

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.608124143410639

max MCSE = 6.31821815693853

all stationary: FALSE

burn: 204

max rel.err.: 1.36835135358739

-- STATS 1D --

min ESS = 133.261024732155

max BMK = 0.0654669919210499

max MCSE = 6.4369212014753

all stationary: FALSE

burn: 0

max rel.err.: 2.81210486295946

-- STATS 2D --

min ESS = 935.113543390868

max BMK = 0.0787826810775219

max MCSE = 3.86209544591462

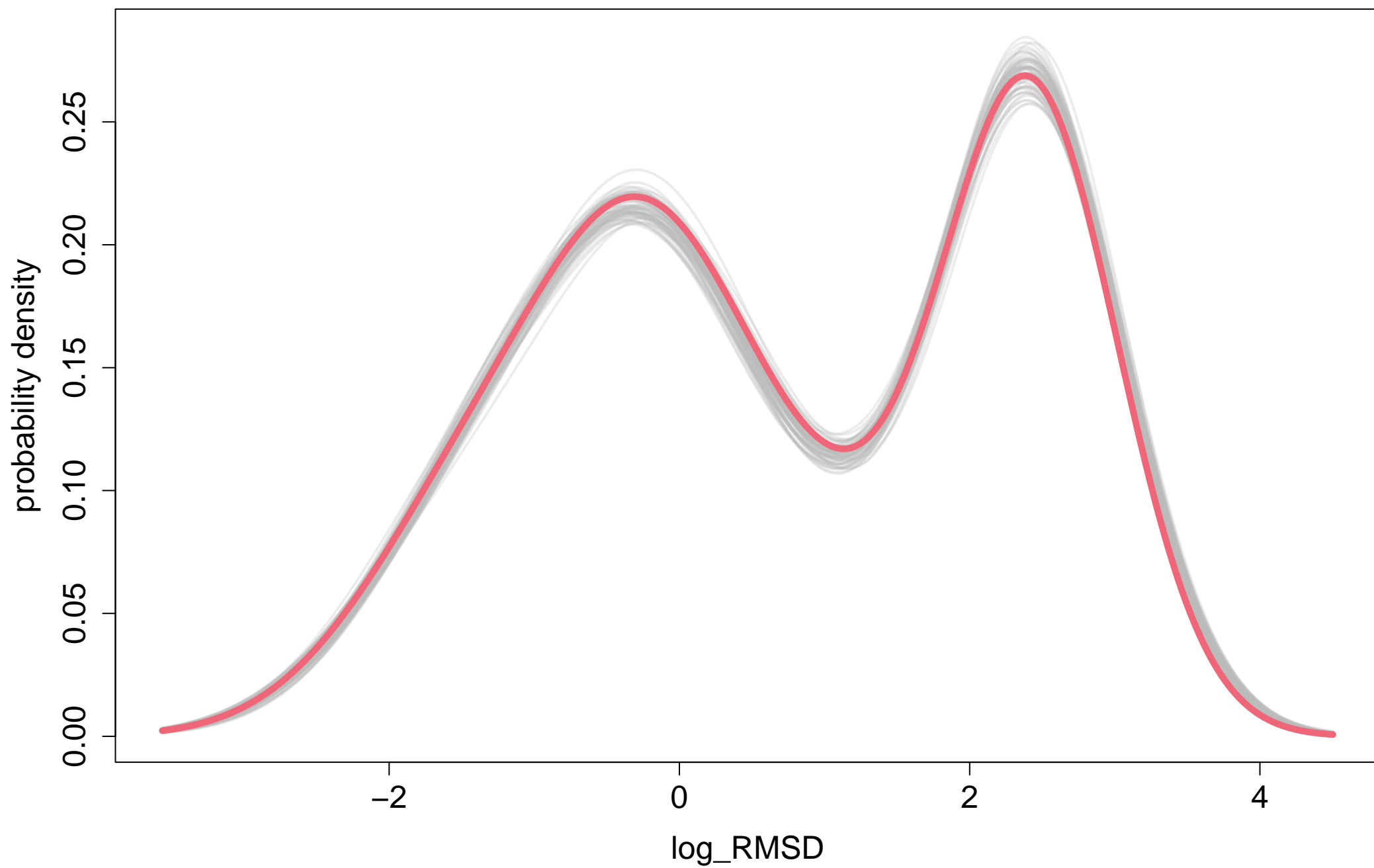
all stationary: TRUE

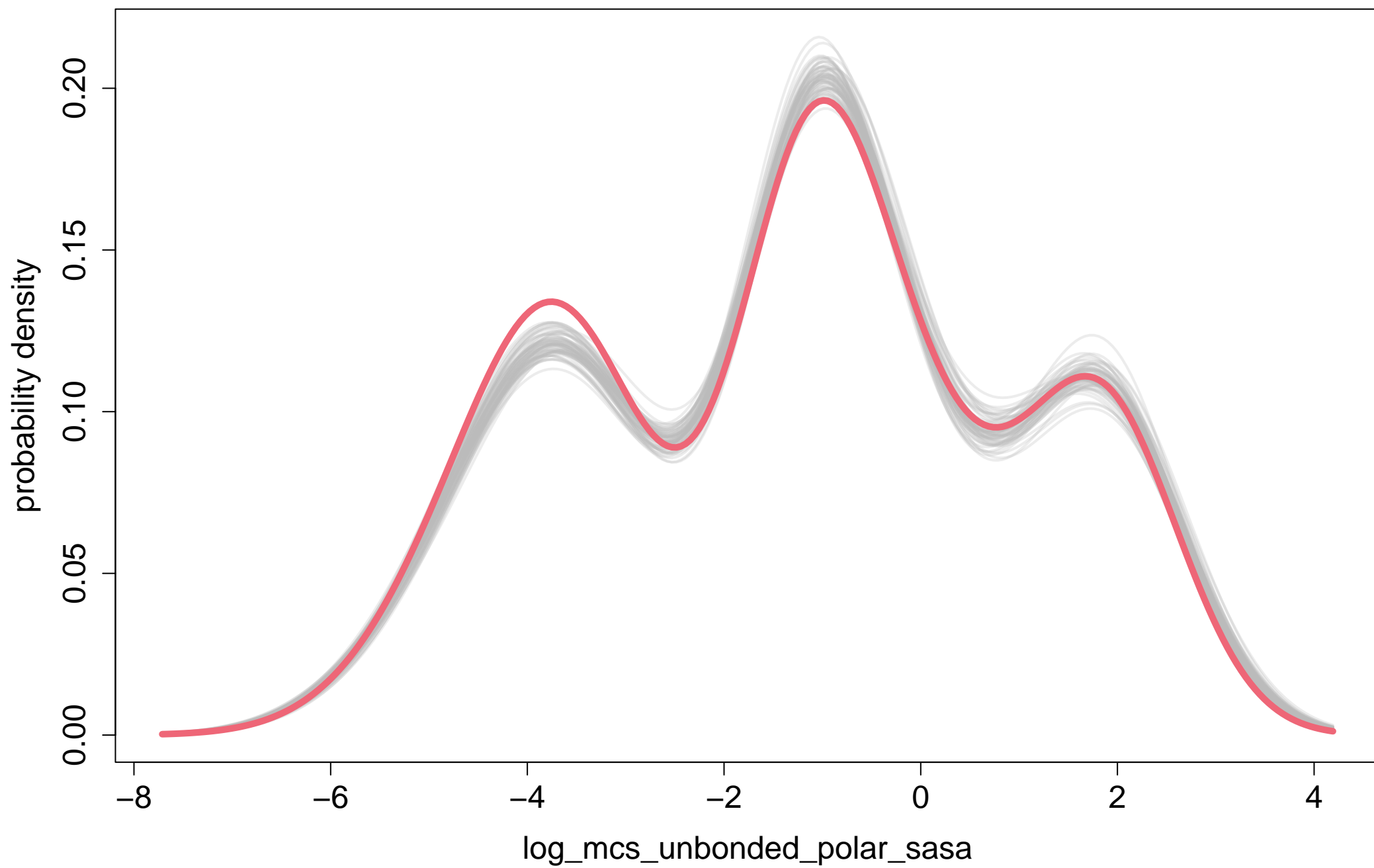
burn: 0

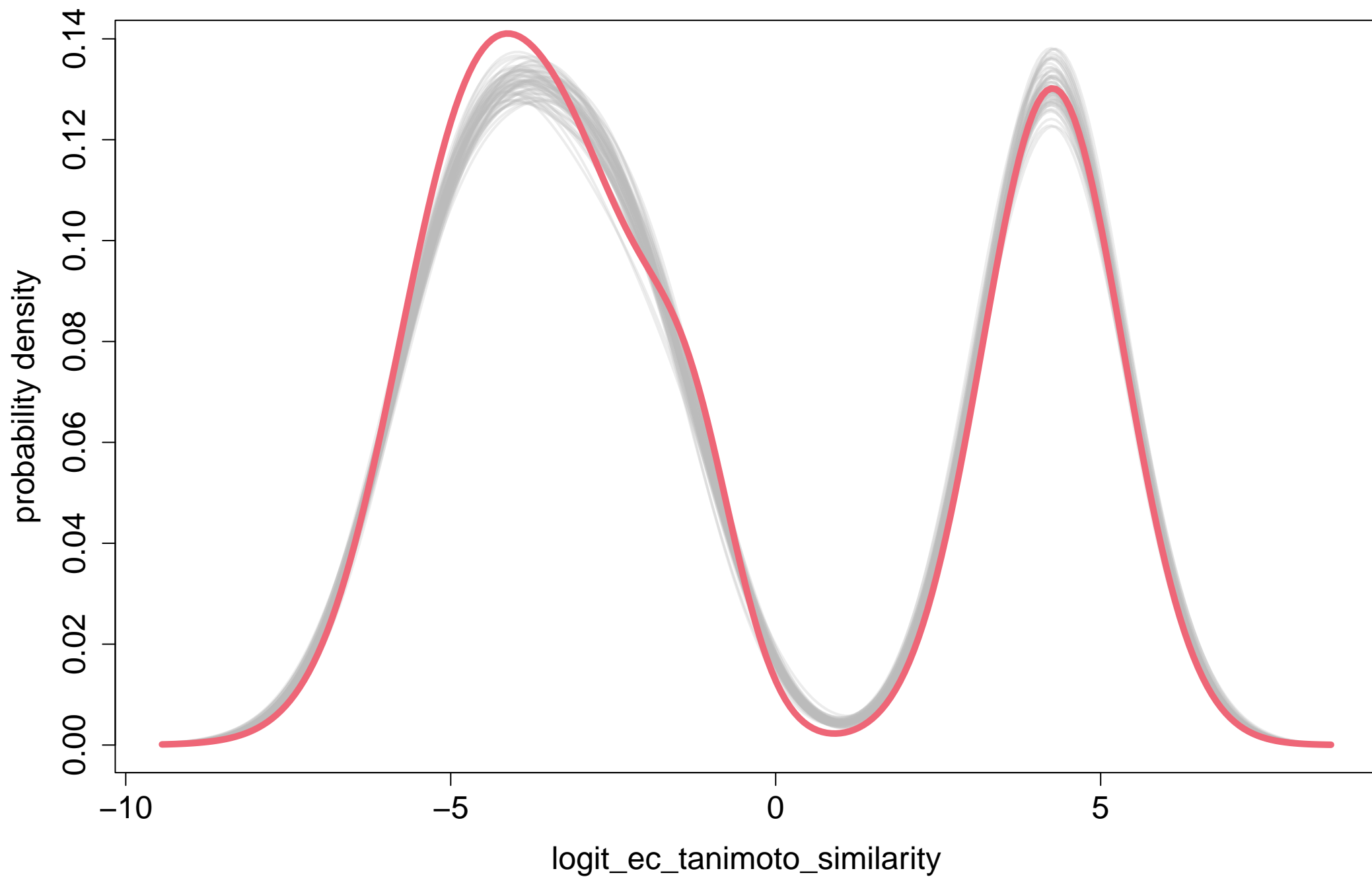
max rel.err.: 2.11280045160449

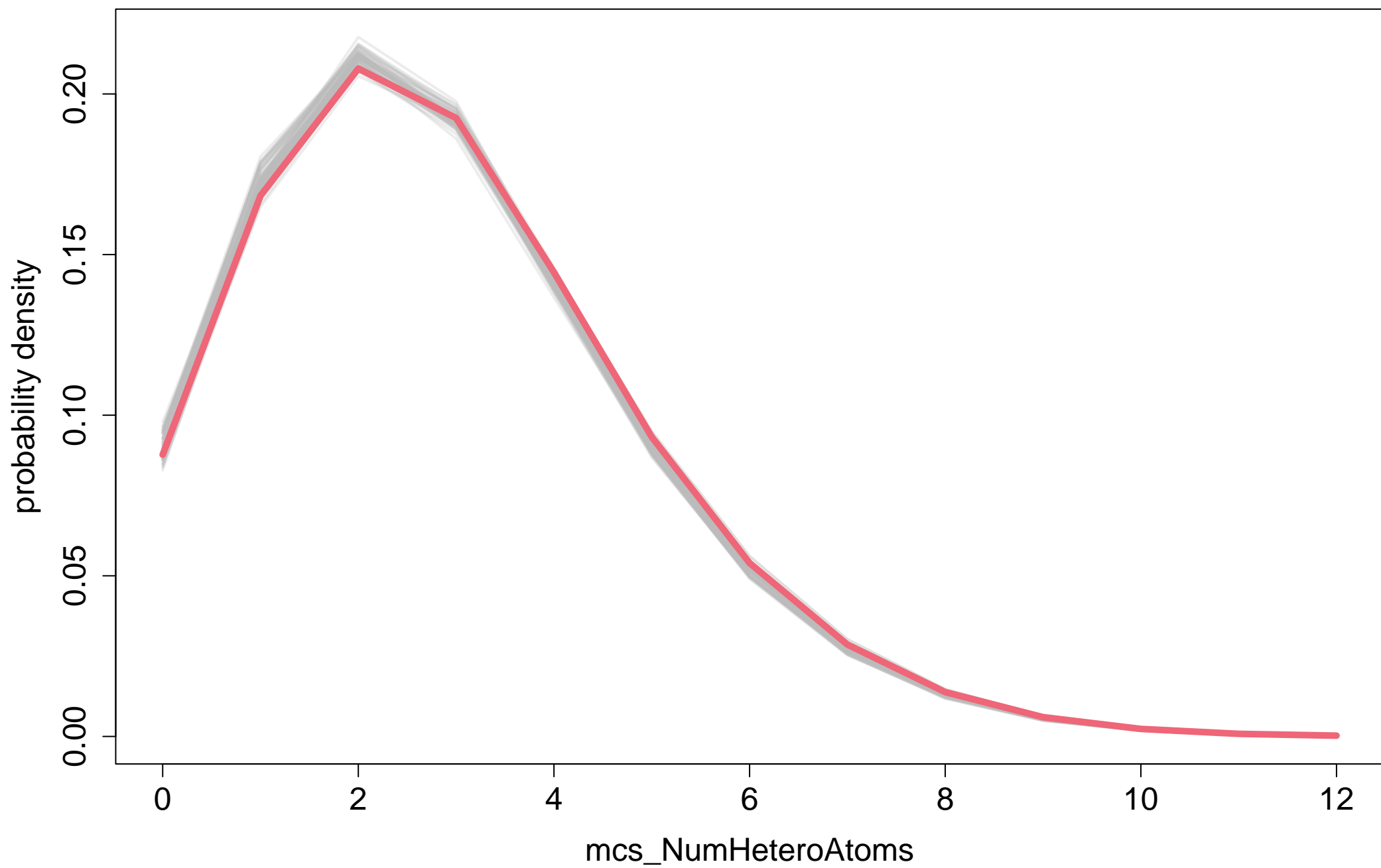
Occupied clusters: 8 of 64

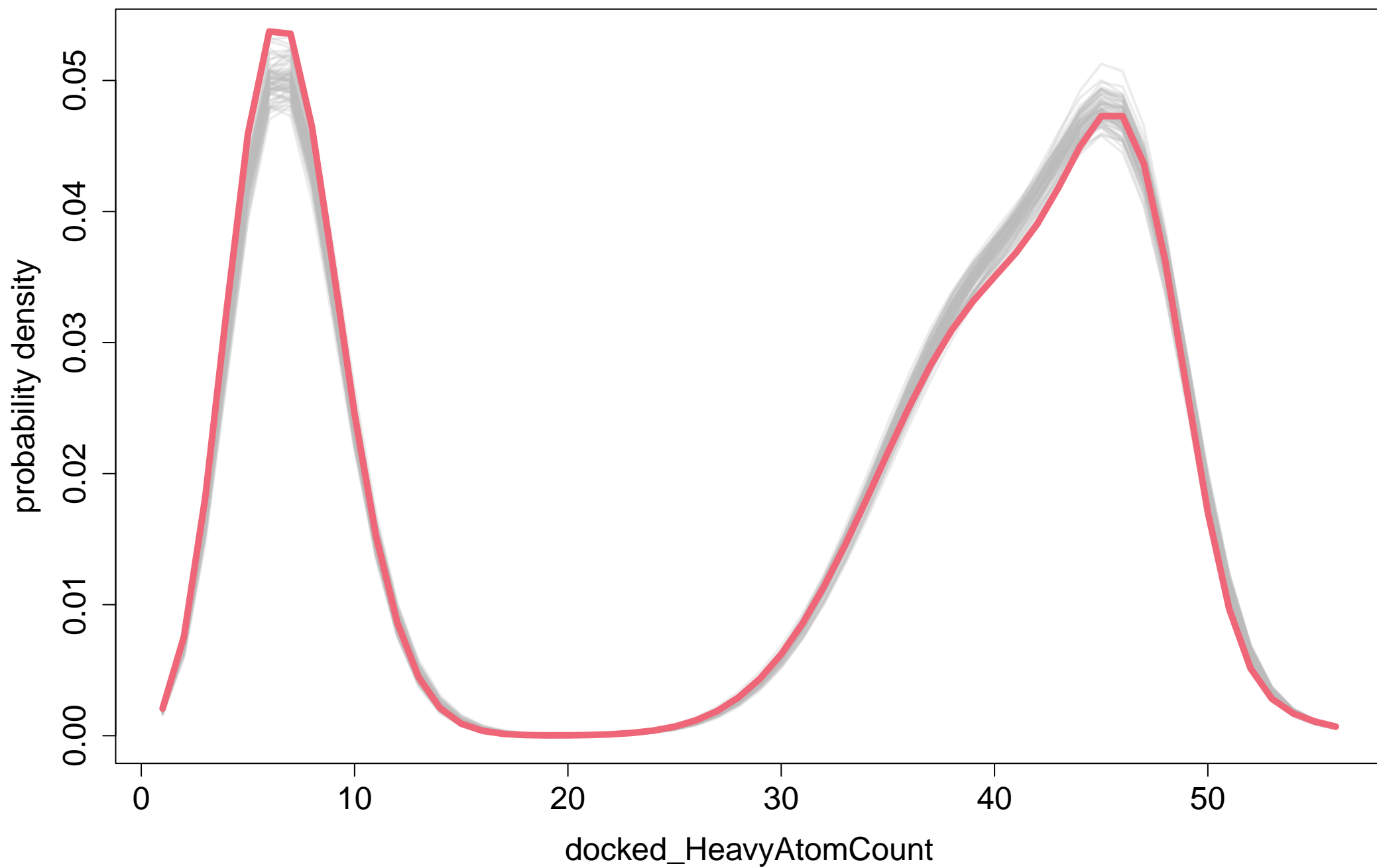
LL: -62500 +- 13.8

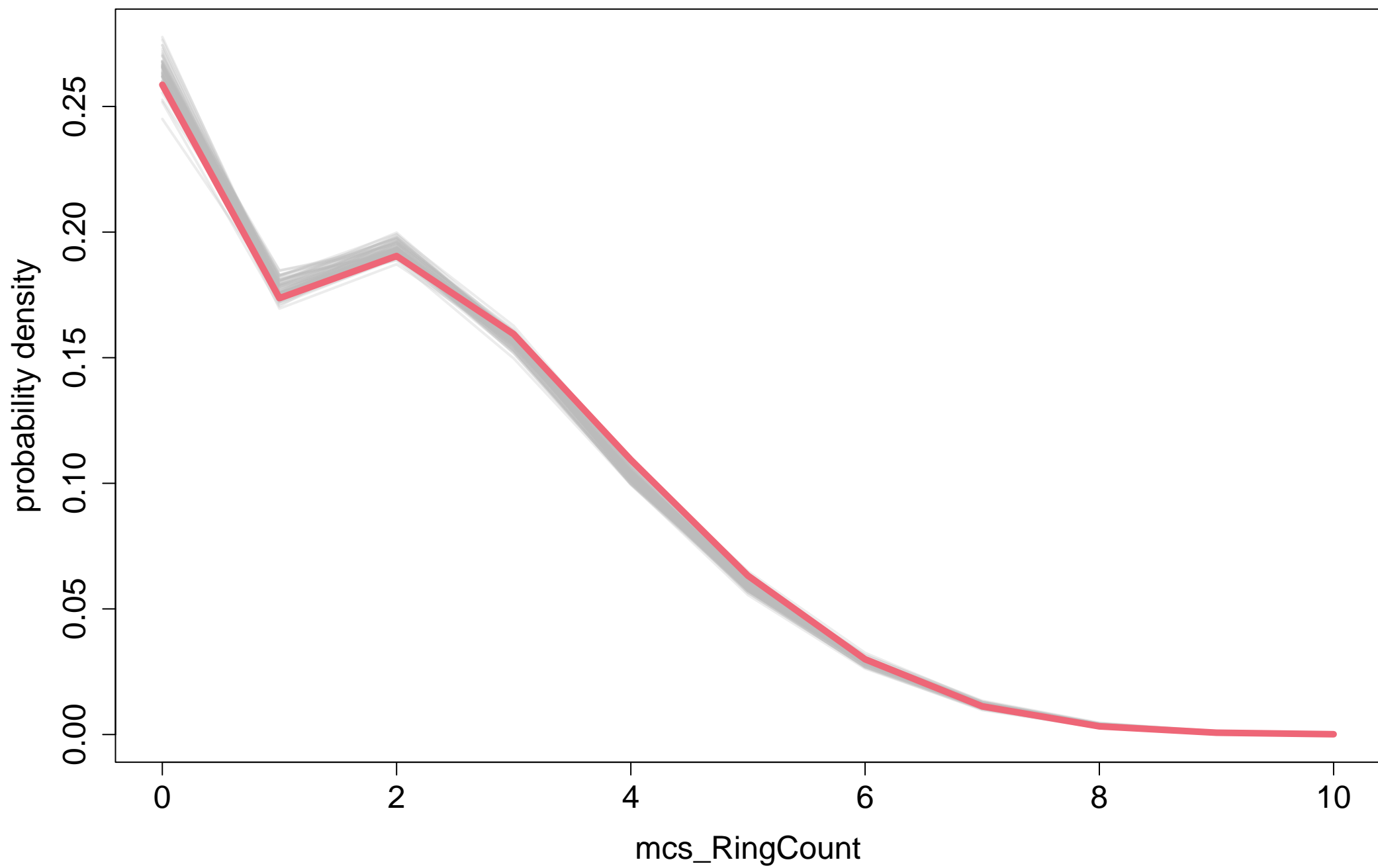


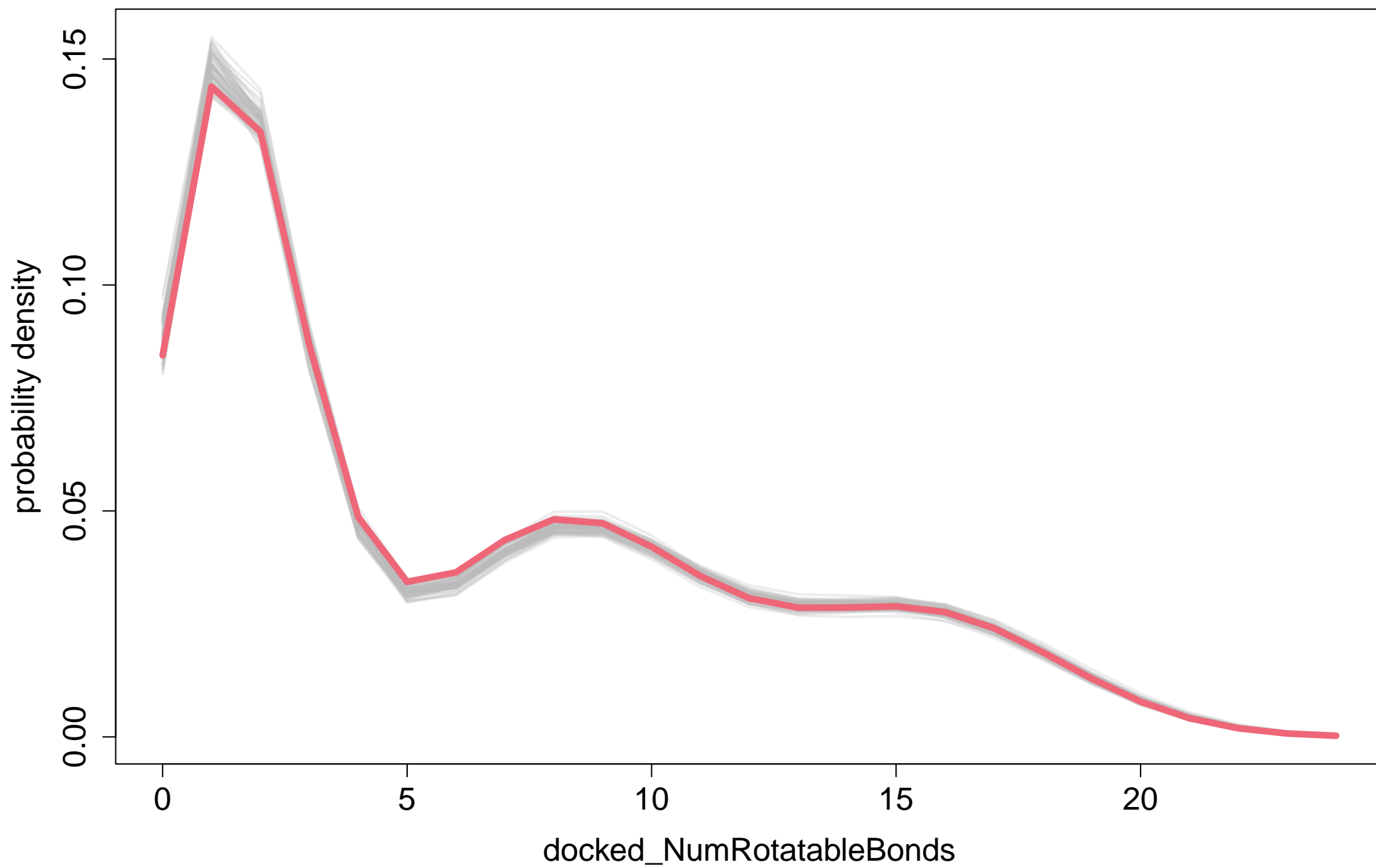




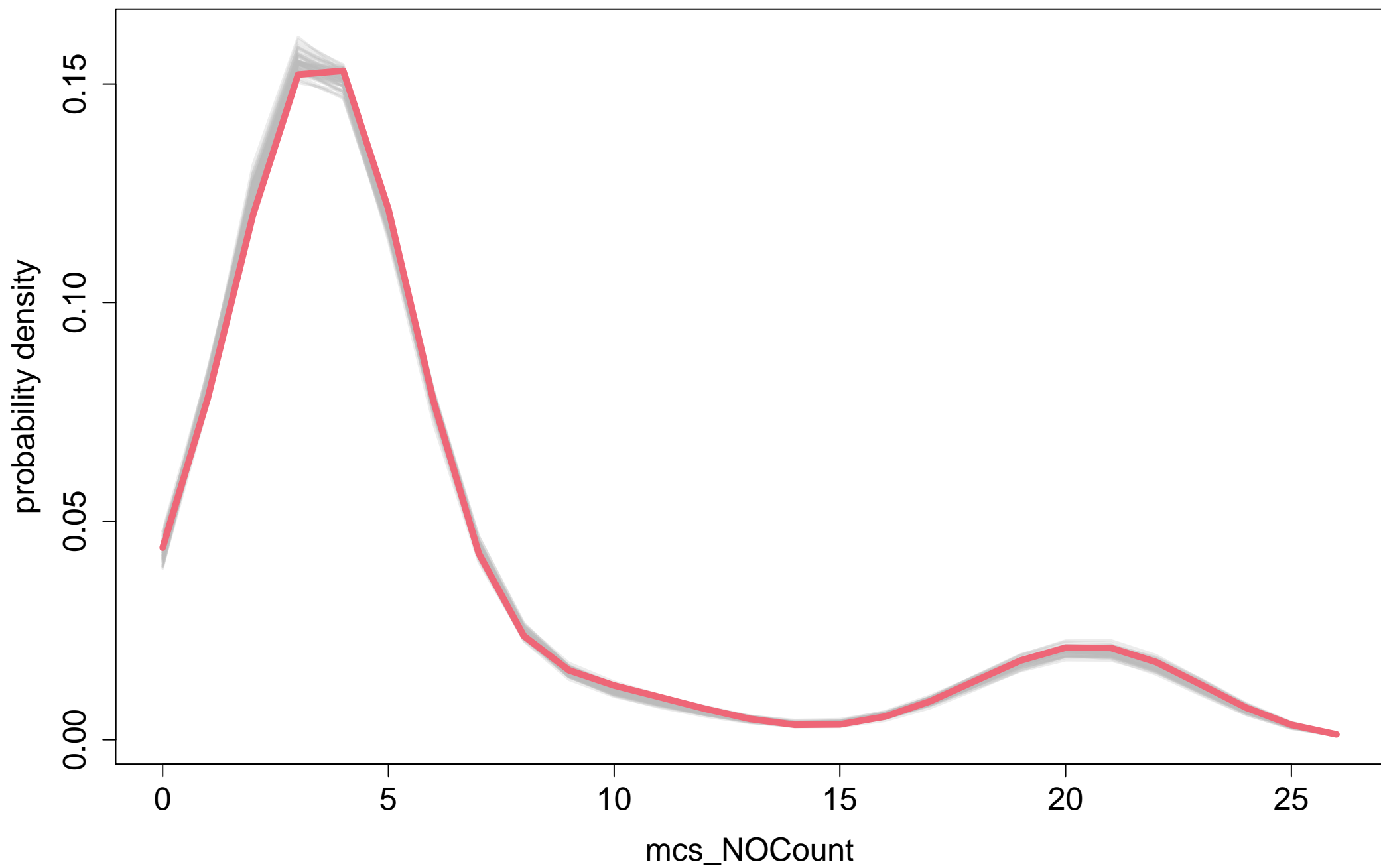


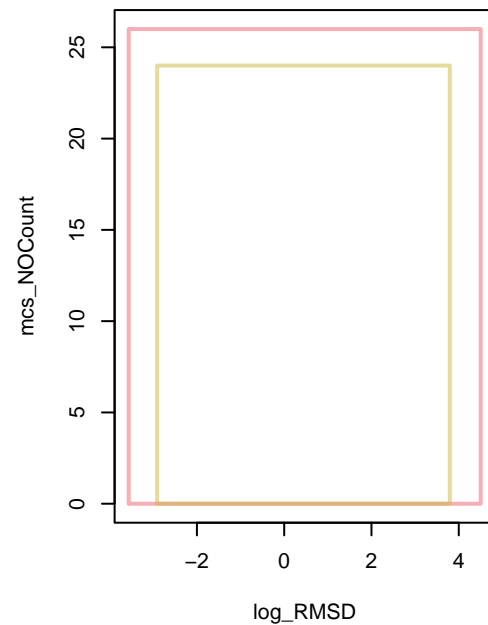
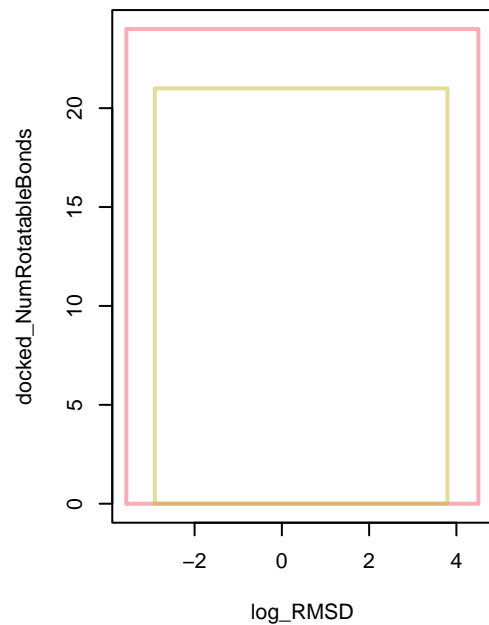
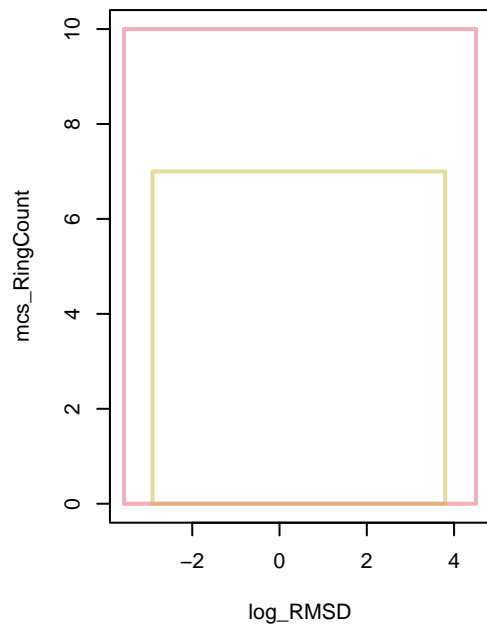
