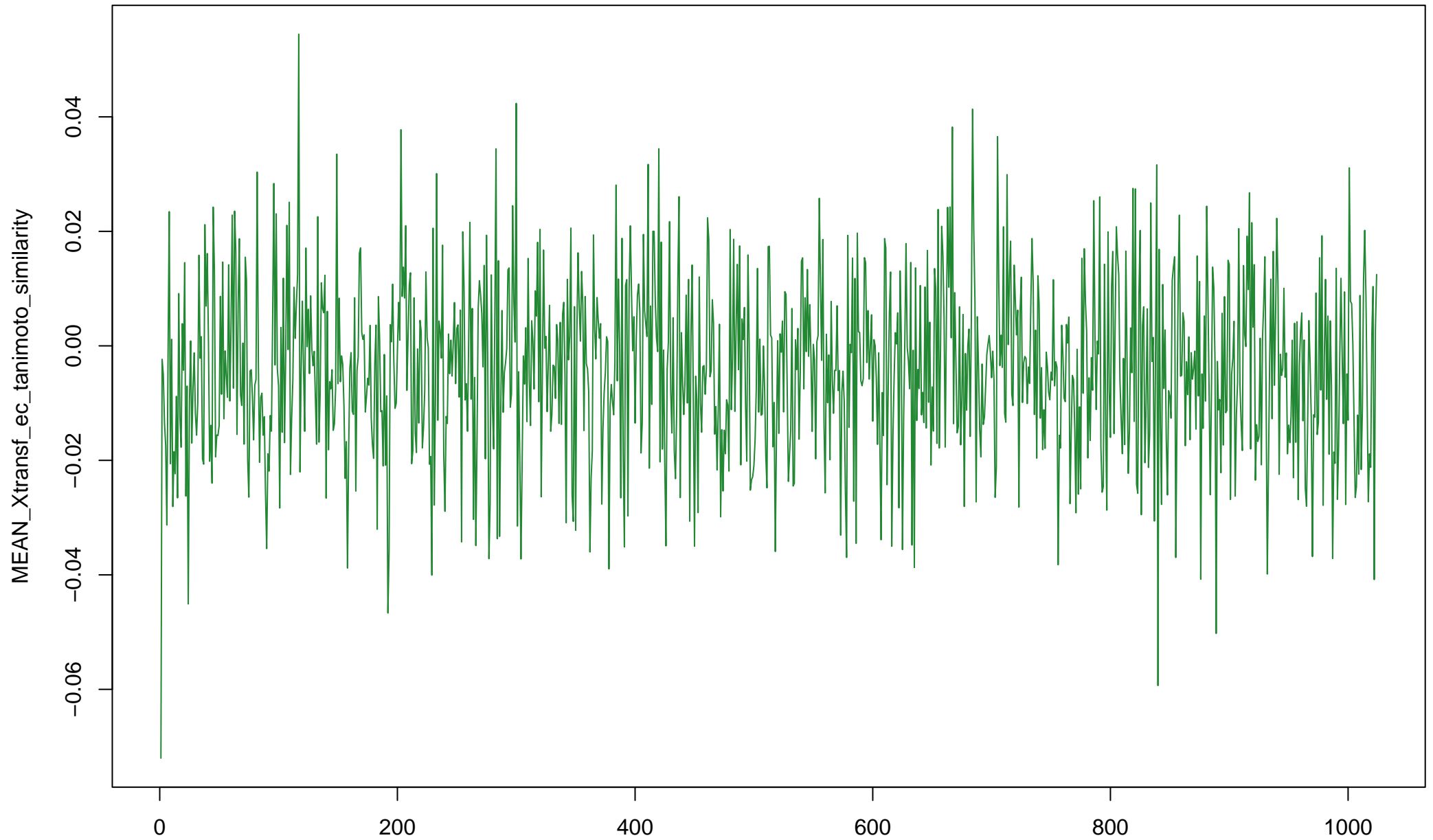
Dcov
ESS = 792 | BMK = 0.167 | MCSE(6.27) = 3.91 | stat: FALSE | burn: 0



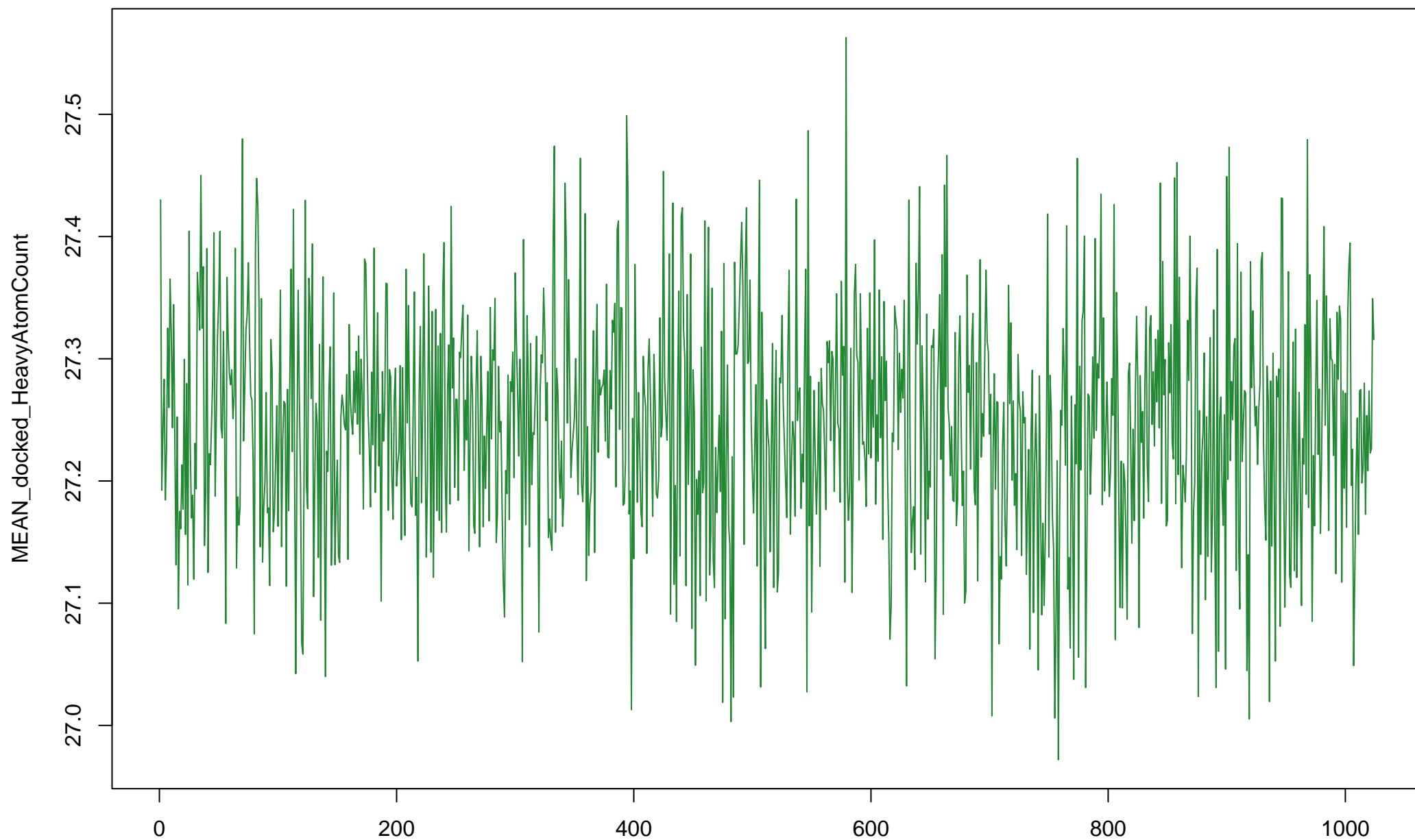
MEAN_log_RMSD
ESS = 1020 | BMK = 0.0515 | MCSE(6.27) = 3.78 | stat: TRUE | burn: 0



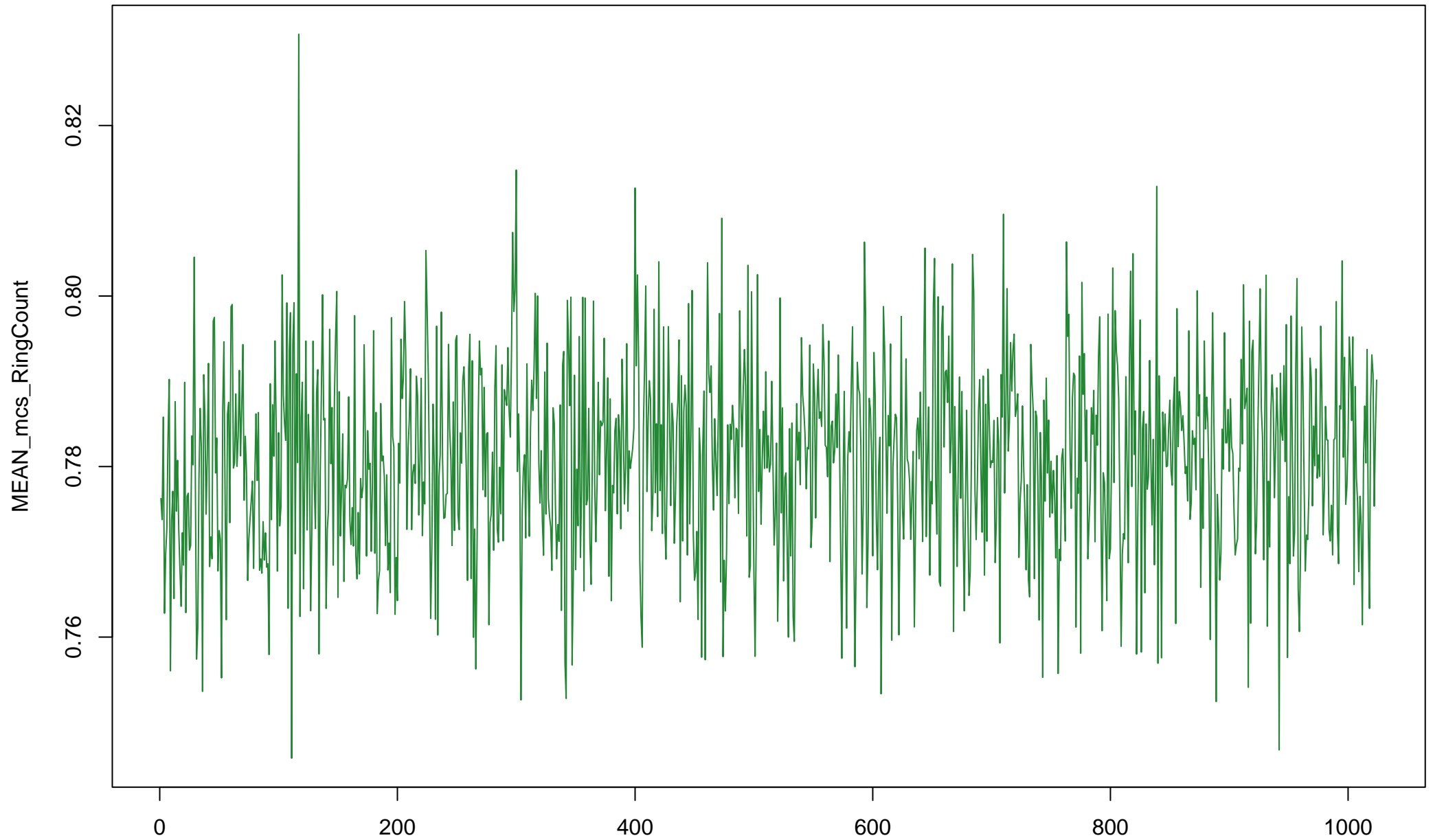
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0402 | MCSE(6.27) = 3.7 | stat: TRUE | burn: 0



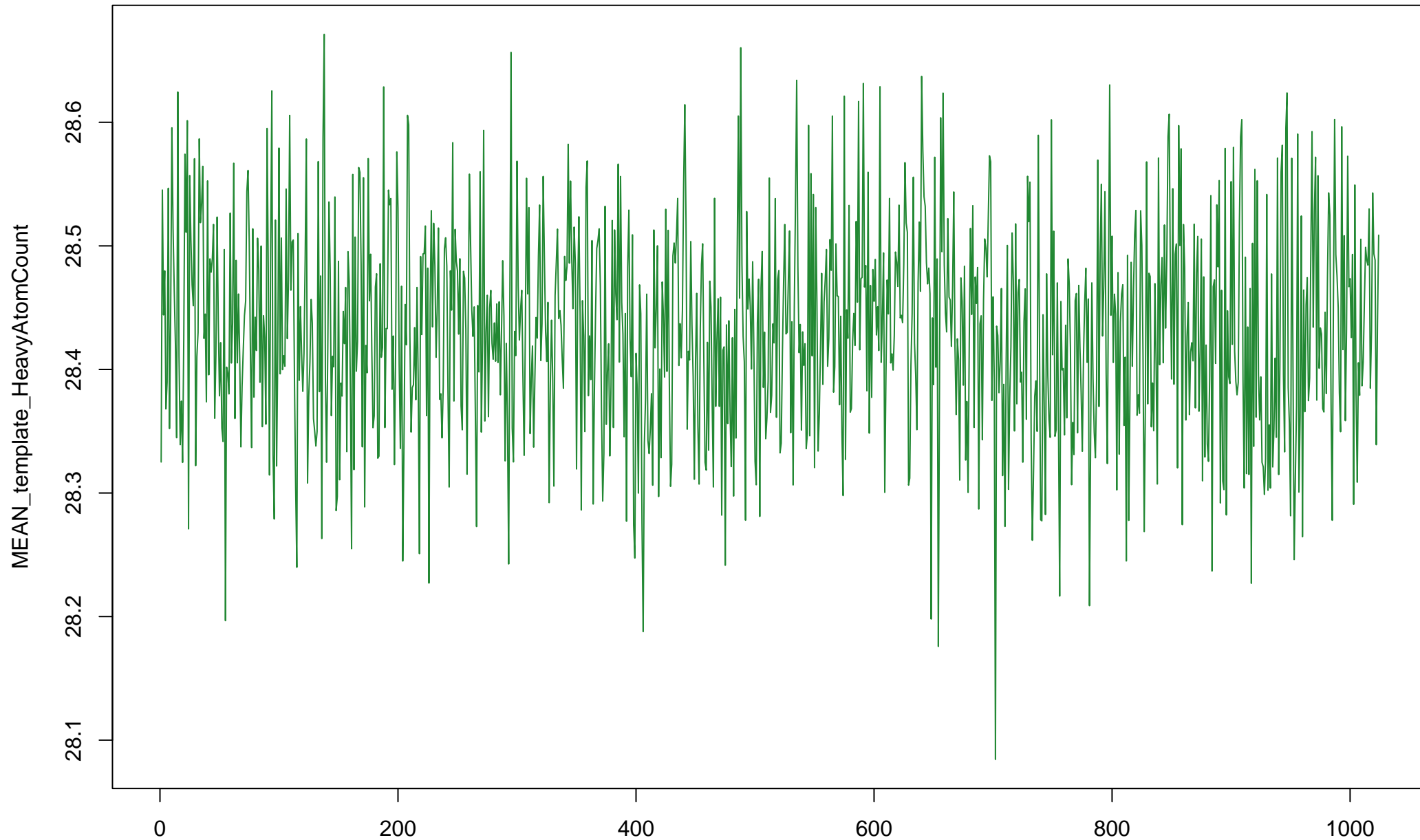
MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0598 | MCSE(6.27) = 3.93 | stat: TRUE | burn: 0



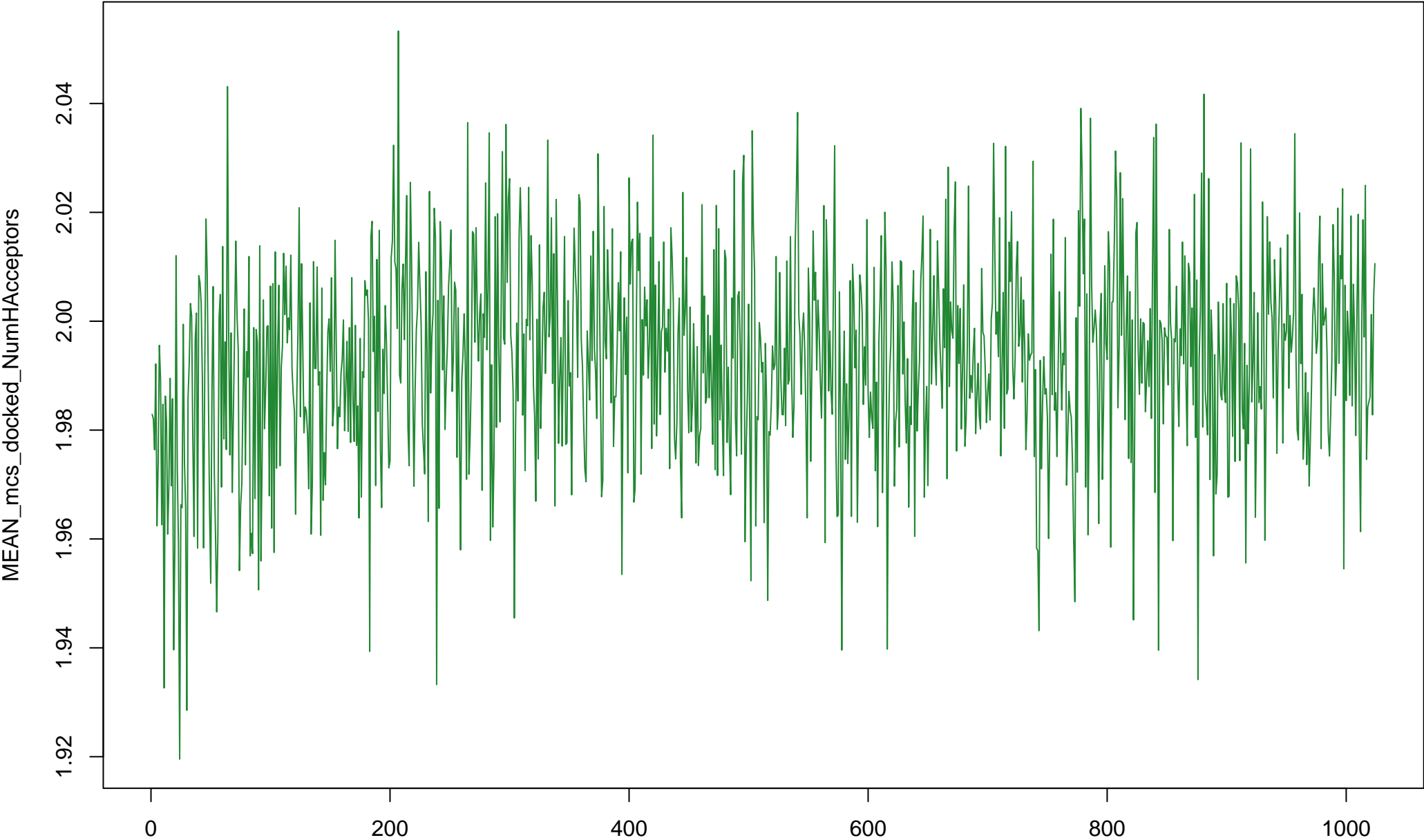
MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0641 | MCSE(6.27) = 3.75 | stat: FALSE | burn: 0



