

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.240512672745537

max MCSE = 7.9571091208364

all stationary: FALSE

burn: 306

min percent.: 0

-- STATS 1D --

min ESS = 78.1667595873139

max BMK = 0.134646883434025

max MCSE = 7.31760927760607

all stationary: FALSE

burn: 0

min percent.: 0.29296875

-- STATS 2D --

min ESS = 793.631340216794

max BMK = 0.0731393066435078

max MCSE = 3.82019069854667

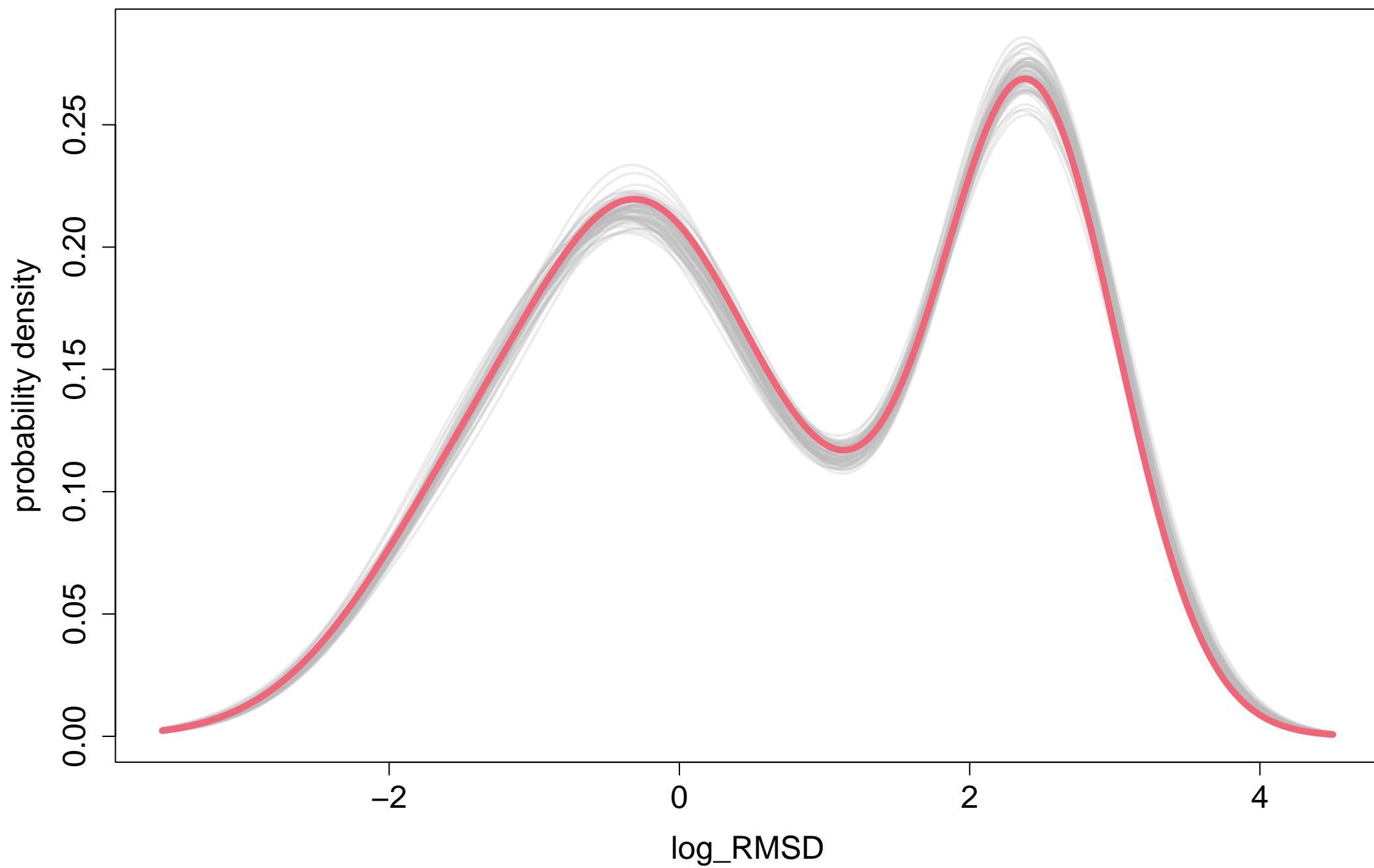
all stationary: TRUE

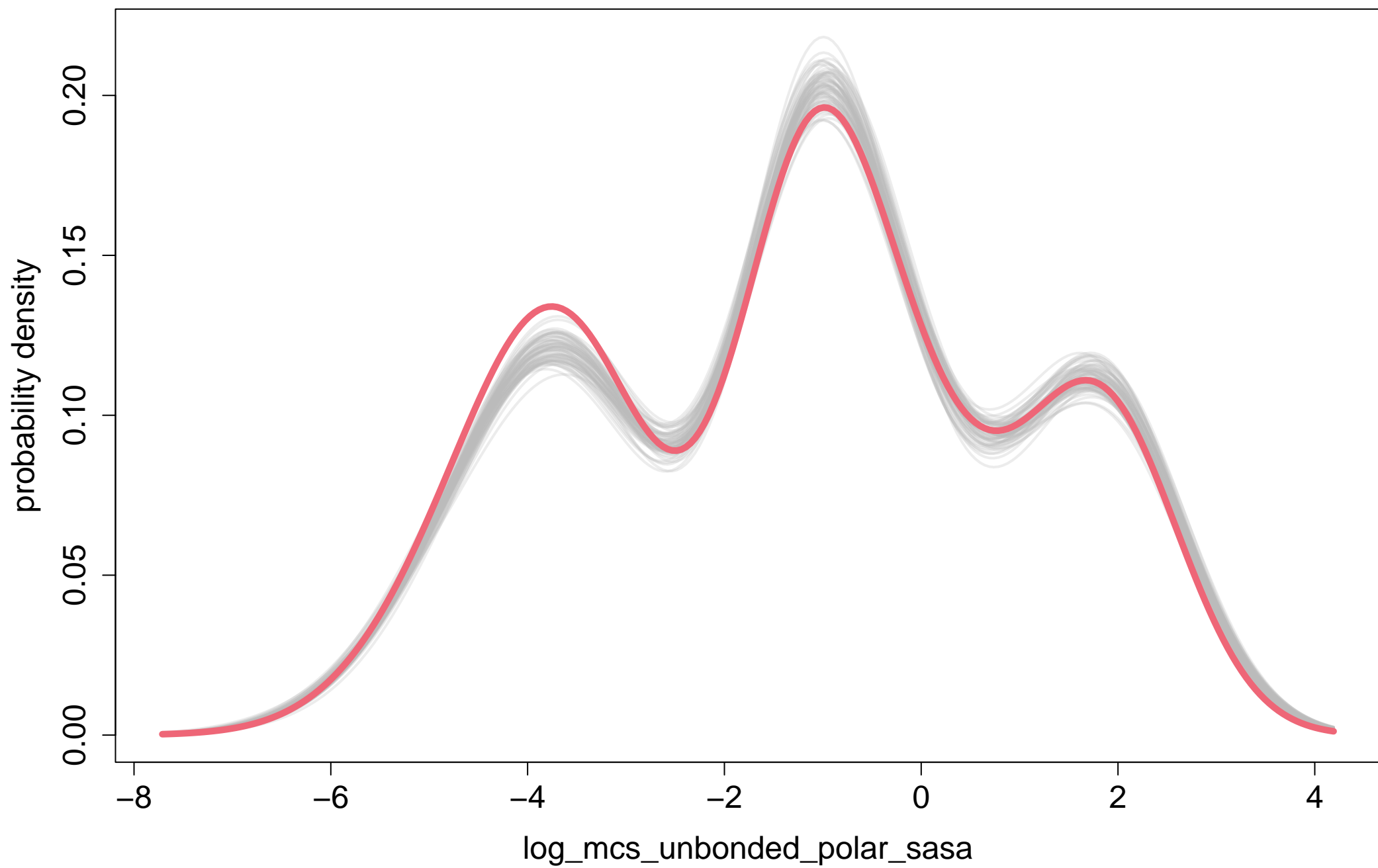
burn: 0

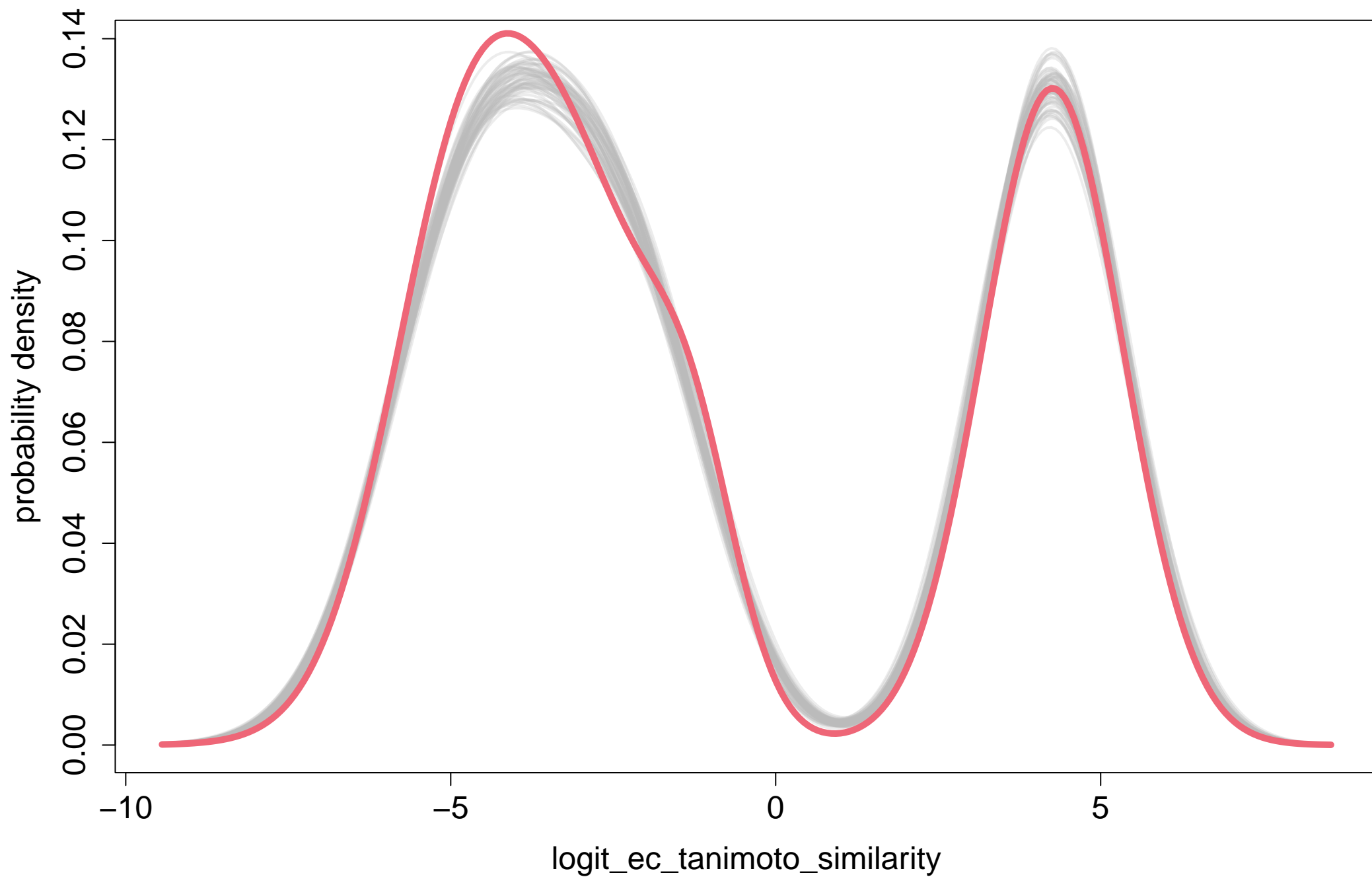
