

-- STATS maxD --

min ESS = 66.2745200170564

max BMK = 1

max MCSE = 10.4869624531837

all stationary: FALSE

burn: 816

-- STATS 2D --

min ESS = 67.0005669649057

max BMK = 0.236605146837599

max MCSE = 8.62045384632206

all stationary: FALSE

burn: 714

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 1

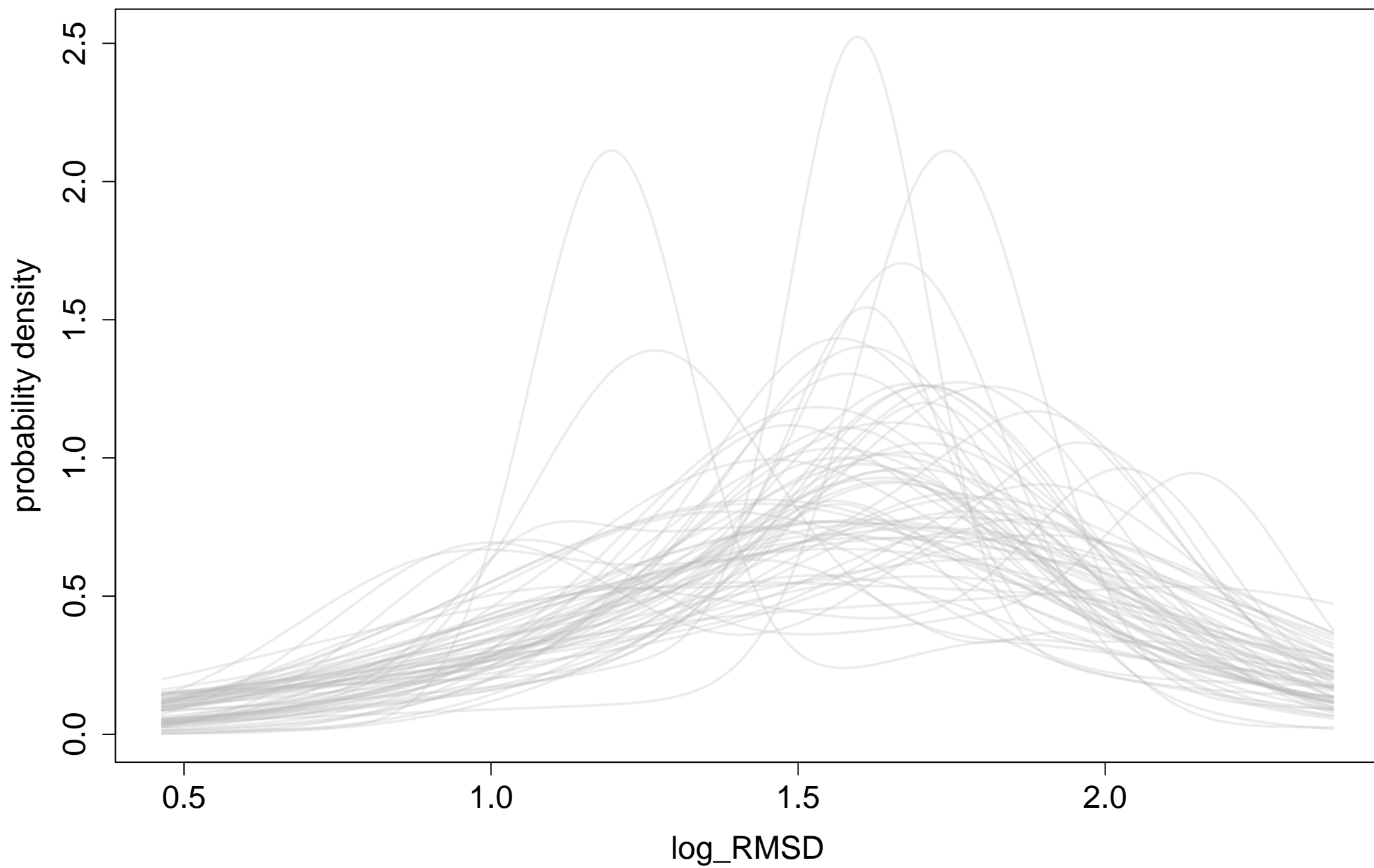
max MCSE = NaN

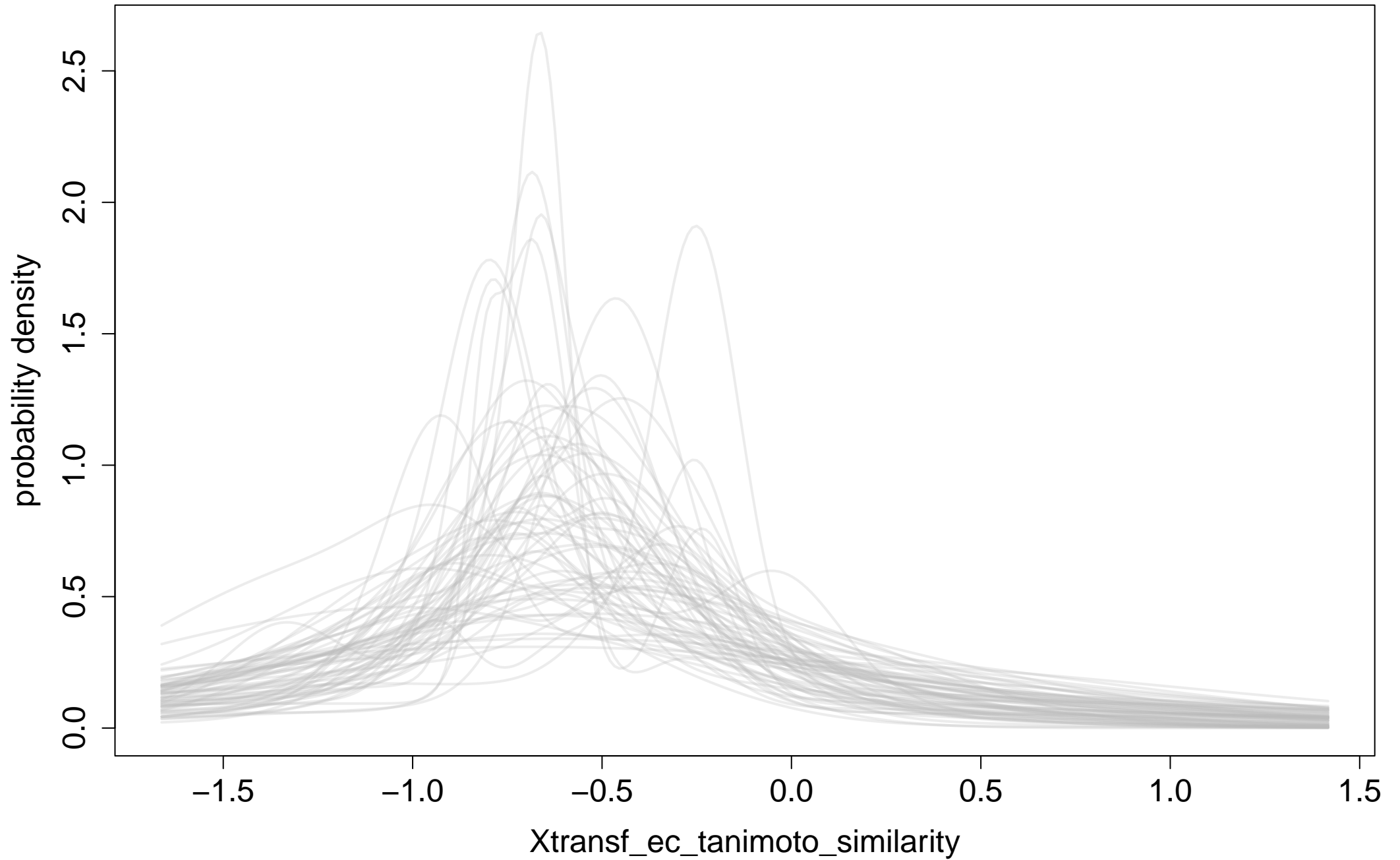
all stationary: FALSE

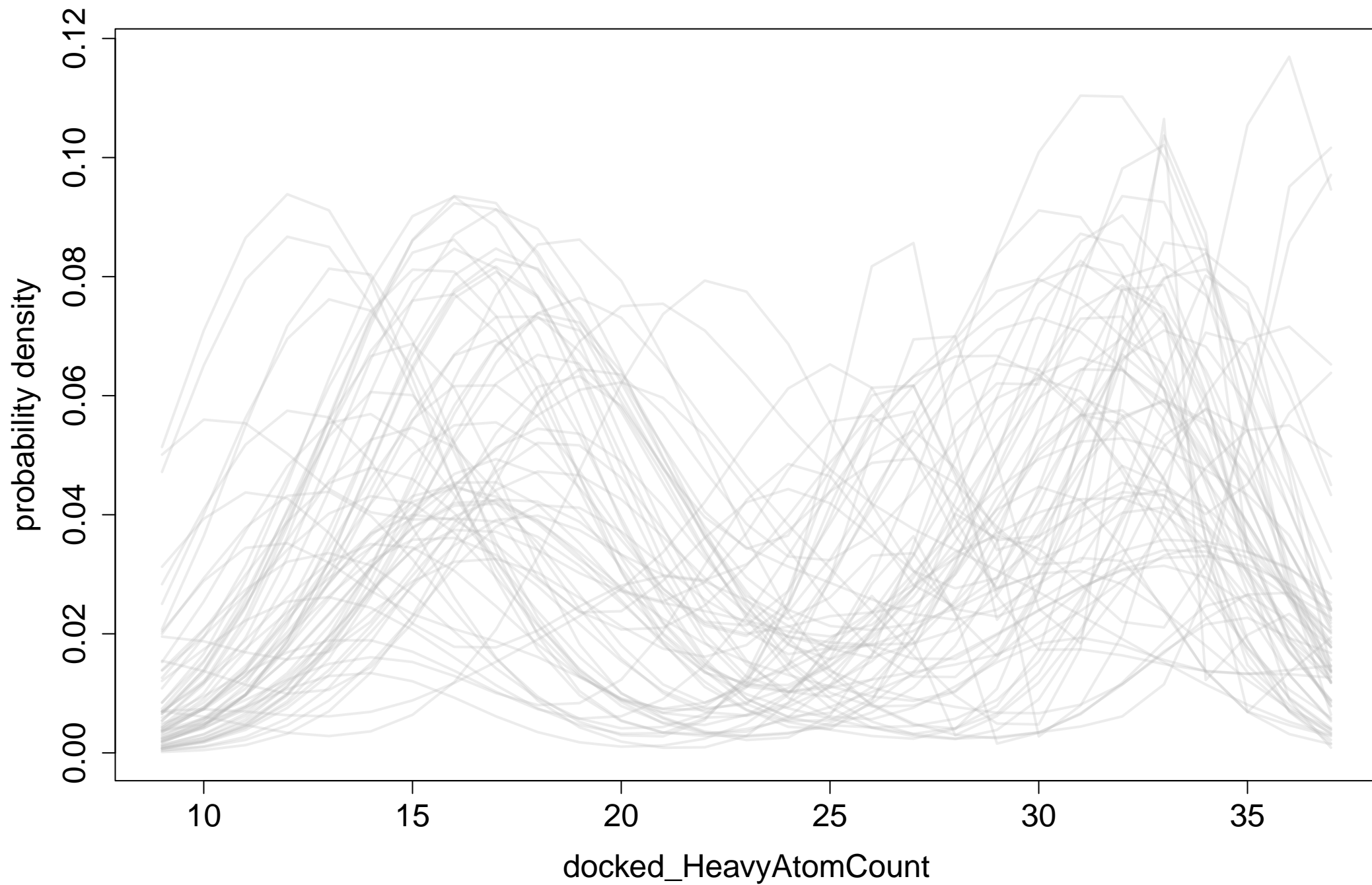
burn: 816

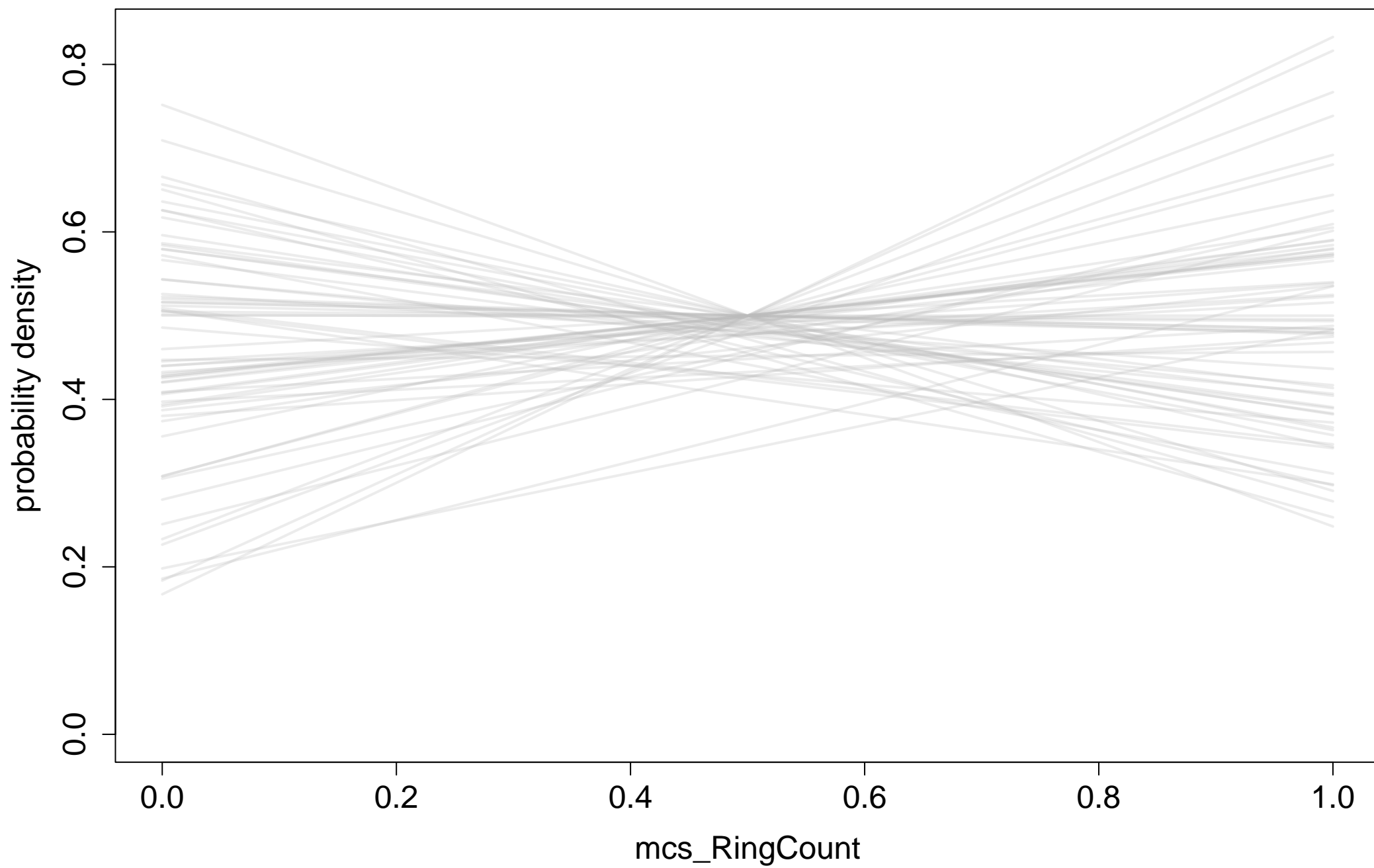
Occupied clusters: 4 of 4

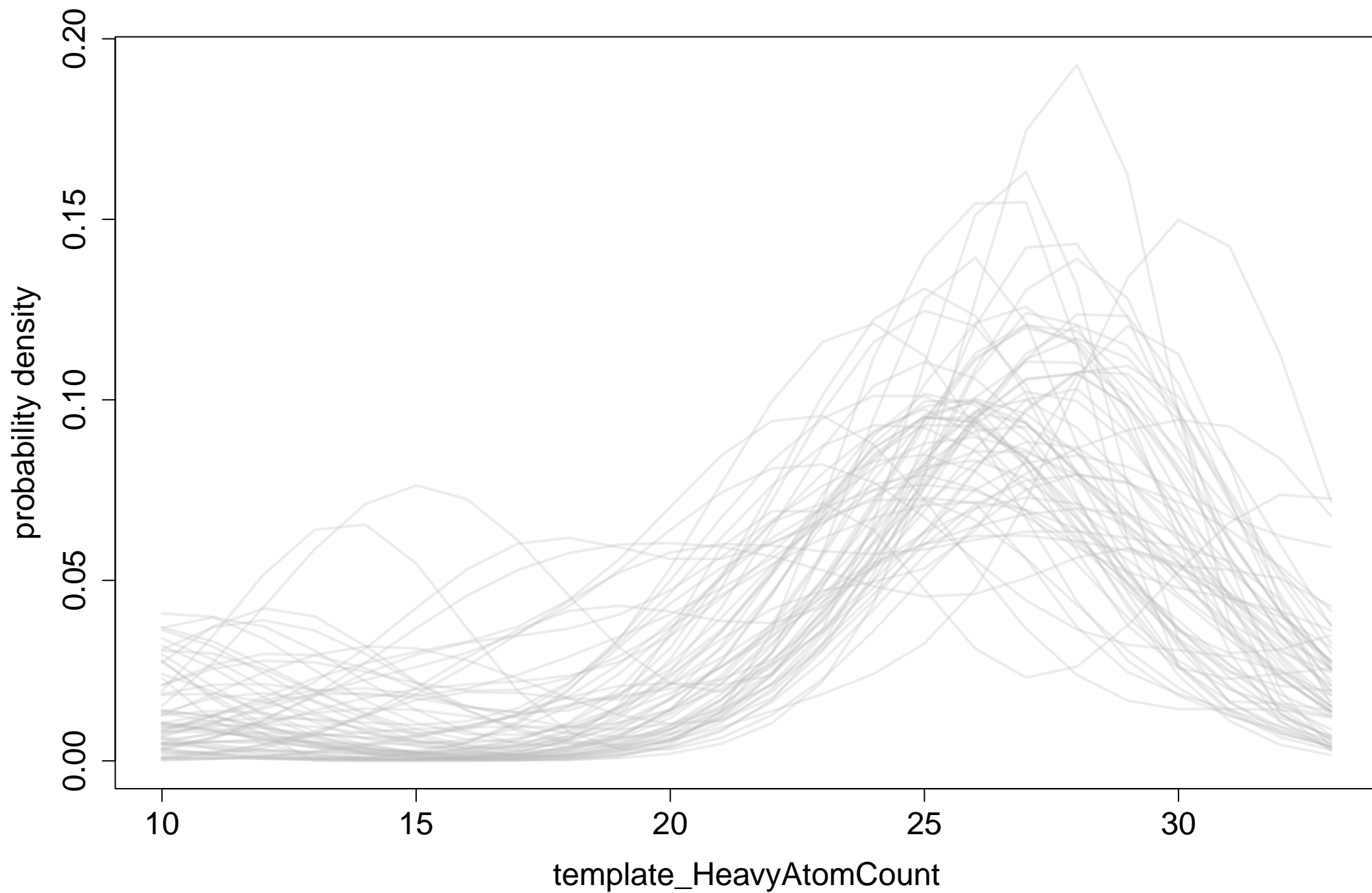
LL: -90.1 +- 4.92

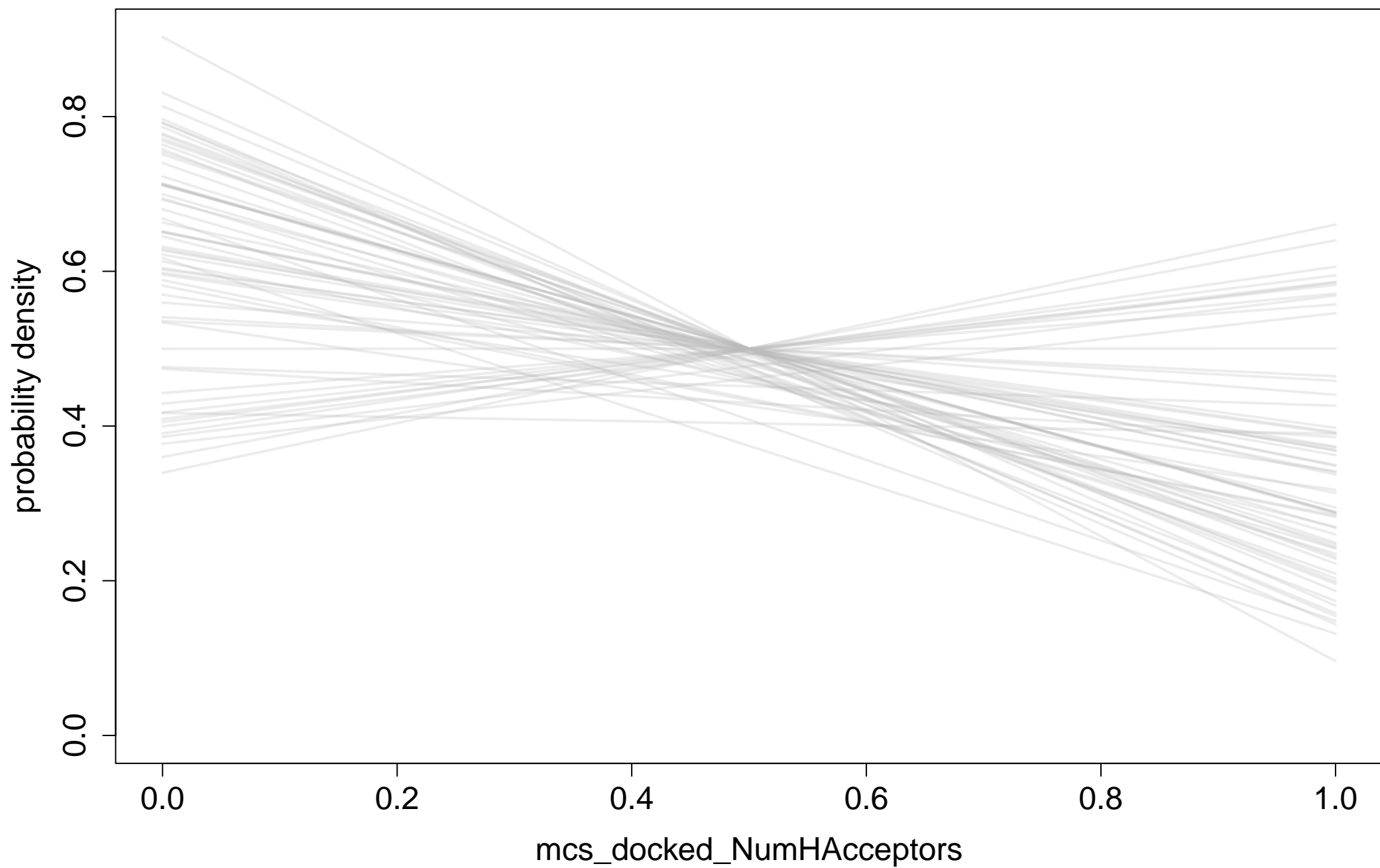


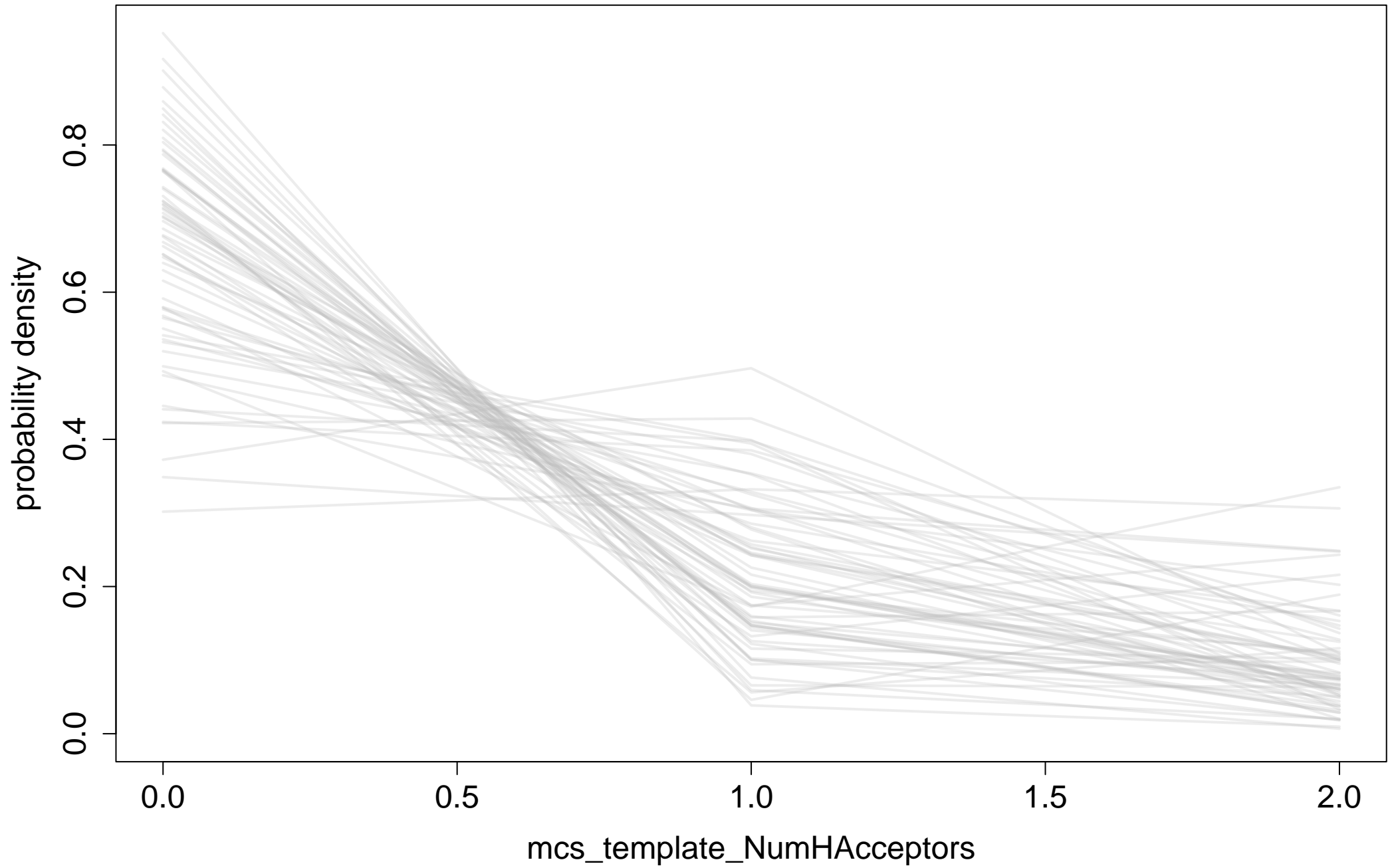


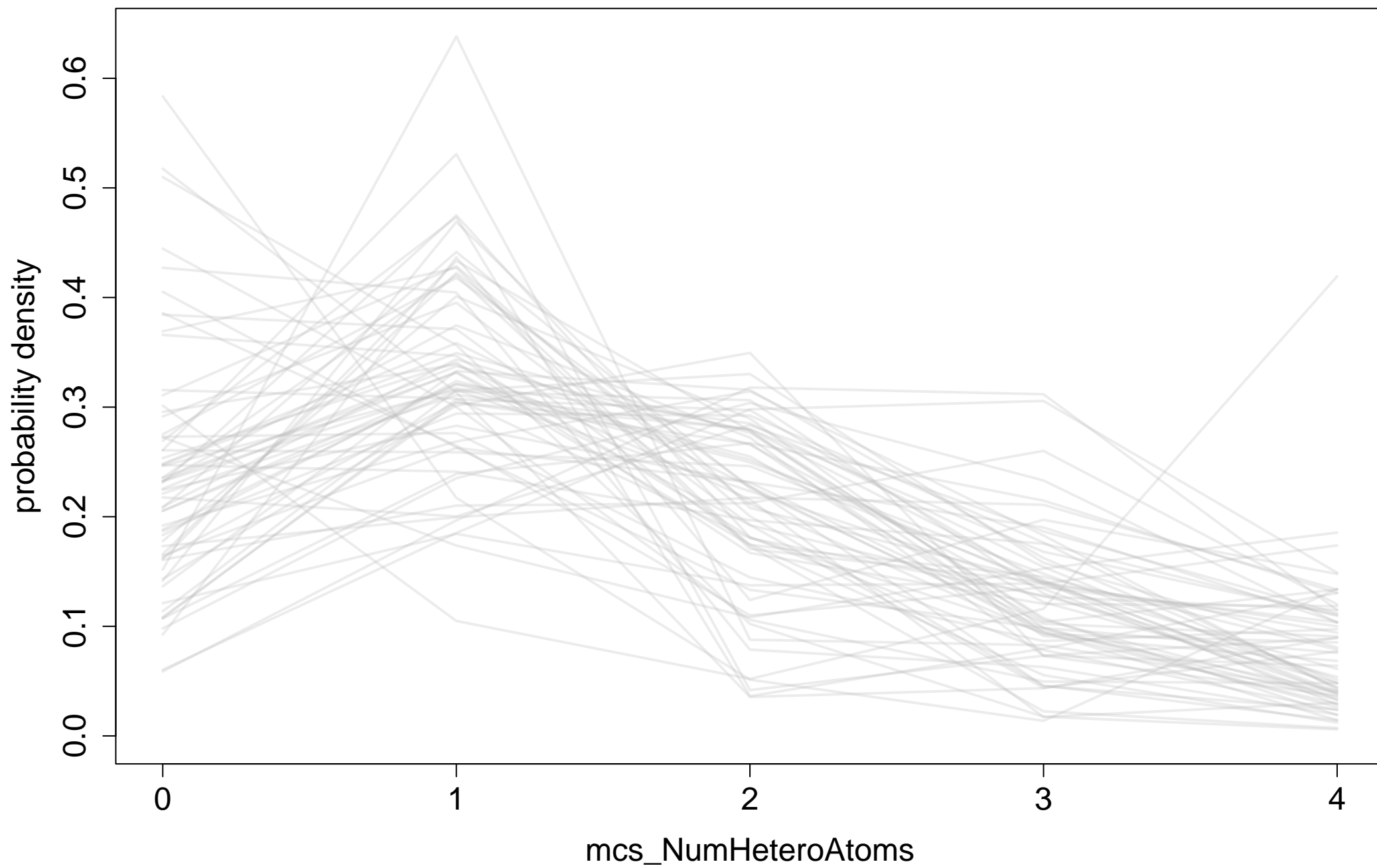


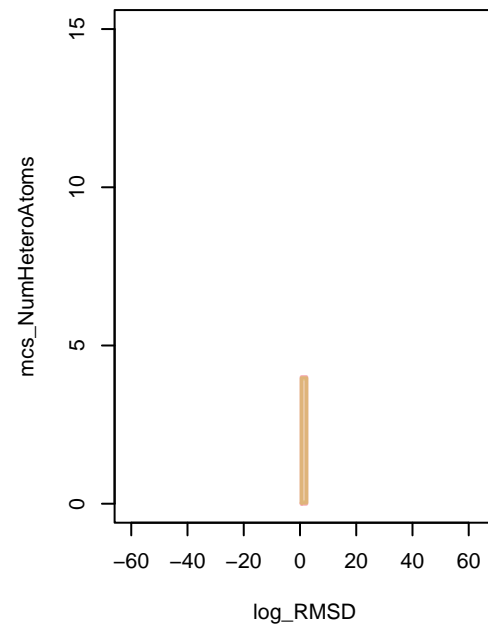
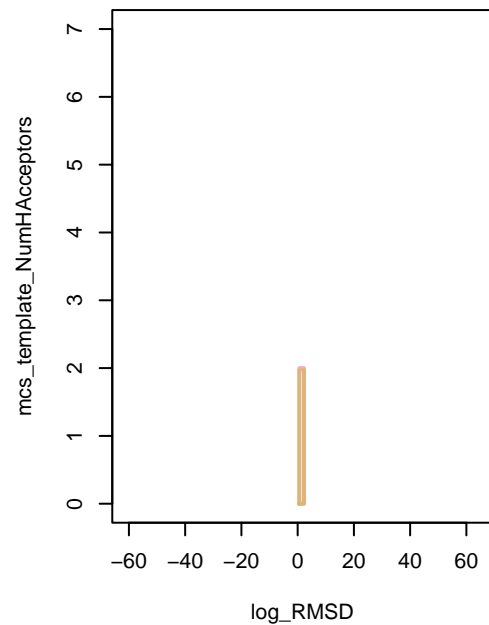
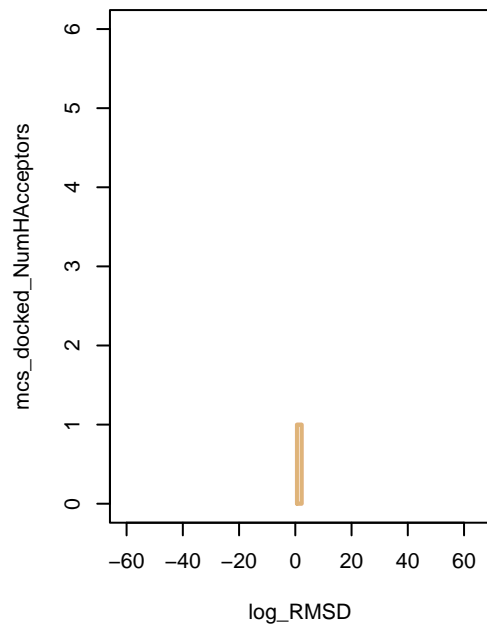
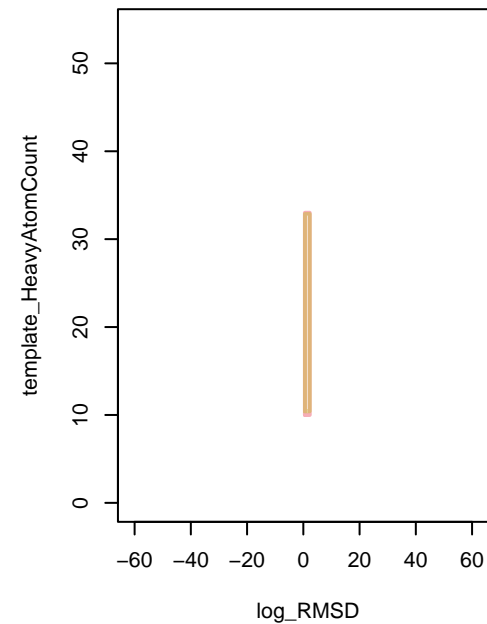
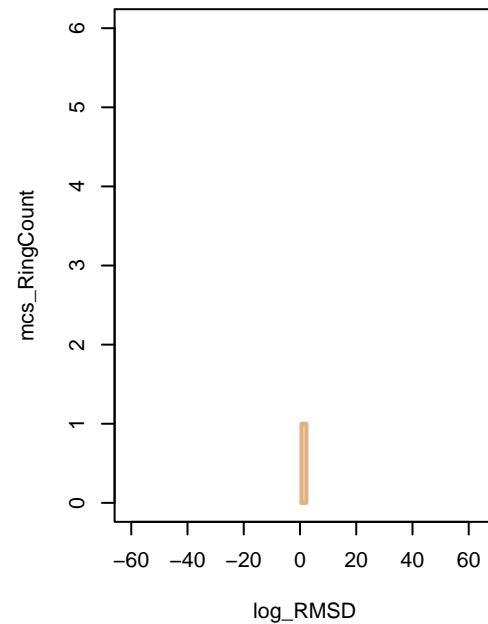
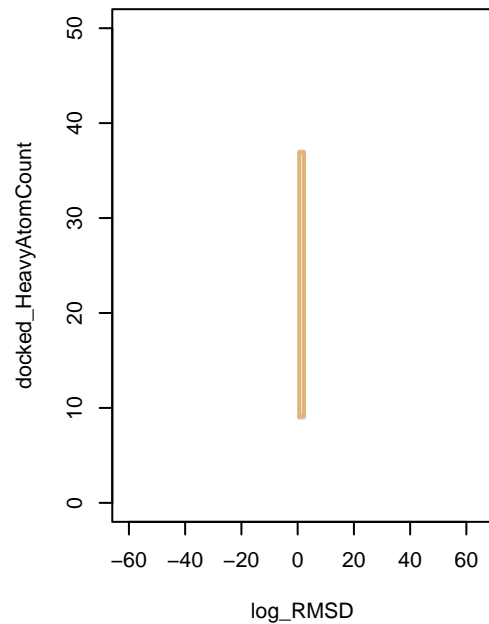
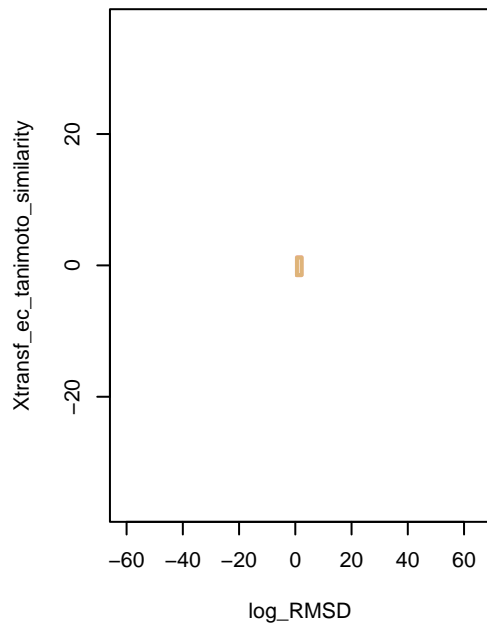




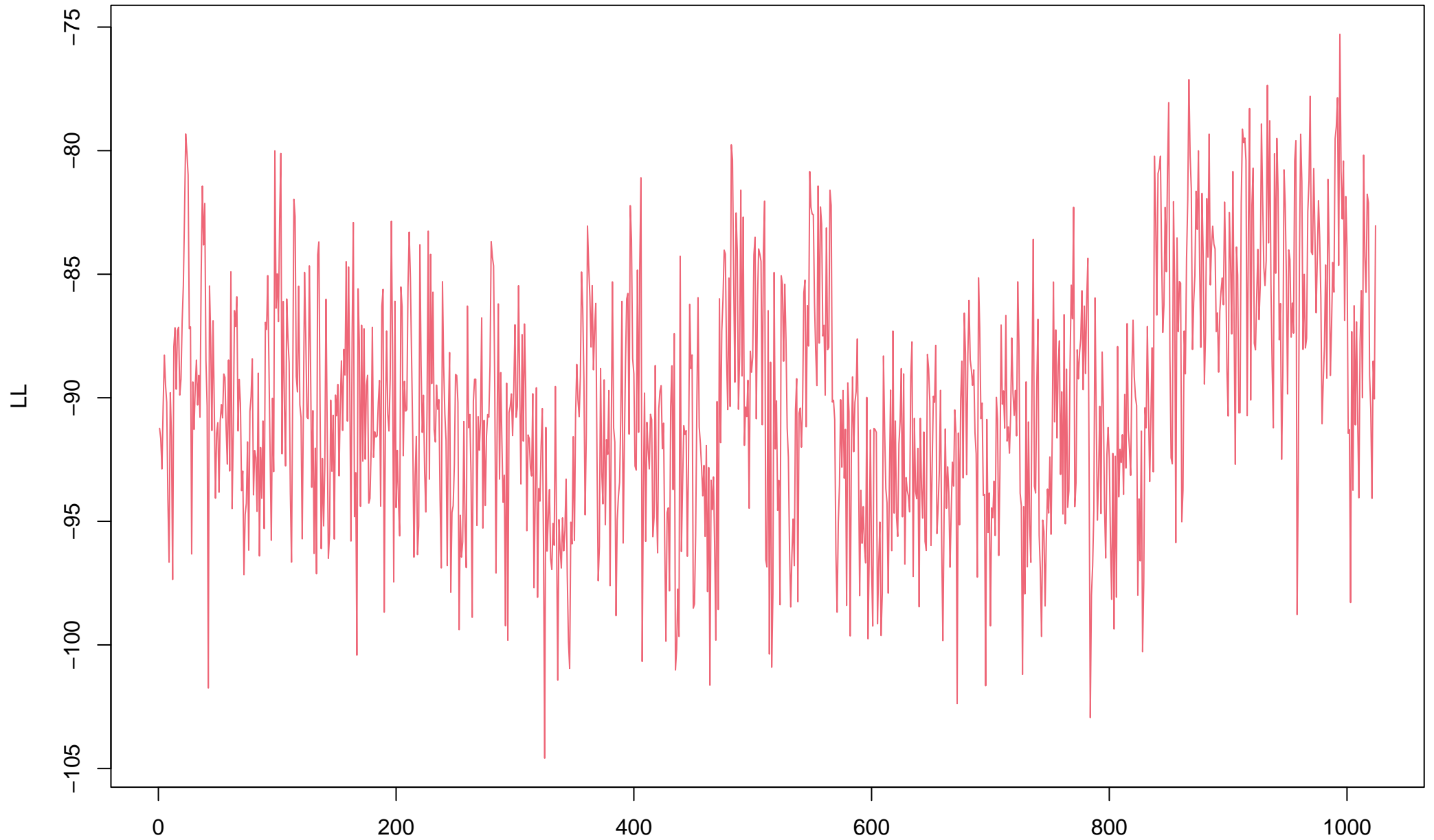




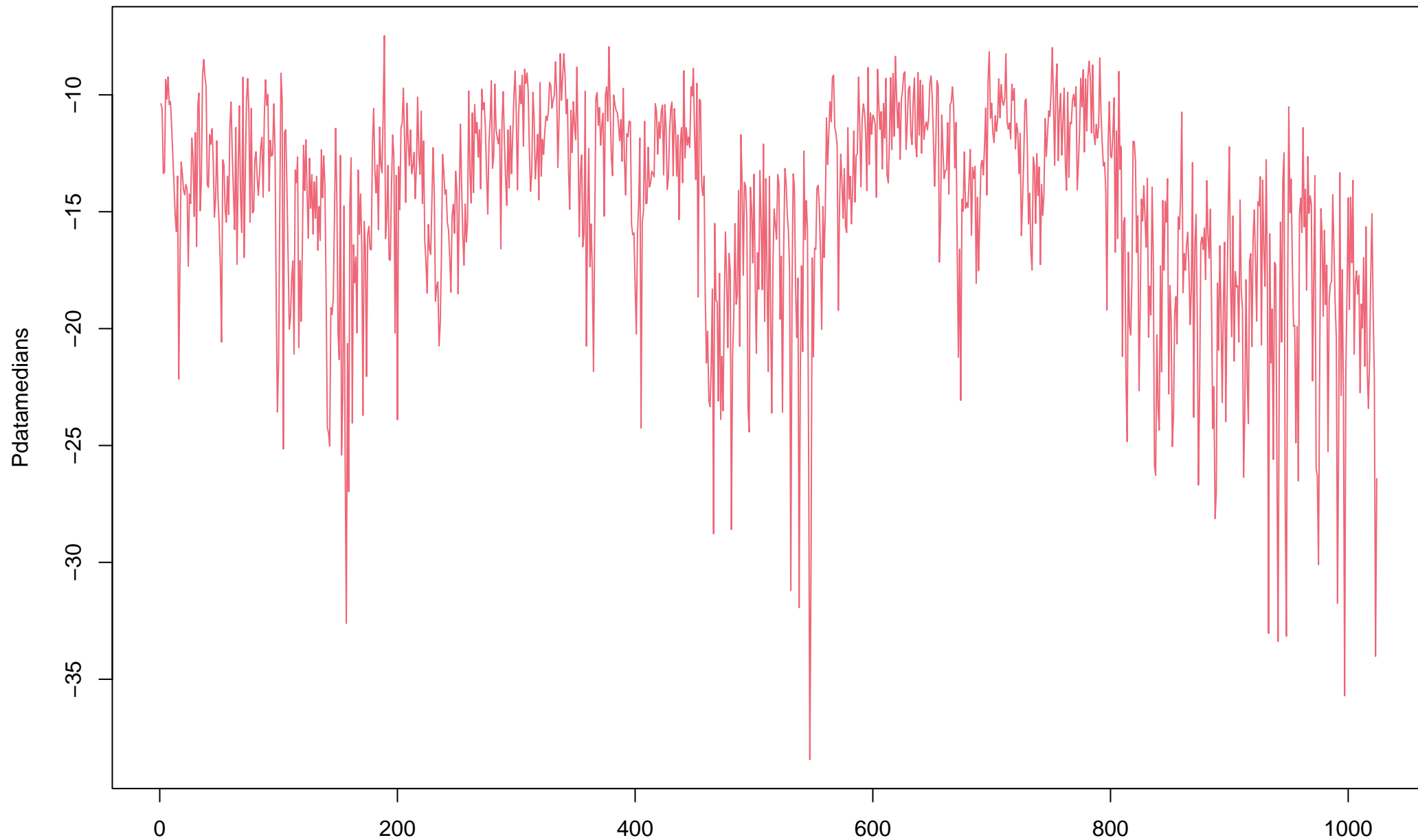




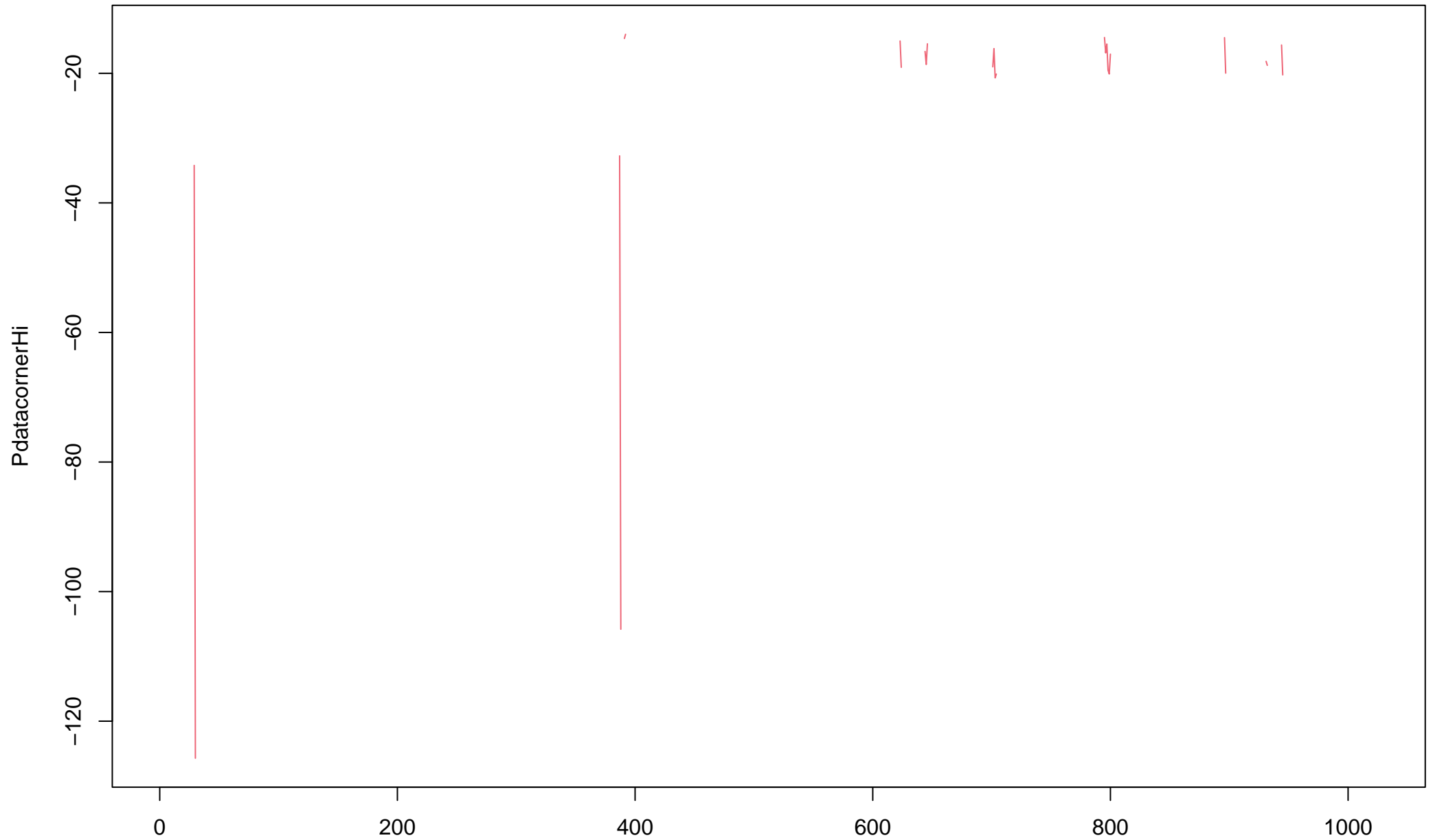
LL
ESS = 66.3 | BMK = 0.149 | MCSE(6.27) = 10.5 | stat: TRUE | burn: 0