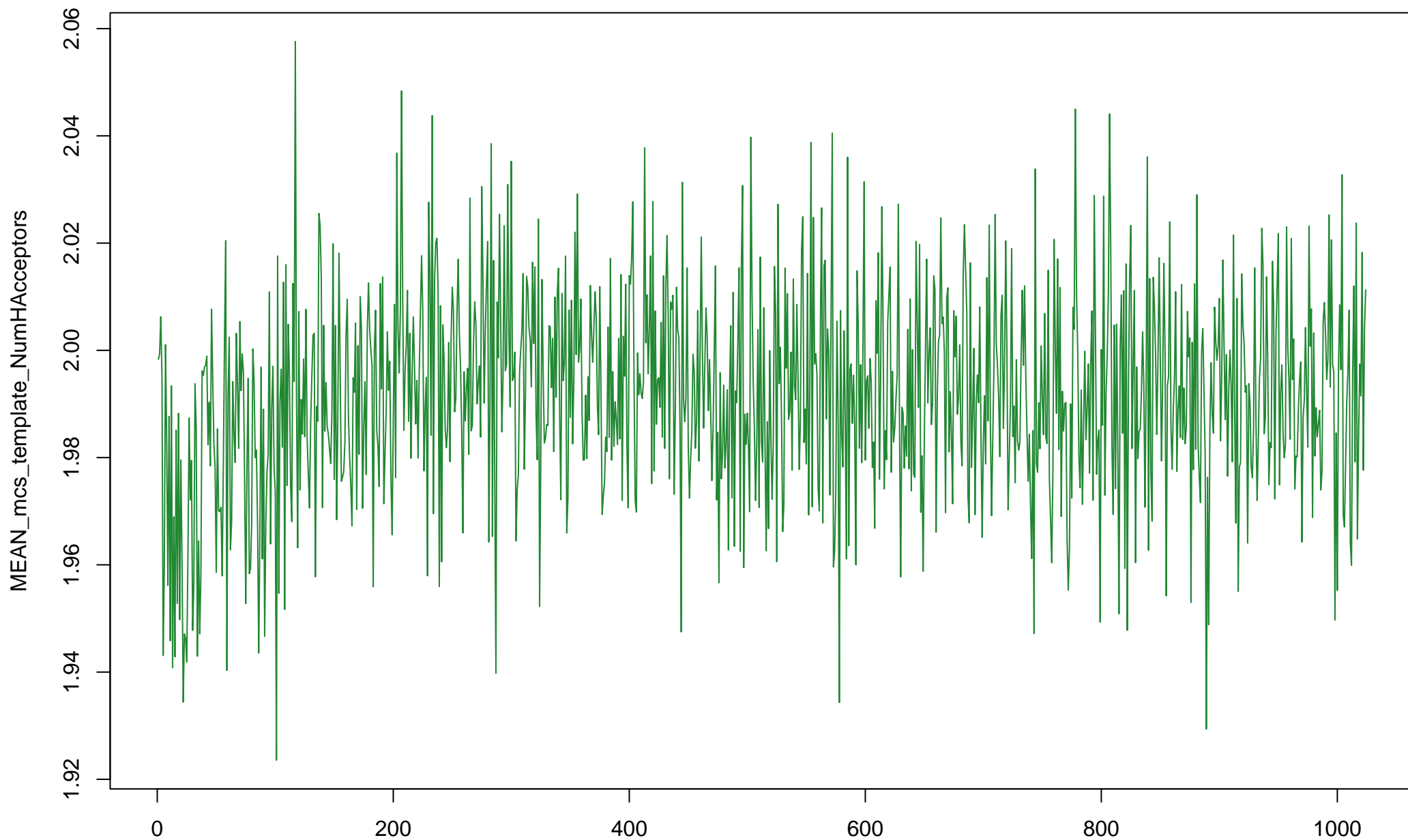
MEAN_template_HeavyAtomCount
ESS = 1020 | BMK = 0.0447 | MCSE(6.27) = 3.81 | stat: TRUE | burn: 0



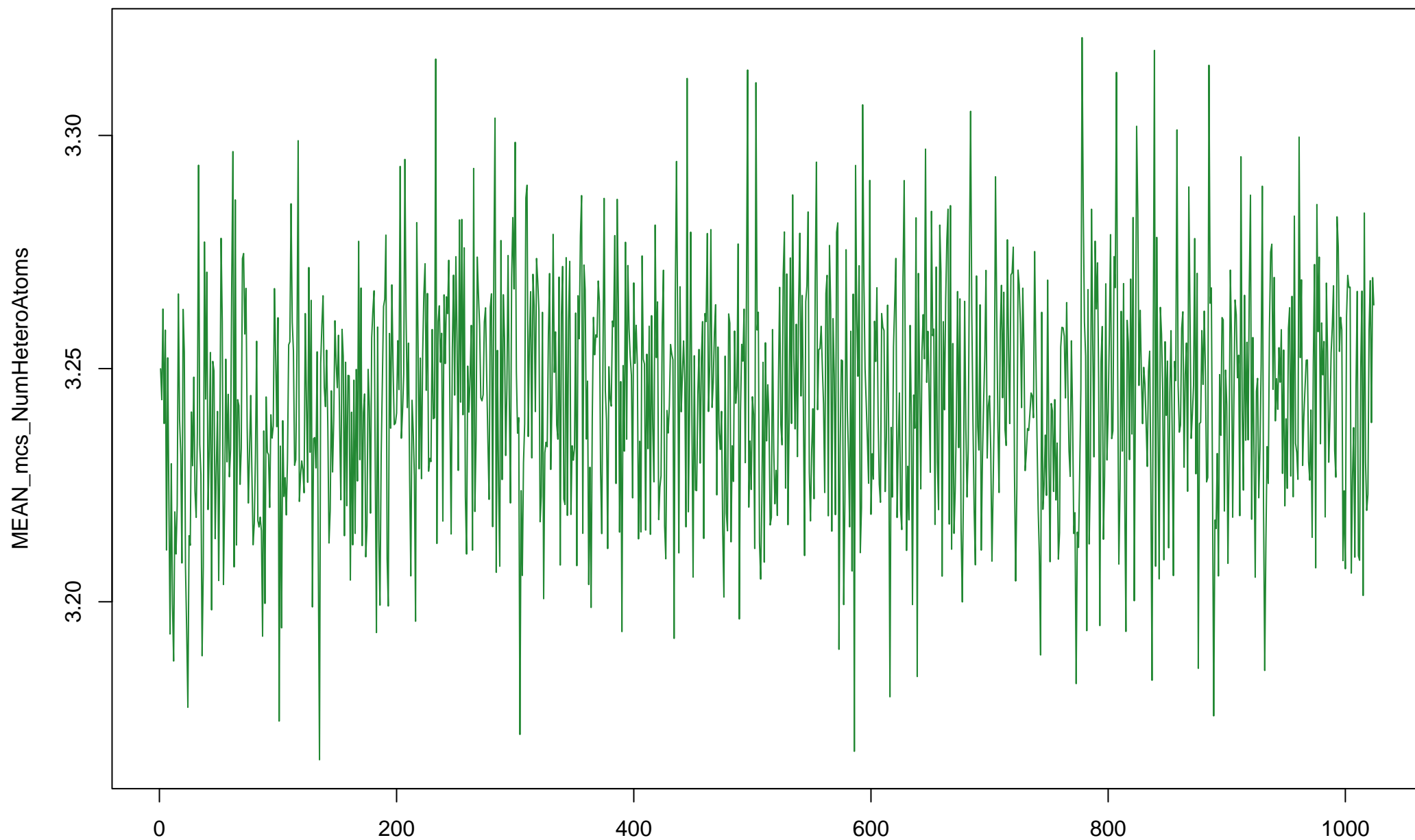
MEAN_mcs_docked_NumHAcceptors
ESS = 516 | BMK = 0.086 | MCSE(6.27) = 5.31 | stat: FALSE | burn: 0



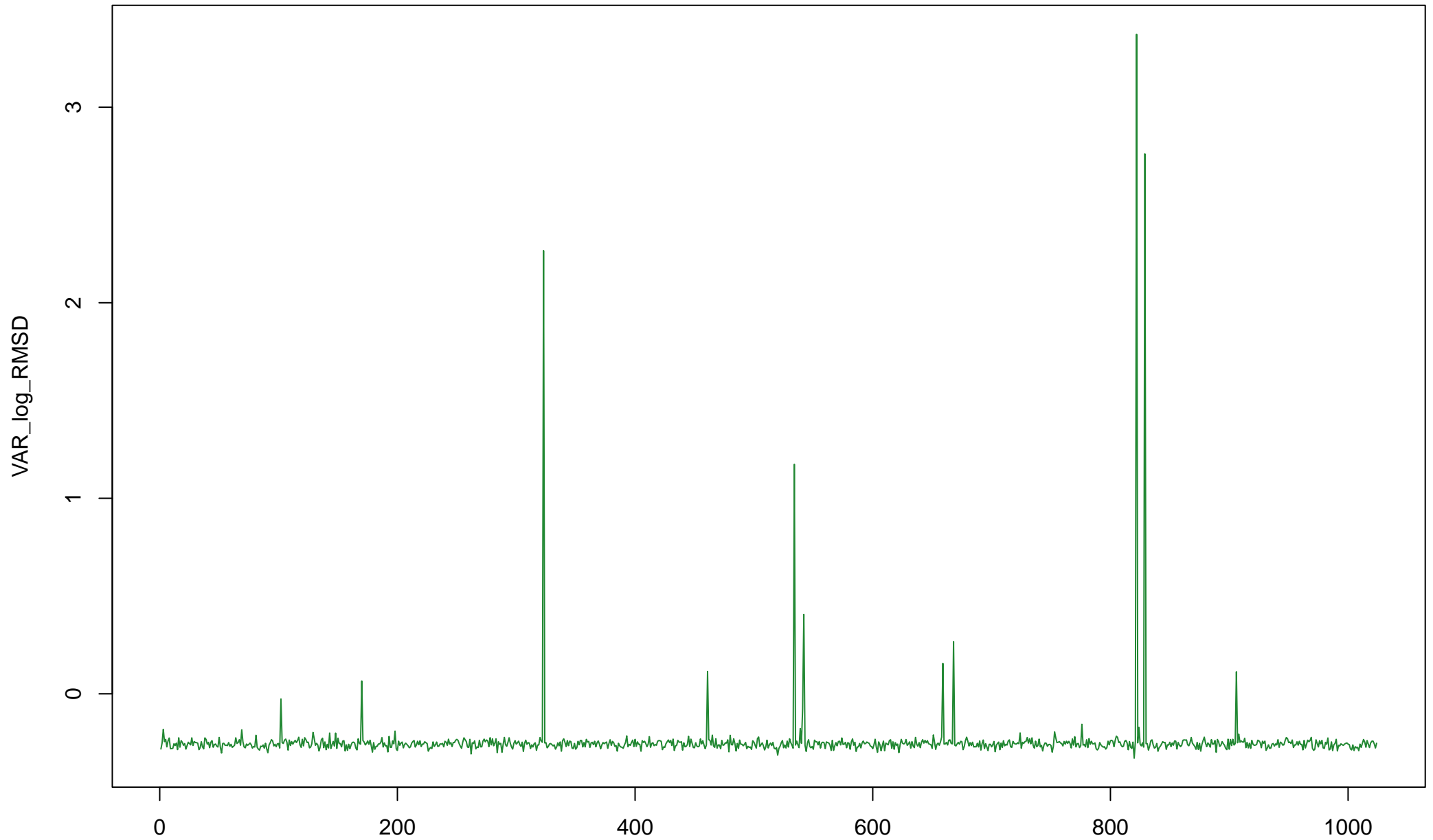
MEAN_mcs_template_NumHAcceptors
ESS = 179 | BMK = 0.0698 | MCSE(6.27) = 5.68 | stat: FALSE | burn: 0



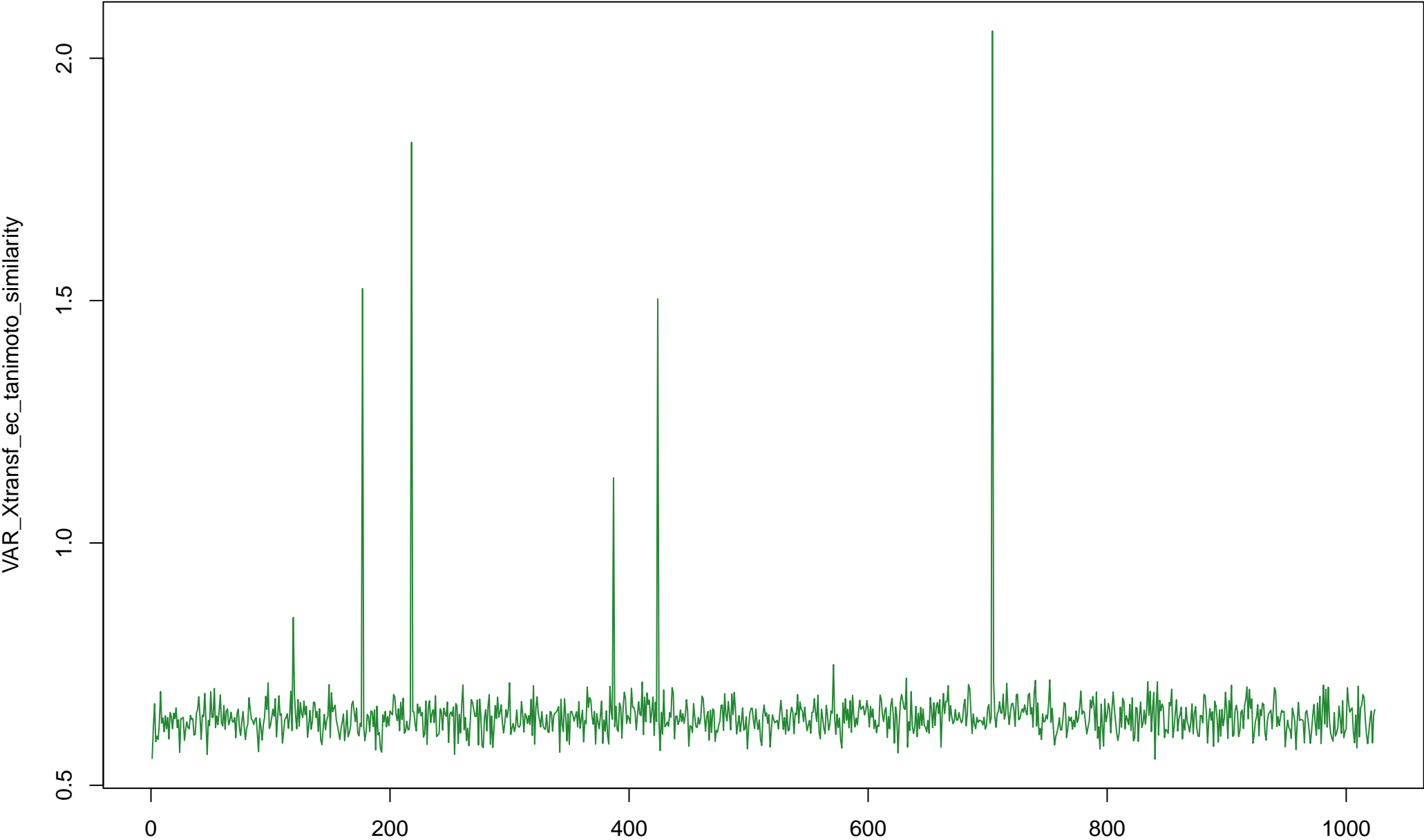
MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0461 | MCSE(6.27) = 3.96 | stat: FALSE | burn: 0



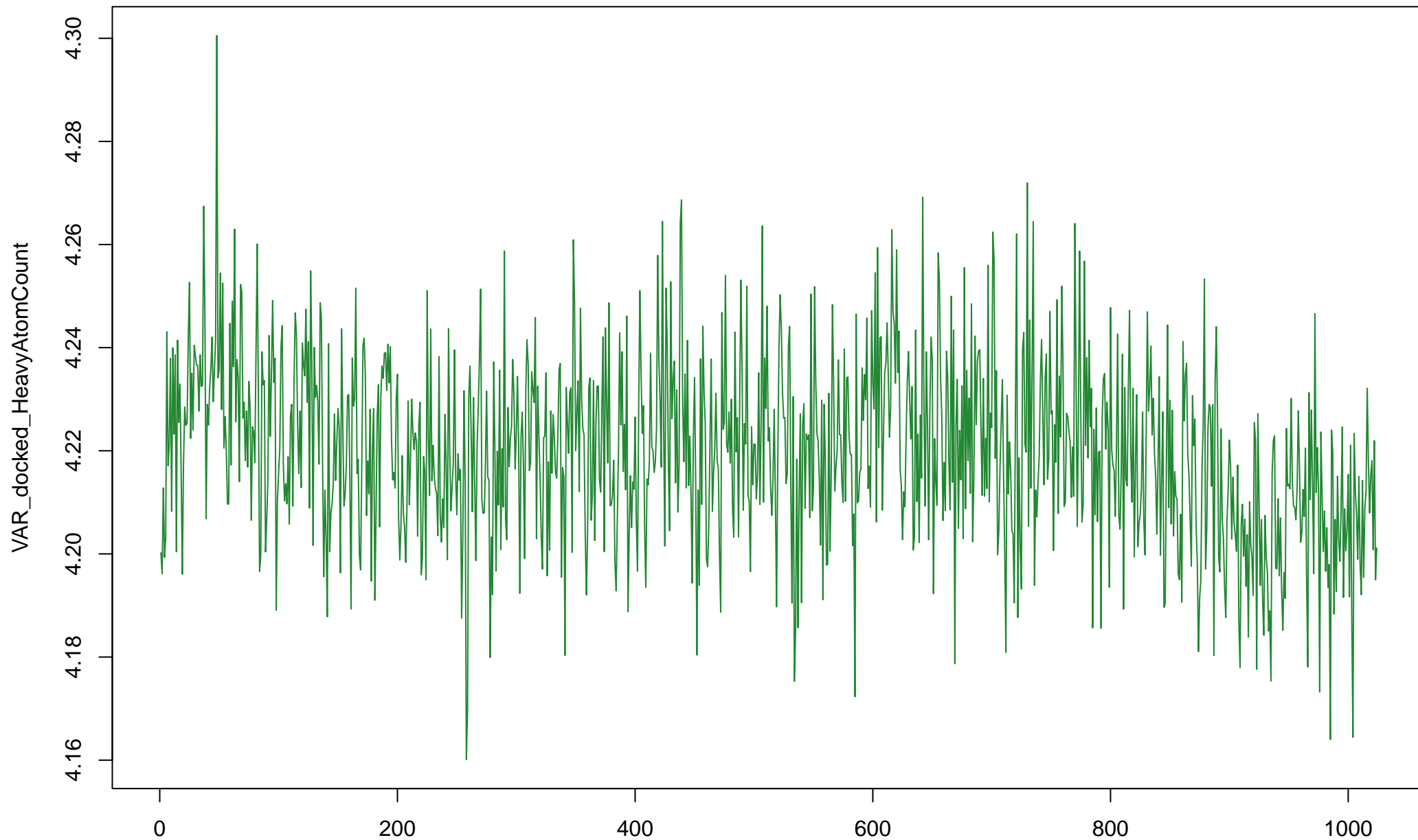
VAR_log_RMSD
ESS = 678 | BMK = 0.206 | MCSE(6.27) = 4.12 | stat: TRUE | burn: 0



