

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 1

max MCSE = 10.7648099073685

all stationary: FALSE

burn: 1020

min percent.: 0.48828125

-- STATS 2D --

min ESS = 921.595433918259

max BMK = 0.0769731039480665

max MCSE = 4.05749787427369

all stationary: TRUE

burn: 0

min percent.: 0.9765625

-- STATS 1D --

min ESS = 104.005496338473

max BMK = 1

max MCSE = 7.34499115563367

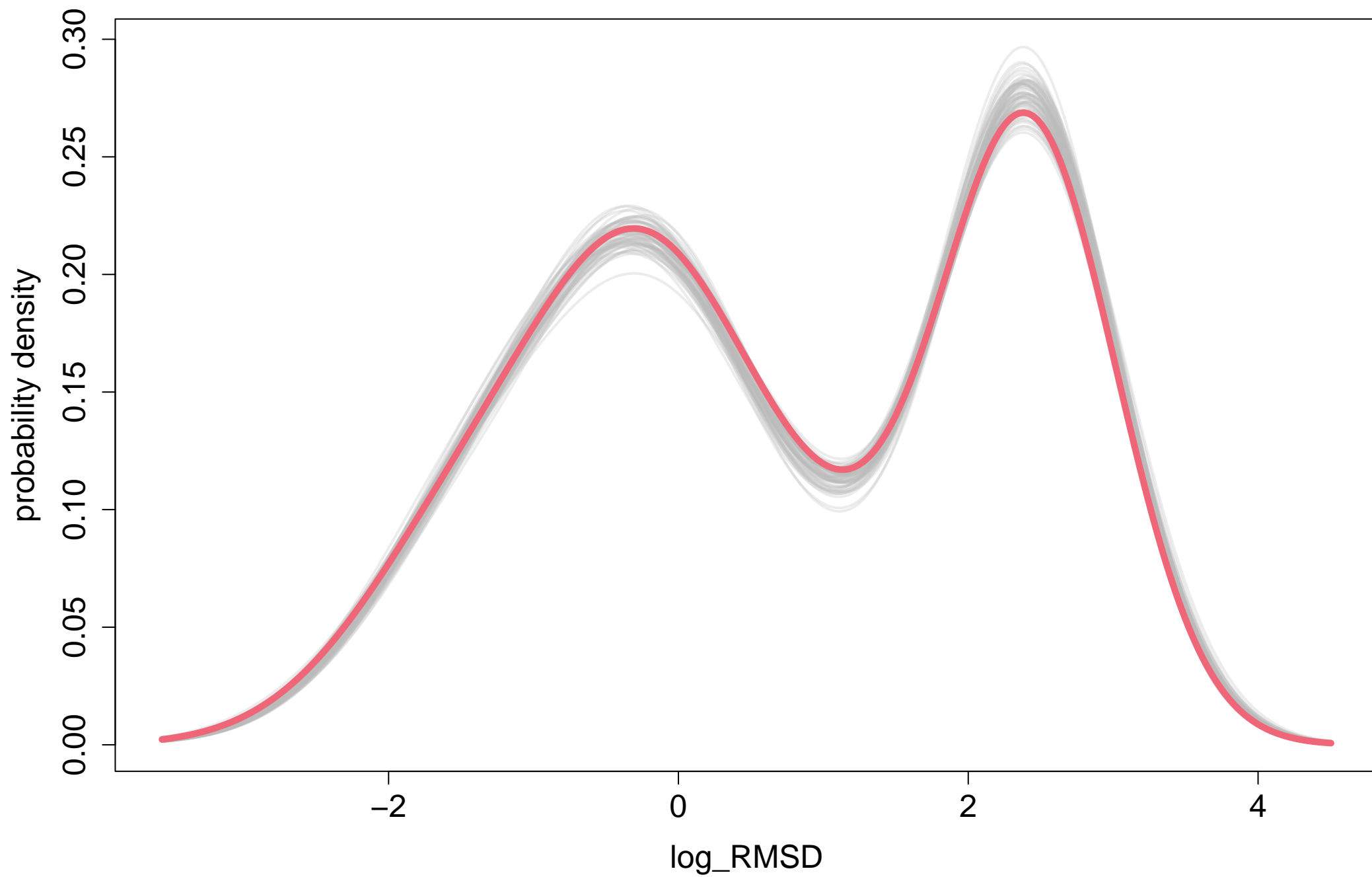
all stationary: FALSE

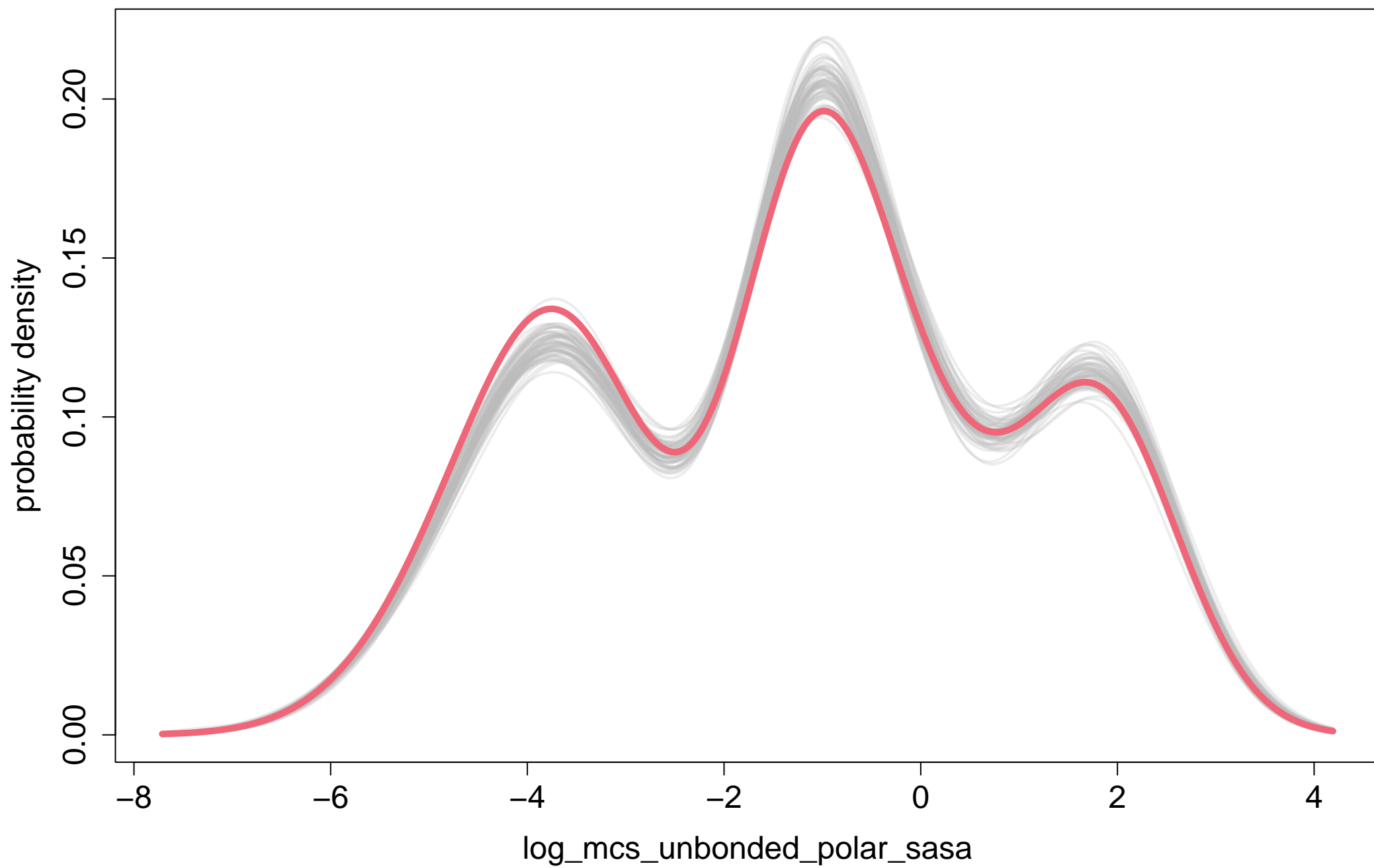
burn: 714

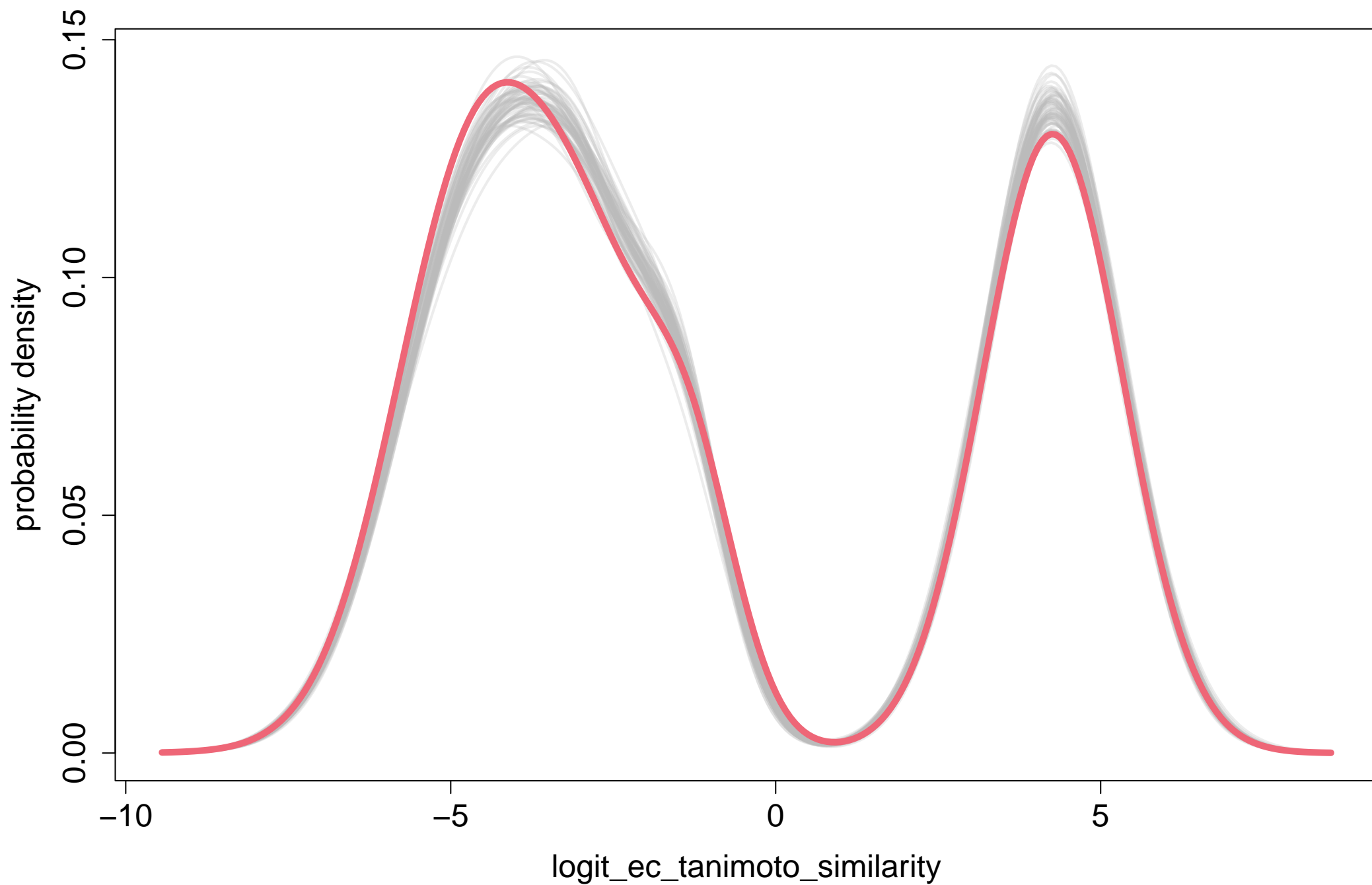
min percent.: 0.1953125

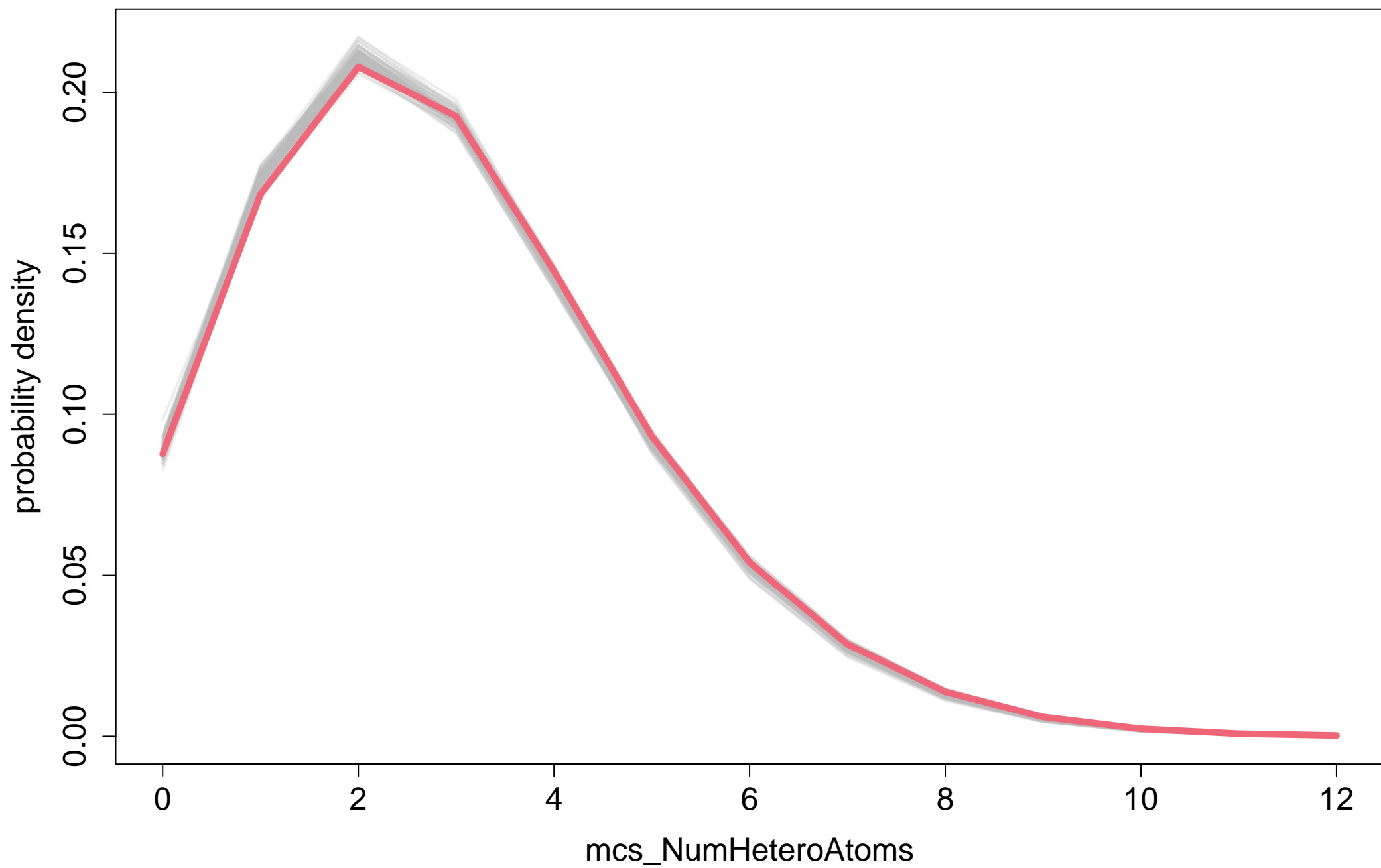
Occupied clusters: 9 of 64

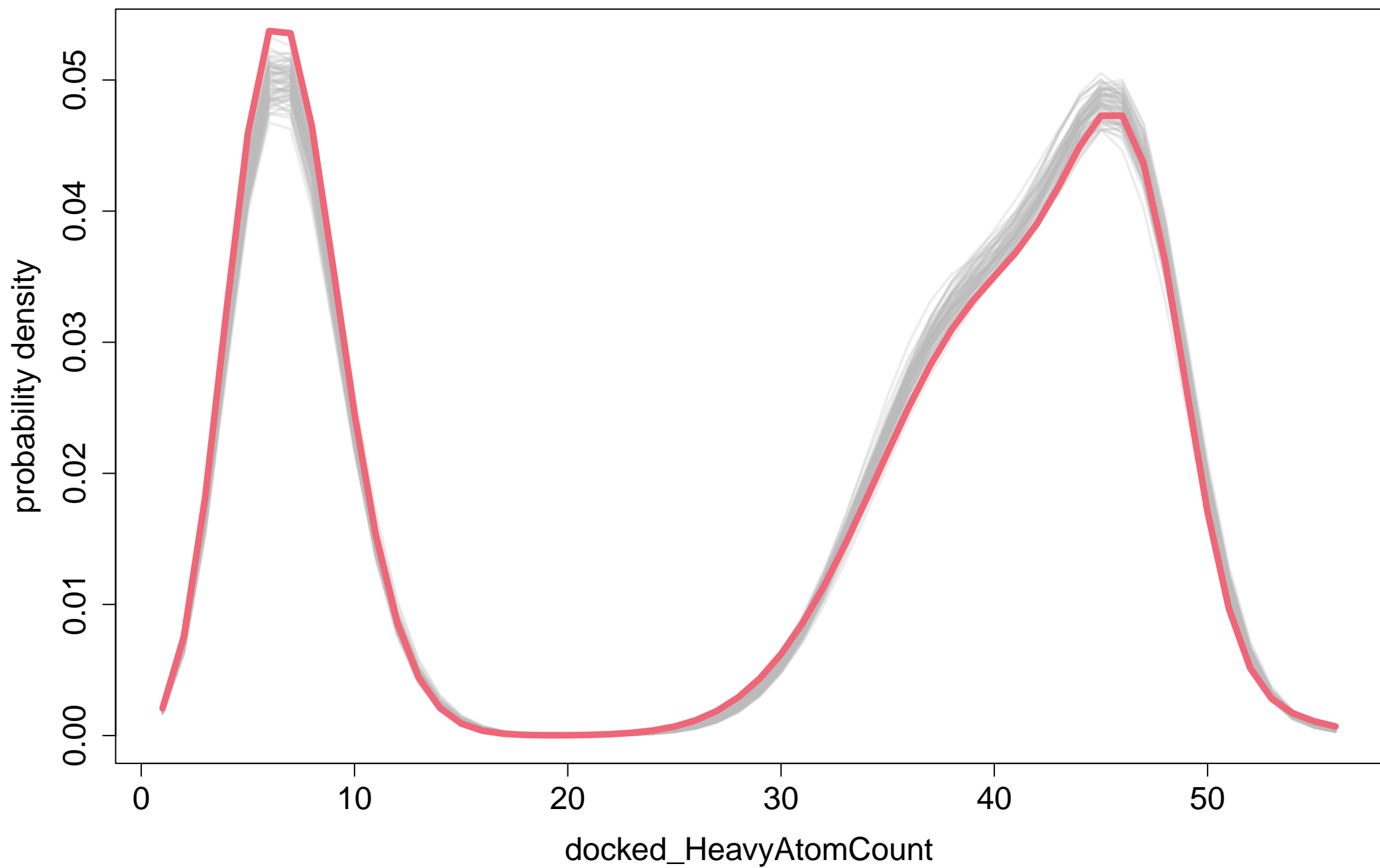
LL: -62400 +- 10.1

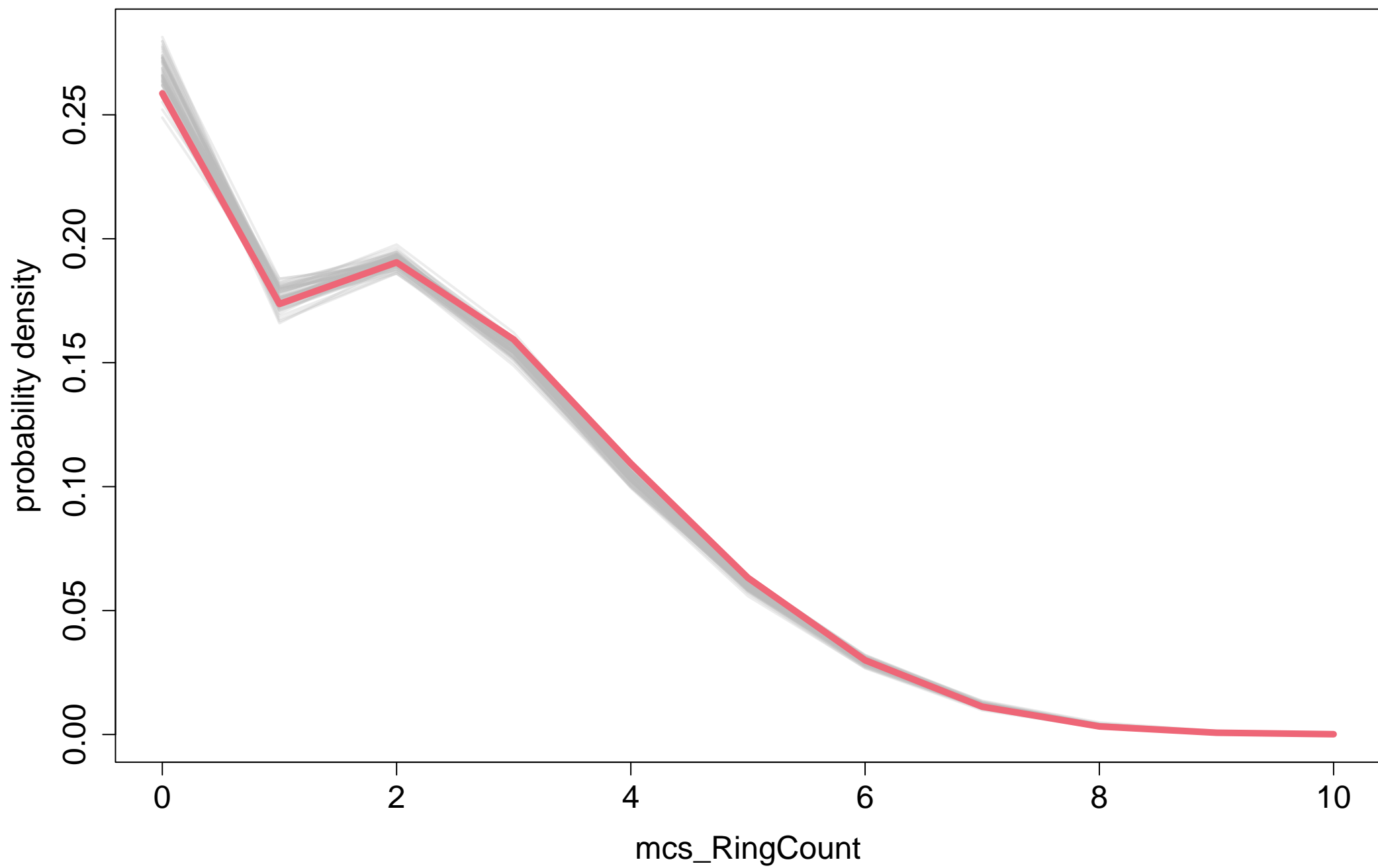


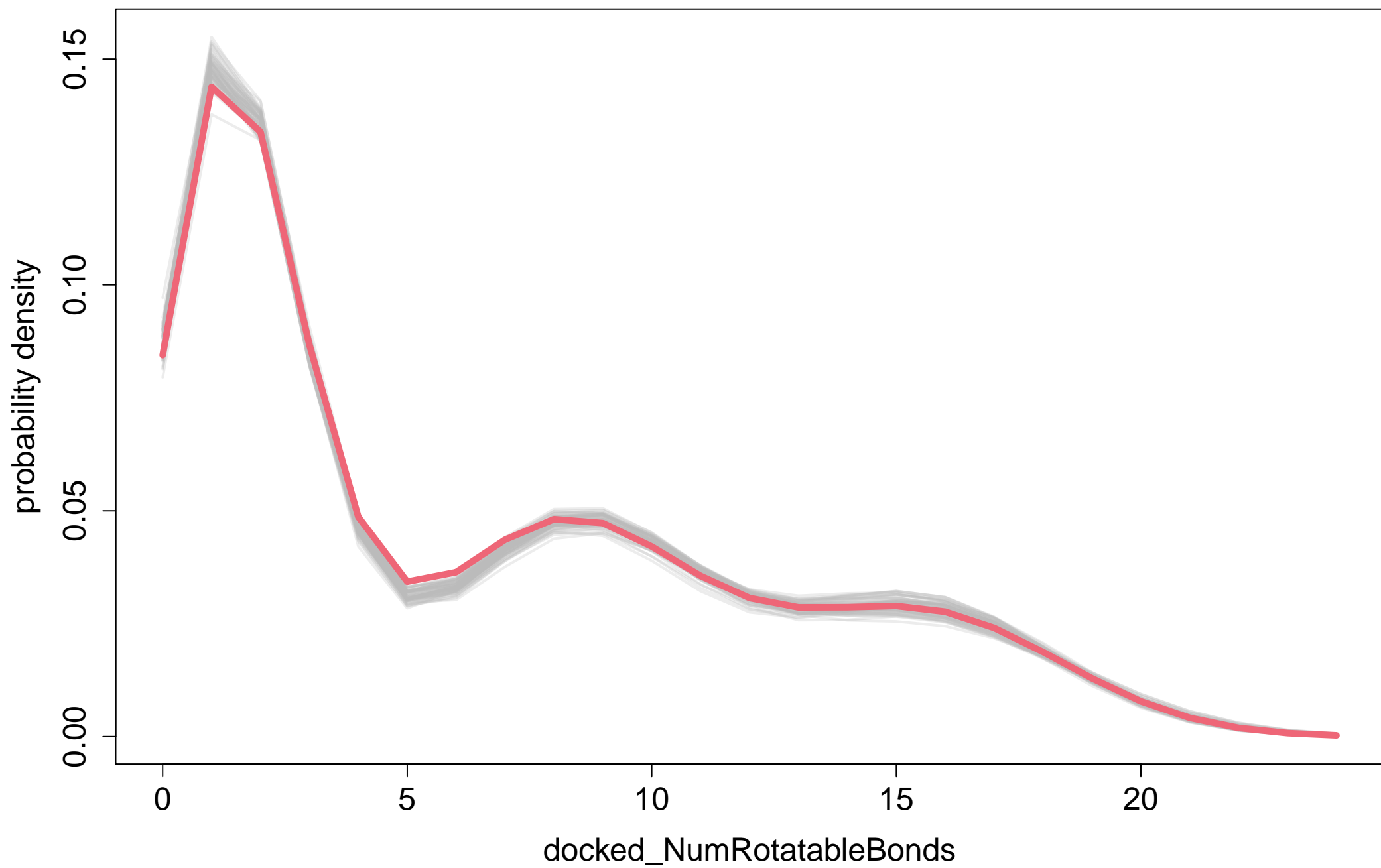




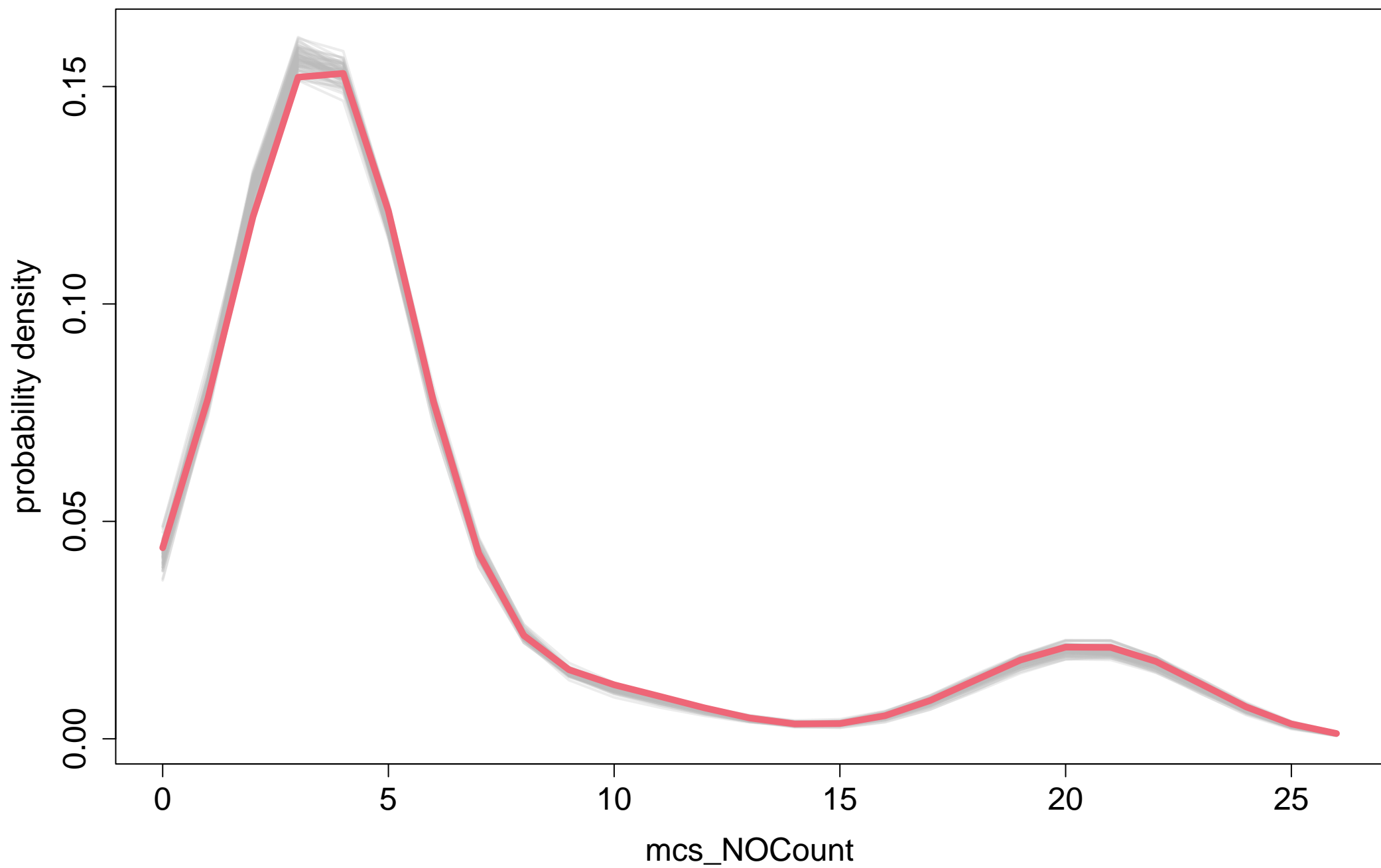


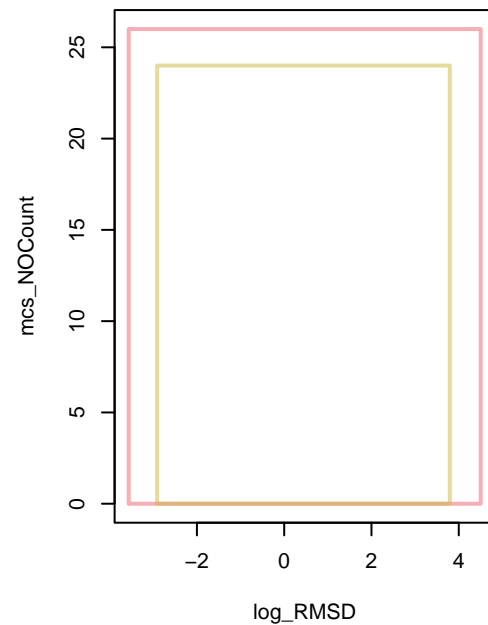
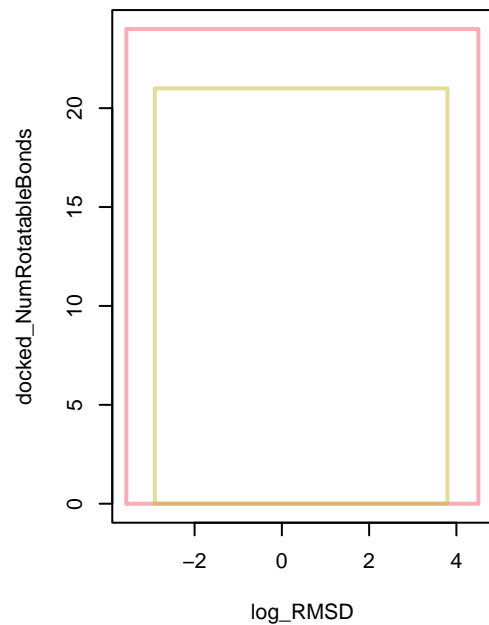
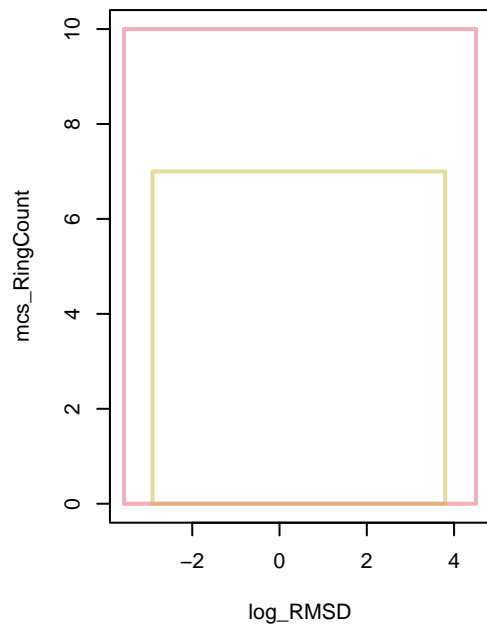
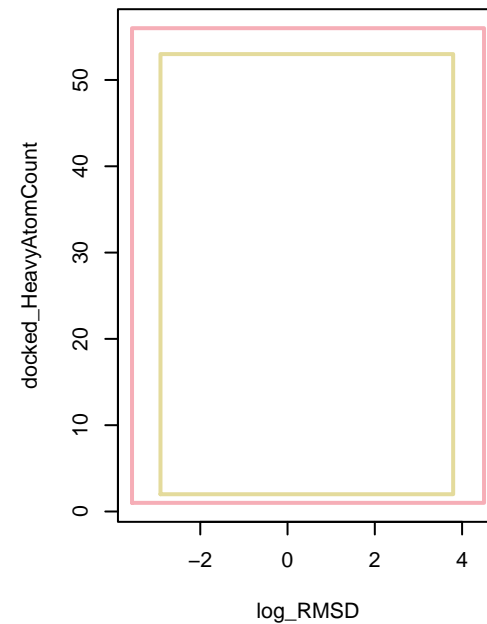
