

-- STATS maxD --

min ESS = 15.4546624110554

max BMK = 1

max MCSE = 18.8292132694745

all stationary: FALSE

burn: 100

-- STATS 2D --

min ESS = 12.0796622960778

max BMK = 0.567647738233113

max MCSE = 33.6876097070107

all stationary: FALSE

burn: 100

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.488796925405854

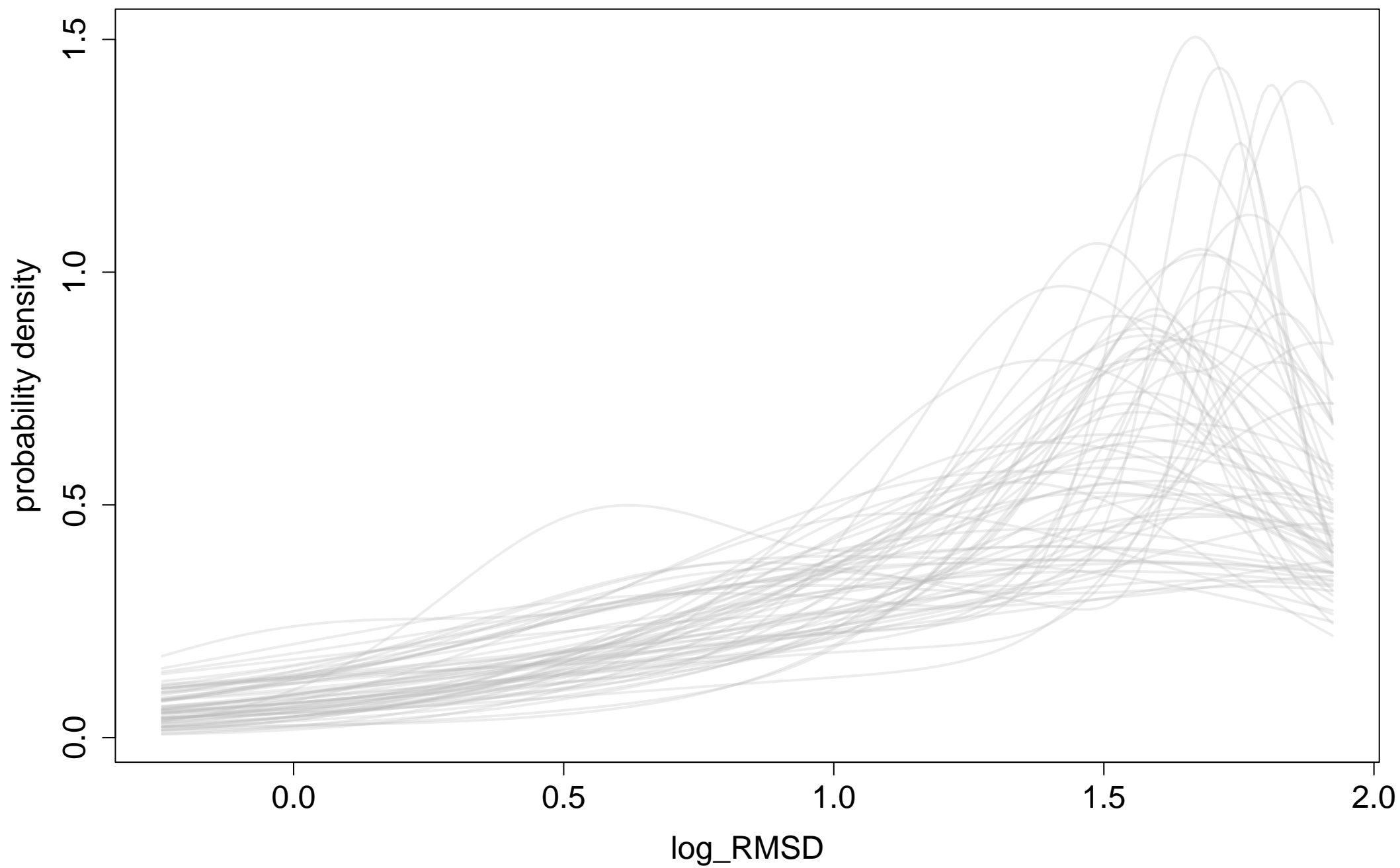
max MCSE = NaN

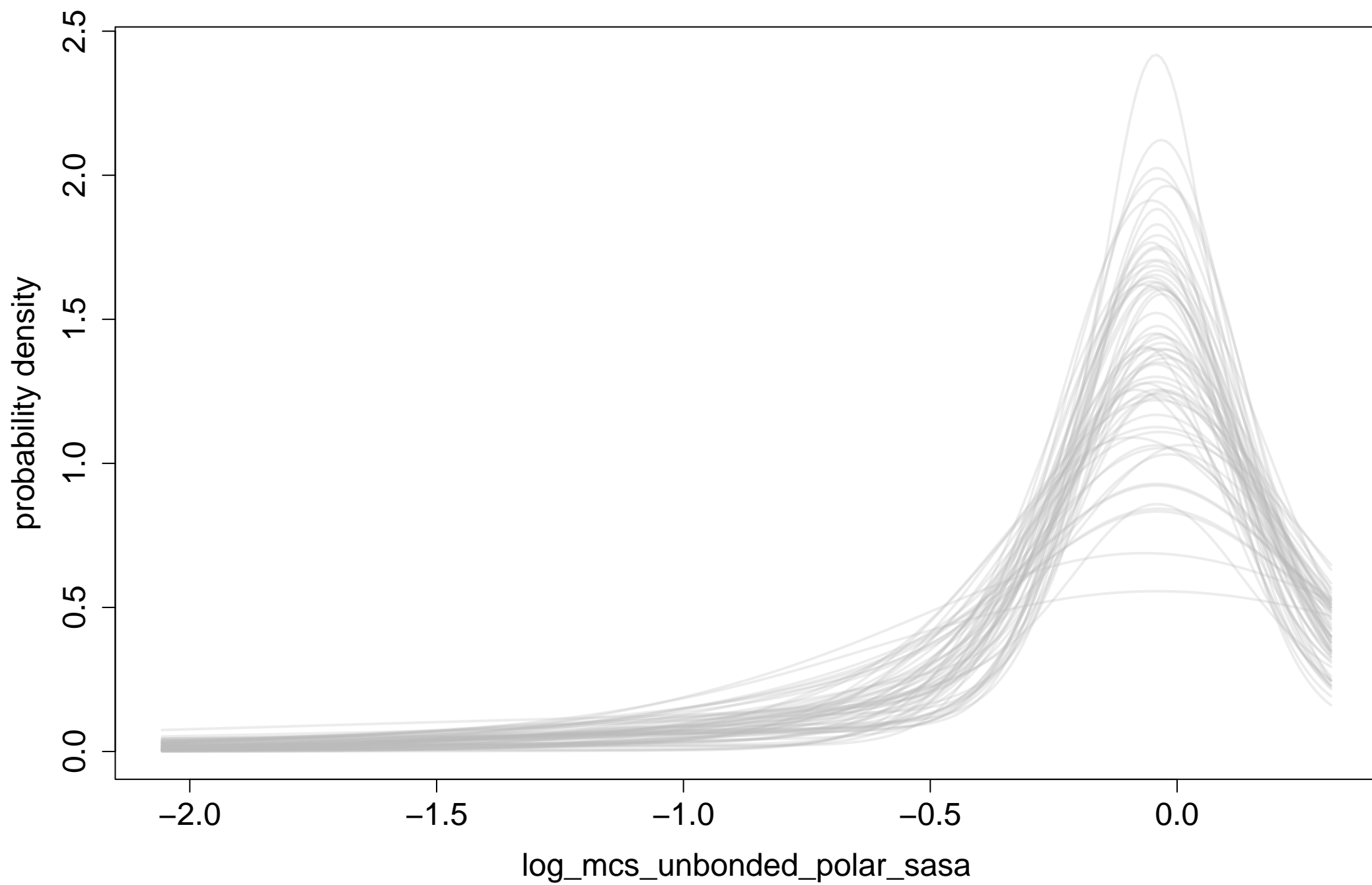
all stationary: FALSE

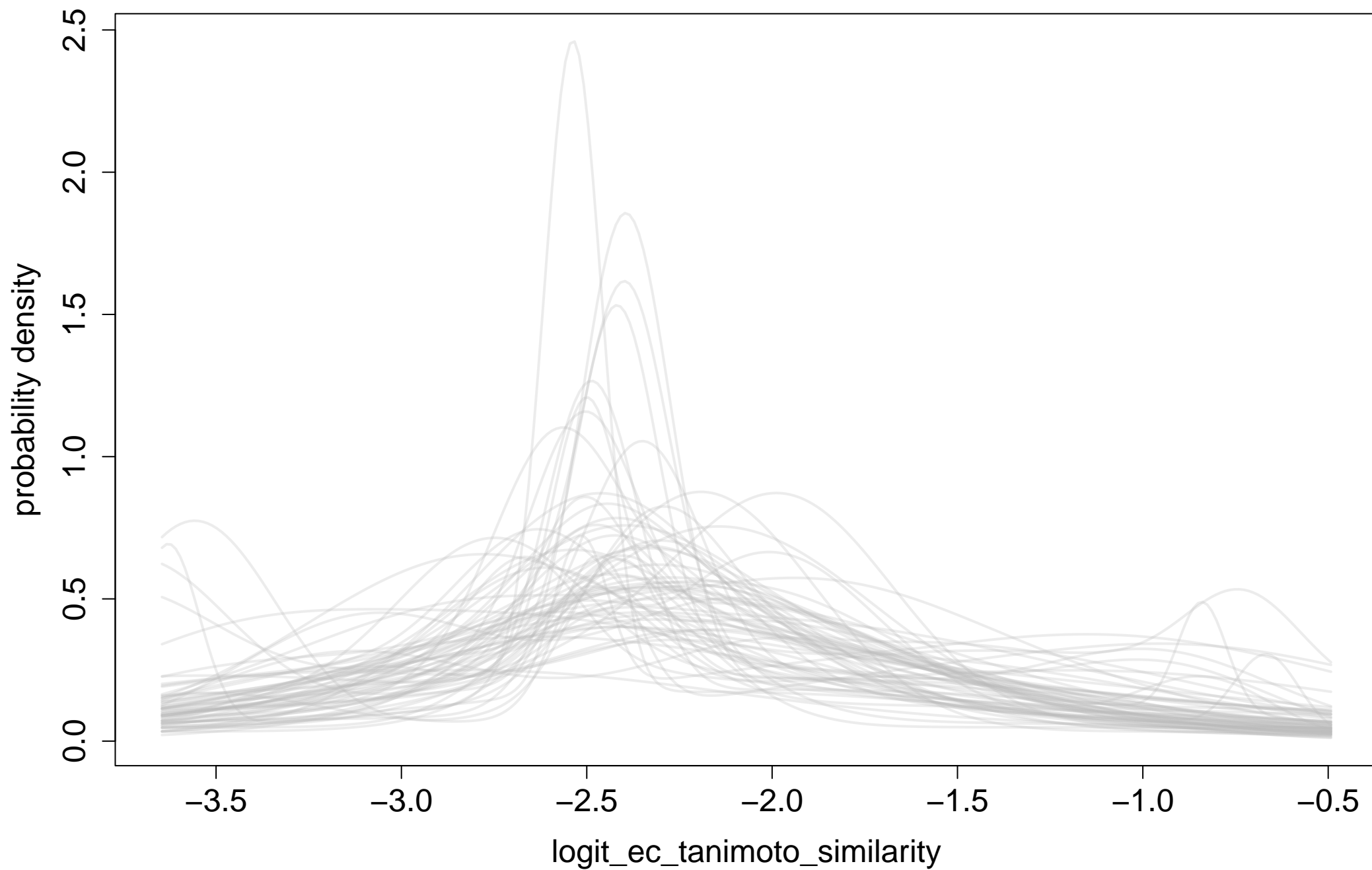
burn: 100

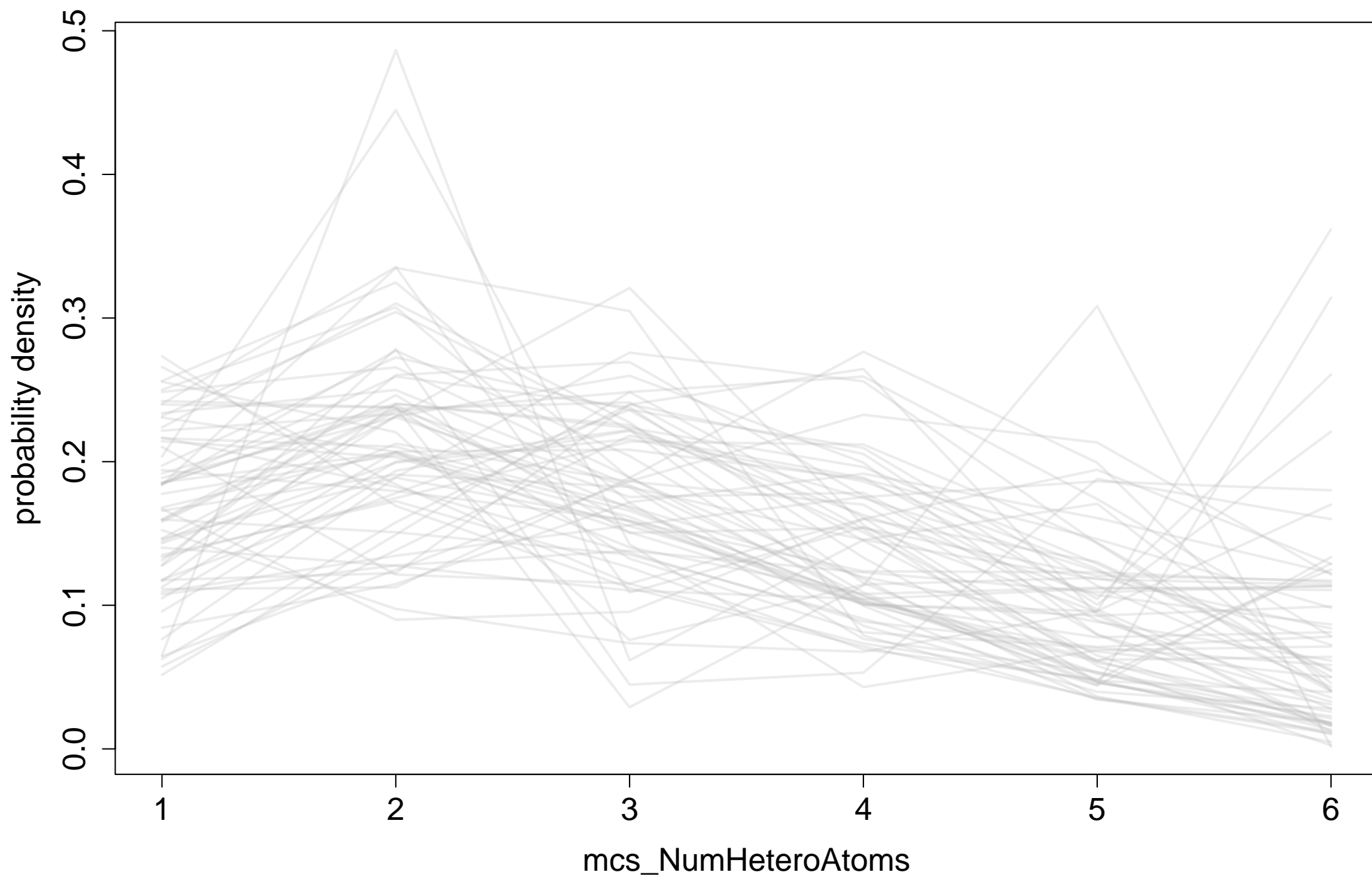
Occupied clusters: 4 of 4

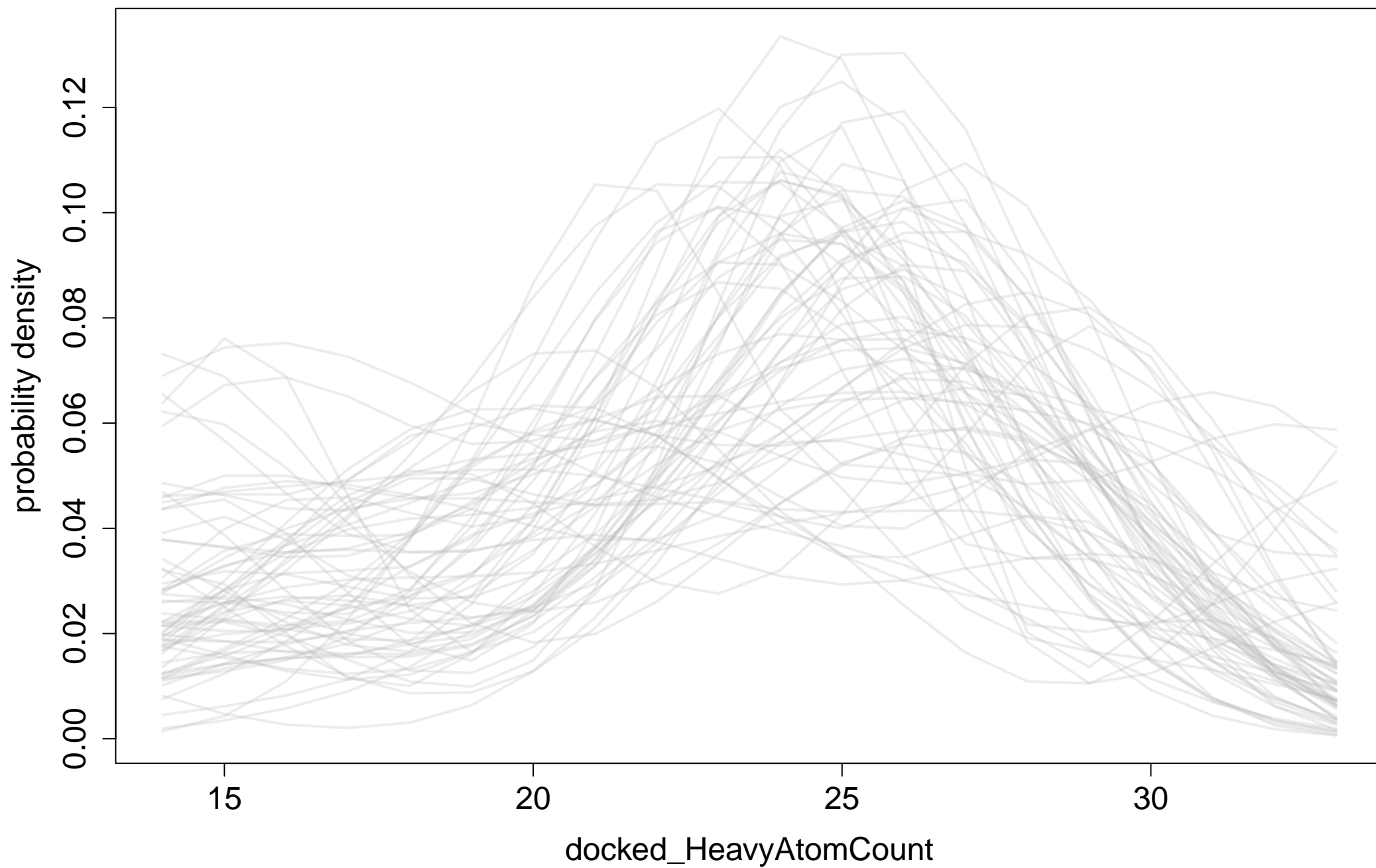
LL: -113 +- 5.32

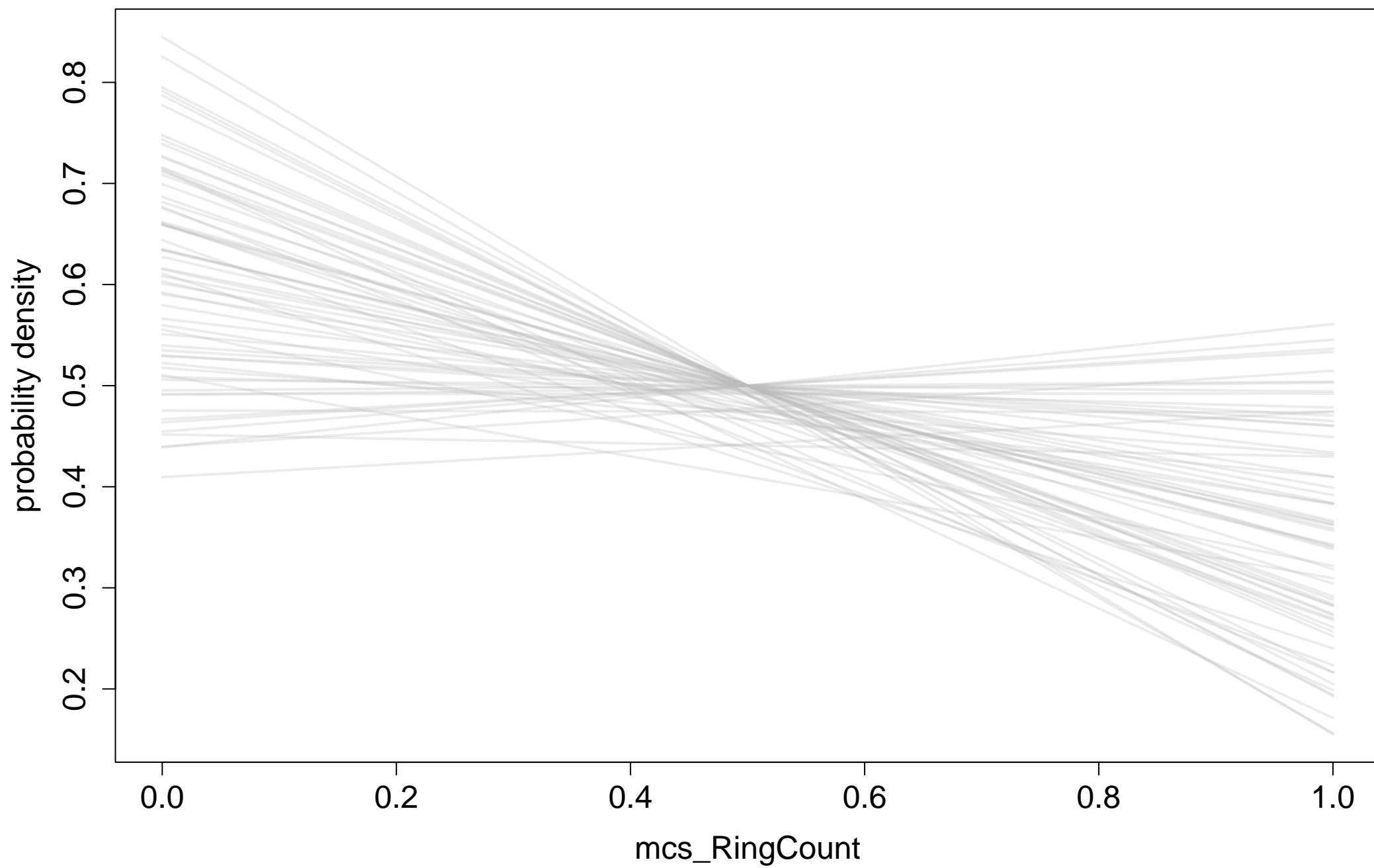


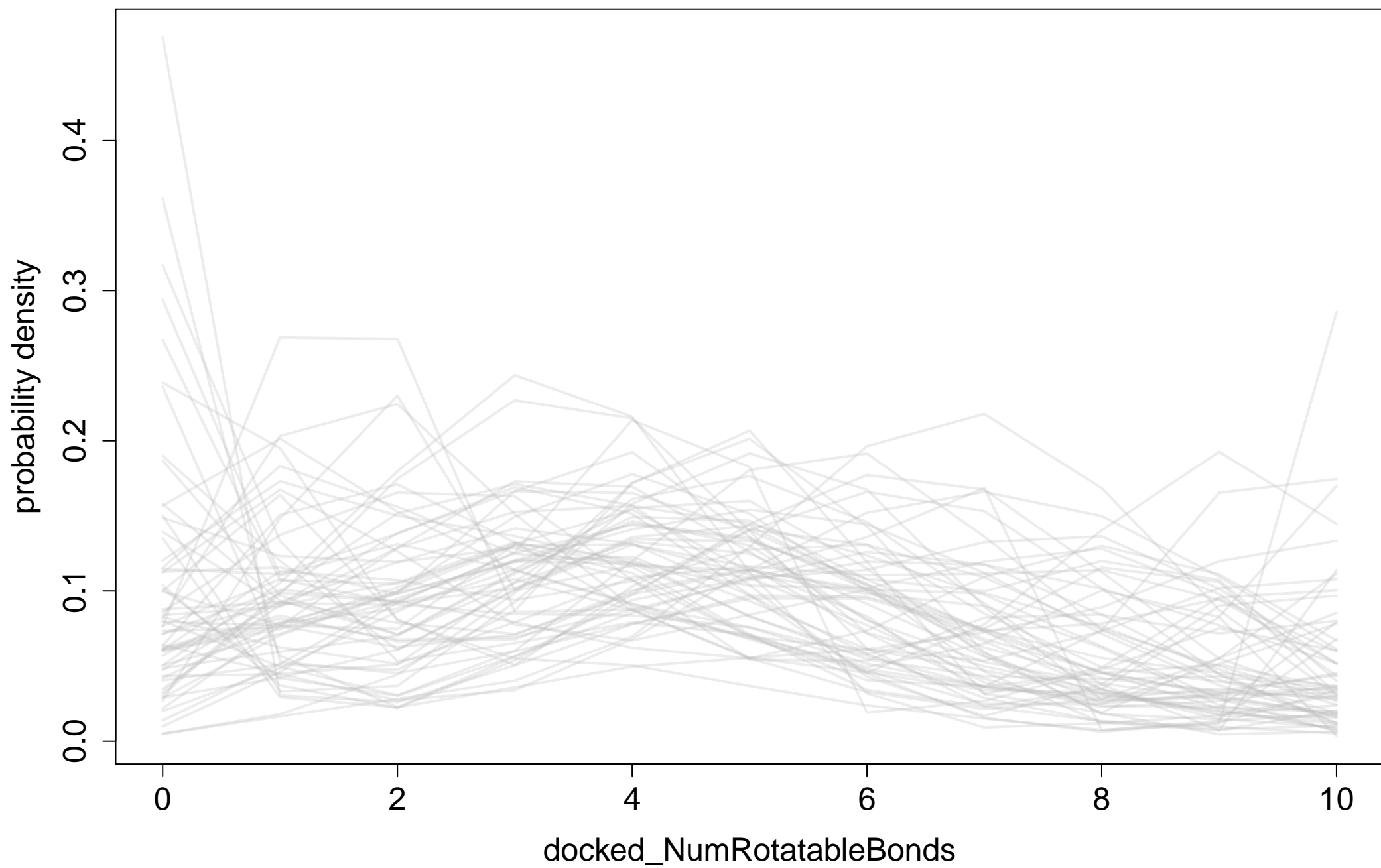


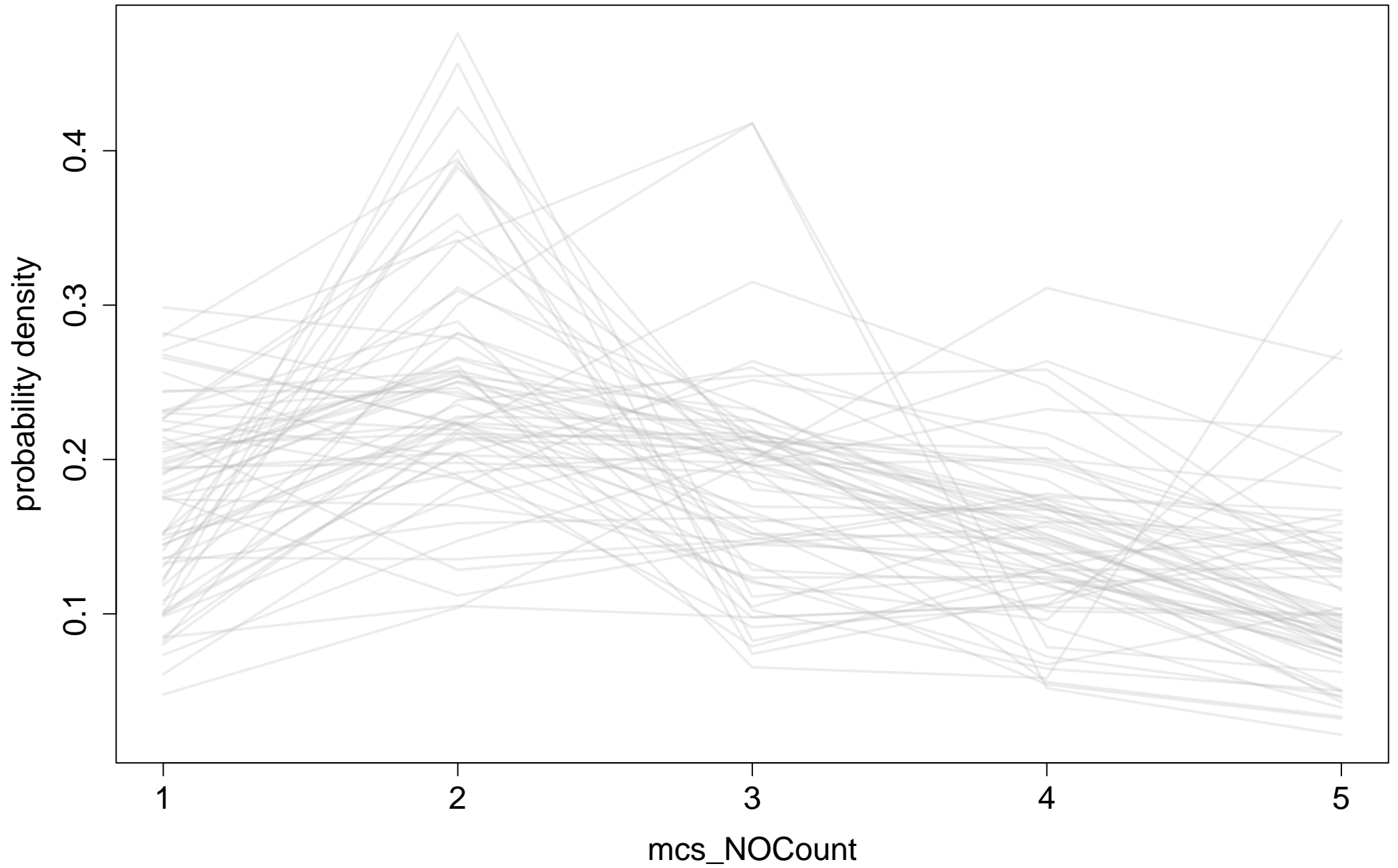


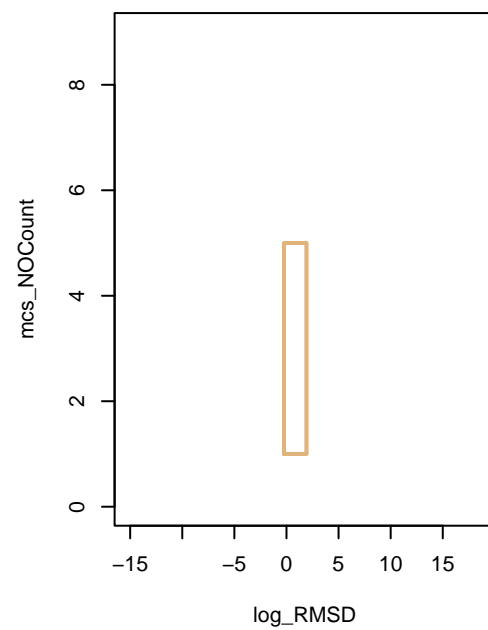
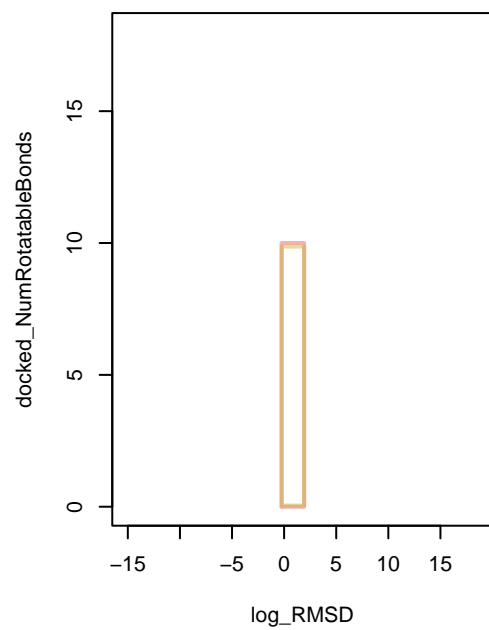
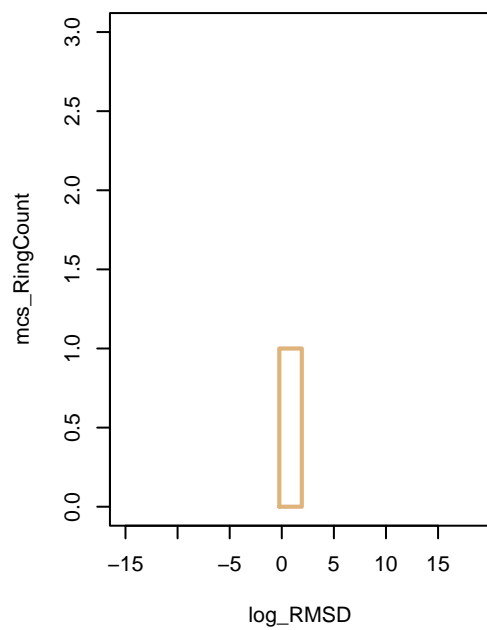
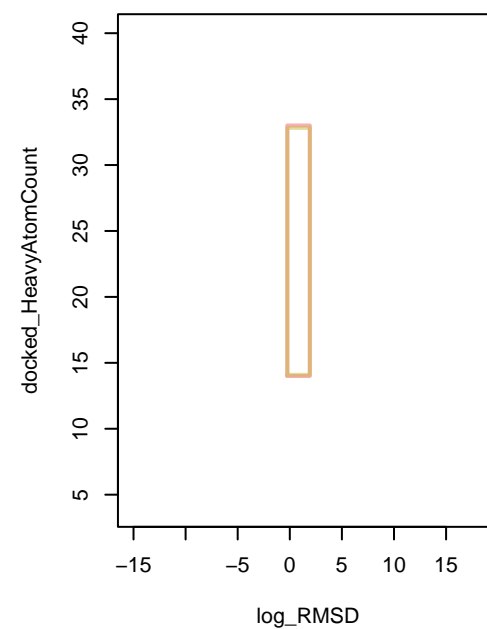
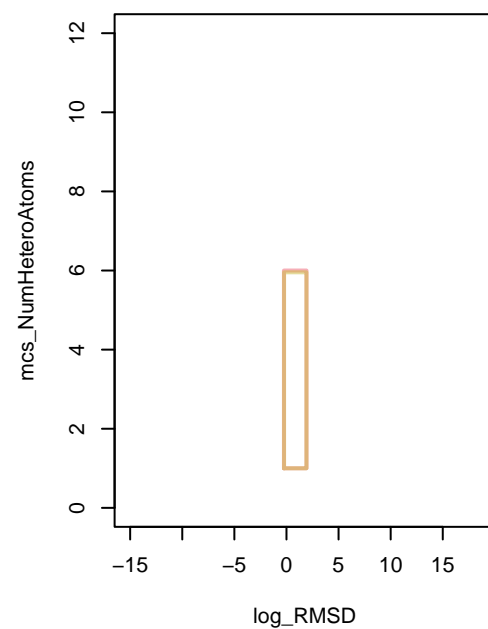
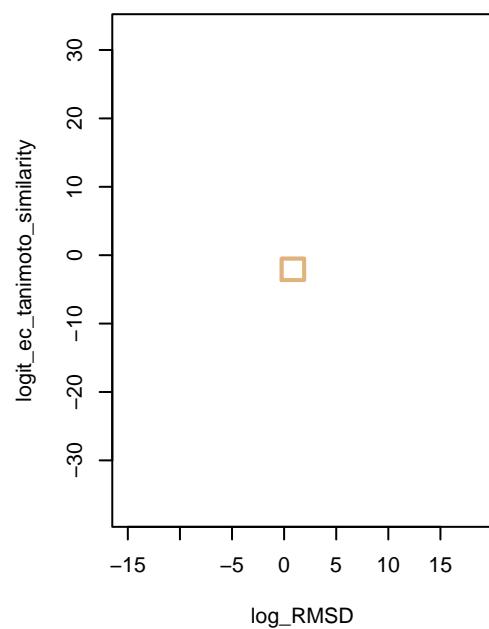
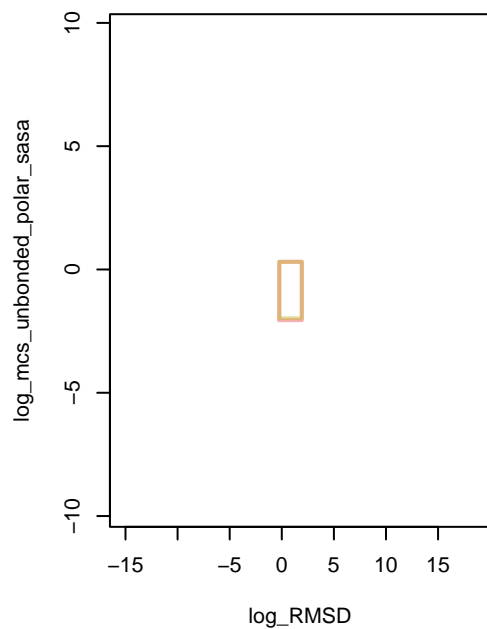




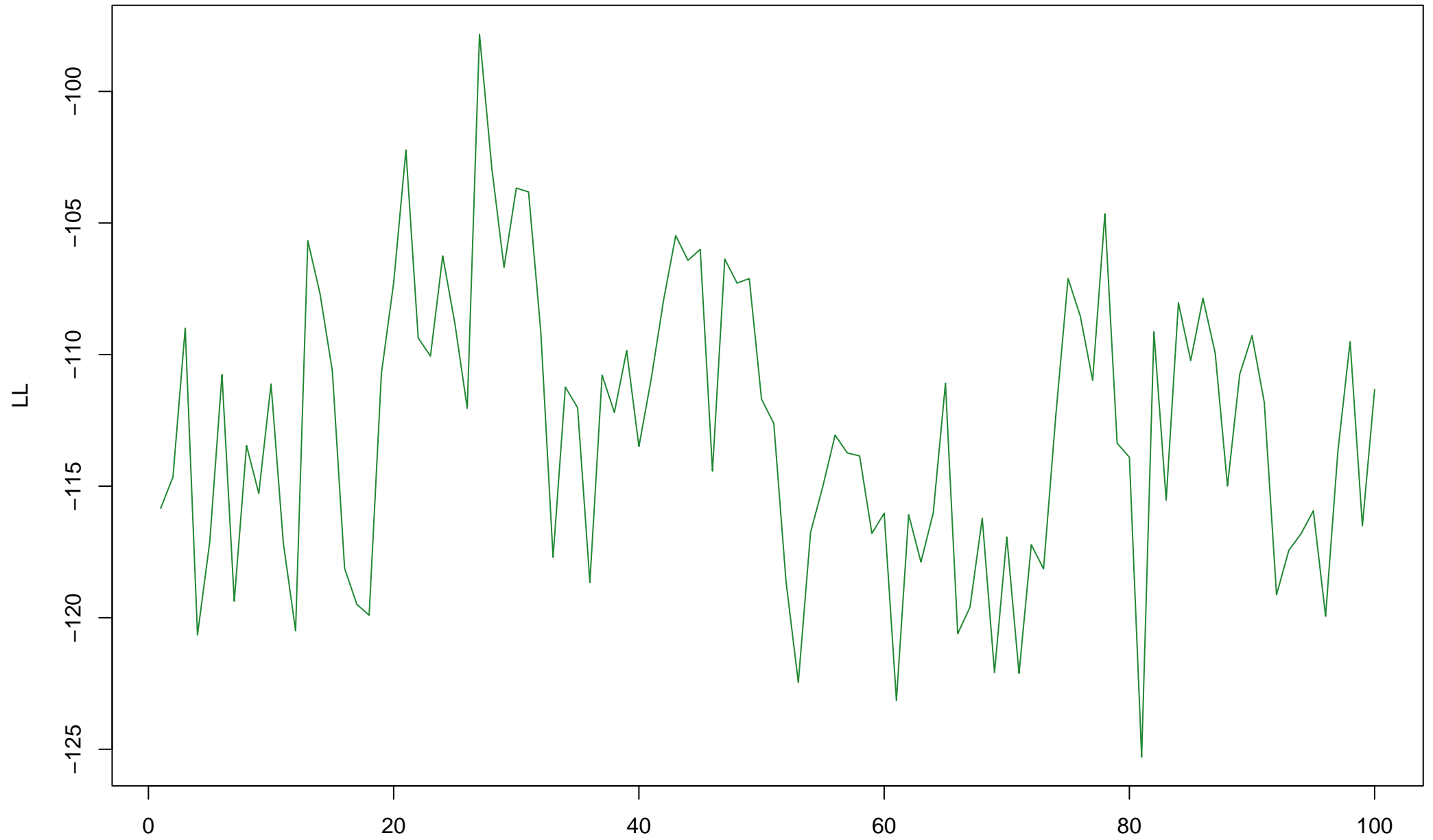




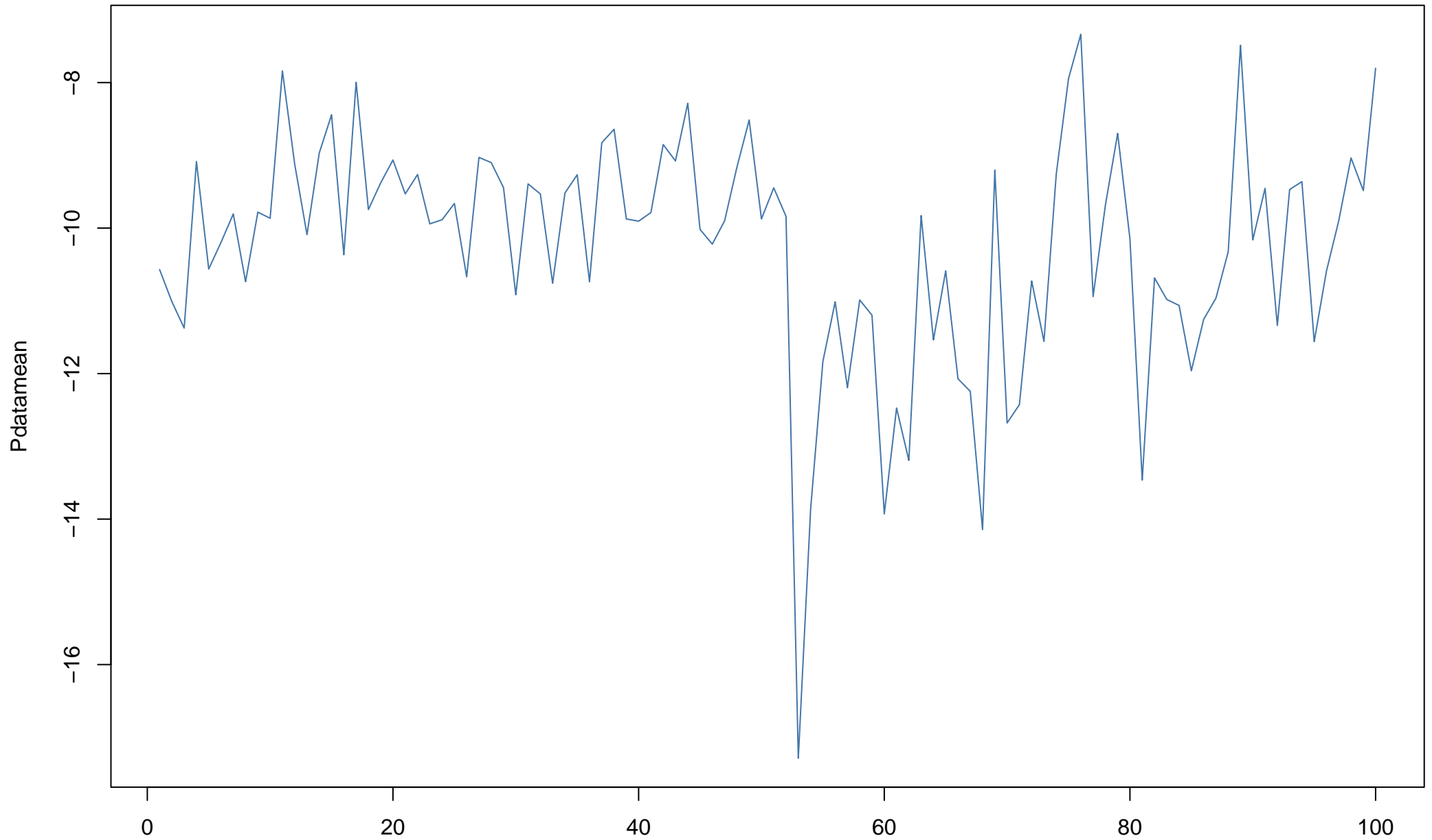




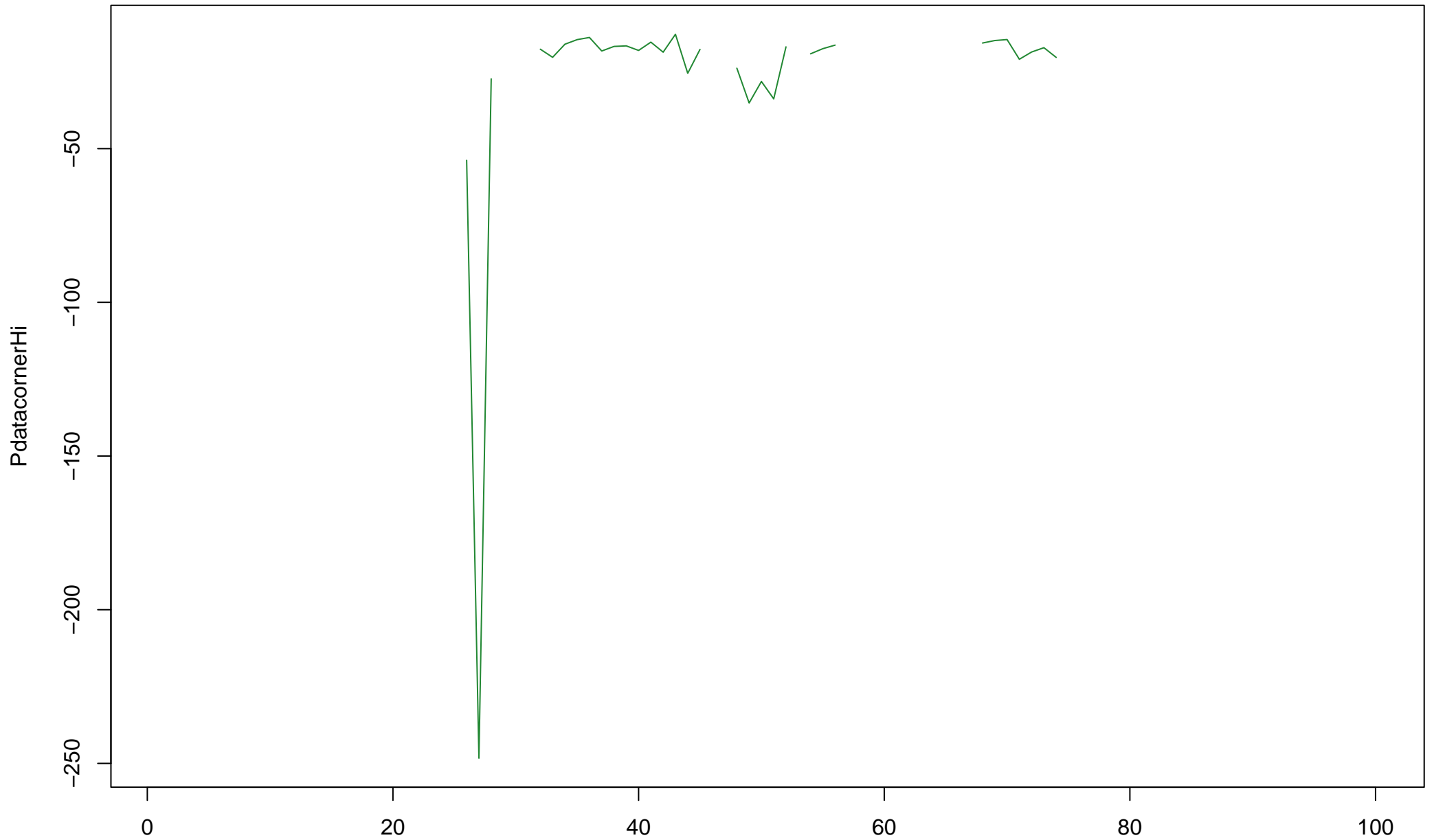
LL



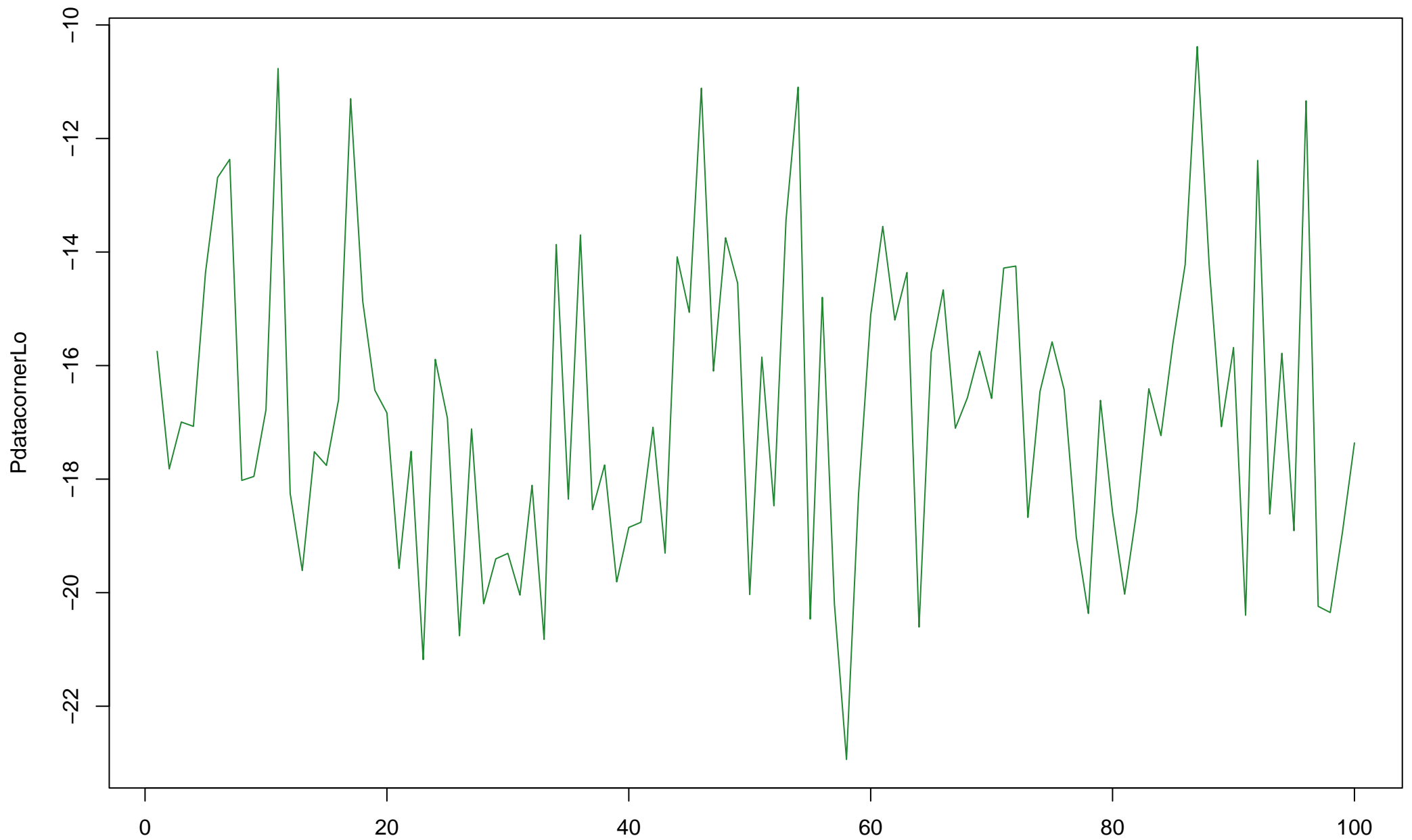
Pdatamean
ESS = 72.1 | BMK = 0.316 | MCSE(6.27) = 13.6 | stat: TRUE | burn: 100



