

-- STATS maxD --

min ESS = 42.7291007268077

max BMK = 1

max MCSE = 11.5307794684758

all stationary: FALSE

burn: 1020

-- STATS 2D --

min ESS = 68.3396660527278

max BMK = 0.154452428950239

max MCSE = 8.26770604869434

all stationary: FALSE

burn: 102

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.711340484520845

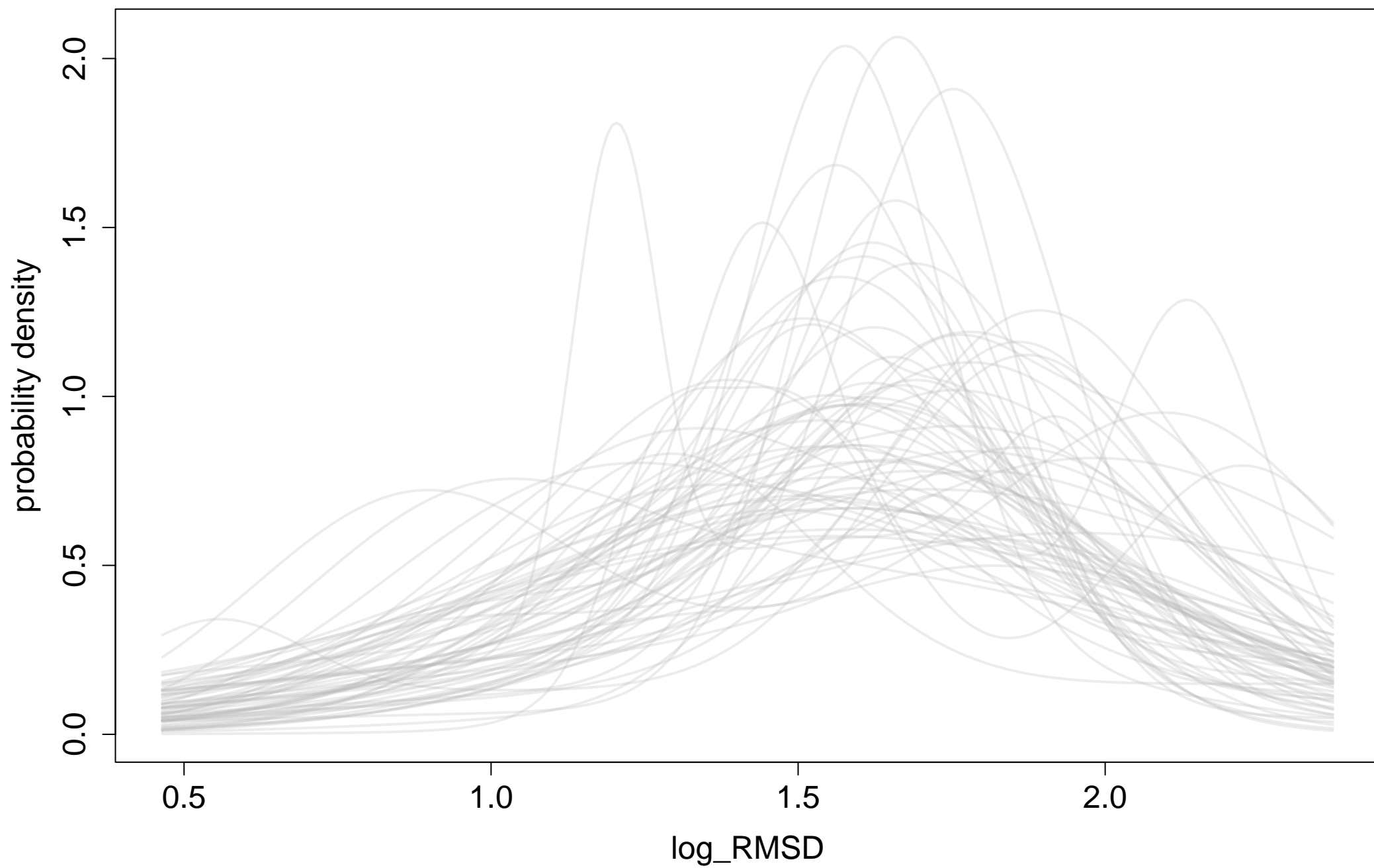
max MCSE = NaN

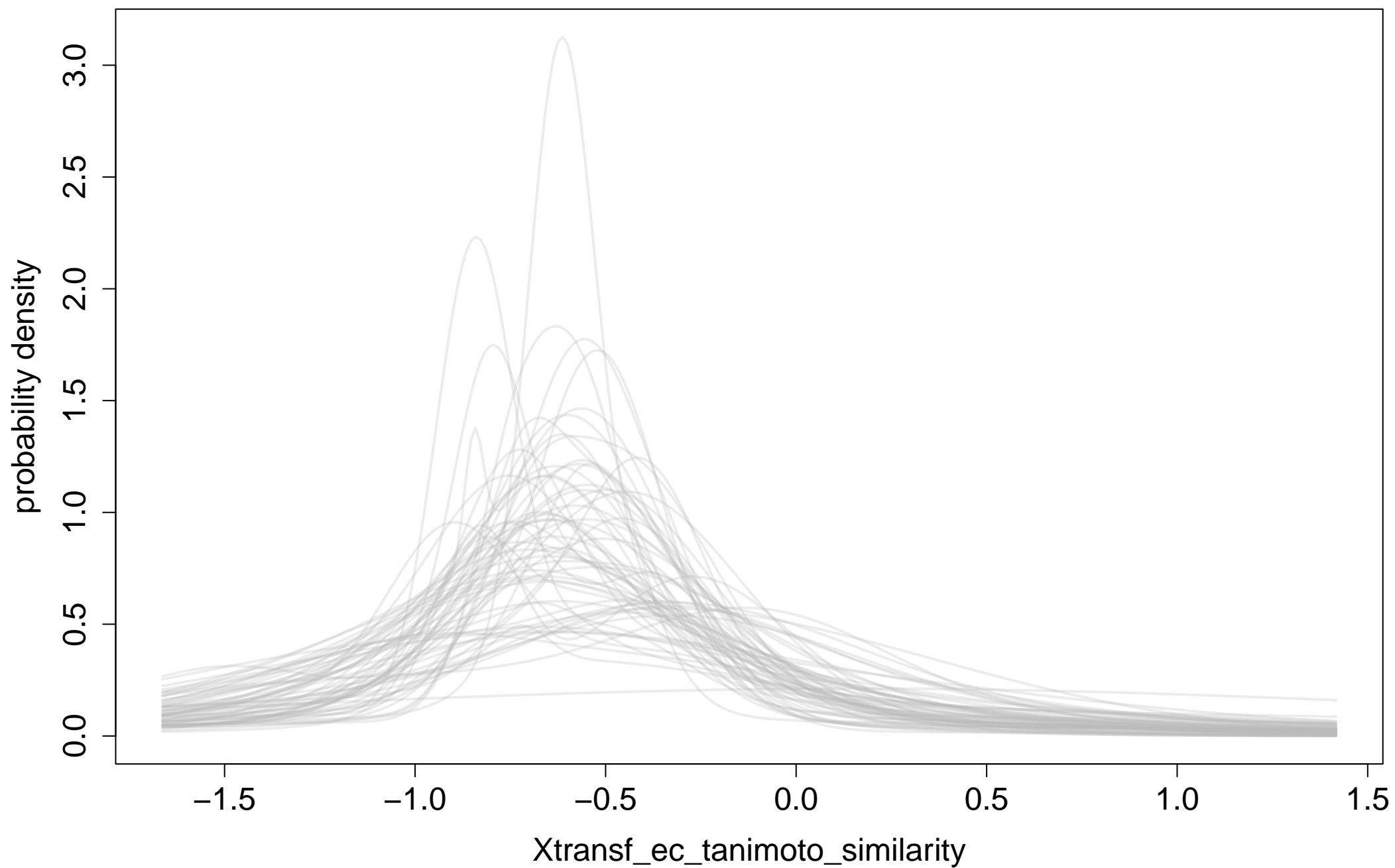
all stationary: FALSE

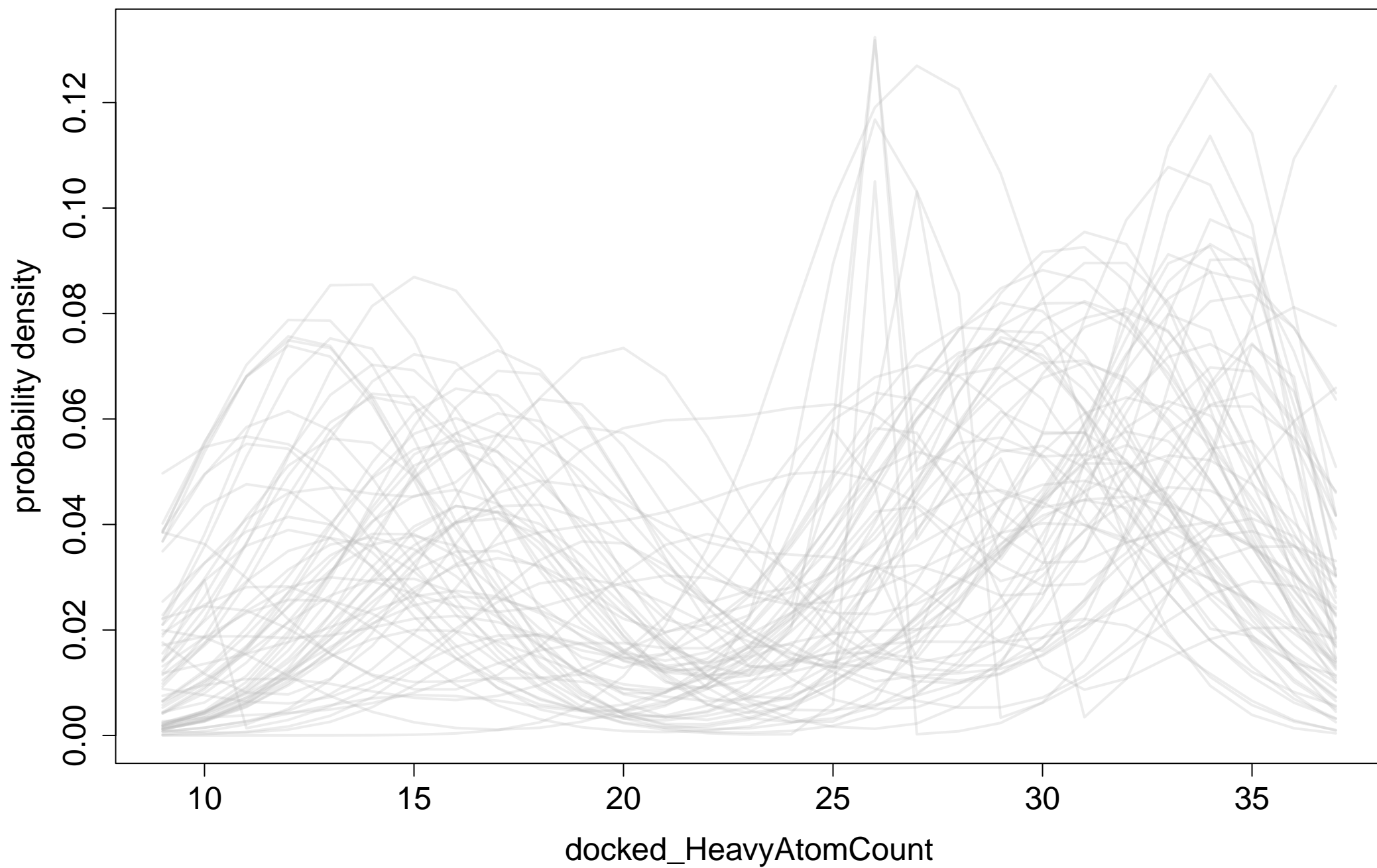
burn: 1020

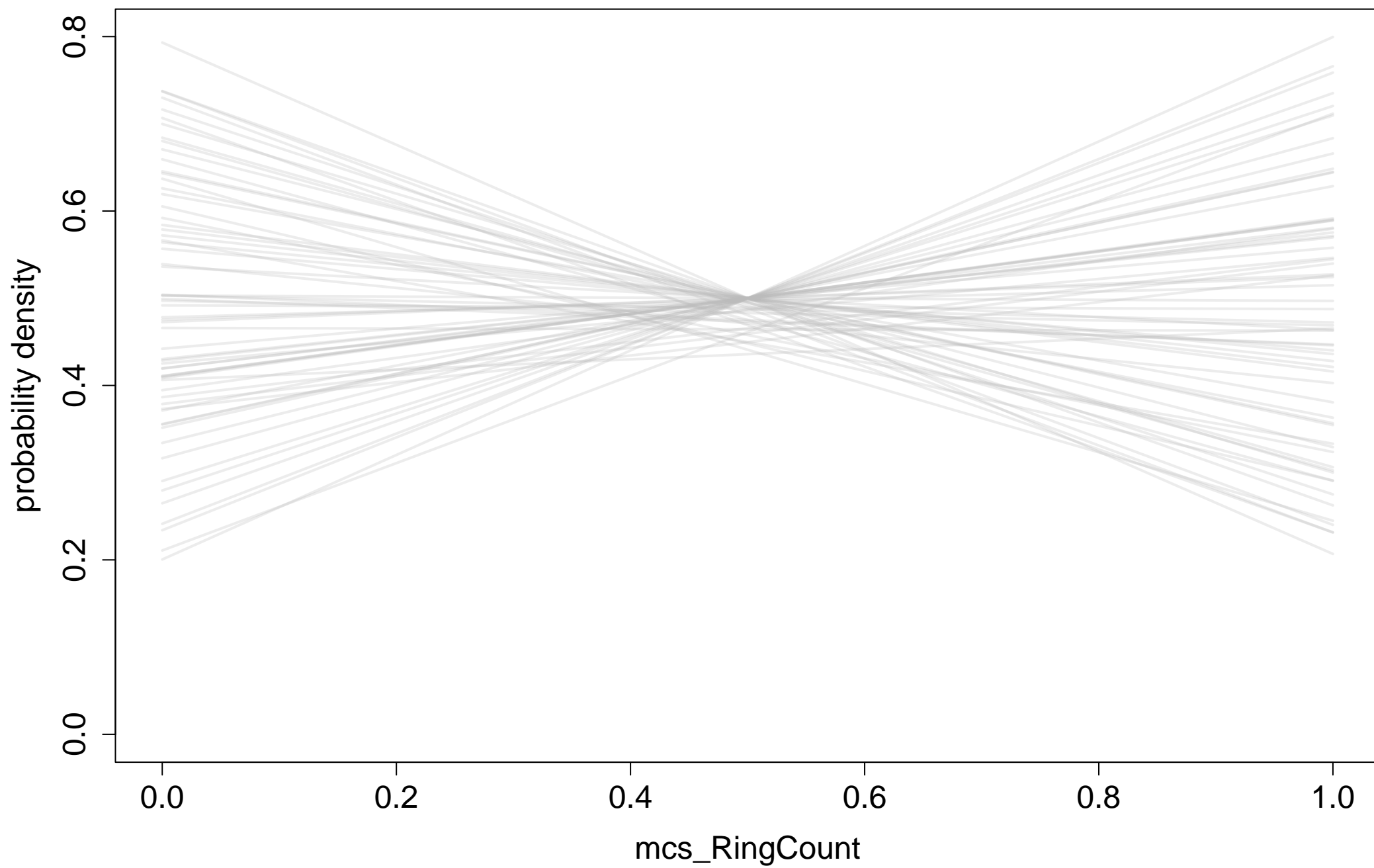
Occupied clusters: 3 of 4

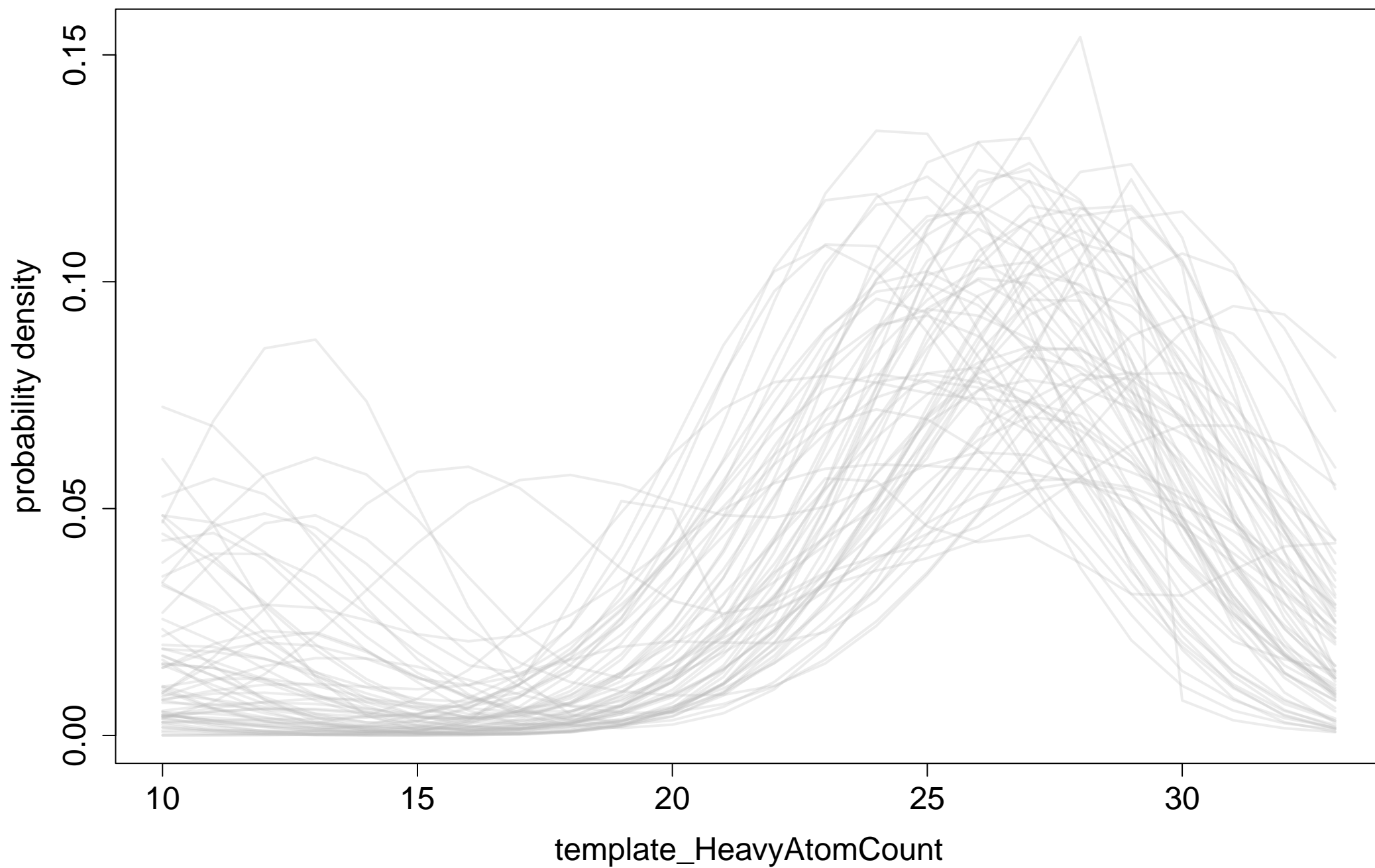
LL: -92.4 +- 5.41

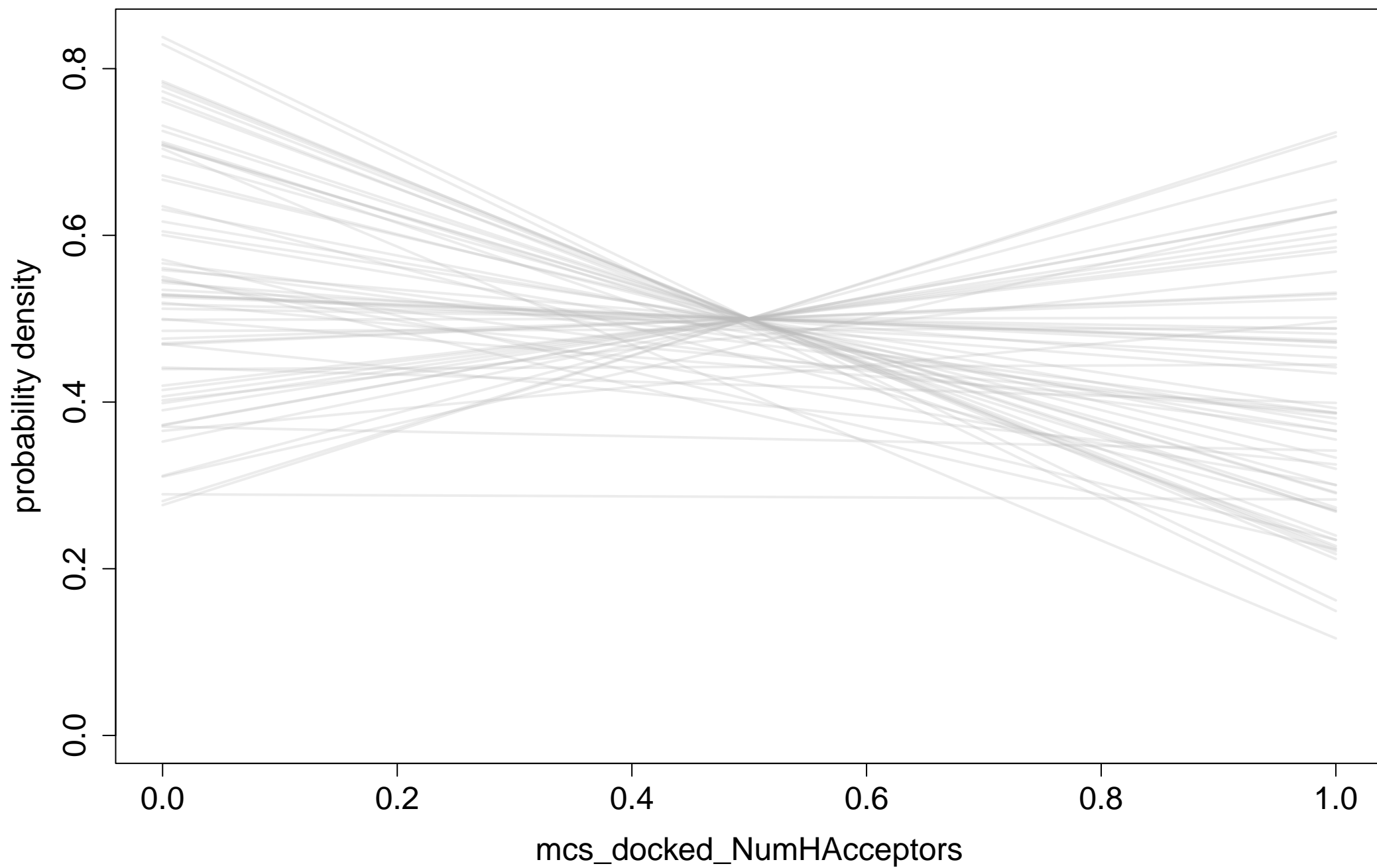


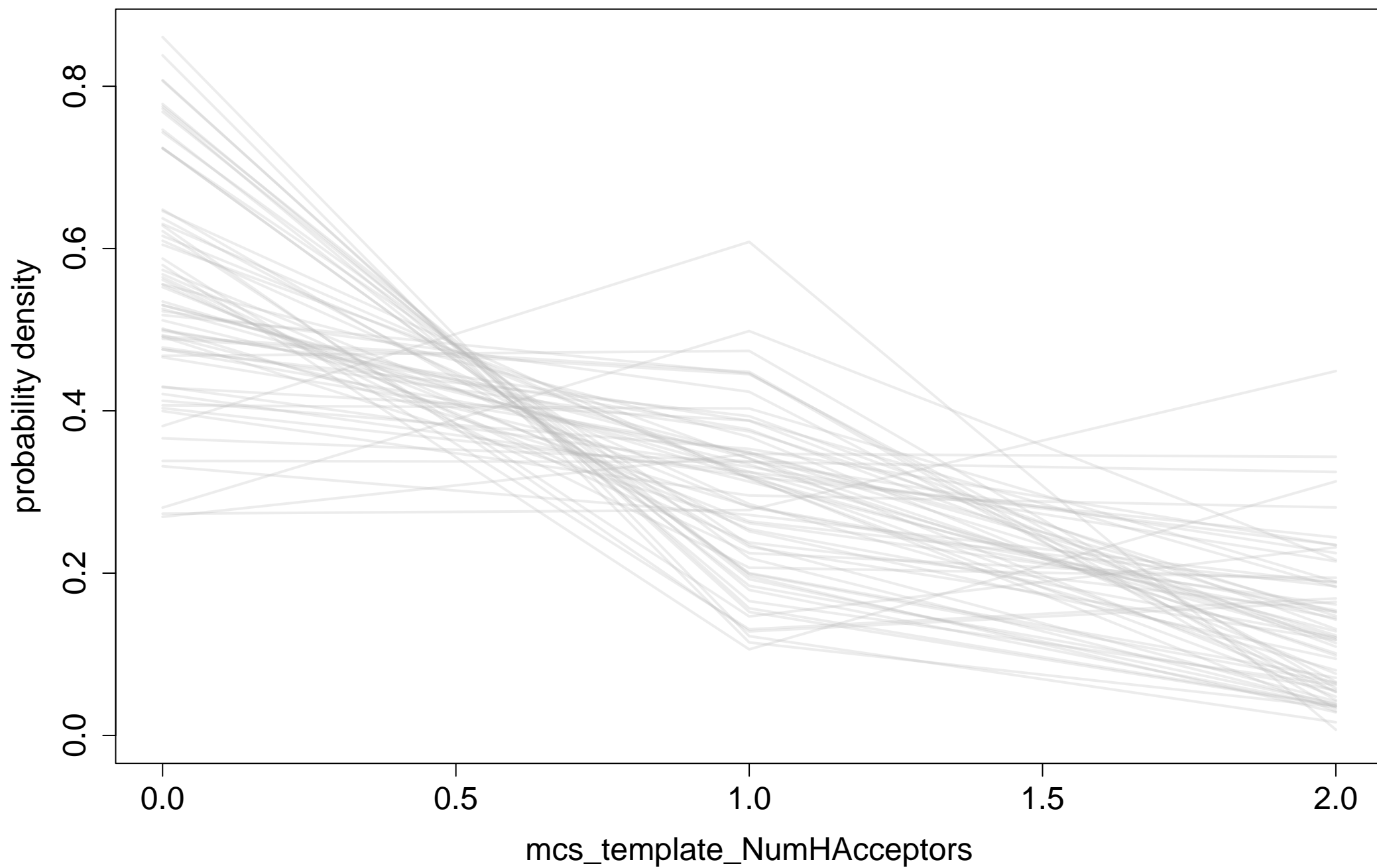


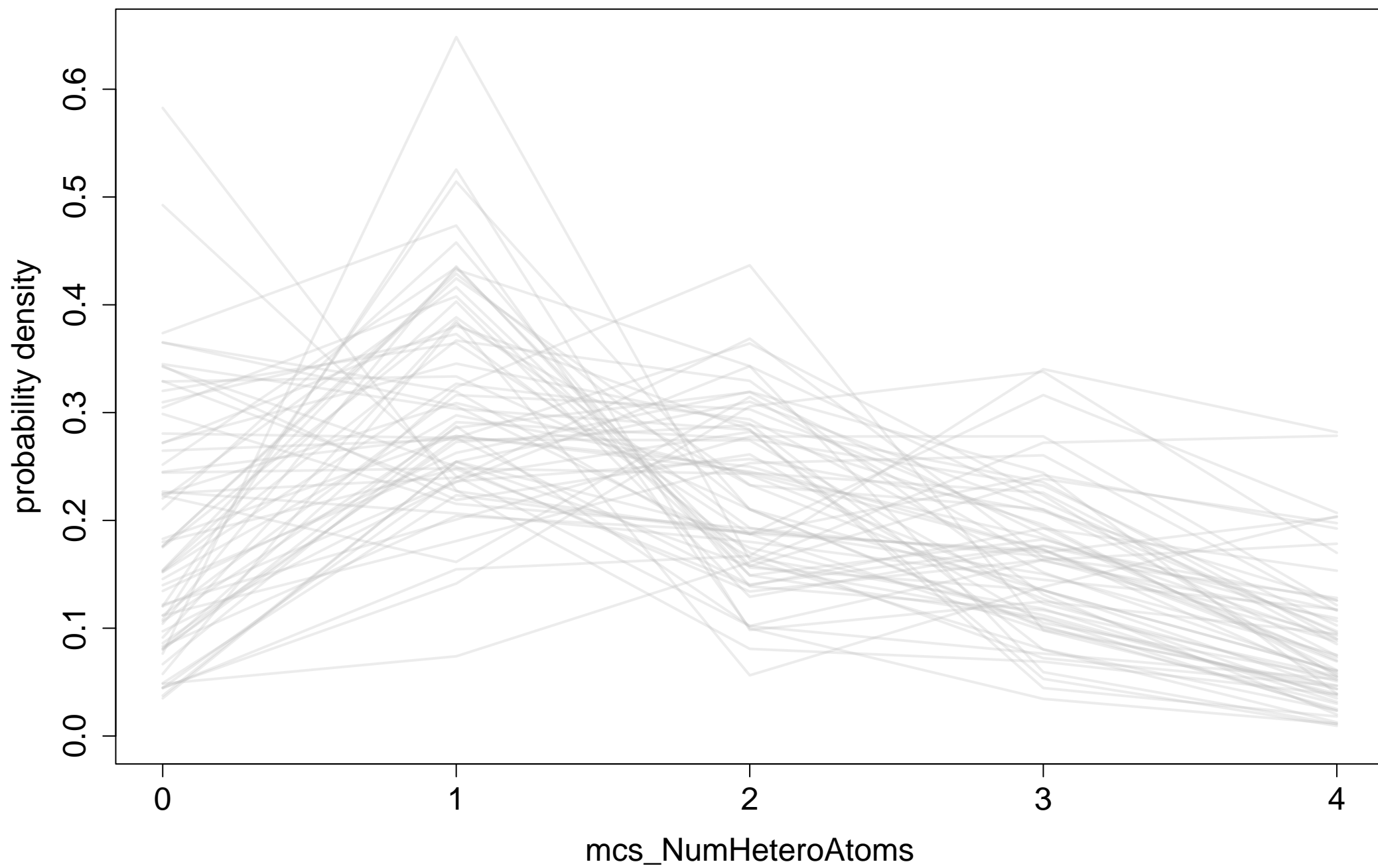


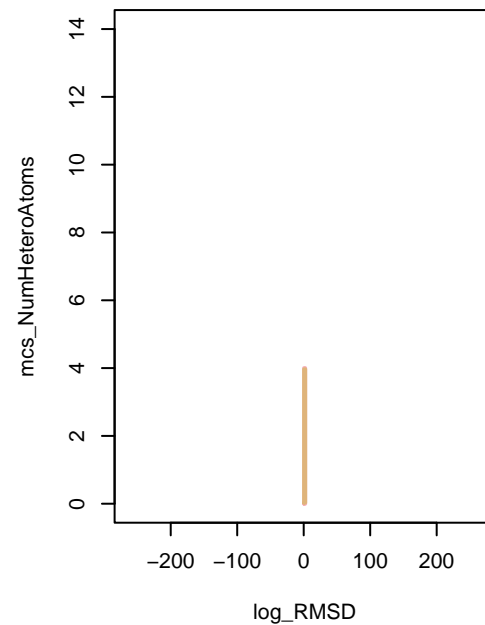
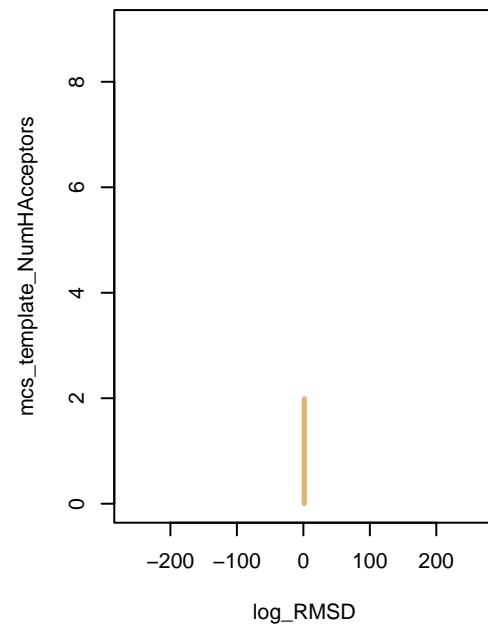
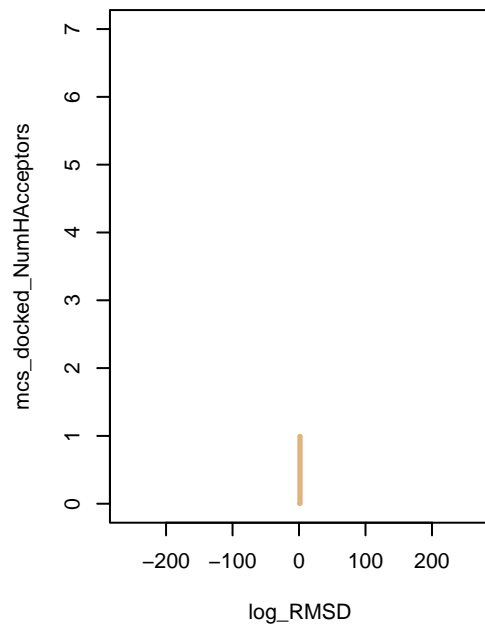
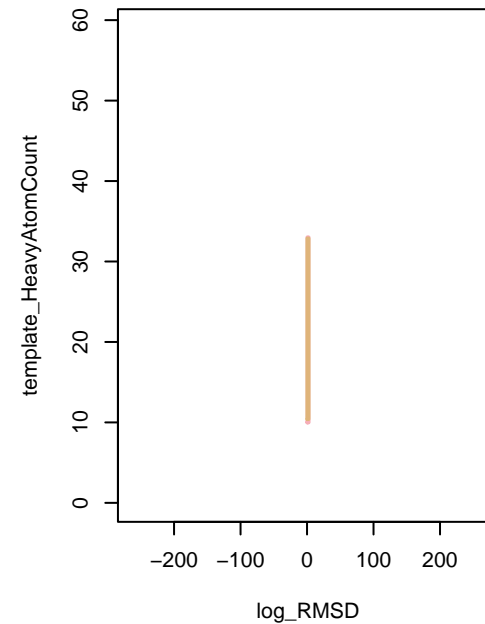
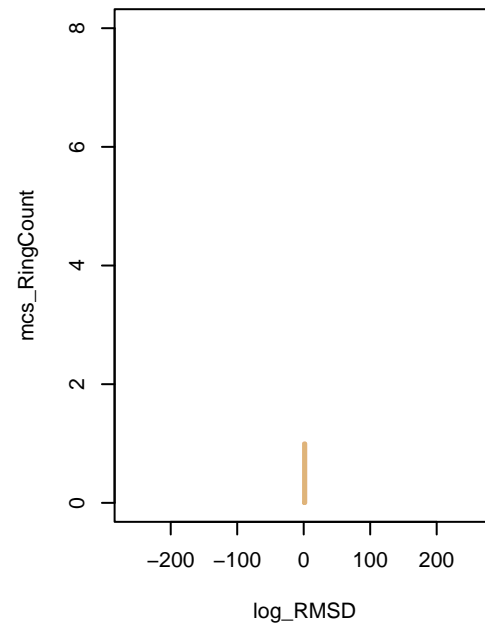
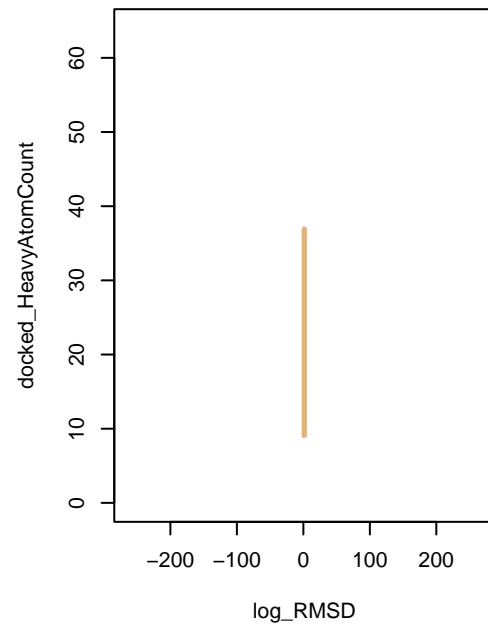
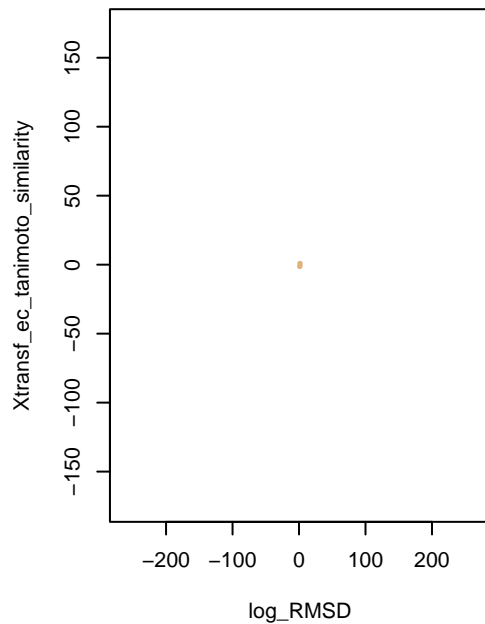




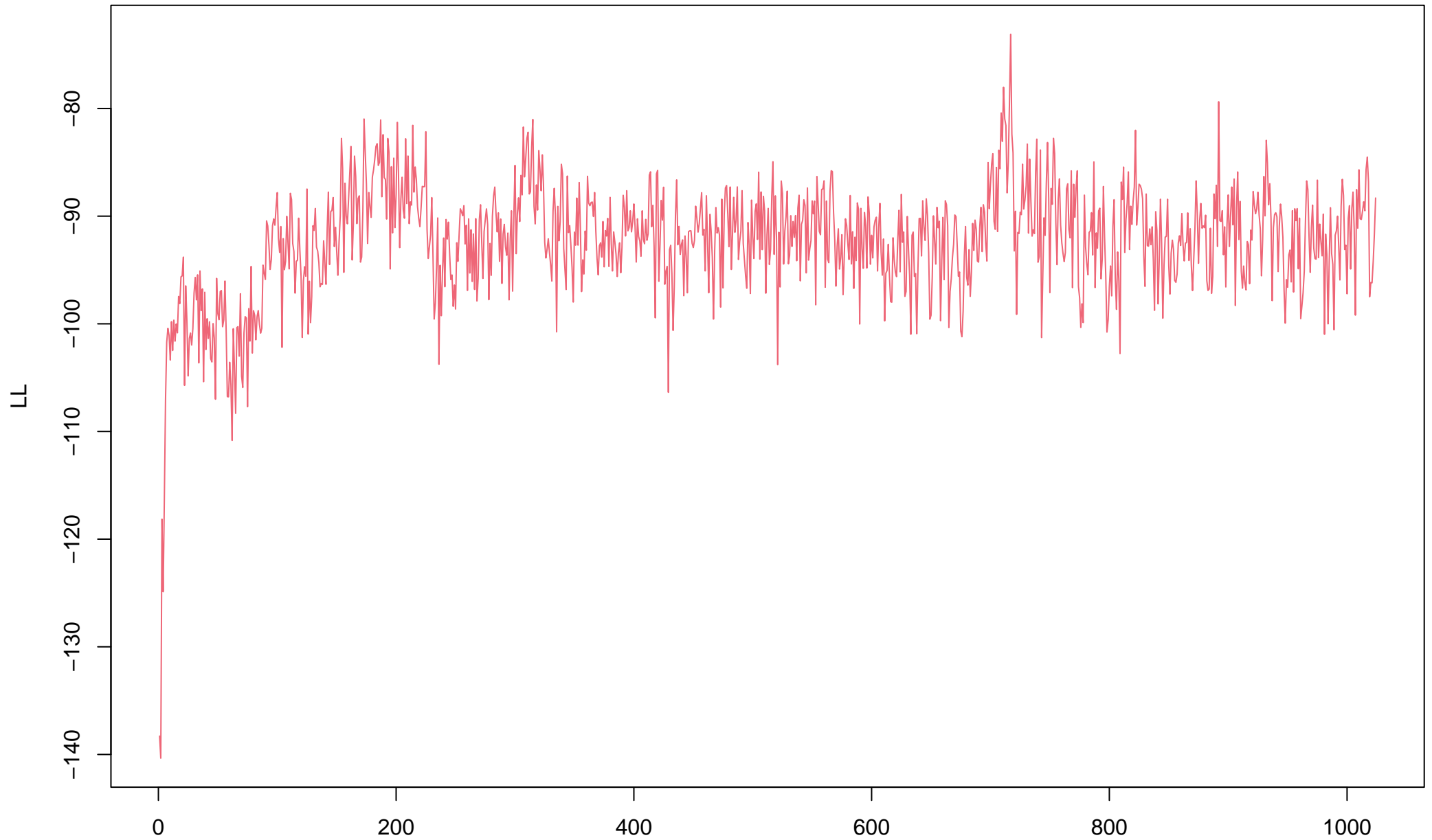




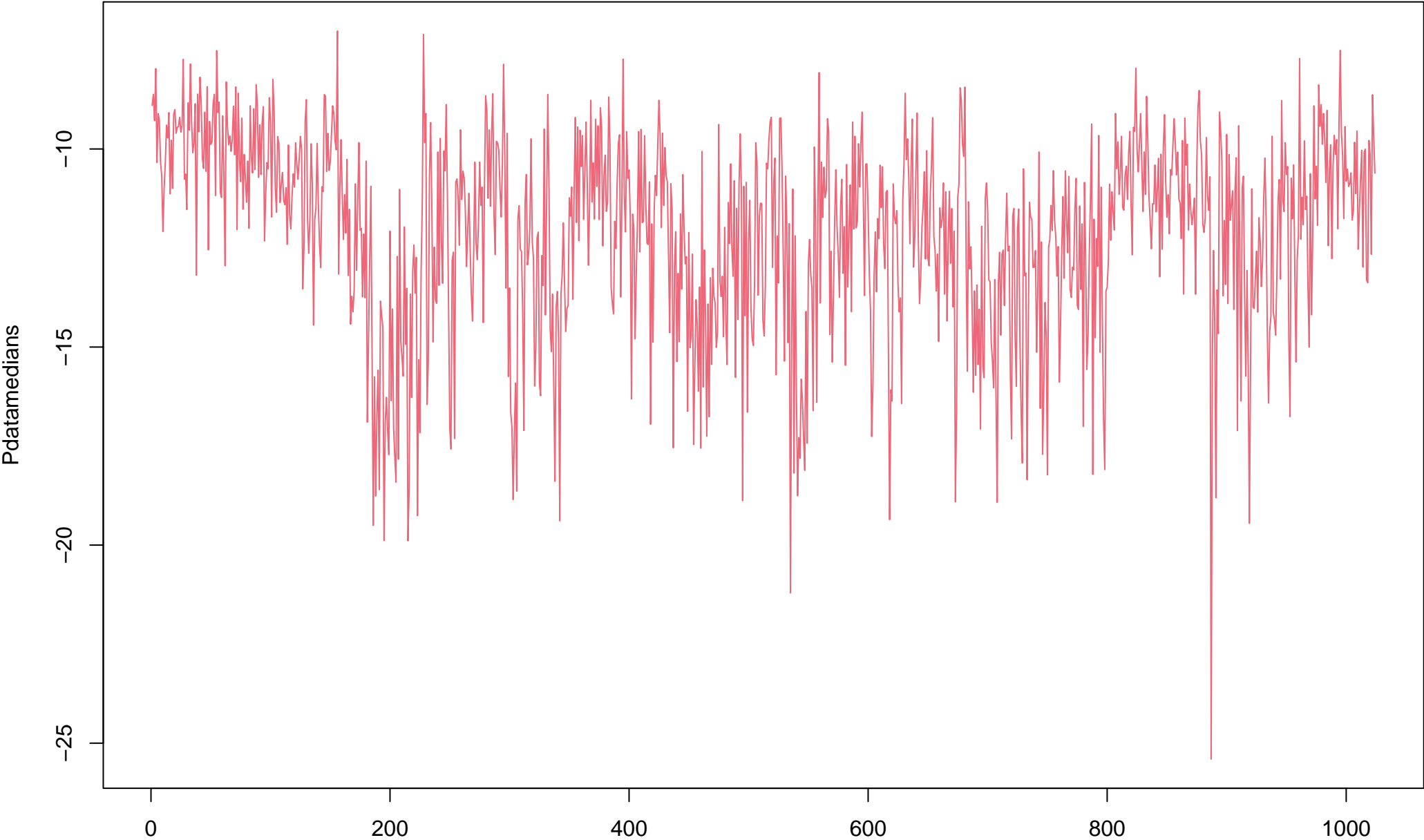




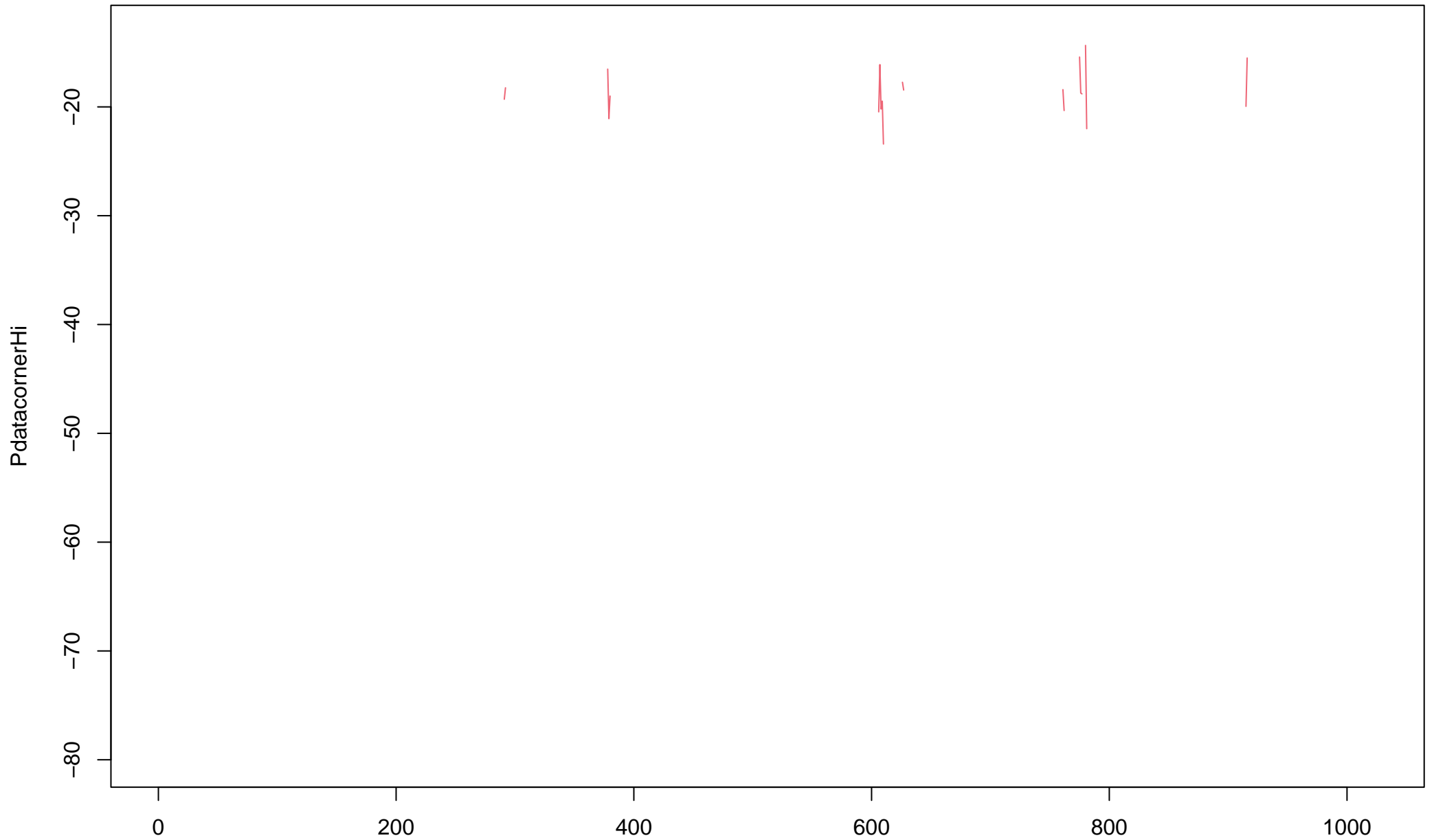
LL
ESS = 42.7 | BMK = 0.166 | MCSE(6.27) = 11.5 | stat: FALSE | burn: 102