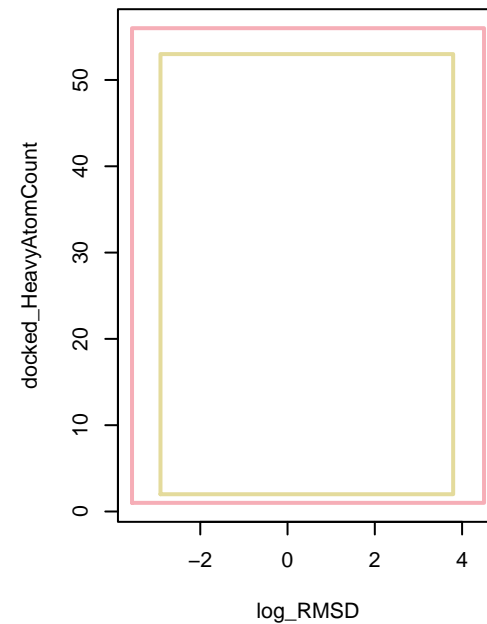
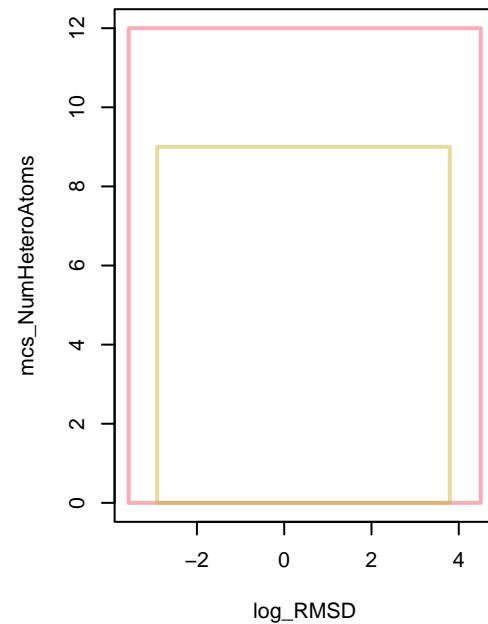
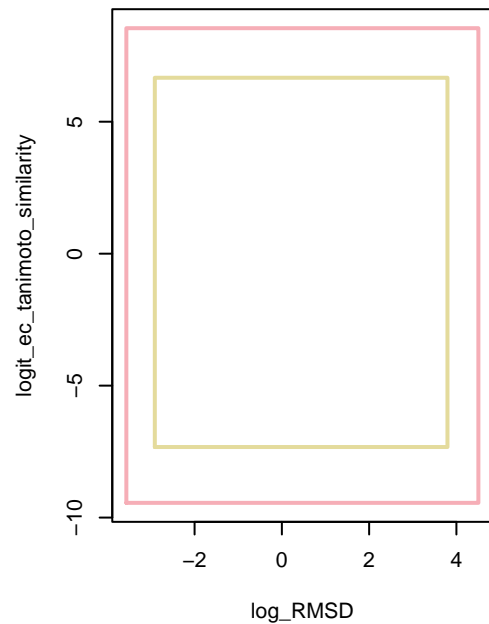
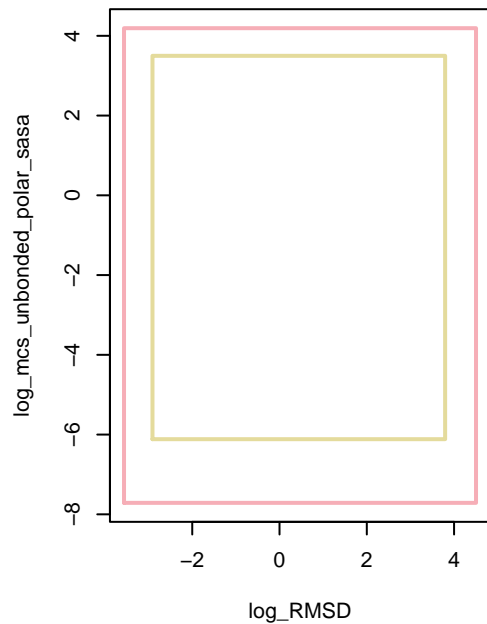




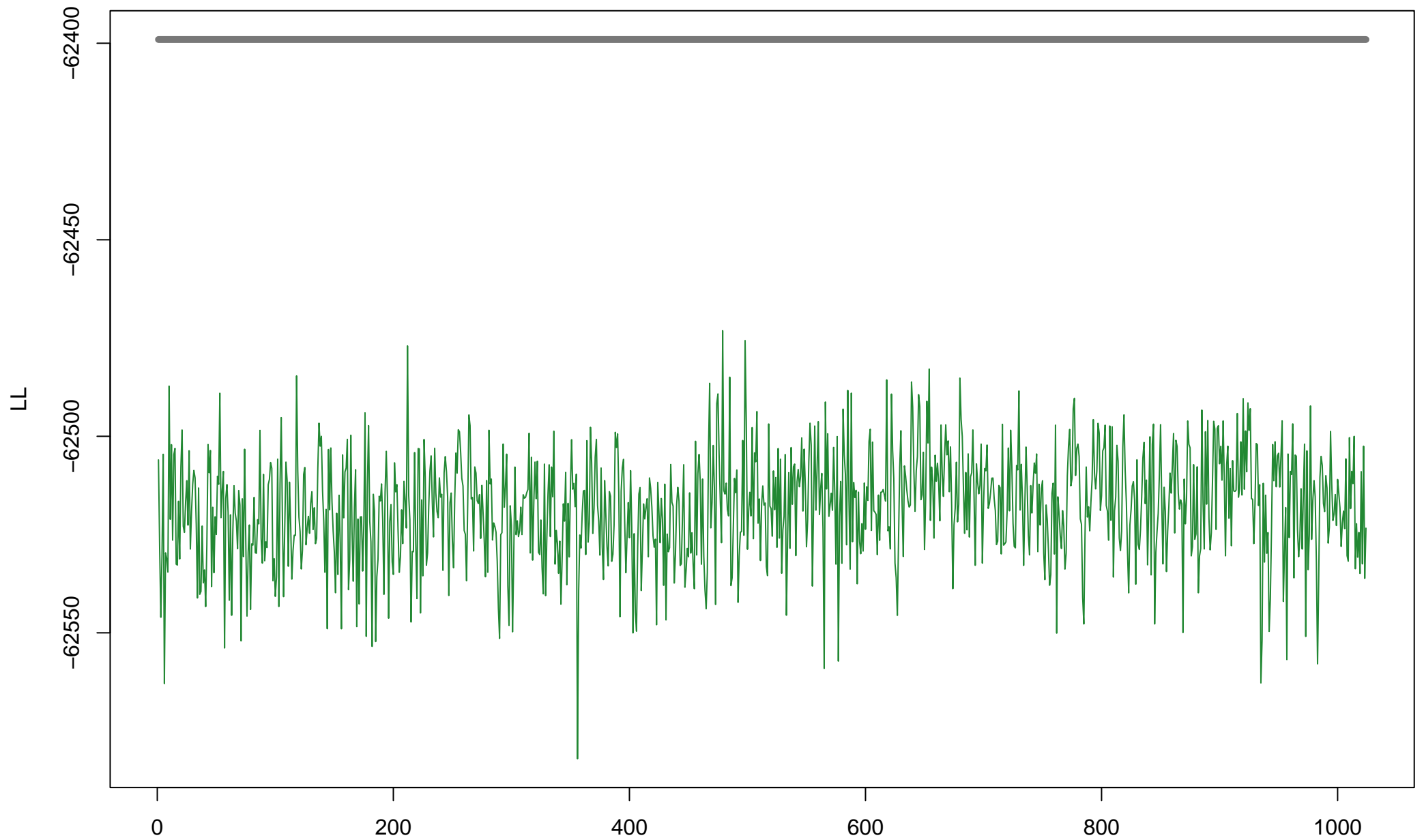






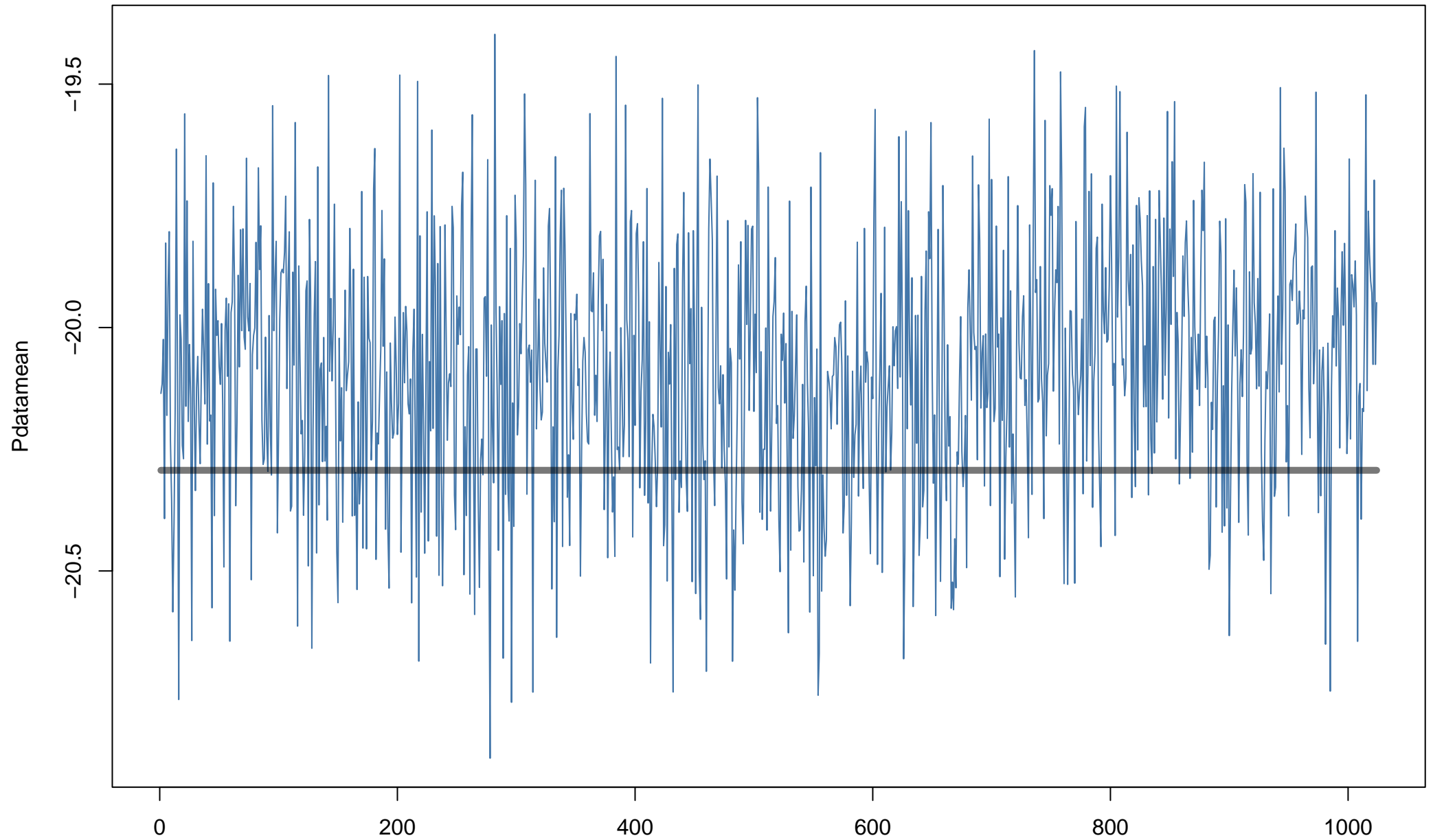


LL



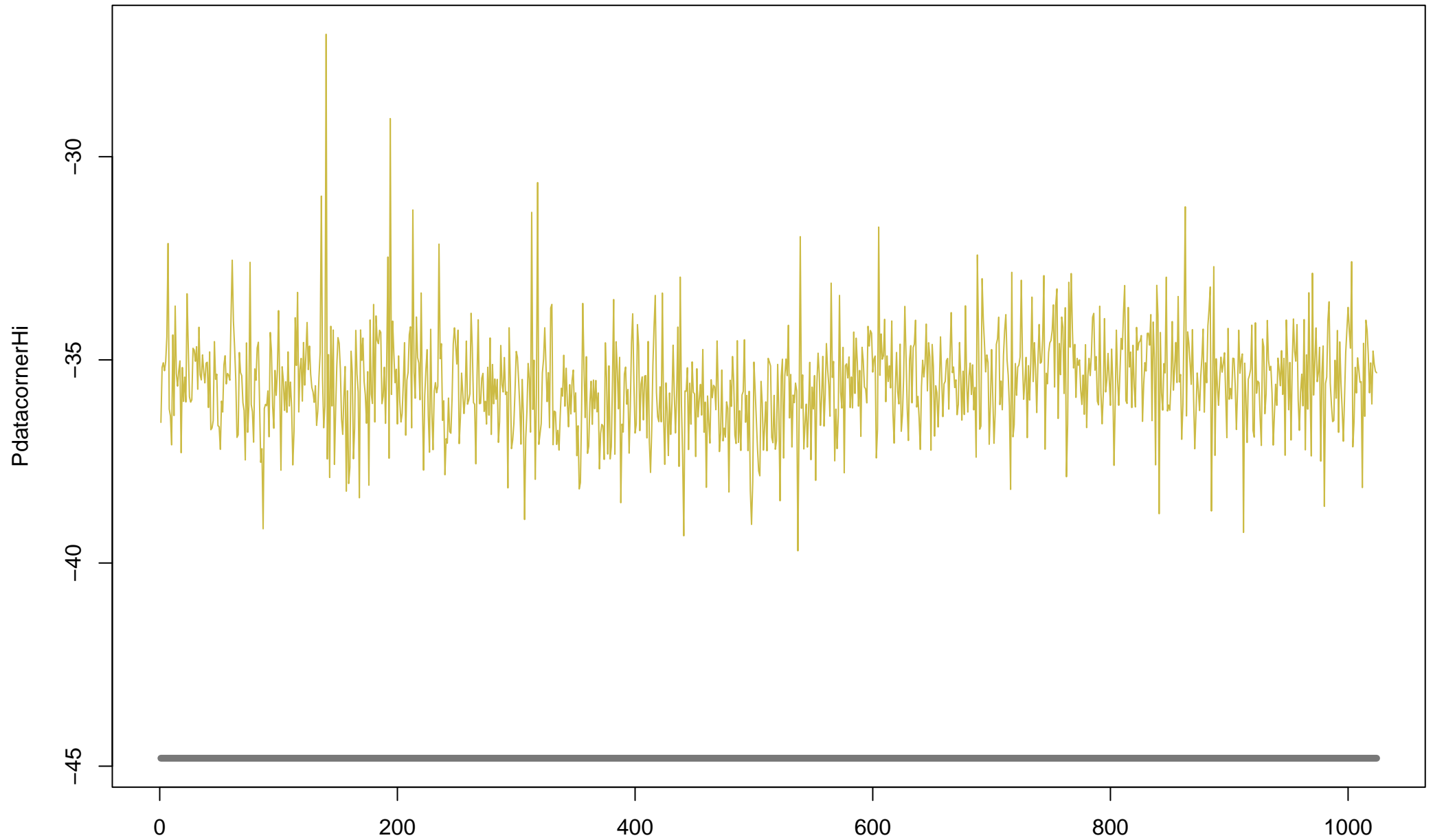
**Pdatamean**

**ESS = 2.22e-16 | BMK = 0.0469 | MCSE(6.27) = 3.91 | stat: TRUE | burn: 0 | rel.err: 0.816**



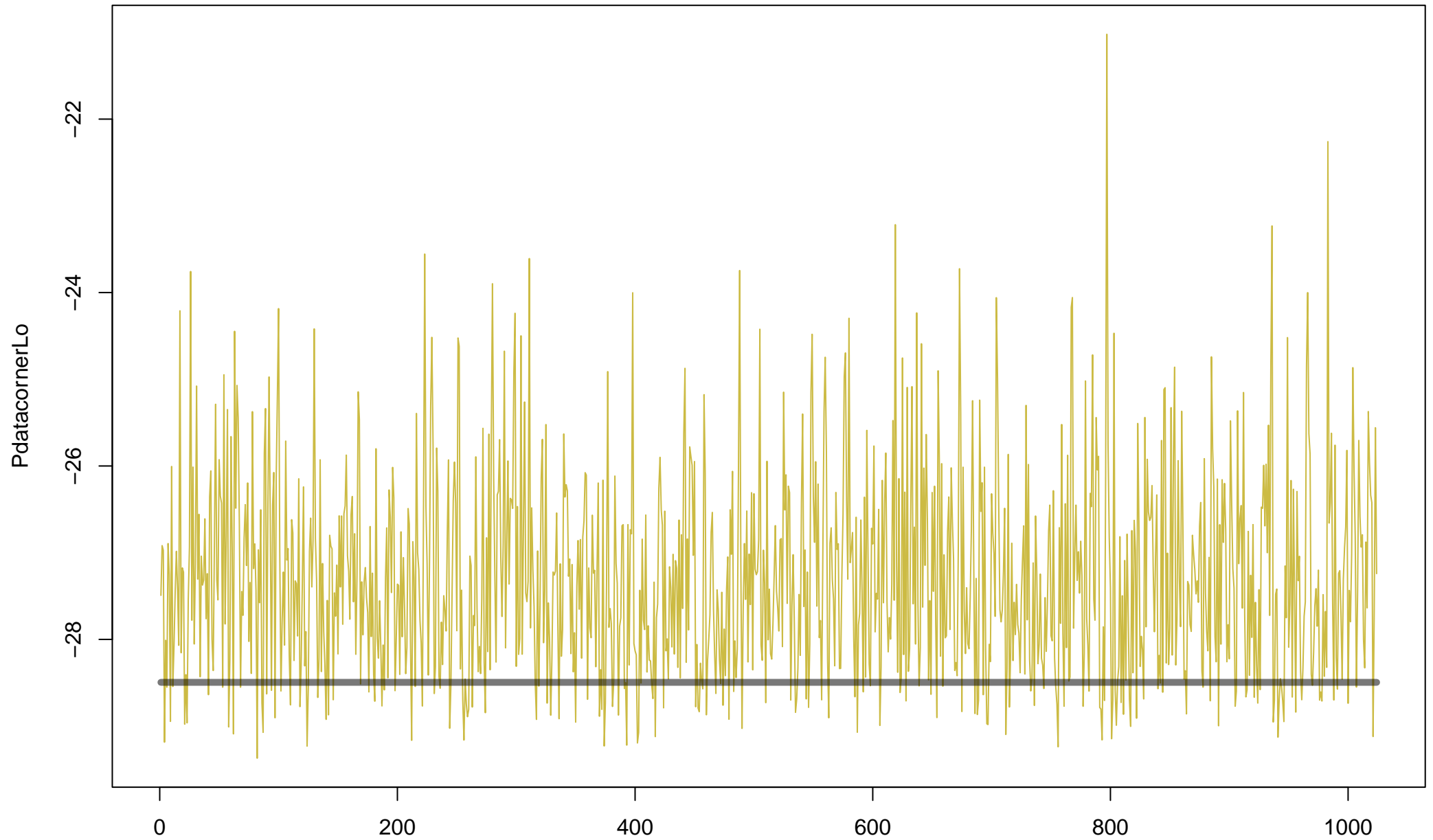
# PdatacornerHi

ESS = 2.22e-16 | BMK = 0.608 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 204 | rel.err: 0.0485

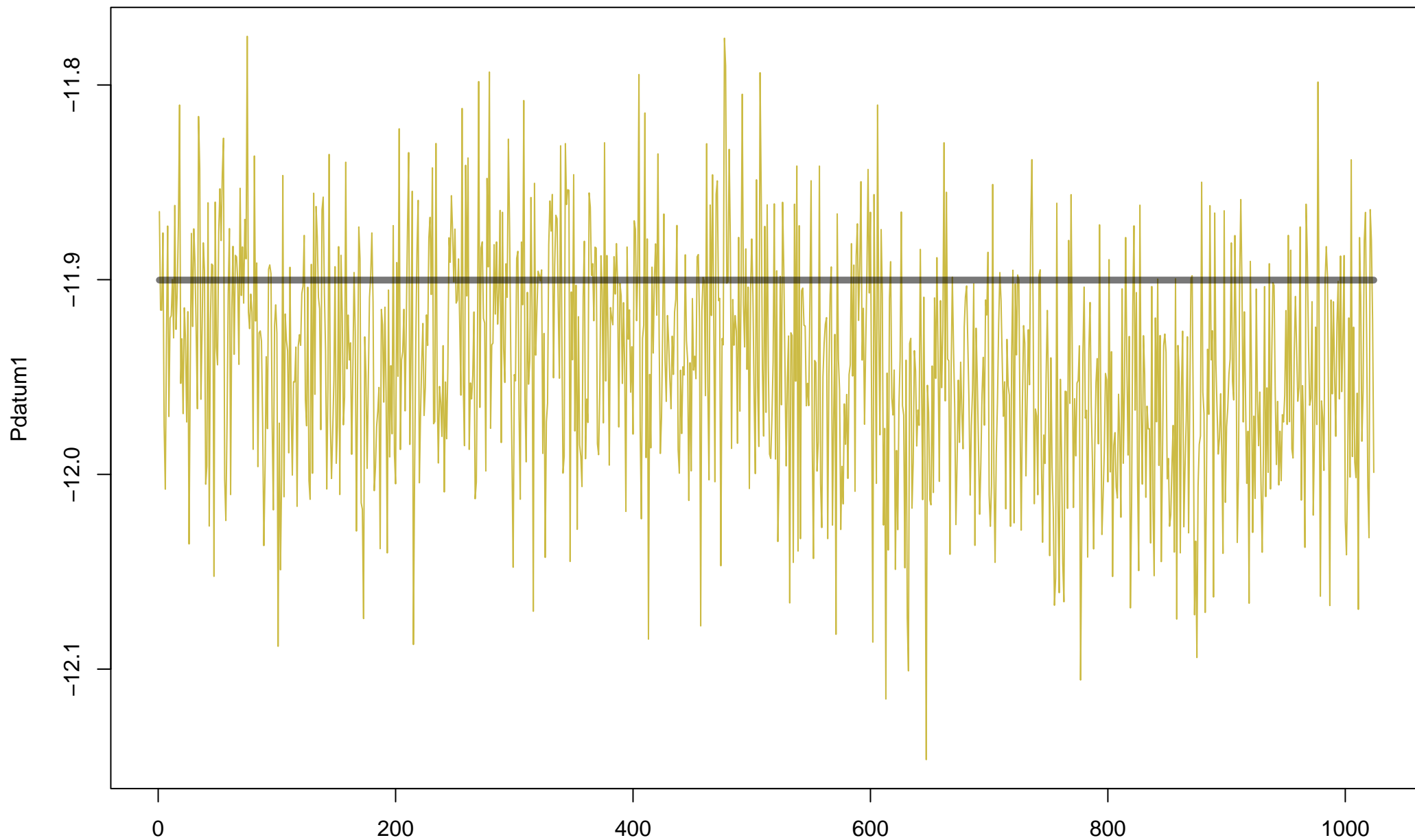


# PdatacornerLo

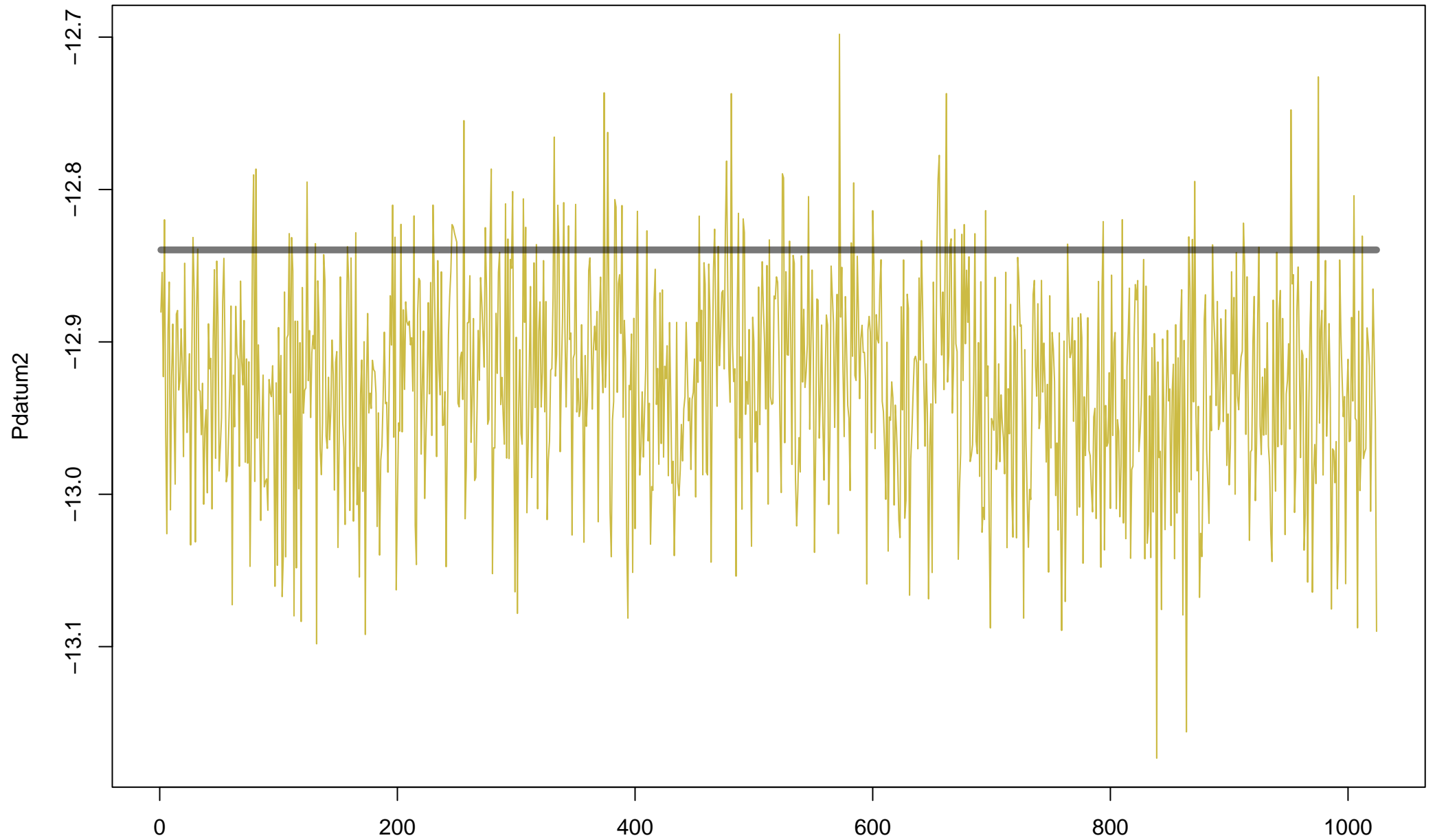
ESS = 2.22e-16 | BMK = 0.147 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | rel.err: 0.15



**Pdatum1**  
**ESS = 125 | BMK = 0.196 | MCSE(6.27) = 6.32 | stat: FALSE | burn: 0 | rel.err: -0.739**



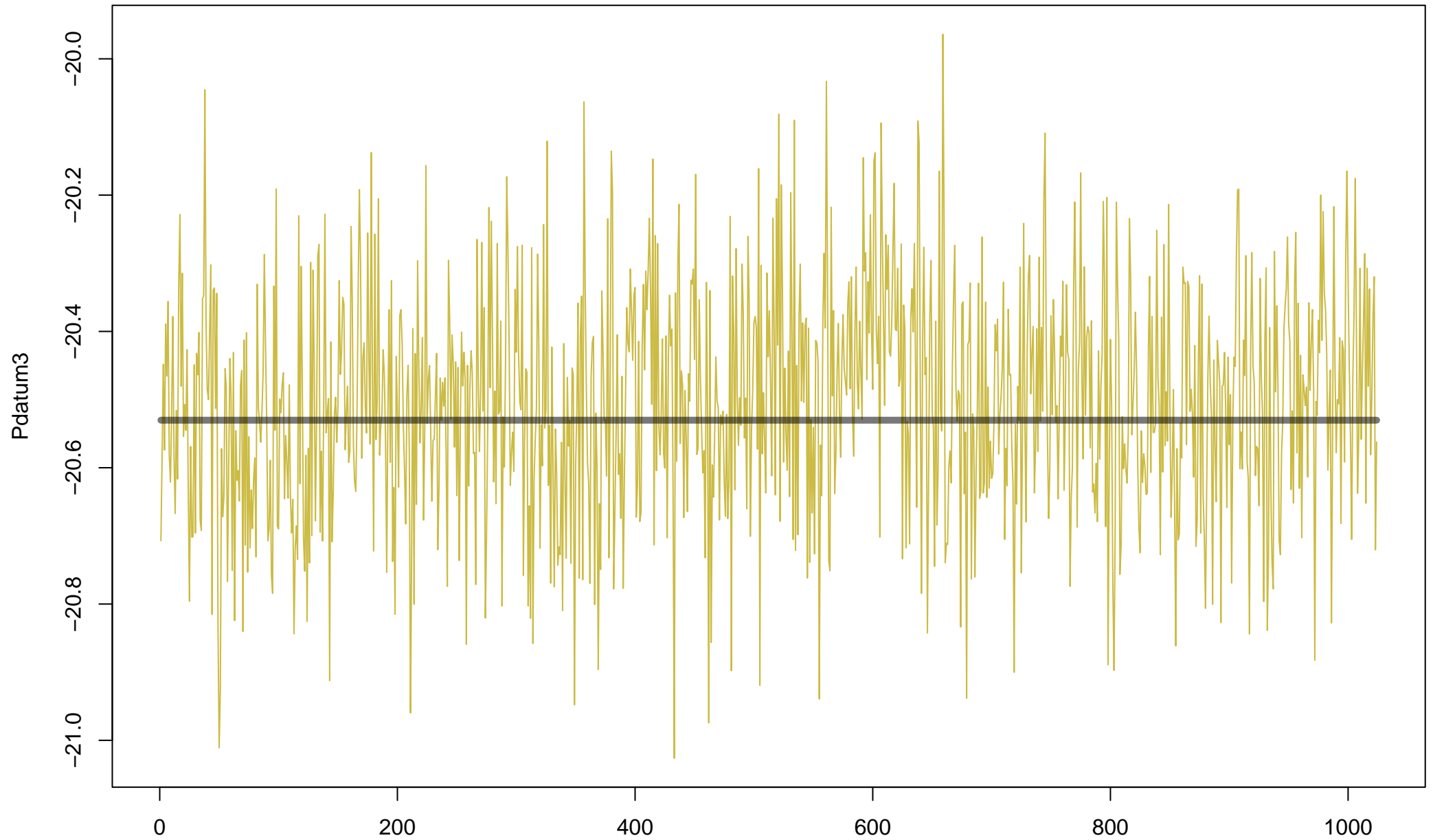
**Pdatum2**  
**ESS = 665 | BMK = 0.0773 | MCSE(6.27) = 5.01 | stat: TRUE | burn: 0 | rel.err: -1.37**





