

-- STATS maxD --

min ESS = 2.63052662078614

max BMK = 0.762699311285285

max MCSE = 17.1590254721933

all stationary: FALSE

burn: 1020

-- STATS 2D --

min ESS = 10.7843612875405

max BMK = 0.586139586526824

max MCSE = 15.0416427888692

all stationary: FALSE

burn: 1020

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 1

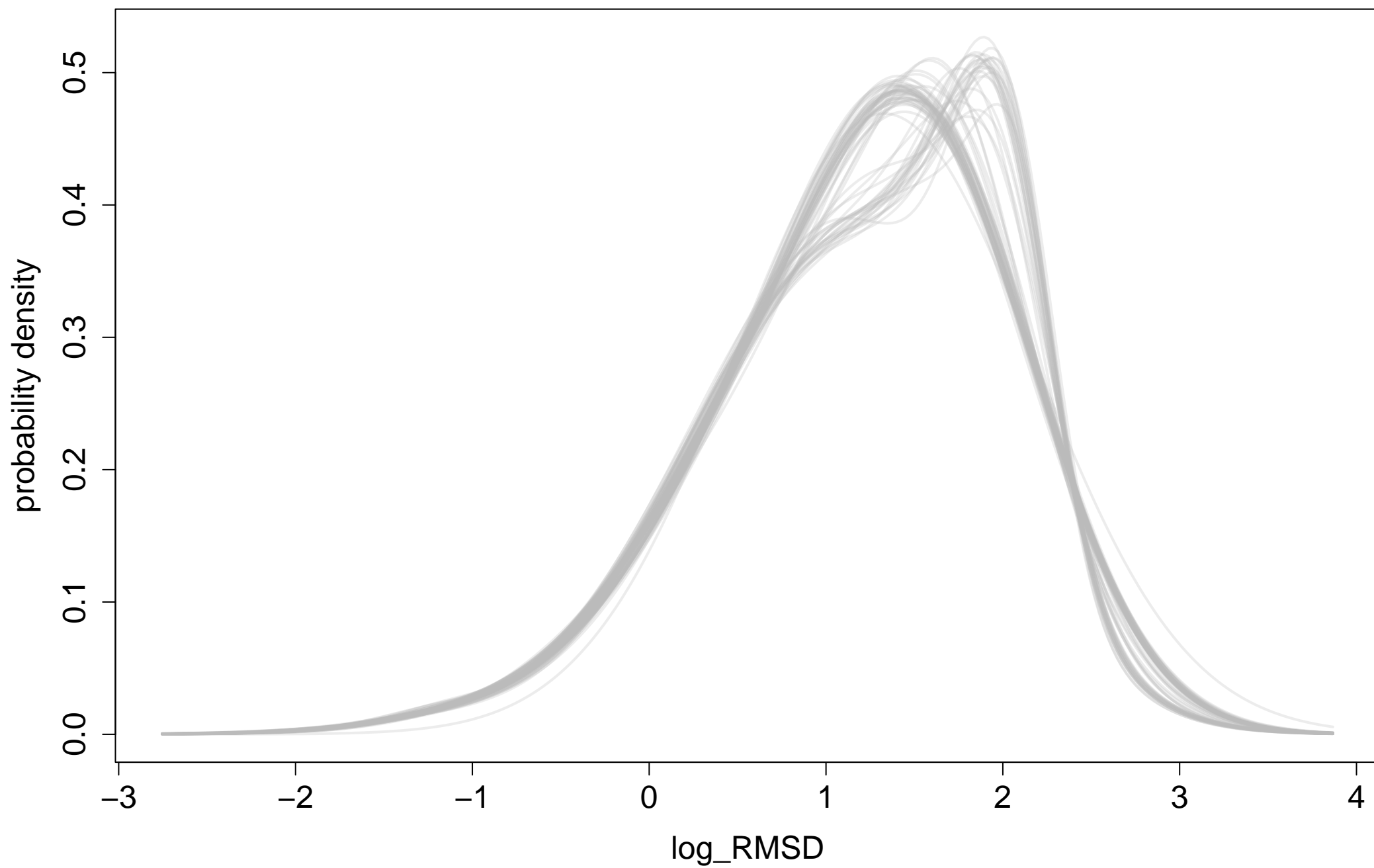
max MCSE = NaN

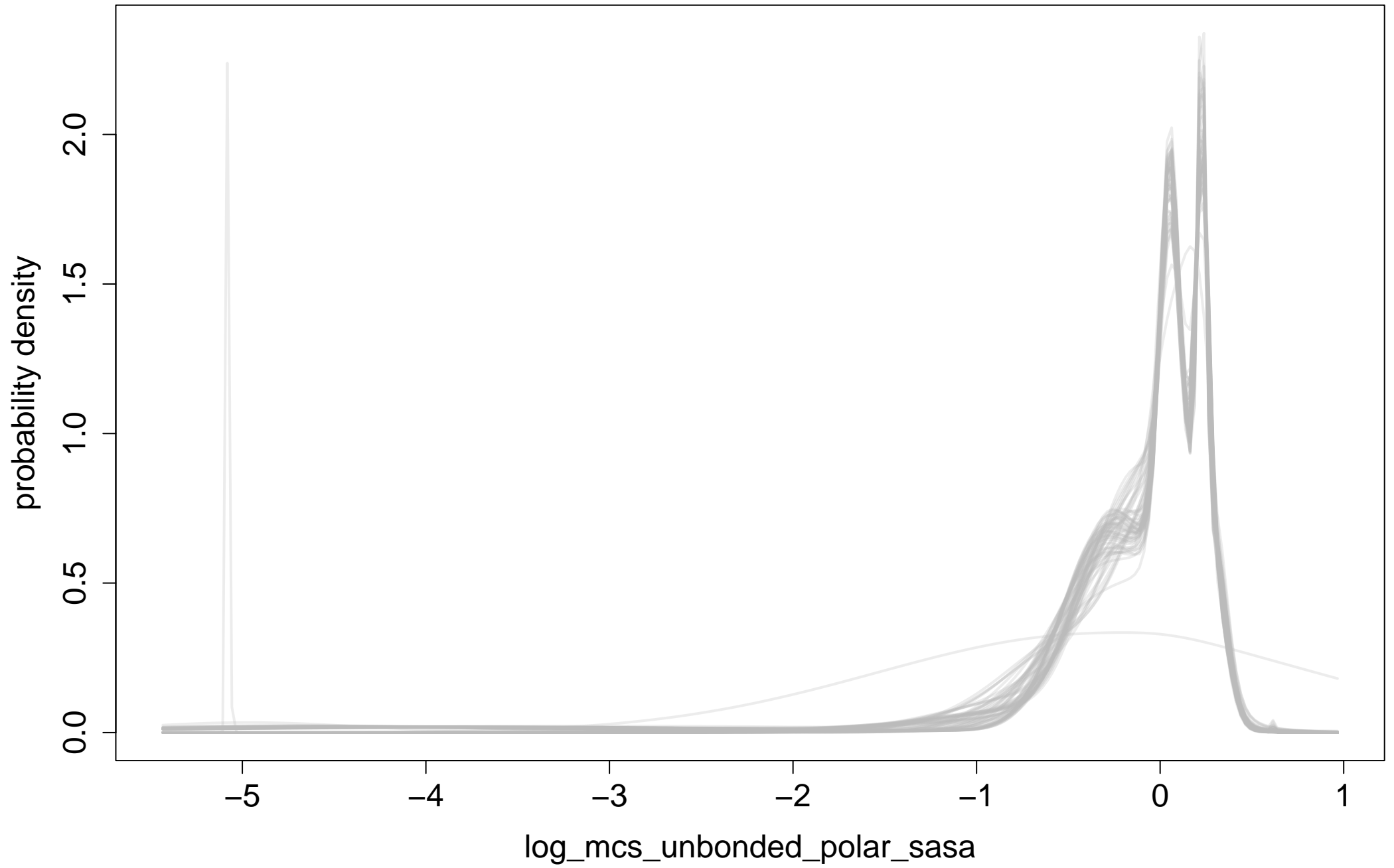
all stationary: FALSE

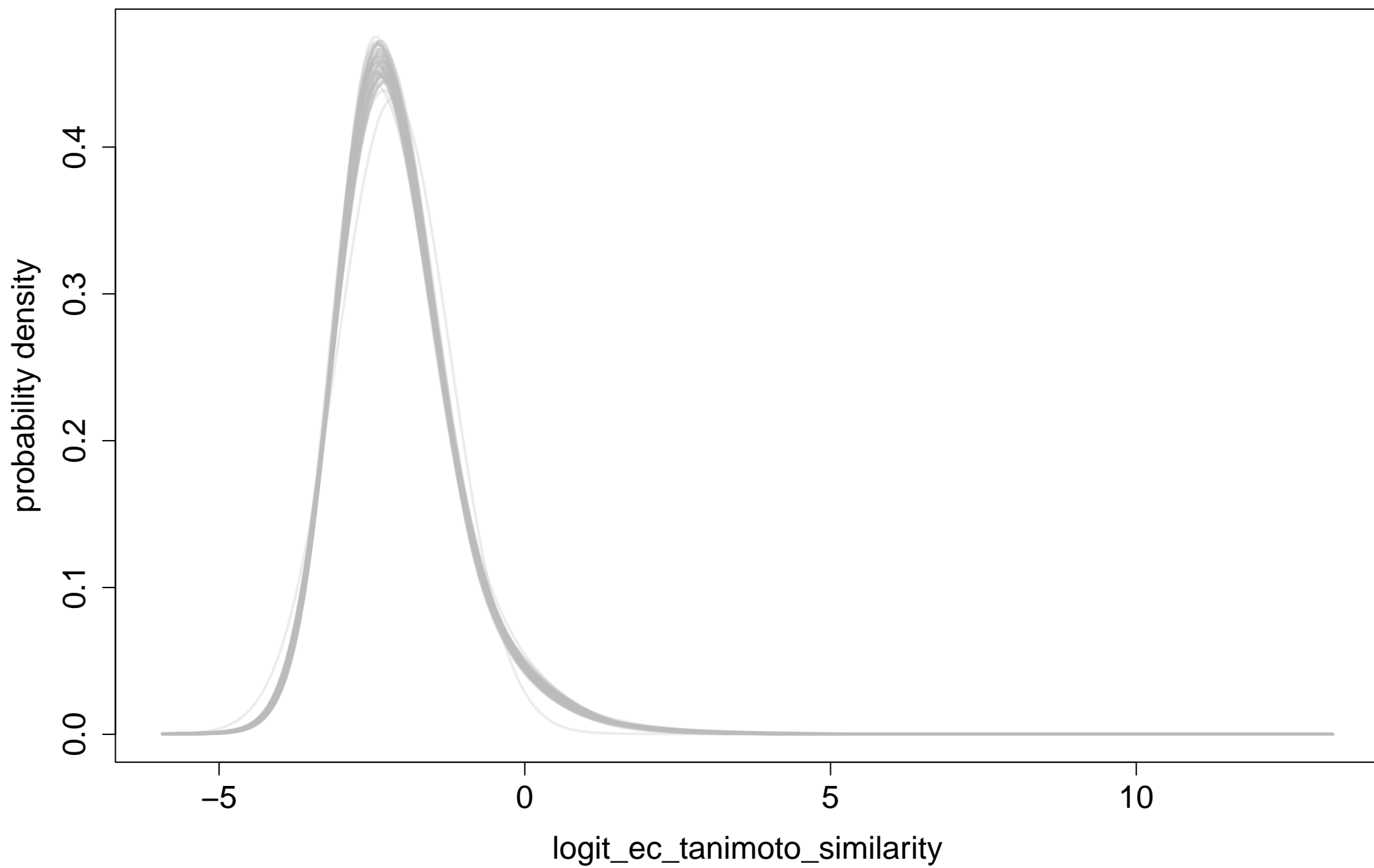
burn: 1020

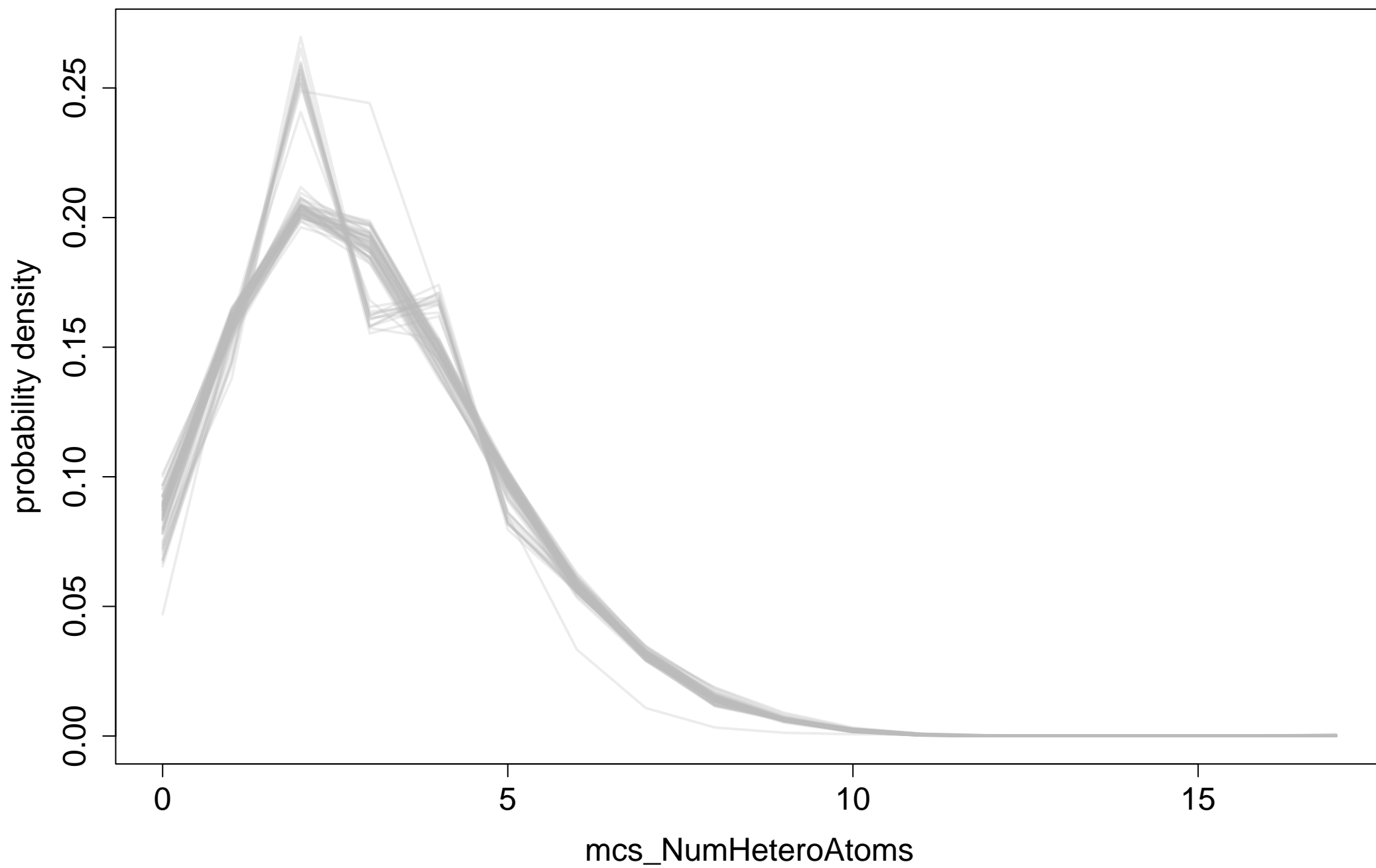
Occupied clusters: 14 of 64

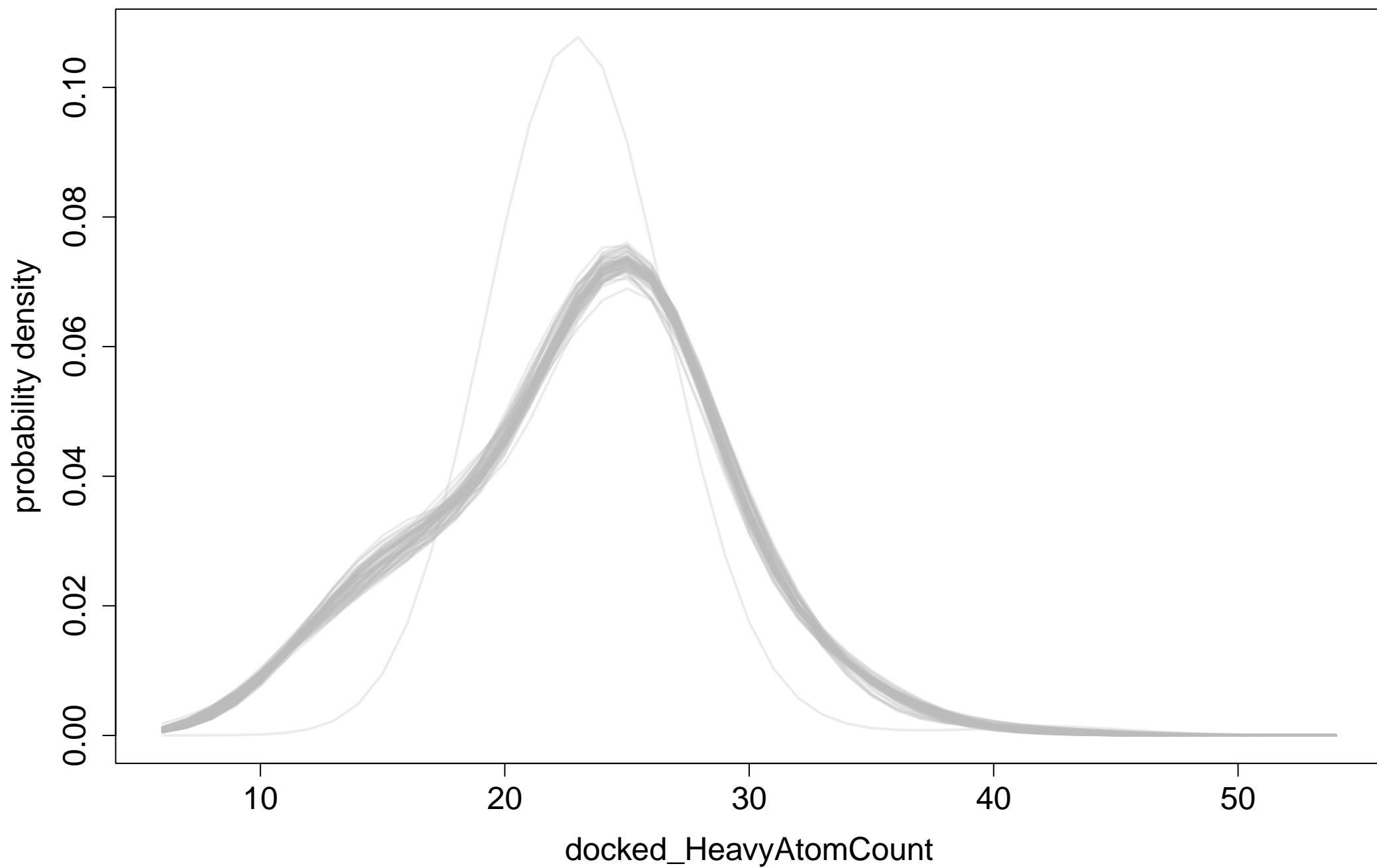
LL: -91300 +- 6840

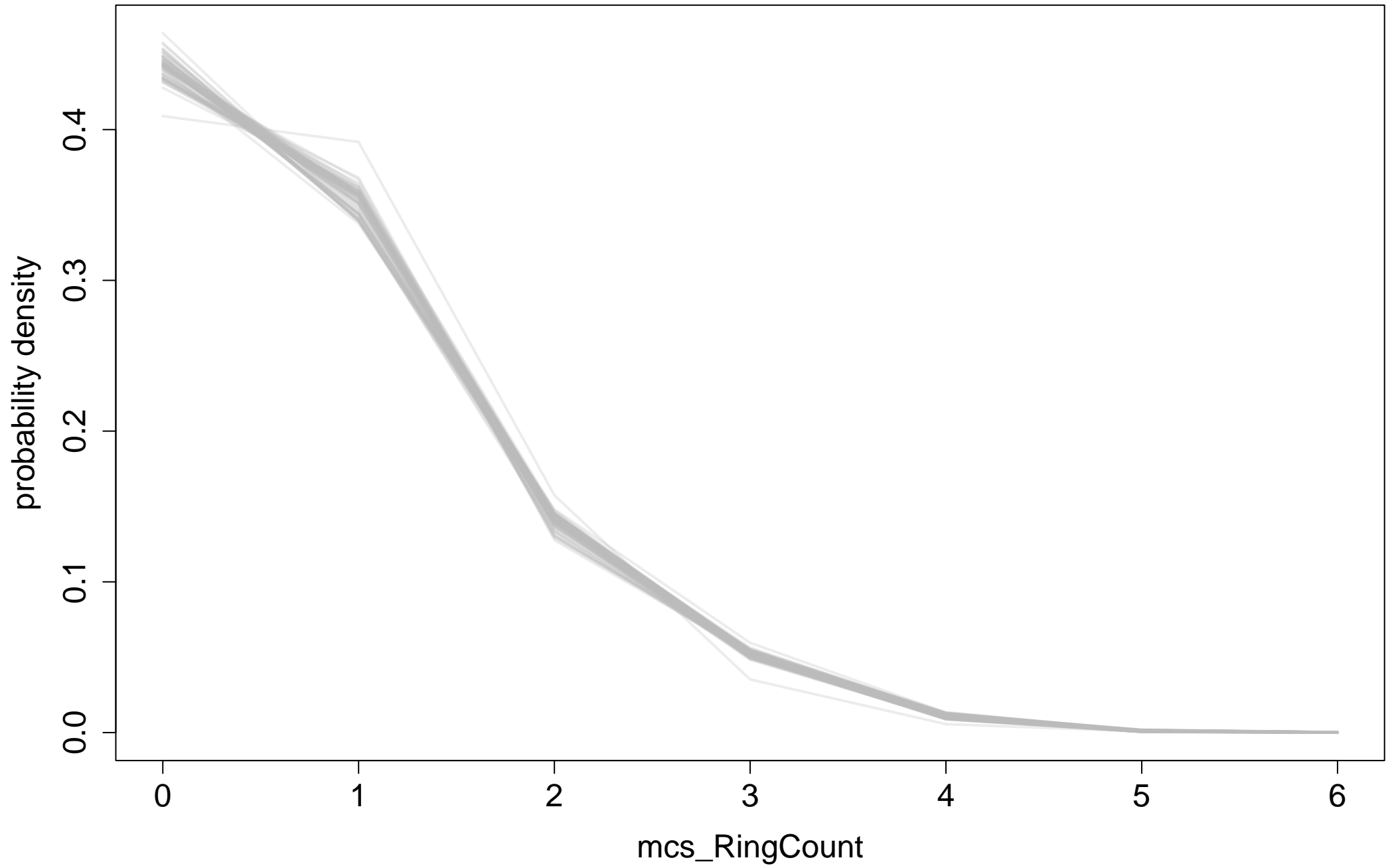


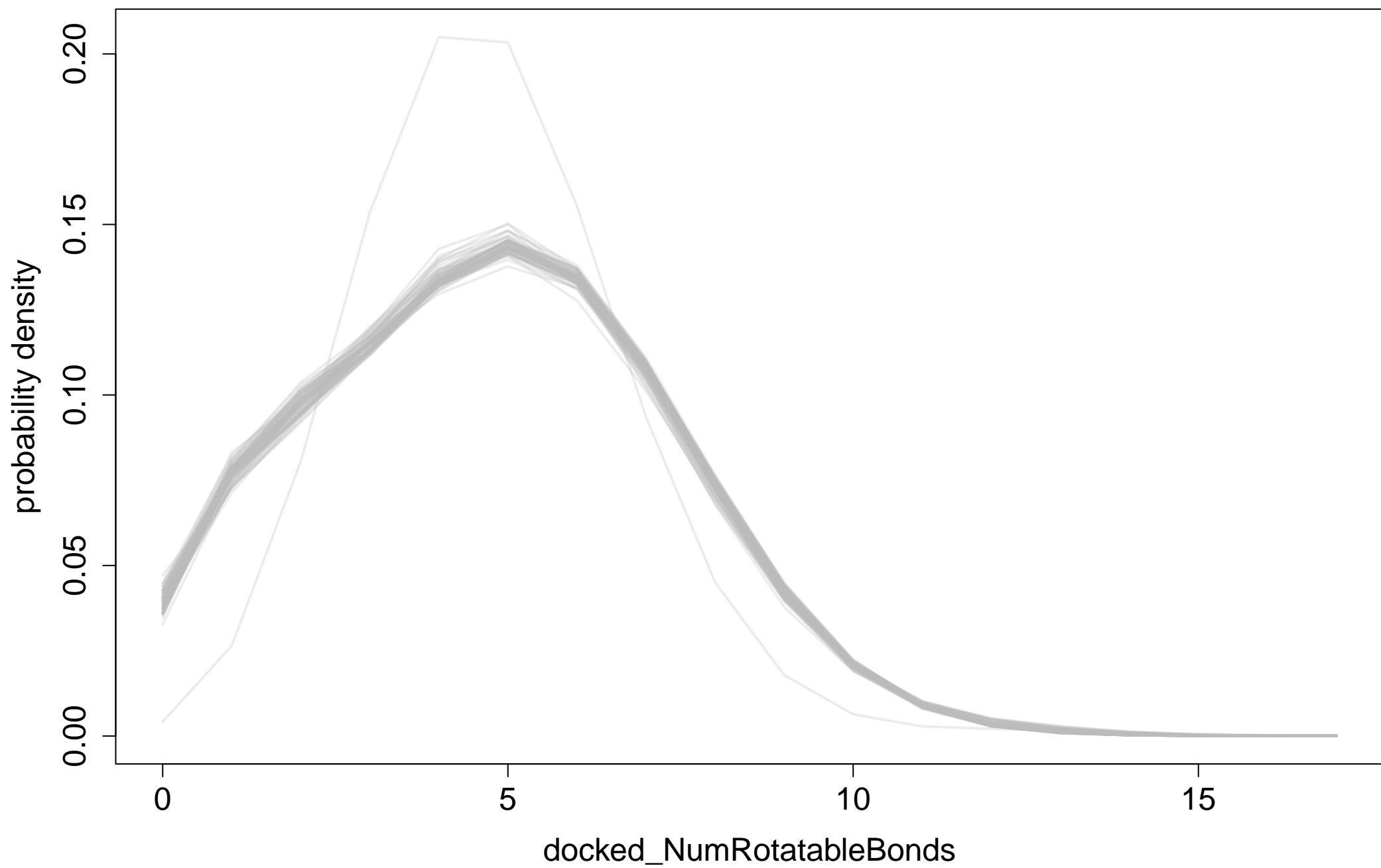


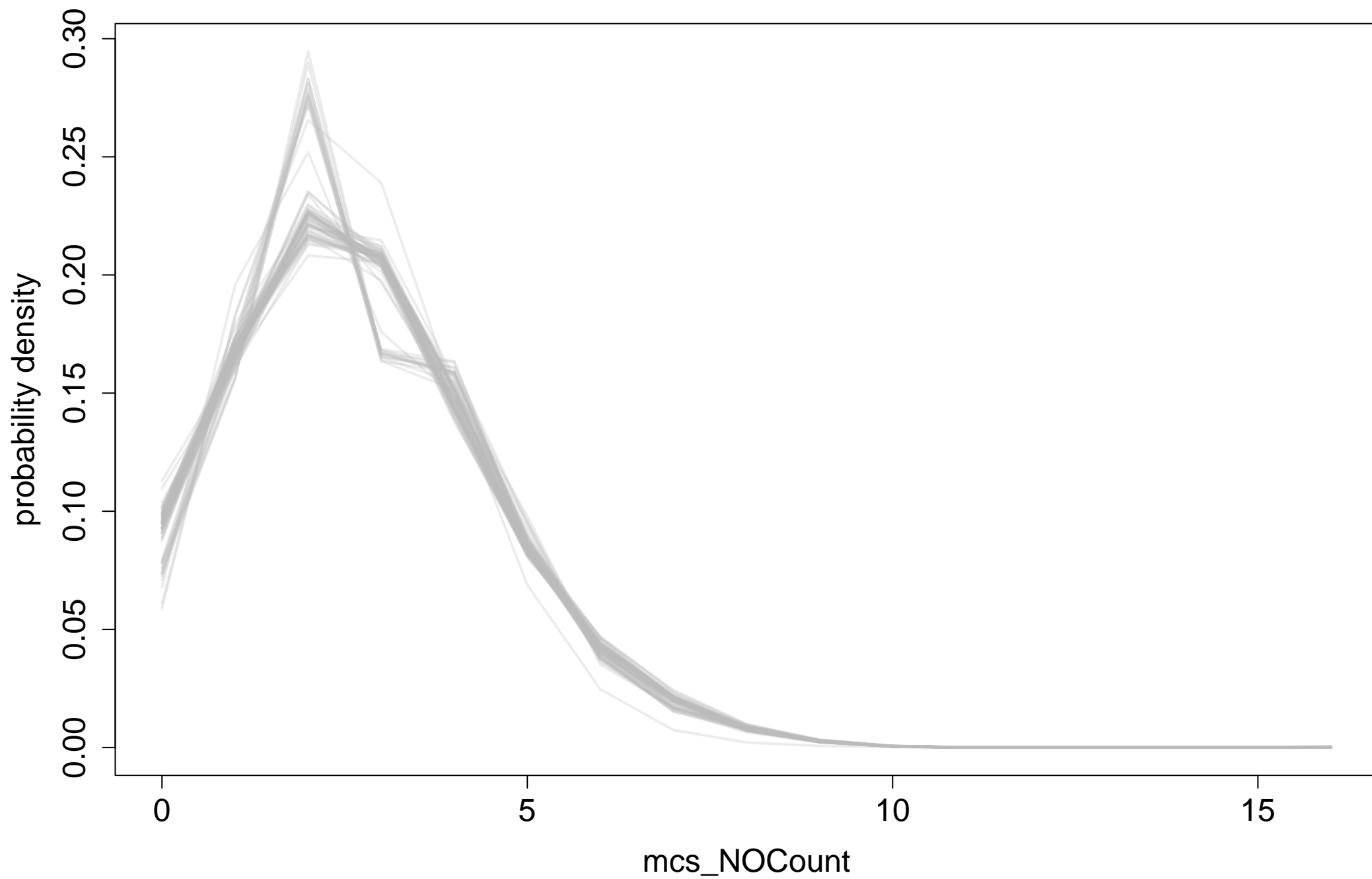


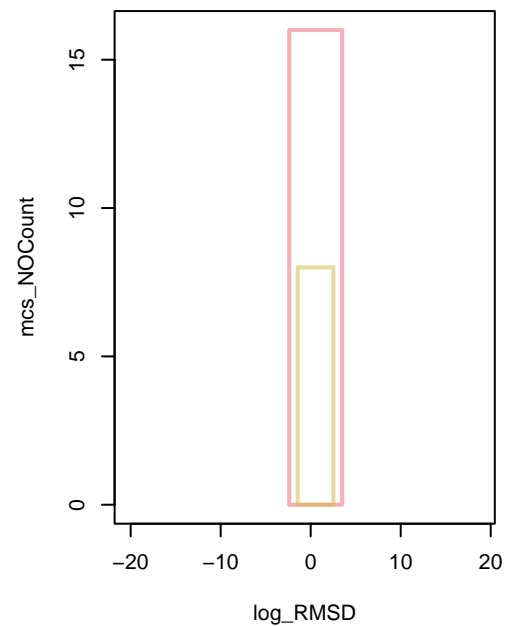
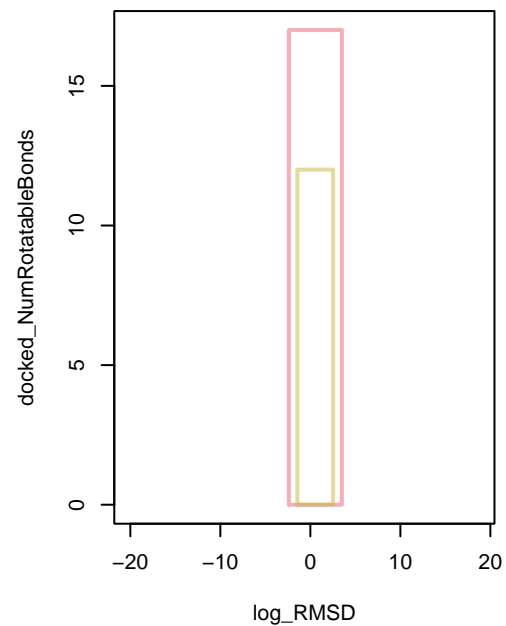
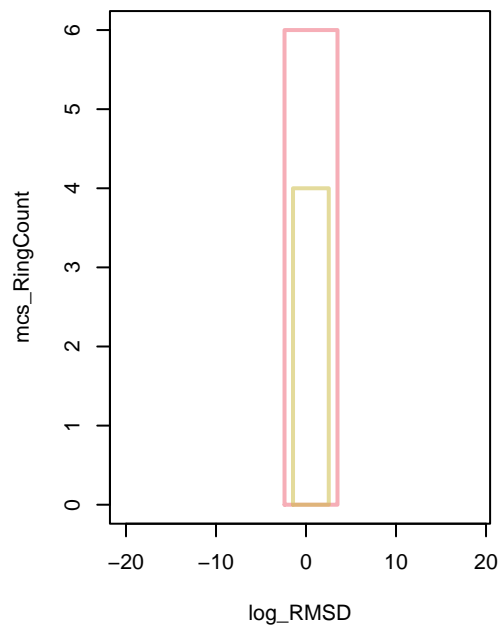
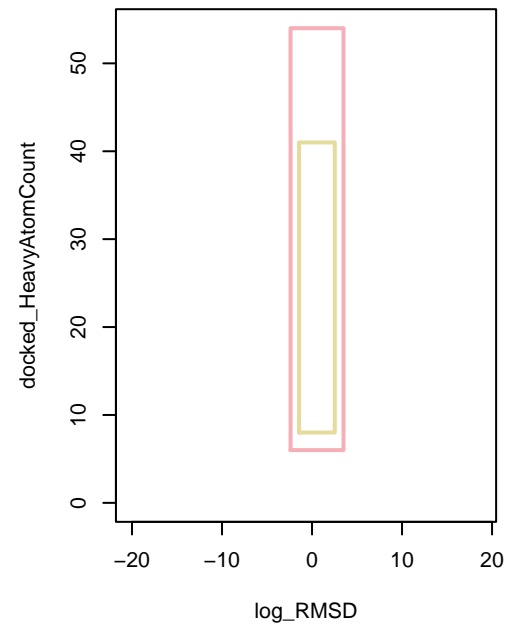
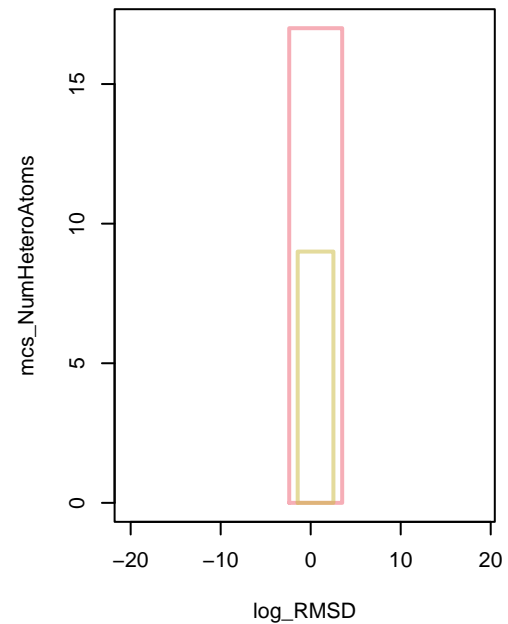
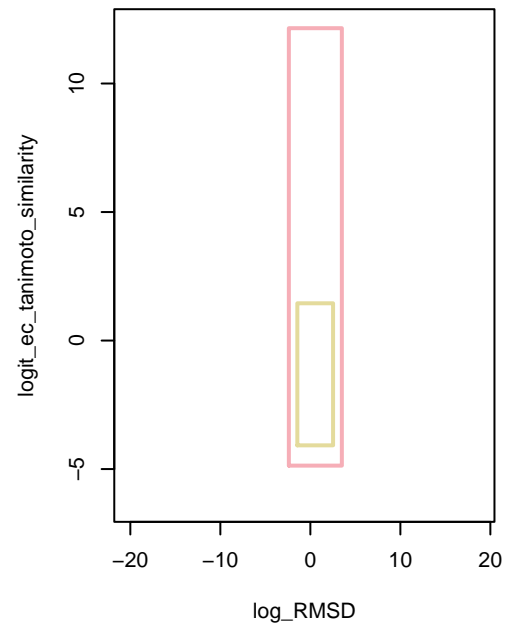
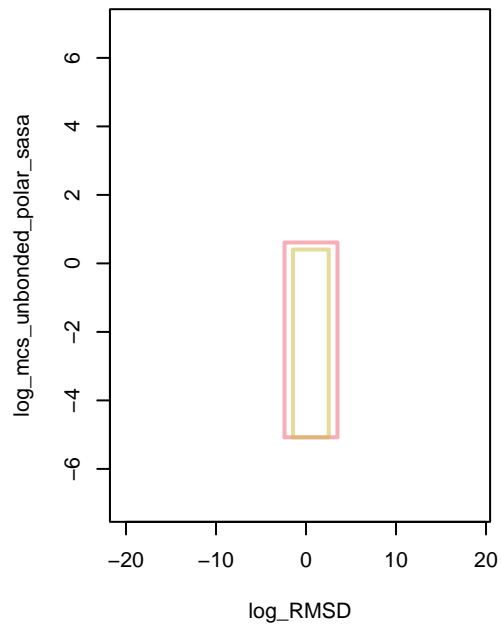




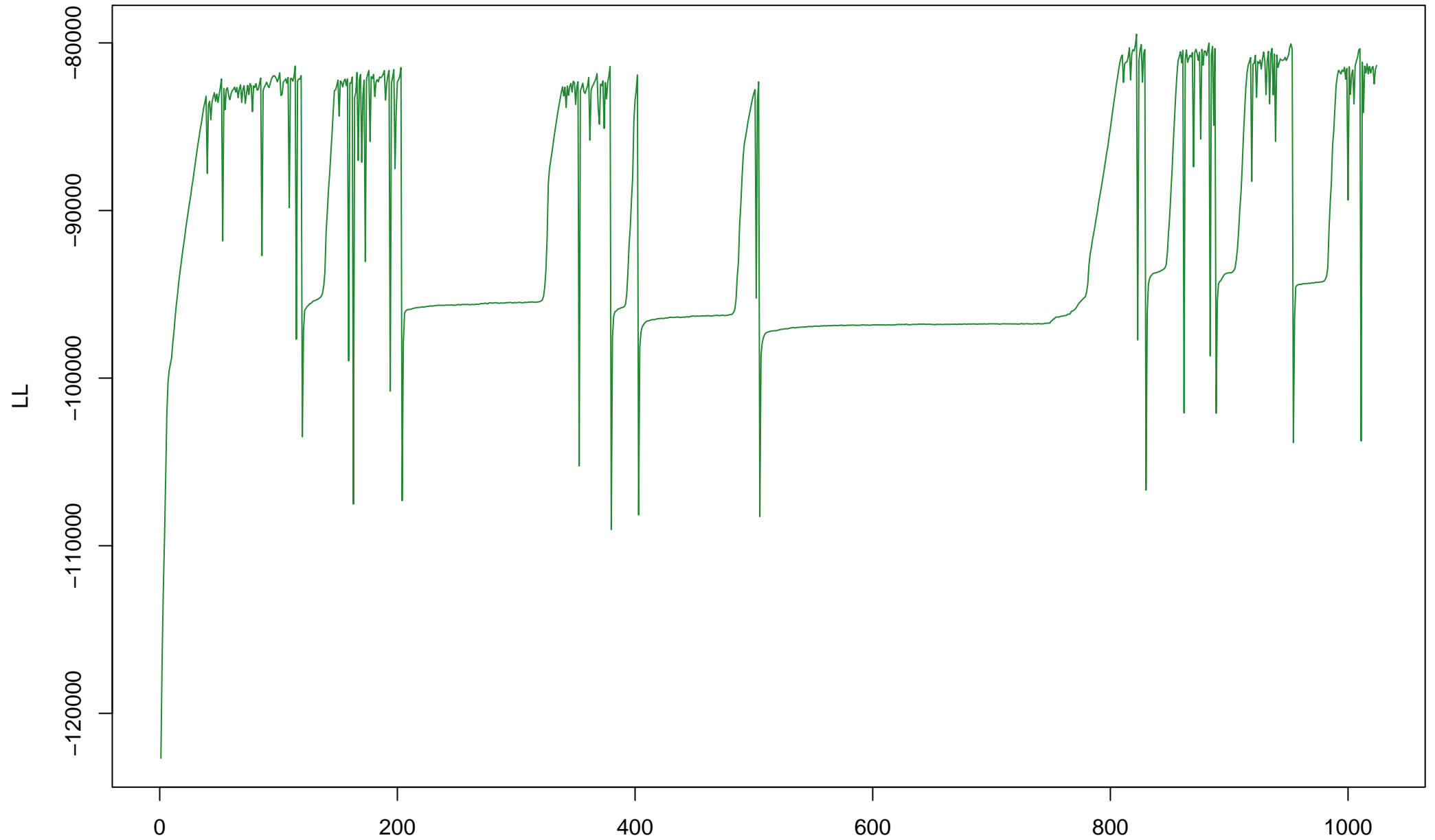




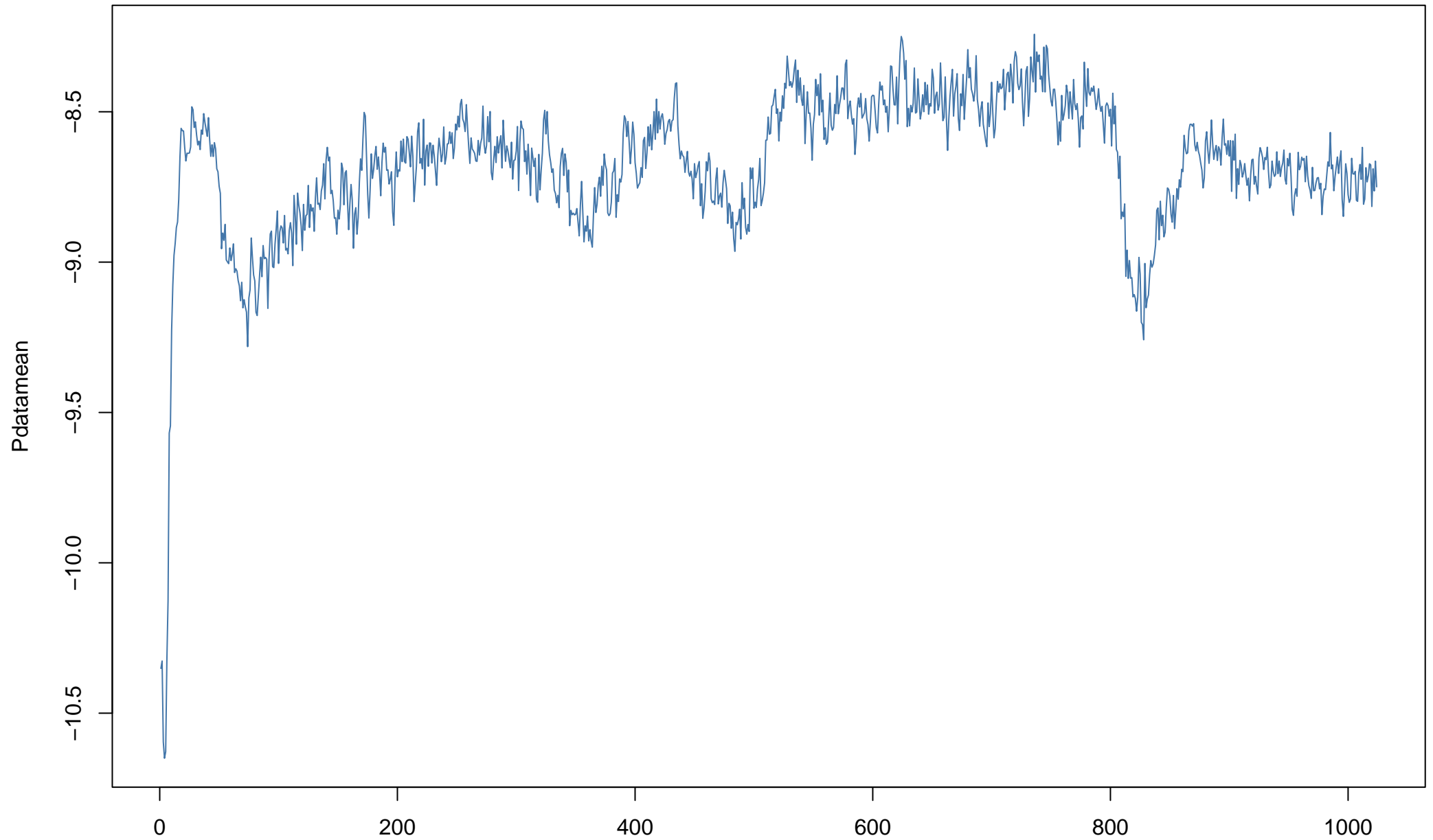




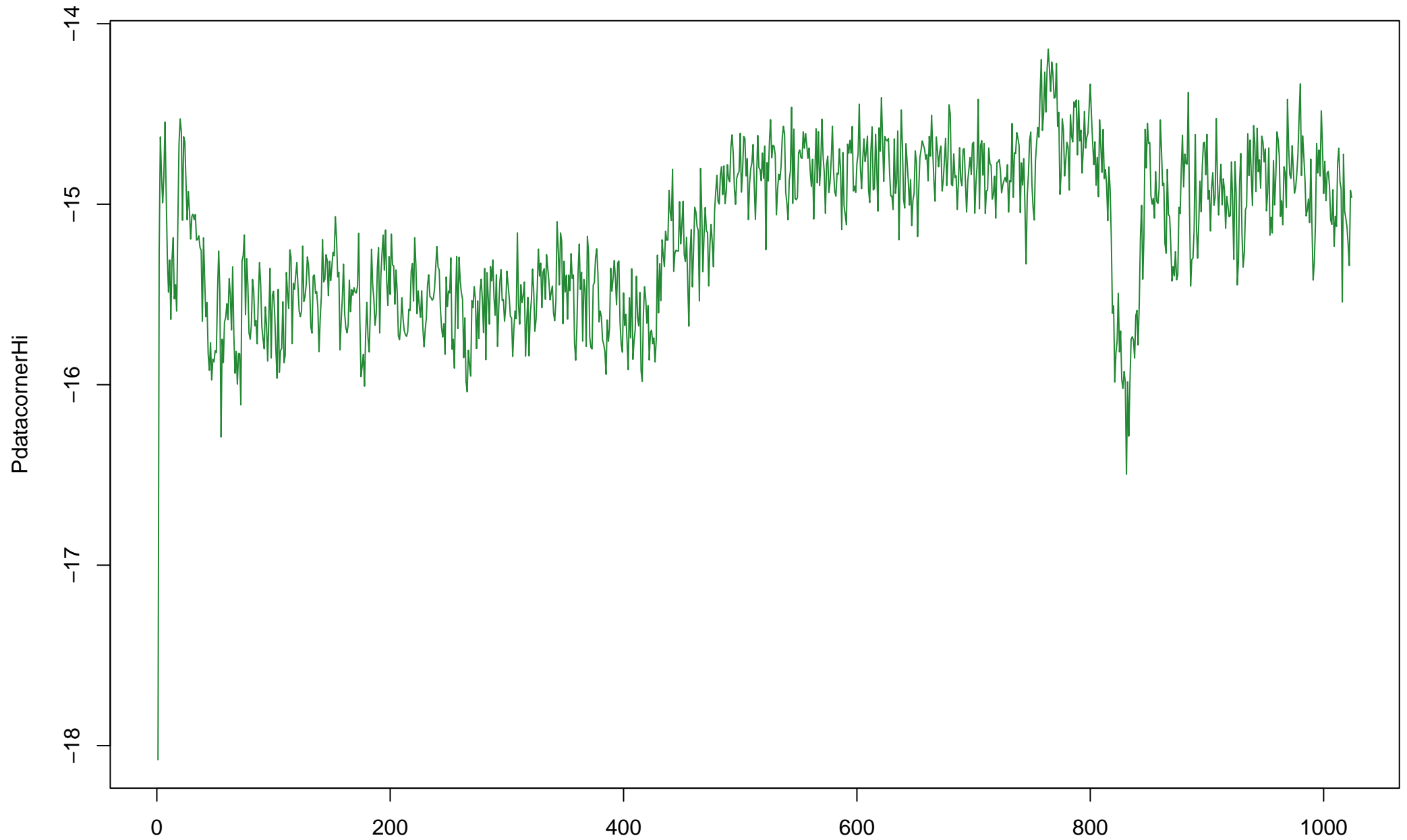
LL



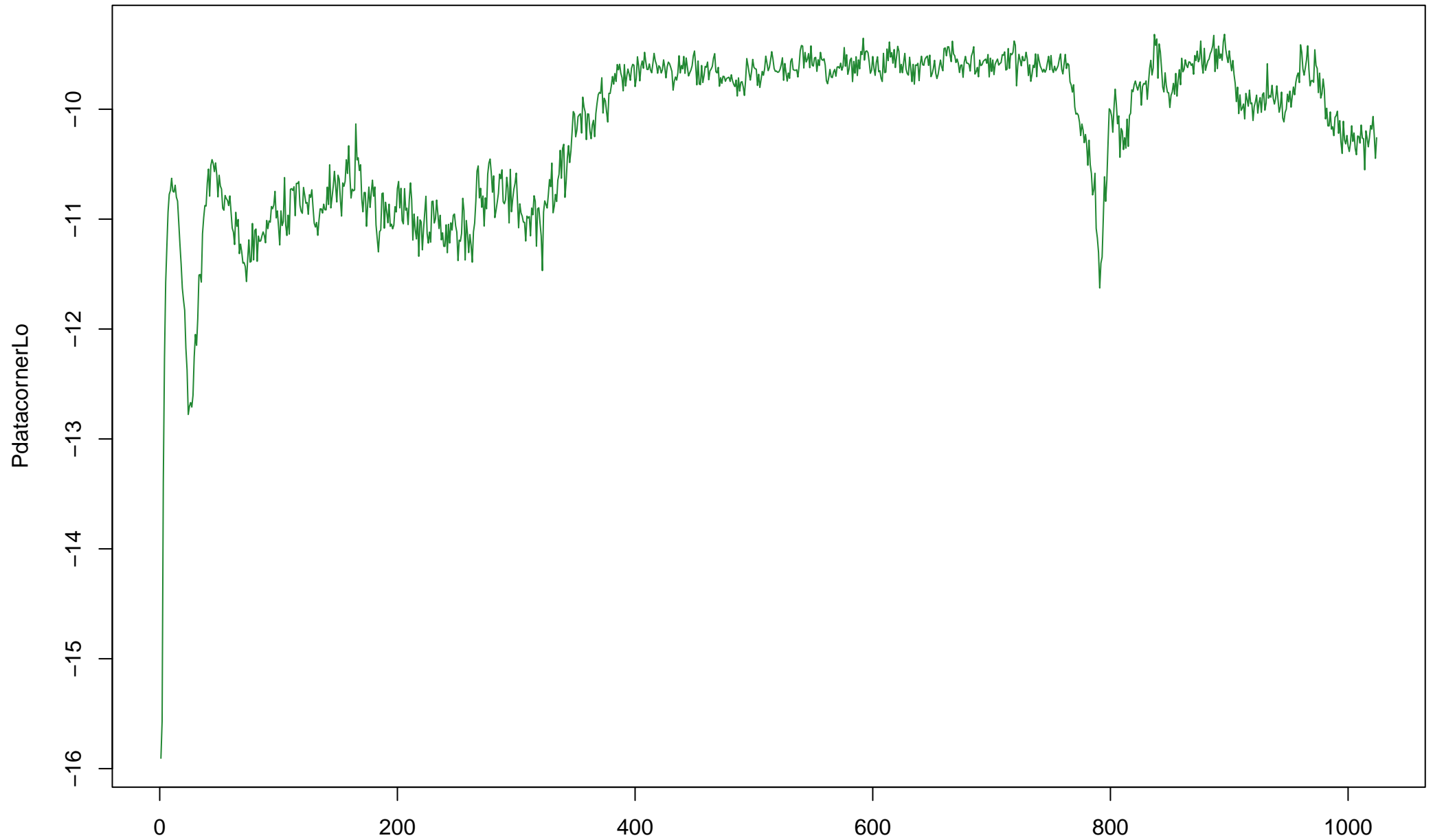
Pdatamean
ESS = 19.4 | BMK = 0.396 | MCSE(6.27) = 14.8 | stat: FALSE | burn: 816