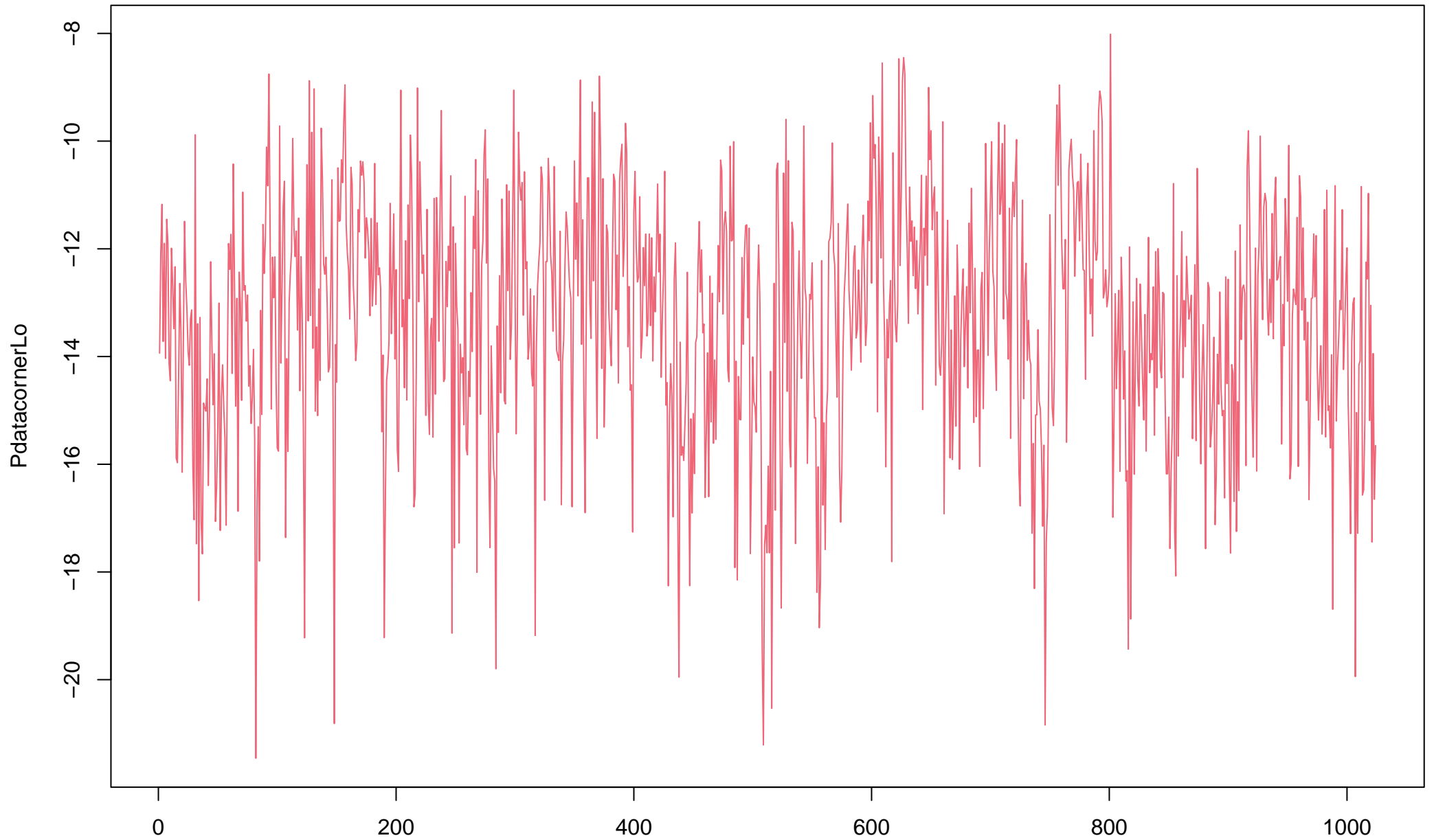
Pdatamedians
ESS = 211 | BMK = 0.153 | MCSE(6.27) = 6.46 | stat: TRUE | burn: 816



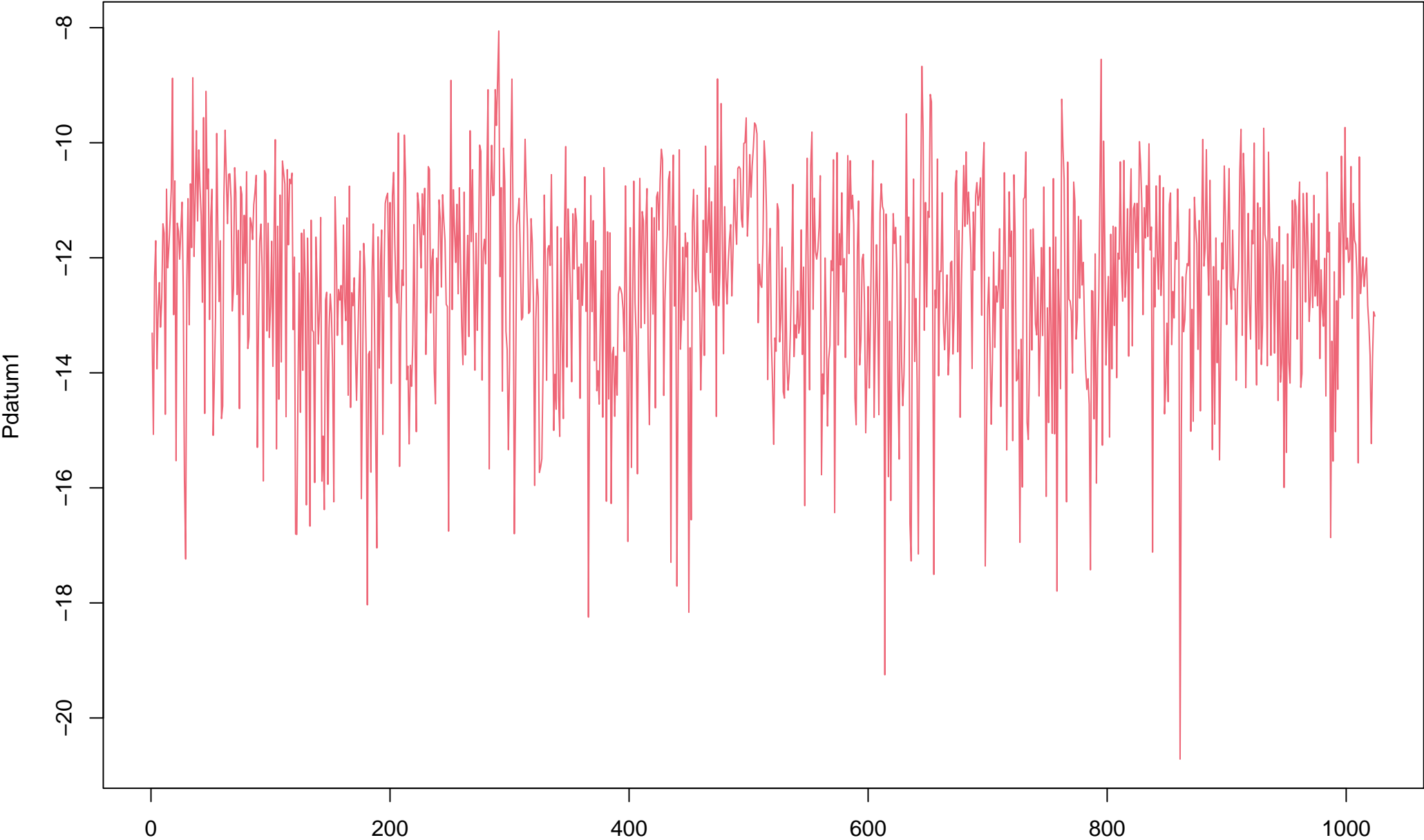
PdatacornerHi
ESS = 626 | BMK = 0.108 | MCSE(6.27) = 3.78 | stat: TRUE | burn: 612



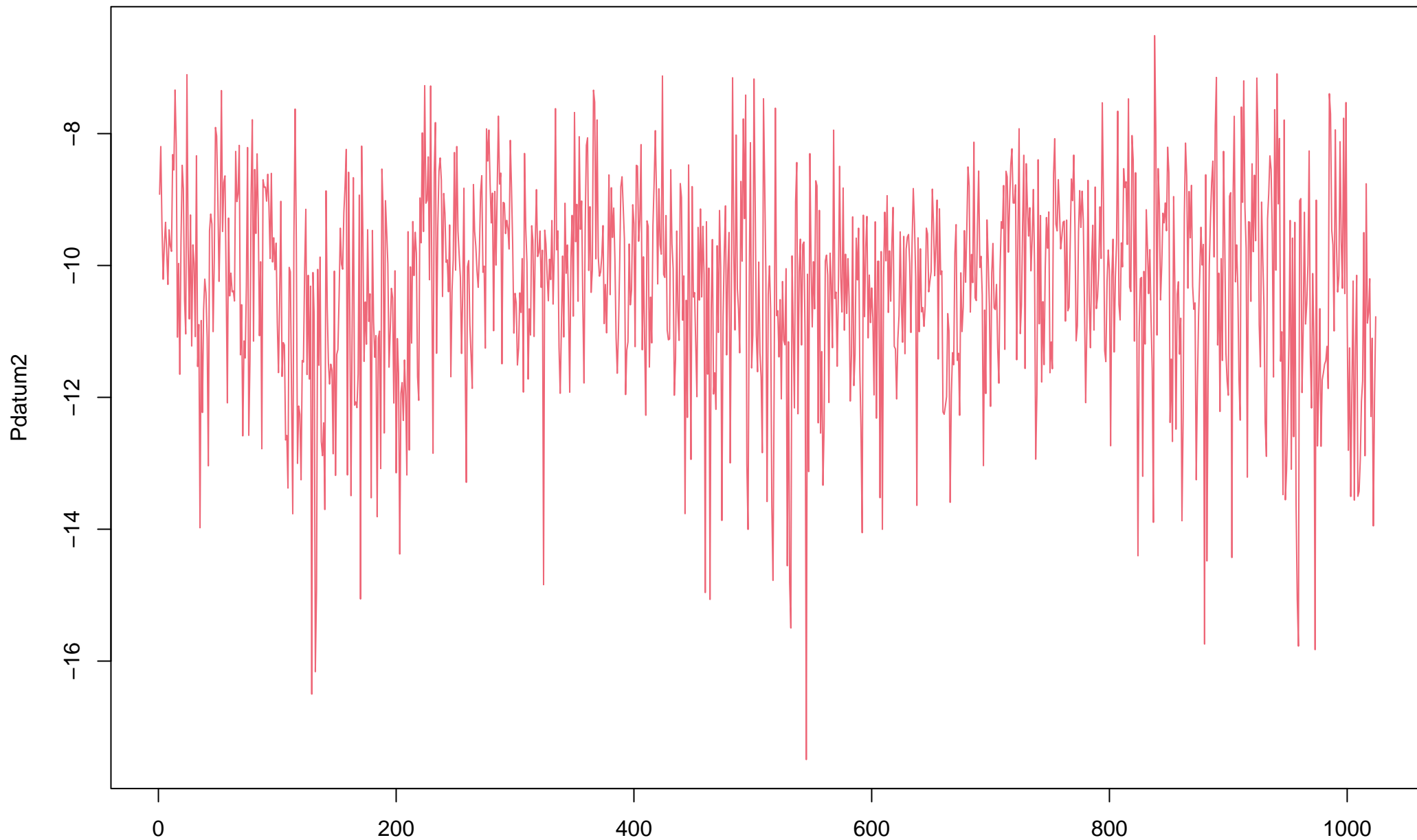
PdatacornerLo
ESS = 169 | BMK = 0.132 | MCSE(6.27) = 4.99 | stat: TRUE | burn: 0



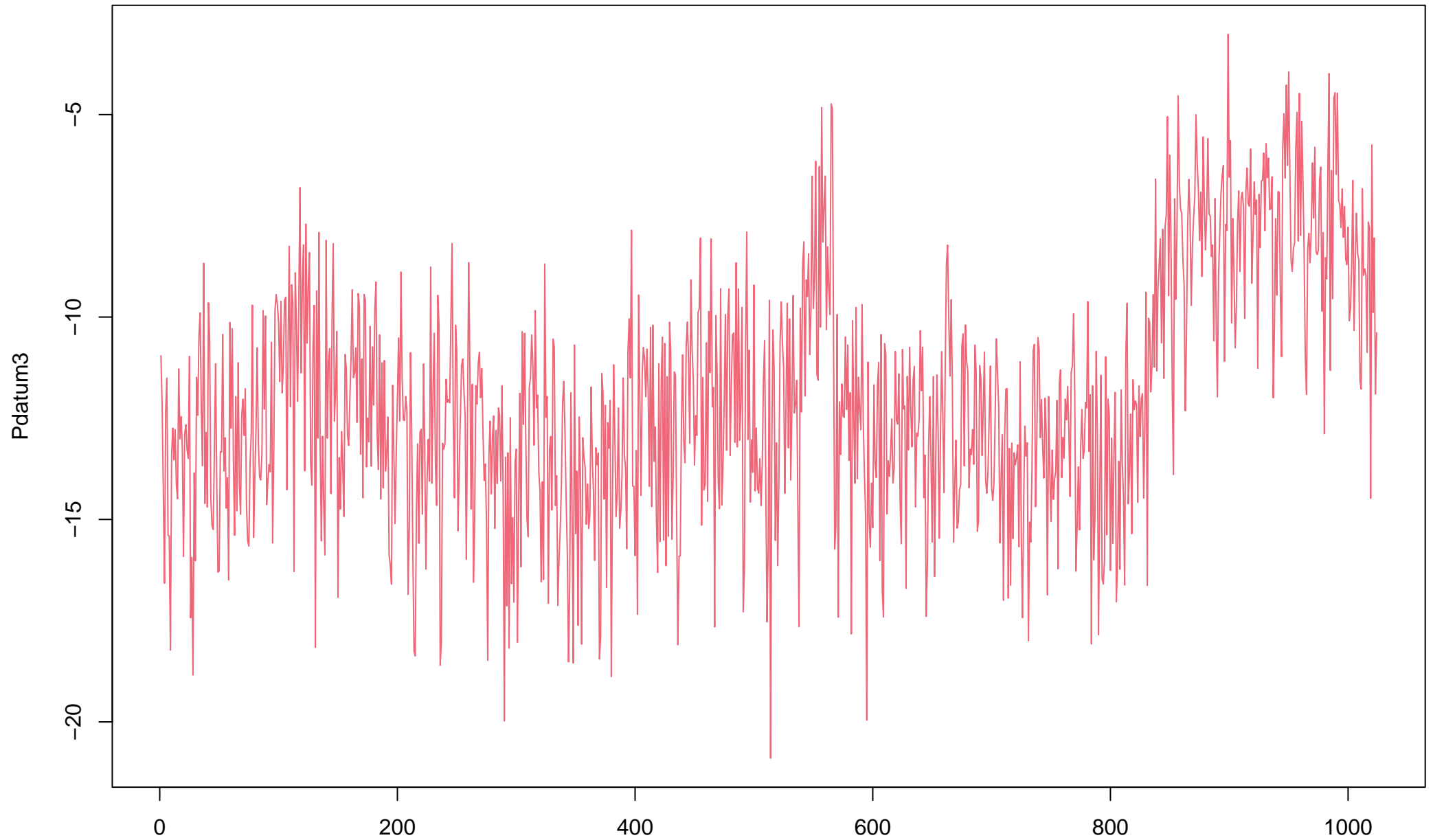
Pdatum1
ESS = 274 | BMK = 0.151 | MCSE(6.27) = 4.97 | stat: FALSE | burn: 0



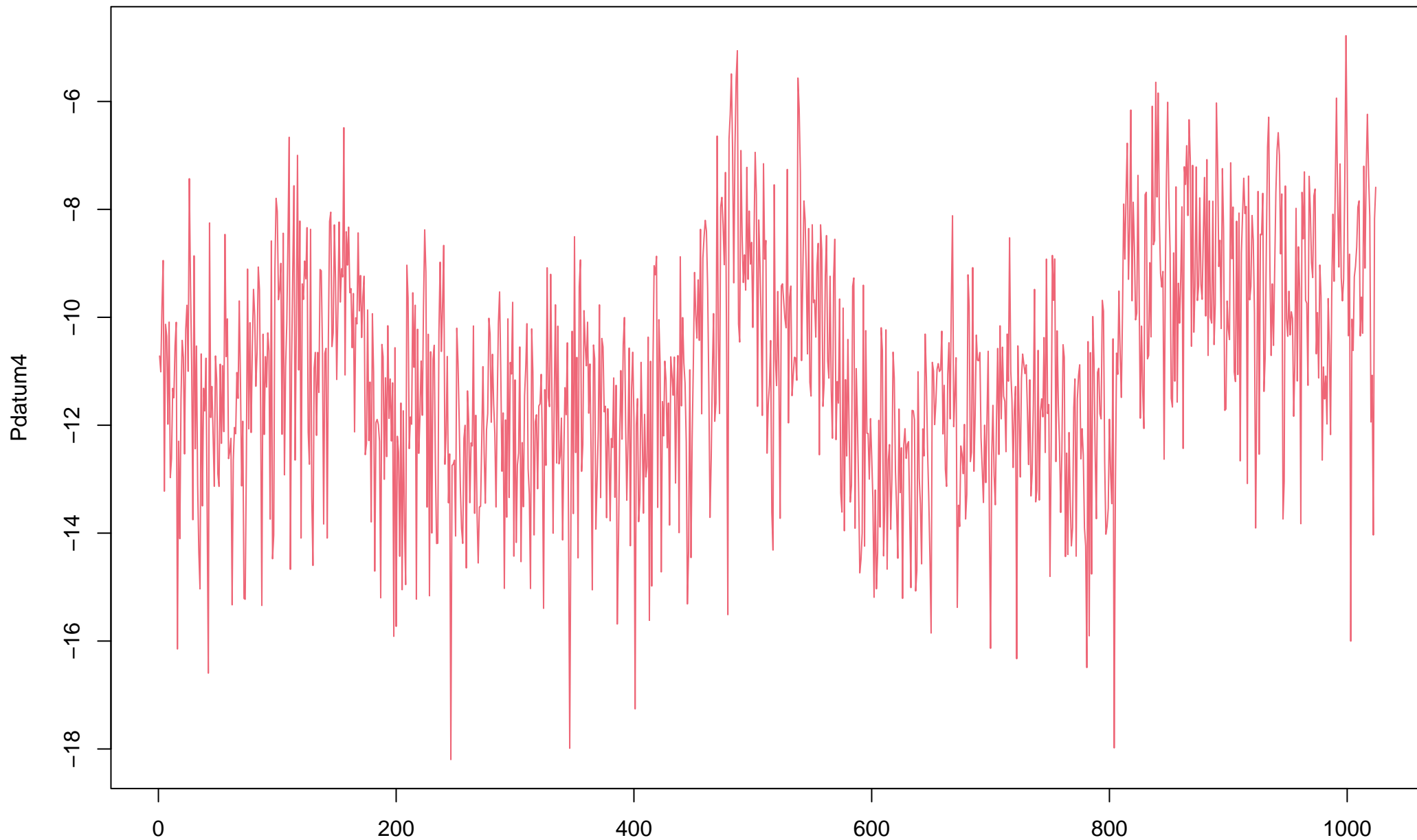
Pdatum2
ESS = 608 | BMK = 0.0822 | MCSE(6.27) = 4.5 | stat: TRUE | burn: 0



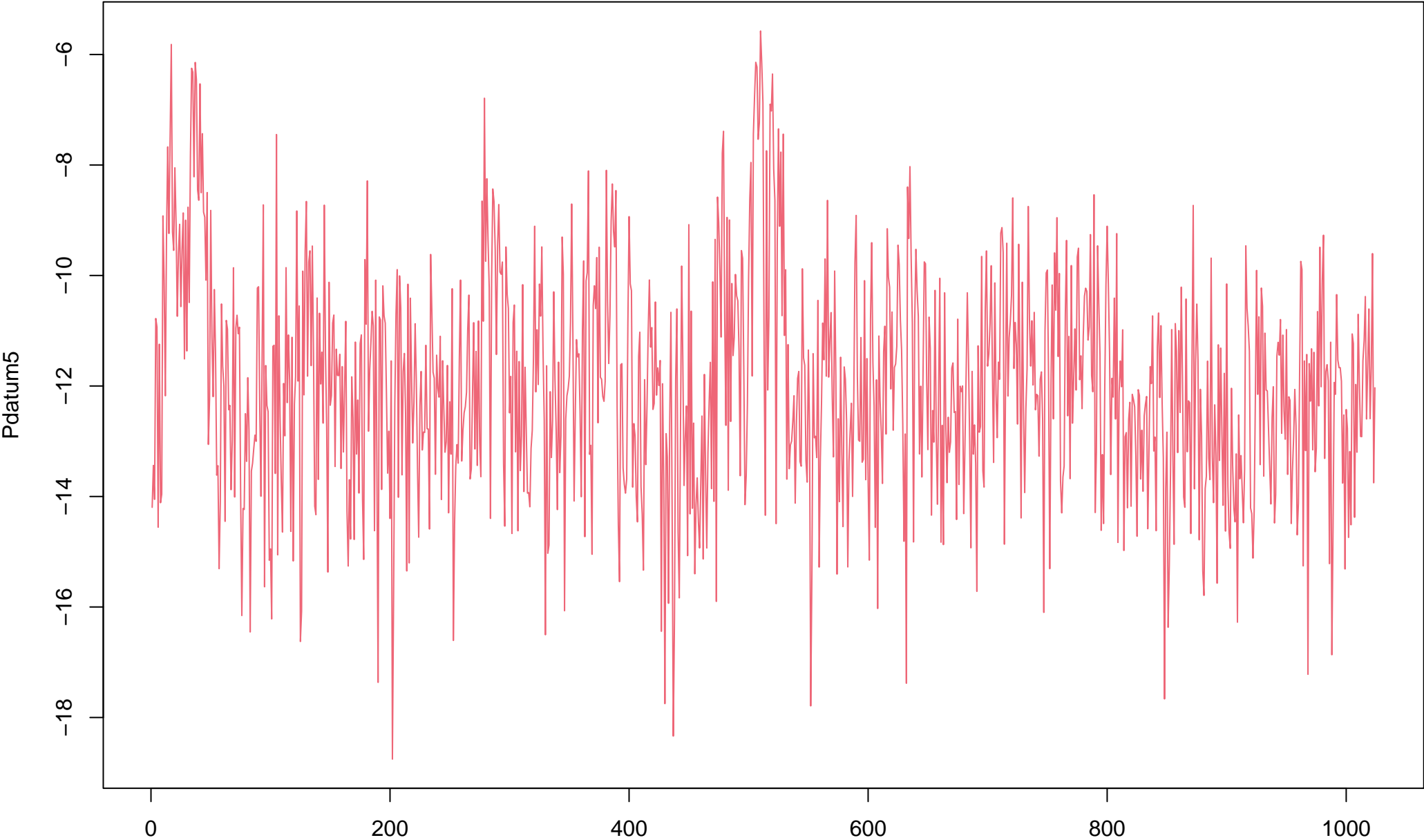
Pdatum3
ESS = 245 | BMK = 1 | MCSE(6.27) = 6.37 | stat: FALSE | burn: 816



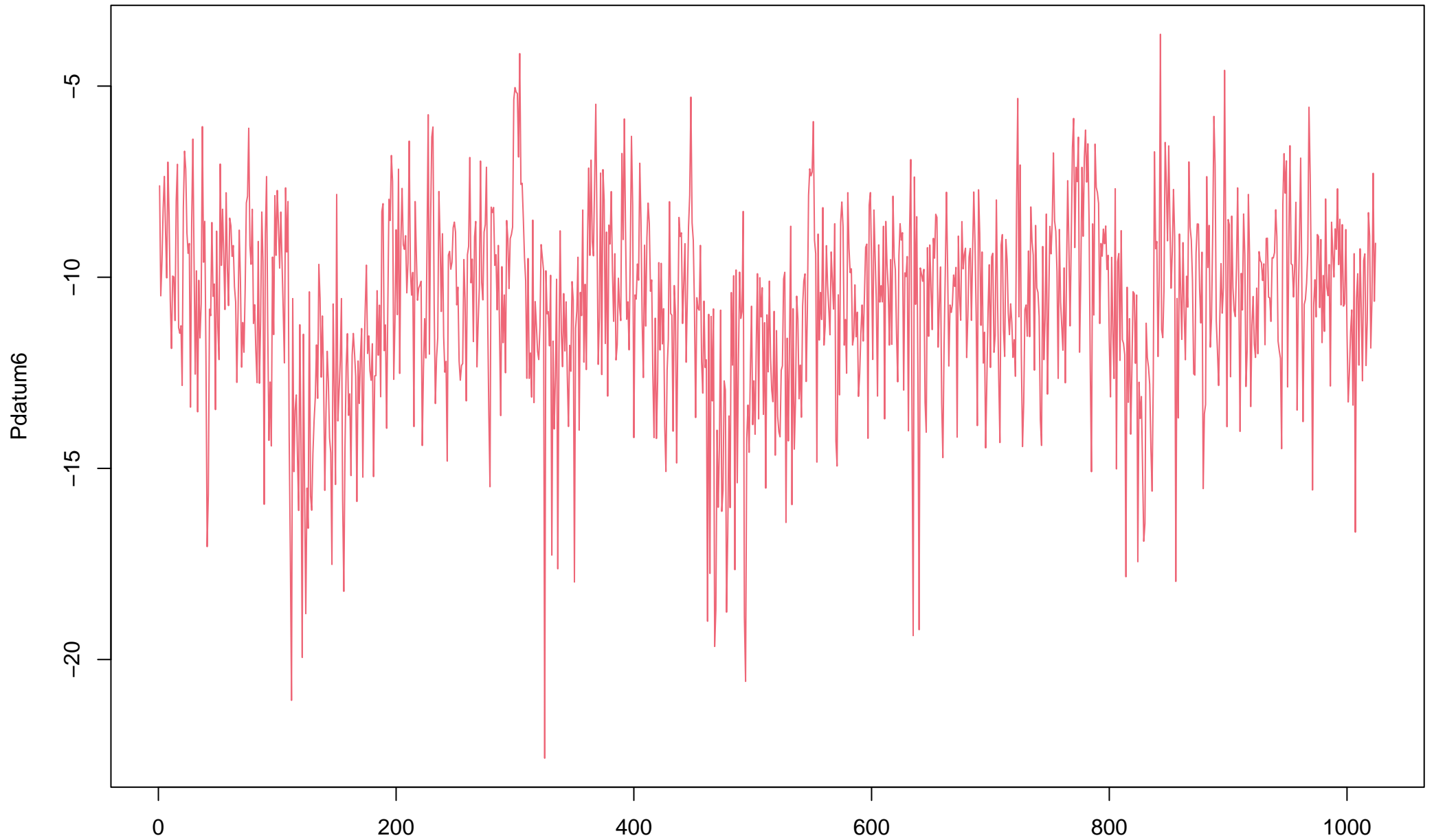
Pdatum4
ESS = 190 | BMK = 0.266 | MCSE(6.27) = 6.85 | stat: FALSE | burn: 816



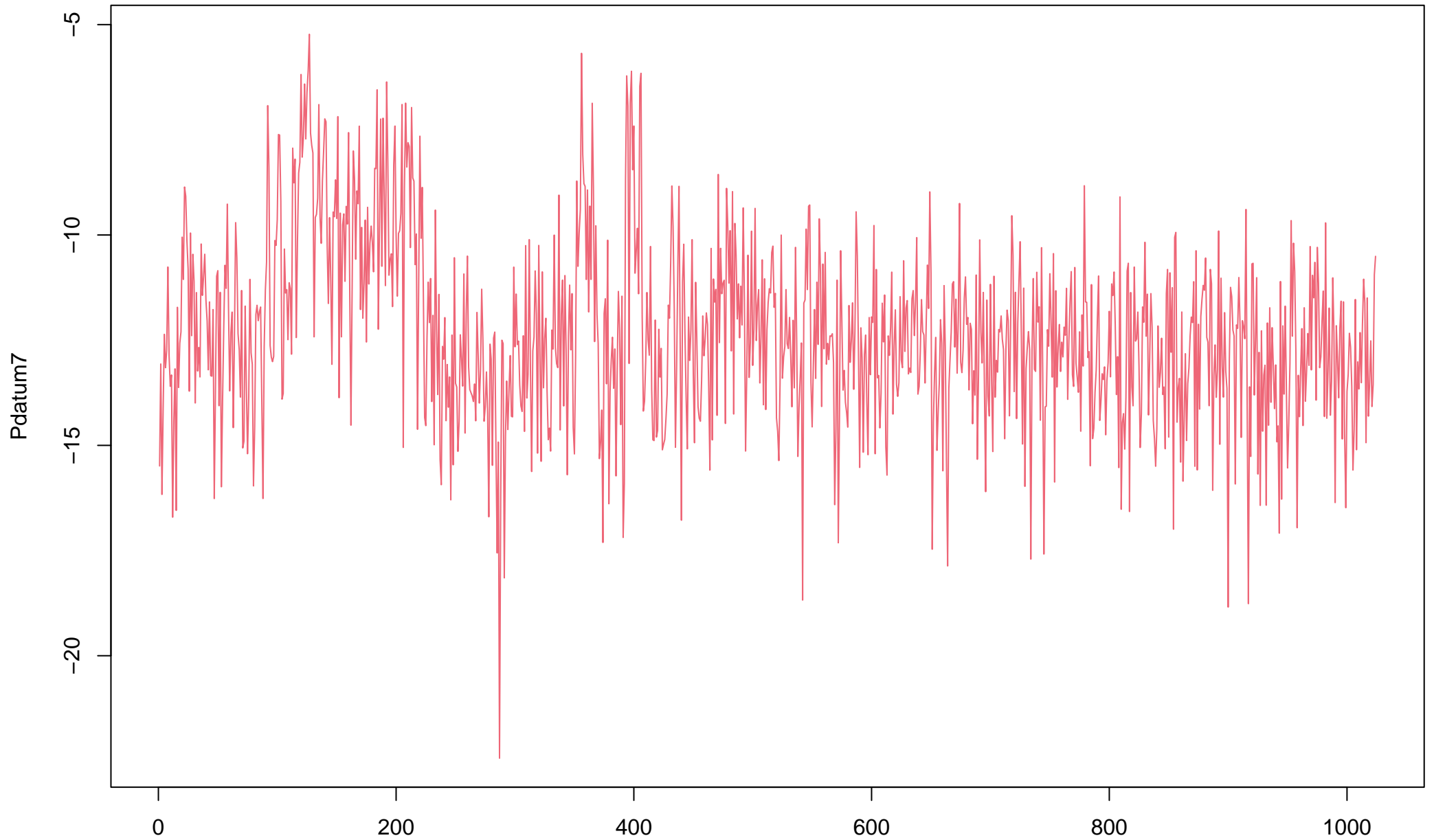
Pdatum5
ESS = 99.6 | BMK = 0.216 | MCSE(6.27) = 7.48 | stat: FALSE | burn: 0



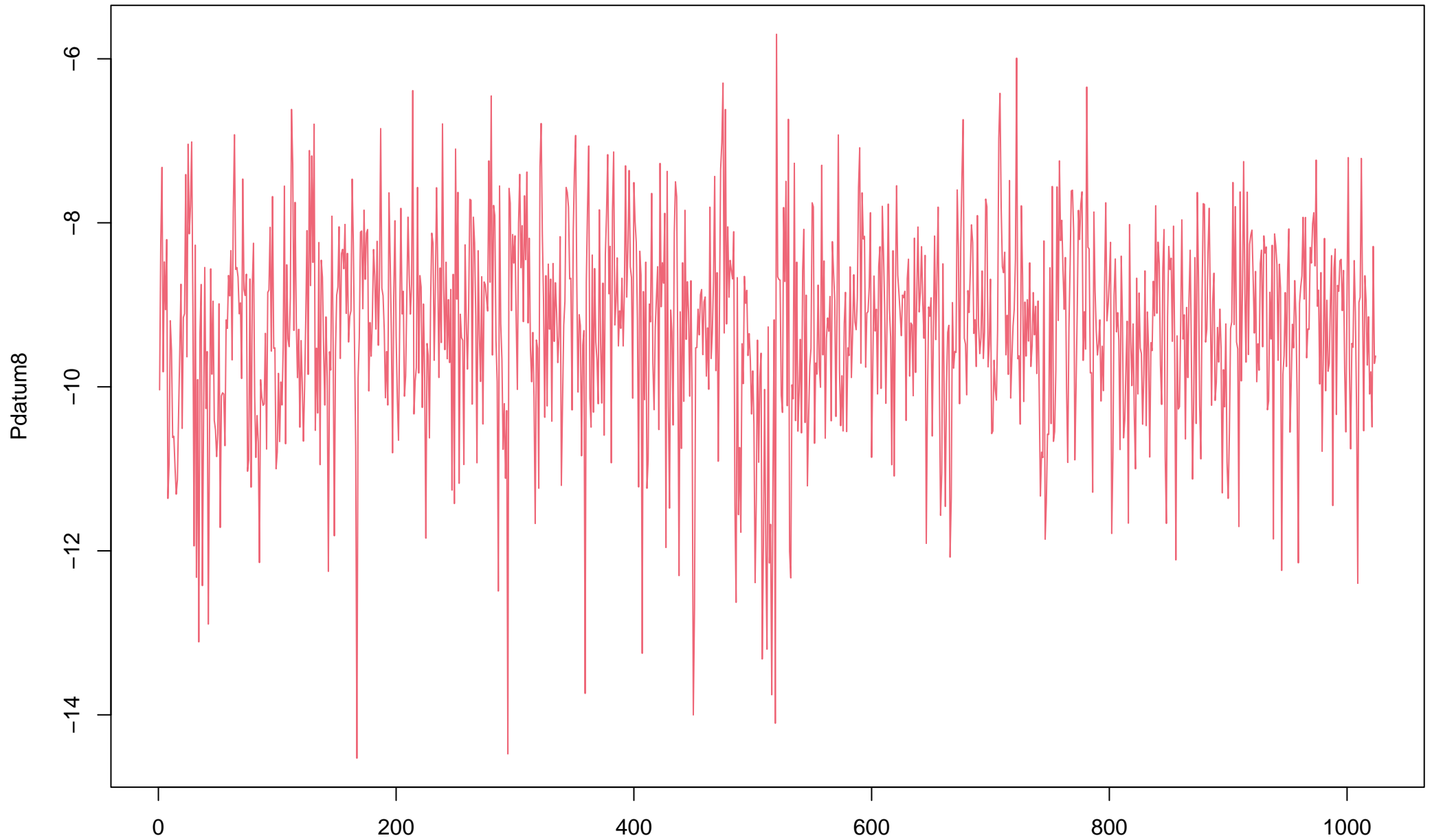
Pdatum6
ESS = 447 | BMK = 0.169 | MCSE(6.27) = 4.31 | stat: TRUE | burn: 204



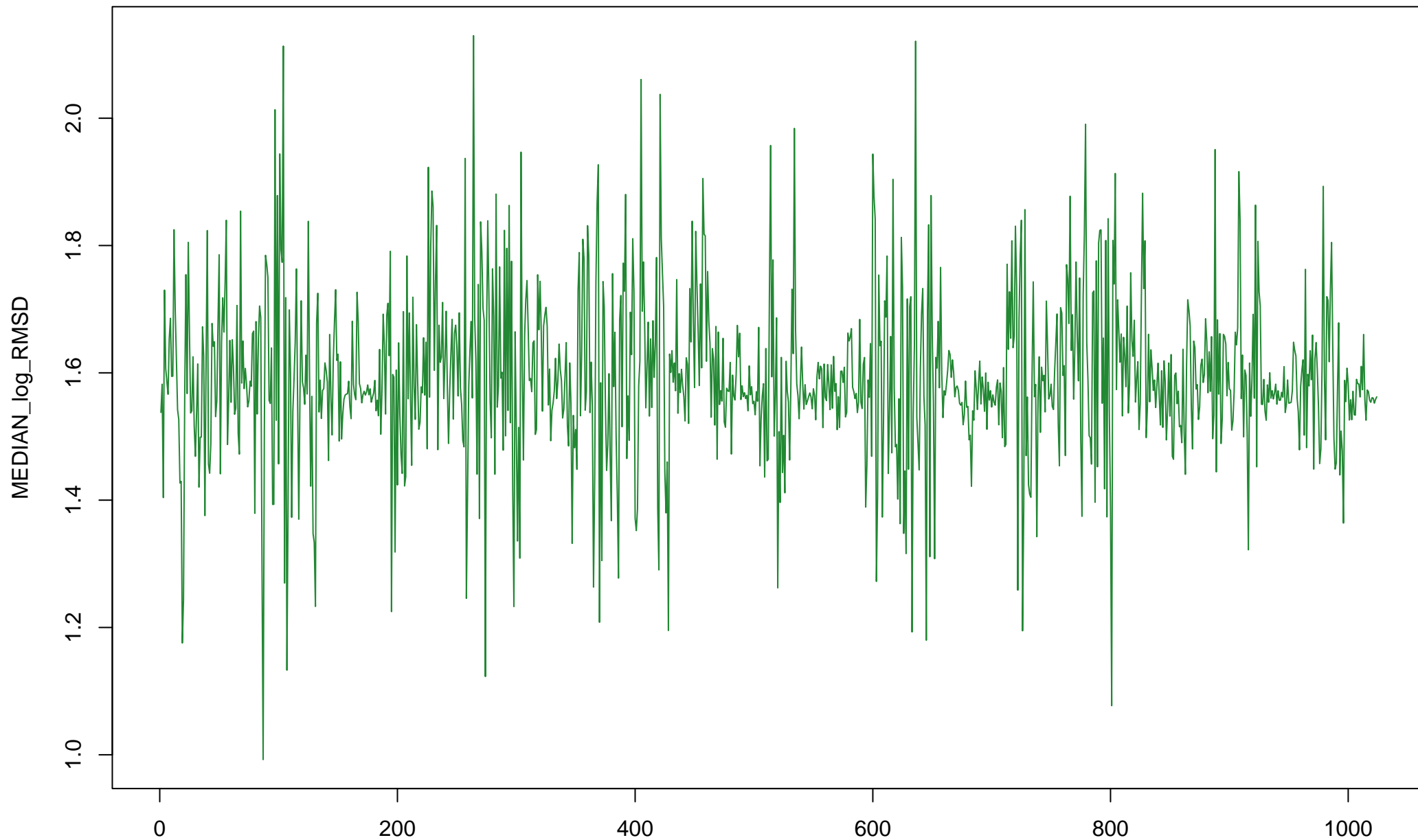
Pdatum7
ESS = 140 | BMK = 0.588 | MCSE(6.27) = 7.27 | stat: TRUE | burn: 306



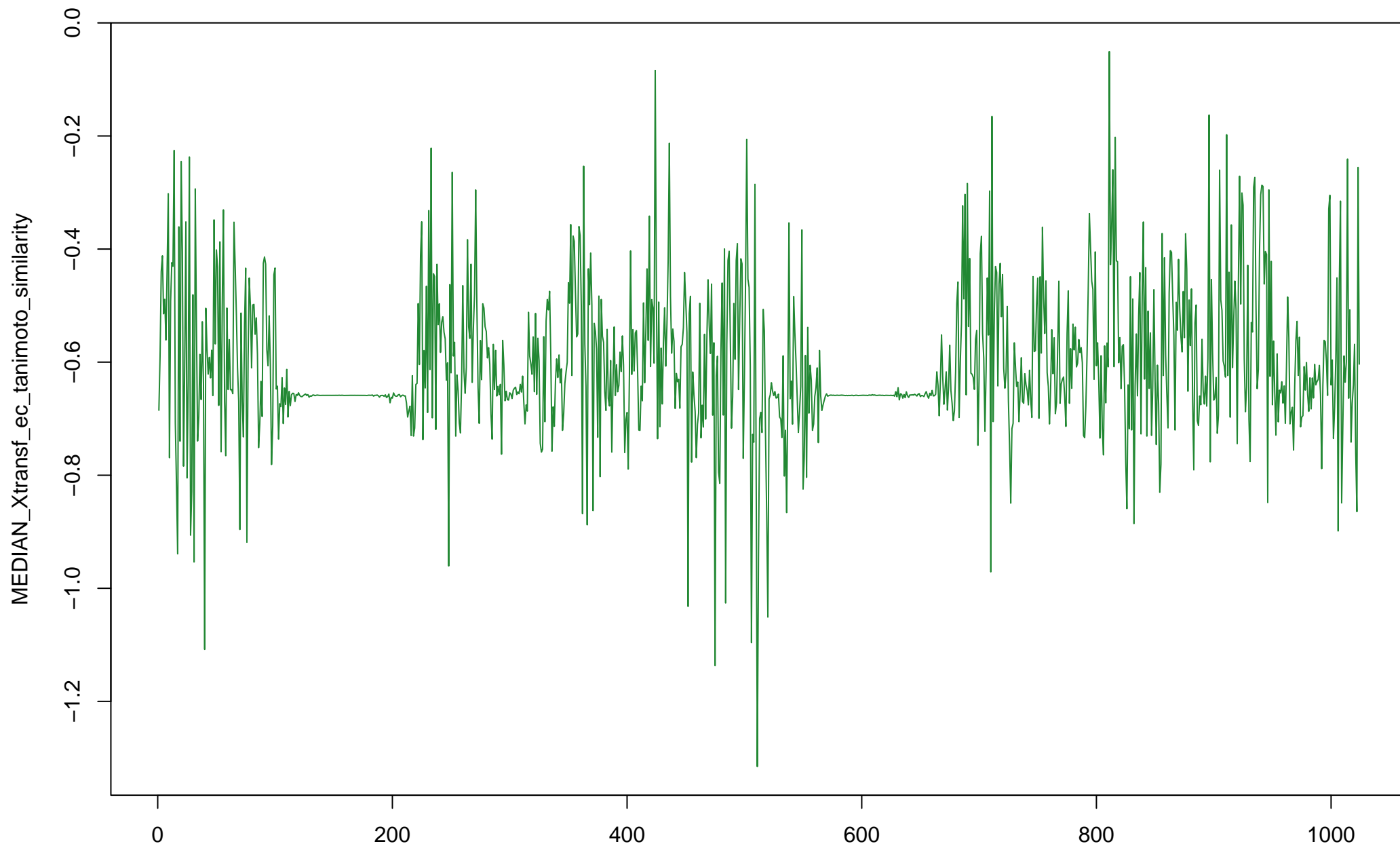
Pdatum8
ESS = 723 | BMK = 0.119 | MCSE(6.27) = 3.48 | stat: TRUE | burn: 0



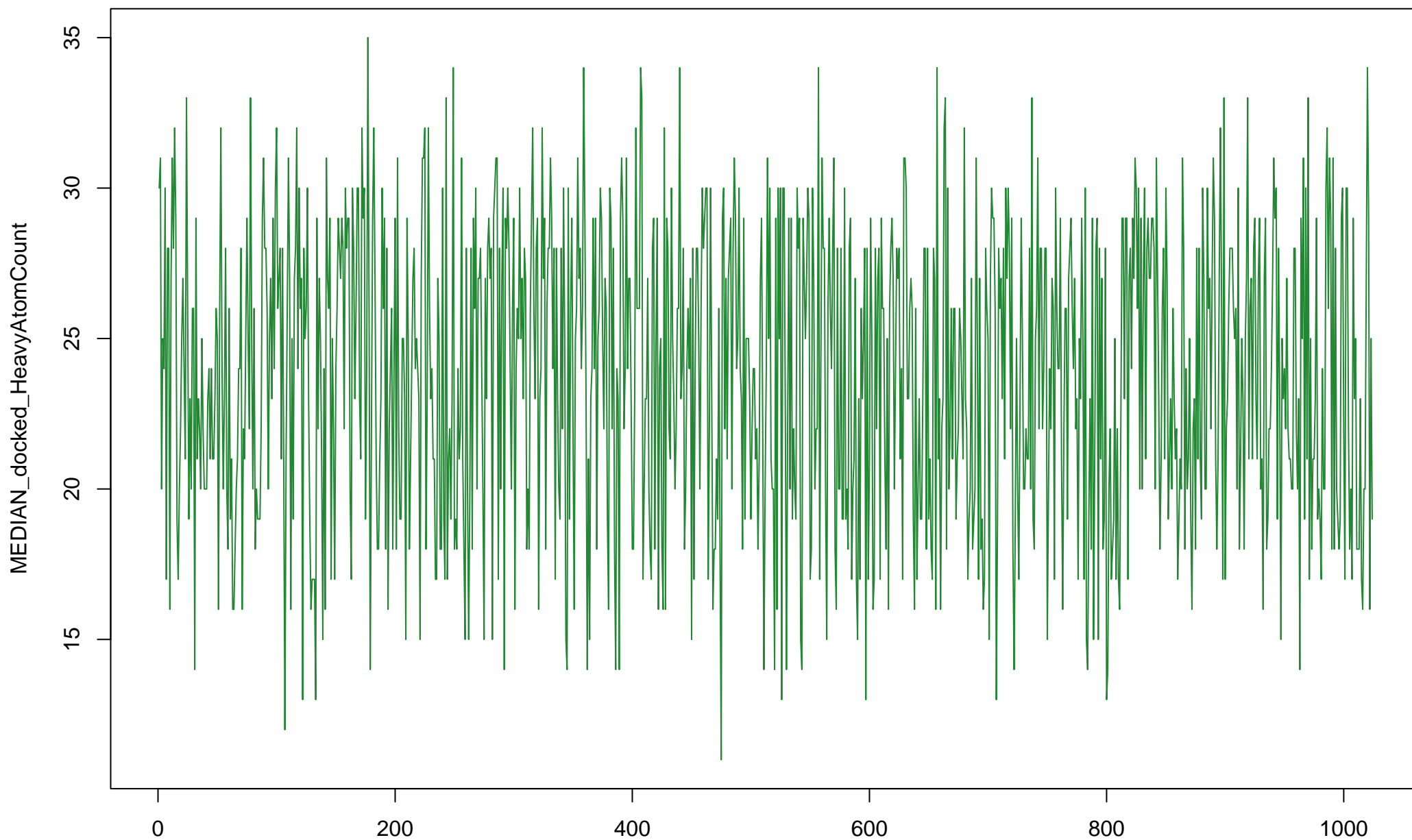
MEDIAN_log_RMSD
ESS = 963 | BMK = 0.108 | MCSE(6.27) = 3.58 | stat: TRUE | burn: 0