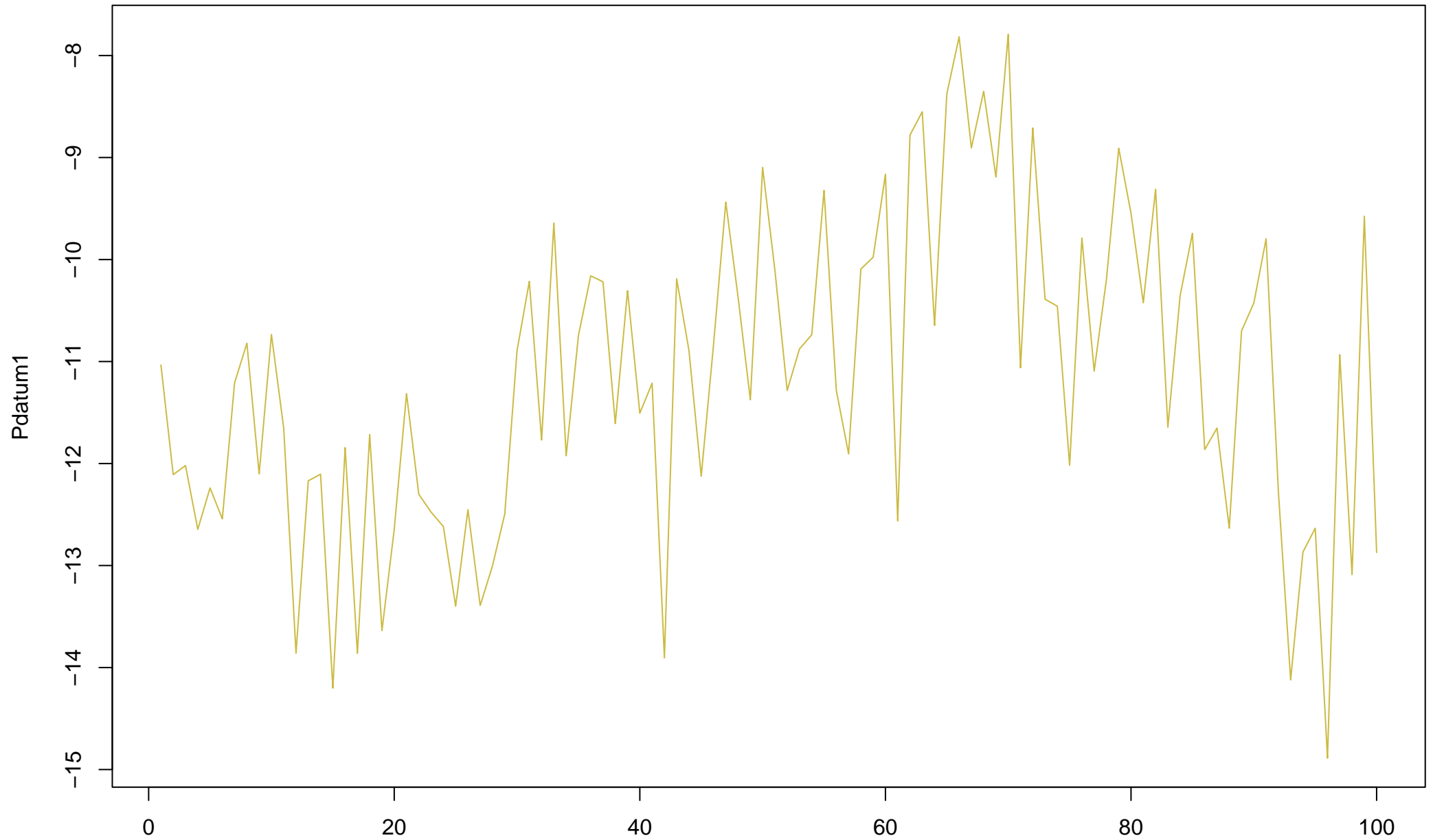
PdatacornerHi
ESS = 100 | BMK = 1 | MCSE(6.27) = 11.6 | stat: TRUE | burn: 100



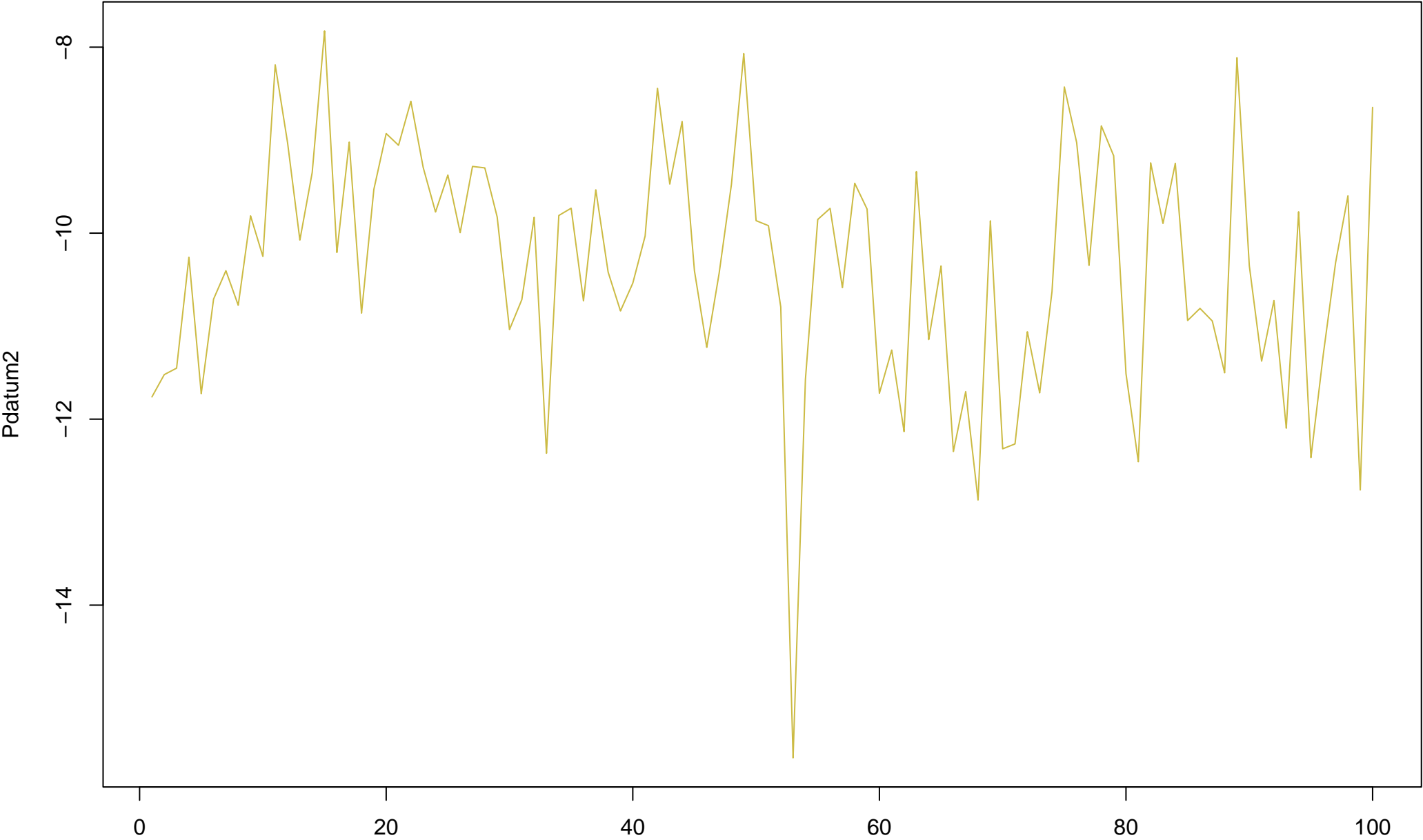
PdatacornerLo
ESS = 100 | BMK = 0.382 | MCSE(6.27) = 9.51 | stat: TRUE | burn: 100



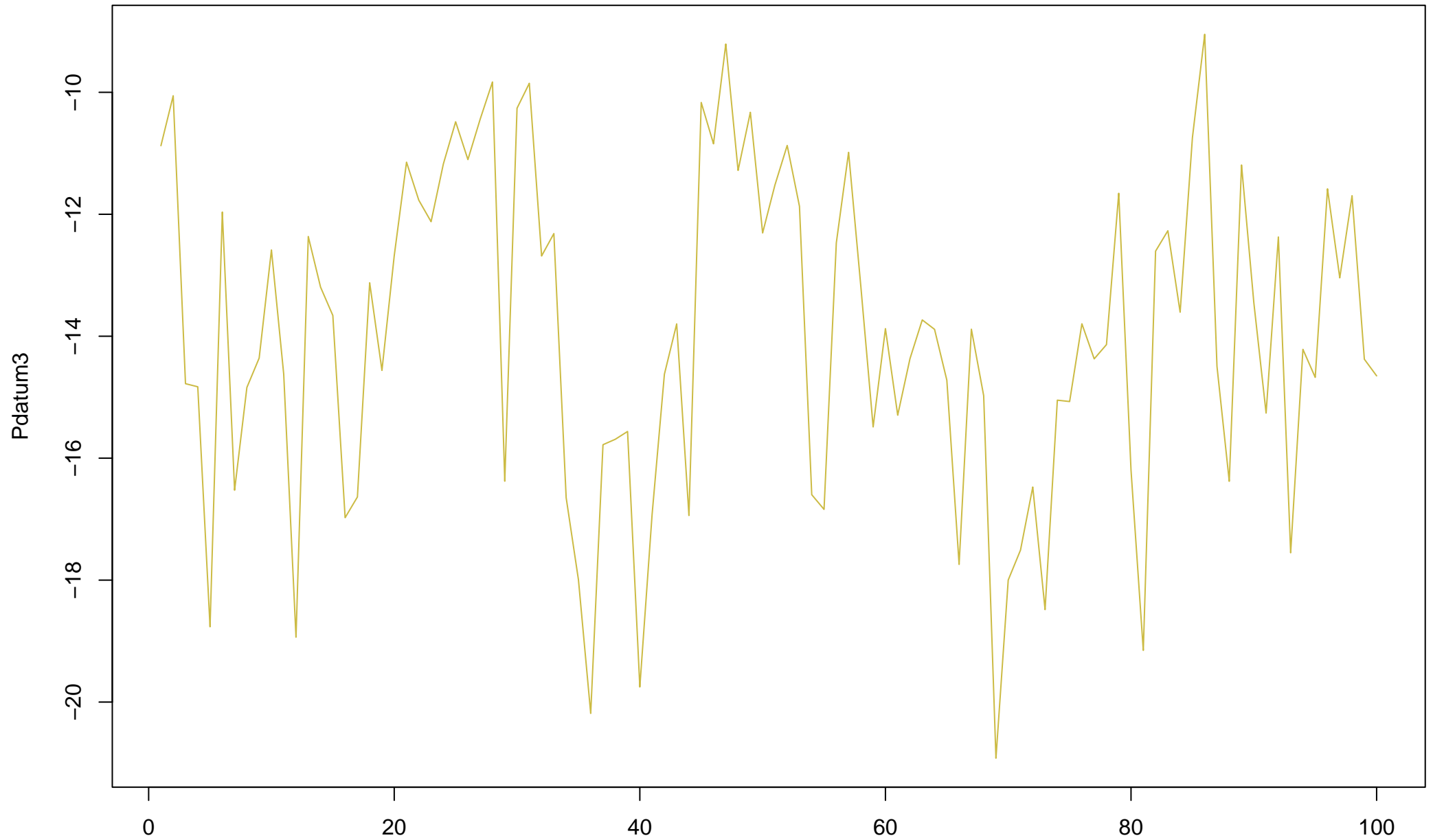
Pdatum1
ESS = 15.5 | BMK = 0.456 | MCSE(6.27) = 18.8 | stat: FALSE | burn: 70



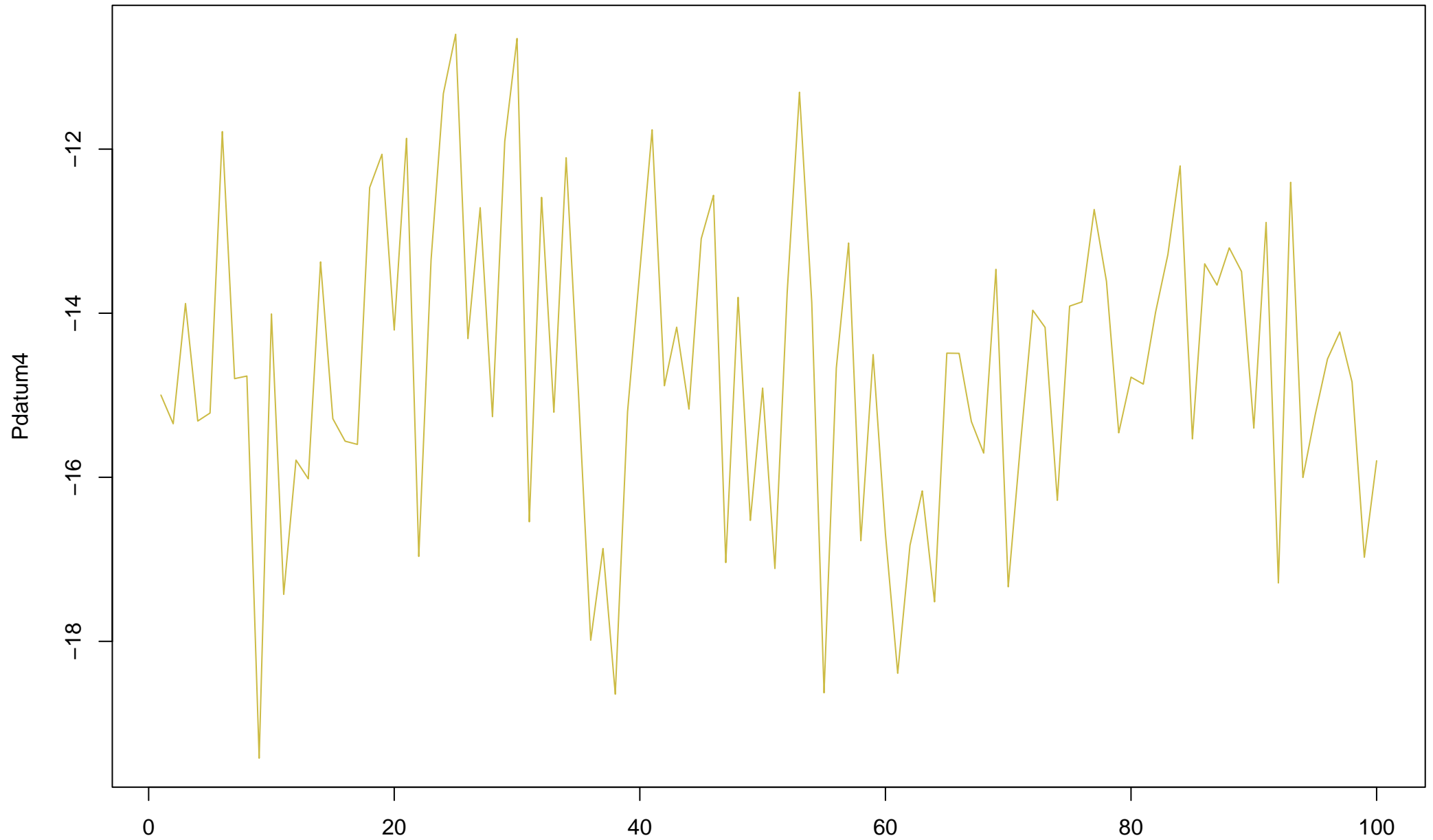
Pdatum2
ESS = 100 | BMK = 0.183 | MCSE(6.27) = 12.9 | stat: TRUE | burn: 10



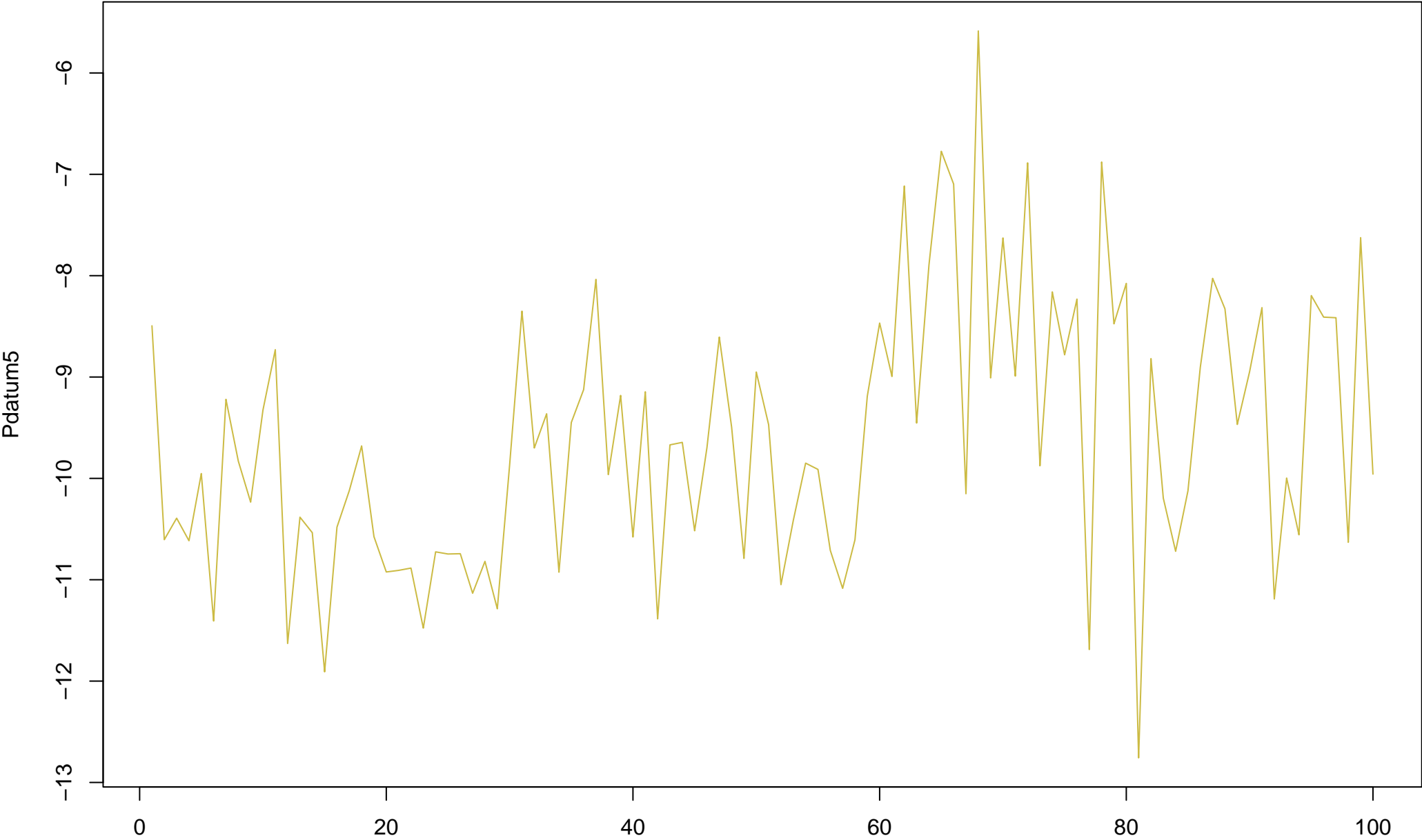
Pdatum3
ESS = 47.1 | BMK = 0.422 | MCSE(6.27) = 18.2 | stat: TRUE | burn: 100



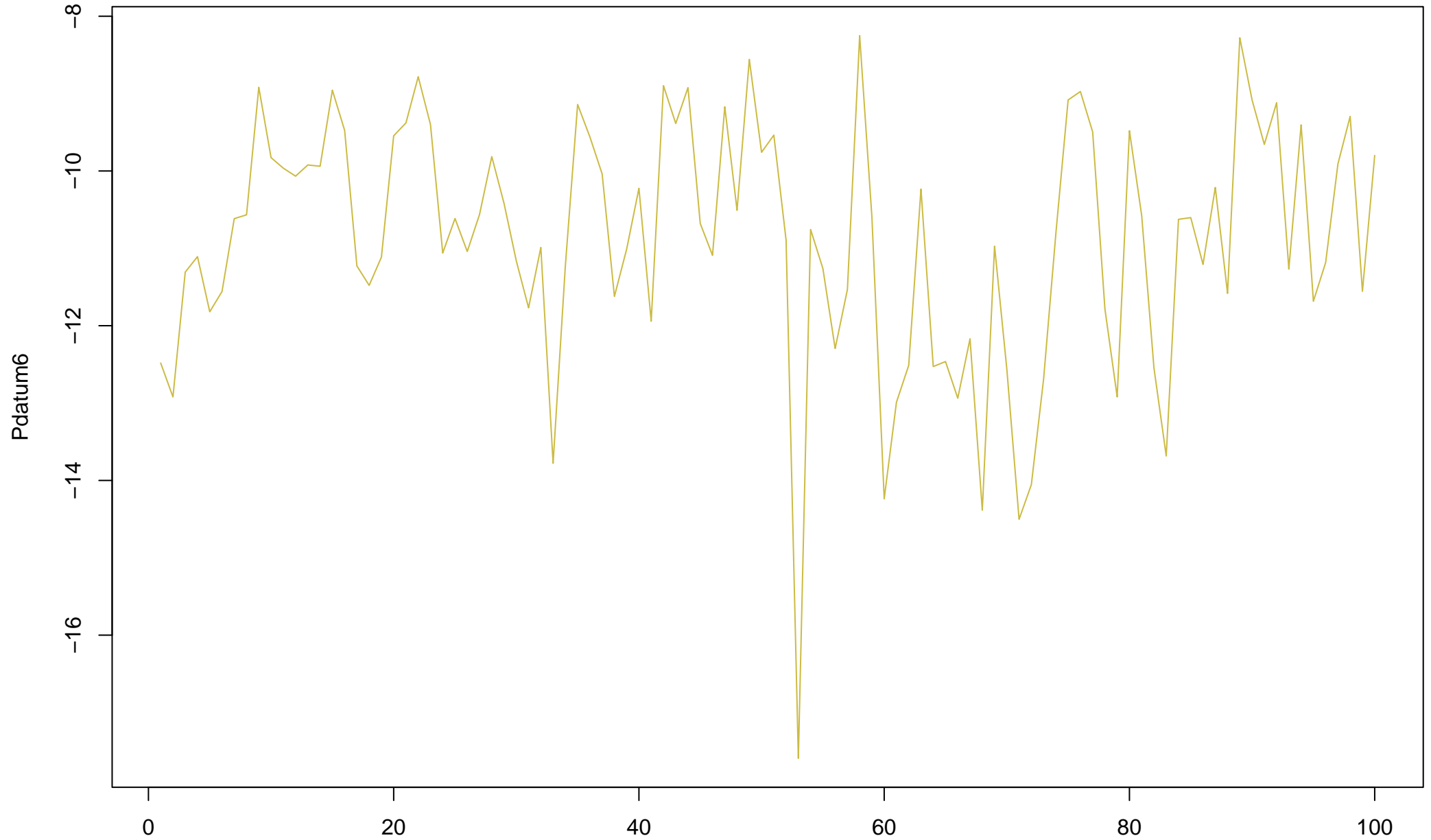
Pdatum4
ESS = 24.3 | BMK = 0.301 | MCSE(6.27) = 13.3 | stat: TRUE | burn: 100



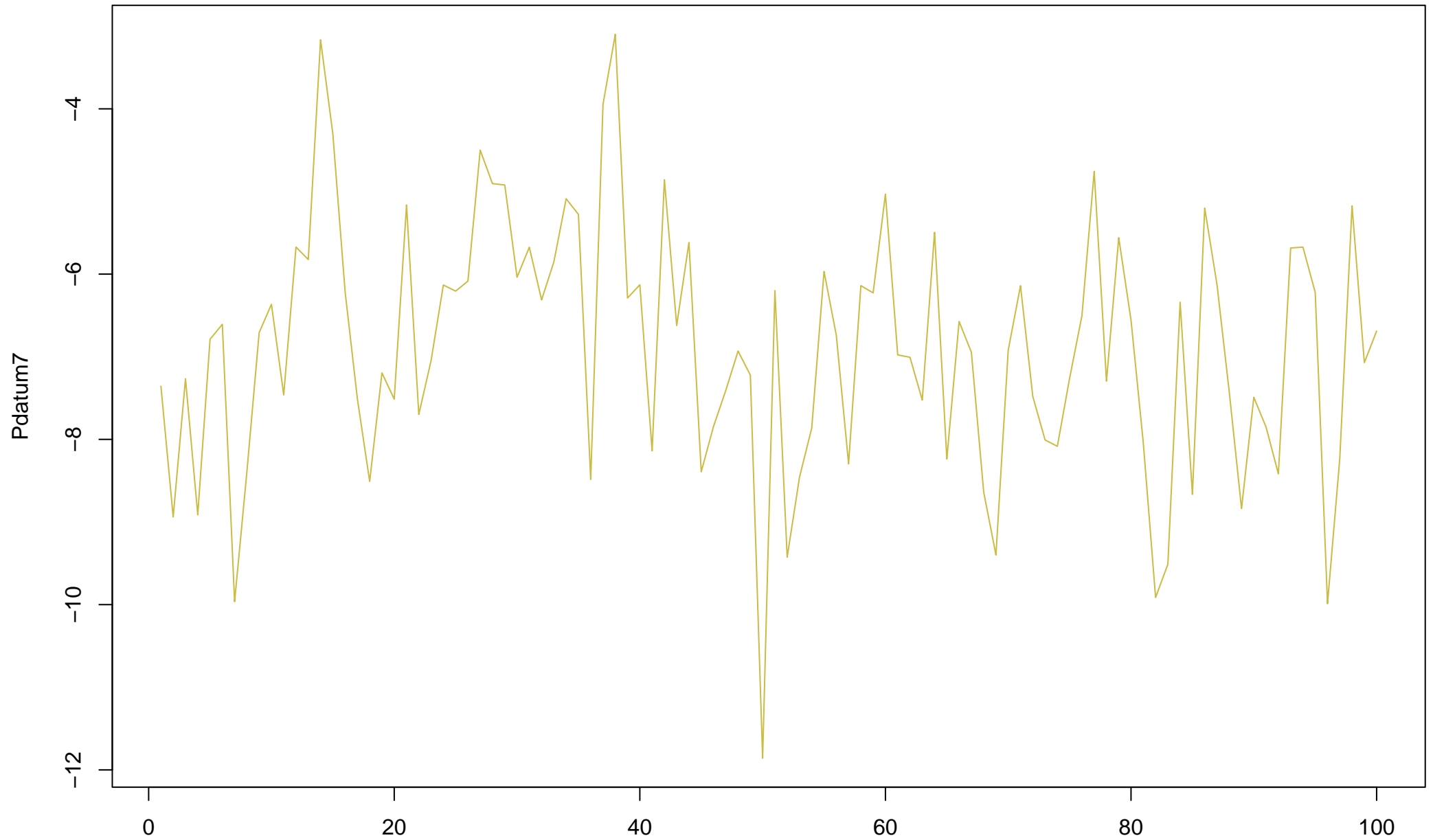
Pdatum5
ESS = 25 | BMK = 0.424 | MCSE(6.27) = 12.8 | stat: FALSE | burn: 60



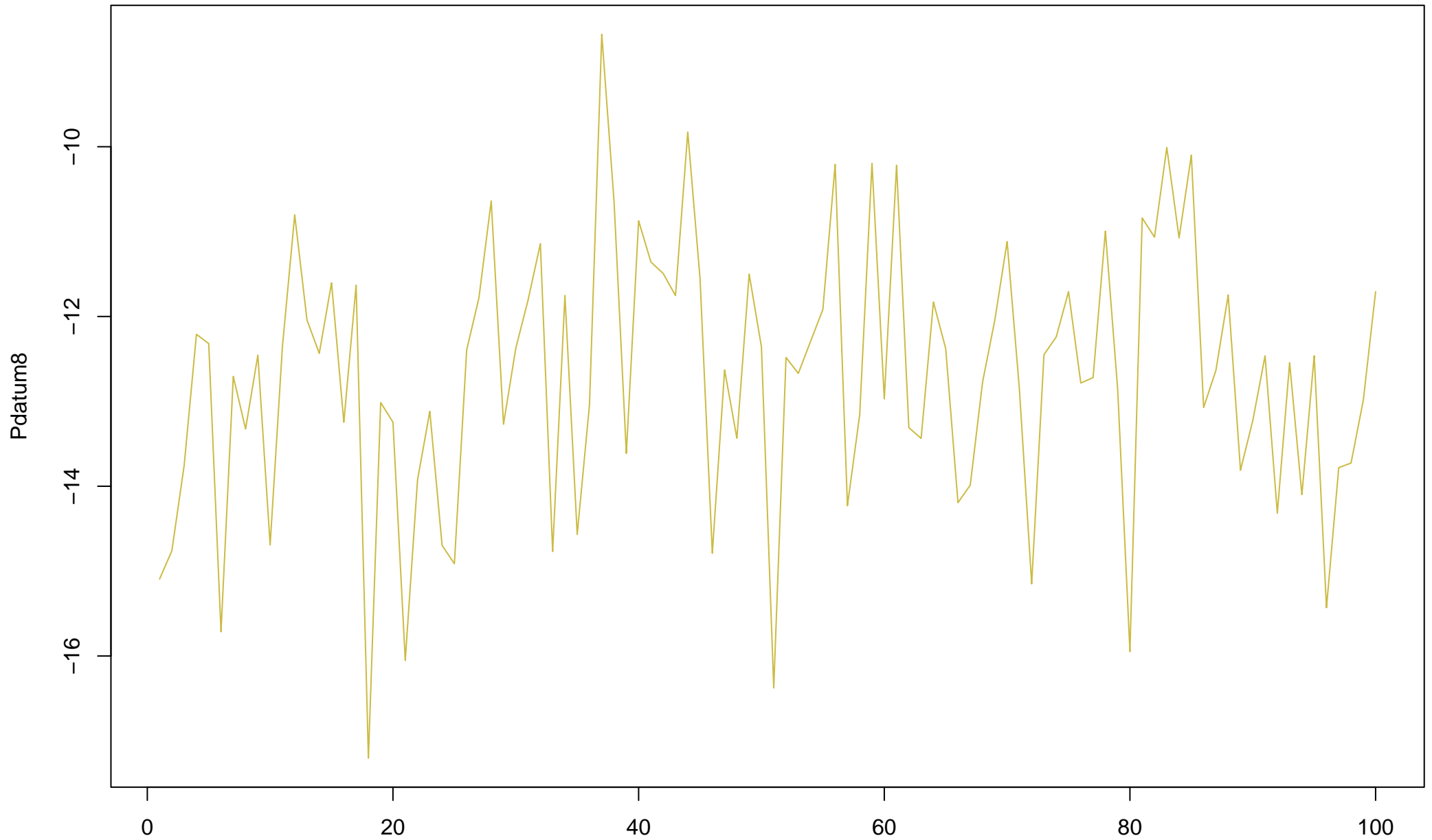
Pdatum6
ESS = 66.1 | BMK = 0.203 | MCSE(6.27) = 13.9 | stat: TRUE | burn: 70



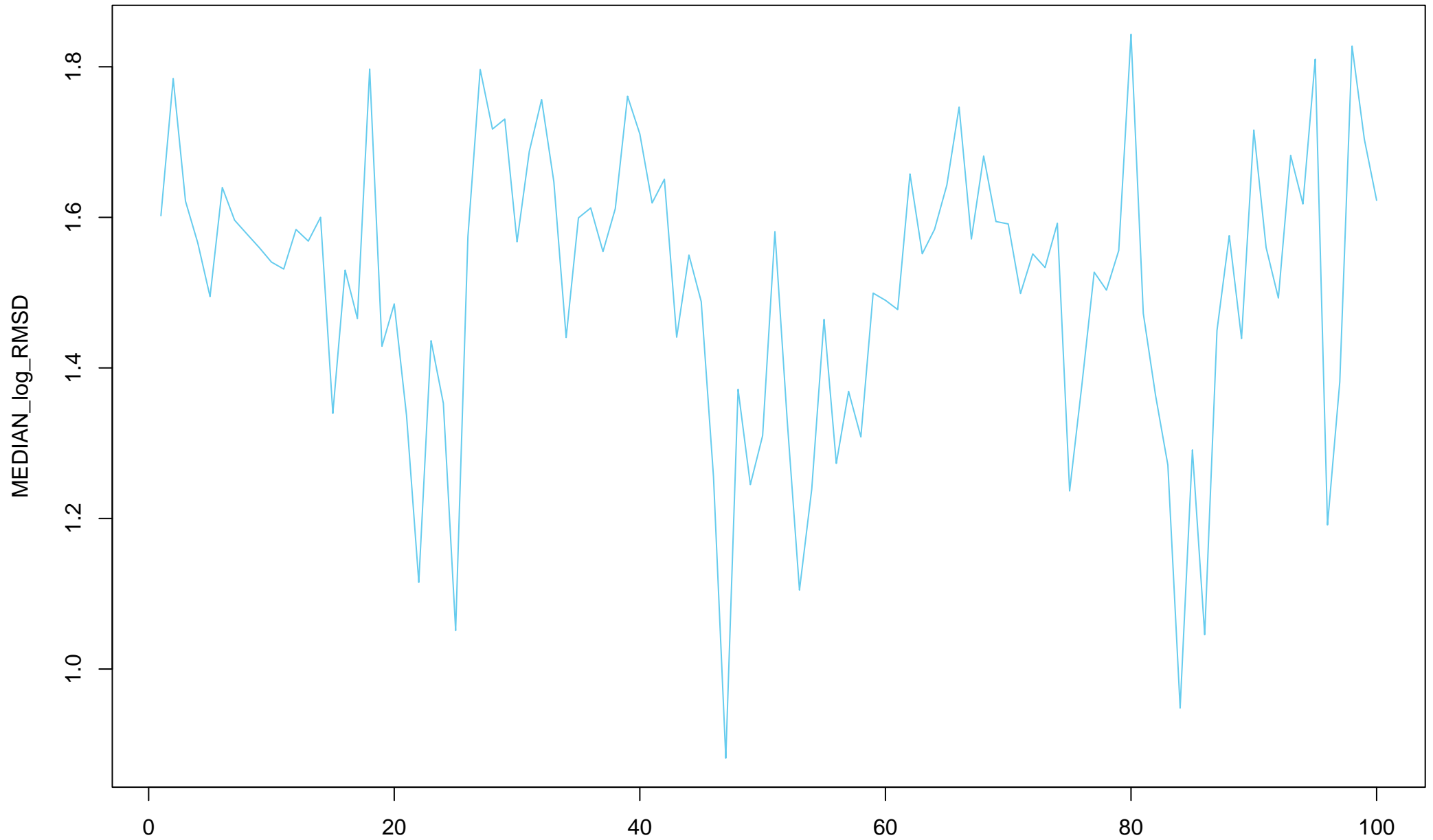
Pdatum7
ESS = 55.1 | BMK = 0.256 | MCSE(6.27) = 14.6 | stat: TRUE | burn: 40



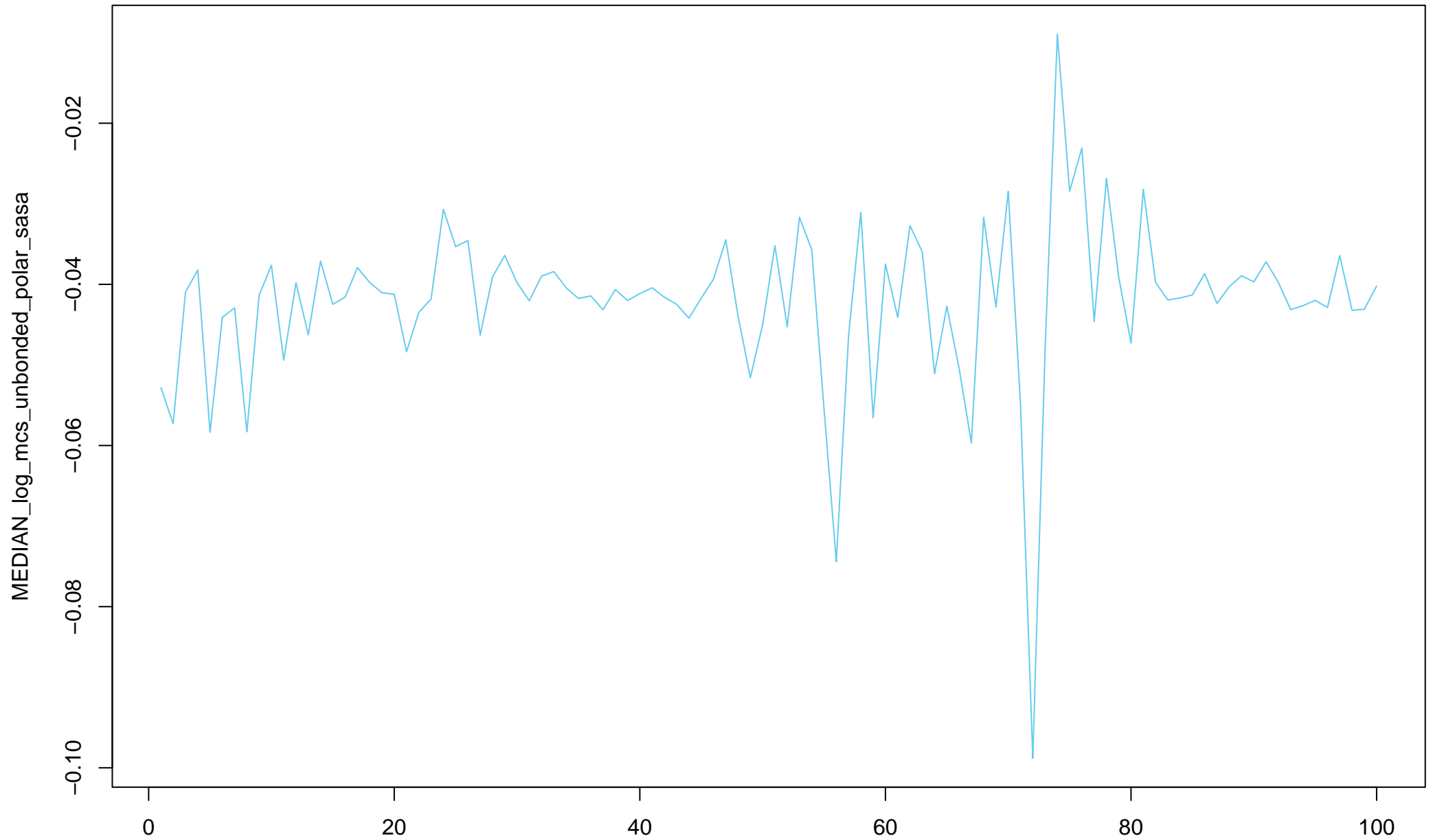
Pdatum8
ESS = 100 | BMK = 0.306 | MCSE(6.27) = 11.2 | stat: FALSE | burn: 100



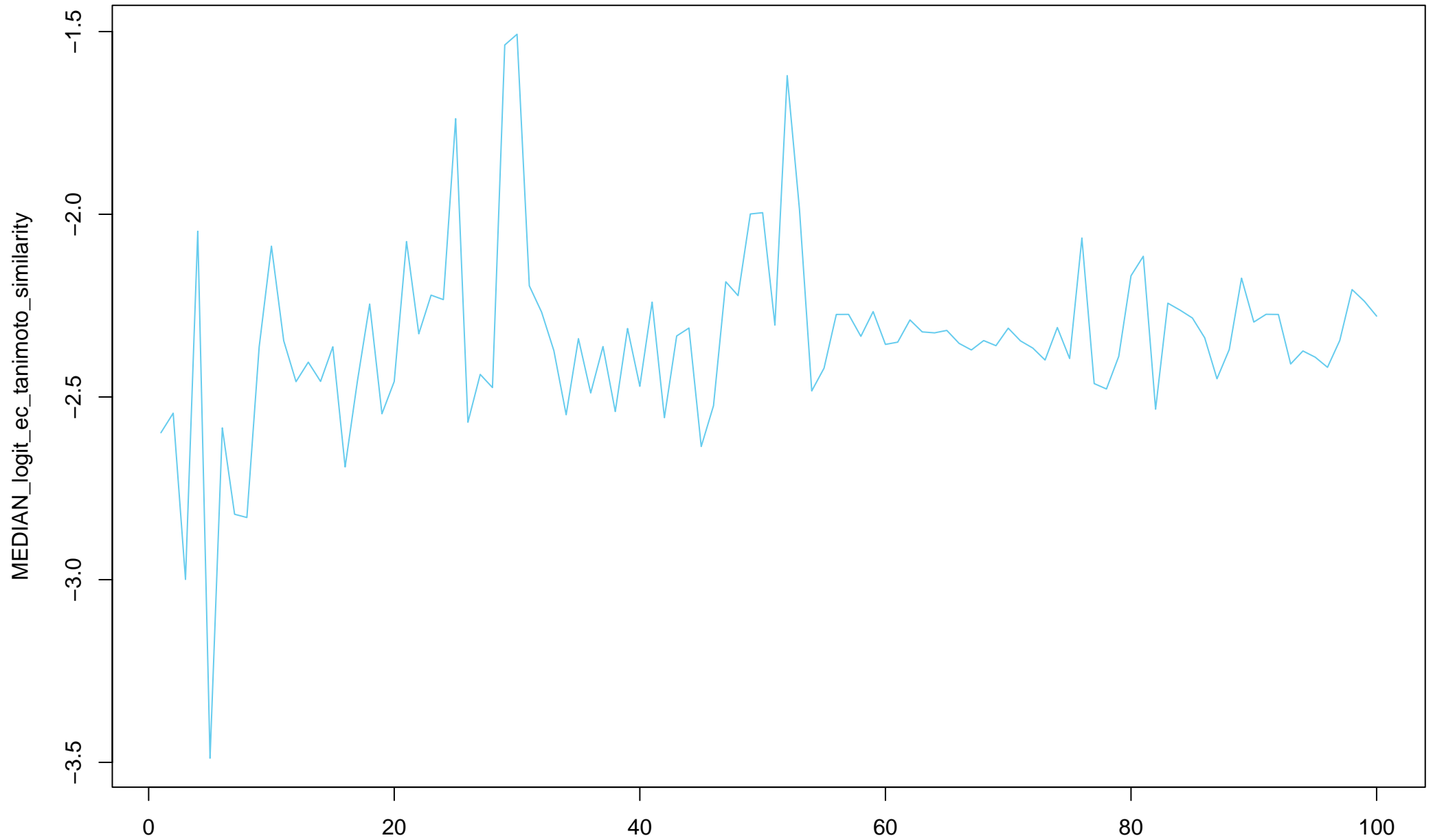
MEDIAN_log_RMSD
ESS = 36.8 | BMK = 0.102 | MCSE(6.27) = 23.3 | stat: FALSE | burn: 80



