

-- STATS maxD --

min ESS = 24.4931859576852

max BMK = 1

max MCSE = 21.8845744009598

all stationary: FALSE

burn: 120

-- STATS 2D --

min ESS = 18.3874466197058

max BMK = 0.615928508956002

max MCSE = 26.0283132129662

all stationary: FALSE

burn: 120

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.488156085651361

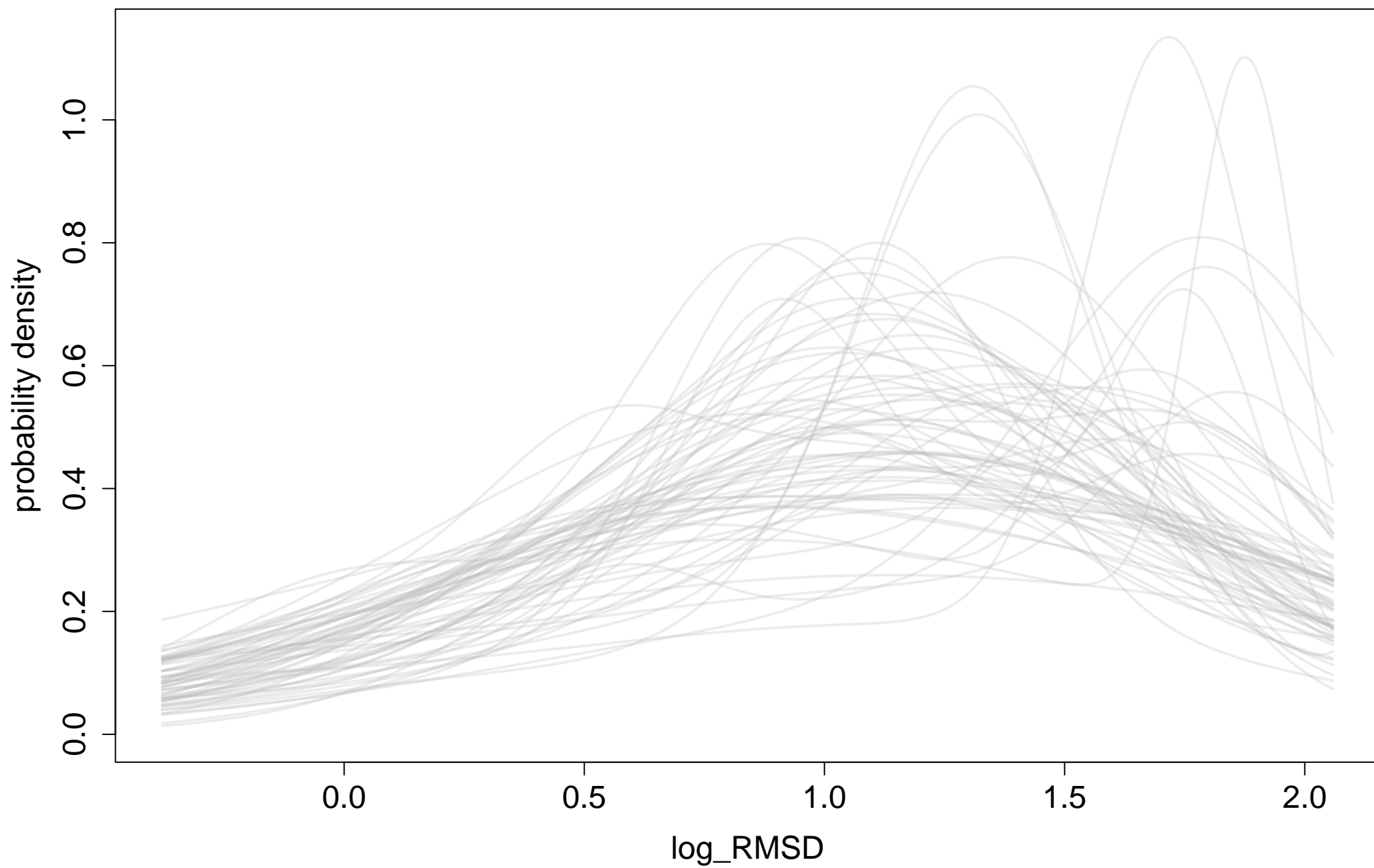
max MCSE = NaN

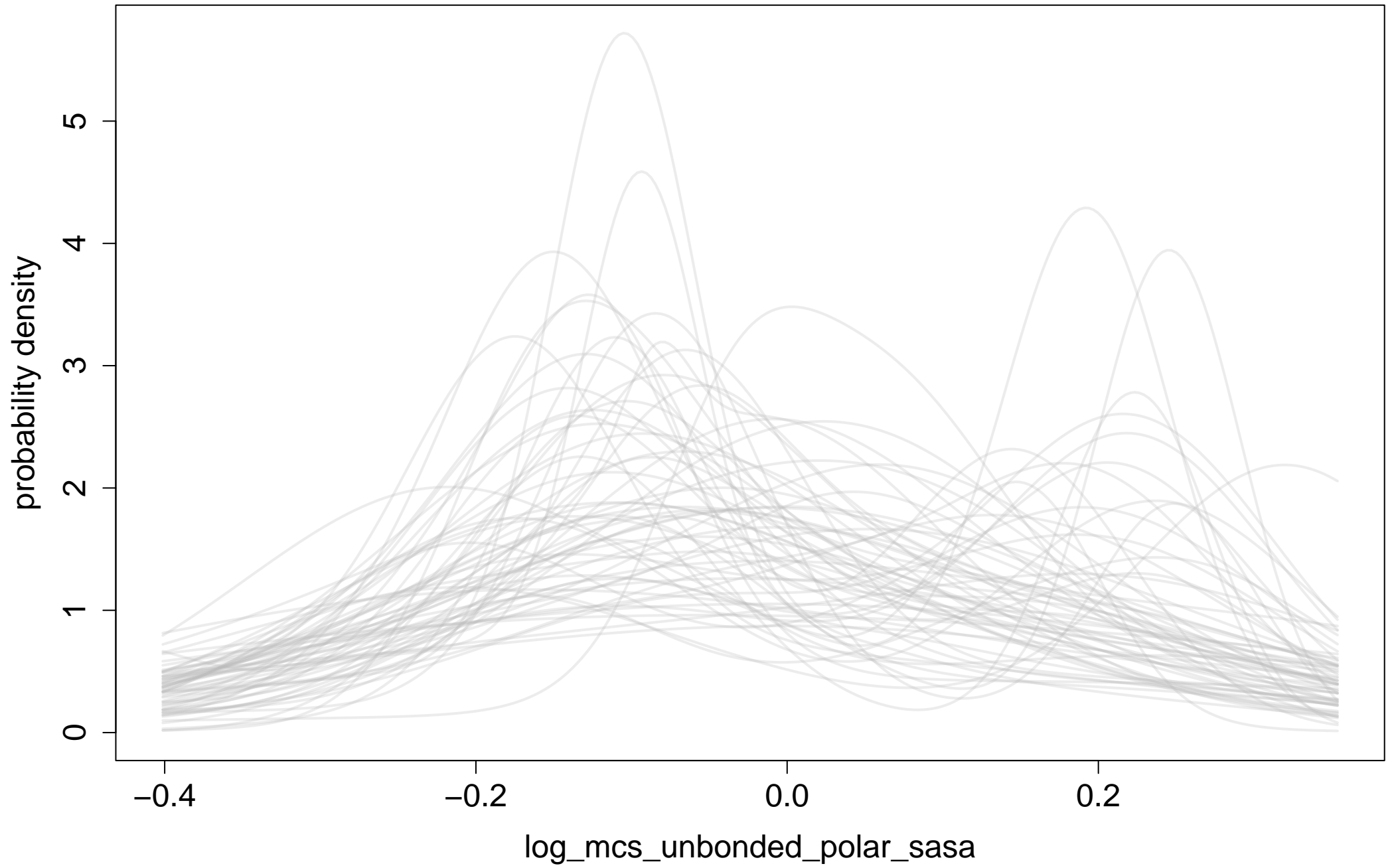
all stationary: FALSE

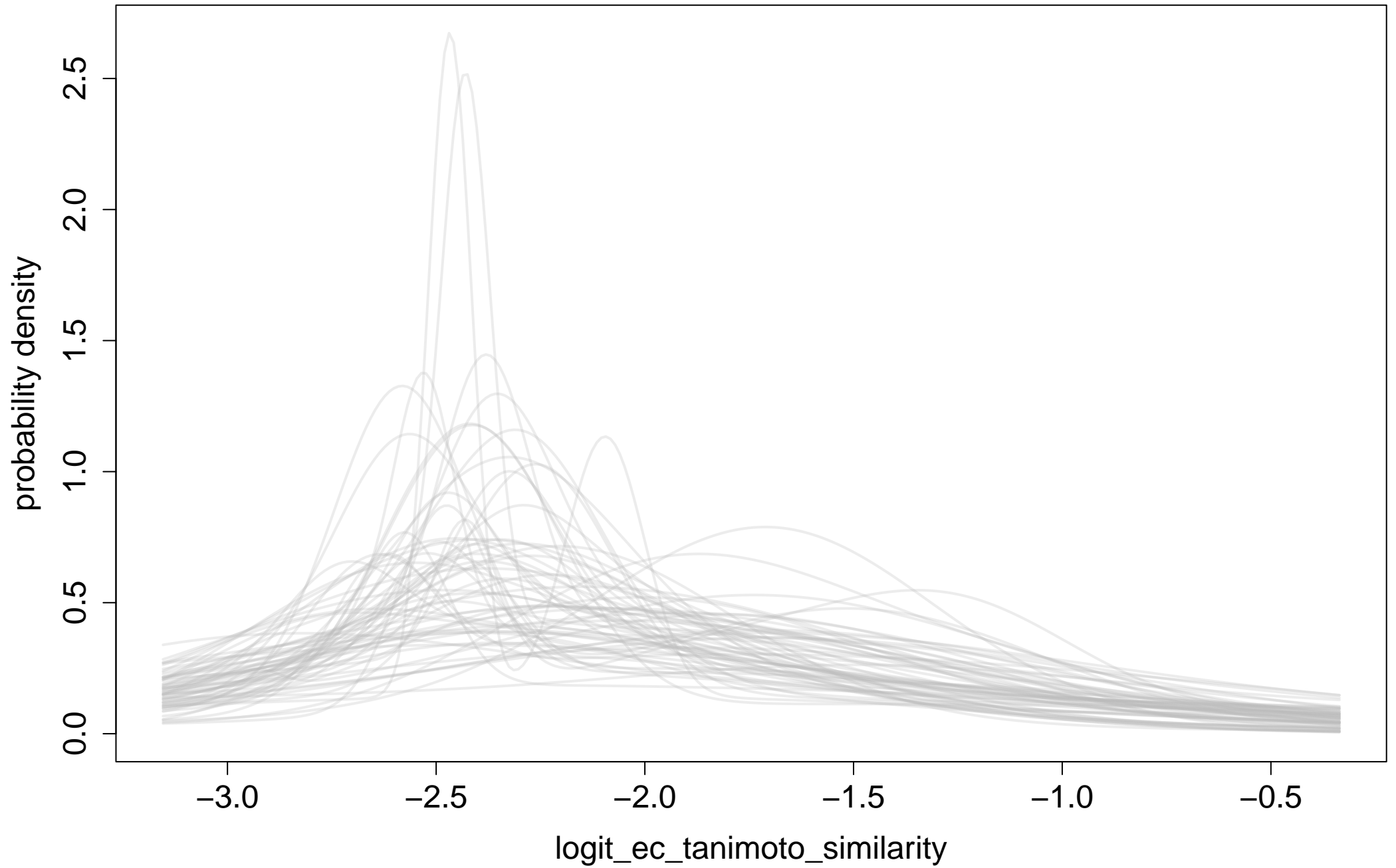
burn: 120

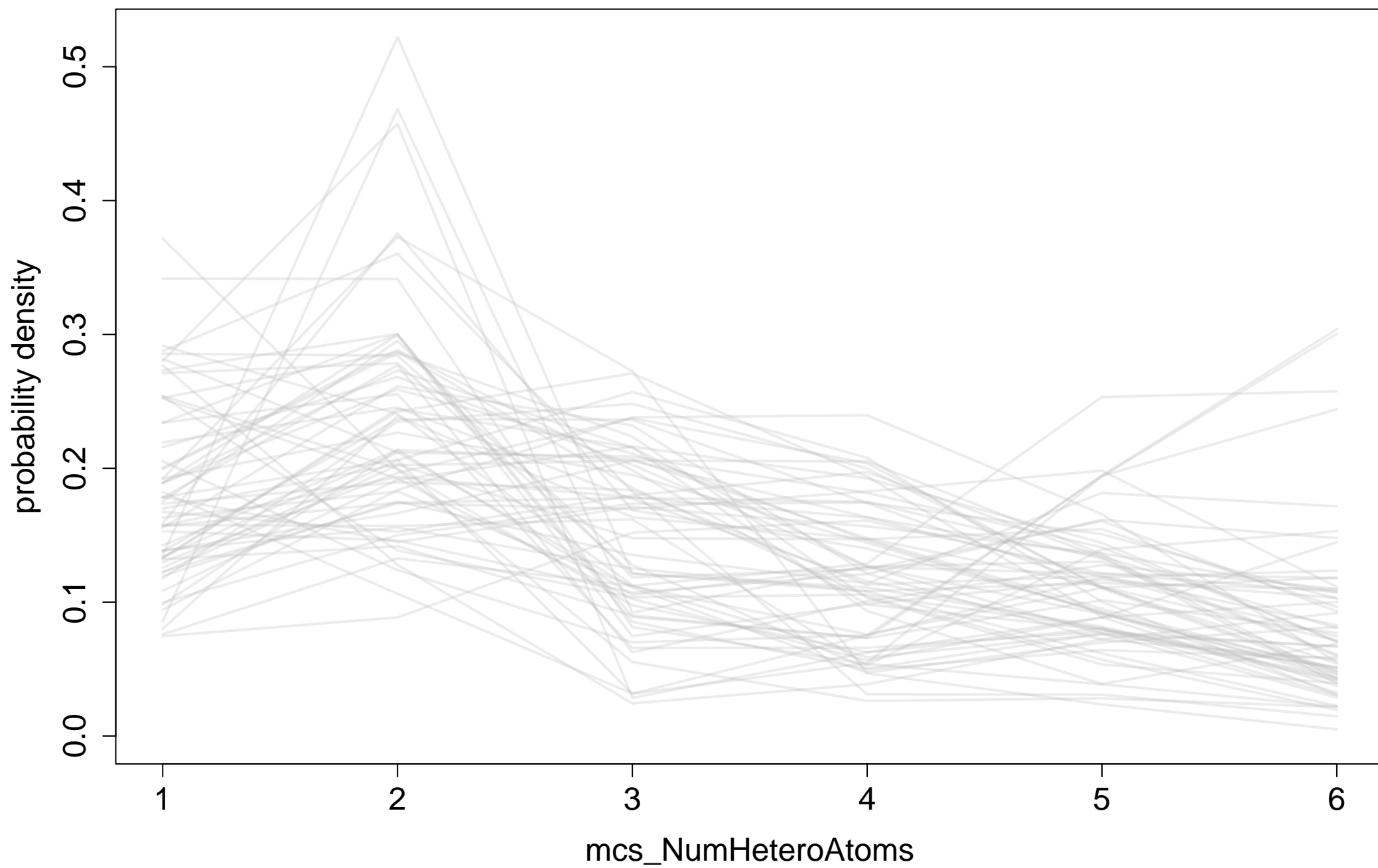
Occupied clusters: 3 of 4

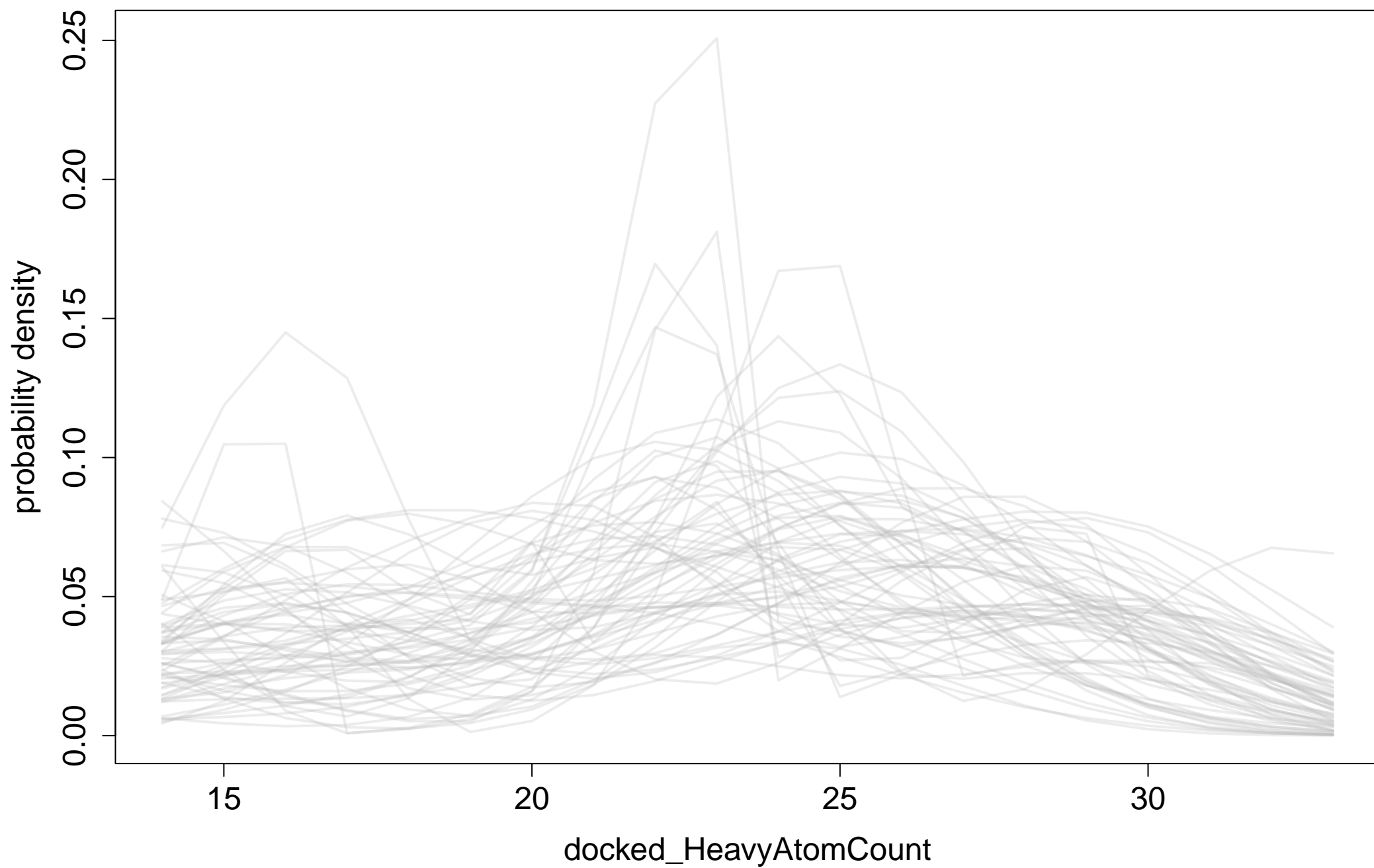
LL: -85.2 +- 4.89

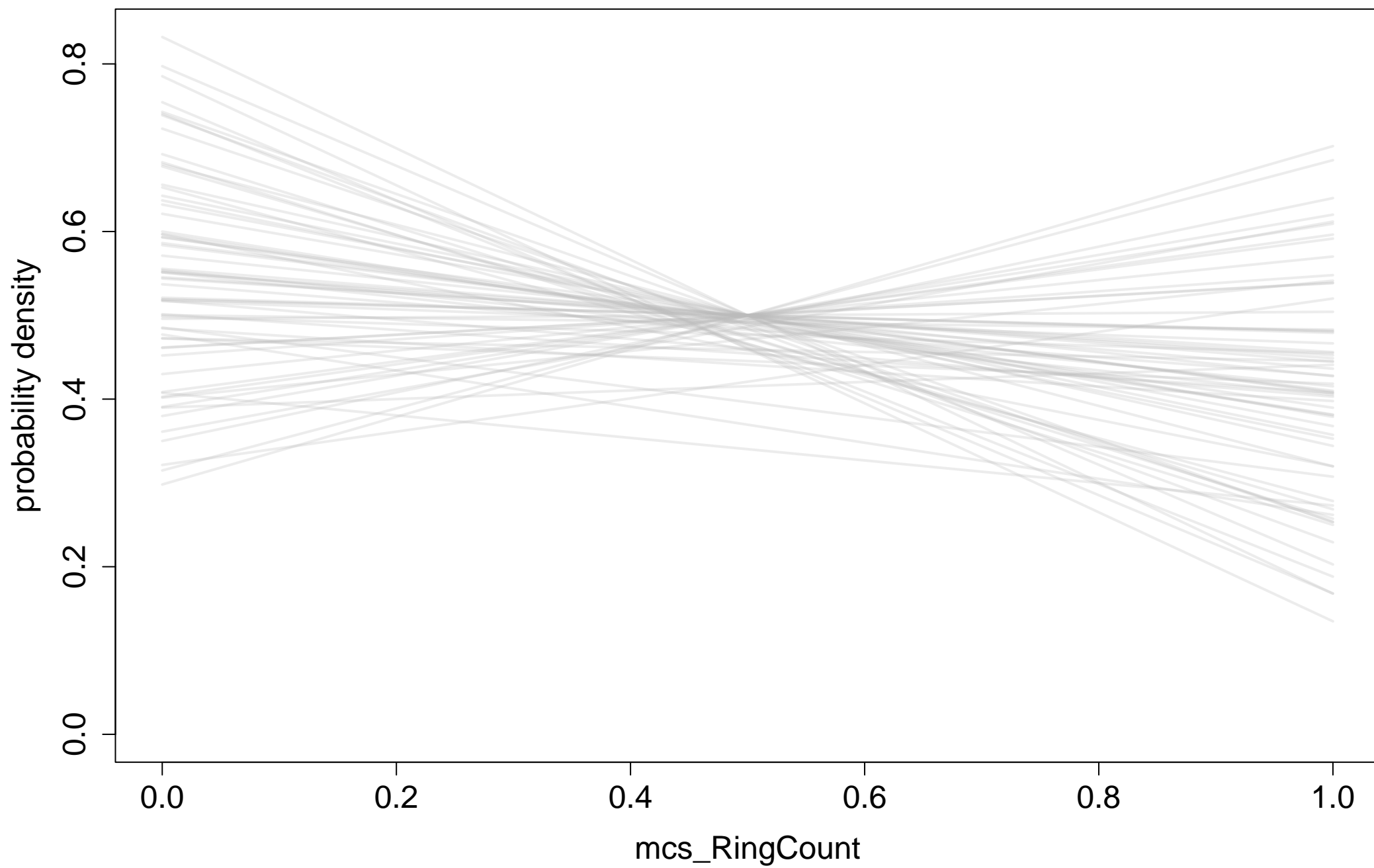


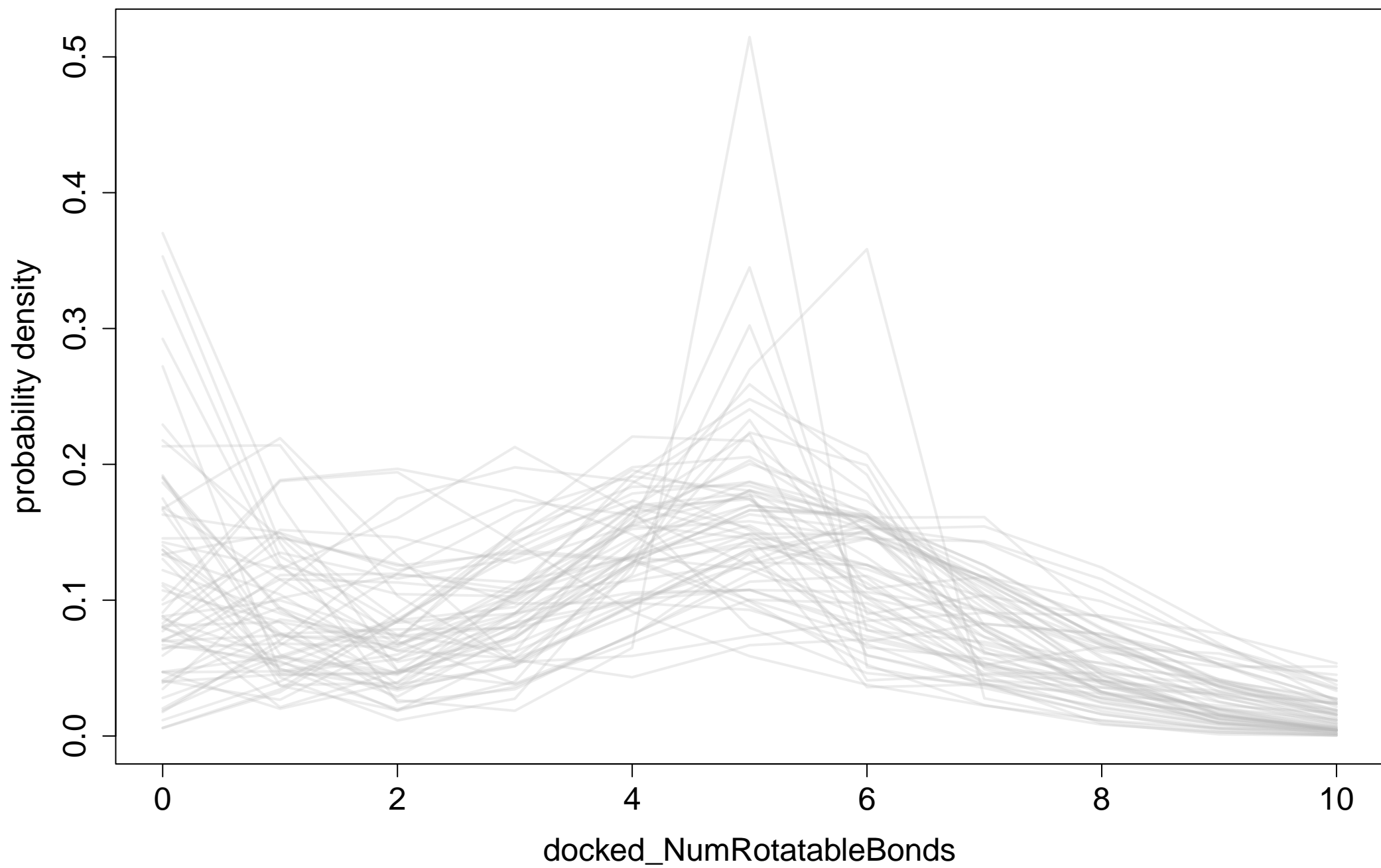


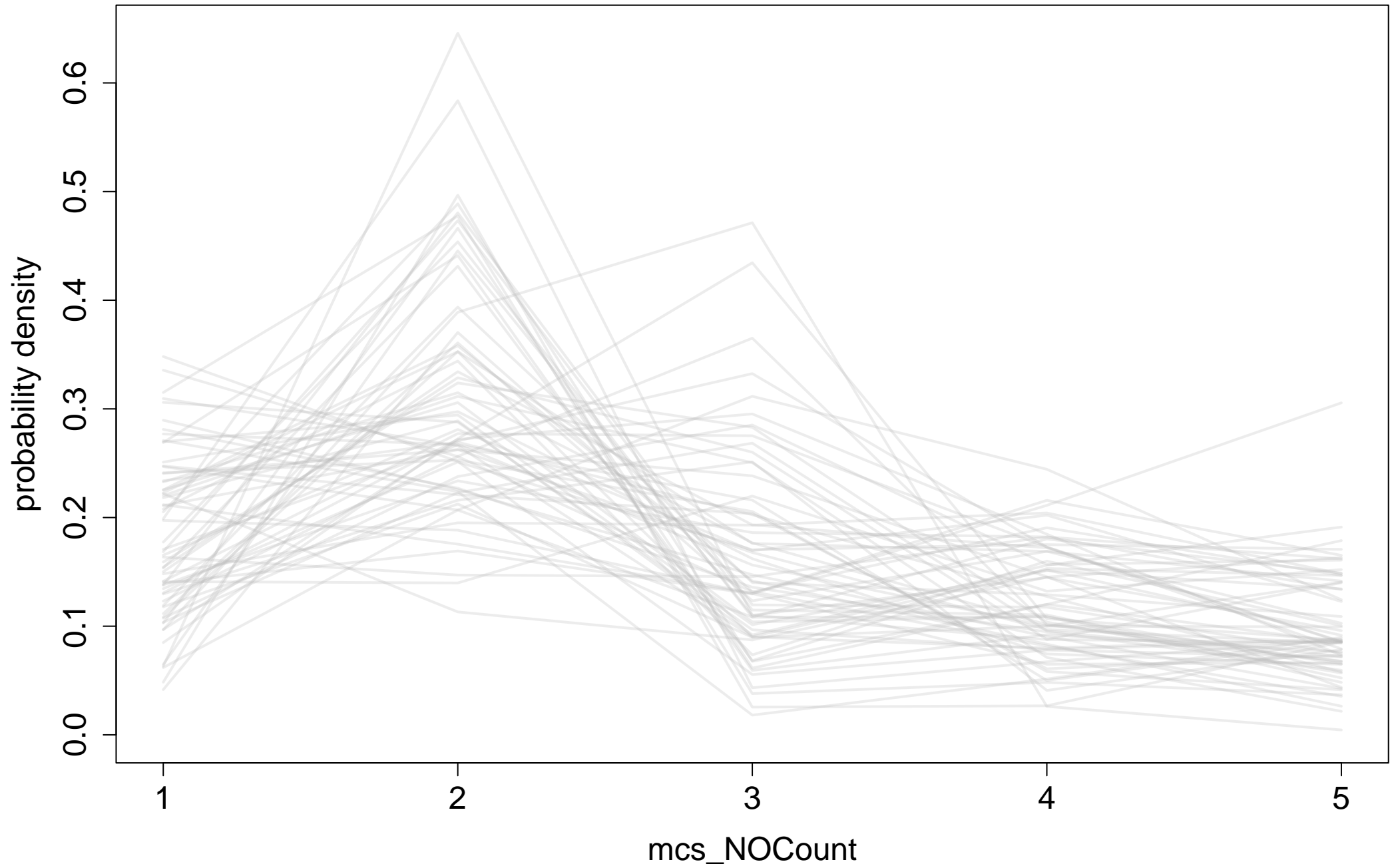


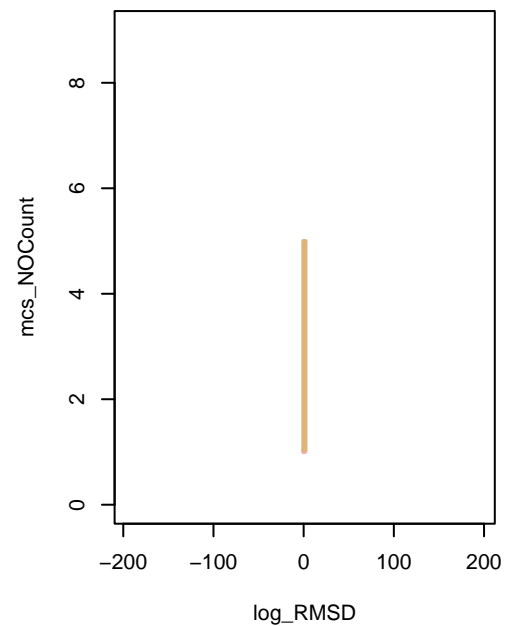
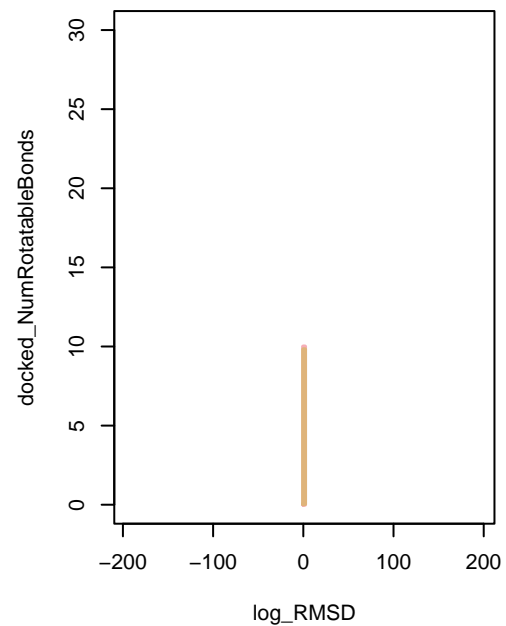
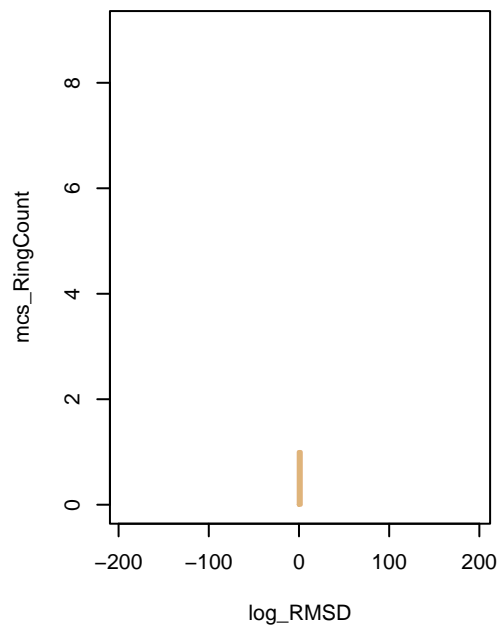
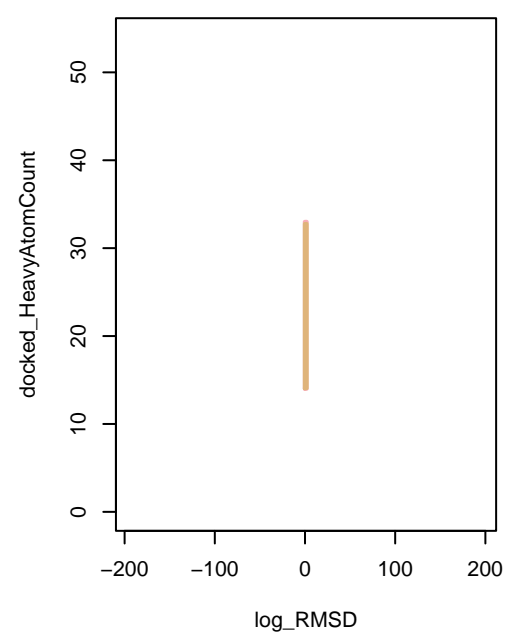
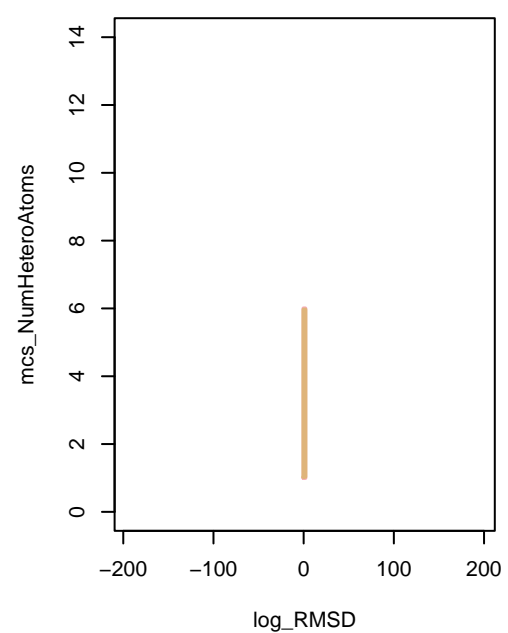
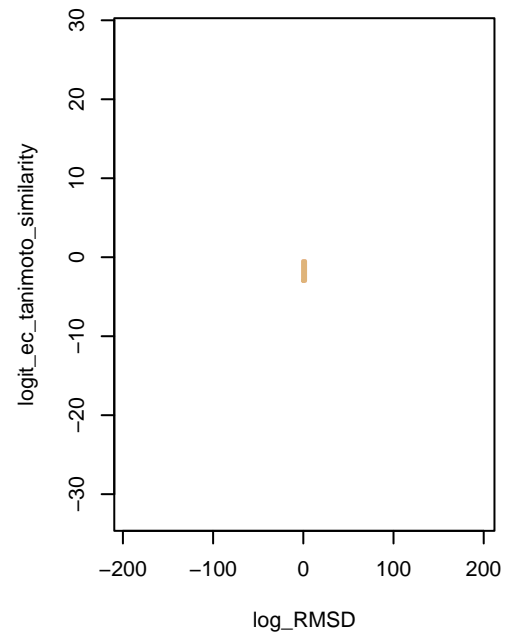
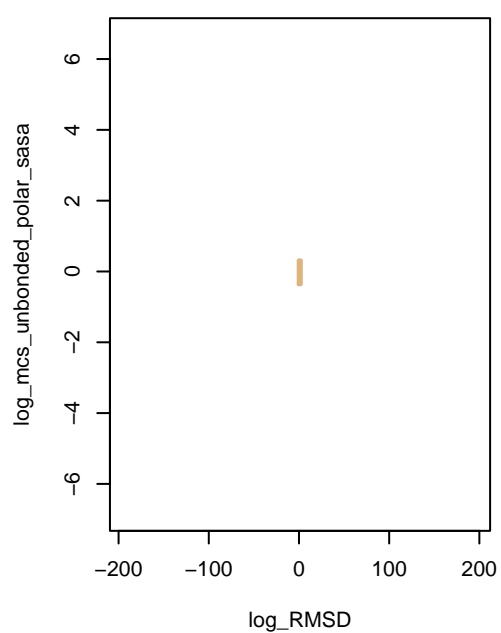




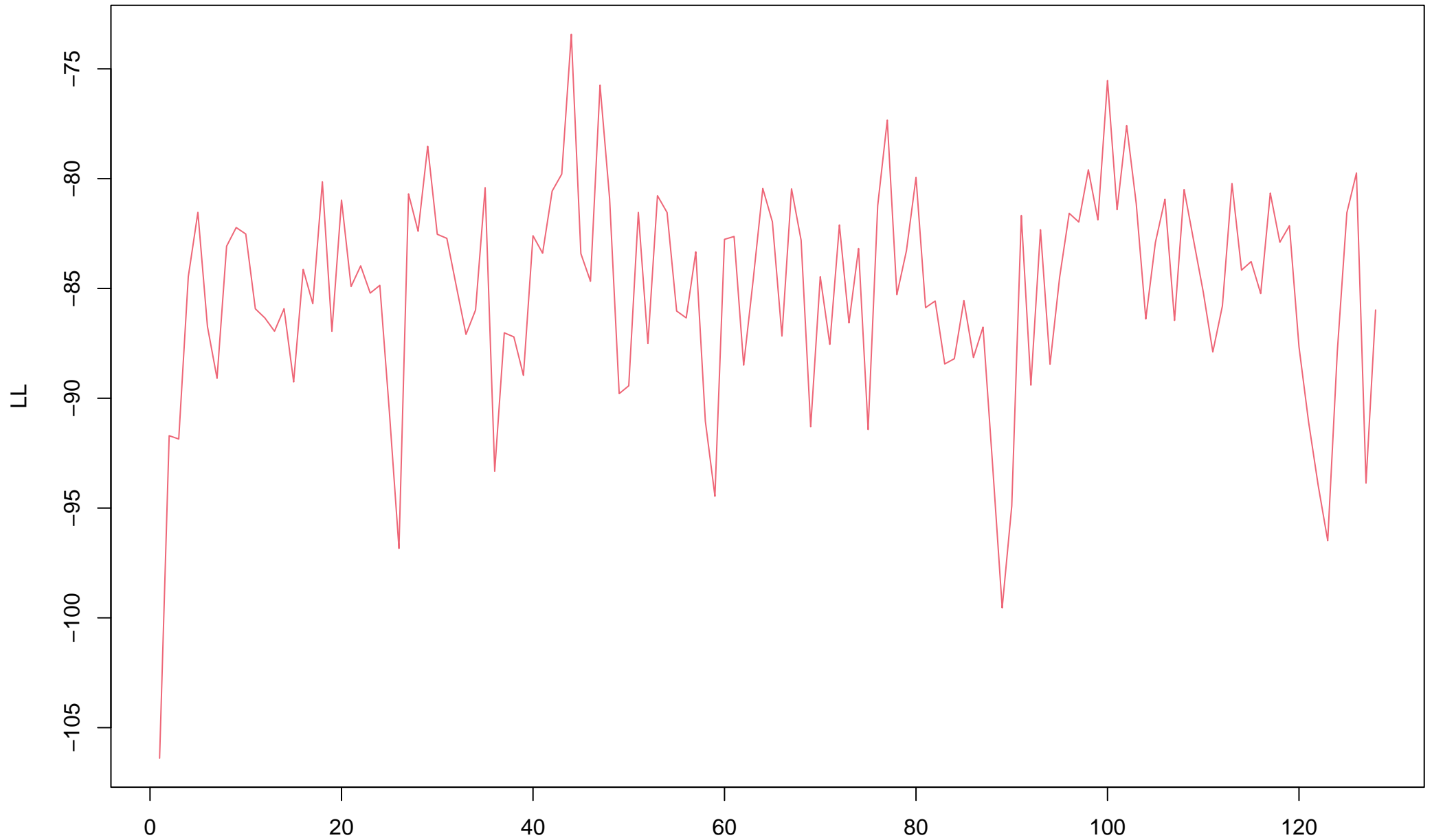




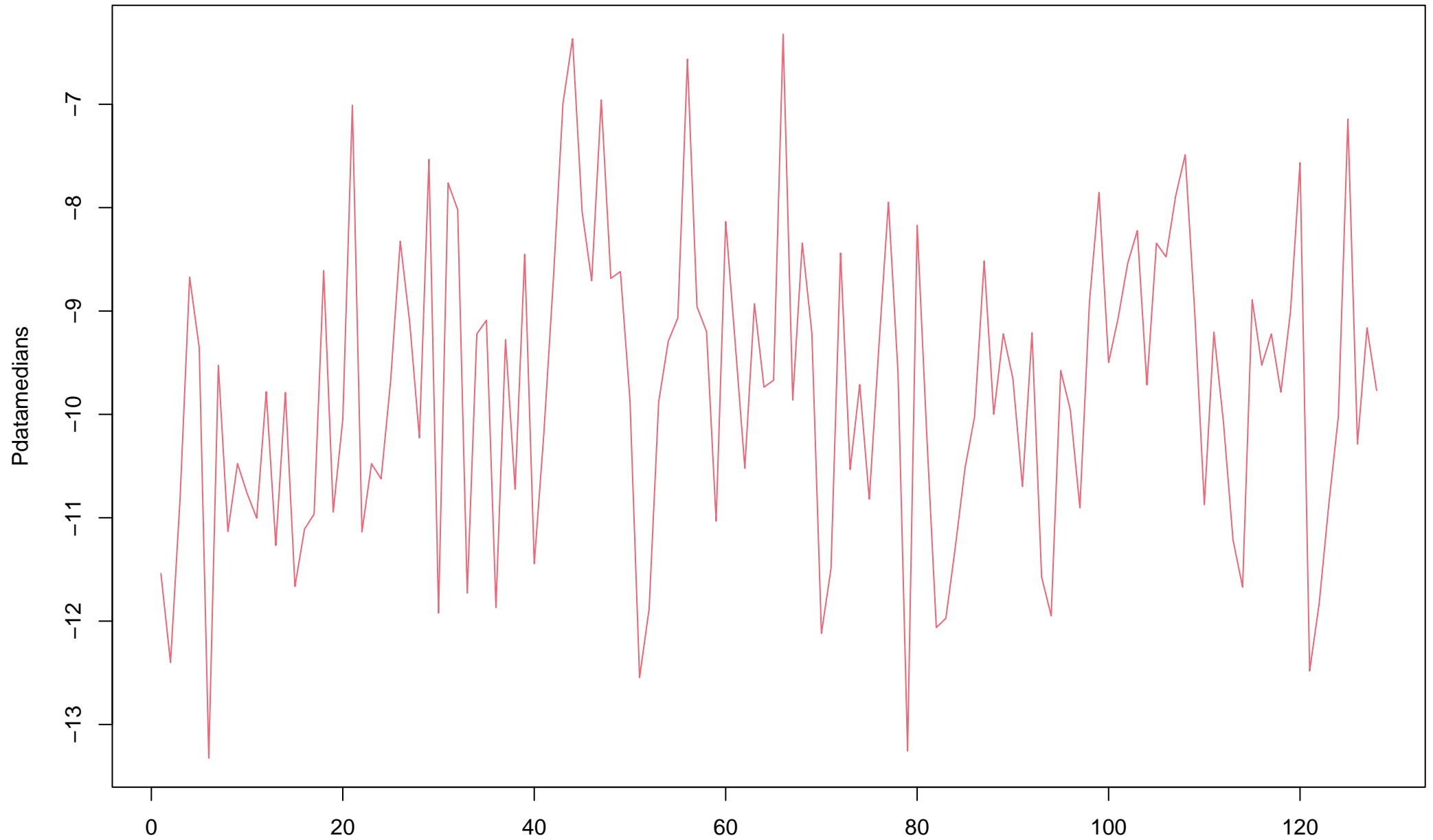




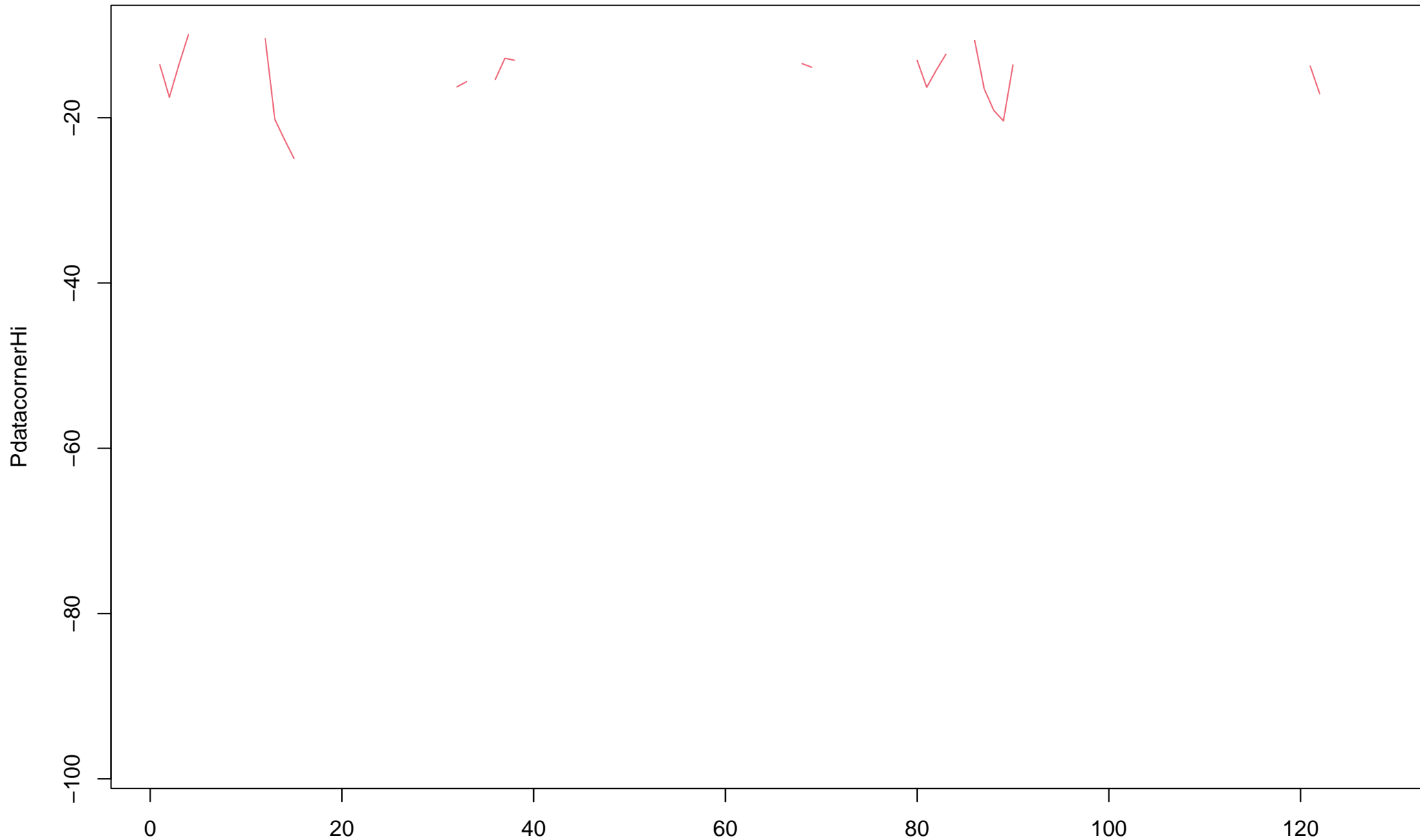
LL
ESS = 67.9 | BMK = 0.108 | MCSE(6.27) = 15.8 | stat: TRUE | burn: 96