min percent.: 1.3671875

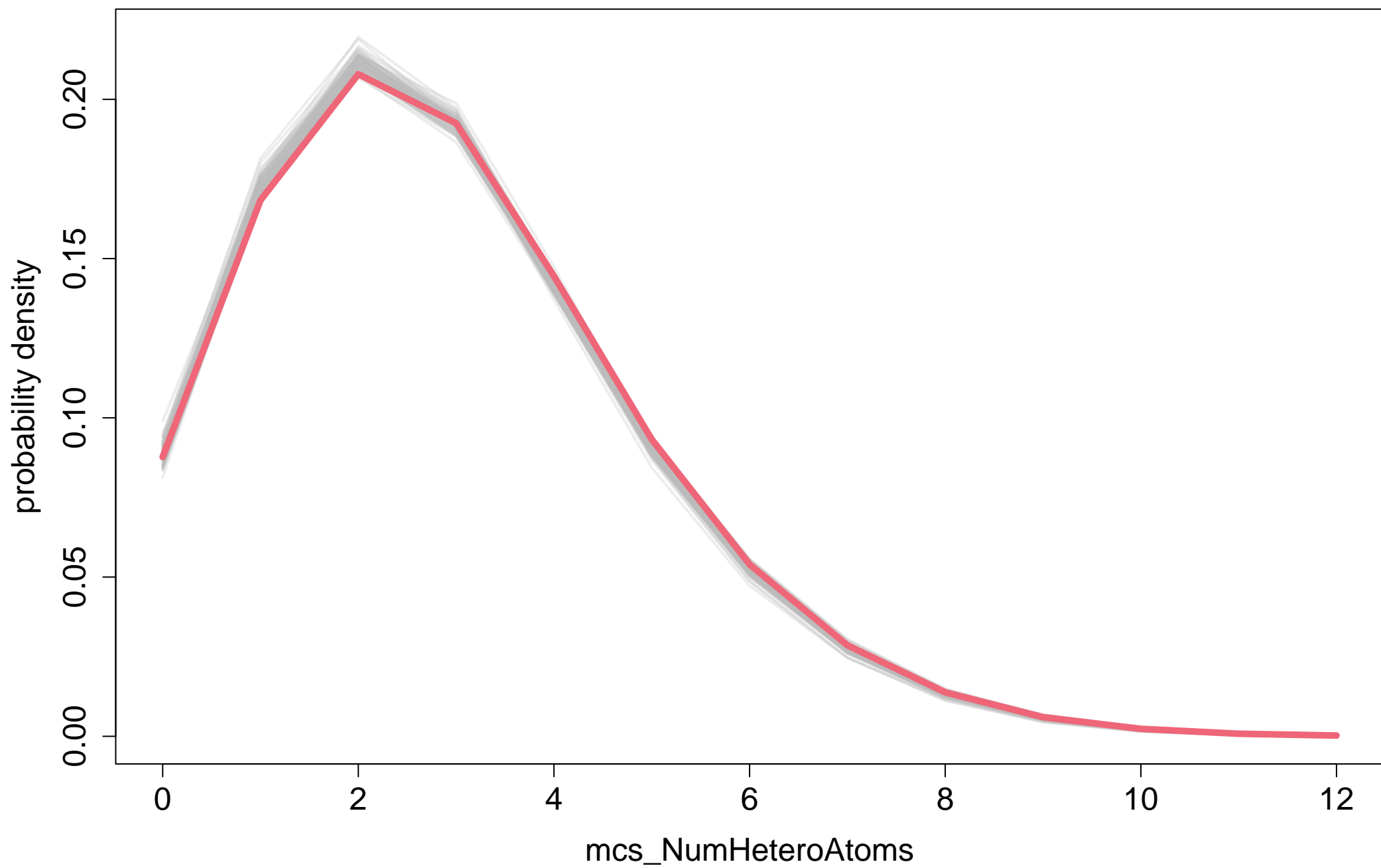
Occupied clusters: 9 of 64

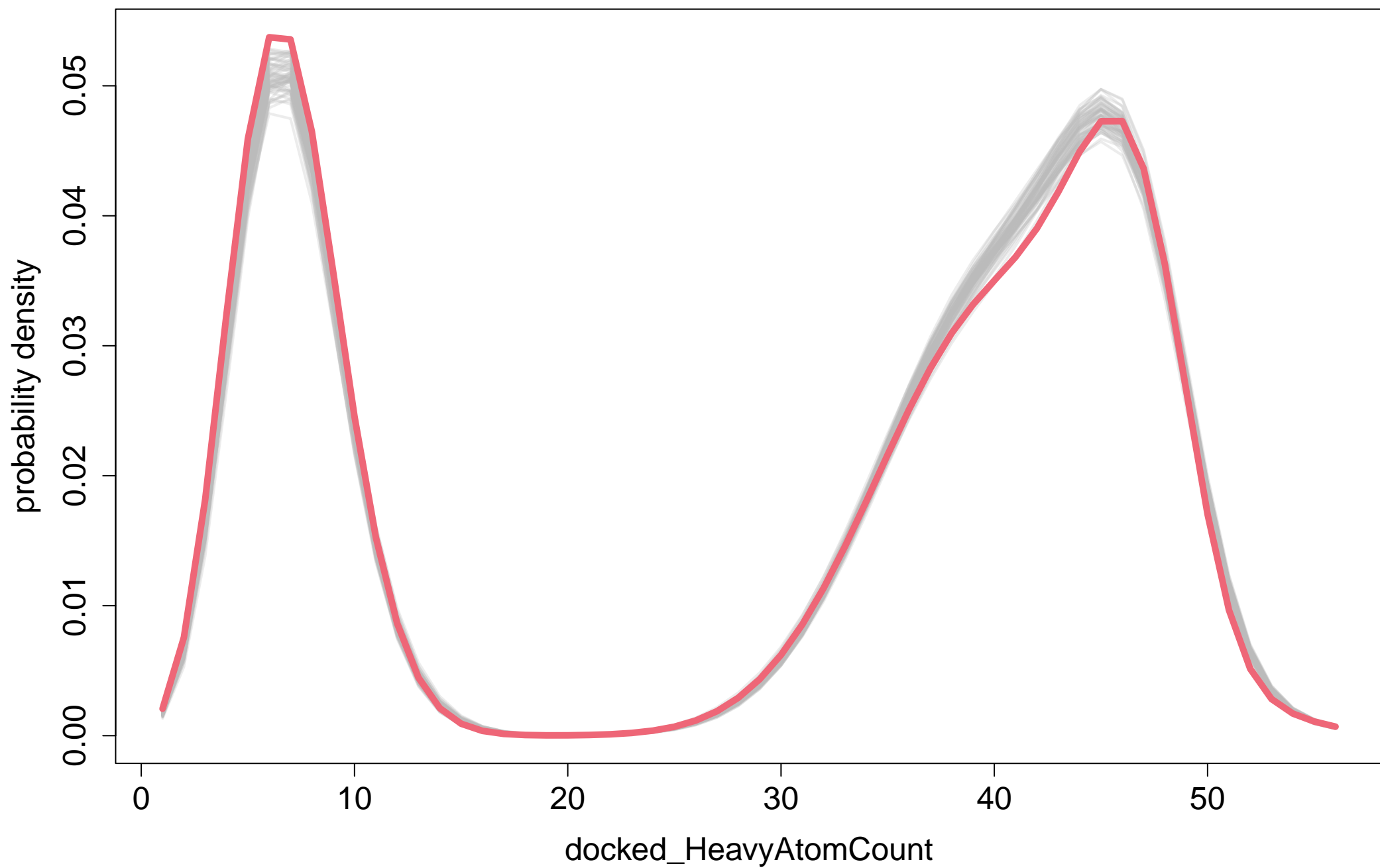
LL: -62500 +- 14.5

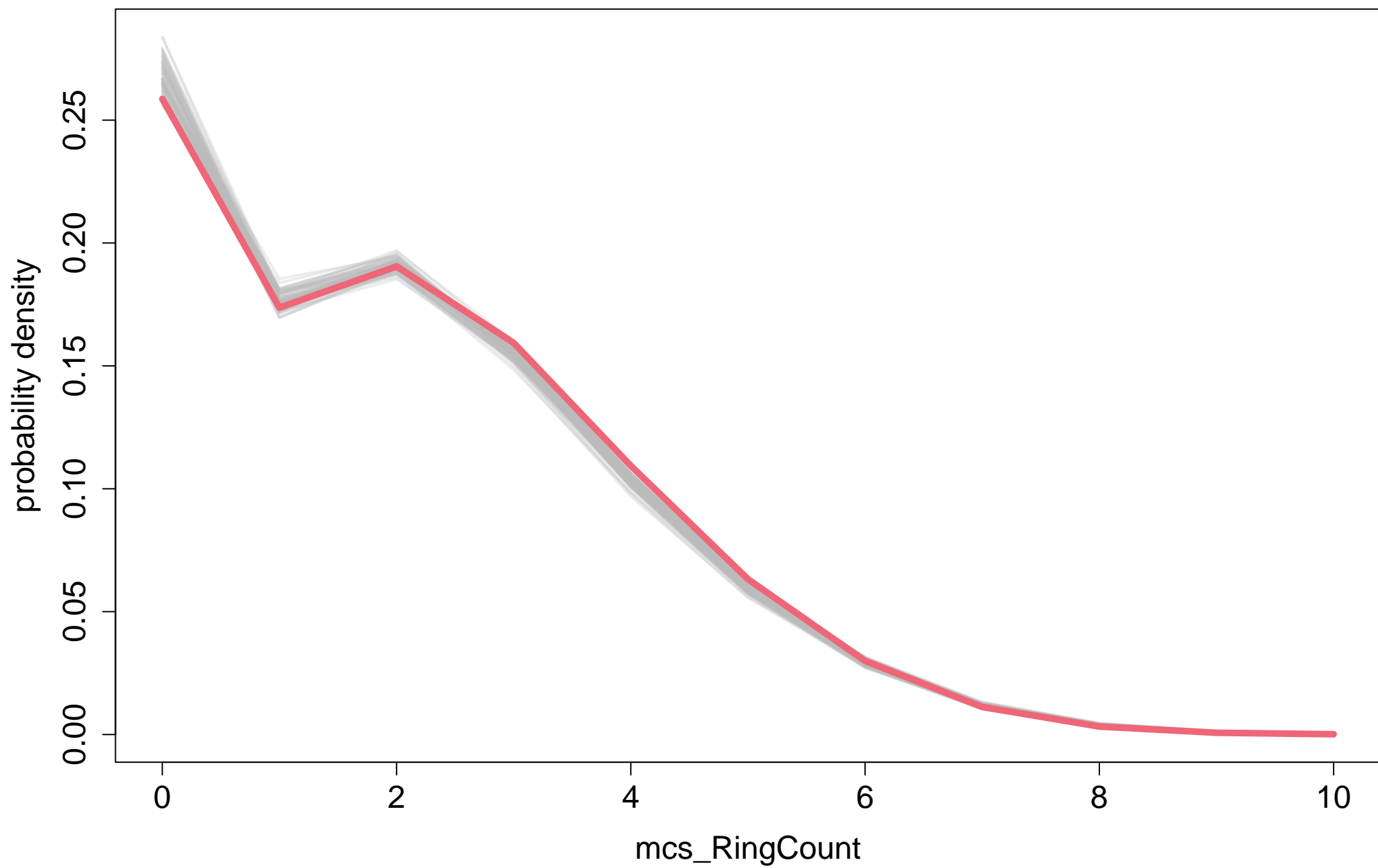


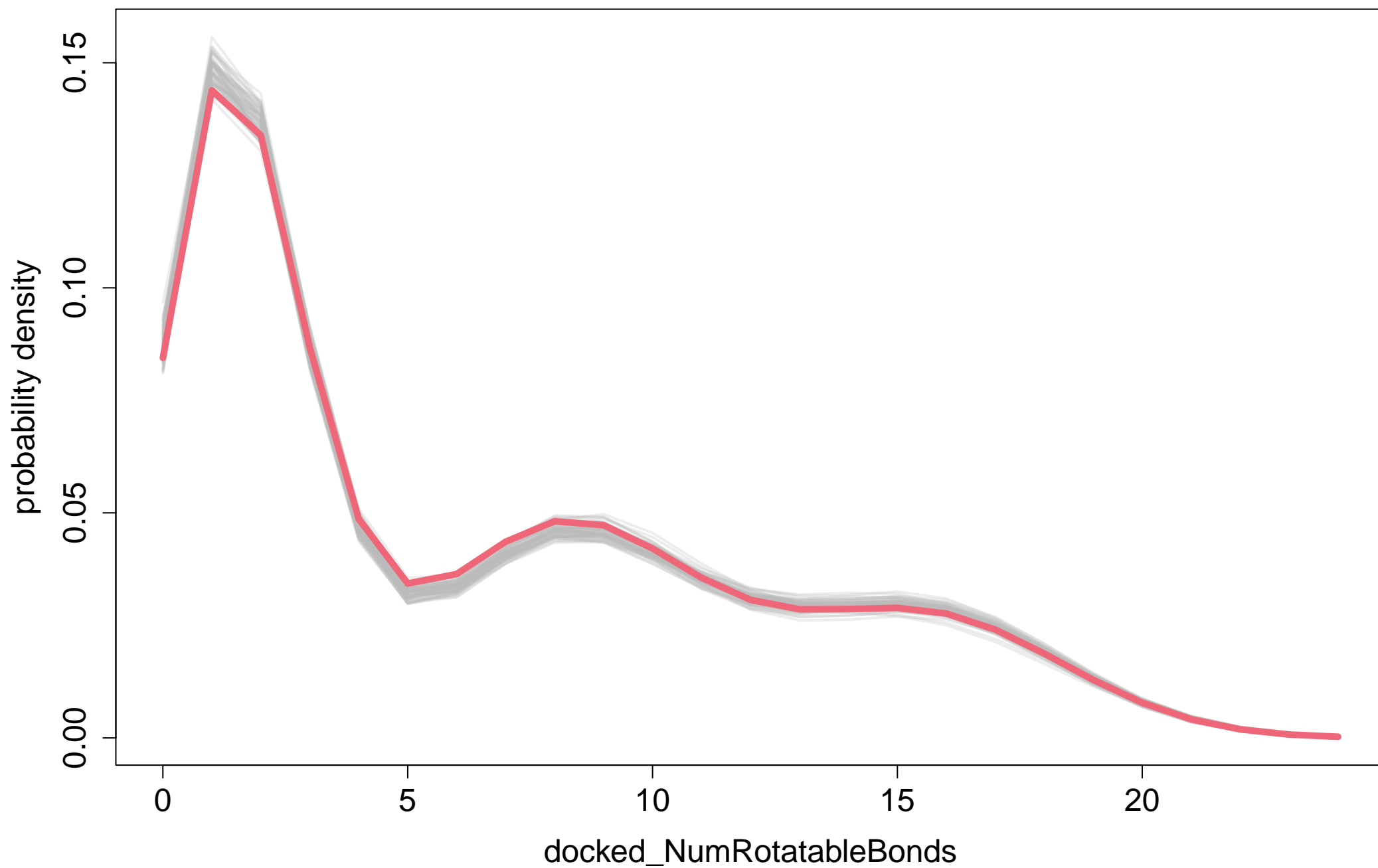




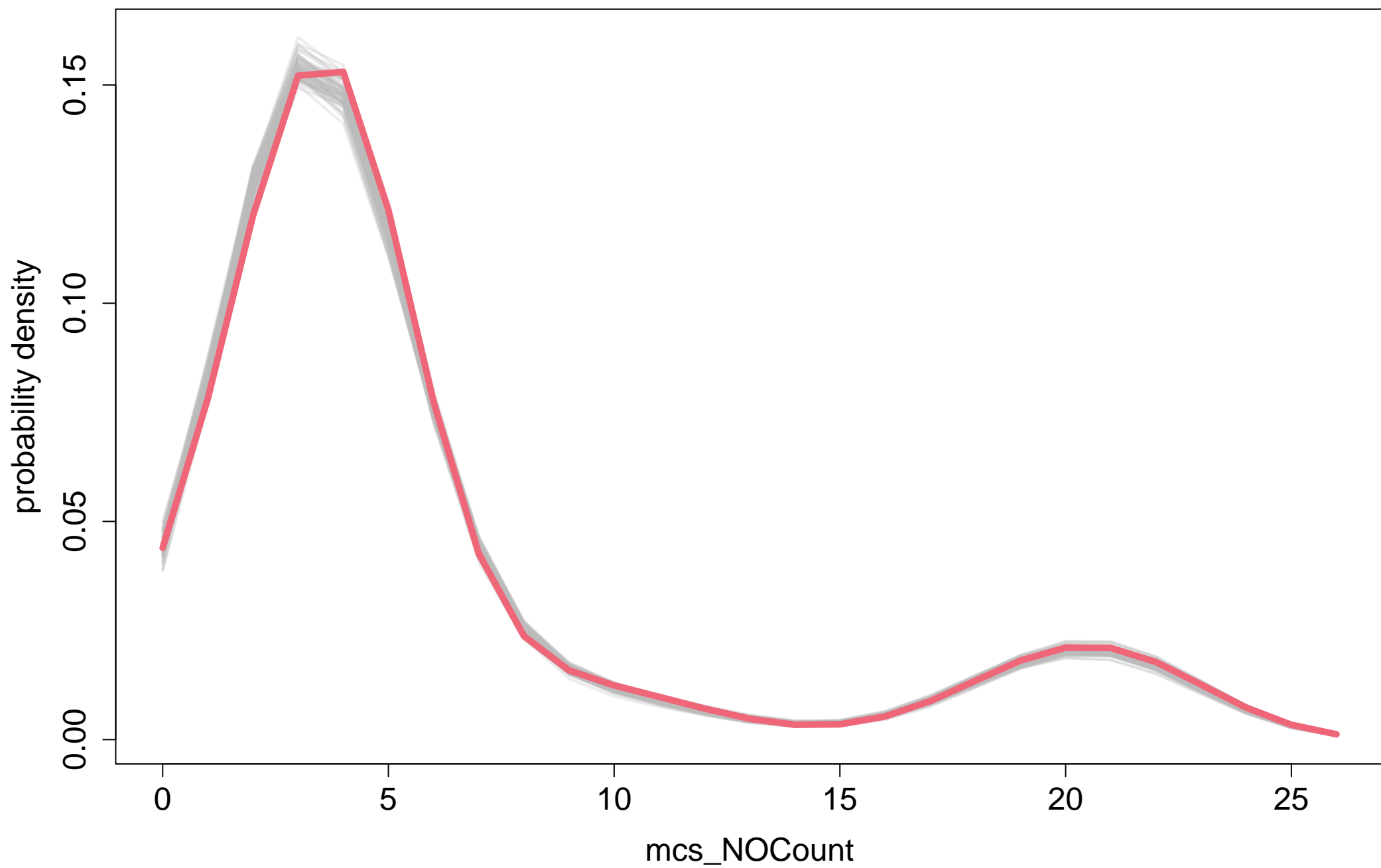


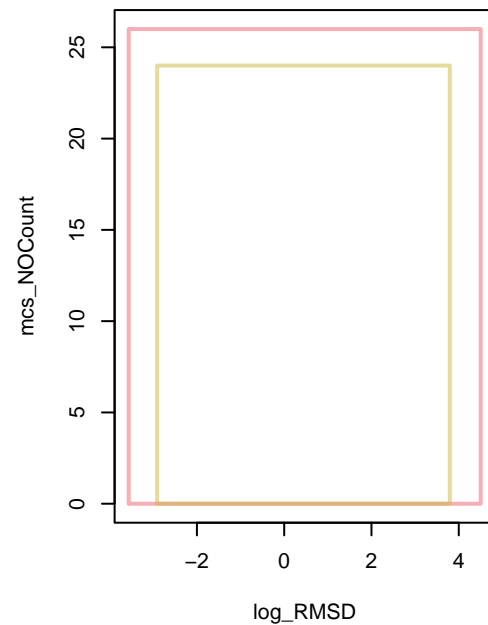
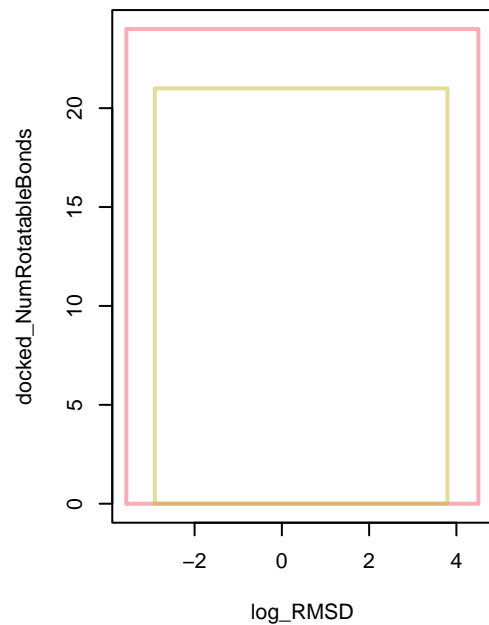
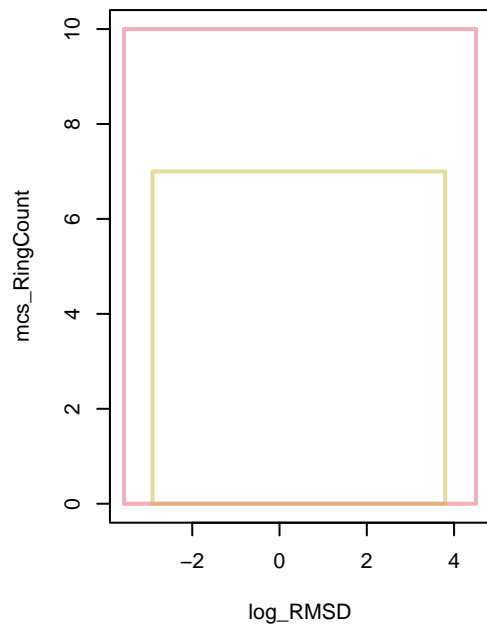
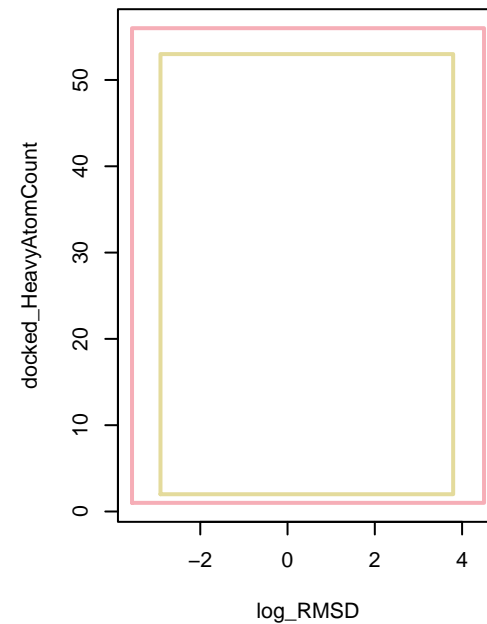
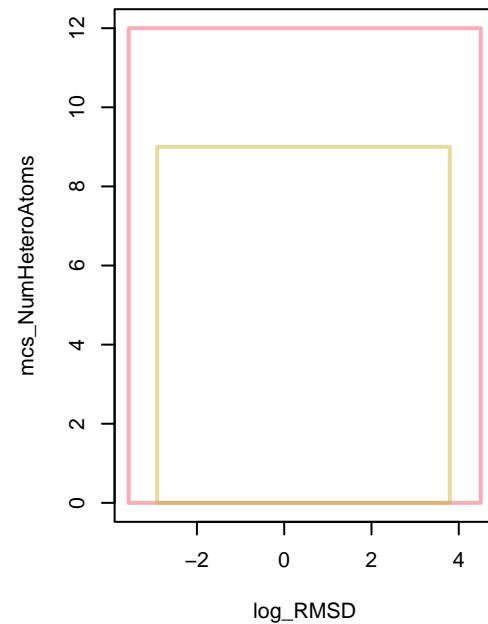
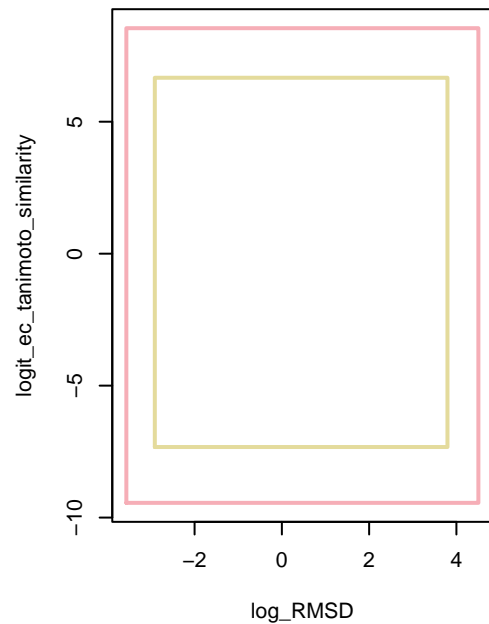
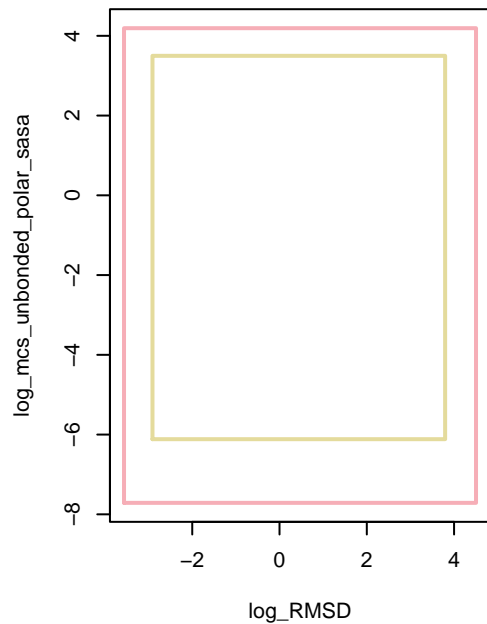




