

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 1

max MCSE = 14.6658772843237

all stationary: FALSE

burn: 816

max rel.err.: 3.92174648035615

-- STATS 1D --

min ESS = 173.133605495916

max BMK = 0.13180154062978

max MCSE = 5.53883745228539

all stationary: FALSE

burn: 0

max rel.err.: 1.91244131970384

-- STATS 2D --

min ESS = 216.700951336012

max BMK = 0.108325599431994

max MCSE = 6.10270937837348

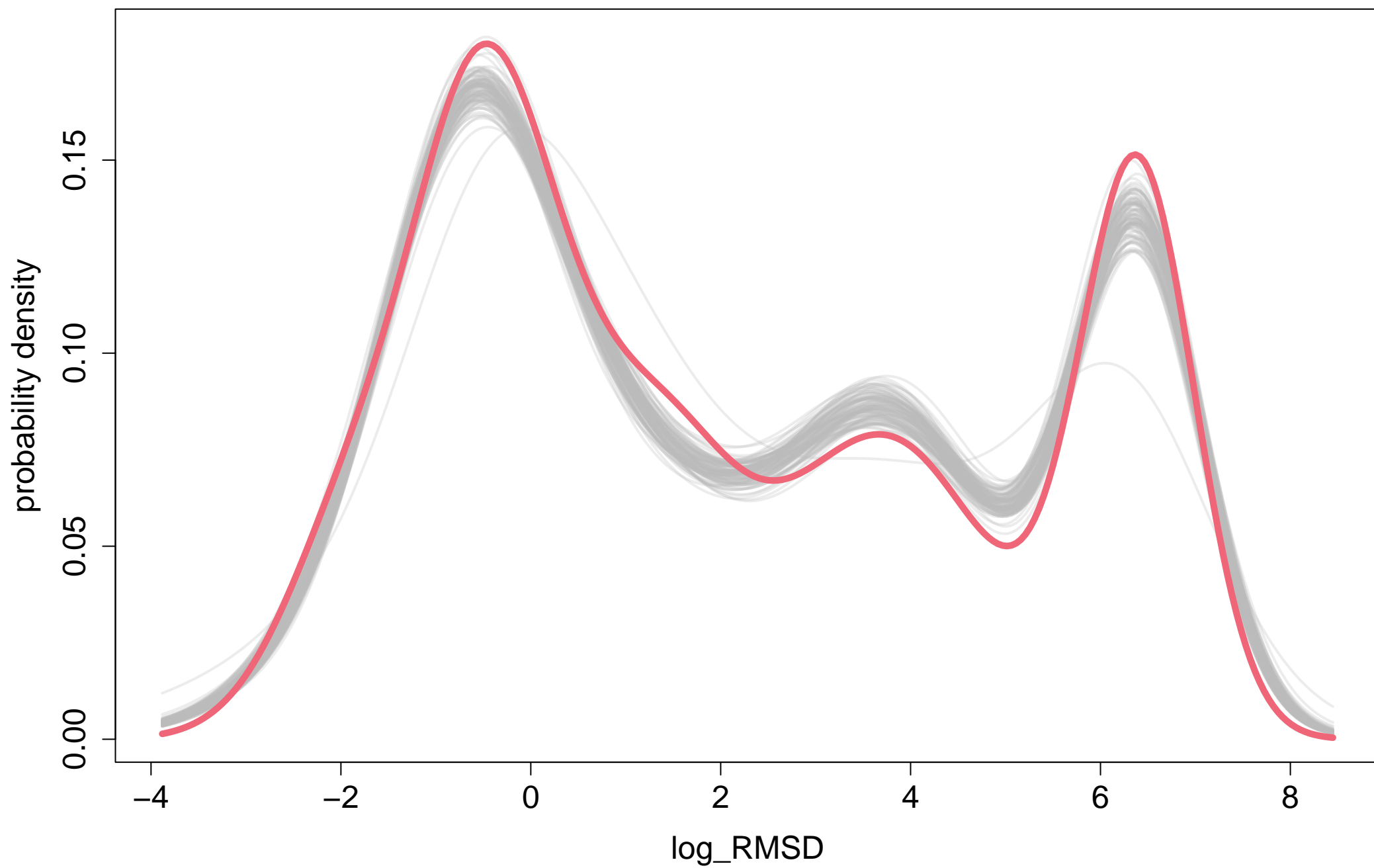
all stationary: FALSE

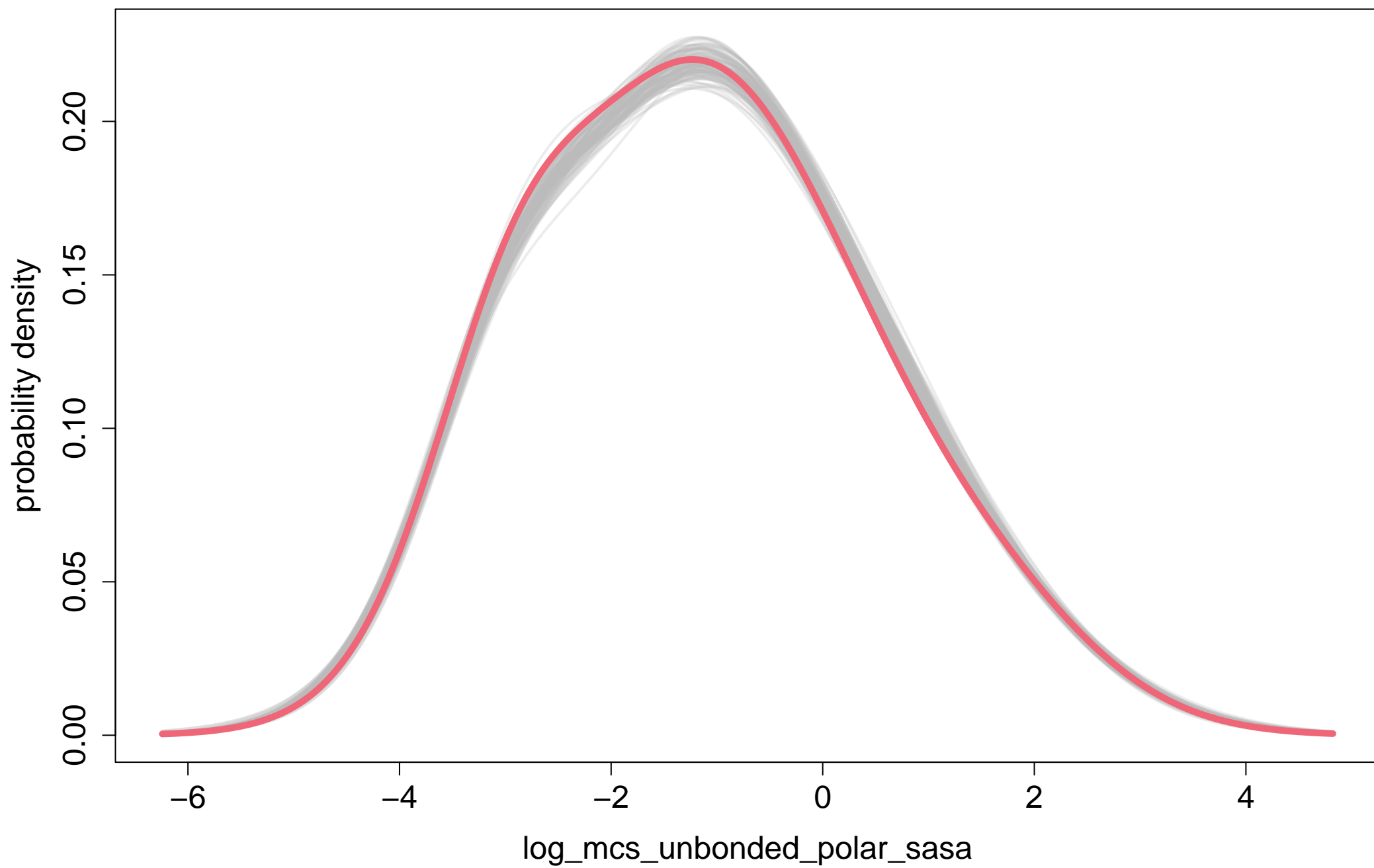
burn: 0

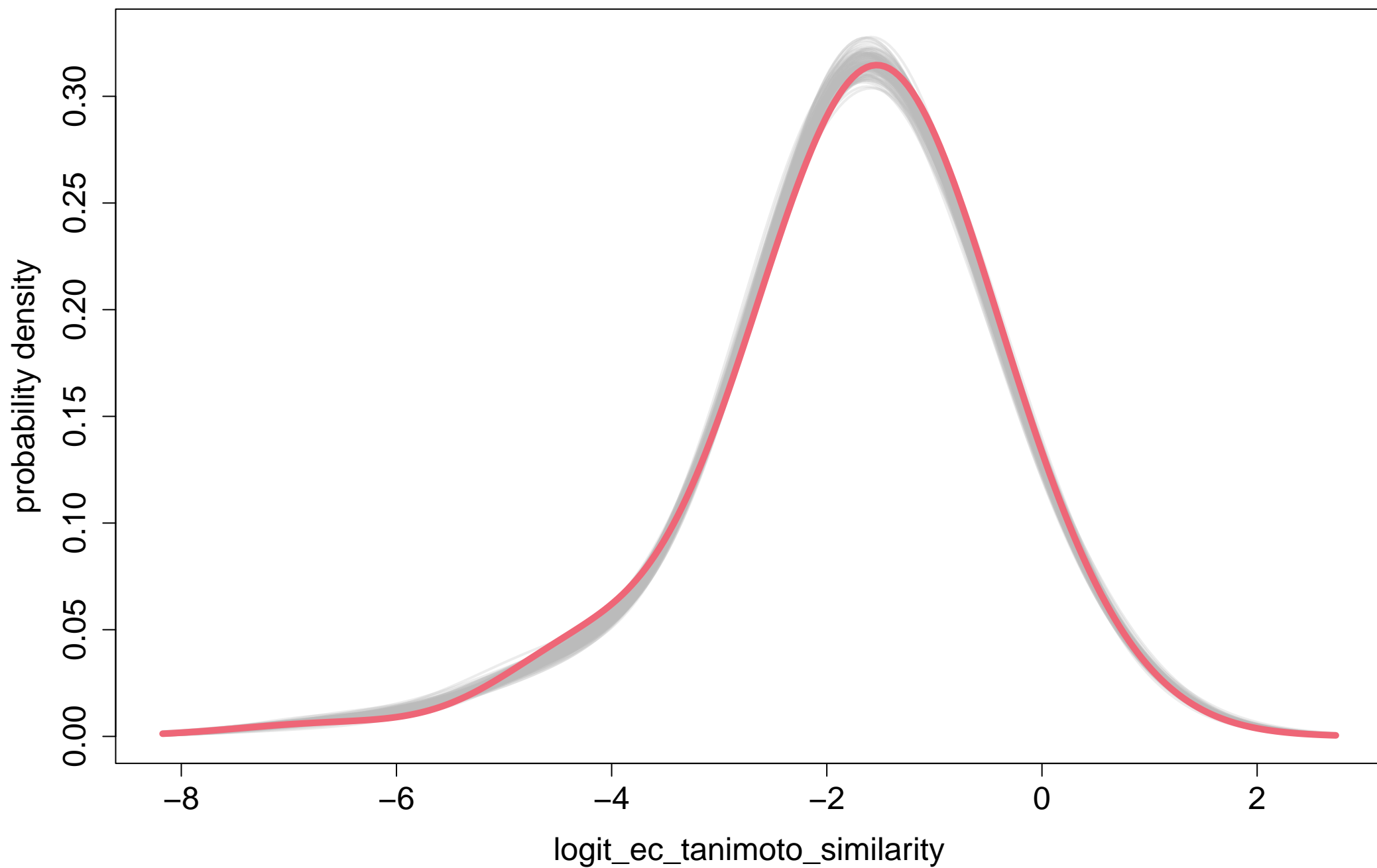
max rel.err.: 2.29698708875017

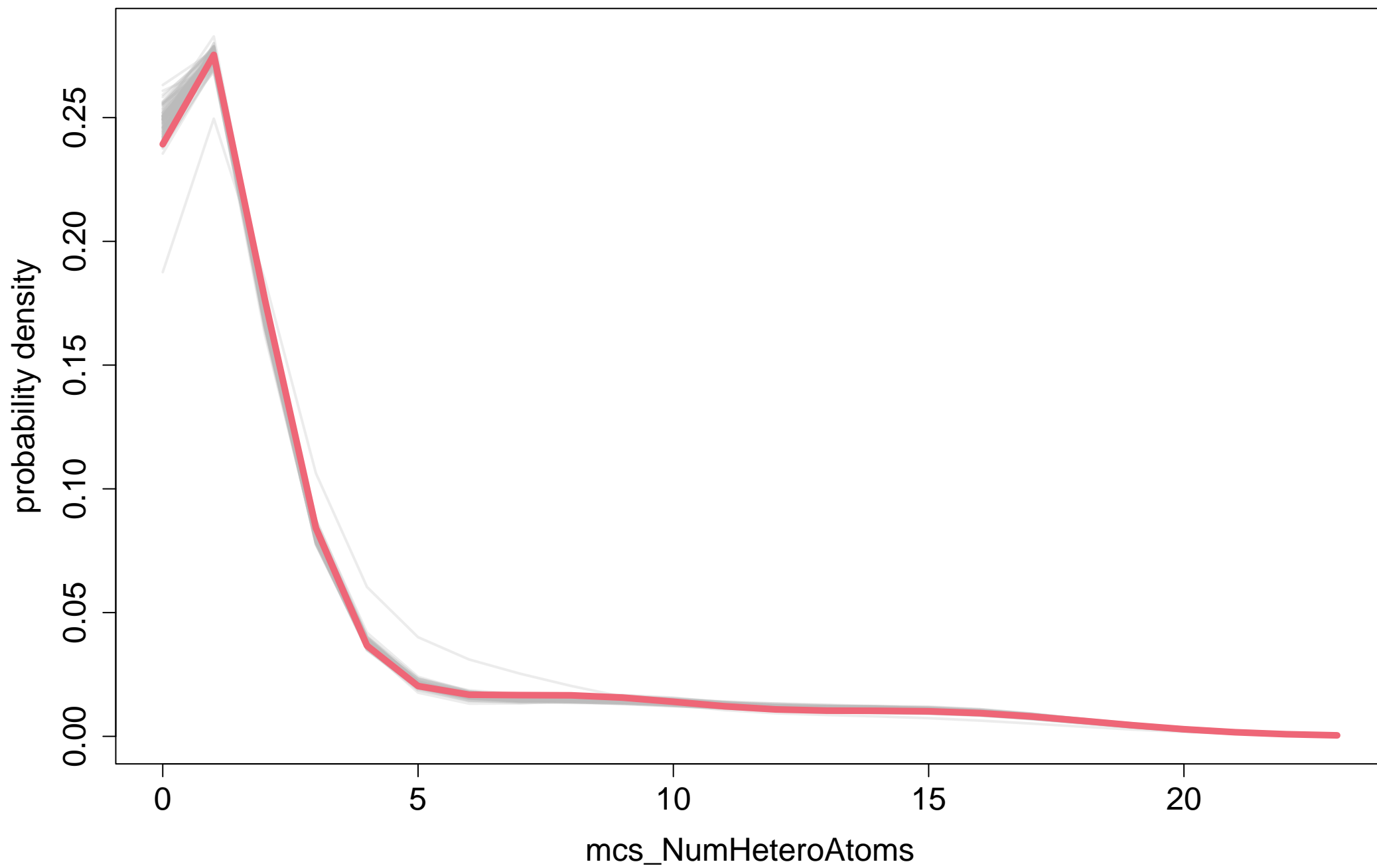
Occupied clusters: 25 of 64

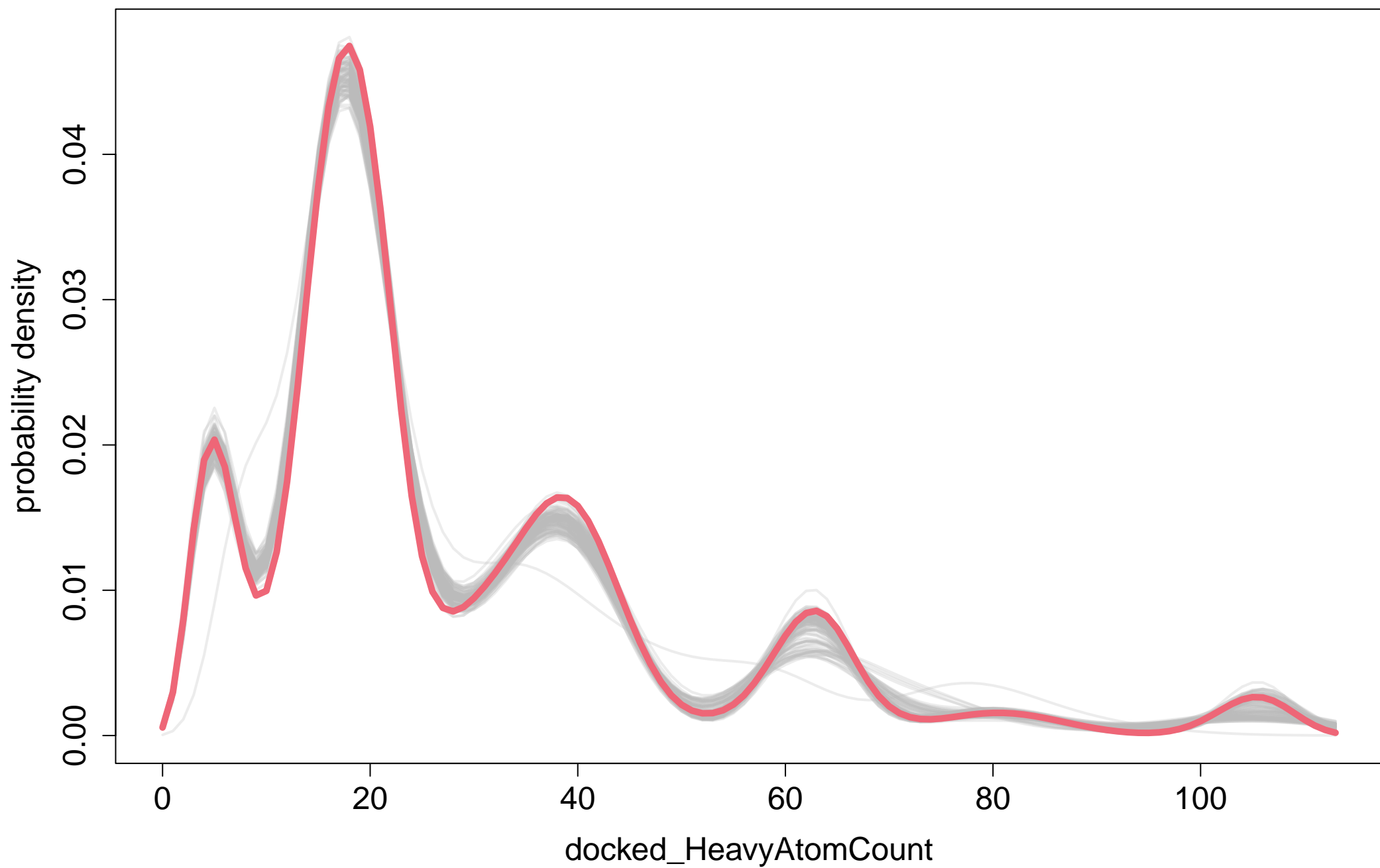
LL: -64300 +- 208

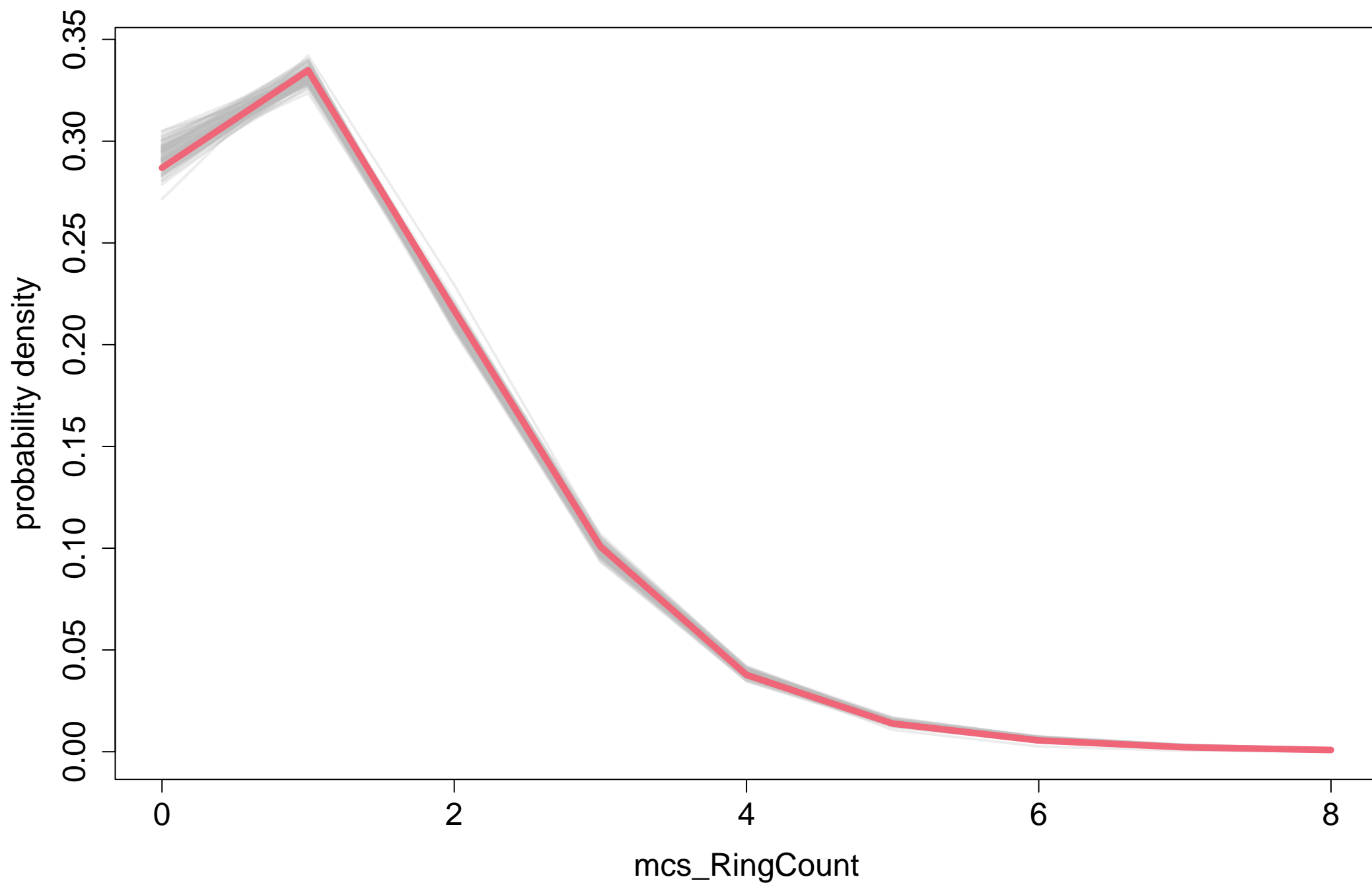


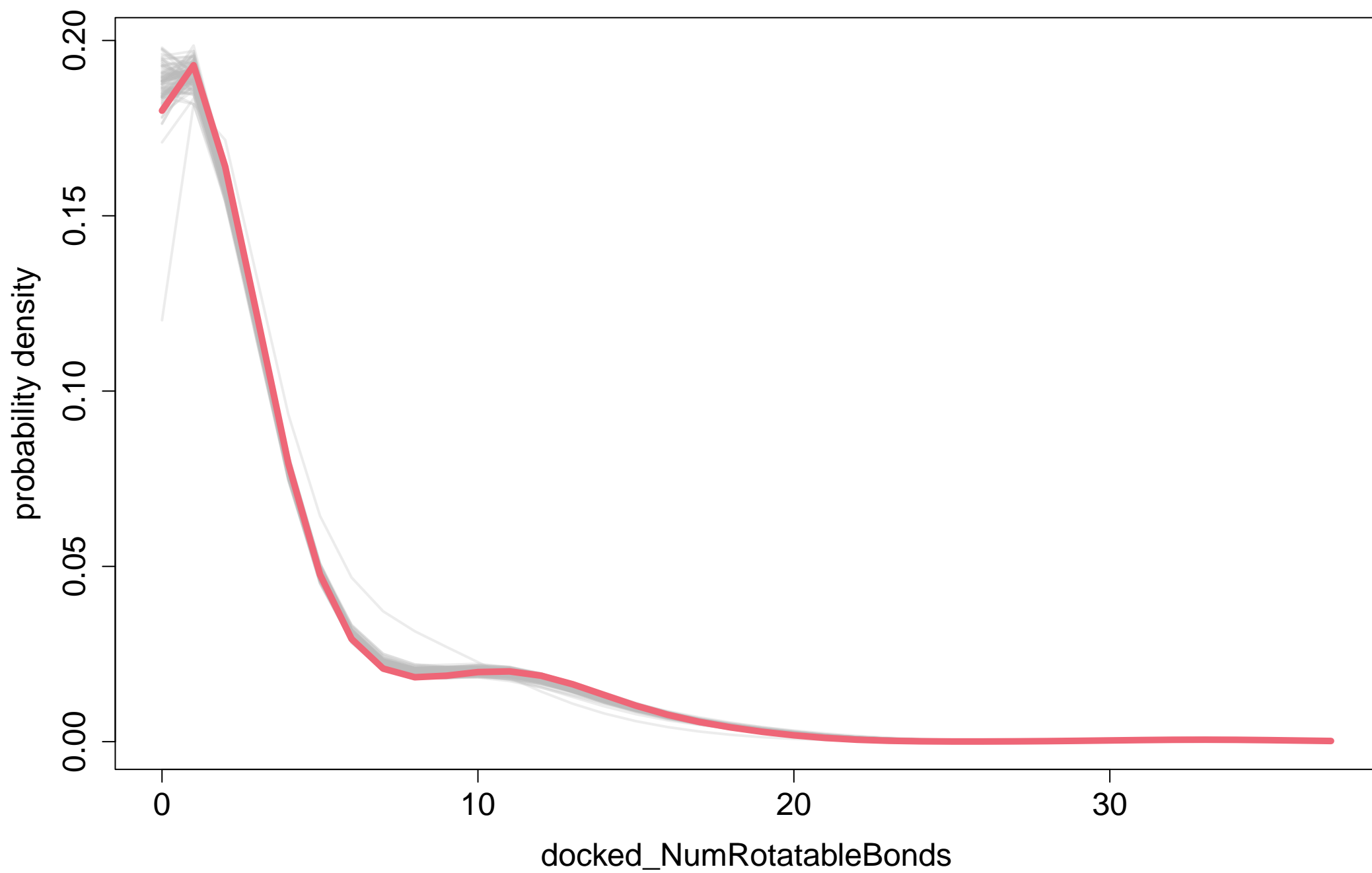


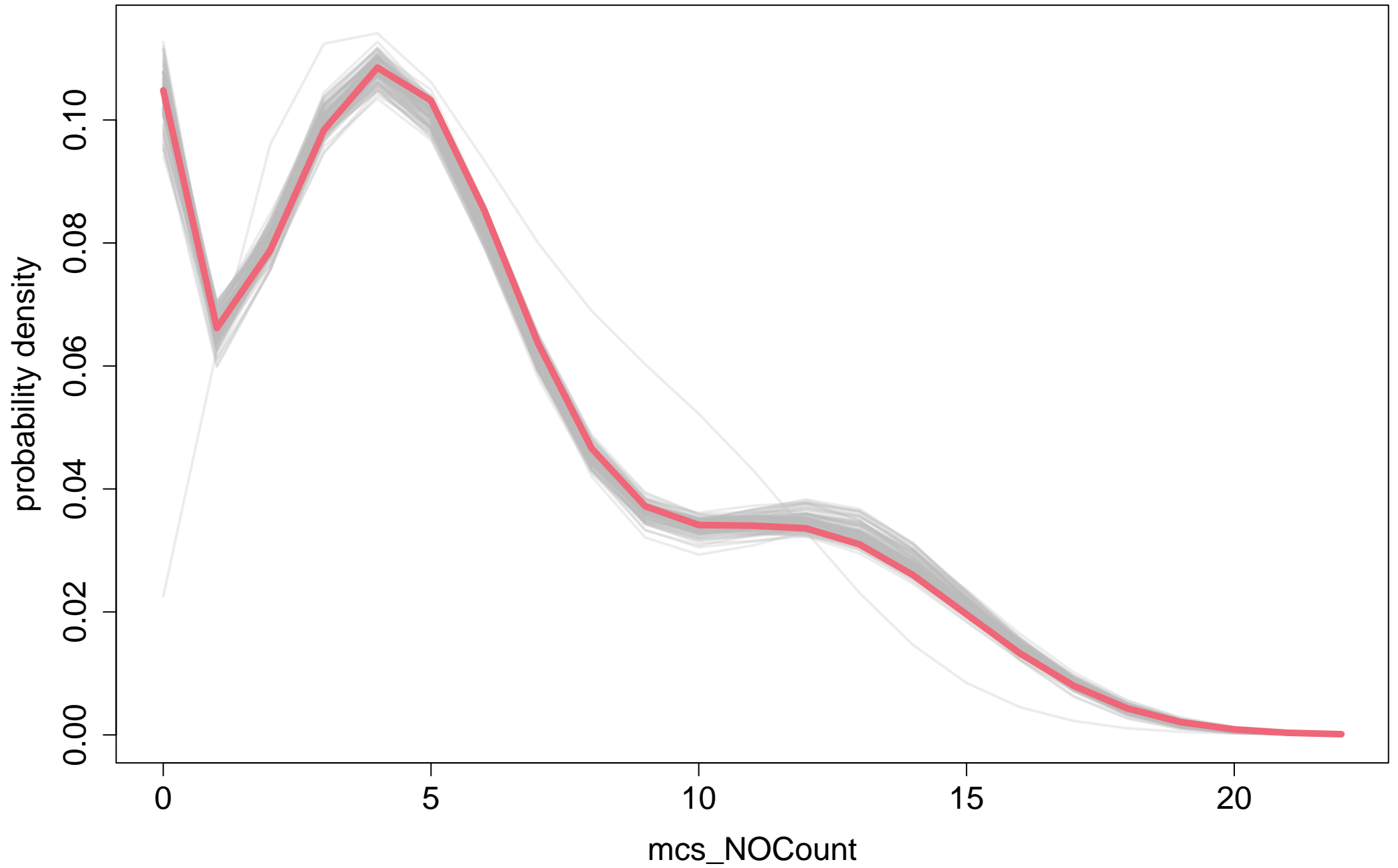


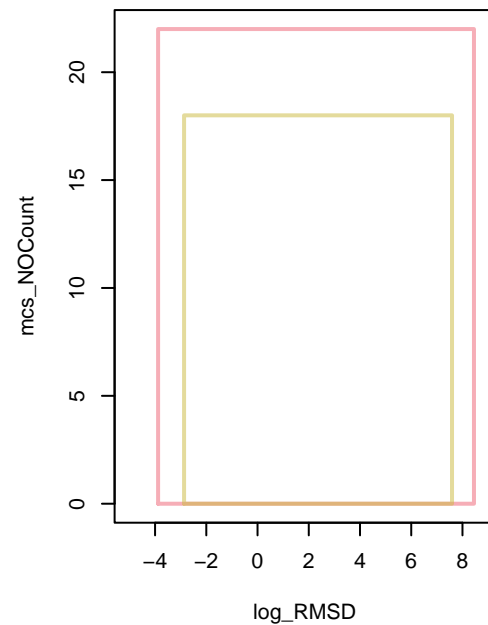
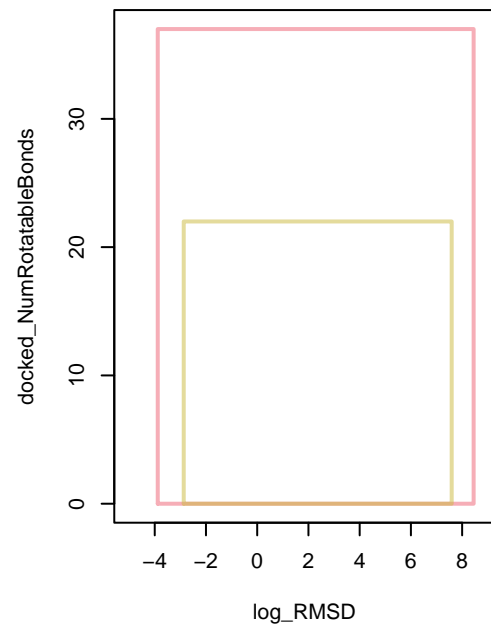
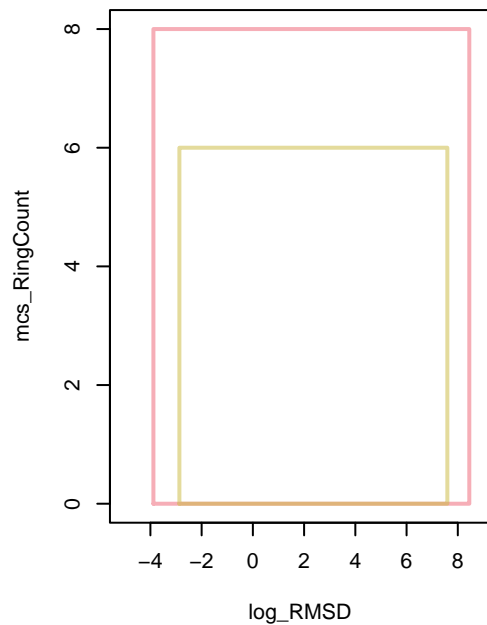