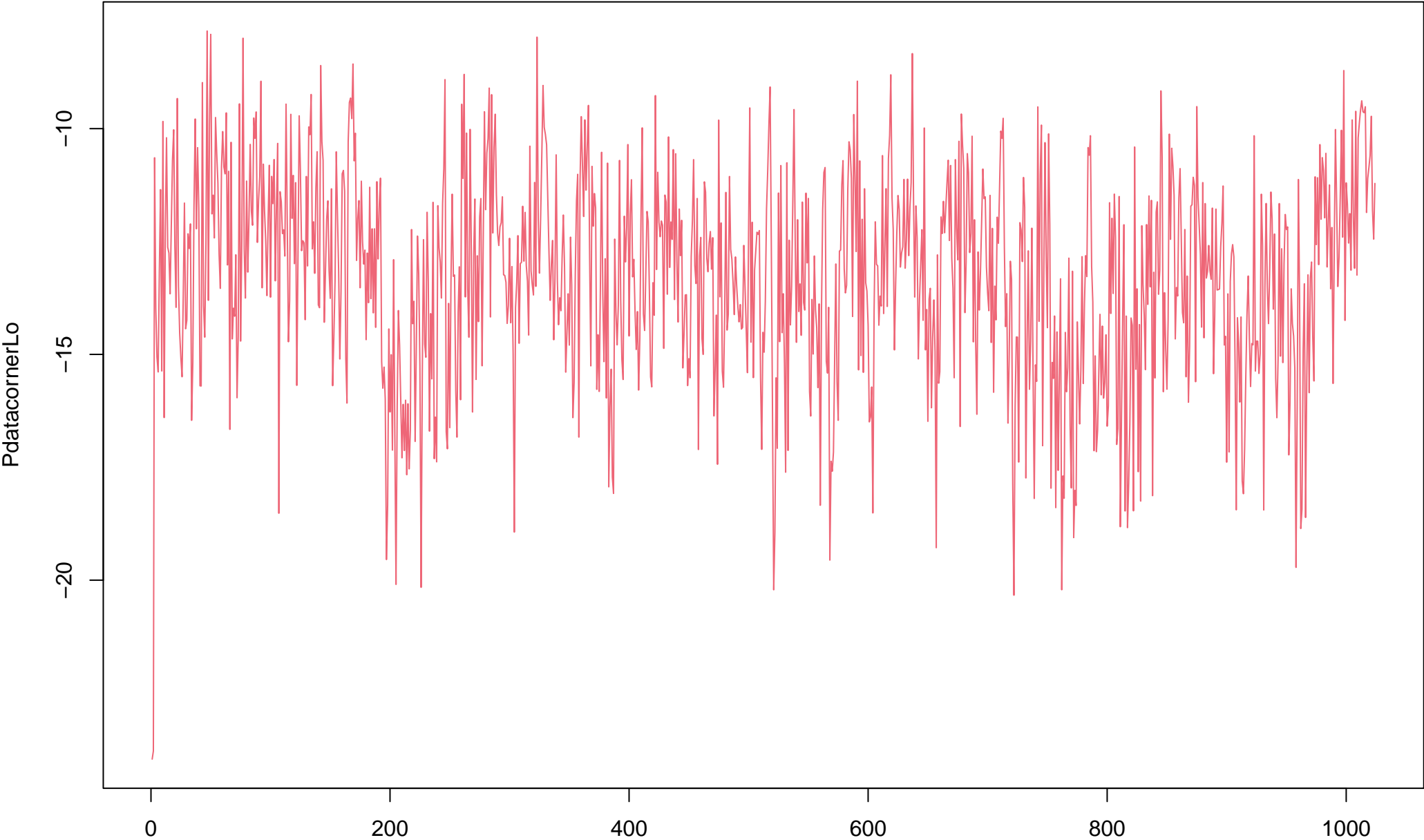
Pdatamedians
ESS = 121 | BMK = 0.156 | MCSE(6.27) = 6.84 | stat: FALSE | burn: 0



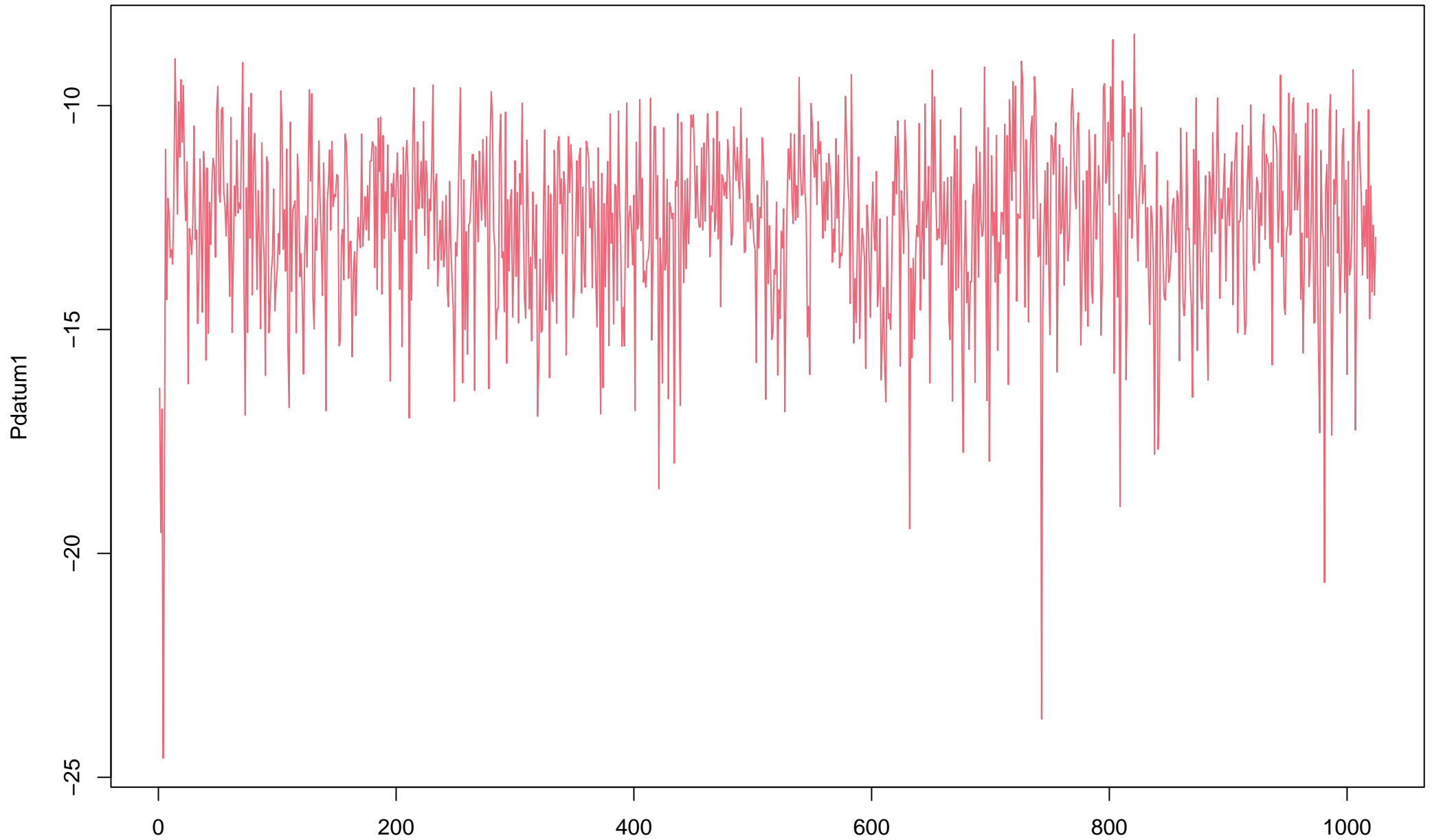
PdatacornerHi
ESS = 1020 | BMK = 0.395 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 1020



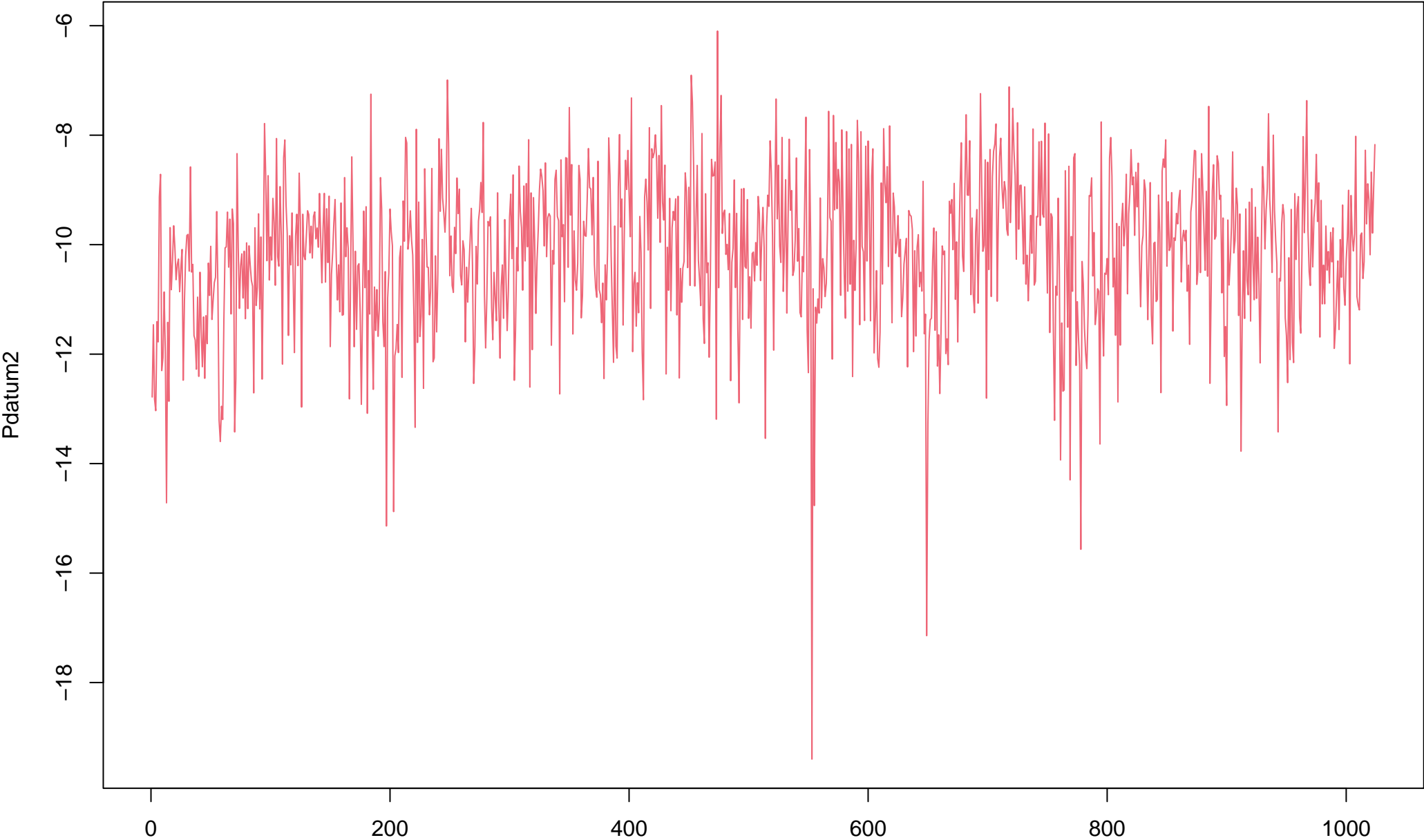
PdatacornerLo
ESS = 439 | BMK = 0.152 | MCSE(6.27) = 5.44 | stat: FALSE | burn: 0



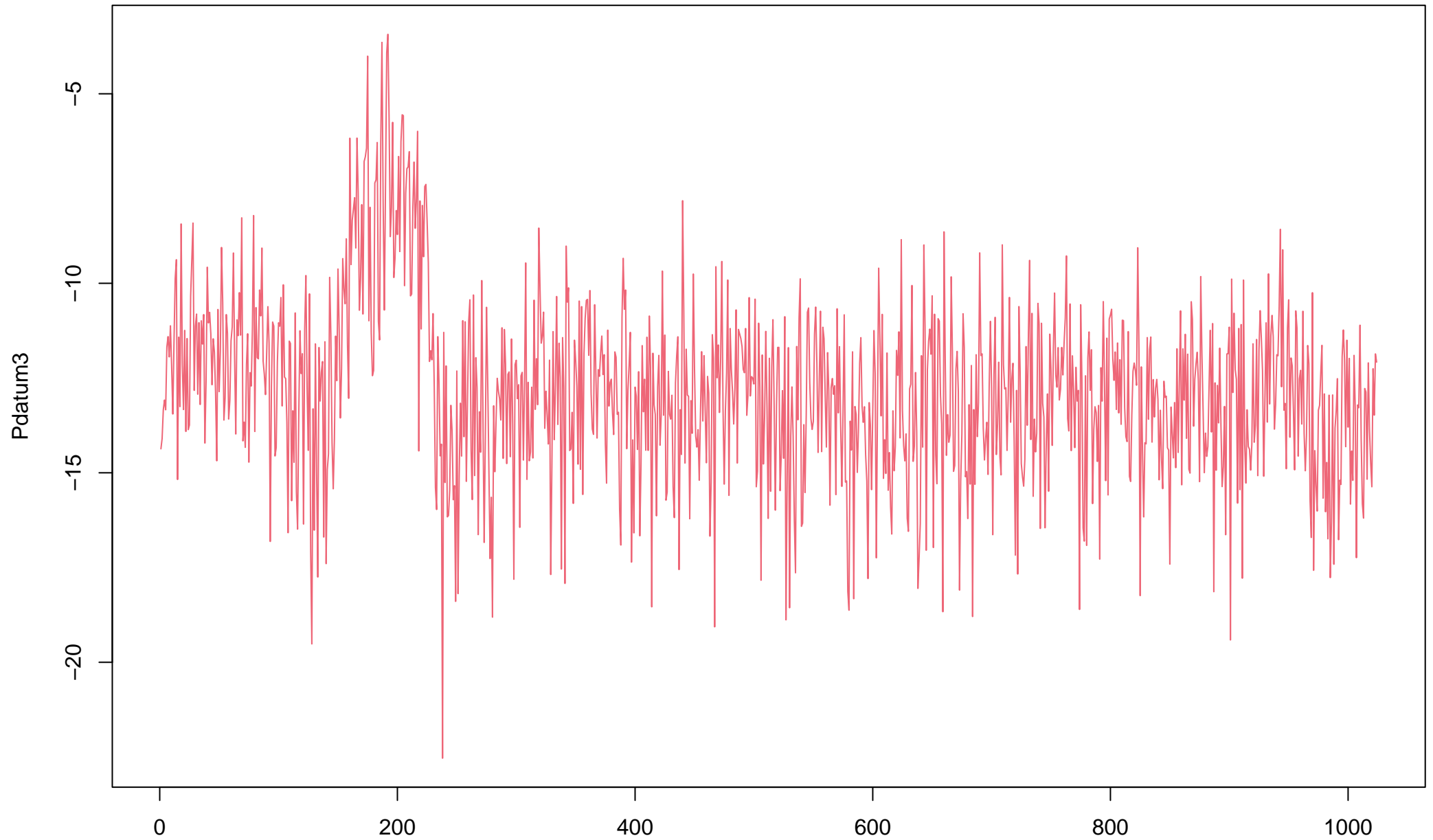
Pdatum1
ESS = 481 | BMK = 0.131 | MCSE(6.27) = 4.25 | stat: TRUE | burn: 0



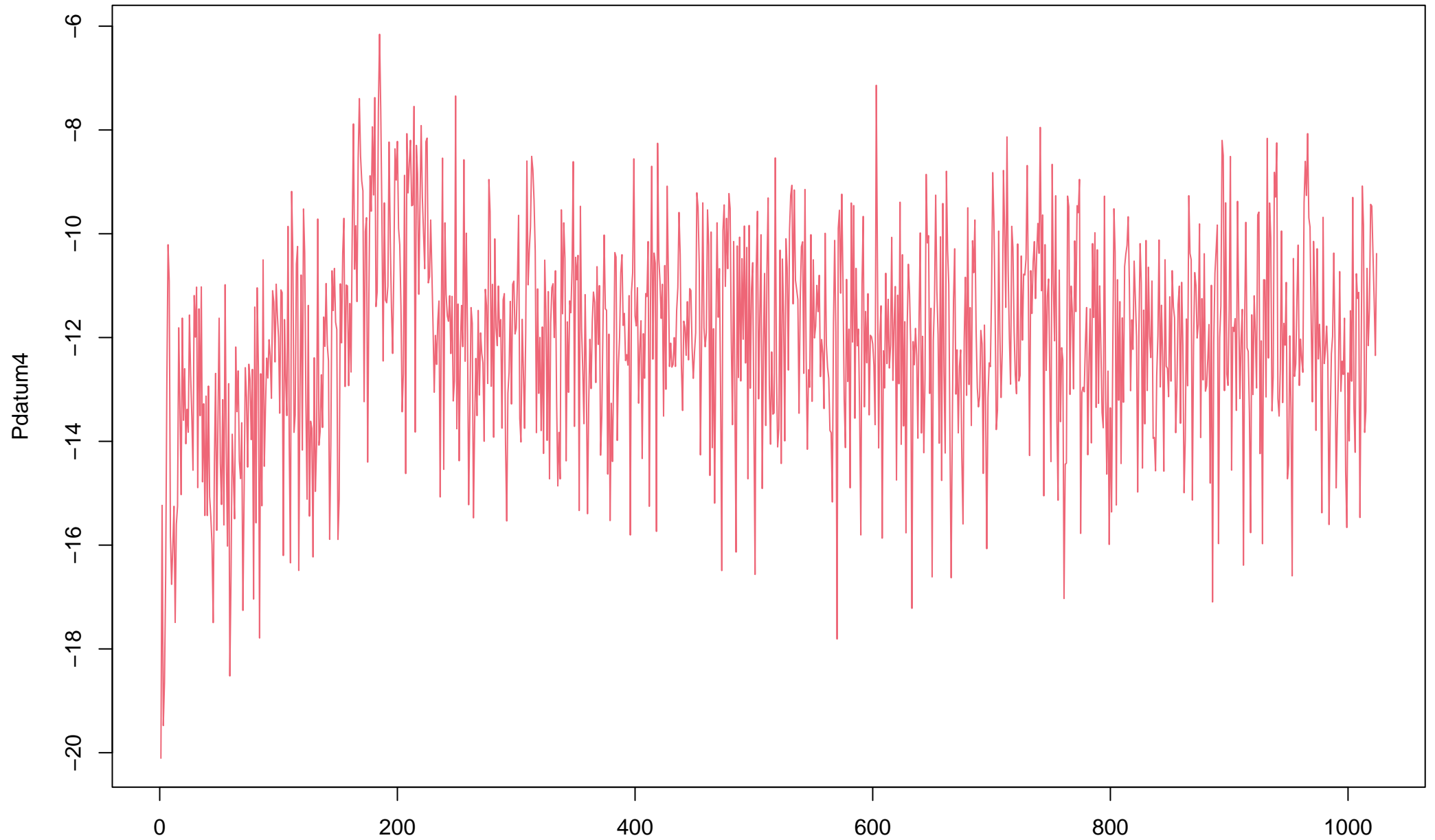
Pdatum2
ESS = 222 | BMK = 0.131 | MCSE(6.27) = 5.34 | stat: FALSE | burn: 0



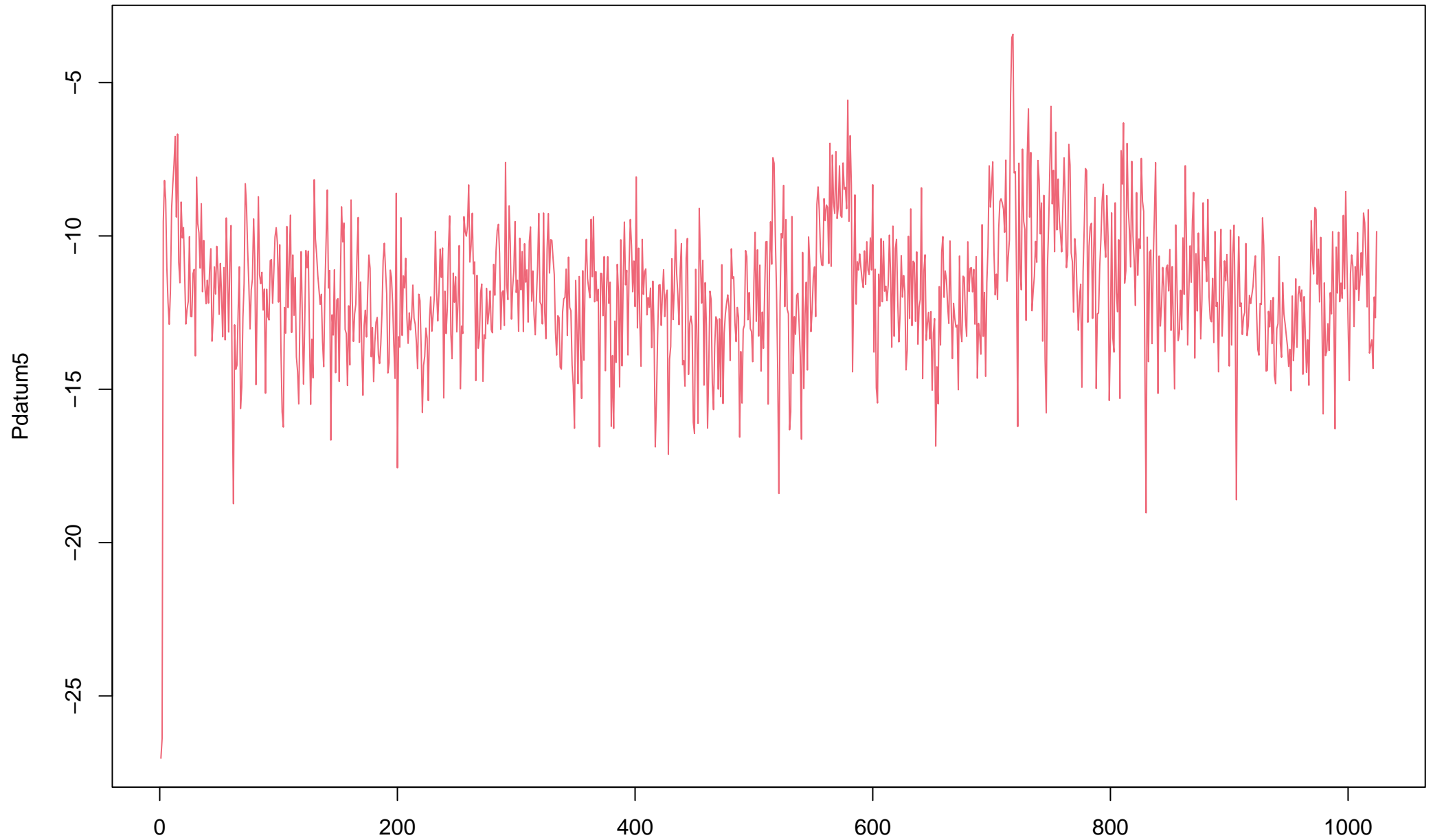
Pdatum3
ESS = 127 | BMK = 1 | MCSE(6.27) = 7.06 | stat: FALSE | burn: 204



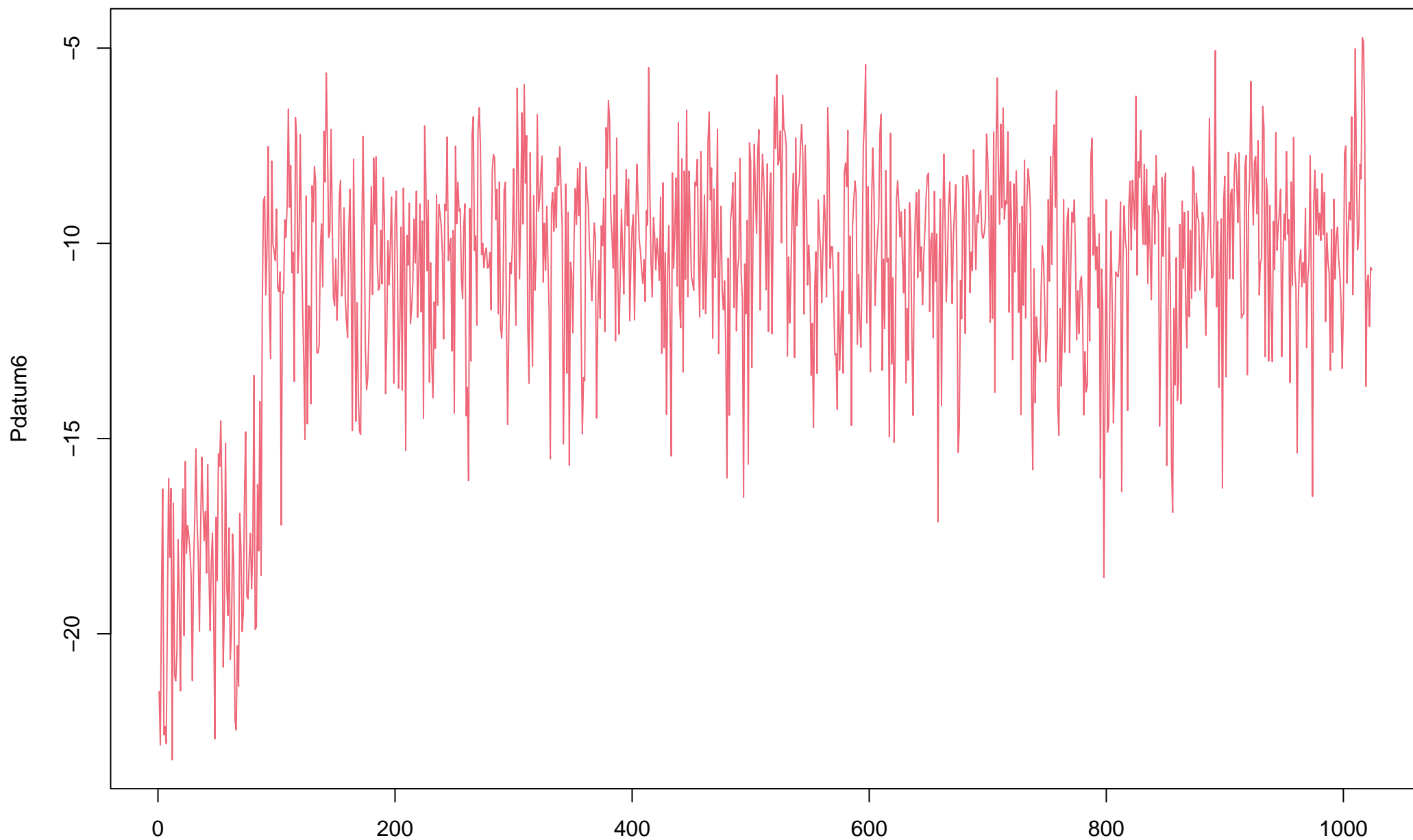
Pdatum4
ESS = 88 | BMK = 0.131 | MCSE(6.27) = 7.09 | stat: FALSE | burn: 102



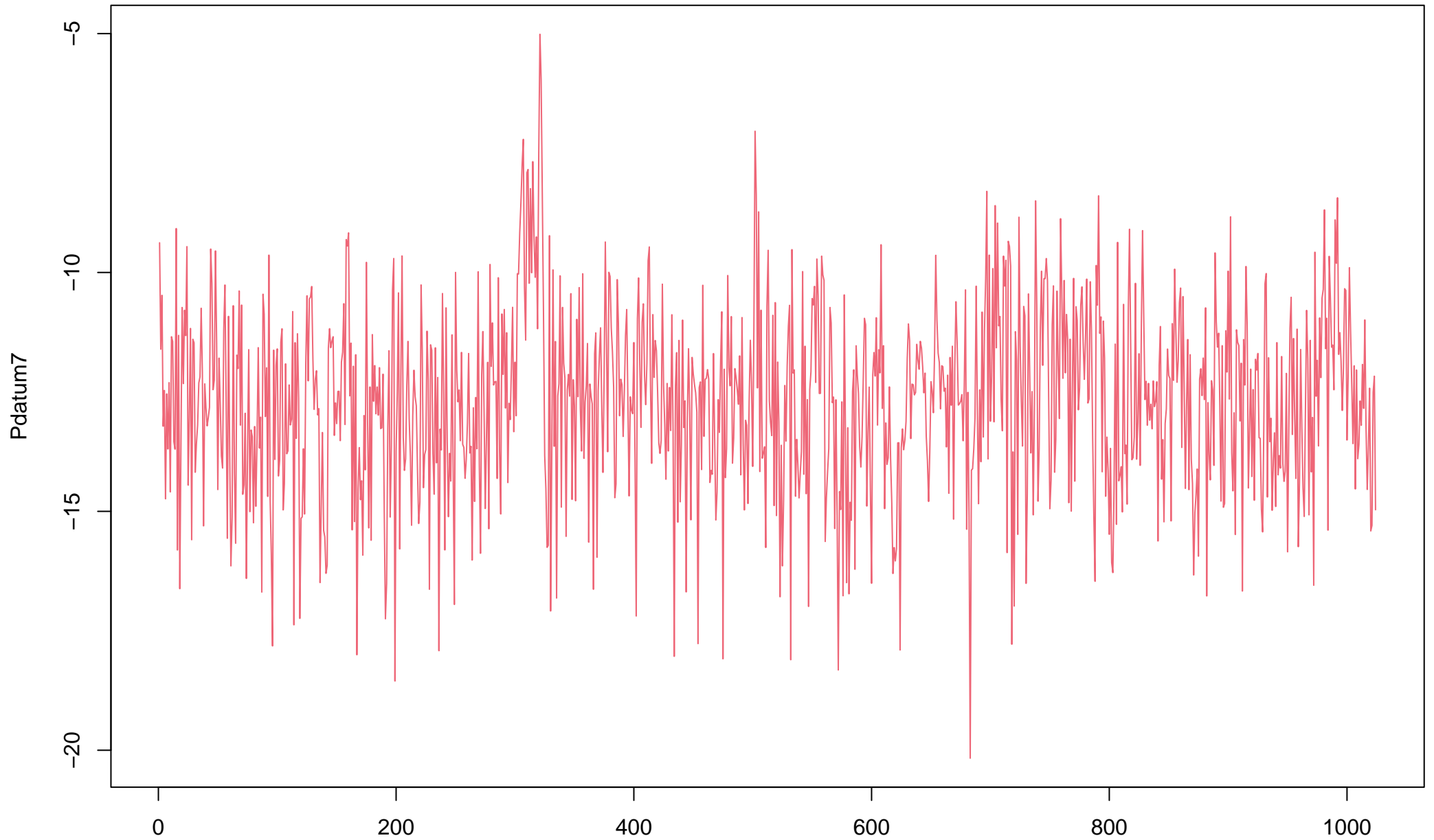
Pdatum5
ESS = 451 | BMK = 0.898 | MCSE(6.27) = 5.15 | stat: TRUE | burn: 816



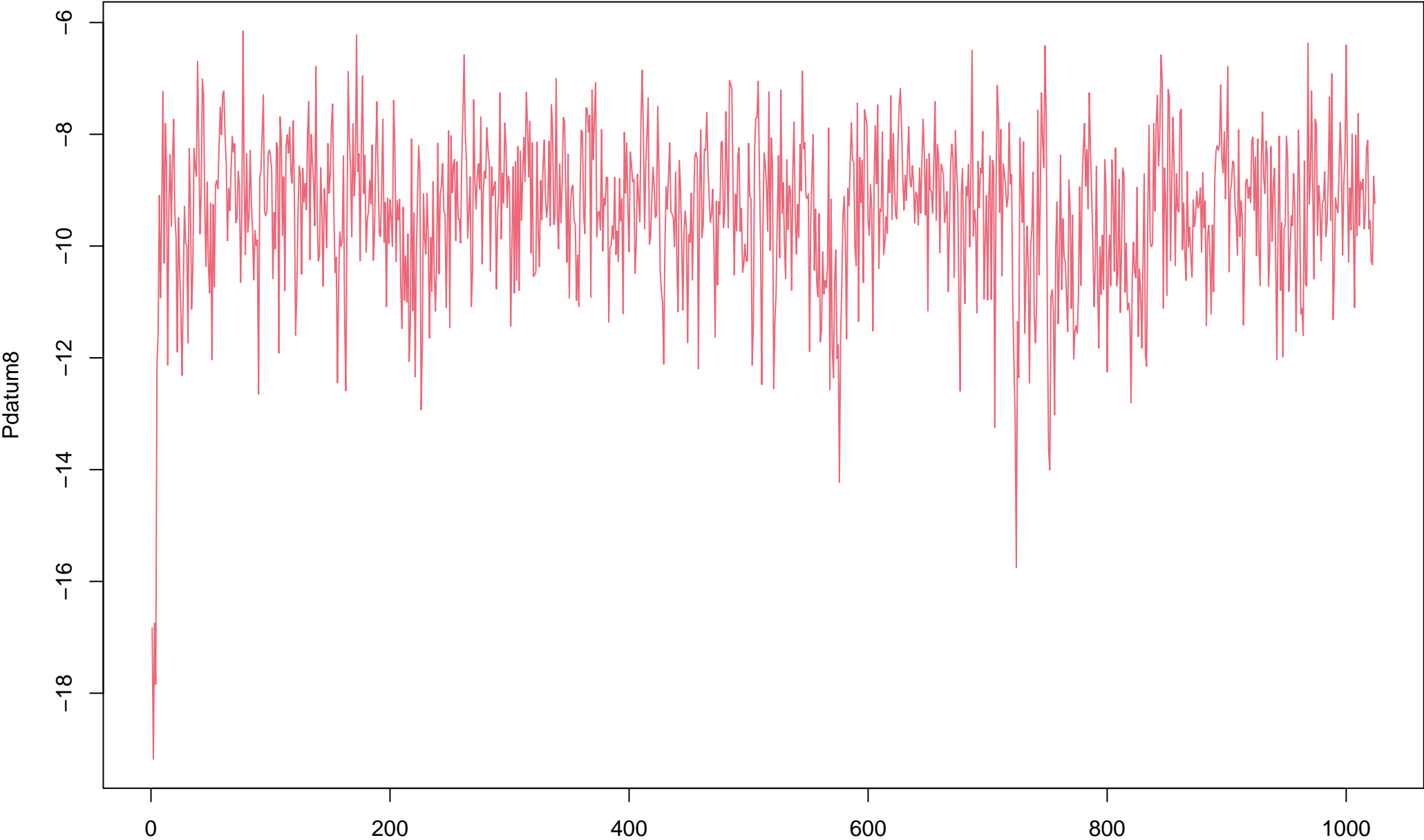
Pdatum6
ESS = 385 | BMK = 0.176 | MCSE(6.27) = 4.87 | stat: FALSE | burn: 102



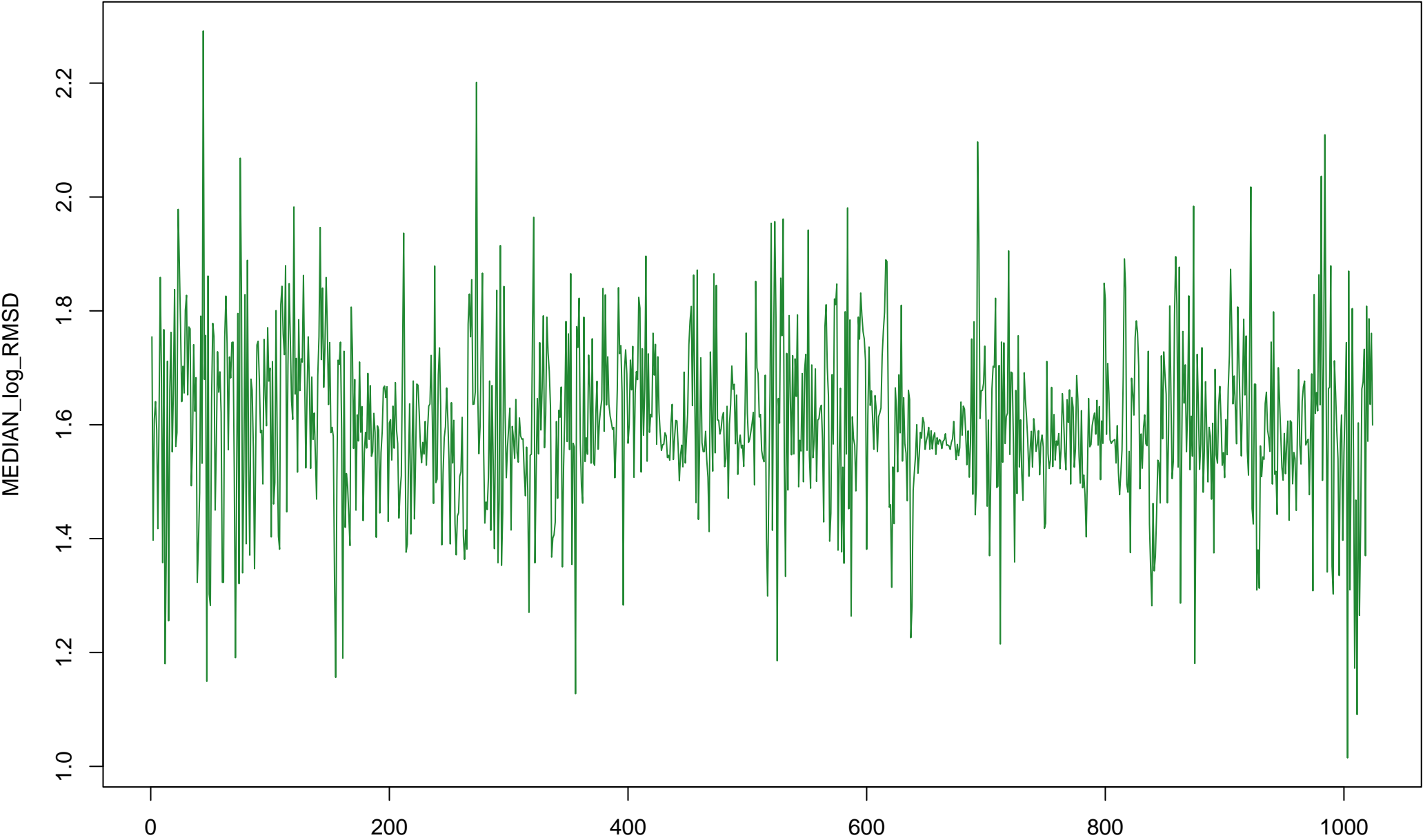
Pdatum7
ESS = 297 | BMK = 0.198 | MCSE(6.27) = 4.31 | stat: TRUE | burn: 408



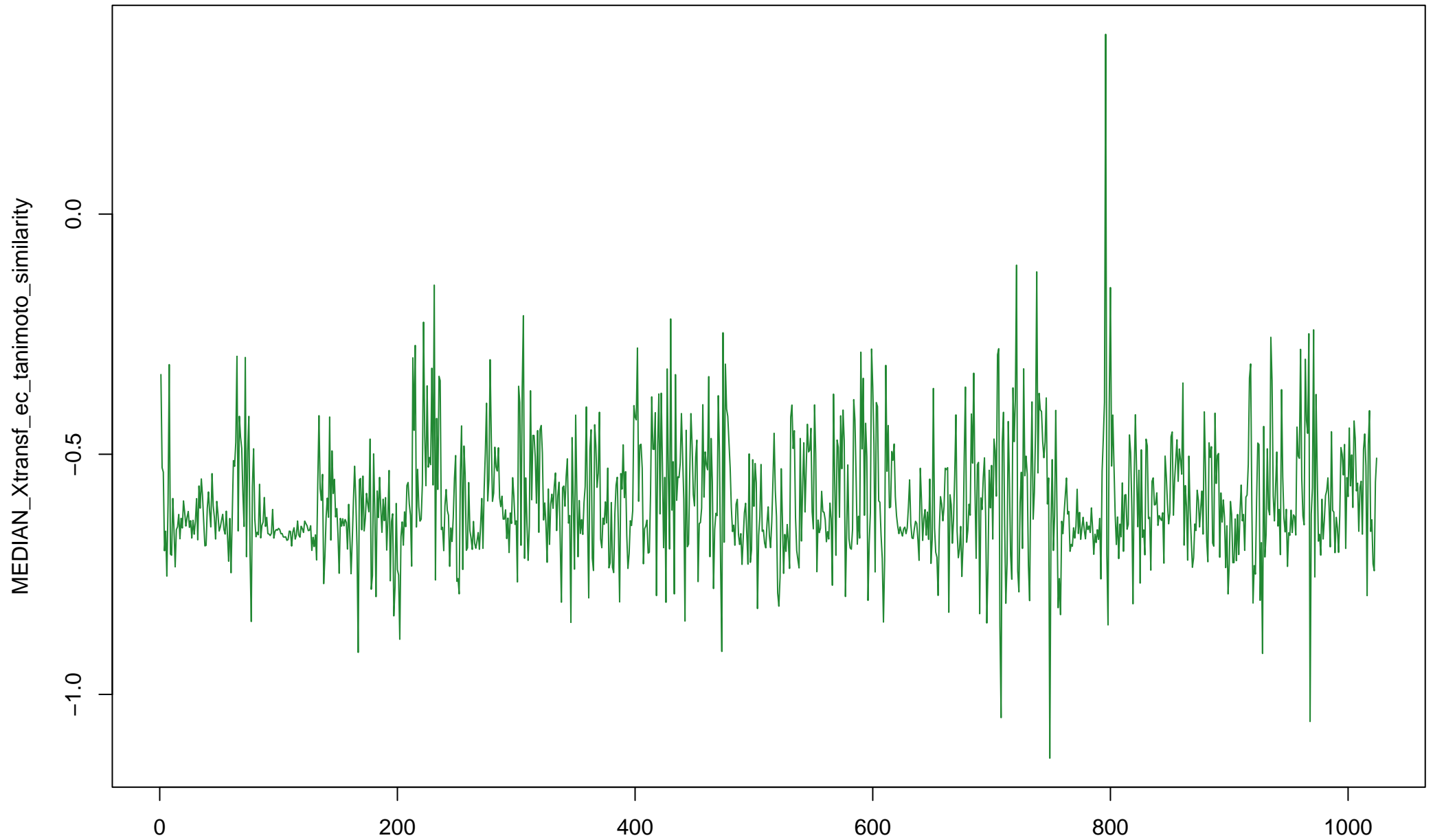
Pdatum8
ESS = 644 | BMK = 0.0973 | MCSE(6.27) = 4.05 | stat: TRUE | burn: 0



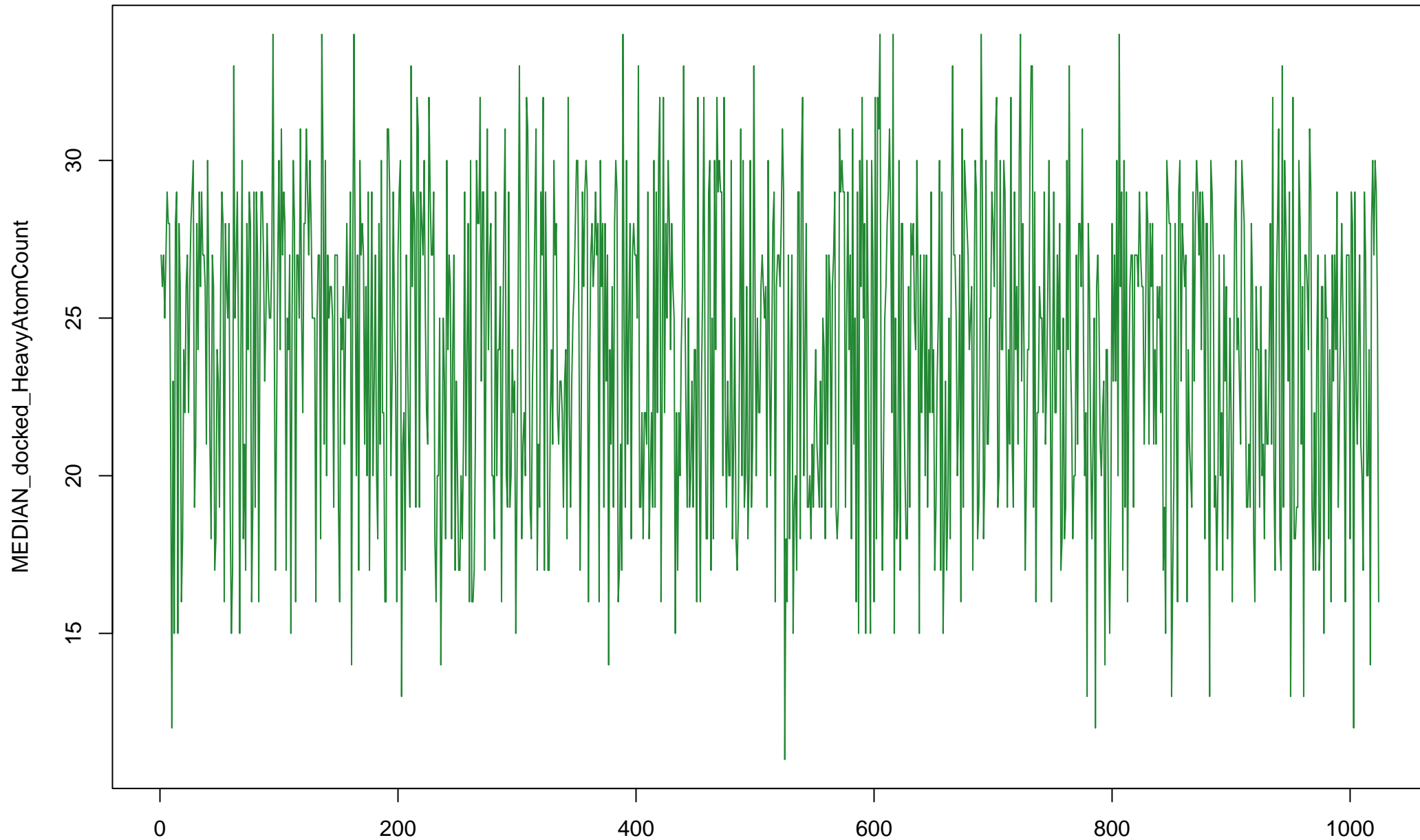
MEDIAN_log_RMSD
ESS = 585 | BMK = 0.0979 | MCSE(6.27) = 3.74 | stat: TRUE | burn: 0