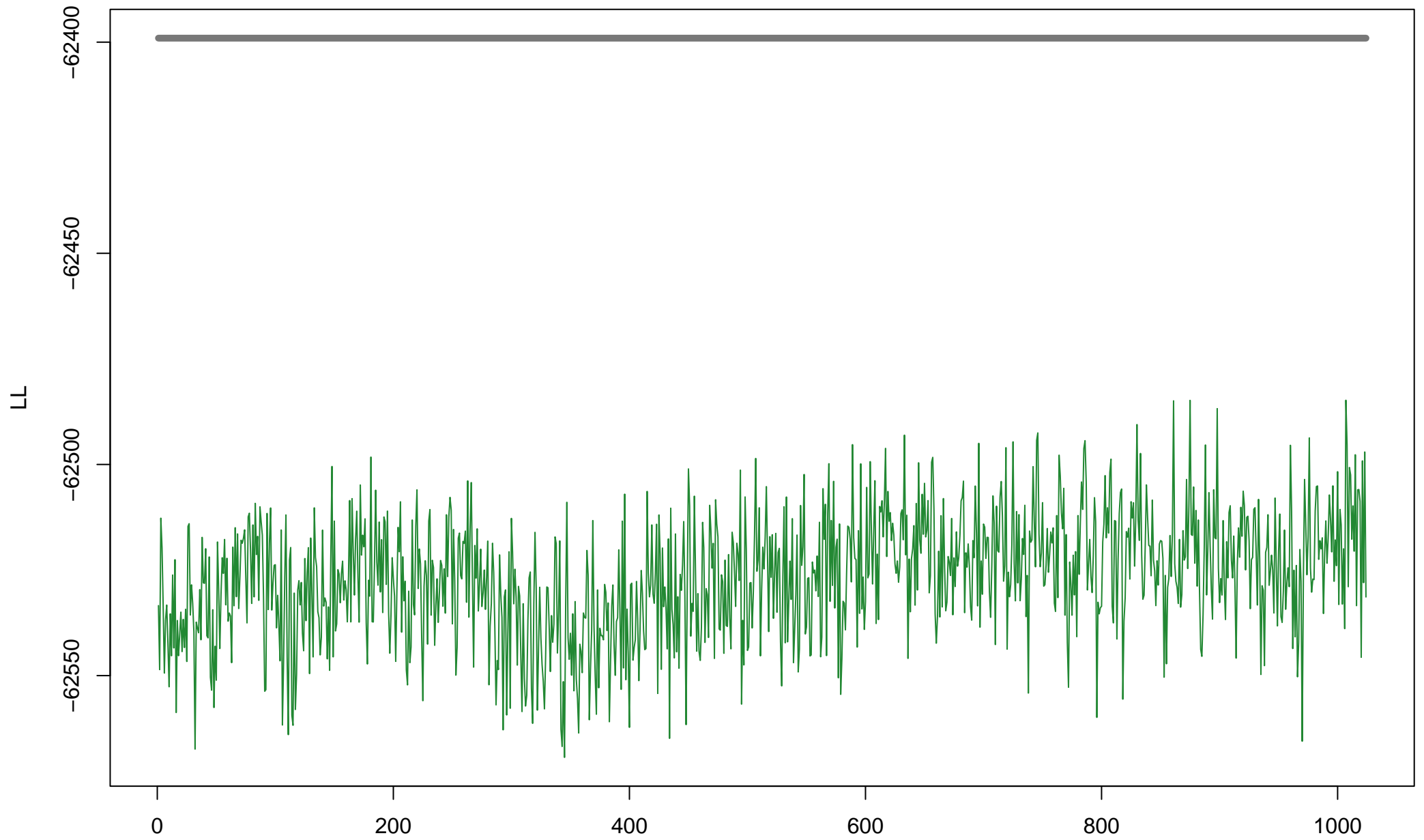






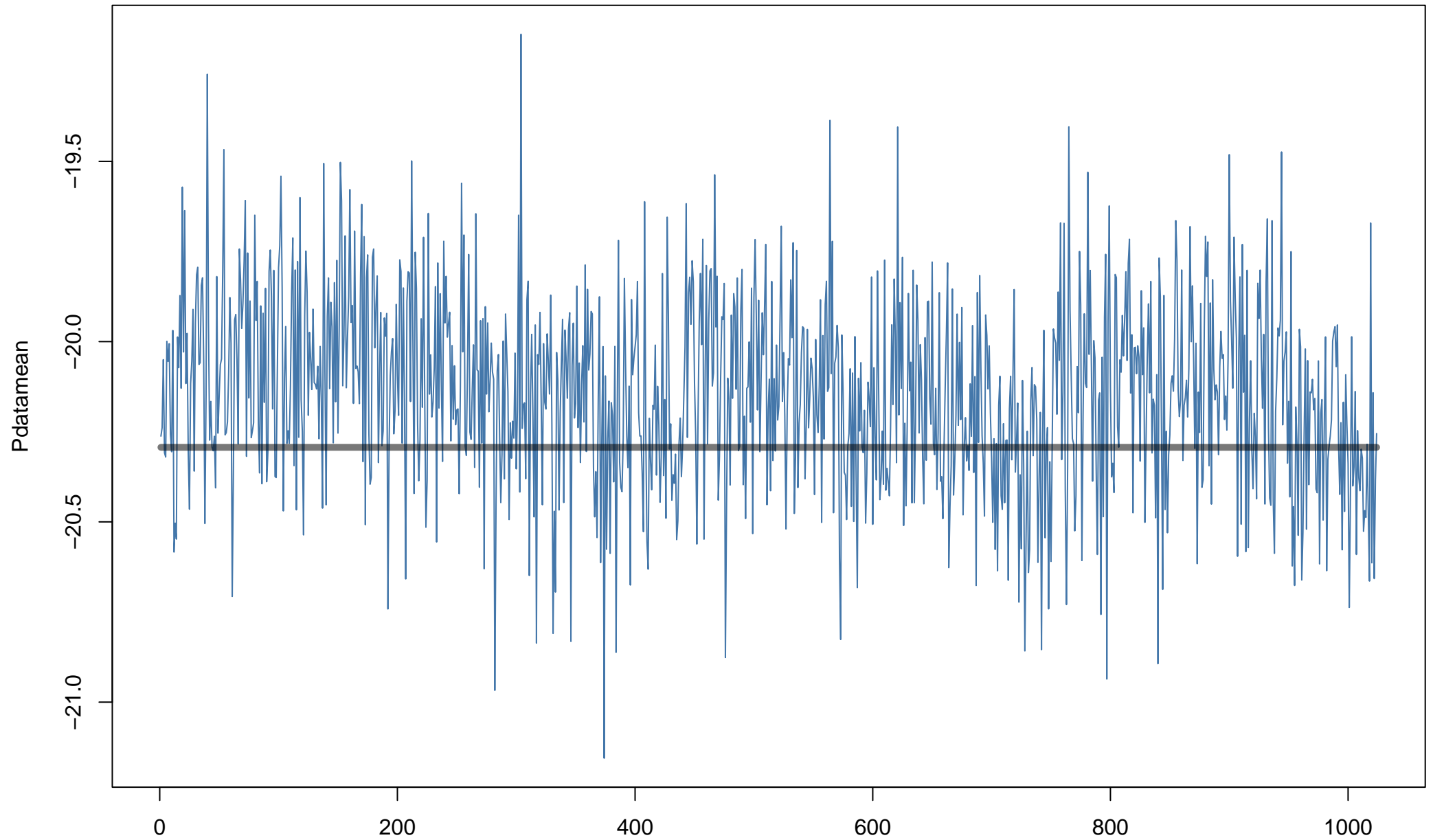


LL



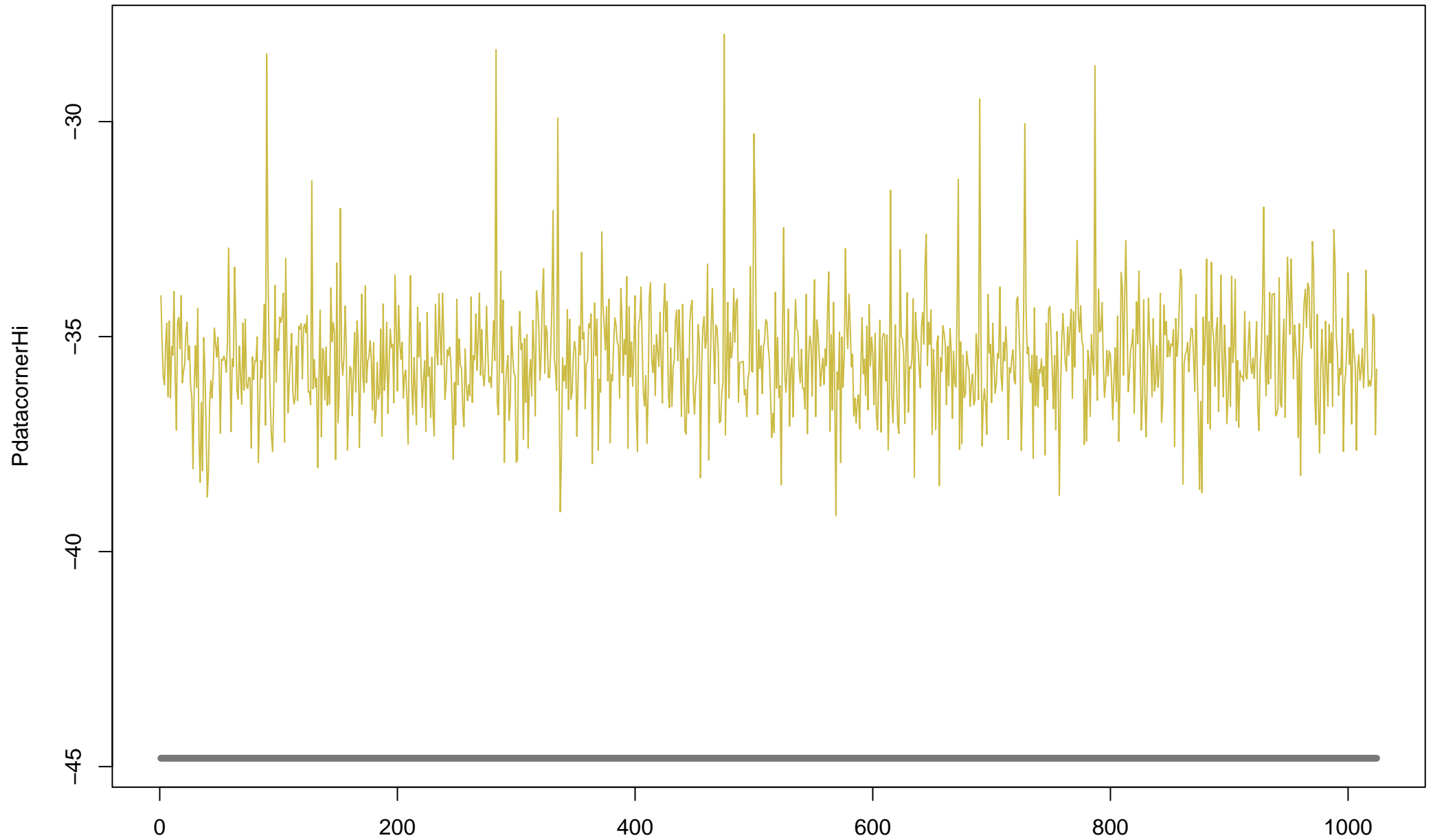
**Pdatamean**

**ESS = 2.22e-16 | BMK = 0.126 | MCSE(6.27) = 5.53 | stat: TRUE | burn: 0 | percentile: 27.5**



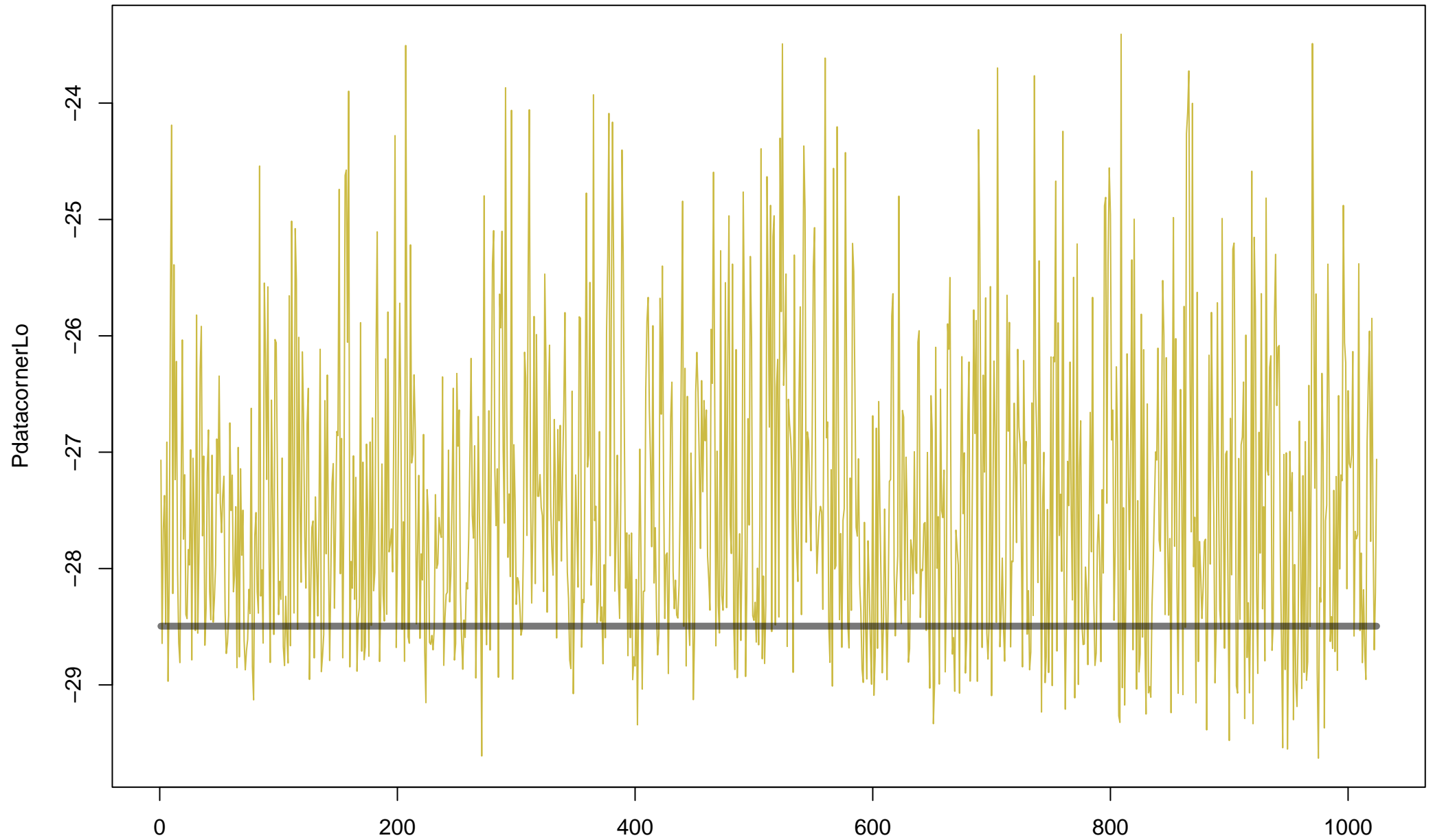
# PdatacornerHi

ESS =  $2.22\text{e-}16$  | BMK = 0.241 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 306 | percentile: 0

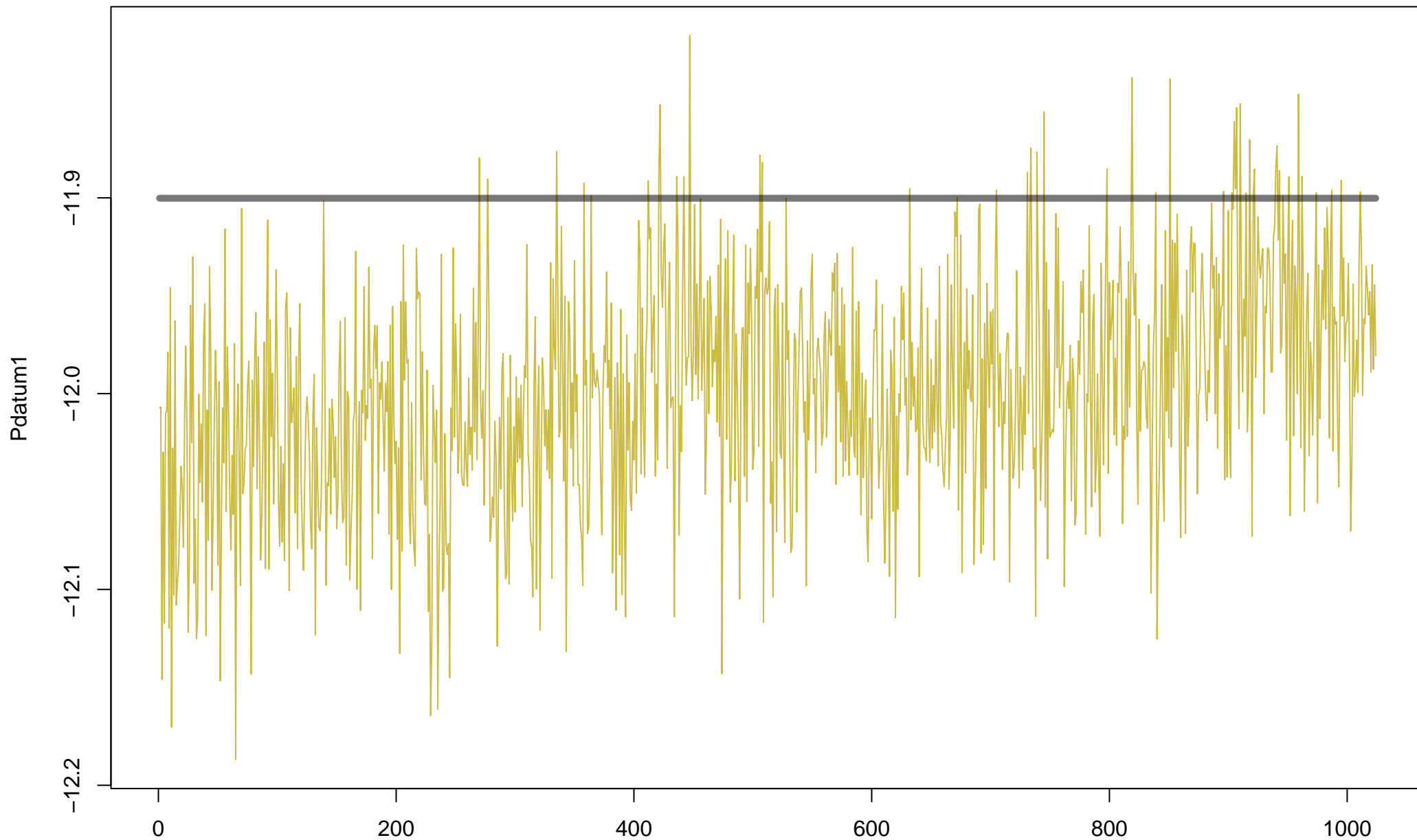


# PdatacornerLo

ESS = 2.22e-16 | BMK = 0.148 | MCSE(6.27) = 3.66 | stat: TRUE | burn: 0 | percentile: 21.7

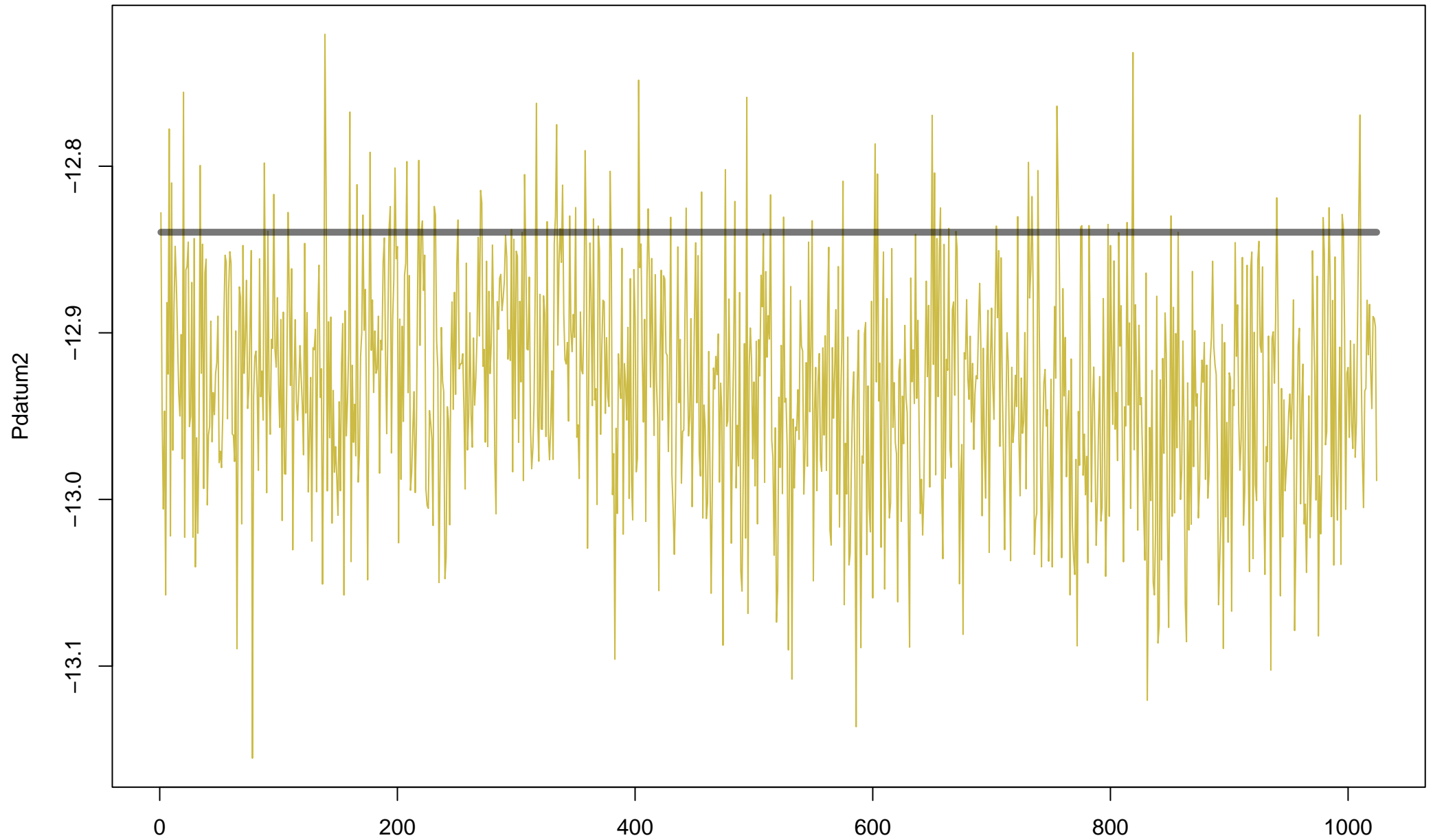


**Pdatum1**  
**ESS = 49.7 | BMK = 0.192 | MCSE(6.27) = 7.96 | stat: FALSE | burn: 0 | percentile: 95.5**



**Pdatum2**

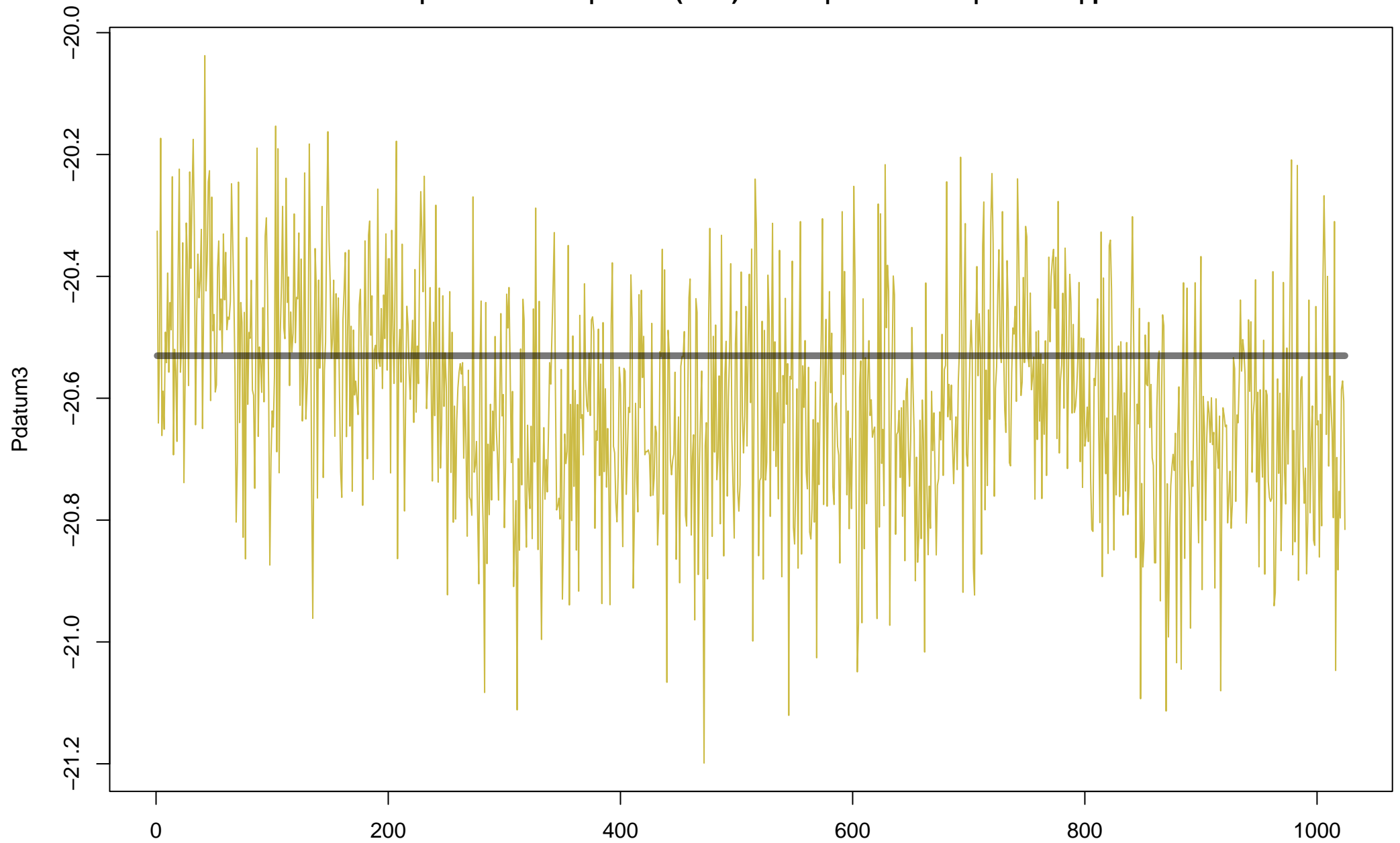
**ESS = 607 | BMK = 0.136 | MCSE(6.27) = 5.11 | stat: FALSE | burn: 0 | percentile: 92.1**