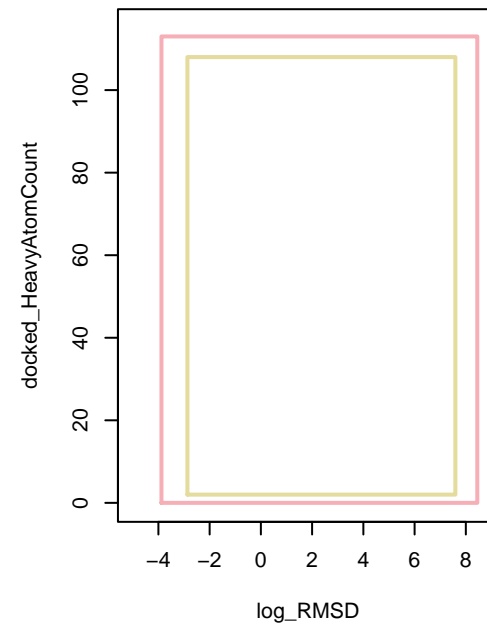
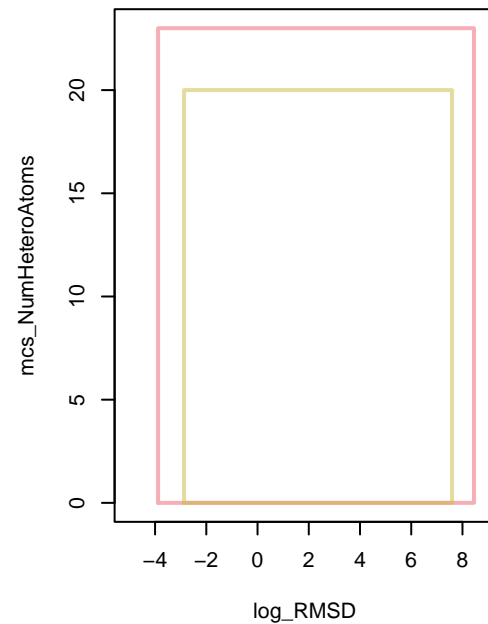
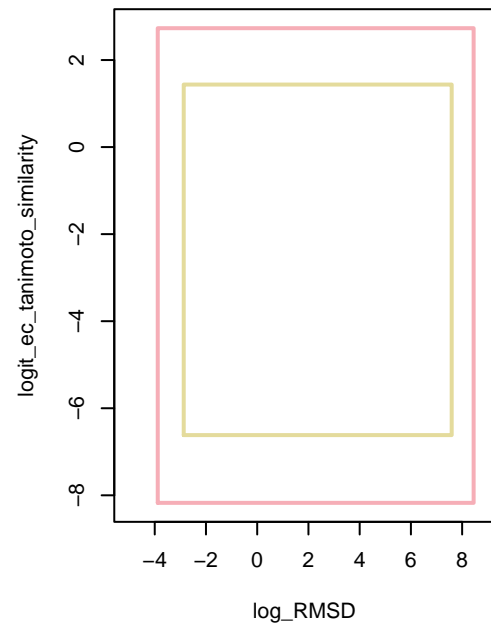
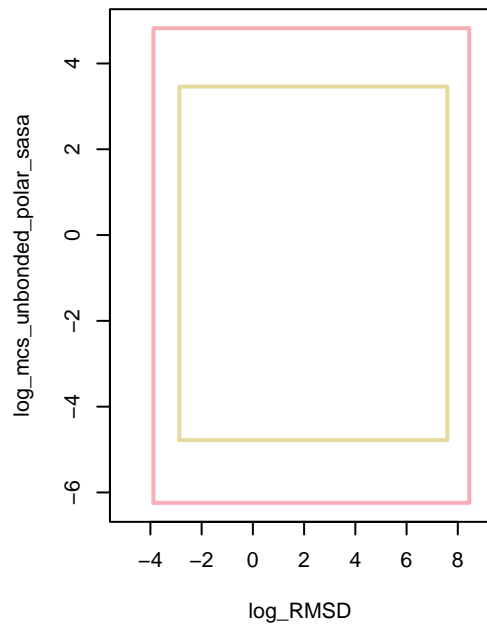




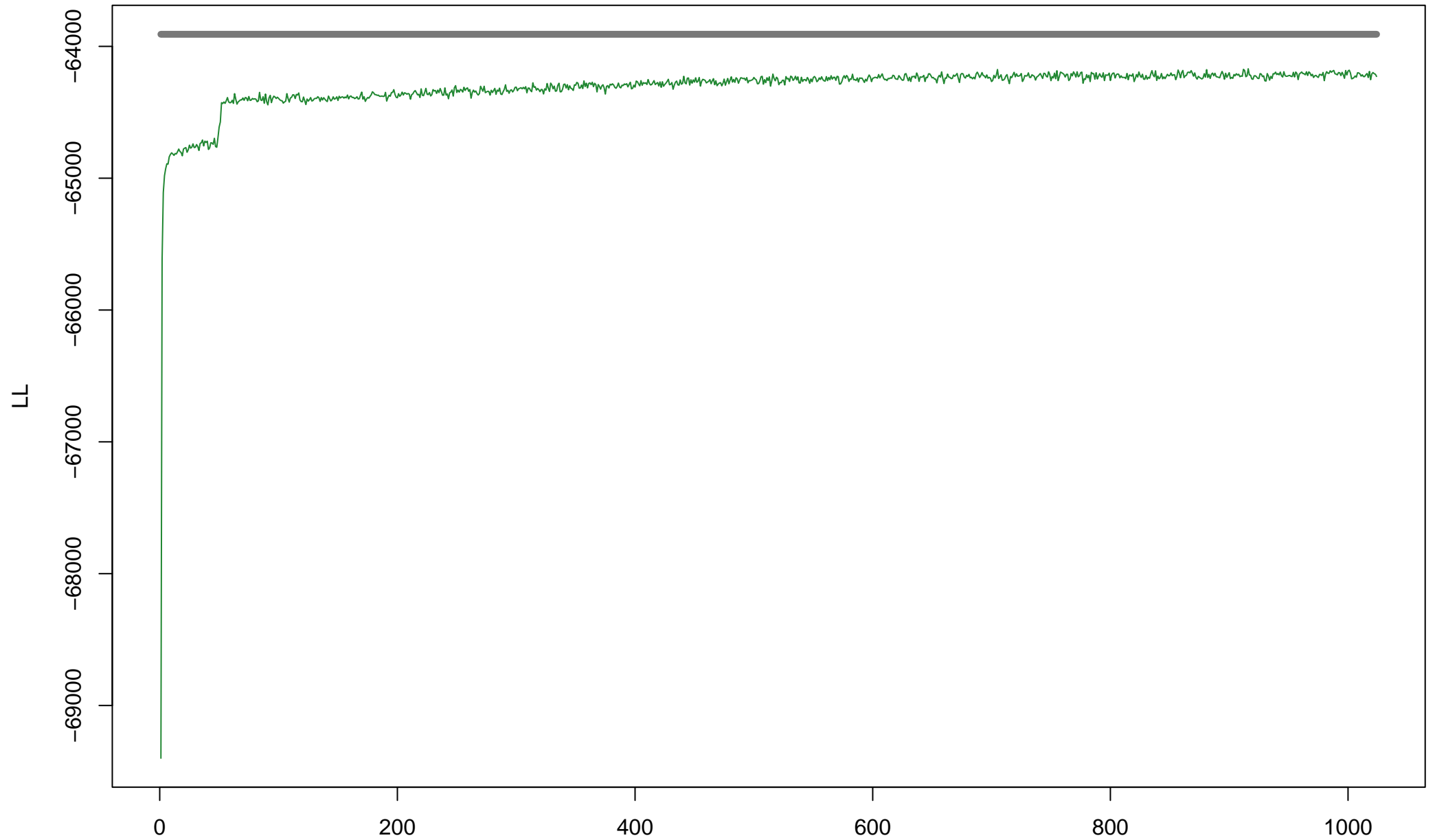






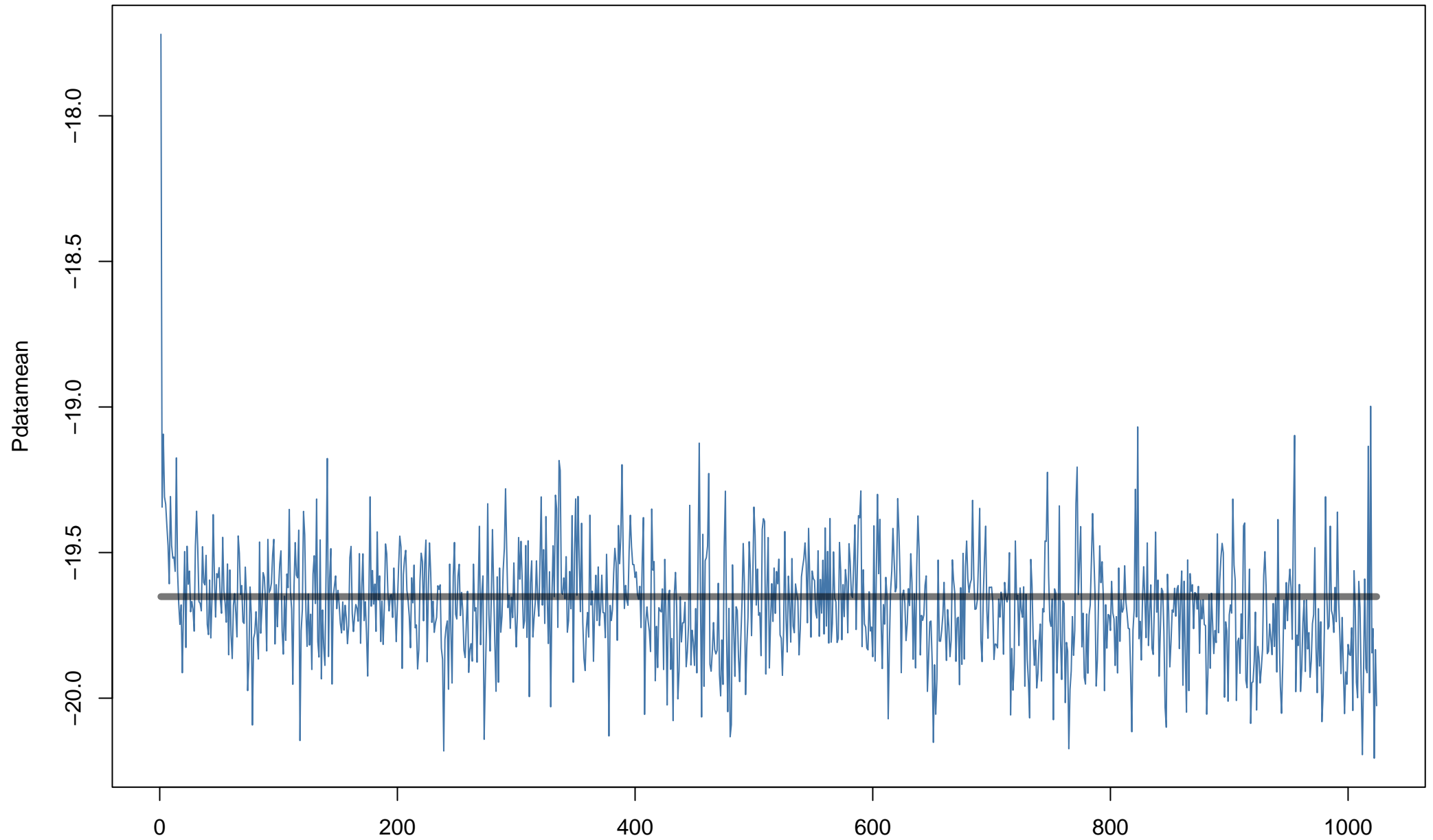


LL



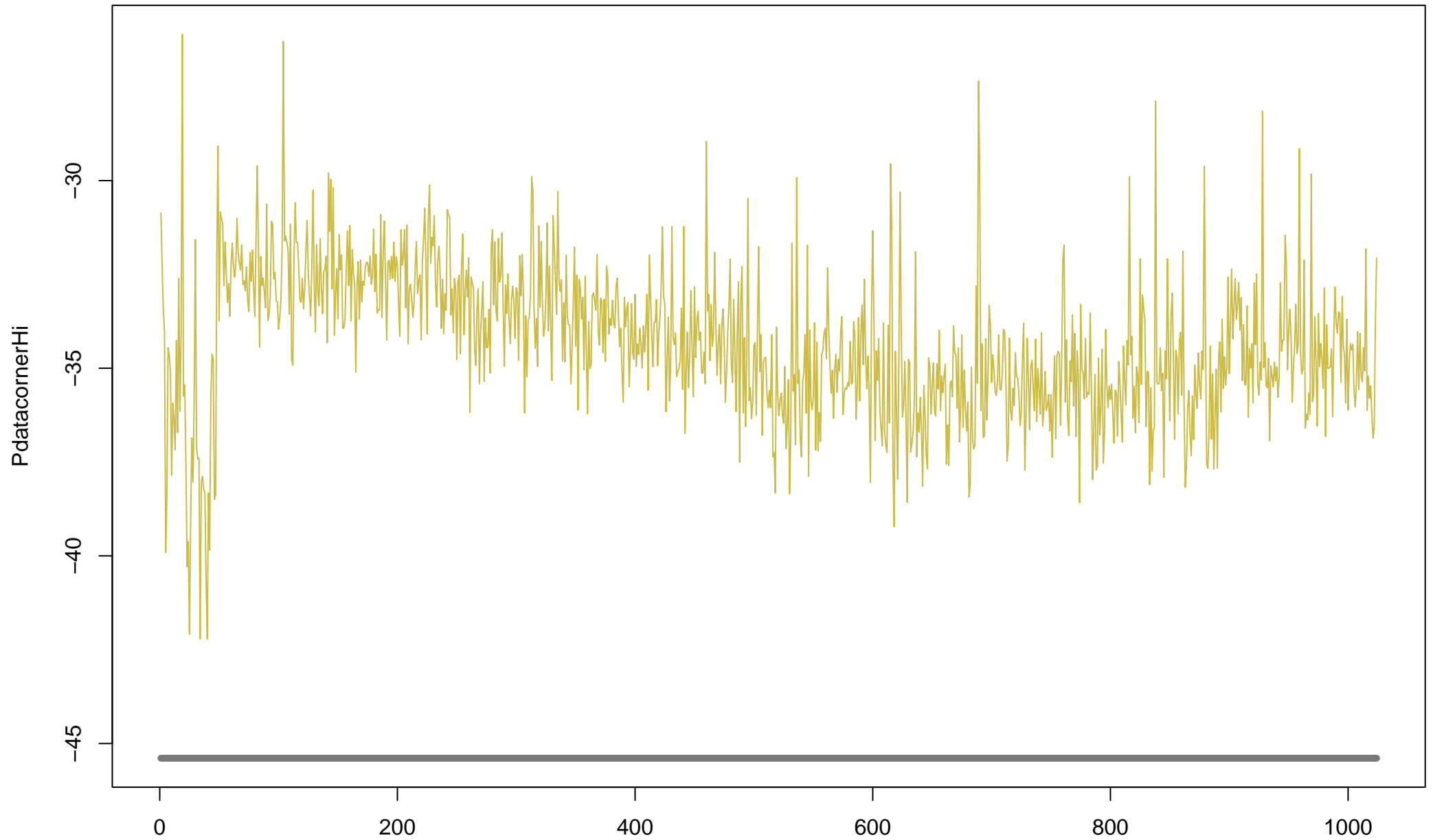
Pdatamean

ESS = 2.22e-16 | BMK = 0.12 | MCSE(6.27) = 5.54 | stat: TRUE | burn: 0 | rel.err: -0.0481



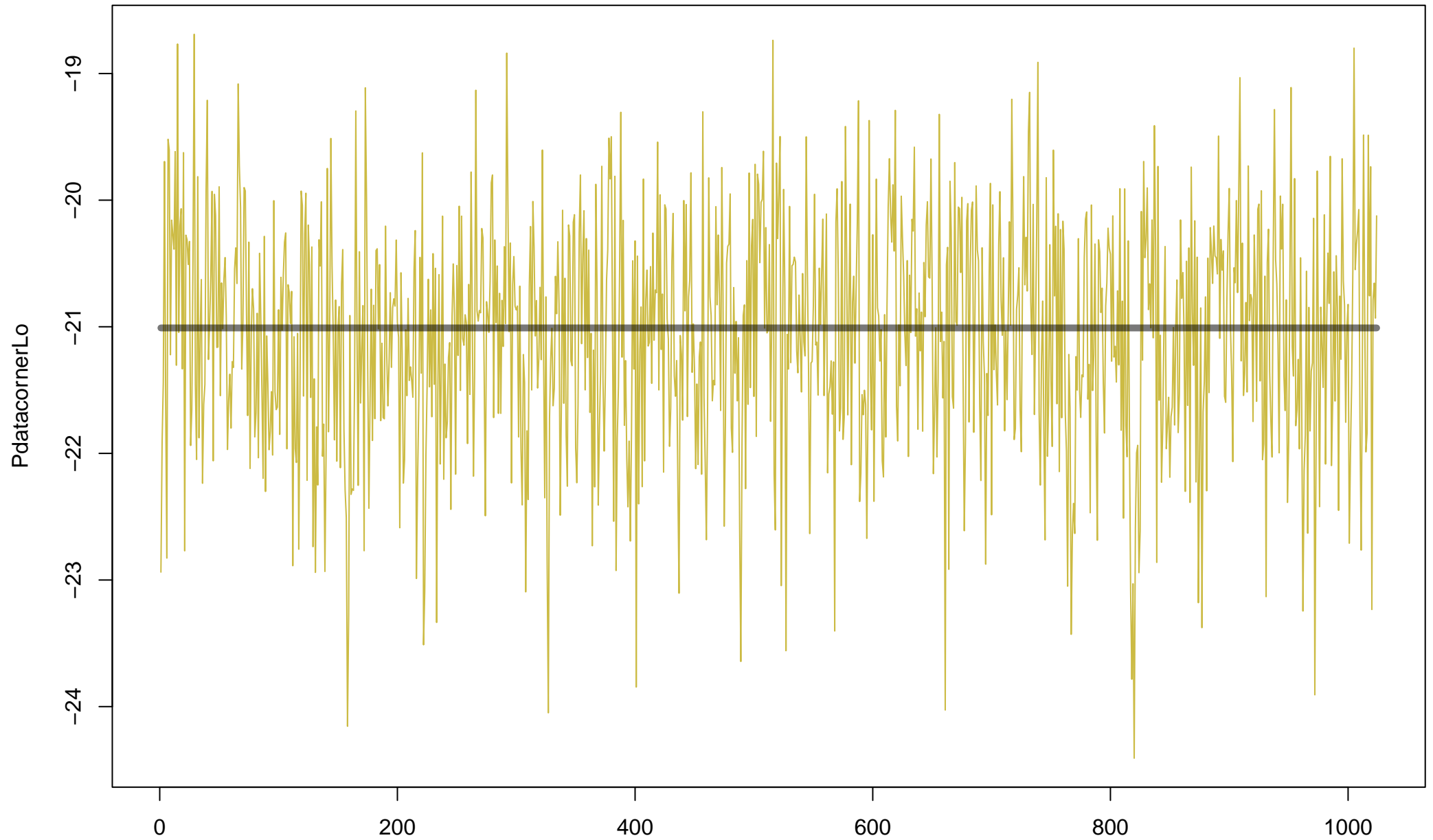
PdatacornerHi

ESS = 2.22e-16 | BMK = 1 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 816 | rel.err: 0.0877



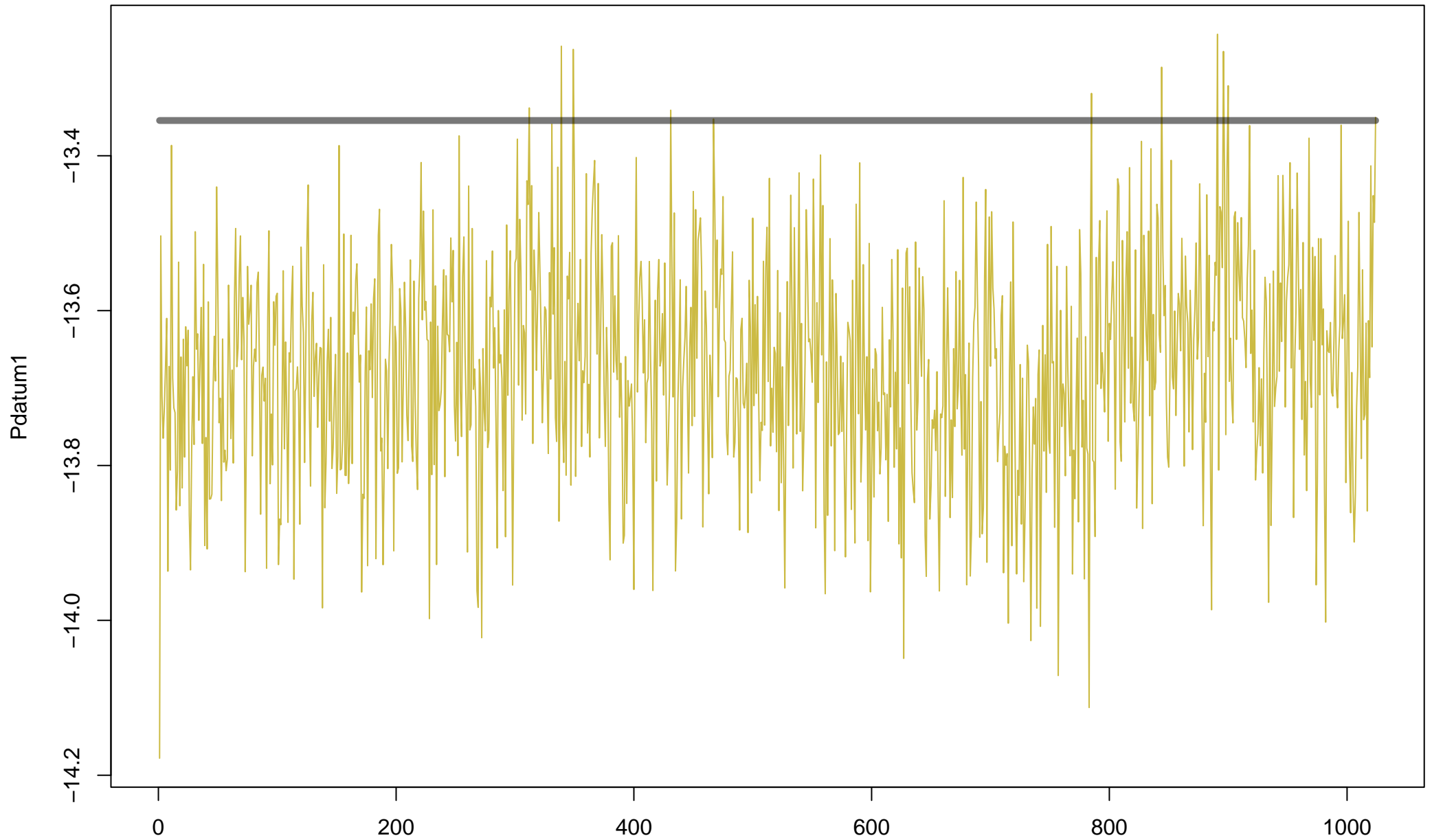
PdatacornerLo

ESS = 2.22e-16 | BMK = 0.0633 | MCSE(6.27) = 3.76 | stat: TRUE | burn: 0 | rel.err: 0.283



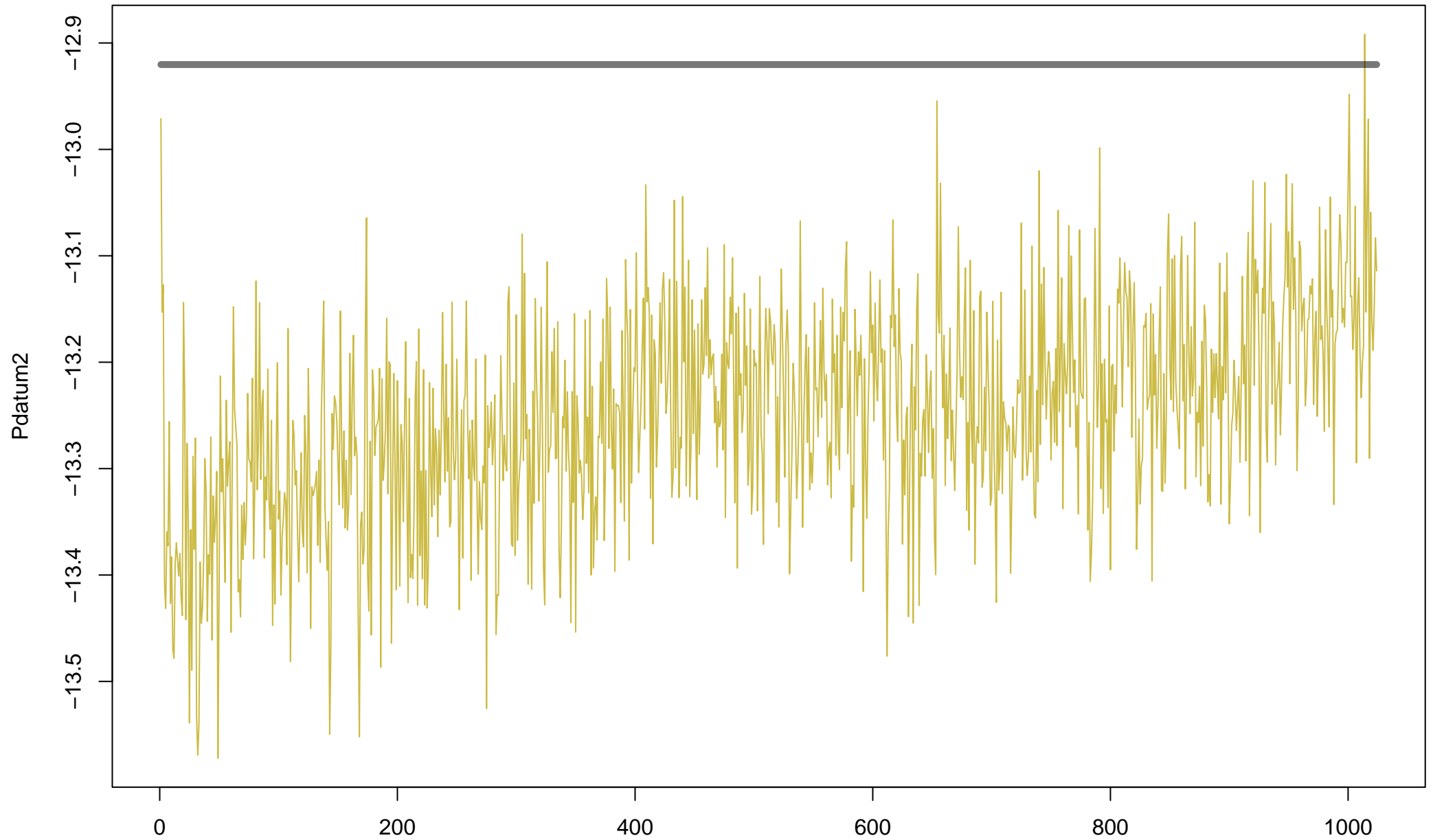
Pdatum1

ESS = 392 | BMK = 0.0516 | MCSE(6.27) = 5.39 | stat: TRUE | burn: 0 | rel.err: -2.6



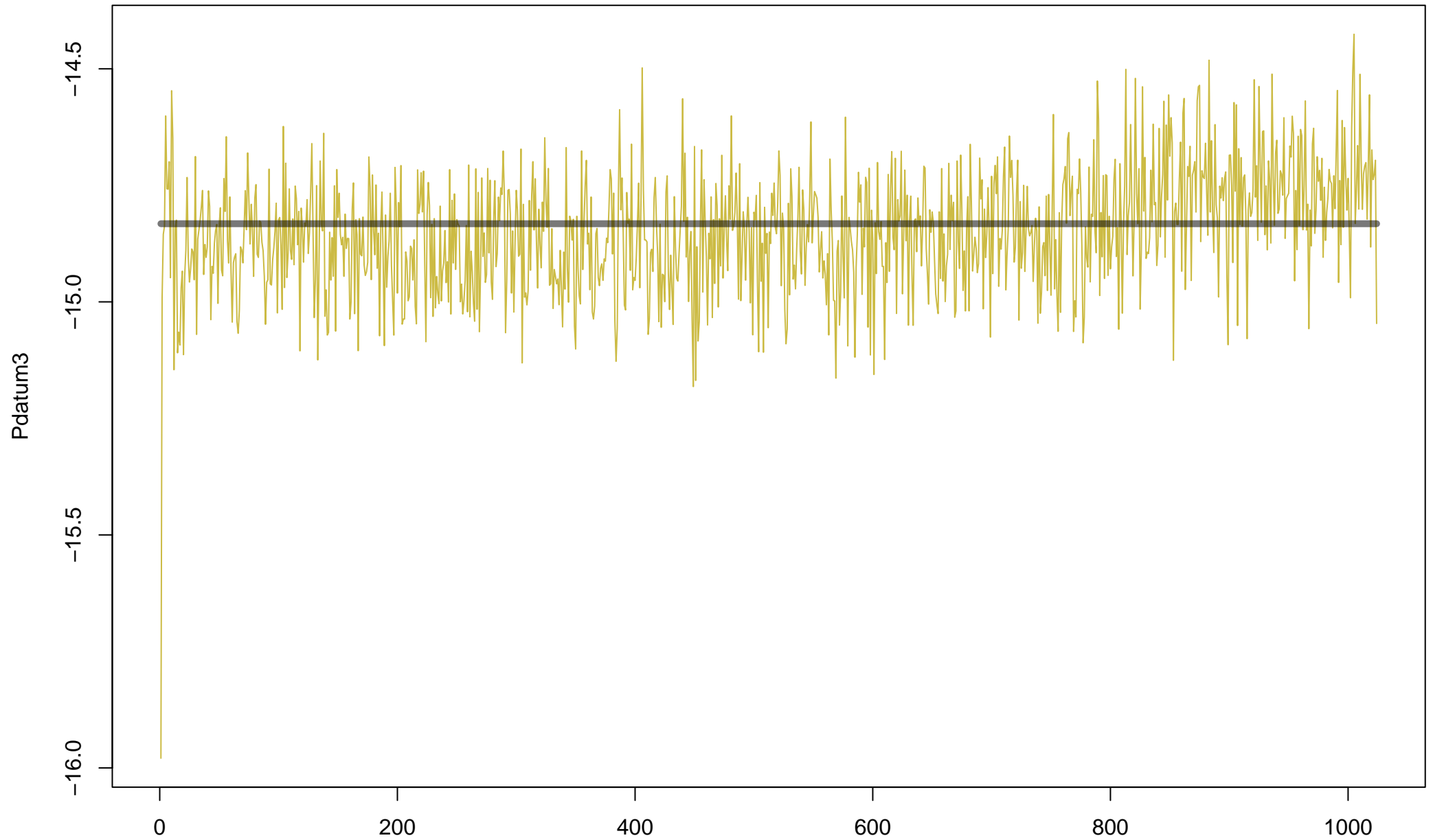
Pdatum2

ESS = 27.7 | BMK = 0.264 | MCSE(6.27) = 9.69 | stat: FALSE | burn: 0 | rel.err: -3.92