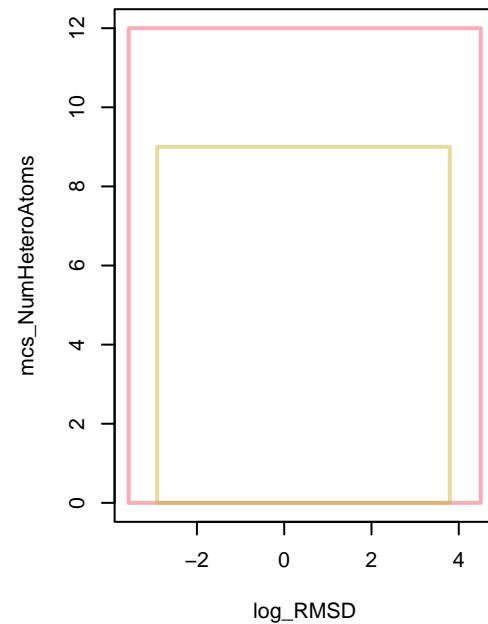
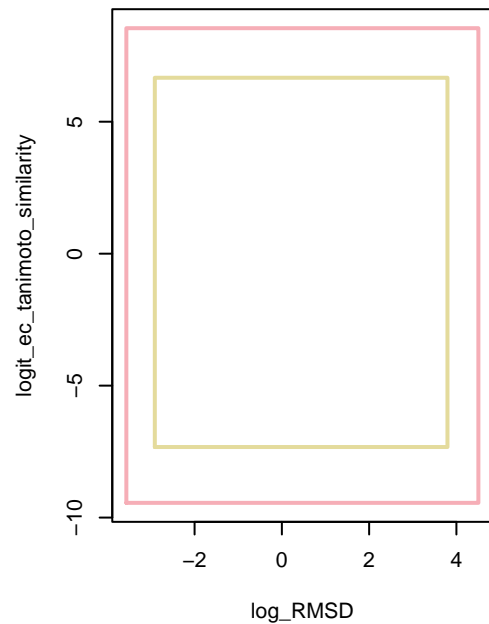
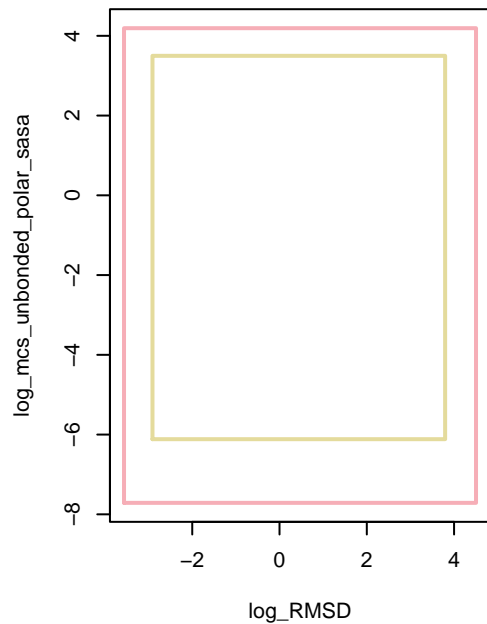




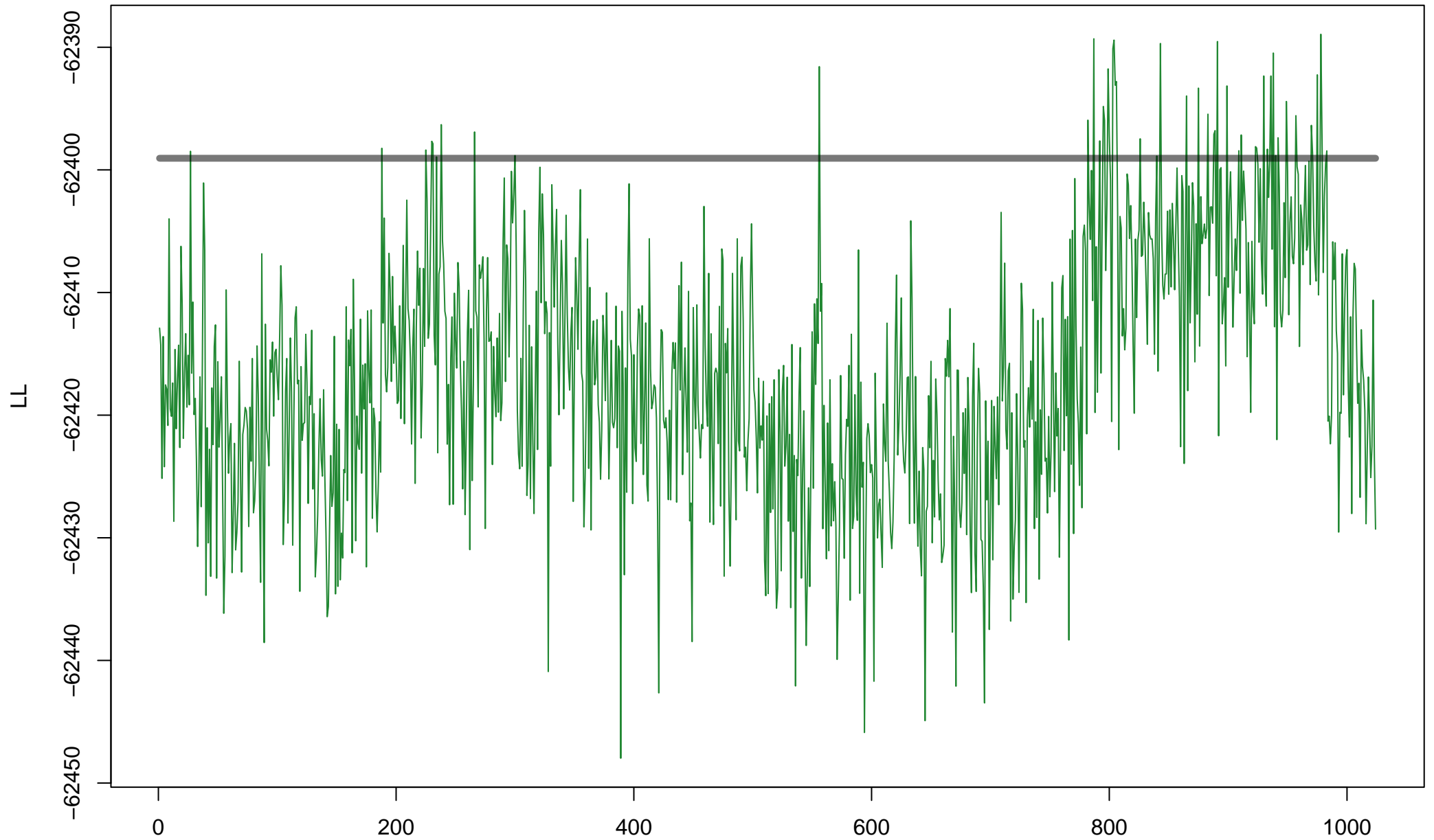






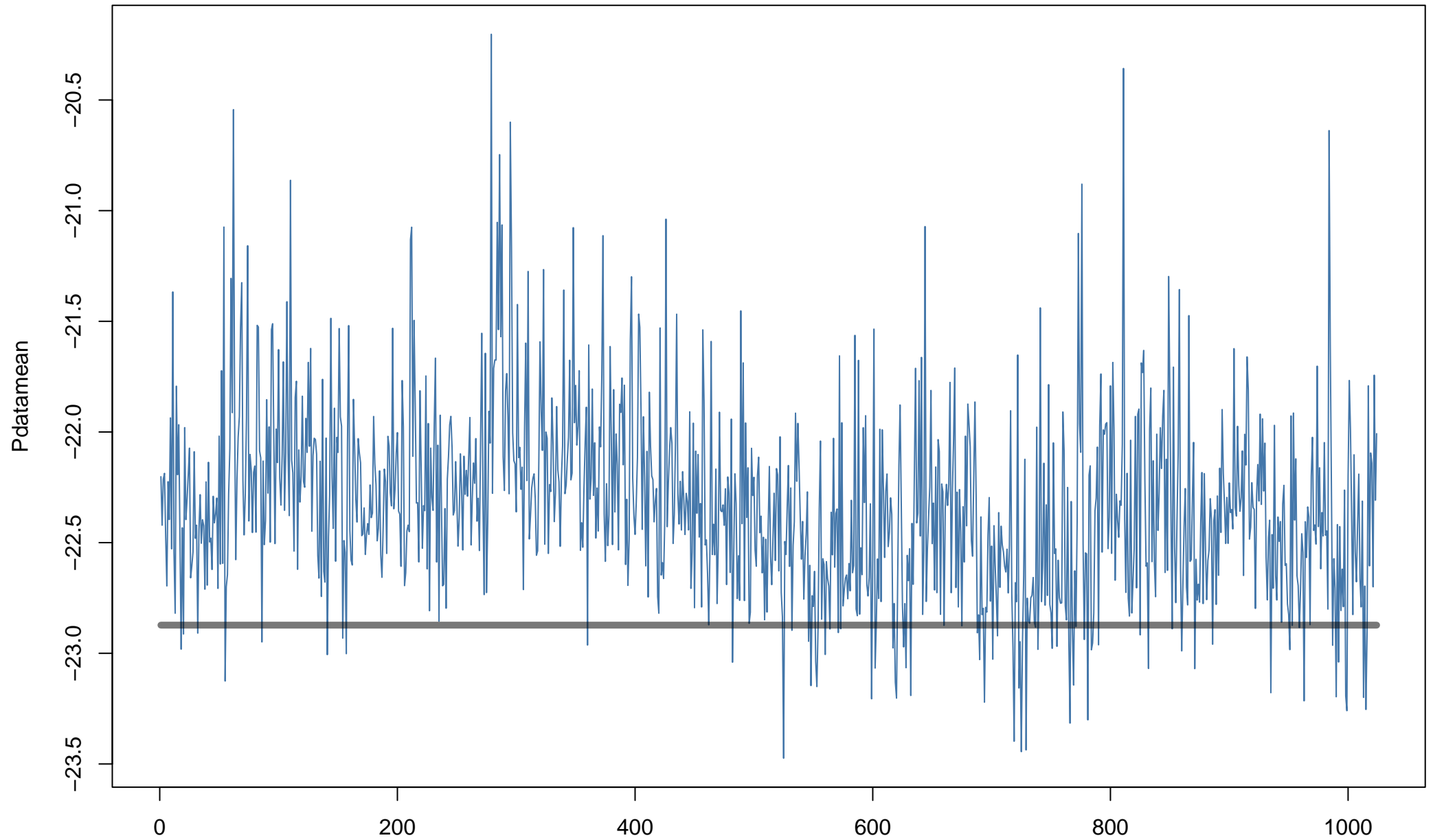


LL



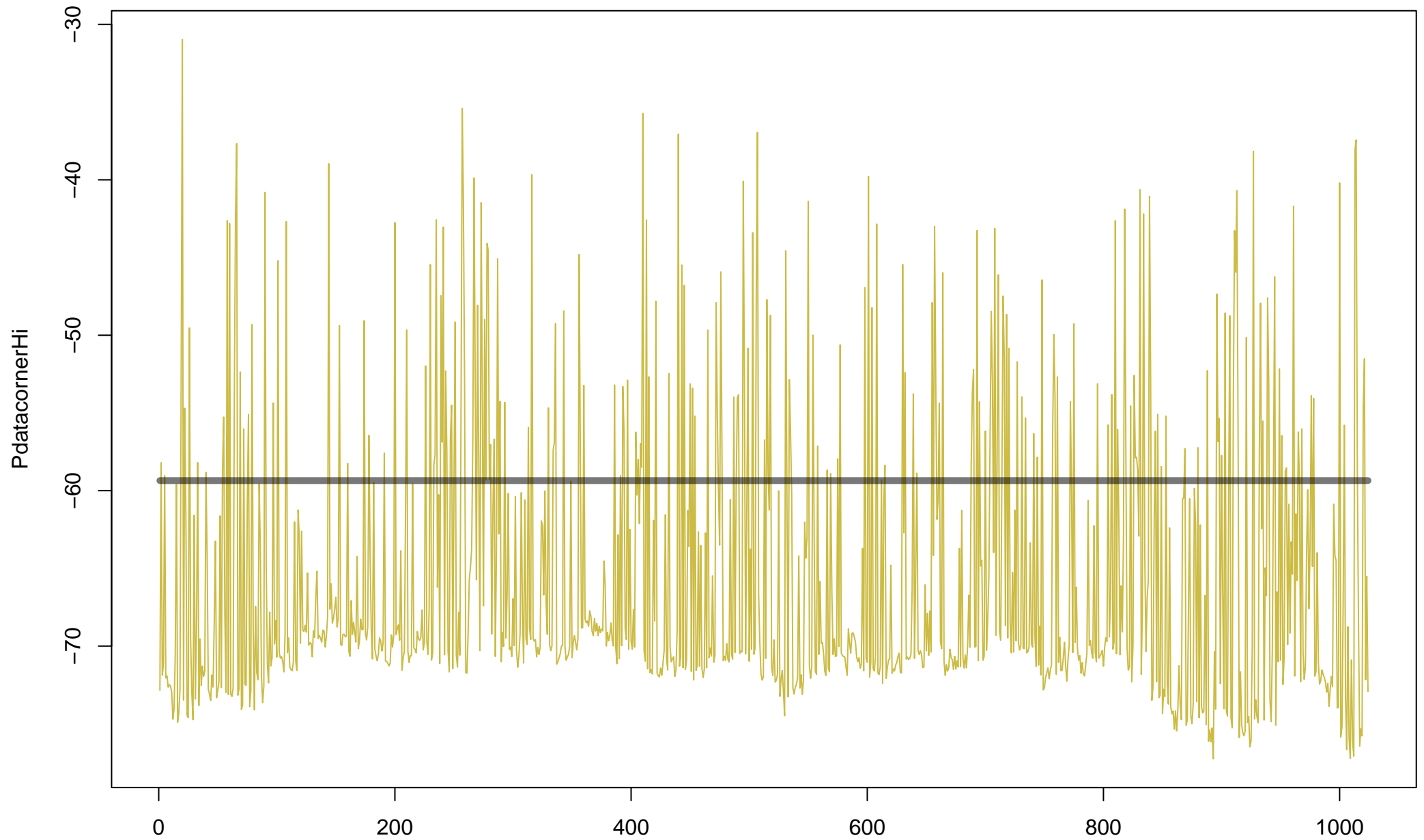
Pdatamean

ESS =  $2.22\text{e-}16$  | BMK = 0.248 | MCSE(6.27) = 6.3 | stat: TRUE | burn: 0 | percentile: 7.42



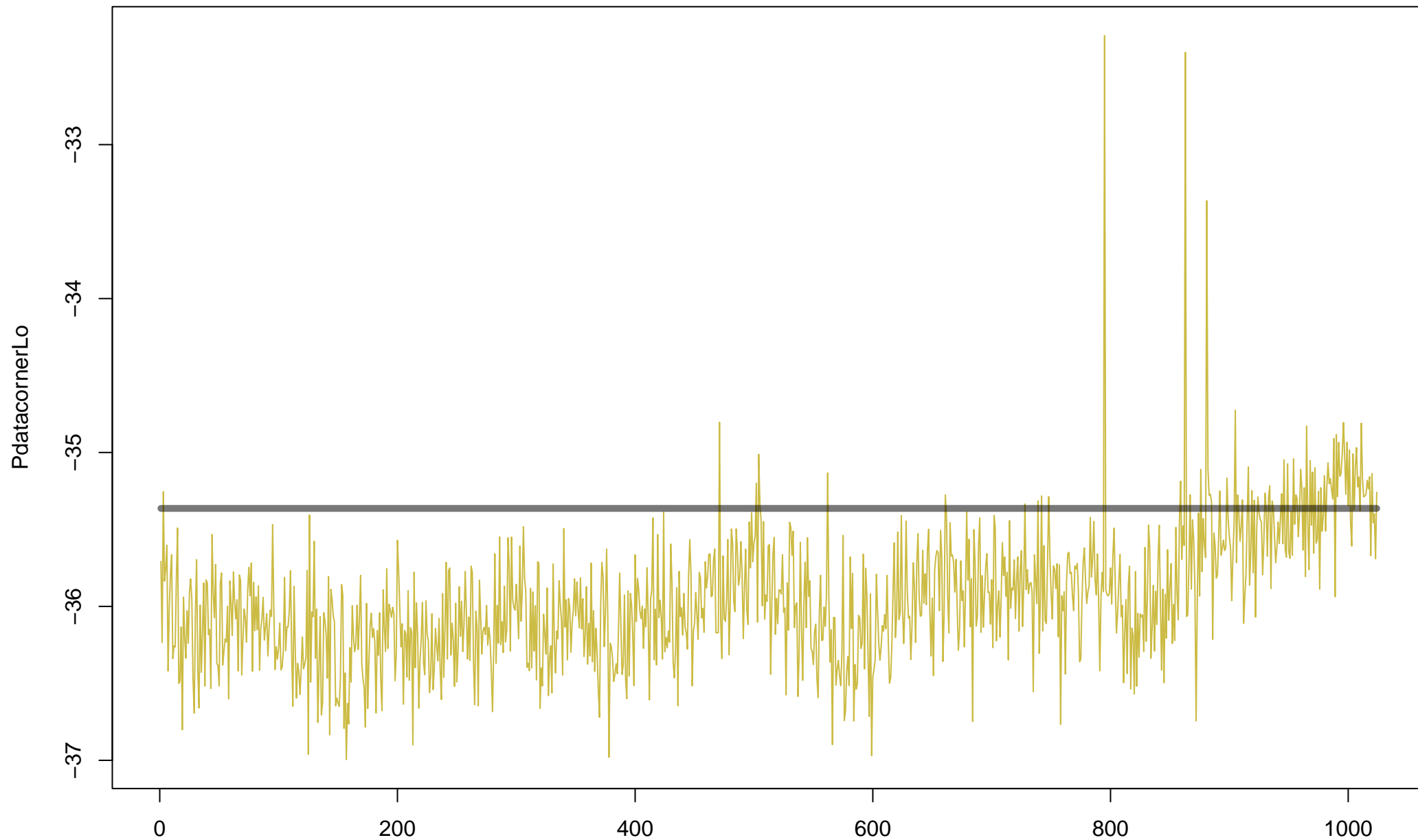
# PdatacornerHi

ESS =  $2.22\text{e-}16$  | BMK = 1 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 1020 | percentile: 77.9

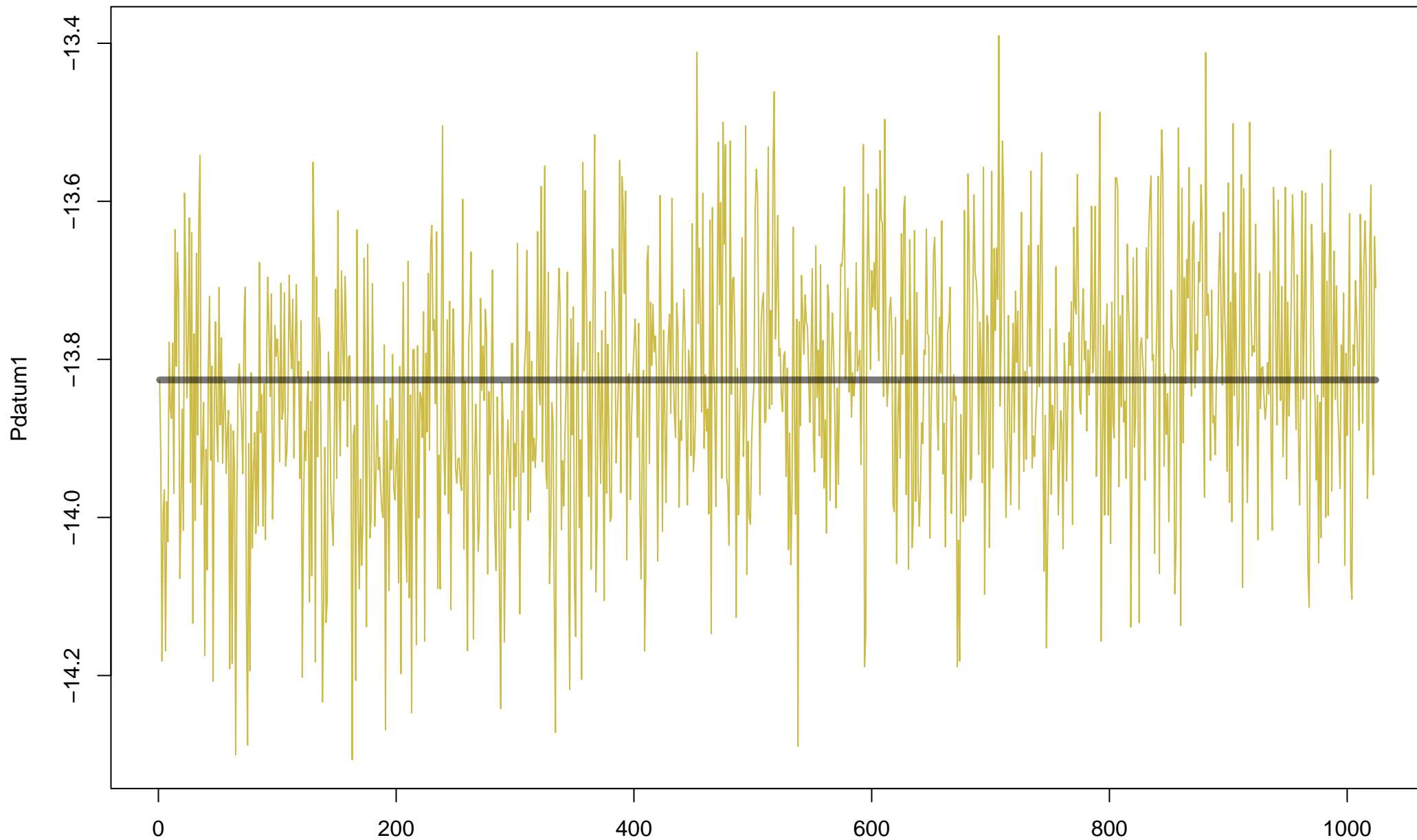


# PdatacornerLo

ESS = 2.22e-16 | BMK = 0.315 | MCSE(6.27) = 4.77 | stat: TRUE | burn: 0 | percentile: 91.7

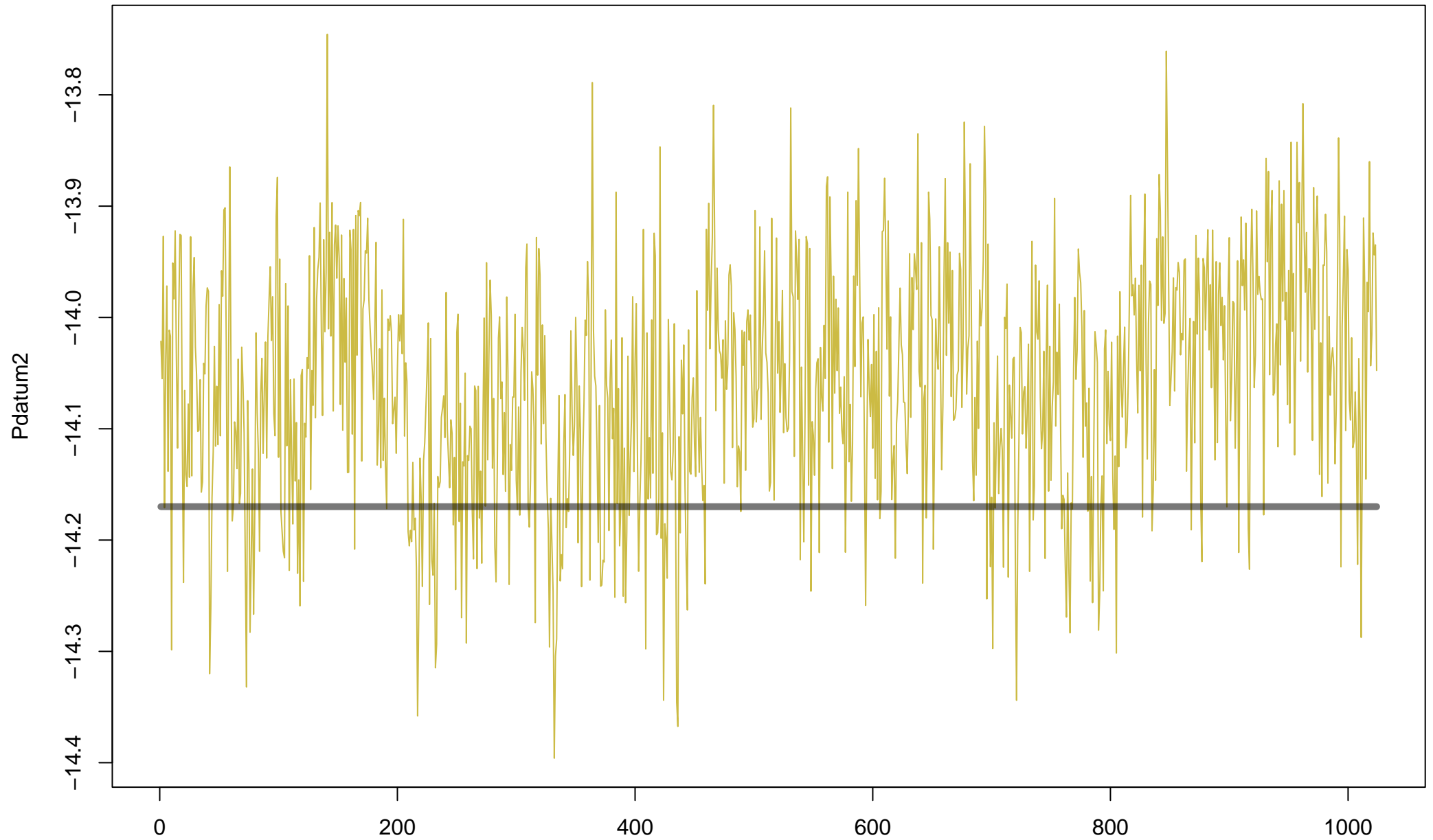


**Pdatum1**  
**ESS = 392 | BMK = 0.15 | MCSE(6.27) = 5.63 | stat: FALSE | burn: 0 | percentile: 52.1**



**Pdatum2**

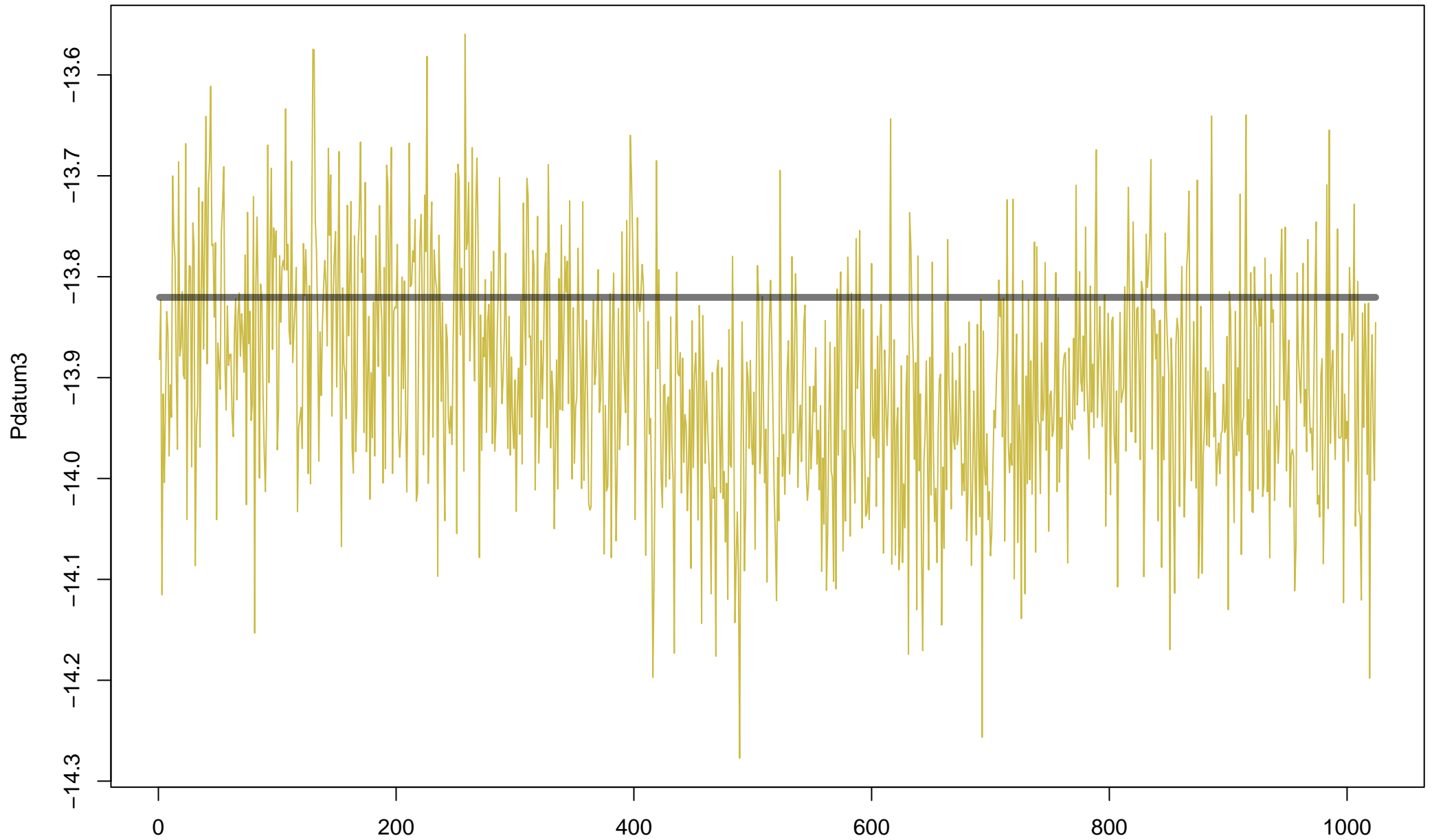
**ESS = 105 | BMK = 0.156 | MCSE(6.27) = 7.91 | stat: FALSE | burn: 0 | percentile: 14.6**