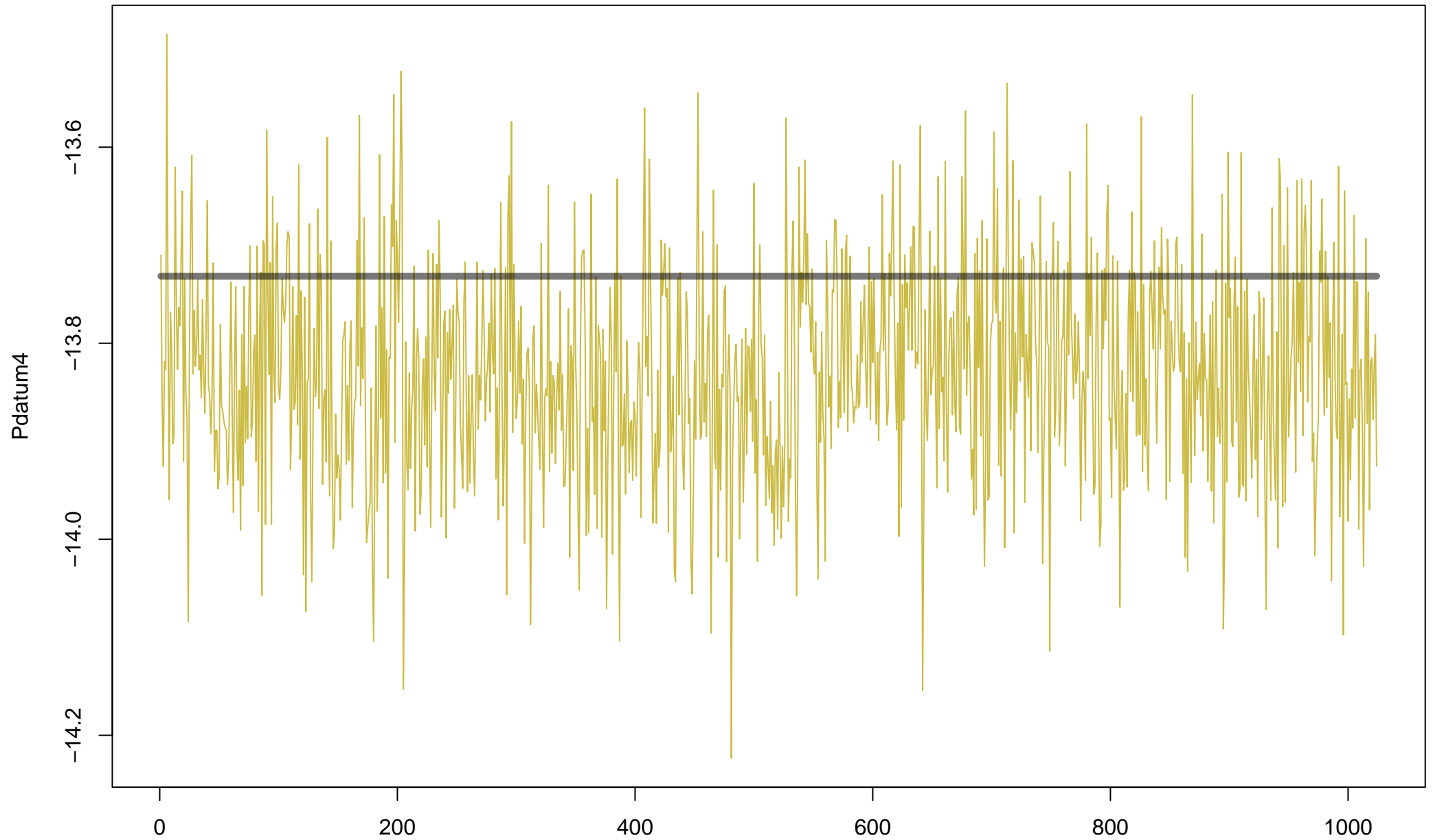
**Pdatum3**

**ESS = 2.22e-16 | BMK = 0.0834 | MCSE(6.27) = 4.9 | stat: TRUE | burn: 0 | rel.err: 0.237**



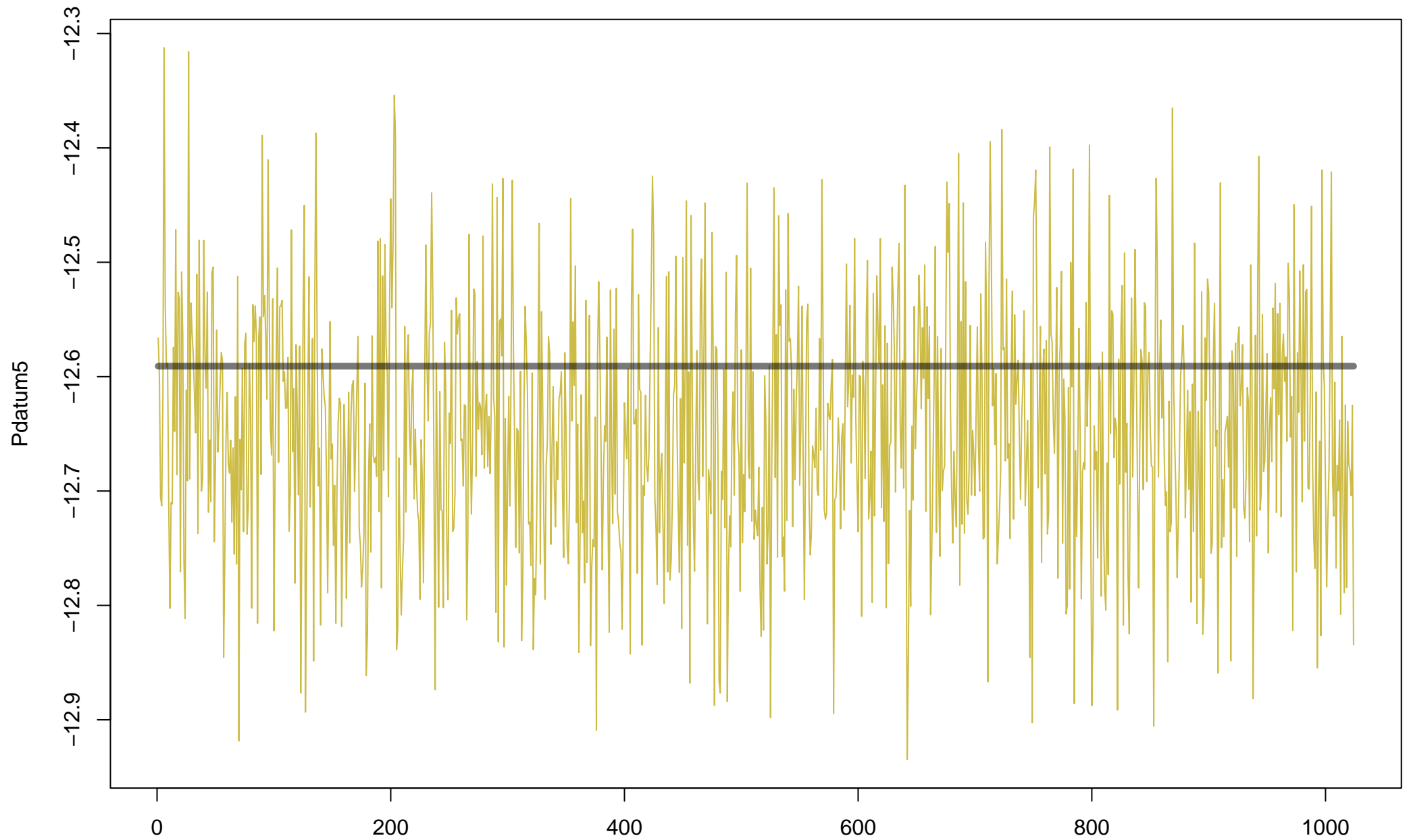
Pdatum4

ESS = 1020 | BMK = 0.0783 | MCSE(6.27) = 3.9 | stat: TRUE | burn: 0 | rel.err: -0.902

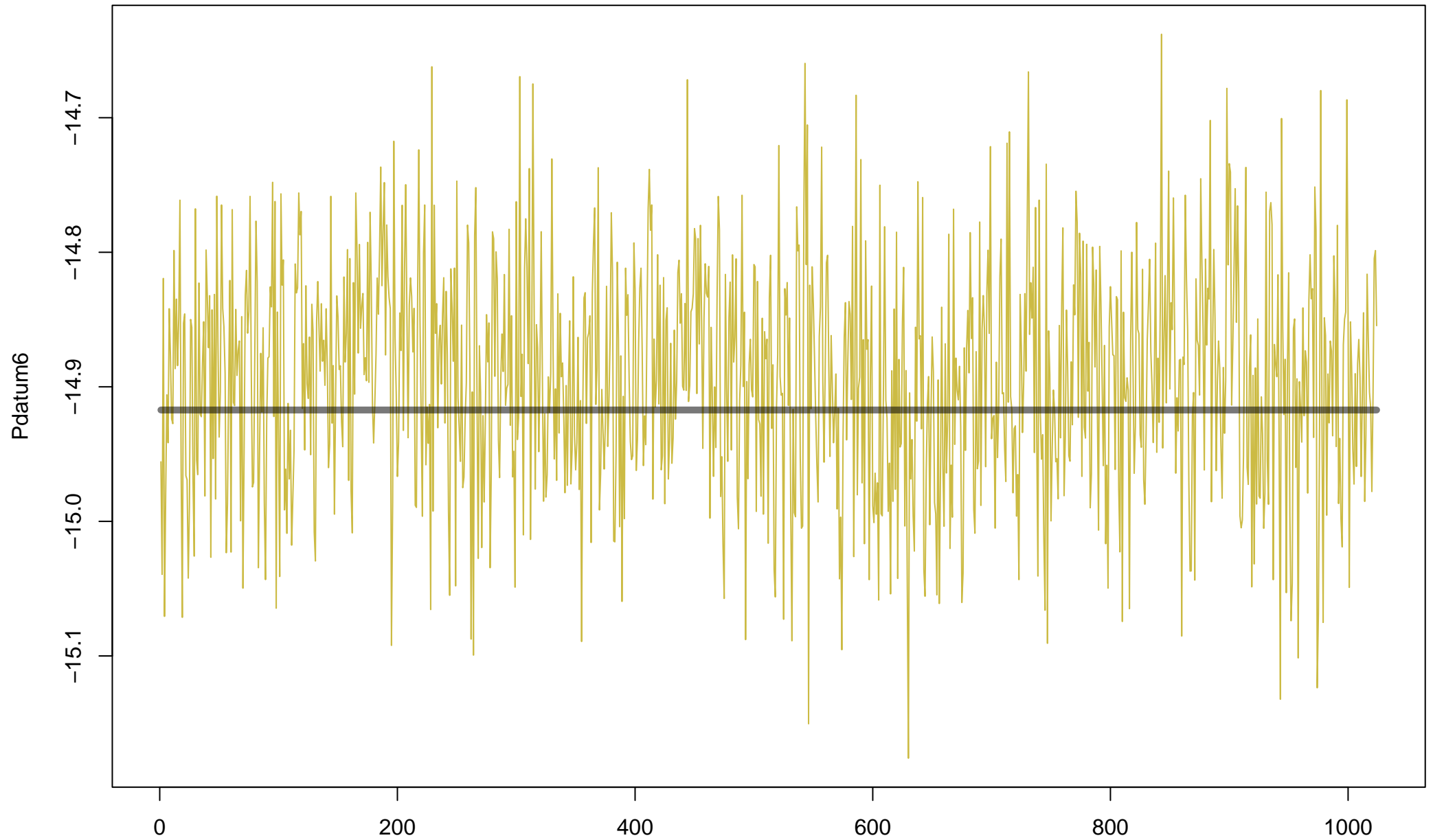


**Pdatum5**

**ESS = 927 | BMK = 0.0478 | MCSE(6.27) = 3.47 | stat: TRUE | burn: 0 | rel.err: -0.491**

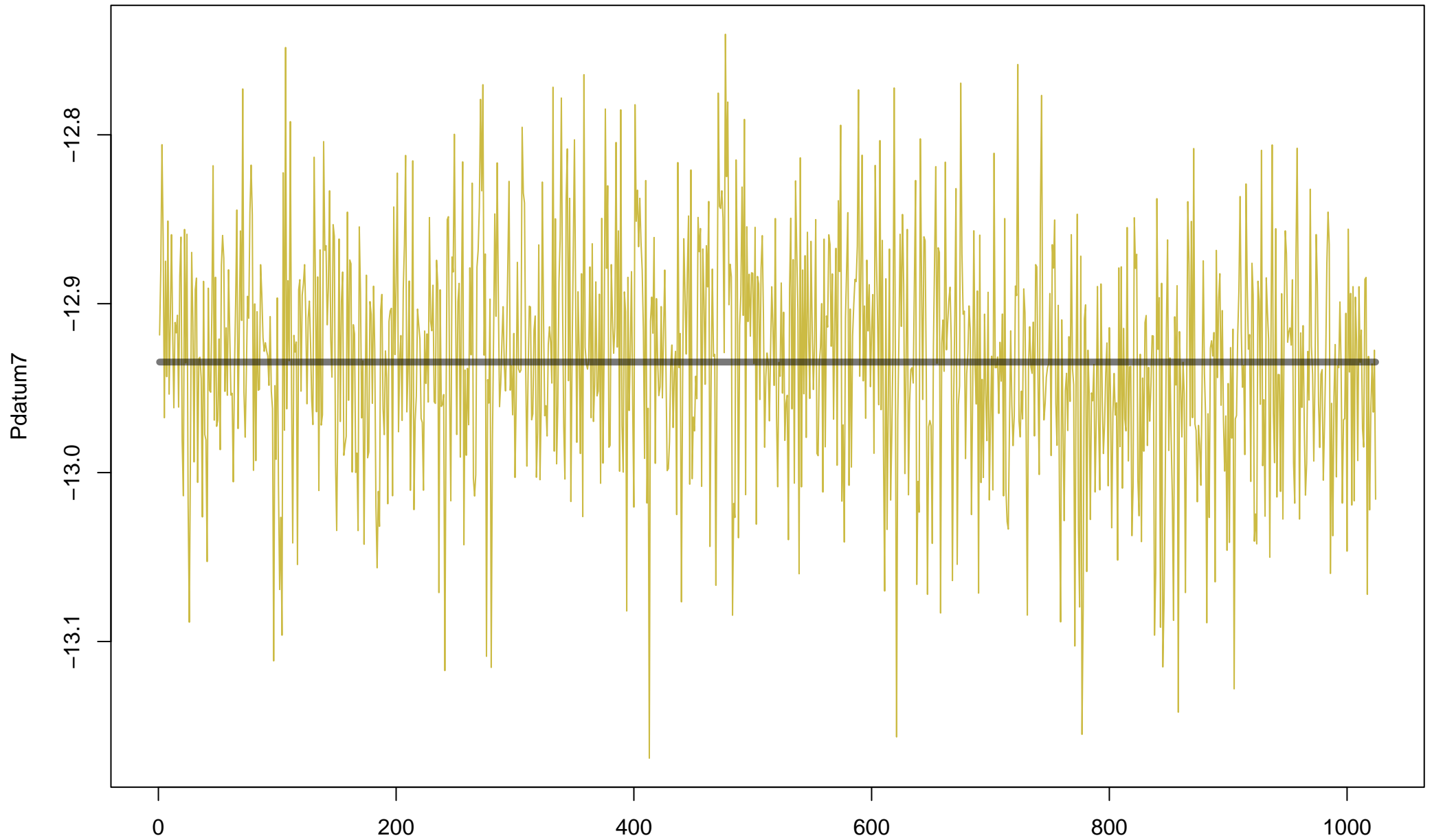


**Pdatum6**  
**ESS = 892 | BMK = 0.0852 | MCSE(6.27) = 3.73 | stat: TRUE | burn: 0 | rel.err: 0.316**



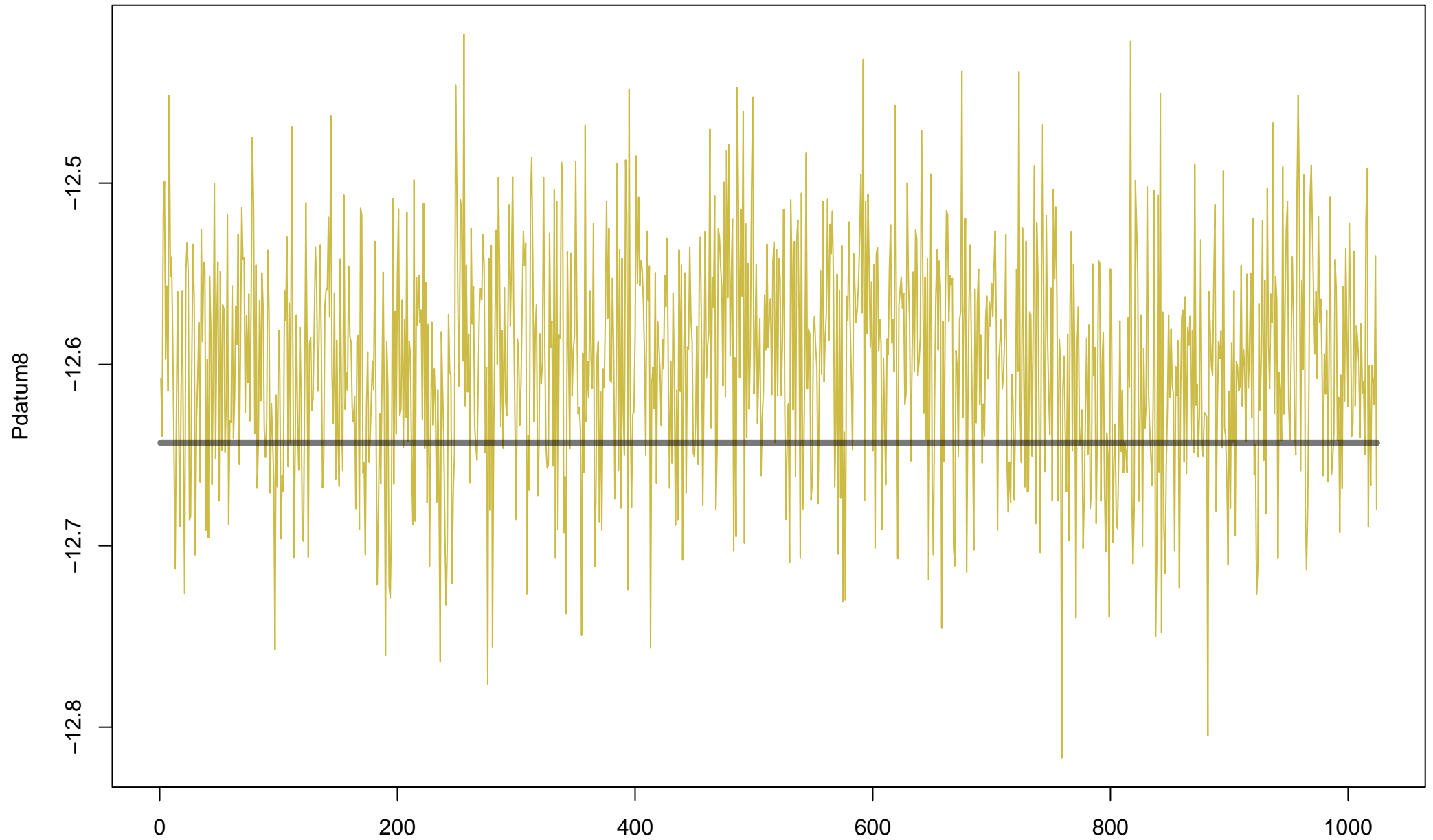
**Pdatum7**

**ESS = 231 | BMK = 0.0976 | MCSE(6.27) = 4.57 | stat: TRUE | burn: 0 | rel.err: 0.0614**



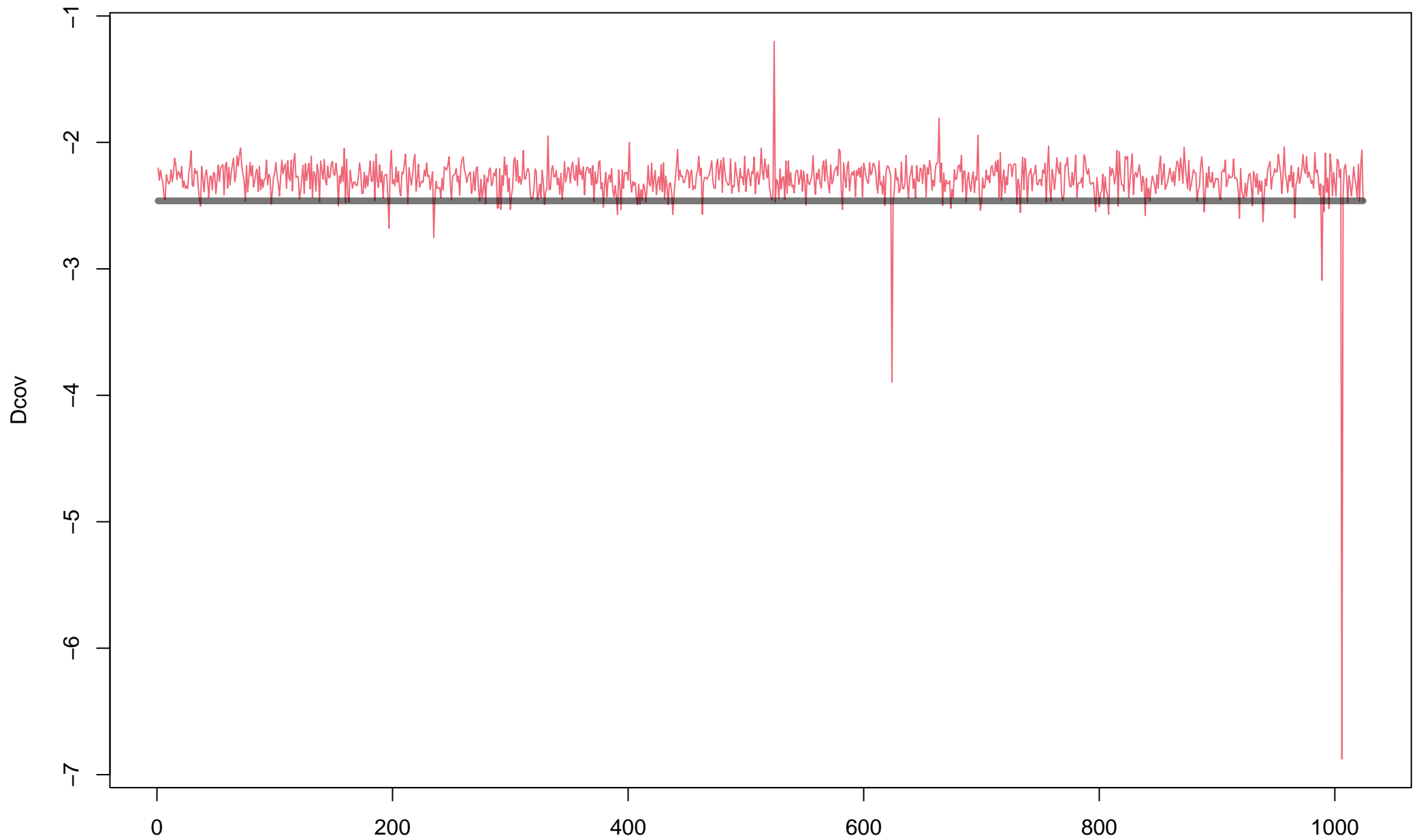
**Pdatum8**

**ESS = 1020 | BMK = 0.0363 | MCSE(6.27) = 4.15 | stat: TRUE | burn: 0 | rel.err: 0.716**

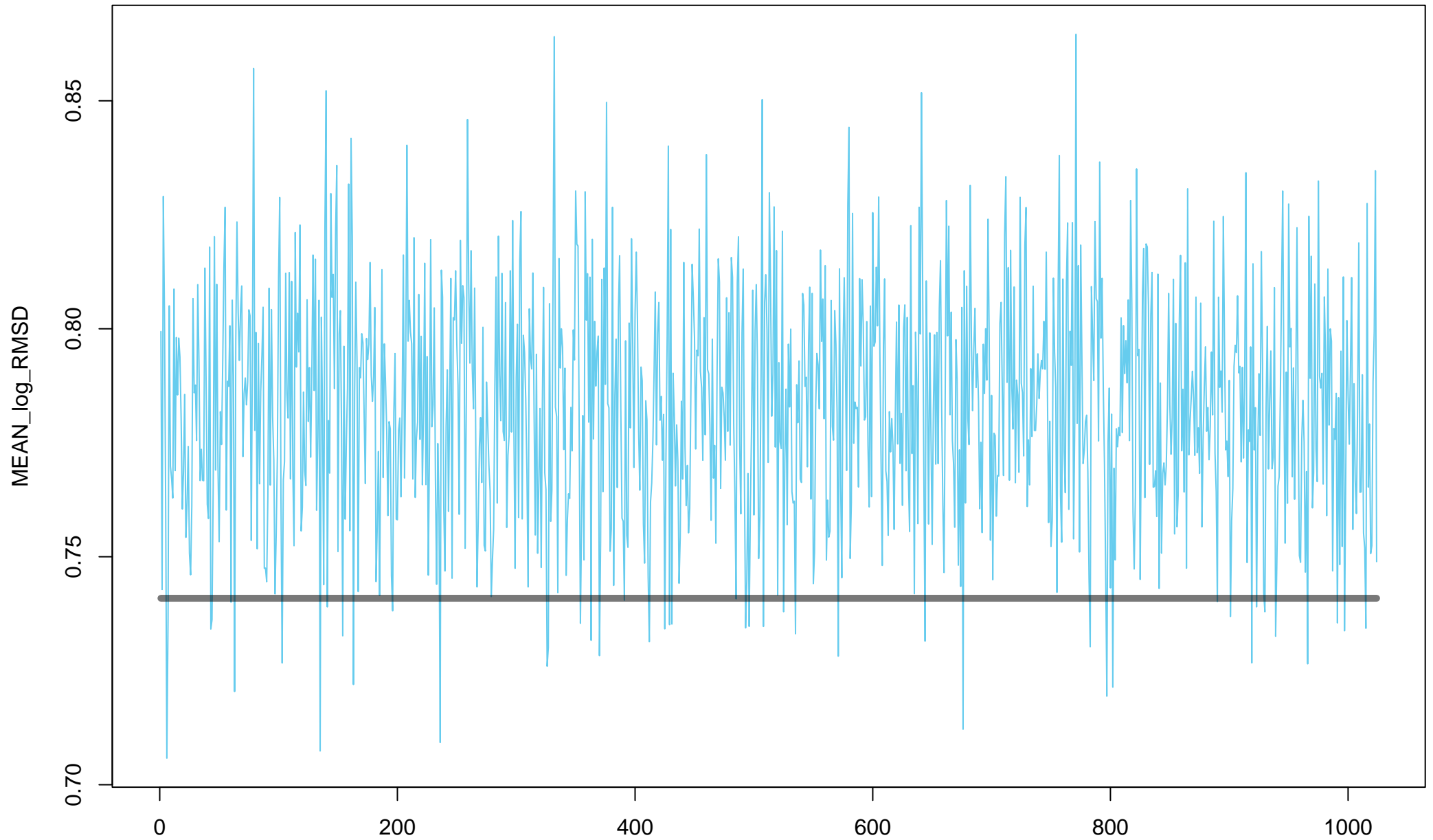


Dcov

ESS = 1020 | BMK = 0.0799 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | rel.err: -1.28

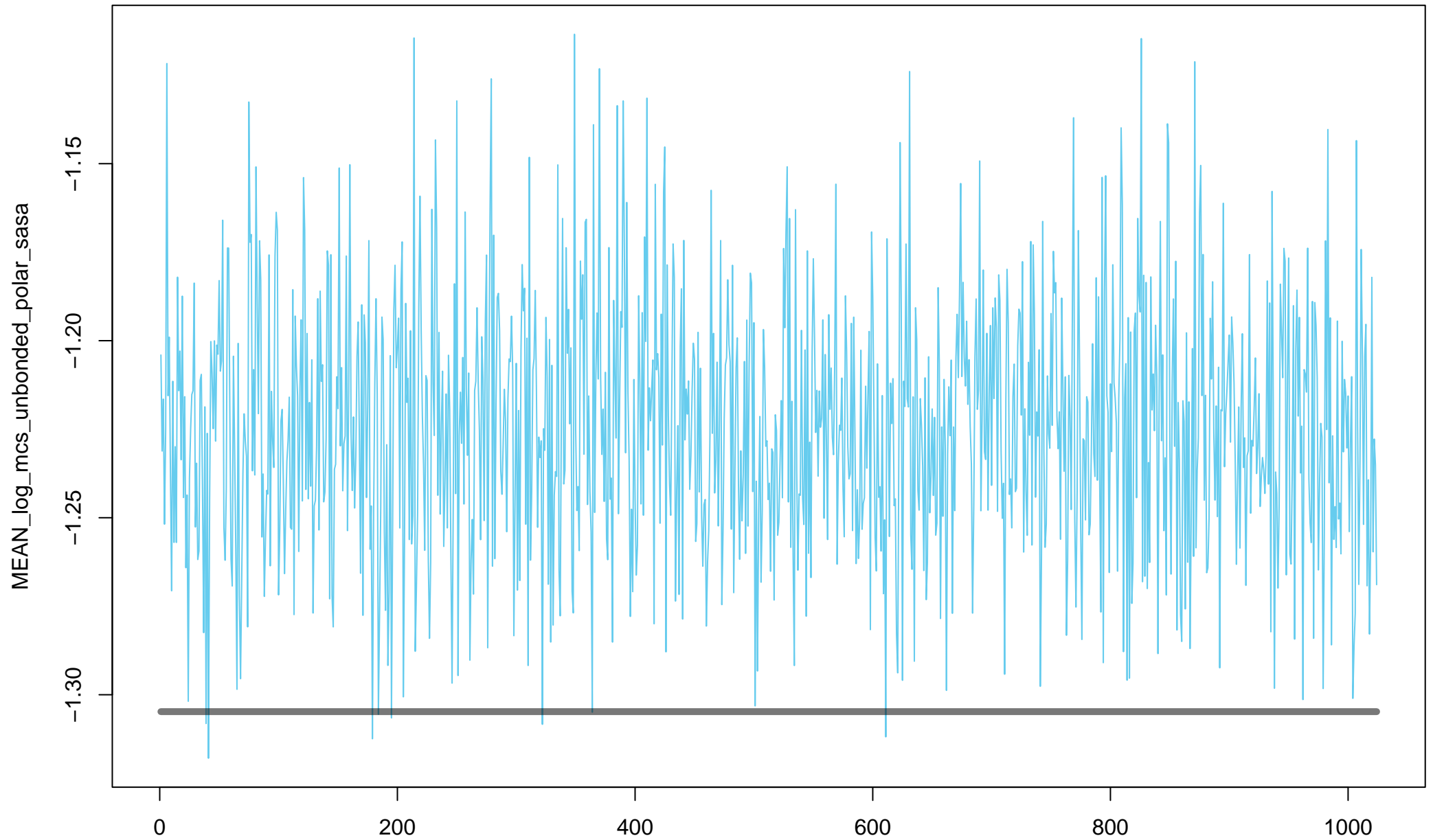


**MEAN\_log\_RMSD**  
**ESS = 1020 | BMK = 0.0575 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0 | rel.err: 1.67**