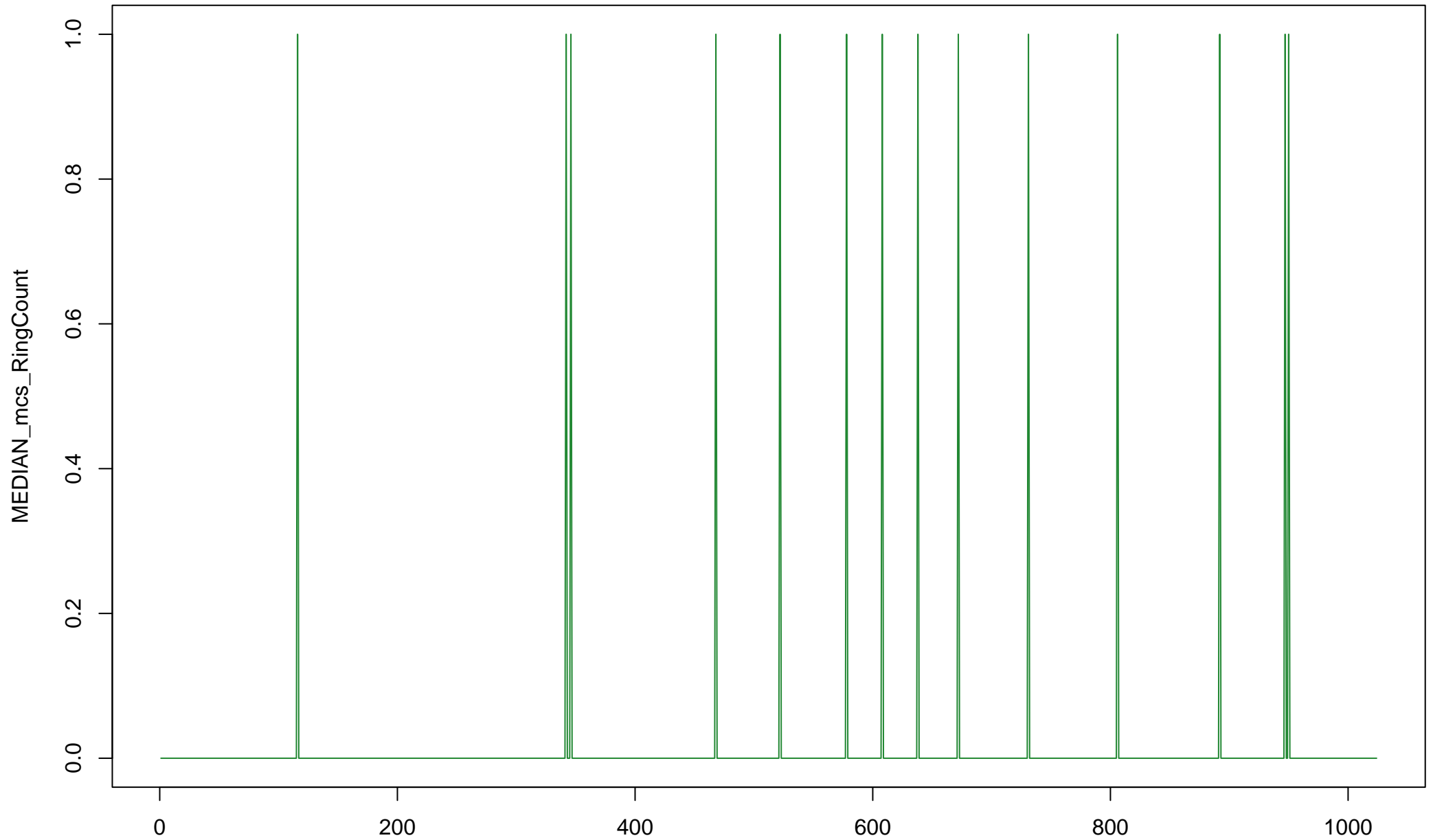
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 235 | BMK = 0.103 | MCSE(6.27) = 5.95 | stat: TRUE | burn: 510



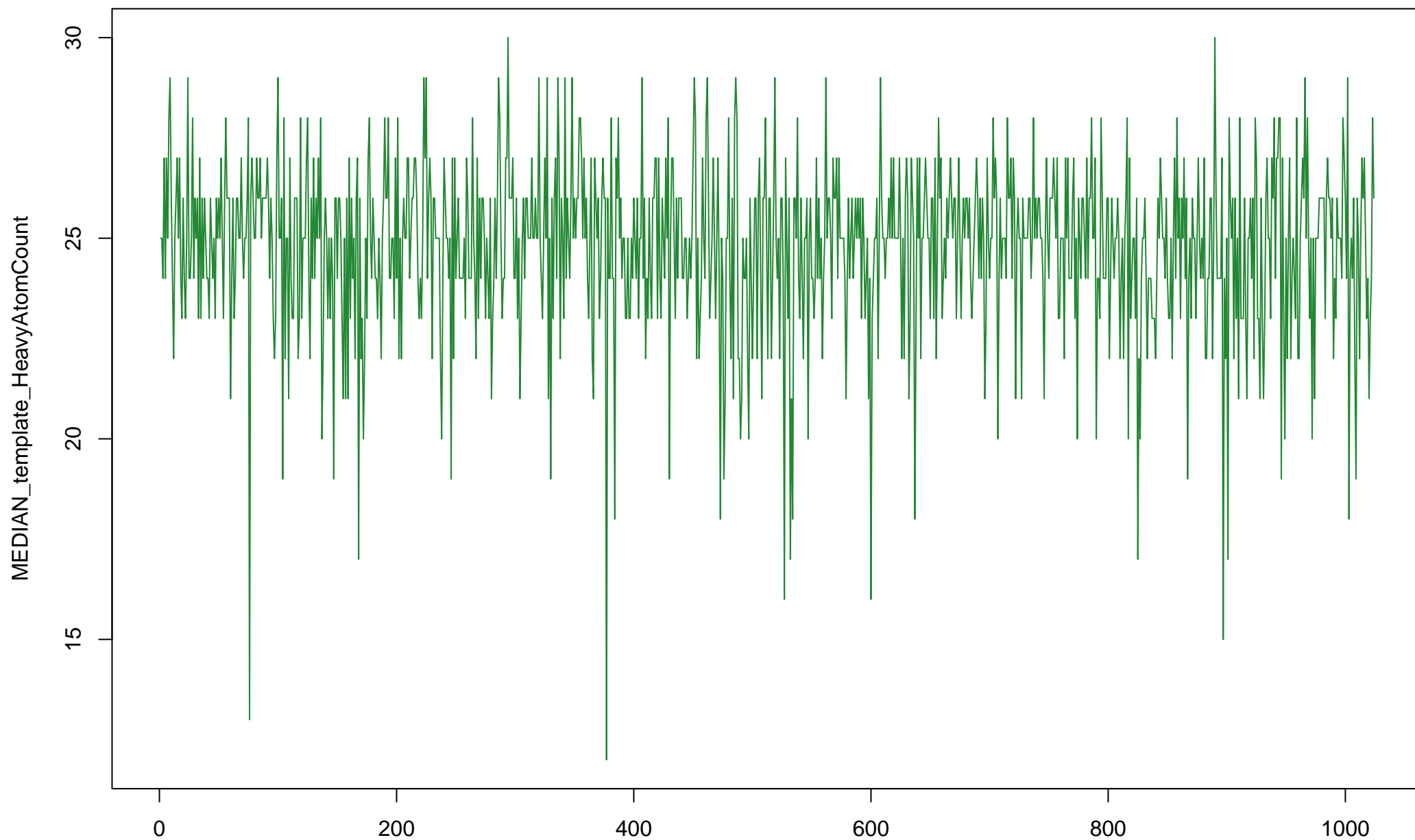
MEDIAN_docked_HeavyAtomCount
ESS = 885 | BMK = 0.0659 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0



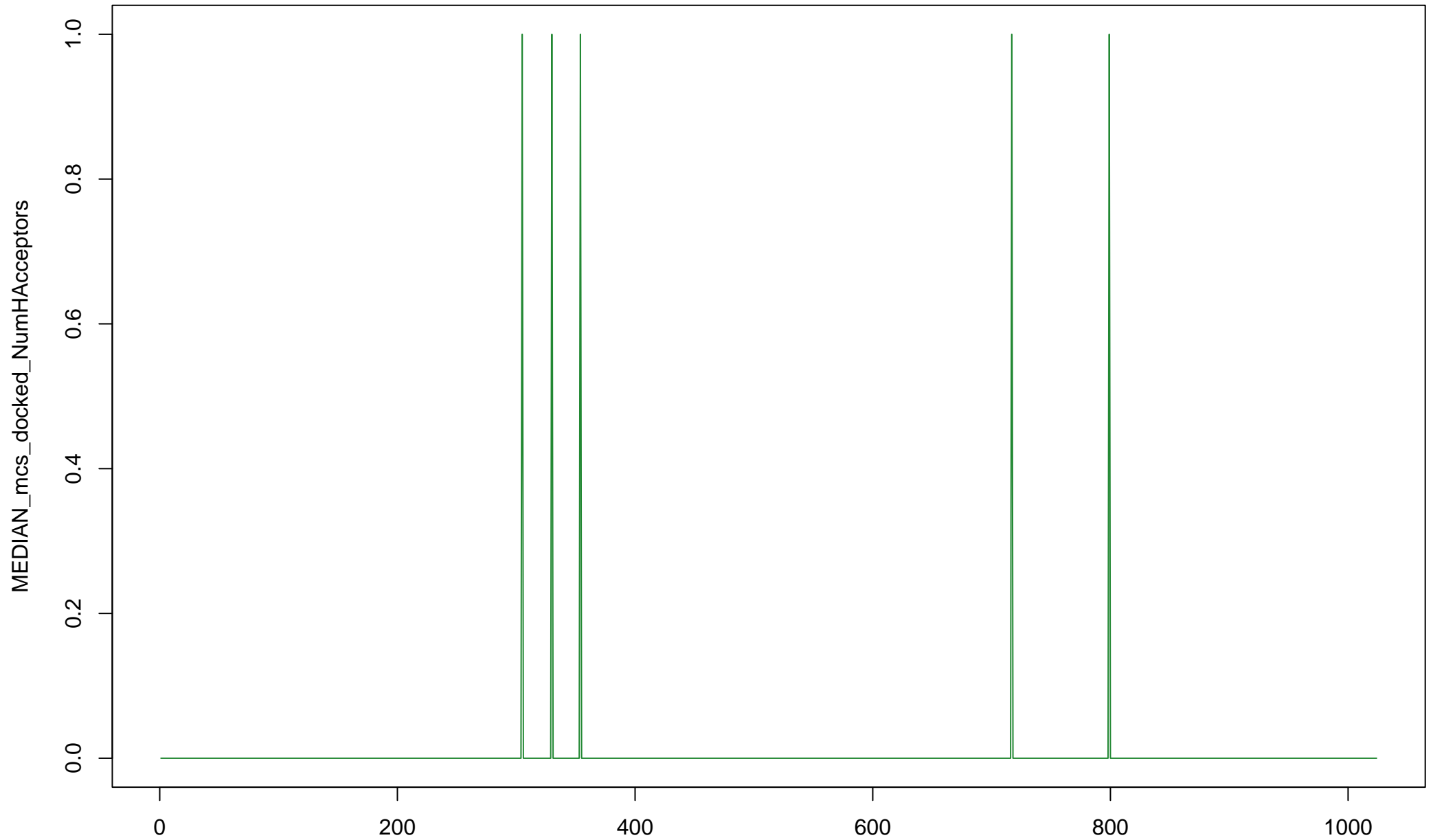
MEDIAN_mcs_RingCount
ESS = 1020 | BMK = 0.158 | MCSE(6.27) = 3.18 | stat: FALSE | burn: 204



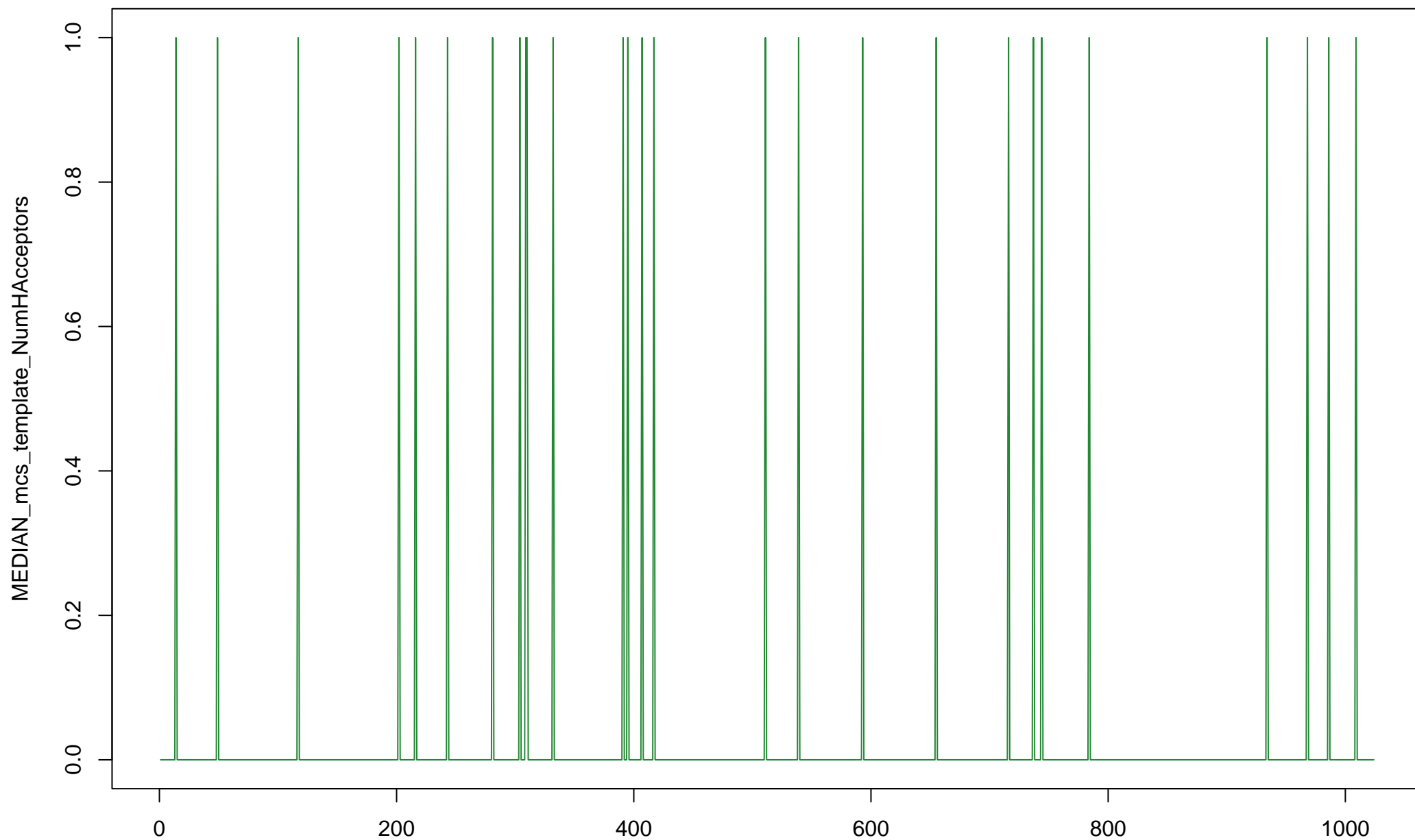
MEDIAN_template_HeavyAtomCount
ESS = 1020 | BMK = 0.0919 | MCSE(6.27) = 3.34 | stat: FALSE | burn: 0



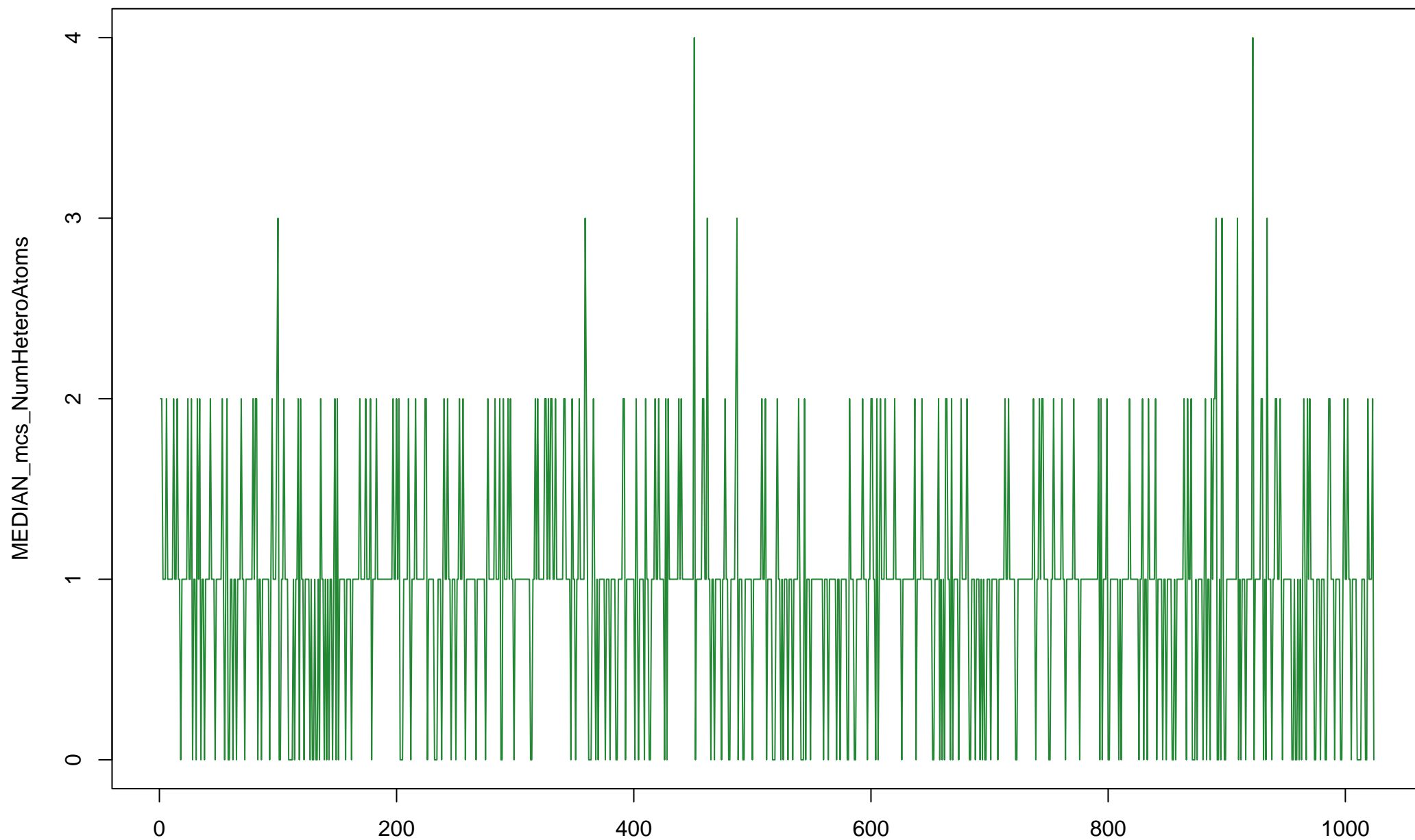
MEDIAN_mcs_docked_NumHAcceptors
ESS = 565 | BMK = 0.0717 | MCSE(6.27) = 2.92 | stat: FALSE | burn: 204



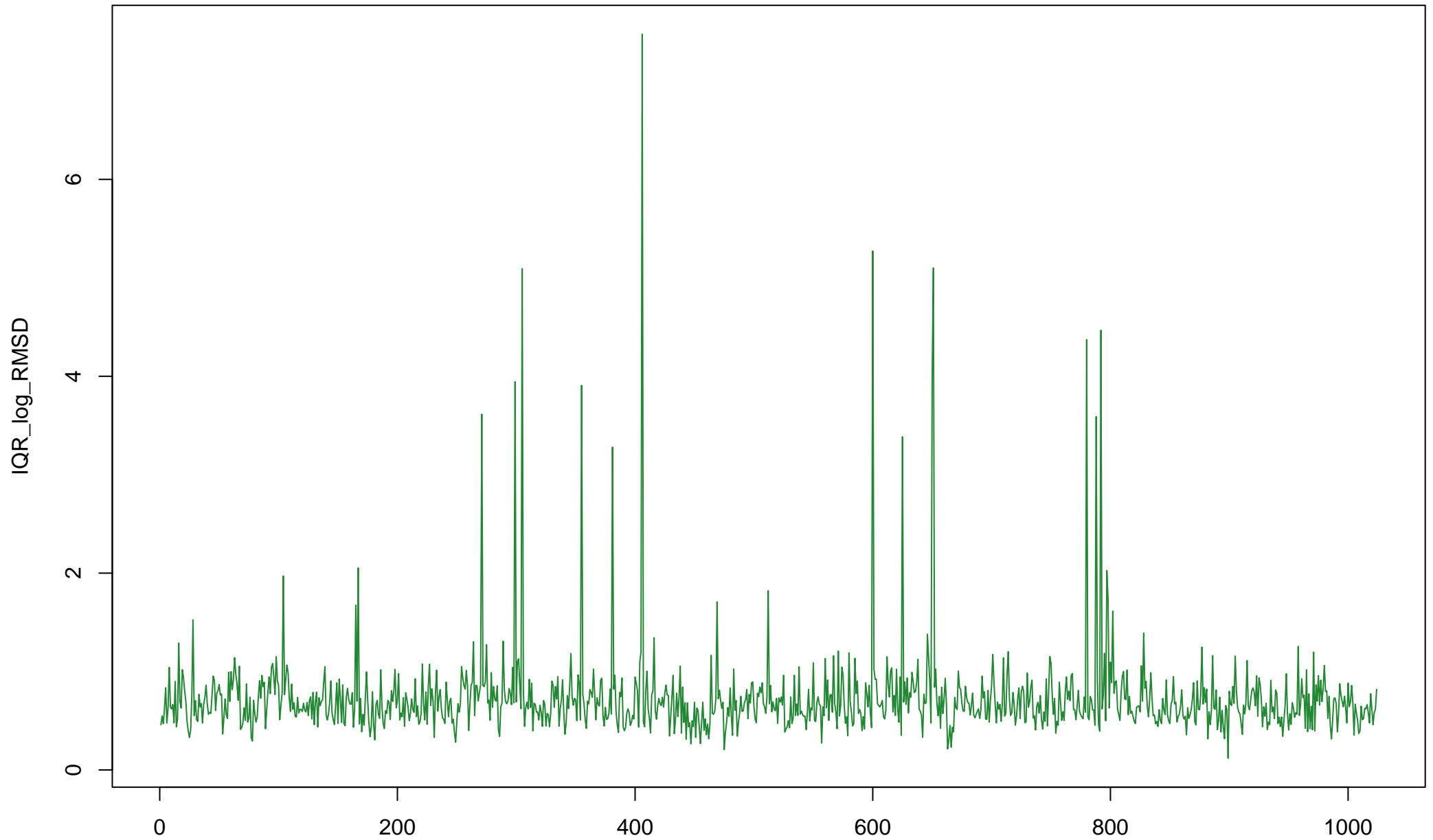
MEDIAN_mcs_template_NumHAcceptors
ESS = 1020 | BMK = 0.0664 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0



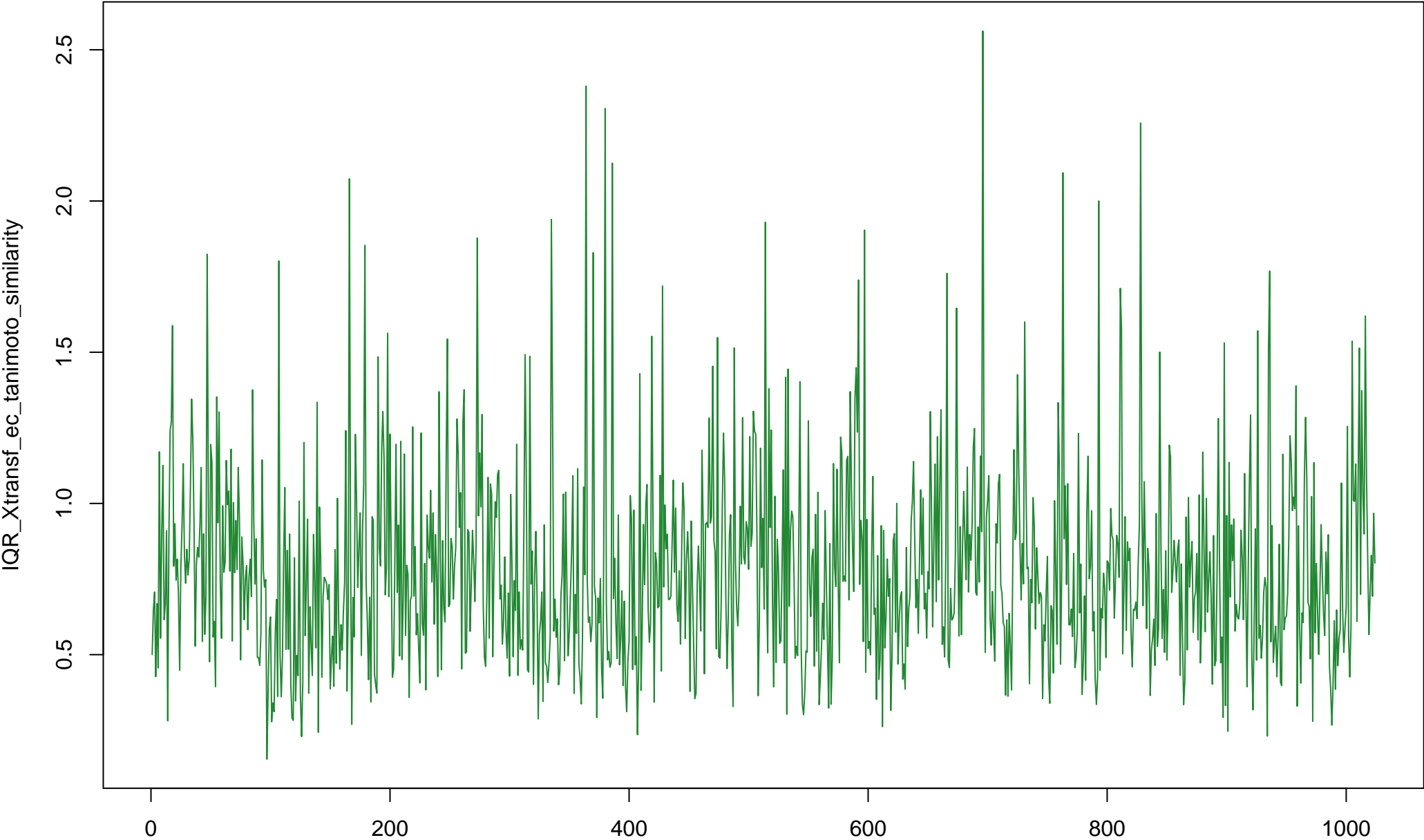
MEDIAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0432 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0



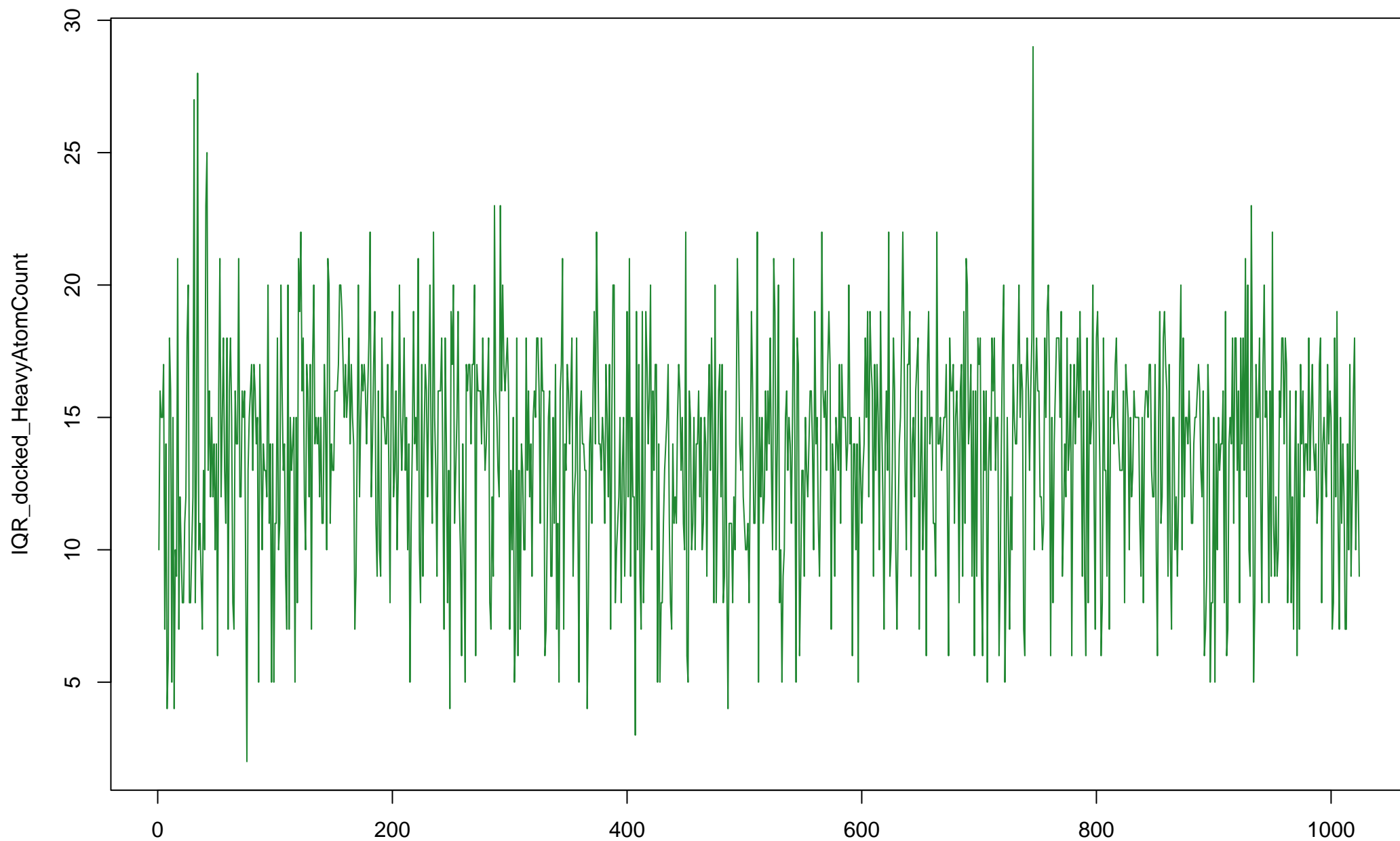
IQR_log_RMSD
ESS = 384 | BMK = 0.1 | MCSE(6.27) = 4.1 | stat: TRUE | burn: 0



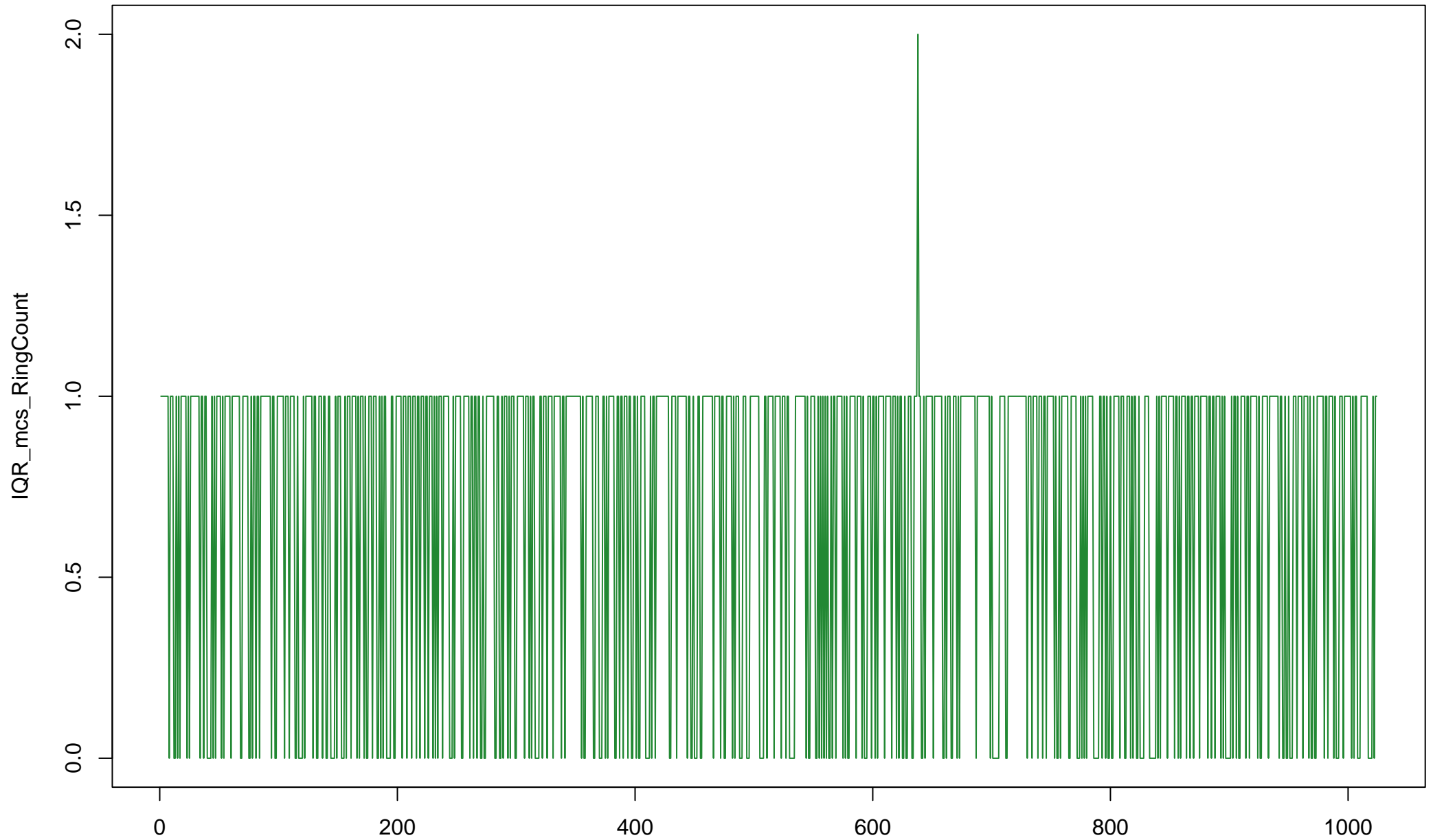
IQR_Xtransf_ec_tanimoto_similarity
ESS = 872 | BMK = 0.0498 | MCSE(6.27) = 4.71 | stat: TRUE | burn: 0



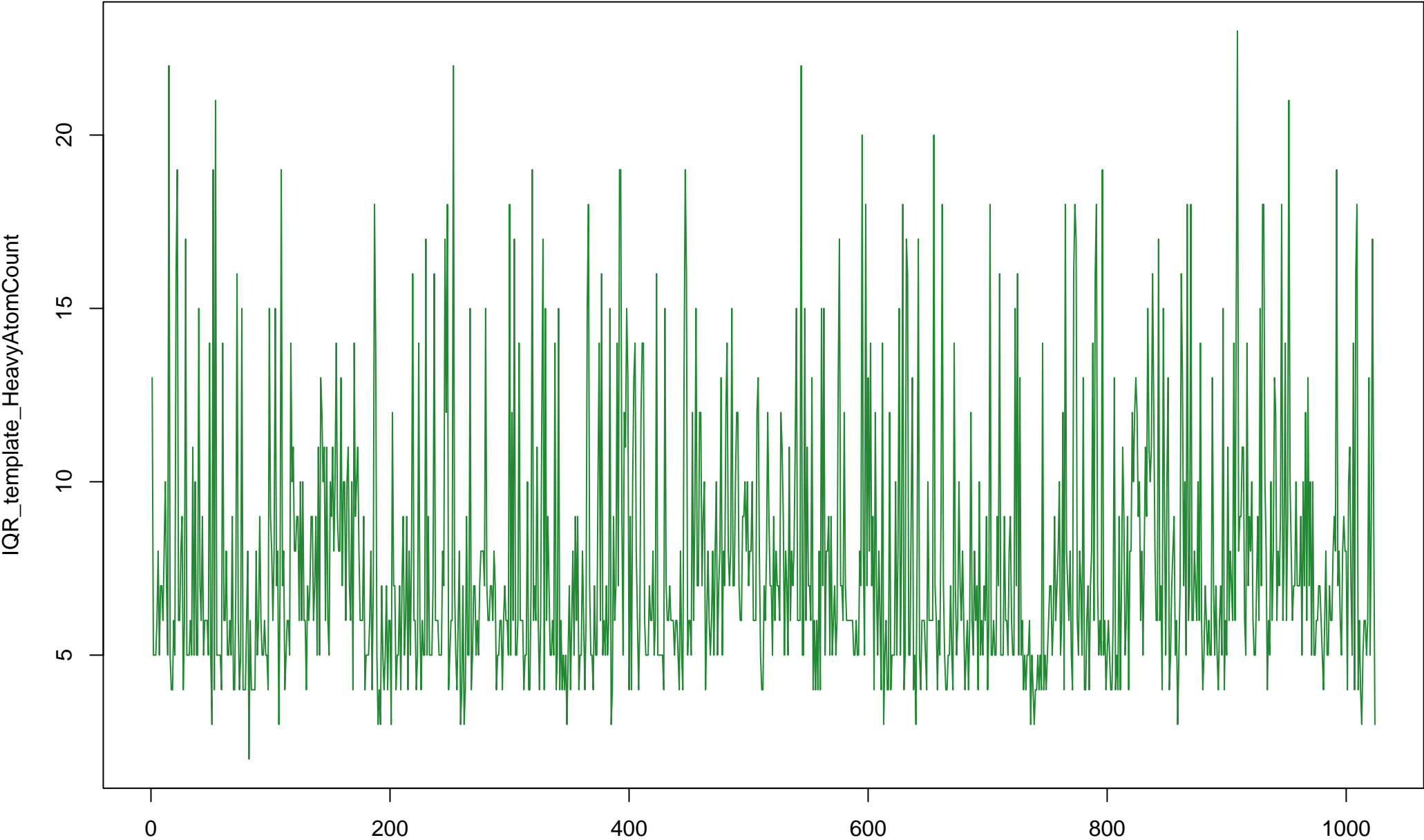
IQR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0789 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0



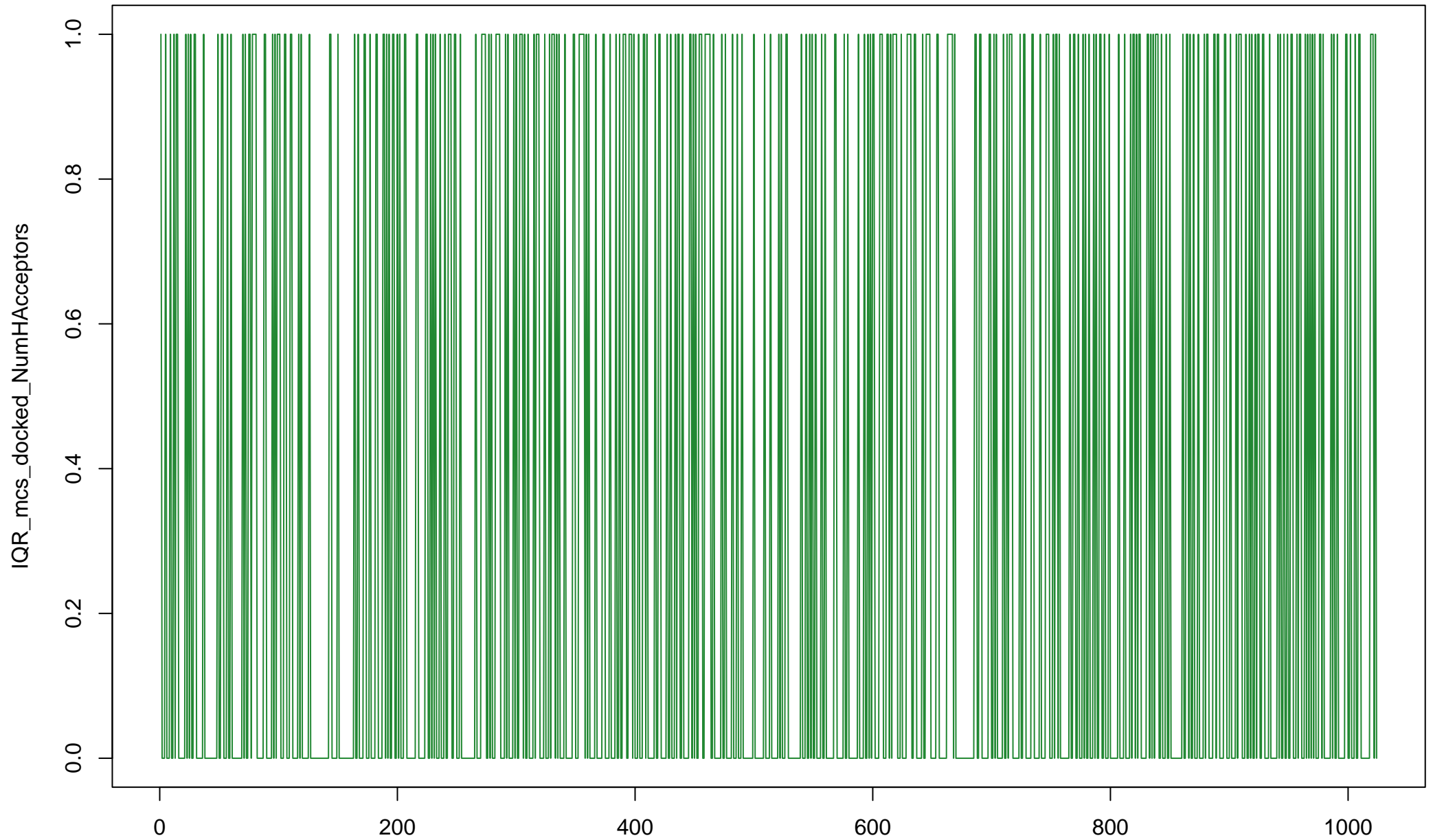
IQR_mcs_RingCount
ESS = 1020 | BMK = 0.0232 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0



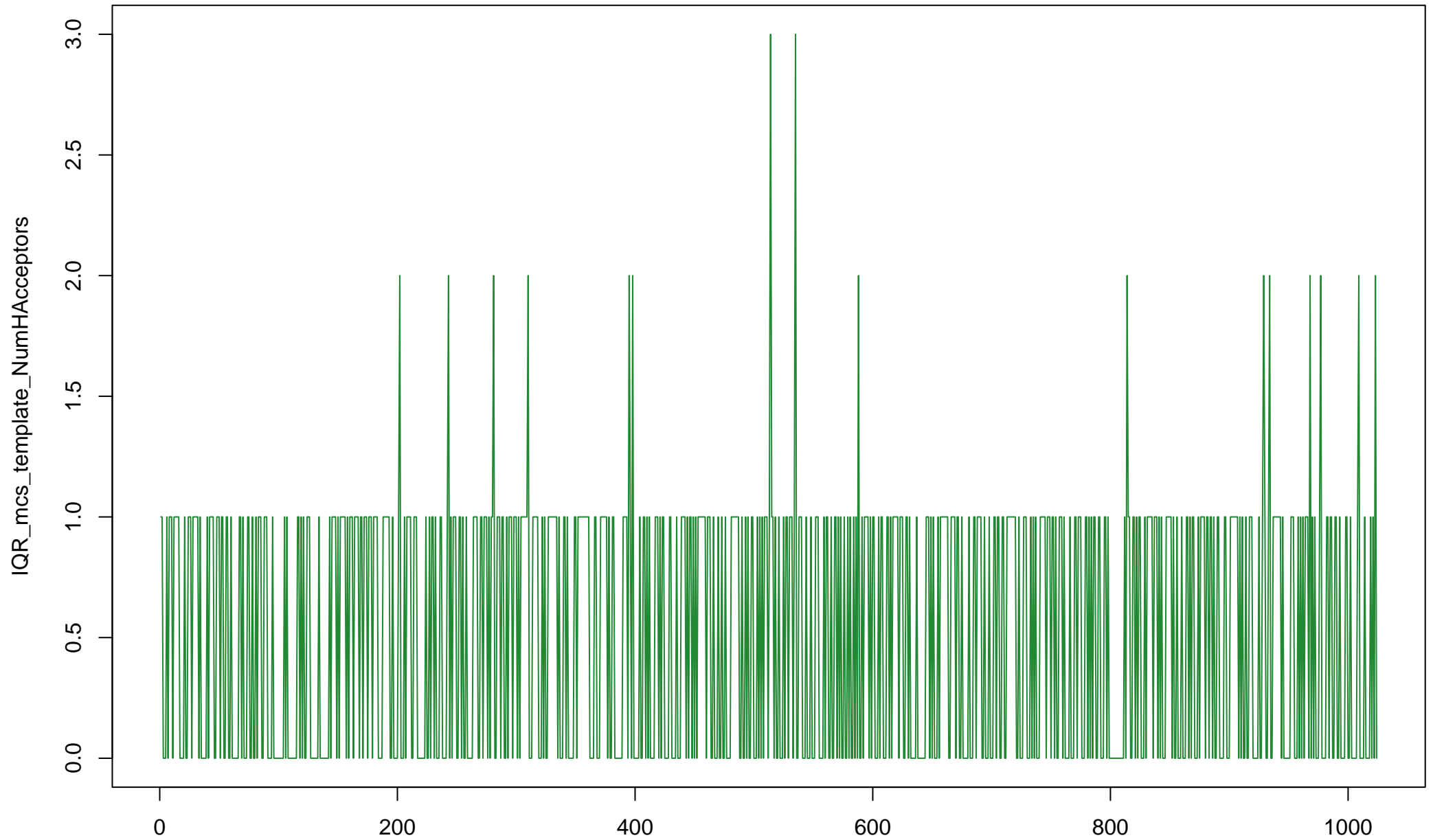
IQR_template_HeavyAtomCount
ESS = 902 | BMK = 0.0411 | MCSE(6.27) = 3.79 | stat: TRUE | burn: 0