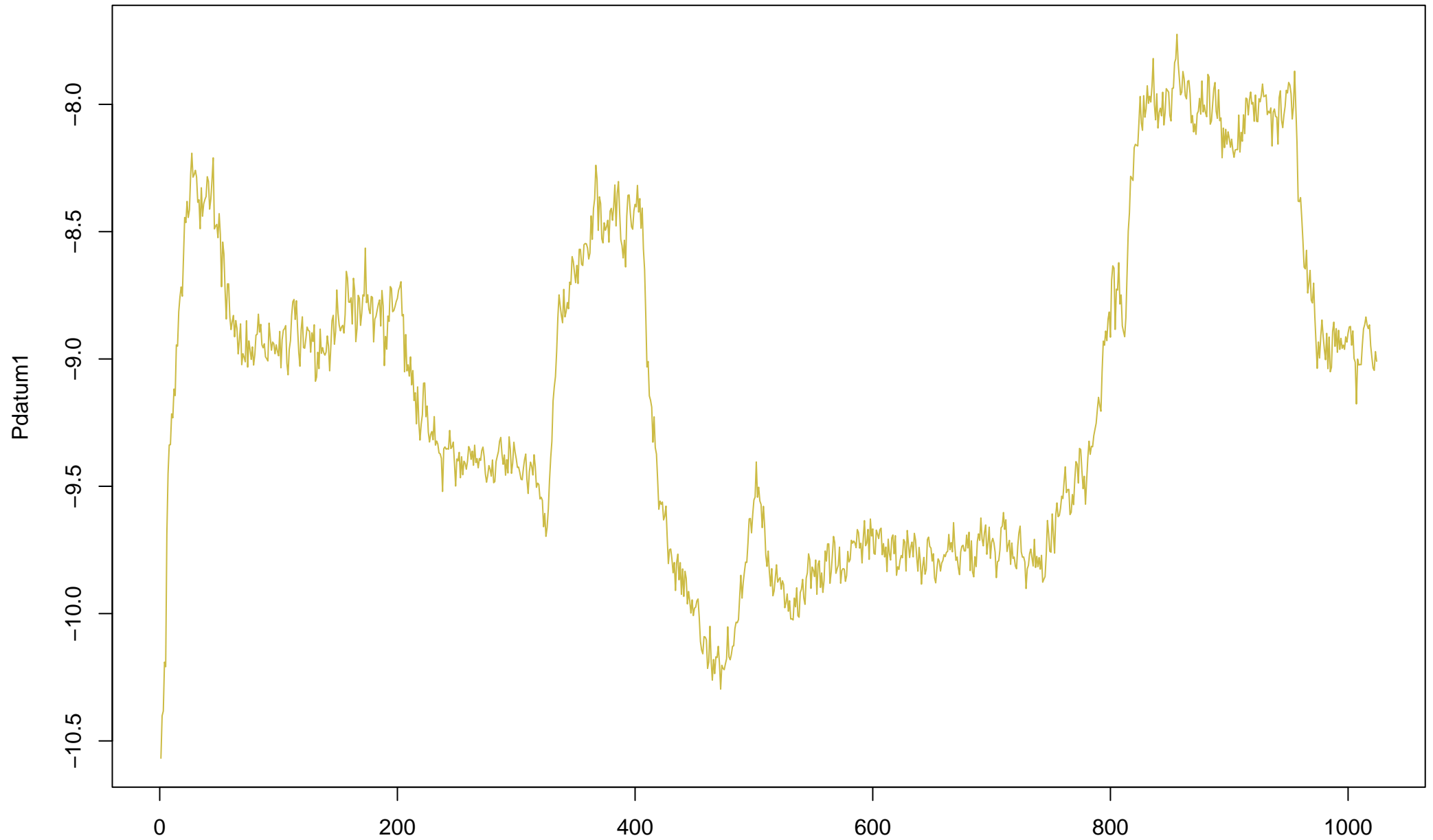
PdatacornerHi
ESS = 8.4 | BMK = 0.595 | MCSE(6.27) = 14.7 | stat: FALSE | burn: 510



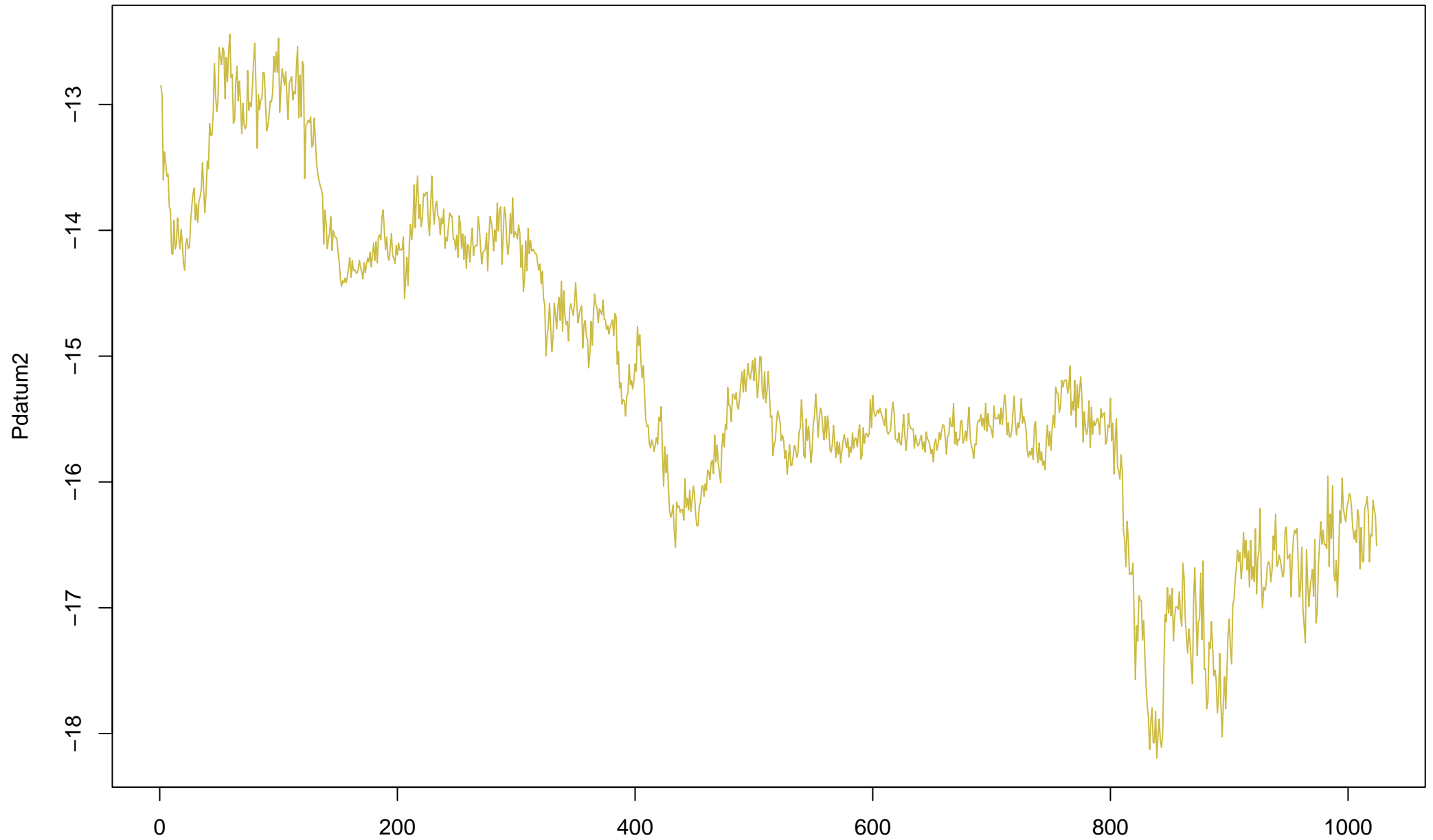
PdatacornerLo
ESS = 4.9 | BMK = 0.514 | MCSE(6.27) = 17.2 | stat: FALSE | burn: 714



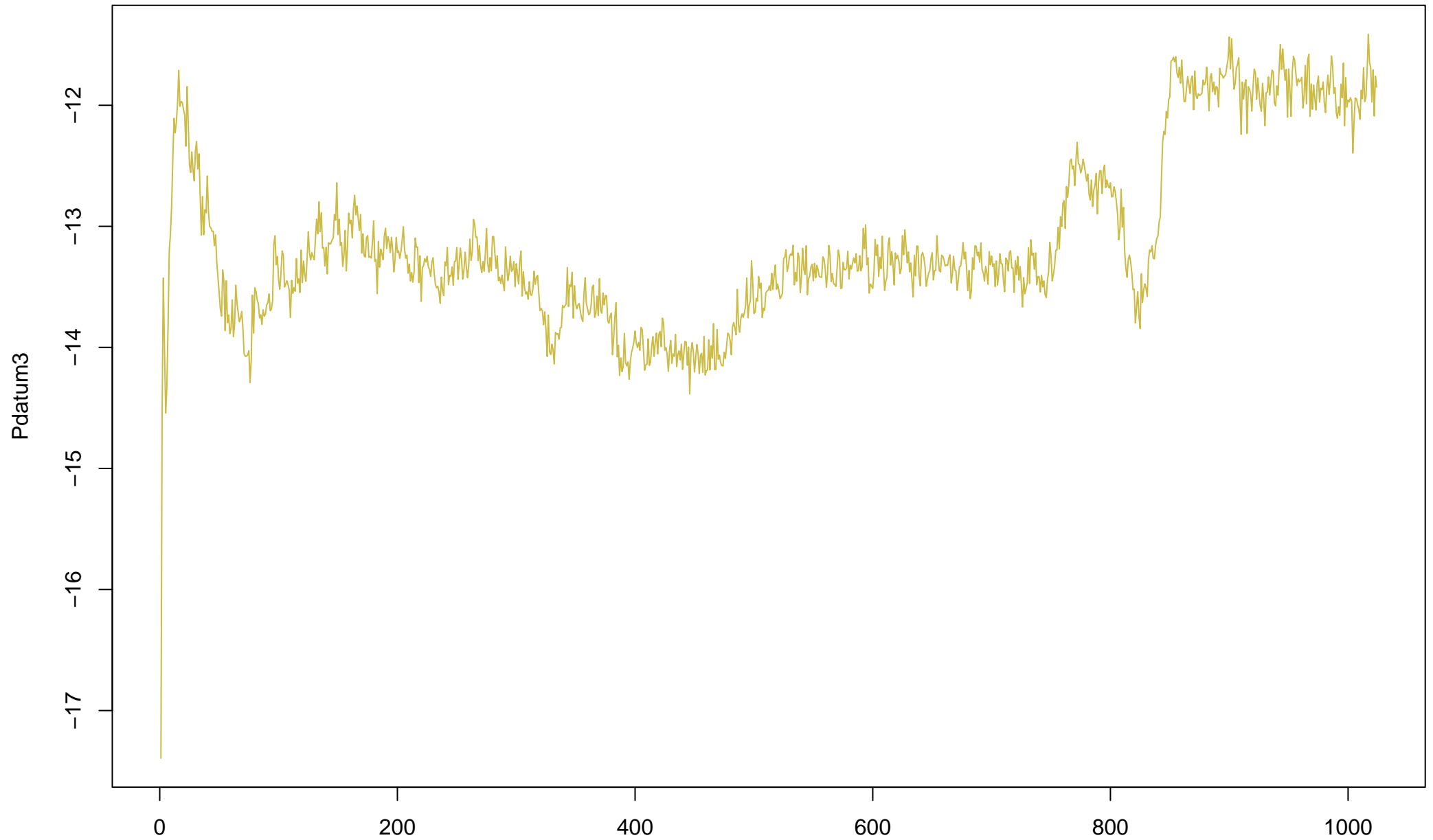
Pdatum1
ESS = 4.34 | BMK = 0.402 | MCSE(6.27) = 17.1 | stat: FALSE | burn: 1020



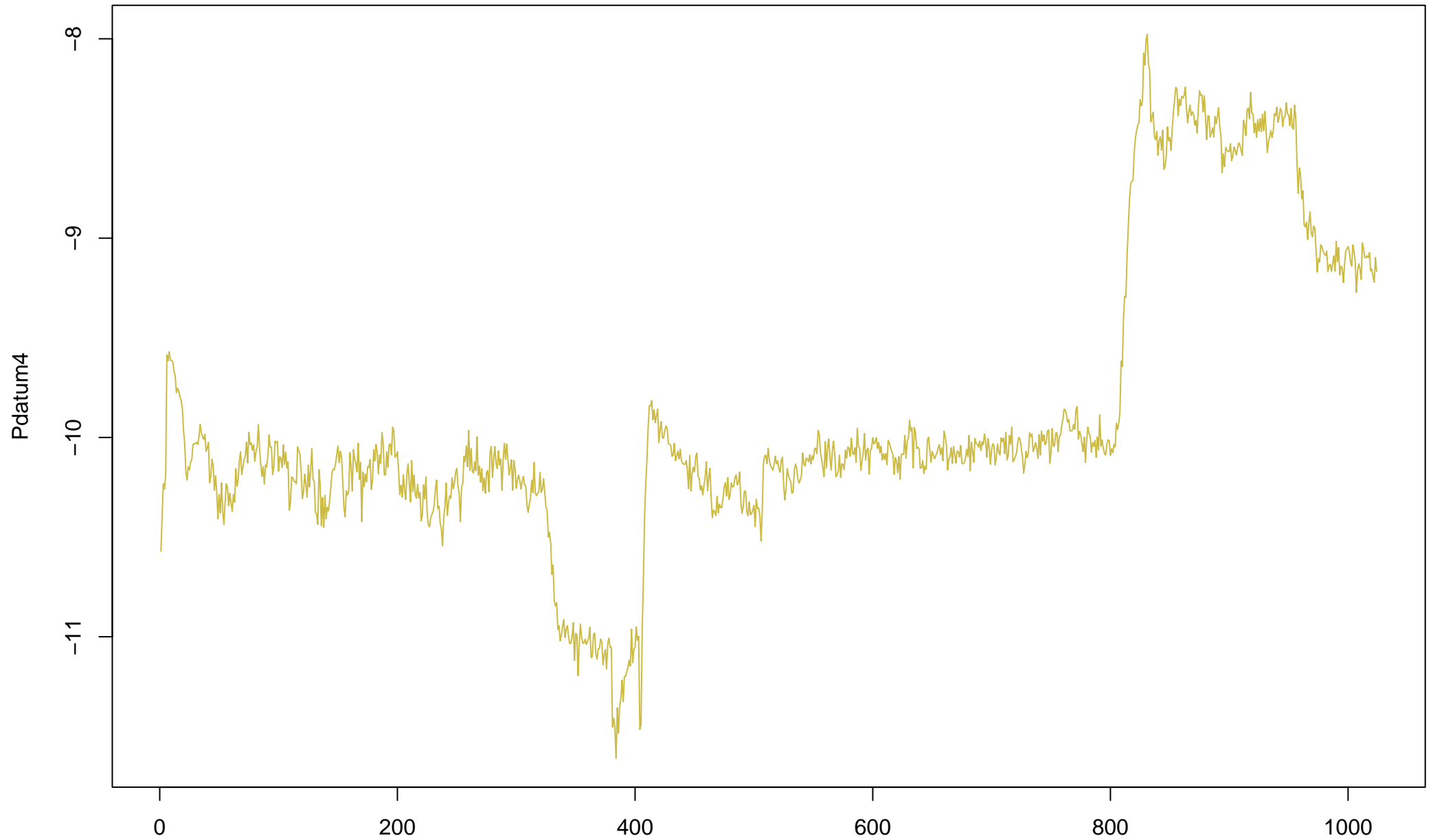
Pdatum2
ESS = 4.1 | BMK = 0.763 | MCSE(6.27) = 16.9 | stat: FALSE | burn: 1020



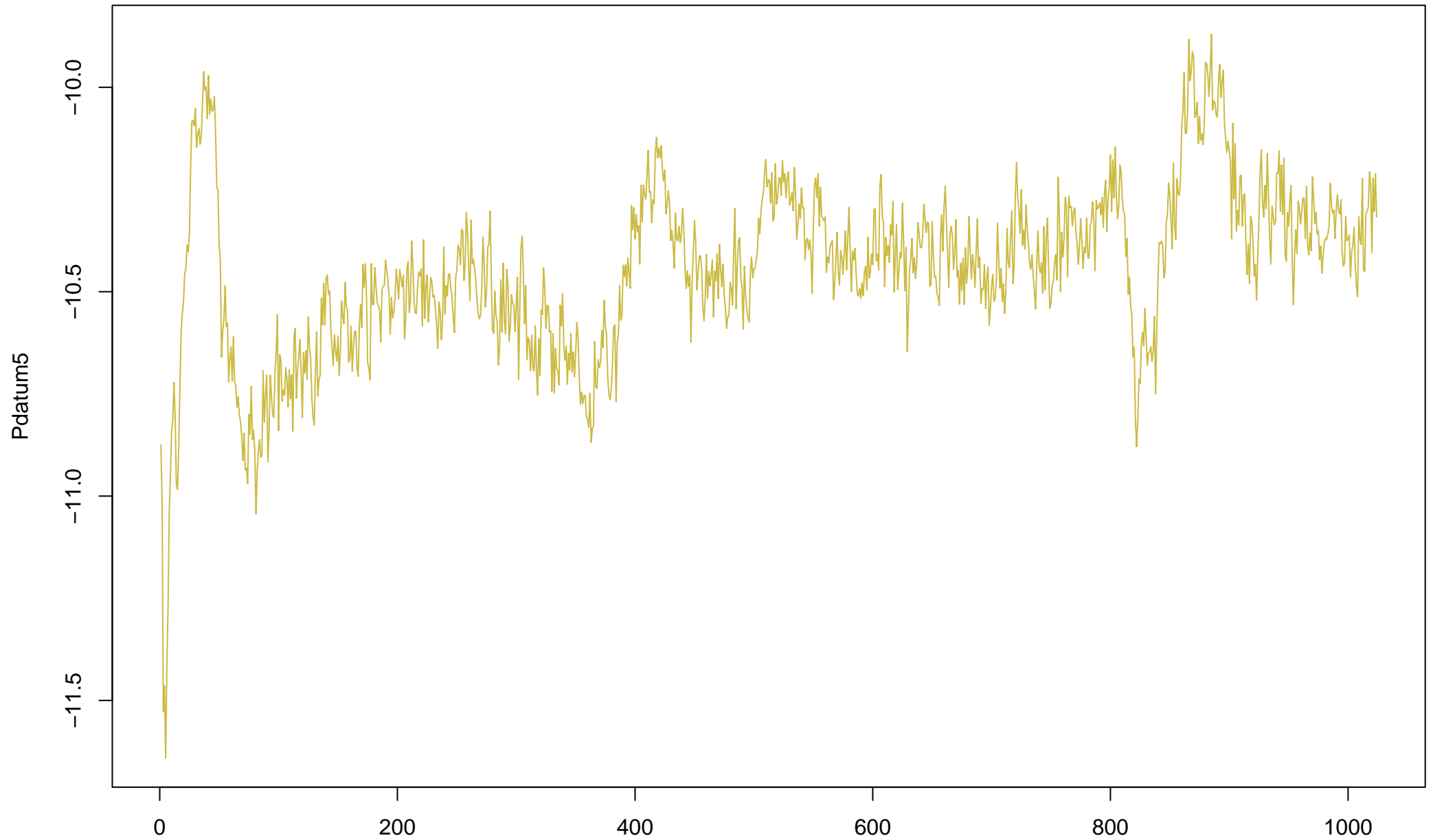
Pdatum3
ESS = 3.49 | BMK = 0.432 | MCSE(6.27) = 16.8 | stat: FALSE | burn: 816



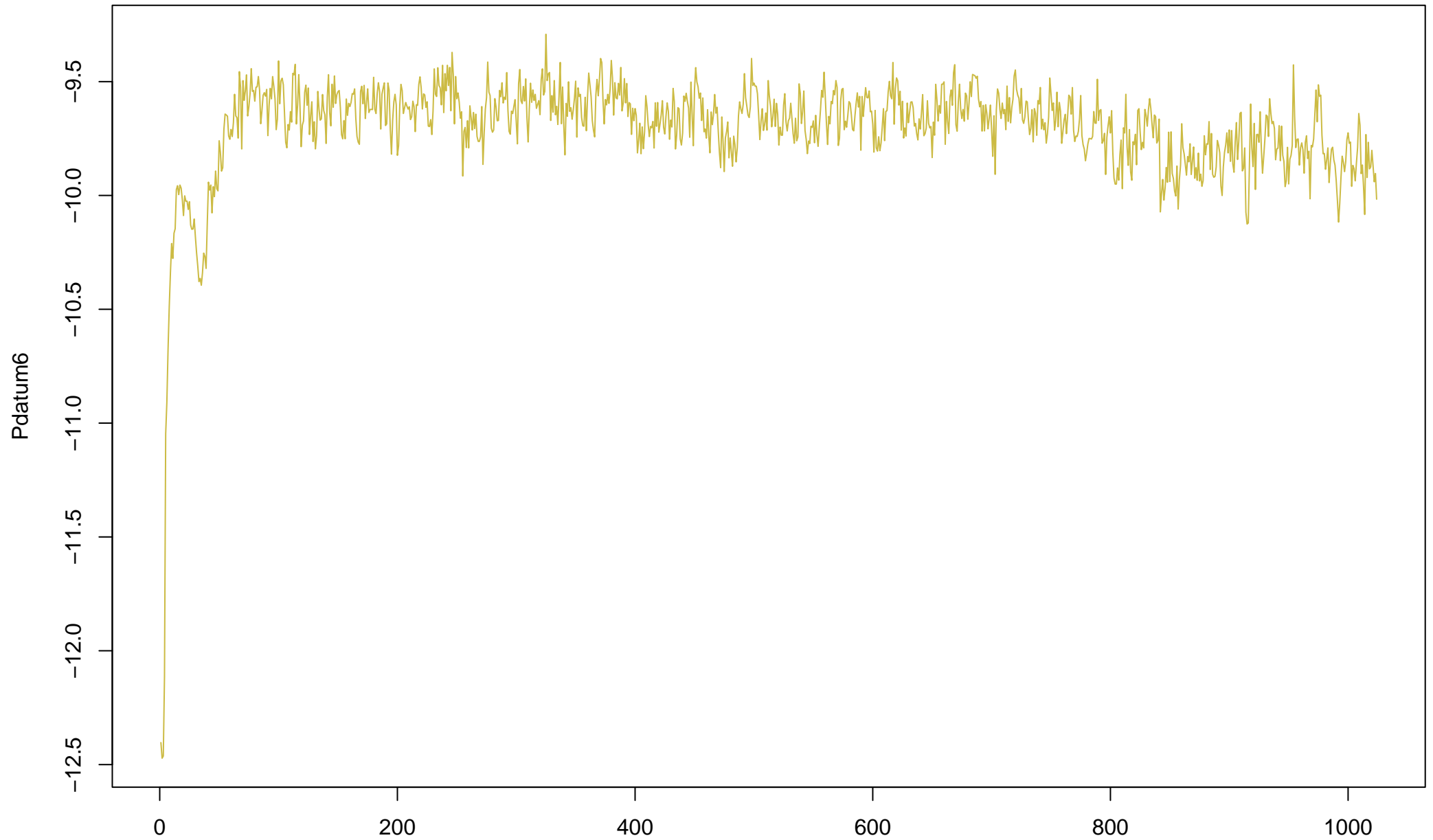
Pdatum4
ESS = 2.63 | BMK = 0.605 | MCSE(6.27) = 17.1 | stat: FALSE | burn: 1020



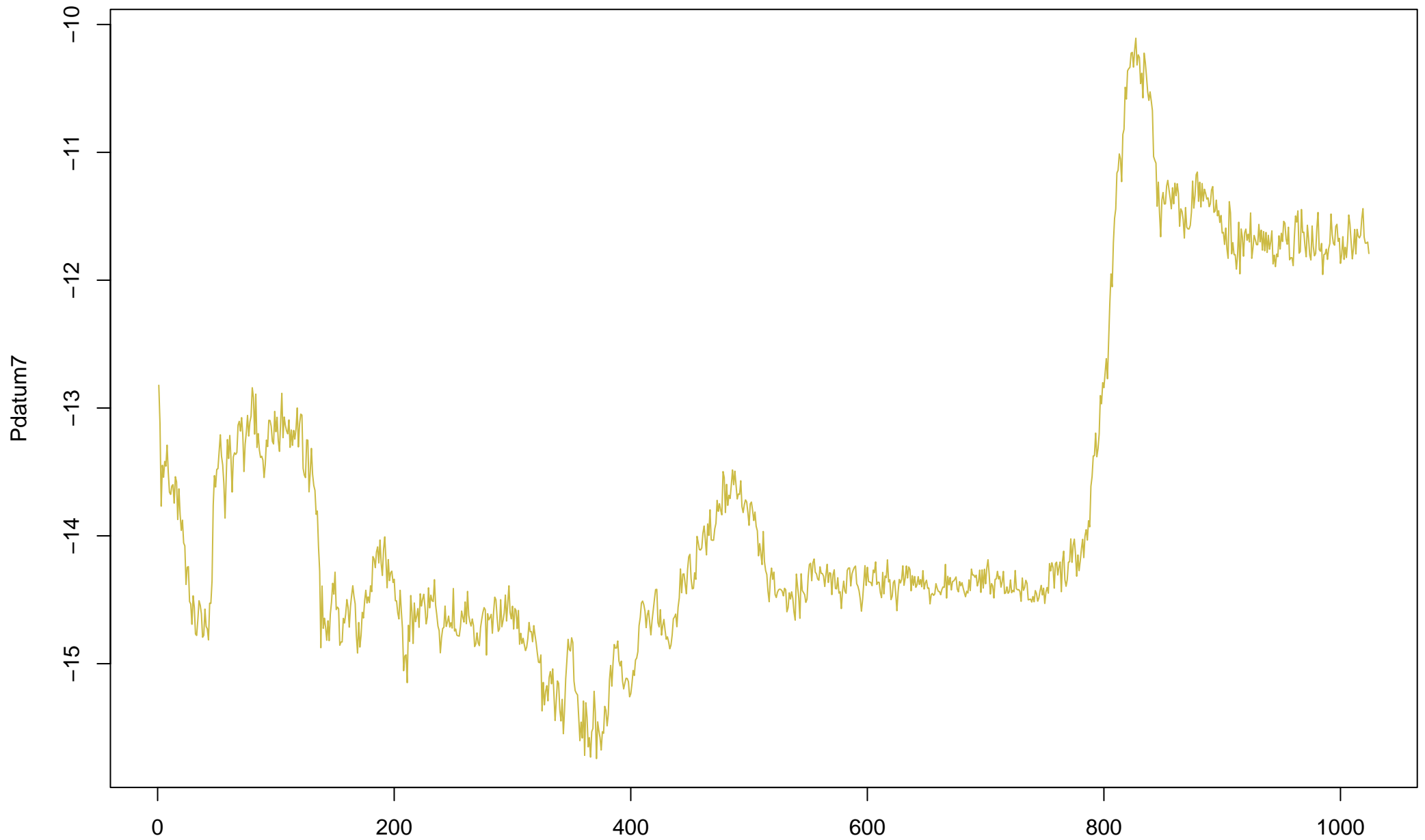
Pdatum5
ESS = 18.7 | BMK = 0.421 | MCSE(6.27) = 13.9 | stat: FALSE | burn: 1020



Pdatum6
ESS = 26.6 | BMK = 0.268 | MCSE(6.27) = 13.4 | stat: FALSE | burn: 102

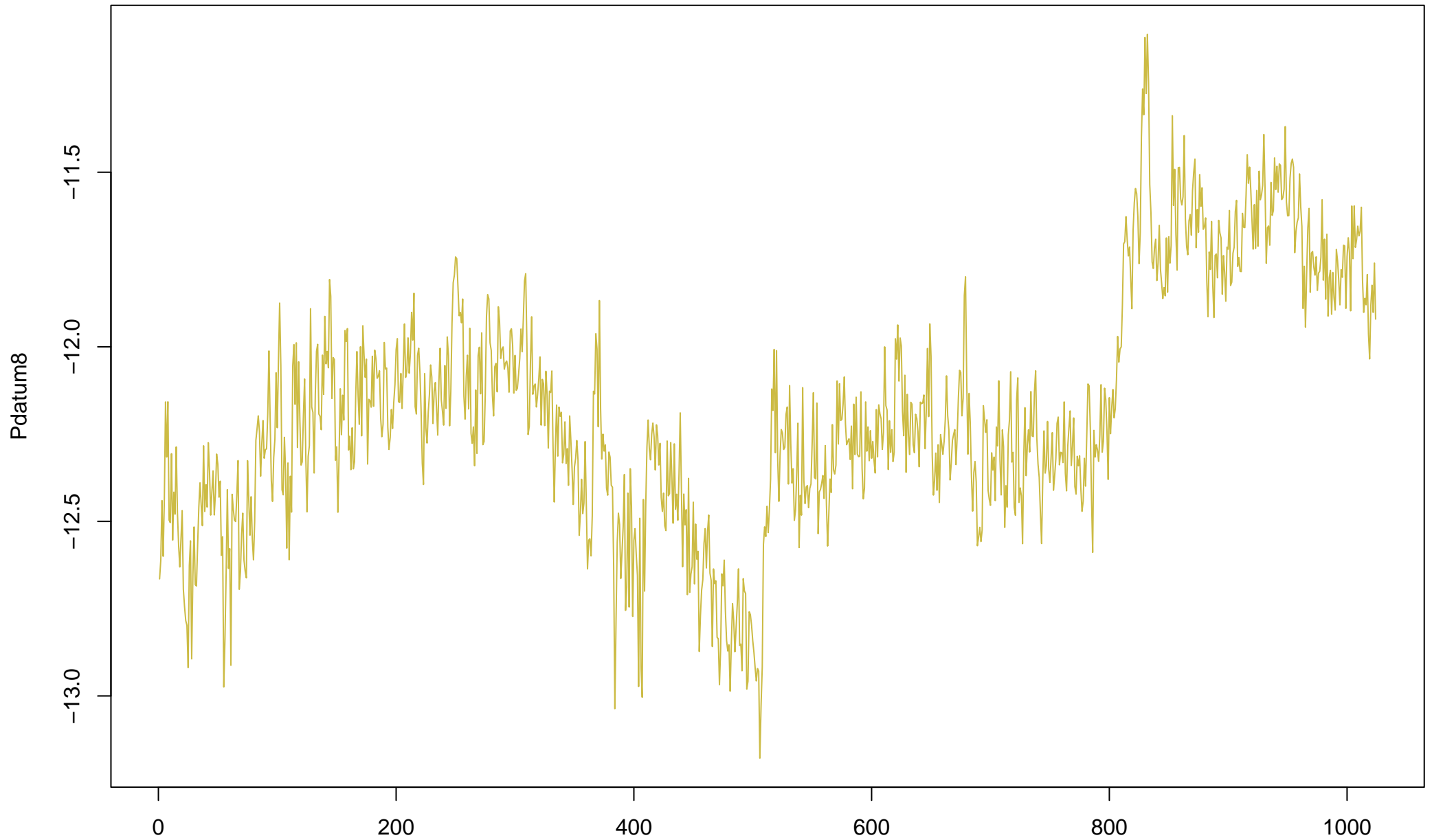


Pdatum7
ESS = 10.1 | BMK = 0.62 | MCSE(6.27) = 16 | stat: FALSE | burn: 1020

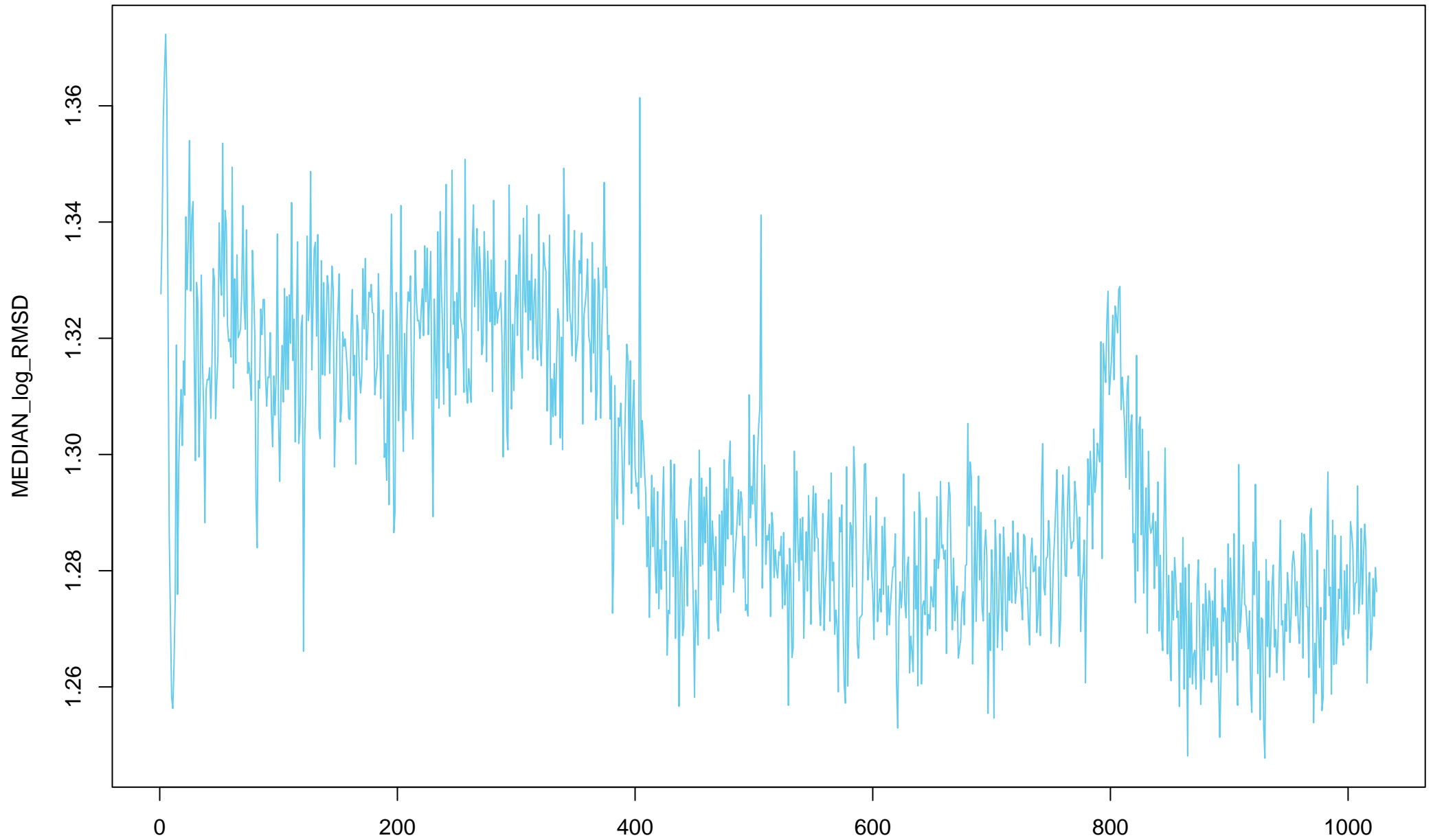


Pdatum8

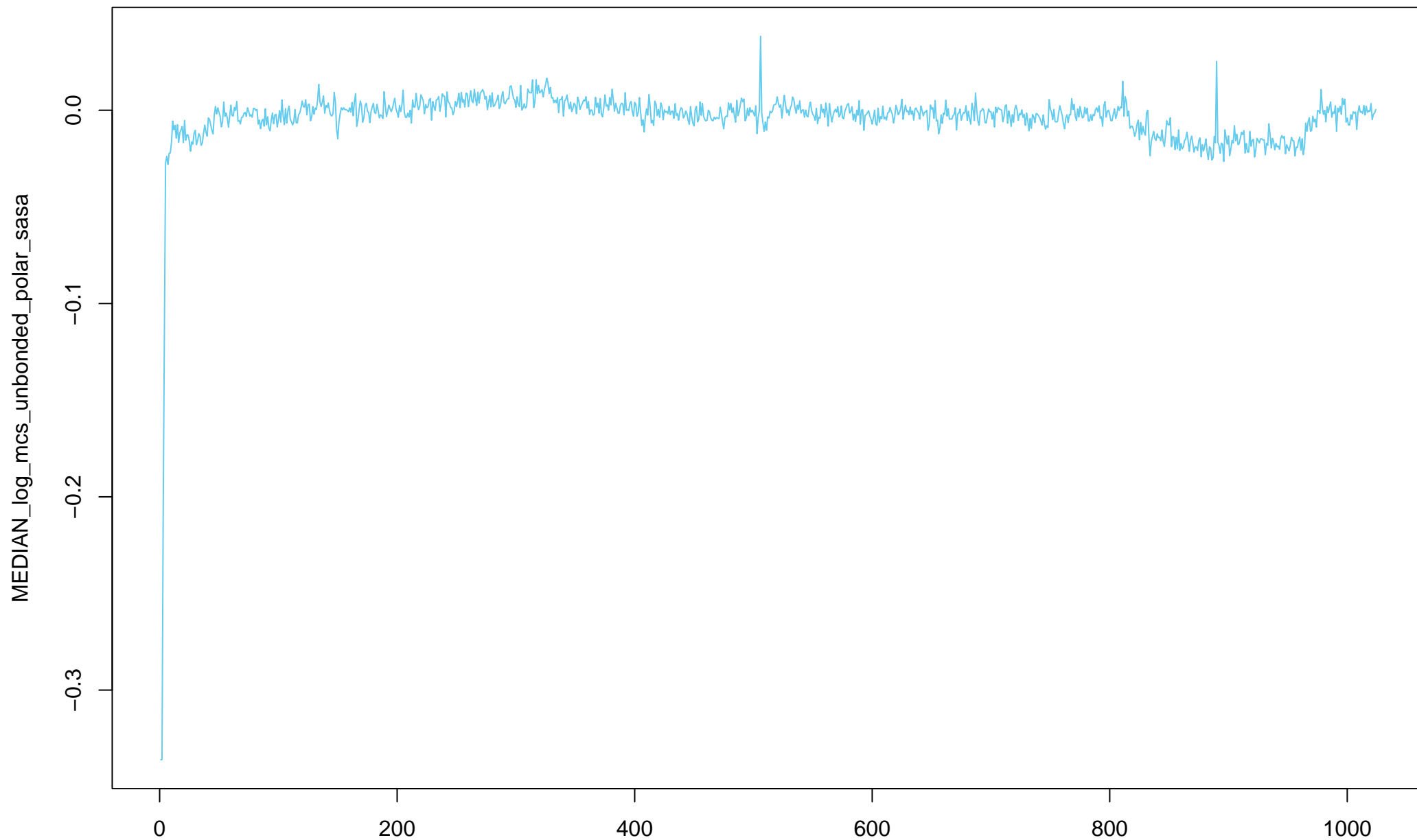
ESS = 7.61 | BMK = 0.43 | MCSE(6.27) = 16.1 | stat: FALSE | burn: 816



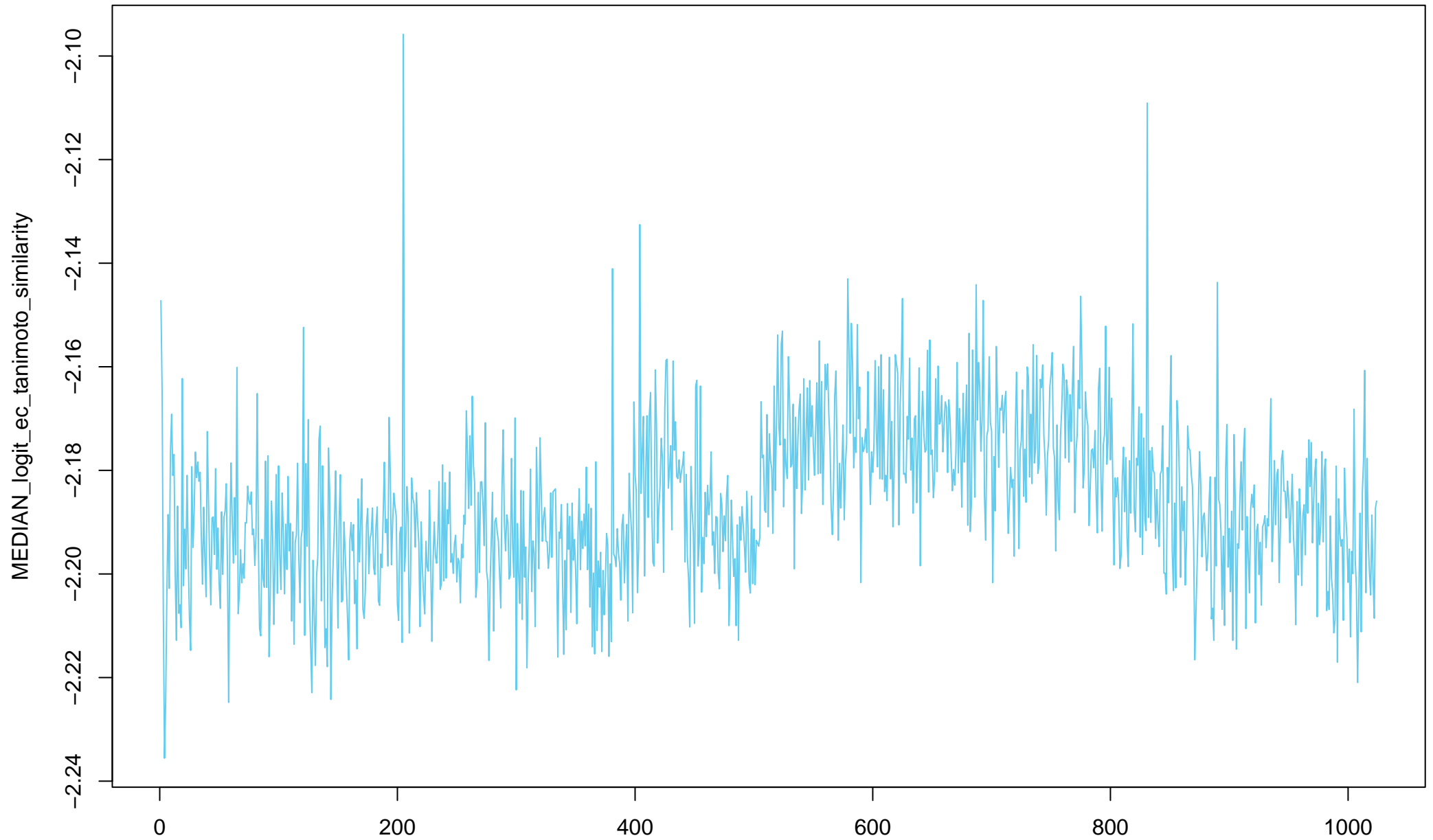
MEDIAN_log_RMSD
ESS = 3.07 | BMK = 0.577 | MCSE(6.27) = 15.1 | stat: FALSE | burn: 408