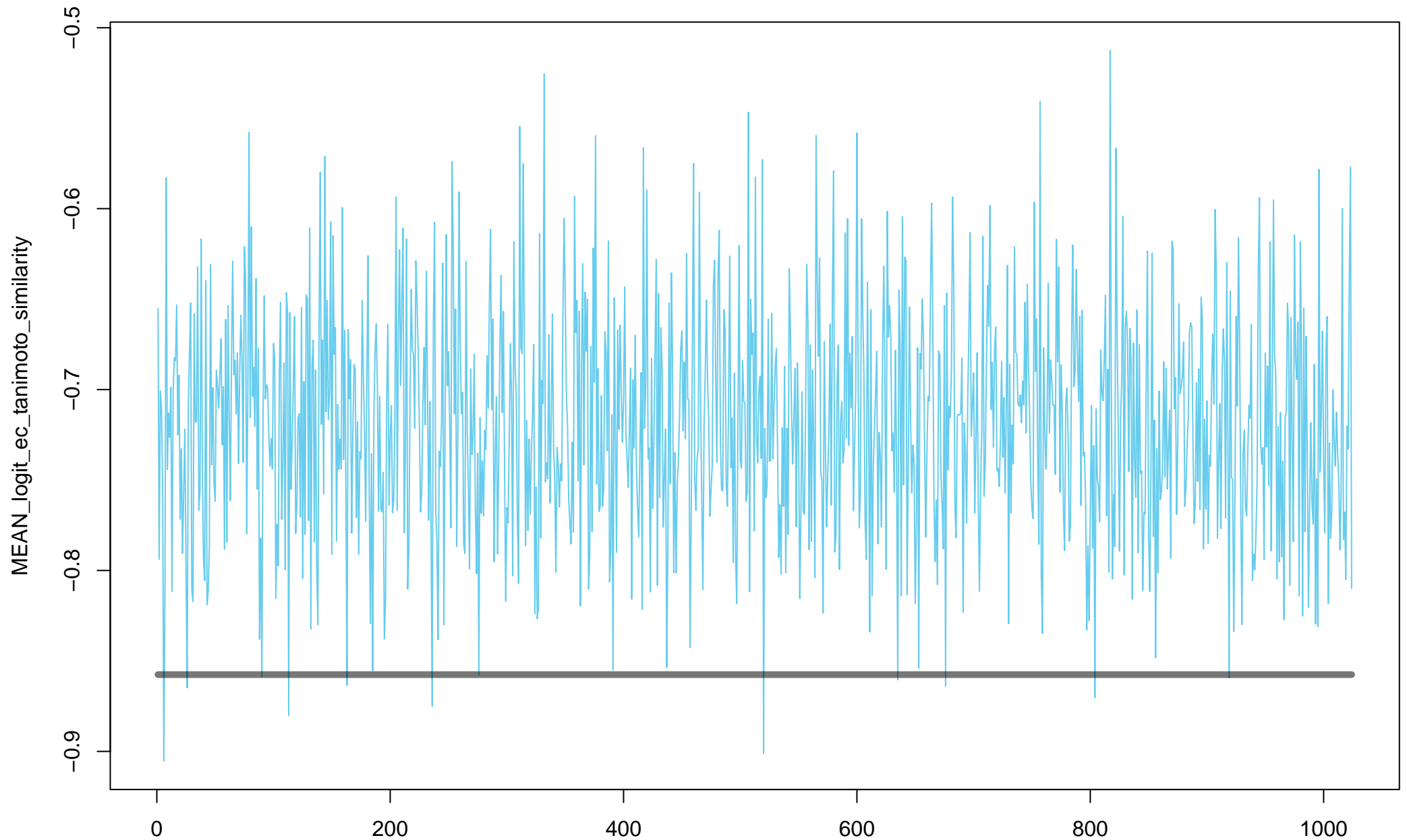




**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1020 | BMK = 0.0445 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | rel.err: 2.24**

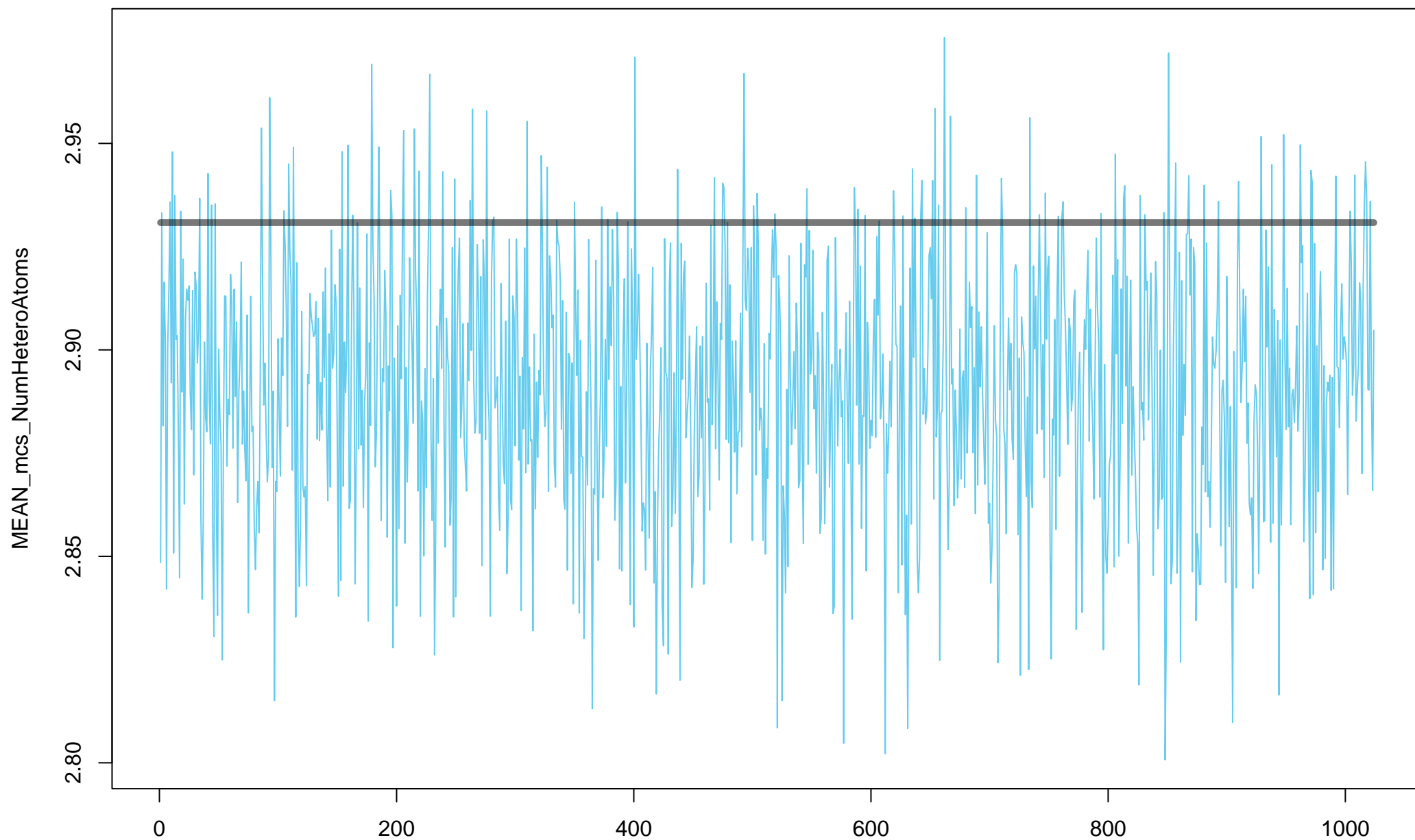


**MEAN\_logit\_ec\_tanimoto\_similarity**  
**ESS = 1020 | BMK = 0.0284 | MCSE(6.27) = 2.67 | stat: TRUE | burn: 0 | rel.err: 2.25**

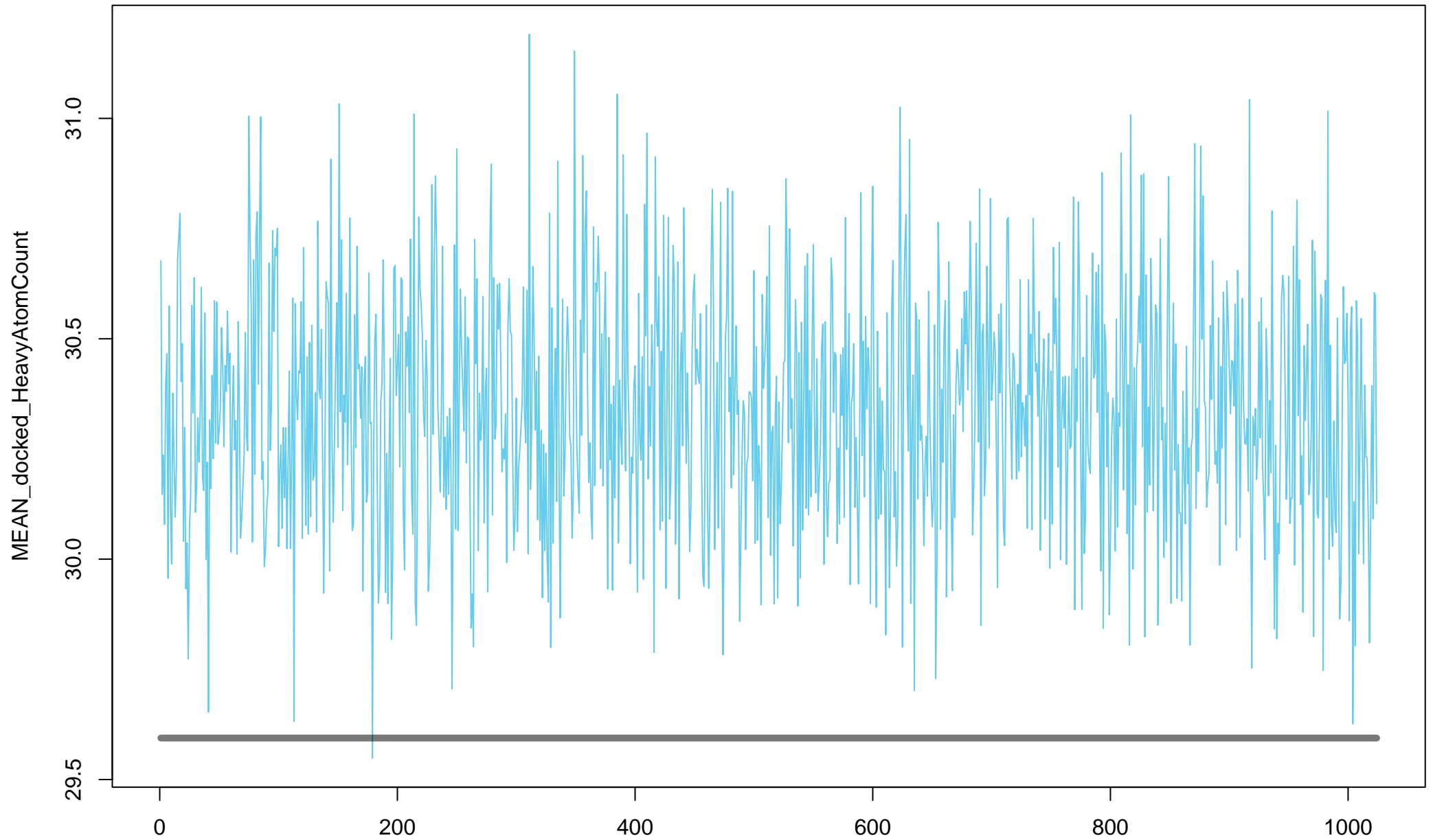


# MEAN\_mcs\_NumHeteroAtoms

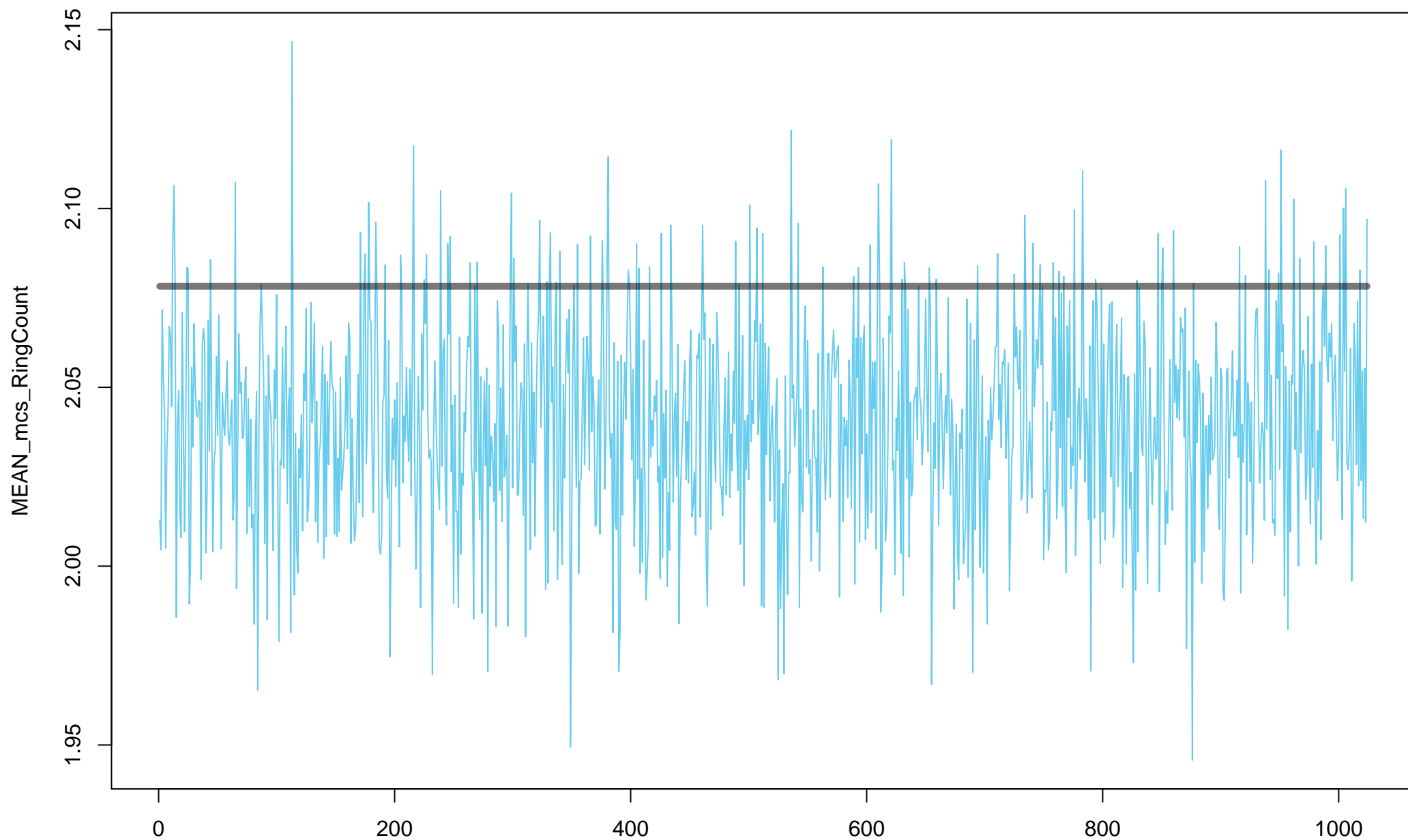
ESS = 1020 | BMK = 0.0508 | MCSE(6.27) = 3.33 | stat: TRUE | burn: 0 | rel.err: -1.31



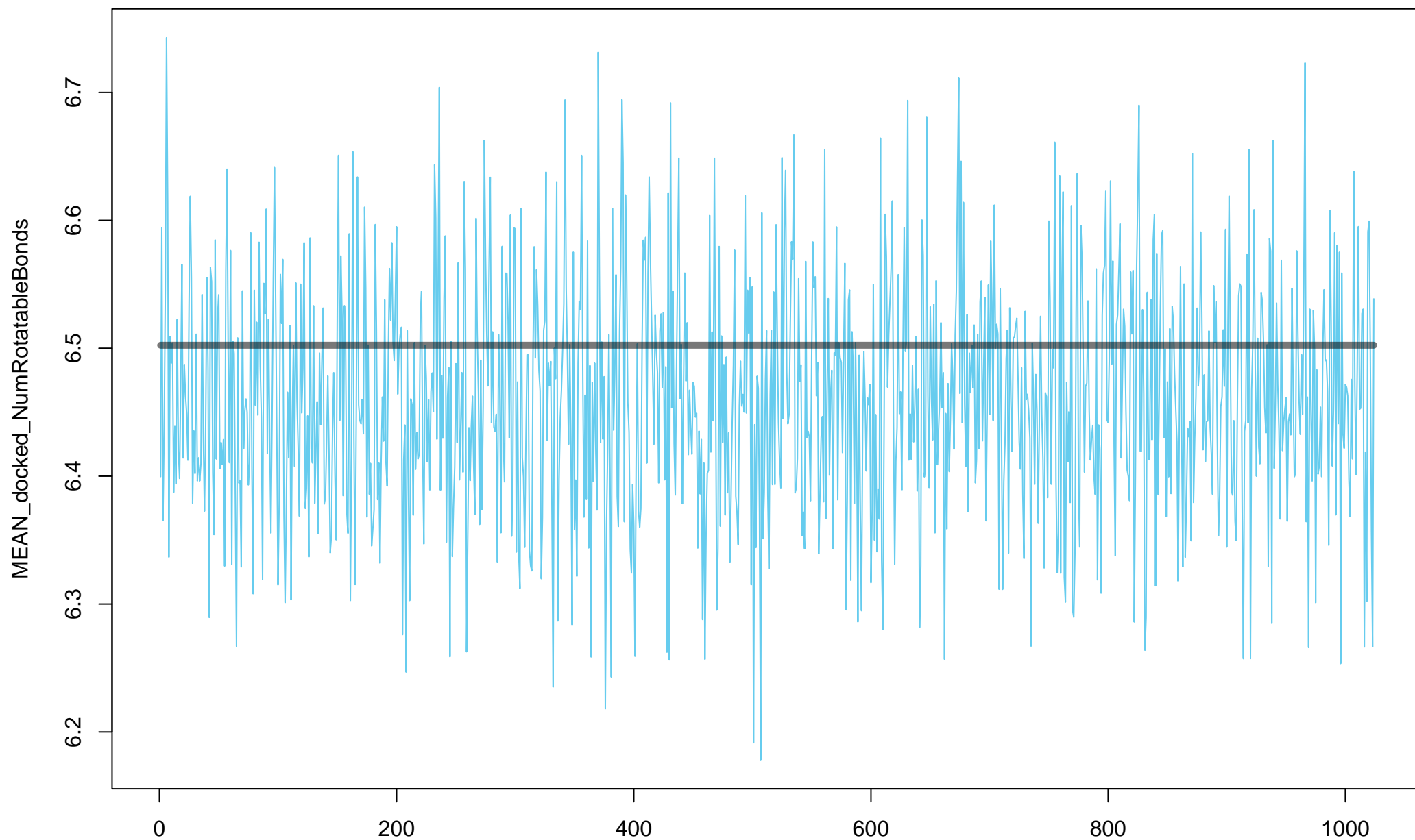
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.0478 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0 | rel.err: 2.81**



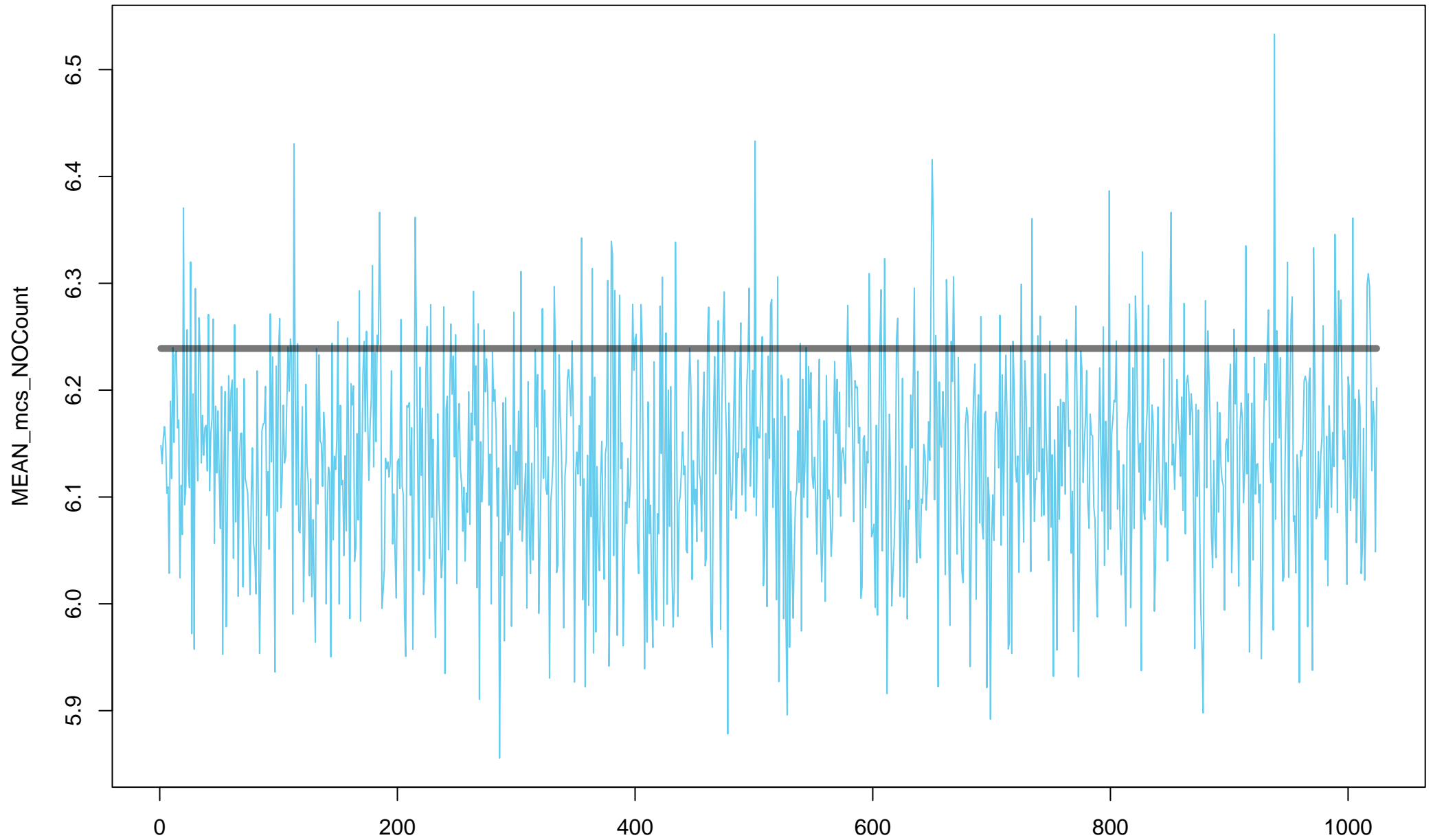
**MEAN\_mcs\_RingCount**  
**ESS = 1020 | BMK = 0.0382 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 0 | rel.err: -1.35**



**MEAN\_docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.056 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0 | rel.err: -0.454**

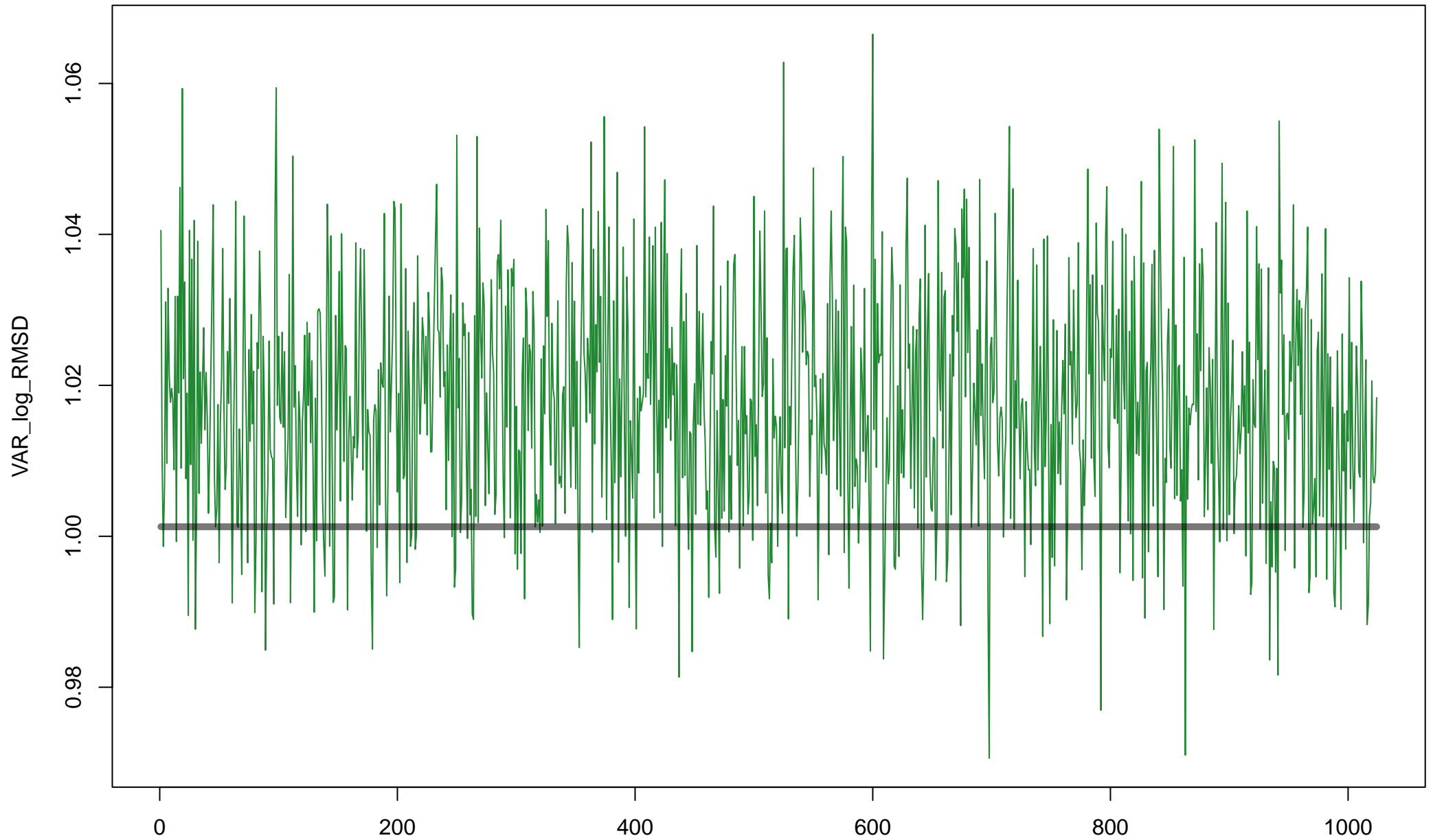


**MEAN\_mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0514 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0 | rel.err: -1.12**



# VAR\_log\_RMSD

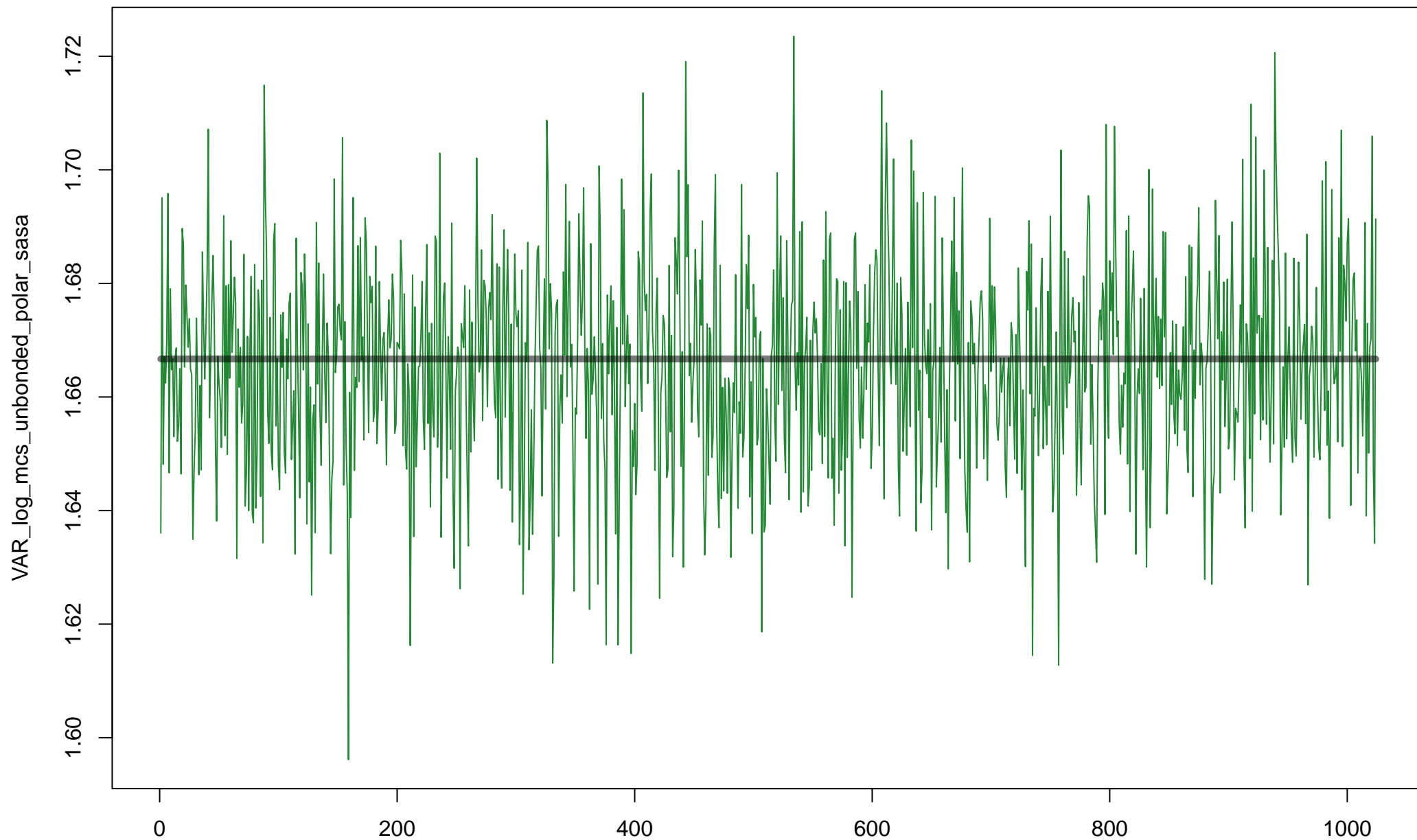
ESS = 1020 | BMK = 0.0495 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | rel.err: 1.08