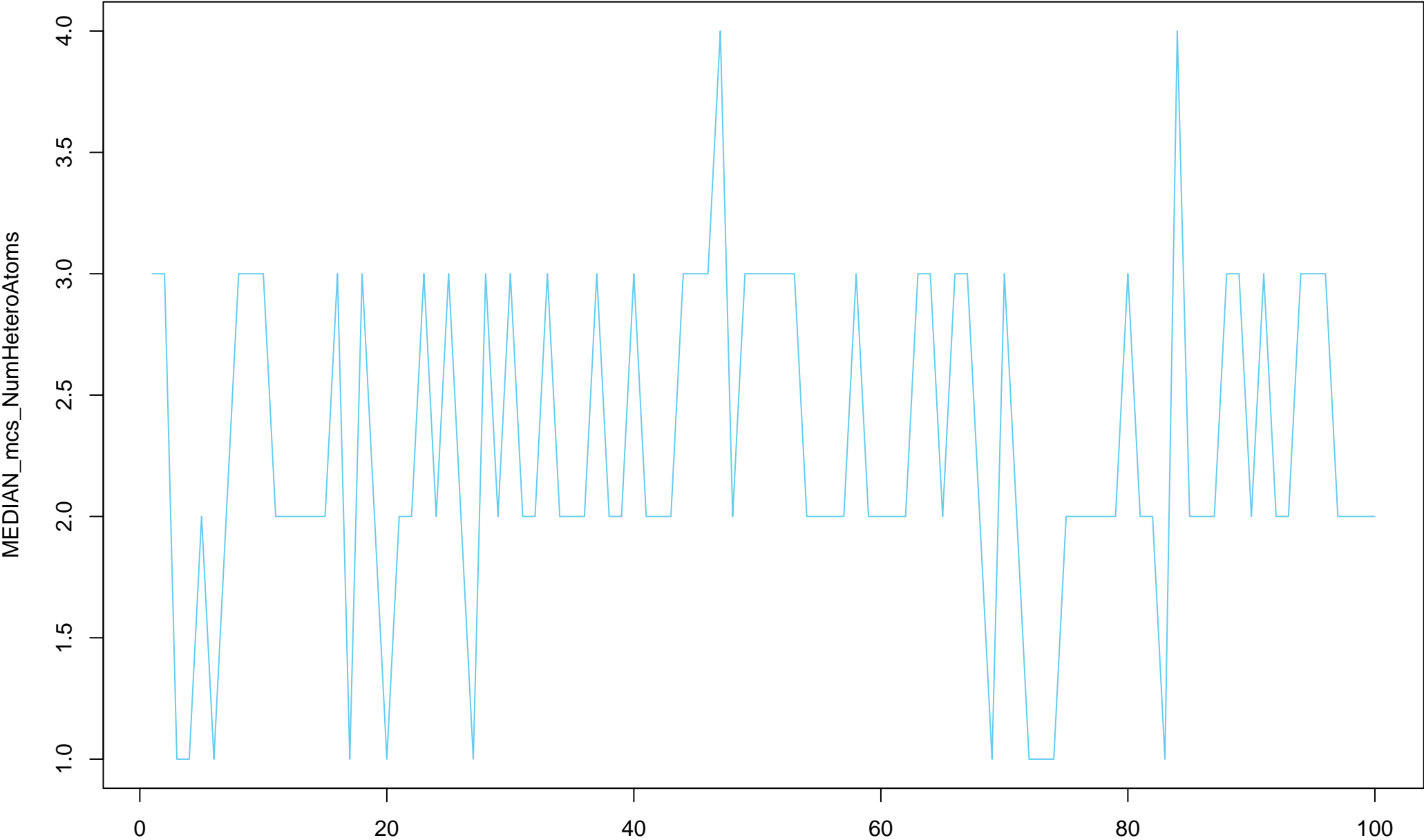
MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 100 | BMK = 0.301 | MCSE(6.27) = 11.6 | stat: TRUE | burn: 80



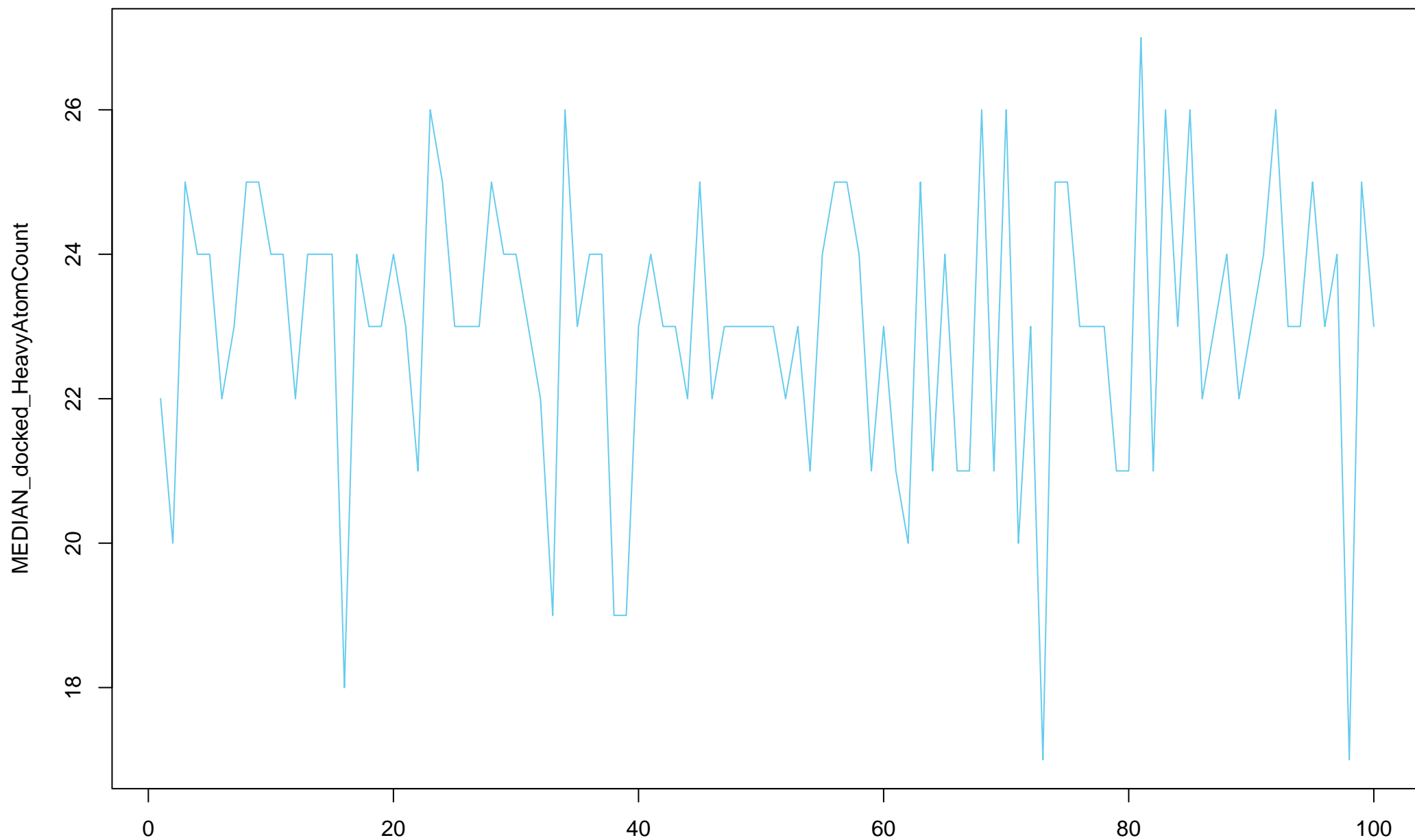
MEDIAN_logit_ec_tanimoto_similarity
ESS = 41.7 | BMK = 0.417 | MCSE(6.27) = 20.8 | stat: FALSE | burn: 70



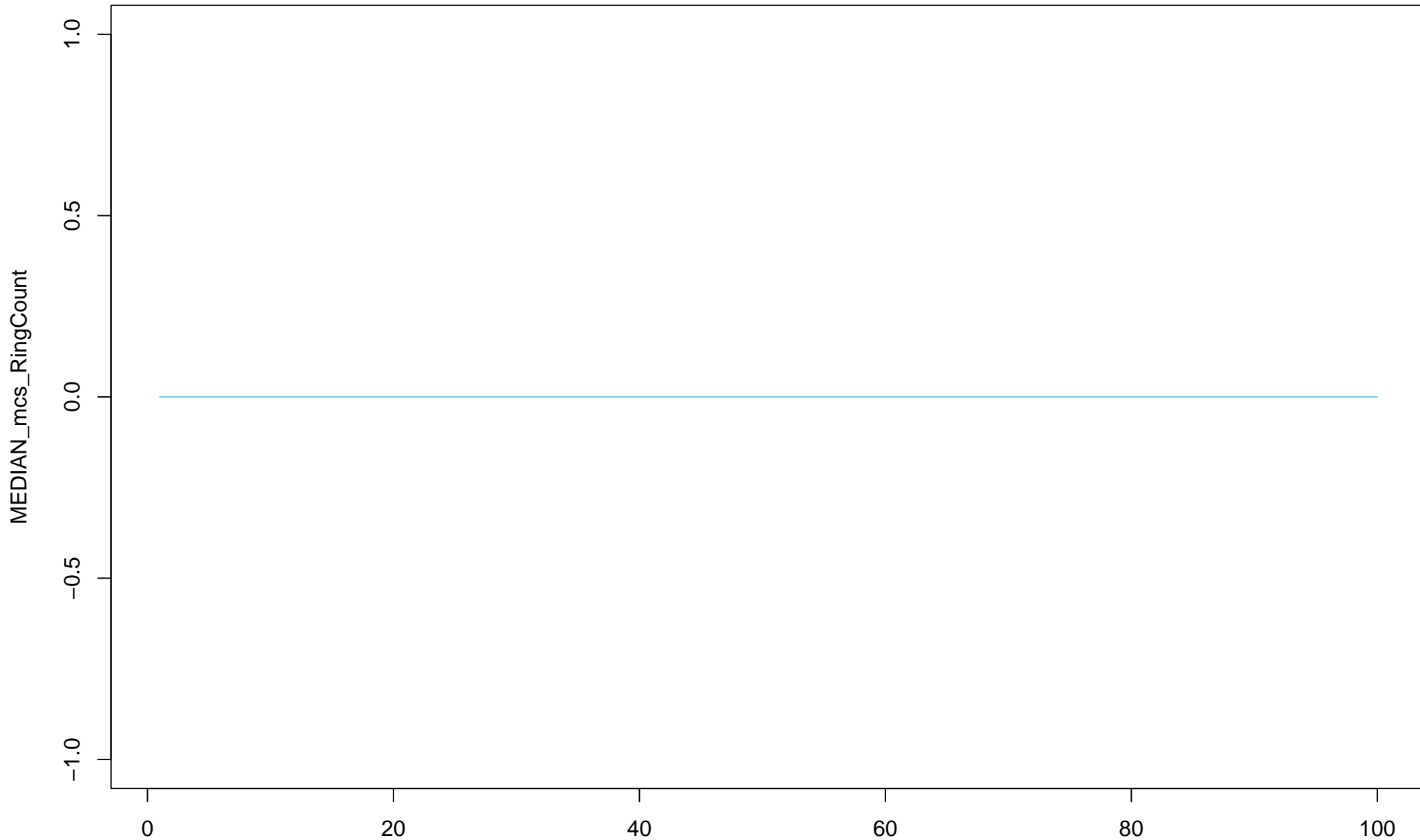
MEDIAN_mcs_NumHeteroAtoms
ESS = 100 | BMK = 0.0565 | MCSE(6.27) = 14.2 | stat: TRUE | burn: 0



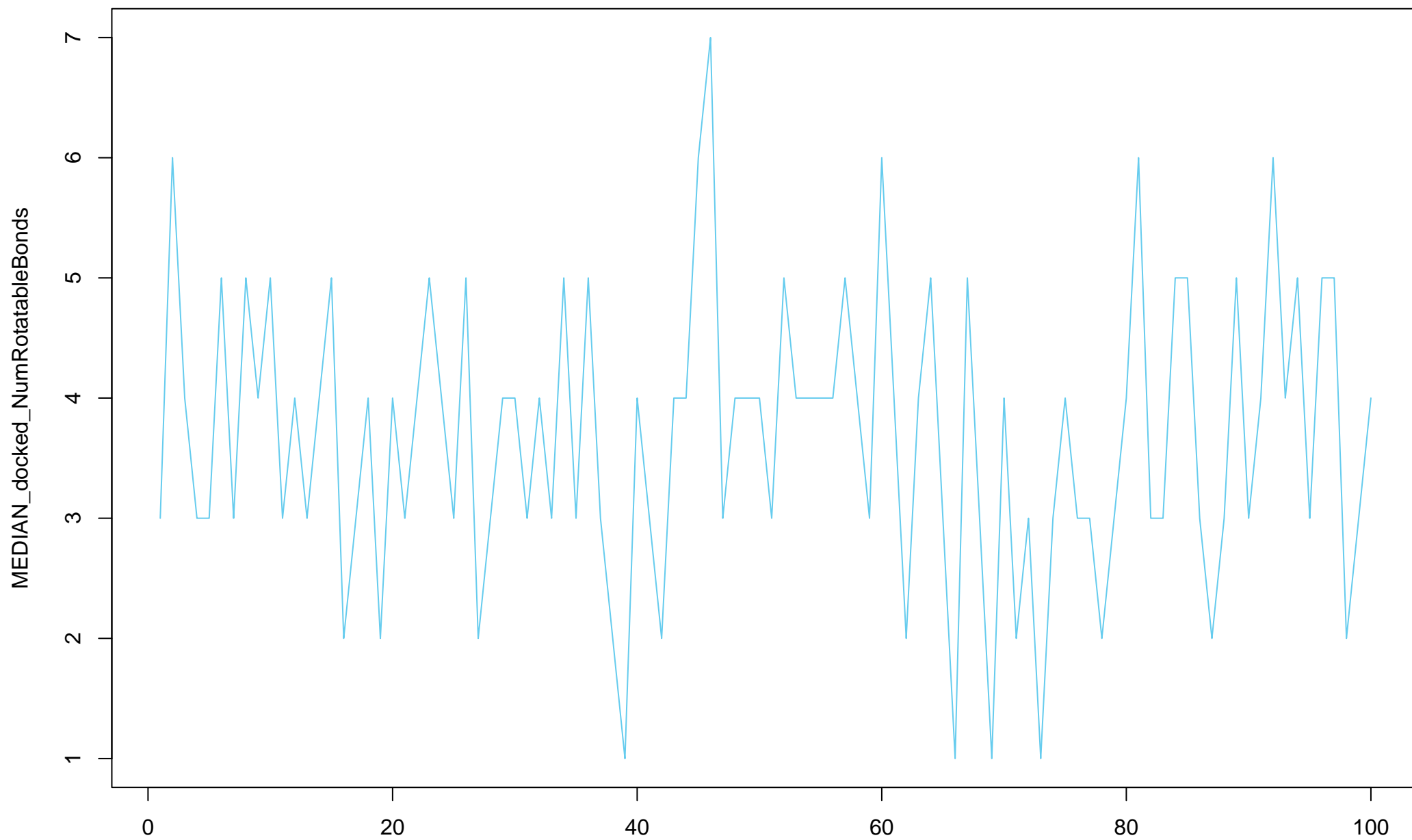
MEDIAN_docked_HeavyAtomCount
ESS = 100 | BMK = 0.265 | MCSE(6.27) = 7.81 | stat: TRUE | burn: 0



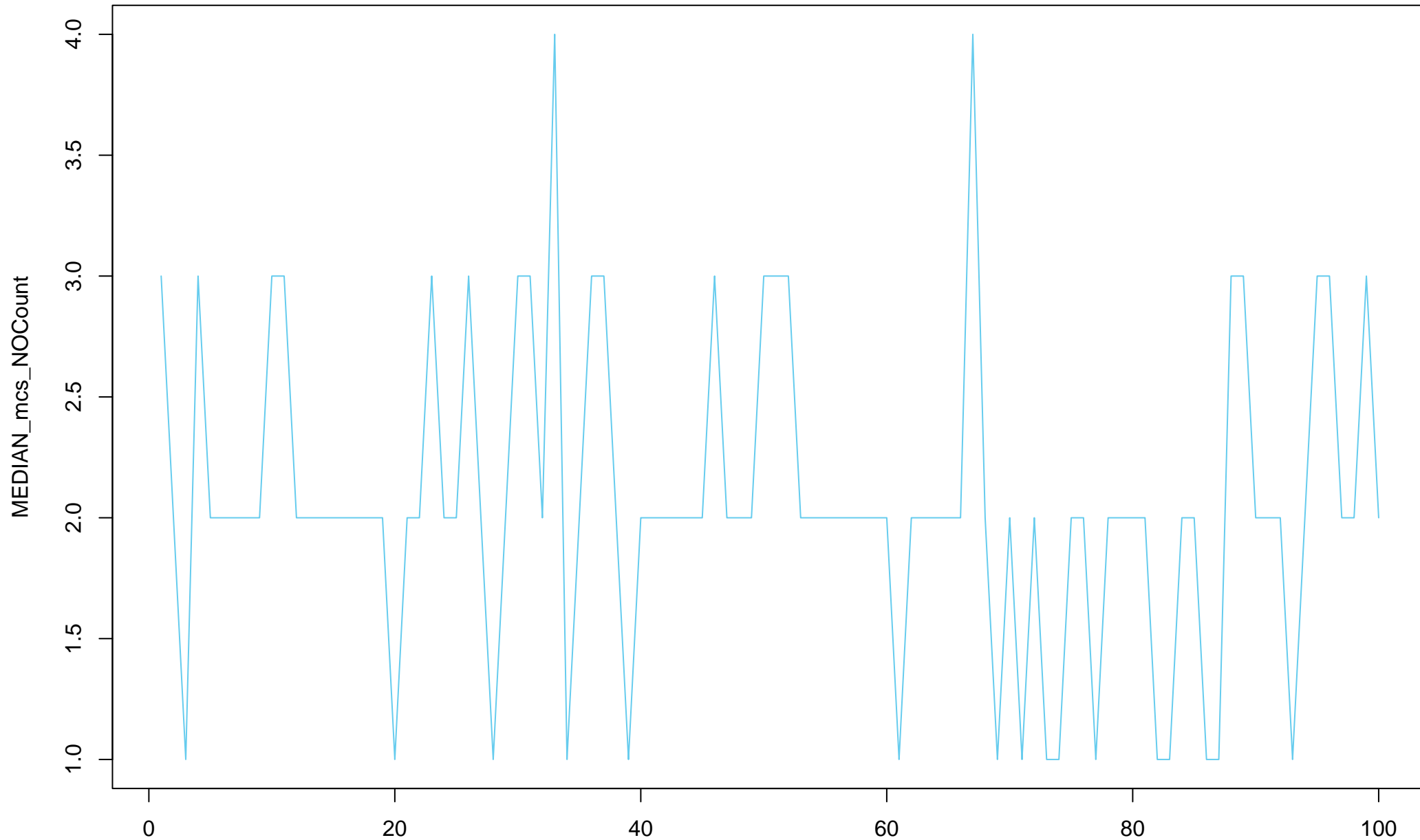
MEDIAN_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



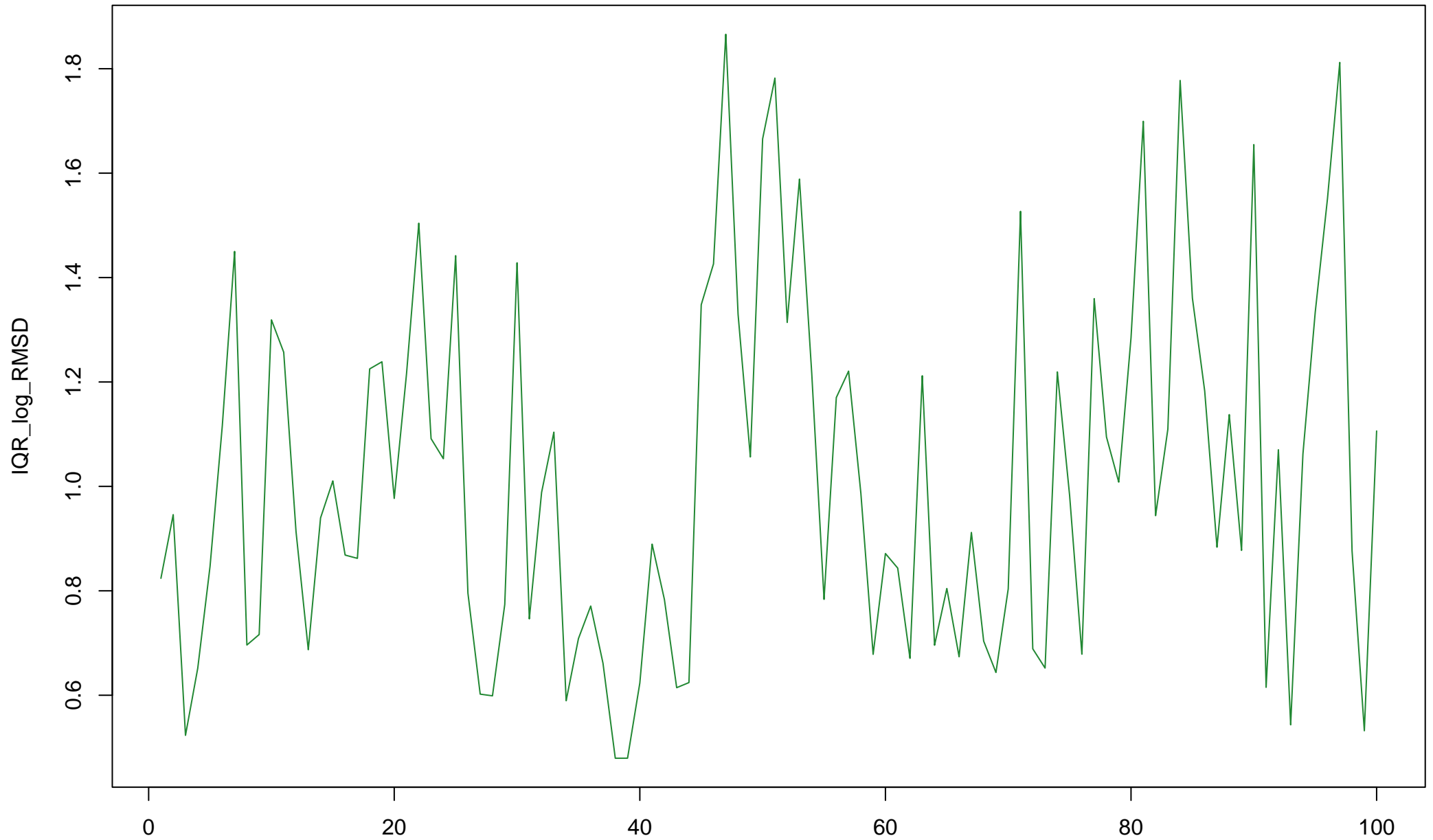
MEDIAN_docked_NumRotatableBonds
ESS = 100 | BMK = 0.119 | MCSE(6.27) = 10.1 | stat: TRUE | burn: 0



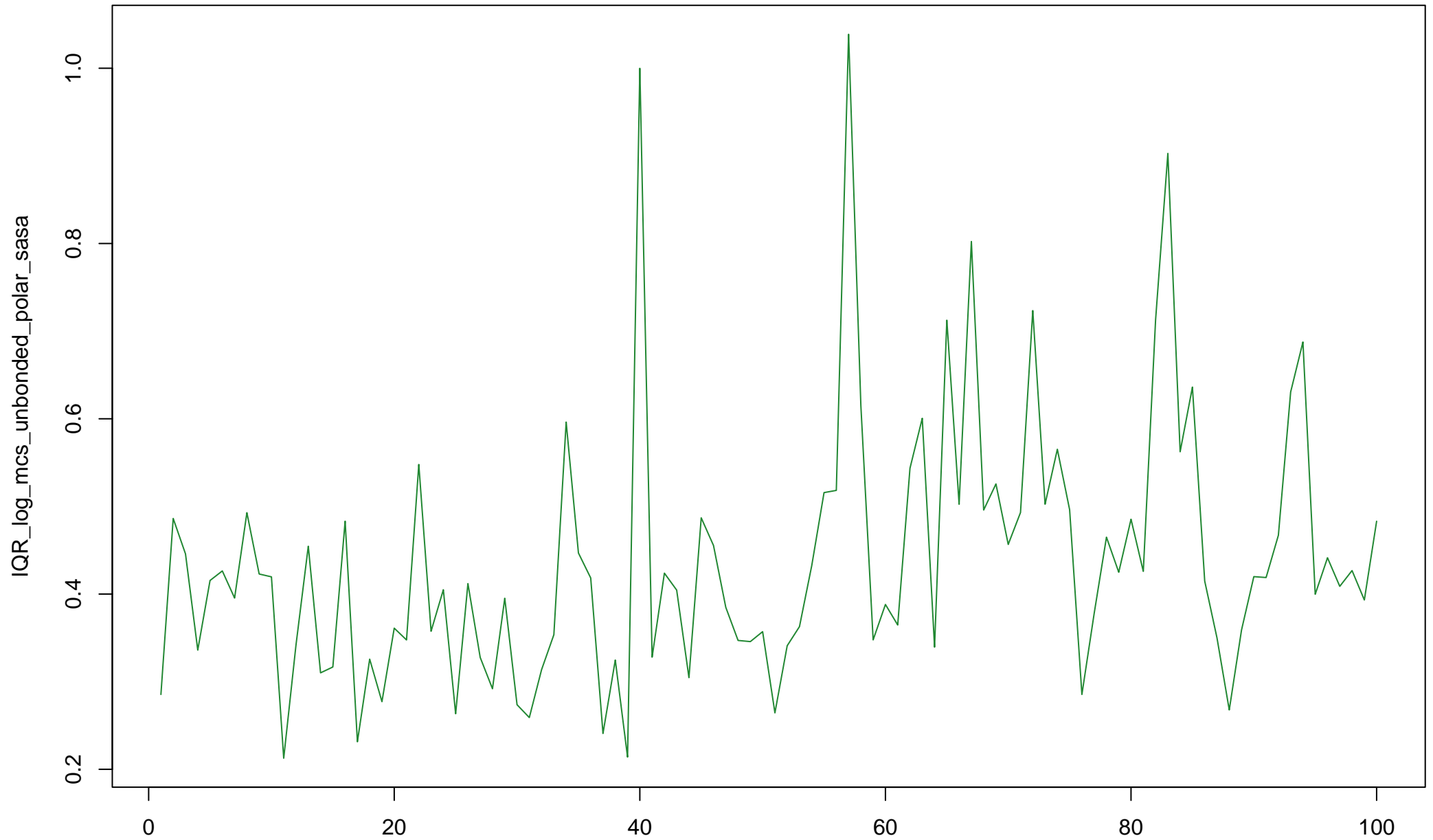
MEDIAN_mcs_NOCount
ESS = 100 | BMK = 0.13 | MCSE(6.27) = 11.2 | stat: TRUE | burn: 0



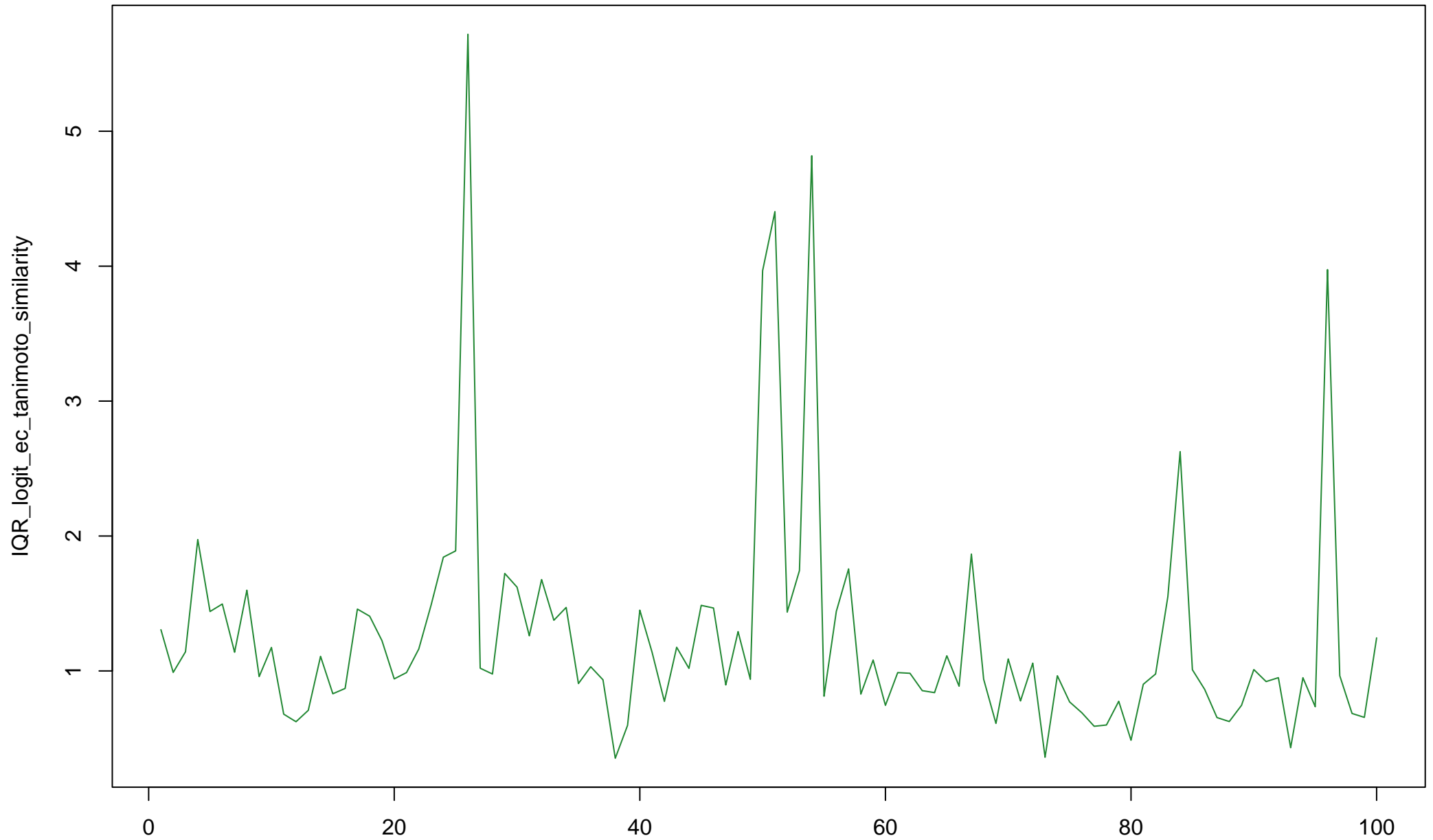
IQR_log_RMSD
ESS = 47.9 | BMK = 0.0969 | MCSE(6.27) = 18.3 | stat: TRUE | burn: 60



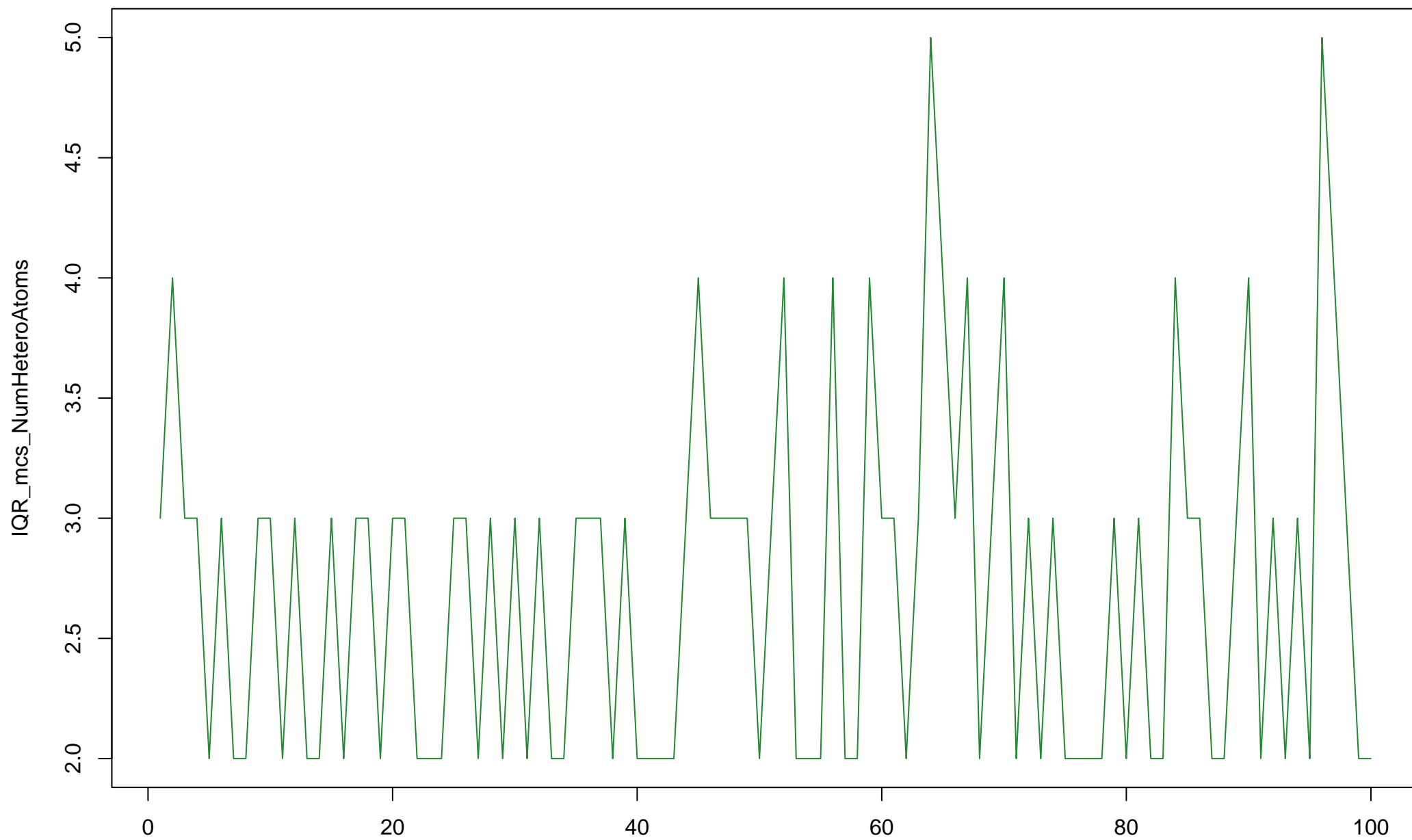
IQR_log_mcs_unbonded_polar_sasa
ESS = 41.3 | BMK = 0.35 | MCSE(6.27) = 17.2 | stat: FALSE | burn: 0



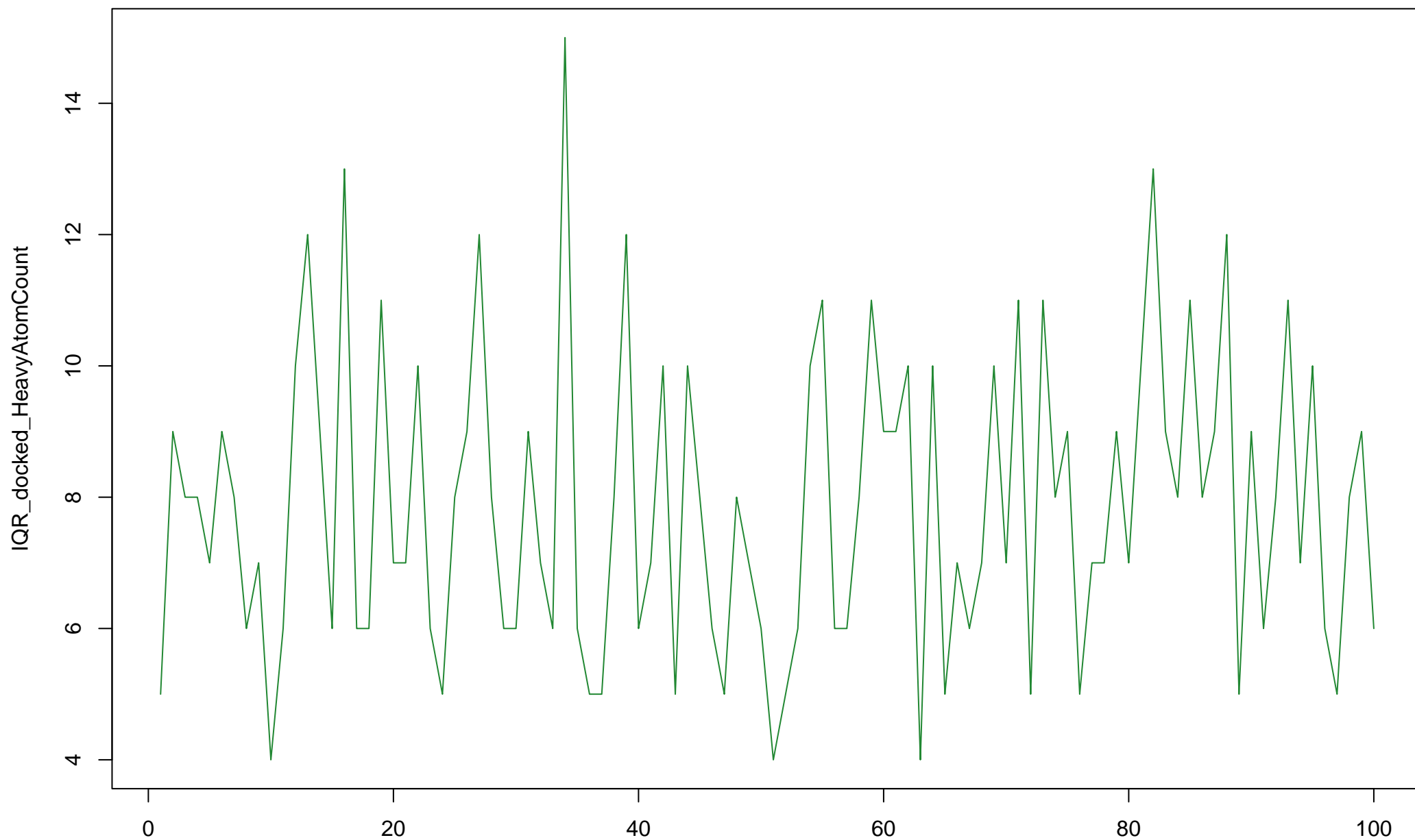
IQR_logit_ec_tanimoto_similarity
ESS = 37.8 | BMK = 0.332 | MCSE(6.27) = 16.3 | stat: TRUE | burn: 60



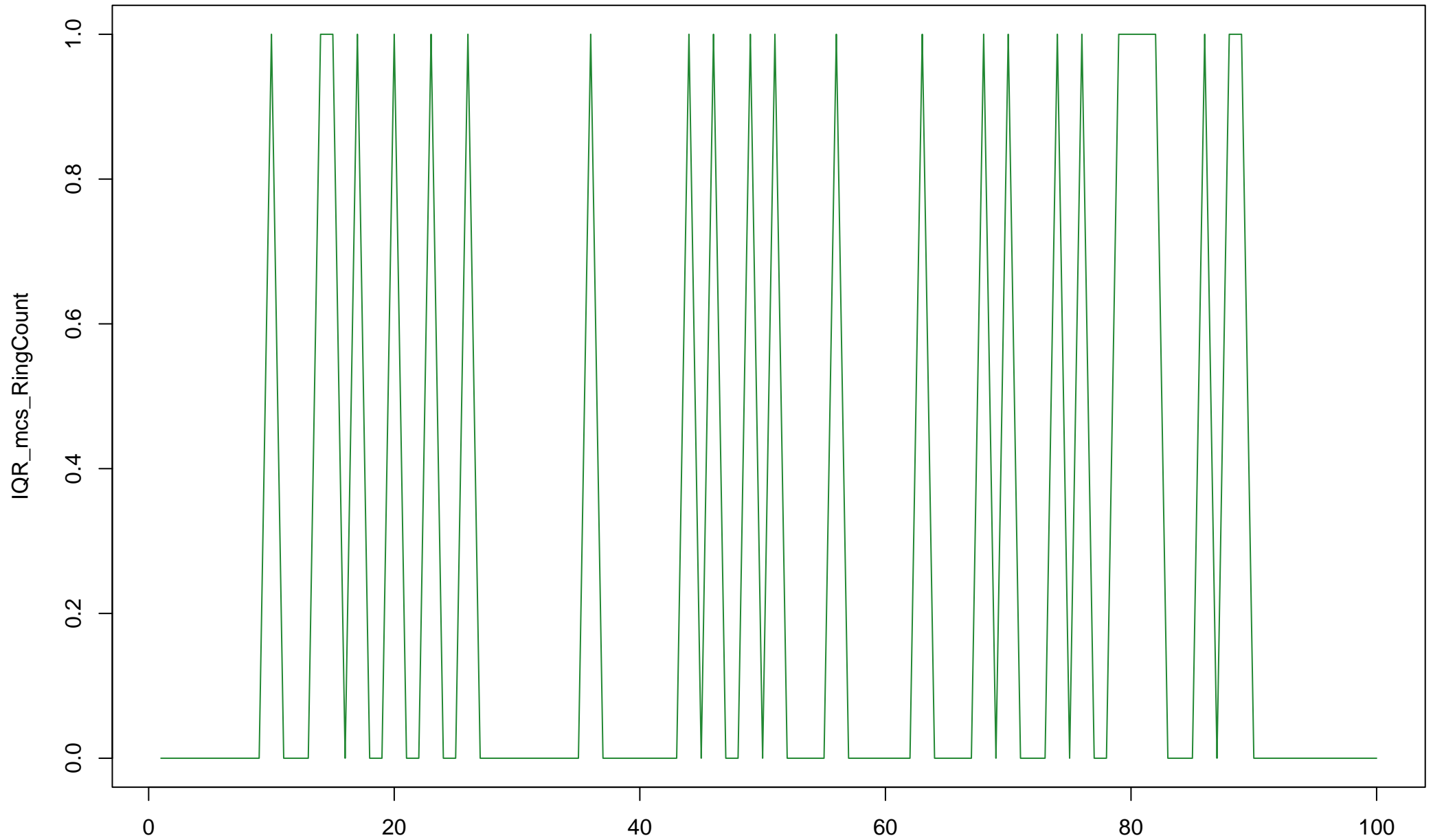
IQR_mcs_NumHeteroAtoms
ESS = 100 | BMK = 0.227 | MCSE(6.27) = 10.6 | stat: TRUE | burn: 0



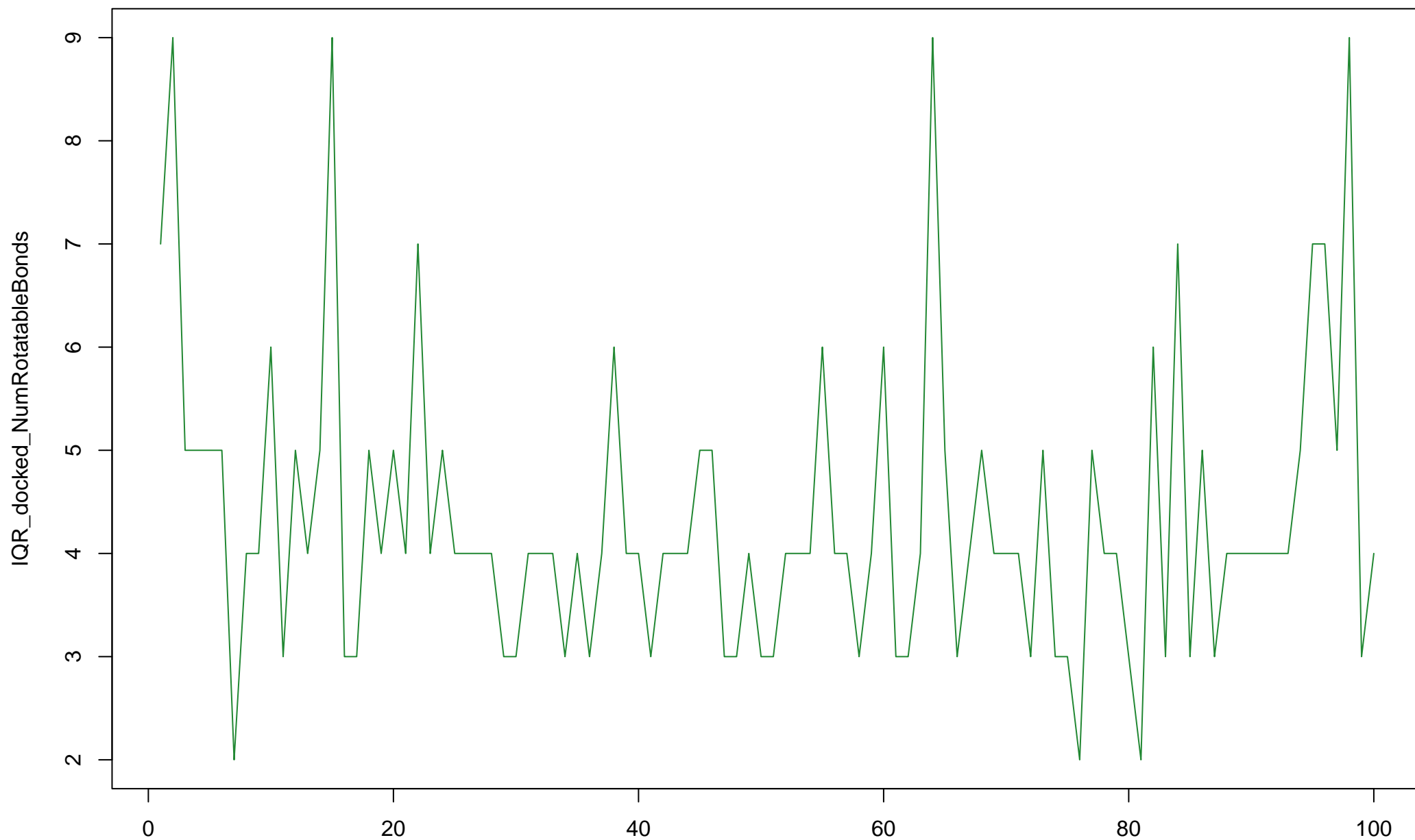
IQR_docked_HeavyAtomCount
ESS = 100 | BMK = 0.12 | MCSE(6.27) = 9.13 | stat: TRUE | burn: 0