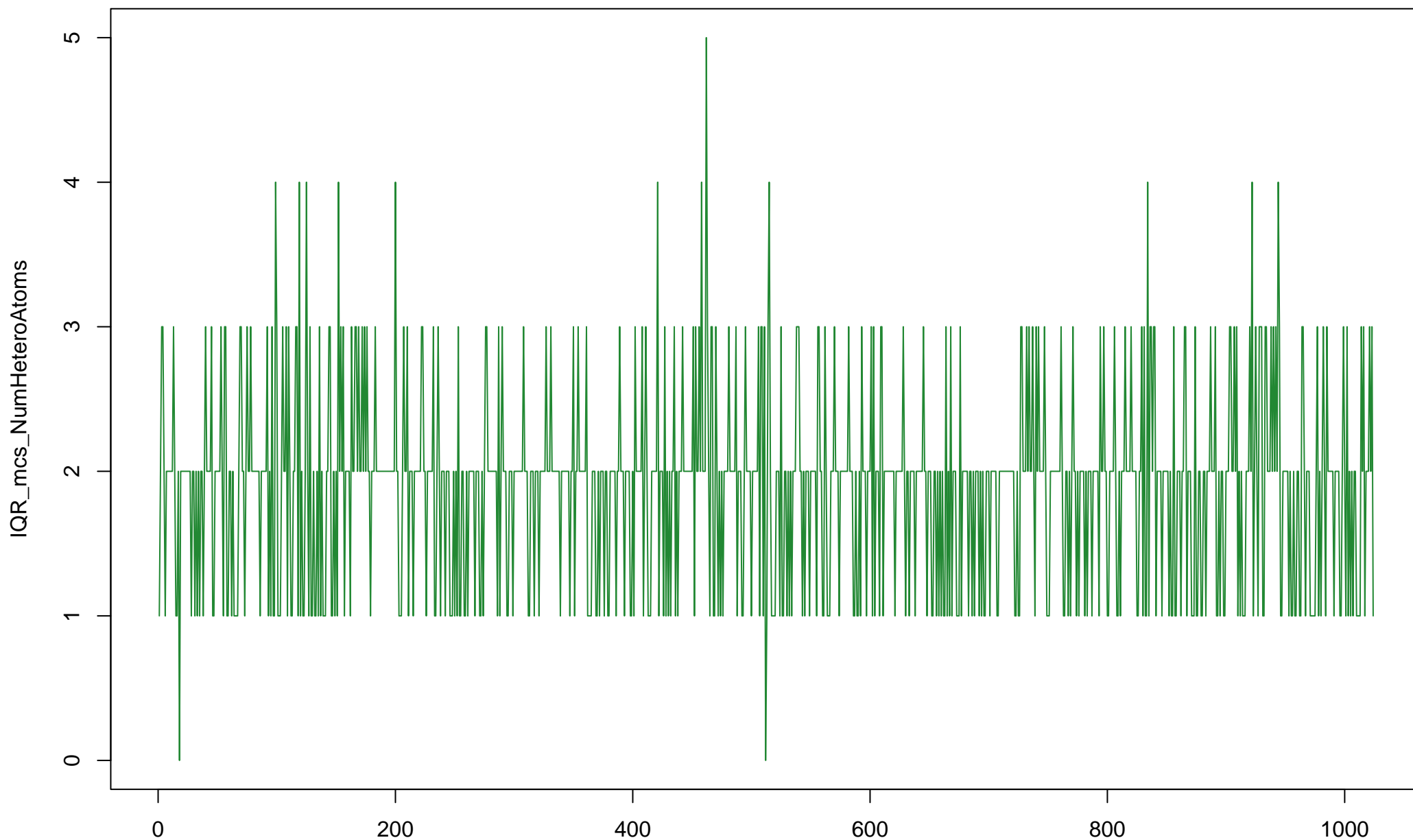
IQR_mcs_docked_NumHAcceptors
ESS = 1020 | BMK = 0.00834 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0



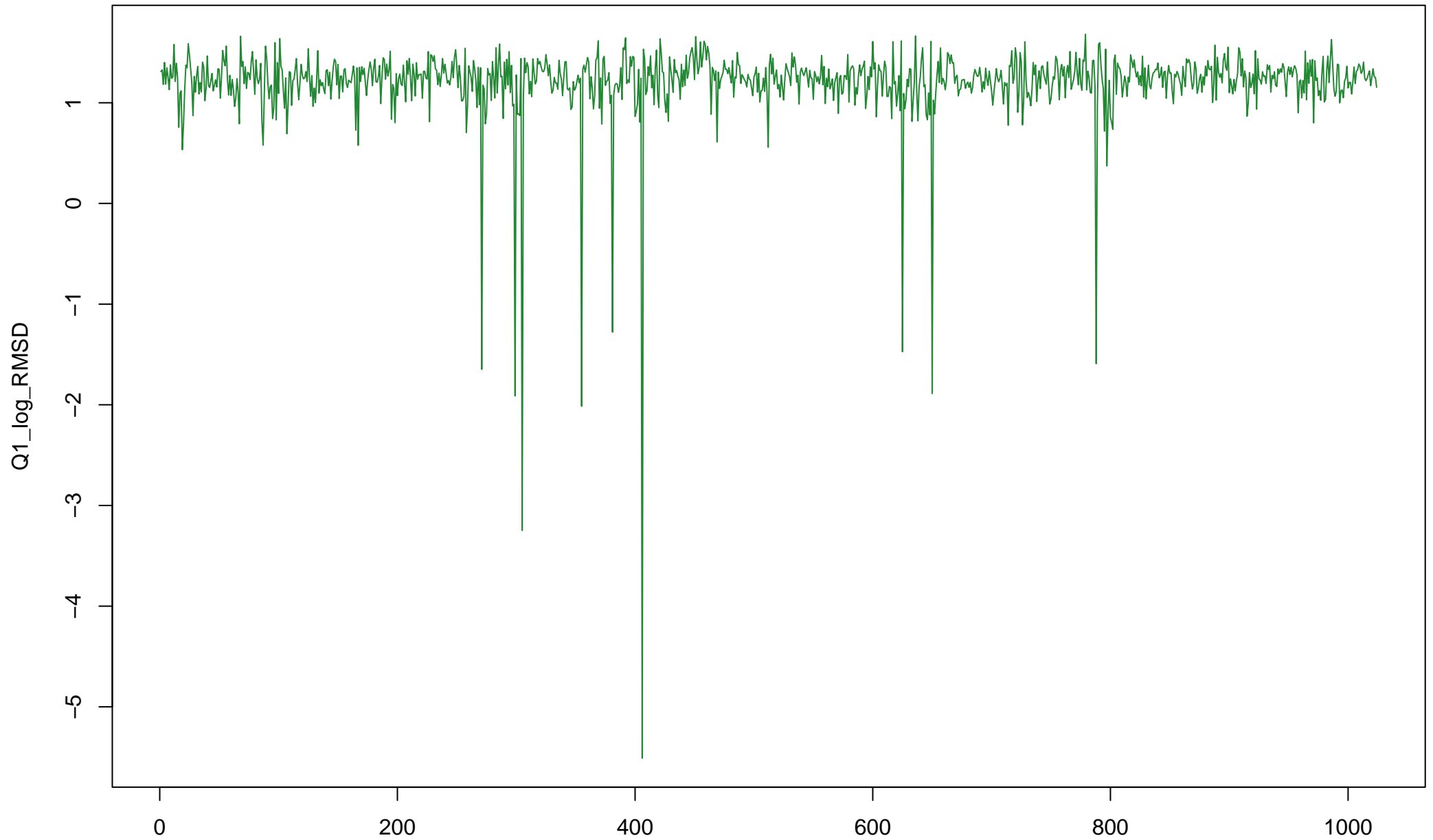
IQR_mcs_template_NumHAcceptors
ESS = 799 | BMK = 0.0448 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0



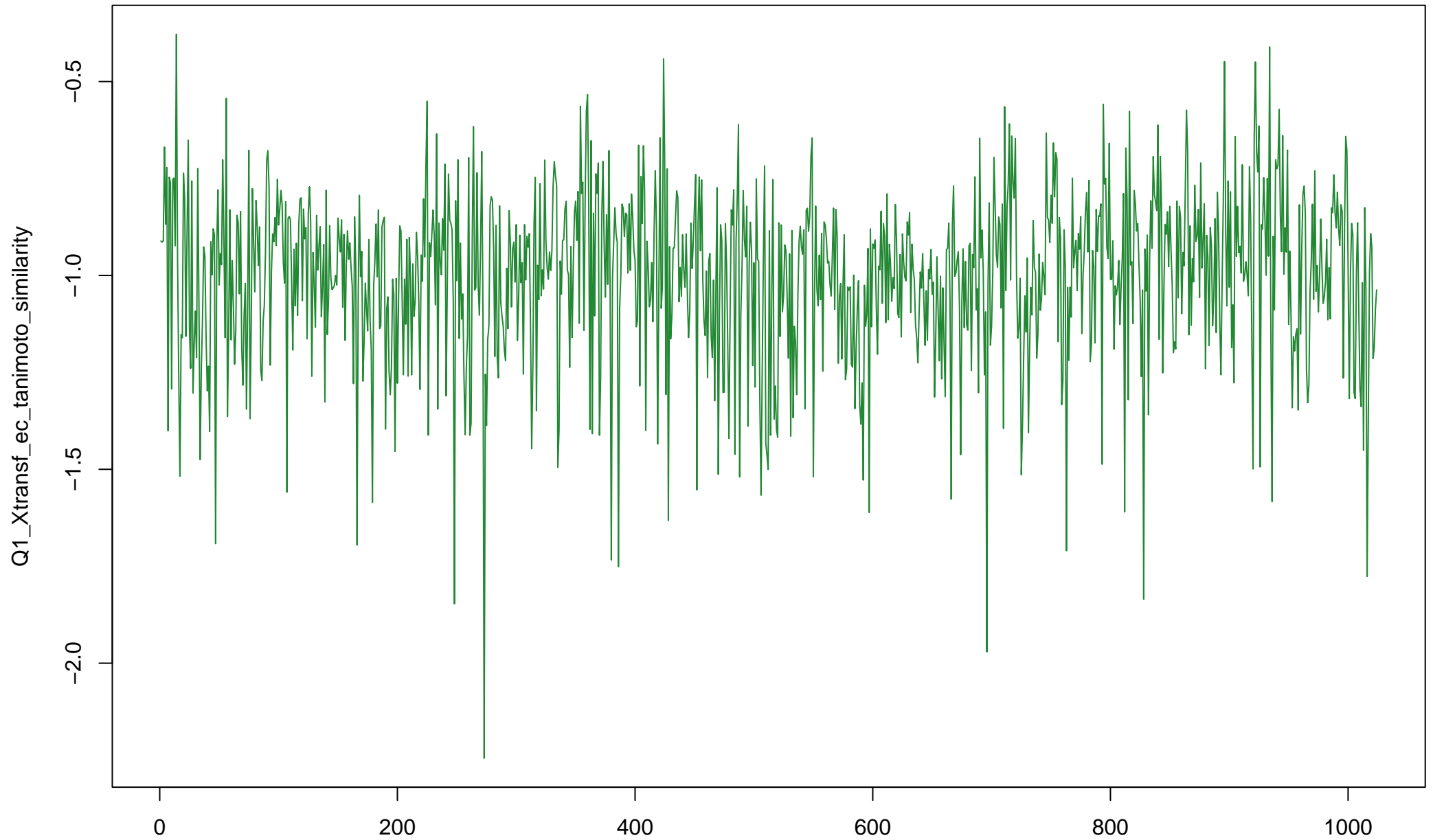
IQR_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0563 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0



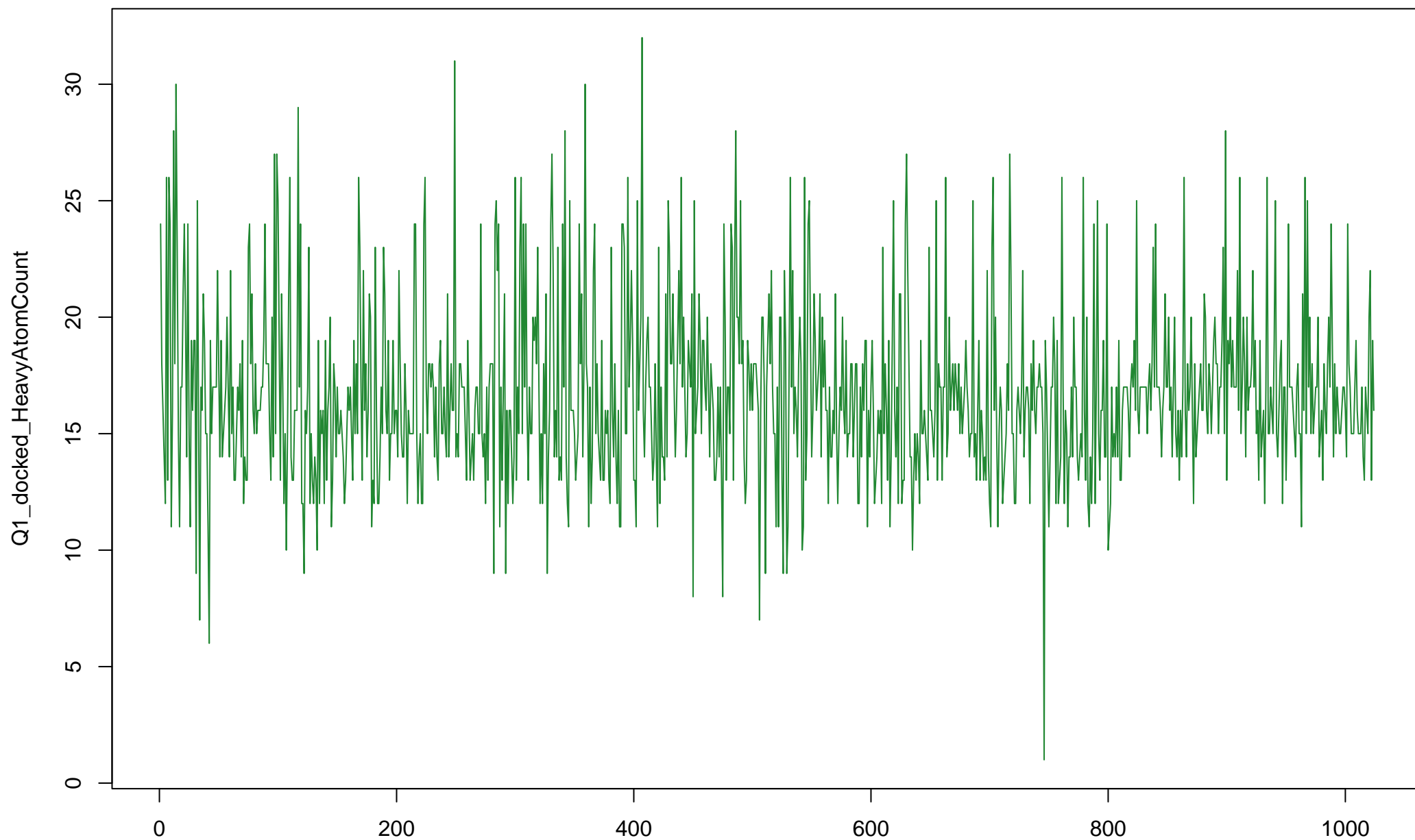
Q1_log_RMSD
ESS = 553 | BMK = 0.114 | MCSE(6.27) = 3.52 | stat: TRUE | burn: 0



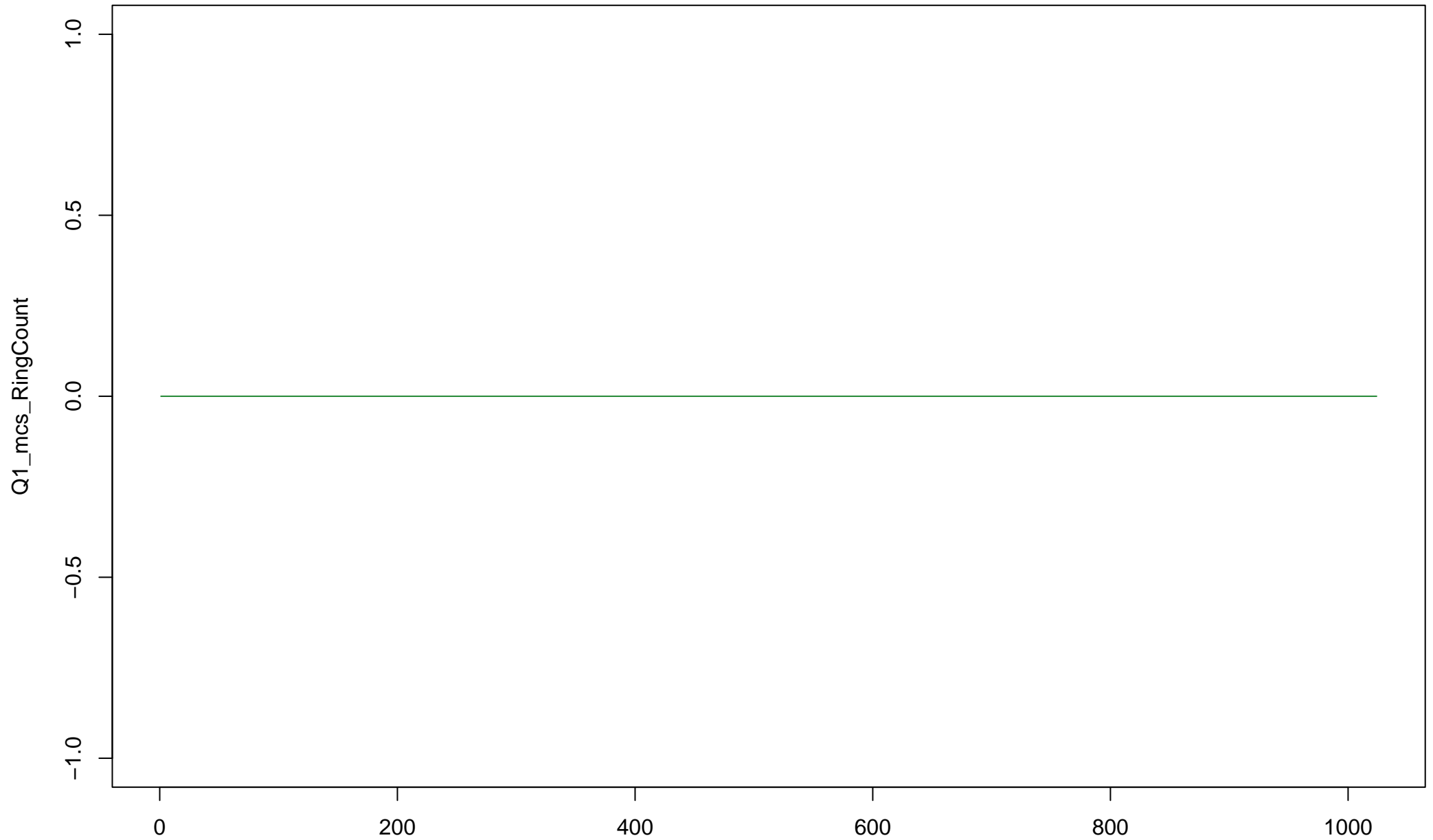
Q1_Xtransf_ec_tanimoto_similarity
ESS = 476 | BMK = 0.0615 | MCSE(6.27) = 4.54 | stat: TRUE | burn: 0



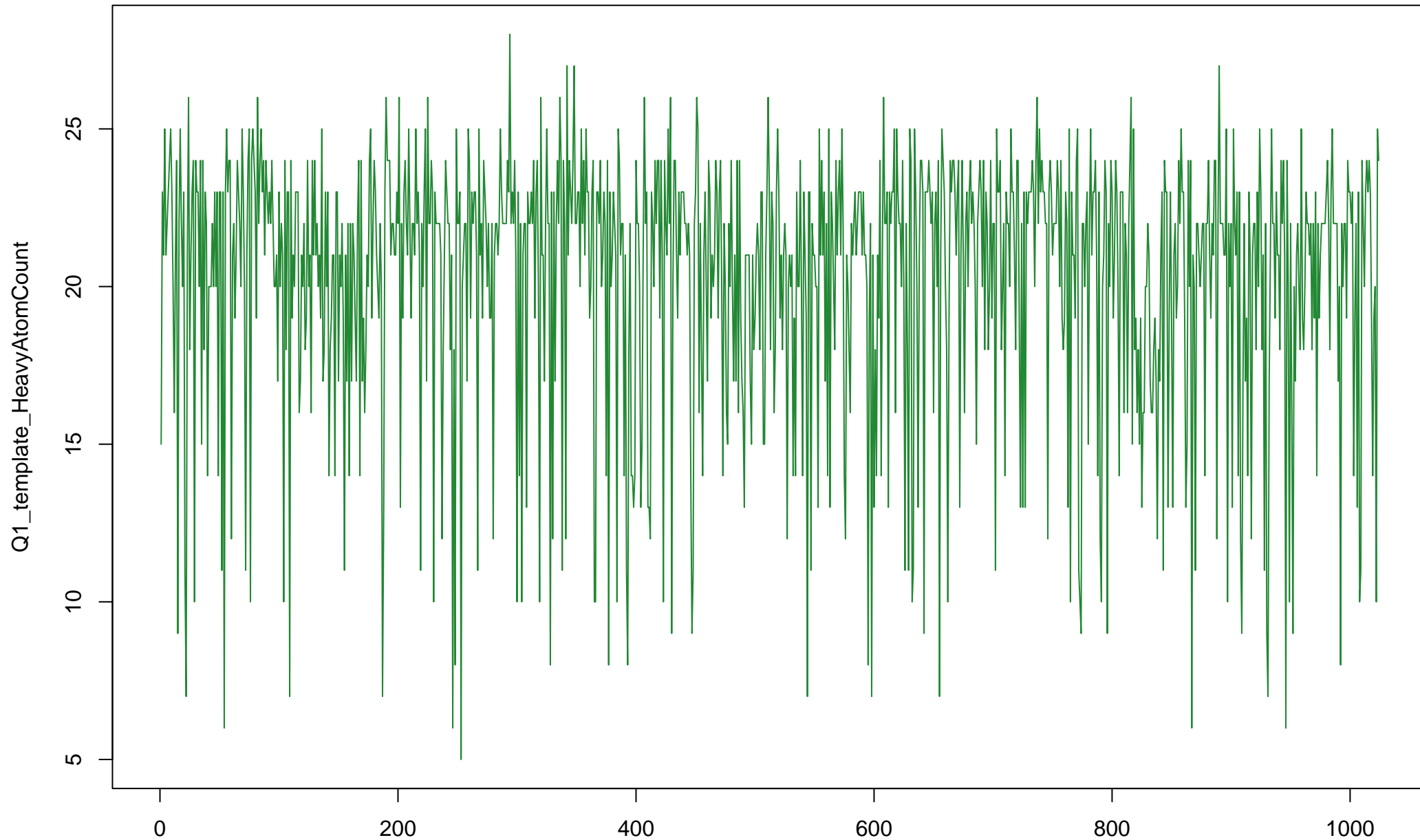
Q1_docked_HeavyAtomCount
ESS = 904 | BMK = 0.139 | MCSE(6.27) = 3.52 | stat: TRUE | burn: 0



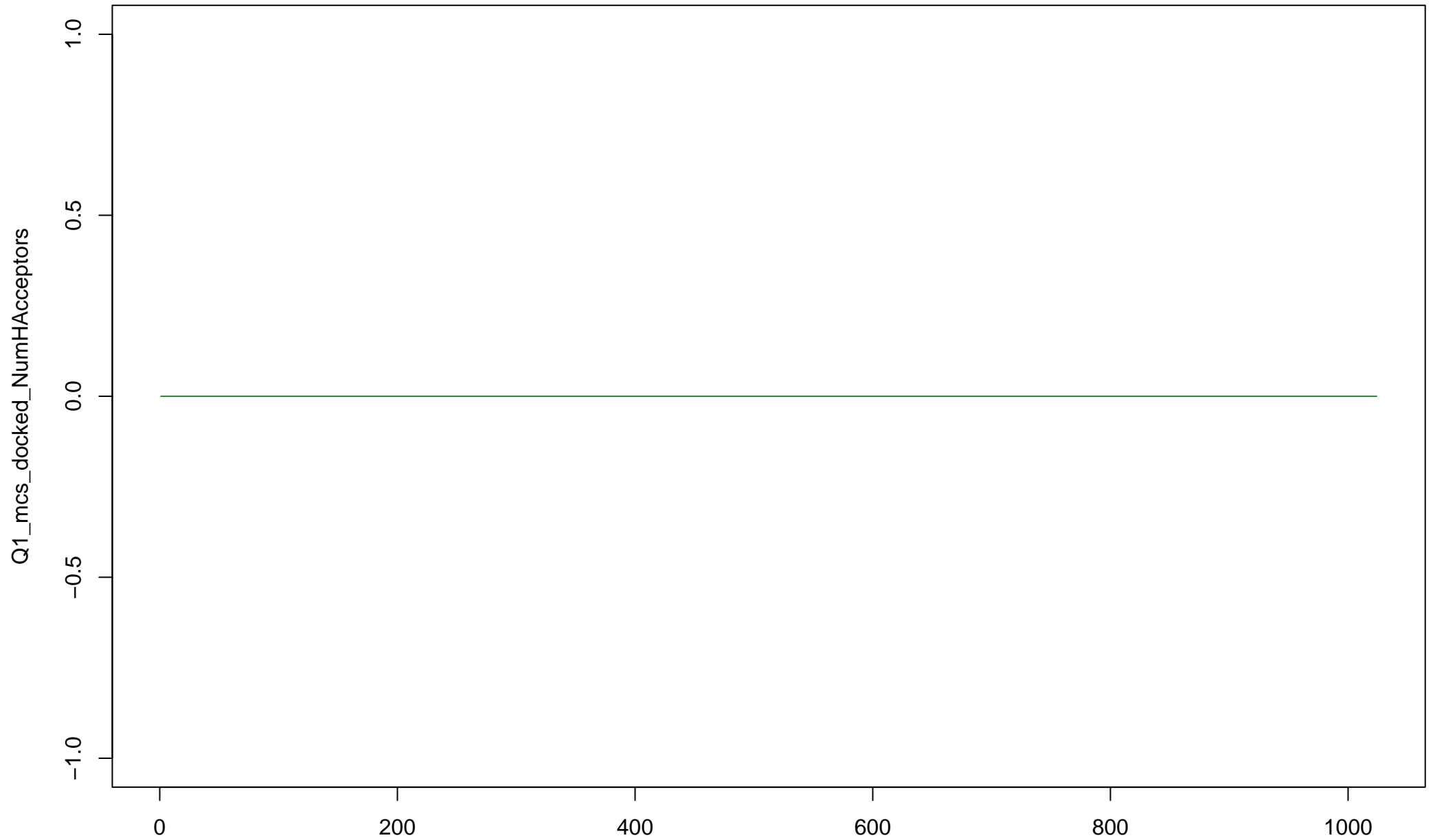
Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



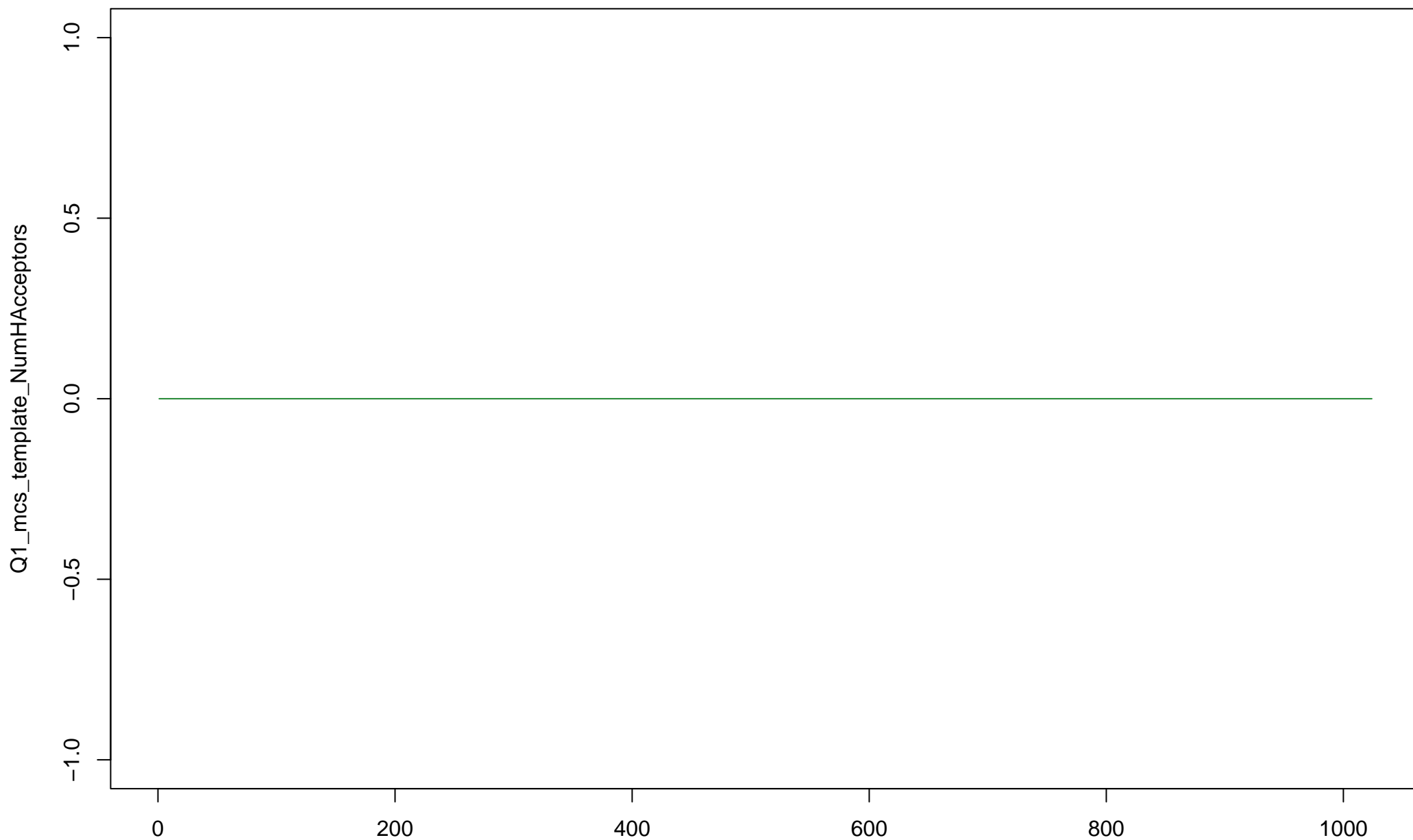
Q1_template_HeavyAtomCount
ESS = 1020 | BMK = 0.0528 | MCSE(6.27) = 3.44 | stat: TRUE | burn: 0



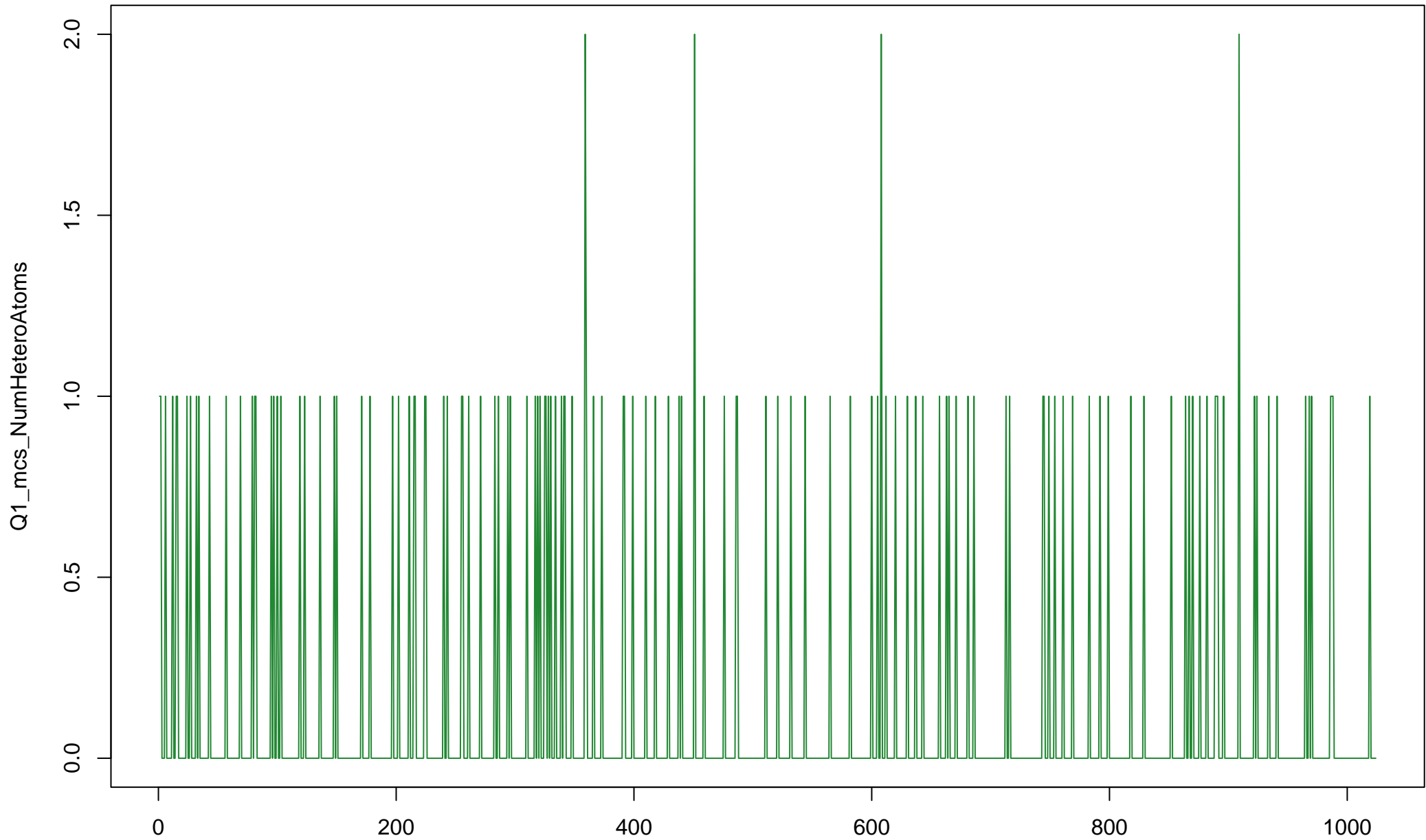
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



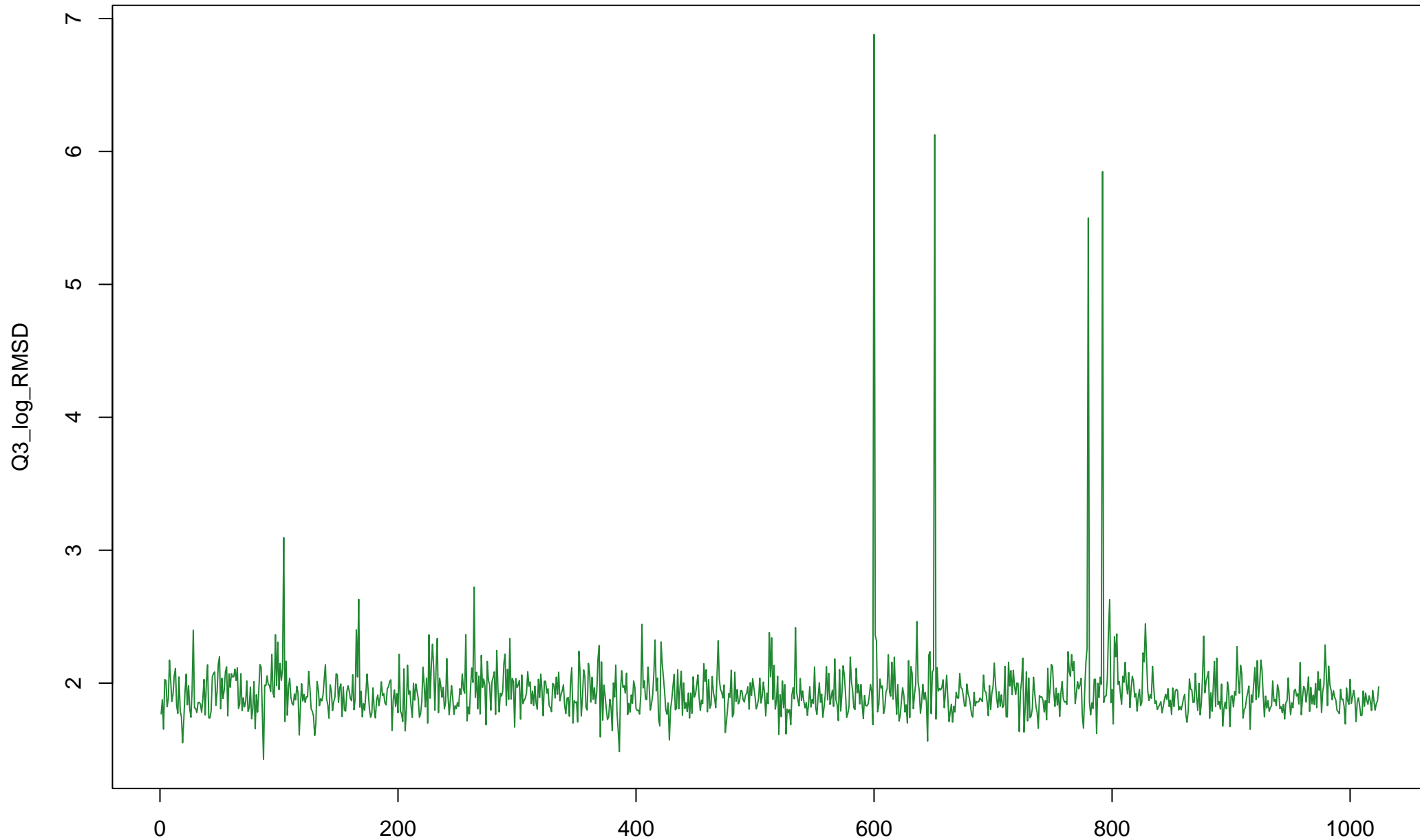
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



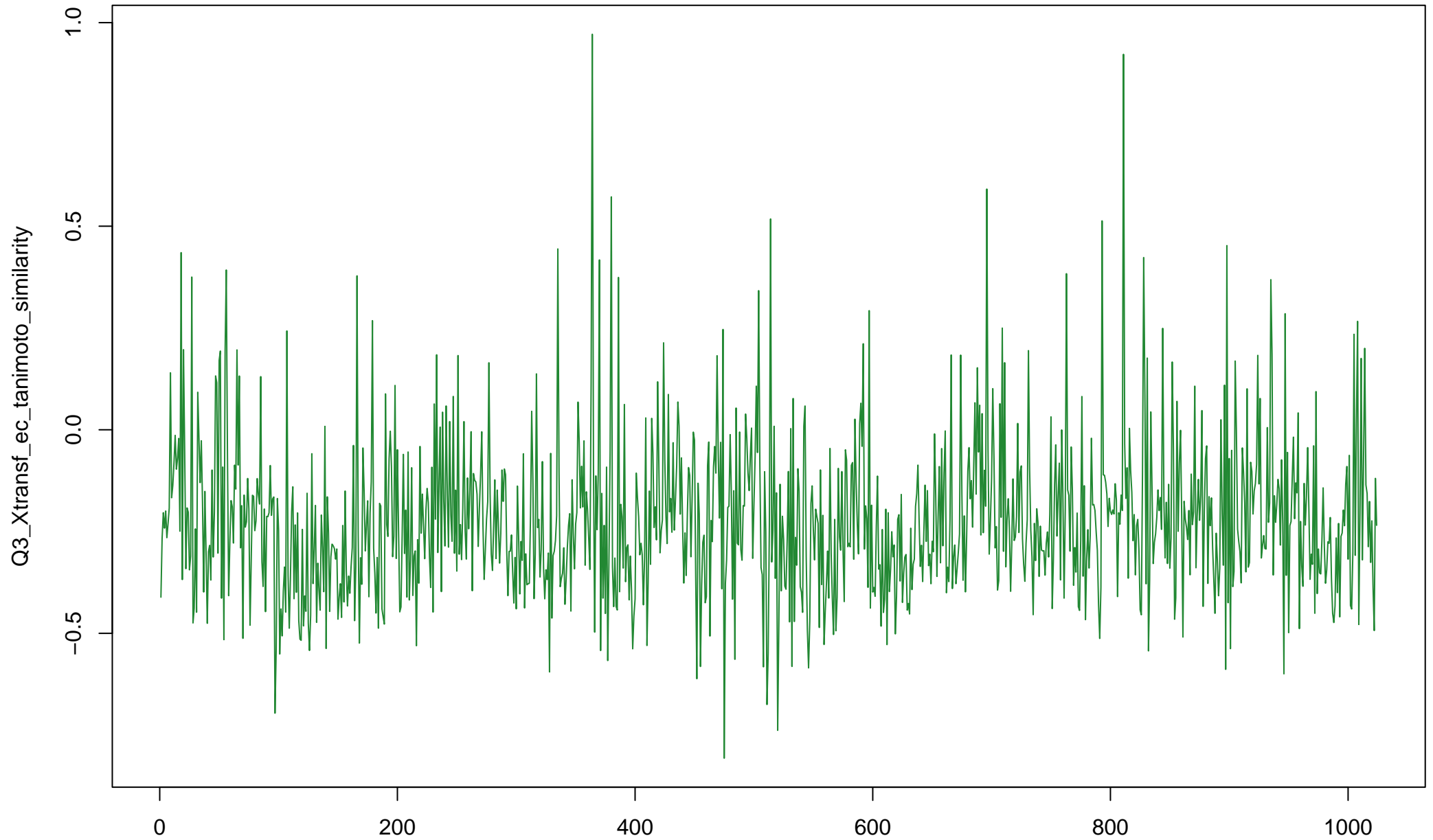
Q1_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0642 | MCSE(6.27) = 3.35 | stat: TRUE | burn: 0



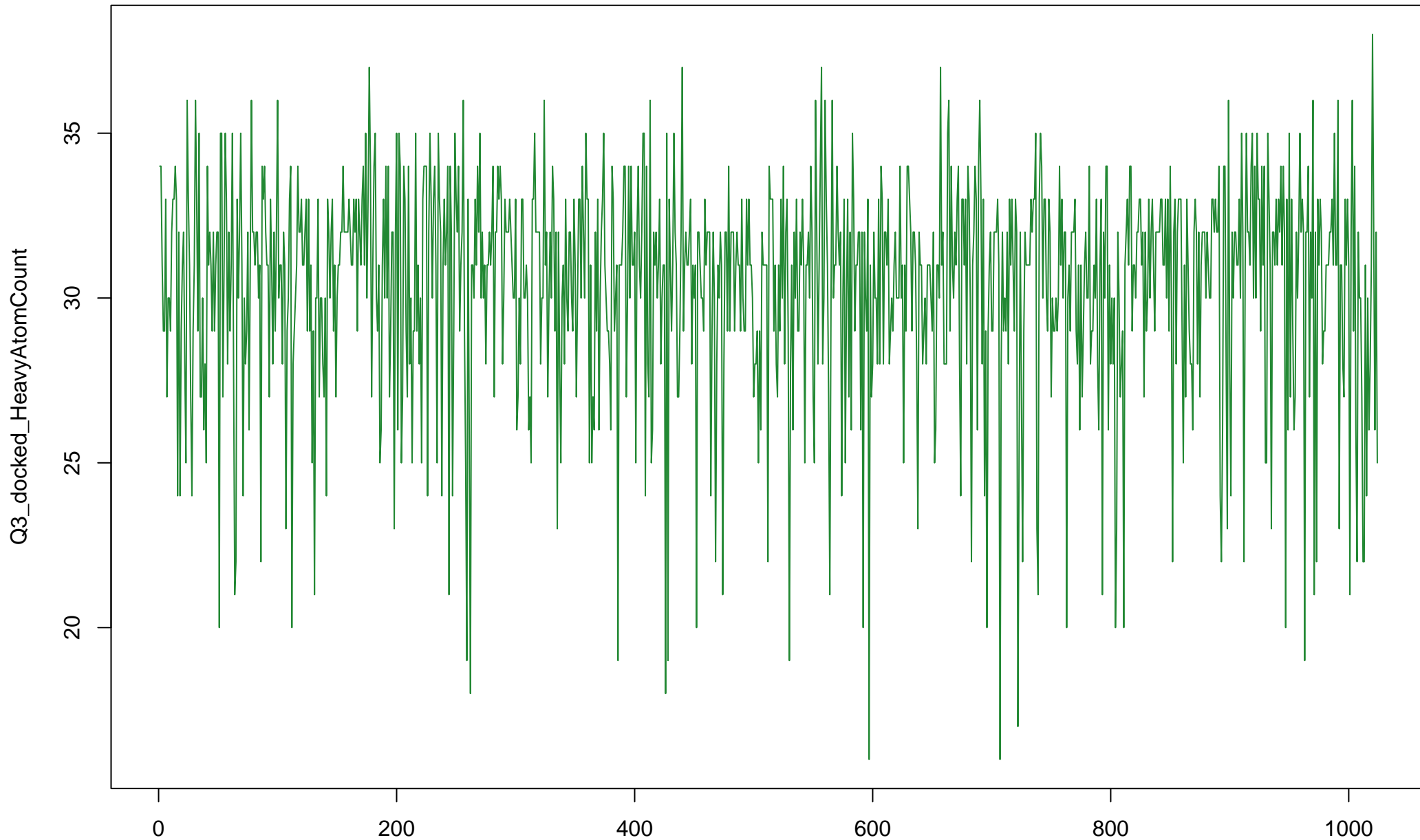
Q3_log_RMSD
ESS = 564 | BMK = 0.11 | MCSE(6.27) = 3.88 | stat: TRUE | burn: 0