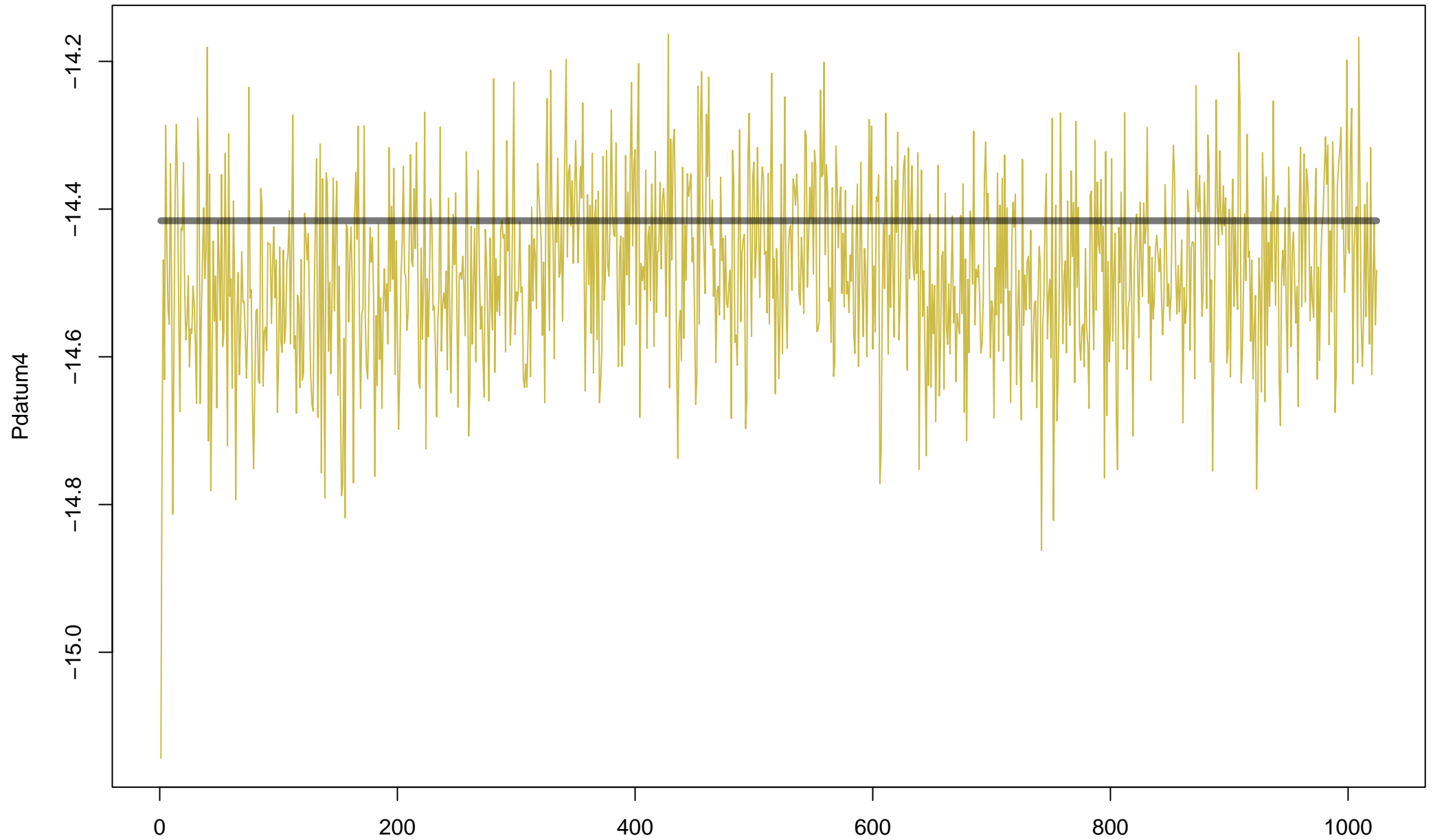
Pdatum3

ESS = 49.3 | BMK = 0.193 | MCSE(6.27) = 7.3 | stat: FALSE | burn: 0 | rel.err: -0.0632



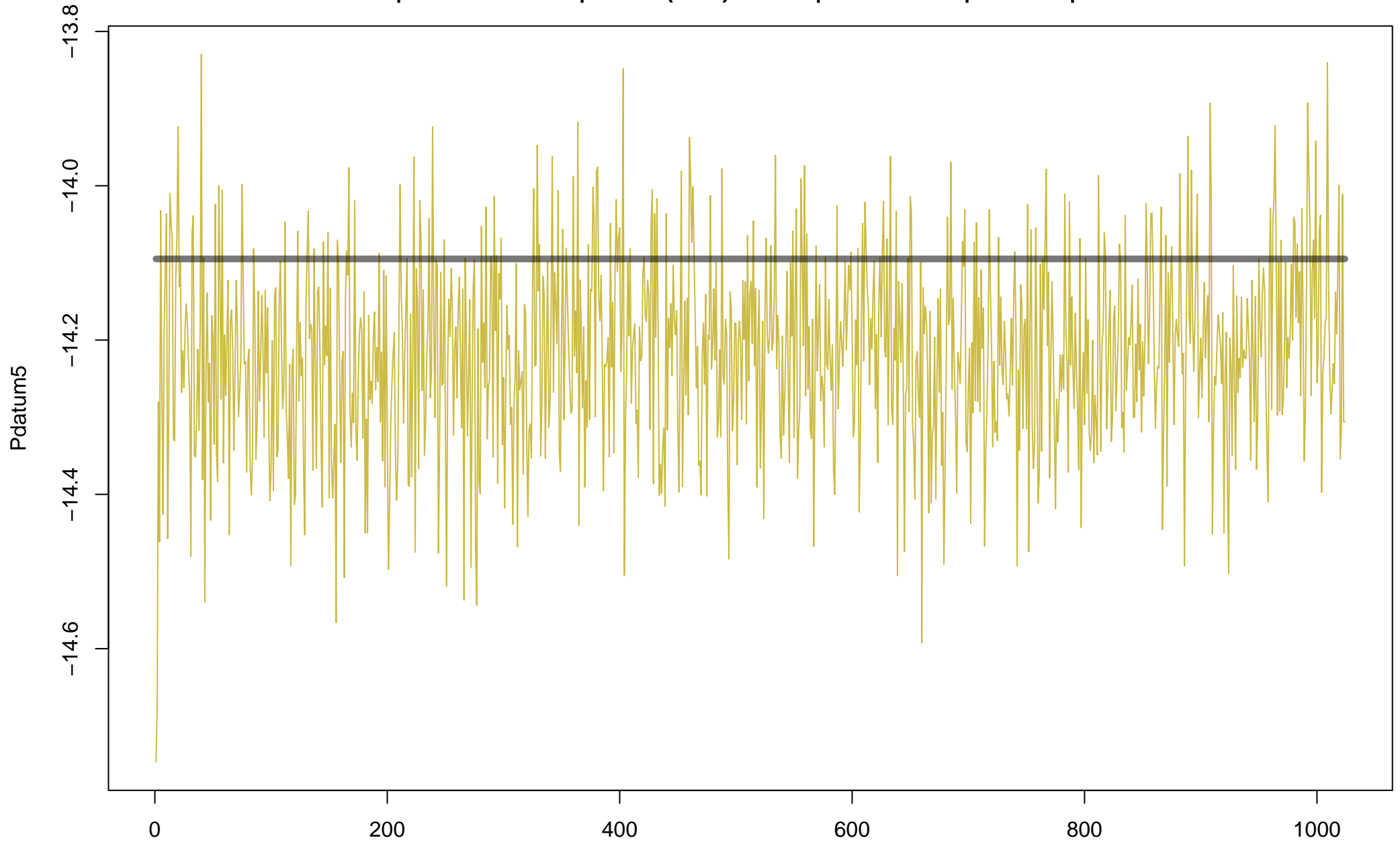
Pdatum4

ESS = 487 | BMK = 0.0535 | MCSE(6.27) = 5.18 | stat: FALSE | burn: 0 | rel.err: -0.537



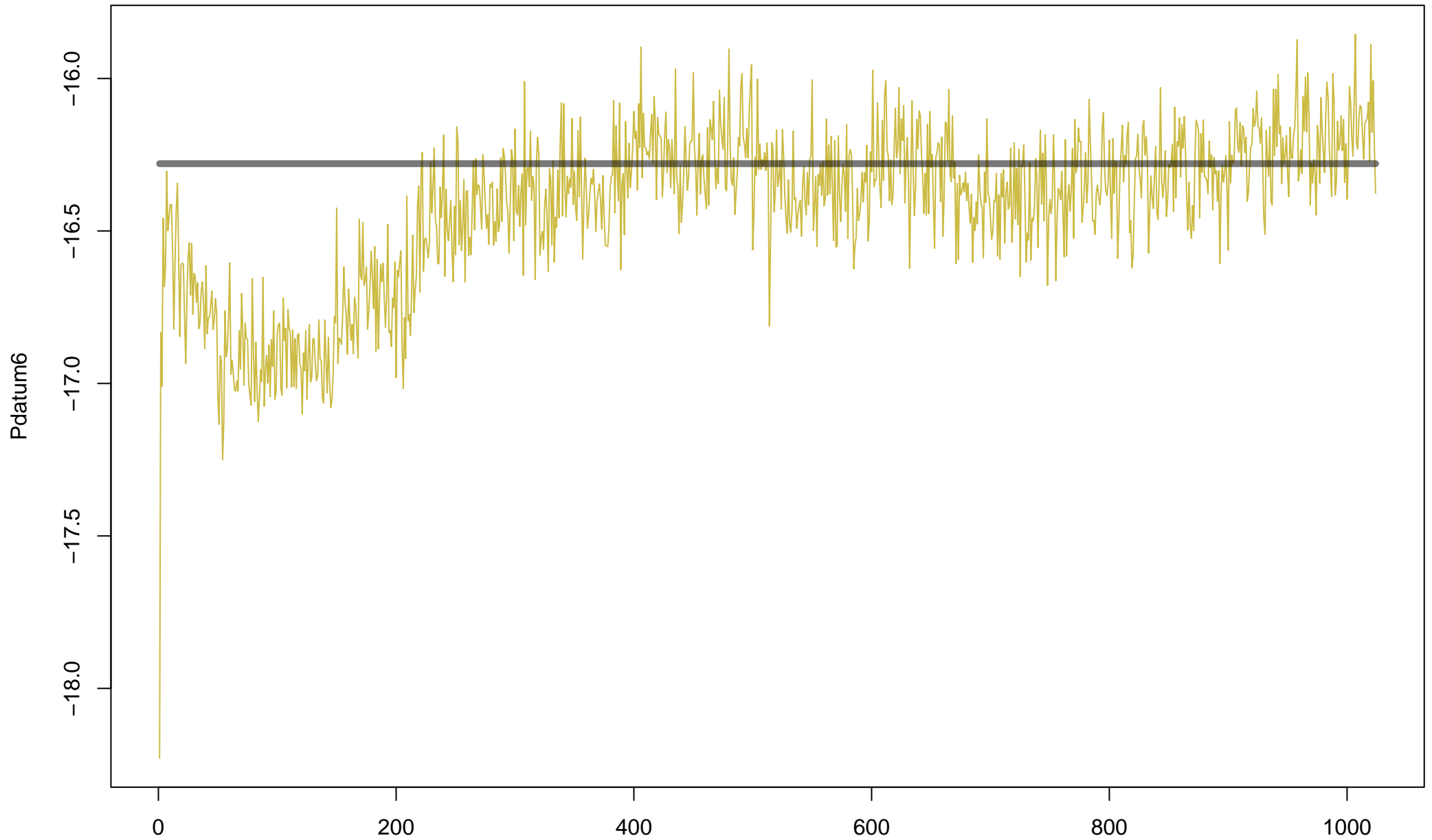
Pdatum5

ESS = 1020 | BMK = 0.0808 | MCSE(6.27) = 3.82 | stat: TRUE | burn: 0 | rel.err: -0.991



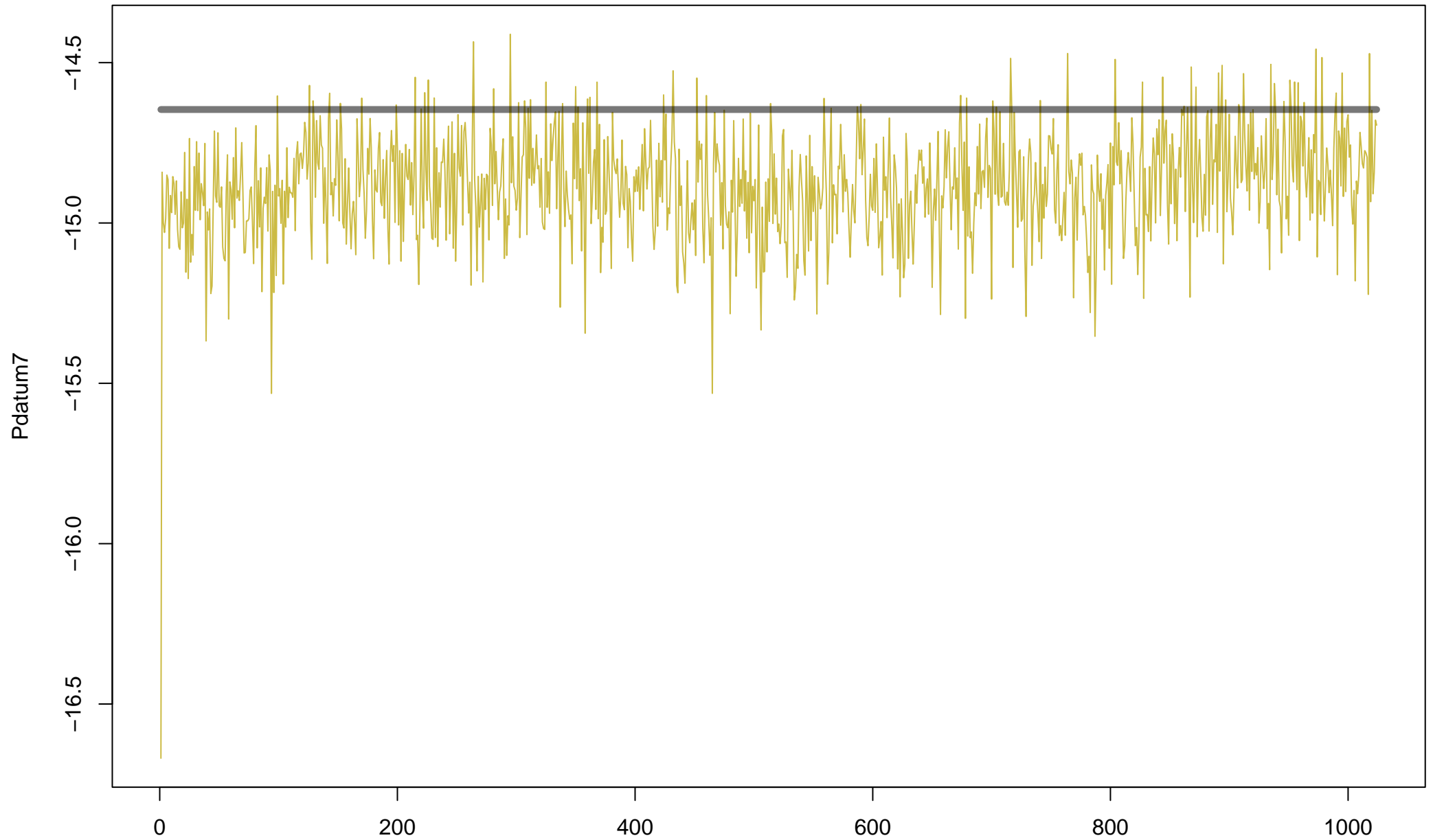
Pdatum6

ESS = 2.22e-16 | BMK = 0.414 | MCSE(6.27) = 14.7 | stat: FALSE | burn: 204 | rel.err: -0.515



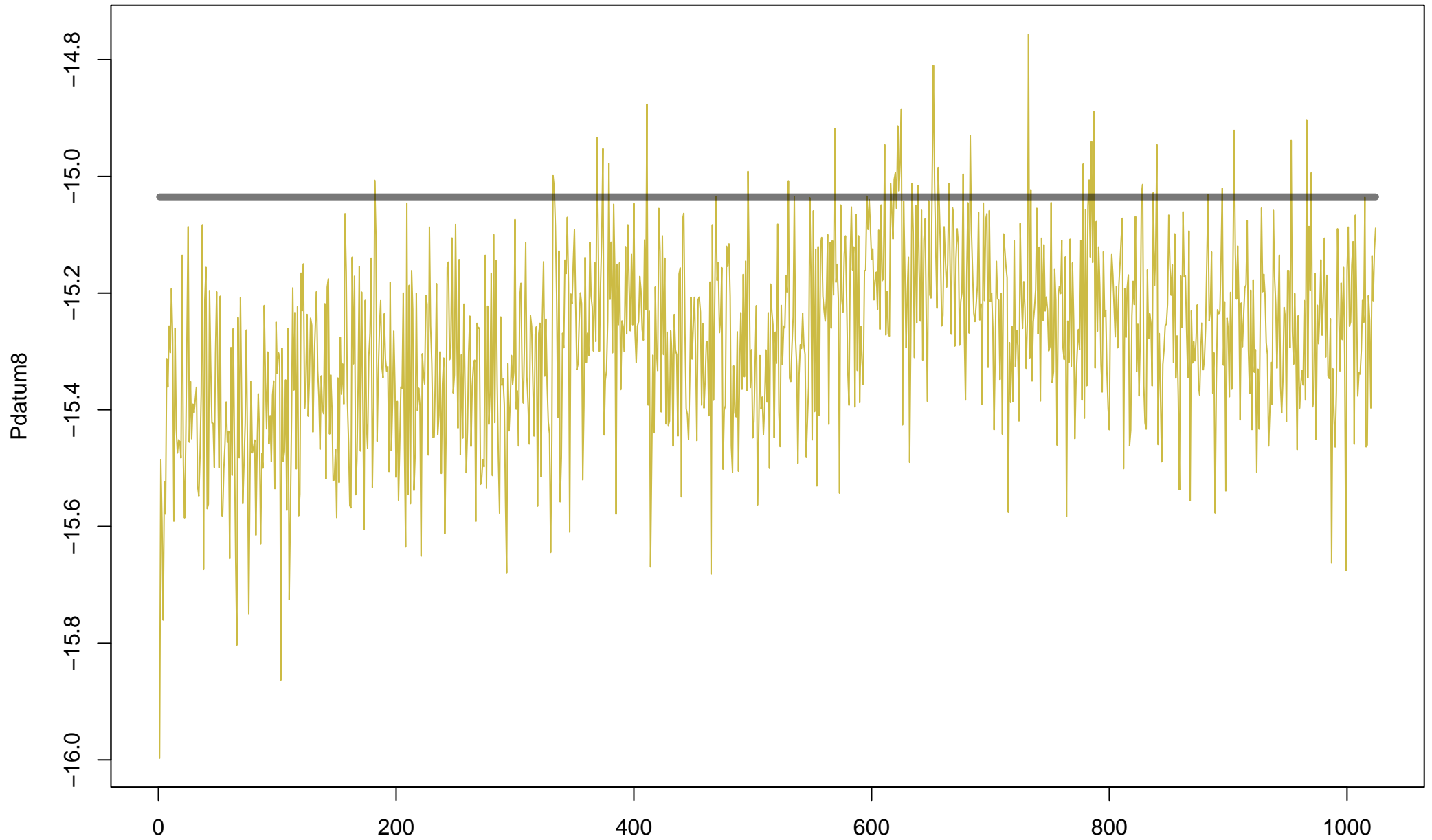
Pdatum7

ESS = 226 | BMK = 0.0847 | MCSE(6.27) = 5.43 | stat: FALSE | burn: 0 | rel.err: -1.57

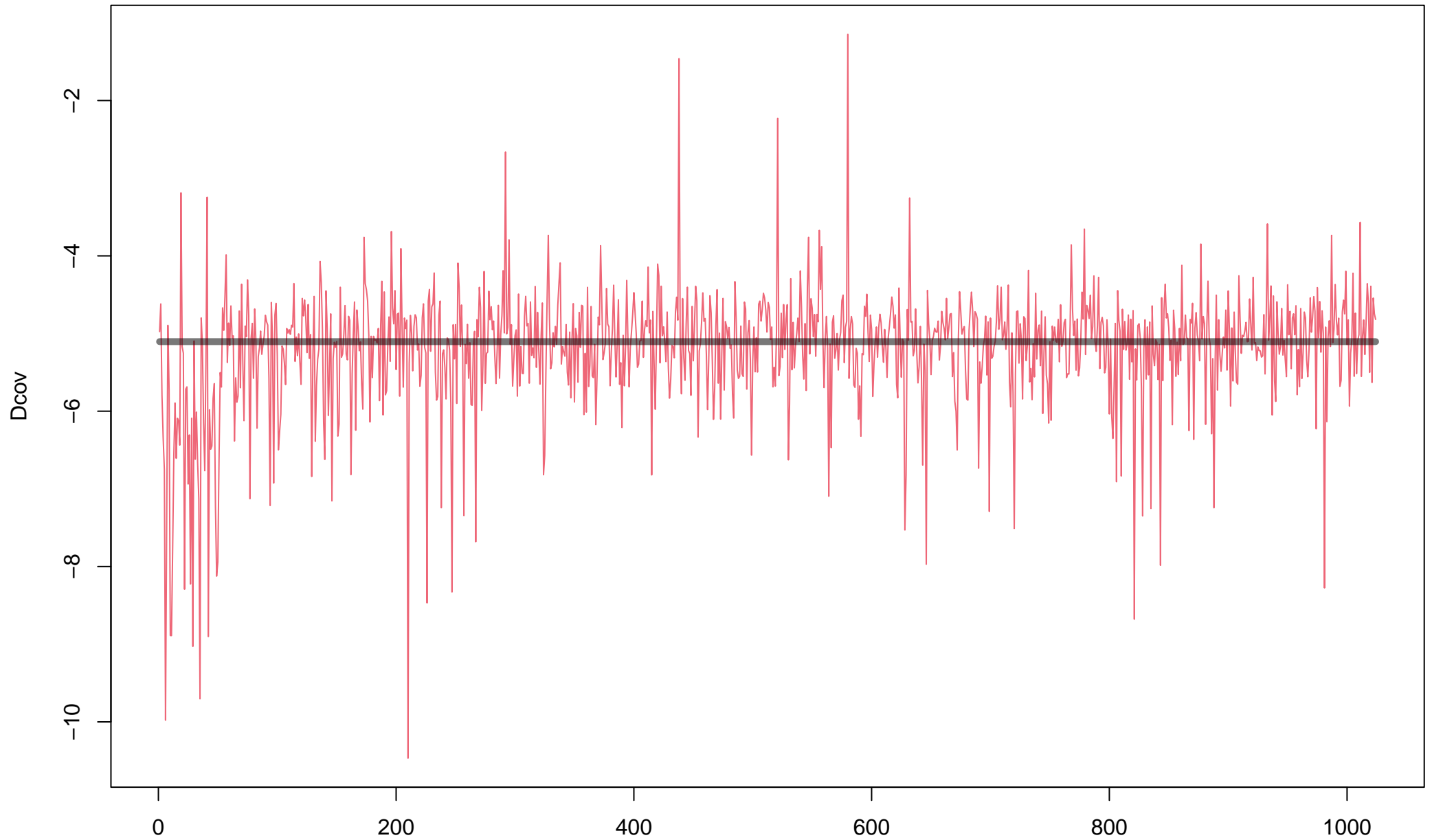


Pdatum8

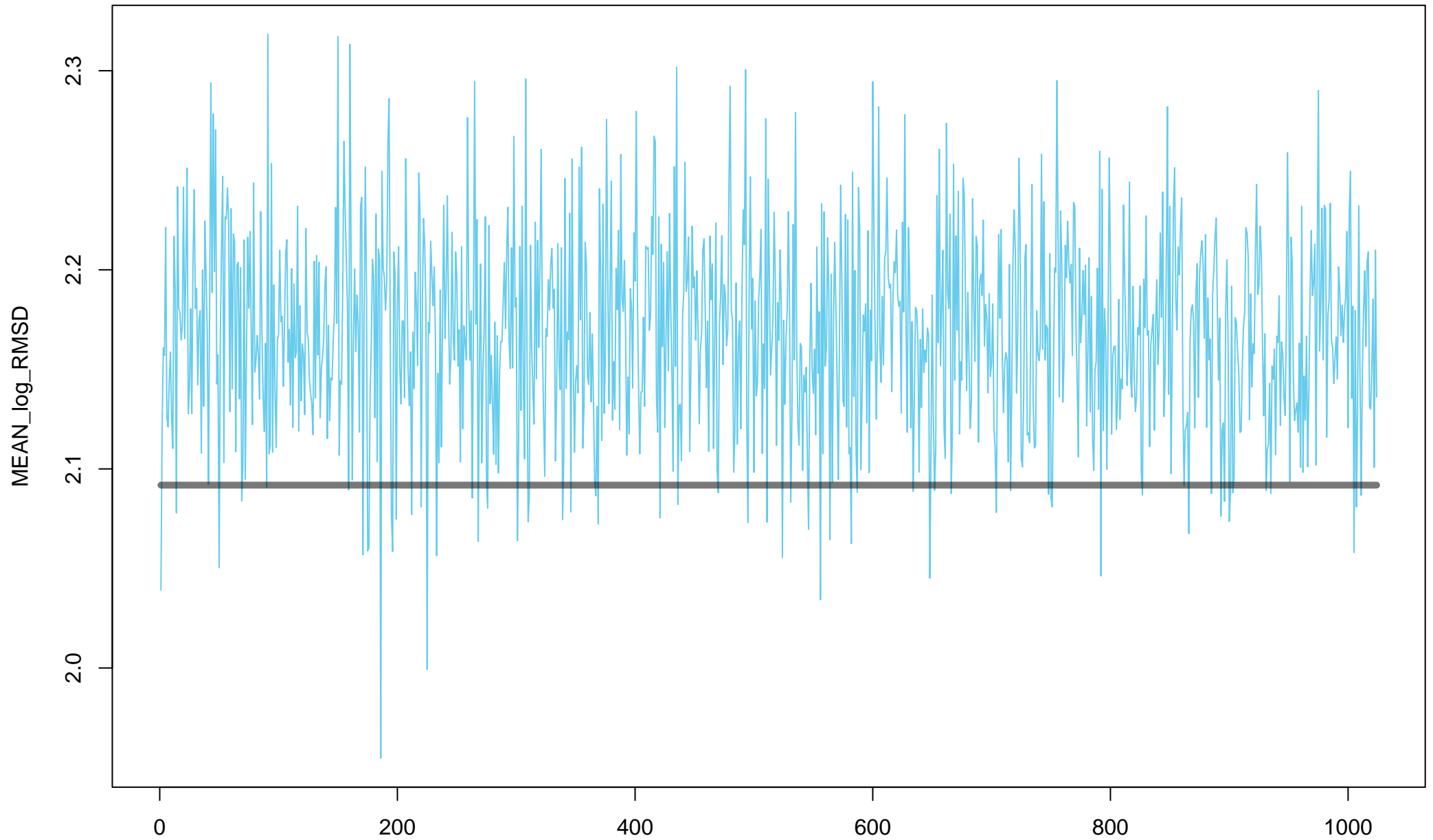
ESS = 46.7 | BMK = 0.26 | MCSE(6.27) = 8.83 | stat: FALSE | burn: 0 | rel.err: -1.72



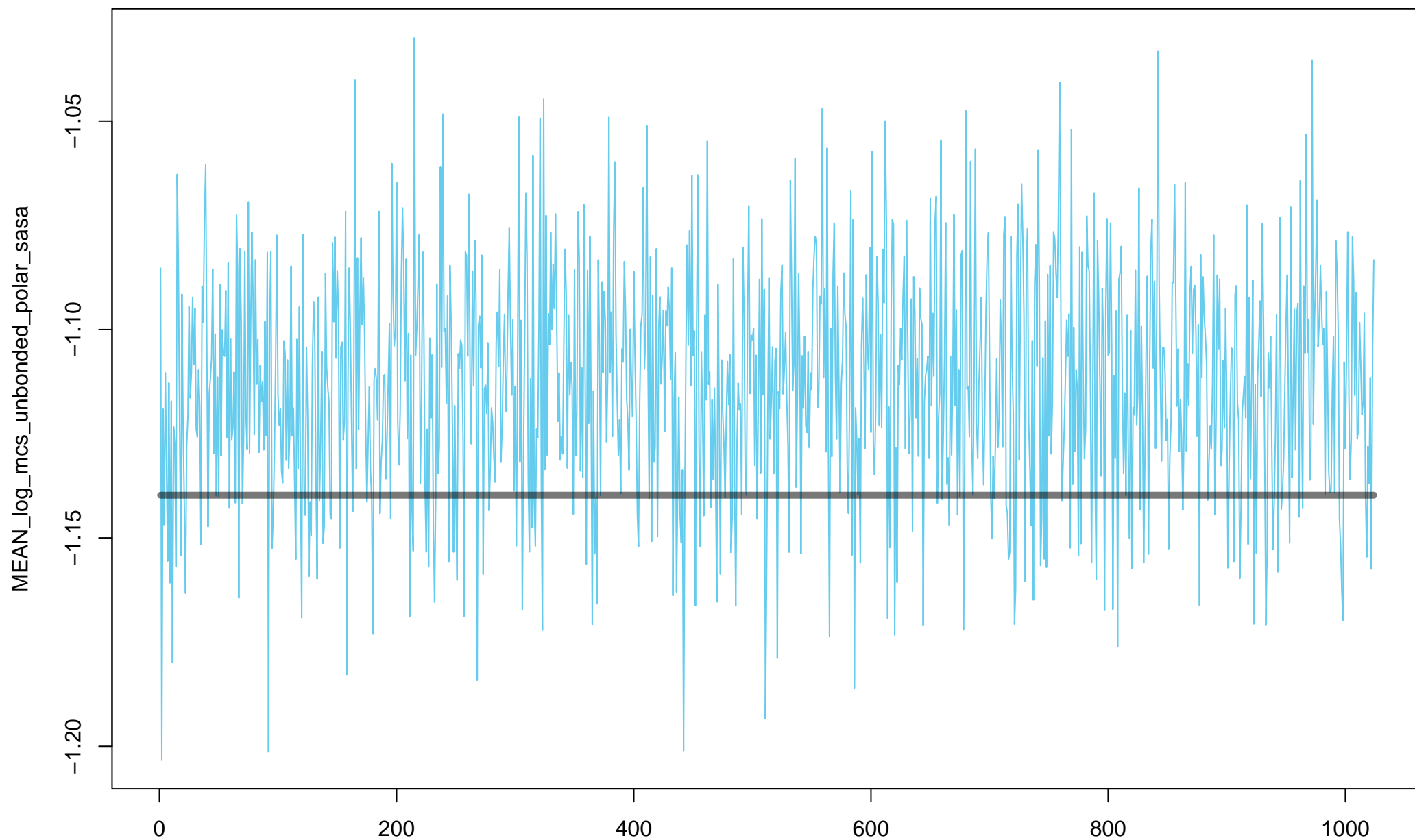
Dcov
ESS = 1020 | BMK = 0.138 | MCSE(6.27) = 3.64 | stat: FALSE | burn: 0 | rel.err: -0.00224