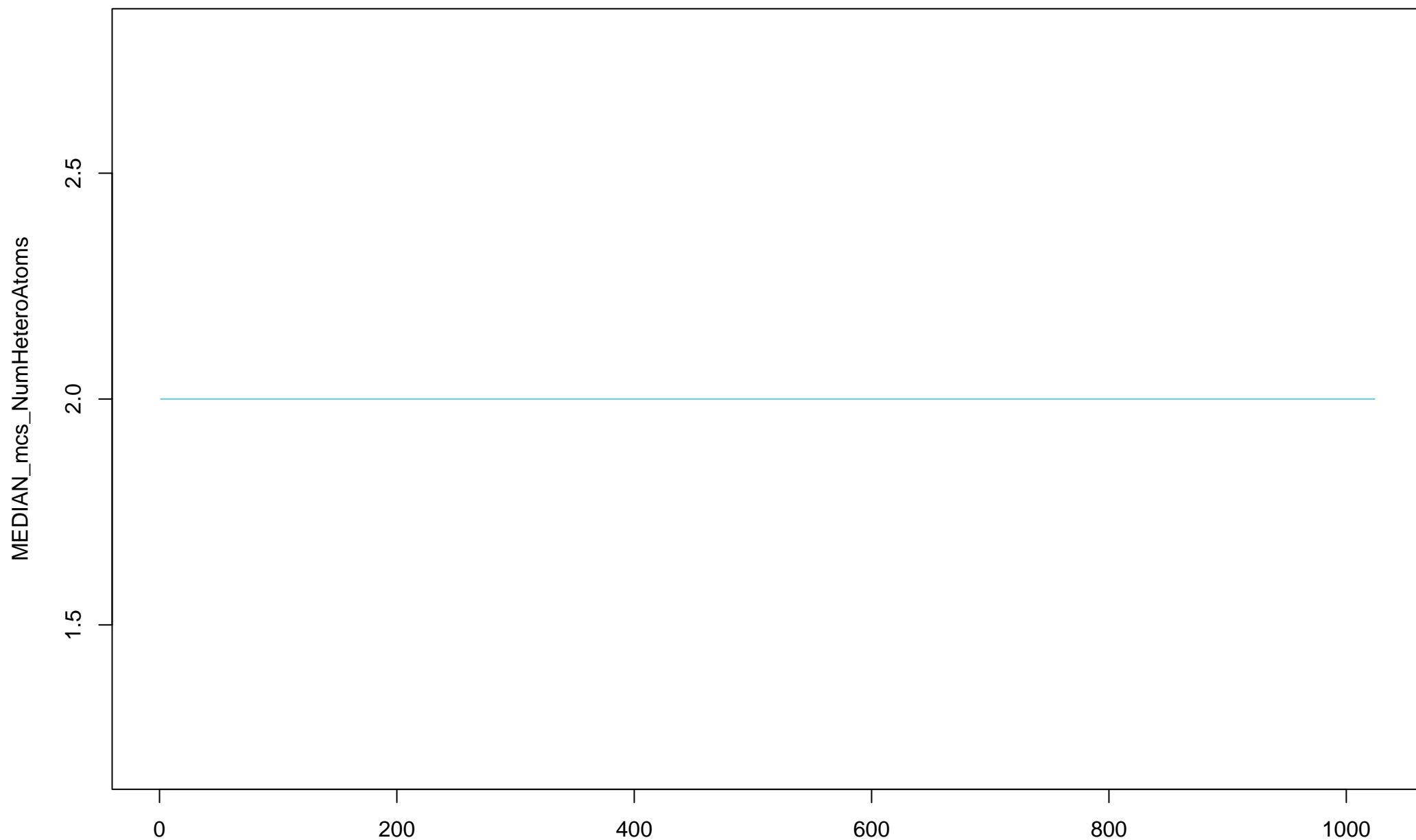
MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 155 | BMK = 0.289 | MCSE(6.27) = 9.28 | stat: TRUE | burn: 816



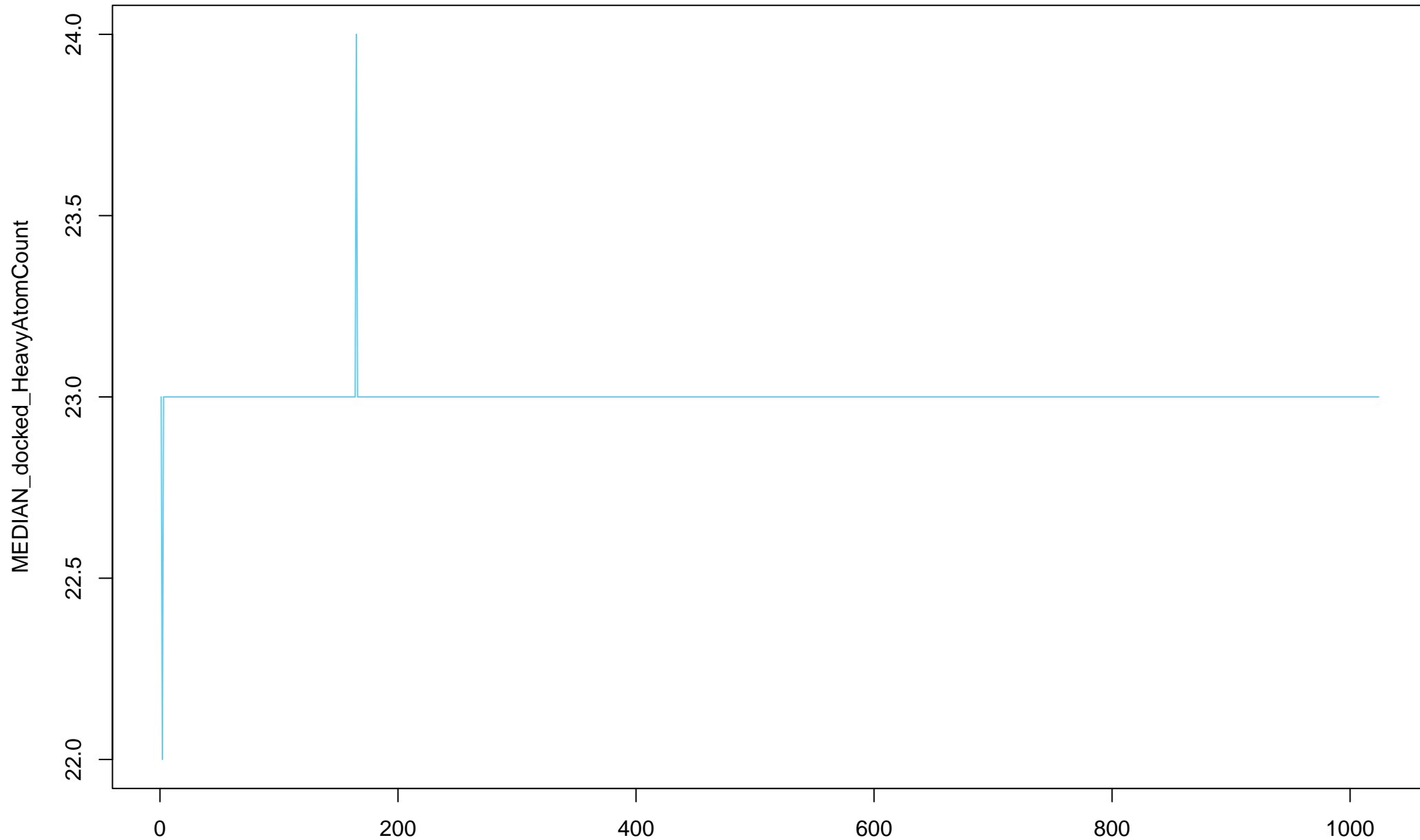
MEDIAN_logit_ec_tanimoto_similarity
ESS = 11.5 | BMK = 0.32 | MCSE(6.27) = 10.5 | stat: FALSE | burn: 0



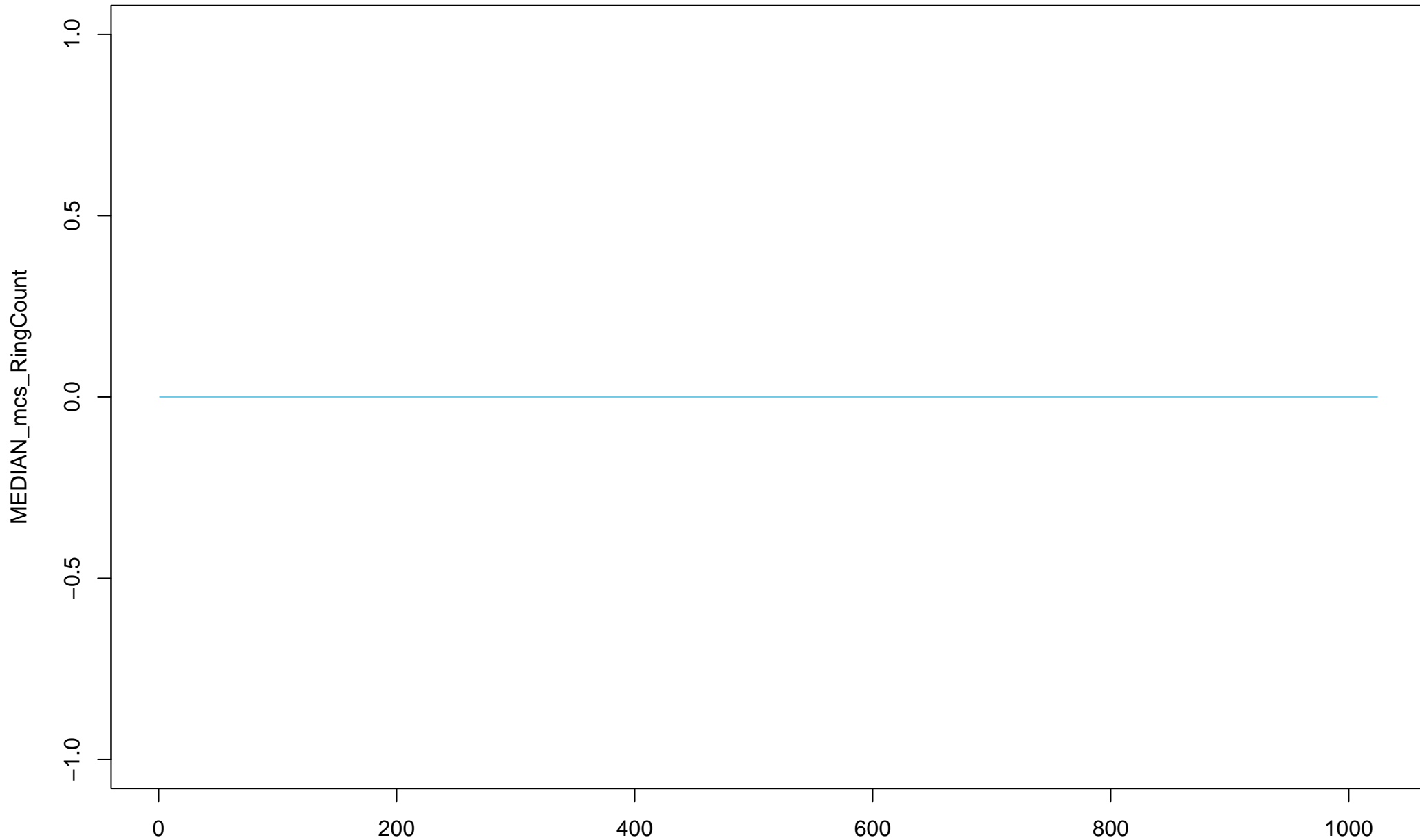
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



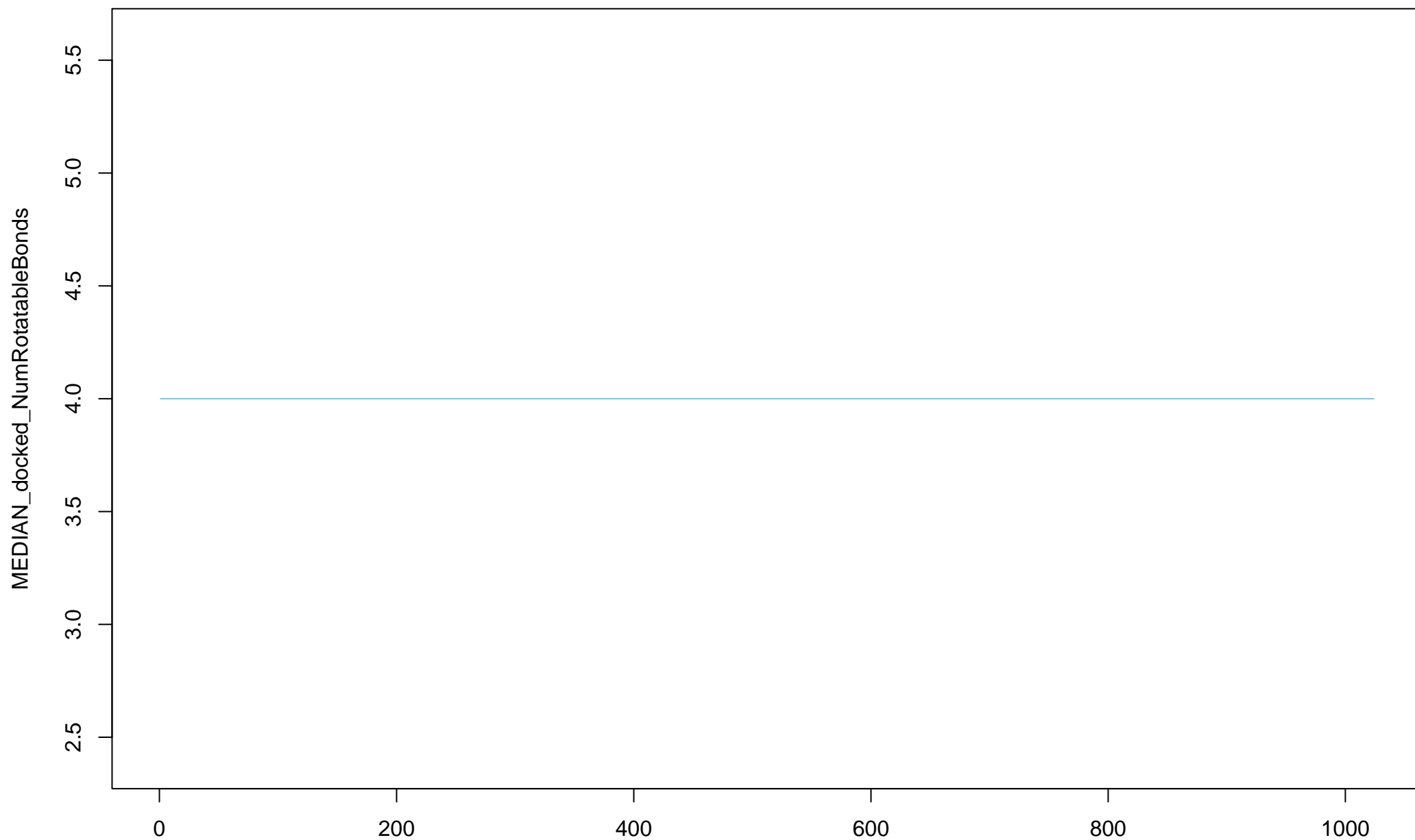
MEDIAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.7 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0



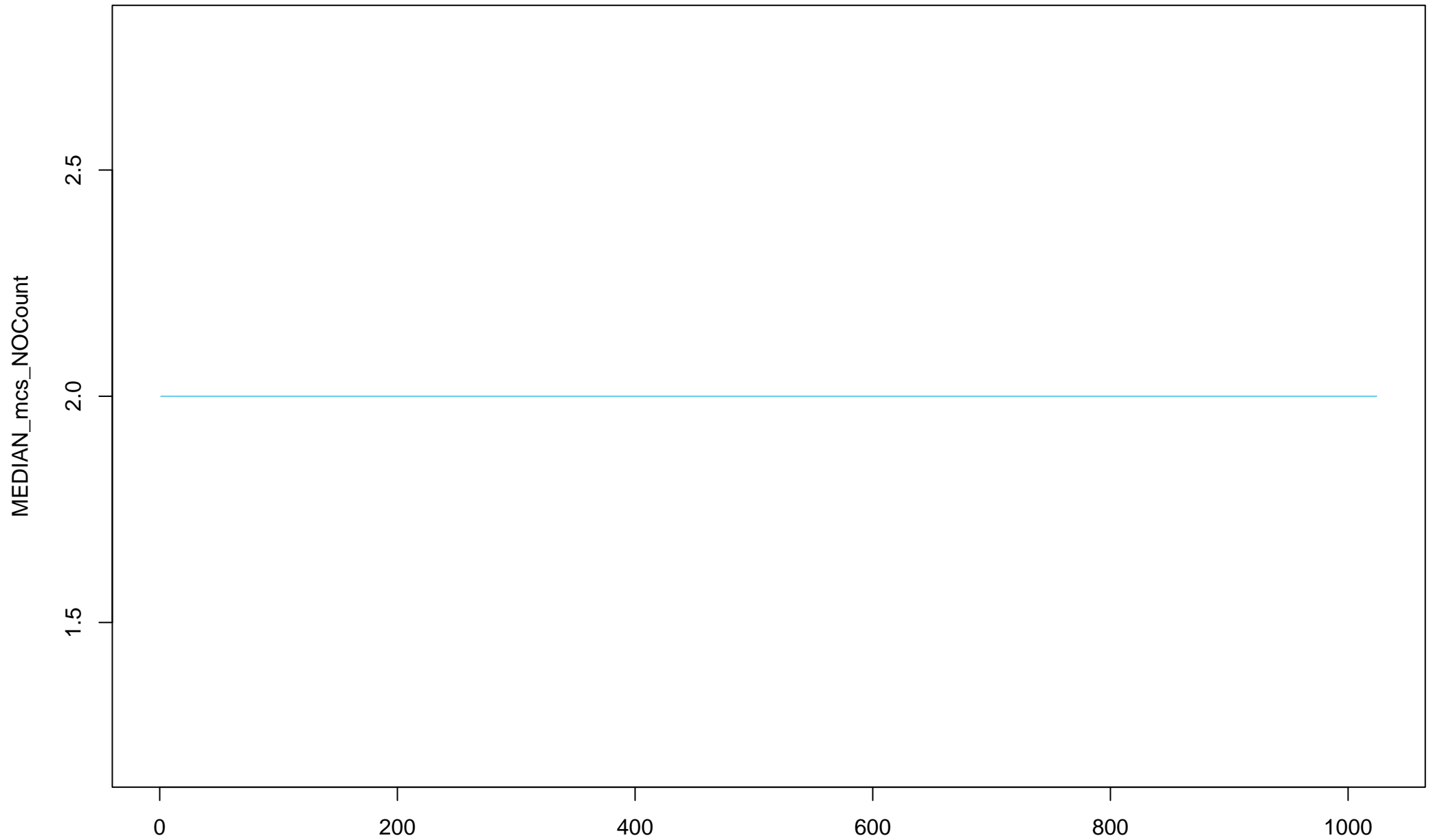
MEDIAN_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



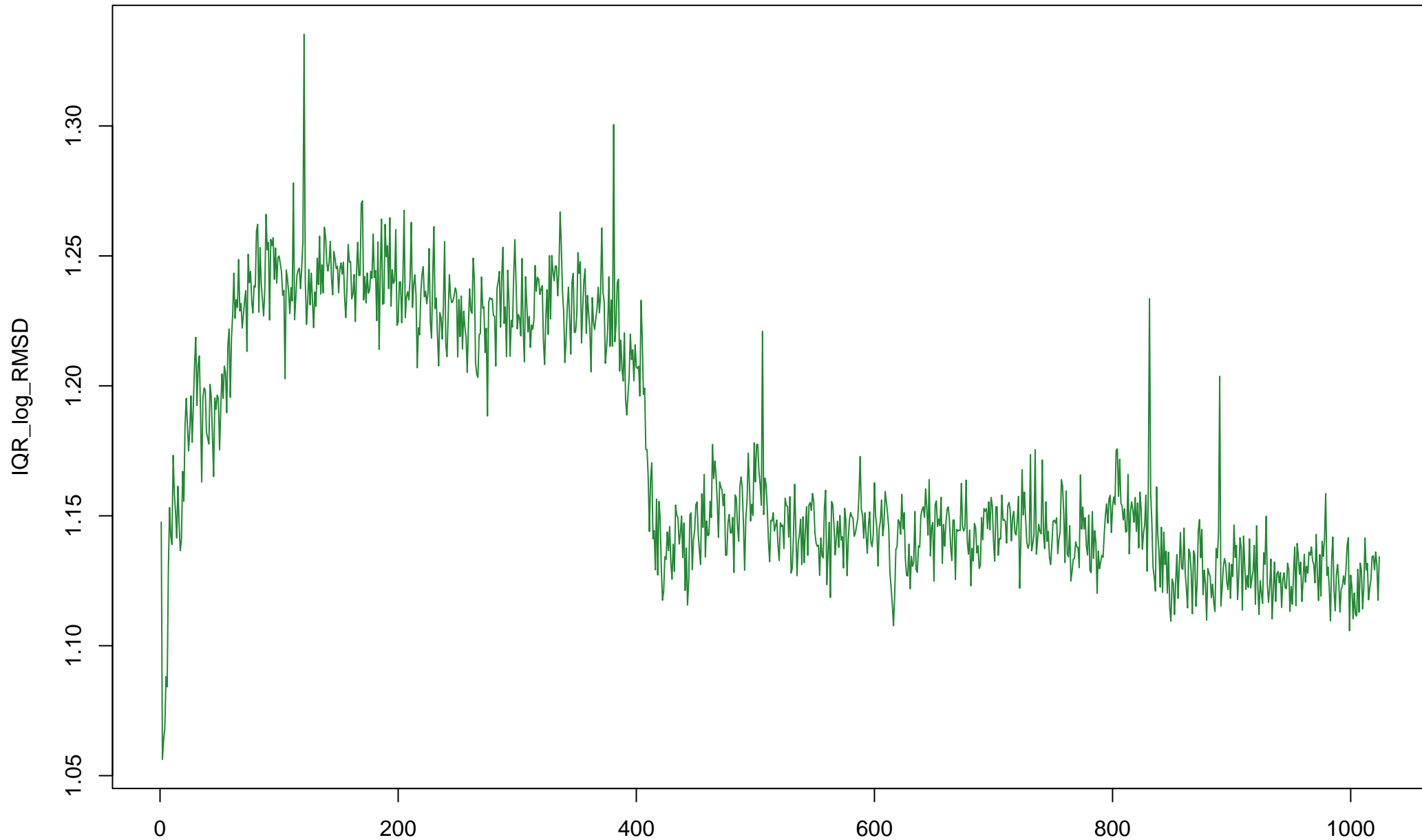
MEDIAN_docked_NumRotatableBonds
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



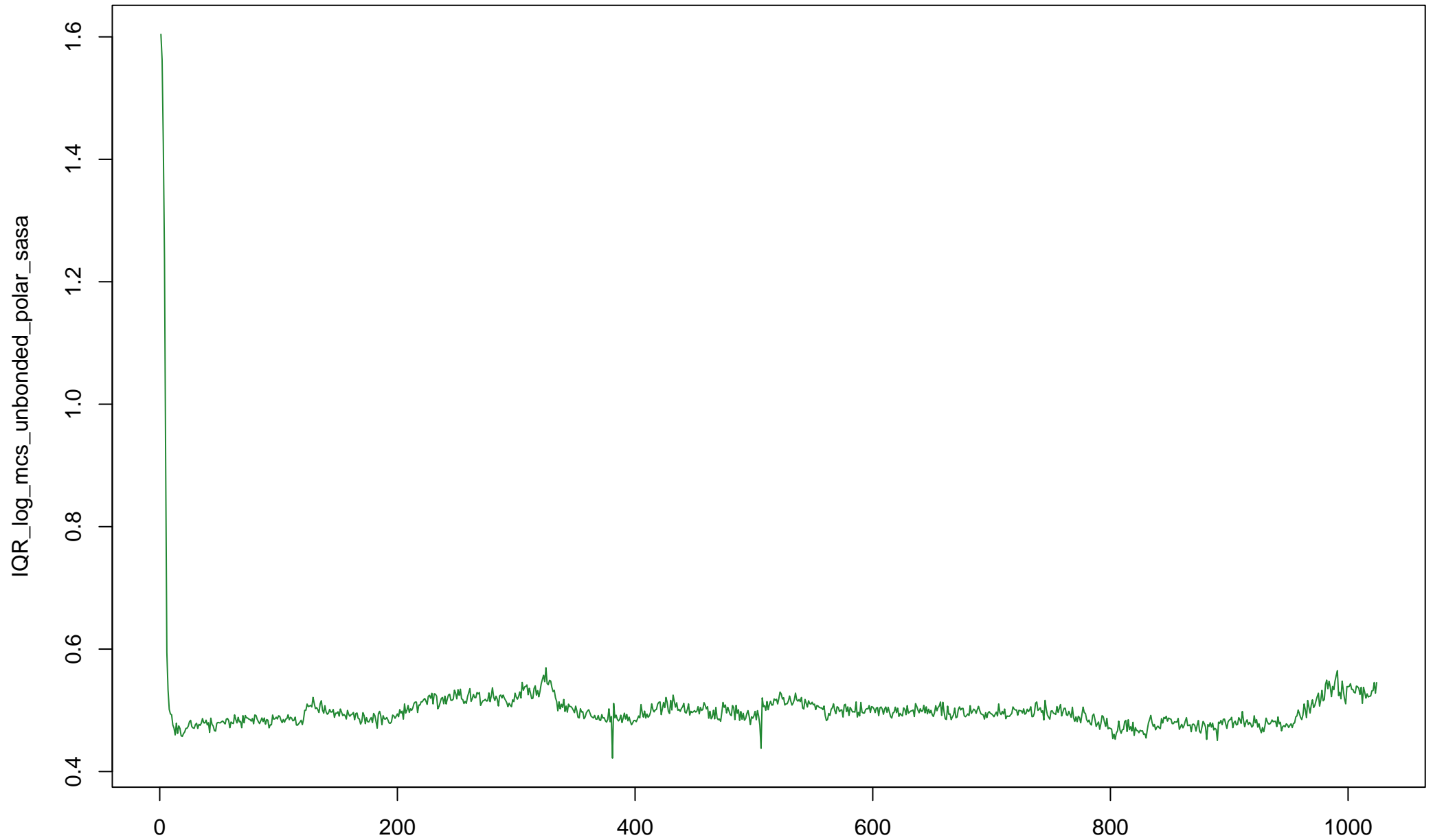
MEDIAN_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



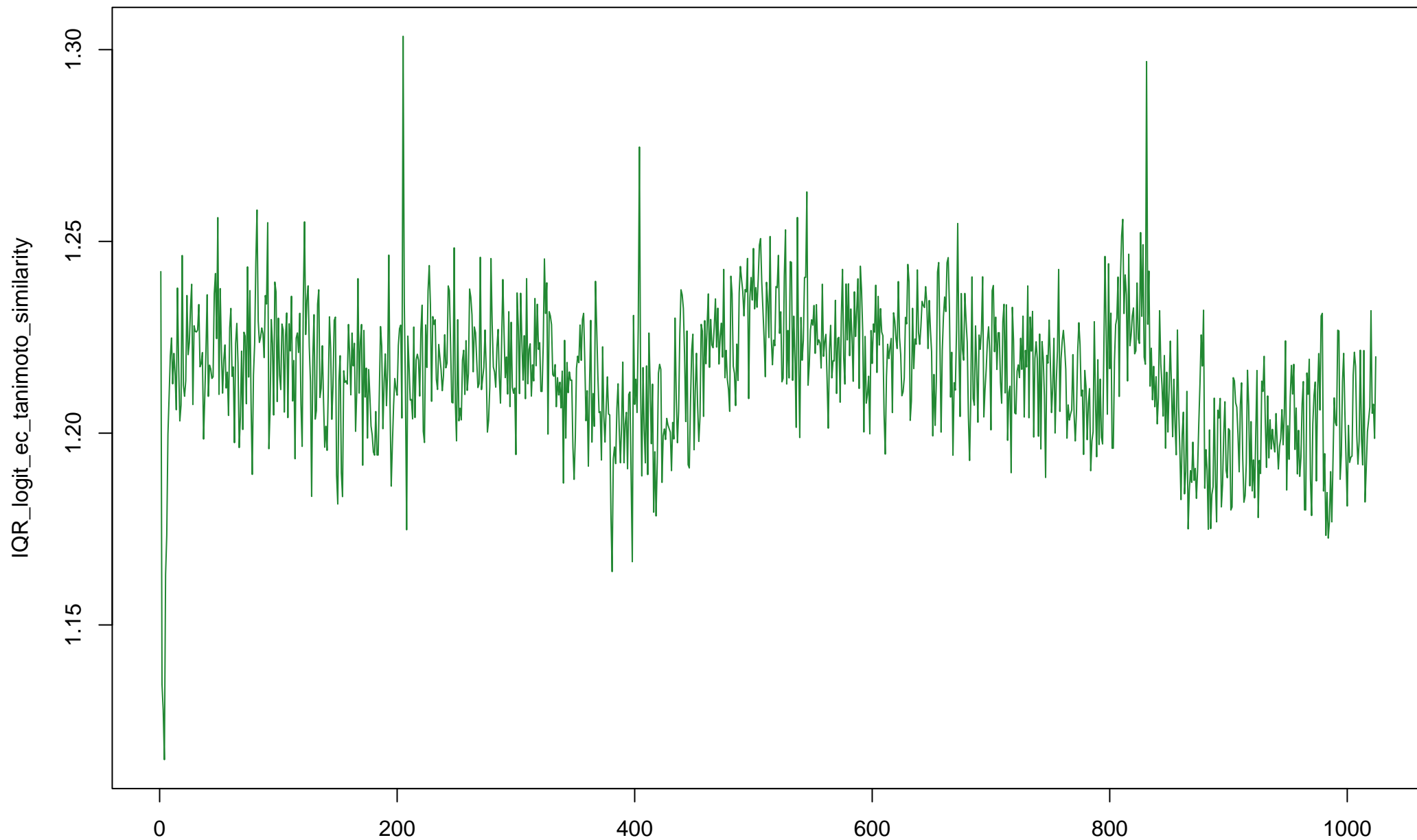
IQR_log_RMSD
ESS = 3.13 | BMK = 0.711 | MCSE(6.27) = 17 | stat: FALSE | burn: 408



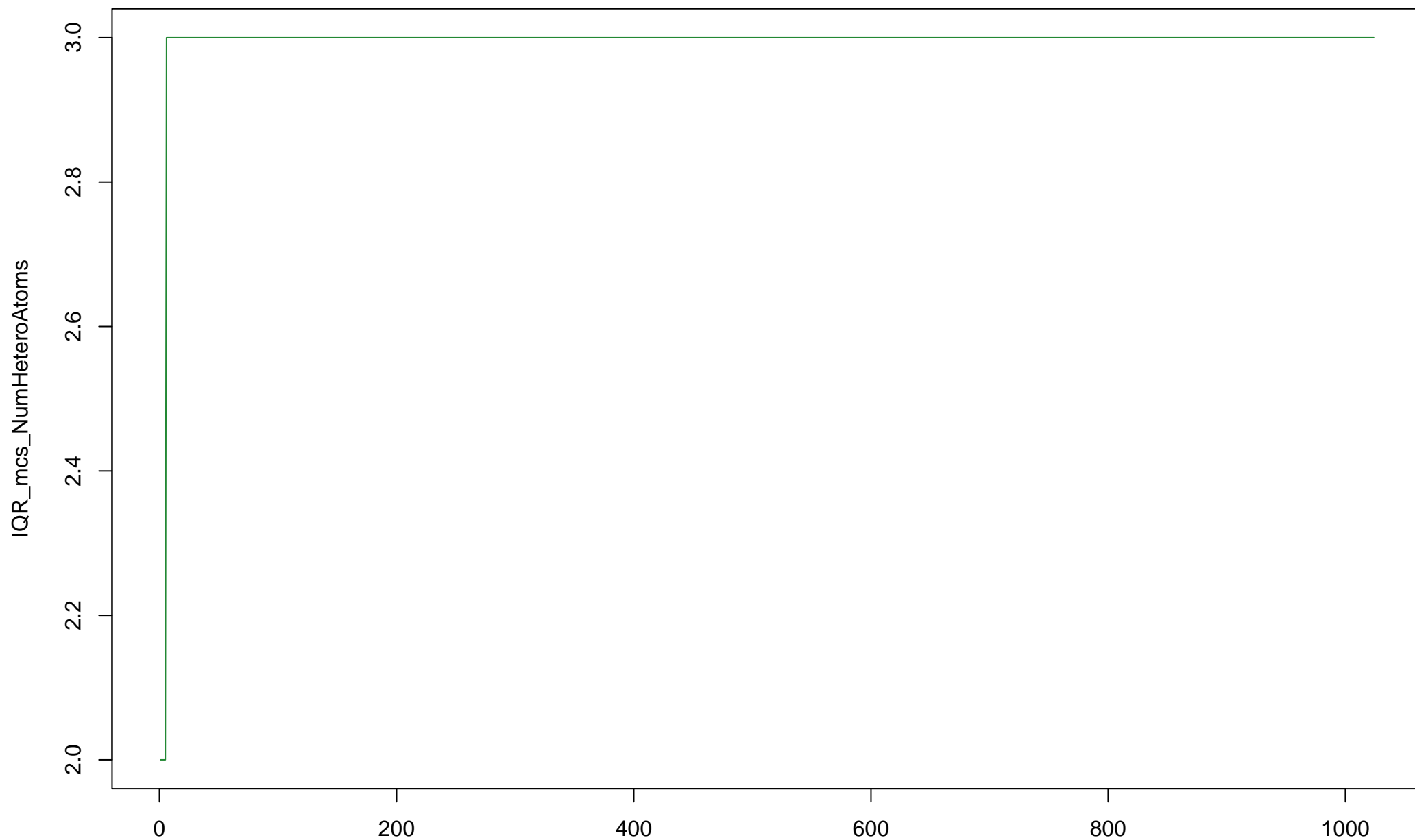
IQR_log_mcs_unbonded_polar_sasa
ESS = 172 | BMK = 0.144 | MCSE(6.27) = 7.17 | stat: TRUE | burn: 1020



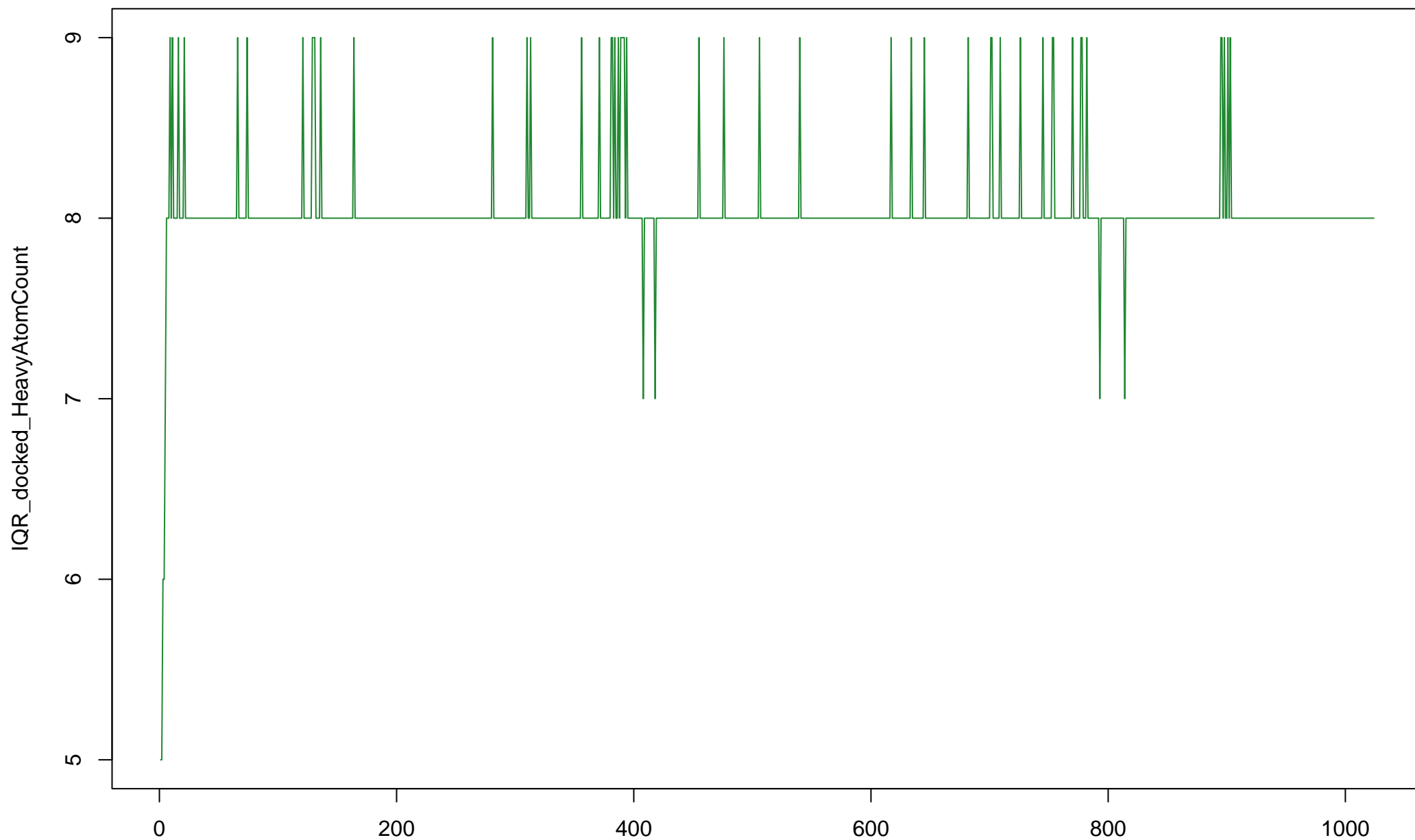
IQR_logit_ec_tanimoto_similarity
ESS = 40.9 | BMK = 0.124 | MCSE(6.27) = 9.74 | stat: TRUE | burn: 0



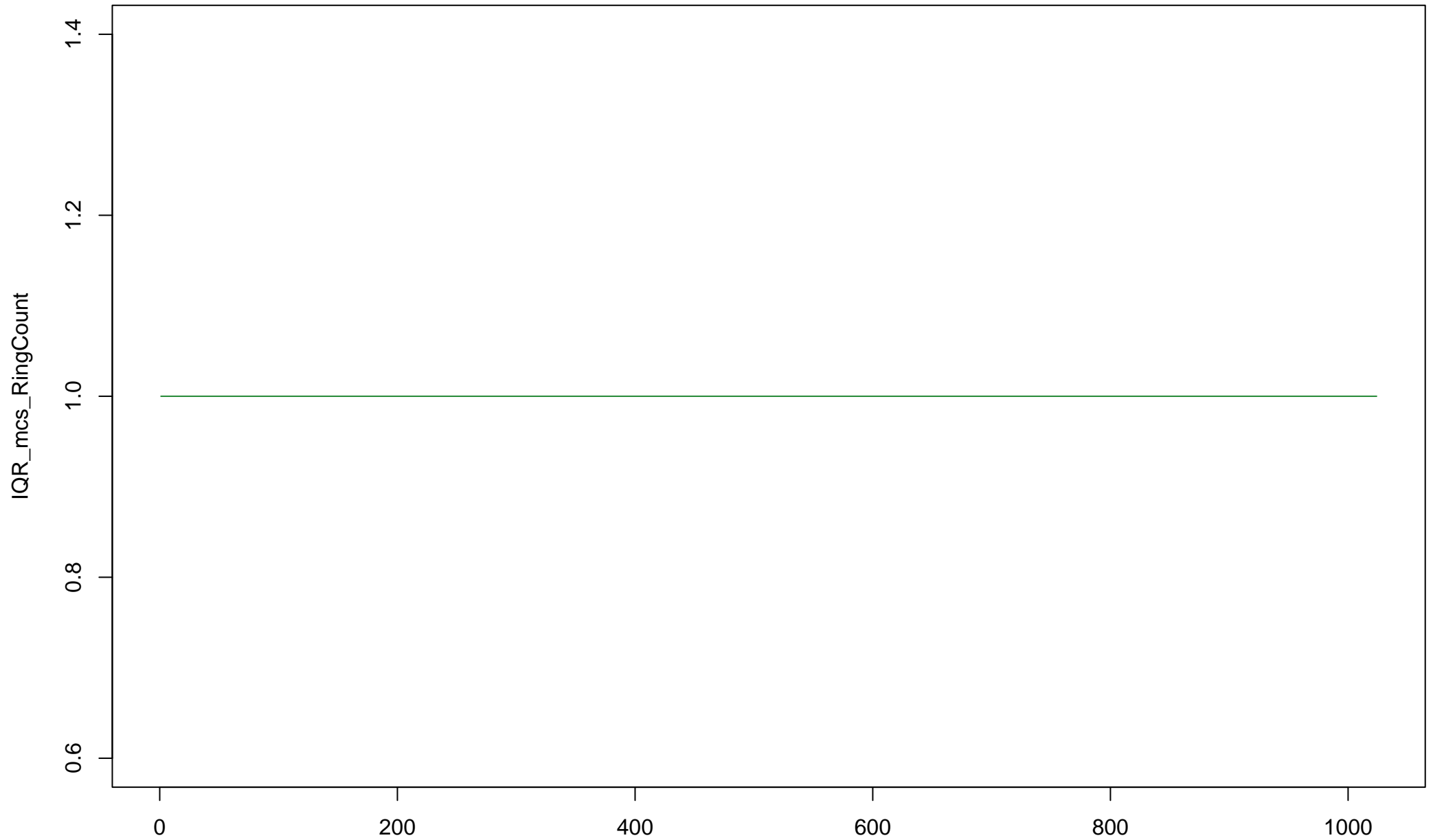
IQR_mcs_NumHeteroAtoms
ESS = 176 | BMK = 0.566 | MCSE(6.27) = 7 | stat: TRUE | burn: 0



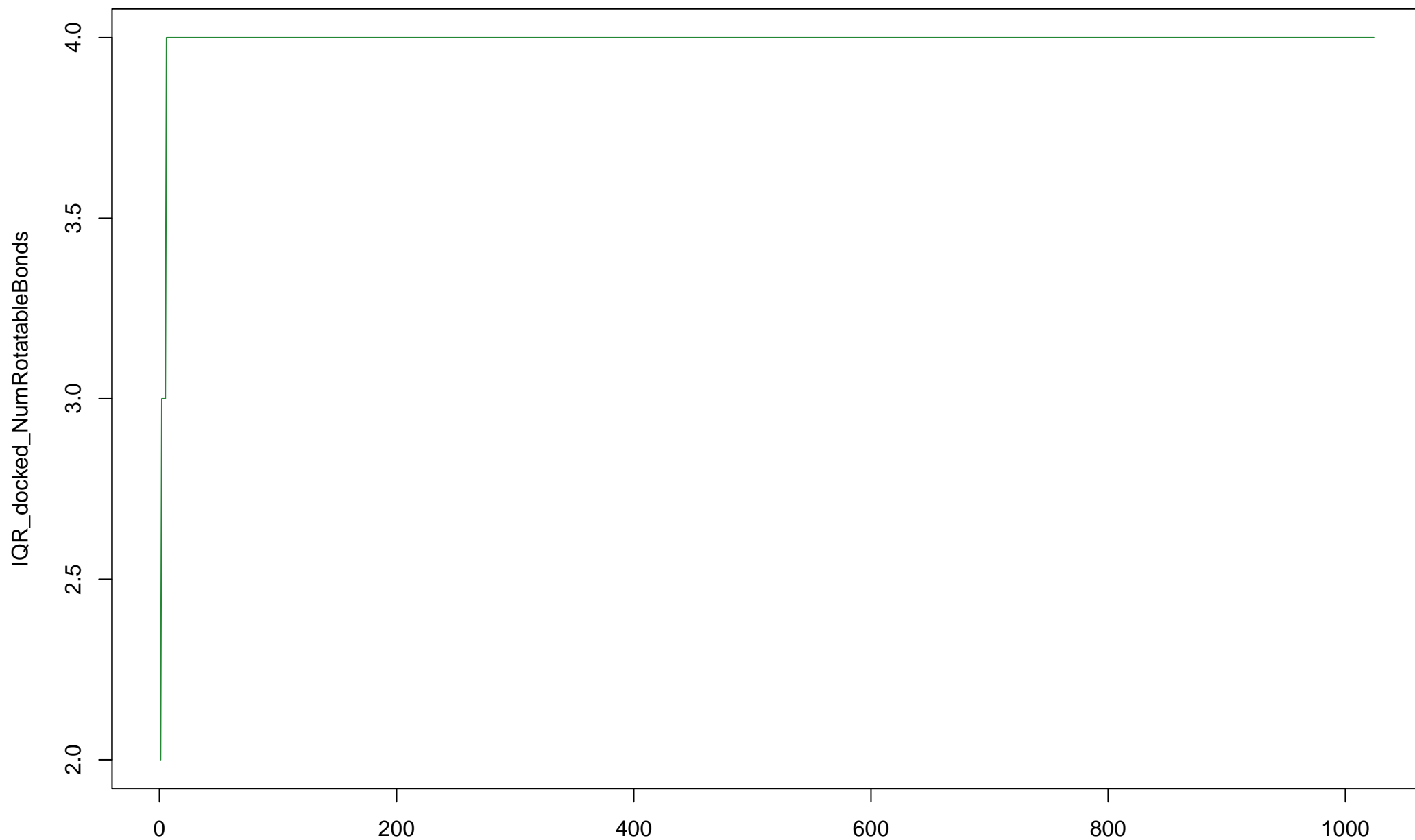
IQR_docked_HeavyAtomCount
ESS = 361 | BMK = 0.233 | MCSE(6.27) = 4.27 | stat: TRUE | burn: 306