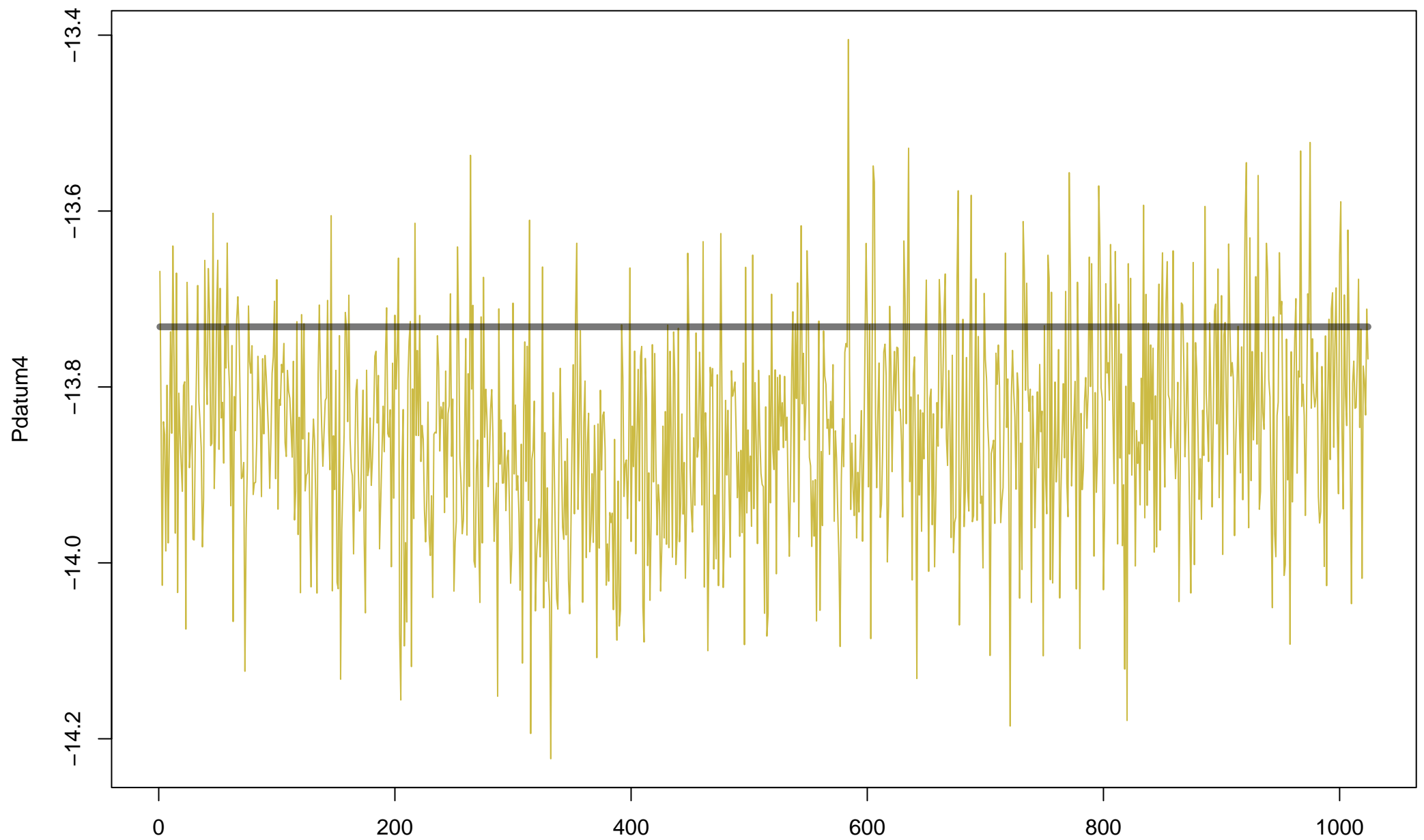


**Pdatum3**

**ESS = 2.22e-16 | BMK = 0.119 | MCSE(6.27) = 7.95 | stat: TRUE | burn: 0 | percentile: 65.8**

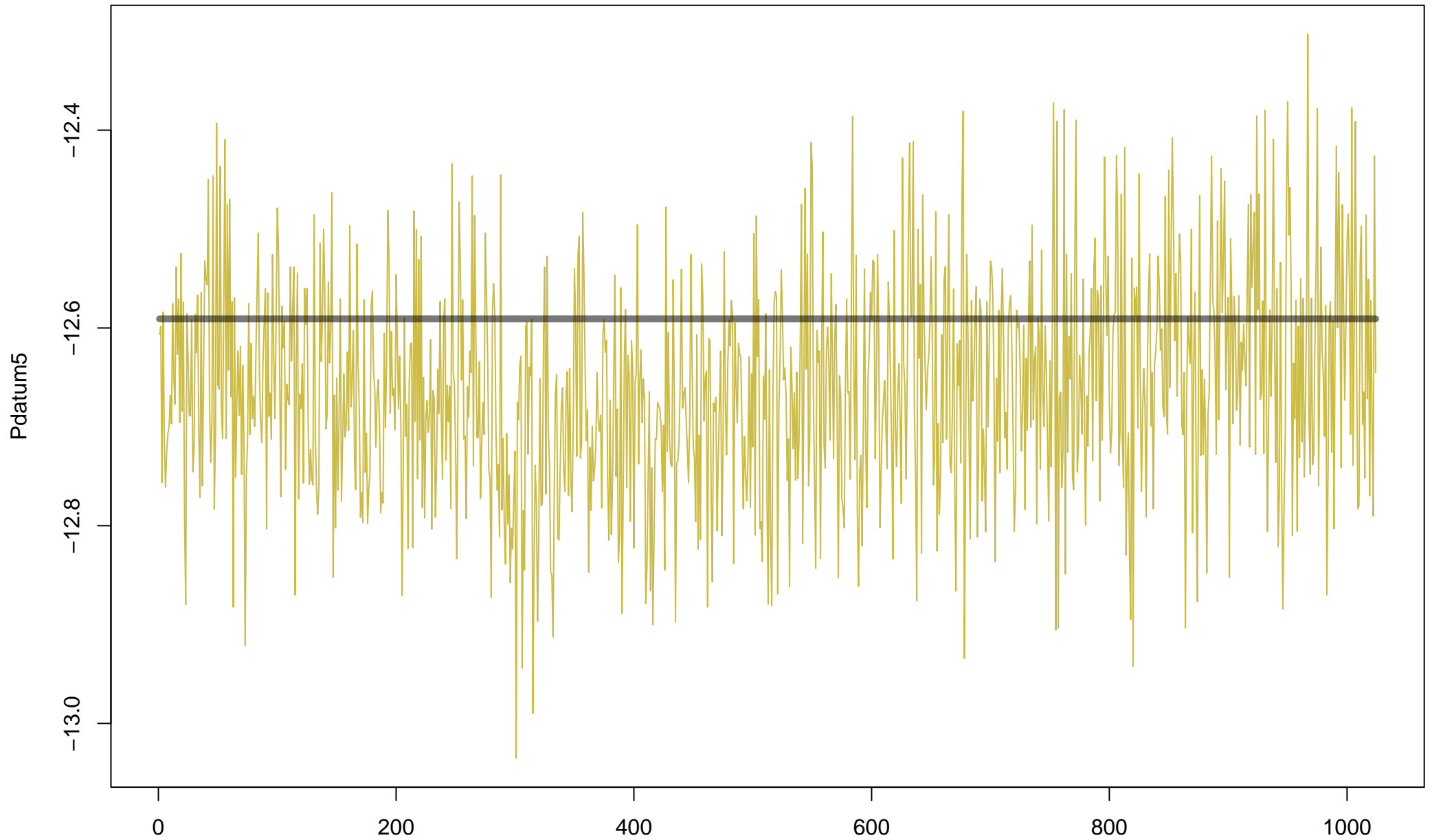


**Pdatum4**  
**ESS = 201 | BMK = 0.131 | MCSE(6.27) = 5.23 | stat: TRUE | burn: 0 | percentile: 85.1**



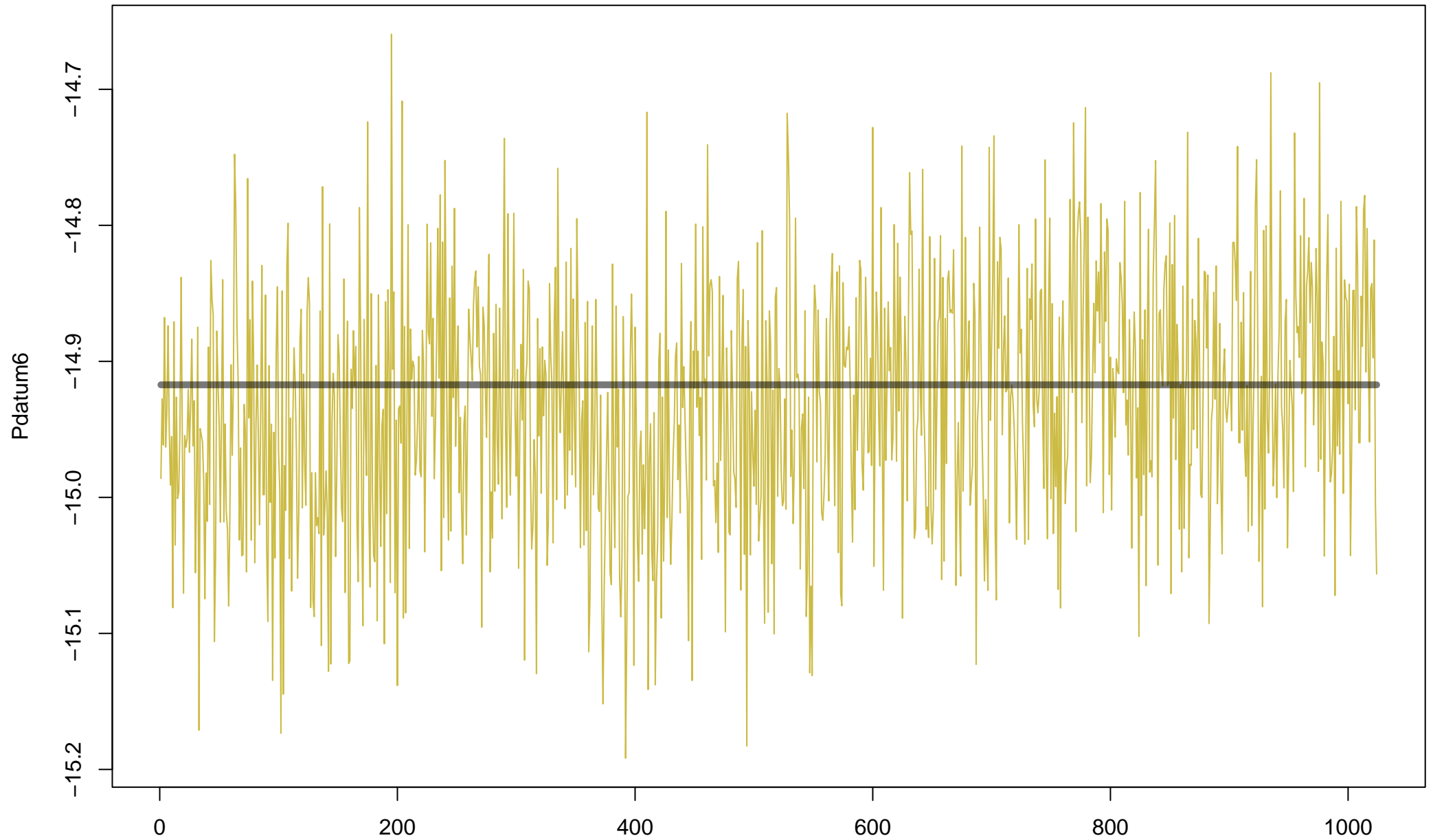
**Pdatum5**

**ESS = 422 | BMK = 0.146 | MCSE(6.27) = 5.51 | stat: TRUE | burn: 0 | percentile: 73.7**



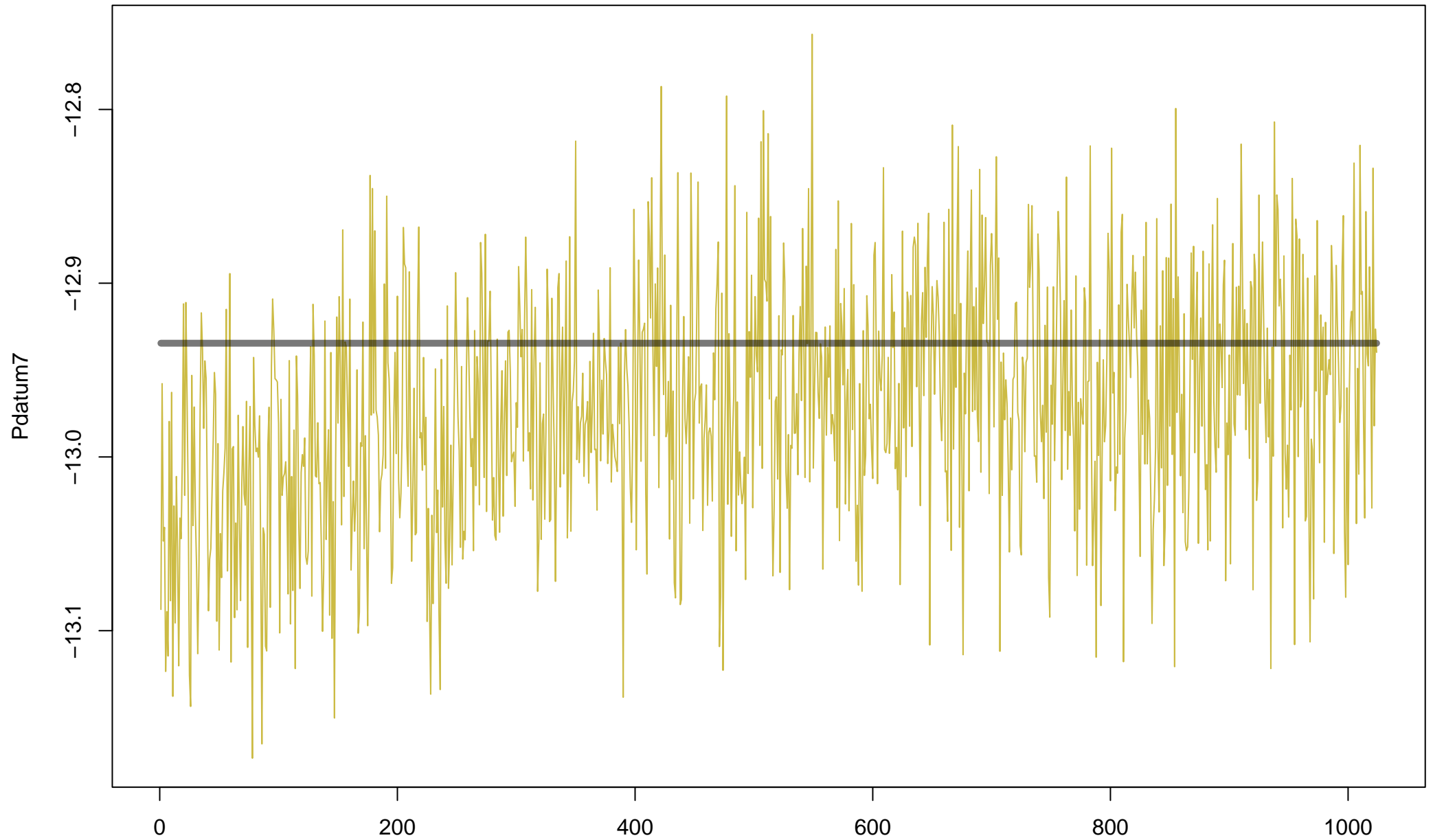
**Pdatum6**

**ESS = 268 | BMK = 0.151 | MCSE(6.27) = 5.65 | stat: FALSE | burn: 0 | percentile: 55.2**



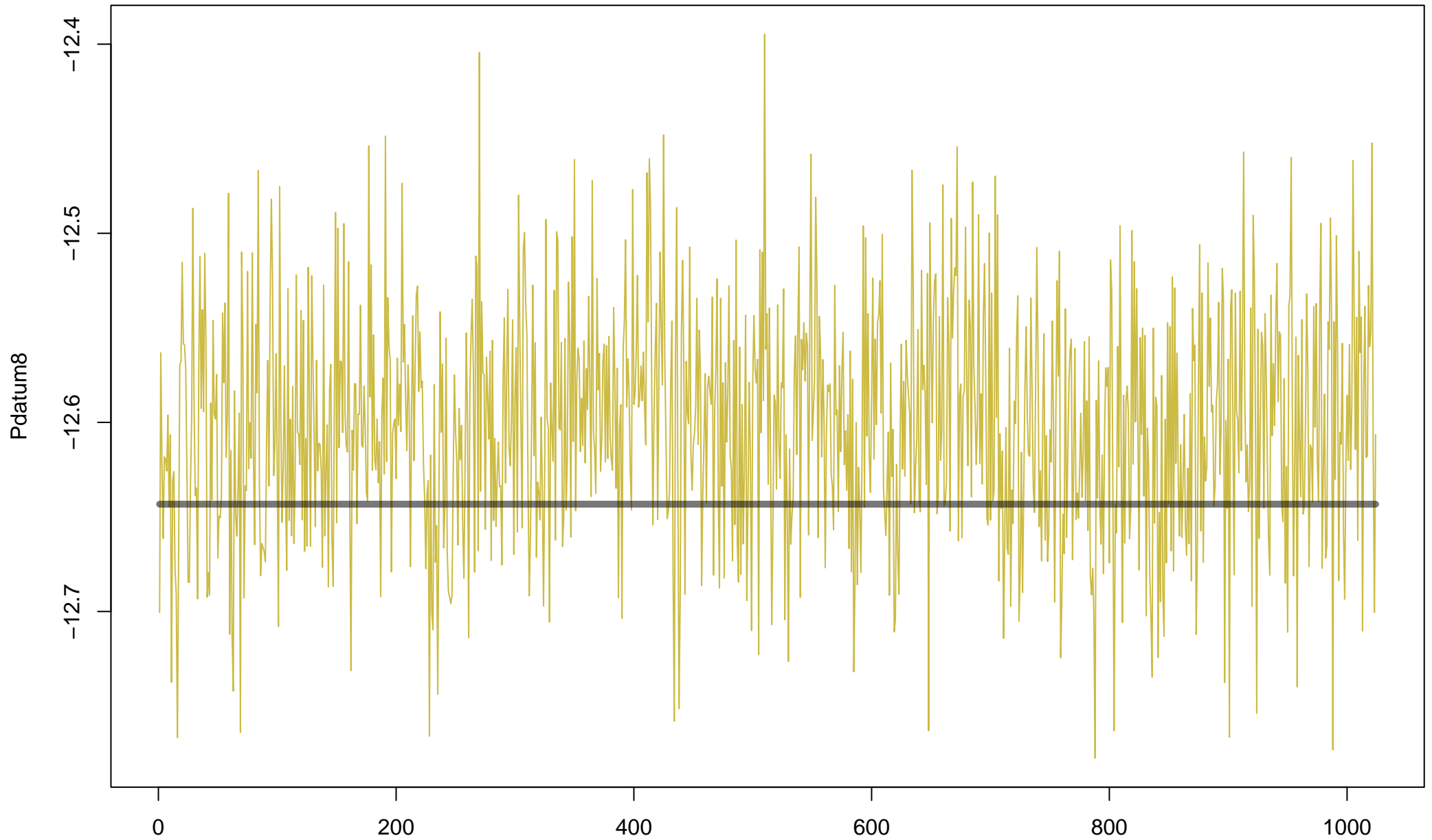
**Pdatum7**

**ESS = 187 | BMK = 0.172 | MCSE(6.27) = 6.92 | stat: FALSE | burn: 0 | percentile: 70.6**



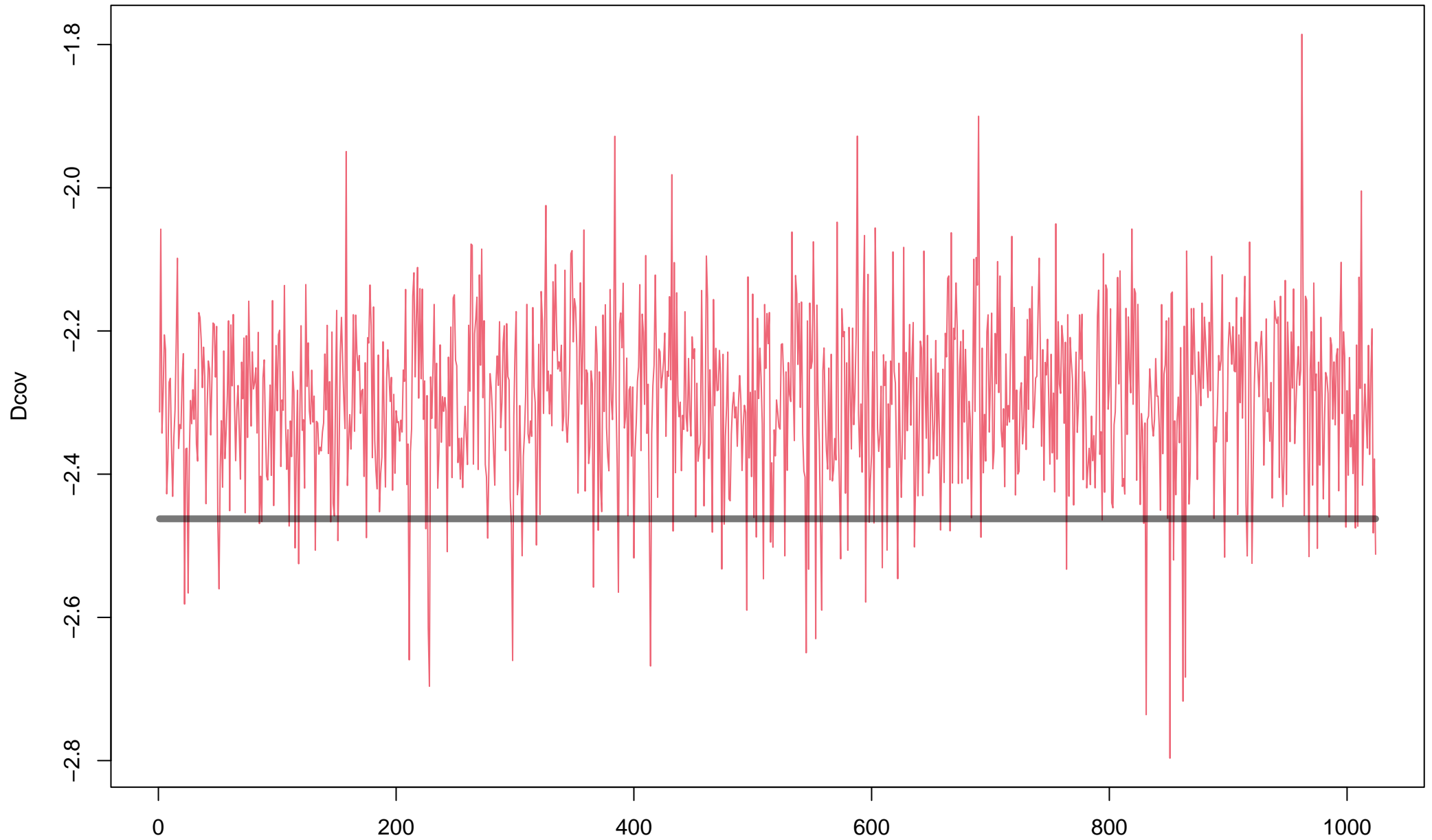
**Pdatum8**

**ESS = 443 | BMK = 0.0598 | MCSE(6.27) = 4.63 | stat: TRUE | burn: 0 | percentile: 24.7**

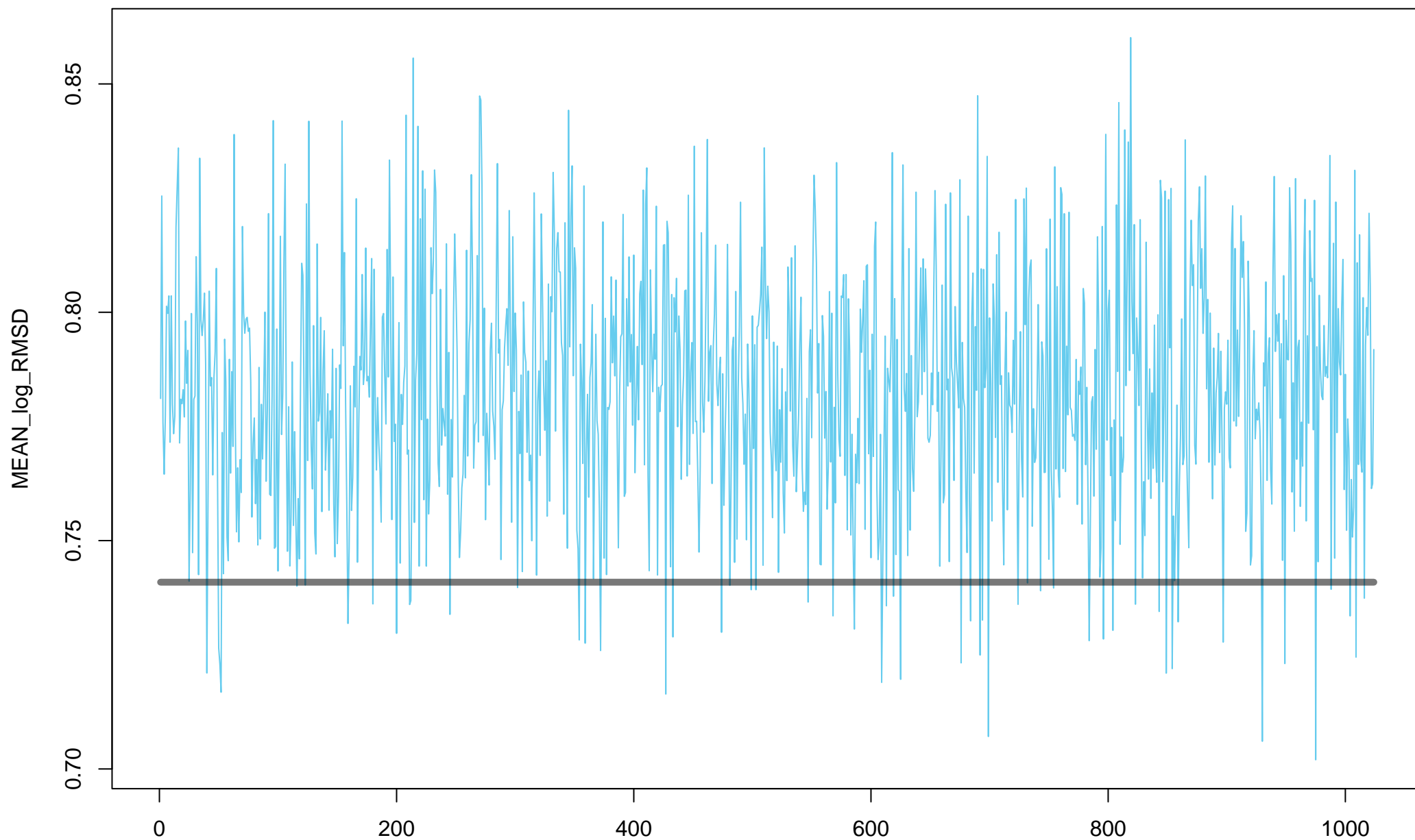


Dcov