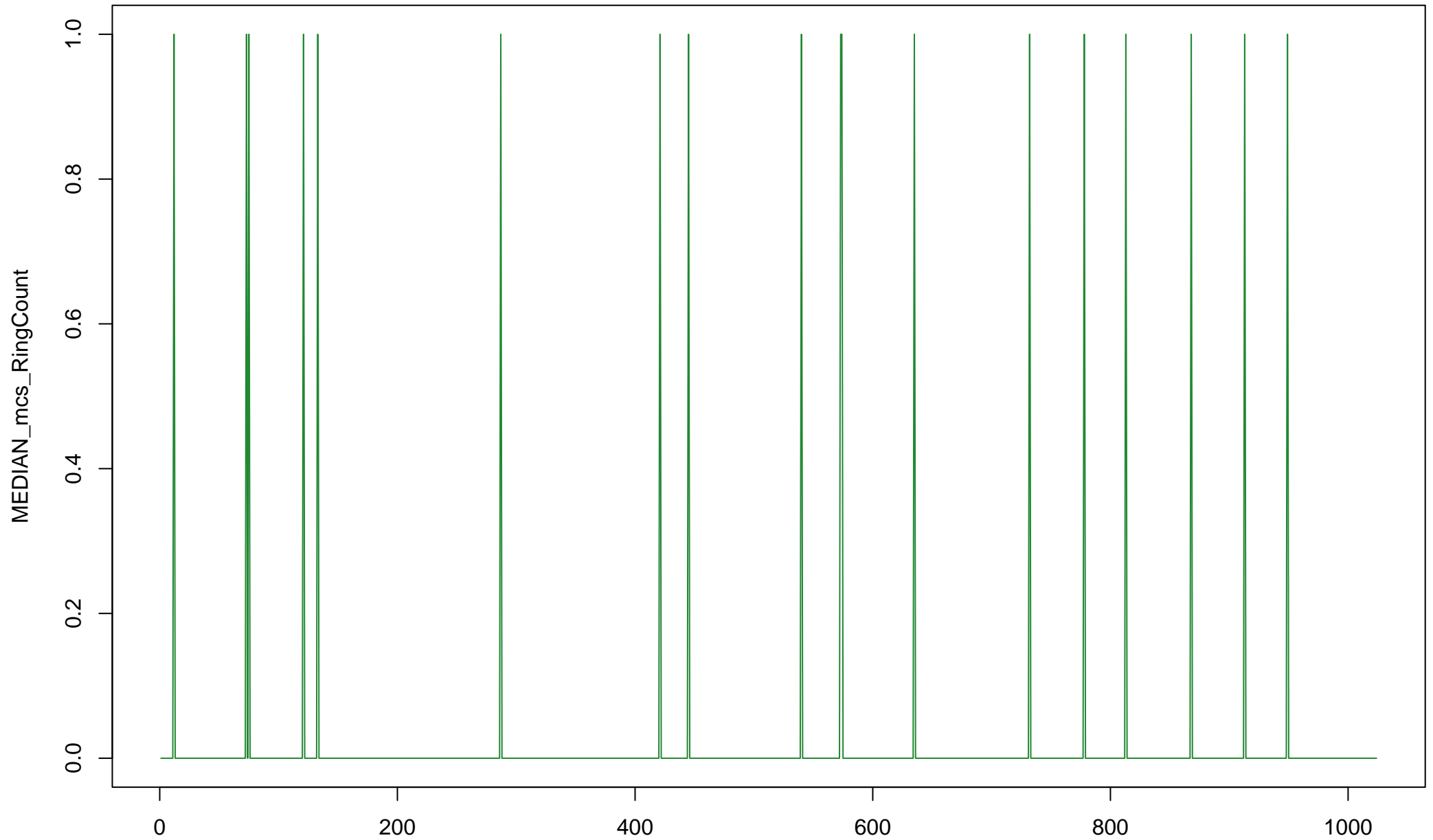
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 403 | BMK = 0.0937 | MCSE(6.27) = 4.08 | stat: TRUE | burn: 0



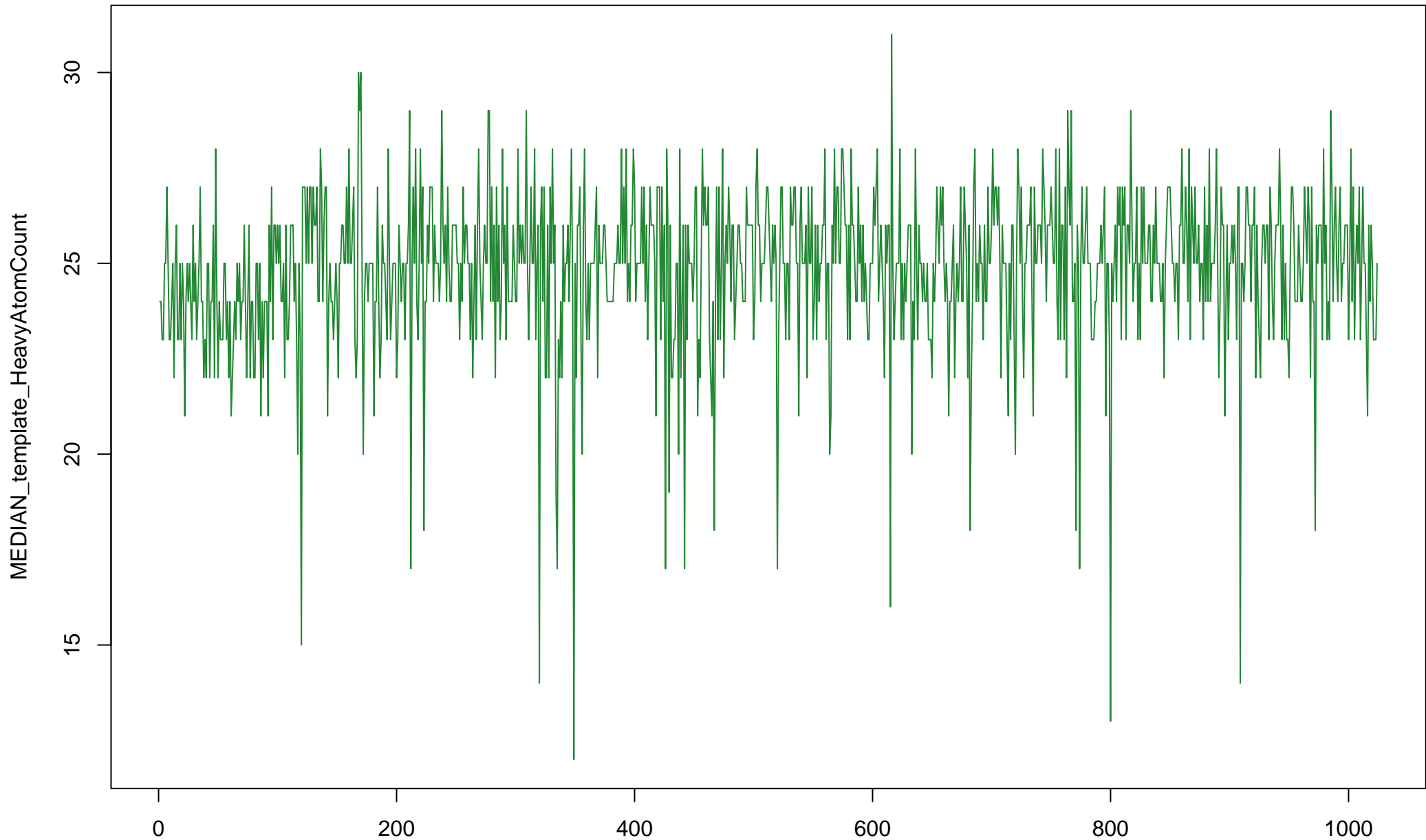
MEDIAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0355 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0



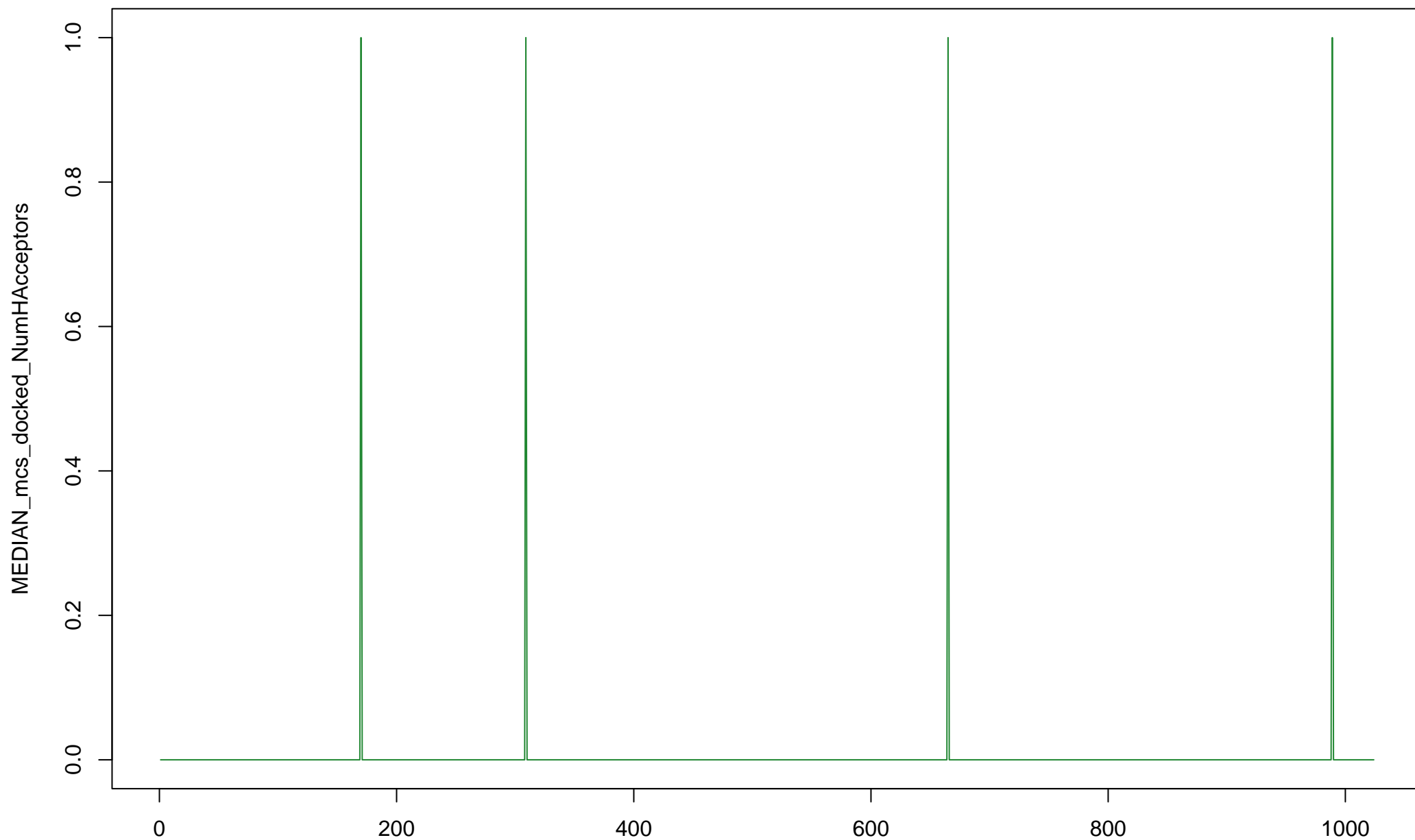
MEDIAN_mcs_RingCount
ESS = 1020 | BMK = 0.0395 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 306



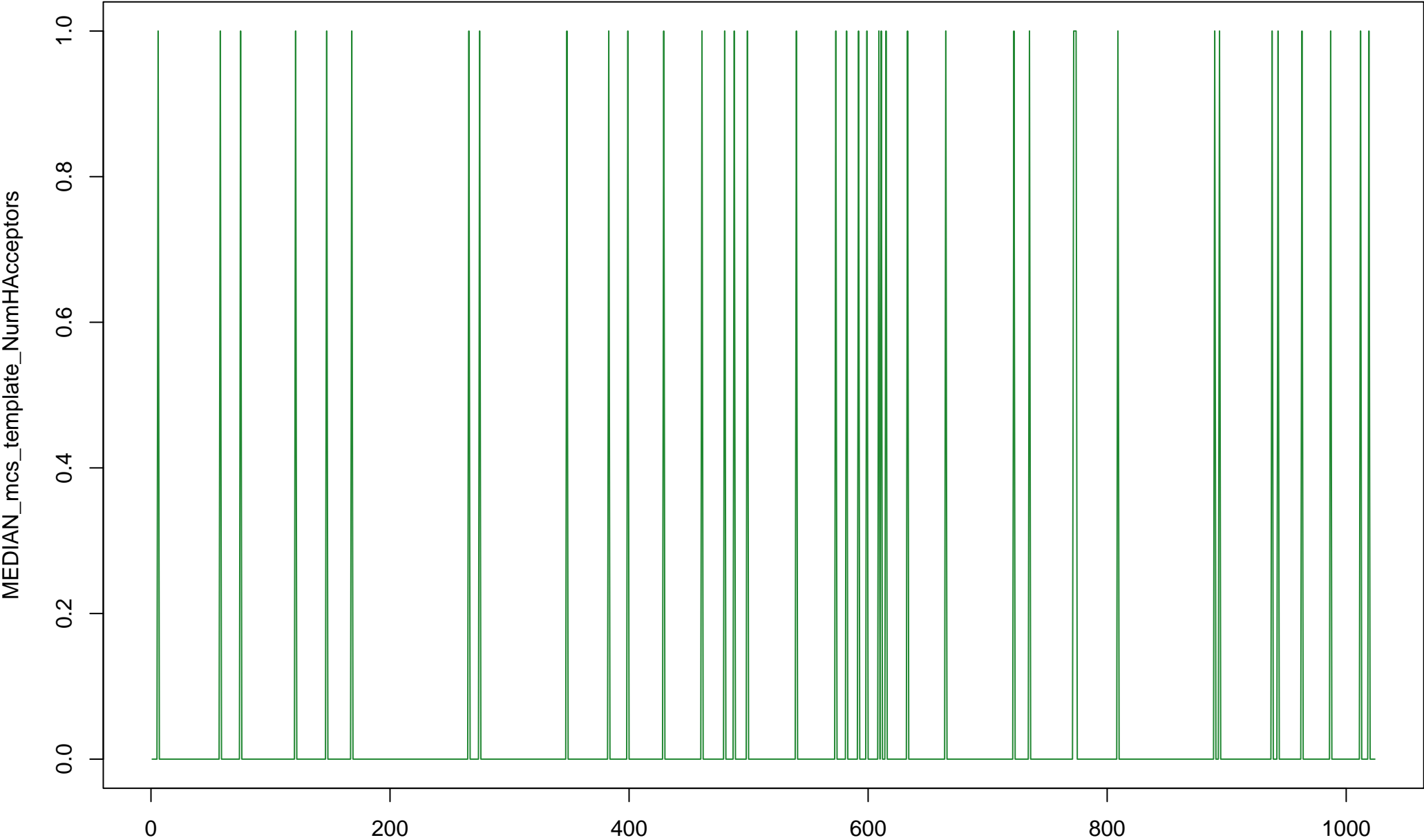
MEDIAN_template_HeavyAtomCount
ESS = 1020 | BMK = 0.0984 | MCSE(6.27) = 4.6 | stat: FALSE | burn: 0



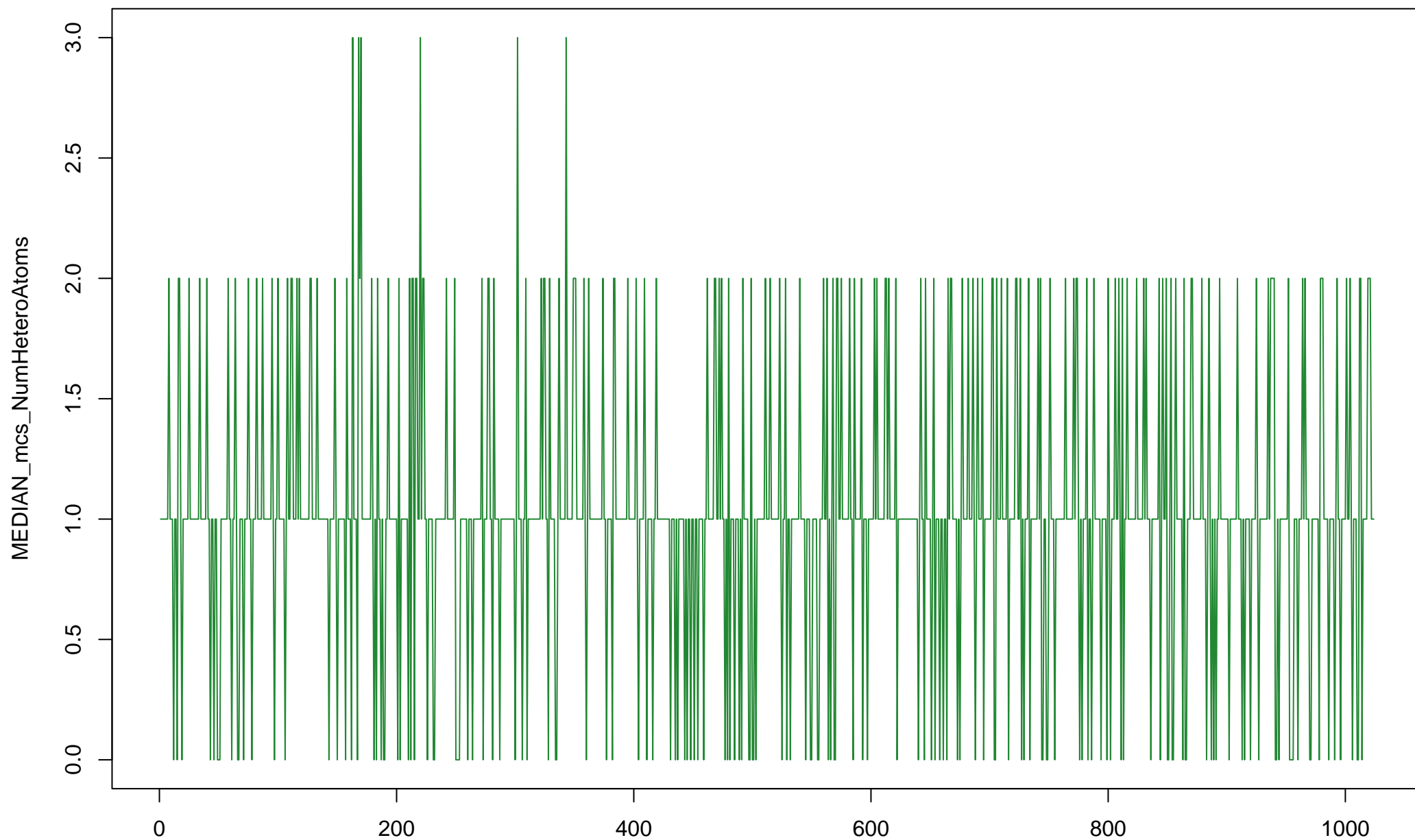
MEDIAN_mcs_docked_NumHAcceptors
ESS = 1020 | BMK = 0 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 1020



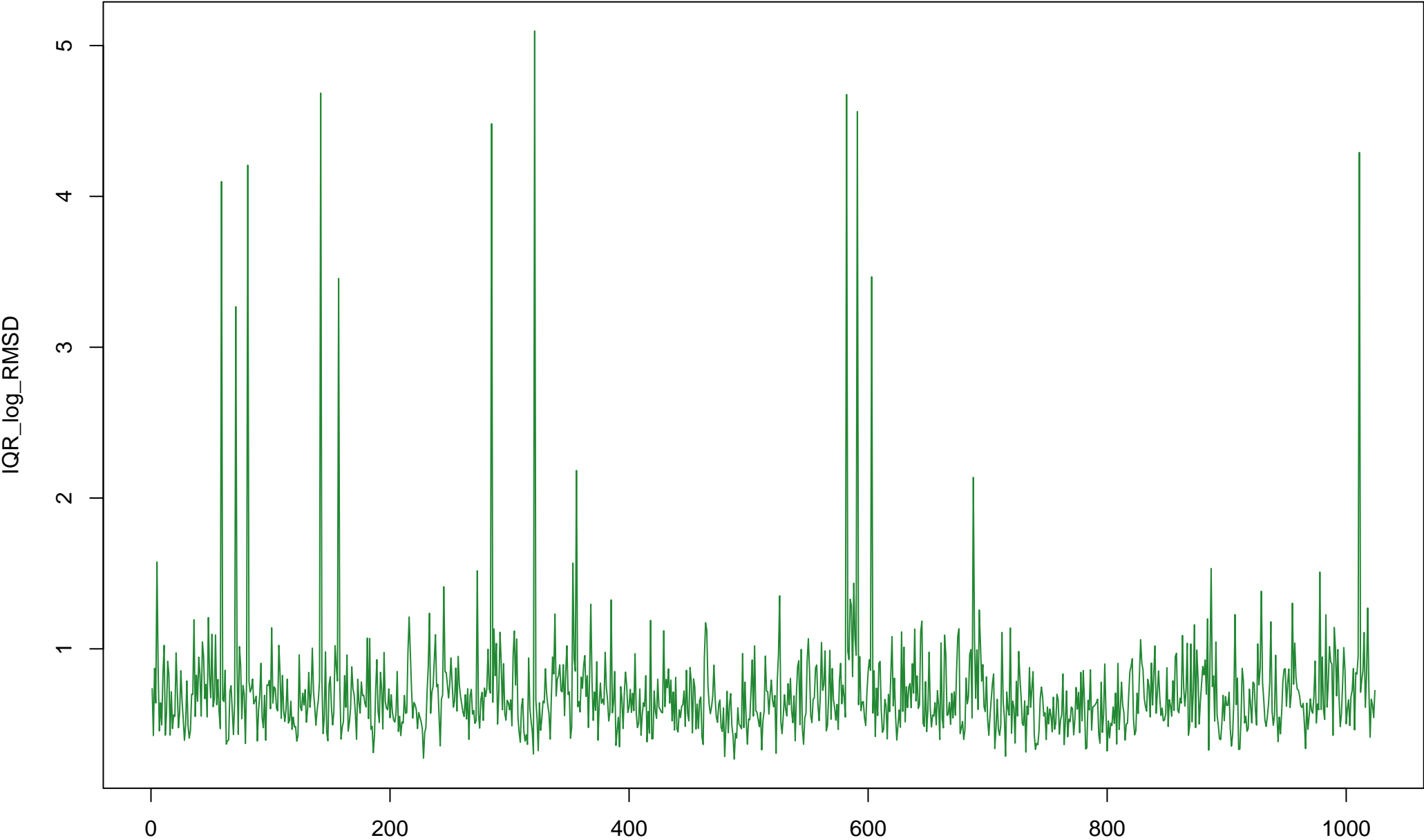
MEDIAN_mcs_template_NumHAcceptors
ESS = 1020 | BMK = 0.0716 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0



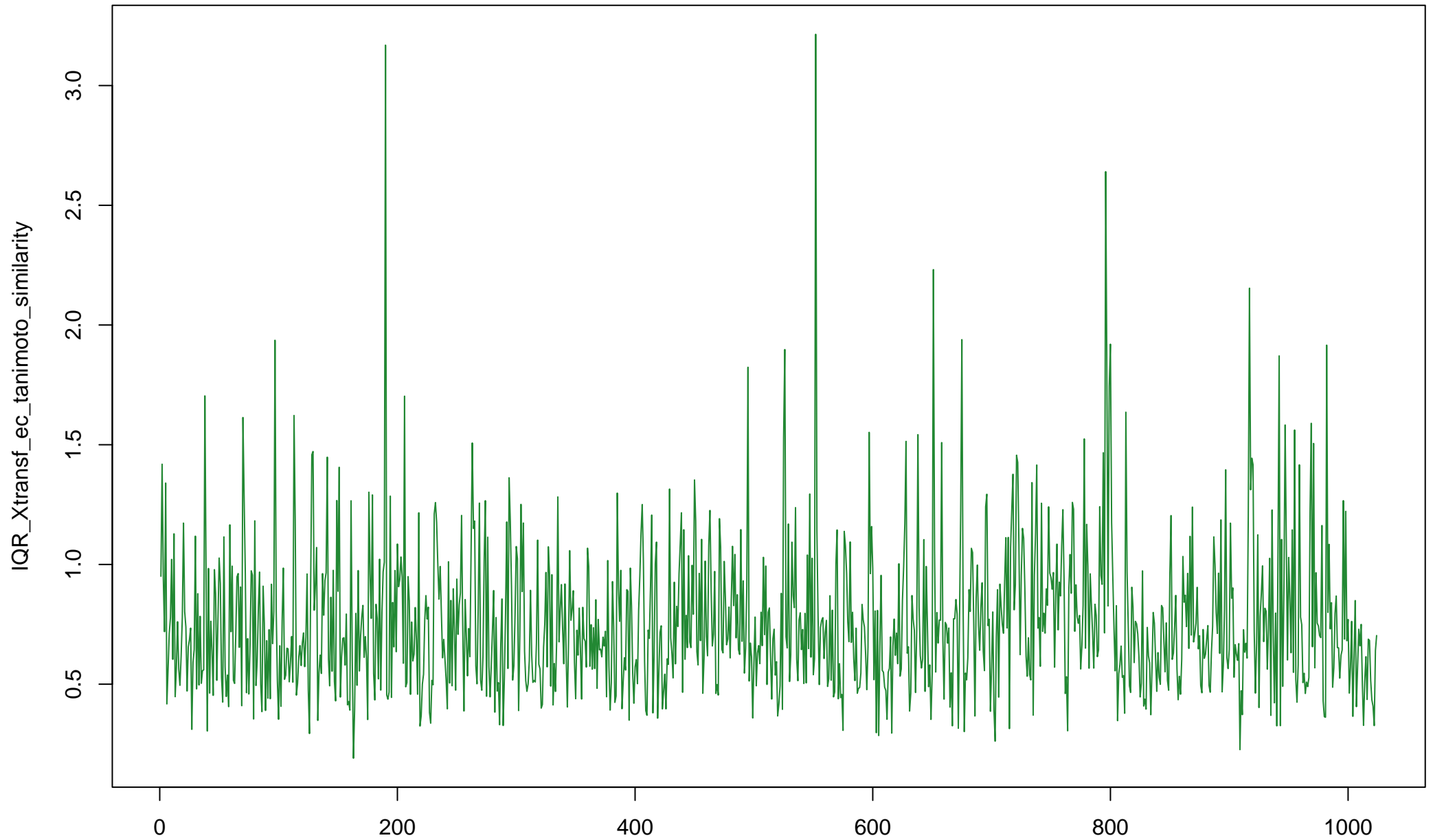
MEDIAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0687 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0



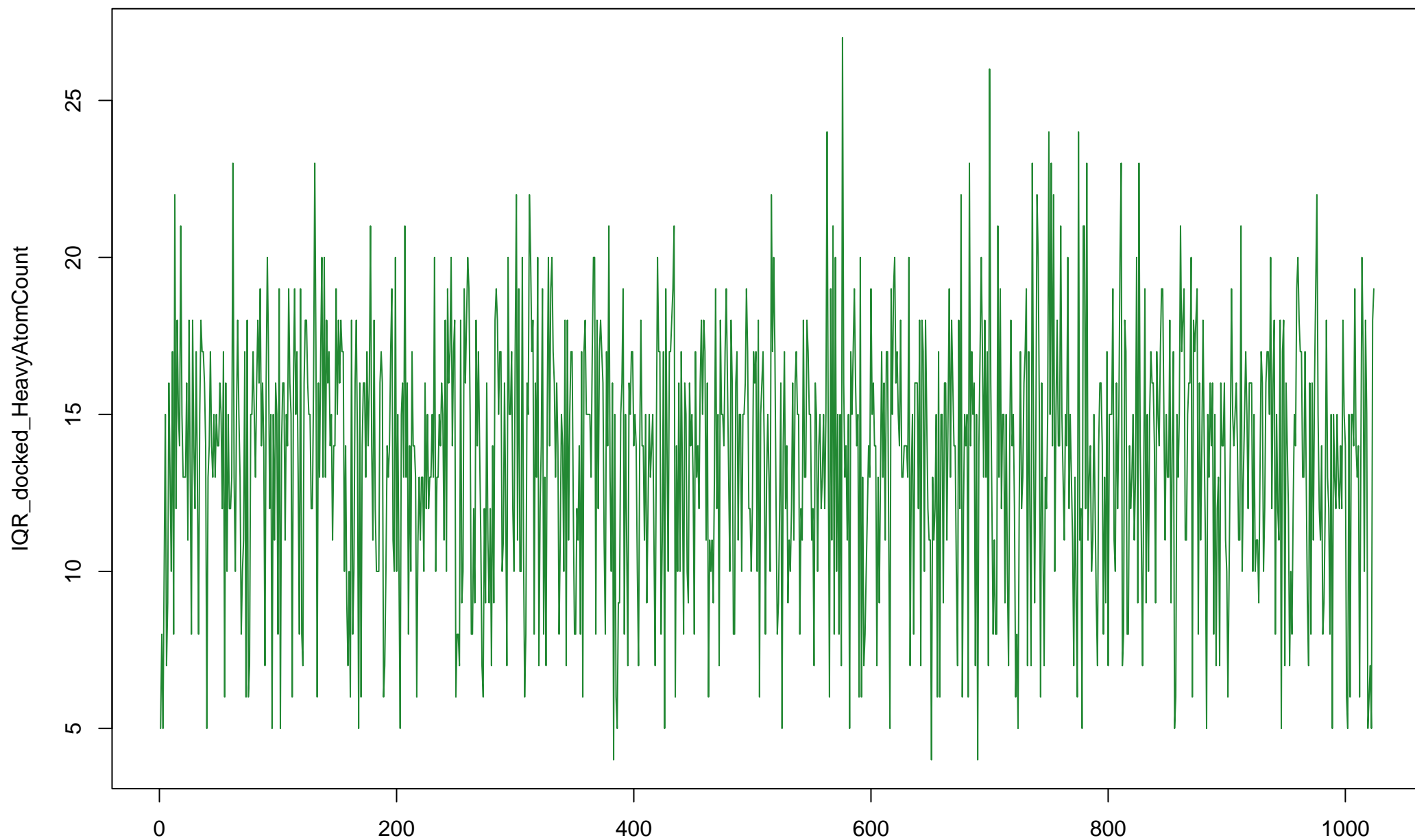
IQR_log_RMSD
ESS = 931 | BMK = 0.0748 | MCSE(6.27) = 4.71 | stat: TRUE | burn: 0



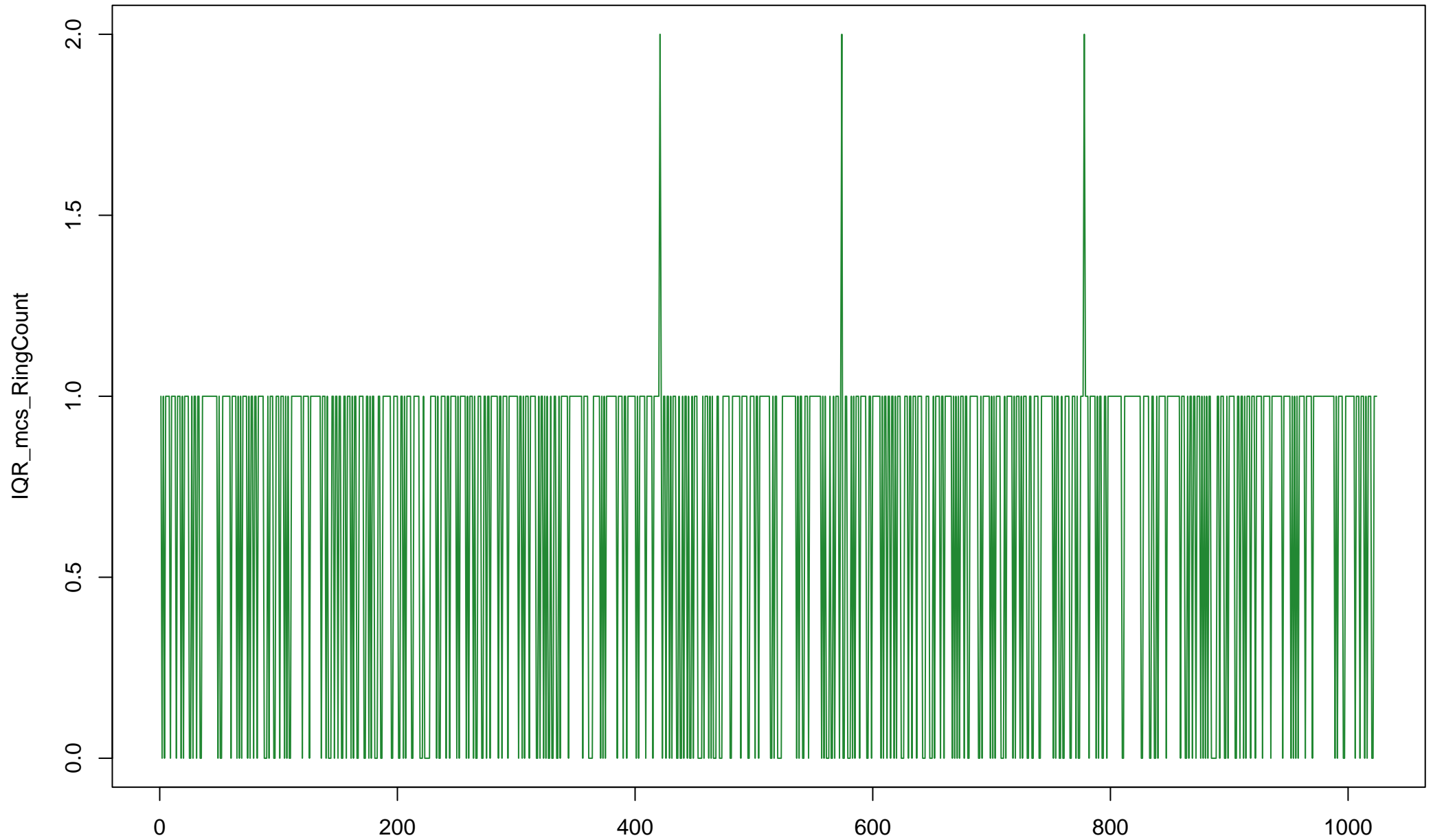
IQR_Xtransf_ec_tanimoto_similarity
ESS = 755 | BMK = 0.0908 | MCSE(6.27) = 4.01 | stat: TRUE | burn: 0



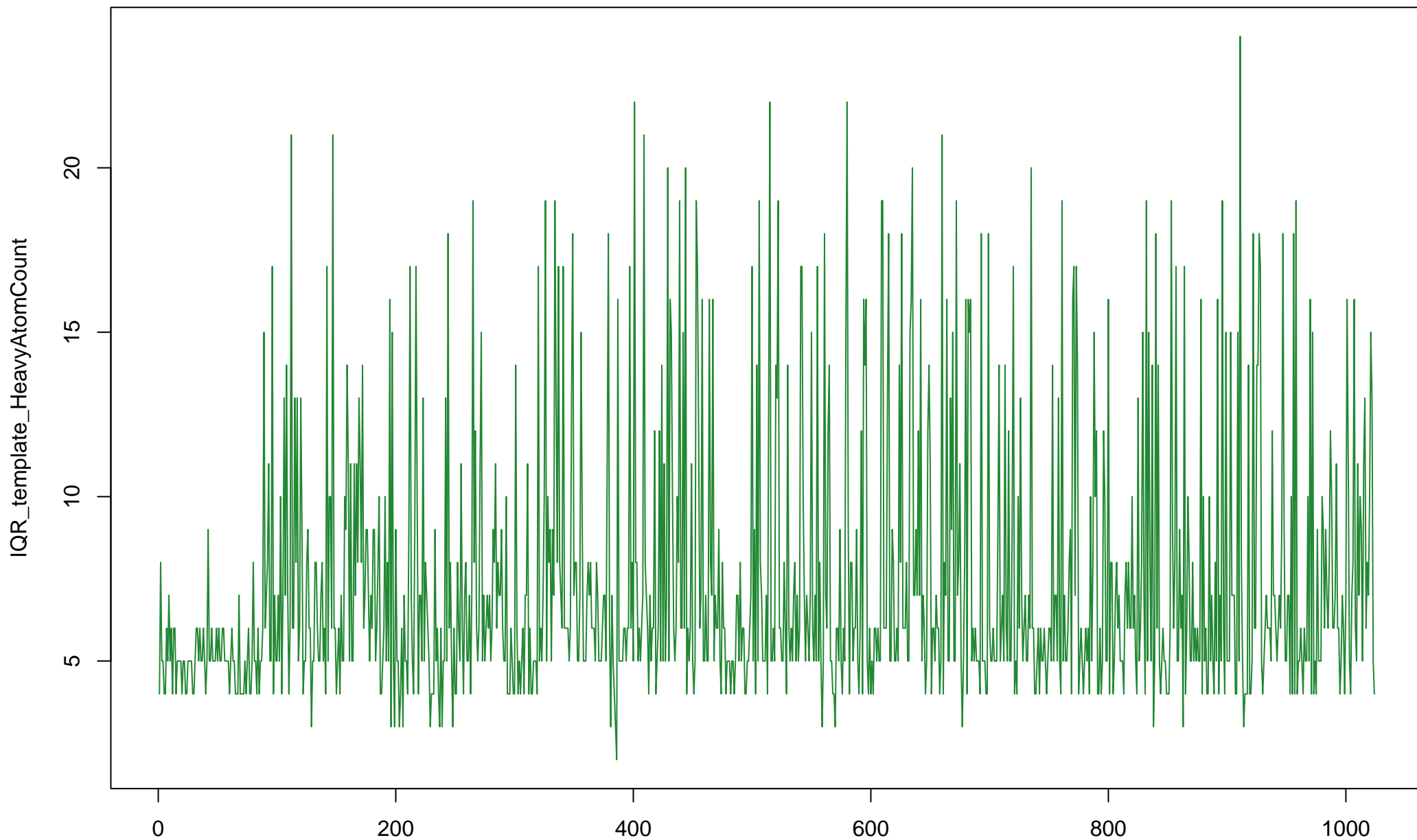
IQR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0781 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0



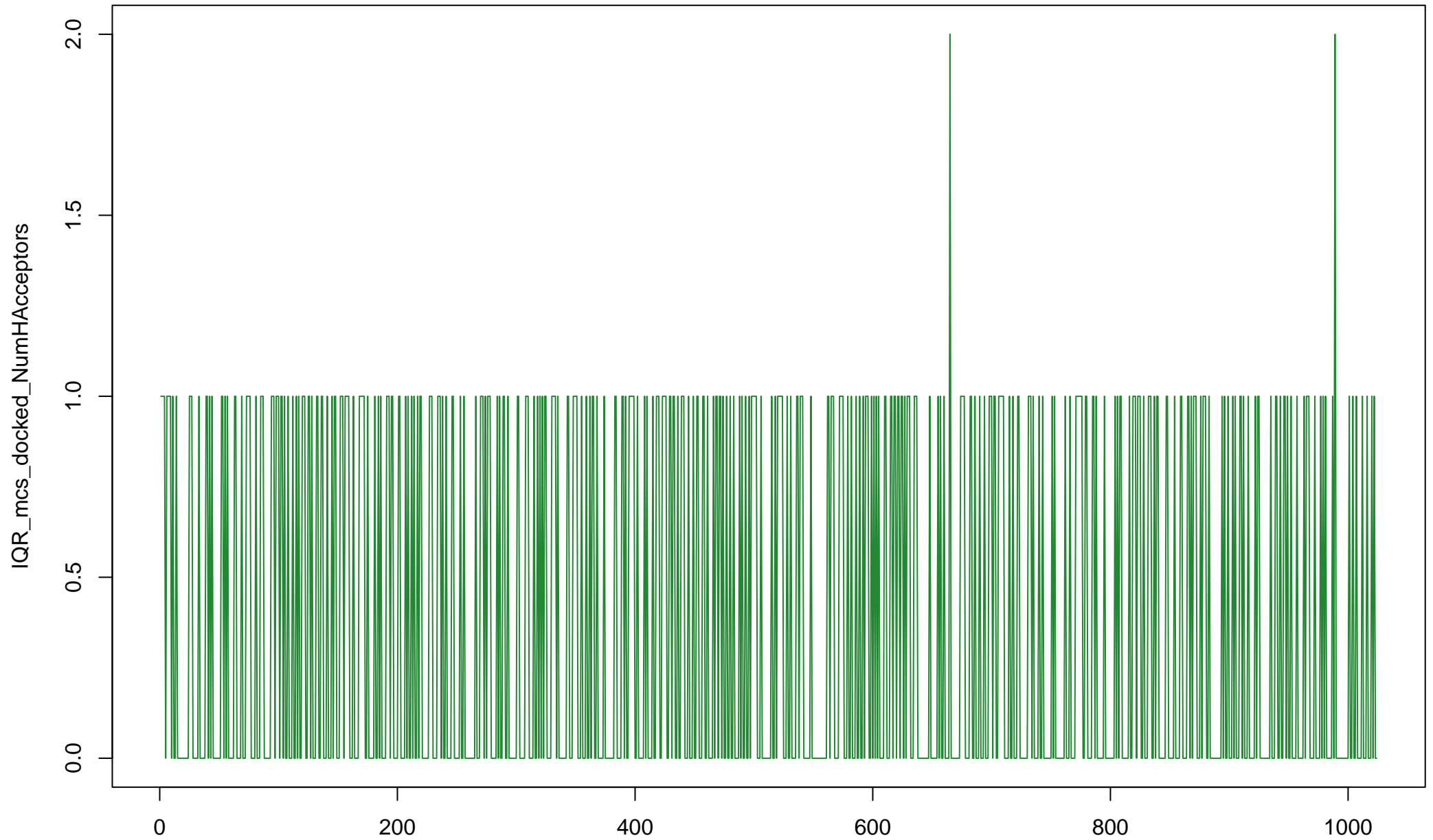
IQR_mcs_RingCount
ESS = 1020 | BMK = 0.0124 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0



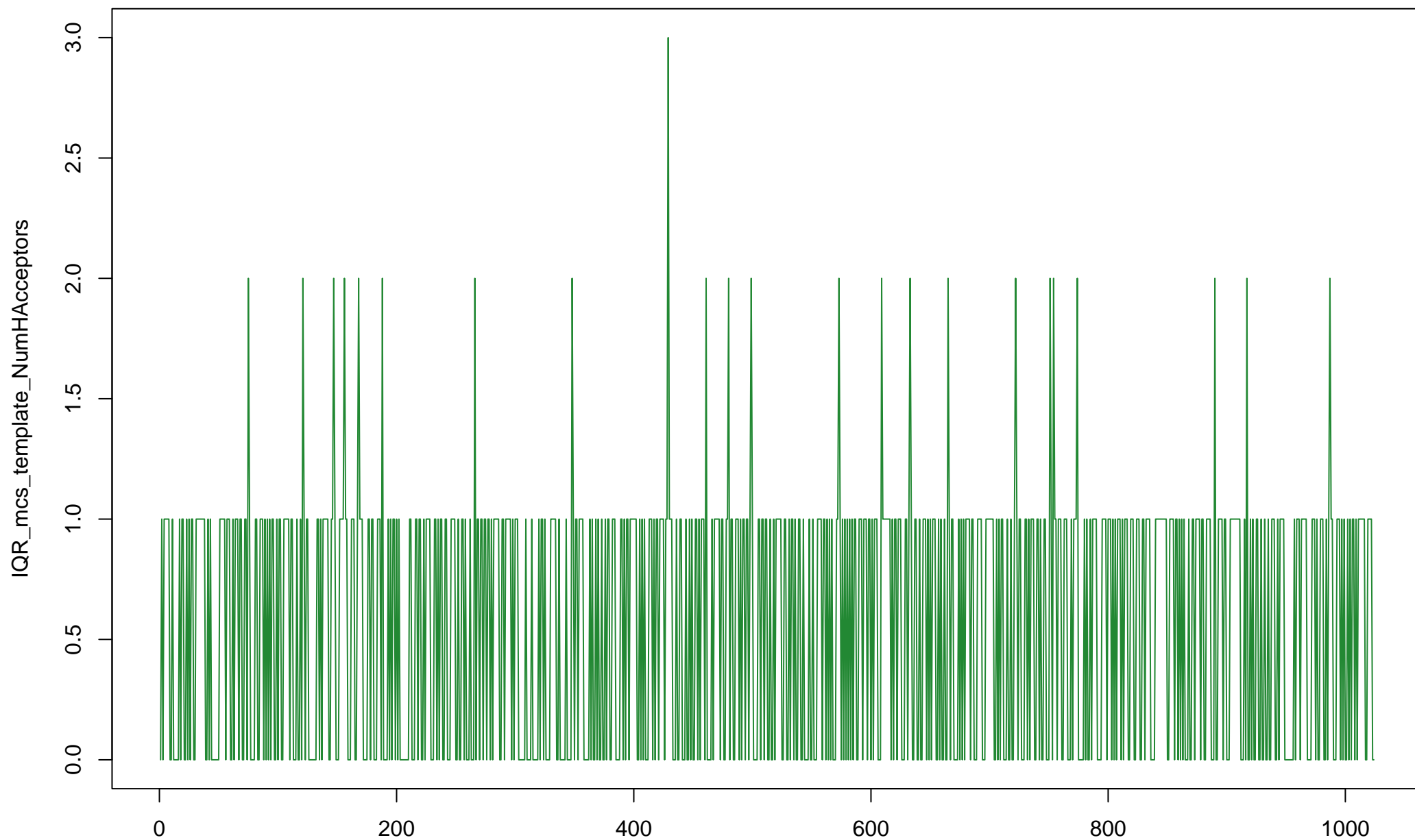
IQR_template_HeavyAtomCount
ESS = 379 | BMK = 0.0844 | MCSE(6.27) = 4.52 | stat: FALSE | burn: 0