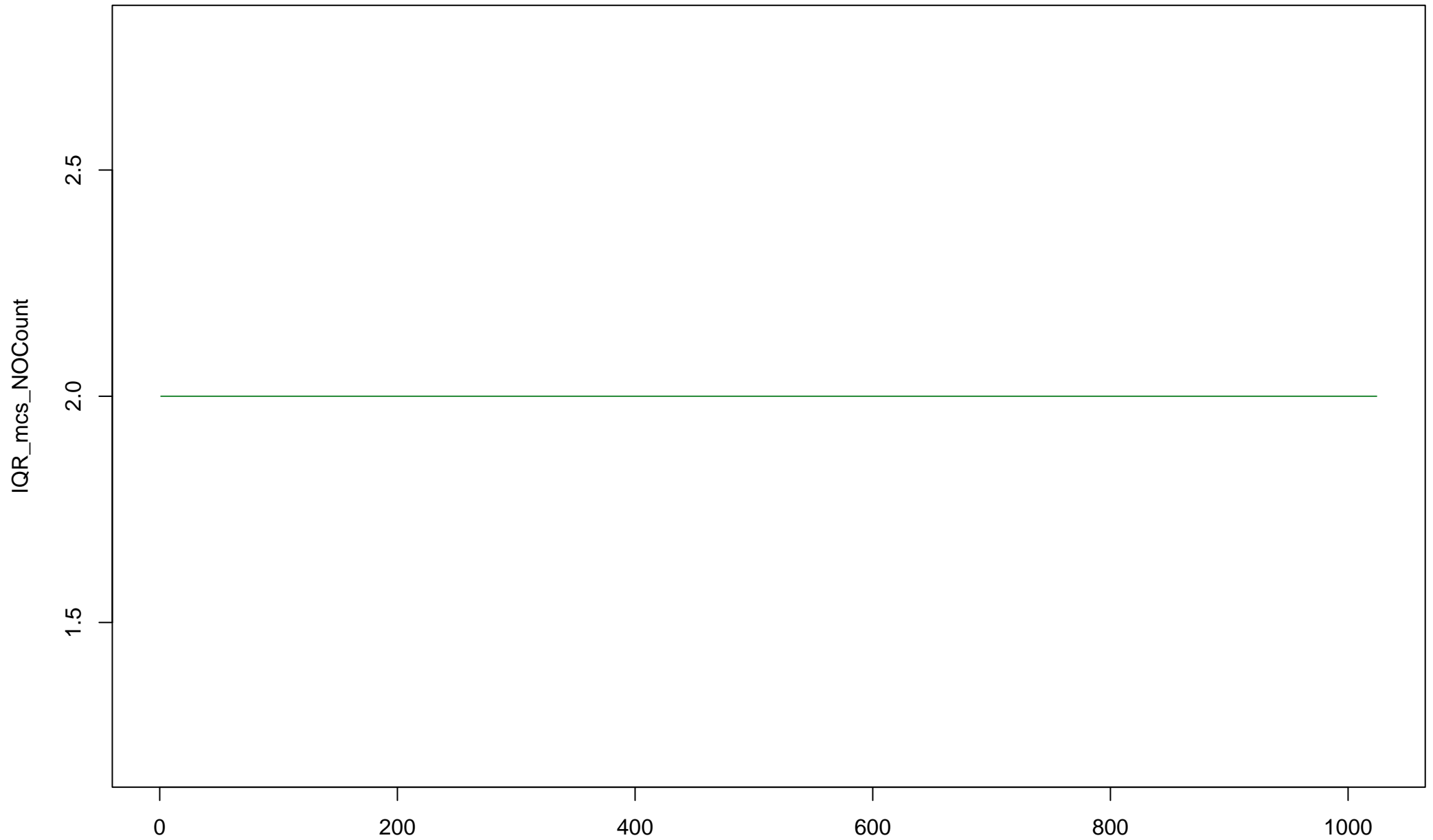
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



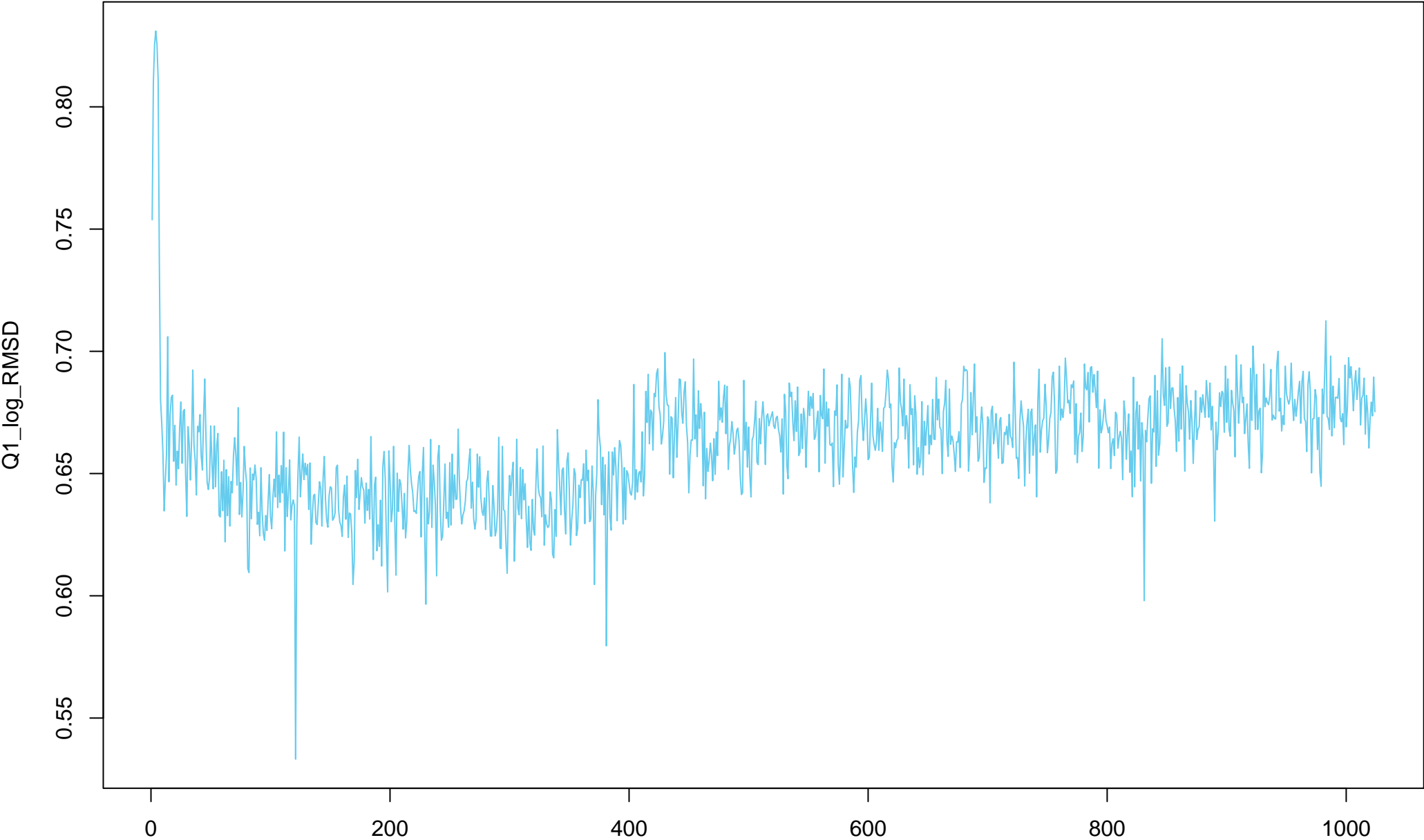
IQR_docked_NumRotatableBonds
ESS = 250 | BMK = 0.594 | MCSE(6.27) = 6.64 | stat: TRUE | burn: 0



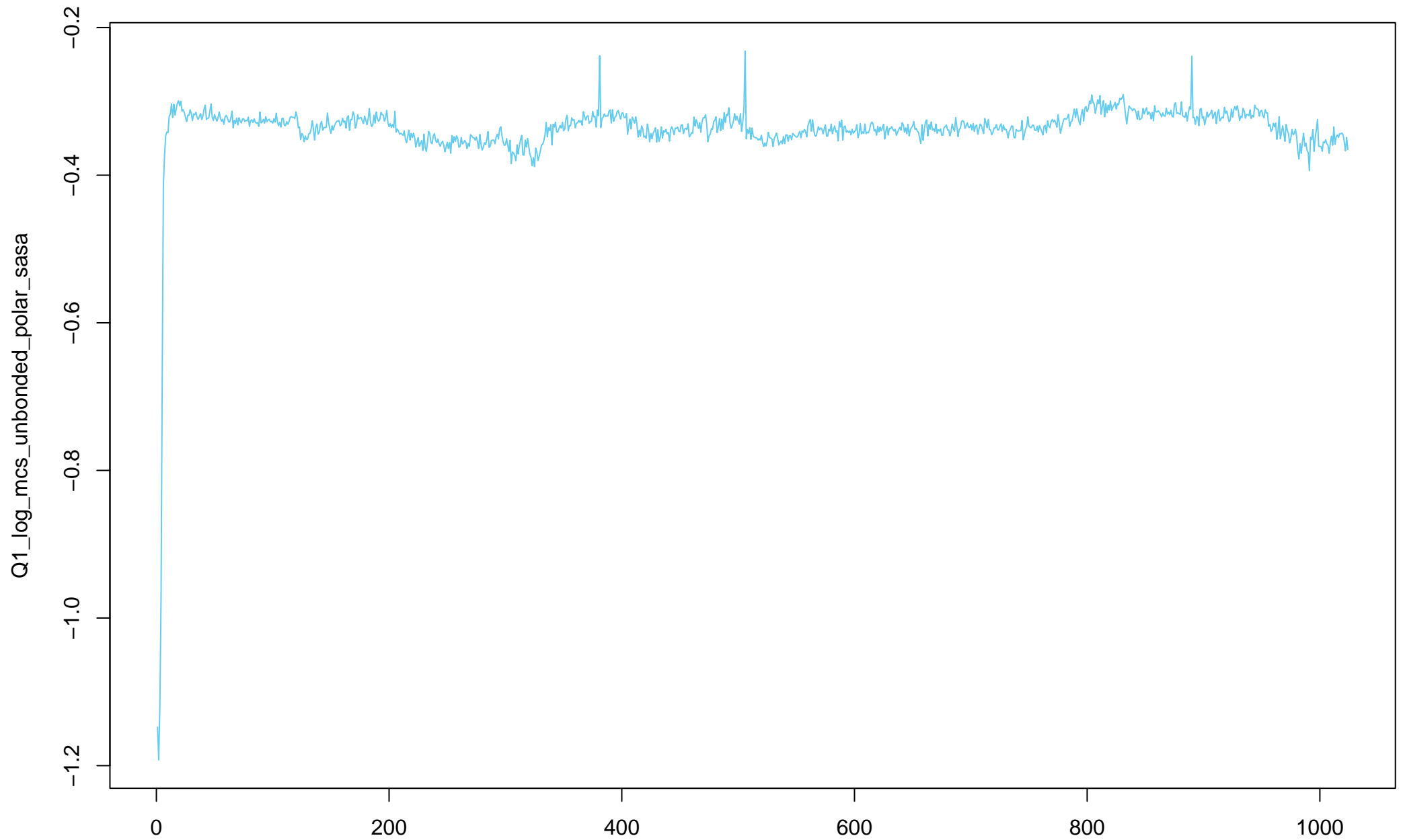
IQR_mcs_NOCCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



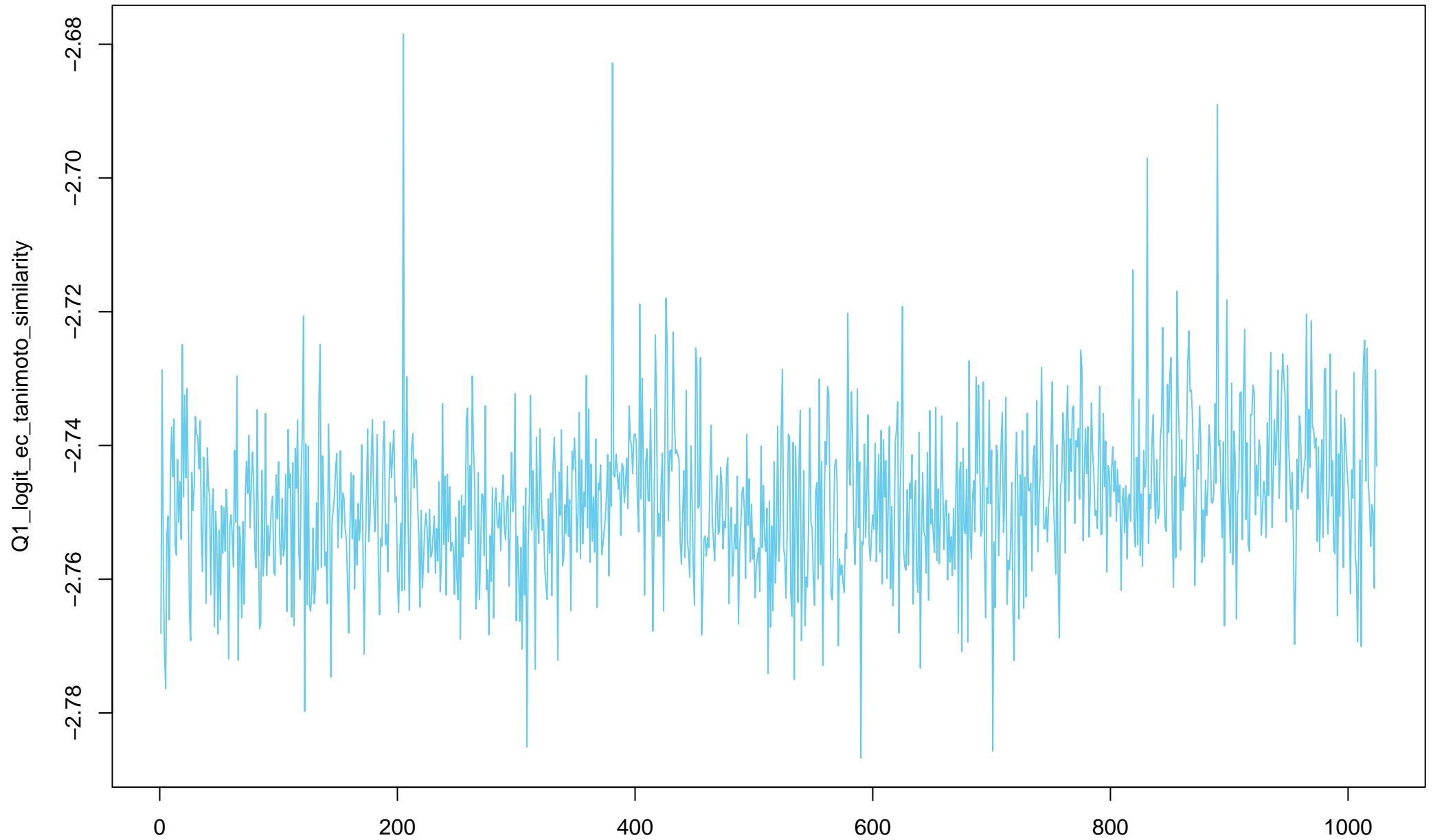
Q1_log_RMSD
ESS = 28 | BMK = 0.519 | MCSE(6.27) = 12.4 | stat: TRUE | burn: 408



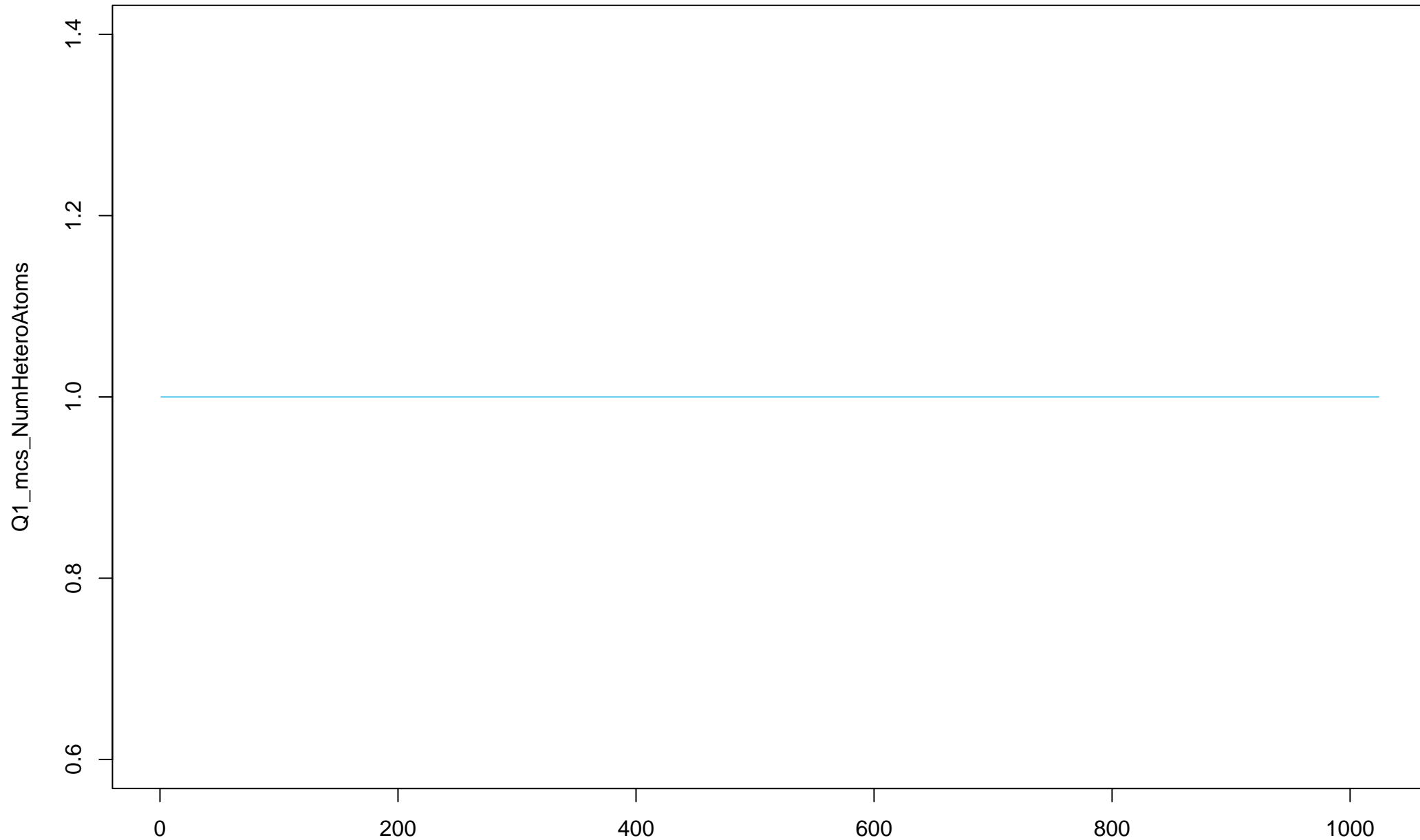
Q1_log_mcs_unbonded_polar_sasa
ESS = 169 | BMK = 0.176 | MCSE(6.27) = 7.38 | stat: TRUE | burn: 1020



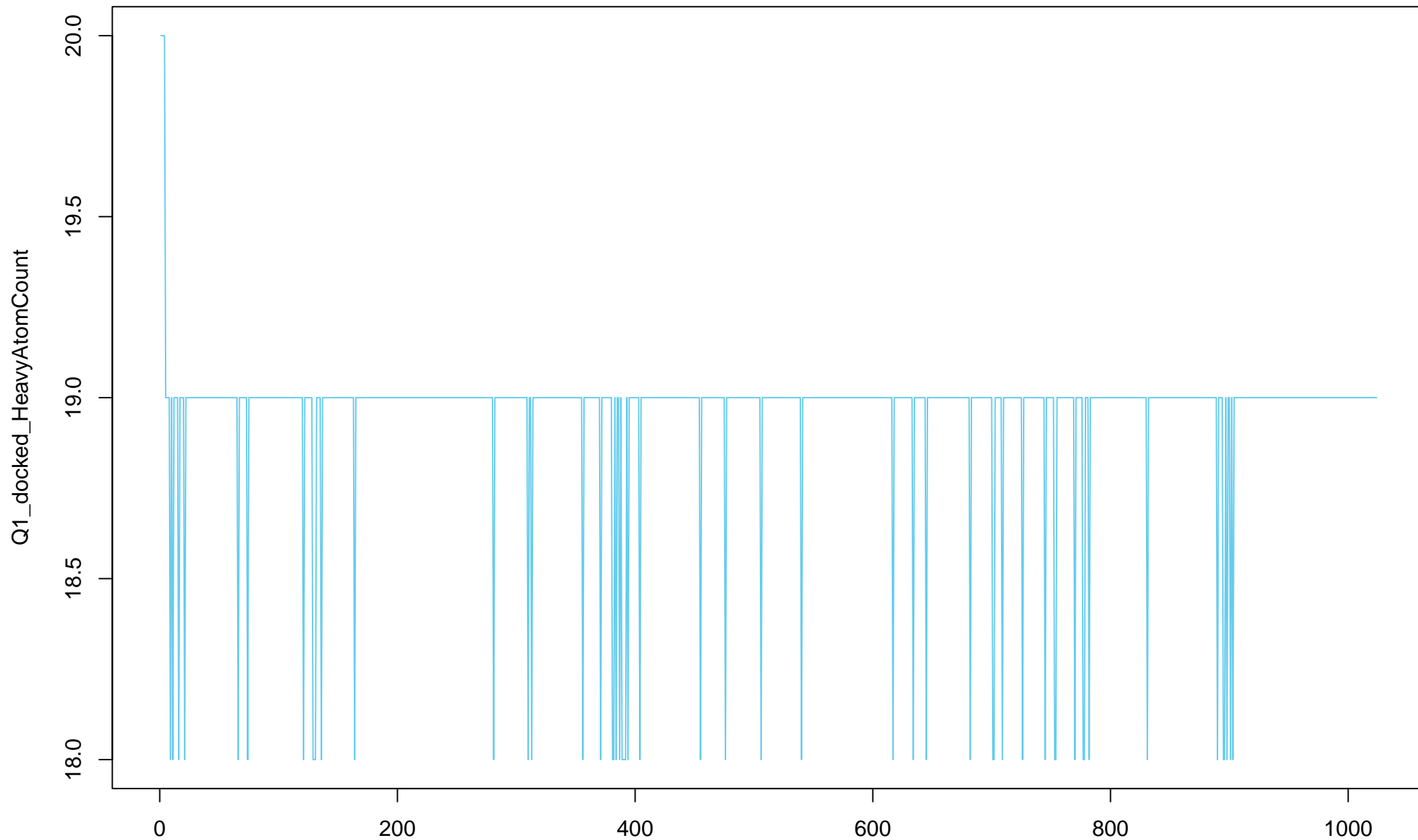
Q1_logit_ec_tanimoto_similarity
ESS = 68.8 | BMK = 0.14 | MCSE(6.27) = 5.91 | stat: FALSE | burn: 0



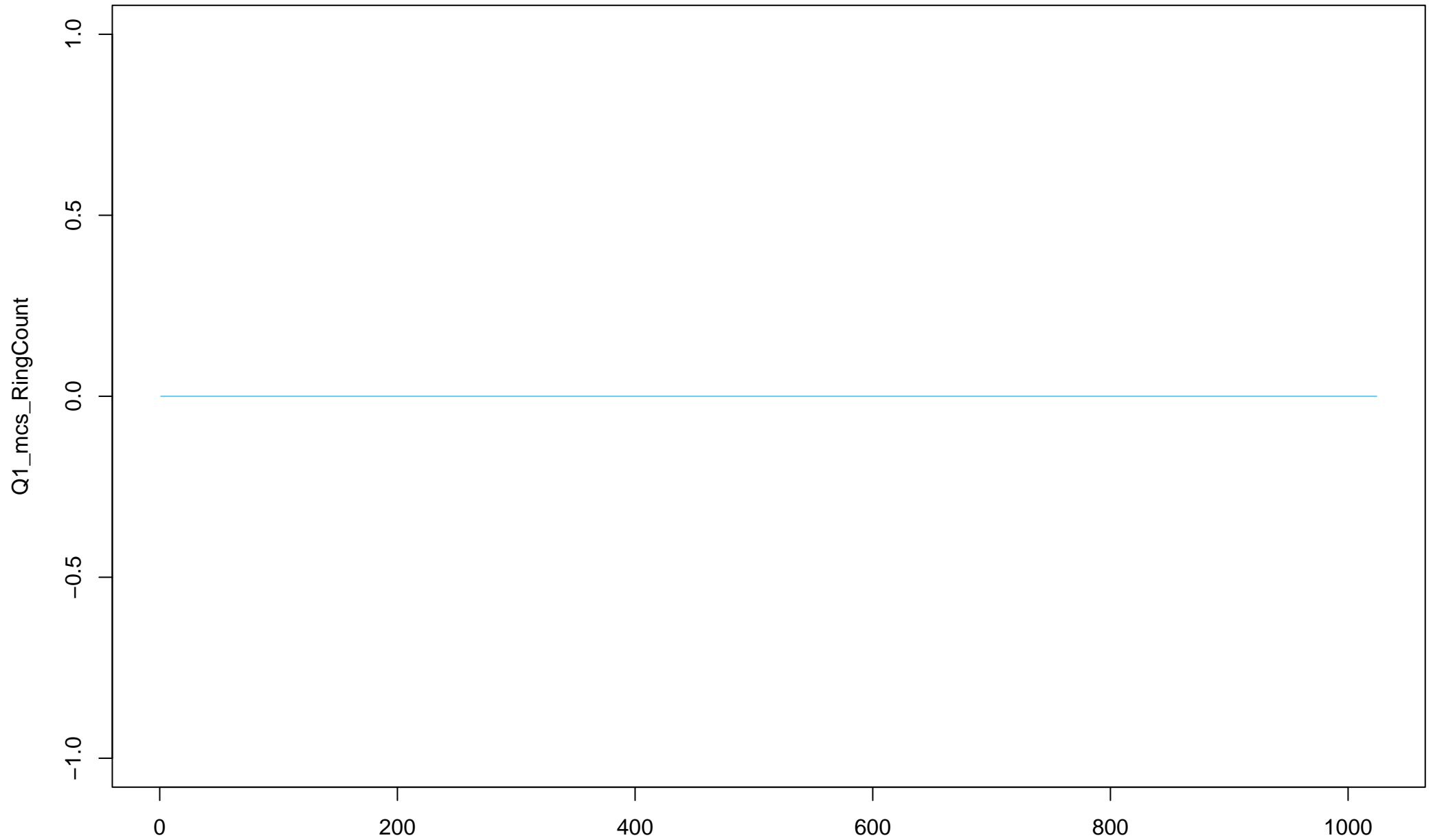
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



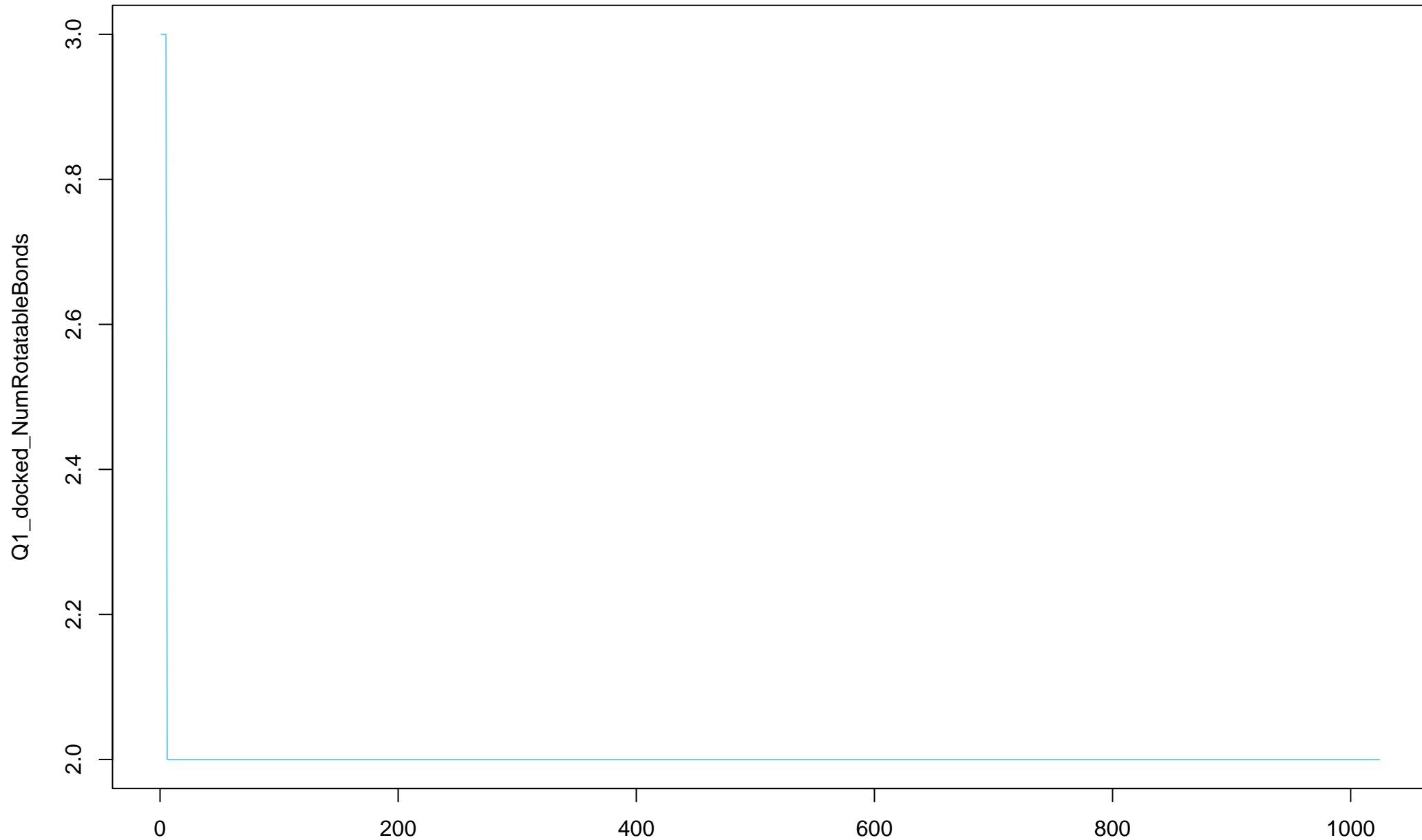
Q1_docked_HeavyAtomCount
ESS = 335 | BMK = 0.108 | MCSE(6.27) = 4.16 | stat: TRUE | burn: 0



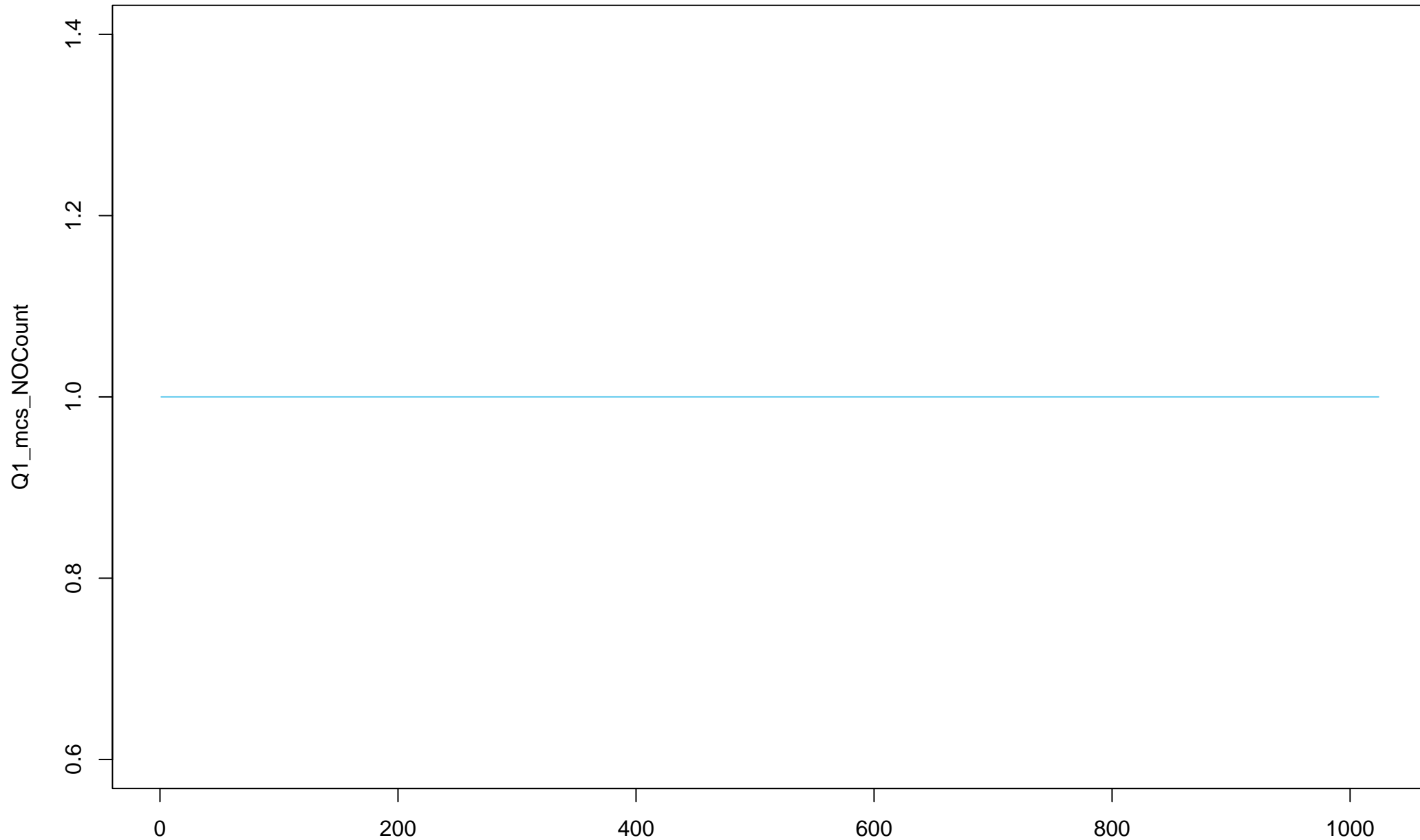
Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



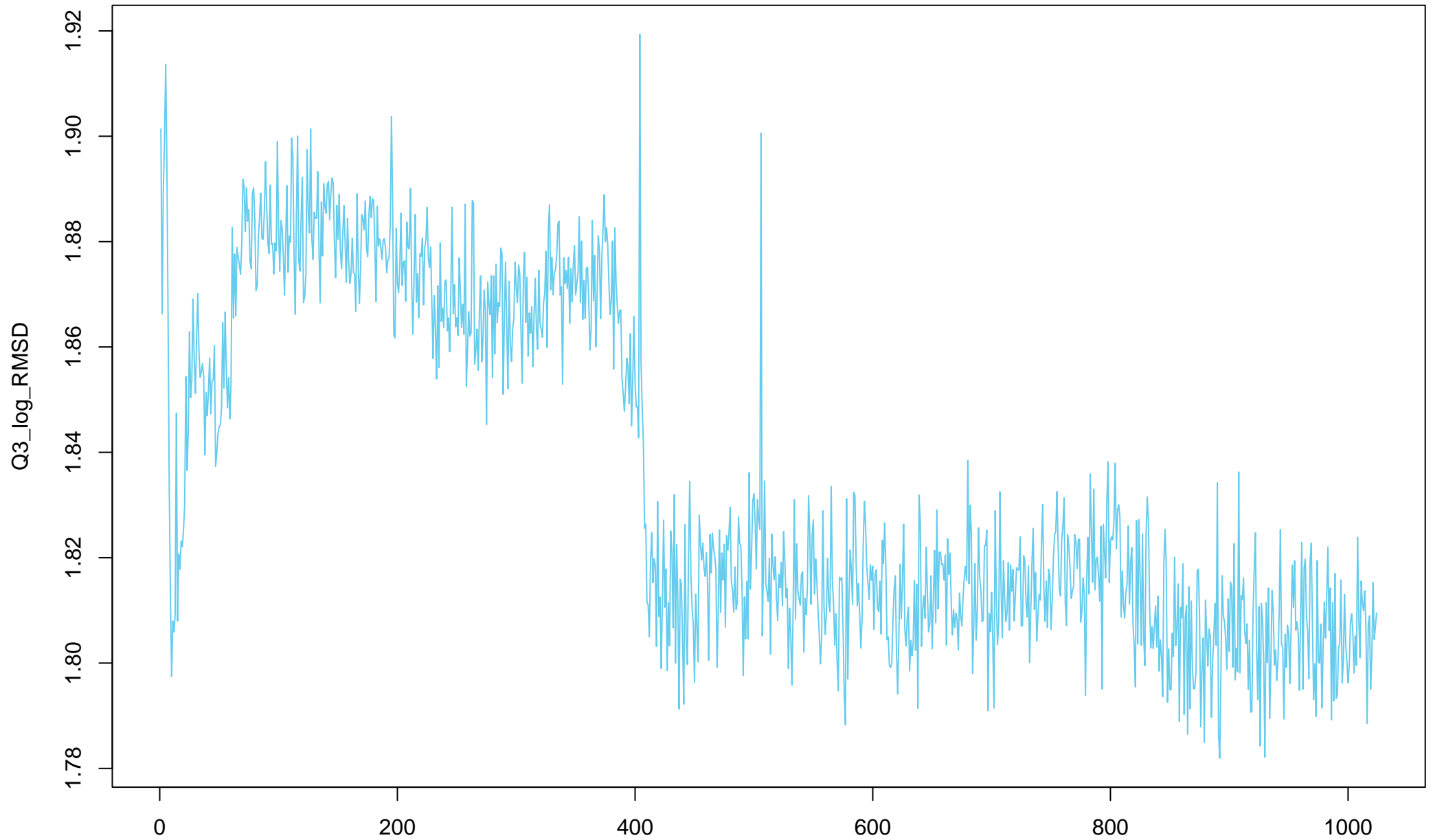
Q1_docked_NumRotatableBonds
ESS = 176 | BMK = 0.574 | MCSE(6.27) = 7 | stat: TRUE | burn: 0



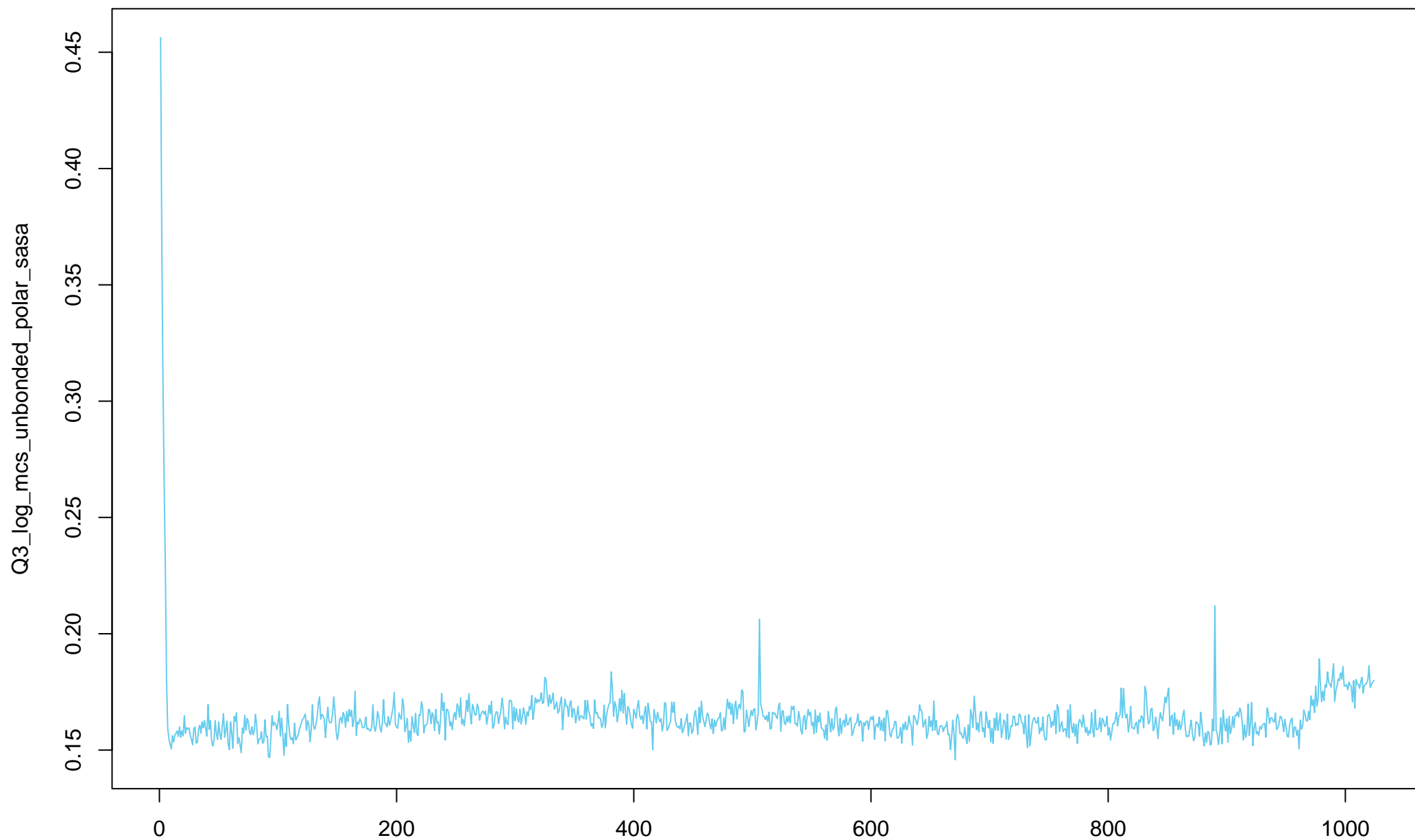
Q1_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



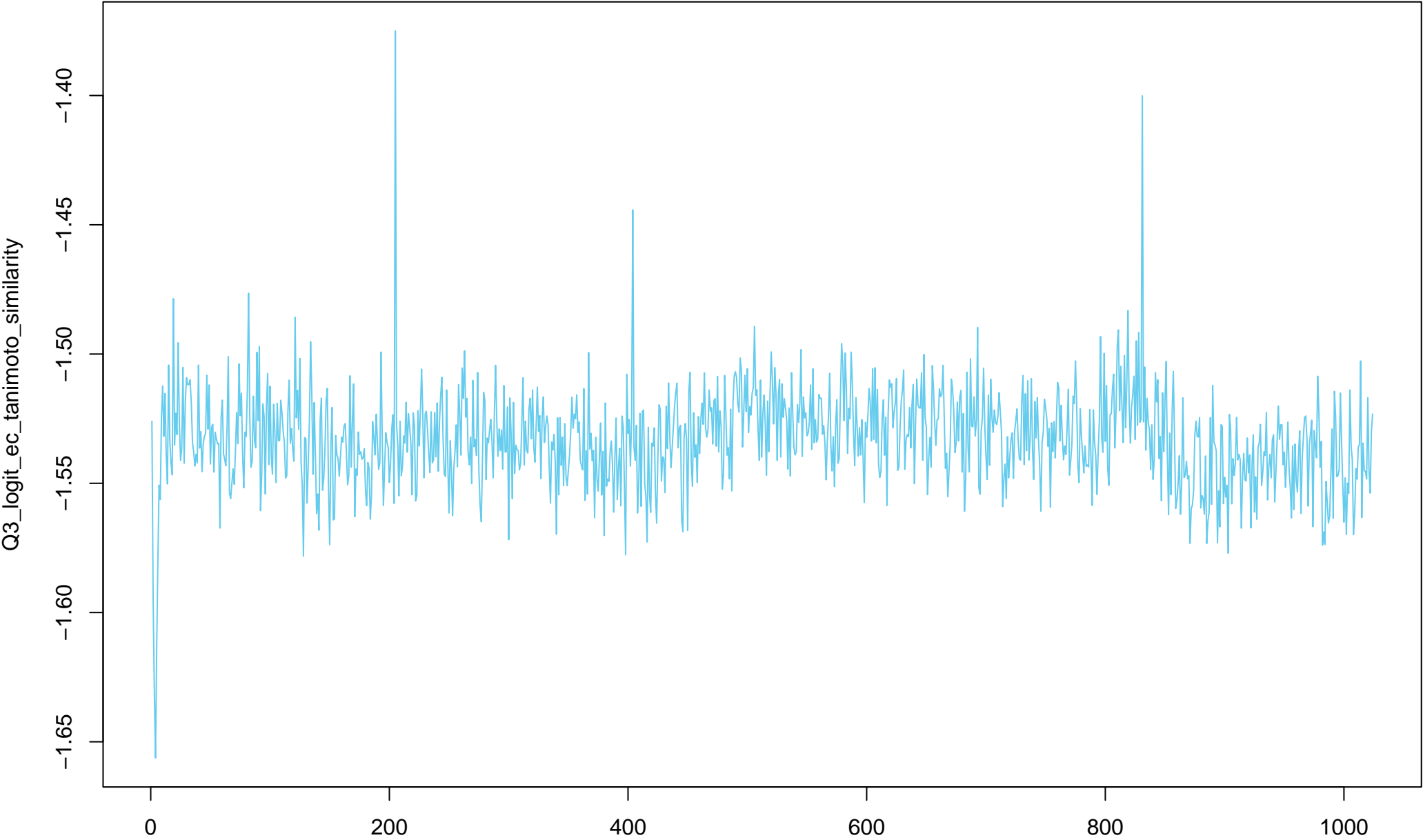
Q3_log_RMSD
ESS = 1.56 | BMK = 0.723 | MCSE(6.27) = 16.8 | stat: FALSE | burn: 408