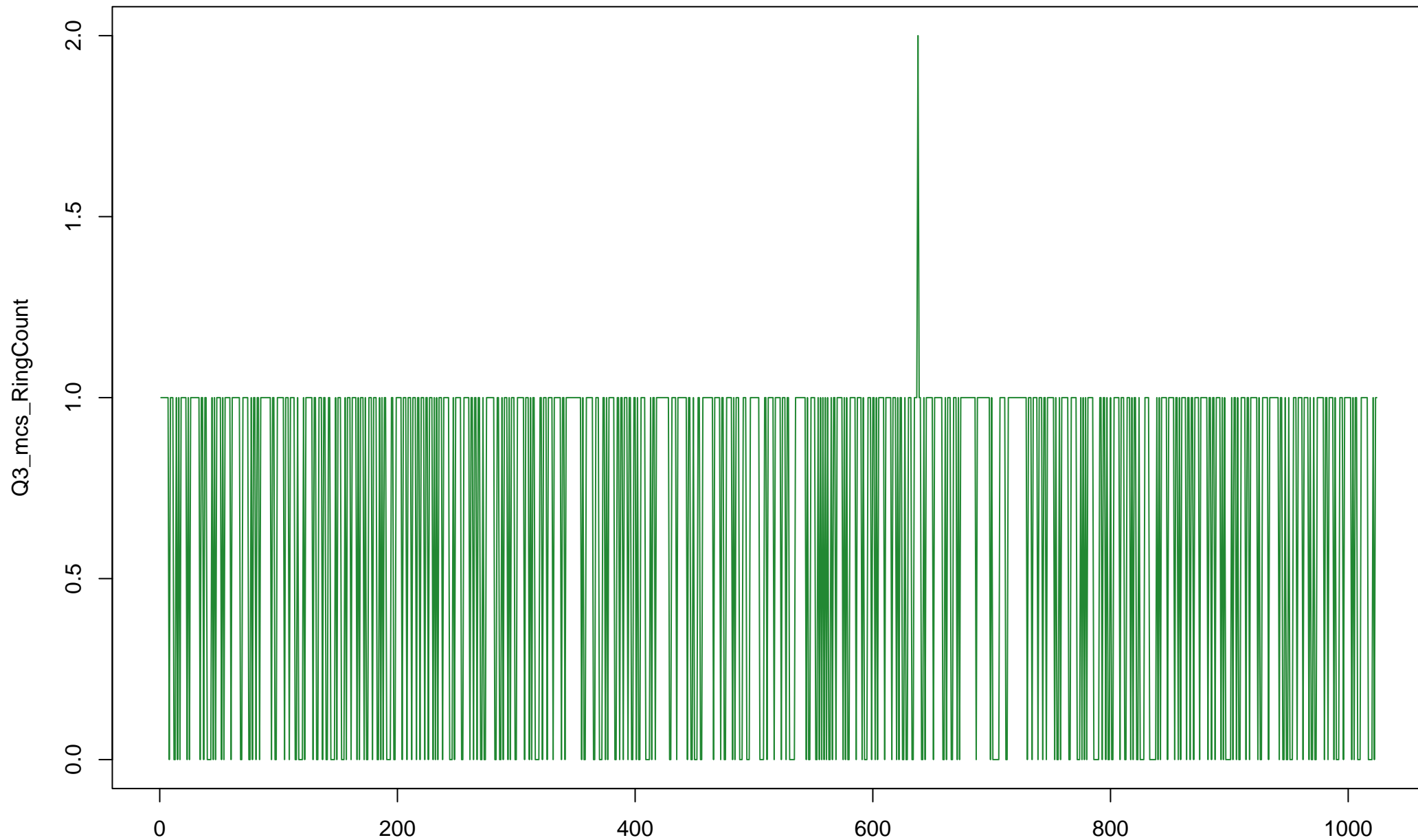
Q3_Xtransf_ec_tanimoto_similarity
ESS = 363 | BMK = 0.0572 | MCSE(6.27) = 5.43 | stat: TRUE | burn: 0



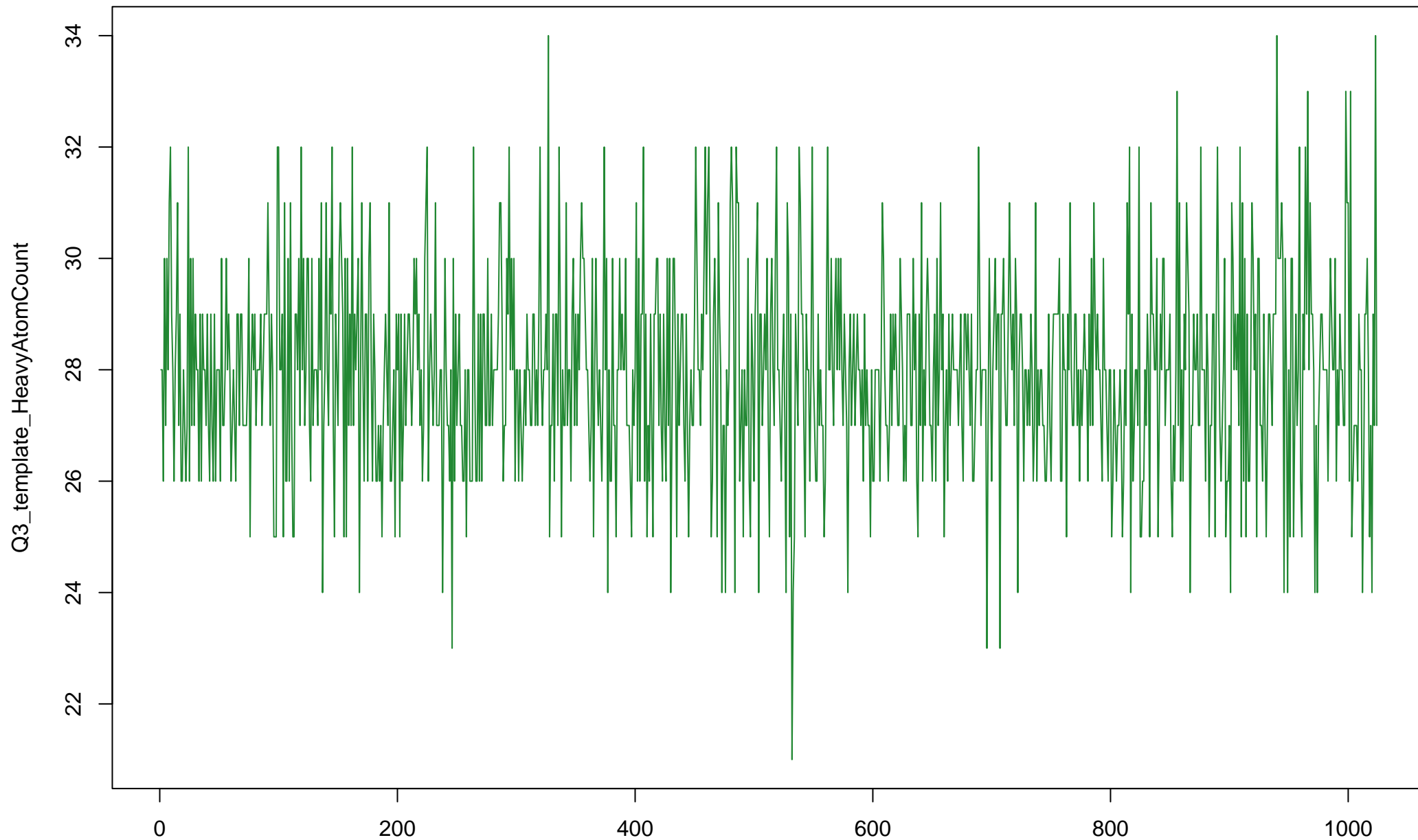
Q3_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0649 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0



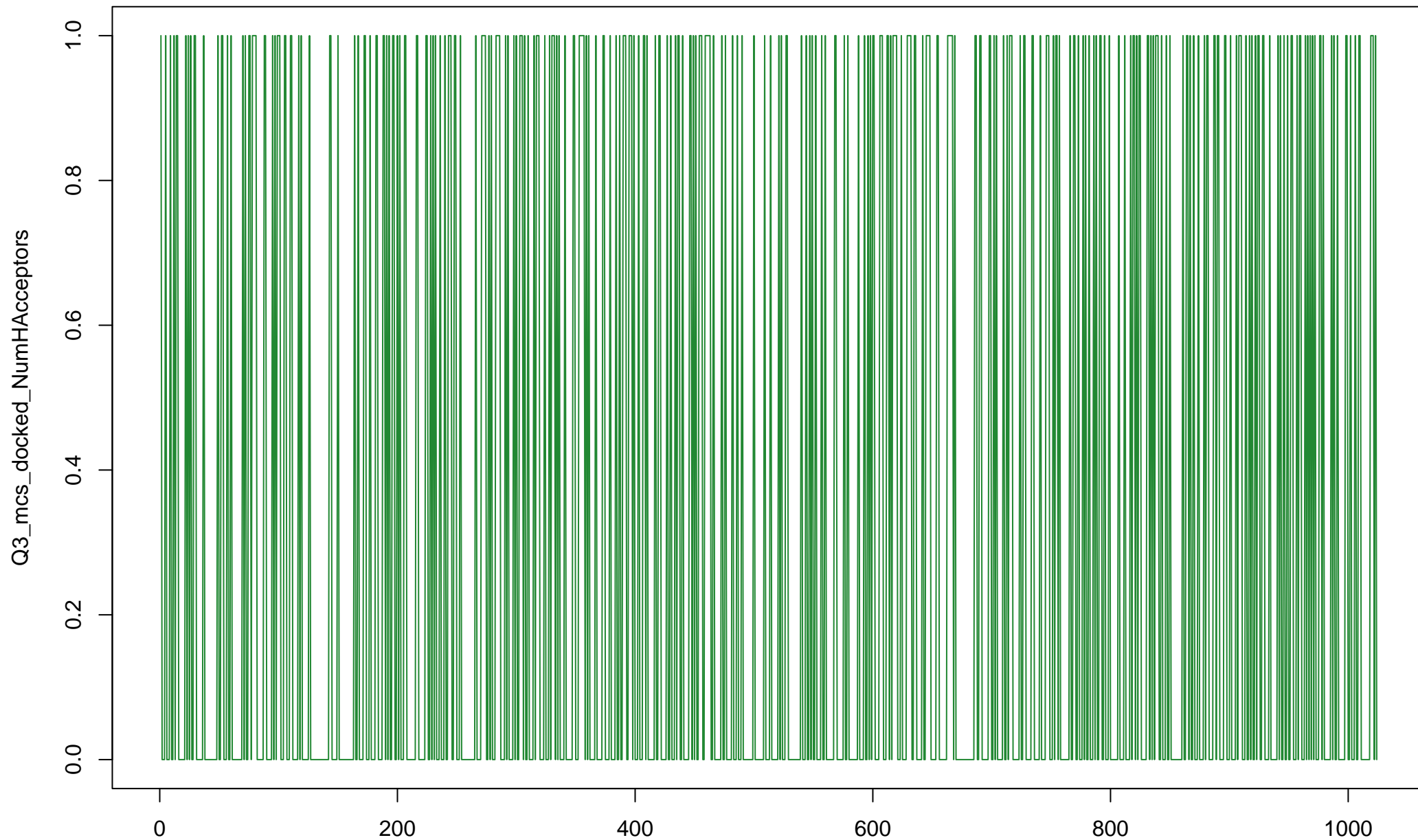
Q3_mcs_RingCount
ESS = 1020 | BMK = 0.0232 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0



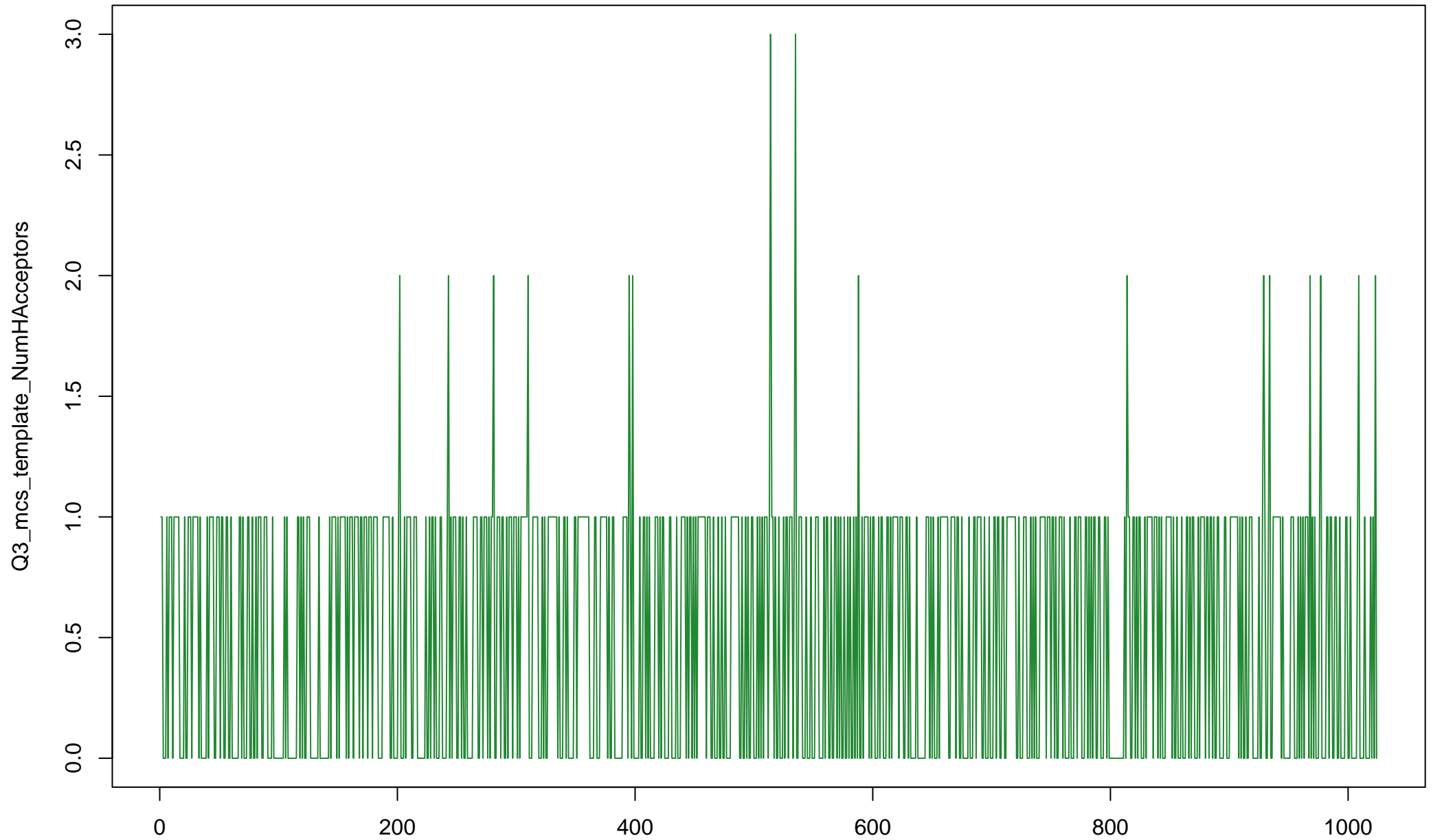
Q3_template_HeavyAtomCount
ESS = 1020 | BMK = 0.0689 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0



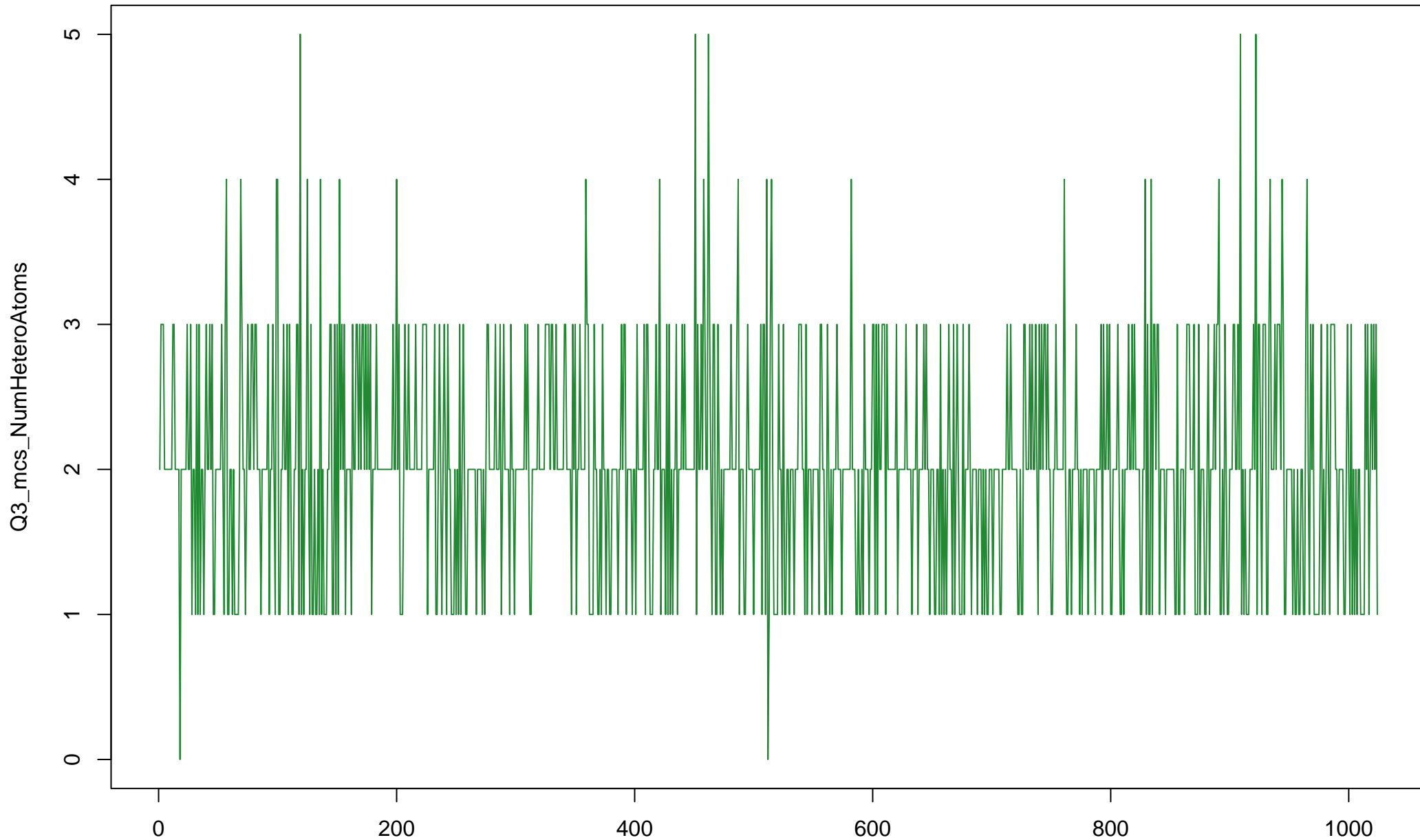
Q3_mcs_docked_NumHAcceptors
ESS = 1020 | BMK = 0.00834 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0



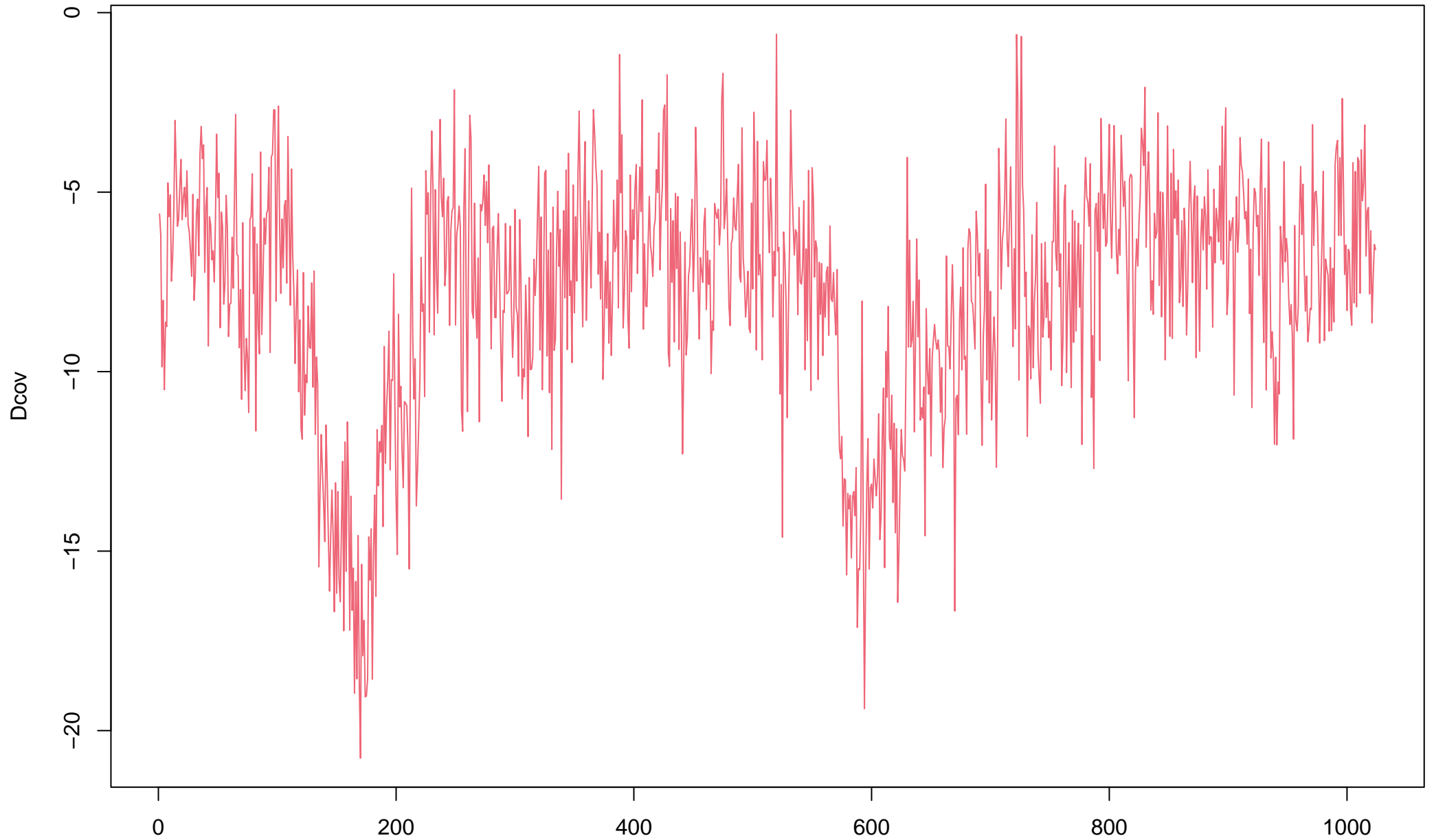
Q3_mcs_template_NumHAcceptors
ESS = 799 | BMK = 0.0448 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0



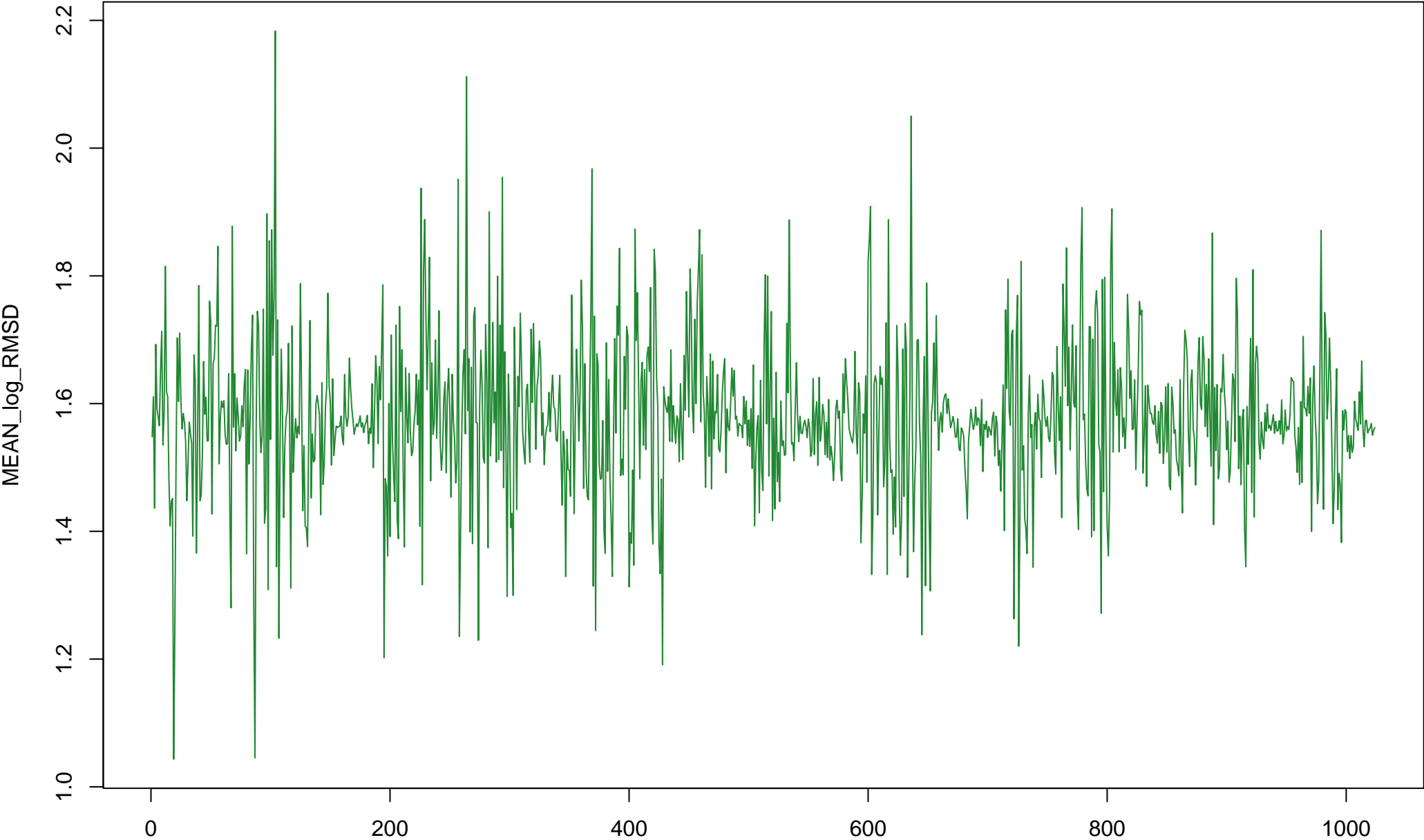
Q3_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0615 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0



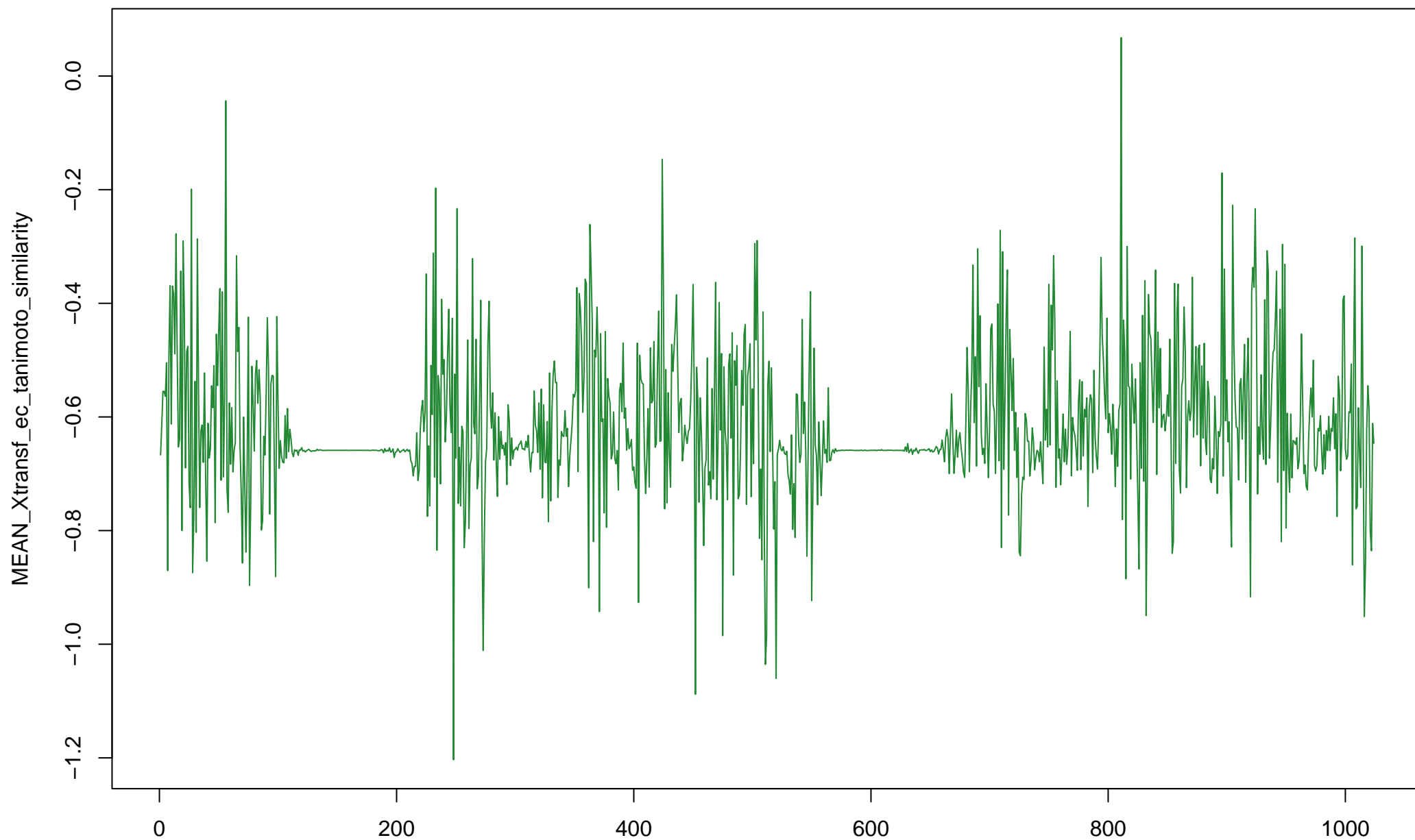
Dcov
ESS = 720 | BMK = 0.309 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 714



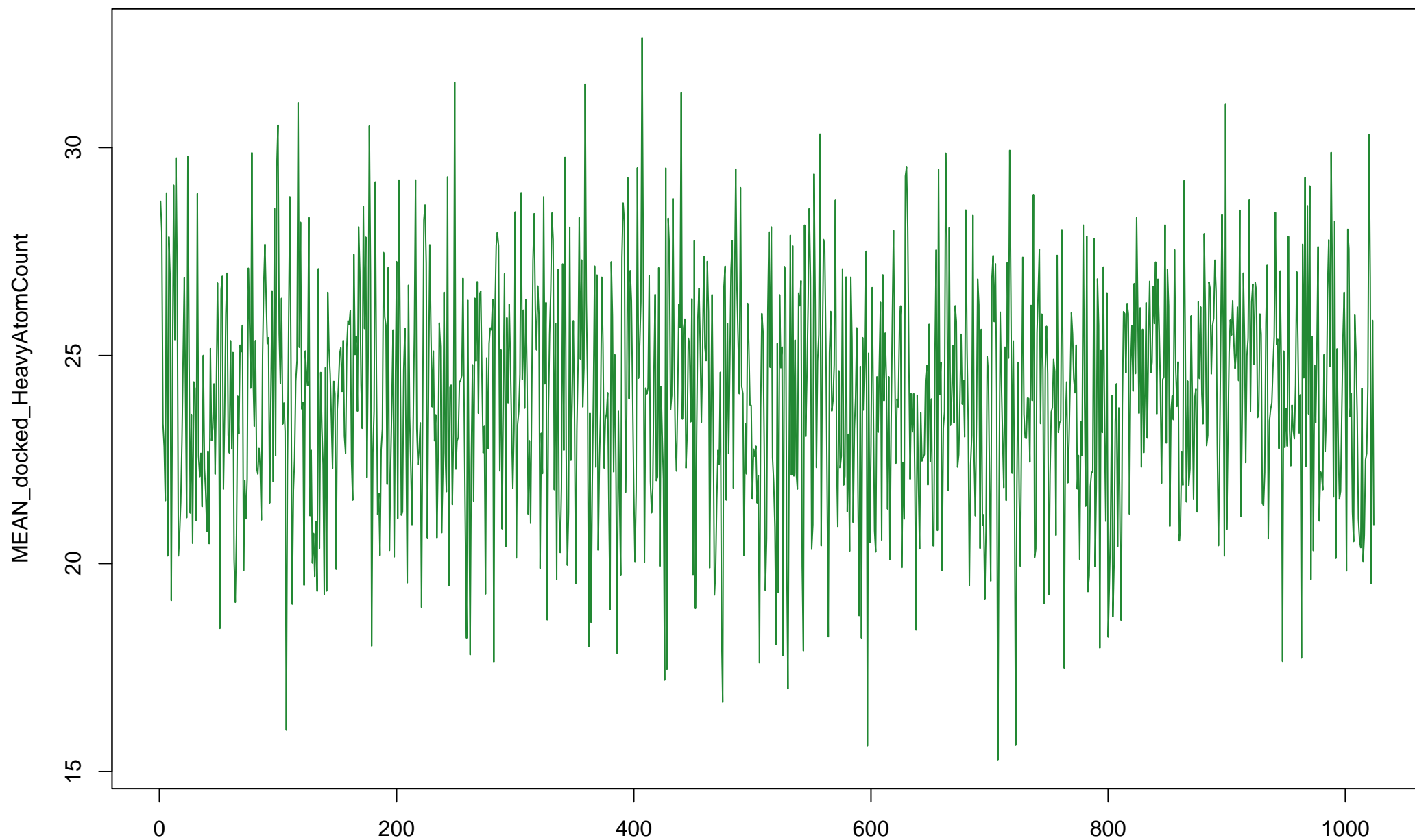
MEAN_log_RMSD
ESS = 1020 | BMK = 0.113 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0



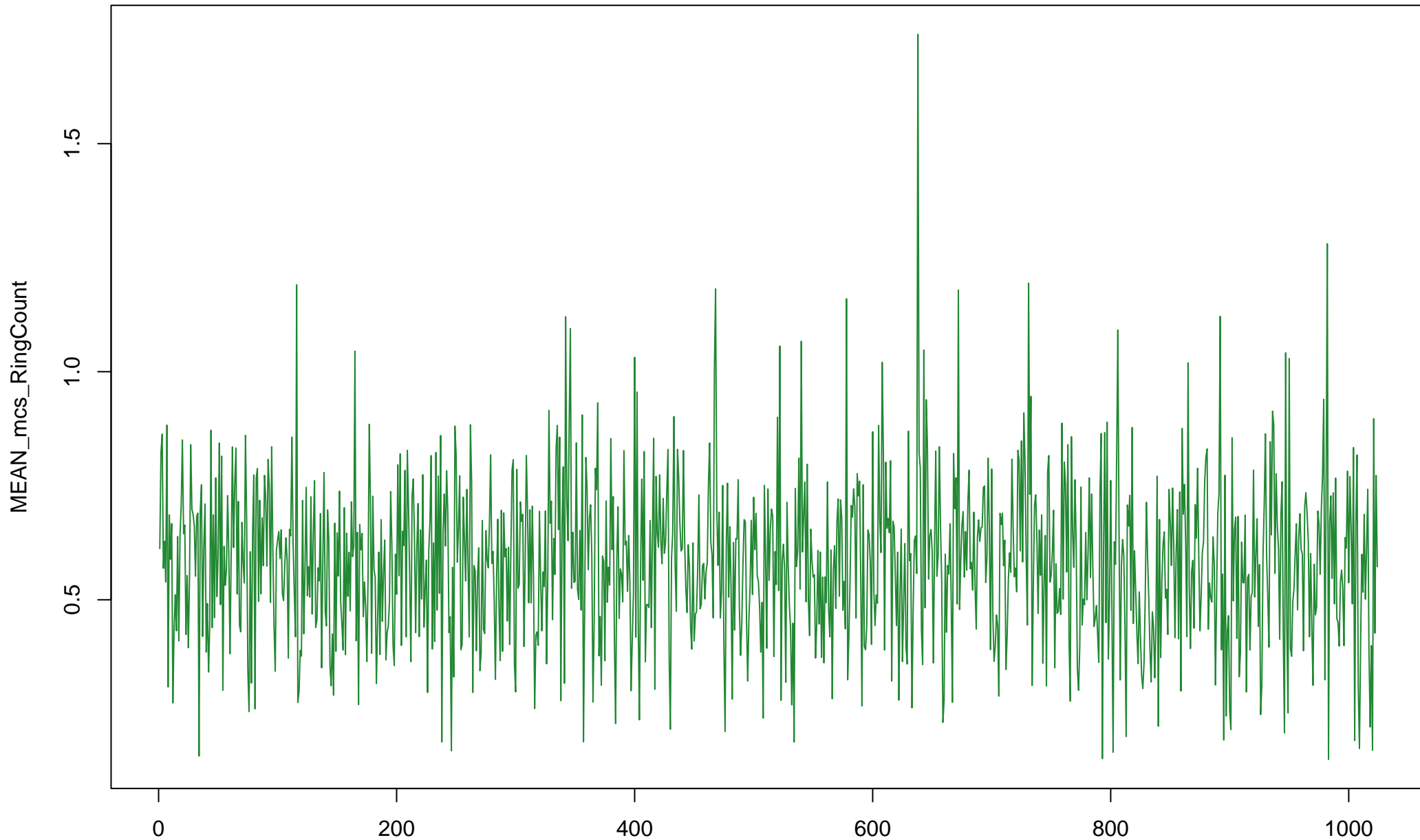
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 272 | BMK = 0.099 | MCSE(6.27) = 5.11 | stat: TRUE | burn: 510



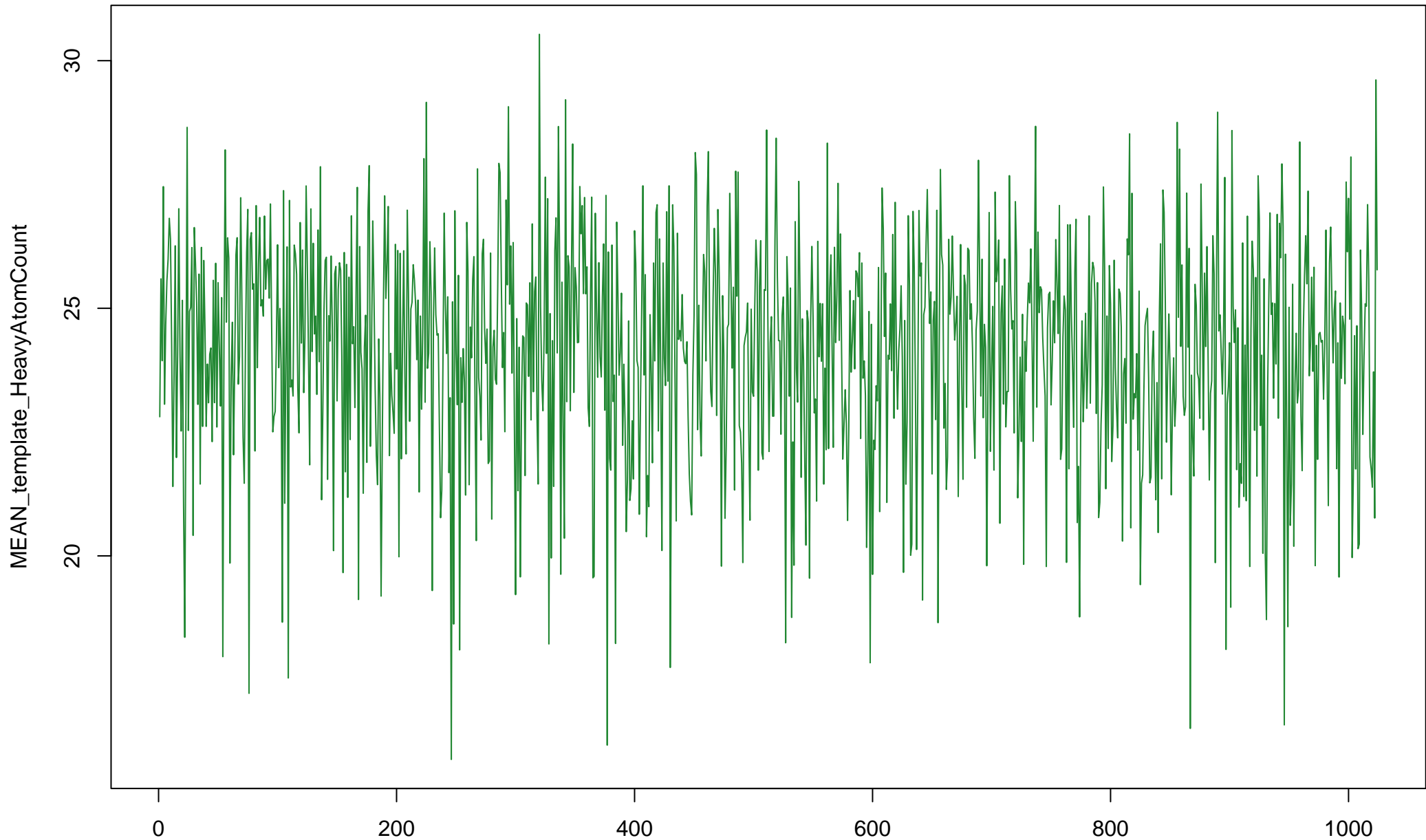
MEAN_docked_HeavyAtomCount
ESS = 913 | BMK = 0.0491 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0



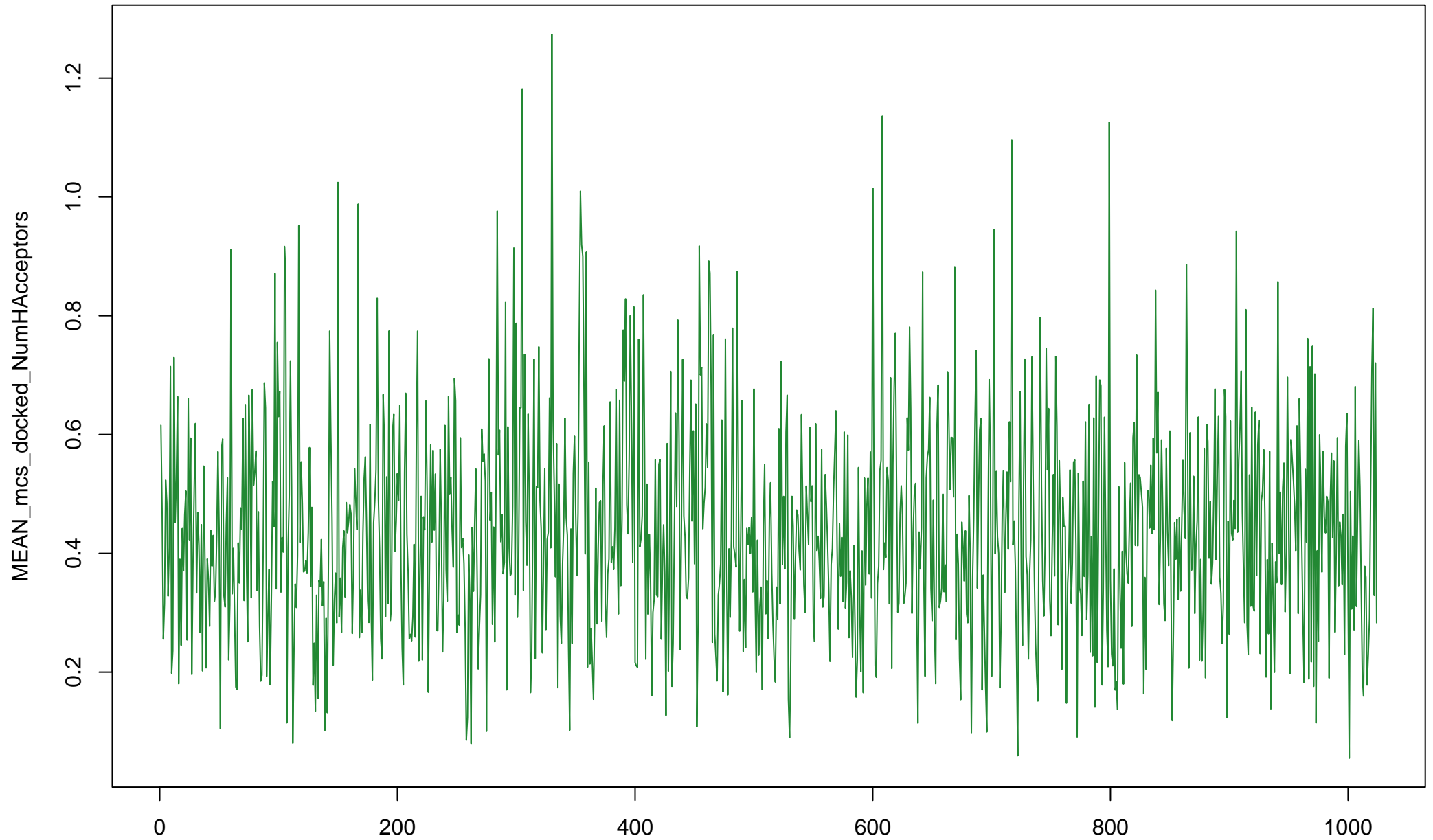
MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0521 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0



