

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 1

max MCSE = 44.3212999857989

all stationary: FALSE

burn: 20

min percent.: 0

-- STATS 2D --

min ESS = 4.34817675241008

max BMK = 0.434362923769908

max MCSE = 45.8361003904253

all stationary: FALSE

burn: 20

min percent.: 0

-- STATS 1D --

min ESS = 20

max BMK = 0.557080352038498

max MCSE = NaN

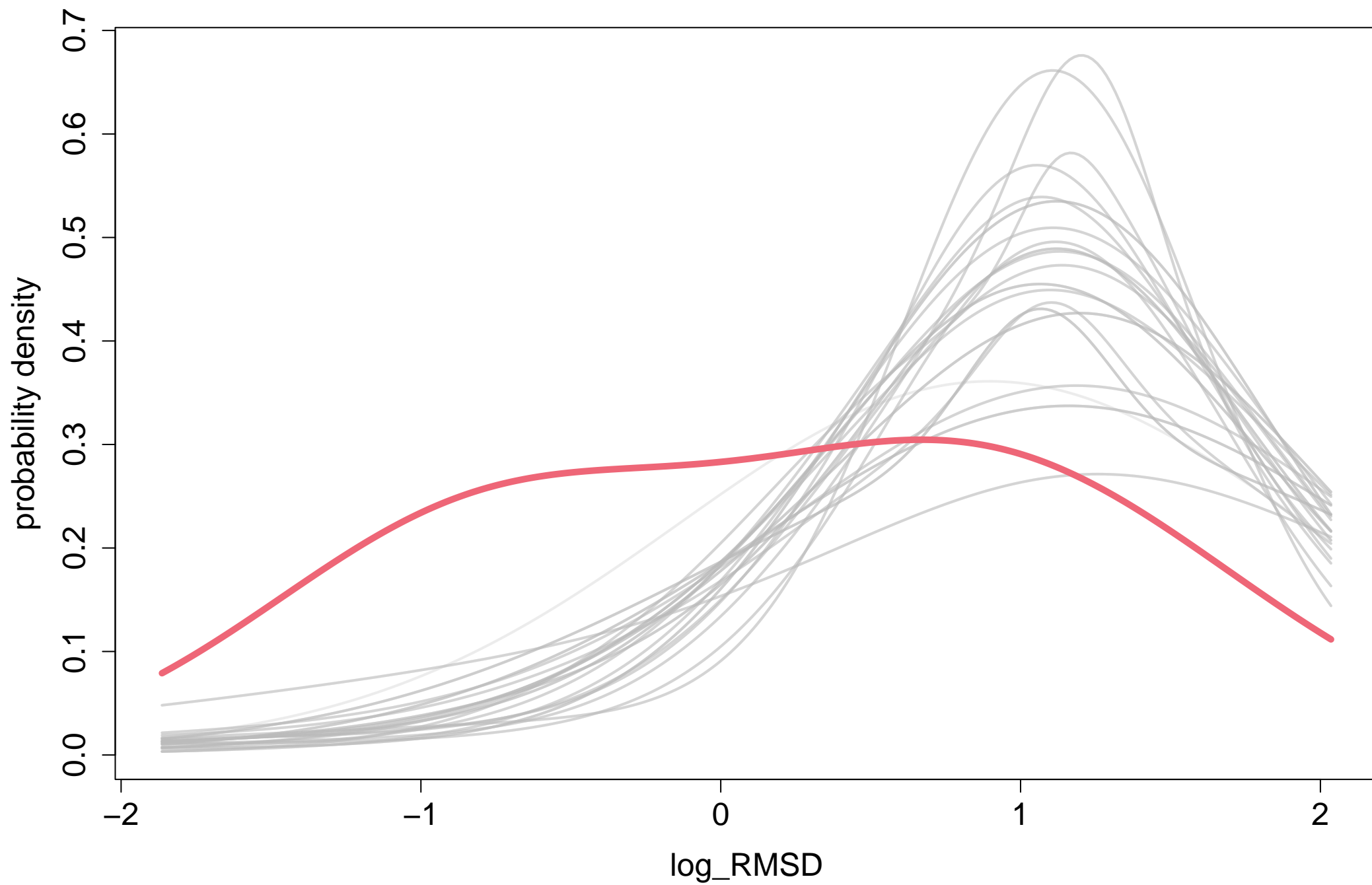
all stationary: FALSE

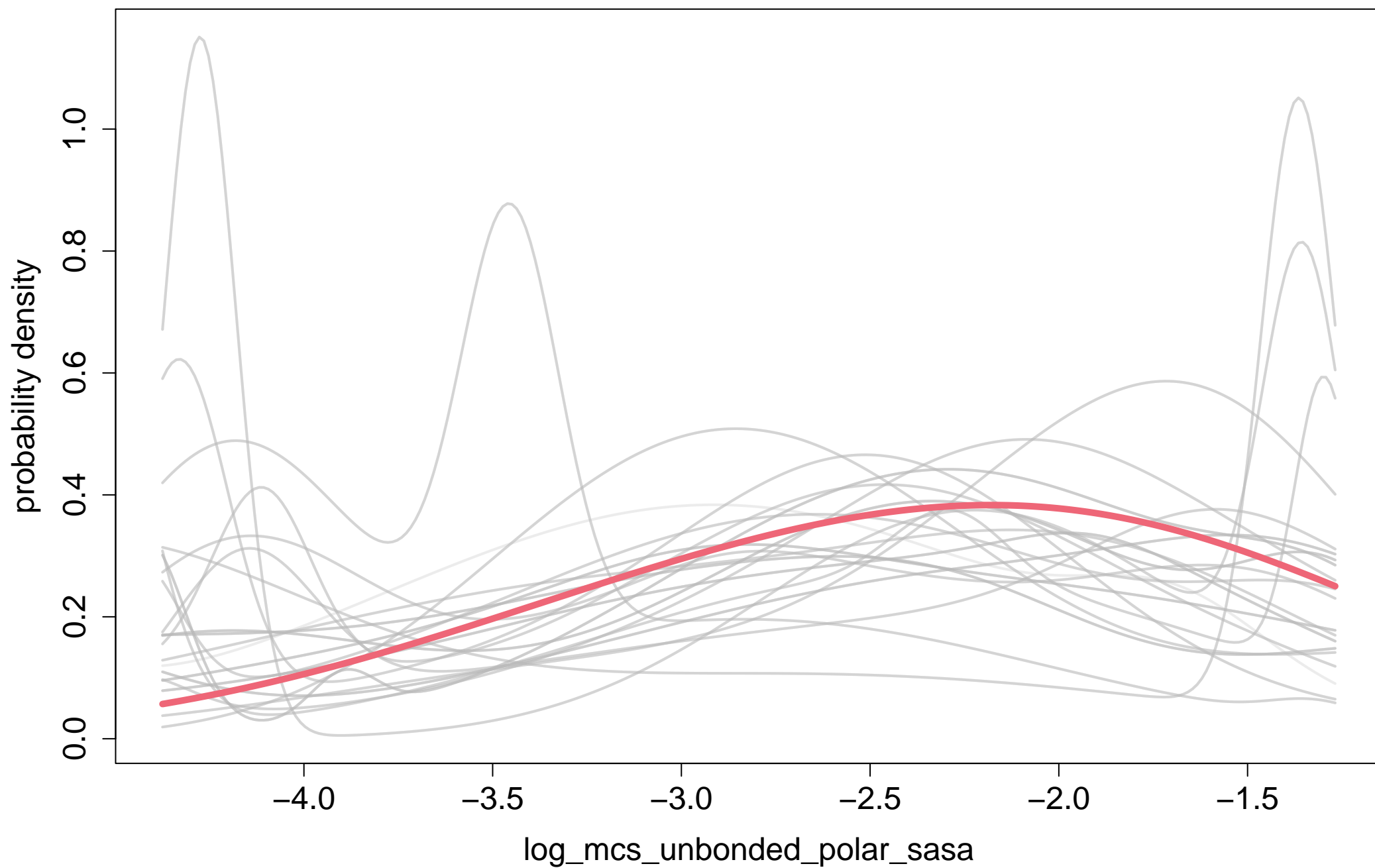
burn: 20

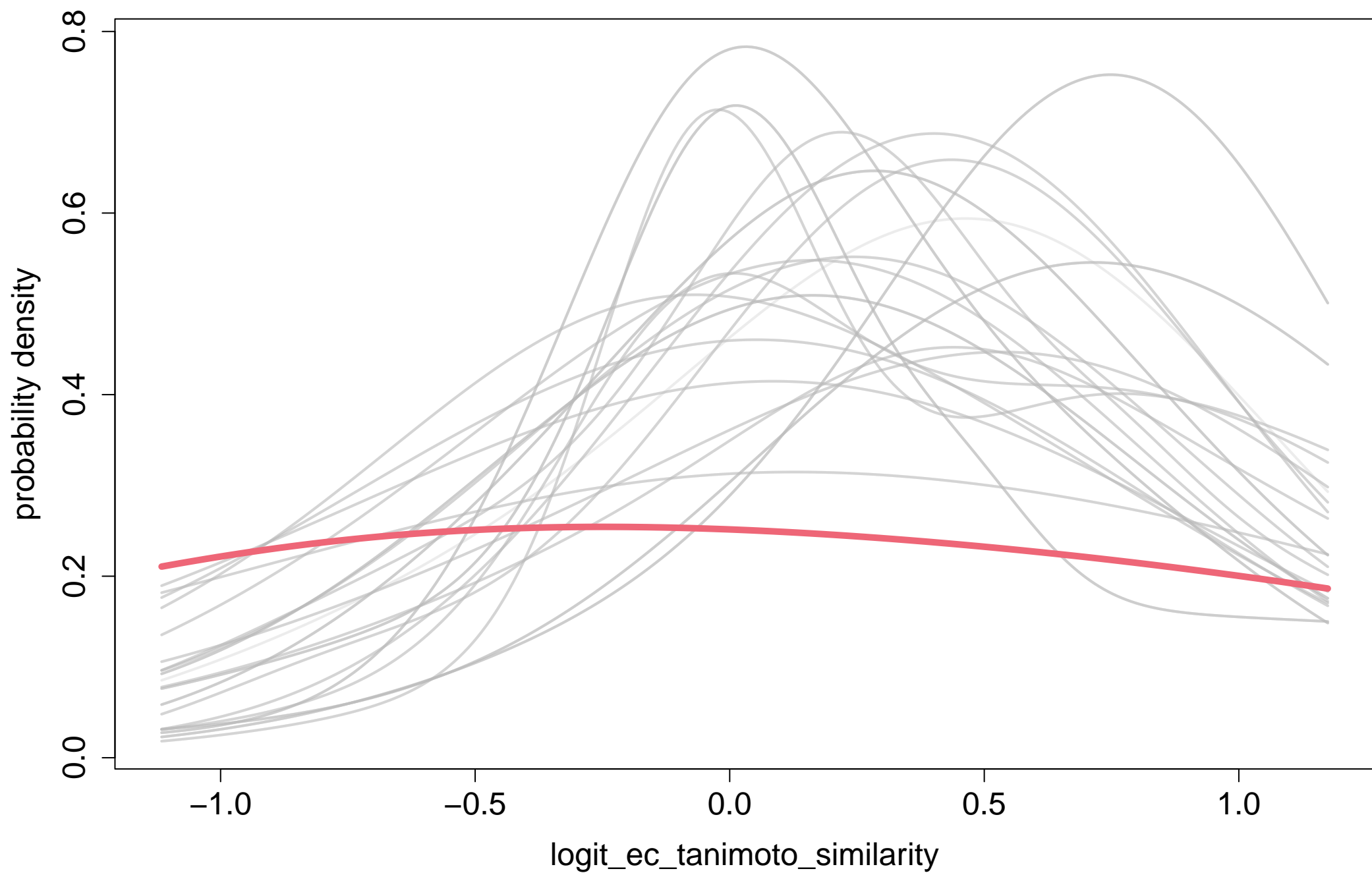
min percent.: 0

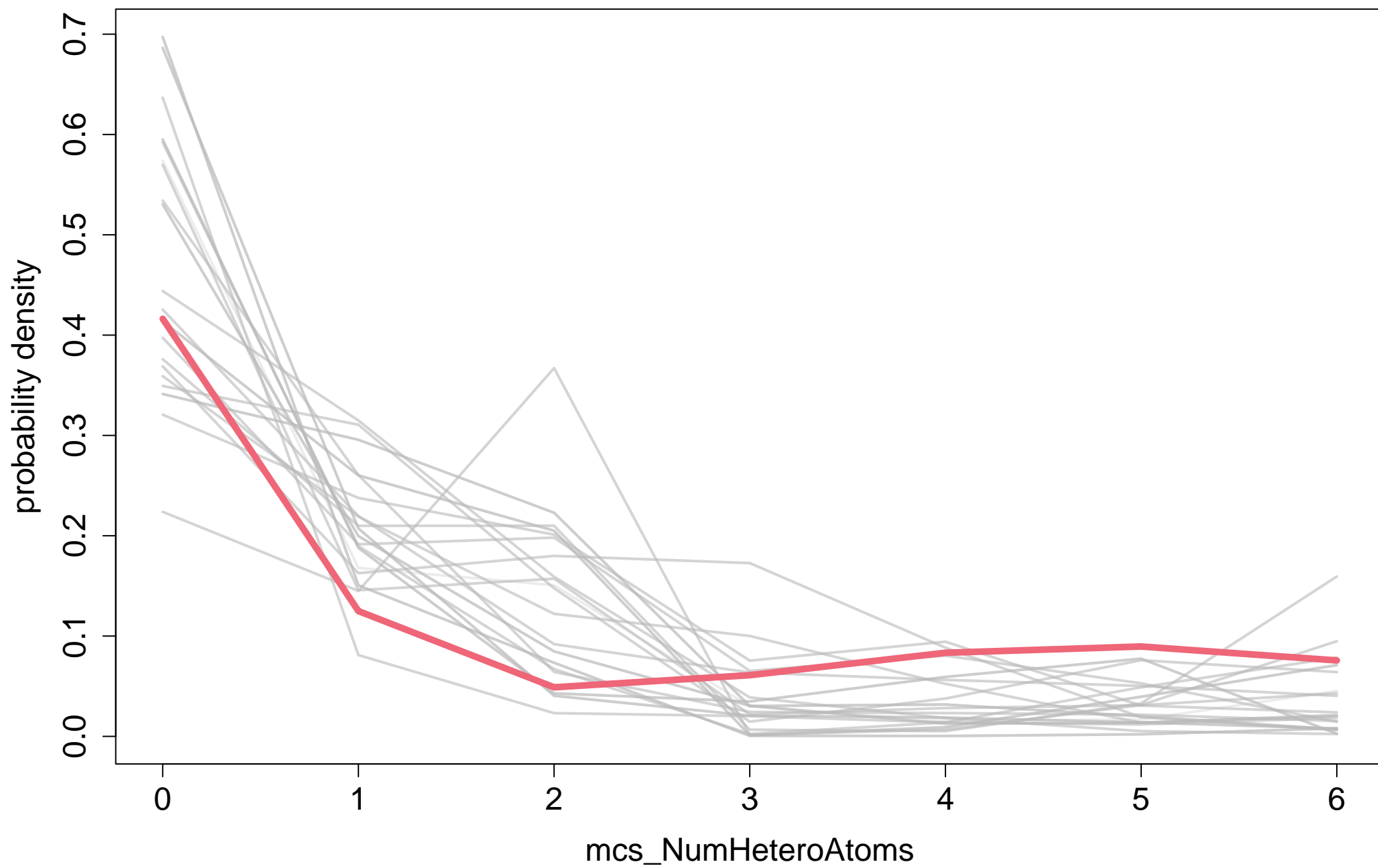
Occupied clusters: 3 of 4

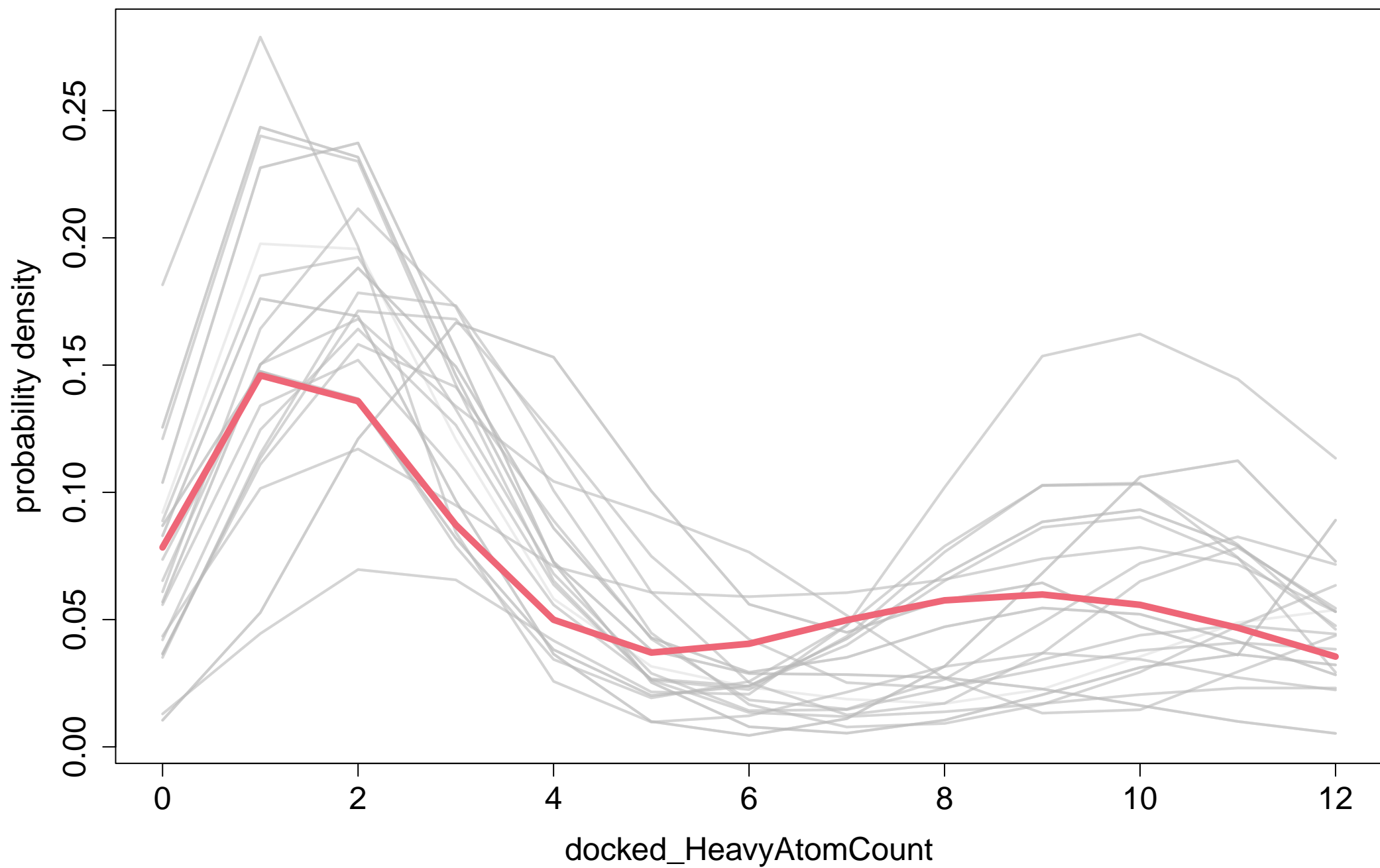
LL: -101 +- 4.97

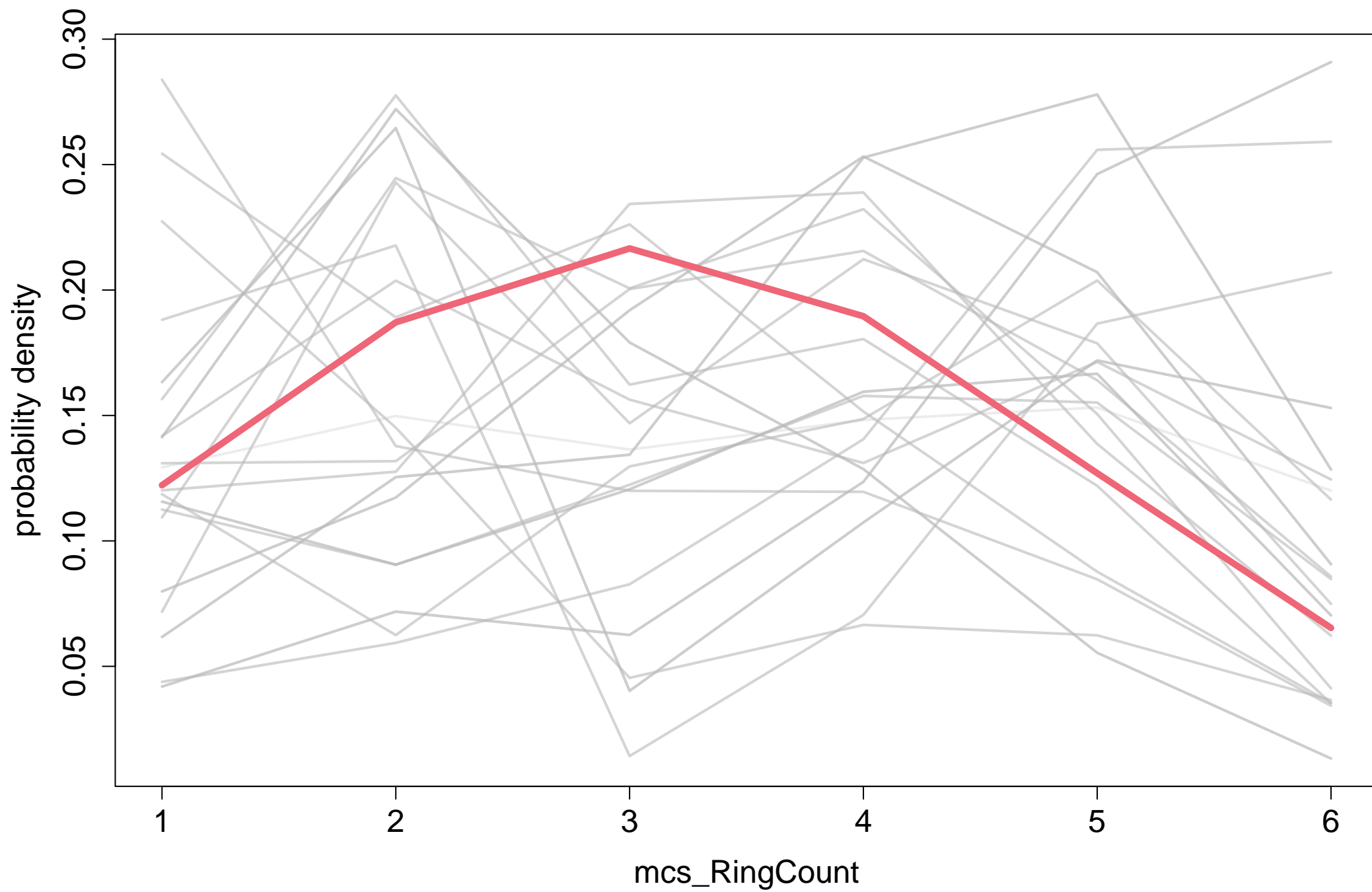


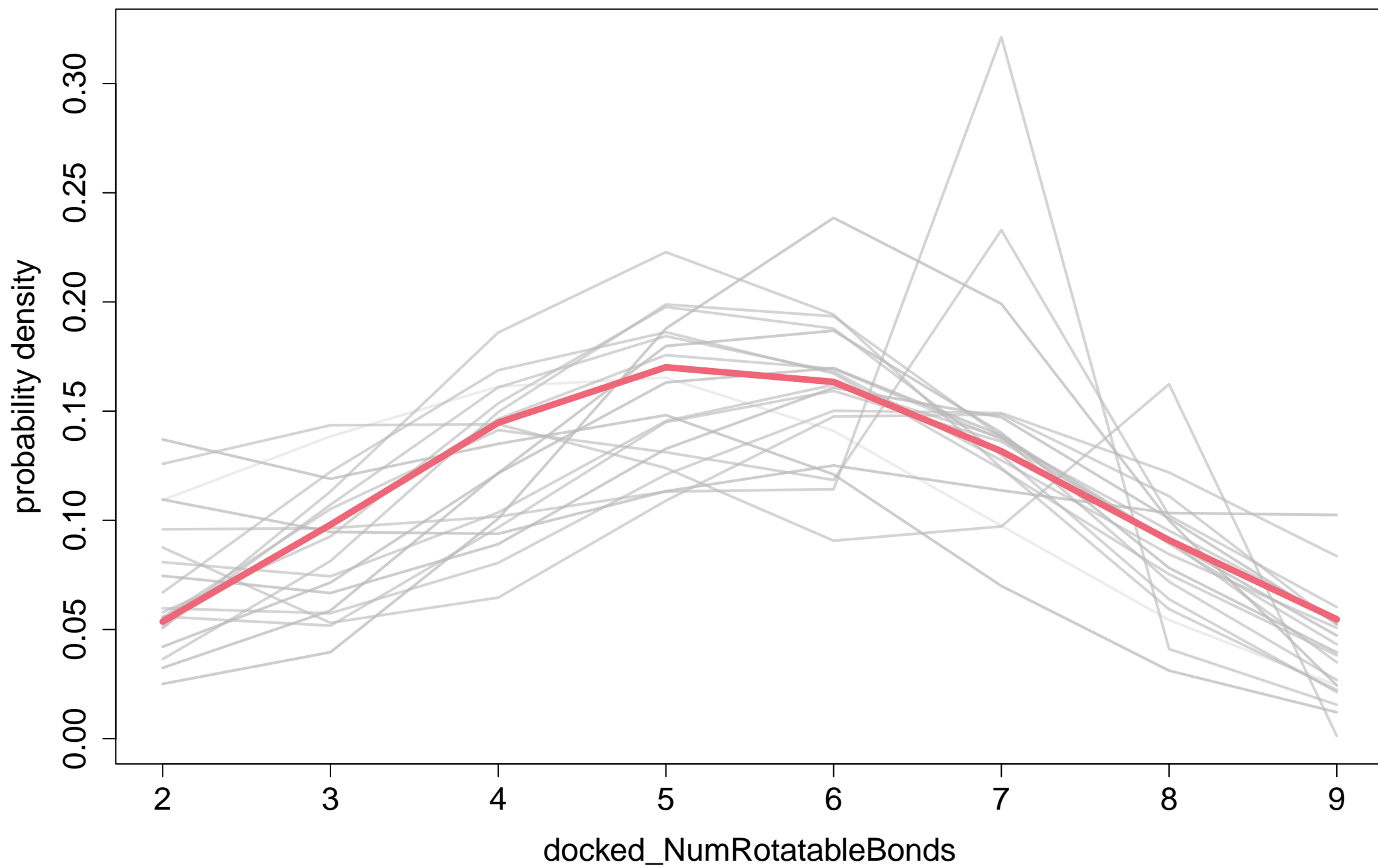


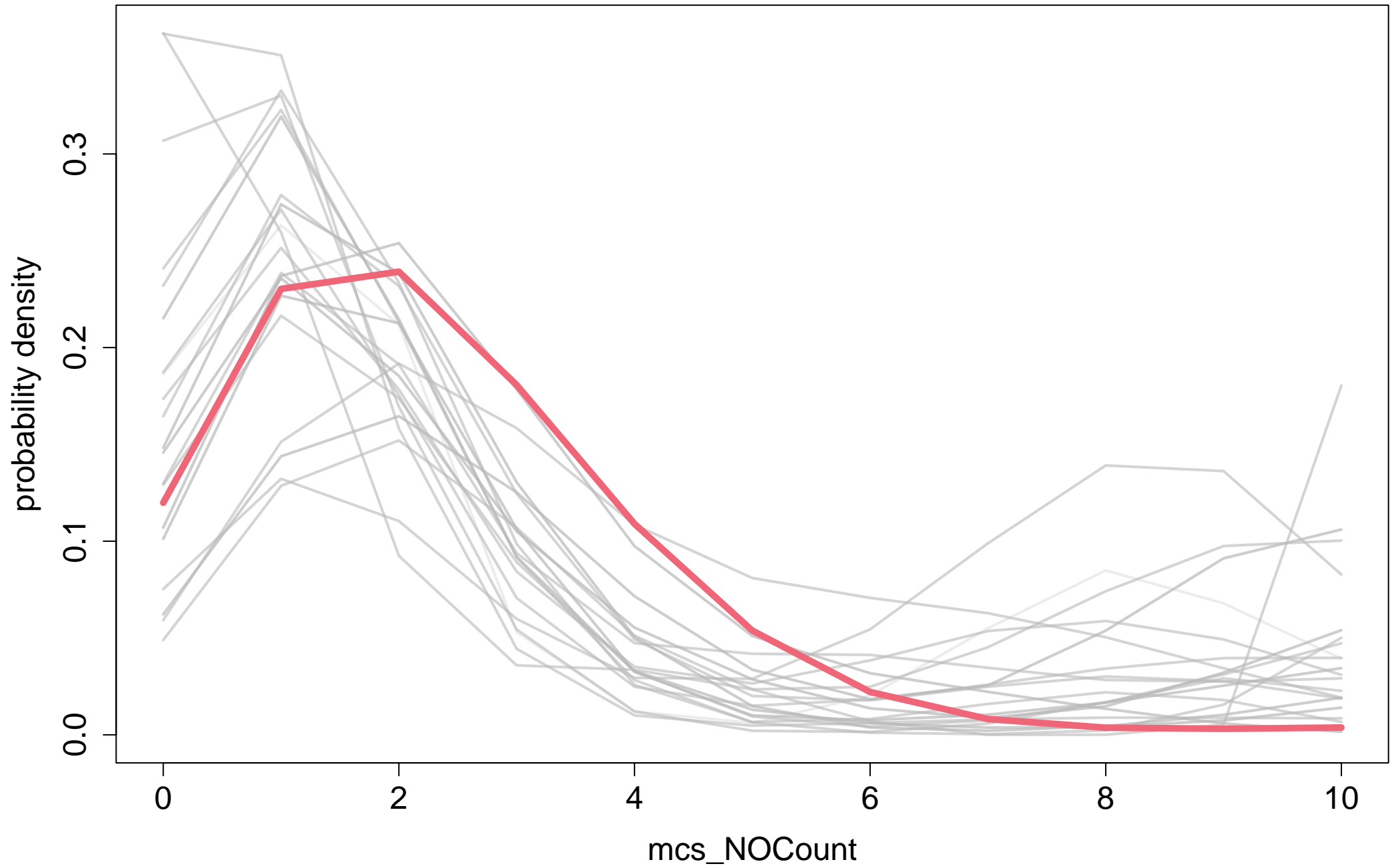


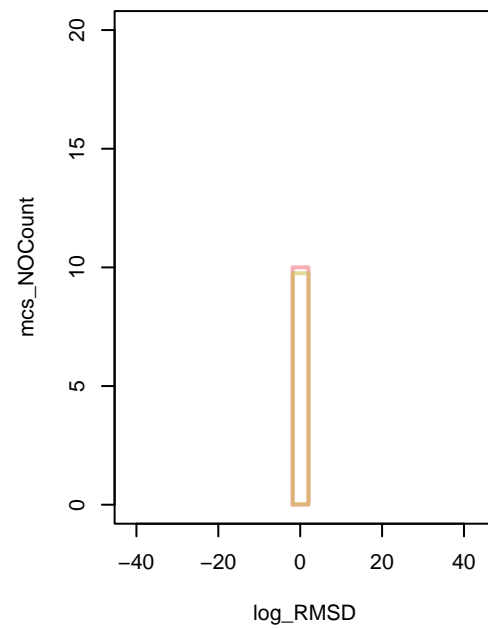
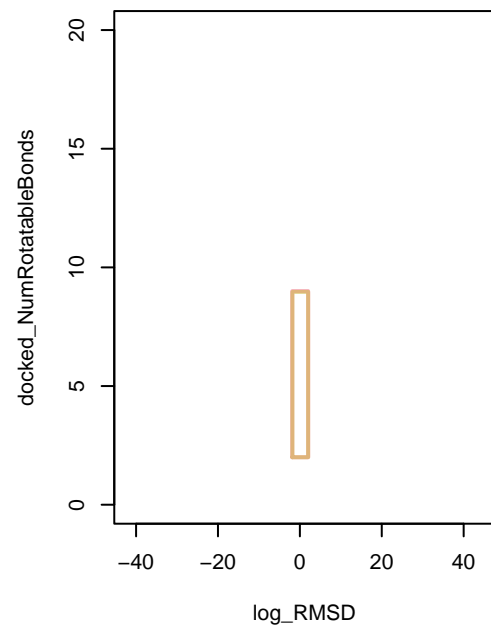