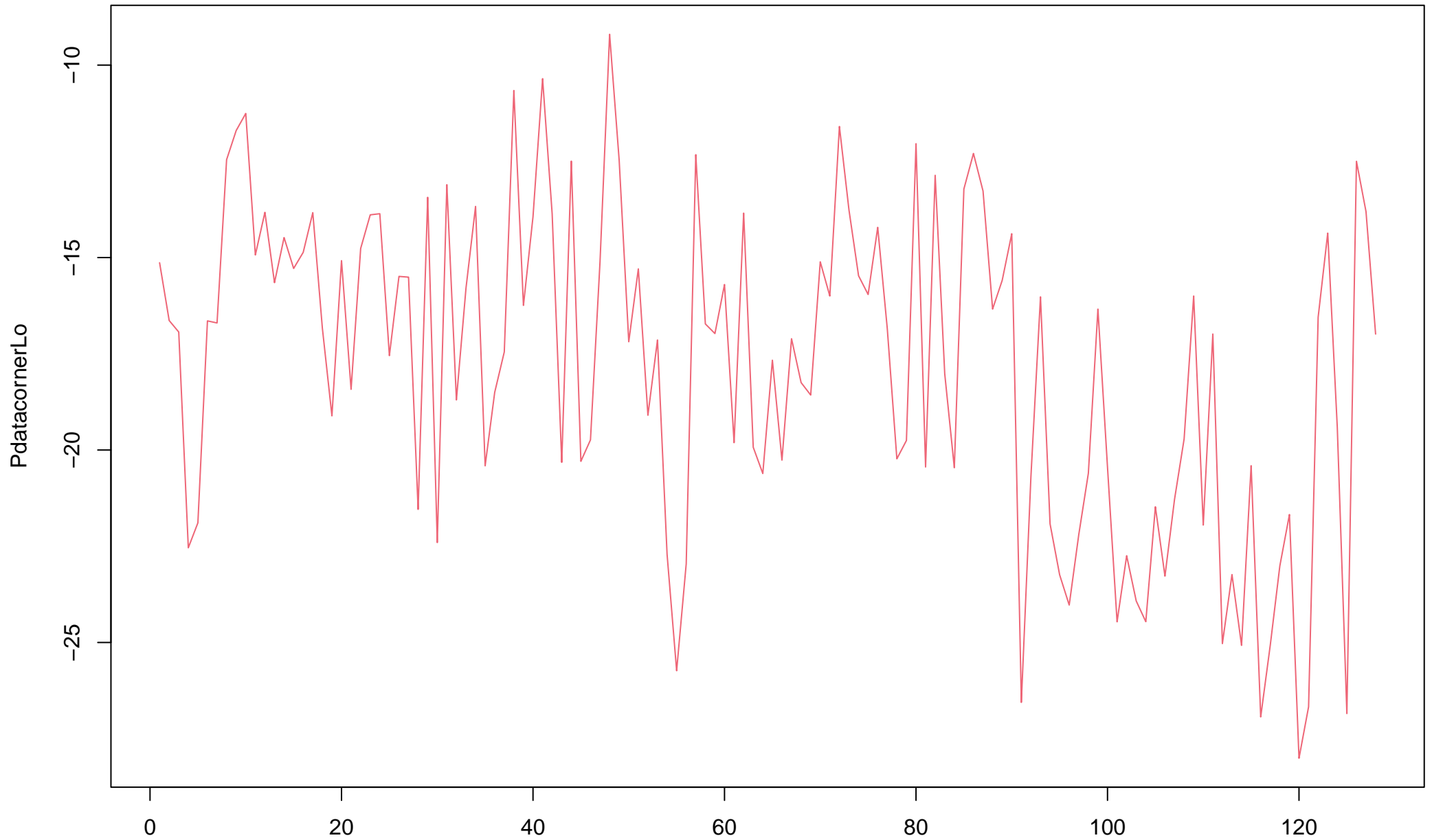
Pdatamedians
ESS = 128 | BMK = 0.207 | MCSE(6.27) = 12 | stat: FALSE | burn: 96



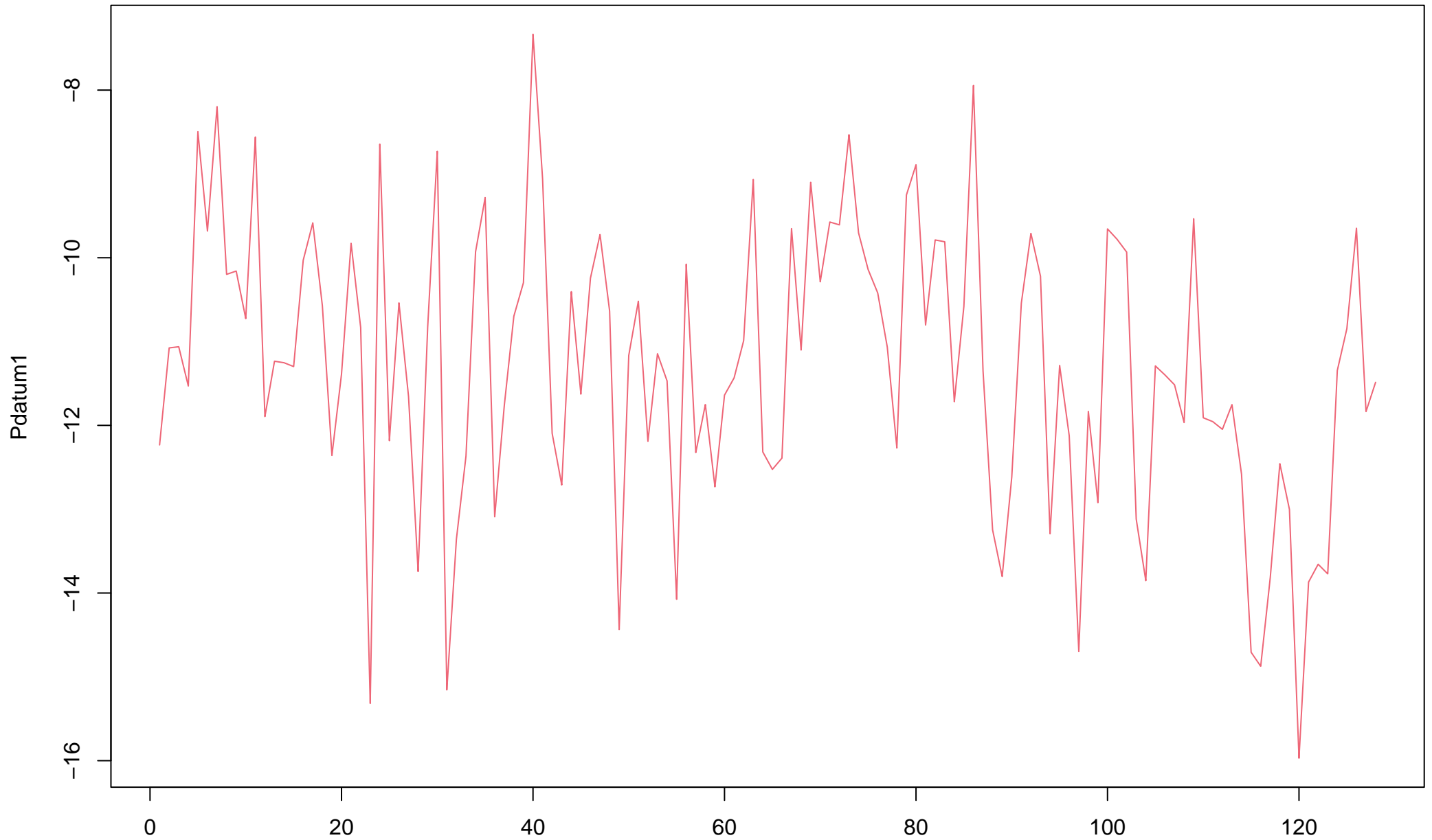
PdatacornerHi
ESS = 76.6 | BMK = 1 | MCSE(6.27) = 8.64 | stat: TRUE | burn: 120



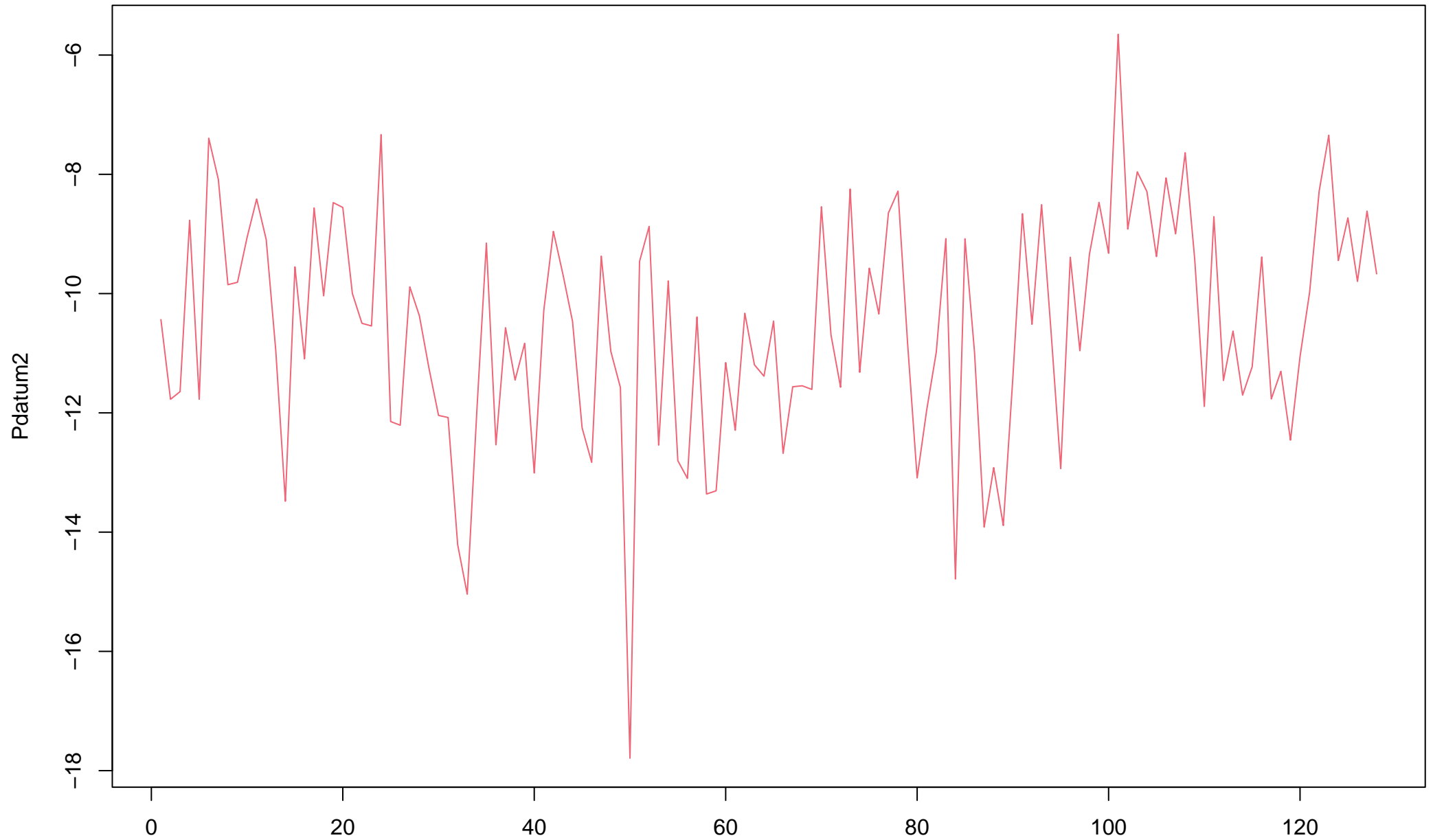
PdatacornerLo
ESS = 128 | BMK = 1 | MCSE(6.27) = 8.94 | stat: TRUE | burn: 120



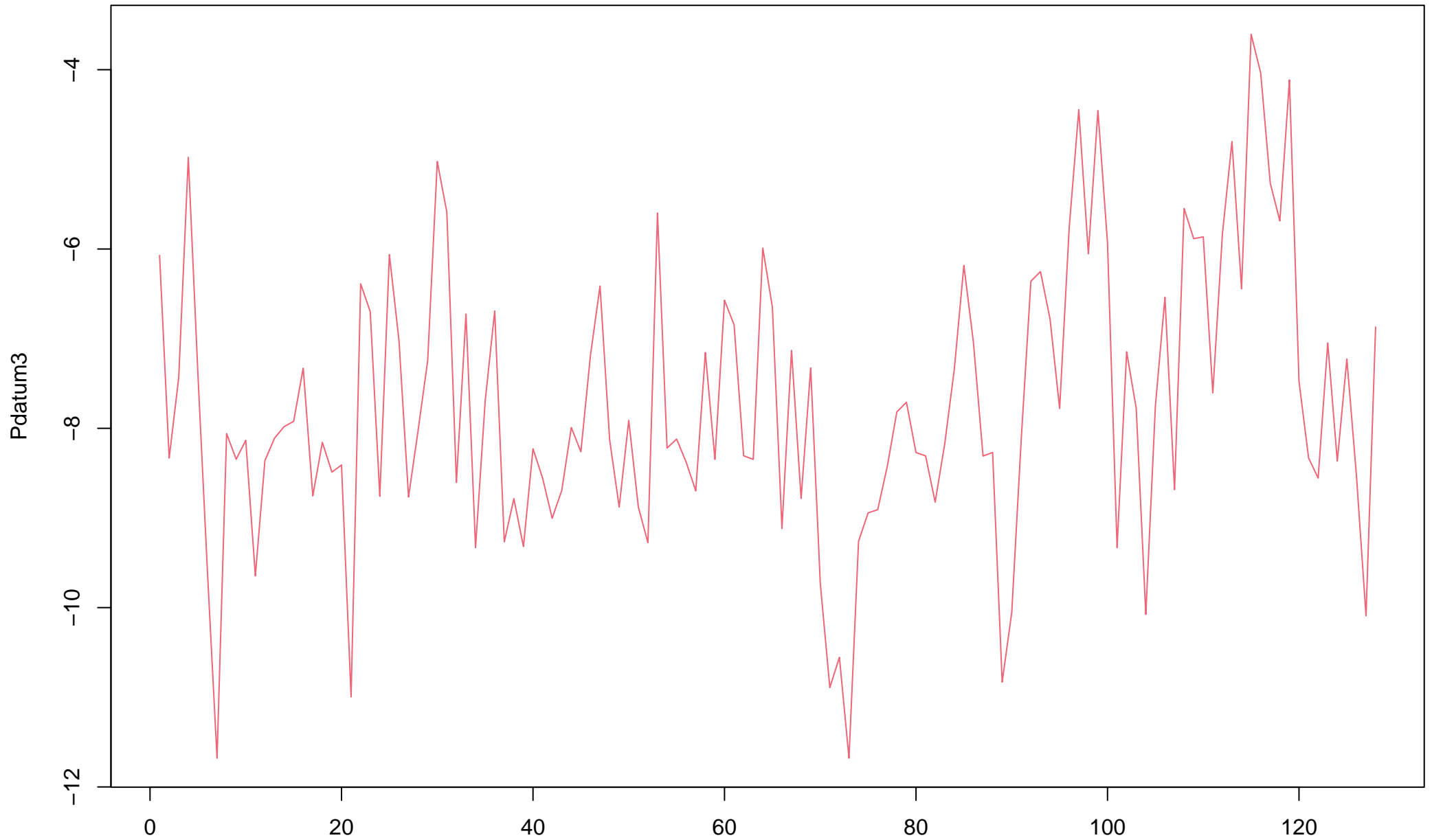
Pdatum1
ESS = 128 | BMK = 0.2 | MCSE(6.27) = 10.2 | stat: TRUE | burn: 120



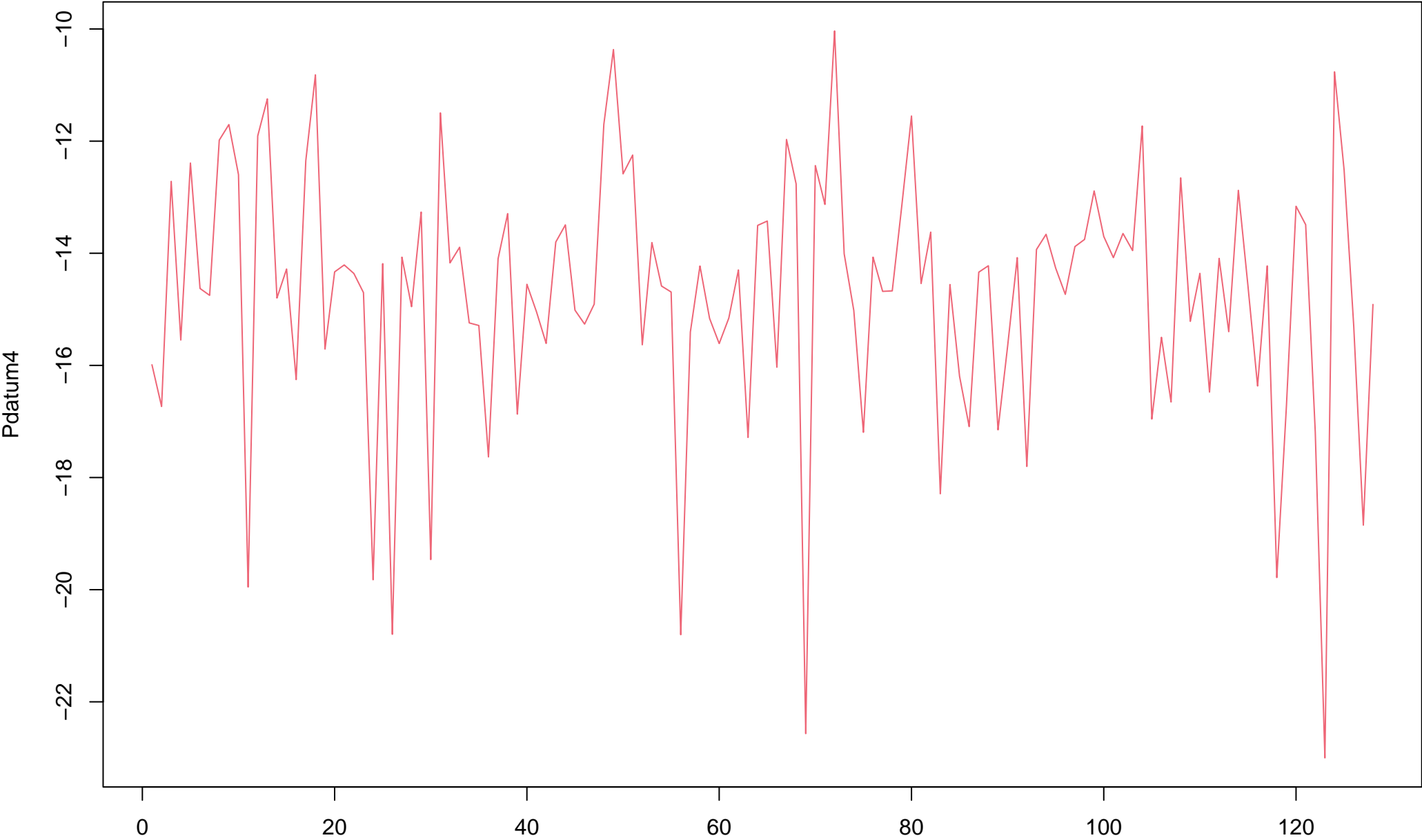
Pdatum2
ESS = 128 | BMK = 0.278 | MCSE(6.27) = 10.2 | stat: TRUE | burn: 120



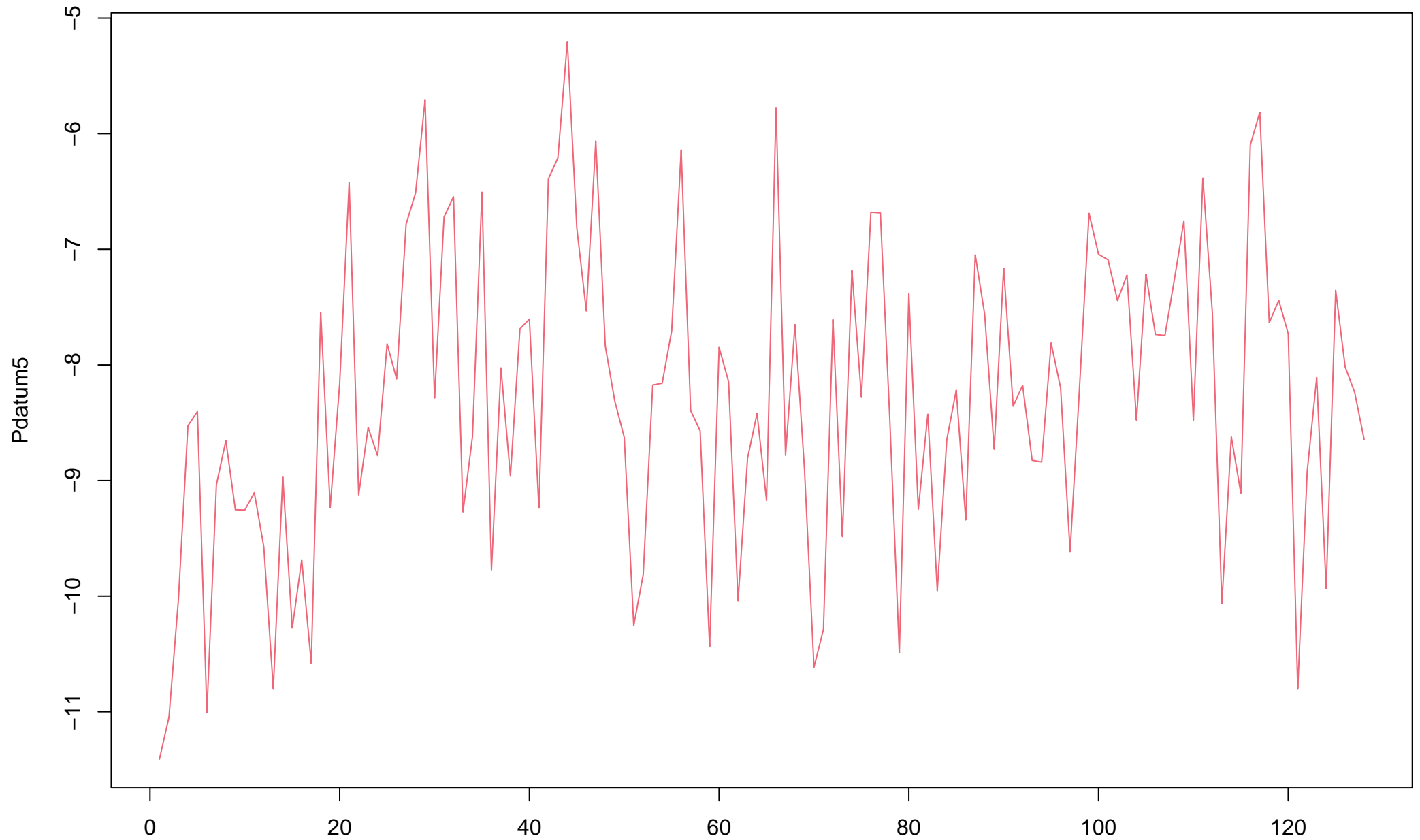
Pdatum3
ESS = 35 | BMK = 0.336 | MCSE(6.27) = 21.9 | stat: TRUE | burn: 84



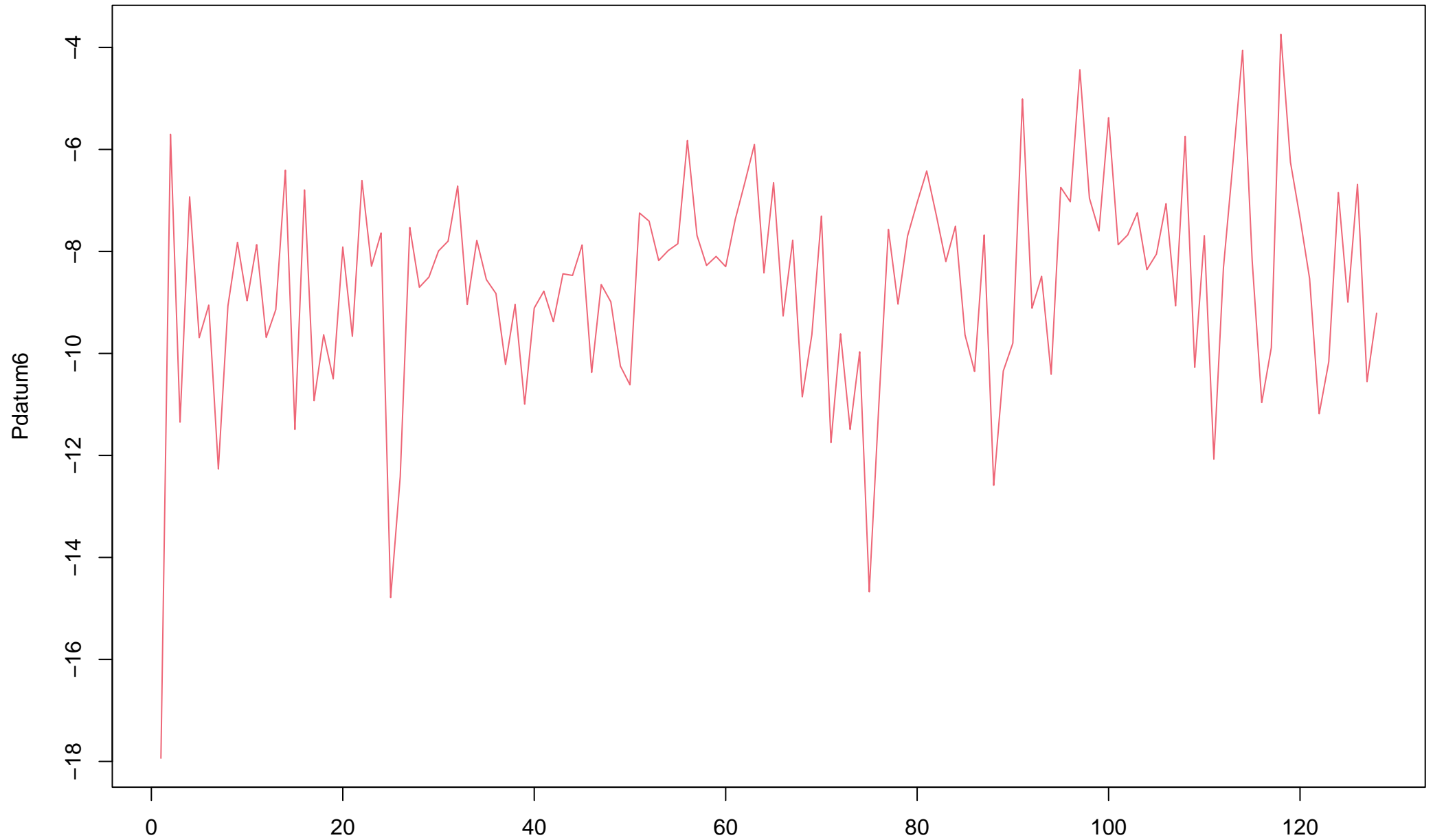
Pdatum4
ESS = 128 | BMK = 0.238 | MCSE(6.27) = 9.93 | stat: TRUE | burn: 72



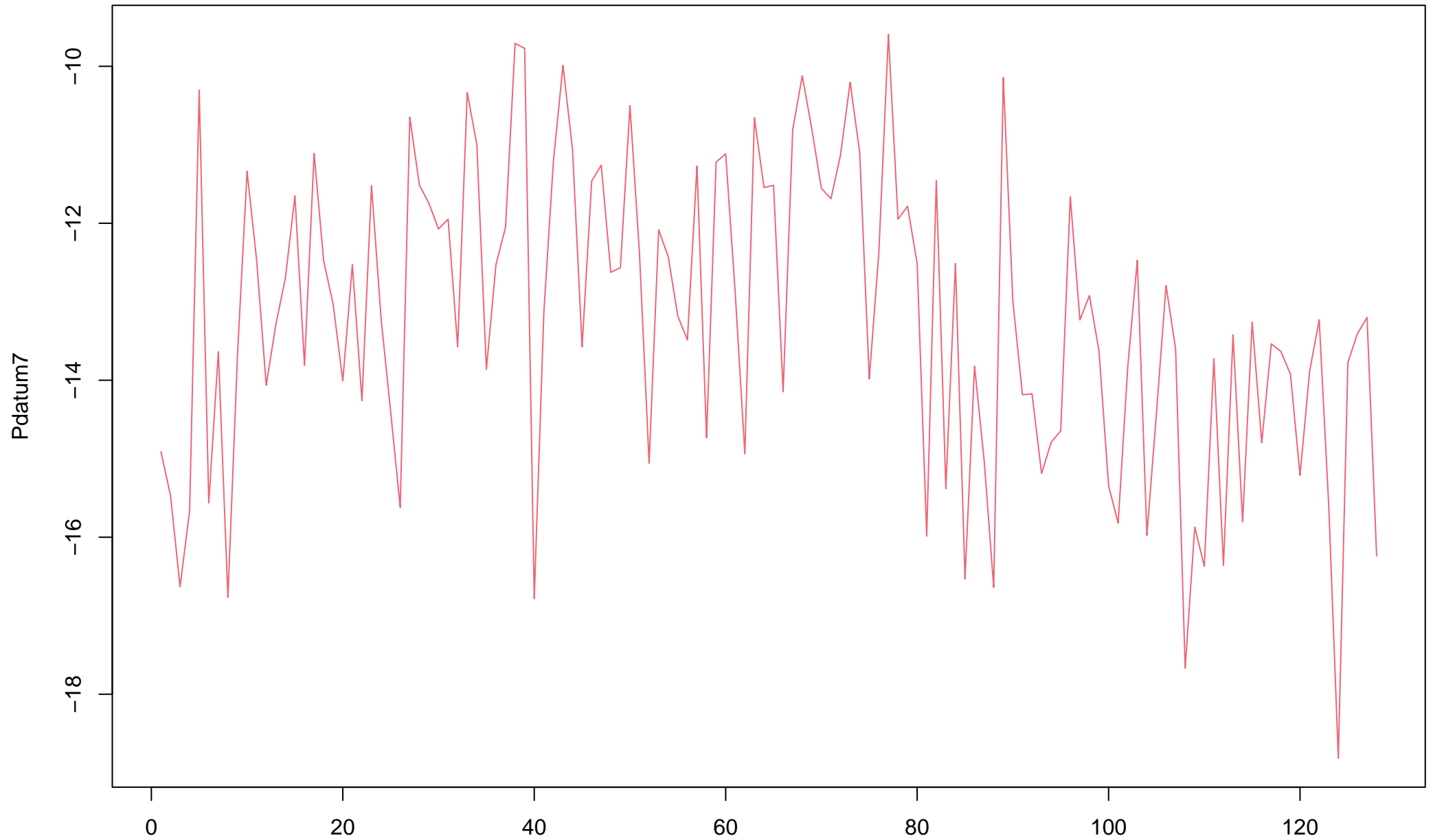
Pdatum5
ESS = 75.1 | BMK = 0.276 | MCSE(6.27) = 15.3 | stat: FALSE | burn: 48



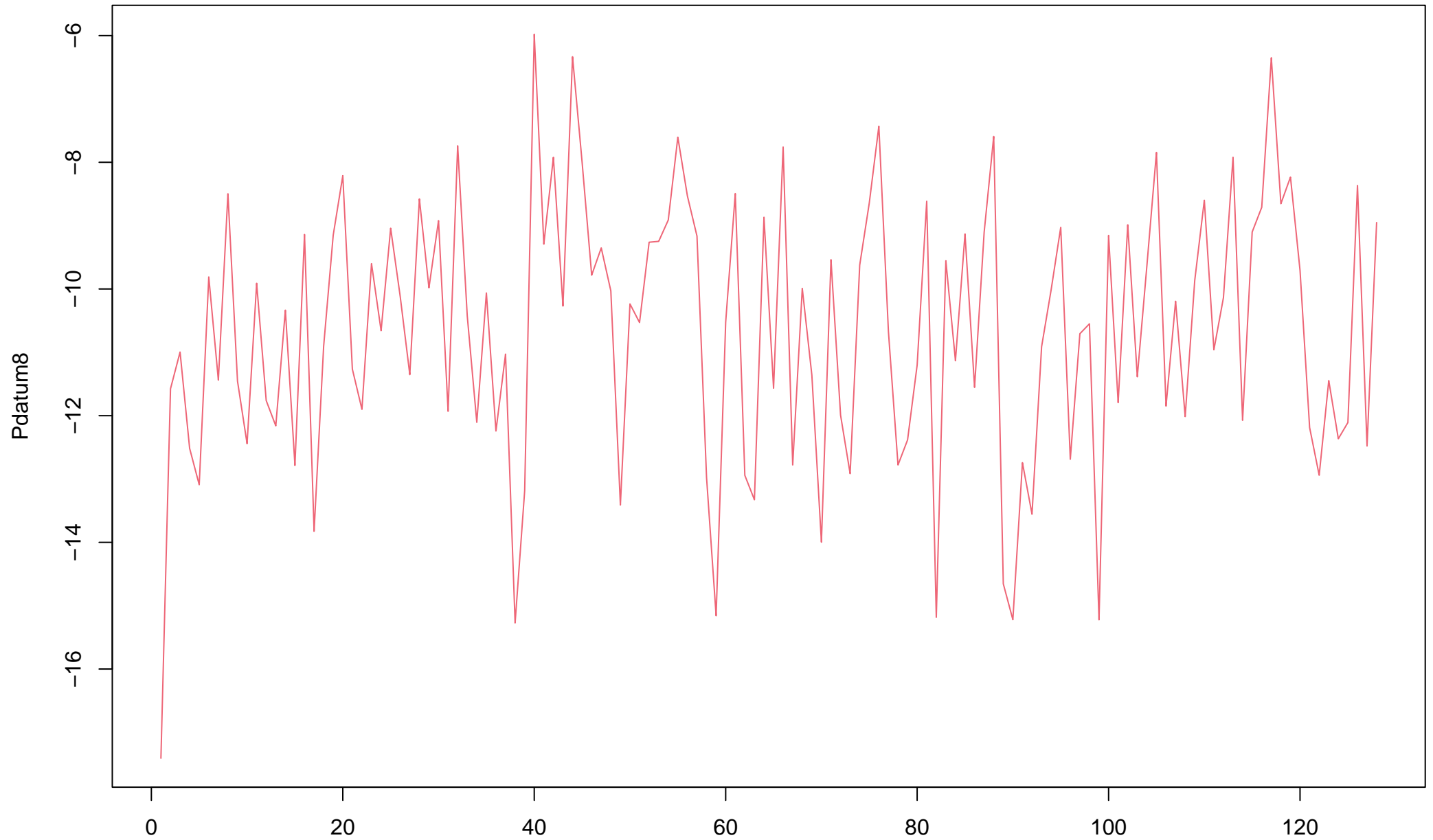
Pdatum6
ESS = 64.7 | BMK = 0.29 | MCSE(6.27) = 8.99 | stat: TRUE | burn: 96



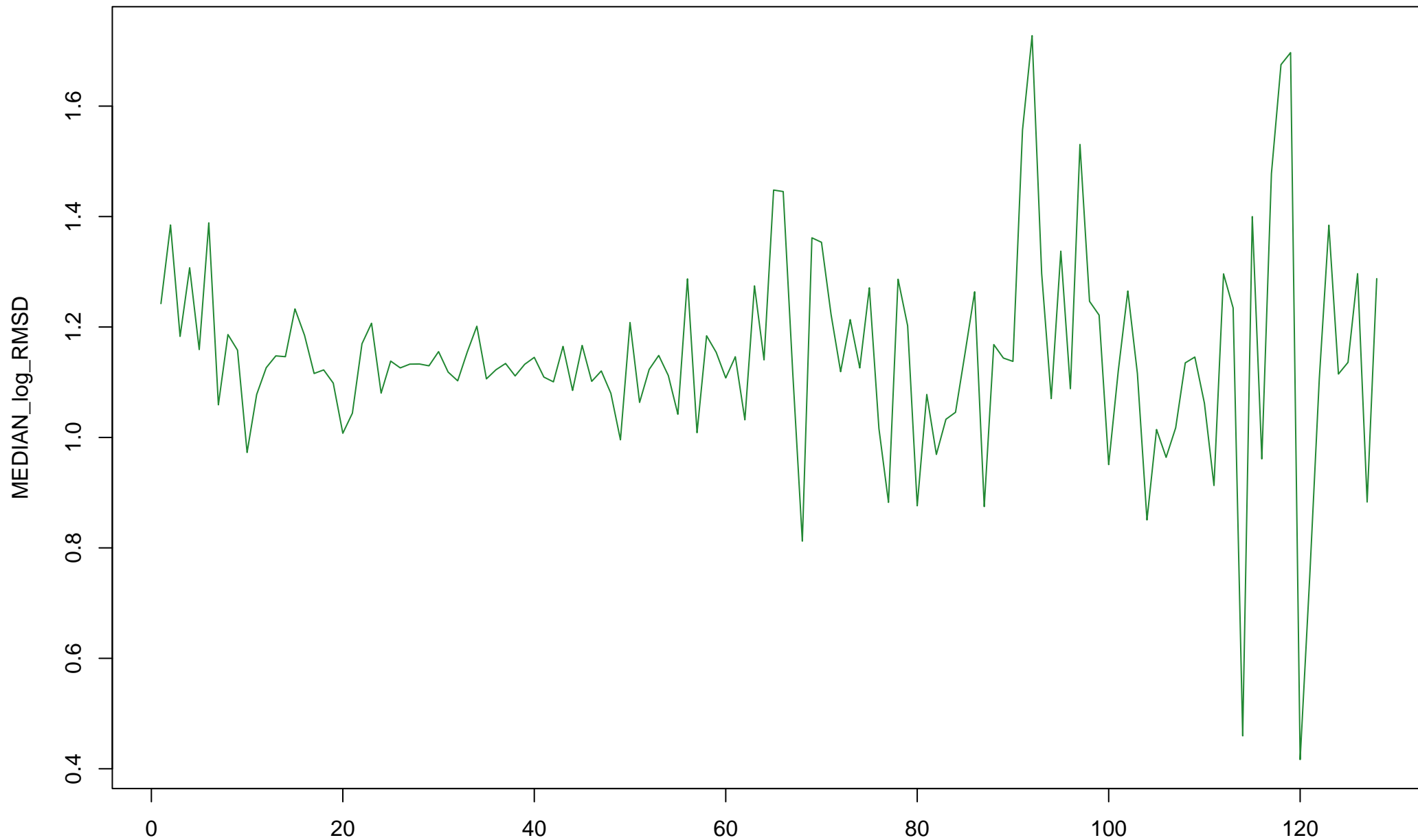
Pdatum7
ESS = 24.5 | BMK = 0.366 | MCSE(6.27) = 11.9 | stat: TRUE | burn: 96



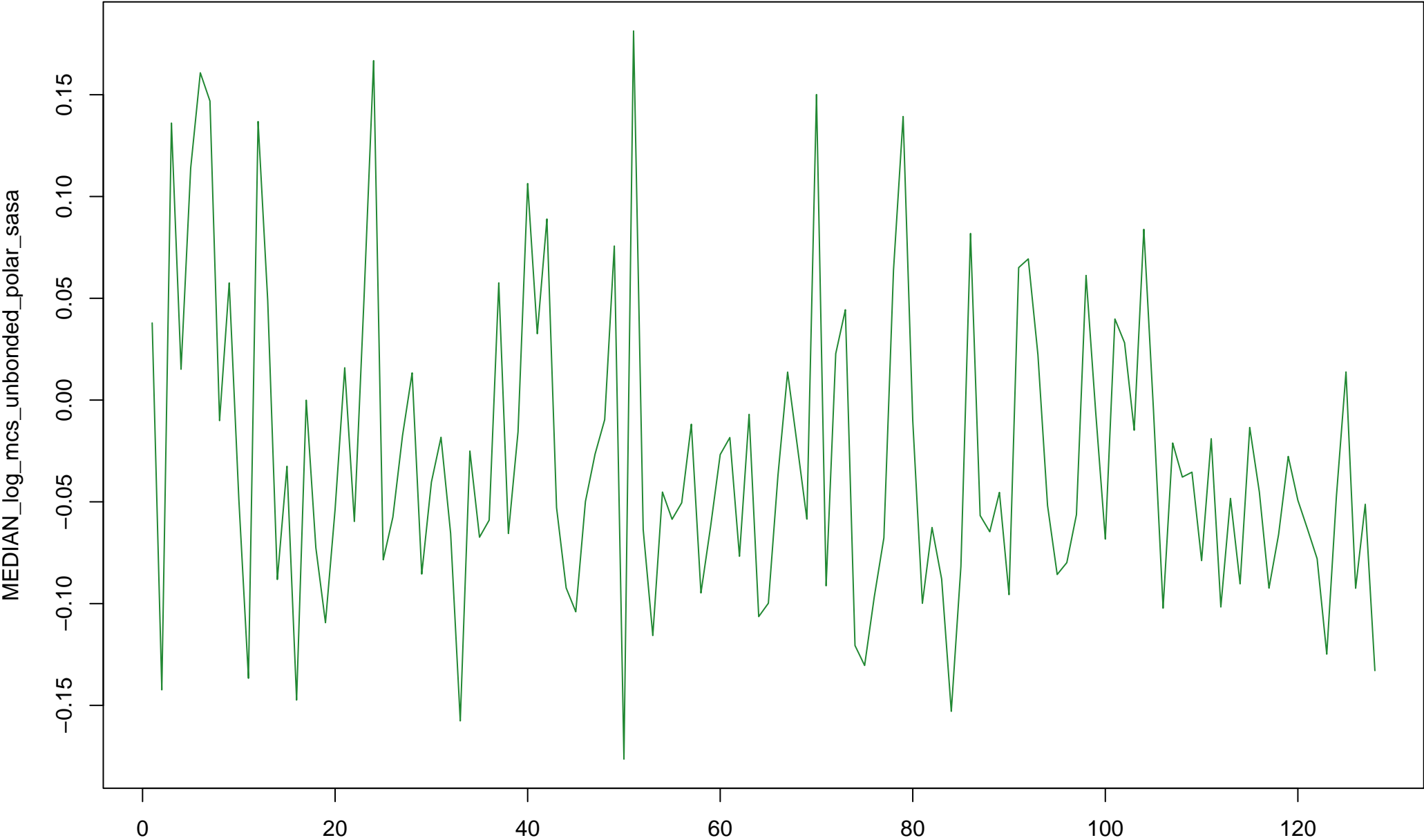
Pdatum8
ESS = 65.2 | BMK = 0.125 | MCSE(6.27) = 9.86 | stat: FALSE | burn: 120



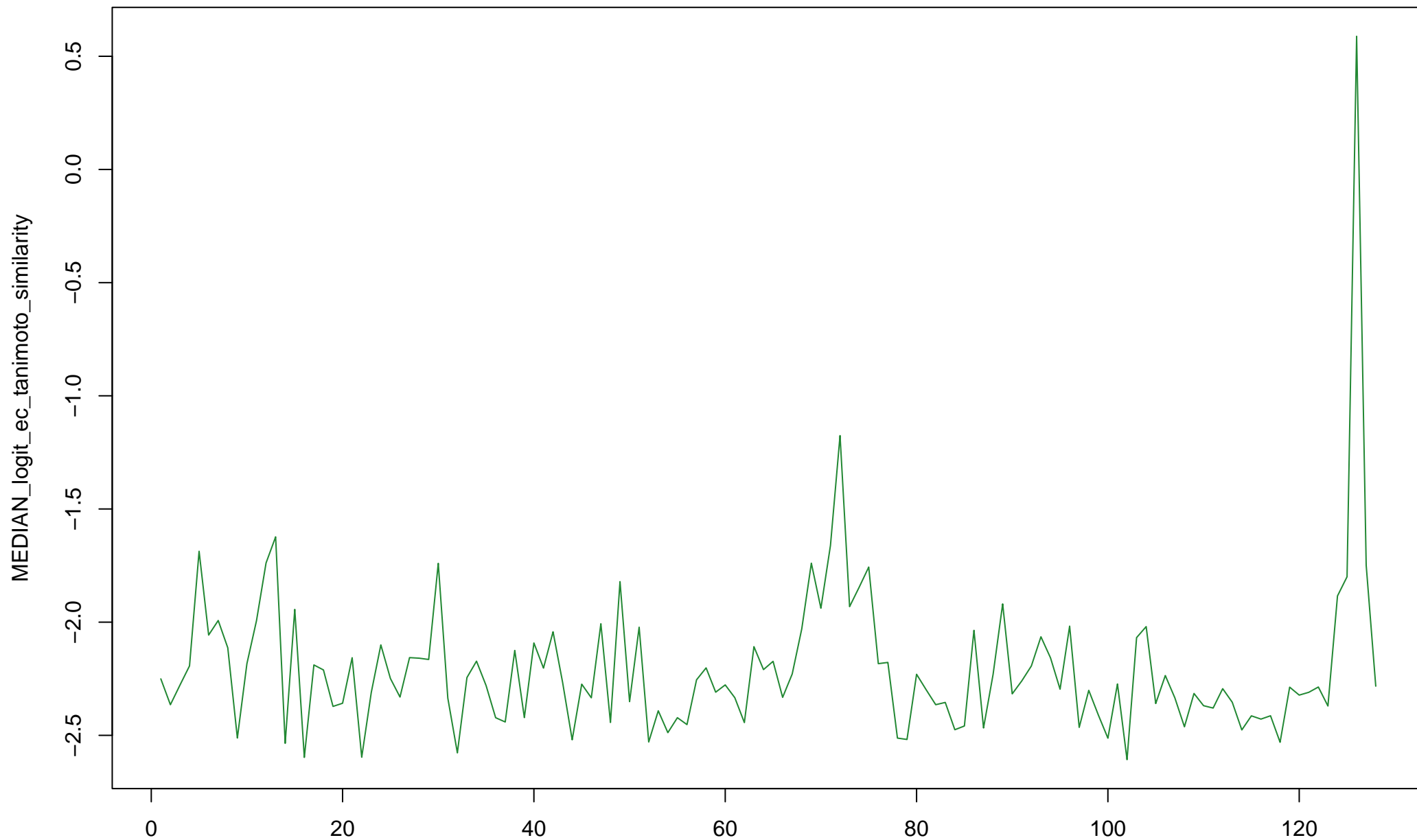
MEDIAN_log_RMSD
ESS = 128 | BMK = 0.472 | MCSE(6.27) = 9.58 | stat: TRUE | burn: 0