ESS = 898 | BMK = 0.0759 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0 | percentile: 92.9

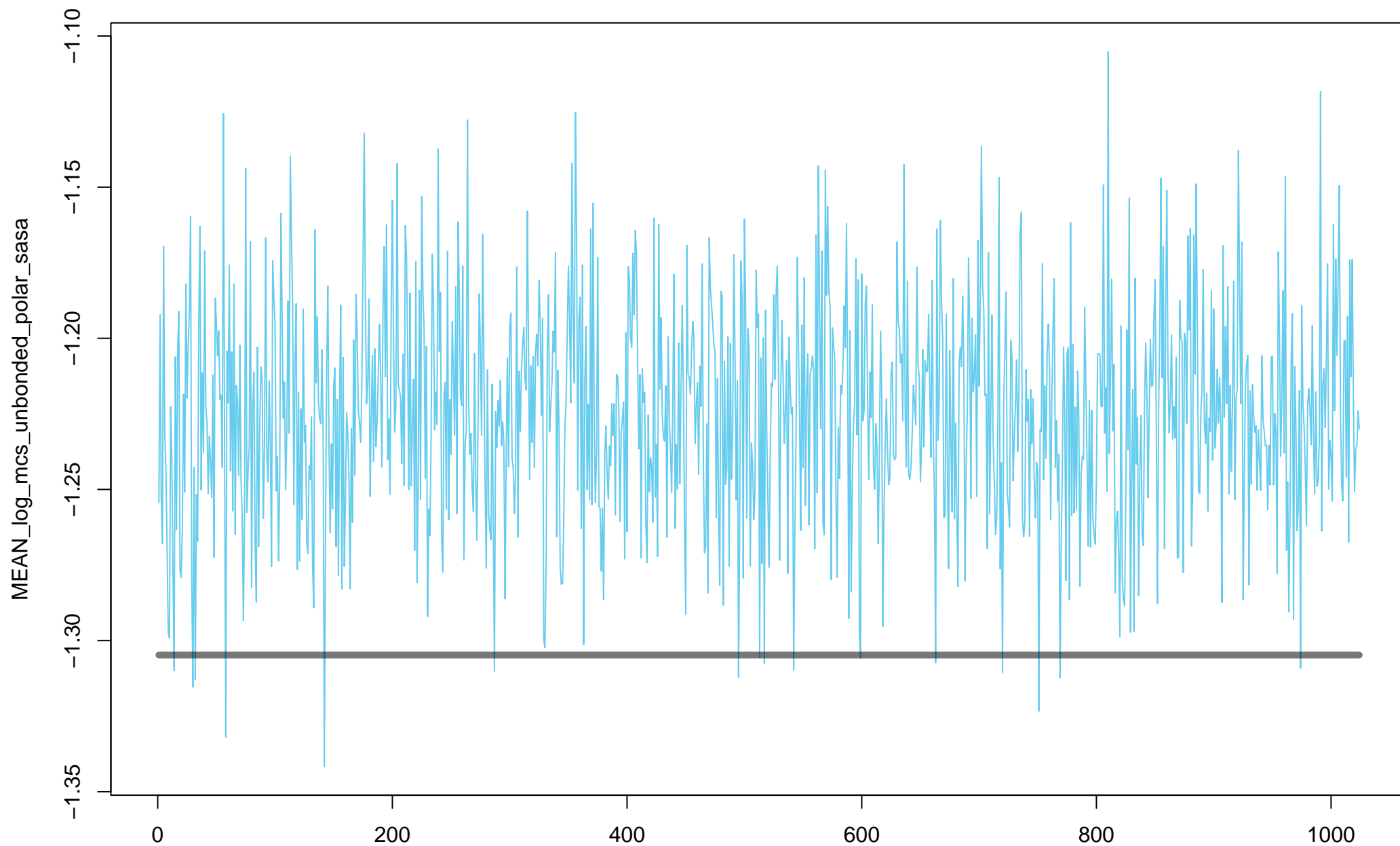


**MEAN\_log\_RMSD**  
**ESS = 951 | BMK = 0.0551 | MCSE(6.27) = 3.55 | stat: TRUE | burn: 0 | percentile: 5.27**

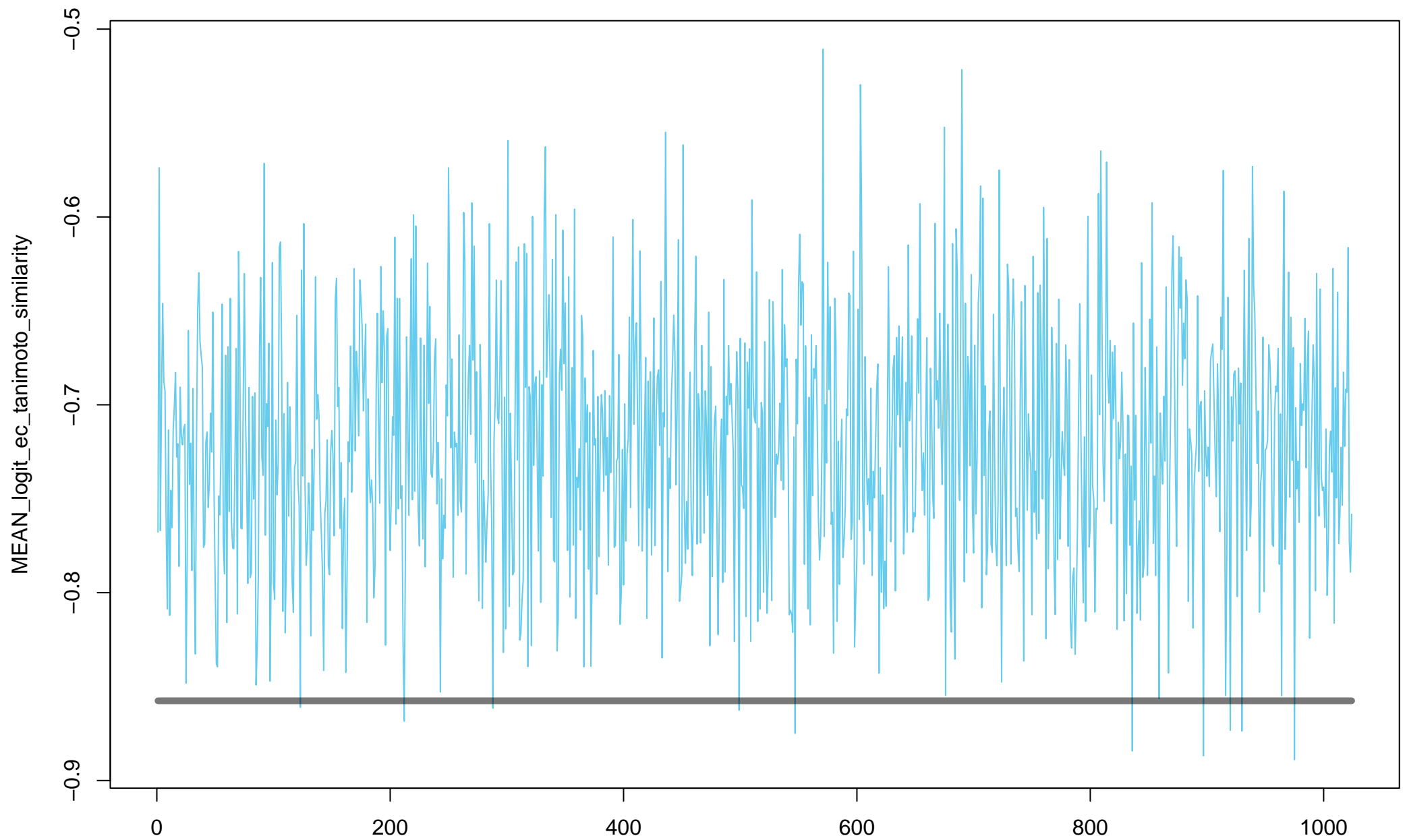




**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 829 | BMK = 0.0519 | MCSE(6.27) = 3.82 | stat: TRUE | burn: 0 | percentile: 1.56**

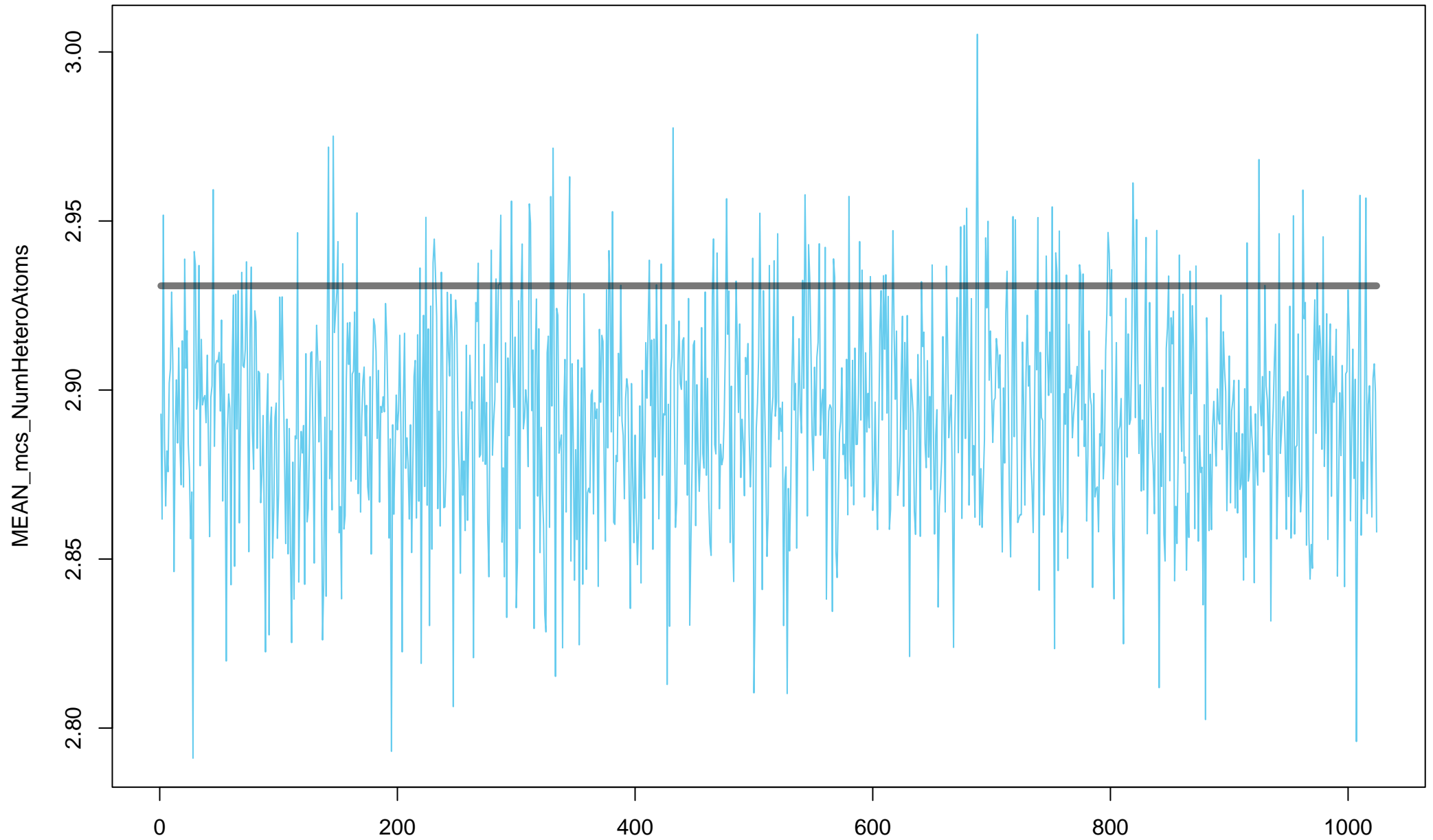


**MEAN\_logit\_ec\_tanimoto\_similarity**  
**ESS = 1020 | BMK = 0.0444 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | percentile: 0.977**



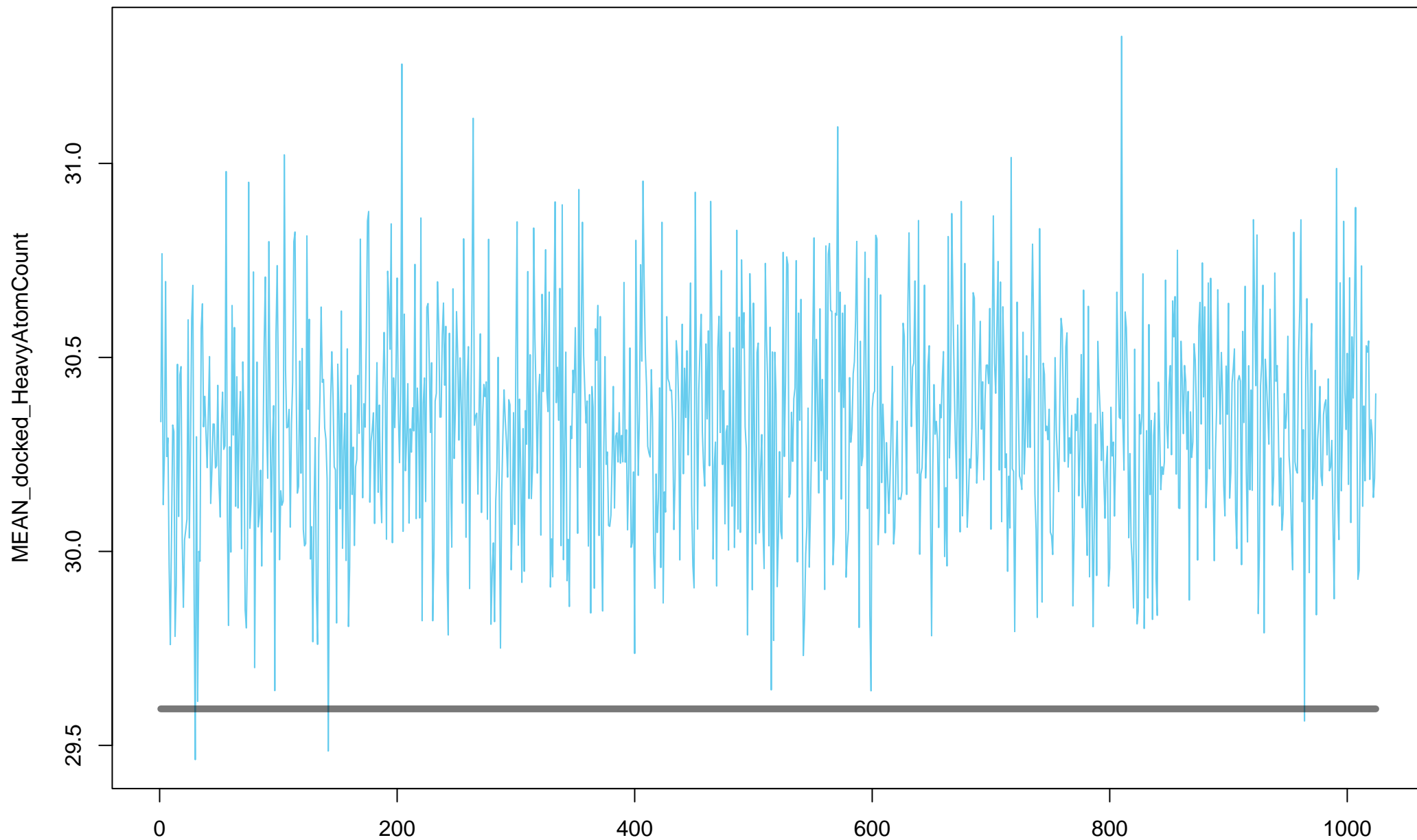
# MEAN\_mcs\_NumHeteroAtoms

ESS = 1020 | BMK = 0.0768 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0 | percentile: 89.3



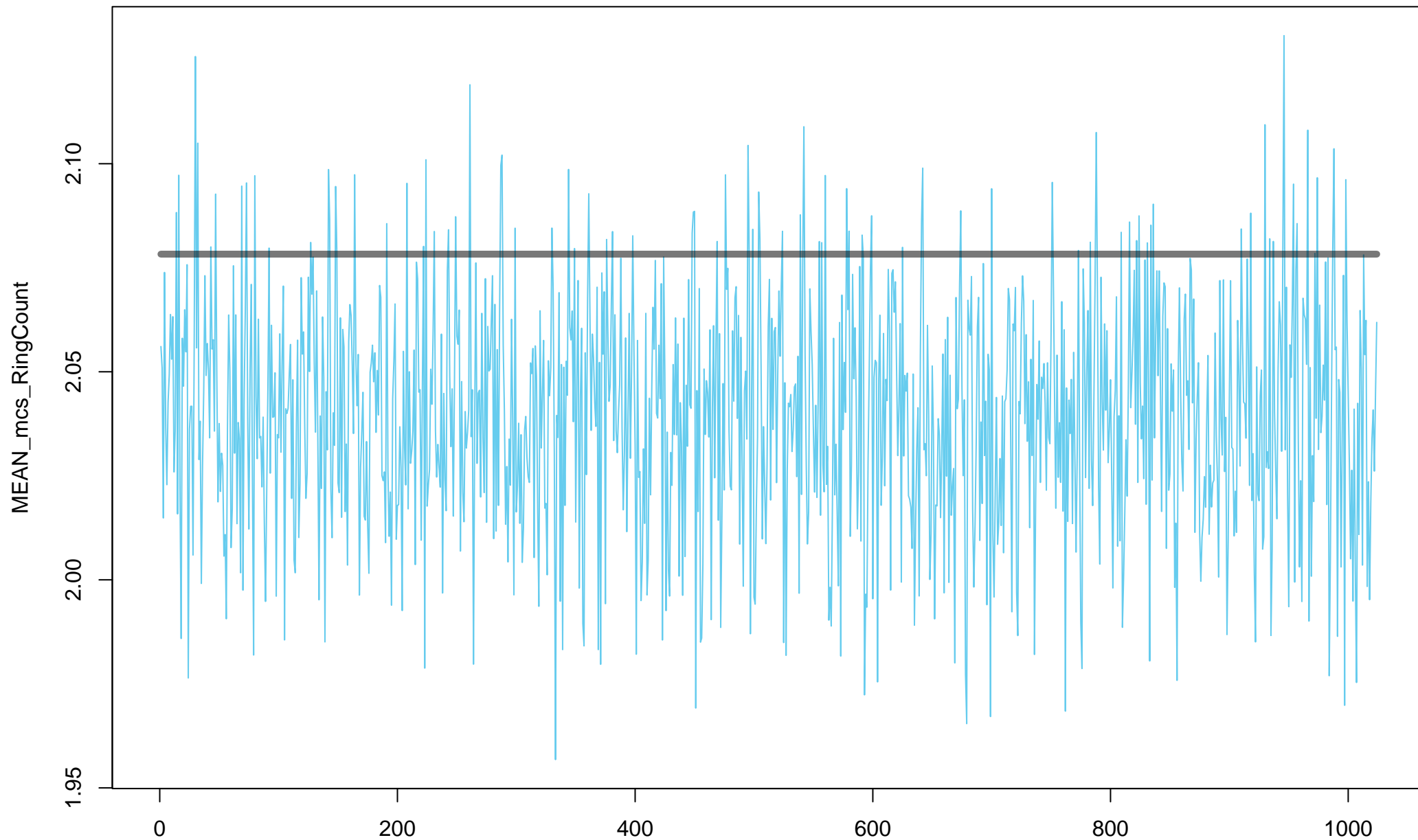
# MEAN\_docked\_HeavyAtomCount

ESS = 924 | BMK = 0.0553 | MCSE(6.27) = 3.62 | stat: FALSE | burn: 0 | percentile: 0.293