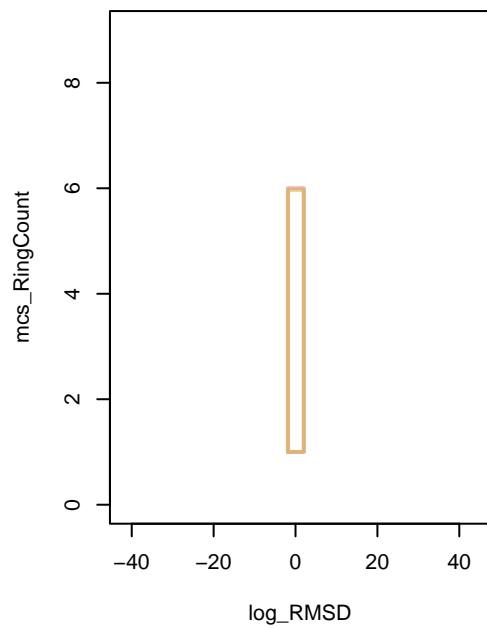
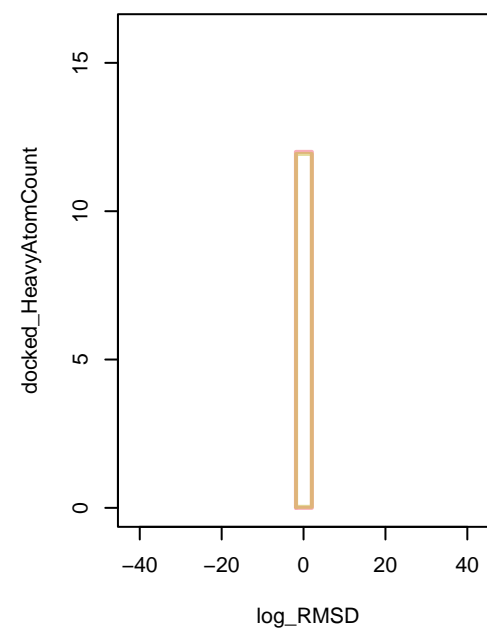
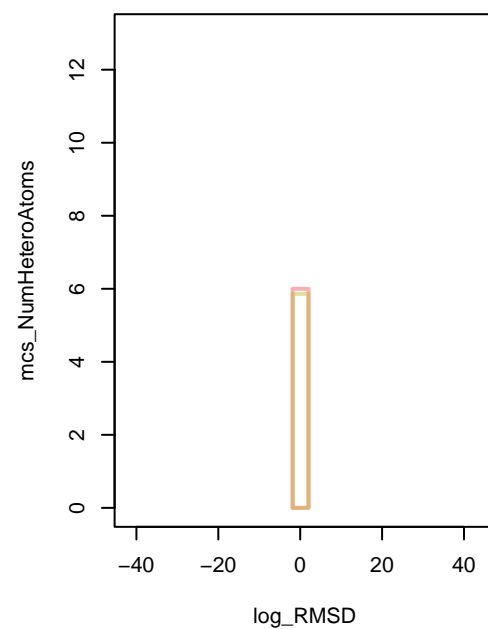
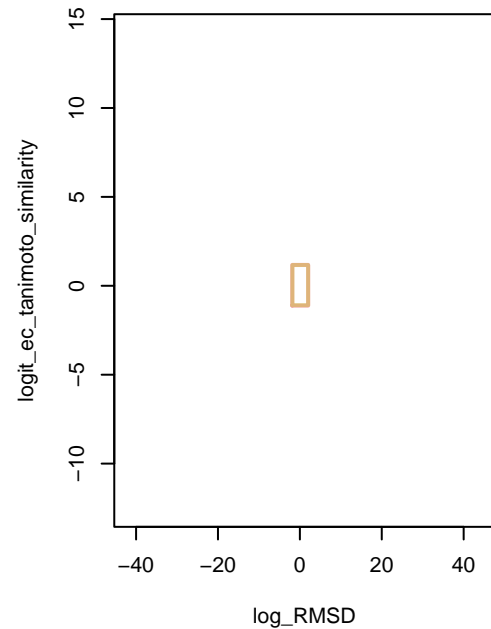
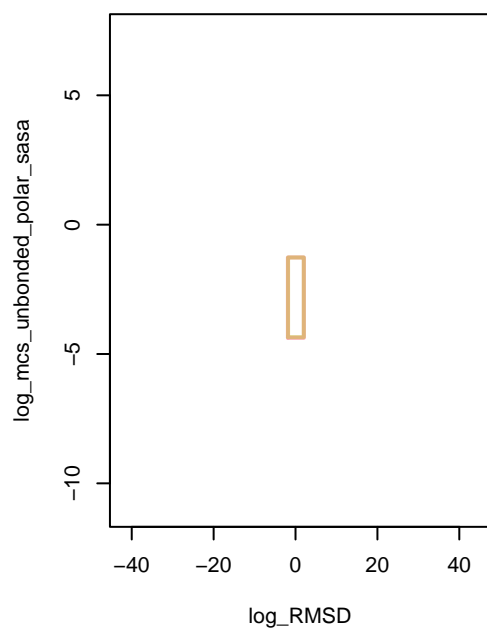




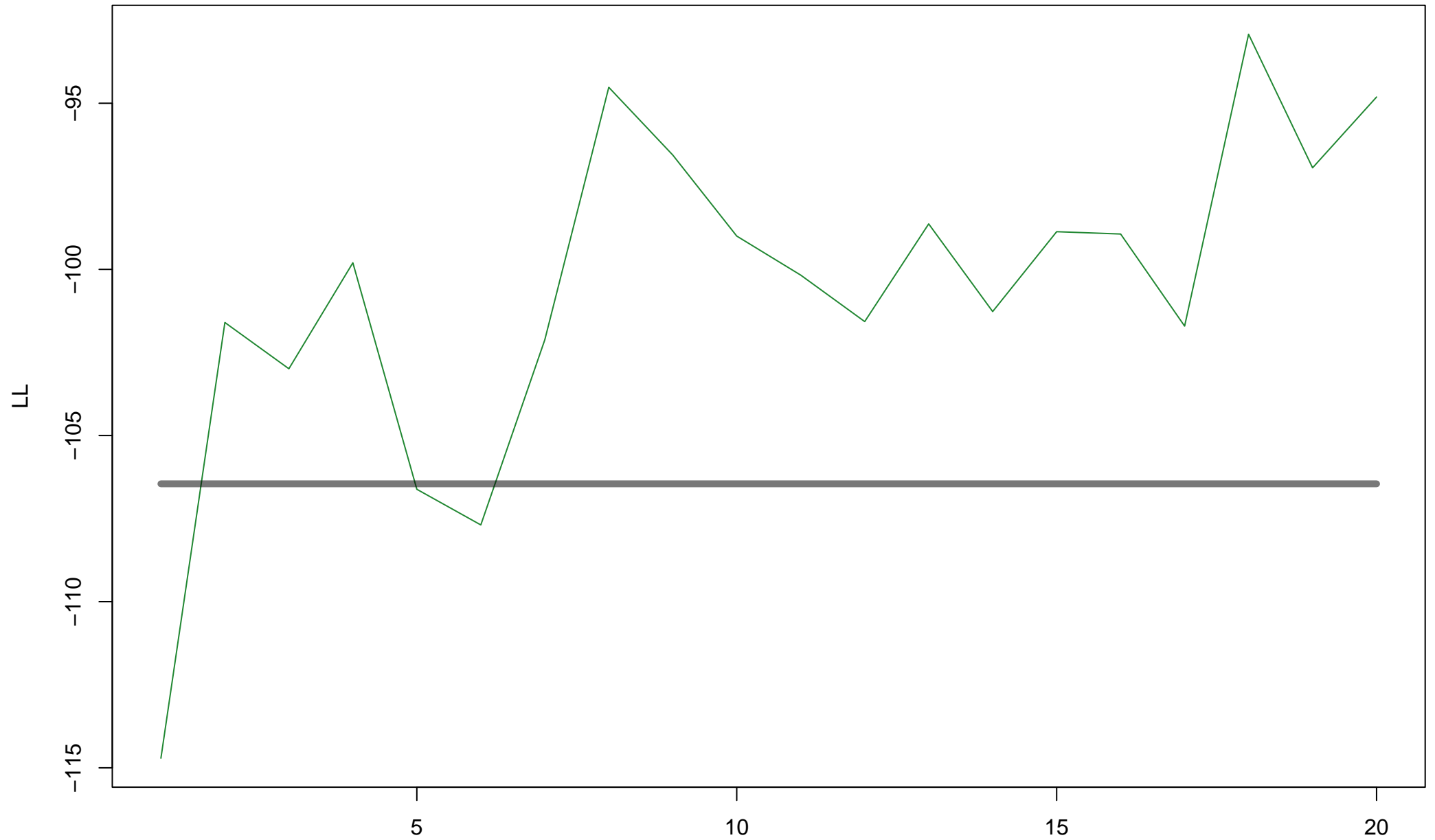




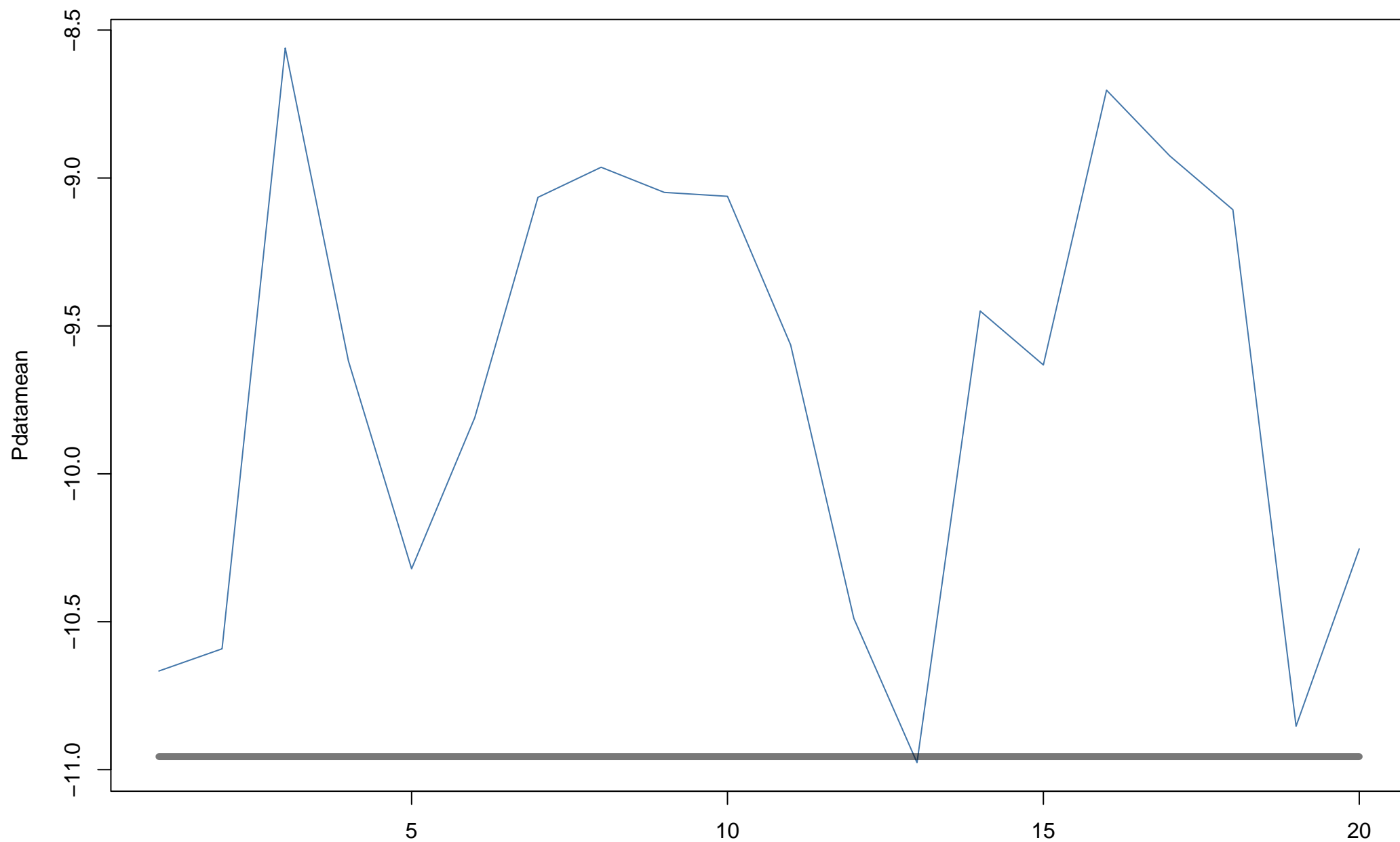




LL

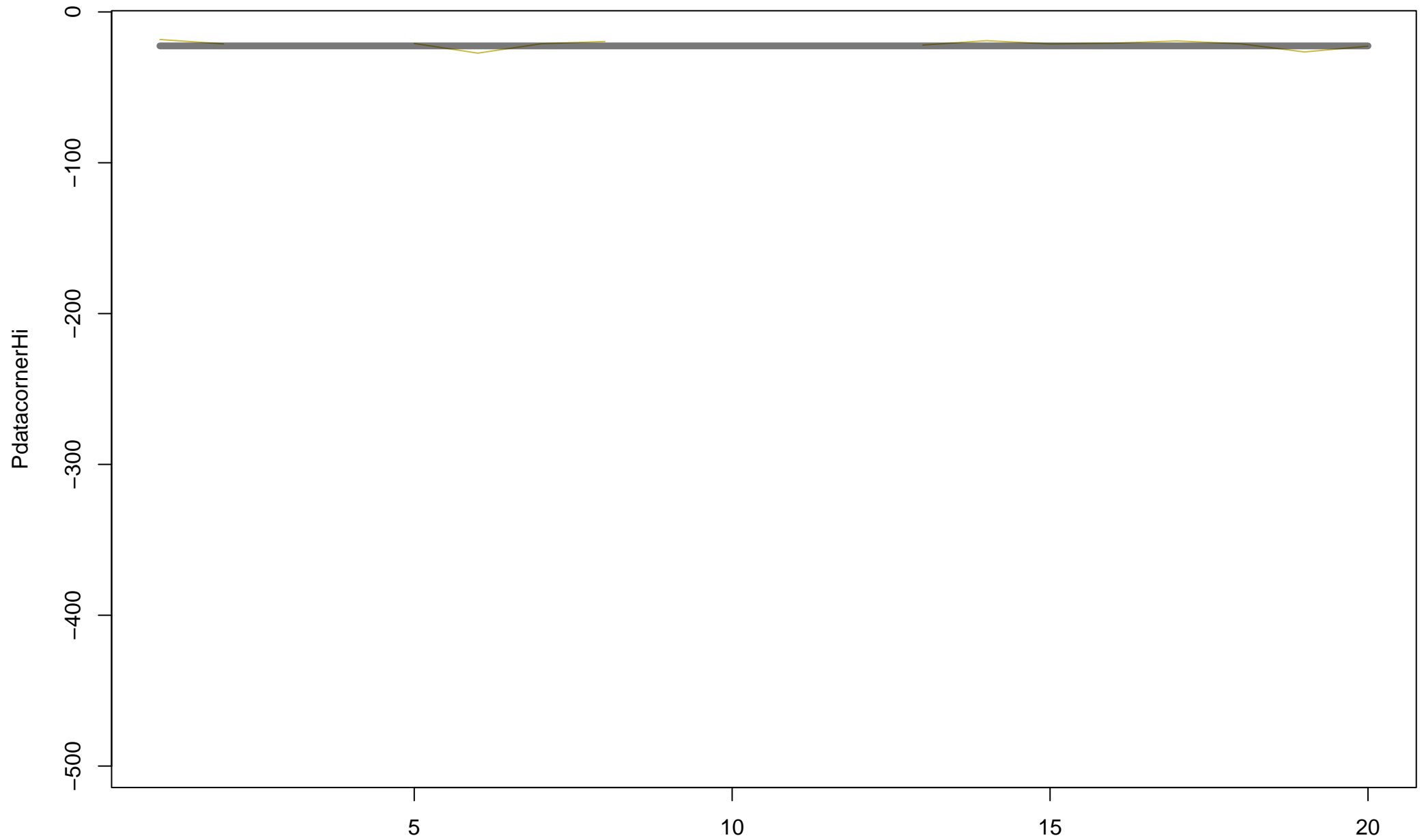


Pdatamean
ESS = 20 | BMK = 0.0736 | MCSE(6.27) = 25.9 | stat: FALSE | burn: 20 | percentile: 5

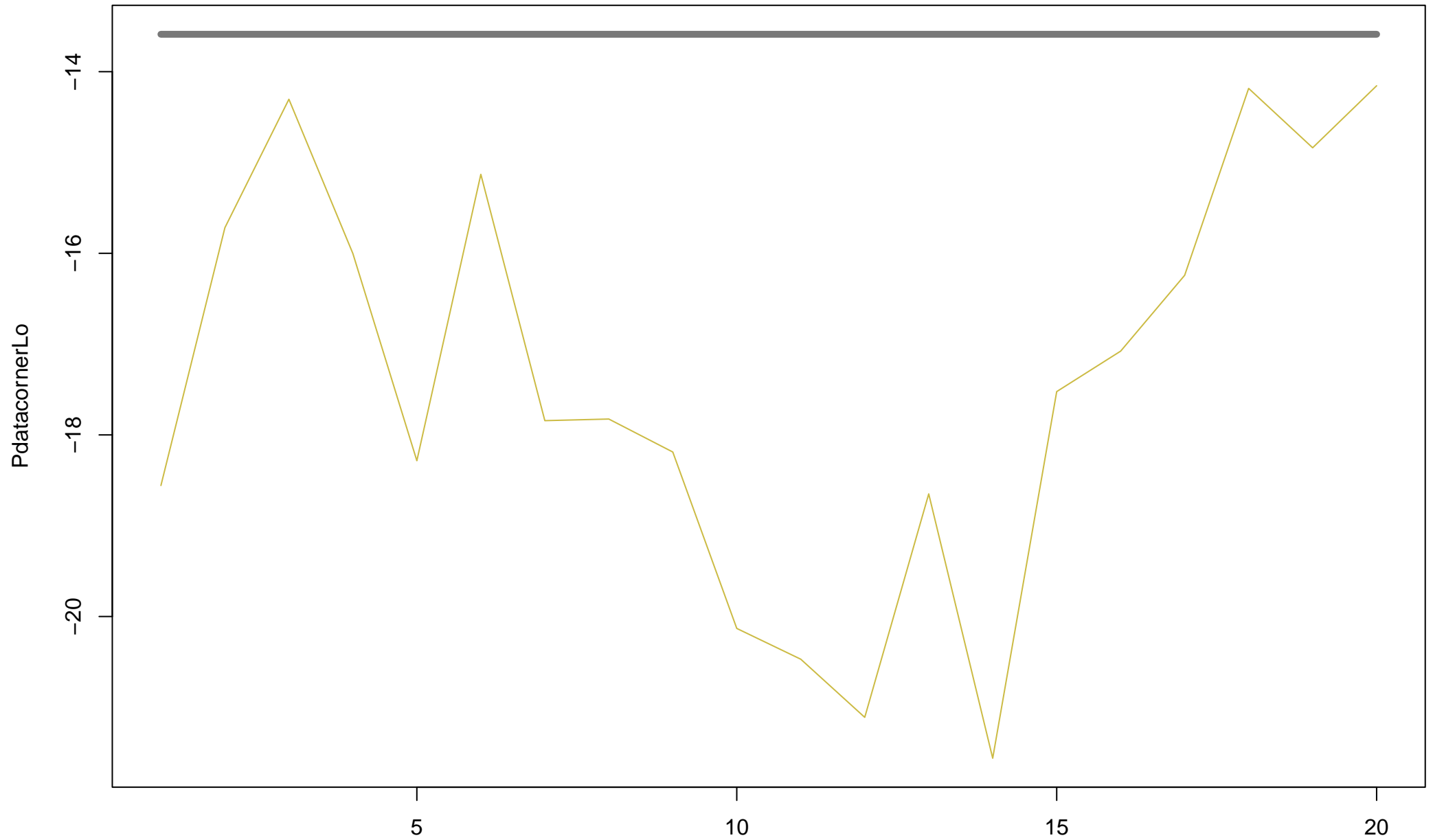


PdatacornerHi

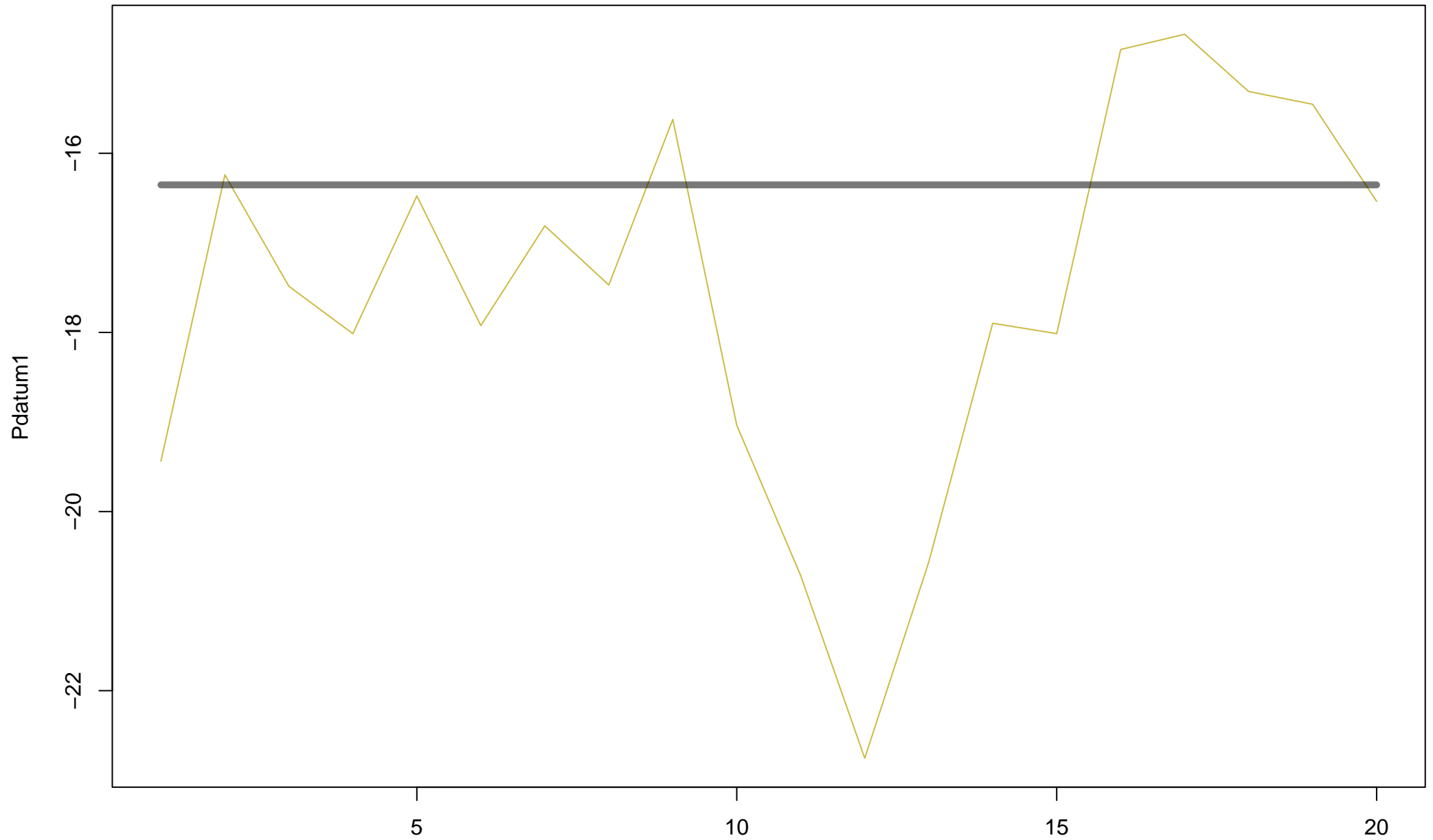
ESS = 2.22e-16 | BMK = 0.414 | MCSE(6.27) = 21 | stat: FALSE | burn: 20 | percentile: 45



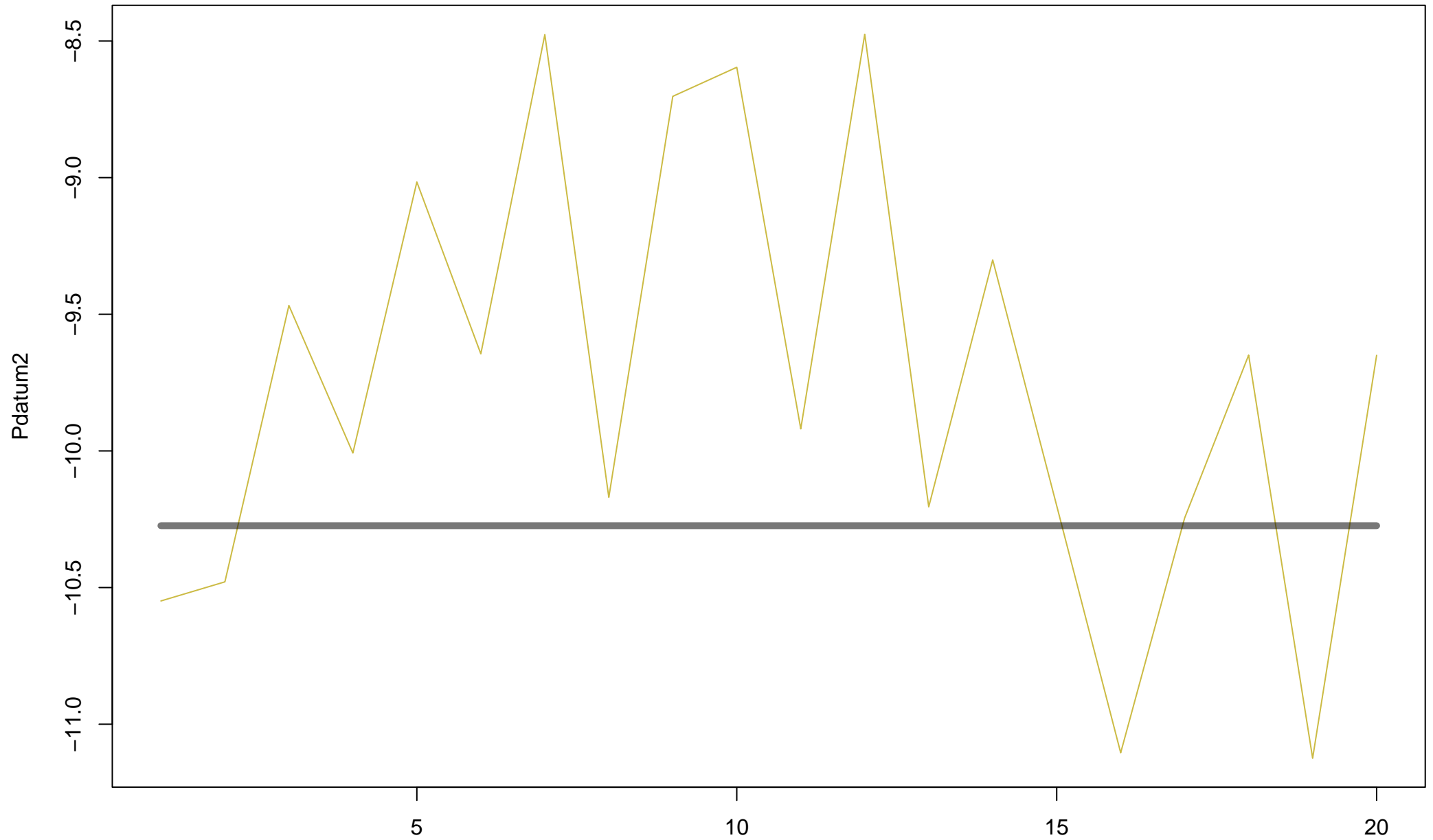
PdatacornerLo
ESS = 20 | BMK = 0.198 | MCSE(6.27) = 40.2 | stat: FALSE | burn: 16 | percentile: 100



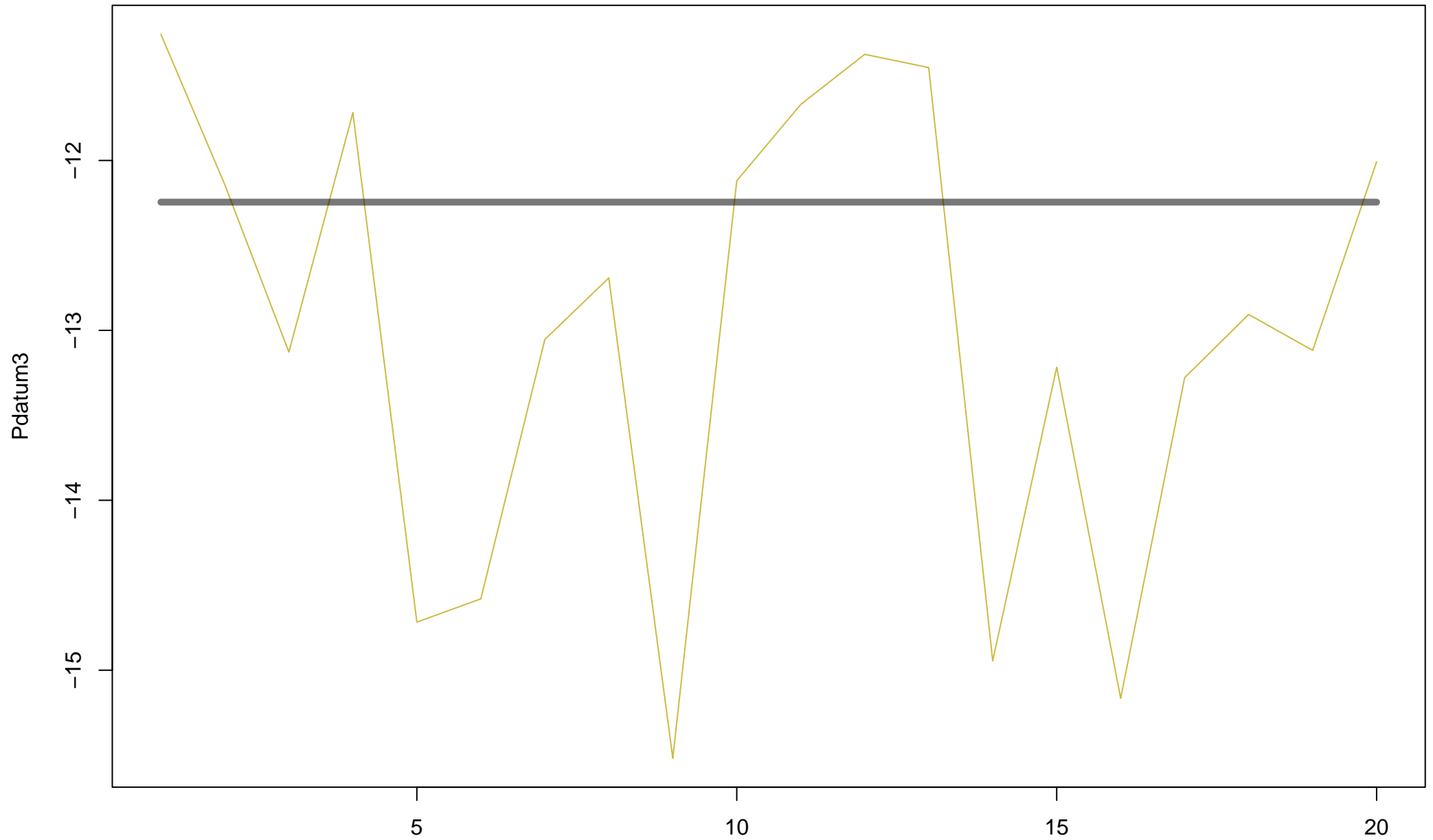
Pdatum1
ESS = 5.24 | BMK = 0.436 | MCSE(6.27) = 44.3 | stat: FALSE | burn: 20 | percentile: 70