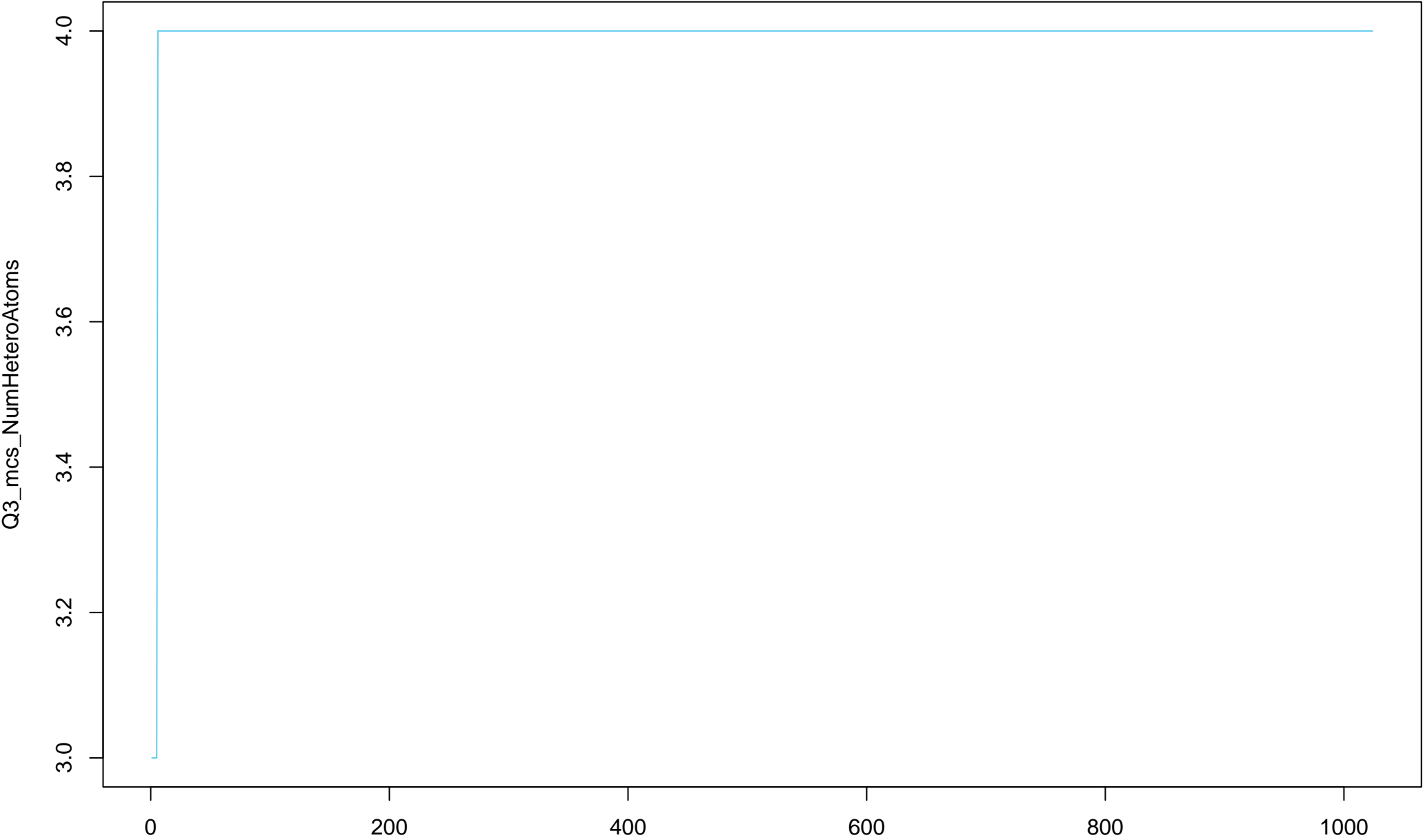
Q3_log_mcs_unbonded_polar_sasa
ESS = 193 | BMK = 0.205 | MCSE(6.27) = 6.91 | stat: TRUE | burn: 0



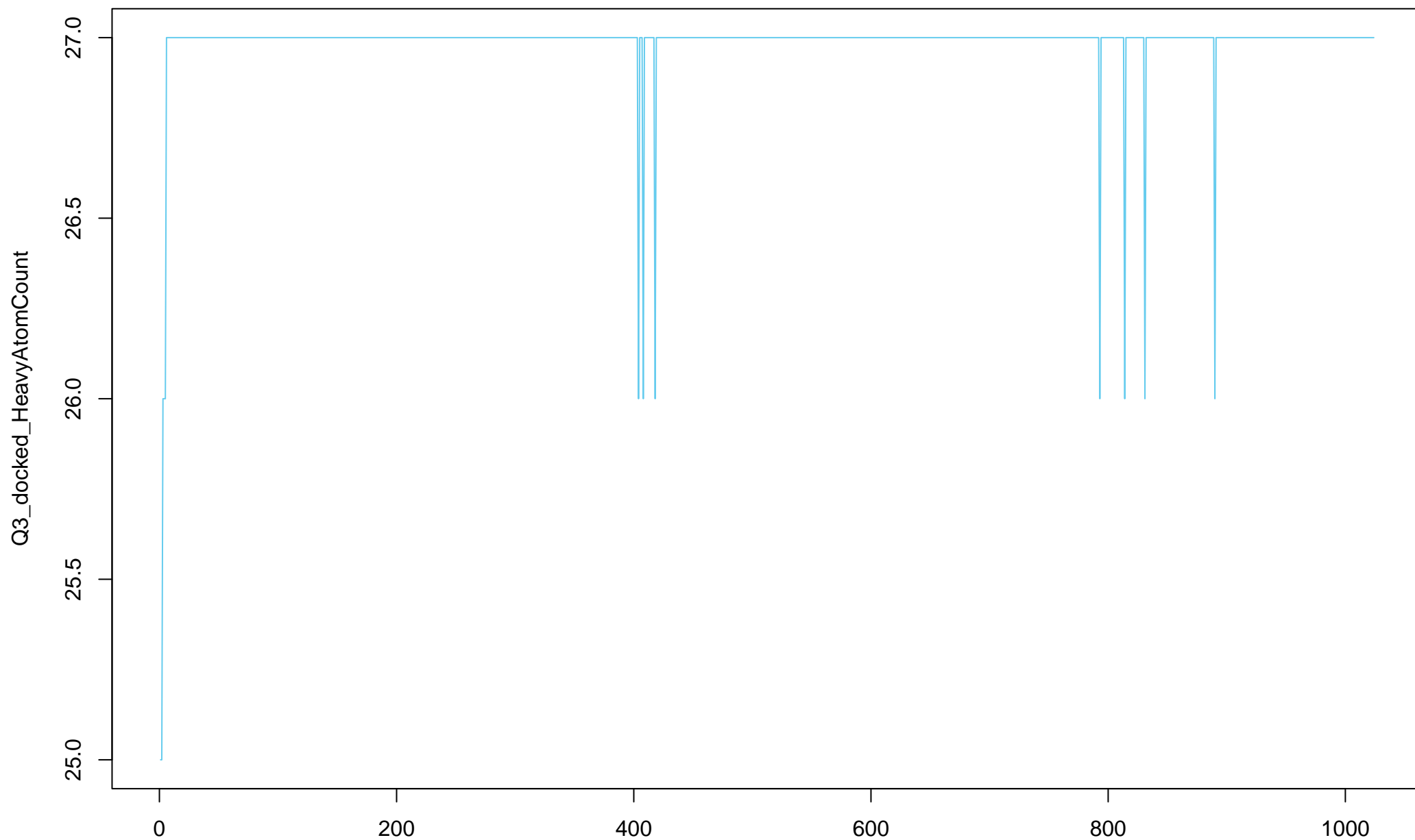
Q3_logit_ec_tanimoto_similarity
ESS = 136 | BMK = 0.0903 | MCSE(6.27) = 6.77 | stat: TRUE | burn: 0



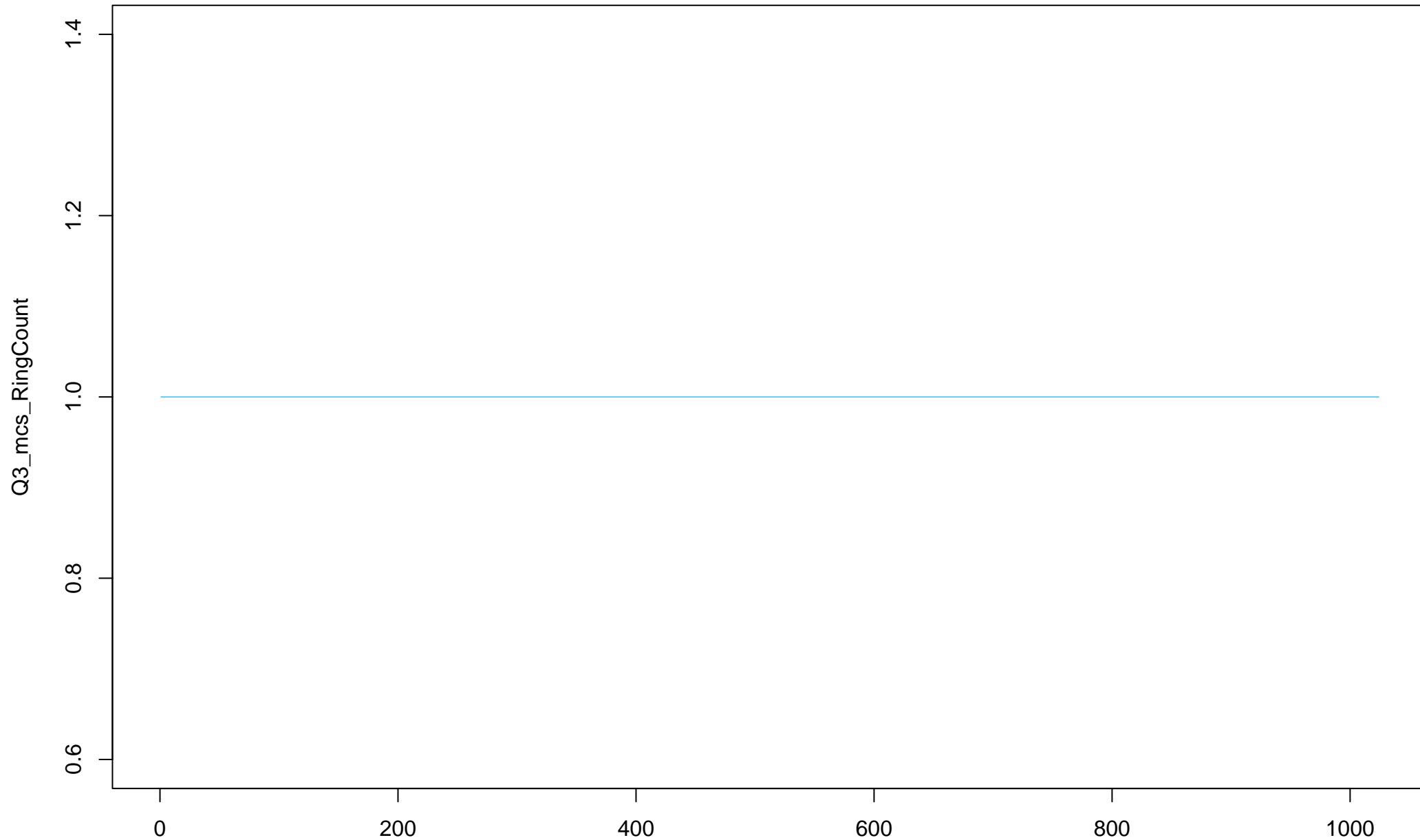
Q3_mcs_NumHeteroAtoms
ESS = 176 | BMK = 0.55 | MCSE(6.27) = 7 | stat: TRUE | burn: 0



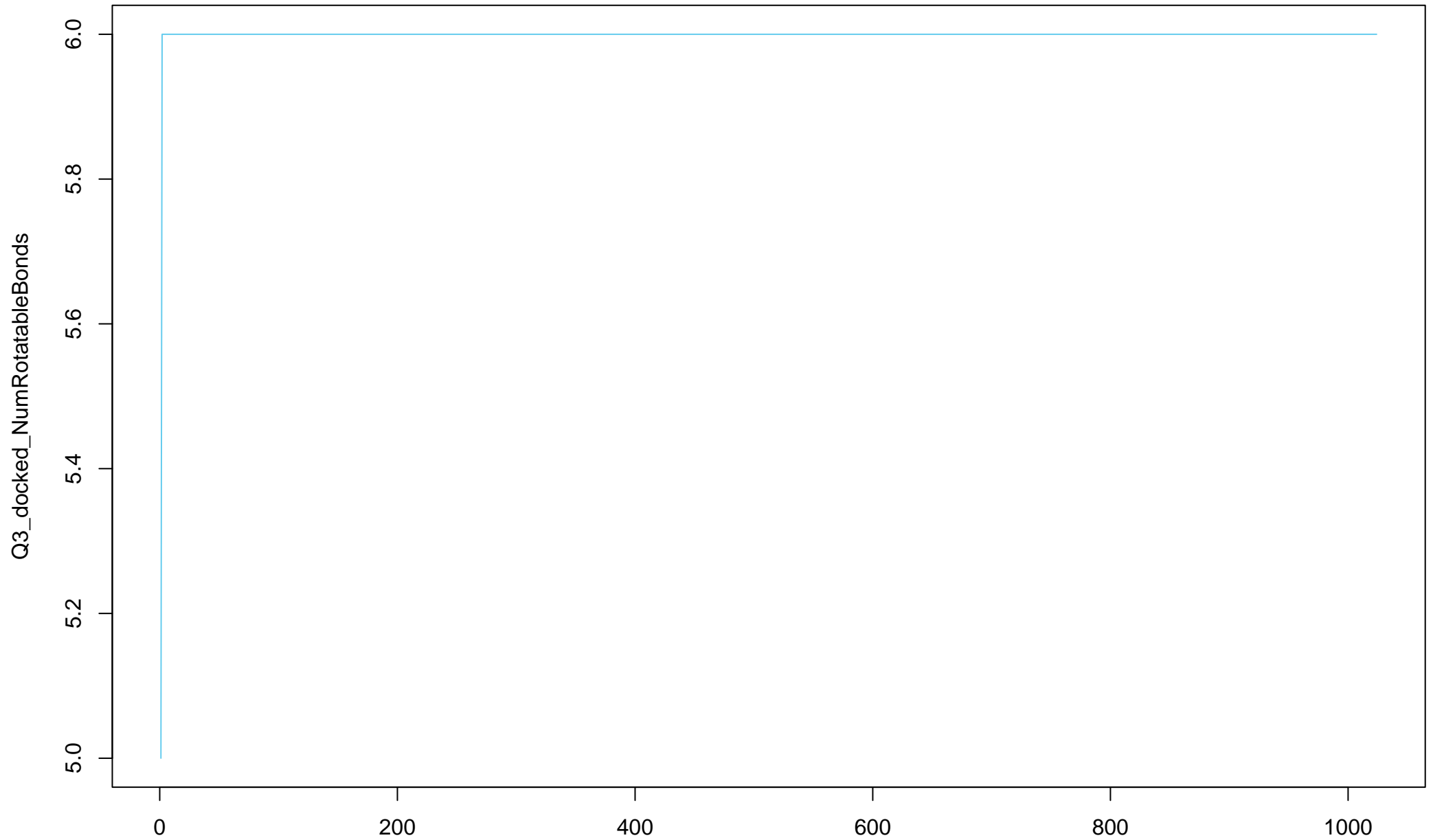
Q3_docked_HeavyAtomCount
ESS = 347 | BMK = 0.214 | MCSE(6.27) = 5.52 | stat: TRUE | burn: 0



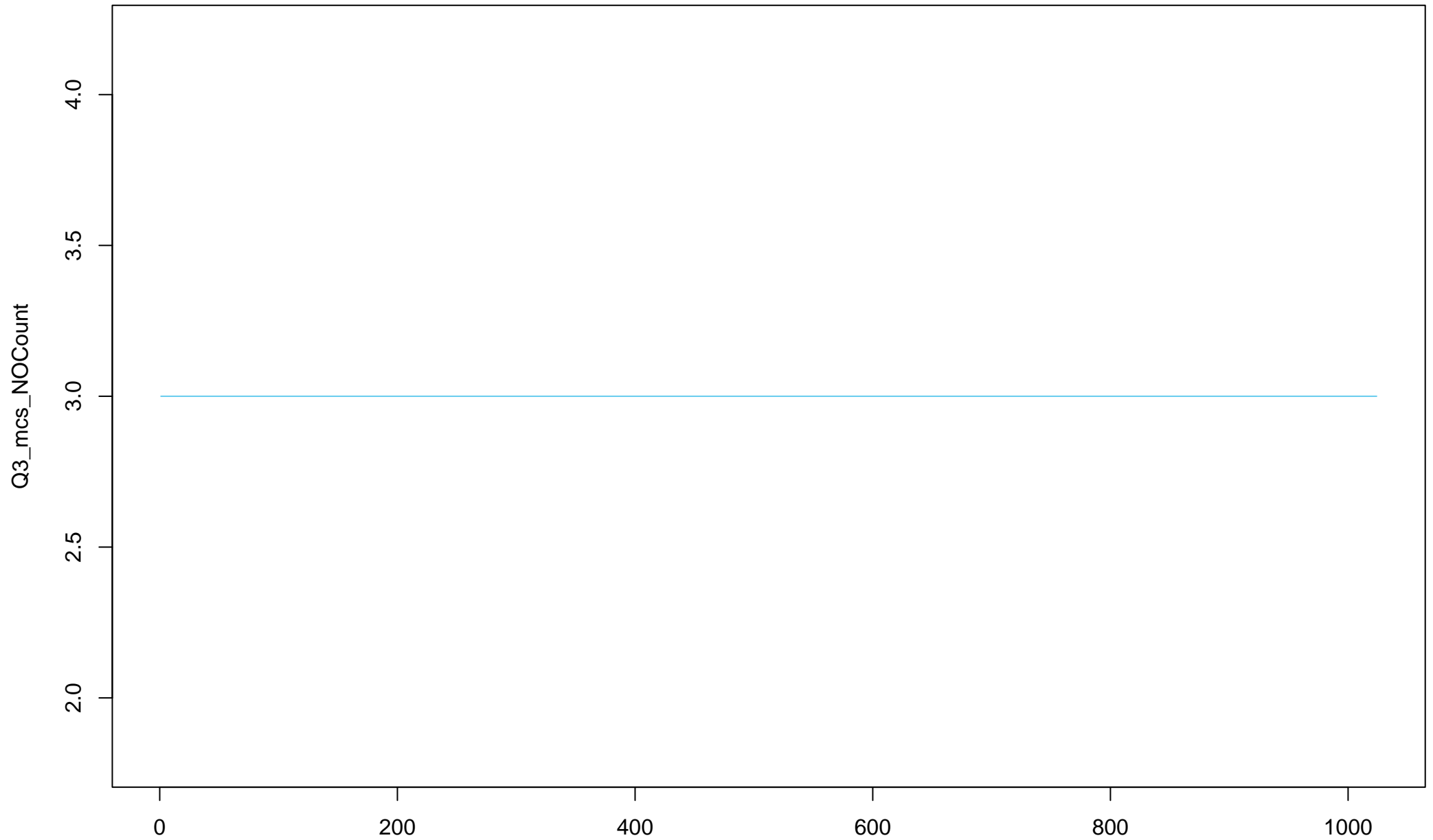
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



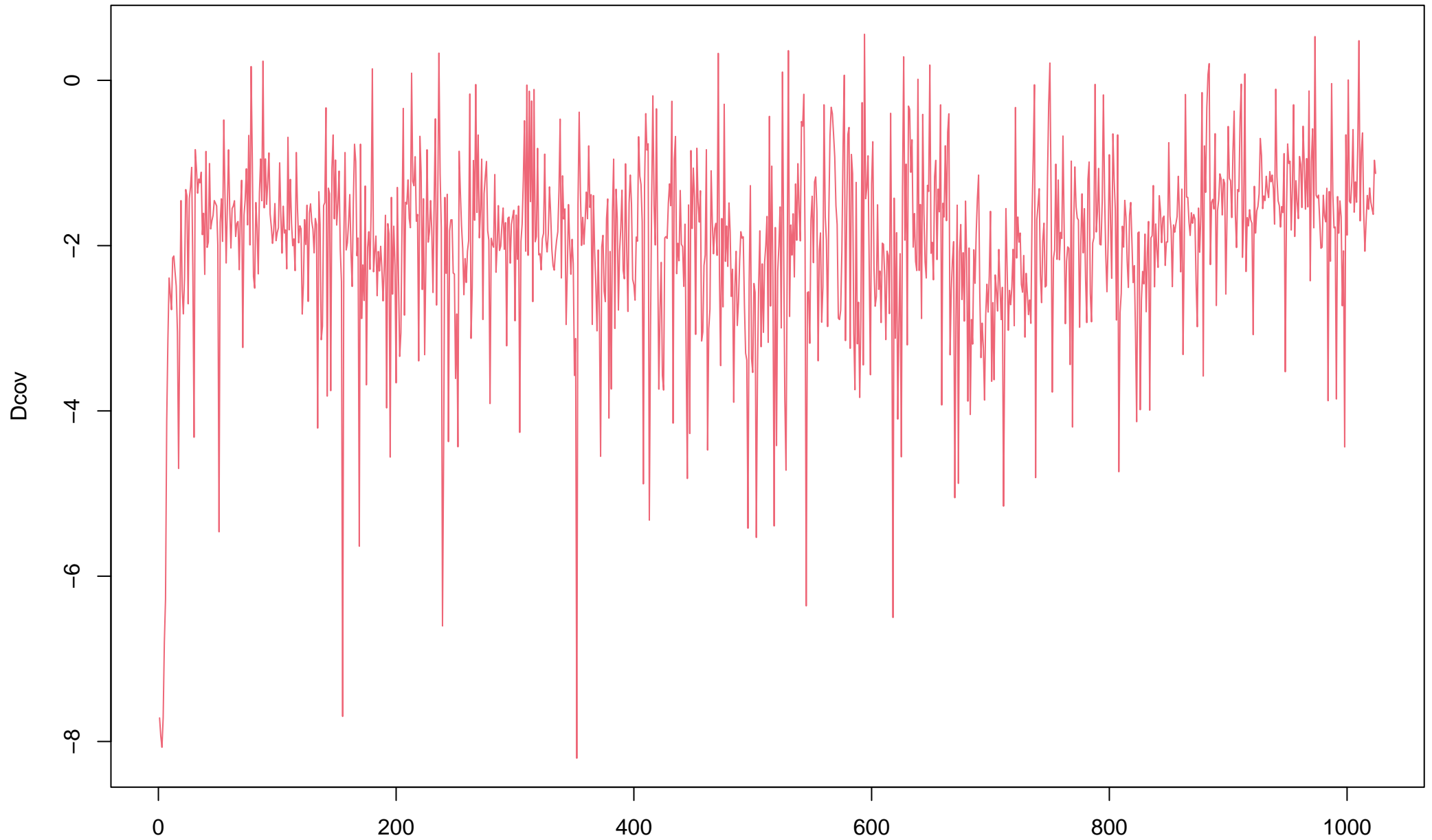
Q3_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.567 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102



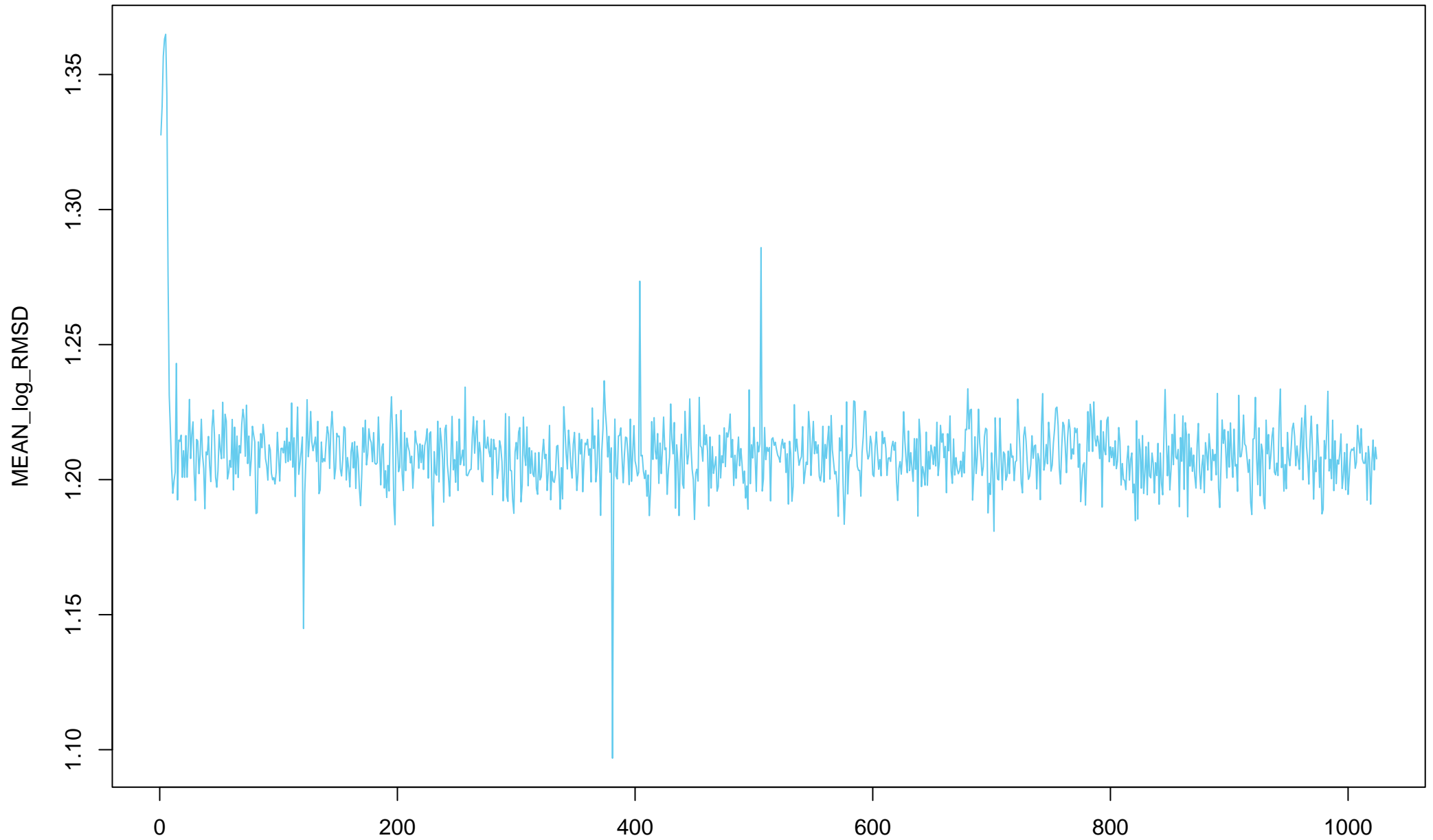
Q3_mcs_NOCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



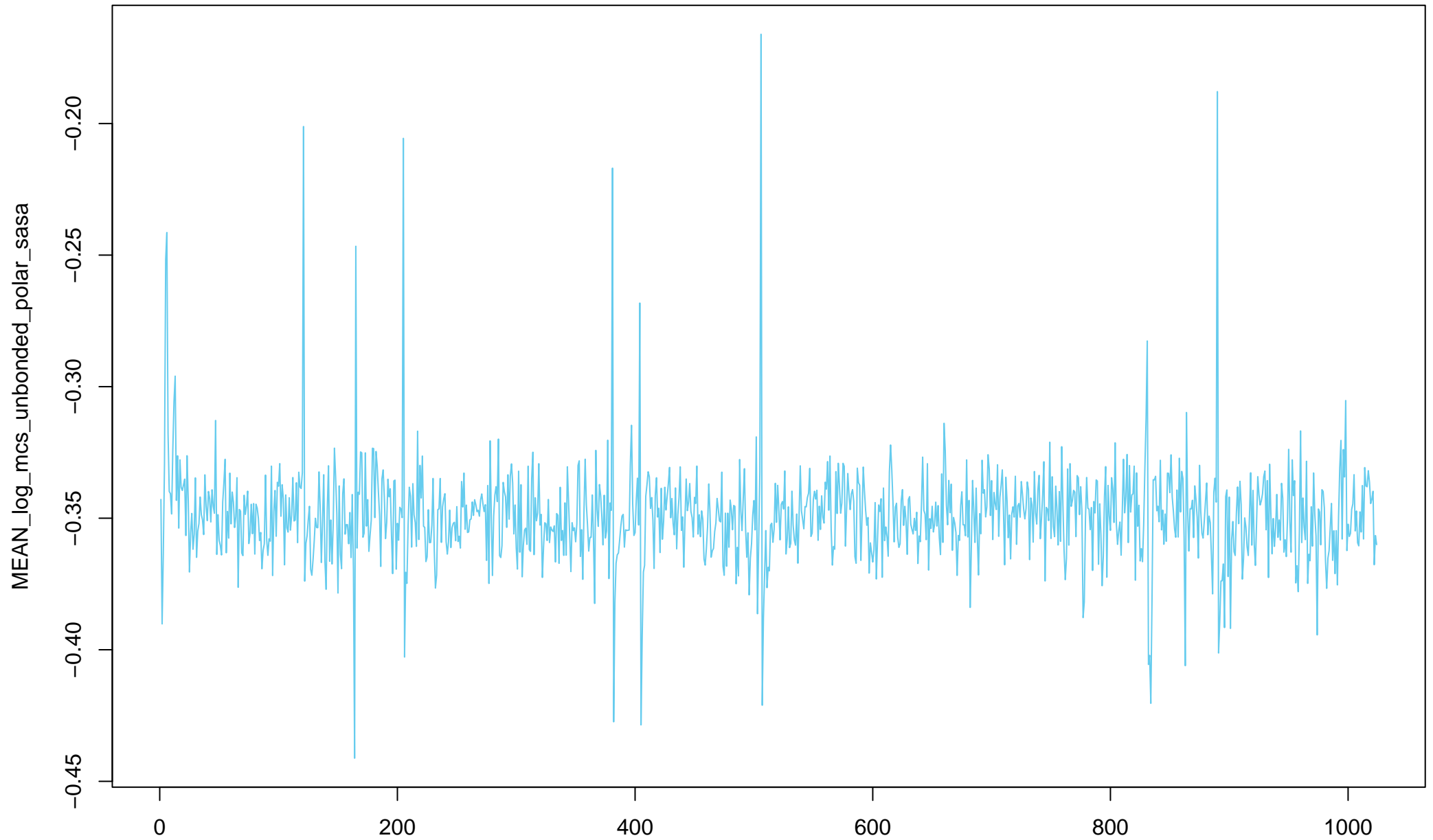
Dcov
ESS = 569 | BMK = 0.13 | MCSE(6.27) = 4.43 | stat: TRUE | burn: 0



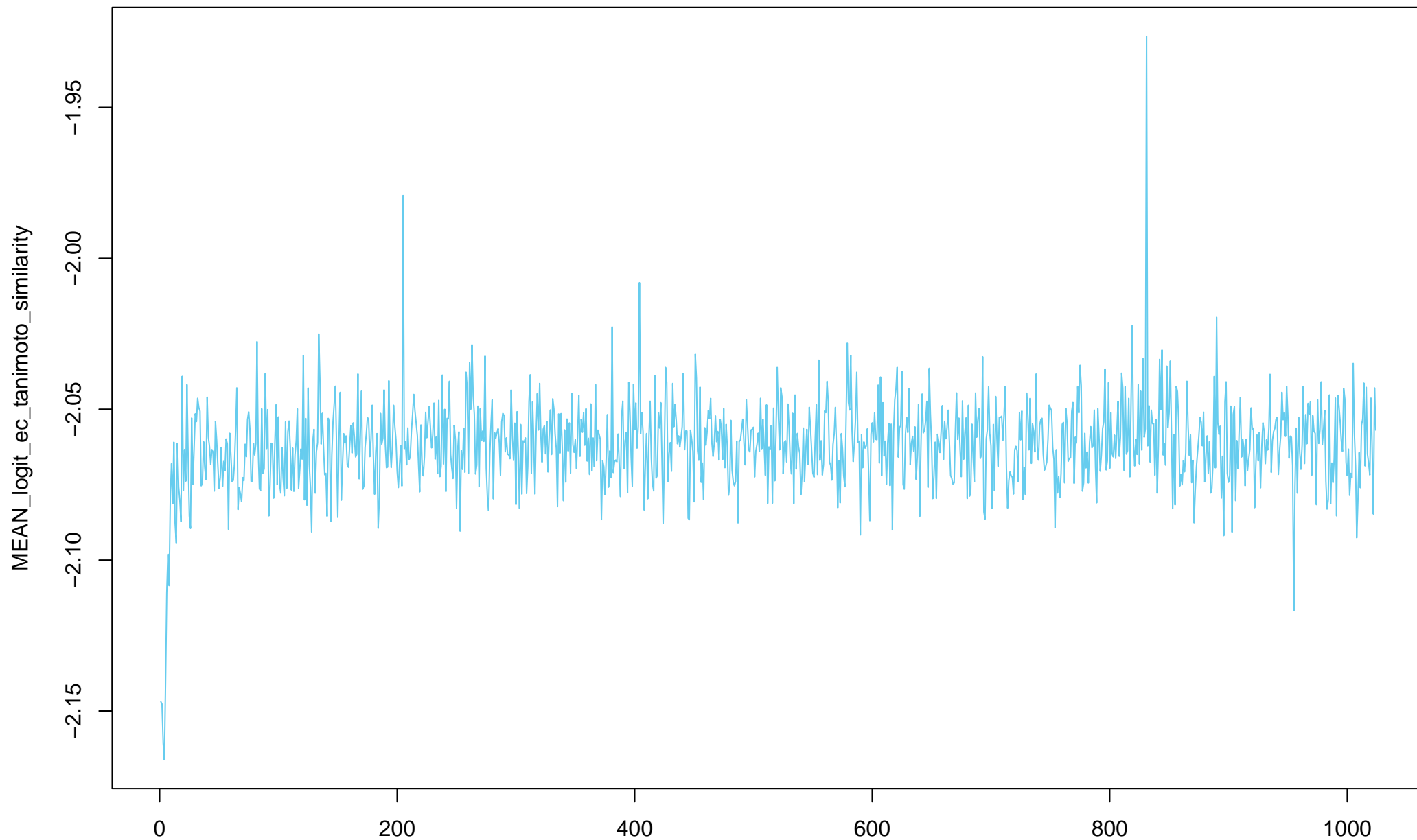
MEAN_log_RMSD
ESS = 282 | BMK = 0.108 | MCSE(6.27) = 6.37 | stat: TRUE | burn: 0



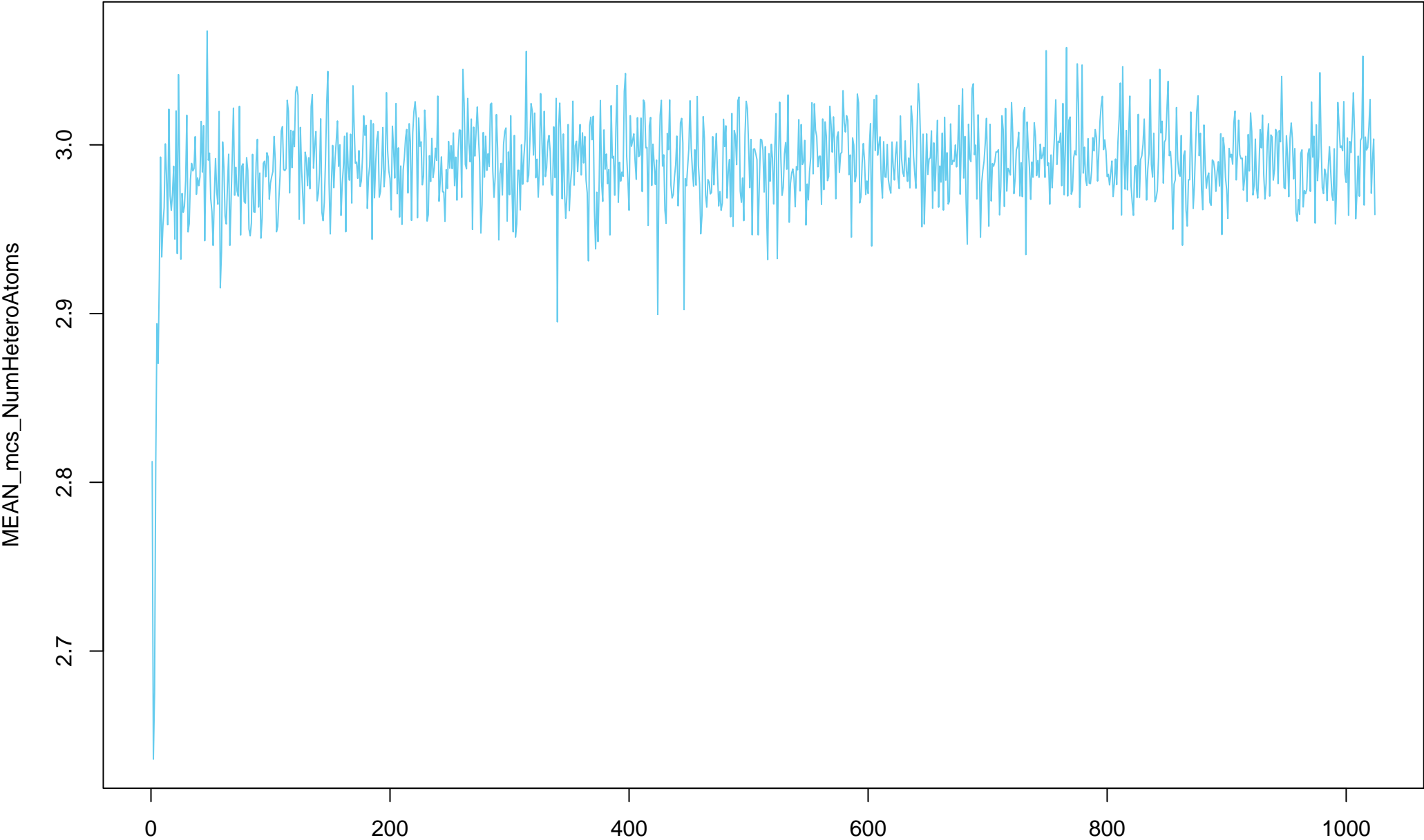
MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.118 | MCSE(6.27) = 3.51 | stat: TRUE | burn: 0



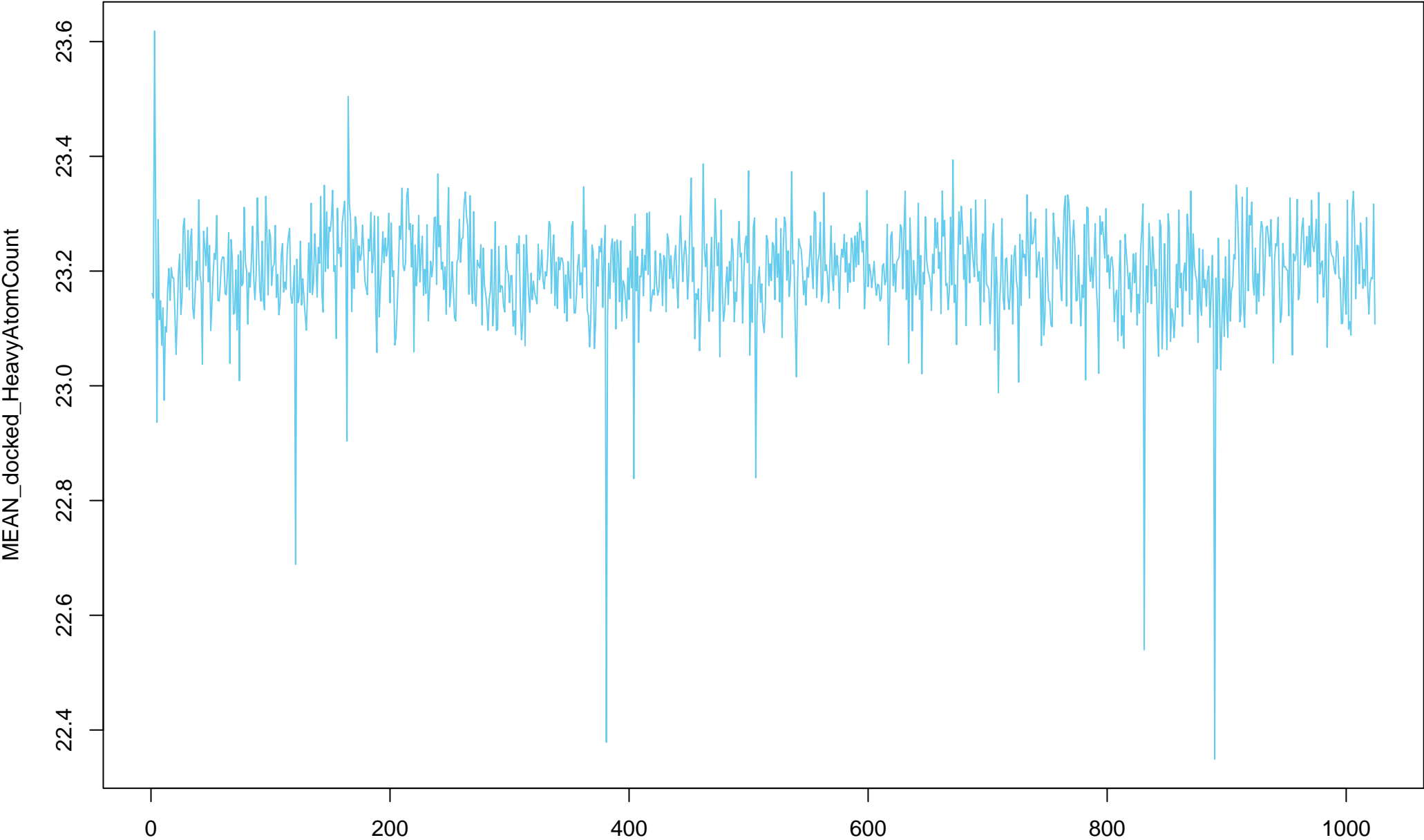
MEAN_logit_ec_tanimoto_similarity
ESS = 408 | BMK = 0.106 | MCSE(6.27) = 5.9 | stat: FALSE | burn: 0



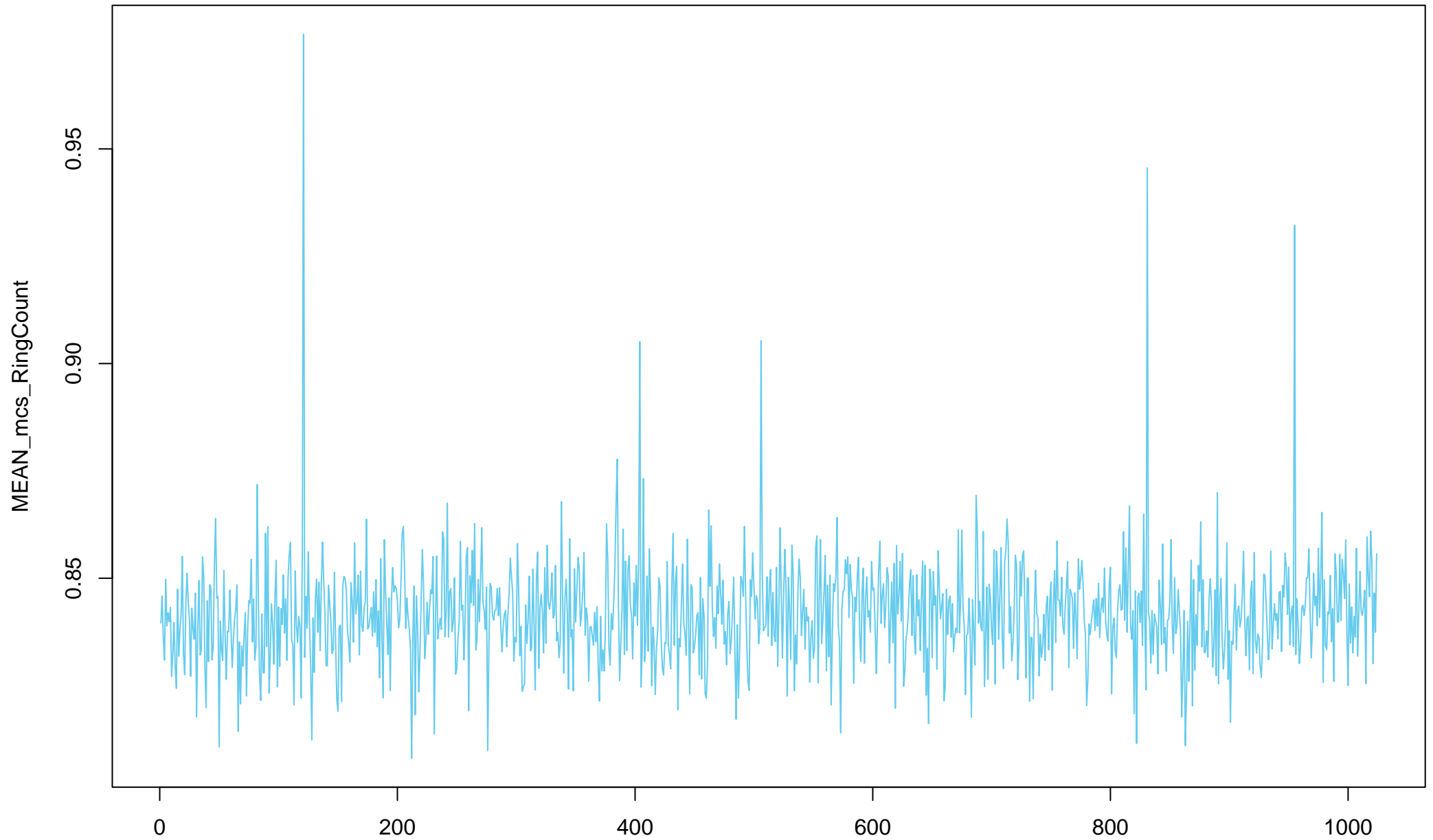
MEAN_mcs_NumHeteroAtoms
ESS = 371 | BMK = 0.137 | MCSE(6.27) = 6.59 | stat: FALSE | burn: 0