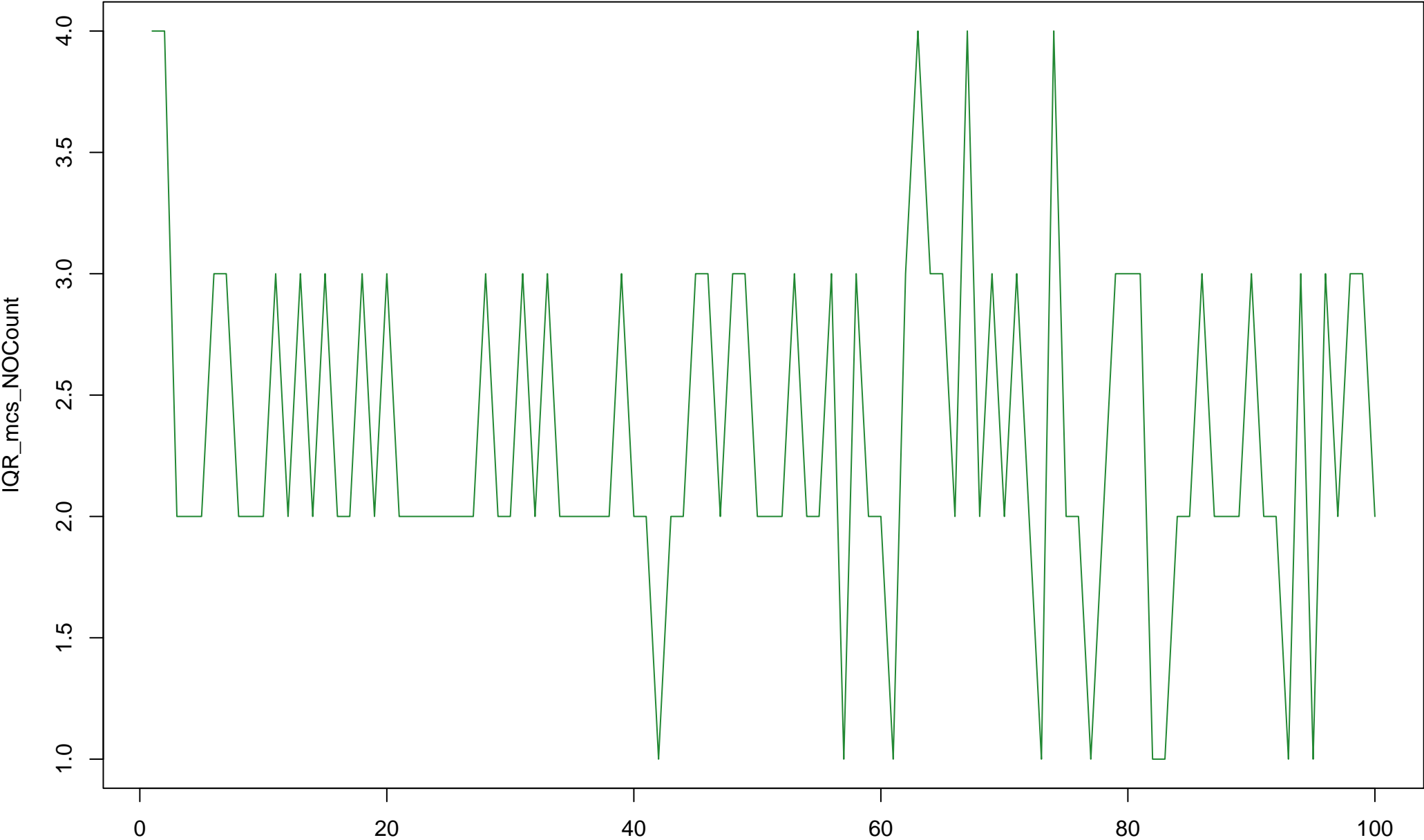
IQR_mcs_RingCount
ESS = 100 | BMK = 0.0452 | MCSE(6.27) = 9.4 | stat: TRUE | burn: 0



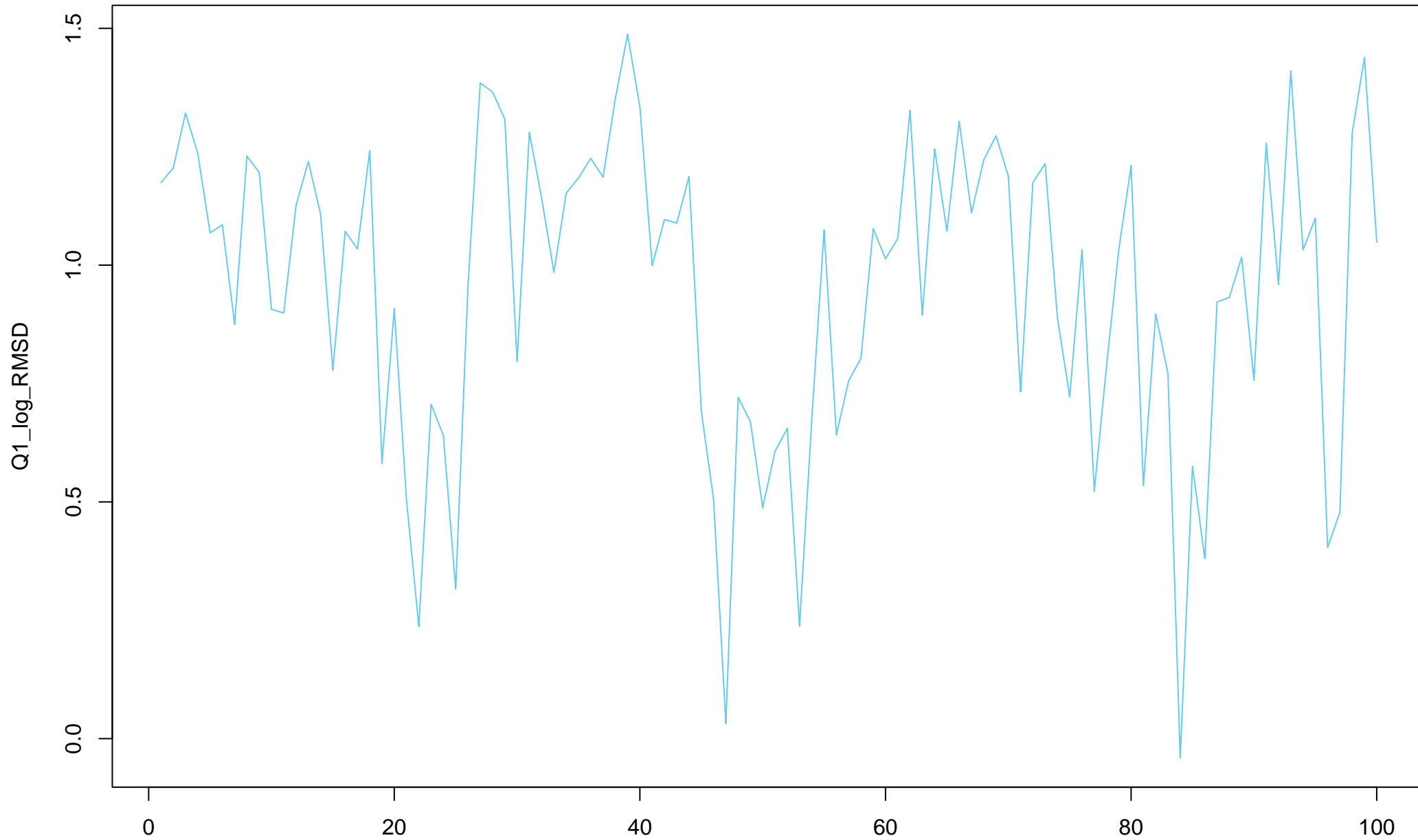
IQR_docked_NumRotatableBonds
ESS = 100 | BMK = 0.147 | MCSE(6.27) = 12.5 | stat: TRUE | burn: 0



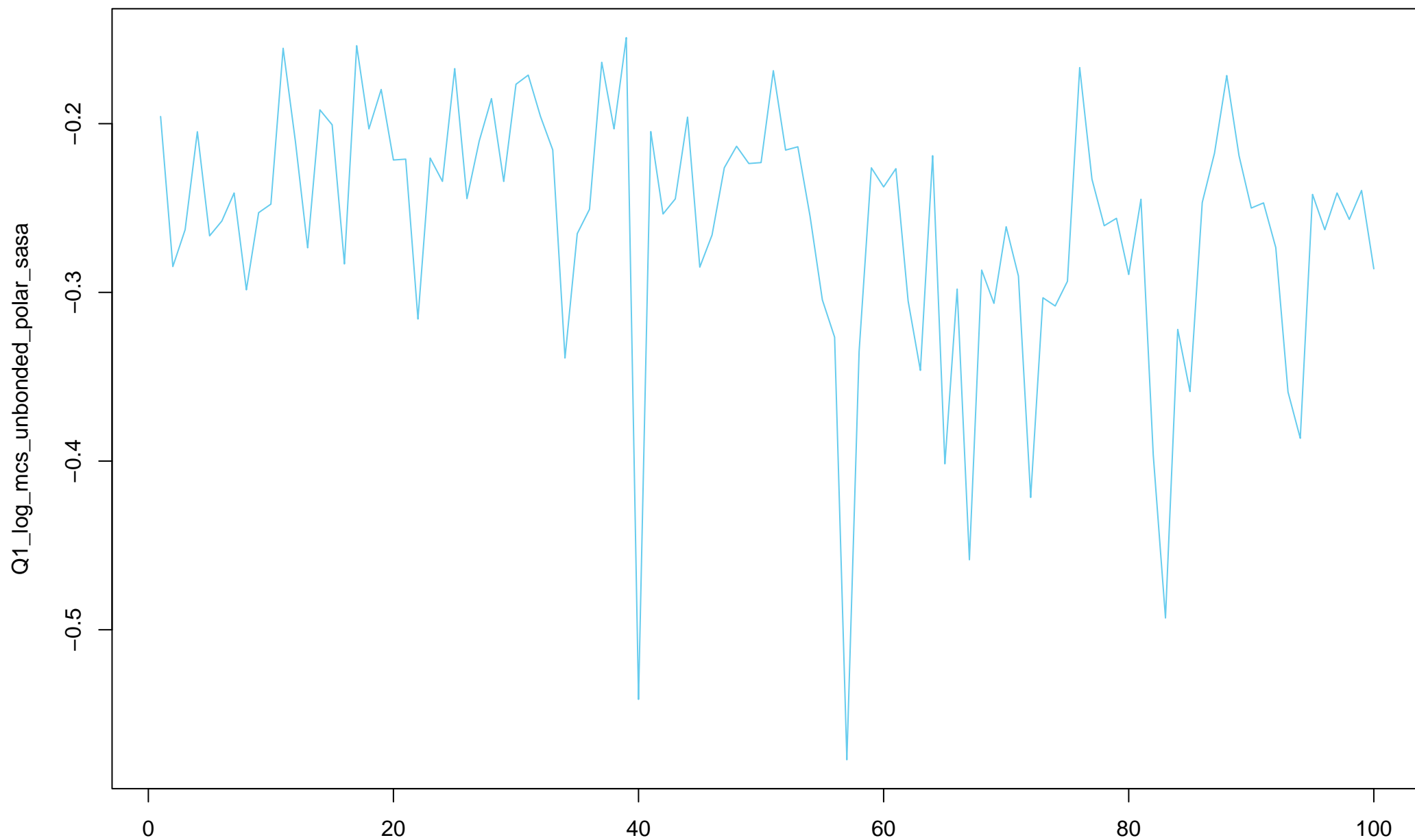
IQR_mcs_NOCount
ESS = 100 | BMK = 0.177 | MCSE(6.27) = 9.26 | stat: FALSE | burn: 0



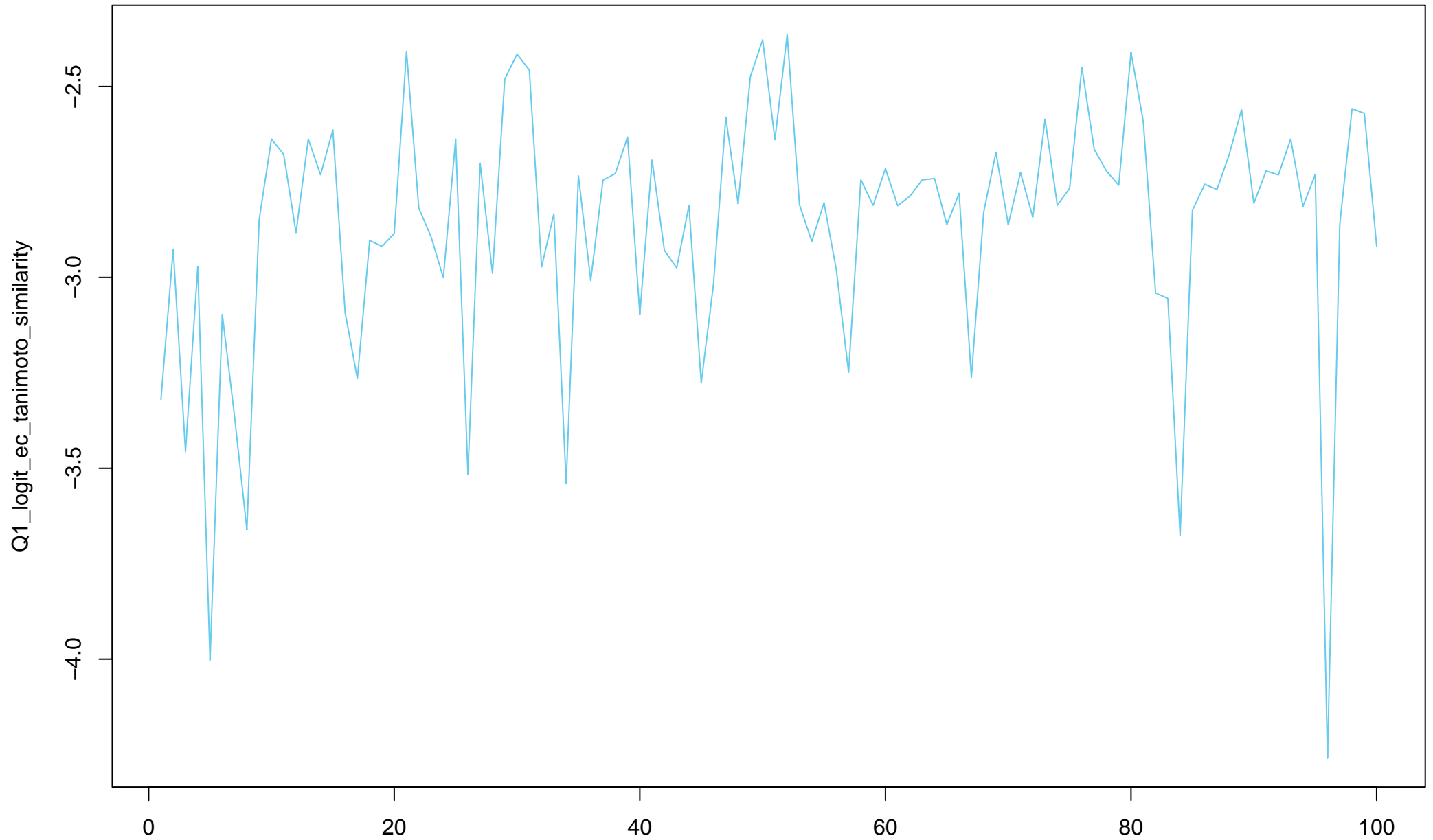
Q1_log_RMSD
ESS = 34.5 | BMK = 0.0918 | MCSE(6.27) = 26.2 | stat: FALSE | burn: 60



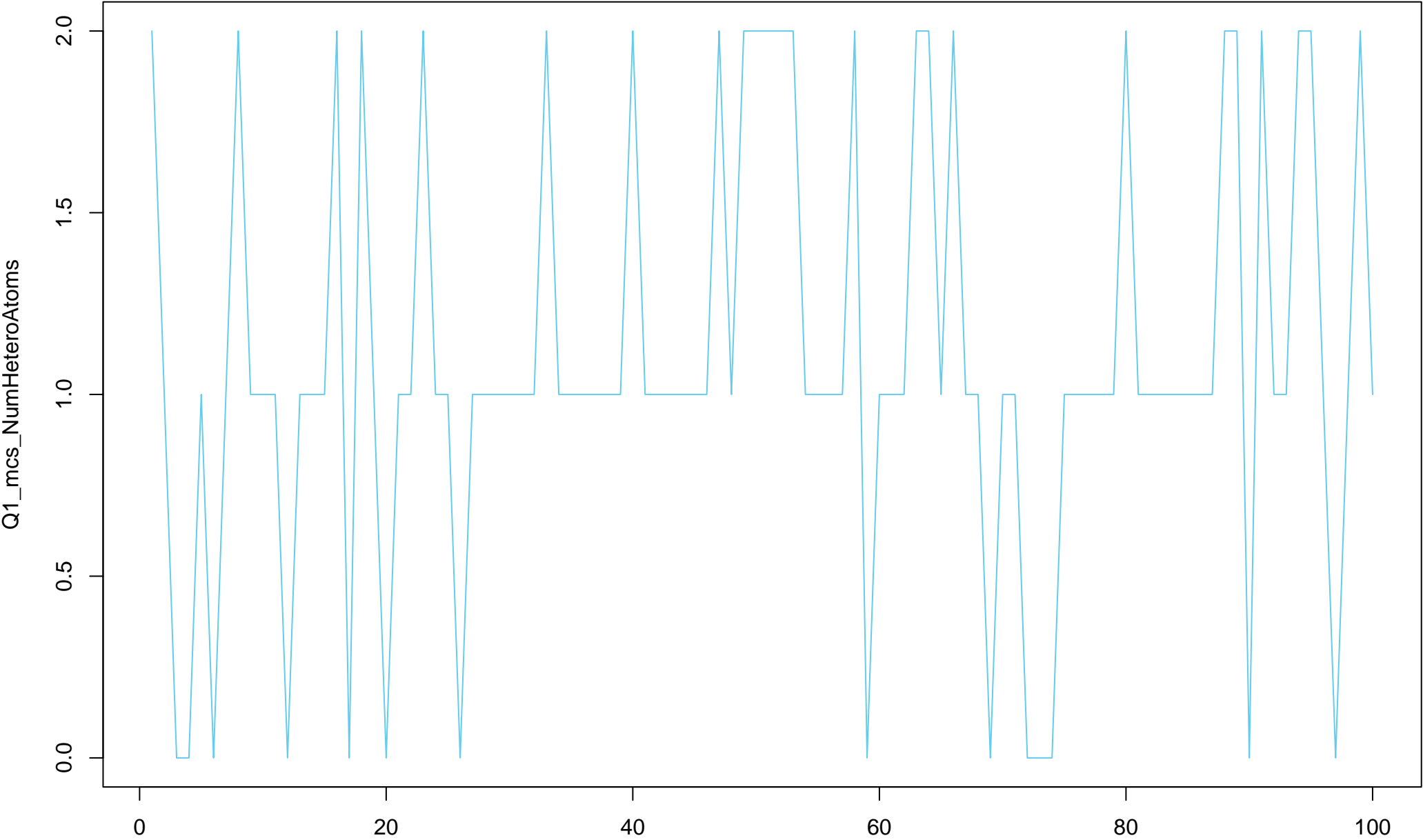
Q1_log_mcs_unbonded_polar_sasa
ESS = 40.2 | BMK = 0.346 | MCSE(6.27) = 17.4 | stat: FALSE | burn: 0



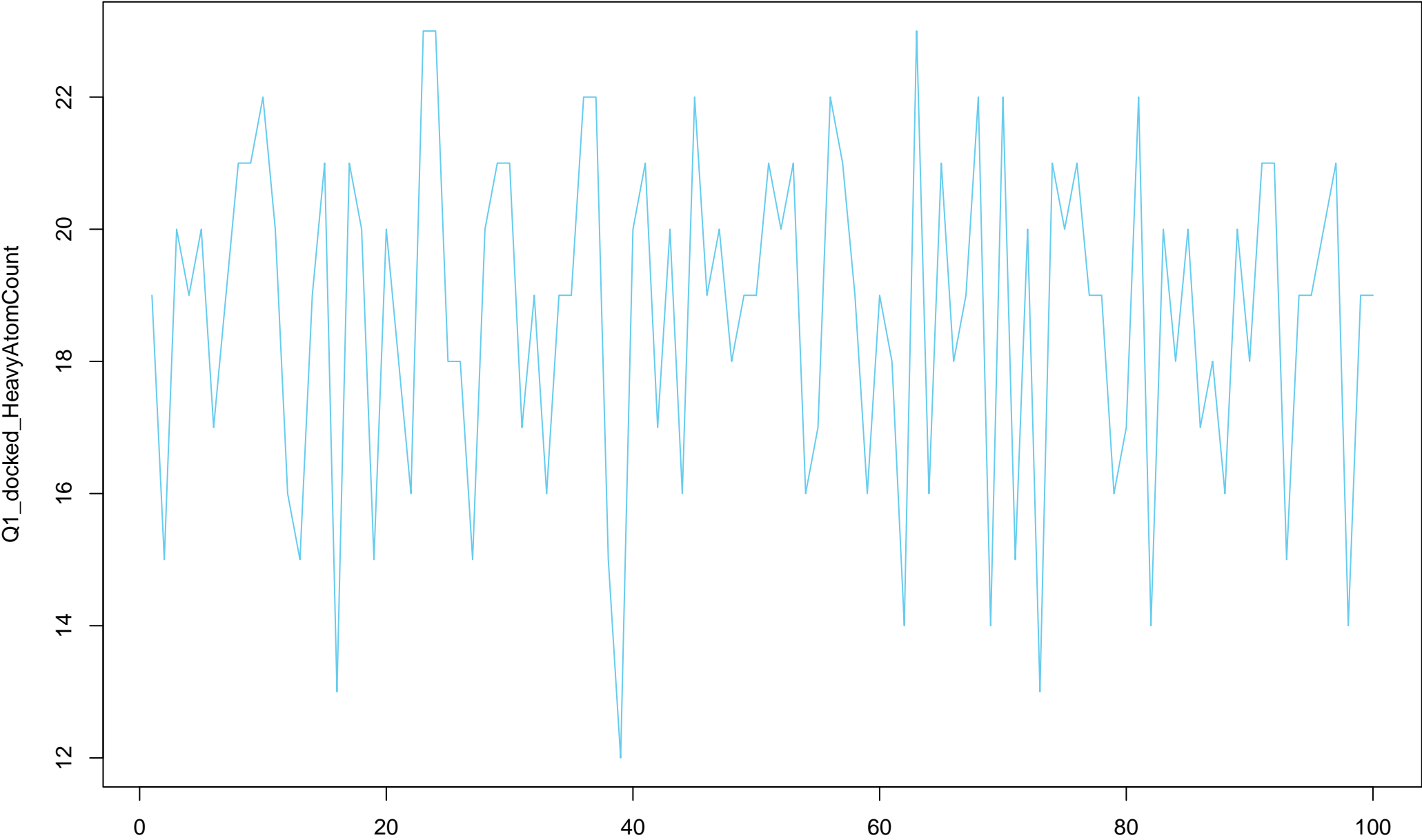
Q1_logit_ec_tanimoto_similarity
ESS = 46 | BMK = 0.316 | MCSE(6.27) = 16 | stat: FALSE | burn: 0



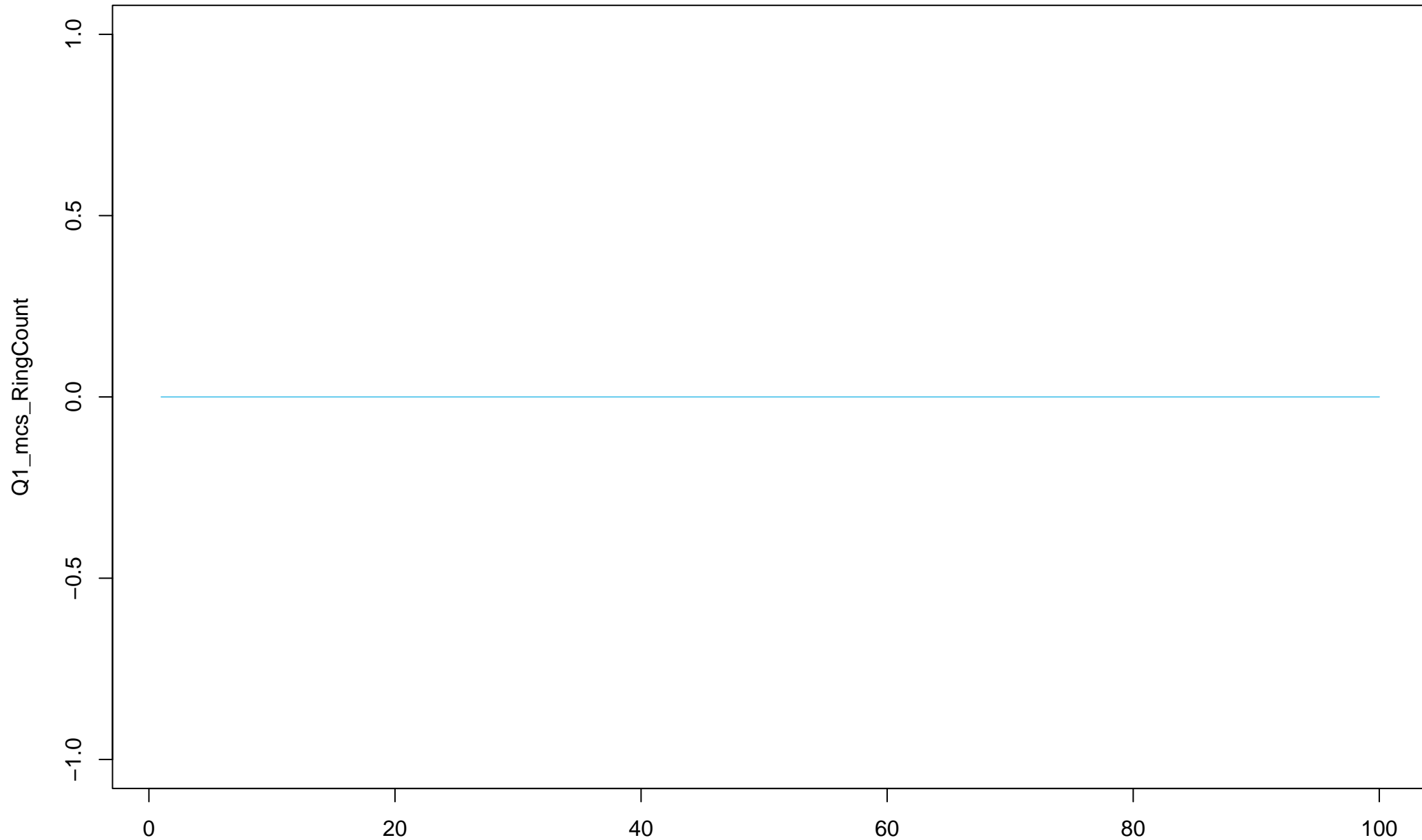
Q1_mcs_NumHeteroAtoms
ESS = 100 | BMK = 0.0625 | MCSE(6.27) = 13.7 | stat: TRUE | burn: 0



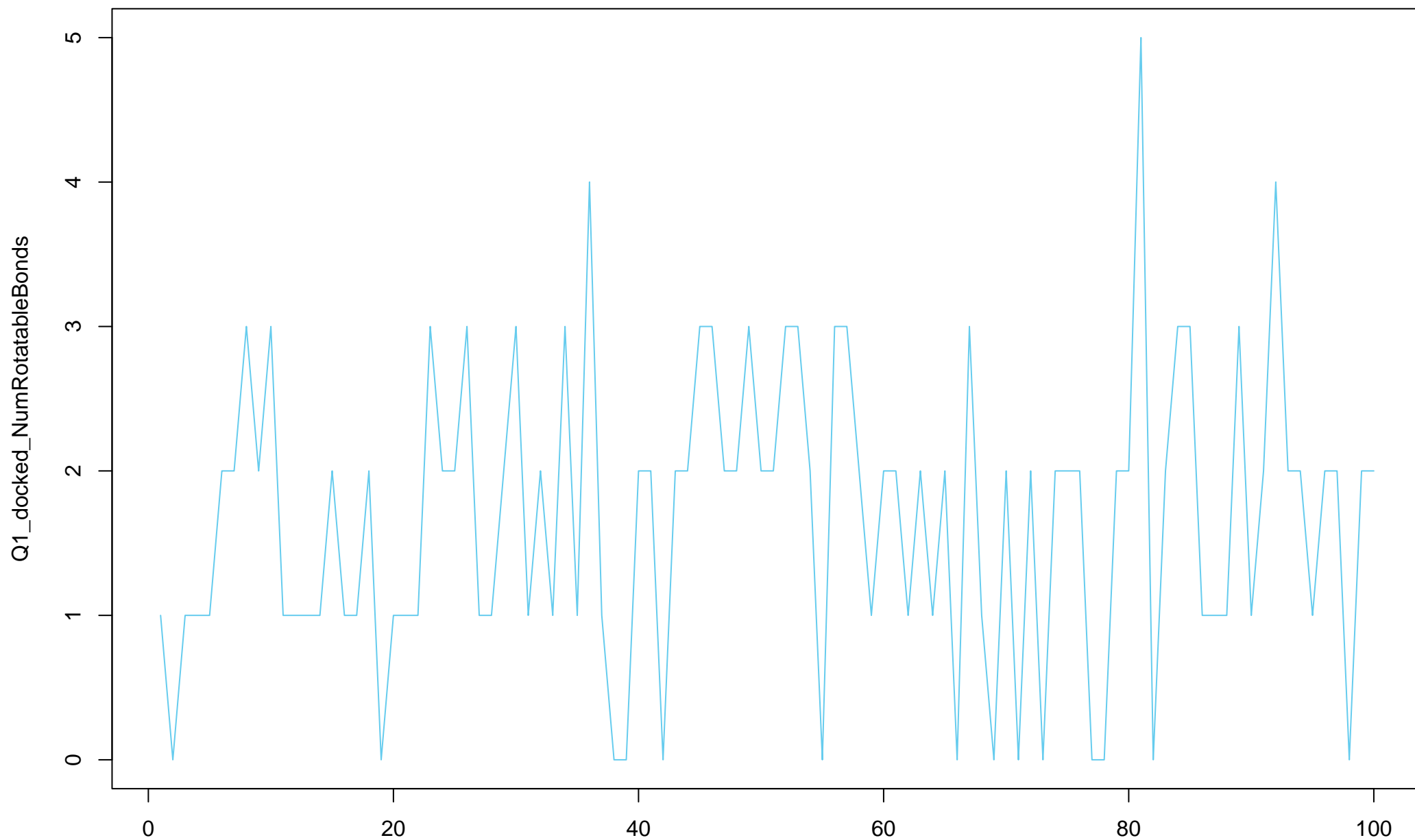
Q1_docked_HeavyAtomCount
ESS = 100 | BMK = 0.0399 | MCSE(6.27) = 7.33 | stat: TRUE | burn: 0



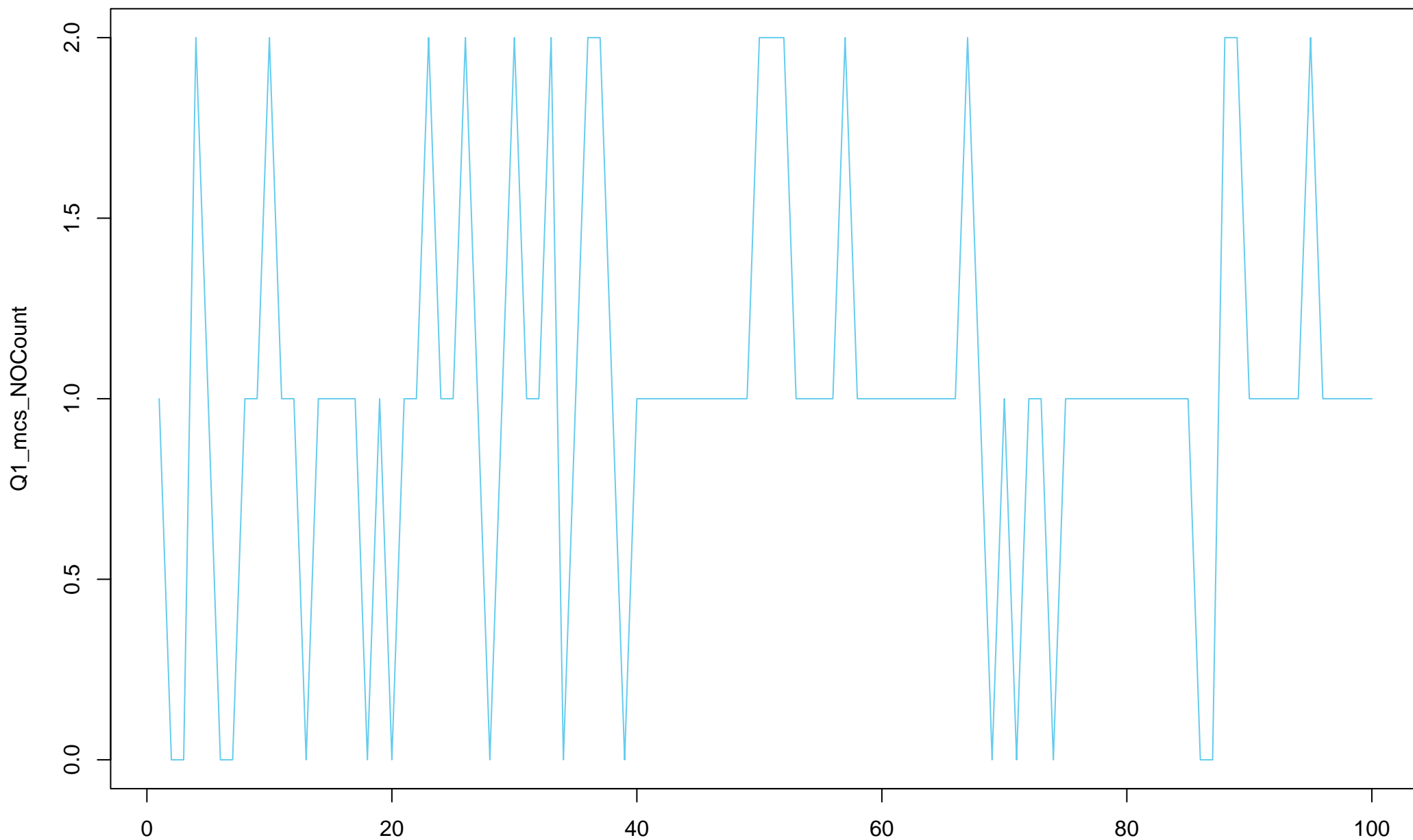
Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



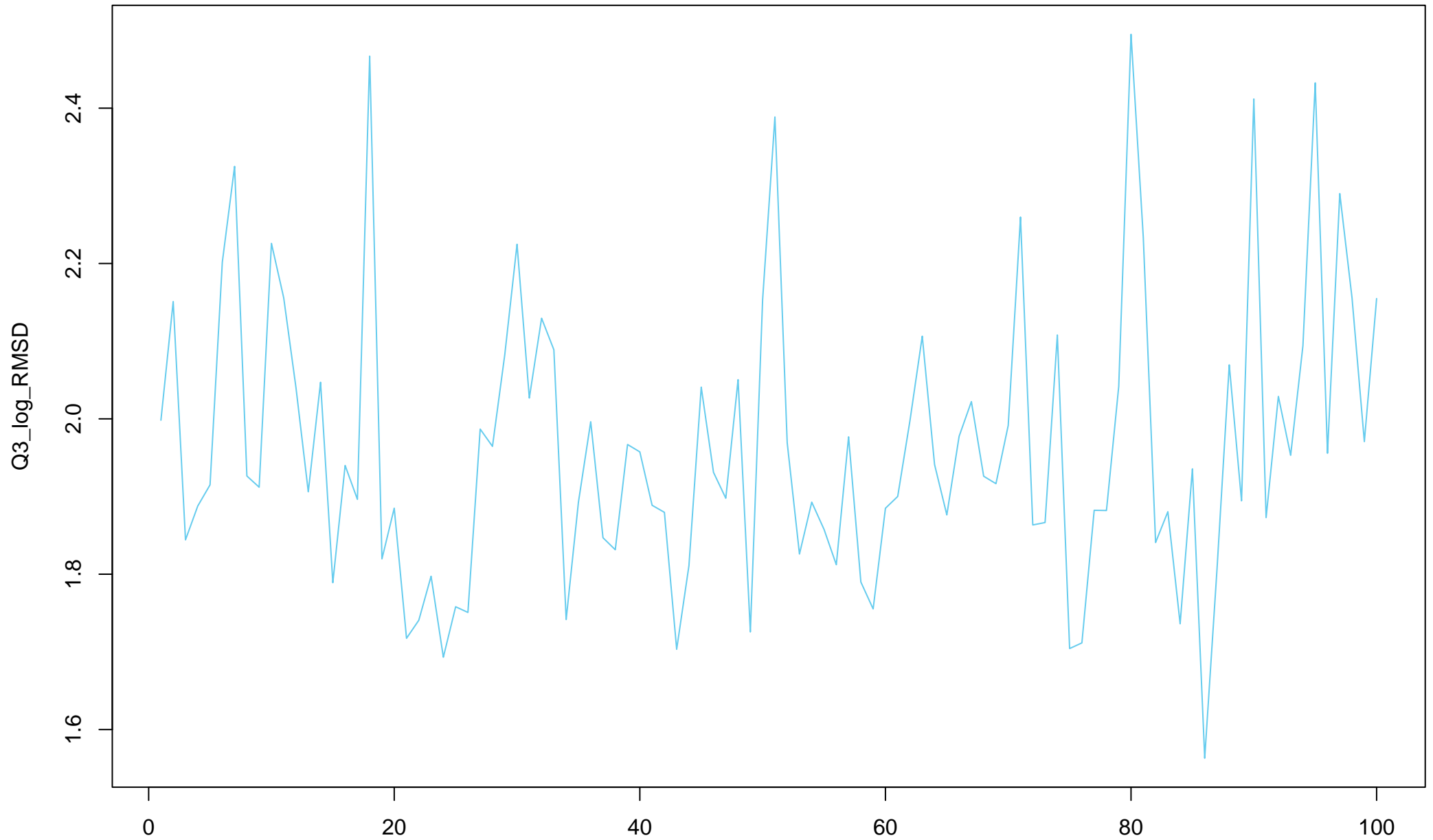
Q1_docked_NumRotatableBonds
ESS = 100 | BMK = 0.152 | MCSE(6.27) = 10.1 | stat: TRUE | burn: 0



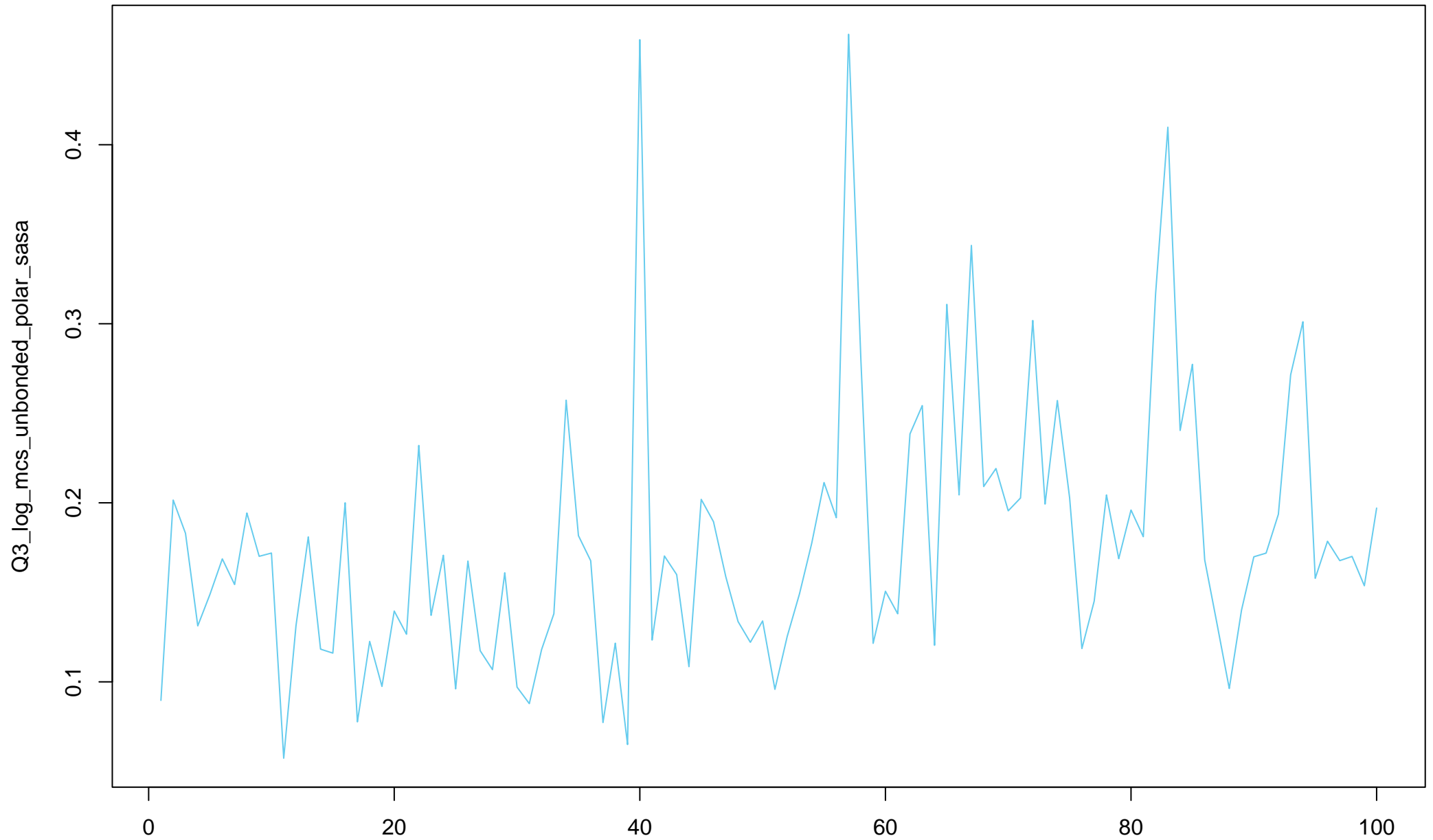
Q1_mcs_NOCount
ESS = 100 | BMK = 0.133 | MCSE(6.27) = 11.2 | stat: TRUE | burn: 0



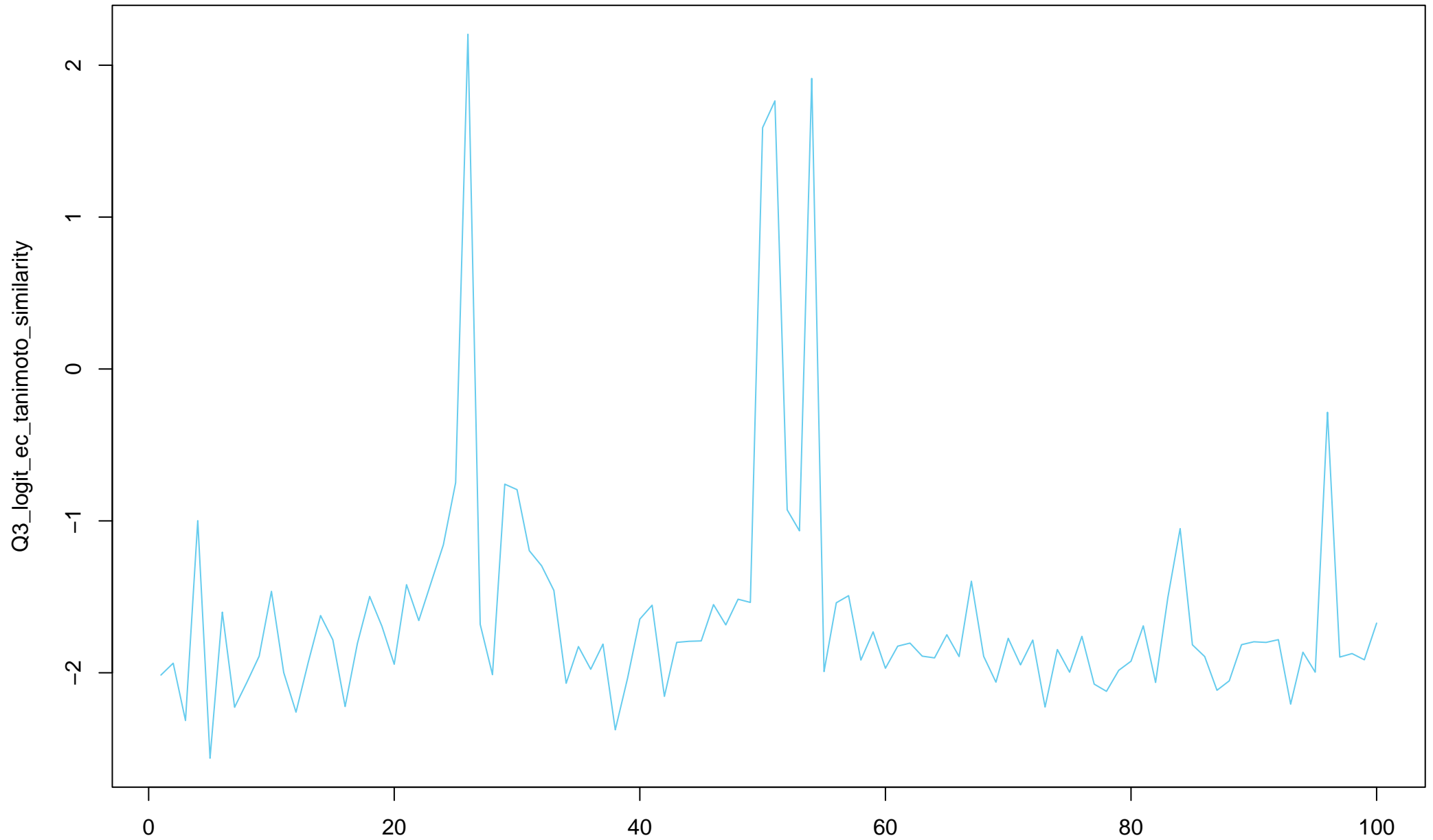
Q3_log_RMSD
ESS = 61.3 | BMK = 0.106 | MCSE(6.27) = 15.5 | stat: TRUE | burn: 0