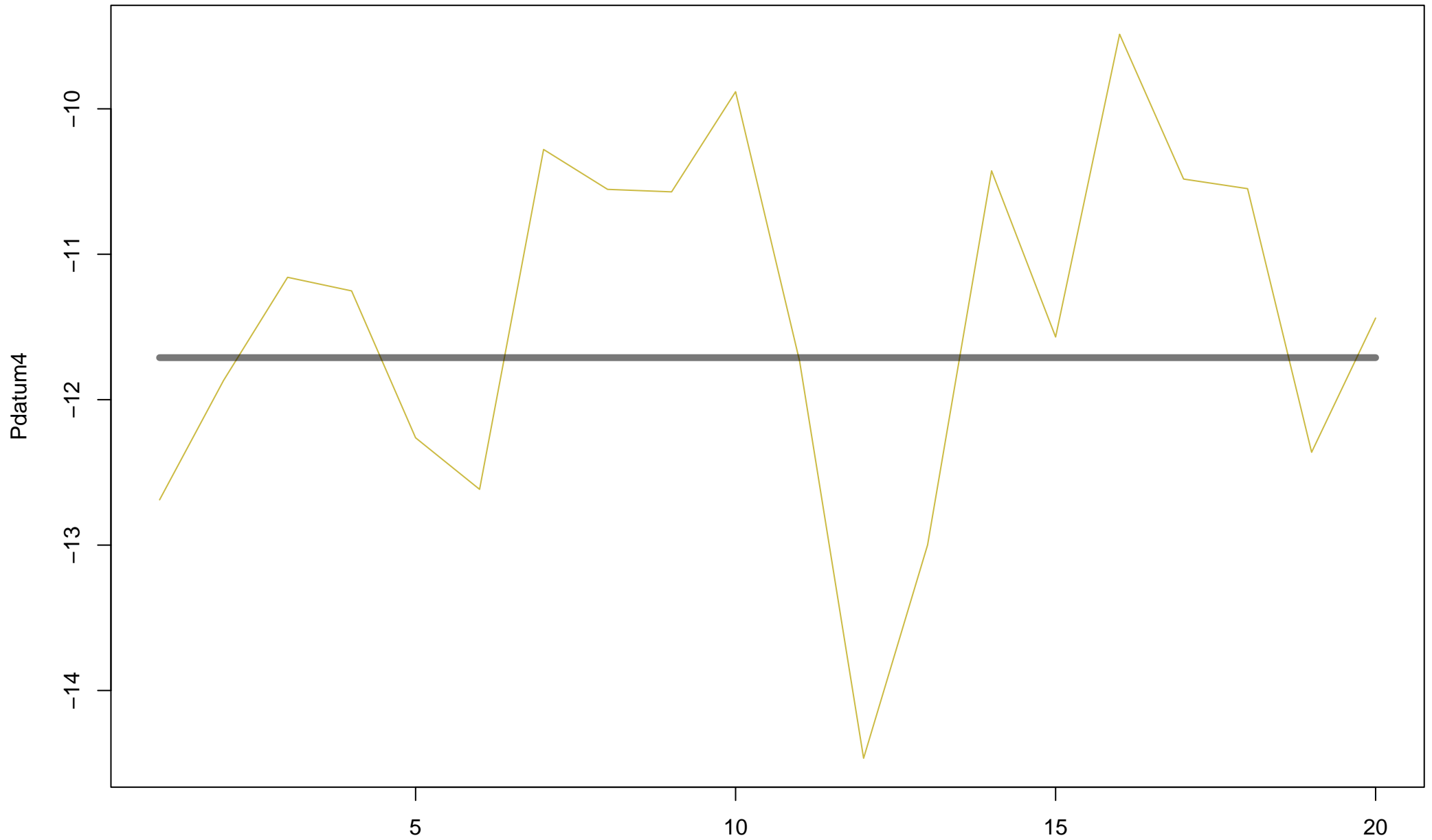
Pdatum2
ESS = 16.3 | BMK = 0.364 | MCSE(6.27) = 27.7 | stat: FALSE | burn: 16 | percentile: 20



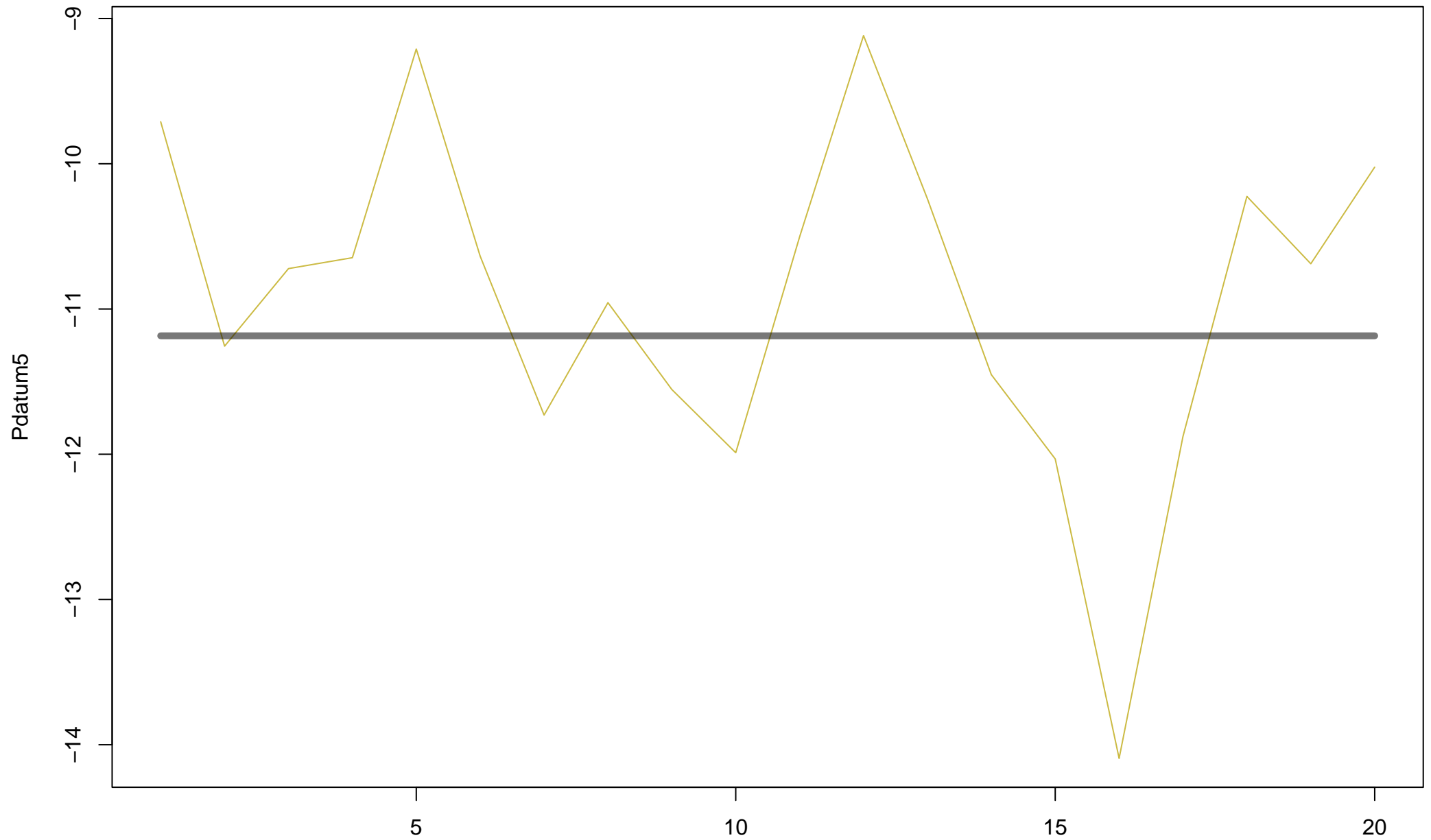
Pdatum3
ESS = 9.9 | BMK = 0.0997 | MCSE(6.27) = 32.9 | stat: FALSE | burn: 20 | percentile: 60



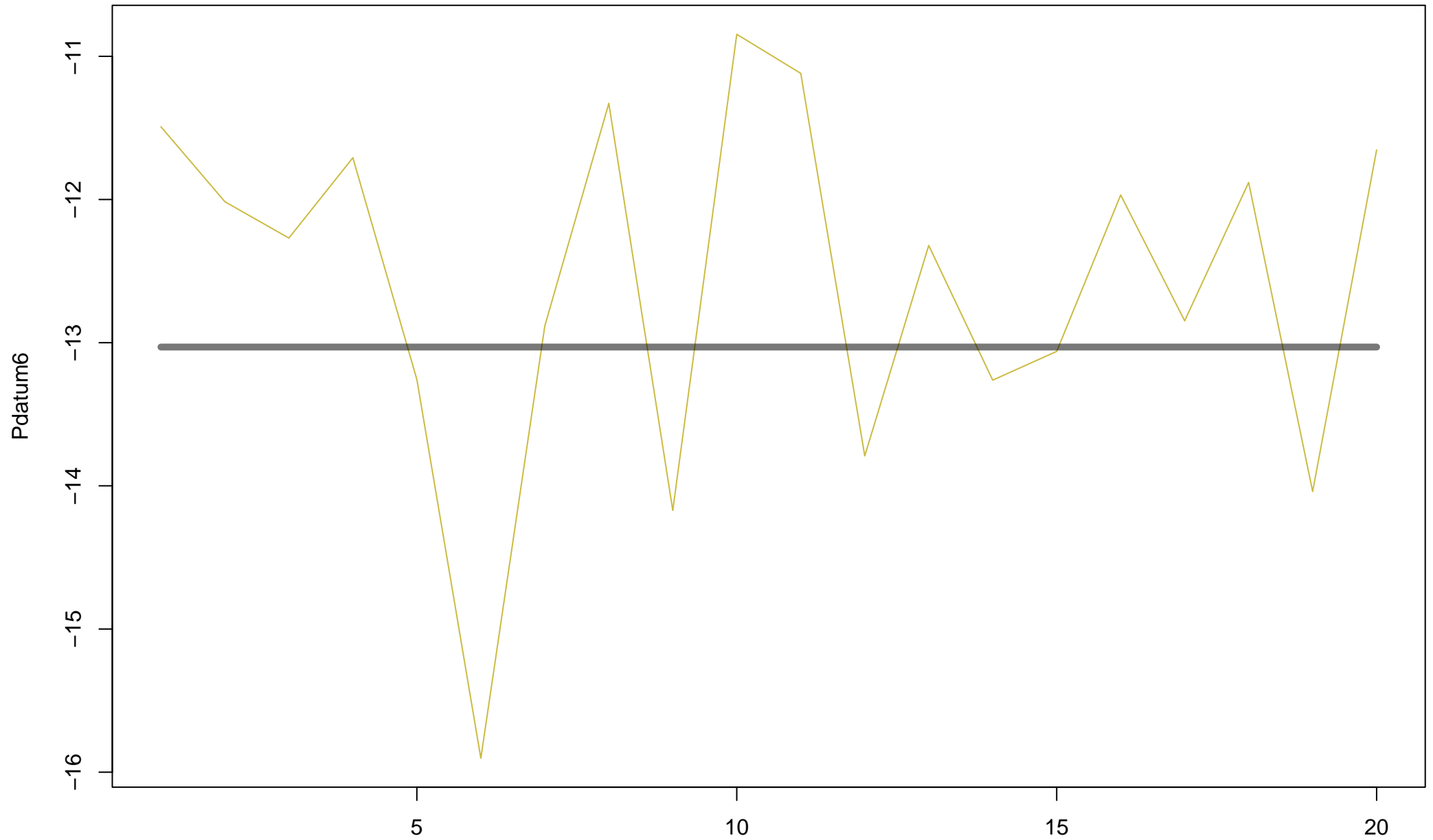
Pdatum4
ESS = 20 | BMK = 0.17 | MCSE(6.27) = 27 | stat: FALSE | burn: 20 | percentile: 40



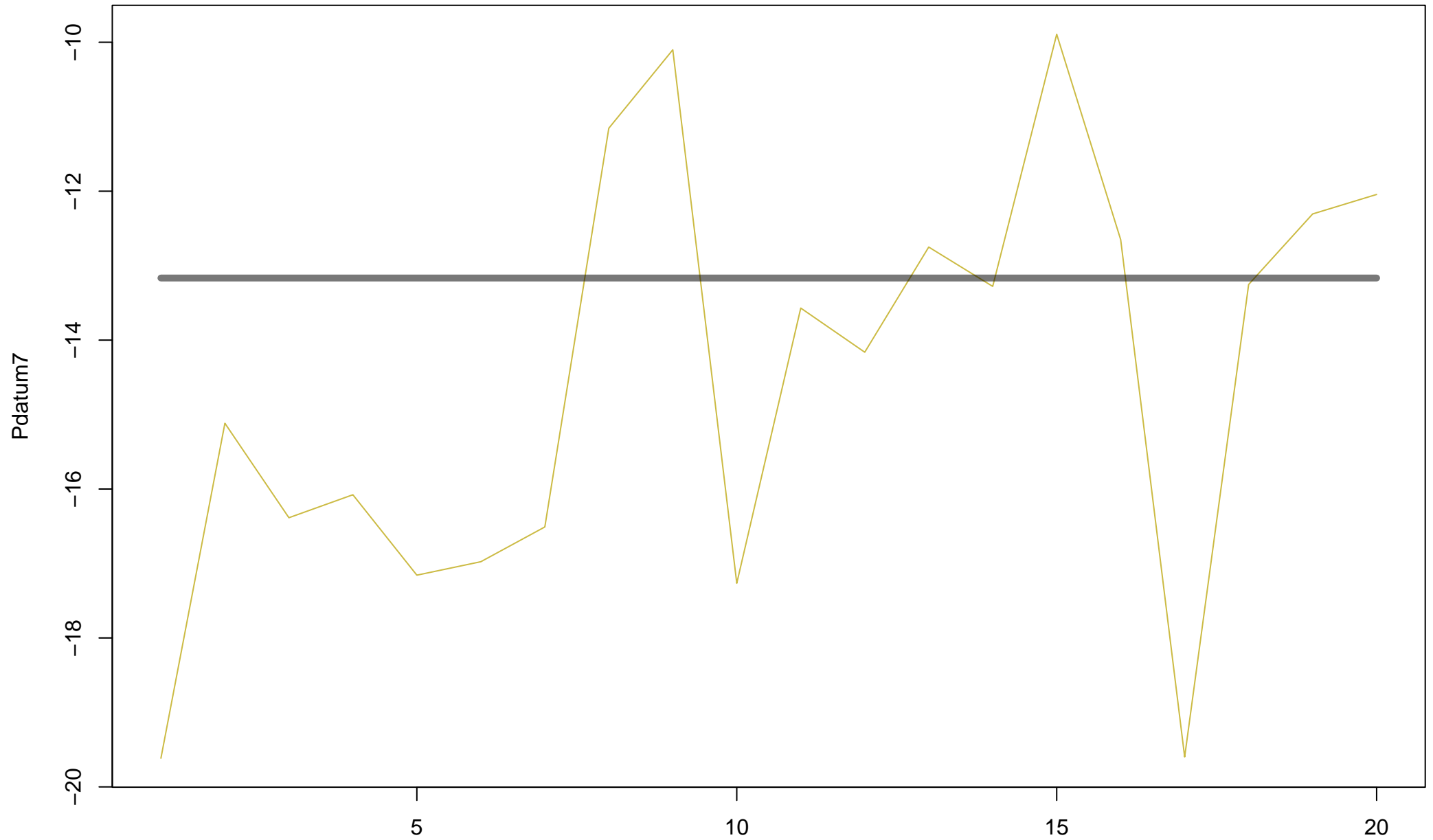
Pdatum5
ESS = 20 | BMK = 0.314 | MCSE(6.27) = 23.8 | stat: FALSE | burn: 20 | percentile: 40



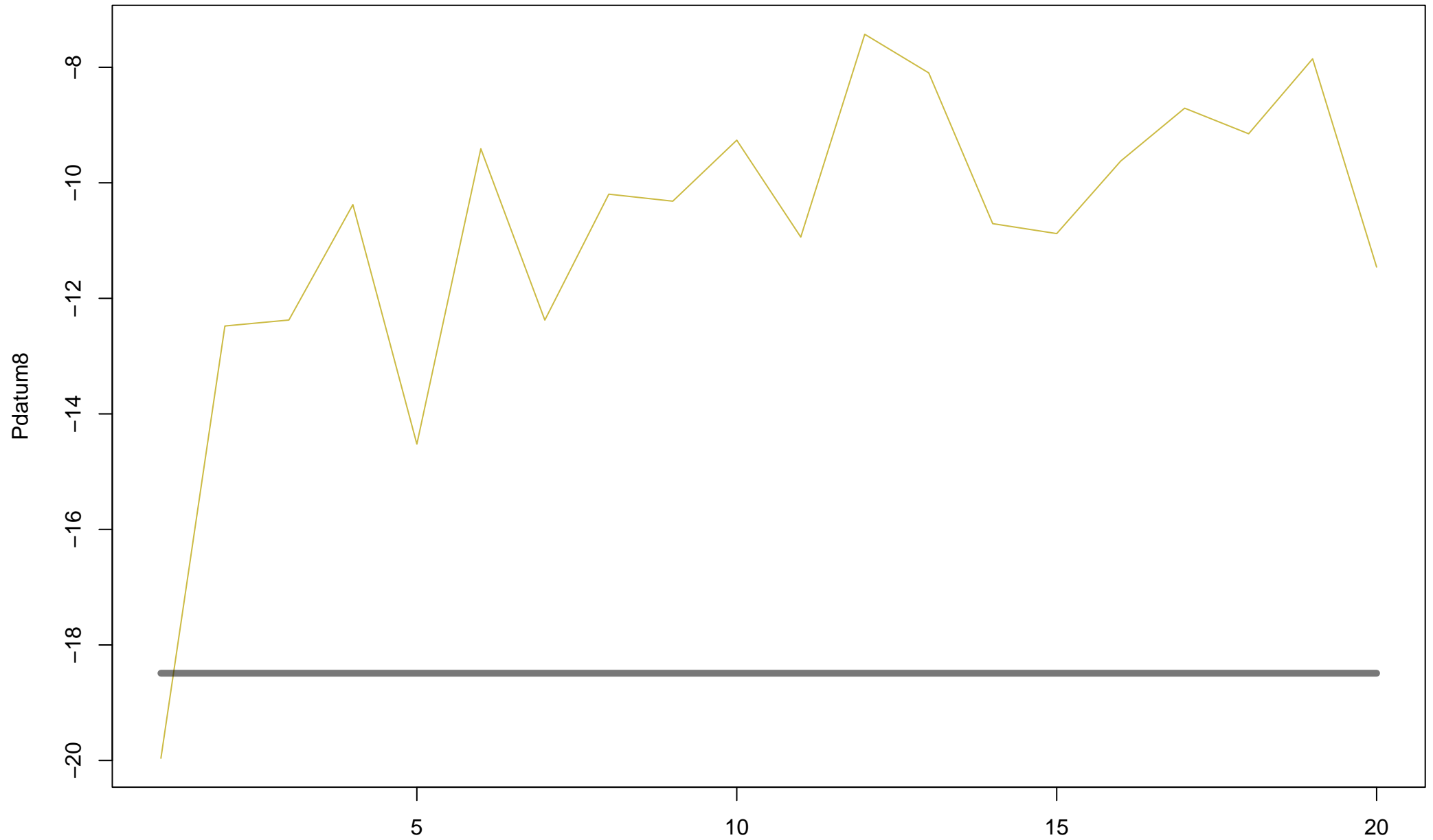
Pdatum6
ESS = 20 | BMK = 0.148 | MCSE(6.27) = 21.3 | stat: FALSE | burn: 12 | percentile: 35



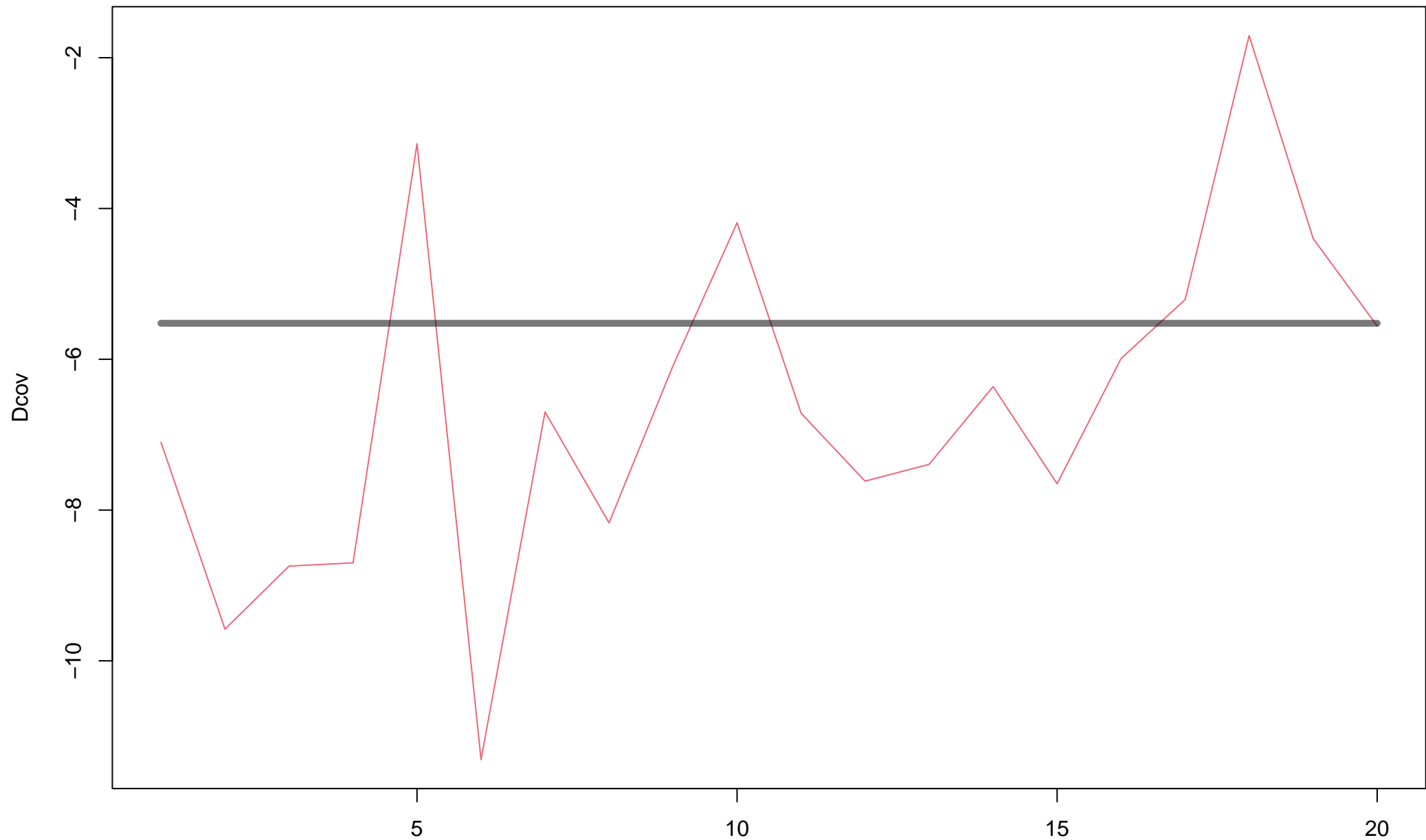
Pdatum7
ESS = 20 | BMK = 1 | MCSE(6.27) = 22.1 | stat: FALSE | burn: 20 | percentile: 65



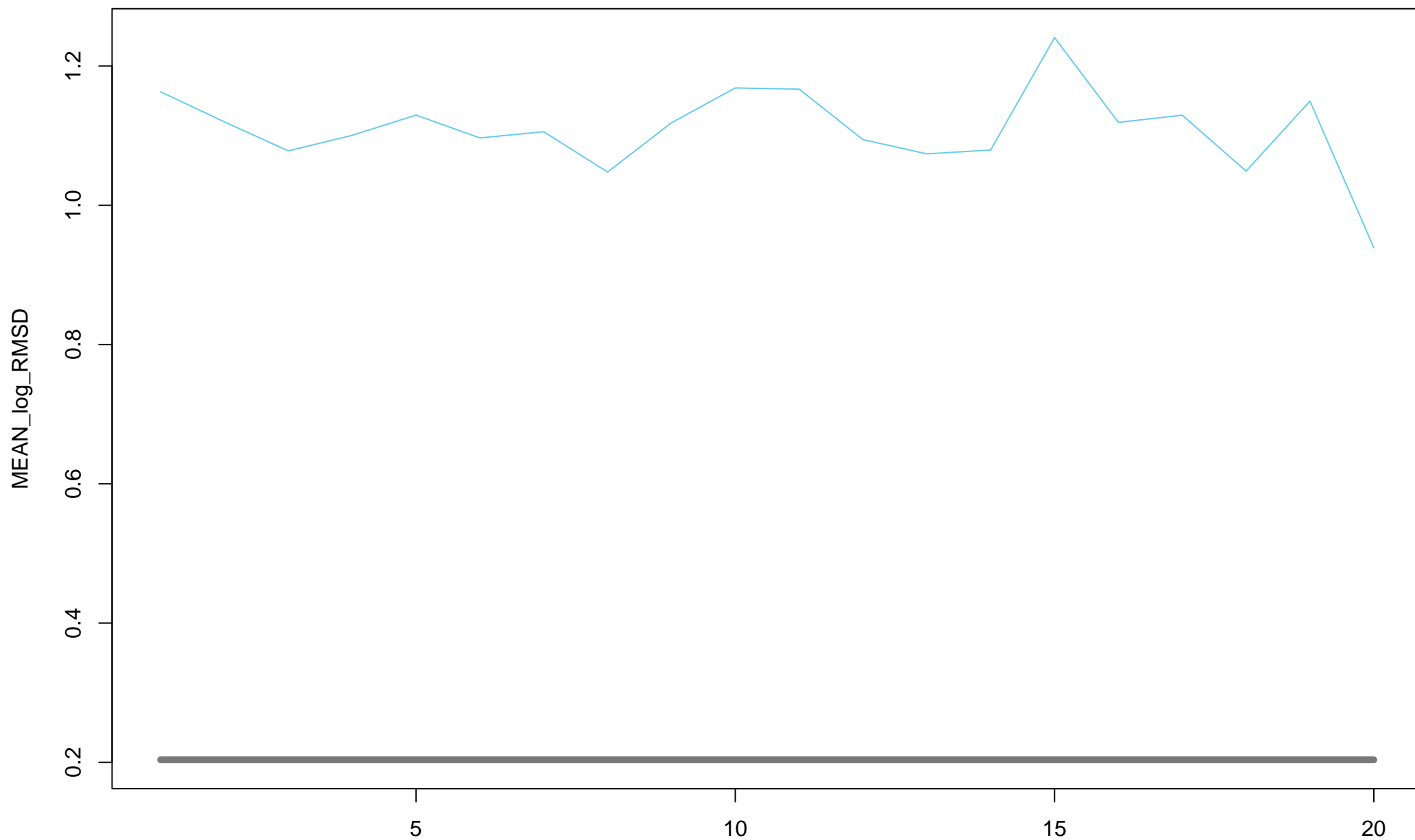
Pdatum8
ESS = 20 | BMK = 0.644 | MCSE(6.27) = 27.6 | stat: FALSE | burn: 20 | percentile: 5



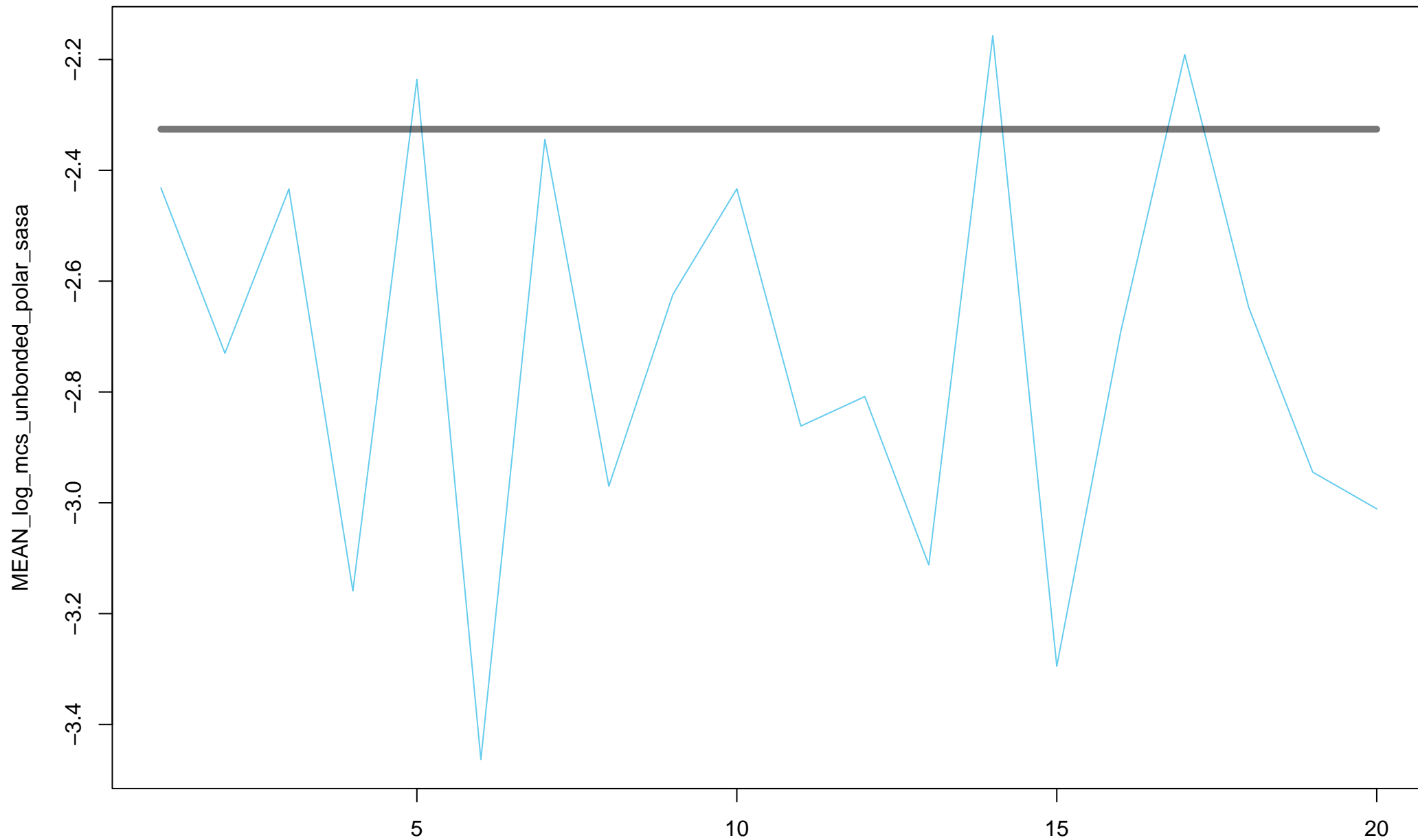
Dcov
ESS = 20 | BMK = 0.806 | MCSE(6.27) = 18.2 | stat: FALSE | burn: 20 | percentile: 90