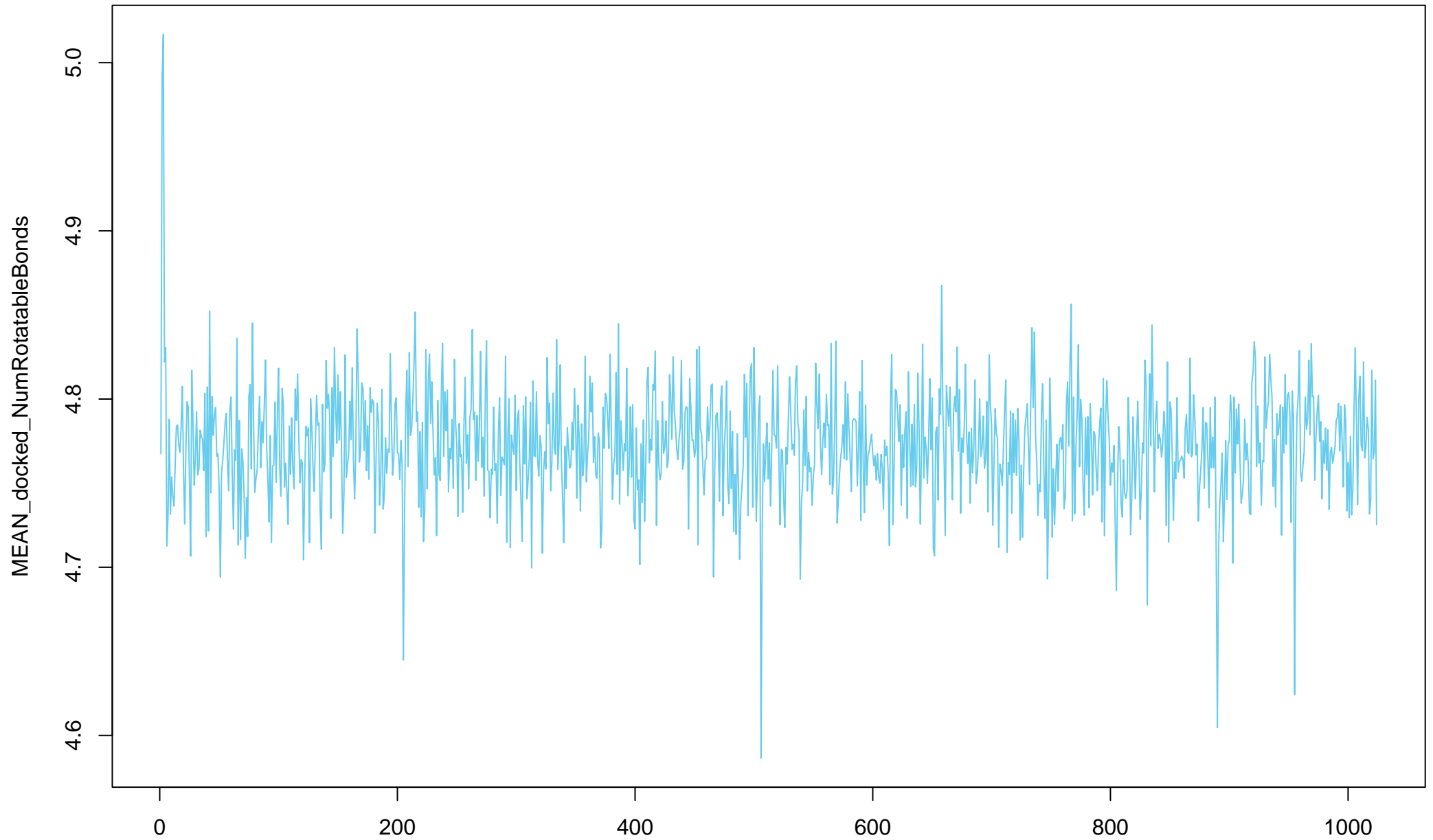
MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.102 | MCSE(6.27) = 4.14 | stat: TRUE | burn: 0



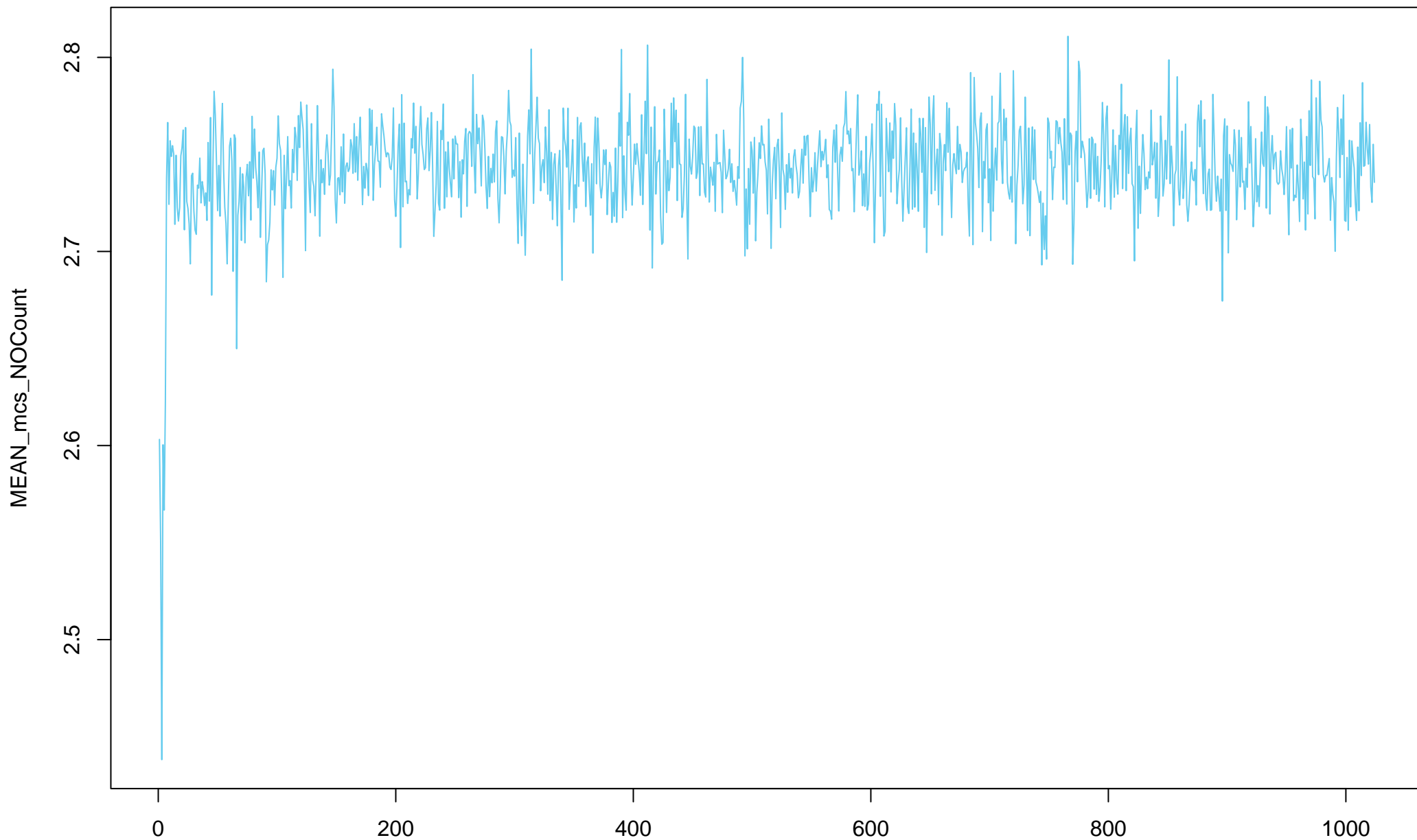
MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0895 | MCSE(6.27) = 3.19 | stat: FALSE | burn: 0



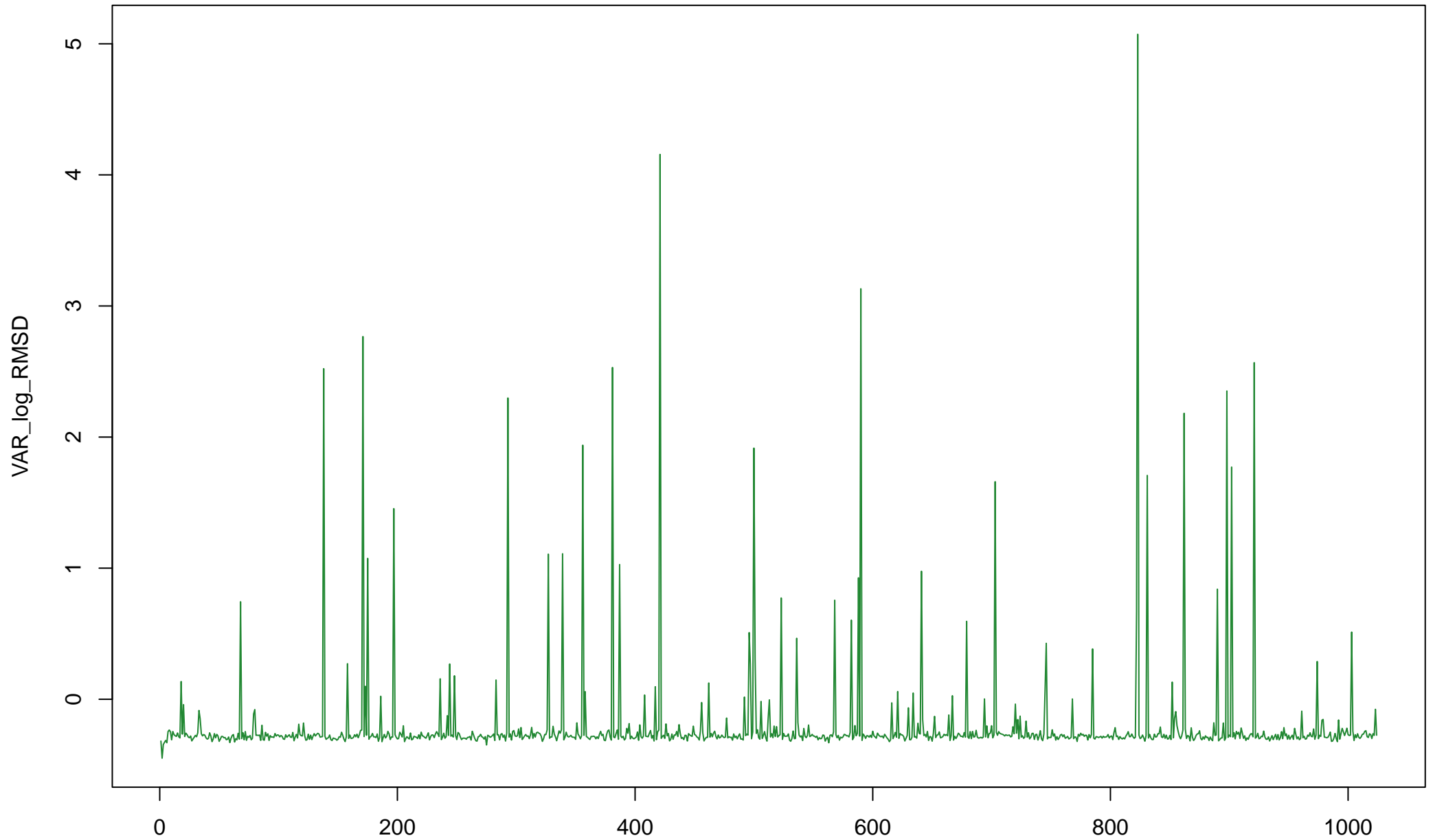
MEAN_docked_NumRotatableBonds
ESS = 861 | BMK = 0.0817 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0



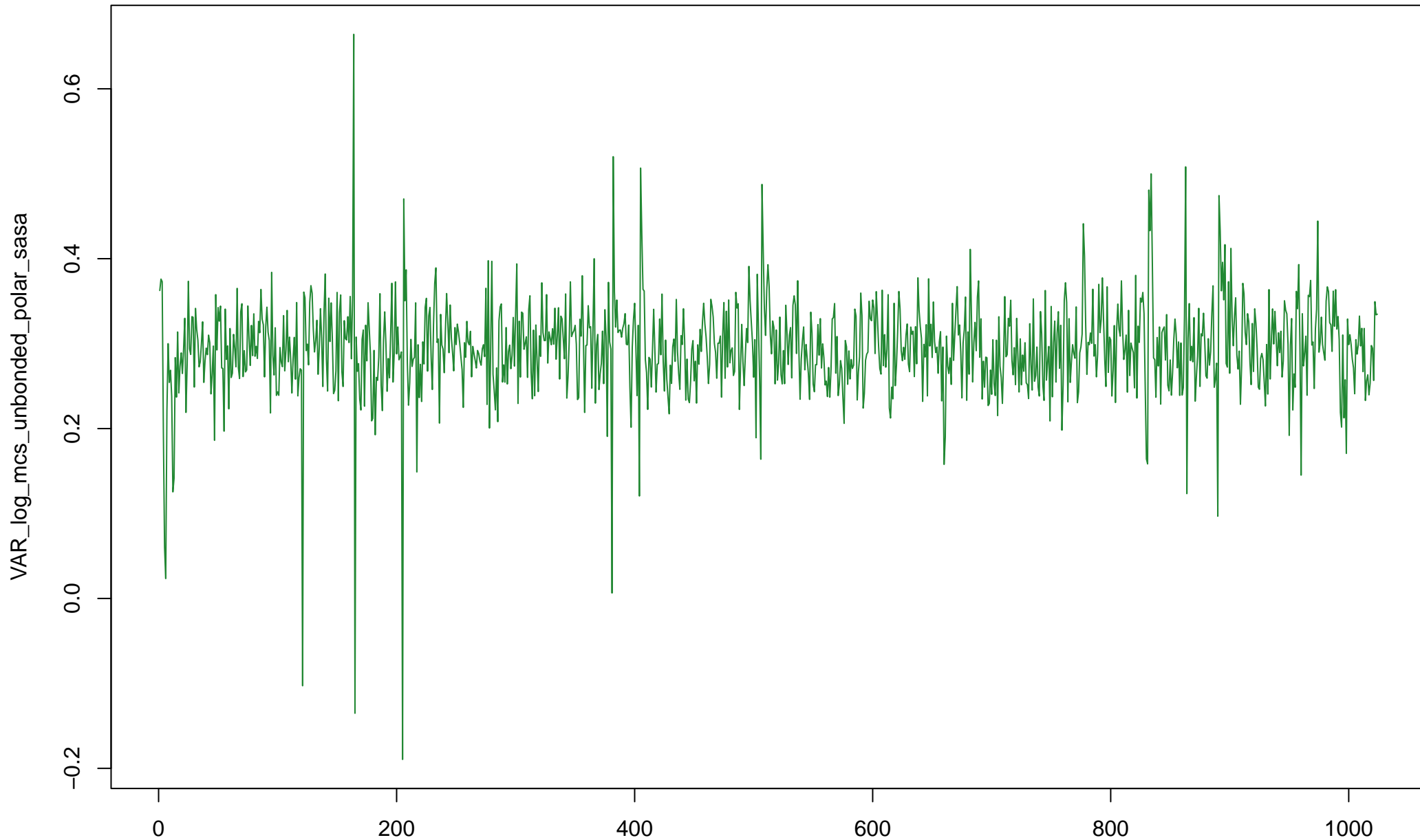
MEAN_mcs_NOCount
ESS = 361 | BMK = 0.0984 | MCSE(6.27) = 5.99 | stat: FALSE | burn: 0



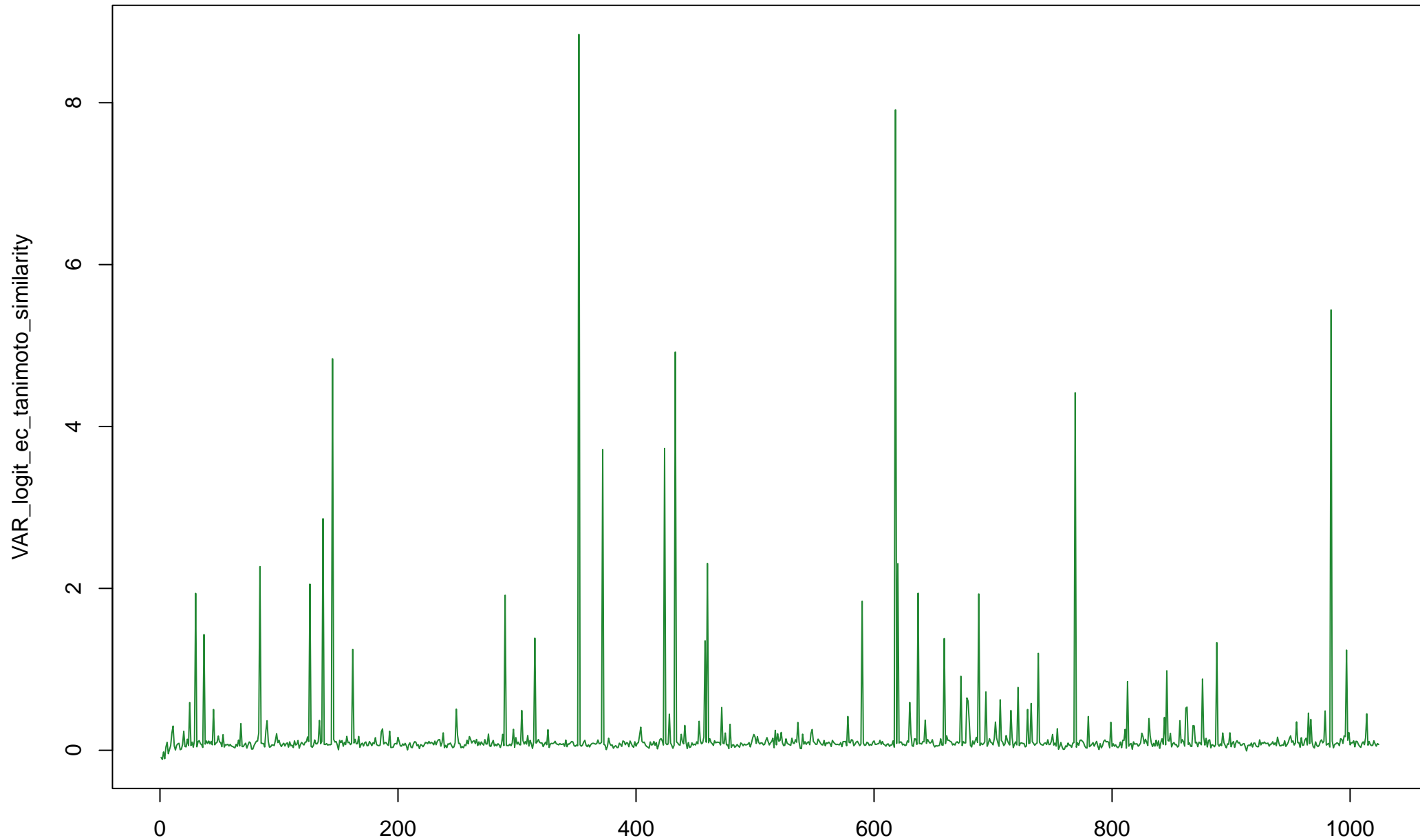
VAR_log_RMSD
ESS = 1020 | BMK = 0.755 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 1020



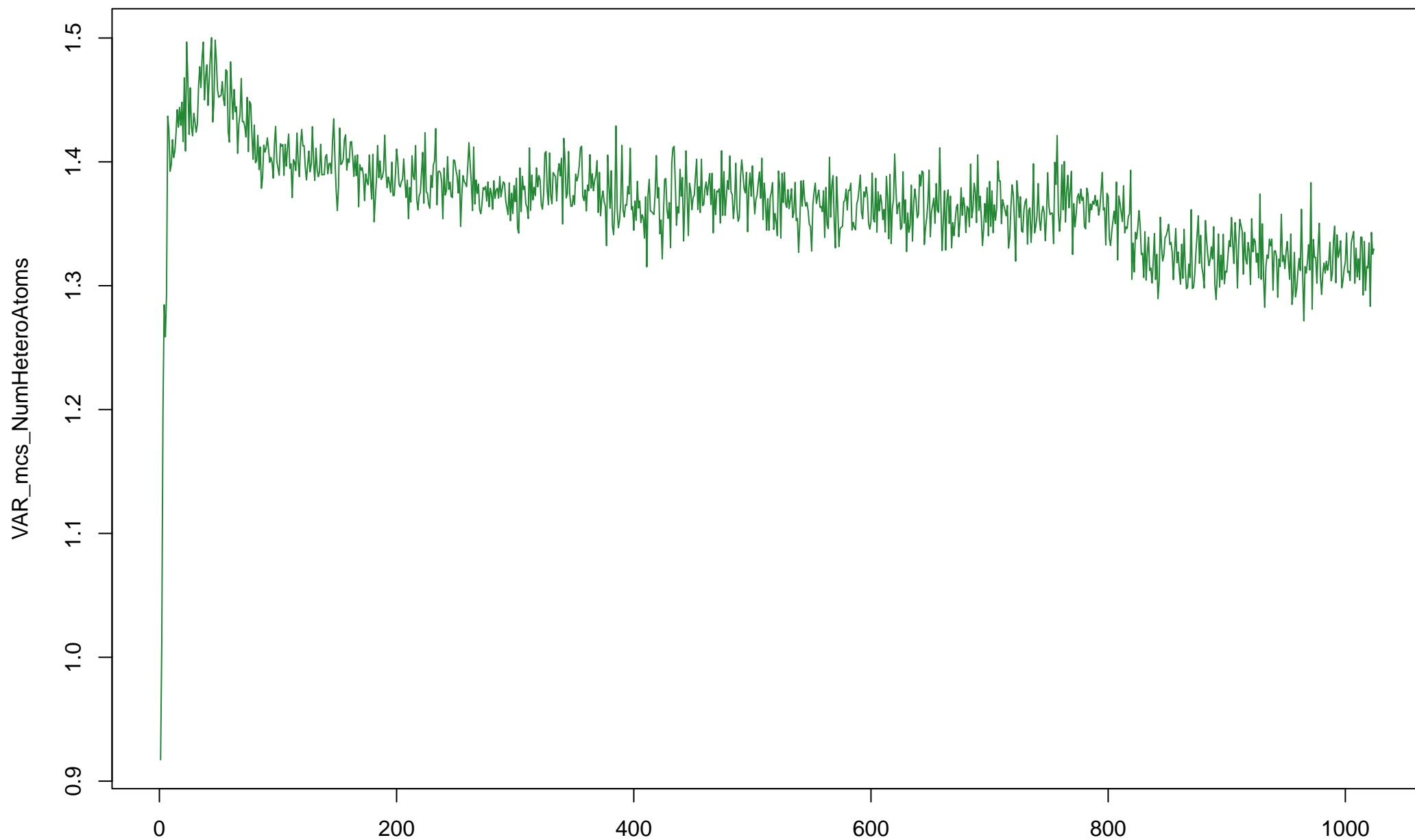
VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0942 | MCSE(6.27) = 3.82 | stat: TRUE | burn: 0



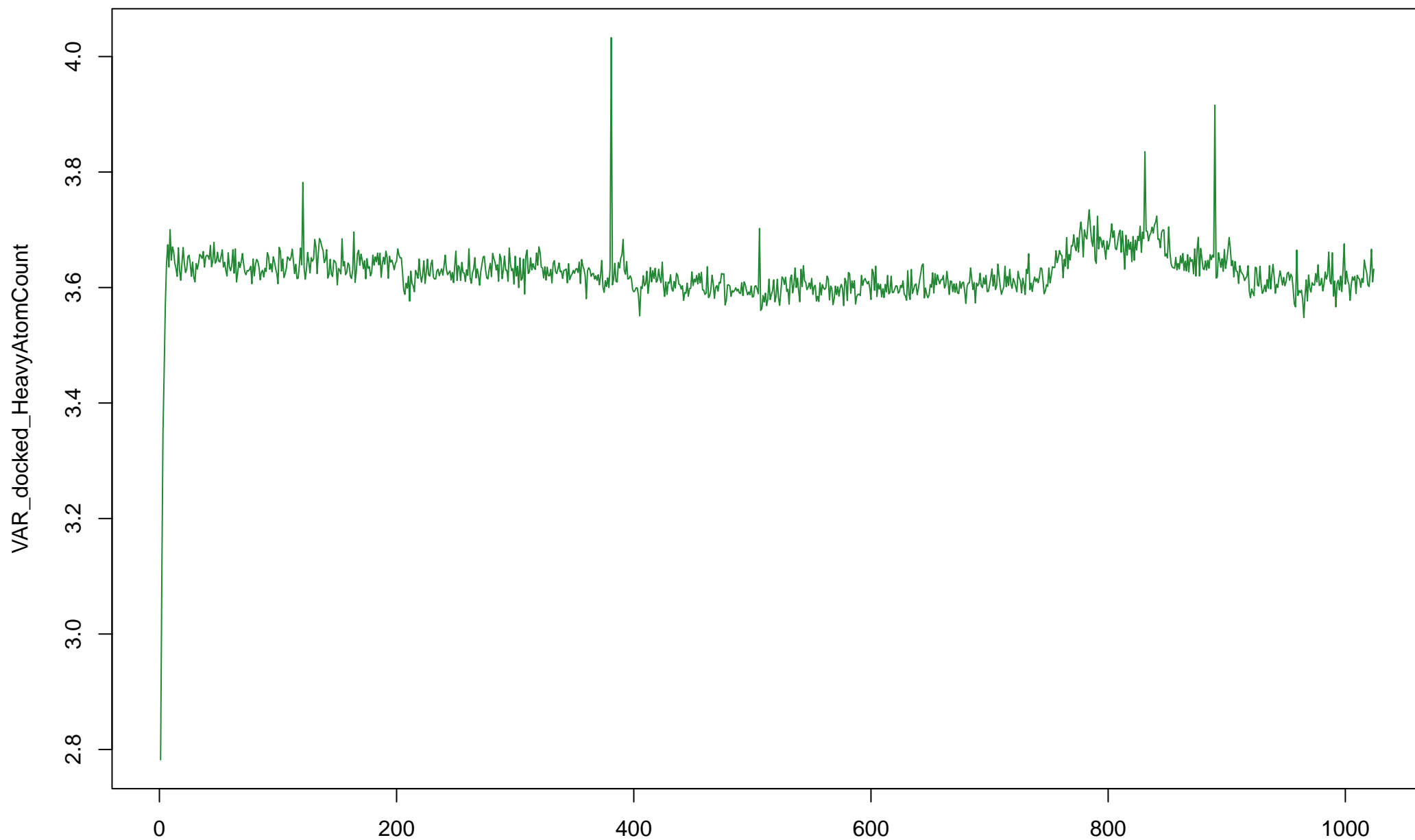
VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 1020



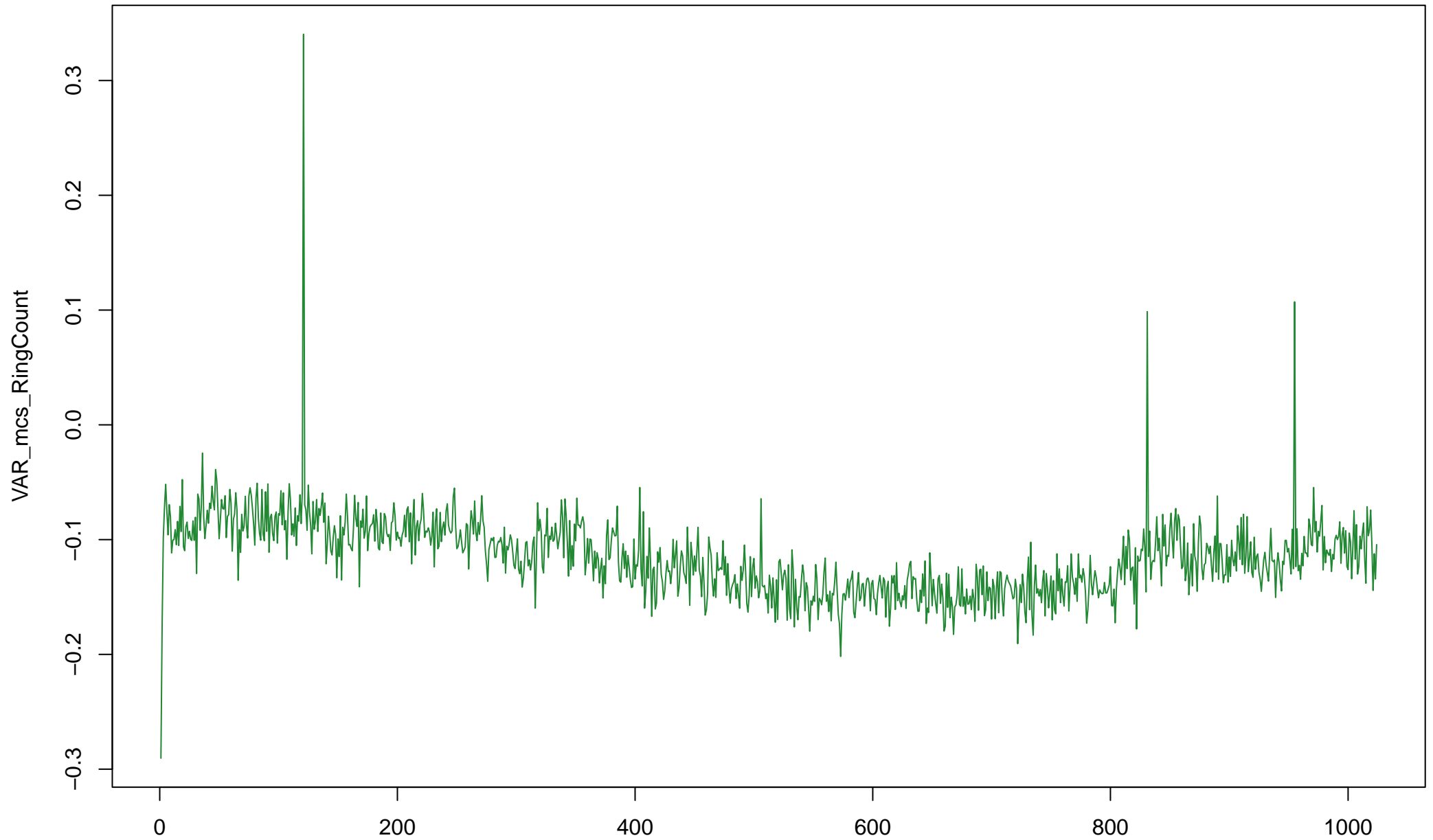
VAR_mcs_NumHeteroAtoms
ESS = 14 | BMK = 0.529 | MCSE(6.27) = 13.6 | stat: FALSE | burn: 816



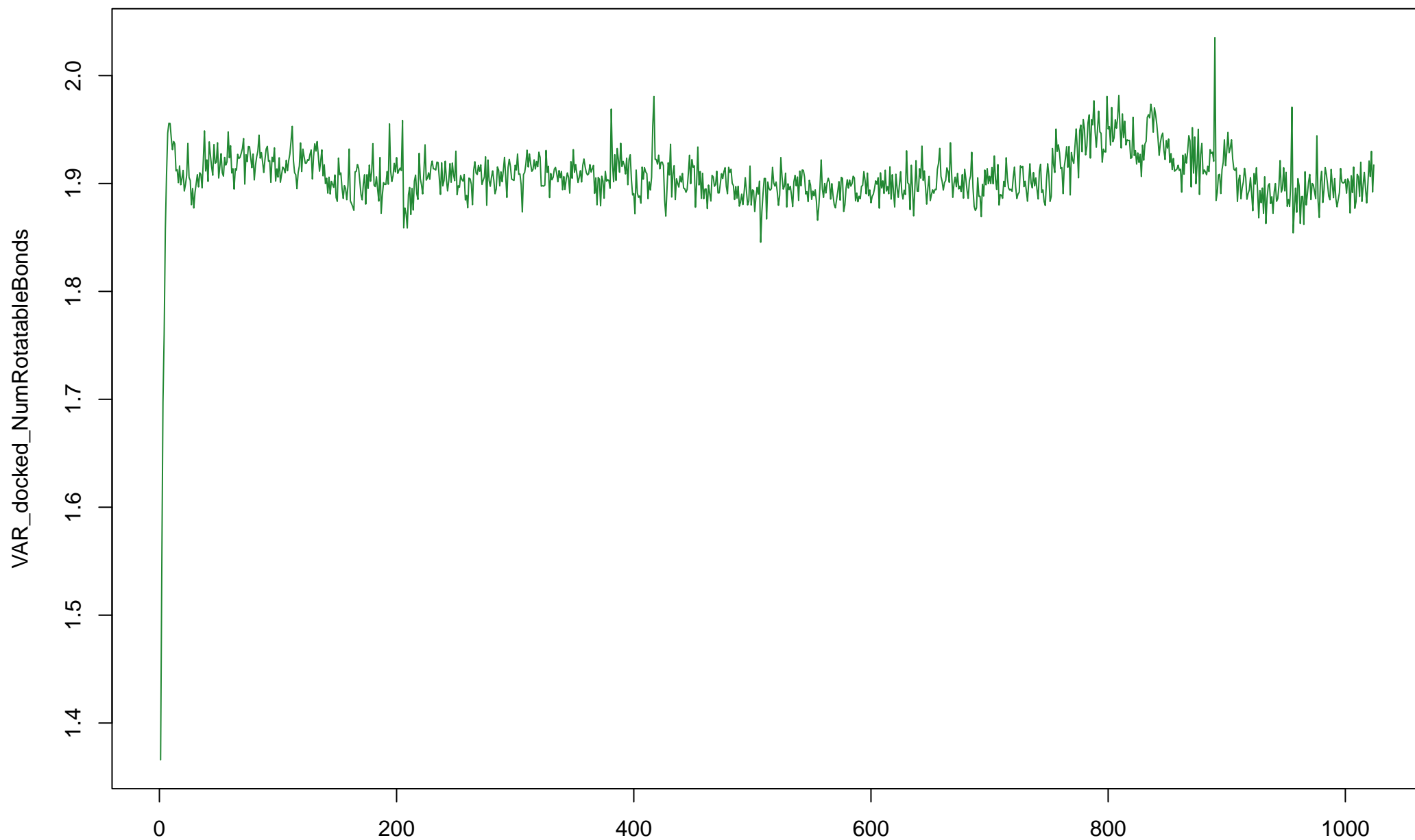
VAR_docked_HeavyAtomCount
ESS = 53.1 | BMK = 0.254 | MCSE(6.27) = 10 | stat: TRUE | burn: 1020



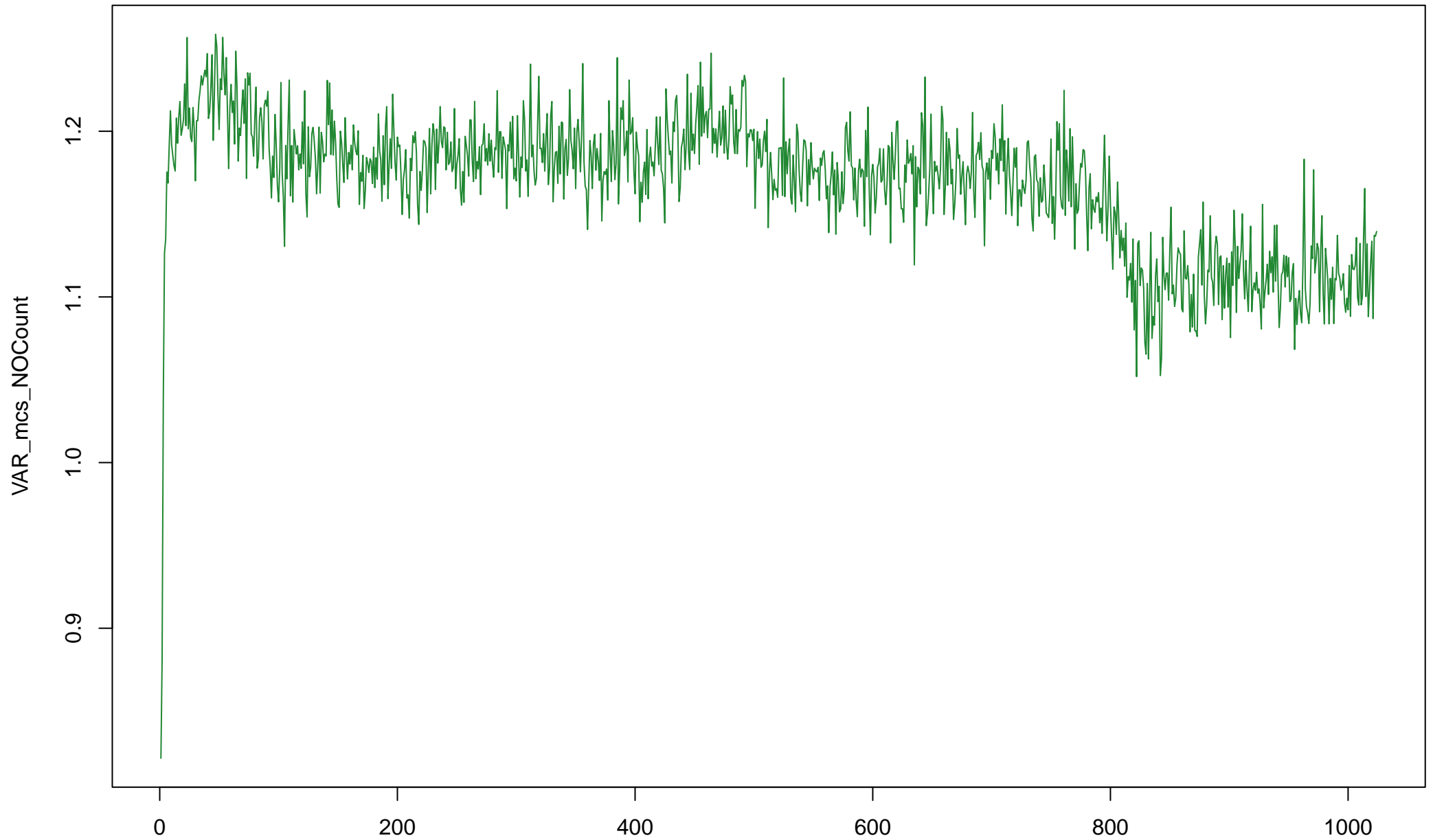
VAR_mcs_RingCount
ESS = 10.1 | BMK = 0.389 | MCSE(6.27) = 11.9 | stat: FALSE | burn: 0



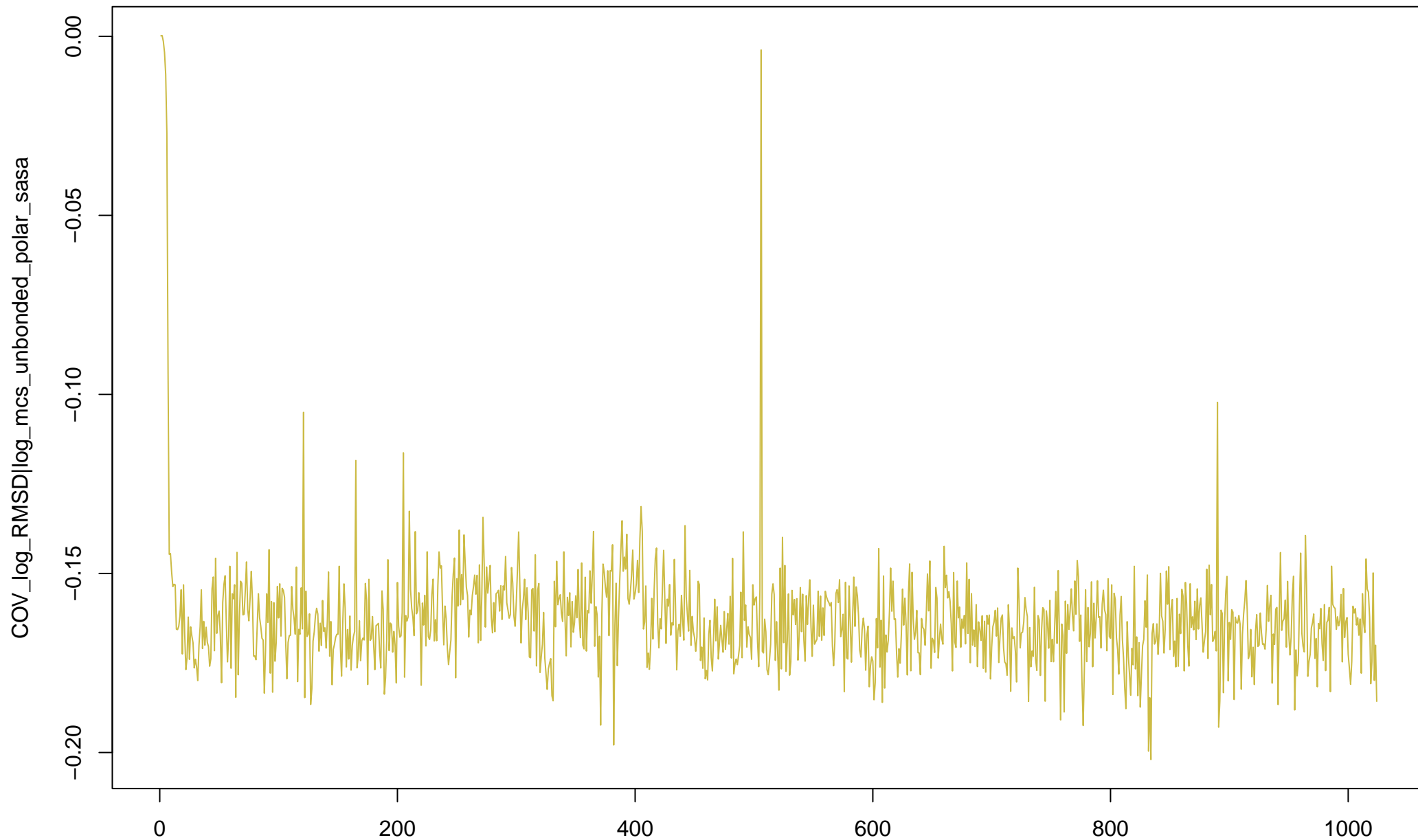
VAR_docked_NumRotatableBonds
ESS = 73.2 | BMK = 0.188 | MCSE(6.27) = 9.28 | stat: TRUE | burn: 1020



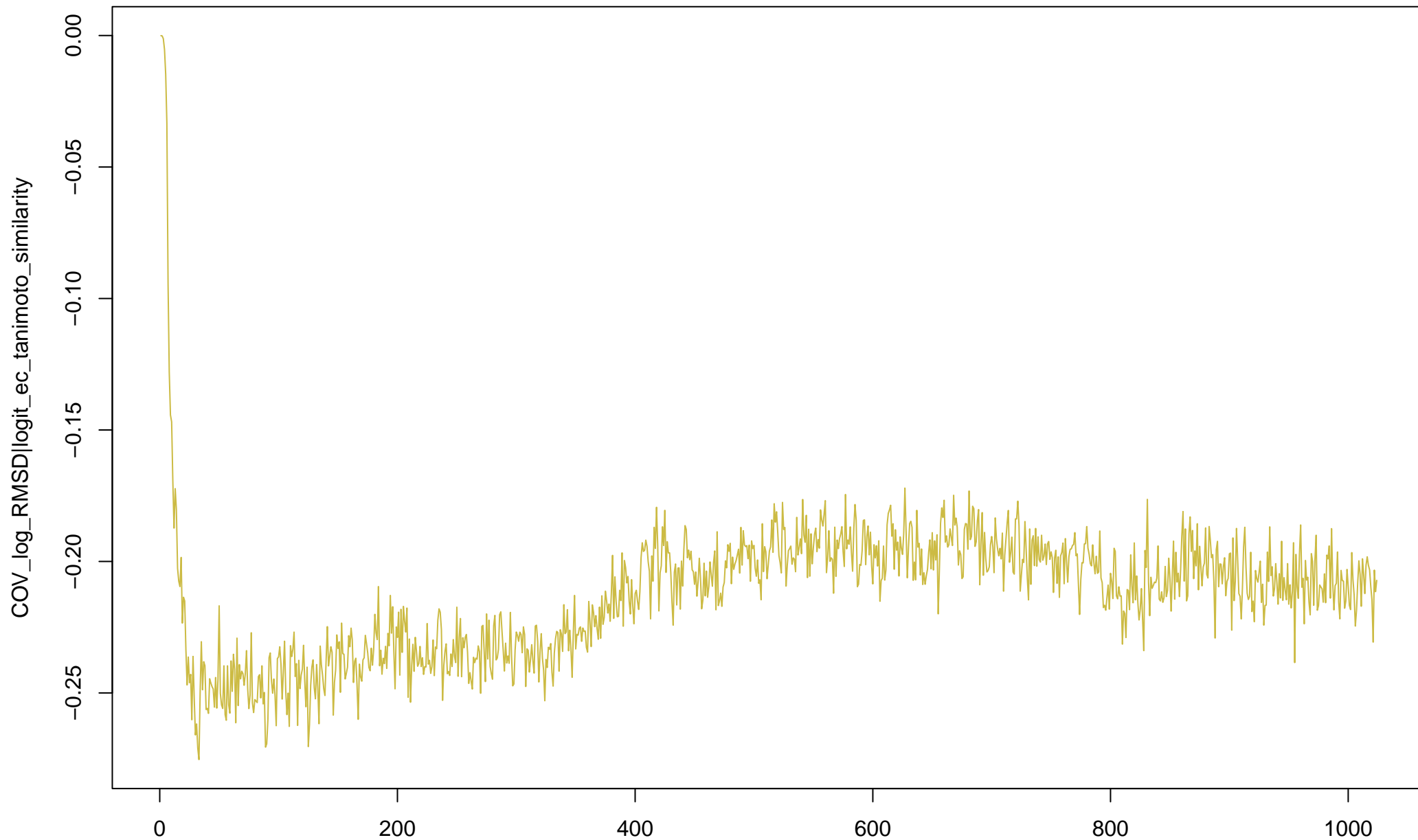
VAR_mcs_NOCount
ESS = 8.55 | BMK = 0.525 | MCSE(6.27) = 14.4 | stat: FALSE | burn: 816



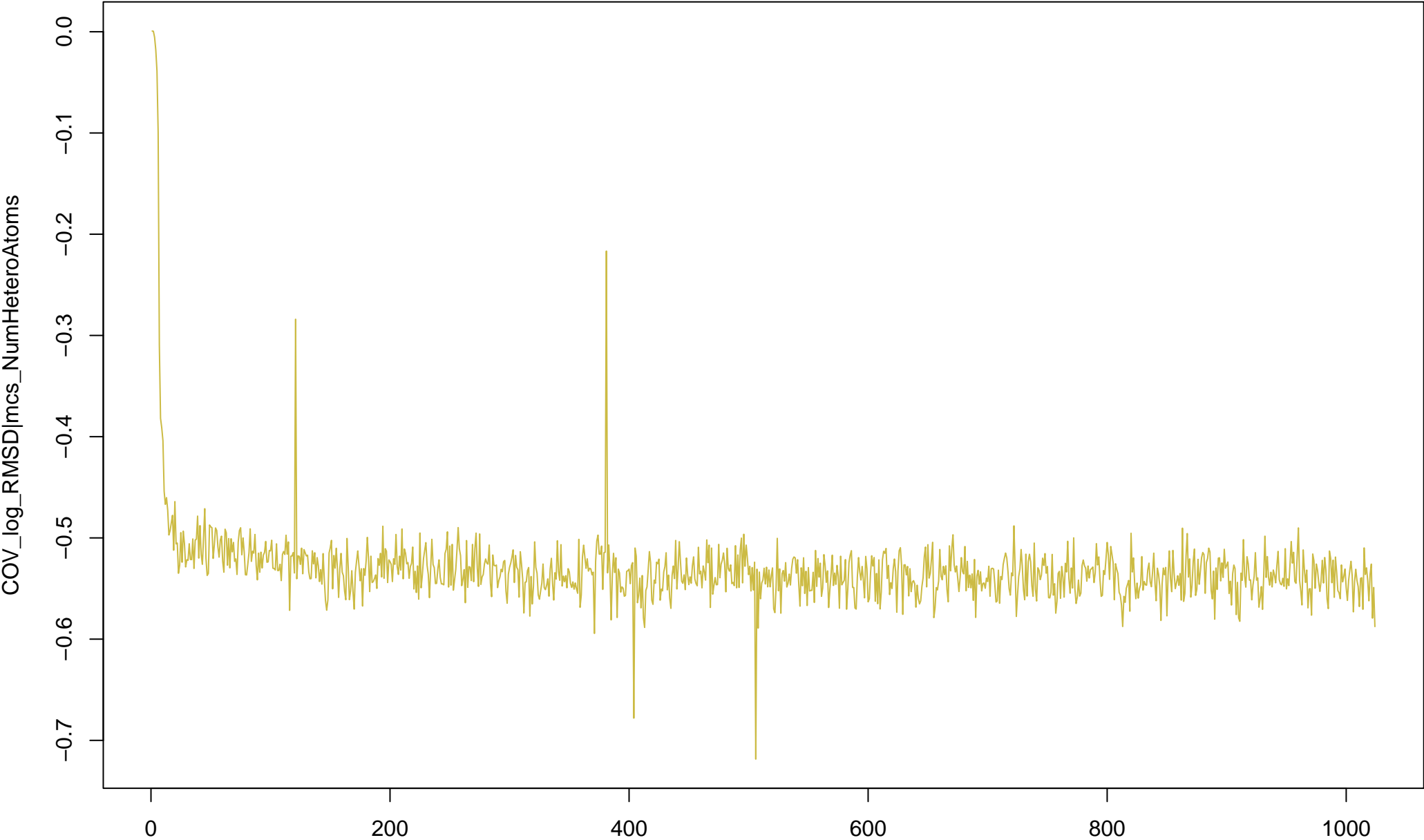
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 181 | BMK = 0.161 | MCSE(6.27) = 6.8 | stat: TRUE | burn: 0