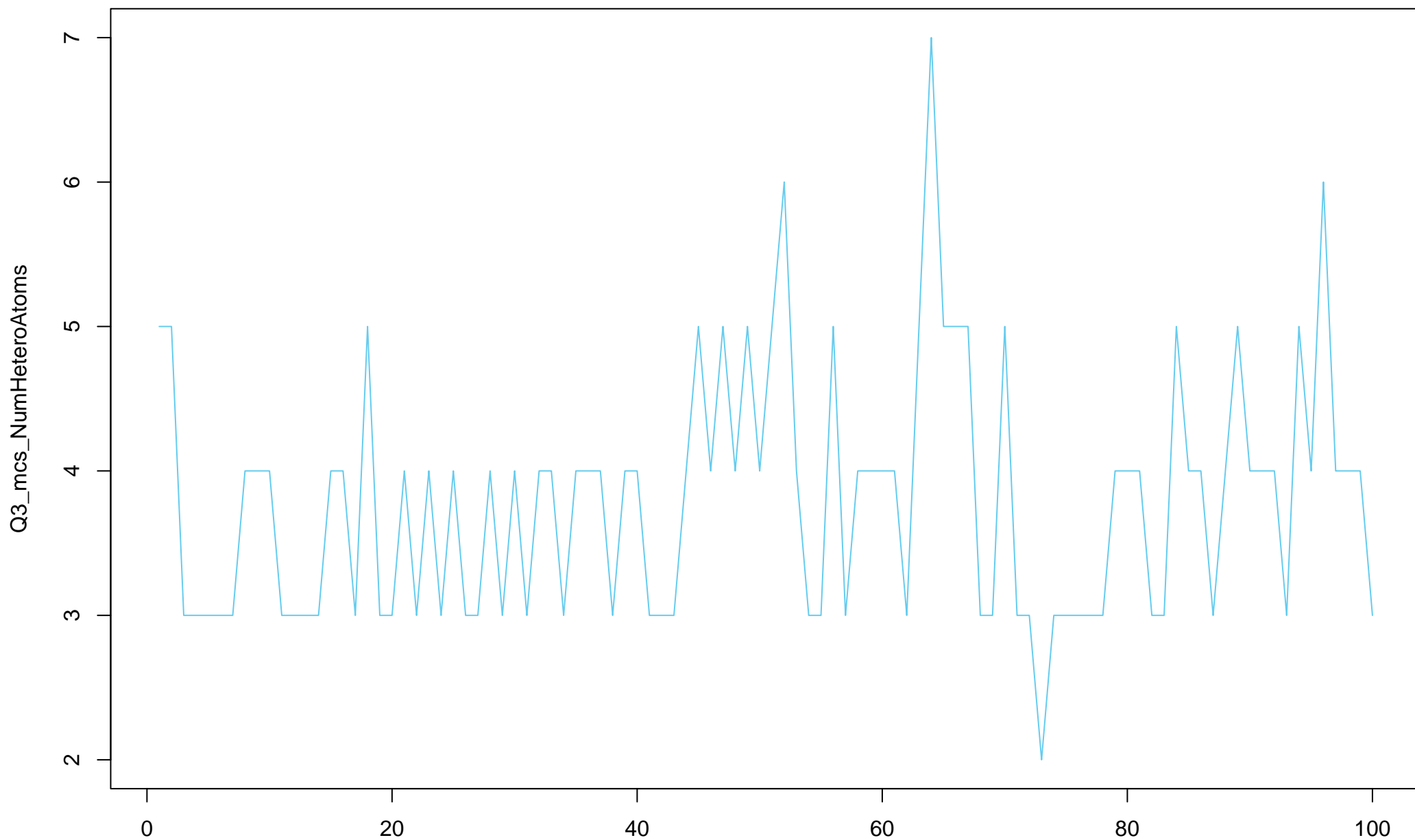
Q3_log_mcs_unbonded_polar_sasa
ESS = 43 | BMK = 0.355 | MCSE(6.27) = 17 | stat: FALSE | burn: 0



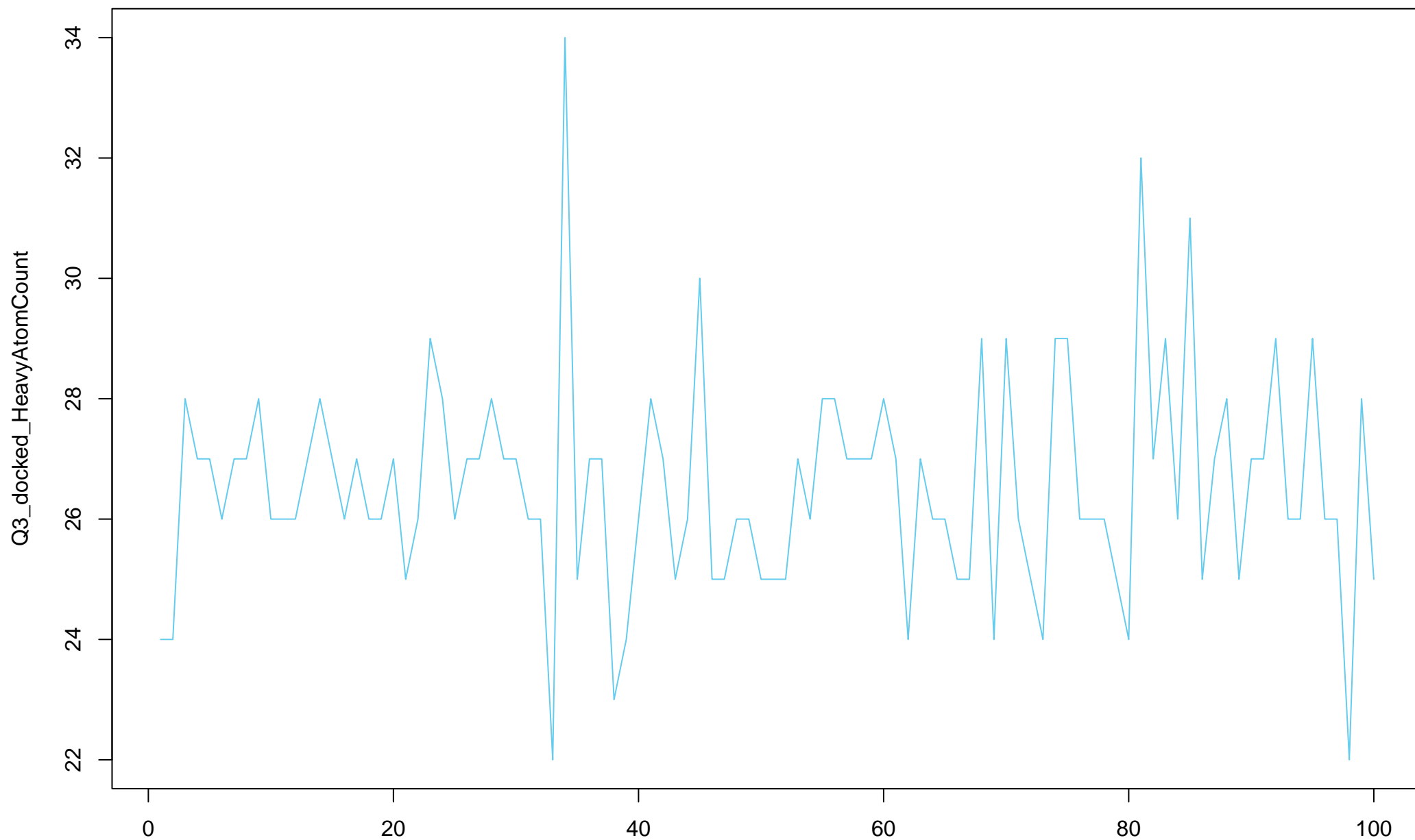
Q3_logit_ec_tanimoto_similarity
ESS = 24.4 | BMK = 0.337 | MCSE(6.27) = 19.1 | stat: TRUE | burn: 60



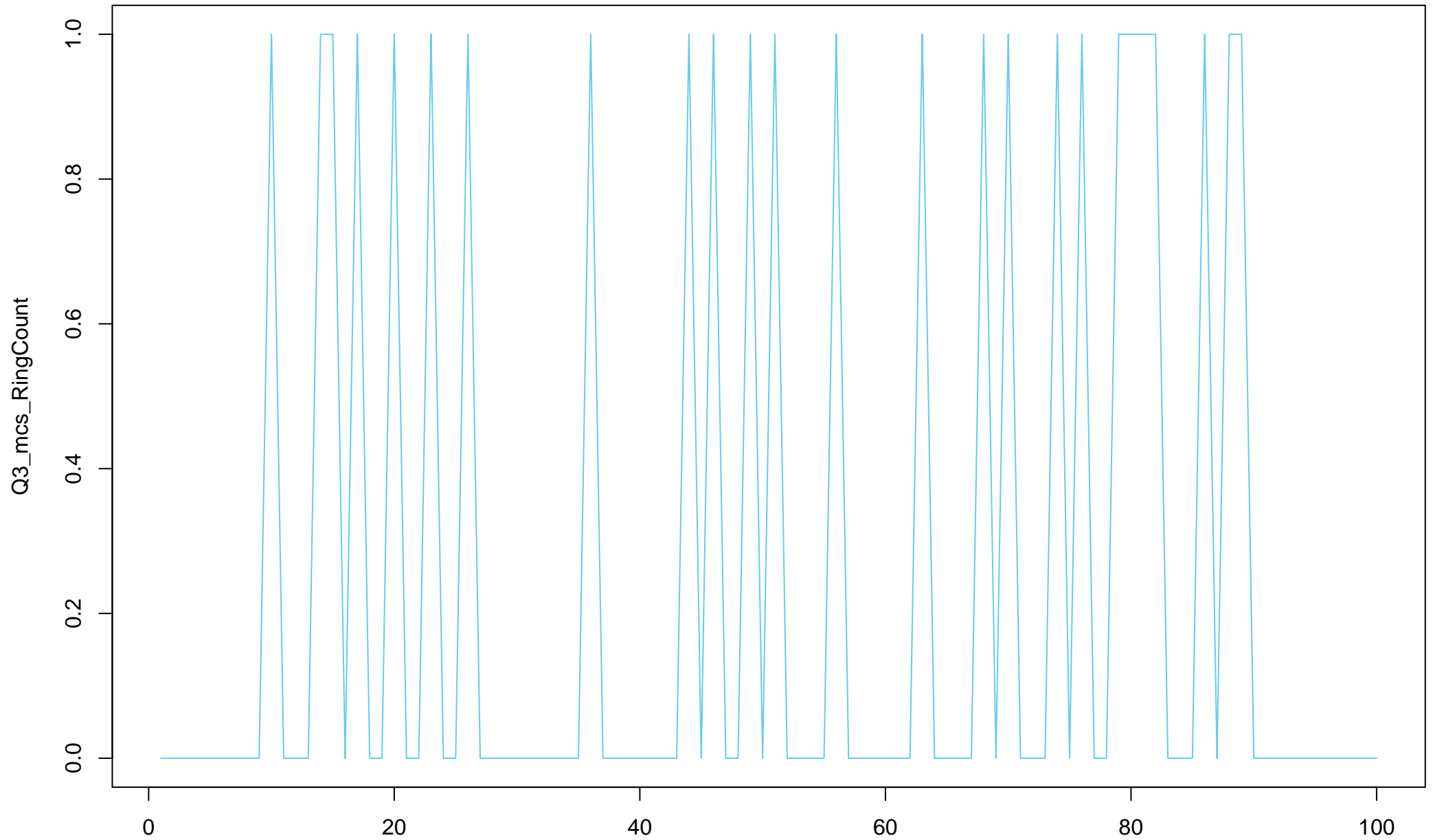
Q3_mcs_NumHeteroAtoms
ESS = 58.6 | BMK = 0.216 | MCSE(6.27) = 17.7 | stat: TRUE | burn: 70



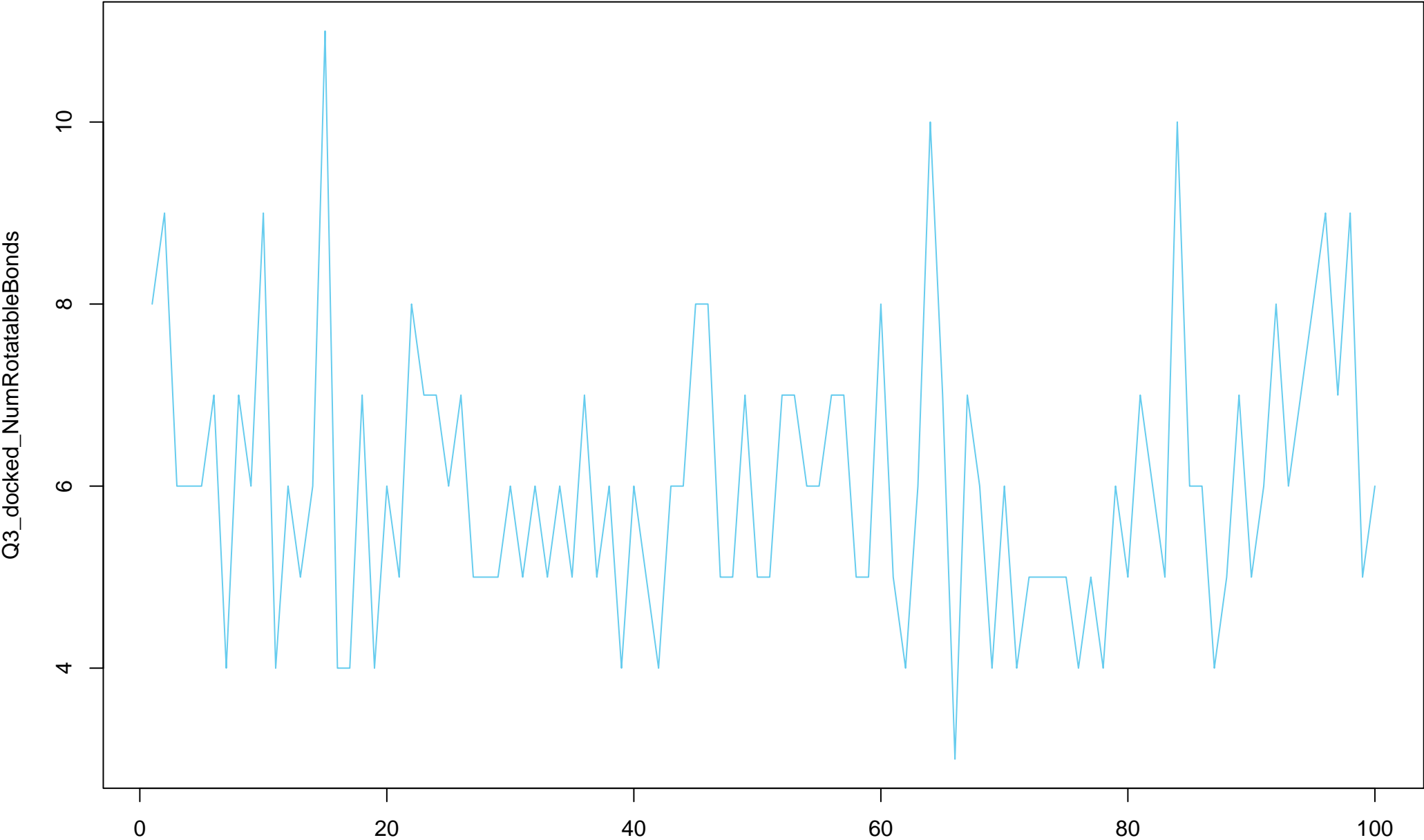
Q3_docked_HeavyAtomCount
ESS = 100 | BMK = 0.23 | MCSE(6.27) = 7.87 | stat: TRUE | burn: 0



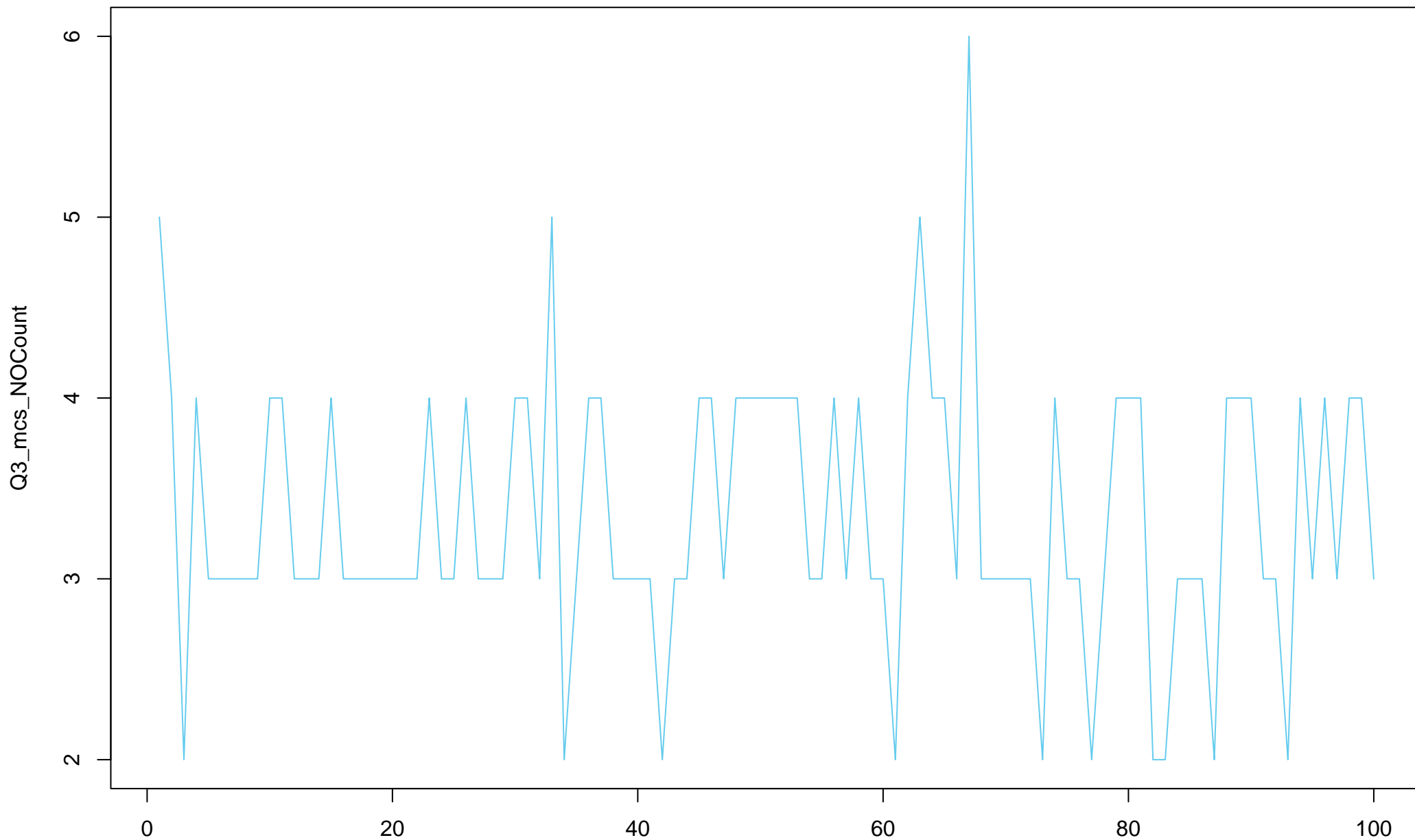
Q3_mcs_RingCount
ESS = 100 | BMK = 0.0452 | MCSE(6.27) = 9.4 | stat: TRUE | burn: 0



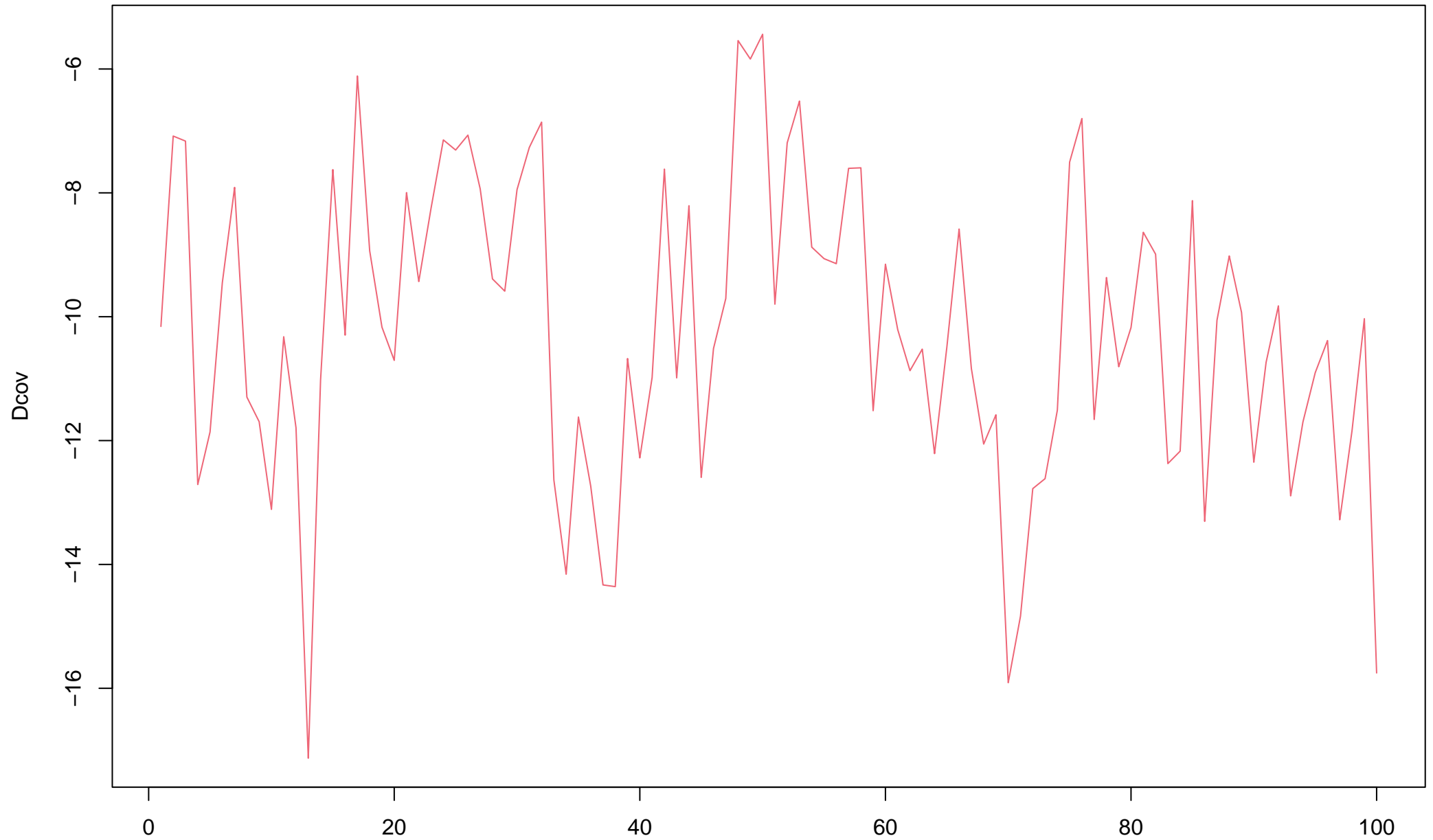
Q3_docked_NumRotatableBonds
ESS = 100 | BMK = 0.0571 | MCSE(6.27) = 10.2 | stat: TRUE | burn: 0



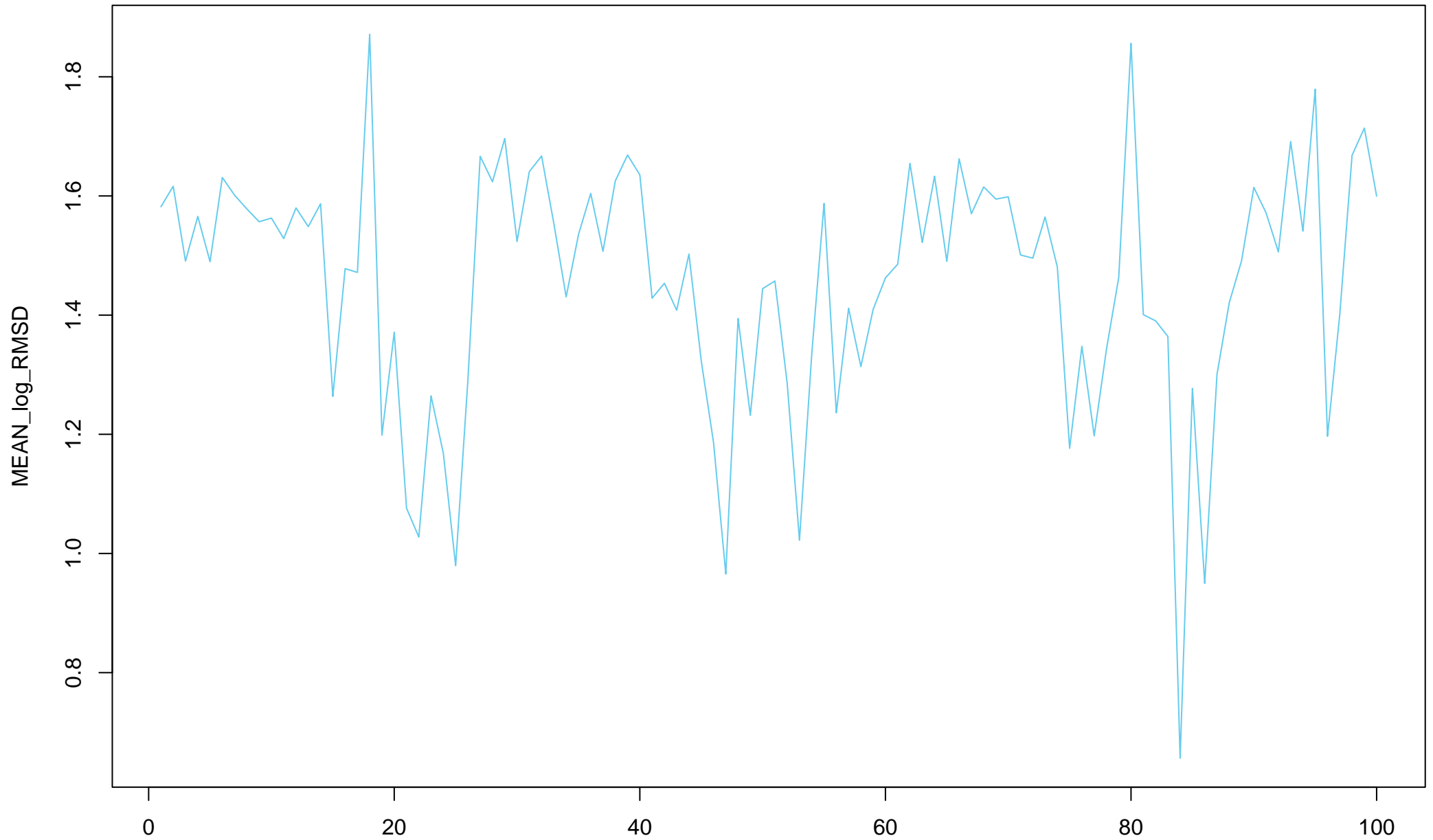
Q3_mcs_NOCount
ESS = 100 | BMK = 0.122 | MCSE(6.27) = 10.6 | stat: TRUE | burn: 0



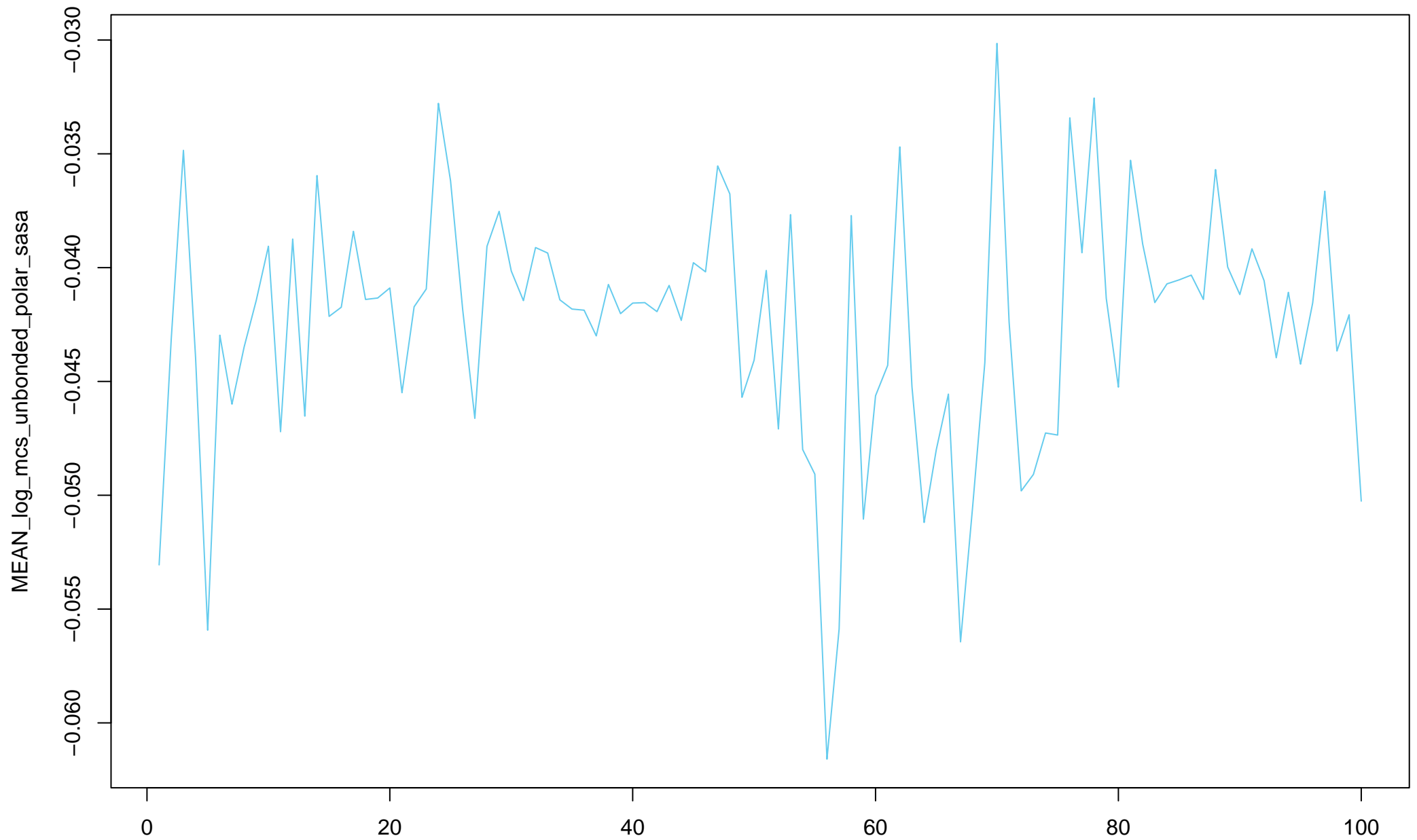
Dcov
ESS = 83.4 | BMK = 0.573 | MCSE(6.27) = 3.64 | stat: TRUE | burn: 80



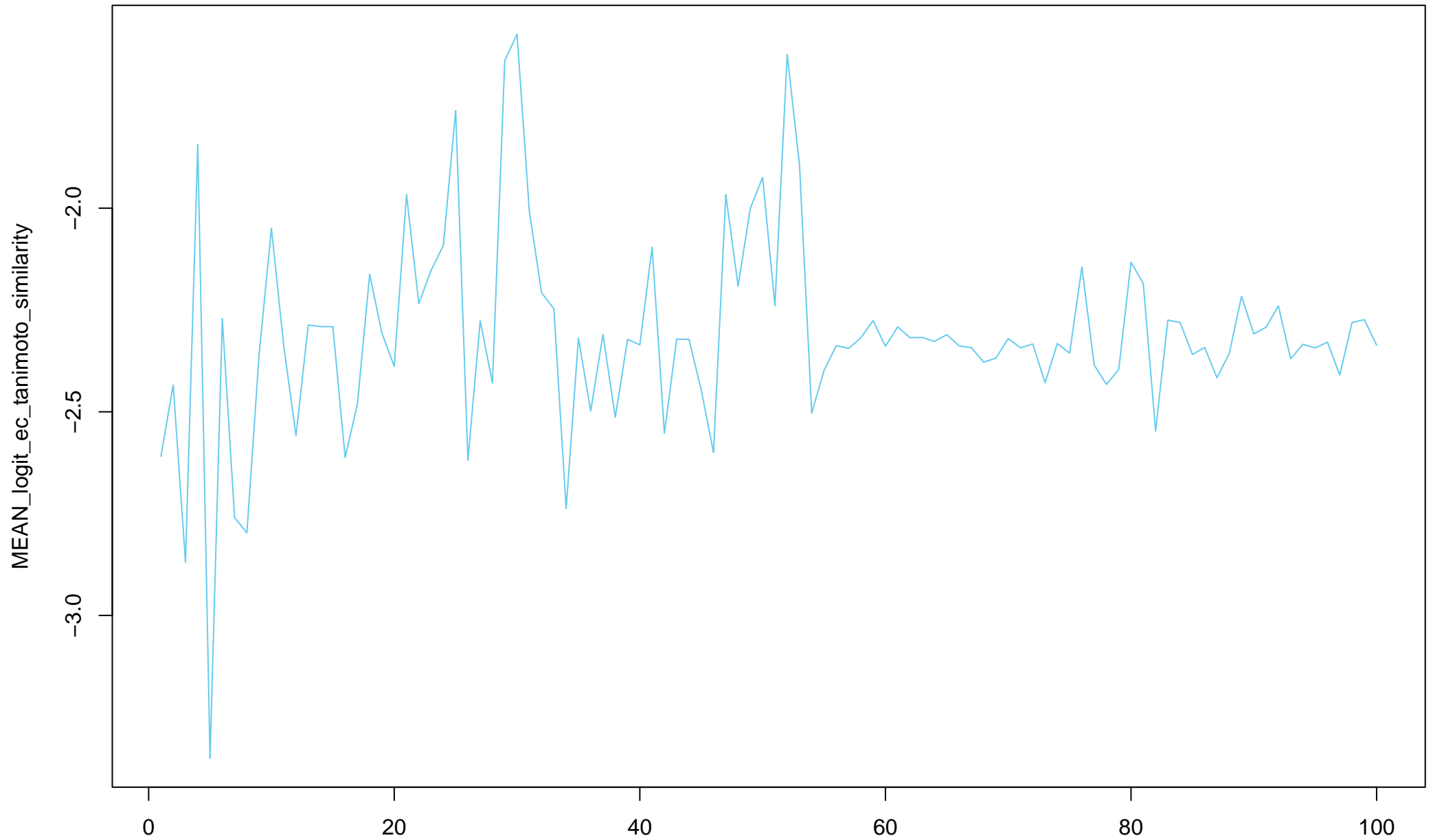
MEAN_log_RMSD
ESS = 24.6 | BMK = 0.128 | MCSE(6.27) = 22.9 | stat: FALSE | burn: 100



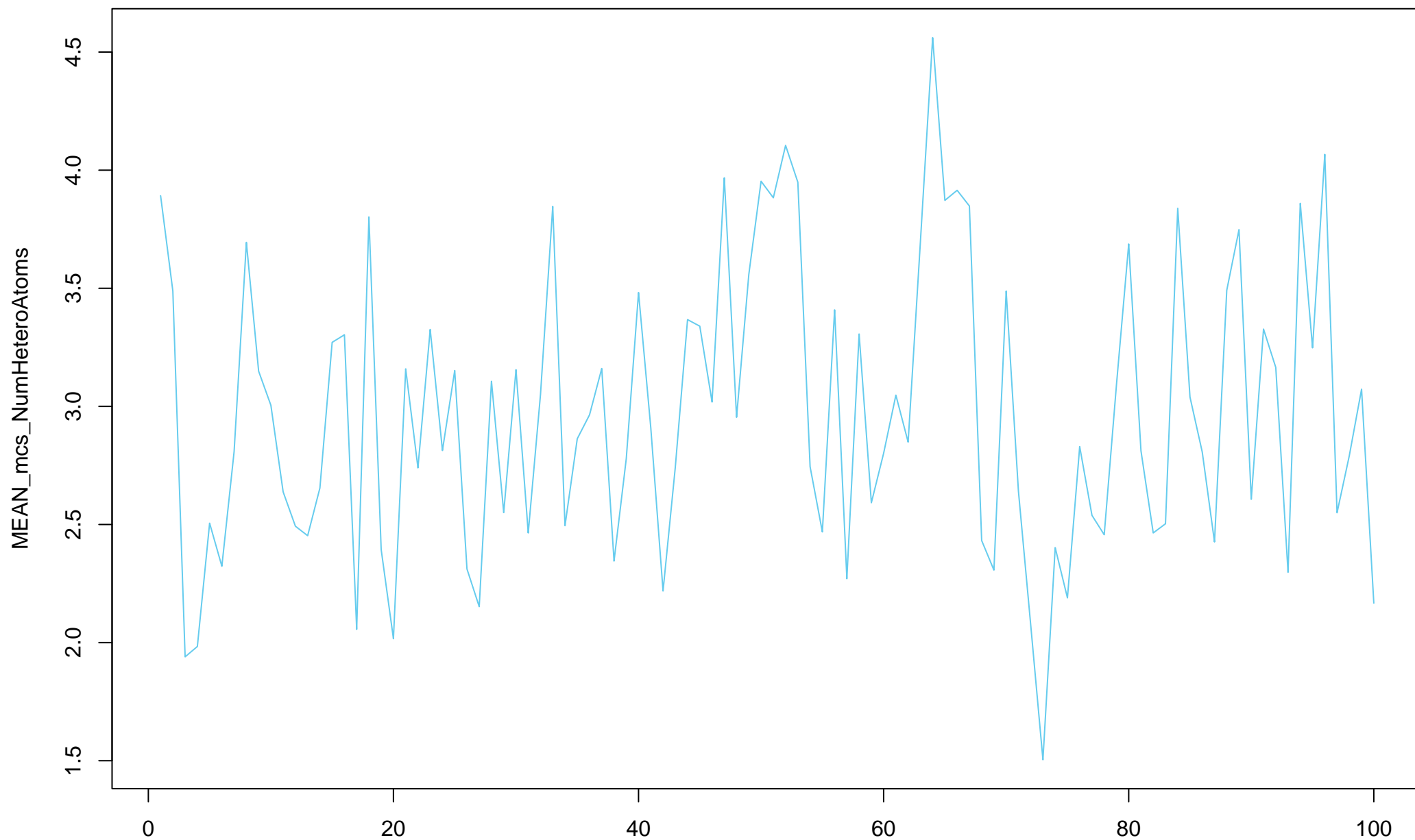
MEAN_log_mcs_unbonded_polar_sasa
ESS = 56.1 | BMK = 0.28 | MCSE(6.27) = 15.5 | stat: TRUE | burn: 80



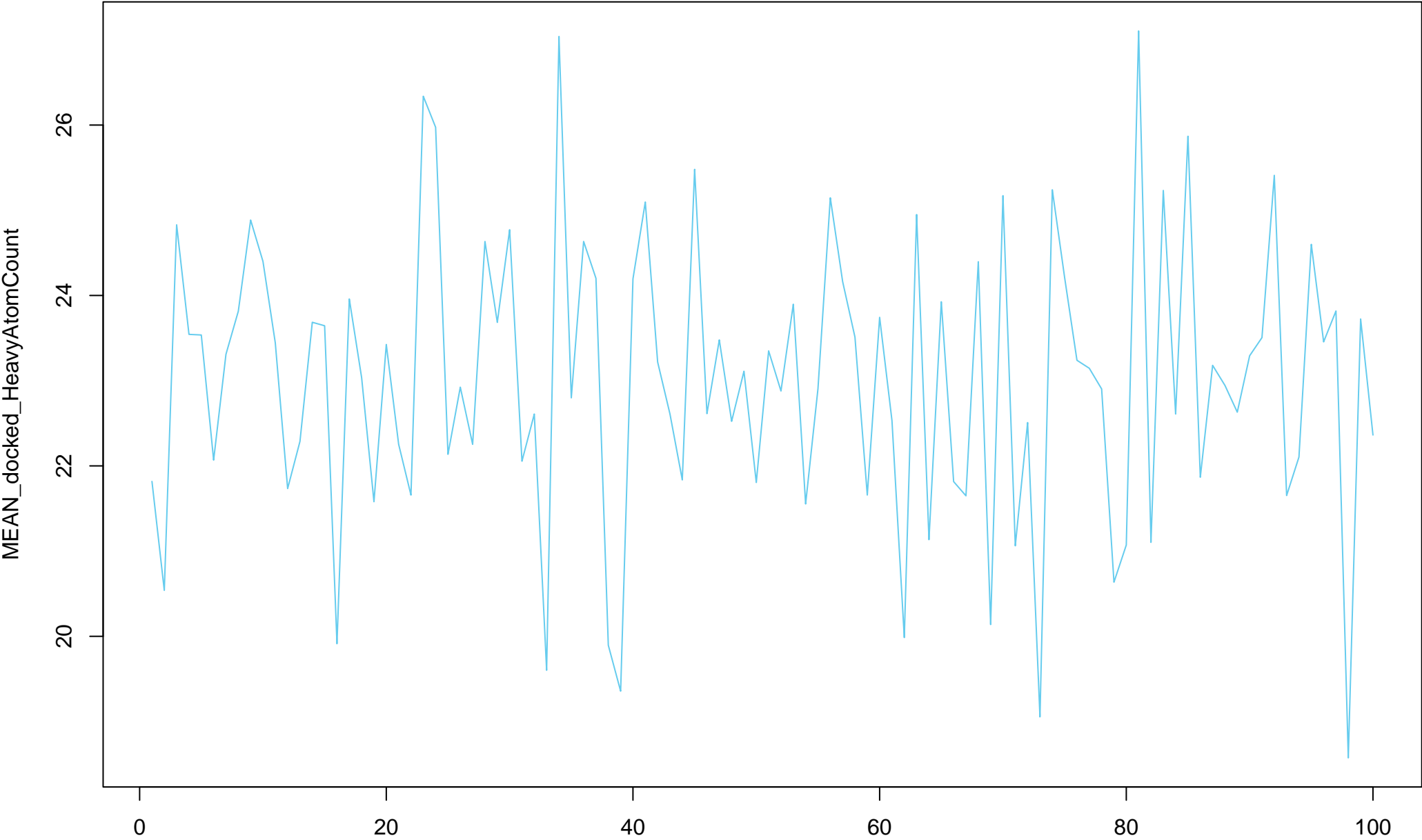
MEAN_logit_ec_tanimoto_similarity
ESS = 48.6 | BMK = 0.489 | MCSE(6.27) = 18.3 | stat: FALSE | burn: 60



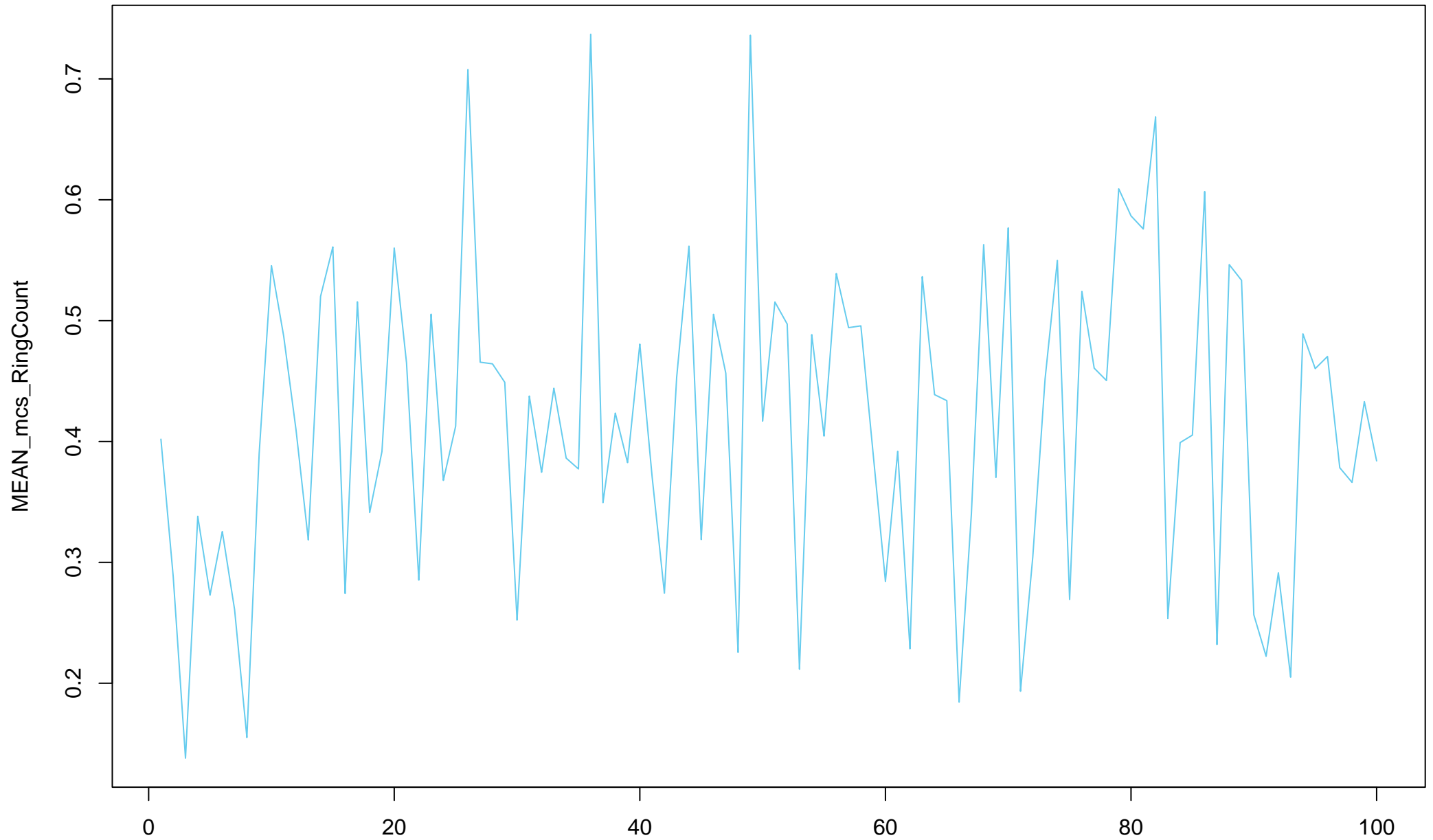
MEAN_mcs_NumHeteroAtoms
ESS = 58.4 | BMK = 0.124 | MCSE(6.27) = 17.2 | stat: TRUE | burn: 0