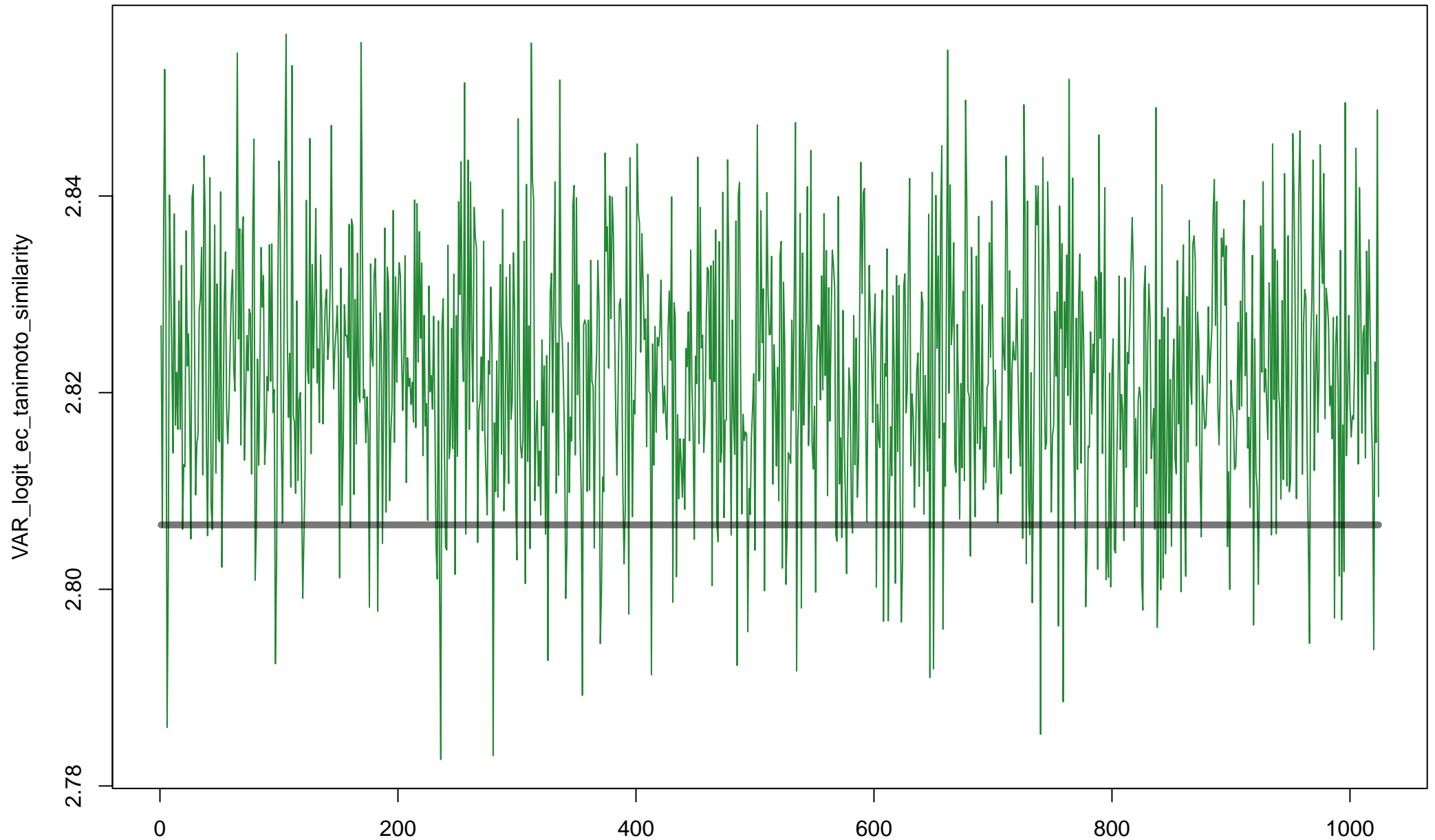


VAR\_log\_mcs\_unbonded\_polar\_sasa

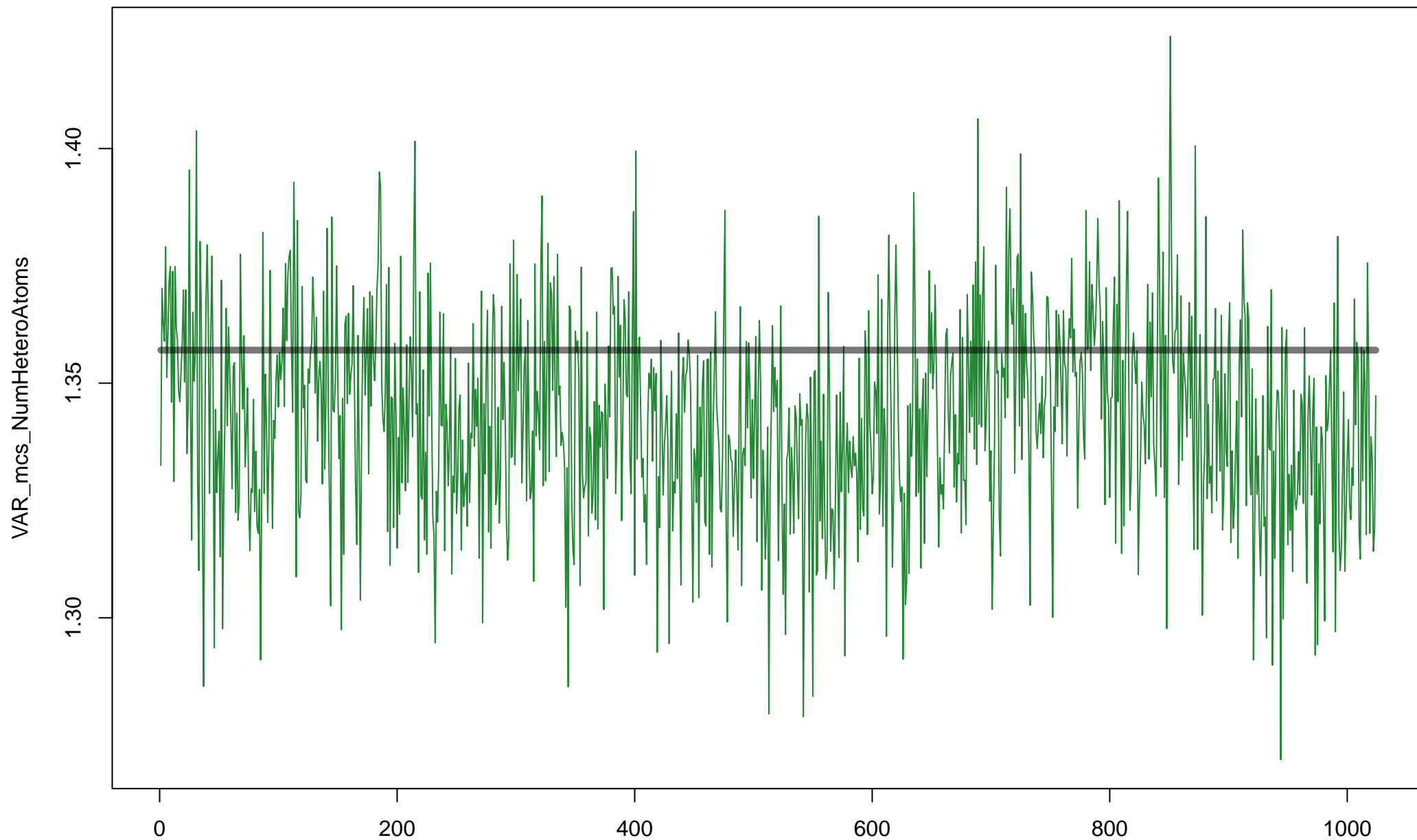
ESS = 1020 | BMK = 0.0632 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | rel.err: -0.0688



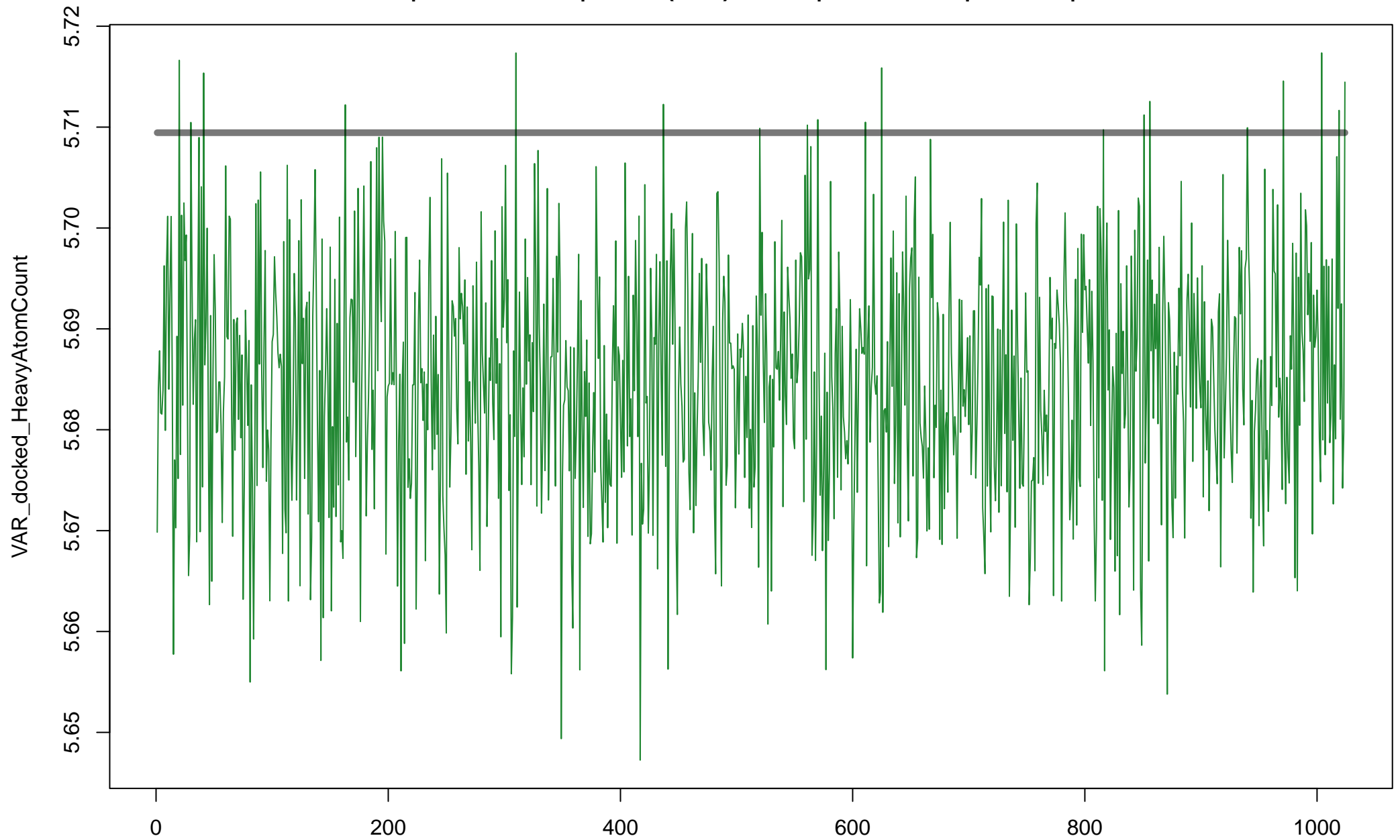
**VAR\_logit\_ec\_tanimoto\_similarity**  
**ESS = 1020 | BMK = 0.0471 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0 | rel.err: 1.23**



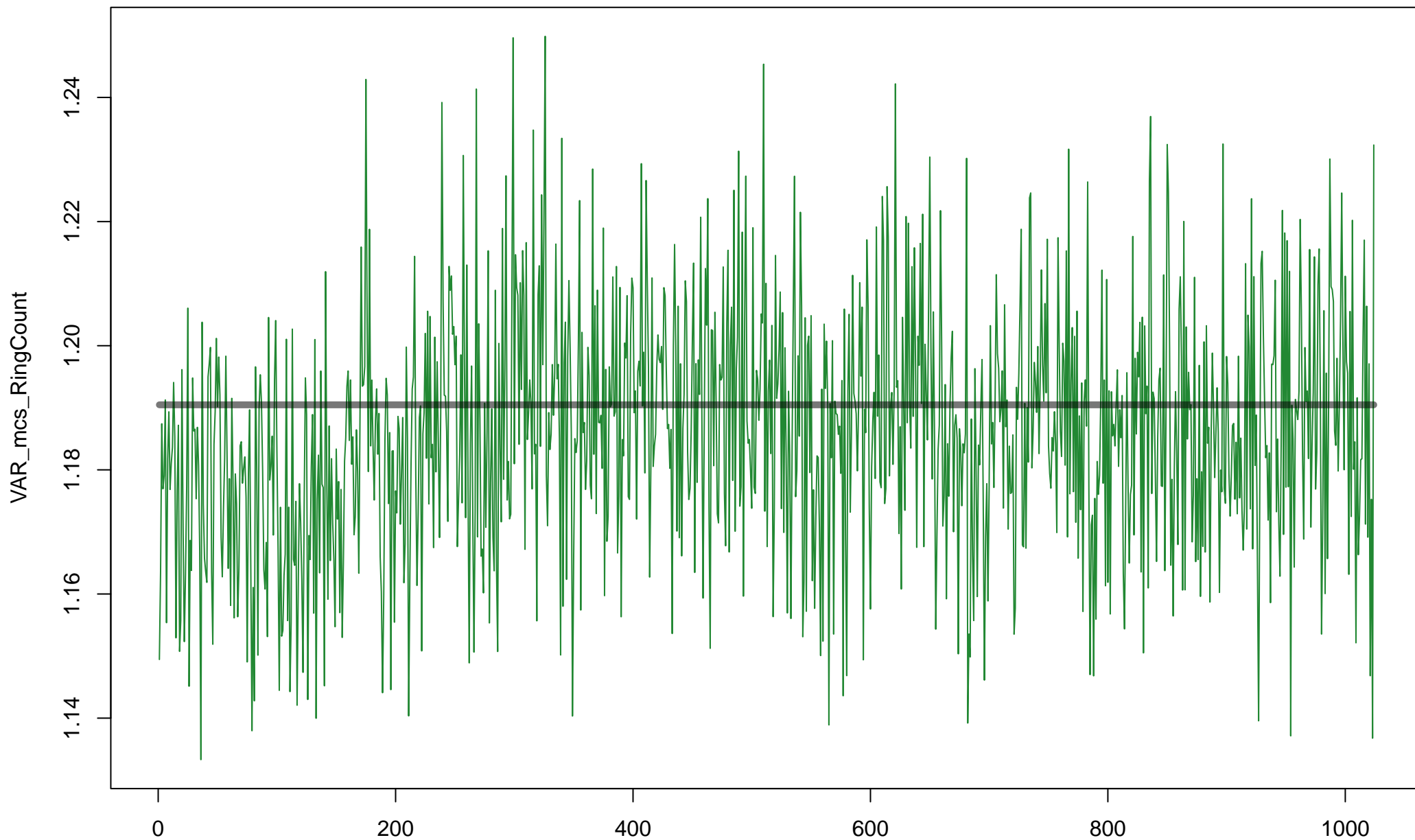
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 179 | BMK = 0.0459 | MCSE(6.27) = 6.44 | stat: TRUE | burn: 0 | rel.err: -0.665**



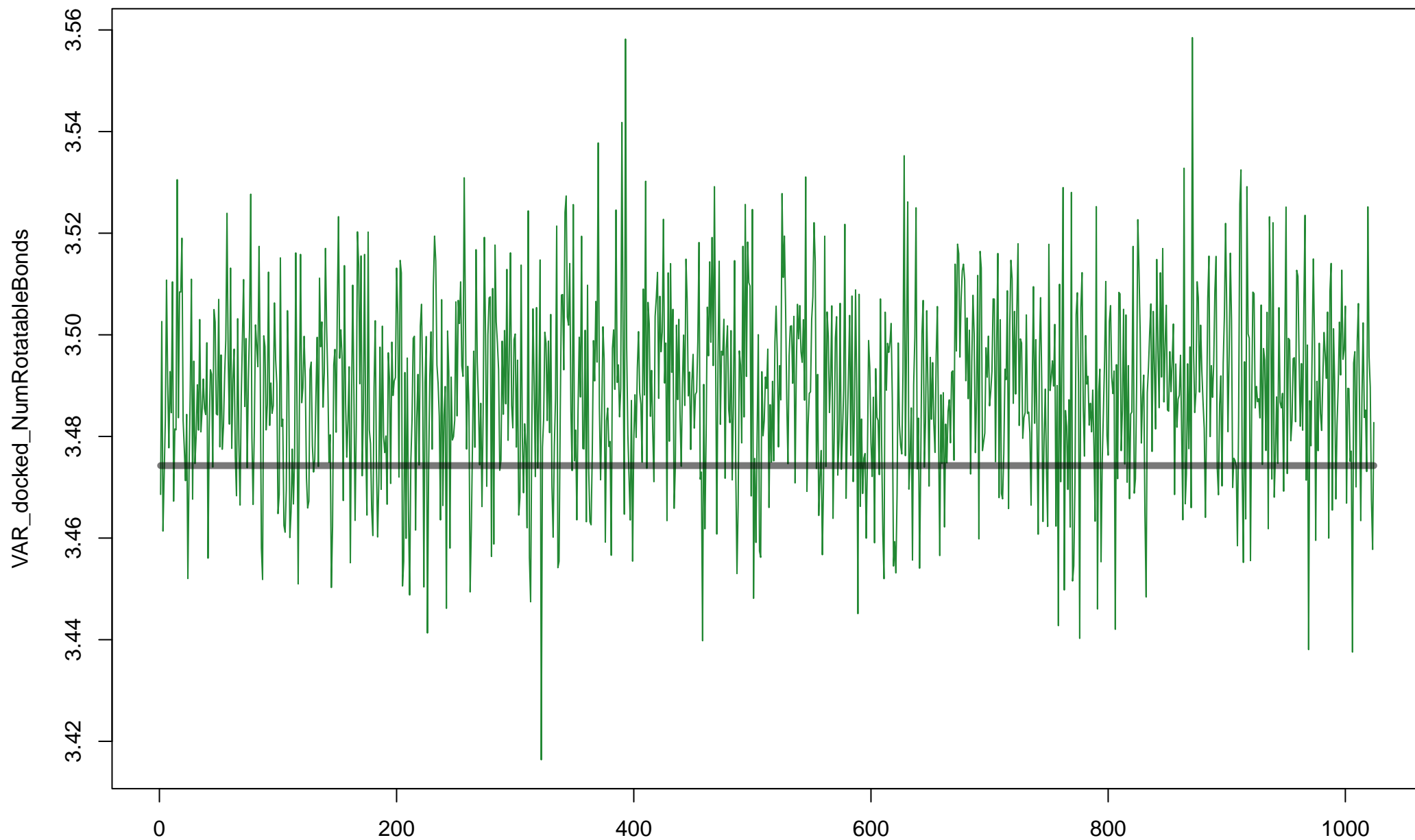
**VAR\_docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.049 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0 | rel.err: -2.15**



**VAR\_mcs\_RingCount**  
**ESS = 133 | BMK = 0.0655 | MCSE(6.27) = 6.4 | stat: FALSE | burn: 0 | rel.err: -0.224**

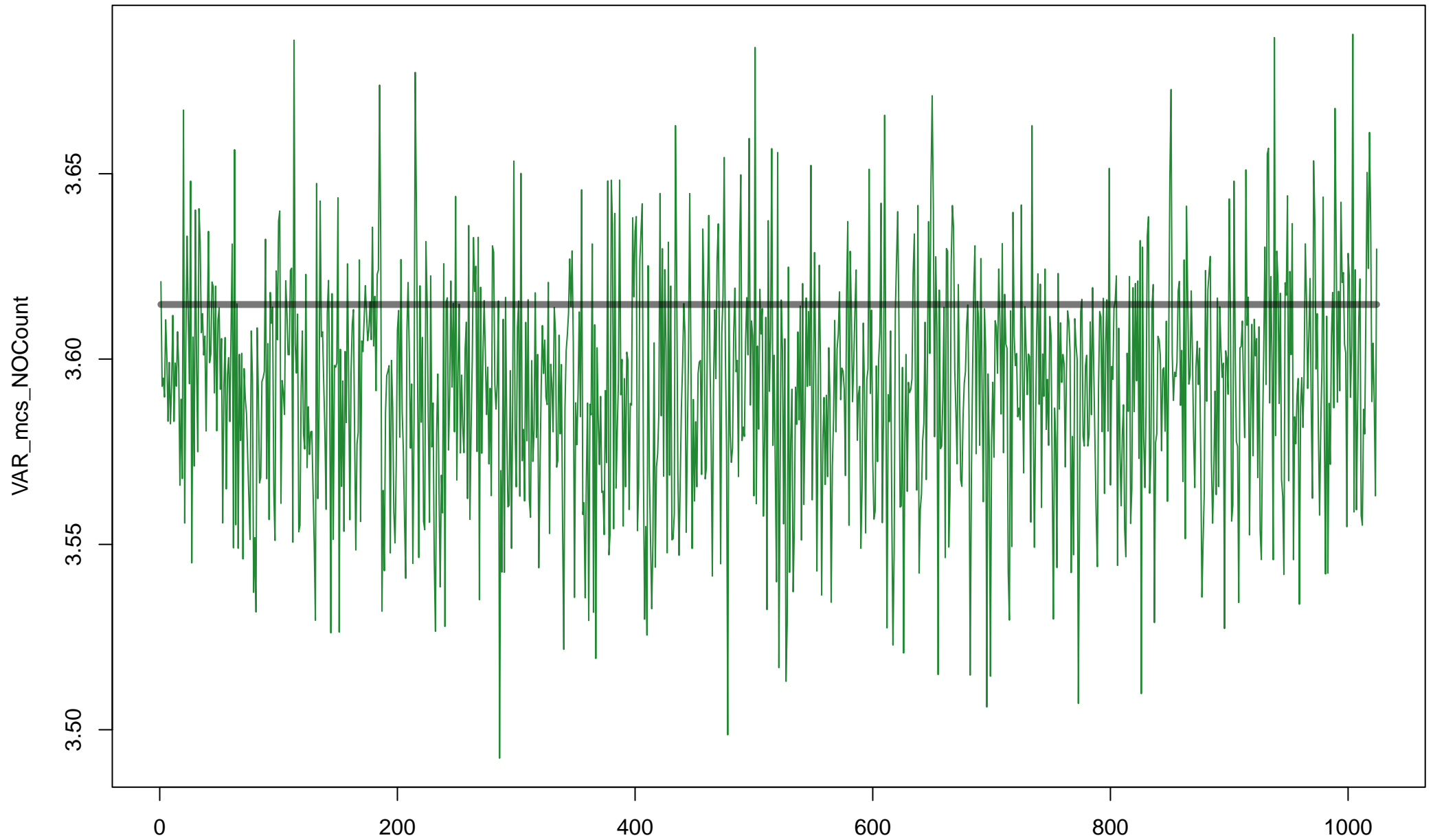


**VAR\_docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.05 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0 | rel.err: 0.8**

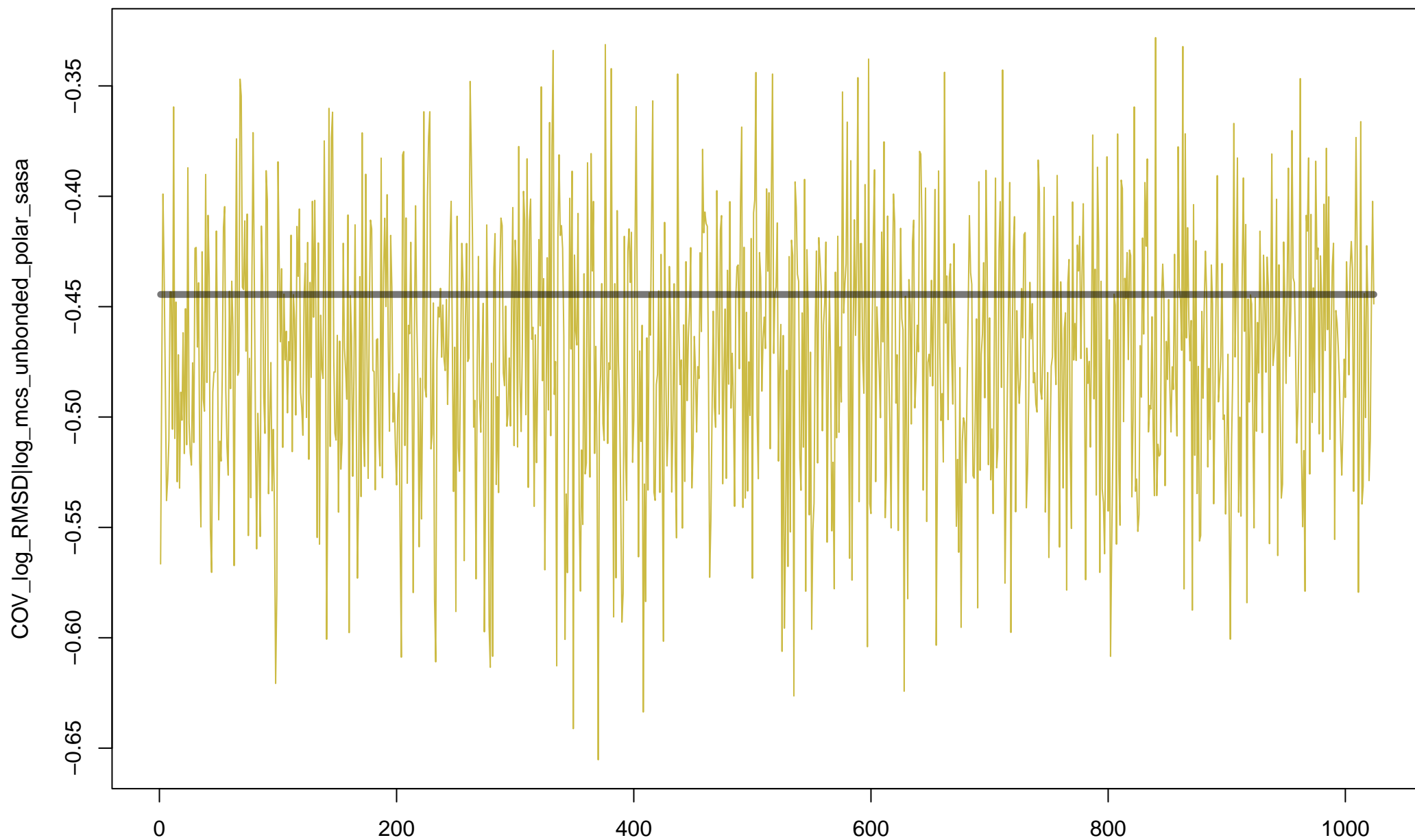


# VAR\_mcs\_NOCount

ESS = 1020 | BMK = 0.0528 | MCSE(6.27) = 3.55 | stat: TRUE | burn: 0 | rel.err: -0.725

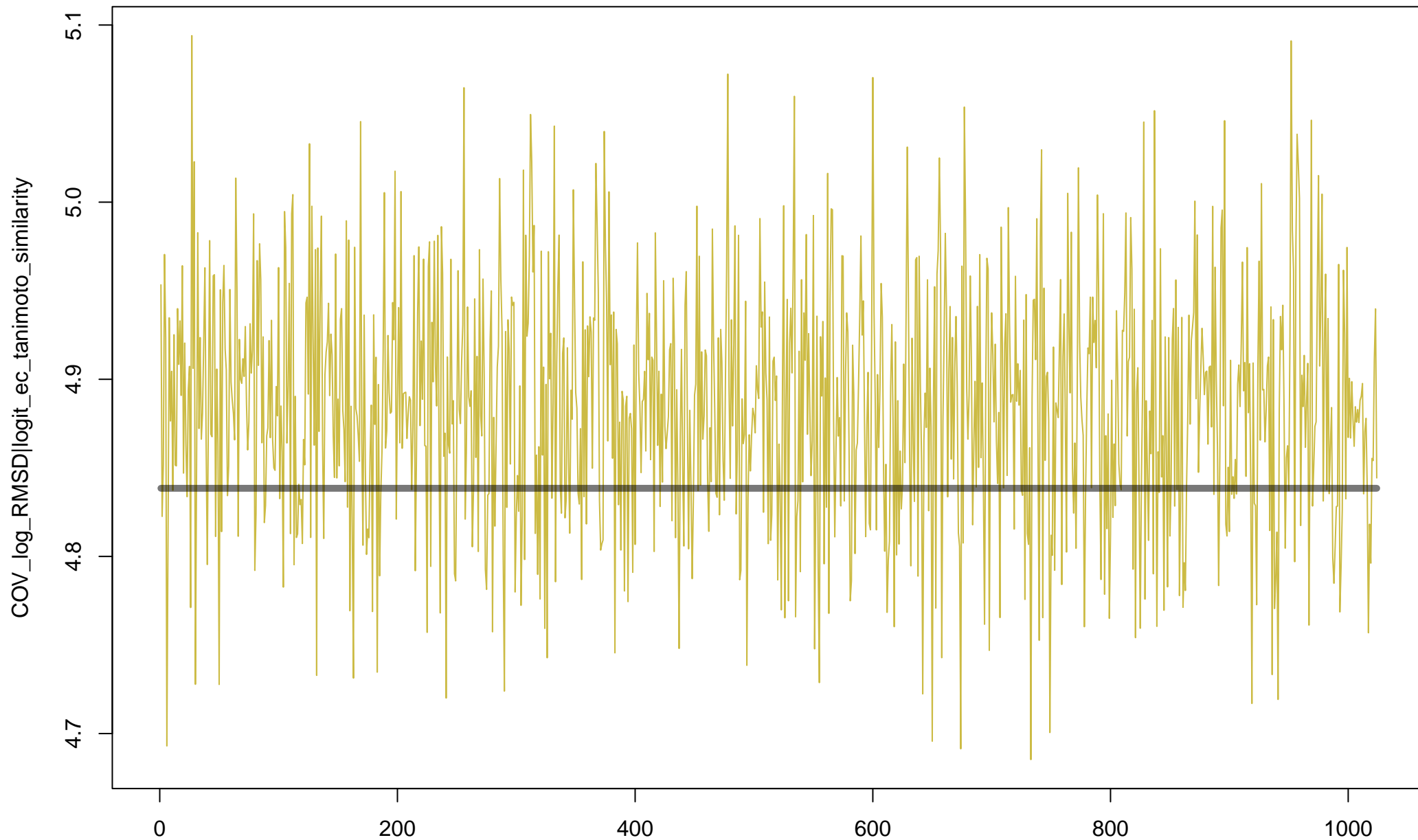


**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1020 | BMK = 0.0499 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0 | rel.err: -0.483**