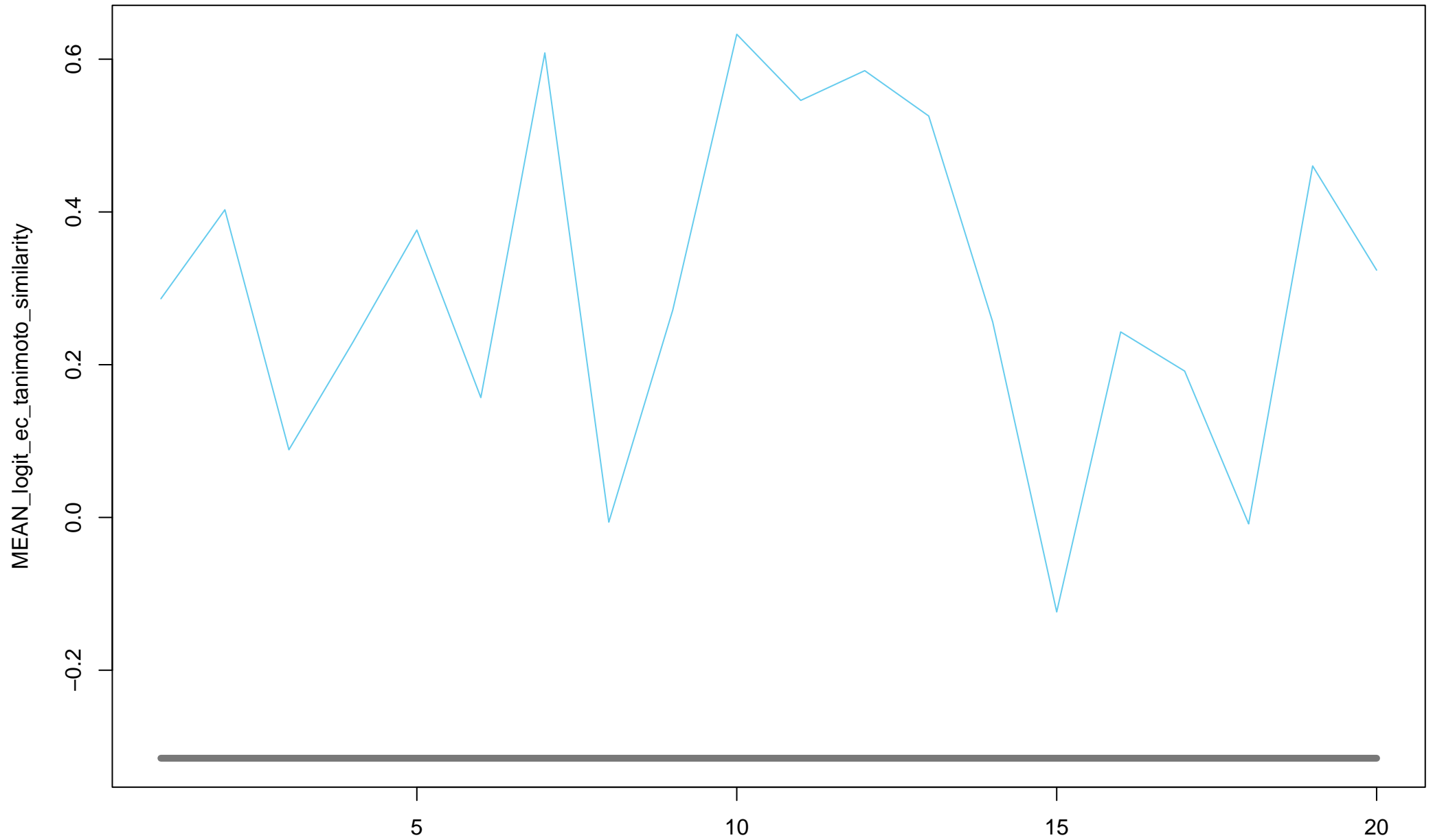
MEAN_log_RMSD
ESS = 20 | BMK = 0.341 | MCSE(6.27) = 19 | stat: FALSE | burn: 20 | percentile: 0



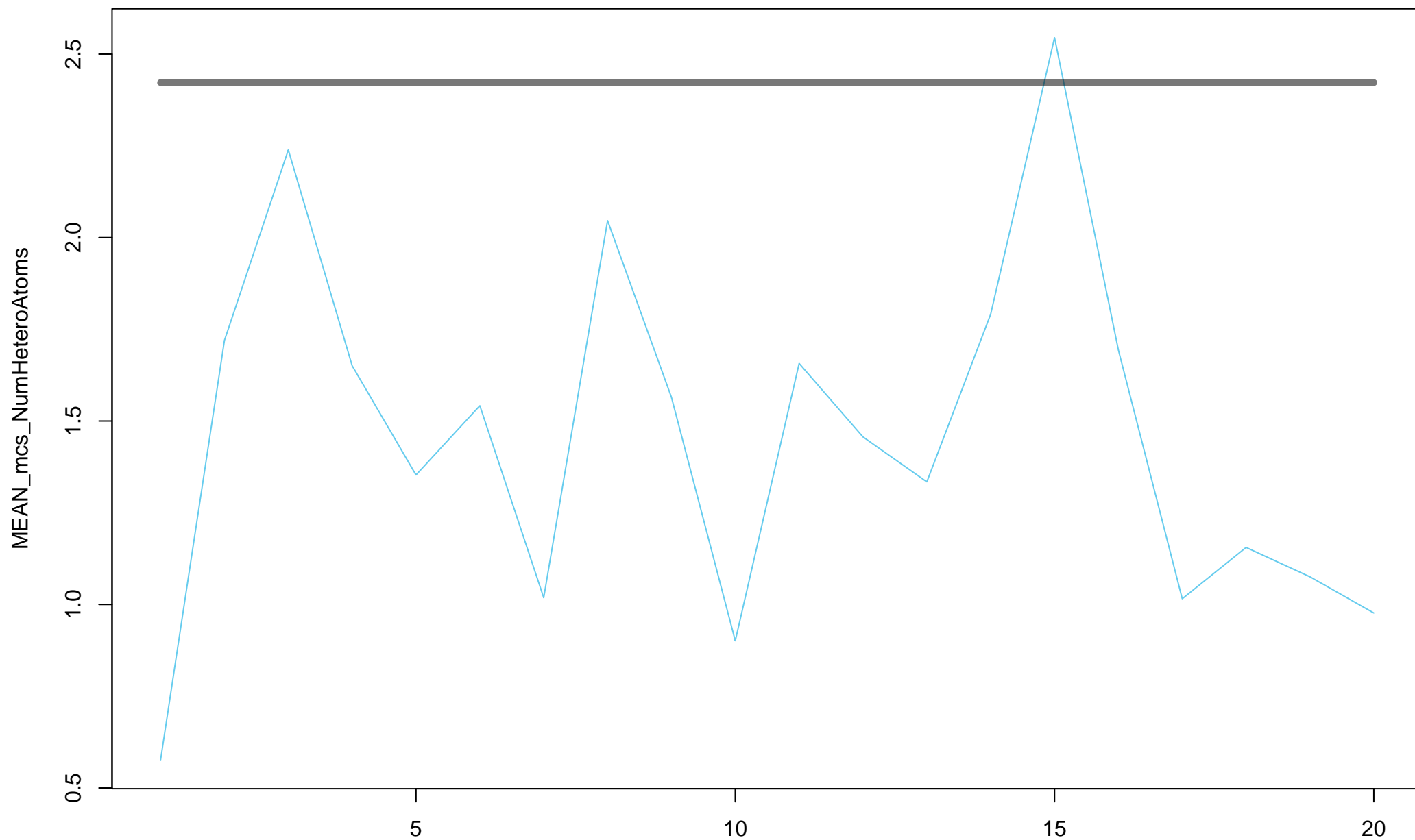
MEAN_log_mcs_unbonded_polar_sasa
ESS = 20 | BMK = 0.235 | MCSE(6.27) = NaN | stat: FALSE | burn: 20 | percentile: 85



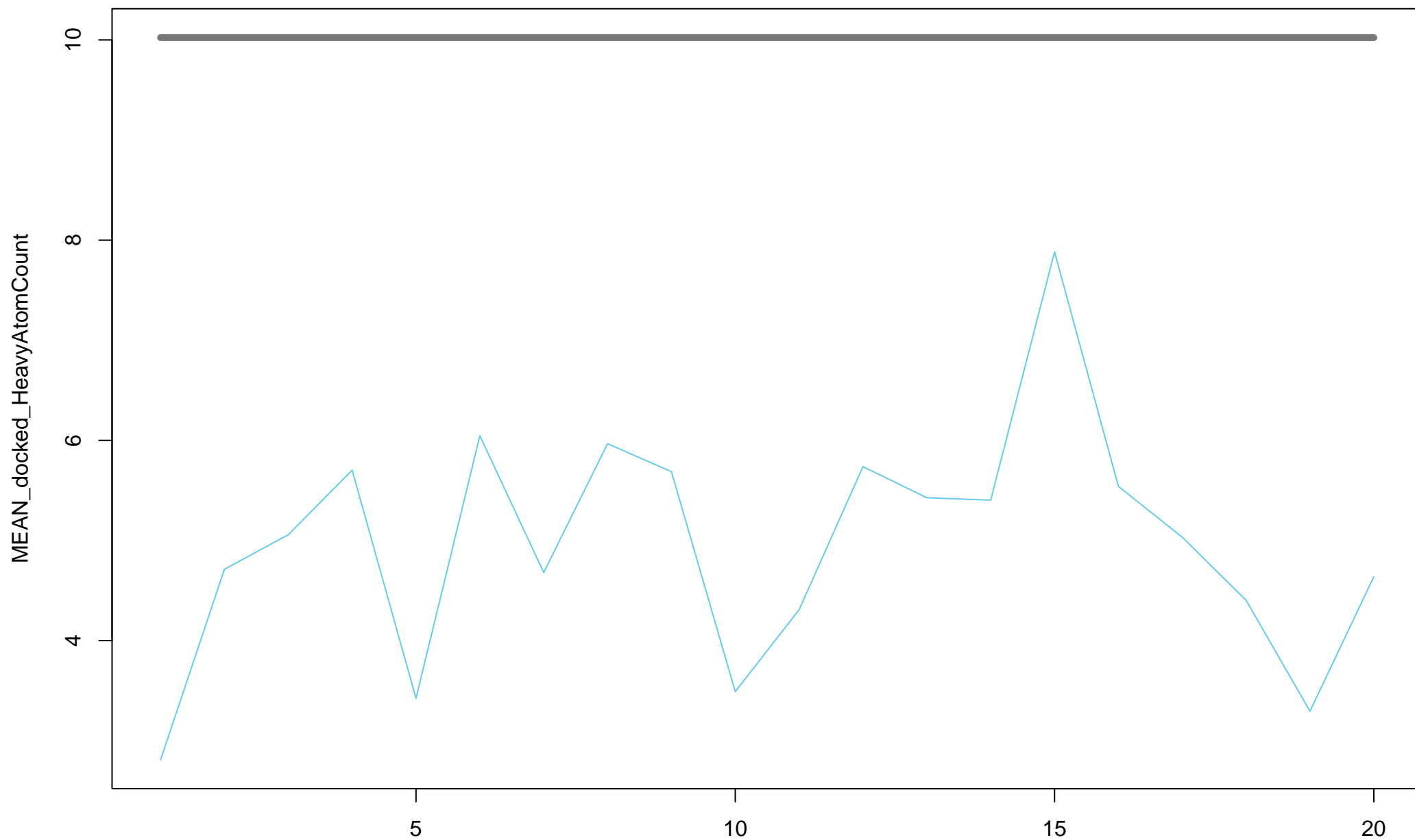
MEAN_logit_ec_tanimoto_similarity
ESS = 20 | BMK = 0.109 | MCSE(6.27) = 27.7 | stat: FALSE | burn: 20 | percentile: 0



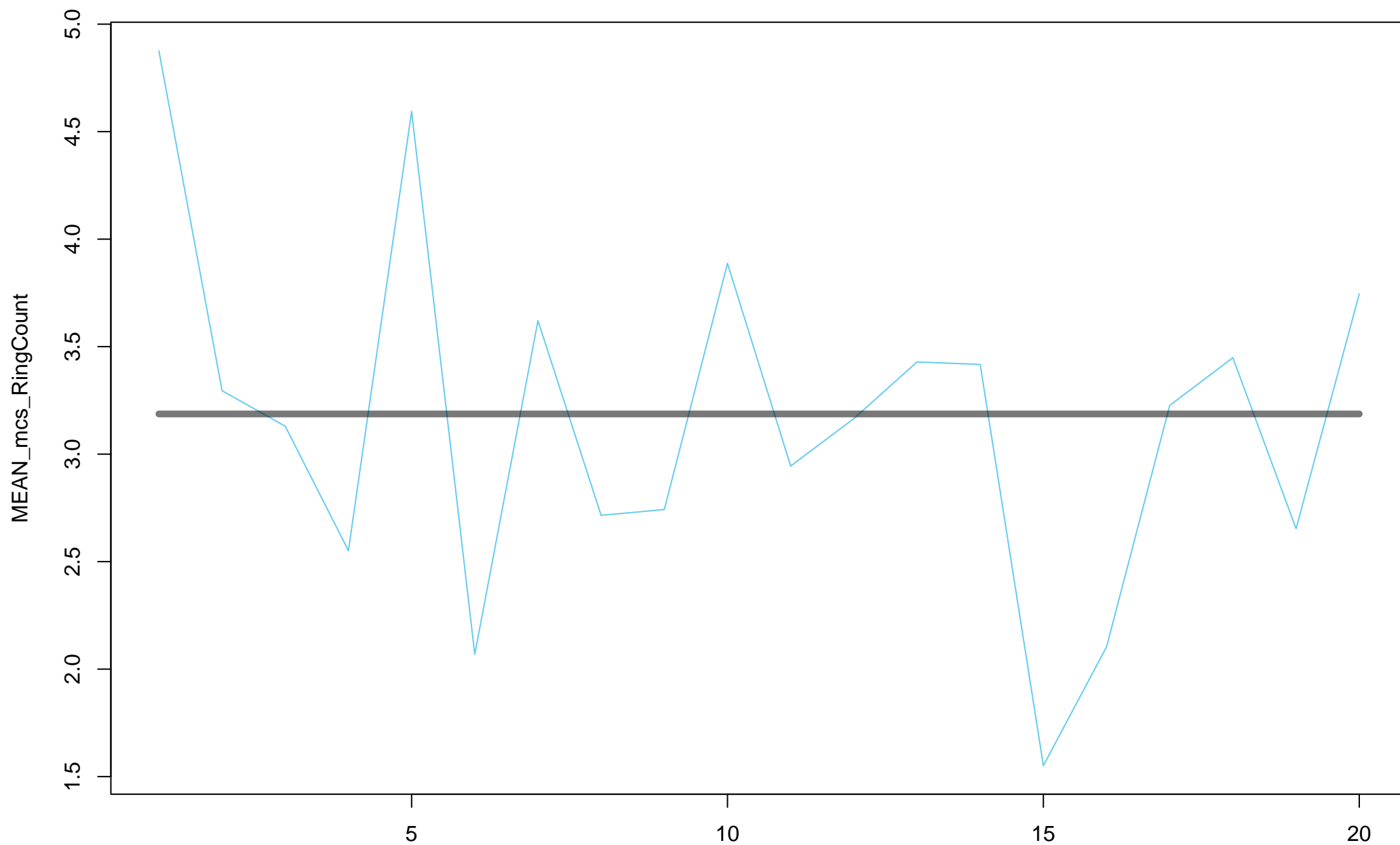
MEAN_mcs_NumHeteroAtoms
ESS = 20 | BMK = 0.139 | MCSE(6.27) = 24.5 | stat: FALSE | burn: 20 | percentile: 95



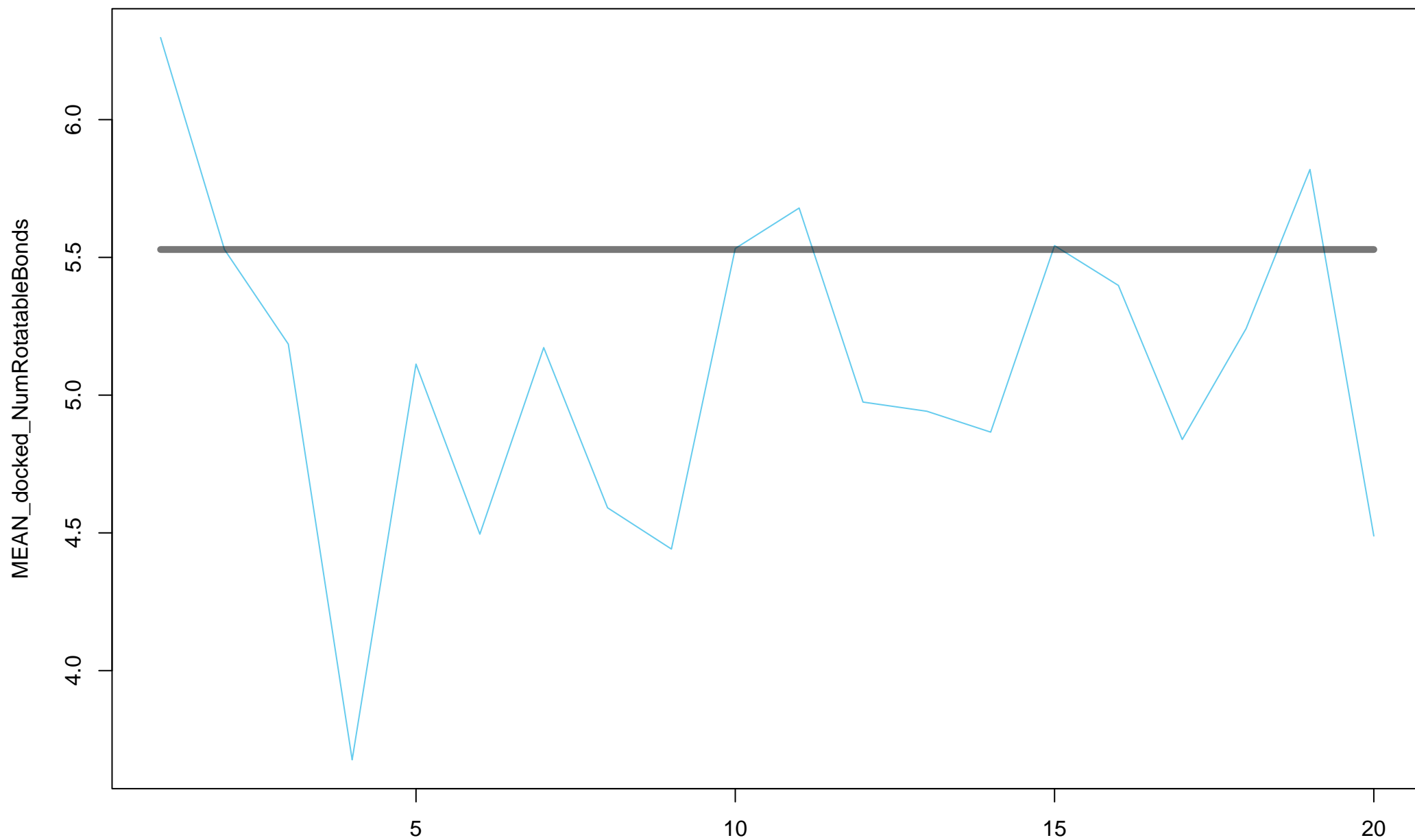
MEAN_docked_HeavyAtomCount
ESS = 20 | BMK = 0.22 | MCSE(6.27) = 25.4 | stat: FALSE | burn: 20 | percentile: 100



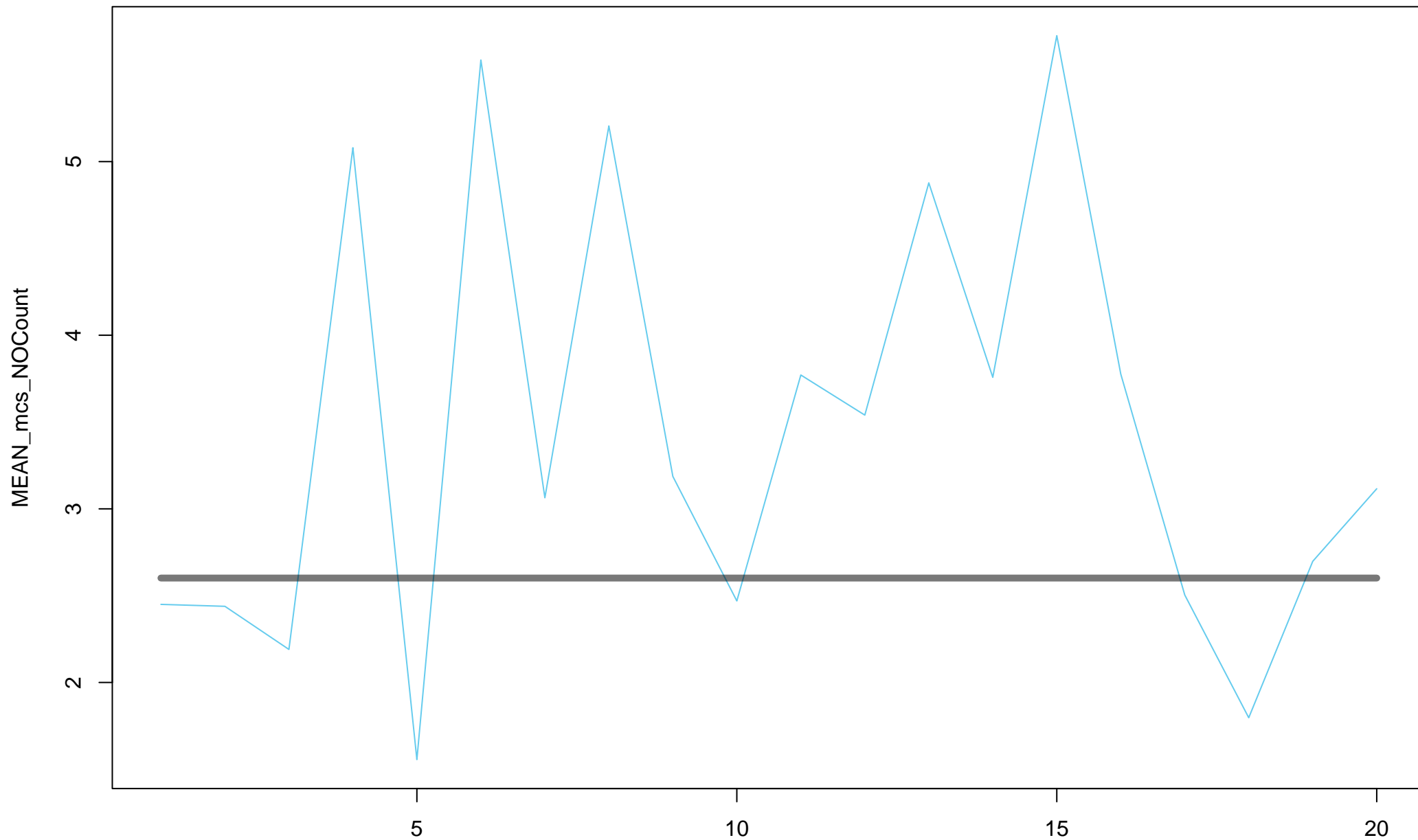
MEAN_mcs_RingCount
ESS = 20 | BMK = 0.291 | MCSE(6.27) = 17.2 | stat: FALSE | burn: 20 | percentile: 50



MEAN_docked_NumRotatableBonds
ESS = 20 | BMK = 0.235 | MCSE(6.27) = 22.4 | stat: FALSE | burn: 20 | percentile: 70

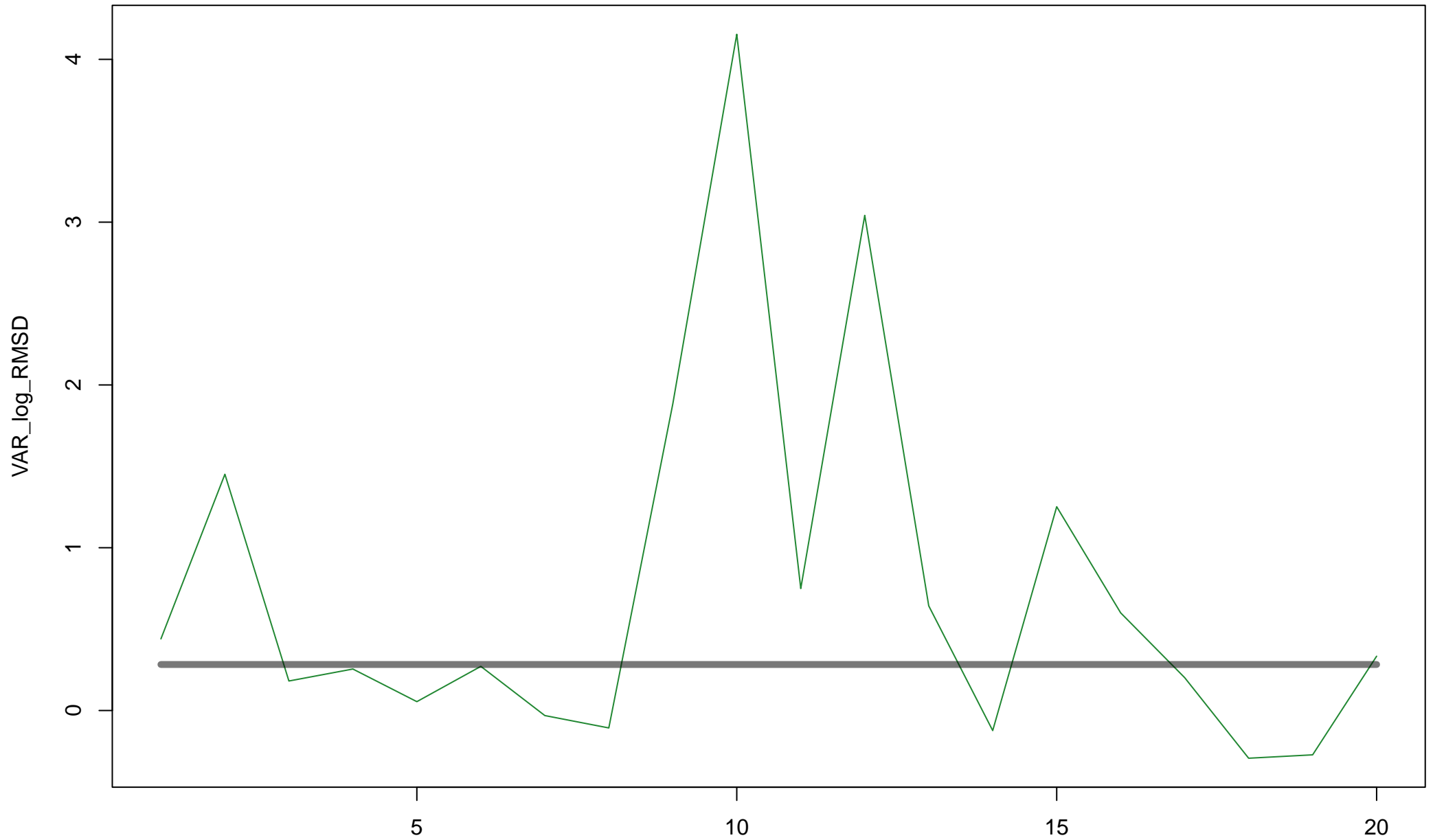


MEAN_mcs_NOCount
ESS = 20 | BMK = 0.174 | MCSE(6.27) = 23.5 | stat: FALSE | burn: 20 | percentile: 35

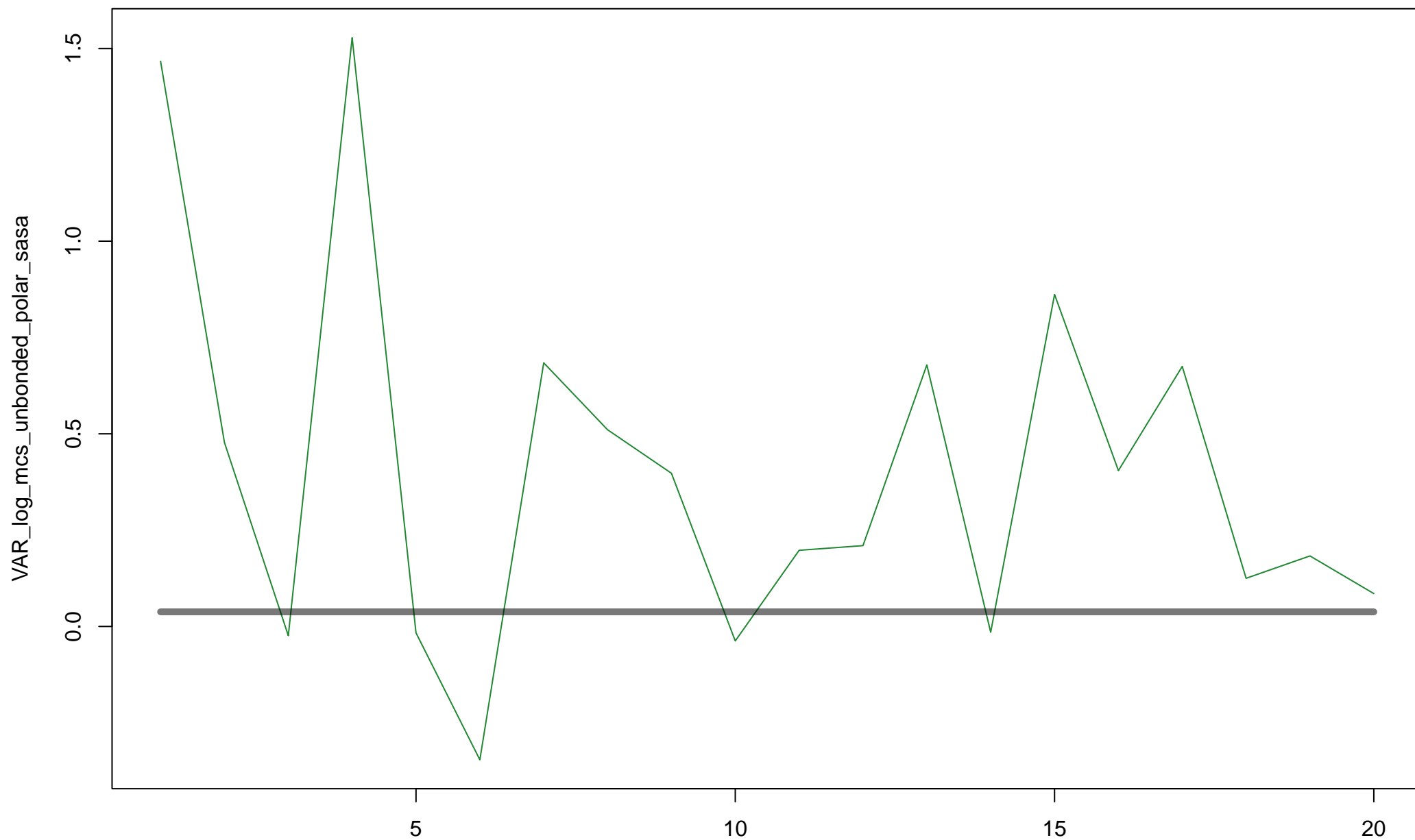


VAR_log_RMSD

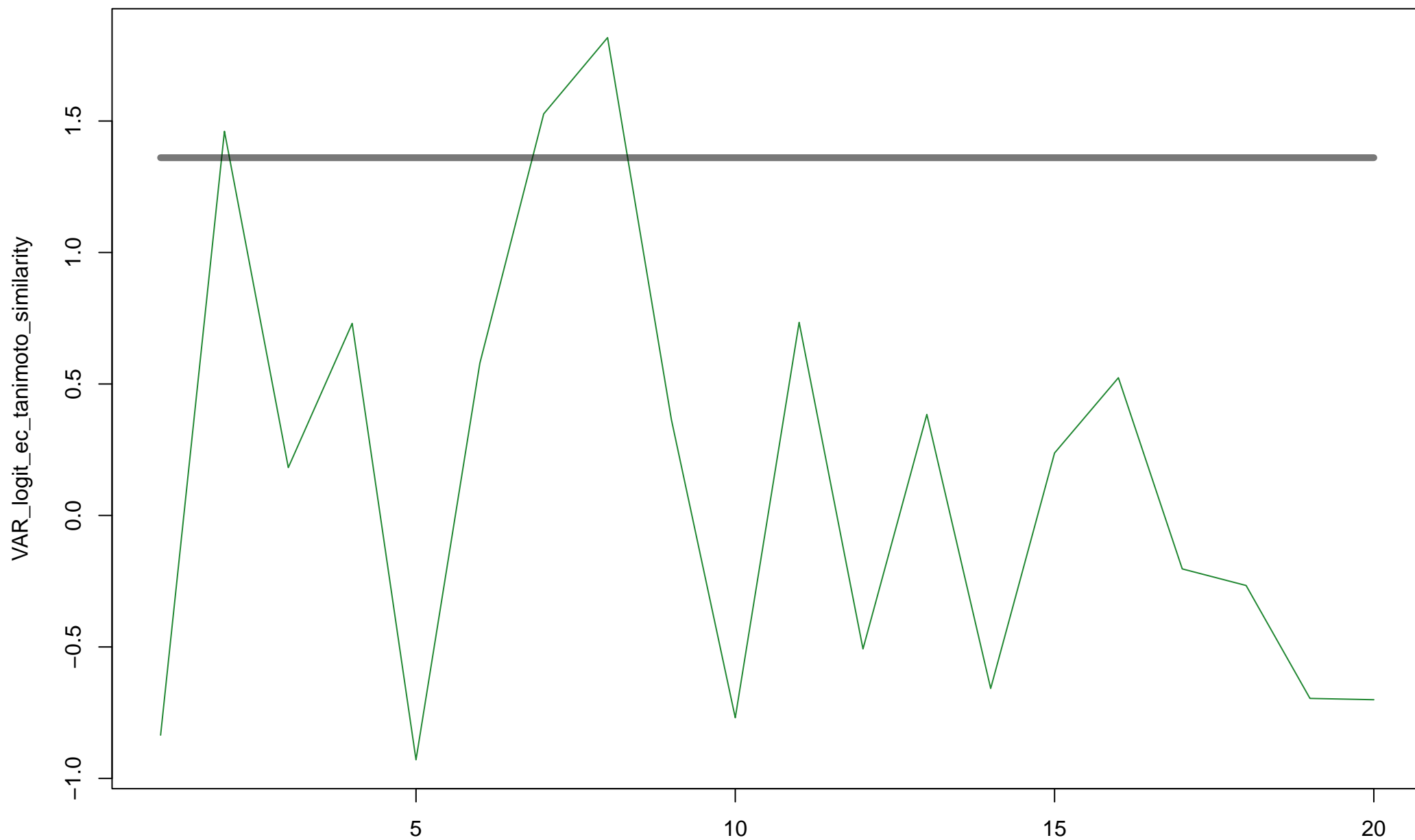
ESS = 20 | BMK = 0.557 | MCSE(6.27) = 27.2 | stat: FALSE | burn: 16 | percentile: 50