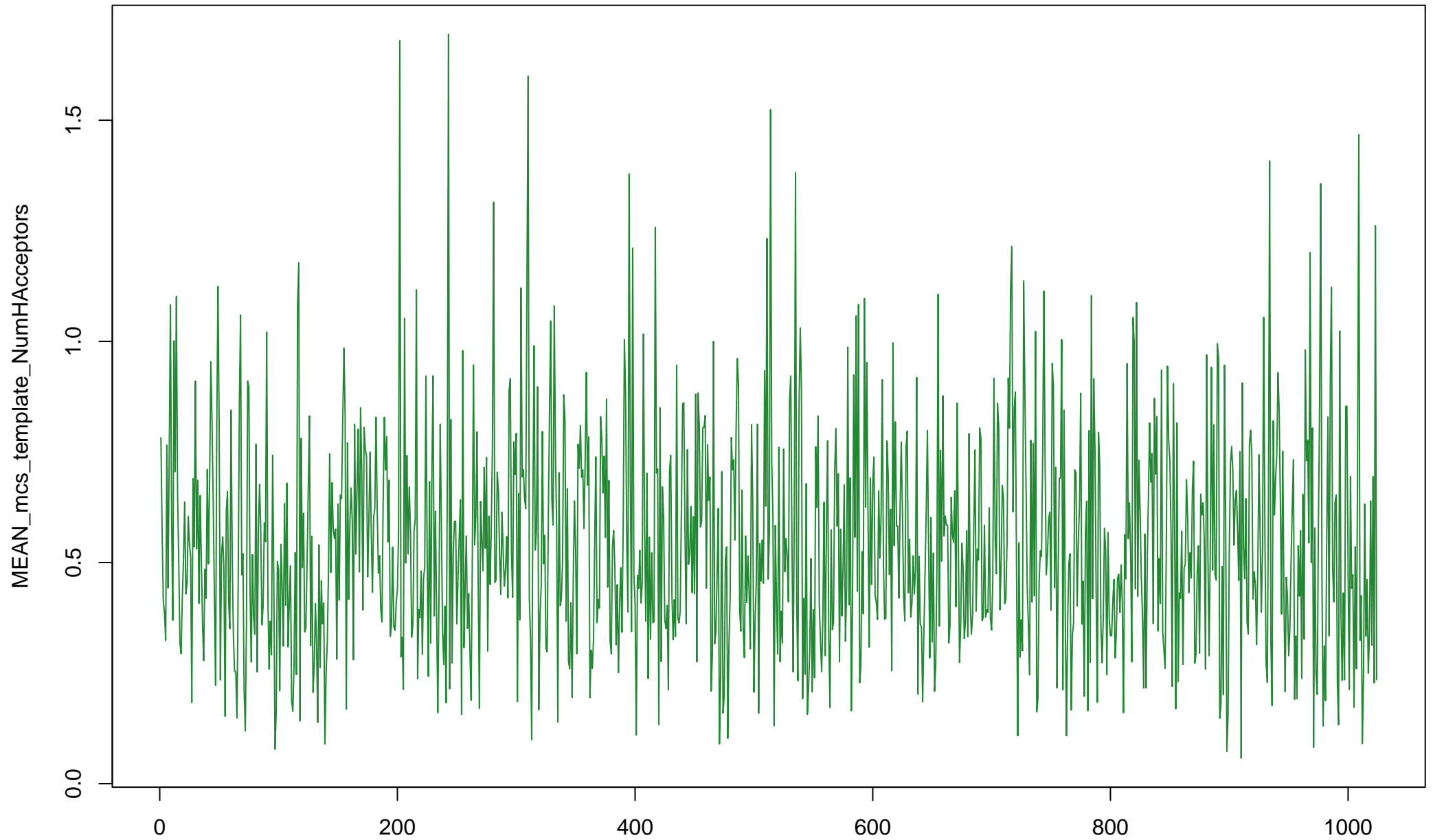
MEAN_template_HeavyAtomCount
ESS = 1020 | BMK = 0.0529 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0



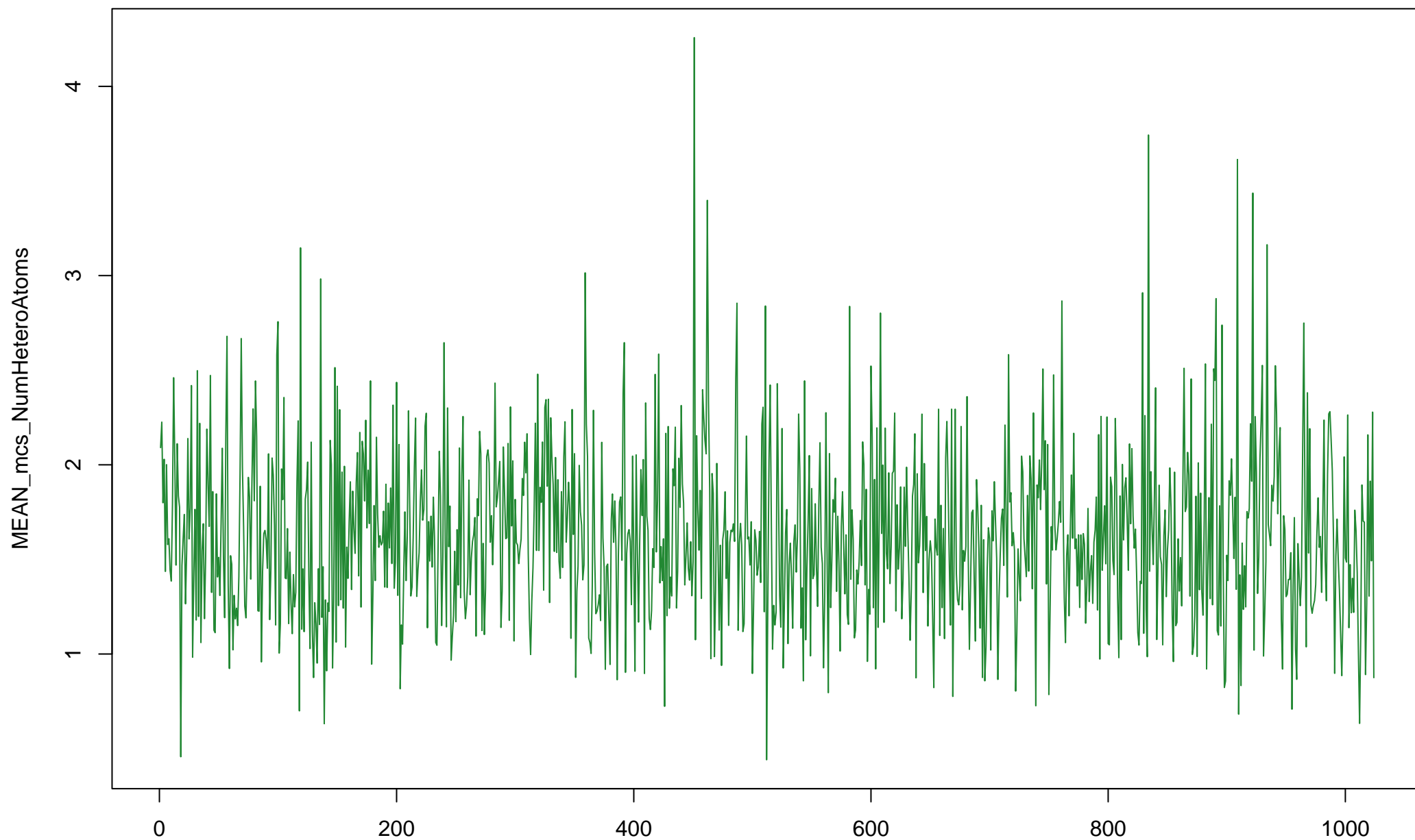
MEAN_mcs_docked_NumHAcceptors
ESS = 885 | BMK = 0.0746 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0



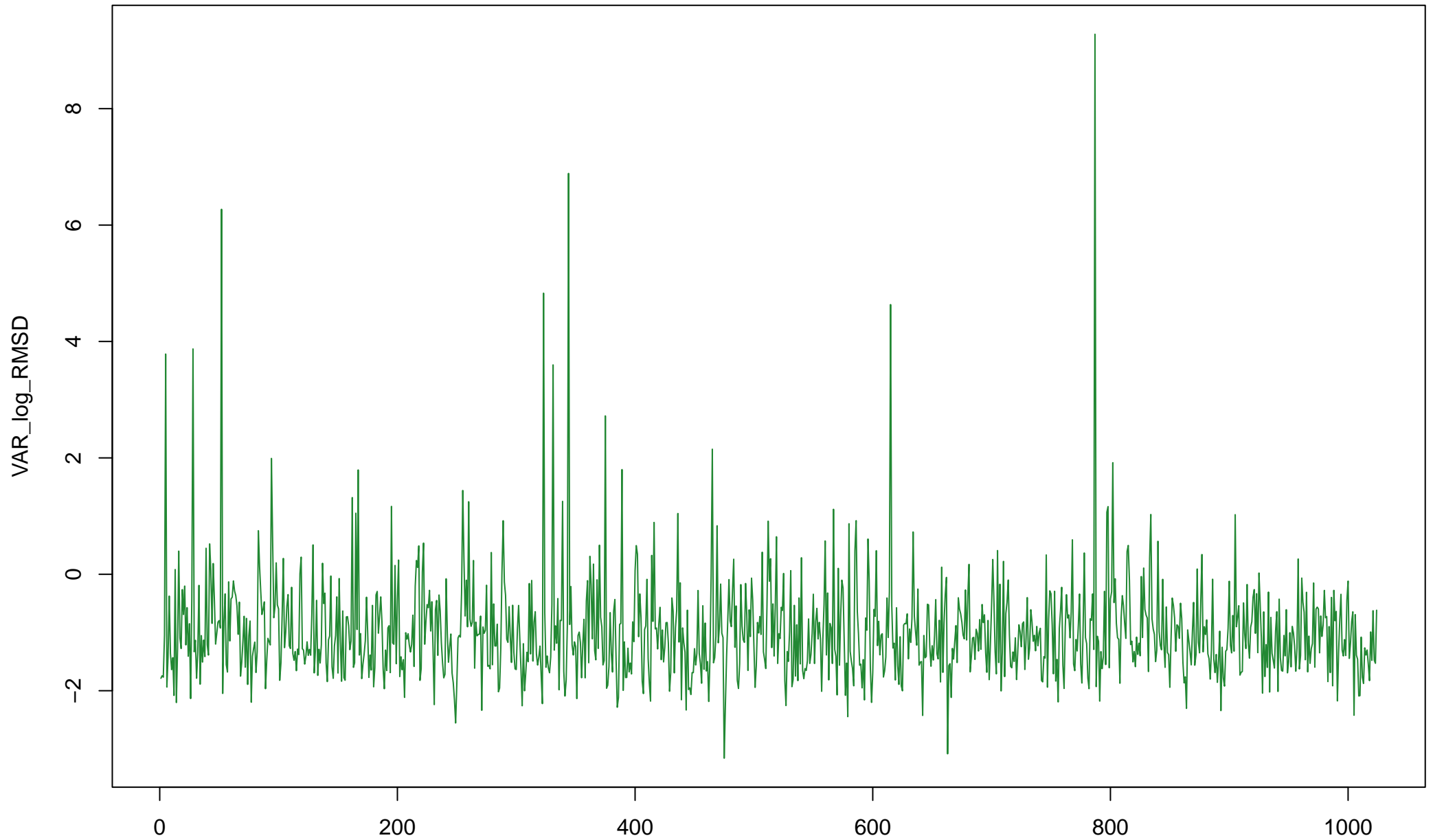
MEAN_mcs_template_NumHAcceptors
ESS = 887 | BMK = 0.0486 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0



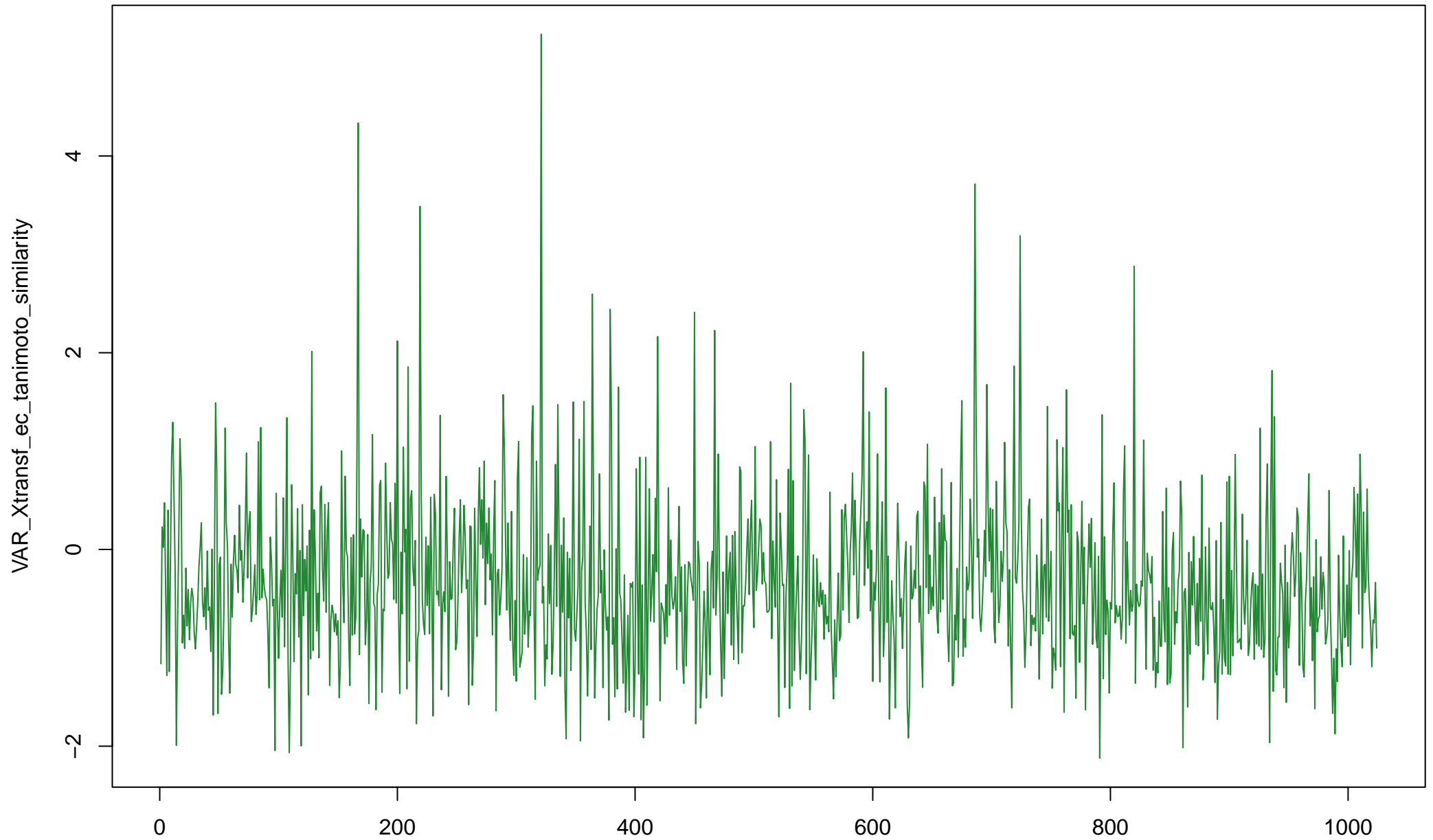
MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0654 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0



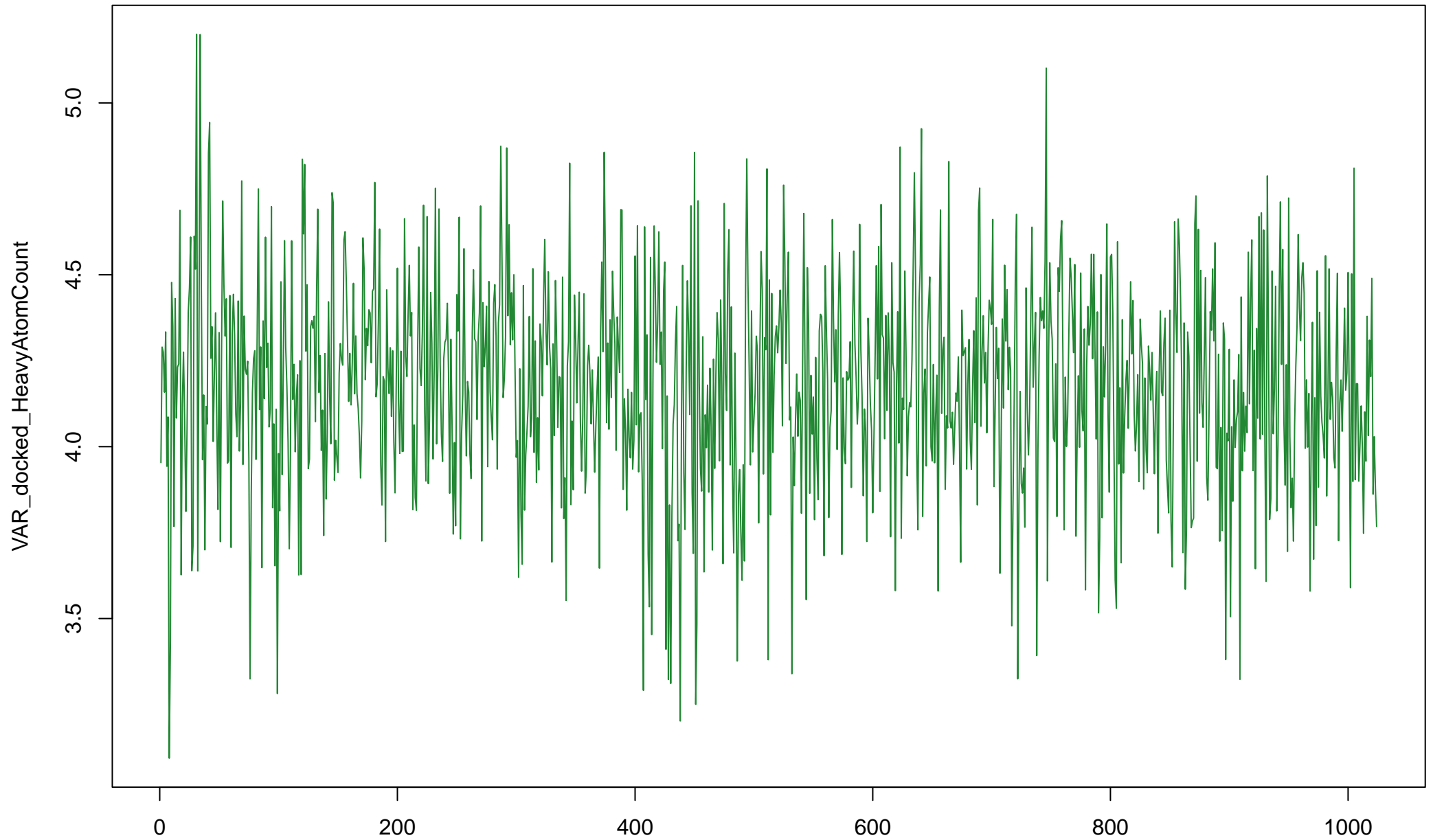
VAR_log_RMSD
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 816



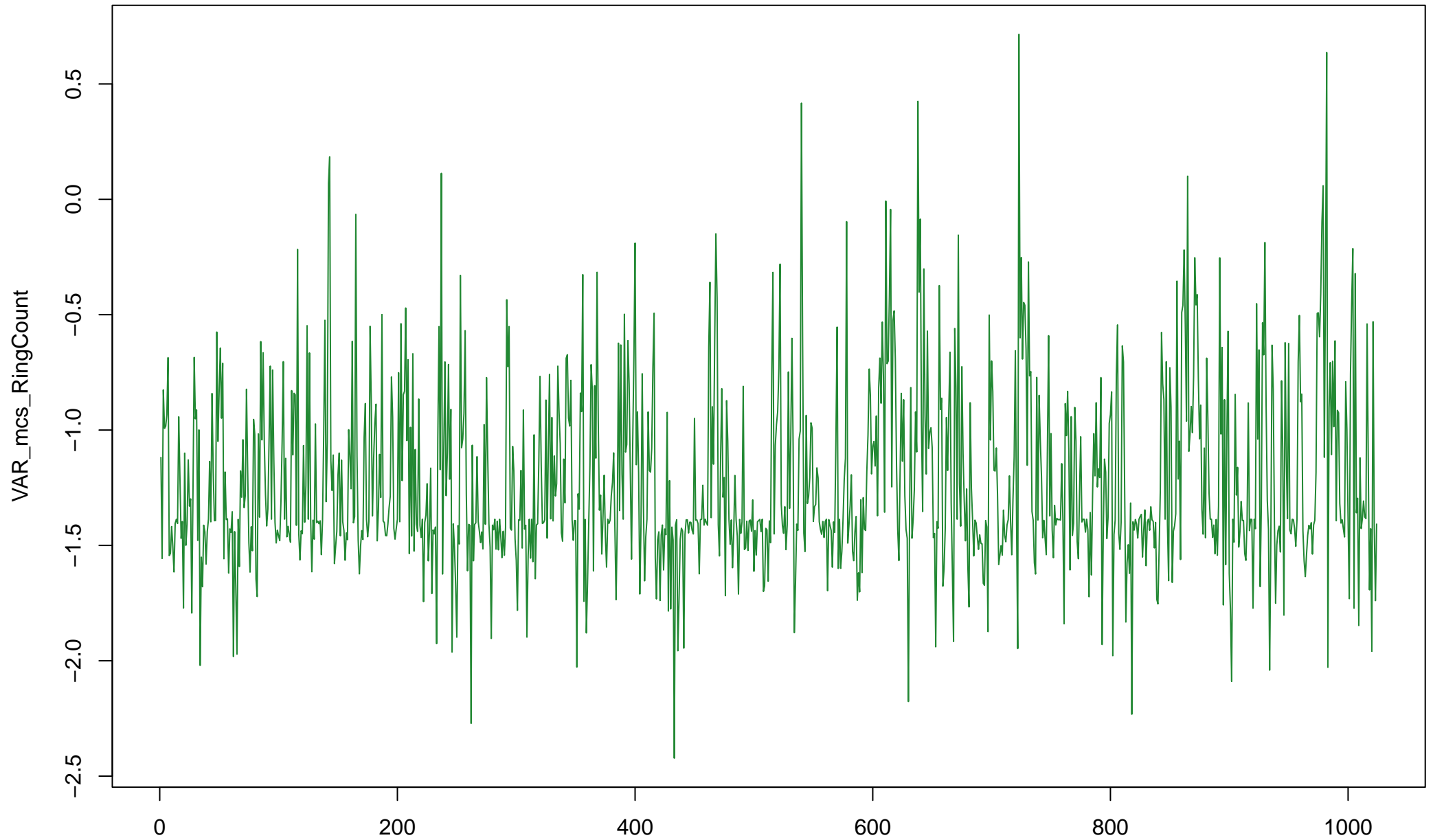
VAR_Xtransf_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.128 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0



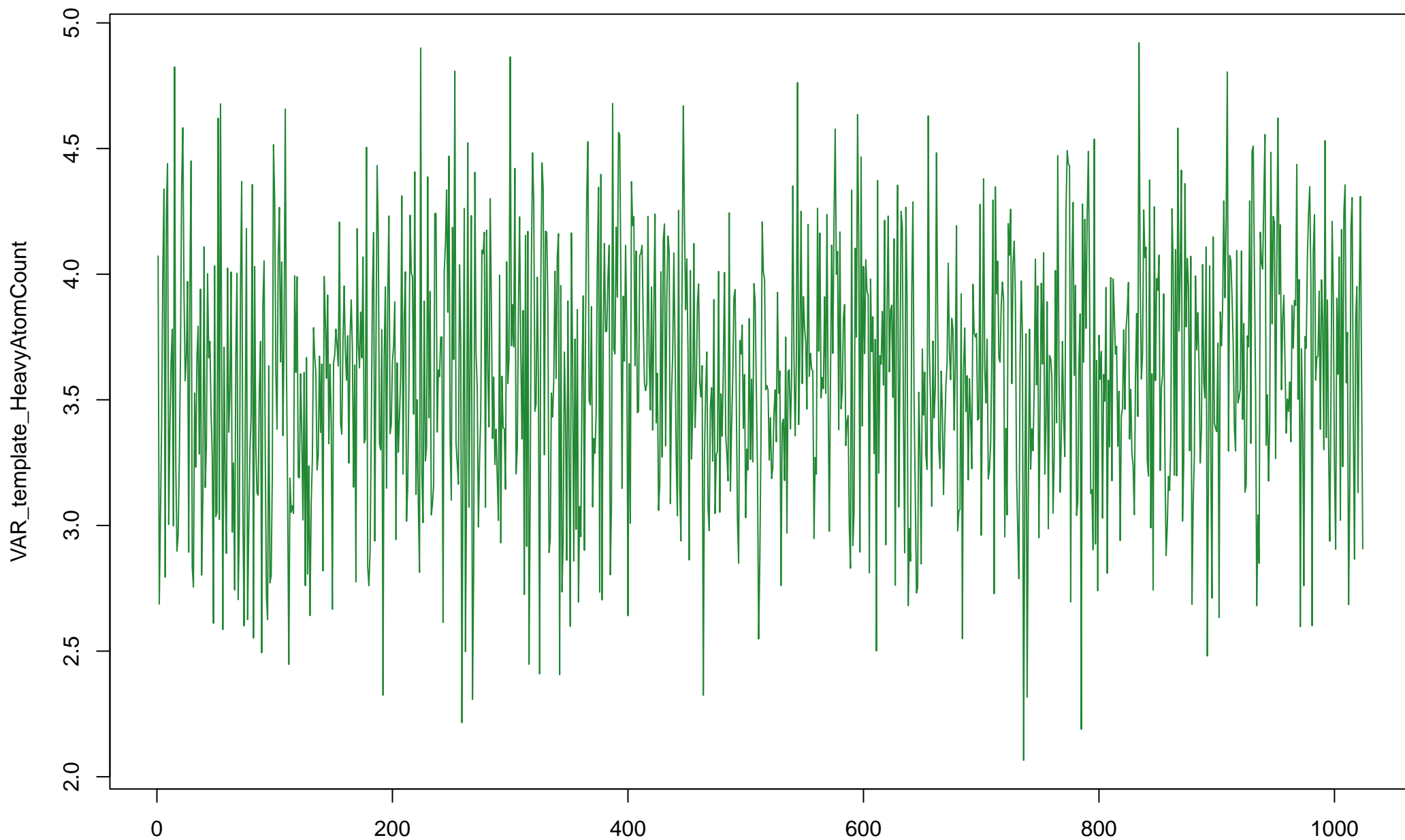
VAR_docked_HeavyAtomCount
ESS = 926 | BMK = 0.0644 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0



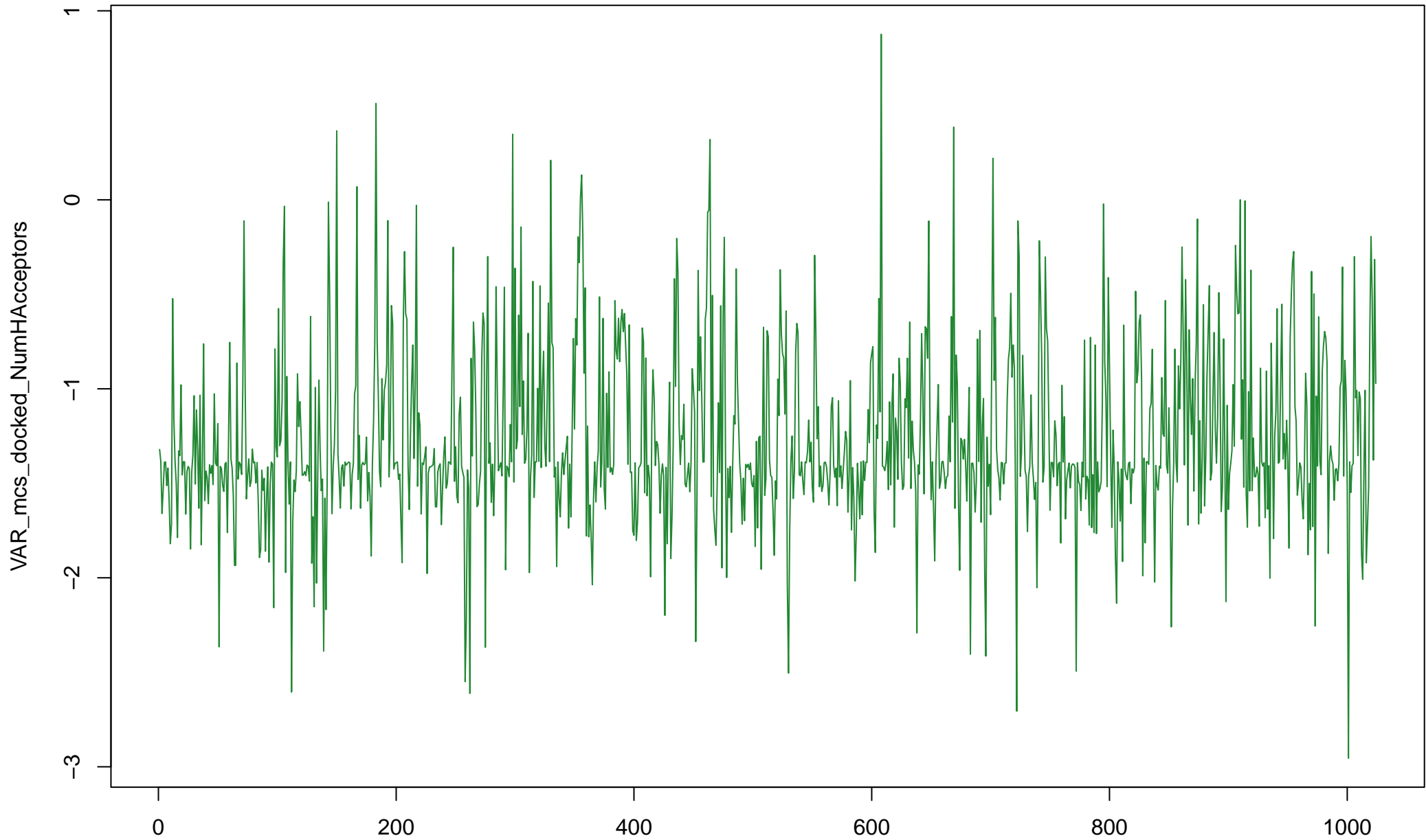
VAR_mcs_RingCount
ESS = 361 | BMK = 0.13 | MCSE(6.27) = 5.55 | stat: FALSE | burn: 0



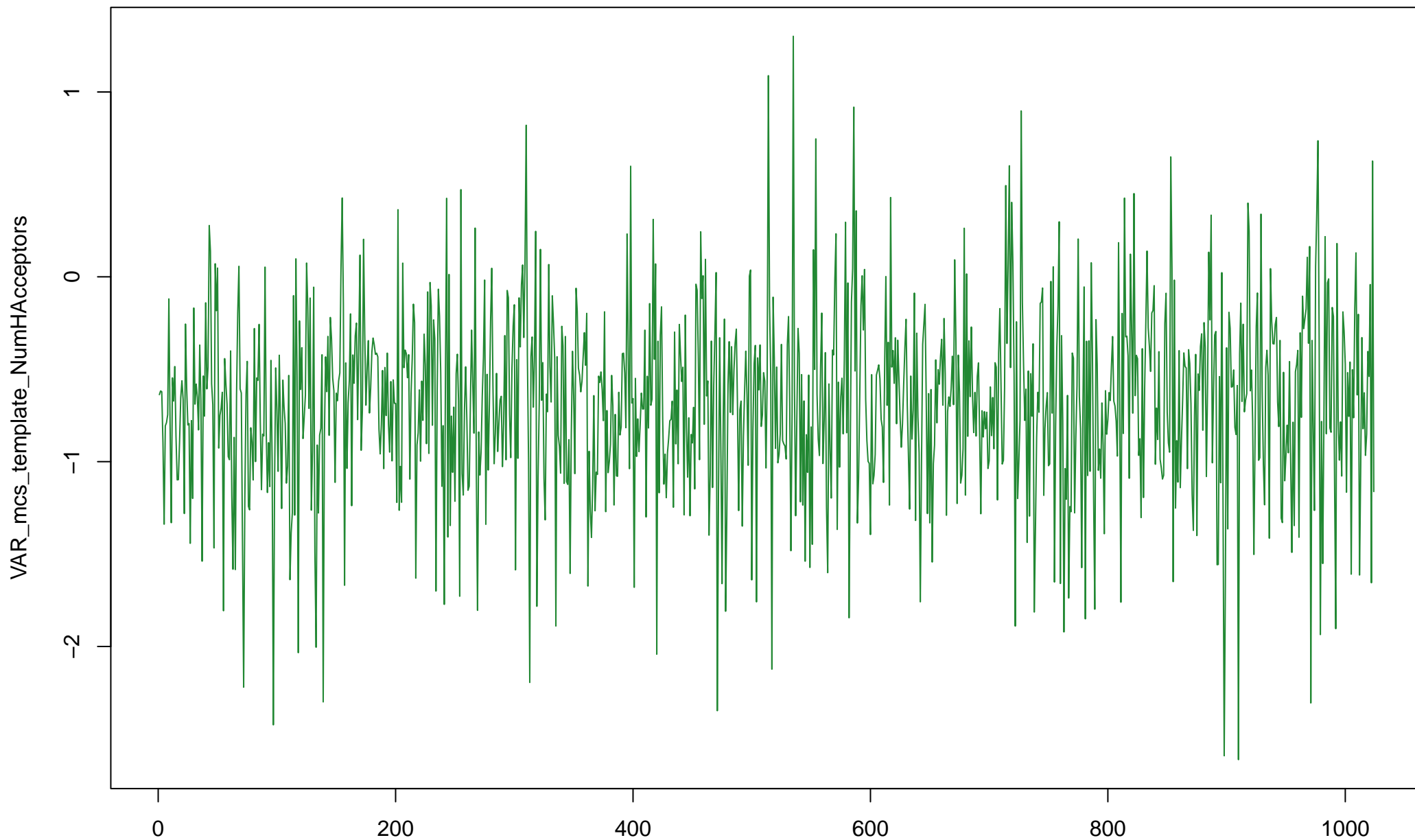
VAR_template_HeavyAtomCount
ESS = 1020 | BMK = 0.0653 | MCSE(6.27) = 3.76 | stat: TRUE | burn: 0



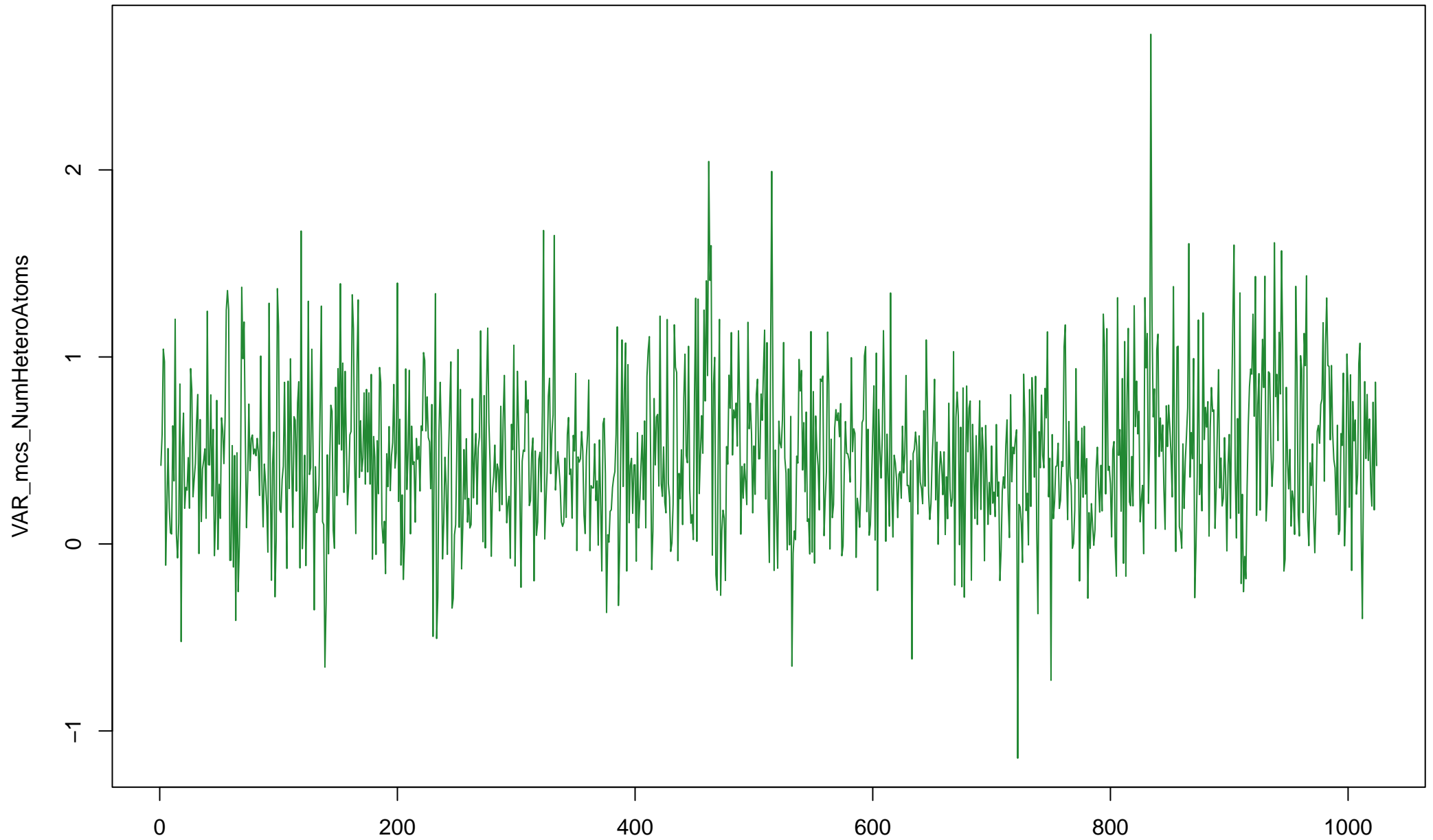
VAR_mcs_docked_NumHAcceptors
ESS = 506 | BMK = 0.0998 | MCSE(6.27) = 3.79 | stat: FALSE | burn: 0



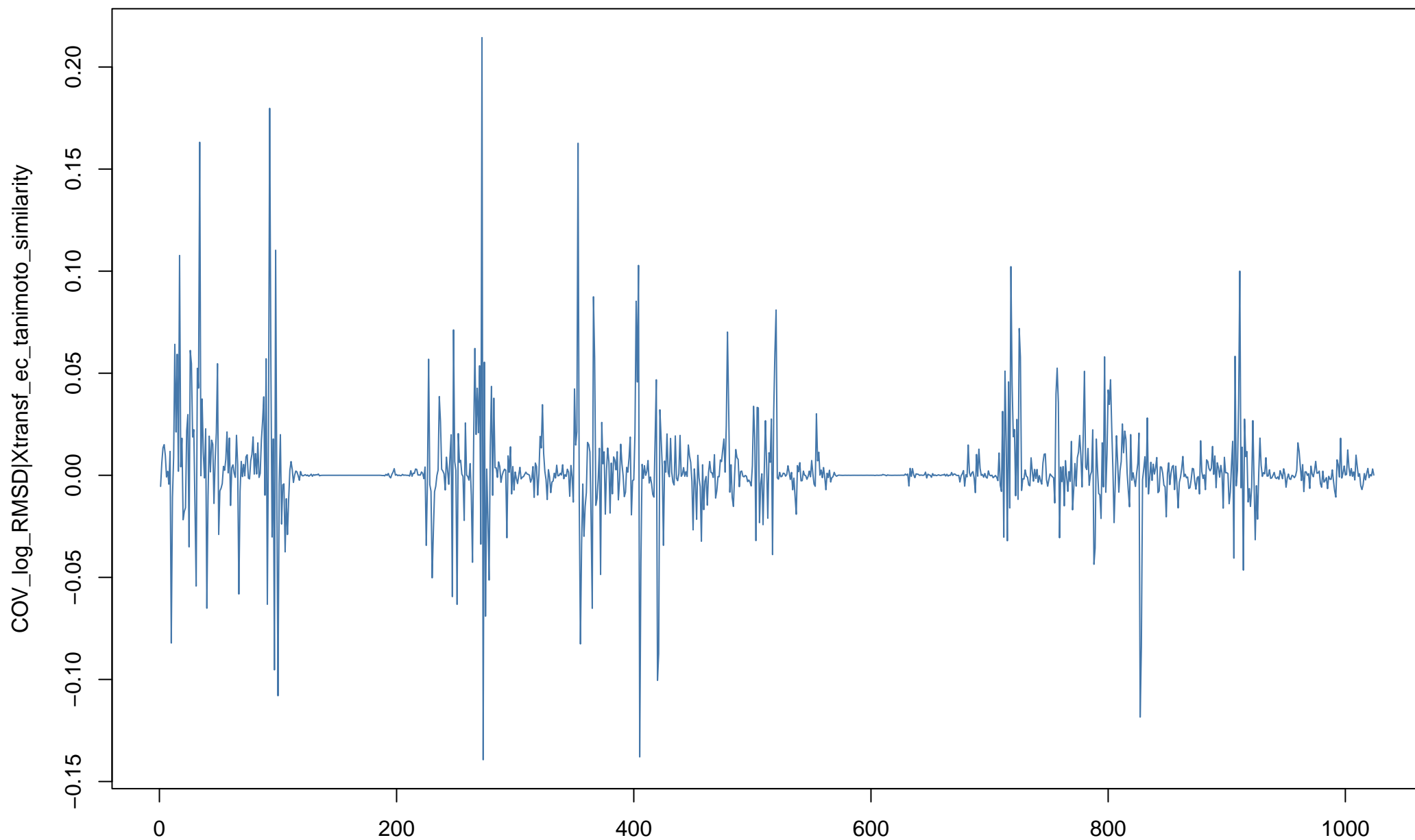
VAR_mcs_template_NumHAcceptors
ESS = 888 | BMK = 0.0918 | MCSE(6.27) = 3.52 | stat: FALSE | burn: 0



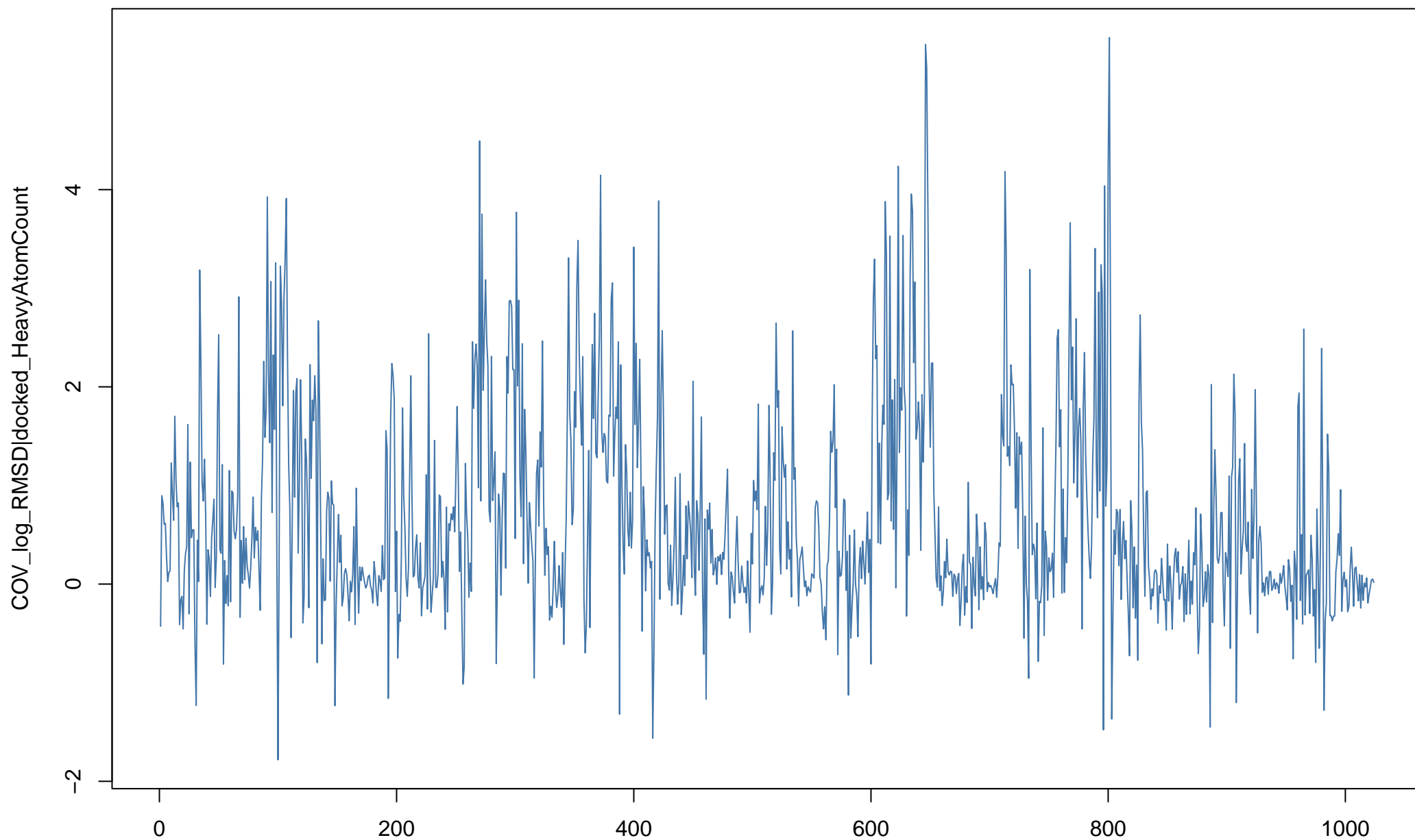
VAR_mcs_NumHeteroAtoms
ESS = 831 | BMK = 0.0756 | MCSE(6.27) = 4.11 | stat: TRUE | burn: 0



