

-- STATS maxD --

min ESS = 11.0585417124343

max BMK = 1

max MCSE = 20.5001570529442

all stationary: FALSE

burn: 100

-- STATS 2D --

min ESS = 11.8076162974727

max BMK = 0.574242311047674

max MCSE = 21.7144348712996

all stationary: FALSE

burn: 100

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.446055909291218

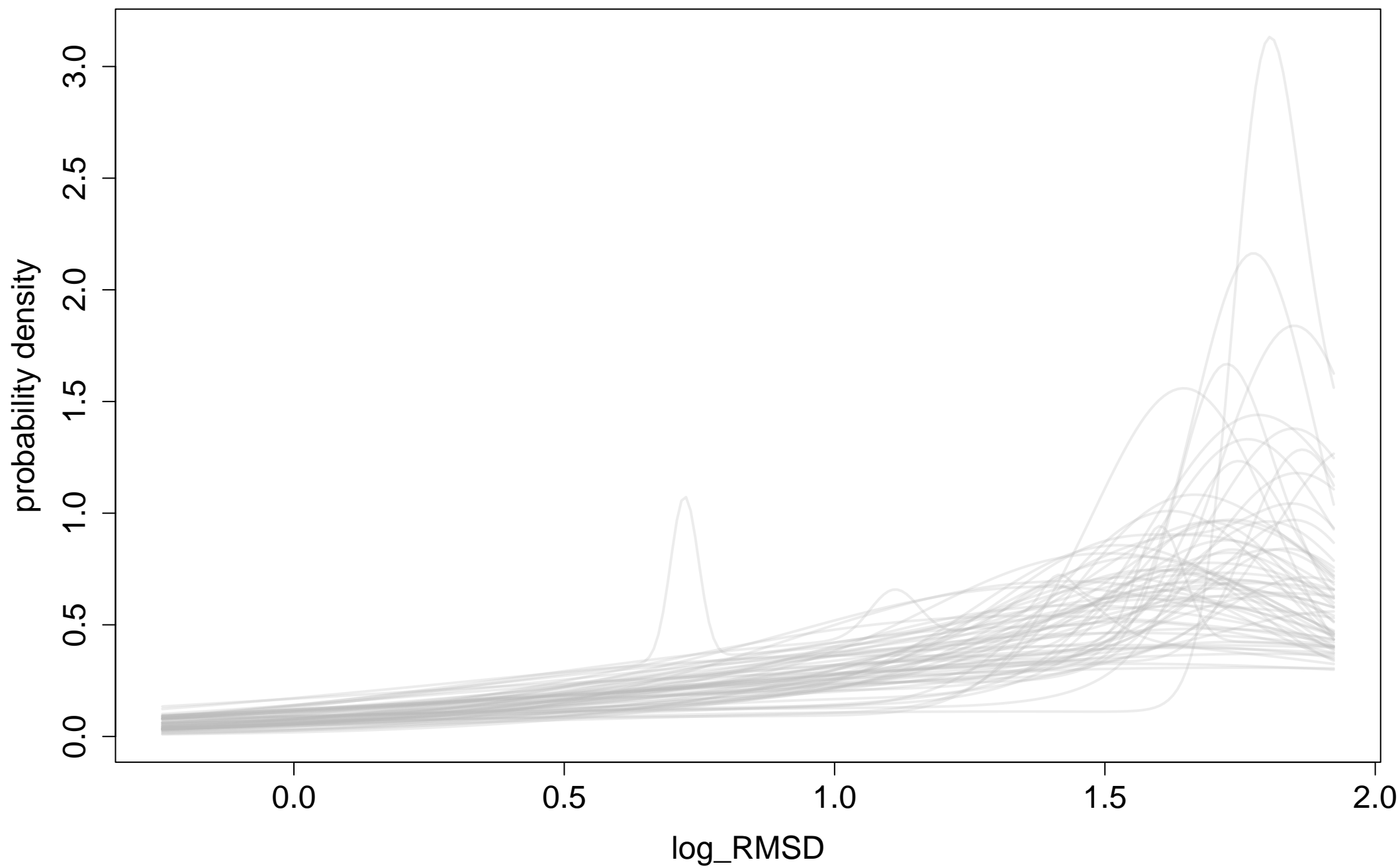
max MCSE = NaN

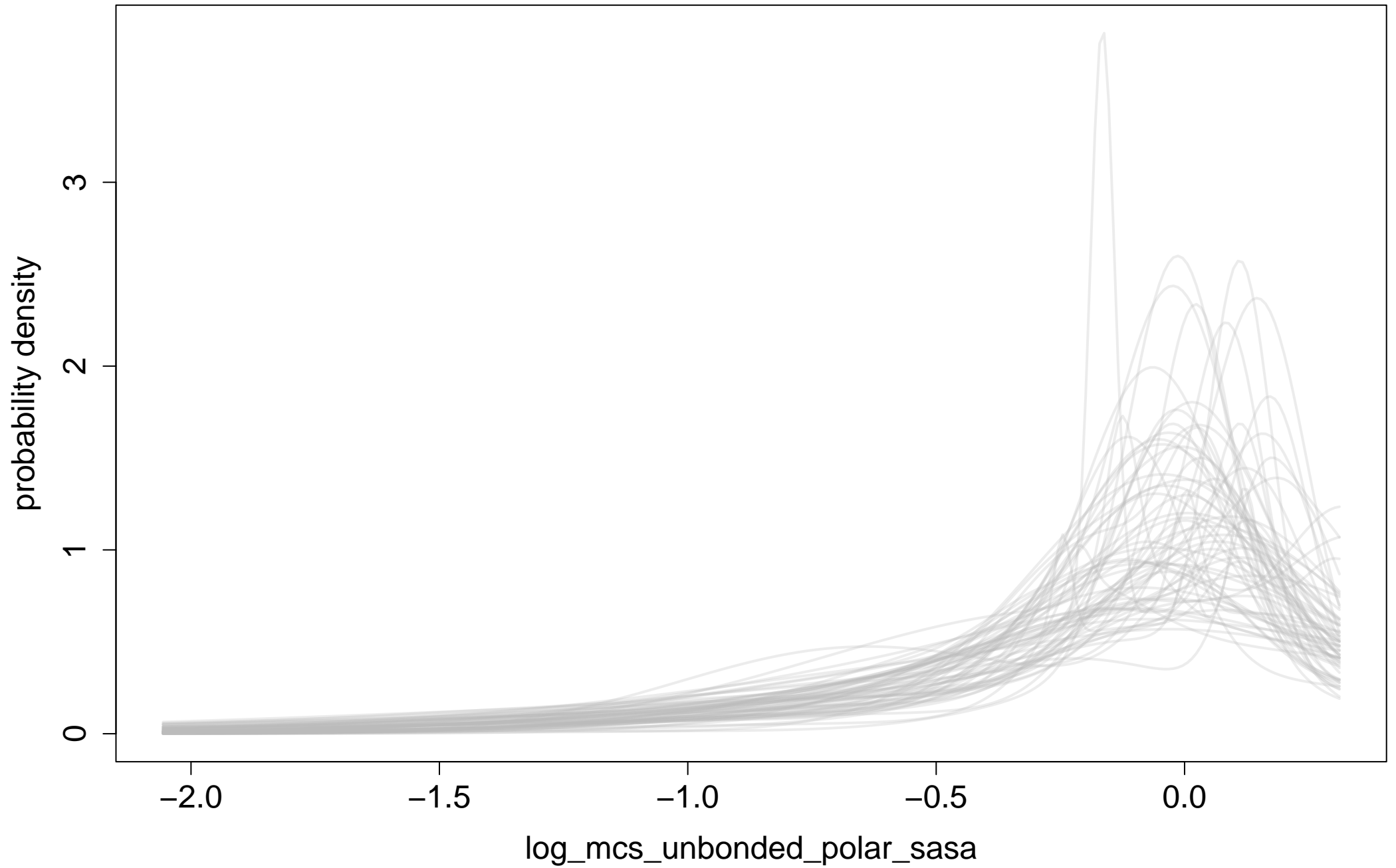
all stationary: FALSE

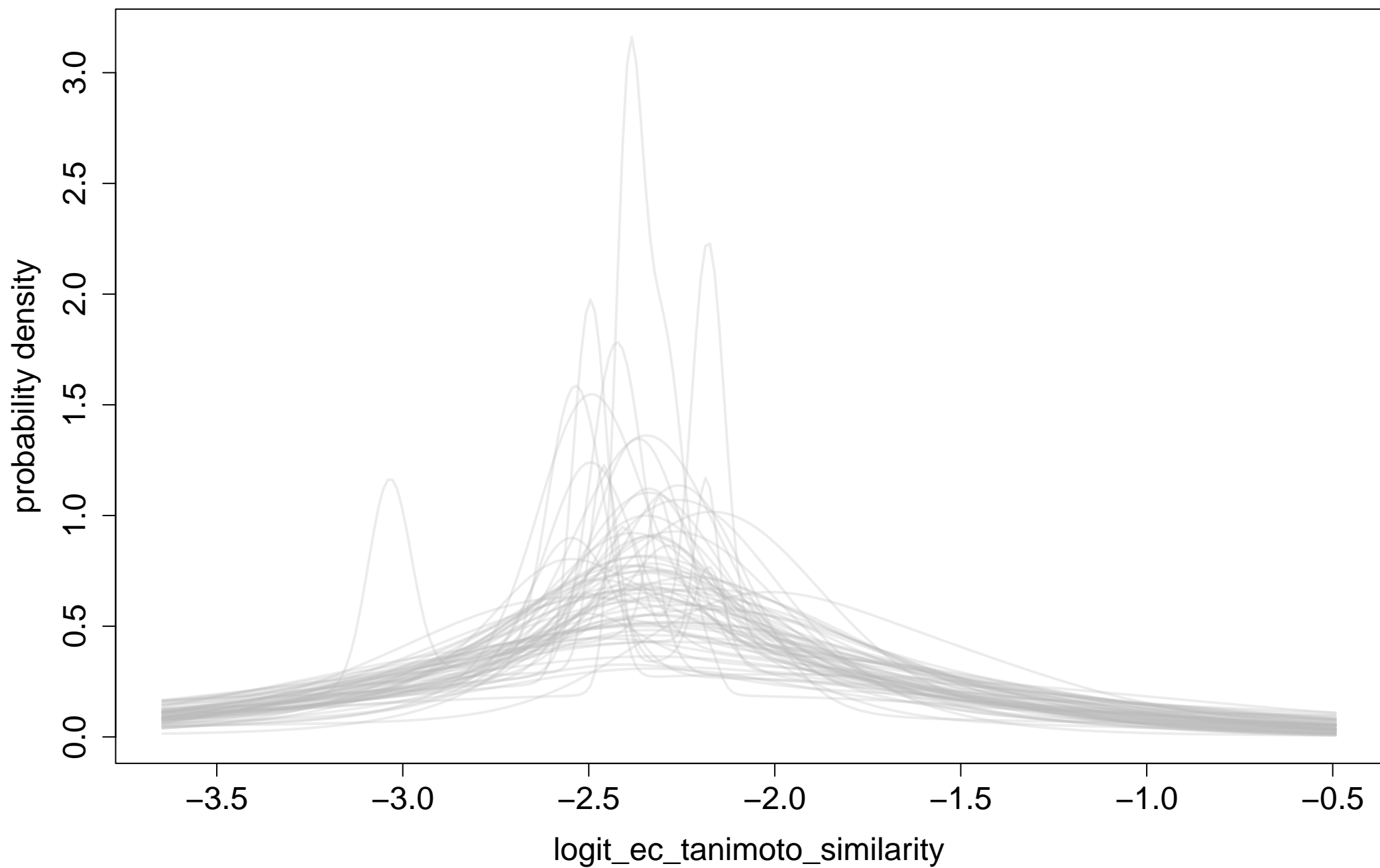
burn: 100

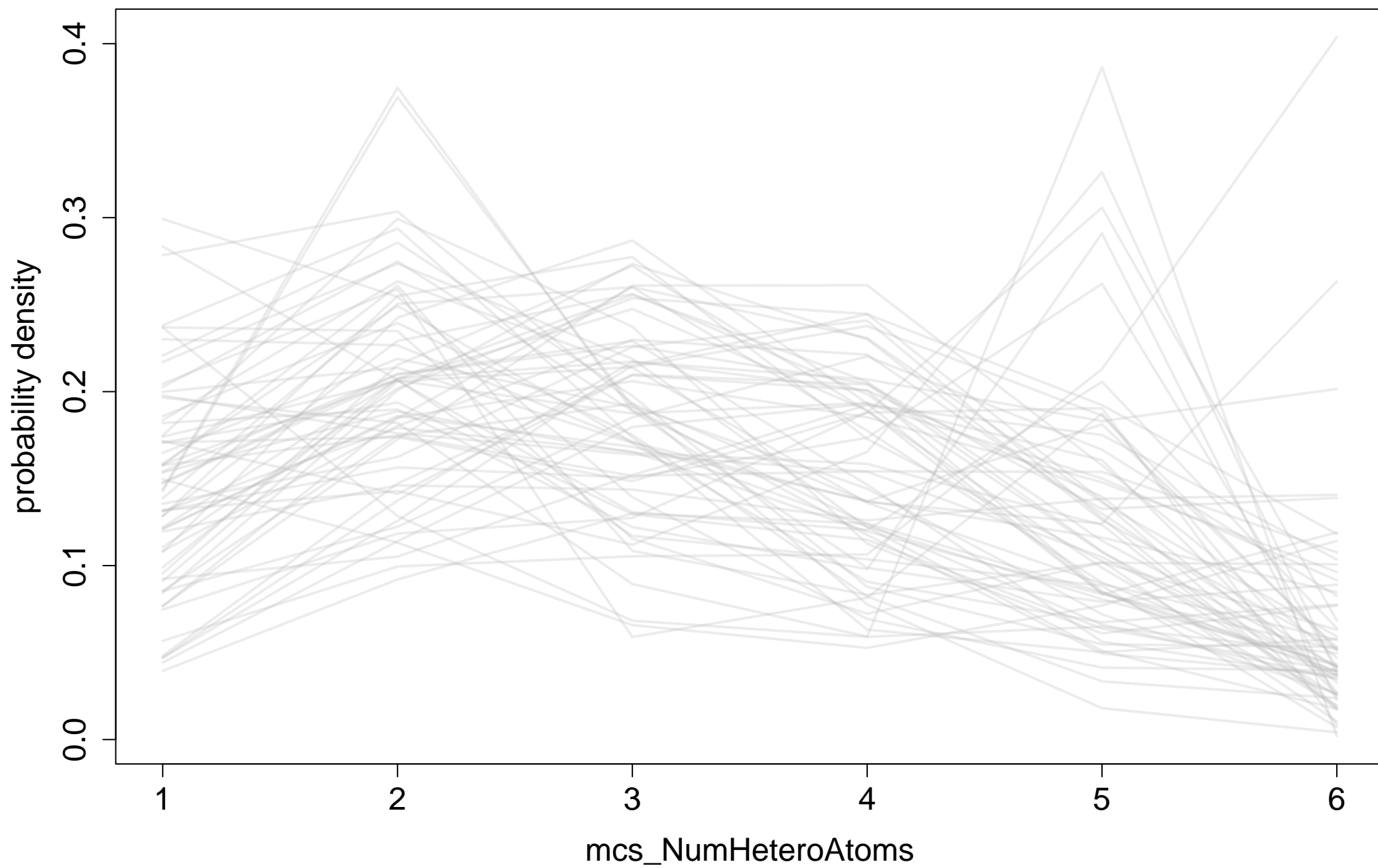
Occupied clusters: 4 of 4

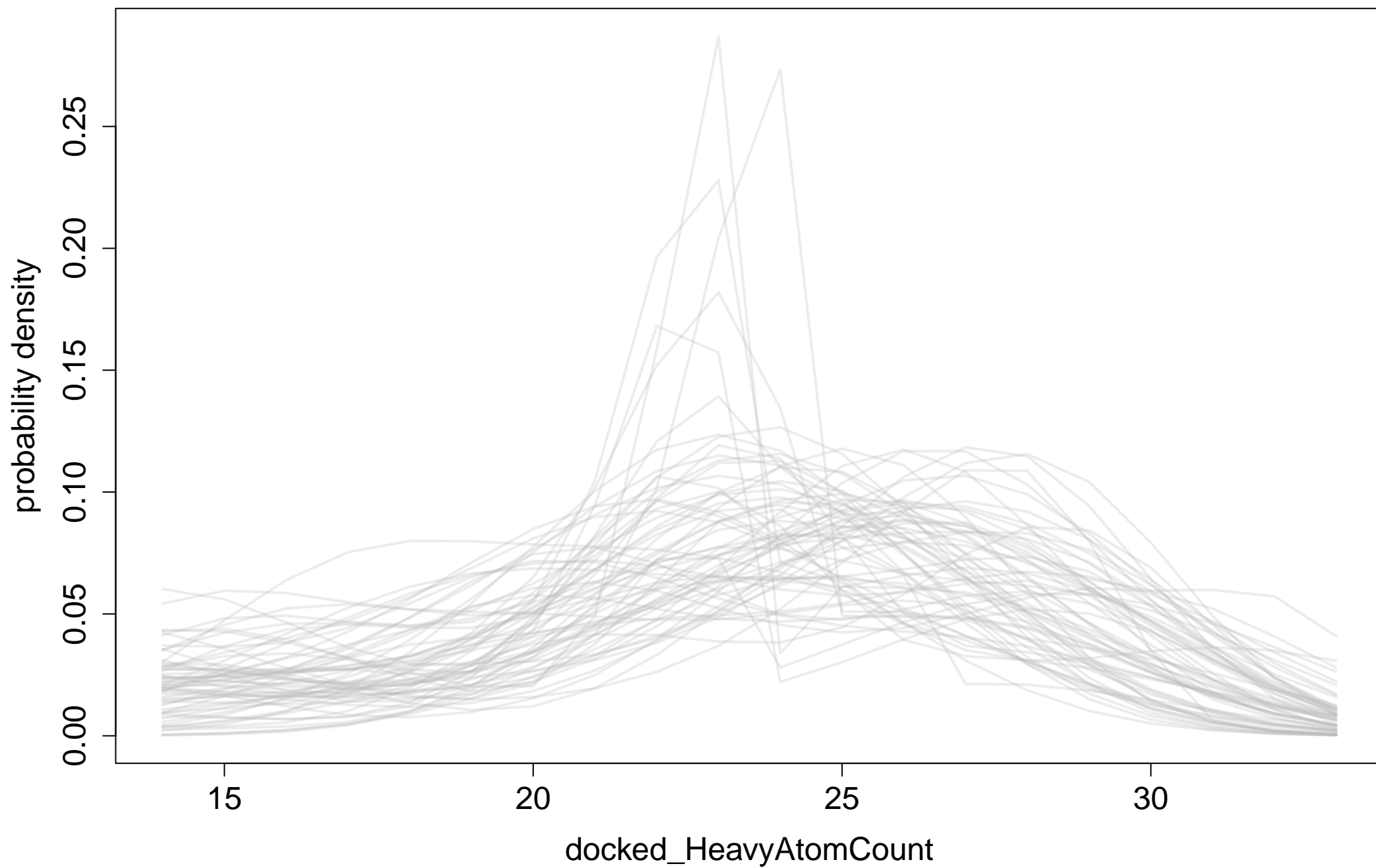
LL: -115 +- 12.4

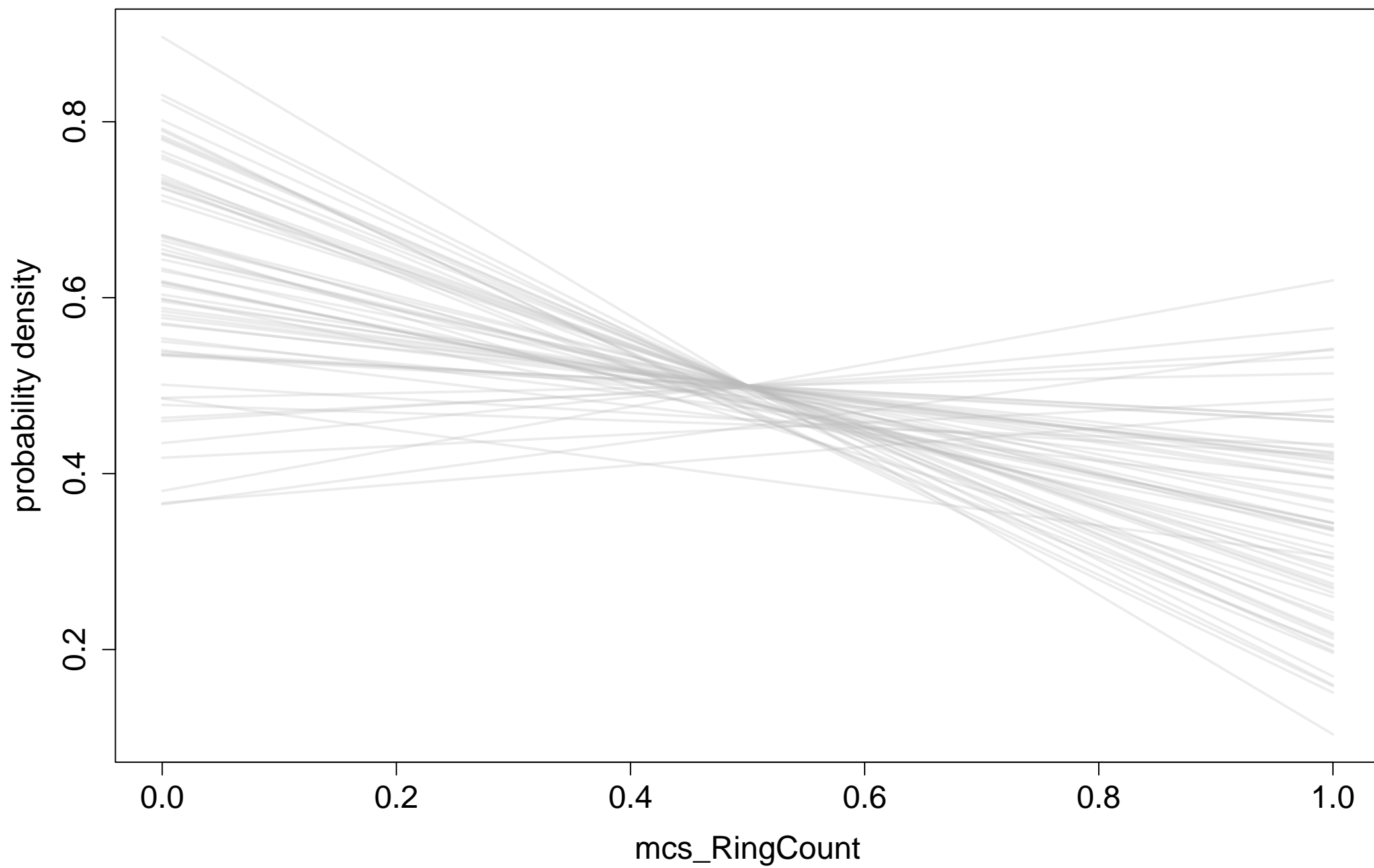


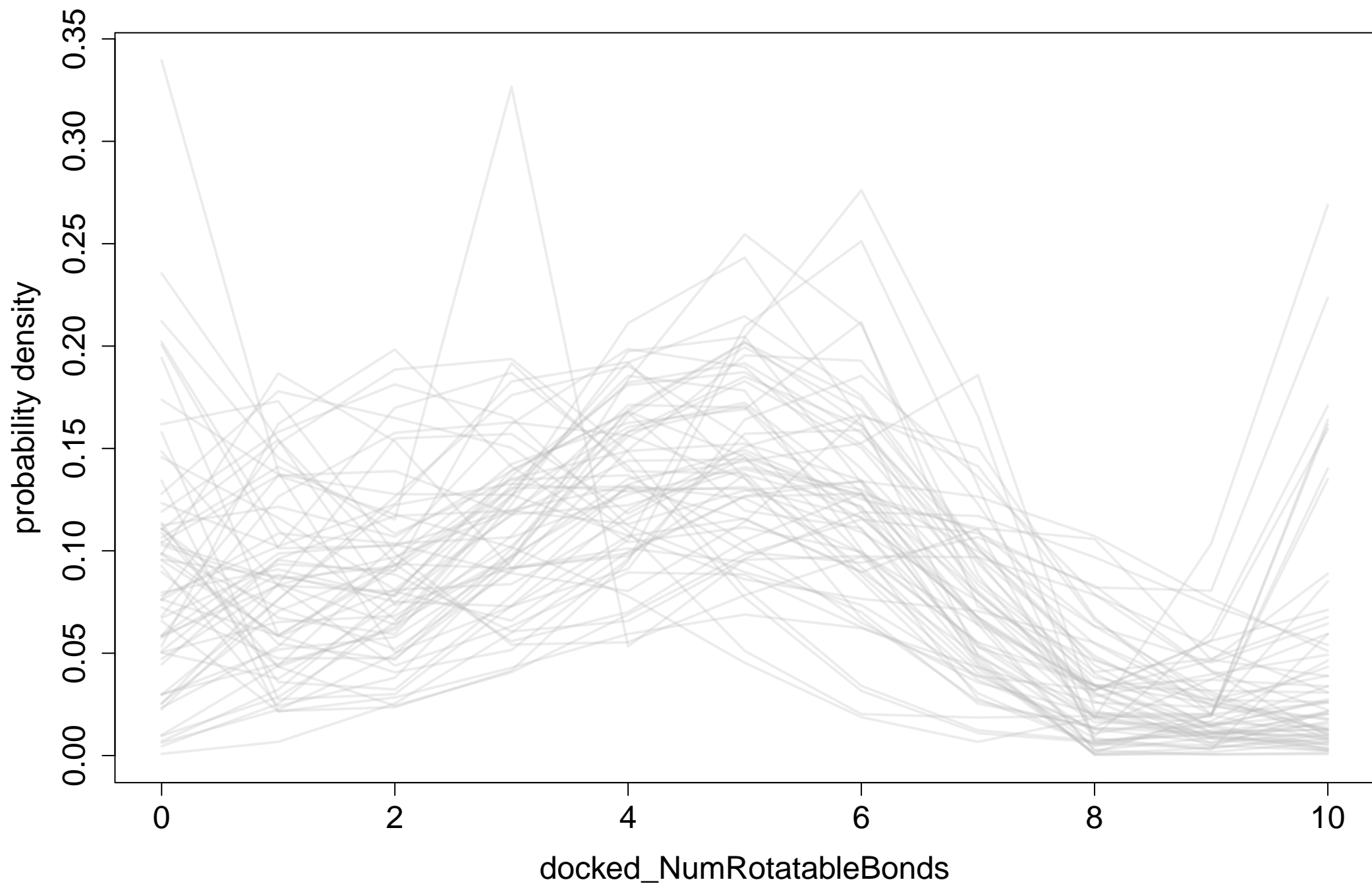


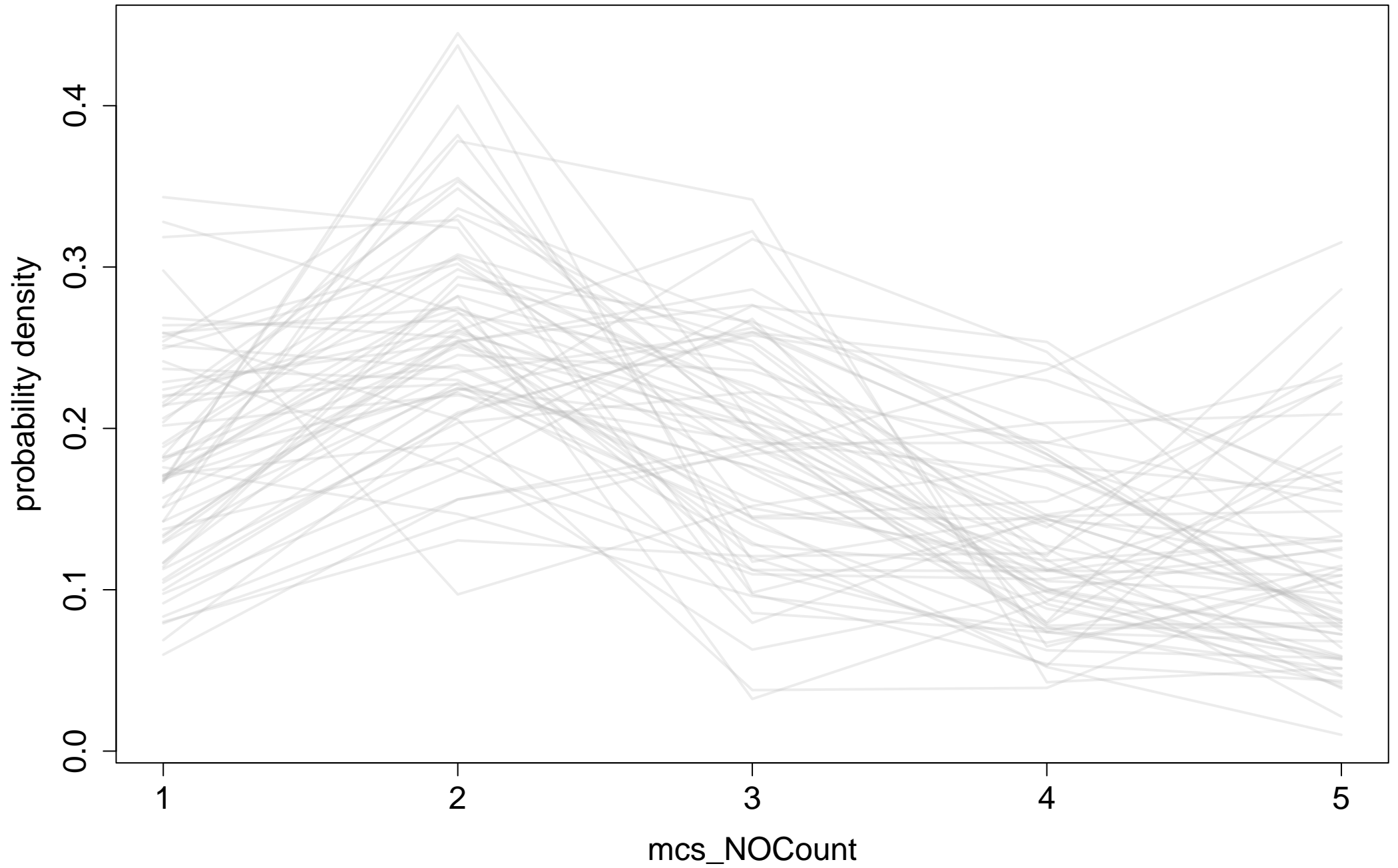


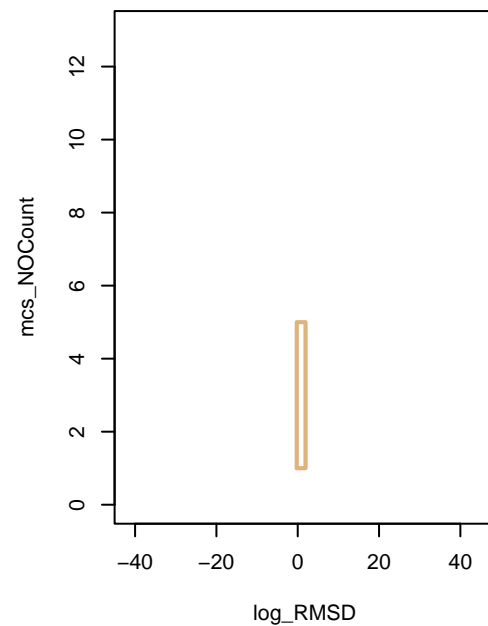
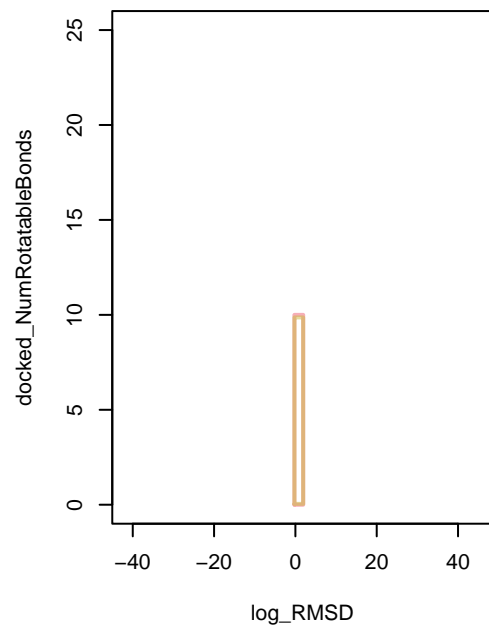
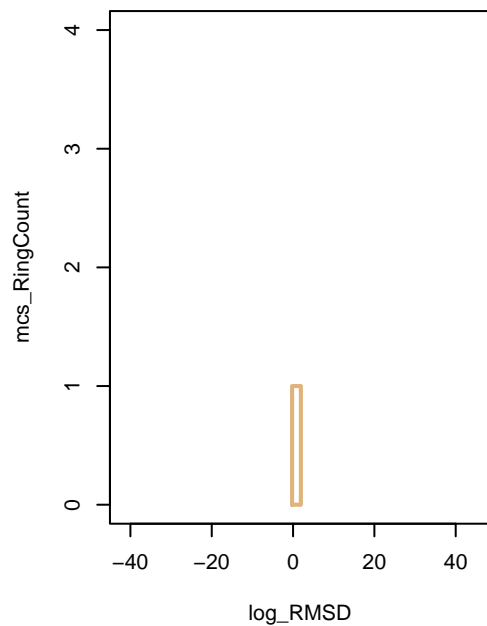
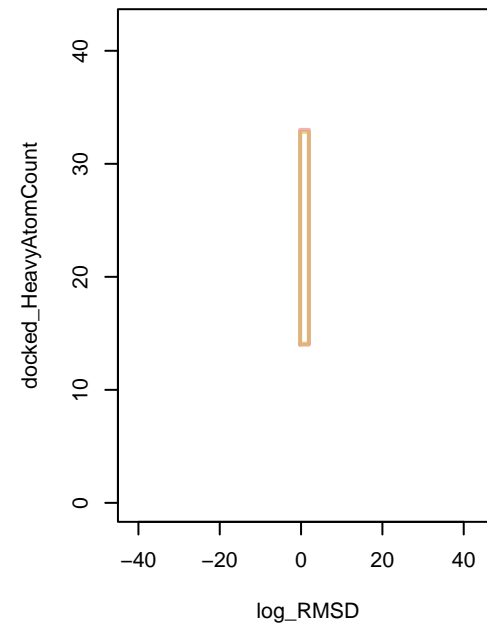
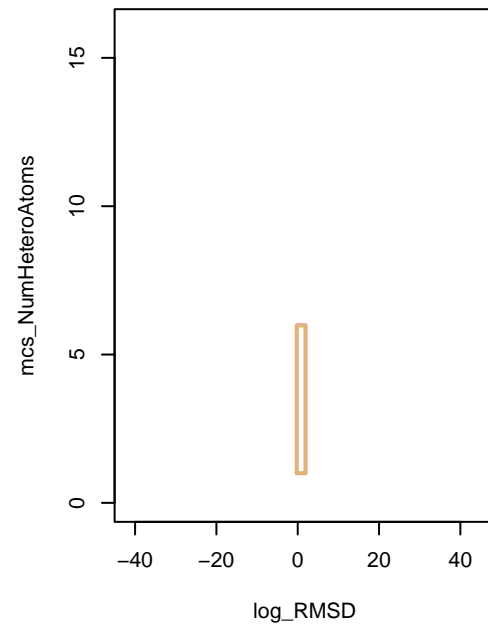
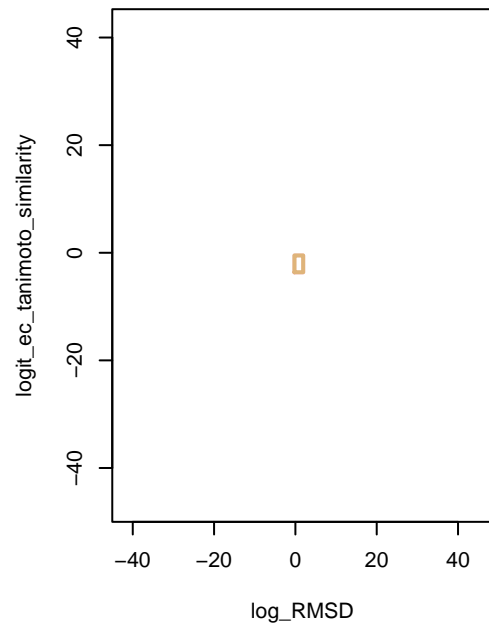
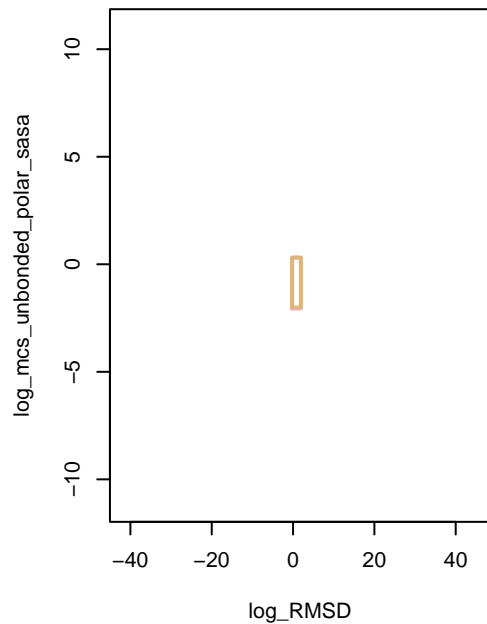




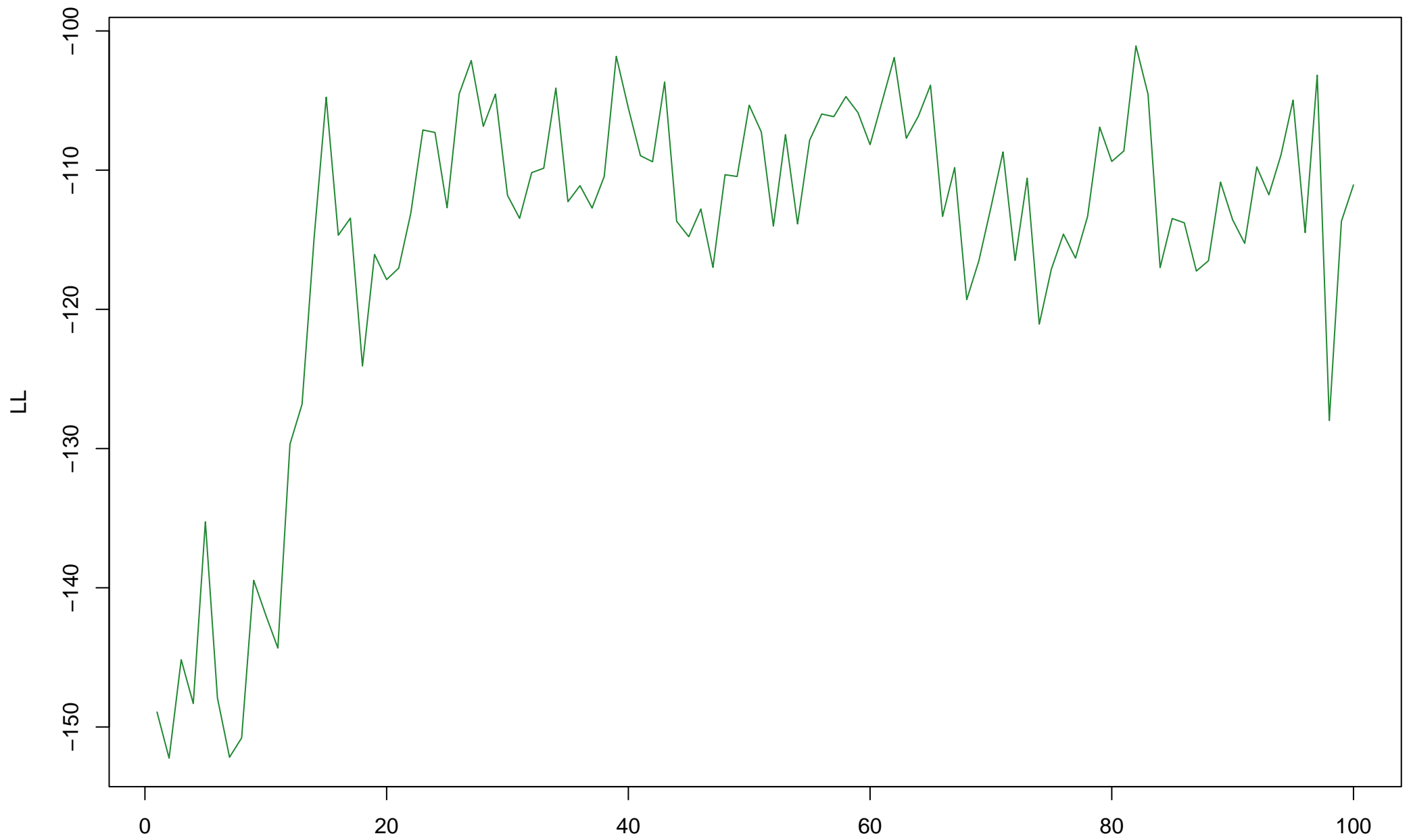




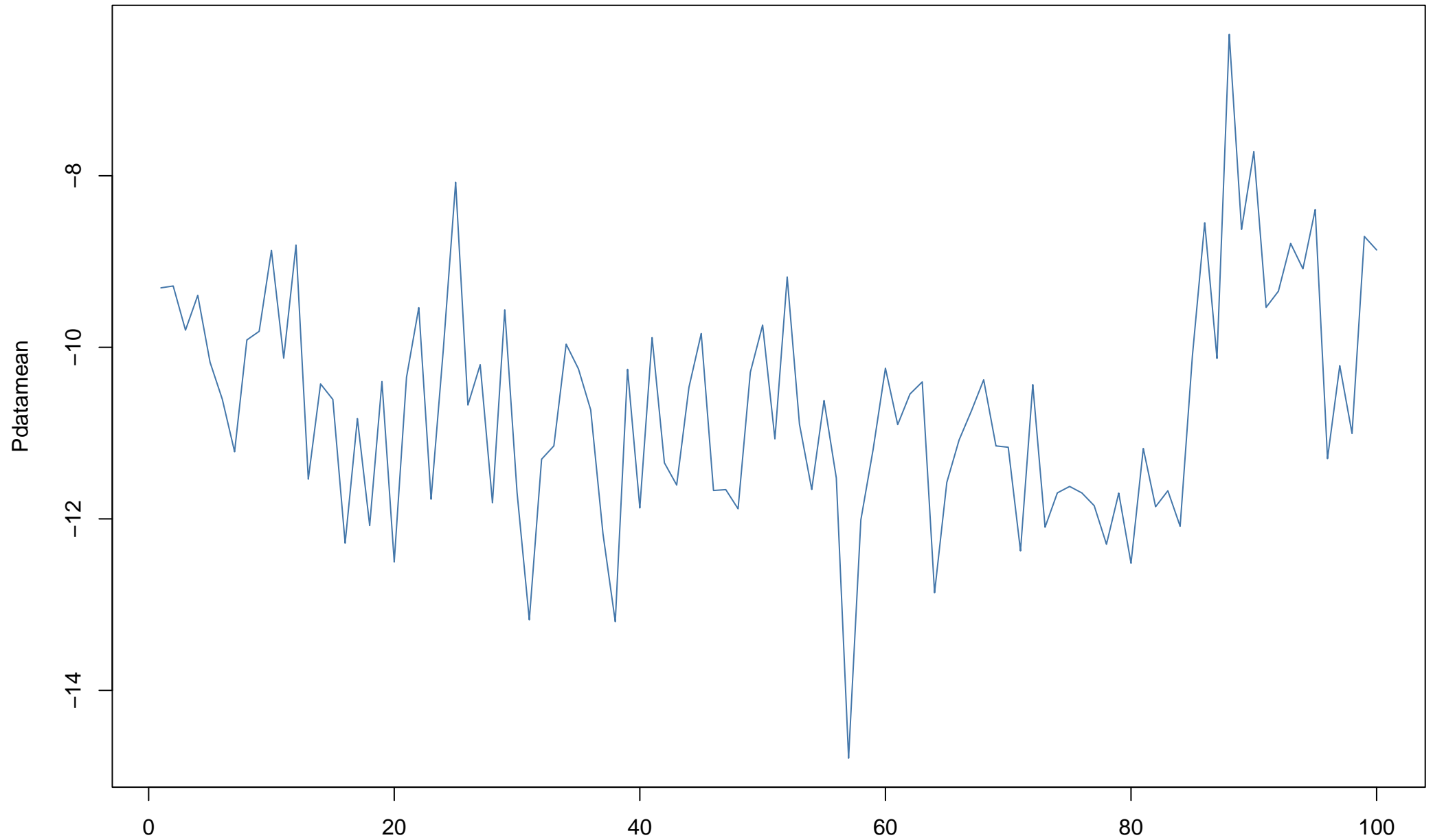




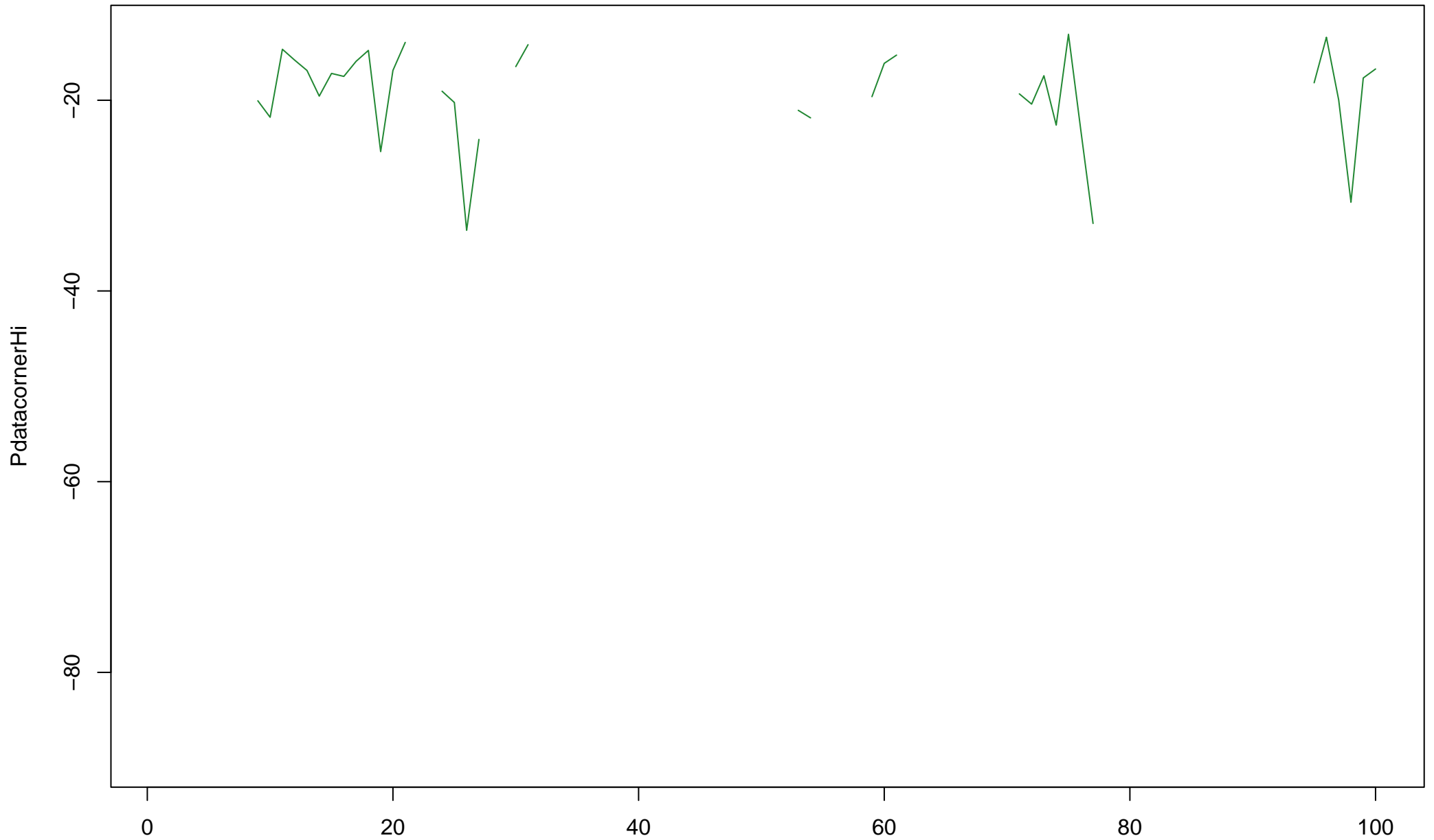
LL



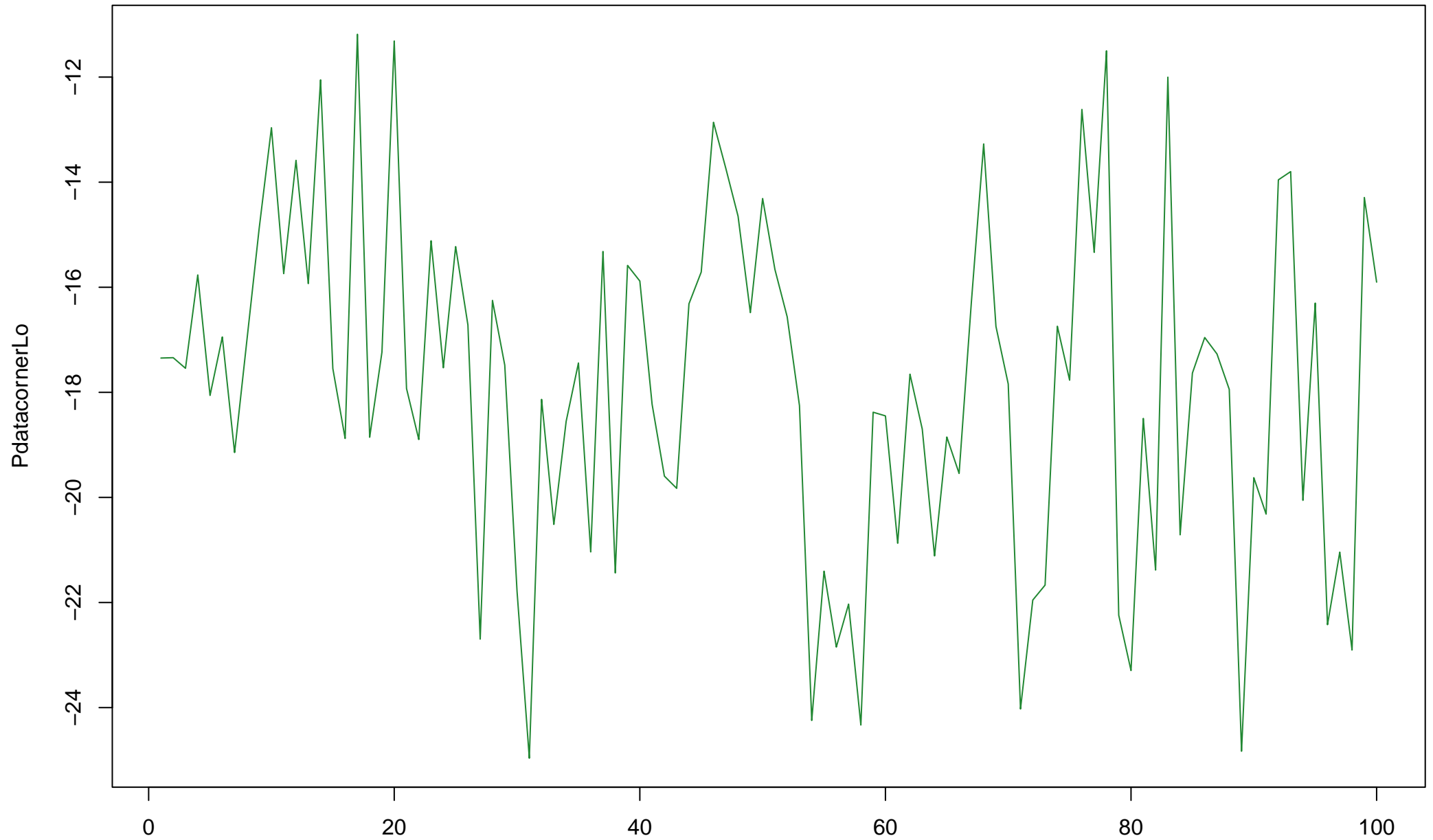
Pdatamean
ESS = 44.4 | BMK = 0.291 | MCSE(6.27) = 16.6 | stat: TRUE | burn: 80