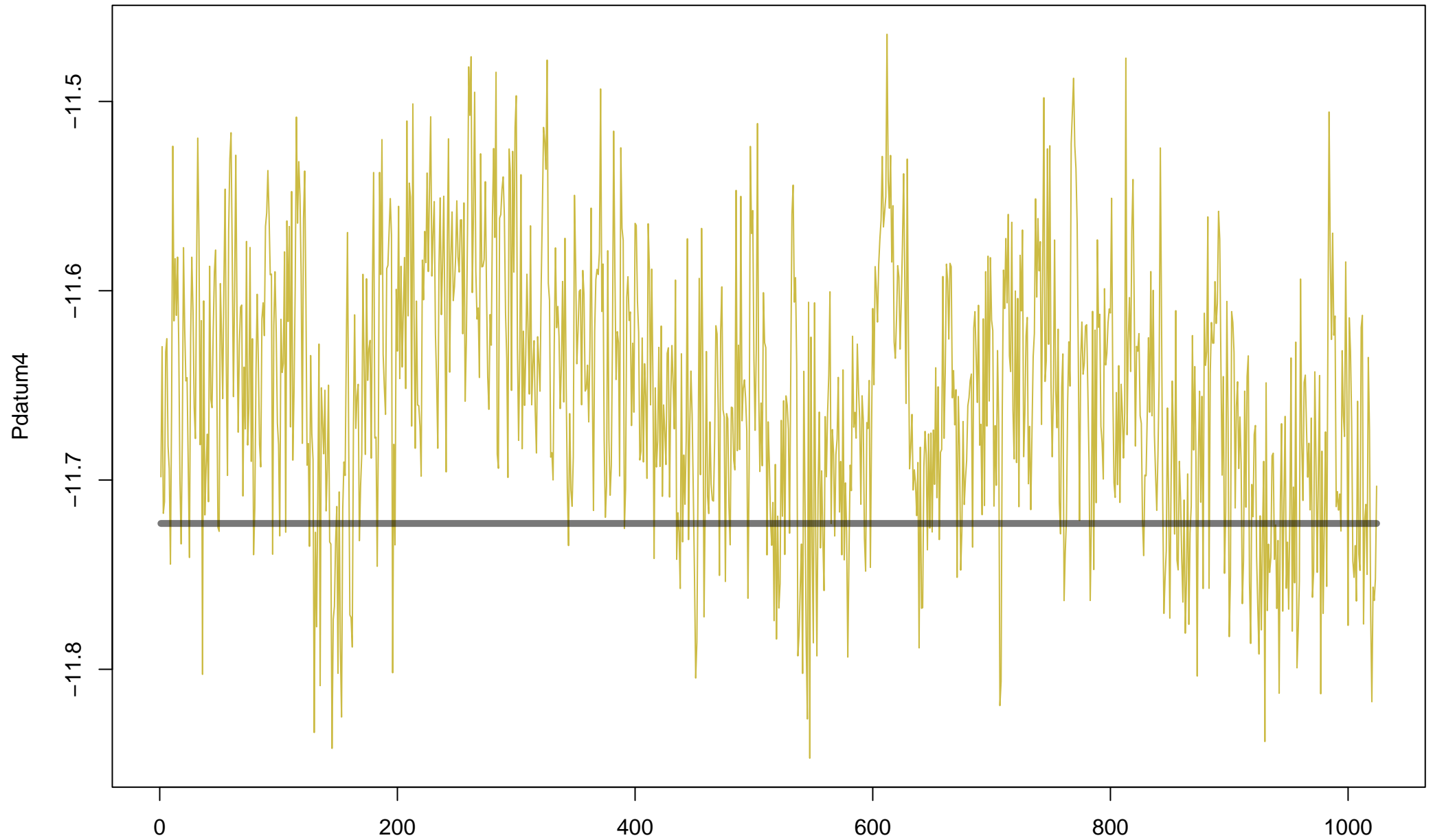
Pdatum3

ESS = 38 | BMK = 0.17 | MCSE(6.27) = 7.39 | stat: FALSE | burn: 0 | percentile: 77.4



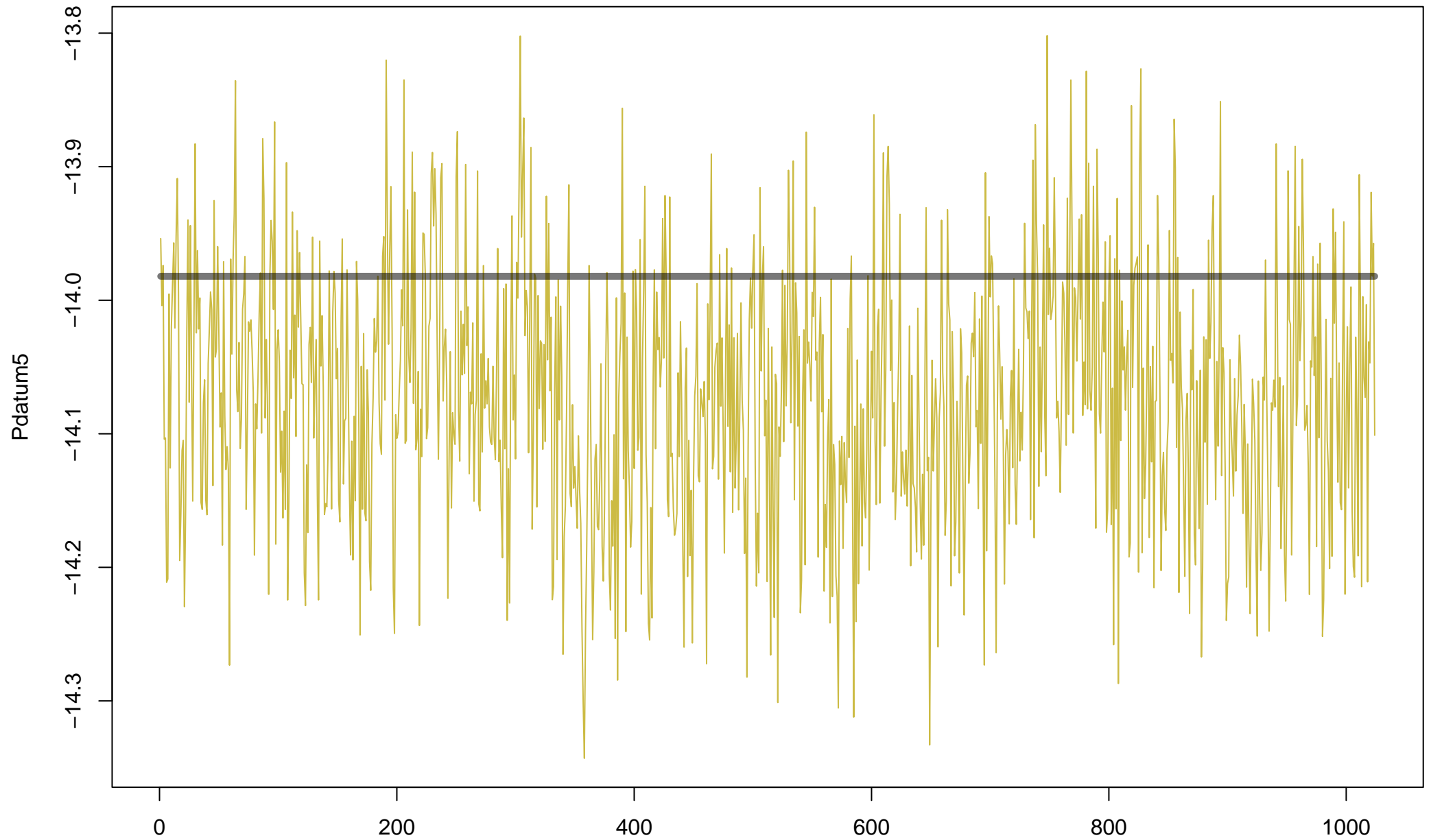
**Pdatum4**

**ESS = 107 | BMK = 0.187 | MCSE(6.27) = 9.51 | stat: FALSE | burn: 0 | percentile: 16.4**



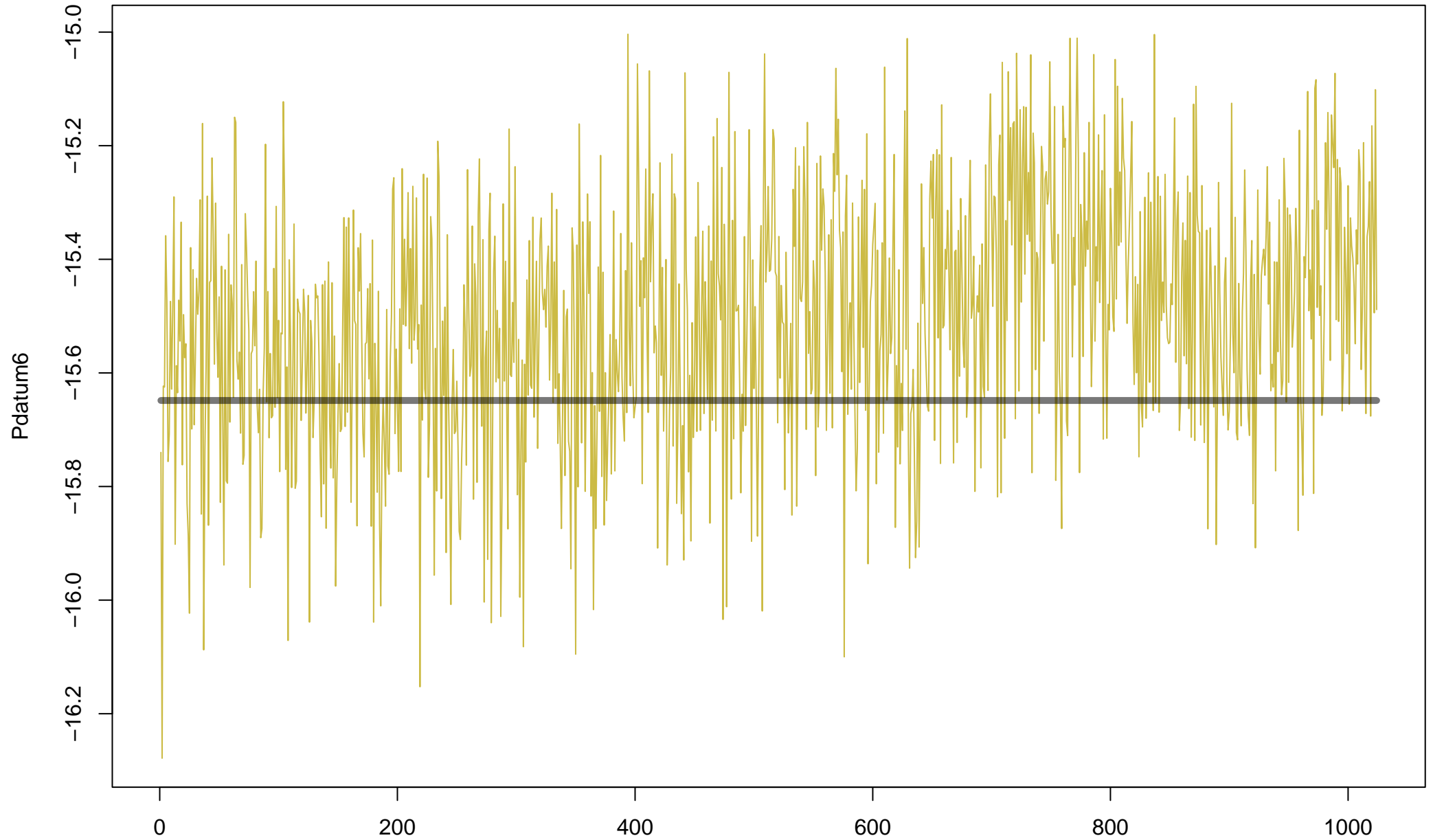
**Pdatum5**

**ESS = 312 | BMK = 0.04 | MCSE(6.27) = 5.4 | stat: FALSE | burn: 0 | percentile: 83.3**



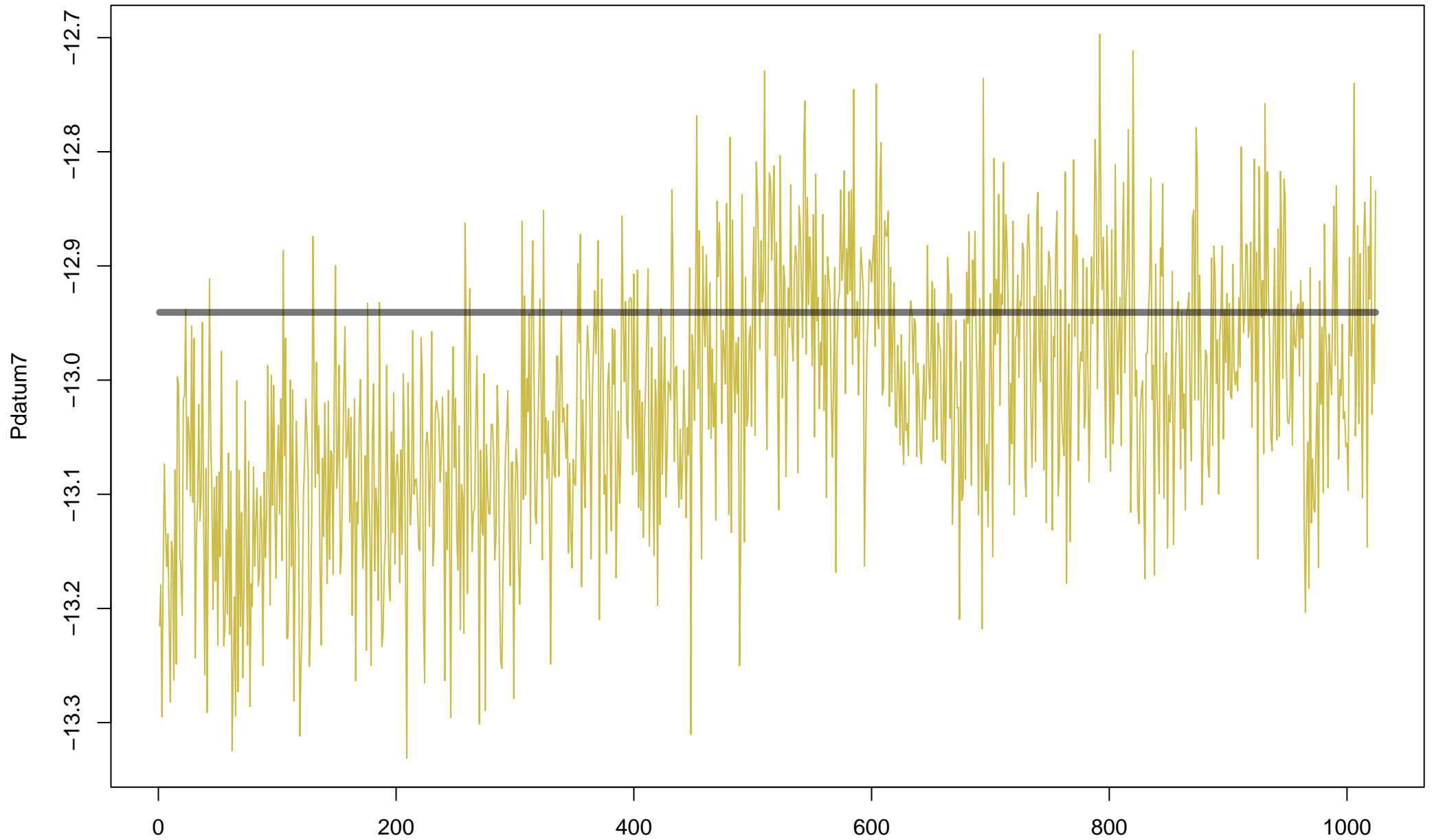
**Pdatum6**

**ESS = 167 | BMK = 0.206 | MCSE(6.27) = 6.88 | stat: FALSE | burn: 0 | percentile: 26.4**



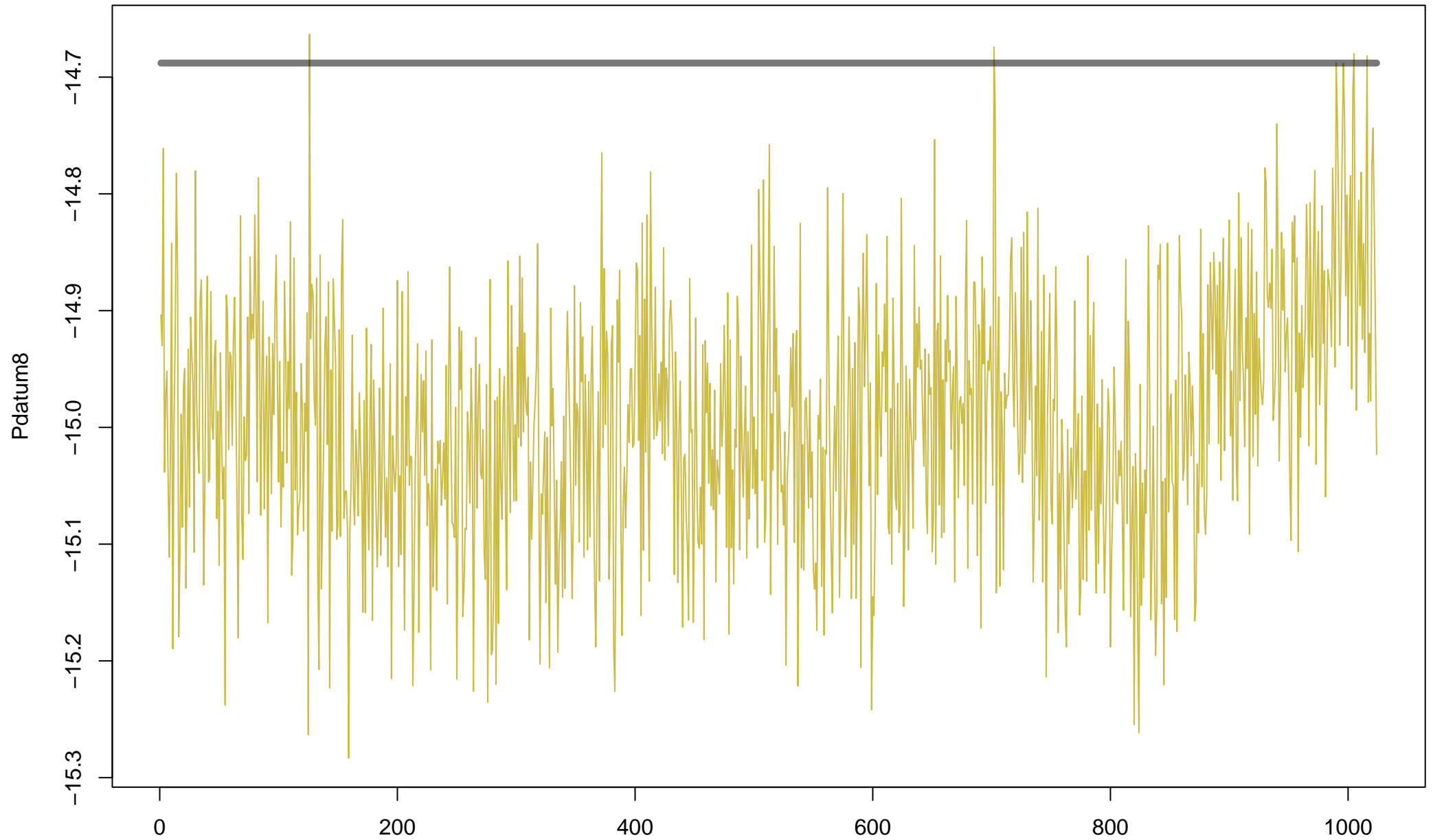
**Pdatum7**

**ESS = 10.1 | BMK = 0.352 | MCSE(6.27) = 10.8 | stat: FALSE | burn: 0 | percentile: 74.2**



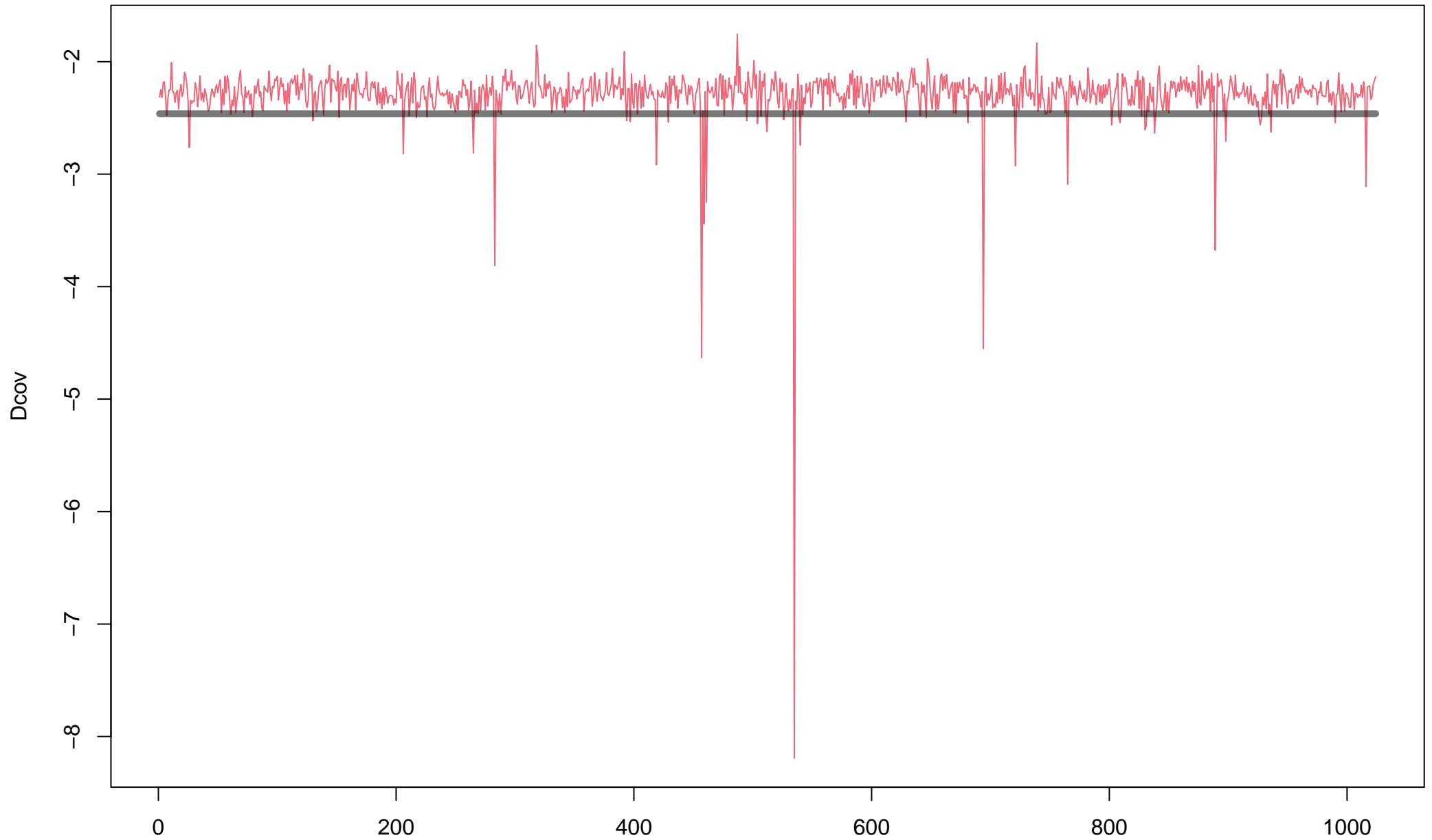
**Pdatum8**

**ESS = 50.8 | BMK = 0.133 | MCSE(6.27) = 8.13 | stat: TRUE | burn: 0 | percentile: 99.5**

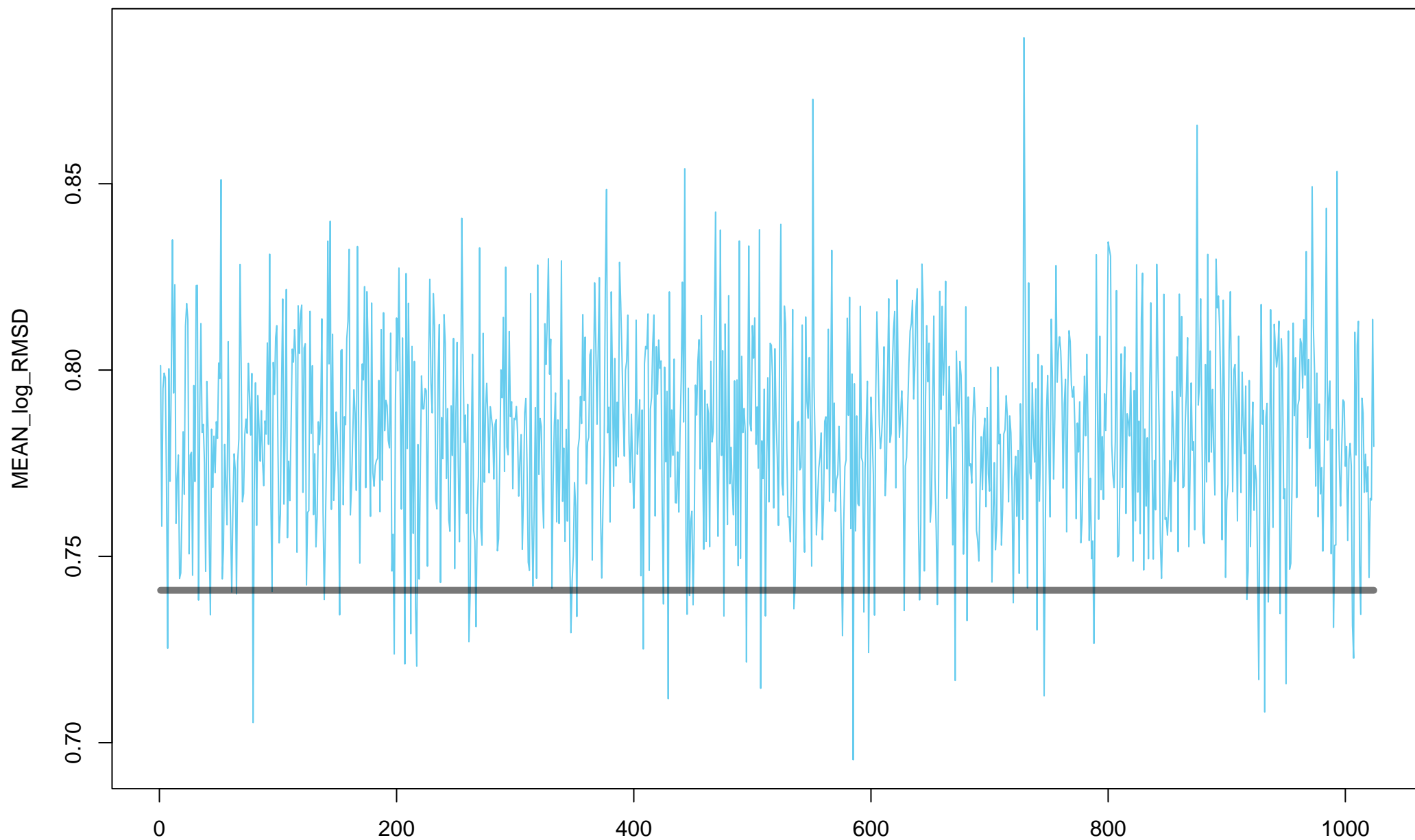


**Dcov**

**ESS = 1020 | BMK = 0.0828 | MCSE(6.27) = 3.76 | stat: TRUE | burn: 0 | percentile: 94.1**

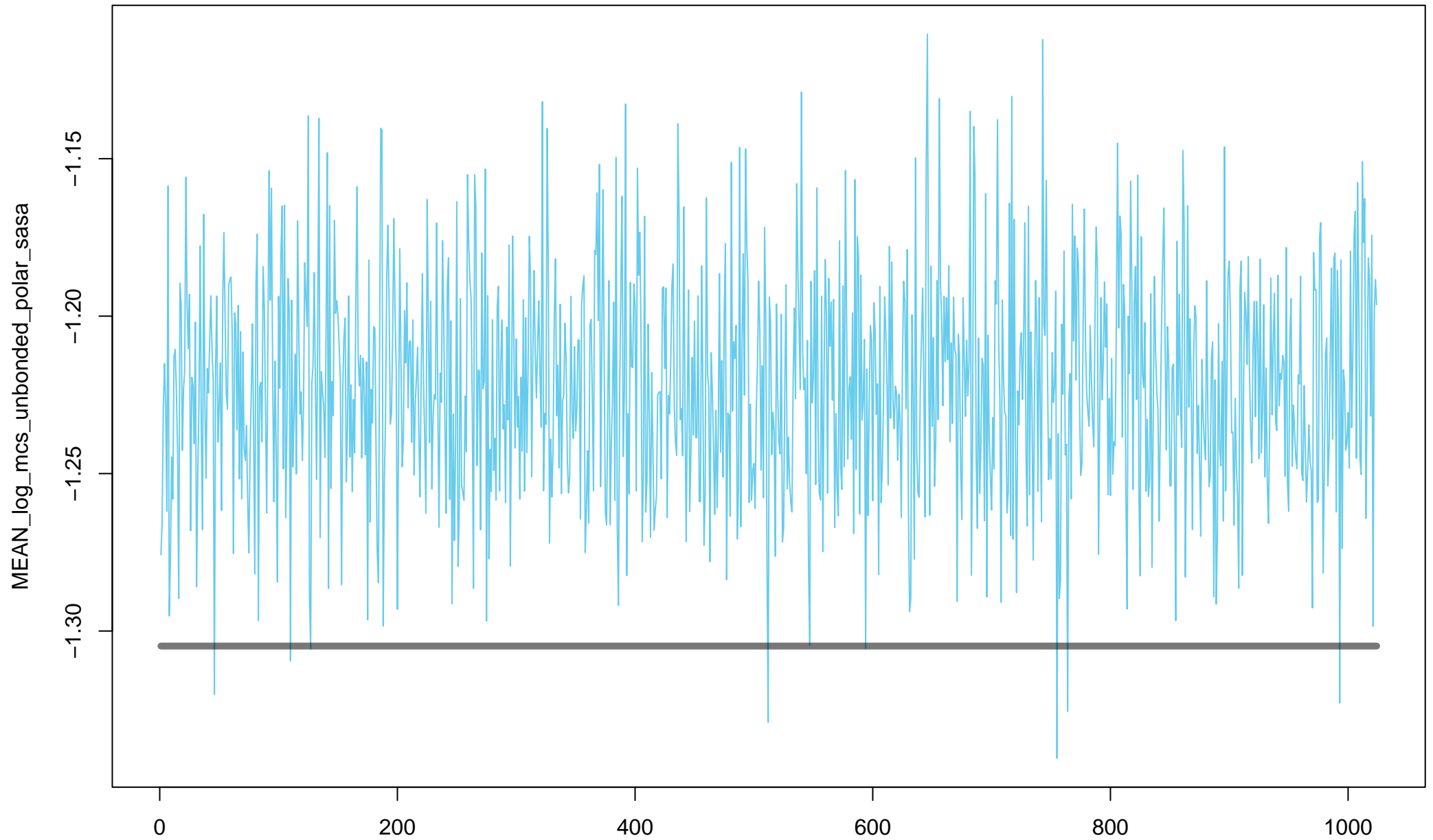


**MEAN\_log\_RMSD**  
**ESS = 896 | BMK = 0.0572 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0 | percentile: 5.27**