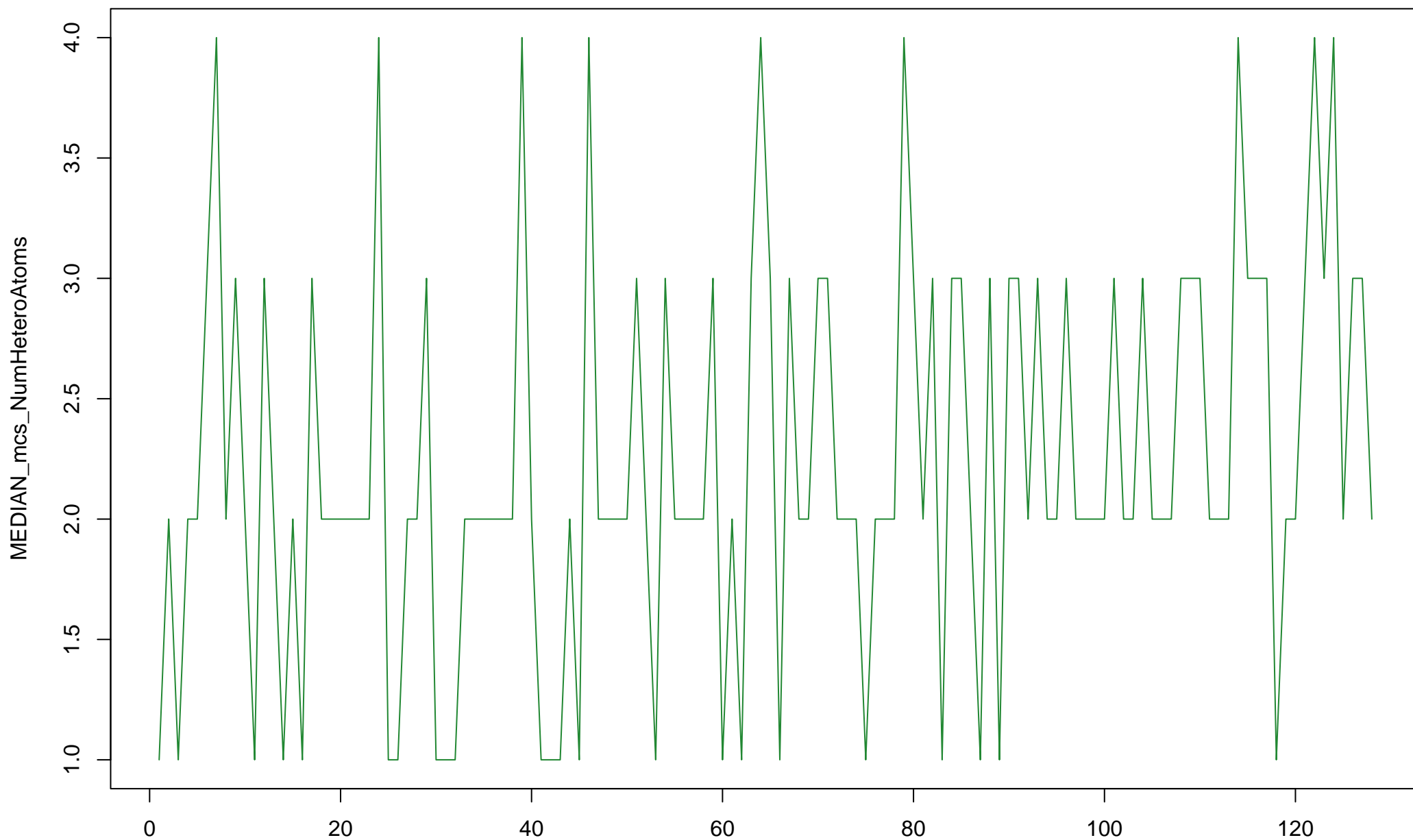
MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 128 | BMK = 0.116 | MCSE(6.27) = 10.9 | stat: FALSE | burn: 0



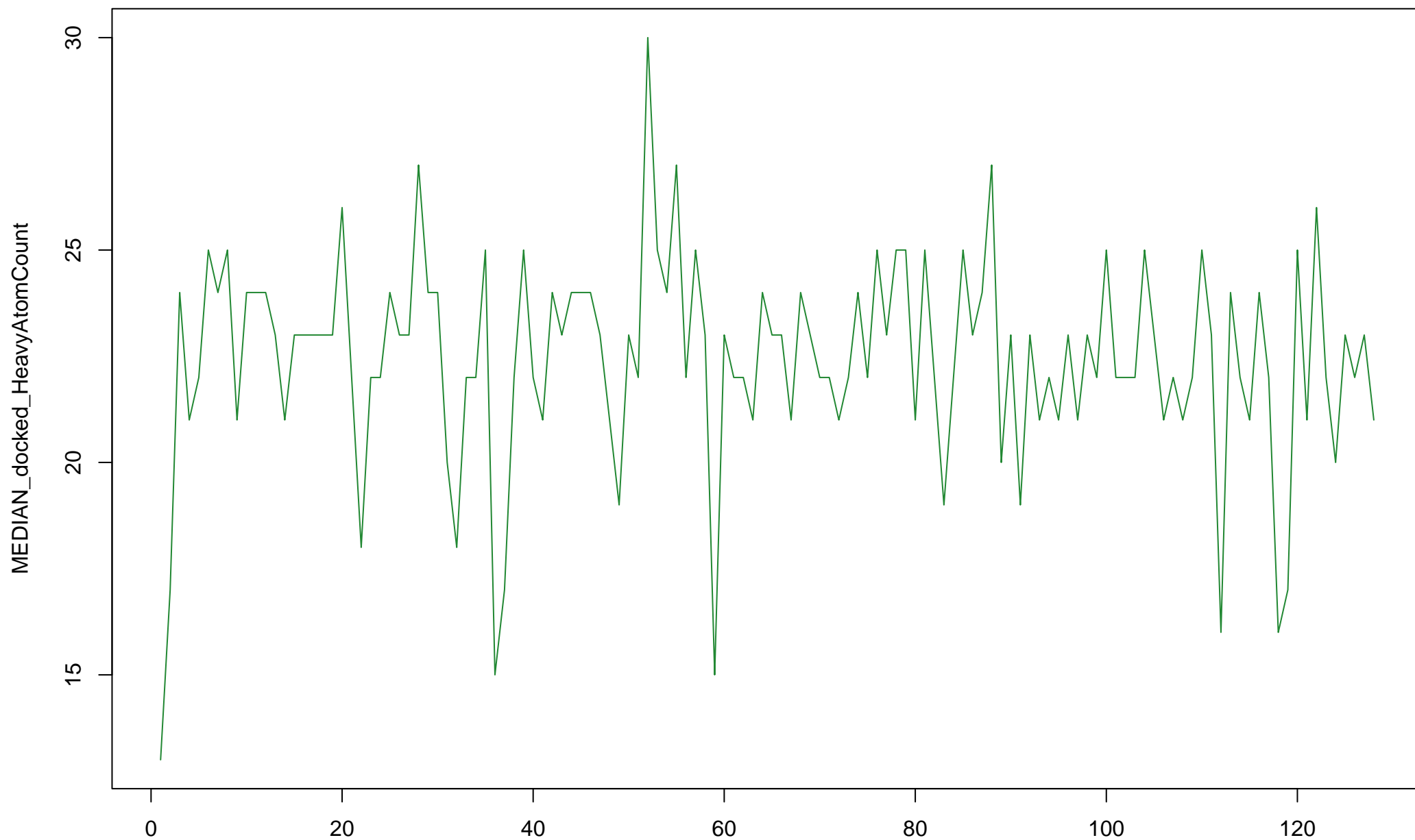
MEDIAN_logit_ec_tanimoto_similarity
ESS = 51.6 | BMK = 0.148 | MCSE(6.27) = 16.6 | stat: TRUE | burn: 0



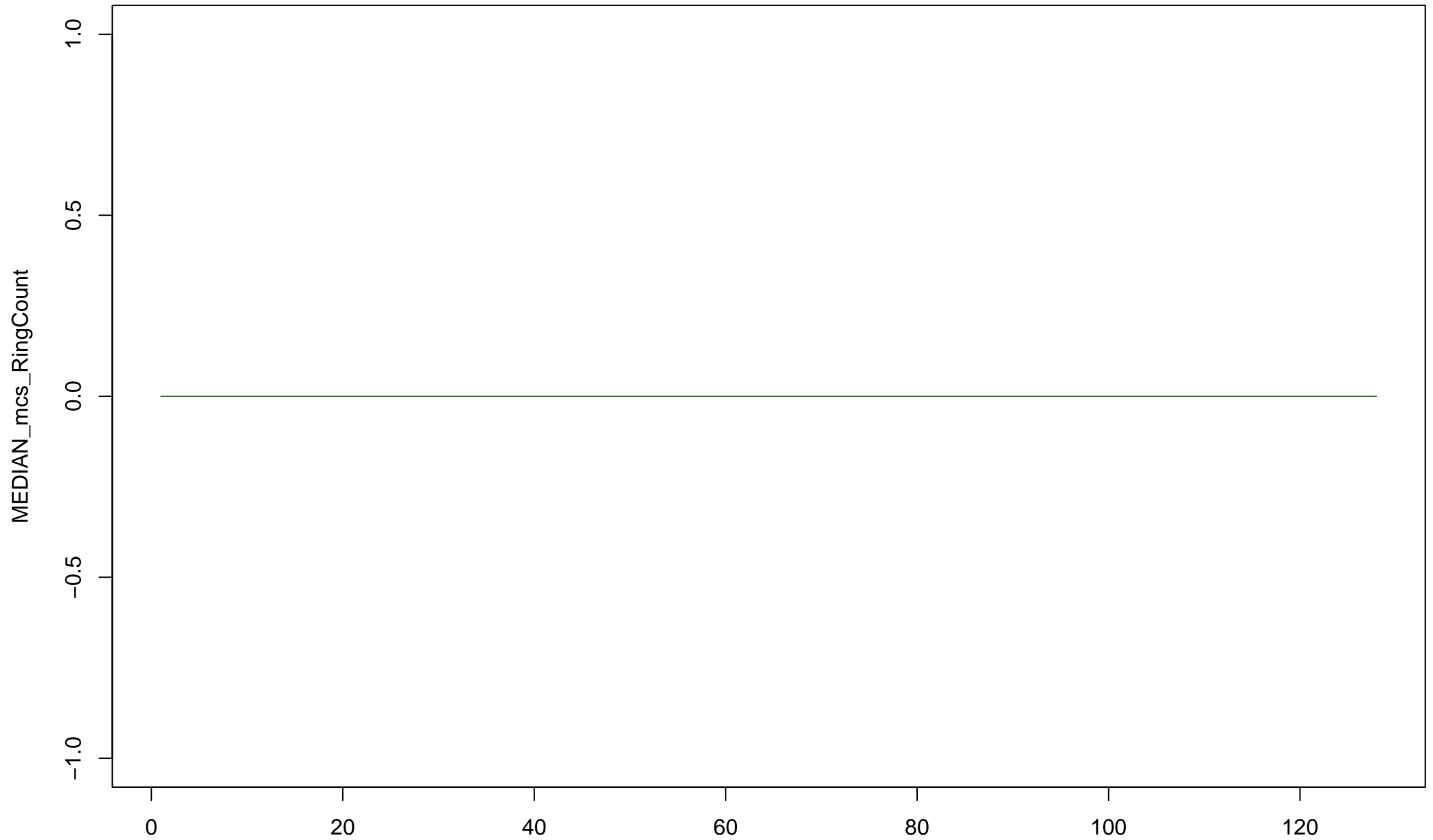
MEDIAN_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.193 | MCSE(6.27) = 10.2 | stat: TRUE | burn: 120



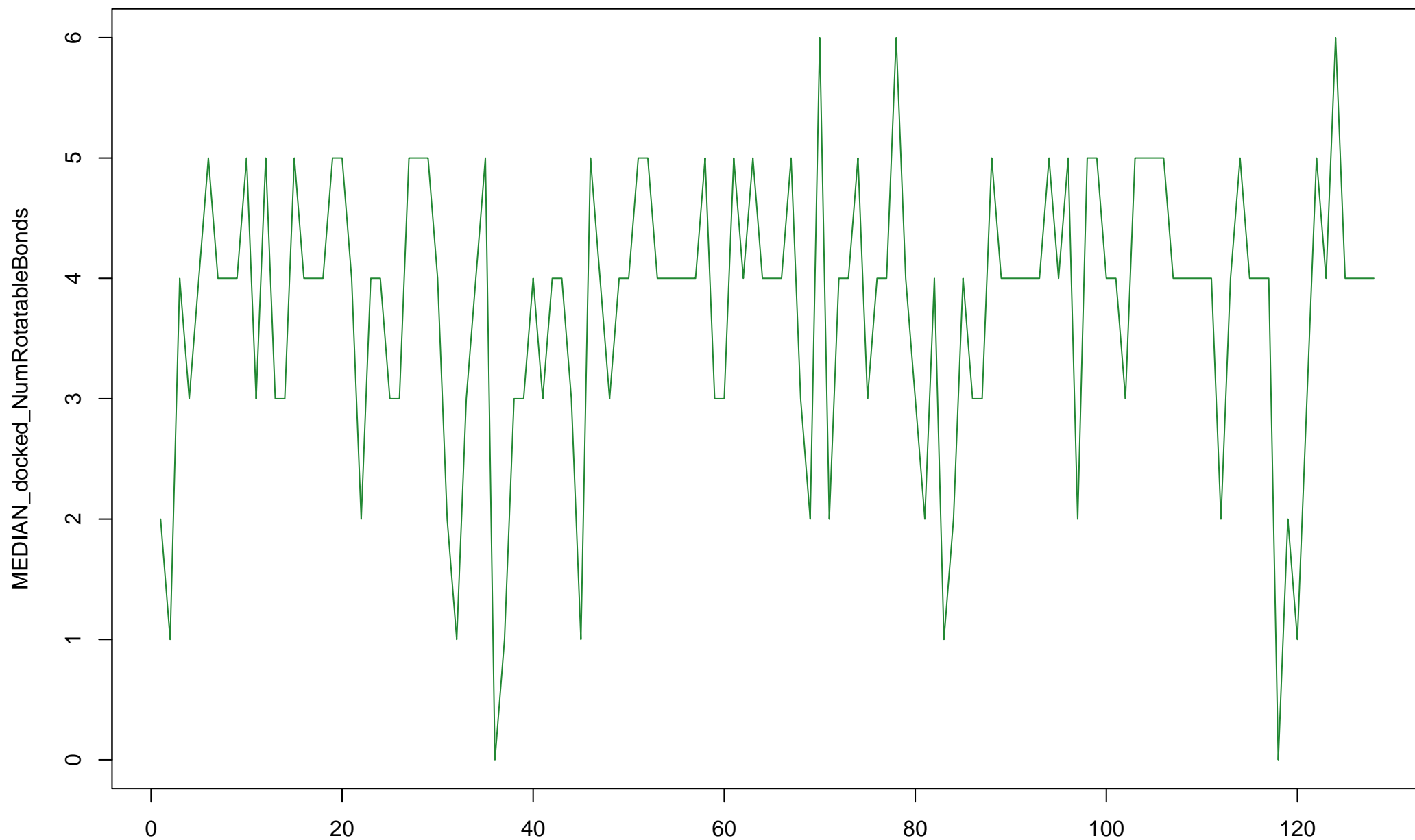
MEDIAN_docked_HeavyAtomCount
ESS = 97.8 | BMK = 0.179 | MCSE(6.27) = 10.6 | stat: TRUE | burn: 0



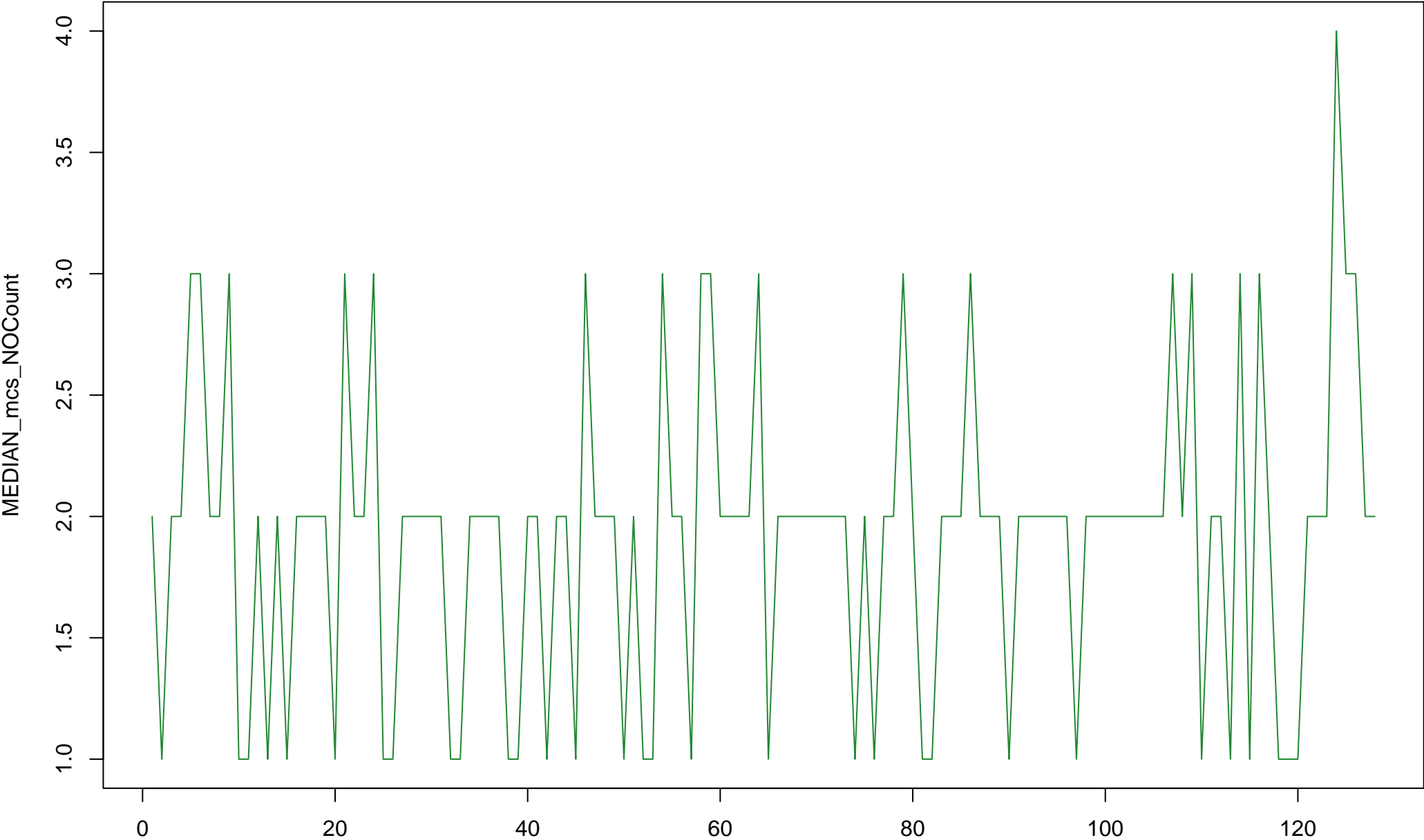
MEDIAN_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



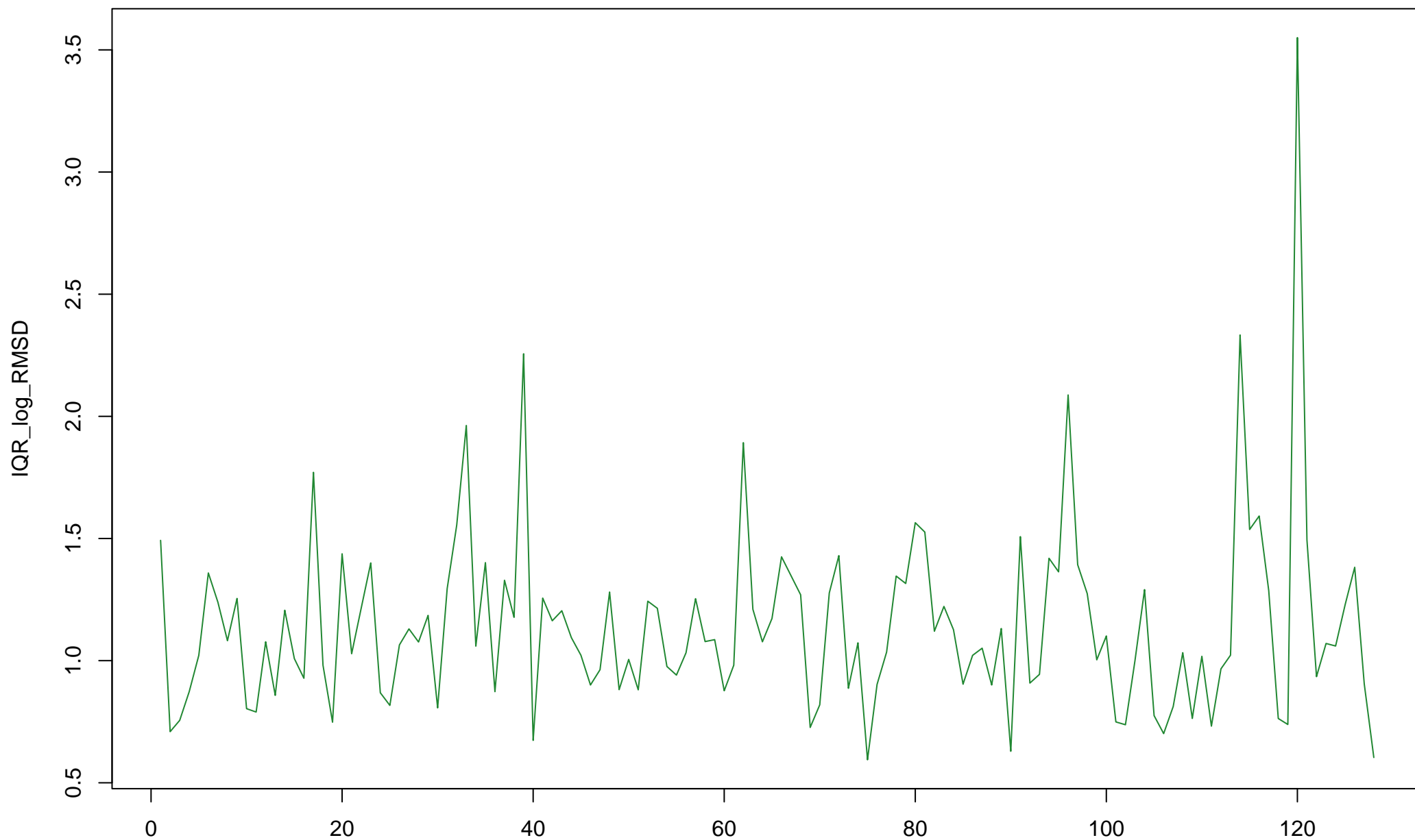
MEDIAN_docked_NumRotatableBonds
ESS = 86.2 | BMK = 0.118 | MCSE(6.27) = 12.5 | stat: TRUE | burn: 84



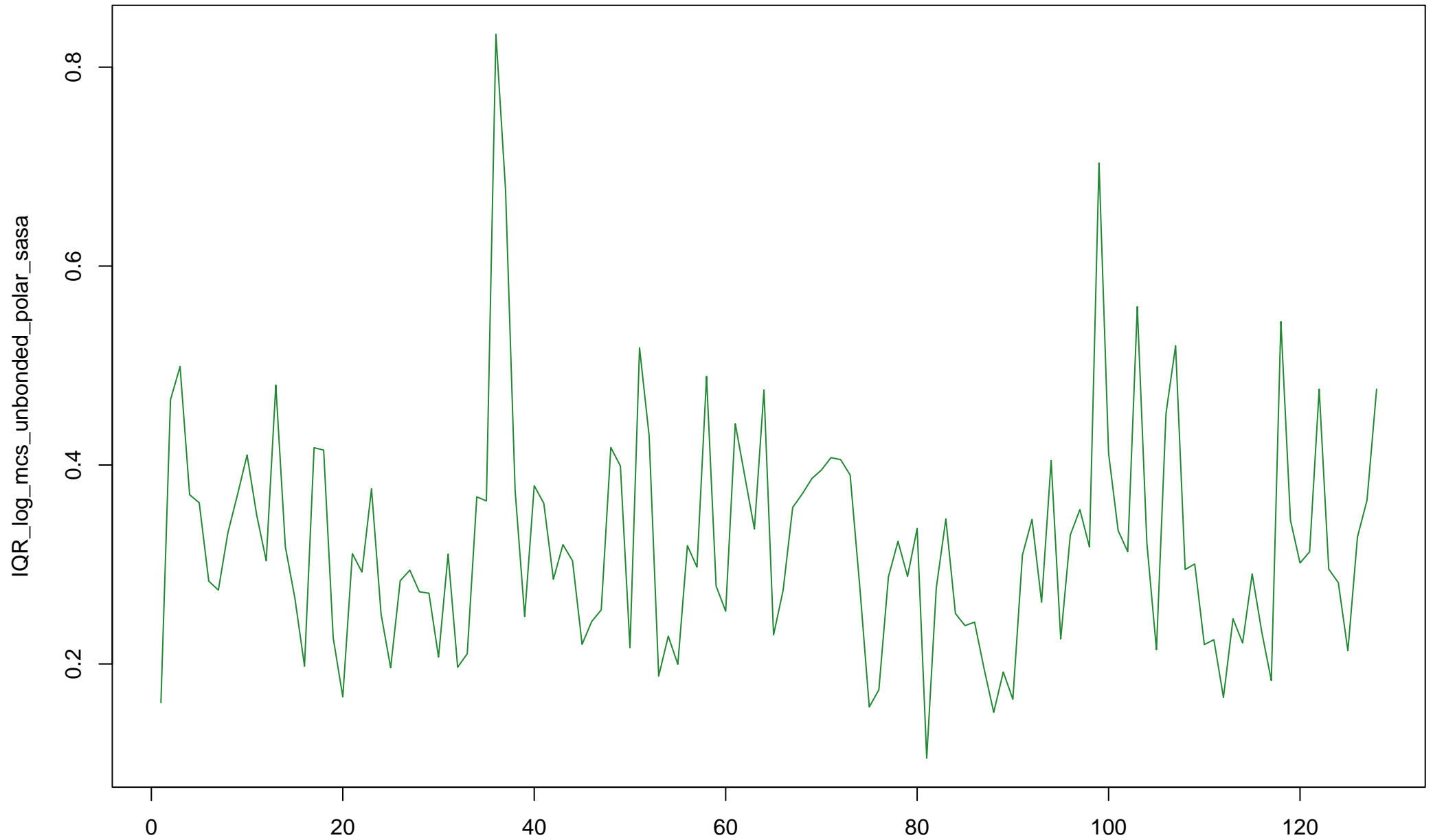
MEDIAN_mcs_NOCount
ESS = 128 | BMK = 0.0797 | MCSE(6.27) = 10.1 | stat: TRUE | burn: 0



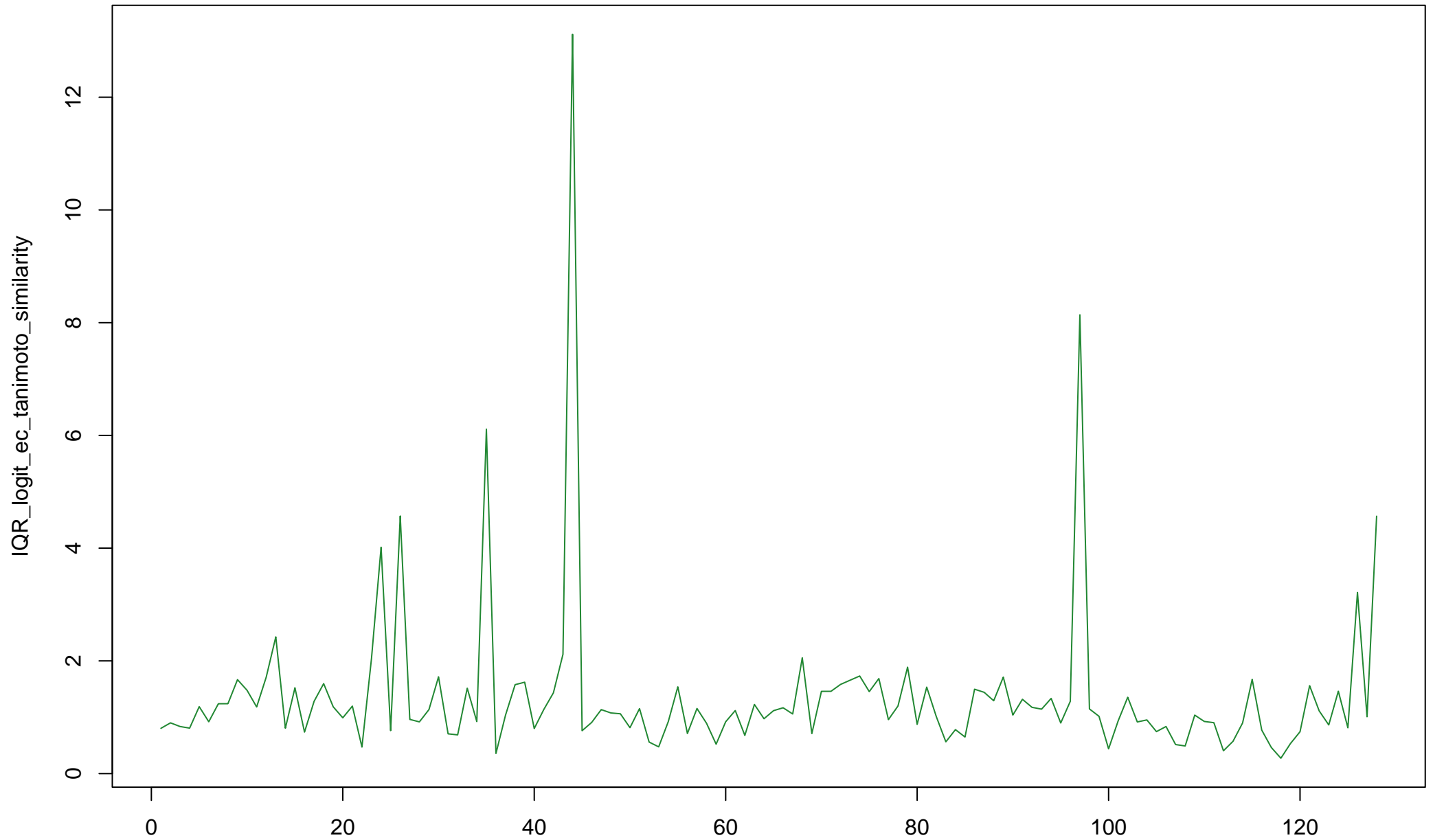
IQR_log_RMSD
ESS = 128 | BMK = 0.16 | MCSE(6.27) = 10.2 | stat: TRUE | burn: 0



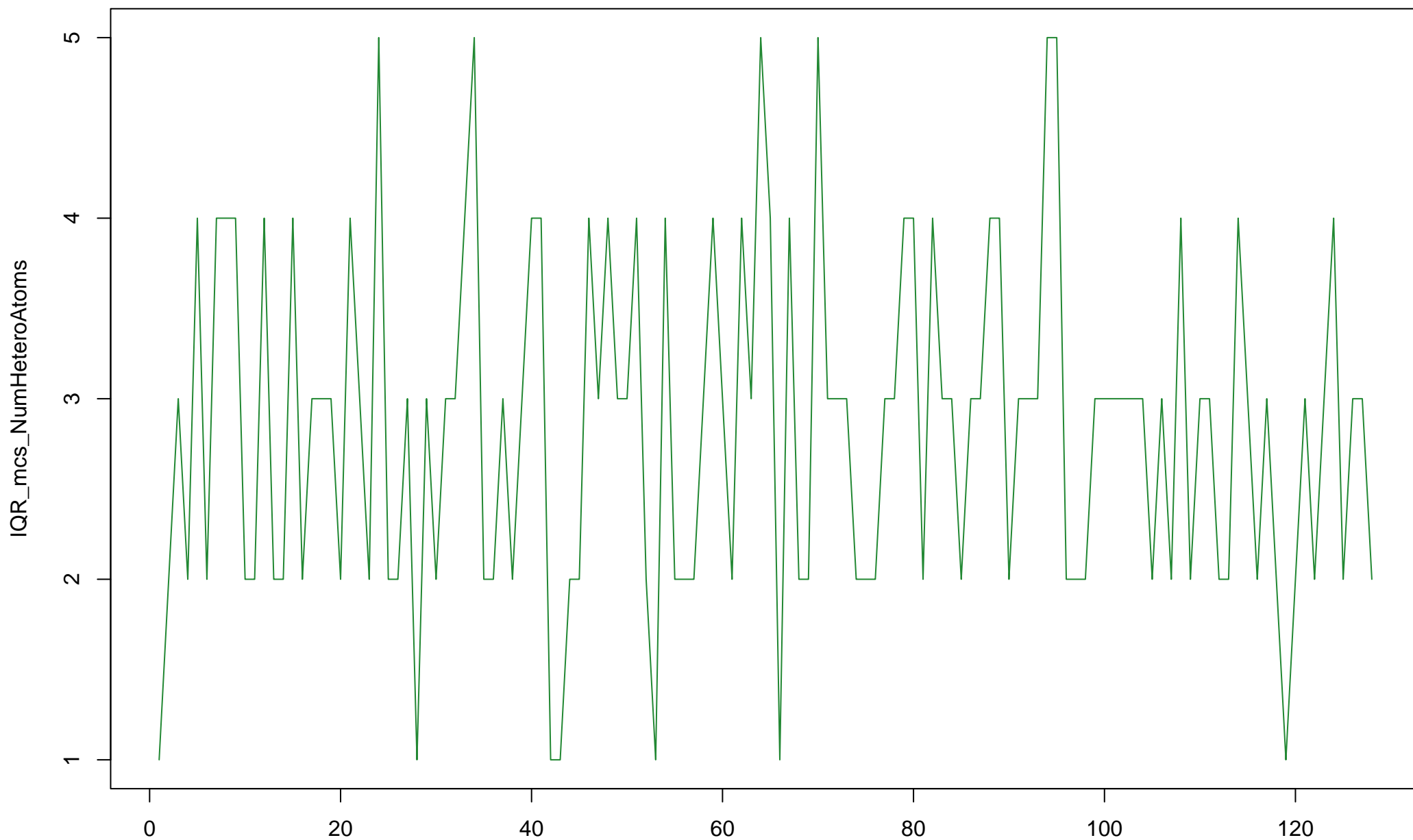
IQR_log_mcs_unbonded_polar_sasa
ESS = 67.7 | BMK = 0.102 | MCSE(6.27) = 13.6 | stat: TRUE | burn: 0



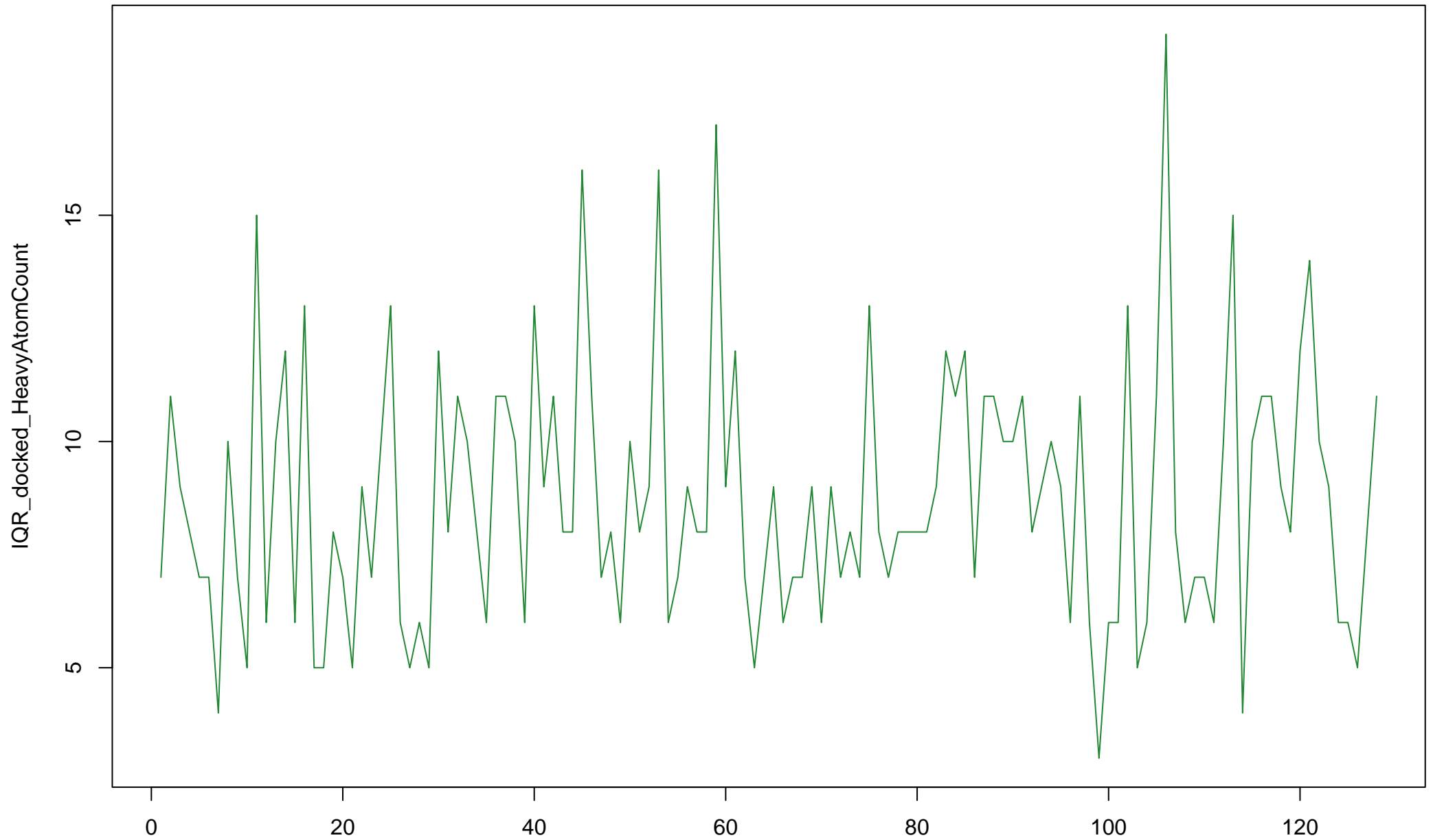
IQR_logit_ec_tanimoto_similarity
ESS = 128 | BMK = 0.197 | MCSE(6.27) = 9.23 | stat: TRUE | burn: 96



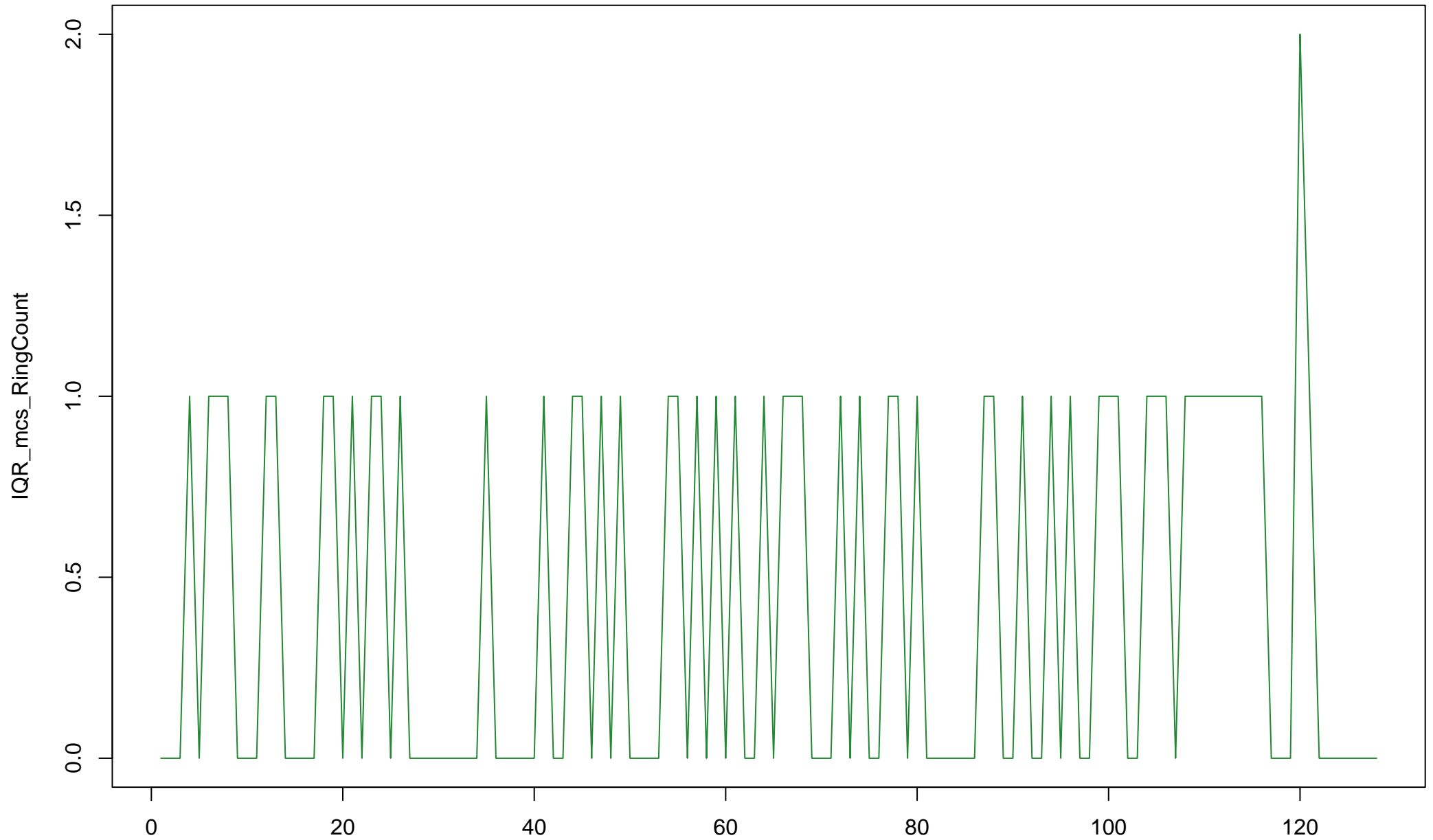
IQR_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.142 | MCSE(6.27) = 8.66 | stat: TRUE | burn: 0



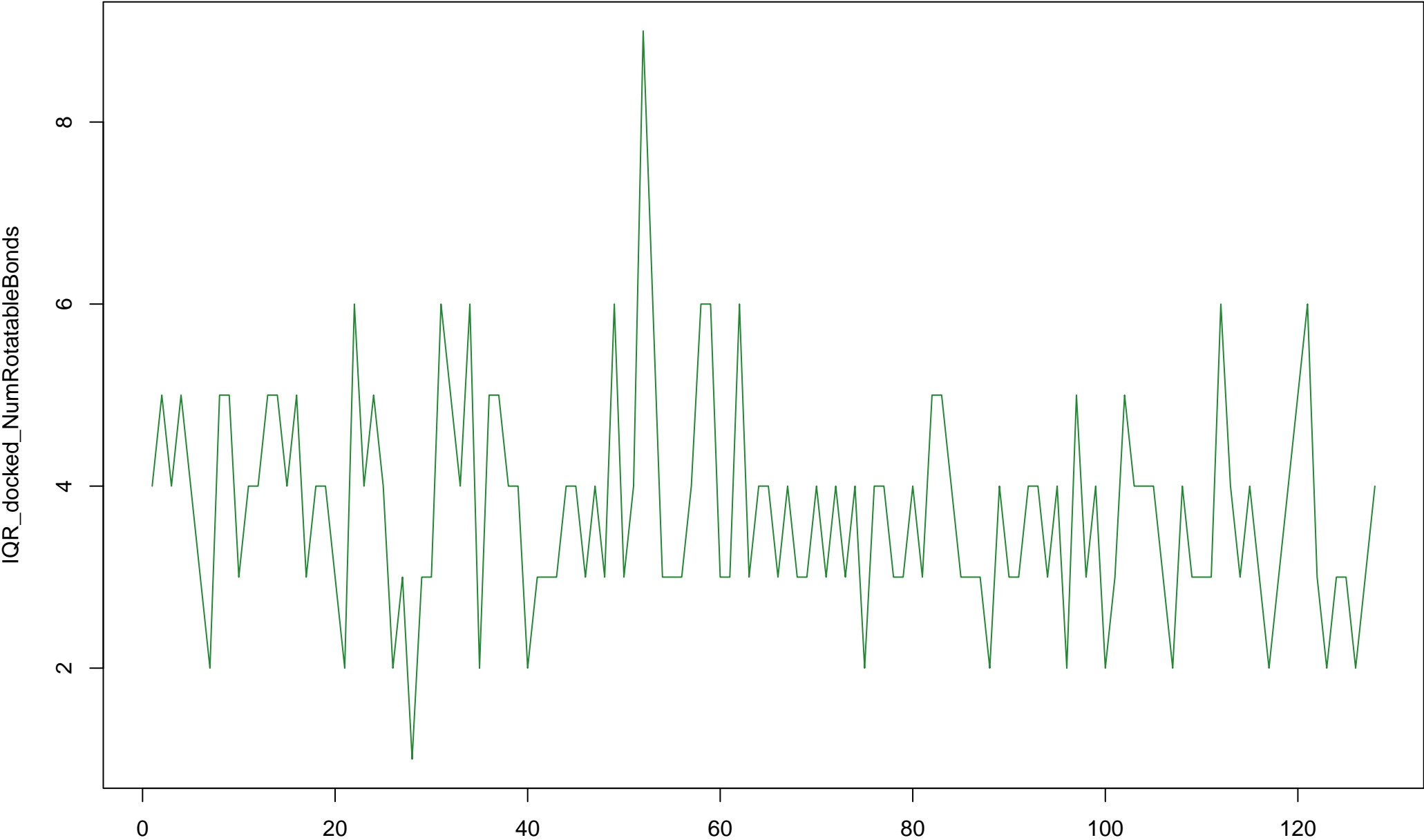
IQR_docked_HeavyAtomCount
ESS = 128 | BMK = 0.0903 | MCSE(6.27) = 8.93 | stat: TRUE | burn: 0