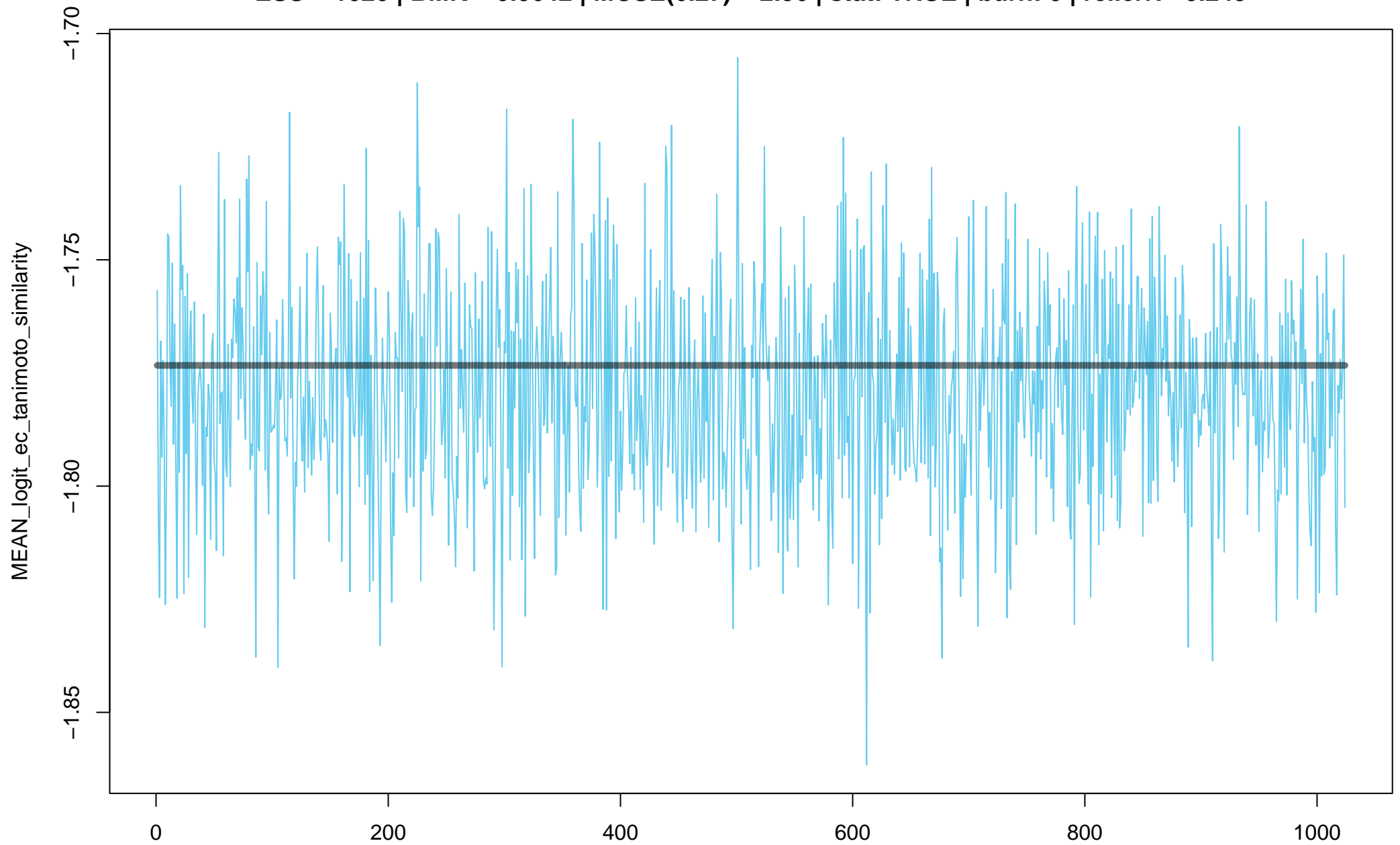
MEAN_log_RMSD
ESS = 1020 | BMK = 0.0654 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0 | rel.err: 1.55



MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0519 | MCSE(6.27) = 3.28 | stat: TRUE | burn: 0 | rel.err: 0.976

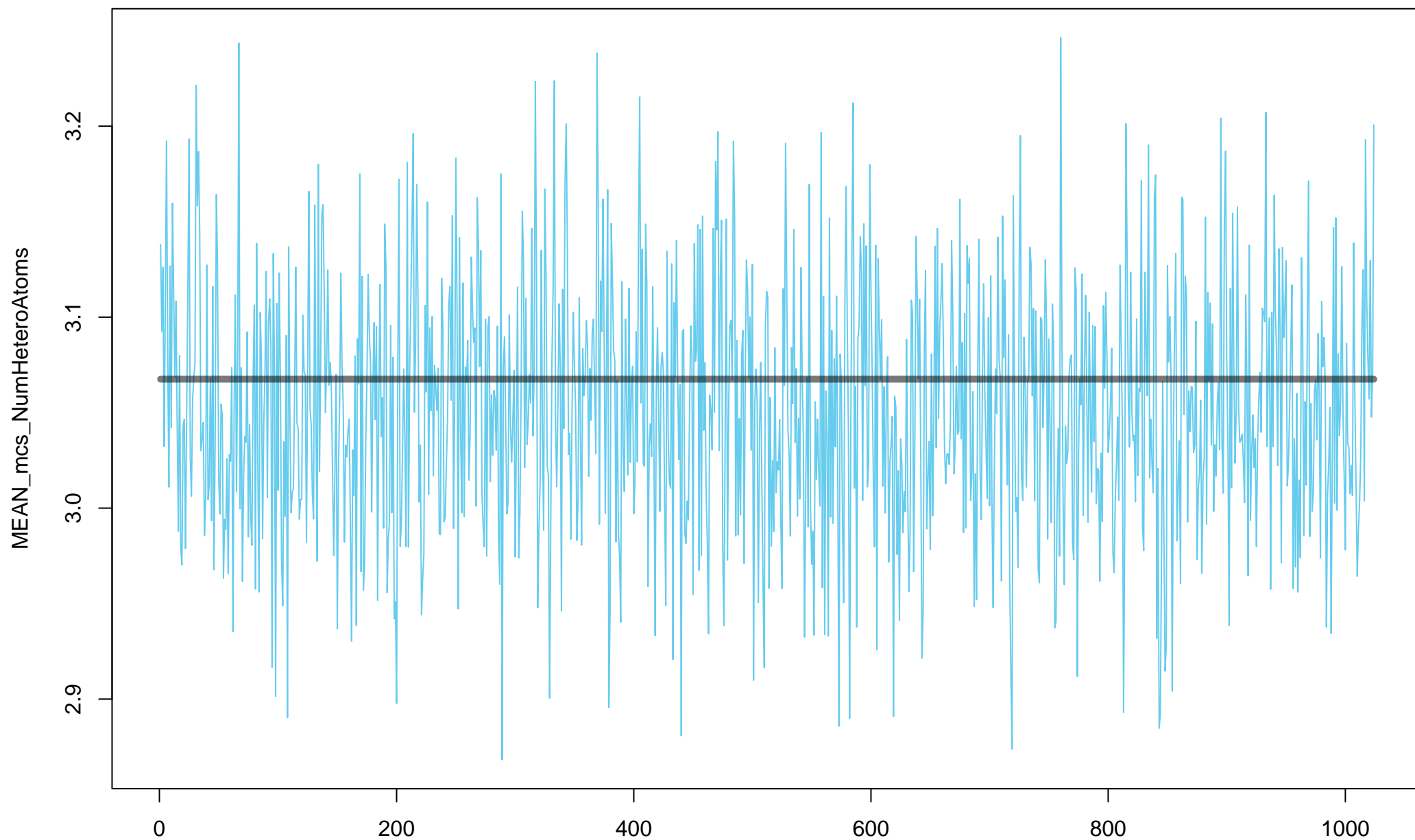


MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0642 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0 | rel.err: -0.245



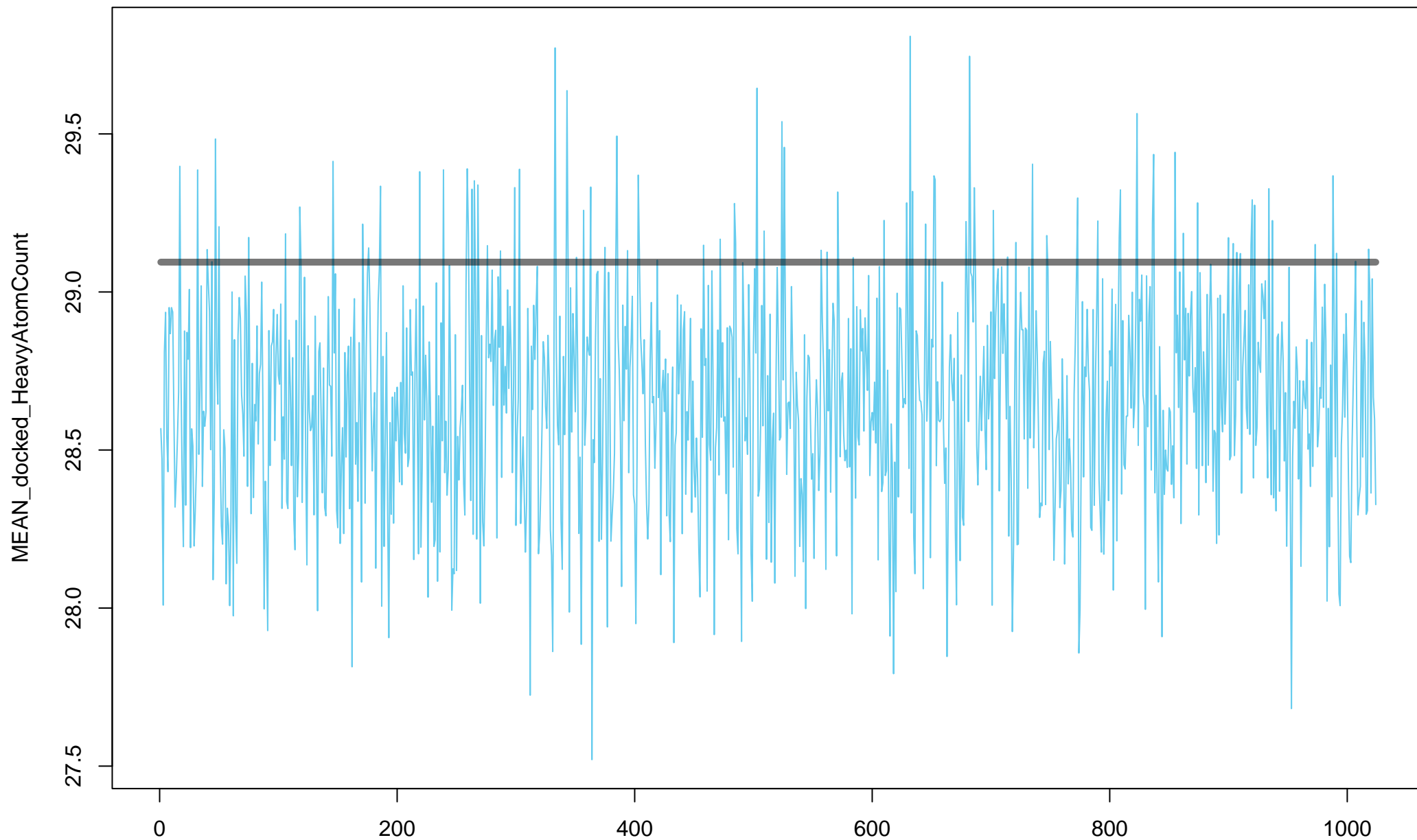
MEAN_mcs_NumHeteroAtoms

ESS = 1020 | BMK = 0.0504 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0 | rel.err: -0.238

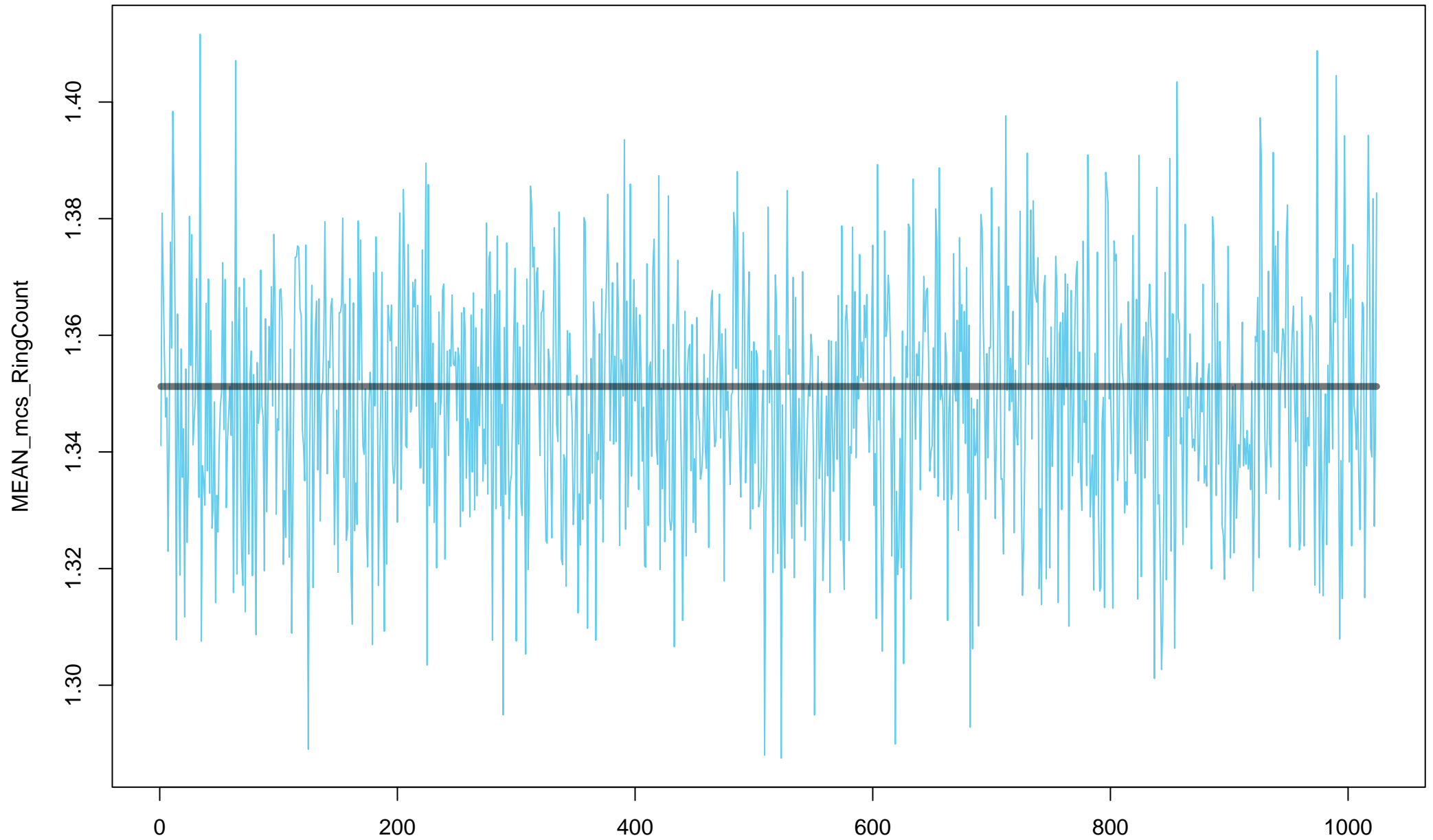


MEAN_docked_HeavyAtomCount

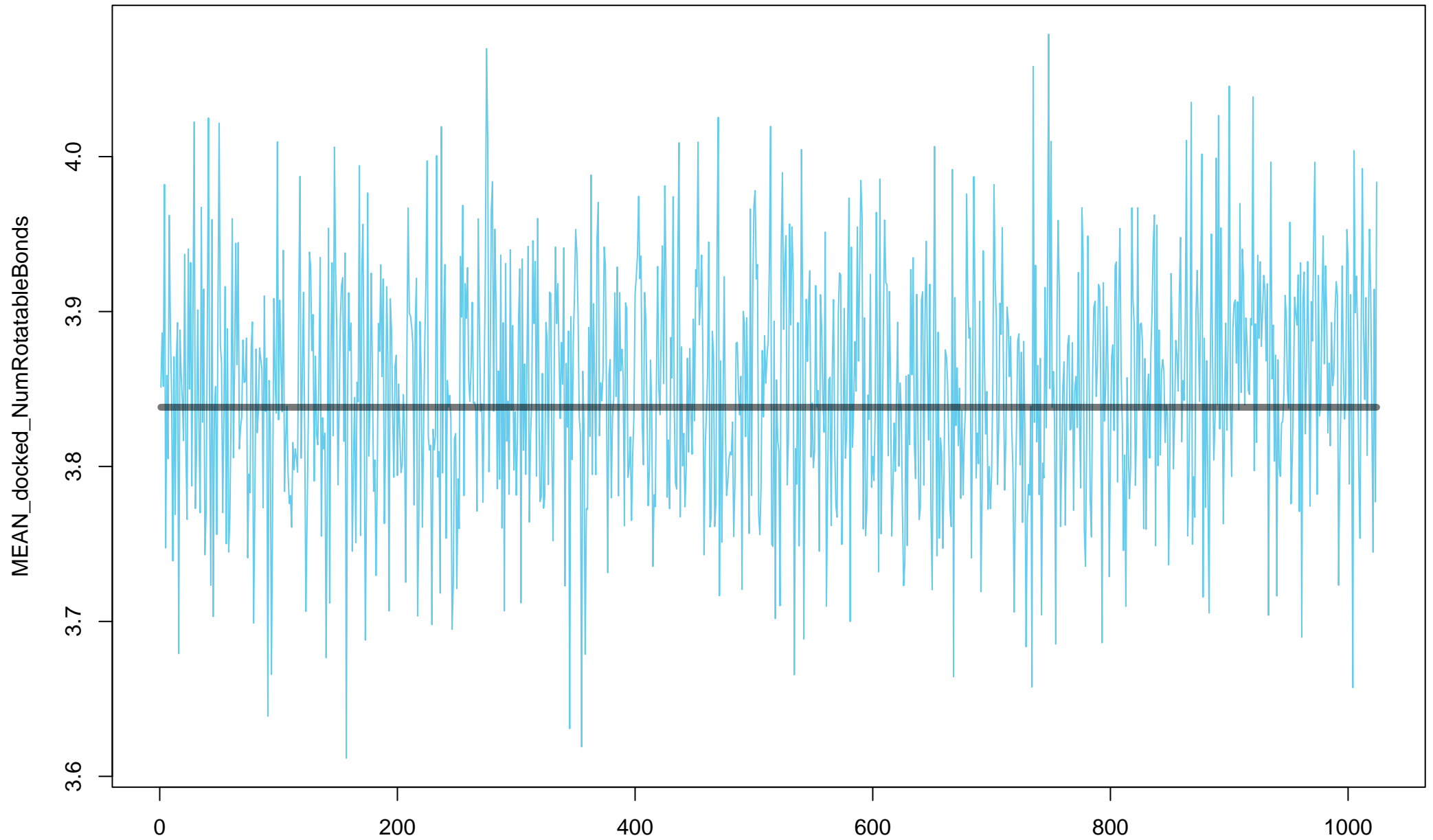
ESS = 1020 | BMK = 0.0536 | MCSE(6.27) = 3.29 | stat: TRUE | burn: 0 | rel.err: -1.31



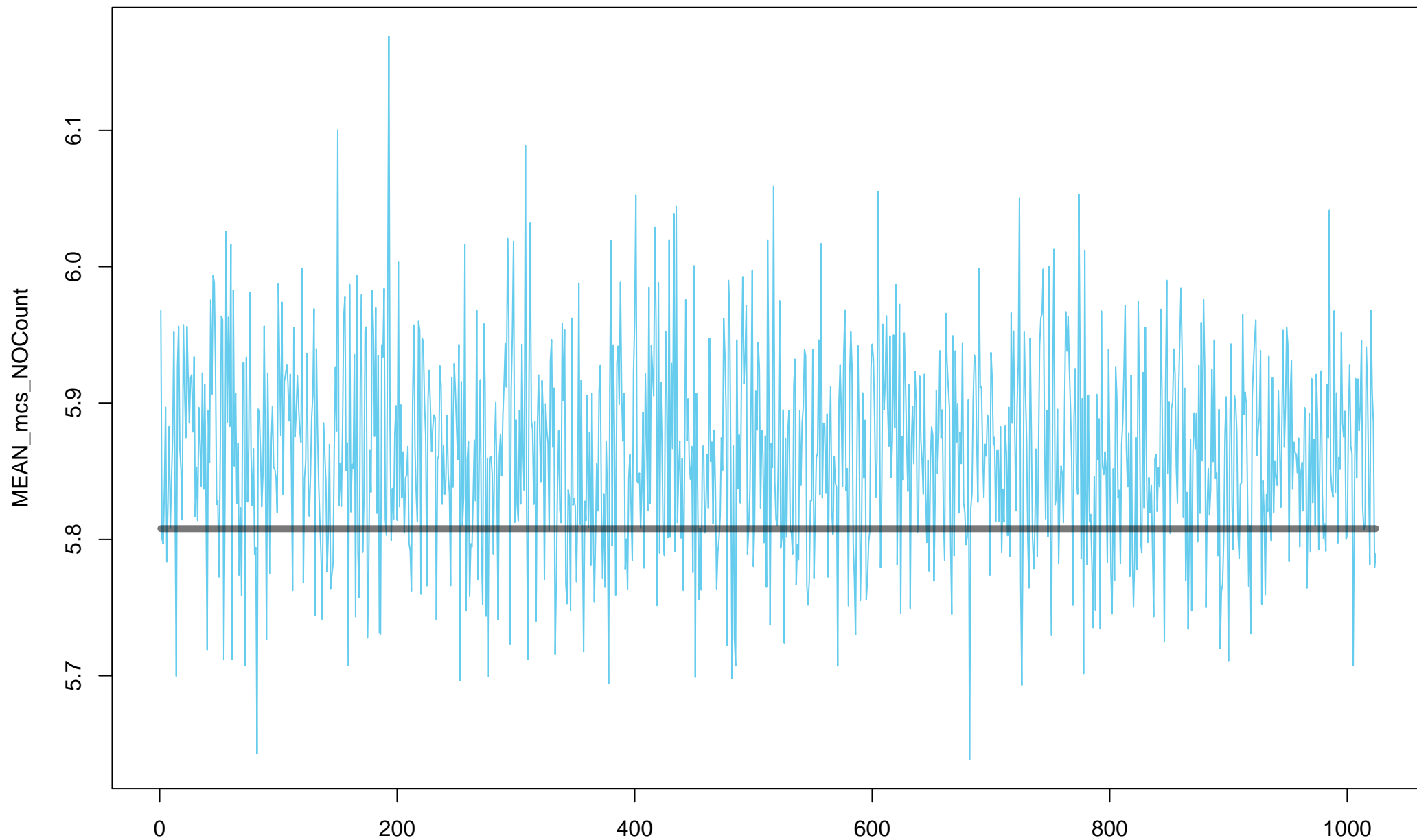
MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0505 | MCSE(6.27) = 2.9 | stat: TRUE | burn: 0 | rel.err: -0.135



MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.043 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 0 | rel.err: 0.175

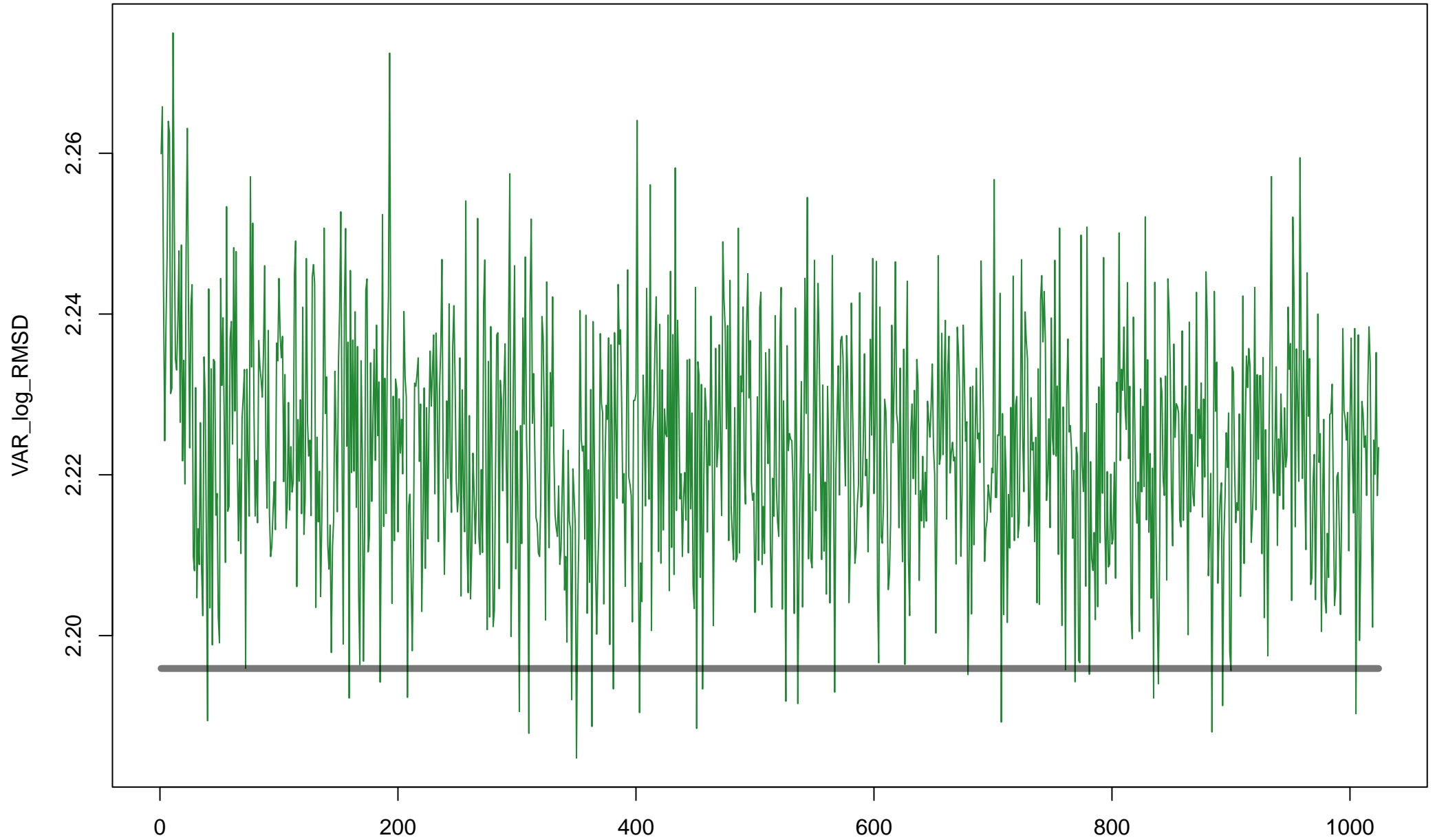


MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0845 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0 | rel.err: 0.769

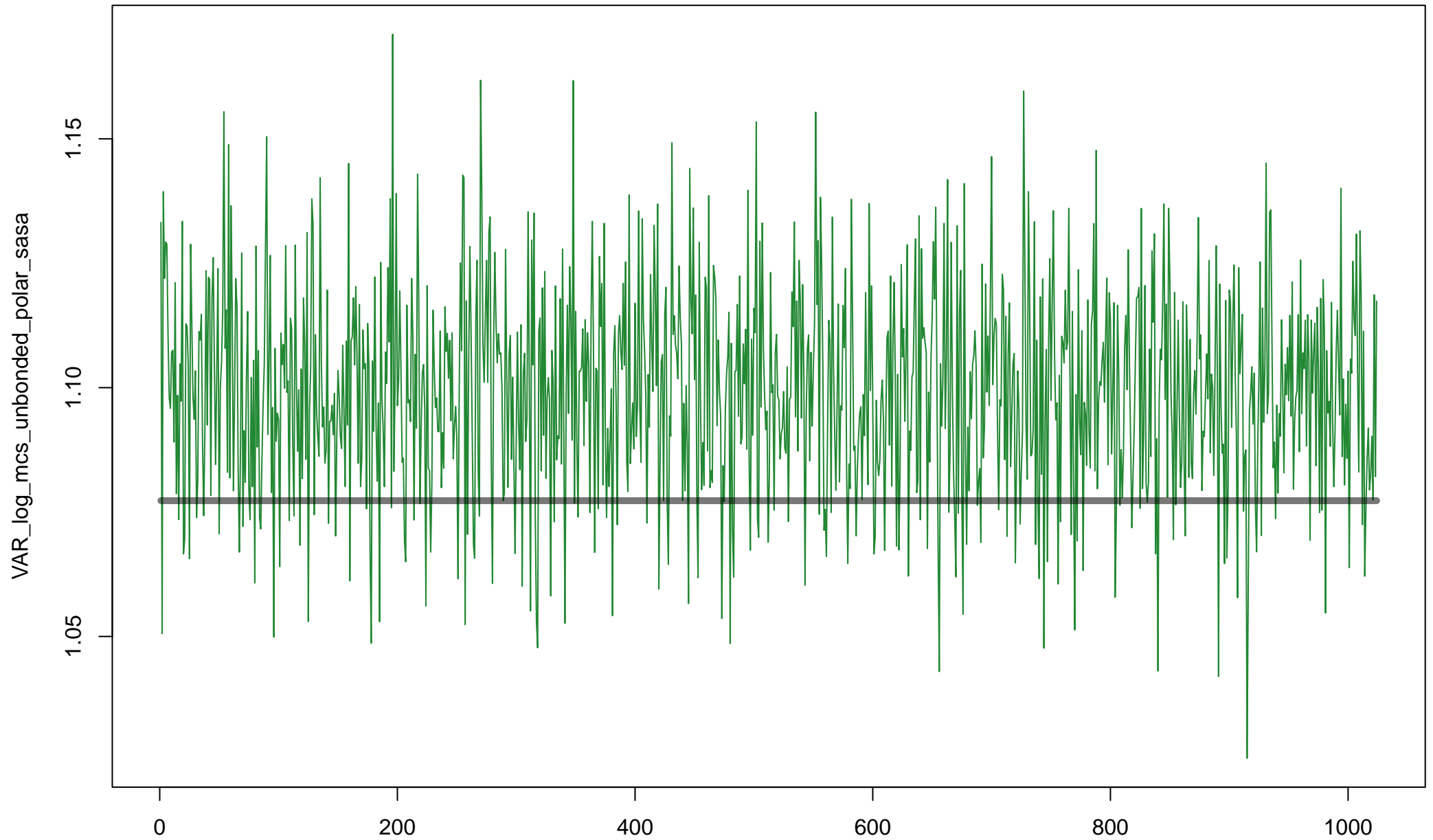


VAR_log_RMSD

ESS = 652 | BMK = 0.101 | MCSE(6.27) = 4.58 | stat: FALSE | burn: 0 | rel.err: 1.91