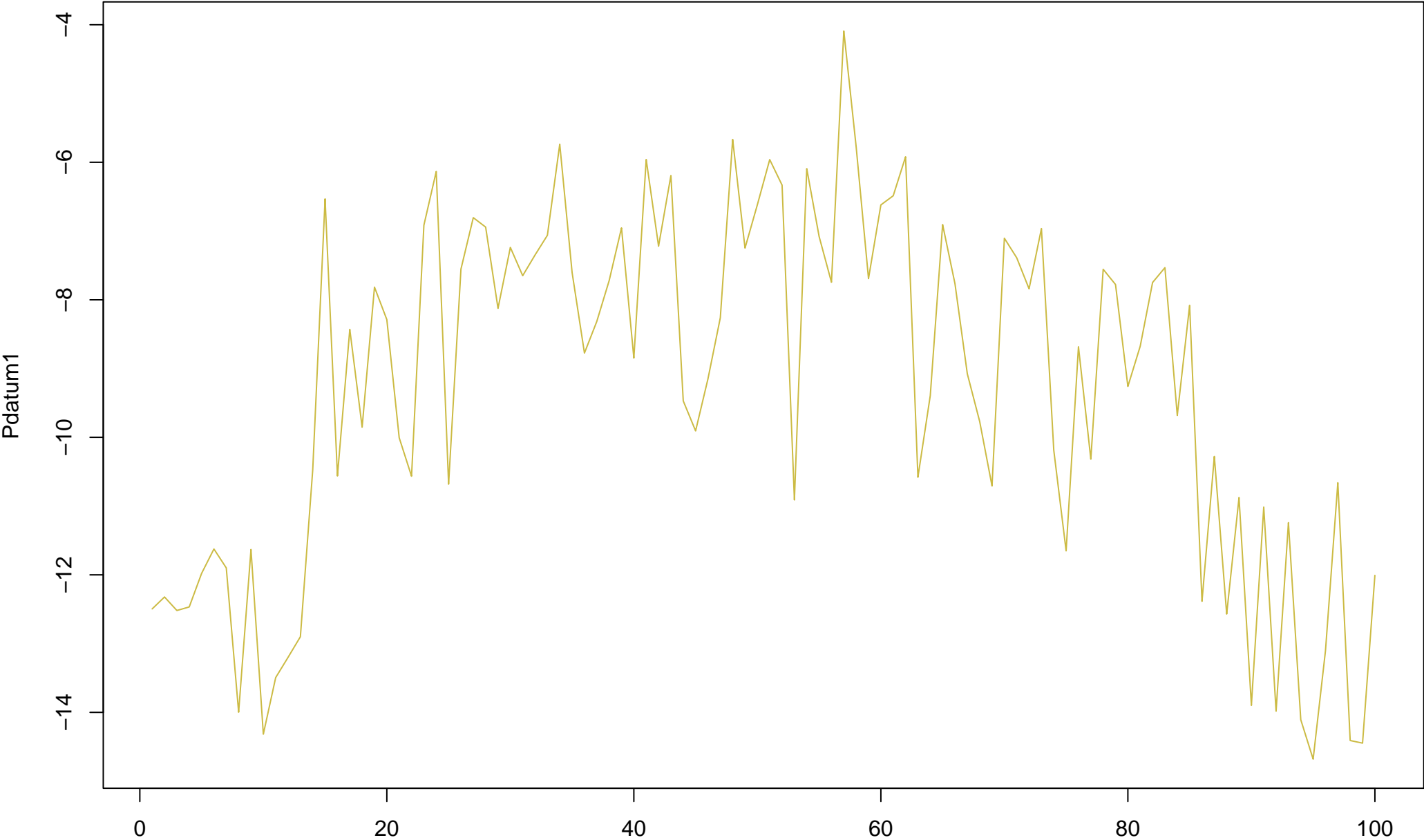
PdatacornerHi
ESS = 100 | BMK = 1 | MCSE(6.27) = 9.62 | stat: TRUE | burn: 100



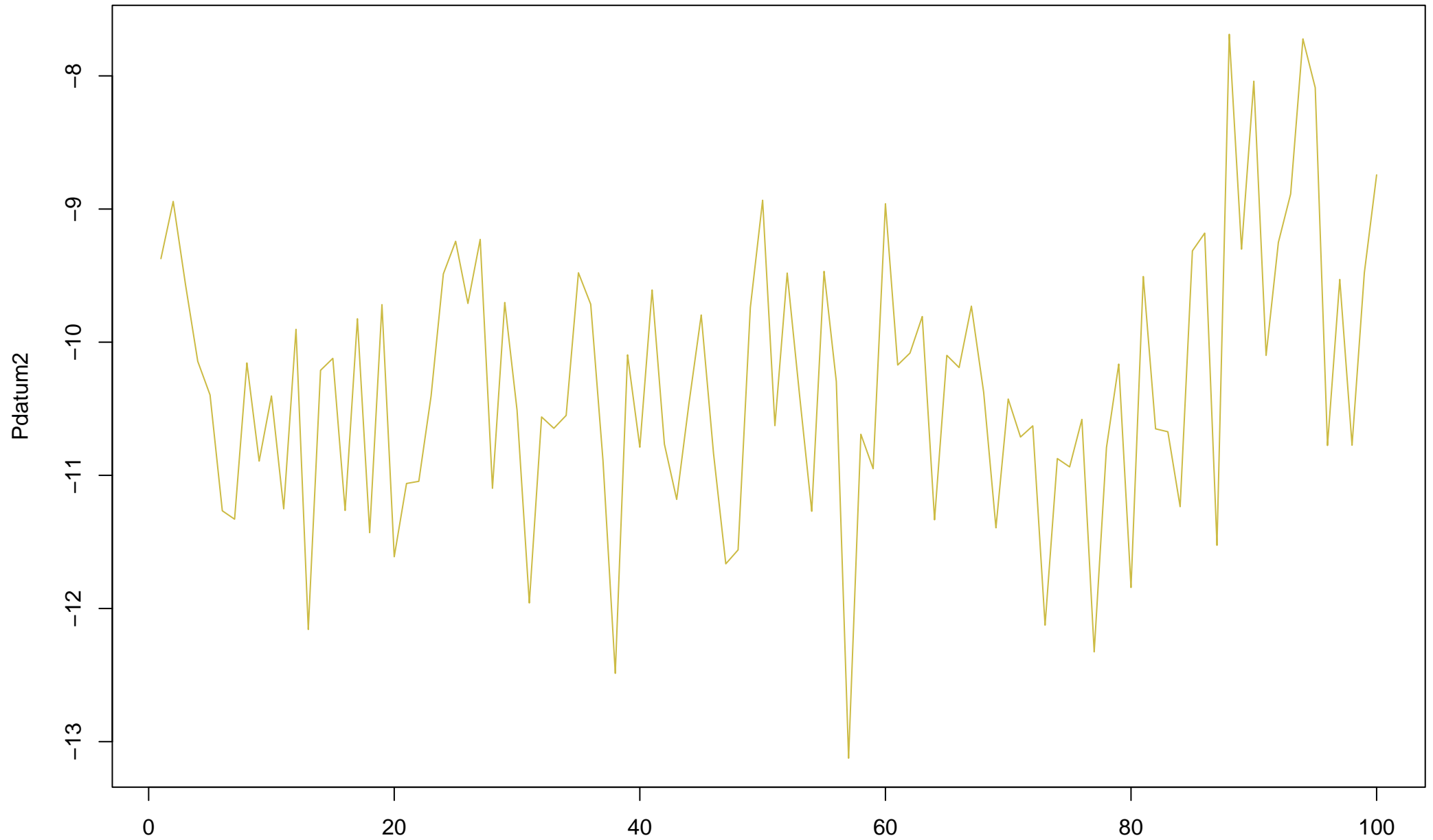
PdatacornerLo
ESS = 45.7 | BMK = 0.678 | MCSE(6.27) = 9.23 | stat: TRUE | burn: 100



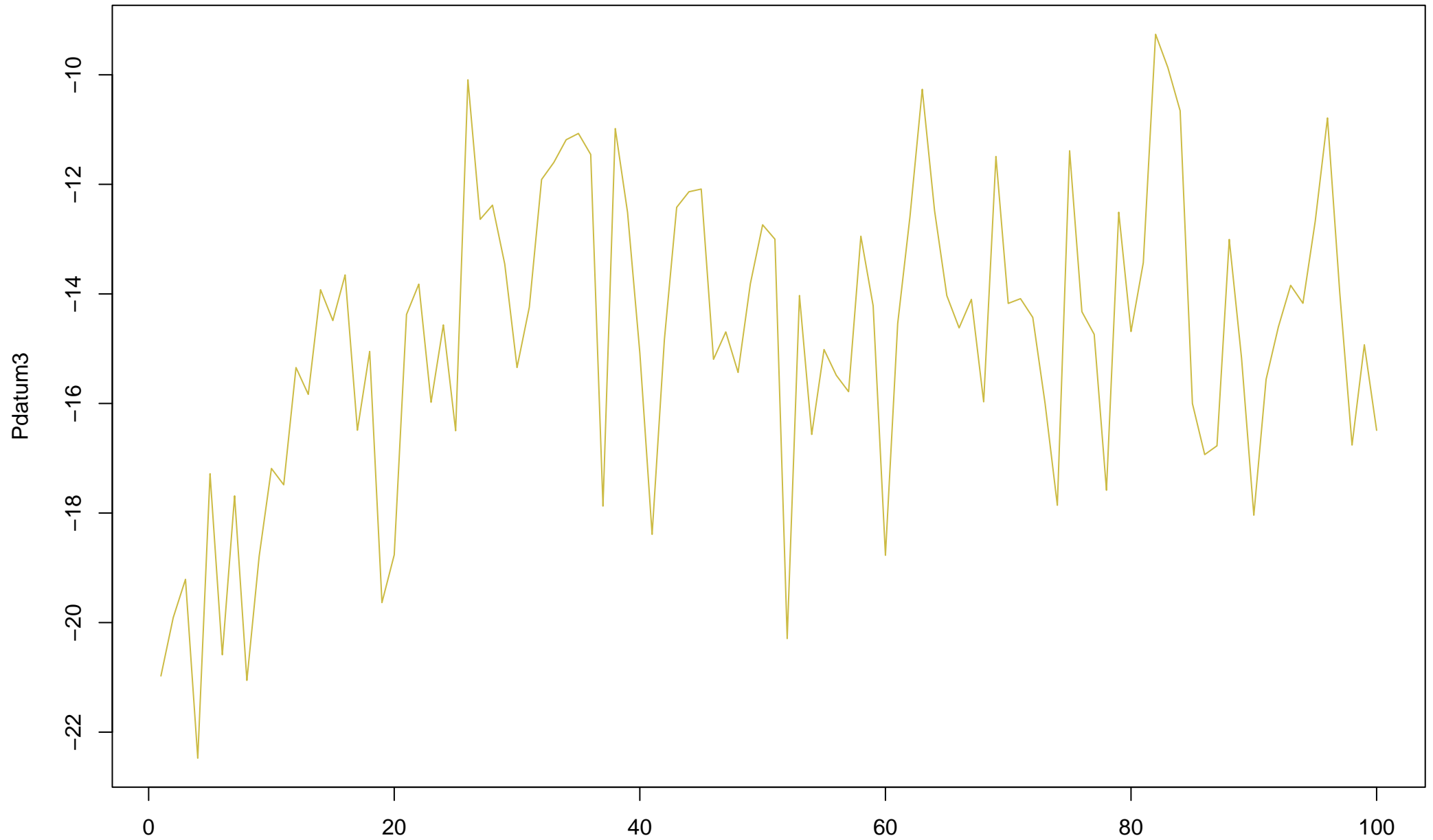
Pdatum1
ESS = 72.2 | BMK = 0.156 | MCSE(6.27) = 13 | stat: TRUE | burn: 100



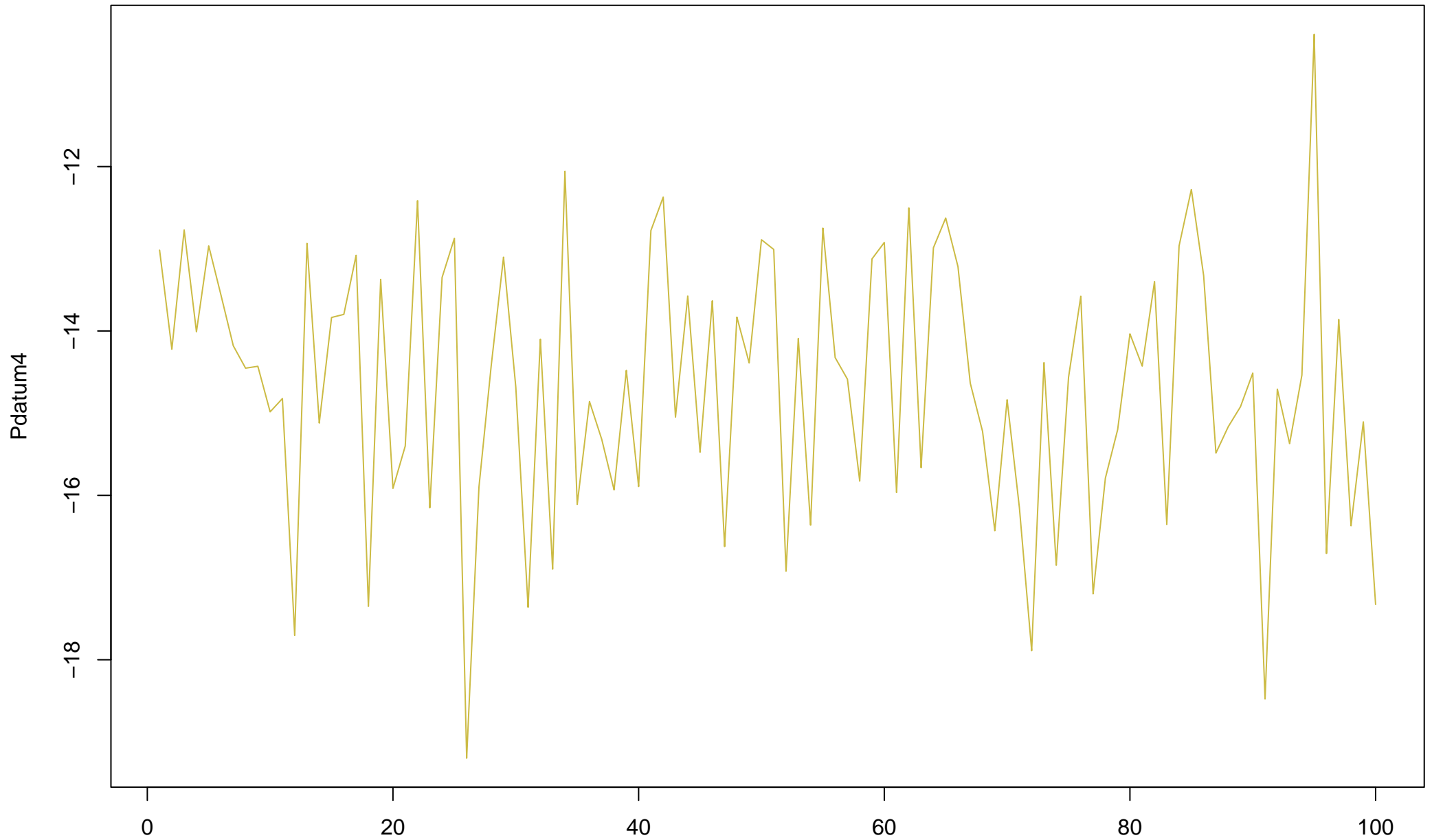
Pdatum2
ESS = 28.9 | BMK = 0.215 | MCSE(6.27) = 20.5 | stat: TRUE | burn: 80



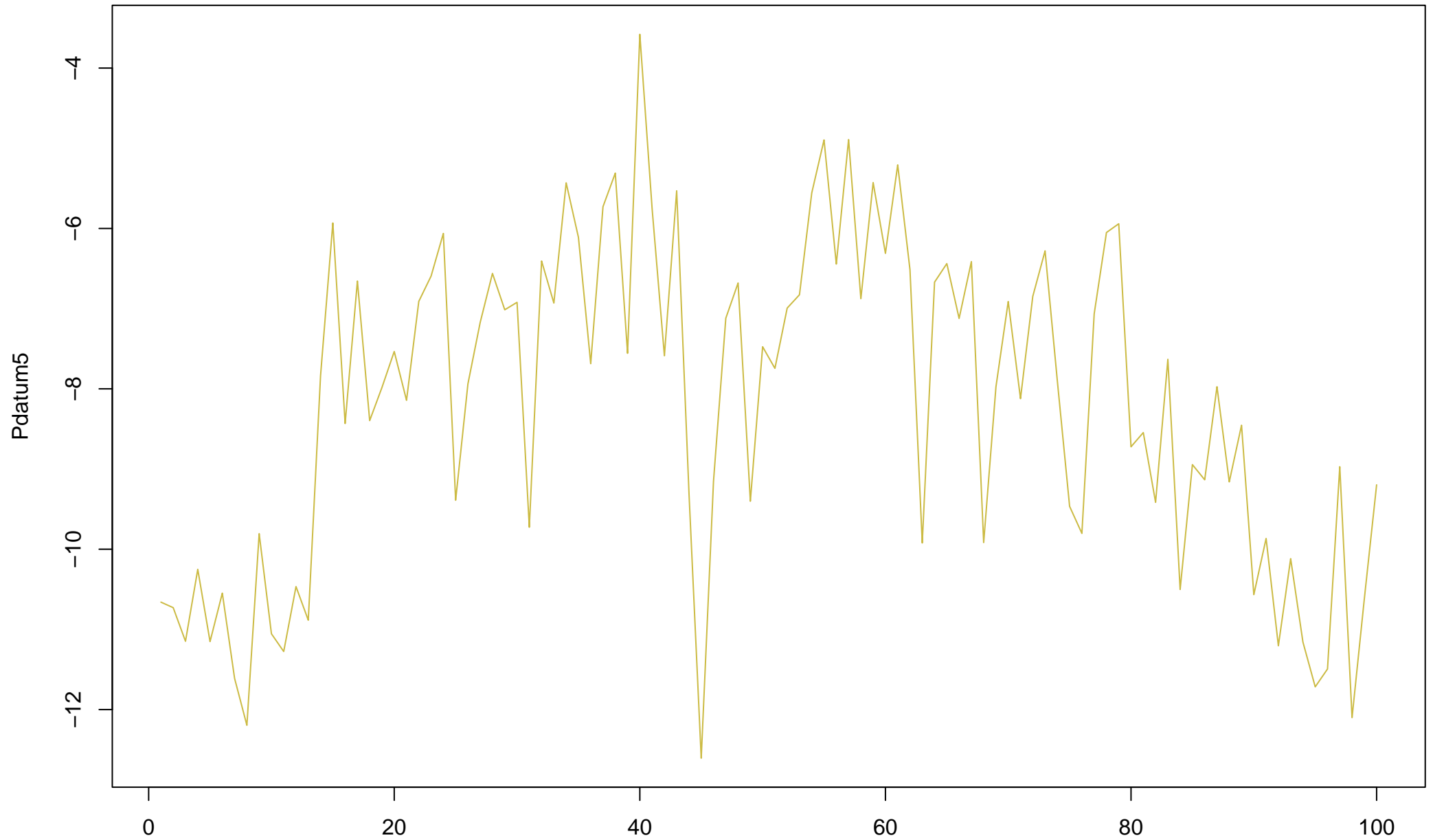
Pdatum3
ESS = 45.6 | BMK = 0.352 | MCSE(6.27) = 16.4 | stat: TRUE | burn: 100



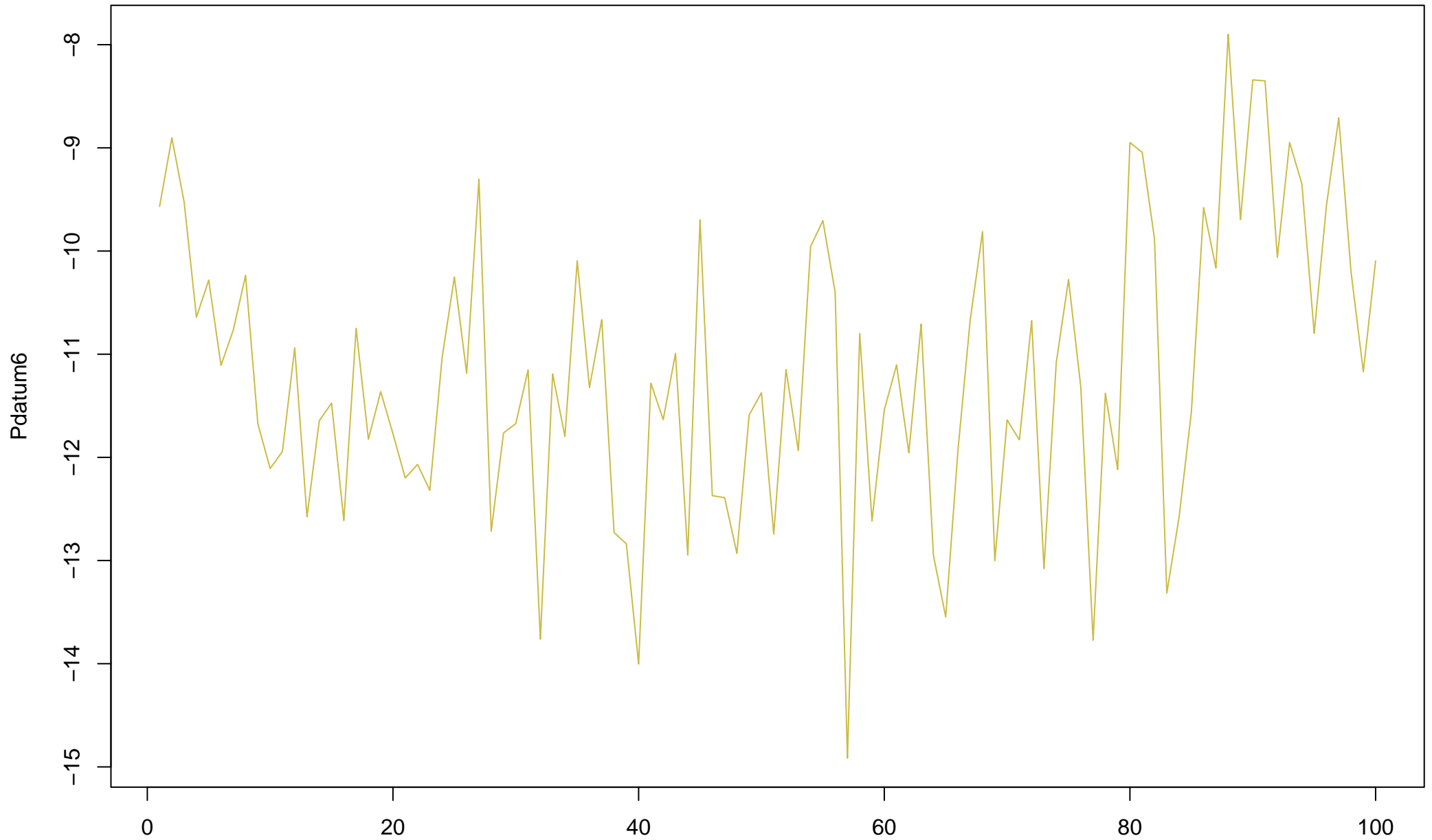
Pdatum4
ESS = 100 | BMK = 0.143 | MCSE(6.27) = 9.42 | stat: TRUE | burn: 100



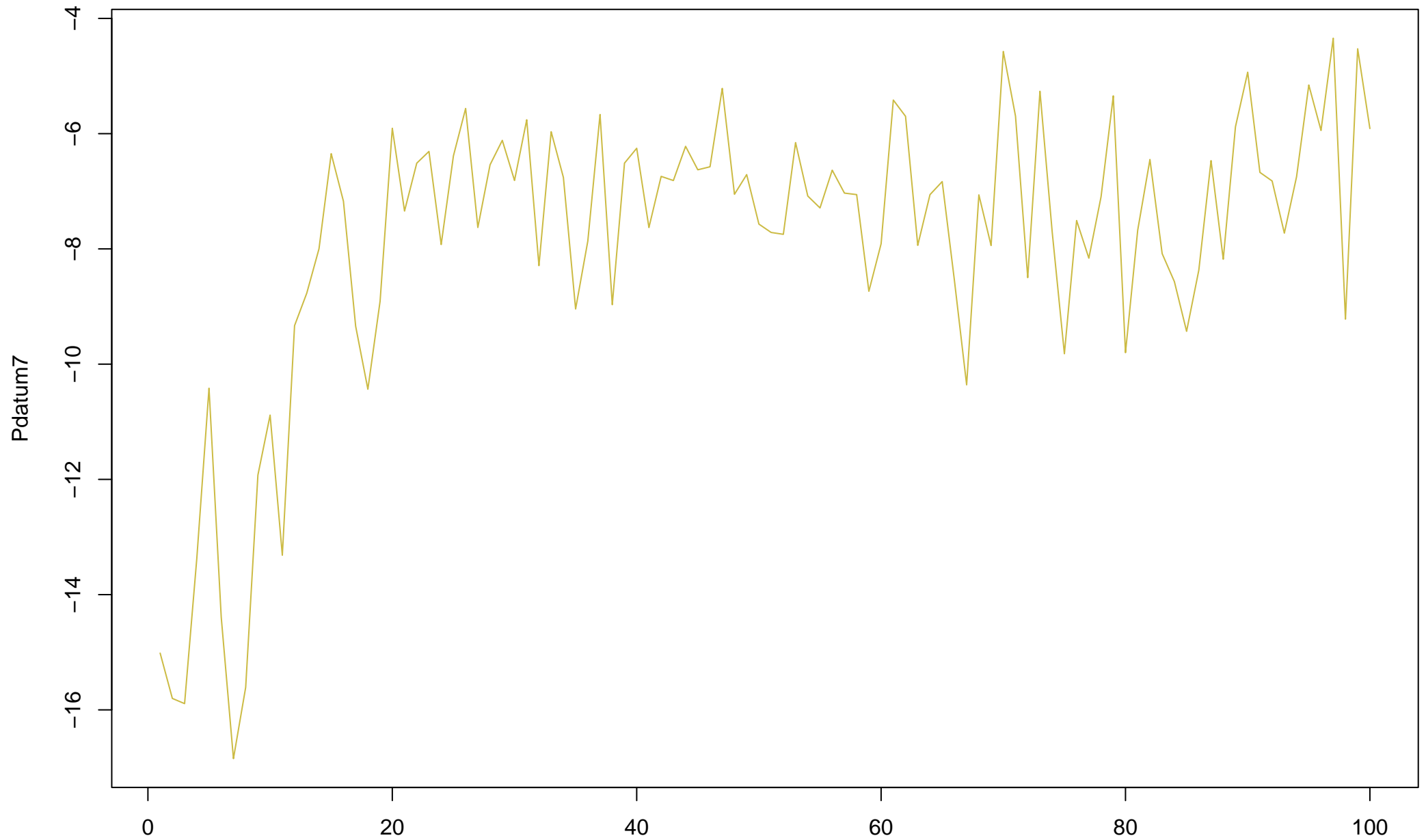
Pdatum5
ESS = 37.7 | BMK = 0.191 | MCSE(6.27) = 13.5 | stat: FALSE | burn: 100



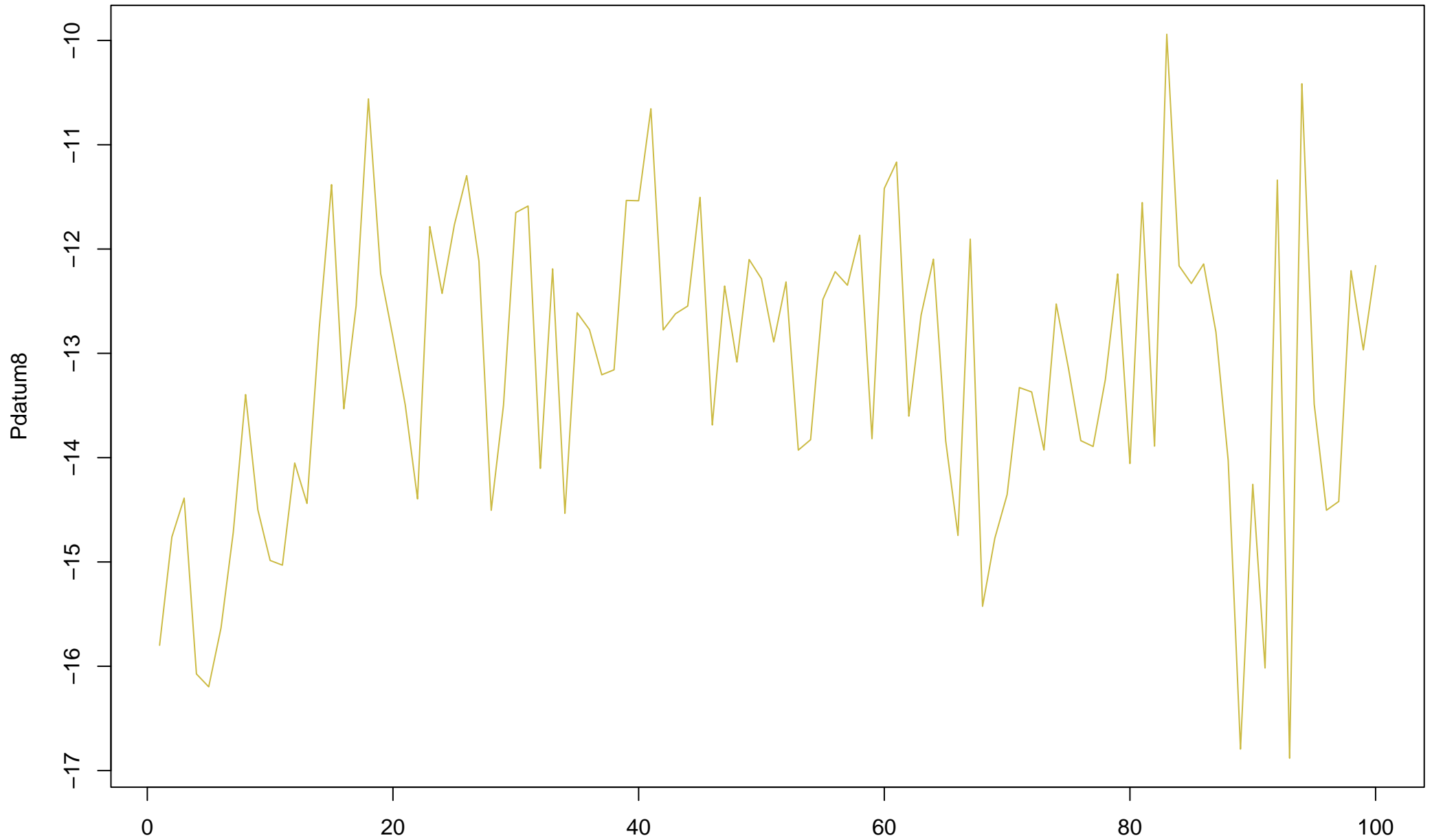
Pdatum6
ESS = 11.1 | BMK = 0.342 | MCSE(6.27) = 18 | stat: TRUE | burn: 80



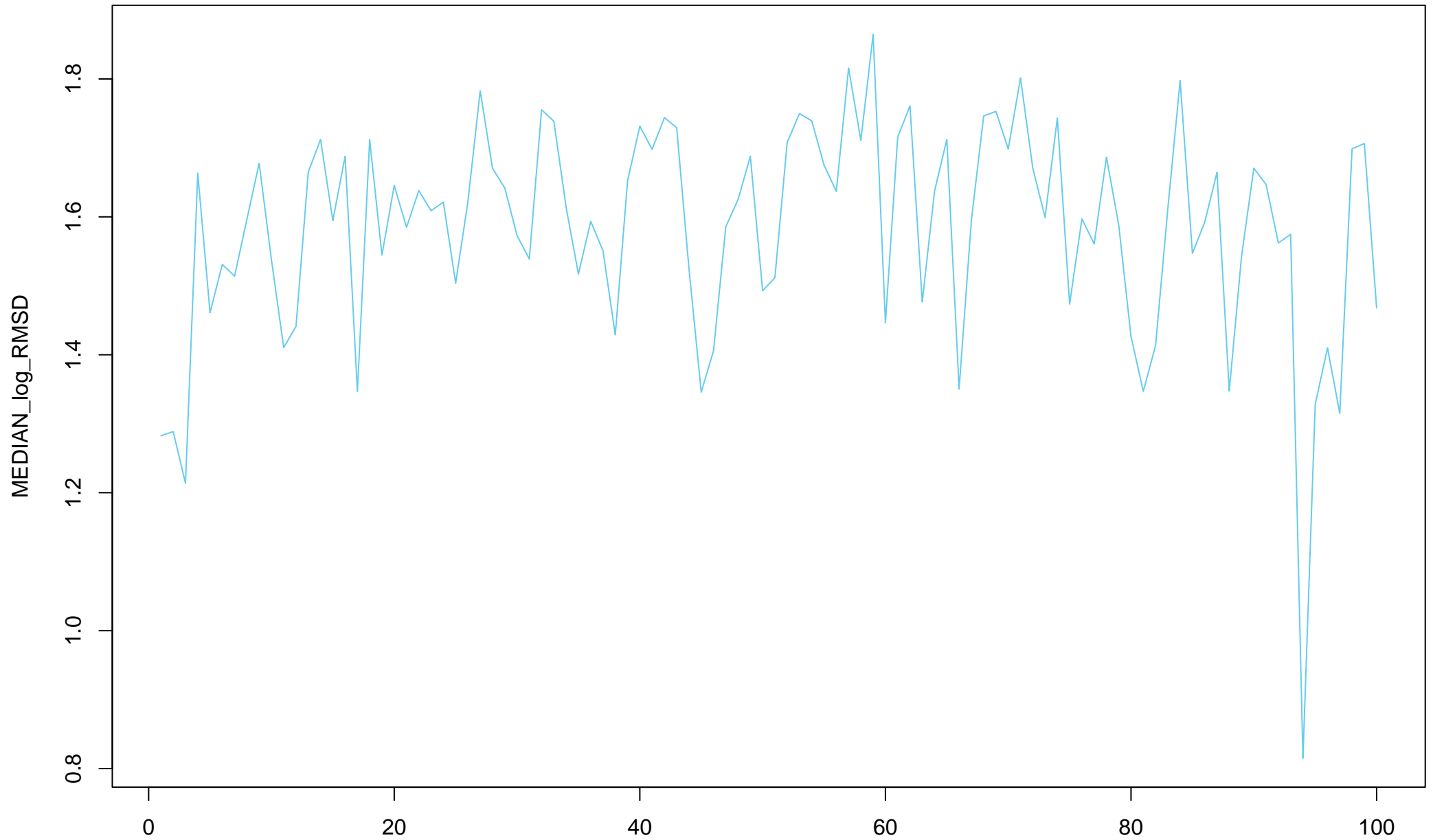
Pdatum7
ESS = 48.3 | BMK = 0.219 | MCSE(6.27) = 13.4 | stat: FALSE | burn: 40



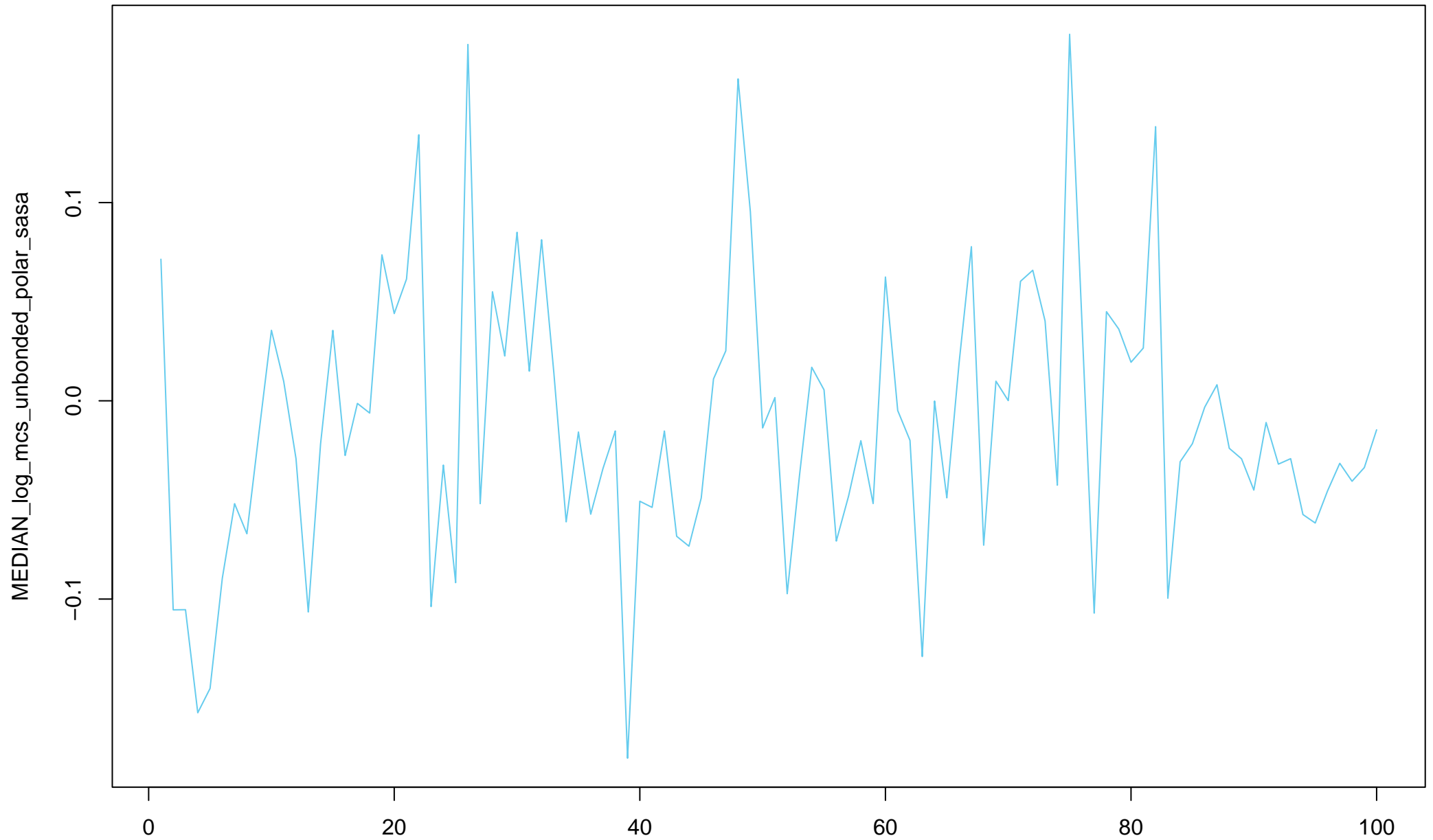
Pdatum8
ESS = 100 | BMK = 0.202 | MCSE(6.27) = 11.8 | stat: FALSE | burn: 10



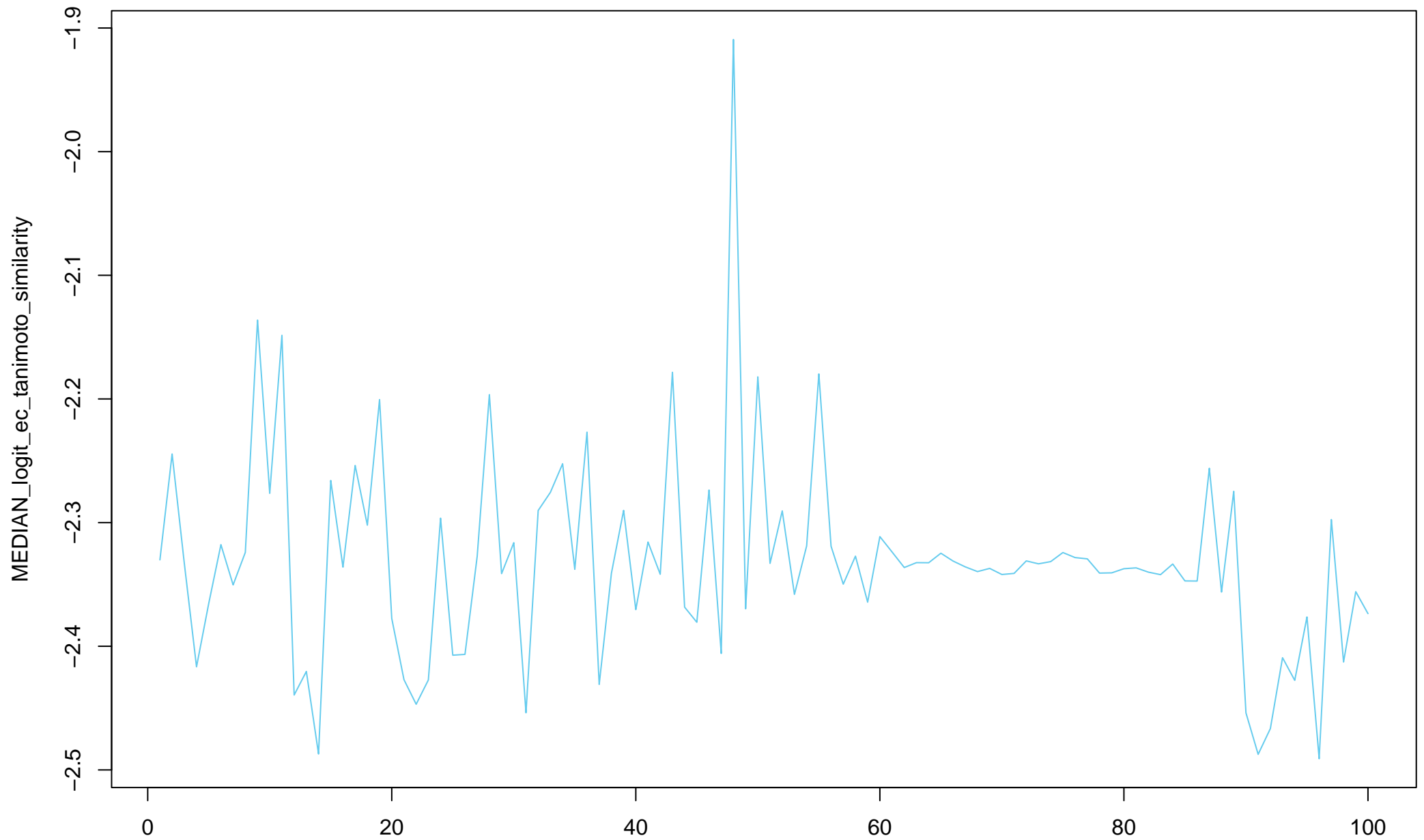
MEDIAN_log_RMSD
ESS = 52.9 | BMK = 0.153 | MCSE(6.27) = 16.8 | stat: TRUE | burn: 0