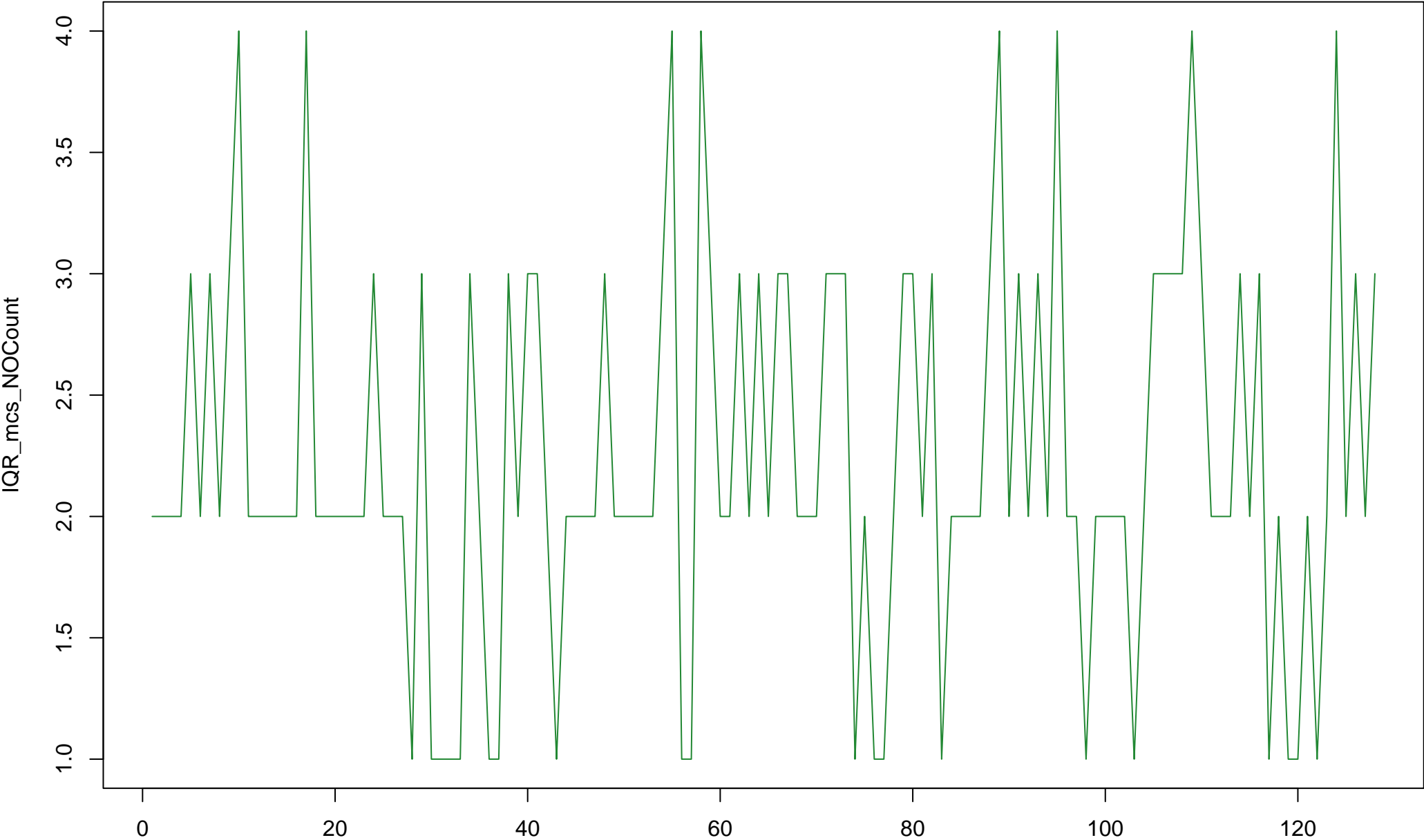
IQR_mcs_RingCount
ESS = 128 | BMK = 0.088 | MCSE(6.27) = 9.65 | stat: TRUE | burn: 0



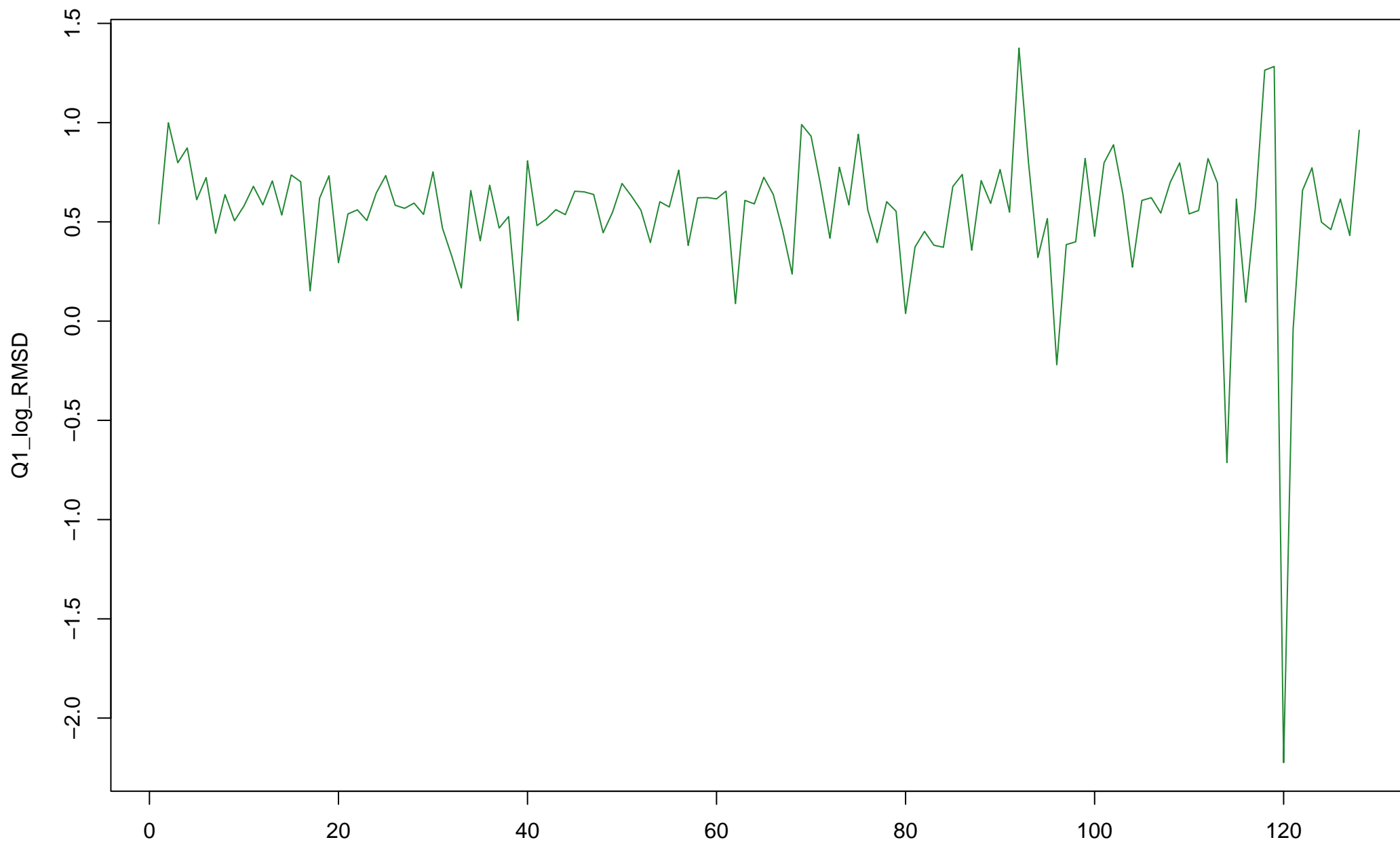
IQR_docked_NumRotatableBonds
ESS = 128 | BMK = 0.233 | MCSE(6.27) = 10.6 | stat: FALSE | burn: 0



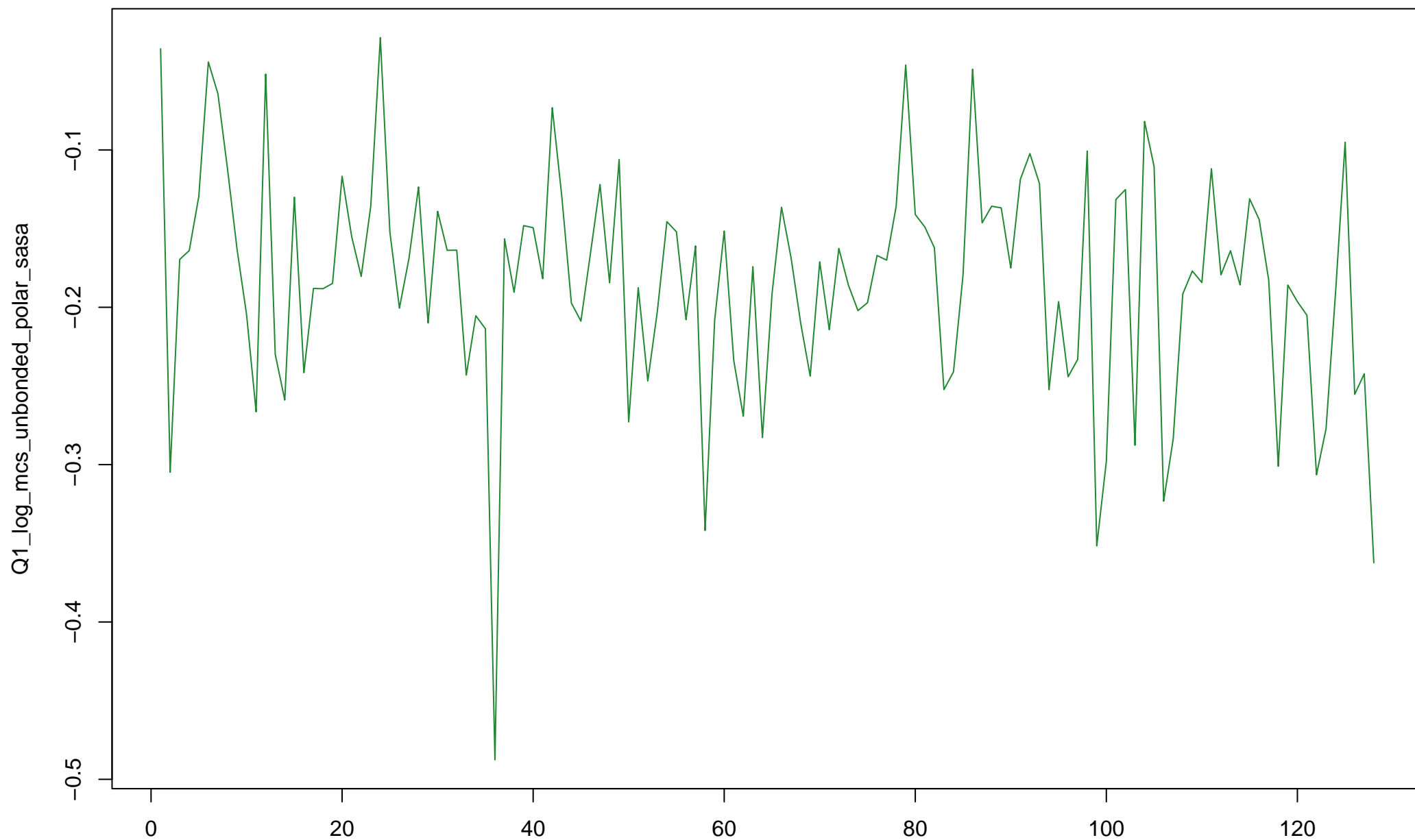
IQR_mcs_NOCount
ESS = 128 | BMK = 0.0724 | MCSE(6.27) = 11.1 | stat: TRUE | burn: 0



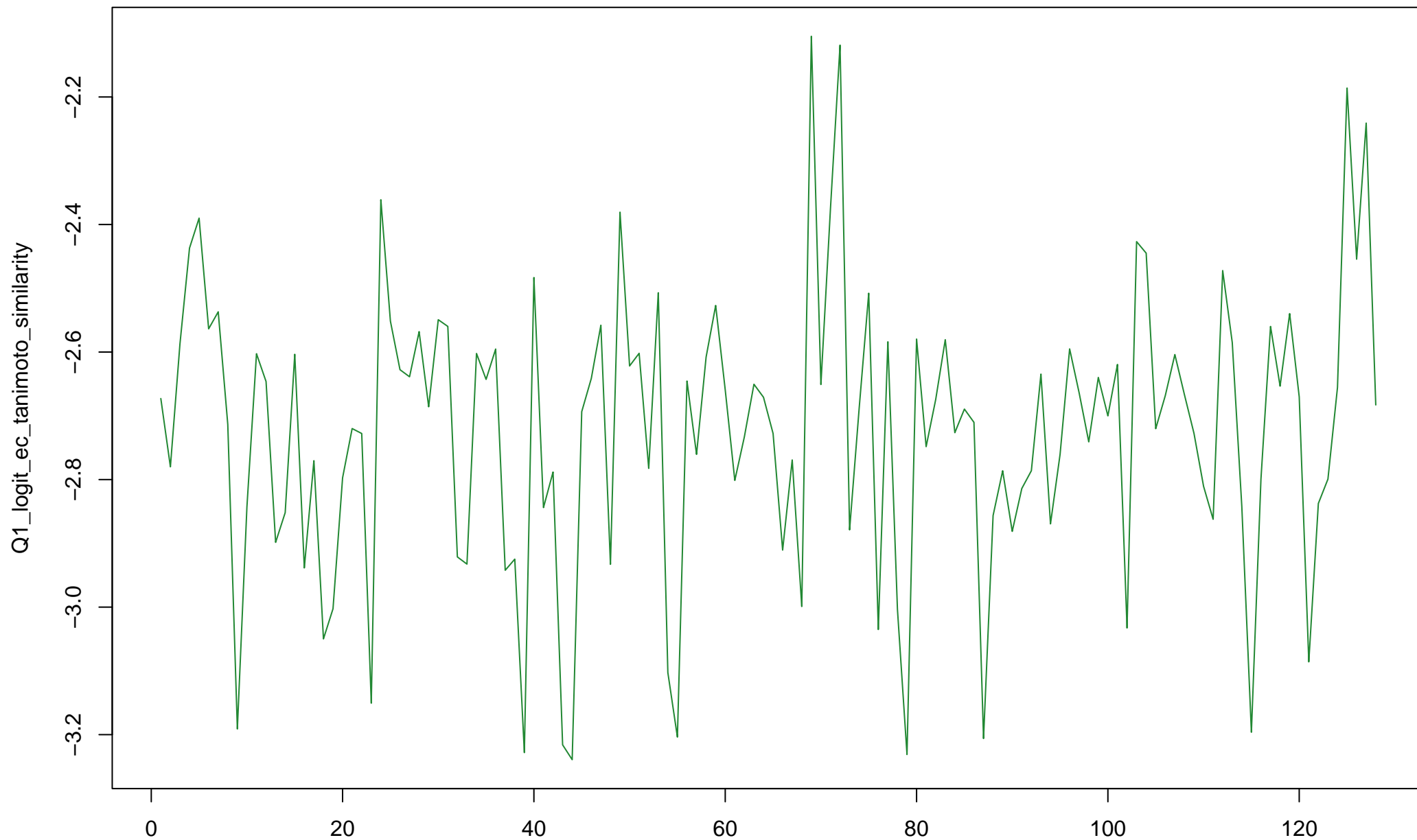
Q1_log_RMSD
ESS = 128 | BMK = 0.288 | MCSE(6.27) = 8.9 | stat: TRUE | burn: 0



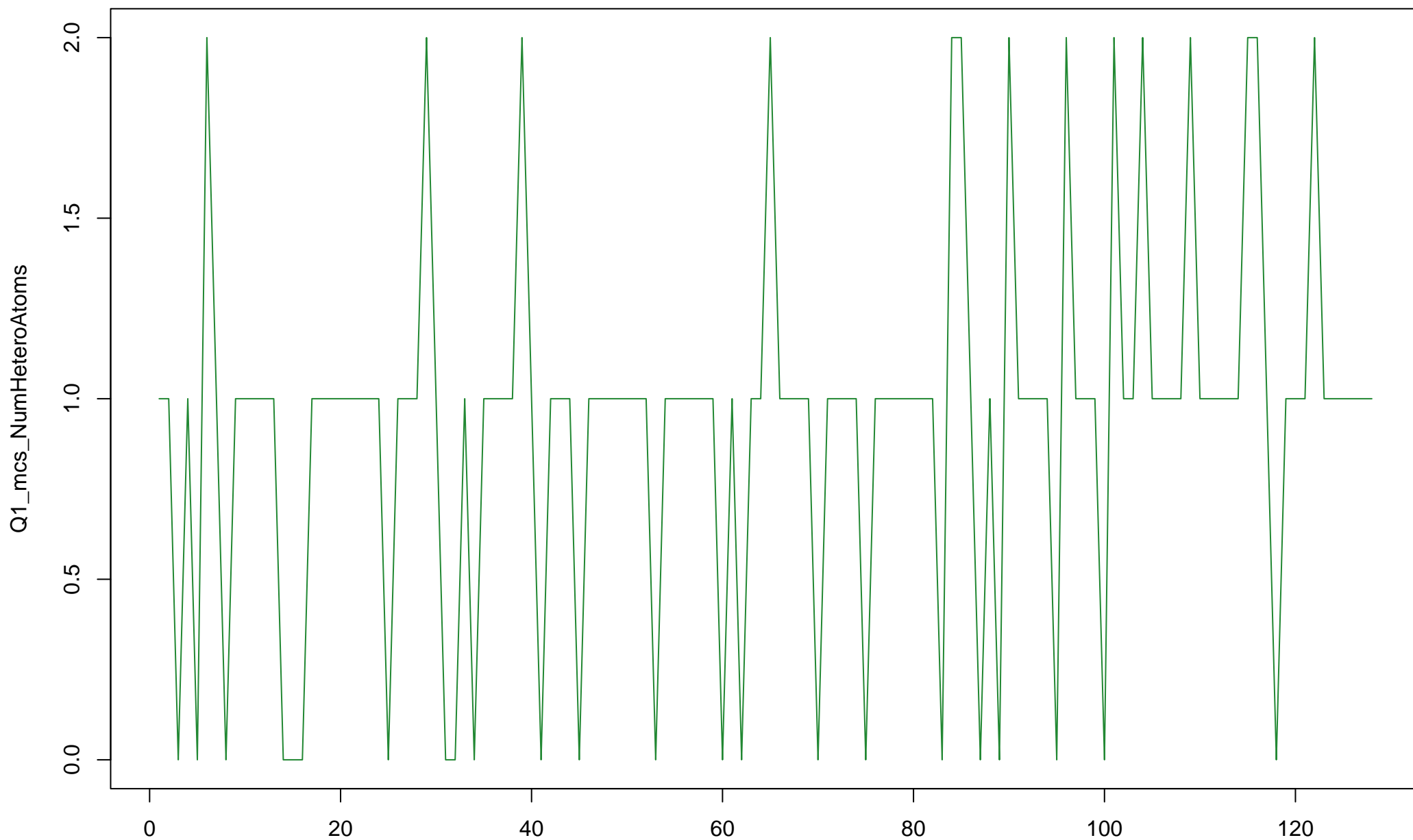
Q1_log_mcs_unbonded_polar_sasa
ESS = 128 | BMK = 0.135 | MCSE(6.27) = 11 | stat: TRUE | burn: 120



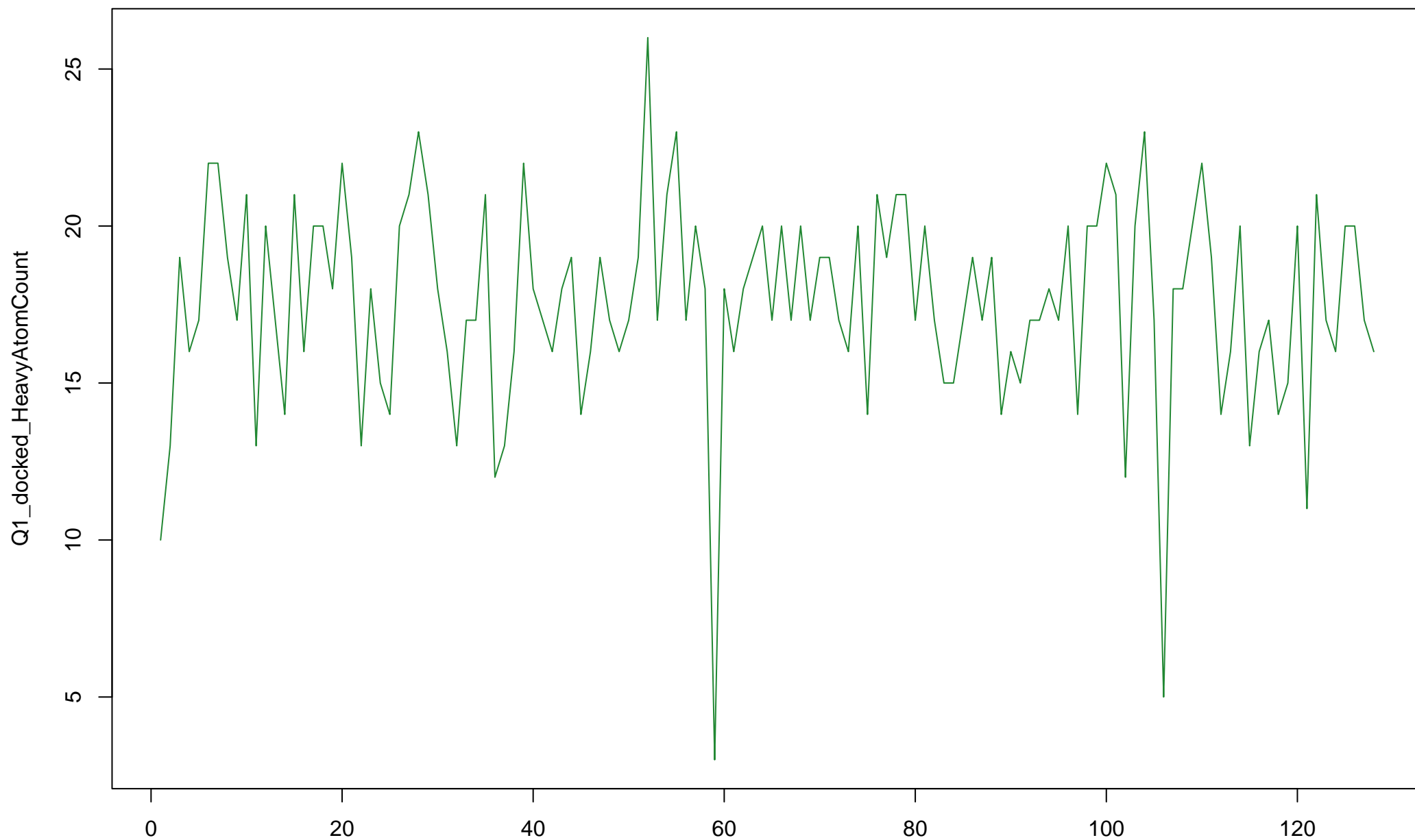
Q1_logit_ec_tanimoto_similarity
ESS = 89.5 | BMK = 0.14 | MCSE(6.27) = 12.1 | stat: TRUE | burn: 96



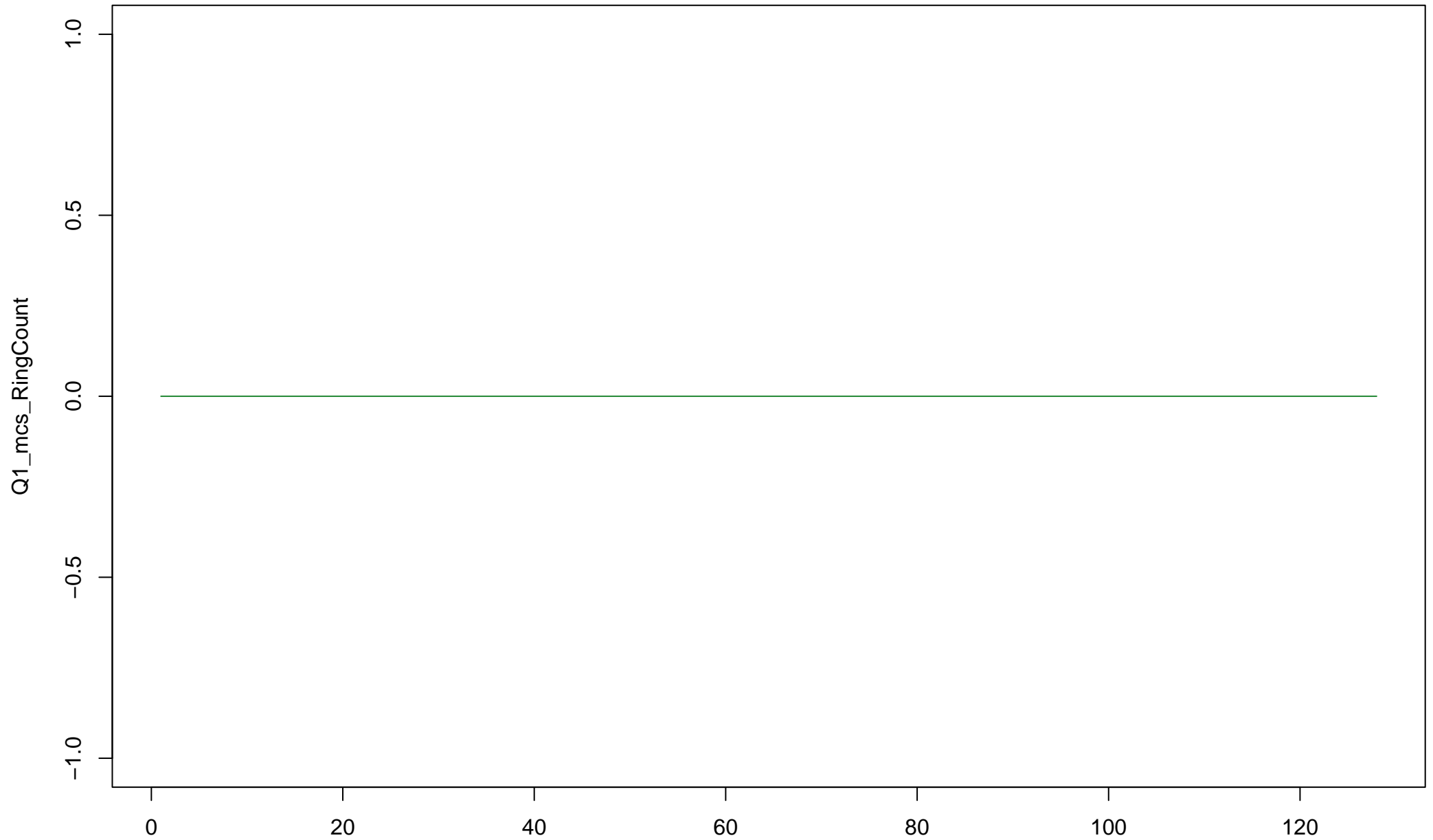
Q1_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.126 | MCSE(6.27) = 8.65 | stat: TRUE | burn: 0



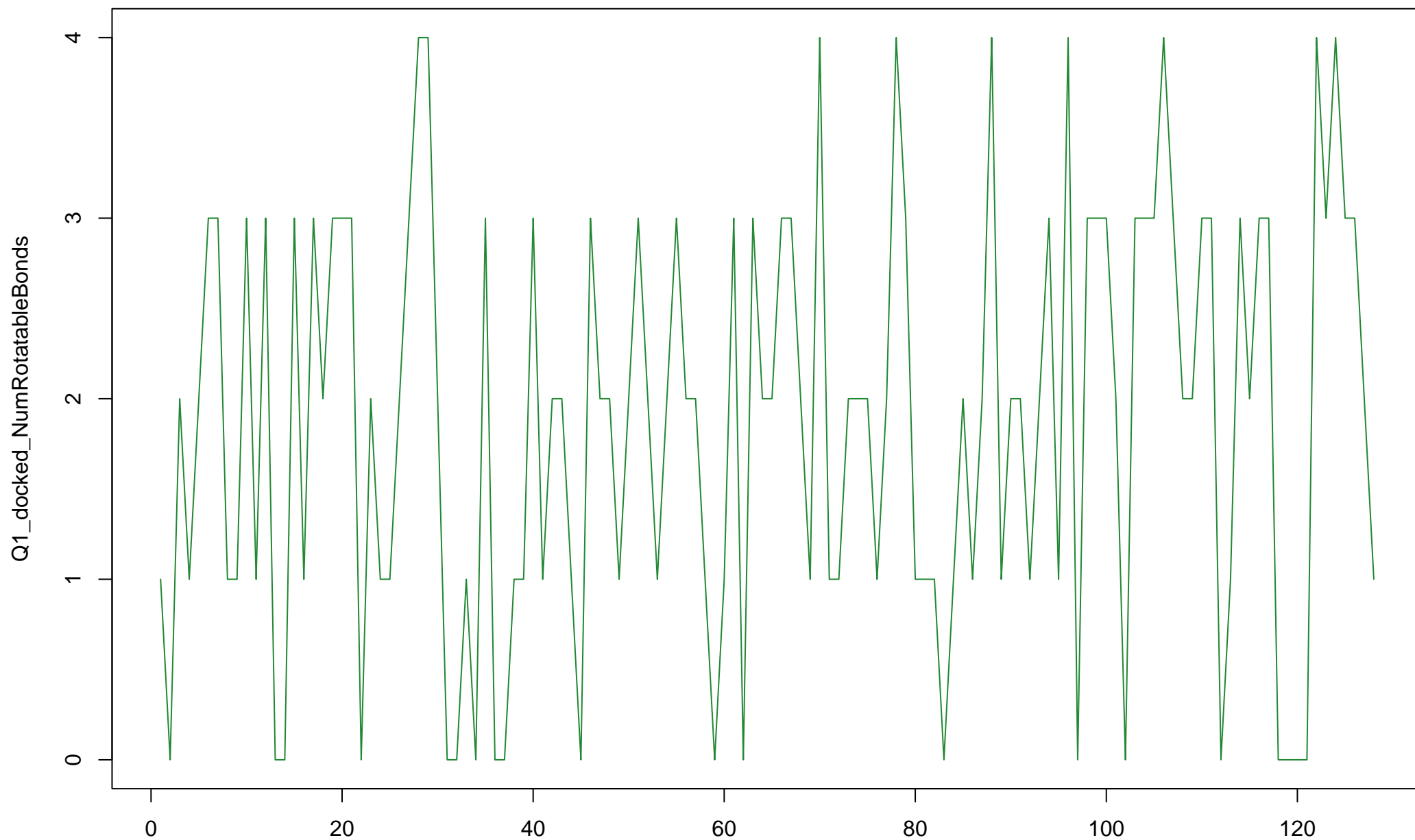
Q1_docked_HeavyAtomCount
ESS = 128 | BMK = 0.095 | MCSE(6.27) = 9.11 | stat: TRUE | burn: 0



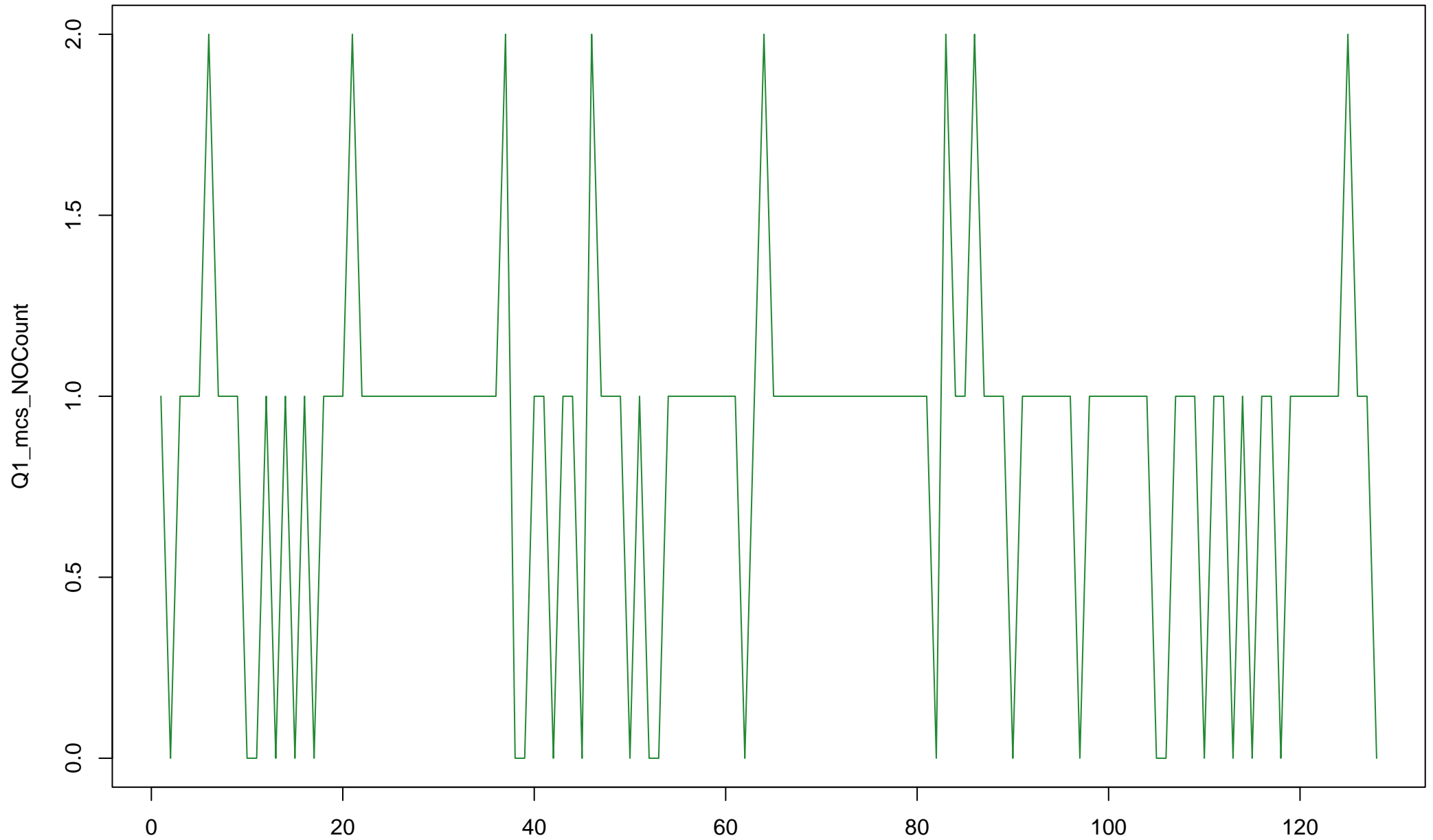
Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



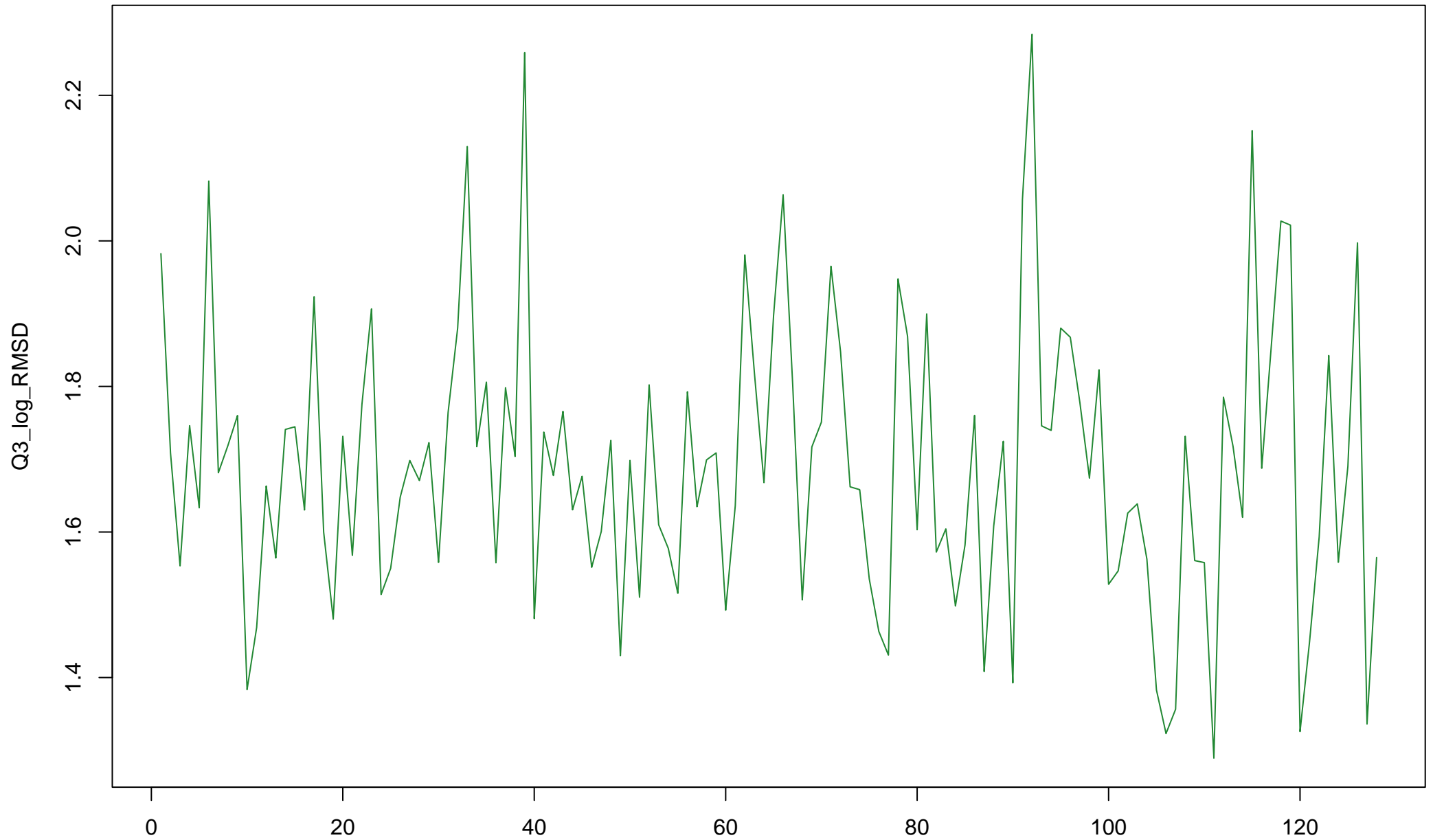
Q1_docked_NumRotatableBonds
ESS = 96.1 | BMK = 0.0764 | MCSE(6.27) = 11.3 | stat: TRUE | burn: 0



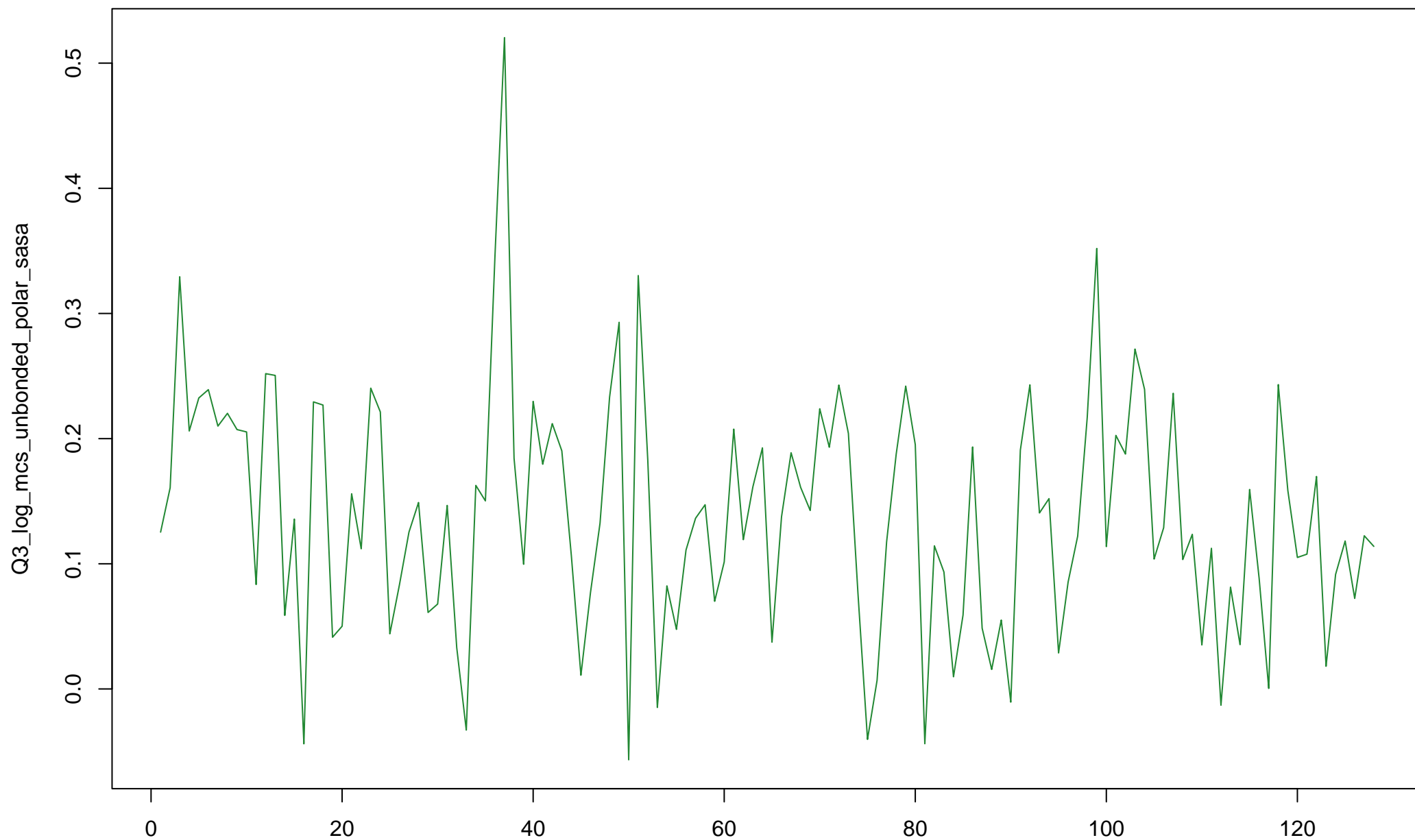
Q1_mcs_NOCount
ESS = 128 | BMK = 0.104 | MCSE(6.27) = 8.64 | stat: TRUE | burn: 48



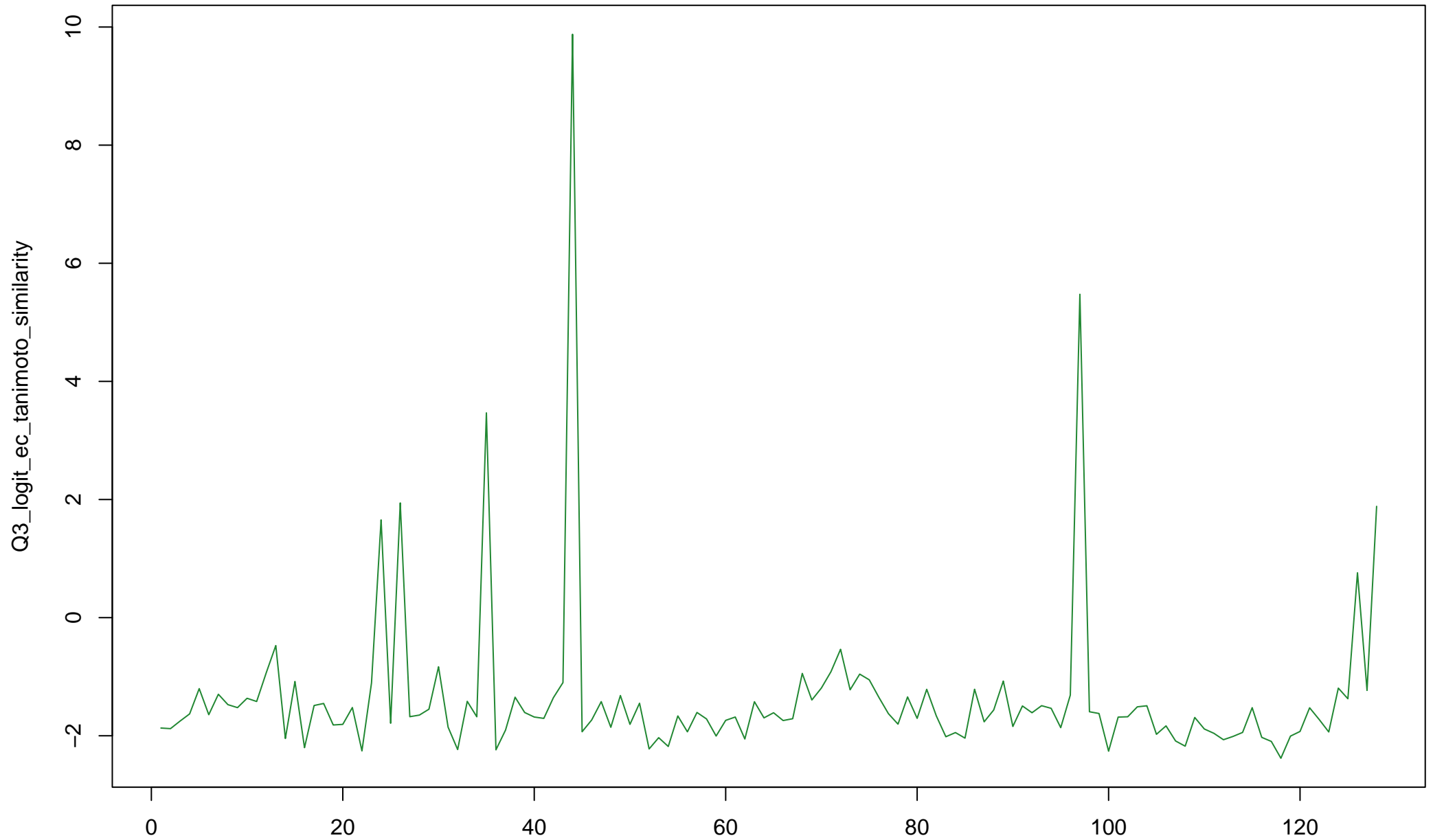
Q3_log_RMSD
ESS = 95.8 | BMK = 0.181 | MCSE(6.27) = 11.8 | stat: TRUE | burn: 0