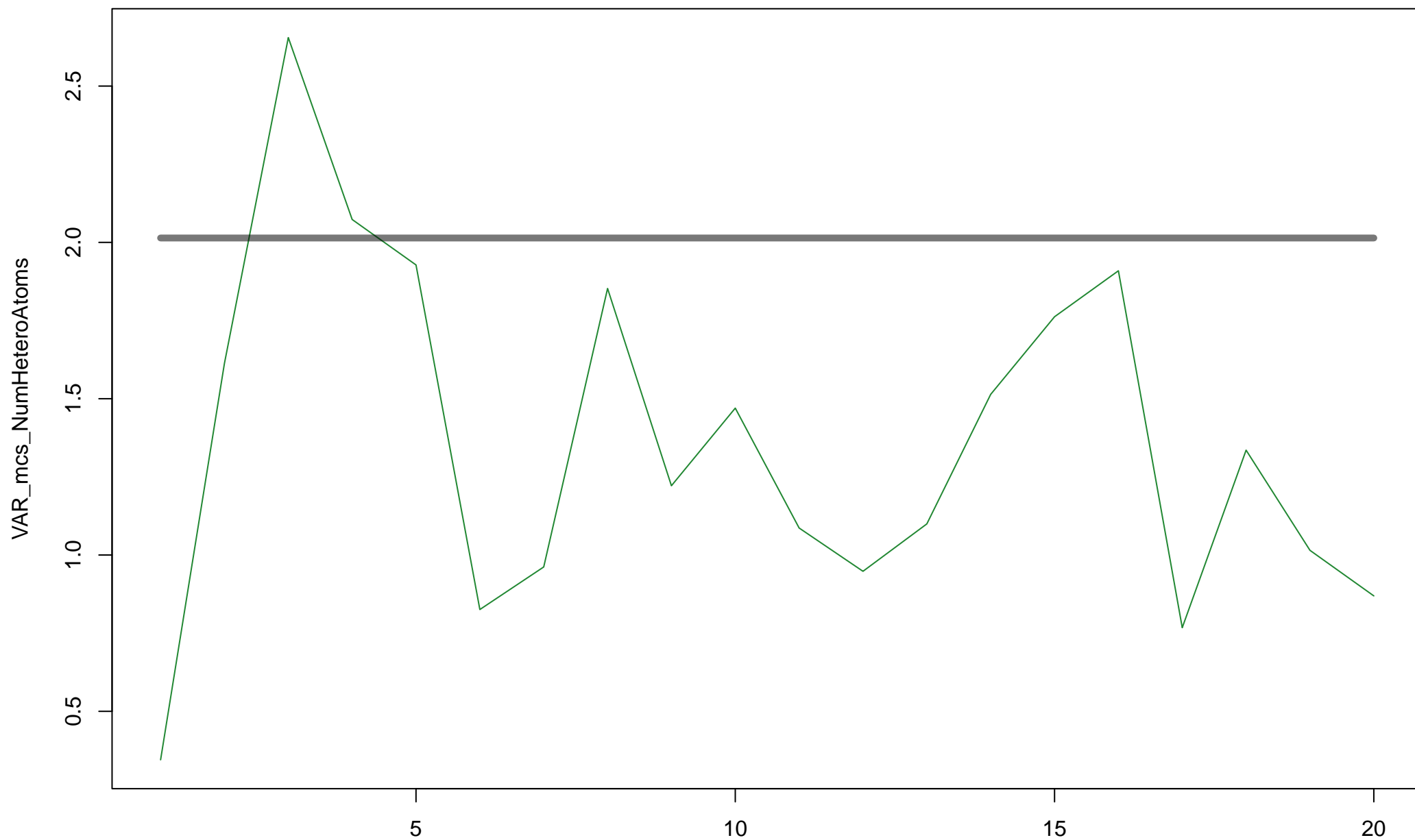
VAR_log_mcs_unbonded_polar_sasa
ESS = 20 | BMK = 0.325 | MCSE(6.27) = 17.4 | stat: FALSE | burn: 20 | percentile: 25



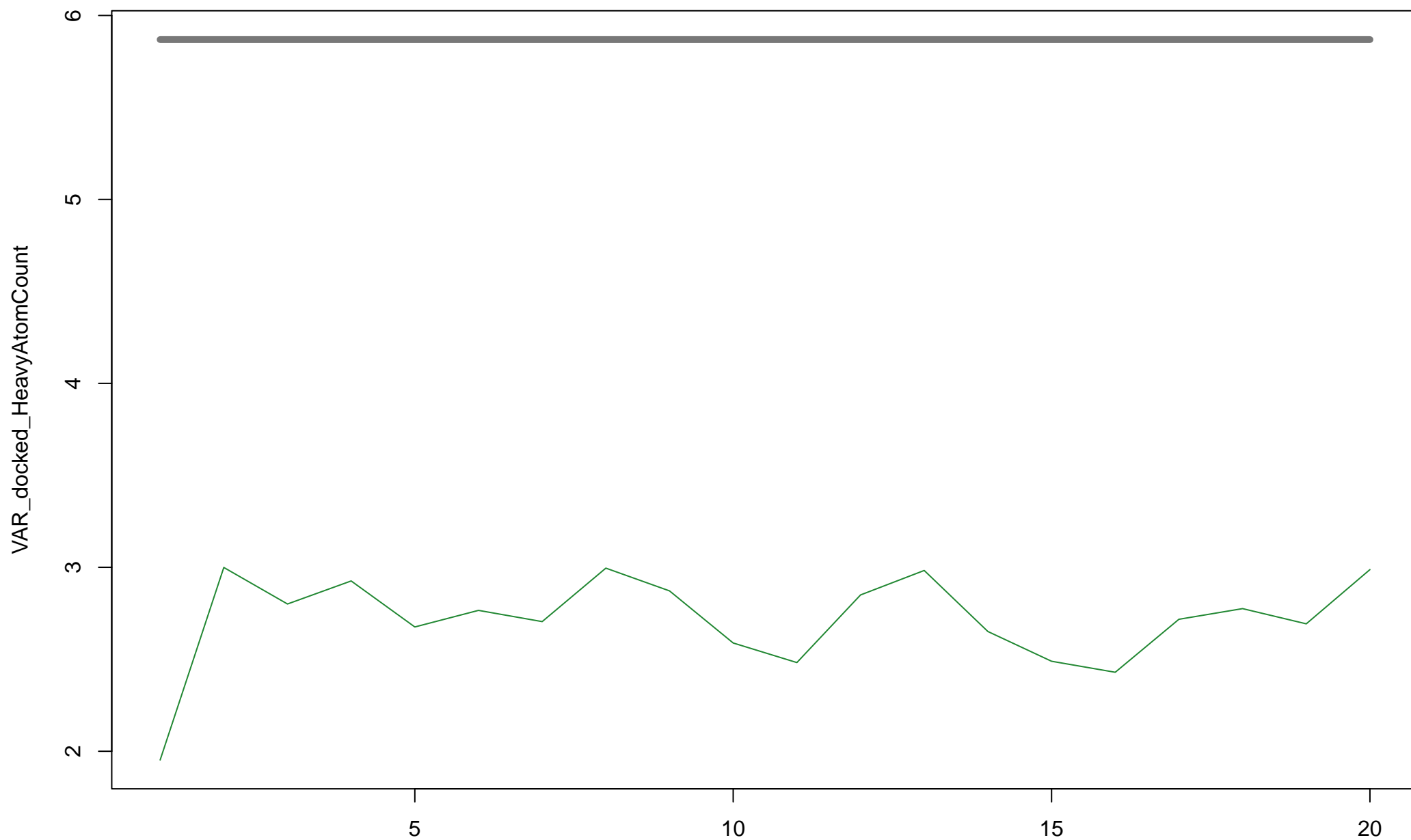
VAR_logit_ec_tanimoto_similarity
ESS = 20 | BMK = 0.462 | MCSE(6.27) = 29.2 | stat: FALSE | burn: 20 | percentile: 85



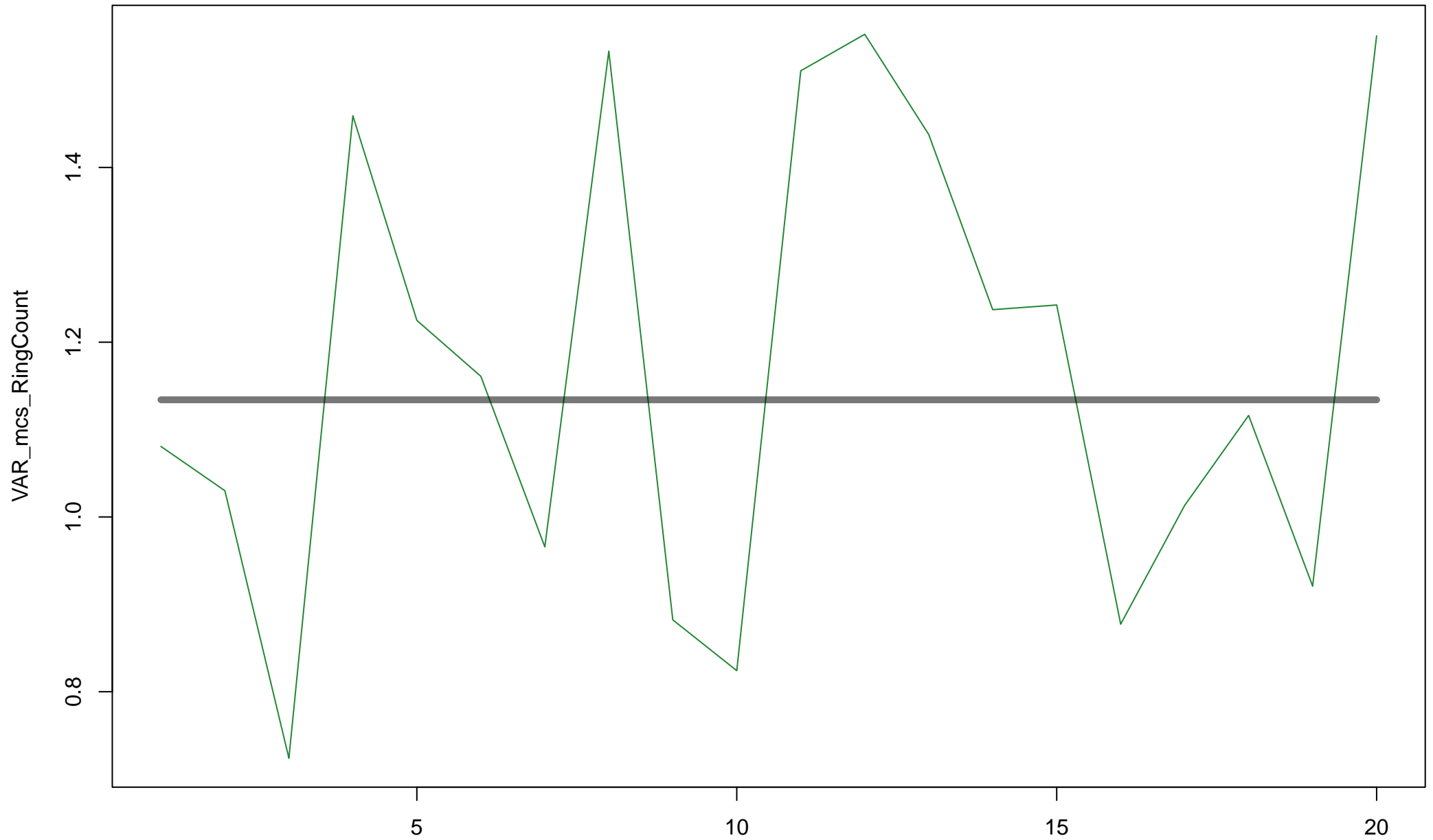
VAR_mcs_NumHeteroAtoms
ESS = 20 | BMK = 0.331 | MCSE(6.27) = 30.7 | stat: FALSE | burn: 20 | percentile: 90



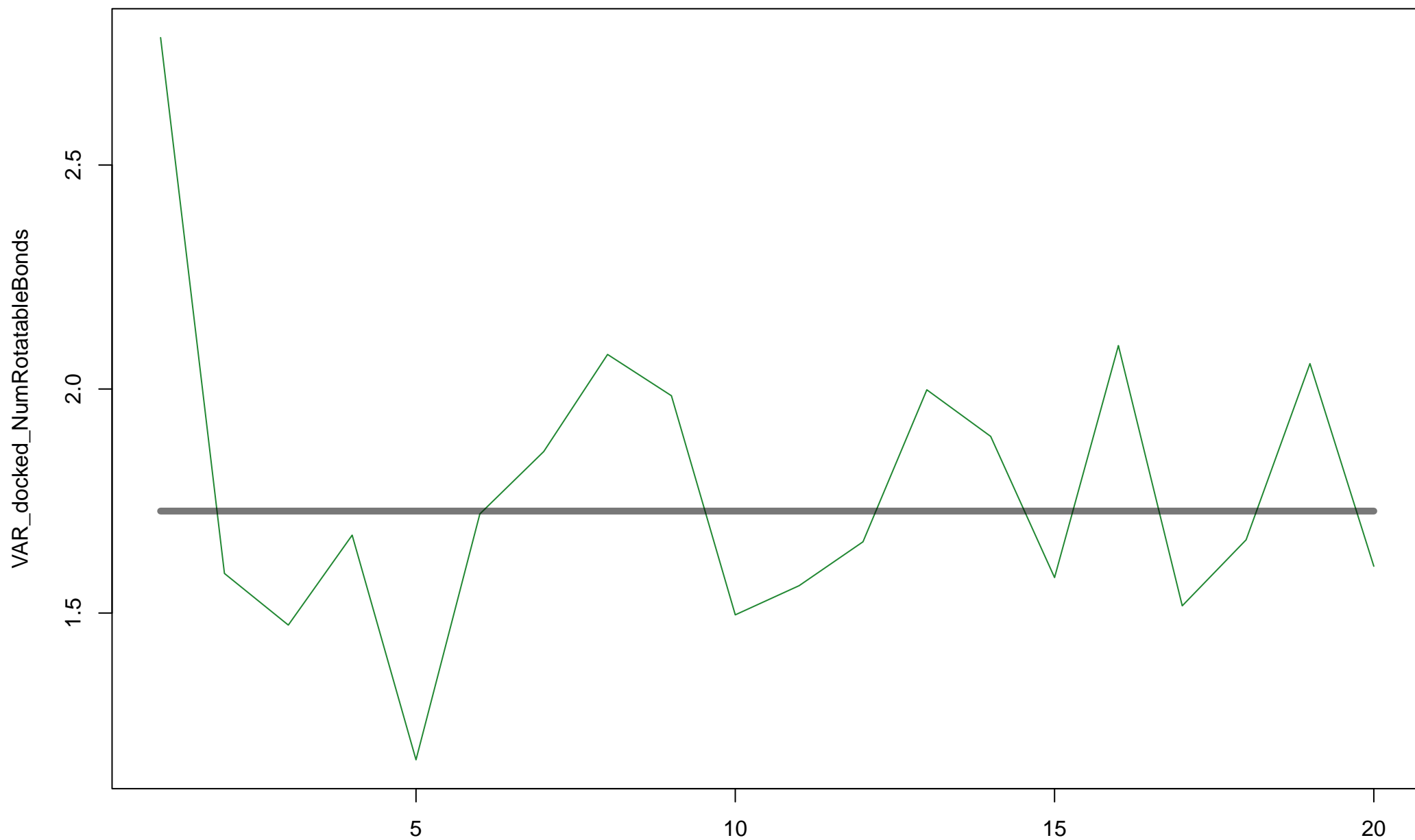
VAR_docked_HeavyAtomCount
ESS = 20 | BMK = 0.21 | MCSE(6.27) = 20.5 | stat: FALSE | burn: 20 | percentile: 100



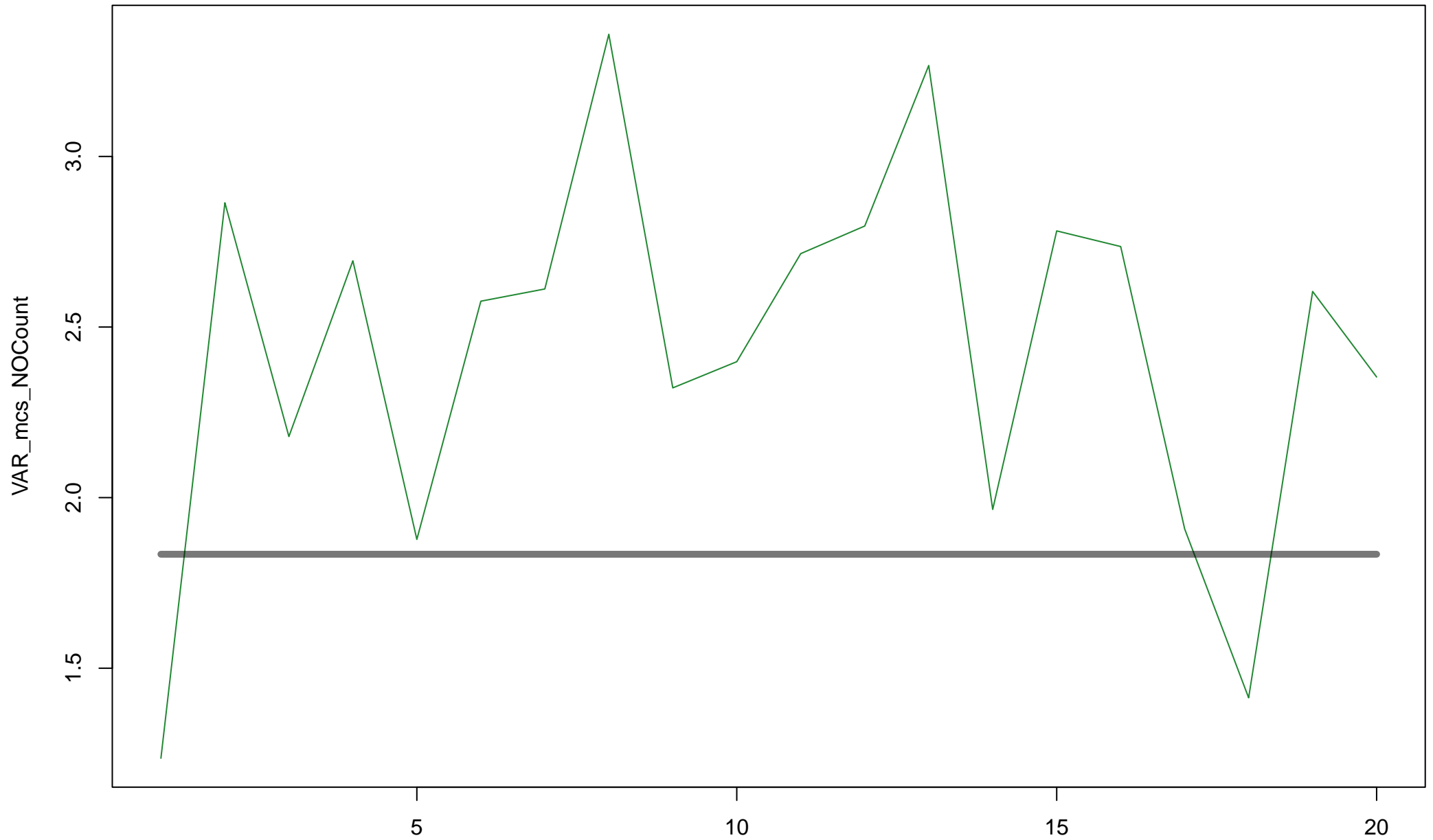
VAR_mcs_RingCount
ESS = 20 | BMK = 0.157 | MCSE(6.27) = 21.9 | stat: FALSE | burn: 20 | percentile: 50



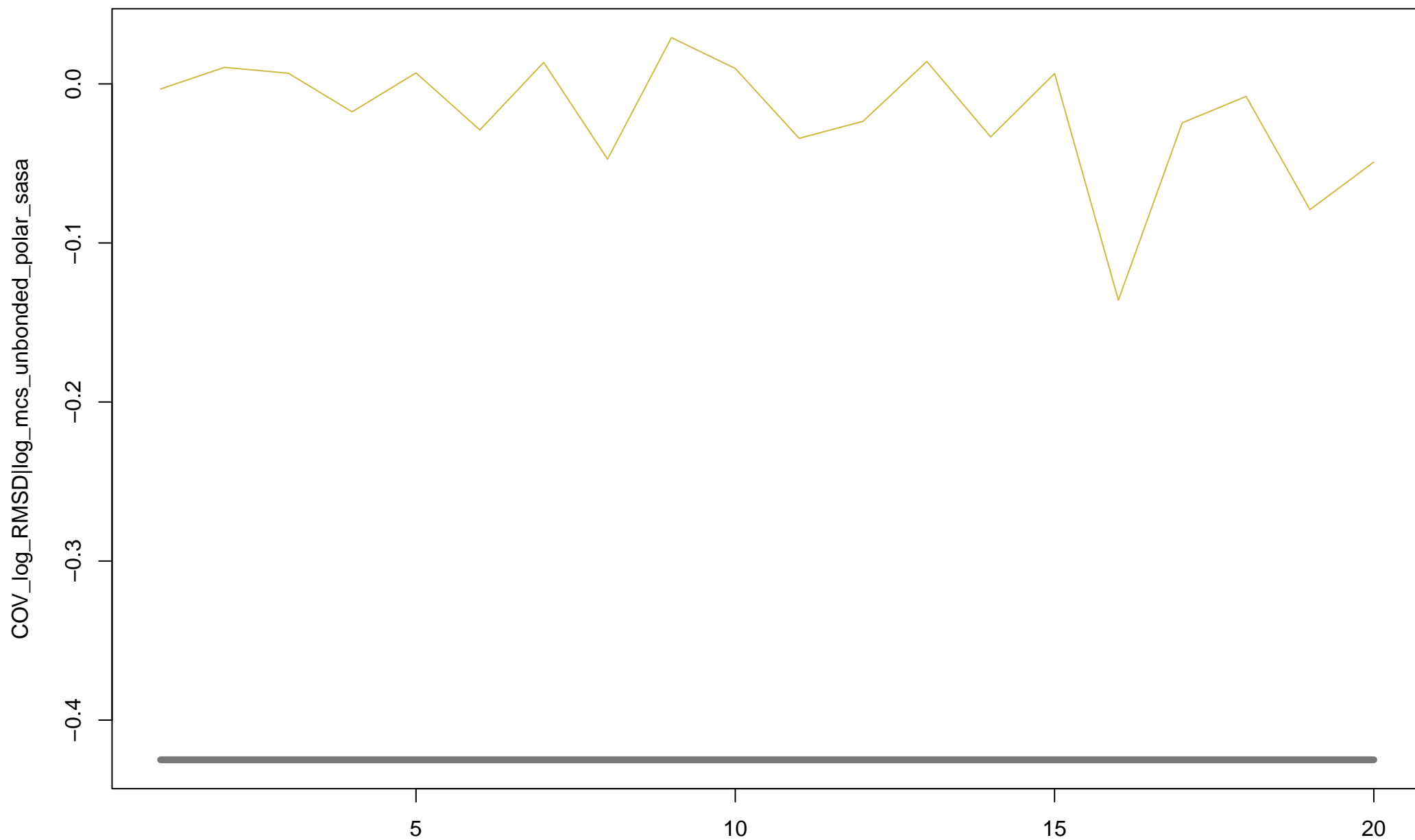
VAR_docked_NumRotatableBonds
ESS = 20 | BMK = 0.248 | MCSE(6.27) = 20.4 | stat: FALSE | burn: 20 | percentile: 60



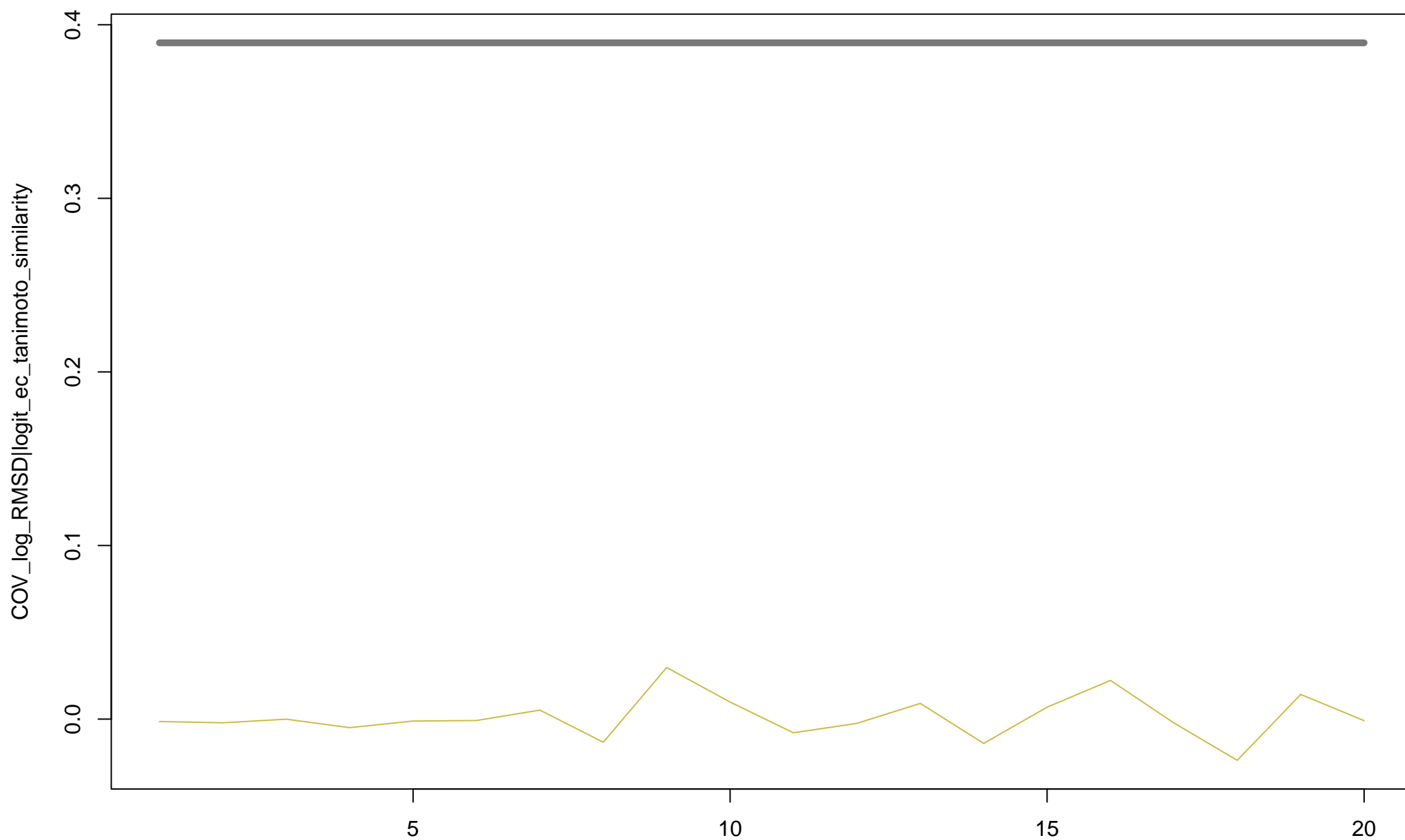
VAR_mcs_NOCCount
ESS = 20 | BMK = 0.142 | MCSE(6.27) = 18.3 | stat: FALSE | burn: 20 | percentile: 10