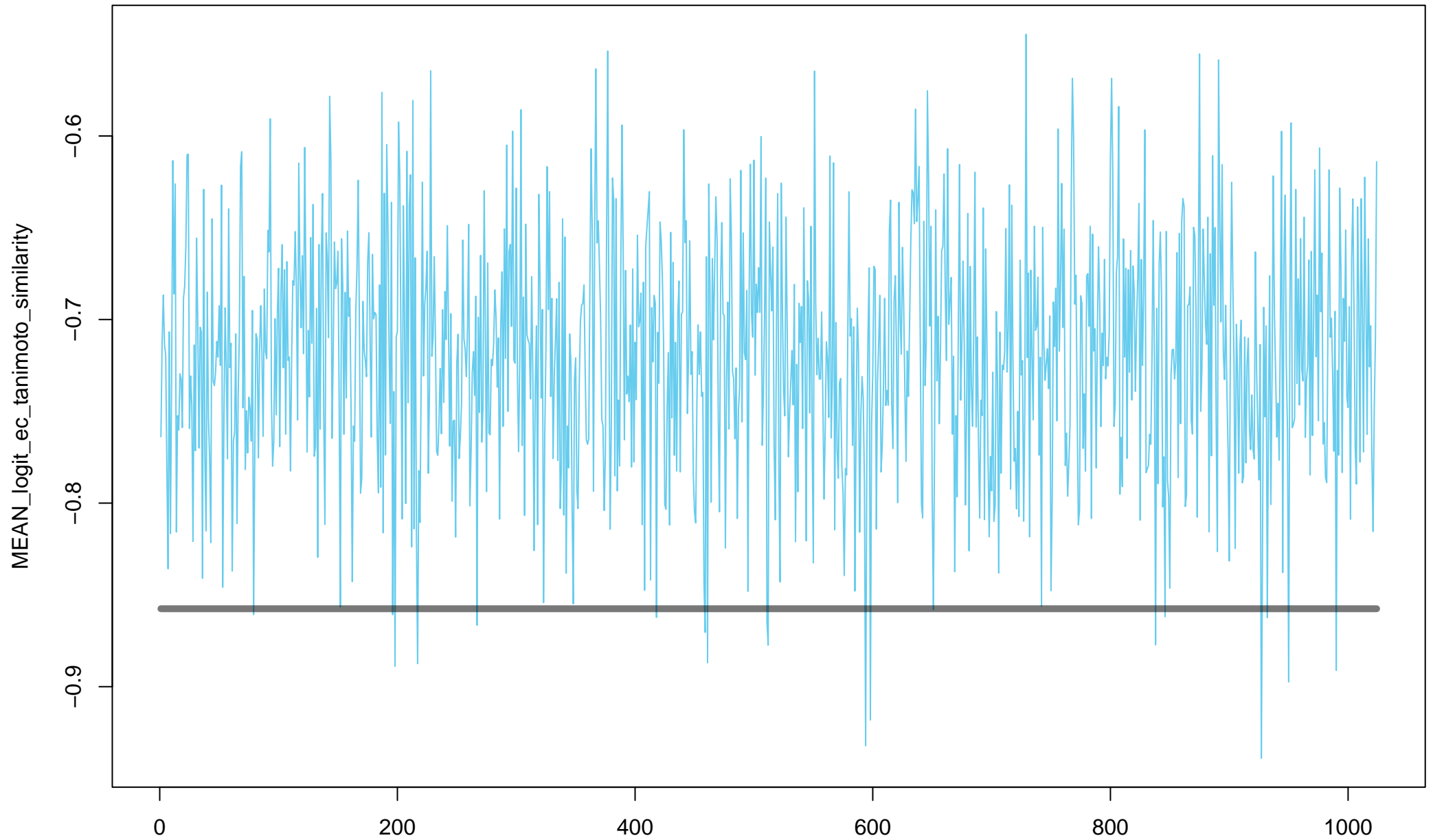


**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1020 | BMK = 0.0343 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0 | percentile: 0.781**



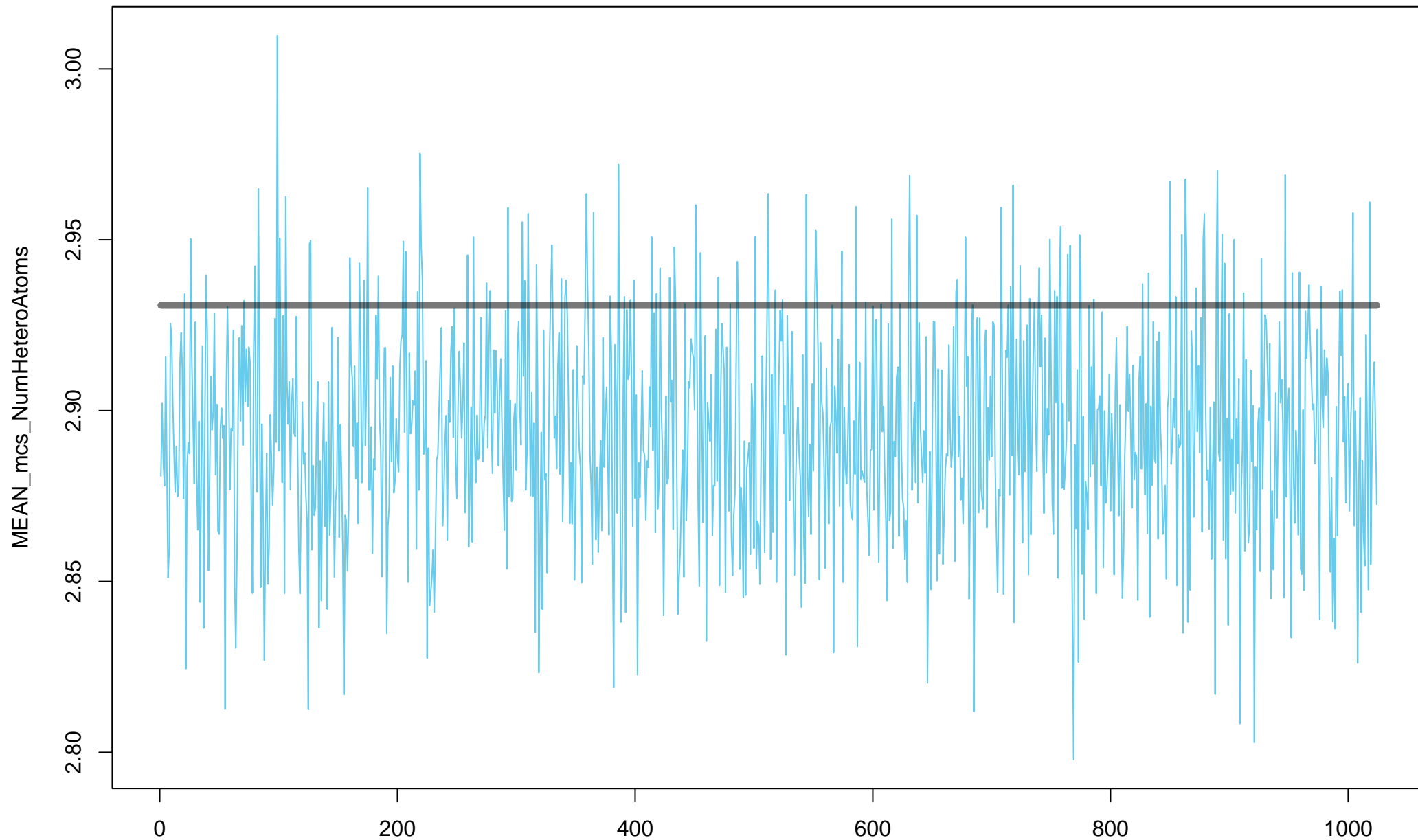
# MEAN\_logit\_ec\_tanimoto\_similarity

ESS = 1020 | BMK = 0.0514 | MCSE(6.27) = 3.97 | stat: TRUE | burn: 0 | percentile: 1.86



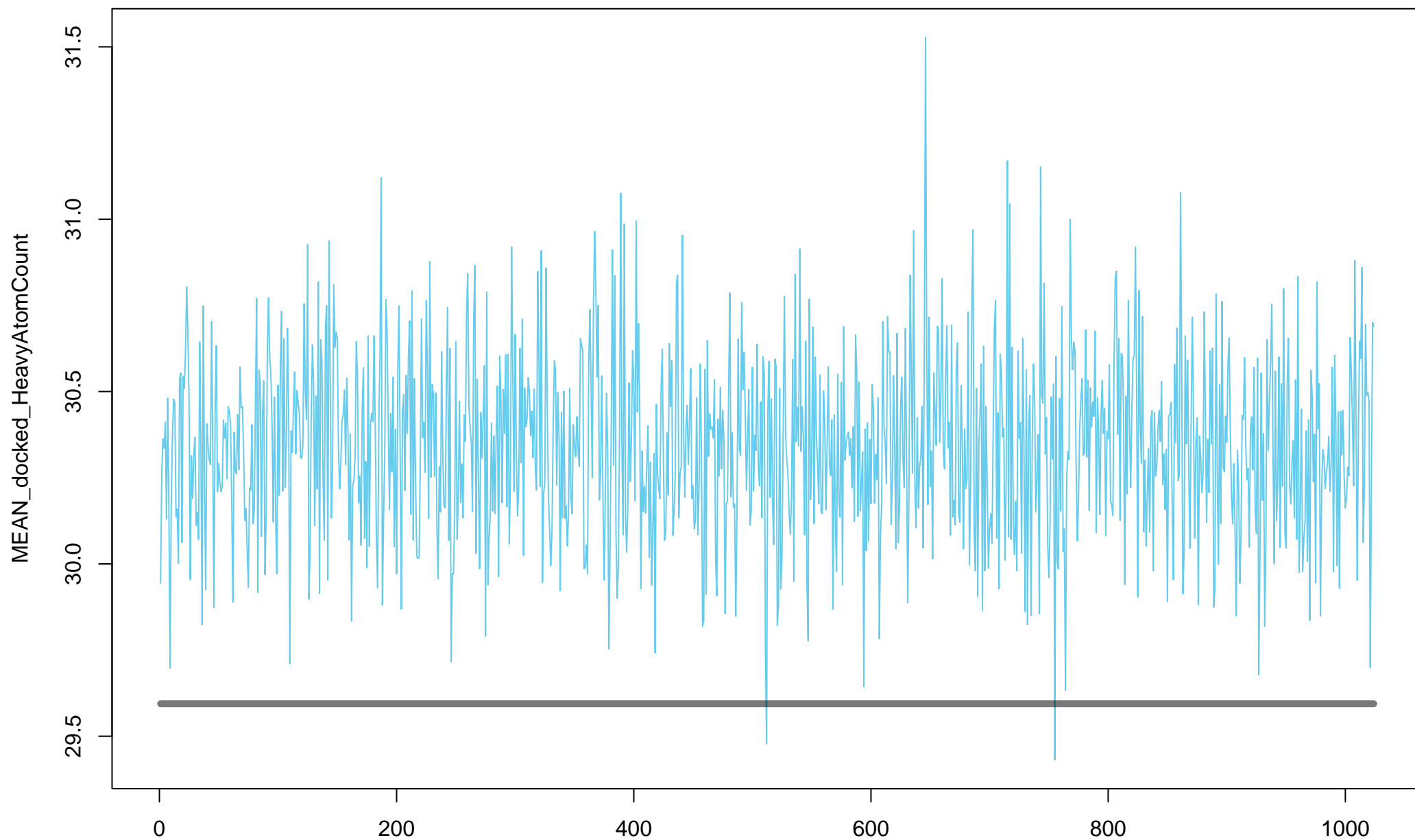
# MEAN\_mcs\_NumHeteroAtoms

ESS = 1020 | BMK = 0.0345 | MCSE(6.27) = 3.22 | stat: TRUE | burn: 0 | percentile: 88.1



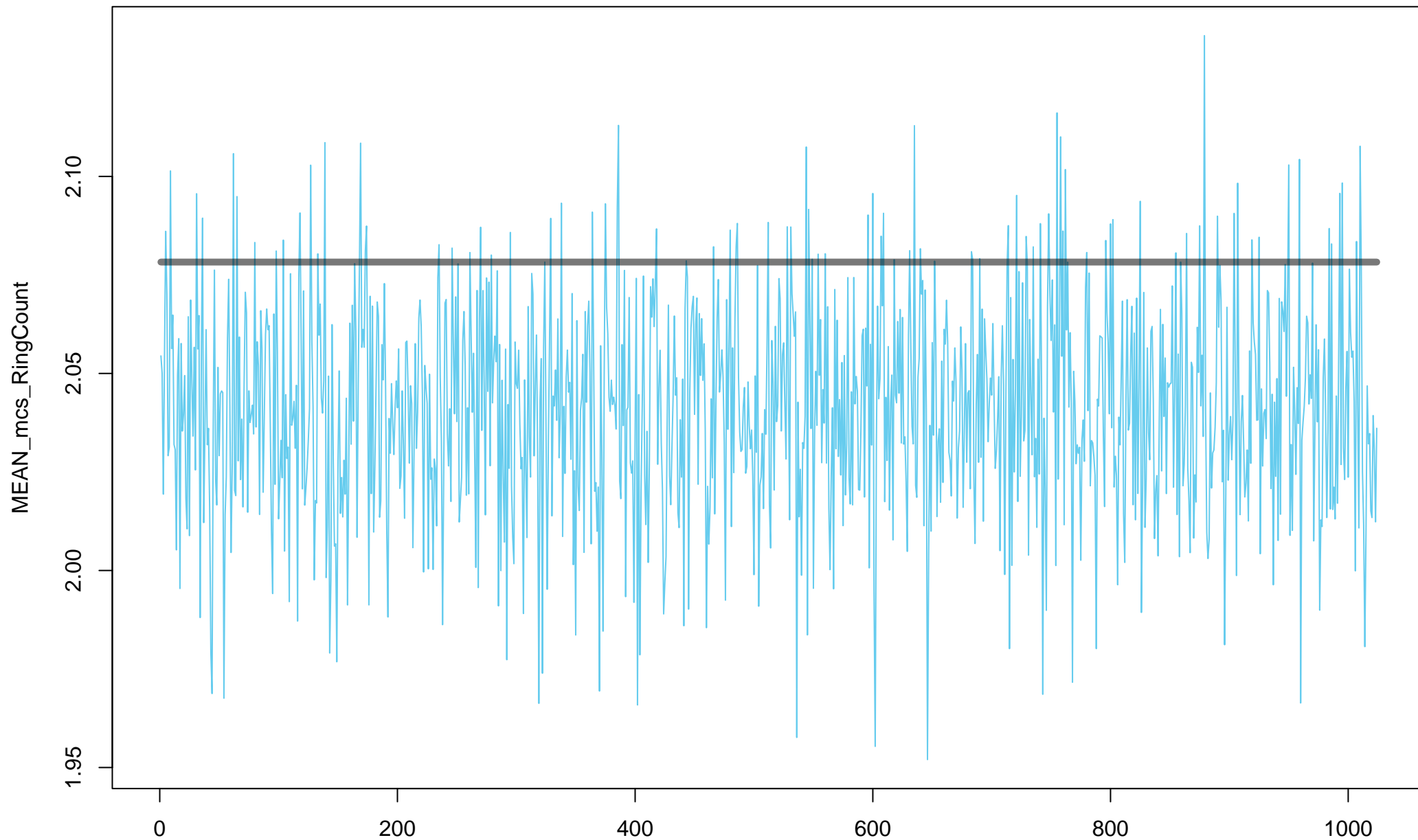
# MEAN\_docked\_HeavyAtomCount

ESS = 1020 | BMK = 0.041 | MCSE(6.27) = 3.29 | stat: TRUE | burn: 0 | percentile: 0.195



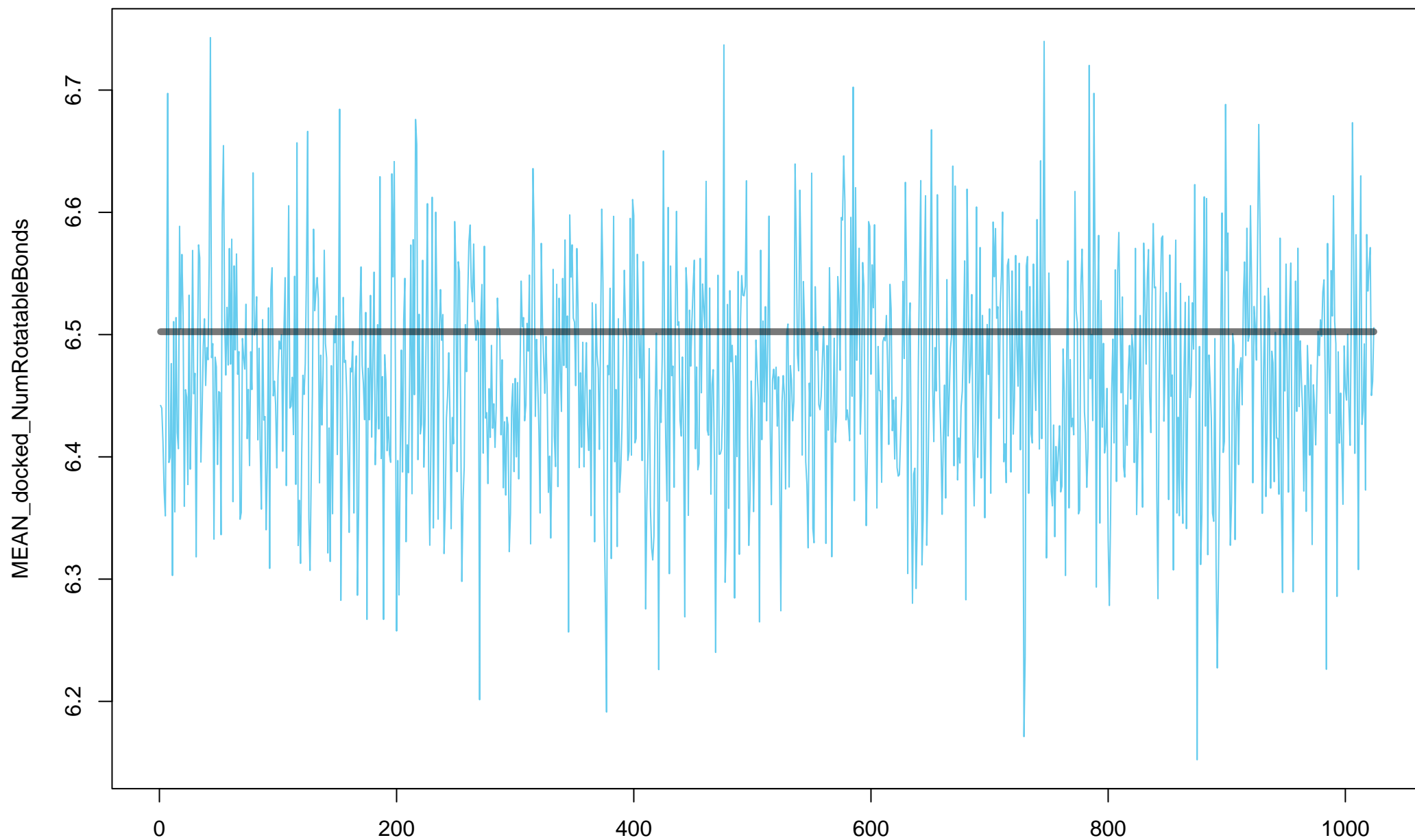
# MEAN\_mcs\_RingCount

ESS = 1020 | BMK = 0.0658 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0 | percentile: 91.5



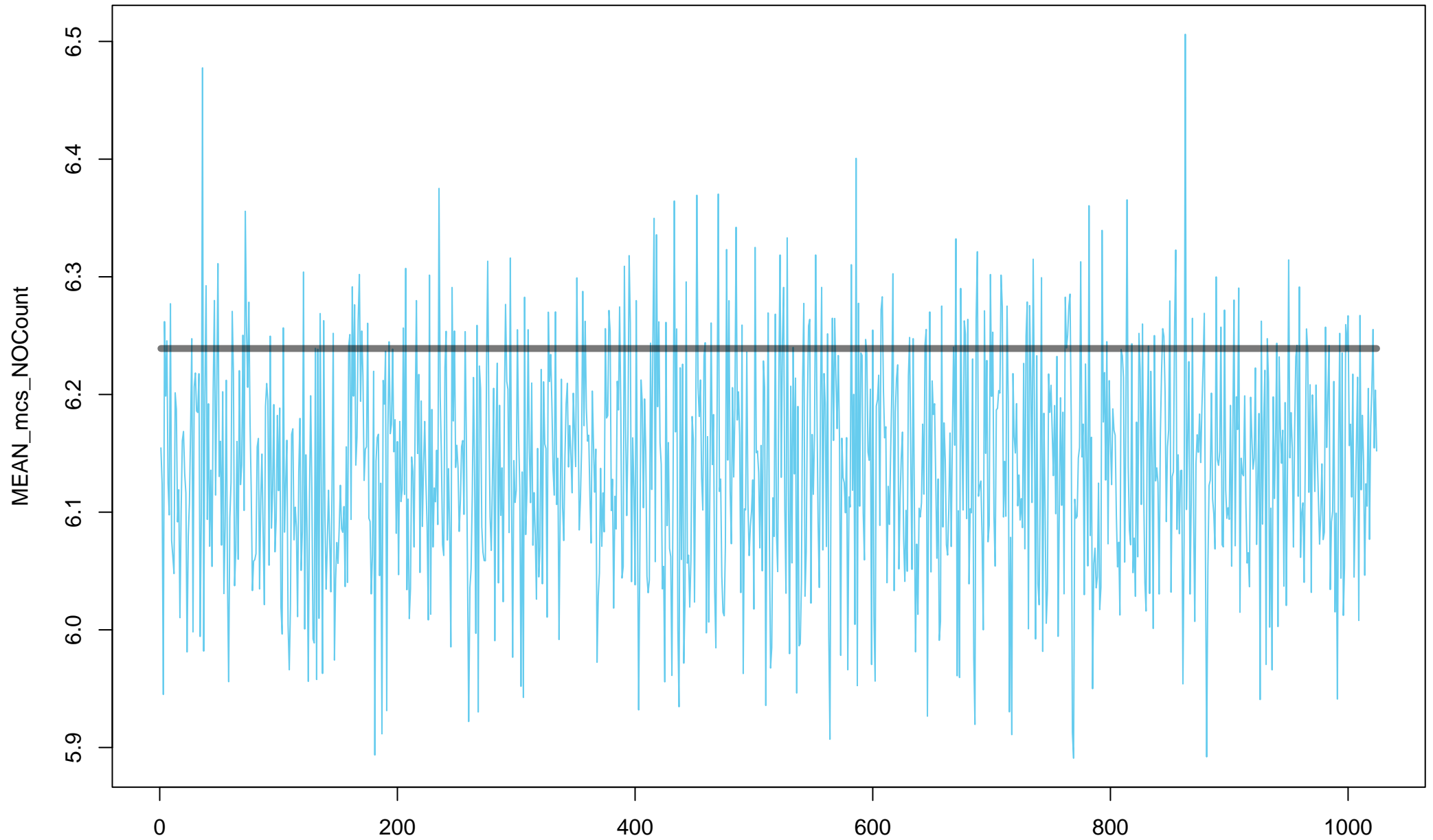
# MEAN\_docked\_NumRotatableBonds

ESS = 992 | BMK = 0.0453 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 0 | percentile: 67.8



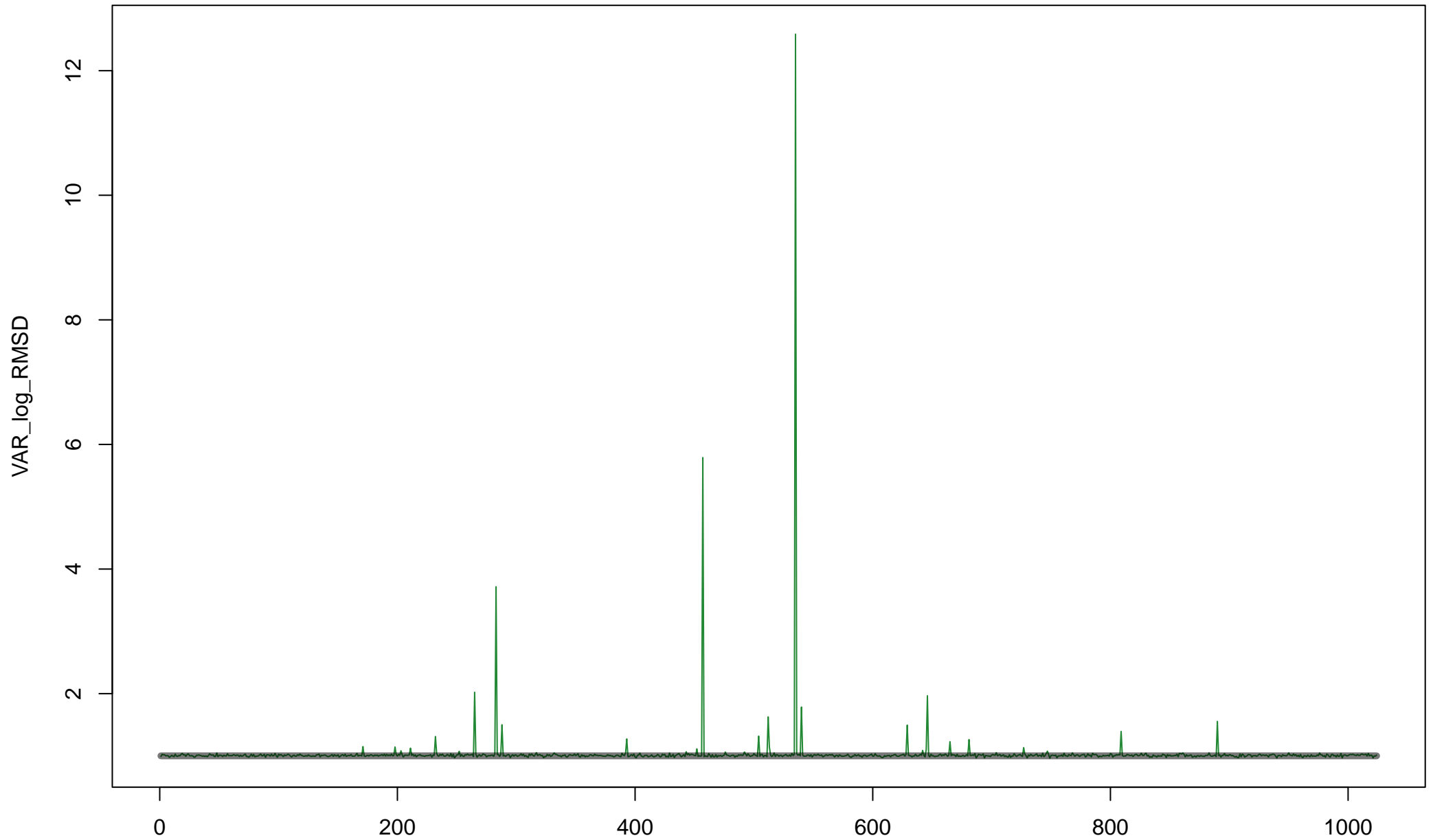
MEAN\_mcs\_NOCount

ESS = 1020 | BMK = 0.0439 | MCSE(6.27) = 2.79 | stat: TRUE | burn: 0 | percentile: 83.8