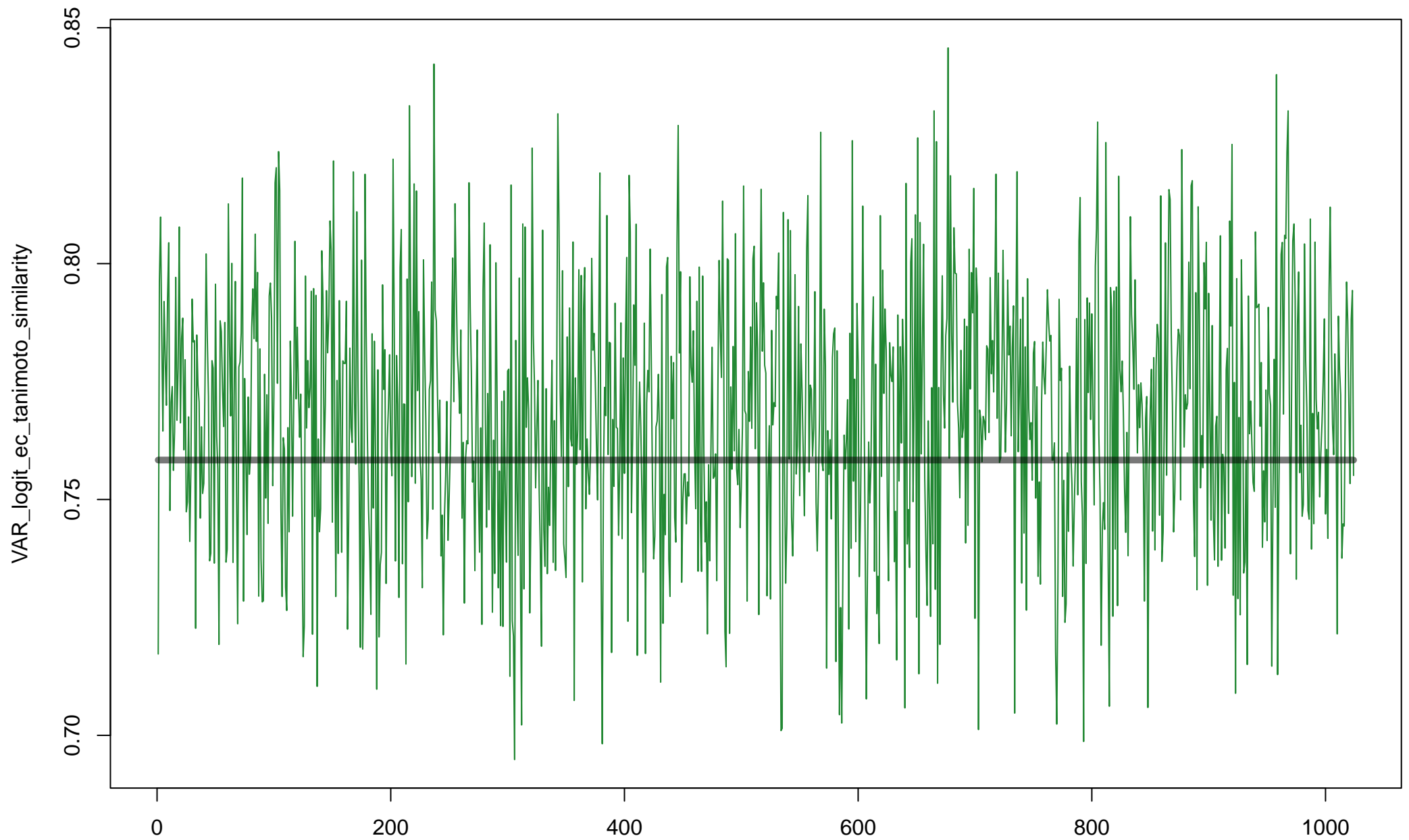


VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0591 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0 | rel.err: 1.06

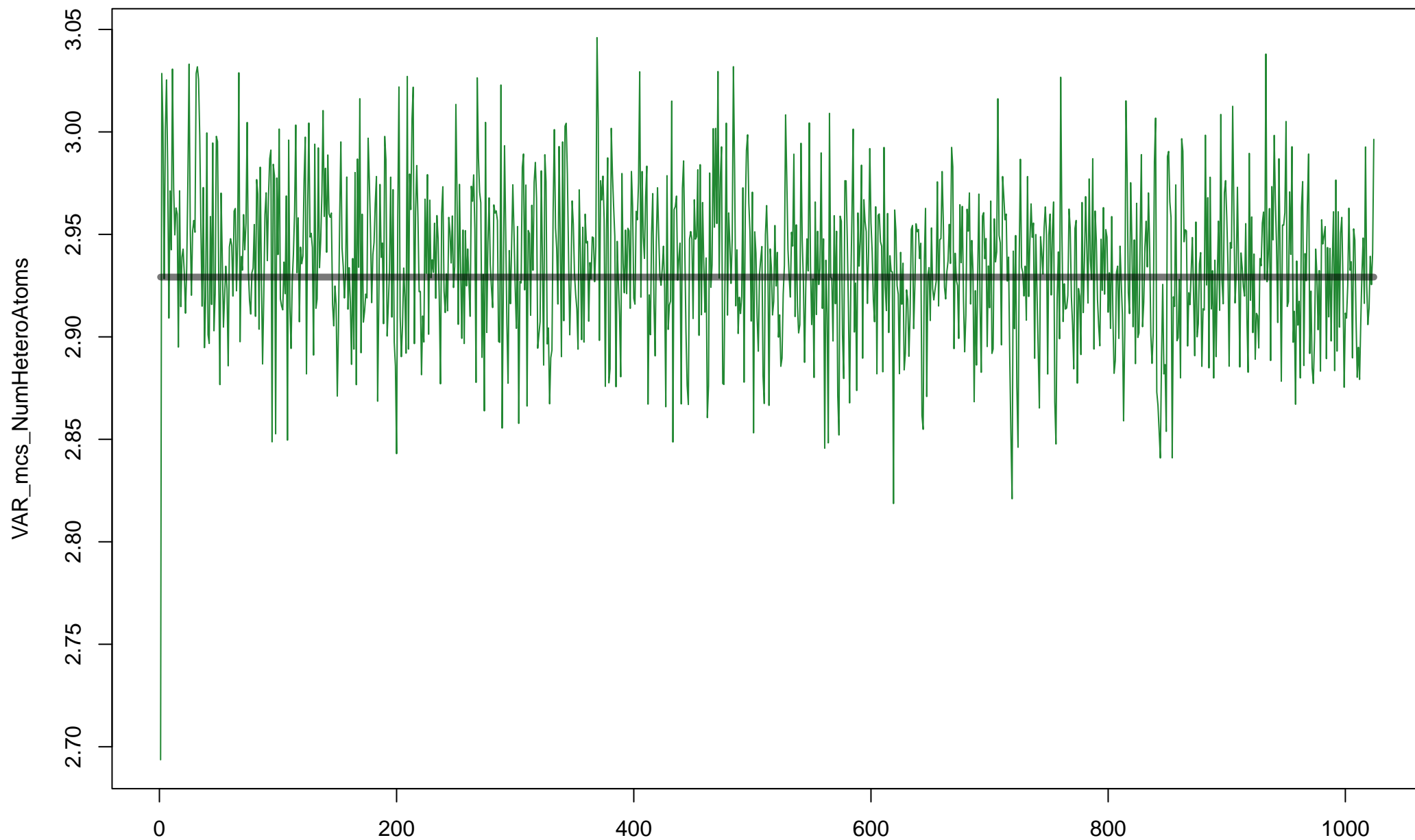


VAR_logit_ec_tanimoto_similarity

ESS = 1020 | BMK = 0.0456 | MCSE(6.27) = 3.97 | stat: TRUE | burn: 0 | rel.err: 0.349

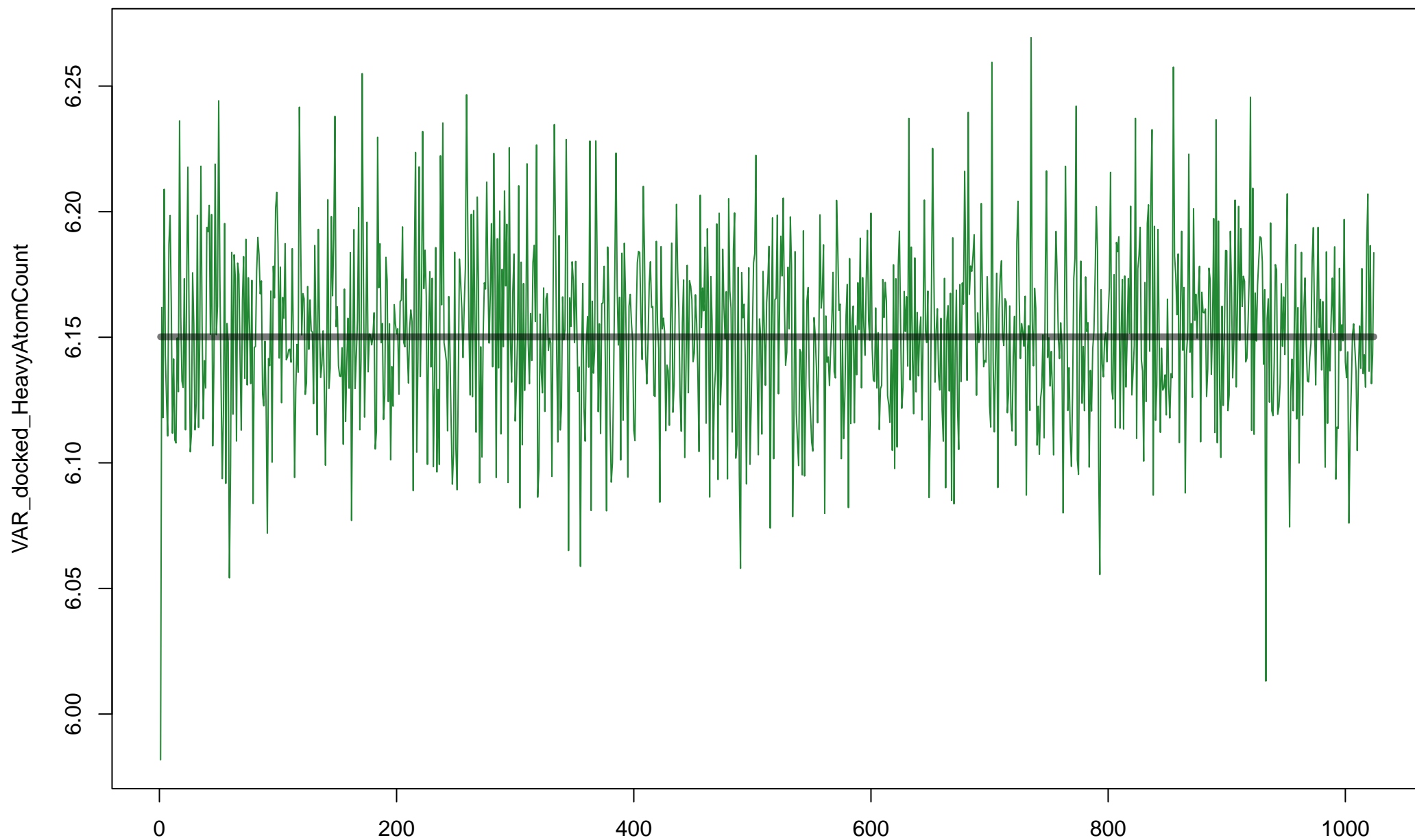


VAR_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.132 | MCSE(6.27) = 3.68 | stat: FALSE | burn: 0 | rel.err: 0.191

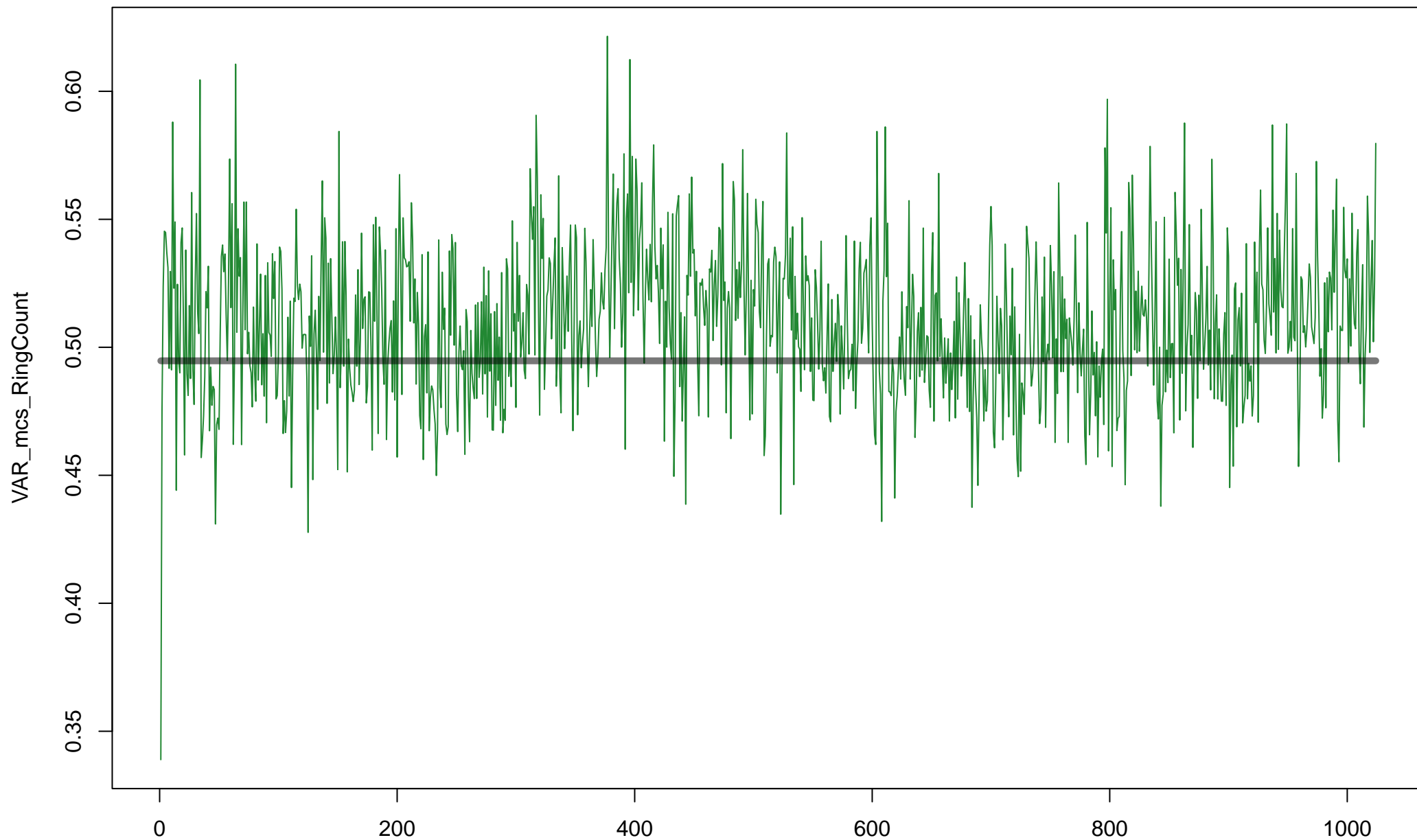


VAR_docked_HeavyAtomCount

ESS = 1020 | BMK = 0.0713 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0 | rel.err: 0.055

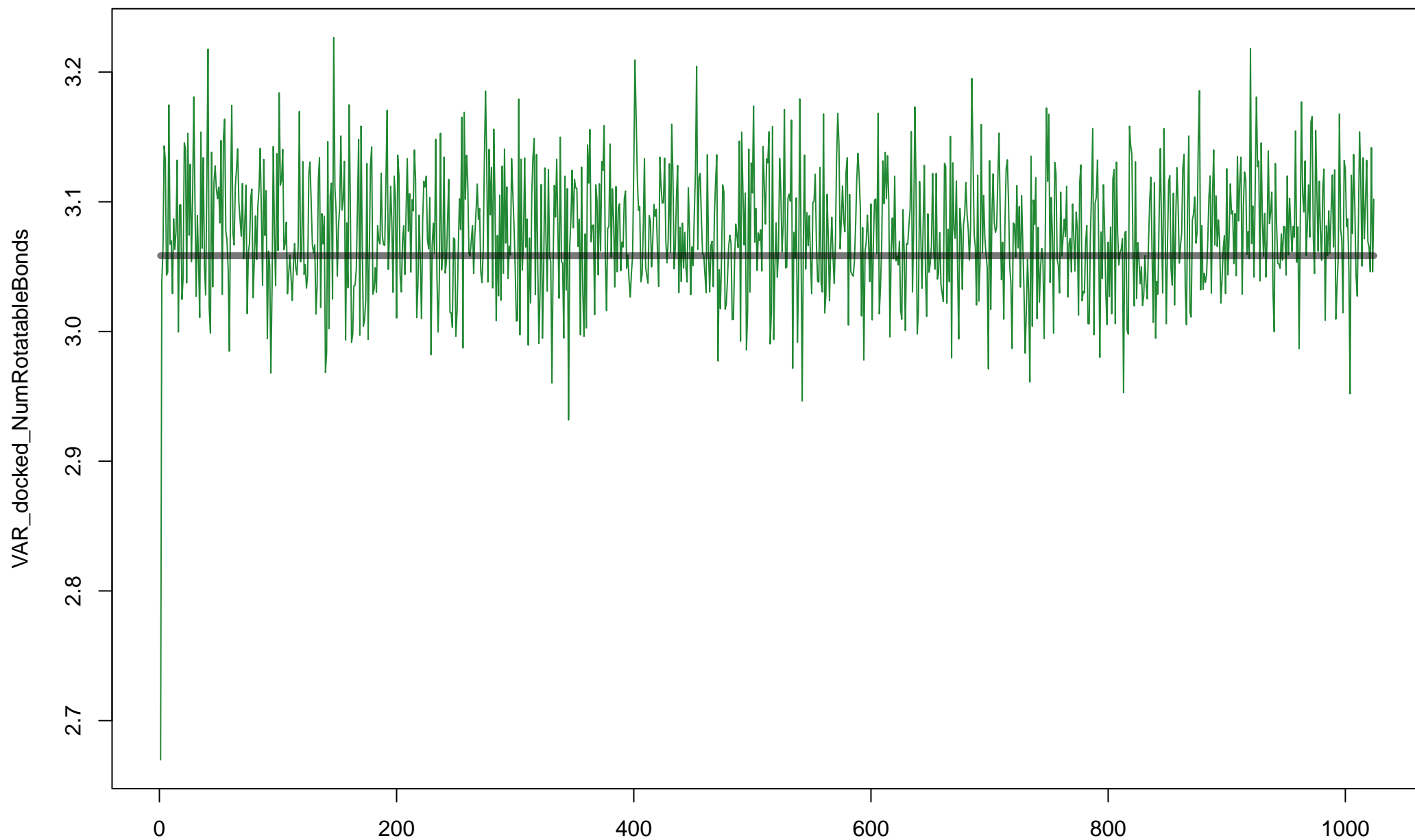


VAR_mcs_RingCount
ESS = 173 | BMK = 0.102 | MCSE(6.27) = 5.54 | stat: TRUE | burn: 0 | rel.err: 0.505

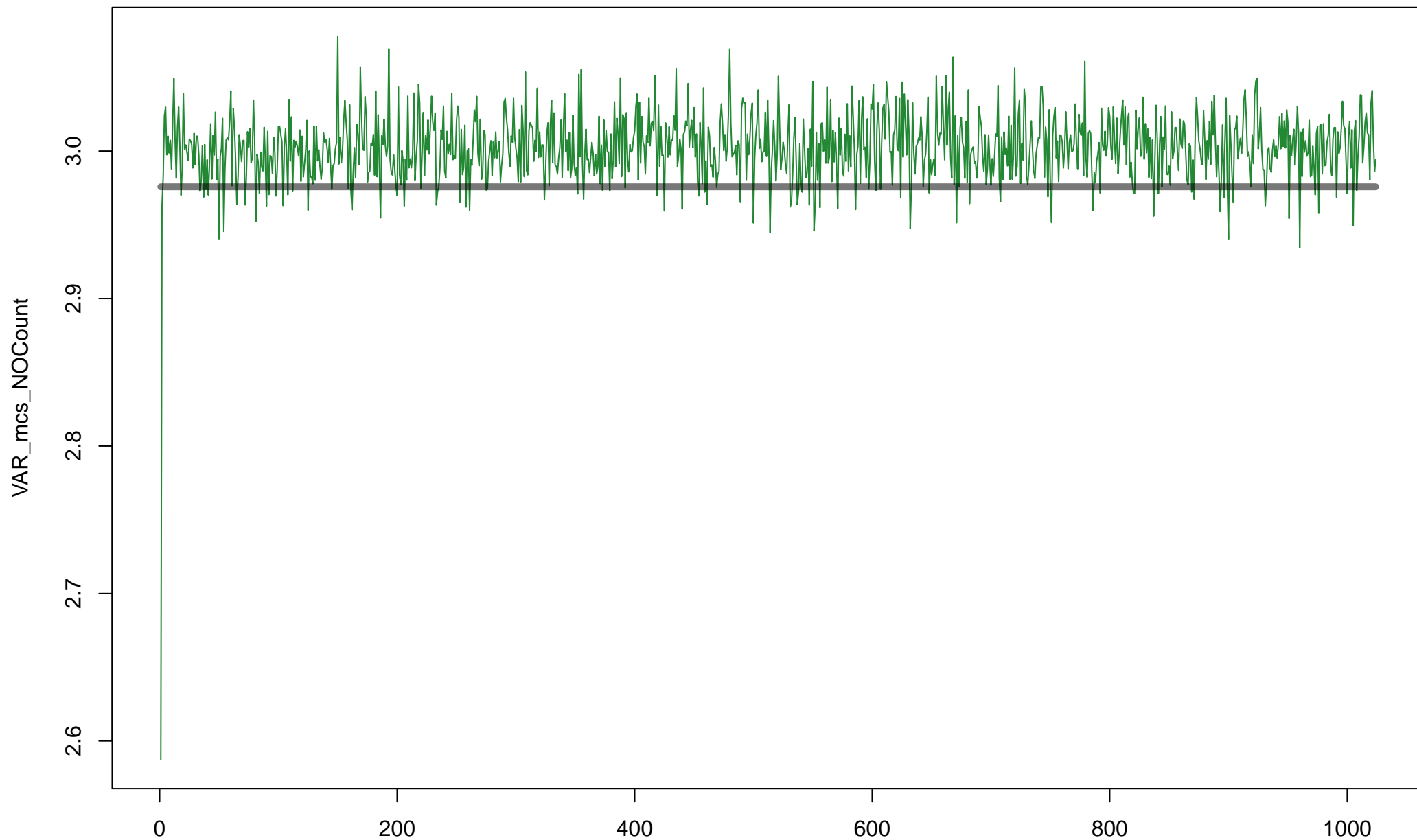


VAR_docked_NumRotatableBonds

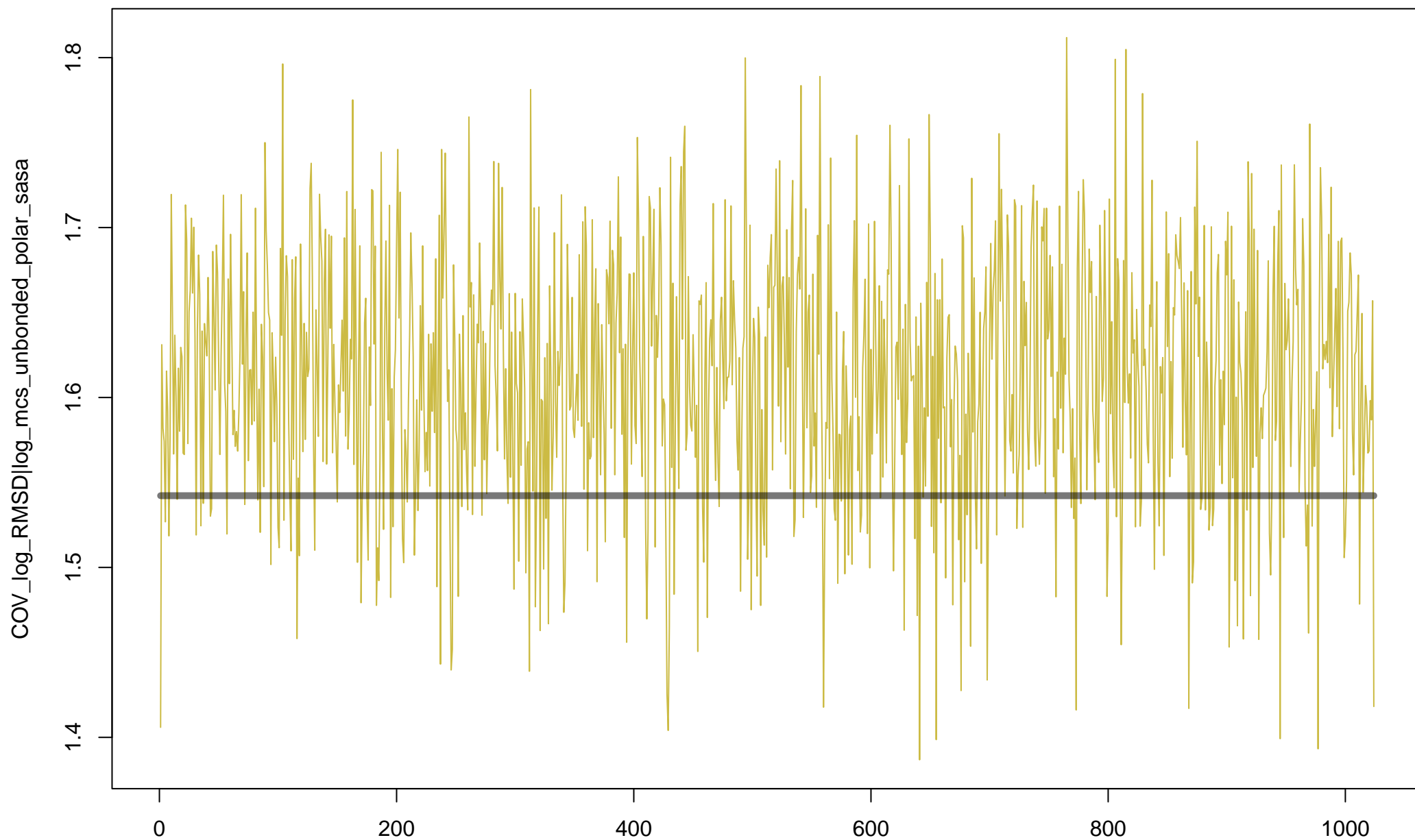
ESS = 1020 | BMK = 0.0502 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | rel.err: 0.396



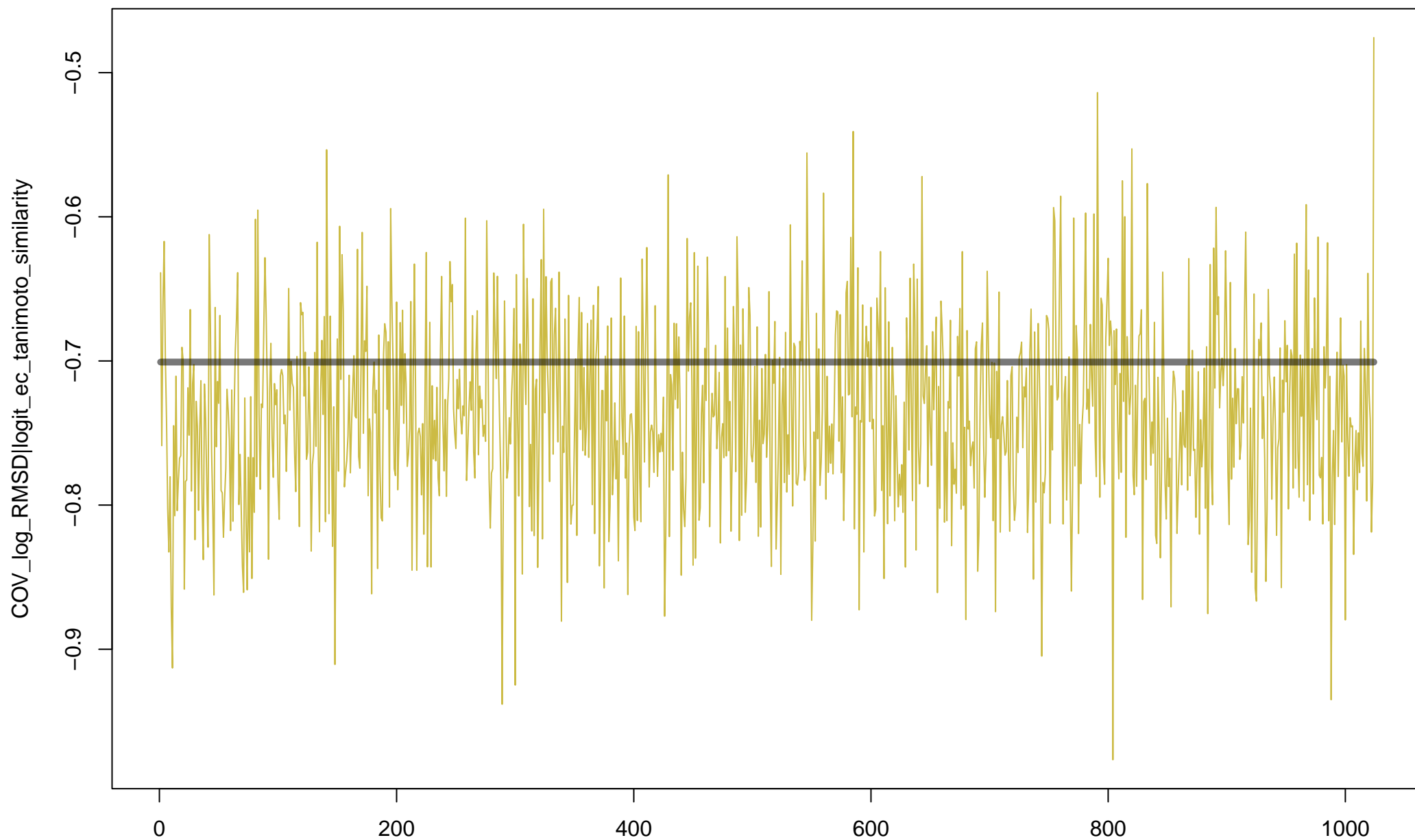
VAR_mcs_NOCount
ESS = 1020 | BMK = 0.0629 | MCSE(6.27) = 3.6 | stat: TRUE | burn: 0 | rel.err: 1.11