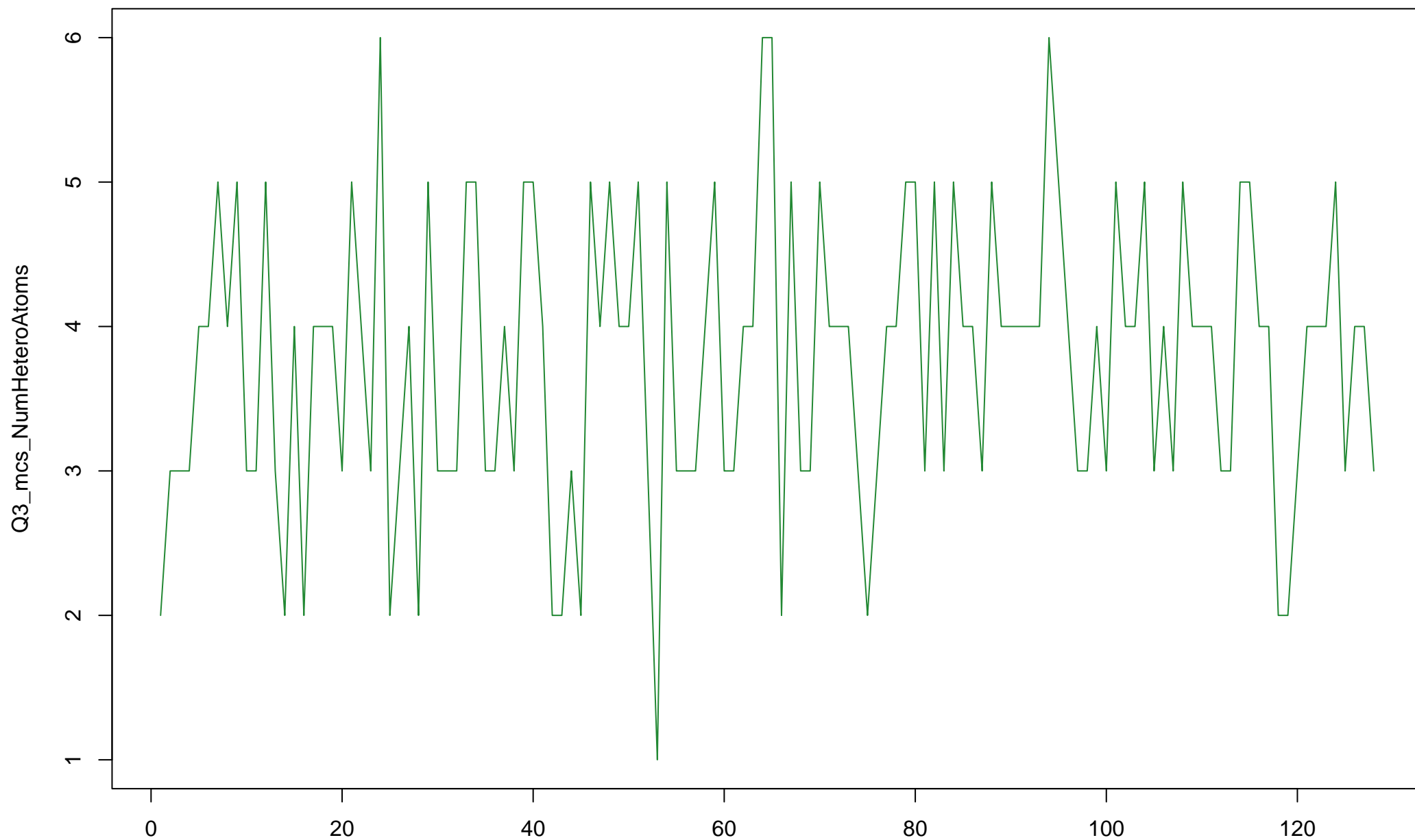
Q3_log_mcs_unbonded_polar_sasa
ESS = 76.2 | BMK = 0.123 | MCSE(6.27) = 13.3 | stat: FALSE | burn: 0



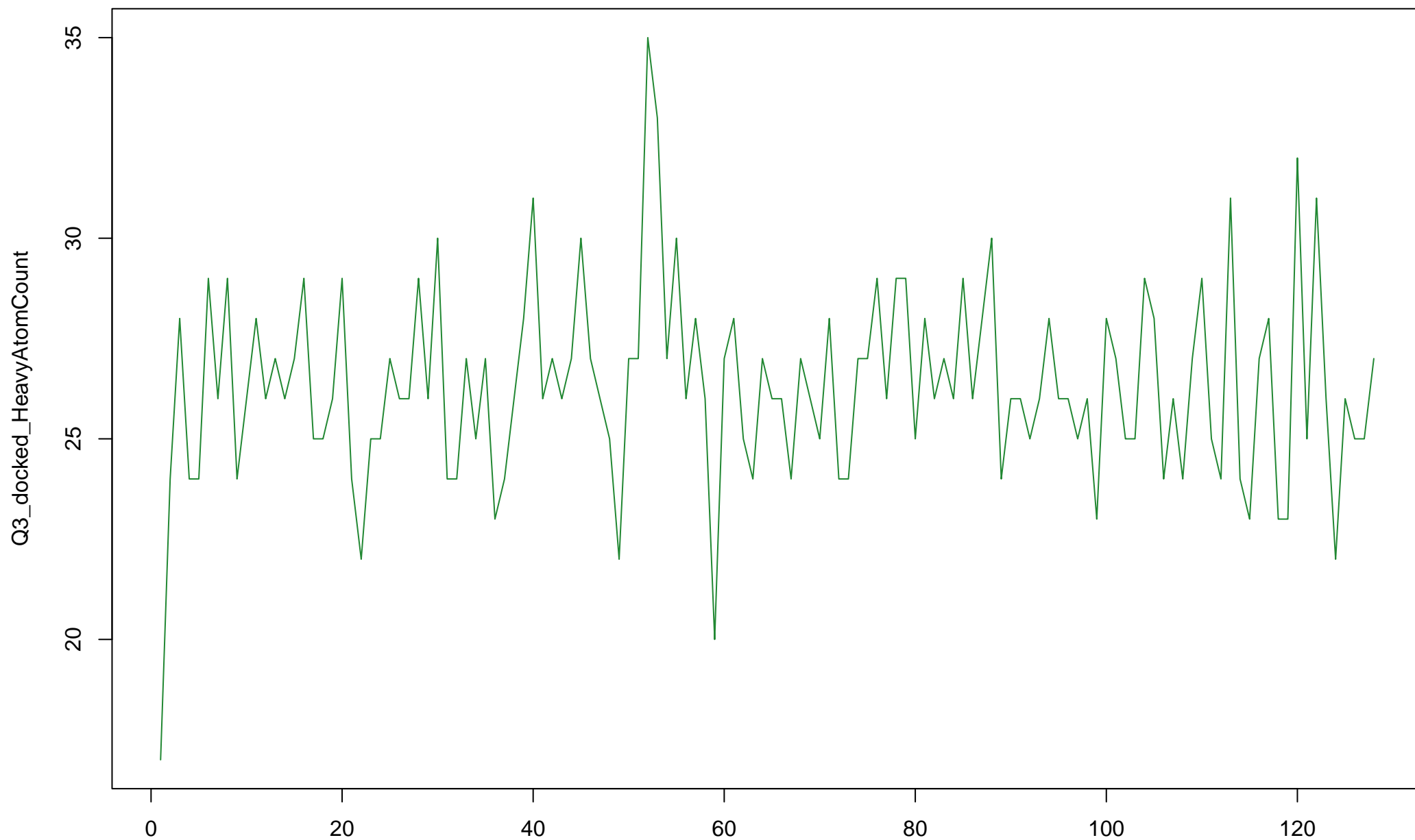
Q3_logit_ec_tanimoto_similarity
ESS = 128 | BMK = 0.189 | MCSE(6.27) = 9.54 | stat: TRUE | burn: 48



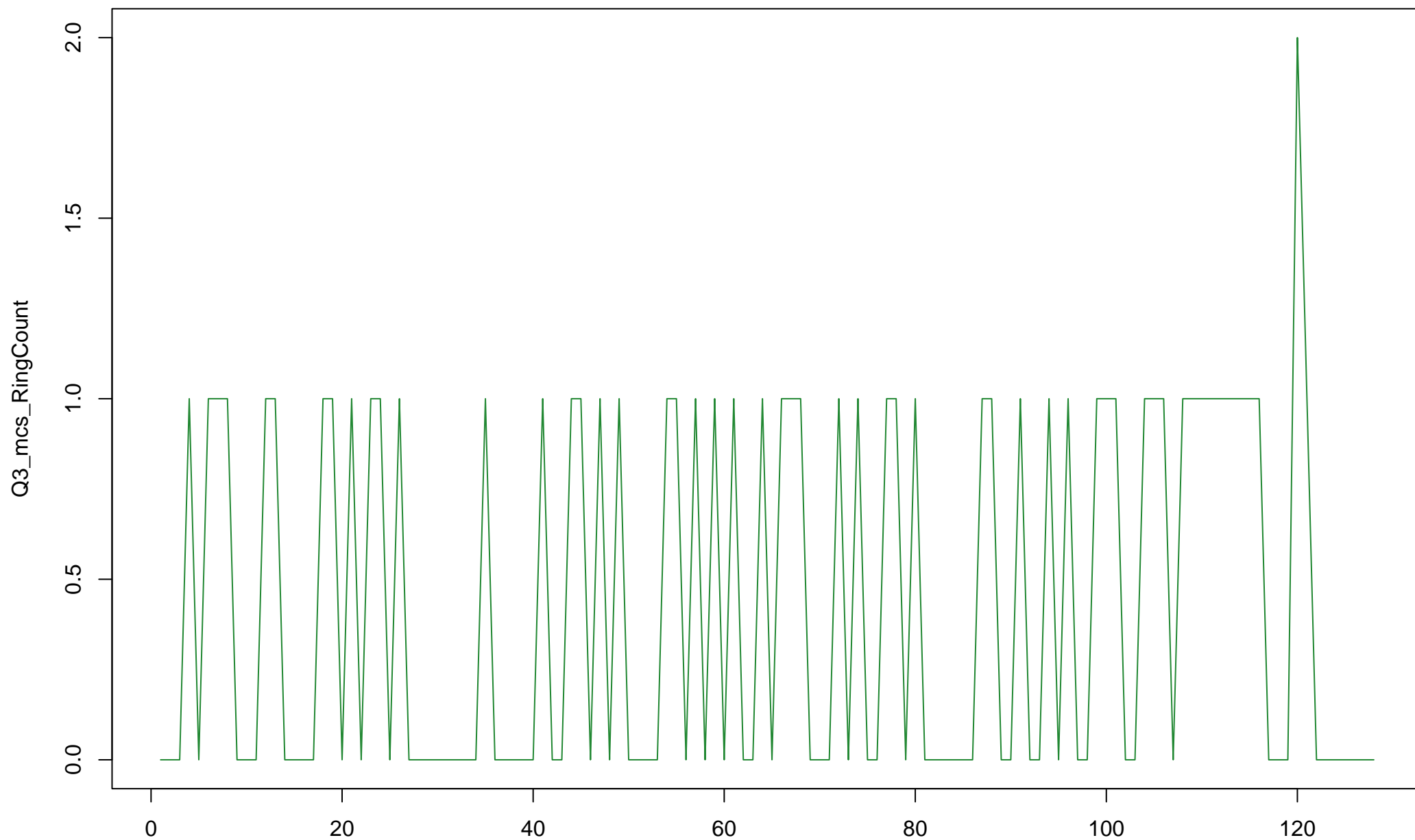
Q3_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.122 | MCSE(6.27) = 8.94 | stat: TRUE | burn: 96



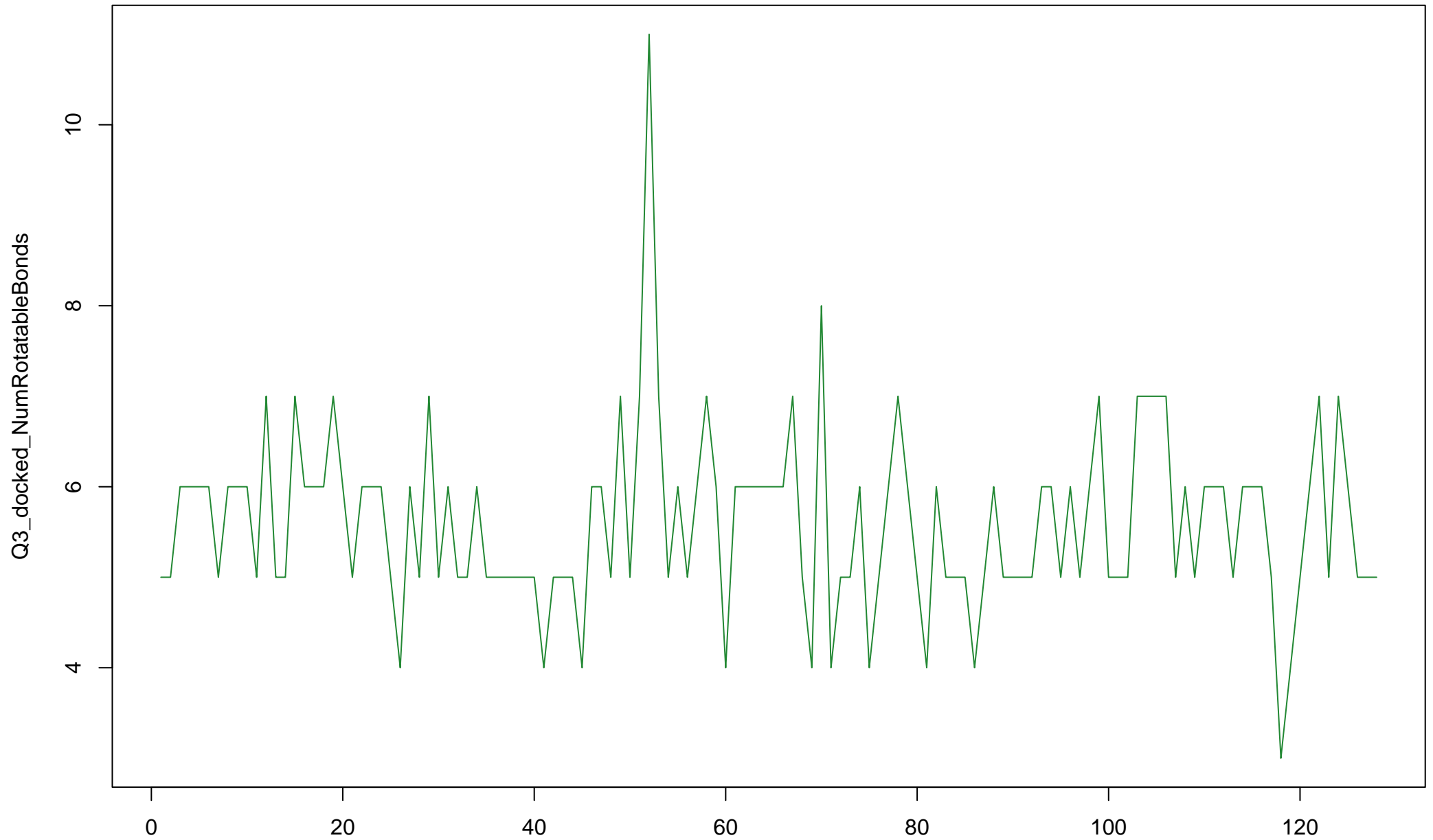
Q3_docked_HeavyAtomCount
ESS = 128 | BMK = 0.135 | MCSE(6.27) = 9.28 | stat: TRUE | burn: 0



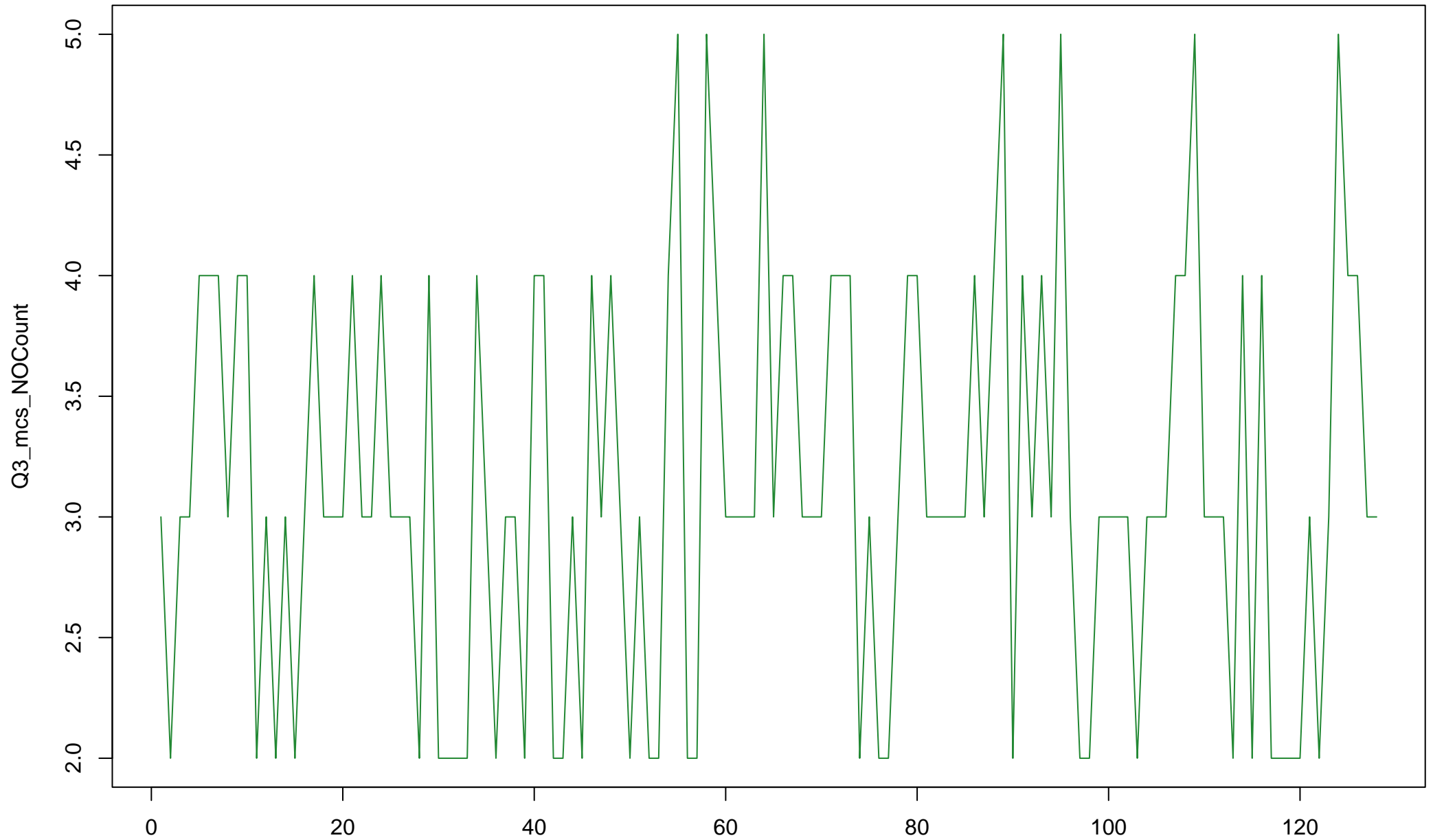
Q3_mcs_RingCount
ESS = 128 | BMK = 0.088 | MCSE(6.27) = 9.65 | stat: TRUE | burn: 0



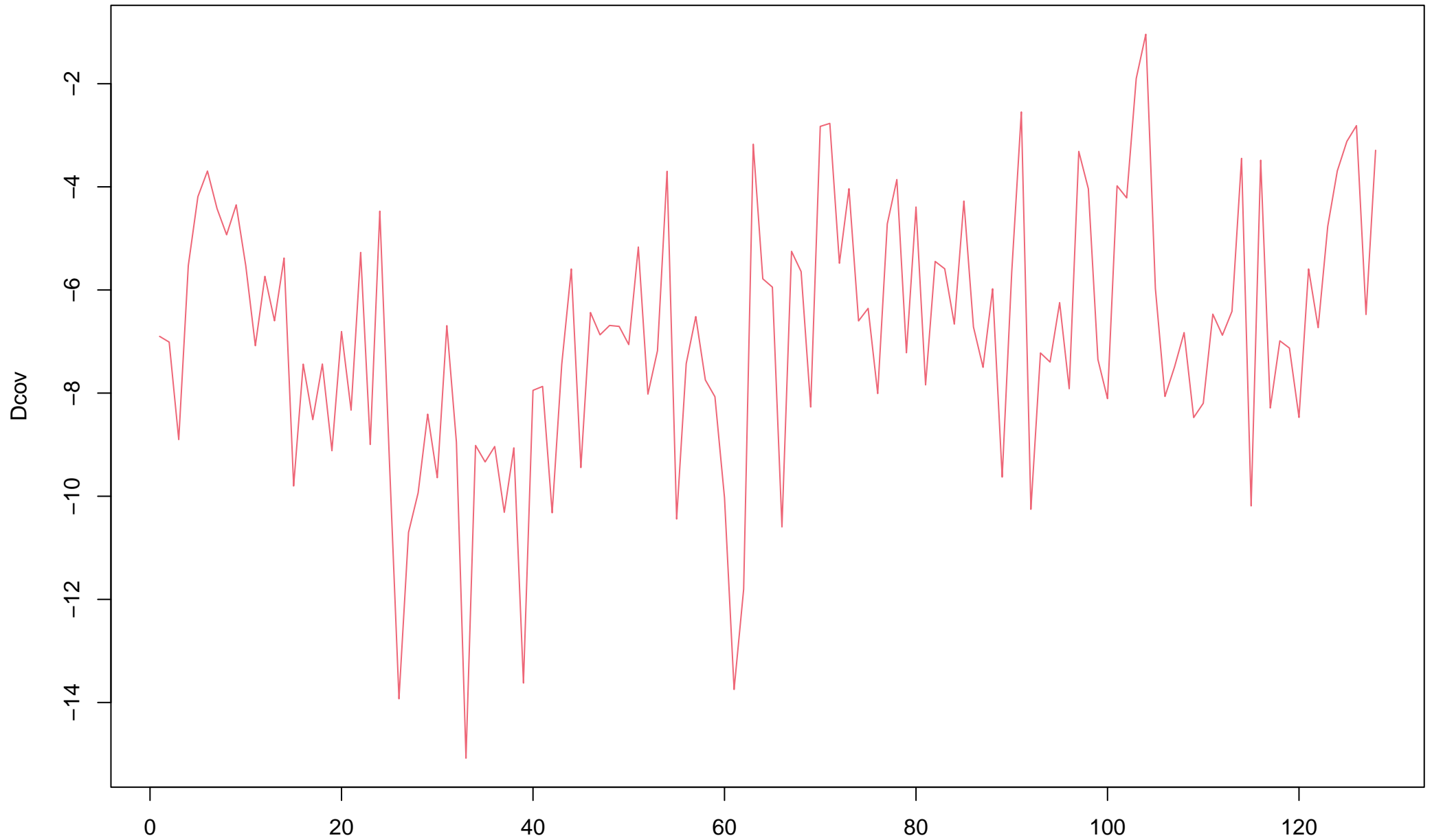
Q3_docked_NumRotatableBonds
ESS = 90.4 | BMK = 0.129 | MCSE(6.27) = 12.3 | stat: TRUE | burn: 24



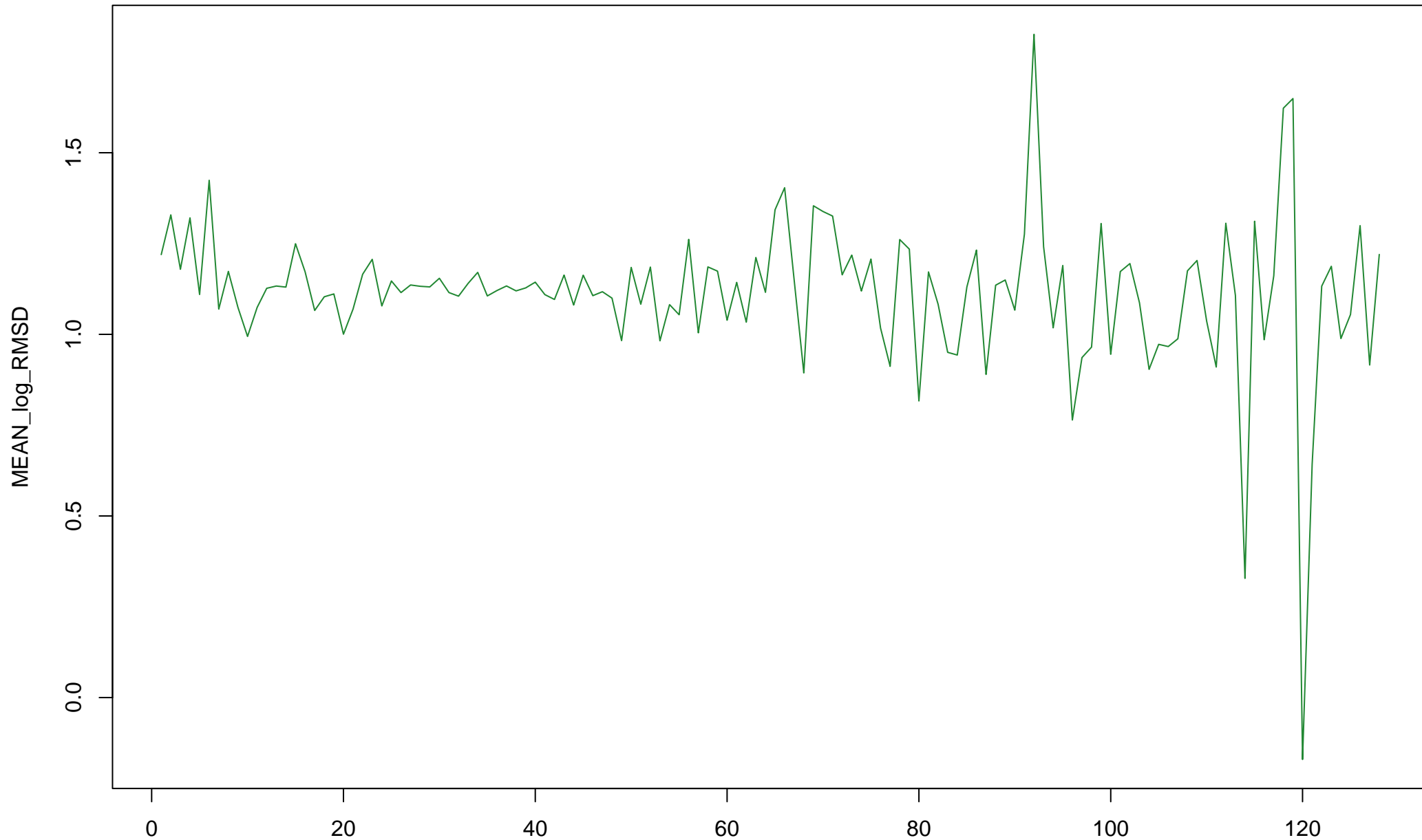
Q3_mcs_NOCount
ESS = 128 | BMK = 0.0601 | MCSE(6.27) = 10.9 | stat: TRUE | burn: 120



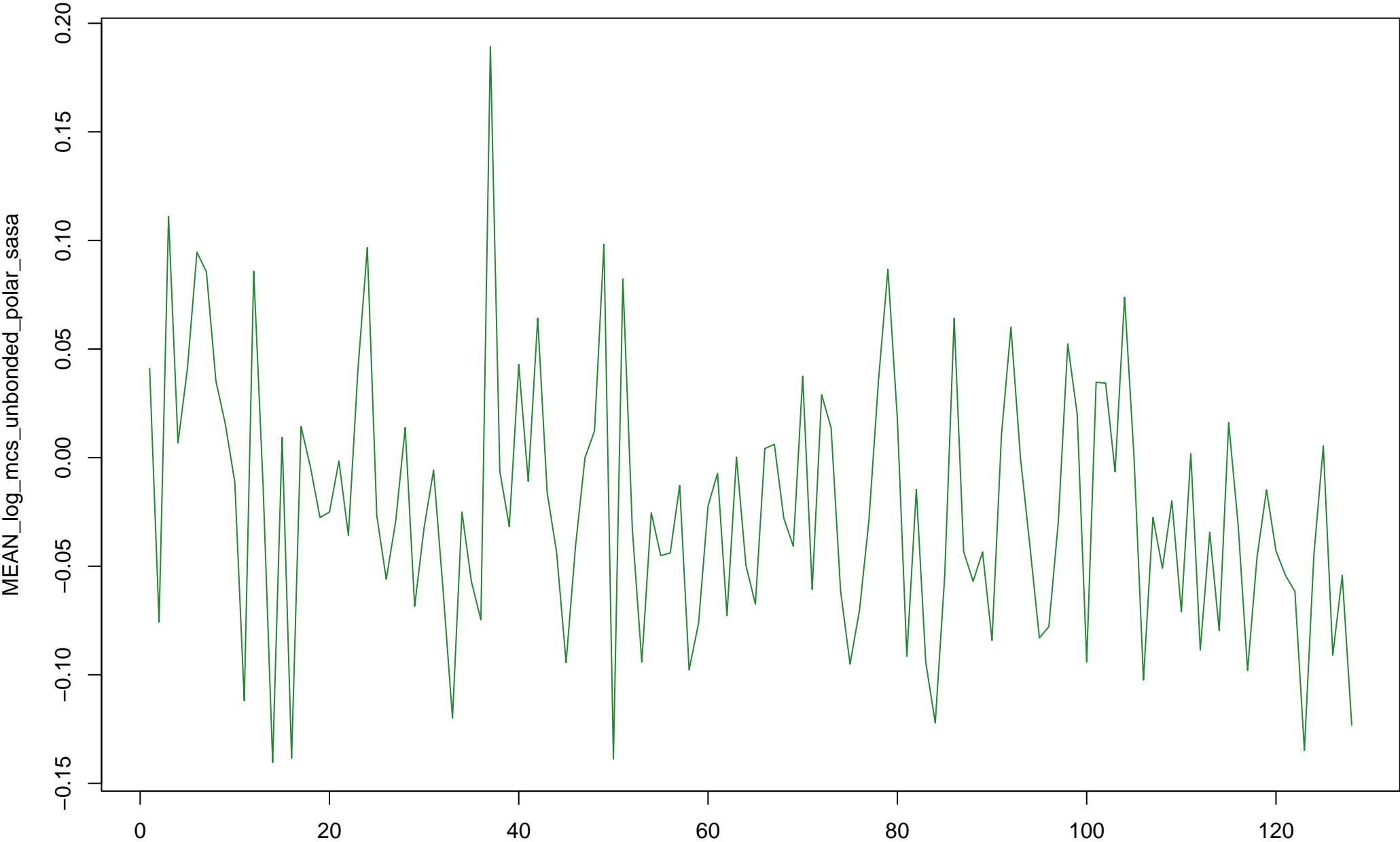
Dcov
ESS = 63.7 | BMK = 0.489 | MCSE(6.27) = 13.5 | stat: TRUE | burn: 120



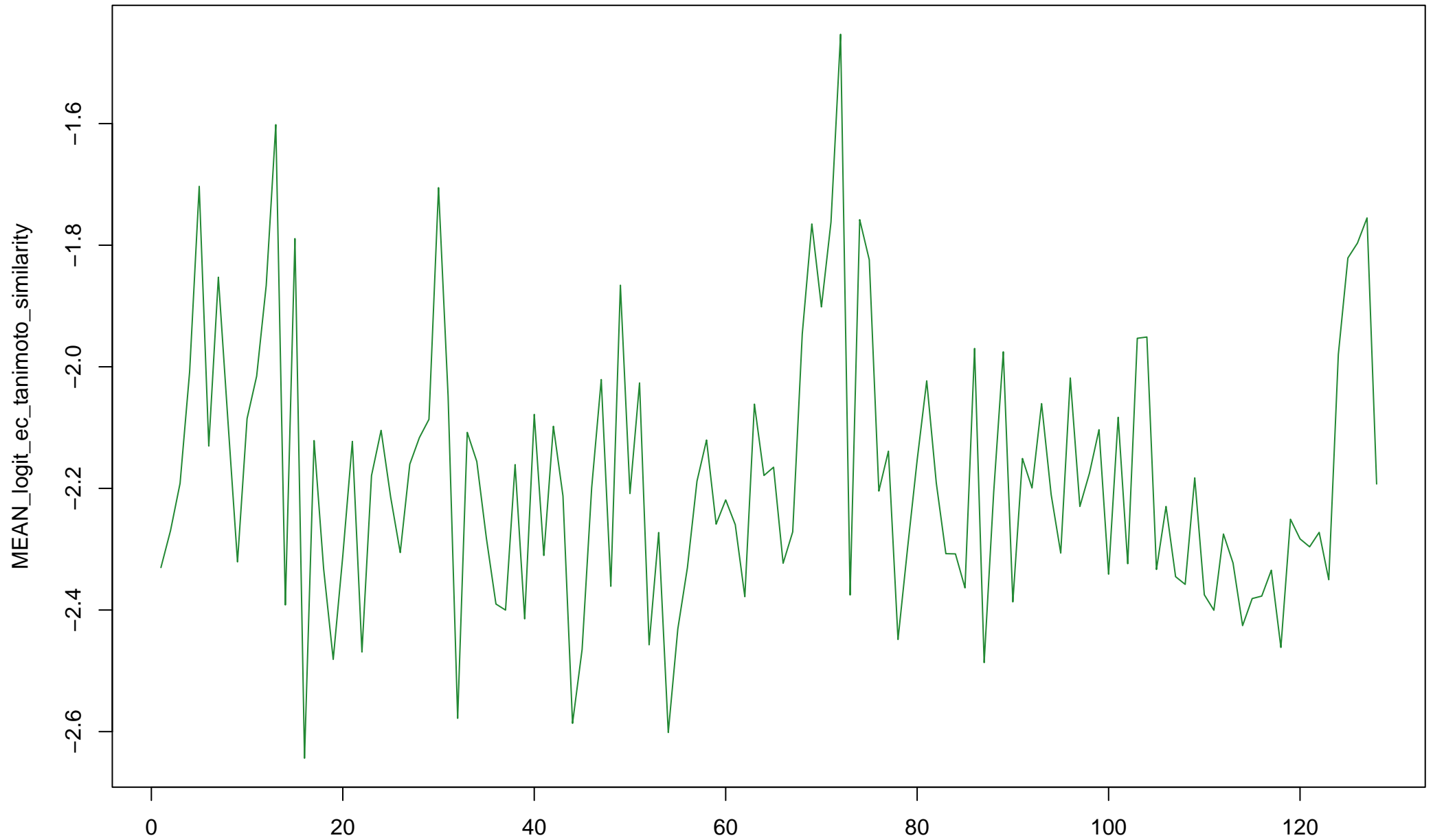
MEAN_log_RMSD
ESS = 128 | BMK = 0.45 | MCSE(6.27) = 9.19 | stat: TRUE | burn: 48



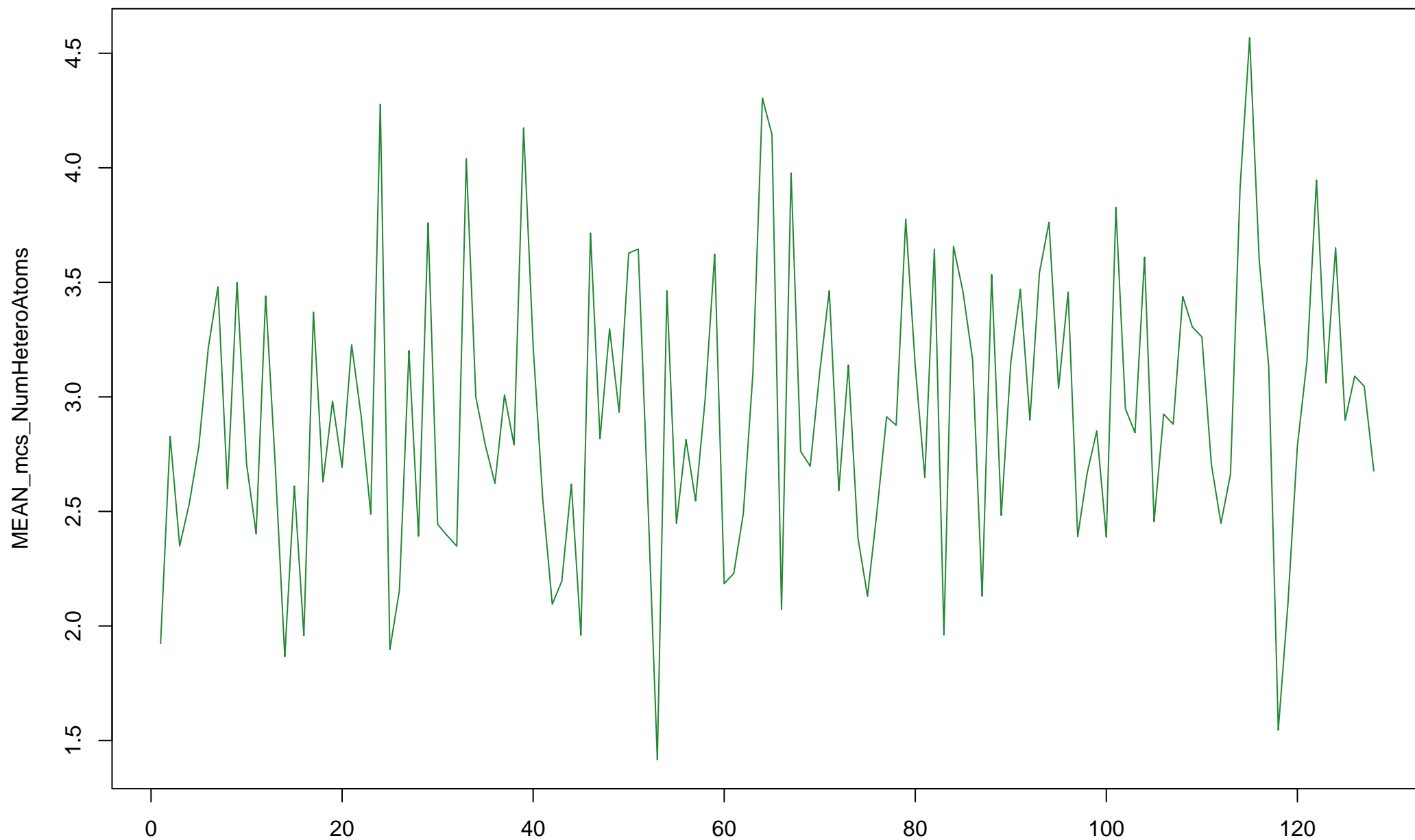
MEAN_log_mcs_unbonded_polar_sasa
ESS = 111 | BMK = 0.163 | MCSE(6.27) = 9.97 | stat: FALSE | burn: 0



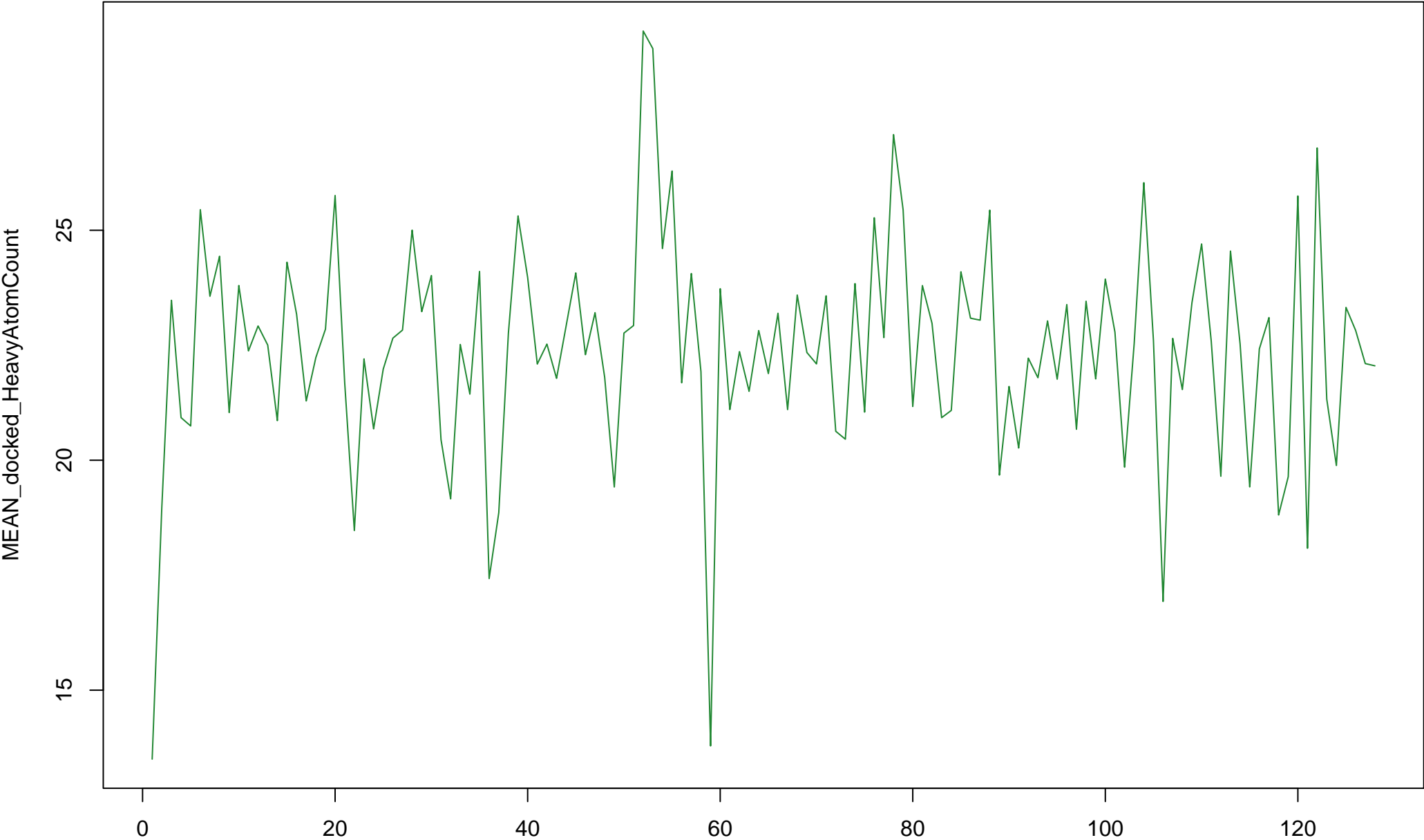
MEAN_logit_ec_tanimoto_similarity
ESS = 48.3 | BMK = 0.136 | MCSE(6.27) = 17.2 | stat: TRUE | burn: 0



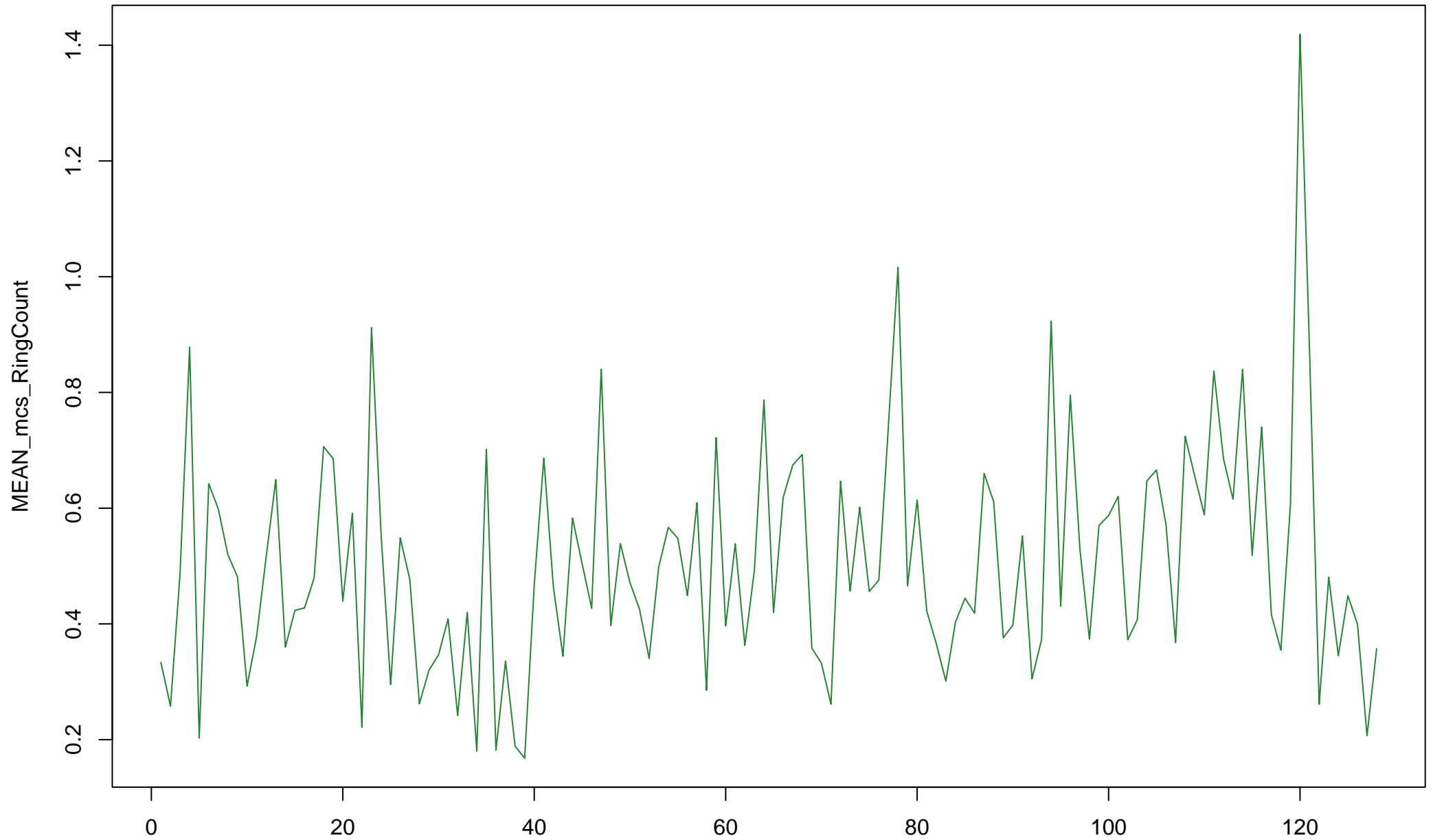
MEAN_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.133 | MCSE(6.27) = 9.18 | stat: TRUE | burn: 0