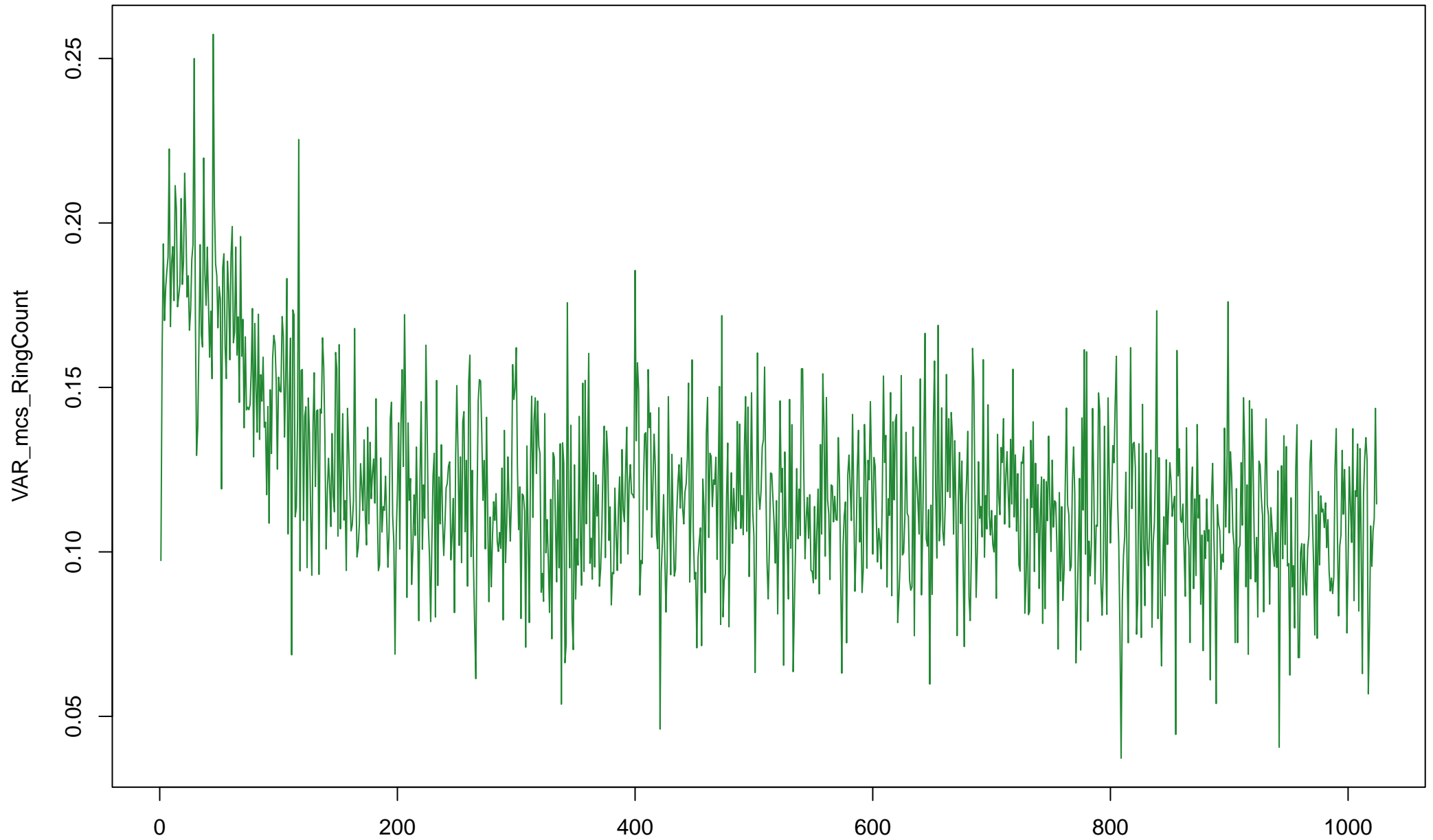
VAR_Xtransf_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.103 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0



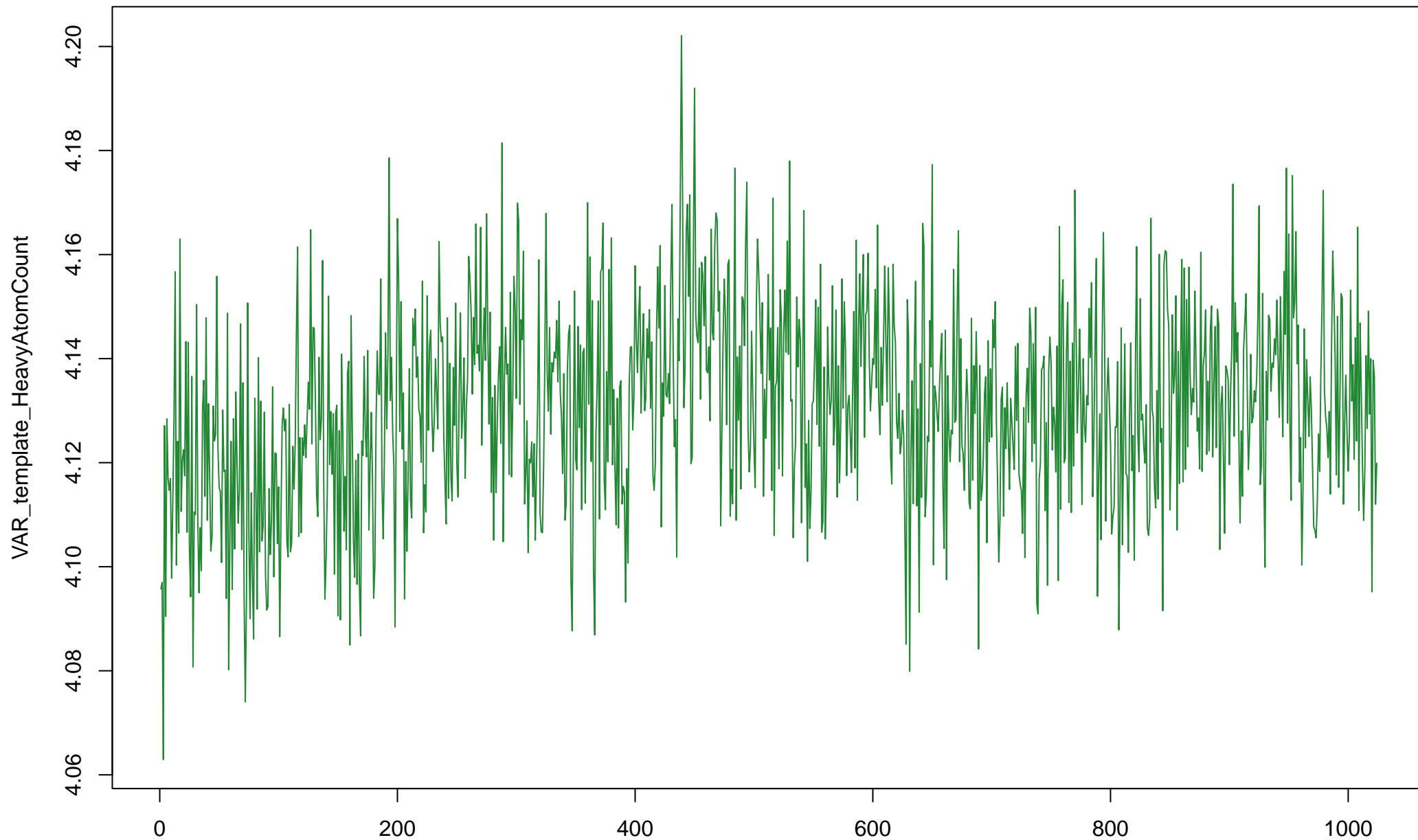
VAR_docked_HeavyAtomCount
ESS = 64.9 | BMK = 0.117 | MCSE(6.27) = 7.29 | stat: FALSE | burn: 0



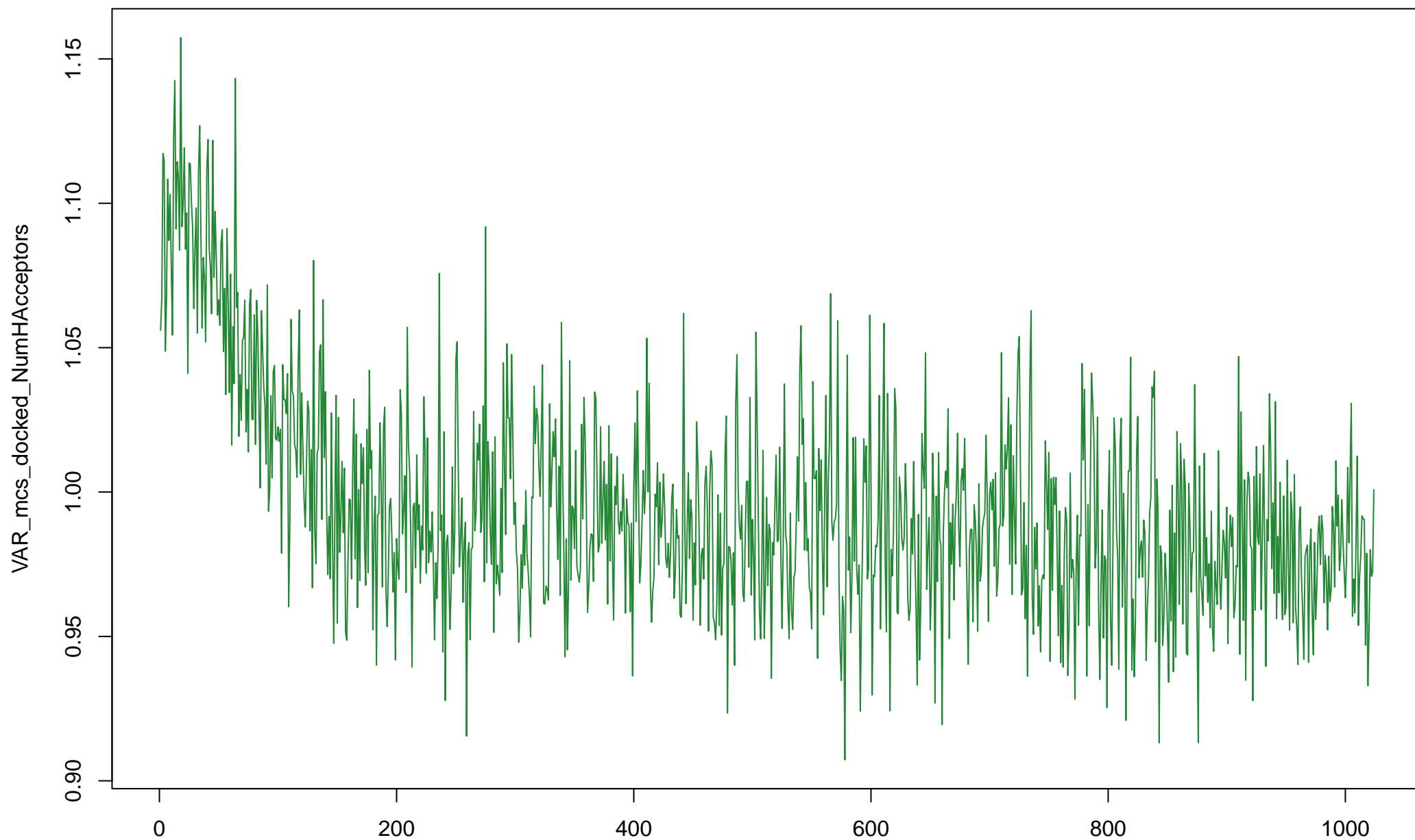
VAR_mcs_RingCount
ESS = 14.1 | BMK = 0.261 | MCSE(6.27) = 11.7 | stat: FALSE | burn: 102



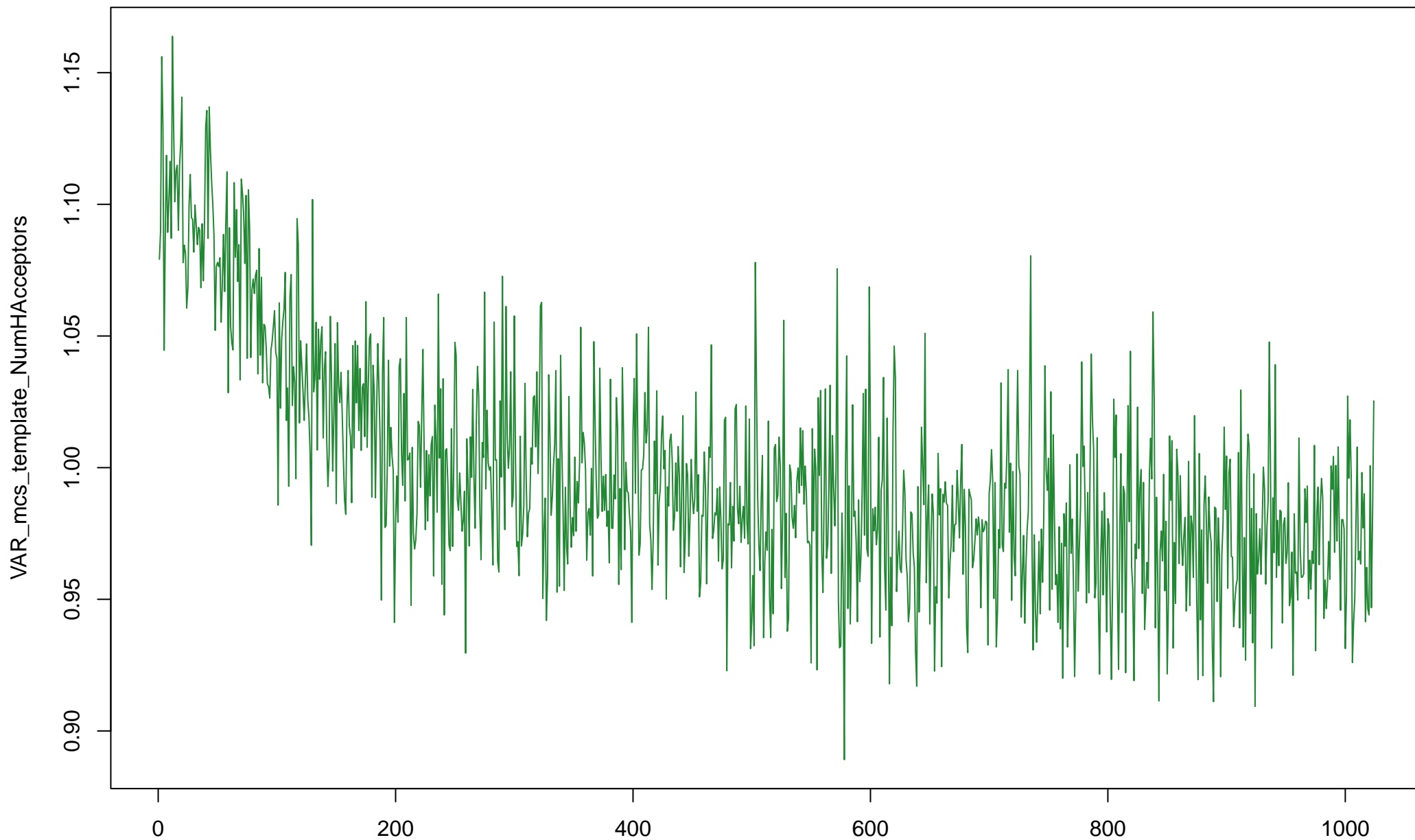
VAR_template_HeavyAtomCount
ESS = 119 | BMK = 0.11 | MCSE(6.27) = 7.49 | stat: FALSE | burn: 0



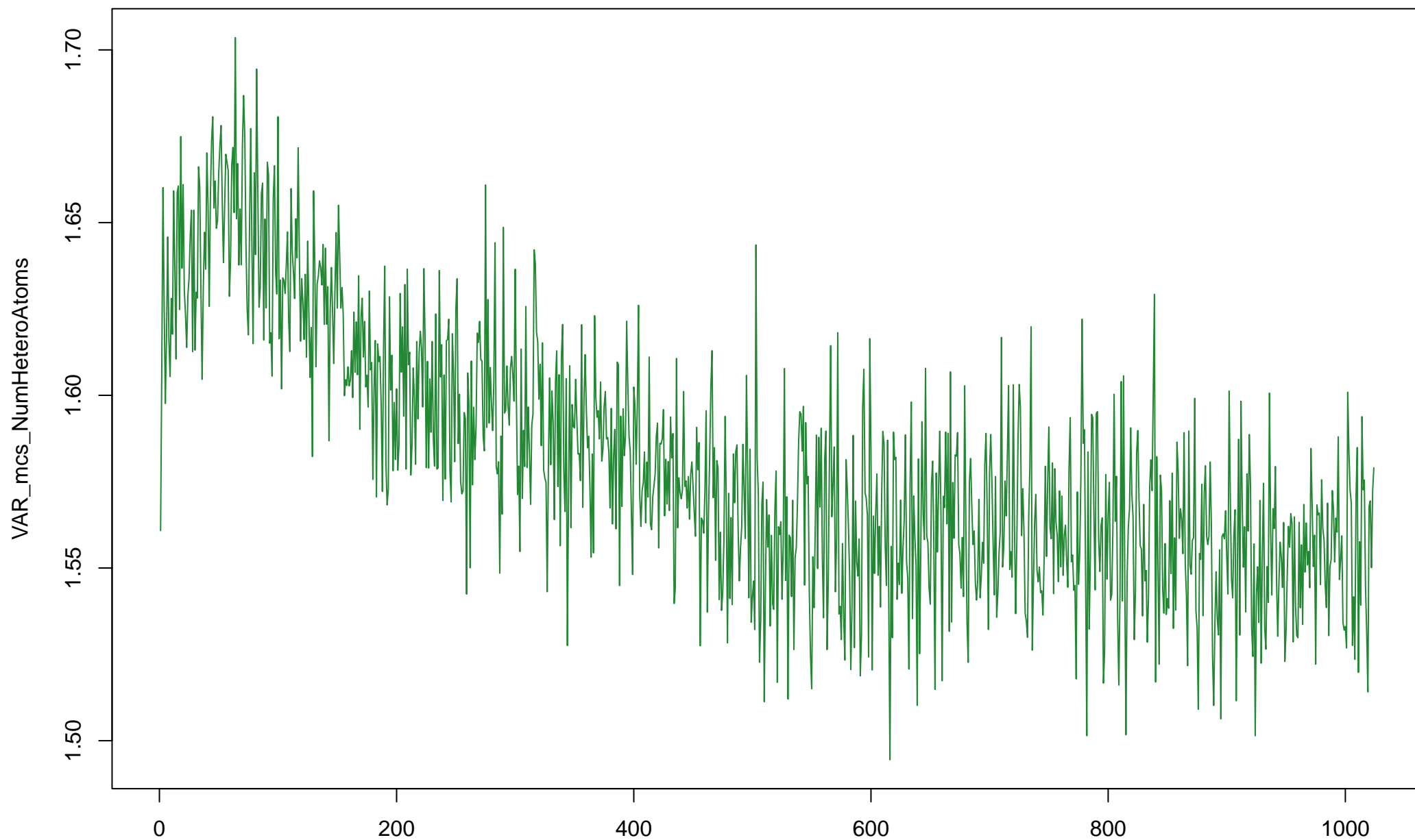
VAR_mcs_docked_NumHAcceptors
ESS = 14.1 | BMK = 0.268 | MCSE(6.27) = 12.7 | stat: FALSE | burn: 102



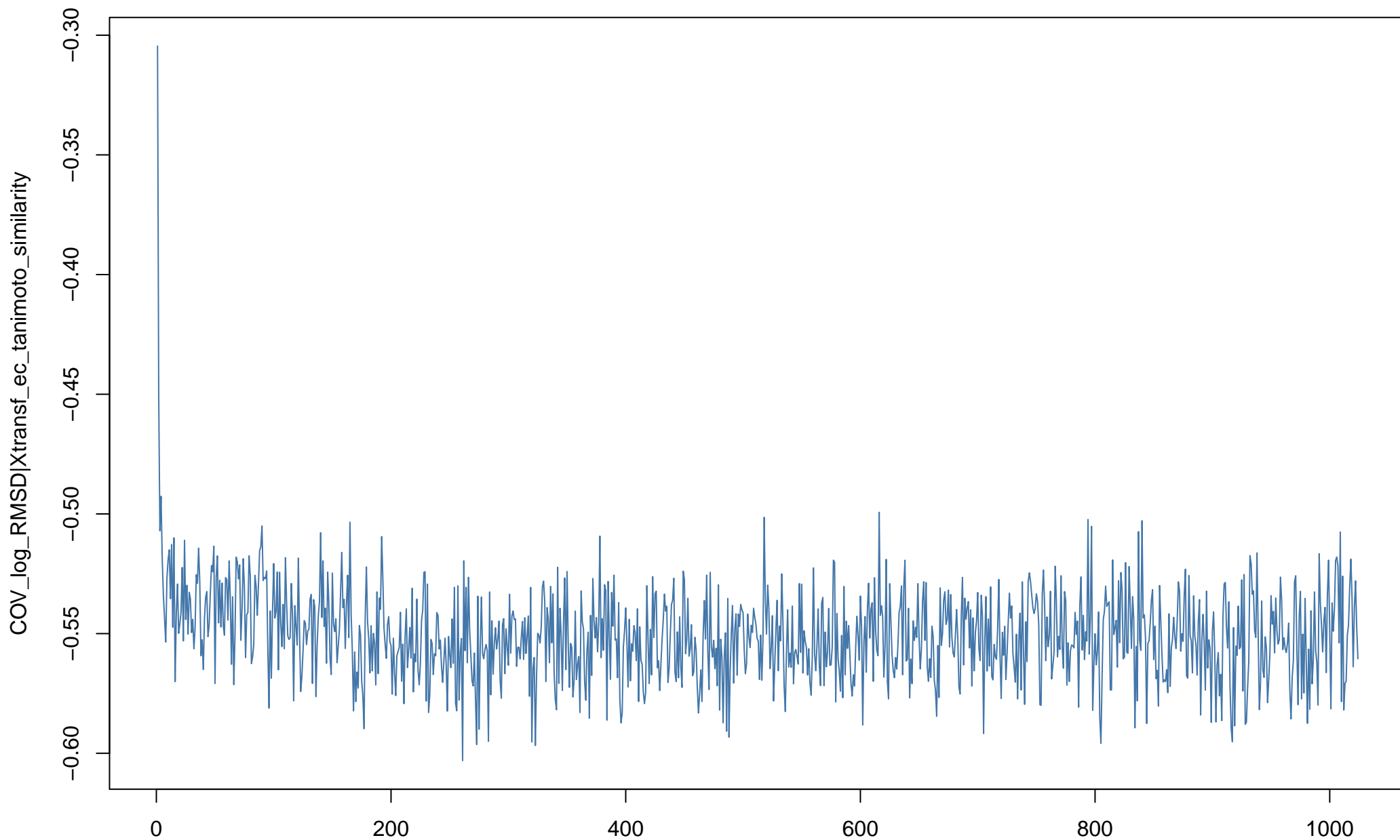
VAR_mcs_template_NumHAcceptors
ESS = 8.44 | BMK = 0.388 | MCSE(6.27) = 13.9 | stat: FALSE | burn: 102