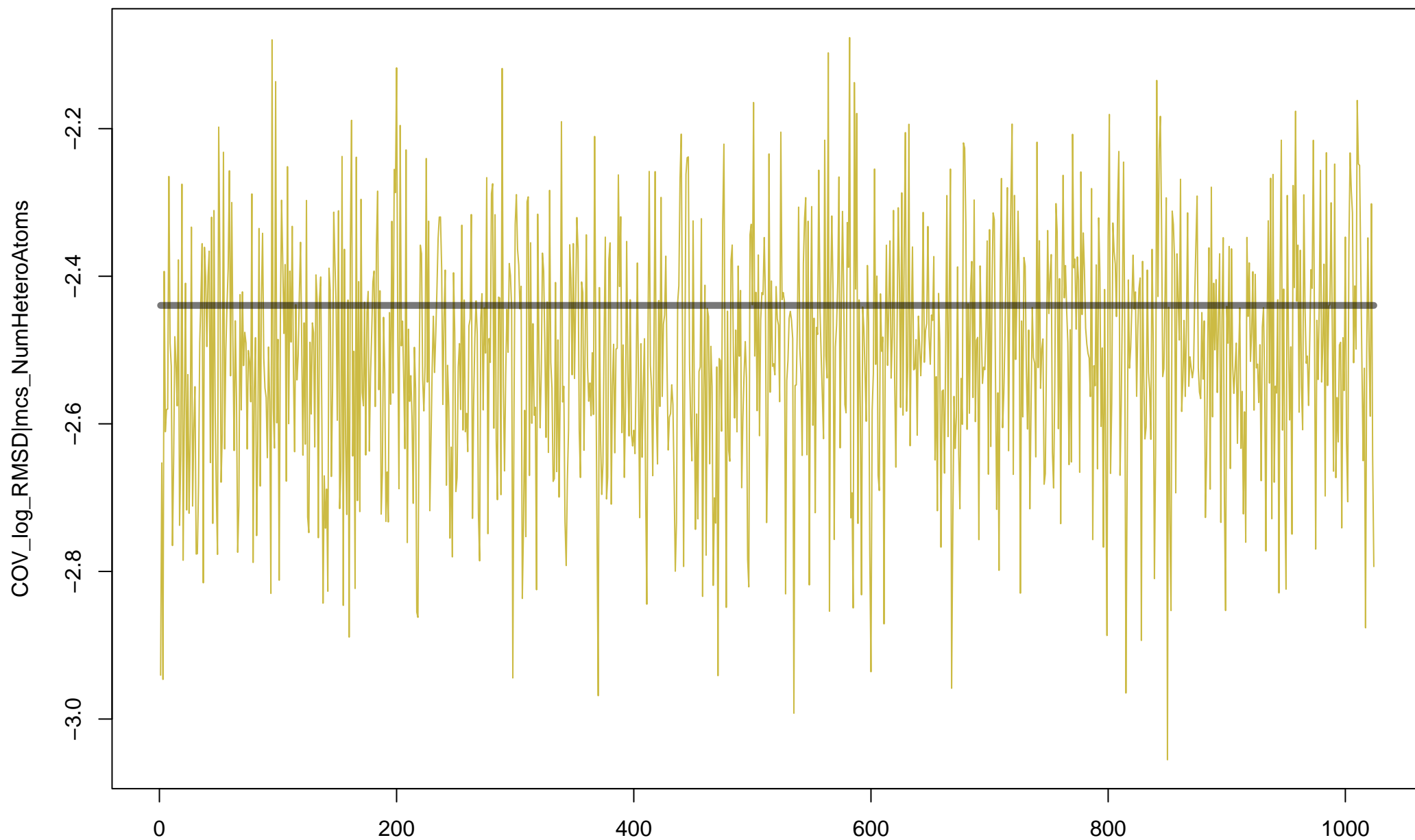
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0486 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0 | rel.err: 0.952



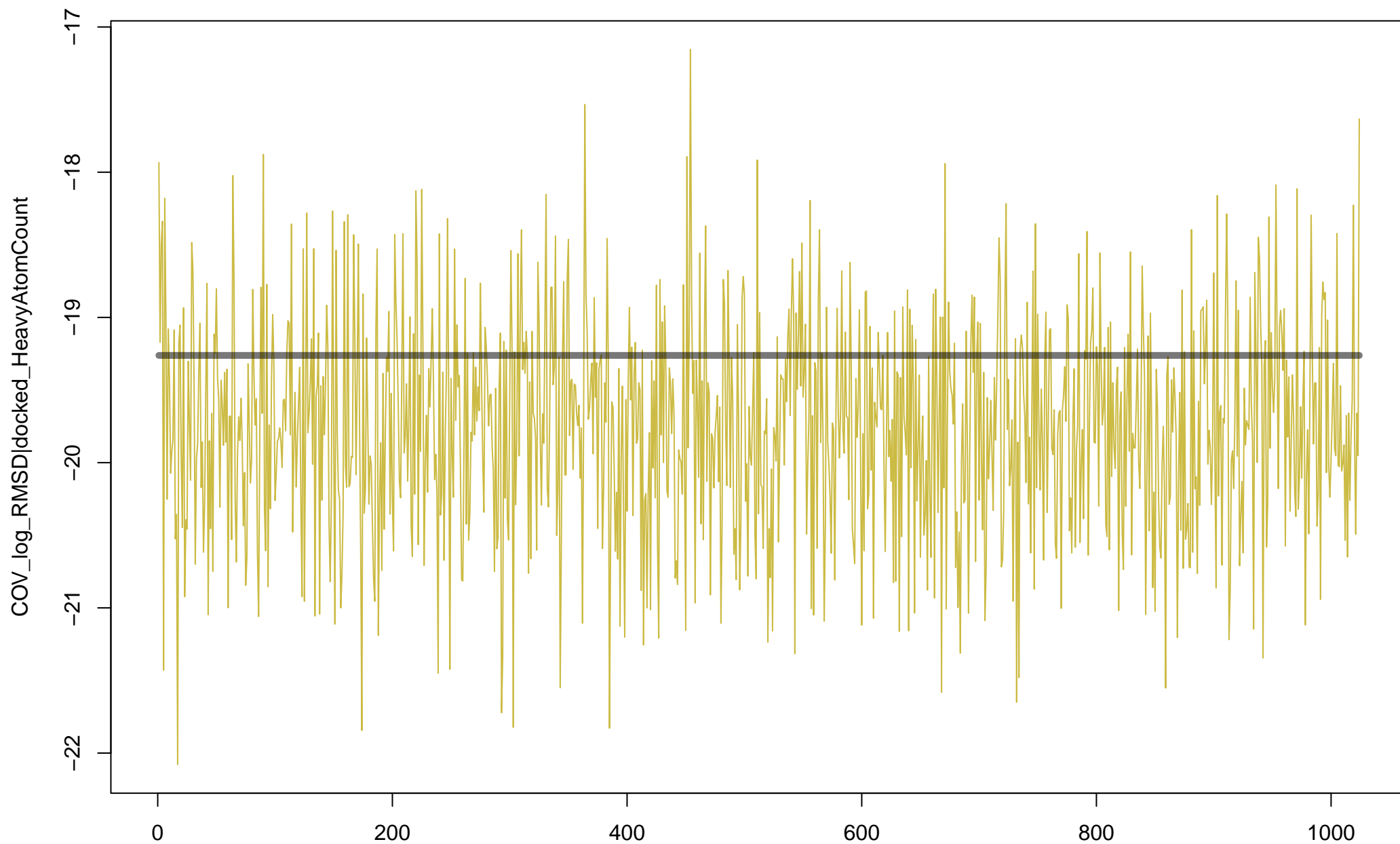
COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0654 | MCSE(6.27) = 2.73 | stat: FALSE | burn: 0 | rel.err: -0.553



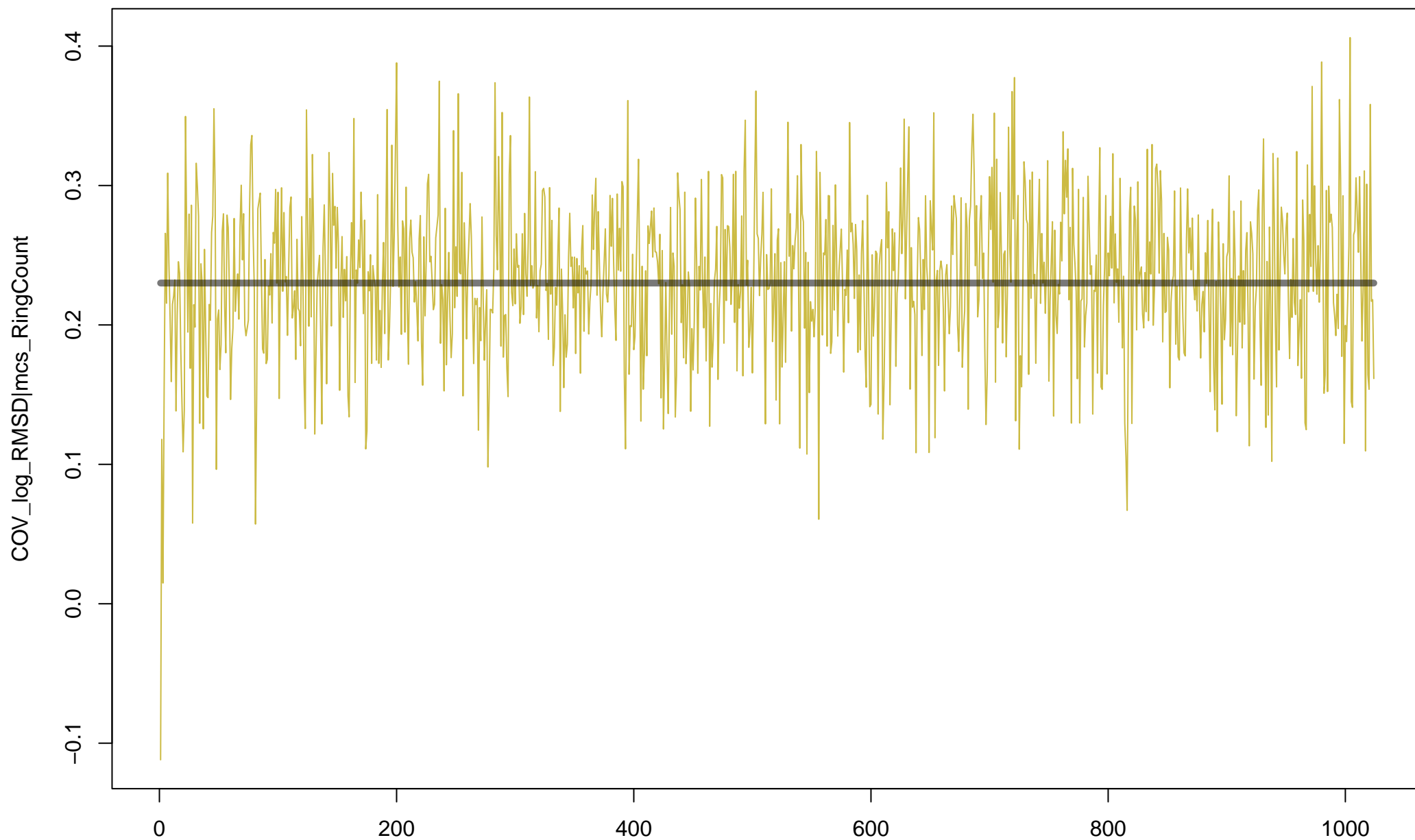
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.095 | MCSE(6.27) = 3.4 | stat: FALSE | burn: 0 | rel.err: -0.433



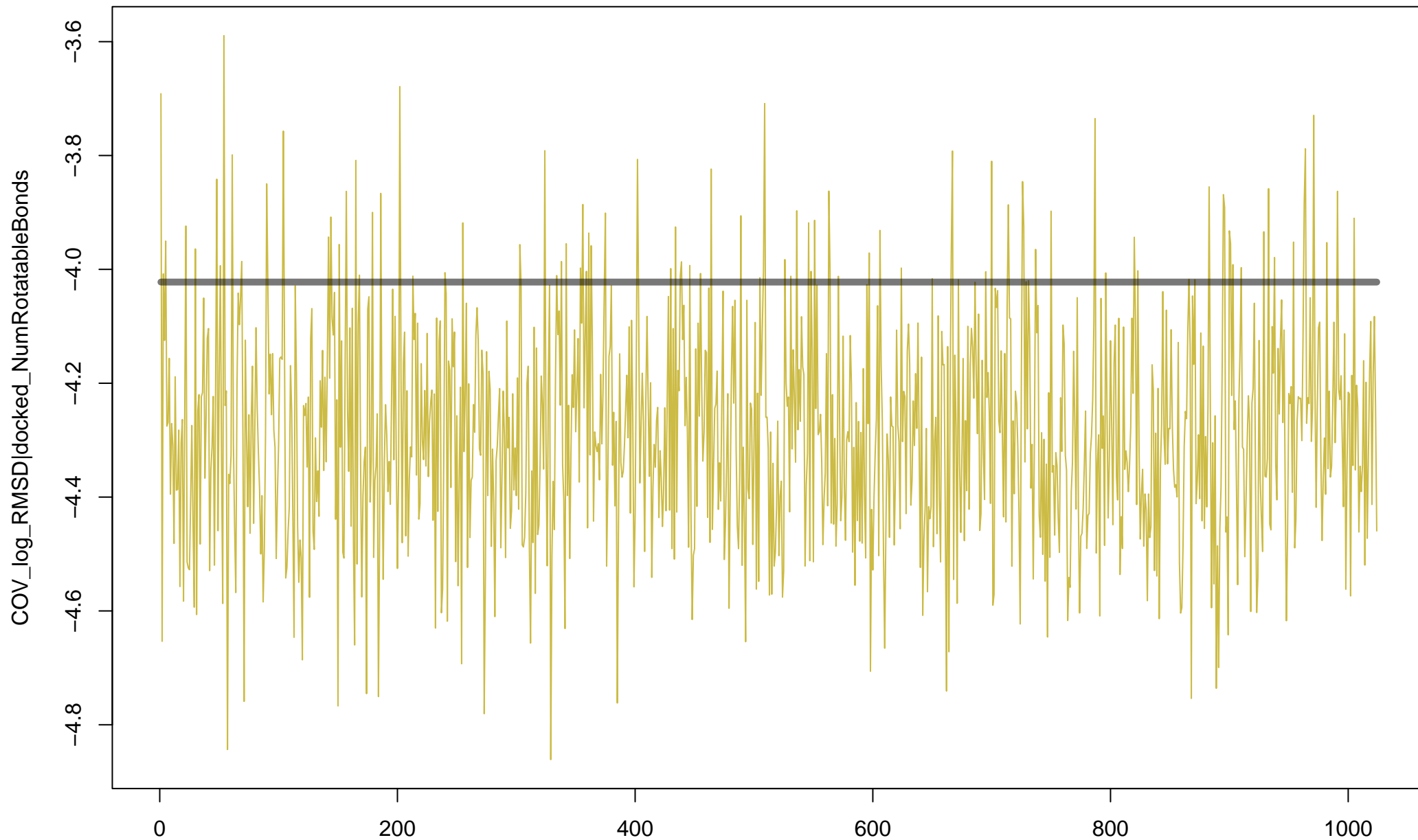
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0596 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | rel.err: -0.672



COV_log_RMSD|mcs_RingCount
ESS = 905 | BMK = 0.0659 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | rel.err: 0.0453

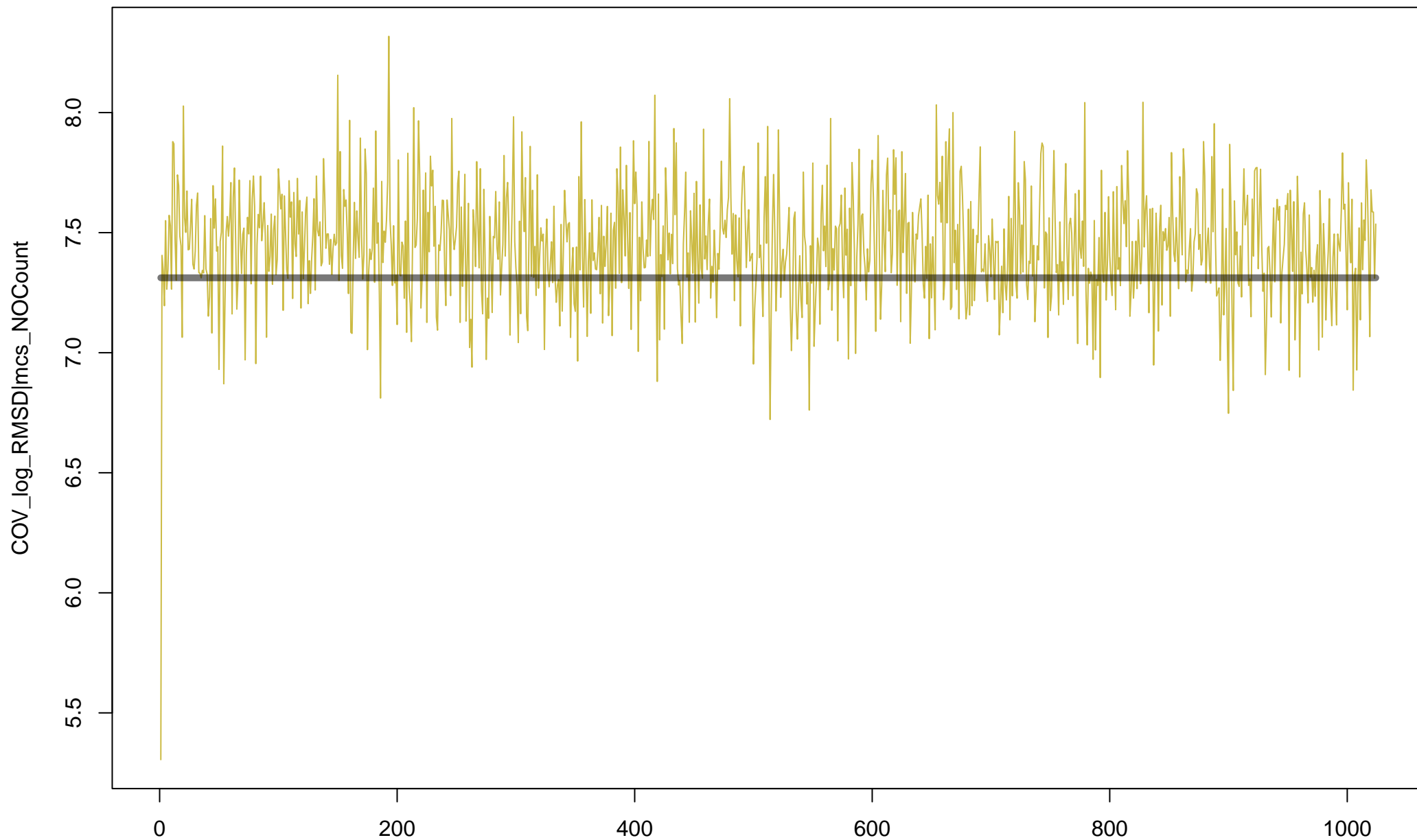


COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0524 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0 | rel.err: -1.37

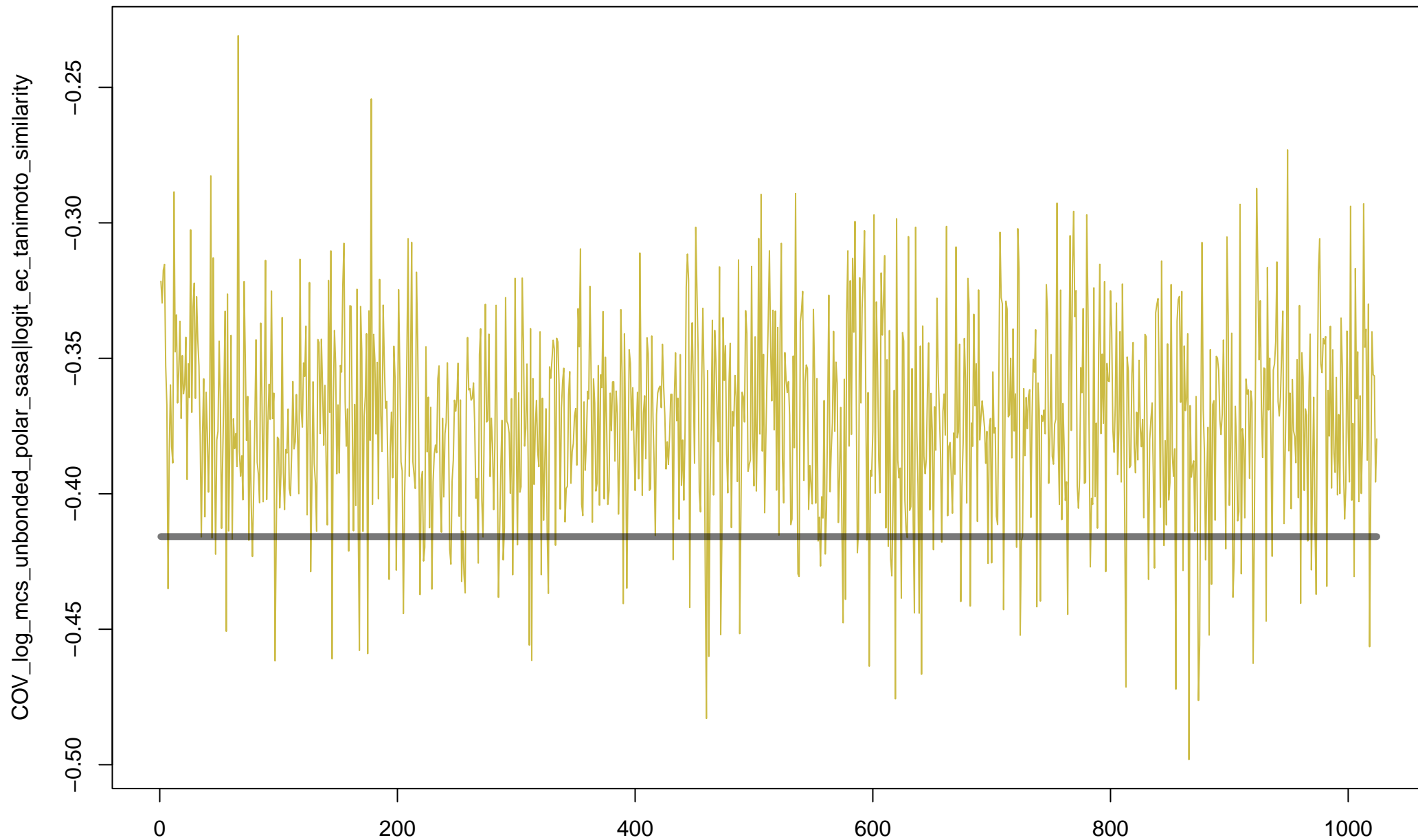


COV_log_RMSD|mcs_NOCount

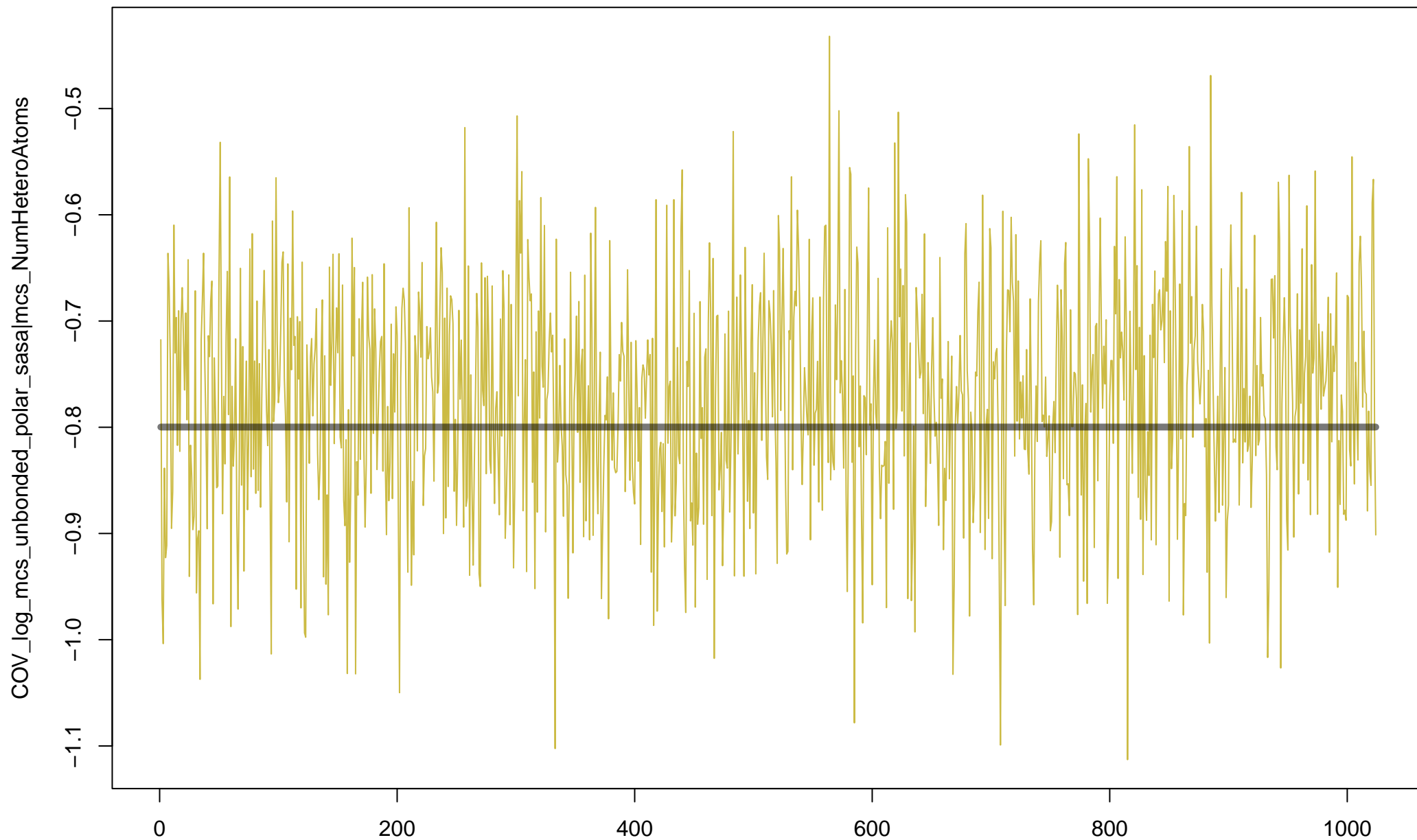
ESS = 1020 | BMK = 0.0783 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0 | rel.err: 0.555



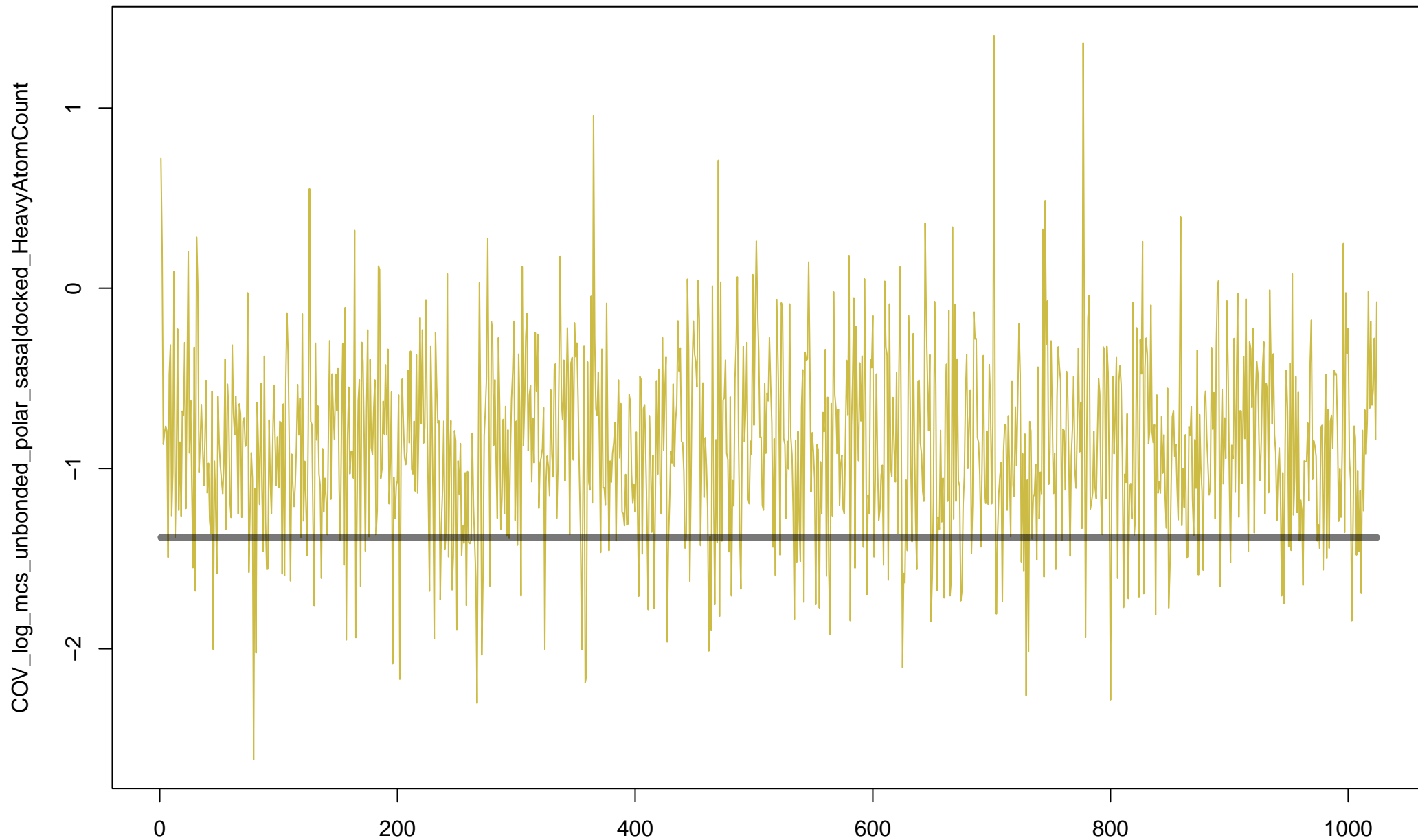
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0805 | MCSE(6.27) = 3.9 | stat: TRUE | burn: 0 | rel.err: 1.2