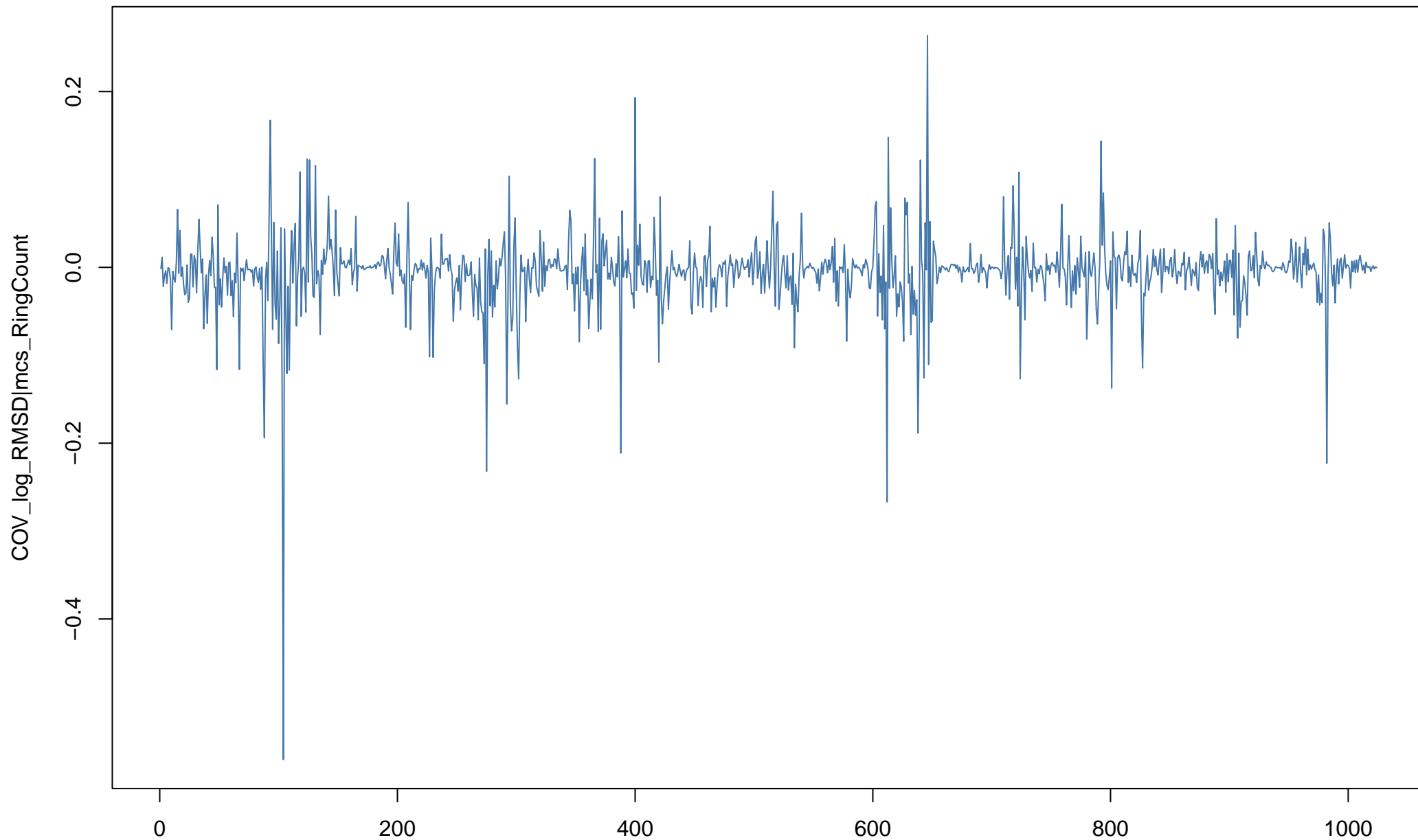
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.237 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 714



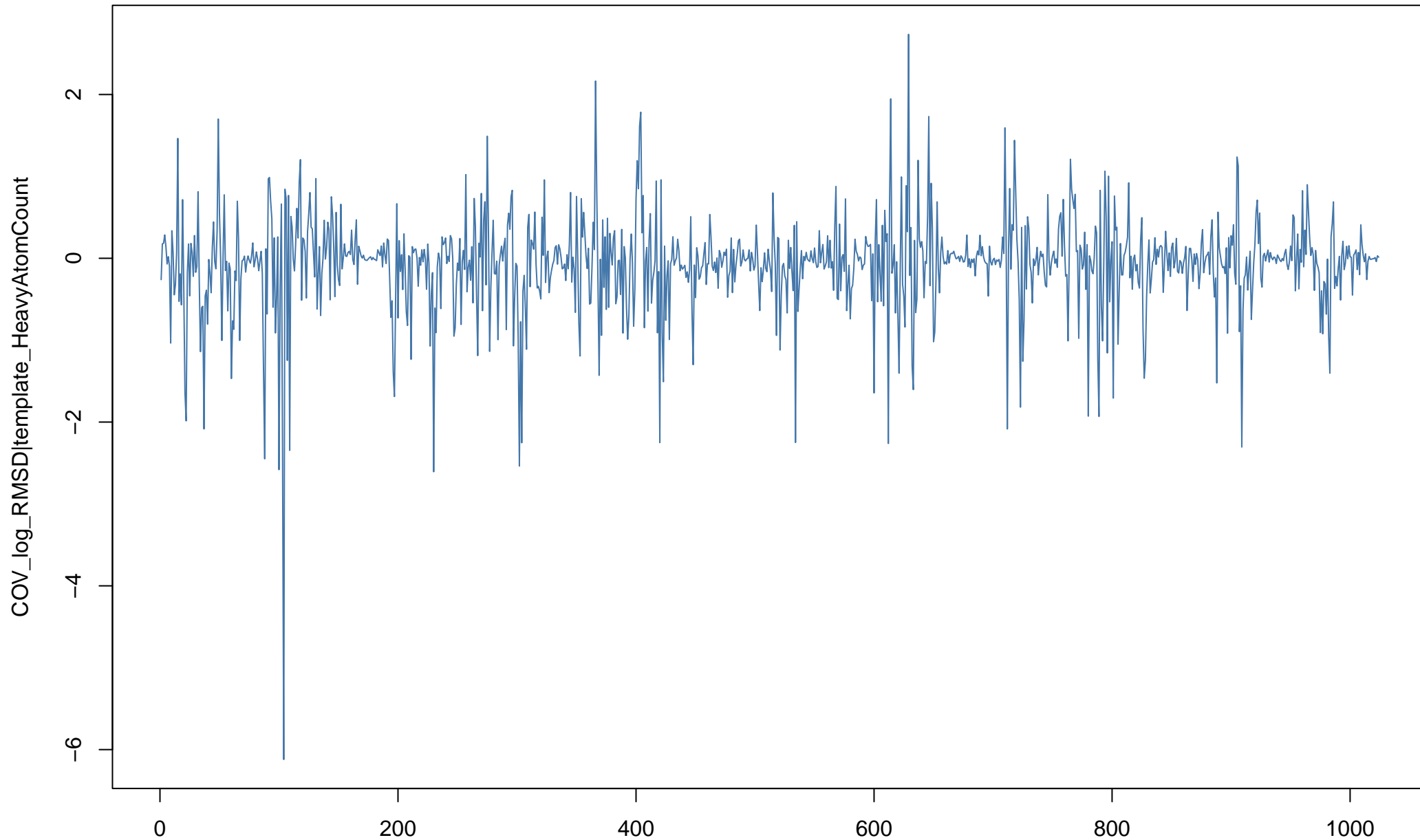
COV_log_RMSD|docked_HeavyAtomCount
ESS = 67 | BMK = 0.112 | MCSE(6.27) = 8.62 | stat: TRUE | burn: 0



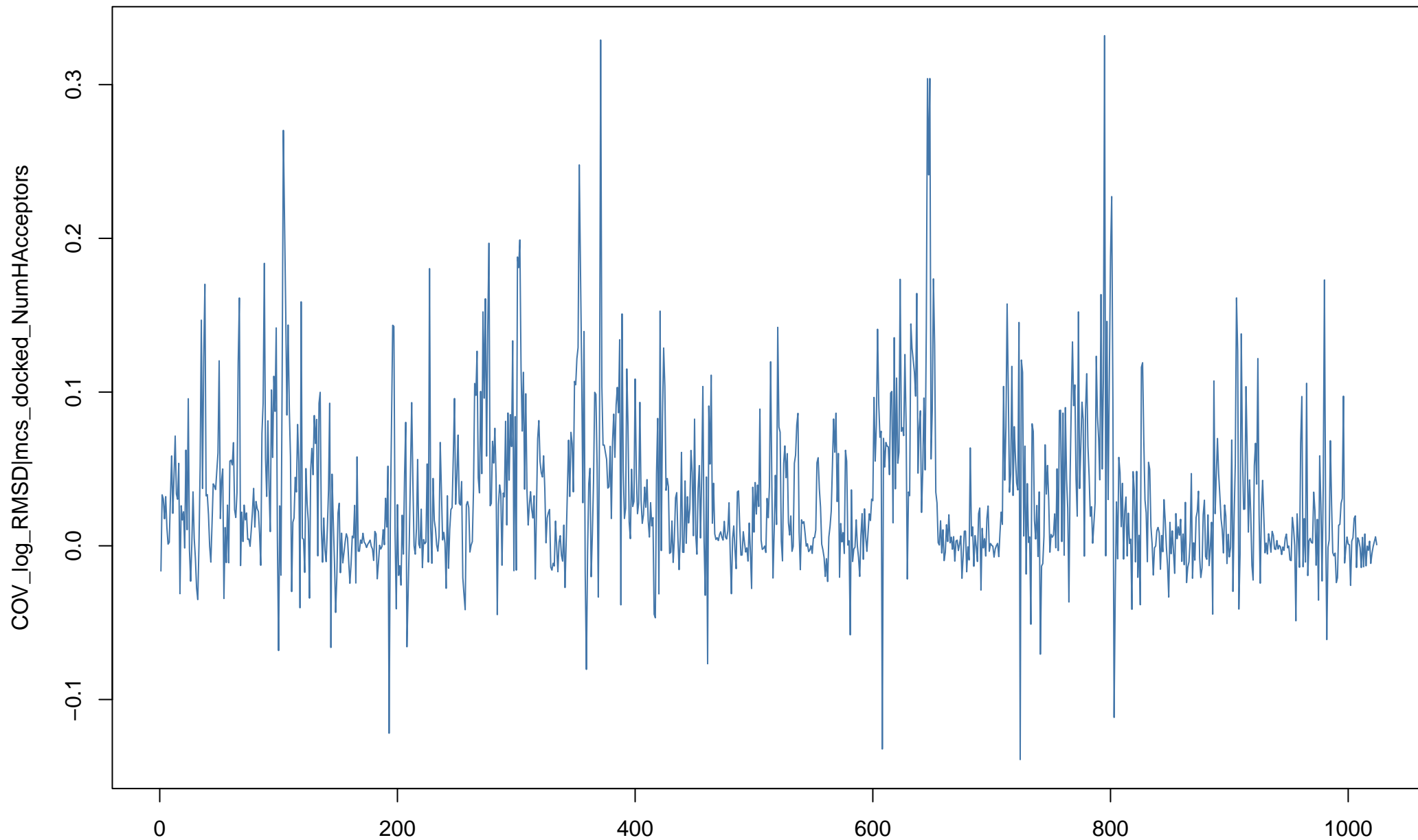
COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.143 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0



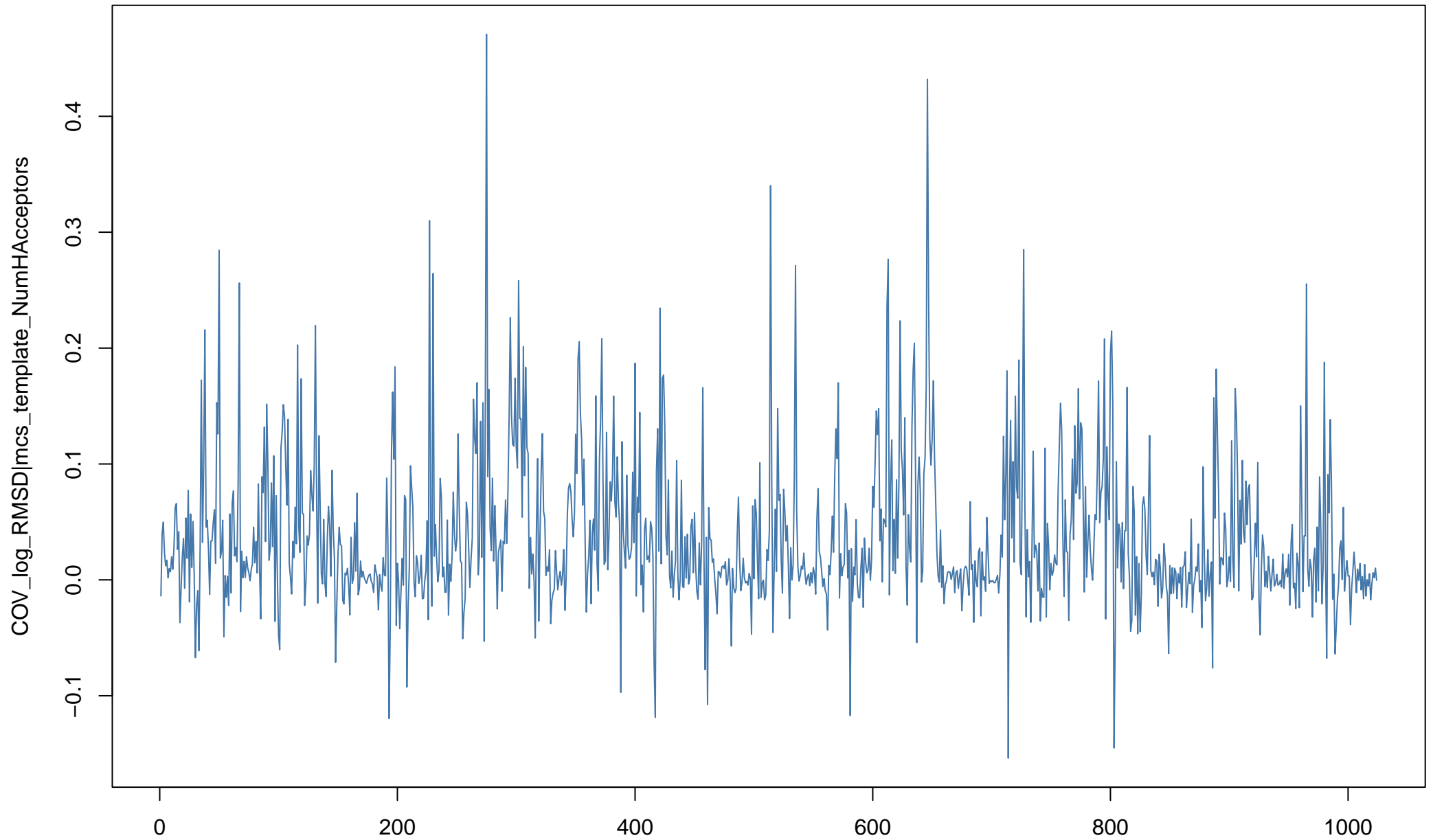
COV_log_RMSD|template_HeavyAtomCount
ESS = 688 | BMK = 0.12 | MCSE(6.27) = 3.38 | stat: TRUE | burn: 0



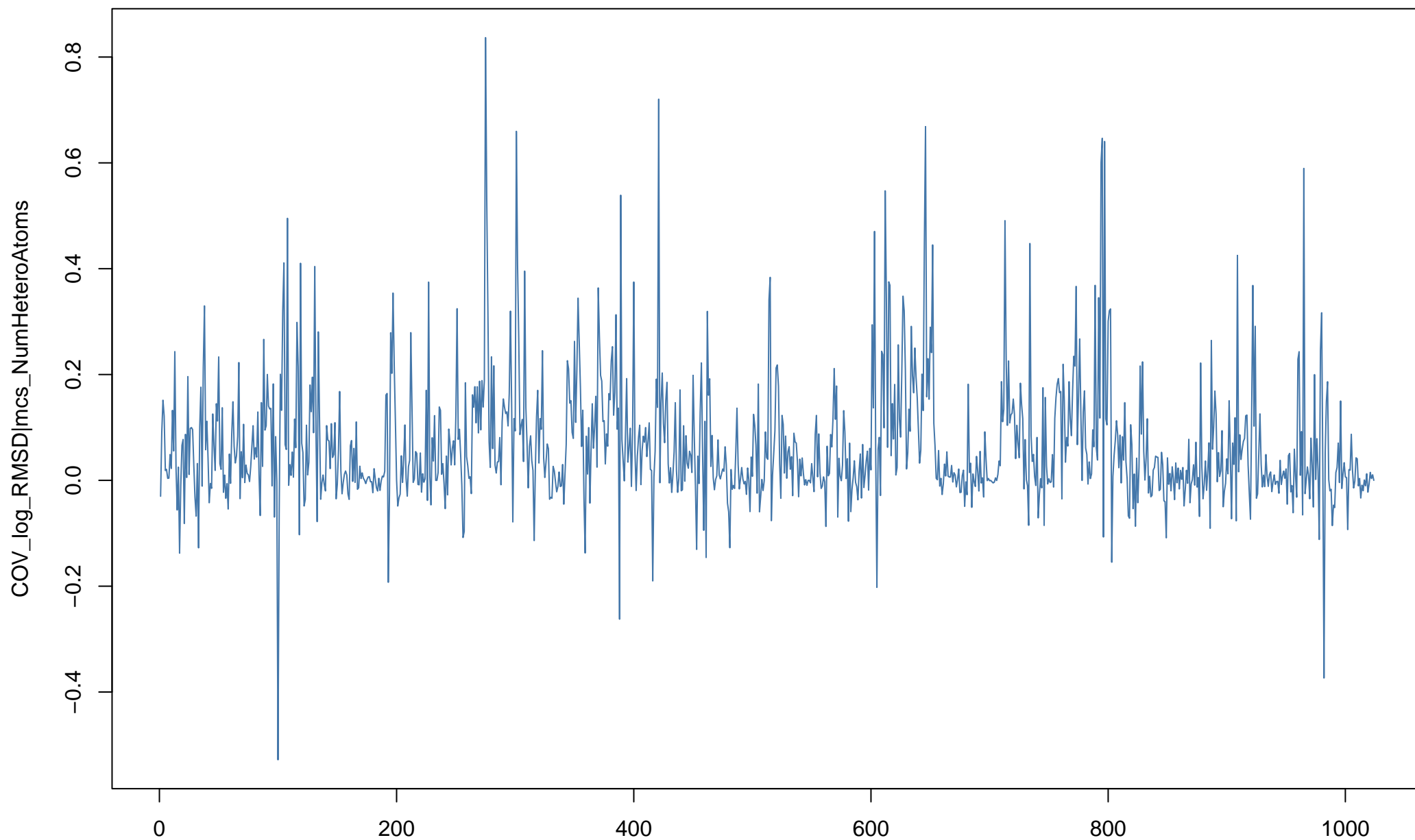
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 195 | BMK = 0.103 | MCSE(6.27) = 7.59 | stat: TRUE | burn: 0



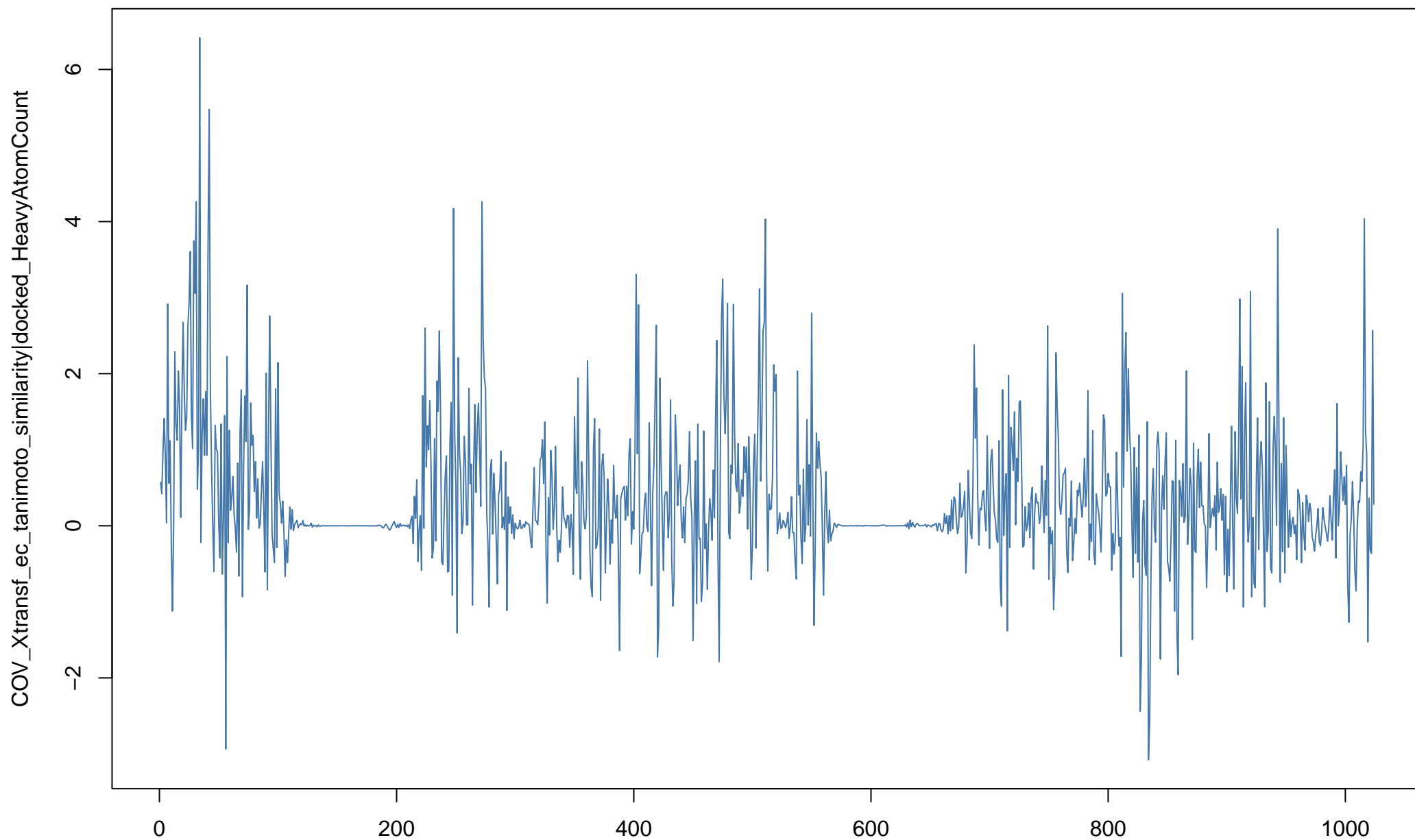
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 180 | BMK = 0.0853 | MCSE(6.27) = 6.55 | stat: TRUE | burn: 0



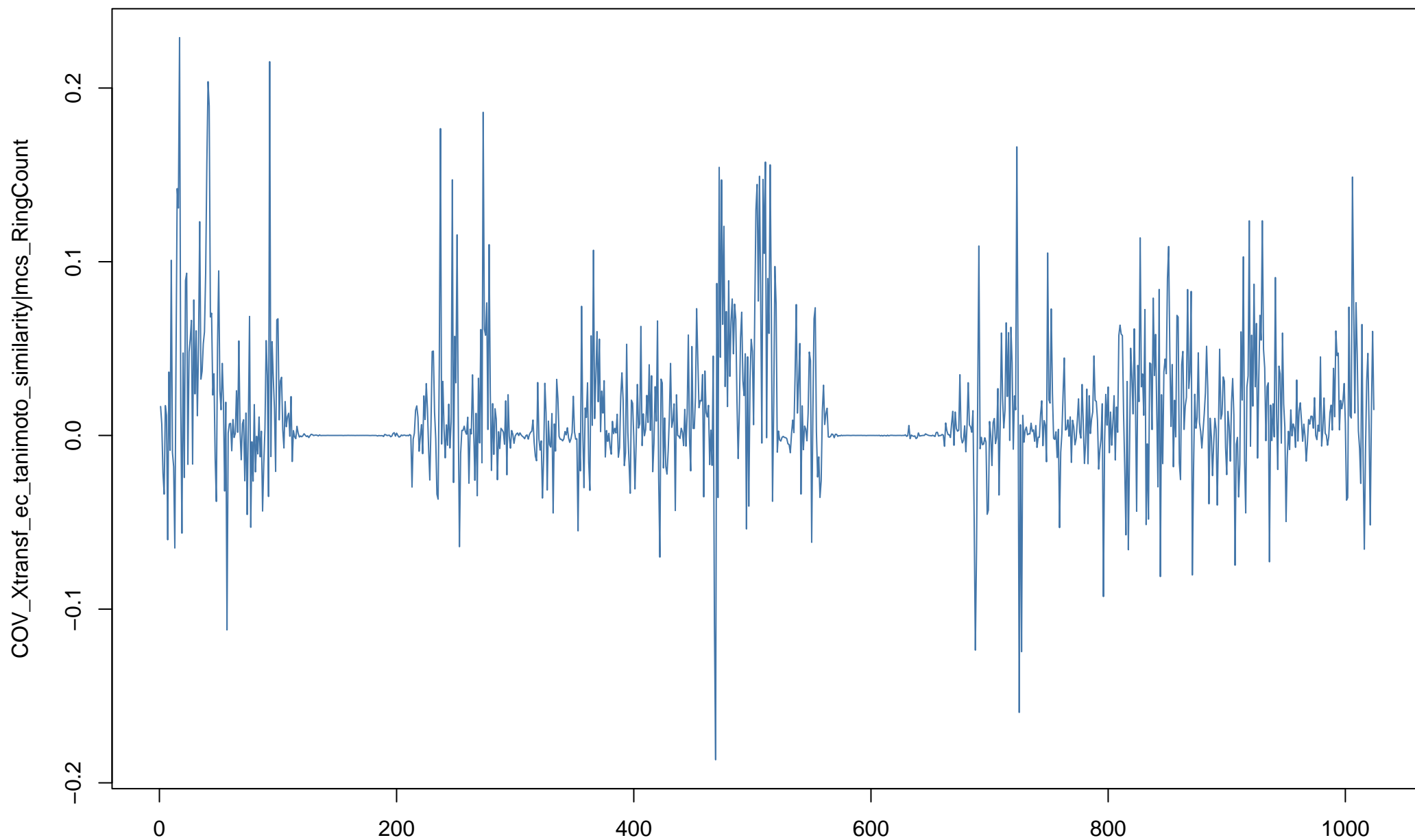
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 248 | BMK = 0.116 | MCSE(6.27) = 6.77 | stat: TRUE | burn: 0



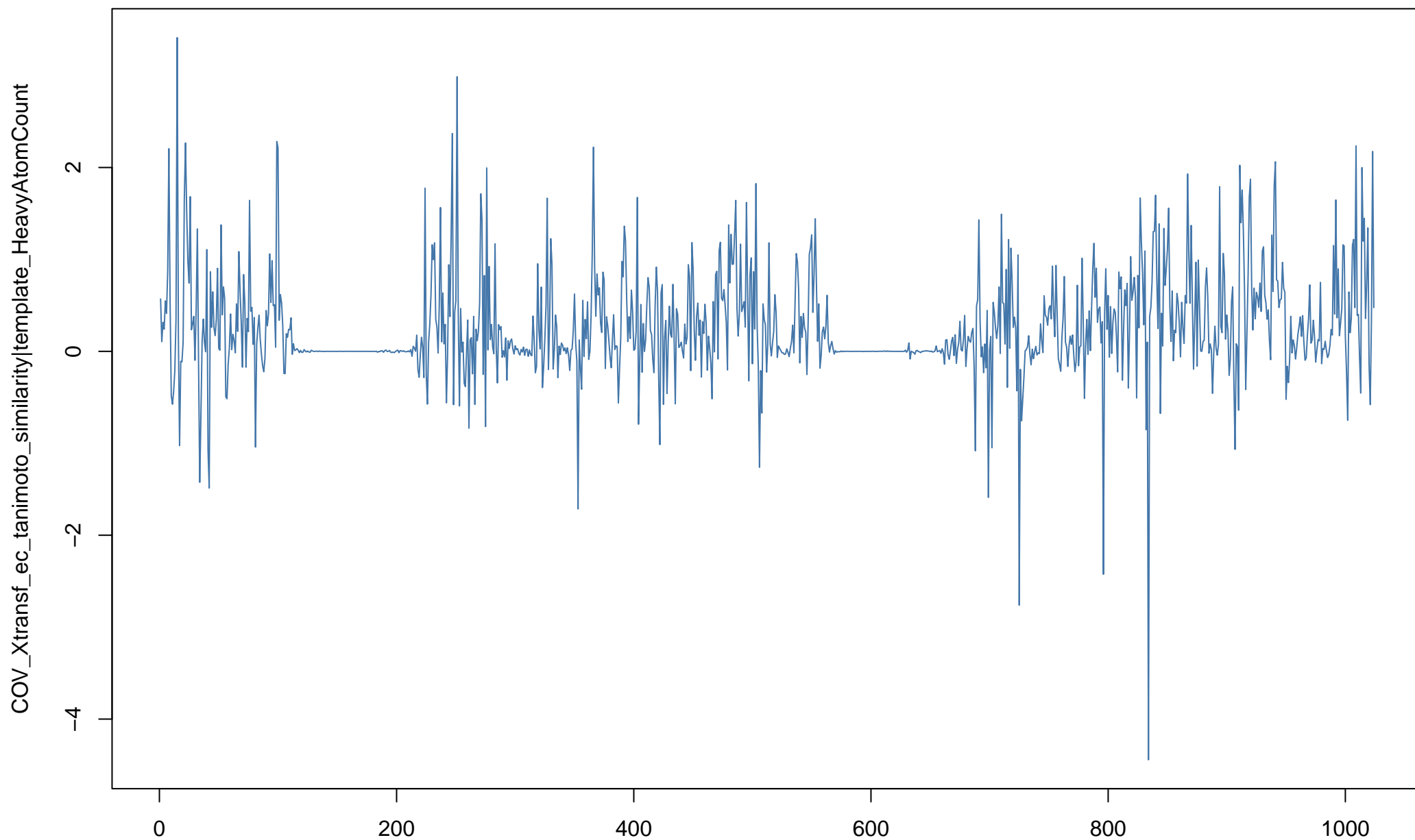
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 151 | BMK = 0.134 | MCSE(6.27) = 6.66 | stat: FALSE | burn: 510



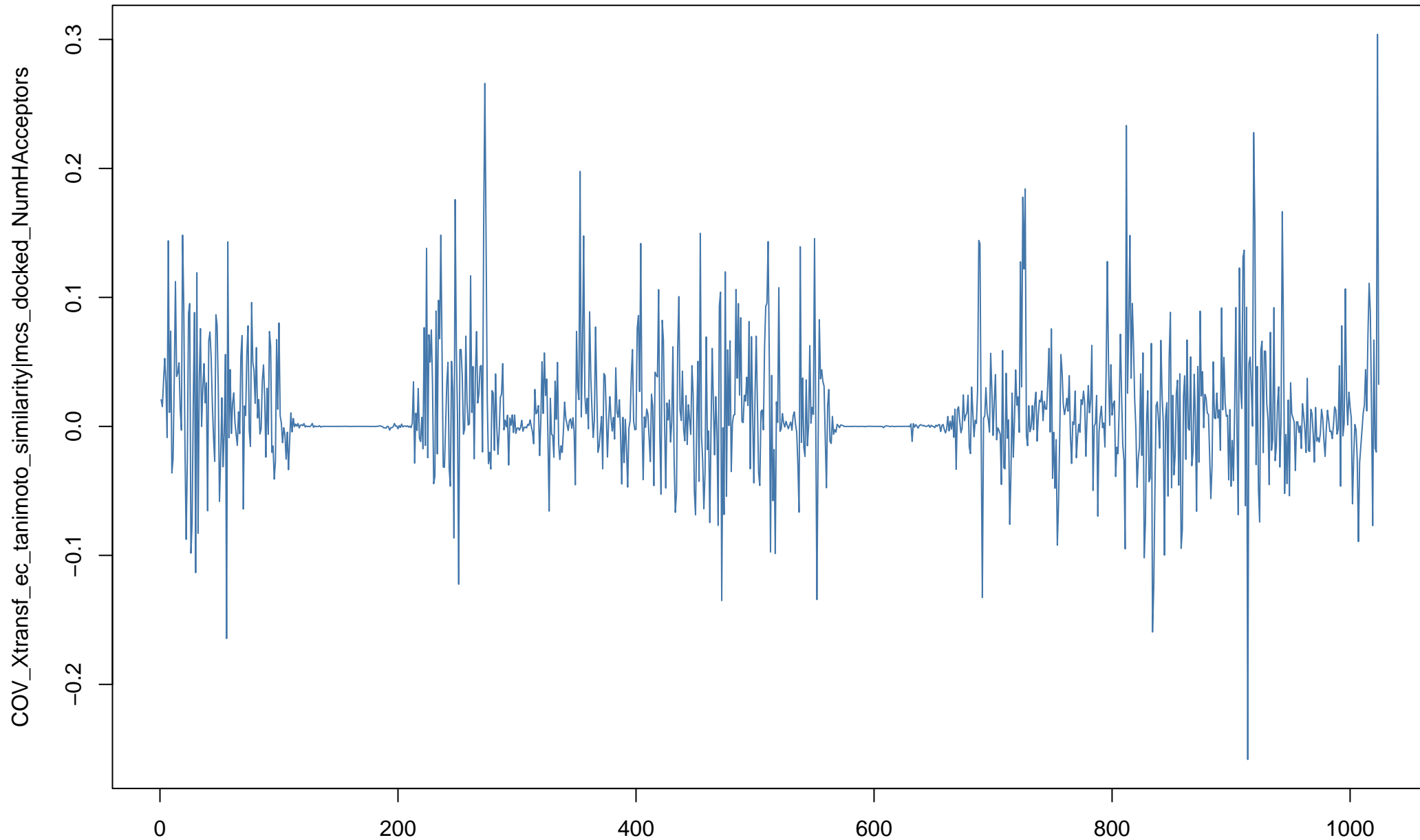
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 203 | BMK = 0.139 | MCSE(6.27) = 6.03 | stat: FALSE | burn: 510



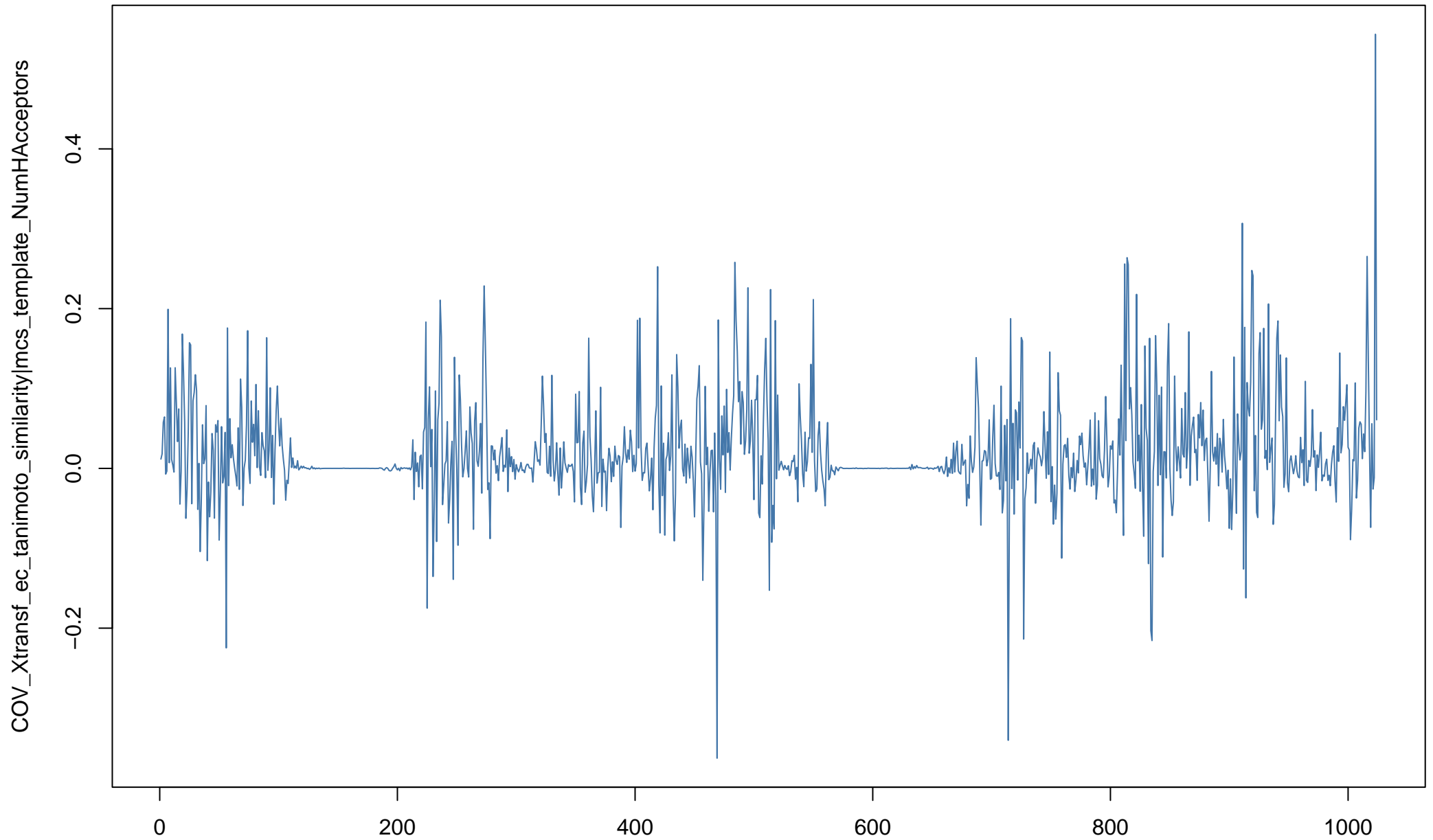
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 263 | BMK = 0.103 | MCSE(6.27) = 5.82 | stat: TRUE | burn: 204



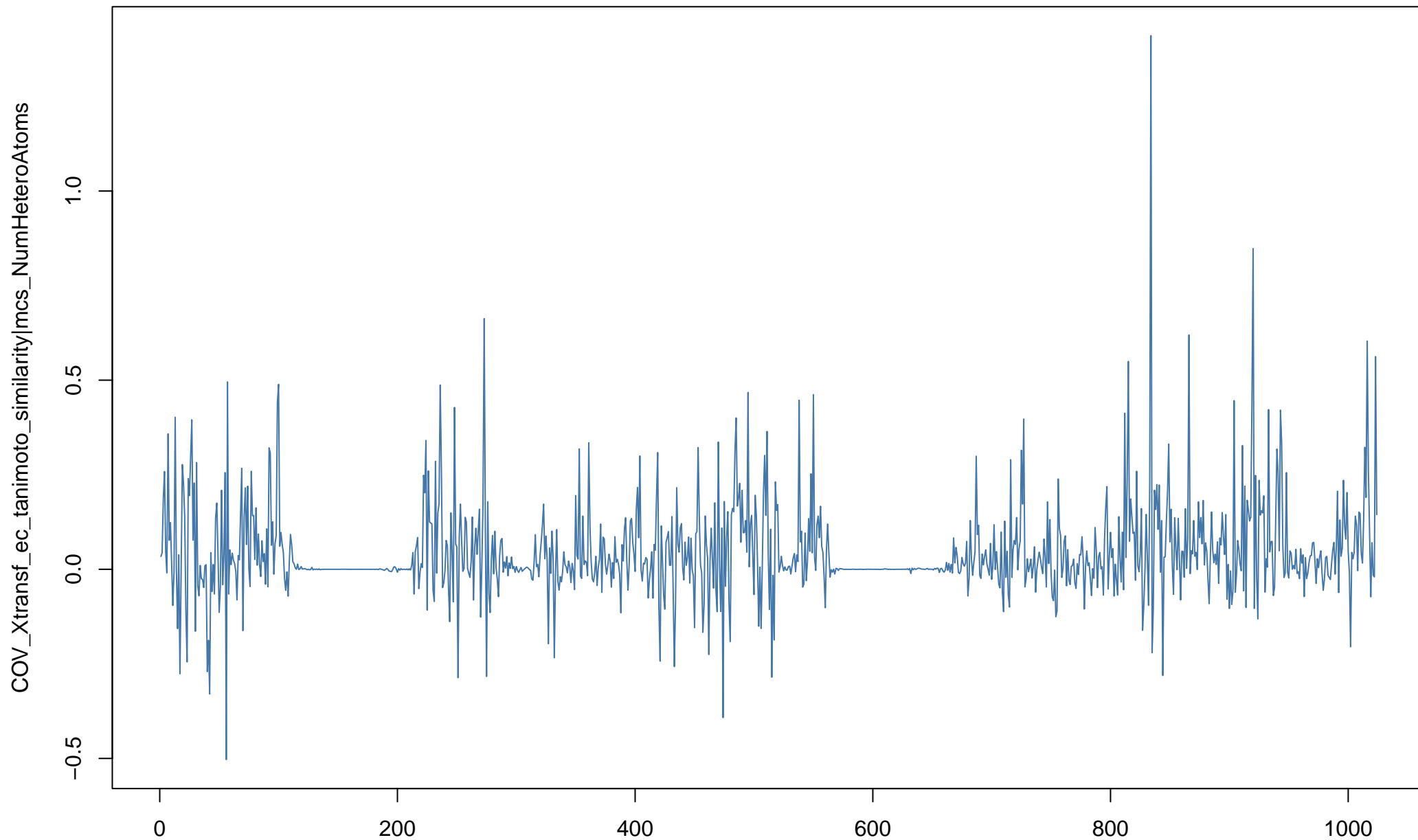
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 880 | BMK = 0.12 | MCSE(6.27) = 4.09 | stat: FALSE | burn: 510



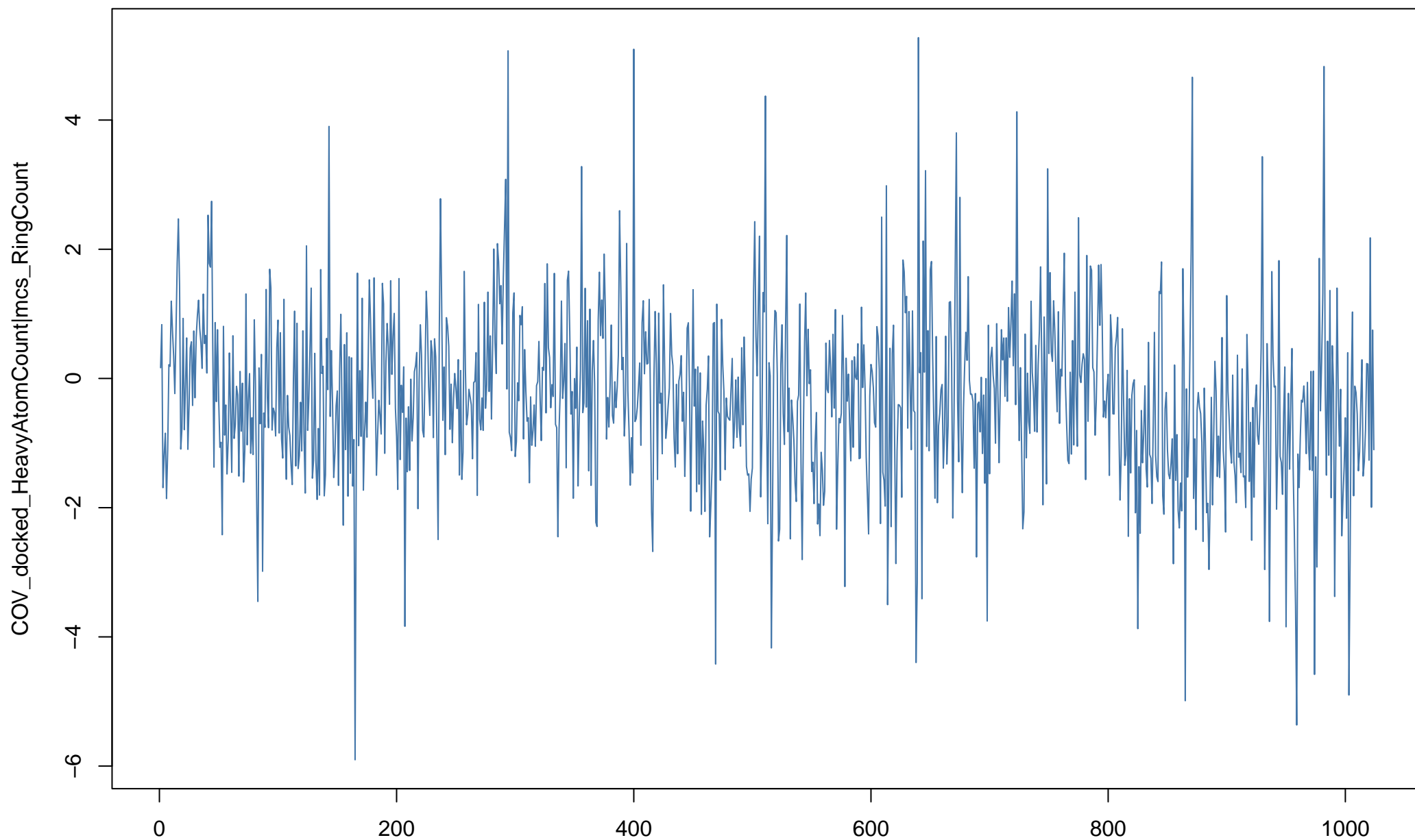
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 452 | BMK = 0.0963 | MCSE(6.27) = 5.11 | stat: TRUE | burn: 714



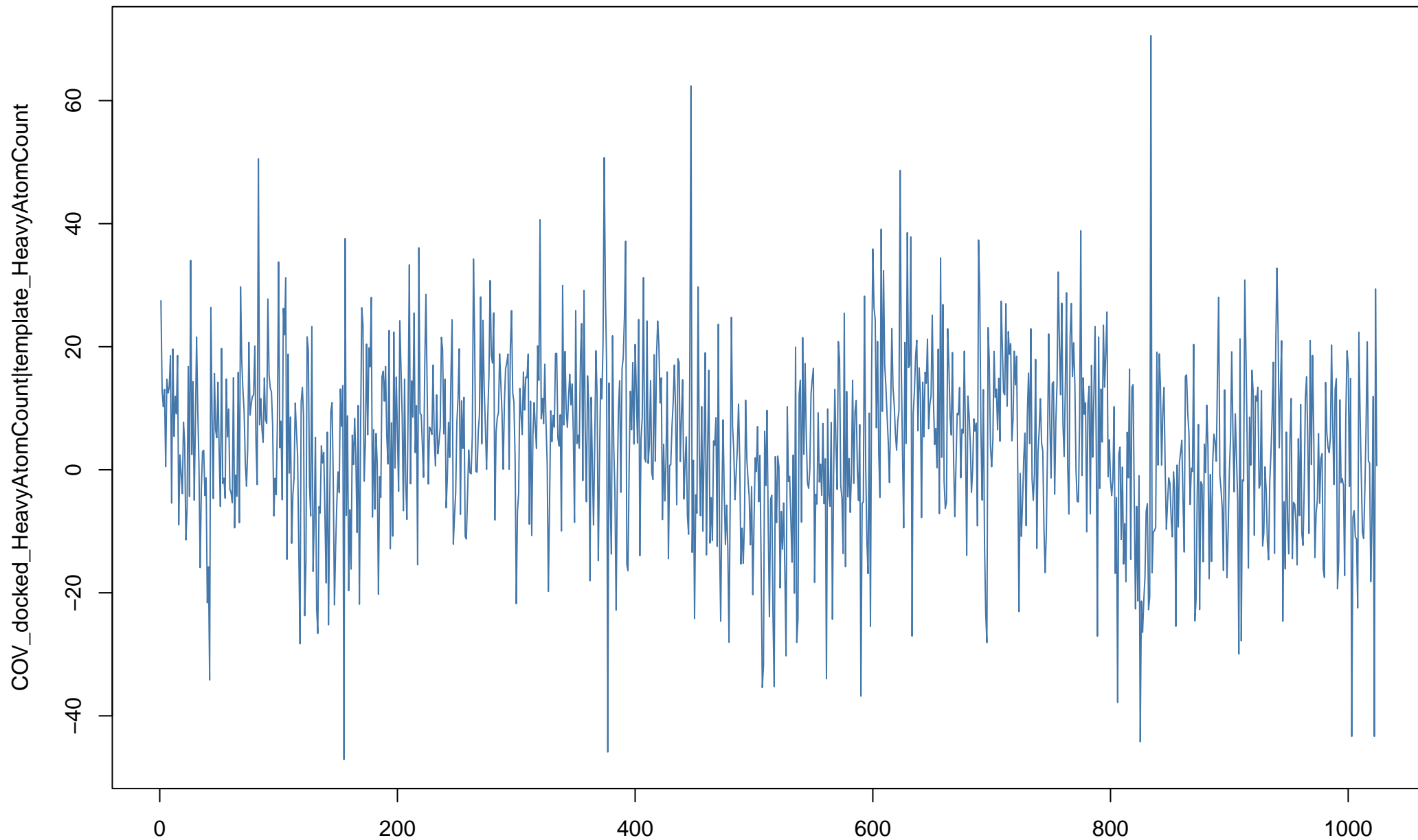
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 357 | BMK = 0.134 | MCSE(6.27) = 5.39 | stat: TRUE | burn: 204