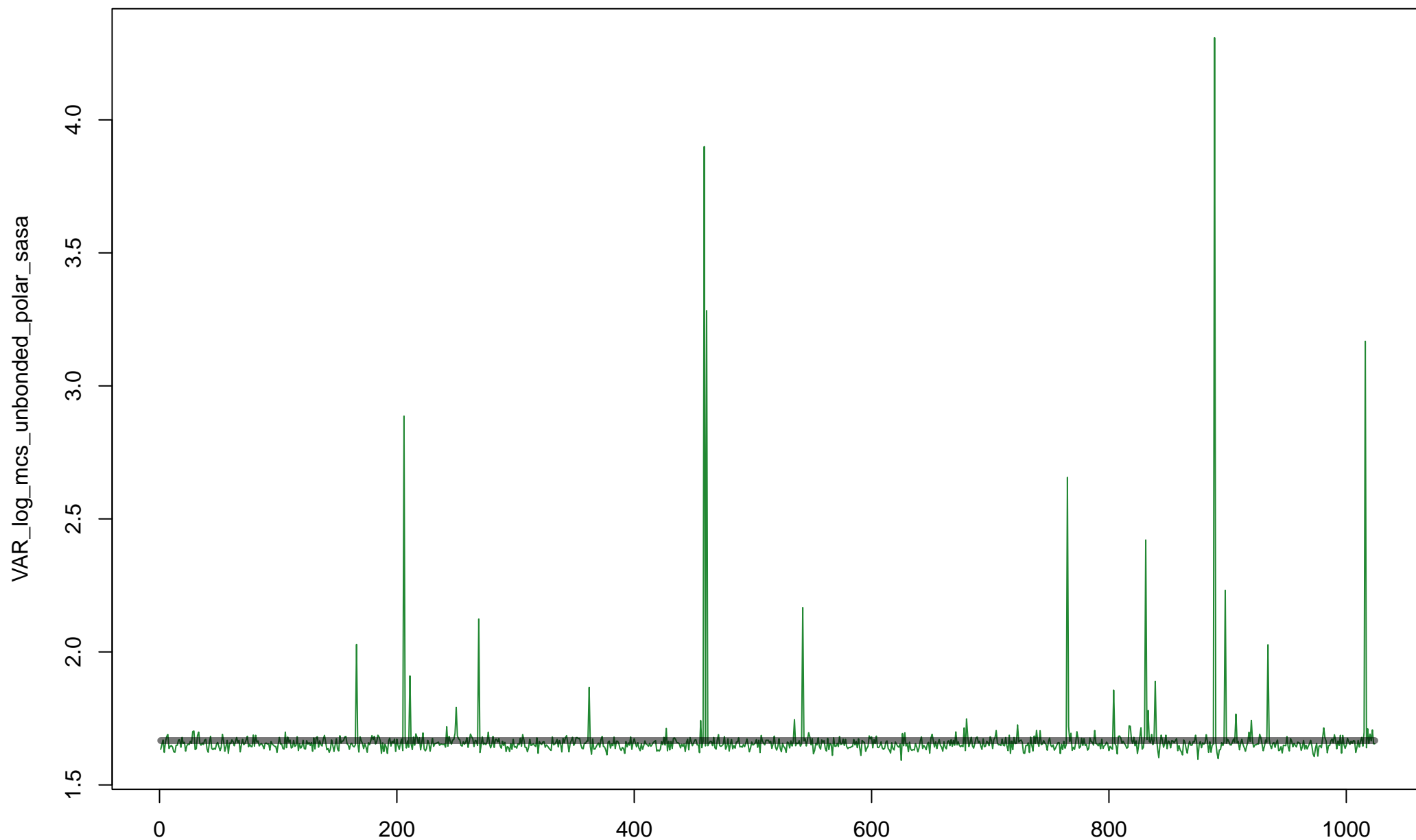
# VAR\_log\_RMSD

ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 612 | percentile: 33.4



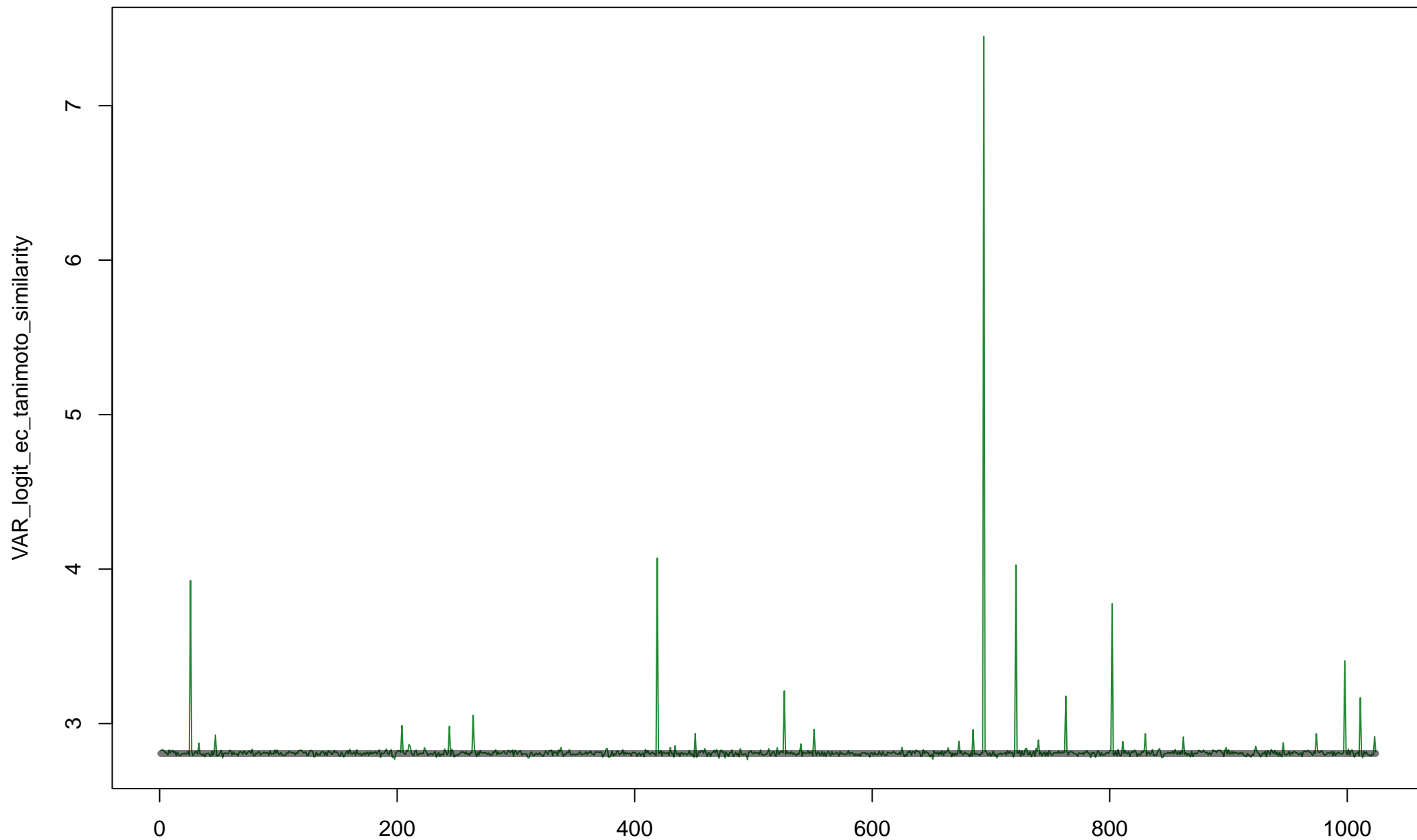


**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 819 | BMK = 0.174 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0 | percentile: 74.3**

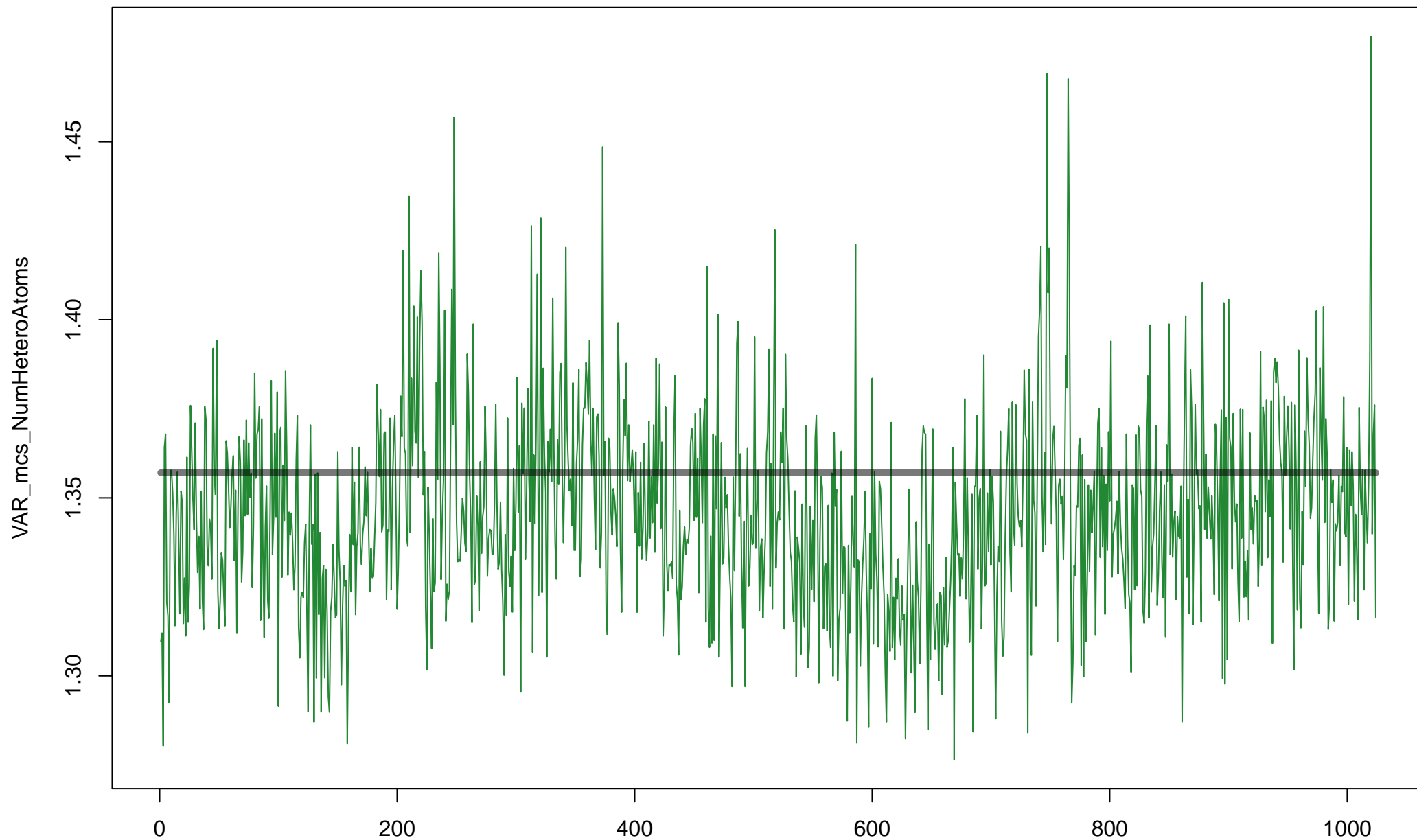


# VAR\_logit\_ec\_tanimoto\_similarity

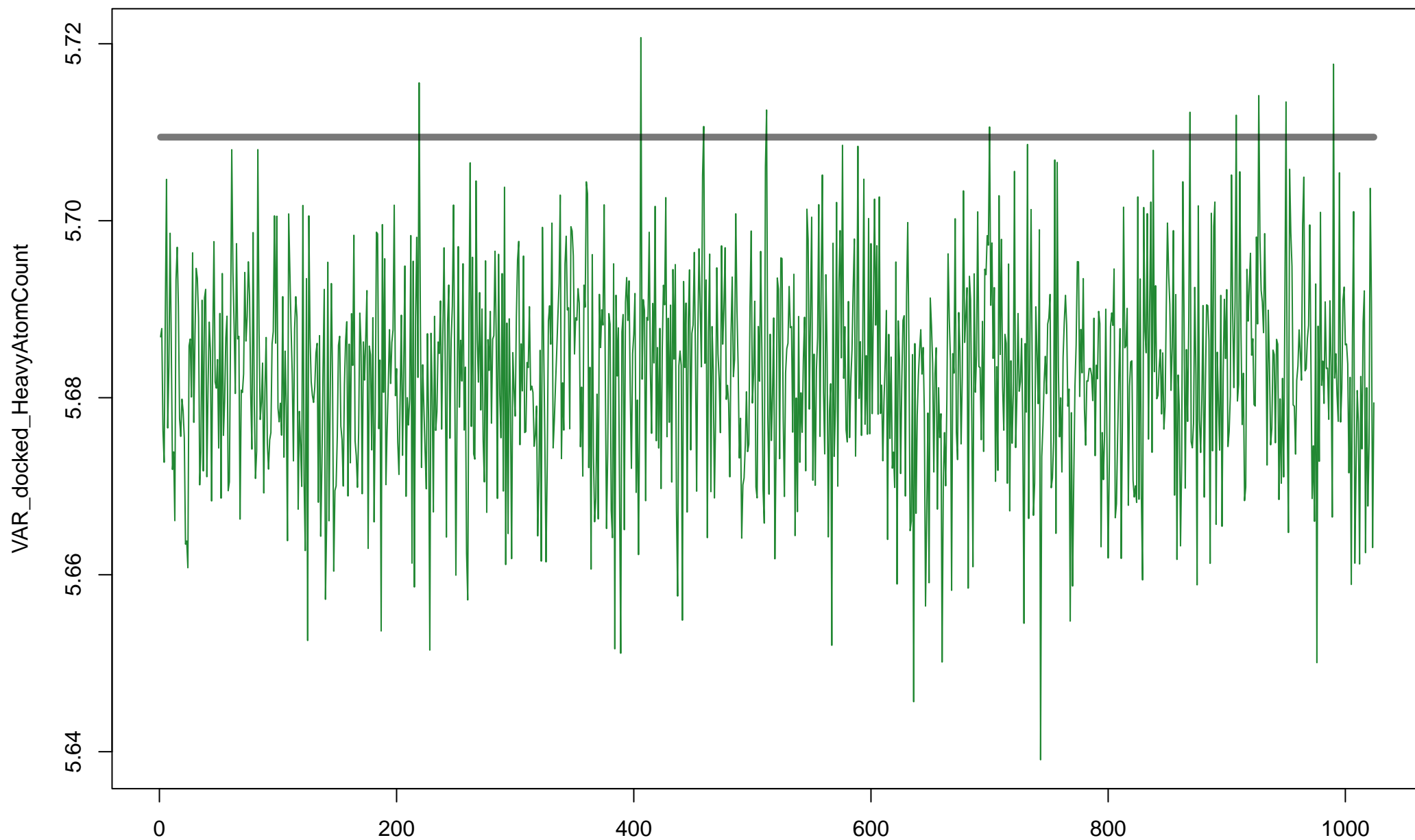
ESS = 1020 | BMK = 0.366 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 714 | percentile: 44.8



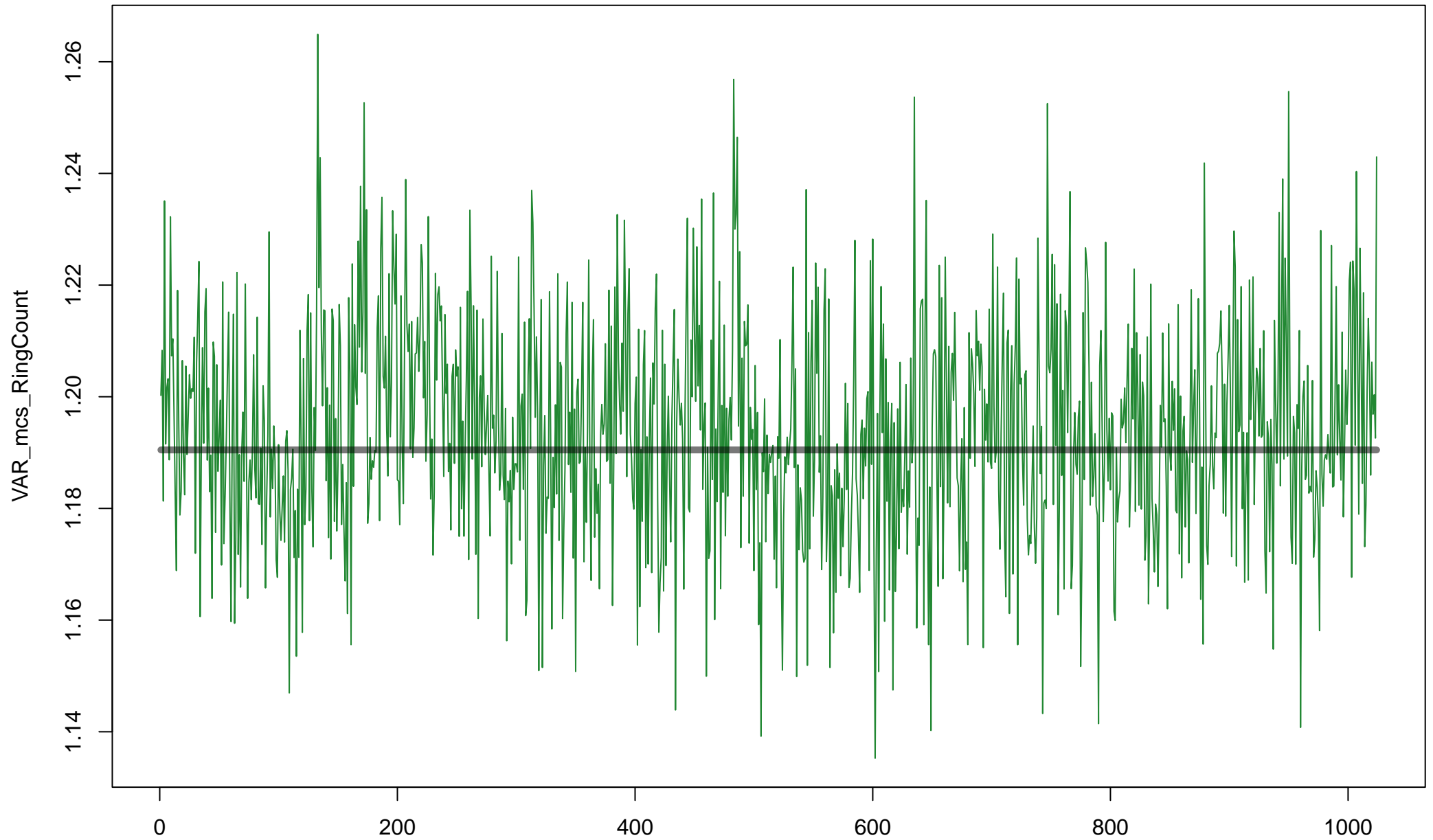
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 104 | BMK = 0.0855 | MCSE(6.27) = 7.34 | stat: TRUE | burn: 0 | percentile: 69.3**



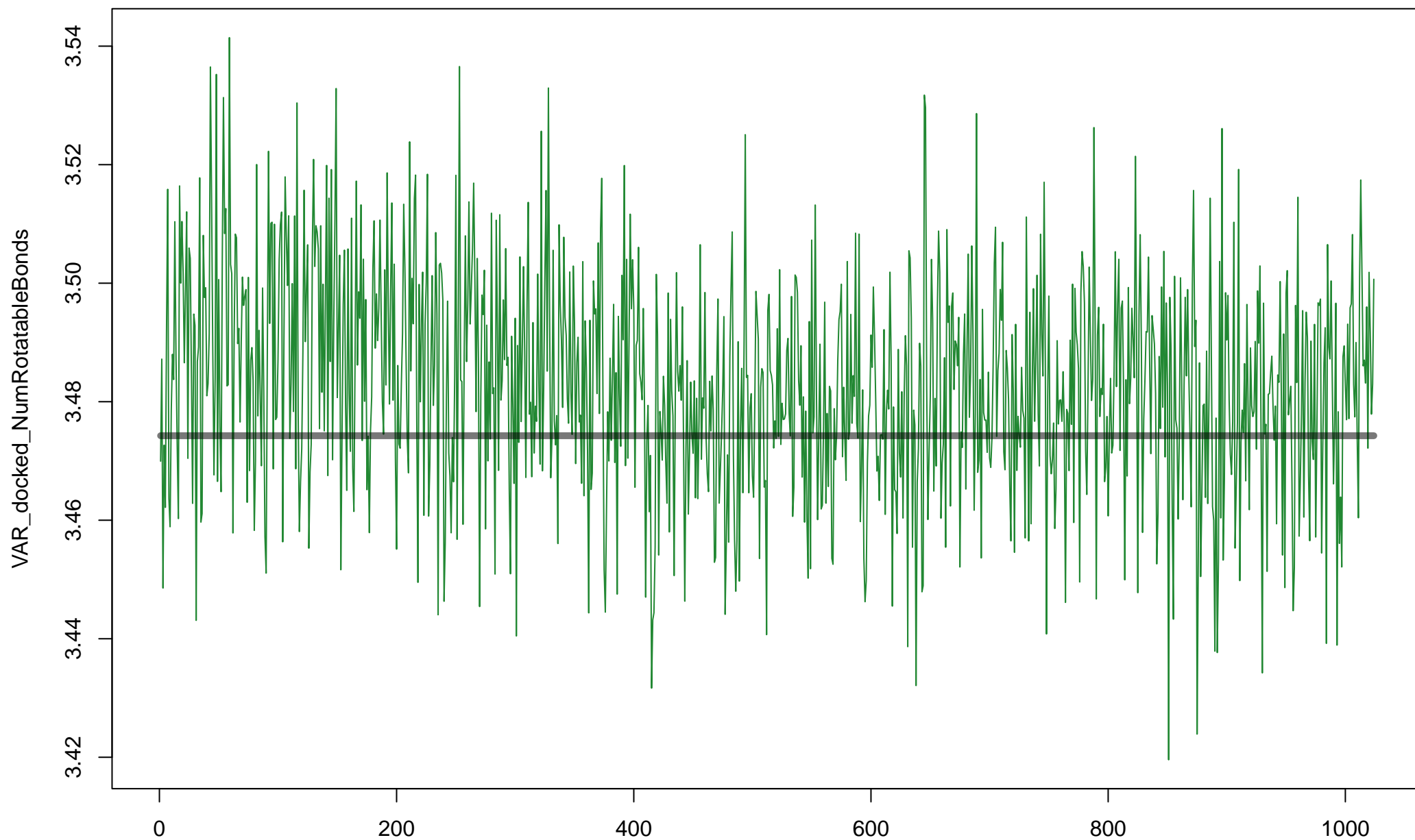
**VAR\_docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.0656 | MCSE(6.27) = 3.78 | stat: TRUE | burn: 0 | percentile: 99**



**VAR\_mcs\_RingCount**  
**ESS = 493 | BMK = 0.061 | MCSE(6.27) = 4.66 | stat: TRUE | burn: 0 | percentile: 45**

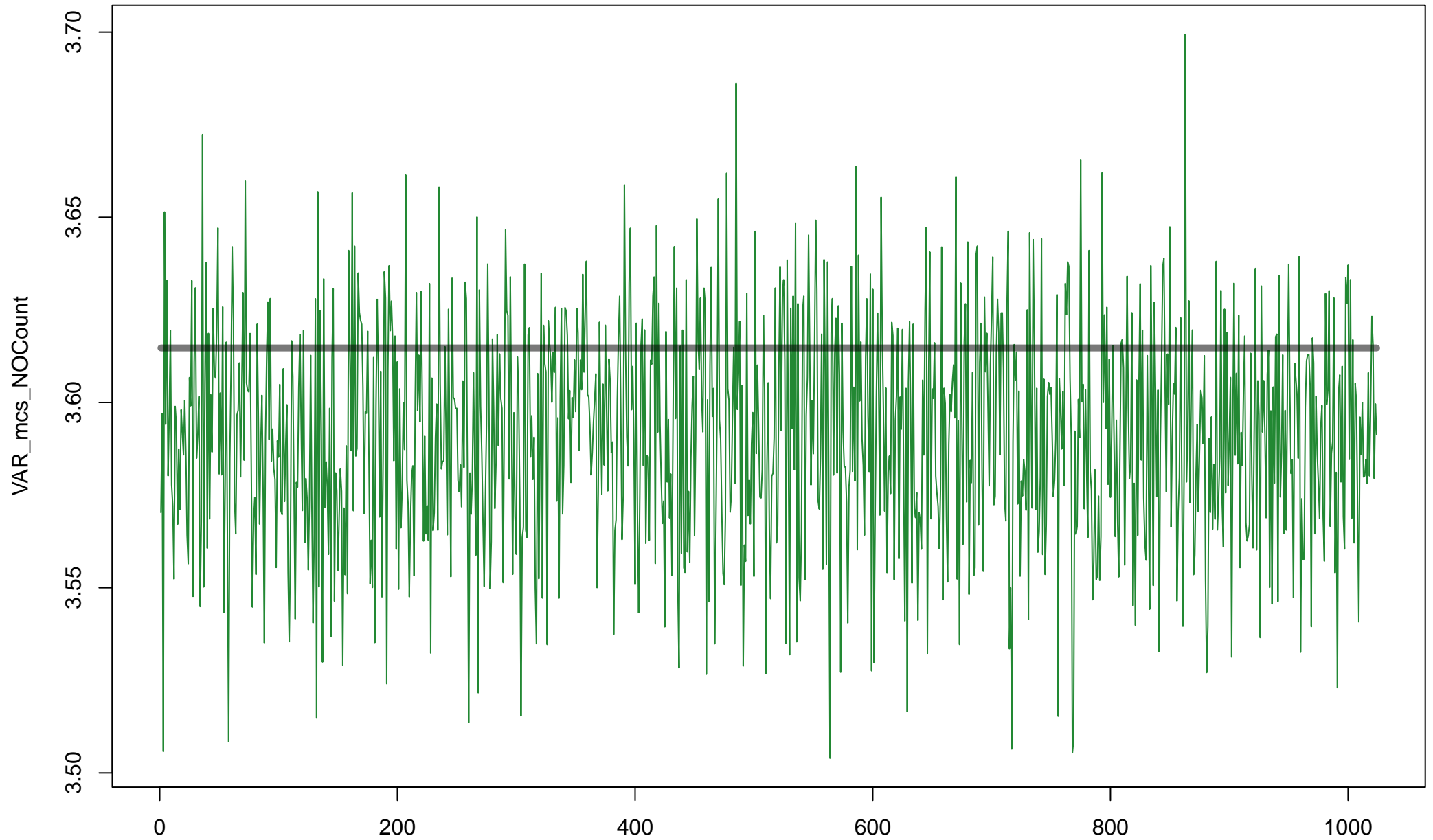


**VAR\_docked\_NumRotatableBonds**  
**ESS = 255 | BMK = 0.131 | MCSE(6.27) = 5.3 | stat: FALSE | burn: 0 | percentile: 31**

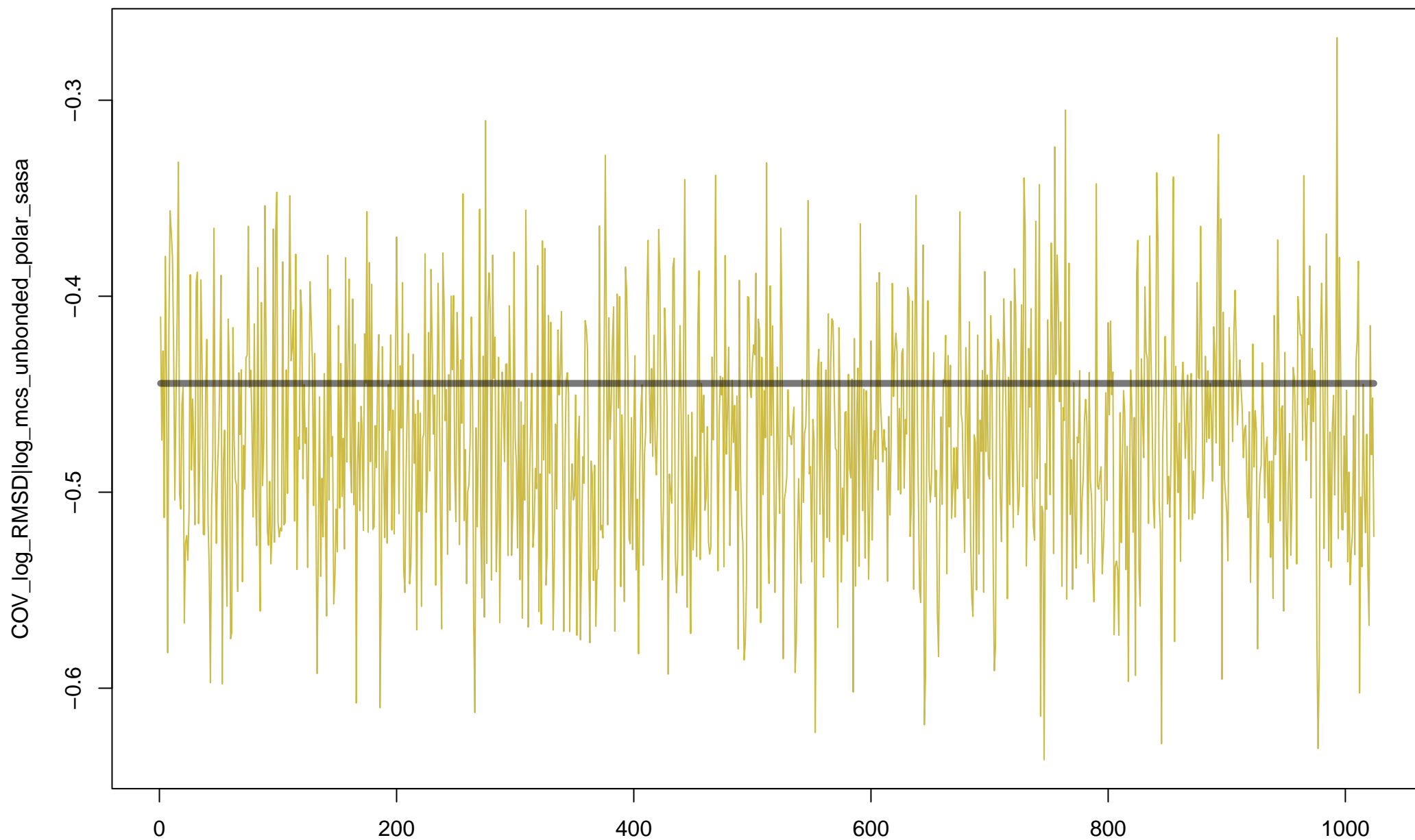


# VAR\_mcs\_NOCount

ESS = 1020 | BMK = 0.036 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0 | percentile: 77

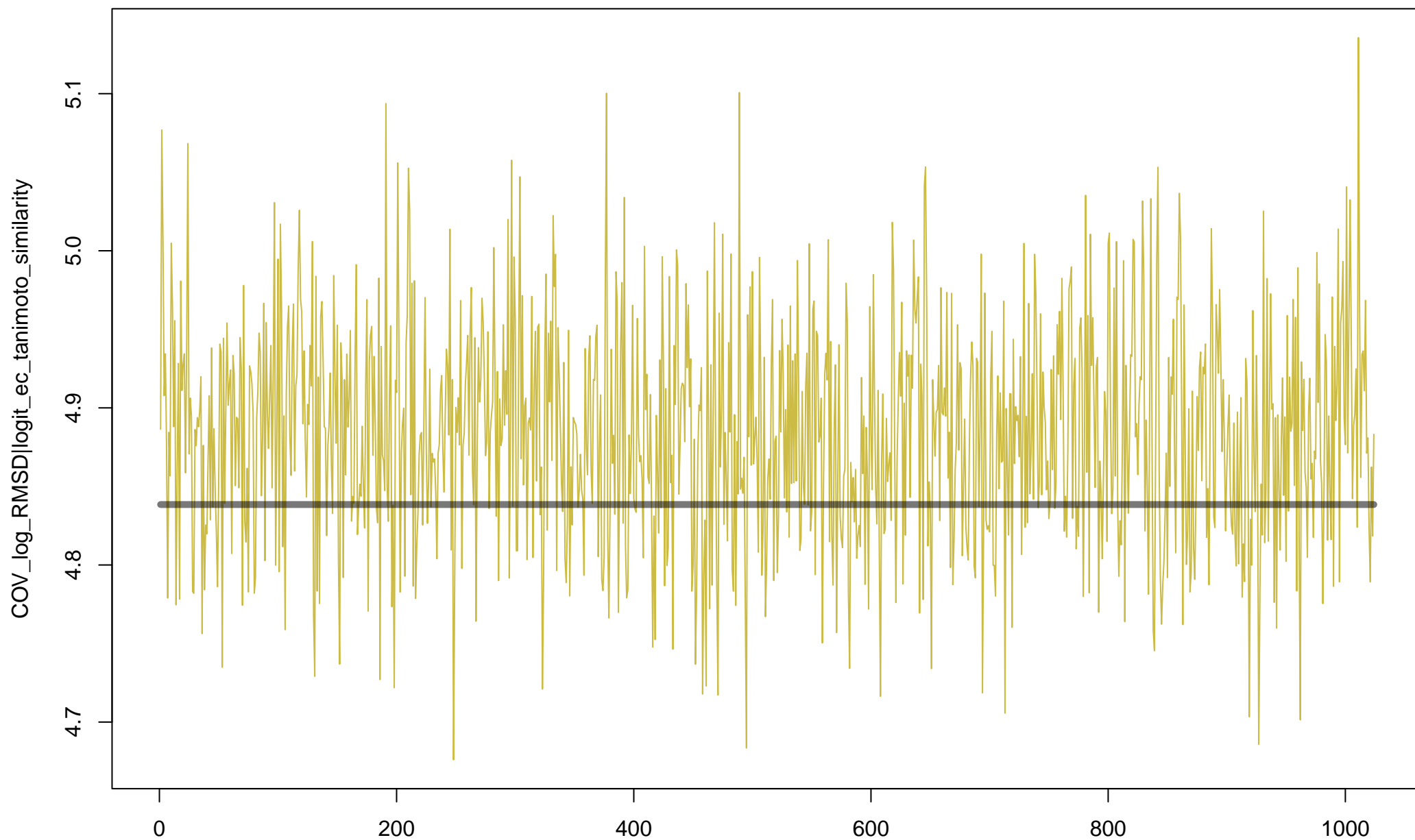


**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1020 | BMK = 0.077 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | percentile: 68**