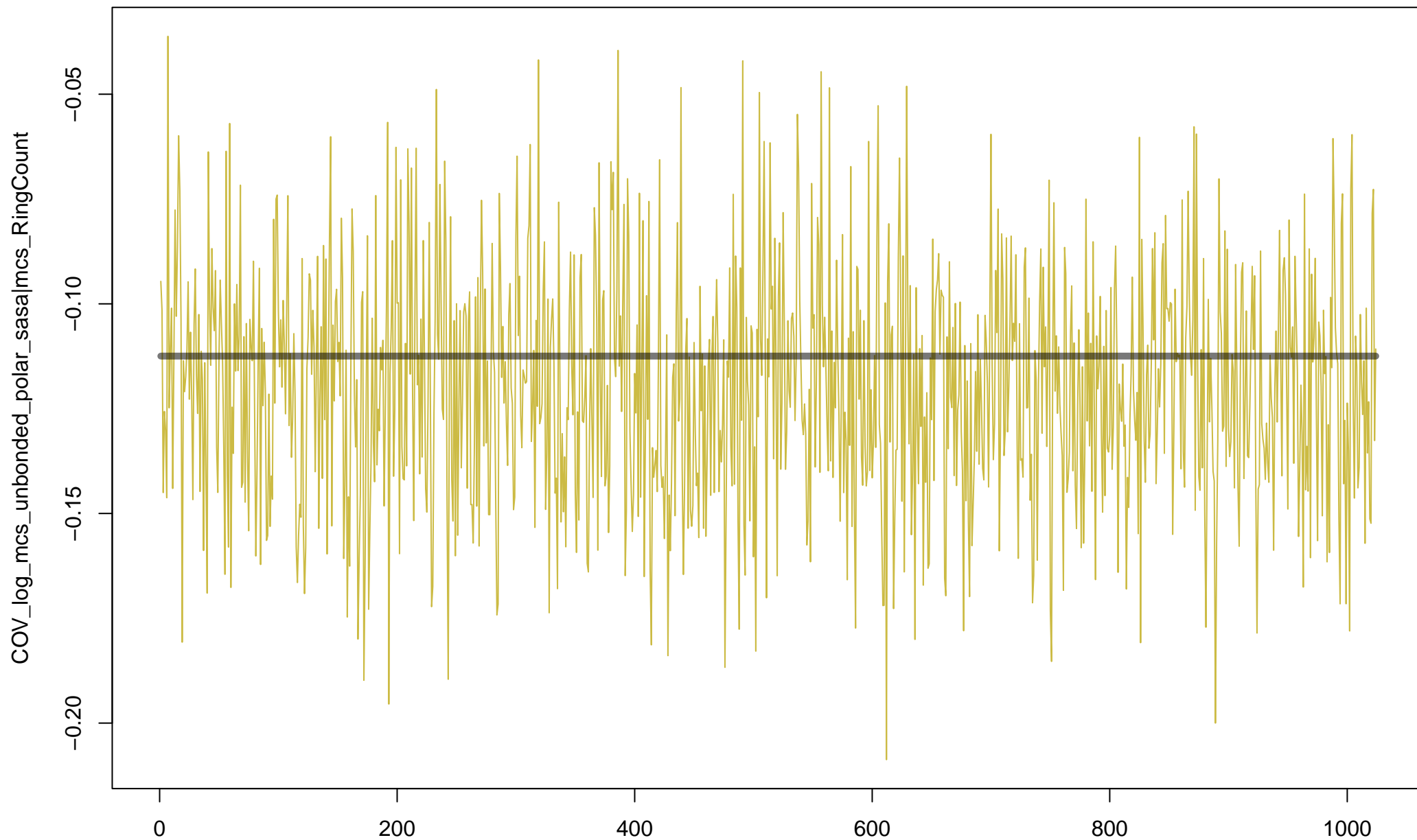
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0846 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0 | rel.err: 0.262



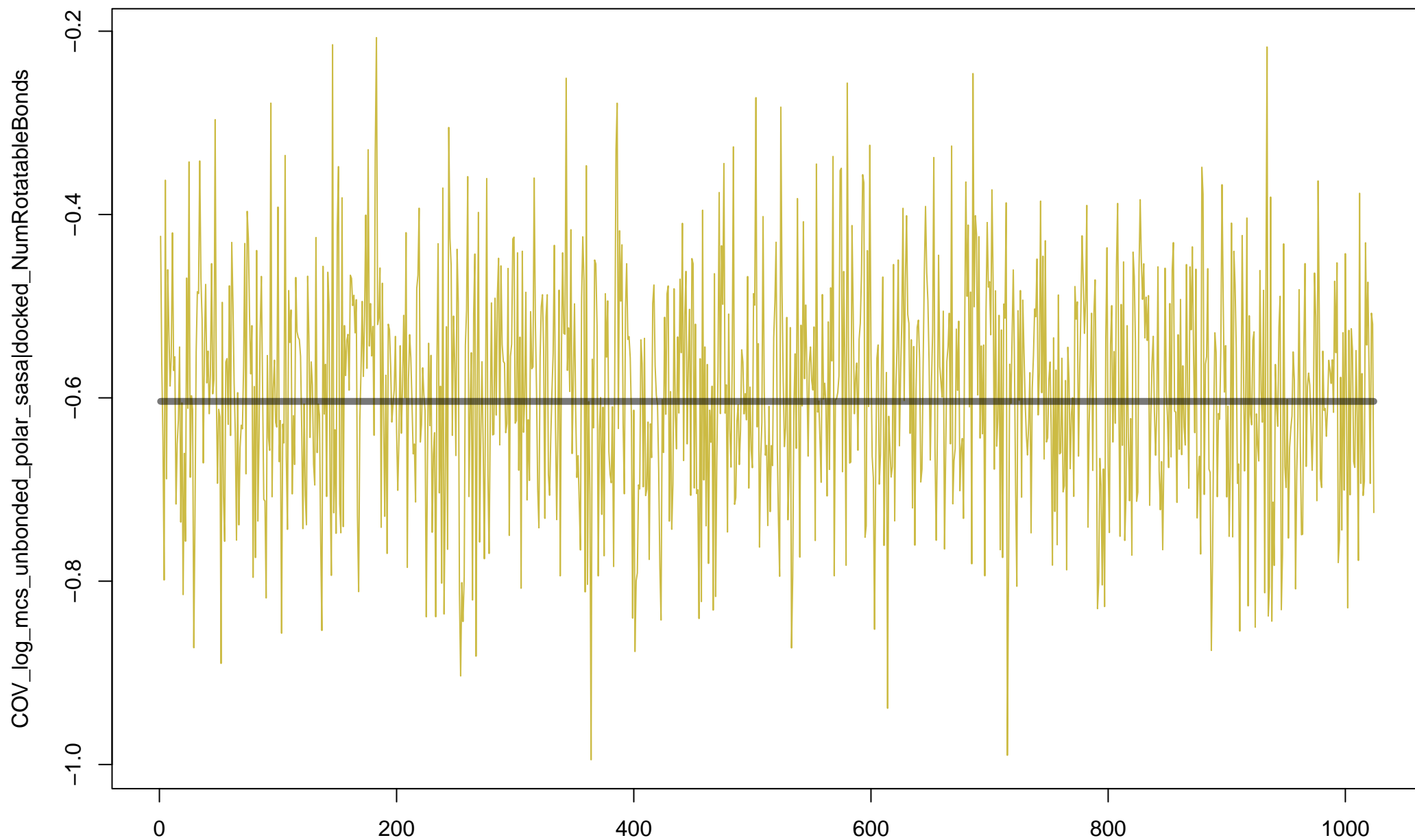
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0707 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 0 | rel.err: 1



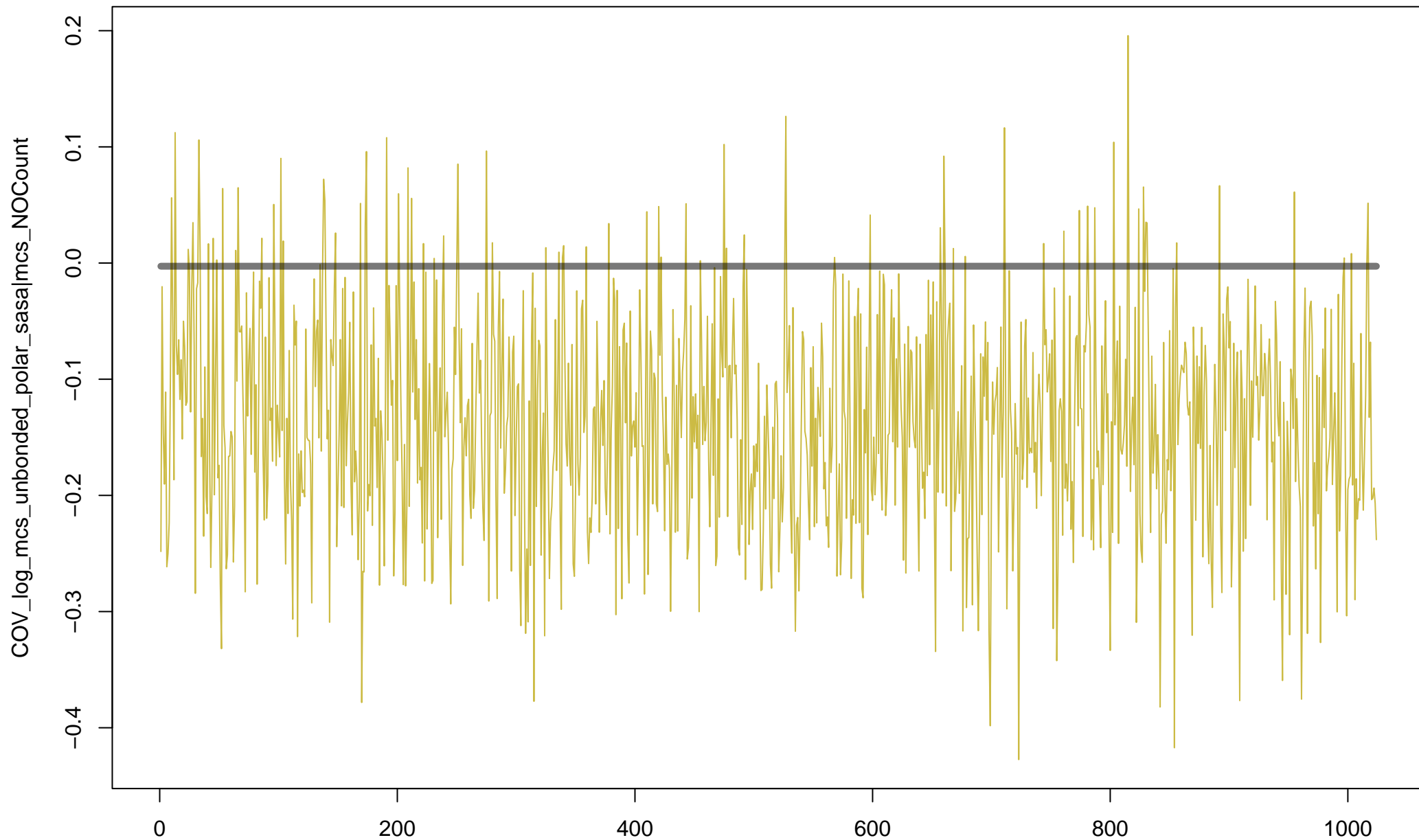
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0696 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 0 | rel.err: -0.275



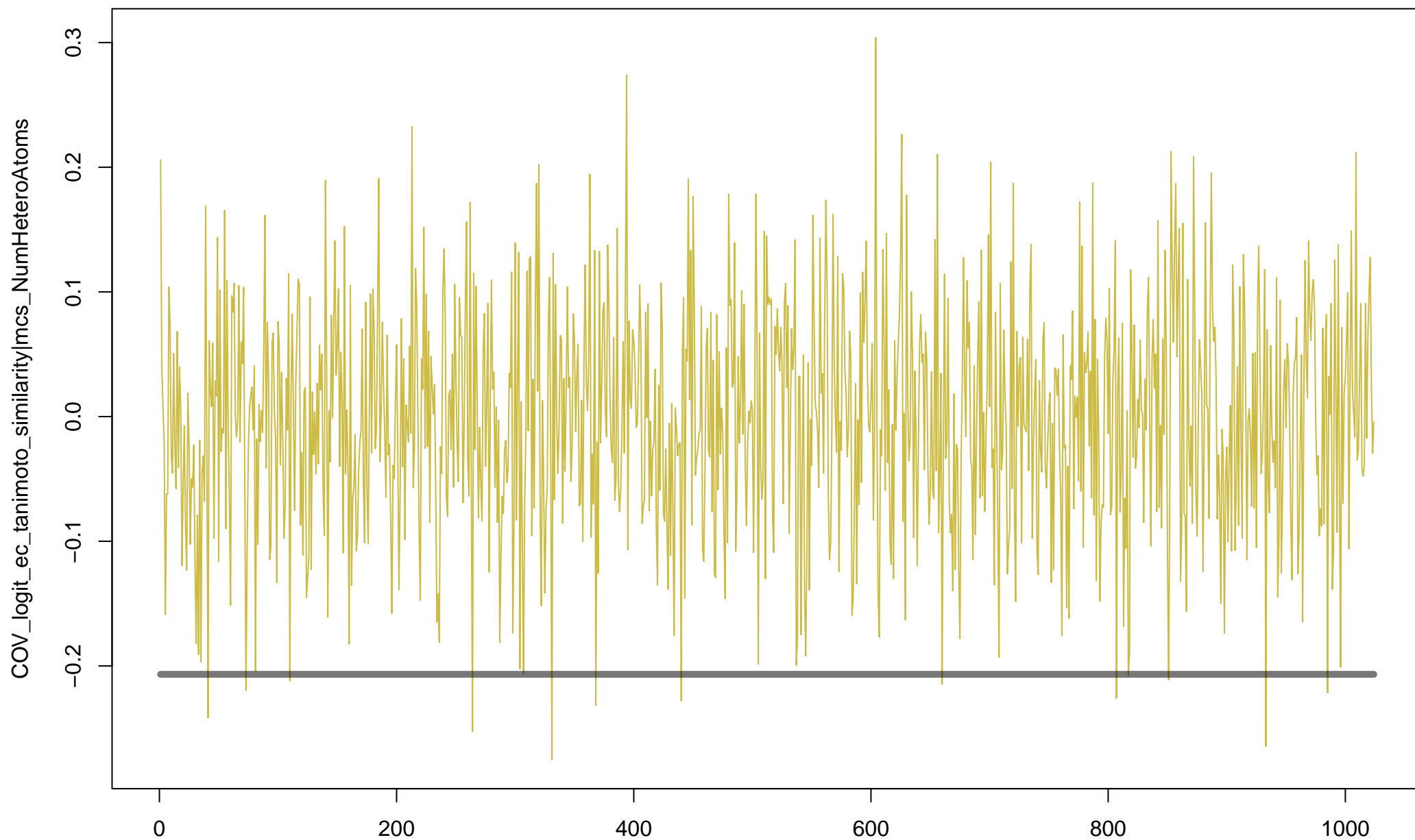
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0389 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0 | rel.err: 0.0947



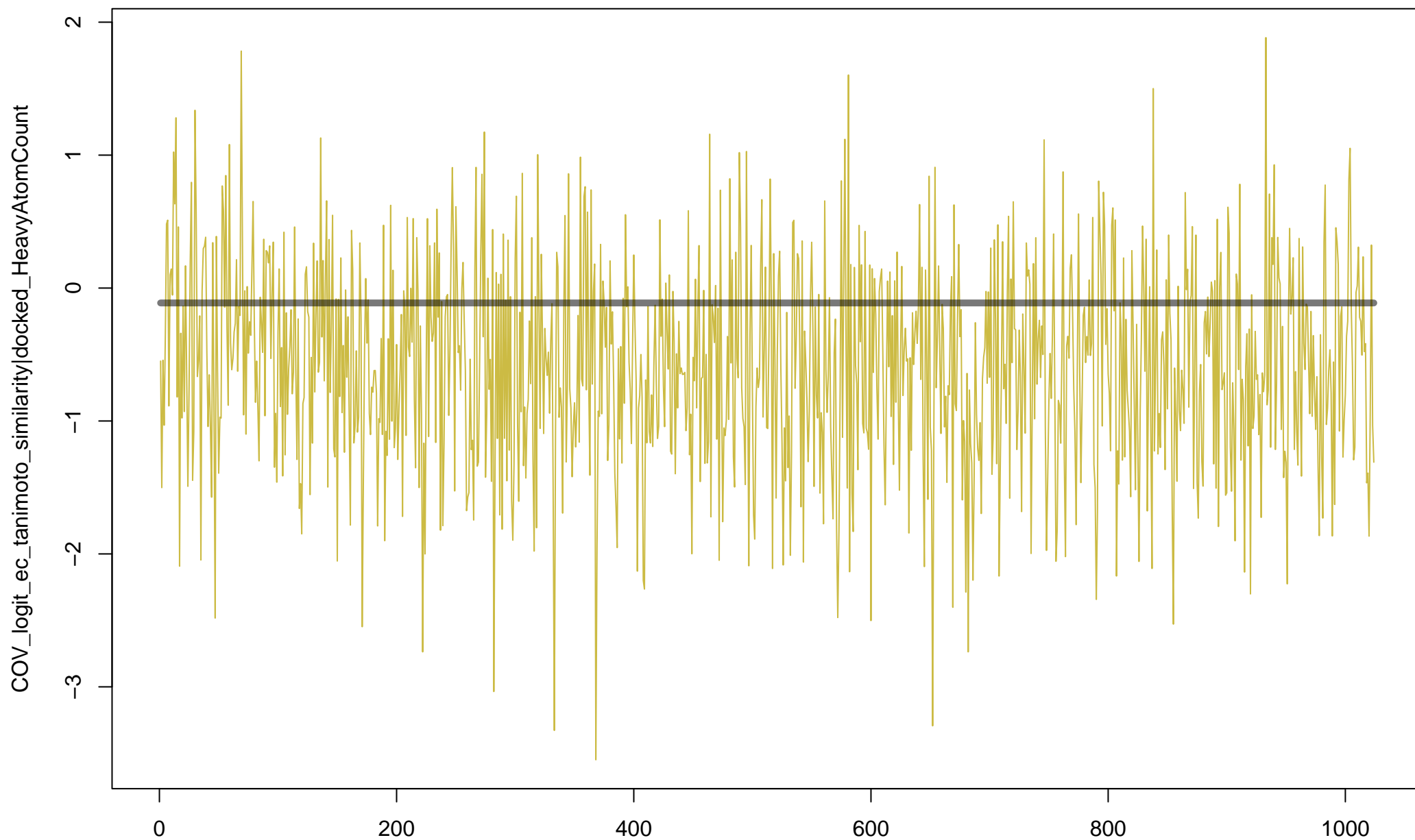
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0761 | MCSE(6.27) = 3.68 | stat: FALSE | burn: 0 | rel.err: -1.45



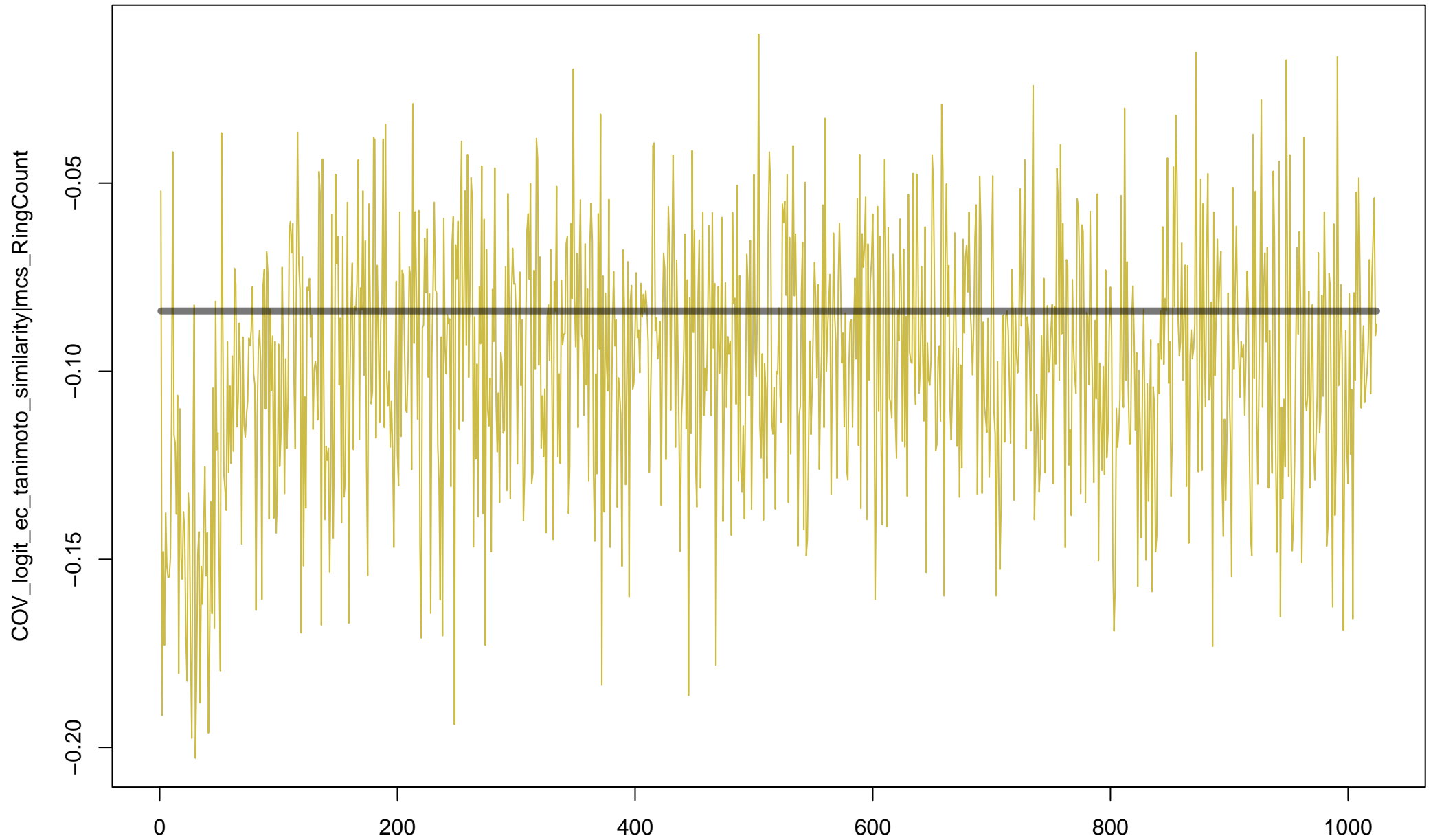
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0505 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0 | rel.err: 2.3



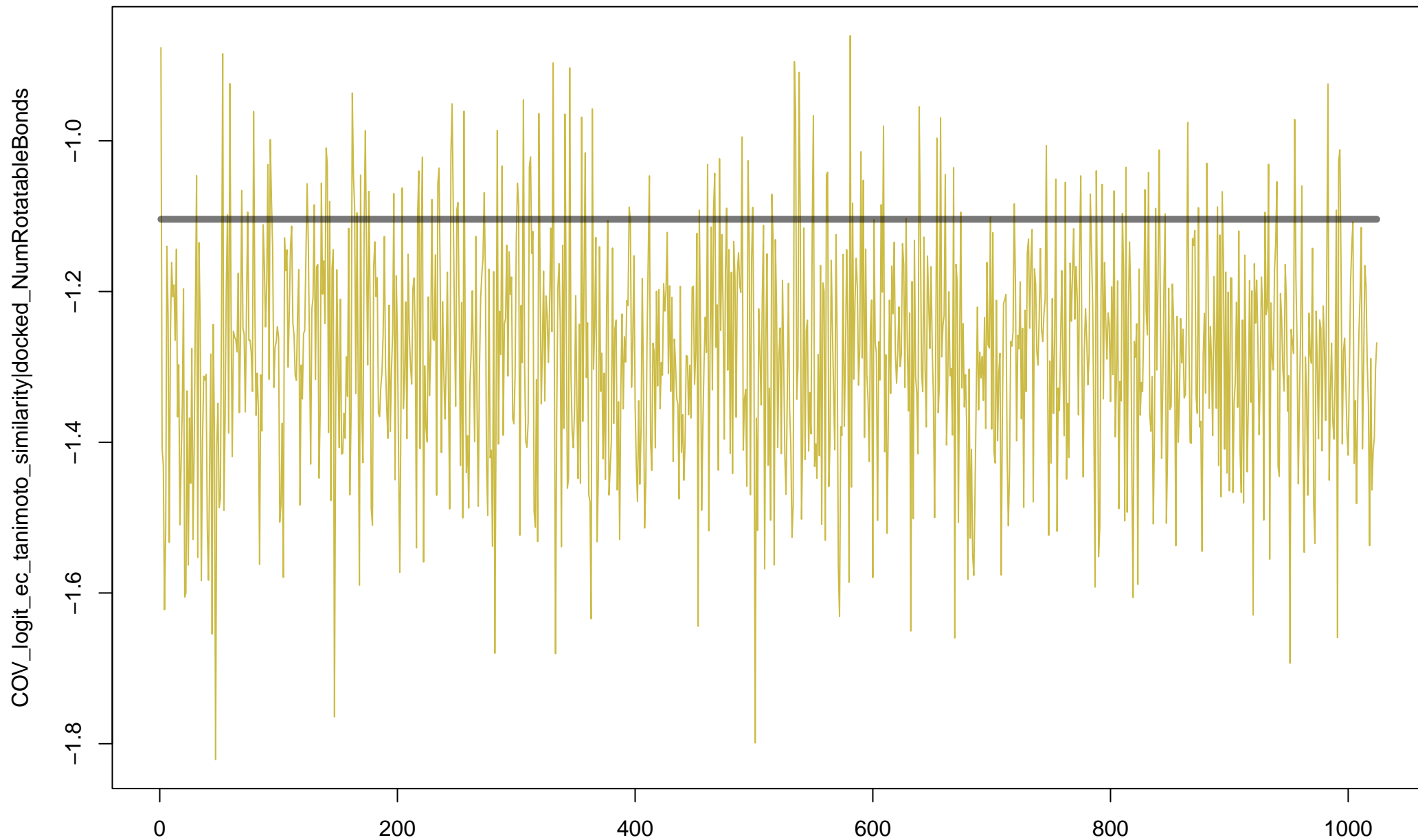
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0549 | MCSE(6.27) = 3.87 | stat: FALSE | burn: 0 | rel.err: -0.62



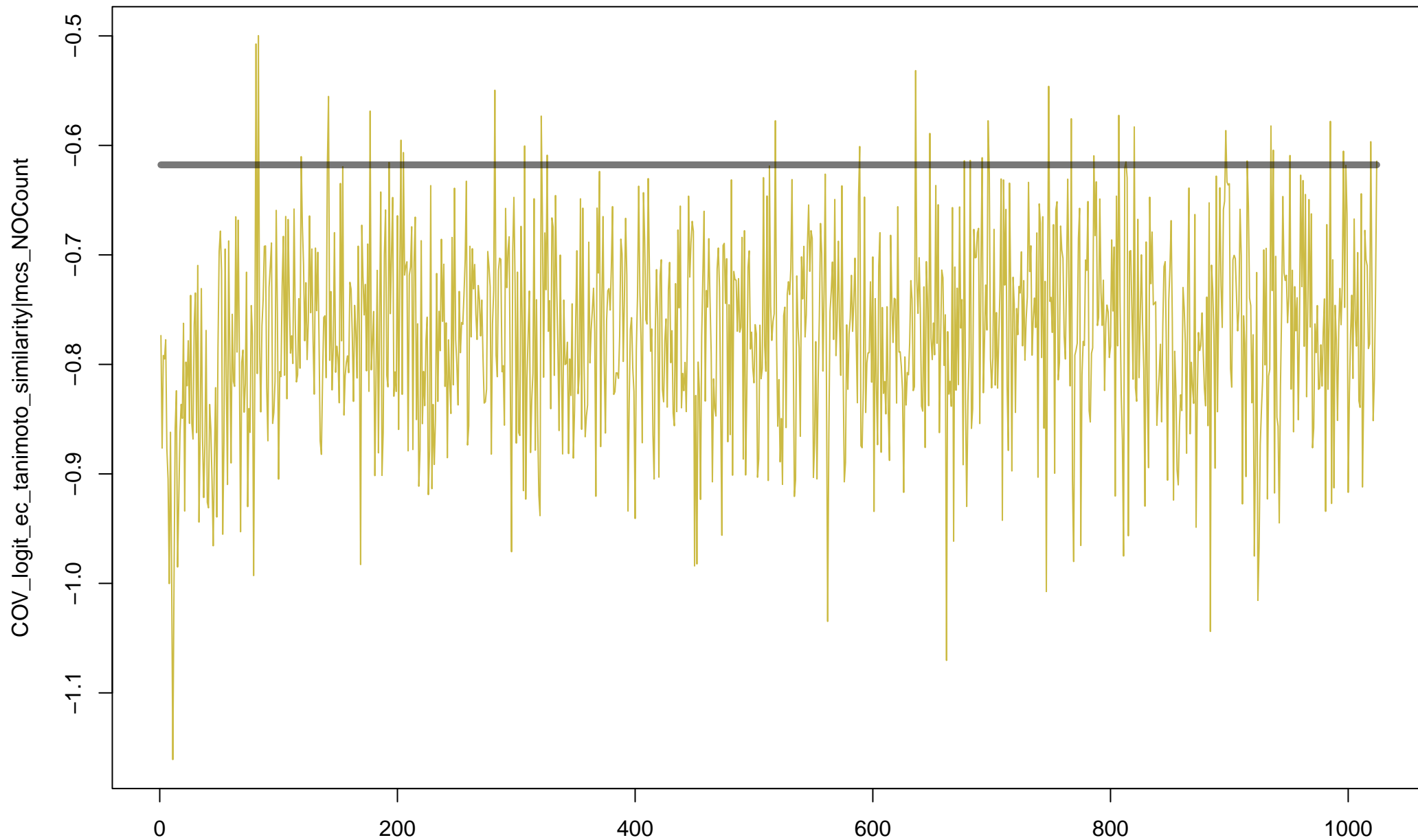
COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 217 | BMK = 0.108 | MCSE(6.27) = 6.1 | stat: FALSE | burn: 0 | rel.err: -0.432



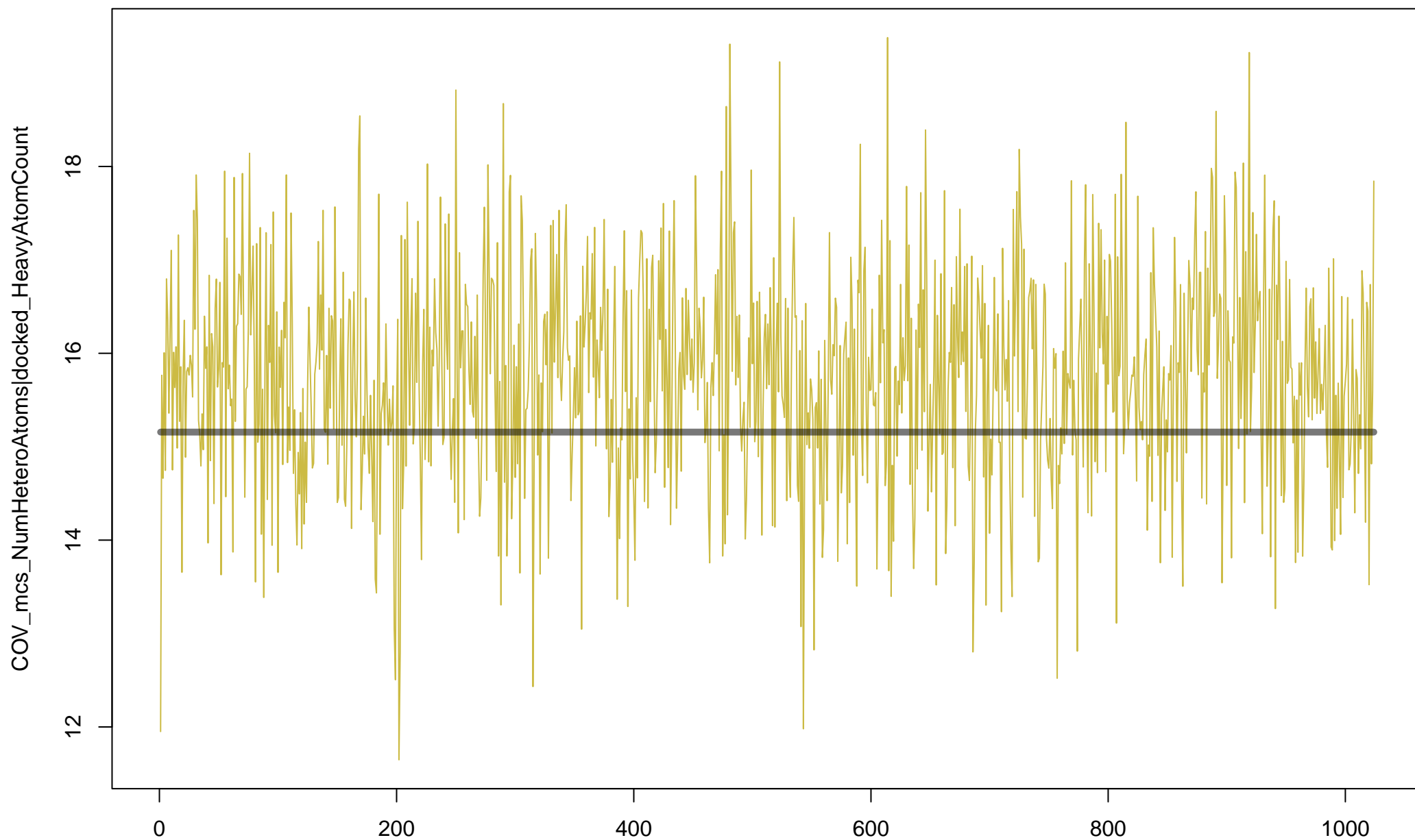
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0541 | MCSE(6.27) = 3.32 | stat: TRUE | burn: 0 | rel.err: -1.2