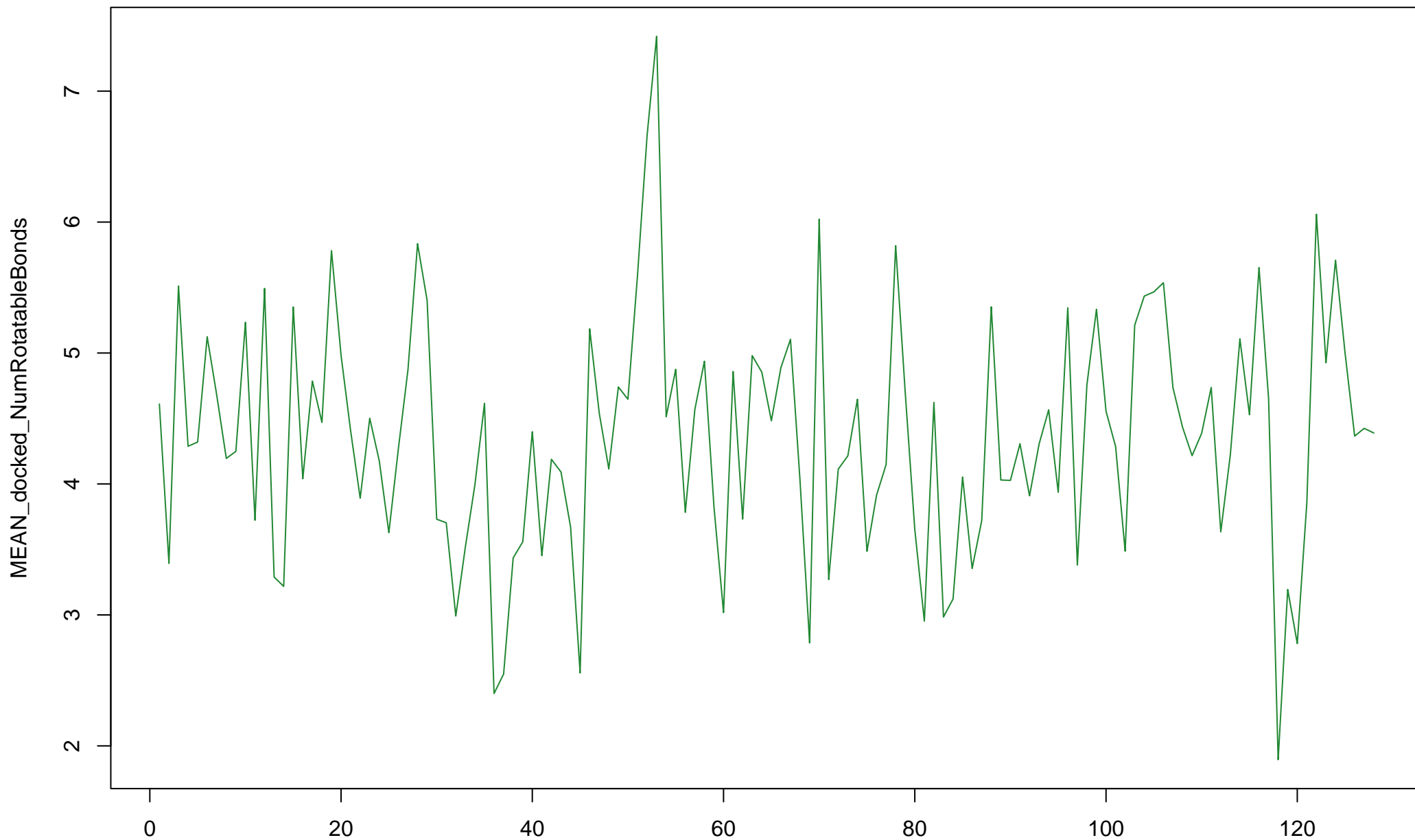
MEAN_docked_HeavyAtomCount
ESS = 128 | BMK = 0.151 | MCSE(6.27) = 10.3 | stat: TRUE | burn: 60



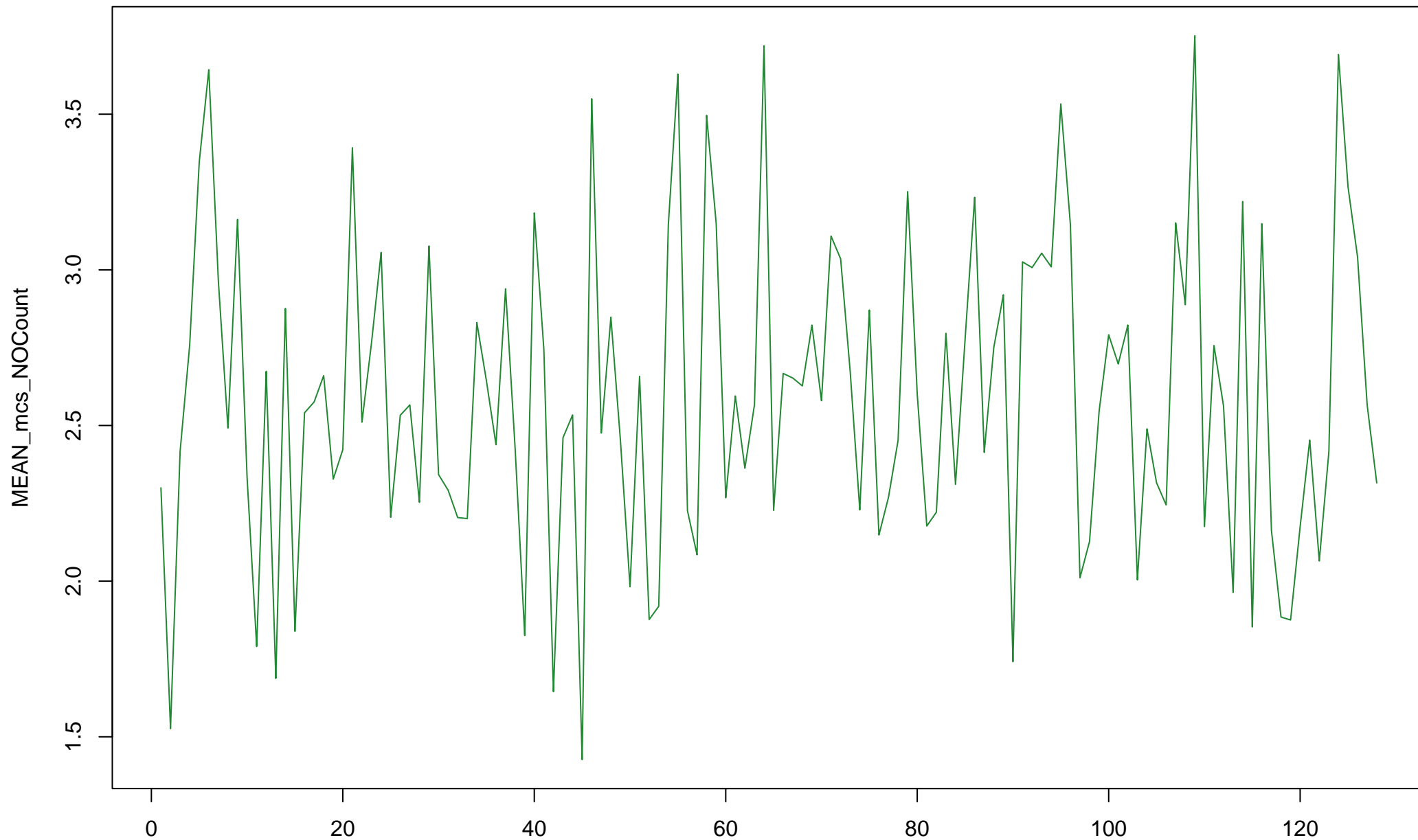
MEAN_mcs_RingCount
ESS = 128 | BMK = 0.144 | MCSE(6.27) = 11.5 | stat: TRUE | burn: 0



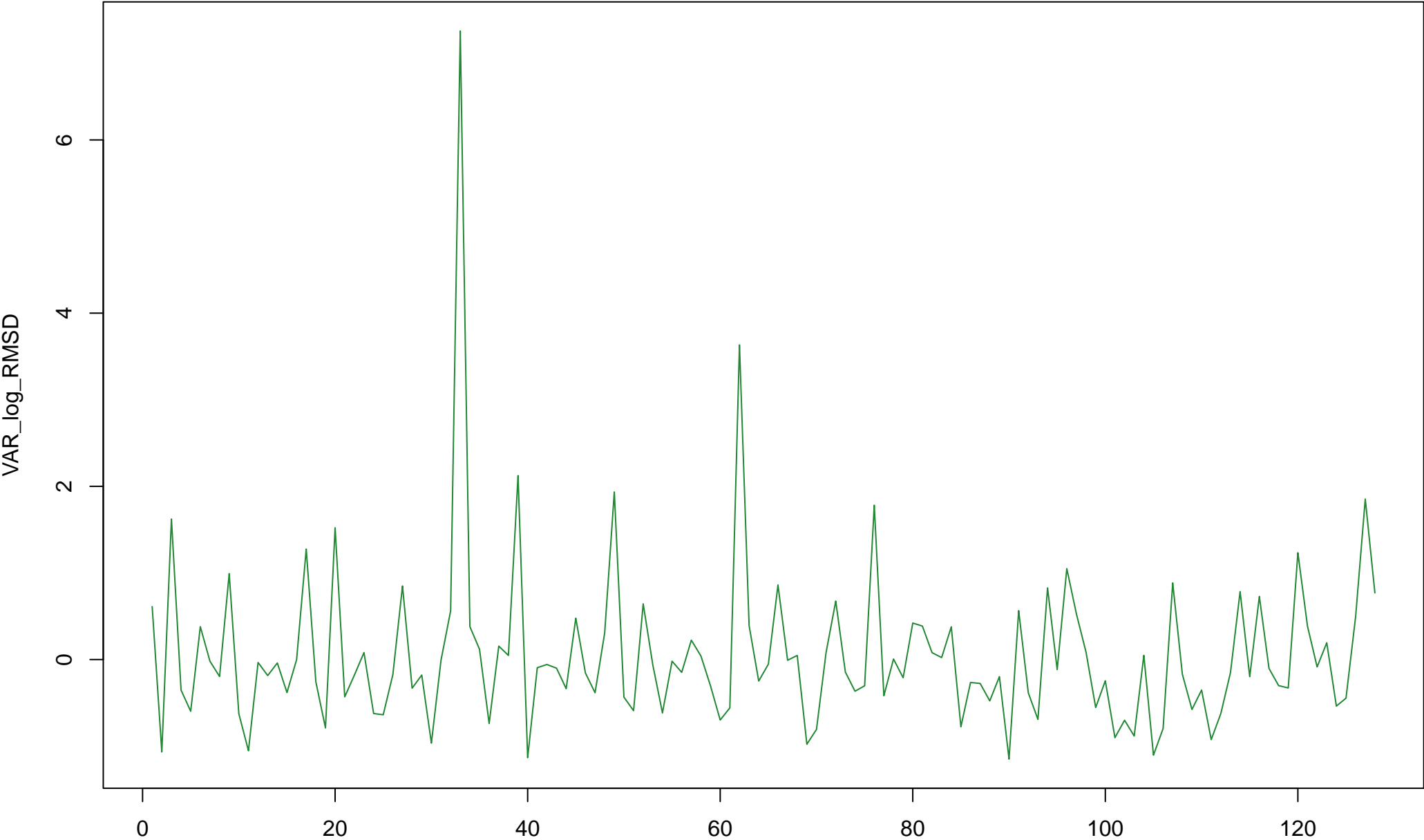
MEAN_docked_NumRotatableBonds
ESS = 76.9 | BMK = 0.0998 | MCSE(6.27) = 14.3 | stat: TRUE | burn: 0



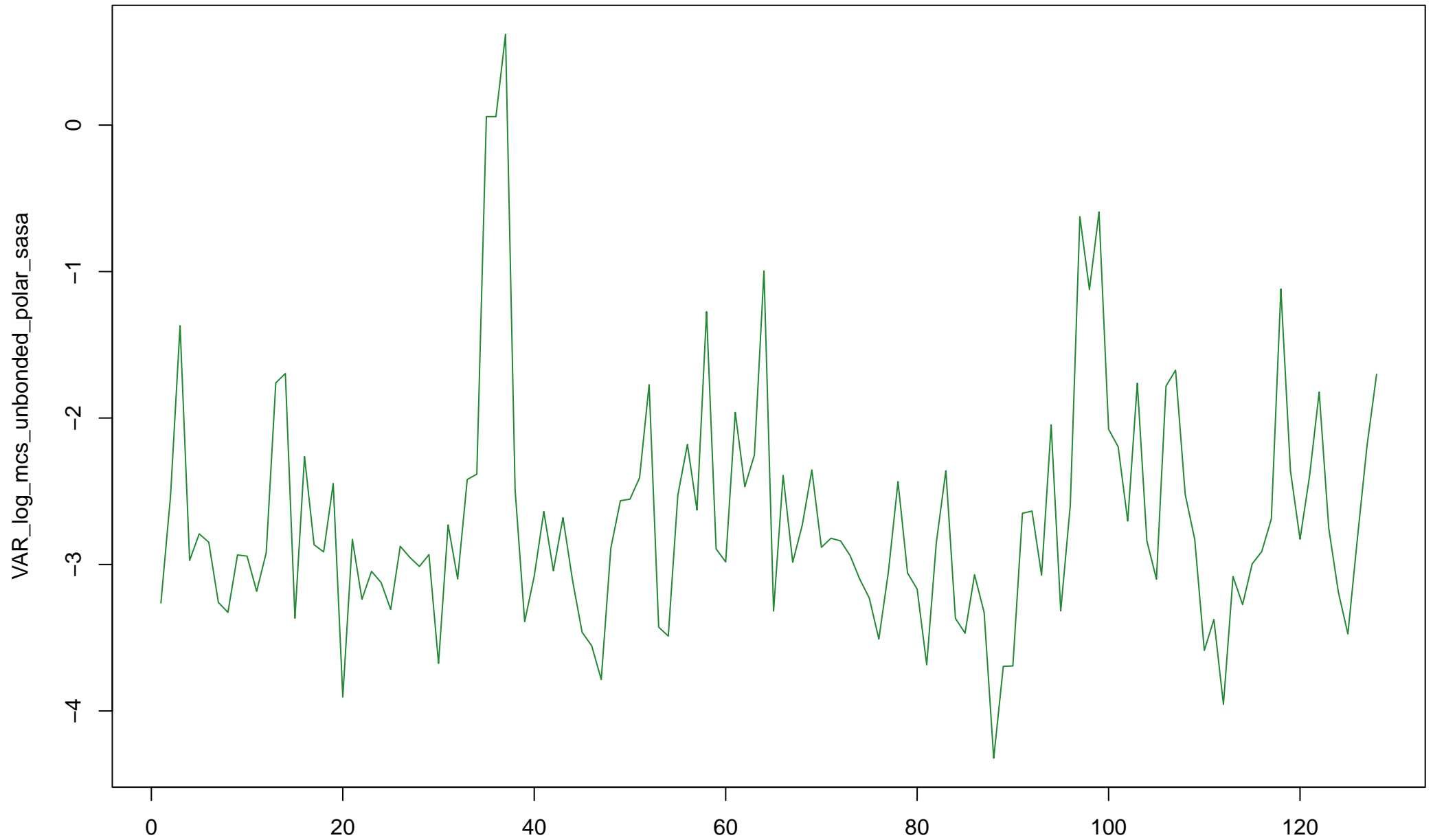
MEAN_mcs_NOCount
ESS = 128 | BMK = 0.118 | MCSE(6.27) = 8.98 | stat: TRUE | burn: 0



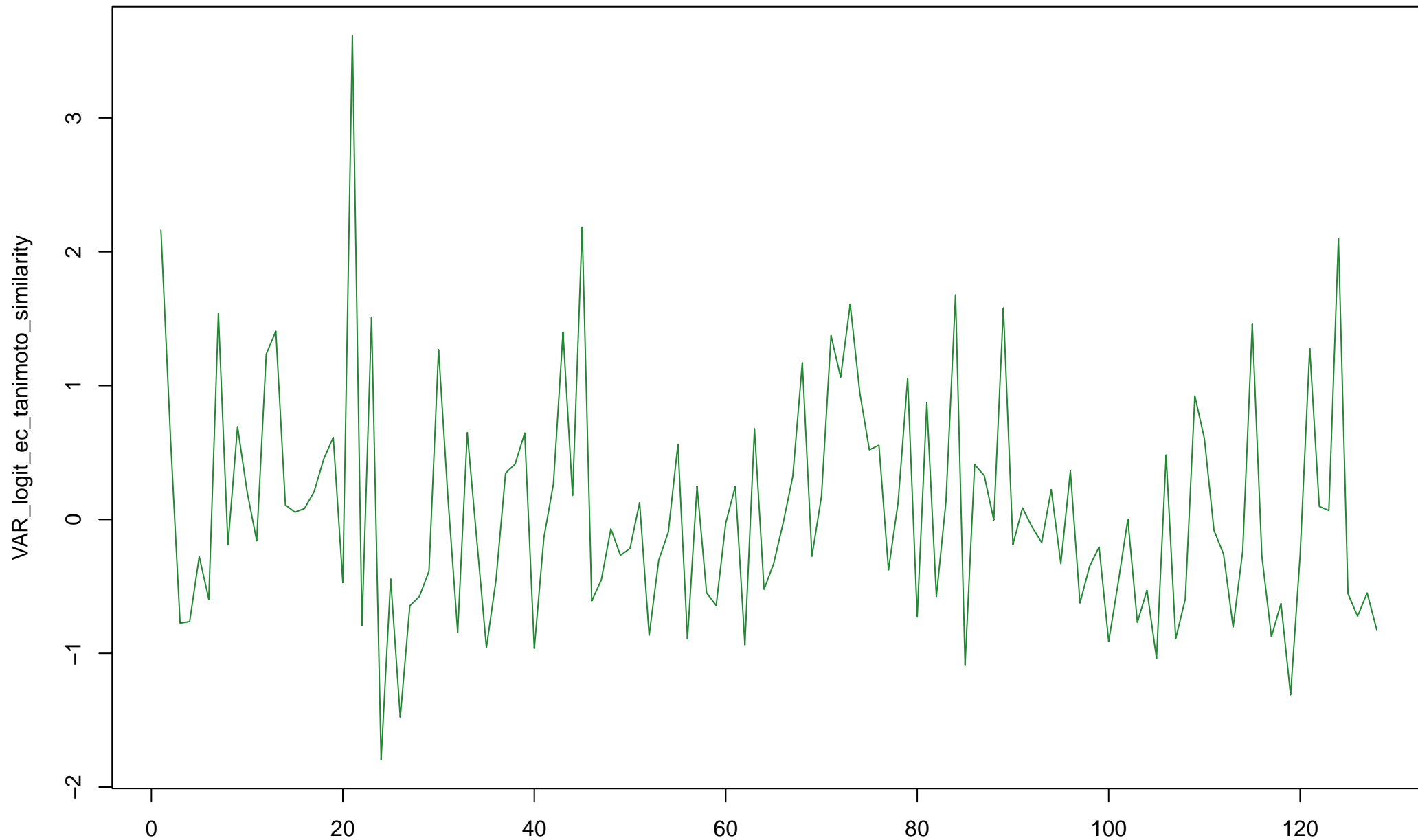
VAR_log_RMSD
ESS = 128 | BMK = 0.488 | MCSE(6.27) = 8.73 | stat: TRUE | burn: 60



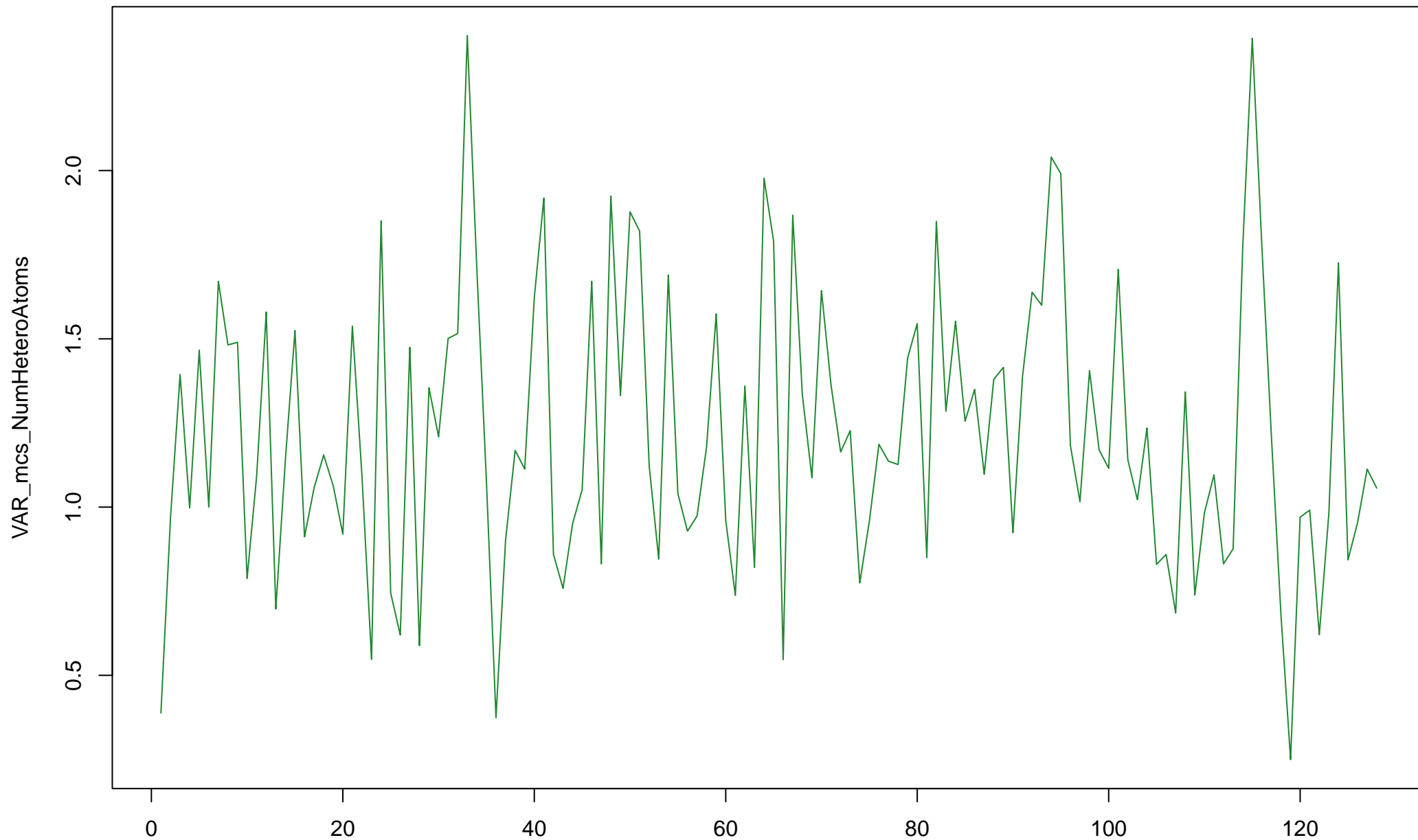
VAR_log_mcs_unbonded_polar_sasa
ESS = 62.8 | BMK = 0.269 | MCSE(6.27) = 17.9 | stat: TRUE | burn: 120



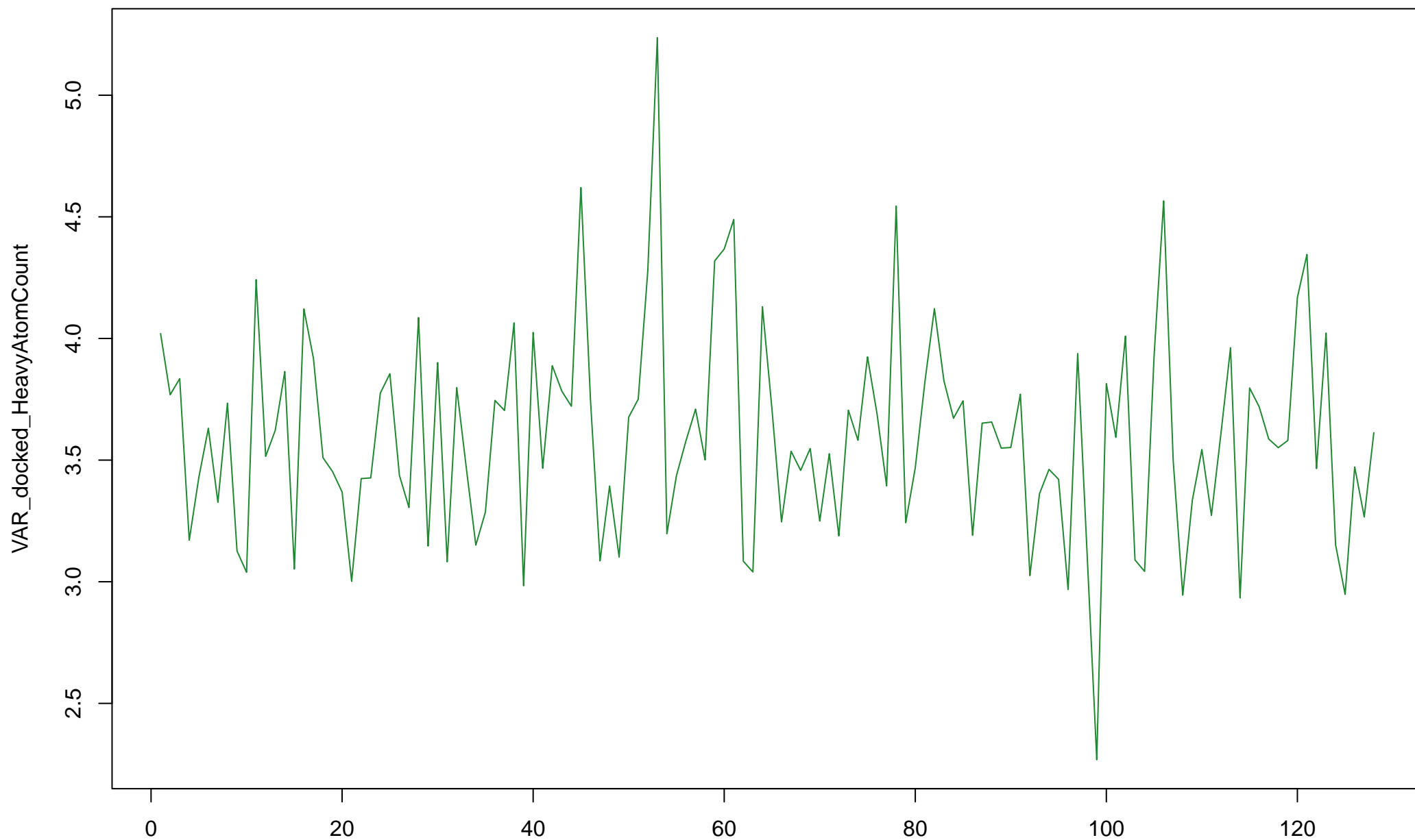
VAR_logit_ec_tanimoto_similarity
ESS = 128 | BMK = 0.194 | MCSE(6.27) = 8.55 | stat: TRUE | burn: 0



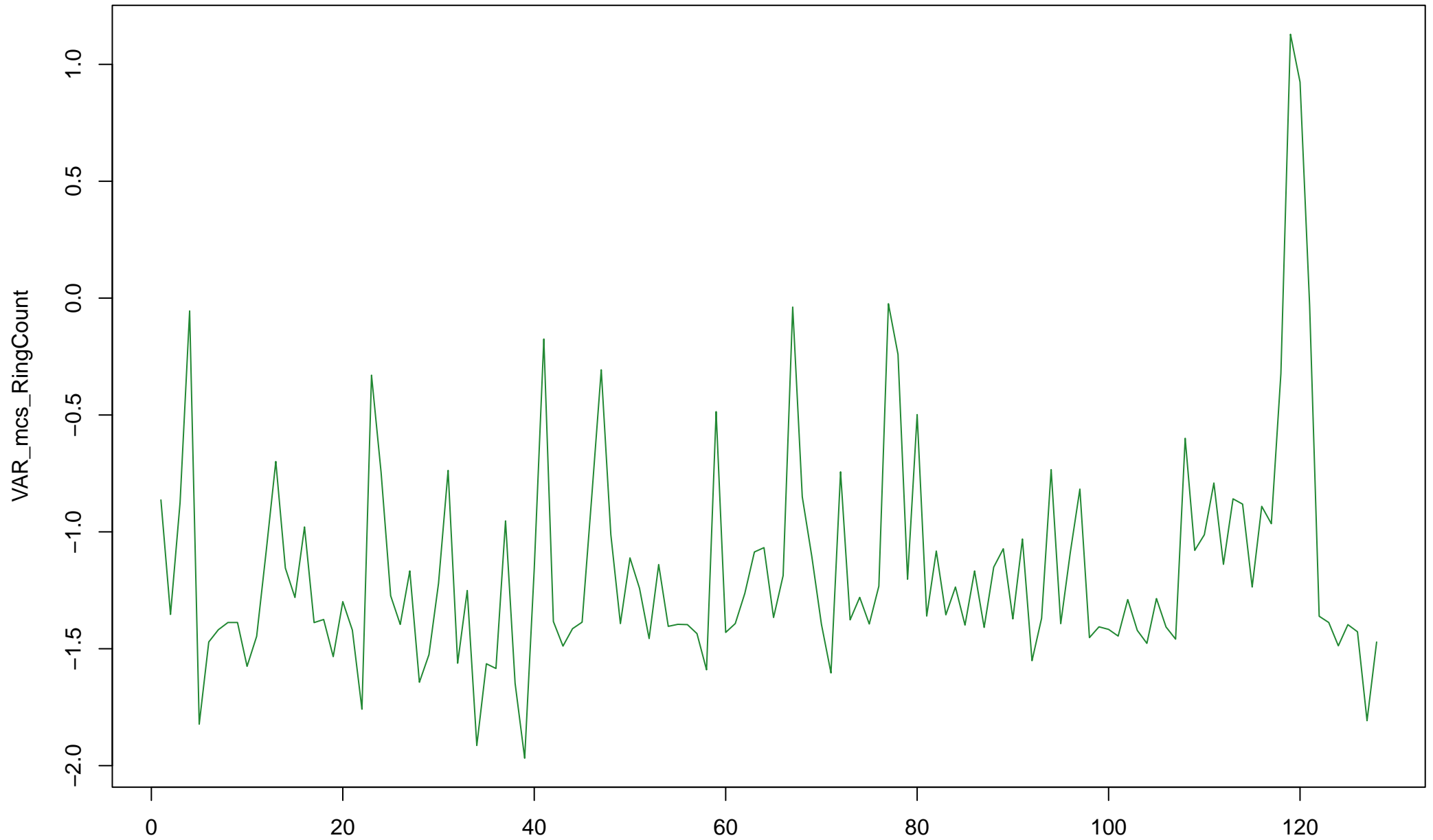
VAR_mcs_NumHeteroAtoms
ESS = 85.6 | BMK = 0.085 | MCSE(6.27) = 11.9 | stat: TRUE | burn: 0



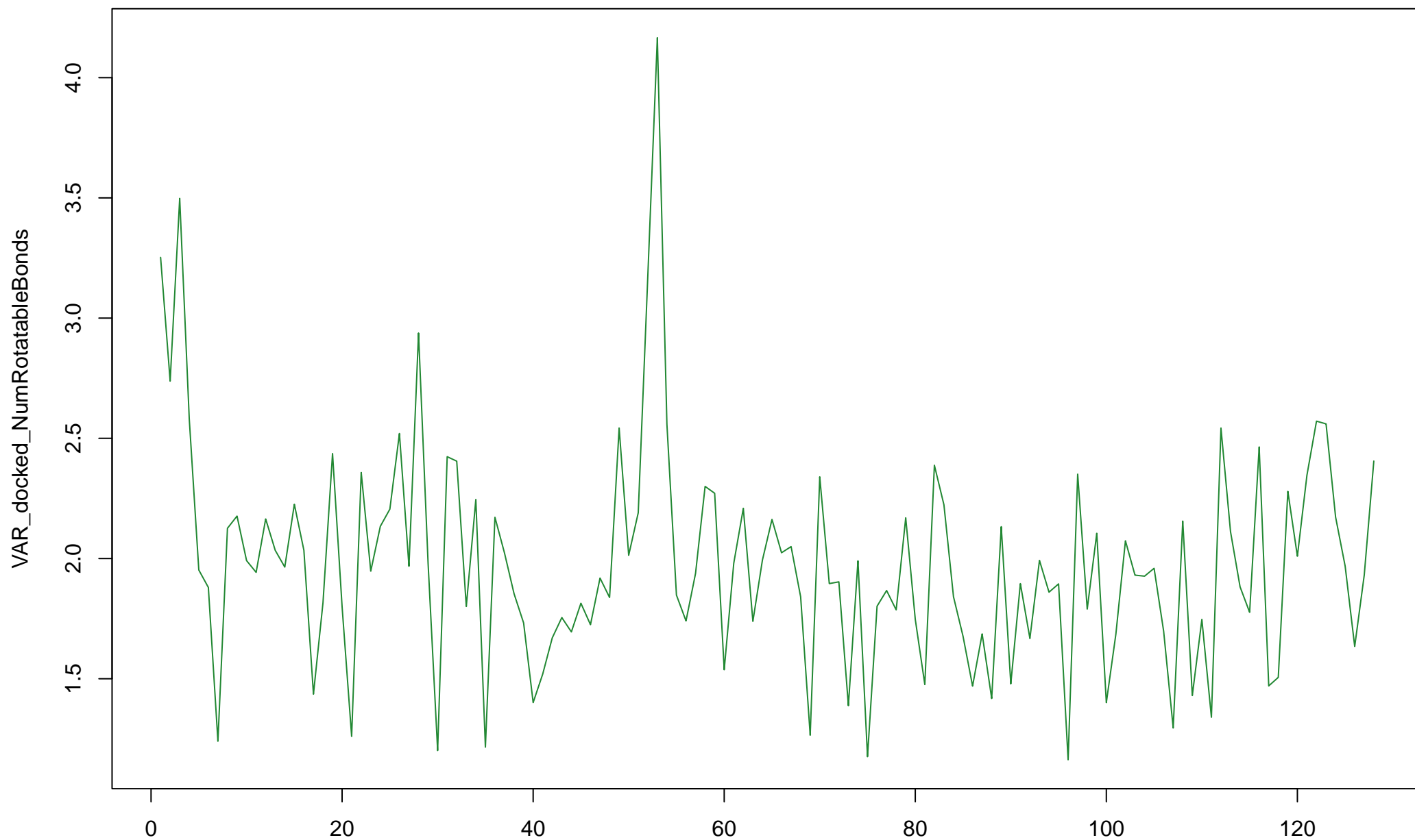
VAR_docked_HeavyAtomCount
ESS = 128 | BMK = 0.133 | MCSE(6.27) = 9.66 | stat: TRUE | burn: 0



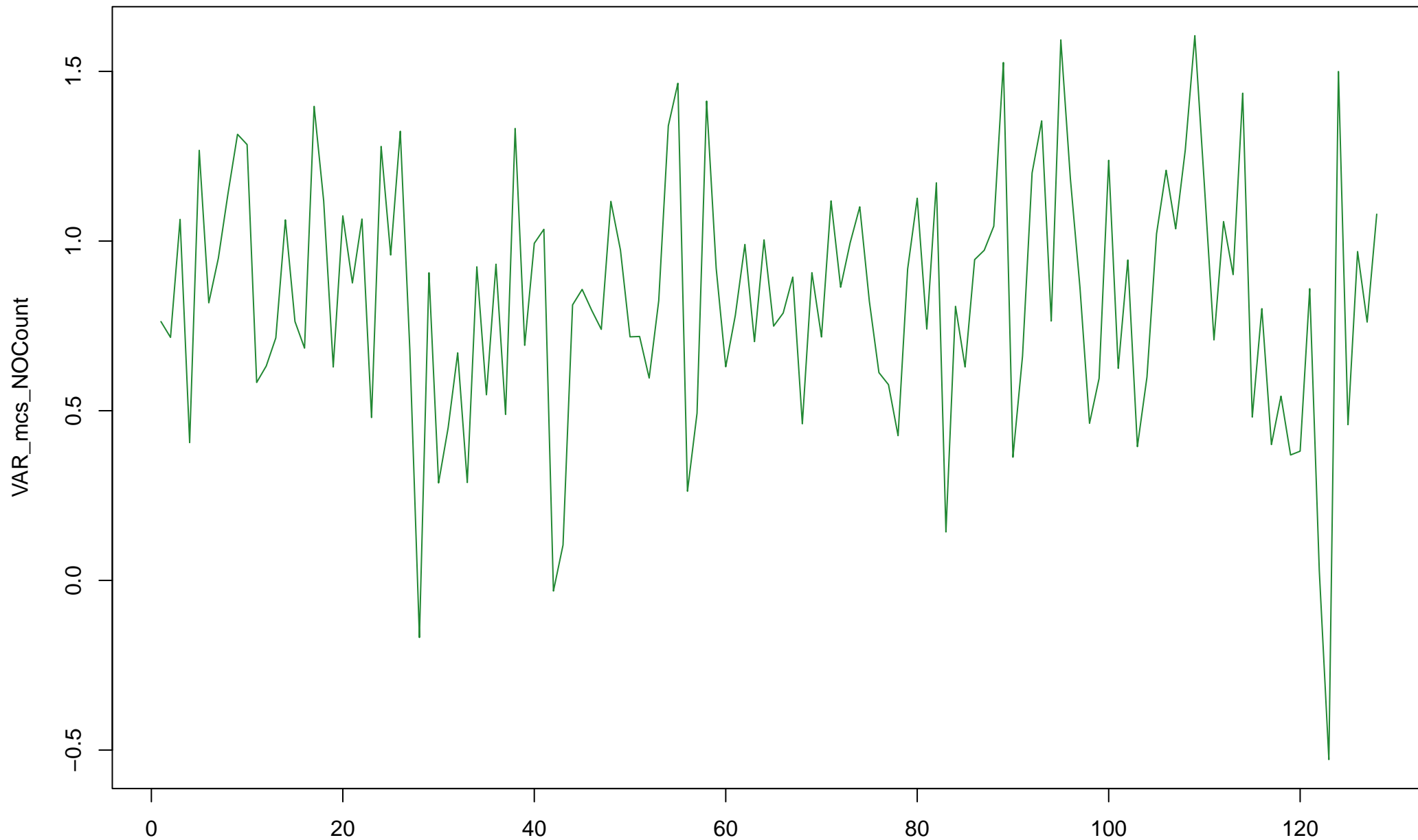
VAR_mcs_RingCount
ESS = 59.8 | BMK = 0.176 | MCSE(6.27) = 17 | stat: TRUE | burn: 120



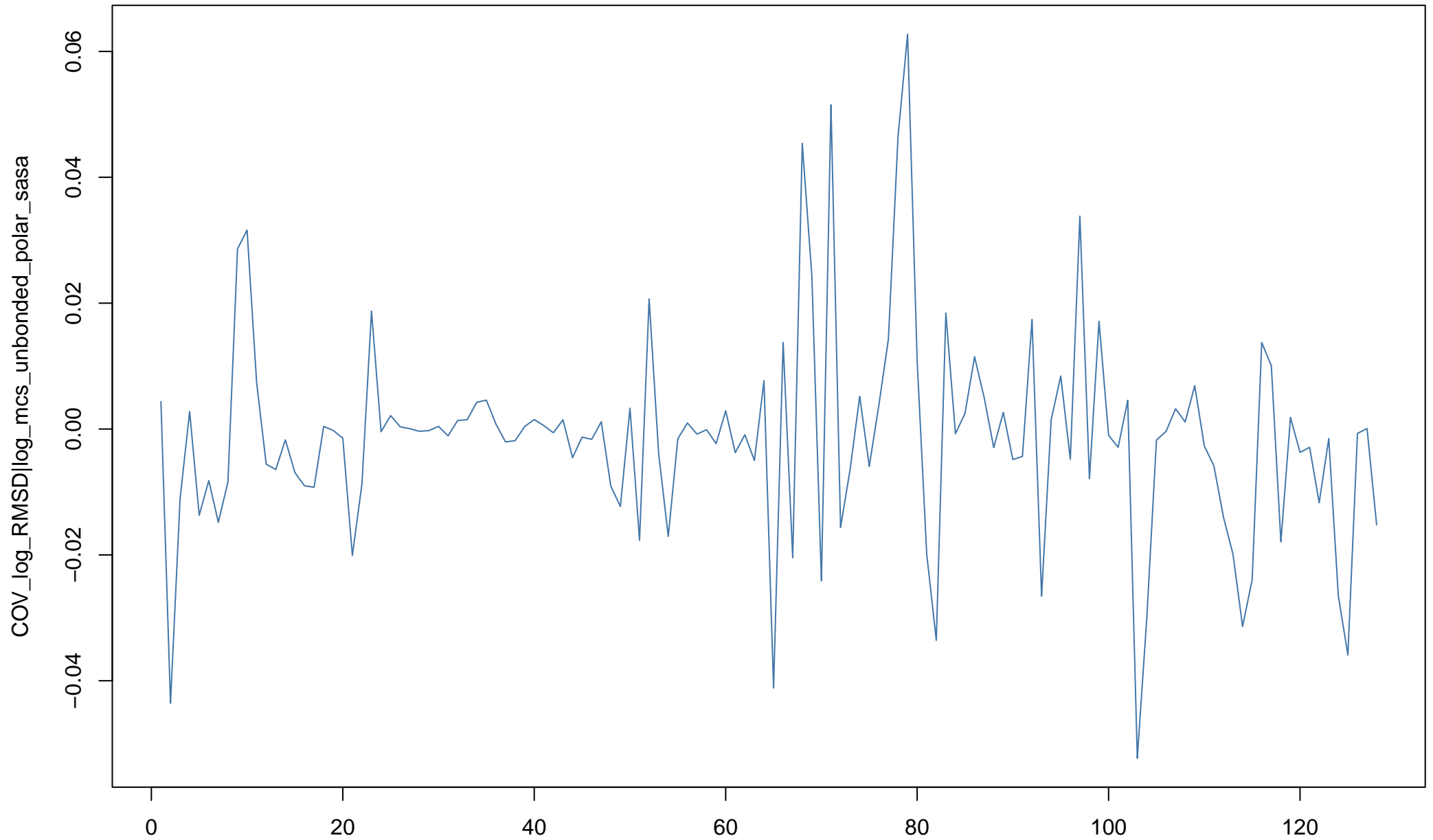
VAR_docked_NumRotatableBonds
ESS = 65 | BMK = 0.223 | MCSE(6.27) = 15.3 | stat: TRUE | burn: 48



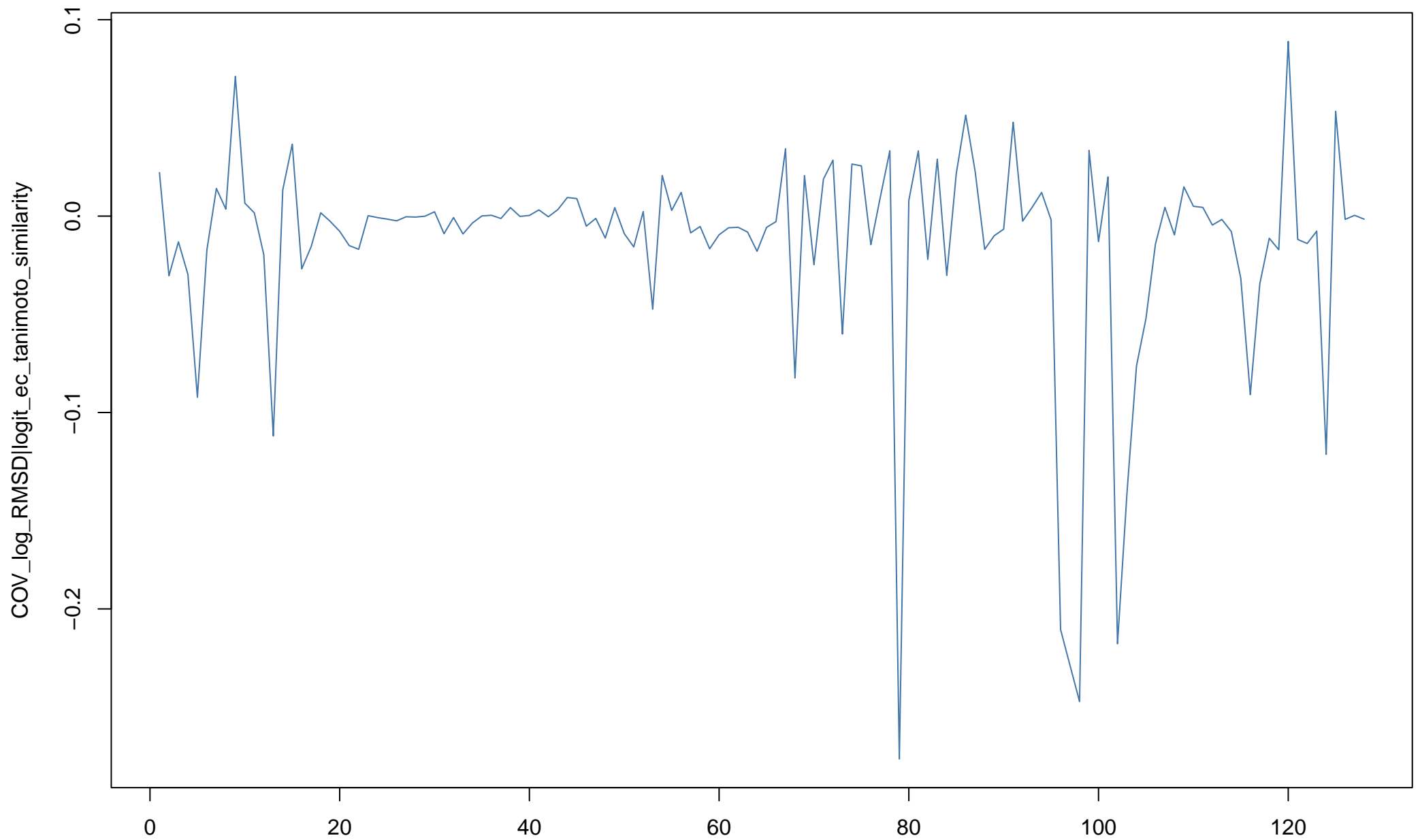
VAR_mcs_NOCount
ESS = 128 | BMK = 0.103 | MCSE(6.27) = 9.89 | stat: TRUE | burn: 0



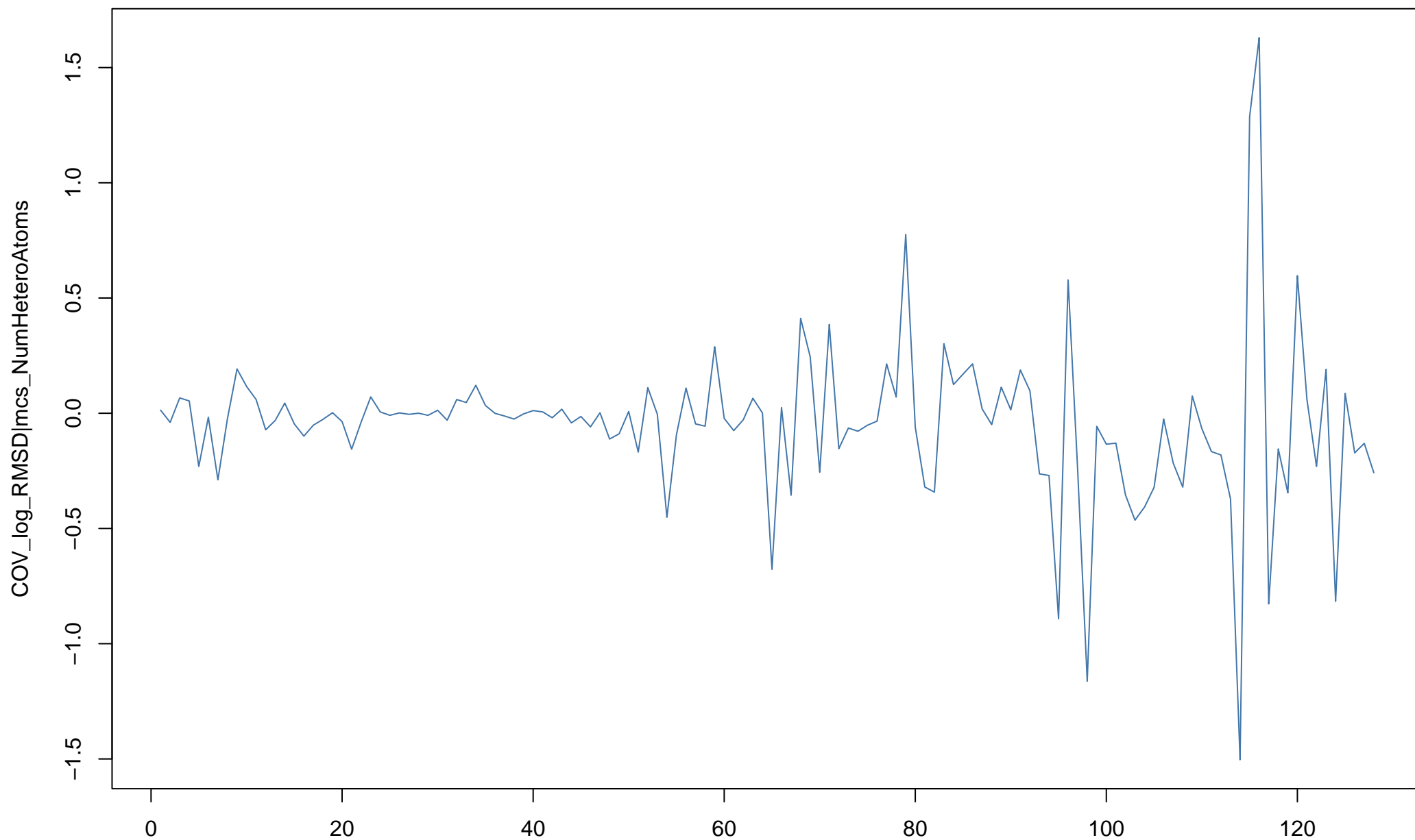
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 128 | BMK = 0.401 | MCSE(6.27) = 11.4 | stat: TRUE | burn: 24