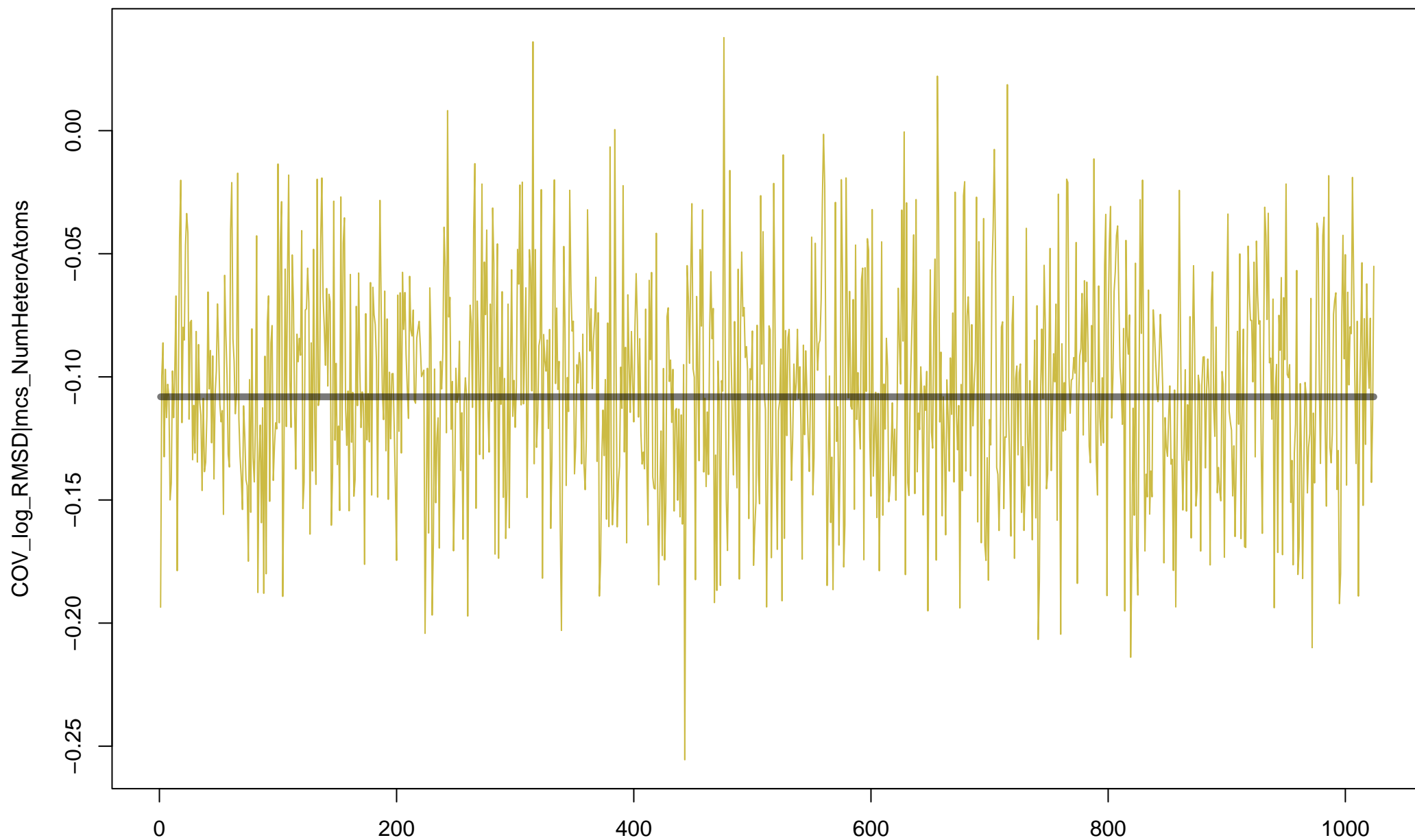




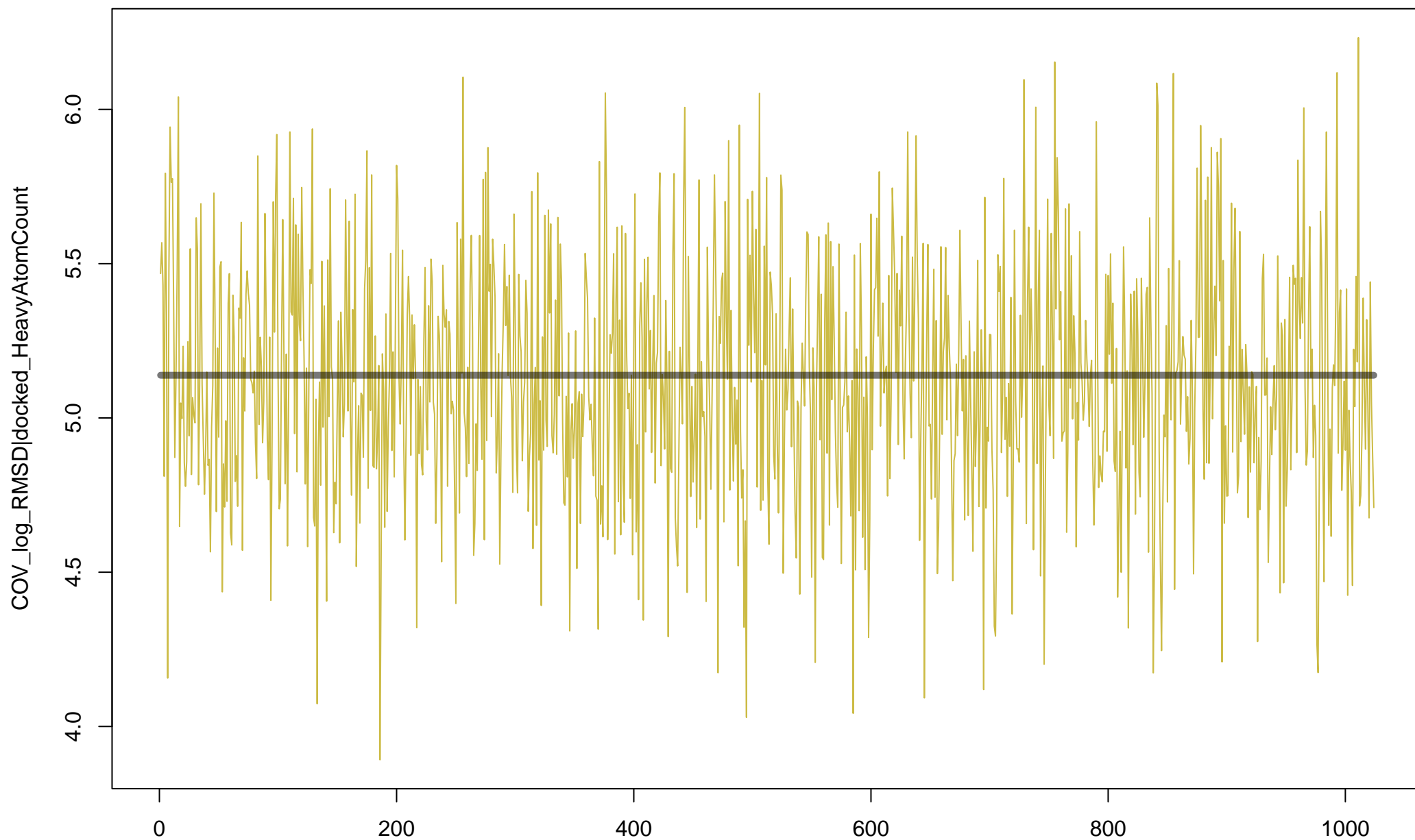
**COV\_log\_RMSD|logit\_ec\_tanimoto\_similarity**  
**ESS = 1020 | BMK = 0.0669 | MCSE(6.27) = 4.06 | stat: TRUE | burn: 0 | percentile: 27.5**



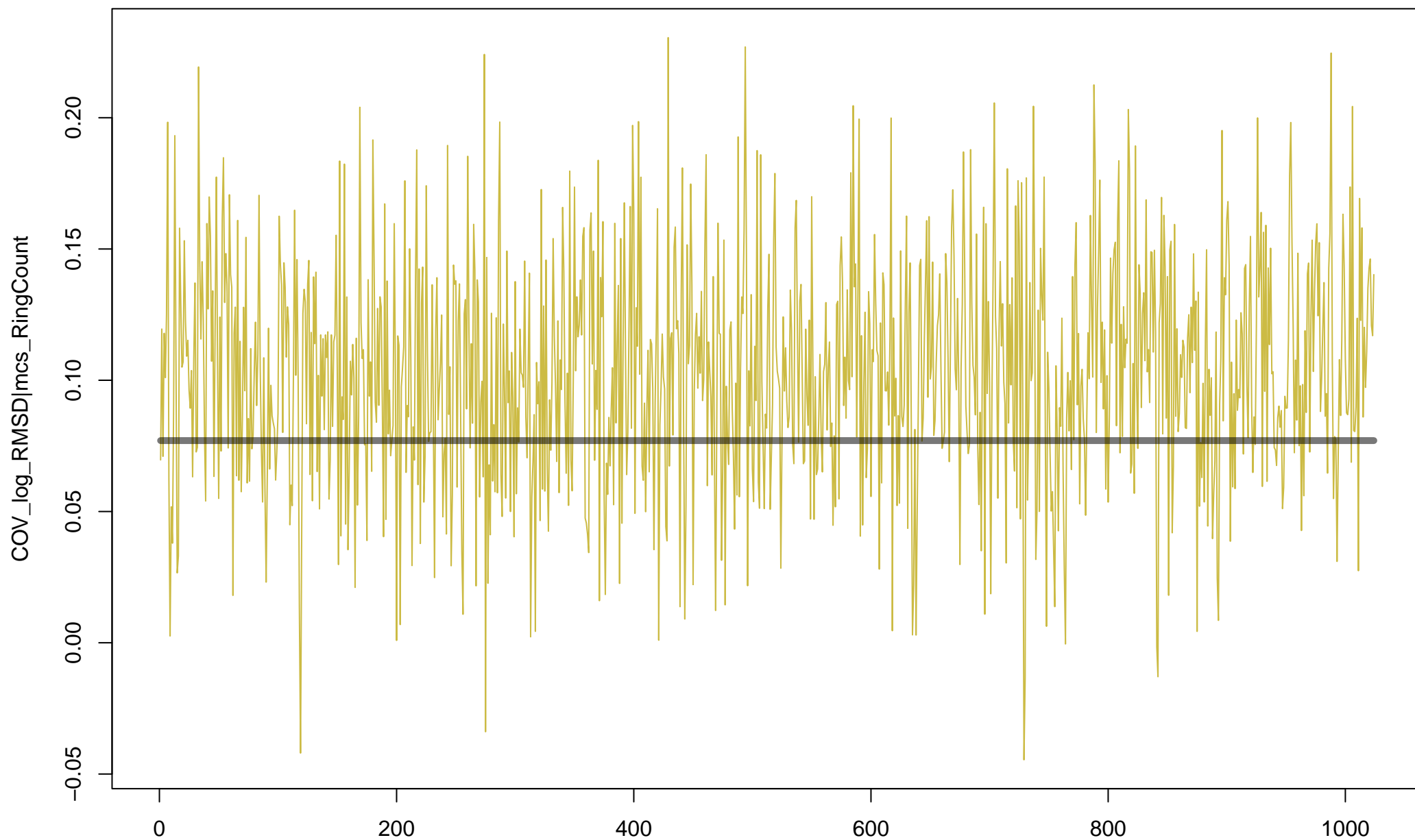
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 1020 | BMK = 0.0515 | MCSE(6.27) = 3.21 | stat: TRUE | burn: 0 | percentile: 47**



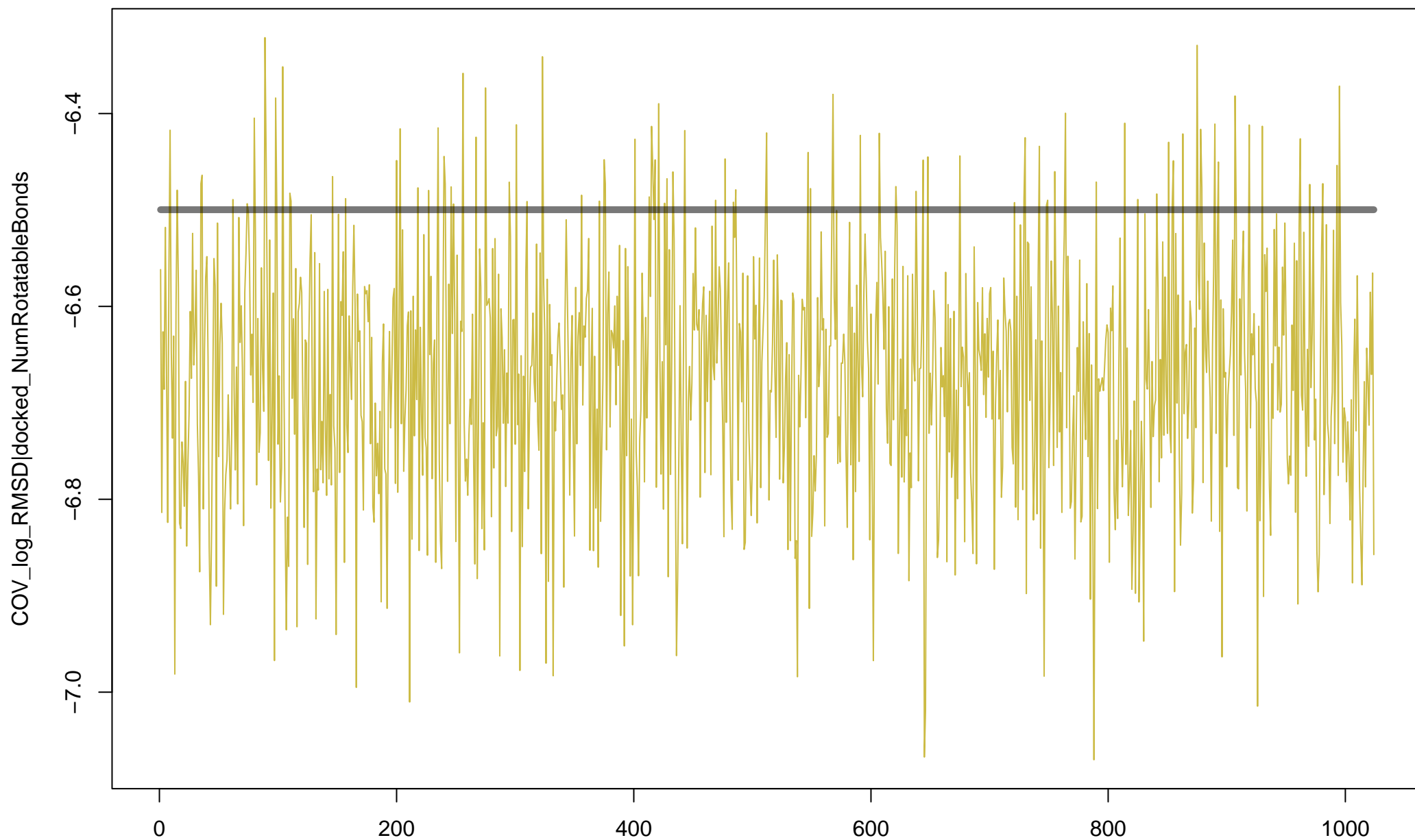
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.0585 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 0 | percentile: 53.6**



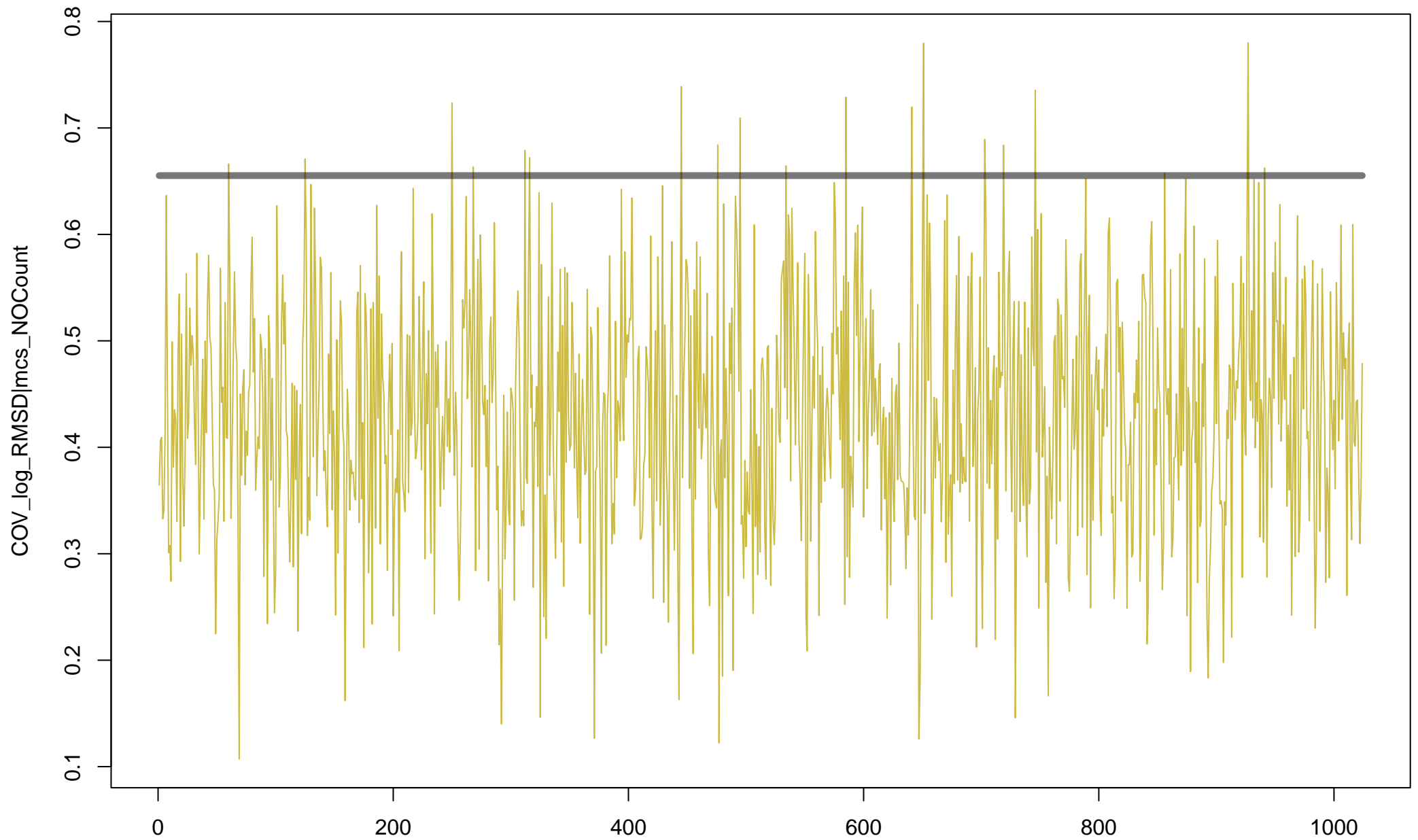
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.0727 | MCSE(6.27) = 3.83 | stat: TRUE | burn: 0 | percentile: 27**



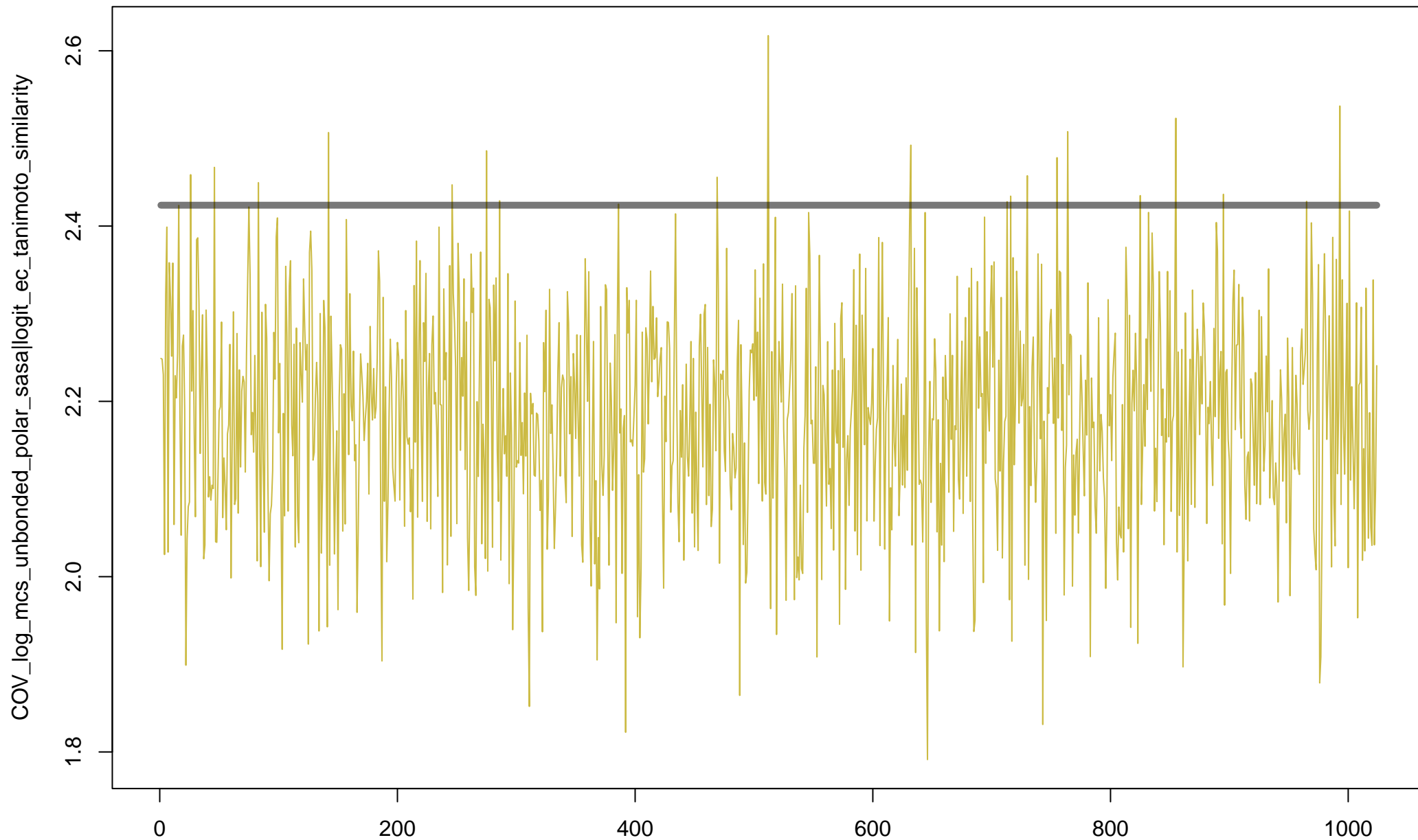
**COV\_log\_RMSD|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0593 | MCSE(6.27) = 3.32 | stat: TRUE | burn: 0 | percentile: 91.1**



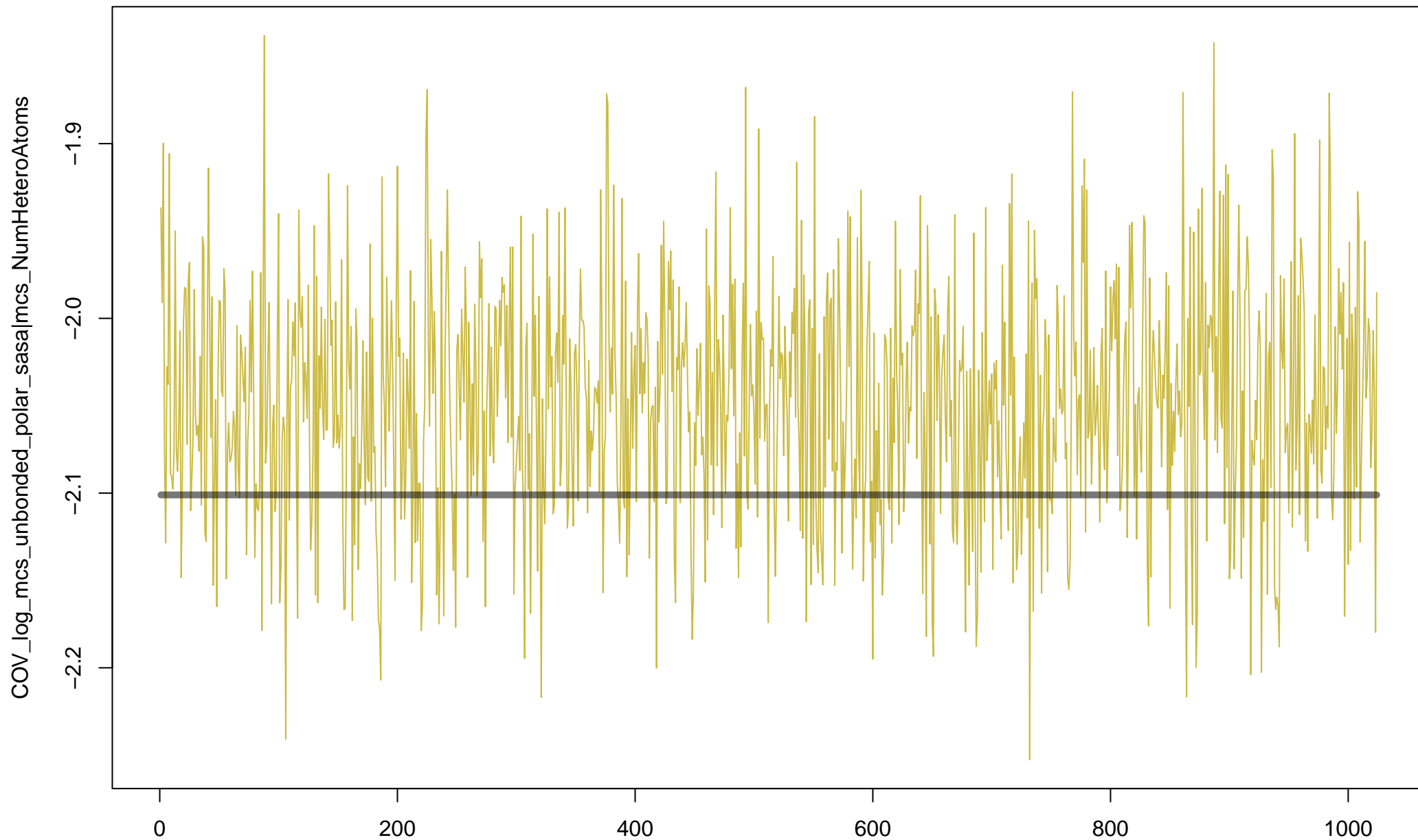
**COV\_log\_RMSD|mcs\_NOCount**  
**ESS = 922 | BMK = 0.0475 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0 | percentile: 98.1**



**COV\_log\_mcs\_unbonded\_polar\_sasa|logit\_ec\_tanimoto\_similarity**  
**ESS = 1020 | BMK = 0.0503 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0 | percentile: 97.9**

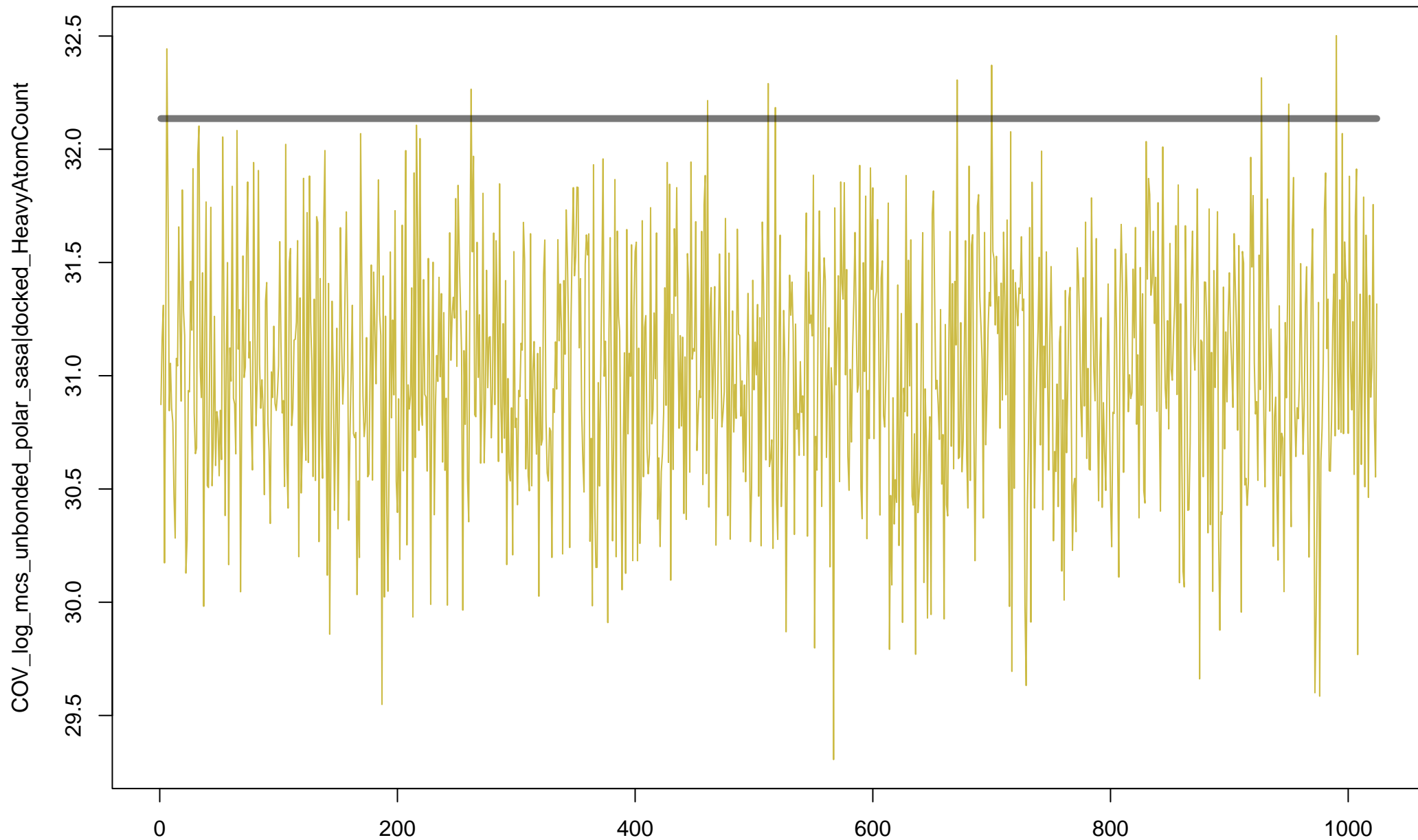


**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 1020 | BMK = 0.0439 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | percentile: 21.9**