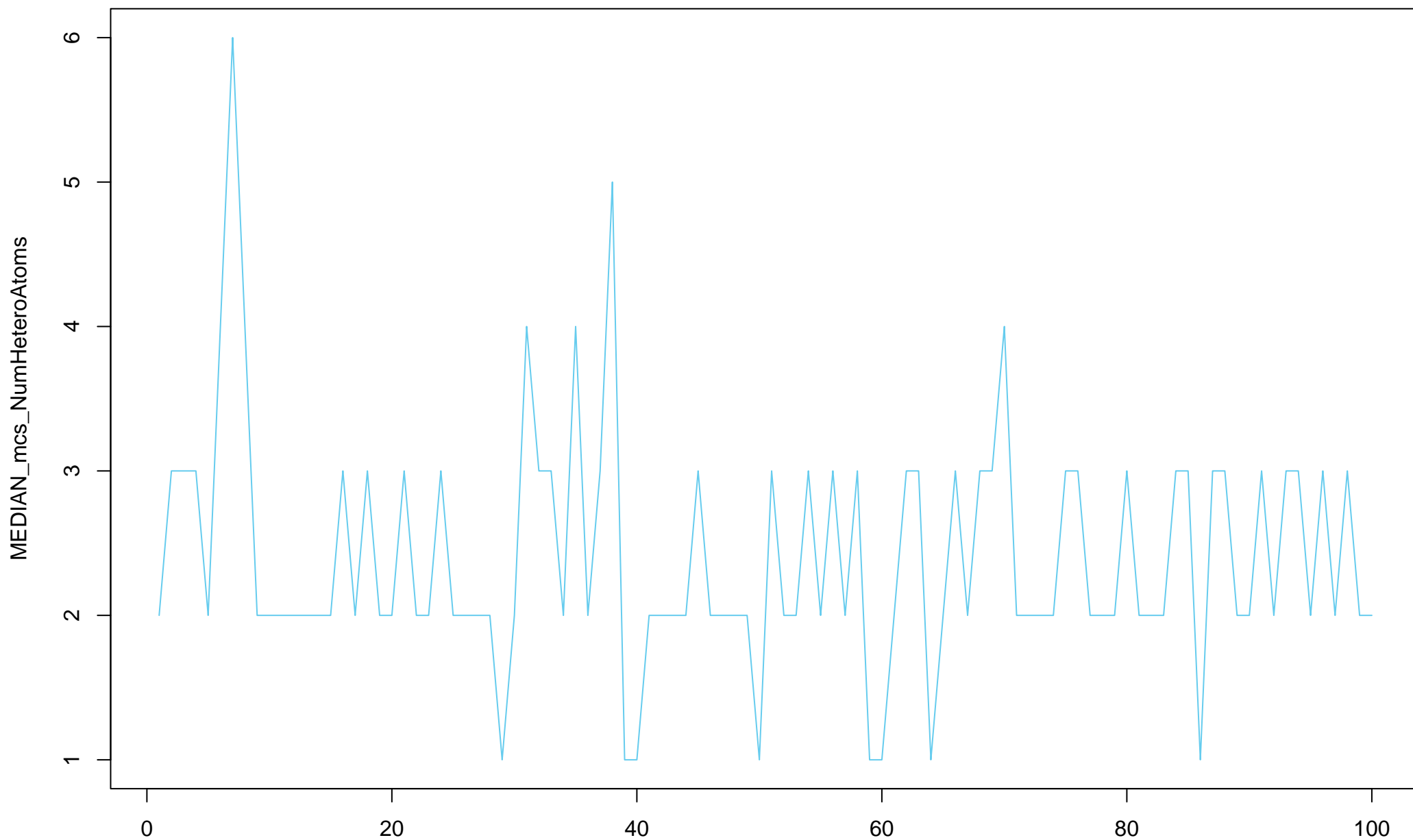
MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 47.4 | BMK = 0.165 | MCSE(6.27) = 17.7 | stat: TRUE | burn: 80



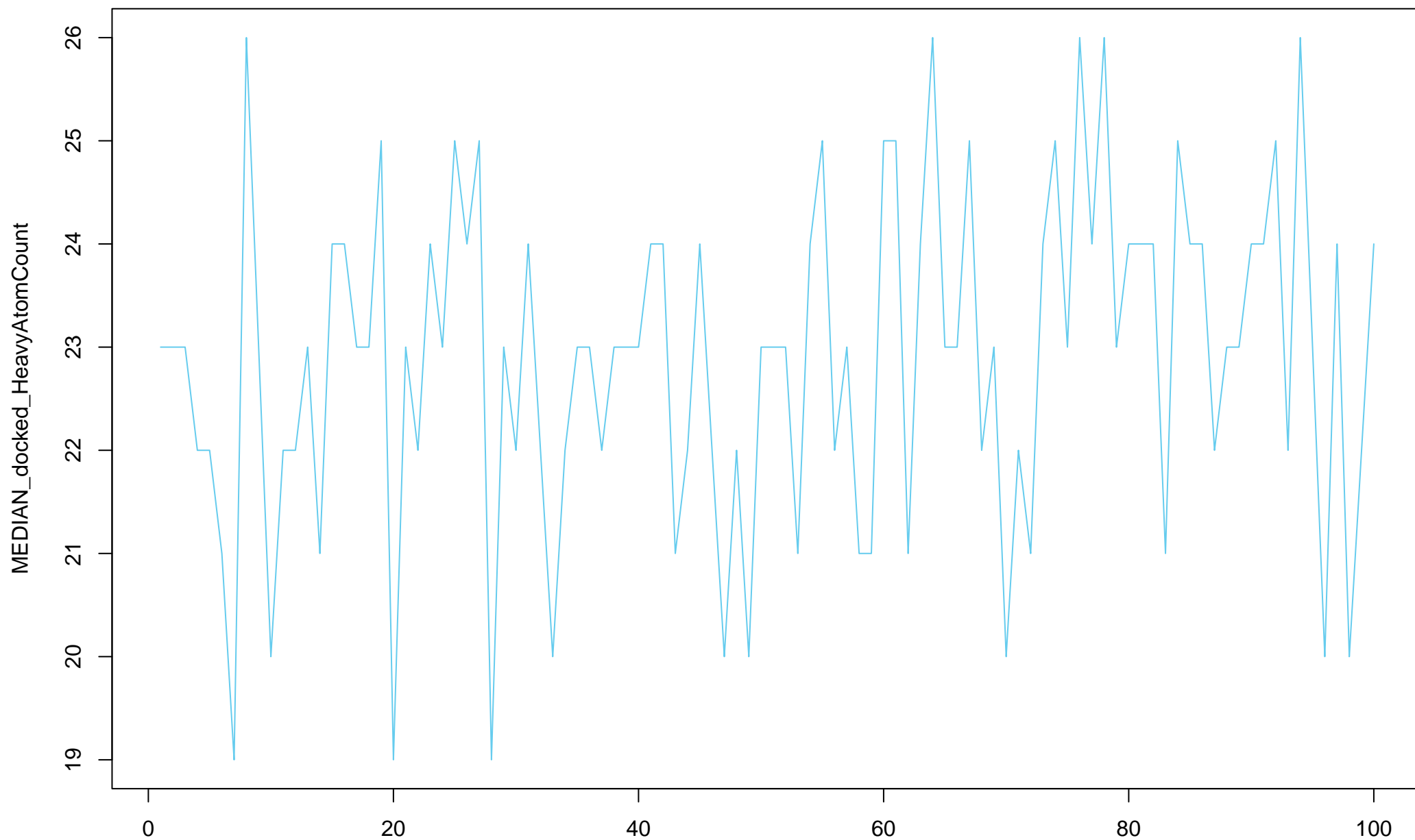
MEDIAN_logit_ec_tanimoto_similarity
ESS = 74.5 | BMK = 0.416 | MCSE(6.27) = 13.8 | stat: TRUE | burn: 100



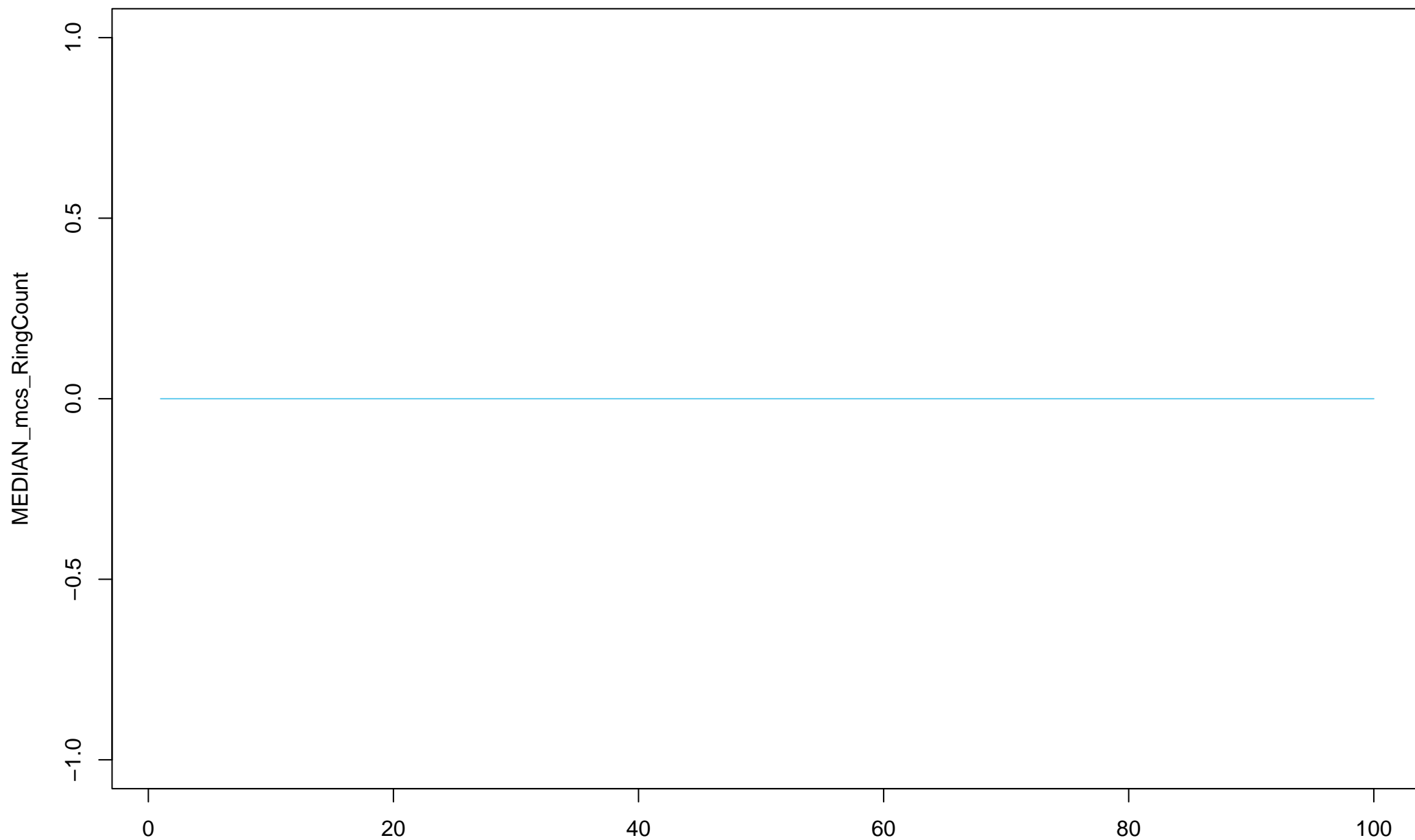
MEDIAN_mcs_NumHeteroAtoms
ESS = 100 | BMK = 0.197 | MCSE(6.27) = 11.6 | stat: TRUE | burn: 0



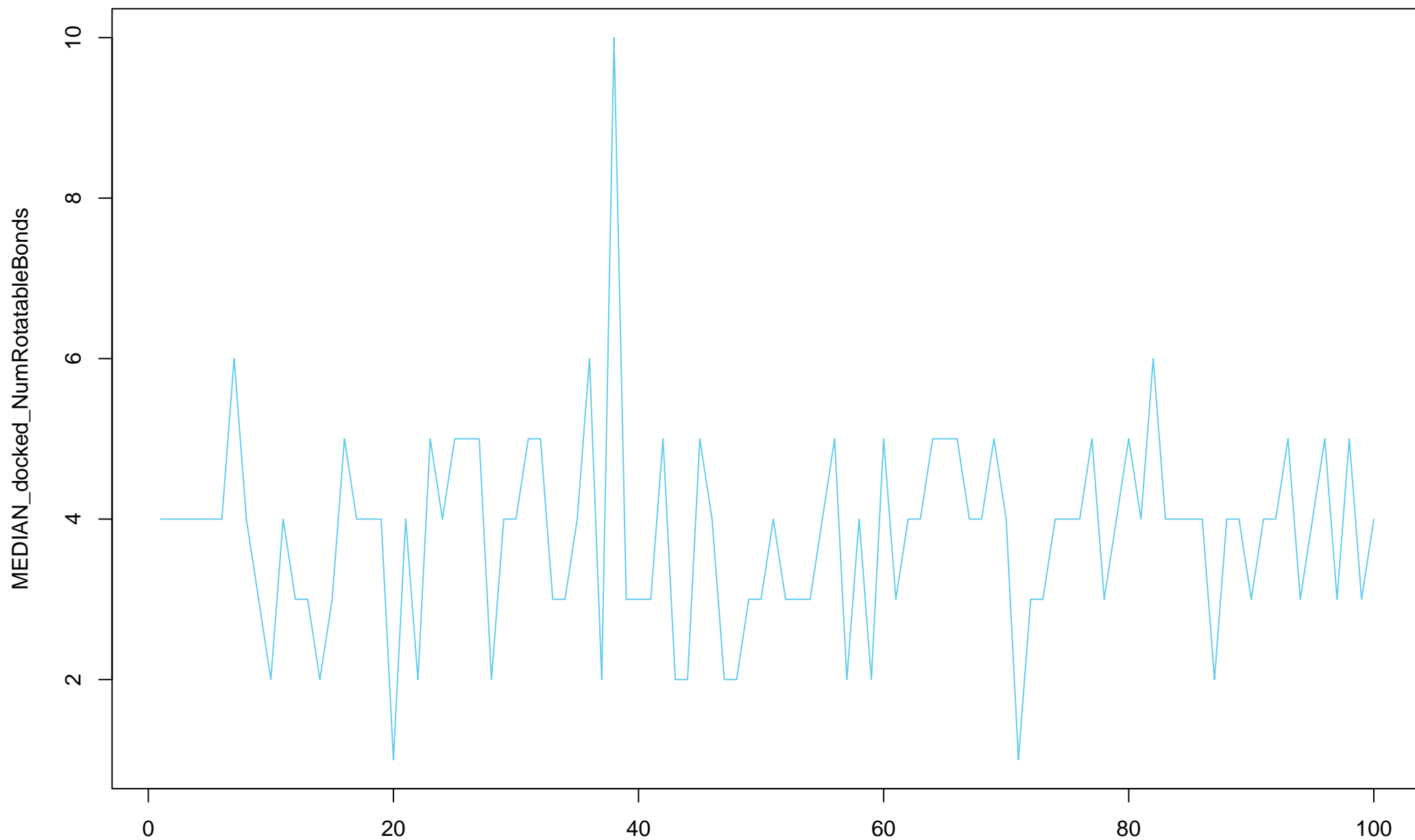
MEDIAN_docked_HeavyAtomCount
ESS = 100 | BMK = 0.208 | MCSE(6.27) = 10.3 | stat: TRUE | burn: 0



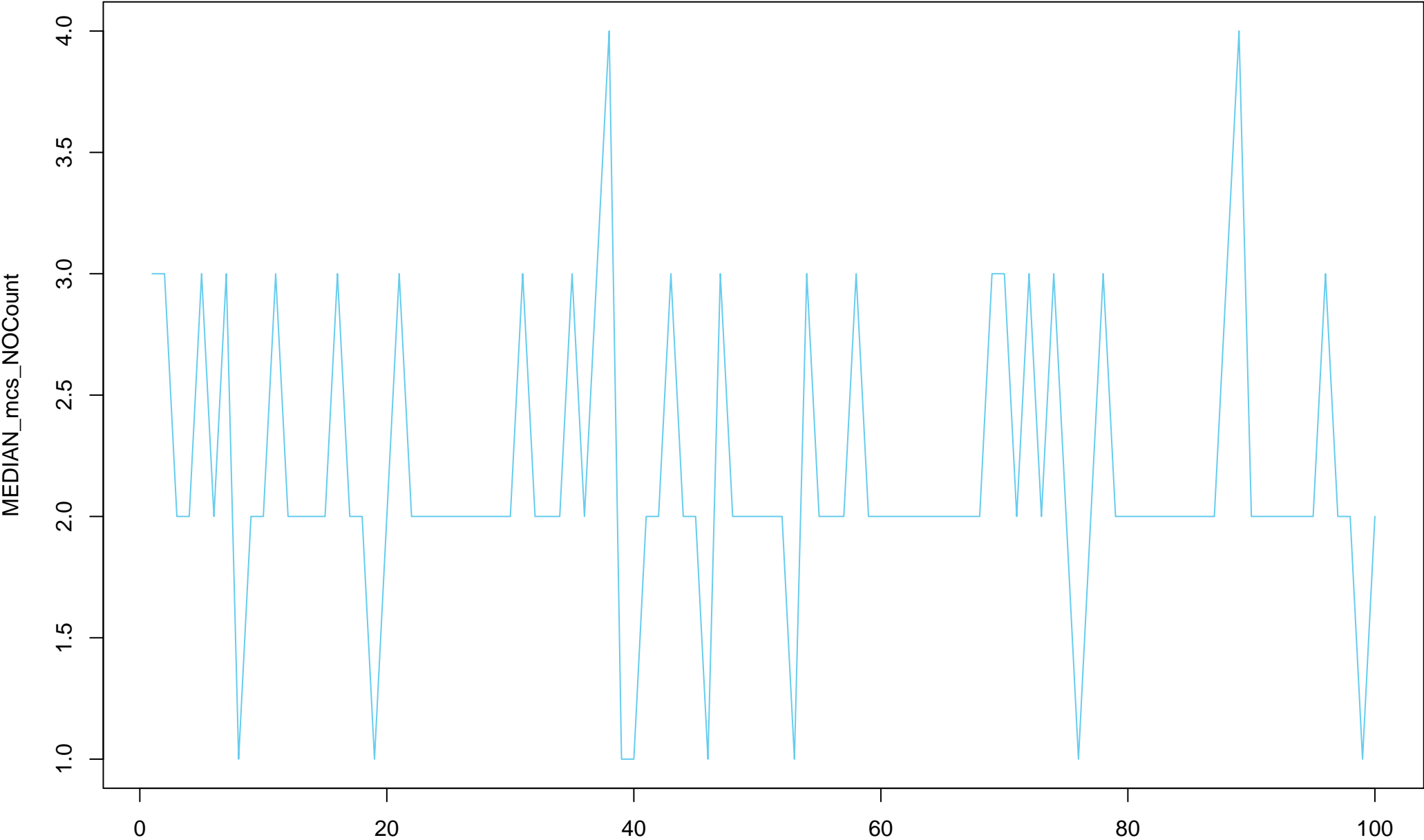
MEDIAN_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



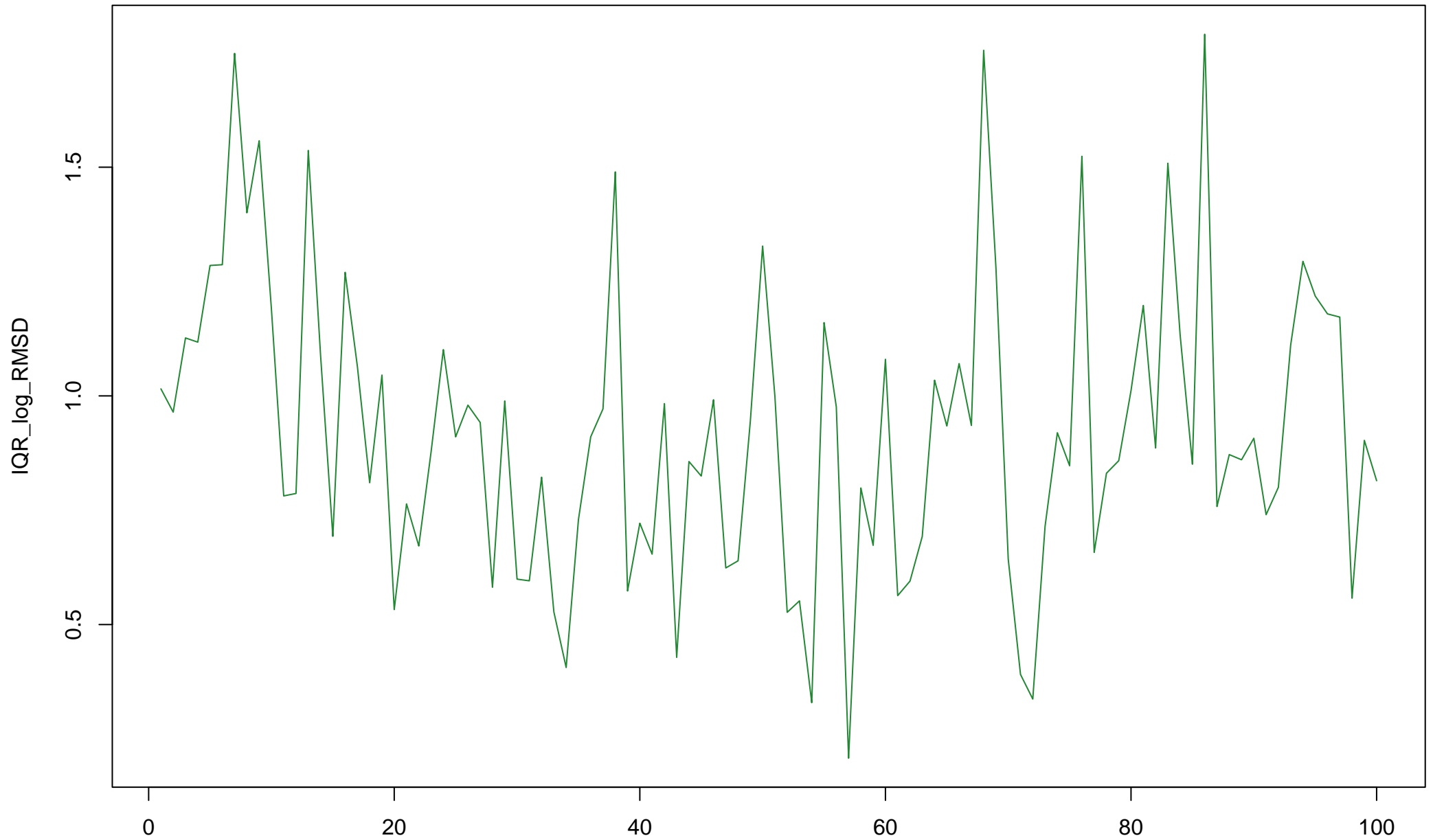
MEDIAN_docked_NumRotatableBonds
ESS = 100 | BMK = 0.163 | MCSE(6.27) = 9.06 | stat: TRUE | burn: 0



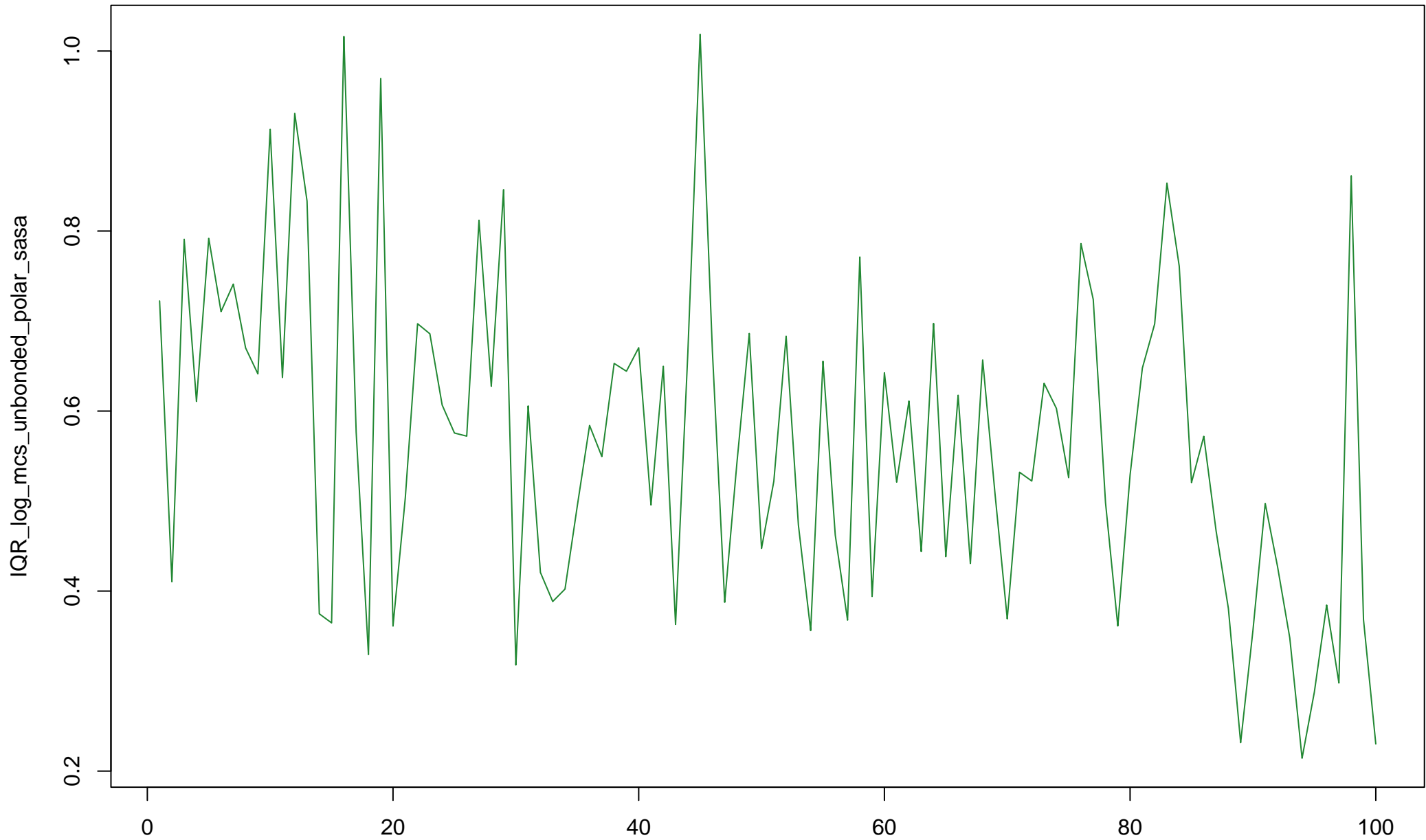
MEDIAN_mcs_NOCount
ESS = 100 | BMK = 0.0713 | MCSE(6.27) = 9.73 | stat: TRUE | burn: 0



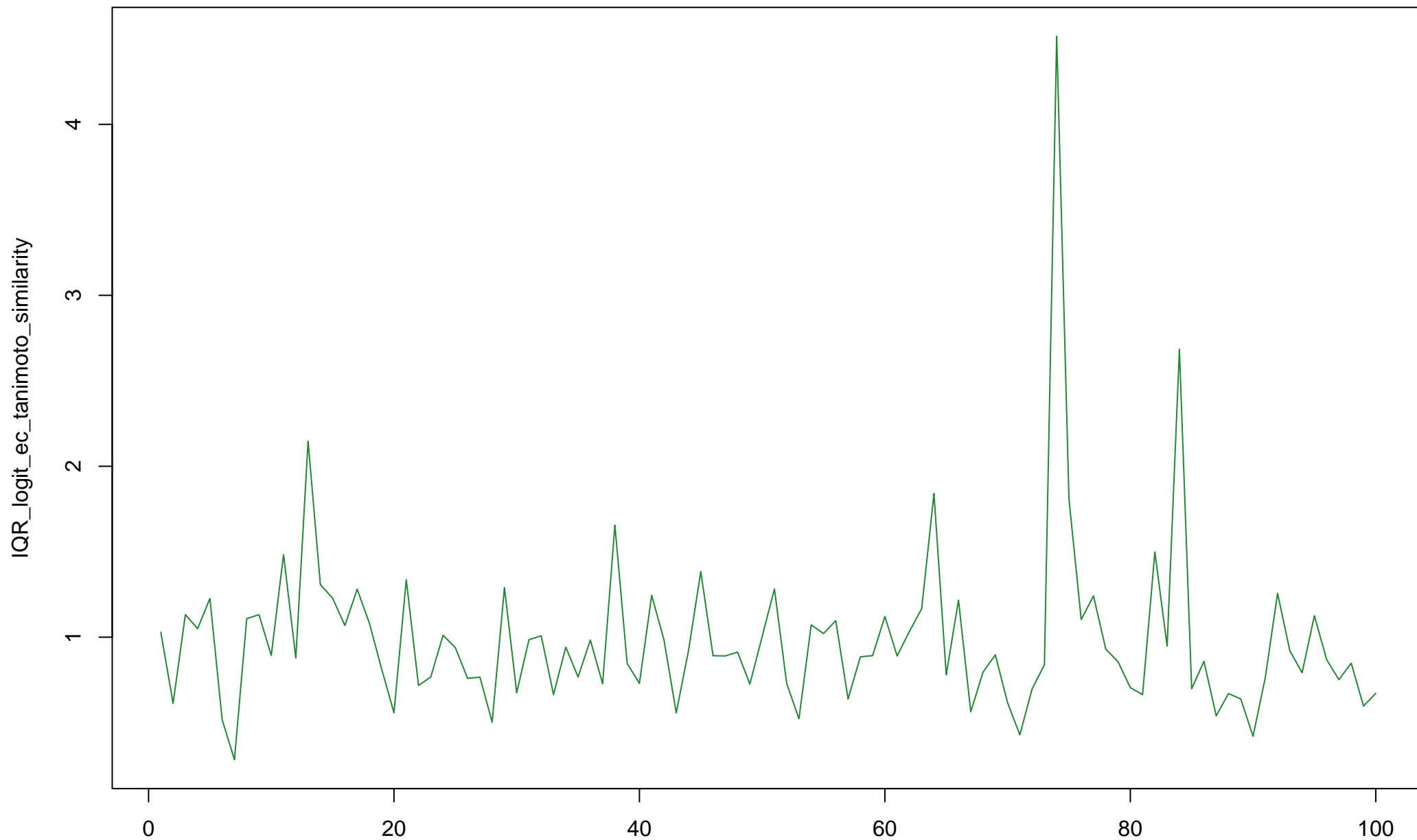
IQR_log_RMSD
ESS = 54.1 | BMK = 0.0728 | MCSE(6.27) = 18.7 | stat: FALSE | burn: 0



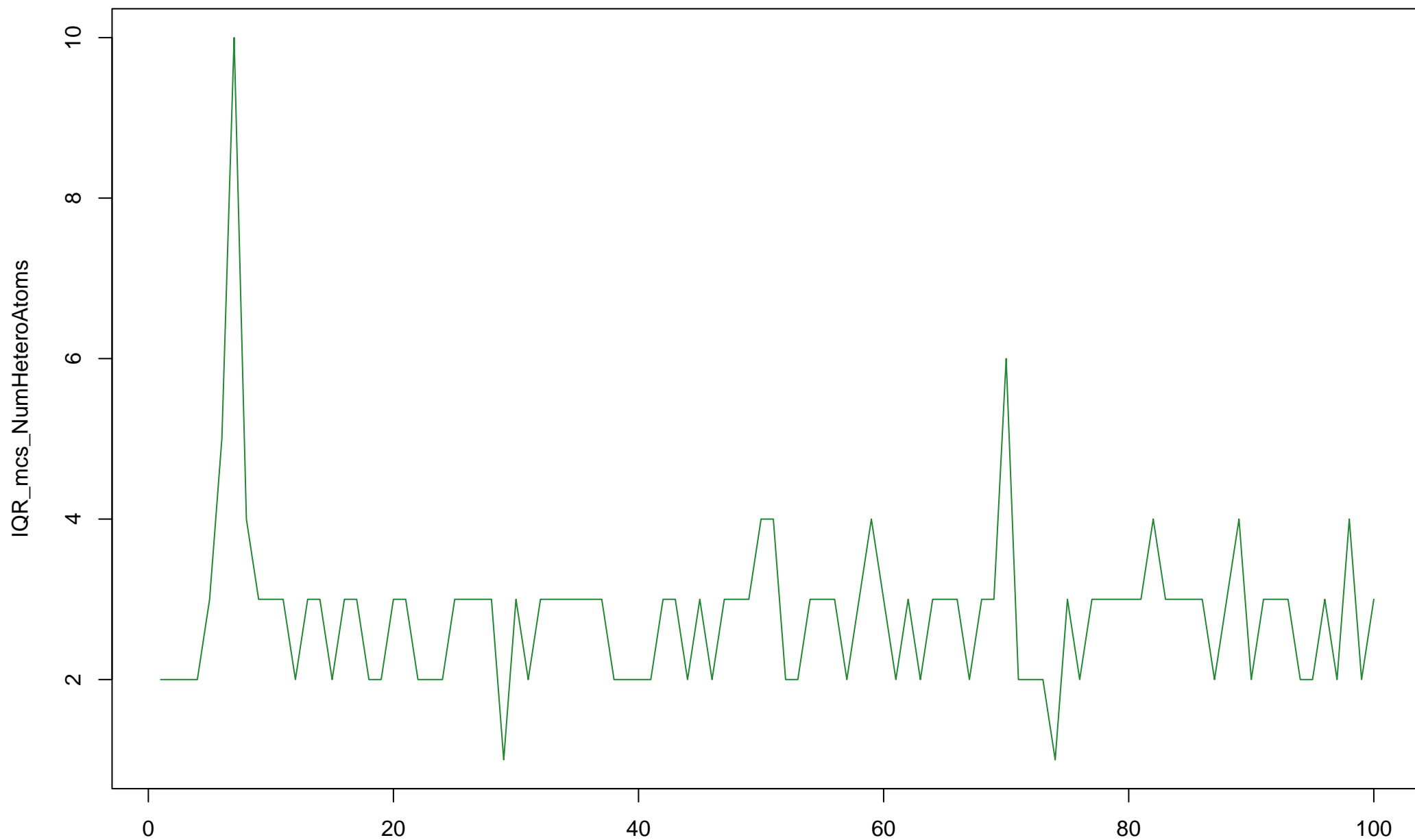
IQR_log_mcs_unbonded_polar_sasa
ESS = 38.9 | BMK = 0.189 | MCSE(6.27) = 12.9 | stat: FALSE | burn: 0



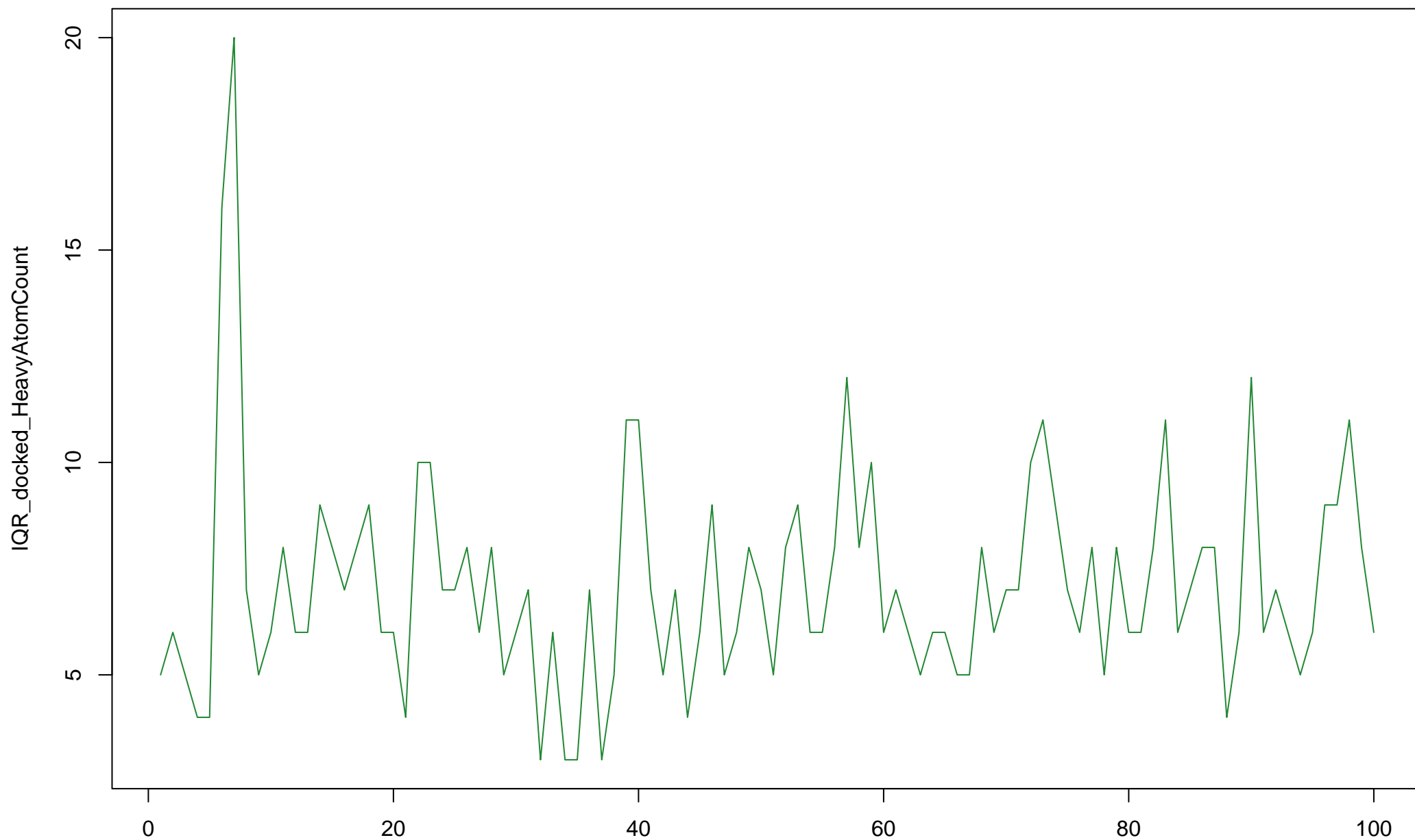
IQR_logit_ec_tanimoto_similarity
ESS = 85.5 | BMK = 0.187 | MCSE(6.27) = 12.5 | stat: TRUE | burn: 0



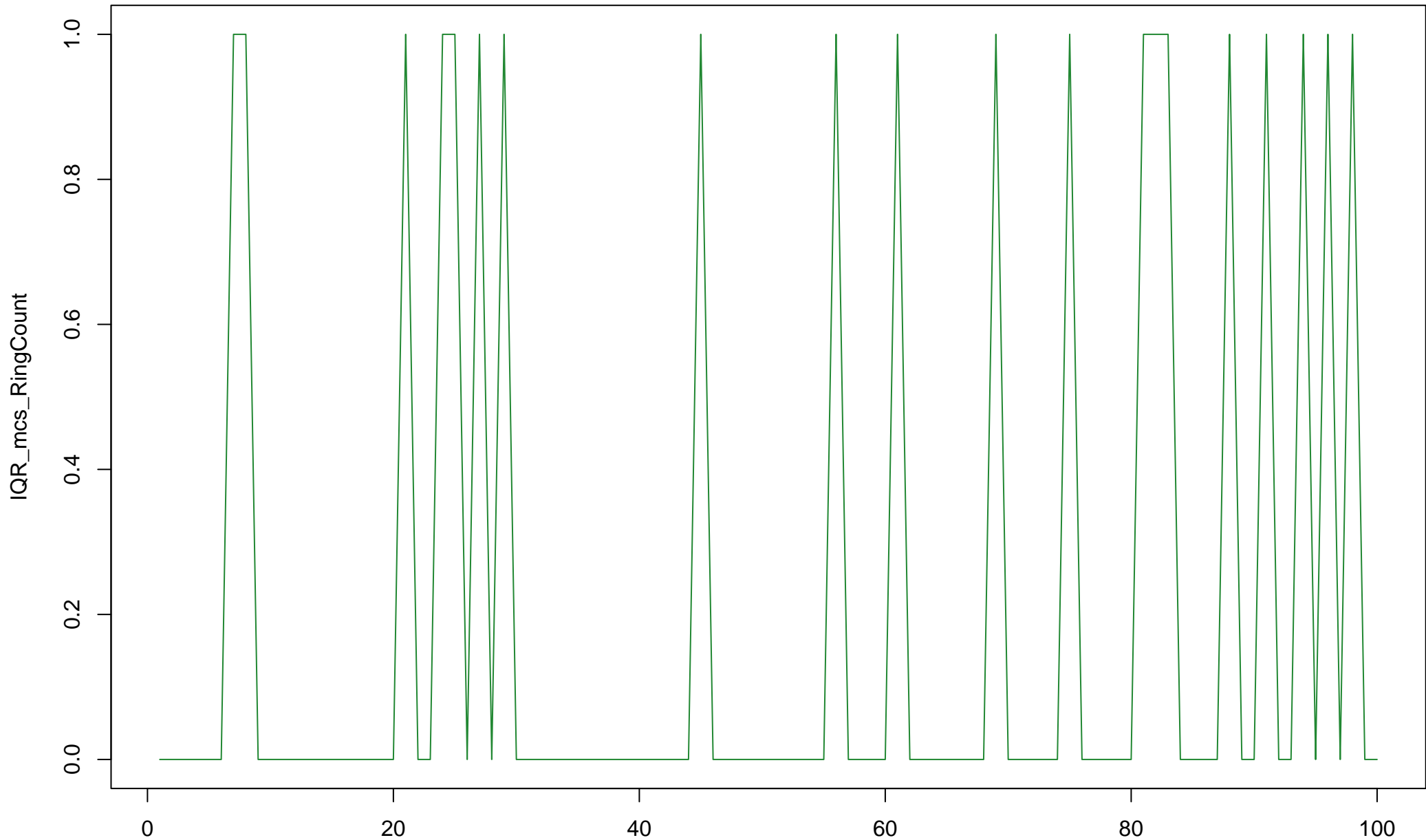
IQR_mcs_NumHeteroAtoms
ESS = 59.8 | BMK = 0.151 | MCSE(6.27) = 14.3 | stat: TRUE | burn: 0



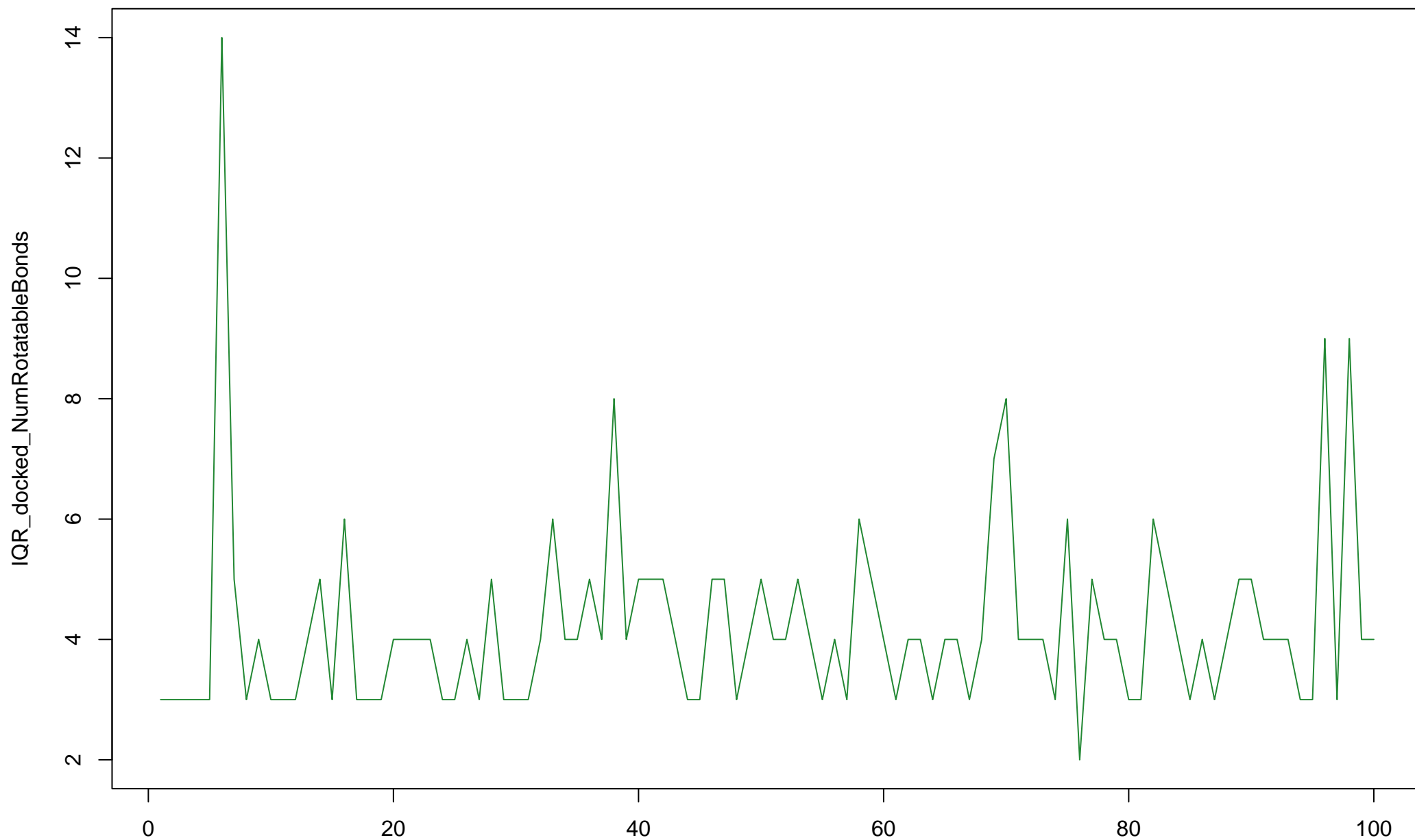
IQR_docked_HeavyAtomCount
ESS = 90.5 | BMK = 0.213 | MCSE(6.27) = 13.6 | stat: TRUE | burn: 10