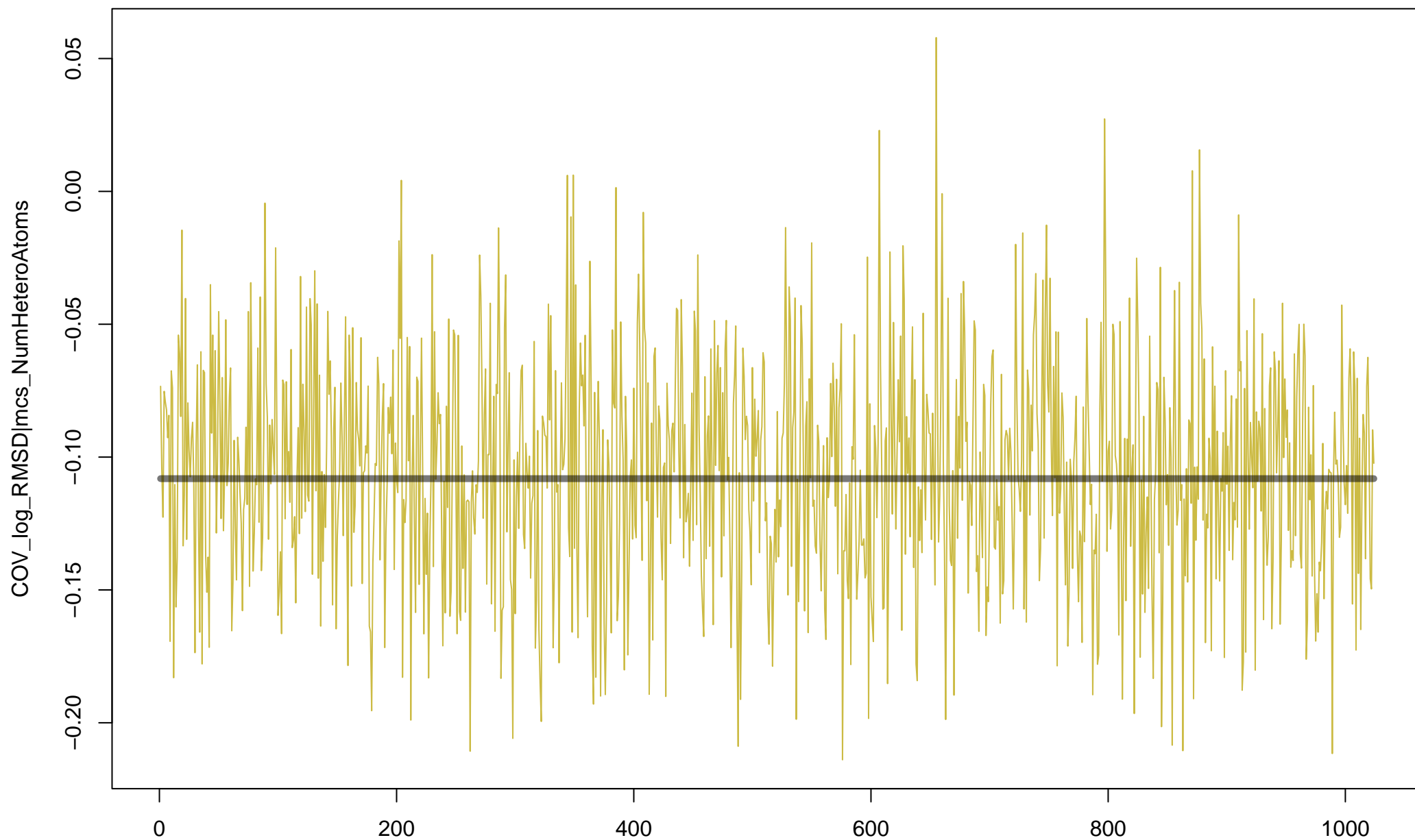




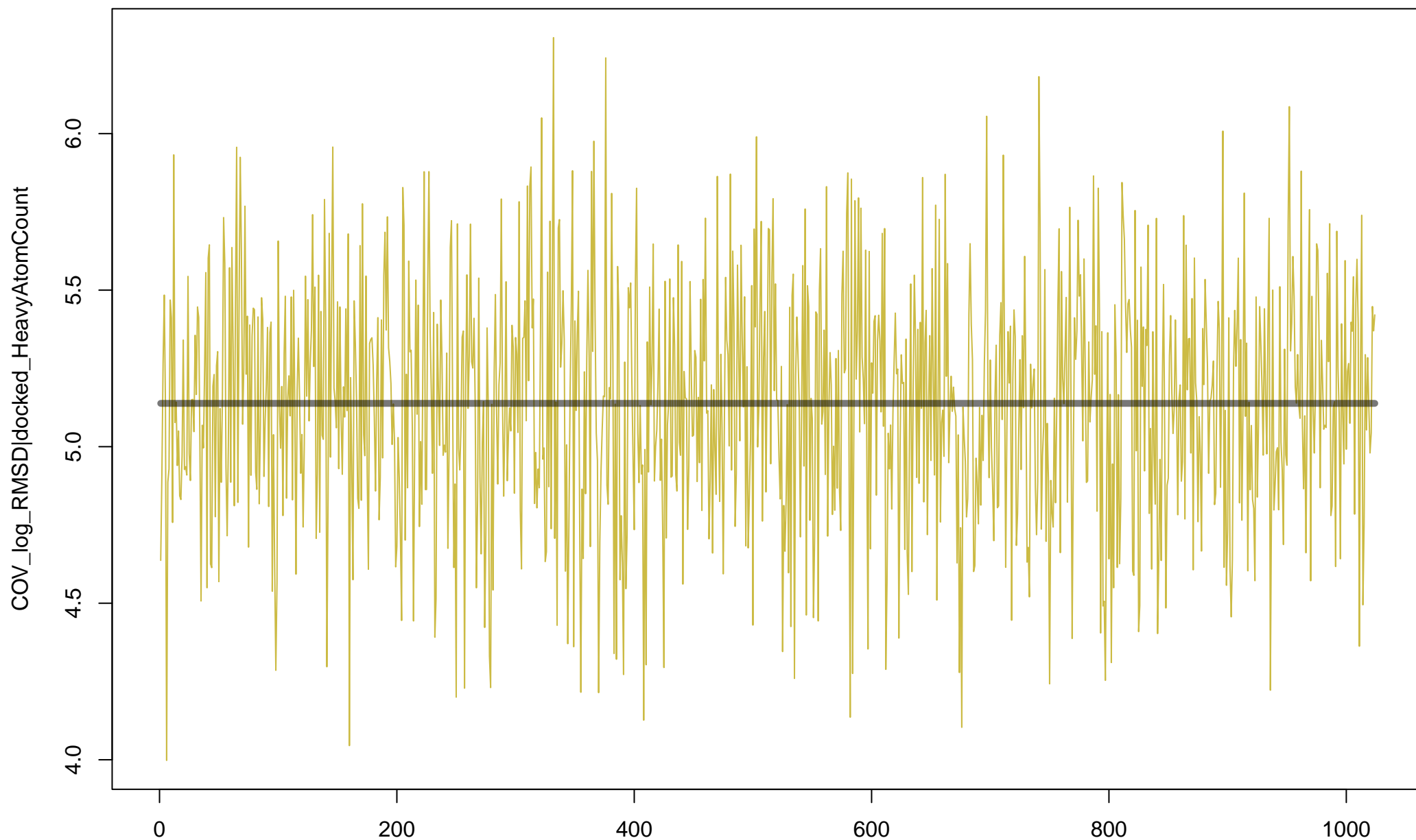
**COV\_log\_RMSD|logit\_ec\_tanimoto\_similarity**  
**ESS = 1020 | BMK = 0.0537 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0 | rel.err: 0.686**



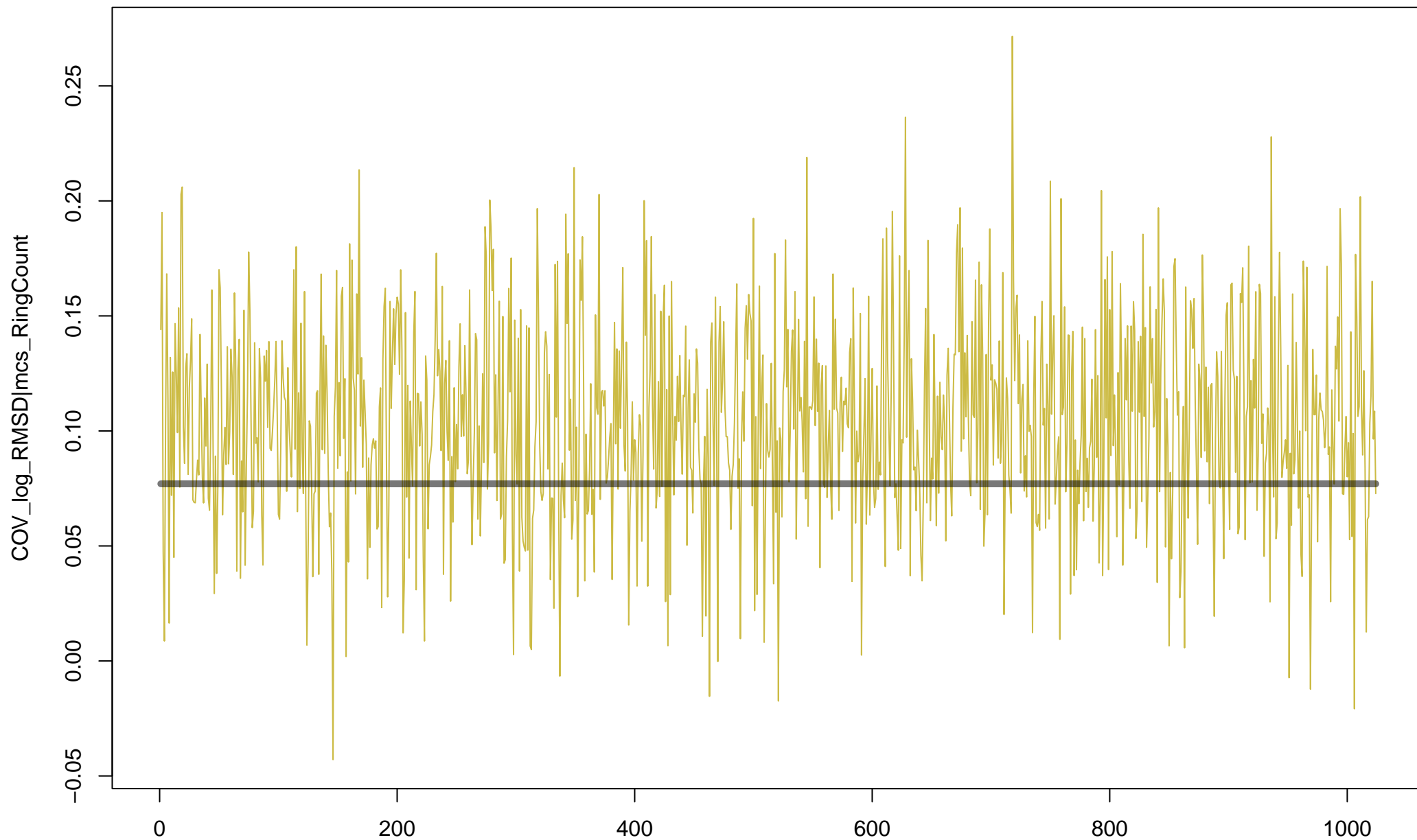
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 1020 | BMK = 0.0575 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0 | rel.err: 0.063**



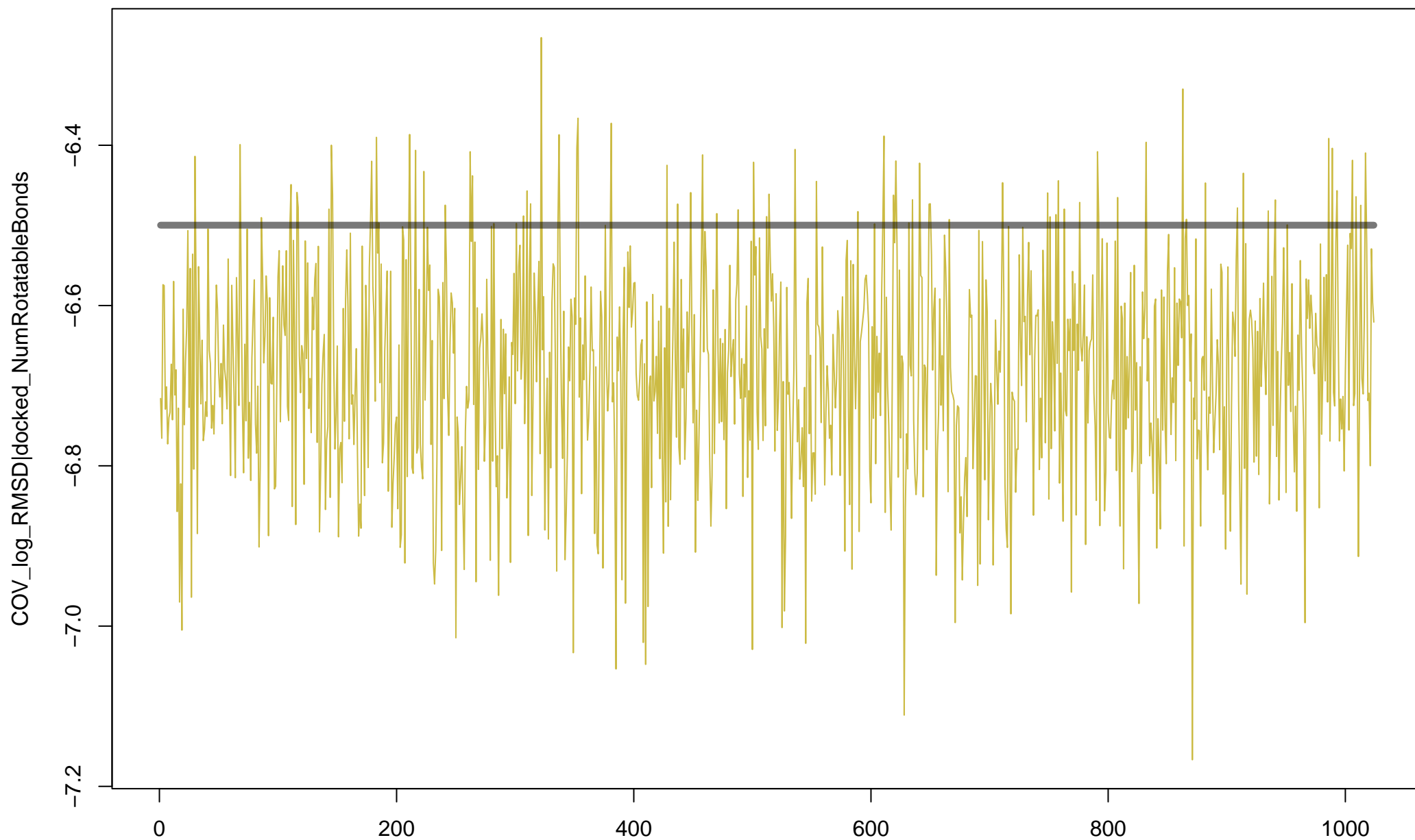
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.047 | MCSE(6.27) = 2.9 | stat: TRUE | burn: 0 | rel.err: -0.0146**



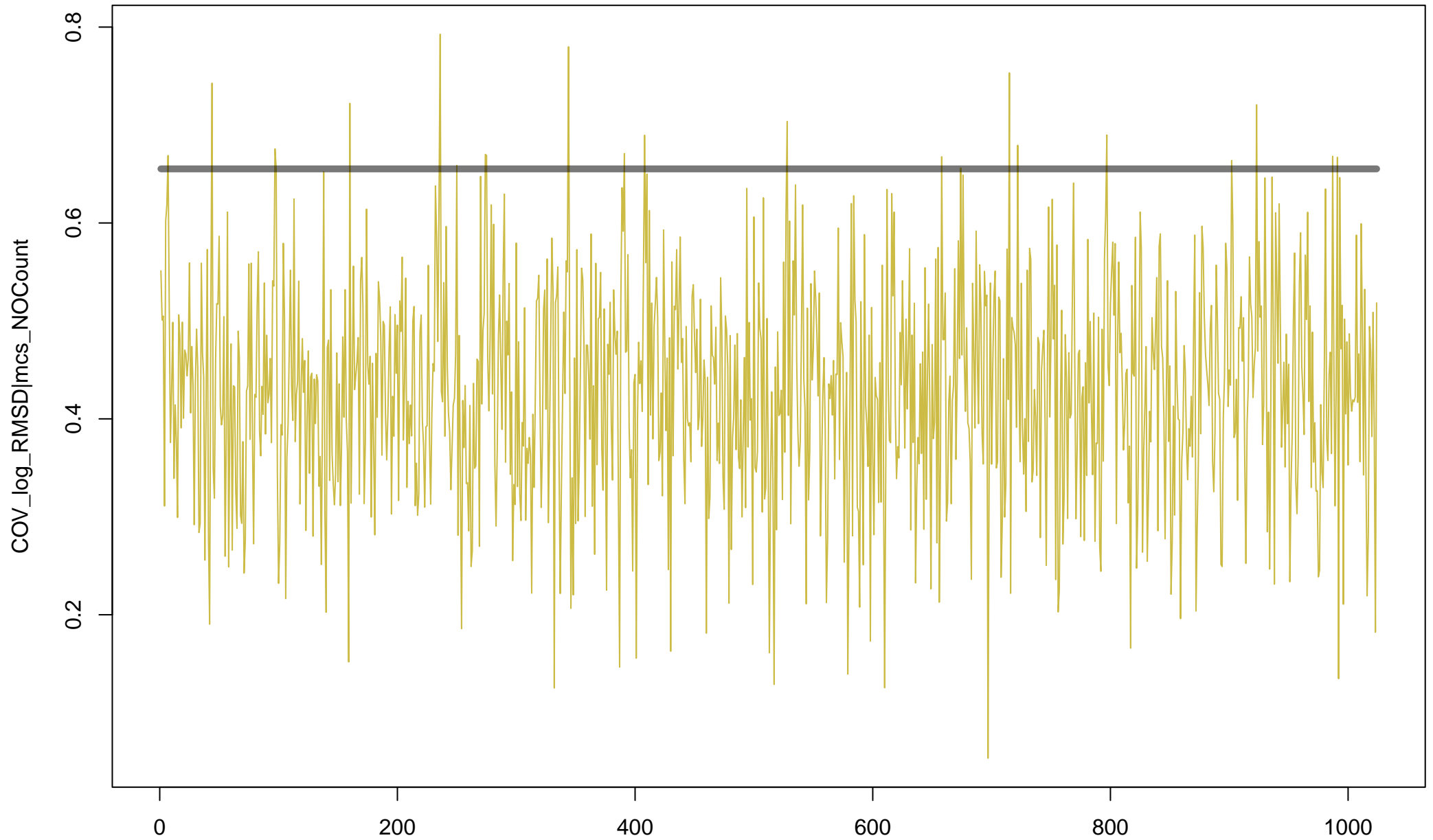
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.0611 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0 | rel.err: 0.625**



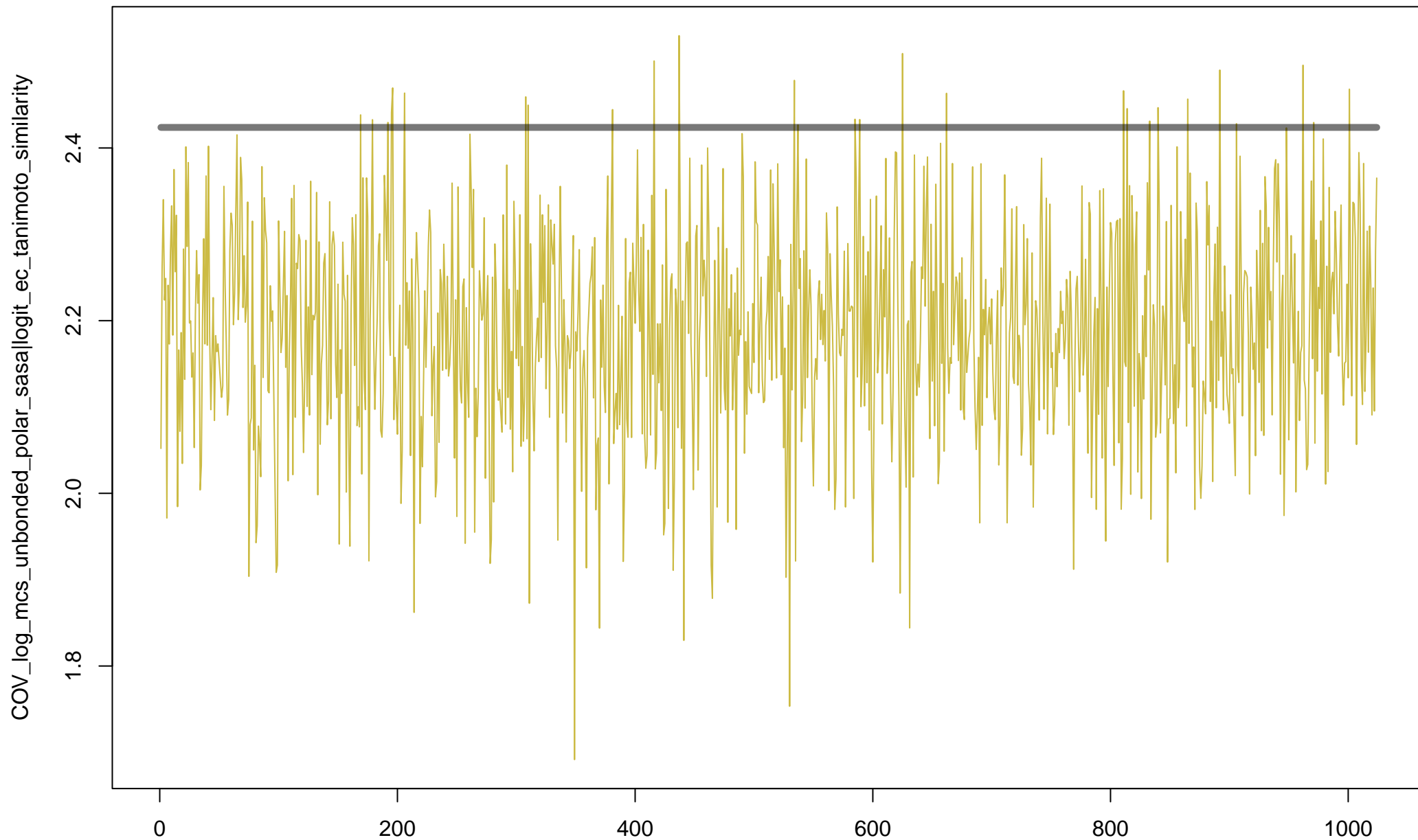
**COV\_log\_RMSD|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0413 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | rel.err: -1.41**



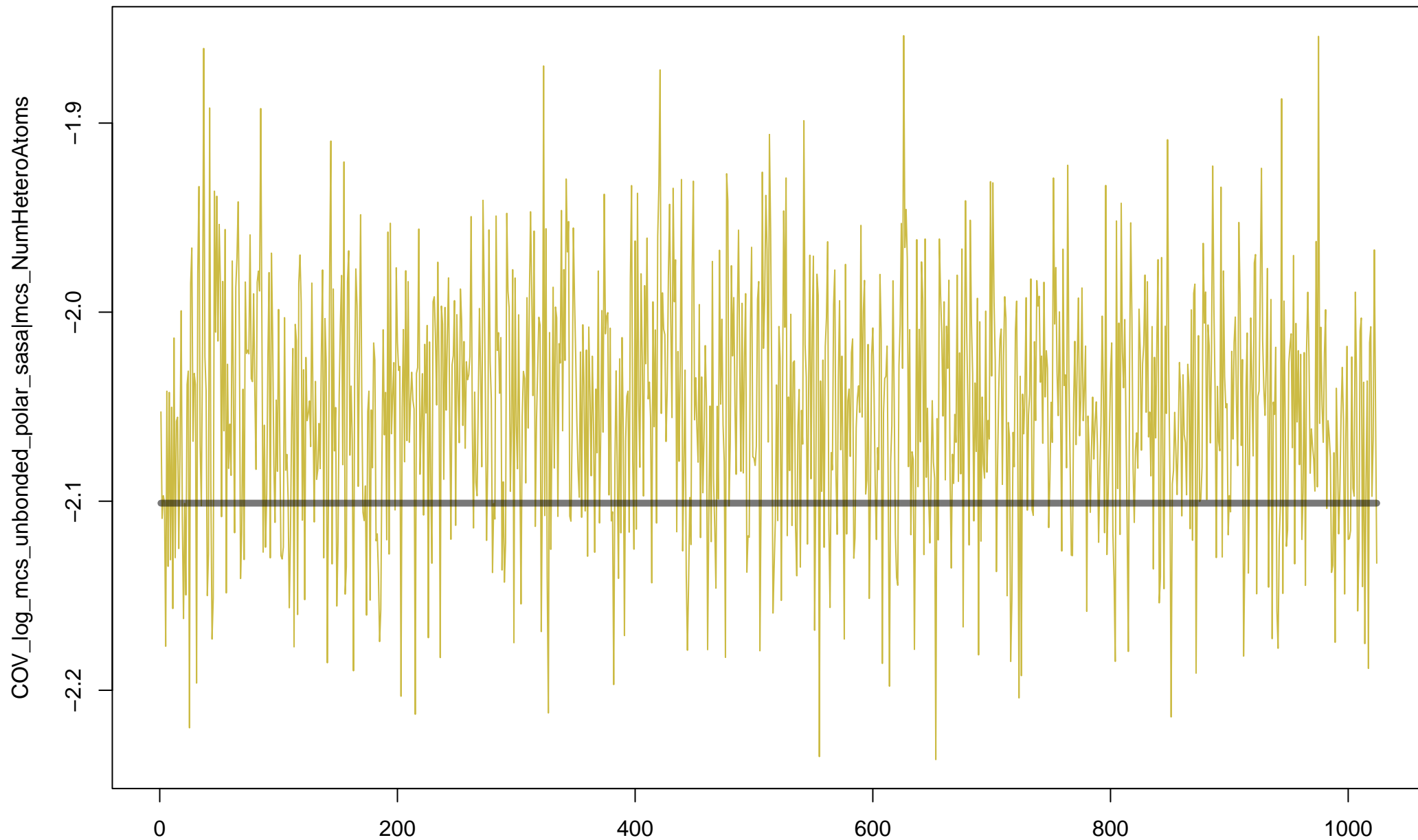
**COV\_log\_RMSD|mcs\_NOCount**  
**ESS = 935 | BMK = 0.0502 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | rel.err: -2.05**



**COV\_log\_mcs\_unbonded\_polar\_sasa|logit\_ec\_tanimoto\_similarity**  
**ESS = 1020 | BMK = 0.0612 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0 | rel.err: -1.94**

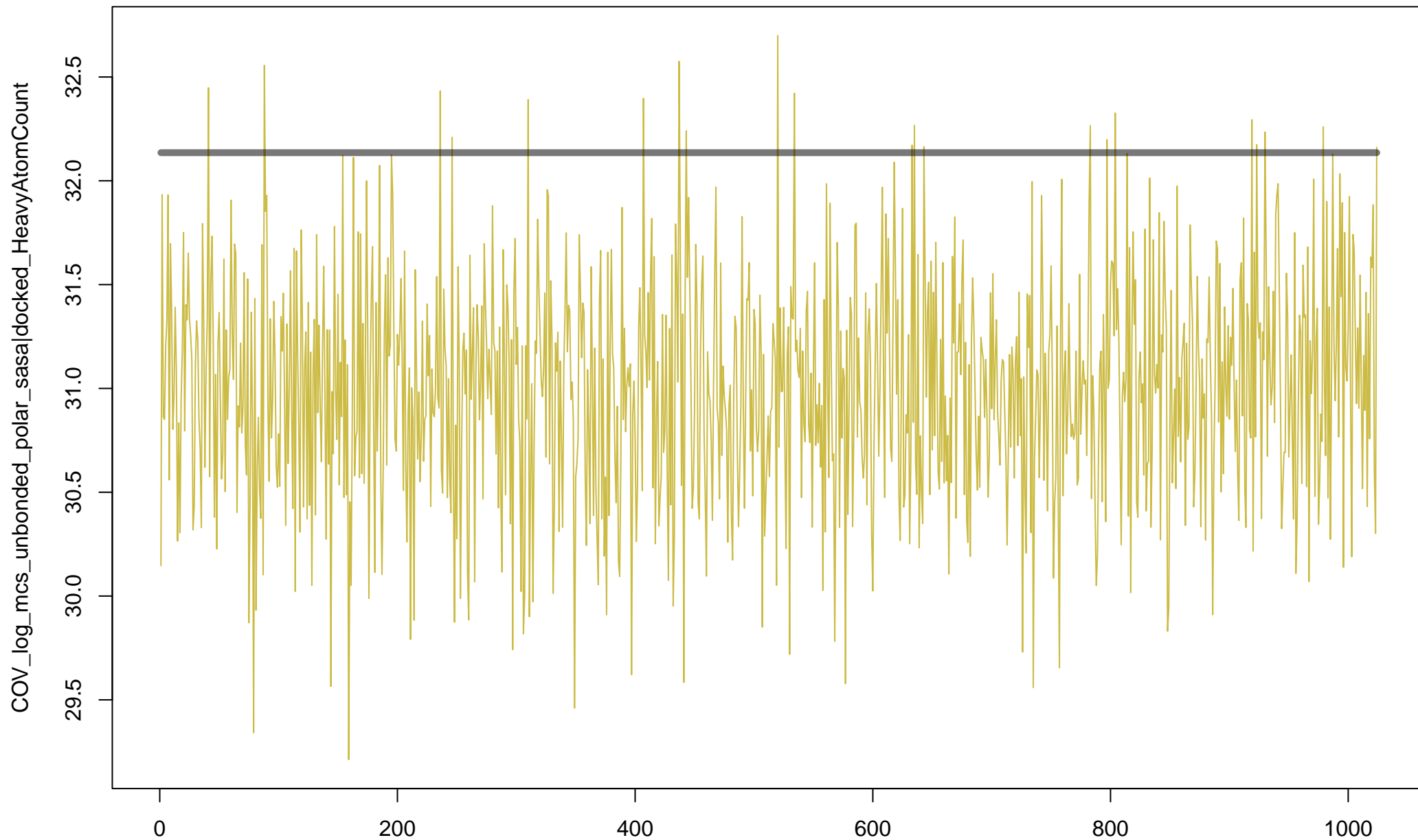


**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 1020 | BMK = 0.0575 | MCSE(6.27) = 3.56 | stat: TRUE | burn: 0 | rel.err: 0.782**