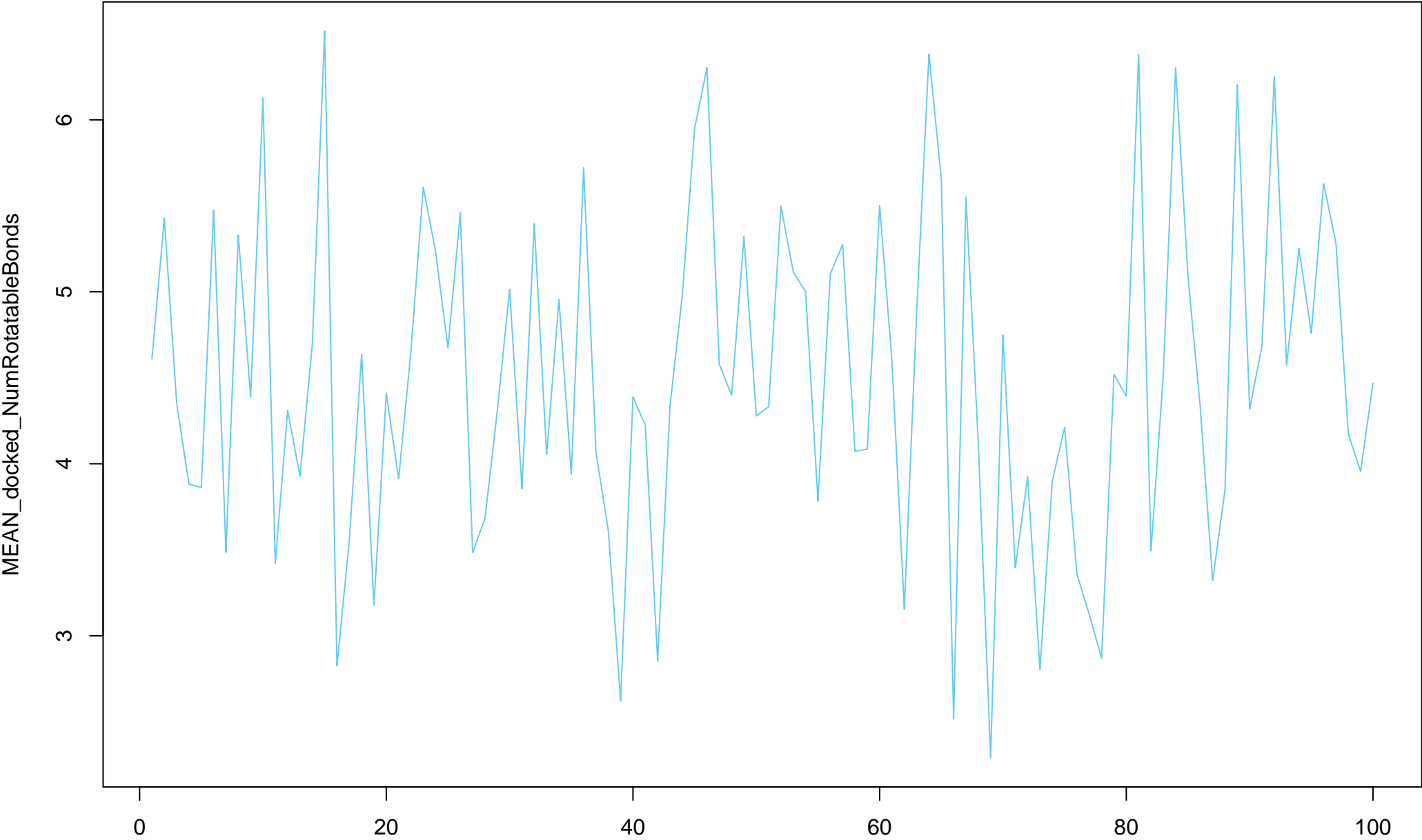
MEAN_docked_HeavyAtomCount
ESS = 100 | BMK = 0.0622 | MCSE(6.27) = 7.32 | stat: TRUE | burn: 0



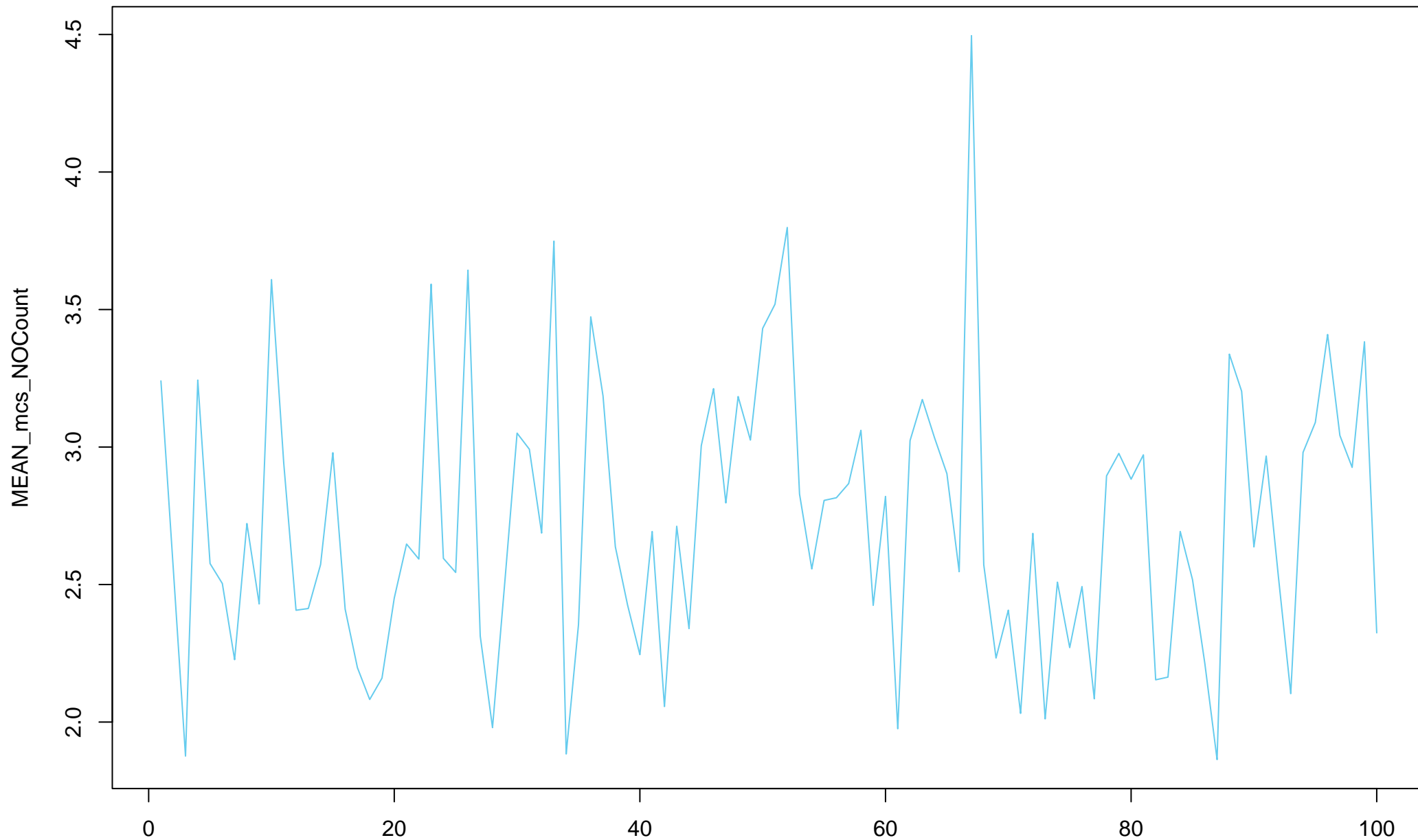
MEAN_mcs_RingCount
ESS = 100 | BMK = 0.151 | MCSE(6.27) = 10.3 | stat: TRUE | burn: 0



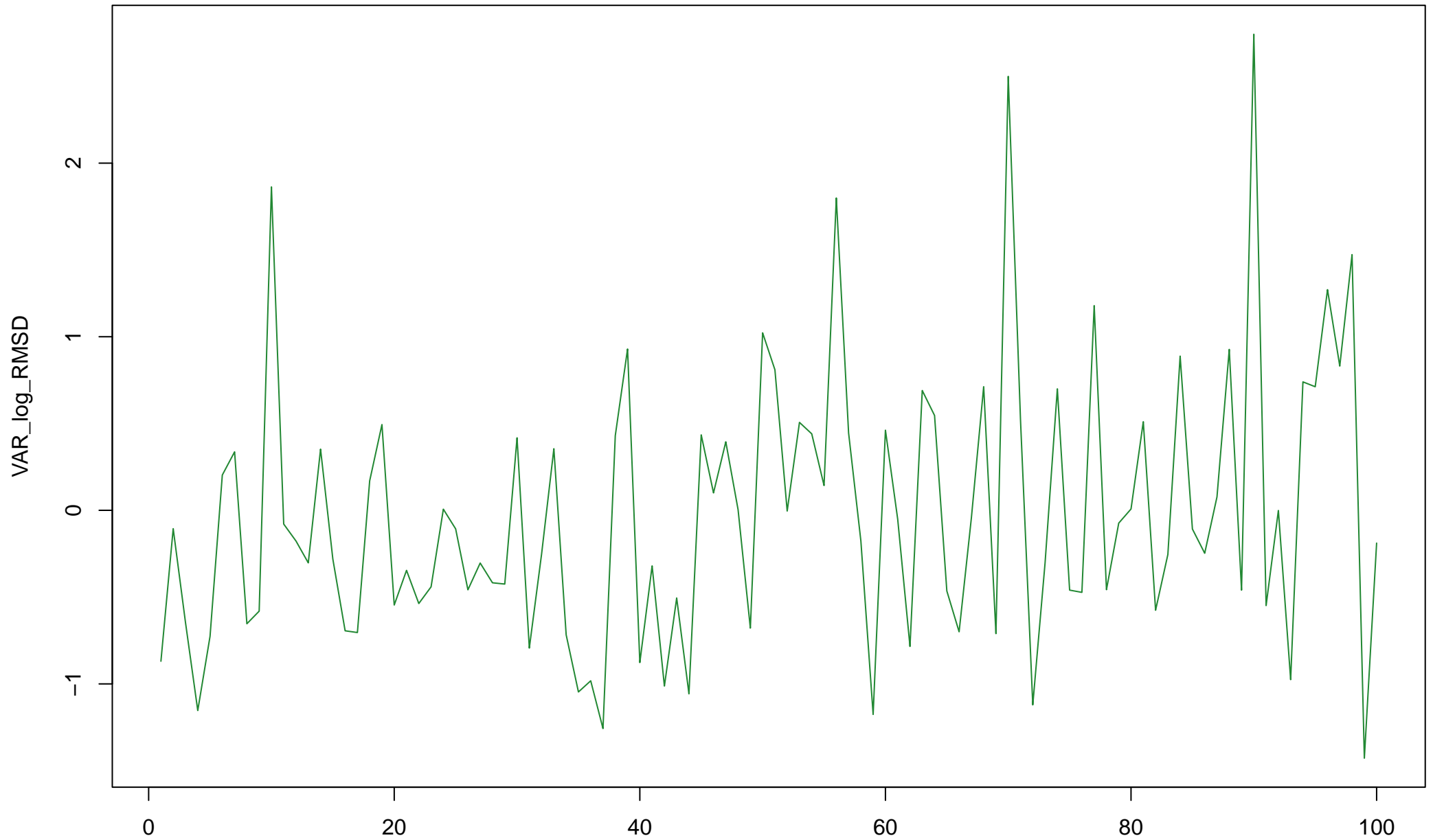
MEAN_docked_NumRotatableBonds
ESS = 100 | BMK = 0.0547 | MCSE(6.27) = 10.5 | stat: TRUE | burn: 0



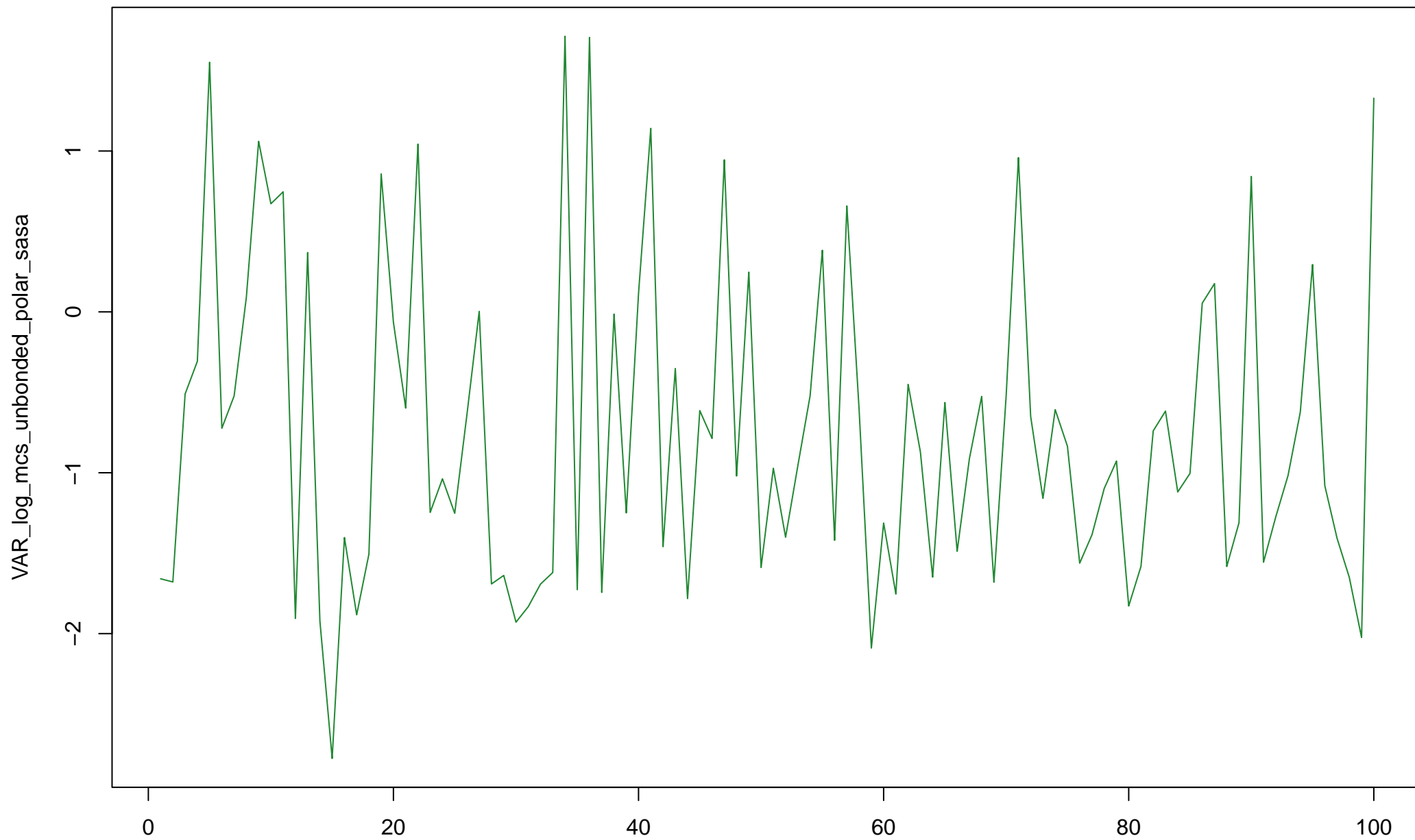
MEAN_mcs_NOCount
ESS = 100 | BMK = 0.125 | MCSE(6.27) = 13.6 | stat: TRUE | burn: 0



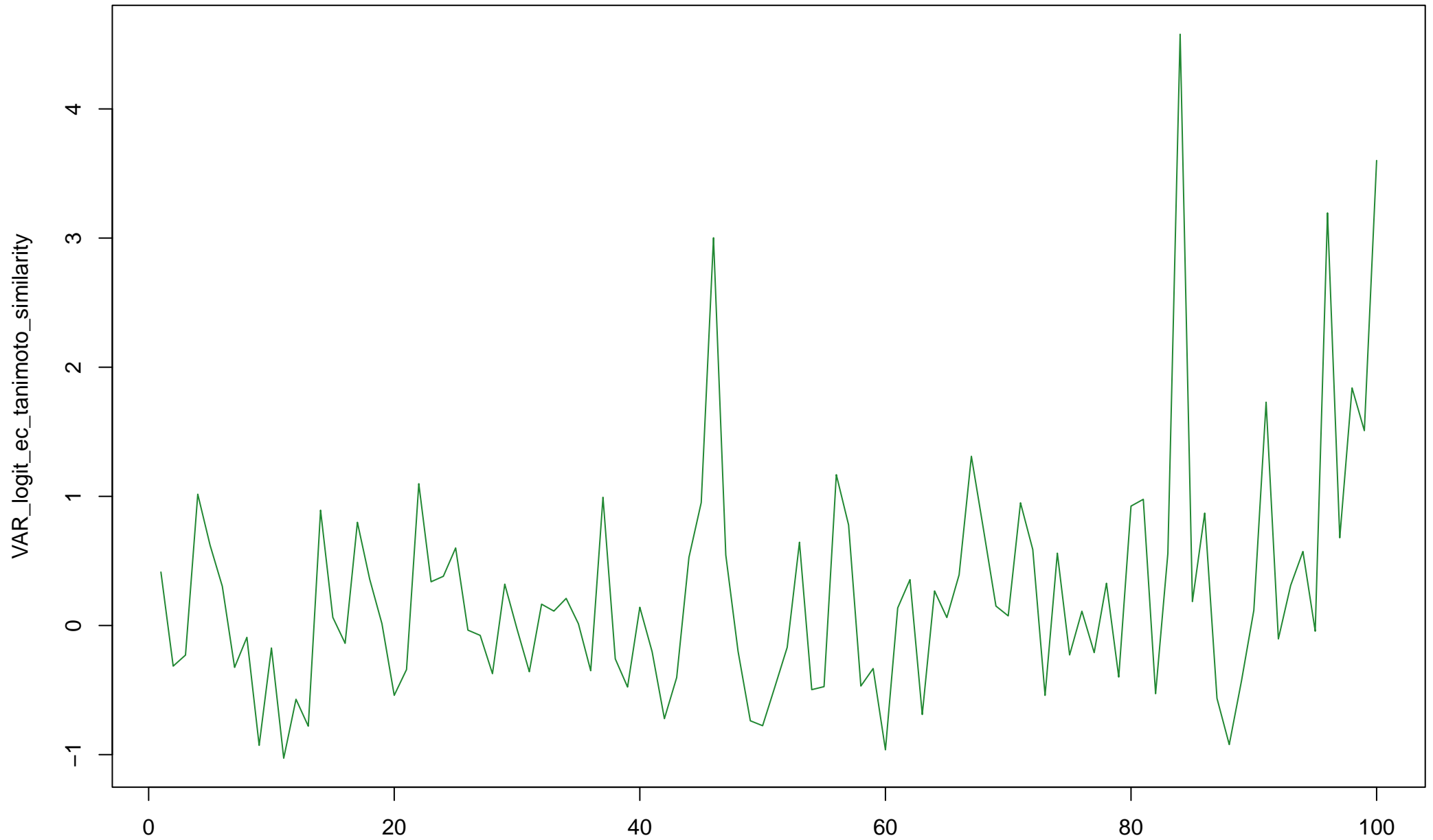
VAR_log_RMSD
ESS = 100 | BMK = 0.325 | MCSE(6.27) = 9.44 | stat: TRUE | burn: 0



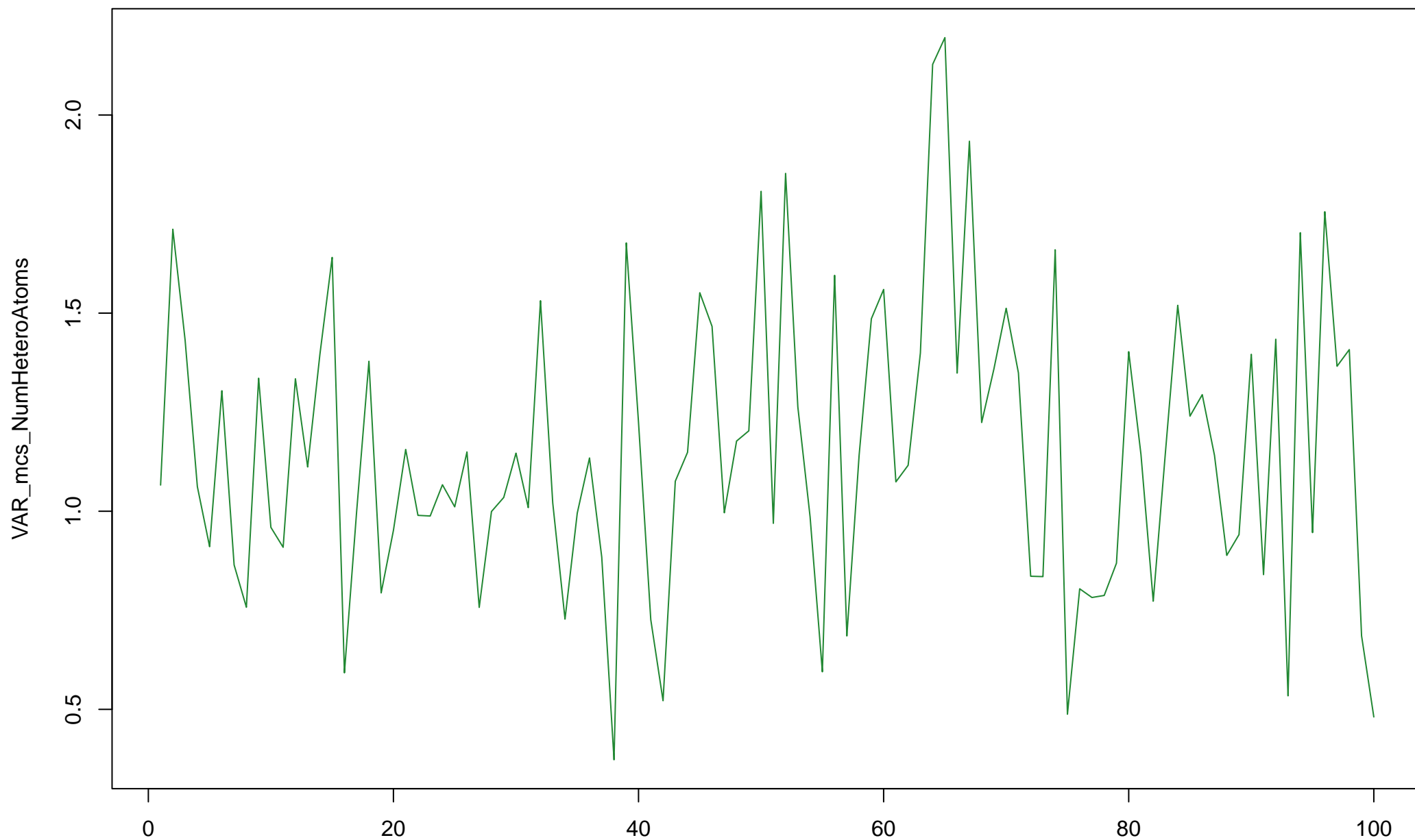
VAR_log_mcs_unbonded_polar_sasa
ESS = 79 | BMK = 0.316 | MCSE(6.27) = 11.1 | stat: TRUE | burn: 0



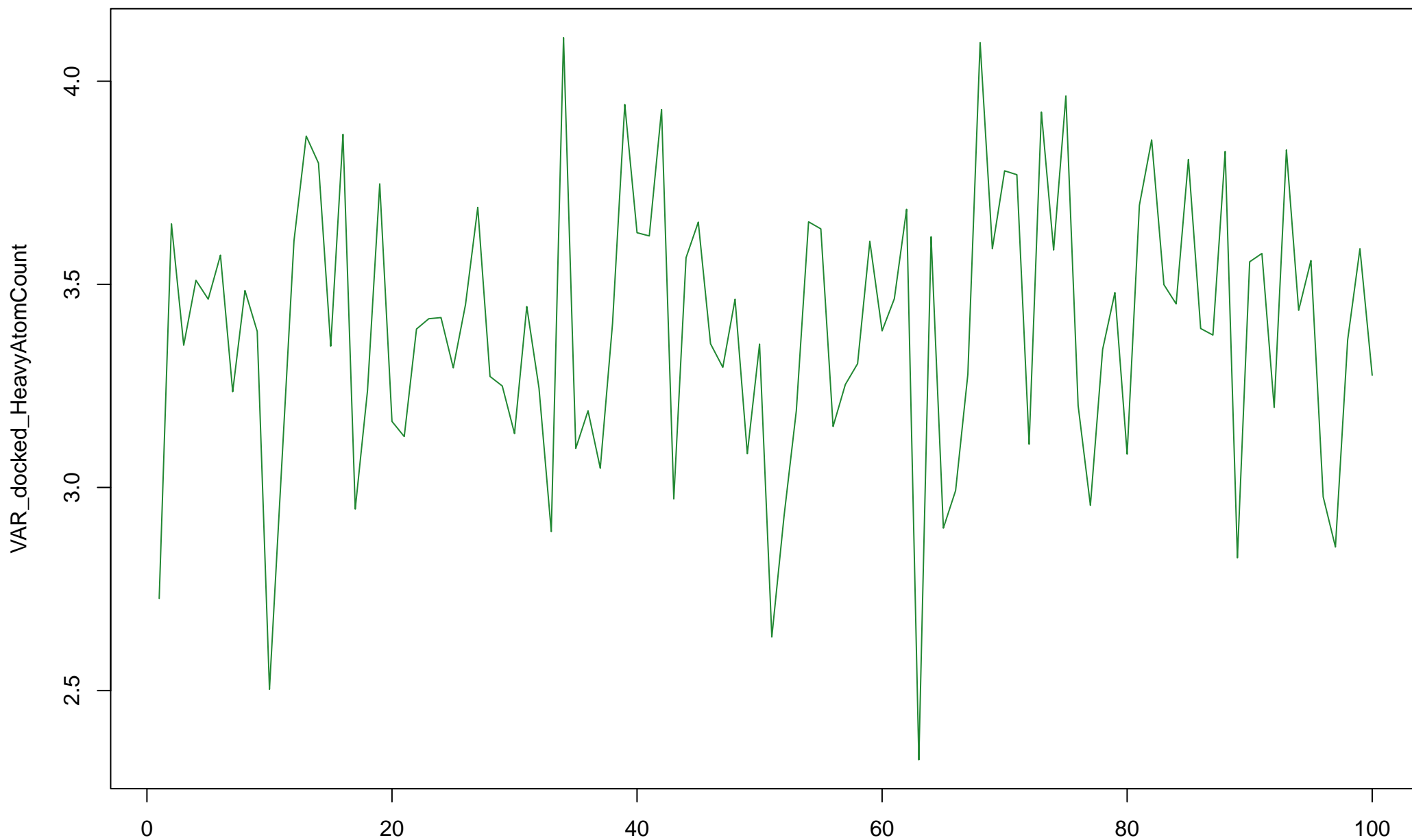
VAR_logit_ec_tanimoto_similarity
ESS = 100 | BMK = 0.364 | MCSE(6.27) = 9.91 | stat: TRUE | burn: 100



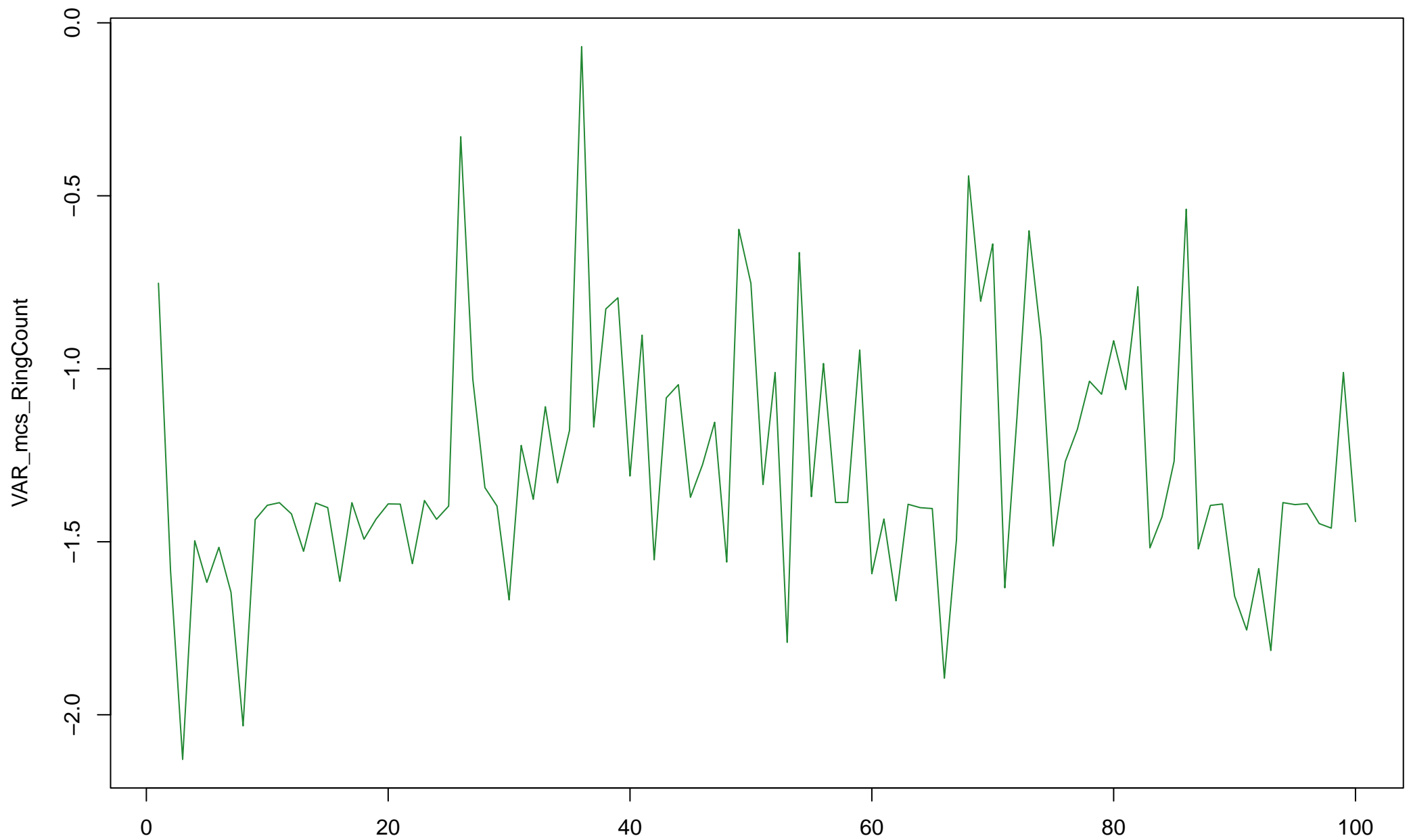
VAR_mcs_NumHeteroAtoms
ESS = 52.4 | BMK = 0.217 | MCSE(6.27) = 18.5 | stat: TRUE | burn: 0



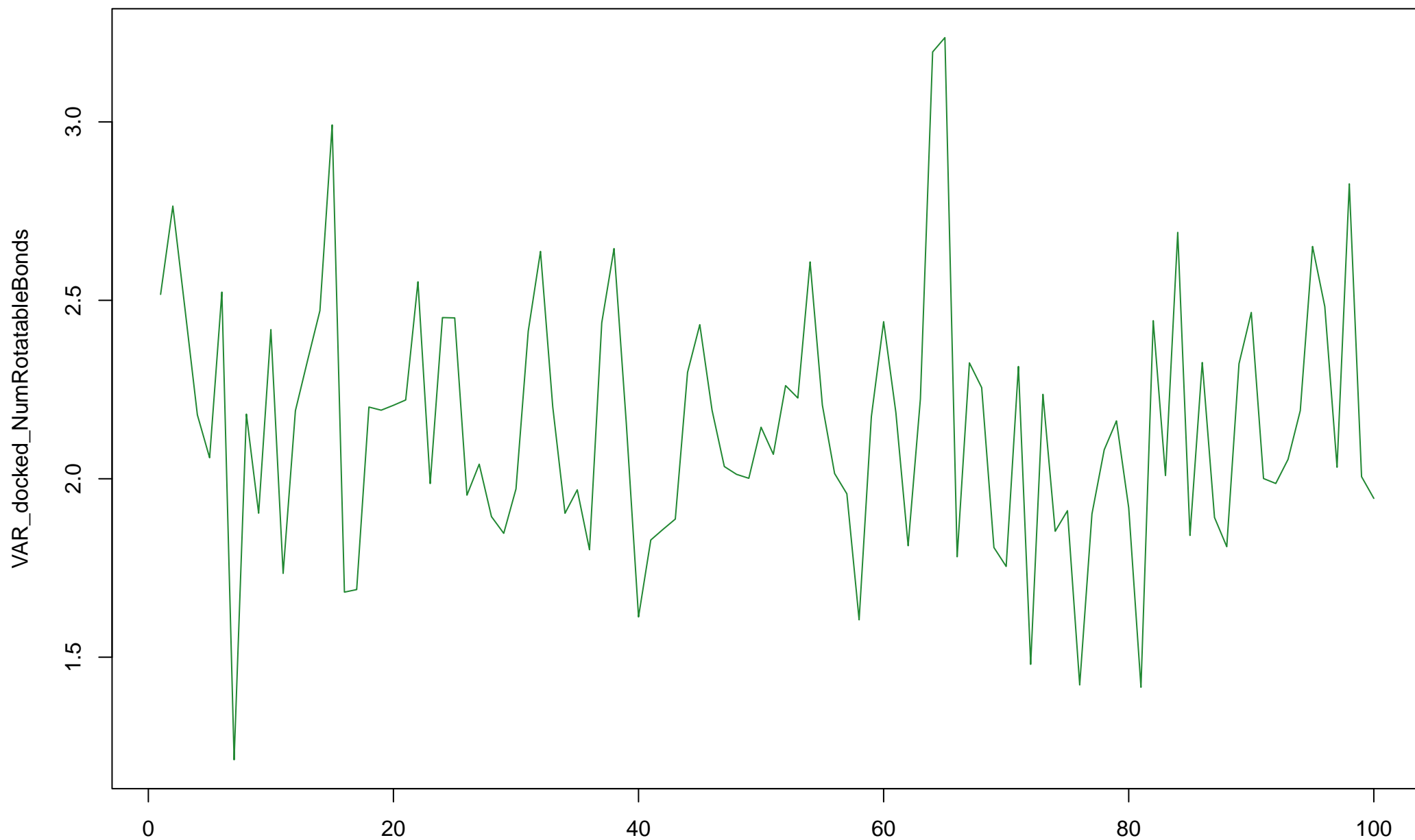
VAR_docked_HeavyAtomCount
ESS = 100 | BMK = 0.0881 | MCSE(6.27) = 9.62 | stat: TRUE | burn: 0



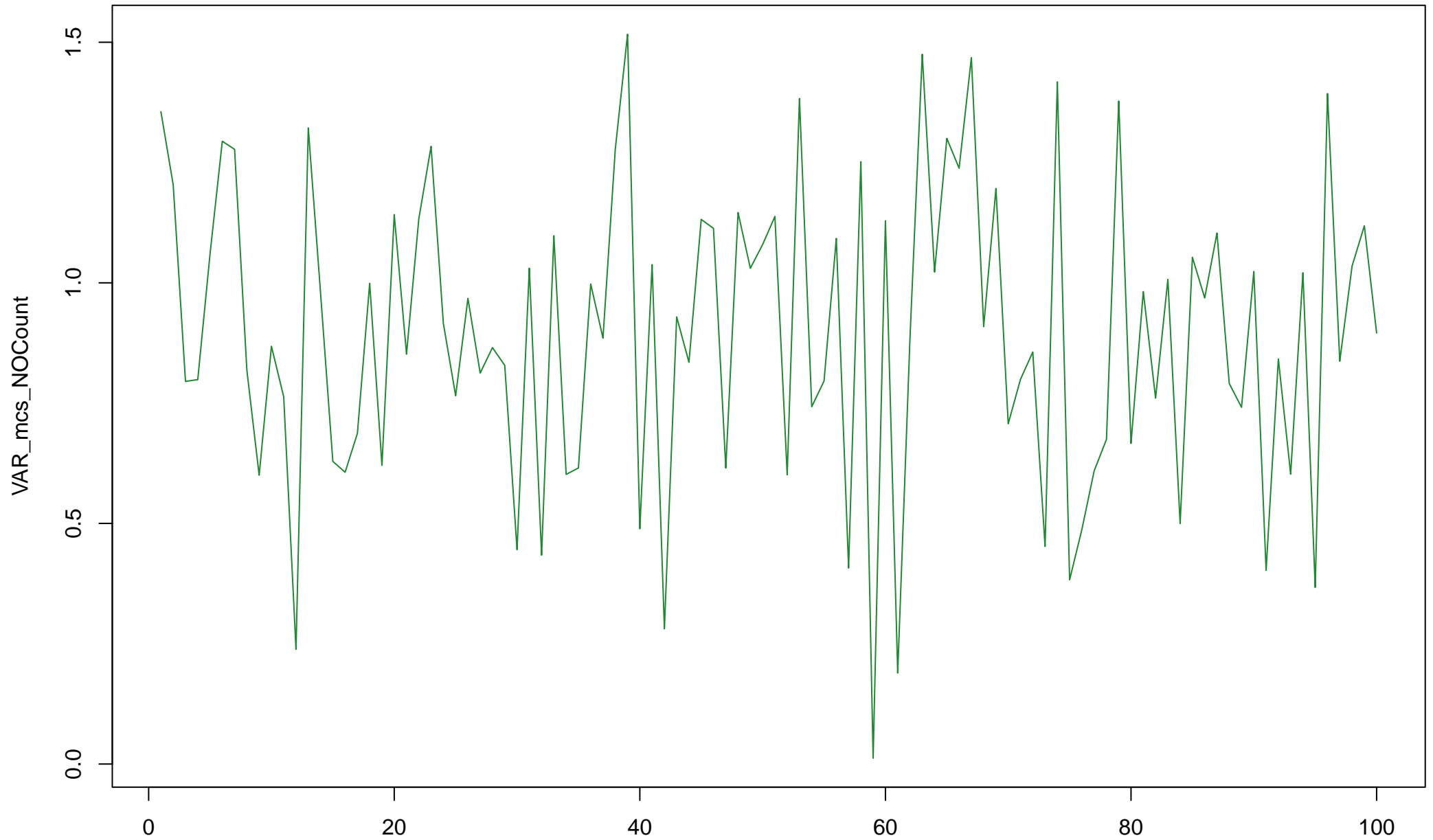
VAR_mcs_RingCount
ESS = 73.8 | BMK = 0.182 | MCSE(6.27) = 15.9 | stat: TRUE | burn: 20



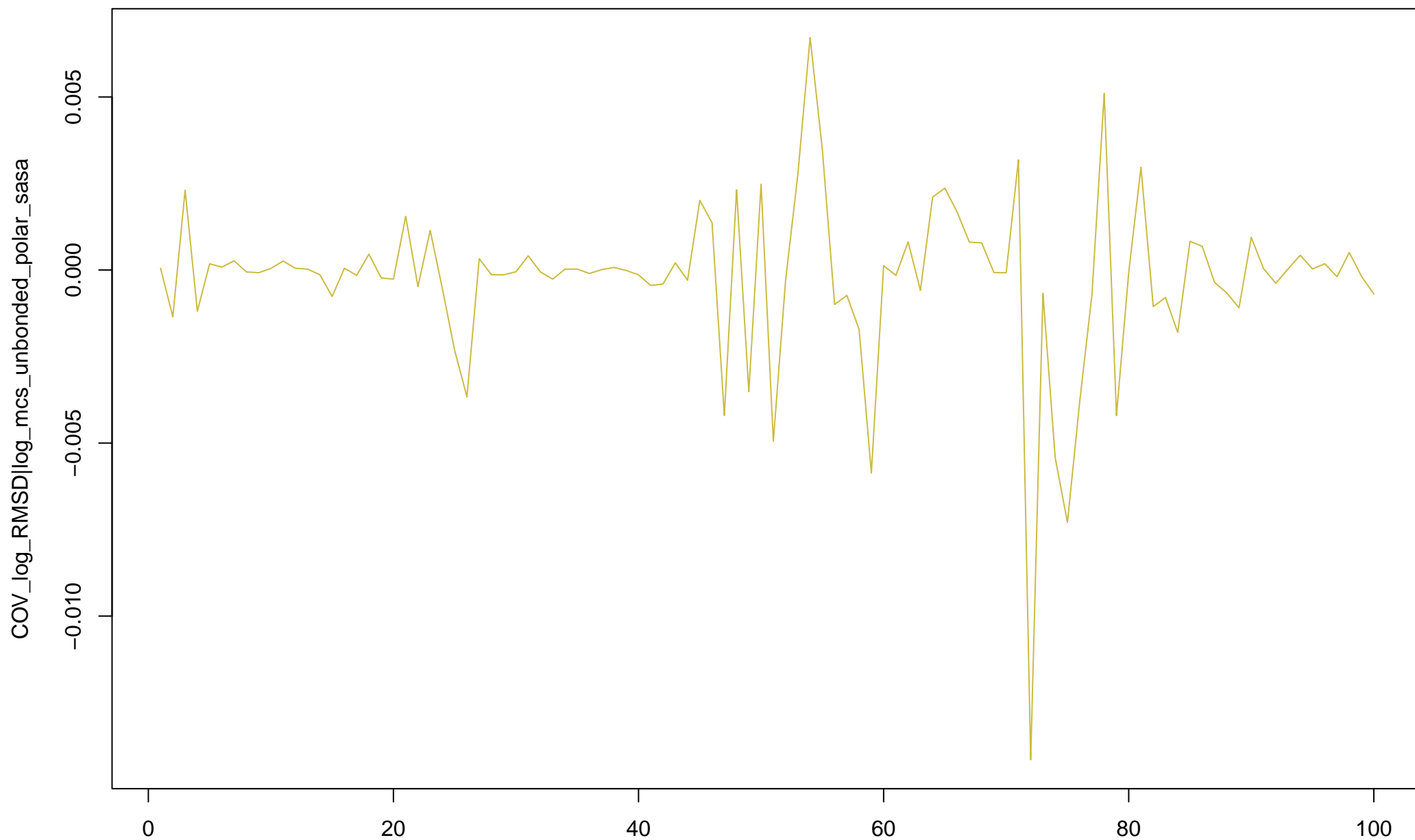
VAR_docked_NumRotatableBonds
ESS = 65 | BMK = 0.156 | MCSE(6.27) = 13 | stat: TRUE | burn: 0



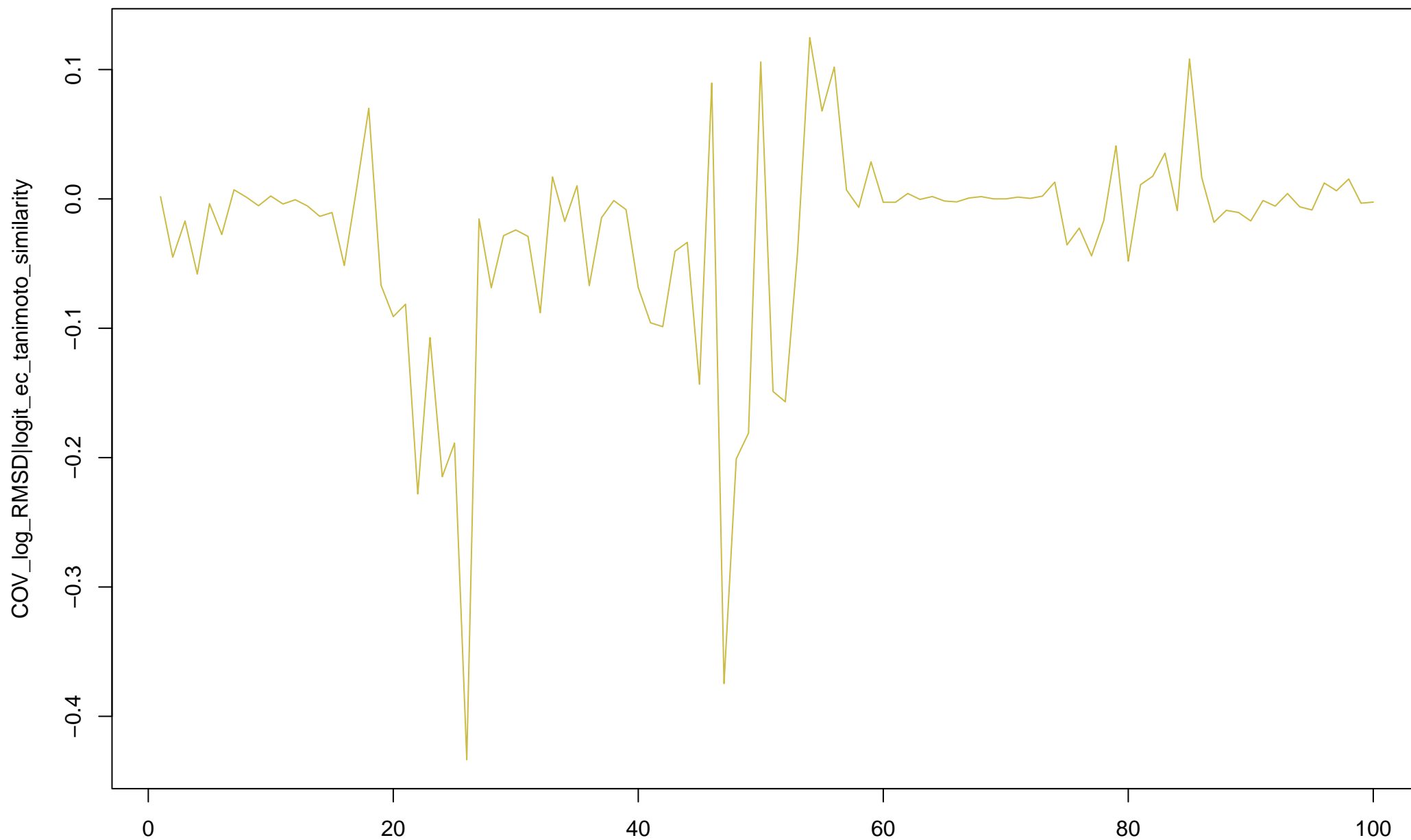
VAR_mcs_NOCount
ESS = 89.5 | BMK = 0.0913 | MCSE(6.27) = 9.13 | stat: TRUE | burn: 0