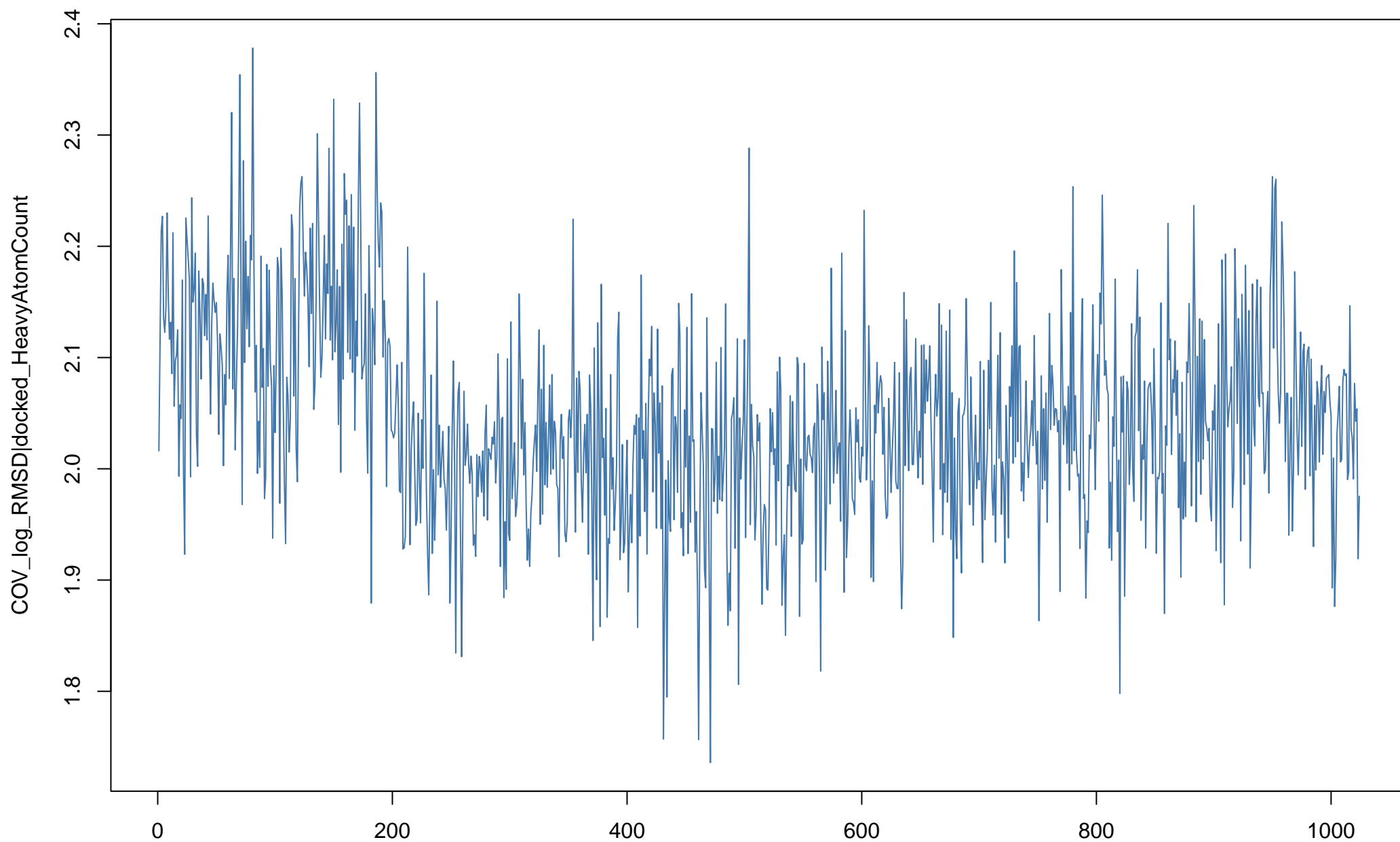
VAR_mcs_NumHeteroAtoms
ESS = 2.74 | BMK = 0.525 | MCSE(6.27) = 14.6 | stat: FALSE | burn: 0



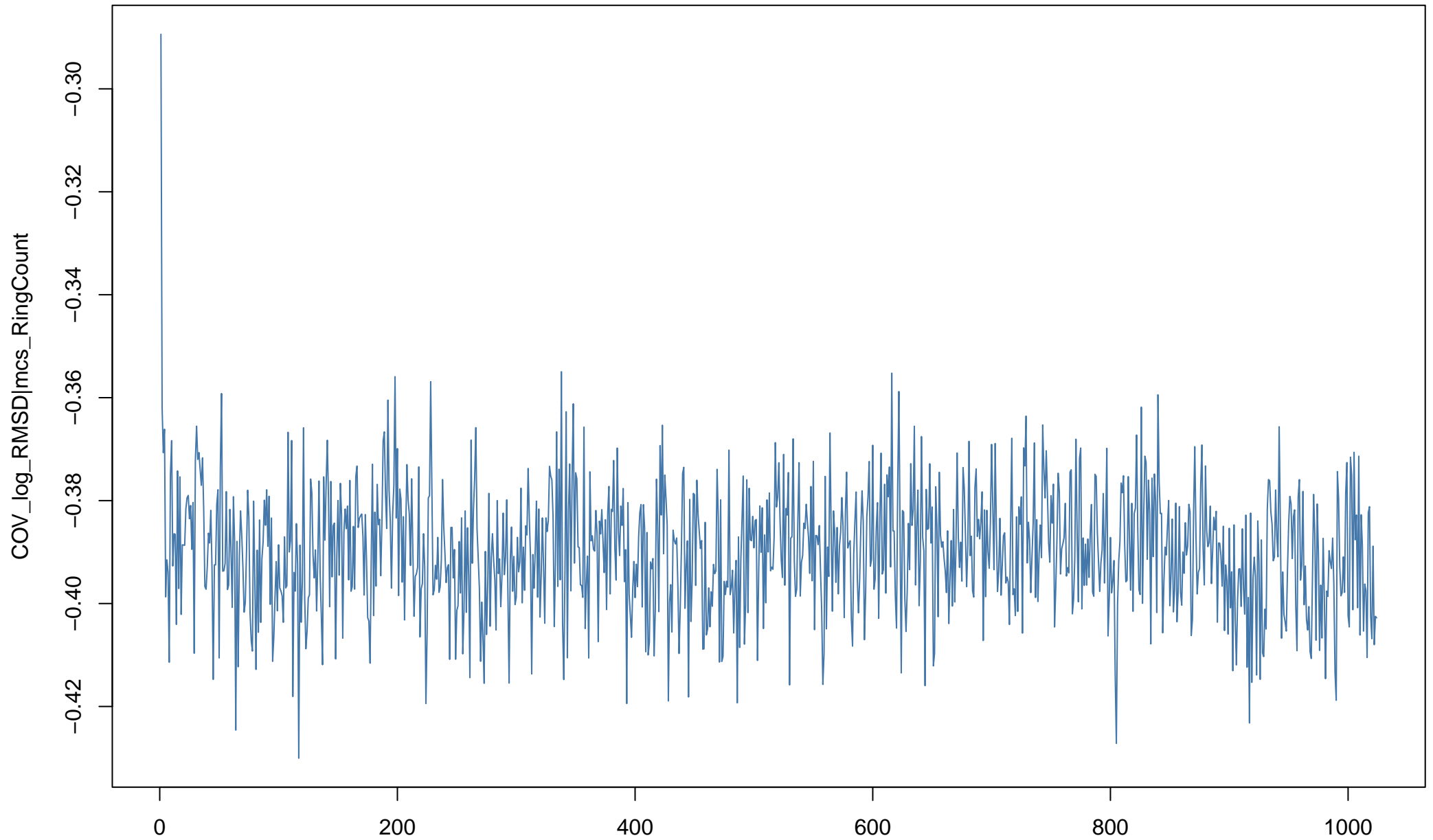
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 453 | BMK = 0.0734 | MCSE(6.27) = 6.48 | stat: FALSE | burn: 0



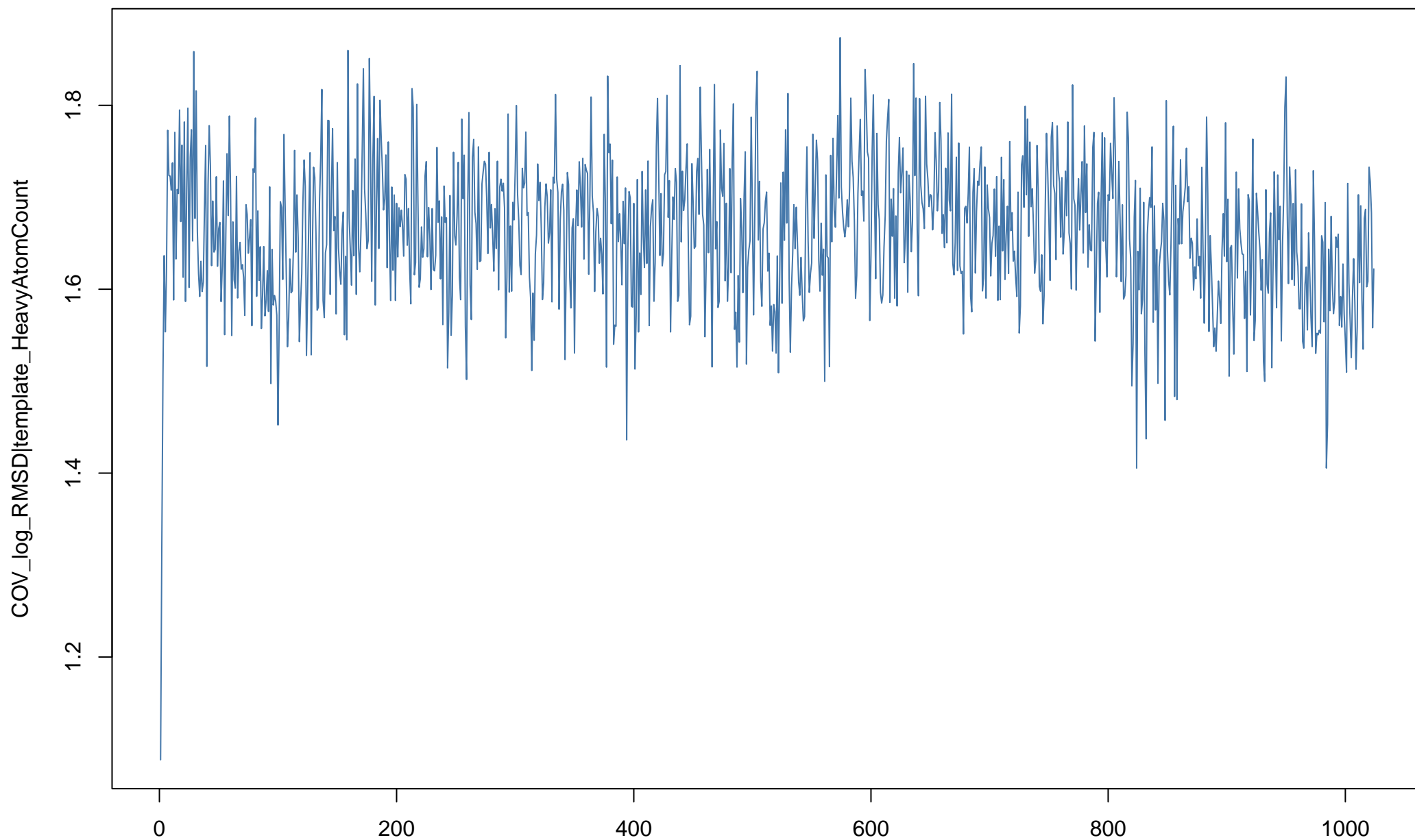
COV_log_RMSD|docked_HeavyAtomCount
ESS = 25.8 | BMK = 0.162 | MCSE(6.27) = 9.69 | stat: FALSE | burn: 204



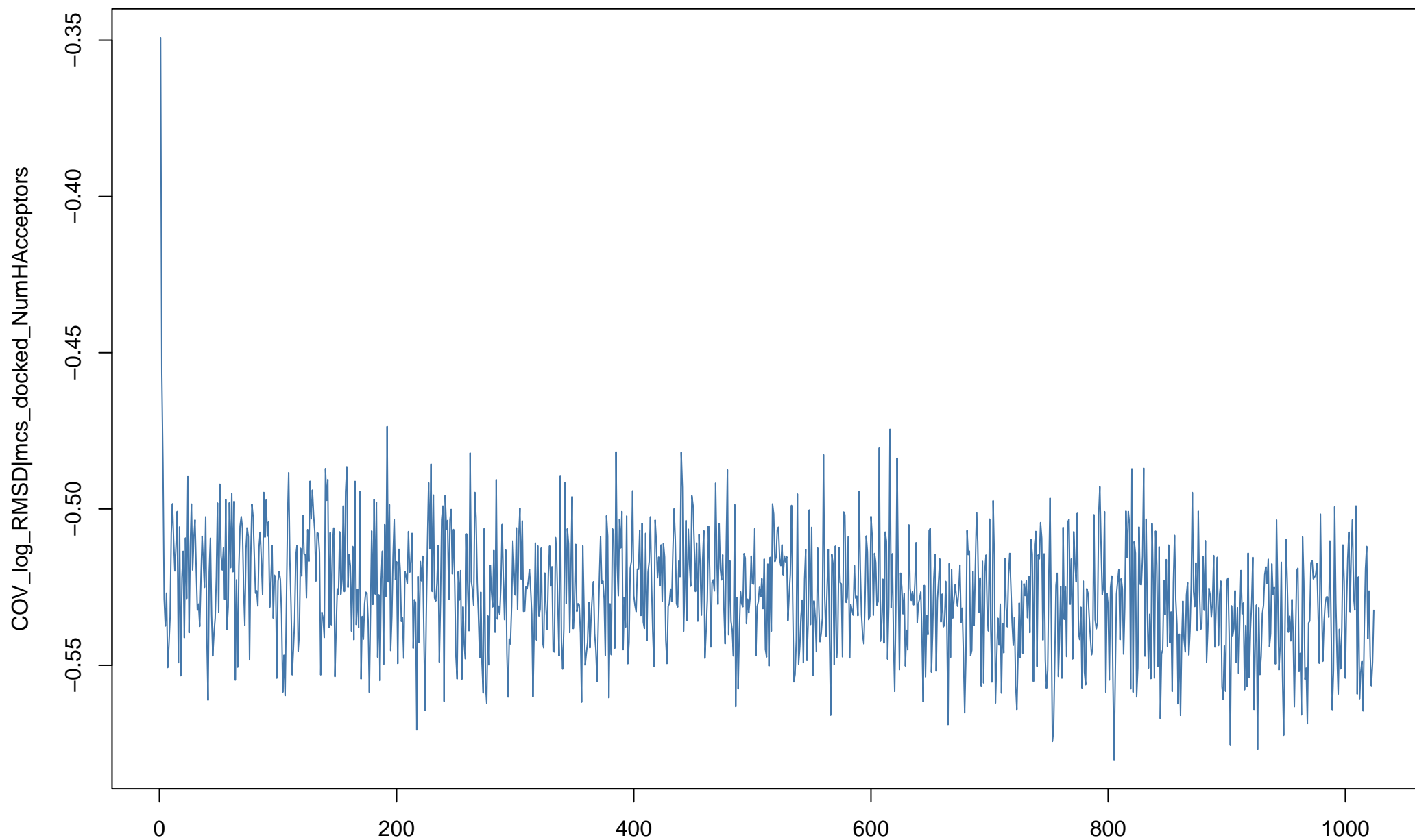
COV_log_RMSD|mcs_RingCount
ESS = 611 | BMK = 0.0517 | MCSE(6.27) = 5.09 | stat: TRUE | burn: 0



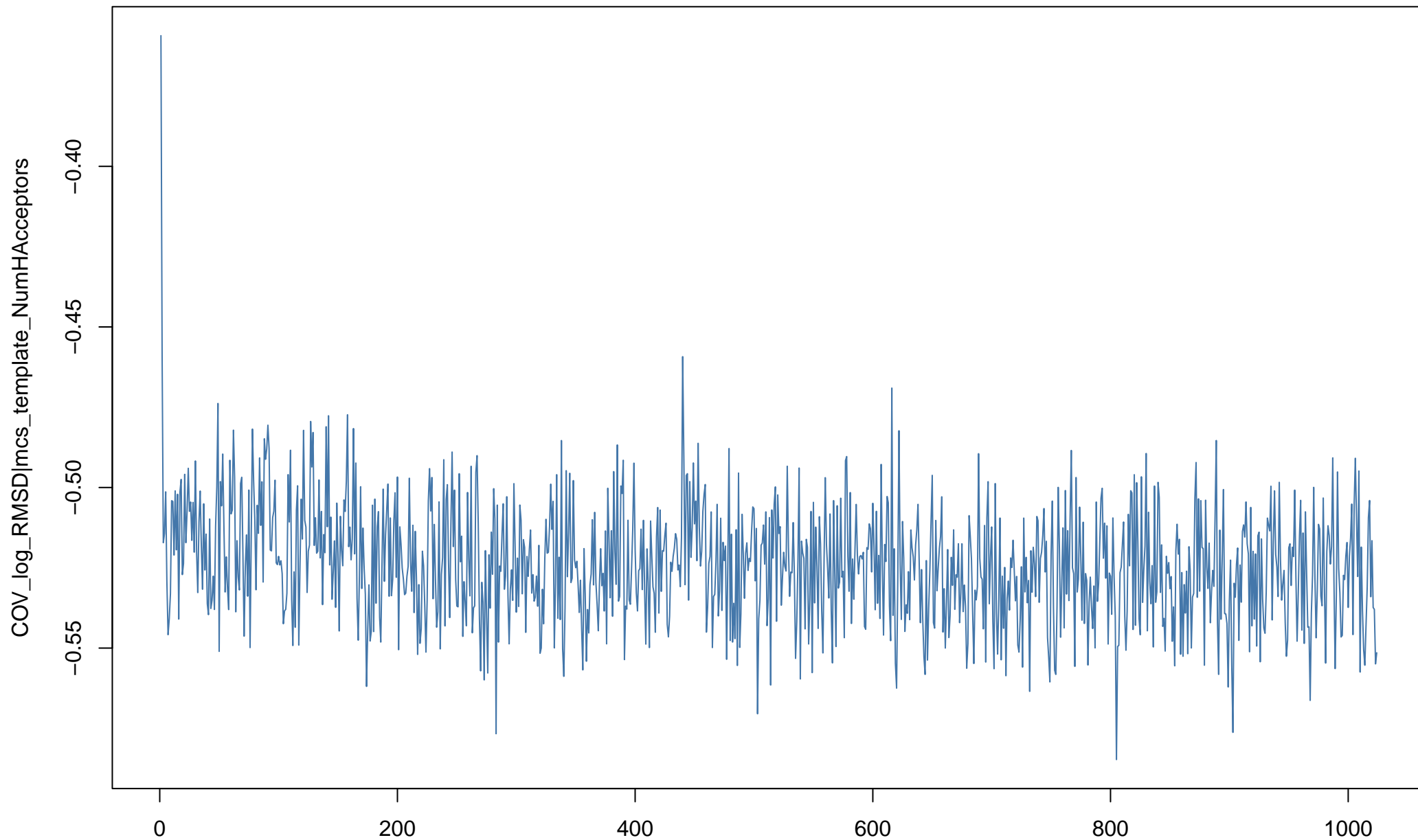
COV_log_RMSD|template_HeavyAtomCount
ESS = 238 | BMK = 0.0655 | MCSE(6.27) = 6.05 | stat: TRUE | burn: 0