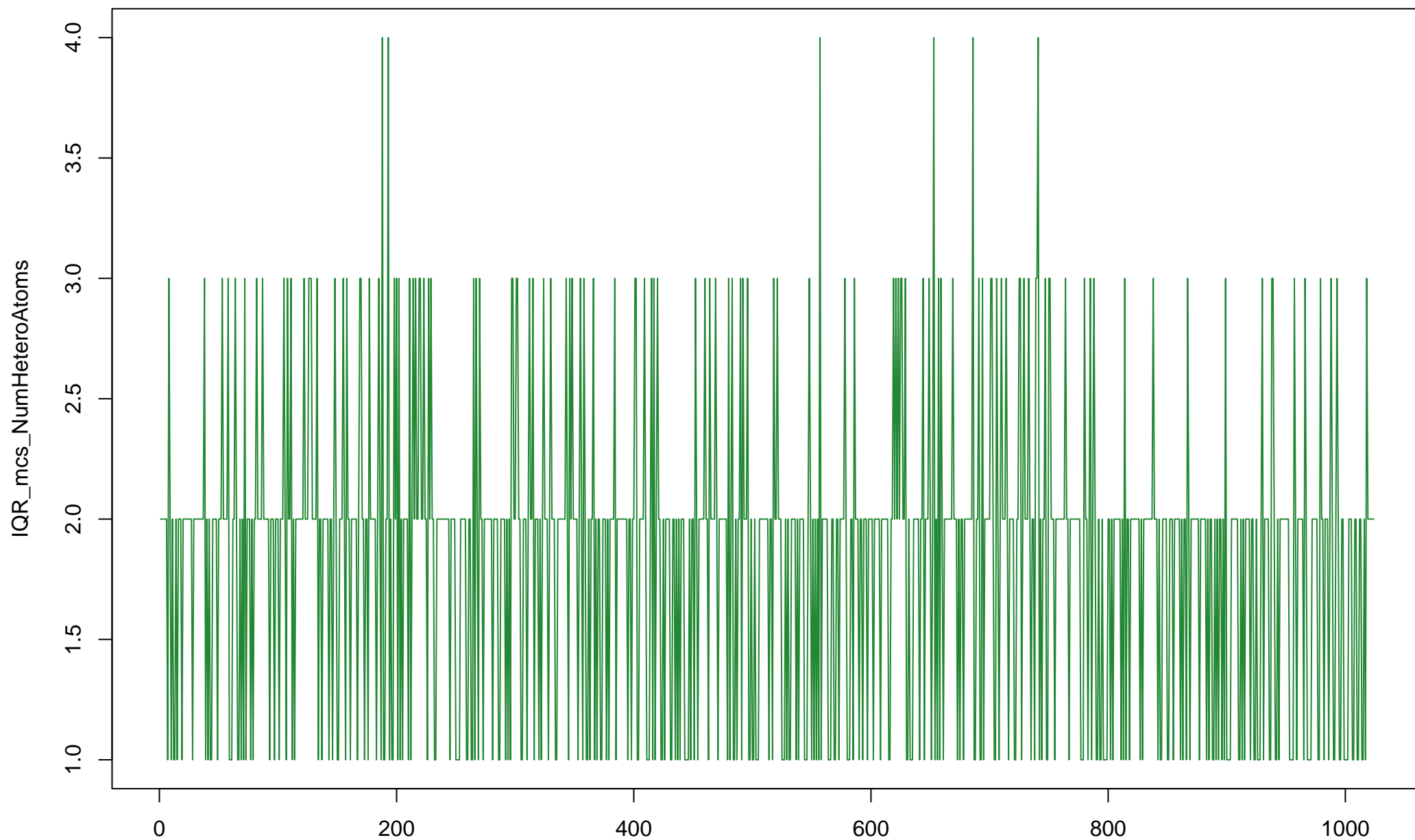
IQR_mcs_docked_NumHAcceptors
ESS = 915 | BMK = 0.0468 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0



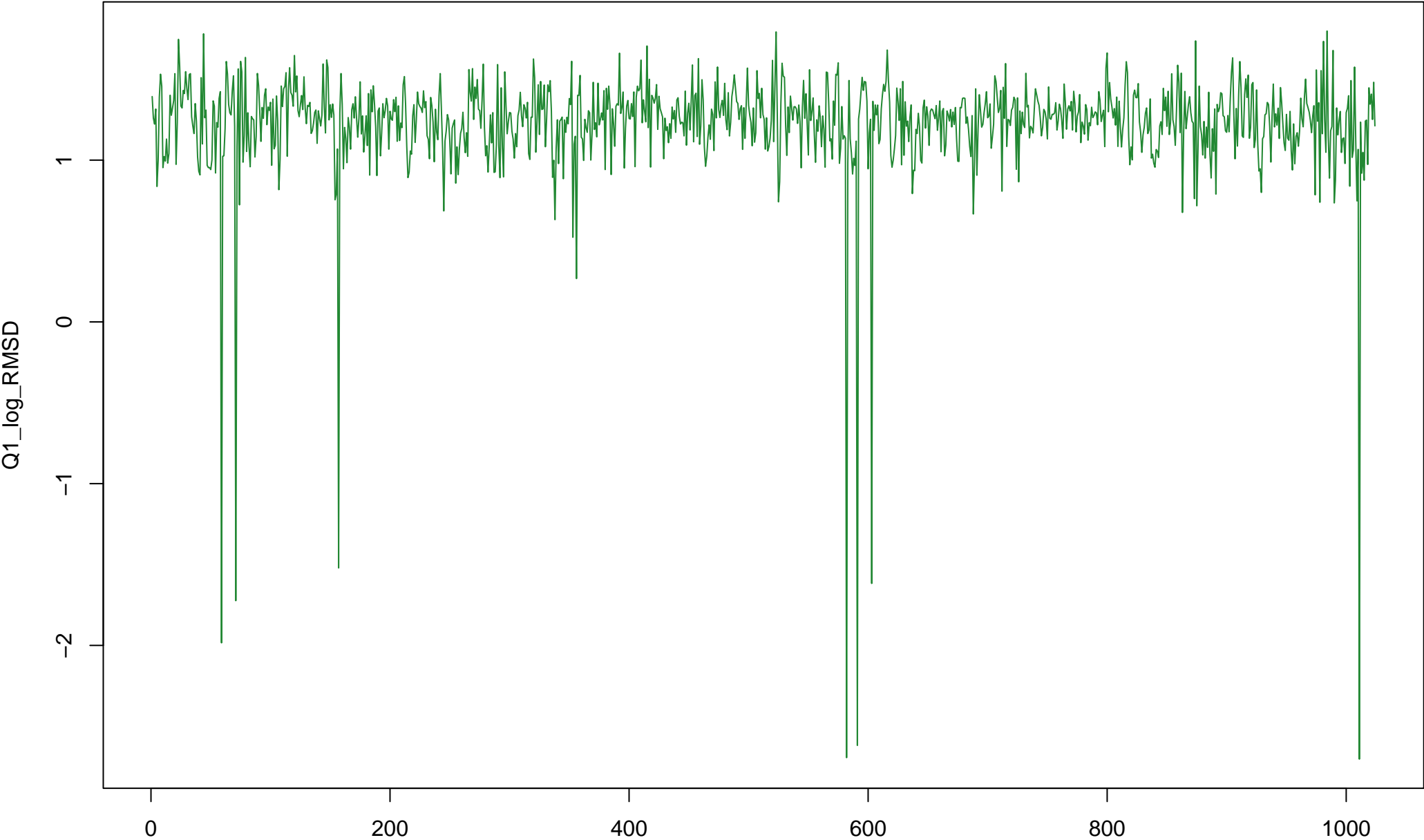
IQR_mcs_template_NumHAcceptors
ESS = 1020 | BMK = 0.0345 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0



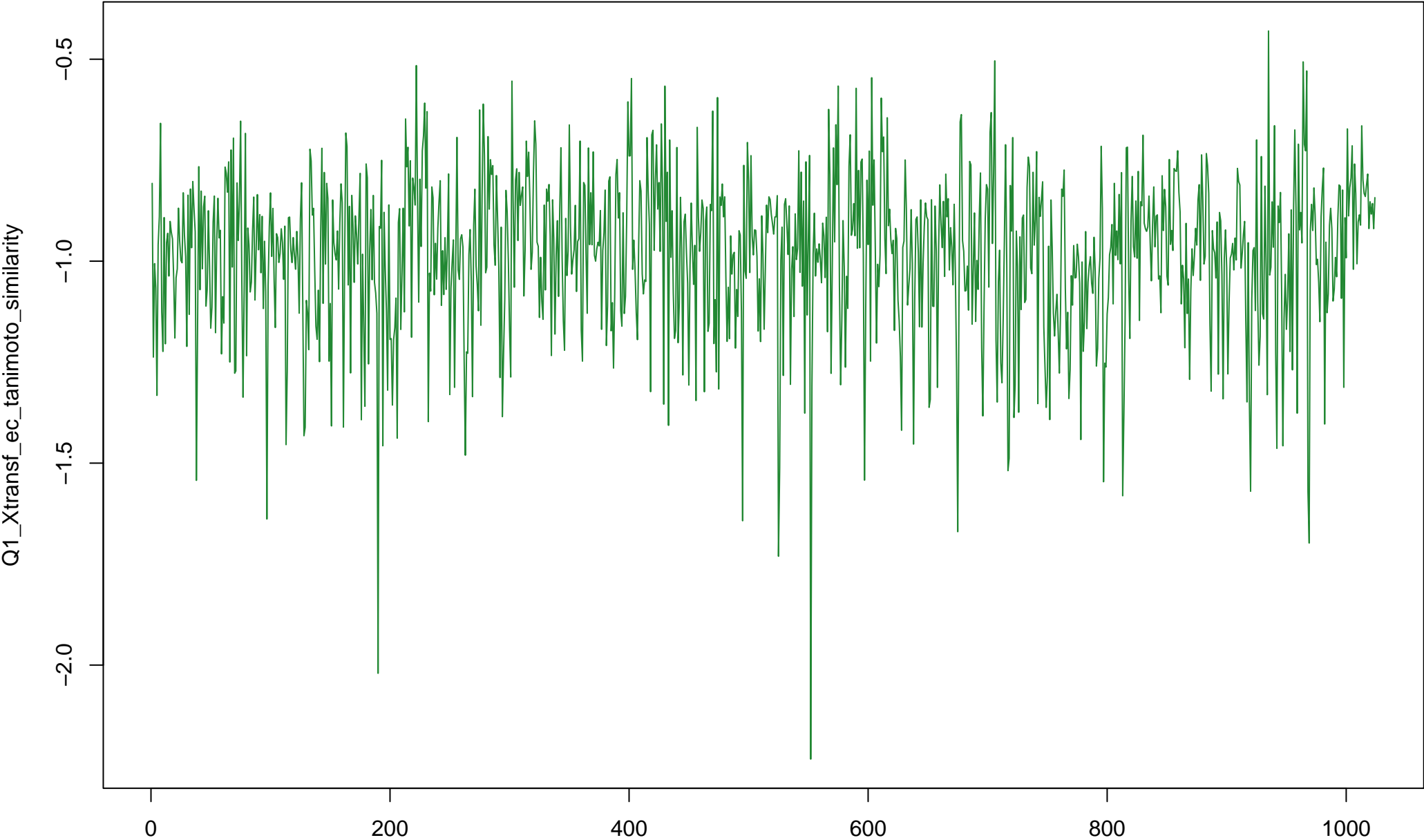
IQR_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0469 | MCSE(6.27) = 3.81 | stat: TRUE | burn: 0



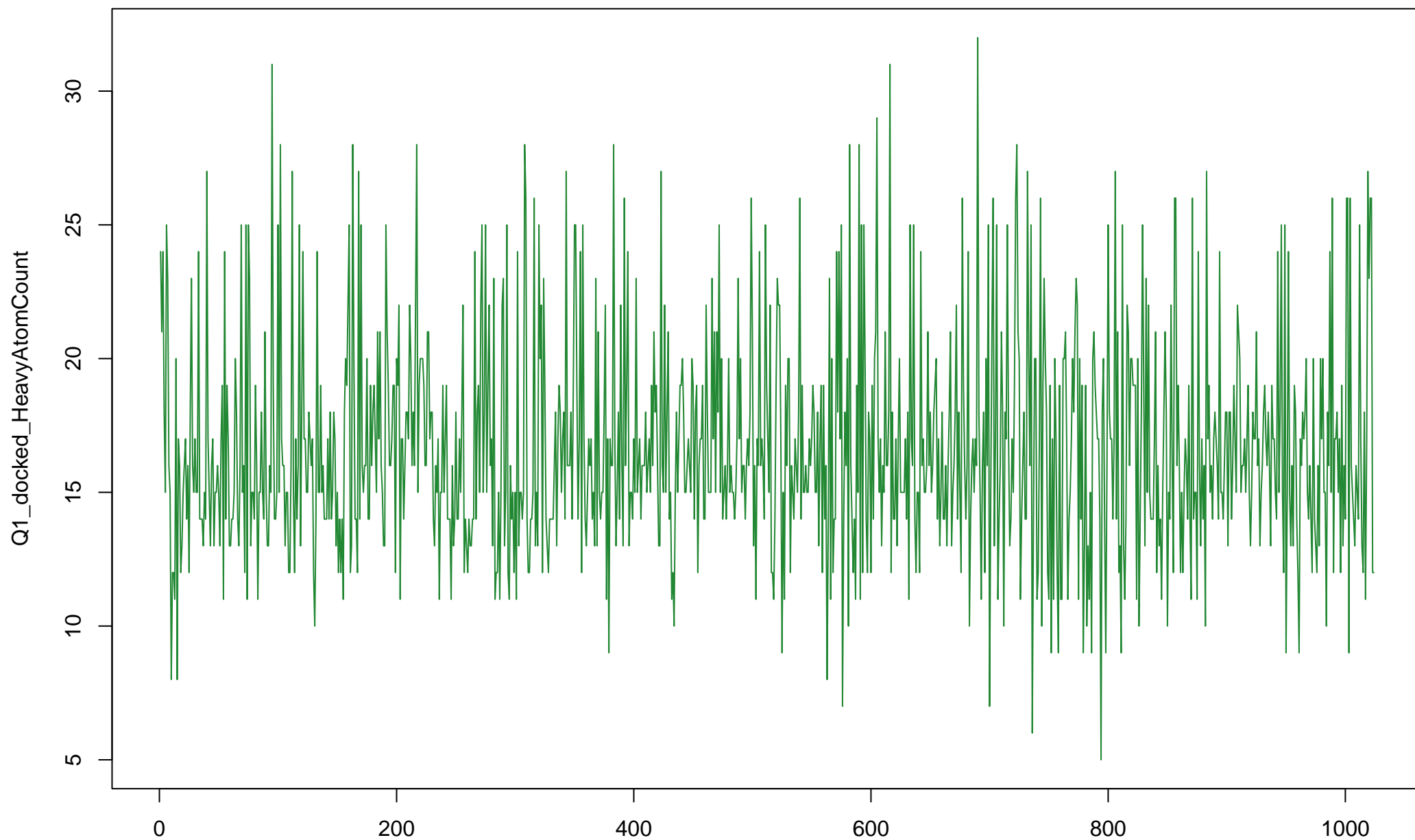
Q1_log_RMSD
ESS = 522 | BMK = 0.0984 | MCSE(6.27) = 4.32 | stat: TRUE | burn: 0



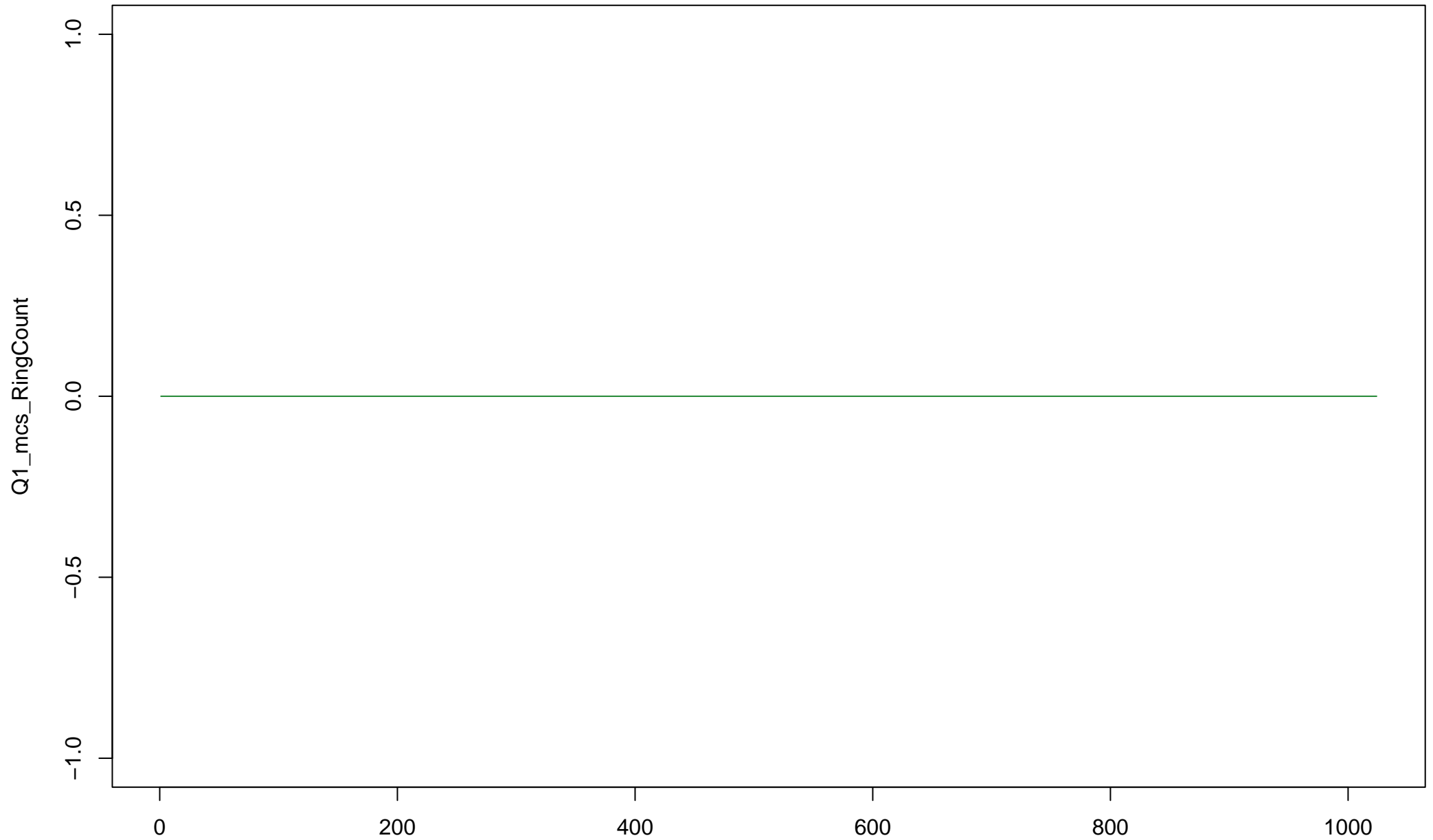
Q1_Xtransf_ec_tanimoto_similarity
ESS = 768 | BMK = 0.0712 | MCSE(6.27) = 3.79 | stat: TRUE | burn: 0



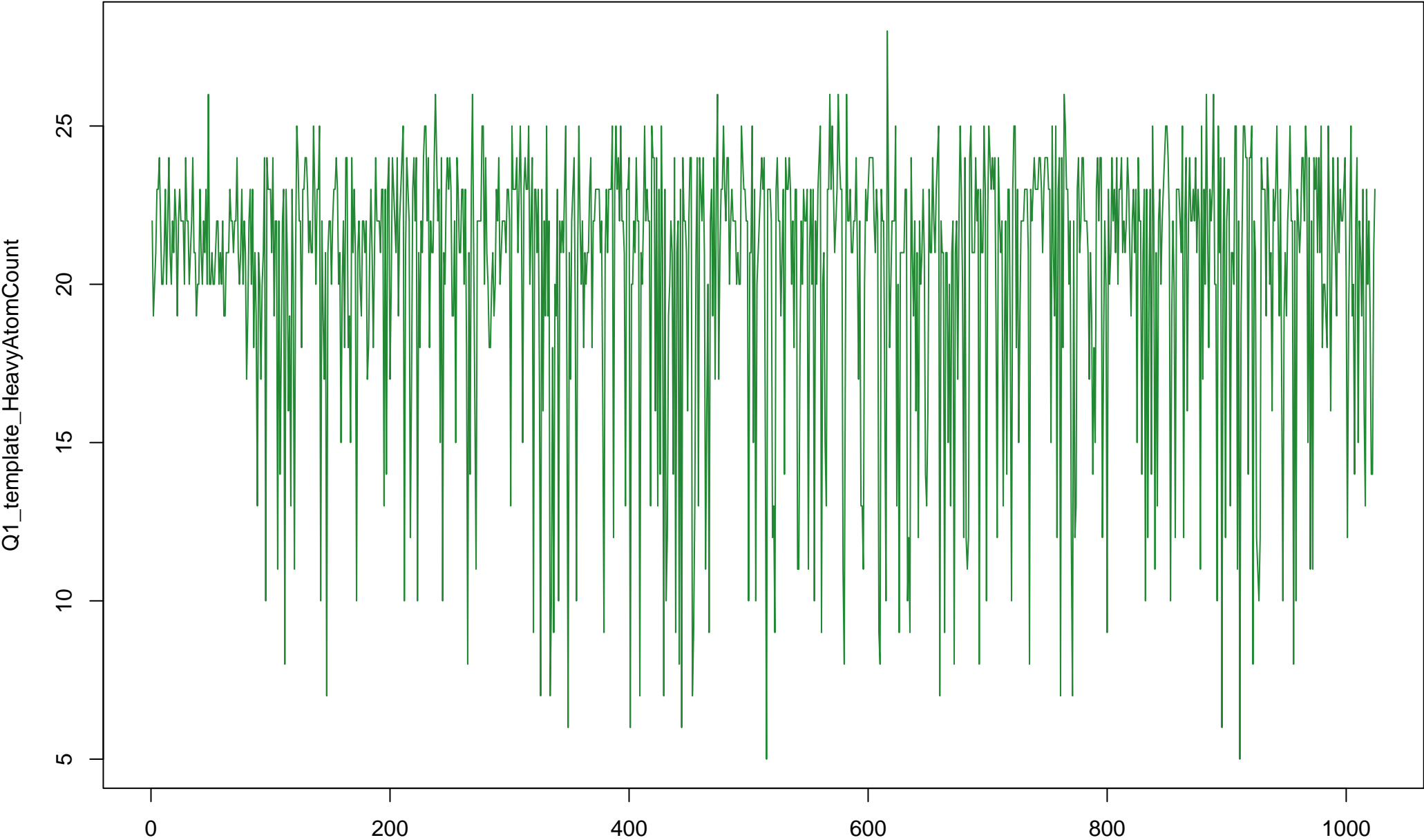
Q1_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.11 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0



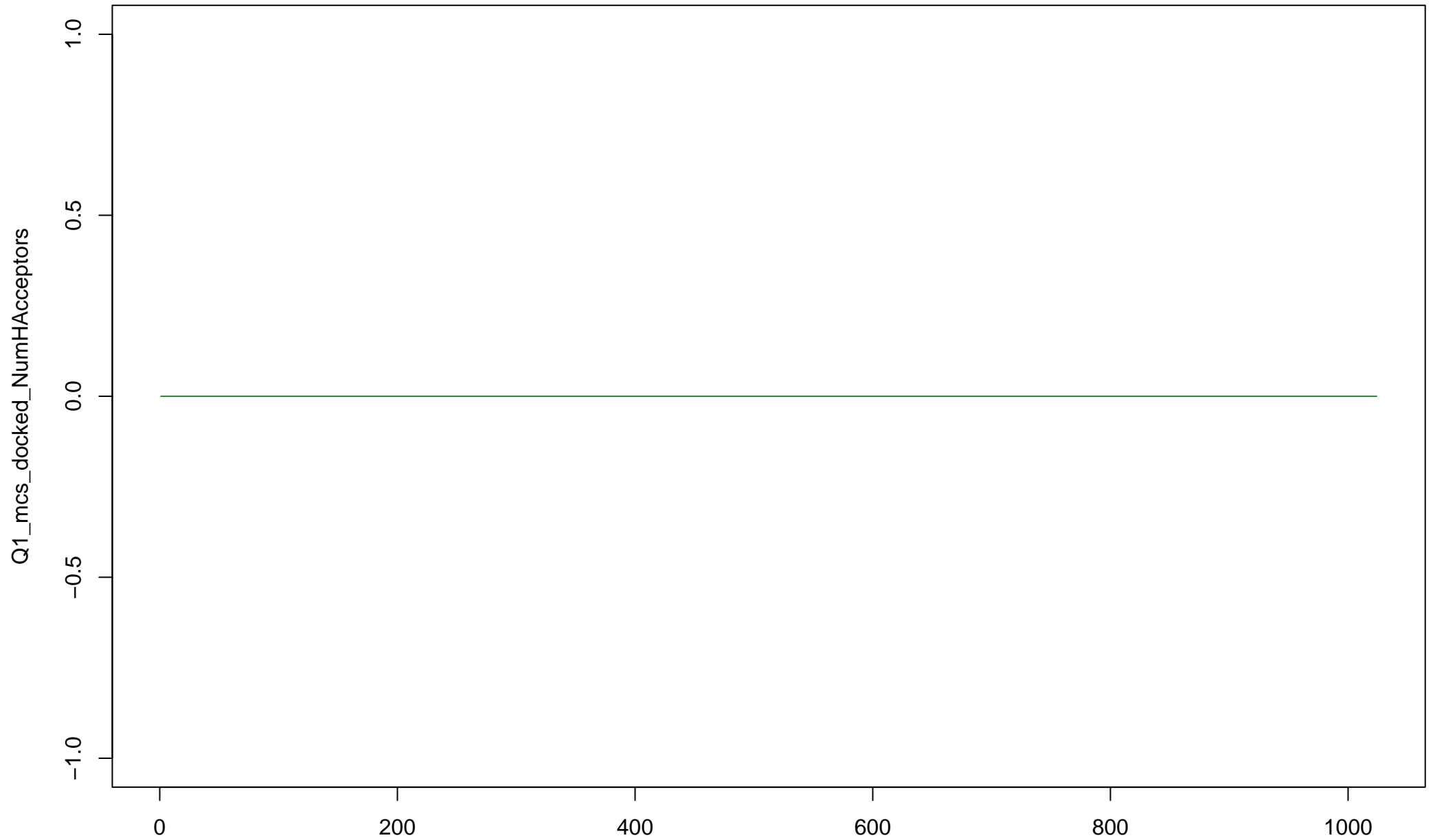
Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



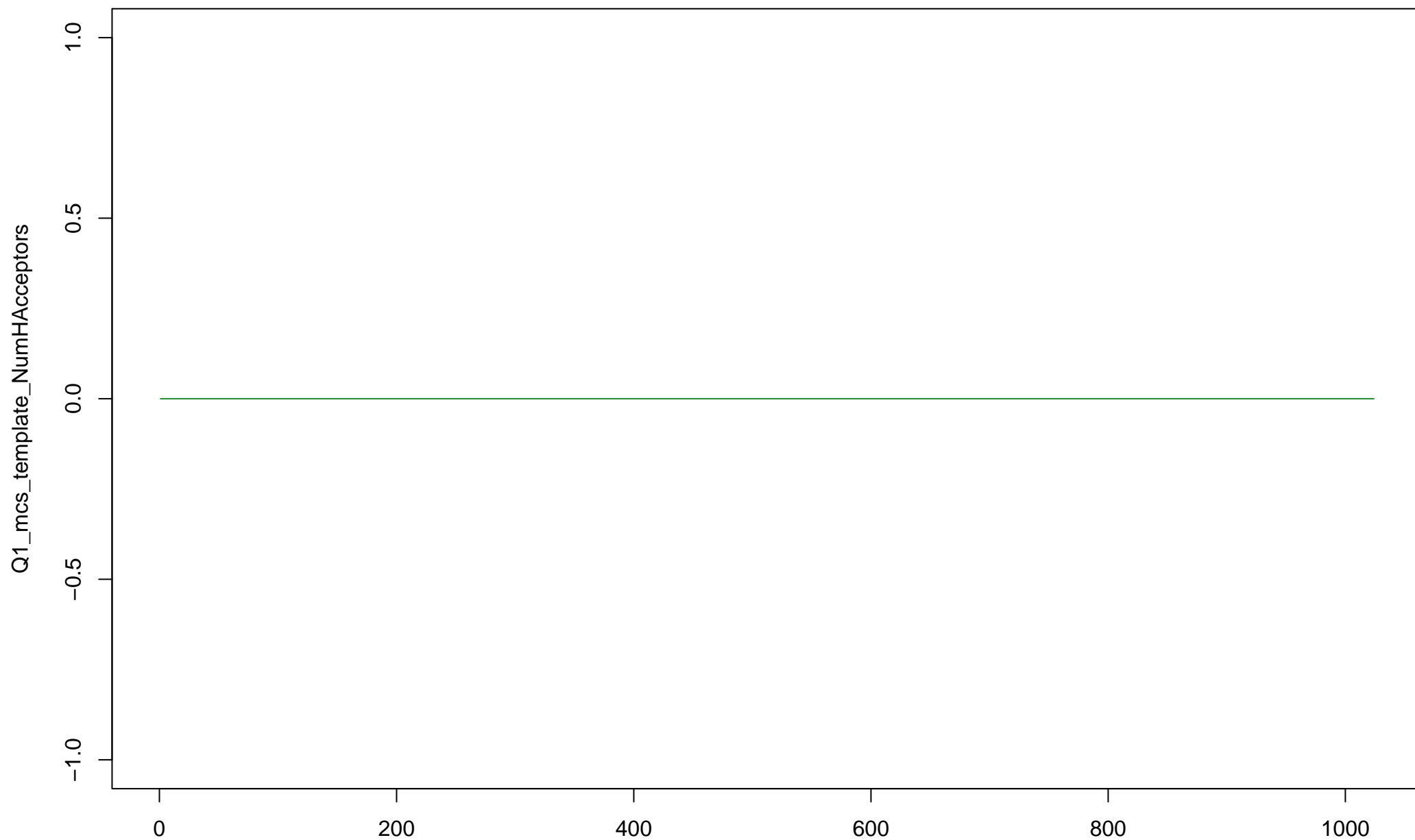
Q1_template_HeavyAtomCount
ESS = 652 | BMK = 0.113 | MCSE(6.27) = 3.81 | stat: FALSE | burn: 0



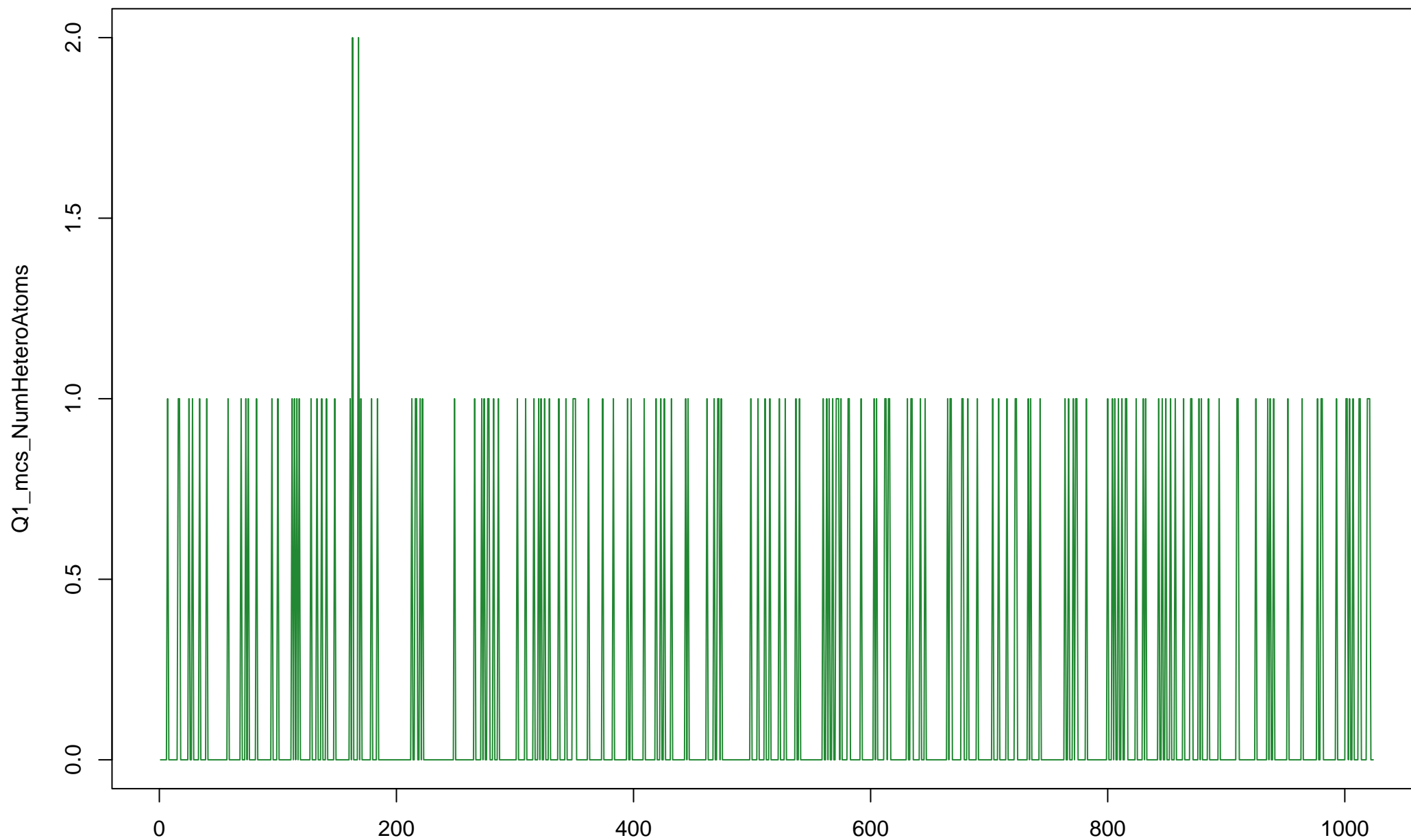
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



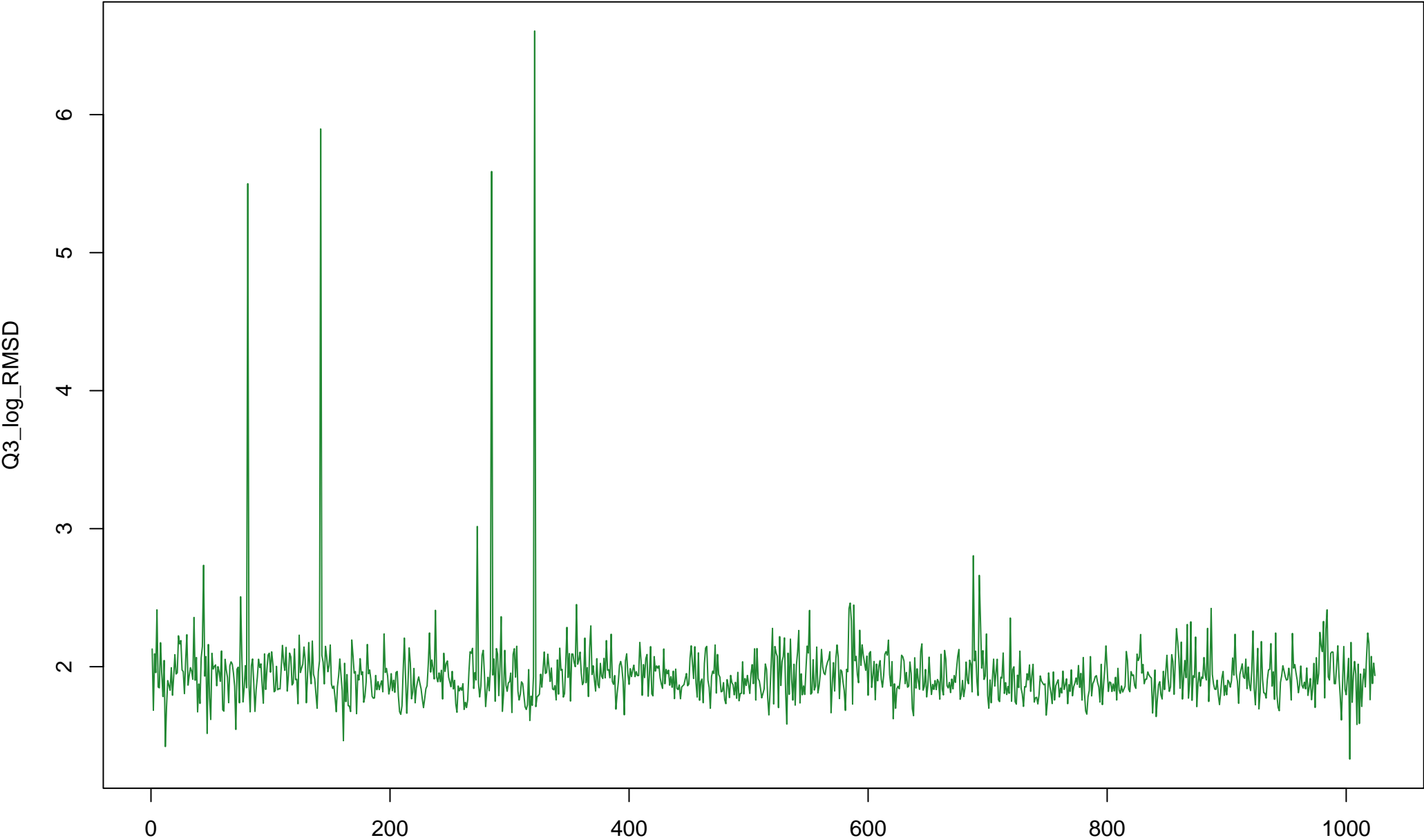
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



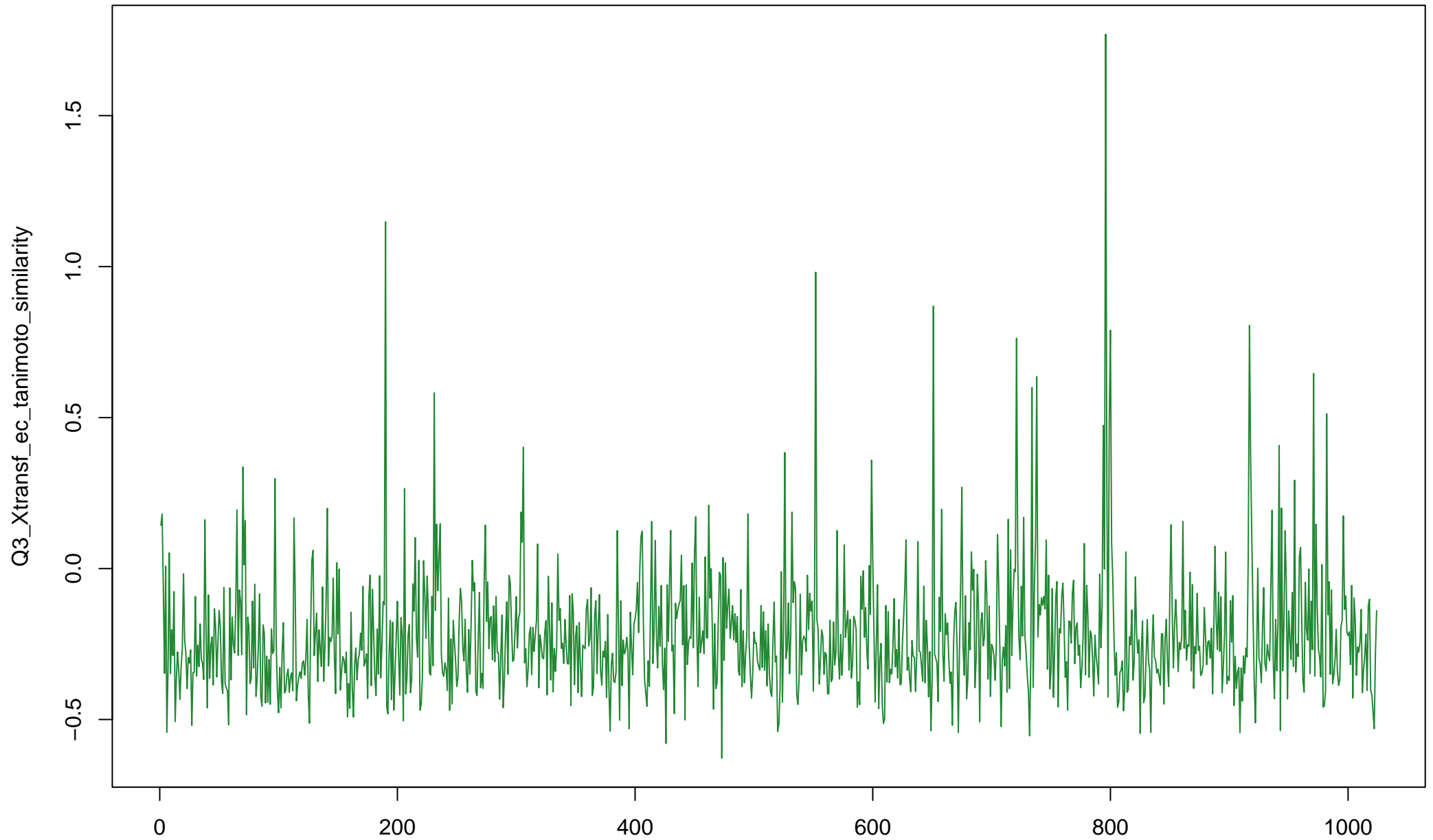
Q1_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0493 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0



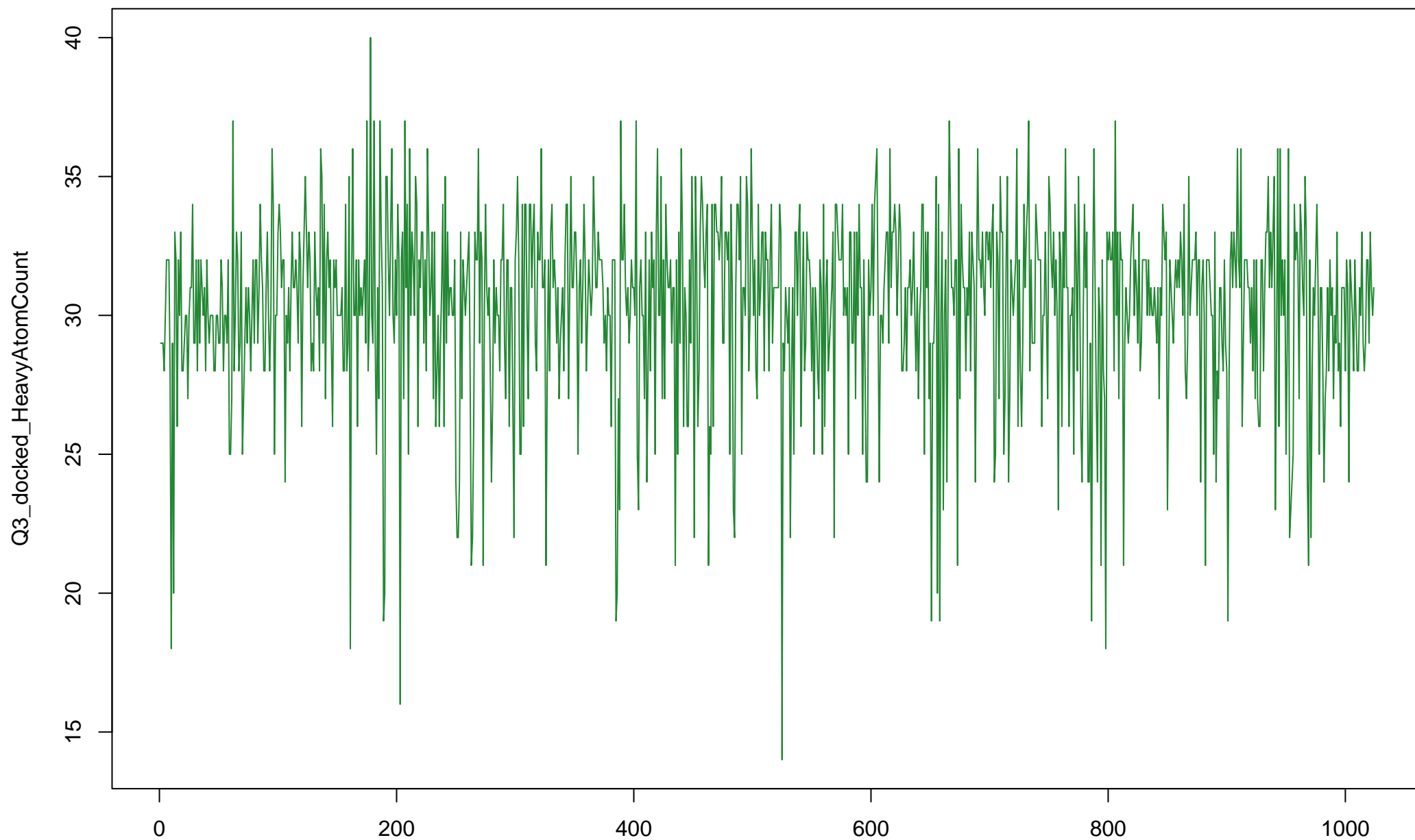
Q3_log_RMSD
ESS = 1020 | BMK = 0.109 | MCSE(6.27) = 3.44 | stat: TRUE | burn: 0