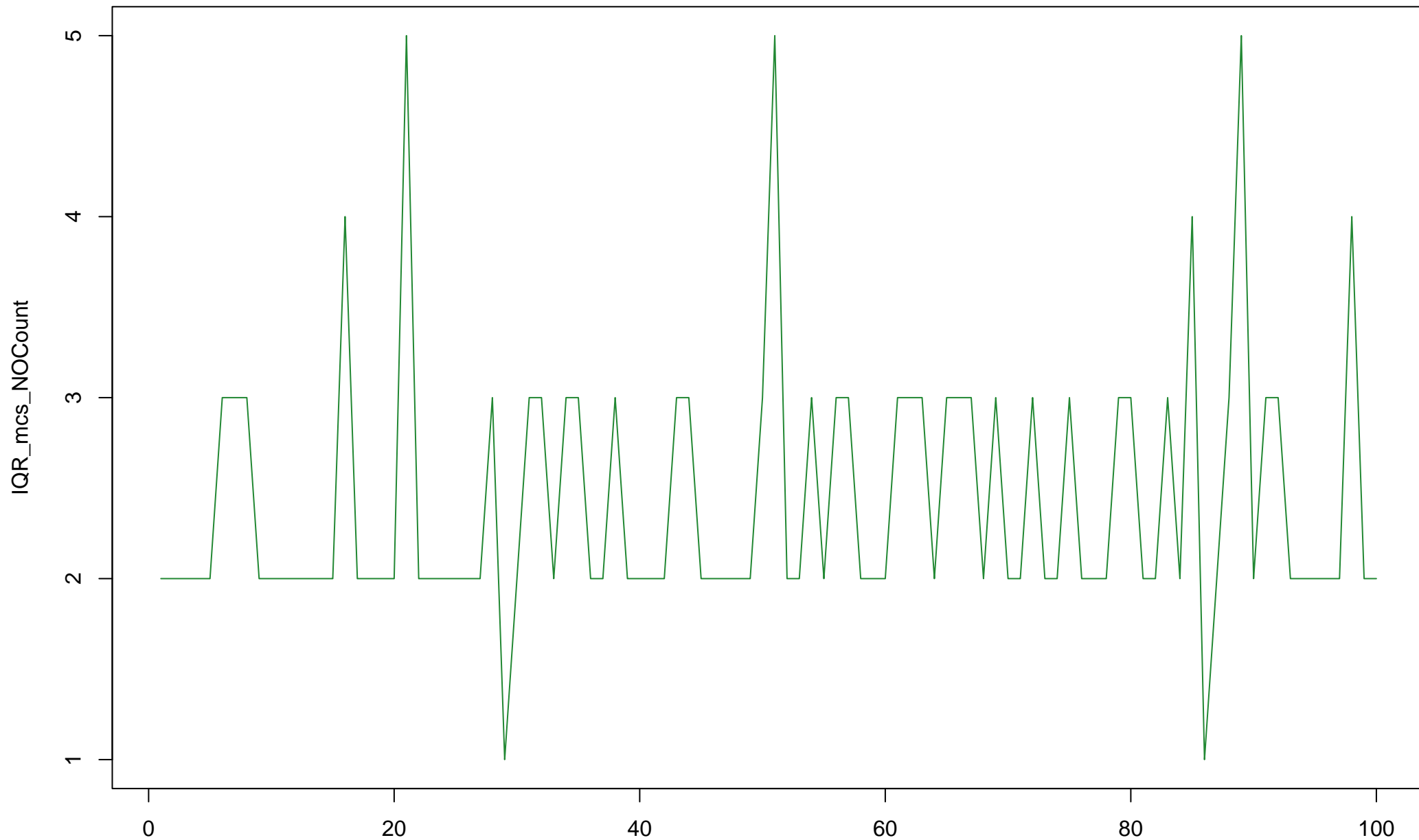
IQR_mcs_RingCount
ESS = 100 | BMK = 0.0744 | MCSE(6.27) = 10.5 | stat: FALSE | burn: 0



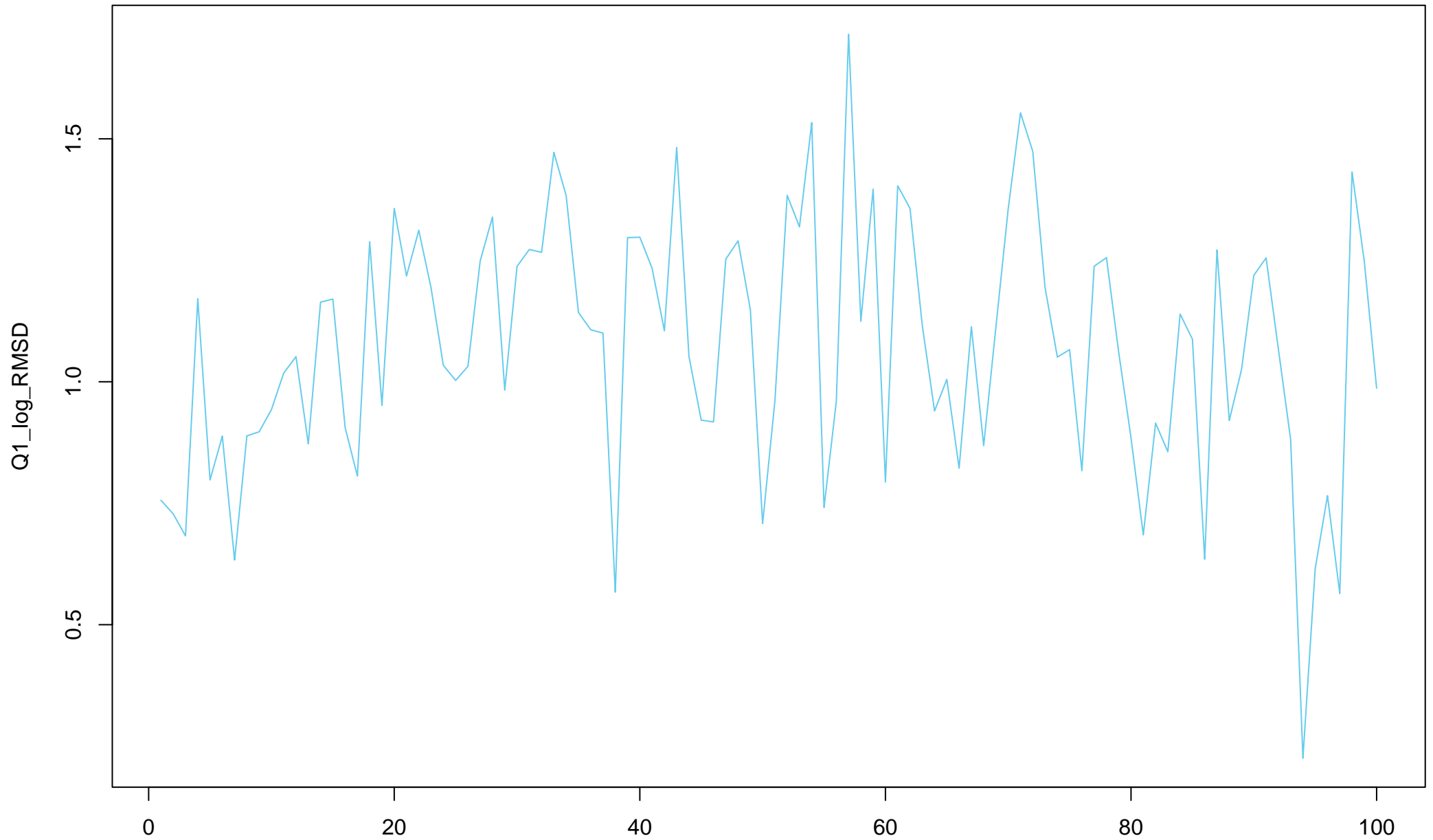
IQR_docked_NumRotatableBonds
ESS = 100 | BMK = 0.155 | MCSE(6.27) = 9.67 | stat: TRUE | burn: 100



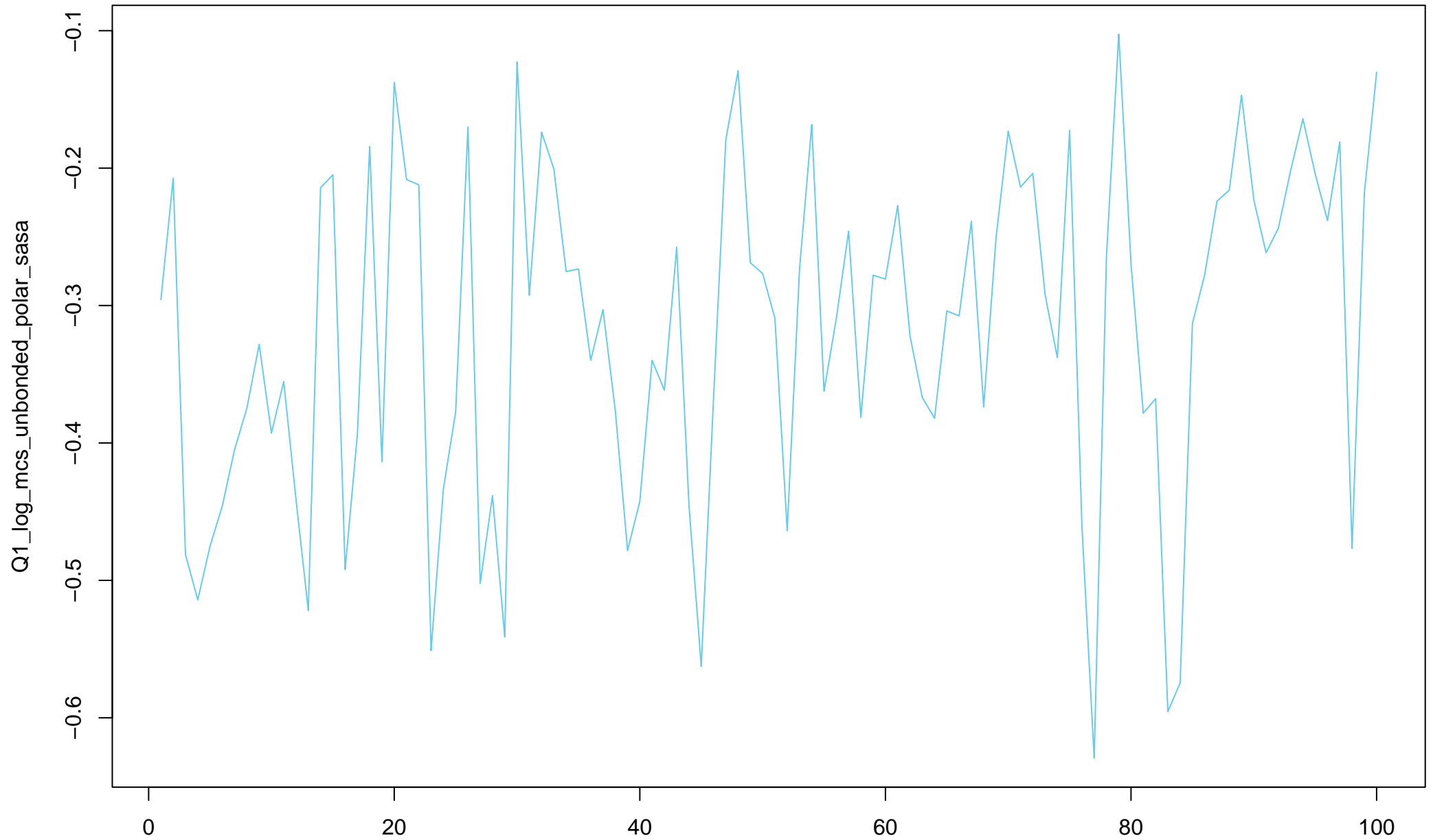
IQR_mcs_NOCCount
ESS = 100 | BMK = 0.125 | MCSE(6.27) = 9.23 | stat: TRUE | burn: 0



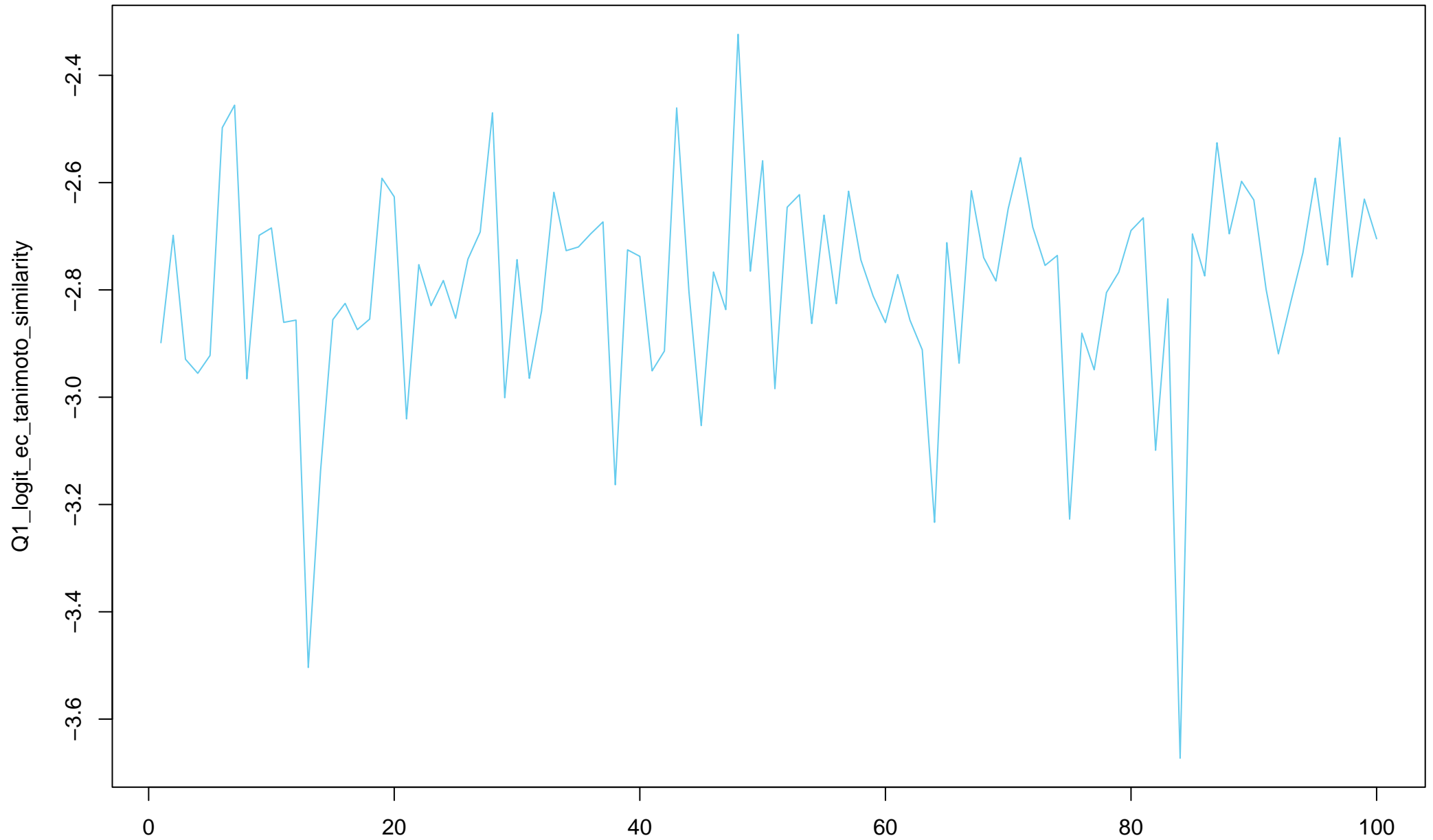
Q1_log_RMSD
ESS = 54.9 | BMK = 0.128 | MCSE(6.27) = 16.7 | stat: FALSE | burn: 0



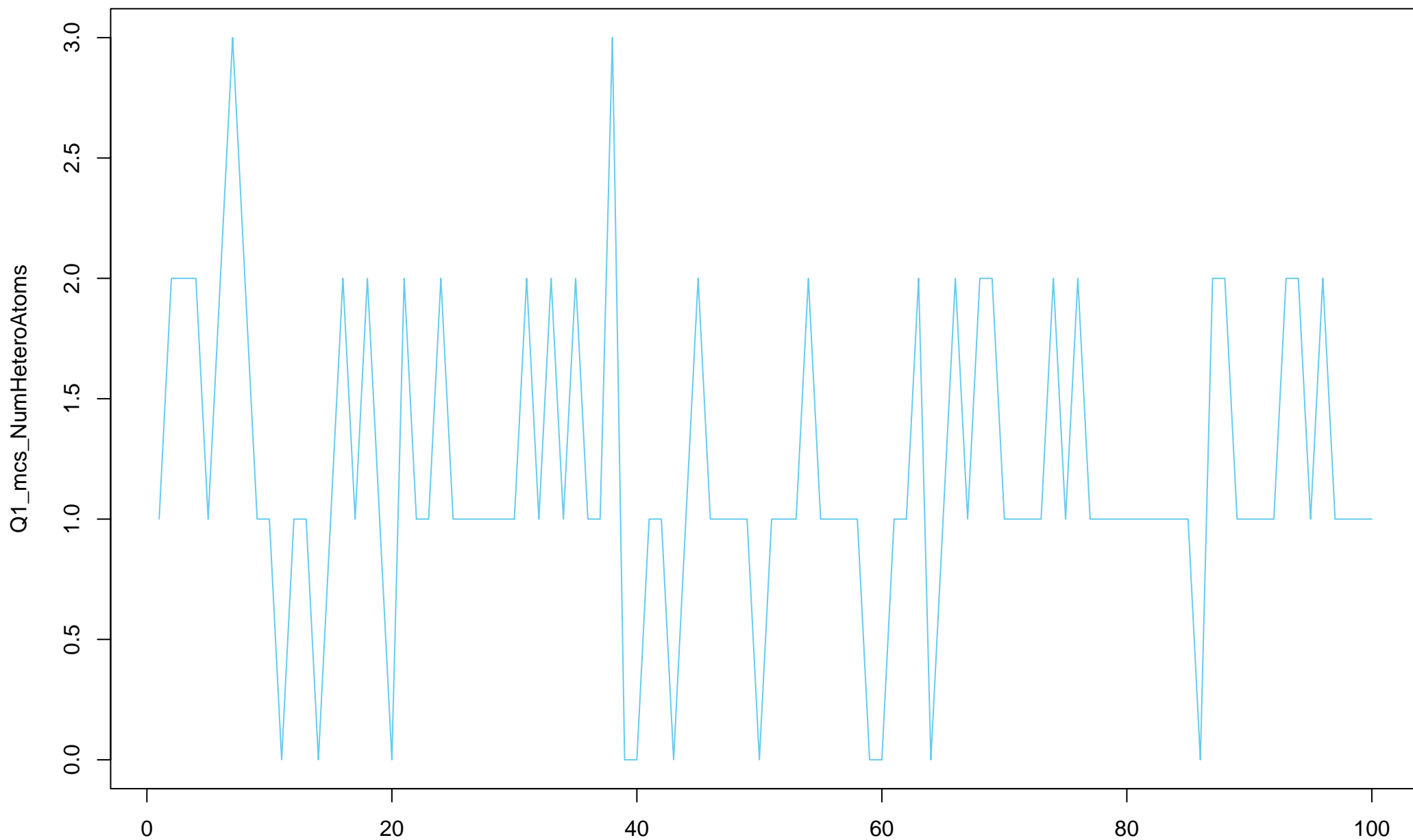
Q1_log_mcs_unbonded_polar_sasa
ESS = 54.1 | BMK = 0.219 | MCSE(6.27) = 14.5 | stat: TRUE | burn: 0



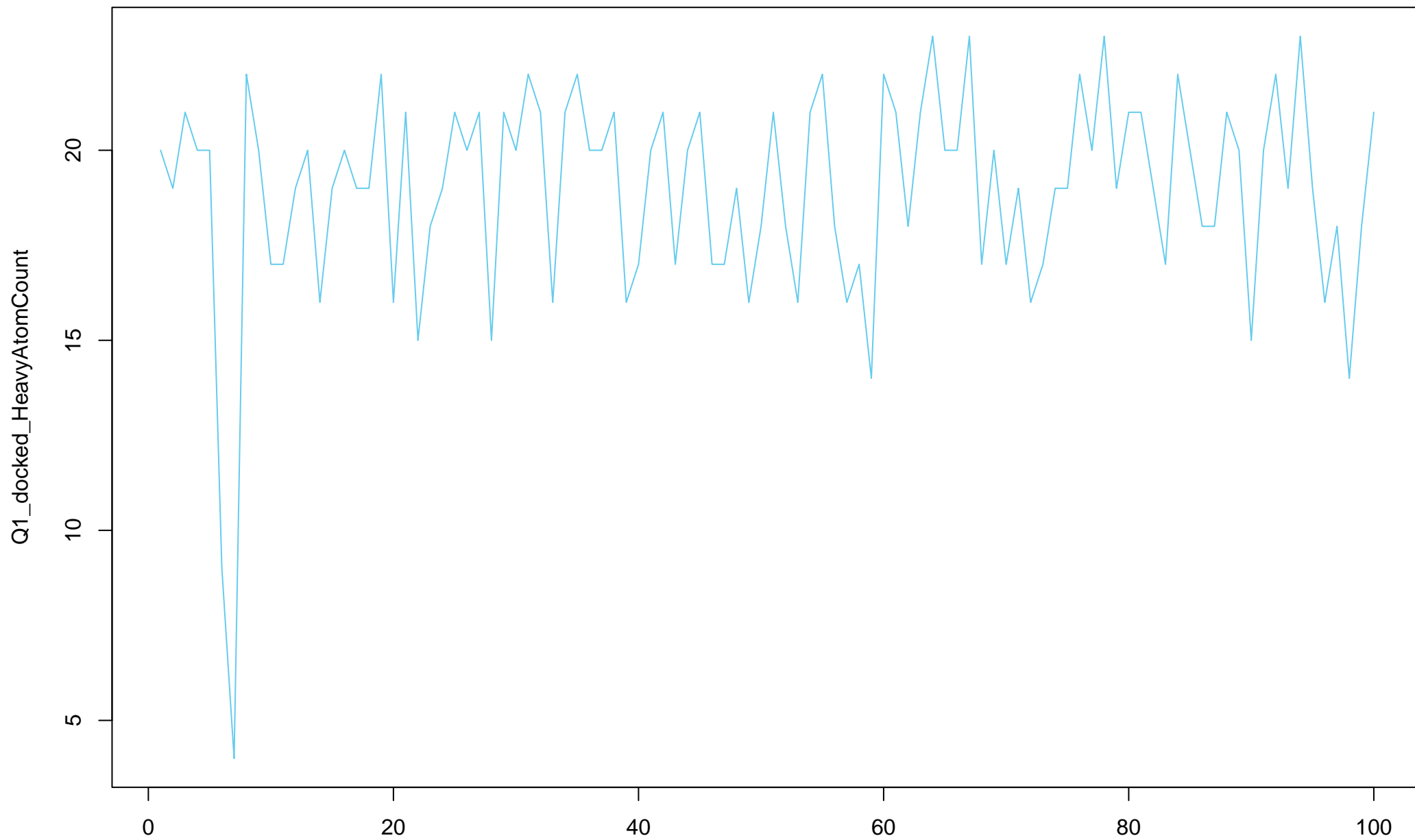
Q1_logit_ec_tanimoto_similarity
ESS = 100 | BMK = 0.203 | MCSE(6.27) = 12.2 | stat: TRUE | burn: 20



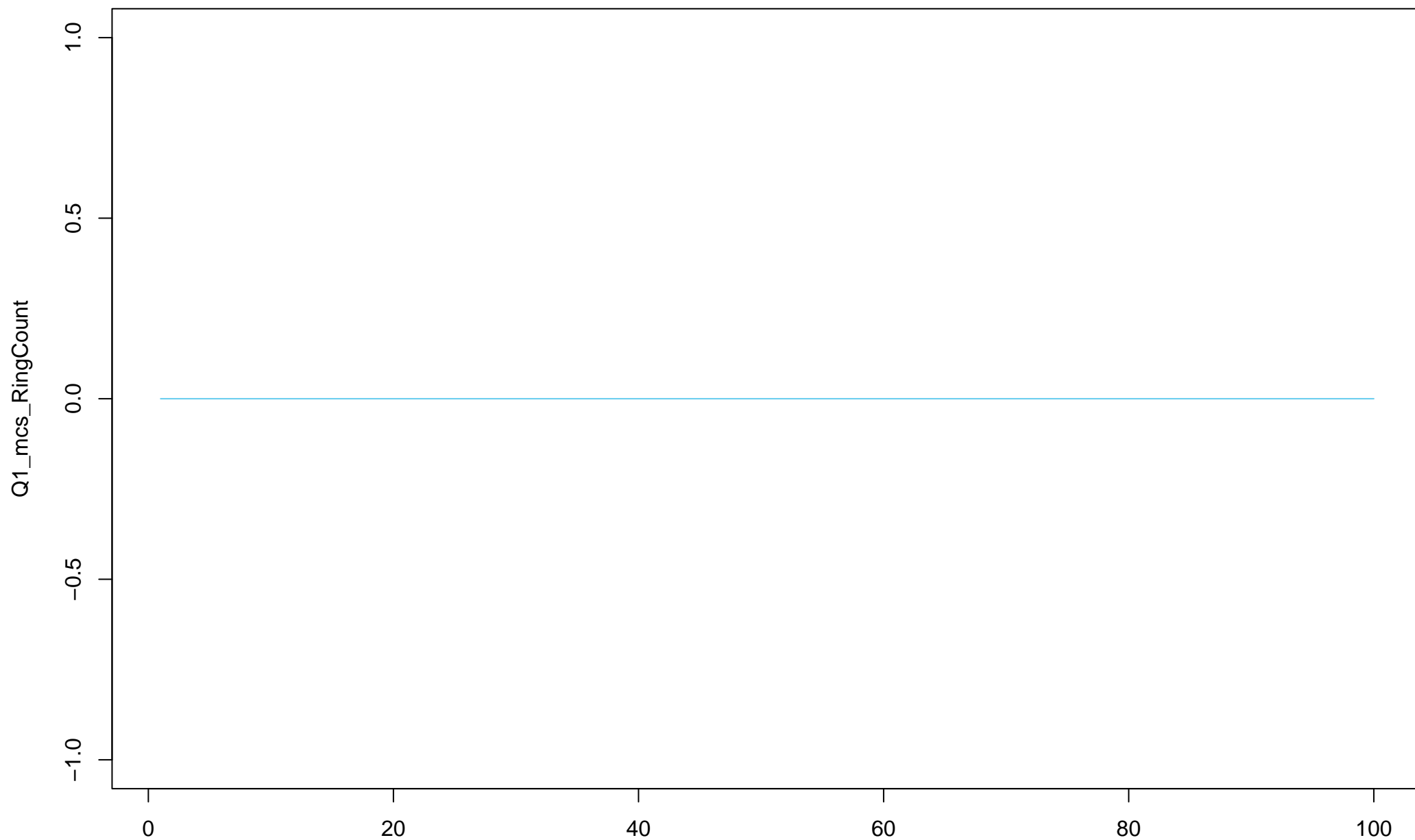
Q1_mcs_NumHeteroAtoms
ESS = 100 | BMK = 0.163 | MCSE(6.27) = 11 | stat: TRUE | burn: 0



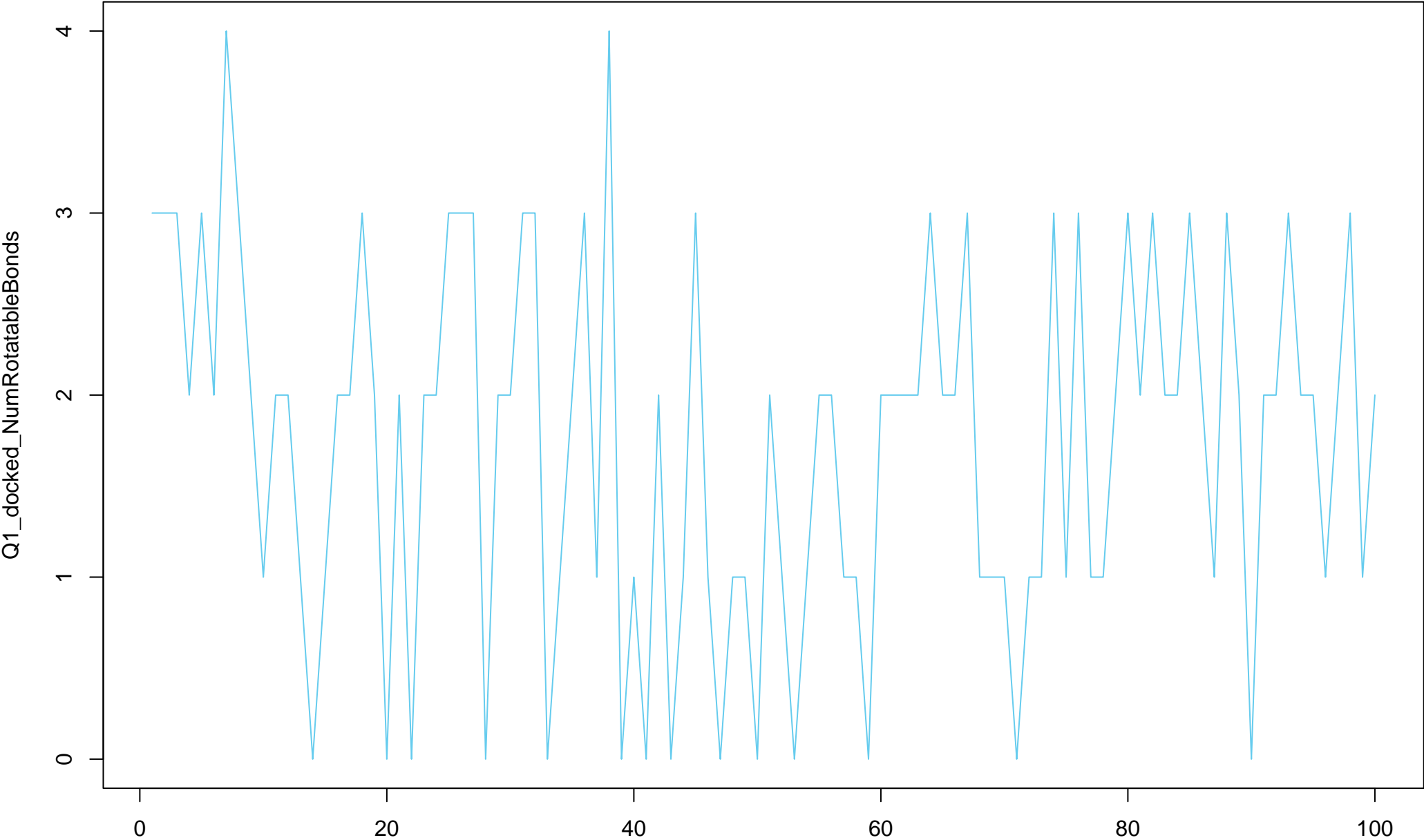
Q1_docked_HeavyAtomCount
ESS = 100 | BMK = 0.136 | MCSE(6.27) = 11.2 | stat: TRUE | burn: 0



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

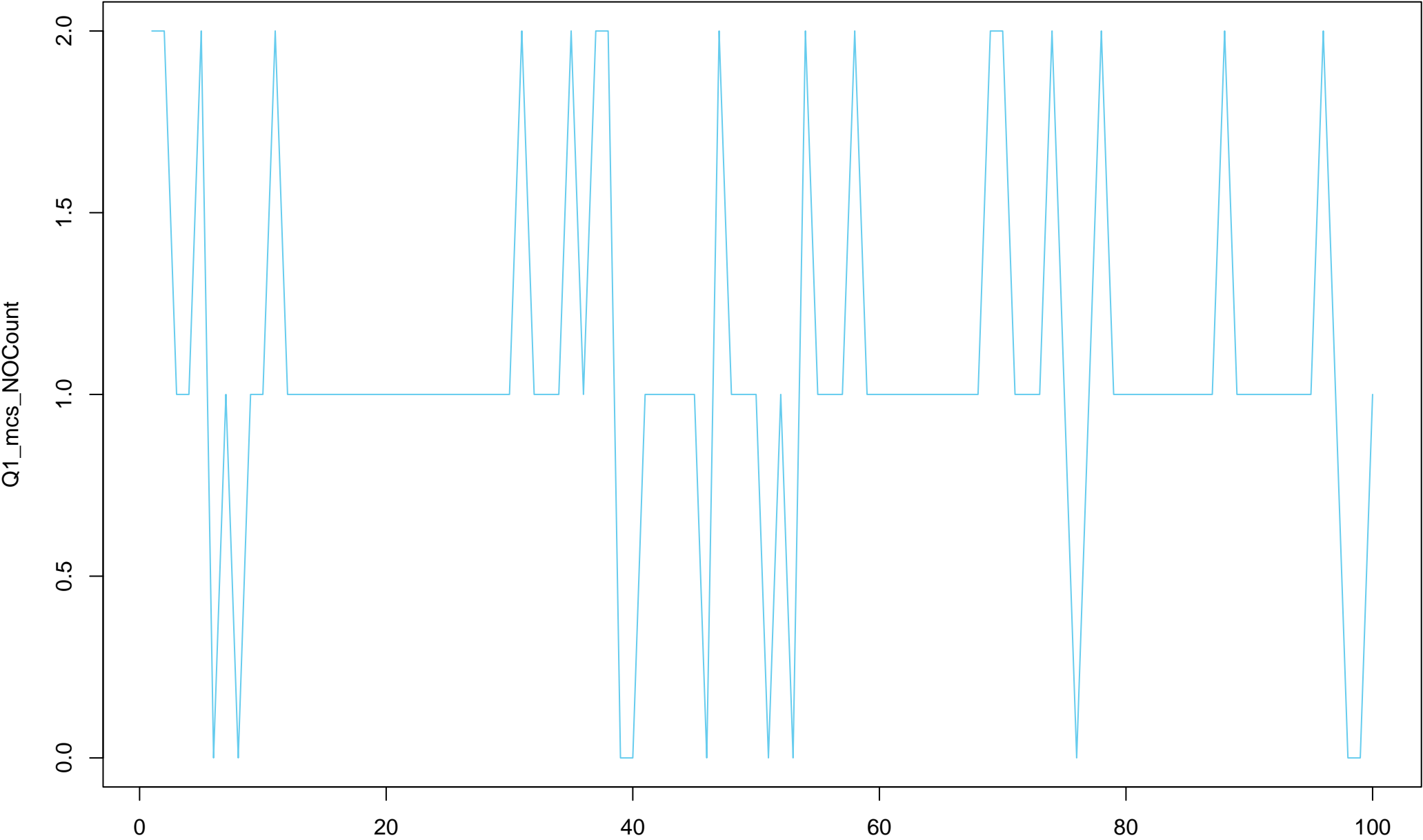


Q1_docked_NumRotatableBonds
ESS = 100 | BMK = 0.167 | MCSE(6.27) = 15.1 | stat: FALSE | burn: 0

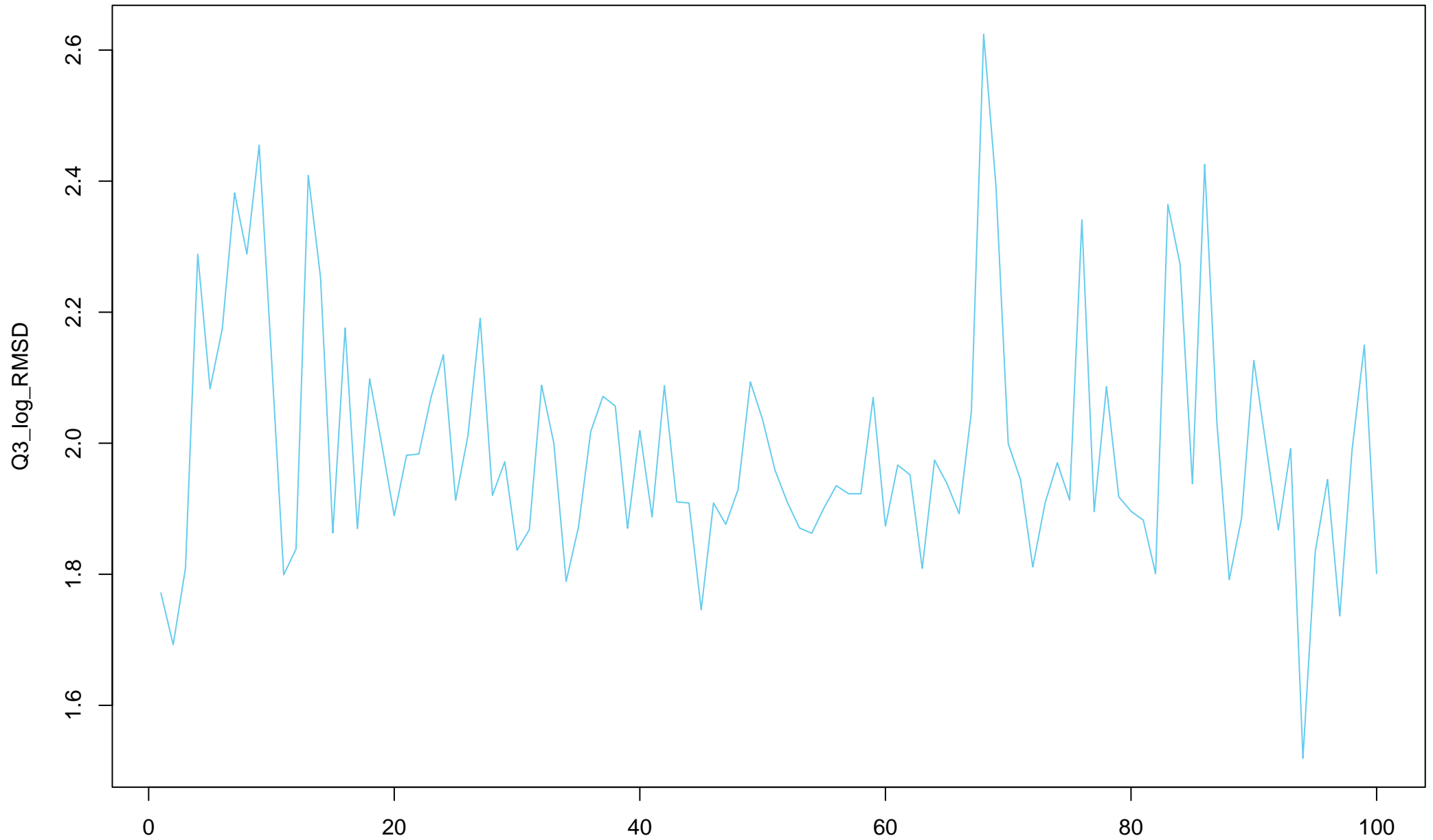


Q1_mcs_NOCount

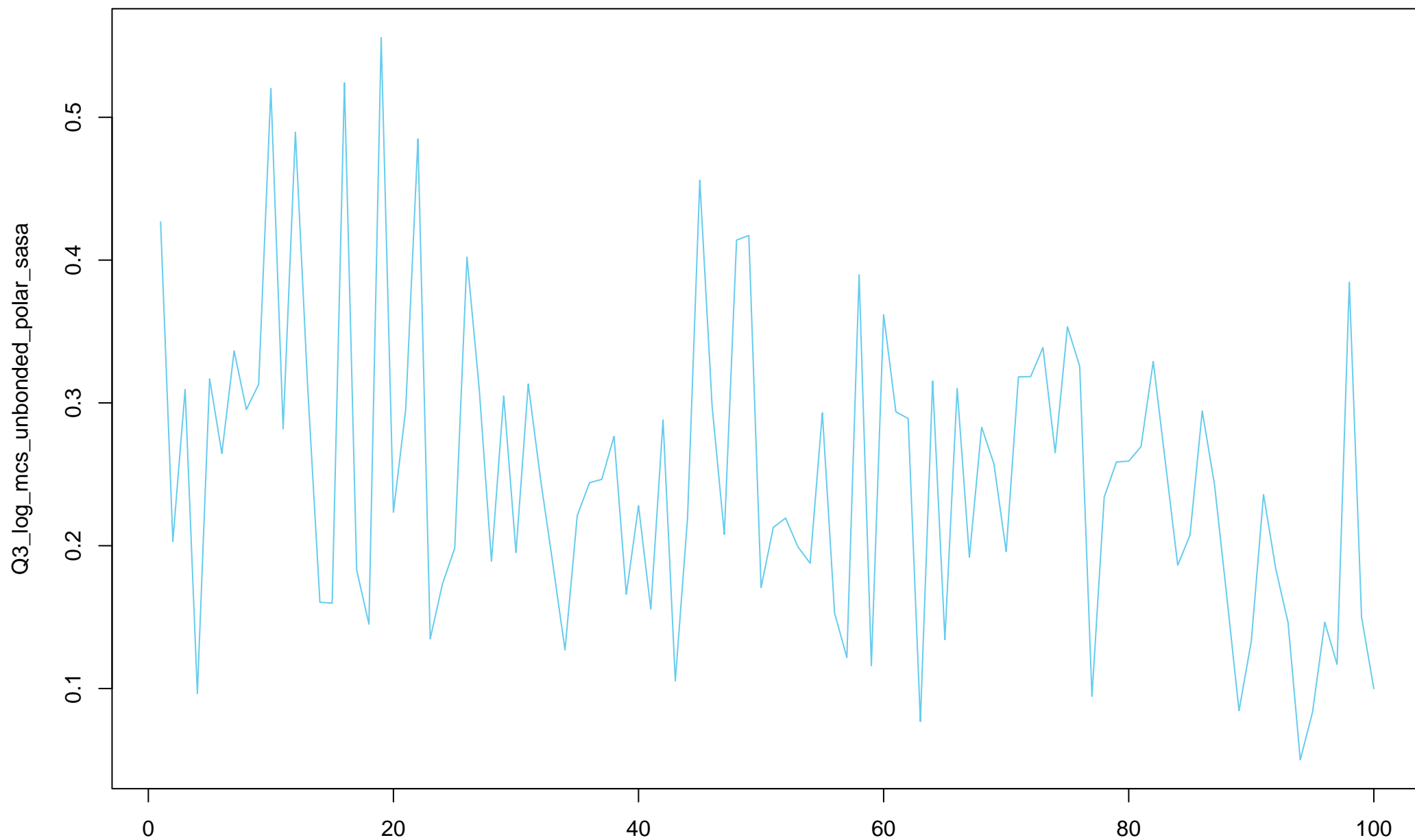
ESS = 100 | BMK = 0.0204 | MCSE(6.27) = 10.2 | stat: TRUE | burn: 0



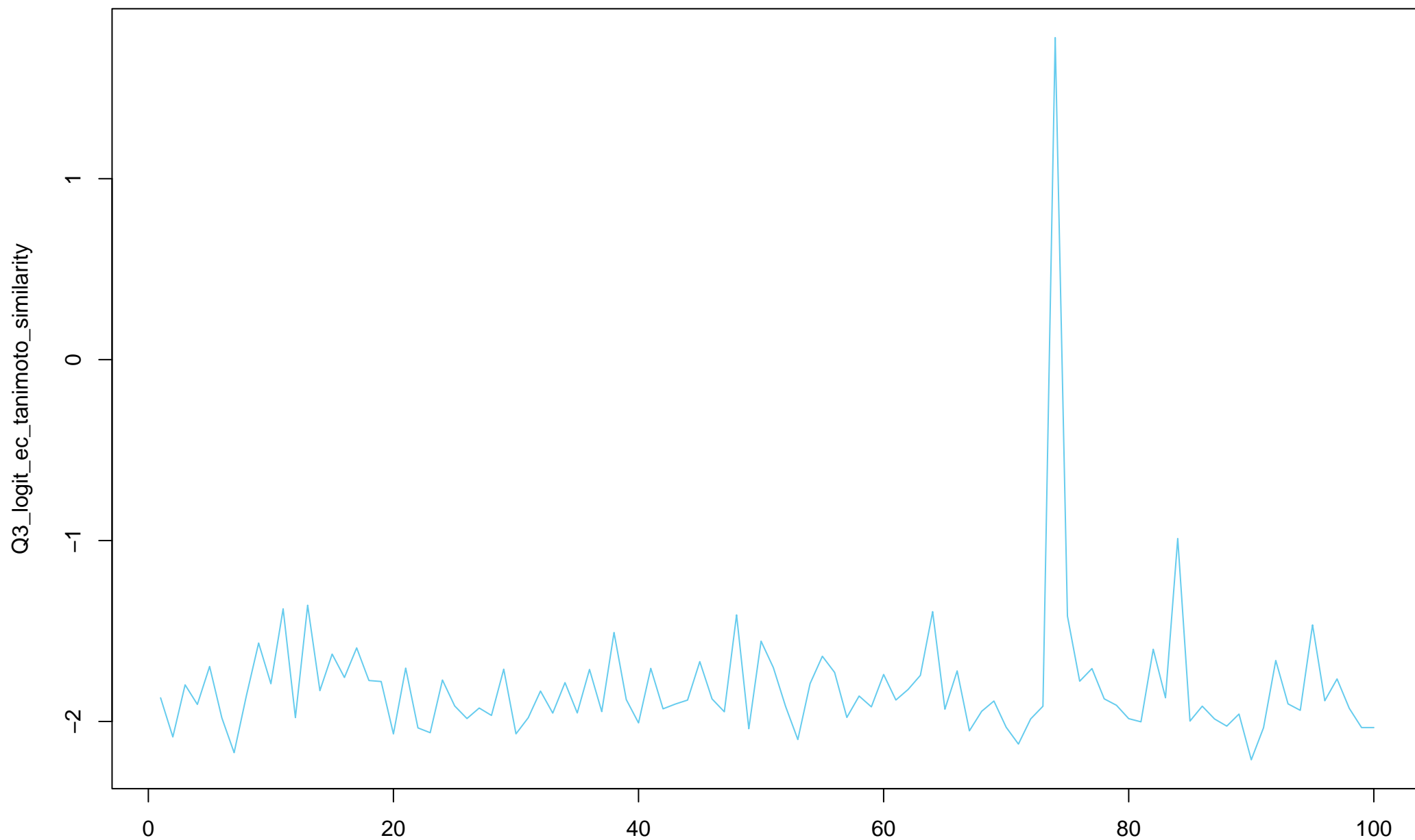
Q3_log_RMSD
ESS = 56 | BMK = 0.231 | MCSE(6.27) = 15.3 | stat: TRUE | burn: 60