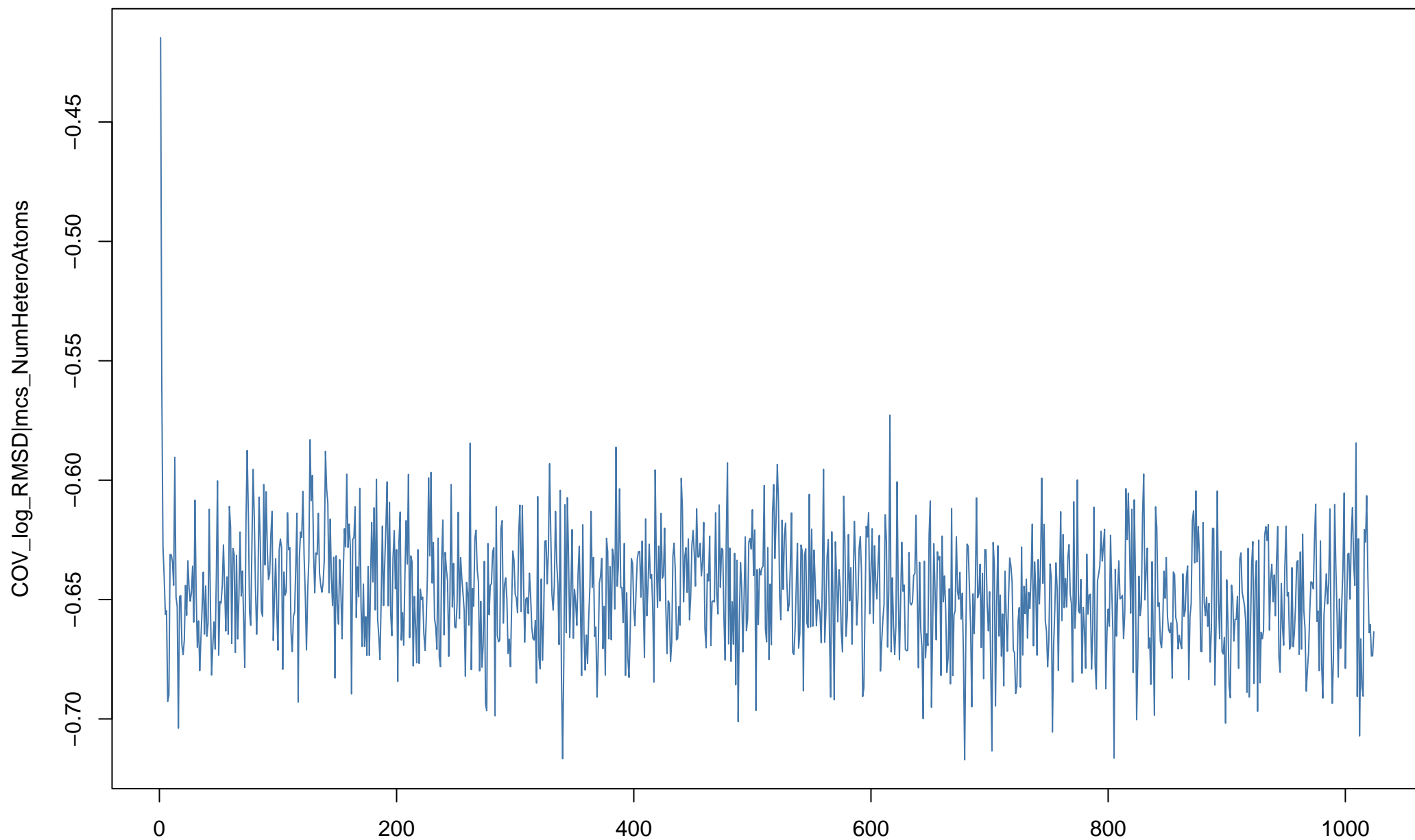
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 491 | BMK = 0.151 | MCSE(6.27) = 5.88 | stat: FALSE | burn: 0



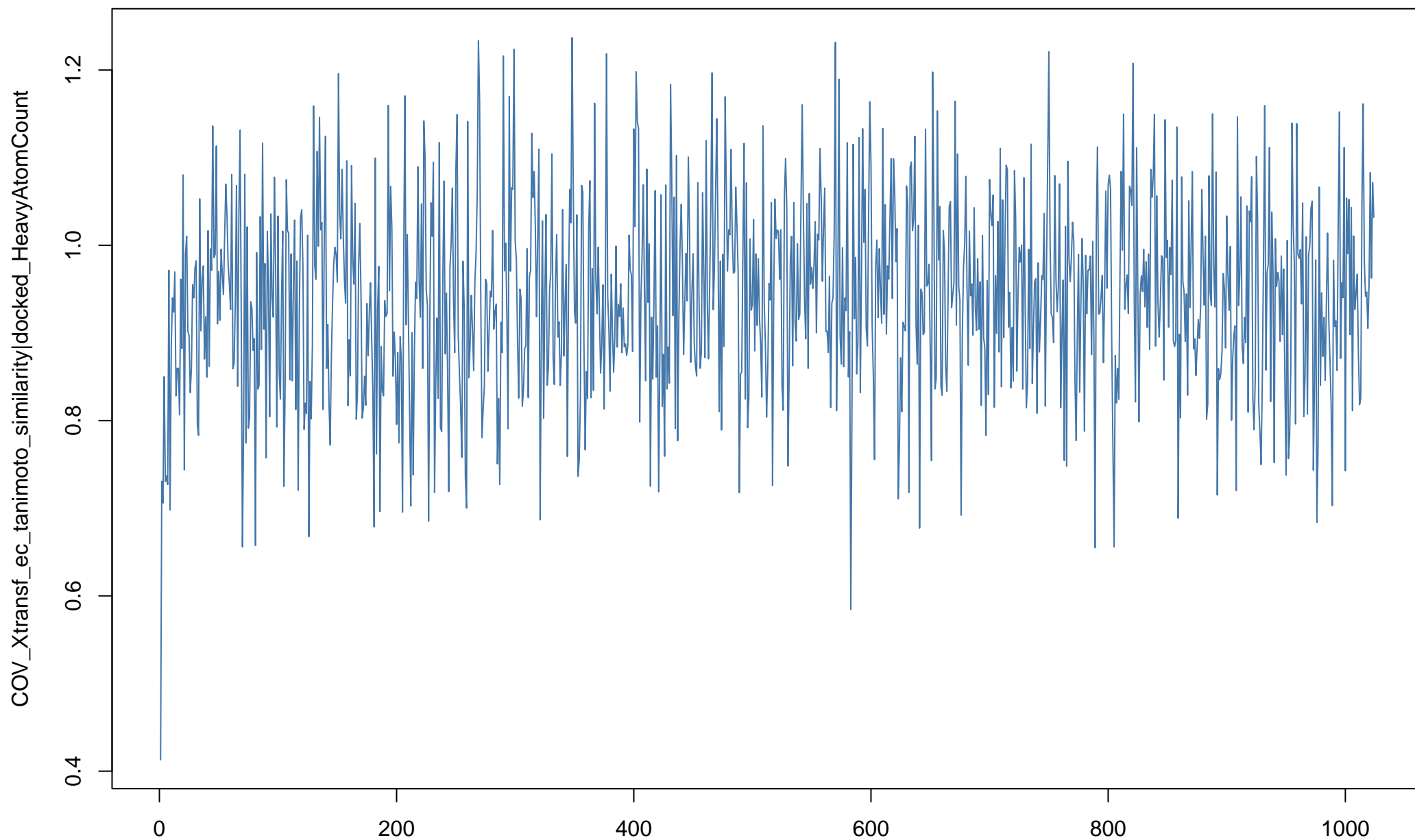
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 465 | BMK = 0.133 | MCSE(6.27) = 5.58 | stat: FALSE | burn: 0



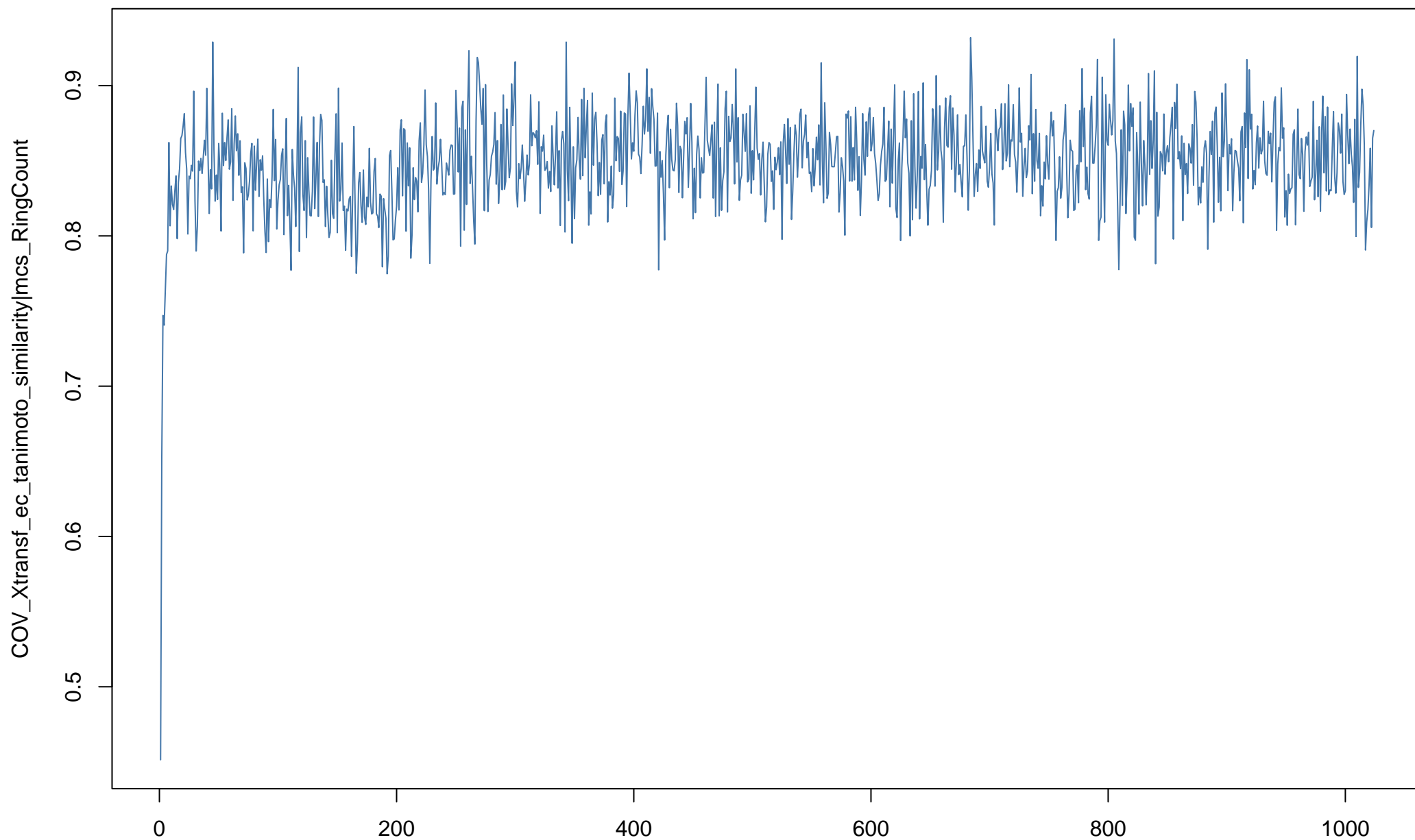
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 814 | BMK = 0.0955 | MCSE(6.27) = 4.45 | stat: TRUE | burn: 0



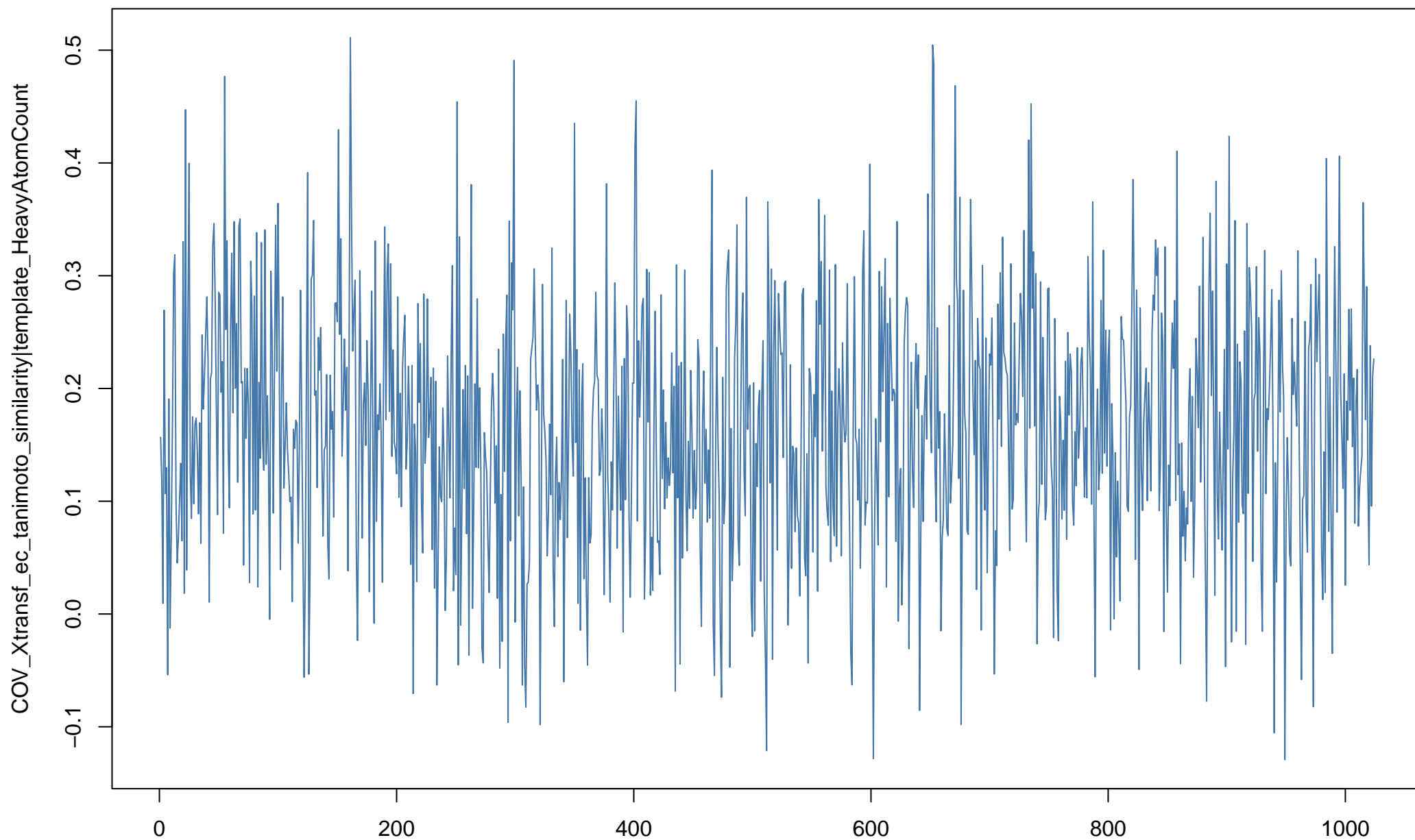
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 855 | BMK = 0.0766 | MCSE(6.27) = 4.32 | stat: FALSE | burn: 0



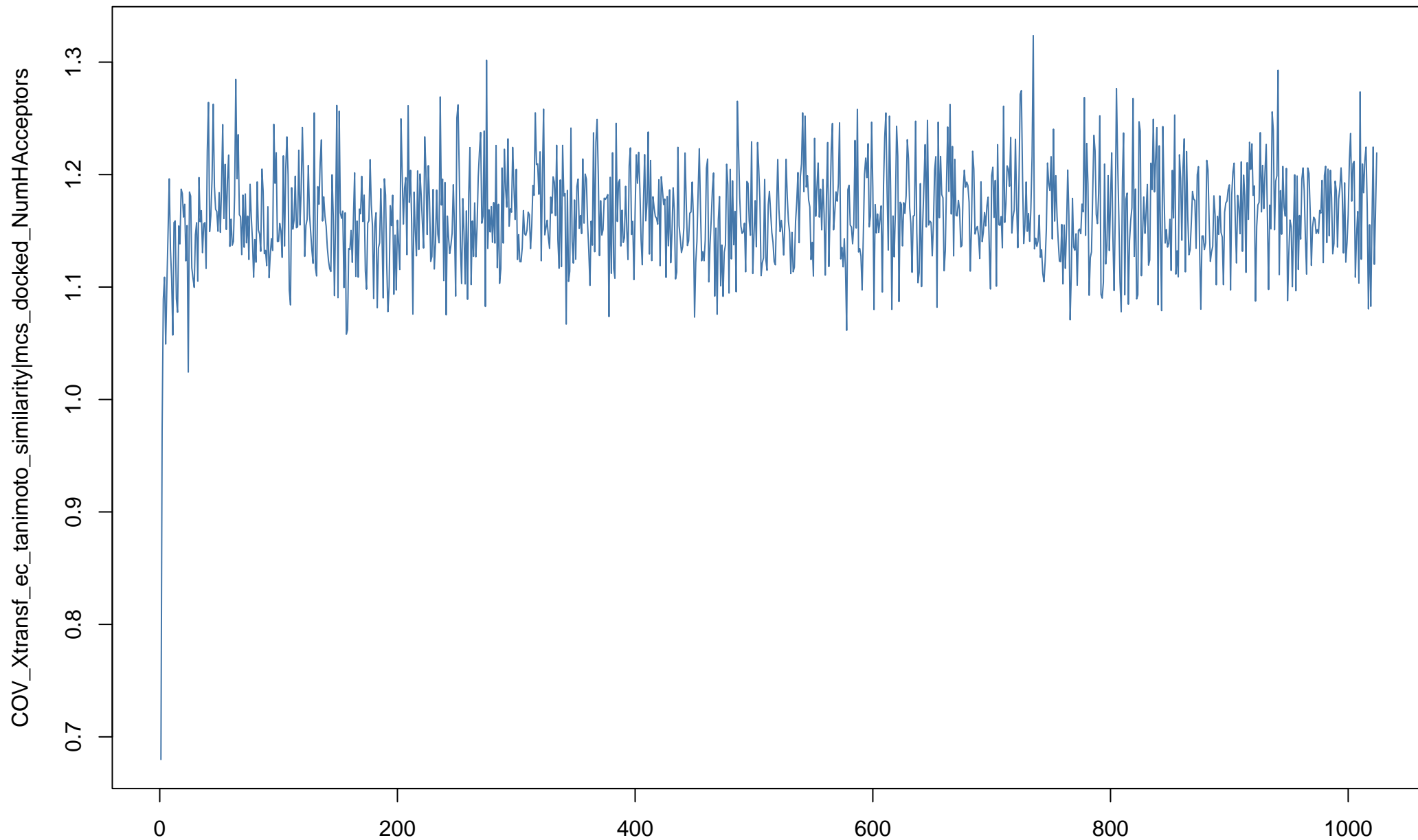
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 353 | BMK = 0.121 | MCSE(6.27) = 6.64 | stat: FALSE | burn: 0