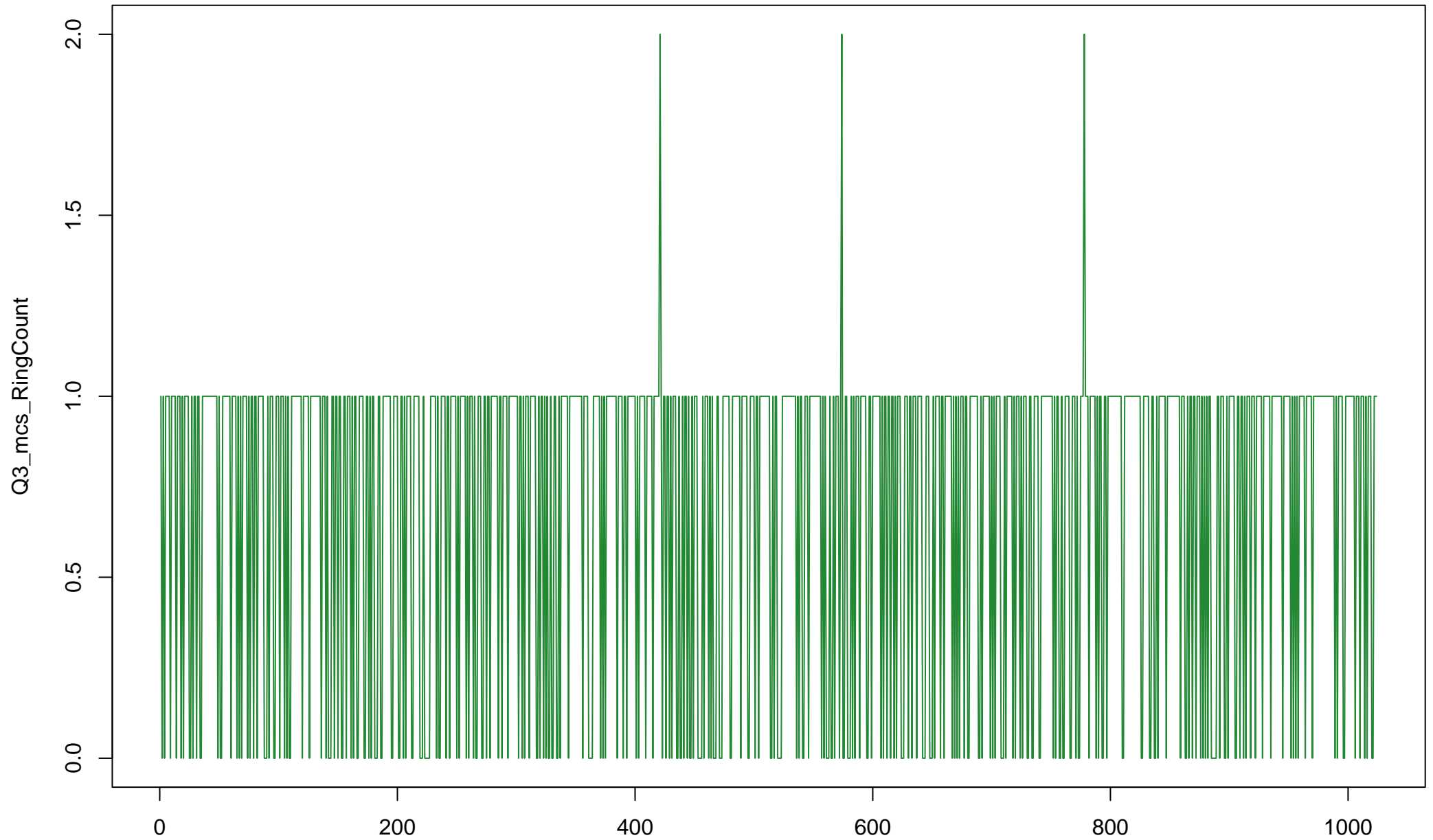
Q3_Xtransf_ec_tanimoto_similarity
ESS = 618 | BMK = 0.0968 | MCSE(6.27) = 3.85 | stat: TRUE | burn: 0



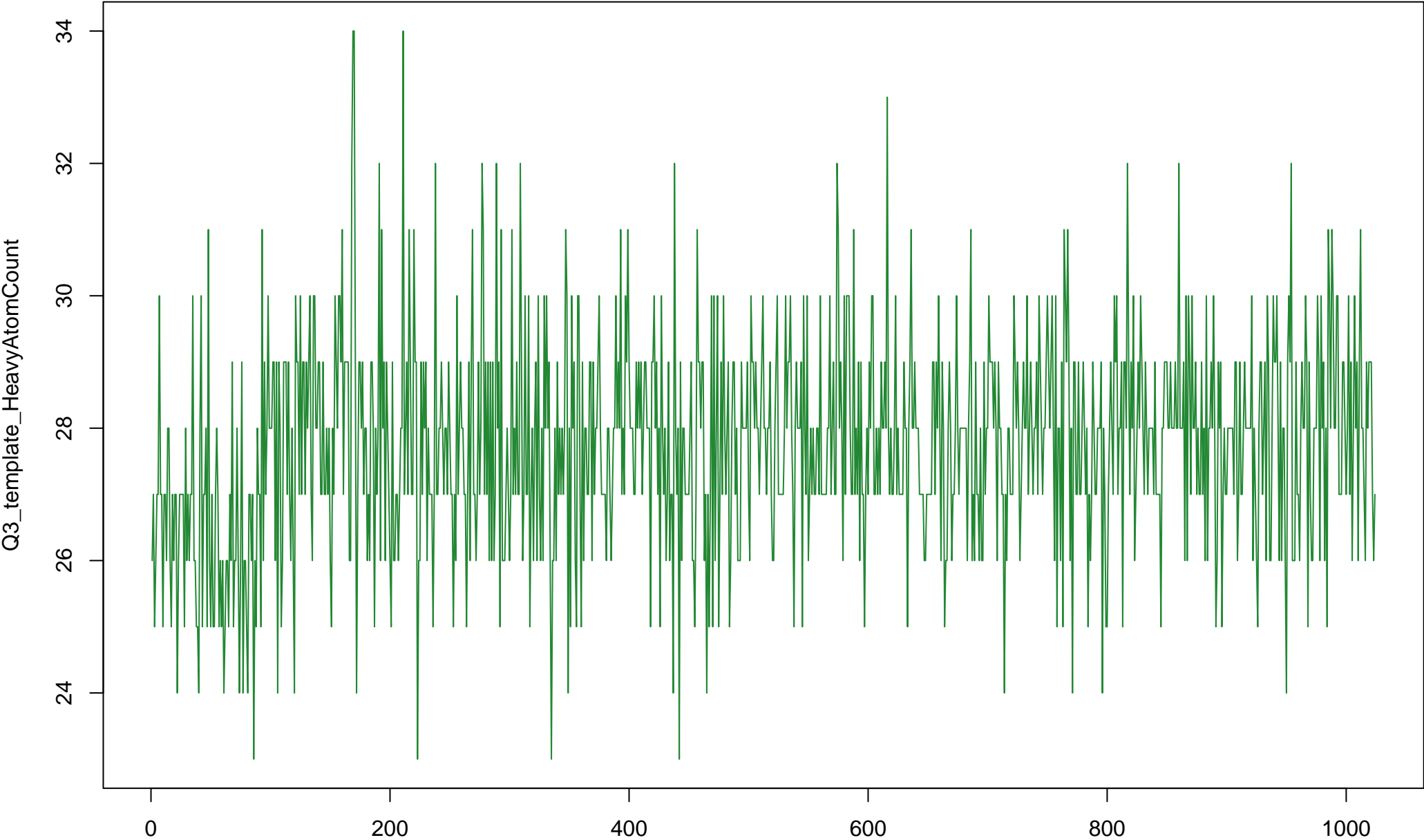
Q3_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0749 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0



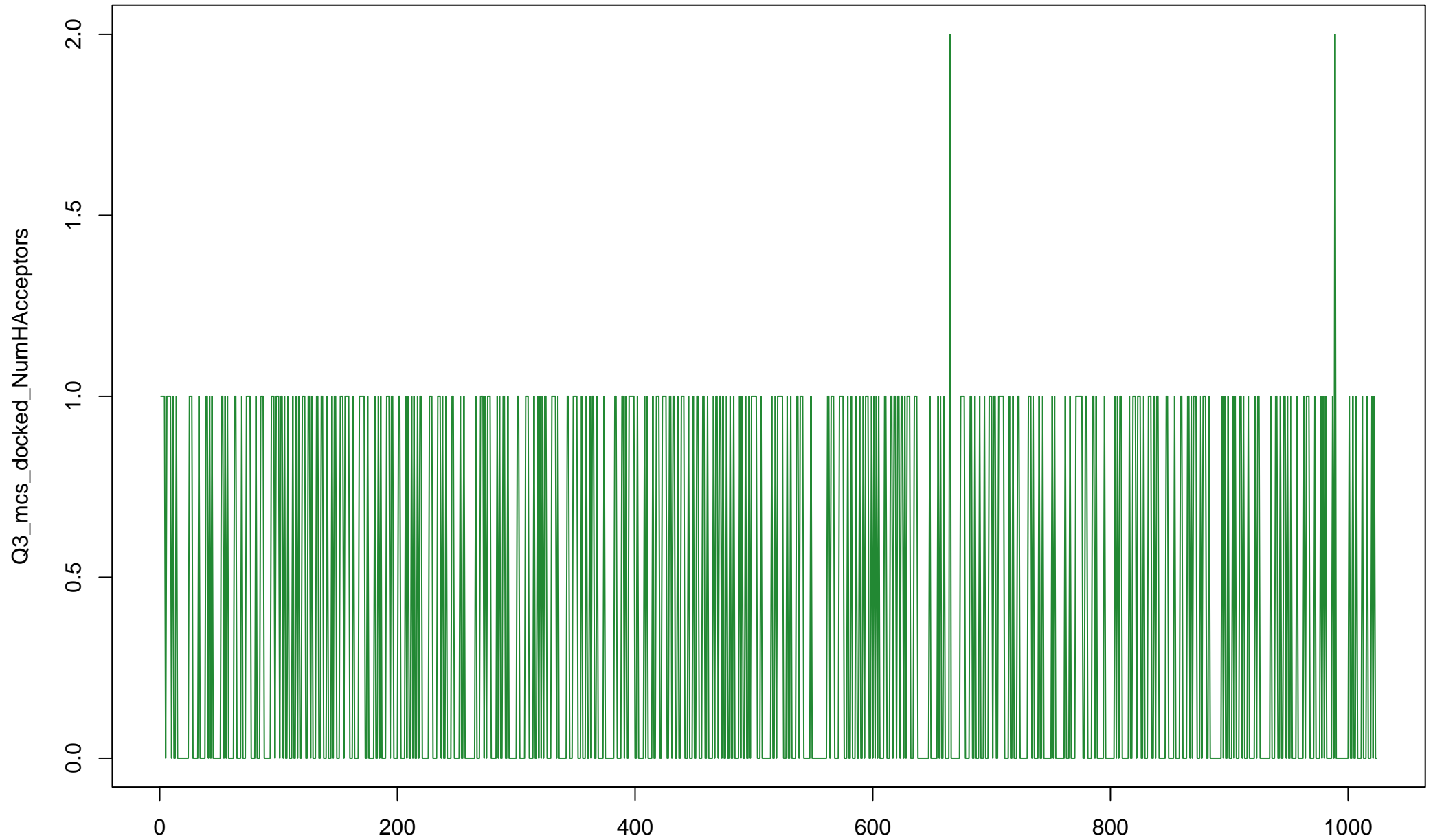
Q3_mcs_RingCount
ESS = 1020 | BMK = 0.0124 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0



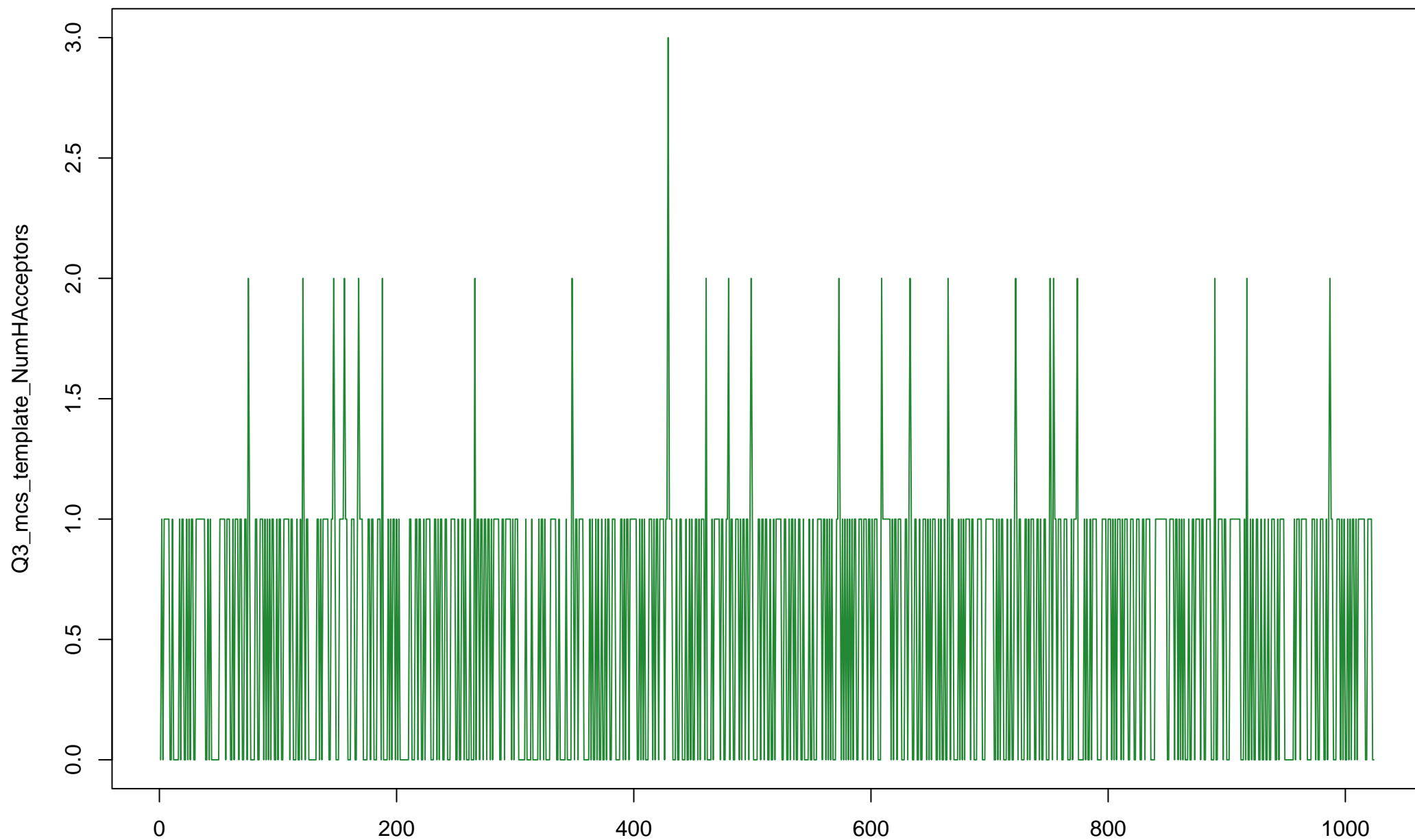
Q3_template_HeavyAtomCount
ESS = 312 | BMK = 0.138 | MCSE(6.27) = 5.65 | stat: FALSE | burn: 0



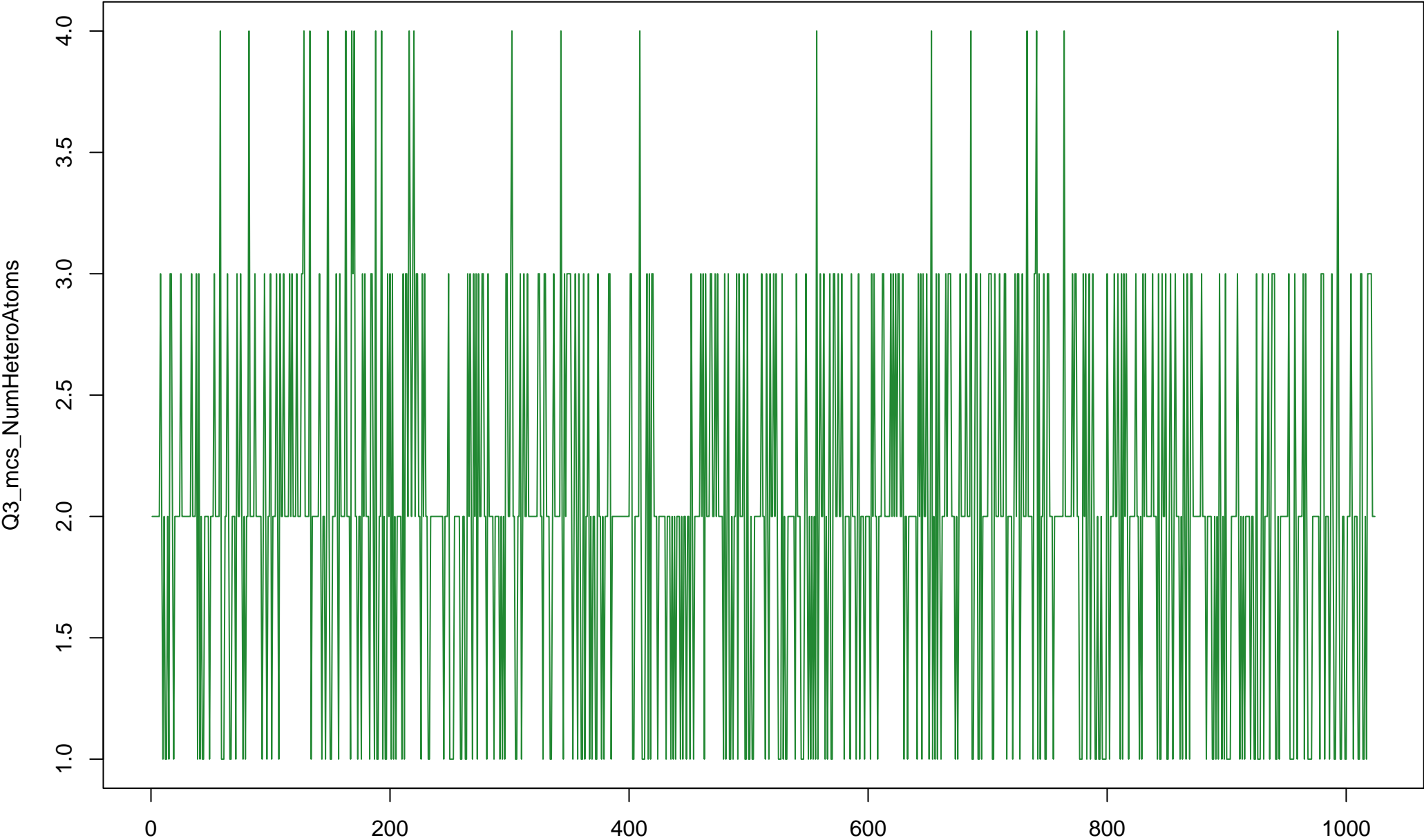
Q3_mcs_docked_NumHAcceptors
ESS = 915 | BMK = 0.0468 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0



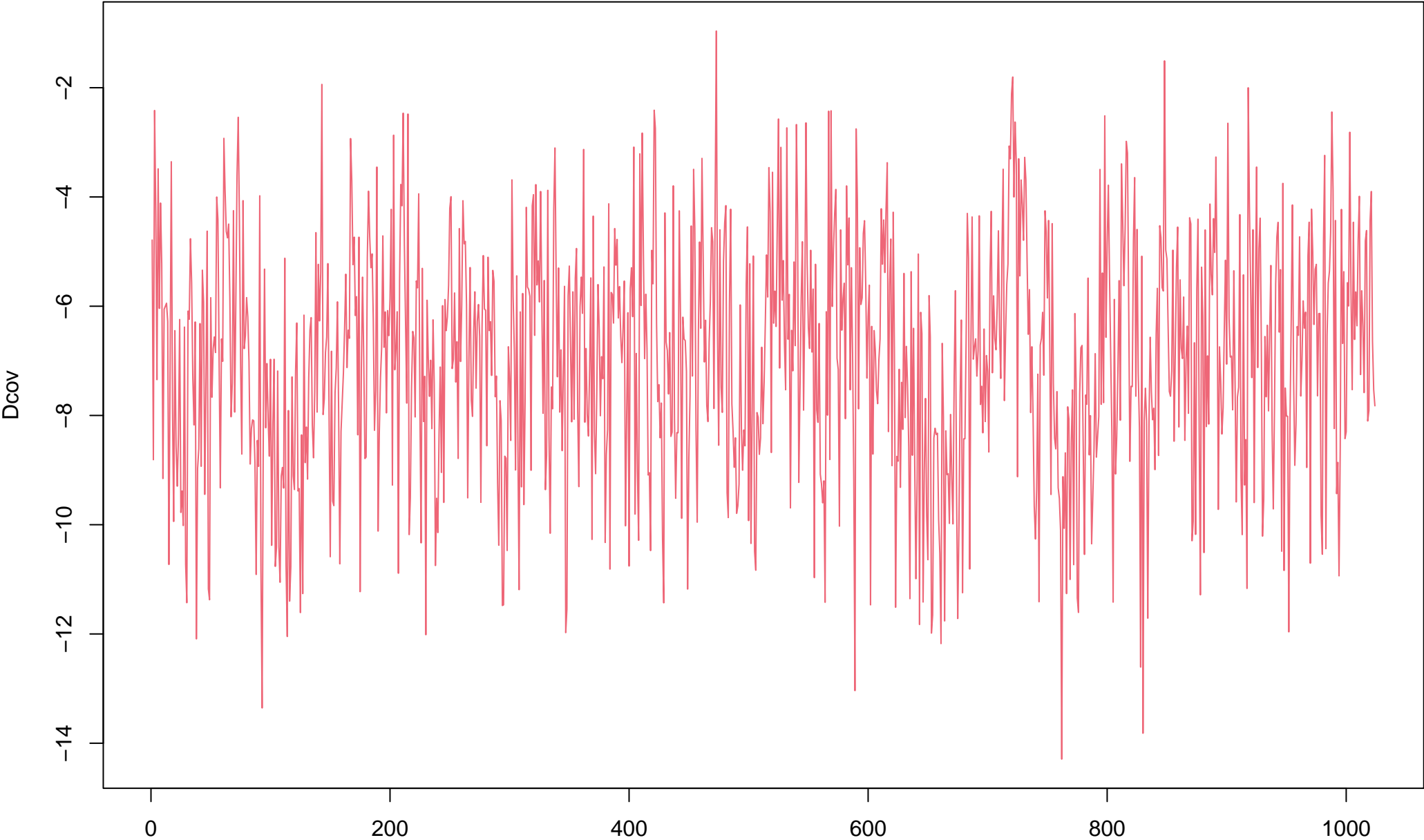
Q3_mcs_template_NumHAcceptors
ESS = 1020 | BMK = 0.0345 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0



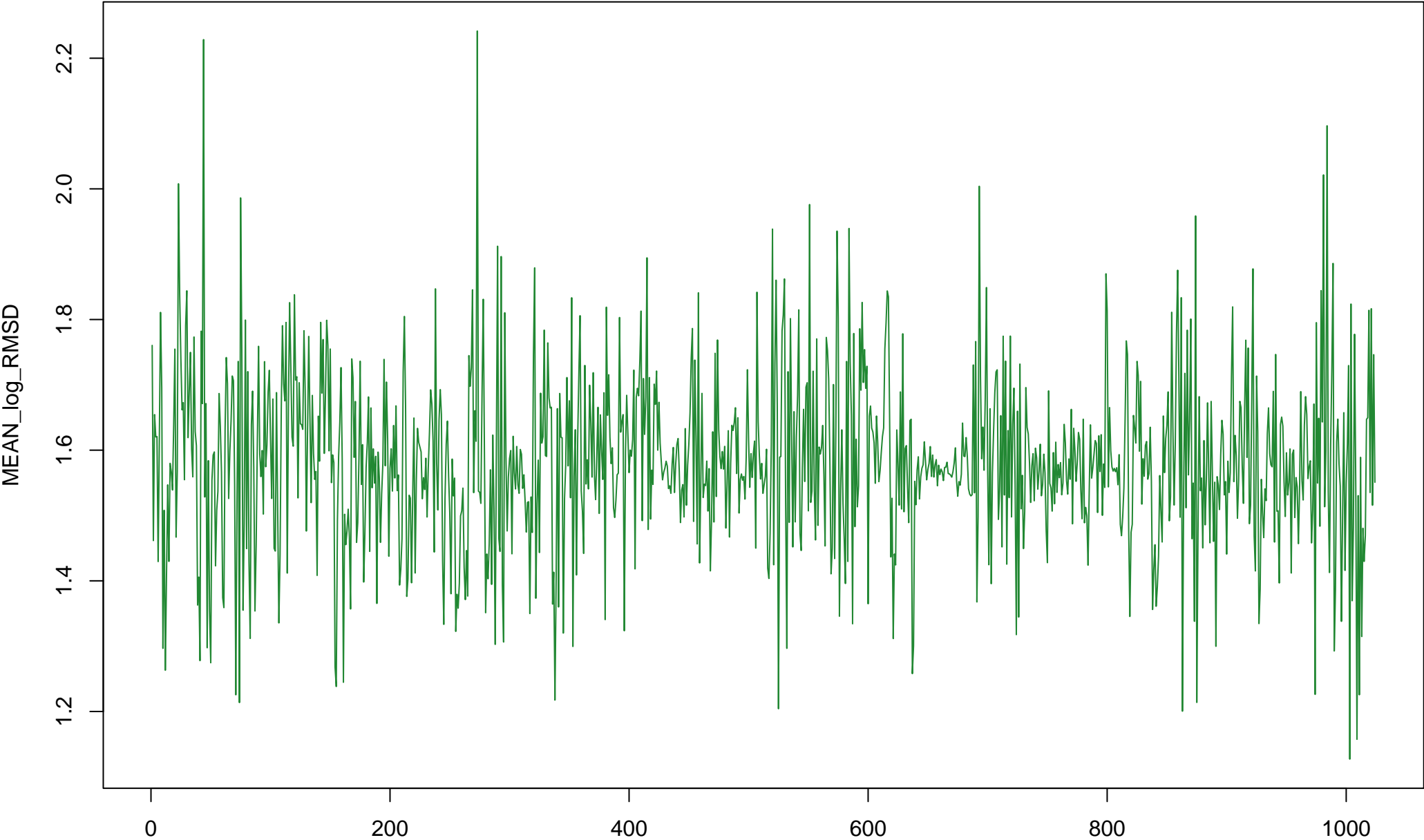
Q3_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0494 | MCSE(6.27) = 3.6 | stat: TRUE | burn: 0



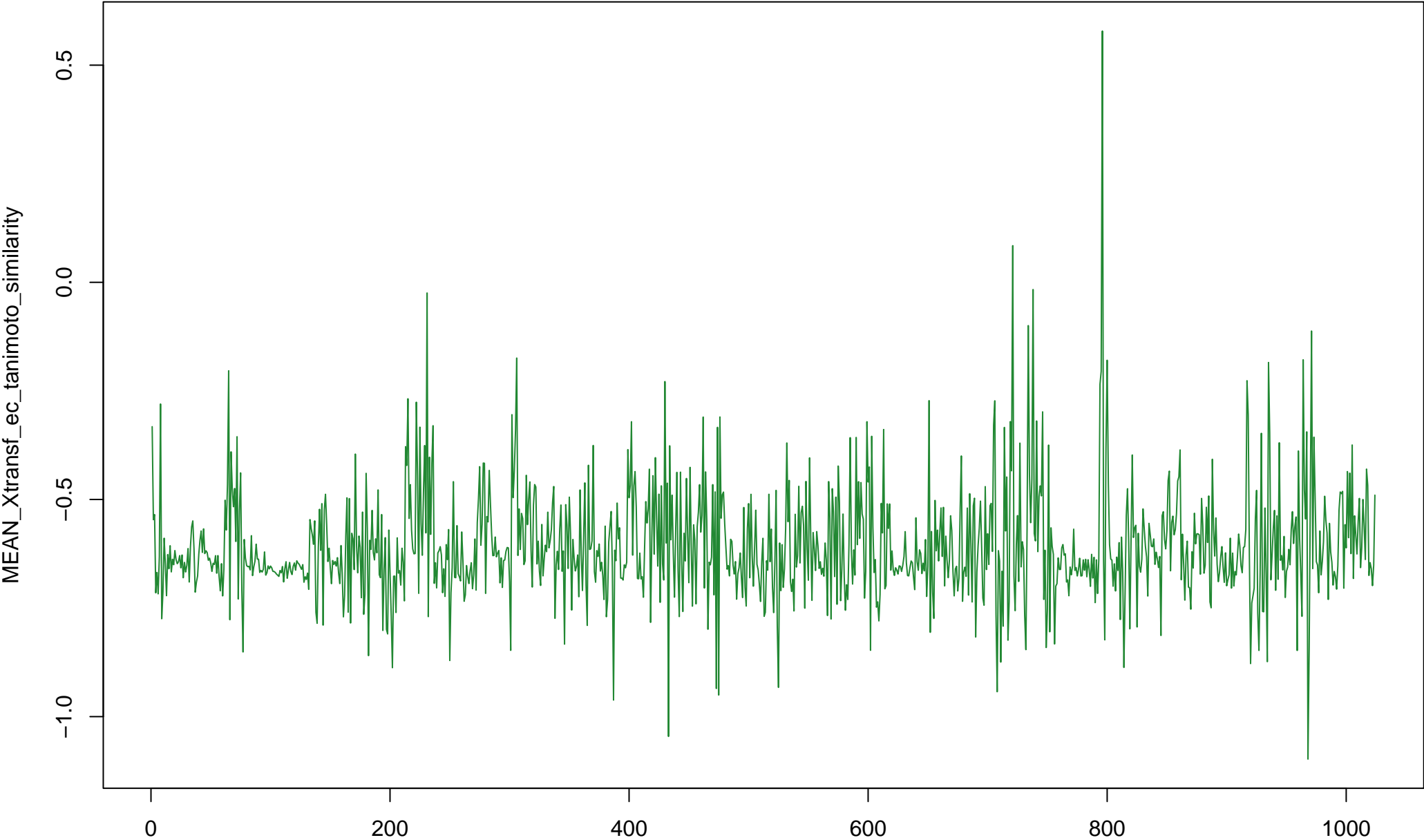
Dcov
ESS = 1020 | BMK = 0.223 | MCSE(6.27) = 3.26 | stat: TRUE | burn: 0



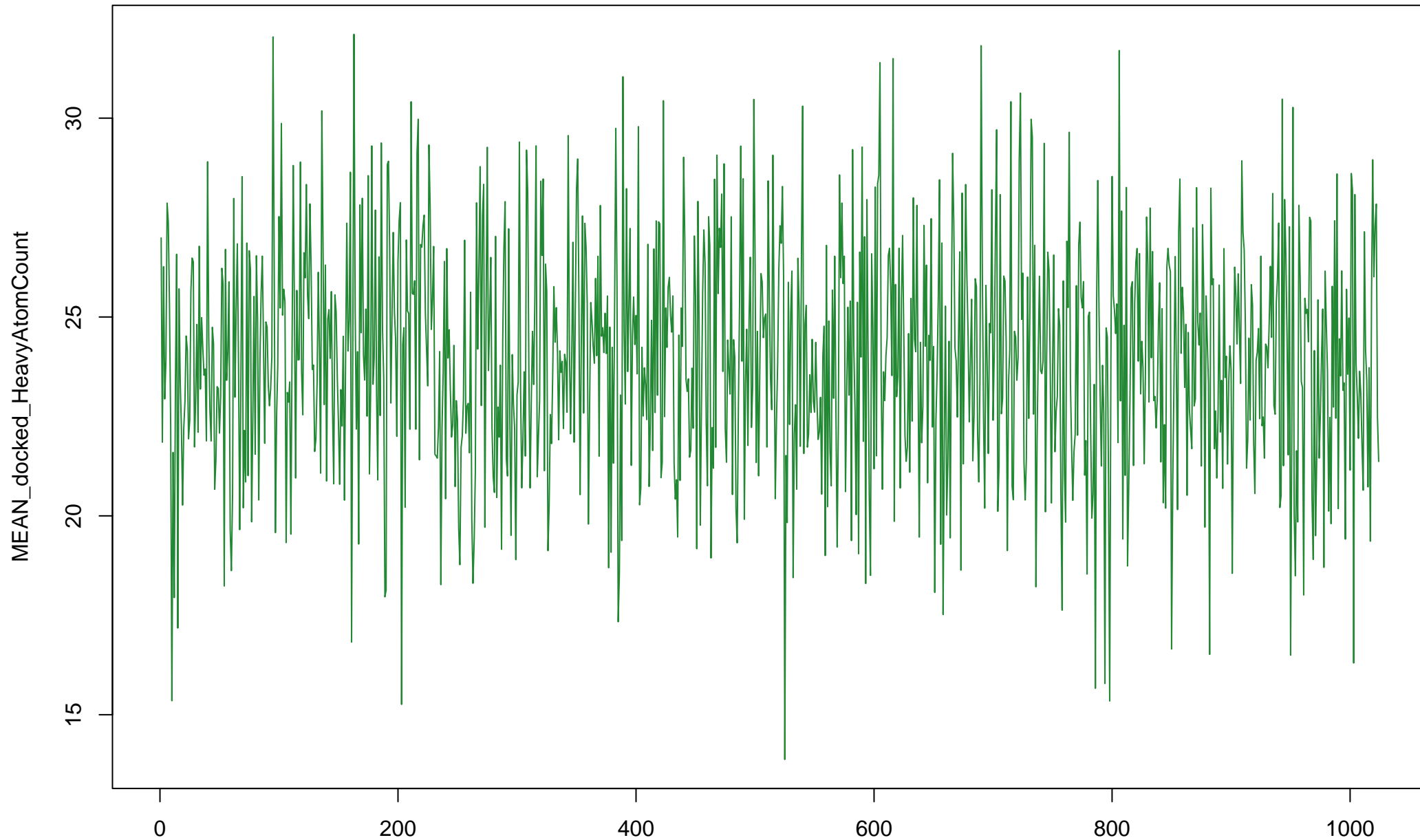
MEAN_log_RMSD
ESS = 890 | BMK = 0.0959 | MCSE(6.27) = 3.28 | stat: TRUE | burn: 0



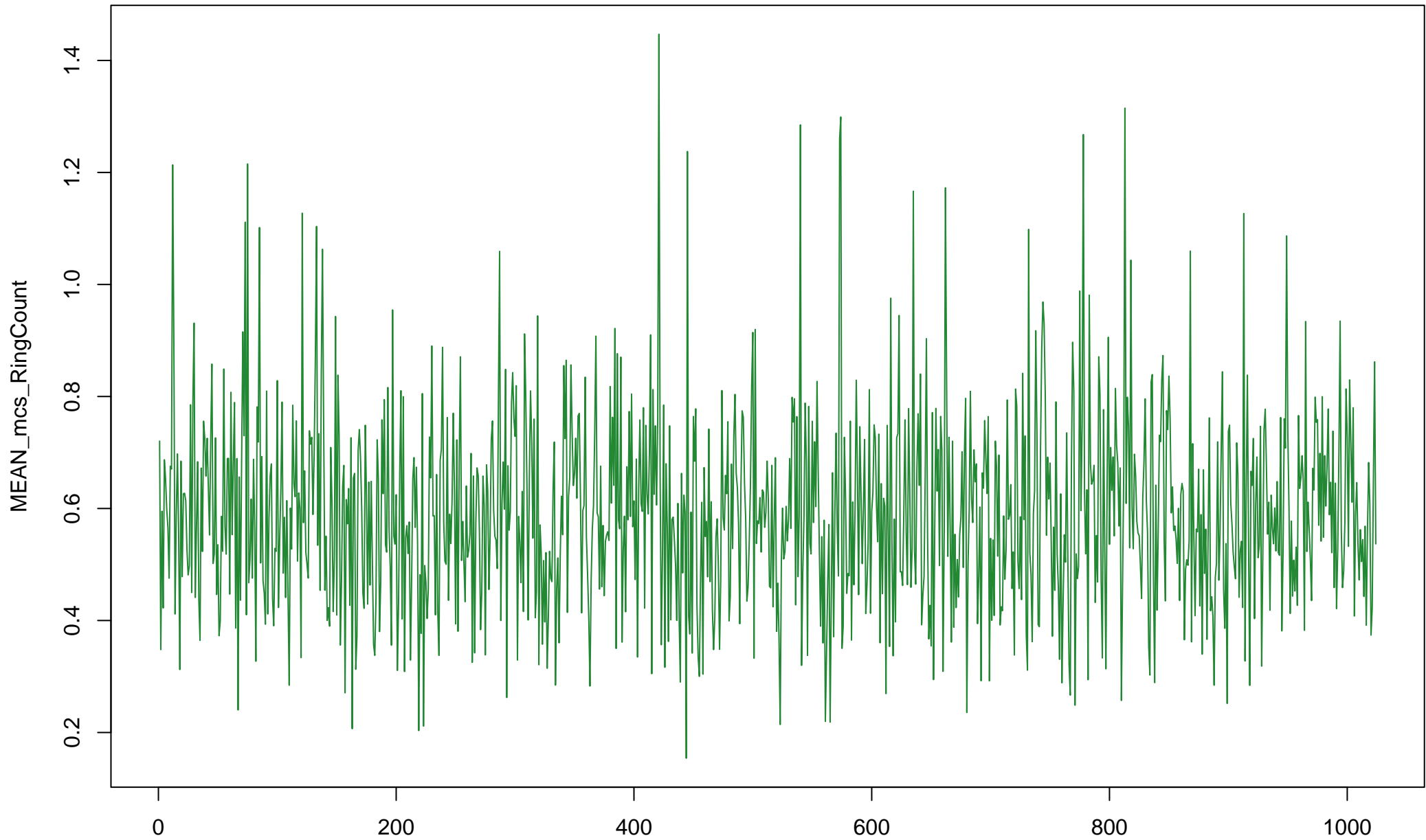
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 446 | BMK = 0.0896 | MCSE(6.27) = 3.38 | stat: TRUE | burn: 0



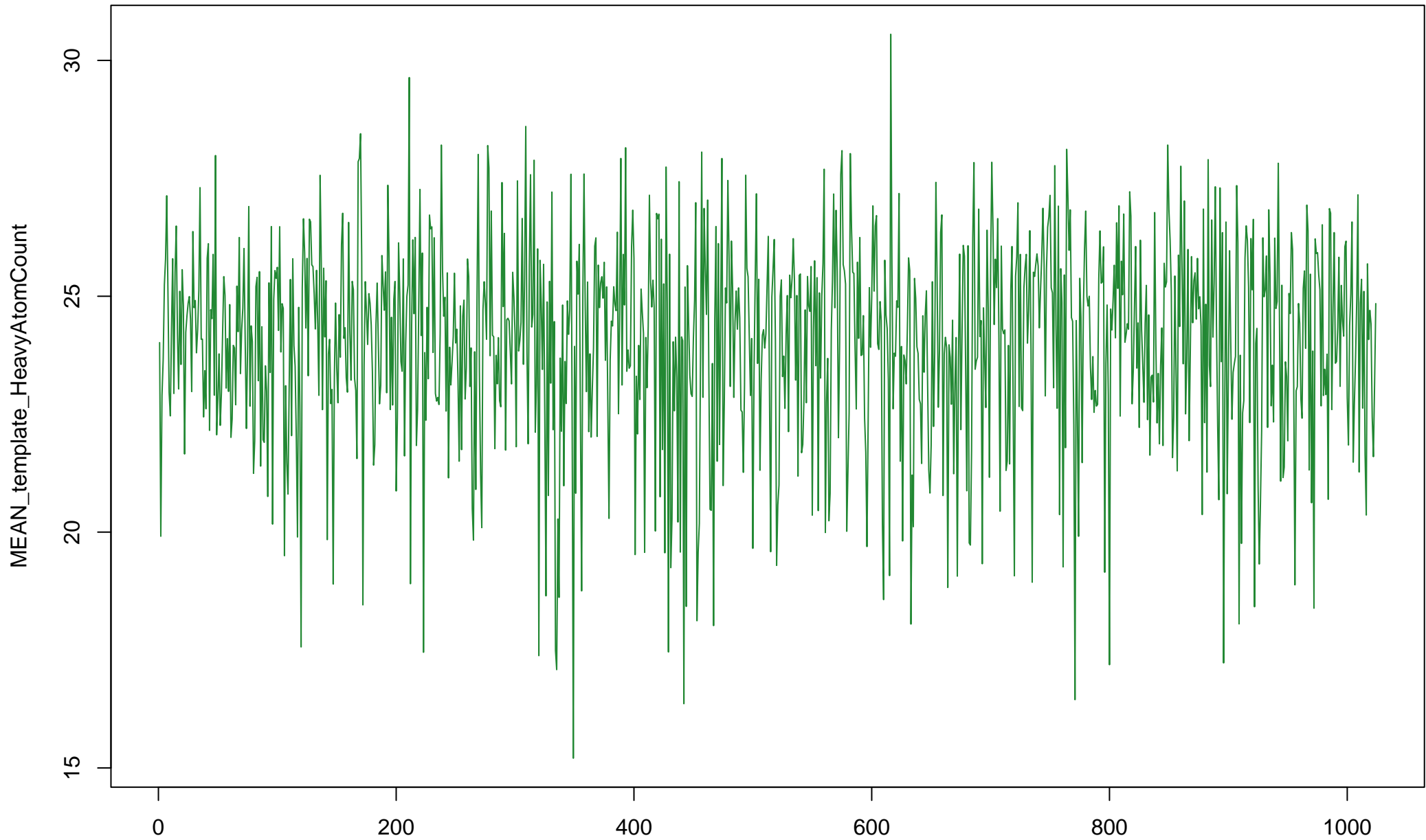
MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0421 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0



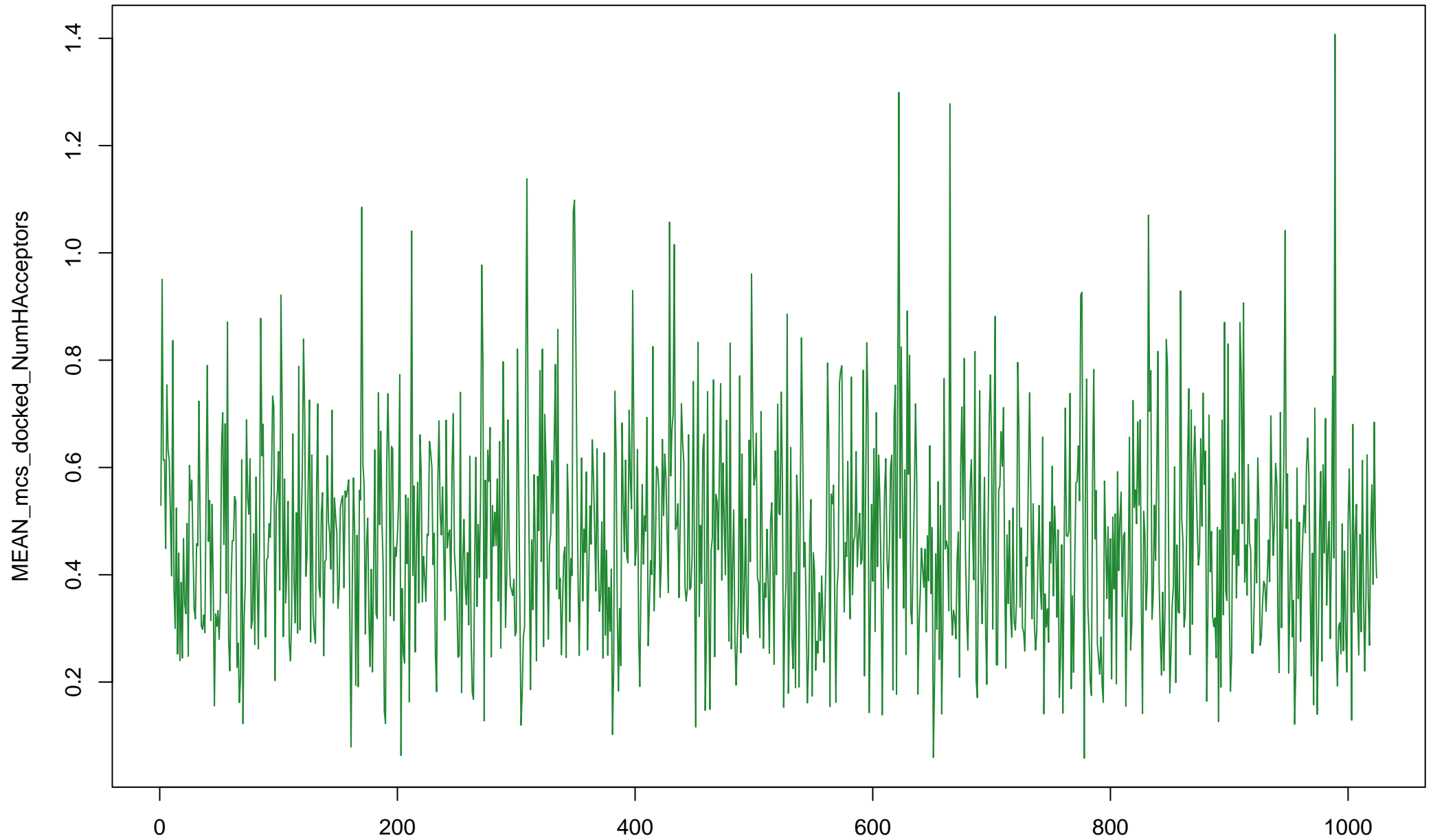
MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0549 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0