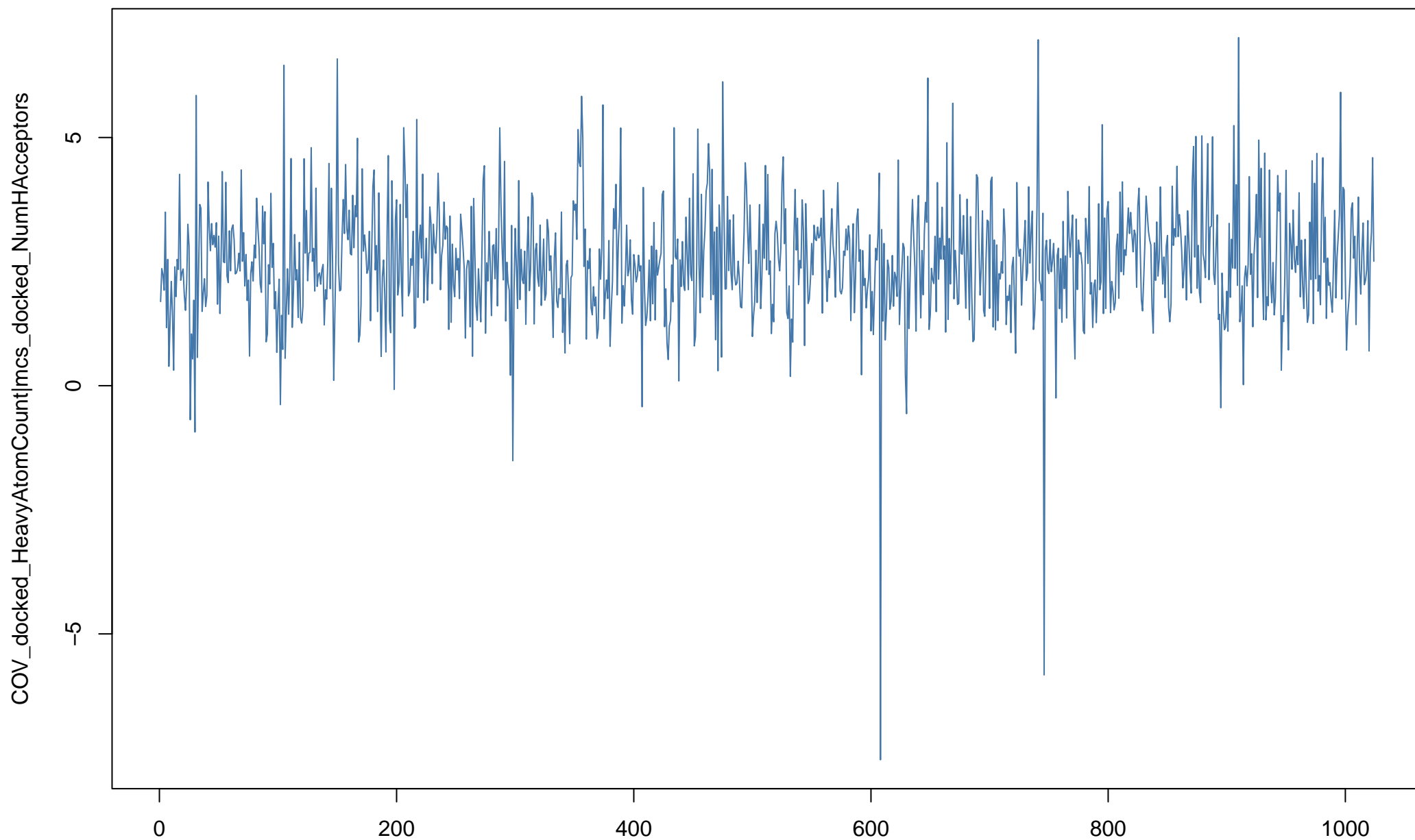
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 370 | BMK = 0.13 | MCSE(6.27) = 5.1 | stat: FALSE | burn: 0



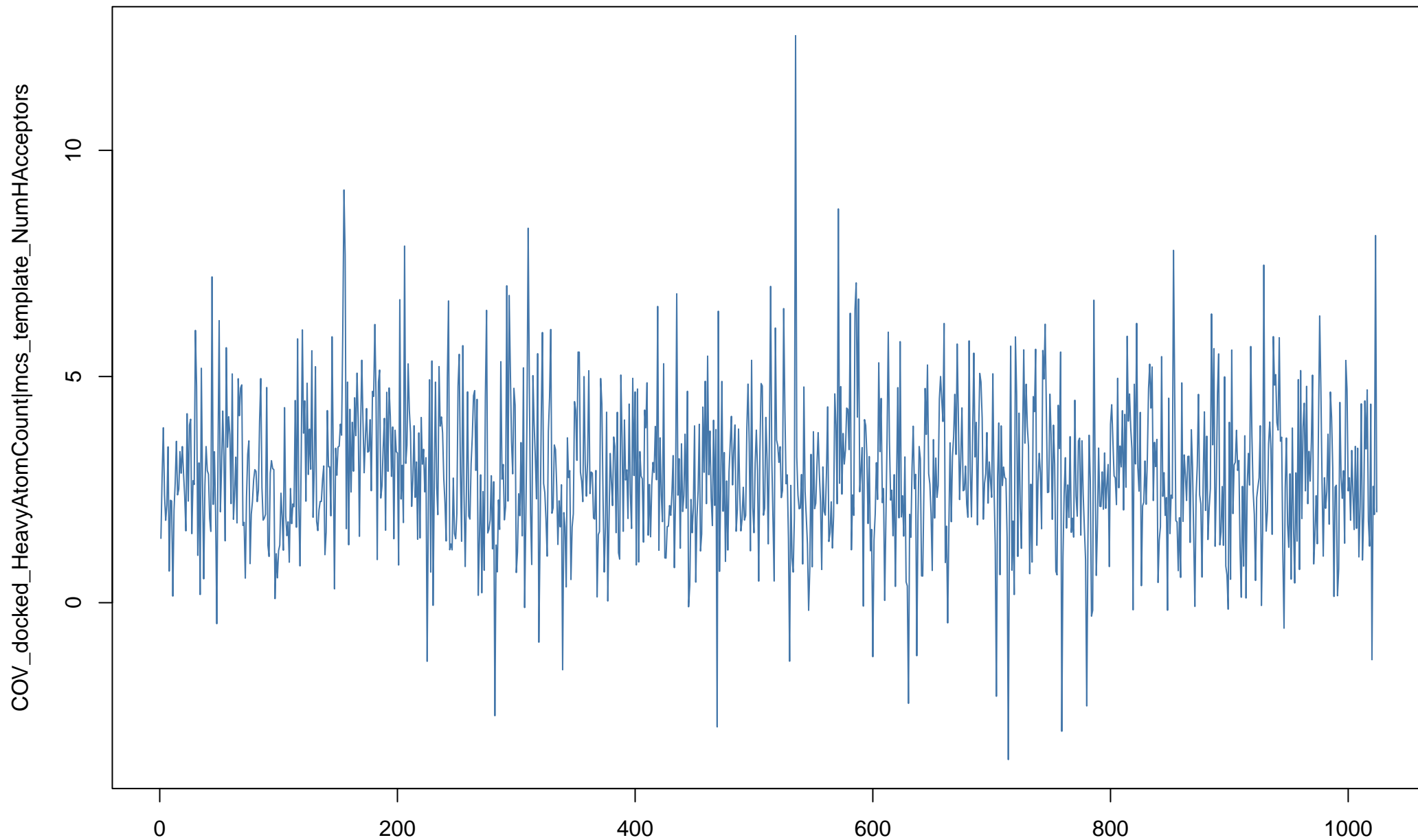
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 124 | BMK = 0.0806 | MCSE(6.27) = 6.79 | stat: FALSE | burn: 0



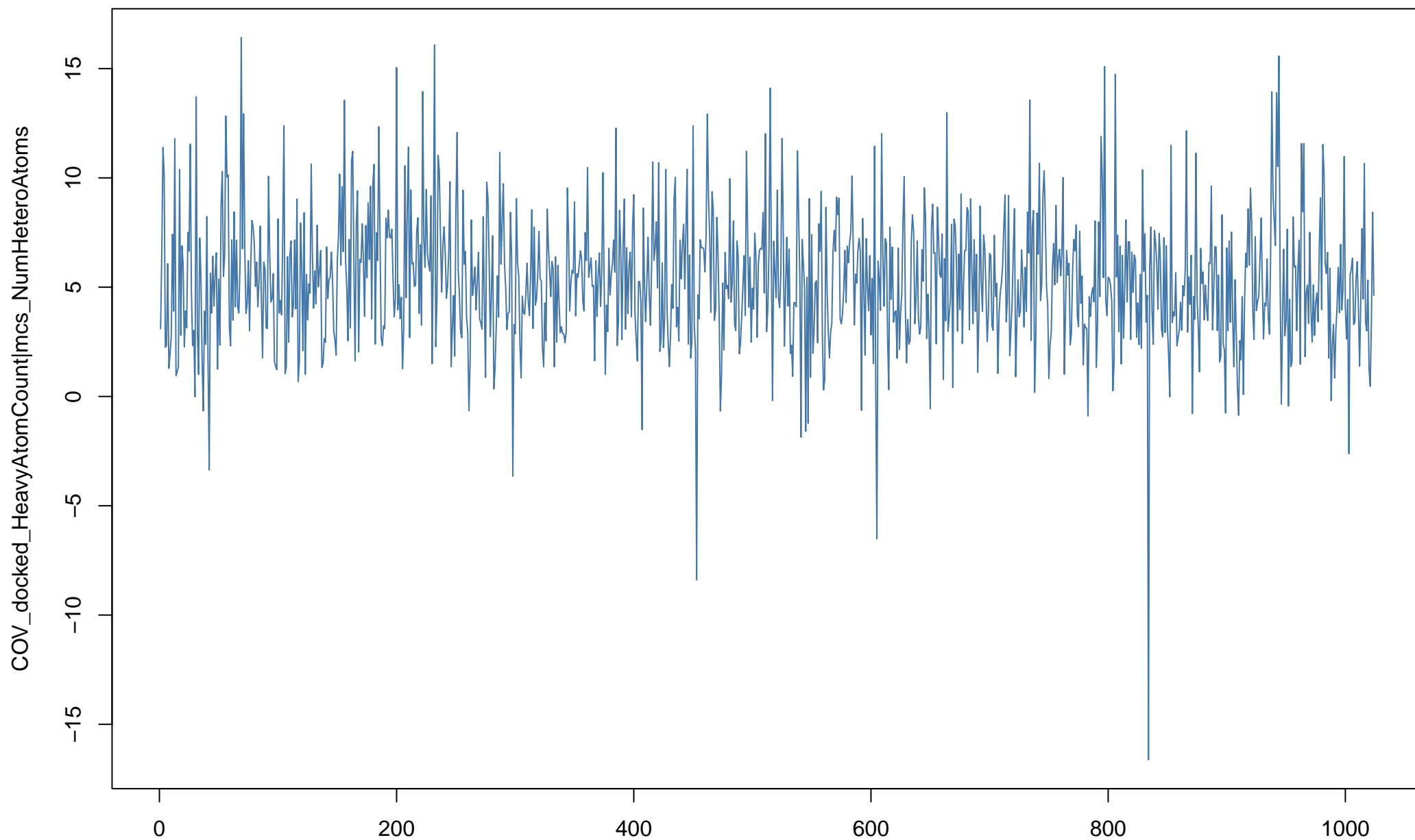
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 859 | BMK = 0.0795 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0



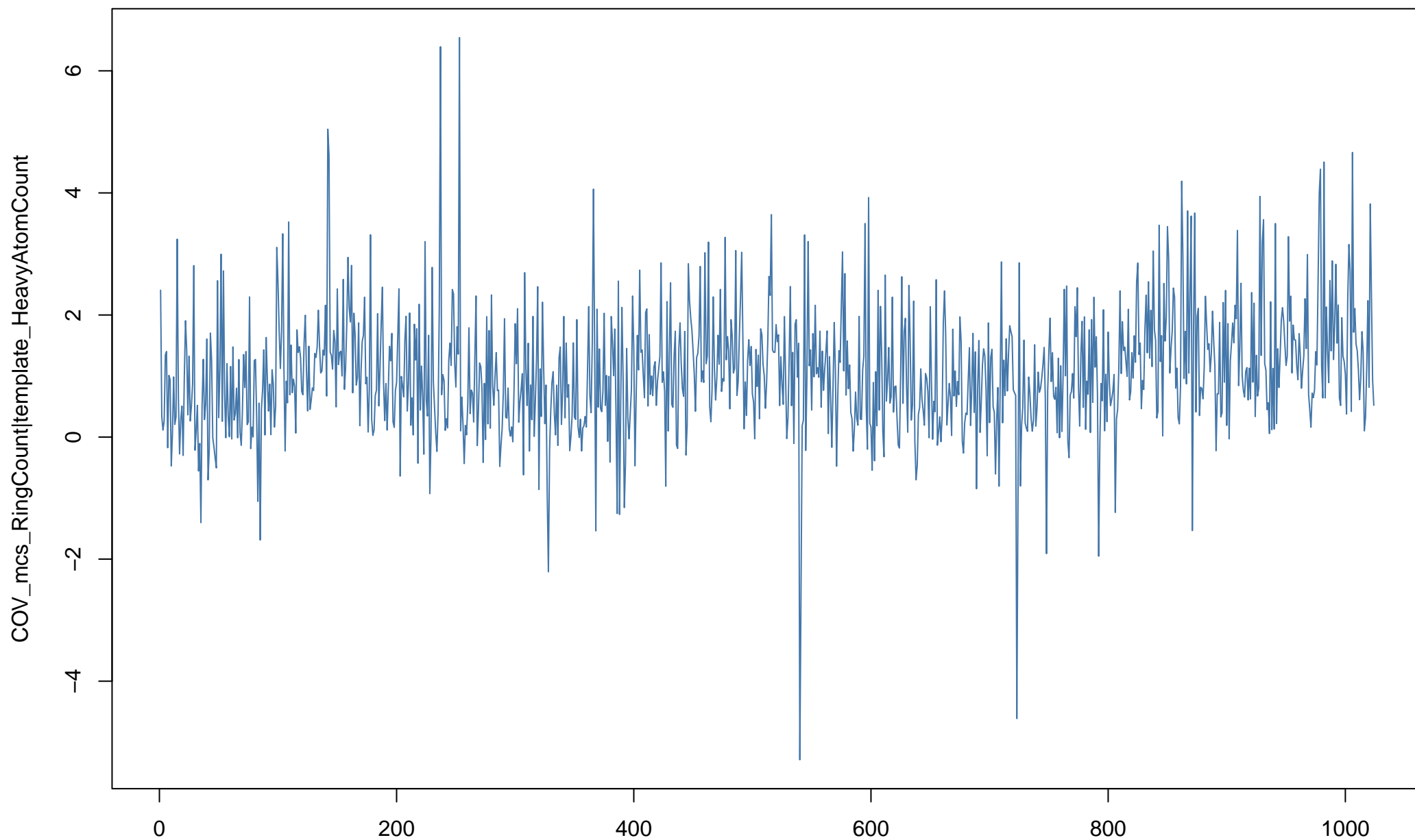
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 769 | BMK = 0.0571 | MCSE(6.27) = 3.41 | stat: TRUE | burn: 0



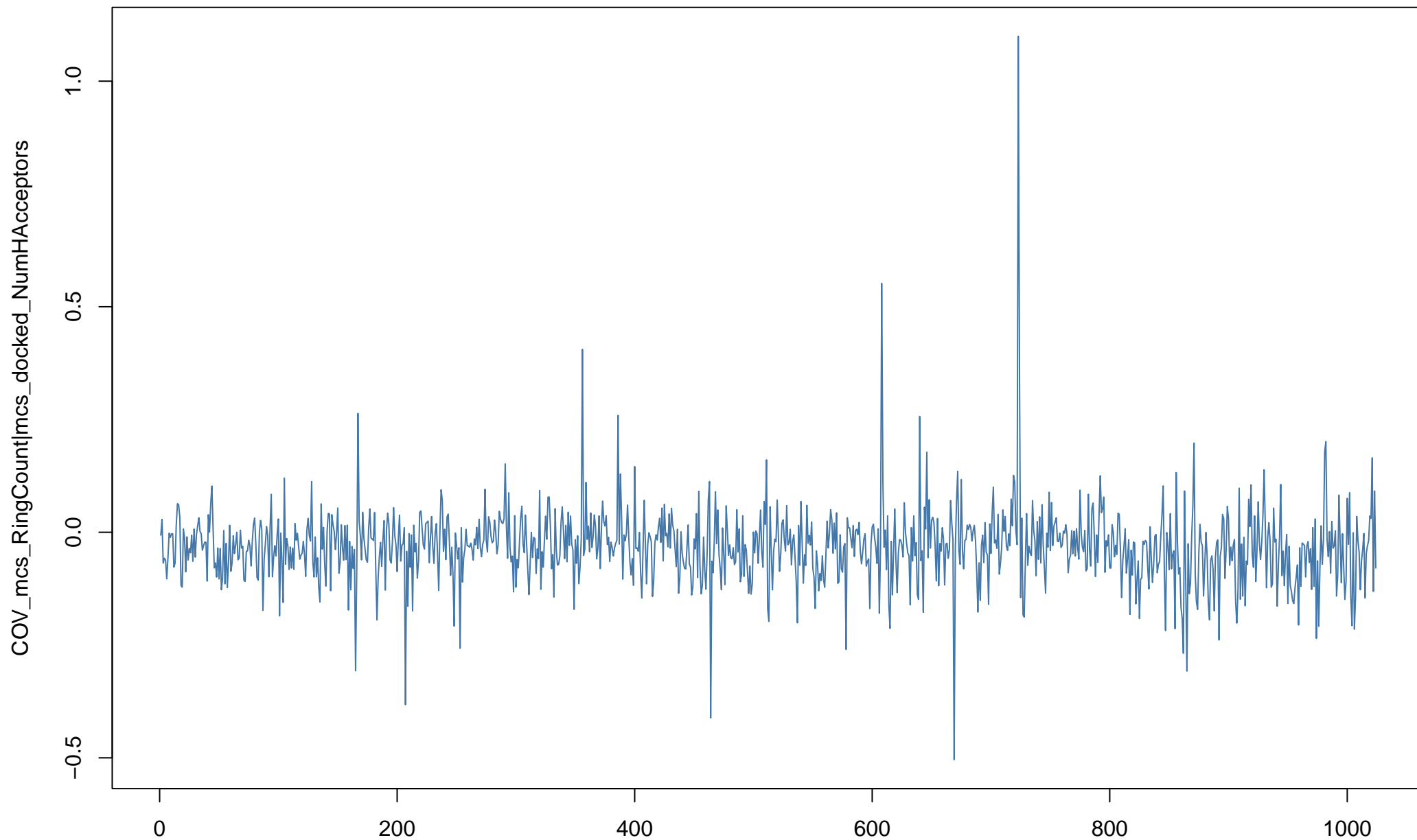
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 889 | BMK = 0.0848 | MCSE(6.27) = 3.38 | stat: TRUE | burn: 0



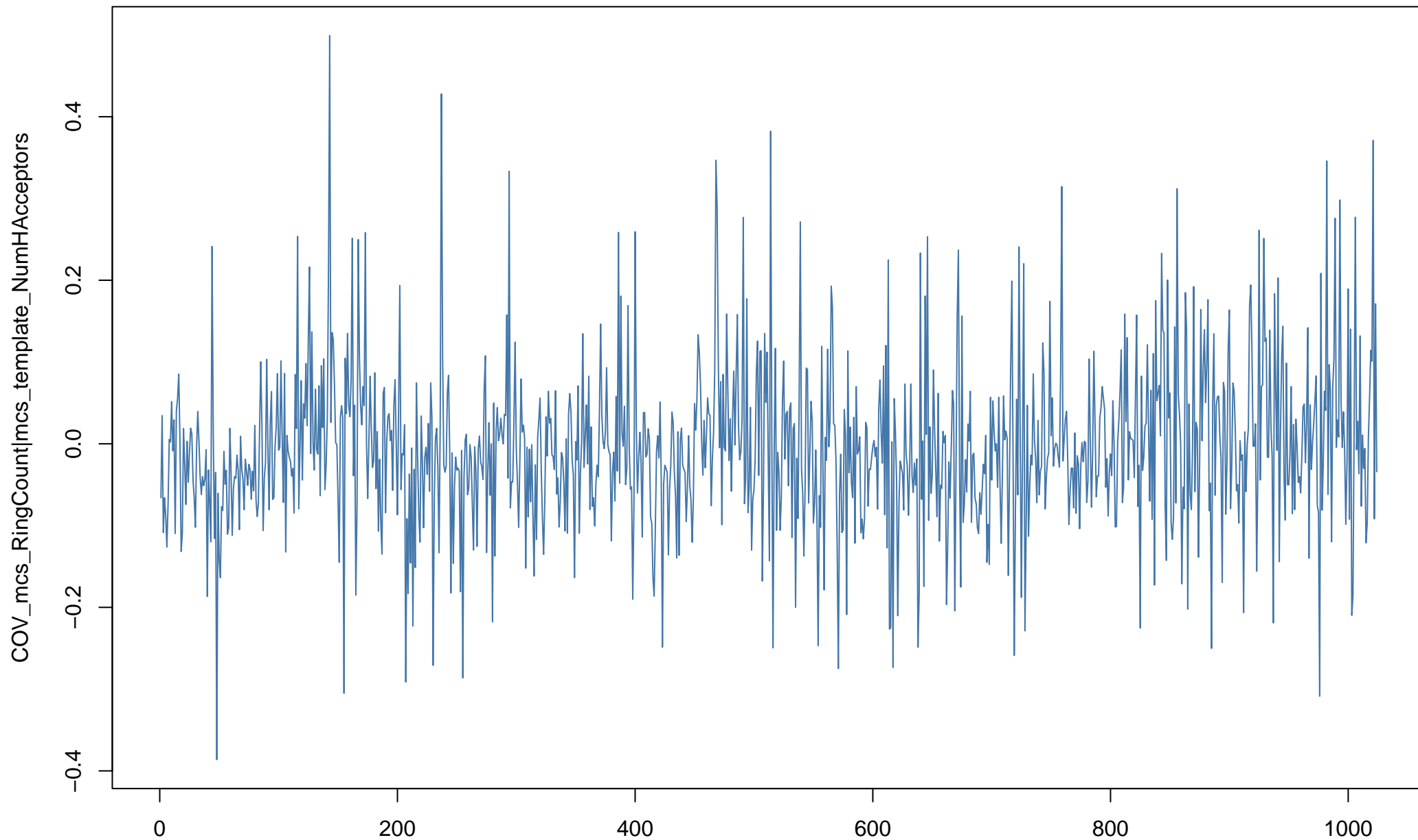
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 173 | BMK = 0.11 | MCSE(6.27) = 5.92 | stat: FALSE | burn: 0



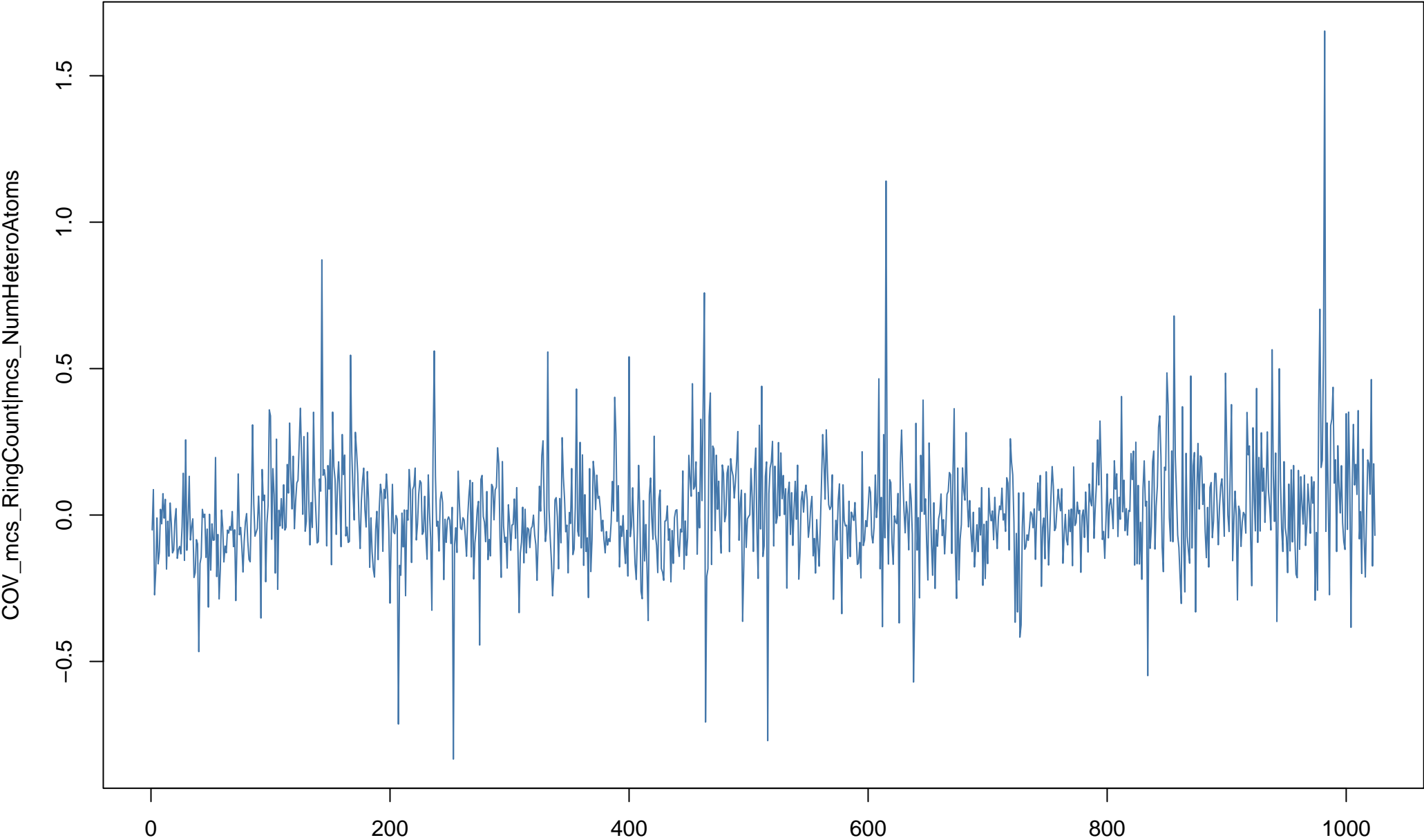
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 789 | BMK = 0.136 | MCSE(6.27) = 3.88 | stat: TRUE | burn: 0



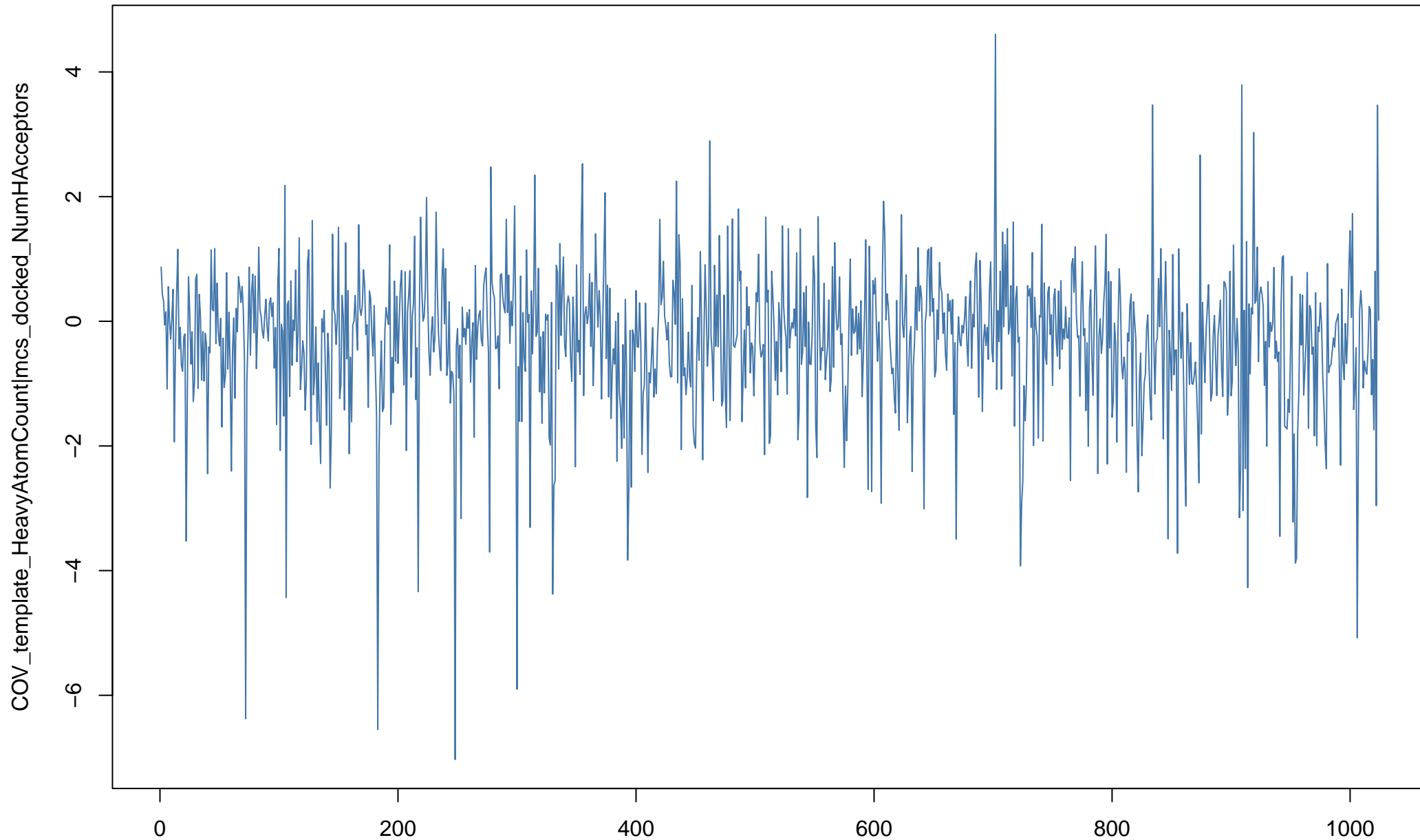
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 575 | BMK = 0.112 | MCSE(6.27) = 4.93 | stat: FALSE | burn: 0



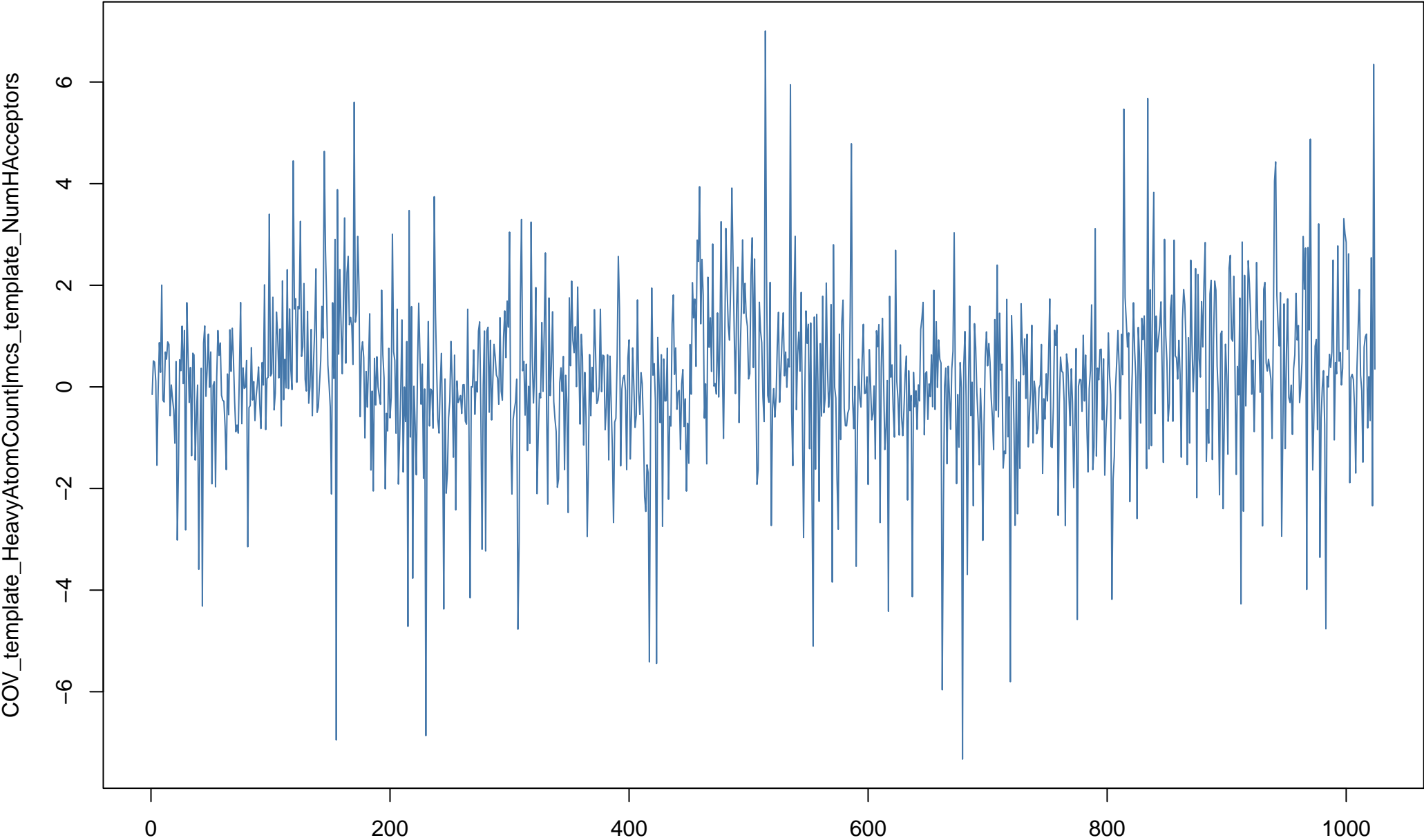
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 312 | BMK = 0.106 | MCSE(6.27) = 5.33 | stat: FALSE | burn: 0



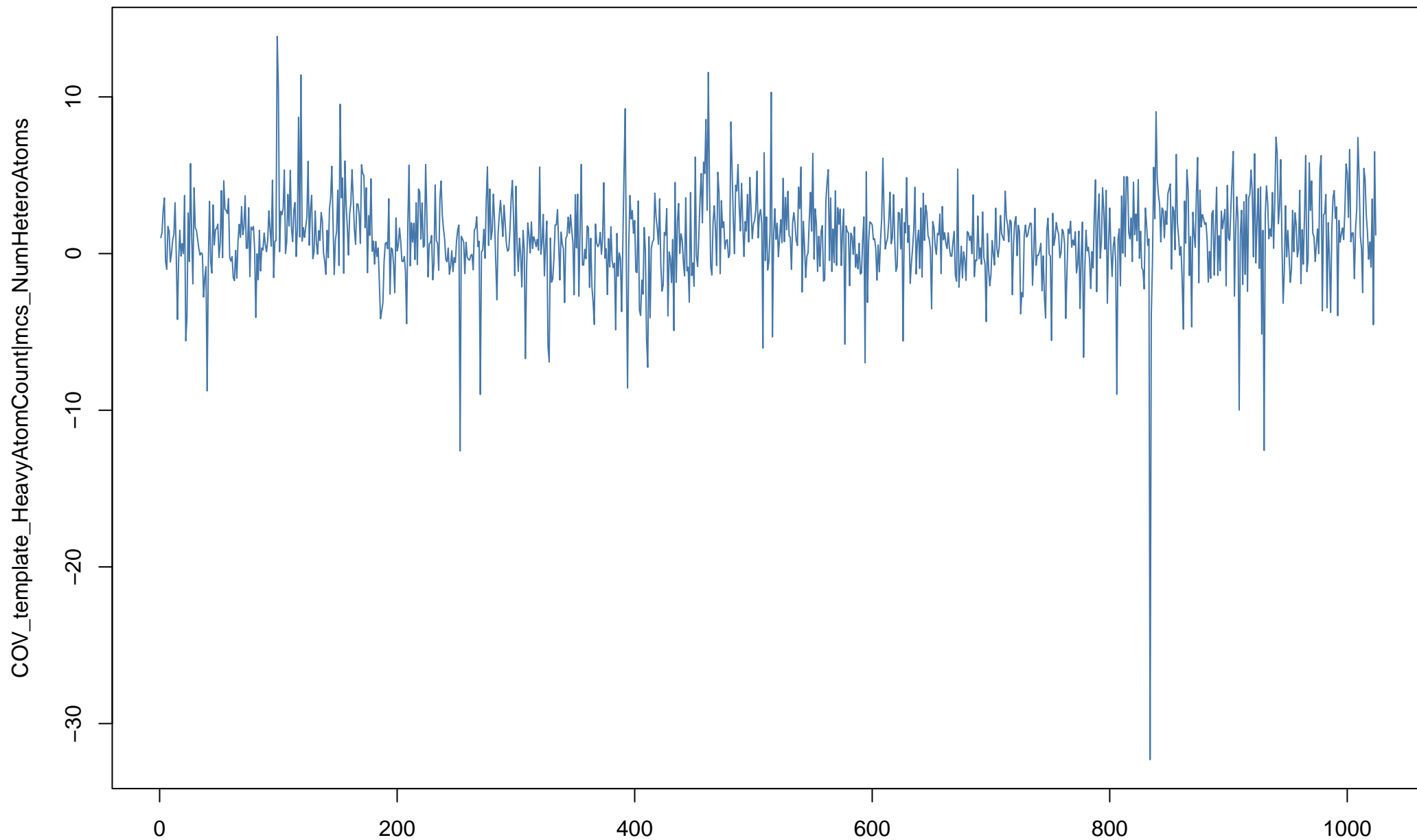
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 854 | BMK = 0.11 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0



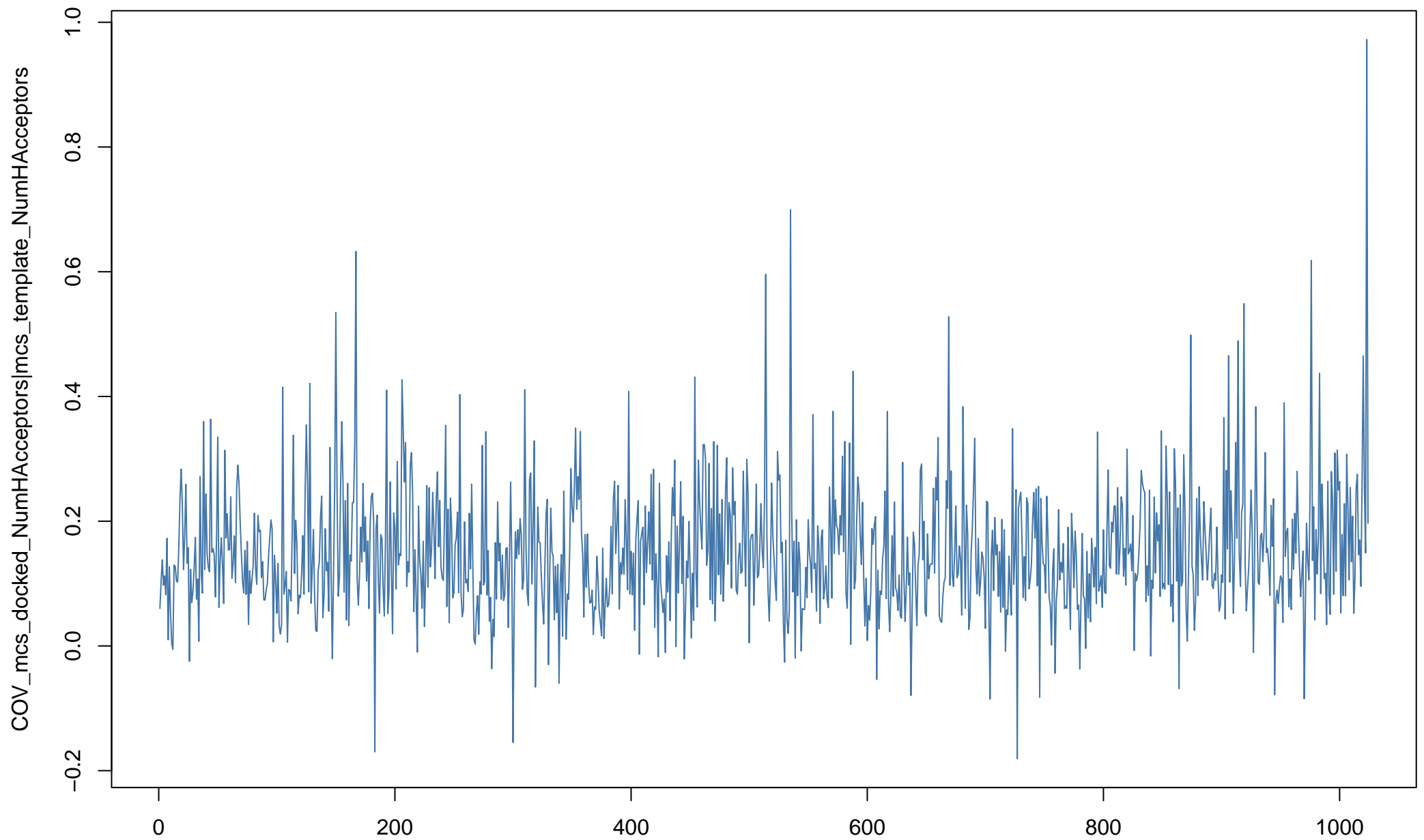
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 509 | BMK = 0.0749 | MCSE(6.27) = 5.65 | stat: TRUE | burn: 0



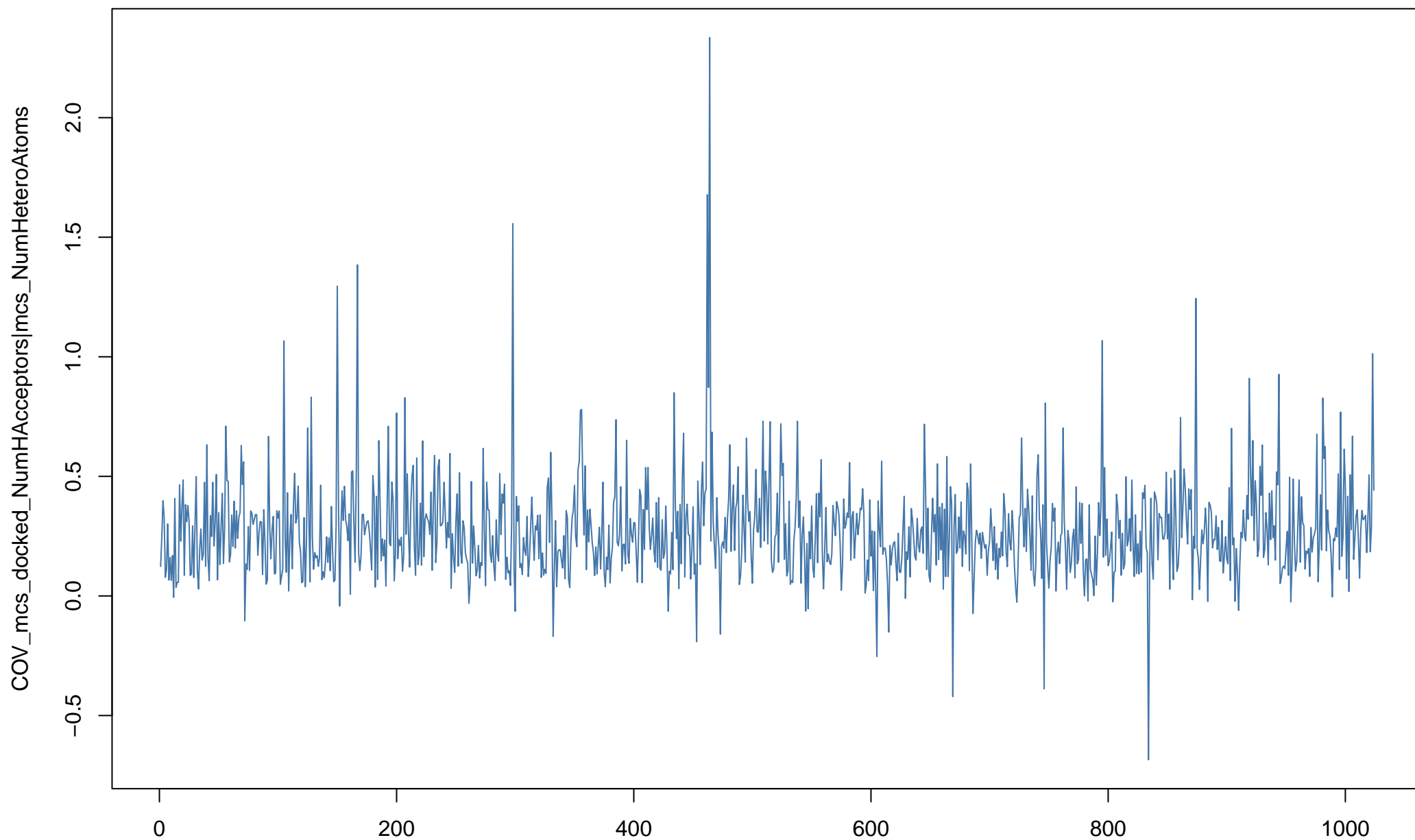
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 554 | BMK = 0.088 | MCSE(6.27) = 4.93 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 913 | BMK = 0.0773 | MCSE(6.27) = 4.16 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 726 | BMK = 0.0991 | MCSE(6.27) = 3.69 | stat: TRUE | burn: 0



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 109 | BMK = 0.108 | MCSE(6.27) = 7.26 | stat: FALSE | burn: 0