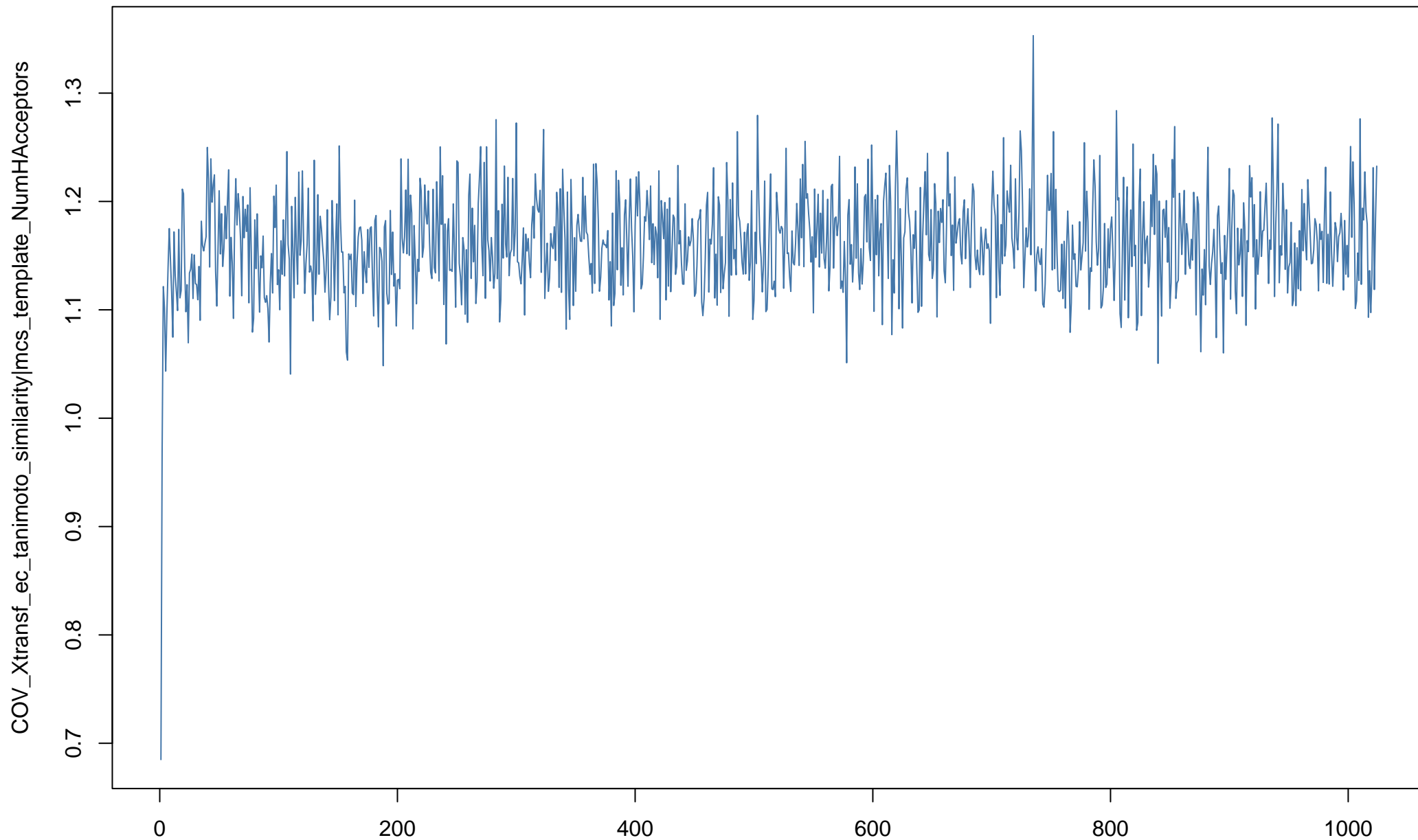
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 925 | BMK = 0.053 | MCSE(6.27) = 3.74 | stat: TRUE | burn: 0



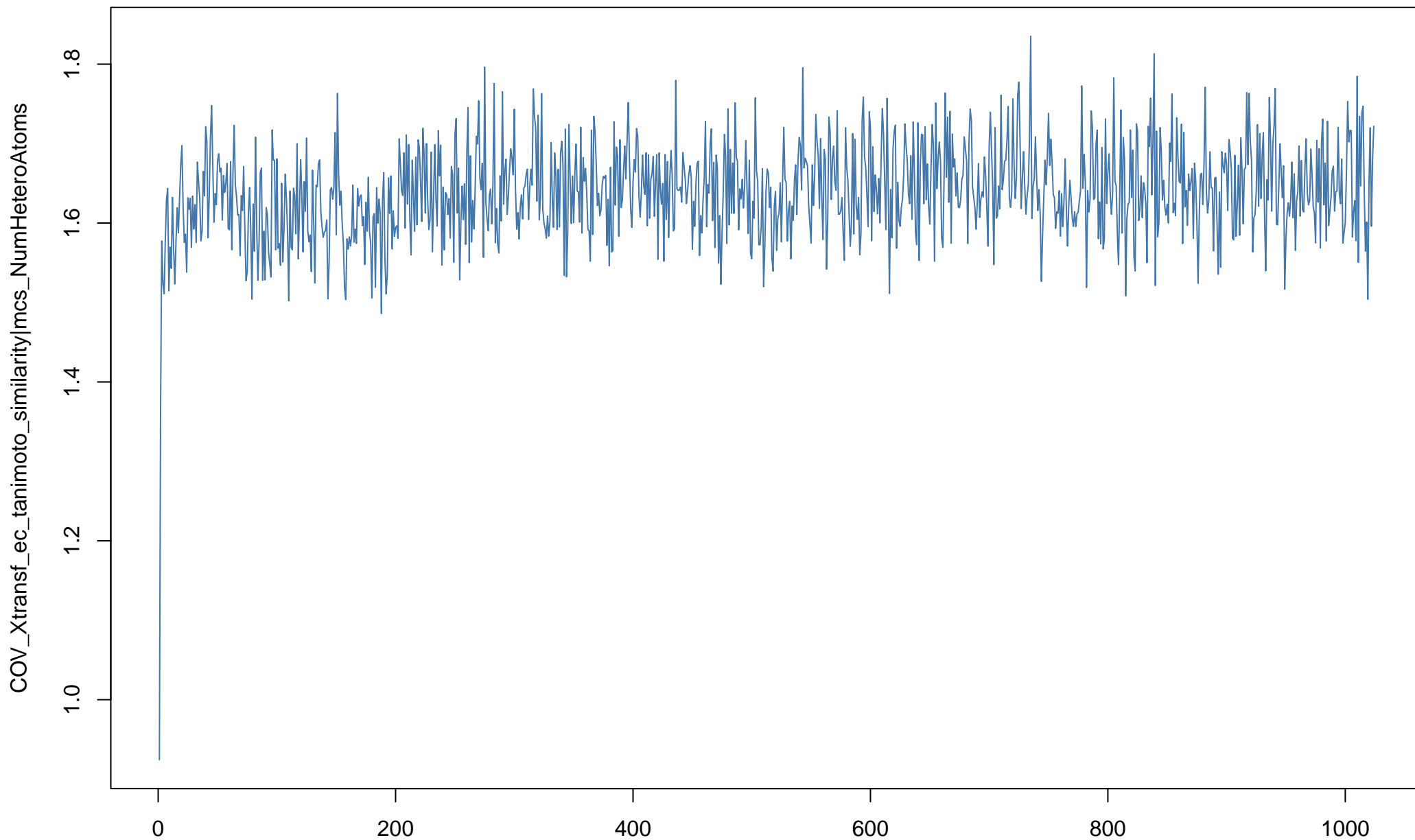
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 506 | BMK = 0.0792 | MCSE(6.27) = 5.14 | stat: TRUE | burn: 0



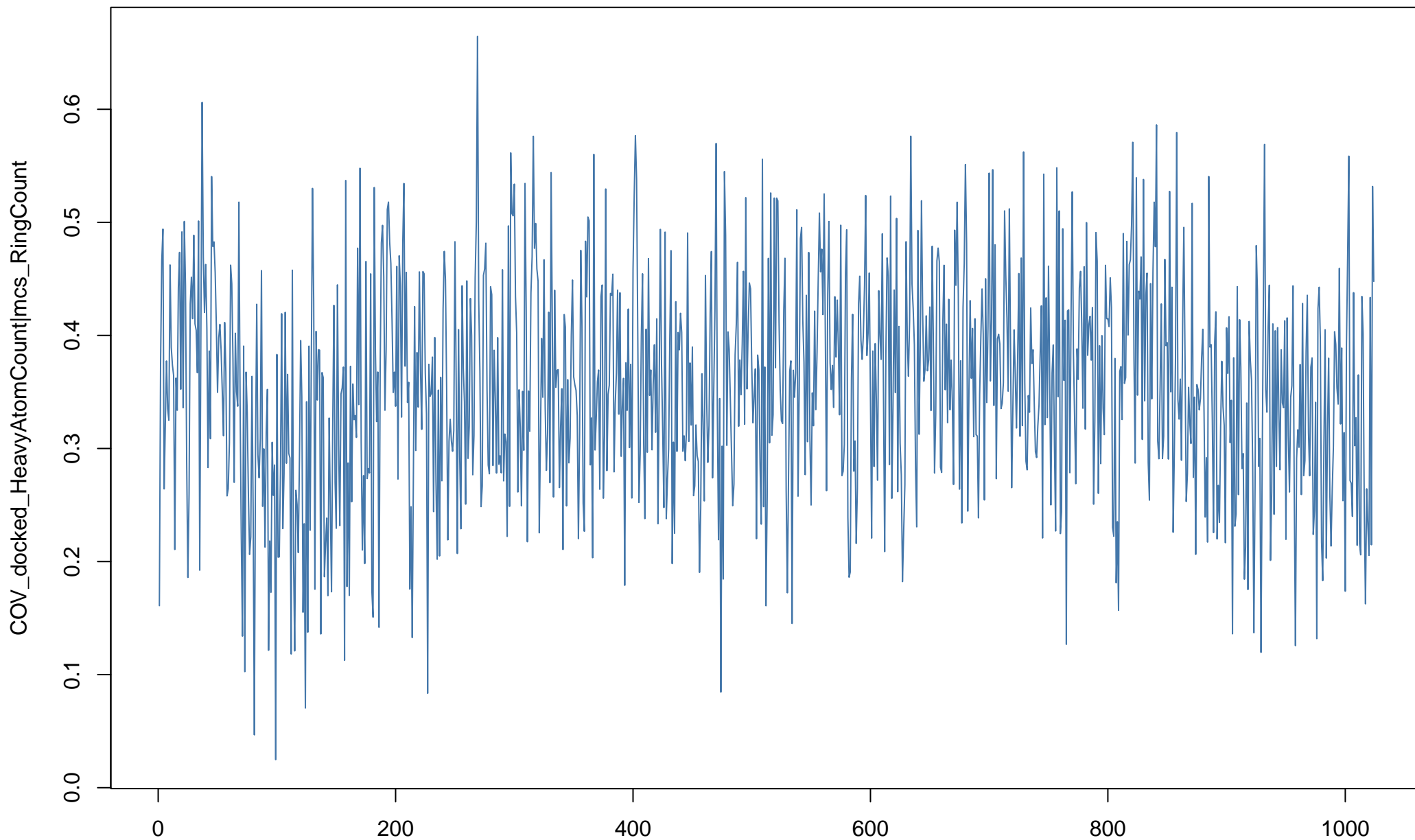
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 853 | BMK = 0.0799 | MCSE(6.27) = 5.01 | stat: FALSE | burn: 0



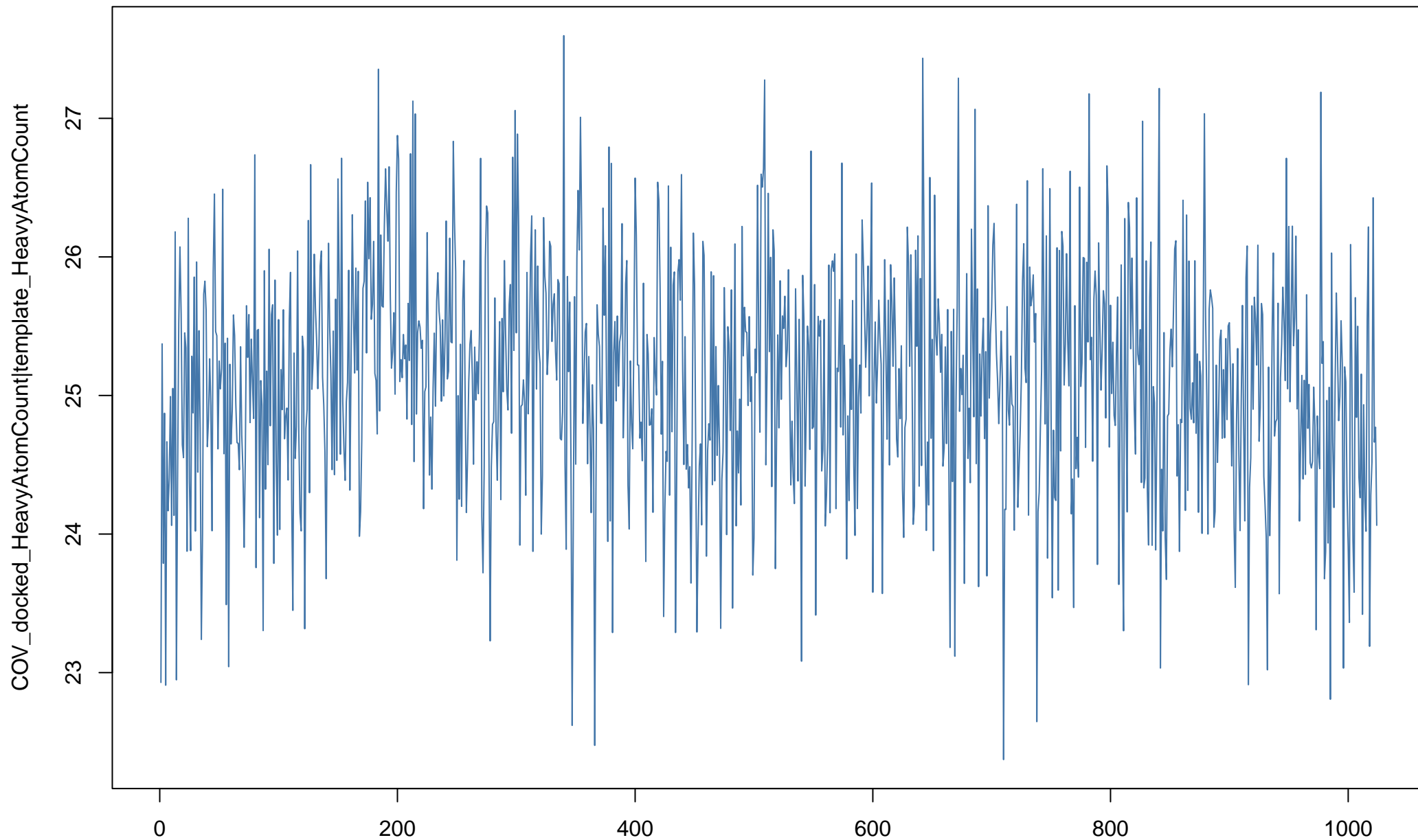
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 195 | BMK = 0.135 | MCSE(6.27) = 6.39 | stat: FALSE | burn: 0



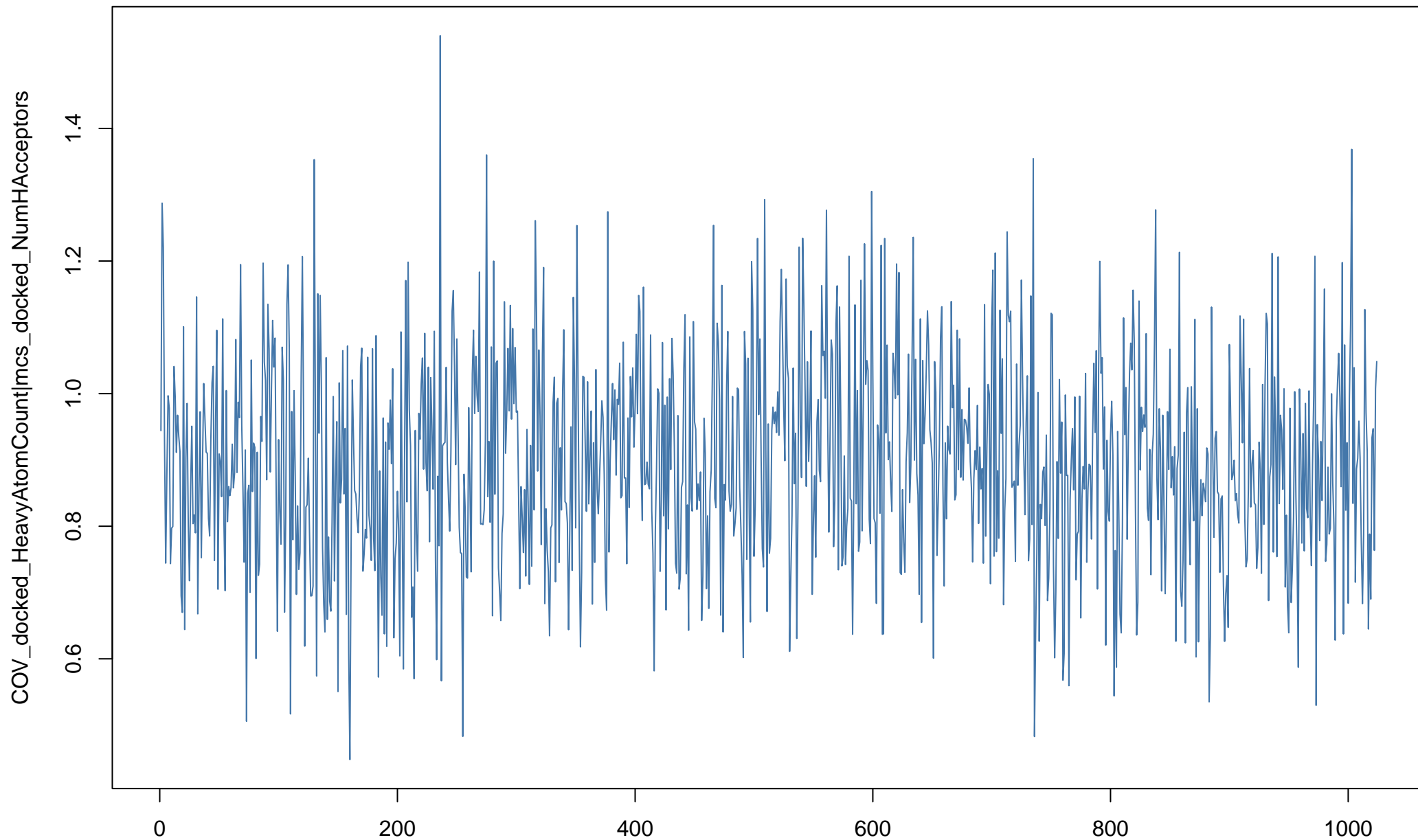
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 370 | BMK = 0.0801 | MCSE(6.27) = 6.03 | stat: TRUE | burn: 0



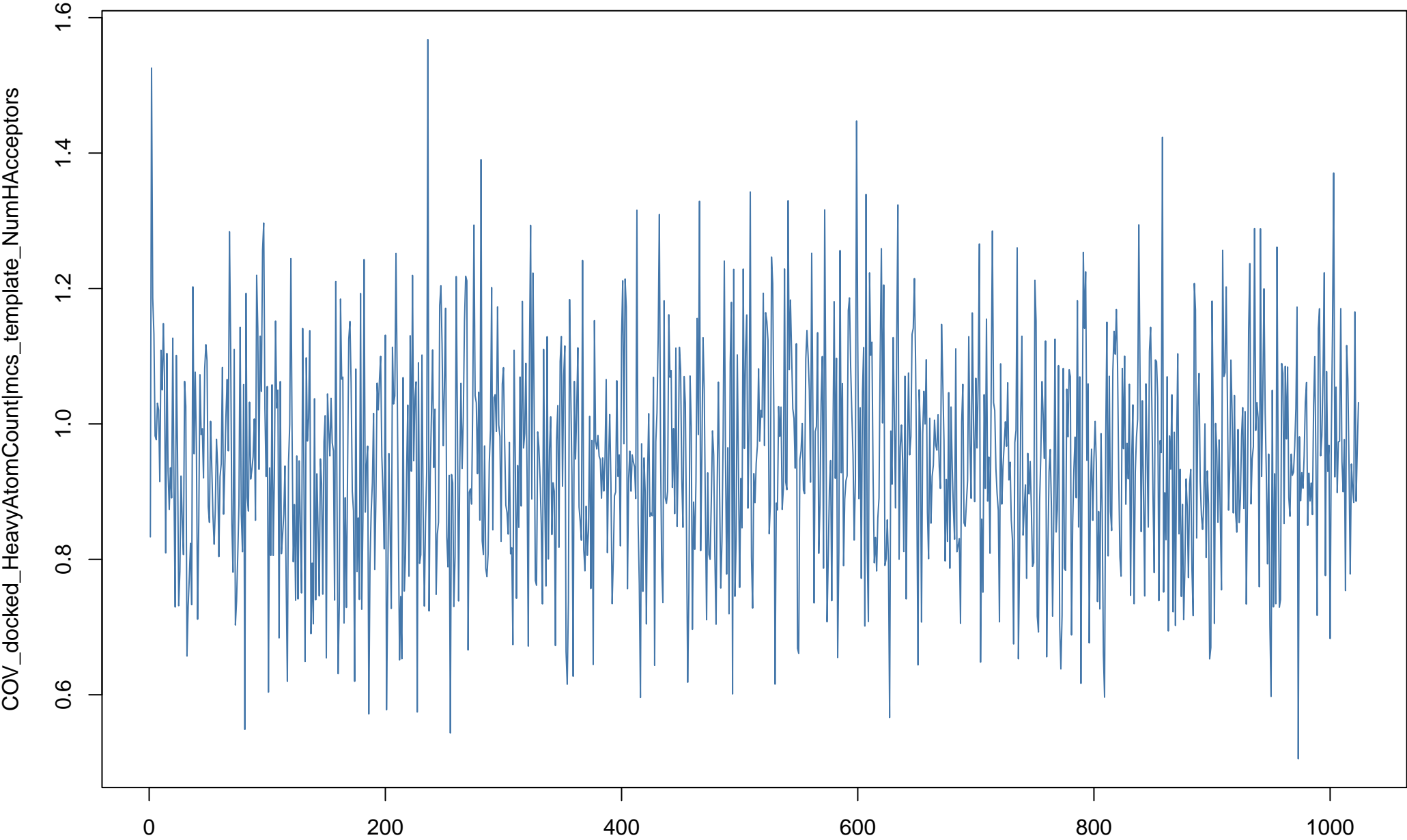
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 803 | BMK = 0.0522 | MCSE(6.27) = 4.65 | stat: FALSE | burn: 0