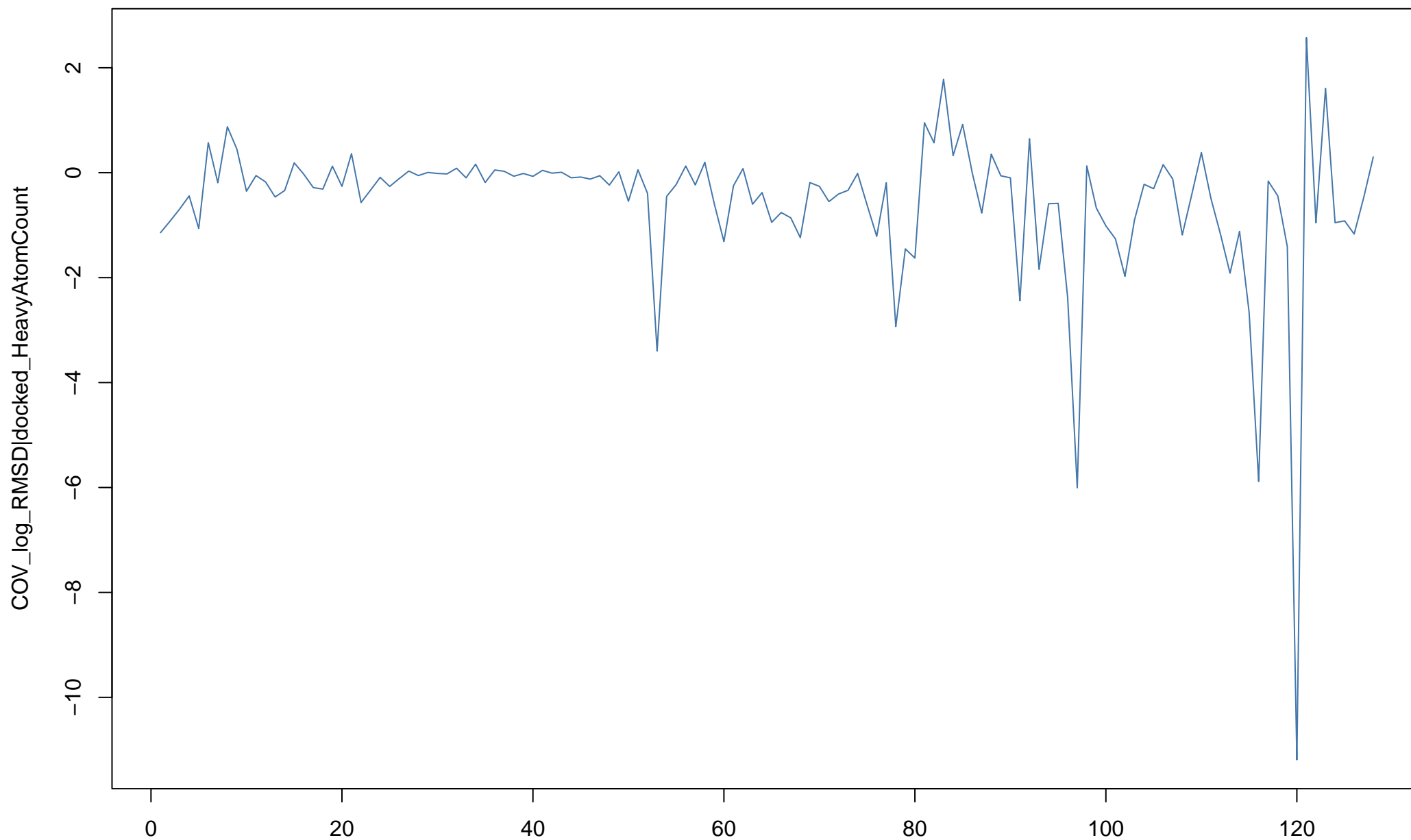
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 76.6 | BMK = 0.409 | MCSE(6.27) = 13.2 | stat: TRUE | burn: 120



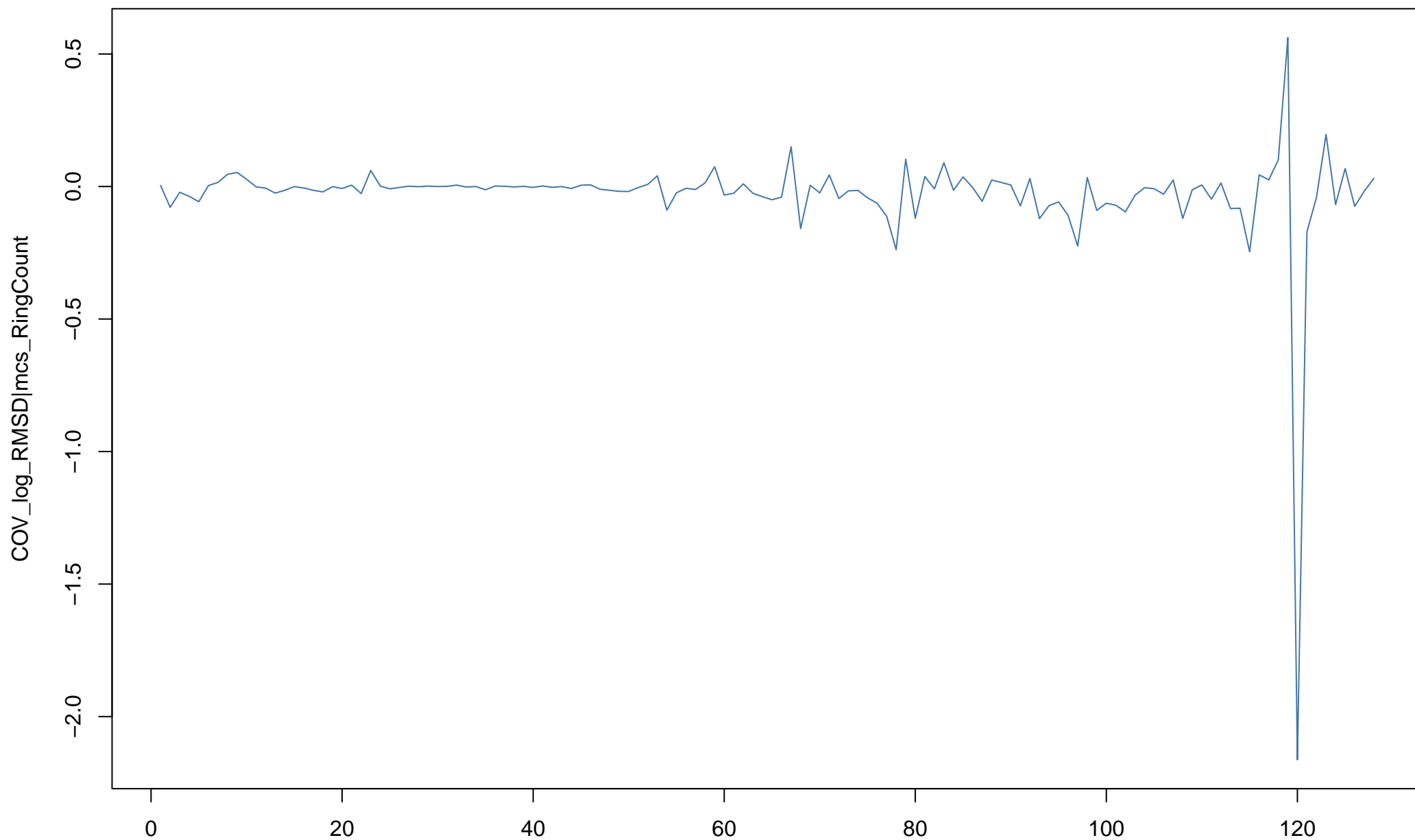
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 88.8 | BMK = 0.542 | MCSE(6.27) = 8.5 | stat: TRUE | burn: 96



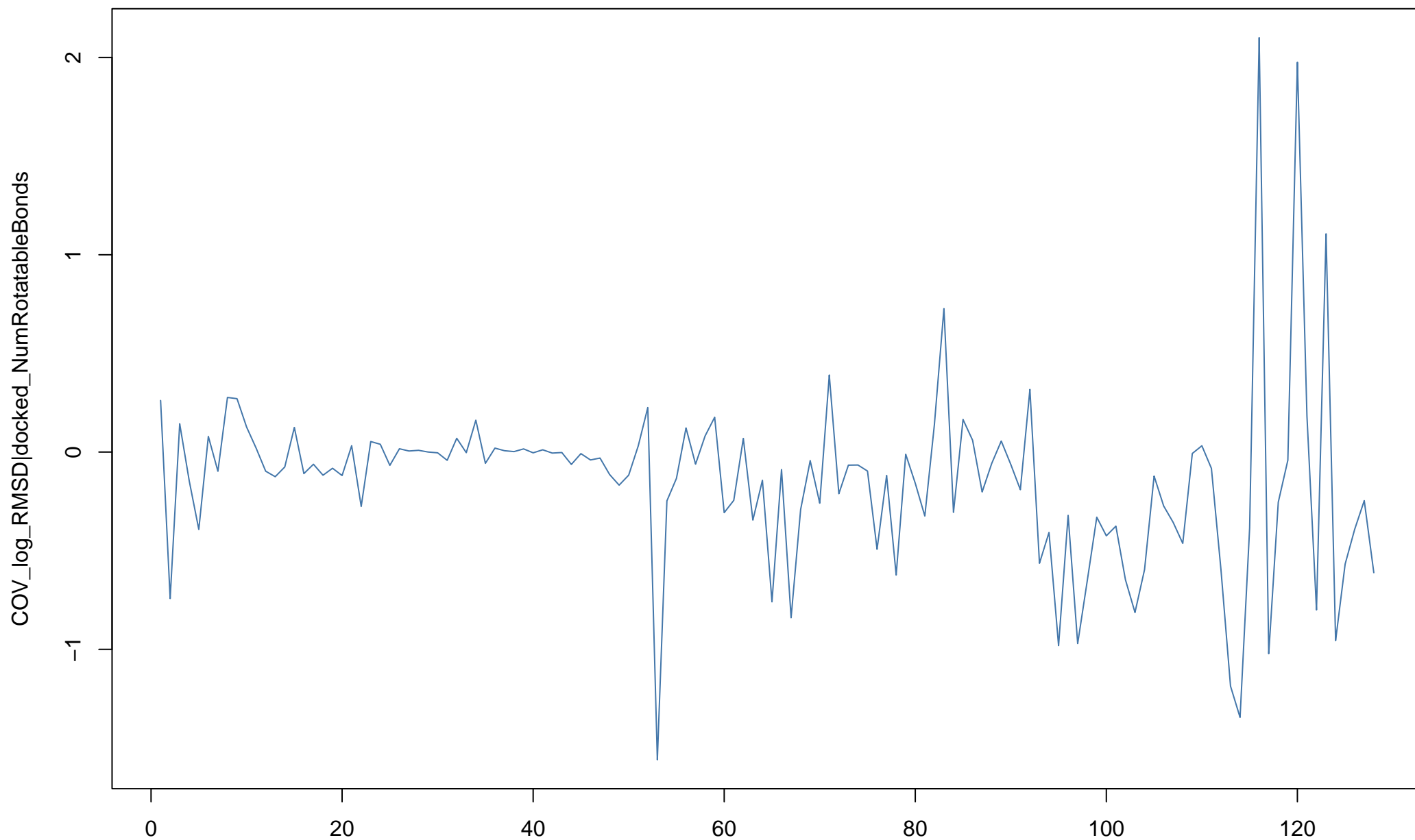
COV_log_RMSD|docked_HeavyAtomCount
ESS = 54.9 | BMK = 0.465 | MCSE(6.27) = 10.9 | stat: TRUE | burn: 72



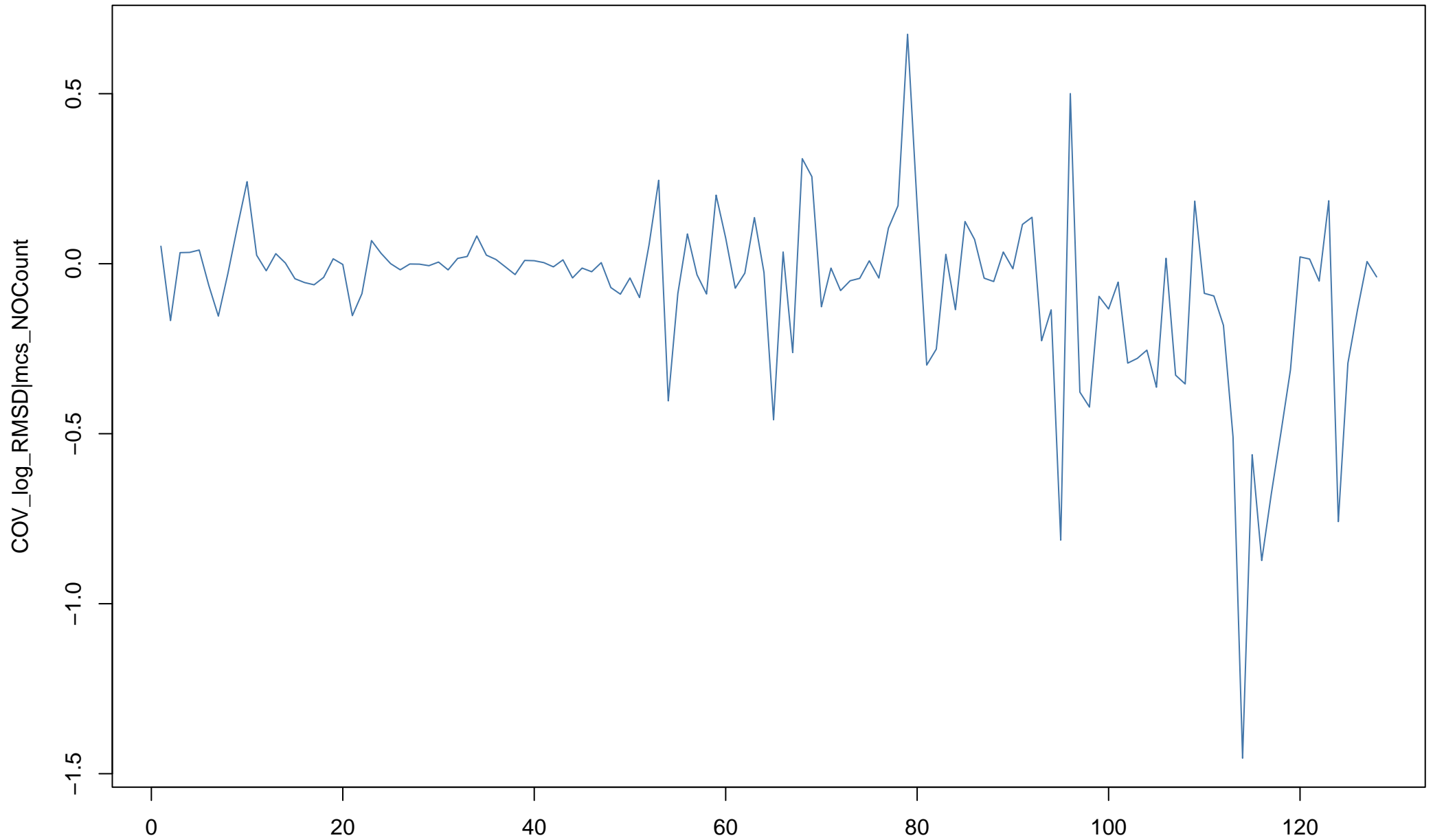
COV_log_RMSD|mcs_RingCount
ESS = 128 | BMK = 0.616 | MCSE(6.27) = 7.2 | stat: TRUE | burn: 48



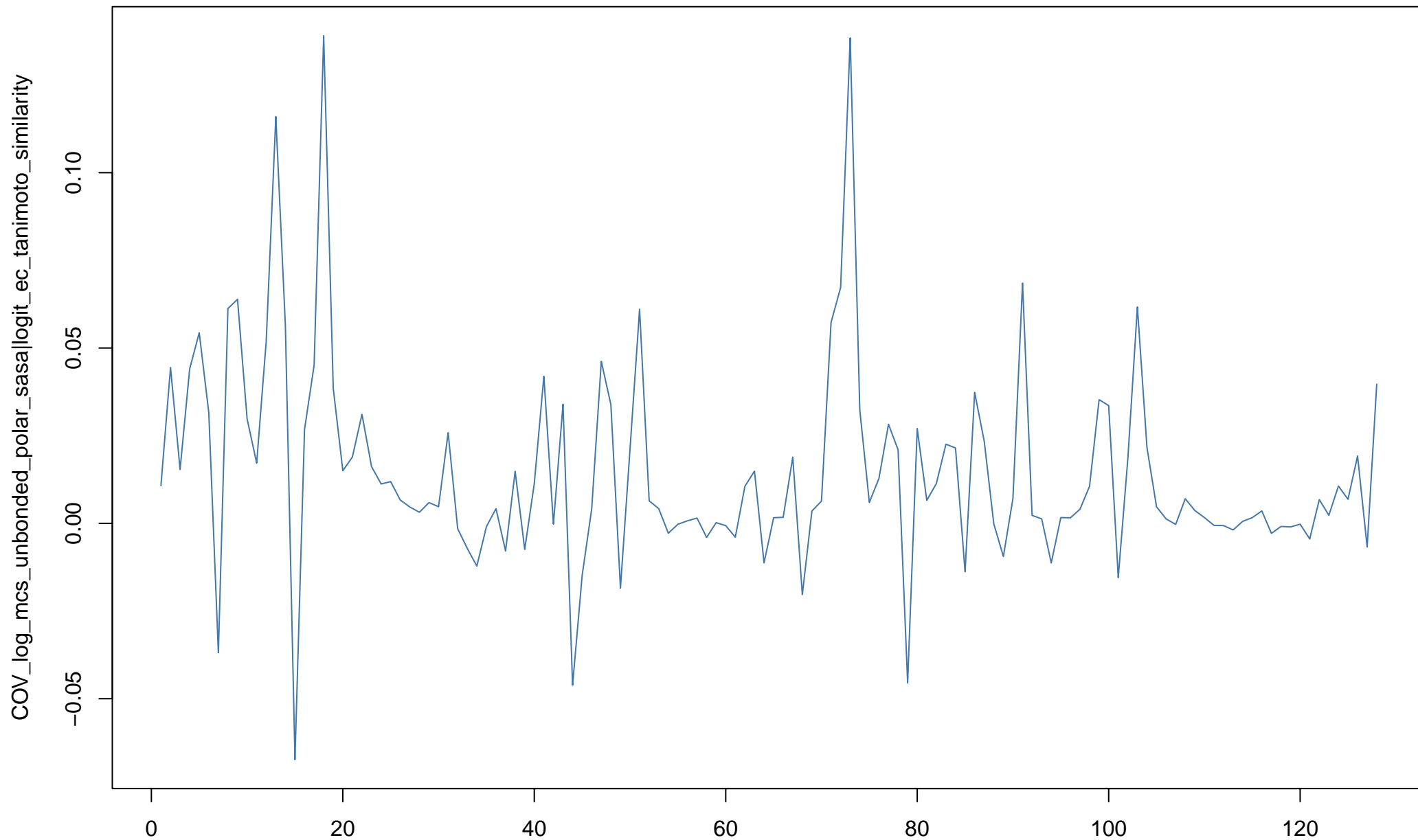
COV_log_RMSD|docked_NumRotatableBonds
ESS = 128 | BMK = 0.501 | MCSE(6.27) = 9.42 | stat: TRUE | burn: 48



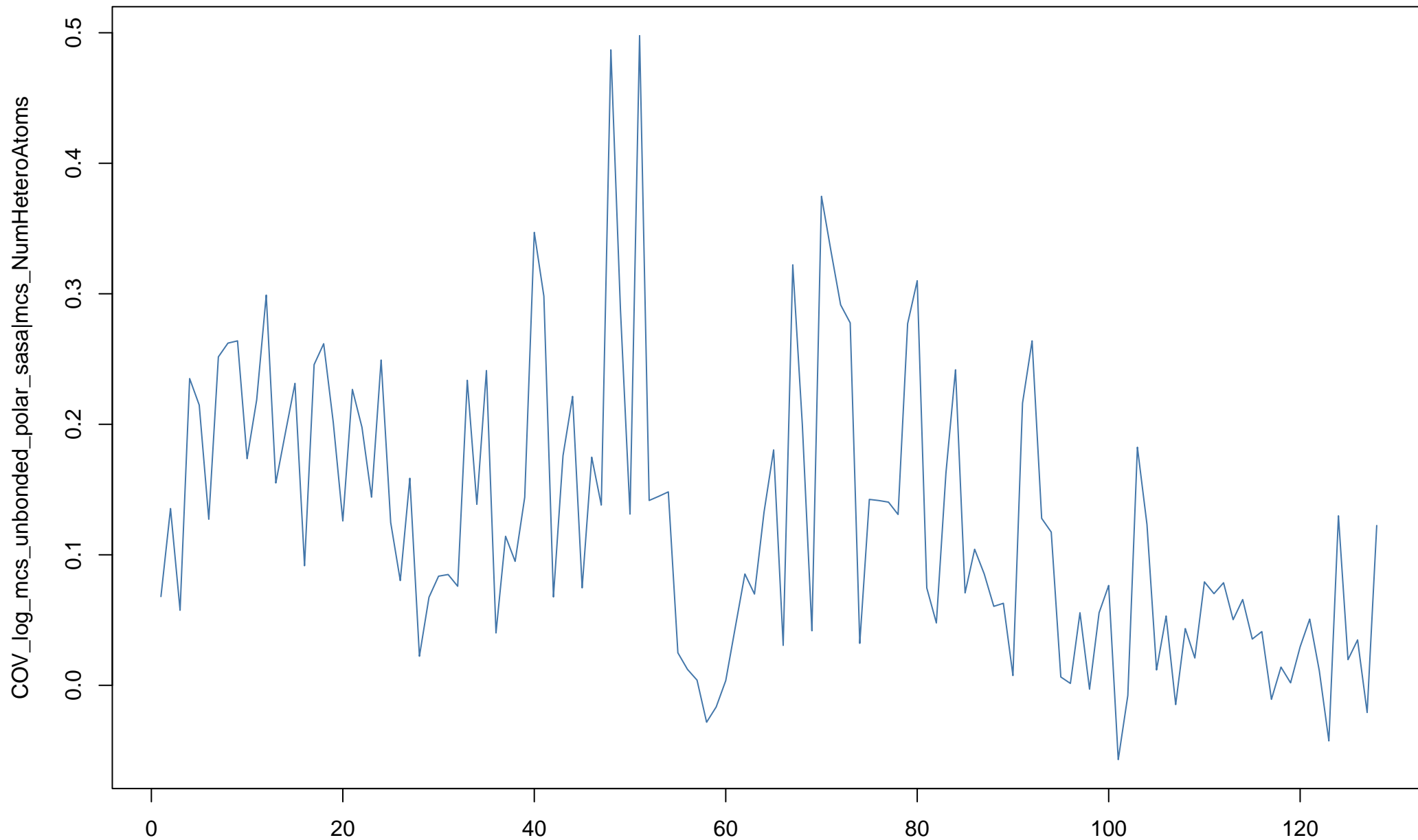
COV_log_RMSD|mcs_NOCount
ESS = 39.5 | BMK = 0.509 | MCSE(6.27) = 21.1 | stat: FALSE | burn: 96



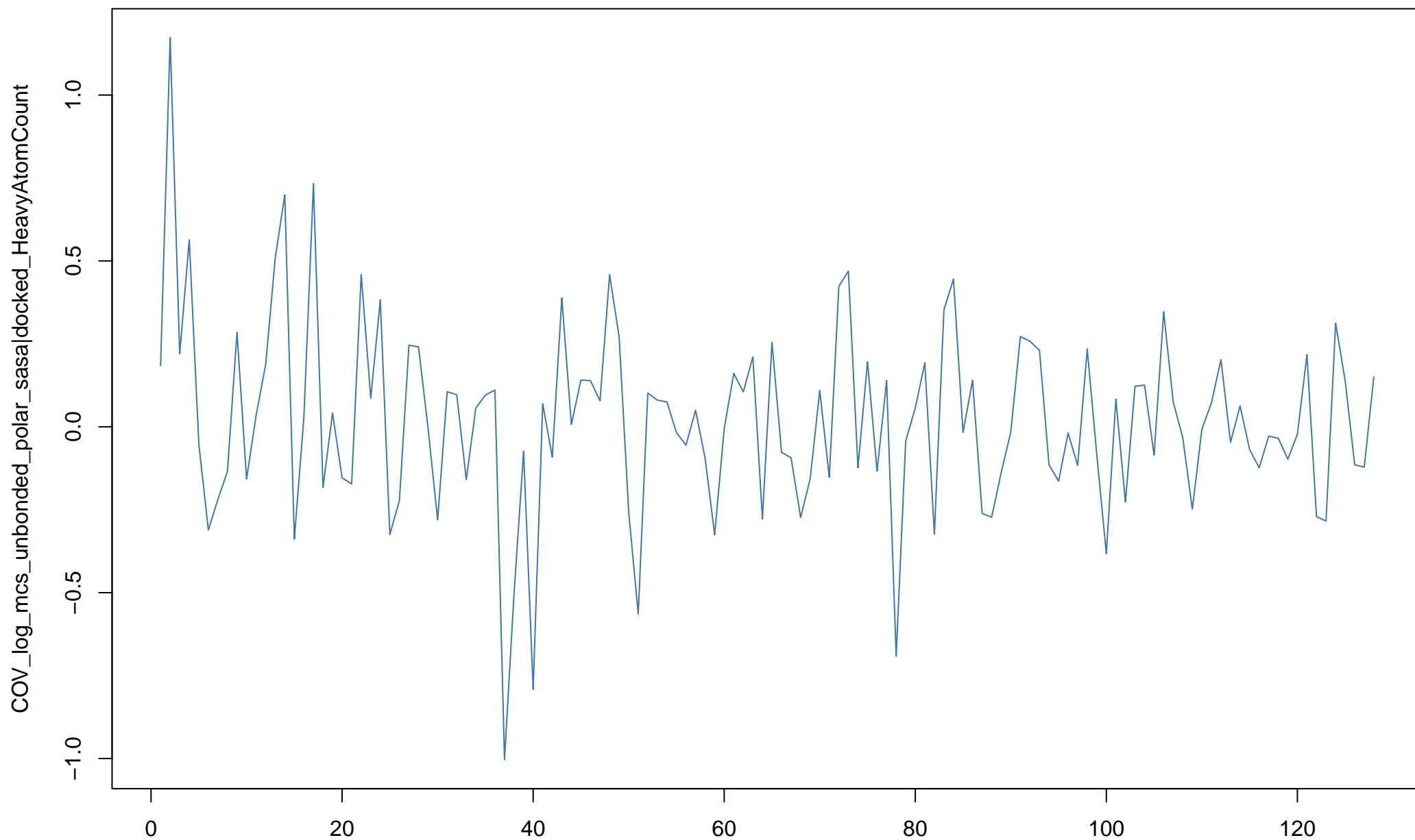
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 48.9 | BMK = 0.189 | MCSE(6.27) = 12.5 | stat: FALSE | burn: 120



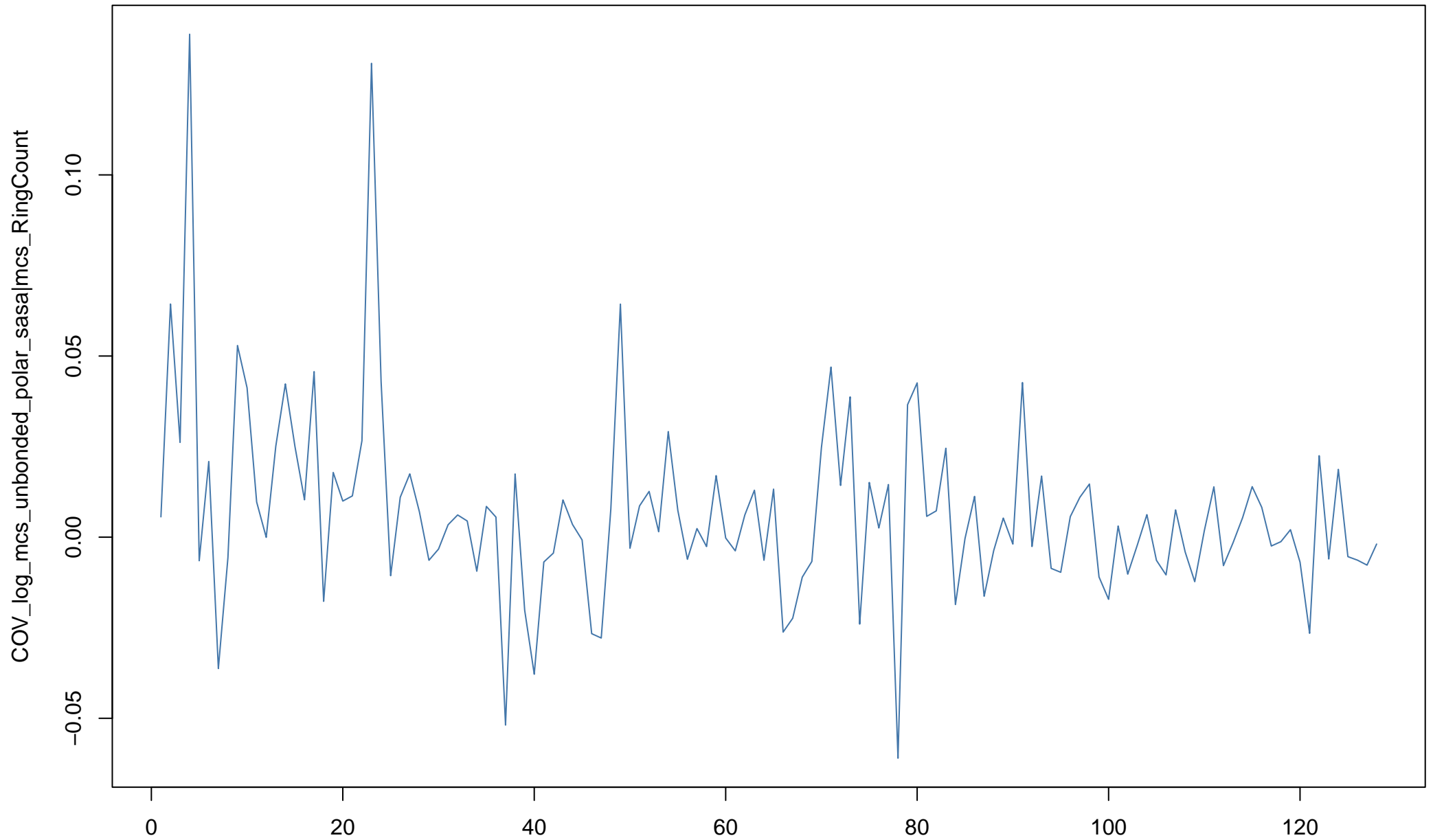
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 18.4 | BMK = 0.242 | MCSE(6.27) = 26 | stat: FALSE | burn: 0



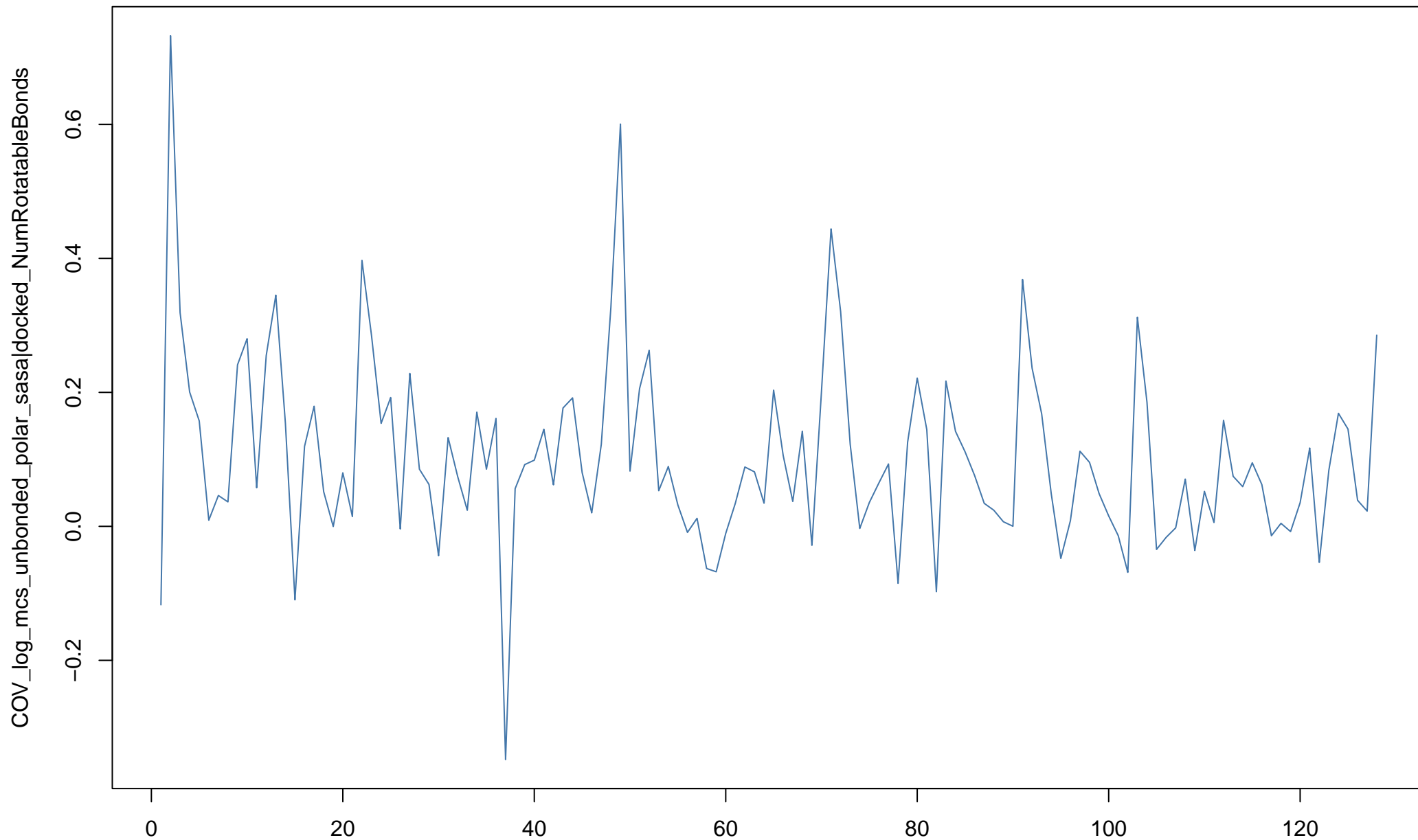
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 128 | BMK = 0.195 | MCSE(6.27) = 10.6 | stat: TRUE | burn: 0



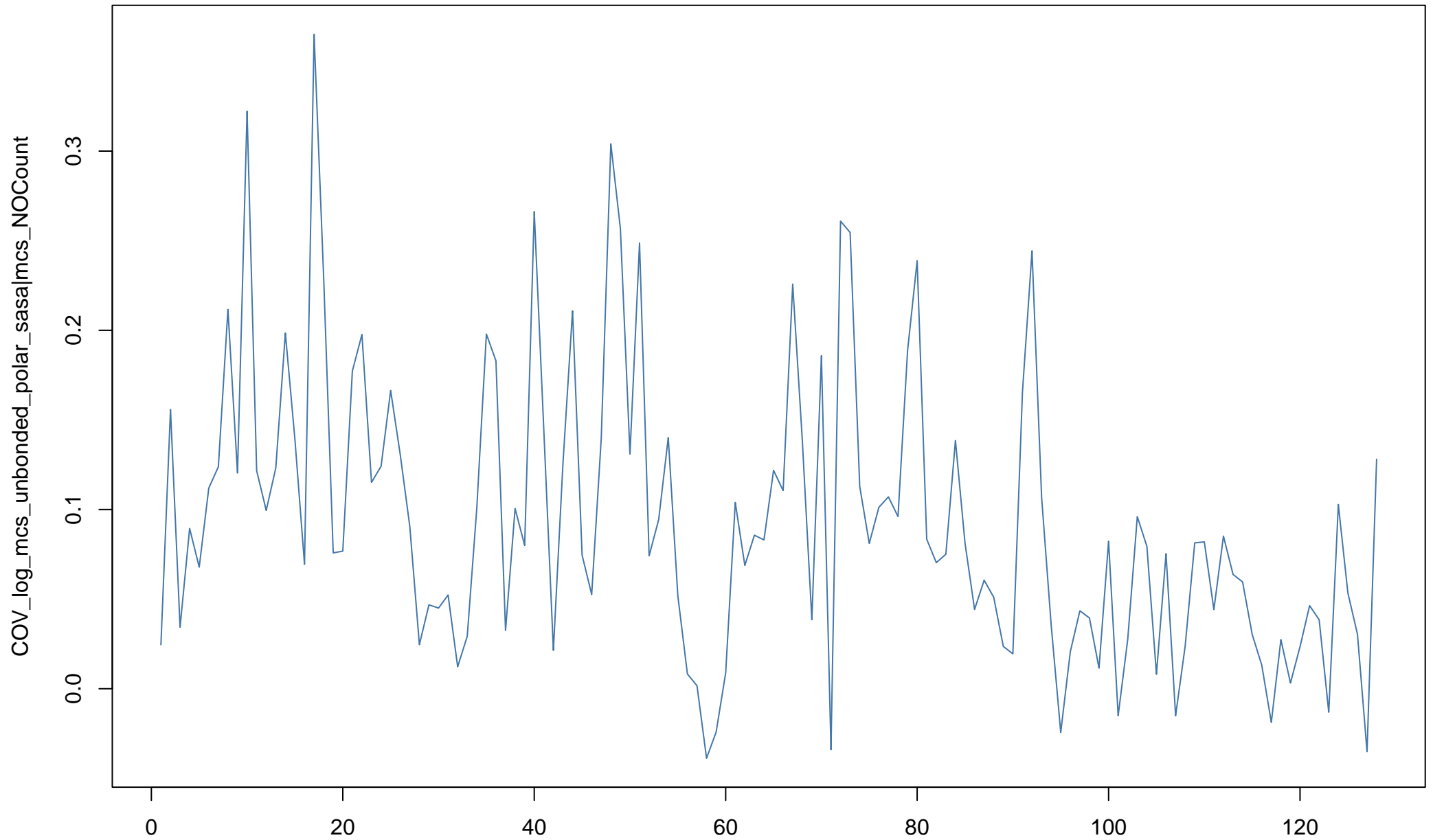
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 97.4 | BMK = 0.211 | MCSE(6.27) = 12.3 | stat: FALSE | burn: 24



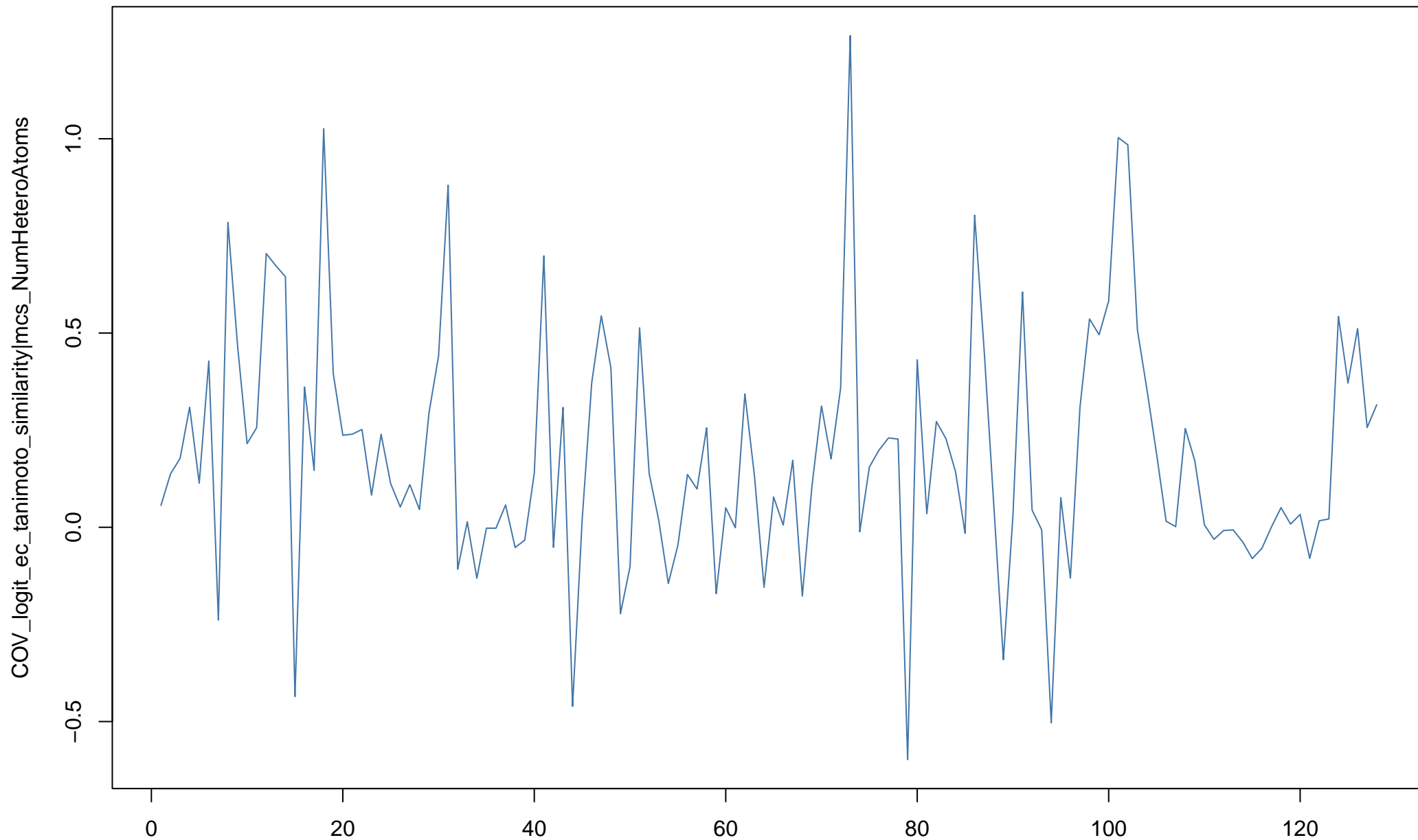
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 84.1 | BMK = 0.161 | MCSE(6.27) = 11.8 | stat: FALSE | burn: 0



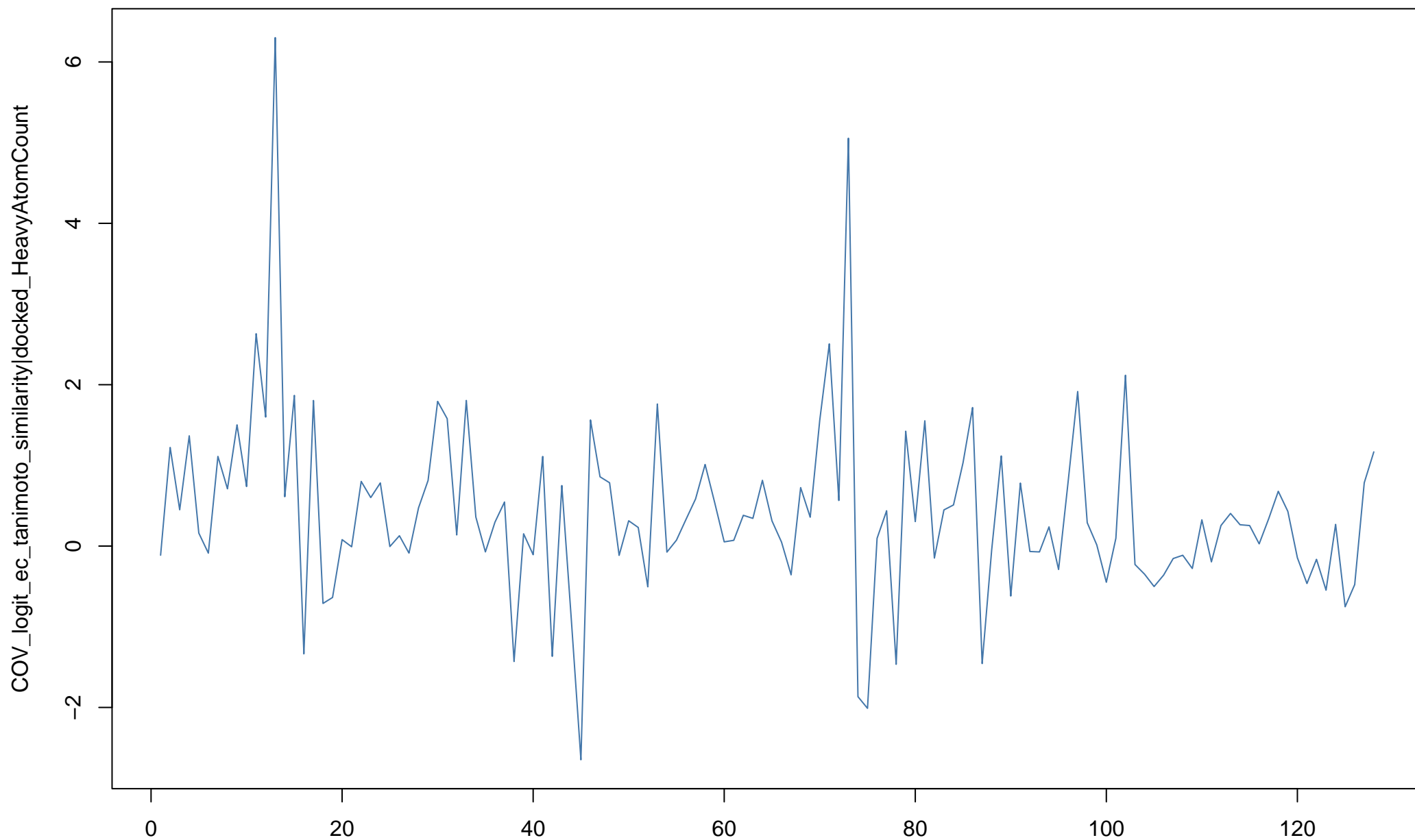
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 25.7 | BMK = 0.205 | MCSE(6.27) = 17.1 | stat: TRUE | burn: 0