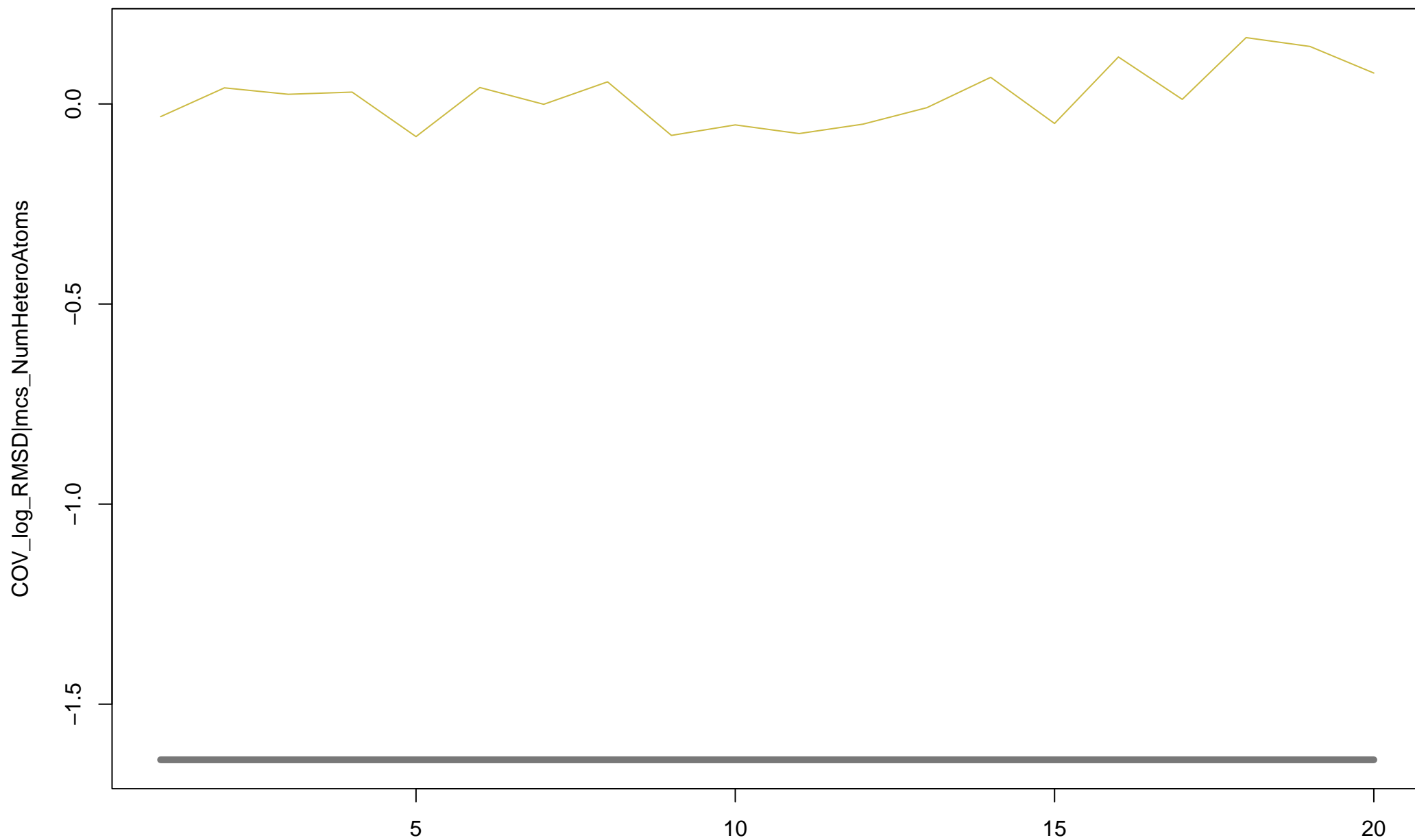
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 20 | BMK = 0.372 | MCSE(6.27) = 19.5 | stat: FALSE | burn: 20 | percentile: 0



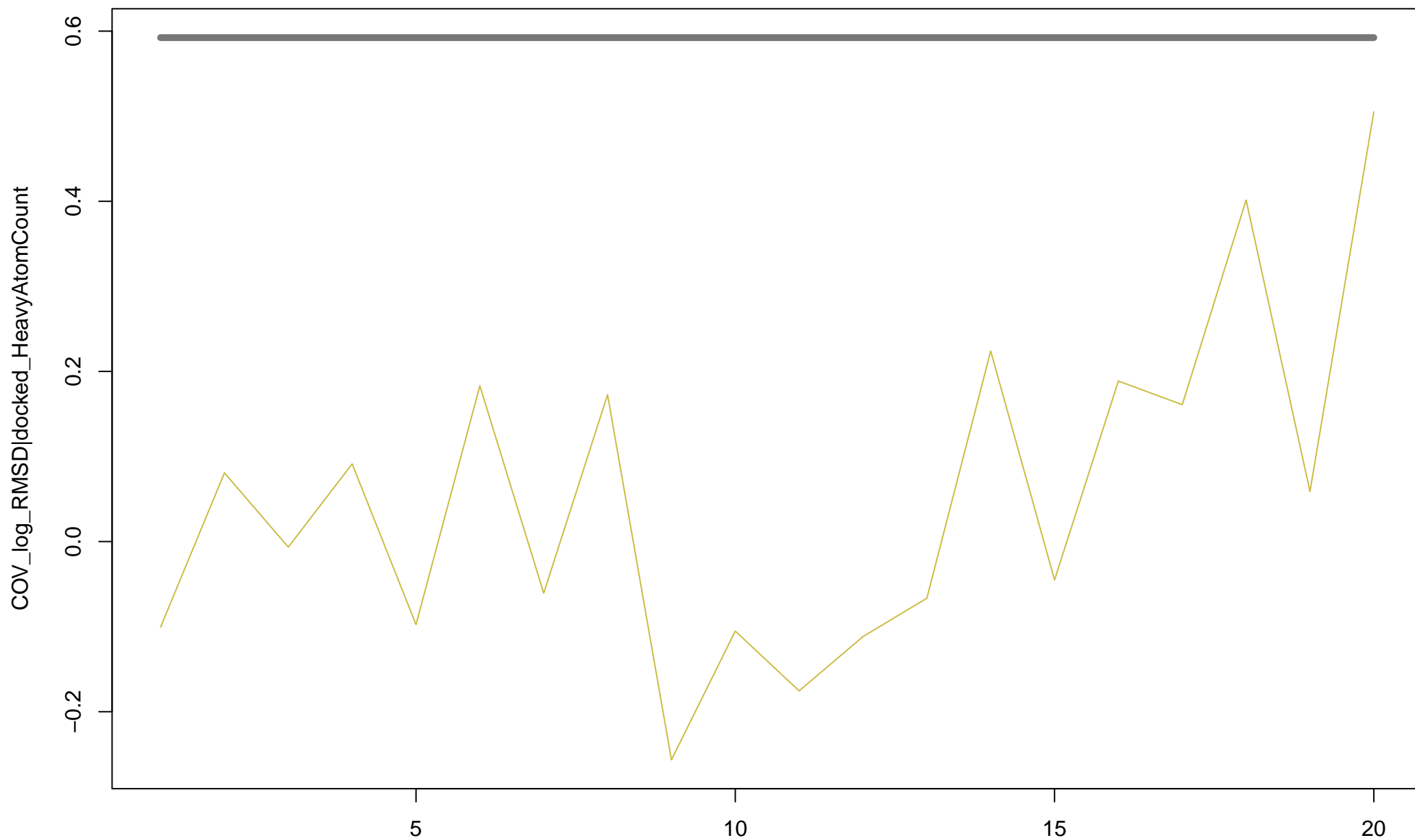
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 20 | BMK = 0.365 | MCSE(6.27) = 15.6 | stat: FALSE | burn: 20 | percentile: 100



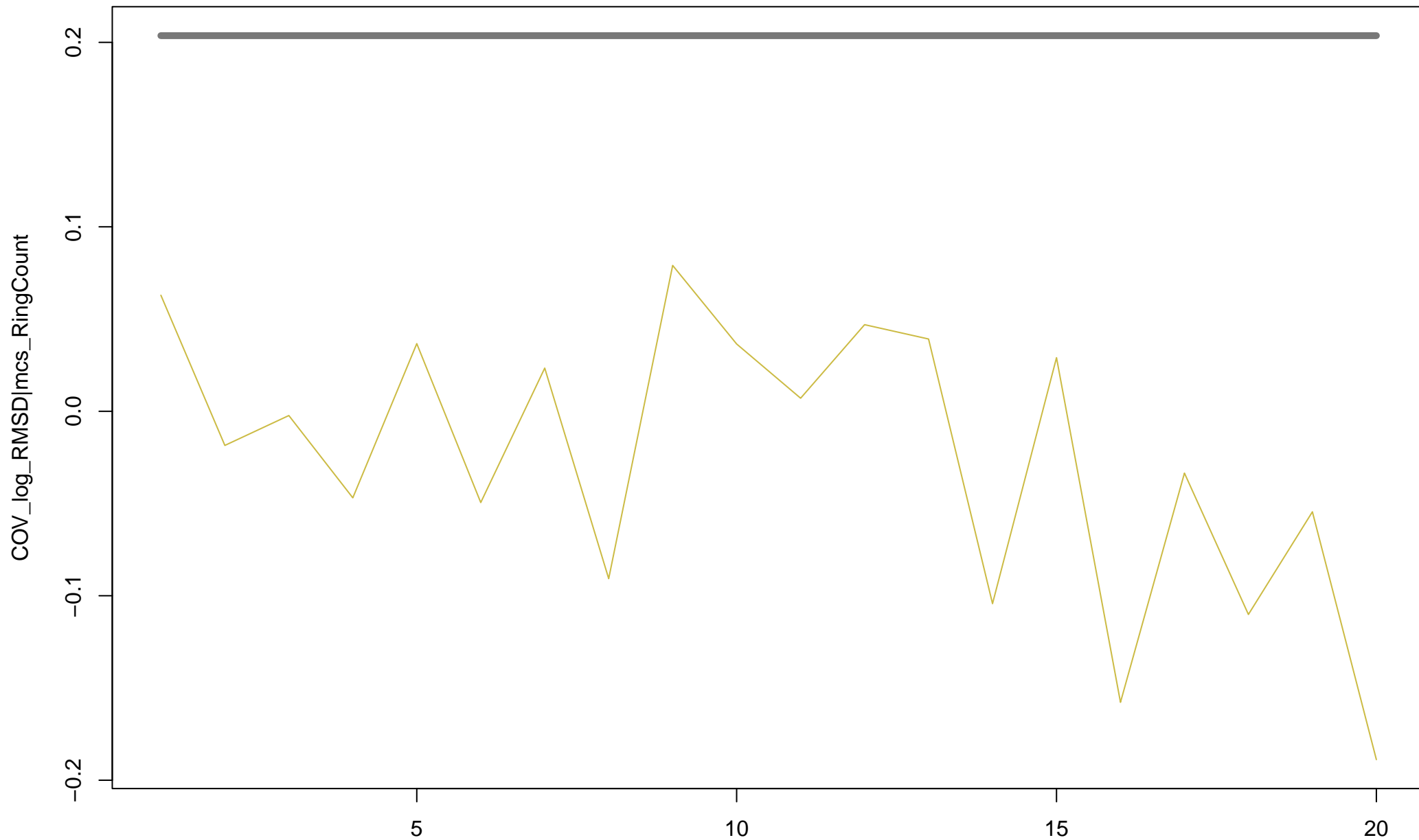
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 4.63 | BMK = 0.322 | MCSE(6.27) = 44.1 | stat: FALSE | burn: 20 | percentile: 0



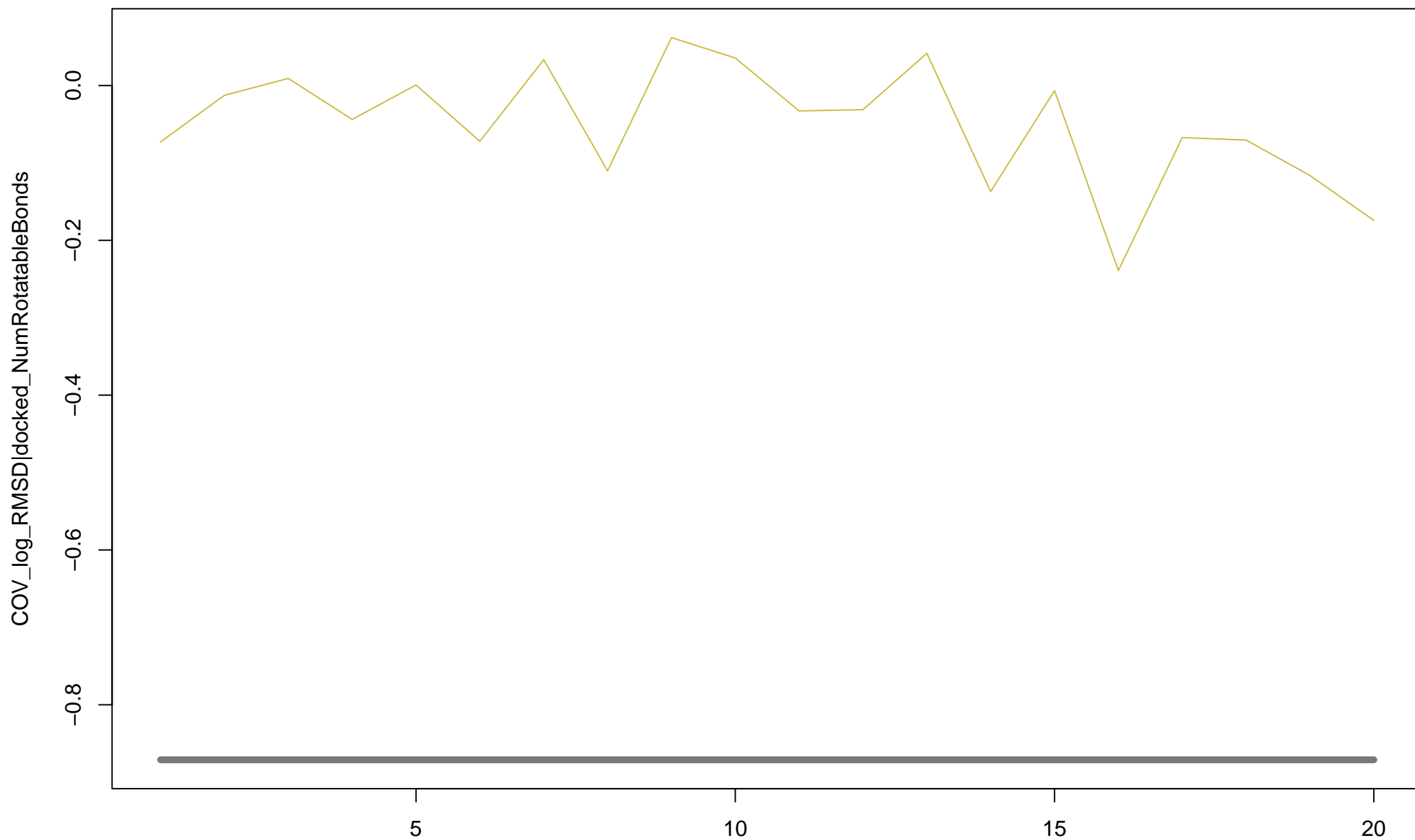
COV_log_RMSD|docked_HeavyAtomCount
ESS = 4.35 | BMK = 0.277 | MCSE(6.27) = 43.2 | stat: FALSE | burn: 16 | percentile: 100



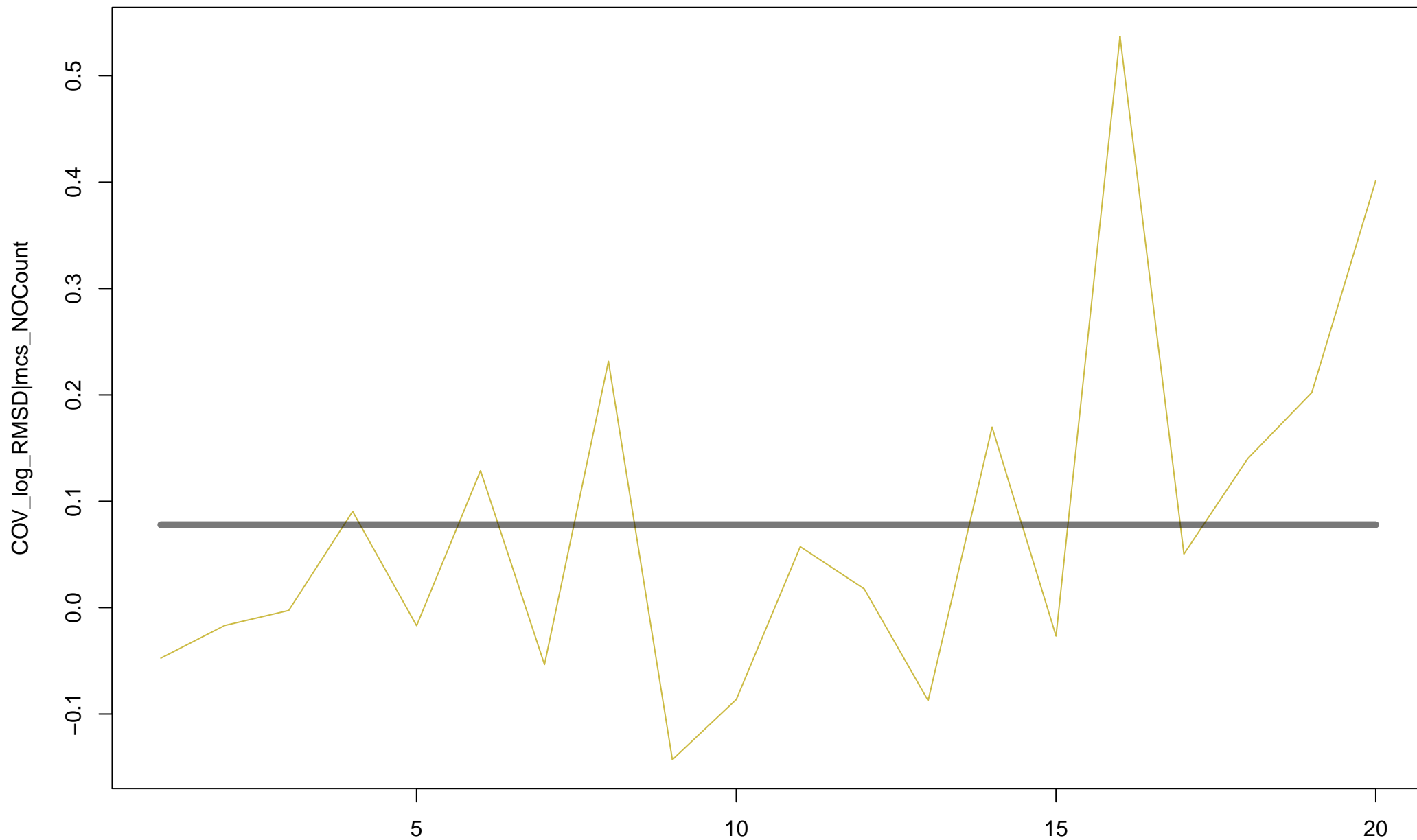
COV_log_RMSD|mcs_RingCount
ESS = 6.83 | BMK = 0.28 | MCSE(6.27) = 28.9 | stat: FALSE | burn: 20 | percentile: 100



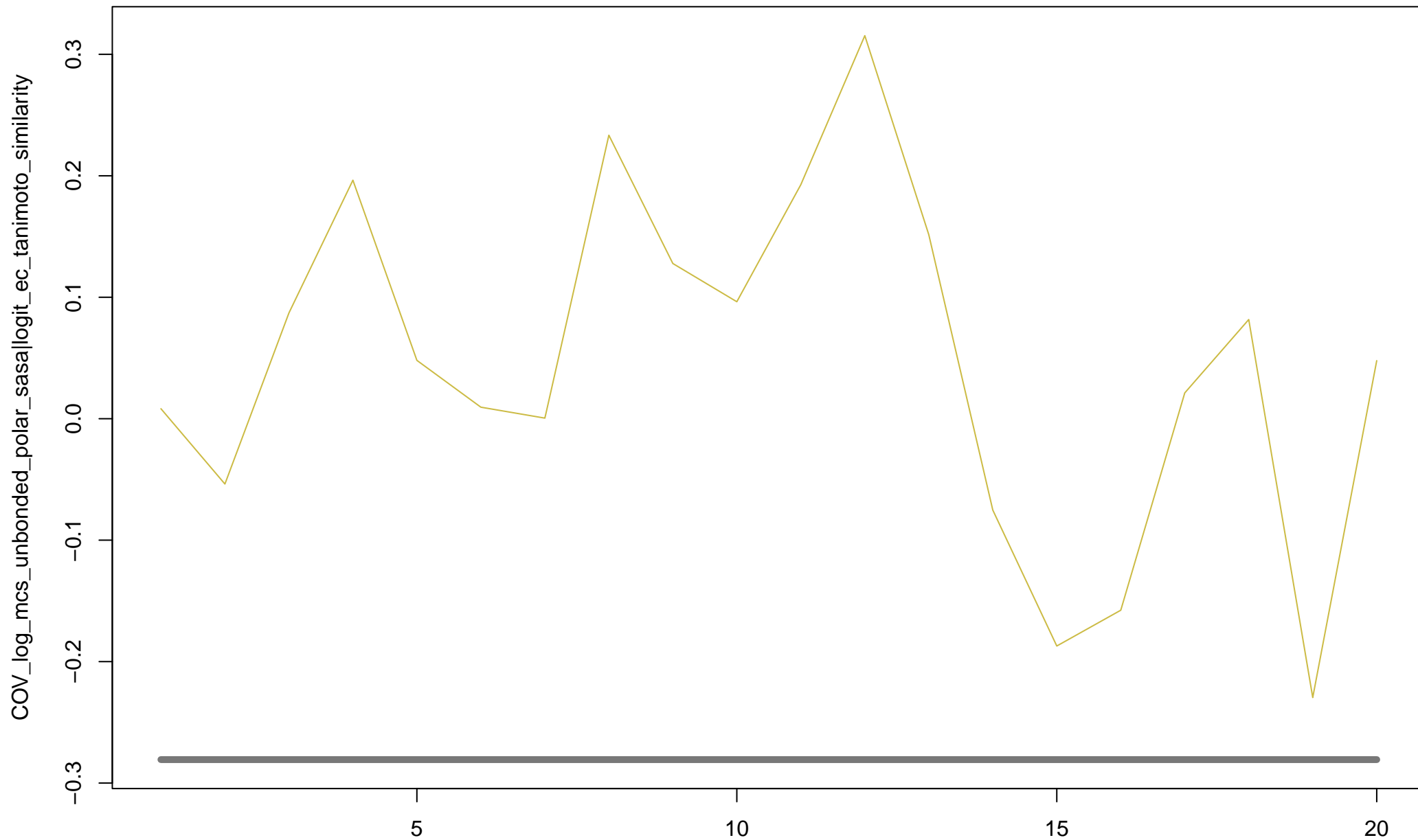
COV_log_RMSD|docked_NumRotatableBonds
ESS = 20 | BMK = 0.316 | MCSE(6.27) = 26.9 | stat: FALSE | burn: 20 | percentile: 0



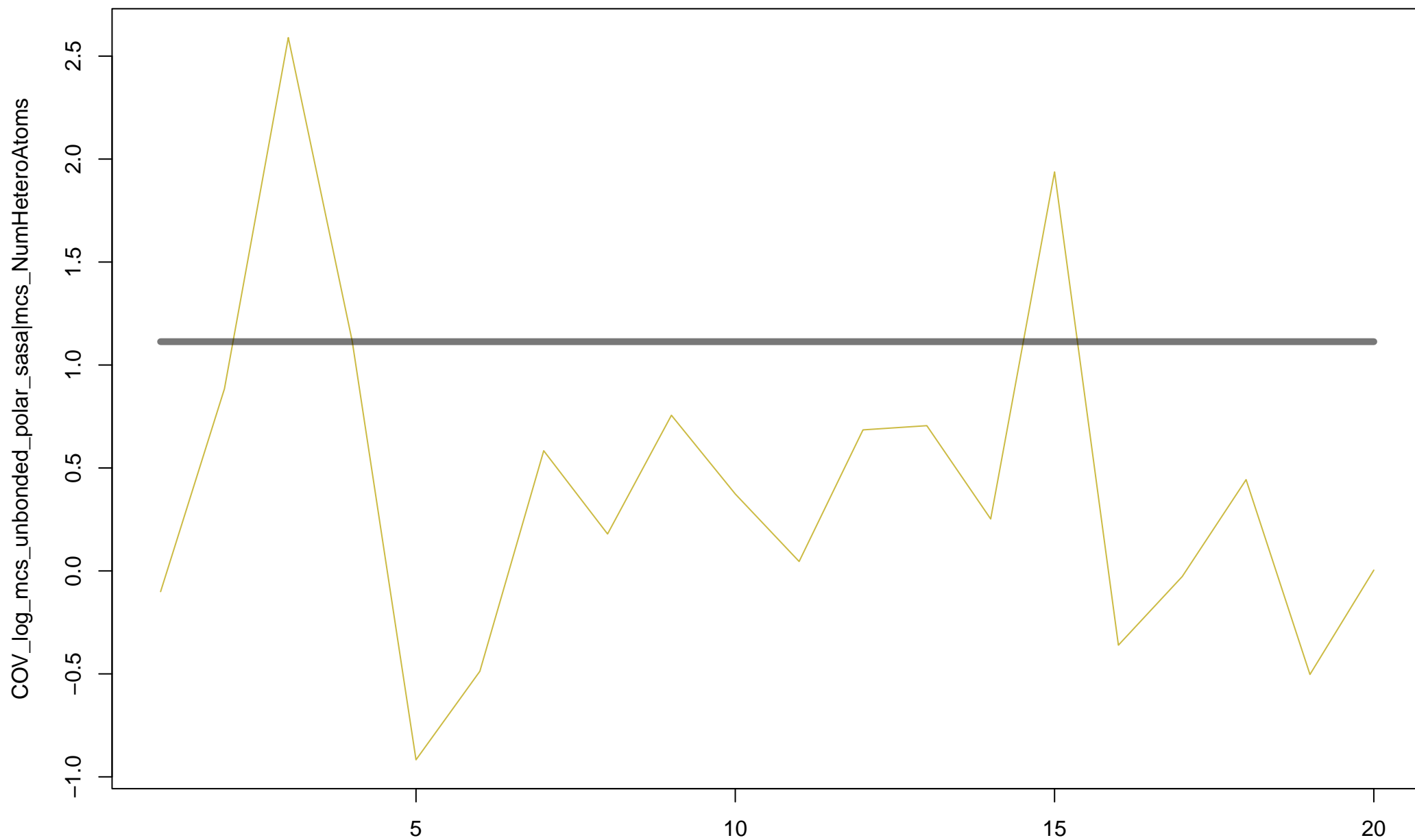
COV_log_RMSD|mcs_NOCount
ESS = 20 | BMK = 0.33 | MCSE(6.27) = 25 | stat: FALSE | burn: 20 | percentile: 60



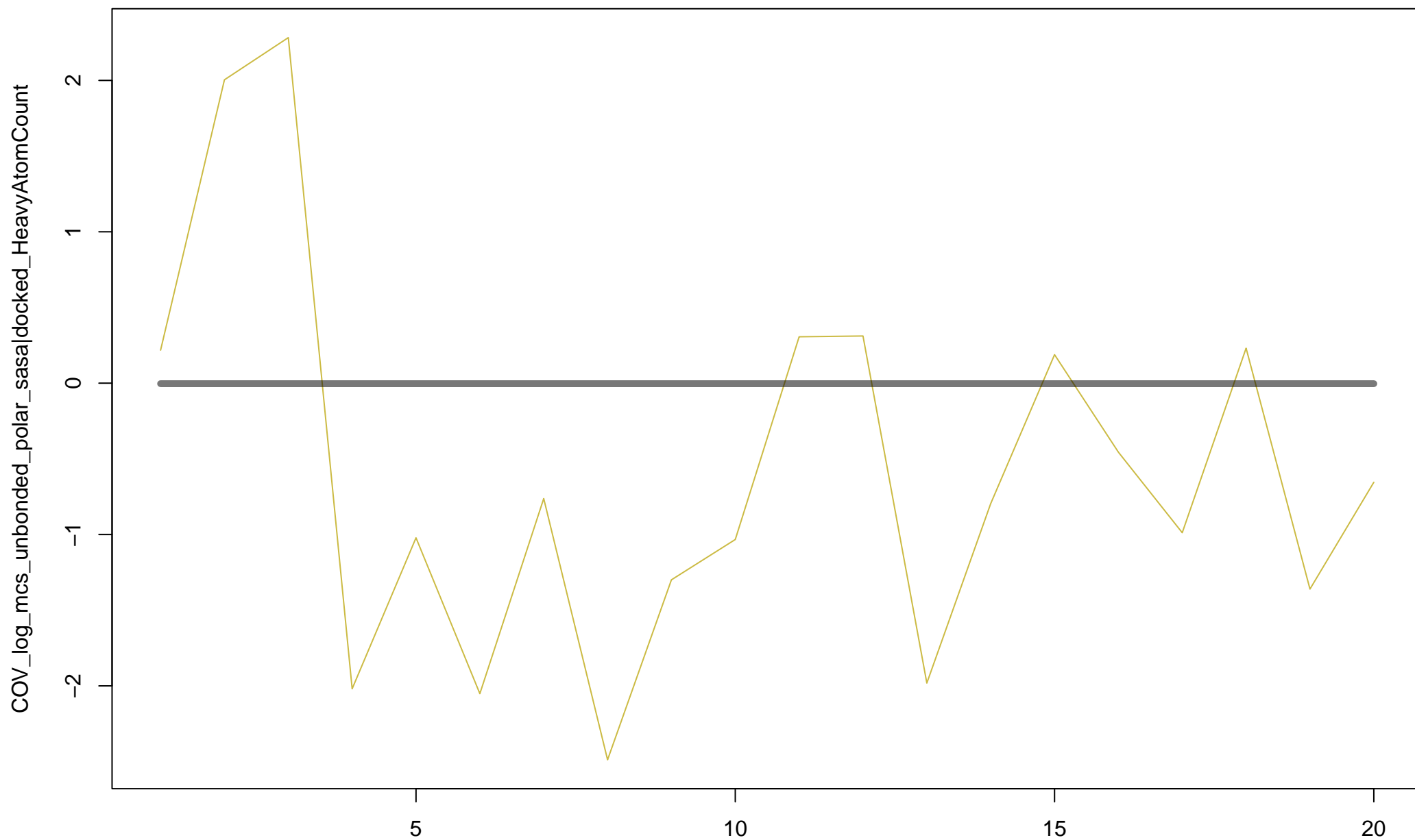
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 8.12 | BMK = 0.327 | MCSE(6.27) = 34.8 | stat: FALSE | burn: 20 | percentile: 0



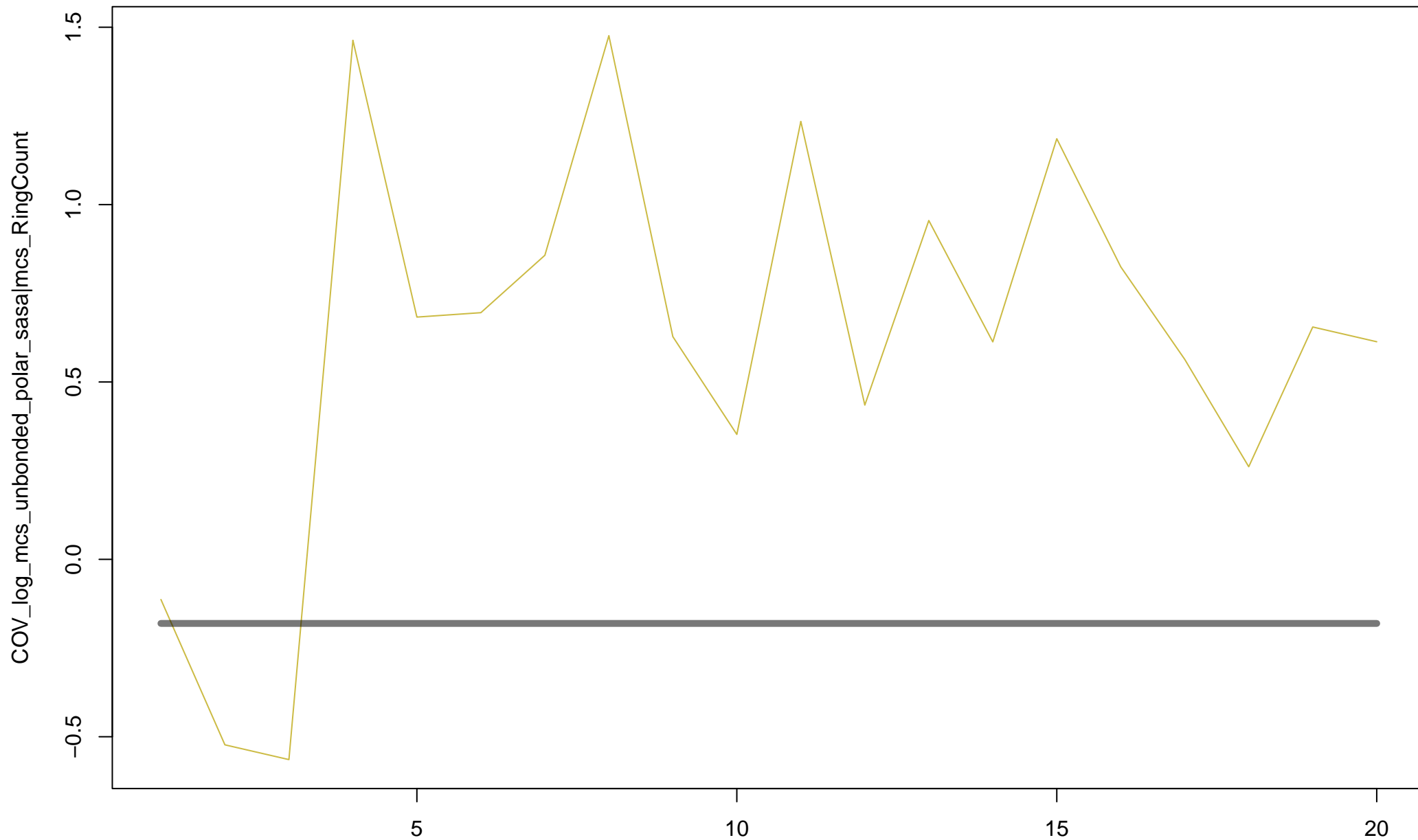
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 20 | BMK = 0.228 | MCSE(6.27) = 24.2 | stat: FALSE | burn: 20 | percentile: 85