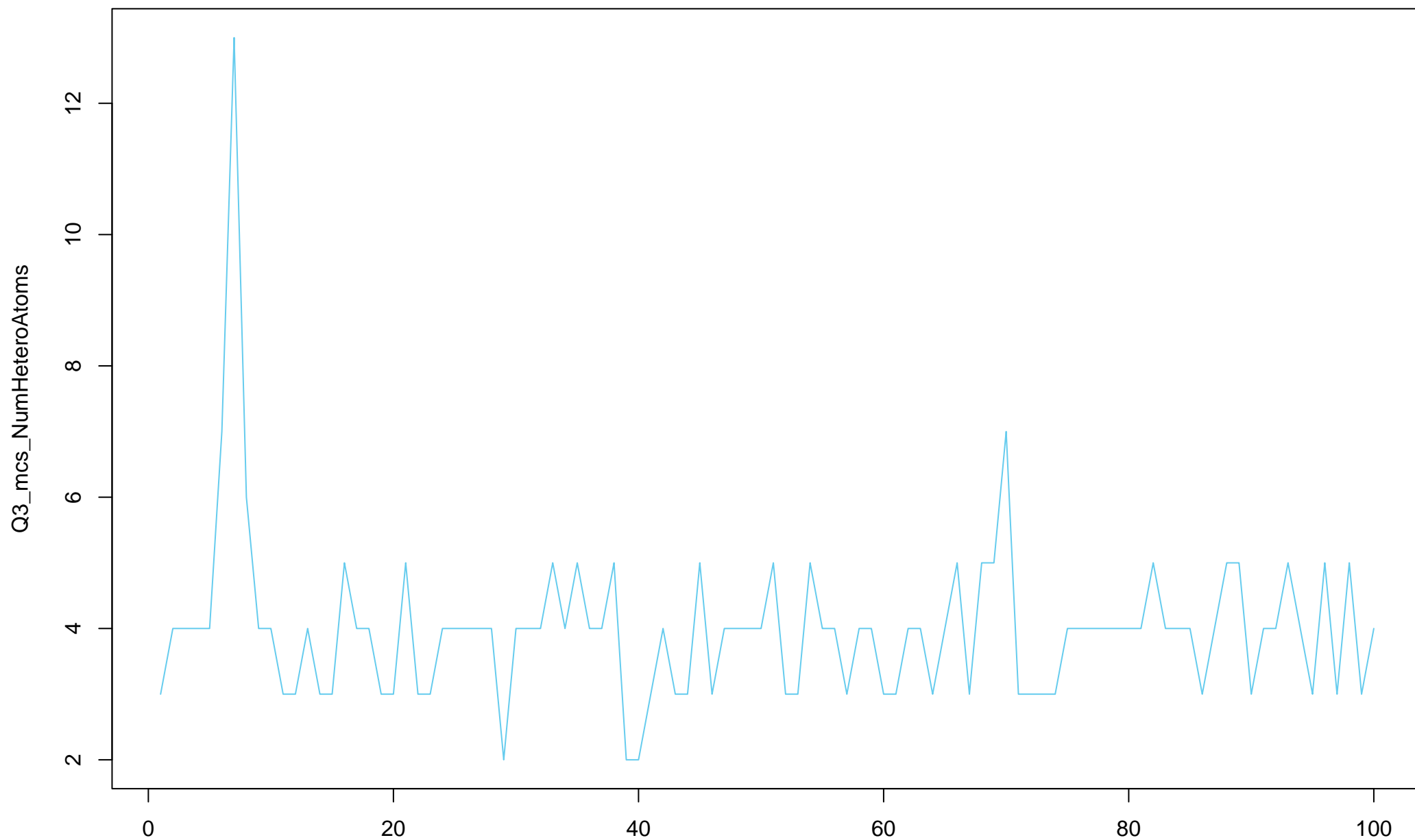
Q3_log_mcs_unbonded_polar_sasa
ESS = 100 | BMK = 0.239 | MCSE(6.27) = 10.6 | stat: TRUE | burn: 0



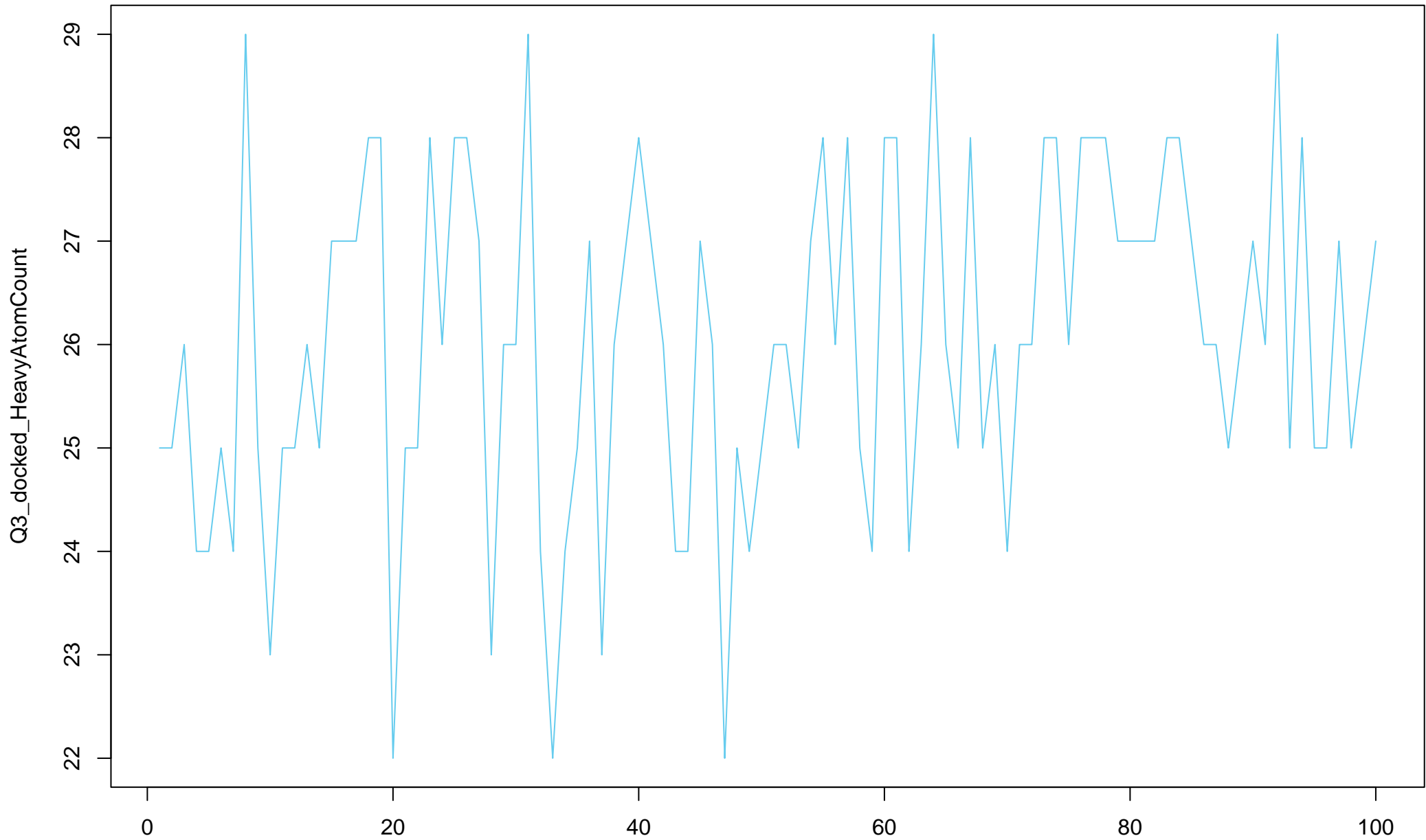
Q3_logit_ec_tanimoto_similarity
ESS = 100 | BMK = 0.15 | MCSE(6.27) = 11.2 | stat: TRUE | burn: 80



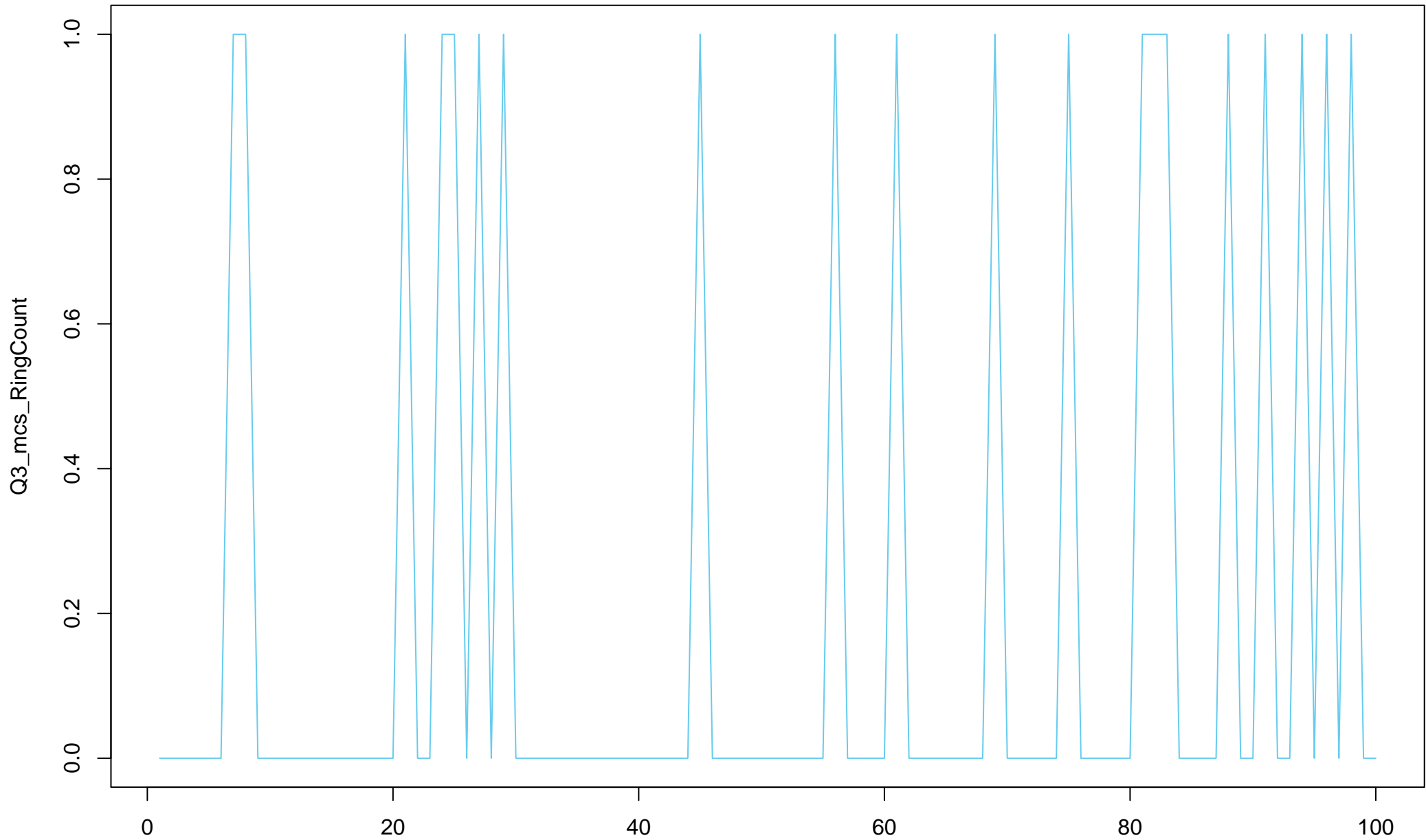
Q3_mcs_NumHeteroAtoms
ESS = 54.3 | BMK = 0.162 | MCSE(6.27) = 15 | stat: TRUE | burn: 0



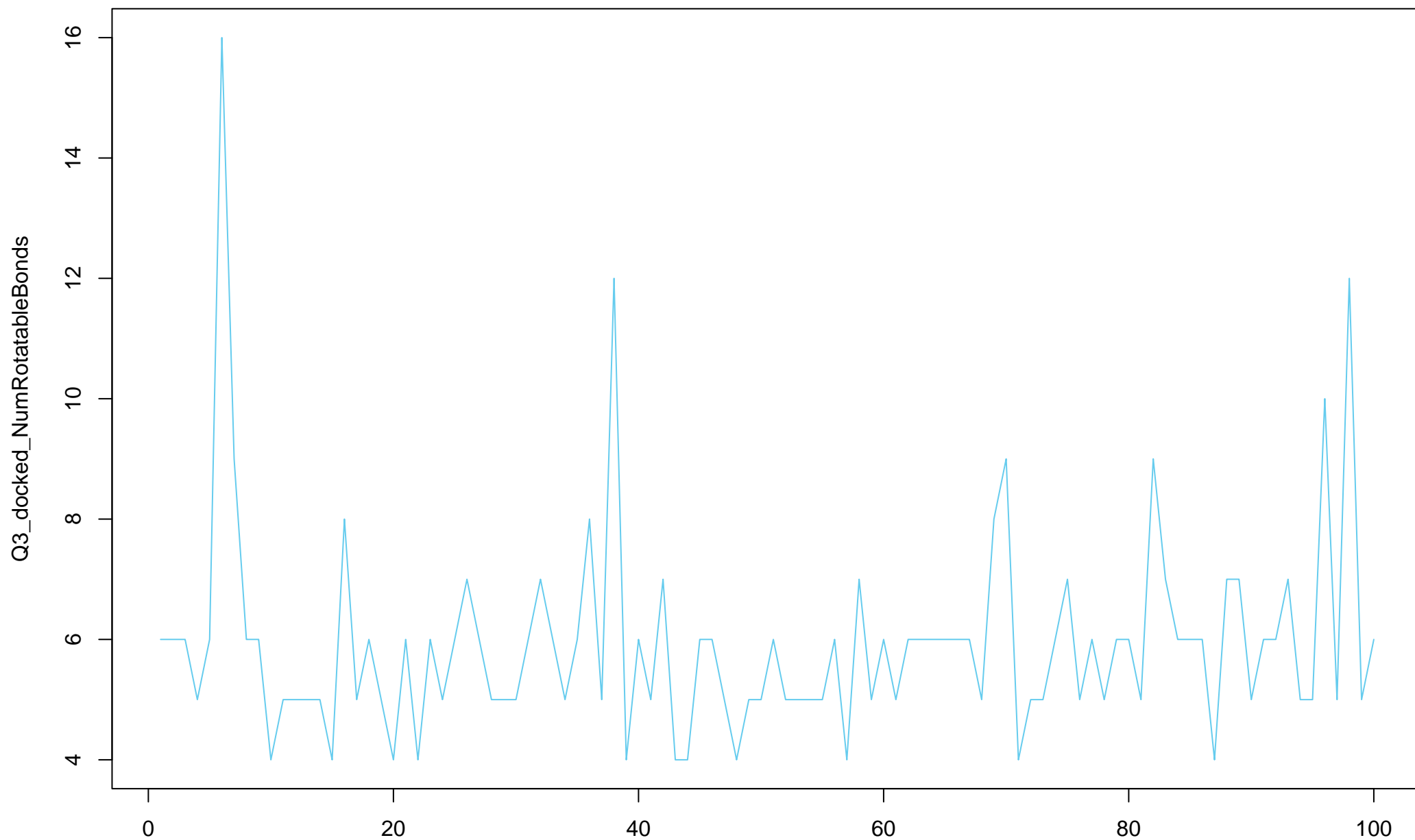
Q3_docked_HeavyAtomCount
ESS = 71.2 | BMK = 0.237 | MCSE(6.27) = 13.2 | stat: FALSE | burn: 0



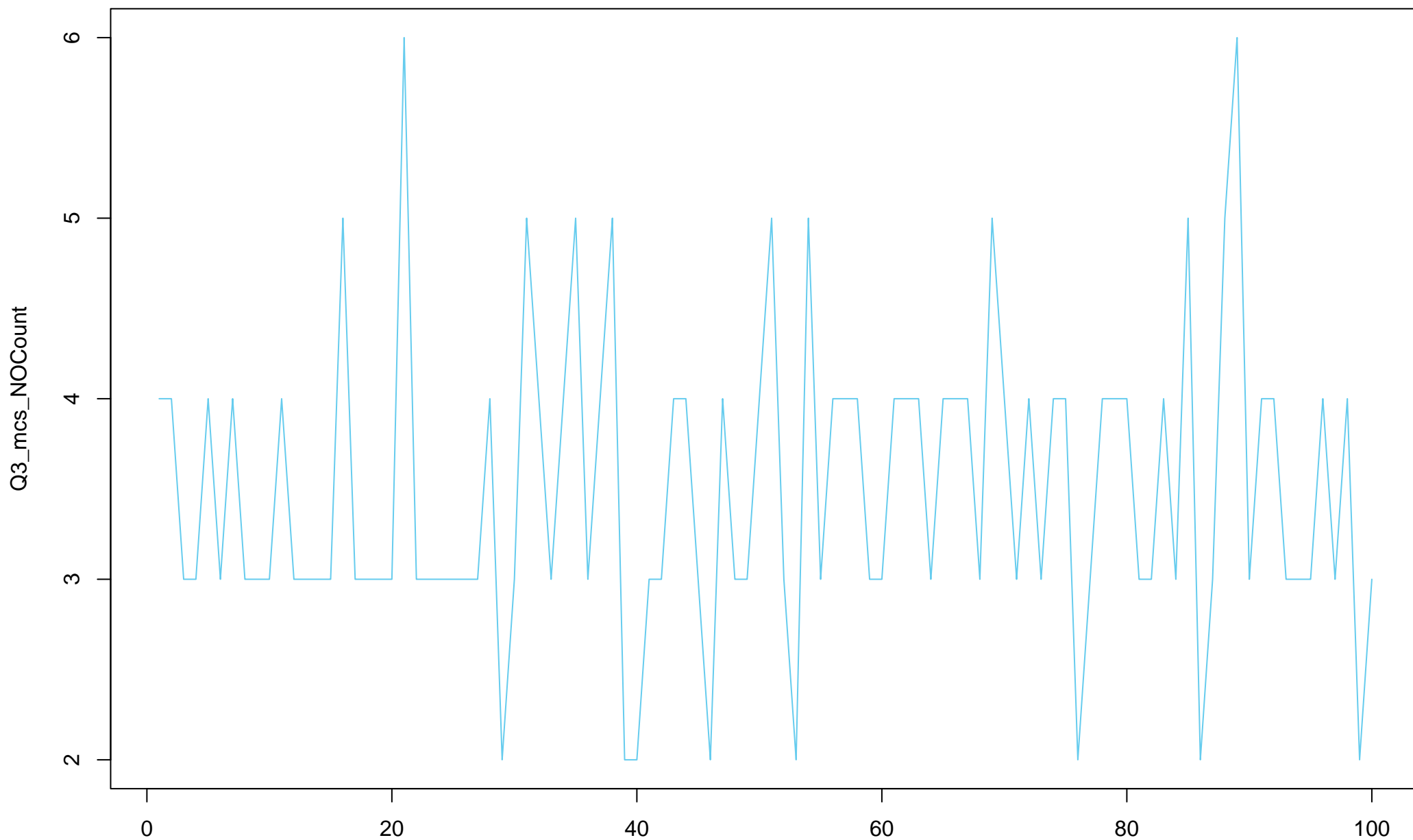
Q3_mcs_RingCount
ESS = 100 | BMK = 0.0744 | MCSE(6.27) = 10.5 | stat: FALSE | burn: 0



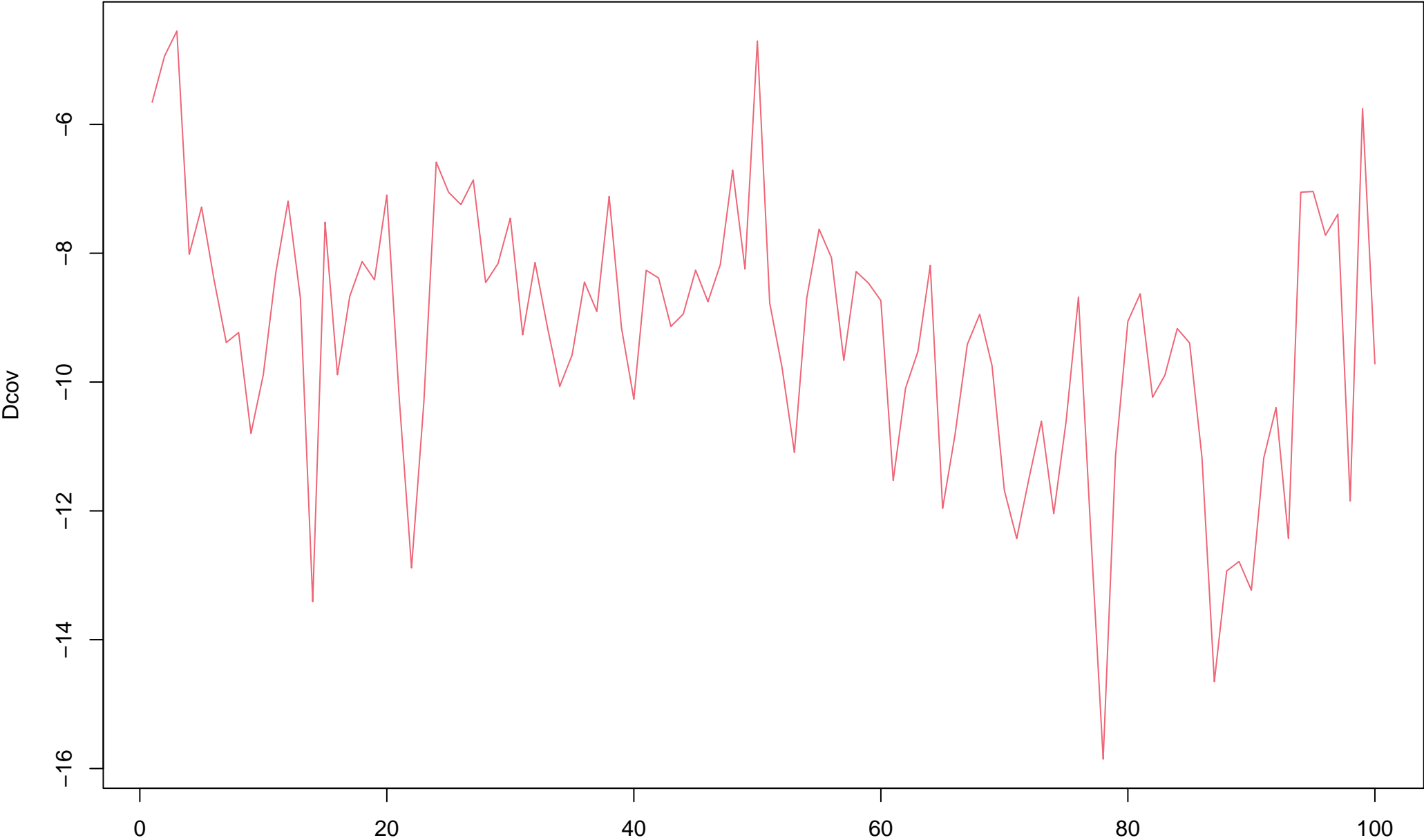
Q3_docked_NumRotatableBonds
ESS = 100 | BMK = 0.167 | MCSE(6.27) = 11.4 | stat: TRUE | burn: 0



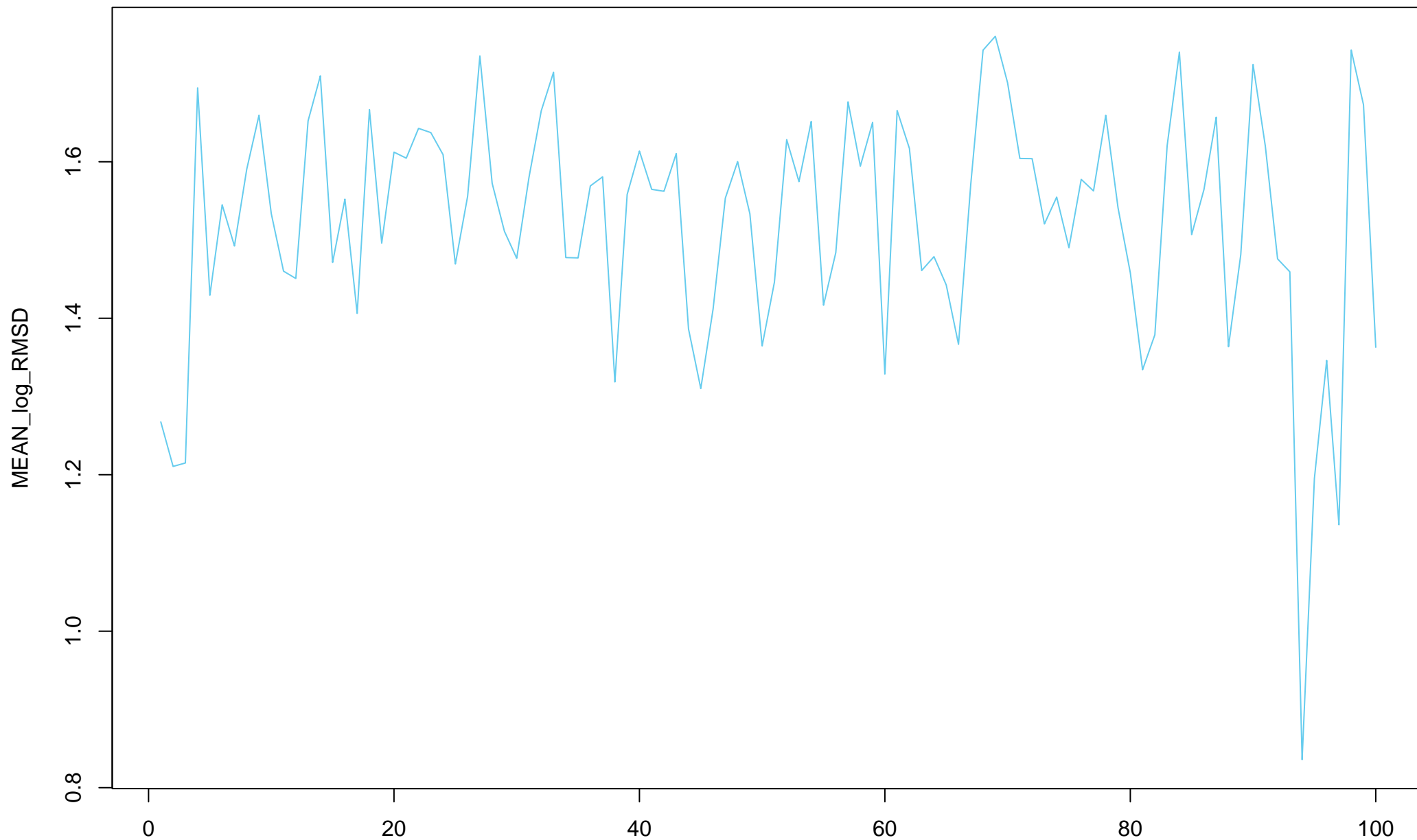
Q3_mcs_NOCount
ESS = 100 | BMK = 0.125 | MCSE(6.27) = 9.11 | stat: TRUE | burn: 0



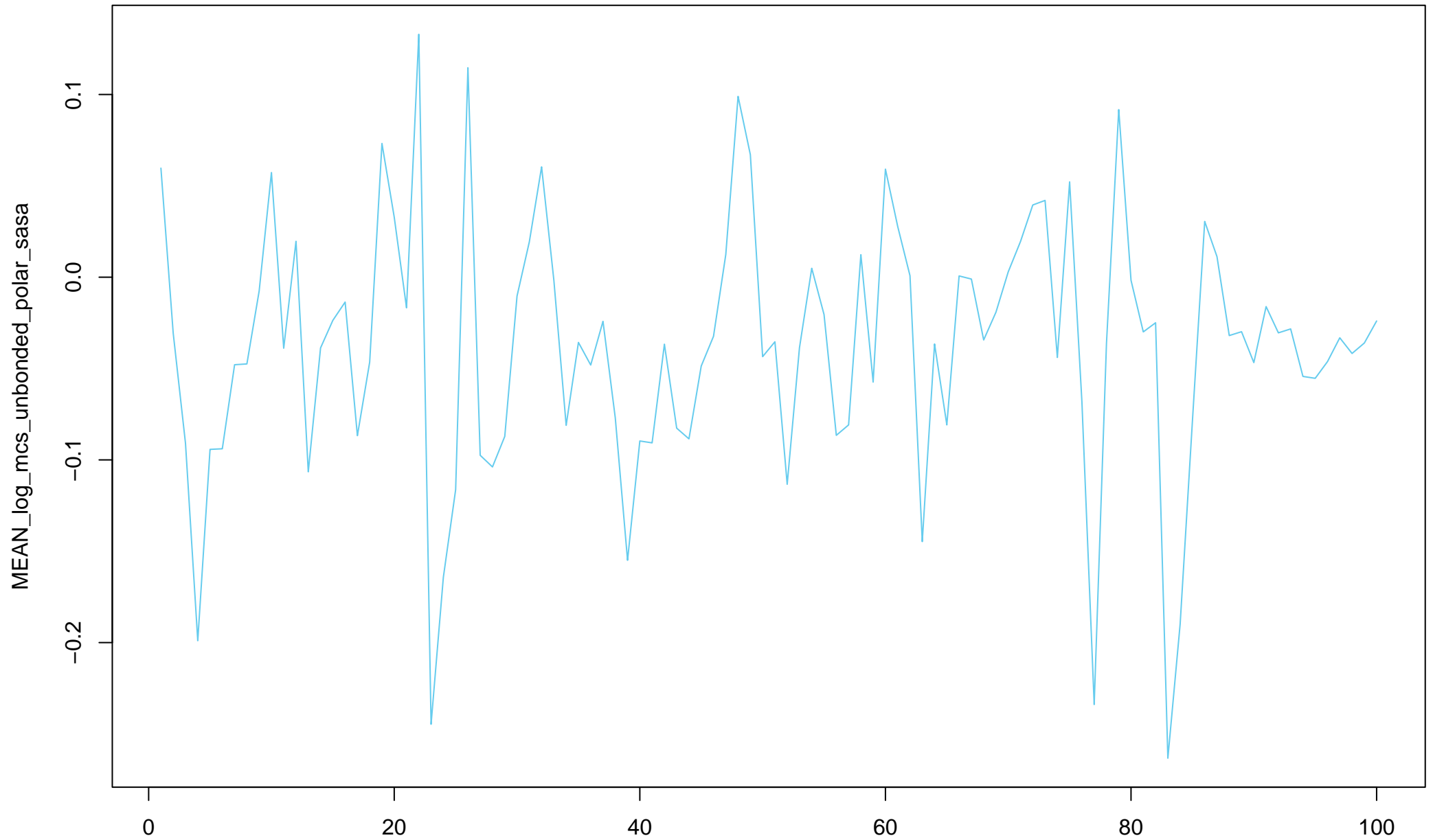
Dcov
ESS = 100 | BMK = 0.467 | MCSE(6.27) = 4.4 | stat: TRUE | burn: 100



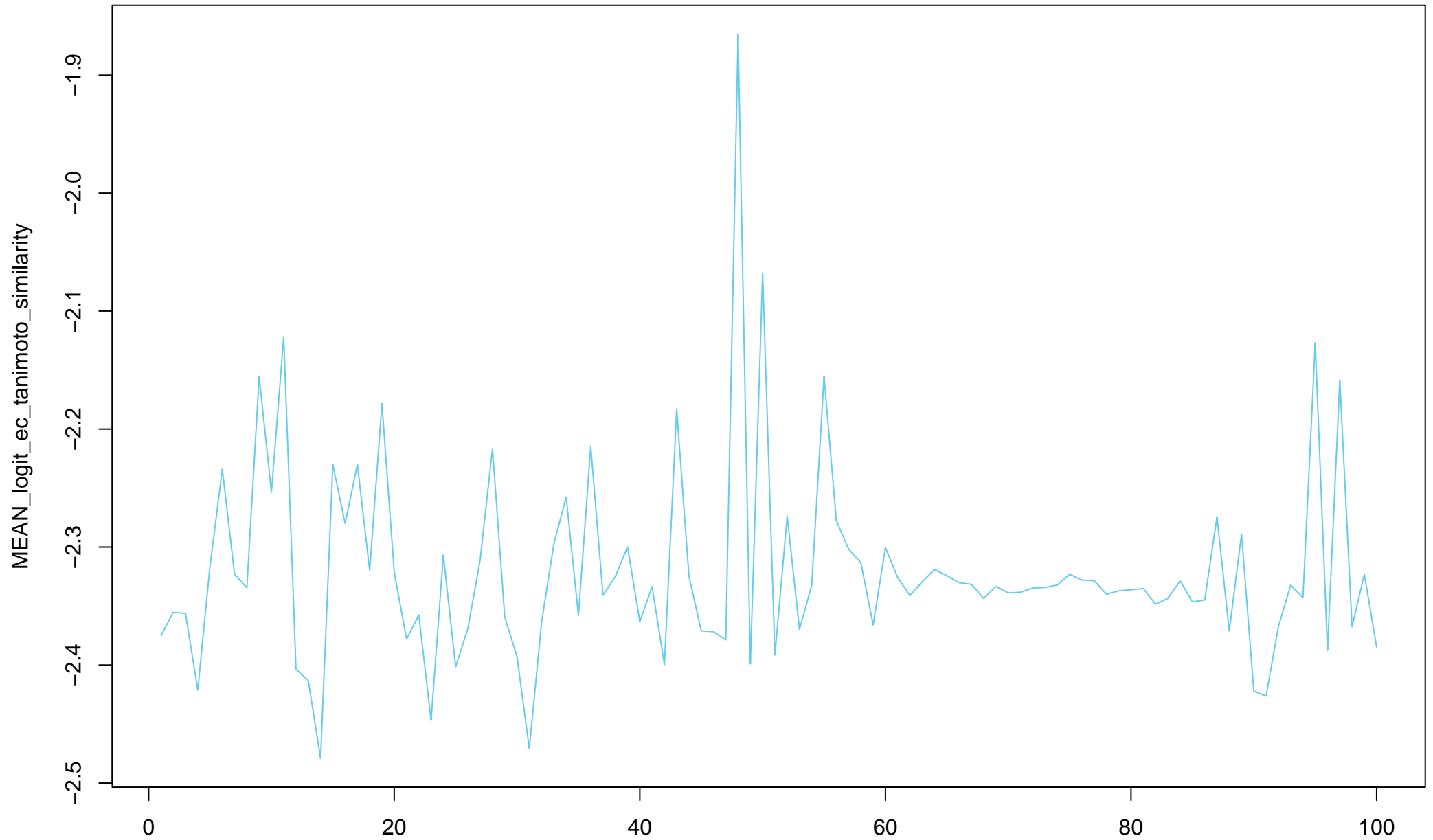
MEAN_log_RMSD
ESS = 52.2 | BMK = 0.137 | MCSE(6.27) = 15.3 | stat: TRUE | burn: 0



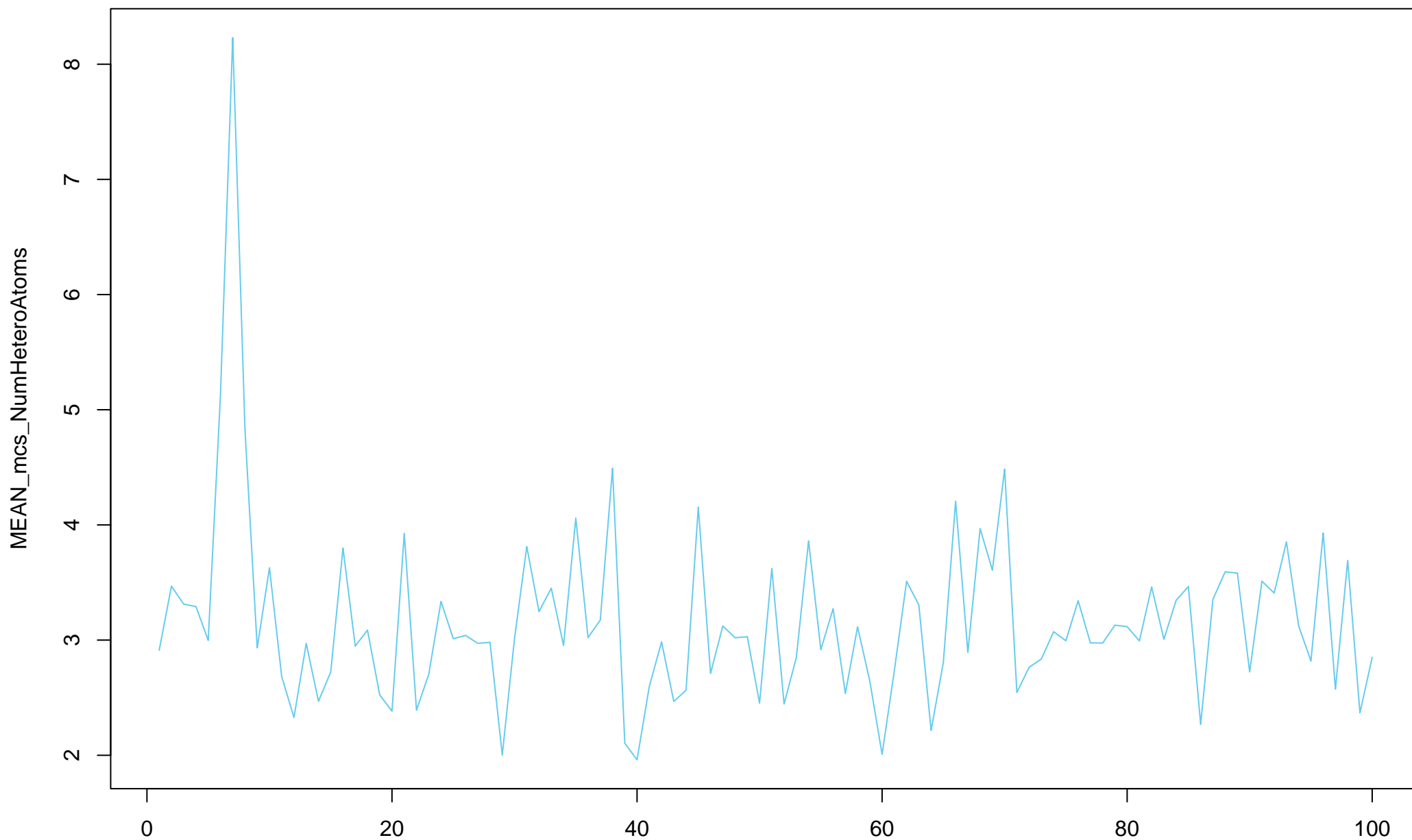
MEAN_log_mcs_unbonded_polar_sasa
ESS = 100 | BMK = 0.217 | MCSE(6.27) = 13.5 | stat: TRUE | burn: 100



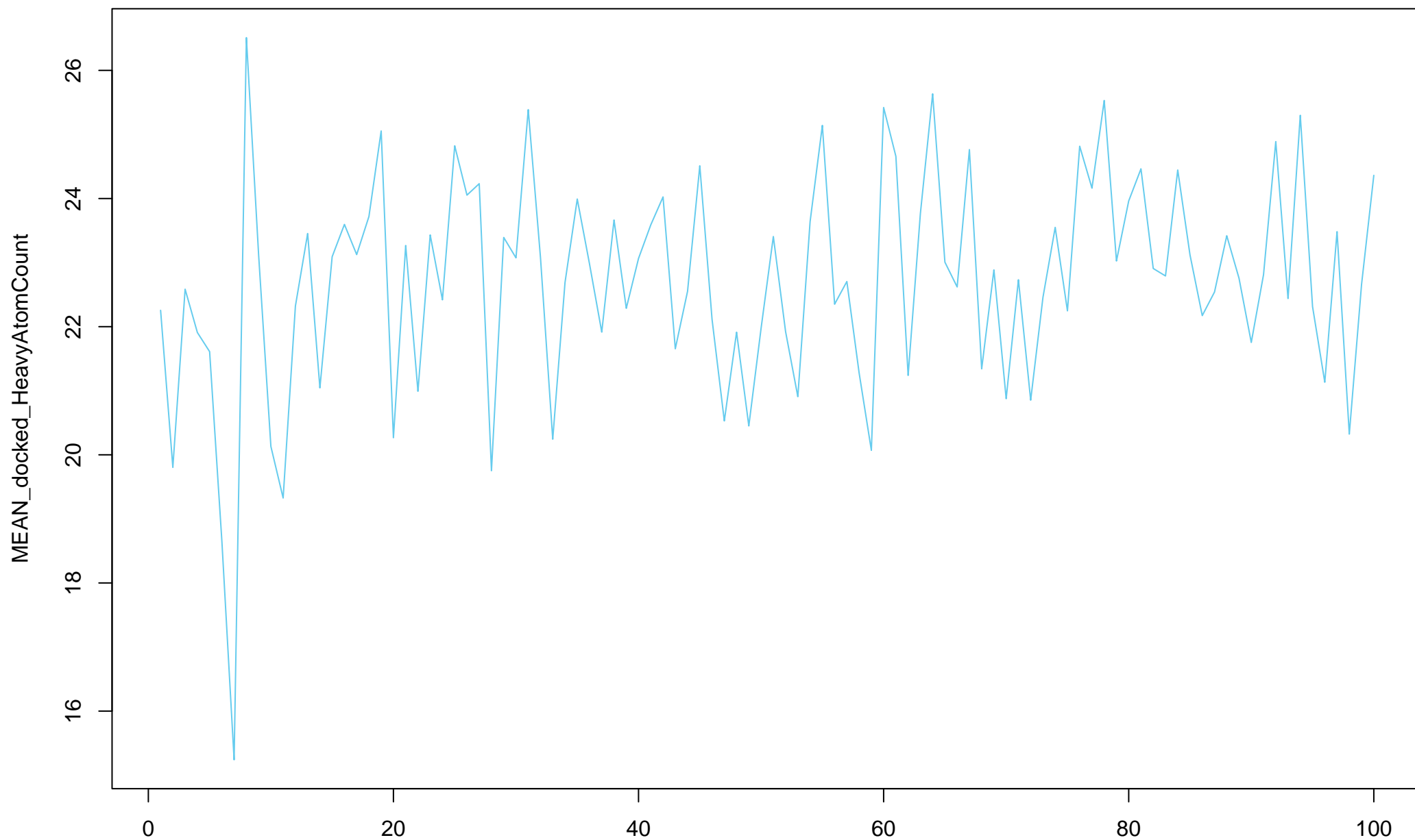
MEAN_logit_ec_tanimoto_similarity
ESS = 100 | BMK = 0.446 | MCSE(6.27) = 10.2 | stat: TRUE | burn: 80



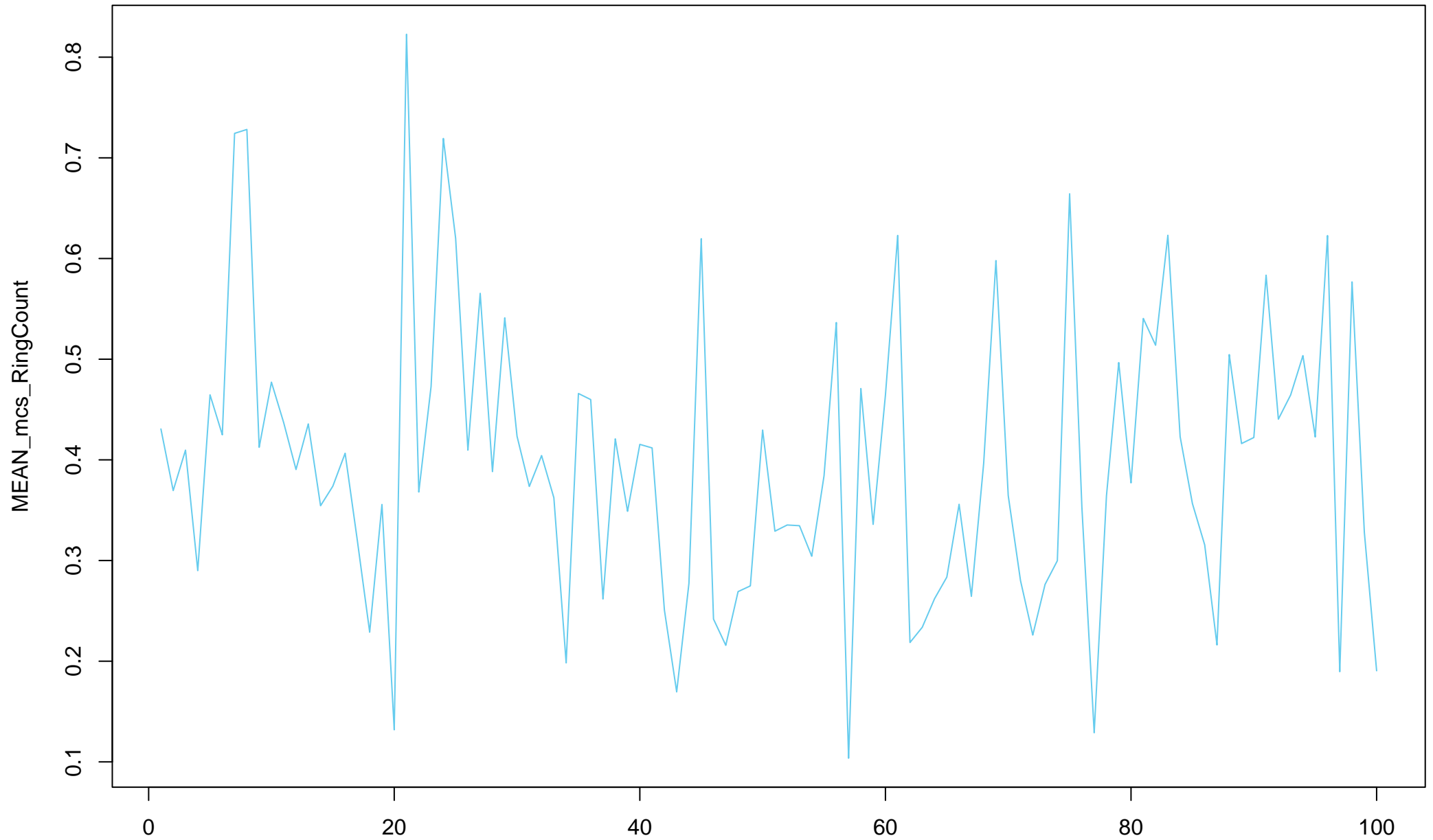
MEAN_mcs_NumHeteroAtoms
ESS = 57.2 | BMK = 0.174 | MCSE(6.27) = 15.9 | stat: TRUE | burn: 70