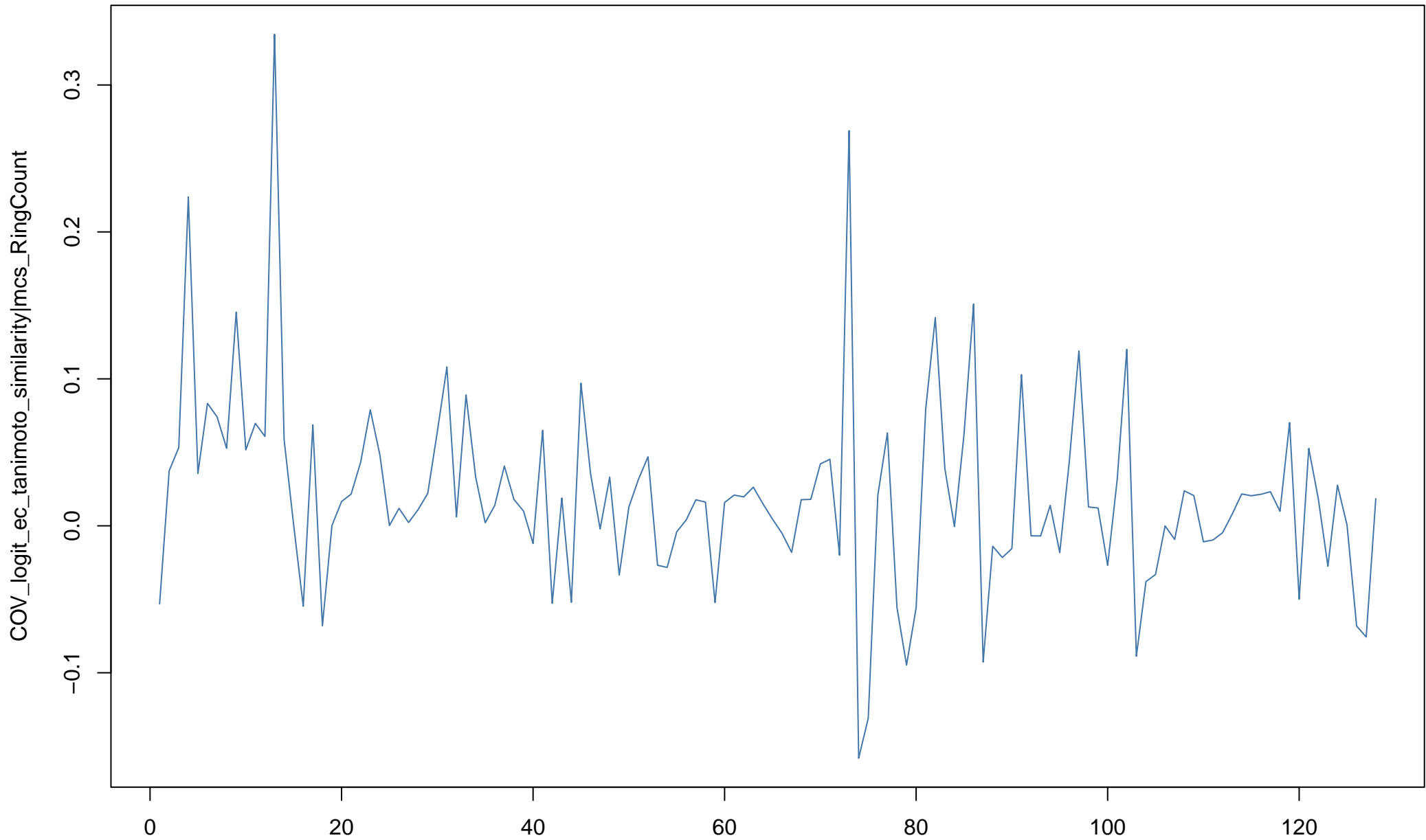
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 100 | BMK = 0.0973 | MCSE(6.27) = 13.7 | stat: TRUE | burn: 120



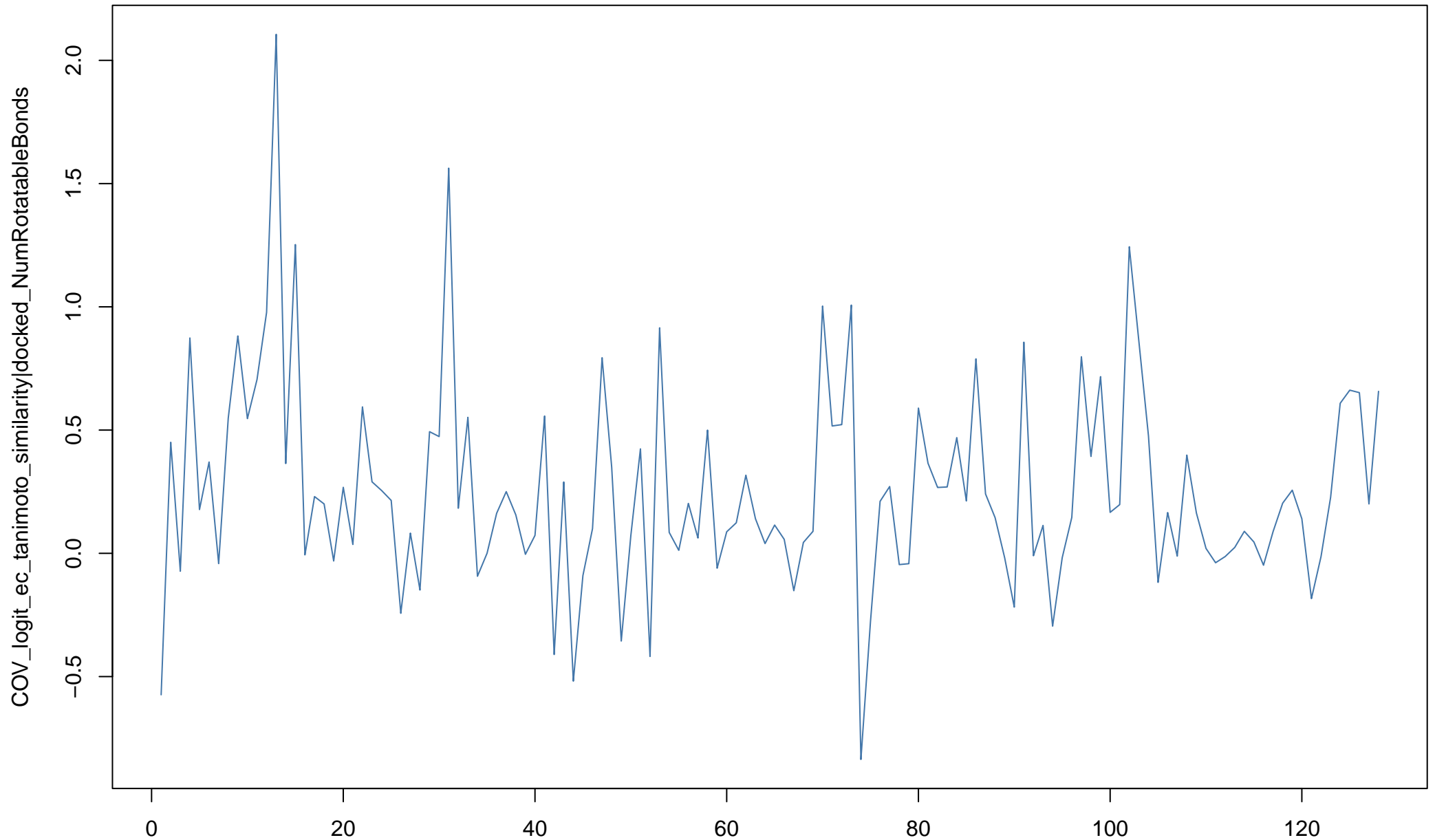
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 80.1 | BMK = 0.201 | MCSE(6.27) = 12.4 | stat: FALSE | burn: 0



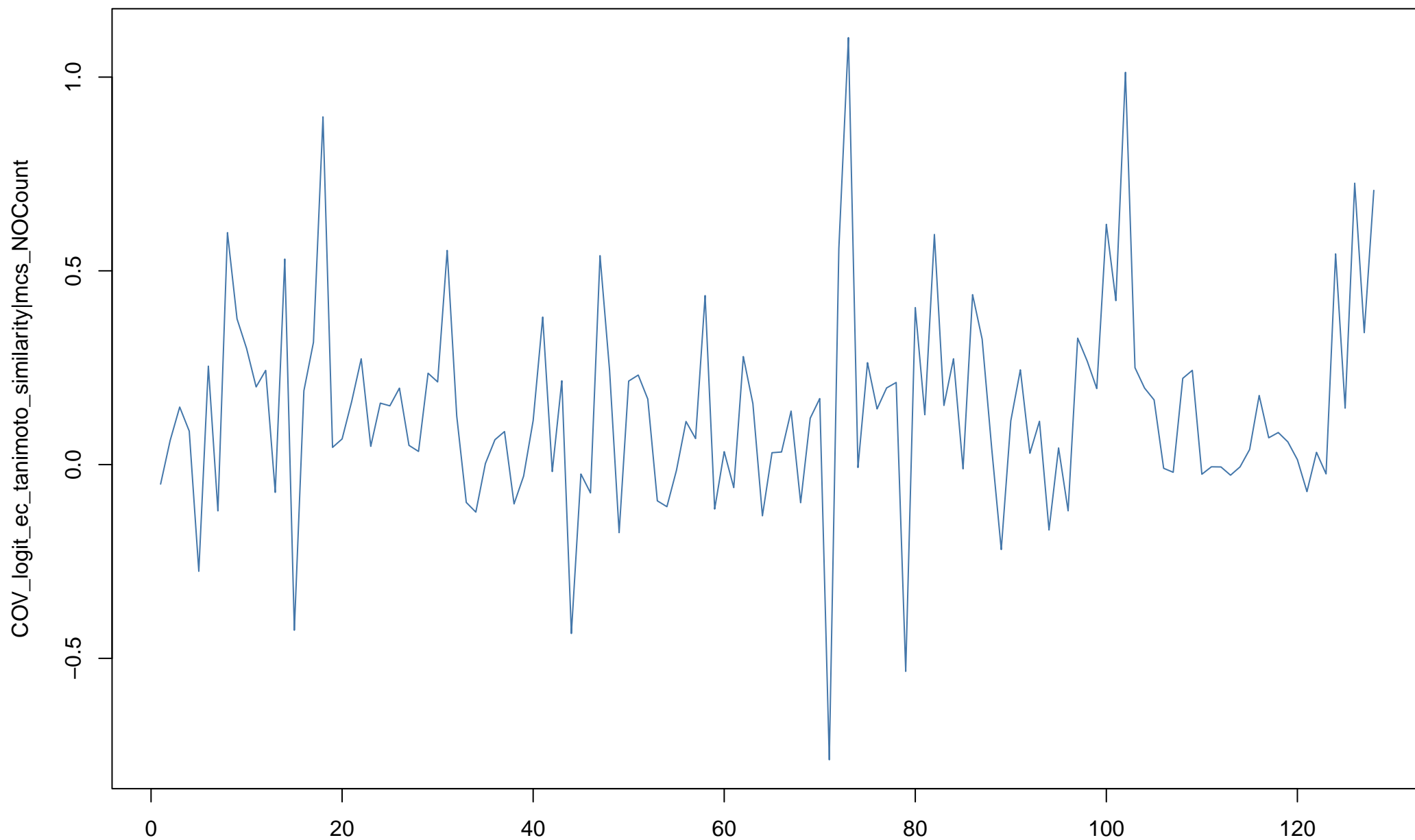
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 128 | BMK = 0.254 | MCSE(6.27) = 9.88 | stat: FALSE | burn: 72



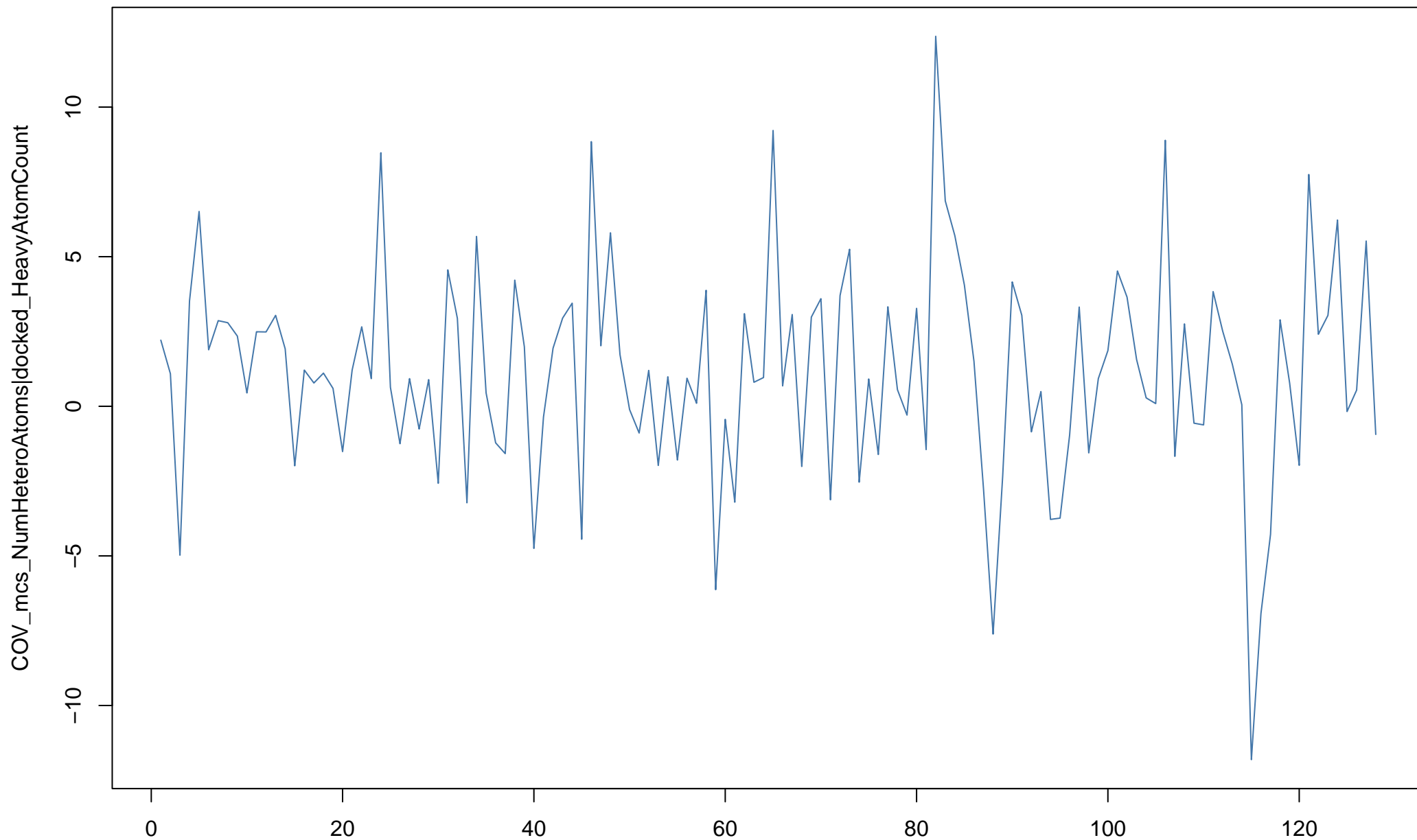
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 59.3 | BMK = 0.132 | MCSE(6.27) = 13.8 | stat: TRUE | burn: 120



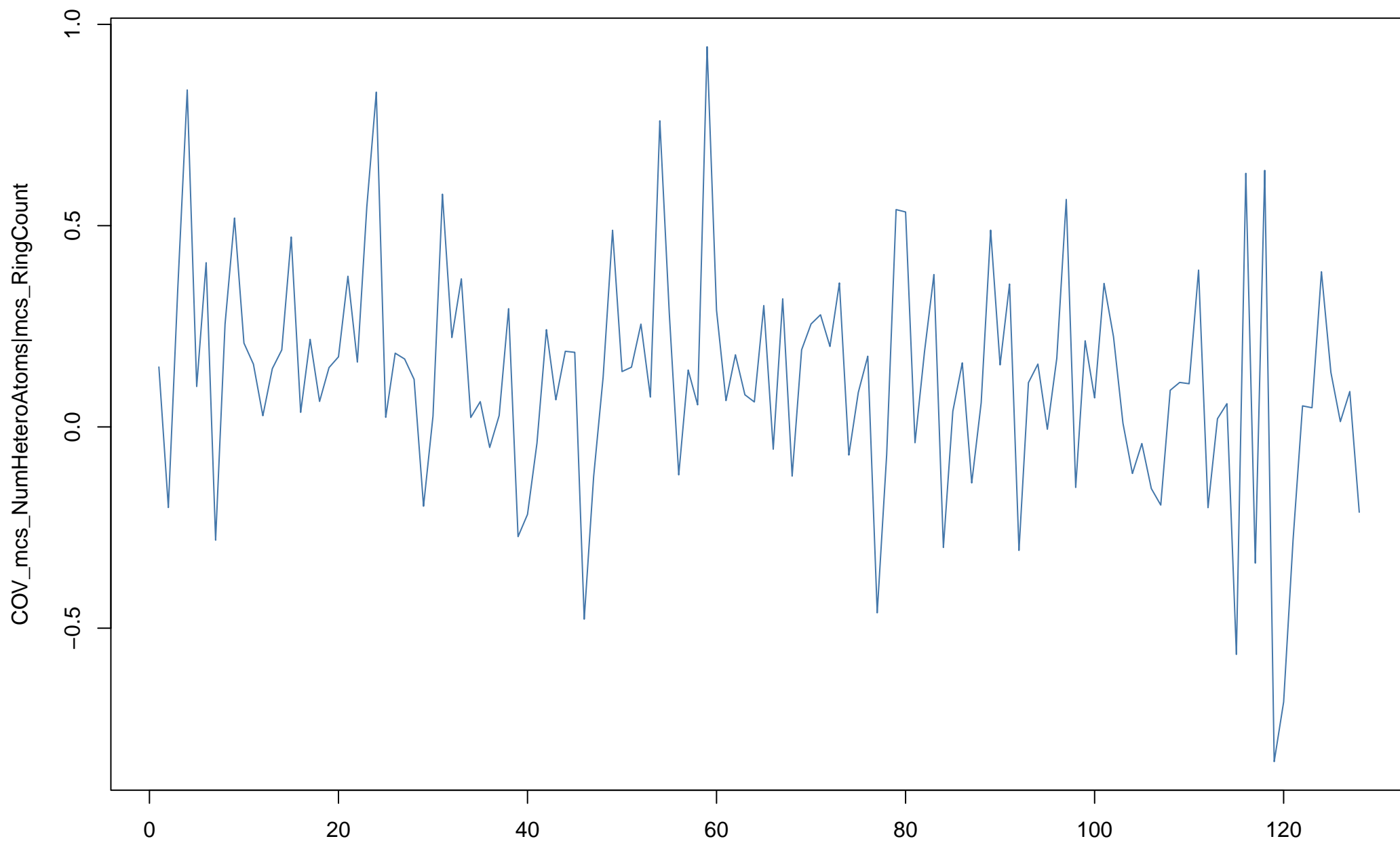
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 128 | BMK = 0.147 | MCSE(6.27) = 10.3 | stat: TRUE | burn: 120



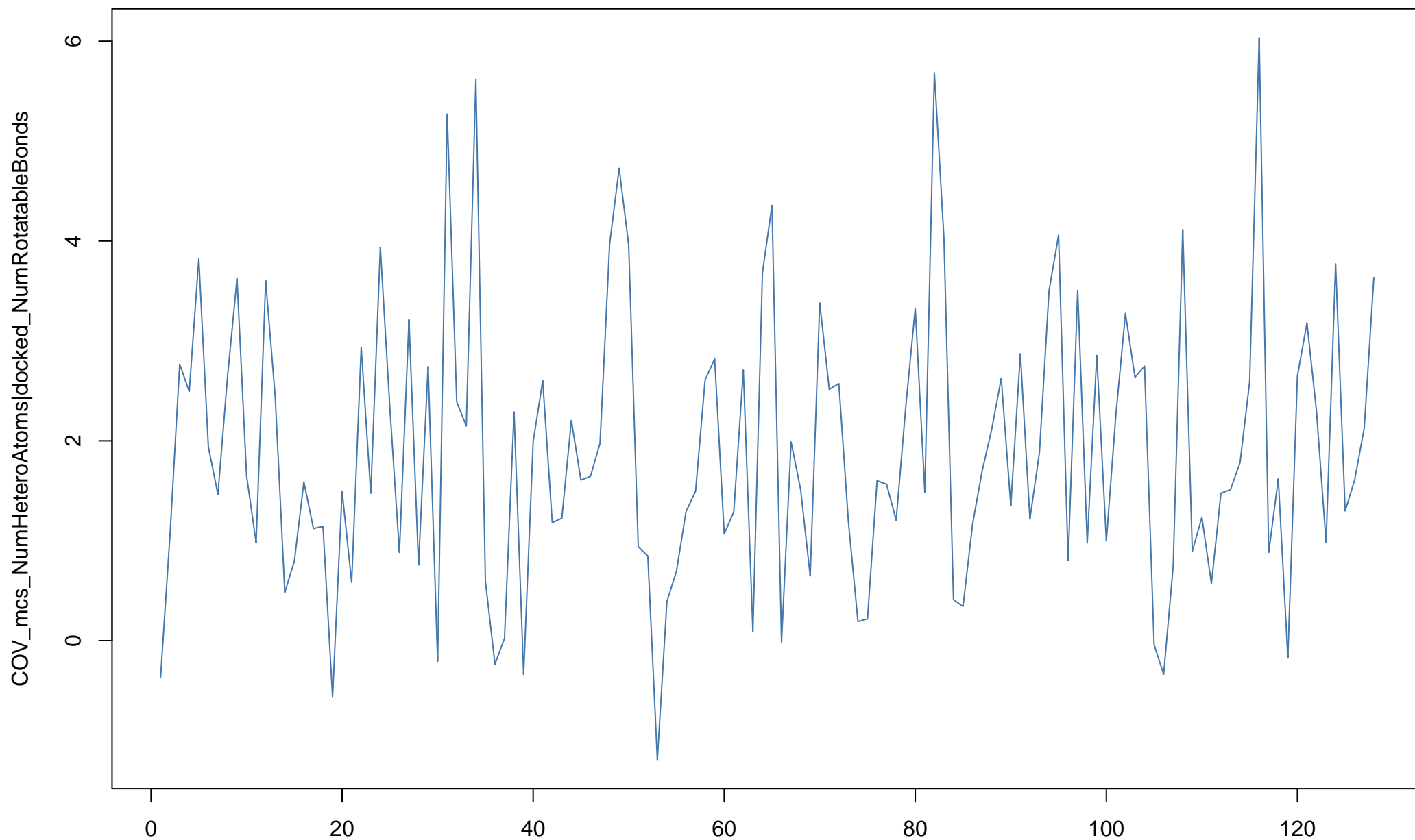
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 128 | BMK = 0.164 | MCSE(6.27) = 11.3 | stat: TRUE | burn: 12



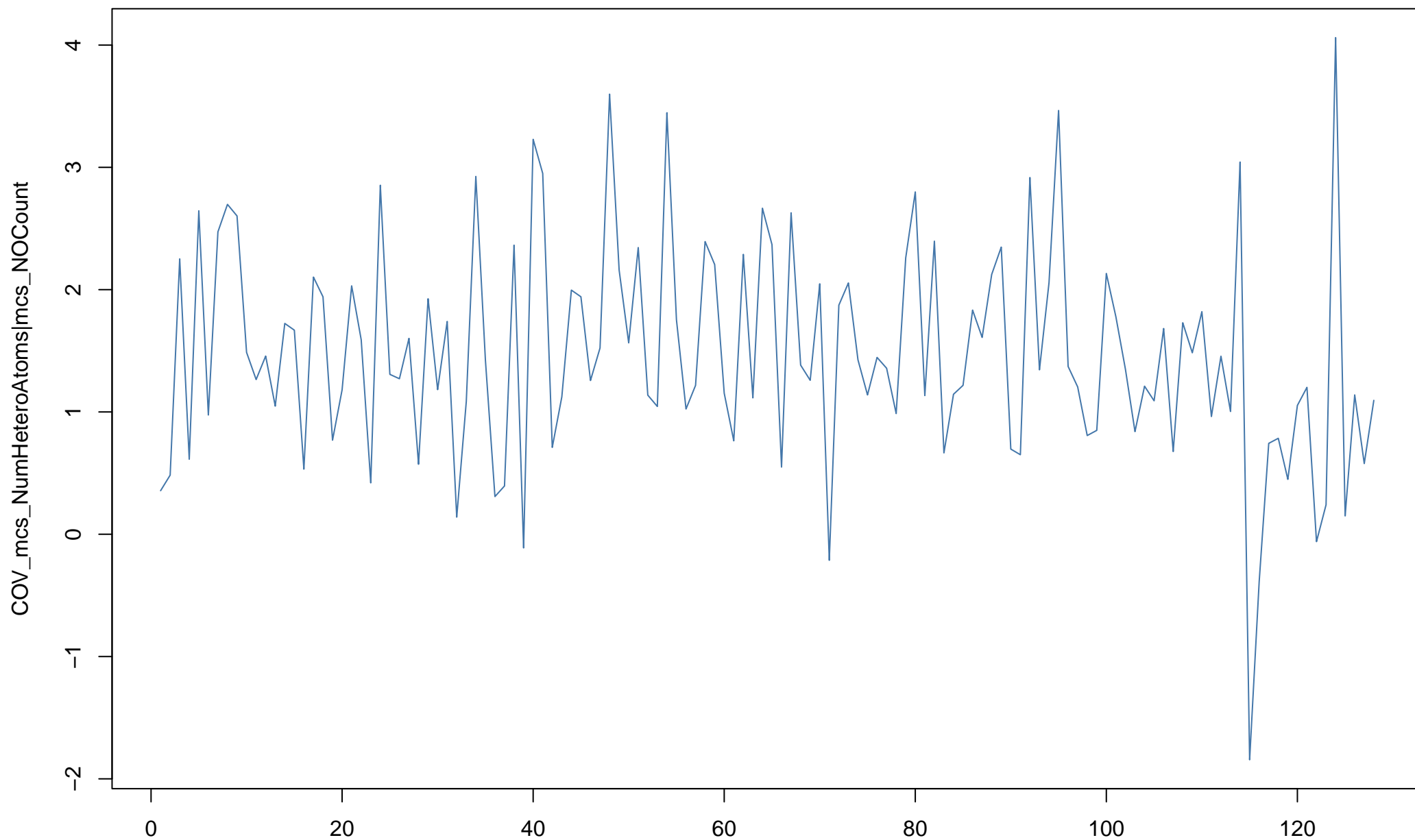
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 128 | BMK = 0.214 | MCSE(6.27) = 9.7 | stat: TRUE | burn: 0



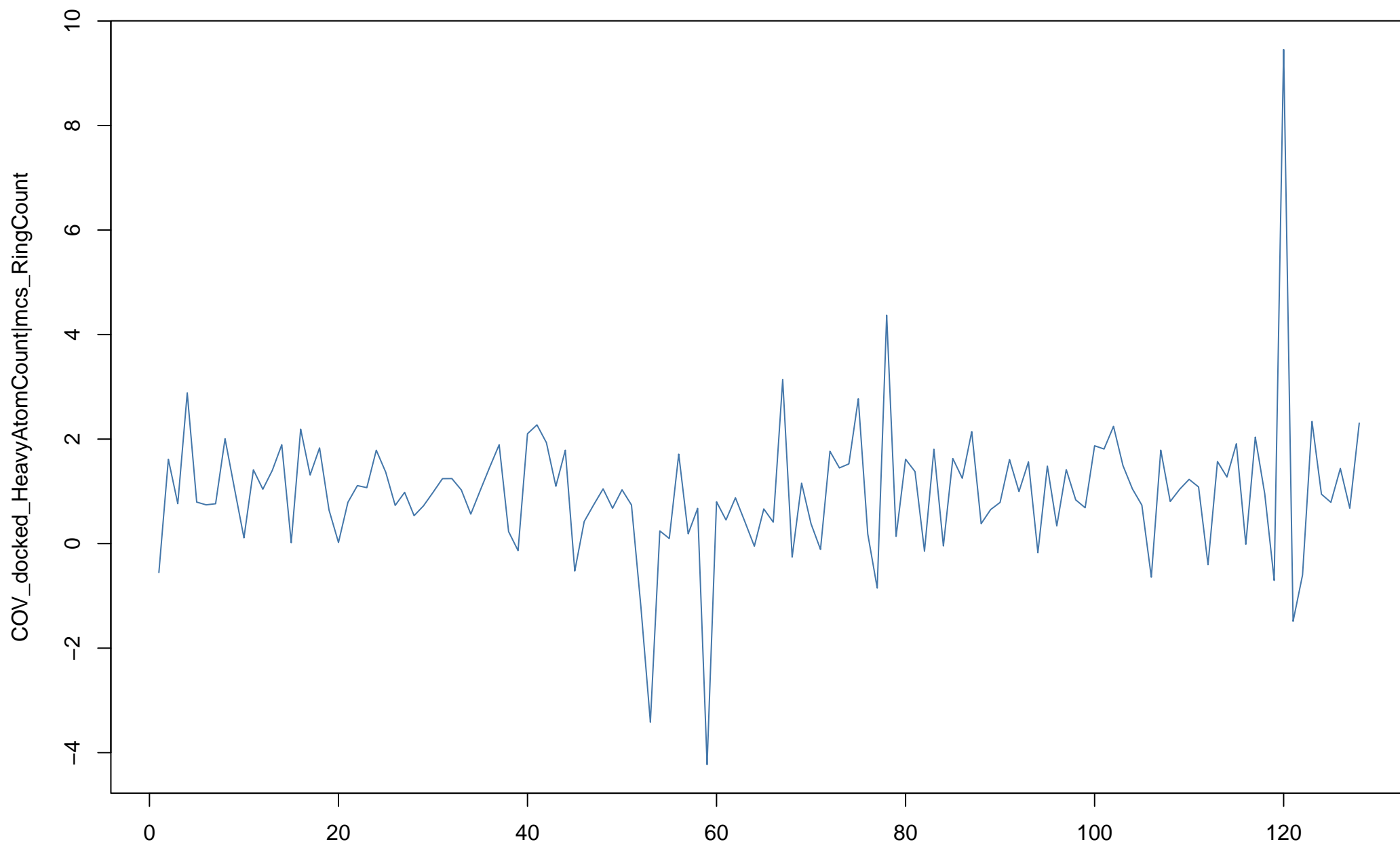
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 128 | BMK = 0.0605 | MCSE(6.27) = 10 | stat: TRUE | burn: 0



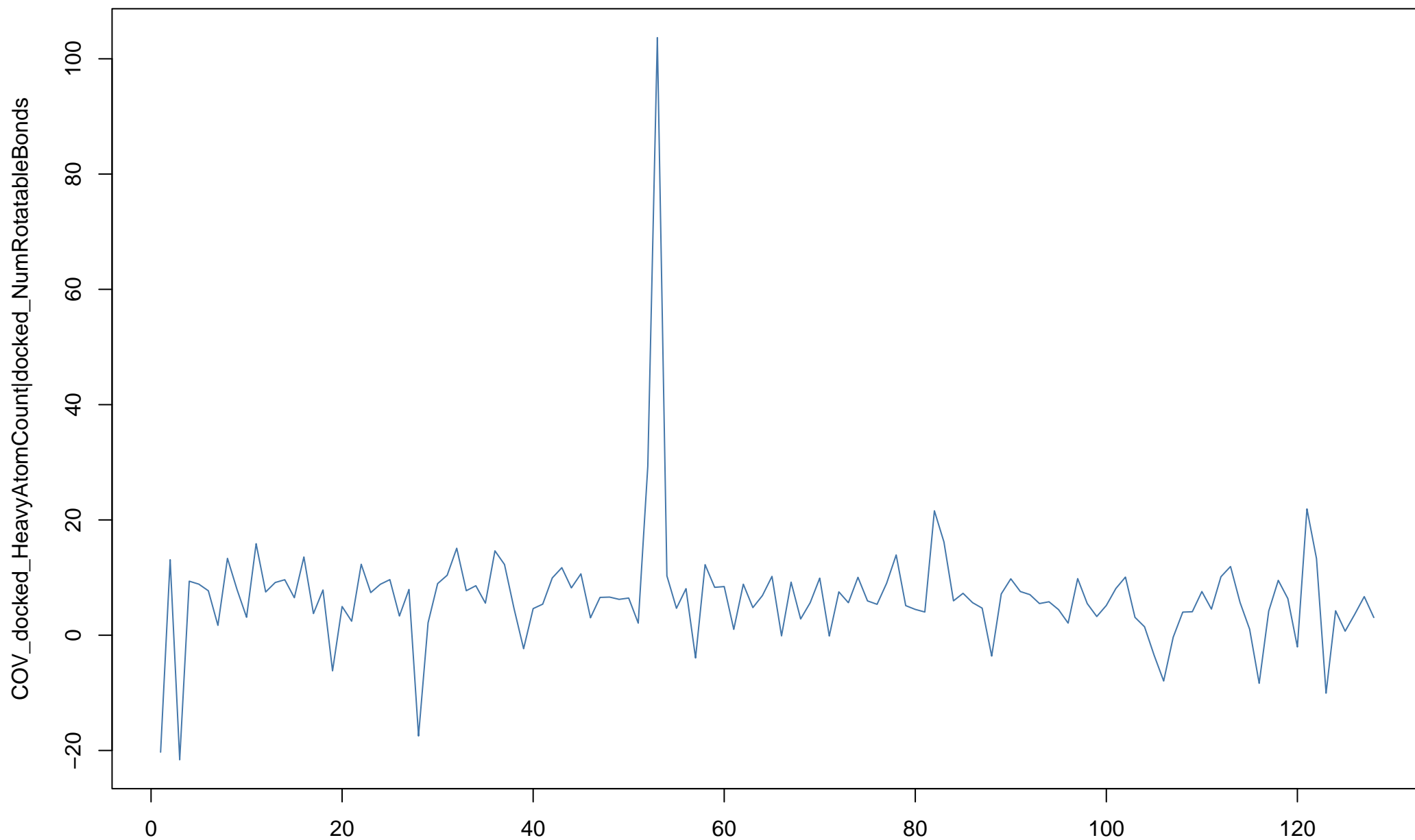
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 128 | BMK = 0.123 | MCSE(6.27) = 8.1 | stat: TRUE | burn: 0



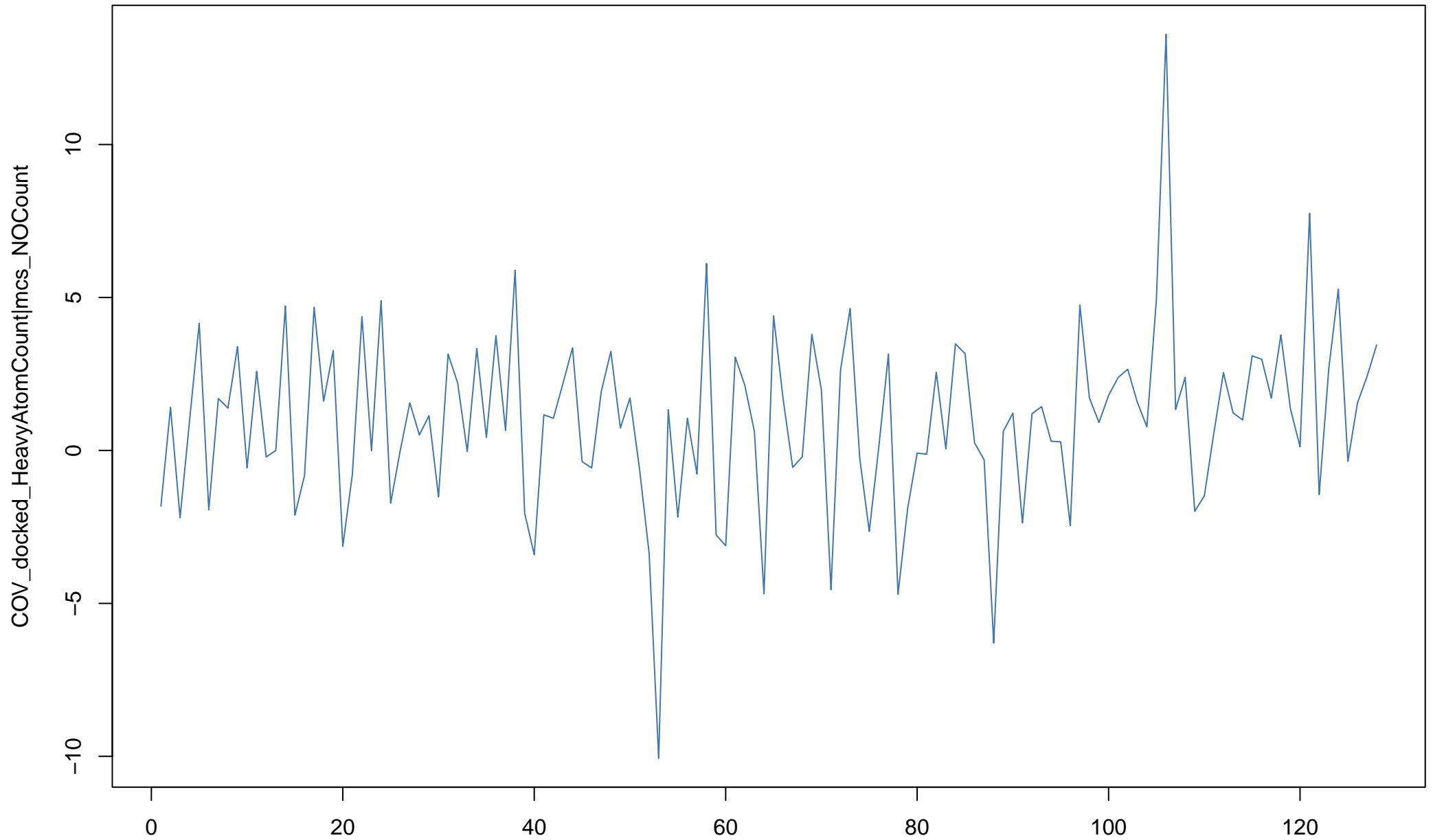
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 62 | BMK = 0.21 | MCSE(6.27) = 7.2 | stat: TRUE | burn: 0



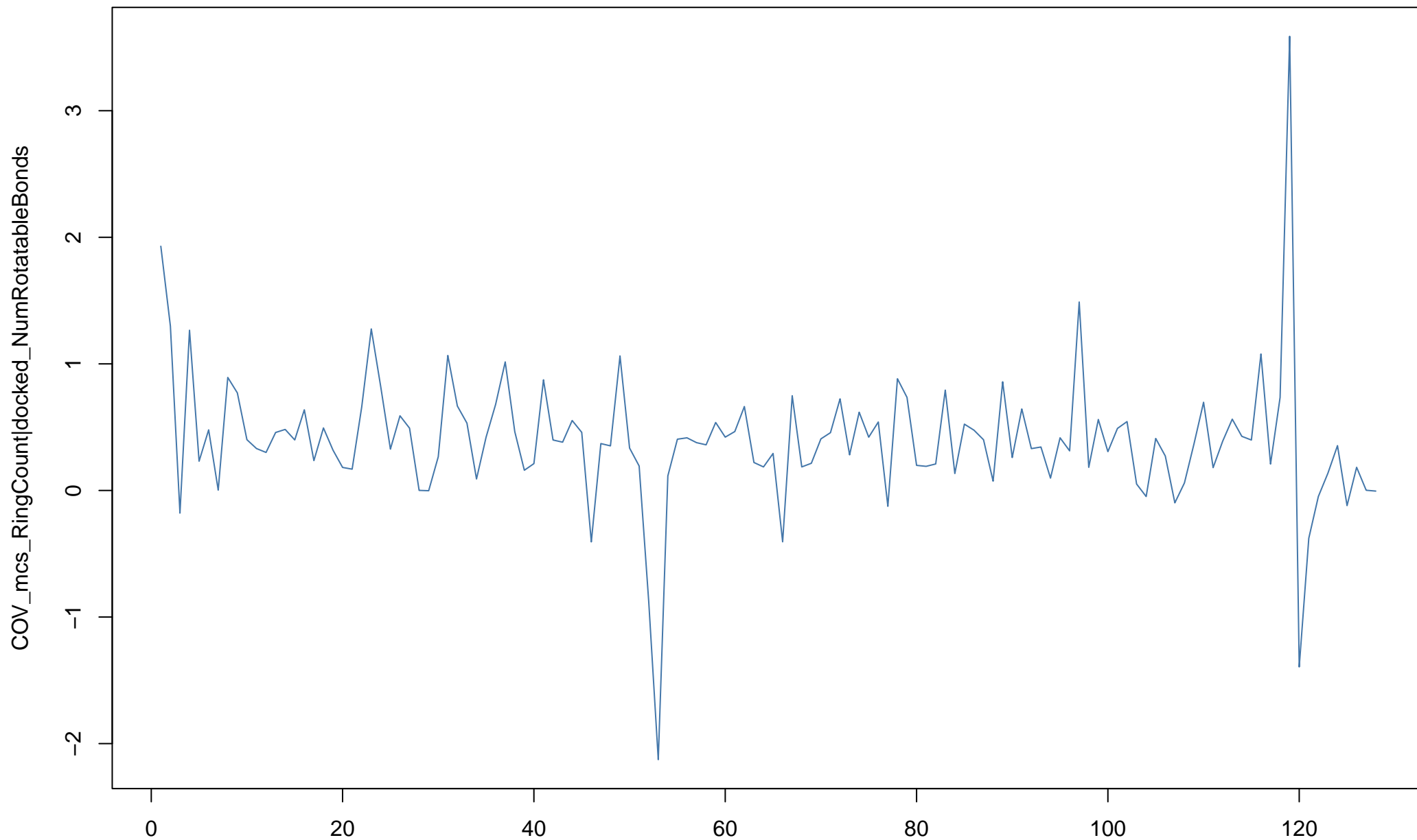
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 91.7 | BMK = 0.289 | MCSE(6.27) = 11.4 | stat: TRUE | burn: 0



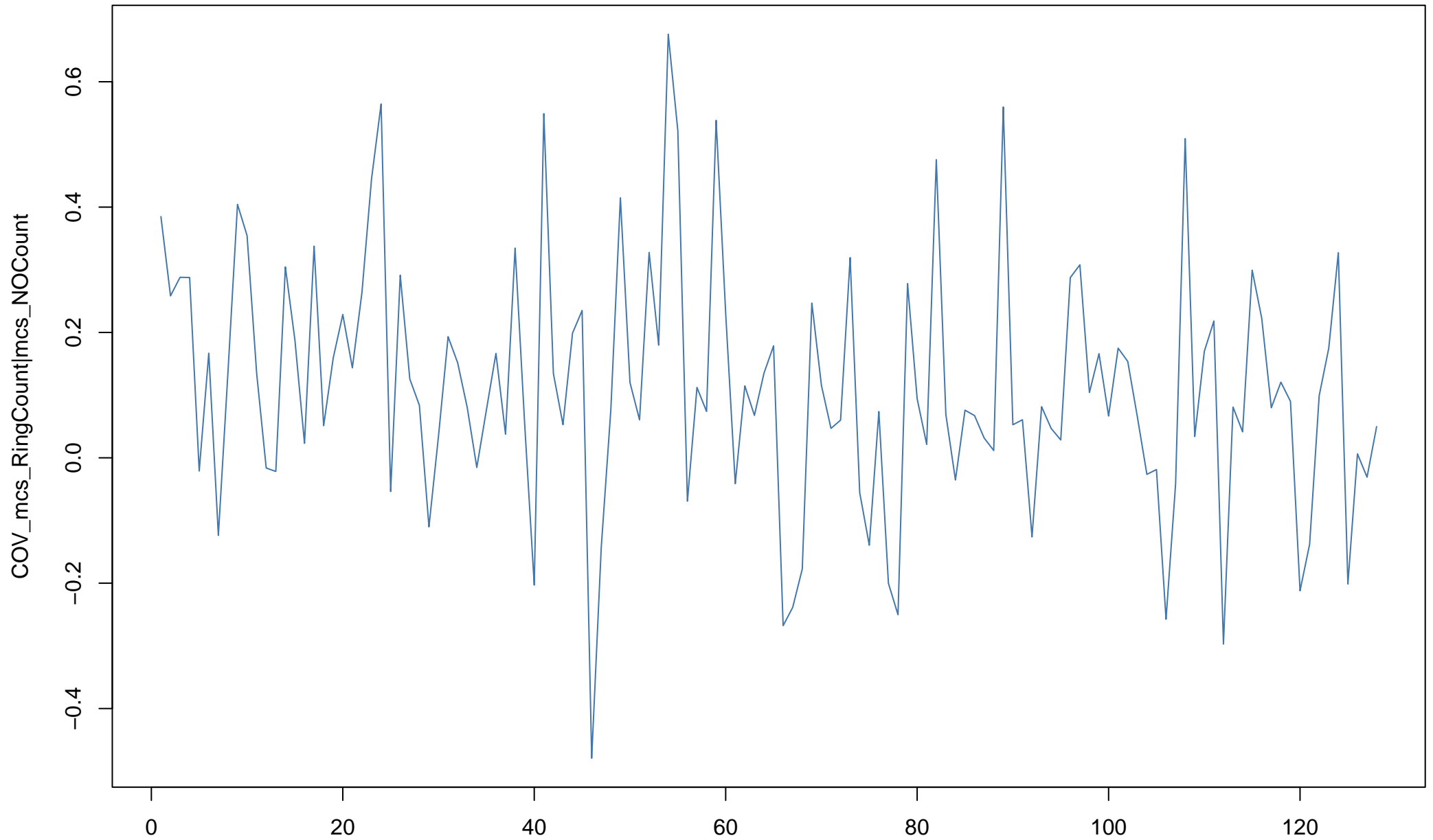
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 128 | BMK = 0.158 | MCSE(6.27) = 8.79 | stat: TRUE | burn: 96



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 128 | BMK = 0.232 | MCSE(6.27) = 9.19 | stat: TRUE | burn: 0



COV_mcs_RingCount|mcs_NOCount
ESS = 96.3 | BMK = 0.211 | MCSE(6.27) = 10.4 | stat: TRUE | burn: 96



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 96.7 | BMK = 0.149 | MCSE(6.27) = 10.9 | stat: TRUE | burn: 0