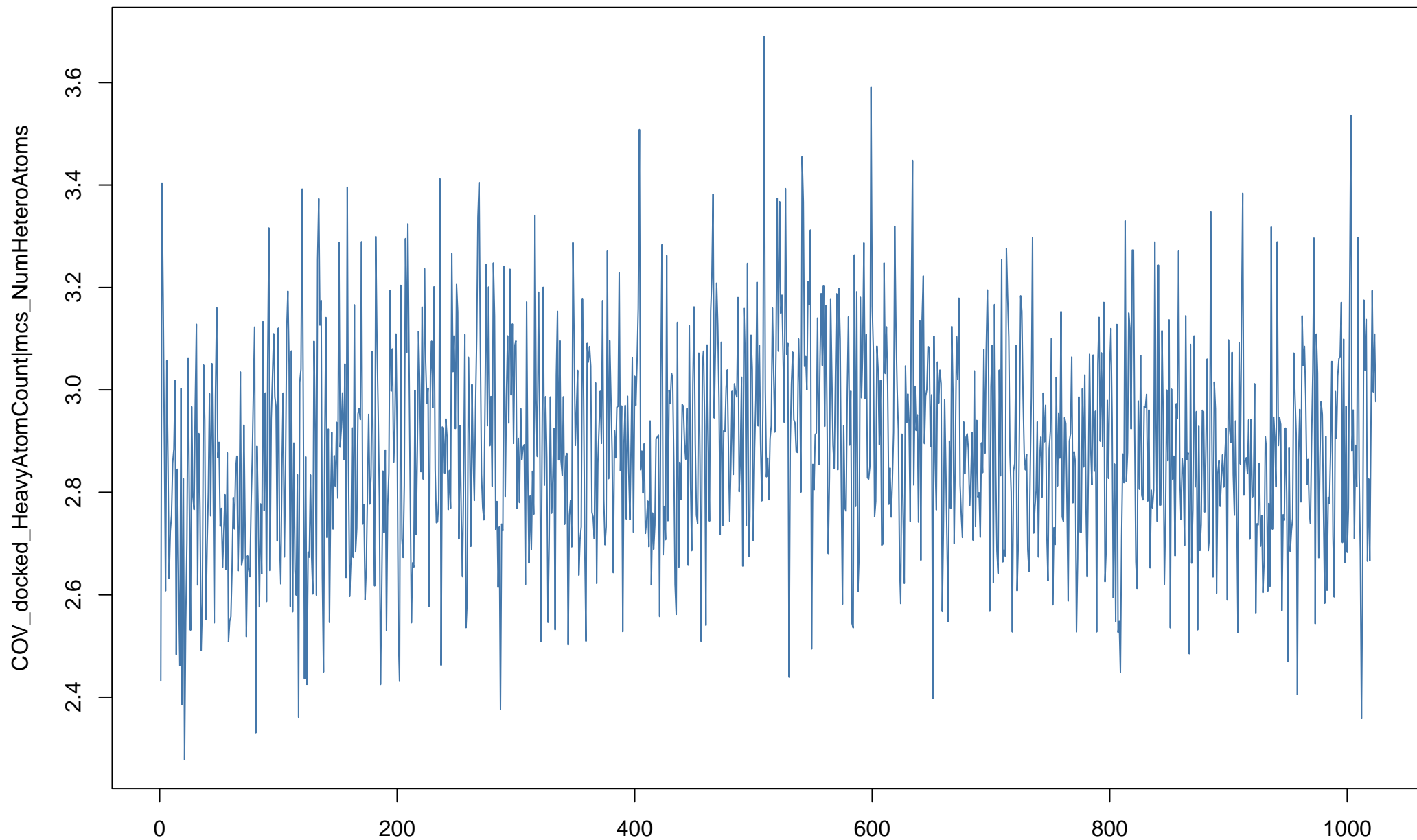
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 910 | BMK = 0.0459 | MCSE(6.27) = 3.7 | stat: TRUE | burn: 0



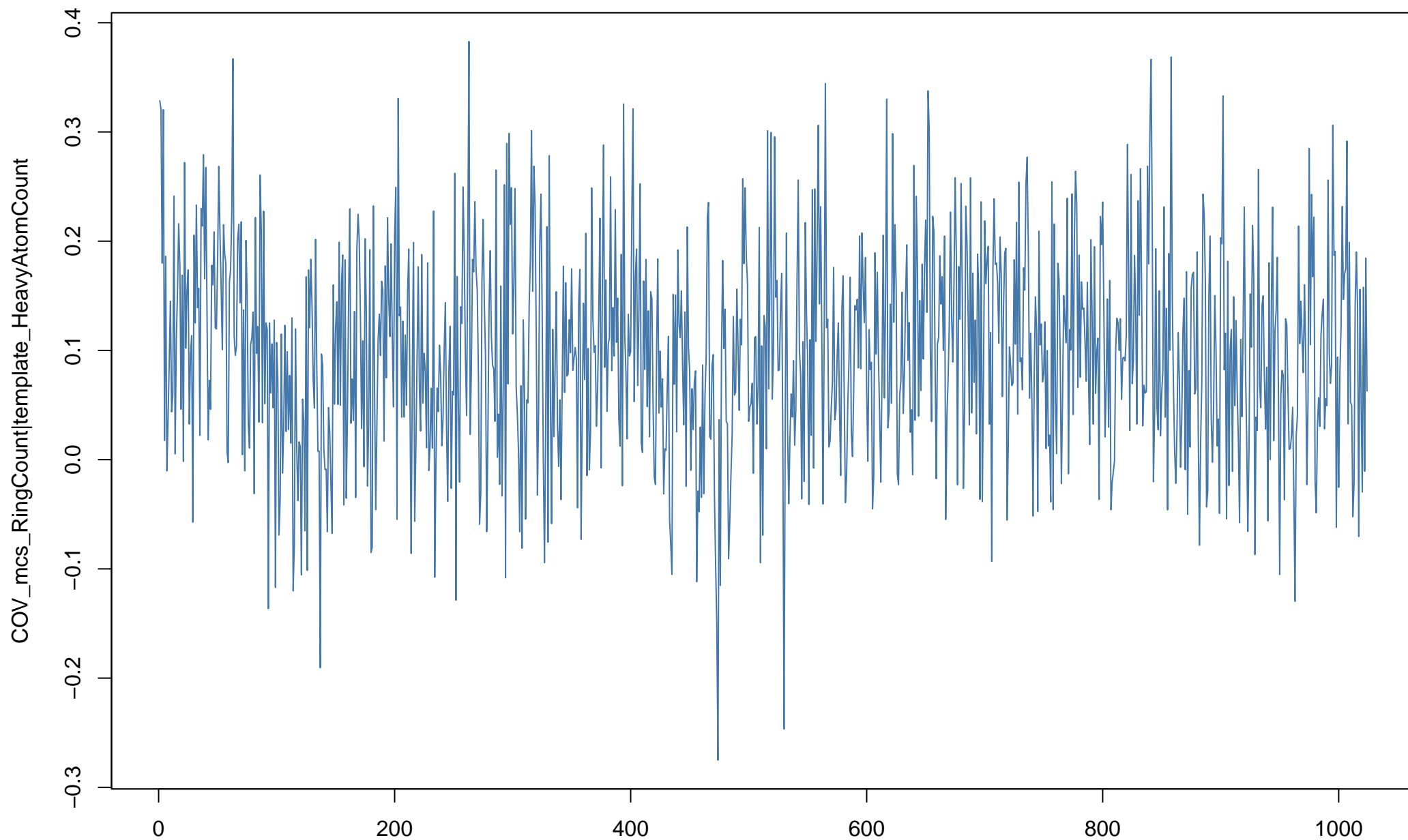
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 932 | BMK = 0.0584 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 0



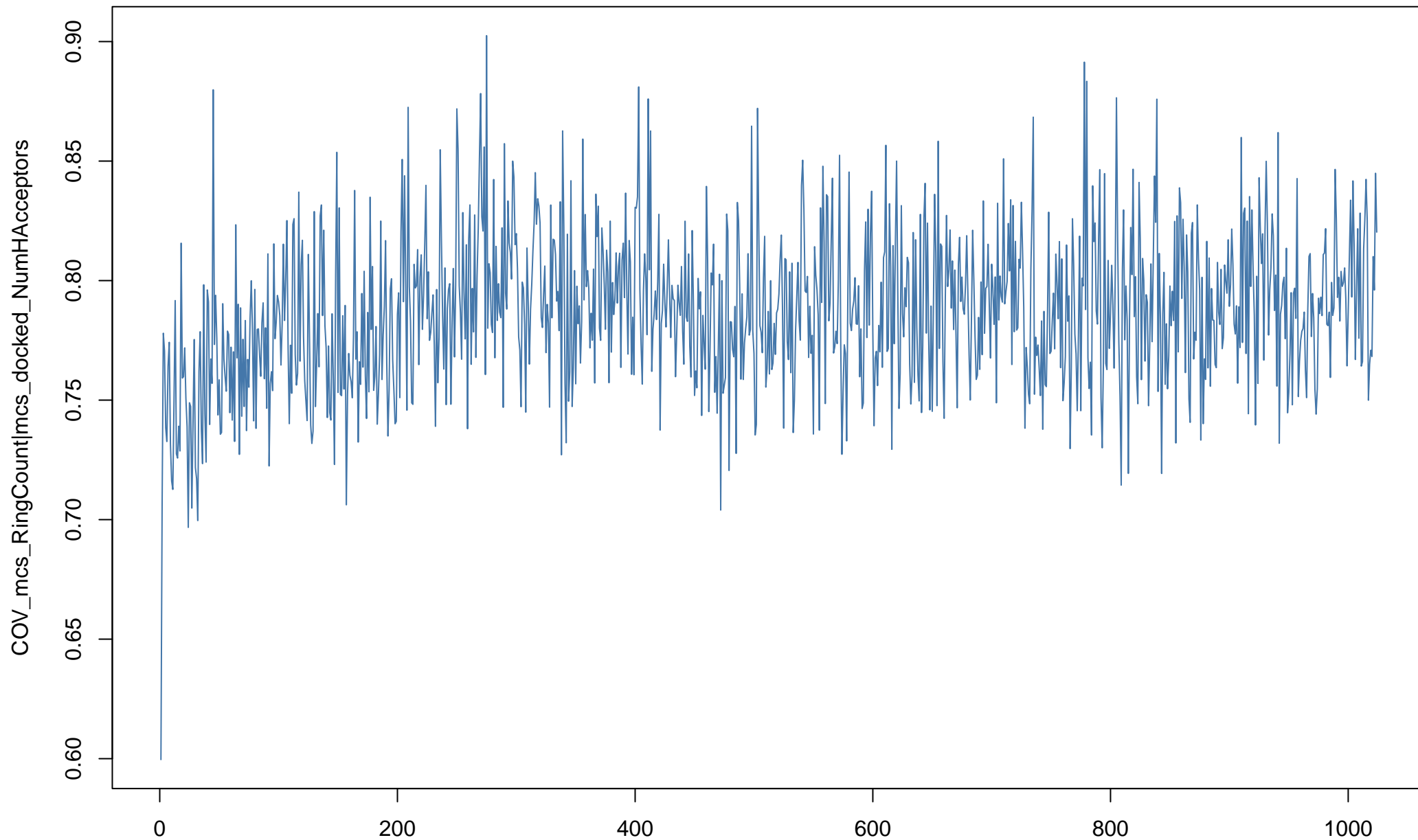
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 175 | BMK = 0.0586 | MCSE(6.27) = 4.85 | stat: FALSE | burn: 0



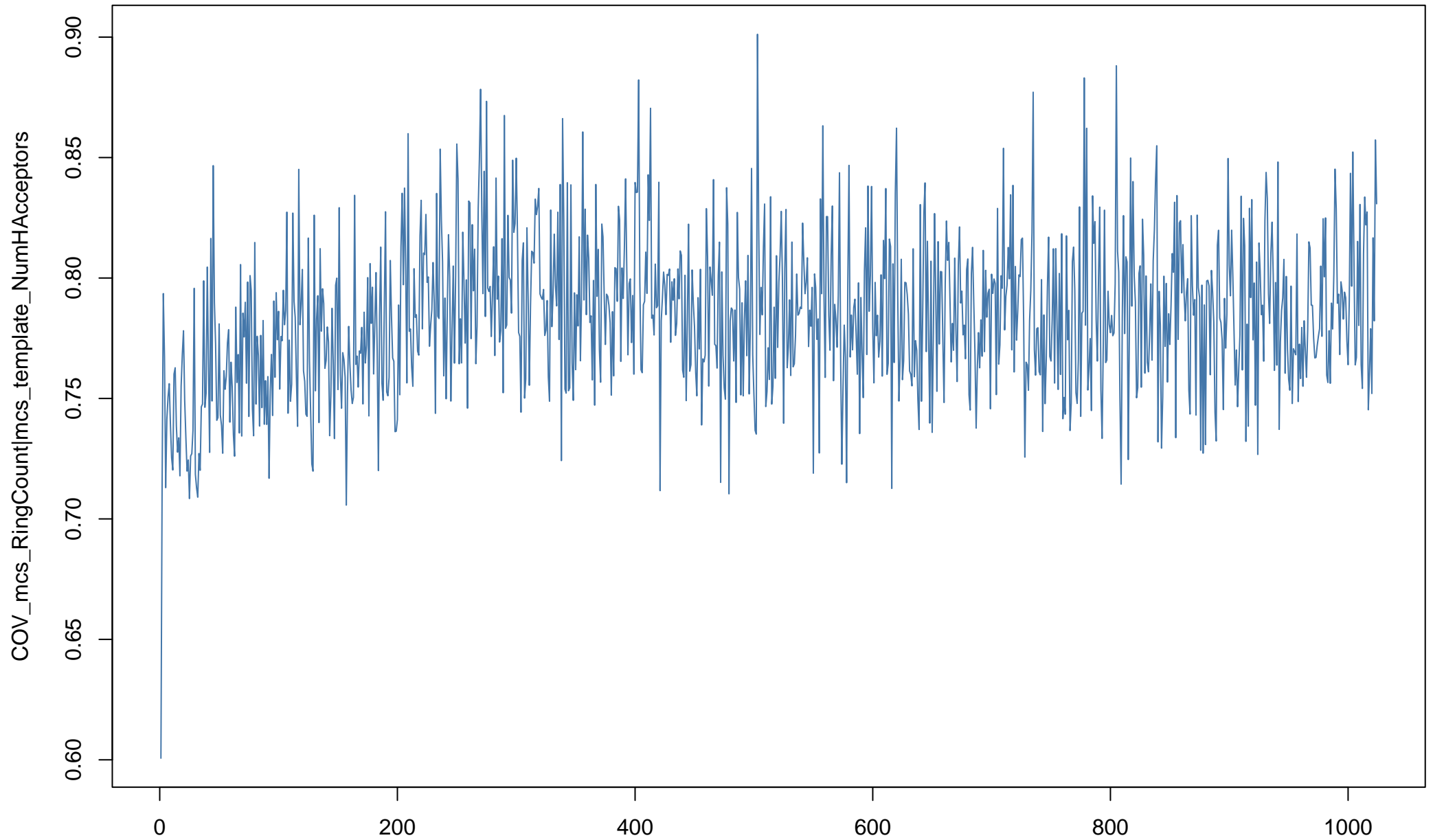
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 462 | BMK = 0.0785 | MCSE(6.27) = 5.4 | stat: TRUE | burn: 0



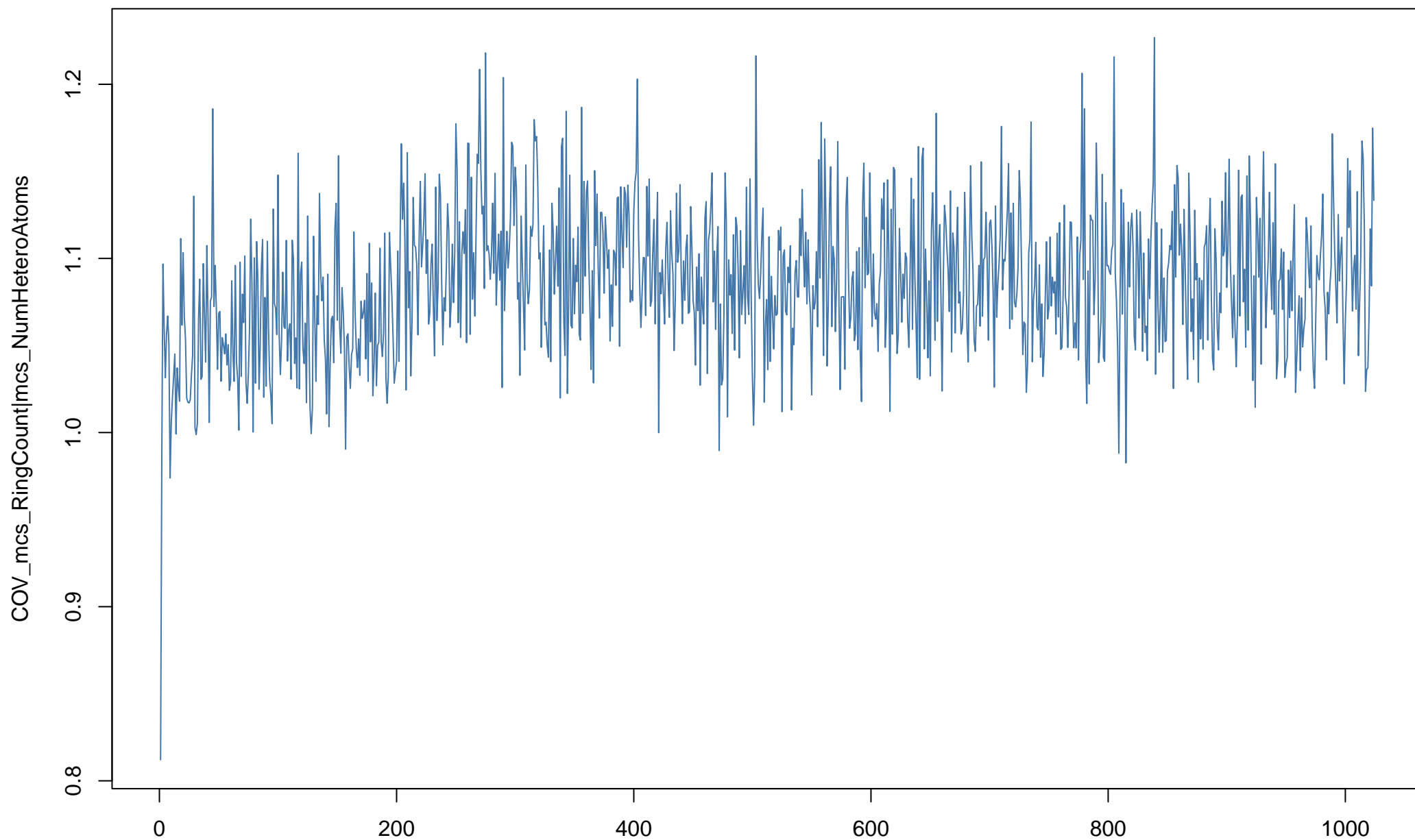
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 77.4 | BMK = 0.109 | MCSE(6.27) = 7.12 | stat: FALSE | burn: 0