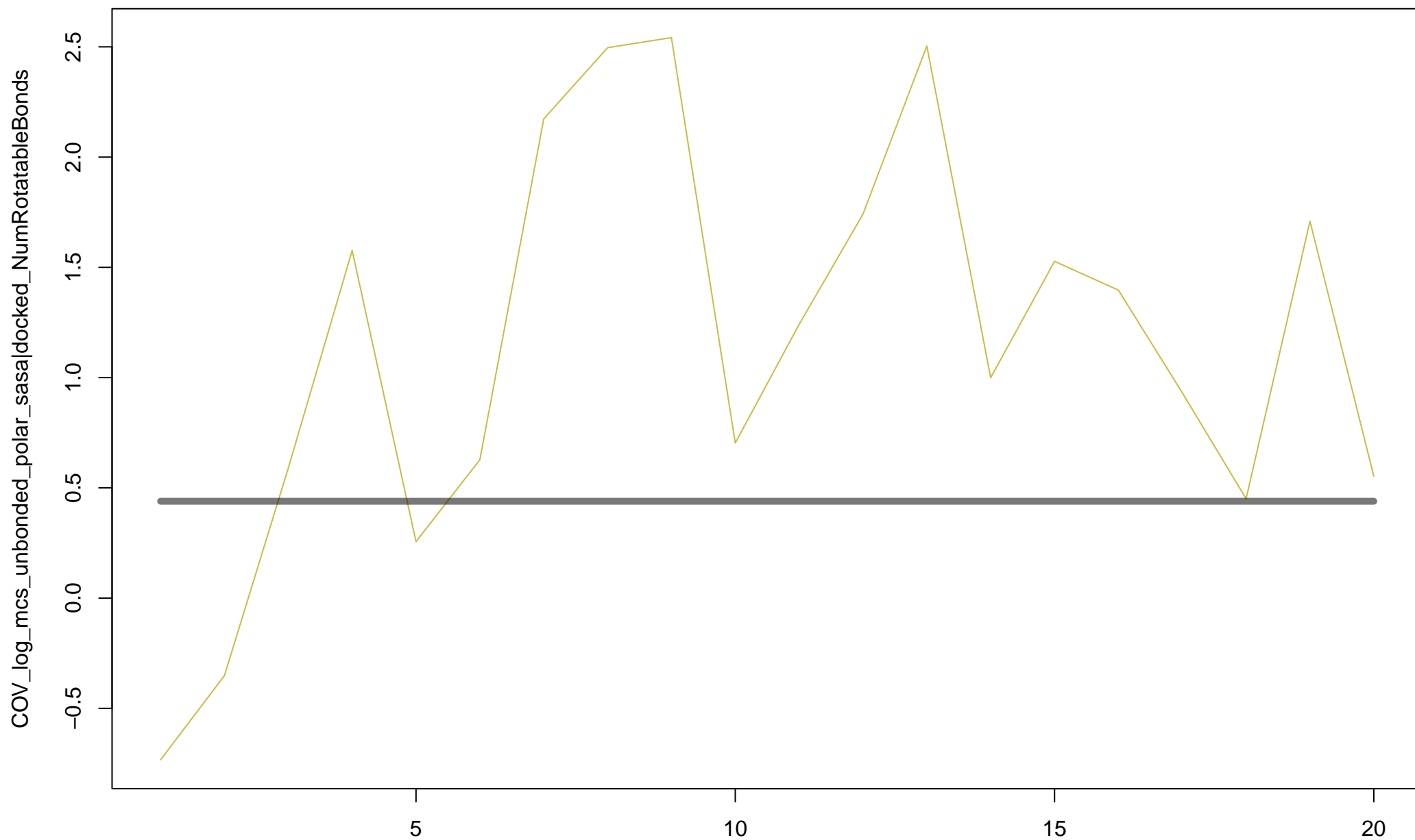
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 20 | BMK = 0.327 | MCSE(6.27) = 30.6 | stat: FALSE | burn: 20 | percentile: 65



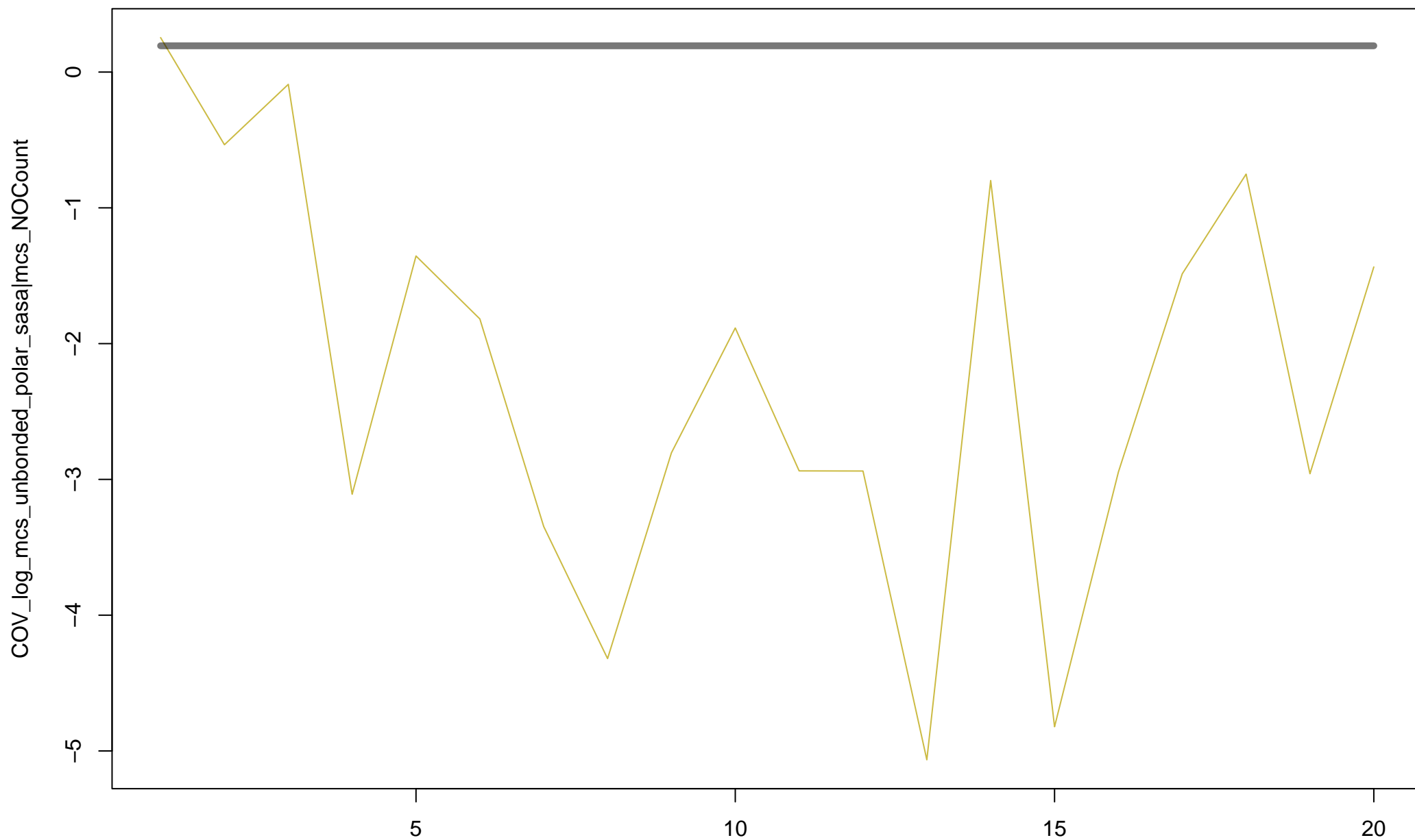
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 20 | BMK = 0.358 | MCSE(6.27) = 29.9 | stat: FALSE | burn: 20 | percentile: 10



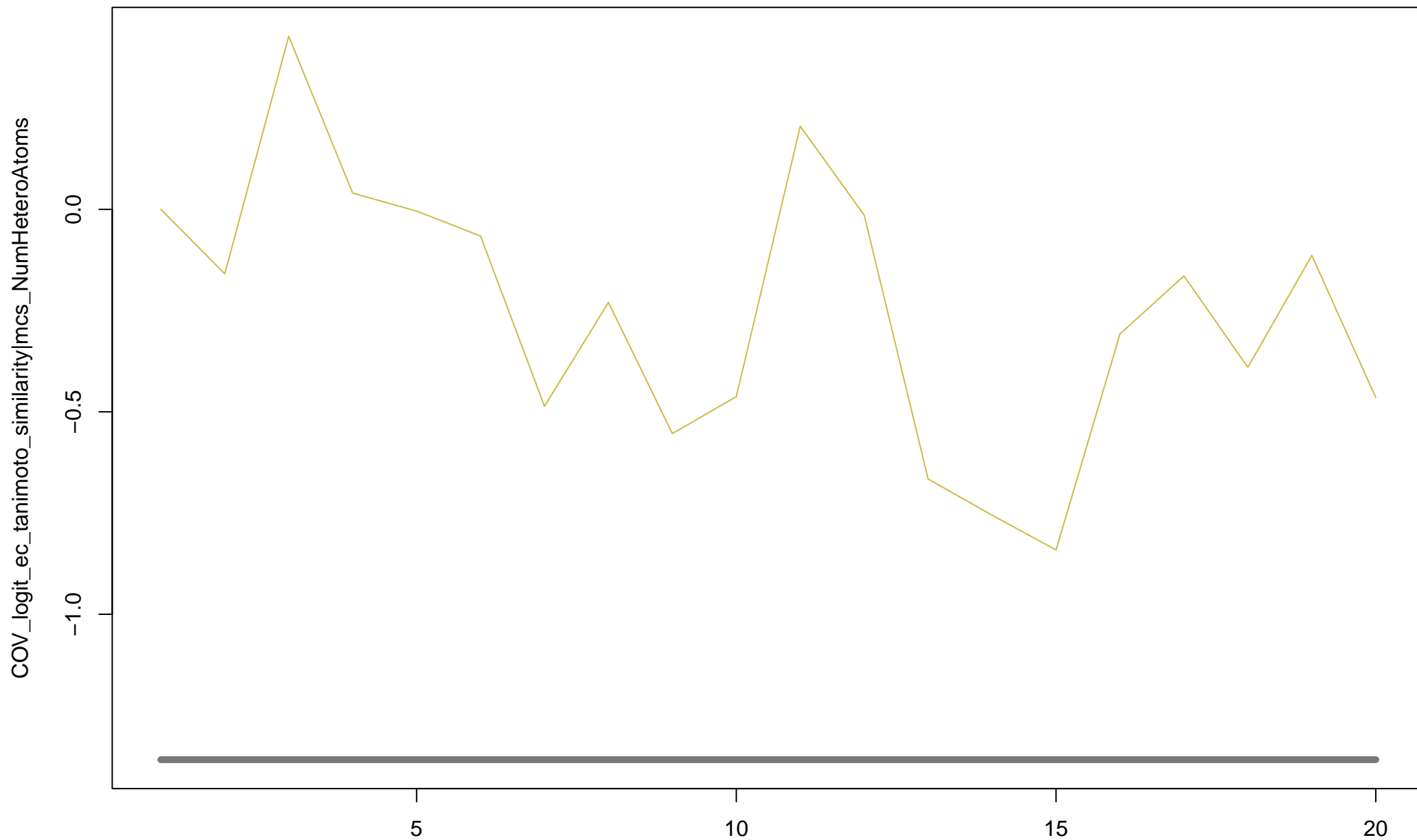
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 9.07 | BMK = 0.321 | MCSE(6.27) = 34.2 | stat: FALSE | burn: 20 | percentile: 15



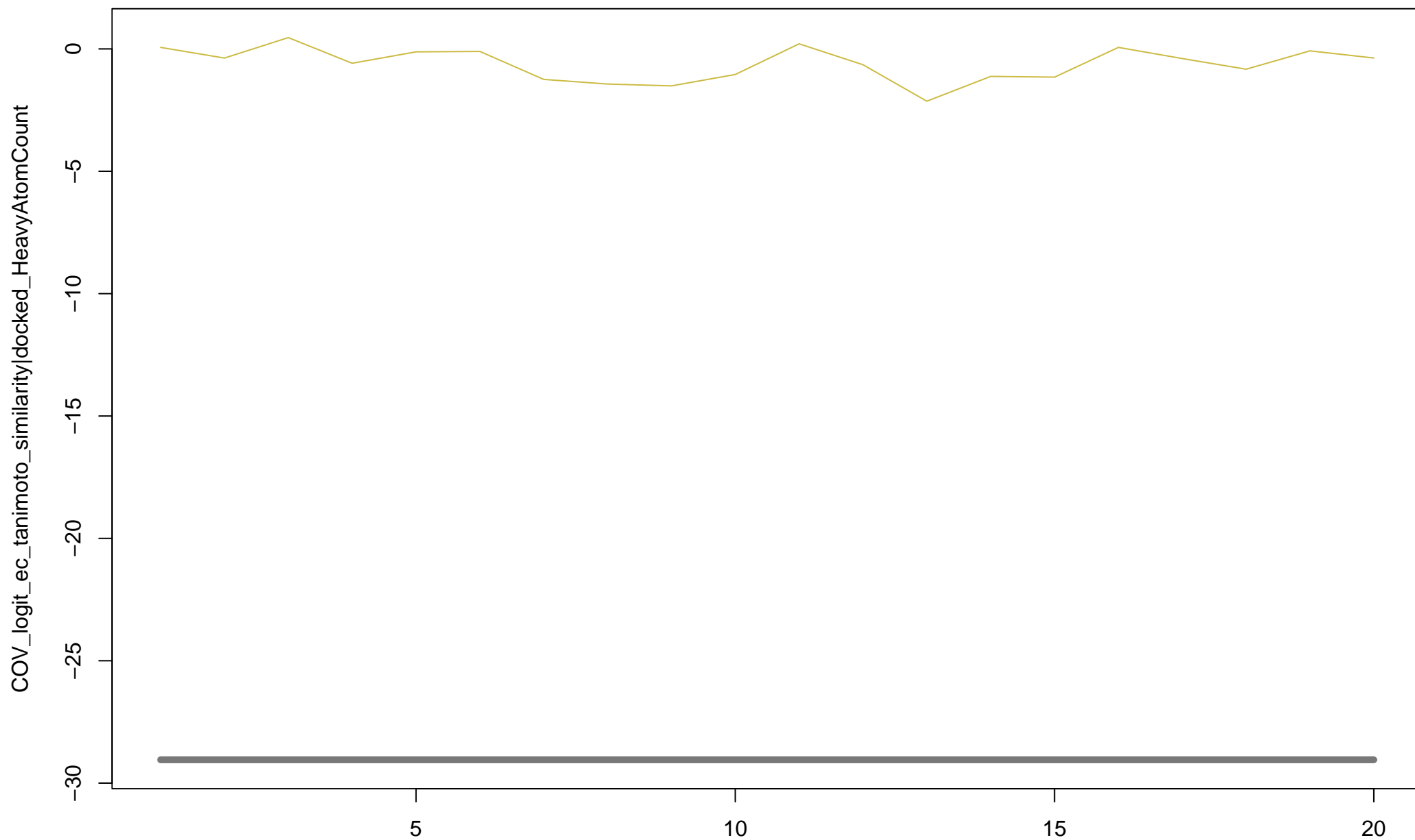
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 20 | BMK = 0.133 | MCSE(6.27) = 31.8 | stat: FALSE | burn: 20 | percentile: 95



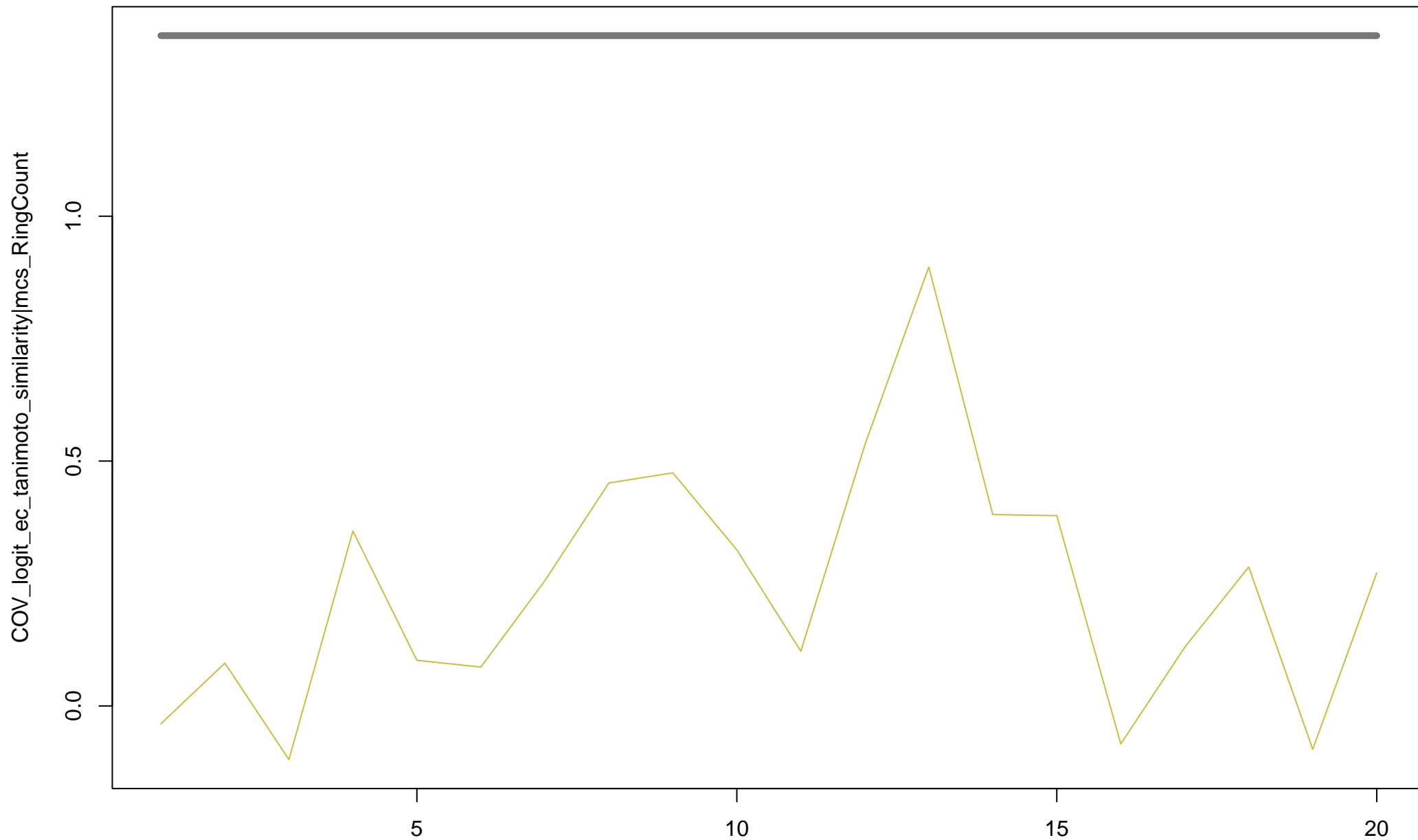
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 8.29 | BMK = 0.169 | MCSE(6.27) = 36.6 | stat: FALSE | burn: 16 | percentile: 0



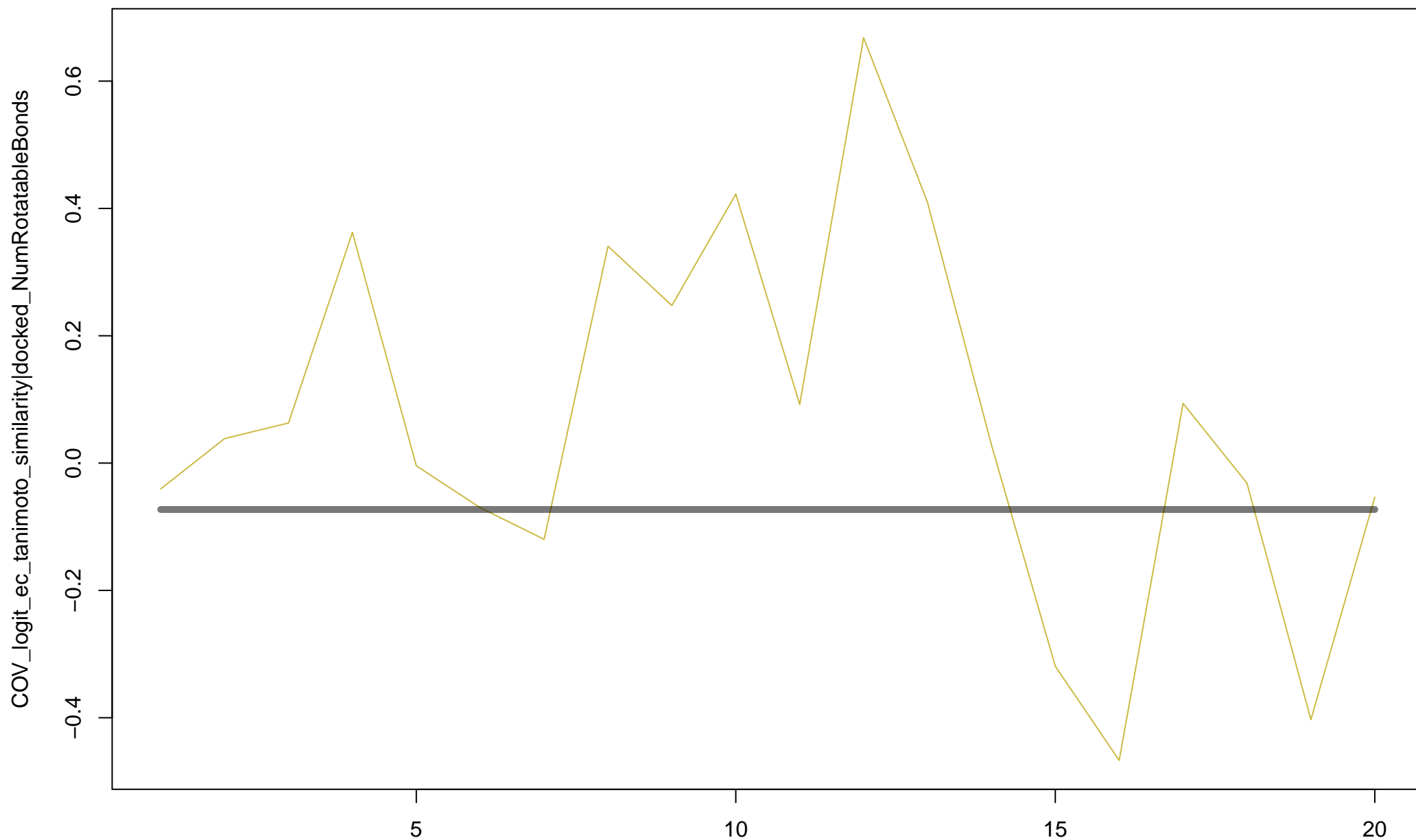
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 20 | BMK = 0.093 | MCSE(6.27) = 31.6 | stat: FALSE | burn: 20 | percentile: 0



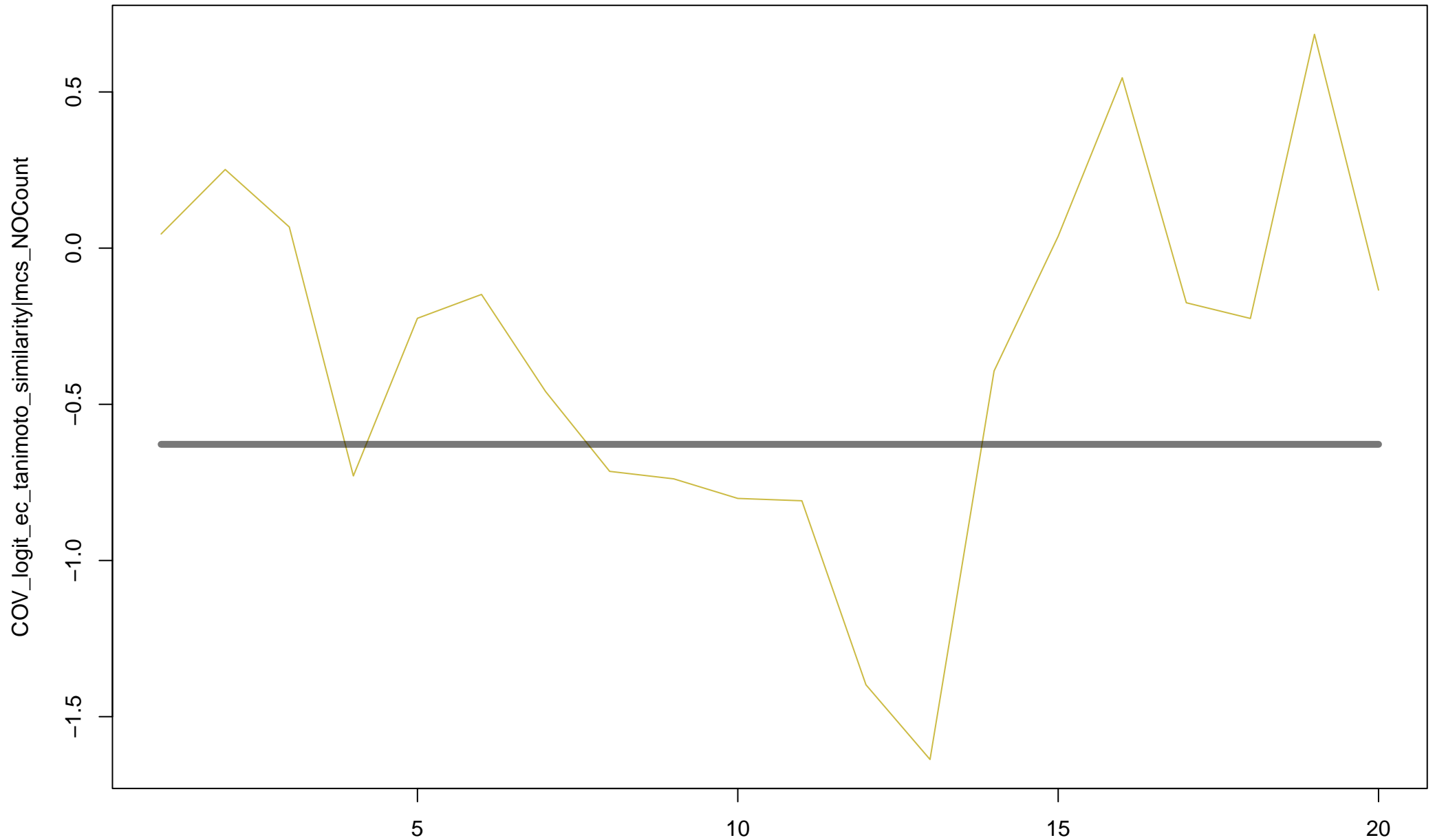
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 20 | BMK = 0.175 | MCSE(6.27) = 34.6 | stat: FALSE | burn: 20 | percentile: 100



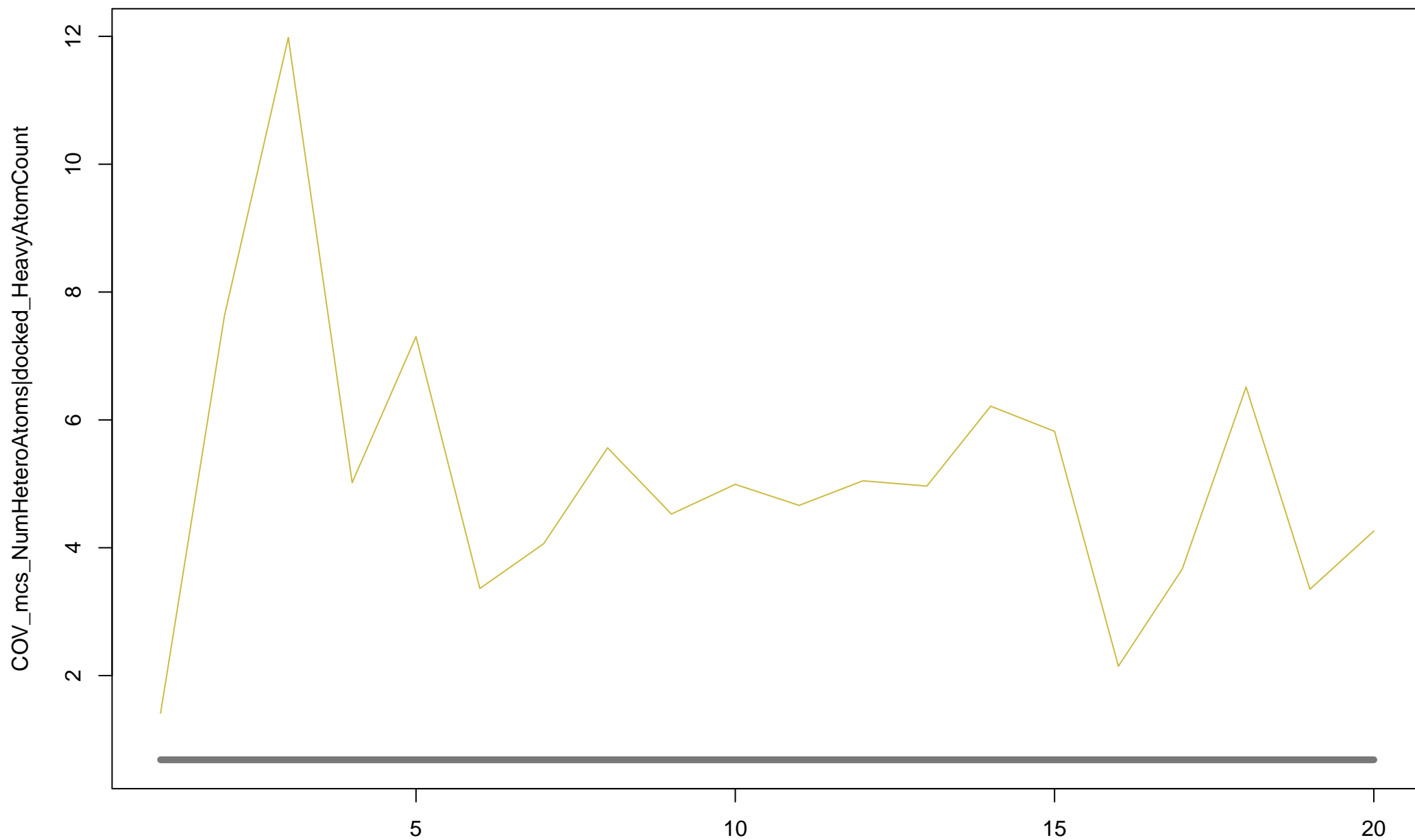
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 8.34 | BMK = 0.305 | MCSE(6.27) = 36.3 | stat: FALSE | burn: 20 | percentile: 20