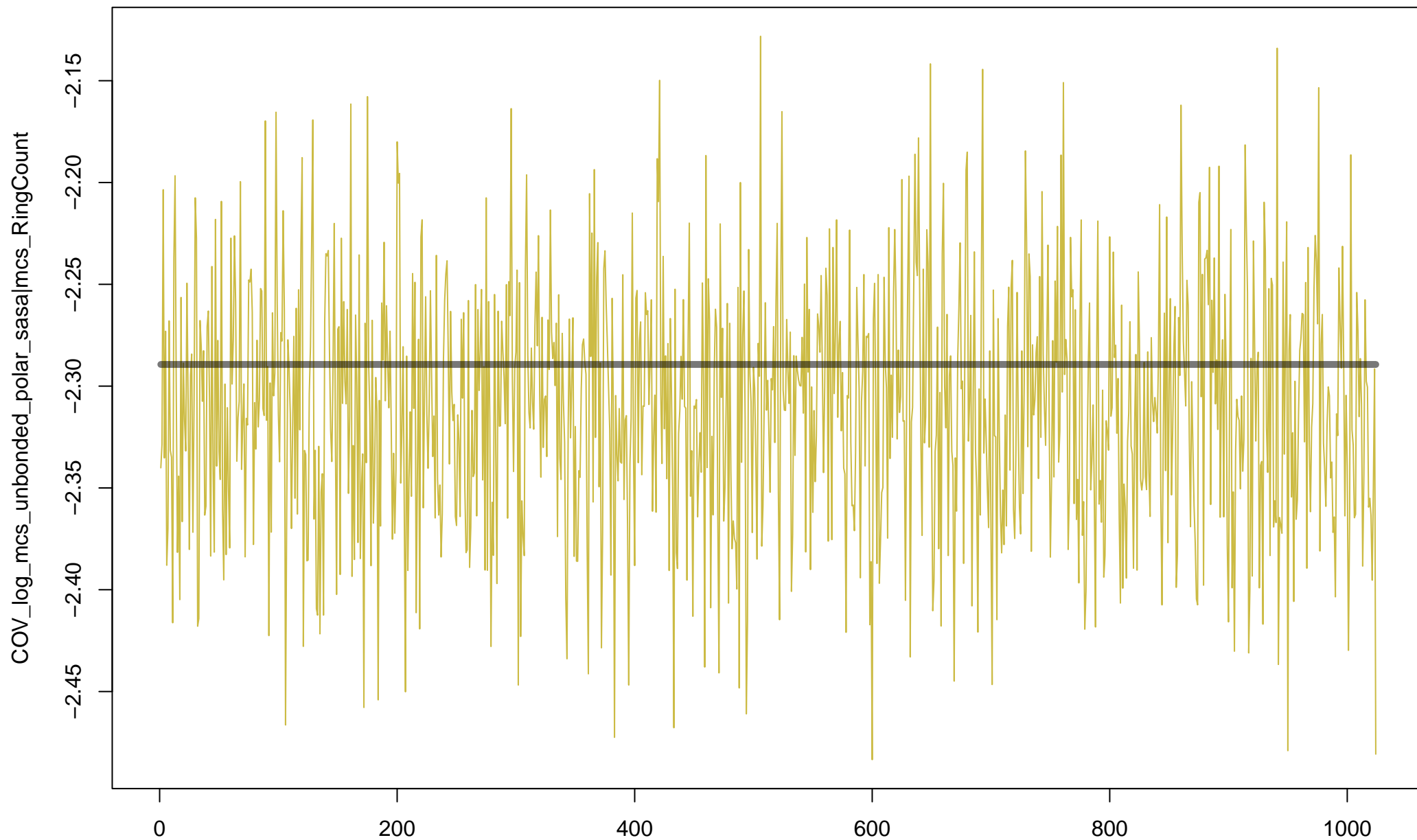




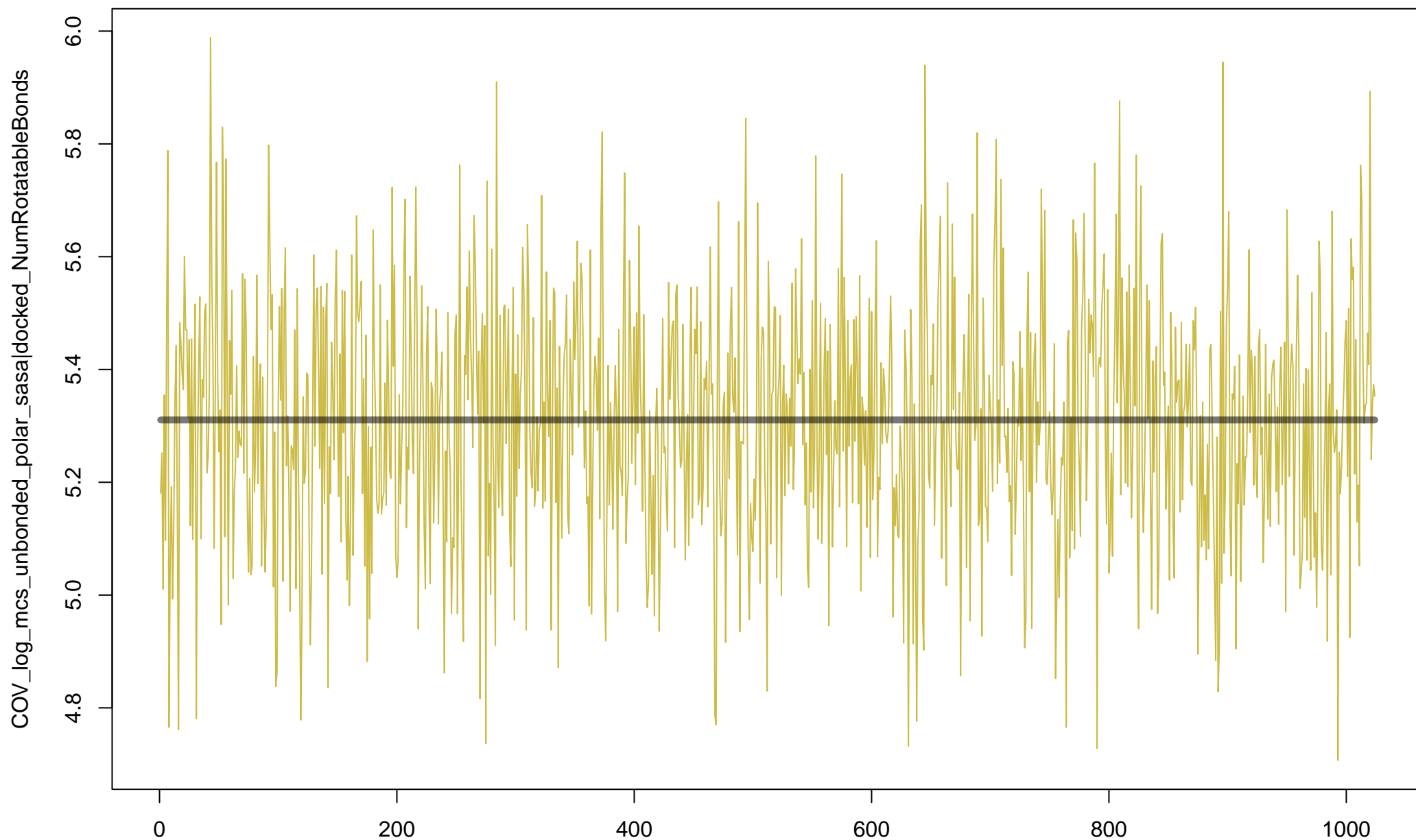
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.0715 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | percentile: 99**



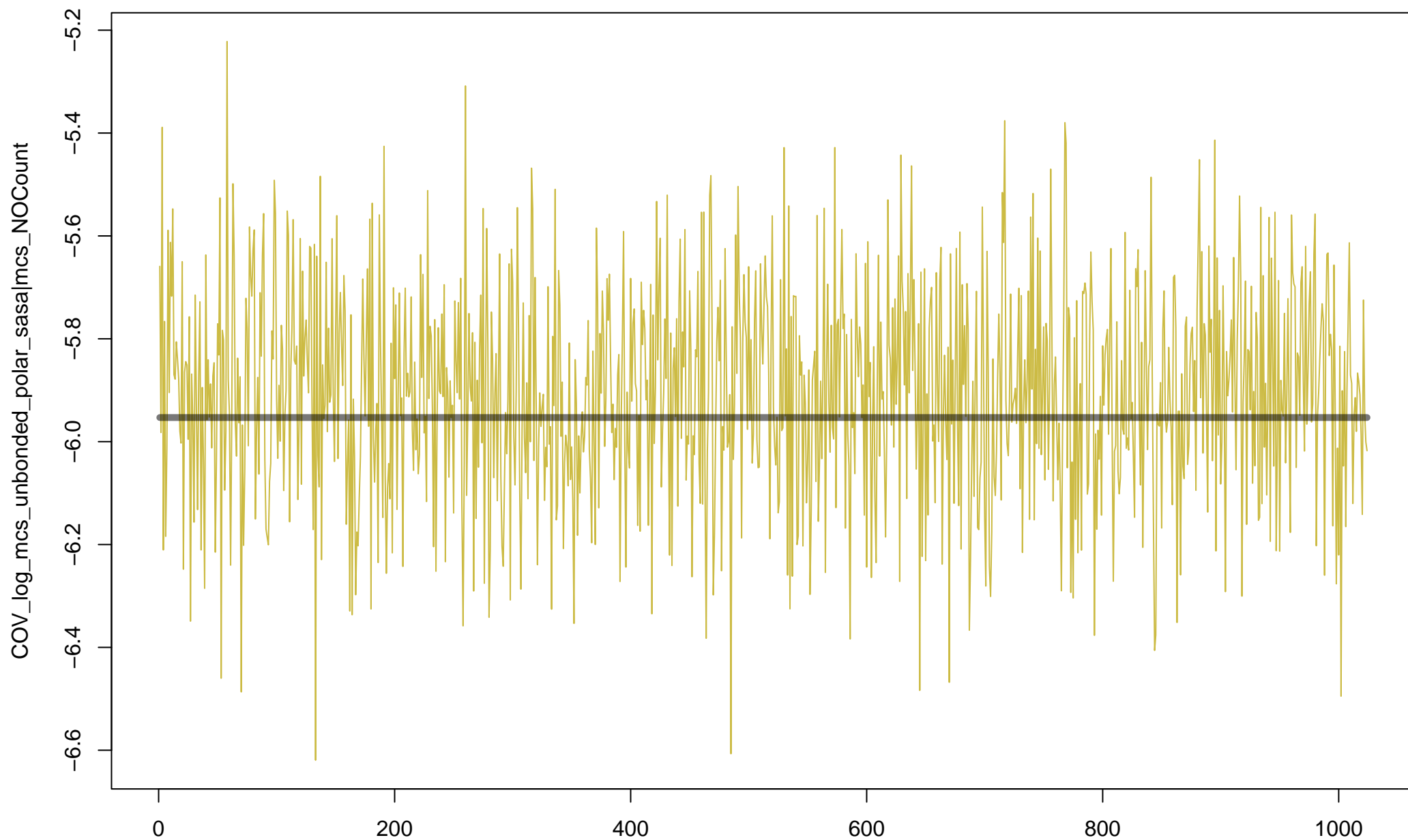
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.0413 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 0 | percentile: 63.3**



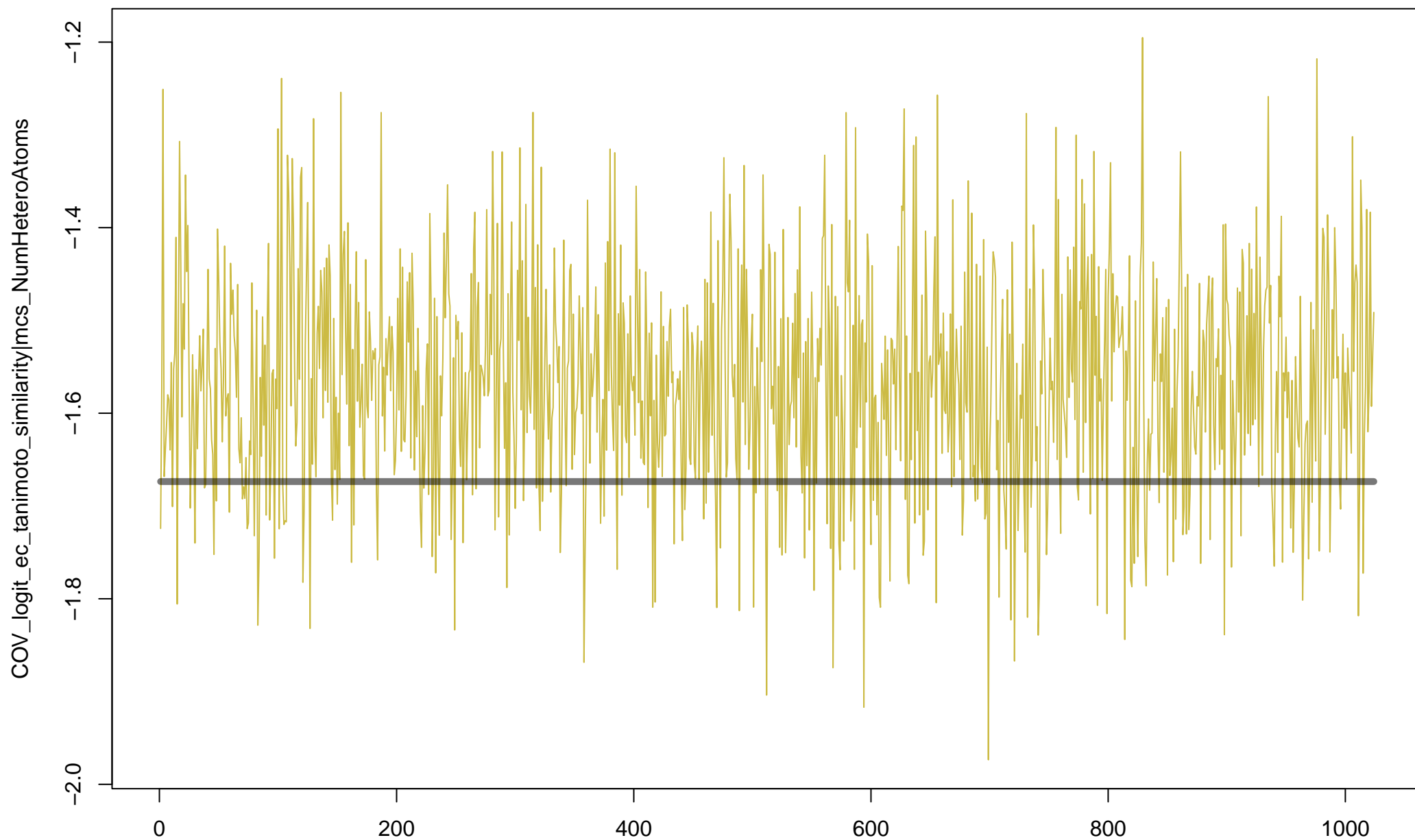
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_NumRotatableBonds**  
**ESS = 981 | BMK = 0.0434 | MCSE(6.27) = 3.73 | stat: TRUE | burn: 0 | percentile: 49.9**



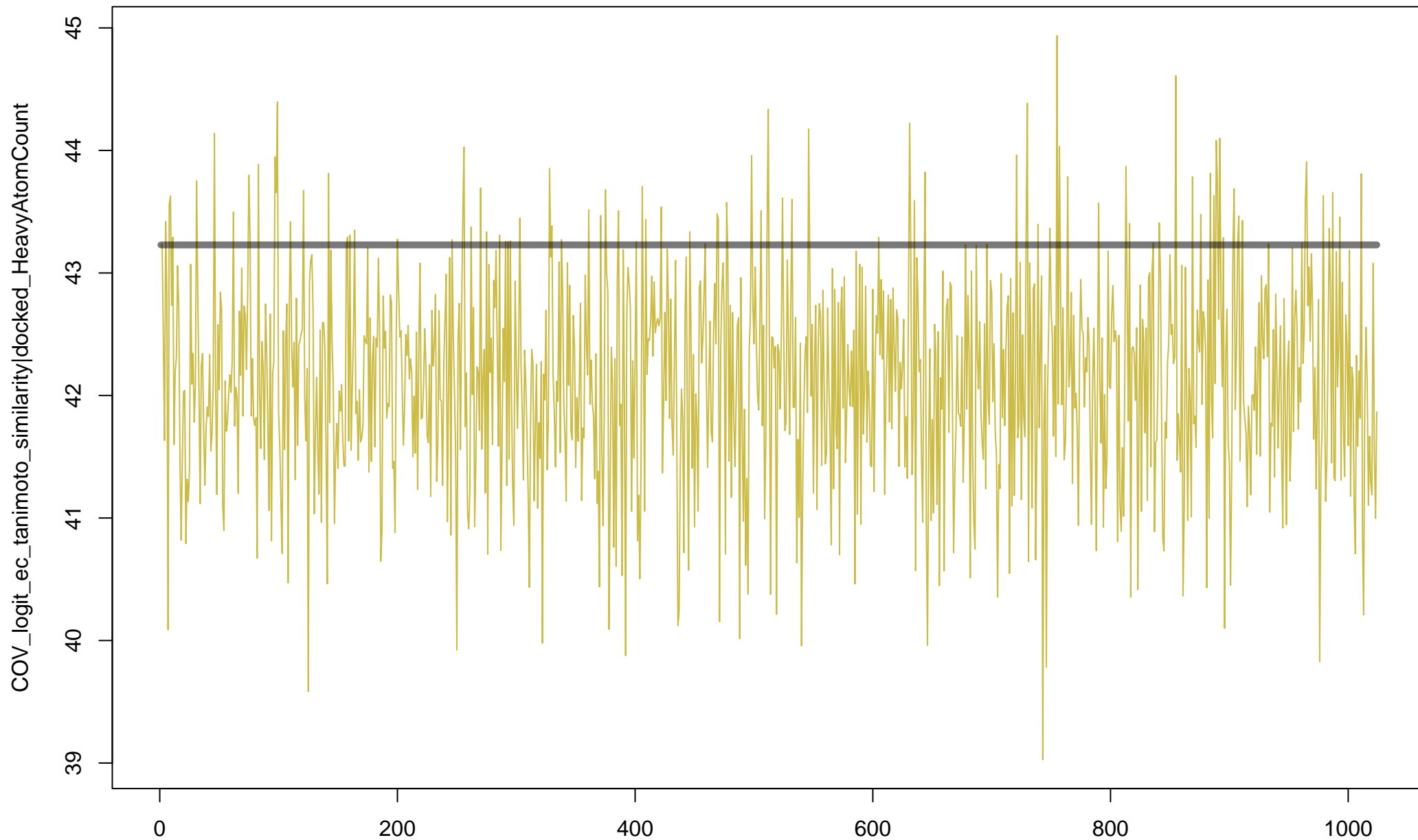
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0492 | MCSE(6.27) = 3.28 | stat: TRUE | burn: 0 | percentile: 40.3**



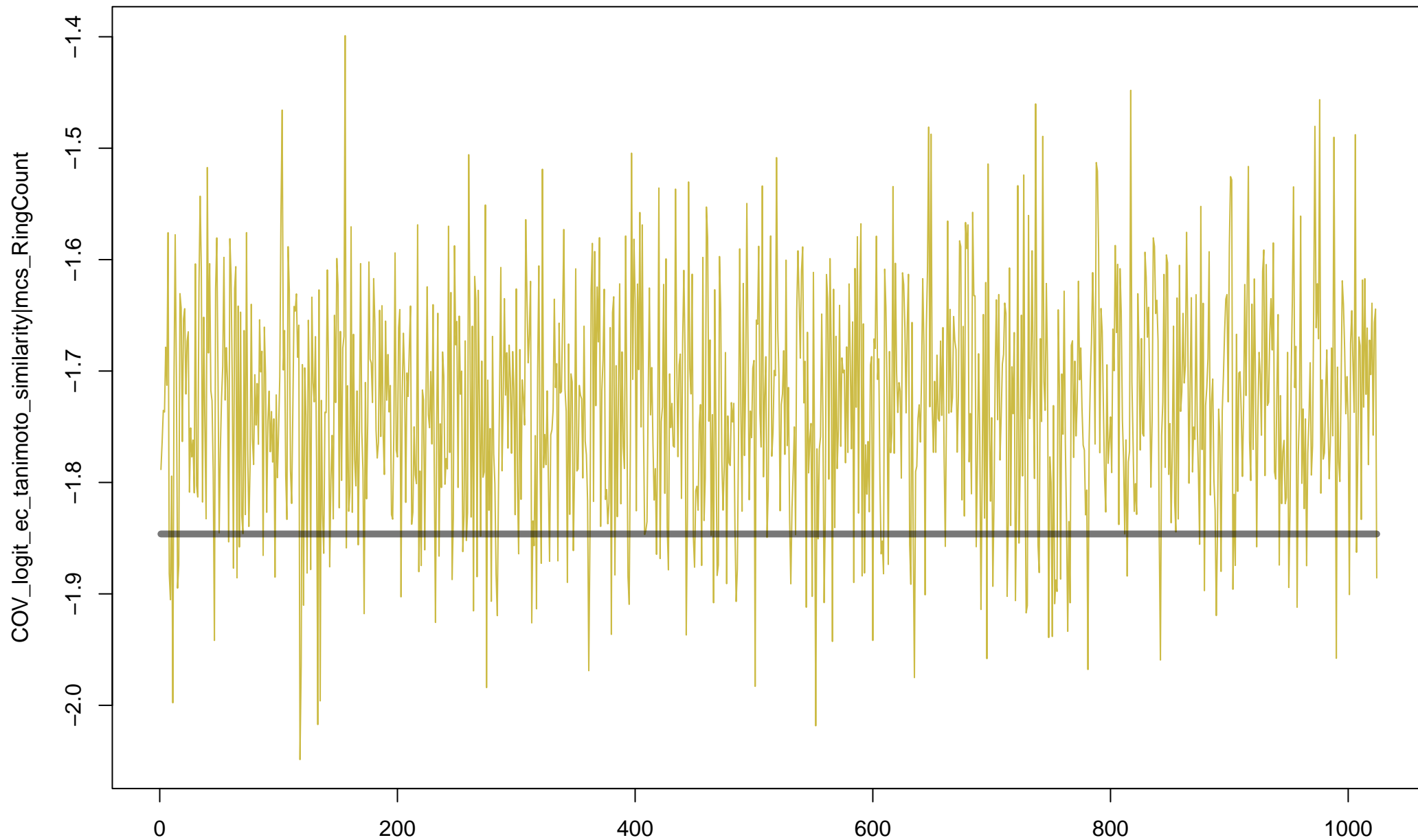
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms**  
**ESS = 1020 | BMK = 0.0651 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | percentile: 18.4**



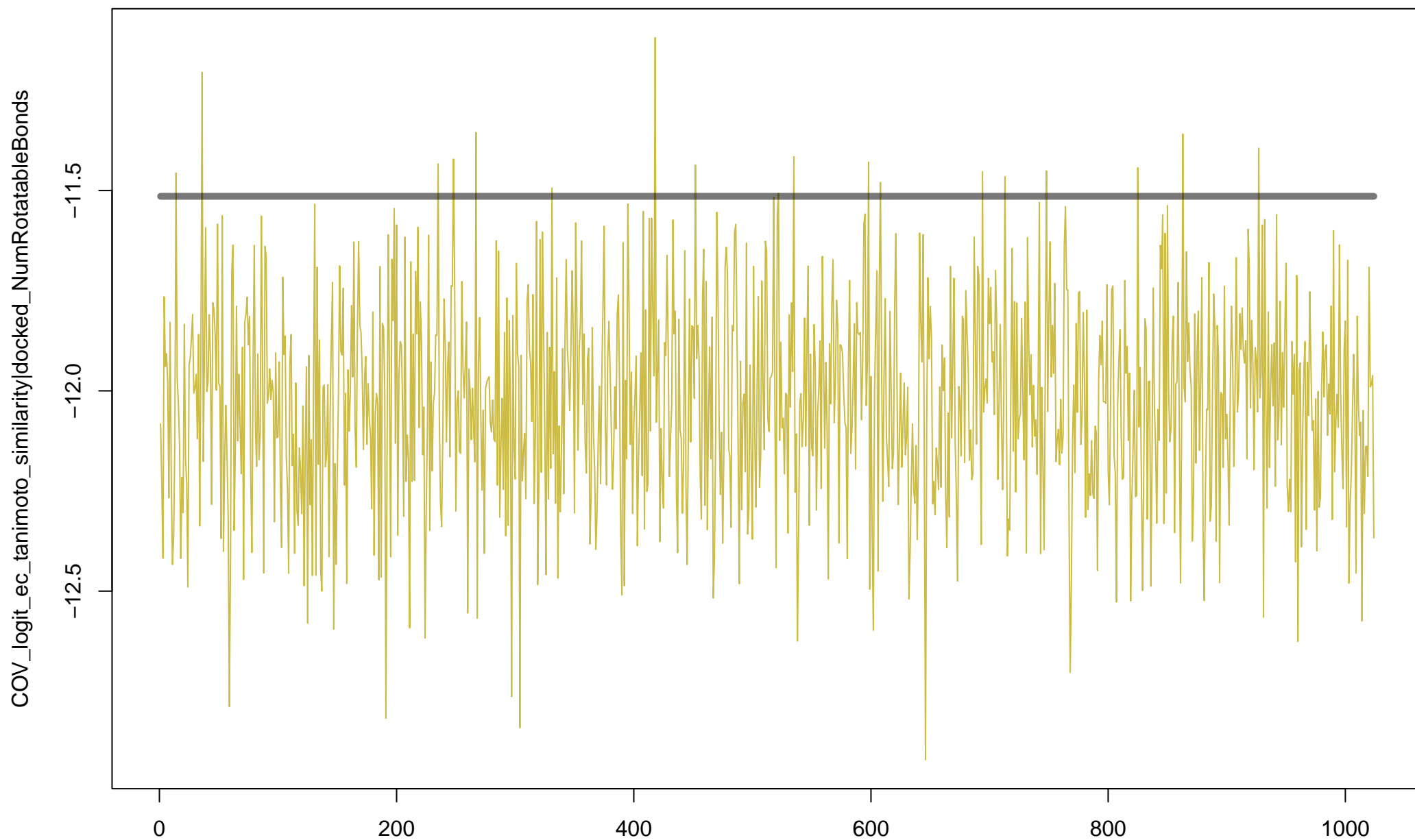
**COV\_logit\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.0415 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | percentile: 90.6**



**COV\_logit\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.0694 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | percentile: 12.9**

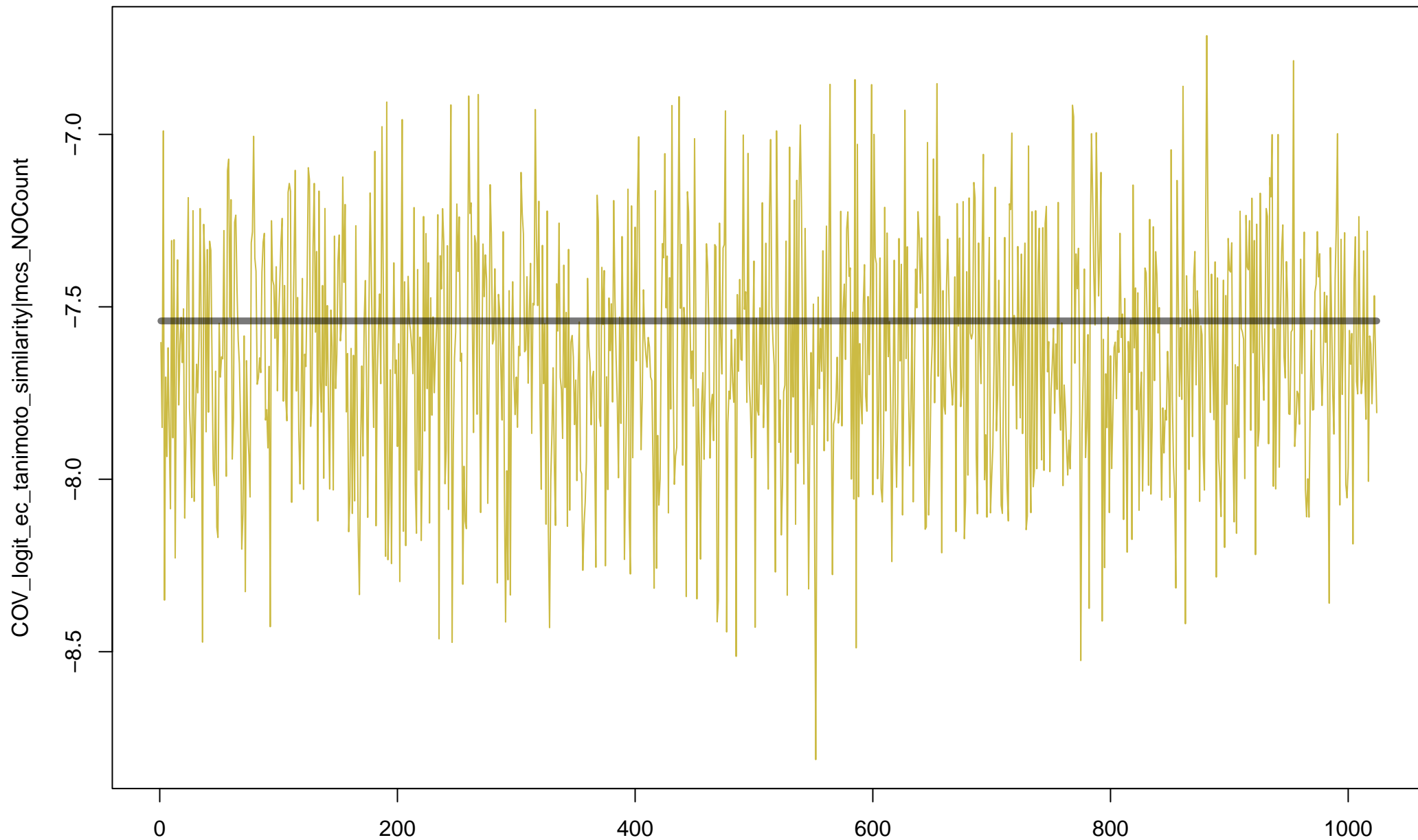


**COV\_logit\_ec\_tanimoto\_similarity|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0664 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0 | percentile: 98.2**