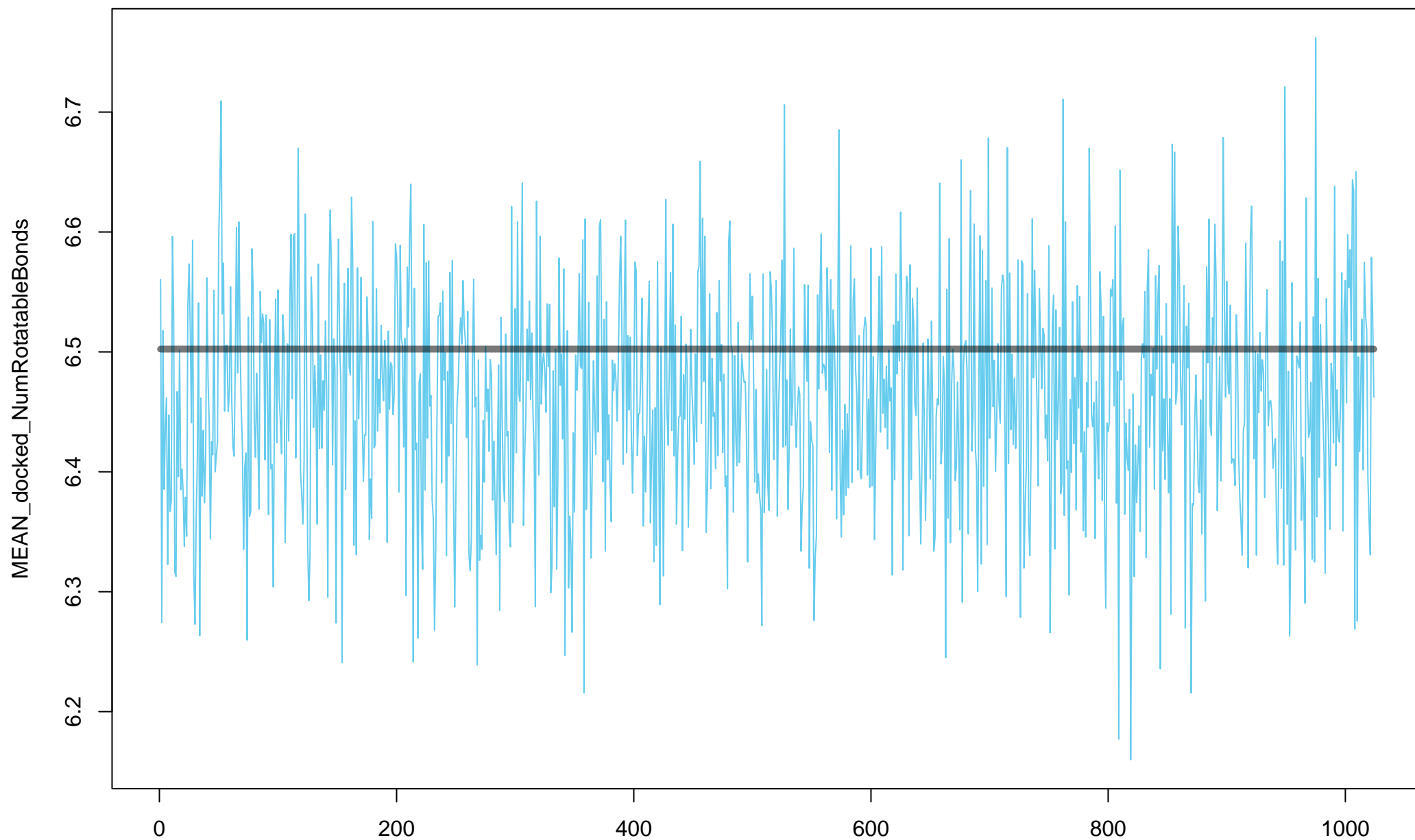


# MEAN\_mcs\_RingCount

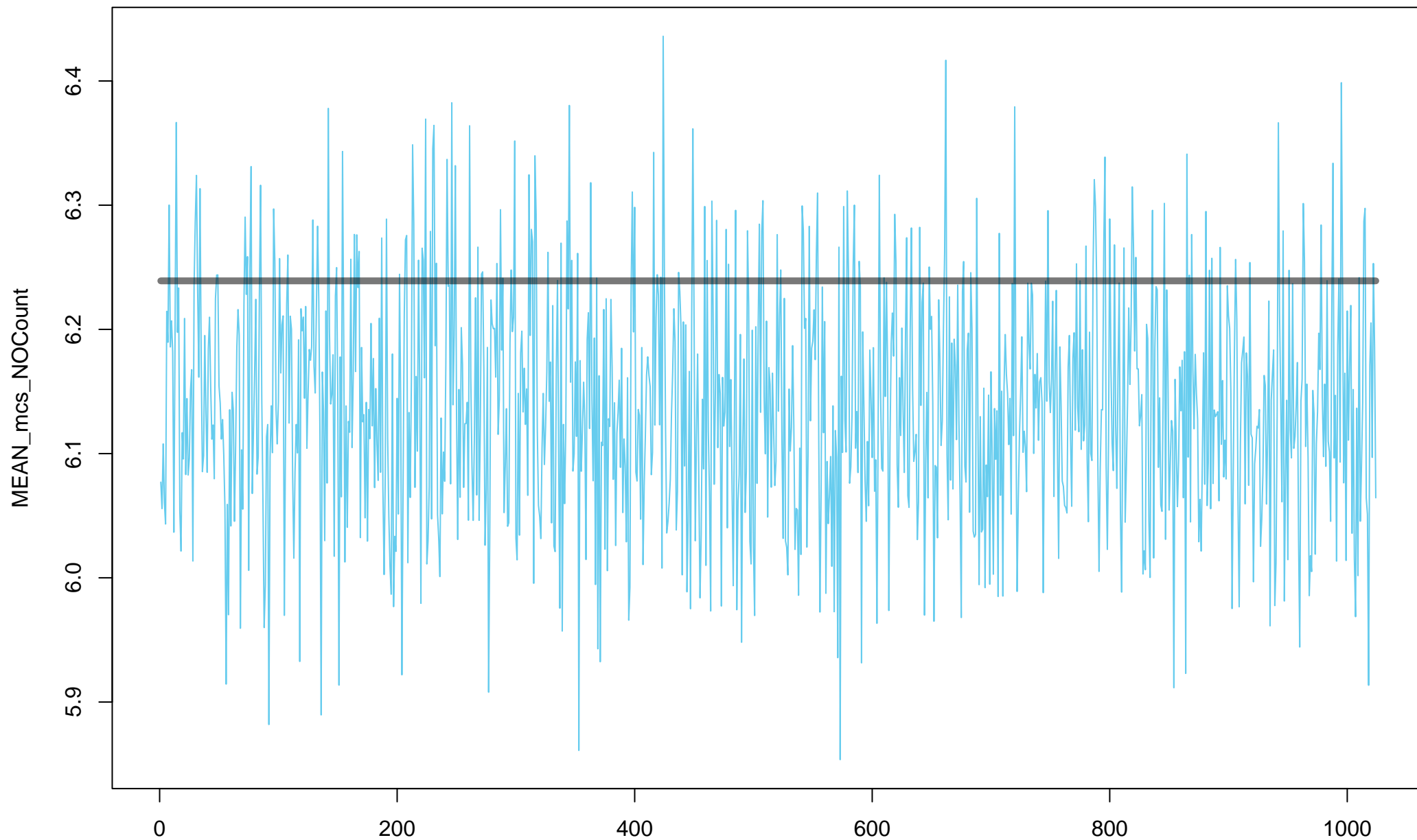
ESS = 1020 | BMK = 0.0496 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | percentile: 91.8



**MEAN\_docked\_NumRotatableBonds**  
**ESS = 963 | BMK = 0.0622 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0 | percentile: 68.2**

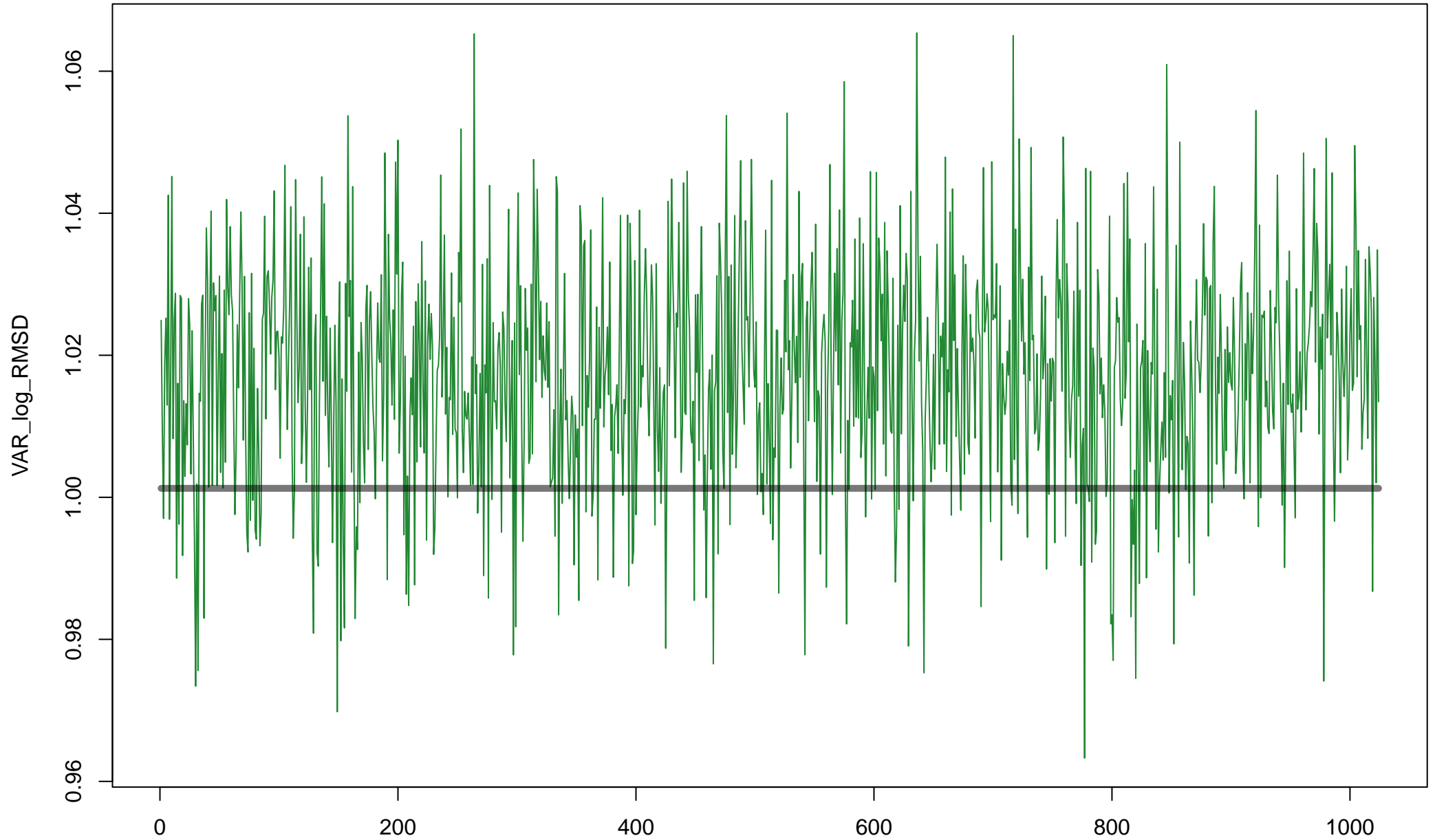


**MEAN\_mcs\_NOCount**  
**ESS = 920 | BMK = 0.0675 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | percentile: 84.9**



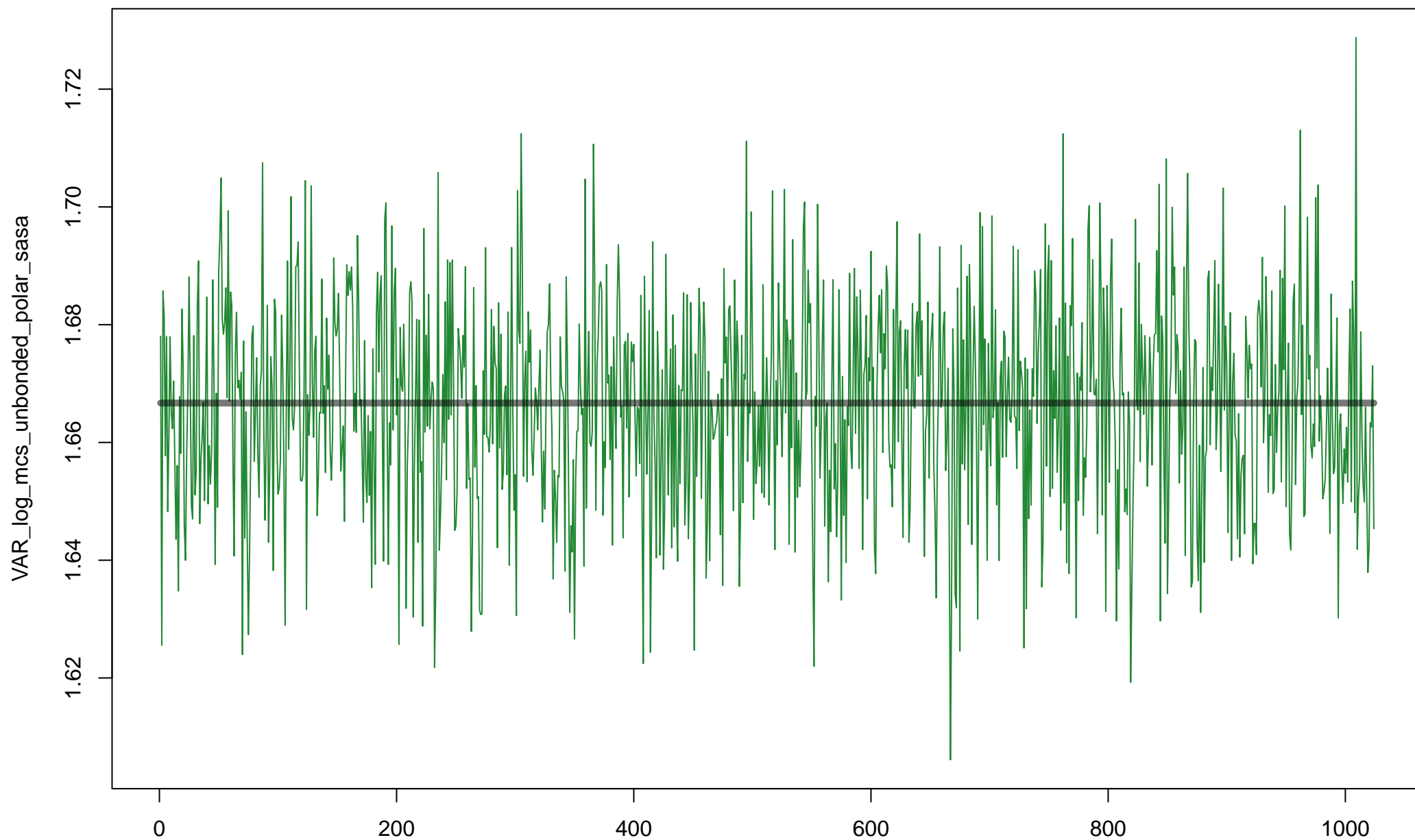
# VAR\_log\_RMSD

ESS = 1020 | BMK = 0.0588 | MCSE(6.27) = 3.38 | stat: TRUE | burn: 0 | percentile: 14.6



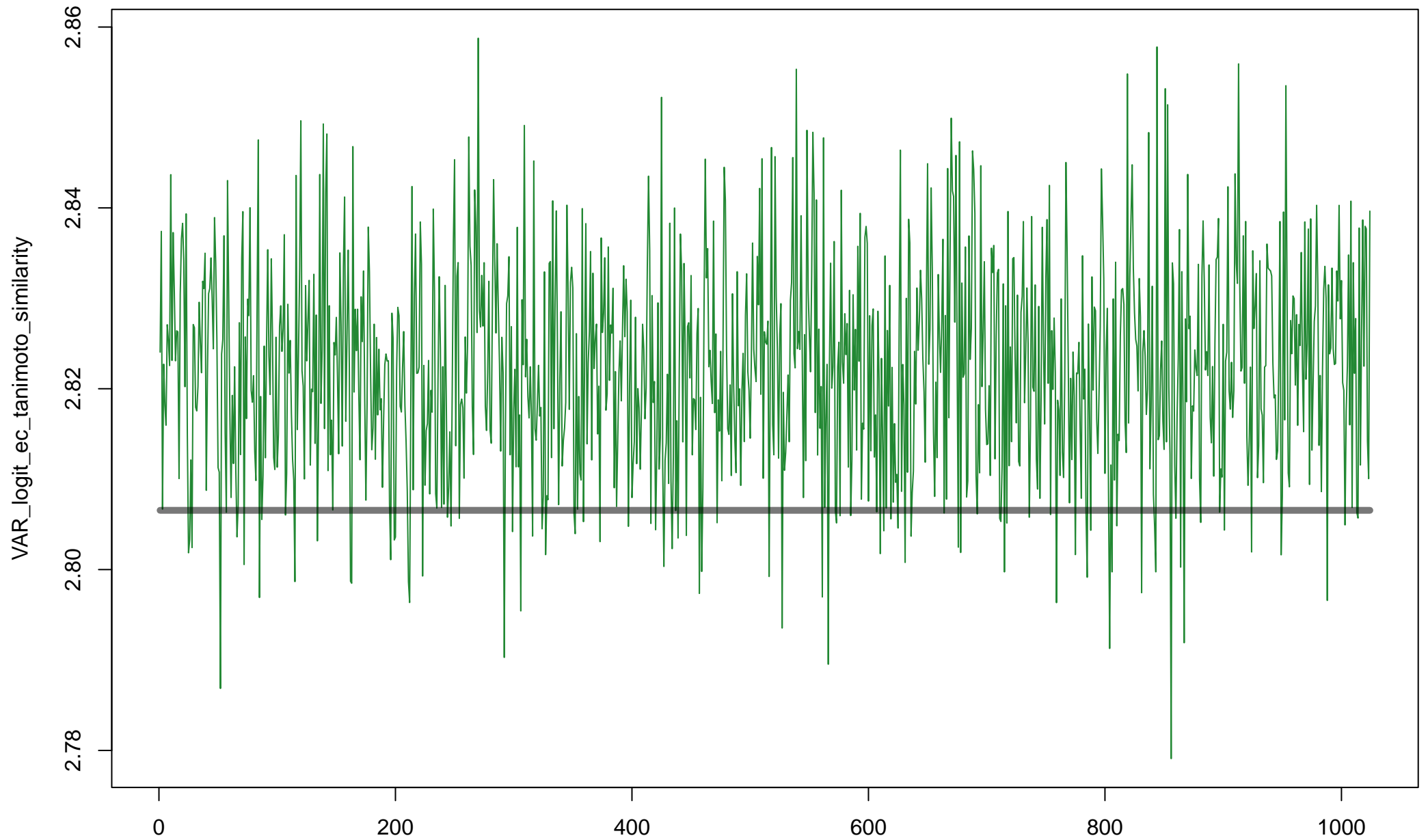


**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 914 | BMK = 0.0515 | MCSE(6.27) = 3.46 | stat: TRUE | burn: 0 | percentile: 49.9**

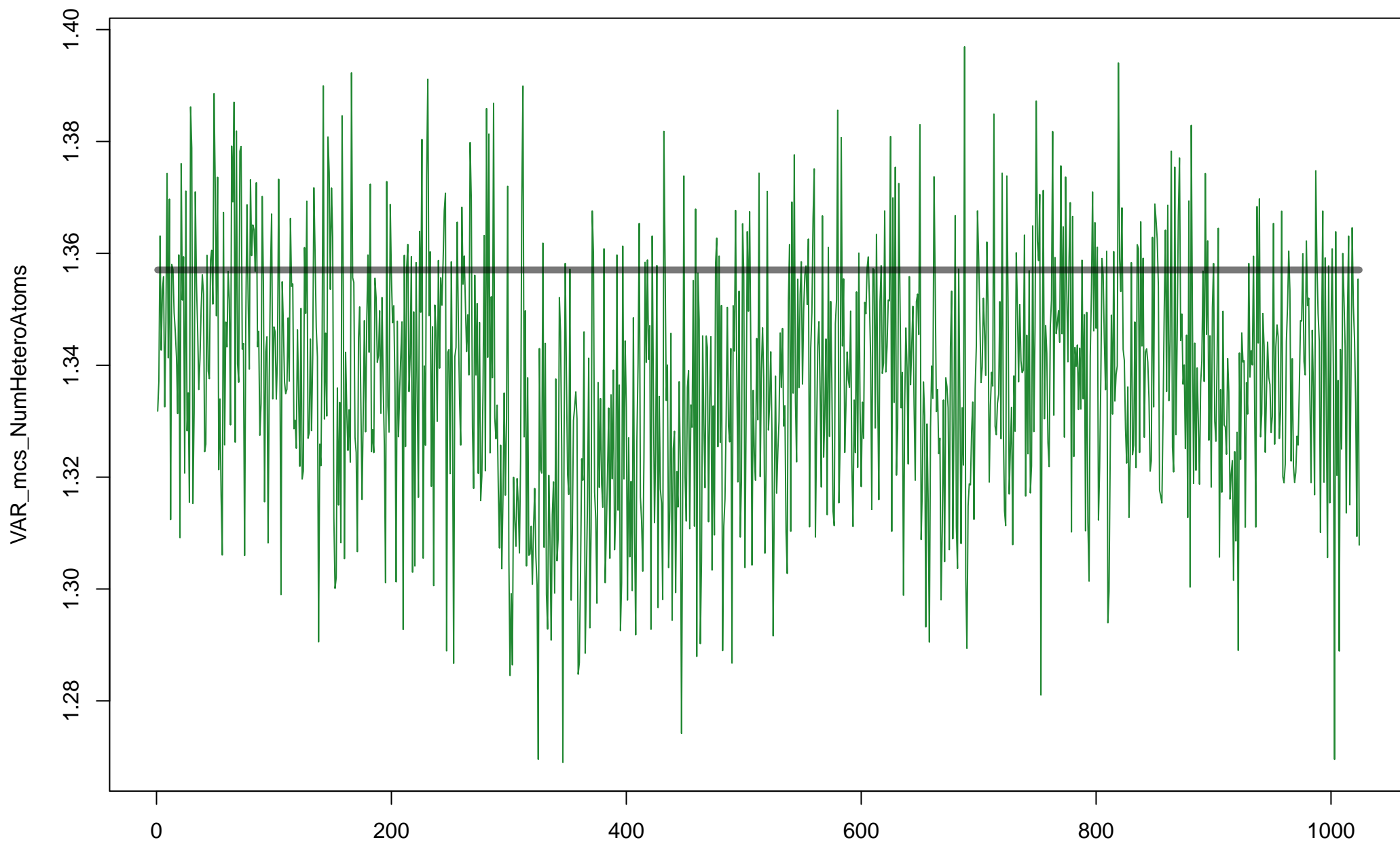


# VAR\_logit\_ec\_tanimoto\_similarity

ESS = 1020 | BMK = 0.0554 | MCSE(6.27) = 3.42 | stat: TRUE | burn: 0 | percentile: 9.08