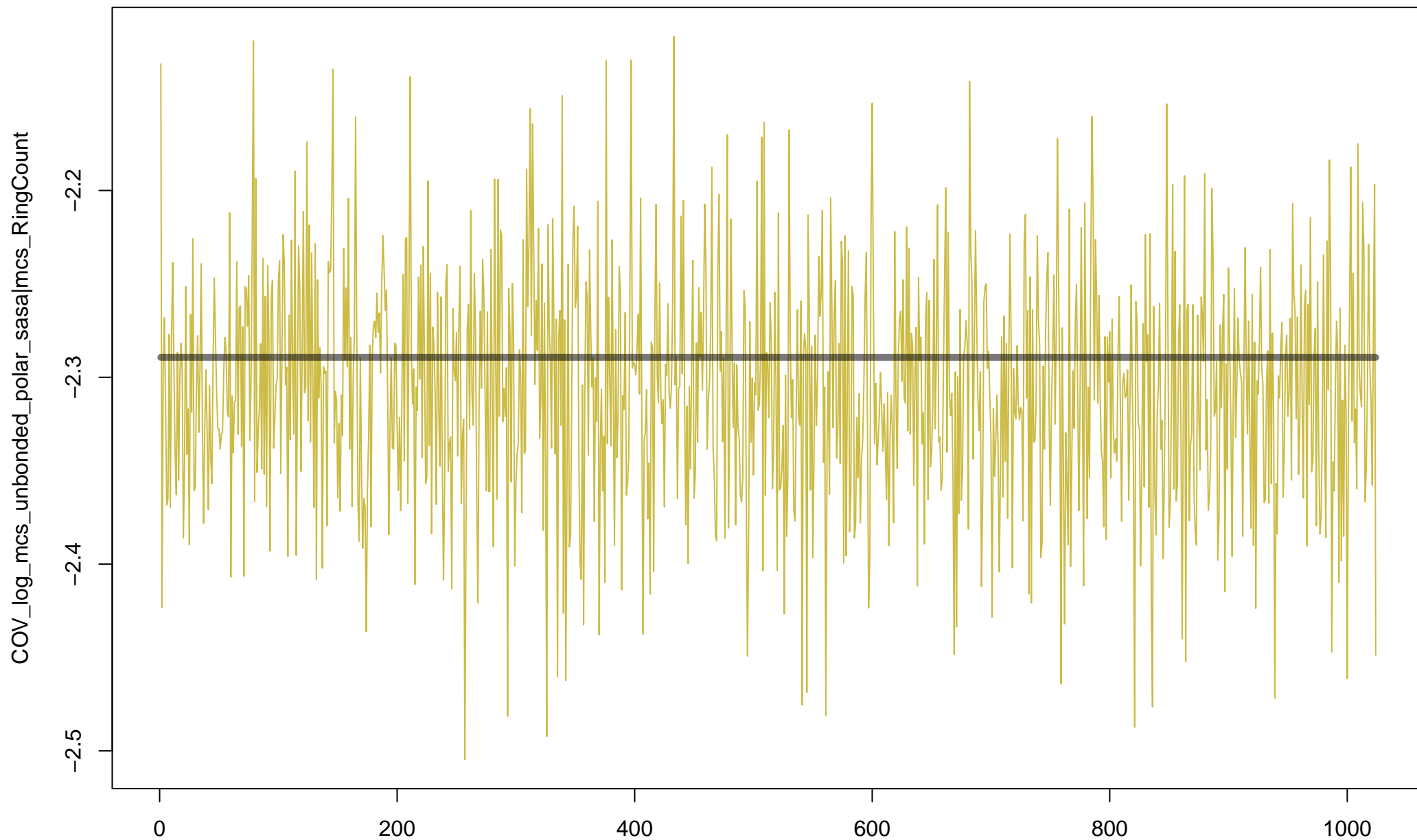




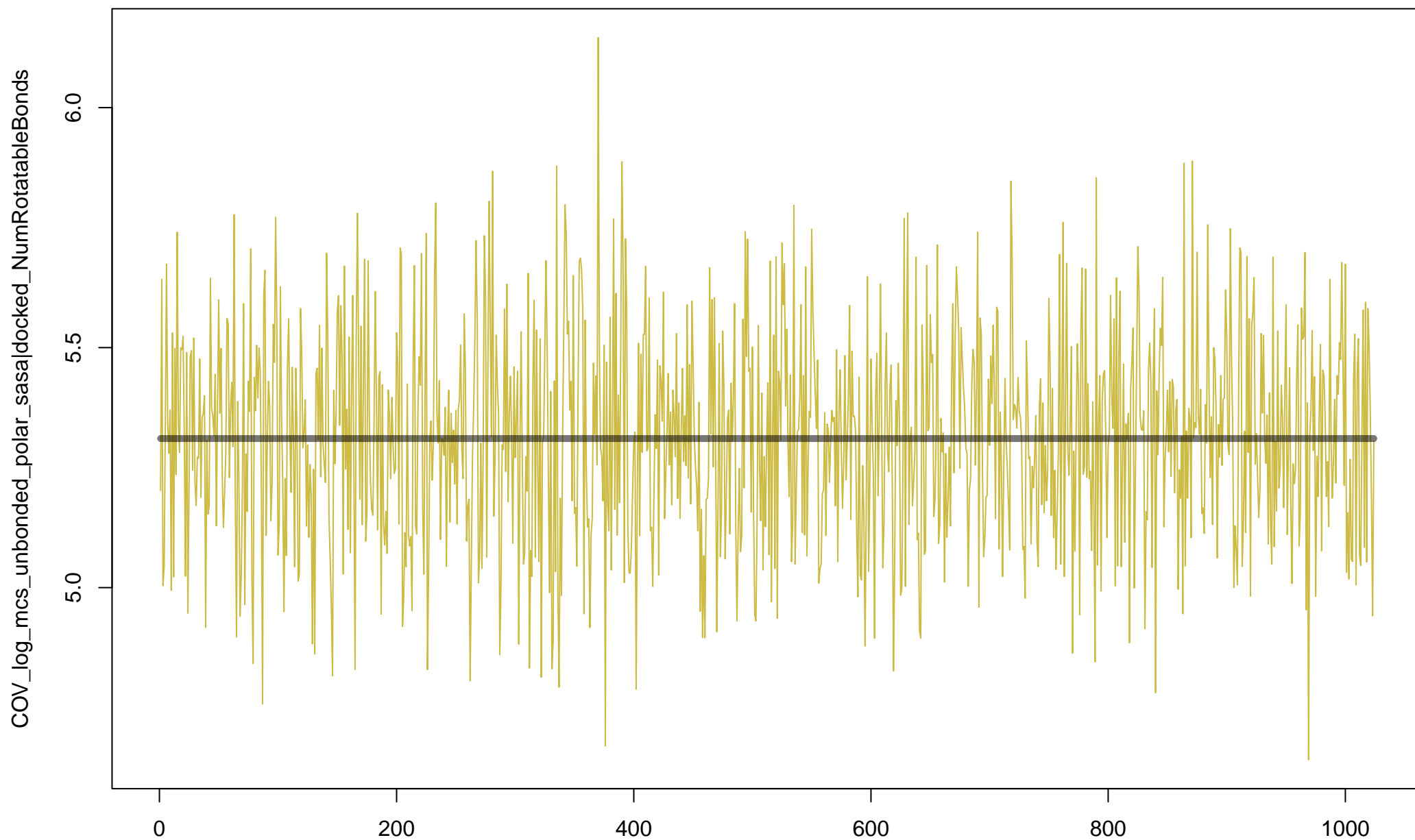
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.0647 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0 | rel.err: -2.11**



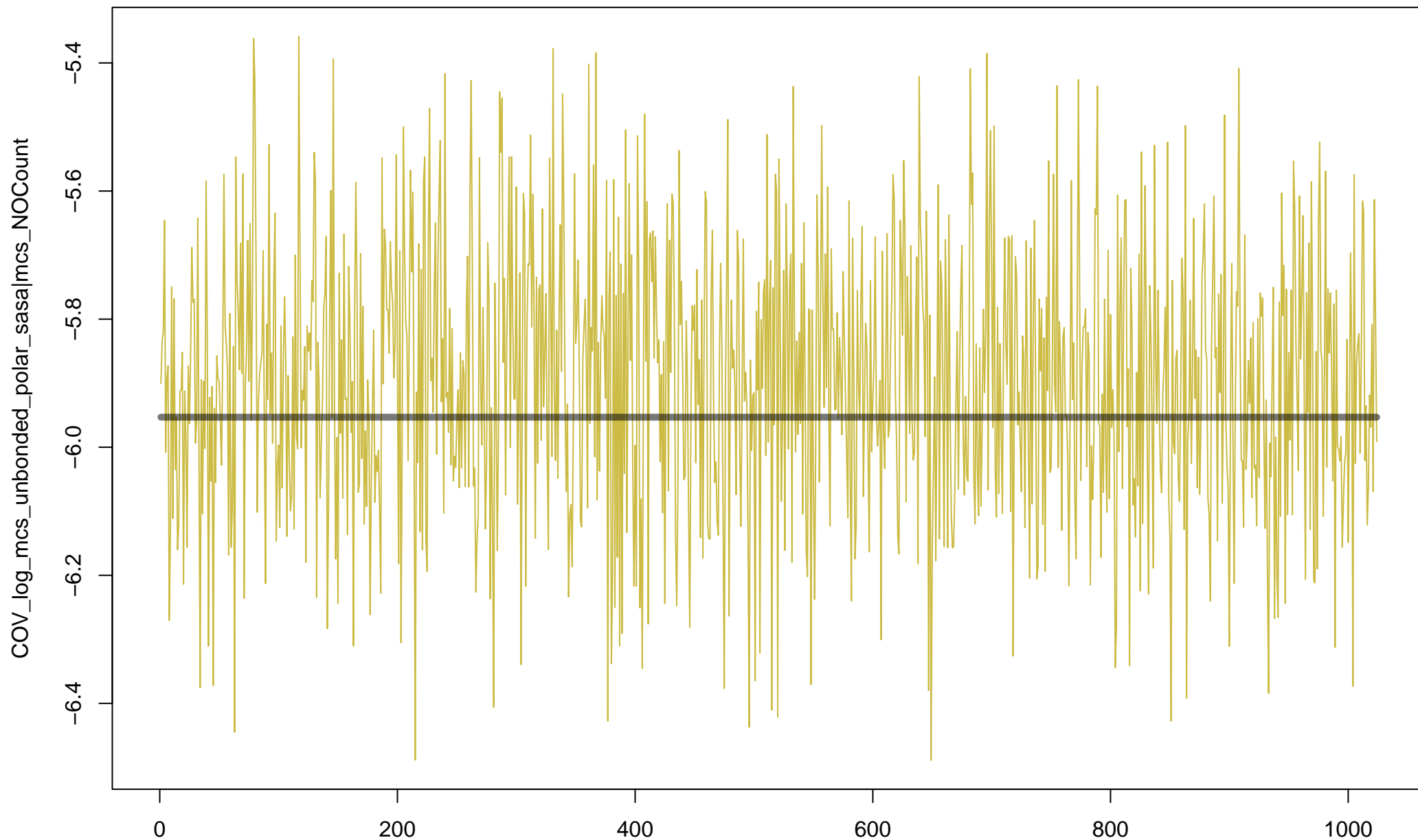
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.06 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0 | rel.err: -0.287**



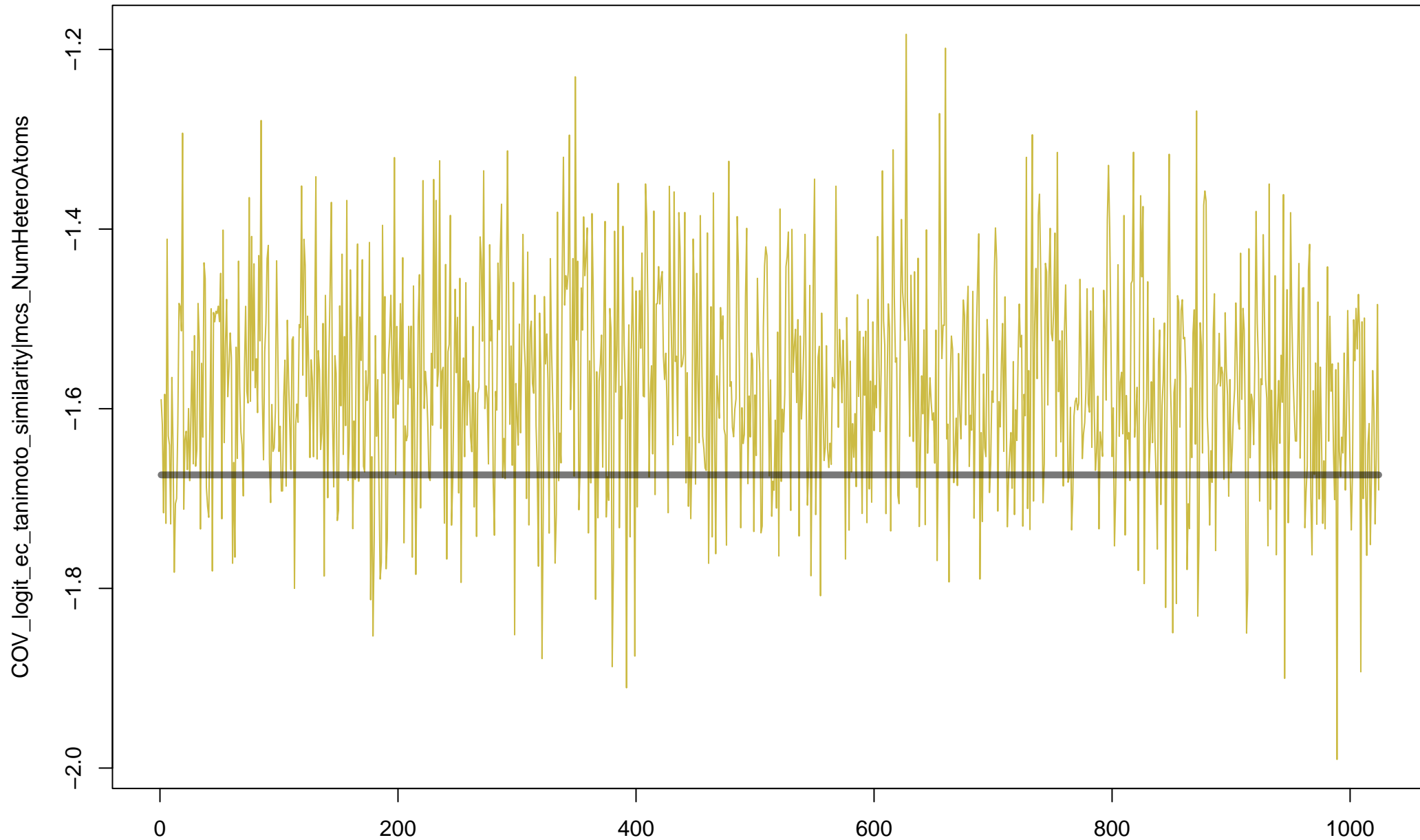
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0699 | MCSE(6.27) = 1.89 | stat: TRUE | burn: 0 | rel.err: 0.0095**



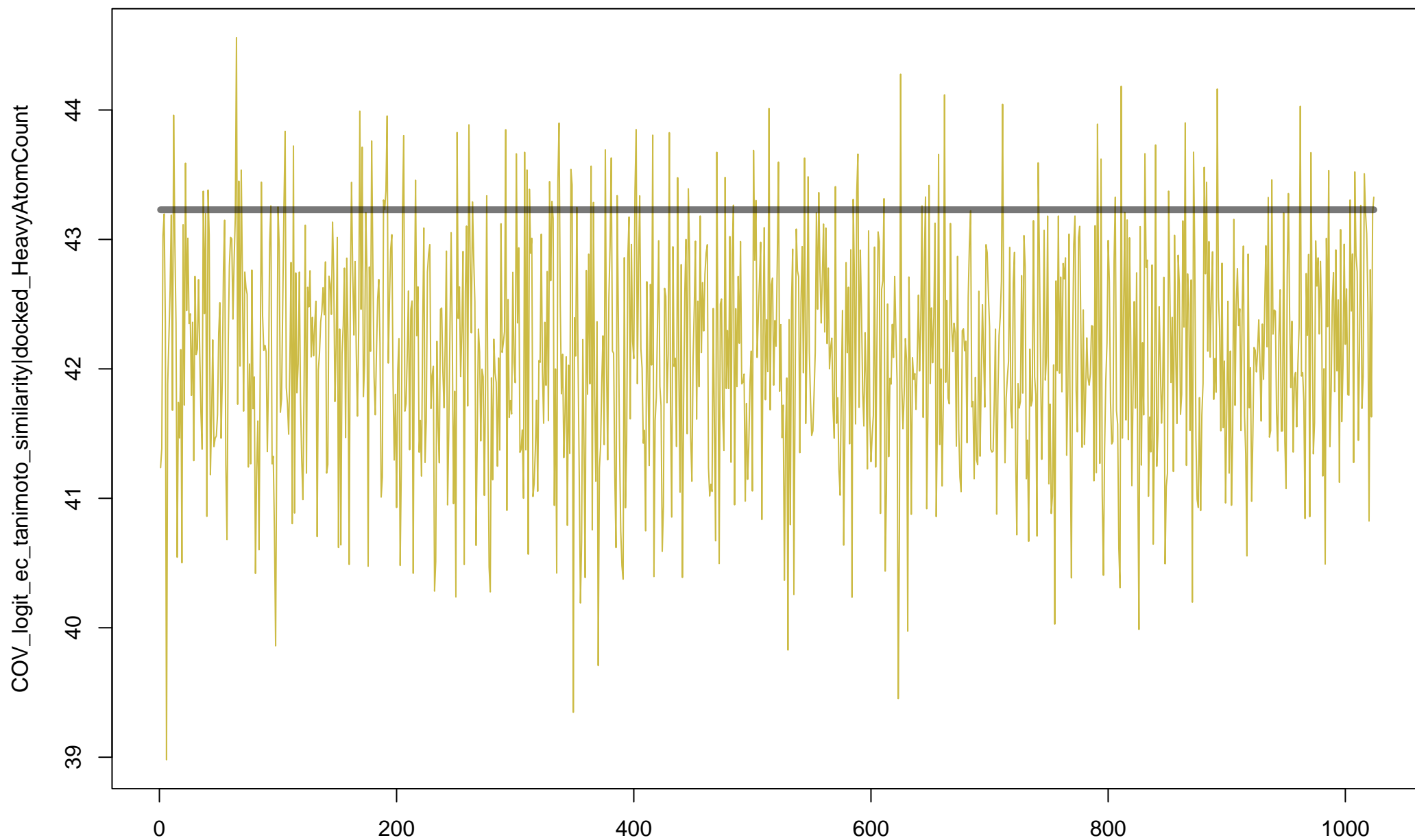
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0467 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | rel.err: 0.271**



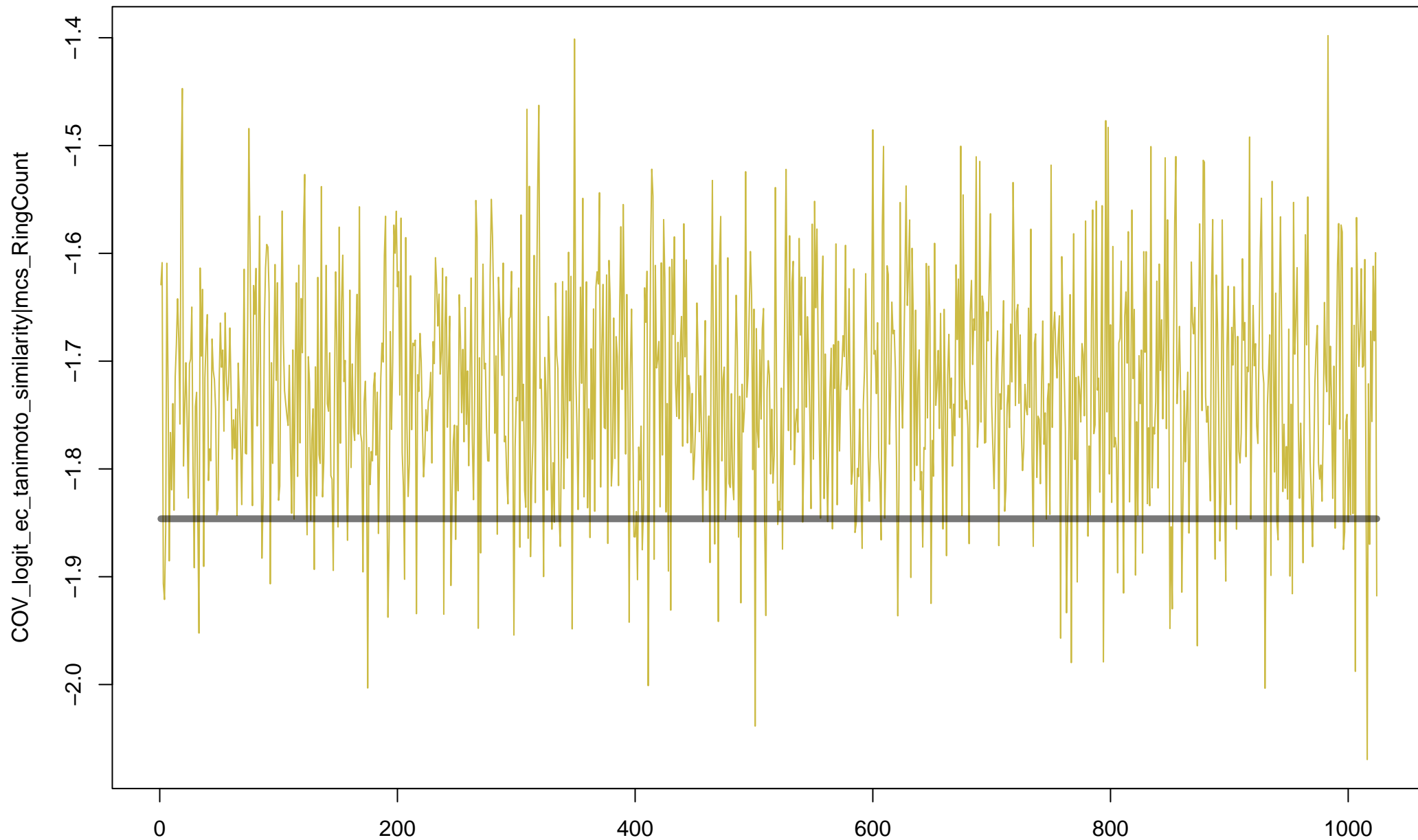
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms**  
**ESS = 1020 | BMK = 0.0596 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | rel.err: 0.869**



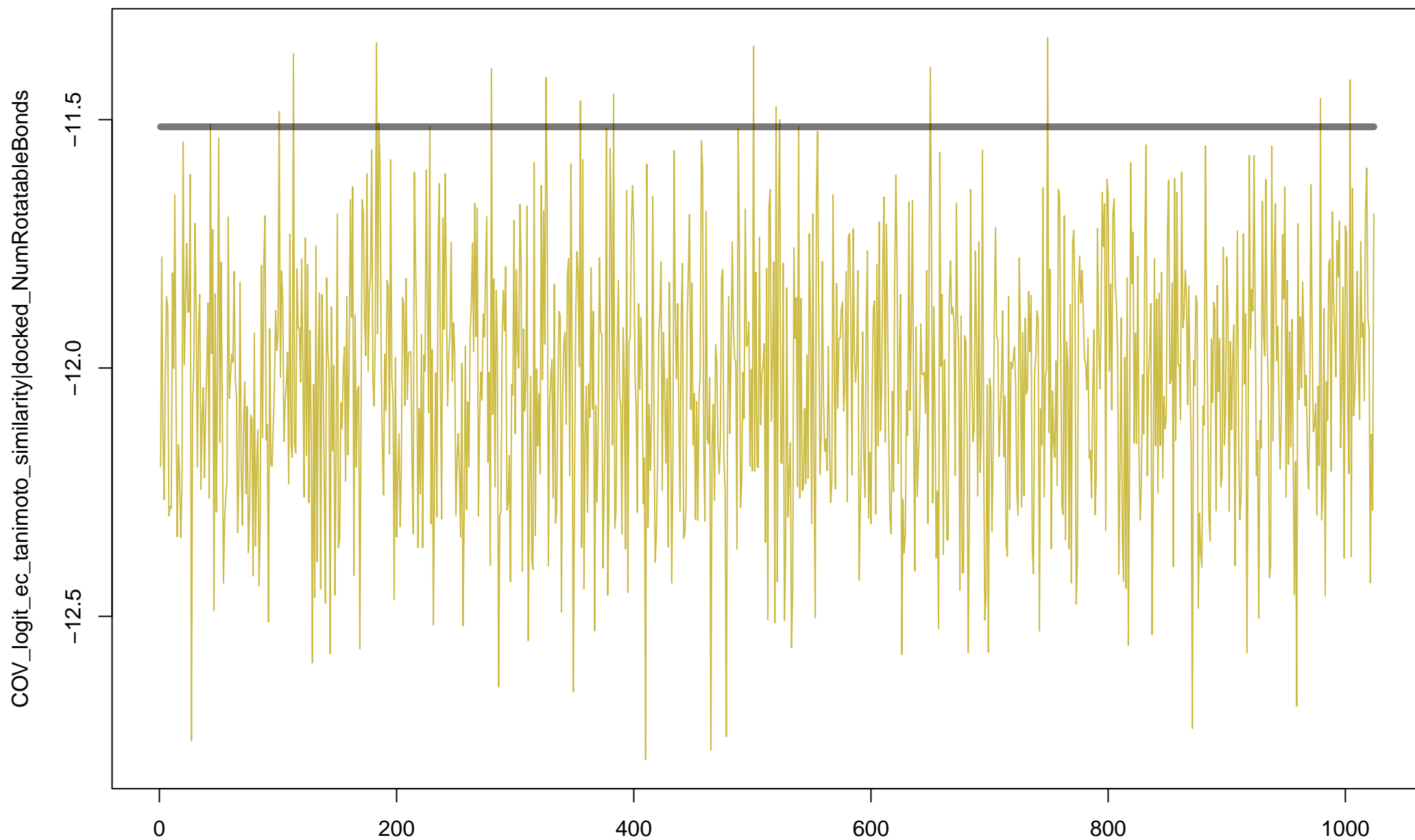
**COV\_logit\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.0666 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0 | rel.err: -1.31**



**COV\_logit\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.0487 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0 | rel.err: 1.2**

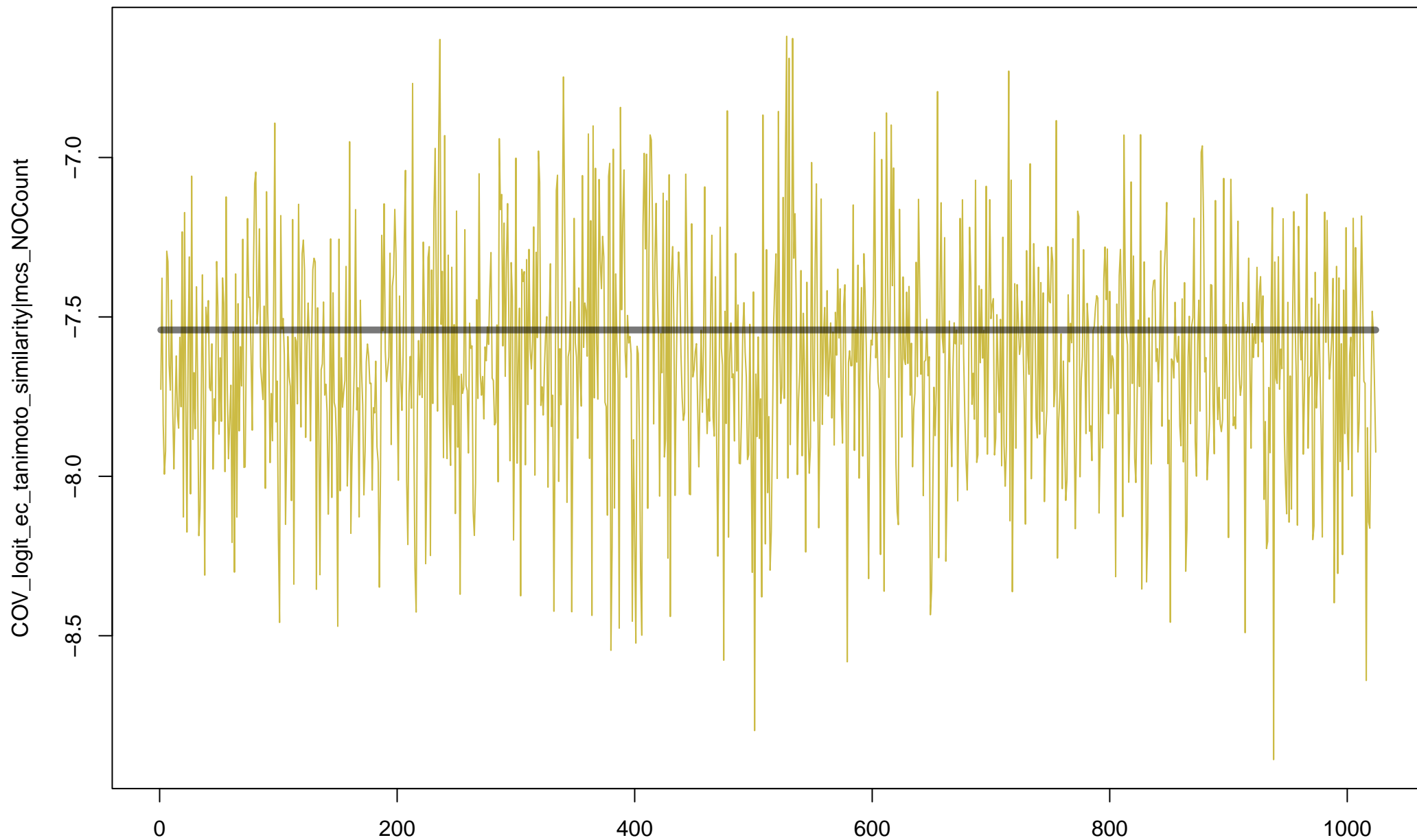


**COV\_logit\_ec\_tanimoto\_similarity|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0517 | MCSE(6.27) = 3.41 | stat: TRUE | burn: 0 | rel.err: -2.06**