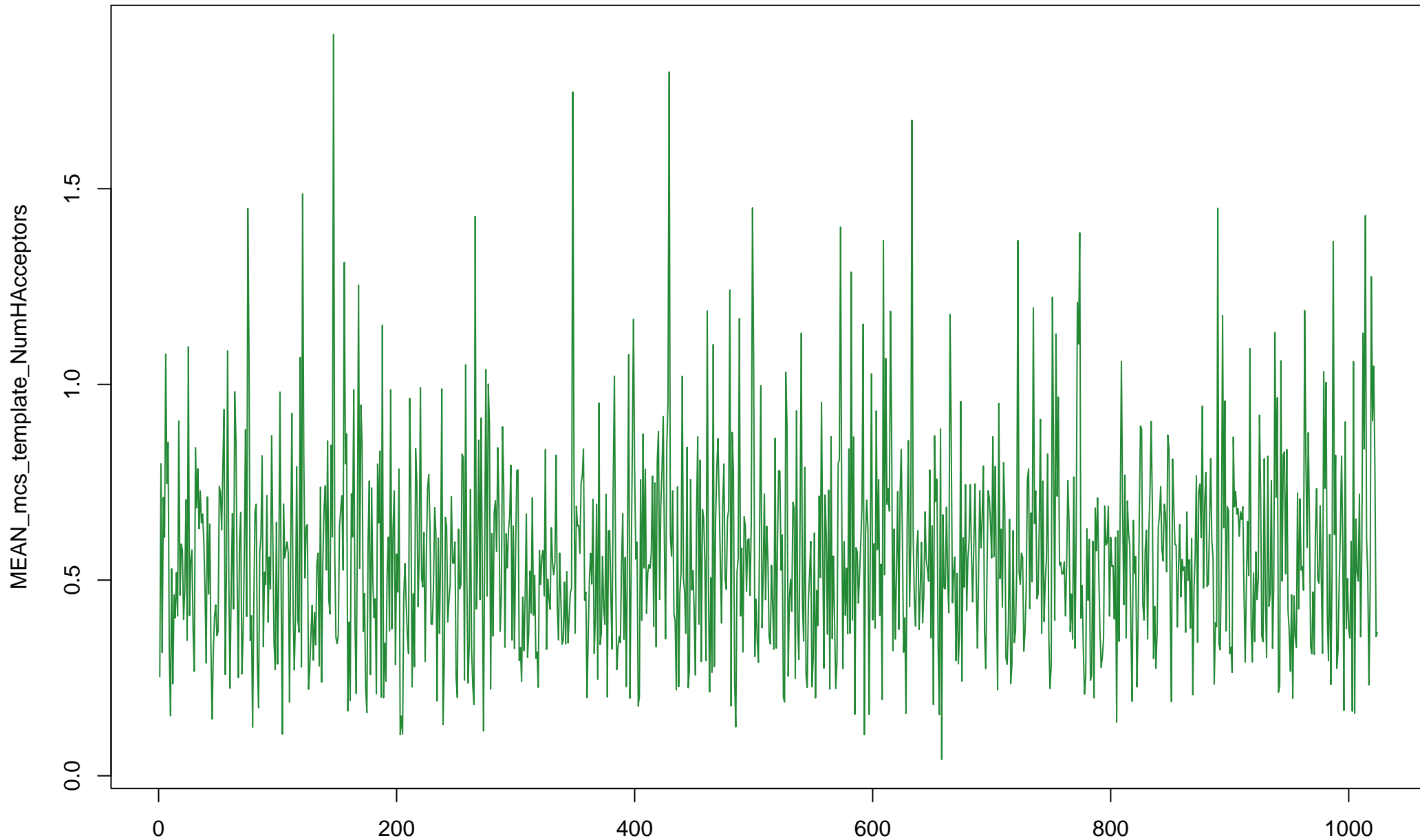
MEAN_template_HeavyAtomCount
ESS = 1010 | BMK = 0.0732 | MCSE(6.27) = 3.78 | stat: TRUE | burn: 0



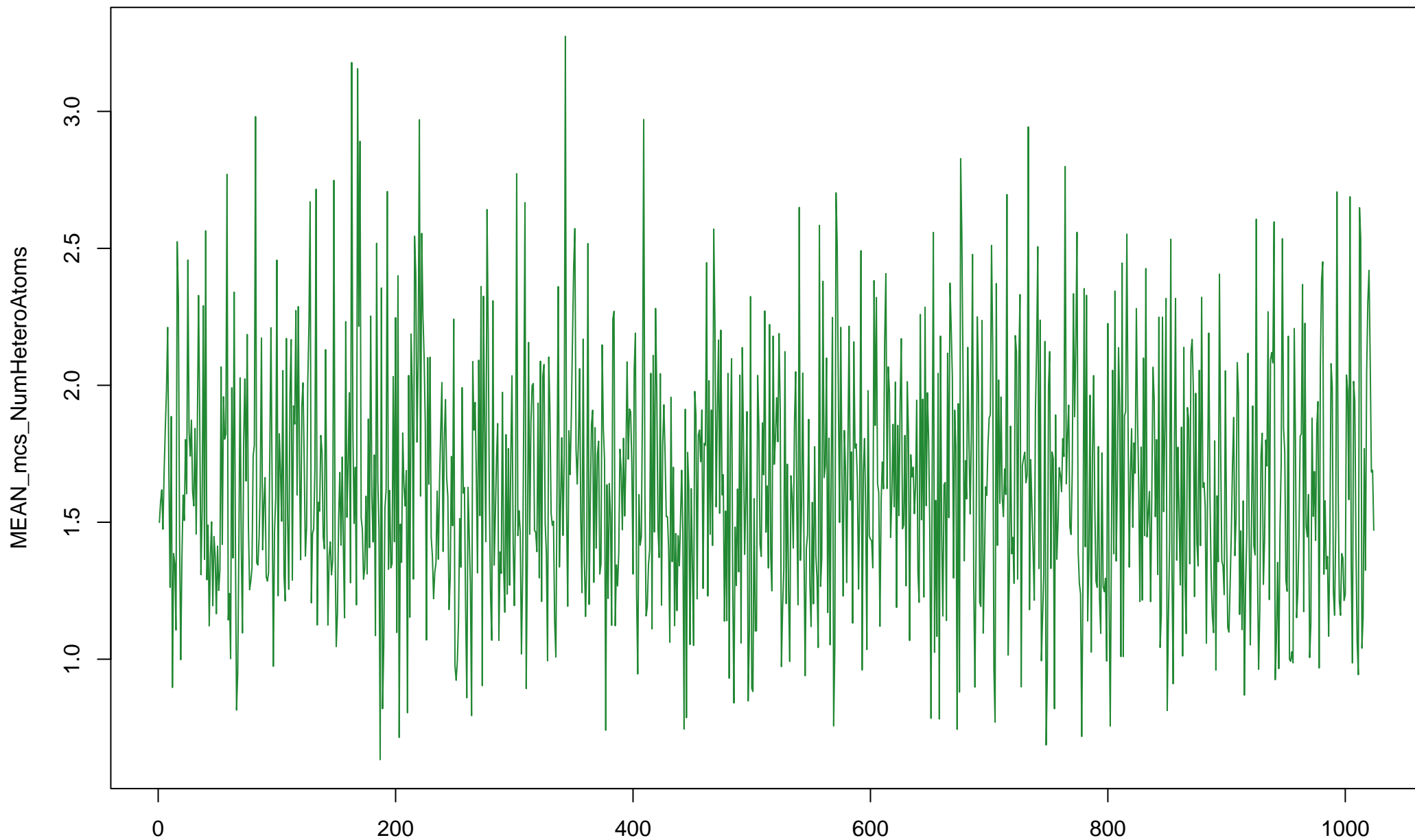
MEAN_mcs_docked_NumHAcceptors
ESS = 831 | BMK = 0.0852 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0



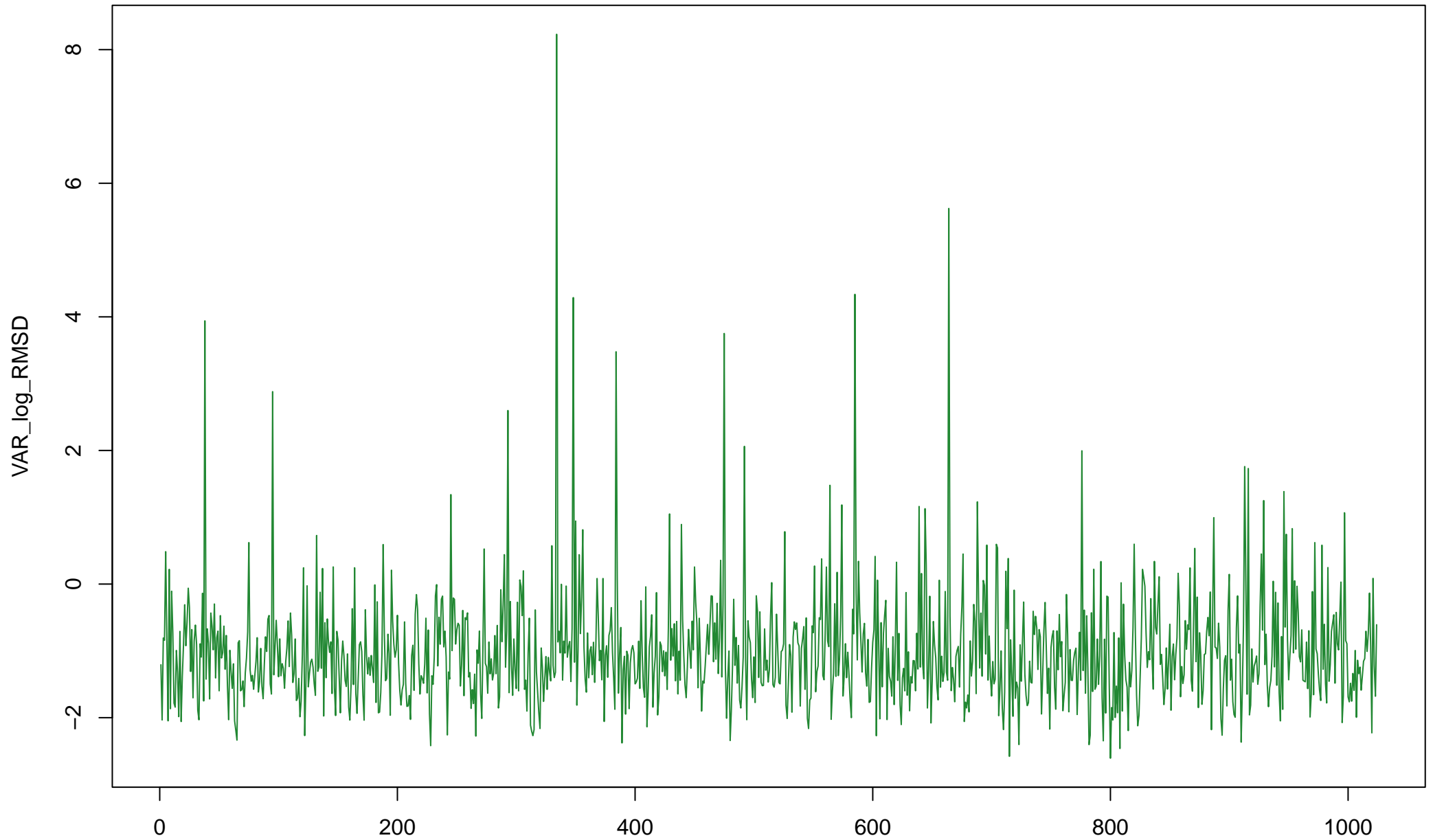
MEAN_mcs_template_NumHAcceptors
ESS = 1020 | BMK = 0.0607 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0



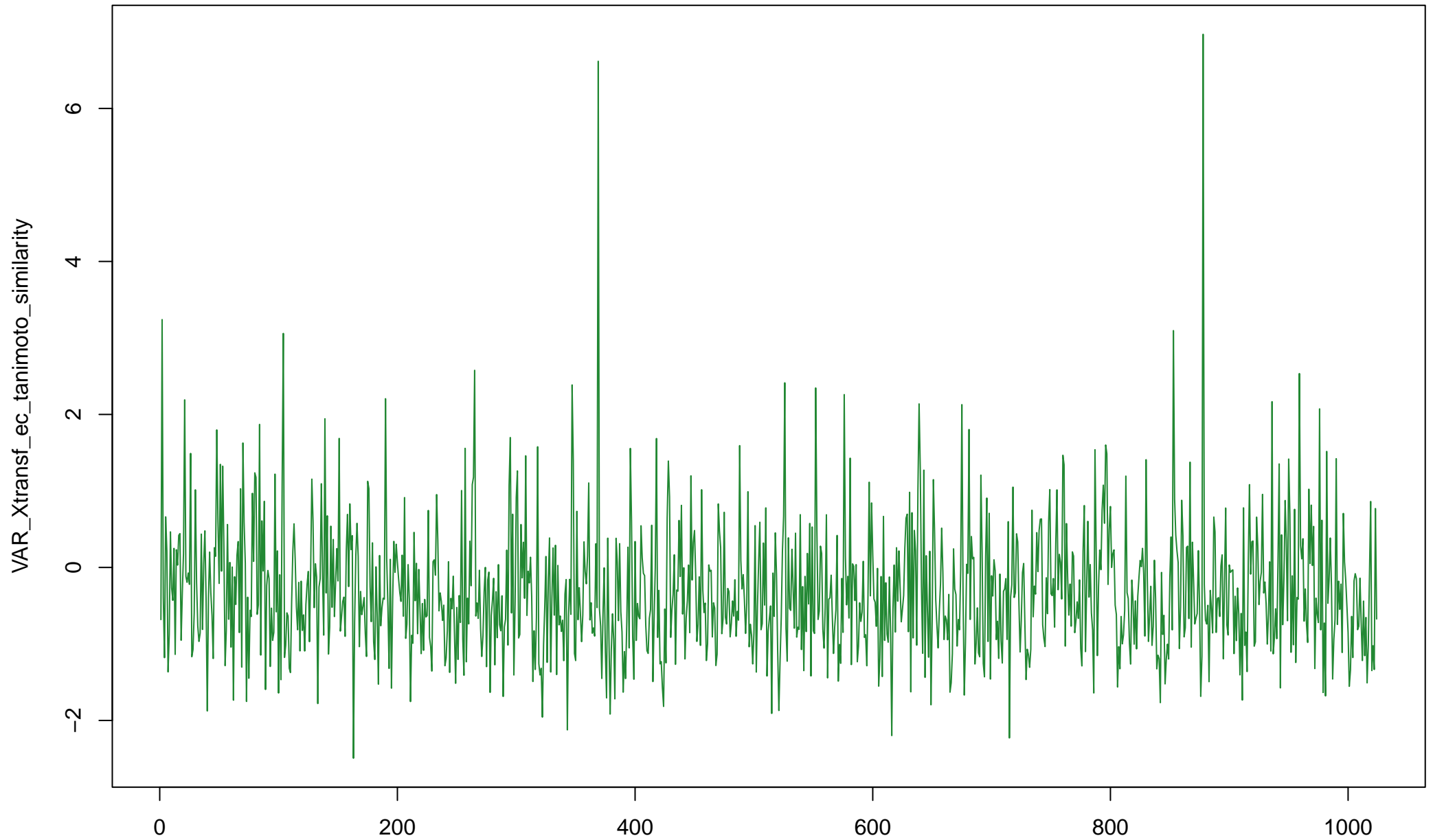
MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0723 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0



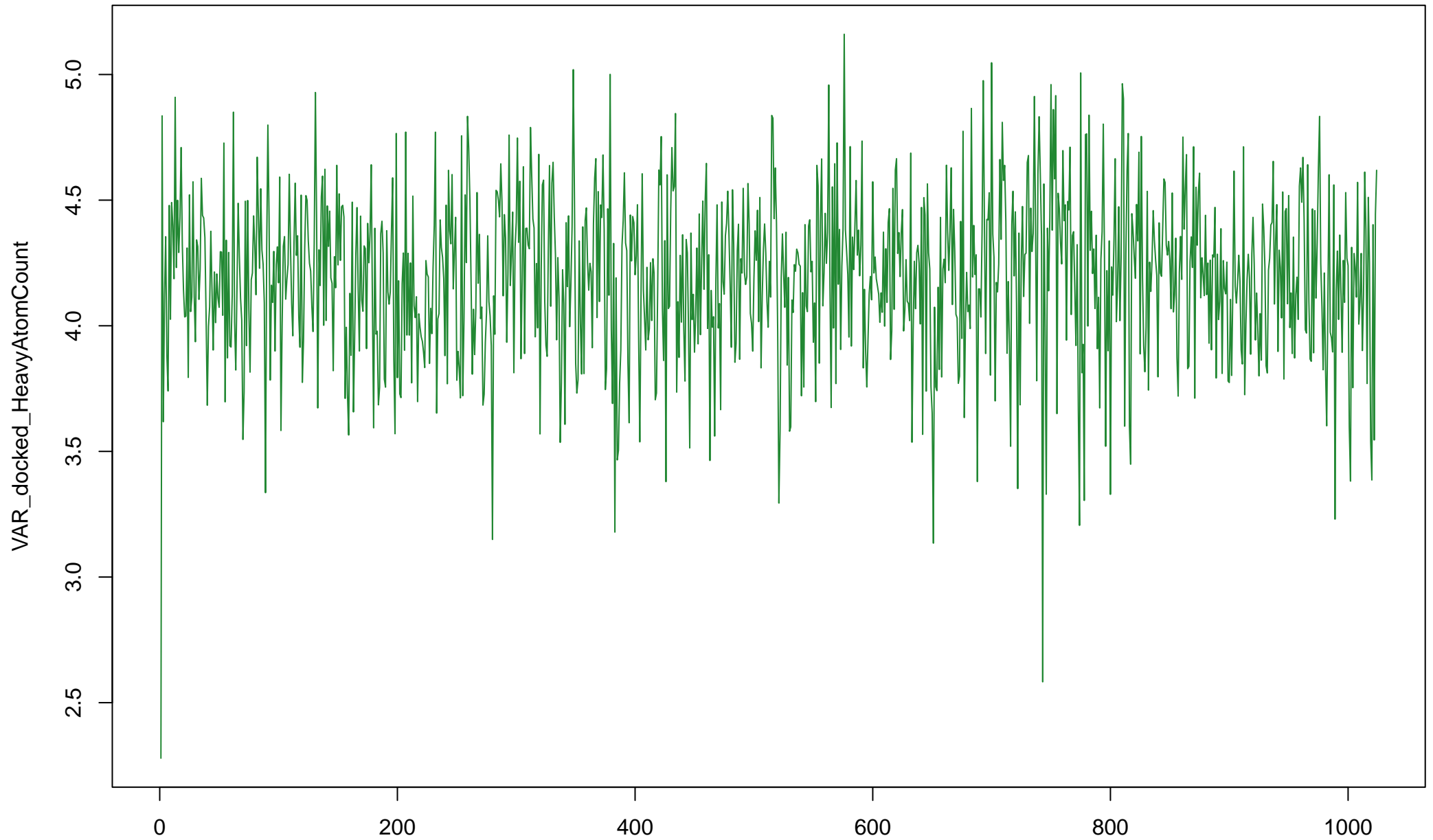
VAR_log_RMSD
ESS = 1020 | BMK = 0.711 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 408



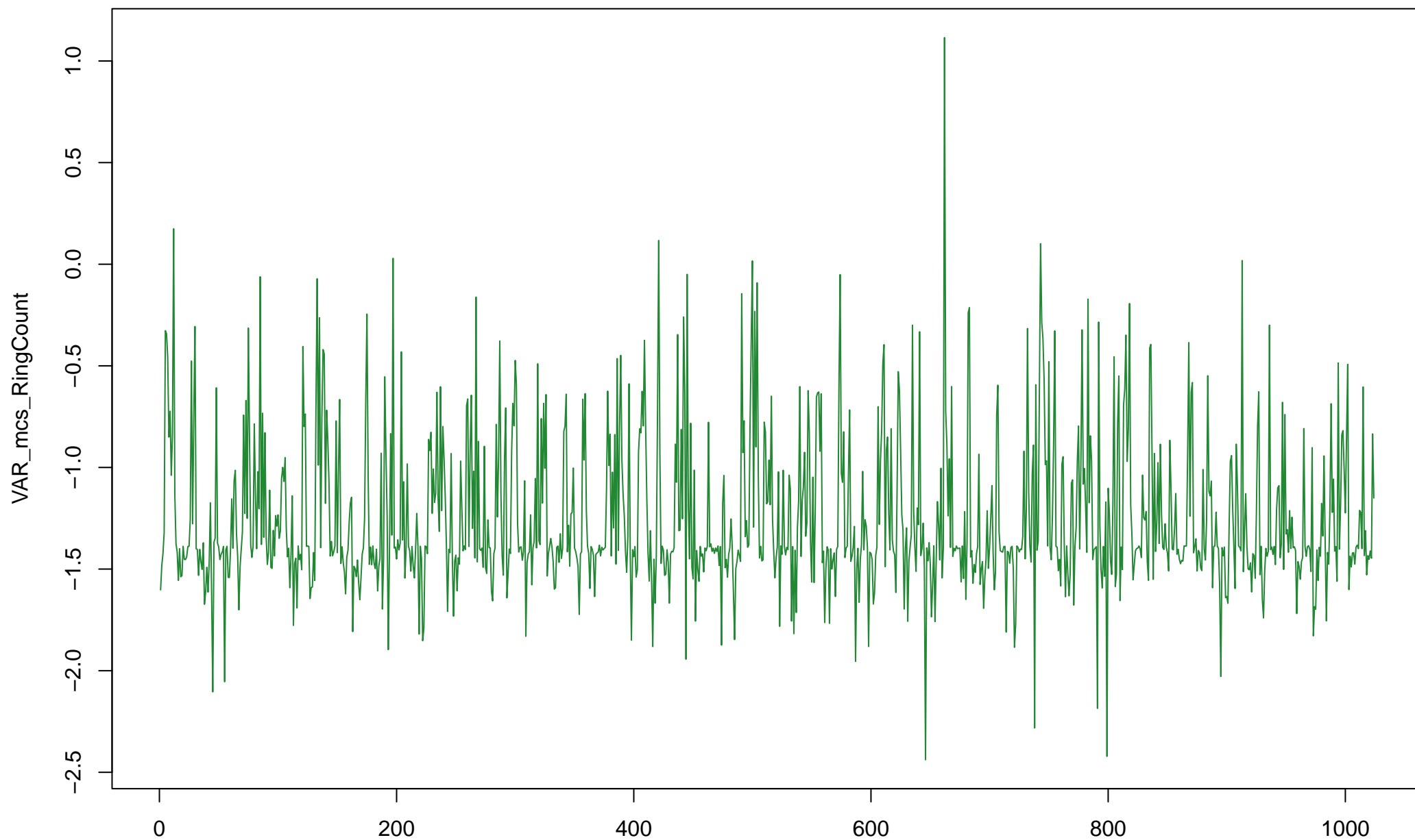
VAR_Xtransf_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.153 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 1020



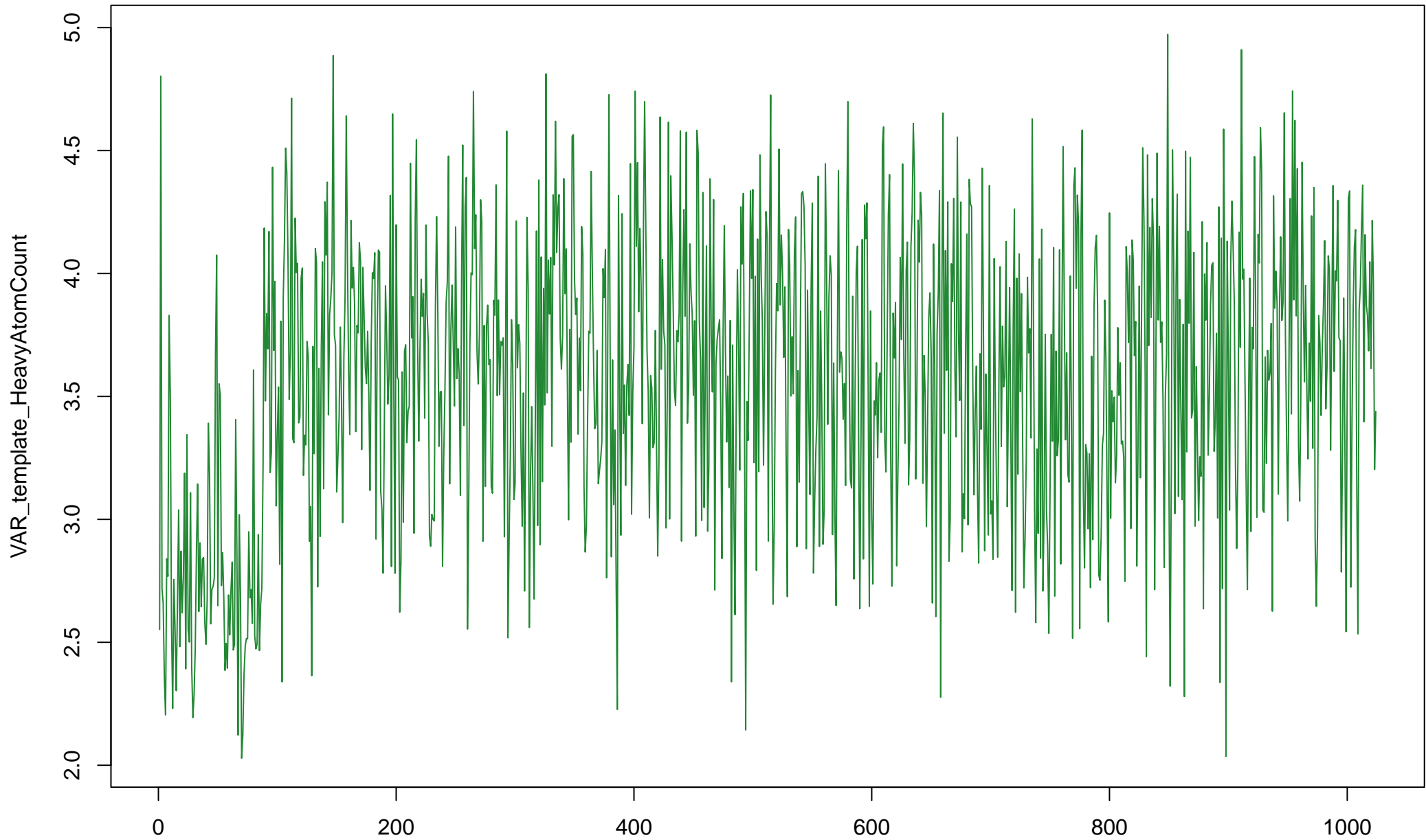
VAR_docked_HeavyAtomCount
ESS = 828 | BMK = 0.0669 | MCSE(6.27) = 3.66 | stat: TRUE | burn: 0



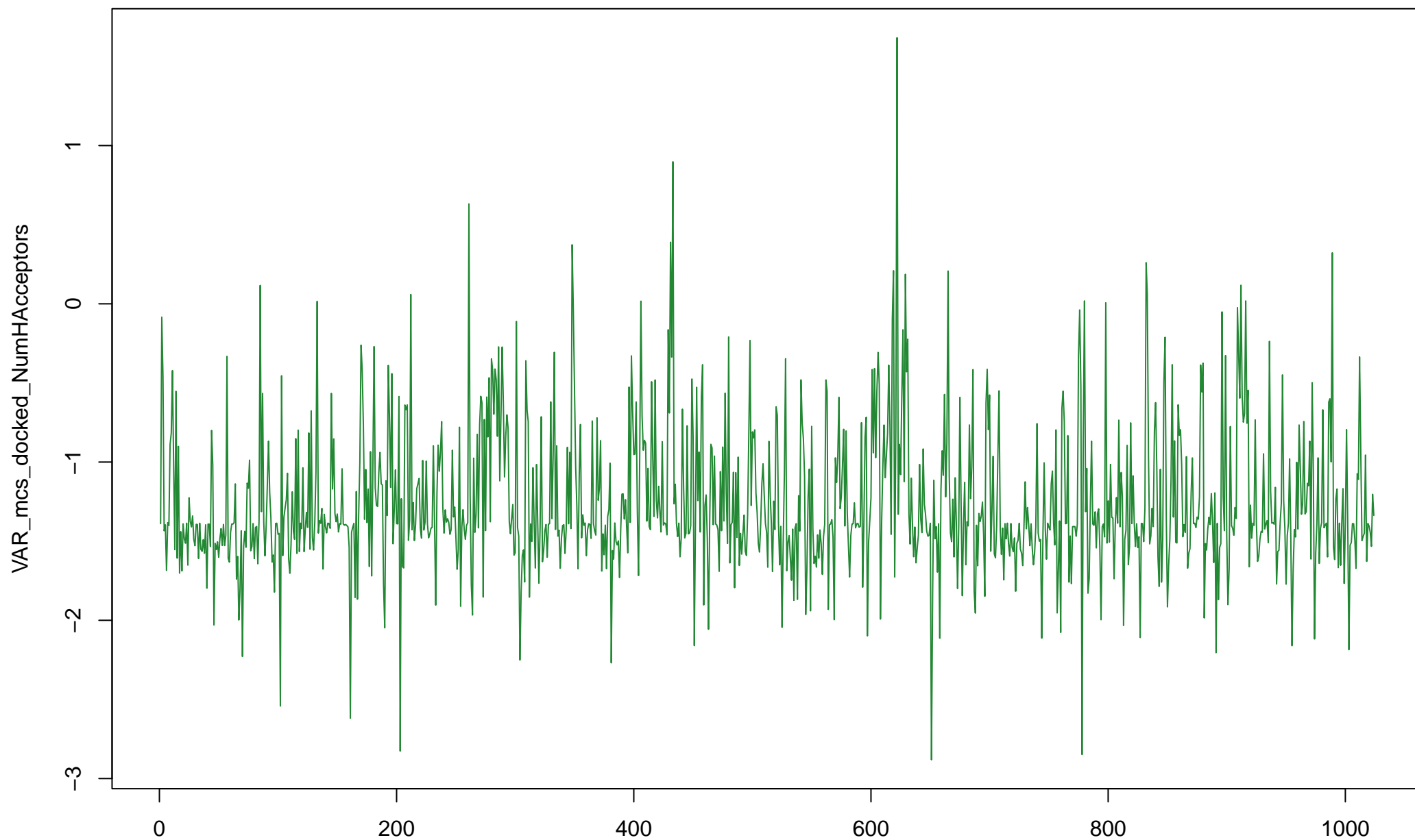
VAR_mcs_RingCount
ESS = 564 | BMK = 0.095 | MCSE(6.27) = 3.9 | stat: TRUE | burn: 0



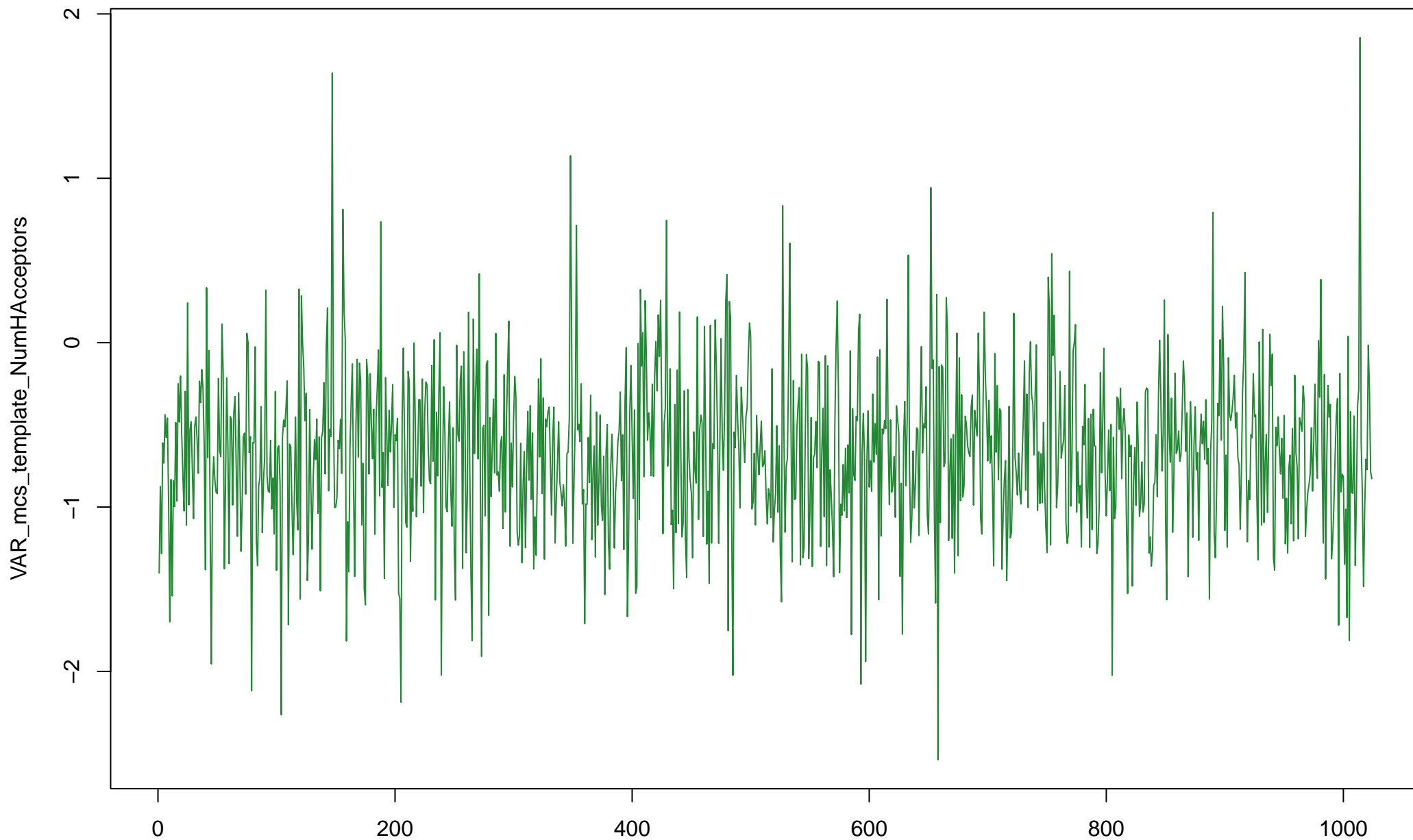
VAR_template_HeavyAtomCount
ESS = 134 | BMK = 0.0725 | MCSE(6.27) = 6.15 | stat: FALSE | burn: 0



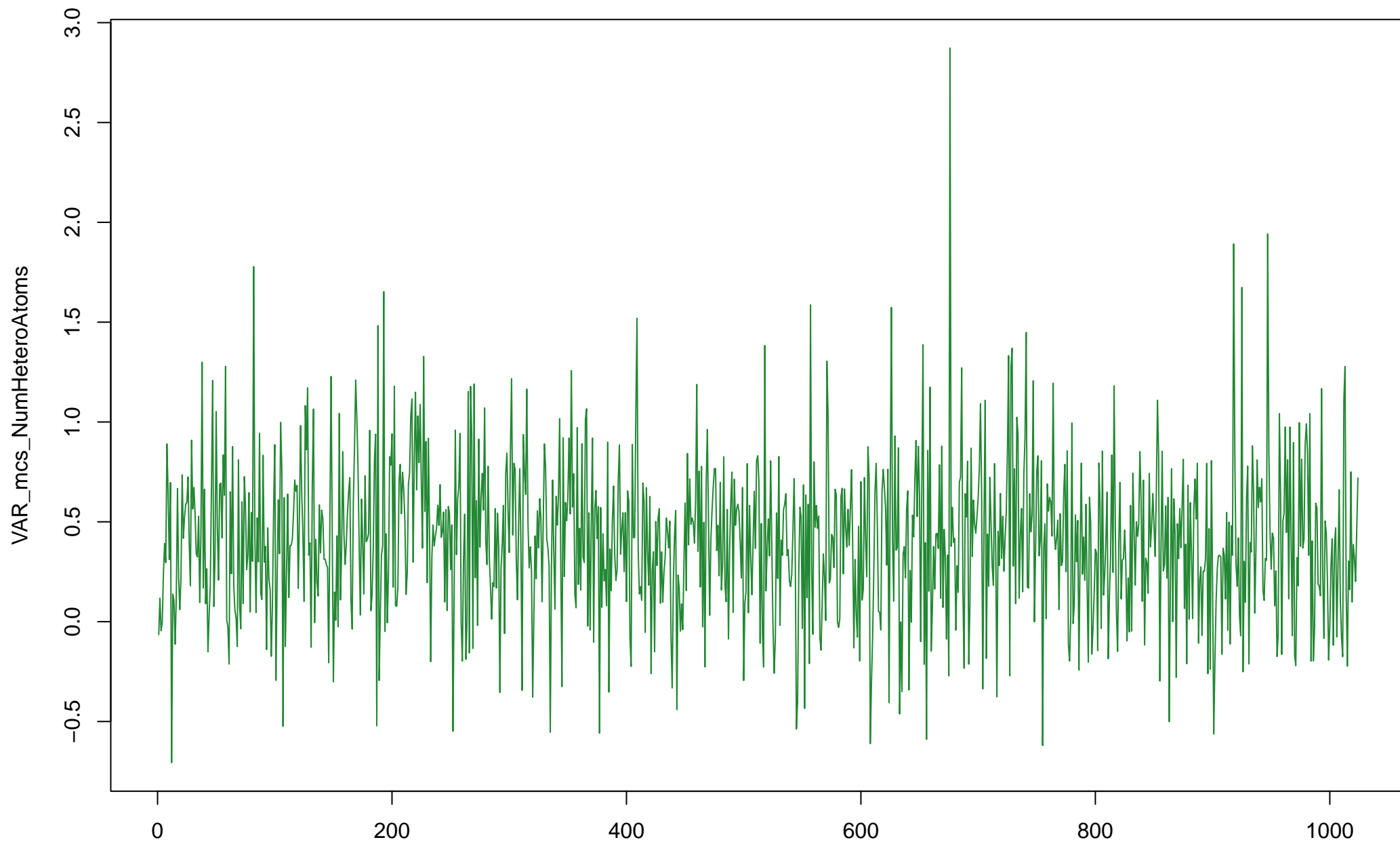
VAR_mcs_docked_NumHAcceptors
ESS = 408 | BMK = 0.104 | MCSE(6.27) = 4.93 | stat: TRUE | burn: 0



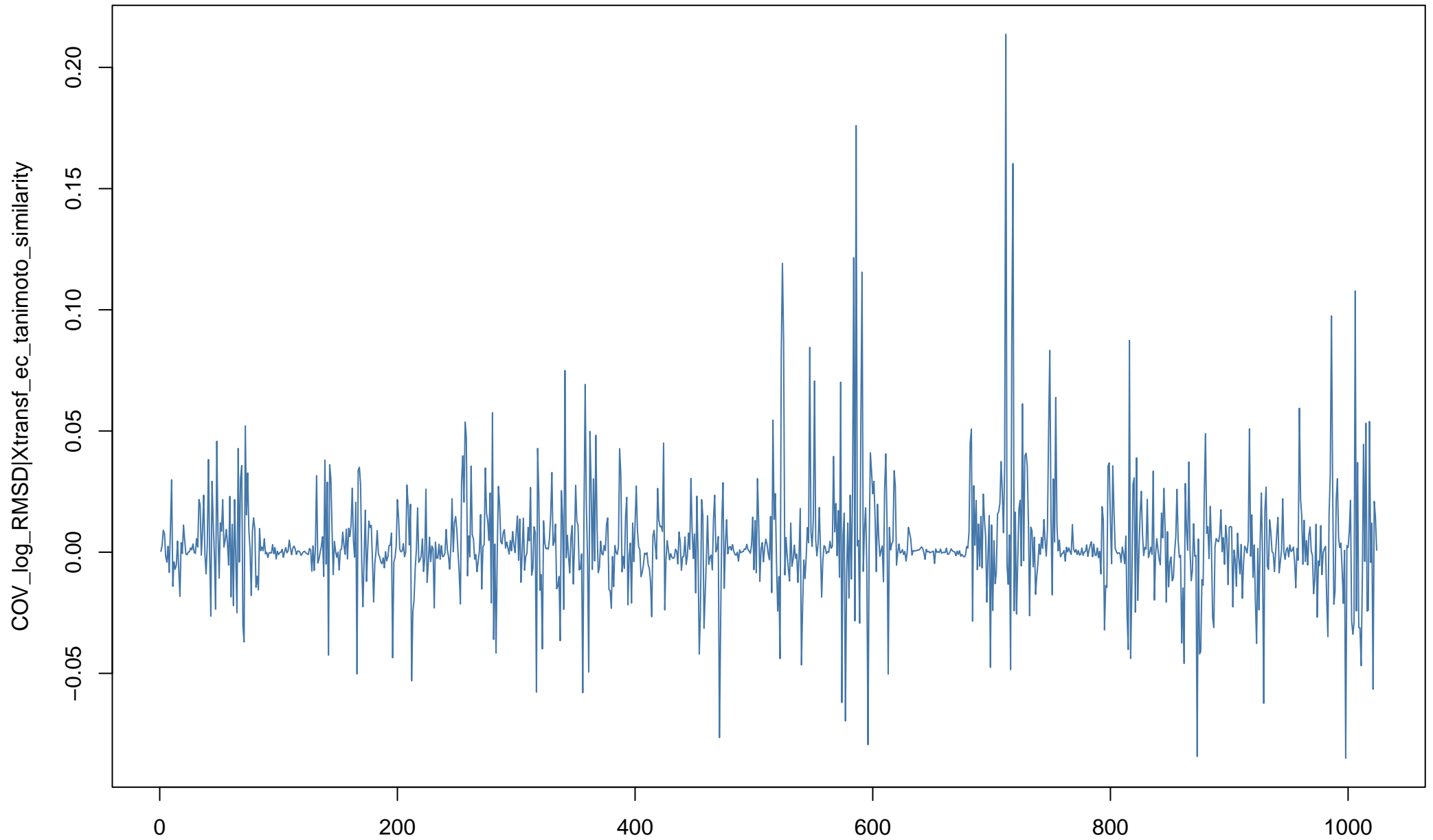
VAR_mcs_template_NumHAcceptors
ESS = 1020 | BMK = 0.0968 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0



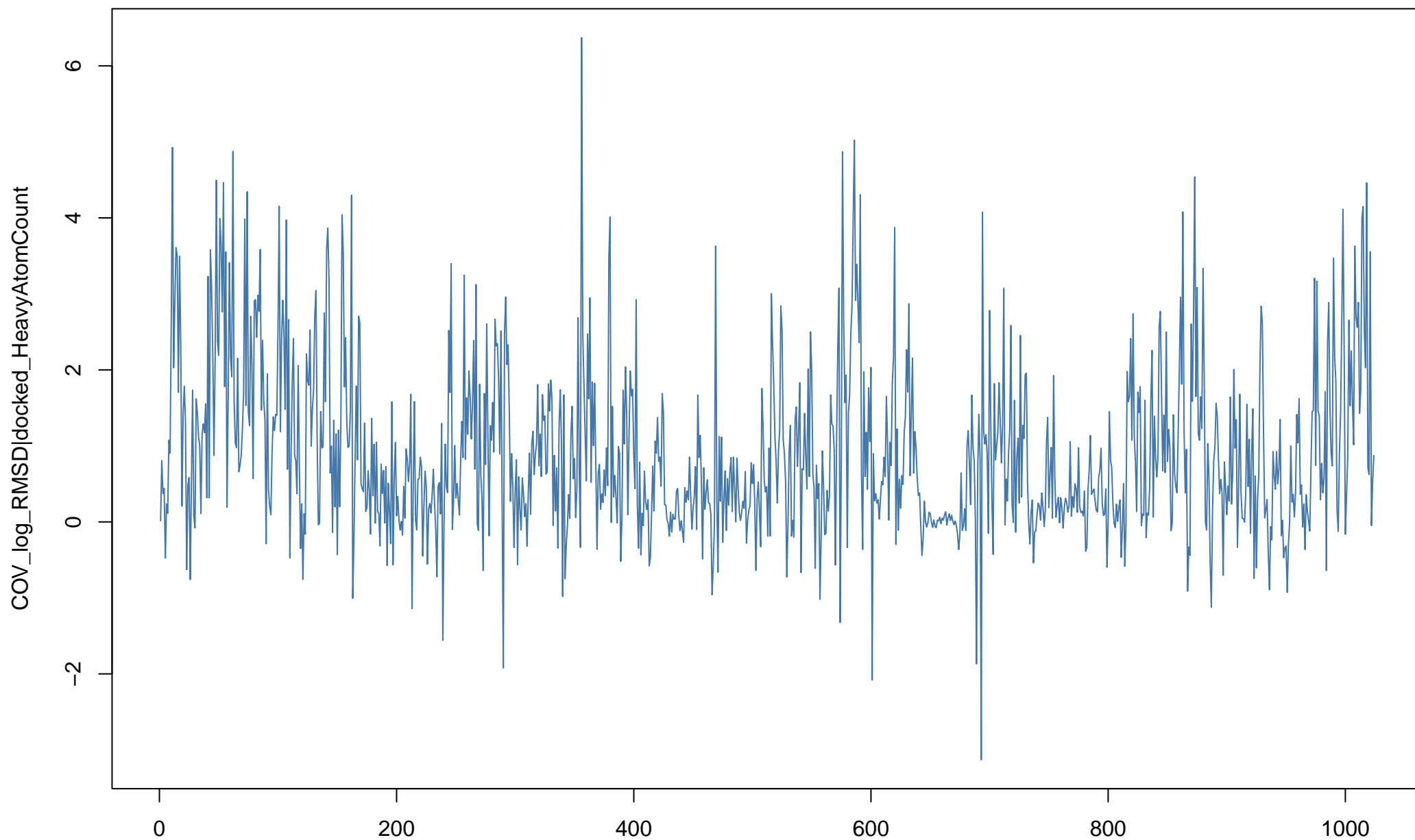
VAR_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.102 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0



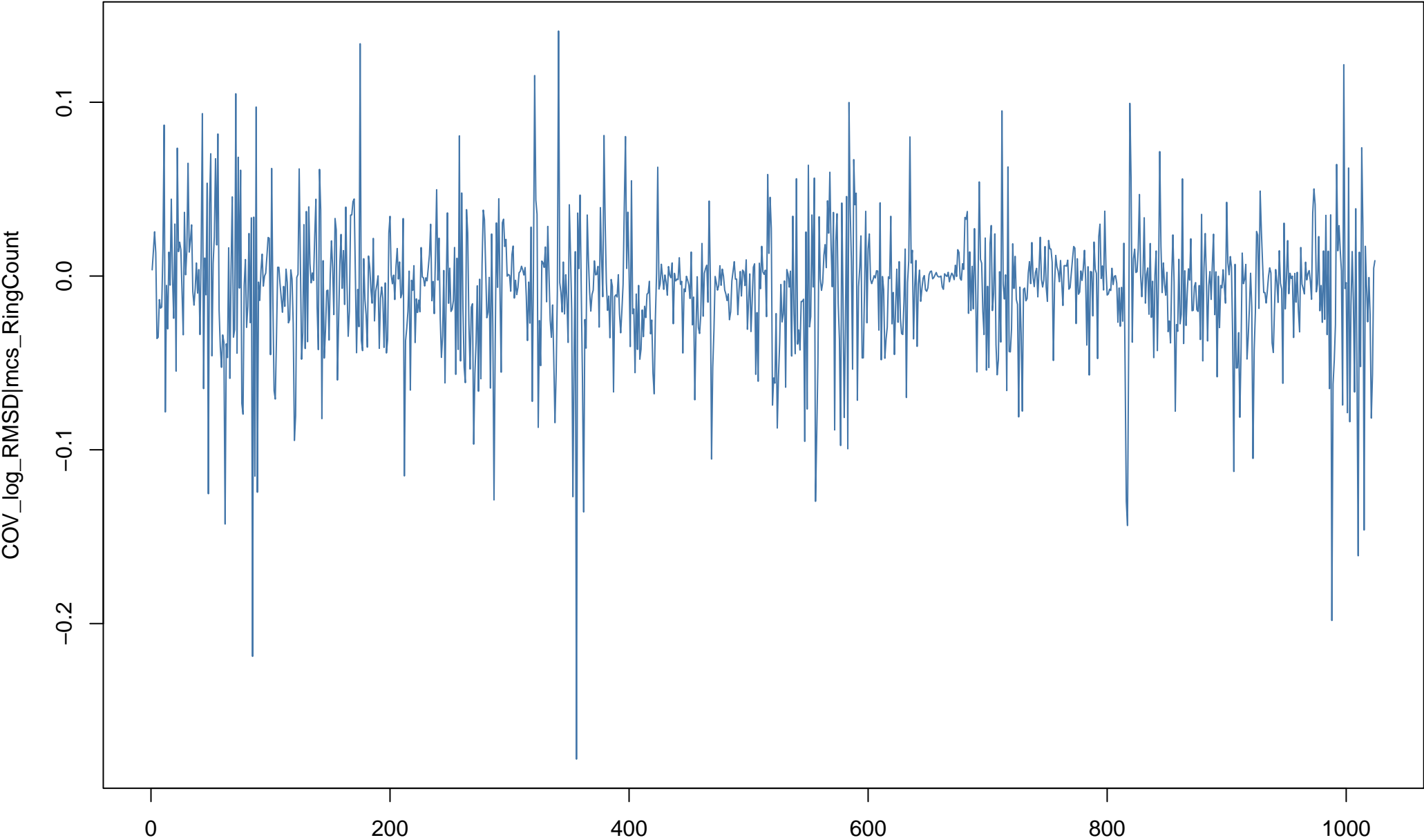
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.149 | MCSE(6.27) = 3.88 | stat: TRUE | burn: 0