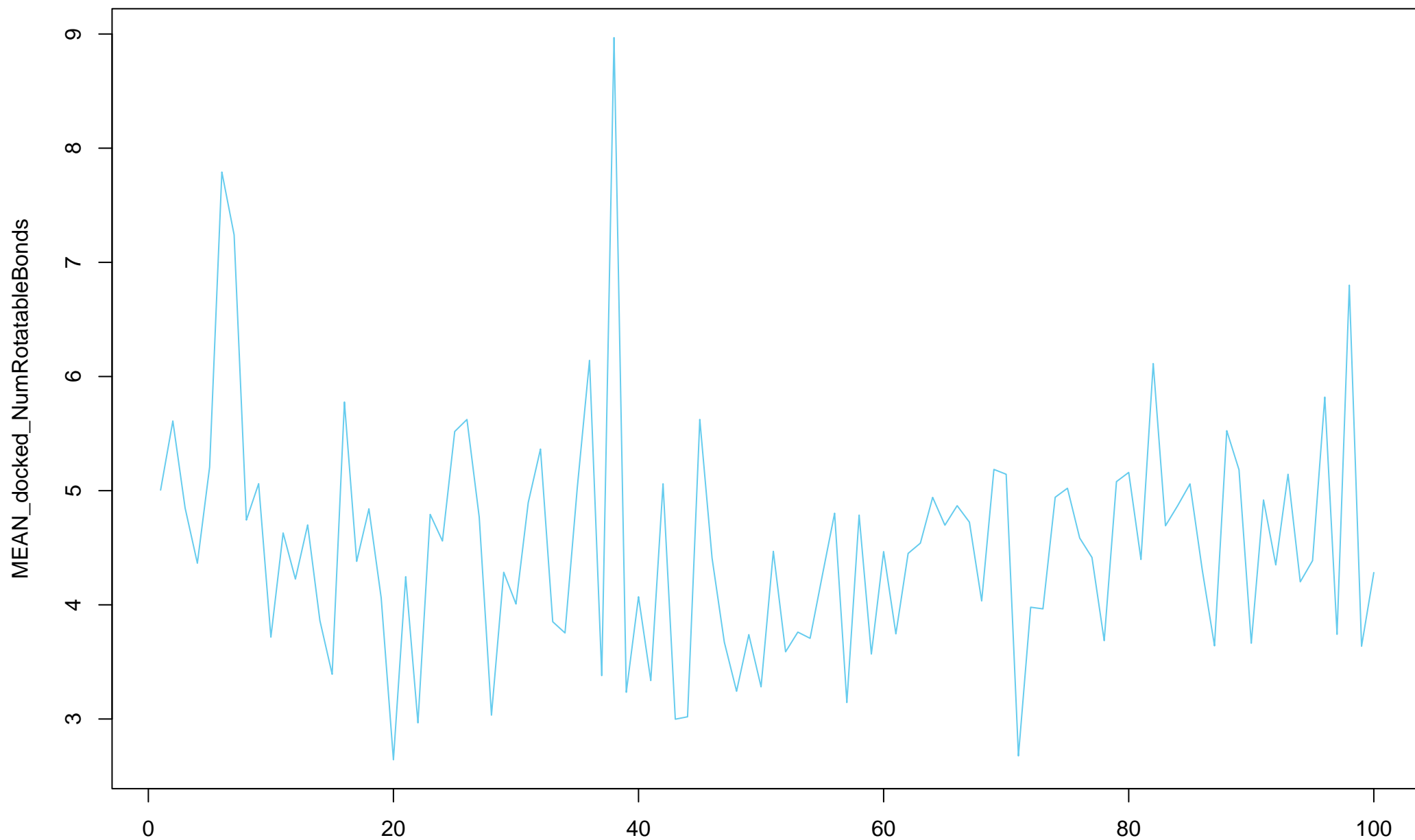
MEAN_docked_HeavyAtomCount
ESS = 100 | BMK = 0.185 | MCSE(6.27) = 10.6 | stat: TRUE | burn: 0



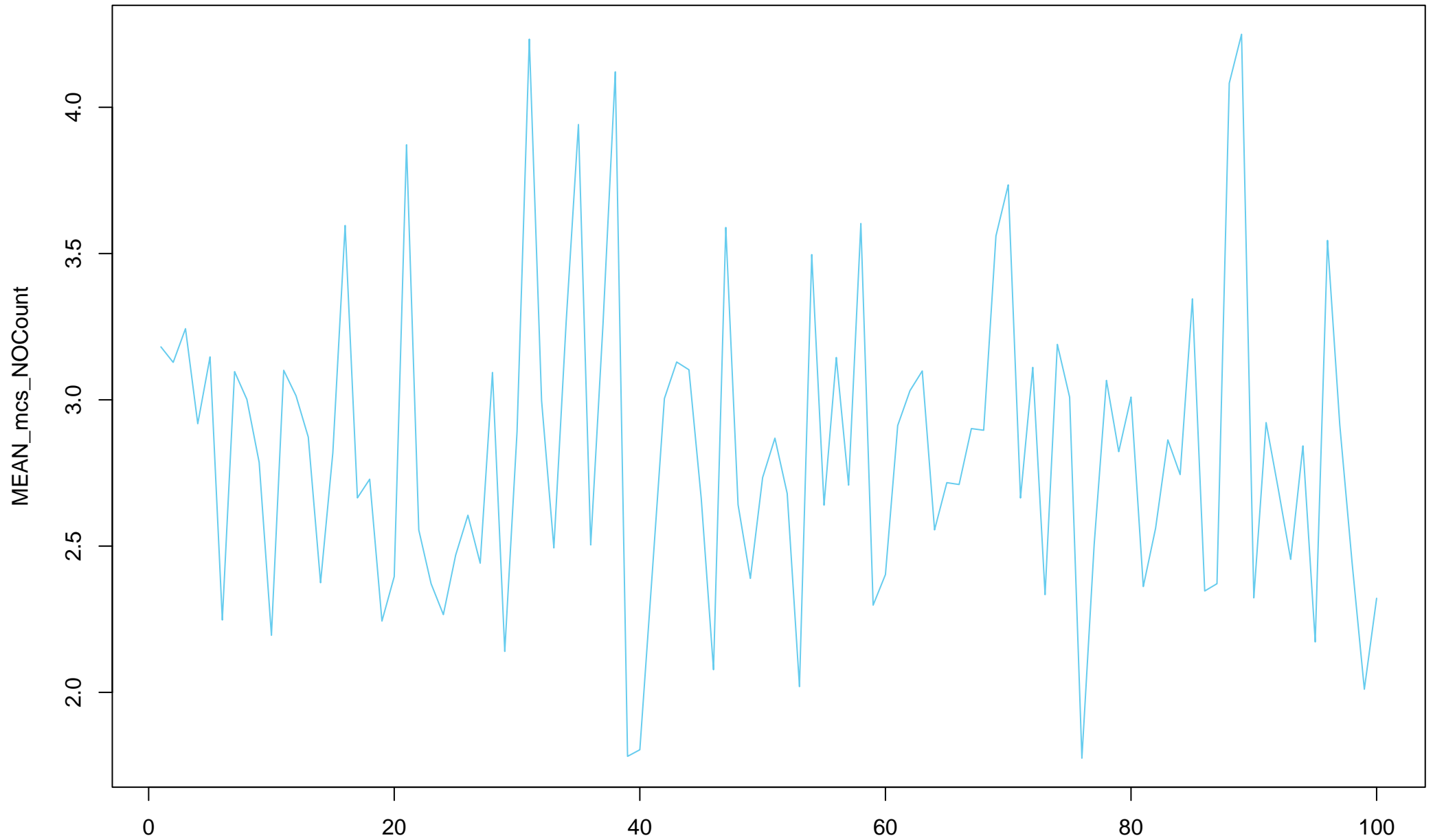
MEAN_mcs_RingCount
ESS = 100 | BMK = 0.179 | MCSE(6.27) = 12.3 | stat: TRUE | burn: 30



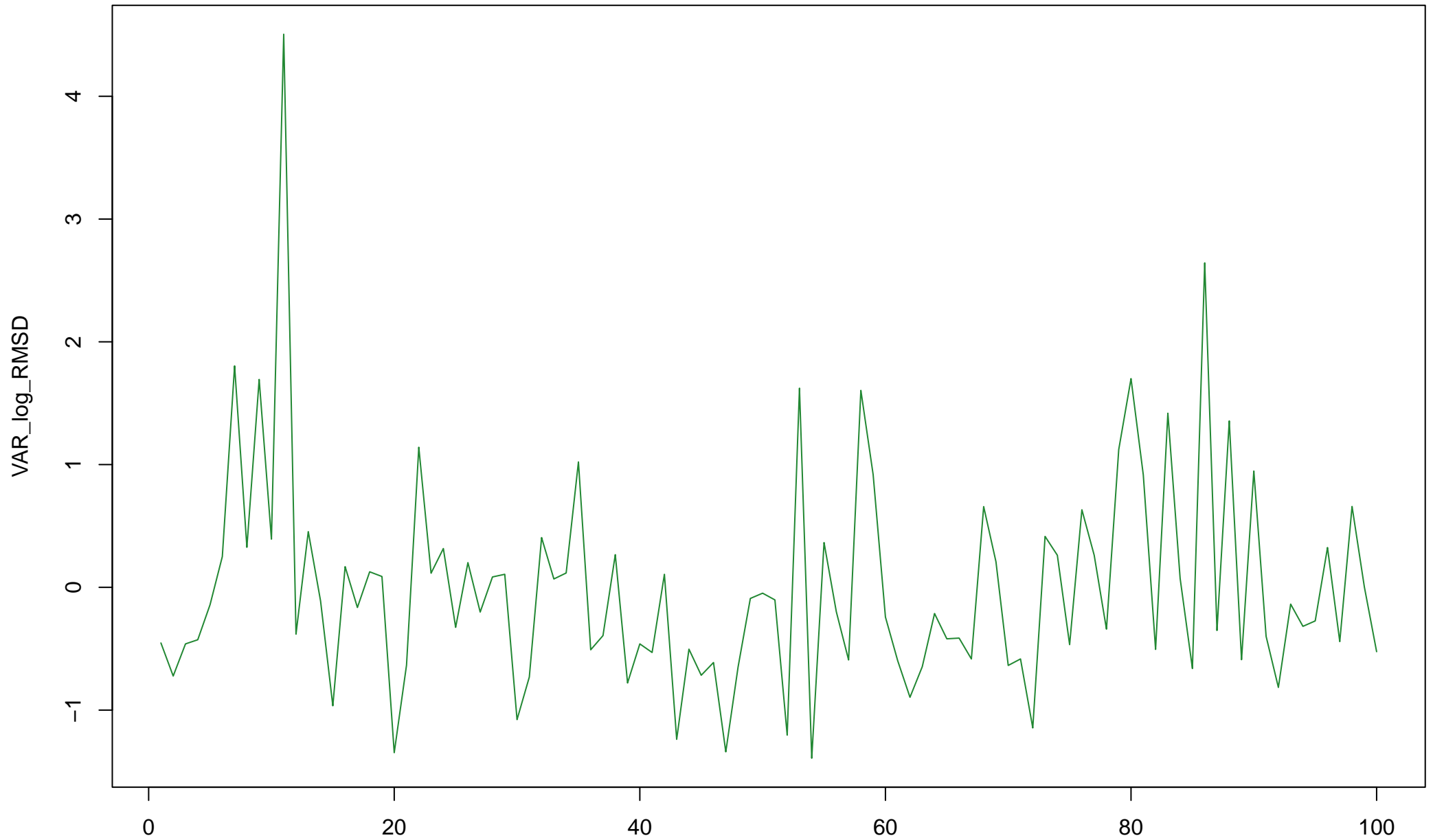
MEAN_docked_NumRotatableBonds
ESS = 100 | BMK = 0.196 | MCSE(6.27) = 12.8 | stat: TRUE | burn: 0



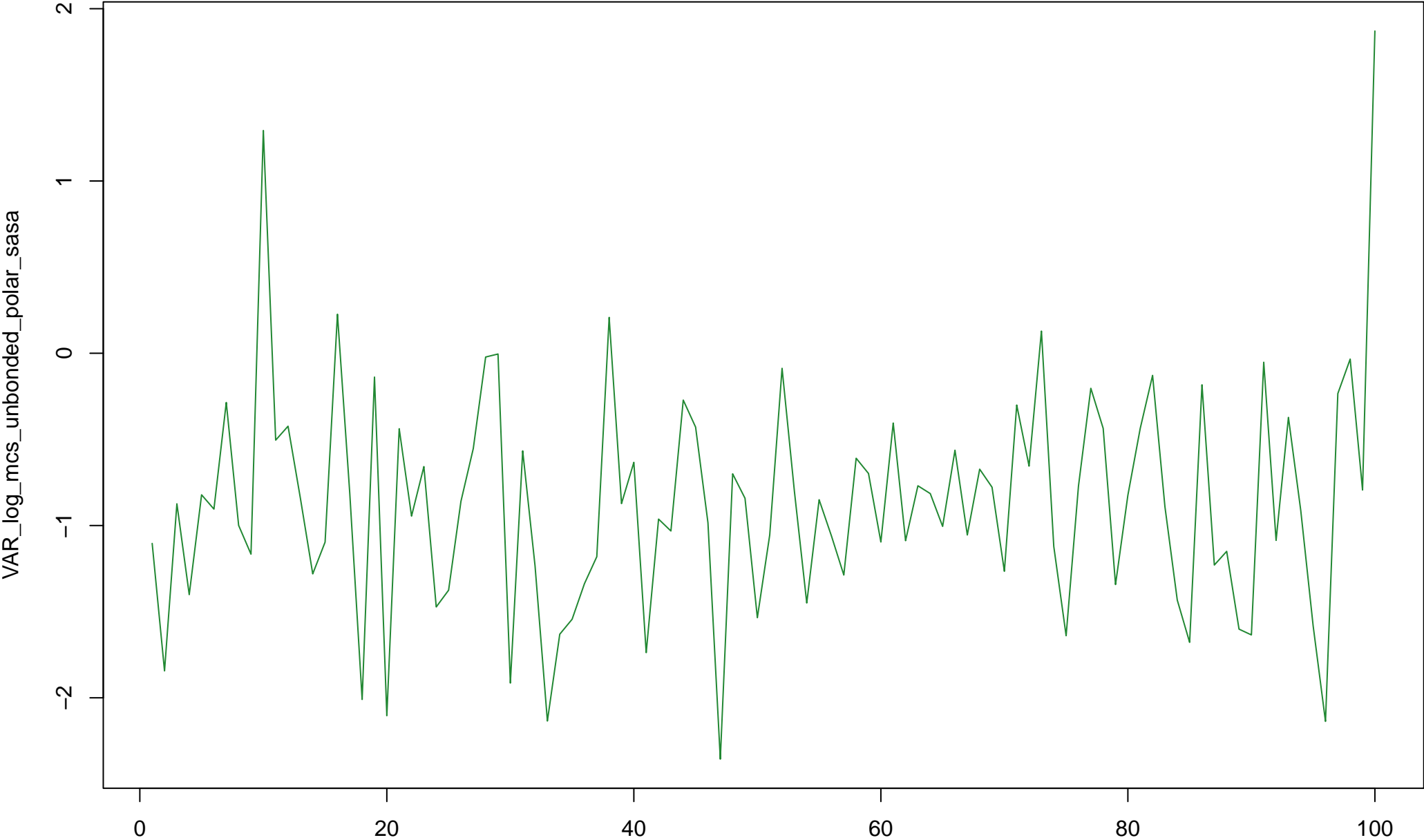
MEAN_mcs_NOCount
ESS = 100 | BMK = 0.0615 | MCSE(6.27) = 10 | stat: TRUE | burn: 0



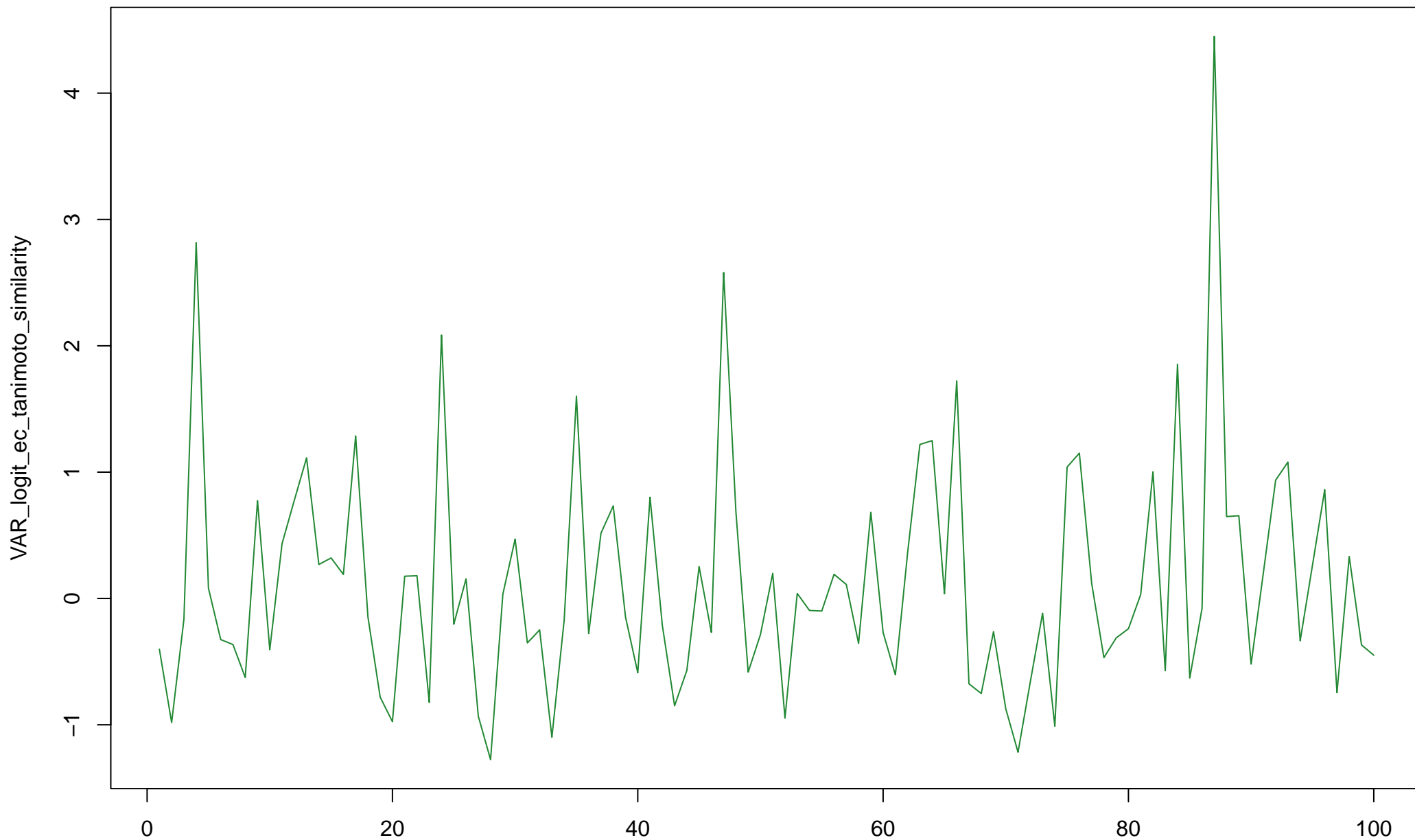
VAR_log_RMSD
ESS = 100 | BMK = 0.366 | MCSE(6.27) = 10 | stat: TRUE | burn: 100



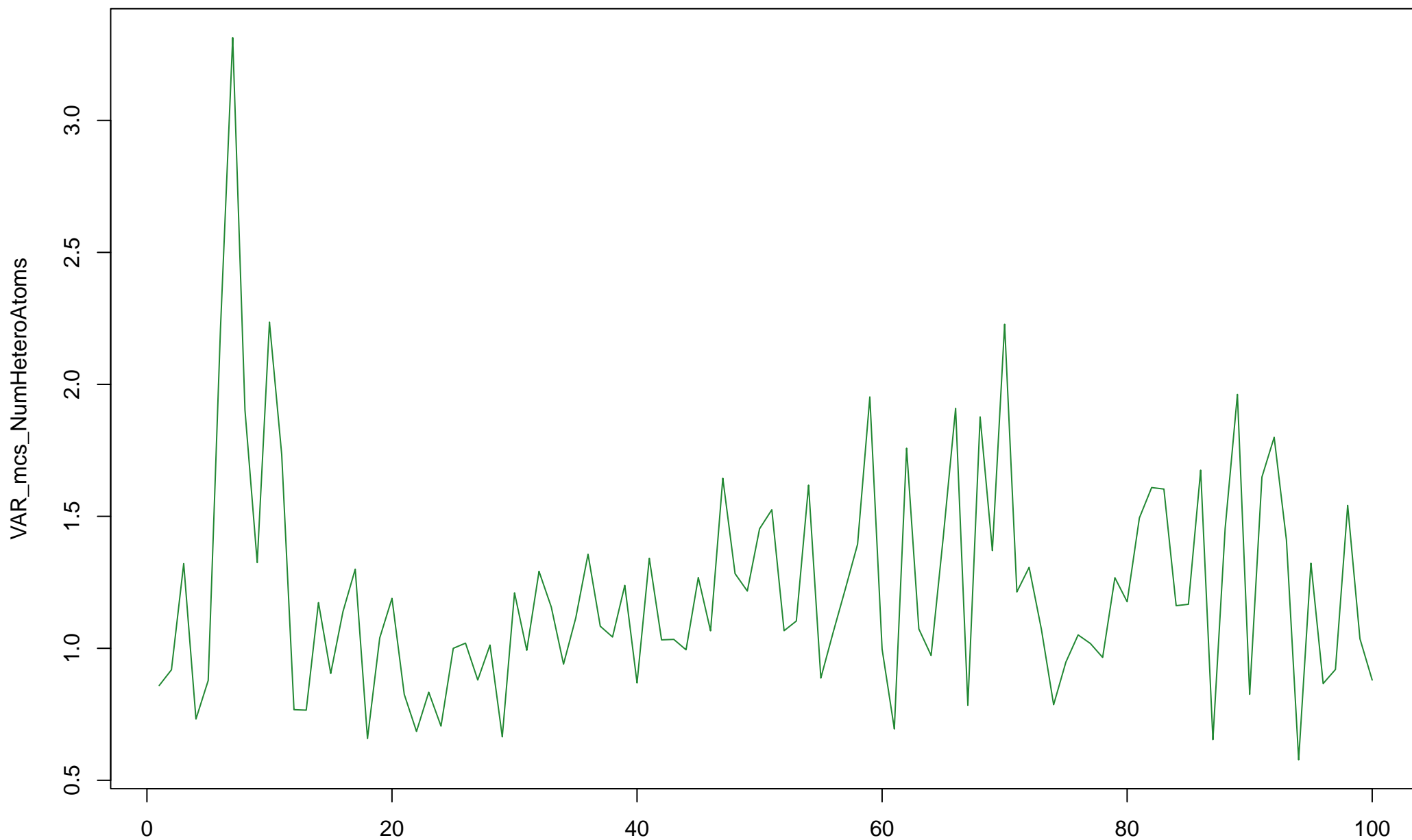
VAR_log_mcs_unbonded_polar_sasa
ESS = 100 | BMK = 0.173 | MCSE(6.27) = 10.1 | stat: TRUE | burn: 10



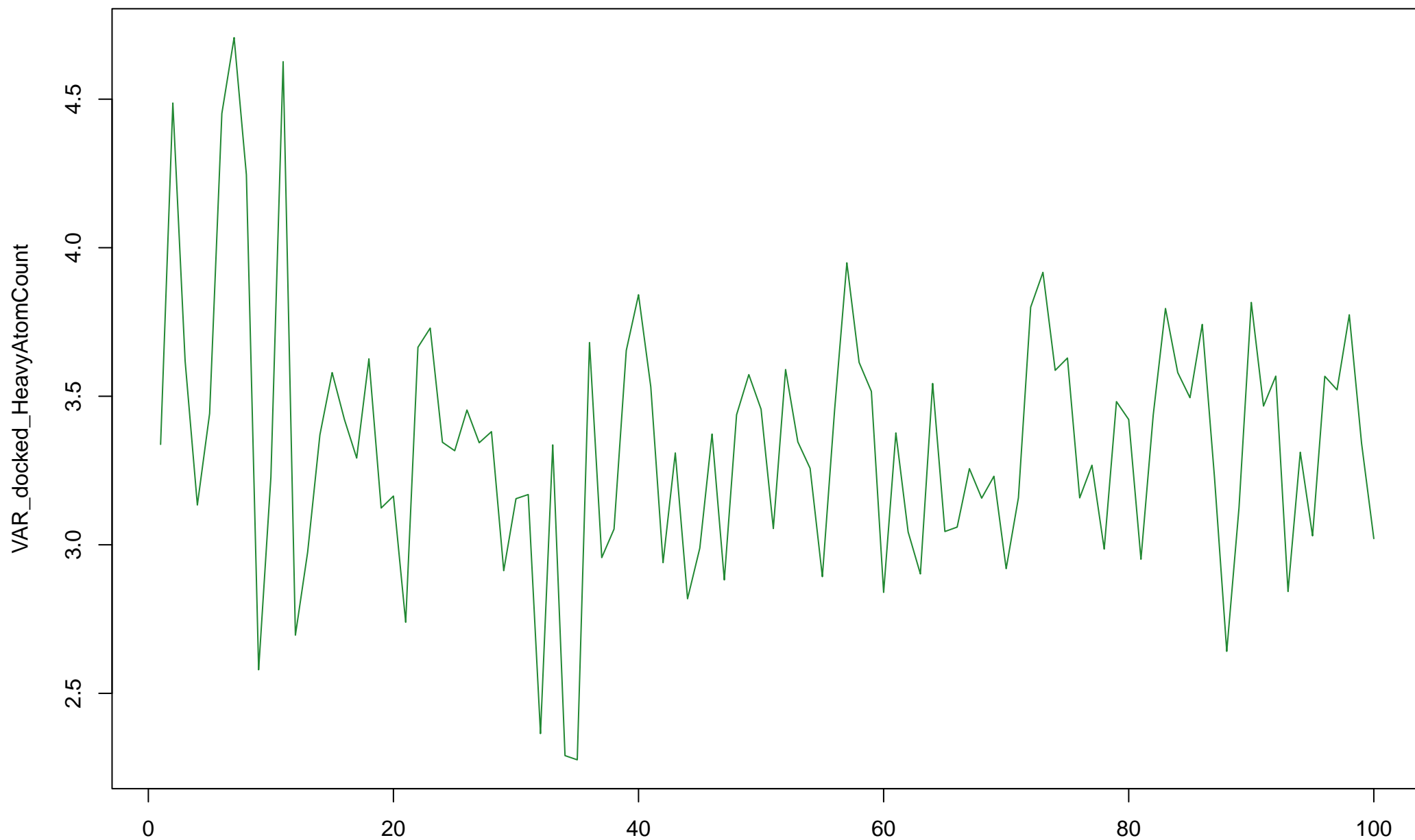
VAR_logit_ec_tanimoto_similarity
ESS = 100 | BMK = 0.169 | MCSE(6.27) = 9.76 | stat: TRUE | burn: 100



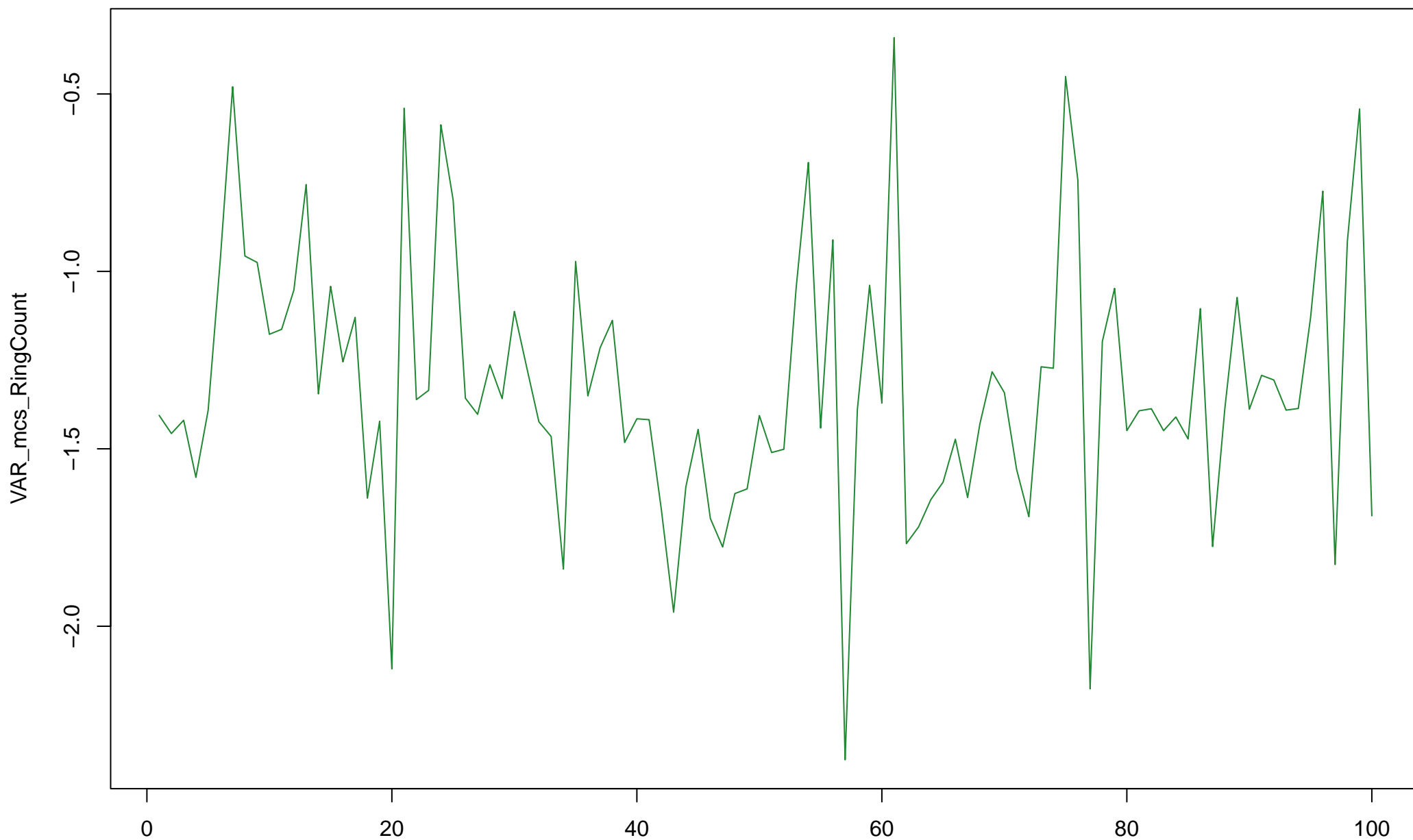
VAR_mcs_NumHeteroAtoms
ESS = 42.8 | BMK = 0.247 | MCSE(6.27) = 15.6 | stat: TRUE | burn: 80



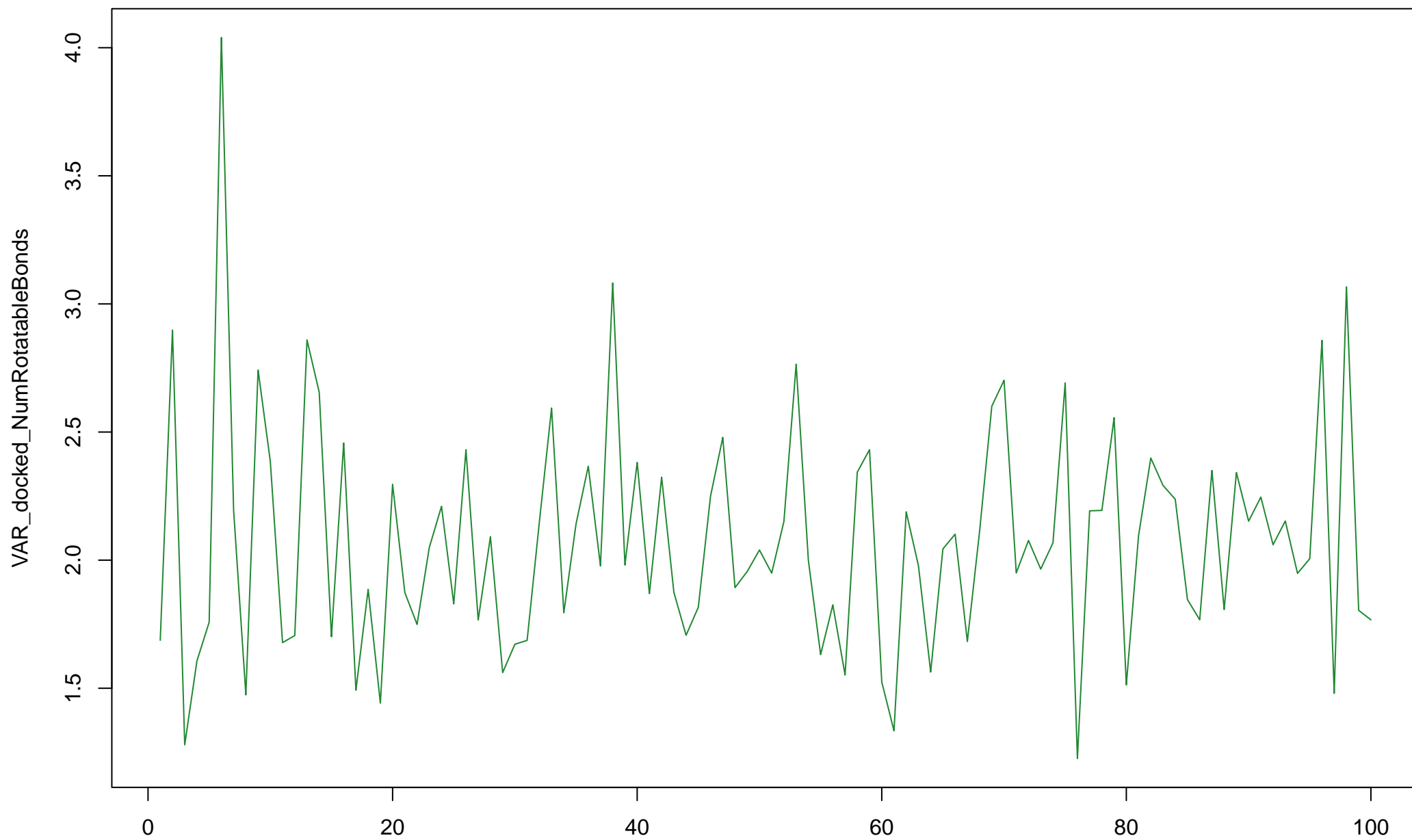
VAR_docked_HeavyAtomCount
ESS = 33.3 | BMK = 0.245 | MCSE(6.27) = 13.9 | stat: TRUE | burn: 0



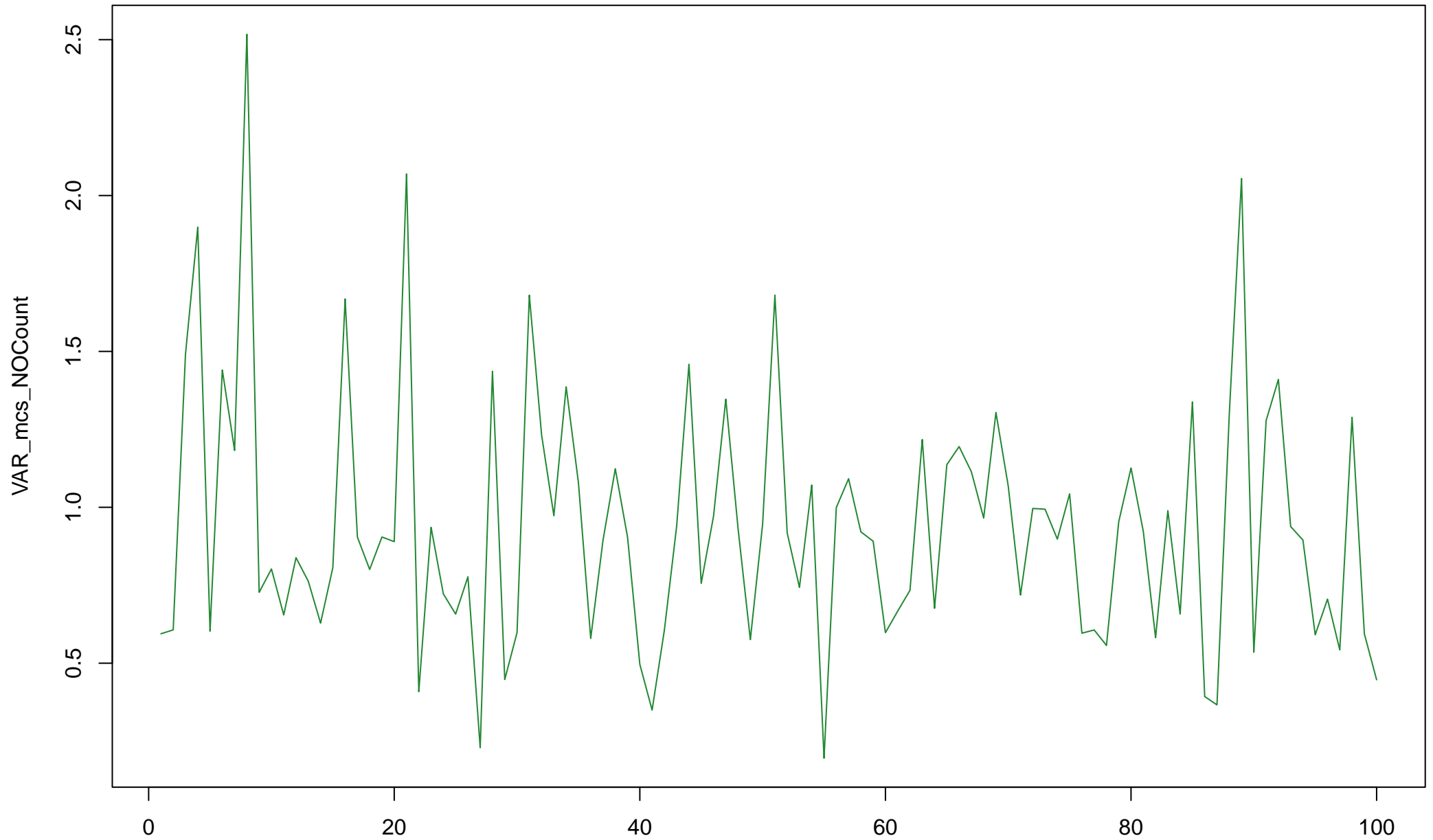
VAR_mcs_RingCount
ESS = 100 | BMK = 0.0948 | MCSE(6.27) = 12.9 | stat: TRUE | burn: 100



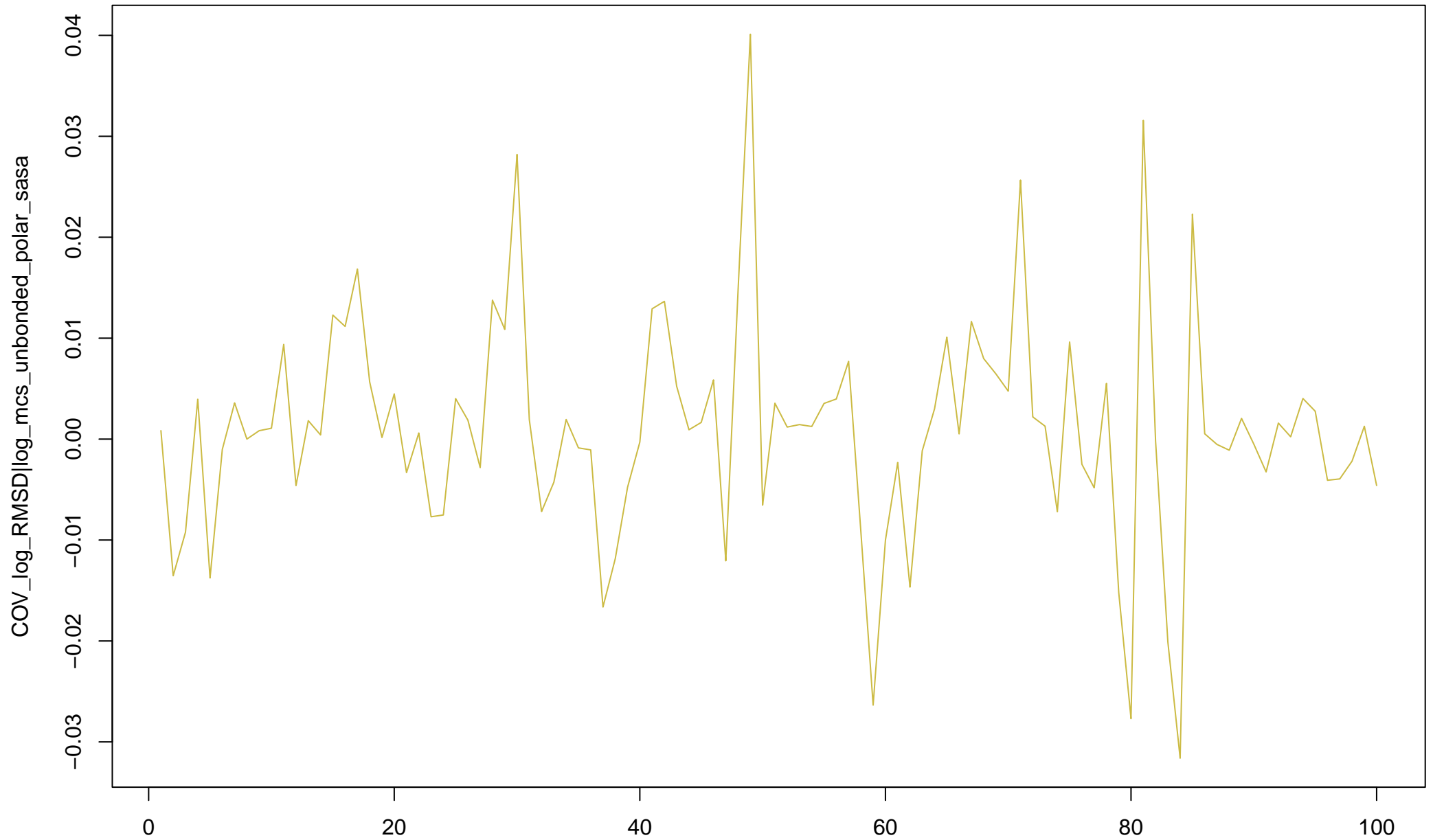
VAR_docked_NumRotatableBonds
ESS = 100 | BMK = 0.125 | MCSE(6.27) = 8.9 | stat: TRUE | burn: 0



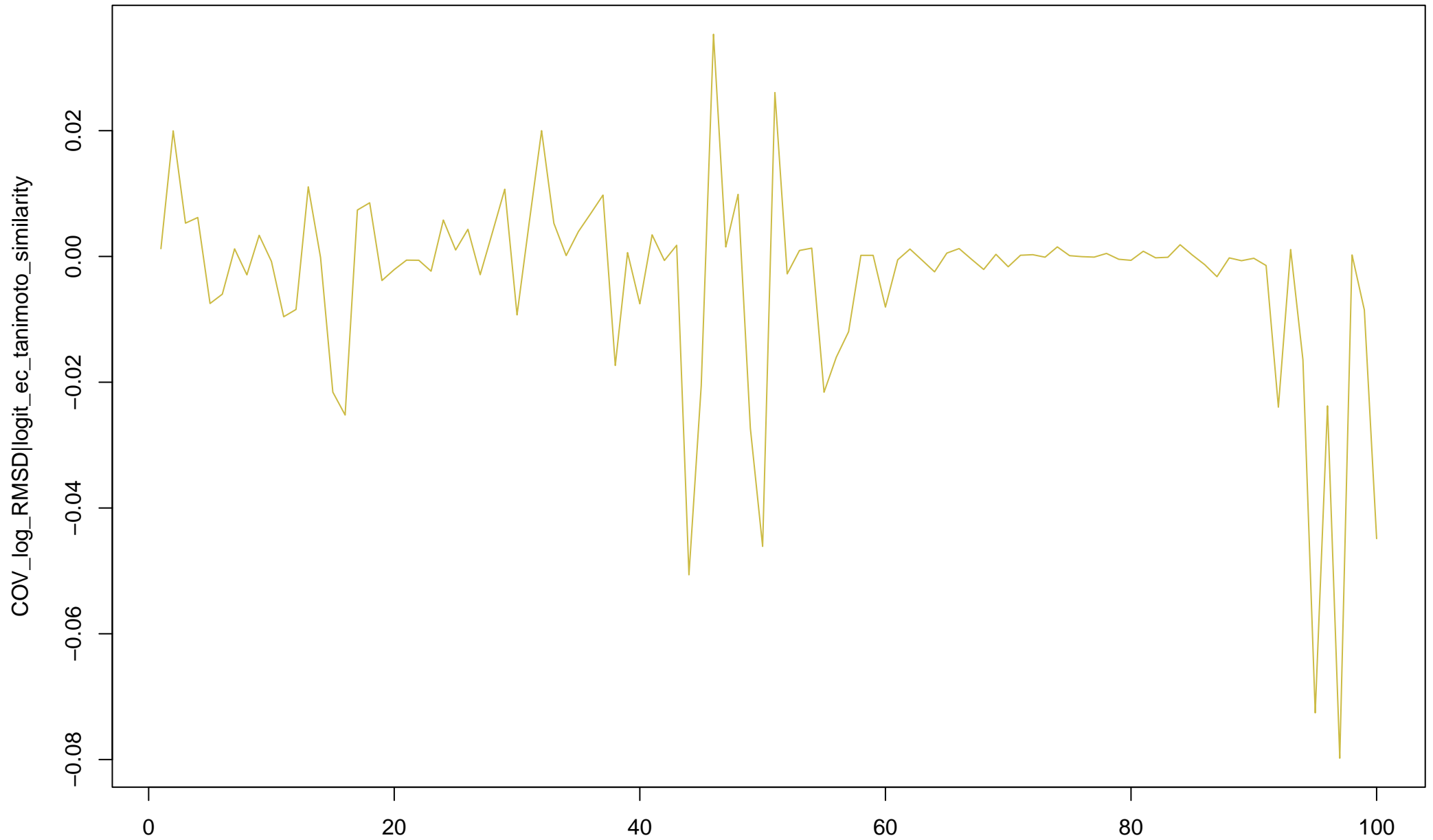
VAR_mcs_NOCount
ESS = 100 | BMK = 0.175 | MCSE(6.27) = 9.67 | stat: TRUE | burn: 10