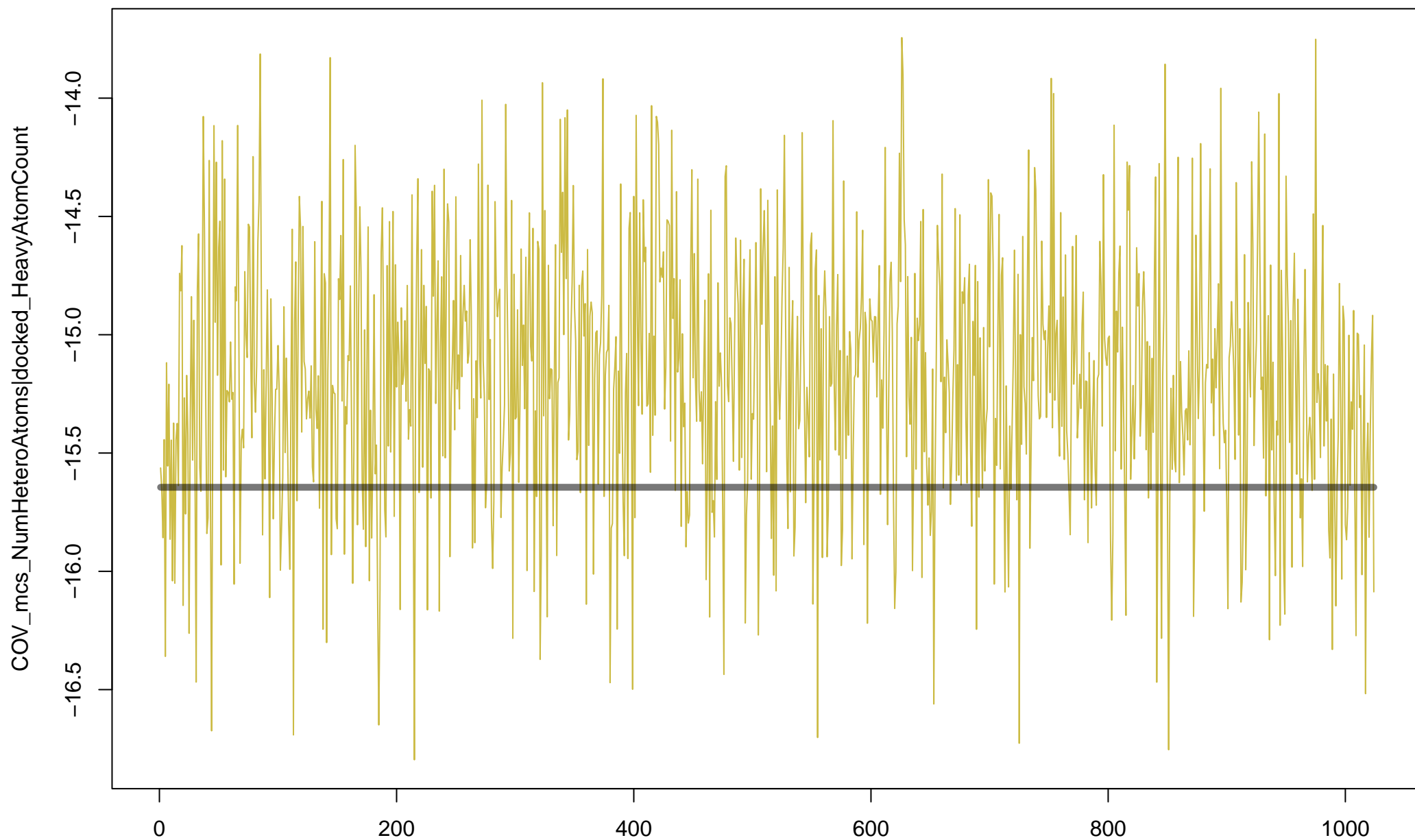




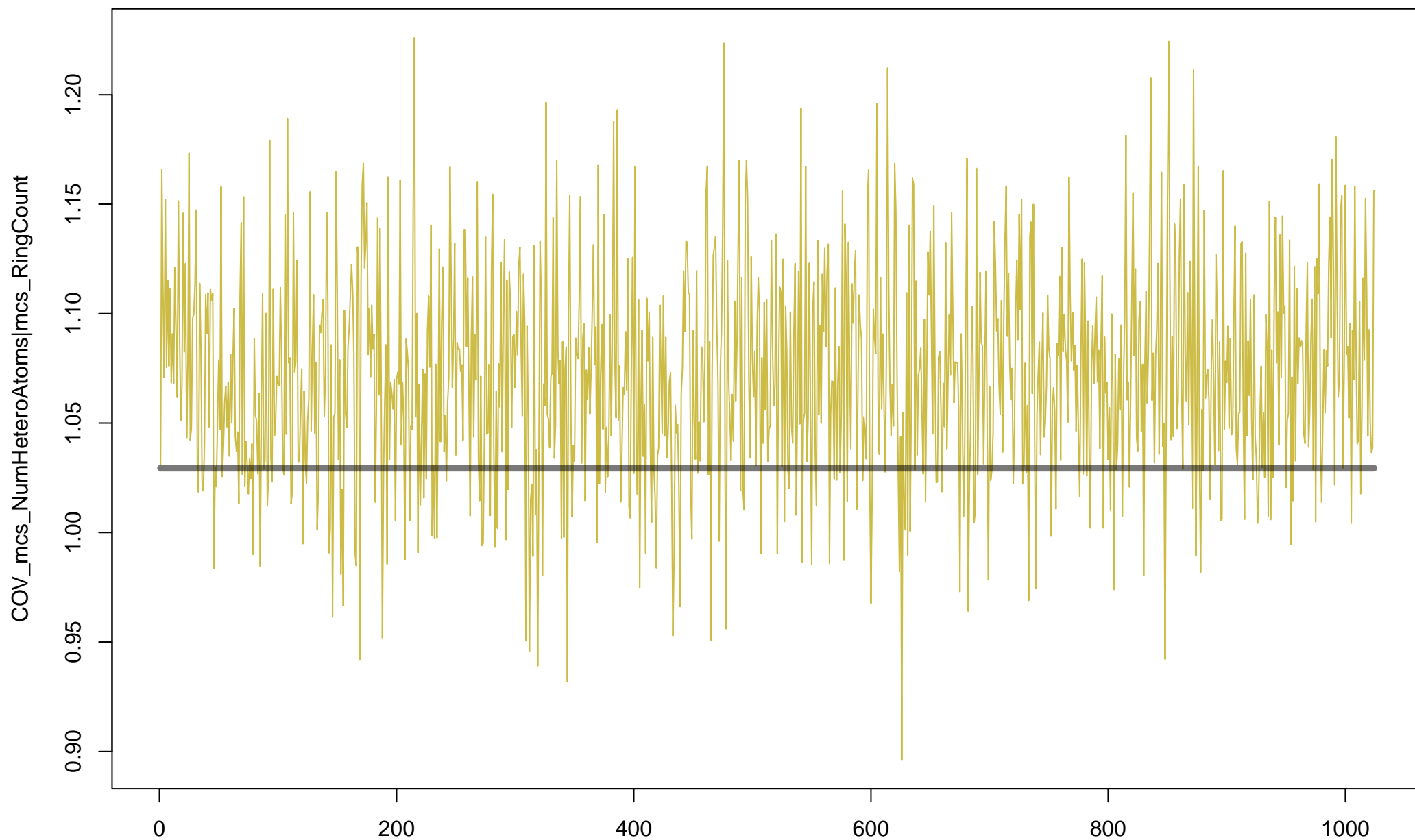
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0703 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | rel.err: -0.293**



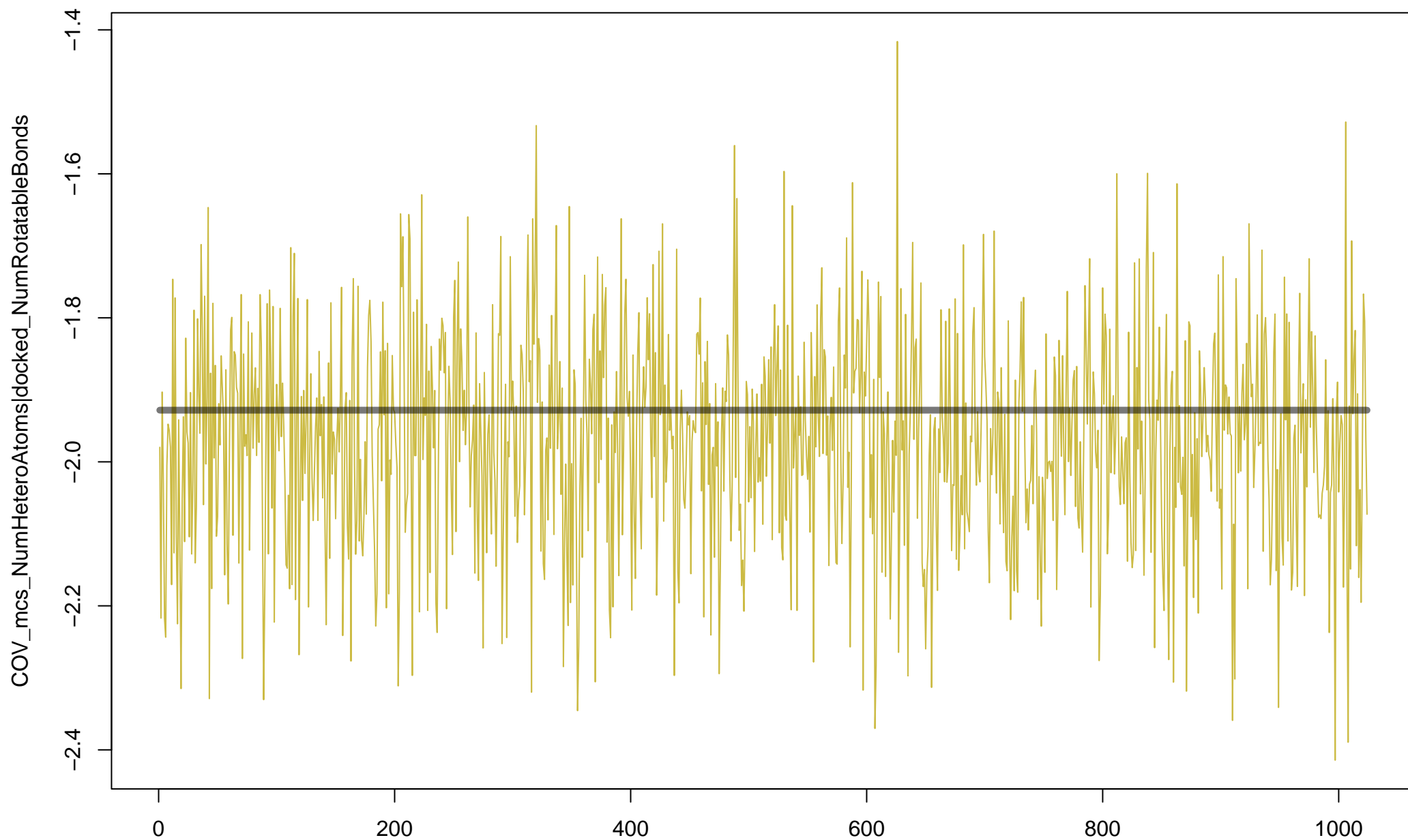
**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.0644 | MCSE(6.27) = 3.84 | stat: TRUE | burn: 0 | rel.err: 0.865**



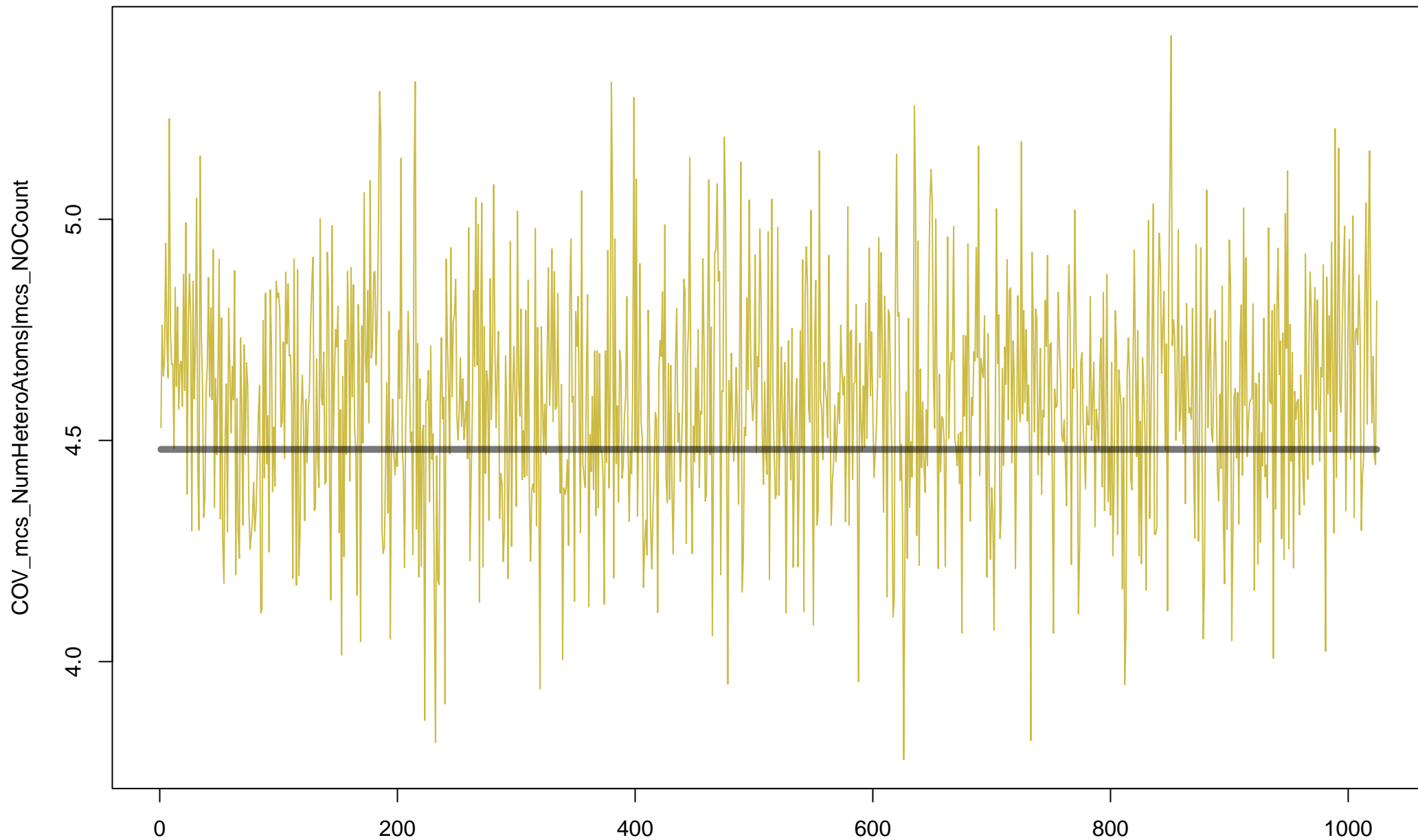
**COV\_mcs\_NumHeteroAtoms|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.0604 | MCSE(6.27) = 3.49 | stat: TRUE | burn: 0 | rel.err: 0.872**



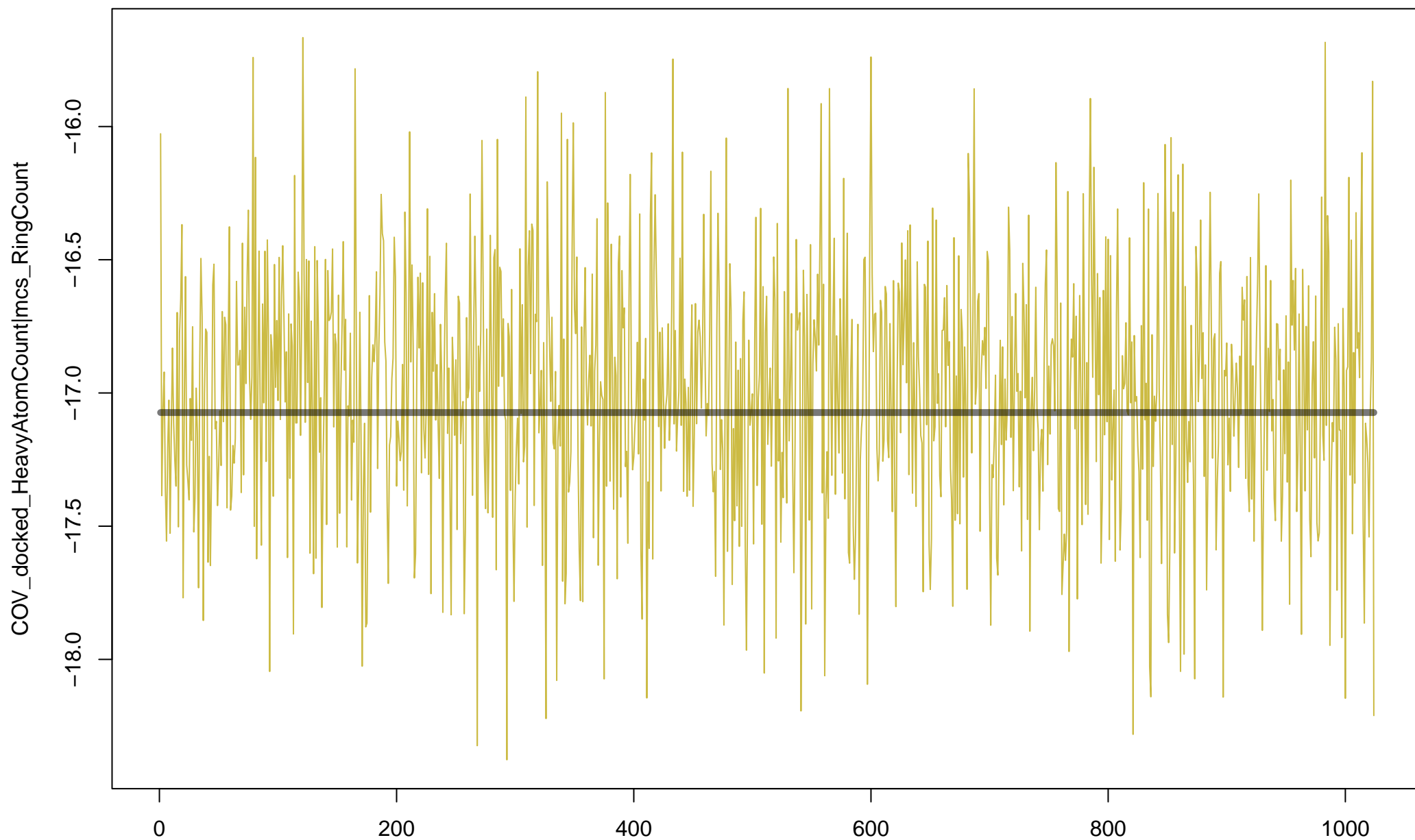
**COV\_mcs\_NumHeteroAtoms|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.059 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0 | rel.err: -0.295**



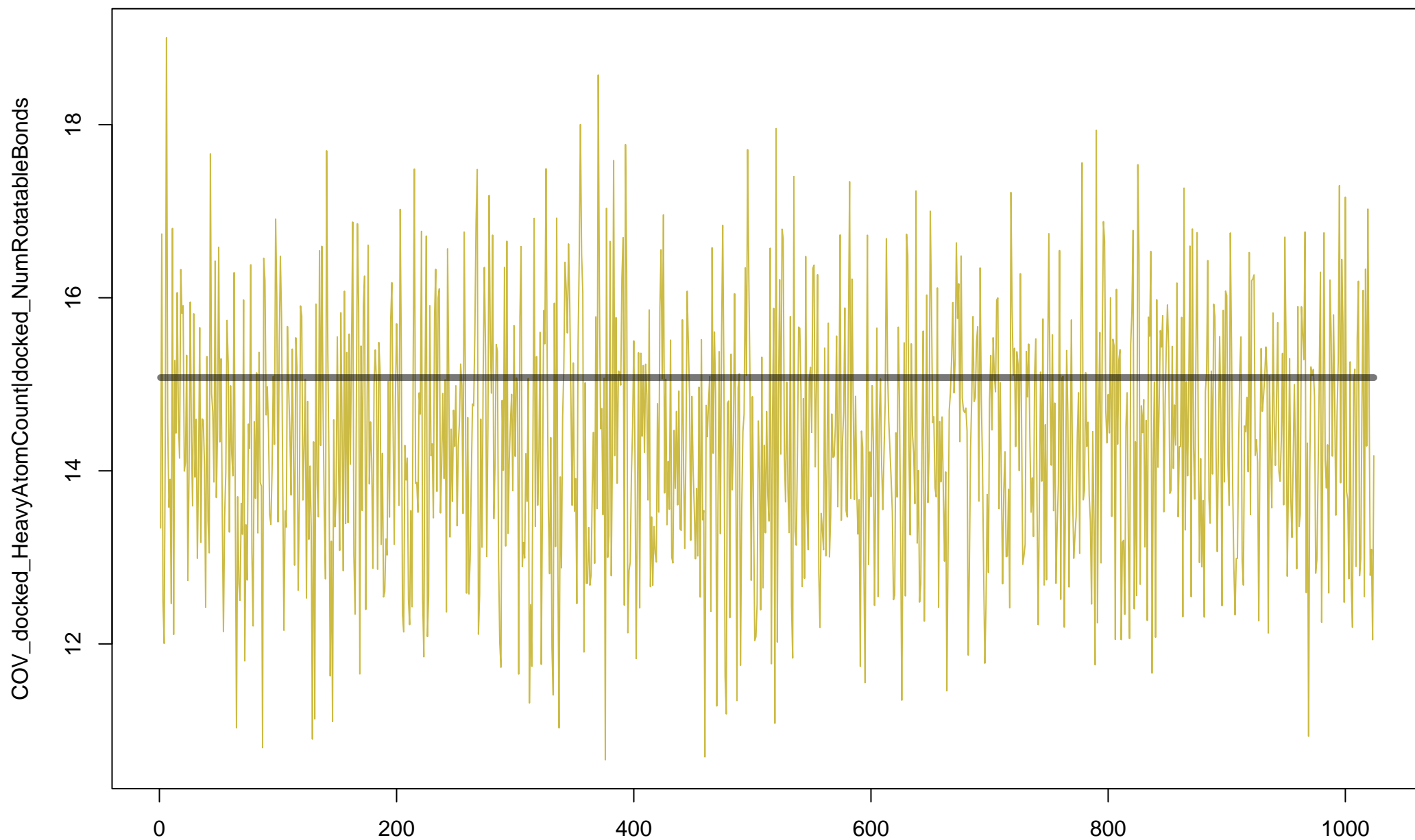
**COV\_mcs\_NumHeteroAtoms|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0484 | MCSE(6.27) = 3.86 | stat: TRUE | burn: 0 | rel.err: 0.442**



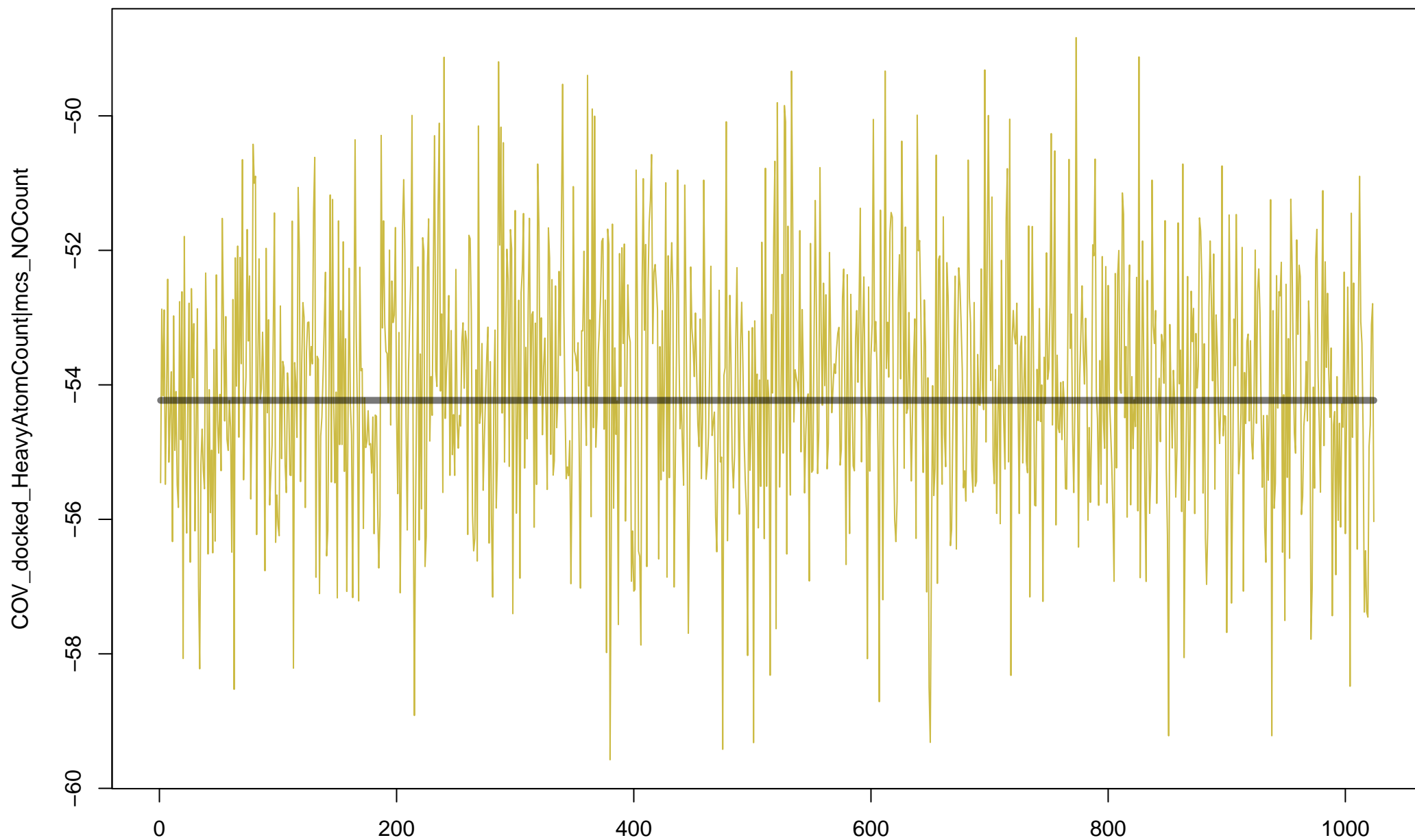
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.0337 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0 | rel.err: 0.165**



**COV\_docked\_HeavyAtomCount|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0598 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0 | rel.err: -0.505**

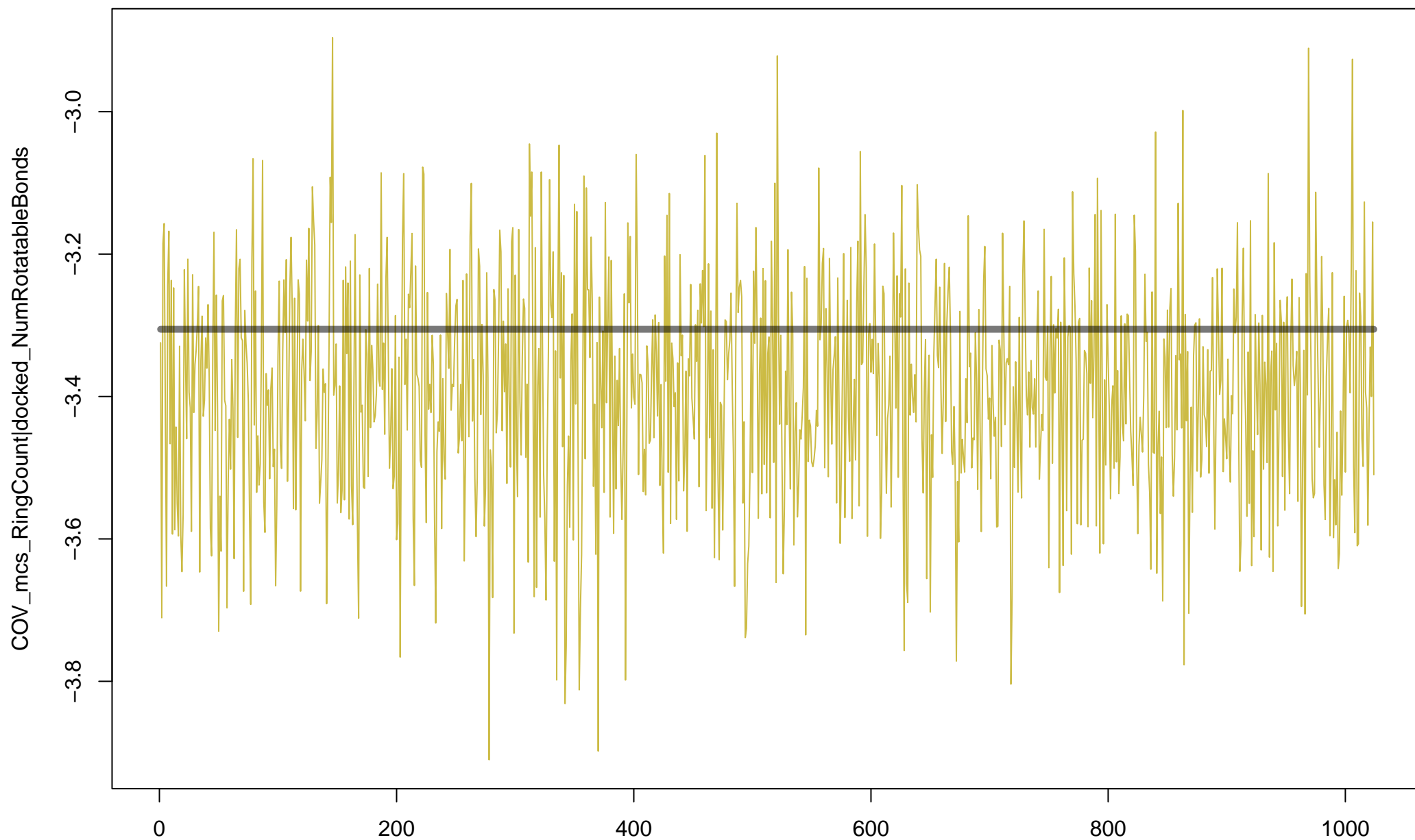


**COV\_docked\_HeavyAtomCount|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0359 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0 | rel.err: 0.137**

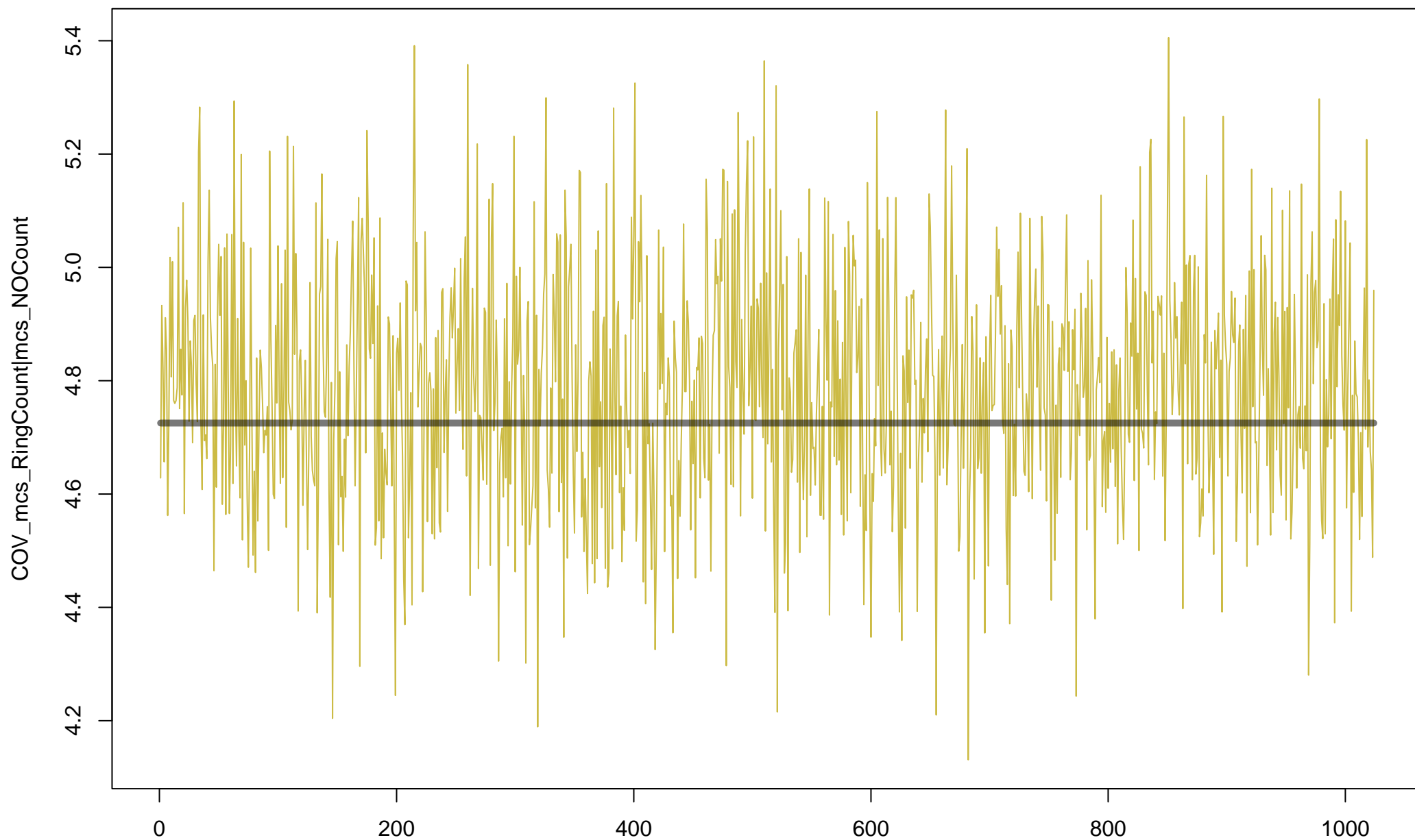




**COV\_mcs\_RingCount|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0788 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: -0.572**



**COV\_mcs\_RingCount|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0617 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 0 | rel.err: 0.304**



**COV\_docked\_NumRotatableBonds|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0603 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | rel.err: 0.998**