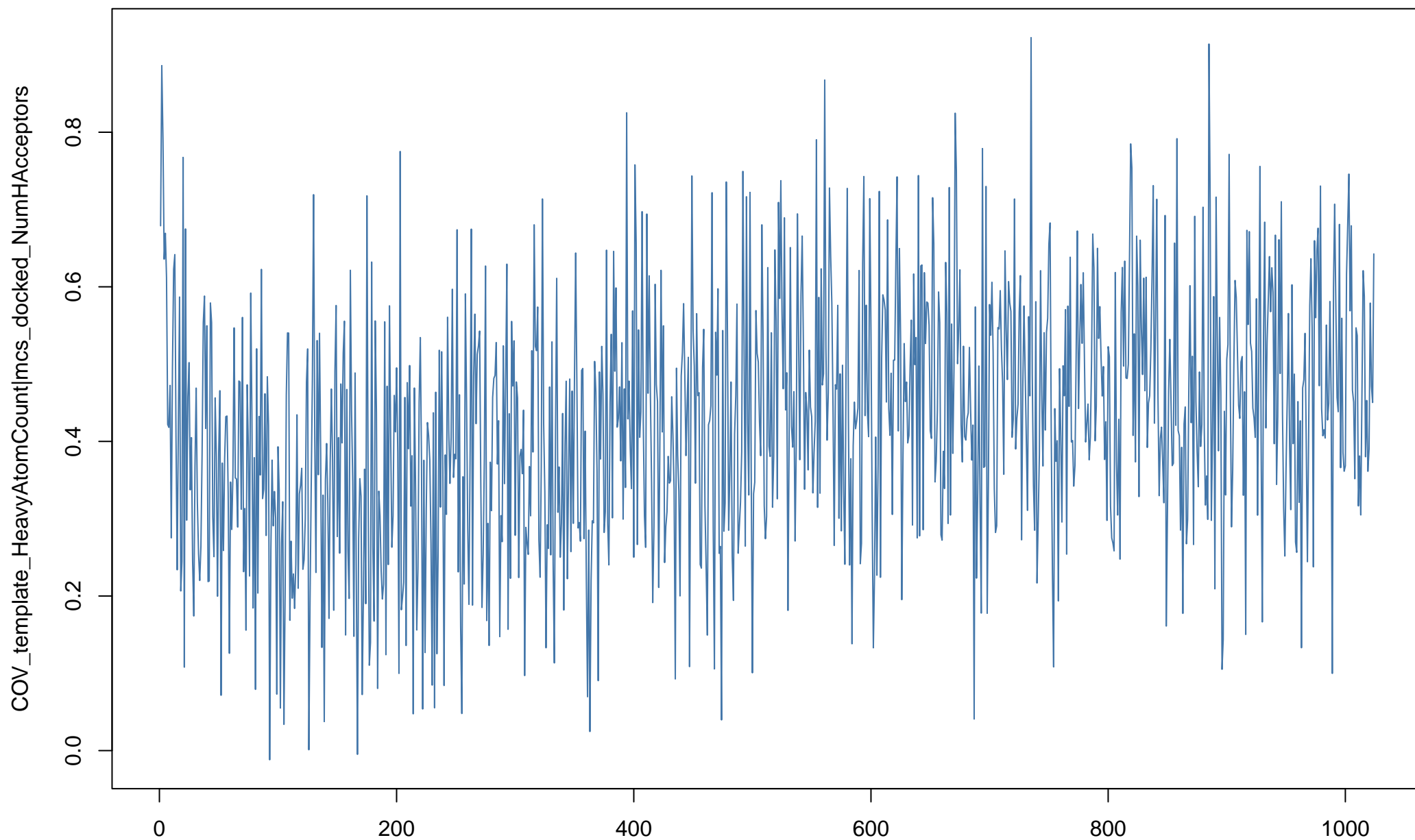
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 88.9 | BMK = 0.0934 | MCSE(6.27) = 7.42 | stat: FALSE | burn: 0



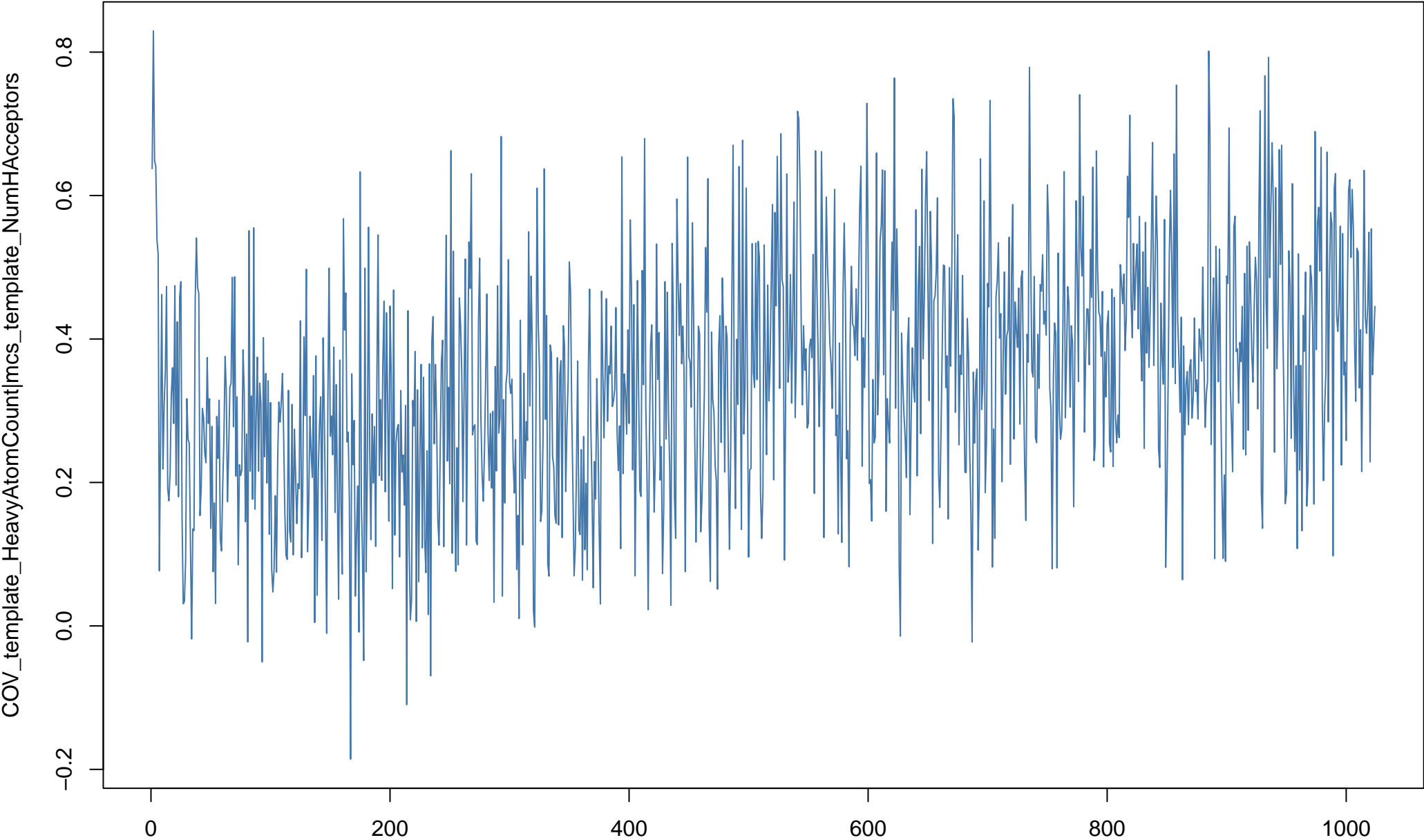
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 58.1 | BMK = 0.108 | MCSE(6.27) = 7.42 | stat: FALSE | burn: 0



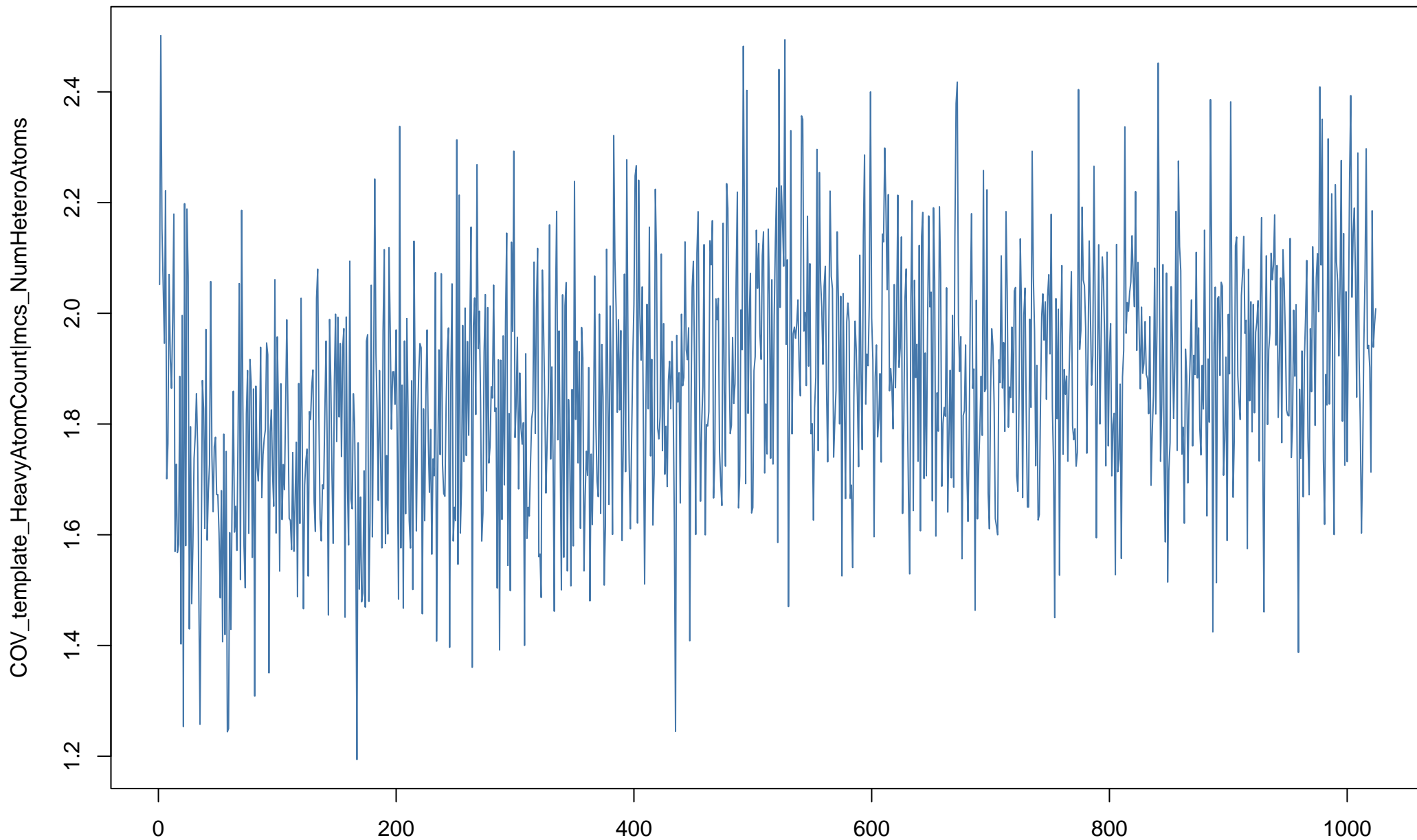
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 90.3 | BMK = 0.22 | MCSE(6.27) = 6.81 | stat: FALSE | burn: 0



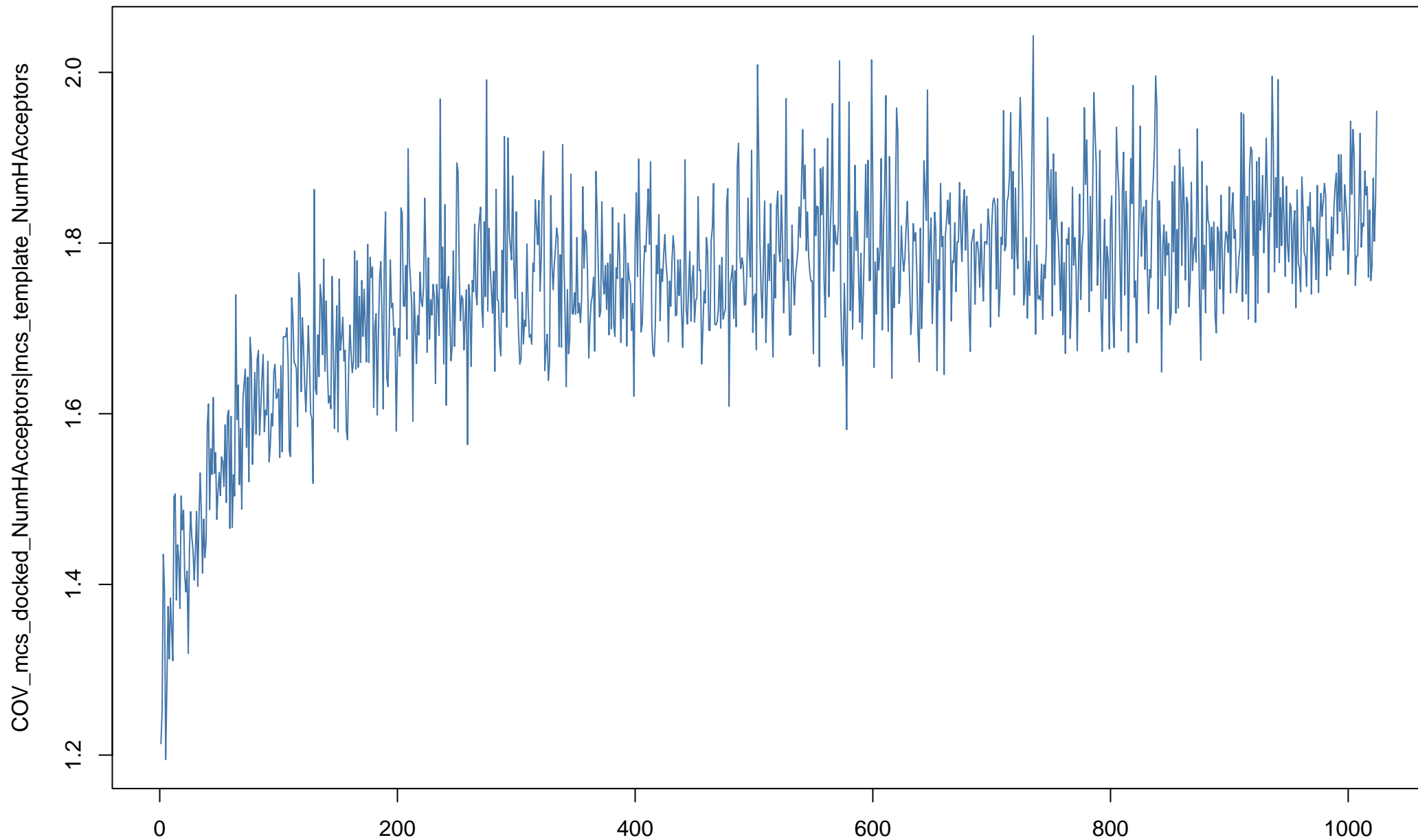
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 148 | BMK = 0.275 | MCSE(6.27) = 7.77 | stat: FALSE | burn: 0



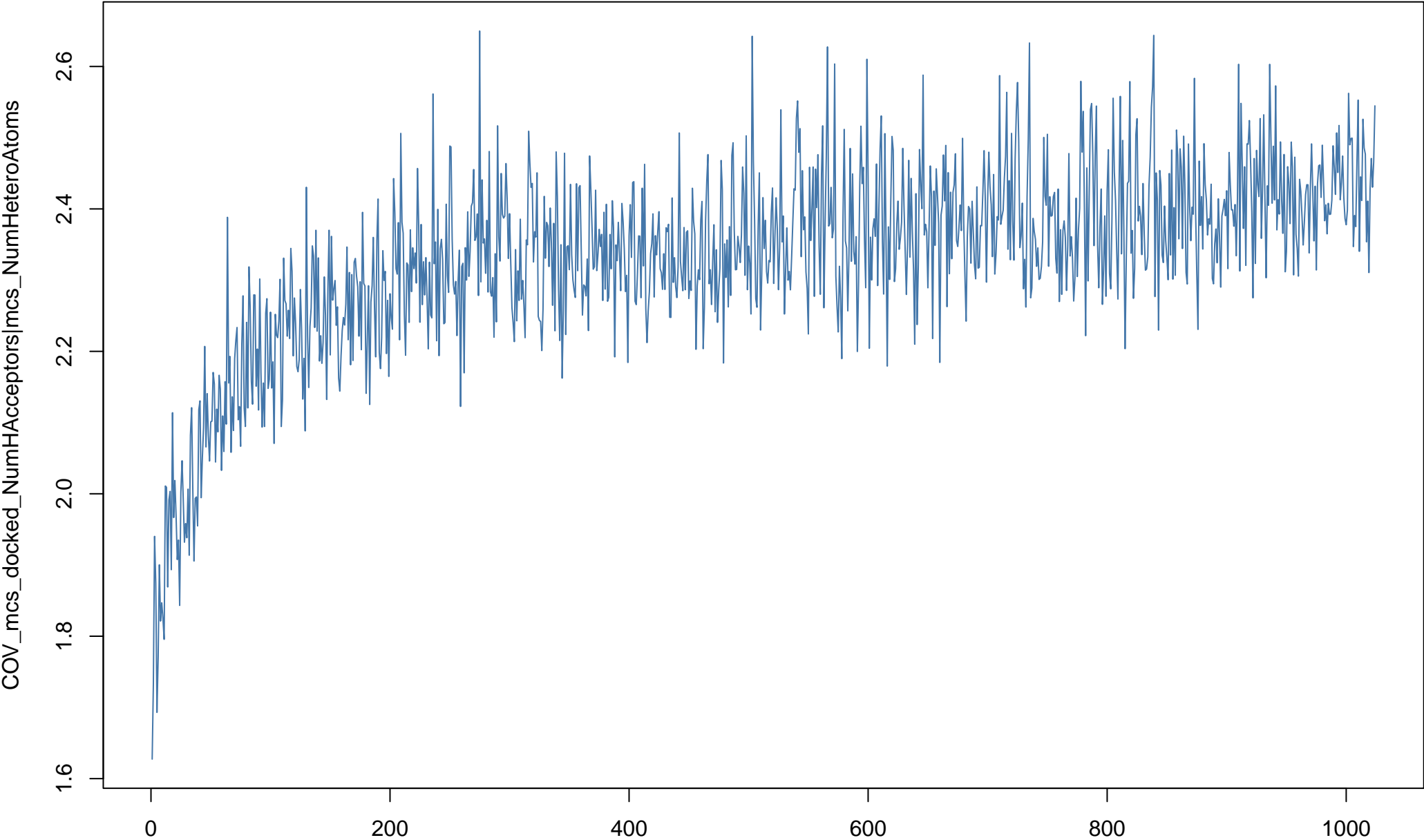
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 109 | BMK = 0.206 | MCSE(6.27) = 7.05 | stat: FALSE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 10.8 | BMK = 0.424 | MCSE(6.27) = 14.4 | stat: FALSE | burn: 102



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 12 | BMK = 0.43 | MCSE(6.27) = 14.4 | stat: FALSE | burn: 102



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 9.92 | BMK = 0.458 | MCSE(6.27) = 14.6 | stat: FALSE | burn: 102