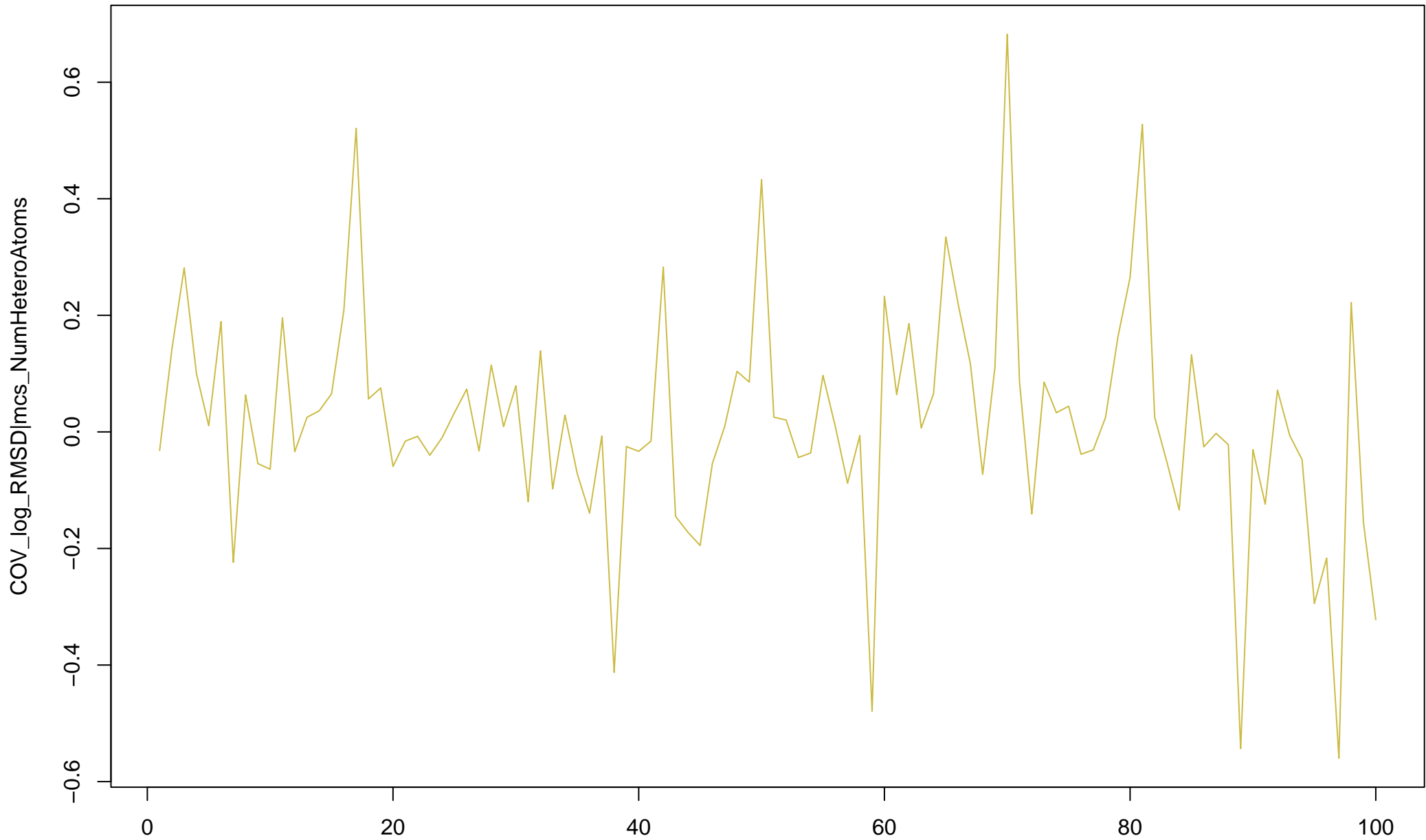
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 74.4 | BMK = 0.241 | MCSE(6.27) = 11.7 | stat: TRUE | burn: 100



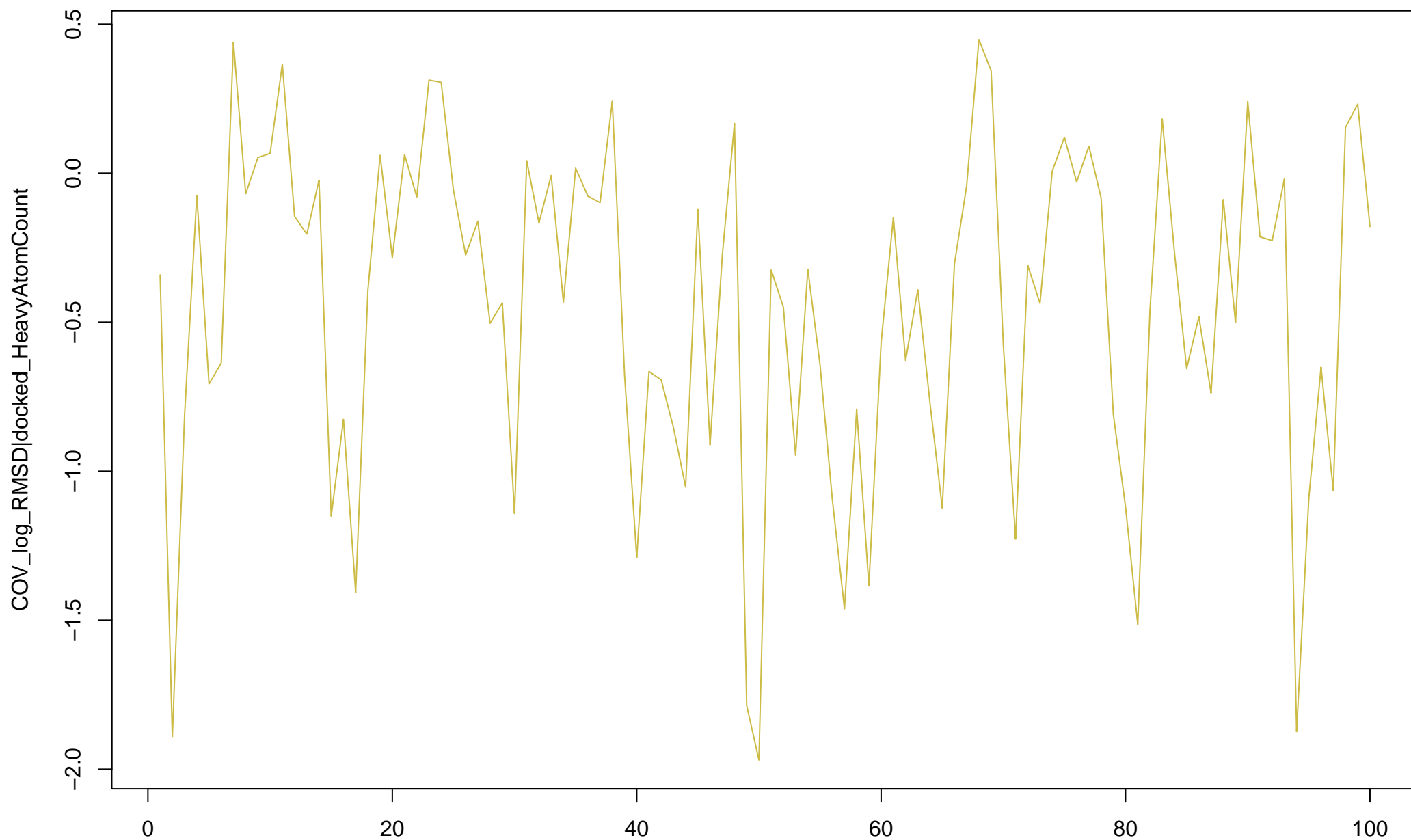
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 22.6 | BMK = 0.574 | MCSE(6.27) = 16.7 | stat: TRUE | burn: 100



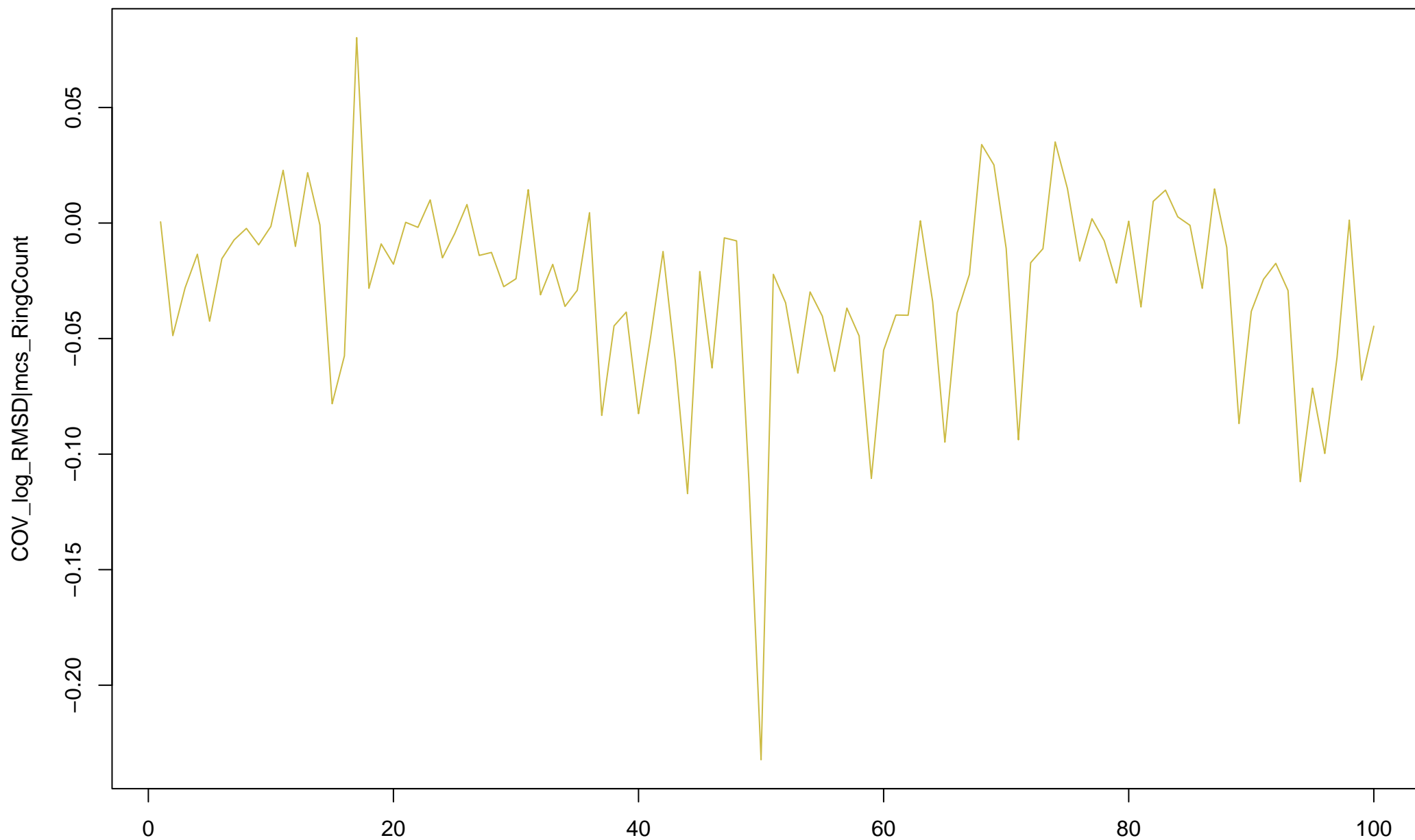
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 70.5 | BMK = 0.17 | MCSE(6.27) = 15.2 | stat: TRUE | burn: 100



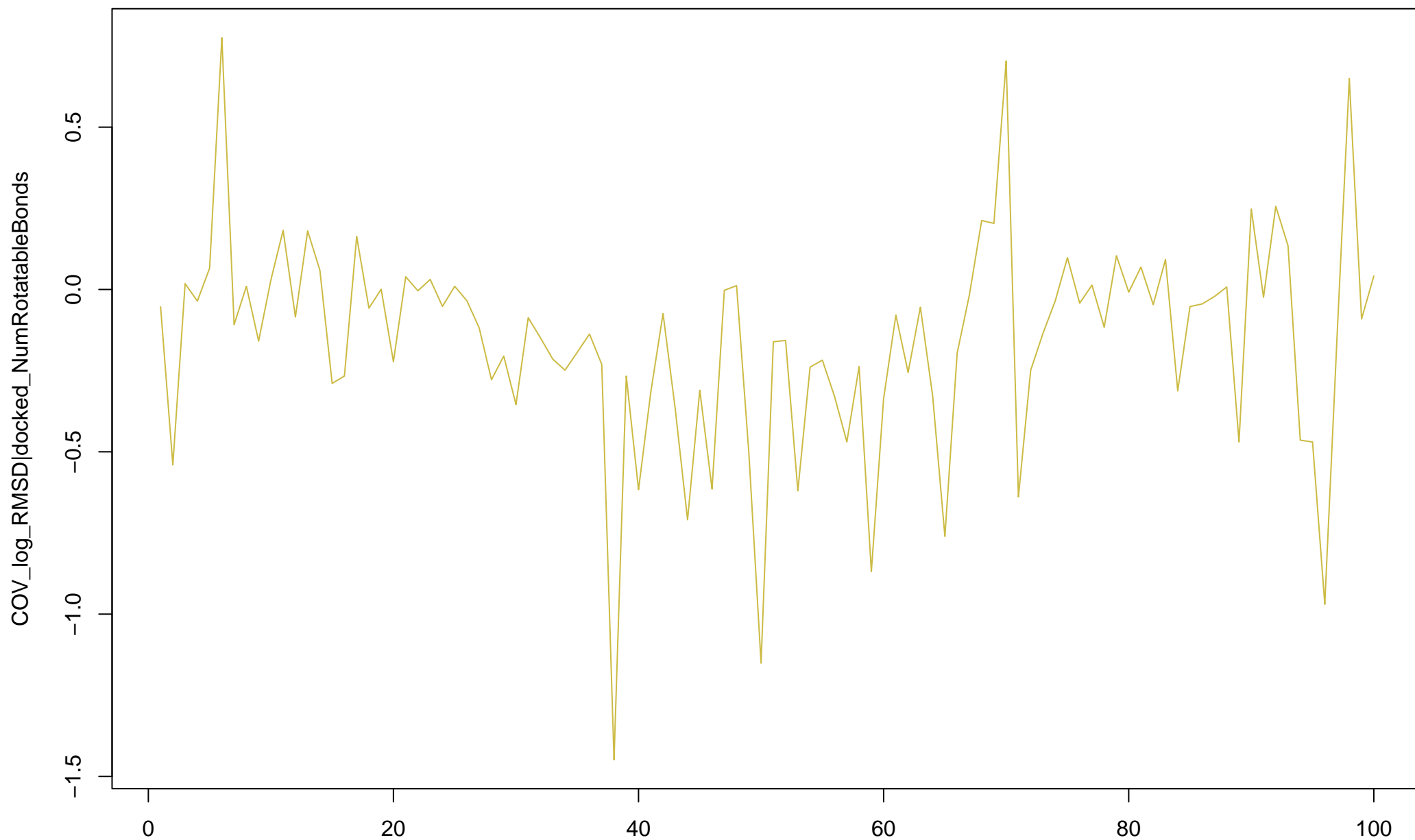
COV_log_RMSD|docked_HeavyAtomCount
ESS = 47.9 | BMK = 0.0964 | MCSE(6.27) = 16.5 | stat: TRUE | burn: 0



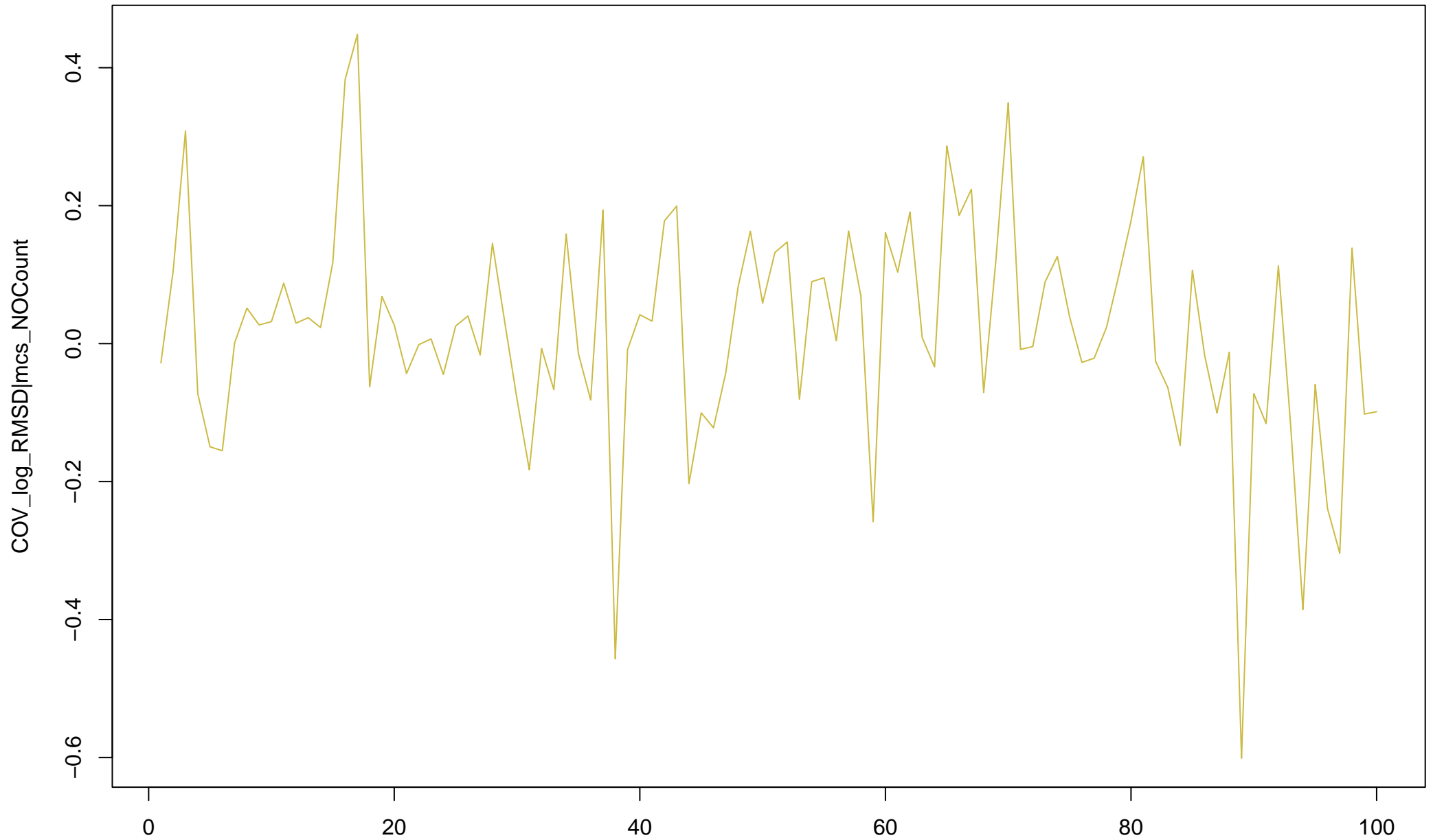
COV_log_RMSD|mcs_RingCount
ESS = 11.8 | BMK = 0.163 | MCSE(6.27) = 16.4 | stat: TRUE | burn: 30



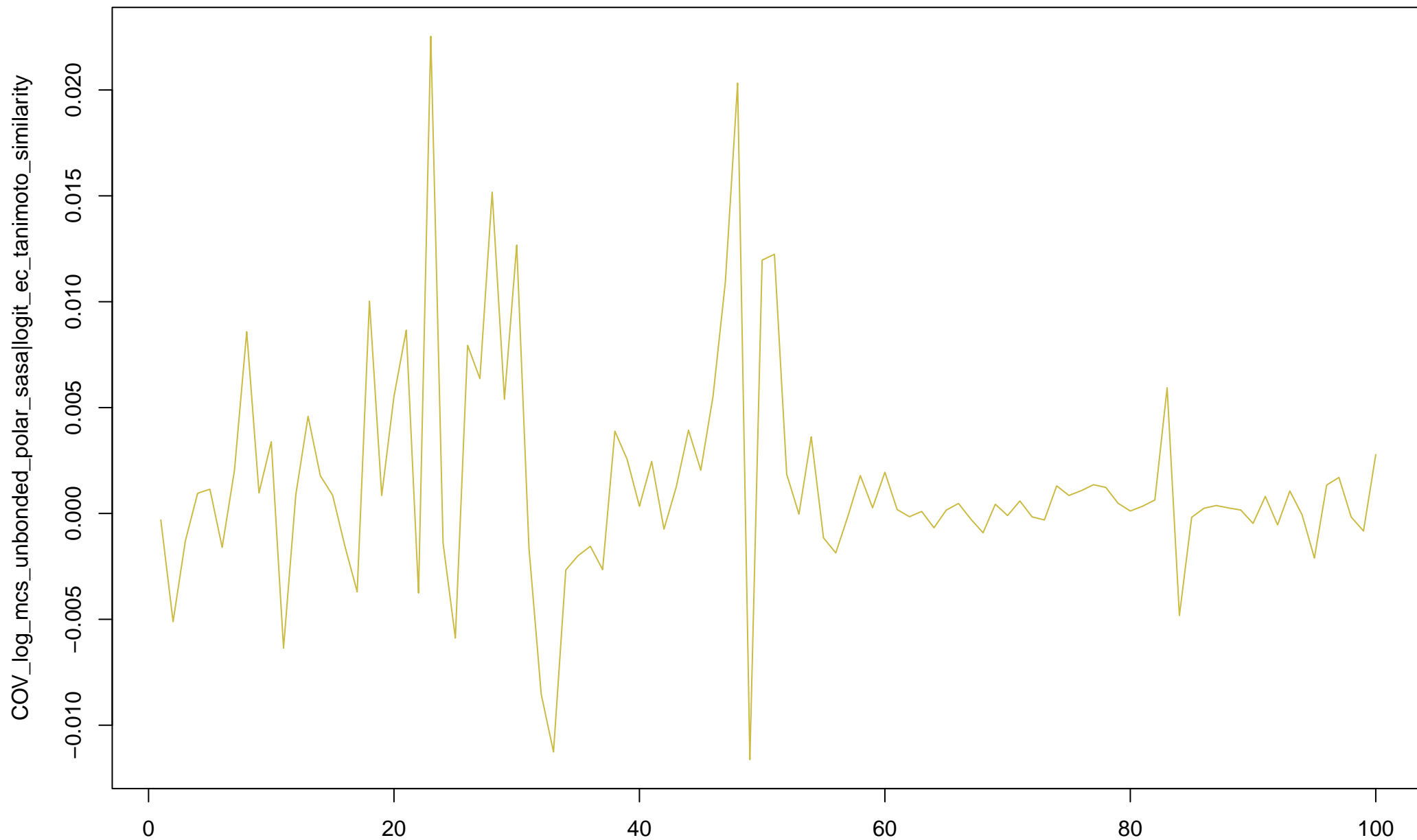
COV_log_RMSD|docked_NumRotatableBonds
ESS = 20.5 | BMK = 0.176 | MCSE(6.27) = 16.3 | stat: TRUE | burn: 40



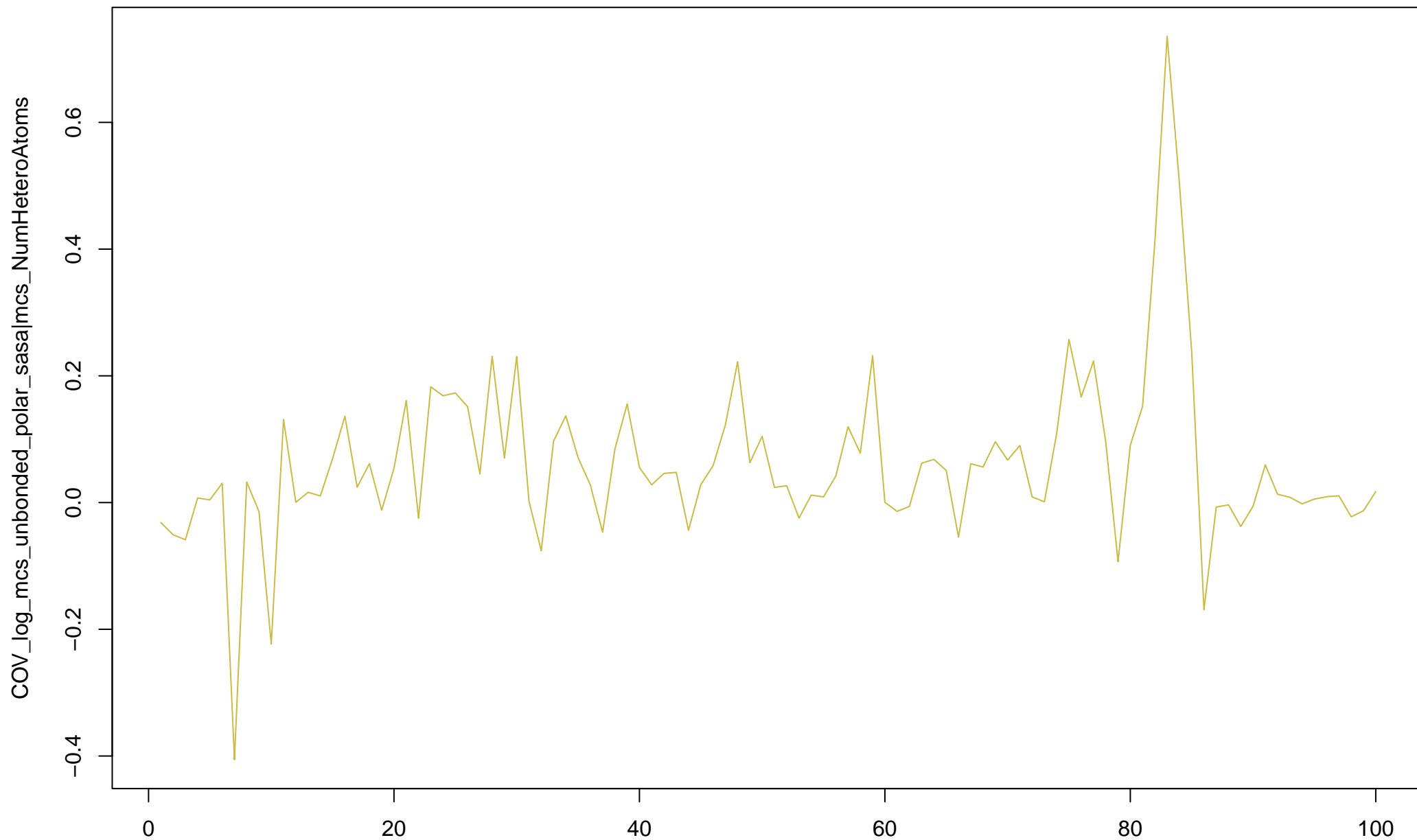
COV_log_RMSD|mcs_NOCount
ESS = 66.7 | BMK = 0.199 | MCSE(6.27) = 15.7 | stat: TRUE | burn: 100



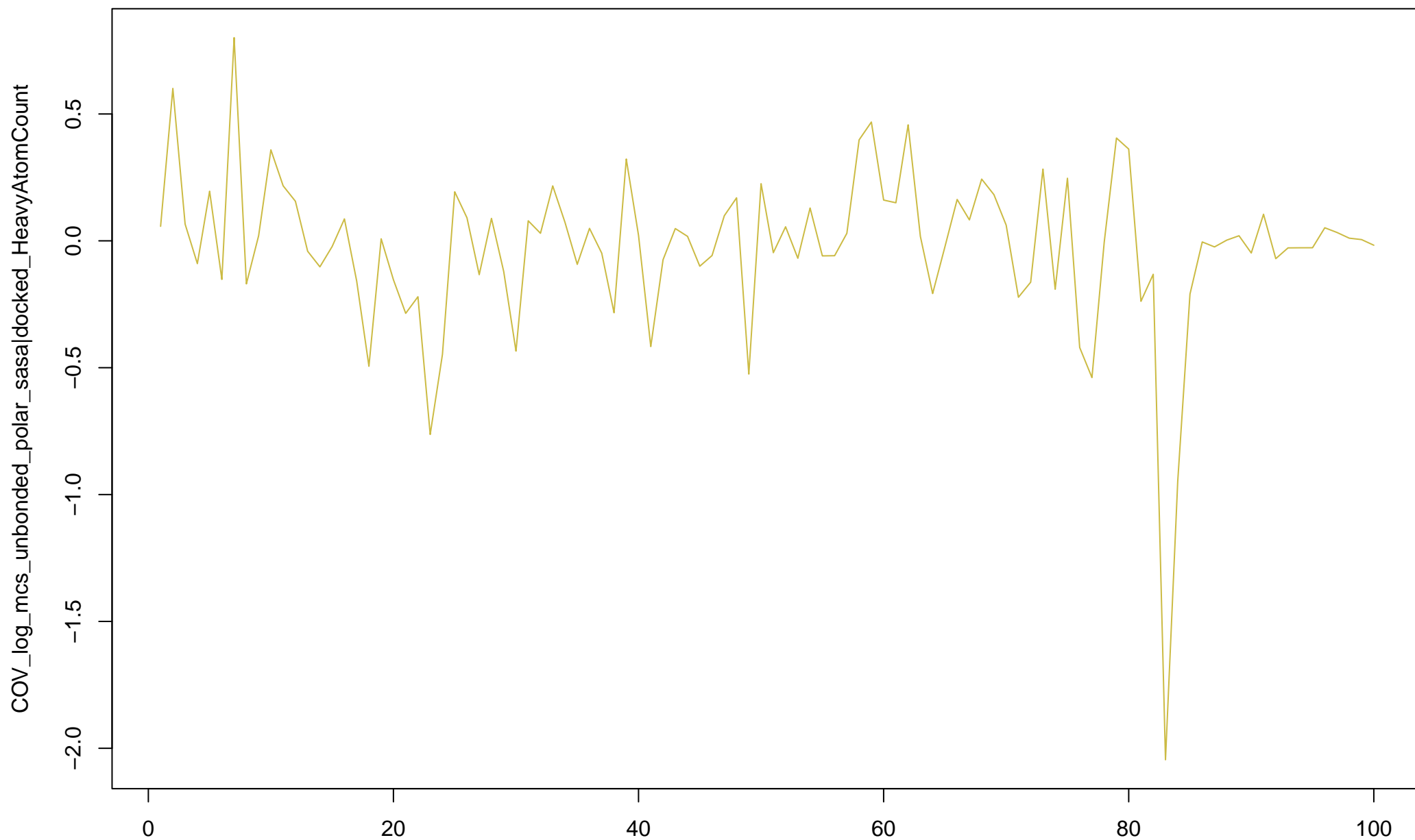
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 100 | BMK = 0.538 | MCSE(6.27) = 11.9 | stat: TRUE | burn: 100



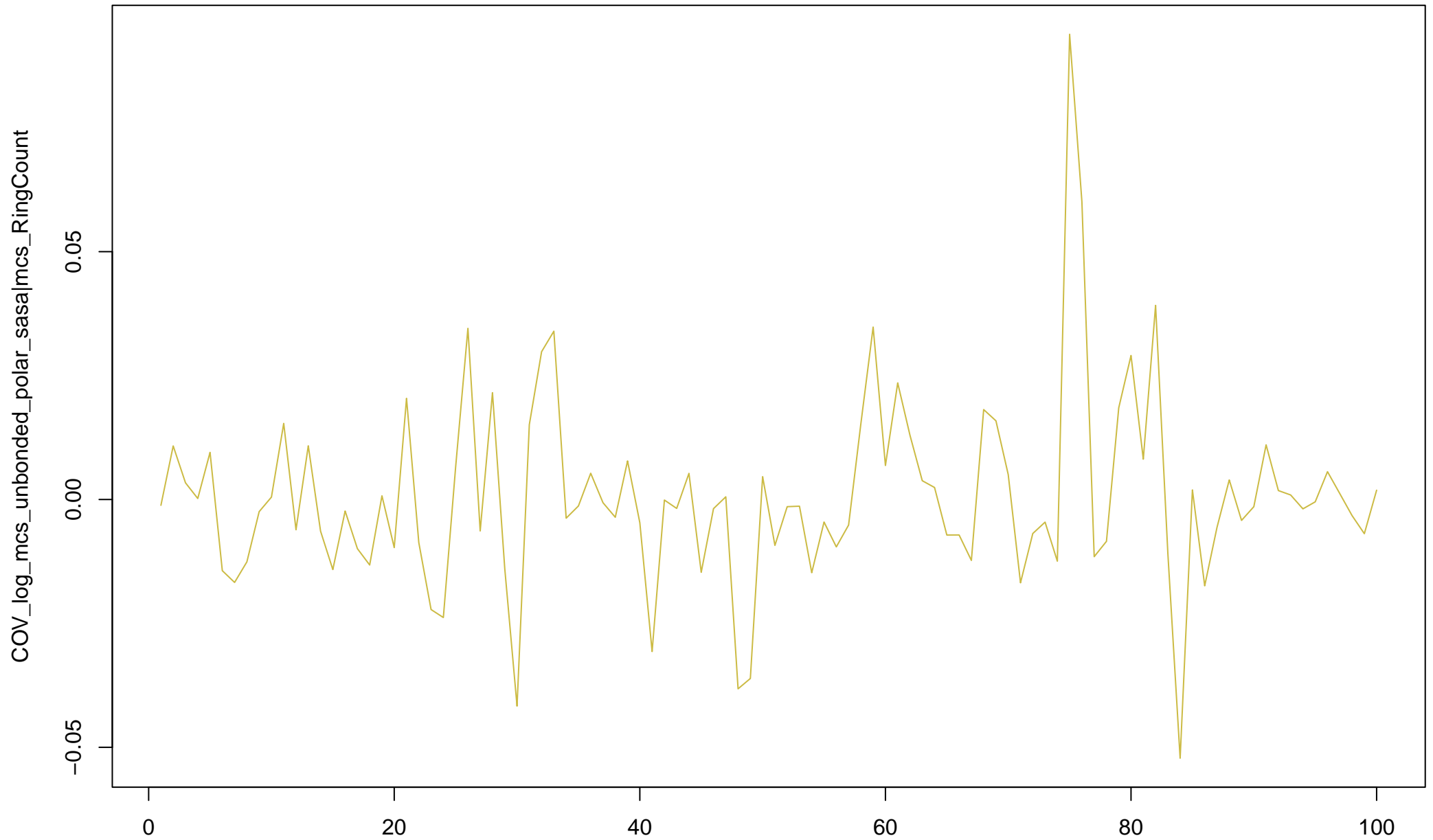
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 34.7 | BMK = 0.231 | MCSE(6.27) = 19.8 | stat: FALSE | burn: 100



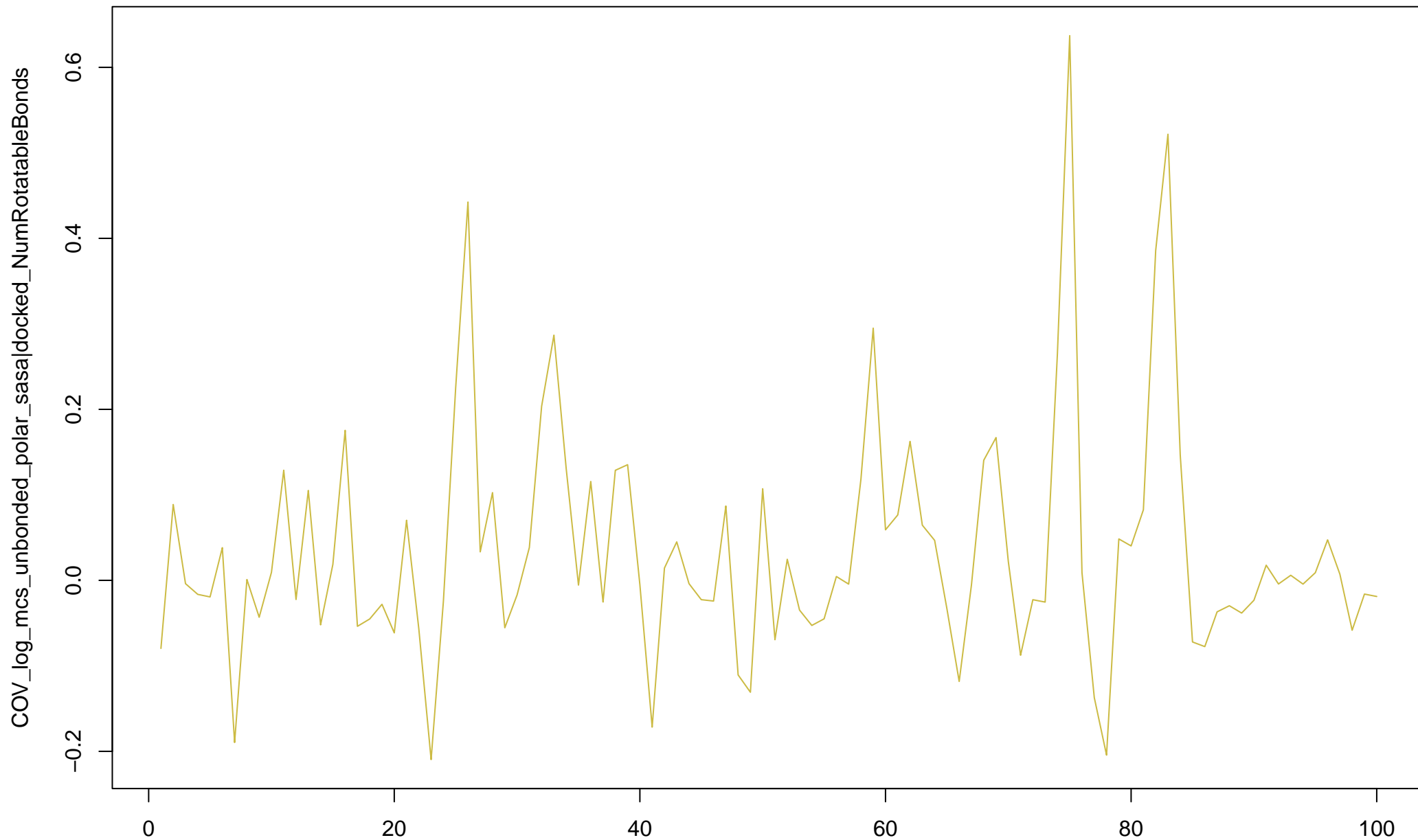
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 54.6 | BMK = 0.229 | MCSE(6.27) = 15.4 | stat: FALSE | burn: 100



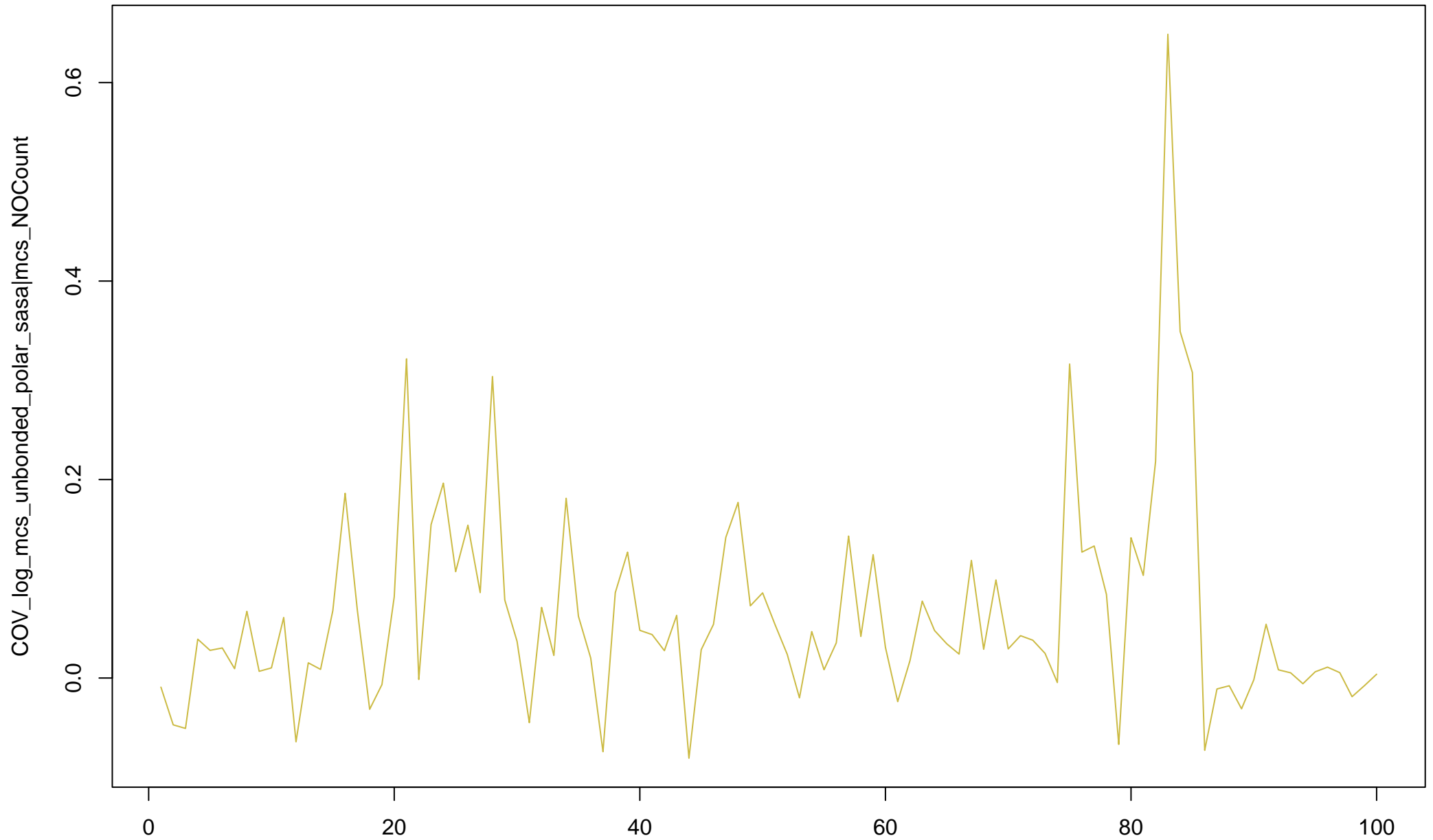
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 71.7 | BMK = 0.232 | MCSE(6.27) = 13.2 | stat: TRUE | burn: 100



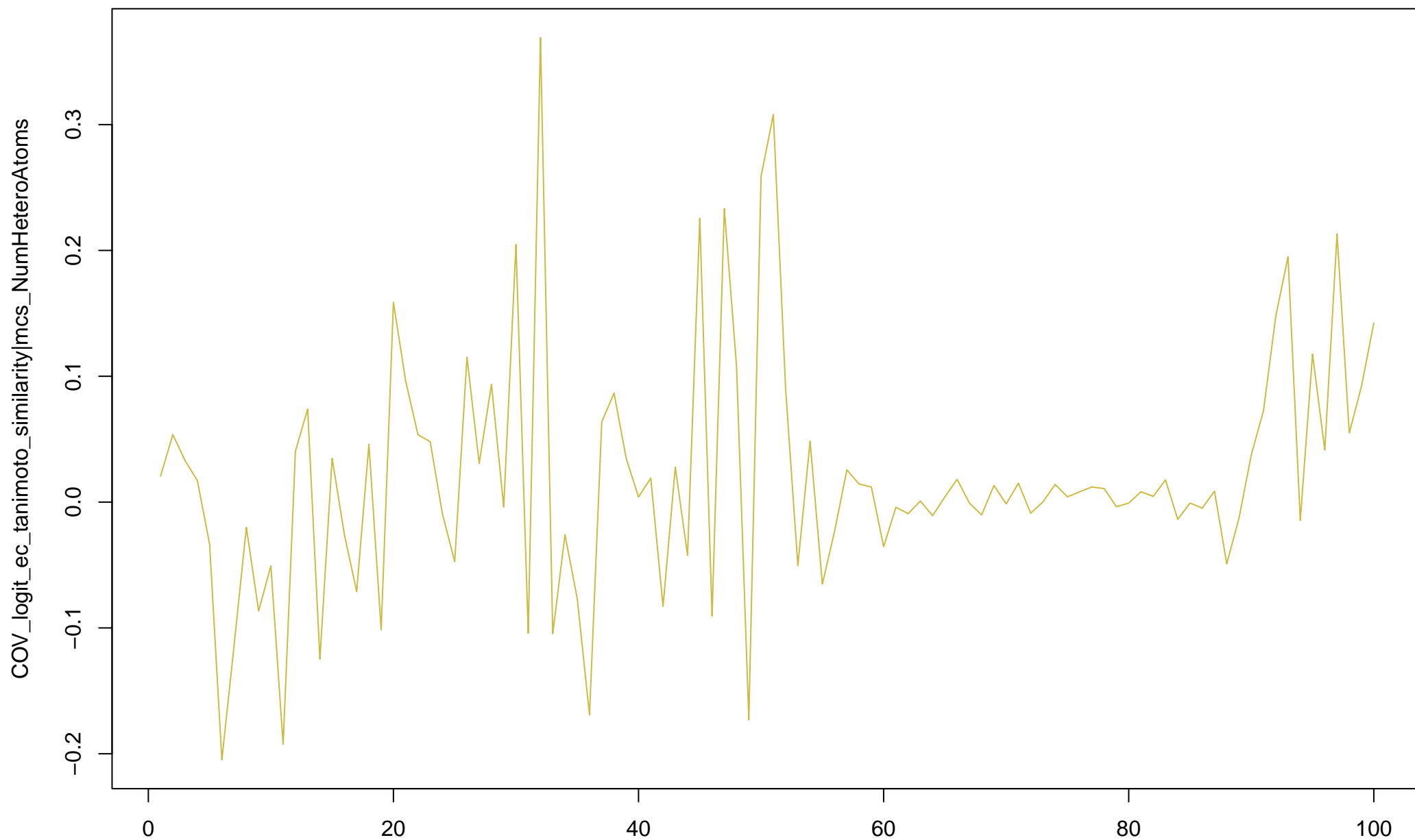
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 75.8 | BMK = 0.151 | MCSE(6.27) = 15.1 | stat: TRUE | burn: 100



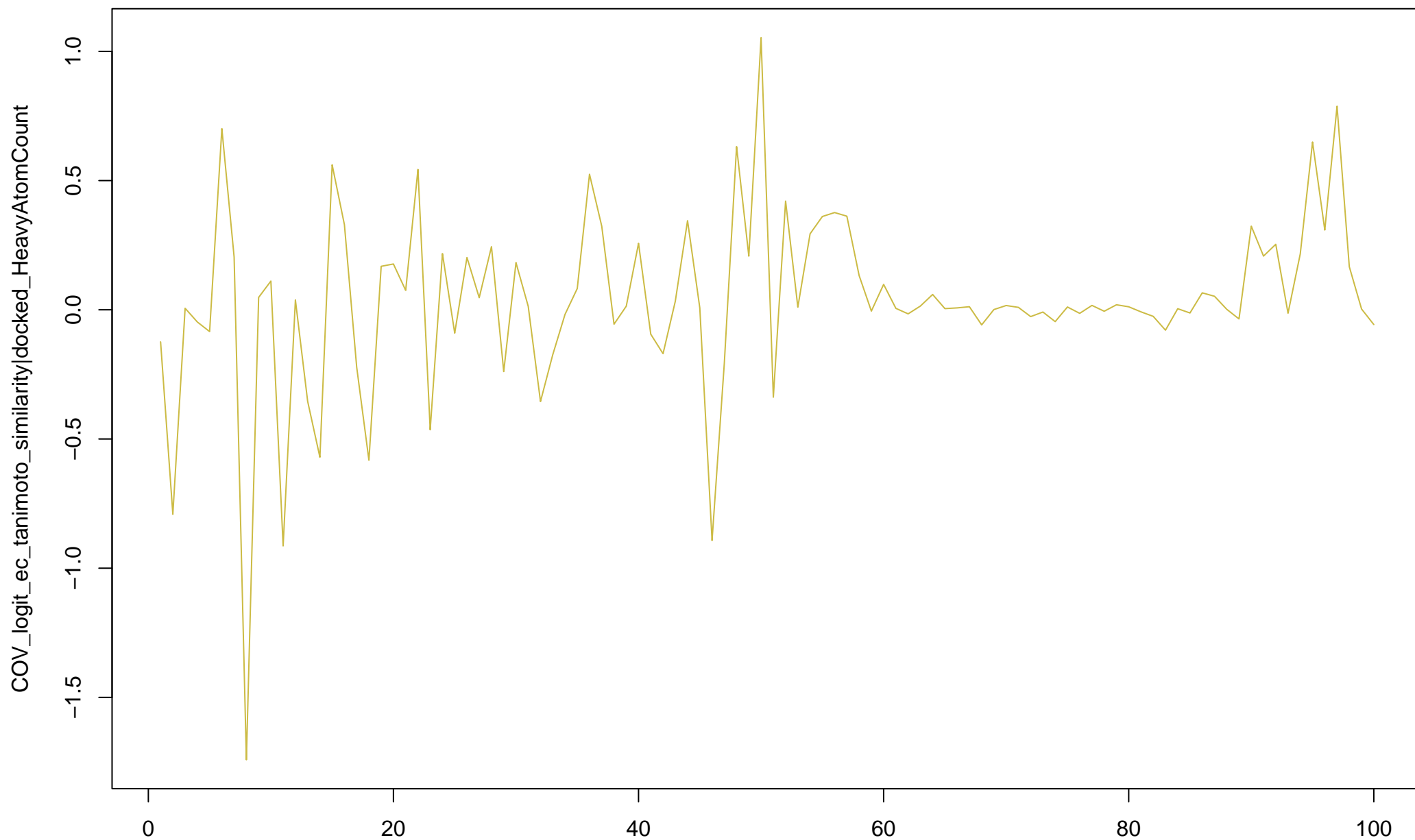
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 42.2 | BMK = 0.169 | MCSE(6.27) = 18.6 | stat: TRUE | burn: 100