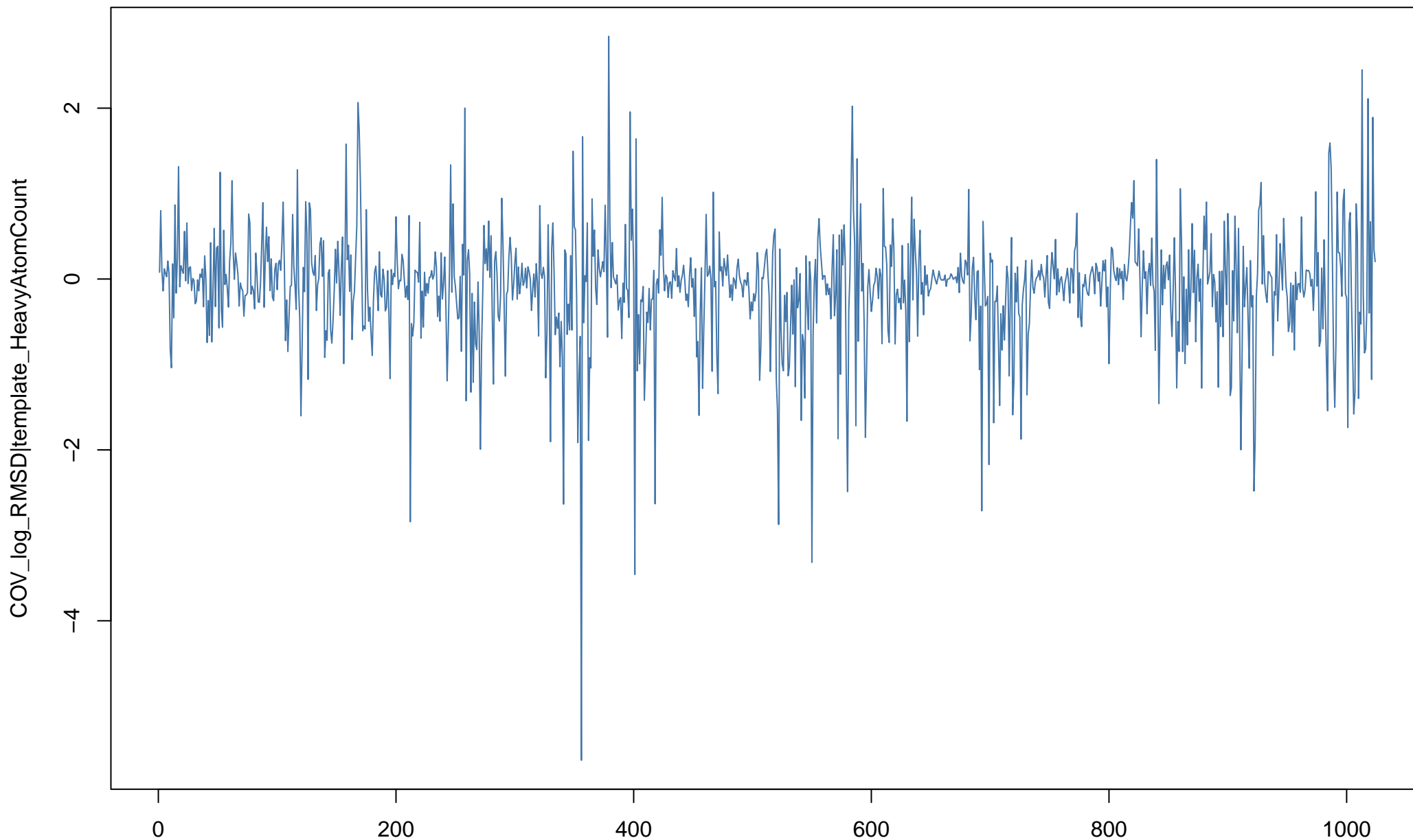
COV_log_RMSD|docked_HeavyAtomCount
ESS = 68.3 | BMK = 0.0629 | MCSE(6.27) = 8.27 | stat: FALSE | burn: 0



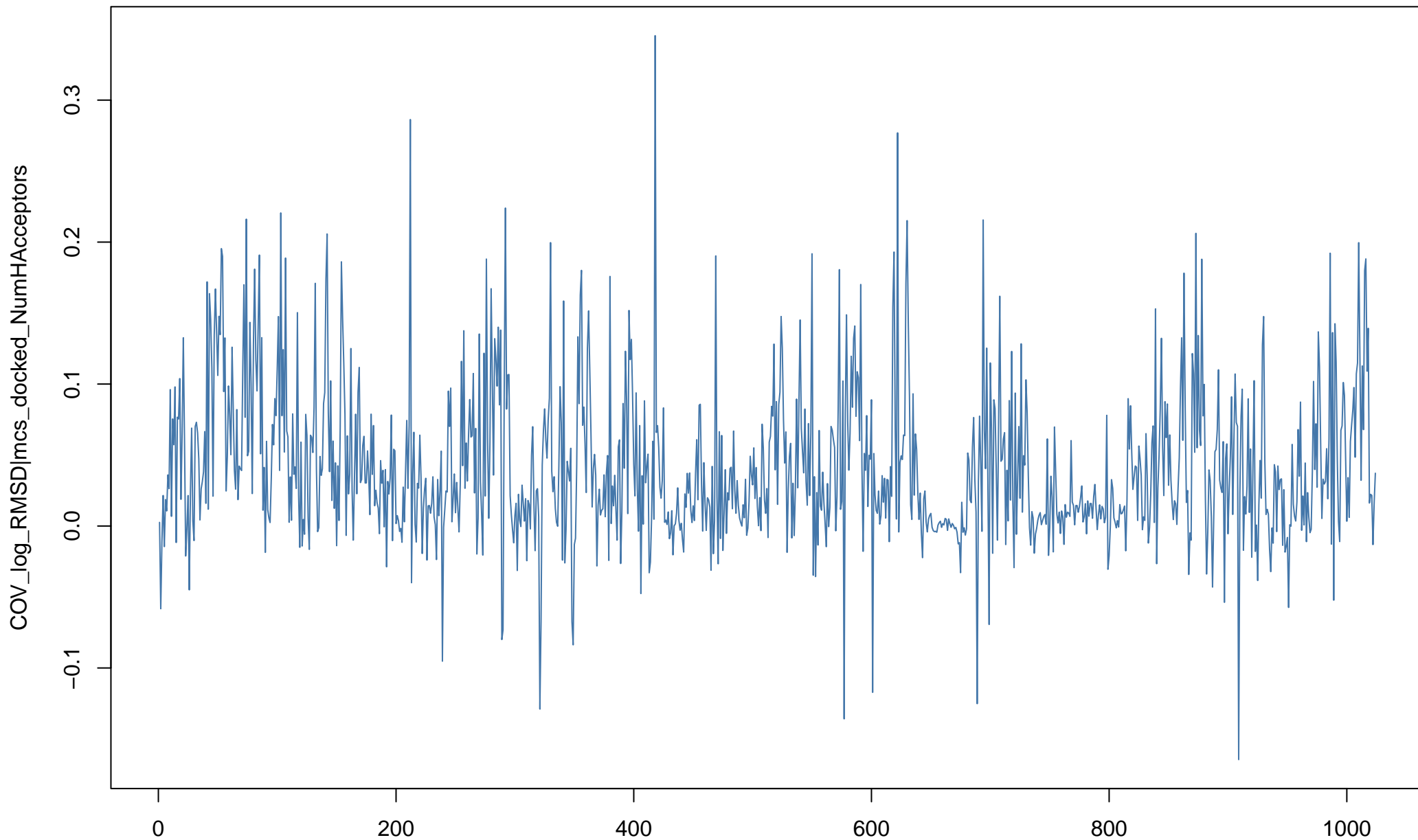
COV_log_RMSD|mcs_RingCount
ESS = 983 | BMK = 0.0954 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0



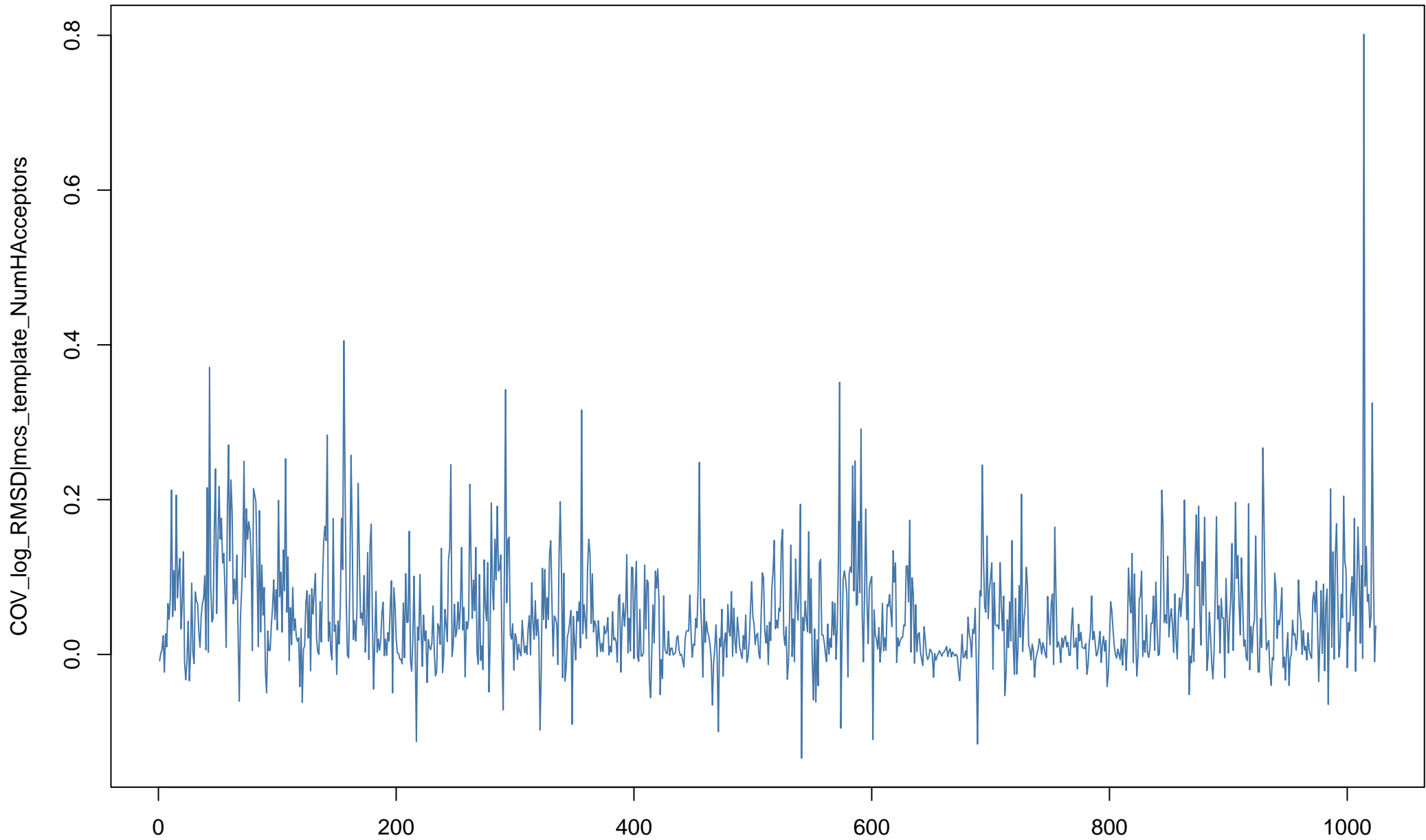
COV_log_RMSD|template_HeavyAtomCount
ESS = 829 | BMK = 0.0899 | MCSE(6.27) = 3.94 | stat: FALSE | burn: 0



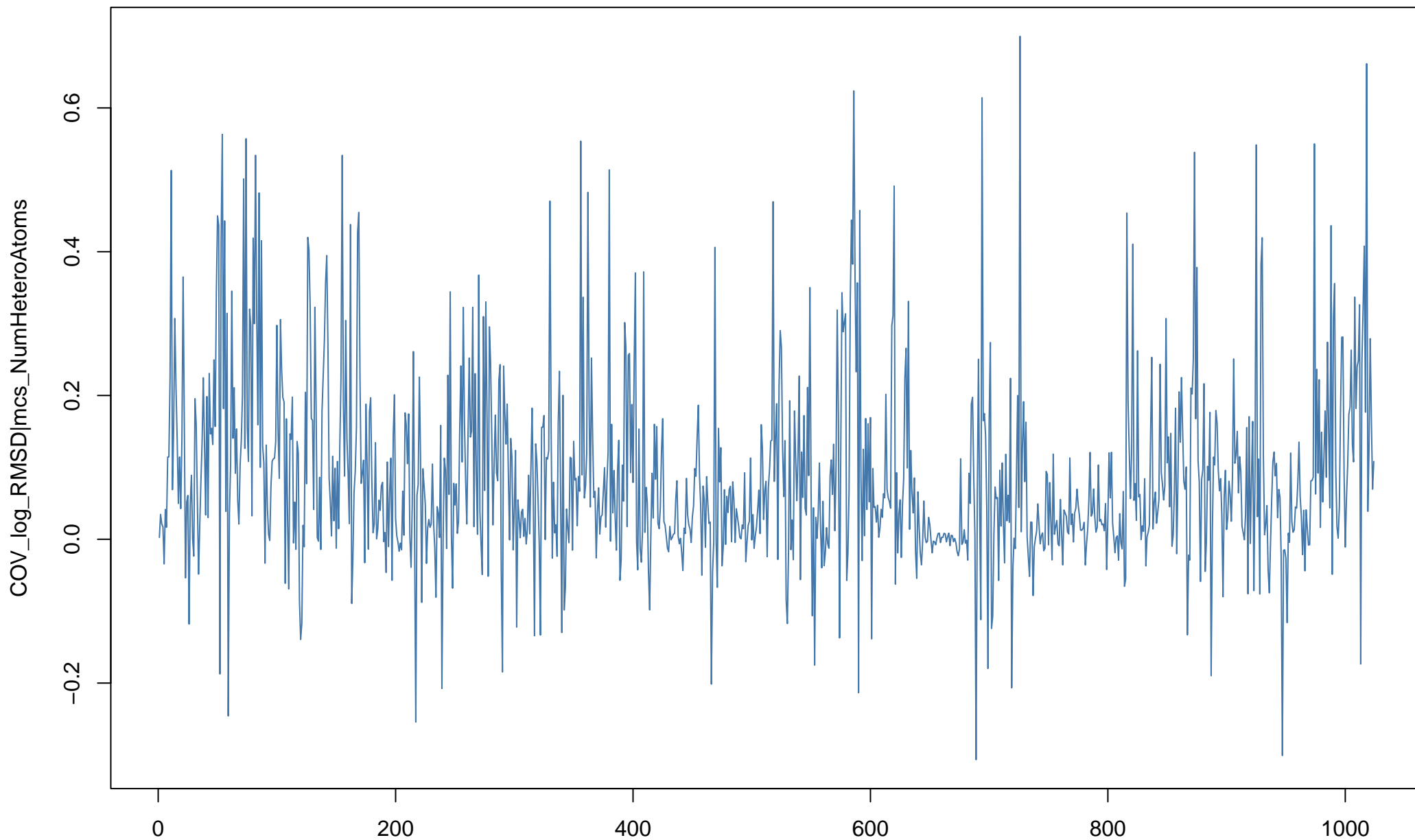
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 292 | BMK = 0.0779 | MCSE(6.27) = 7.01 | stat: FALSE | burn: 0



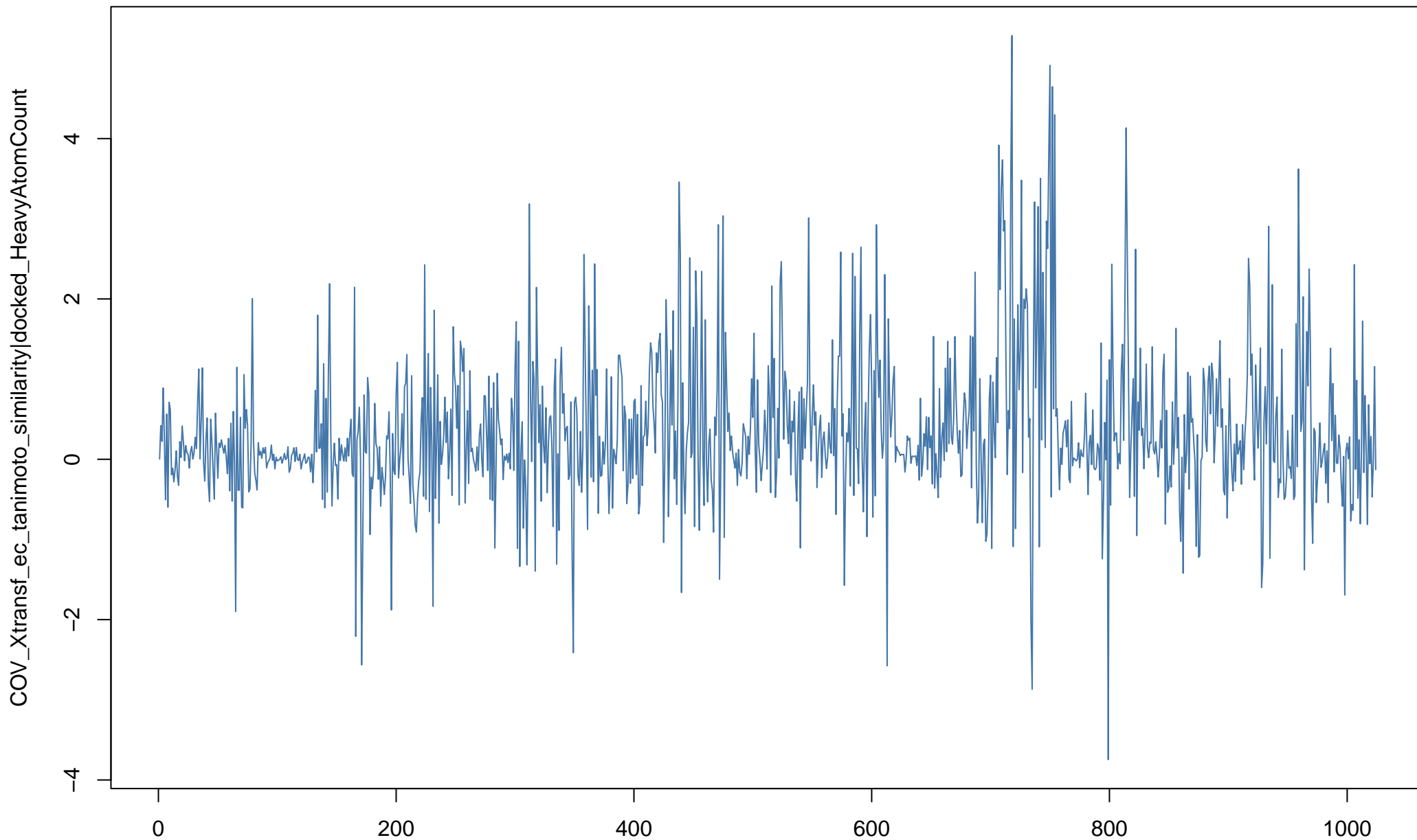
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 206 | BMK = 0.0829 | MCSE(6.27) = 6.39 | stat: FALSE | burn: 0



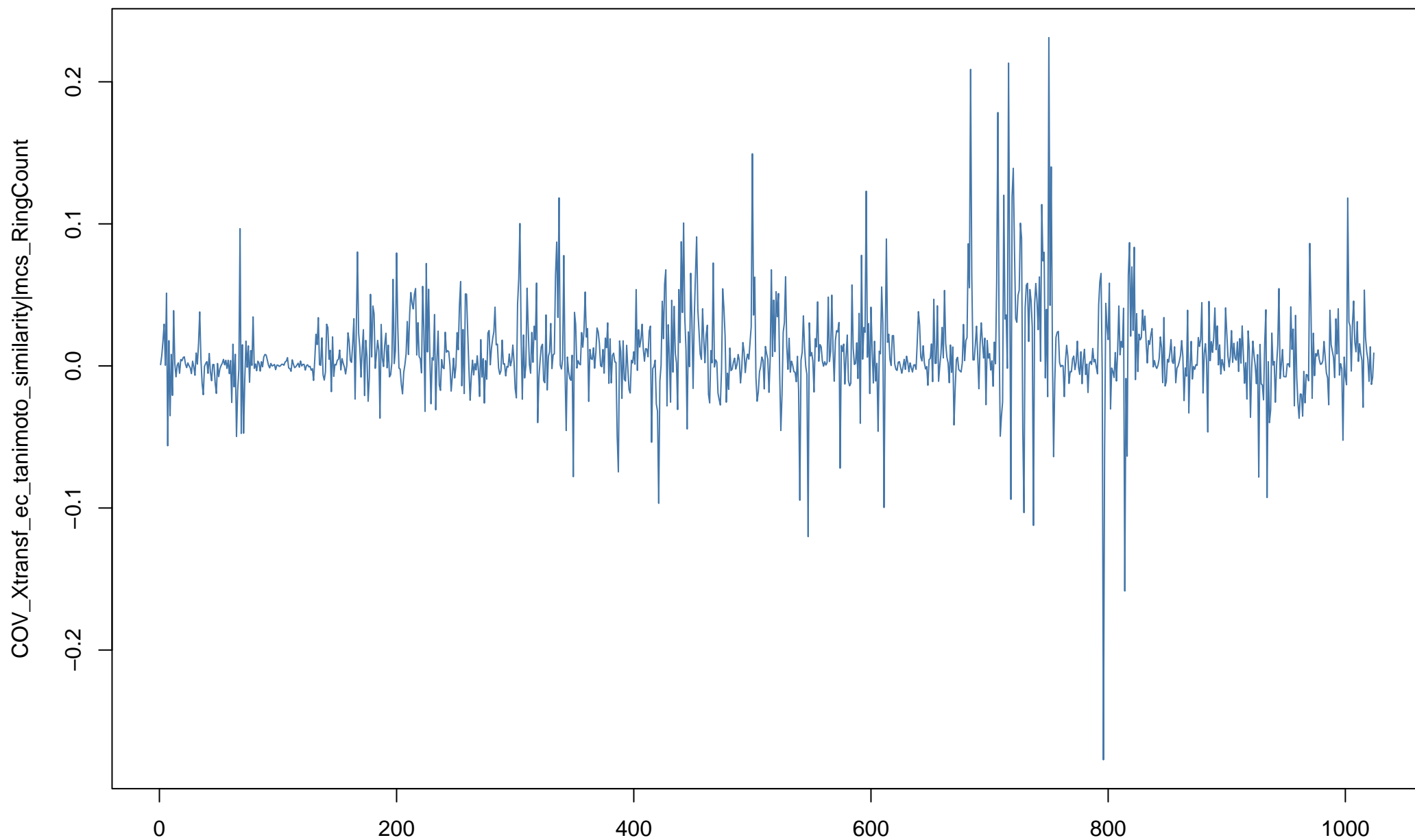
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 309 | BMK = 0.0936 | MCSE(6.27) = 6.55 | stat: FALSE | burn: 0



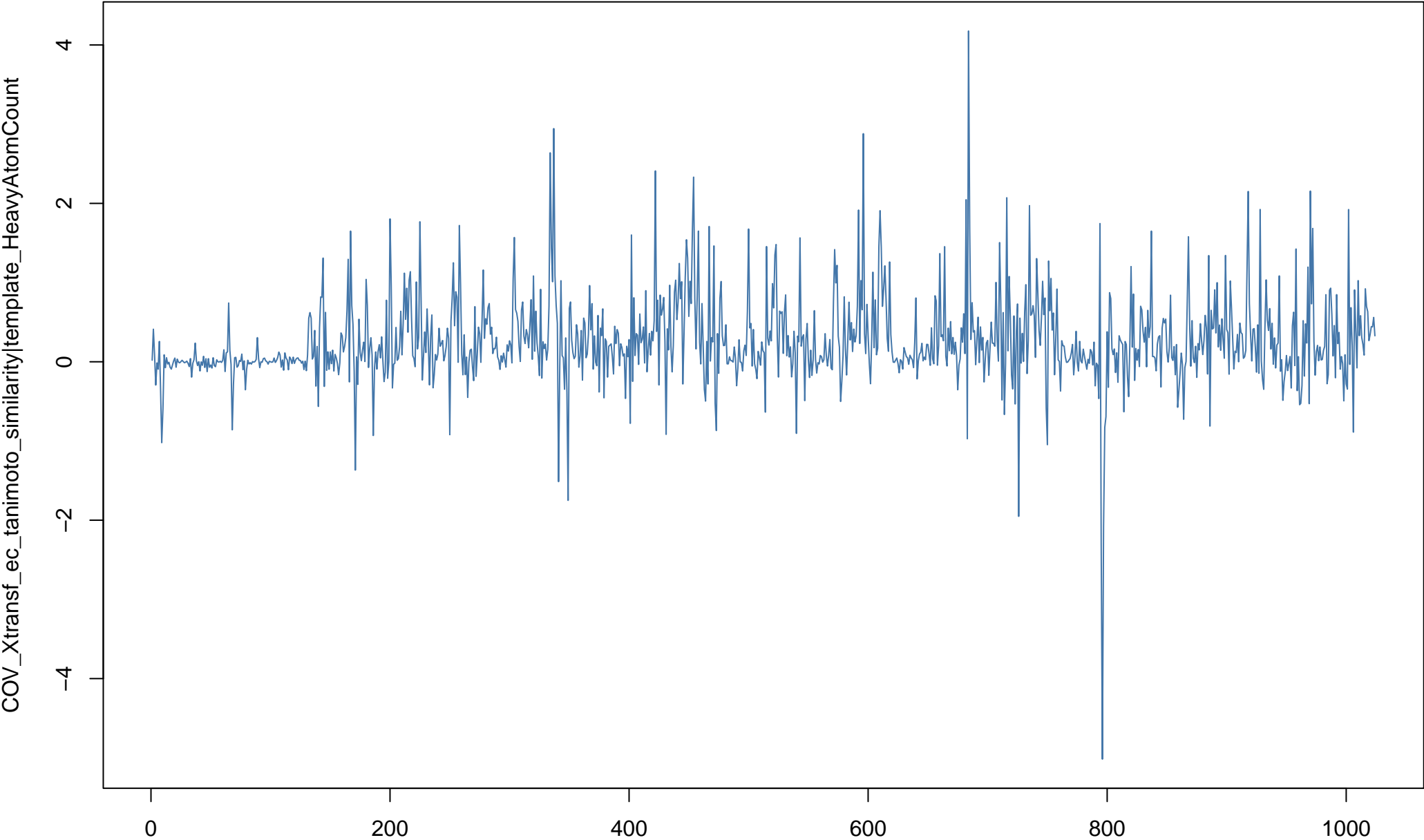
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 299 | BMK = 0.135 | MCSE(6.27) = 6.19 | stat: FALSE | burn: 0



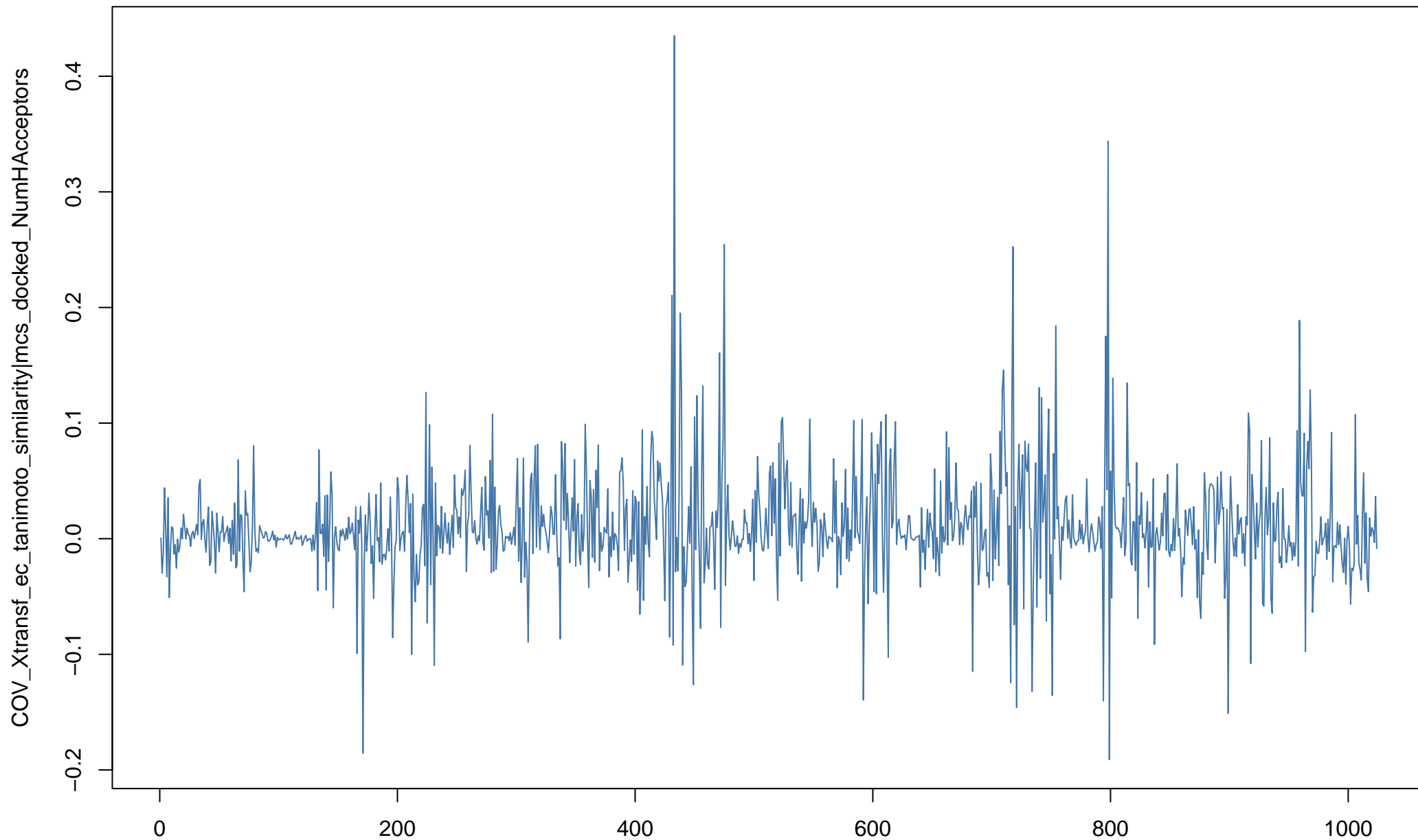
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 298 | BMK = 0.14 | MCSE(6.27) = 4.76 | stat: FALSE | burn: 0



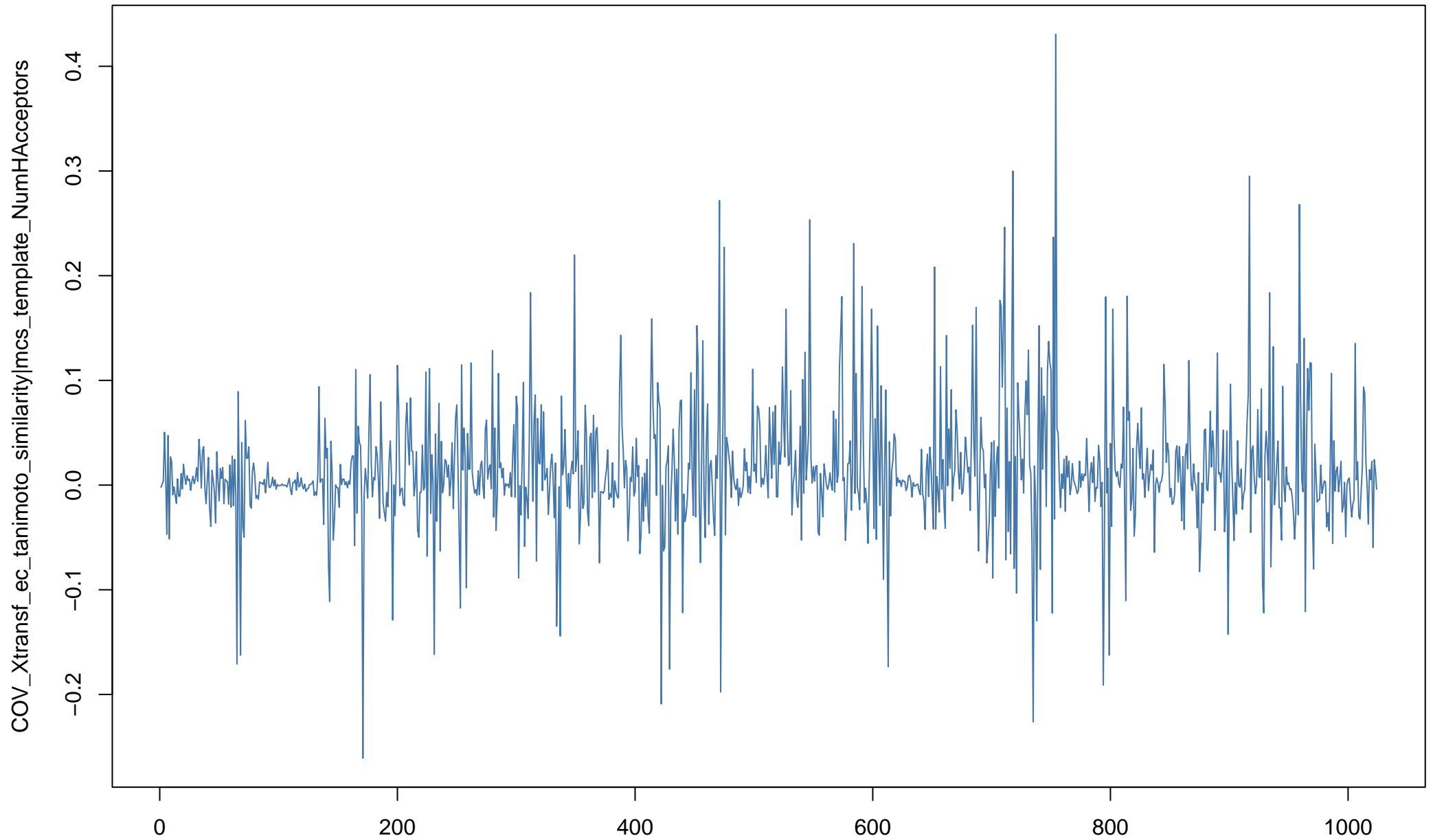
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 344 | BMK = 0.154 | MCSE(6.27) = 5.53 | stat: FALSE | burn: 0



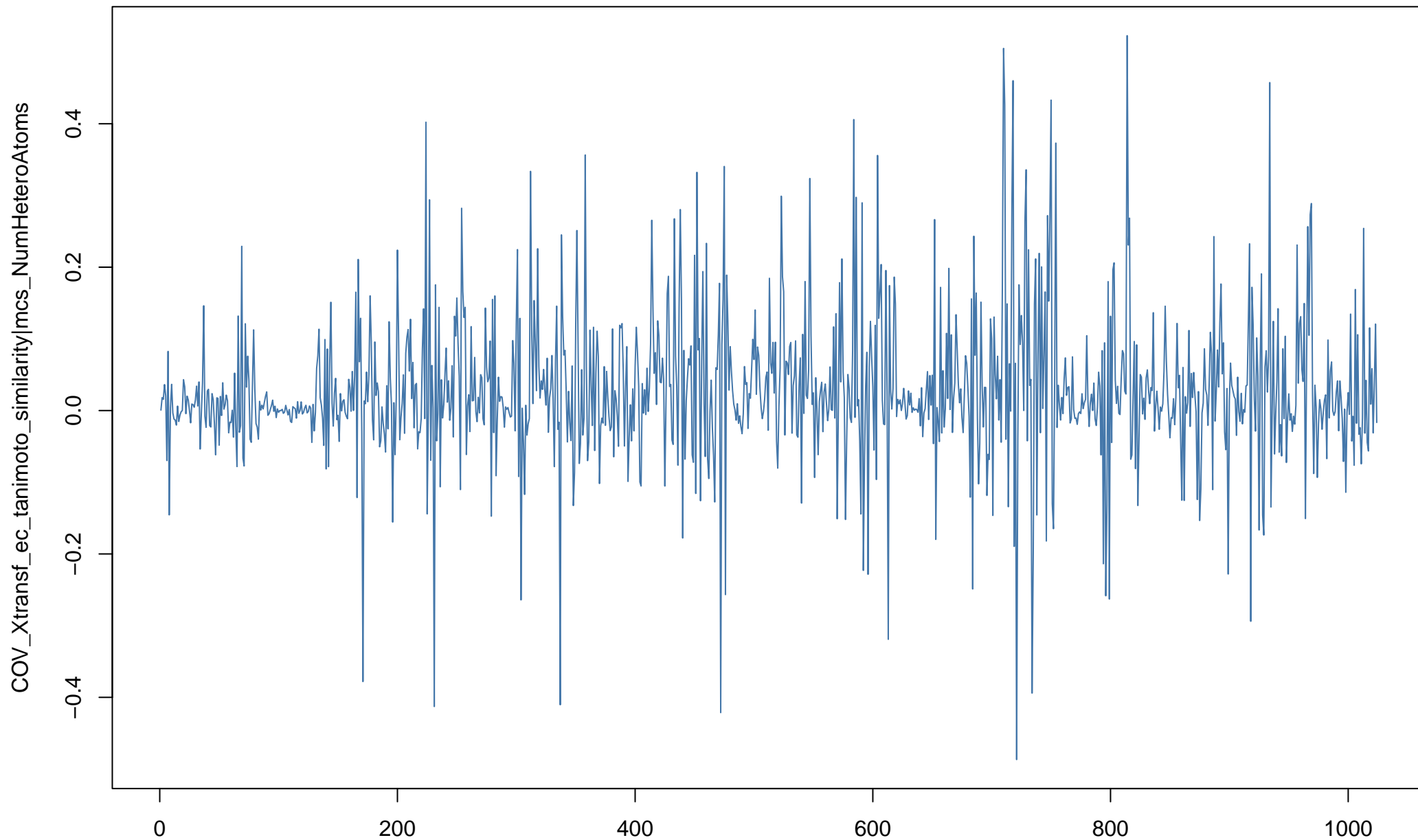
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 626 | BMK = 0.135 | MCSE(6.27) = 3.4 | stat: FALSE | burn: 0



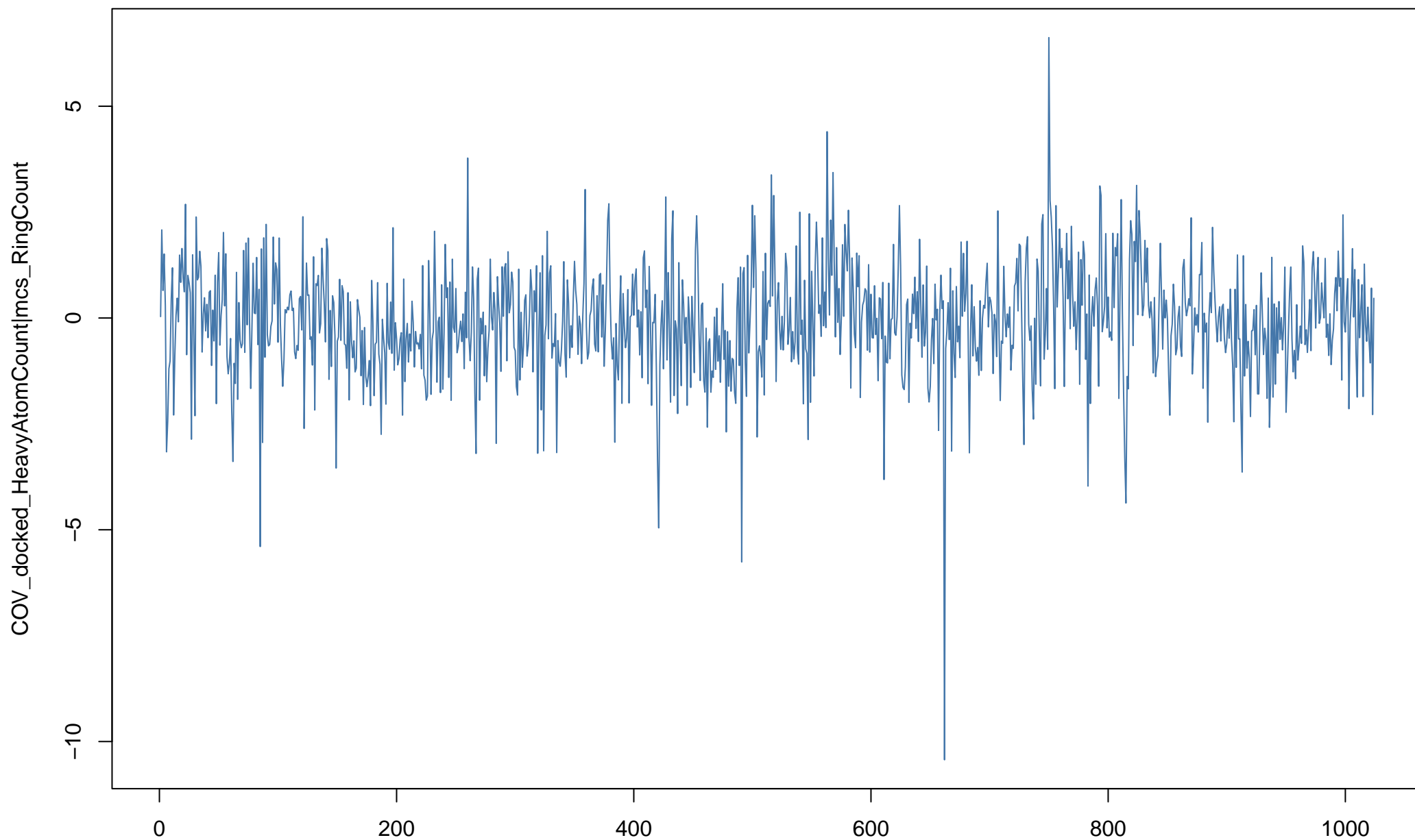
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 1020 | BMK = 0.13 | MCSE(6.27) = 3.83 | stat: FALSE | burn: 0



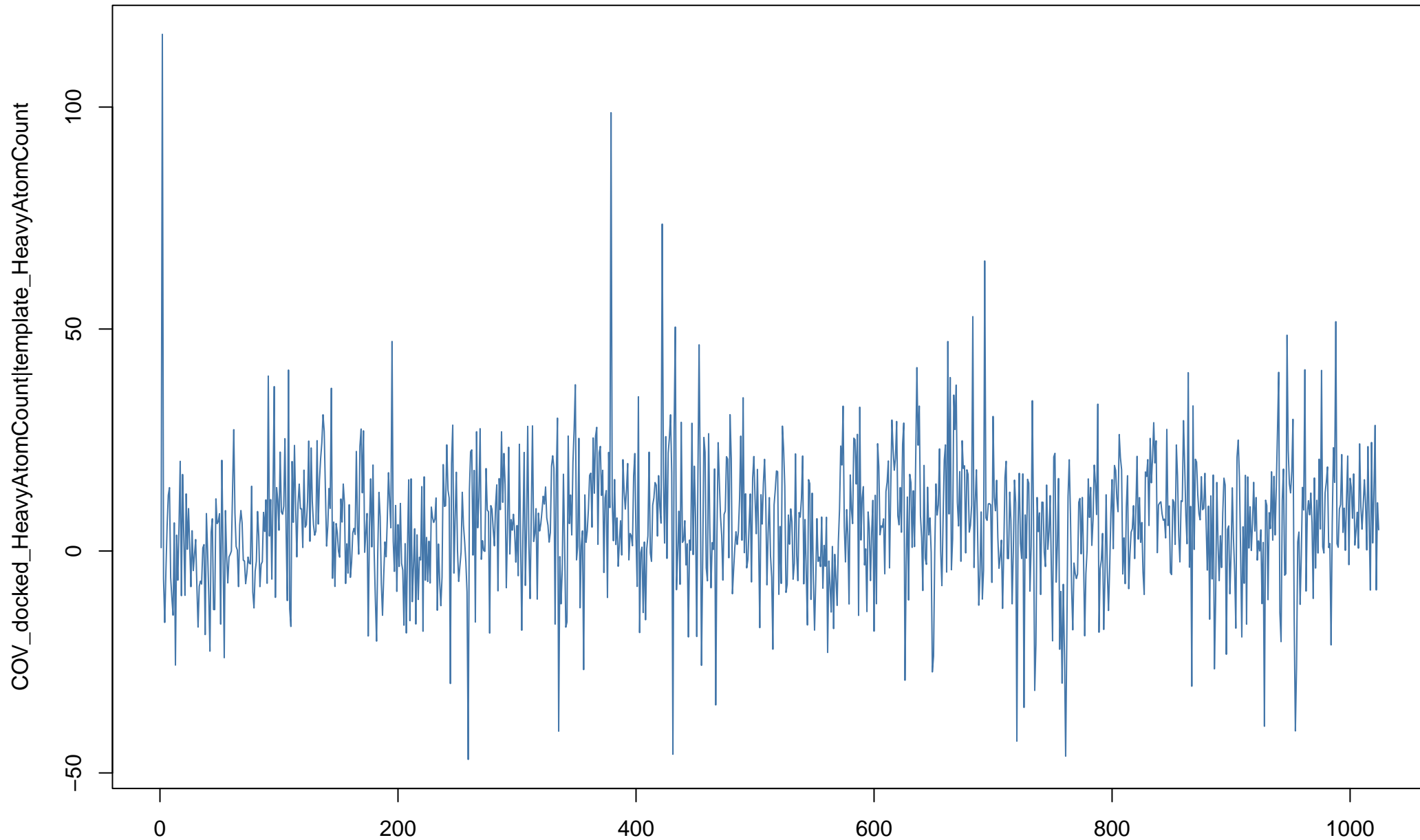
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.138 | MCSE(6.27) = 3.26 | stat: FALSE | burn: 0