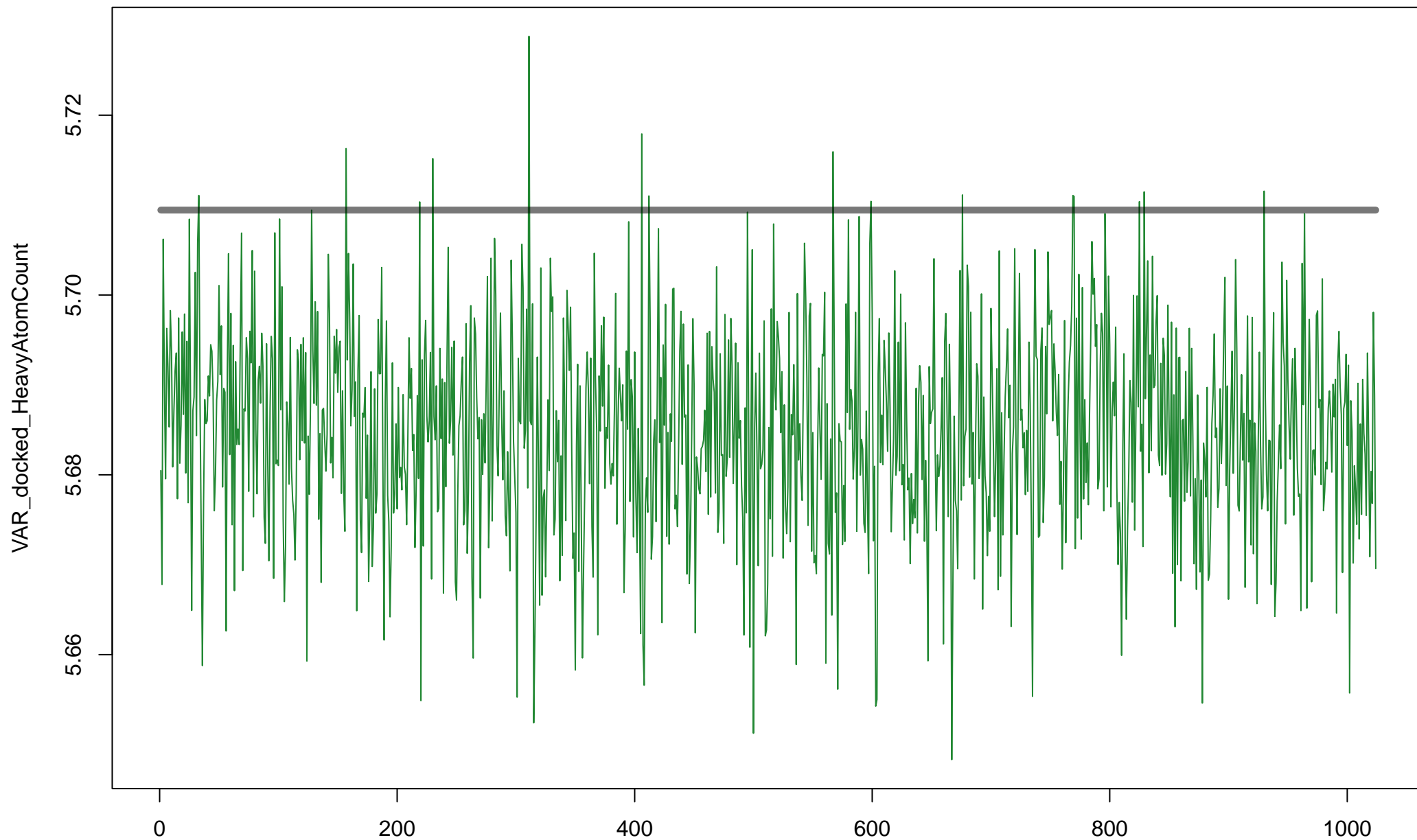


**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 89.4 | BMK = 0.113 | MCSE(6.27) = 6.68 | stat: FALSE | burn: 0 | percentile: 80.1**

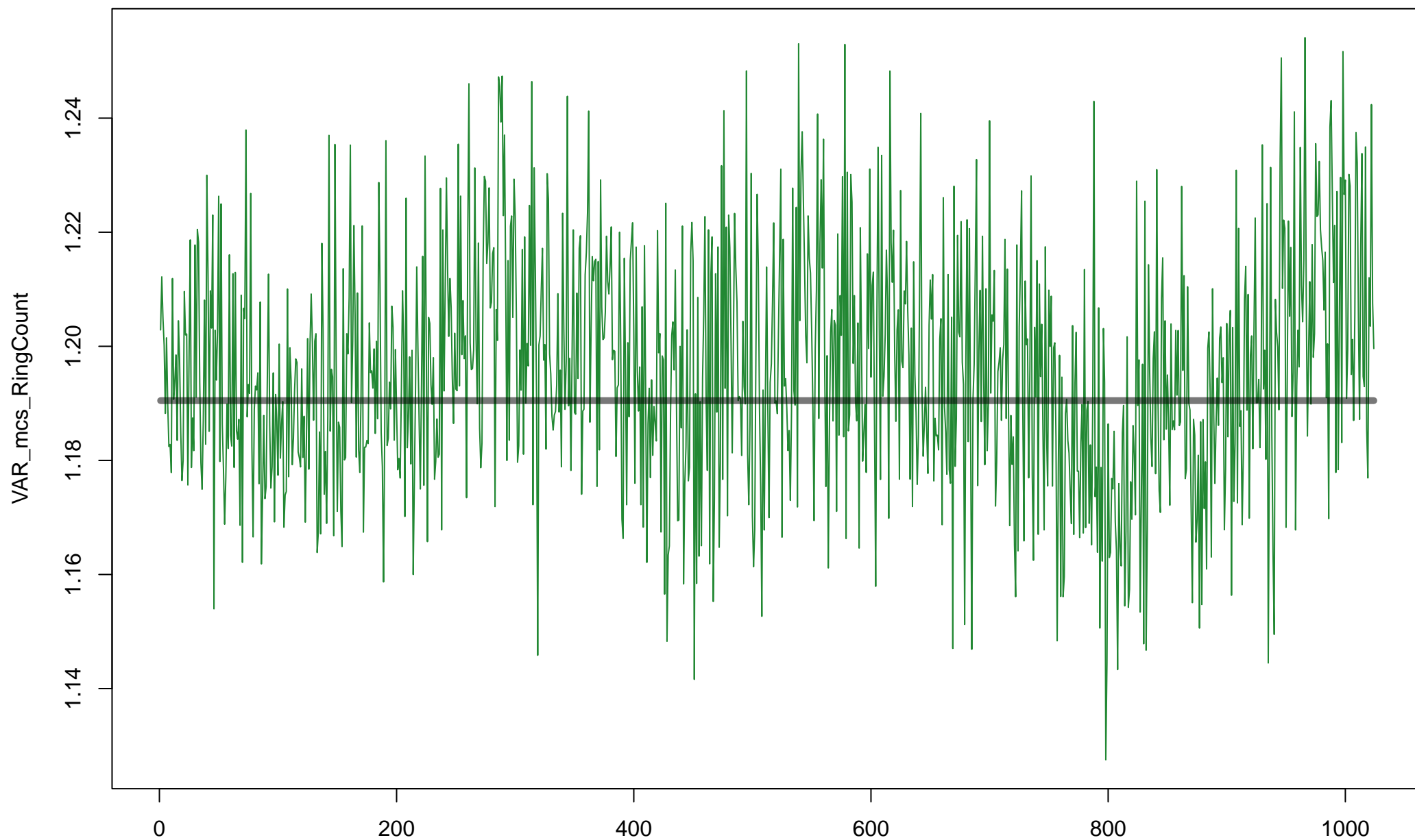


# VAR\_docked\_HeavyAtomCount

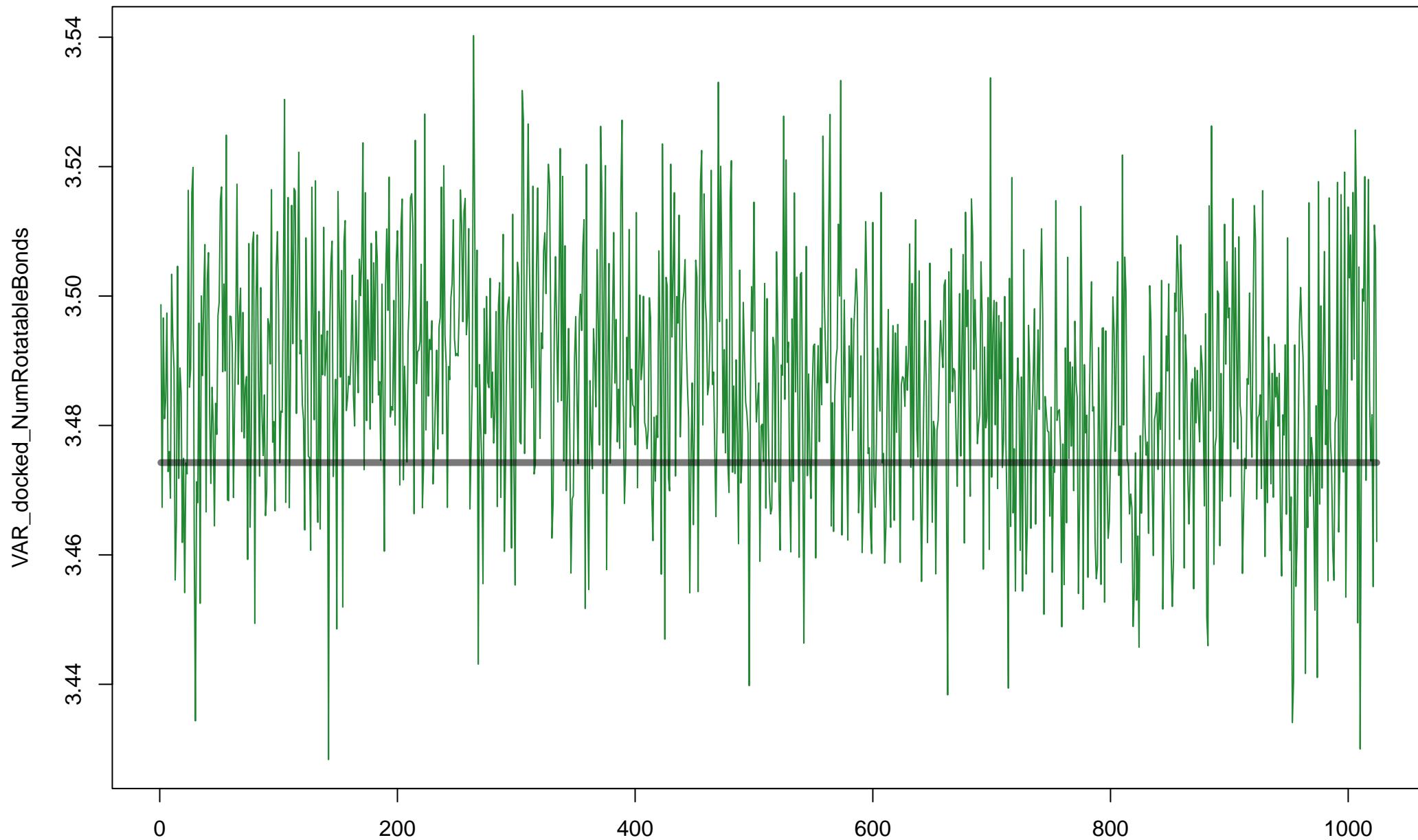
ESS = 1020 | BMK = 0.0473 | MCSE(6.27) = 3.7 | stat: FALSE | burn: 0 | percentile: 98.5



**VAR\_mcs\_RingCount**  
**ESS = 78.2 | BMK = 0.0739 | MCSE(6.27) = 7.32 | stat: TRUE | burn: 0 | percentile: 43.6**

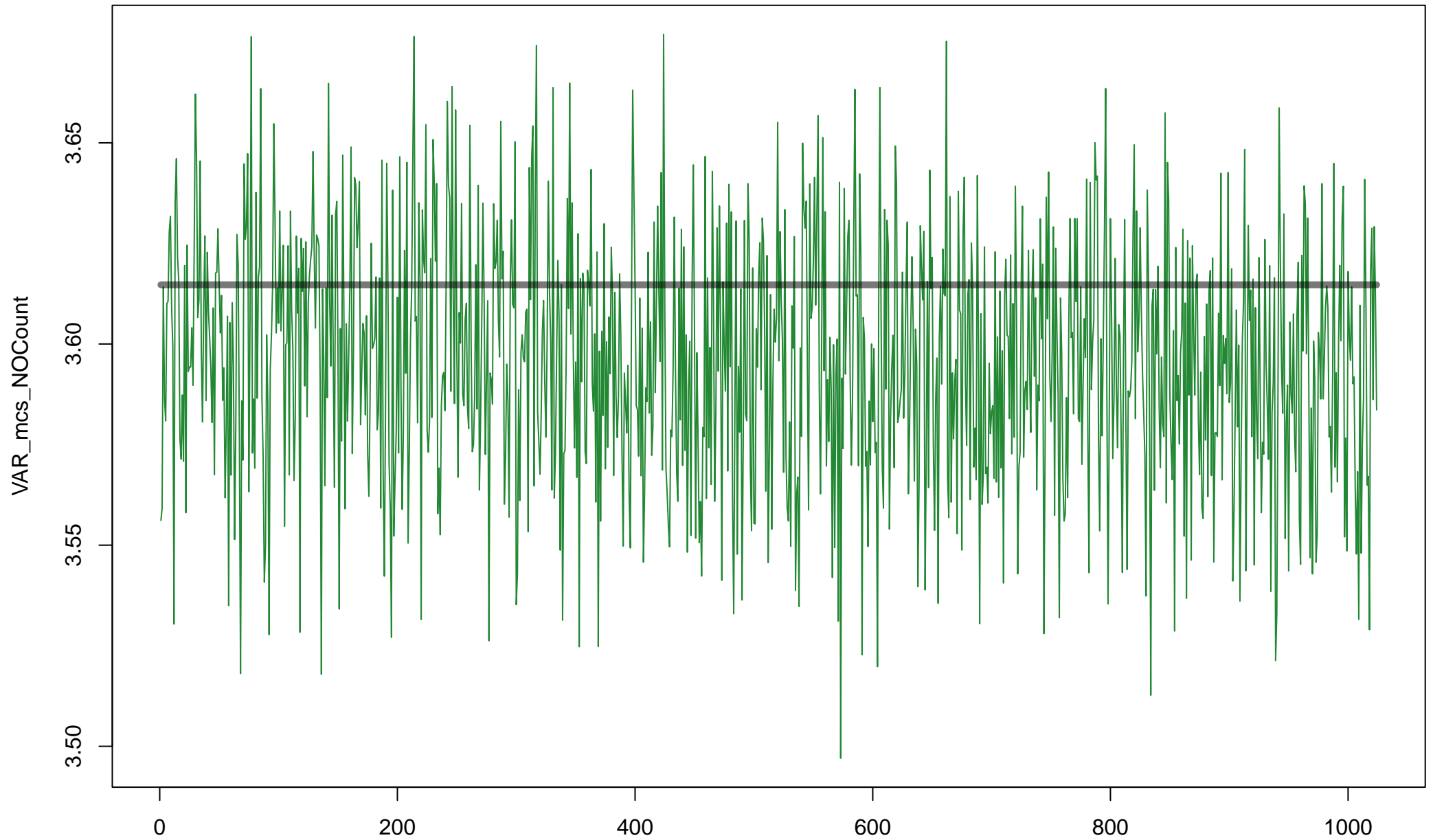


**VAR\_docked\_NumRotatableBonds**  
**ESS = 300 | BMK = 0.135 | MCSE(6.27) = 5.29 | stat: TRUE | burn: 0 | percentile: 25**

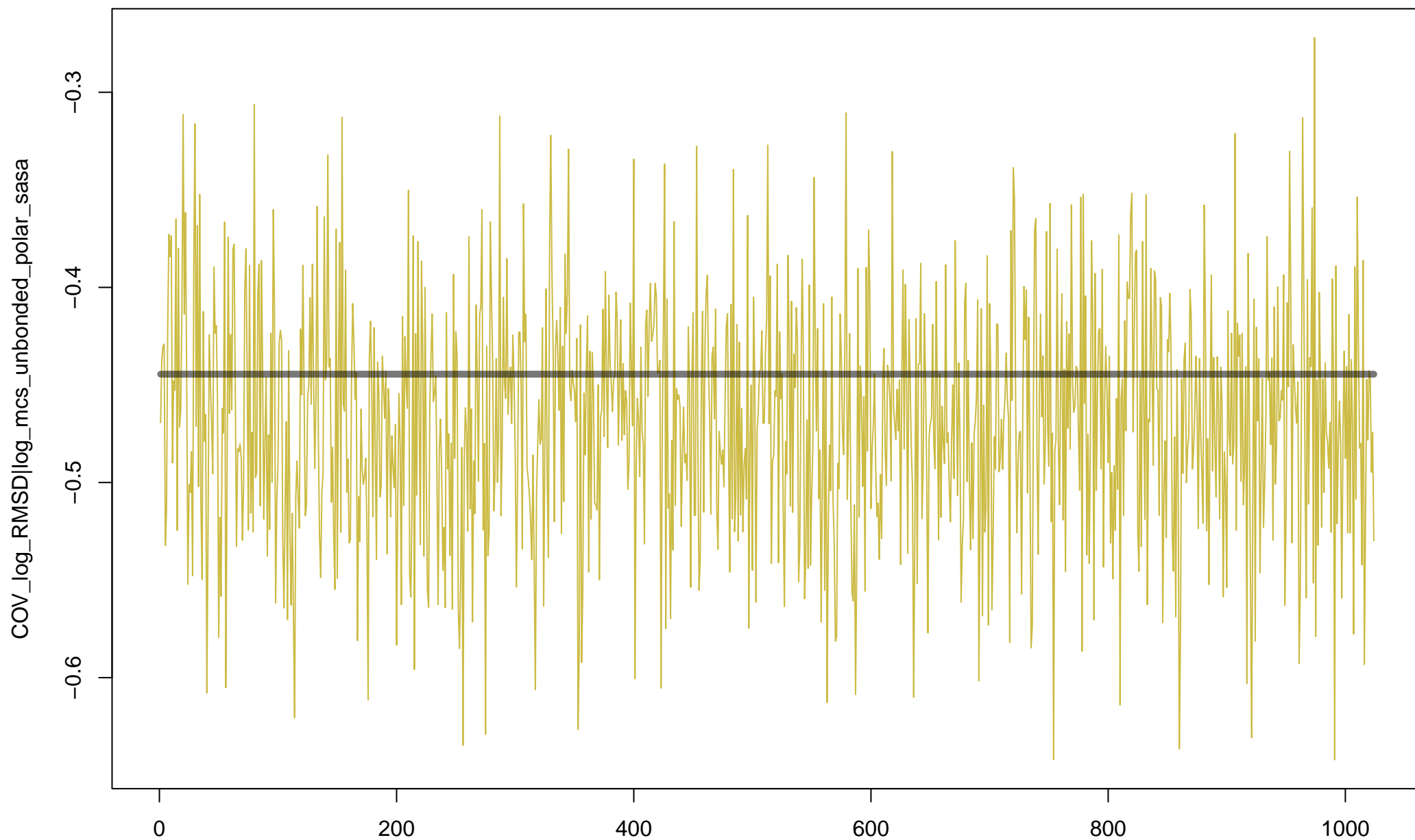


# VAR\_mcs\_NOCount

ESS = 1020 | BMK = 0.0625 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0 | percentile: 72.9