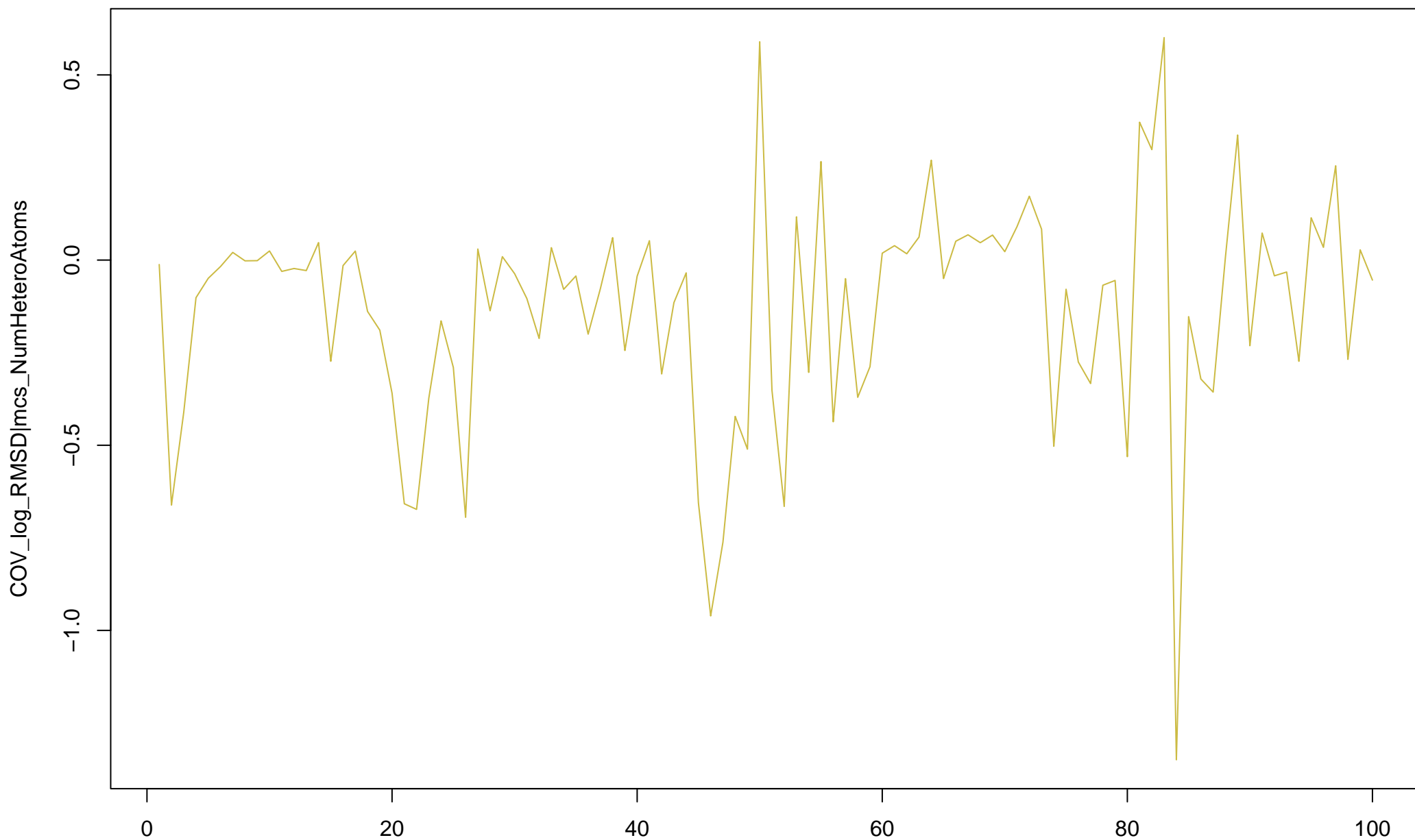
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 100 | BMK = 0.449 | MCSE(6.27) = 13.8 | stat: TRUE | burn: 100



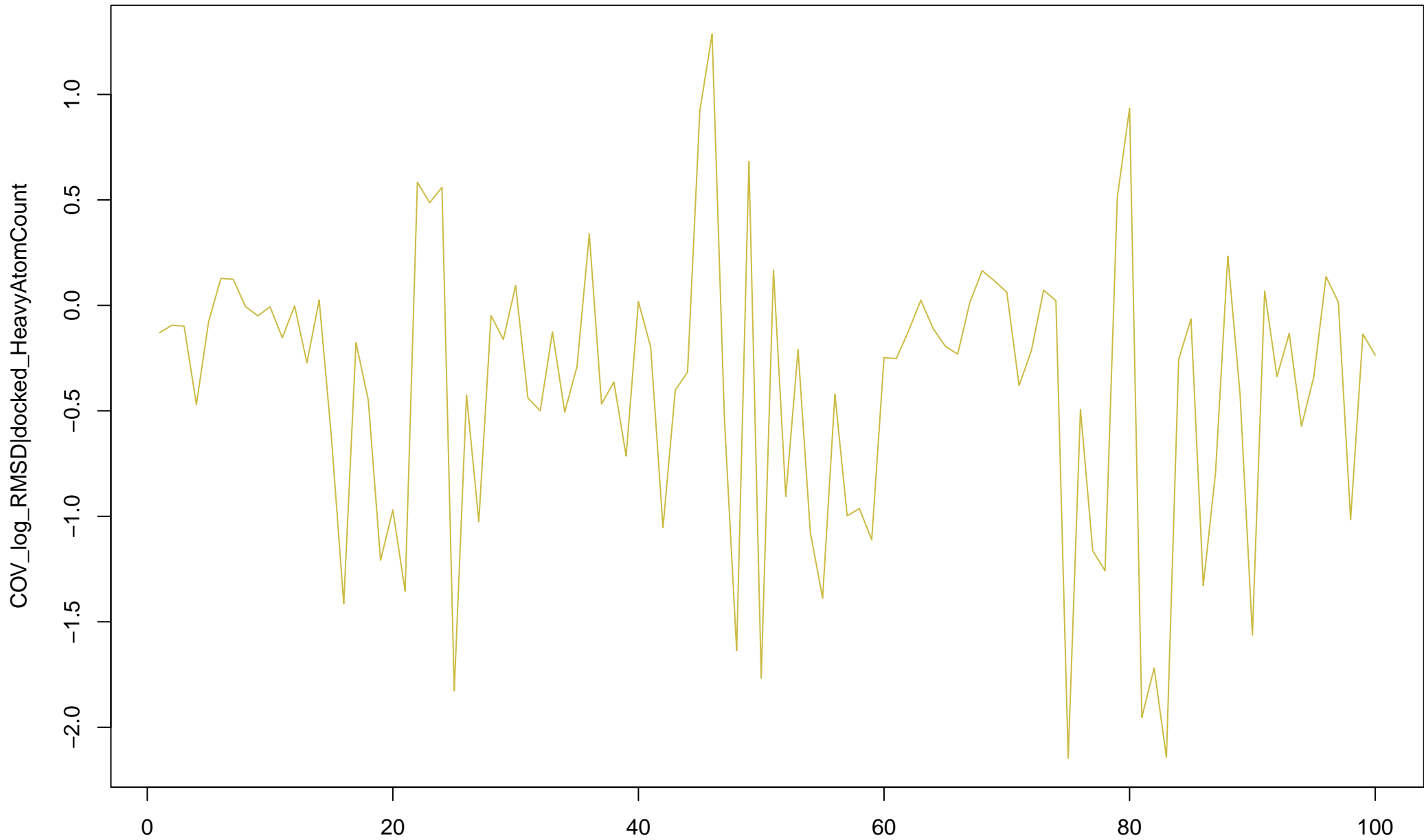
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 16.7 | BMK = 0.492 | MCSE(6.27) = 25.7 | stat: TRUE | burn: 70



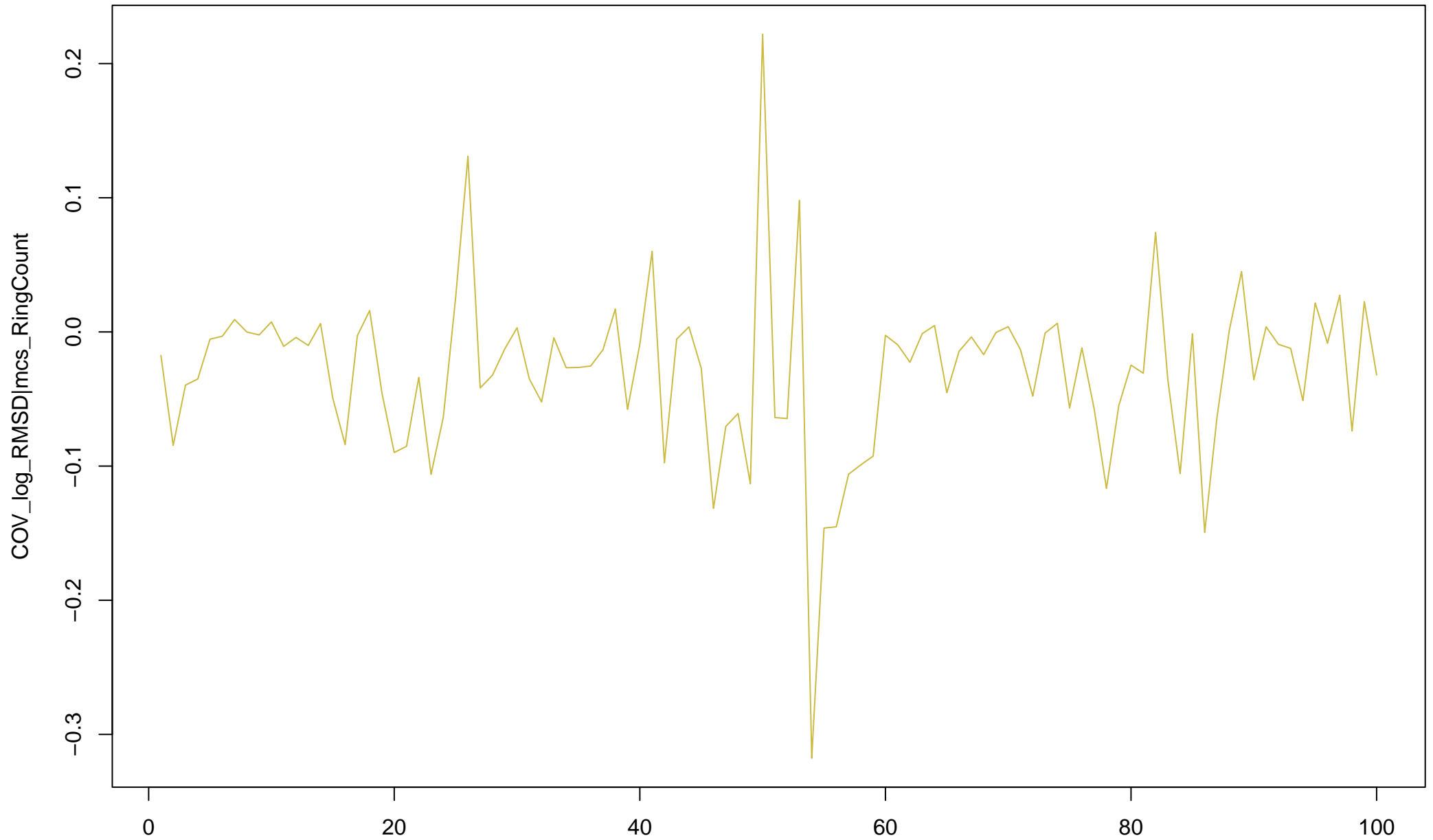
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 100 | BMK = 0.282 | MCSE(6.27) = 14.8 | stat: TRUE | burn: 100



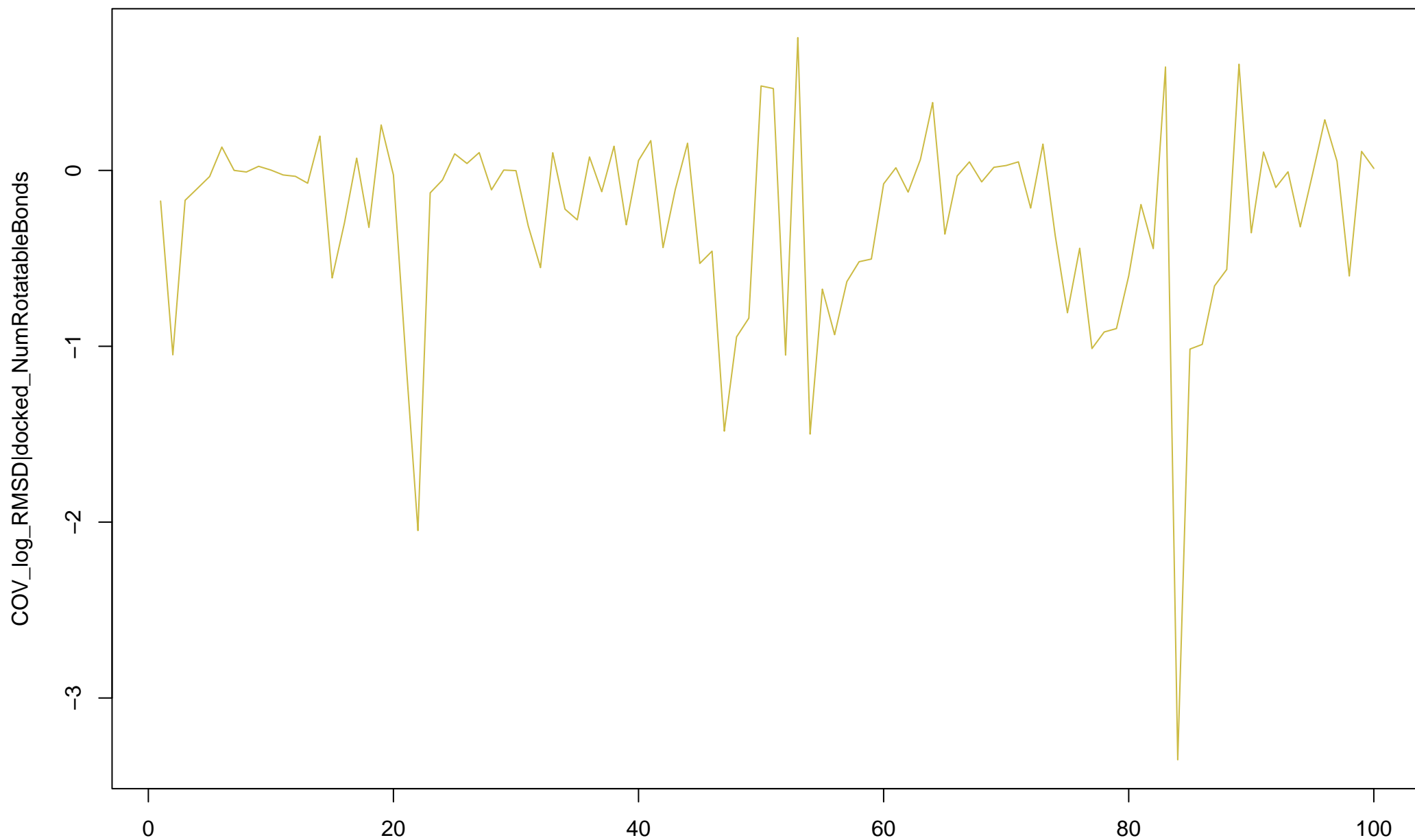
COV_log_RMSD|docked_HeavyAtomCount
ESS = 100 | BMK = 0.123 | MCSE(6.27) = 11.5 | stat: FALSE | burn: 70



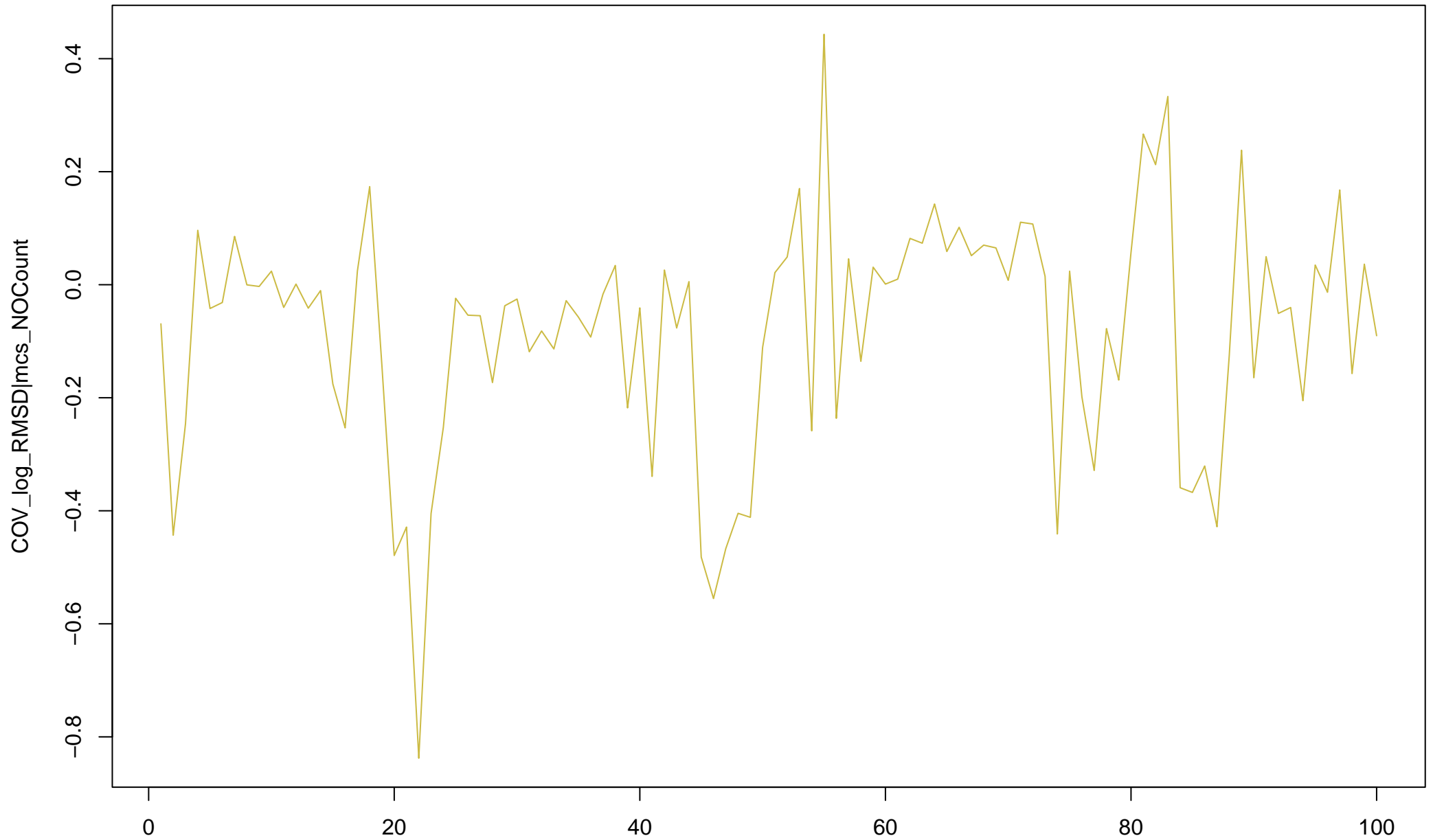
COV_log_RMSD|mcs_RingCount
ESS = 88.8 | BMK = 0.181 | MCSE(6.27) = 11.4 | stat: TRUE | burn: 60



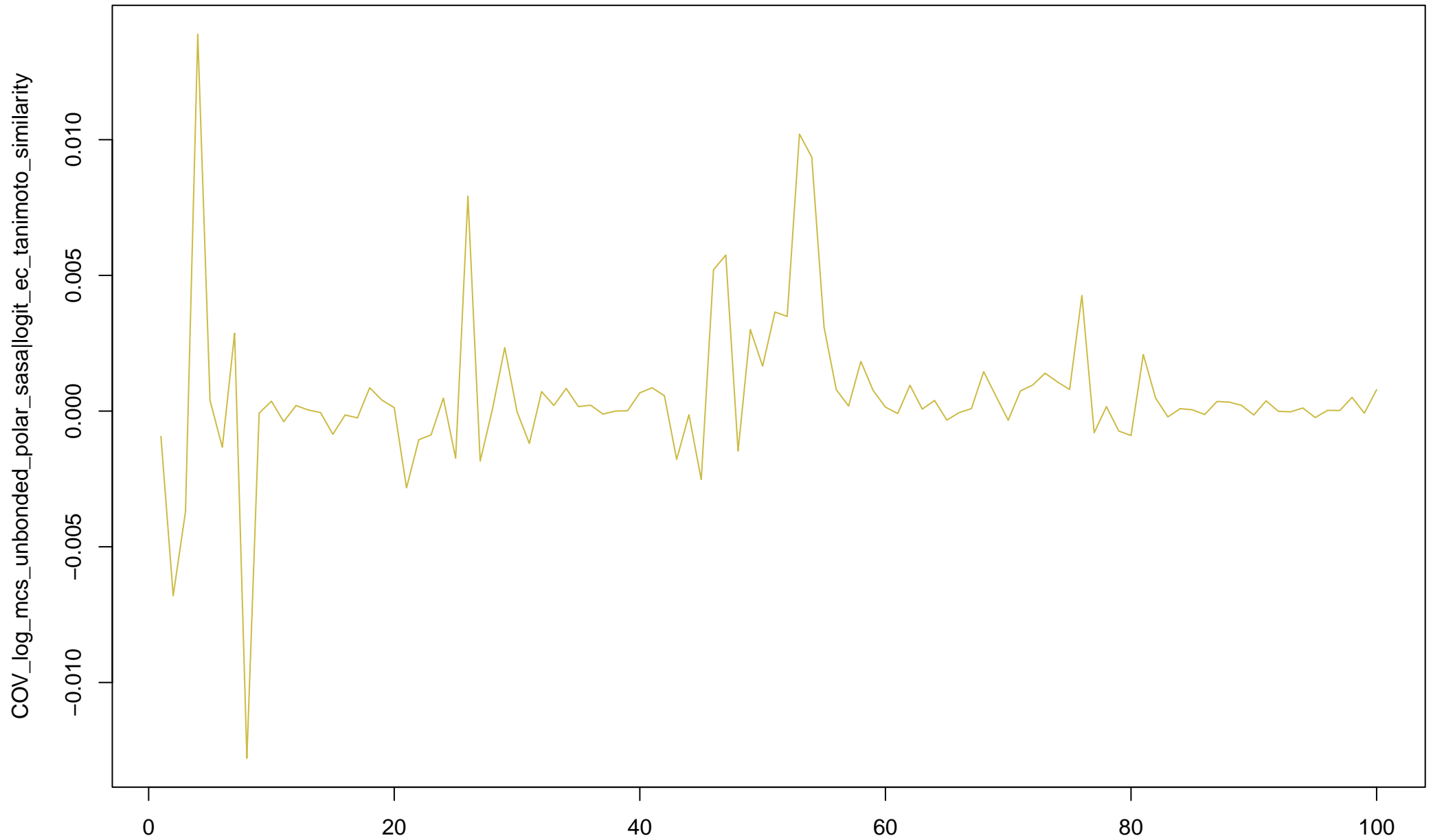
COV_log_RMSD|docked_NumRotatableBonds
ESS = 51.7 | BMK = 0.252 | MCSE(6.27) = 15.3 | stat: TRUE | burn: 100



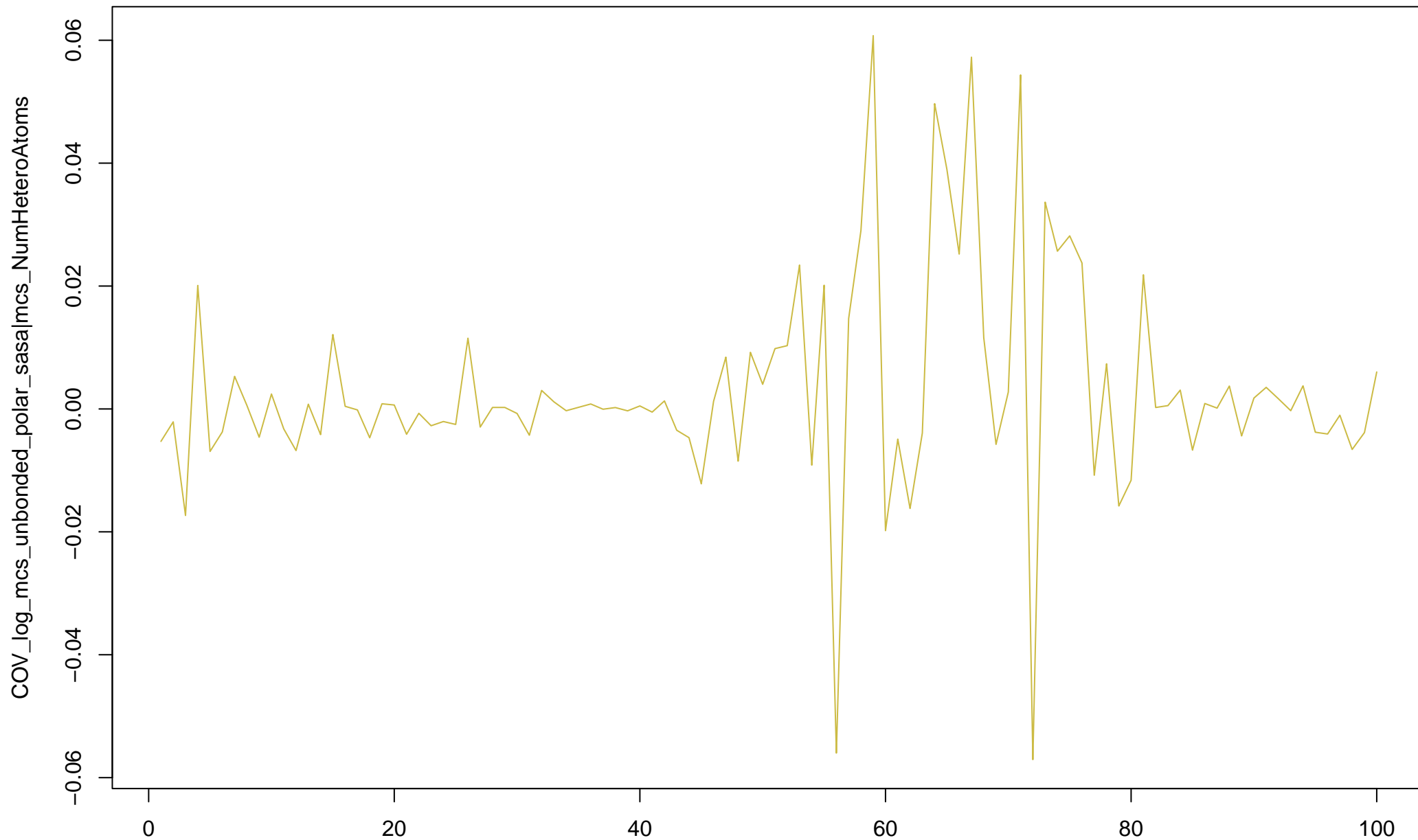
COV_log_RMSD|mcs_NOCount
ESS = 40.7 | BMK = 0.271 | MCSE(6.27) = 19.8 | stat: TRUE | burn: 70



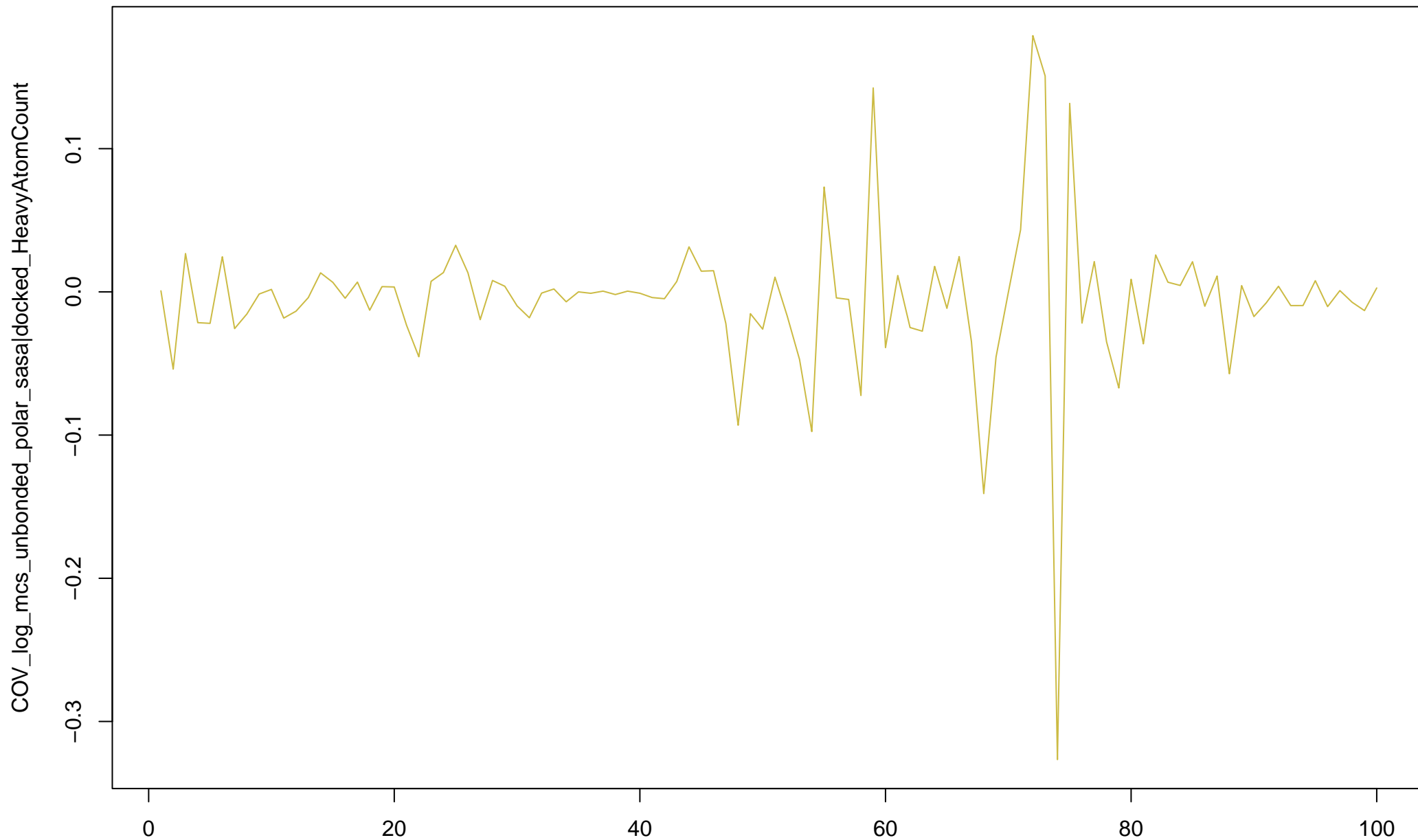
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 100 | BMK = 0.409 | MCSE(6.27) = 11.8 | stat: TRUE | burn: 80



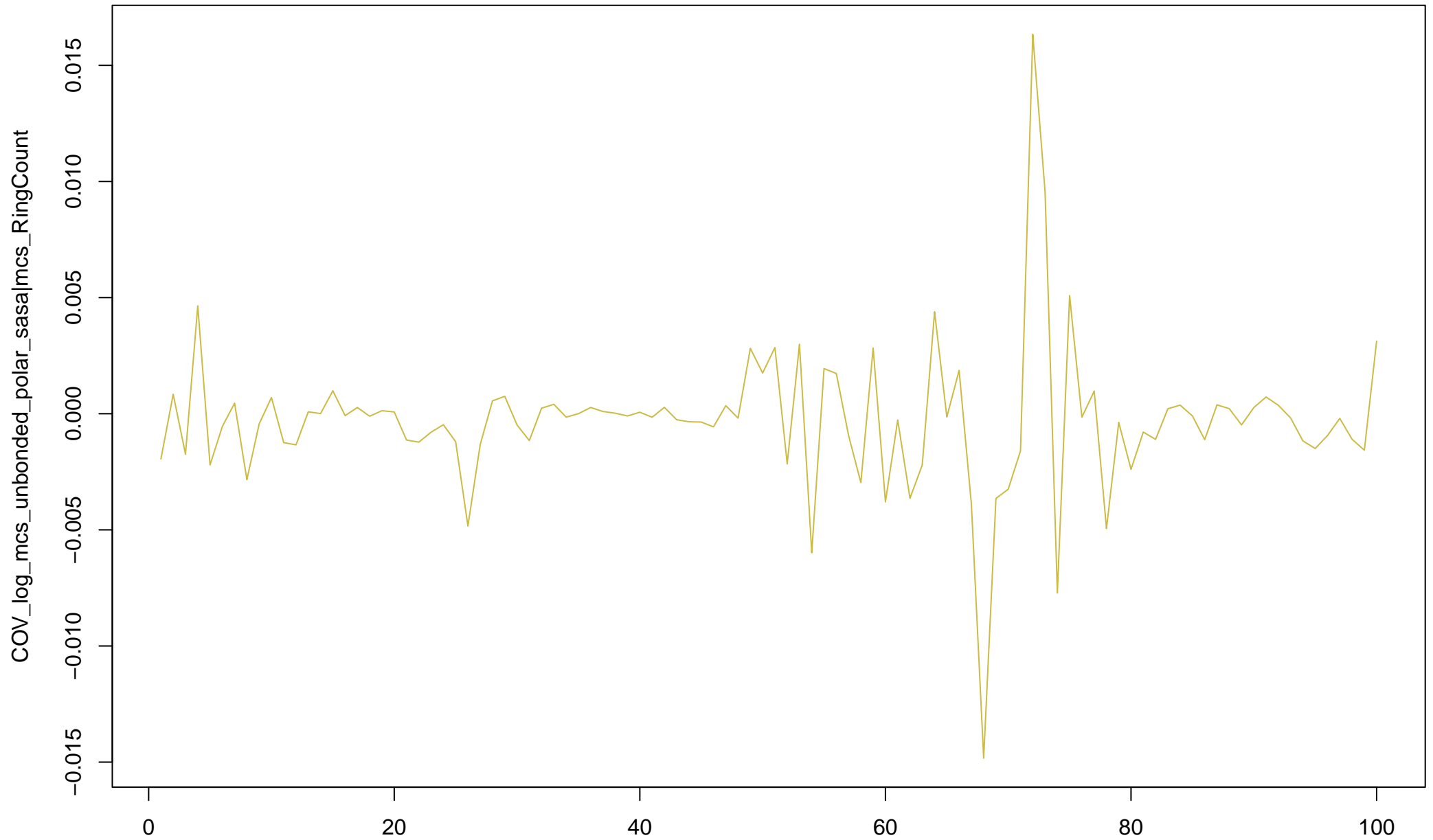
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 100 | BMK = 0.487 | MCSE(6.27) = 10.6 | stat: FALSE | burn: 80



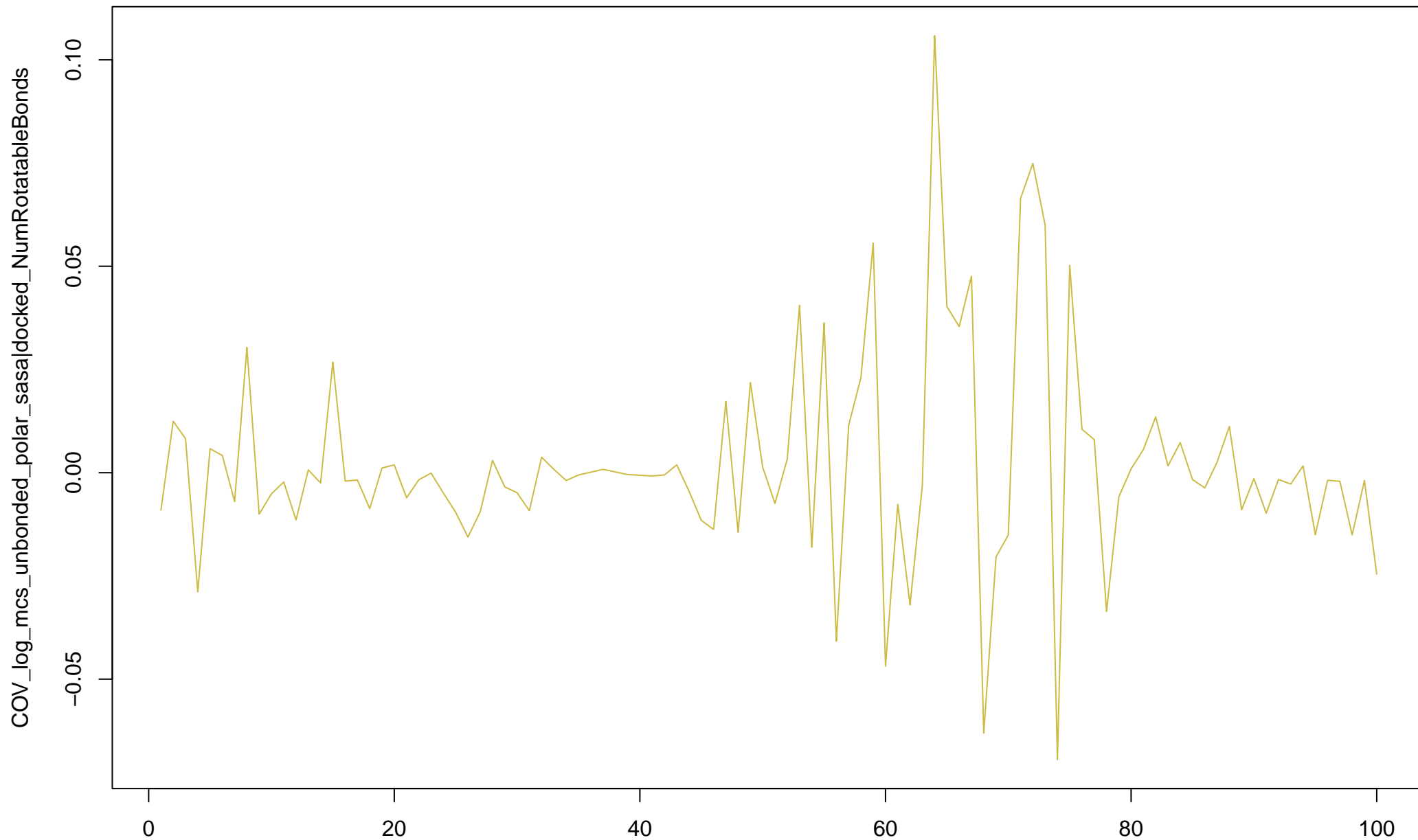
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 100 | BMK = 0.323 | MCSE(6.27) = 7.11 | stat: TRUE | burn: 100



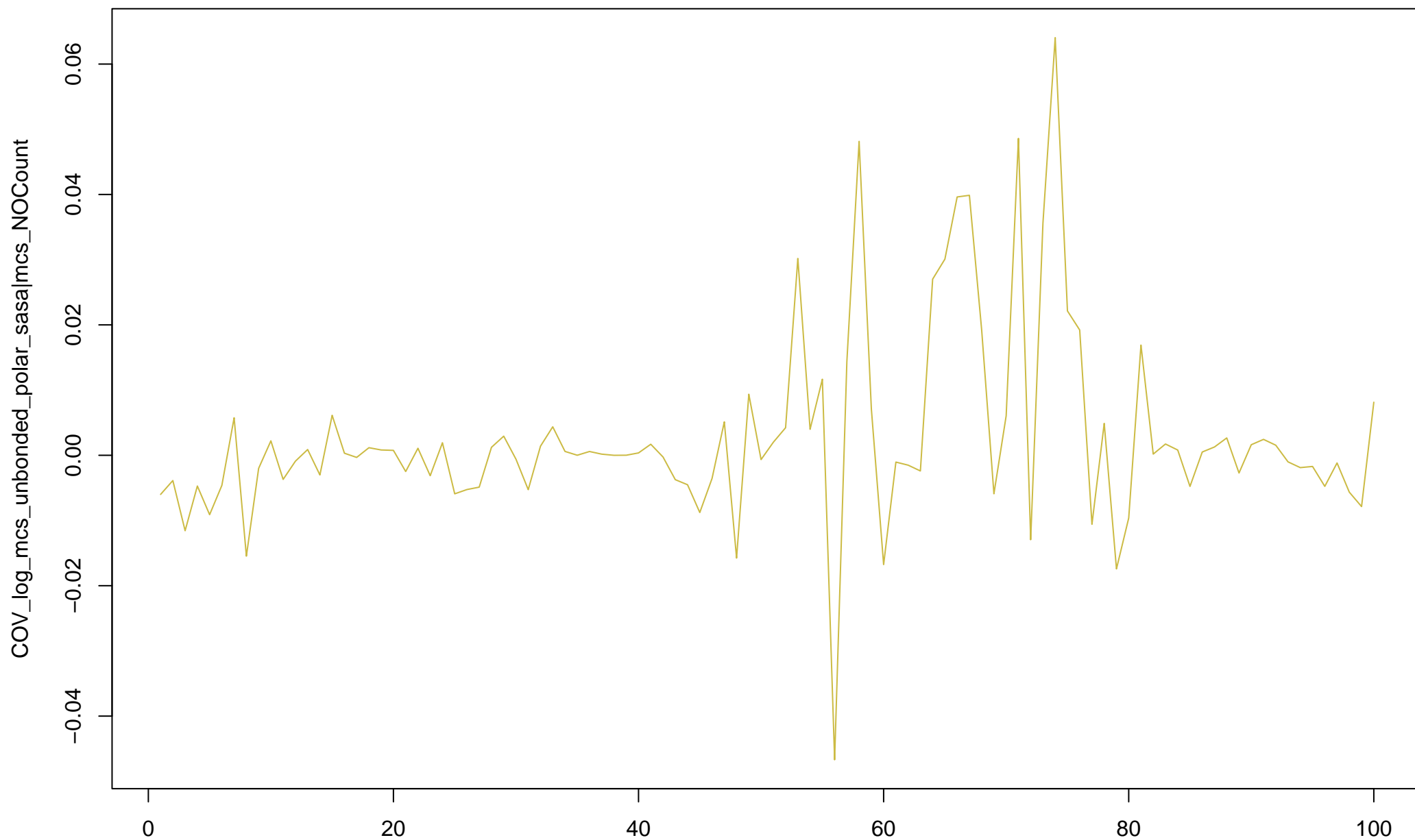
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 100 | BMK = 0.373 | MCSE(6.27) = 10.9 | stat: TRUE | burn: 80



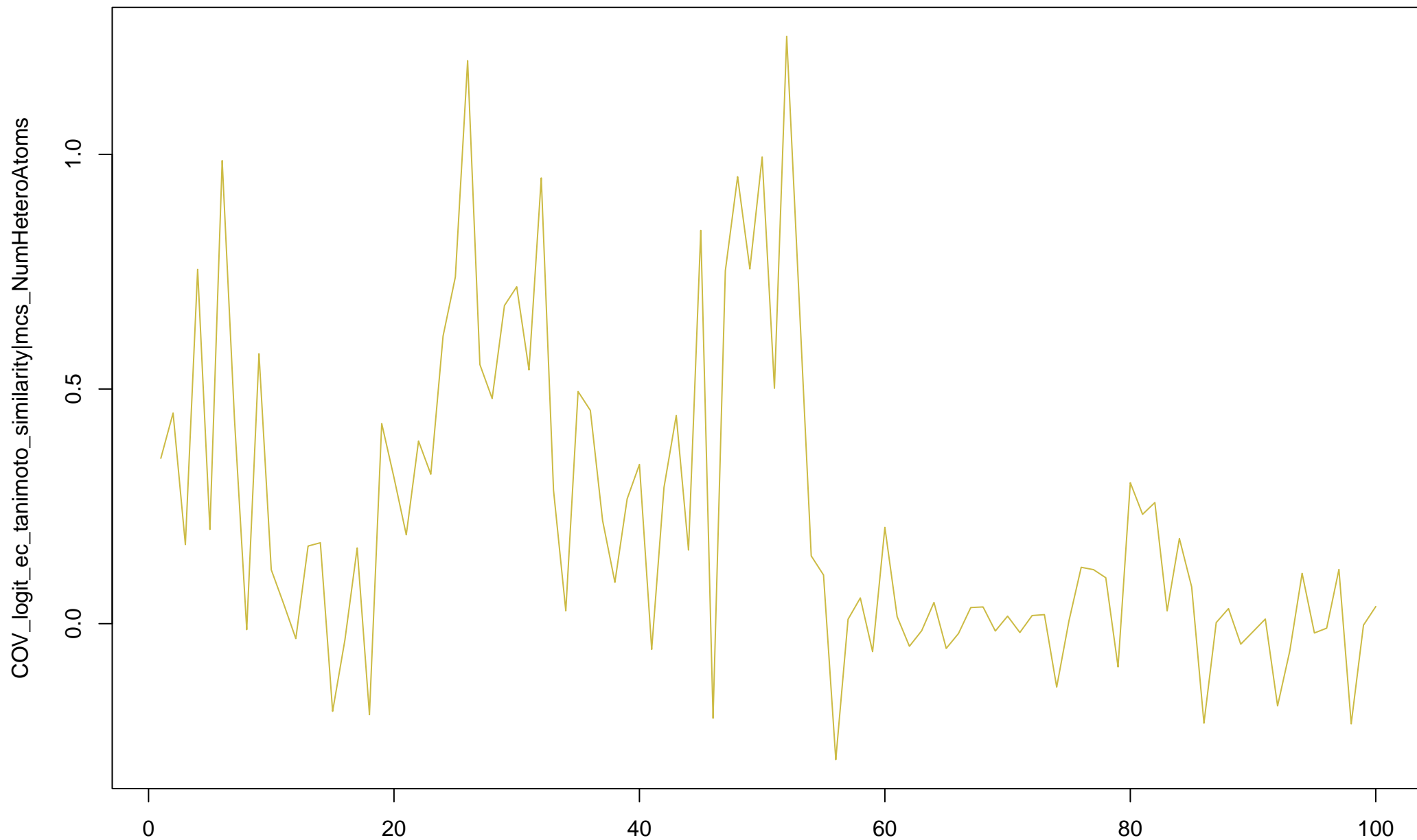
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 30.7 | BMK = 0.442 | MCSE(6.27) = 10.6 | stat: TRUE | burn: 80



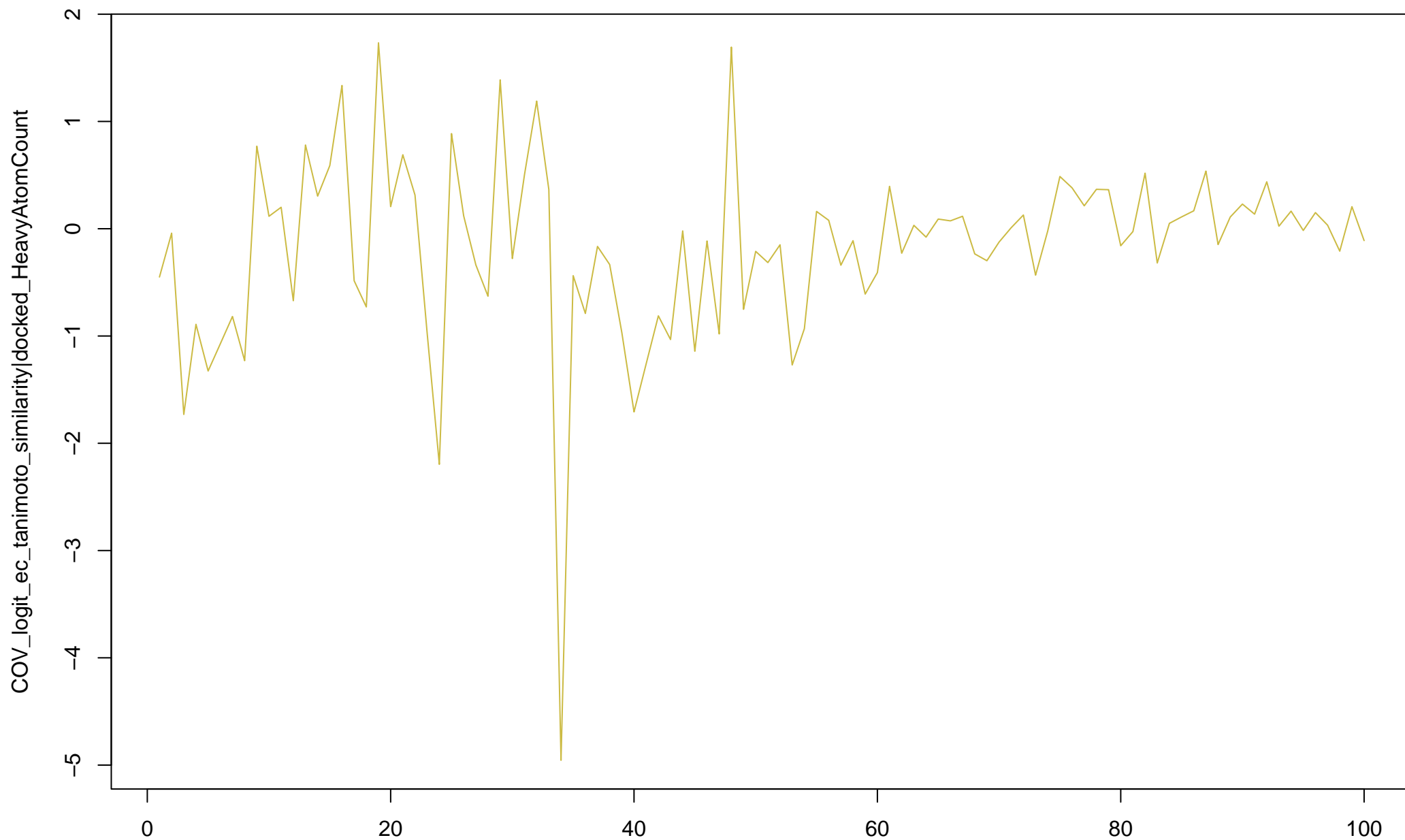
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 54.3 | BMK = 0.461 | MCSE(6.27) = 16.9 | stat: FALSE | burn: 100