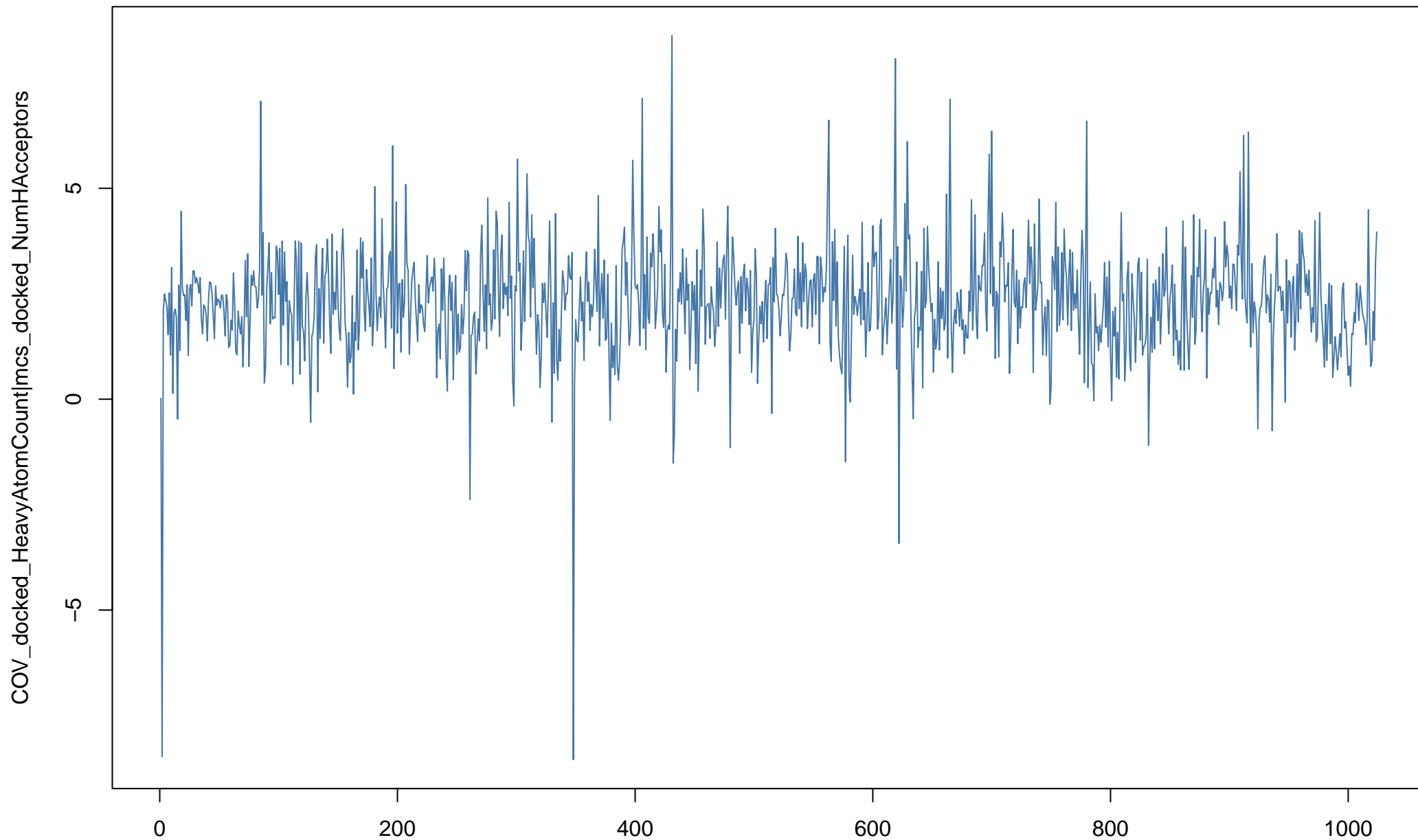
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 417 | BMK = 0.11 | MCSE(6.27) = 4.77 | stat: TRUE | burn: 0



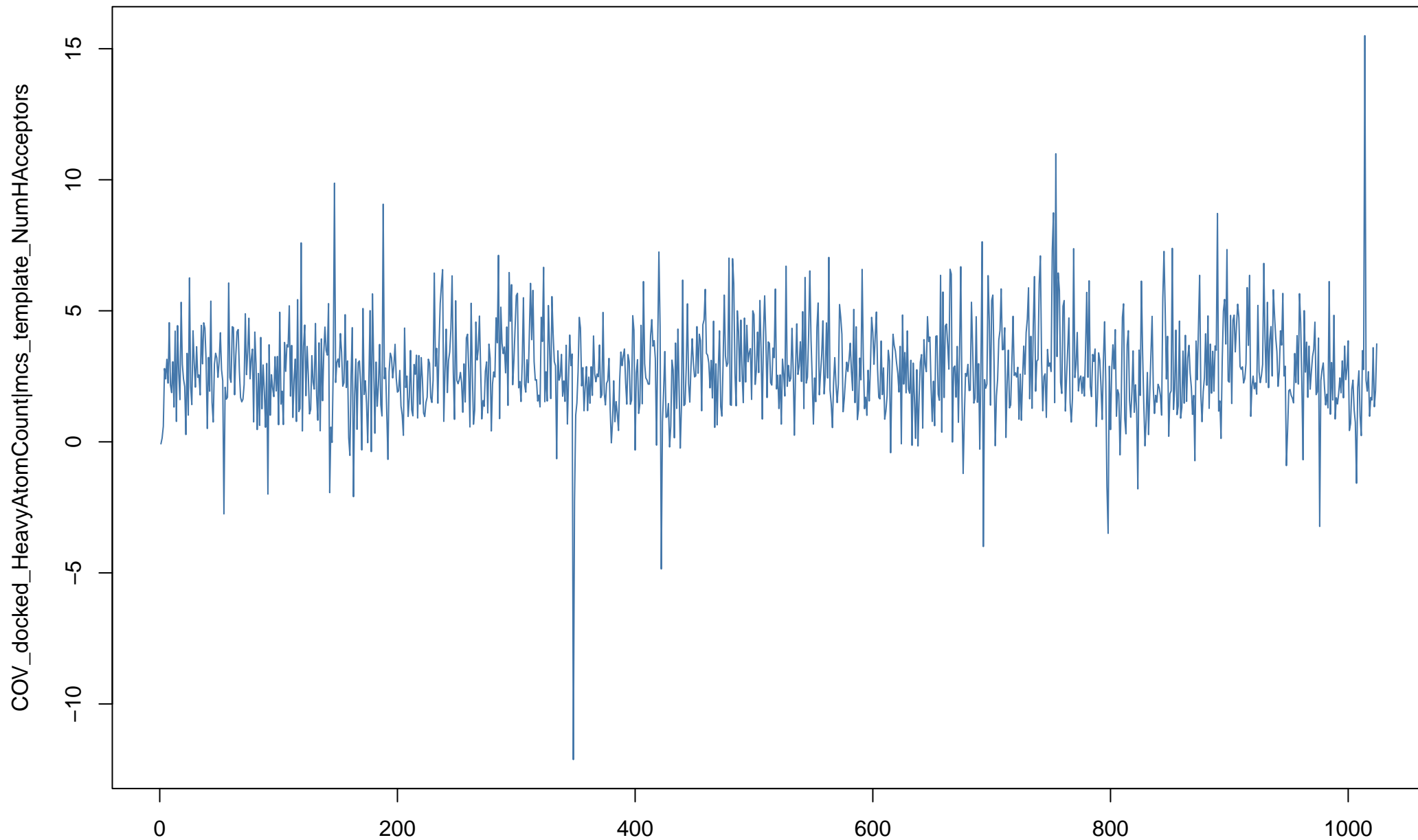
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 538 | BMK = 0.0874 | MCSE(6.27) = 4.7 | stat: FALSE | burn: 0



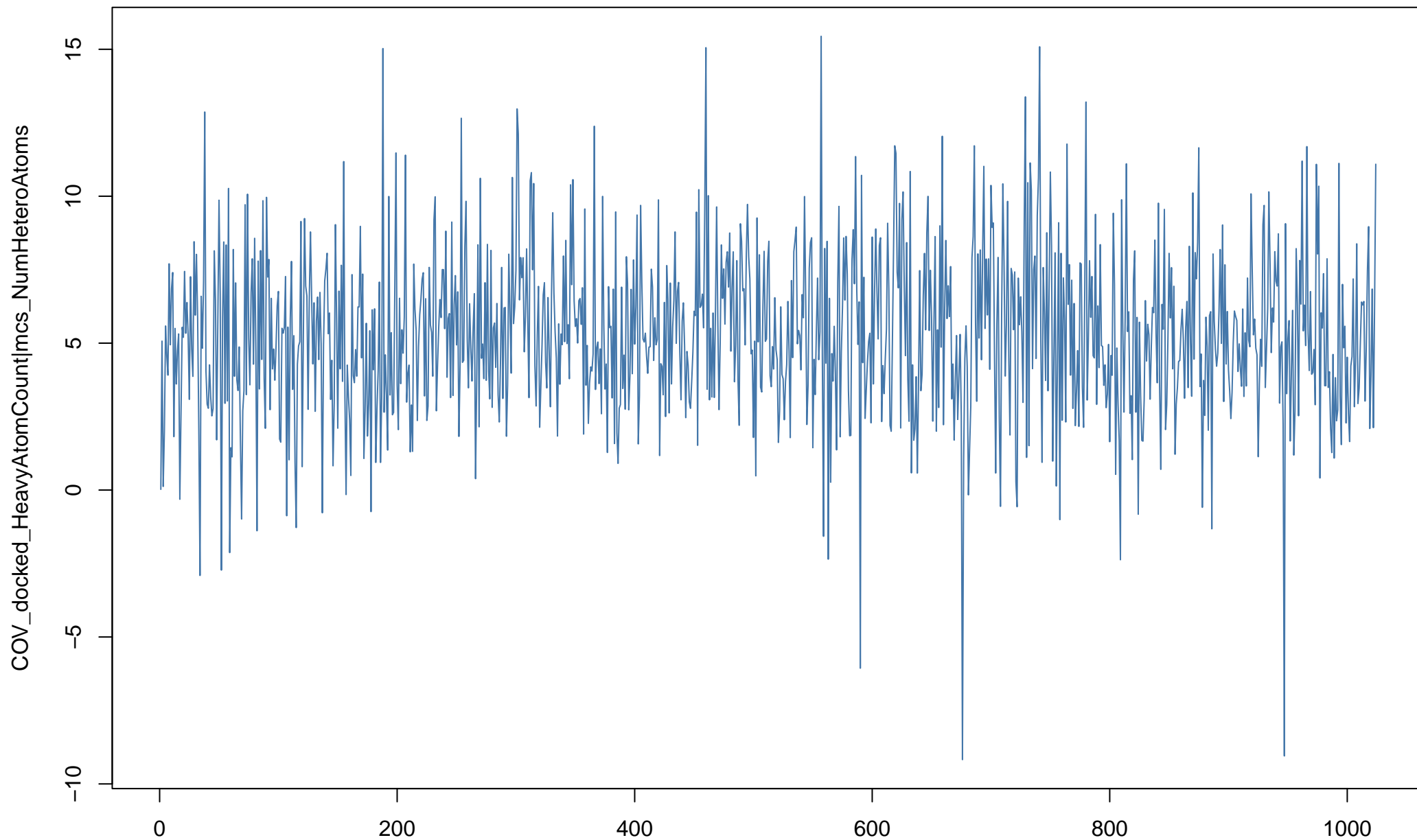
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 858 | BMK = 0.0798 | MCSE(6.27) = 3.69 | stat: TRUE | burn: 0



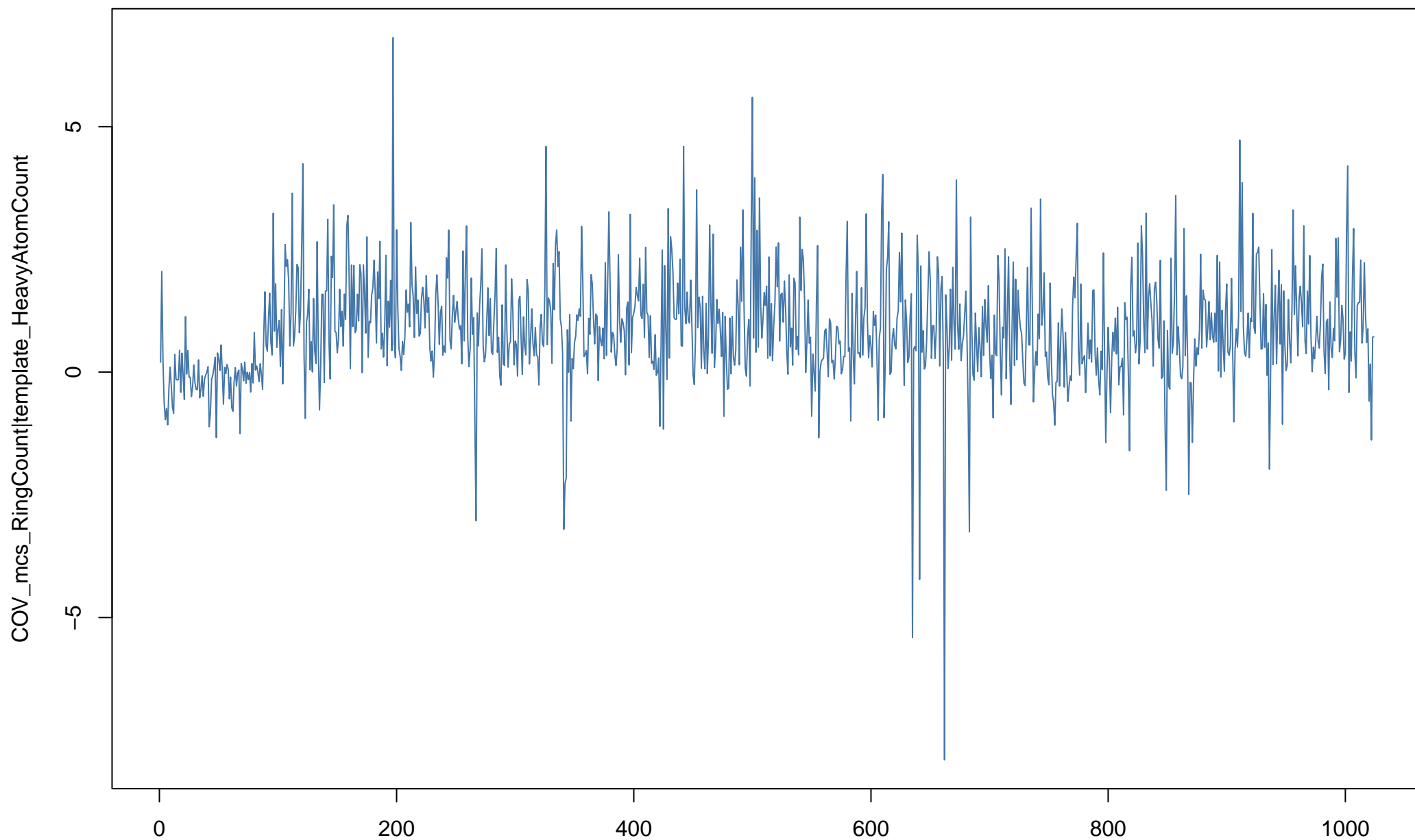
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 535 | BMK = 0.0862 | MCSE(6.27) = 4.1 | stat: TRUE | burn: 0



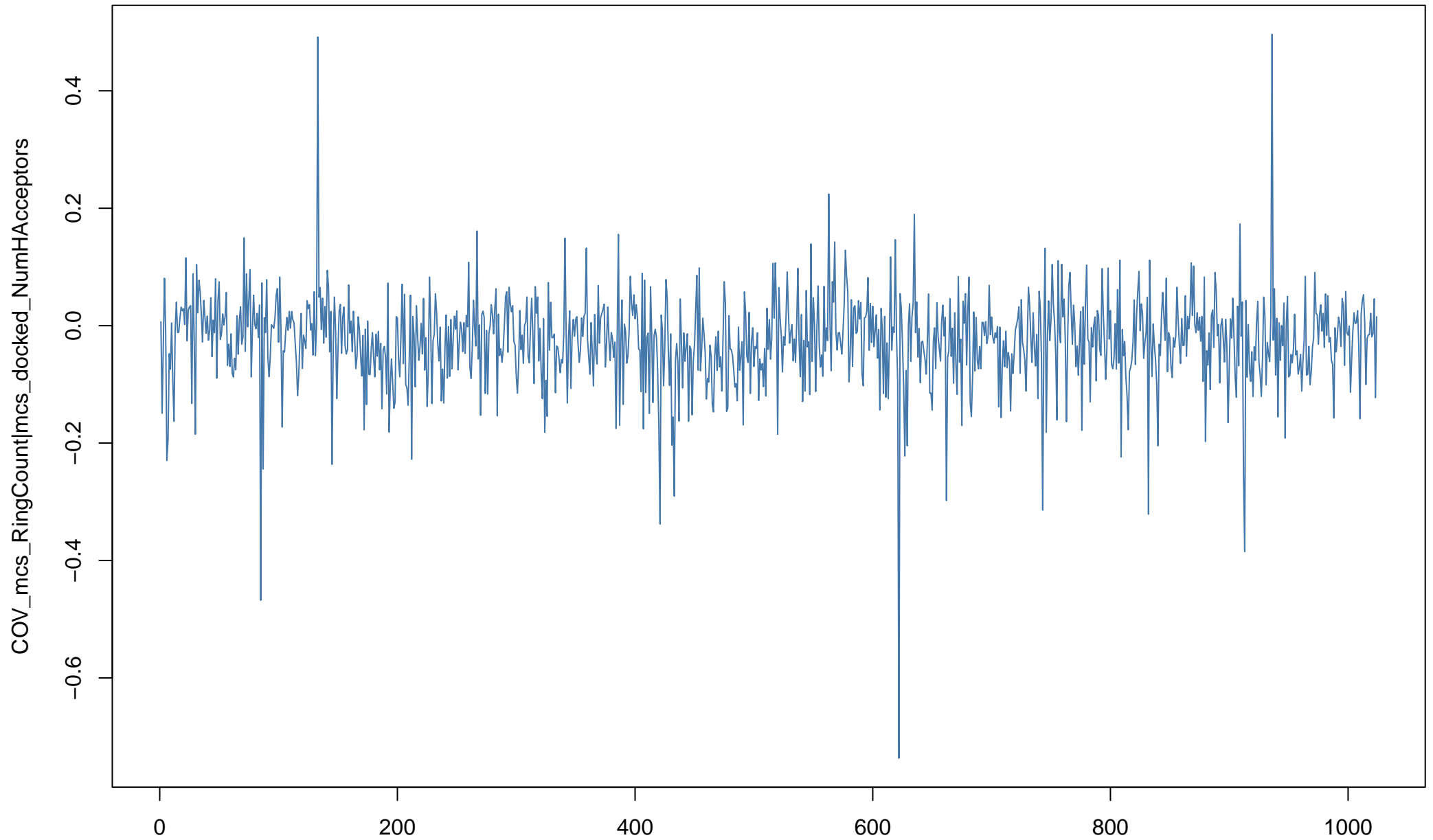
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0708 | MCSE(6.27) = 3.41 | stat: TRUE | burn: 0



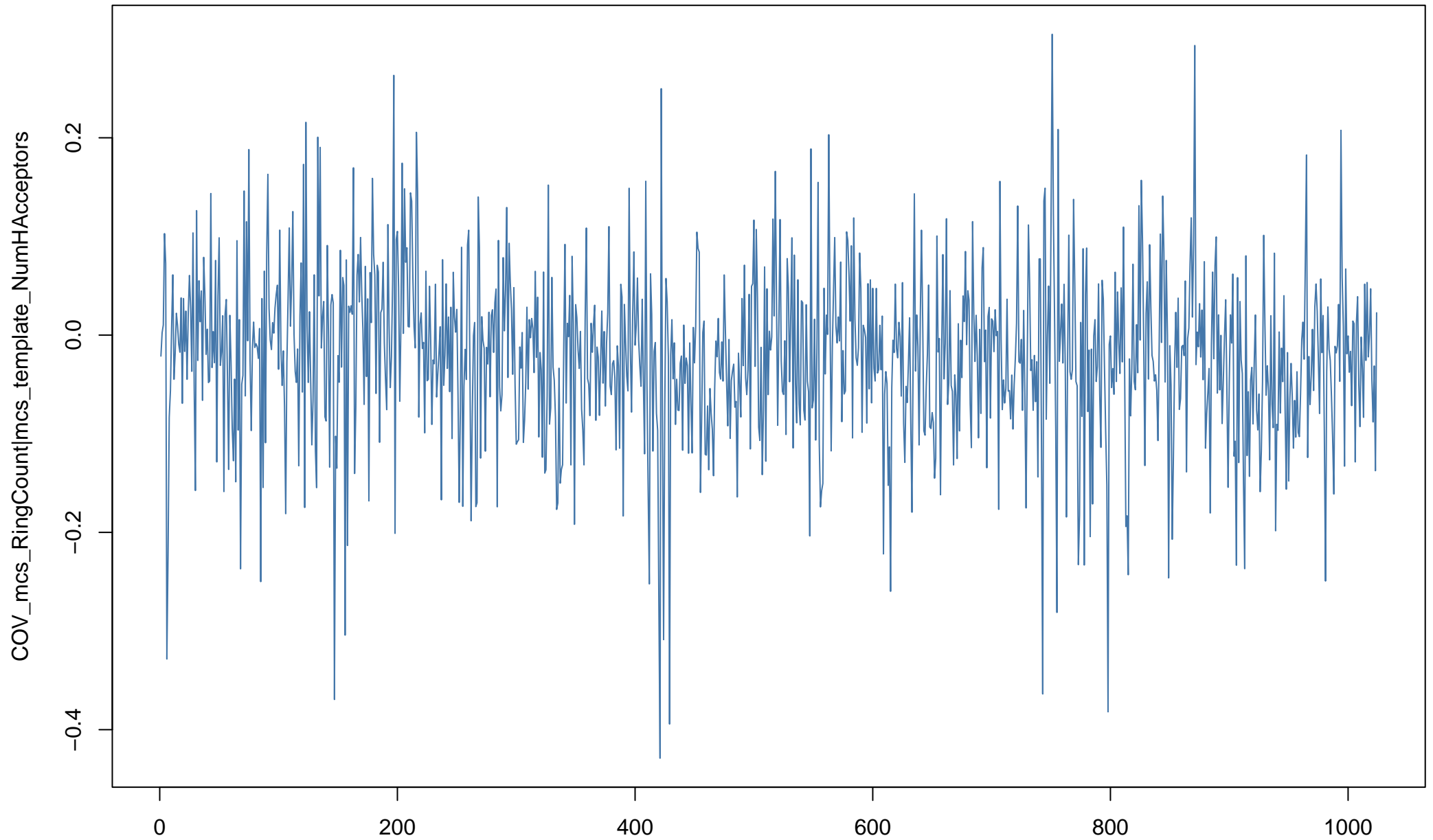
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 341 | BMK = 0.0802 | MCSE(6.27) = 6.2 | stat: FALSE | burn: 102



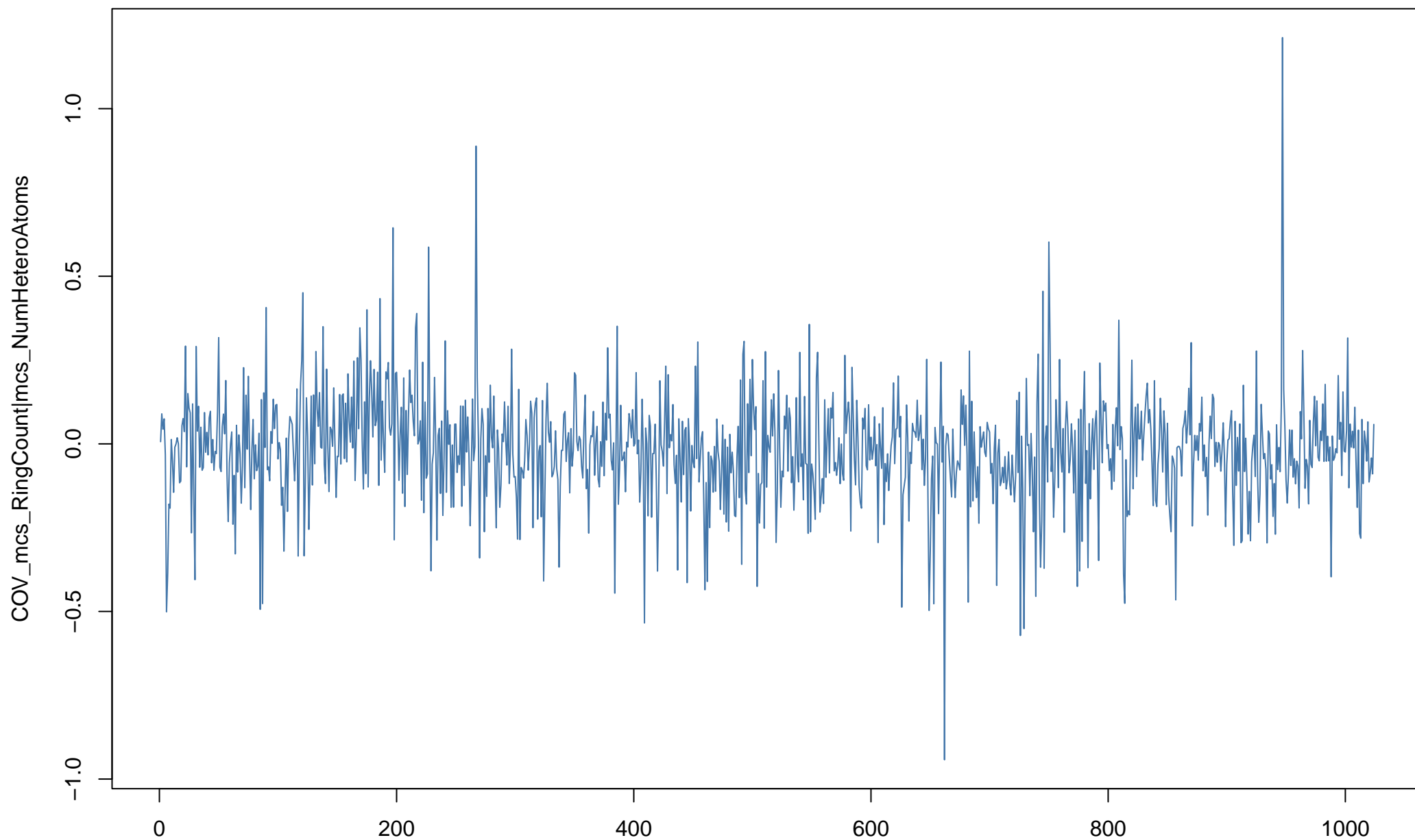
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 840 | BMK = 0.0842 | MCSE(6.27) = 4.29 | stat: TRUE | burn: 0



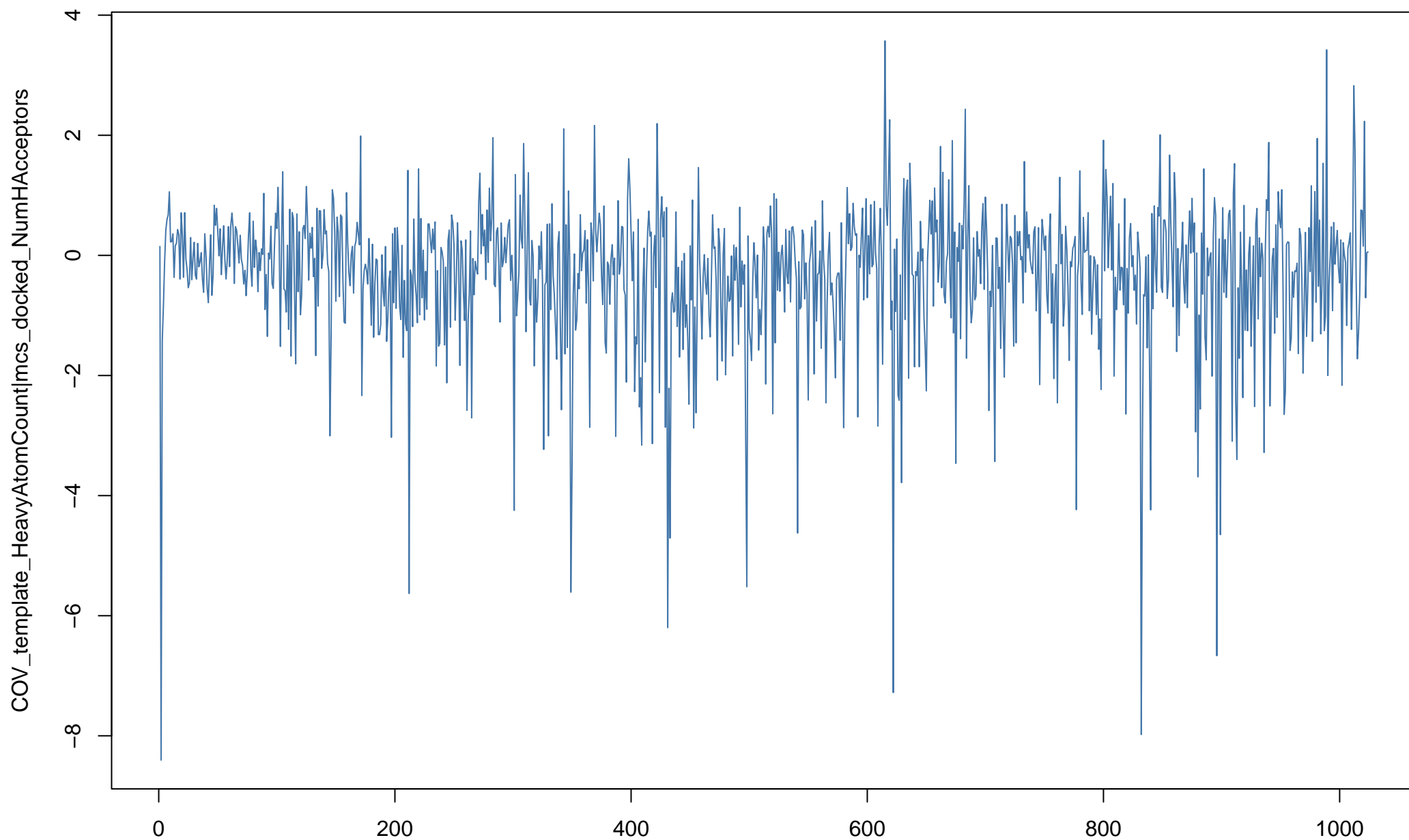
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 691 | BMK = 0.0719 | MCSE(6.27) = 4.79 | stat: TRUE | burn: 0



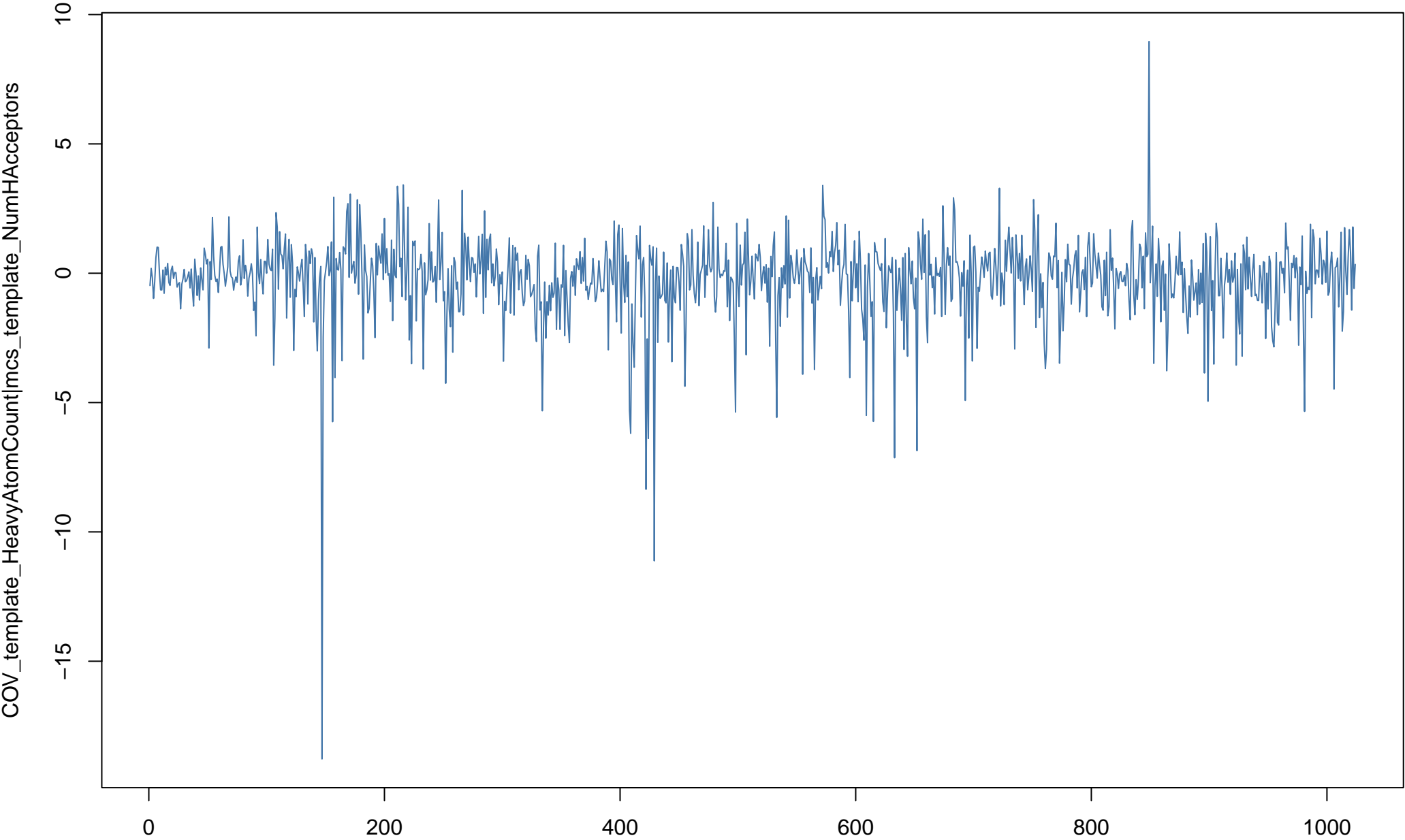
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 640 | BMK = 0.093 | MCSE(6.27) = 4.24 | stat: TRUE | burn: 0



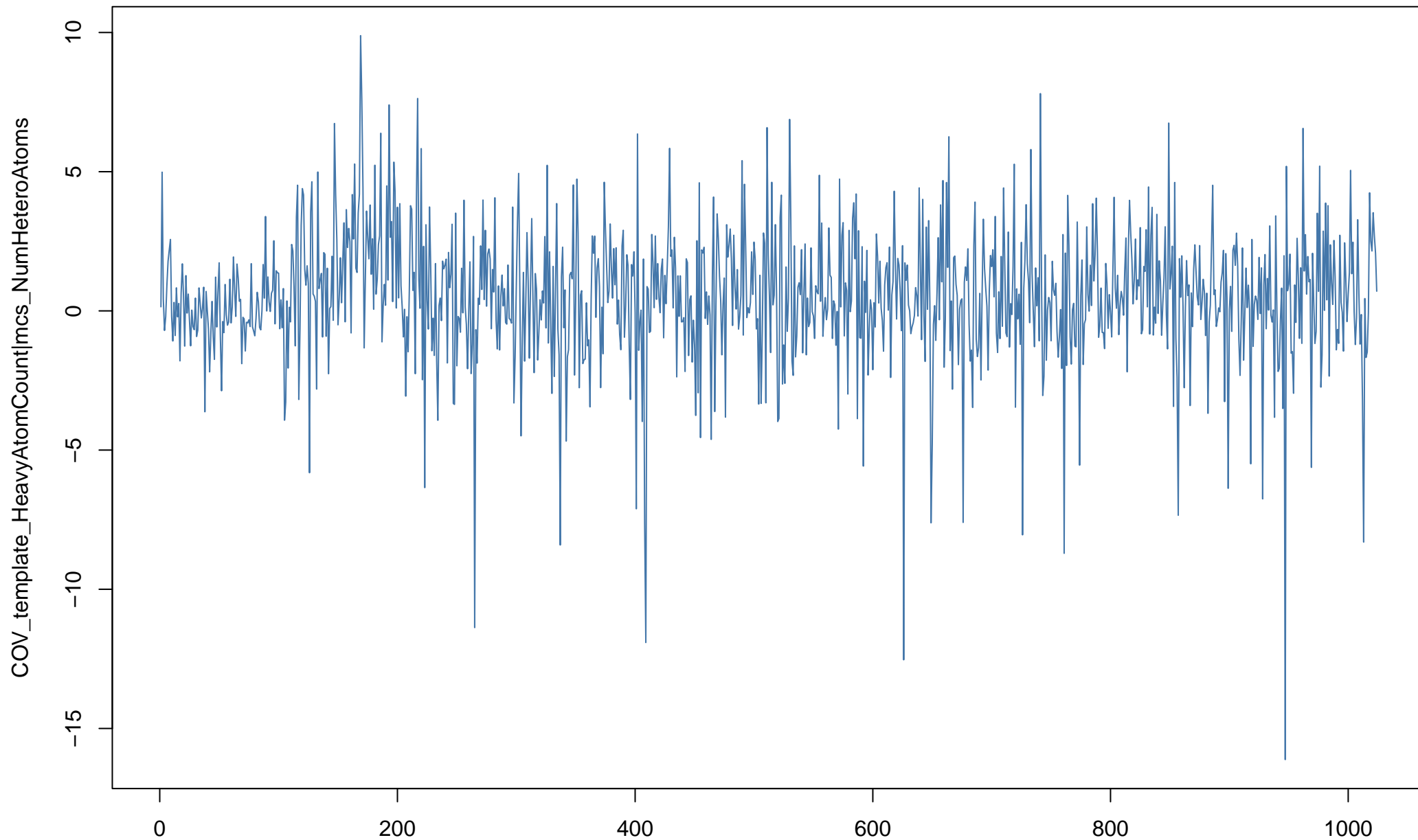
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1020 | BMK = 0.112 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 0



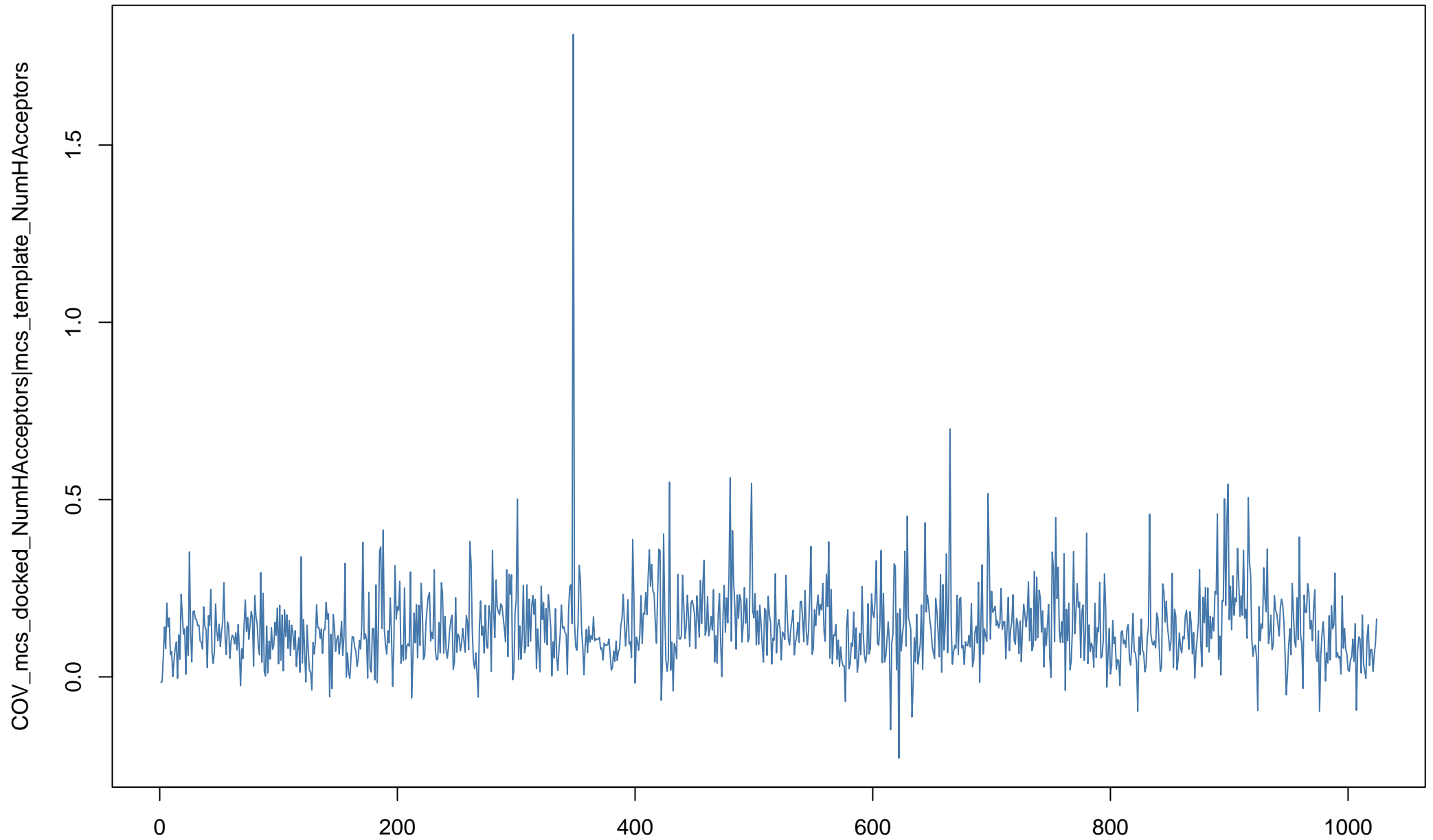
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 754 | BMK = 0.0909 | MCSE(6.27) = 4.07 | stat: TRUE | burn: 0



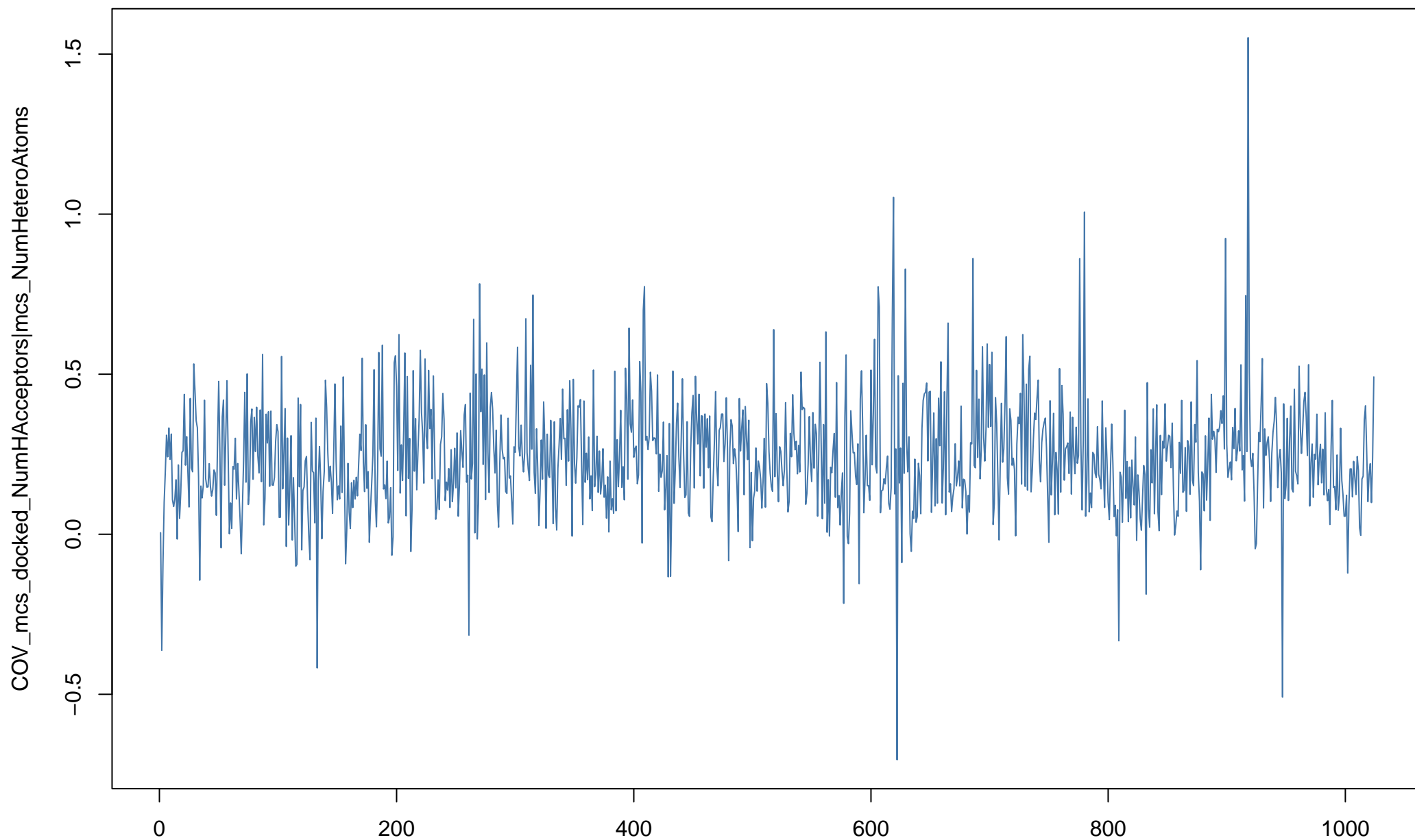
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 675 | BMK = 0.0656 | MCSE(6.27) = 4.18 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 438 | BMK = 0.0931 | MCSE(6.27) = 4.97 | stat: FALSE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 661 | BMK = 0.0914 | MCSE(6.27) = 4.69 | stat: TRUE | burn: 0



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 602 | BMK = 0.0947 | MCSE(6.27) = 4.93 | stat: TRUE | burn: 0