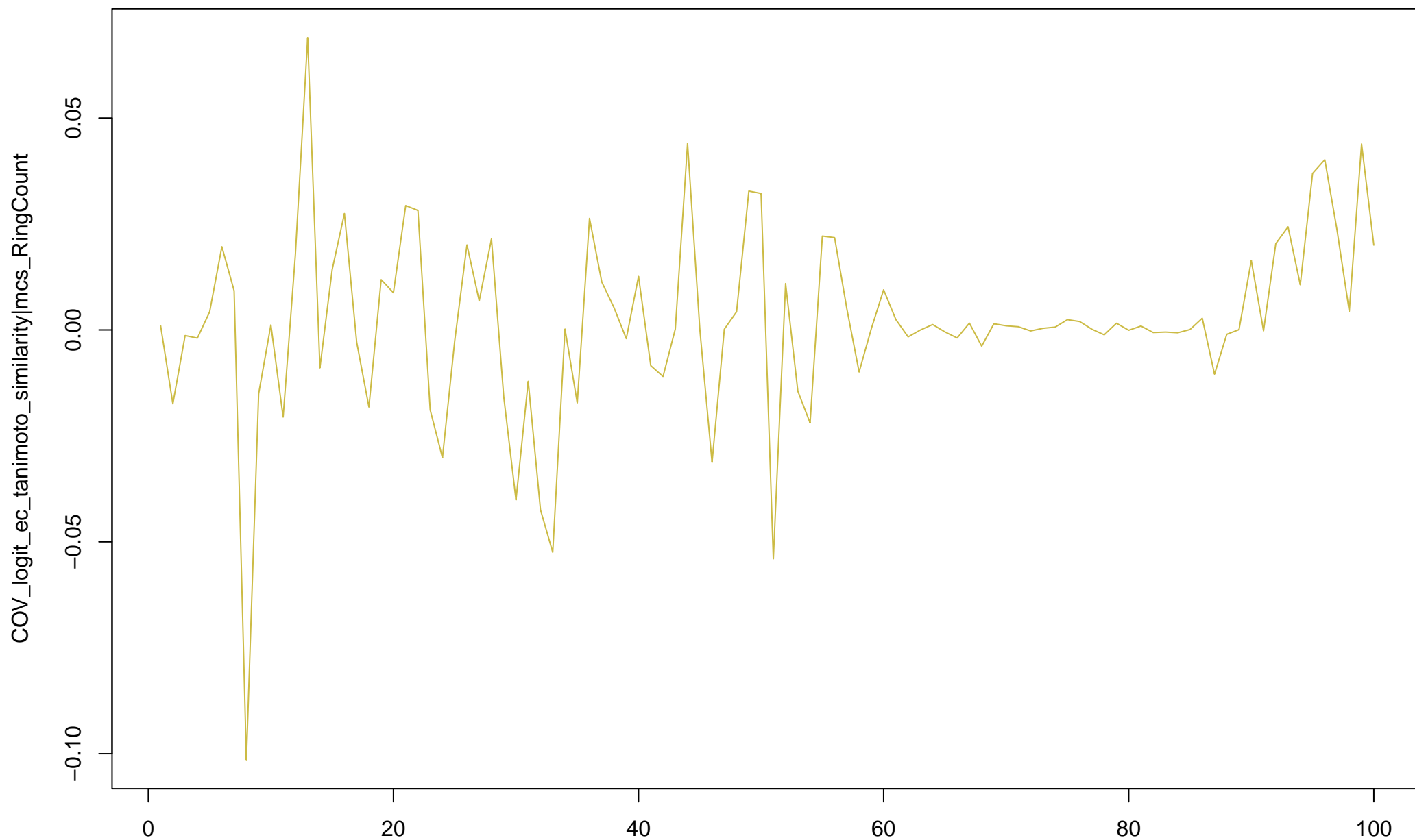
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 65.5 | BMK = 0.431 | MCSE(6.27) = 11.7 | stat: TRUE | burn: 100



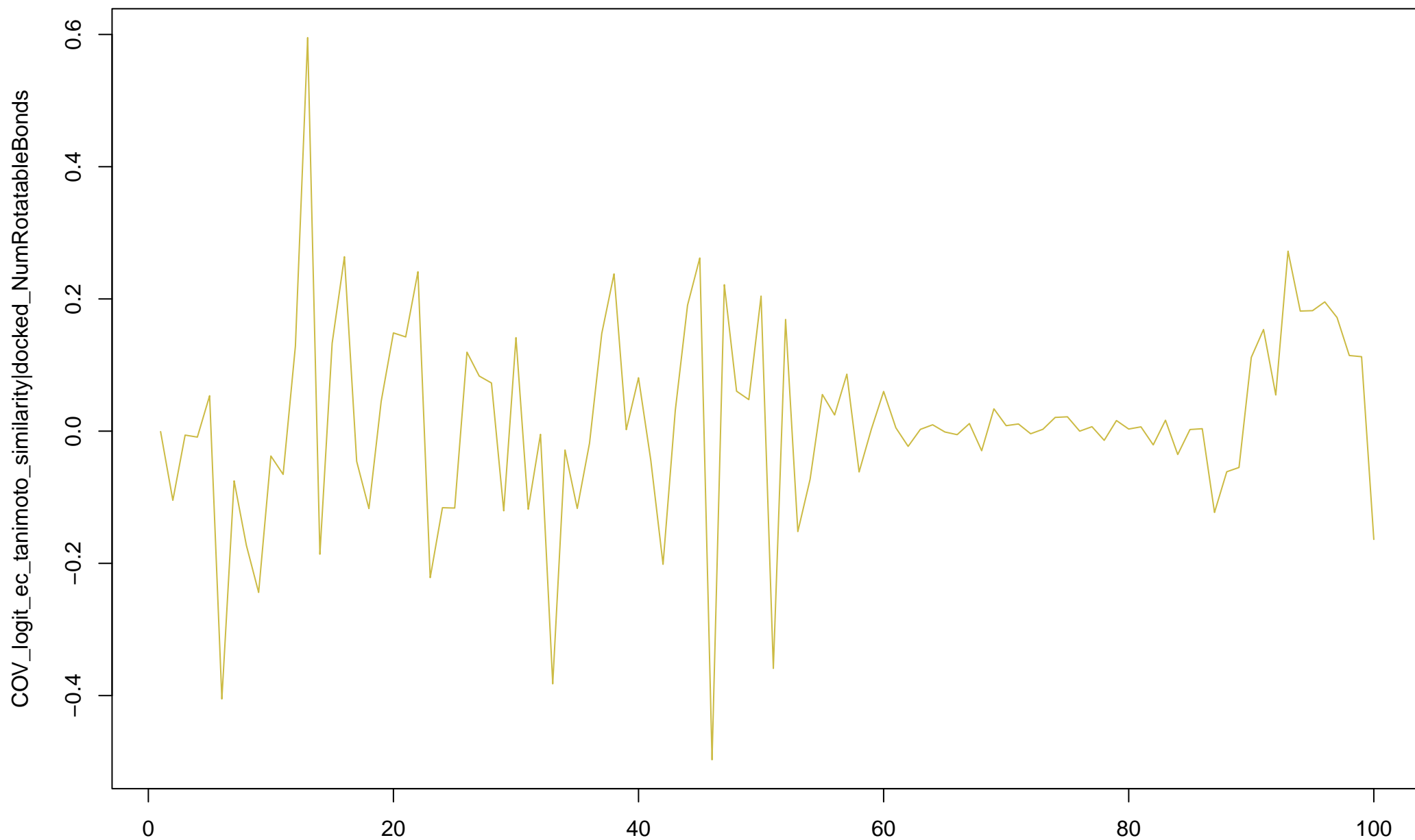
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 100 | BMK = 0.407 | MCSE(6.27) = 10.3 | stat: TRUE | burn: 100



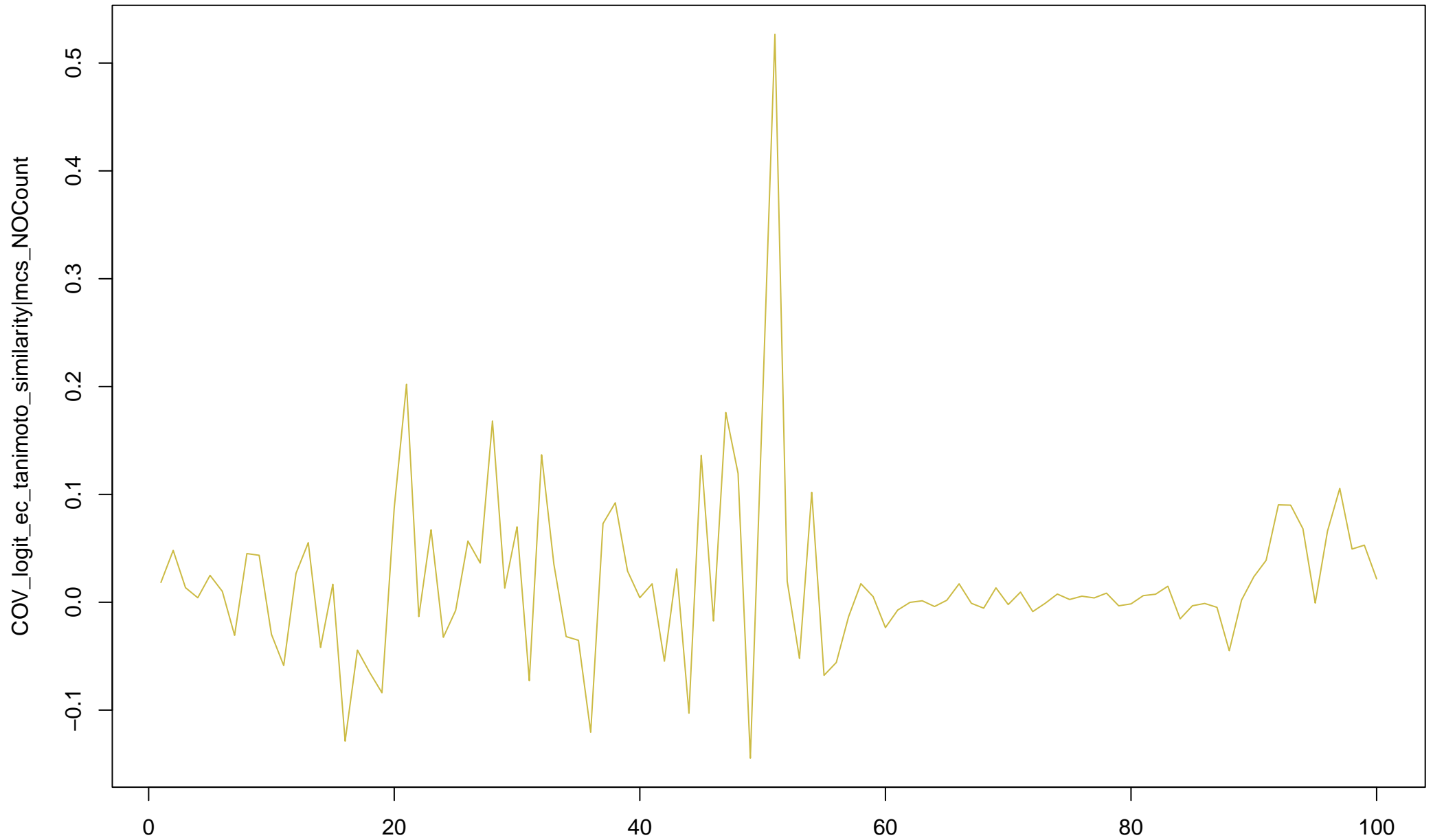
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 53 | BMK = 0.387 | MCSE(6.27) = 14 | stat: TRUE | burn: 100



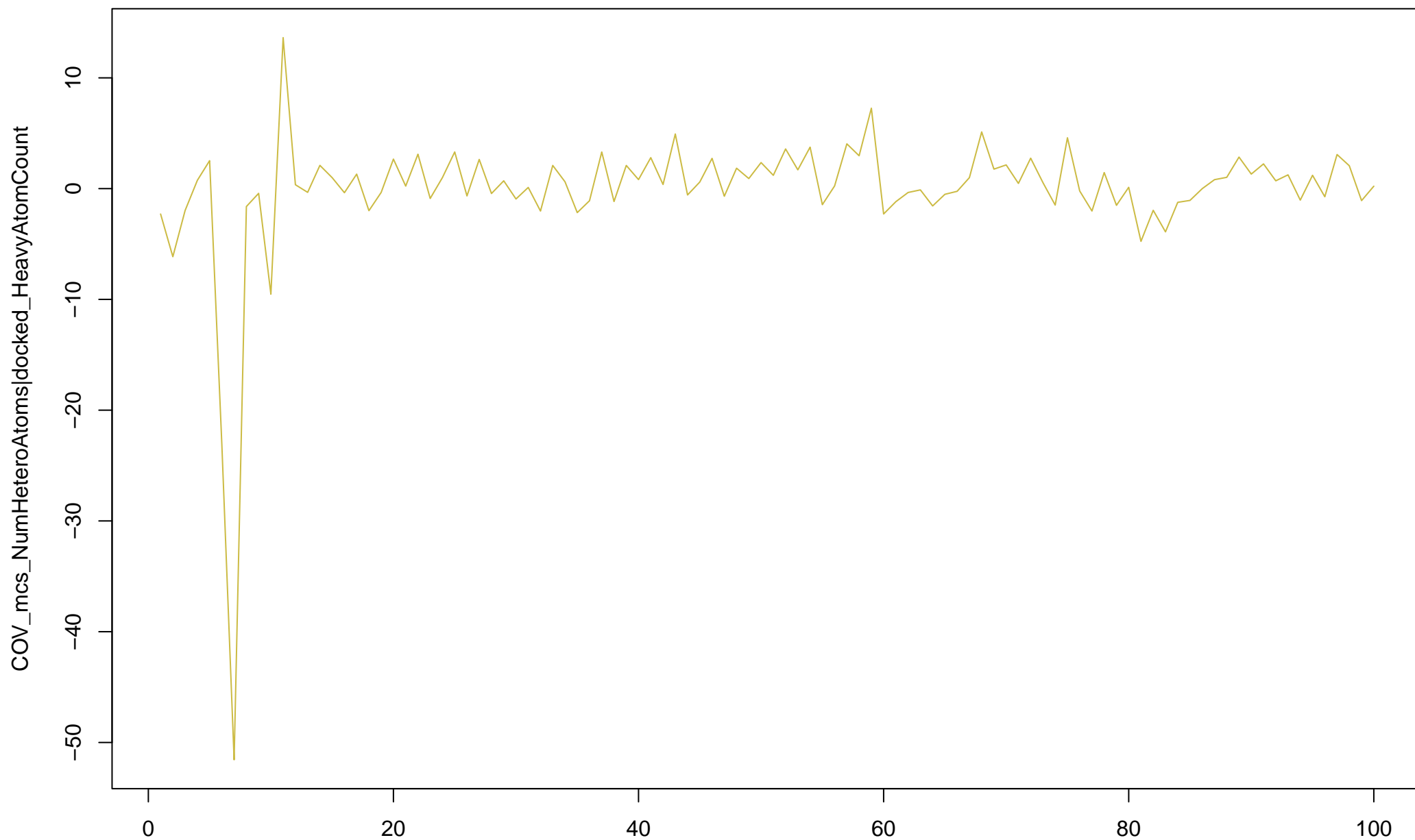
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 100 | BMK = 0.364 | MCSE(6.27) = 10.7 | stat: FALSE | burn: 100



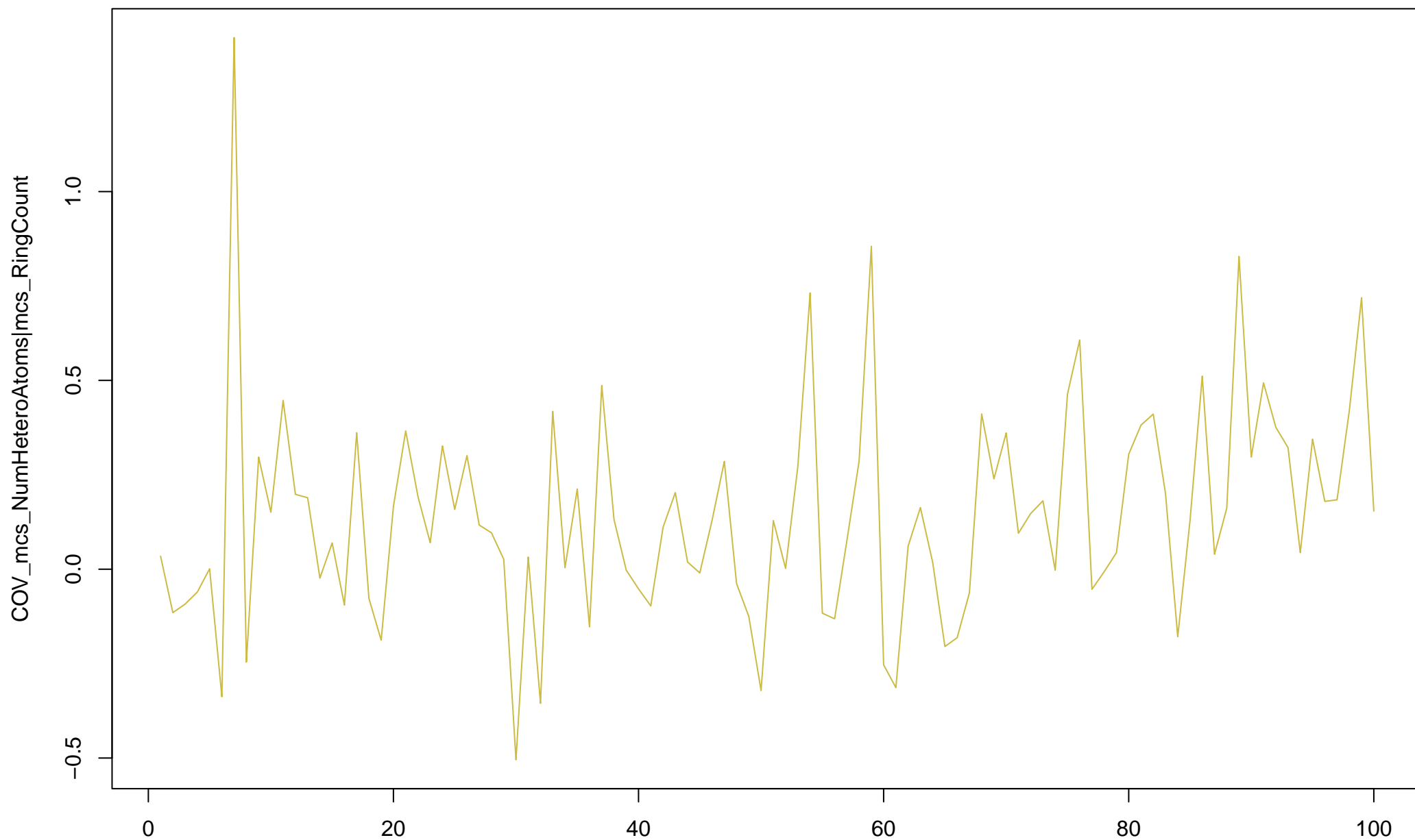
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 100 | BMK = 0.457 | MCSE(6.27) = 11 | stat: TRUE | burn: 100



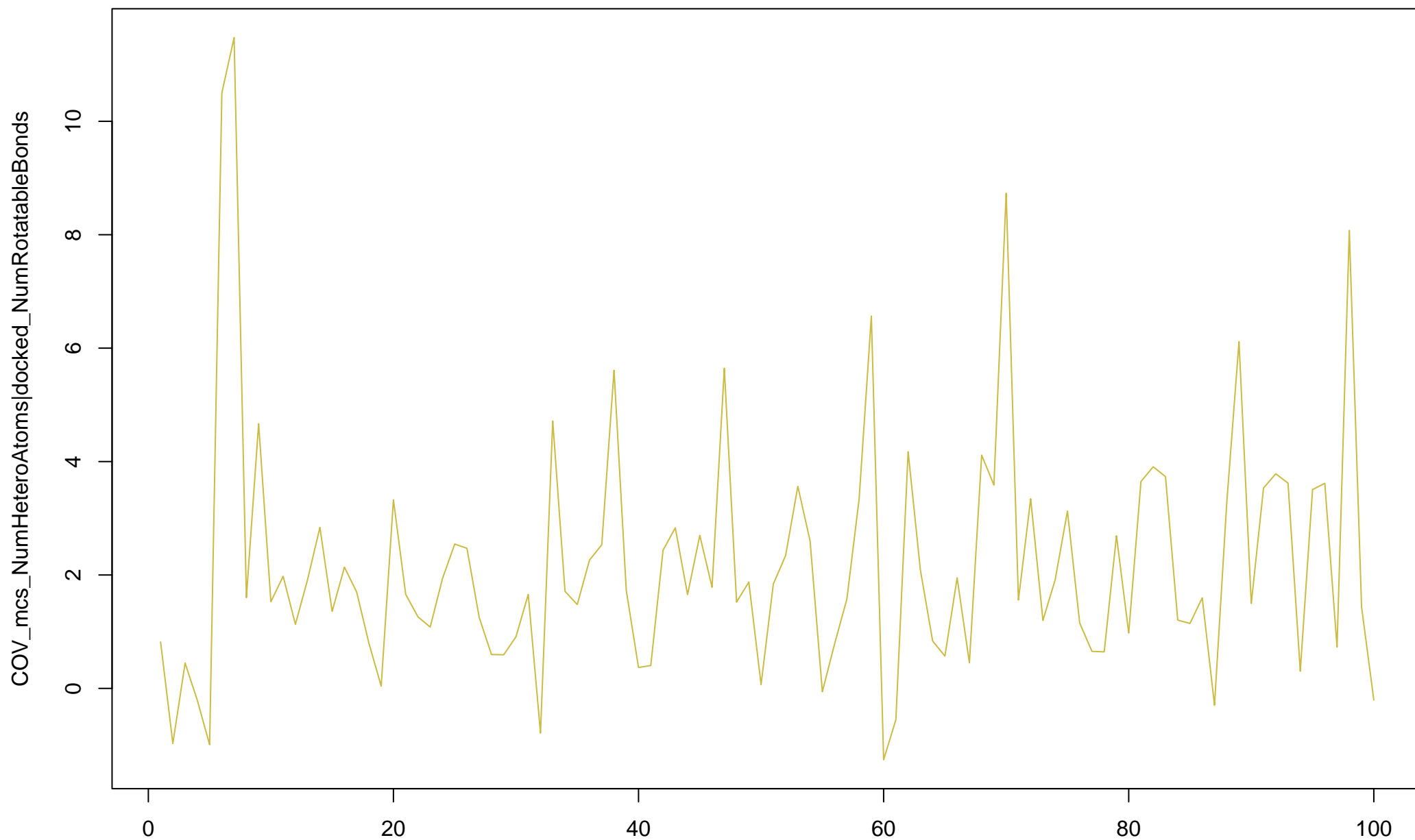
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 60.8 | BMK = 0.223 | MCSE(6.27) = 16.4 | stat: TRUE | burn: 10



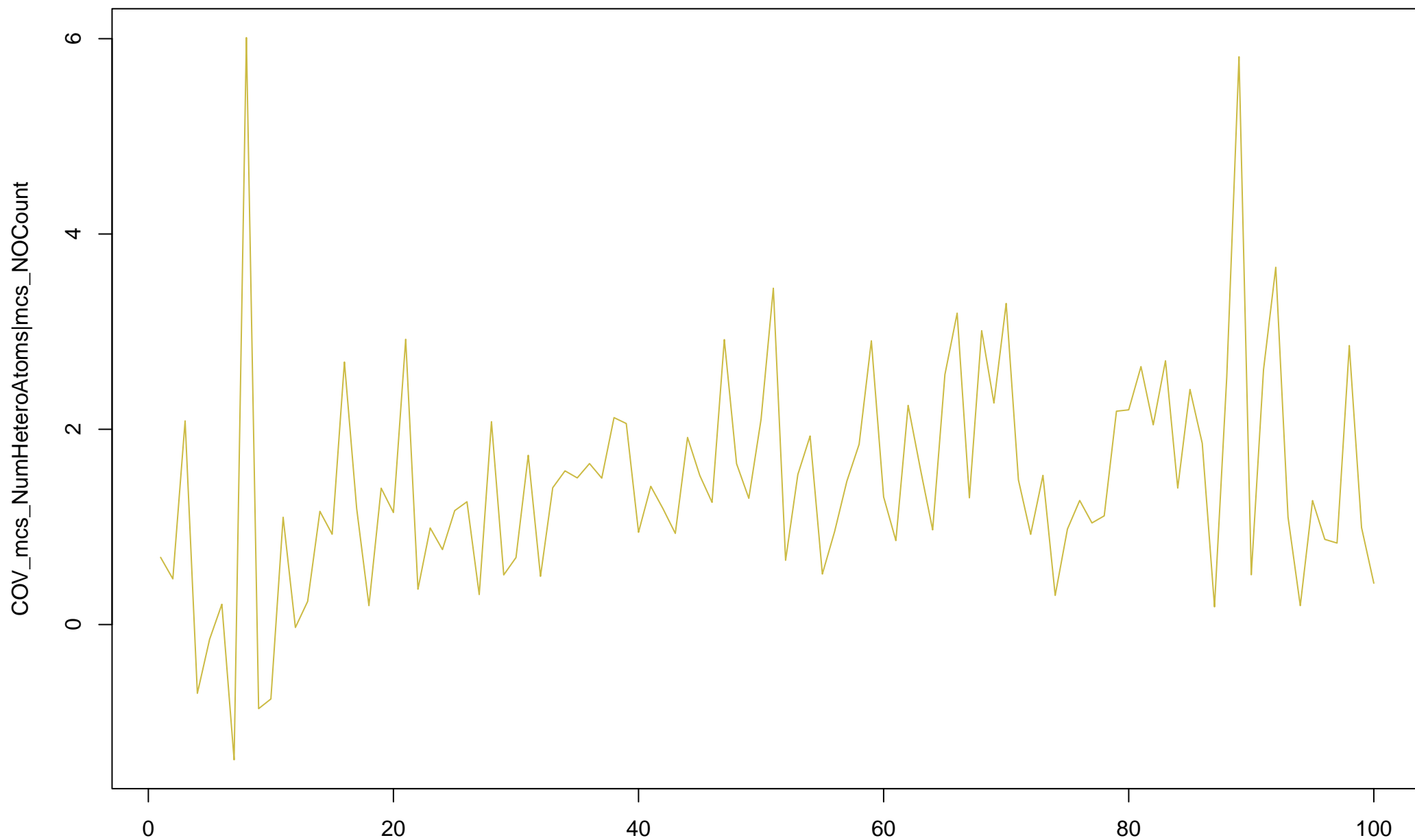
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 100 | BMK = 0.256 | MCSE(6.27) = 10.3 | stat: TRUE | burn: 0



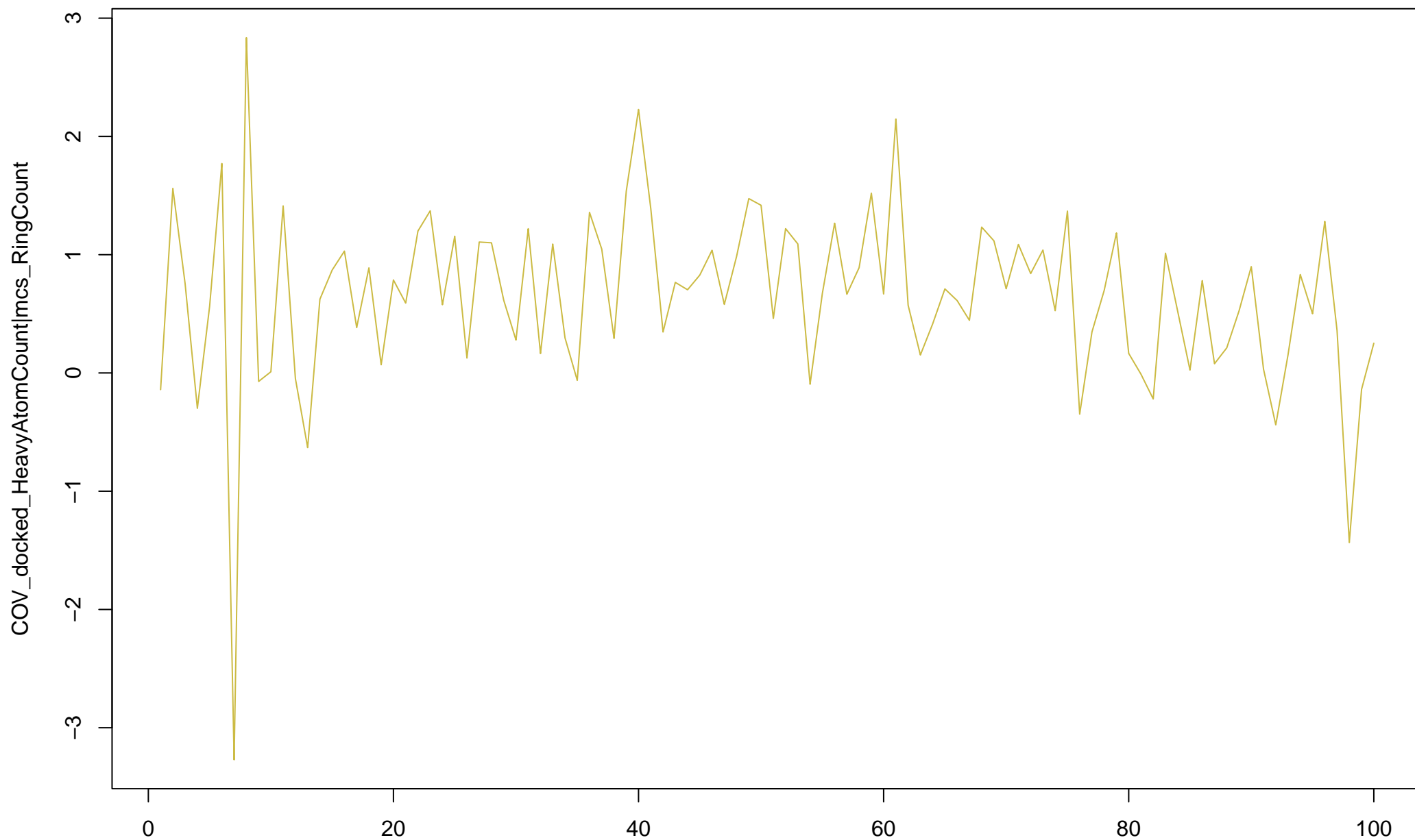
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 100 | BMK = 0.265 | MCSE(6.27) = 11.5 | stat: TRUE | burn: 10



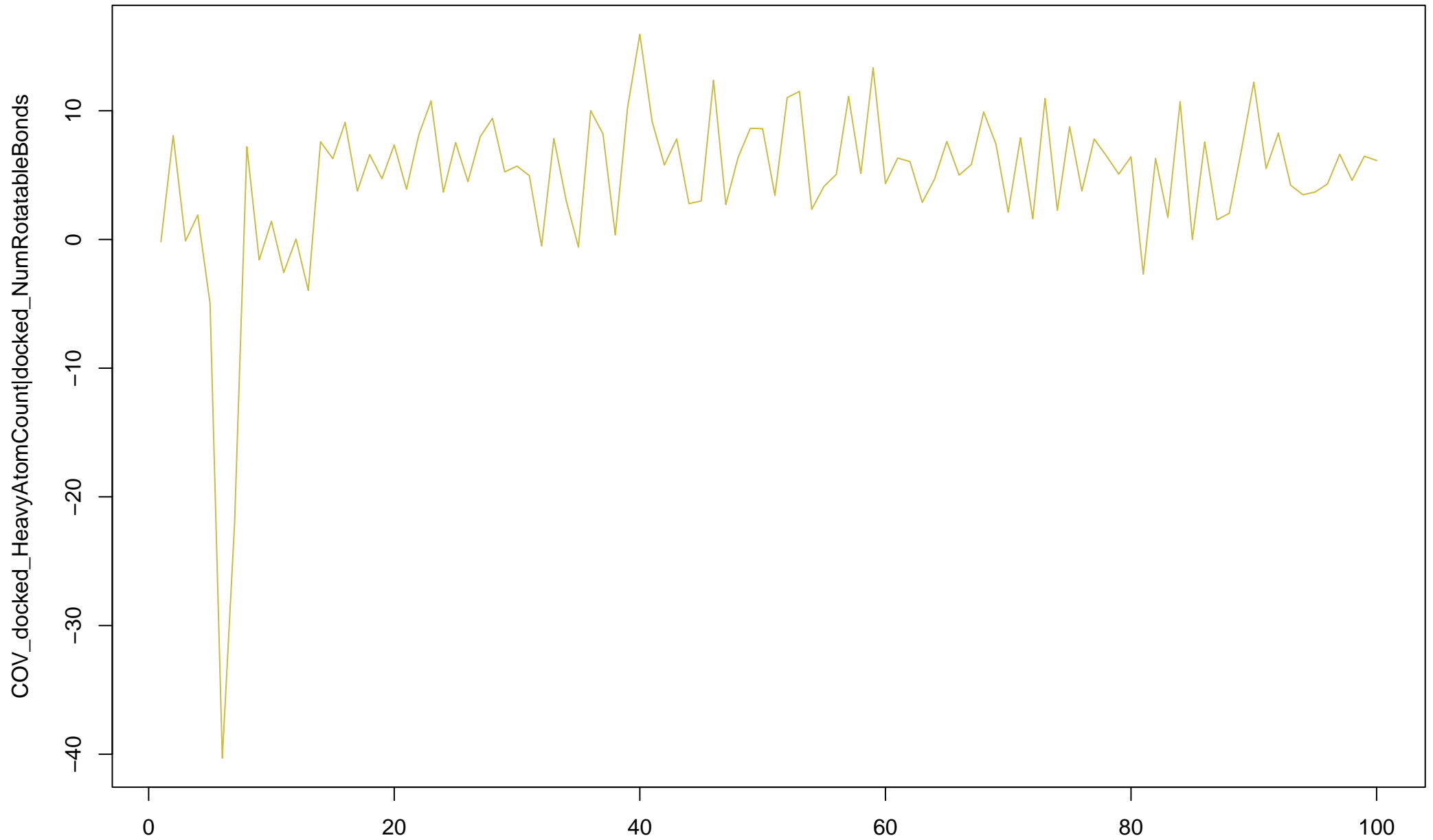
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 52.8 | BMK = 0.246 | MCSE(6.27) = 9.73 | stat: FALSE | burn: 10



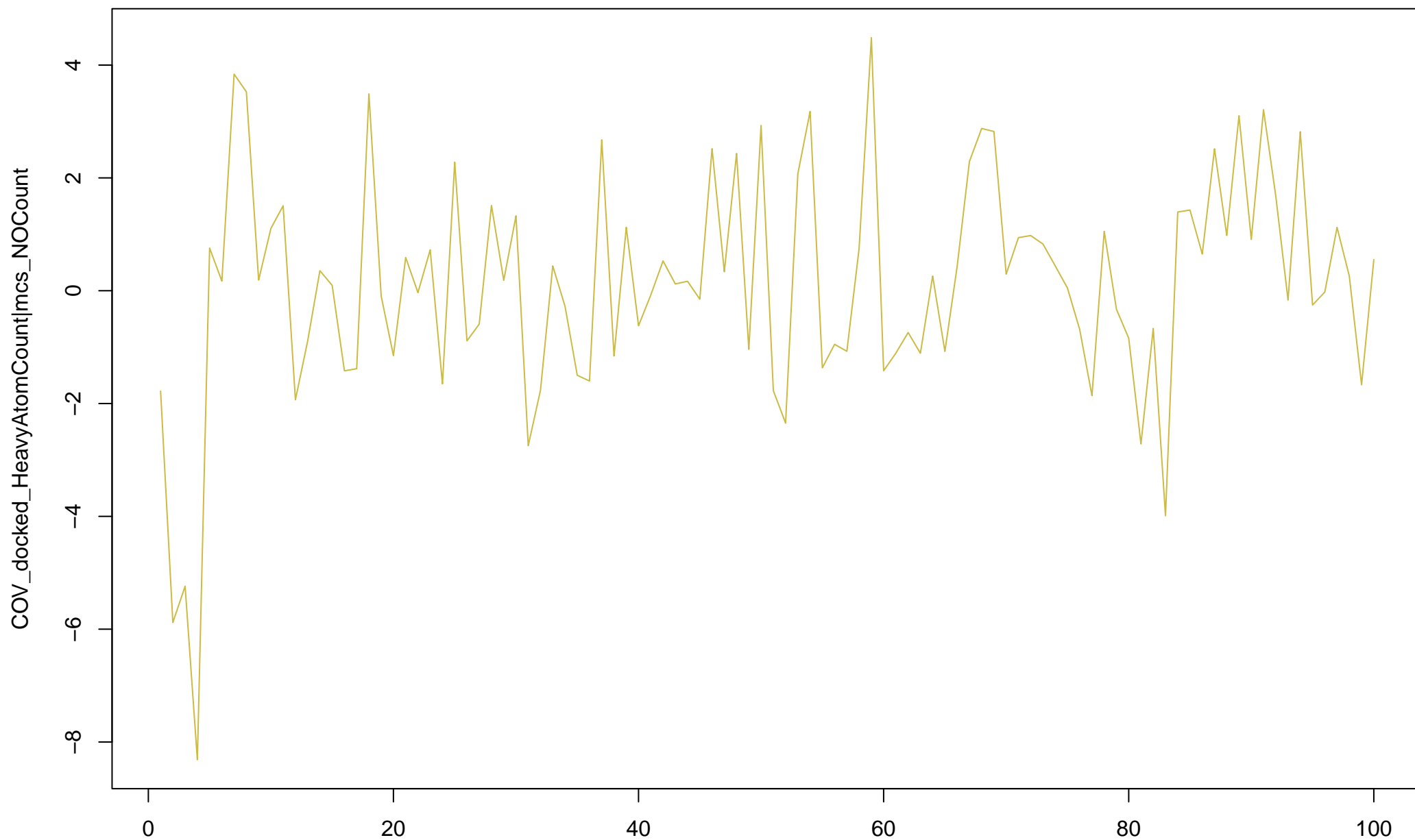
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 91.1 | BMK = 0.17 | MCSE(6.27) = 8 | stat: TRUE | burn: 0



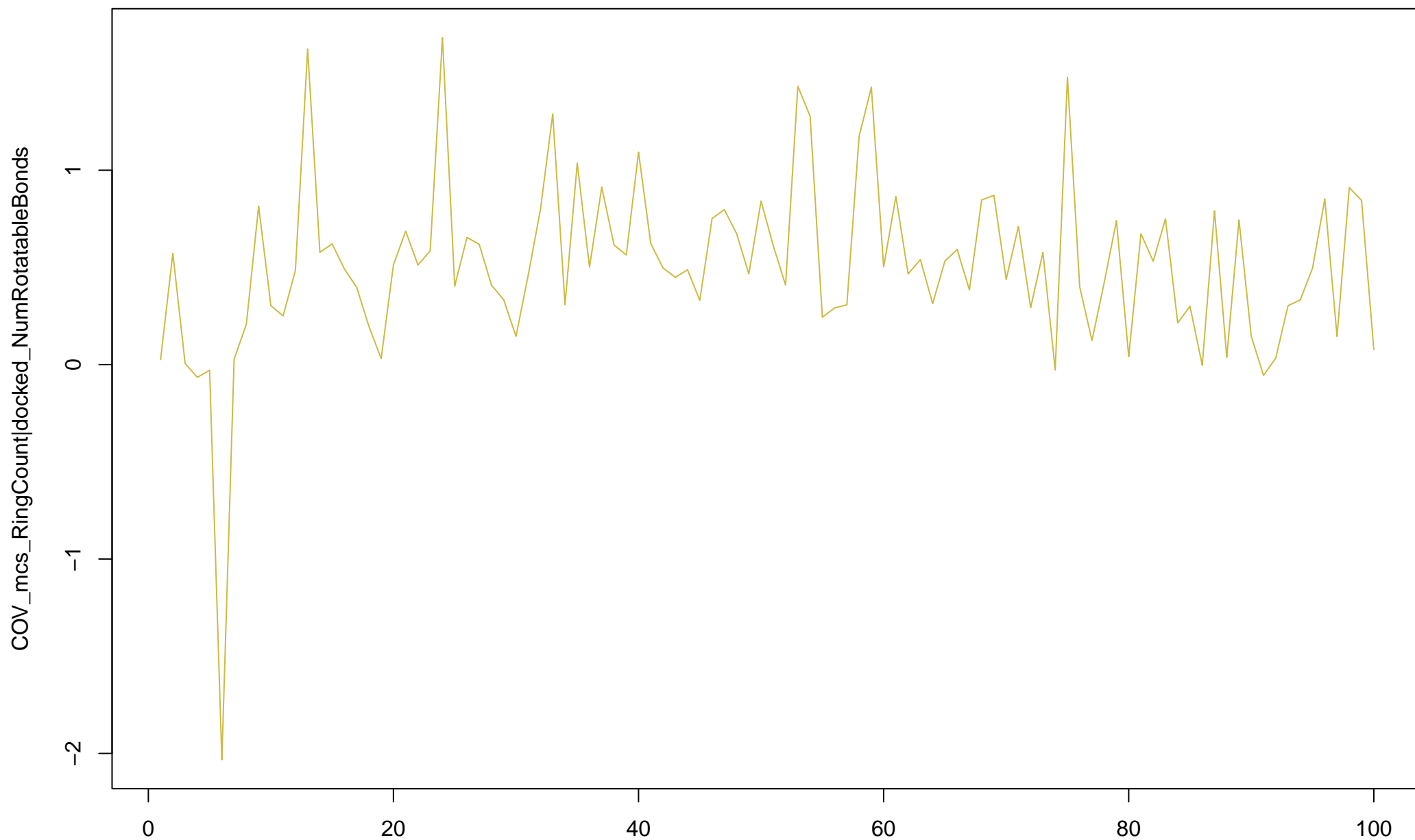
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 44.1 | BMK = 0.234 | MCSE(6.27) = 21.7 | stat: TRUE | burn: 100



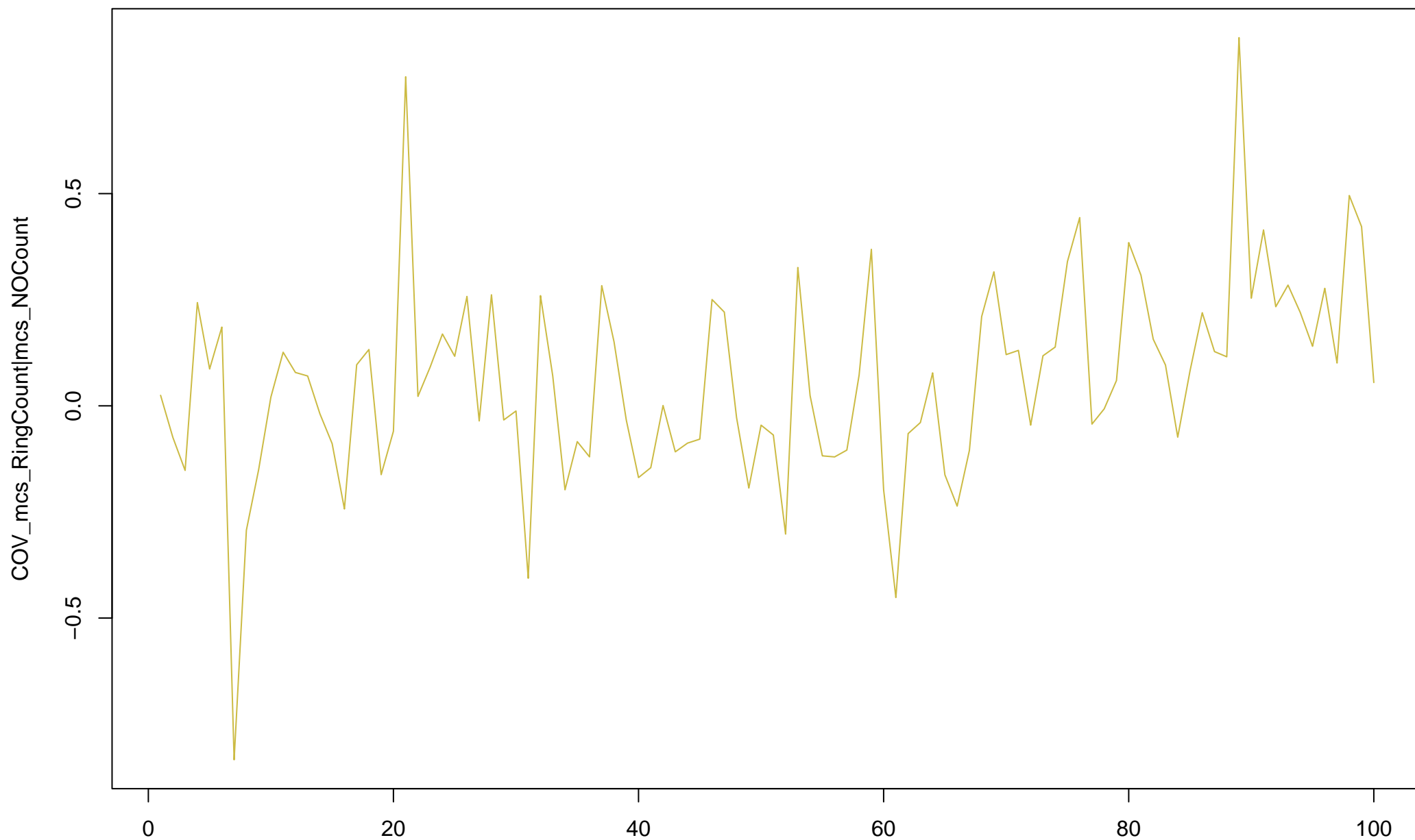
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 57.8 | BMK = 0.145 | MCSE(6.27) = 16.6 | stat: TRUE | burn: 0



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 68.6 | BMK = 0.145 | MCSE(6.27) = 18 | stat: TRUE | burn: 10



COV_mcs_RingCount|mcs_NOCount
ESS = 57 | BMK = 0.249 | MCSE(6.27) = 15.7 | stat: TRUE | burn: 0



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 100 | BMK = 0.178 | MCSE(6.27) = 10.6 | stat: TRUE | burn: 10