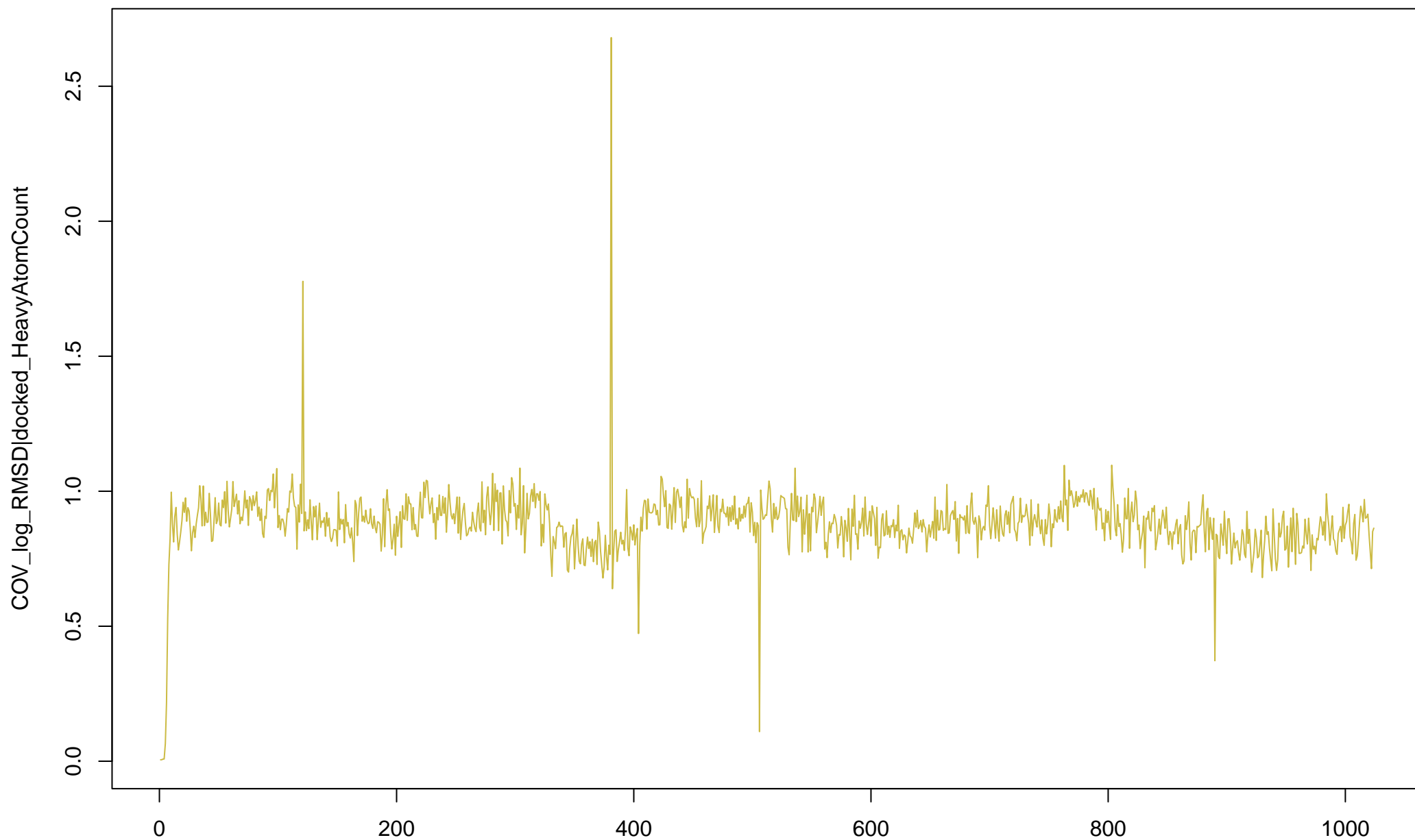
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 38.6 | BMK = 0.586 | MCSE(6.27) = 13.2 | stat: FALSE | burn: 408



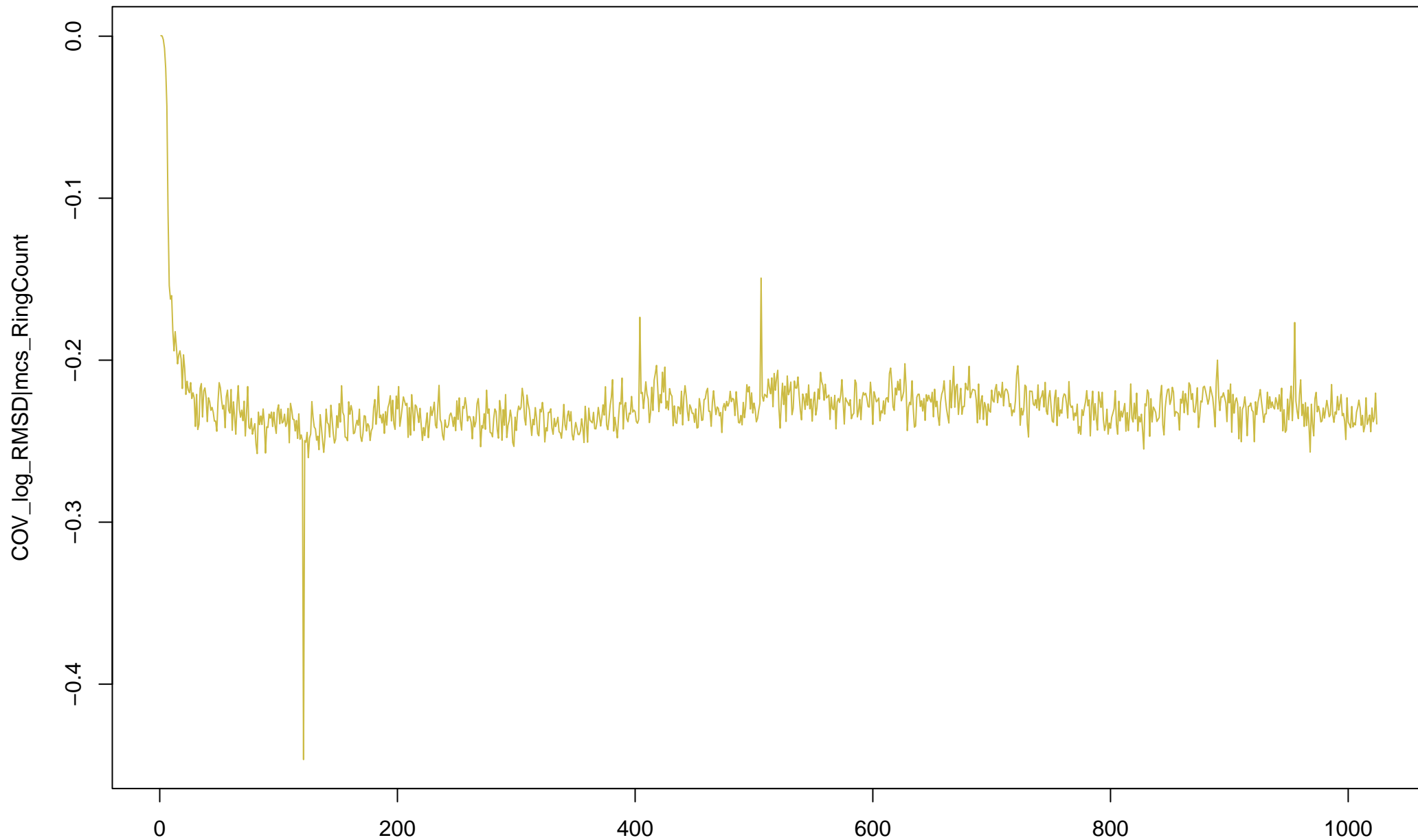
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 107 | BMK = 0.229 | MCSE(6.27) = 9.93 | stat: FALSE | burn: 0



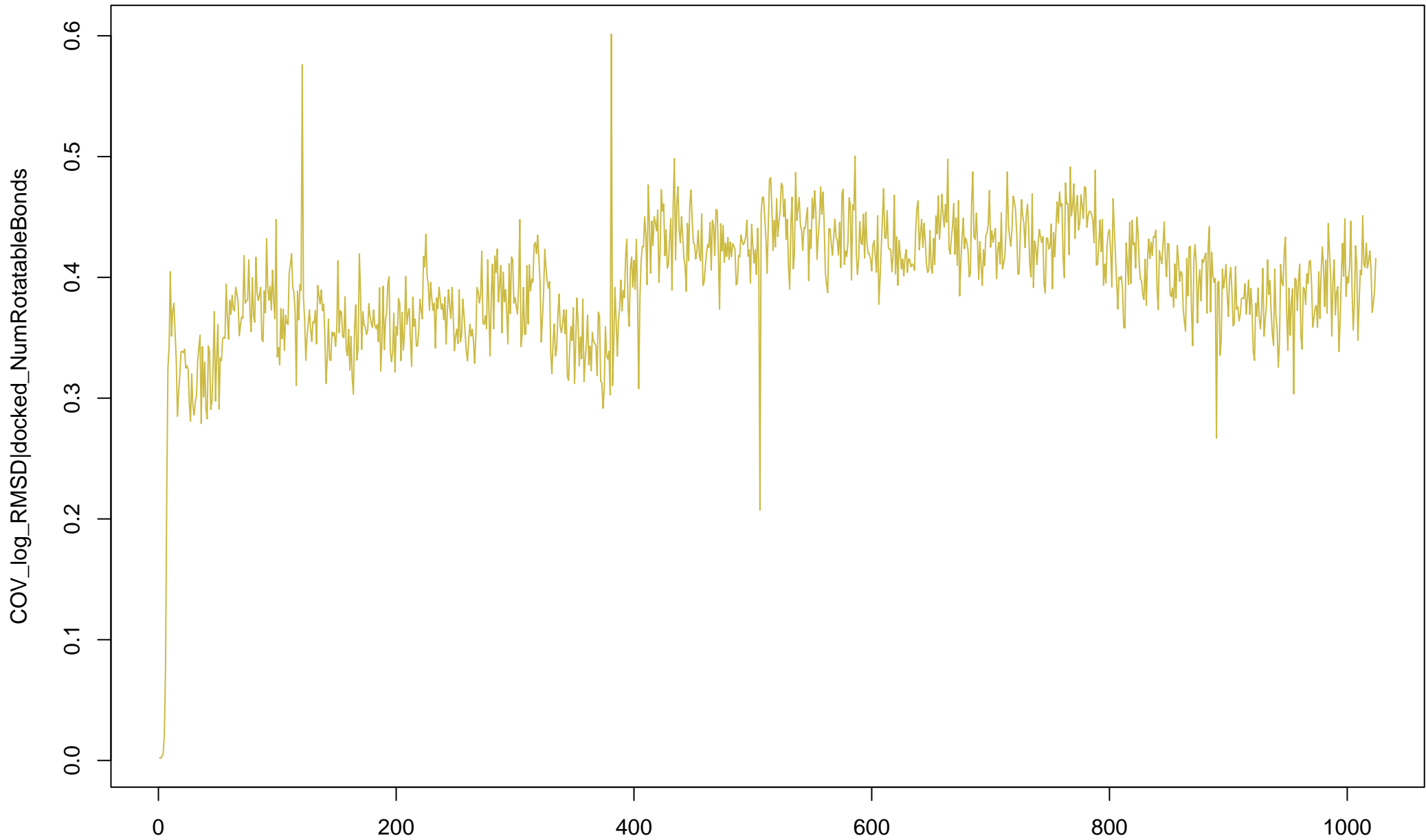
COV_log_RMSD|docked_HeavyAtomCount
ESS = 205 | BMK = 0.173 | MCSE(6.27) = 7.46 | stat: TRUE | burn: 0



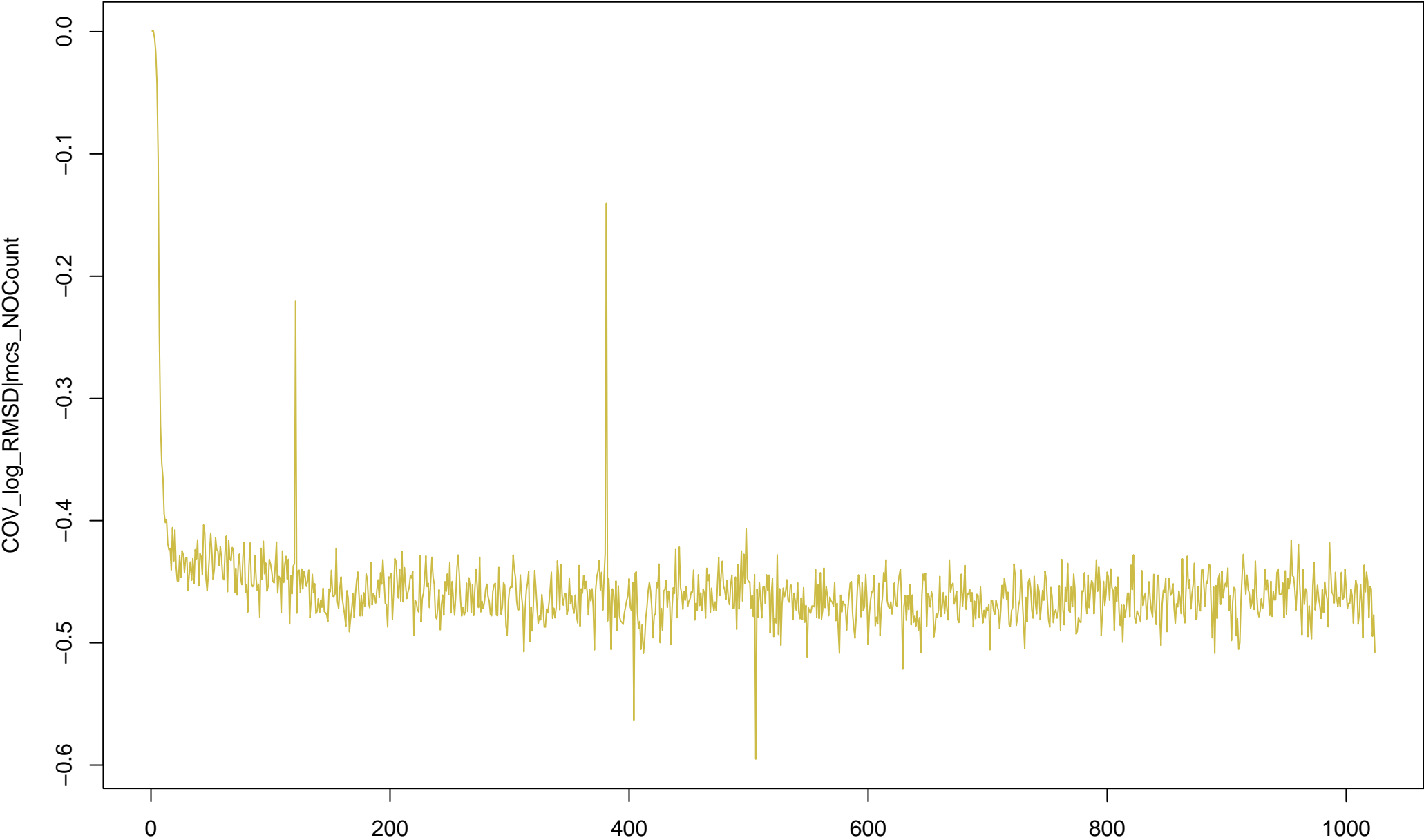
COV_log_RMSD|mcs_RingCount
ESS = 94.4 | BMK = 0.253 | MCSE(6.27) = 10.6 | stat: TRUE | burn: 0



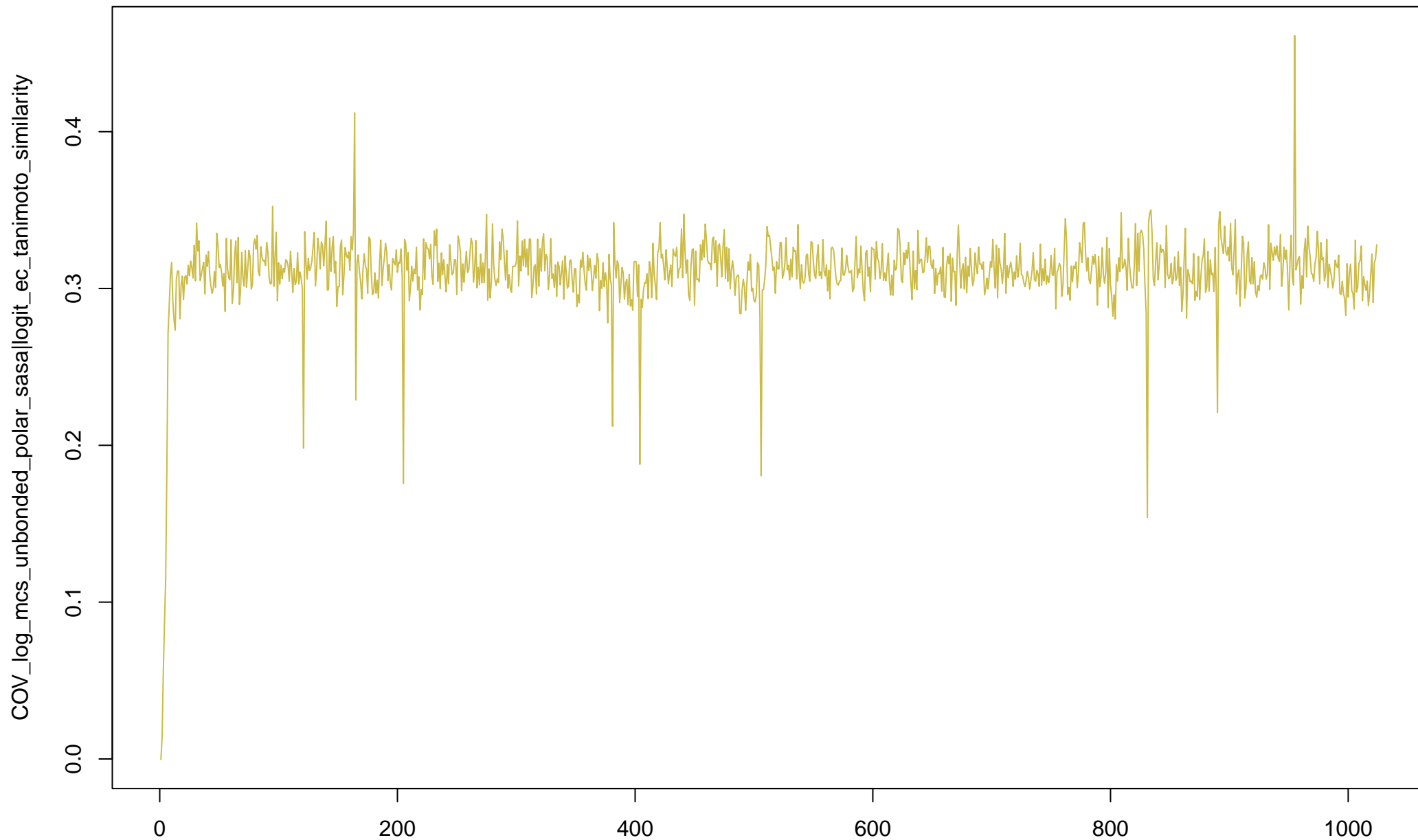
COV_log_RMSD|docked_NumRotatableBonds
ESS = 26 | BMK = 0.375 | MCSE(6.27) = 13.3 | stat: FALSE | burn: 408



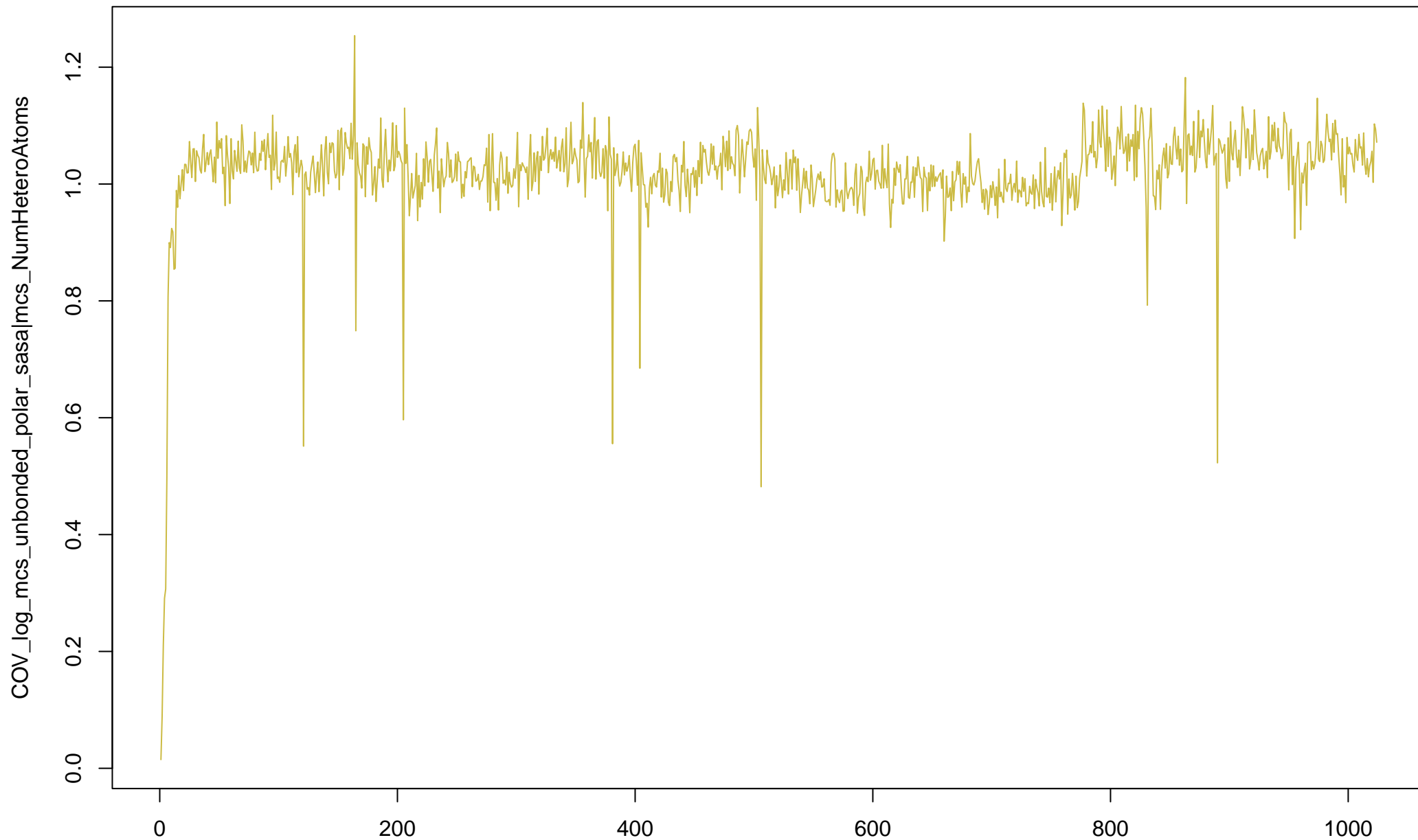
COV_log_RMSD|mcs_NOCount
ESS = 113 | BMK = 0.219 | MCSE(6.27) = 9.96 | stat: FALSE | burn: 0



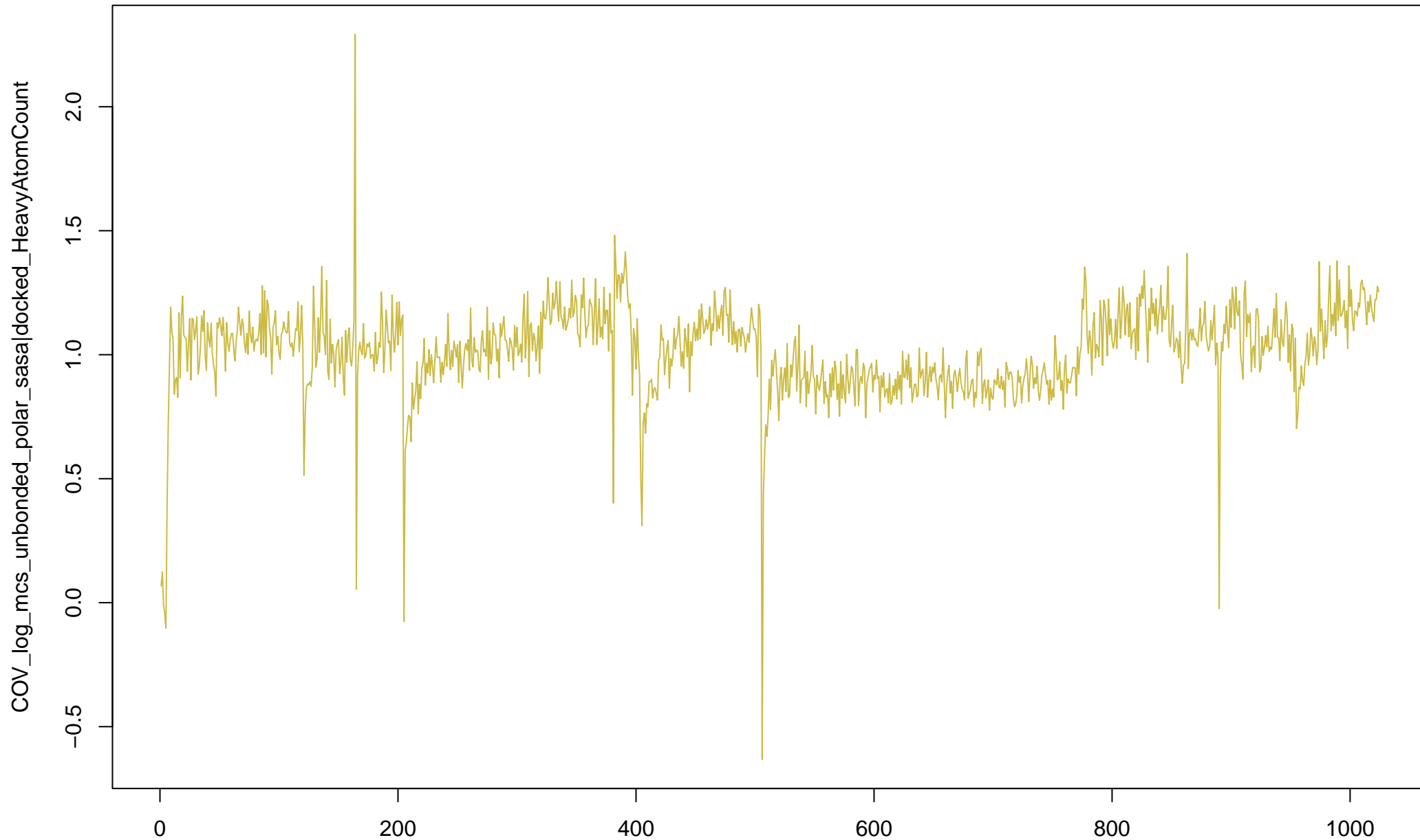
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 251 | BMK = 0.128 | MCSE(6.27) = 6.92 | stat: TRUE | burn: 0



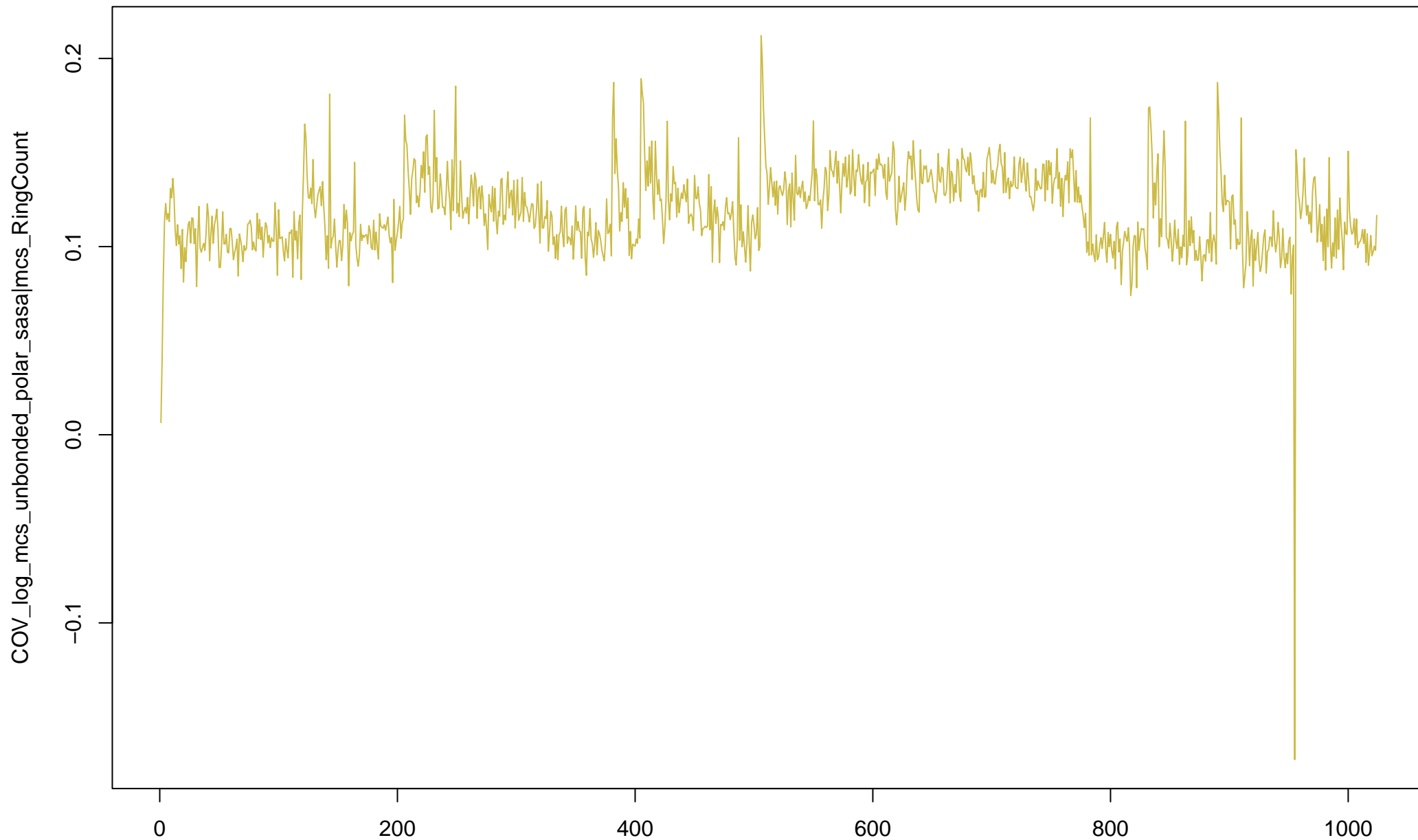
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 161 | BMK = 0.182 | MCSE(6.27) = 8.22 | stat: TRUE | burn: 0



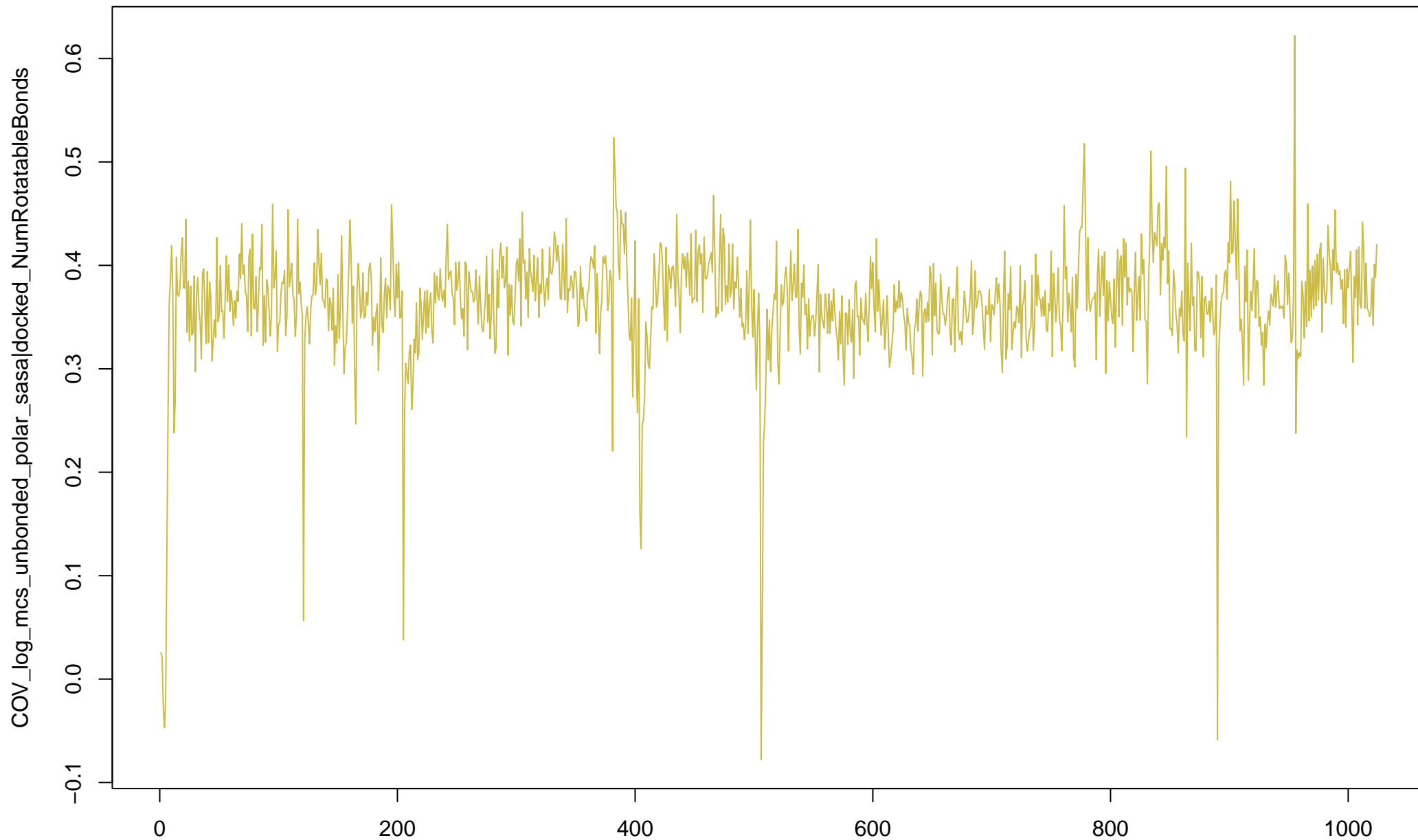
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 113 | BMK = 0.25 | MCSE(6.27) = 9.72 | stat: TRUE | burn: 510



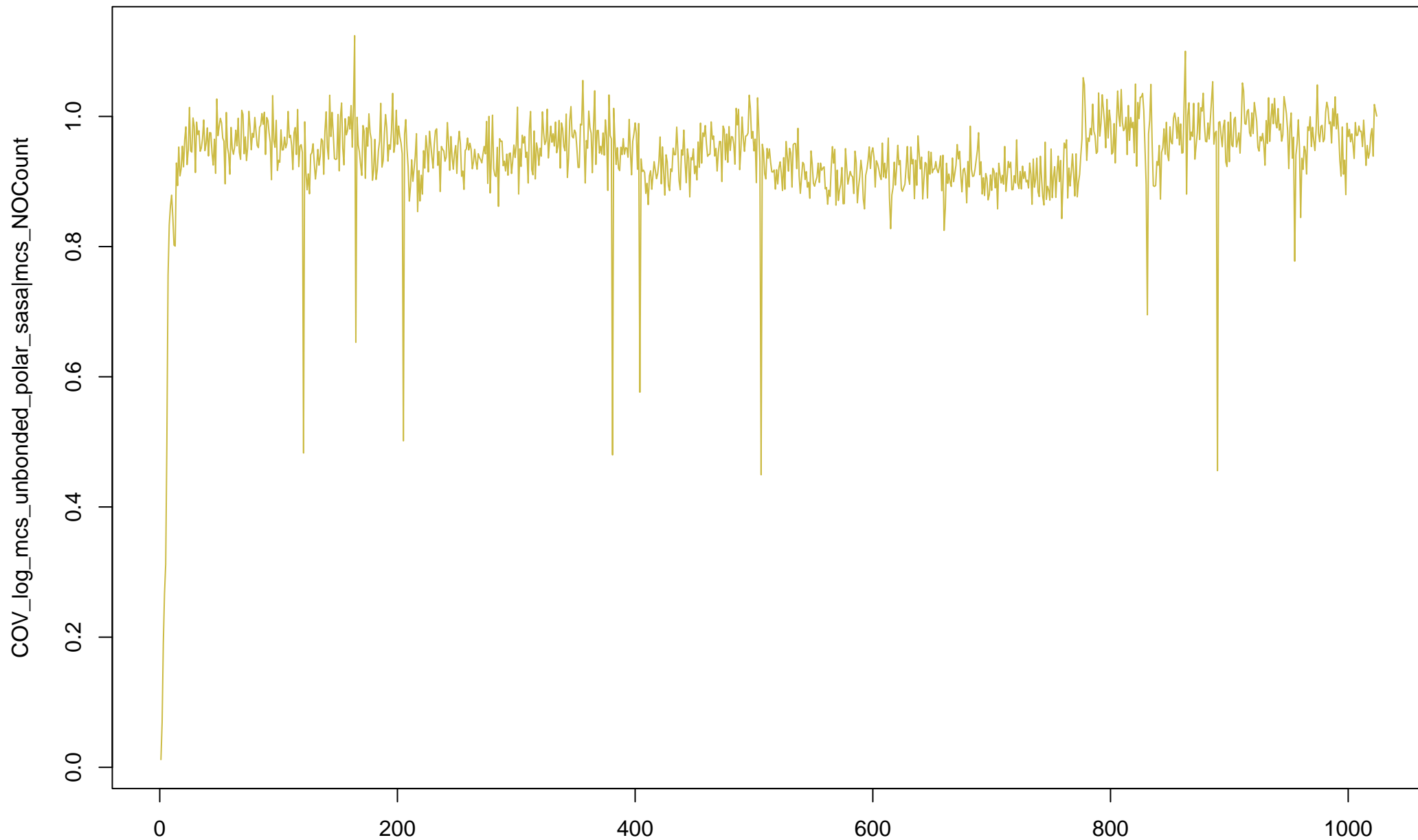
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 47.5 | BMK = 0.226 | MCSE(6.27) = 10.2 | stat: FALSE | burn: 0



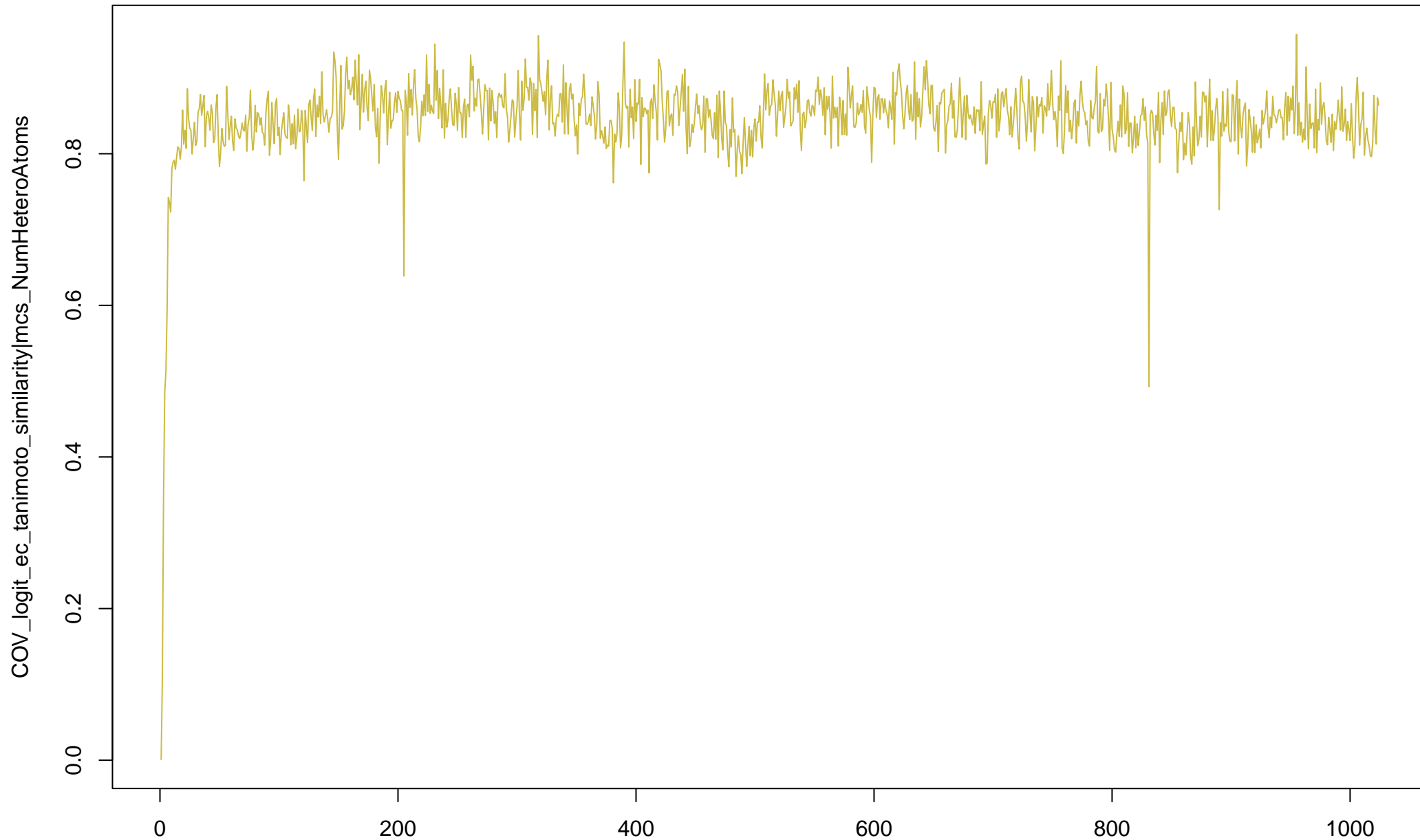
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 202 | BMK = 0.165 | MCSE(6.27) = 6.85 | stat: TRUE | burn: 0



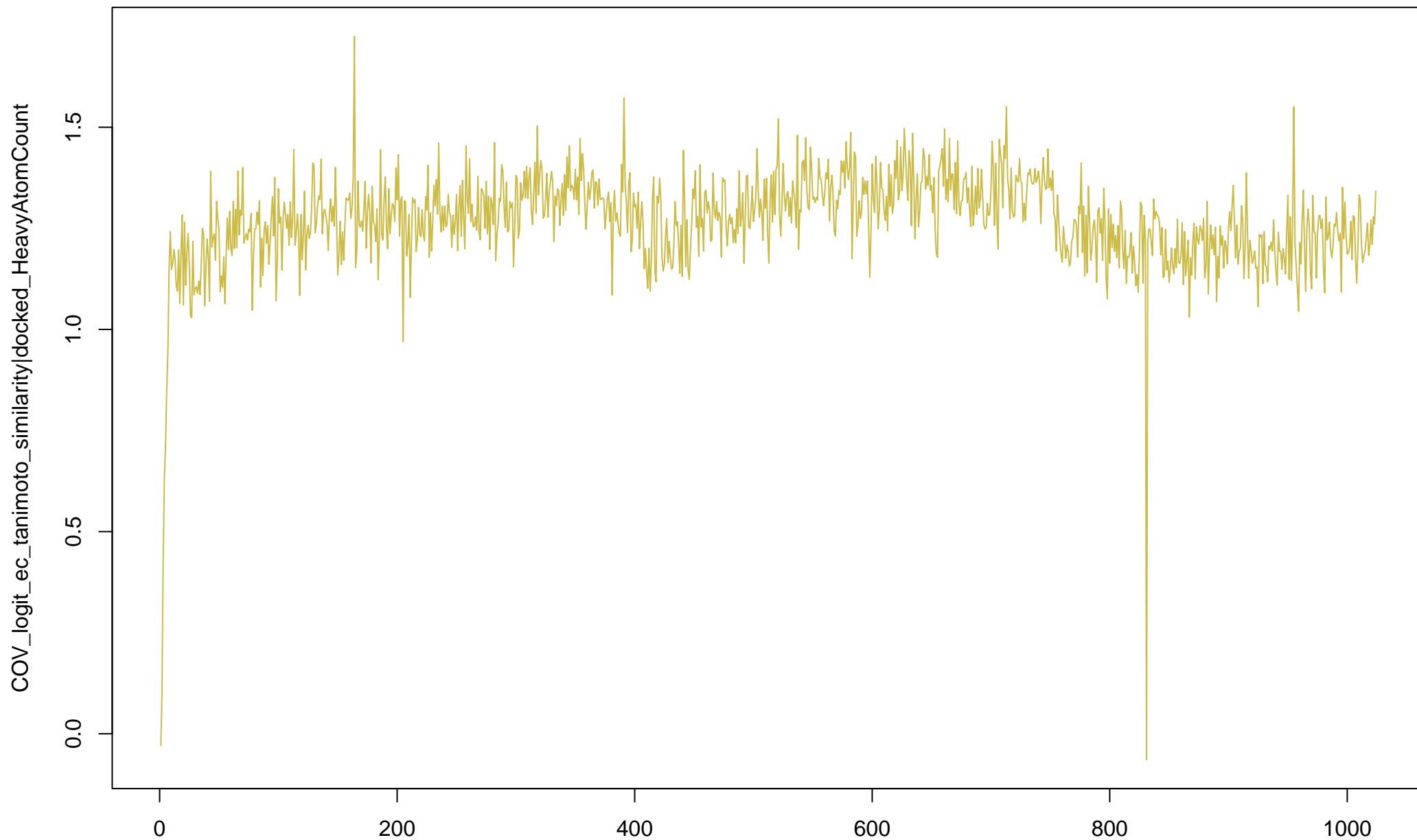
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 162 | BMK = 0.196 | MCSE(6.27) = 8.16 | stat: TRUE | burn: 0