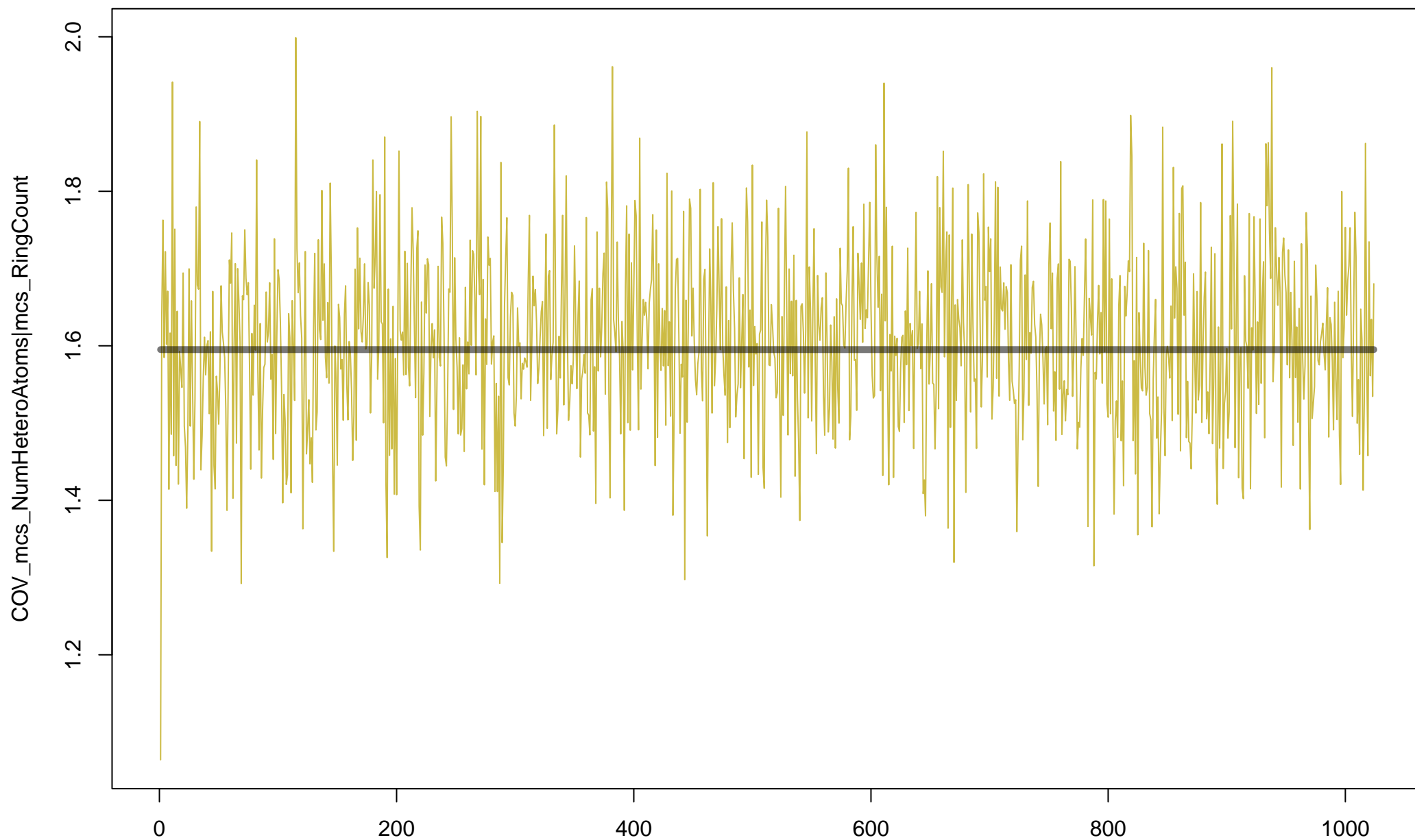
COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 649 | BMK = 0.0922 | MCSE(6.27) = 4.62 | stat: FALSE | burn: 0 | rel.err: -1.74



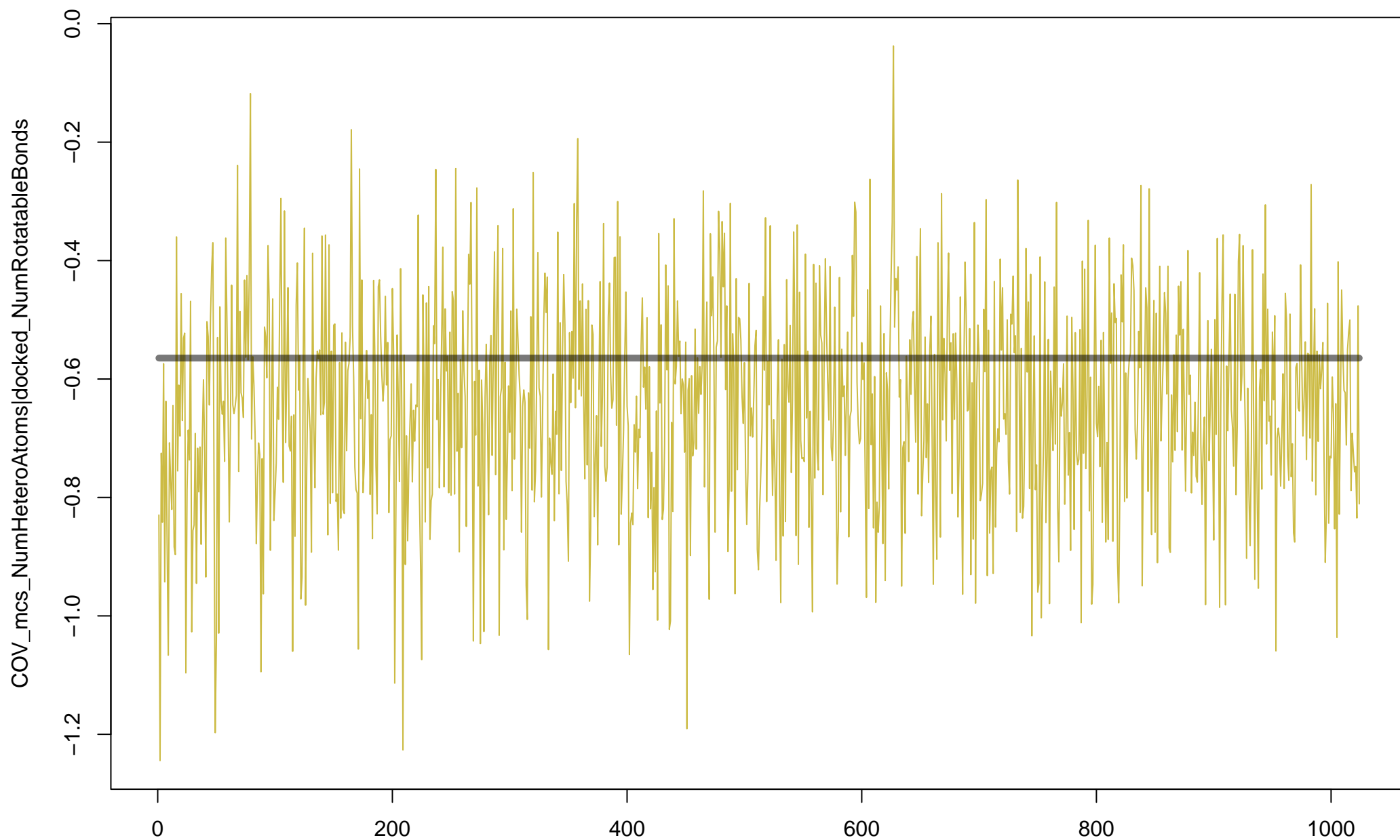
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0398 | MCSE(6.27) = 3.89 | stat: TRUE | burn: 0 | rel.err: 0.519



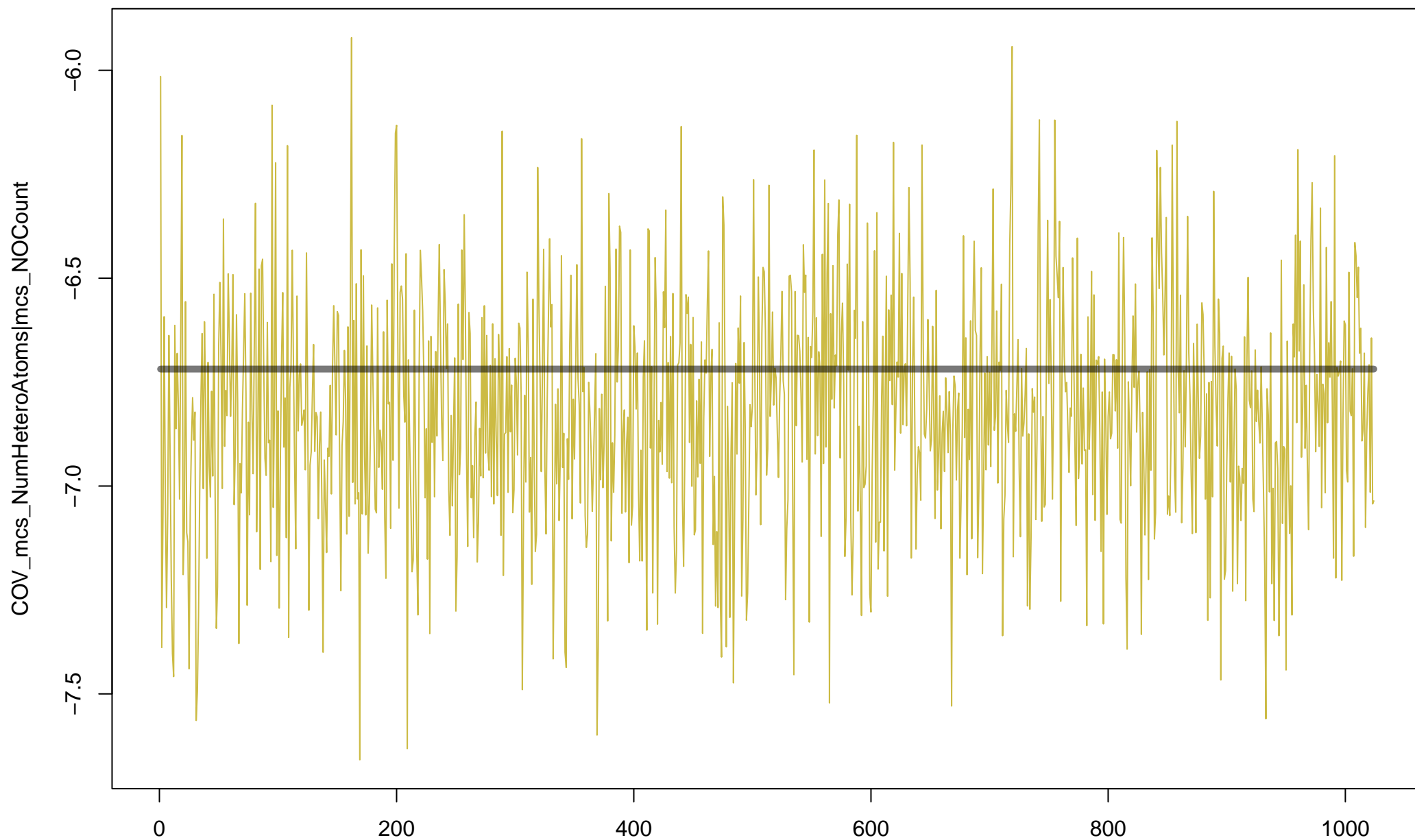
COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0535 | MCSE(6.27) = 3.13 | stat: FALSE | burn: 0 | rel.err: 0.0984



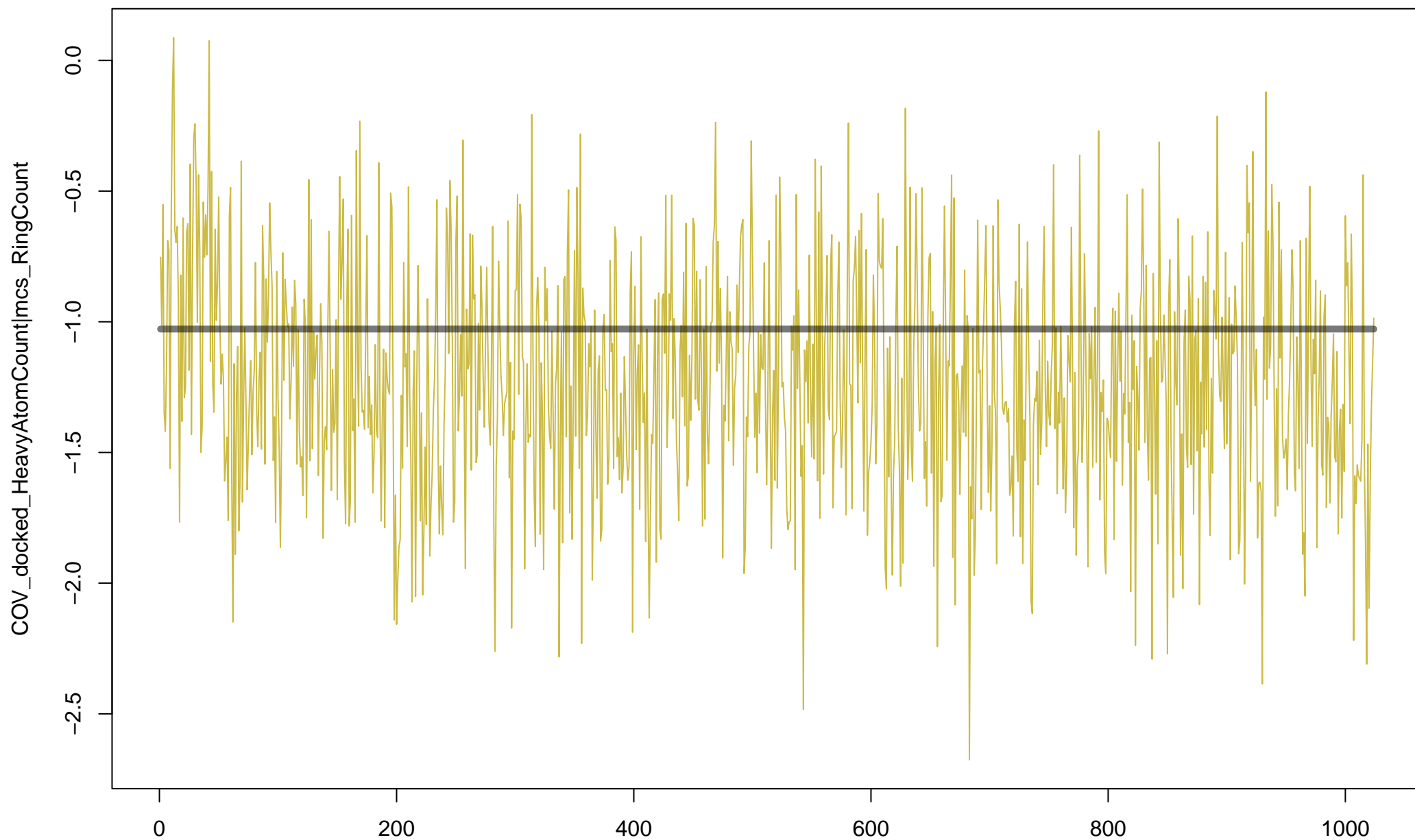
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 903 | BMK = 0.0911 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0 | rel.err: -0.458



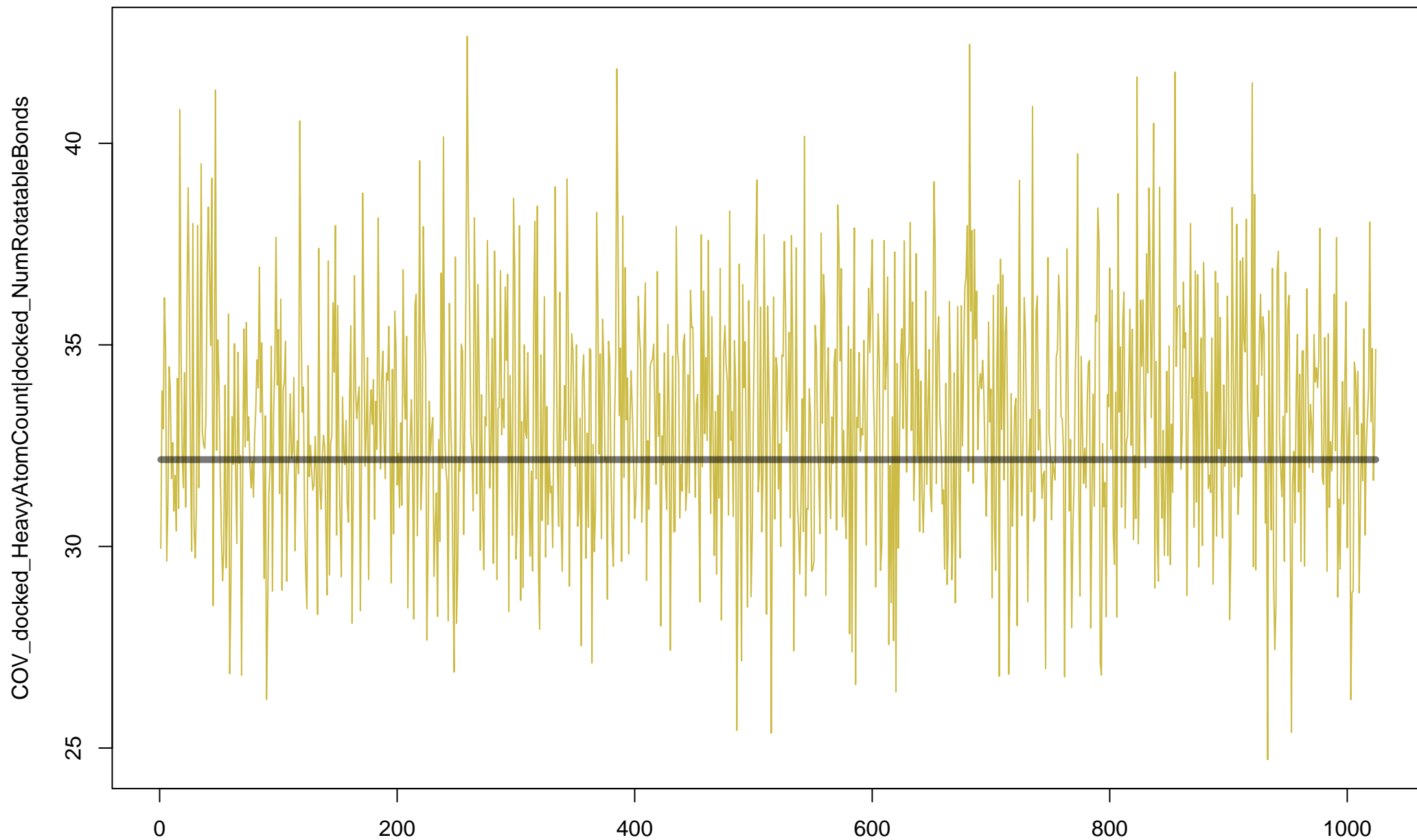
COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 919 | BMK = 0.081 | MCSE(6.27) = 4.02 | stat: TRUE | burn: 0 | rel.err: -0.382



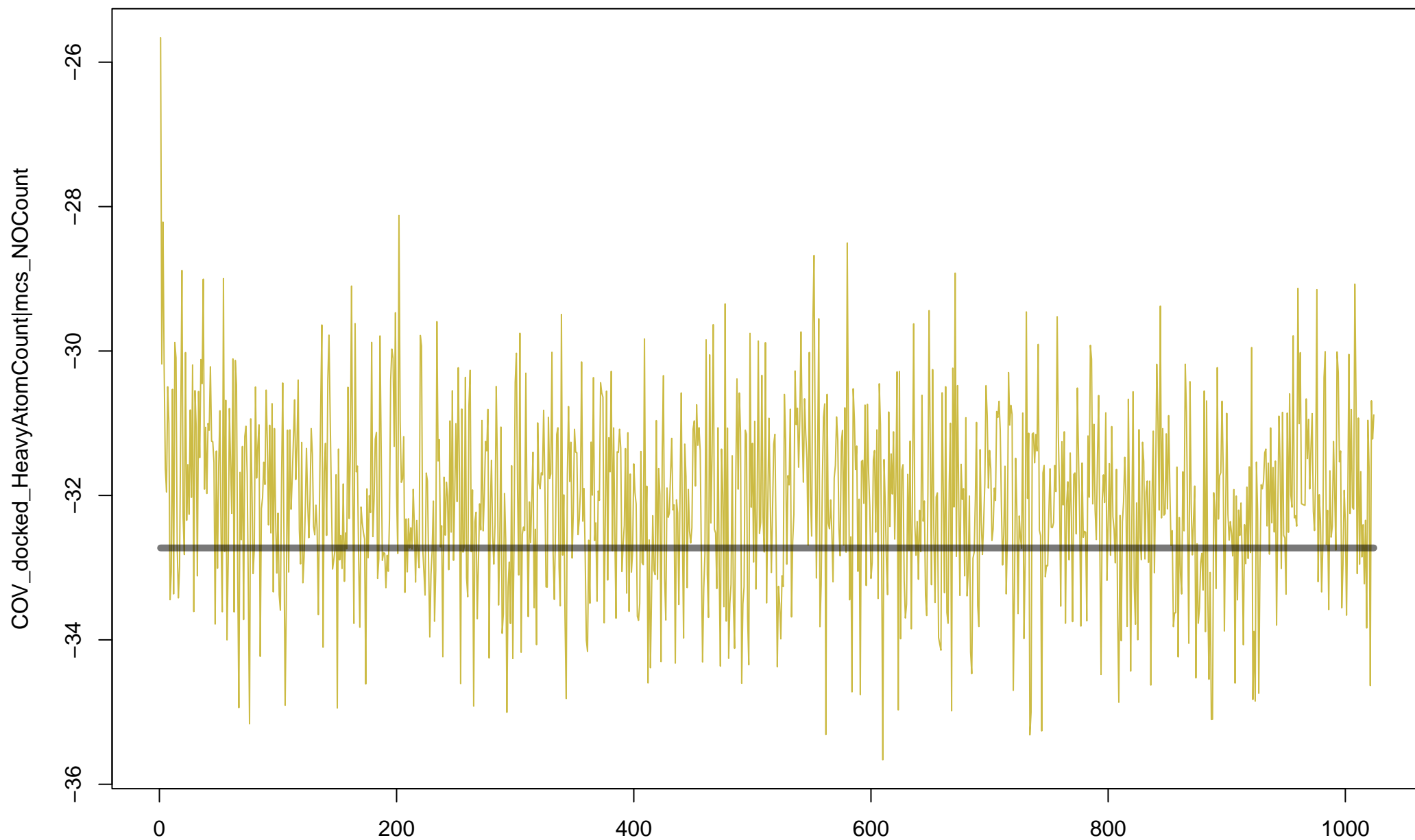
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 796 | BMK = 0.0629 | MCSE(6.27) = 4.52 | stat: FALSE | burn: 0 | rel.err: -0.464



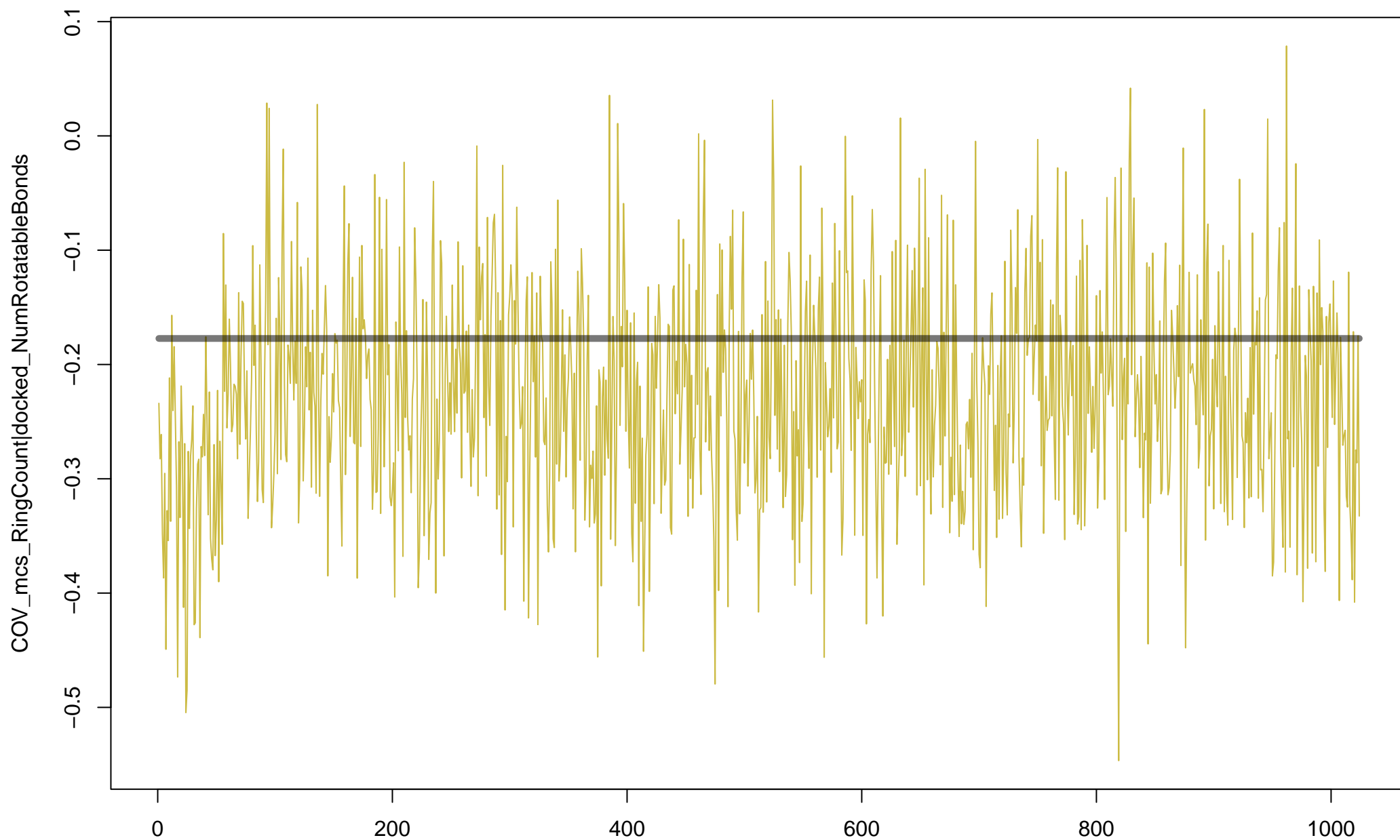
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0531 | MCSE(6.27) = 3.21 | stat: TRUE | burn: 0 | rel.err: 0.331



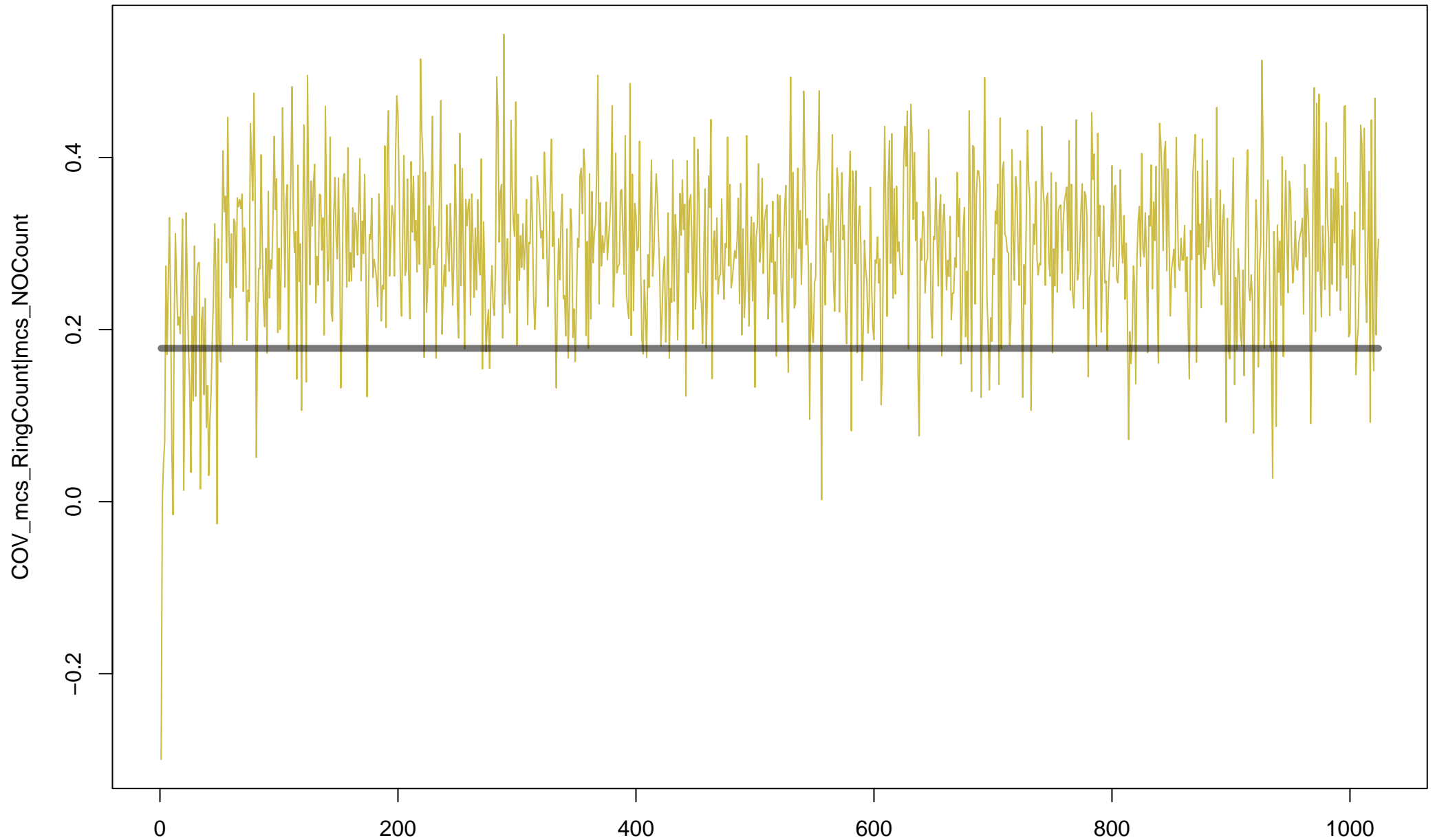
COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 795 | BMK = 0.0675 | MCSE(6.27) = 4.18 | stat: FALSE | burn: 0 | rel.err: 0.502



COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 914 | BMK = 0.0509 | MCSE(6.27) = 4.62 | stat: FALSE | burn: 0 | rel.err: -0.531



COV_mcs_RingCount|mcs_NOCount
ESS = 313 | BMK = 0.0664 | MCSE(6.27) = 5.89 | stat: FALSE | burn: 0 | rel.err: 1.28



COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 925 | BMK = 0.0684 | MCSE(6.27) = 3.35 | stat: TRUE | burn: 0 | rel.err: -1.67