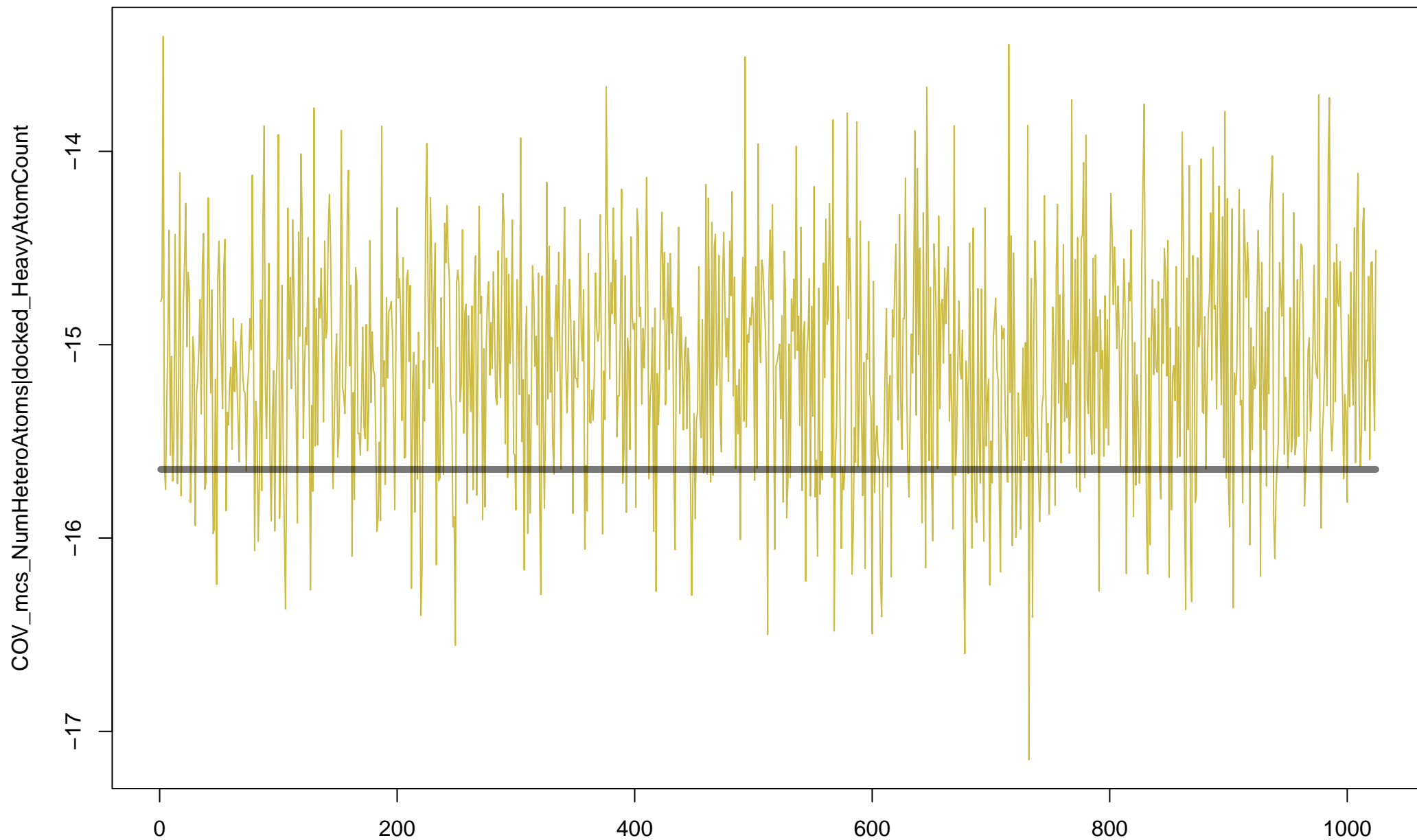




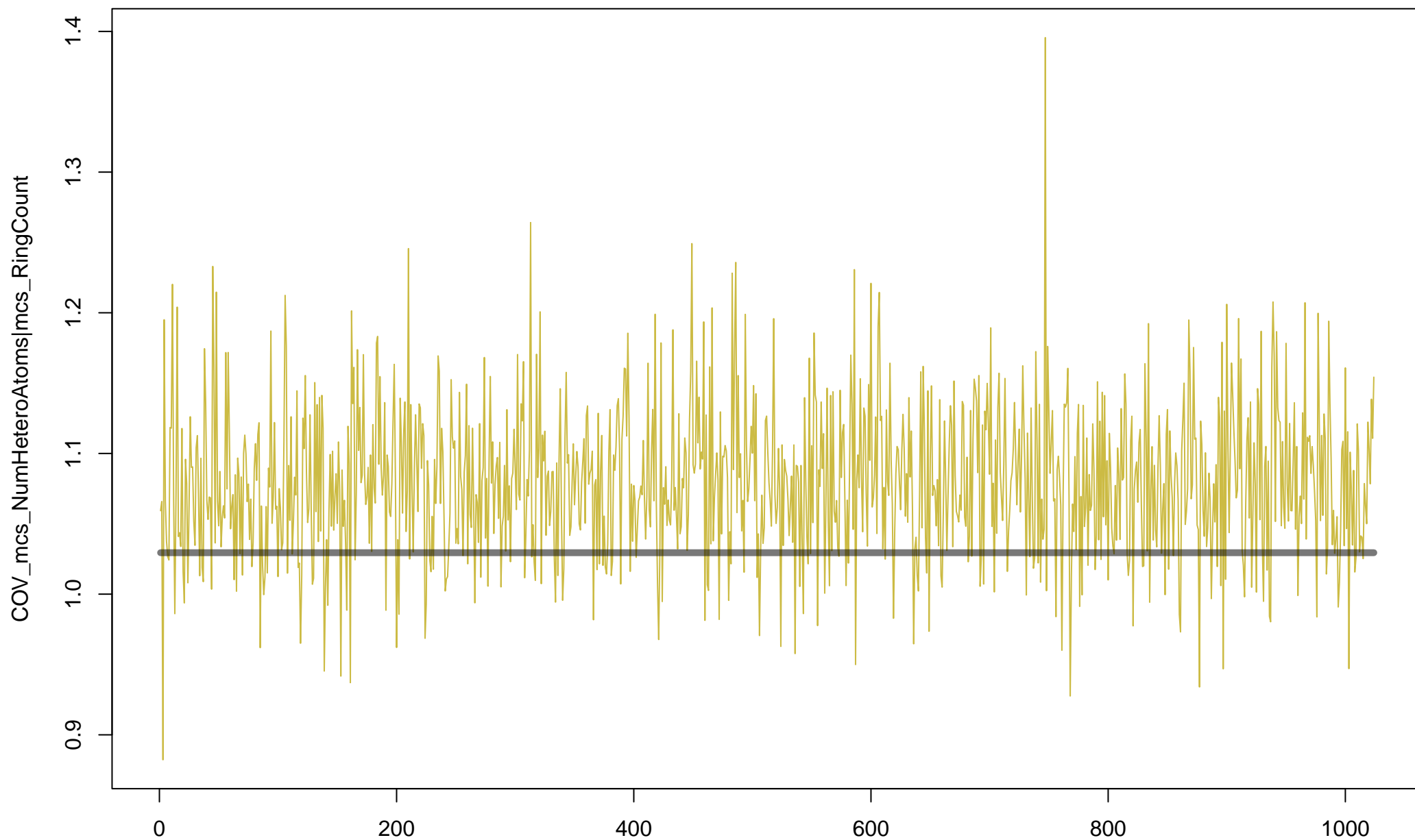
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0605 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0 | percentile: 62.1**



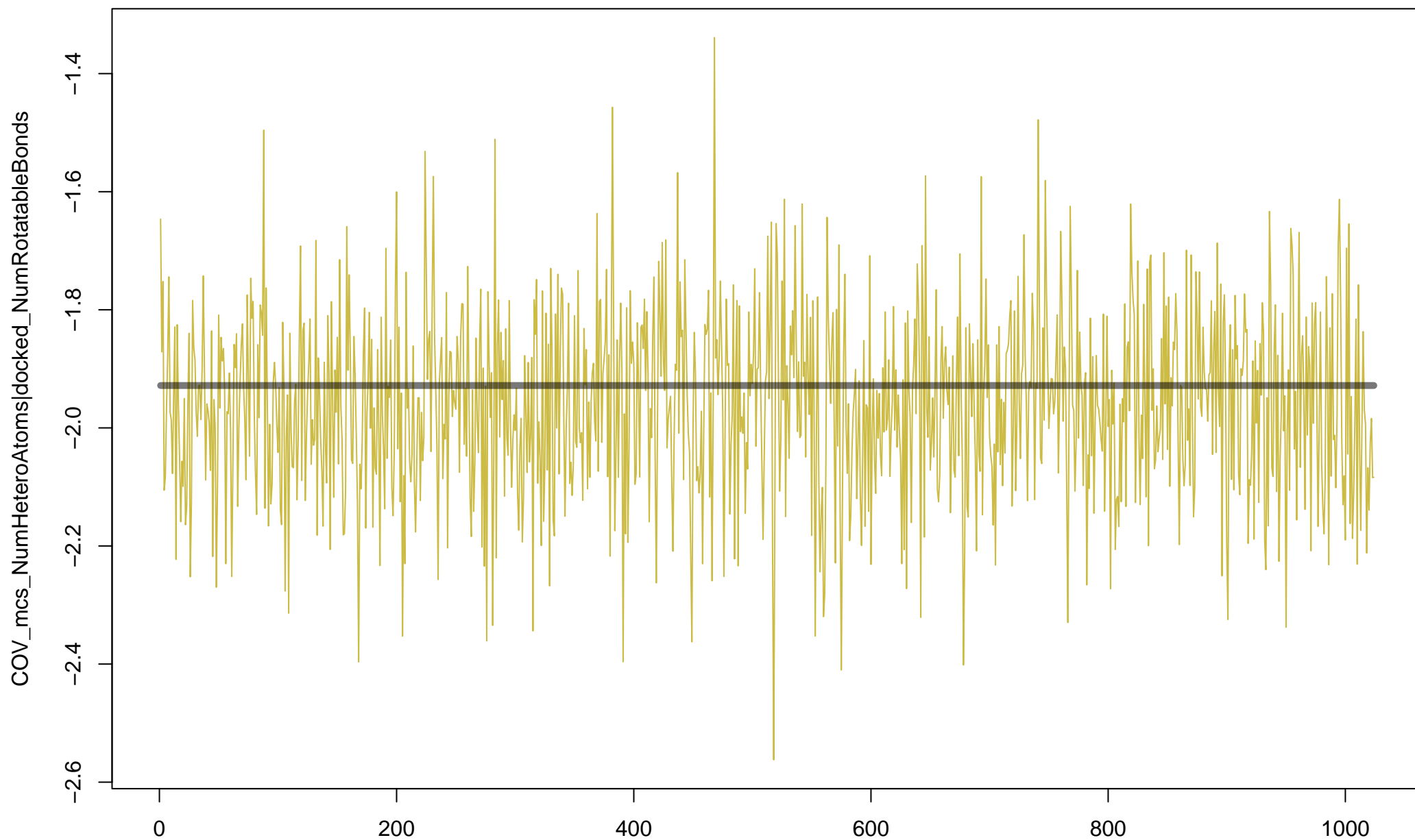
**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.0678 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0 | percentile: 17.3**



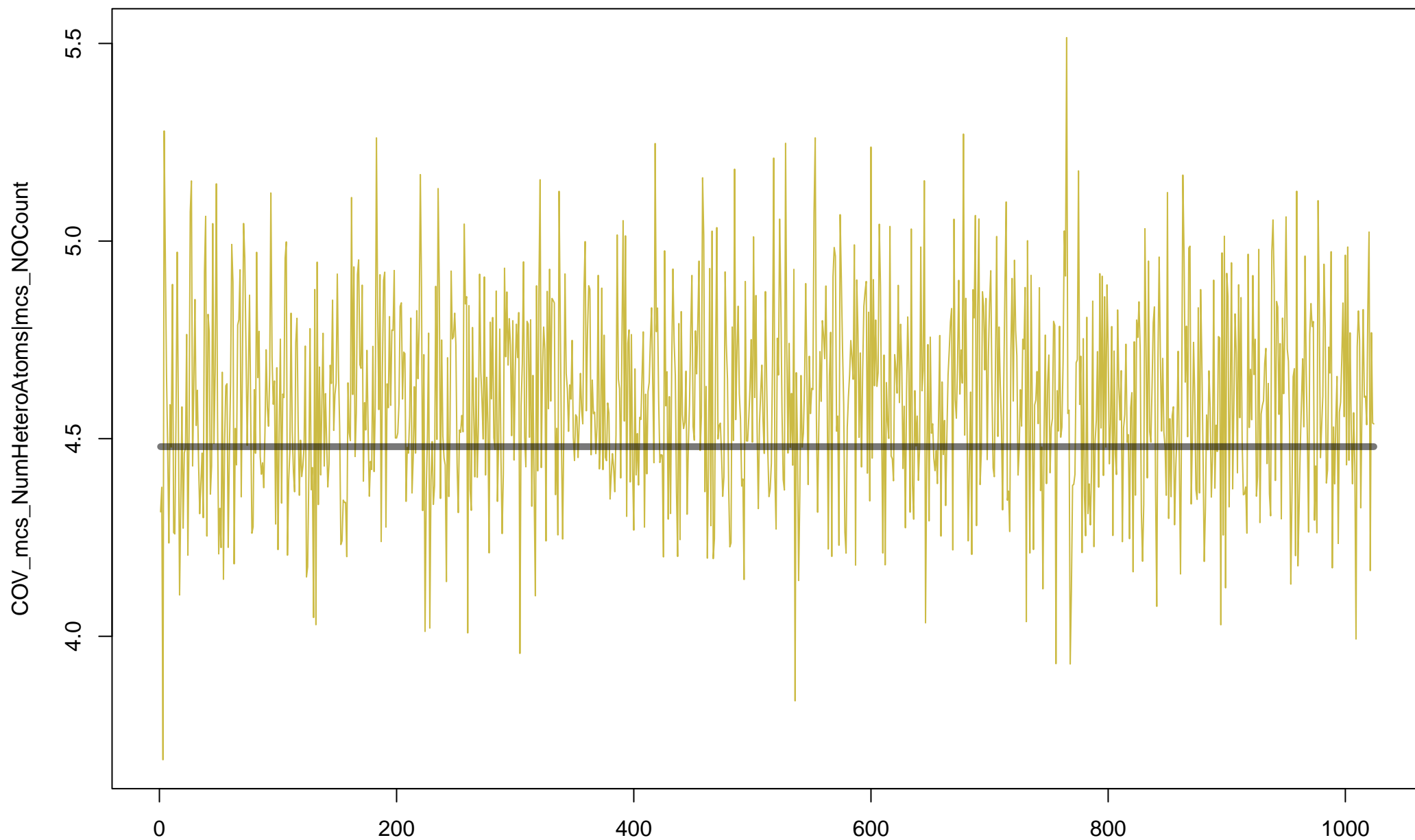
**COV\_mcs\_NumHeteroAtoms|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.0757 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0 | percentile: 16.9**



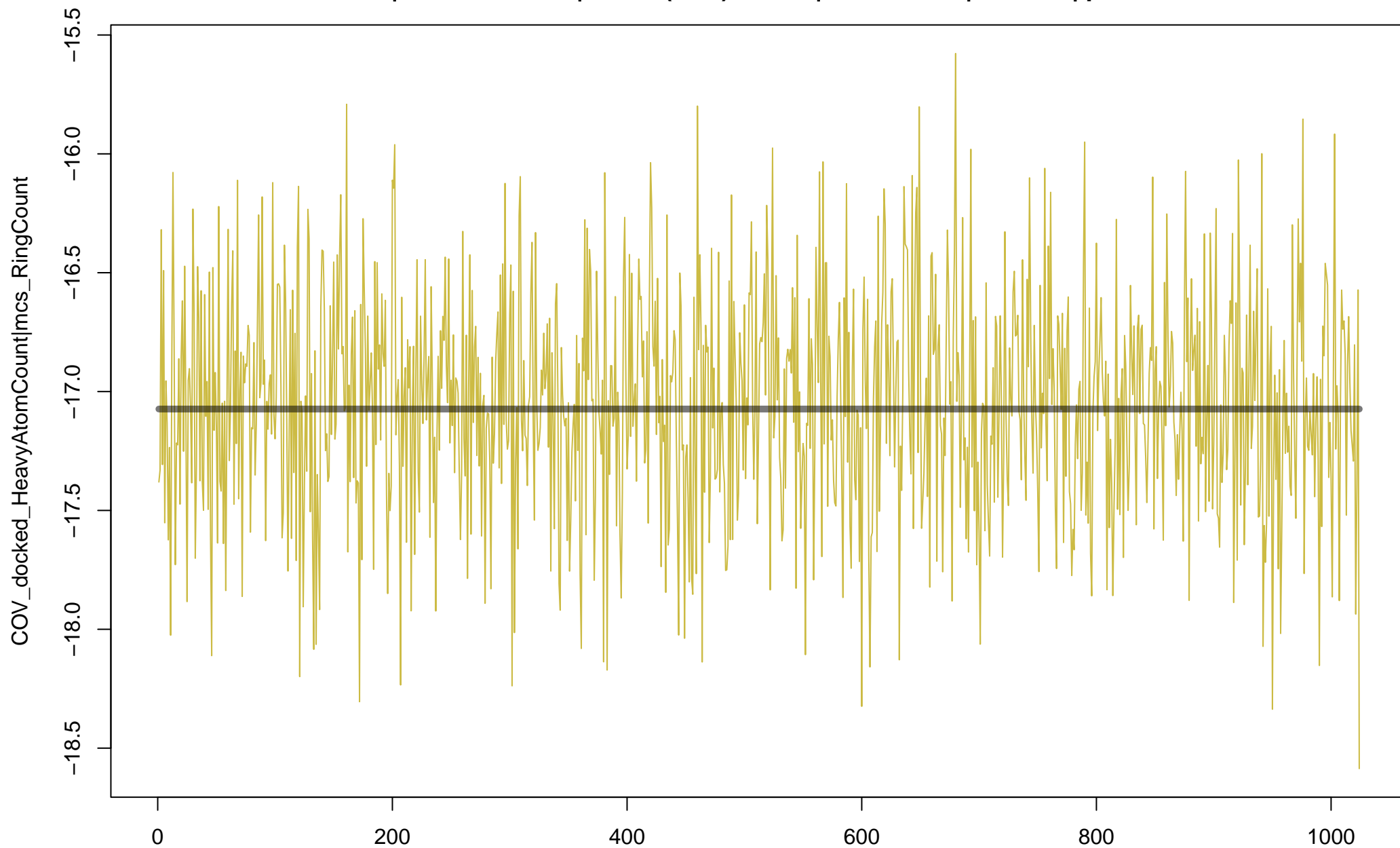
**COV\_mcs\_NumHeteroAtoms|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0648 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0 | percentile: 59.1**



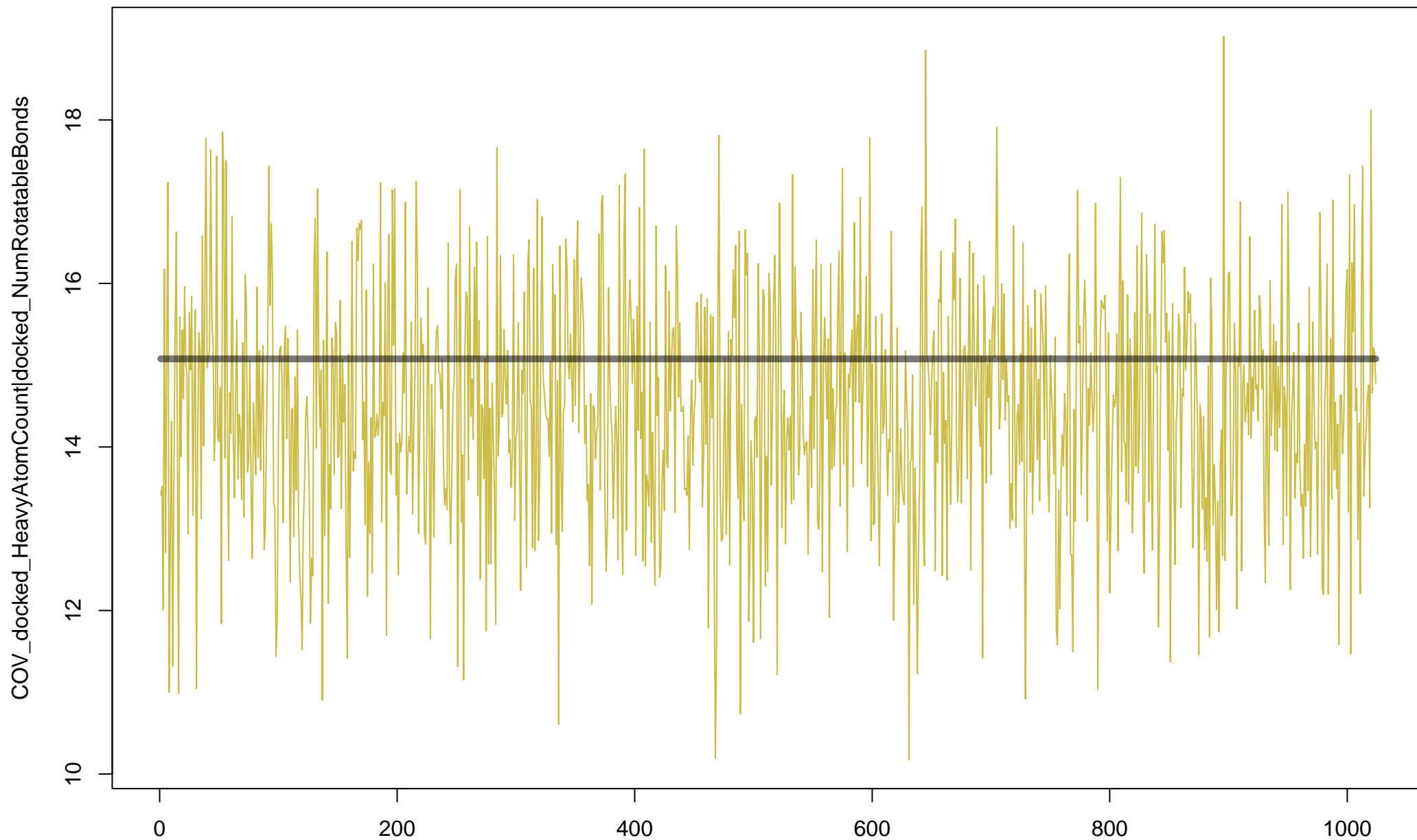
**COV\_mcs\_NumHeteroAtoms|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0485 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0 | percentile: 32.8**



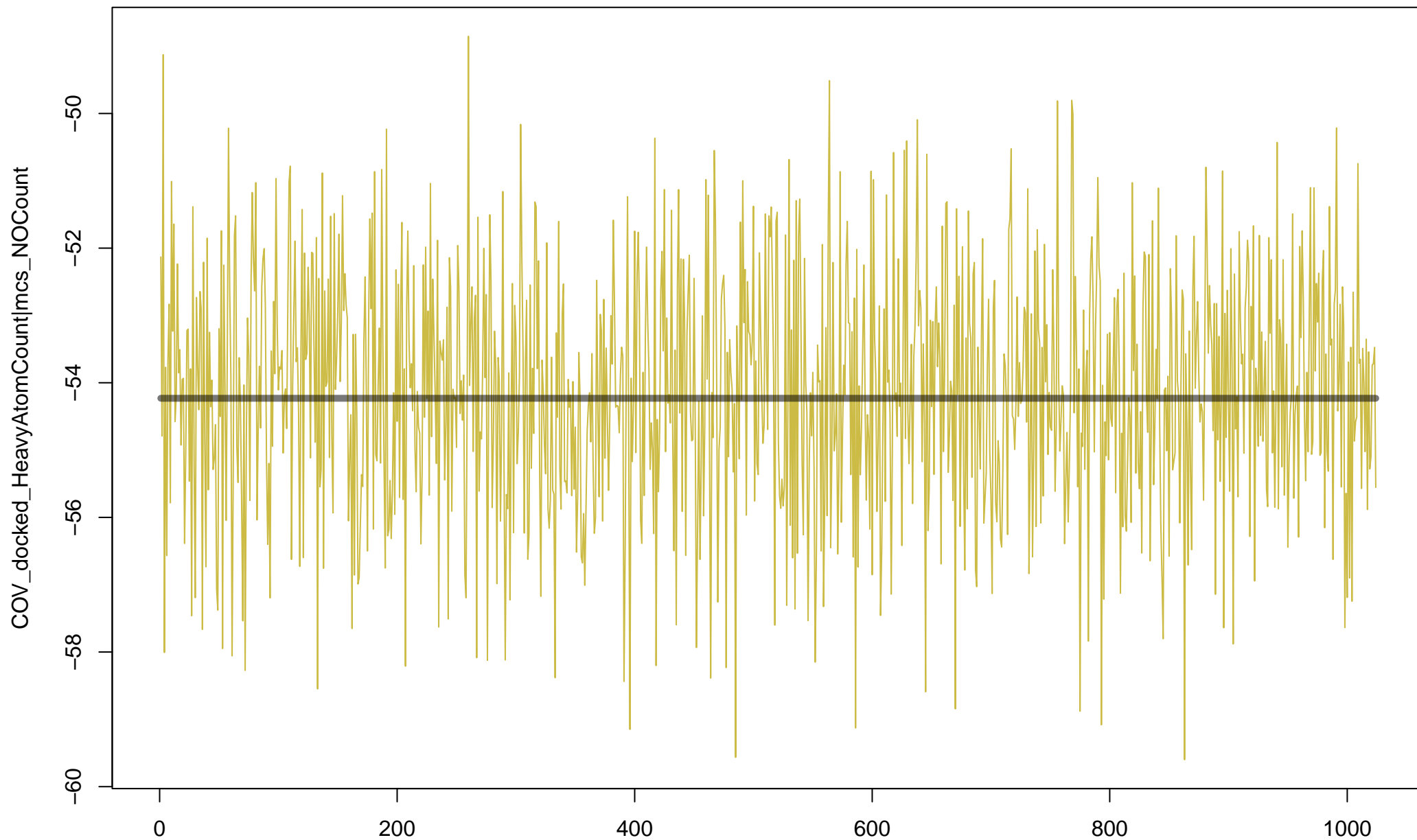
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.0536 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0 | percentile: 47.9**



**COV\_docked\_HeavyAtomCount|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0667 | MCSE(6.27) = 3.87 | stat: TRUE | burn: 0 | percentile: 66.5**

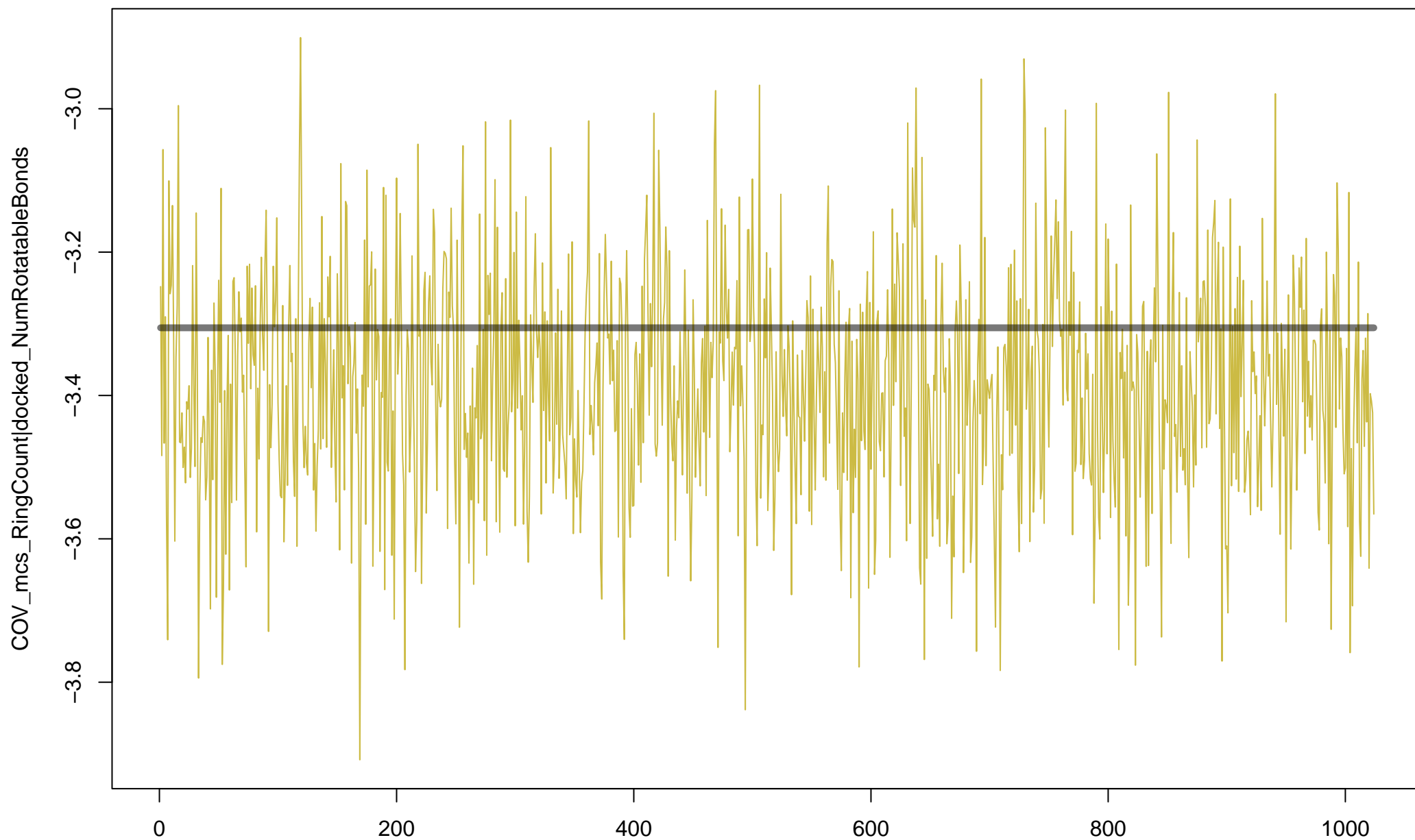


**COV\_docked\_HeavyAtomCount|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.044 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0 | percentile: 46.7**

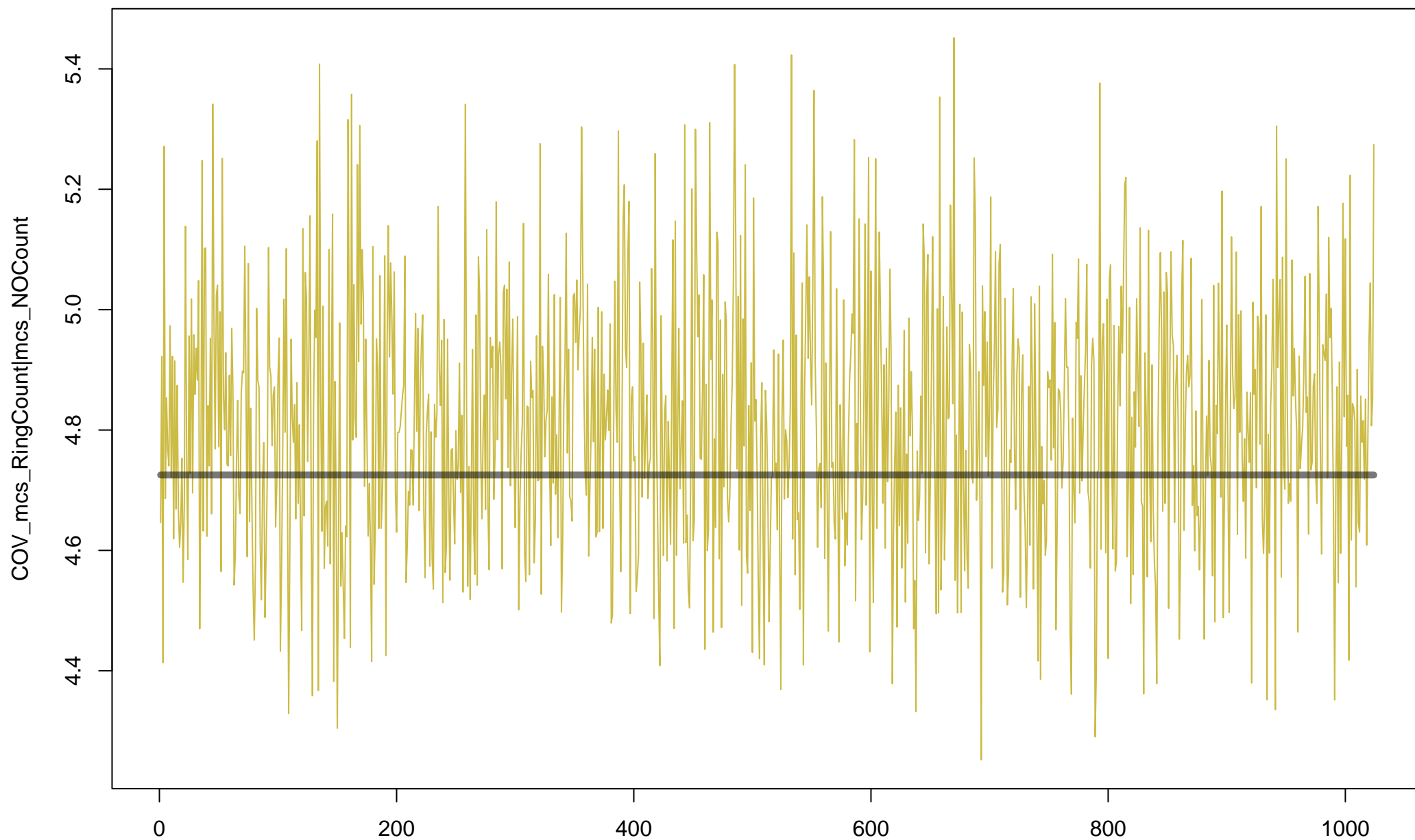




**COV\_mcs\_RingCount|docked\_NumRotatableBonds**  
**ESS = 936 | BMK = 0.0522 | MCSE(6.27) = 3.86 | stat: TRUE | burn: 0 | percentile: 71.2**



**COV\_mcs\_RingCount|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0451 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0 | percentile: 36.2**



**COV\_docked\_NumRotatableBonds|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0356 | MCSE(6.27) = 3.68 | stat: TRUE | burn: 0 | percentile: 16**