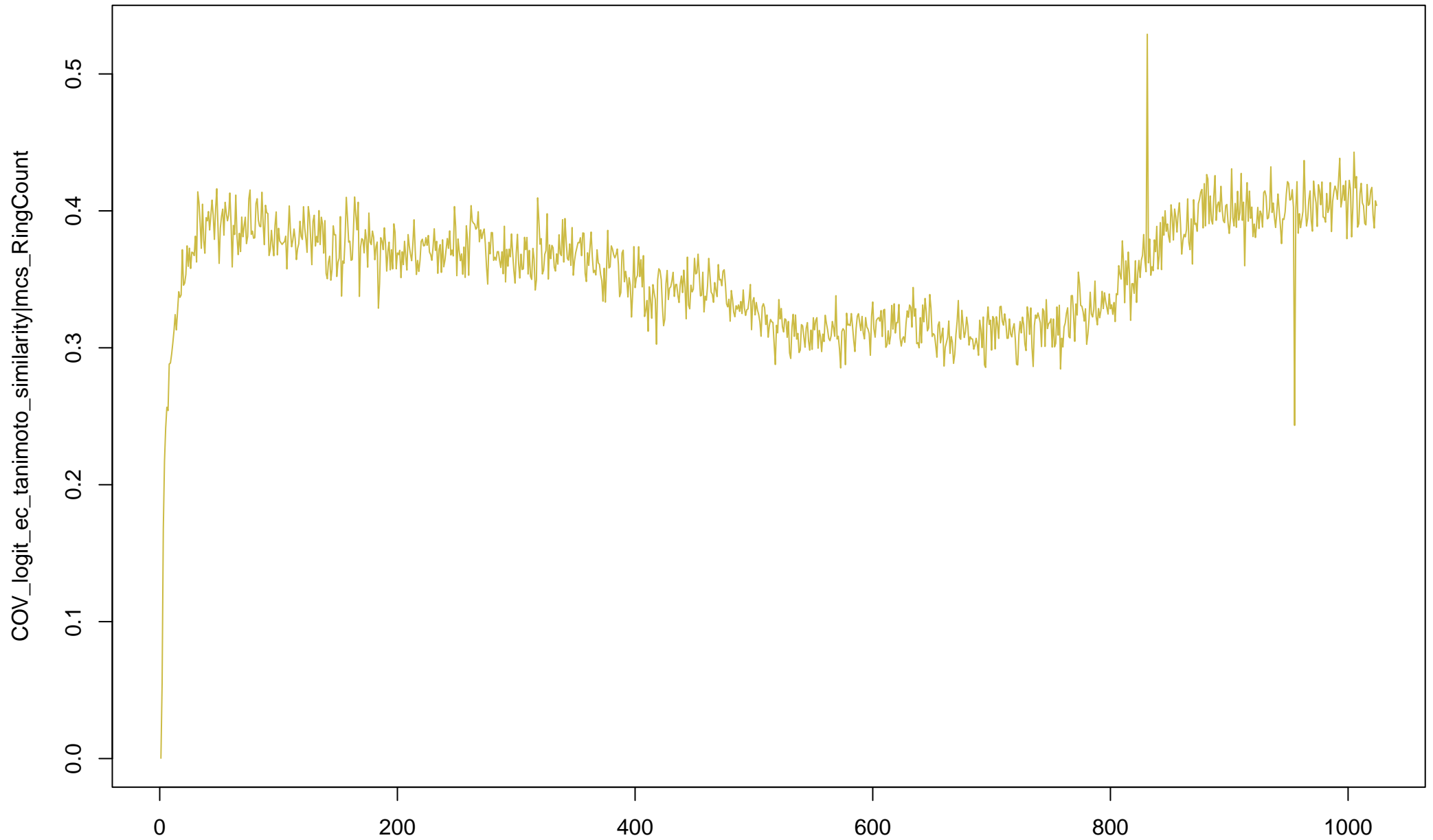
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 167 | BMK = 0.118 | MCSE(6.27) = 8.6 | stat: TRUE | burn: 0



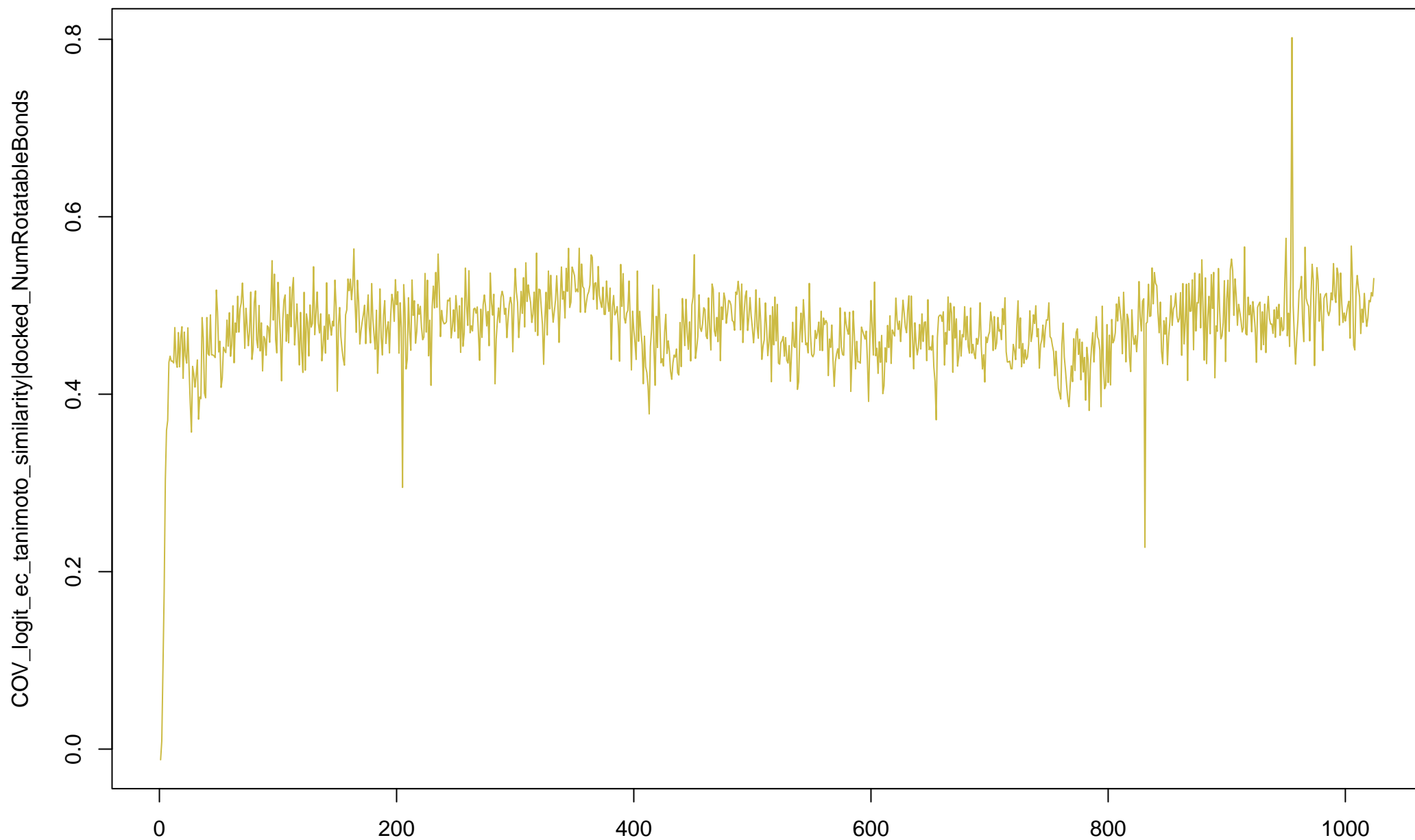
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 51.1 | BMK = 0.136 | MCSE(6.27) = 10.6 | stat: FALSE | burn: 0



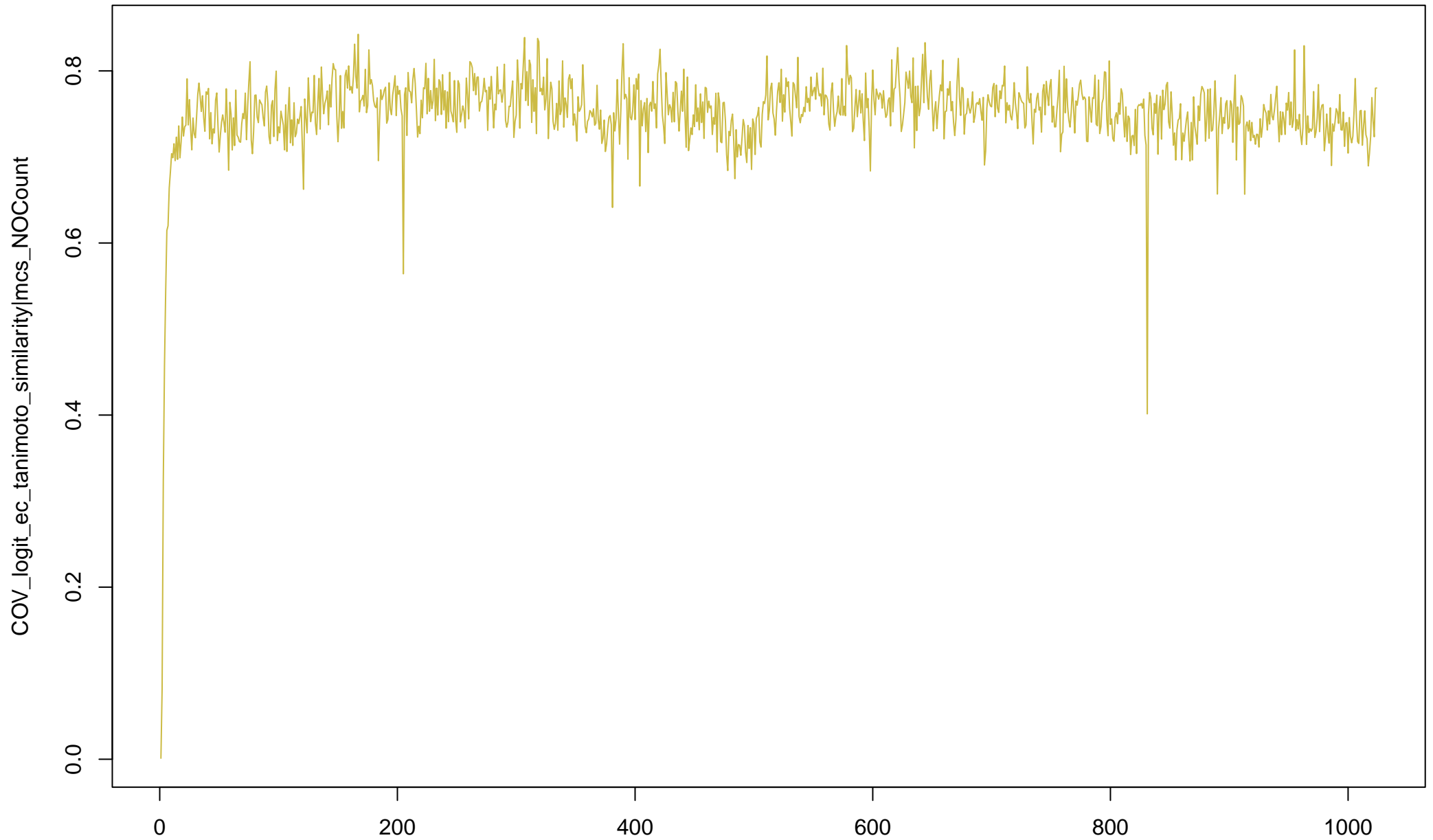
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 10.8 | BMK = 0.459 | MCSE(6.27) = 15 | stat: TRUE | burn: 816



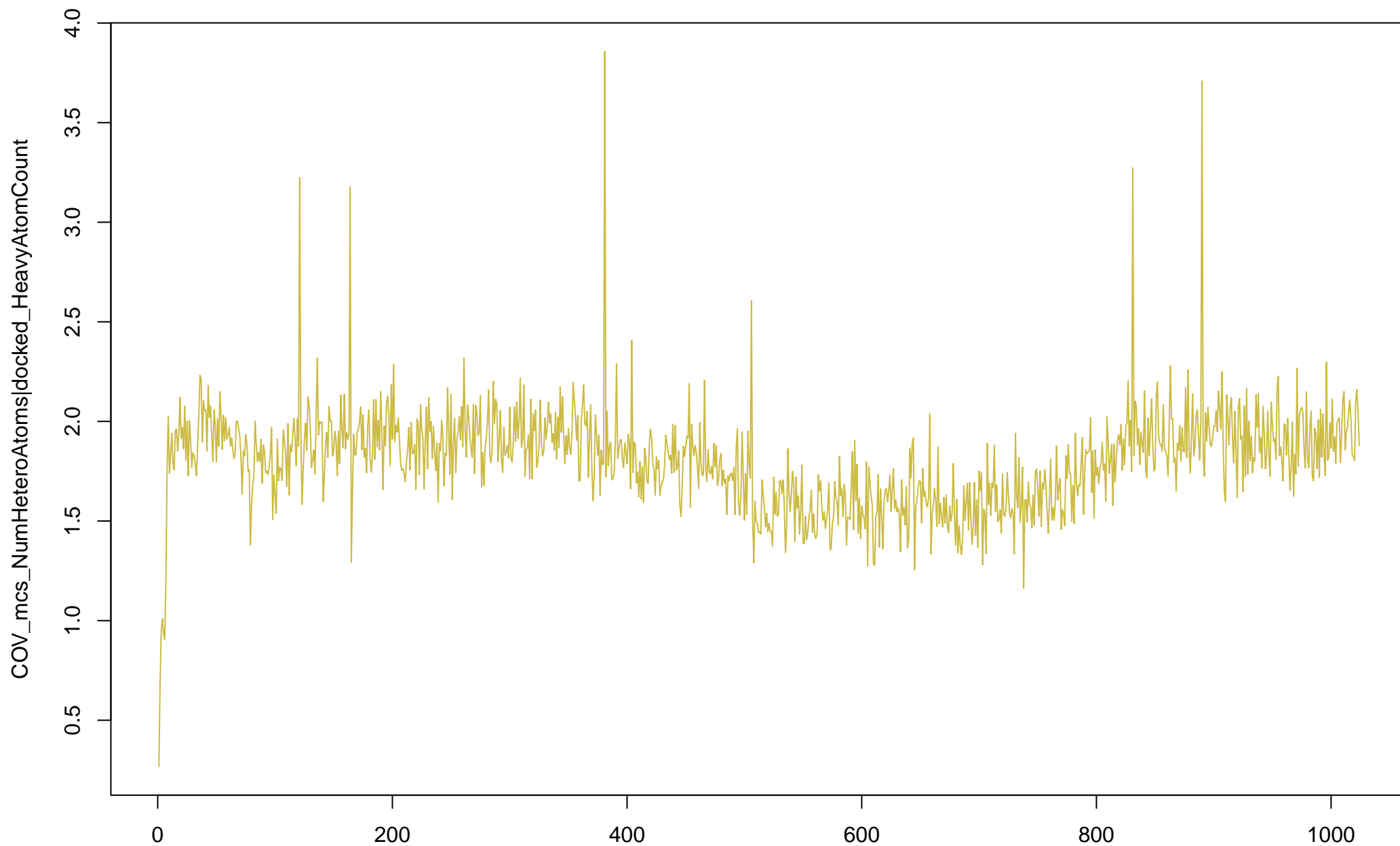
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 91.7 | BMK = 0.139 | MCSE(6.27) = 9.79 | stat: TRUE | burn: 0



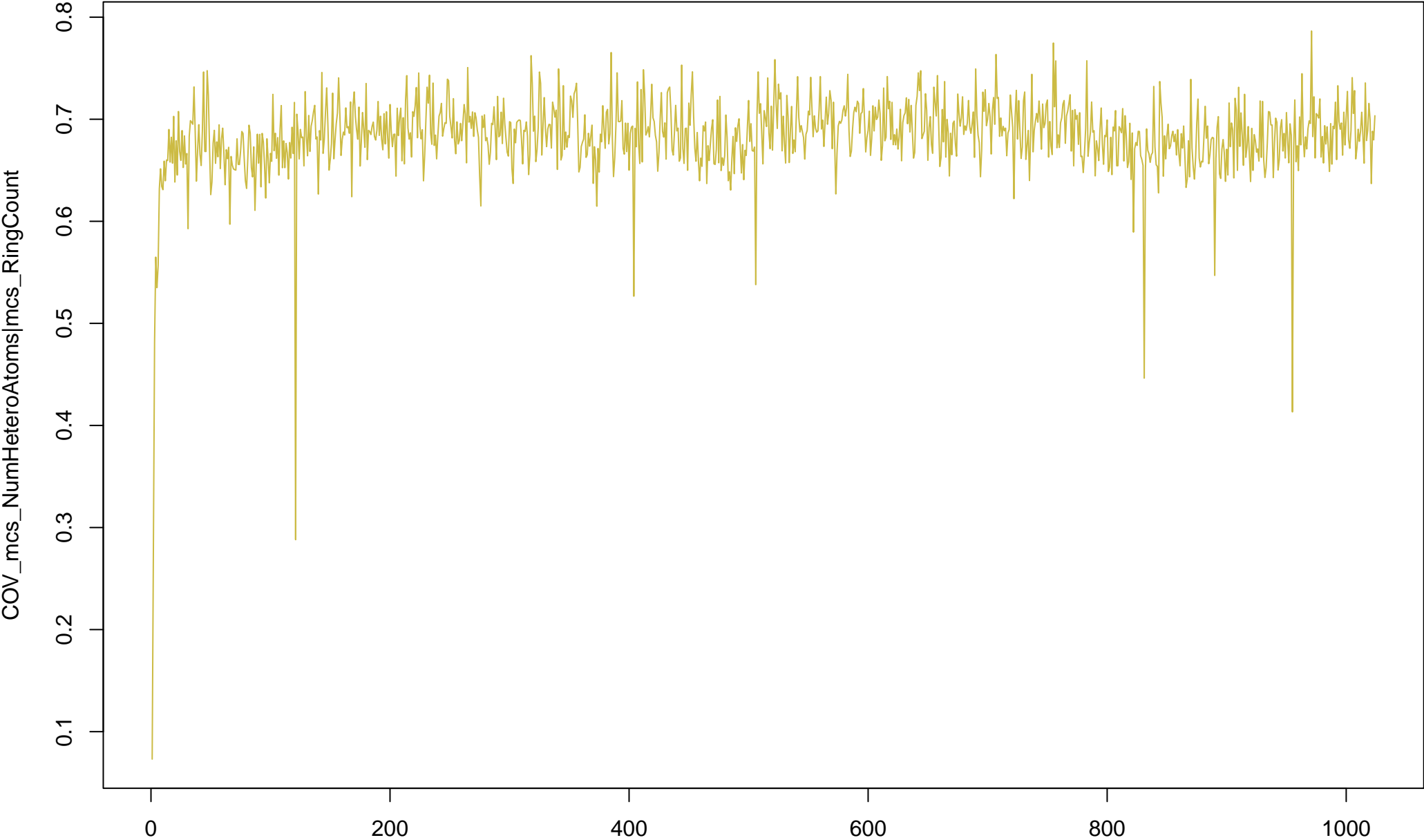
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 196 | BMK = 0.125 | MCSE(6.27) = 8.39 | stat: TRUE | burn: 0



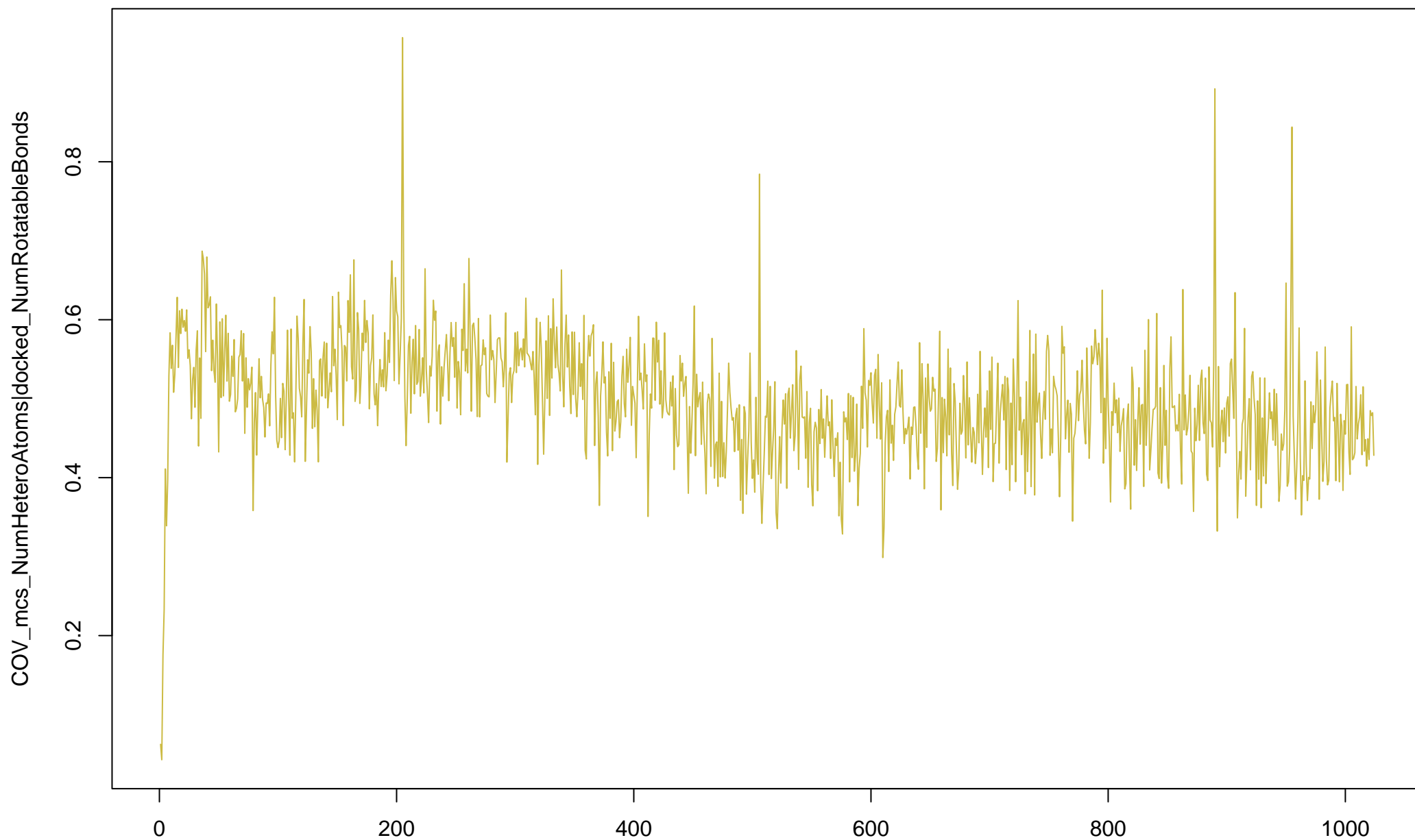
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 31.8 | BMK = 0.309 | MCSE(6.27) = 11 | stat: TRUE | burn: 816



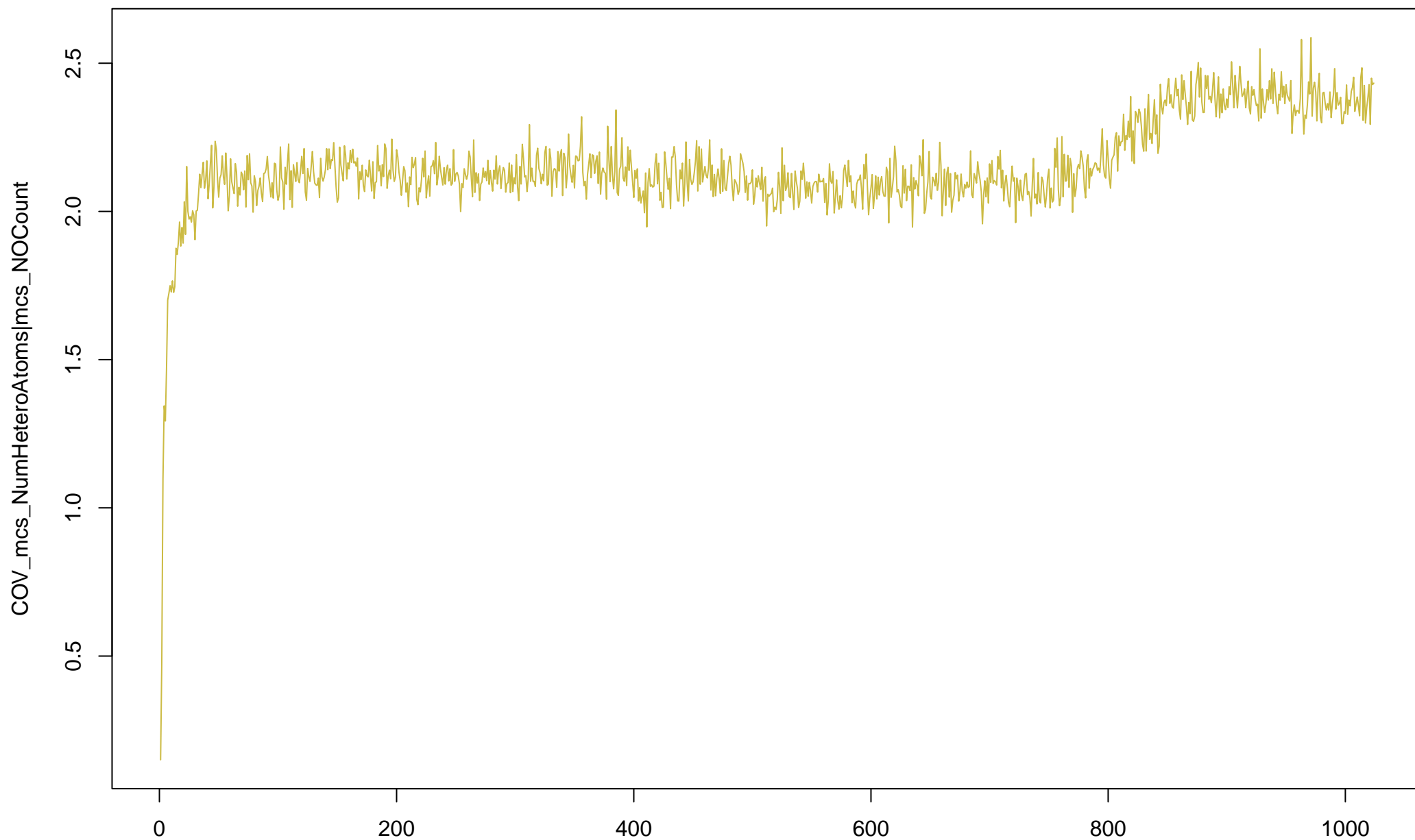
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 188 | BMK = 0.127 | MCSE(6.27) = 7.35 | stat: FALSE | burn: 0



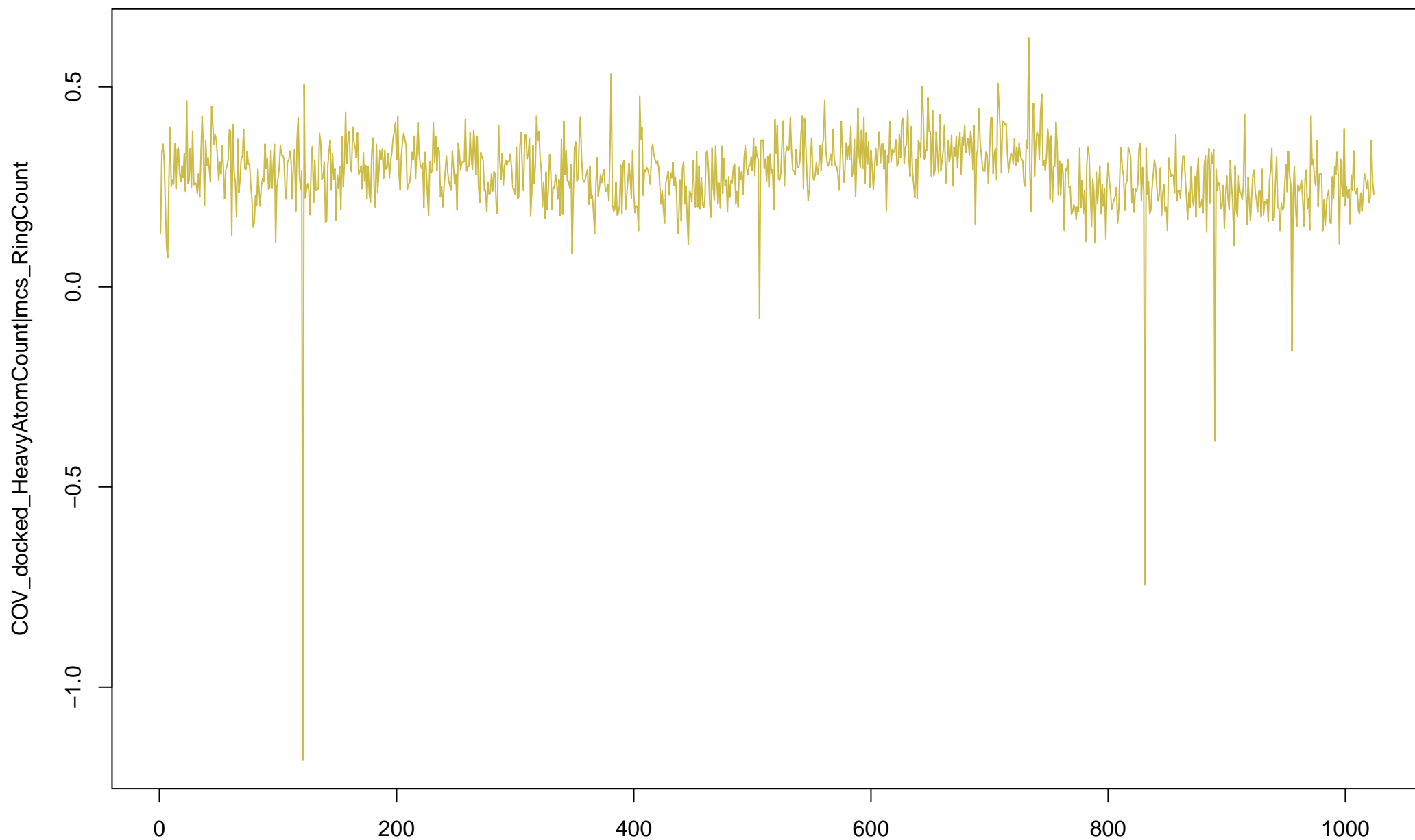
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 27.2 | BMK = 0.325 | MCSE(6.27) = 8.82 | stat: FALSE | burn: 0



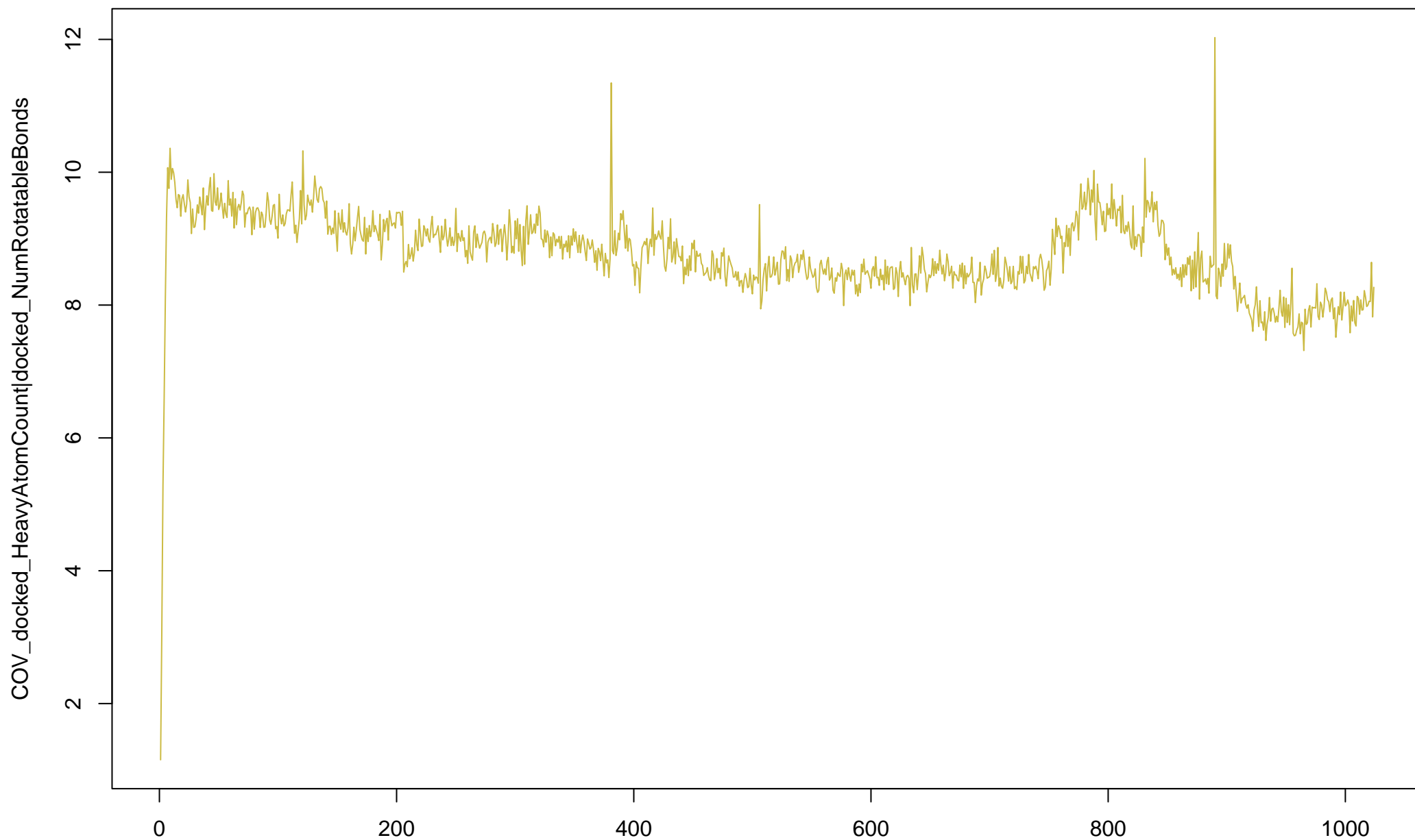
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 18.6 | BMK = 0.457 | MCSE(6.27) = 14.6 | stat: FALSE | burn: 816



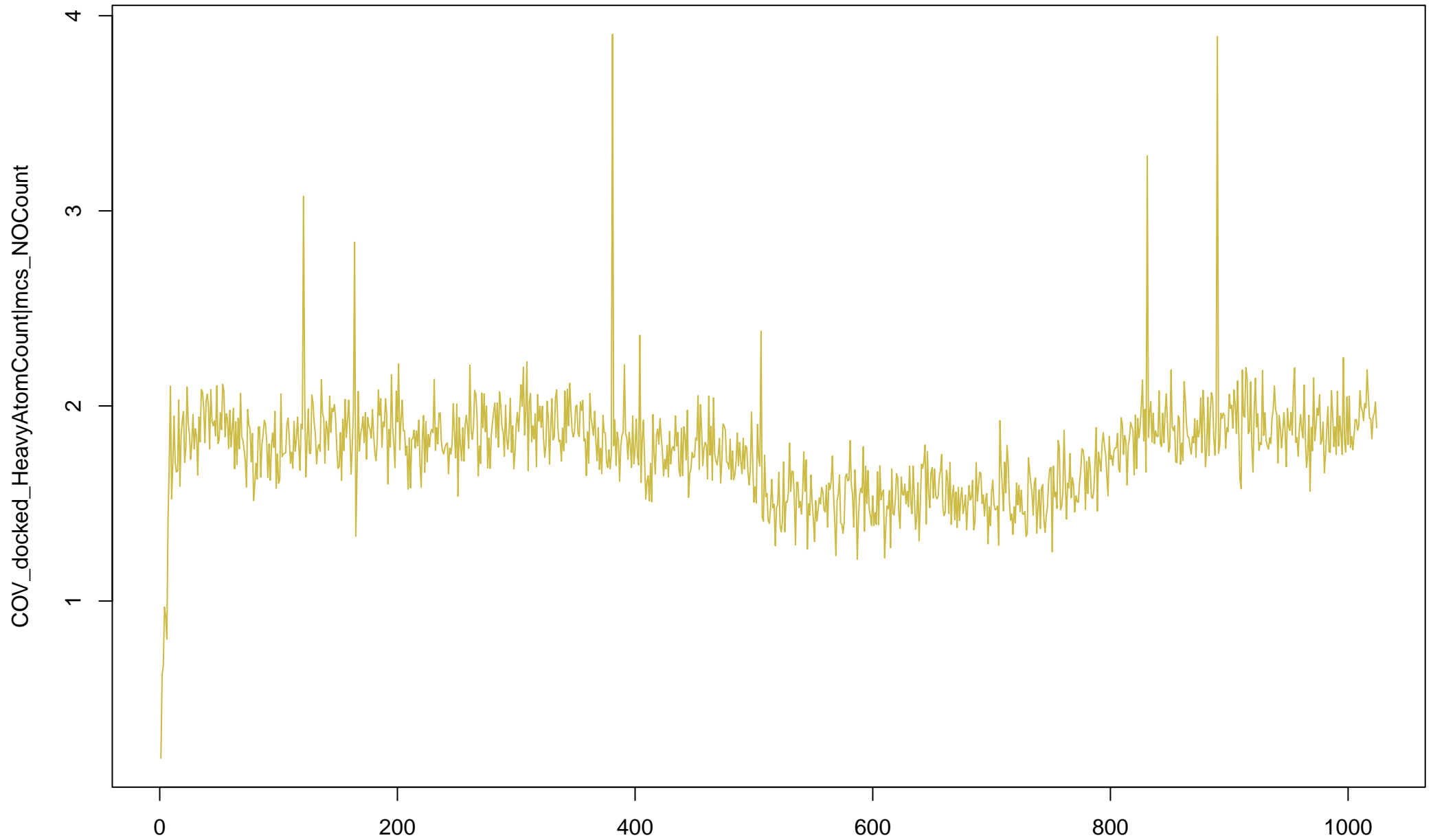
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 120 | BMK = 0.104 | MCSE(6.27) = 7.28 | stat: TRUE | burn: 0



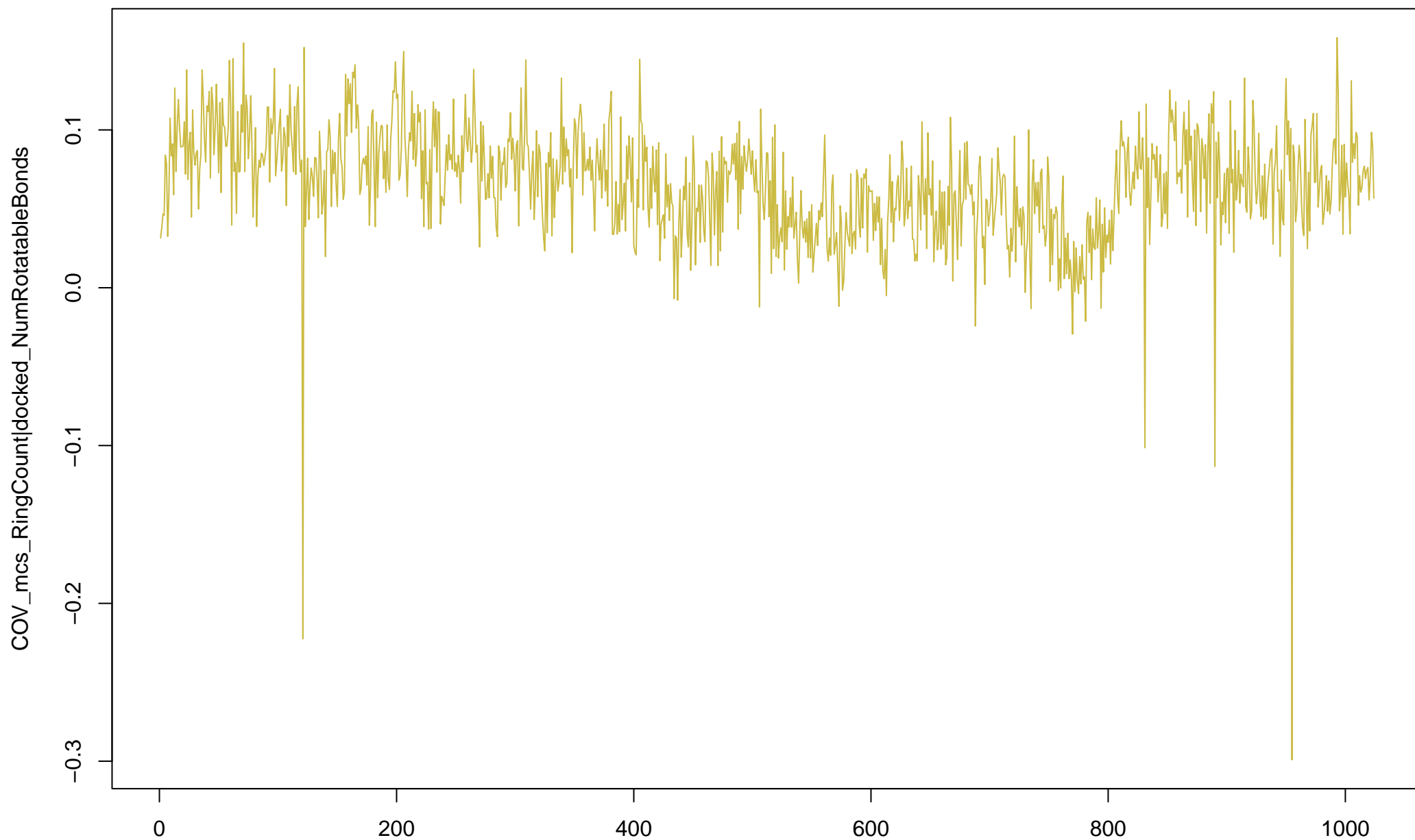
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 26.1 | BMK = 0.454 | MCSE(6.27) = 12.7 | stat: FALSE | burn: 1020



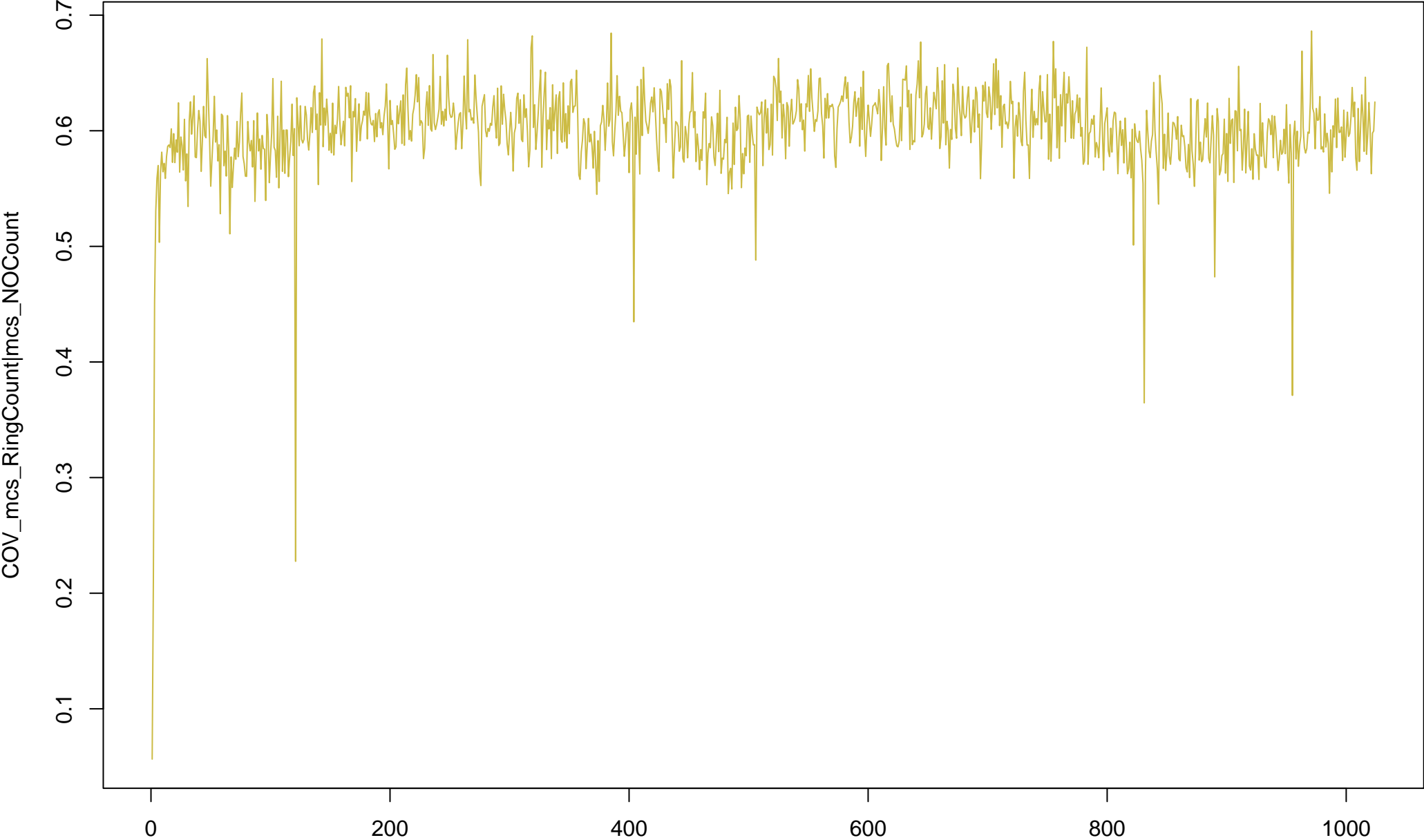
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 20.5 | BMK = 0.333 | MCSE(6.27) = 11.5 | stat: TRUE | burn: 816



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 48.5 | BMK = 0.278 | MCSE(6.27) = 9.54 | stat: FALSE | burn: 0



COV_mcs_RingCount|mcs_NOCount
ESS = 160 | BMK = 0.109 | MCSE(6.27) = 7.63 | stat: FALSE | burn: 0



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 34.3 | BMK = 0.332 | MCSE(6.27) = 8.58 | stat: FALSE | burn: 0