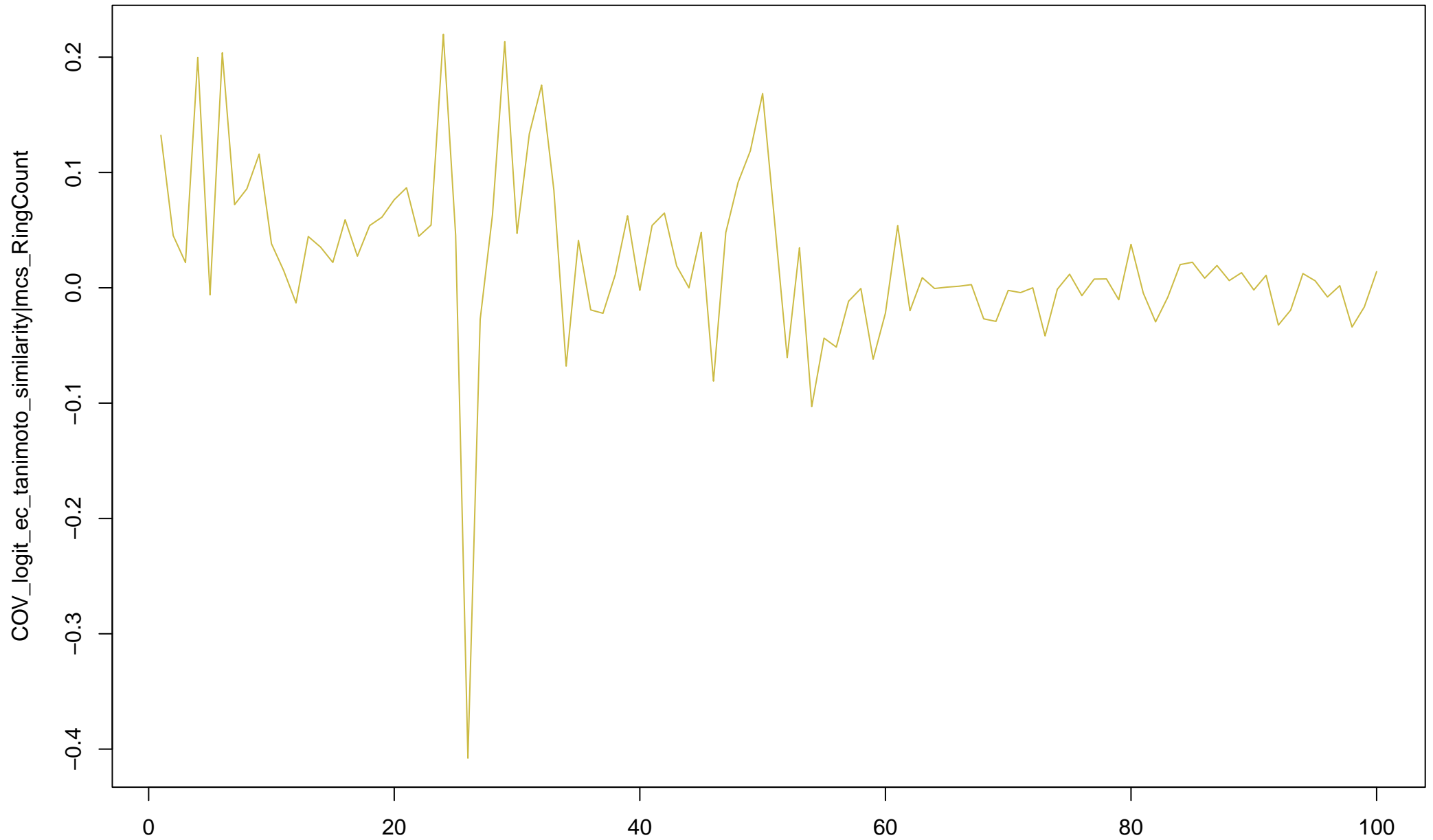
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 15.4 | BMK = 0.504 | MCSE(6.27) = 33.7 | stat: FALSE | burn: 60



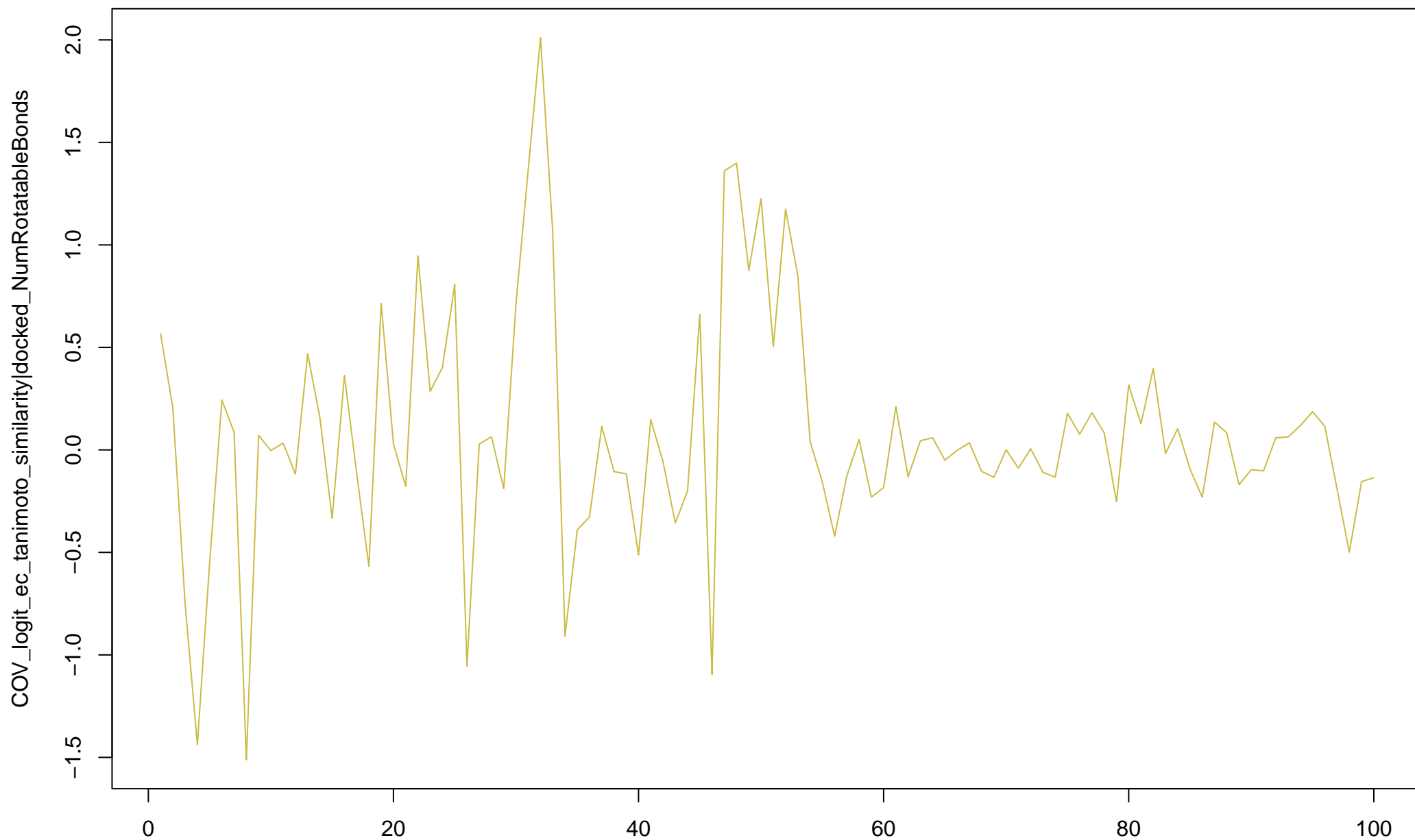
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 45.1 | BMK = 0.497 | MCSE(6.27) = 14 | stat: TRUE | burn: 0



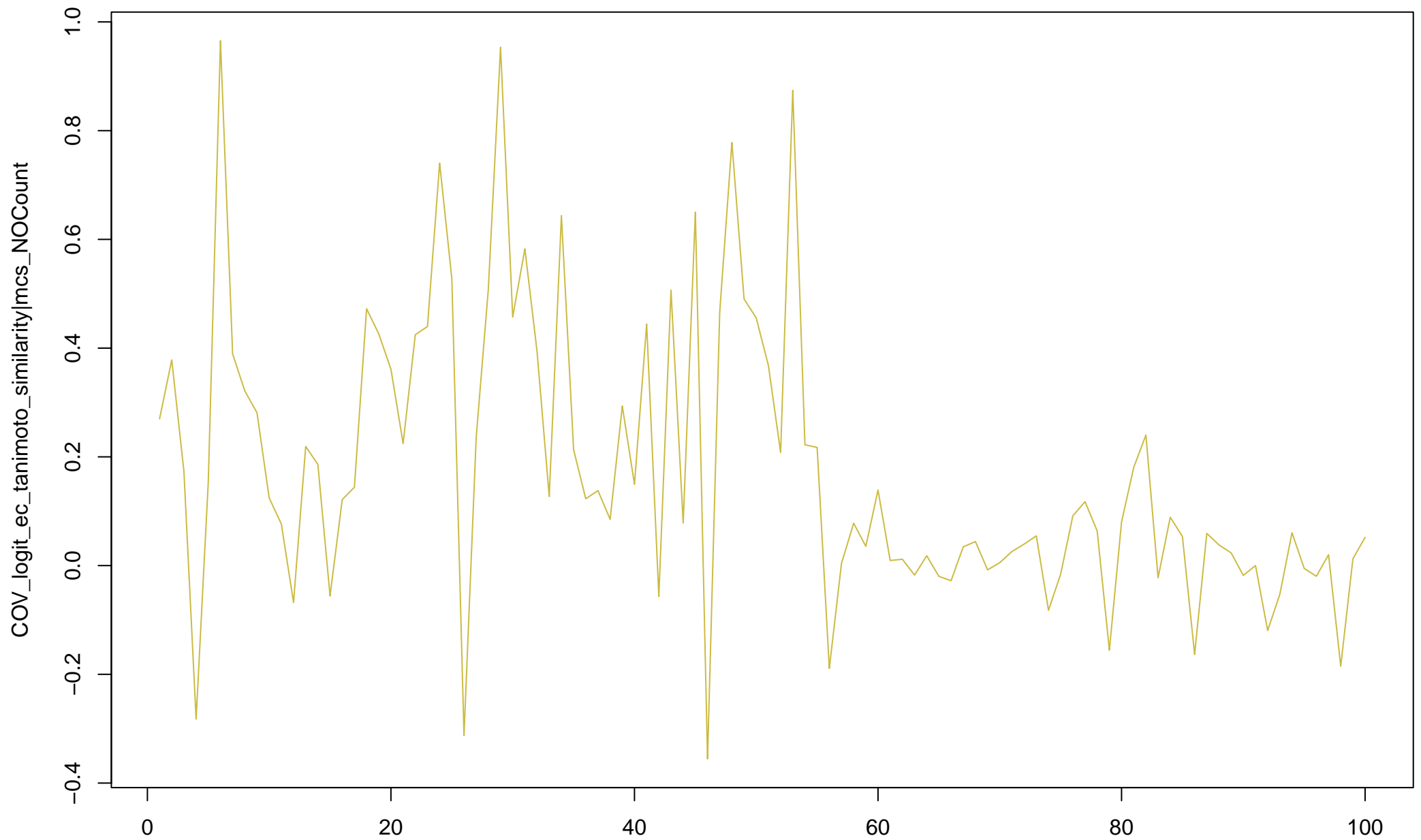
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 60.3 | BMK = 0.549 | MCSE(6.27) = 14.6 | stat: FALSE | burn: 60



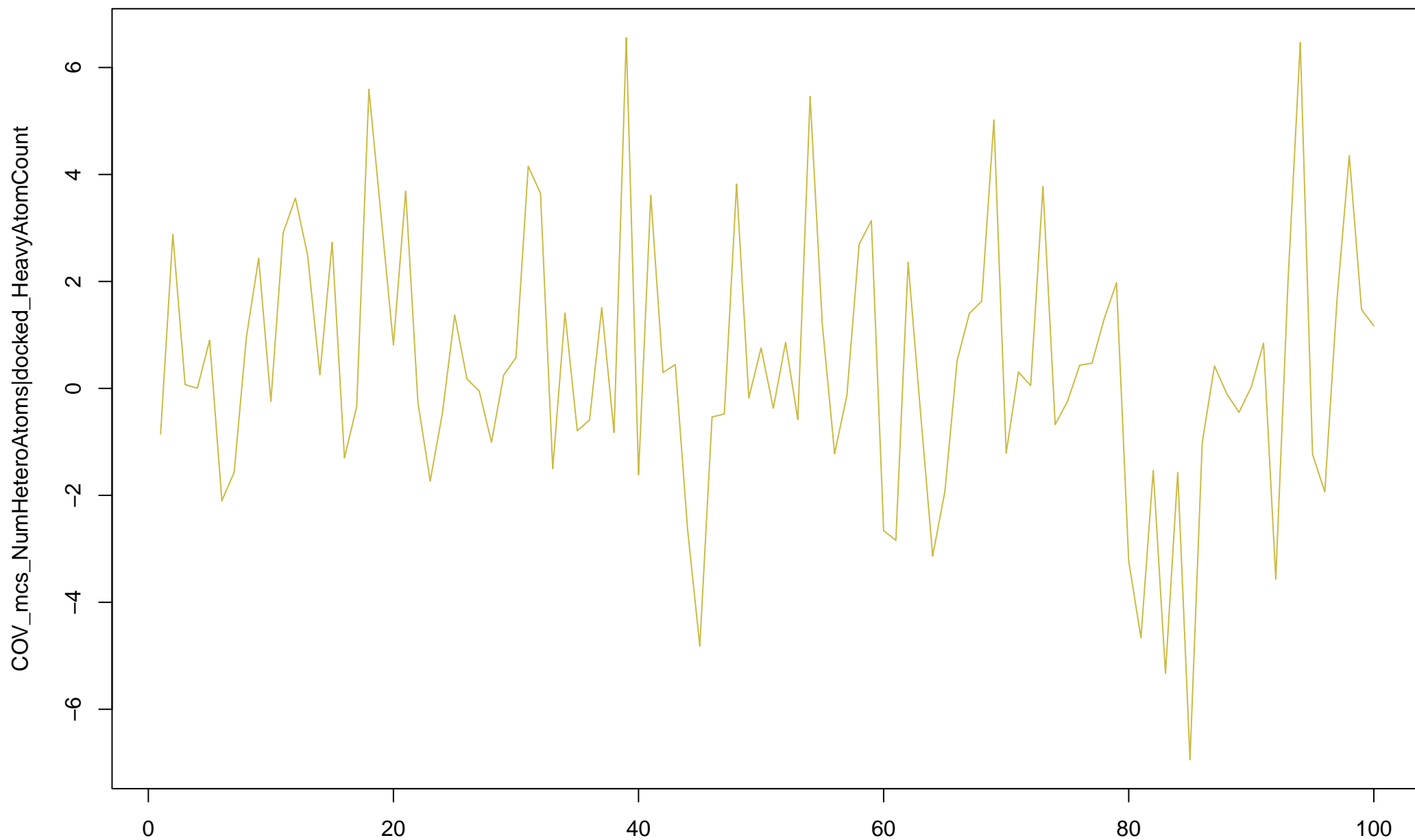
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 50.2 | BMK = 0.436 | MCSE(6.27) = 17.4 | stat: TRUE | burn: 60



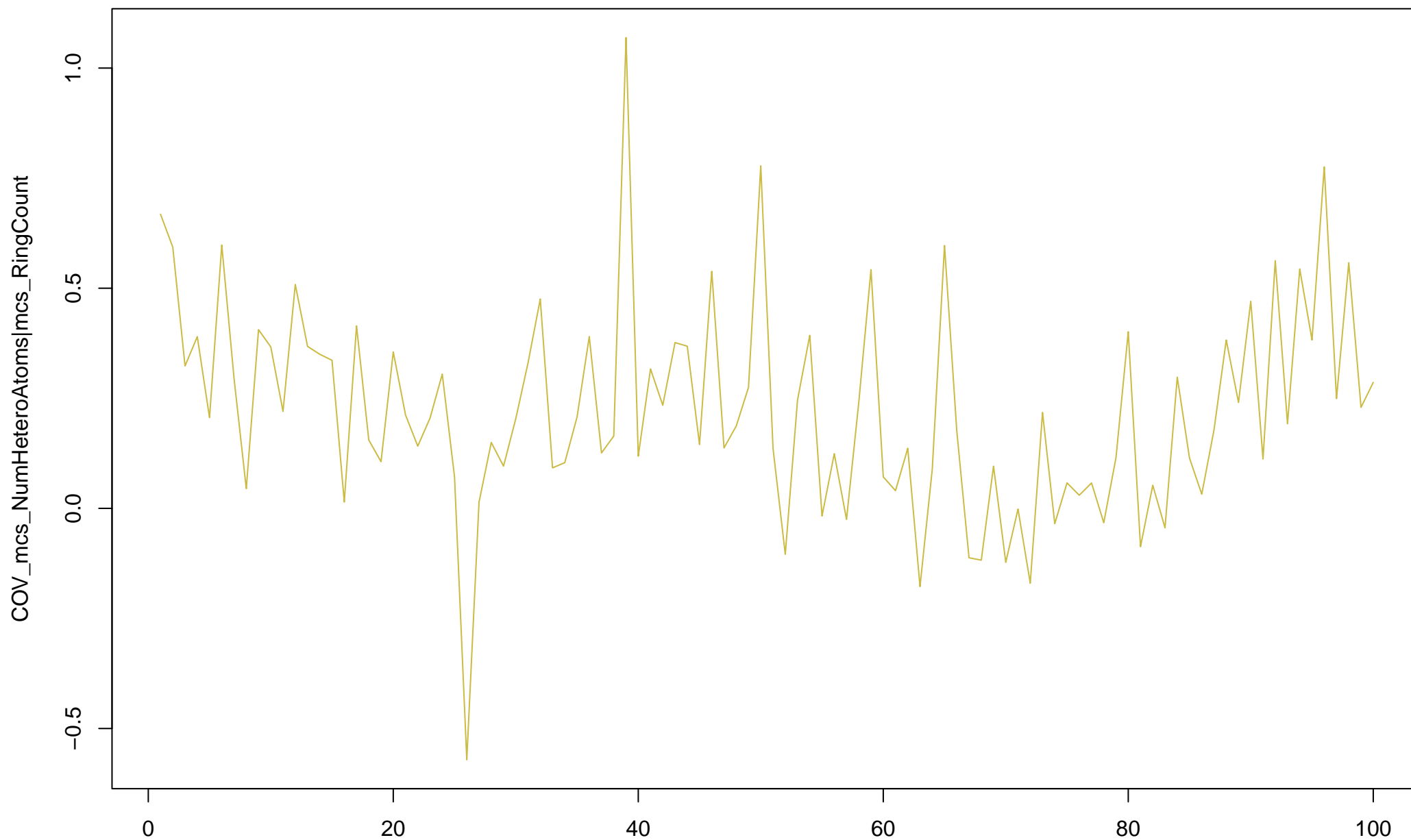
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 12.1 | BMK = 0.568 | MCSE(6.27) = 19.5 | stat: TRUE | burn: 70



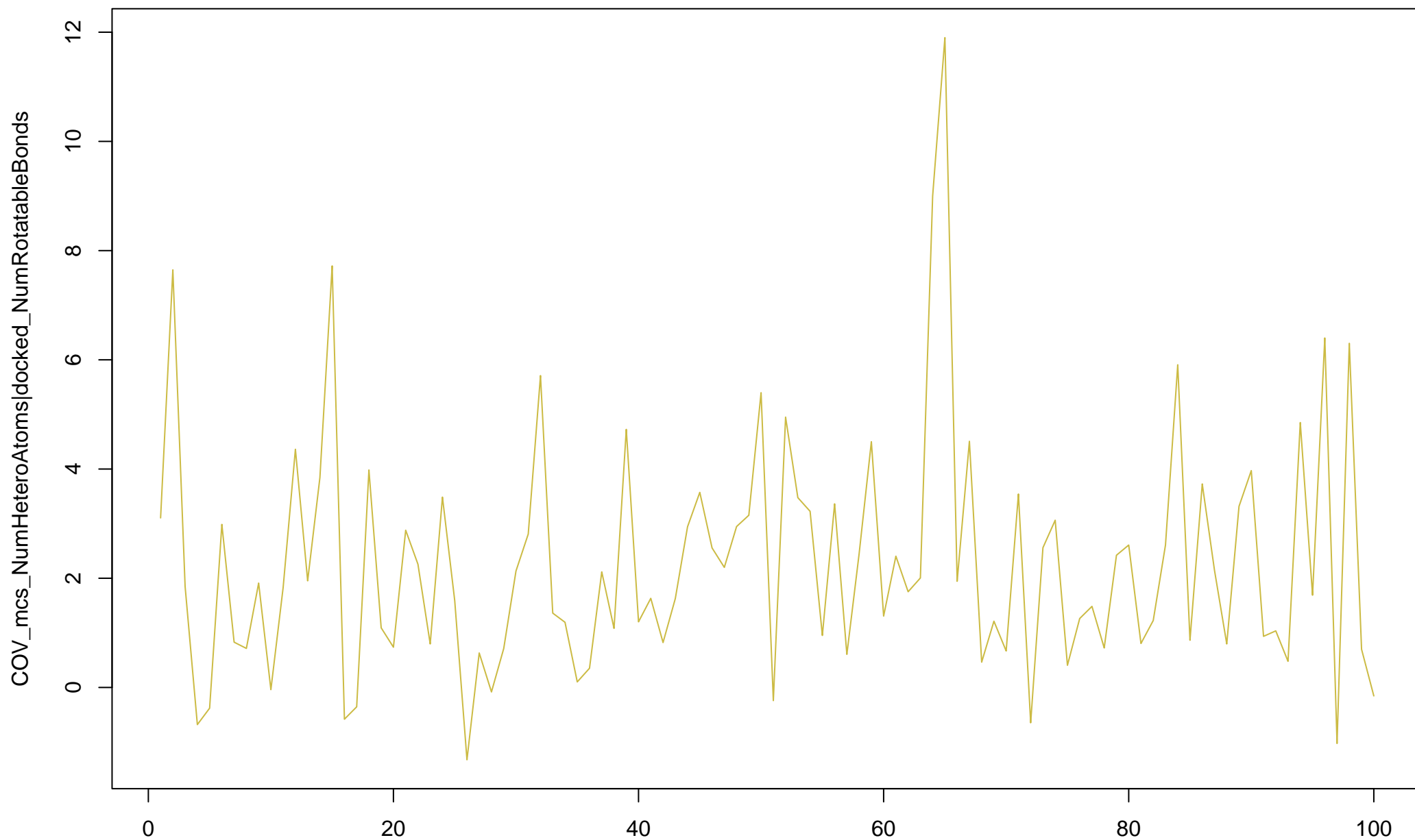
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 72.6 | BMK = 0.139 | MCSE(6.27) = 13.5 | stat: TRUE | burn: 0



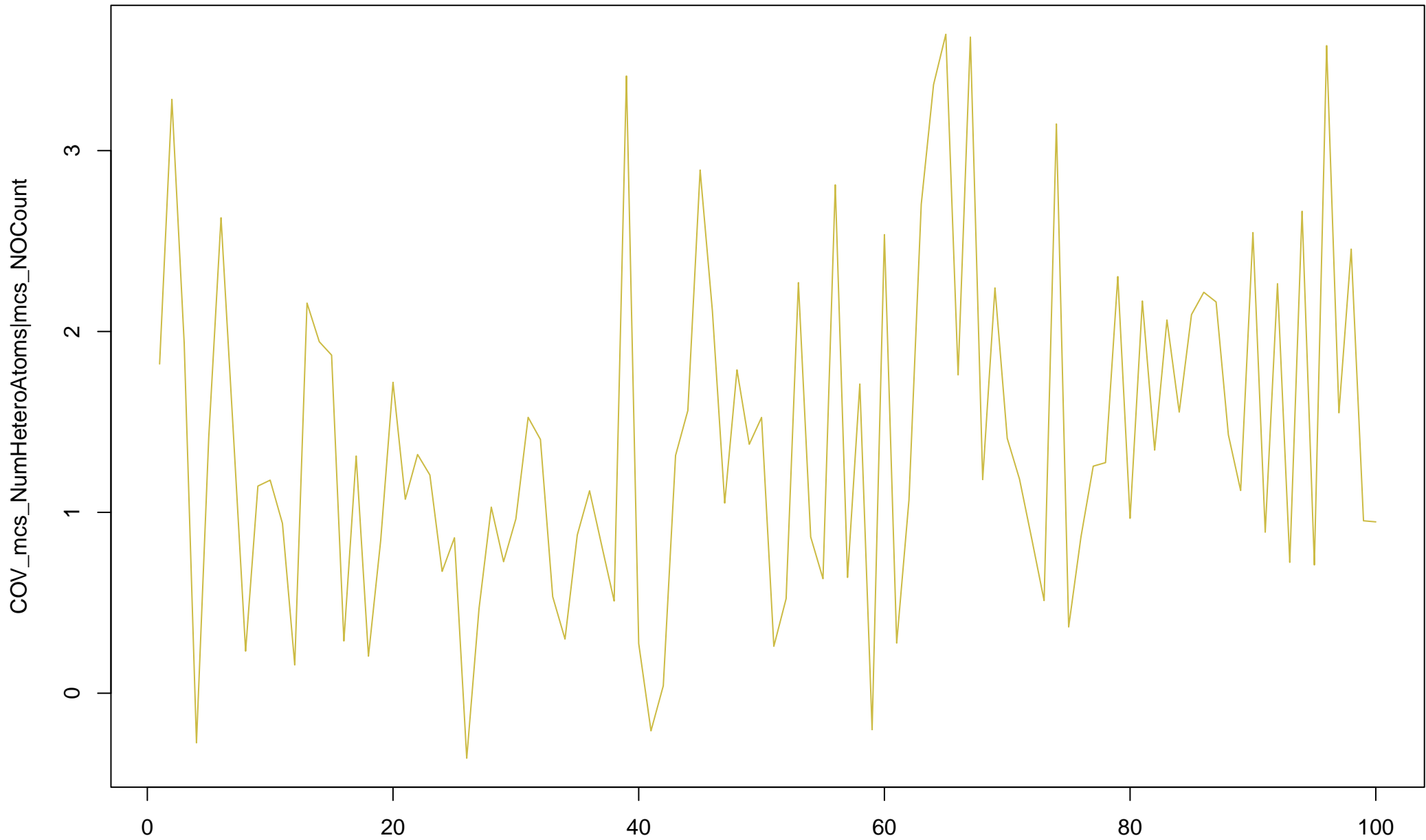
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 38.8 | BMK = 0.305 | MCSE(6.27) = 14.2 | stat: FALSE | burn: 0



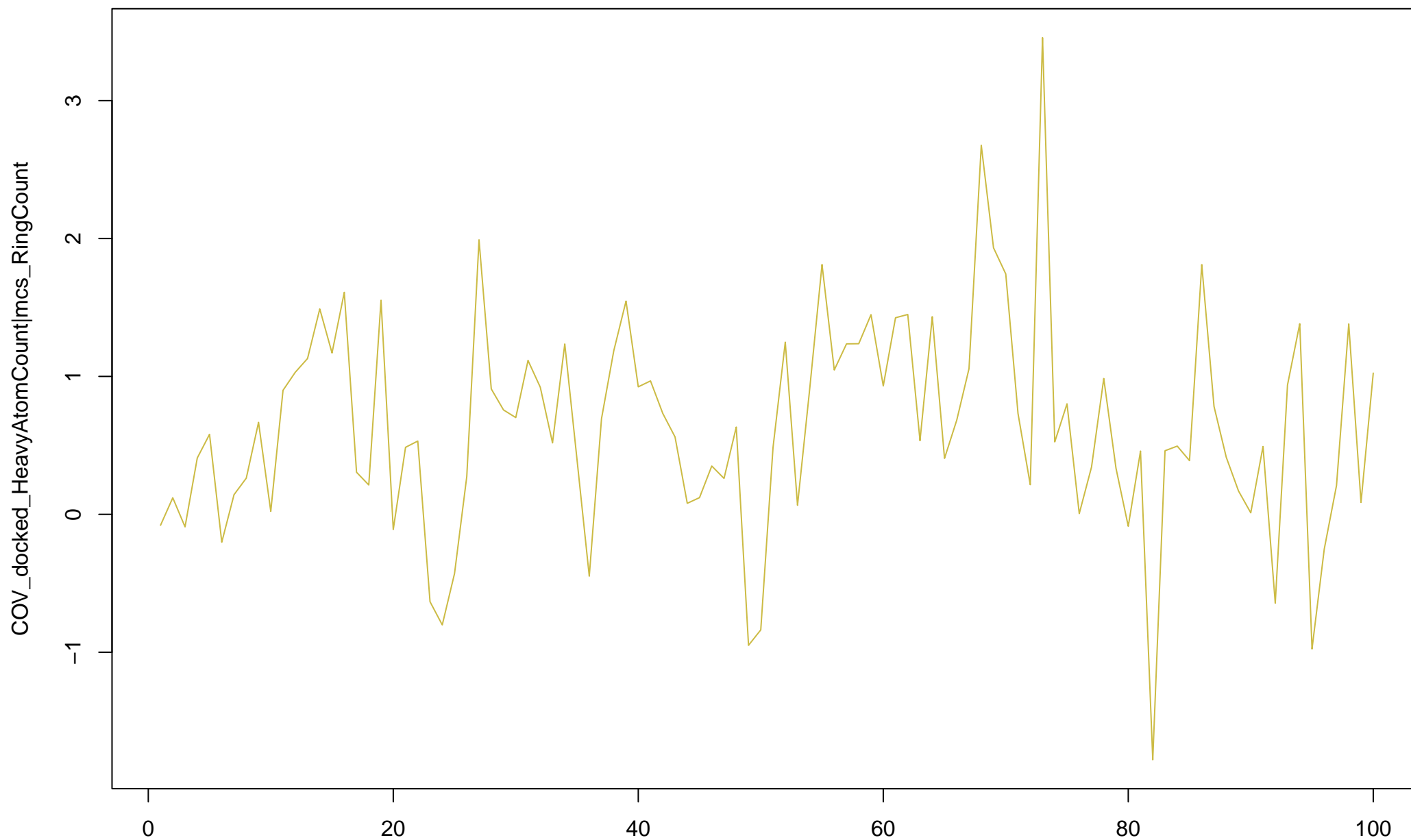
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 100 | BMK = 0.116 | MCSE(6.27) = 11.2 | stat: TRUE | burn: 0



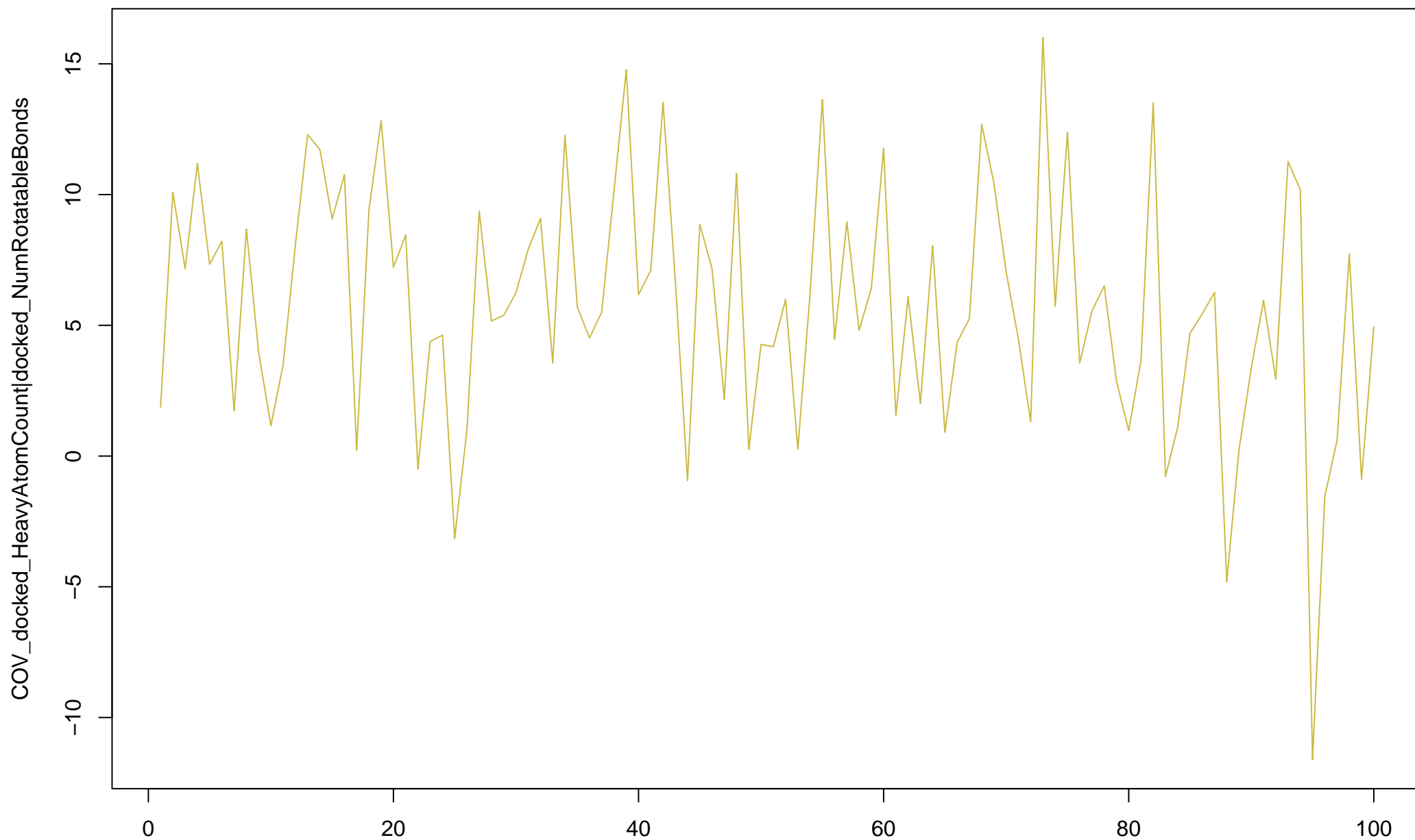
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 38.1 | BMK = 0.173 | MCSE(6.27) = 13.7 | stat: TRUE | burn: 80



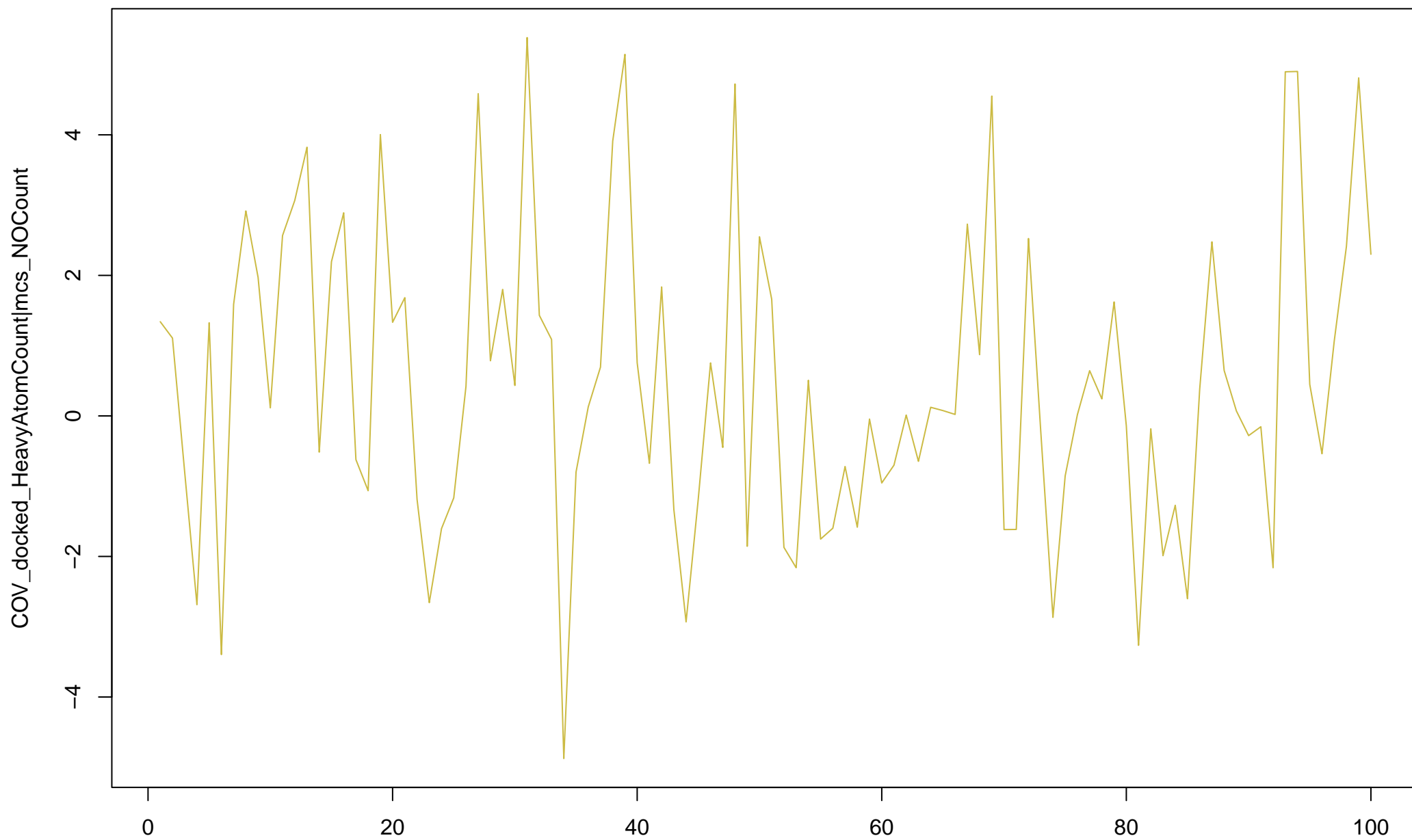
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 56 | BMK = 0.172 | MCSE(6.27) = 20.2 | stat: FALSE | burn: 100



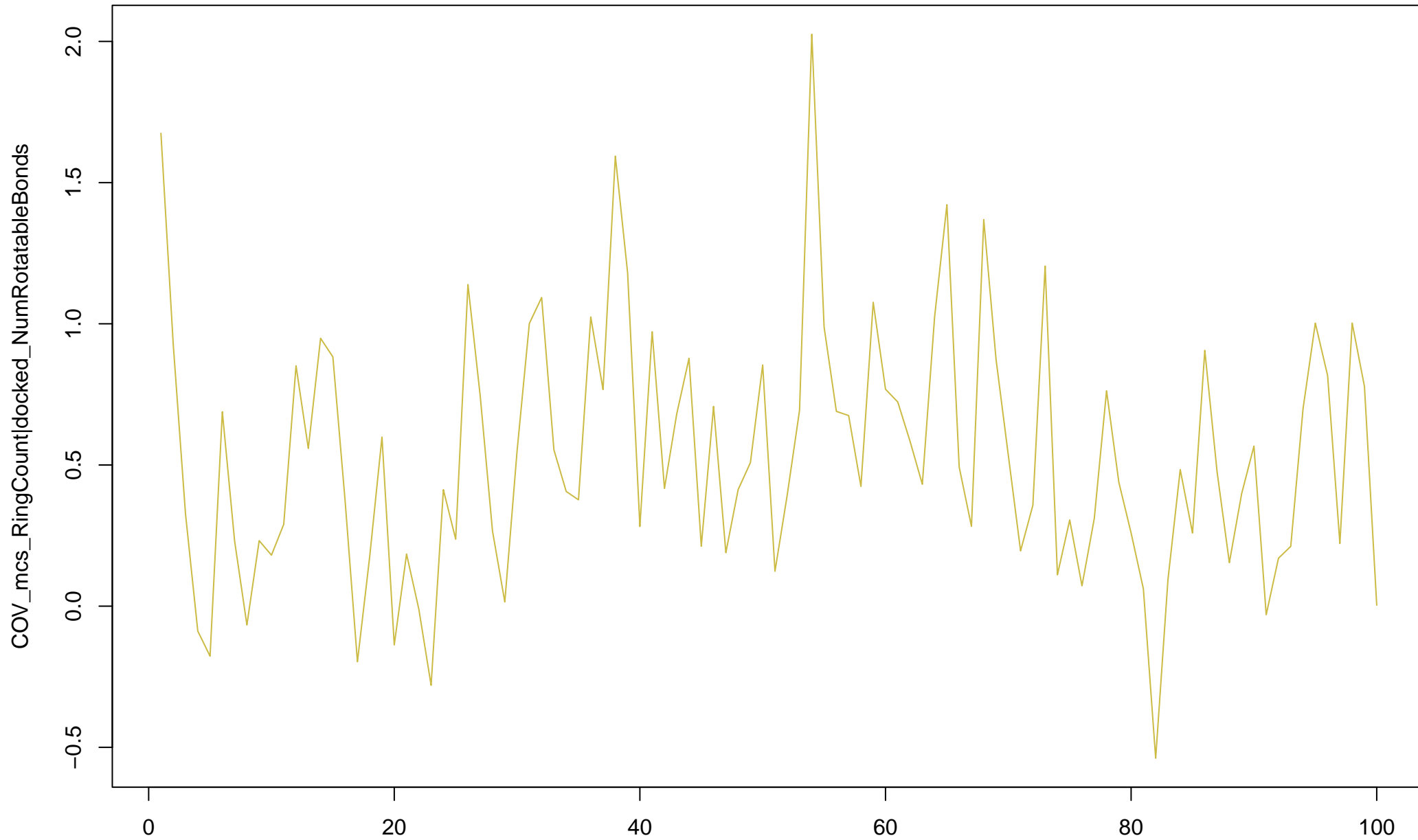
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 100 | BMK = 0.168 | MCSE(6.27) = 11.7 | stat: TRUE | burn: 0



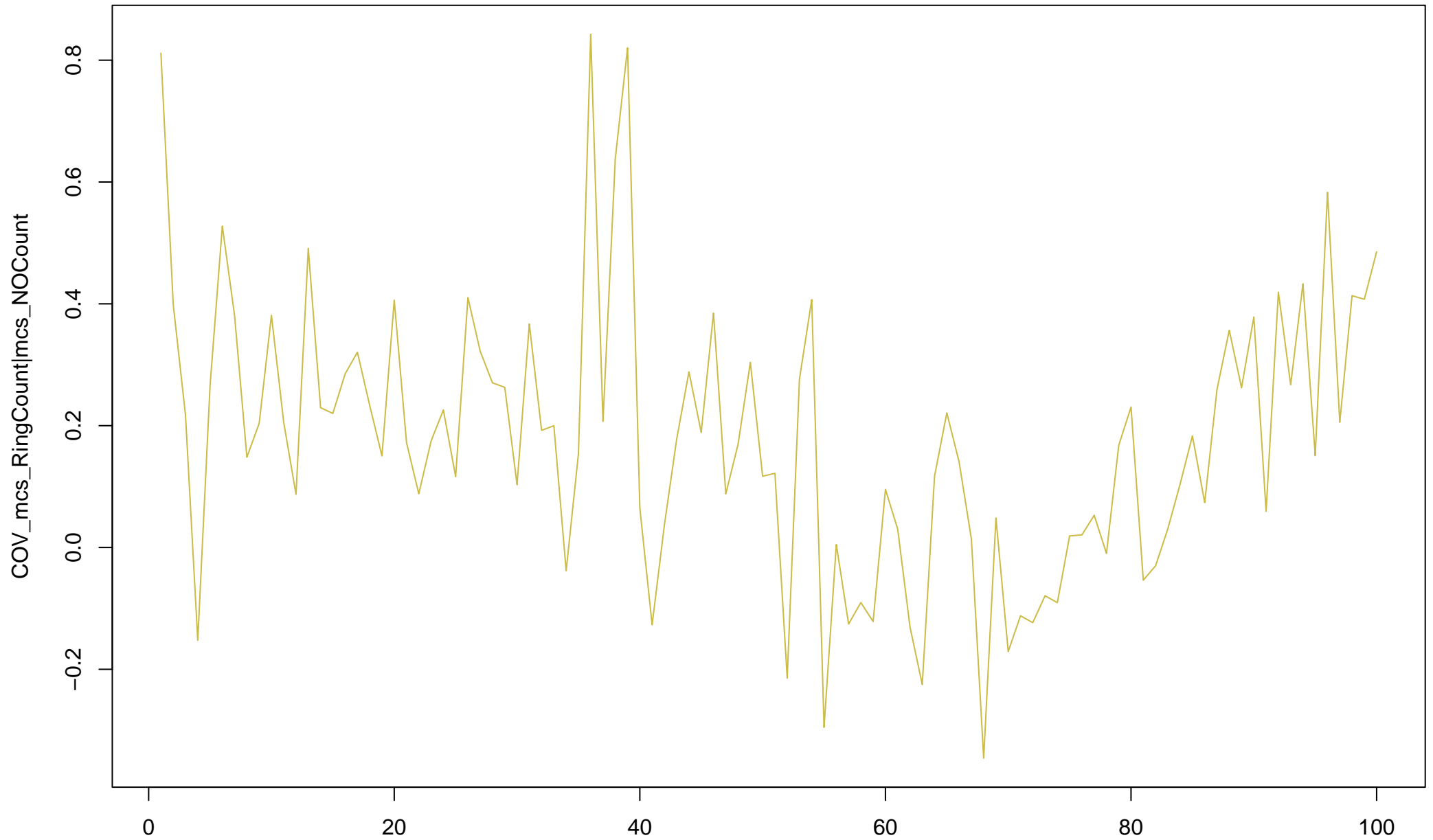
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 63.4 | BMK = 0.177 | MCSE(6.27) = 14 | stat: TRUE | burn: 0



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 51.5 | BMK = 0.0967 | MCSE(6.27) = 15.6 | stat: TRUE | burn: 0



COV_mcs_RingCount|mcs_NOCount
ESS = 18.5 | BMK = 0.313 | MCSE(6.27) = 19.6 | stat: TRUE | burn: 0



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 66.2 | BMK = 0.0287 | MCSE(6.27) = 13.6 | stat: TRUE | burn: 0