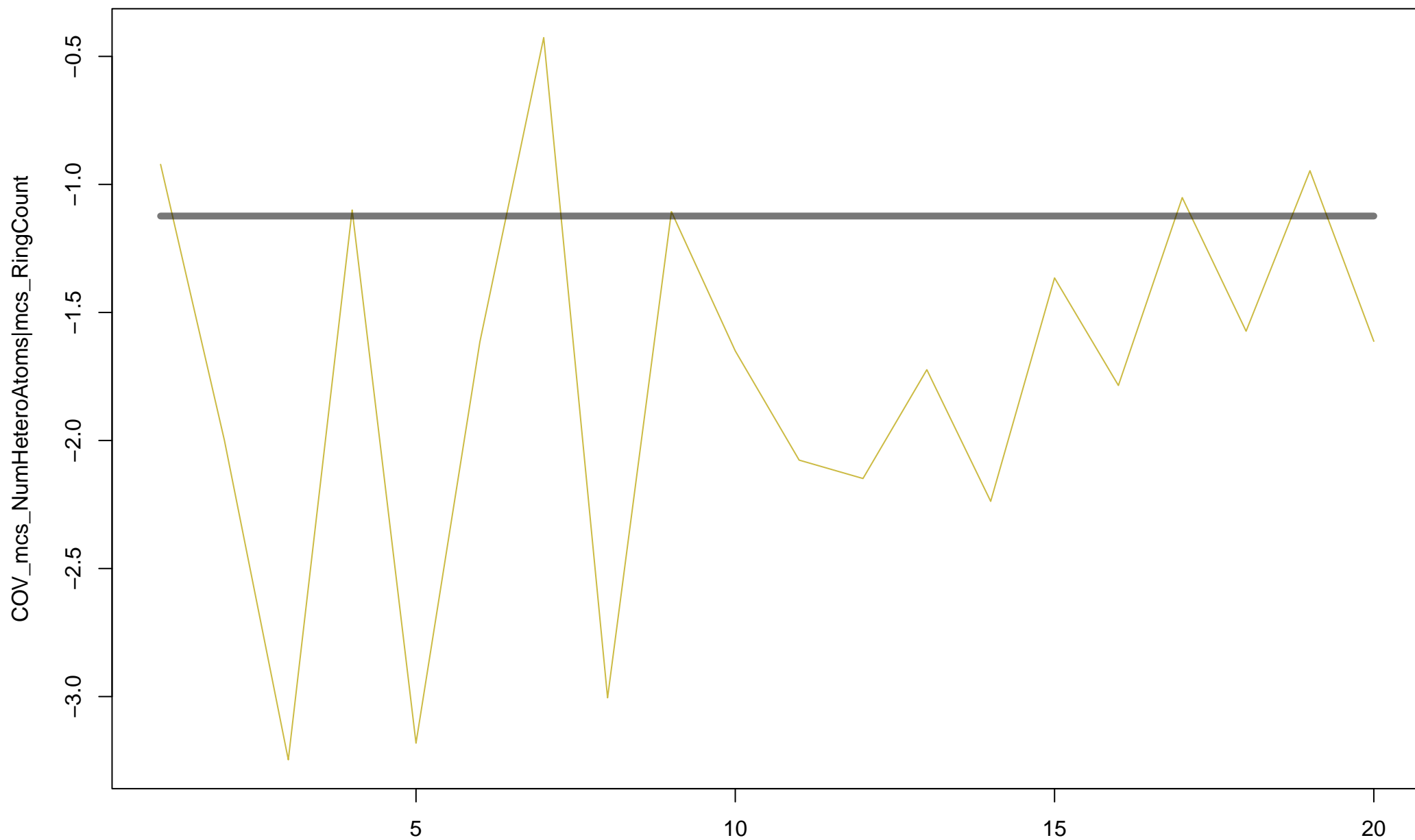
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 5.41 | BMK = 0.298 | MCSE(6.27) = 45.8 | stat: FALSE | burn: 20 | percentile: 35



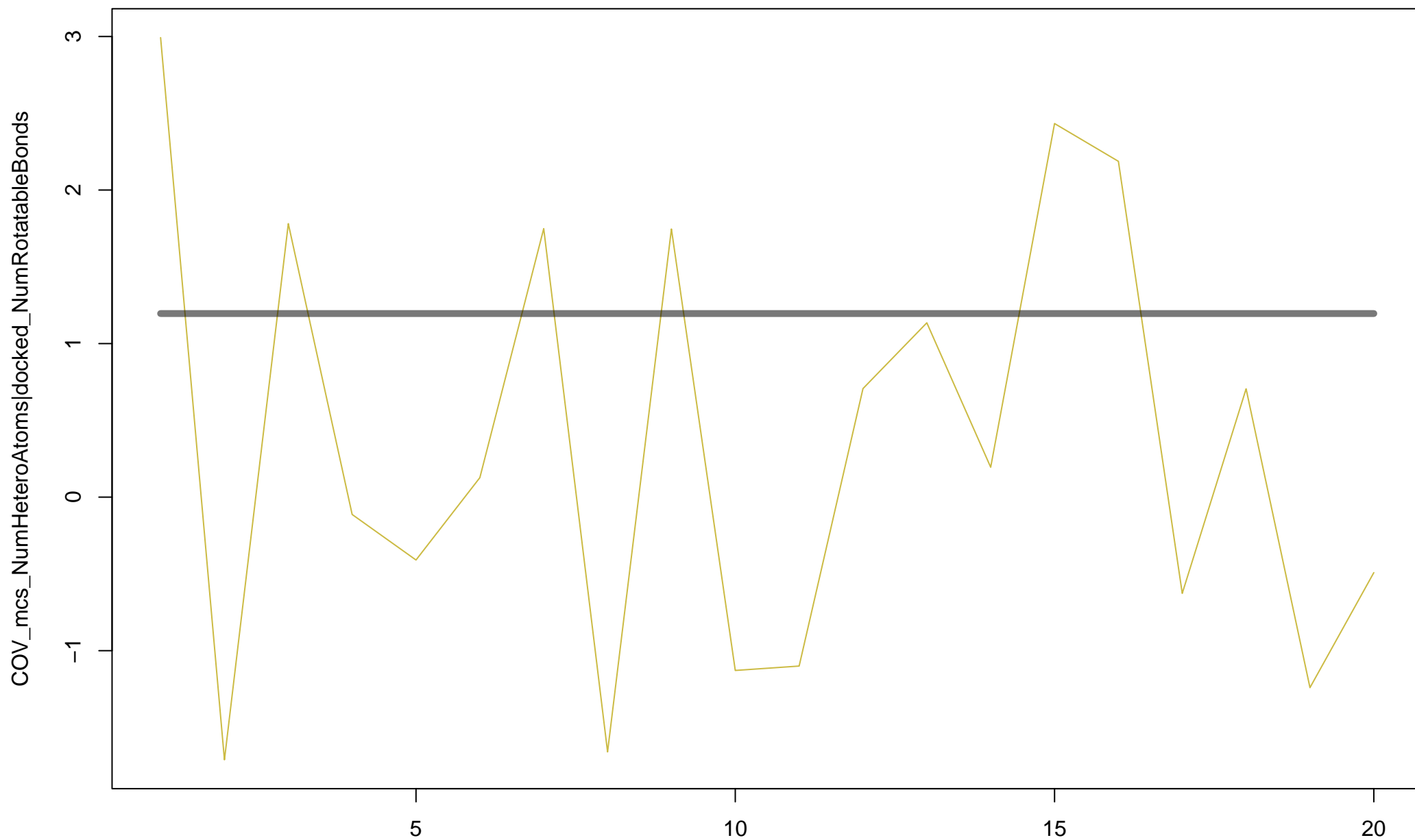
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 20 | BMK = 0.268 | MCSE(6.27) = 22.8 | stat: FALSE | burn: 20 | percentile: 0



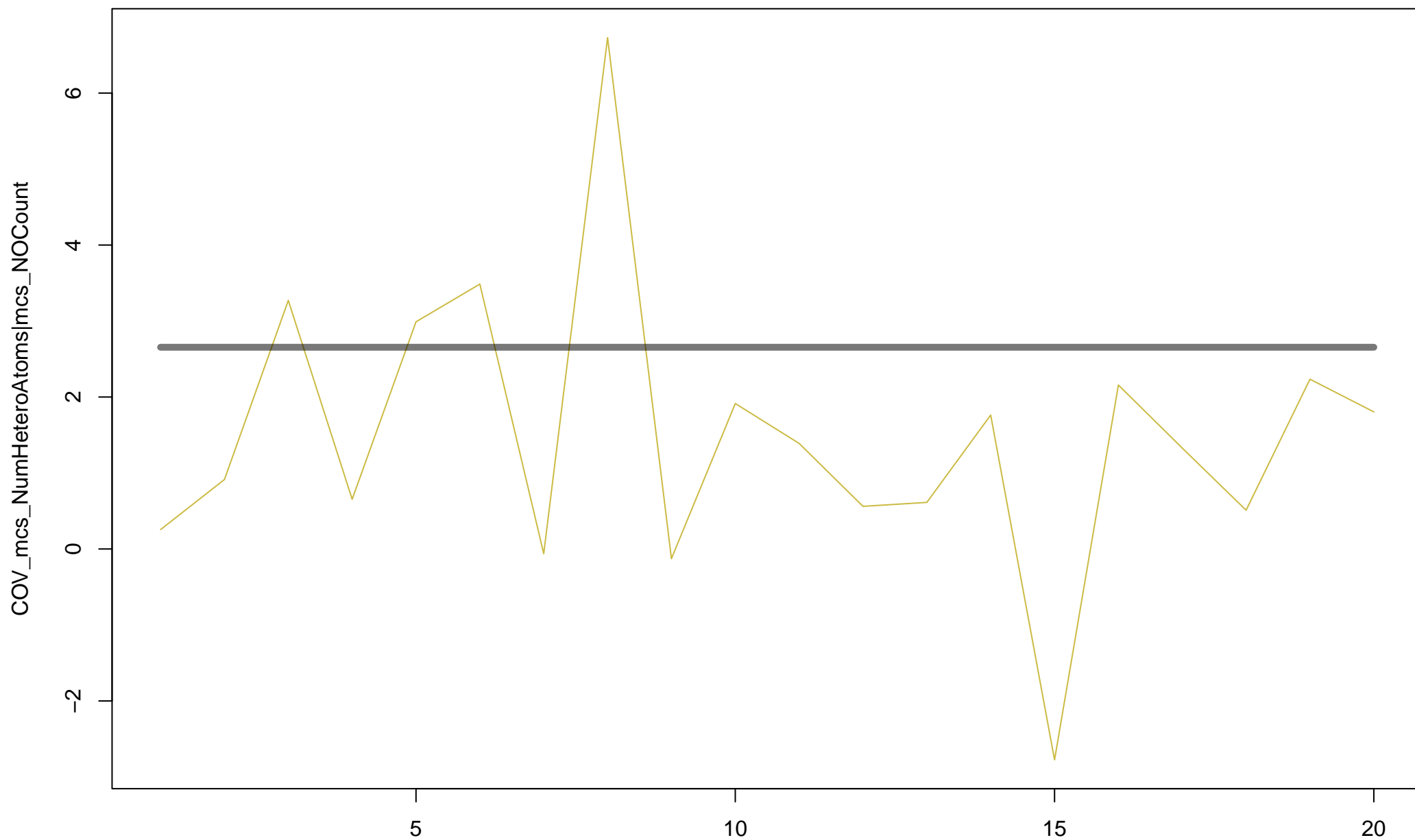
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 20 | BMK = 0.34 | MCSE(6.27) = 11.8 | stat: FALSE | burn: 16 | percentile: 70



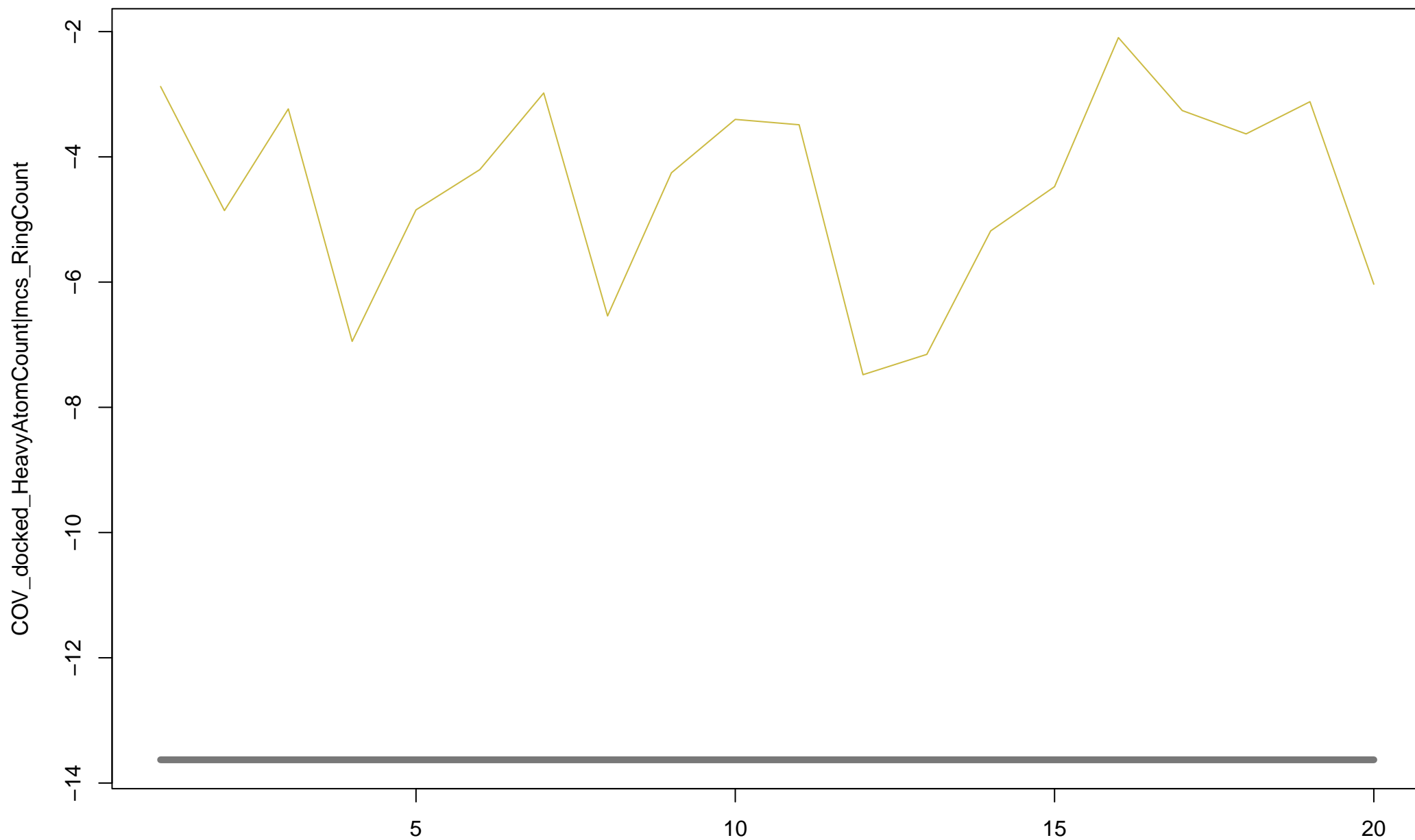
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 20 | BMK = 0.0823 | MCSE(6.27) = 13 | stat: FALSE | burn: 20 | percentile: 70



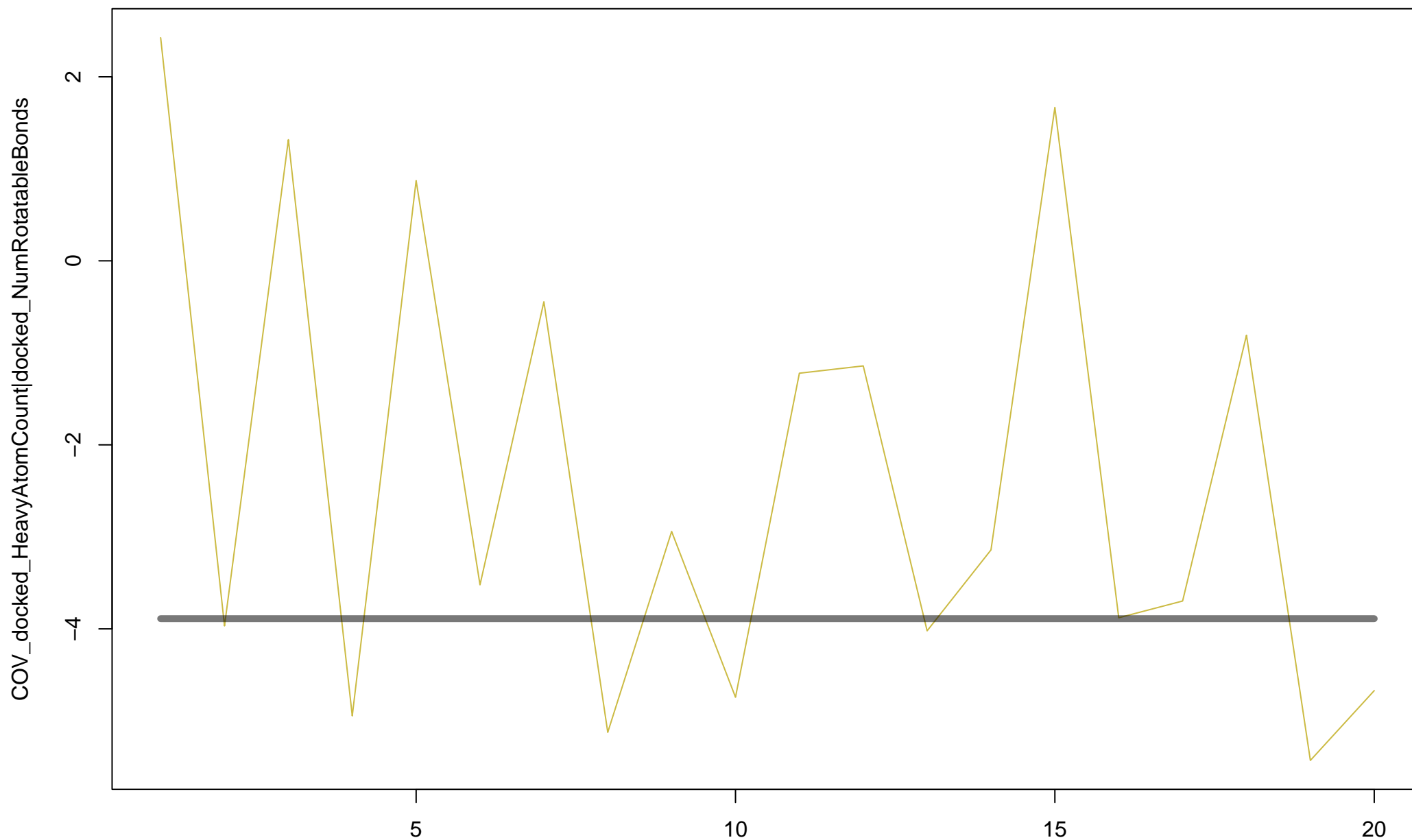
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 11.2 | BMK = 0.434 | MCSE(6.27) = 11.3 | stat: FALSE | burn: 20 | percentile: 80



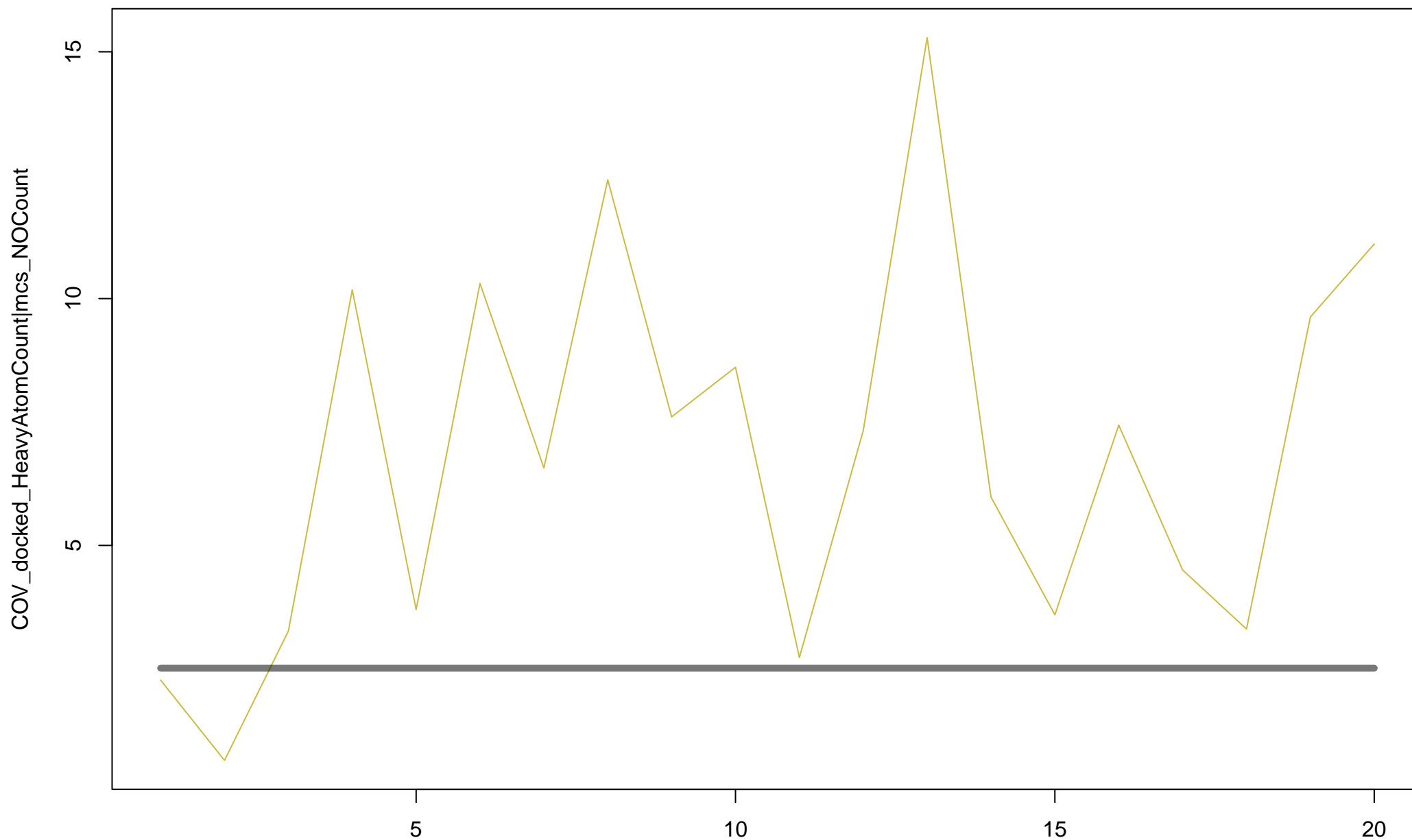
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 20 | BMK = 0.0924 | MCSE(6.27) = 24.1 | stat: FALSE | burn: 20 | percentile: 0



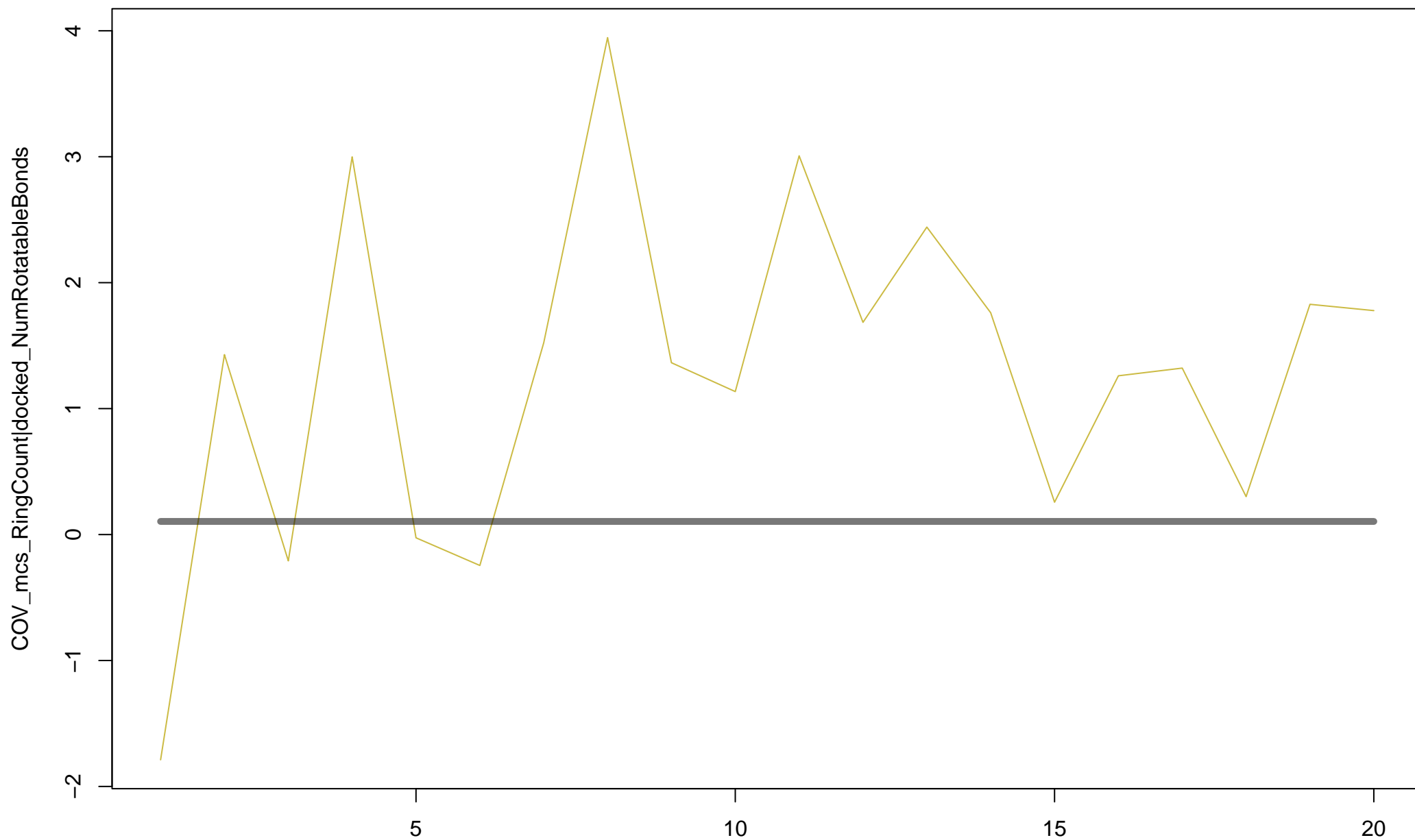
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 20 | BMK = 0.117 | MCSE(6.27) = 9.14 | stat: FALSE | burn: 20 | percentile: 35



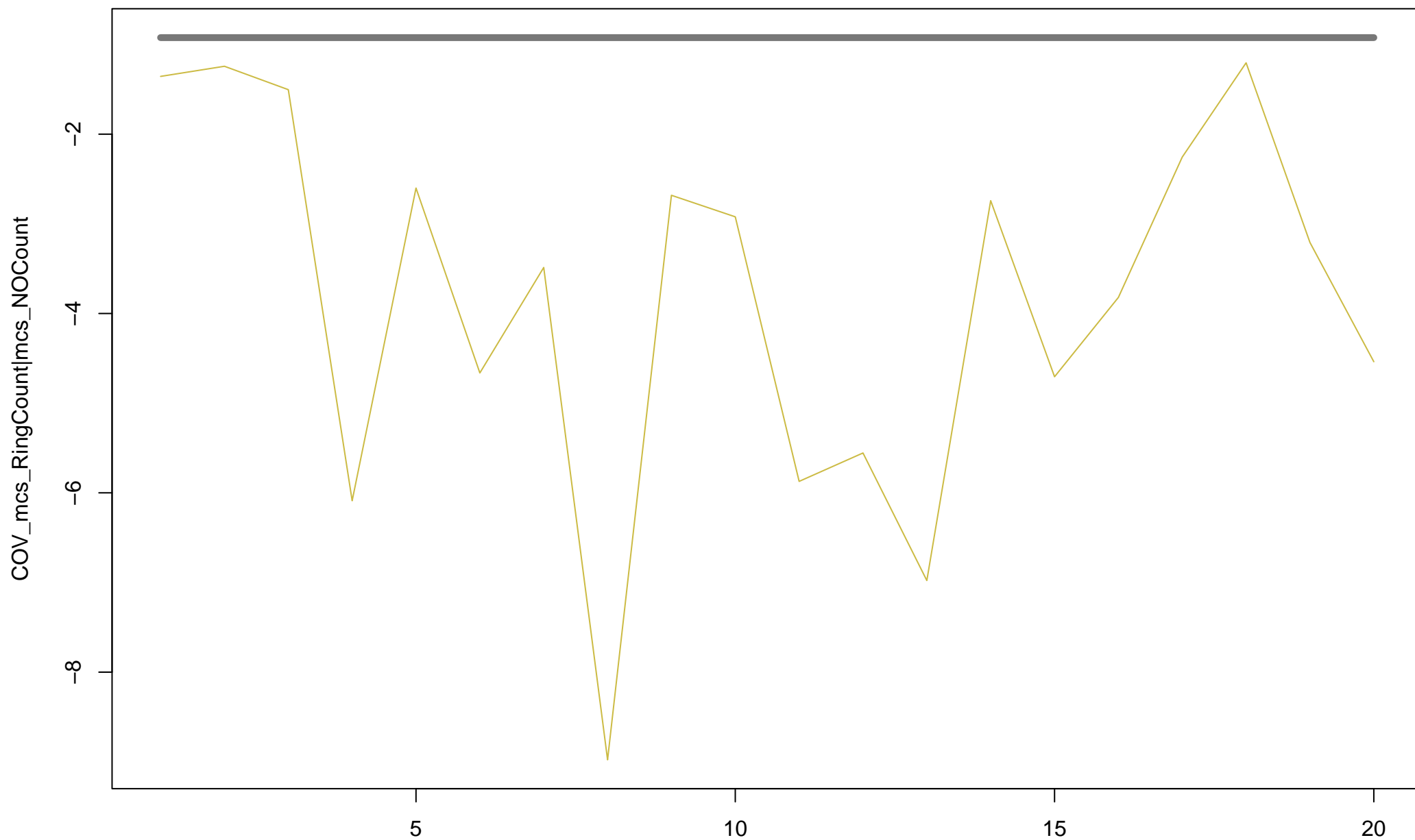
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 20 | BMK = 0.0899 | MCSE(6.27) = 23.1 | stat: FALSE | burn: 20 | percentile: 10



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 20 | BMK = 0.419 | MCSE(6.27) = 20.2 | stat: FALSE | burn: 20 | percentile: 20



COV_mcs_RingCount|mcs_NOCount
ESS = 20 | BMK = 0.189 | MCSE(6.27) = 25.5 | stat: FALSE | burn: 20 | percentile: 100



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 20 | BMK = 0.17 | MCSE(6.27) = 24.8 | stat: FALSE | burn: 20 | percentile: 85