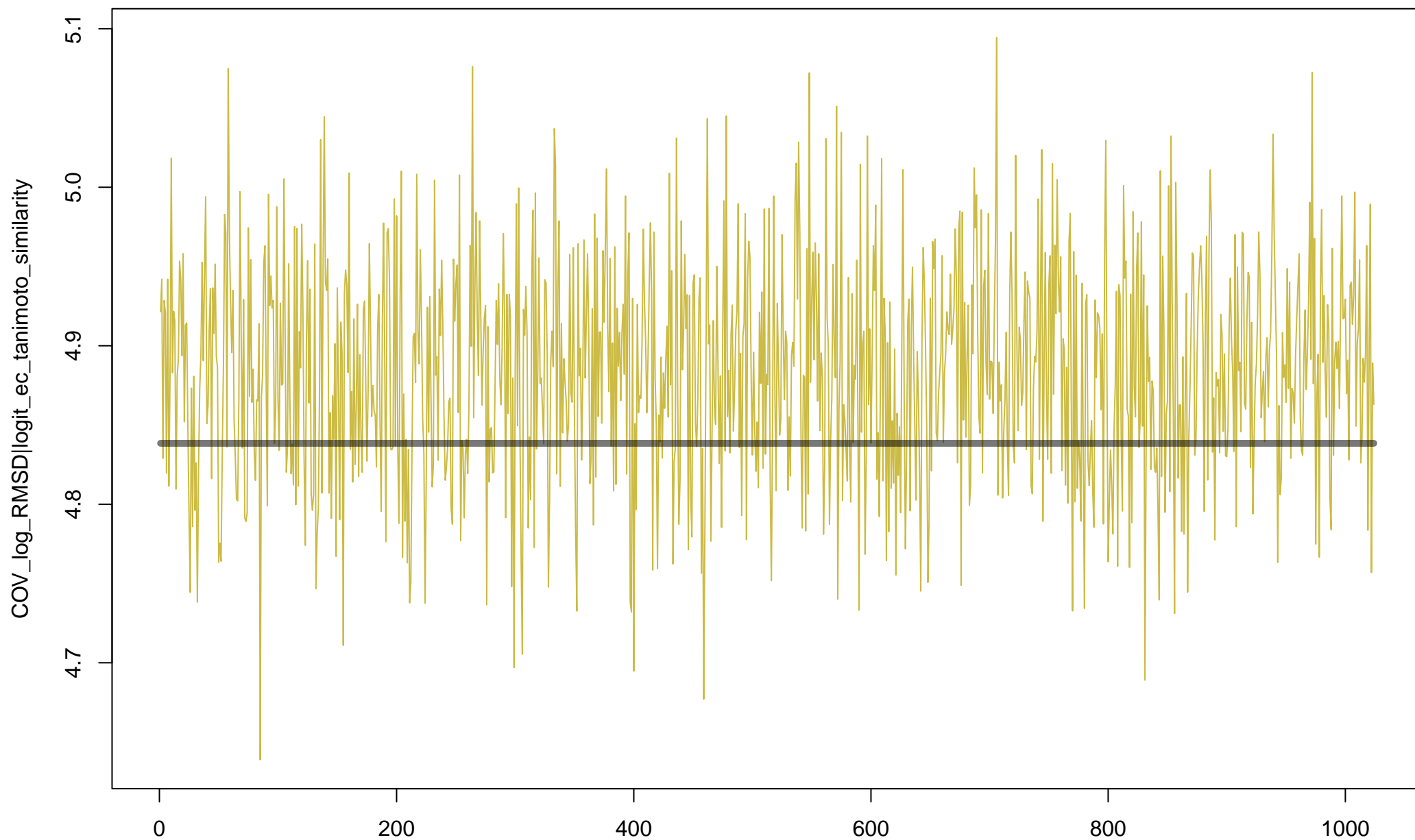


**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1020 | BMK = 0.0334 | MCSE(6.27) = 3.82 | stat: TRUE | burn: 0 | percentile: 66.1**

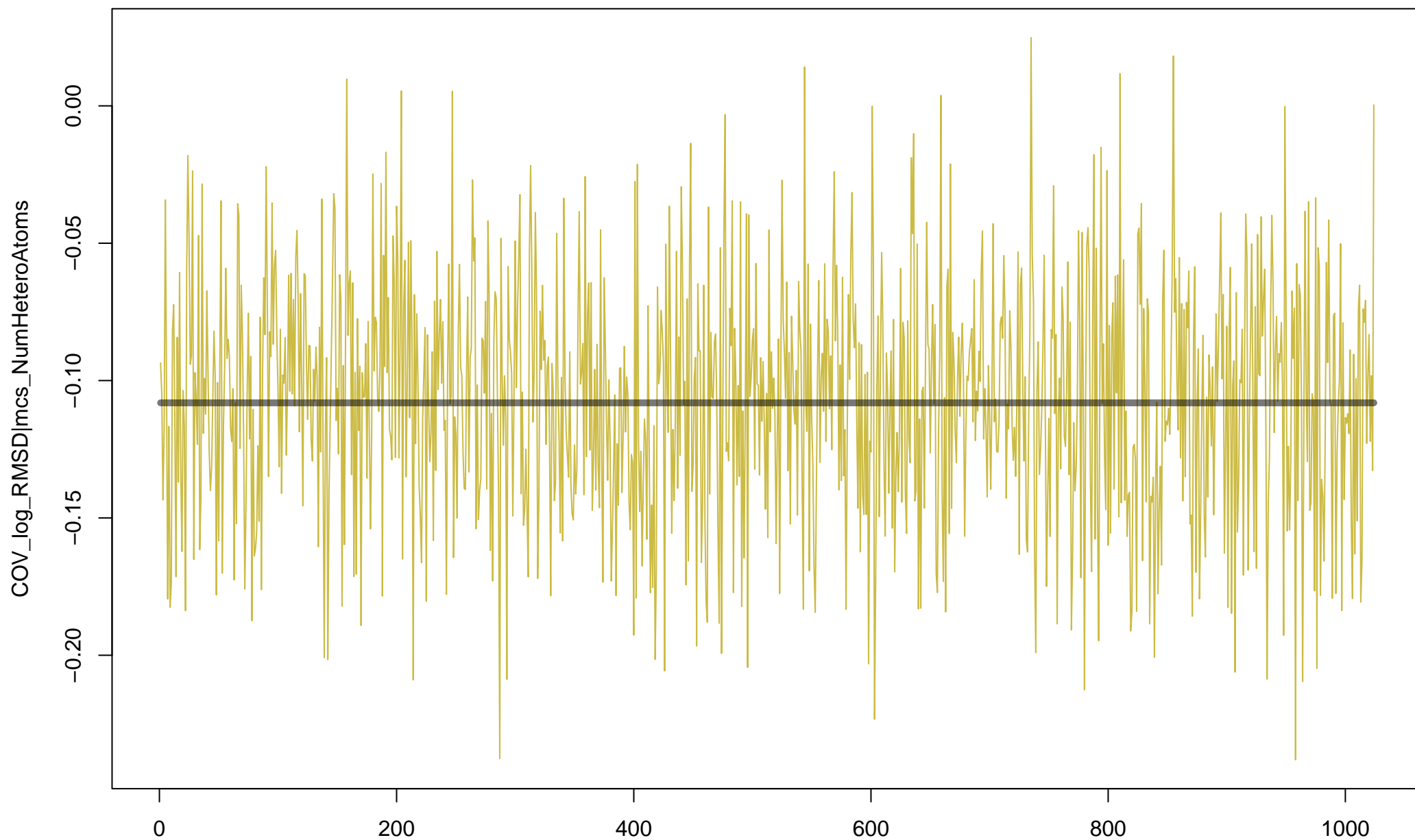




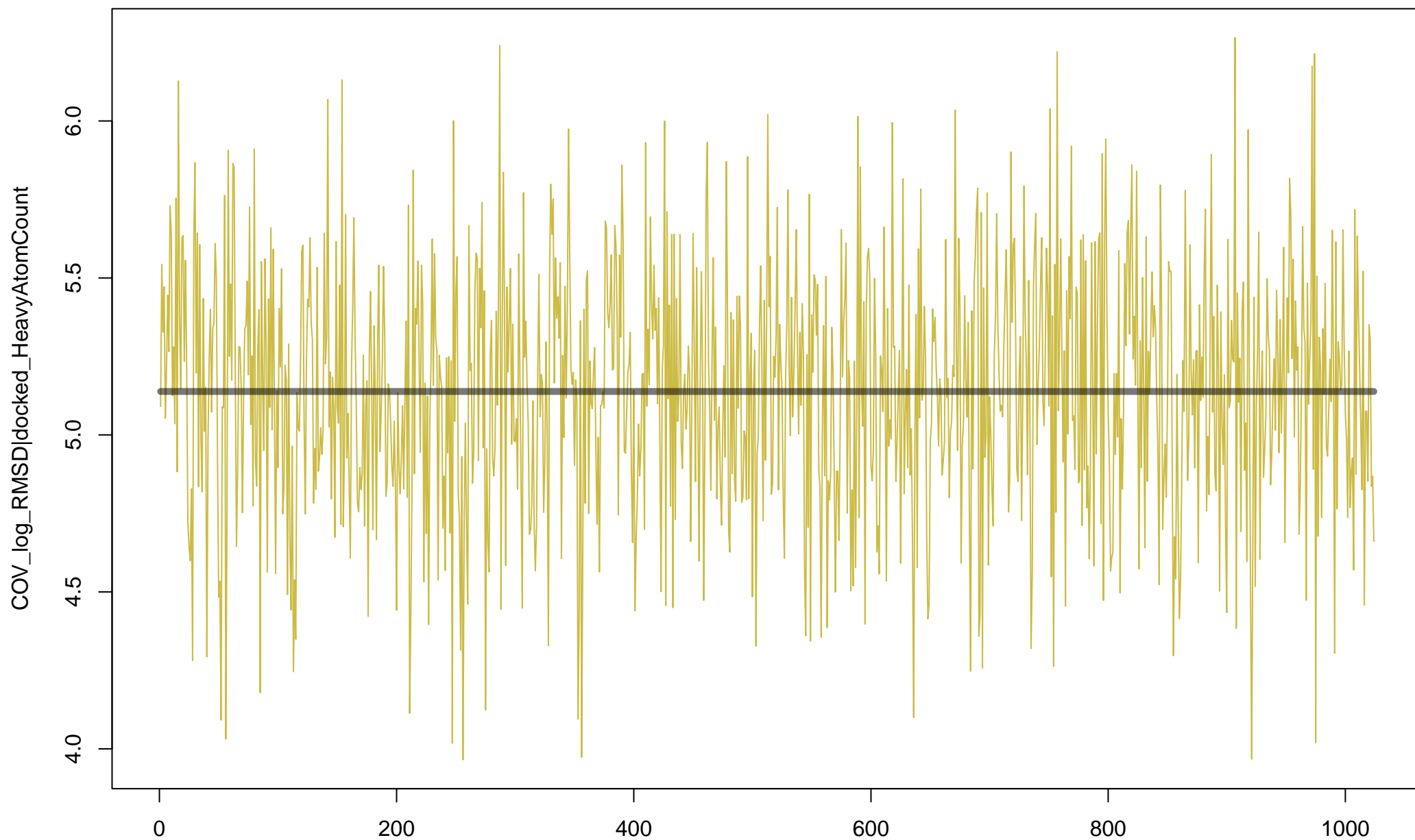
**COV\_log\_RMSD|logit\_ec\_tanimoto\_similarity**  
**ESS = 1020 | BMK = 0.0437 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | percentile: 27.1**



**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 1020 | BMK = 0.0489 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | percentile: 46.5**

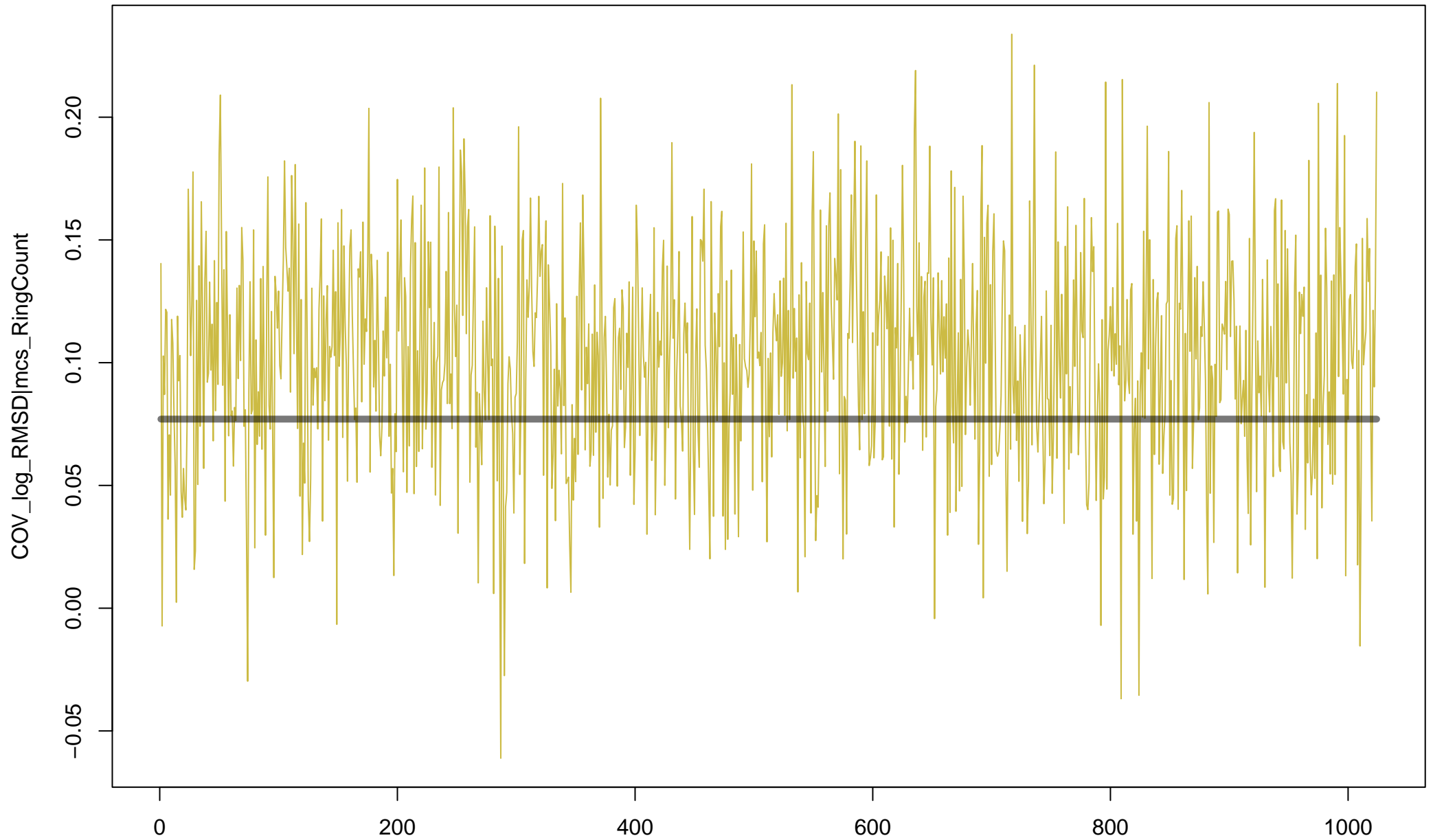


**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 794 | BMK = 0.0358 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0 | percentile: 48.6**

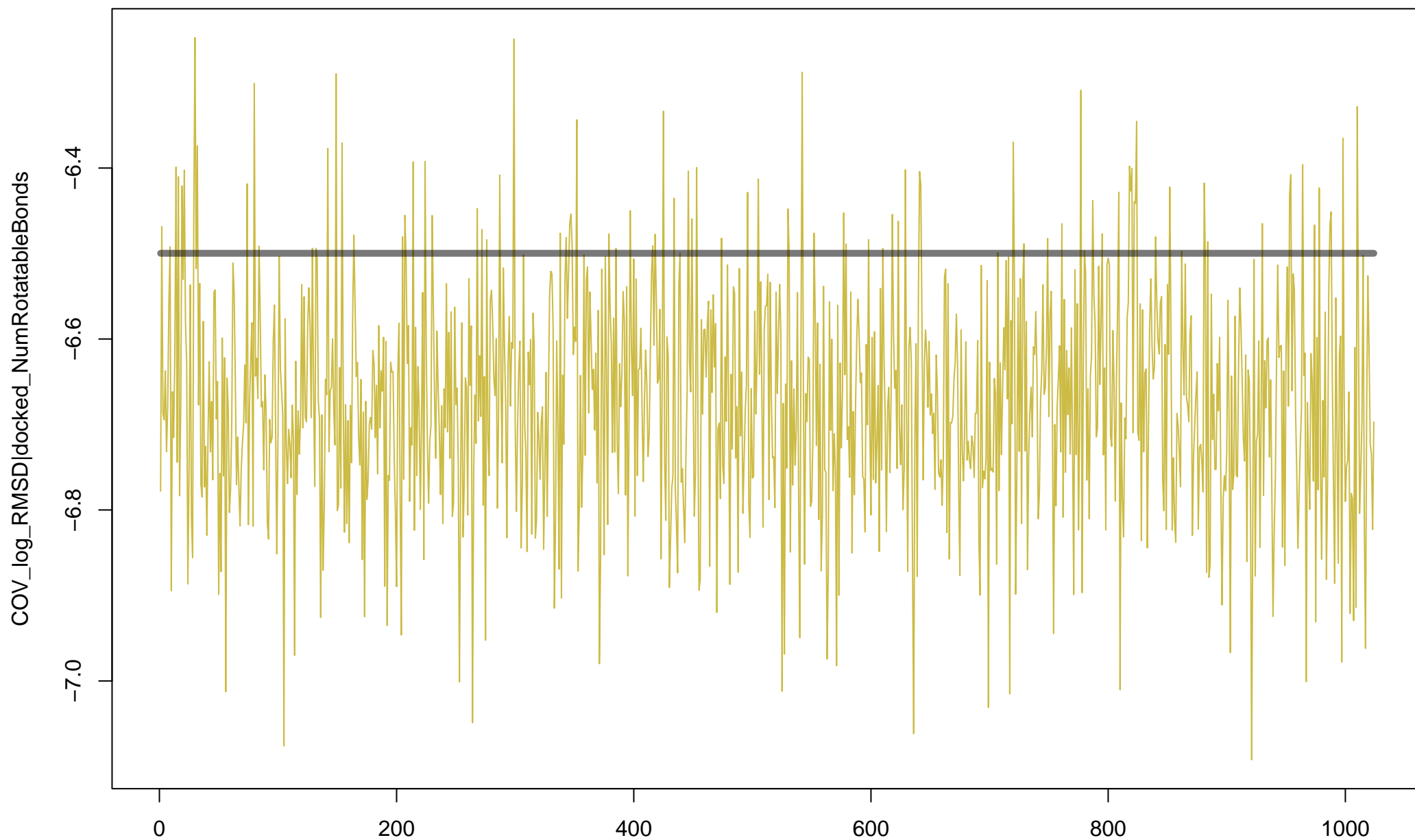


COV\_log\_RMSD|mcs\_RingCount

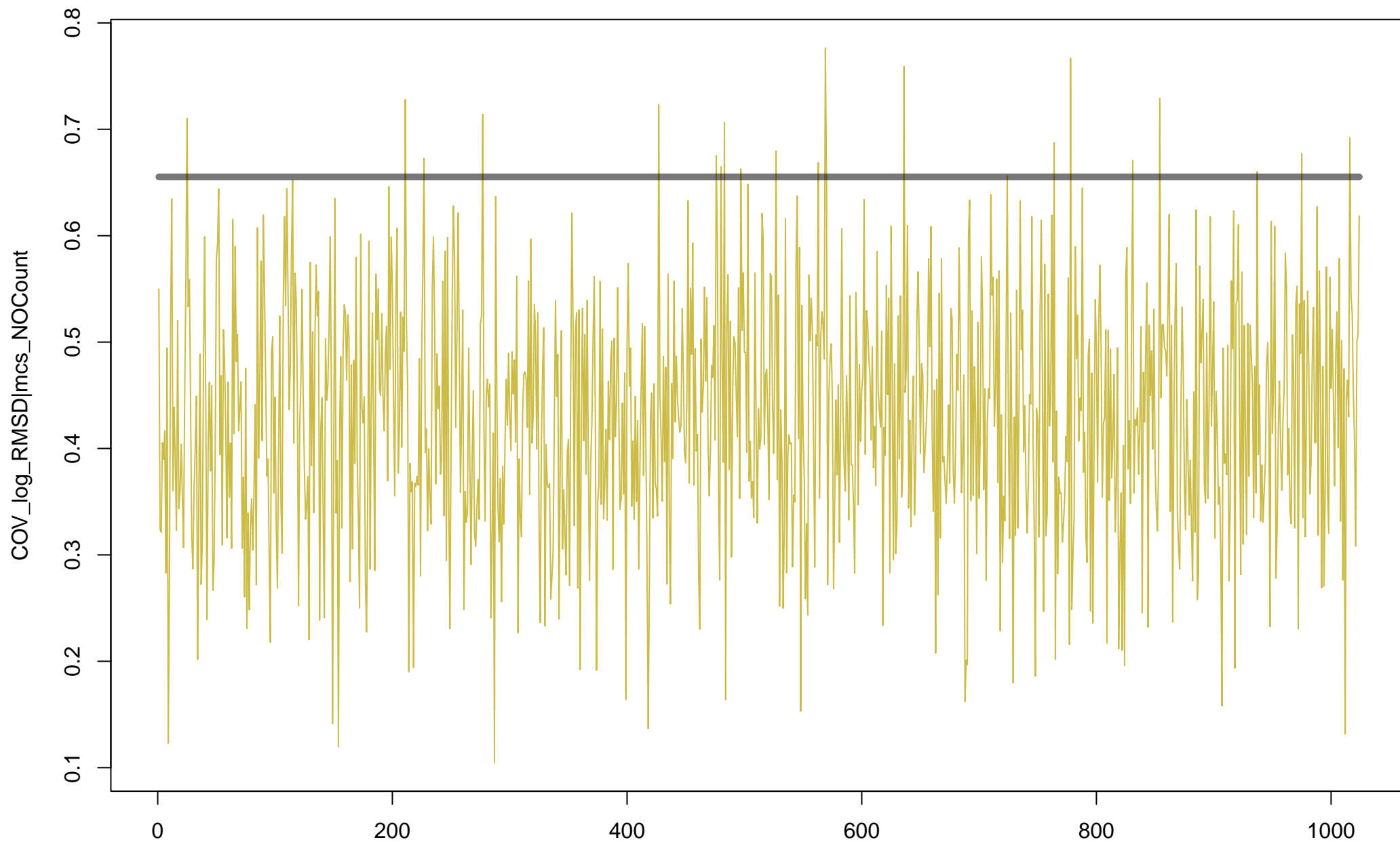
ESS = 1020 | BMK = 0.0496 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0 | percentile: 28.9



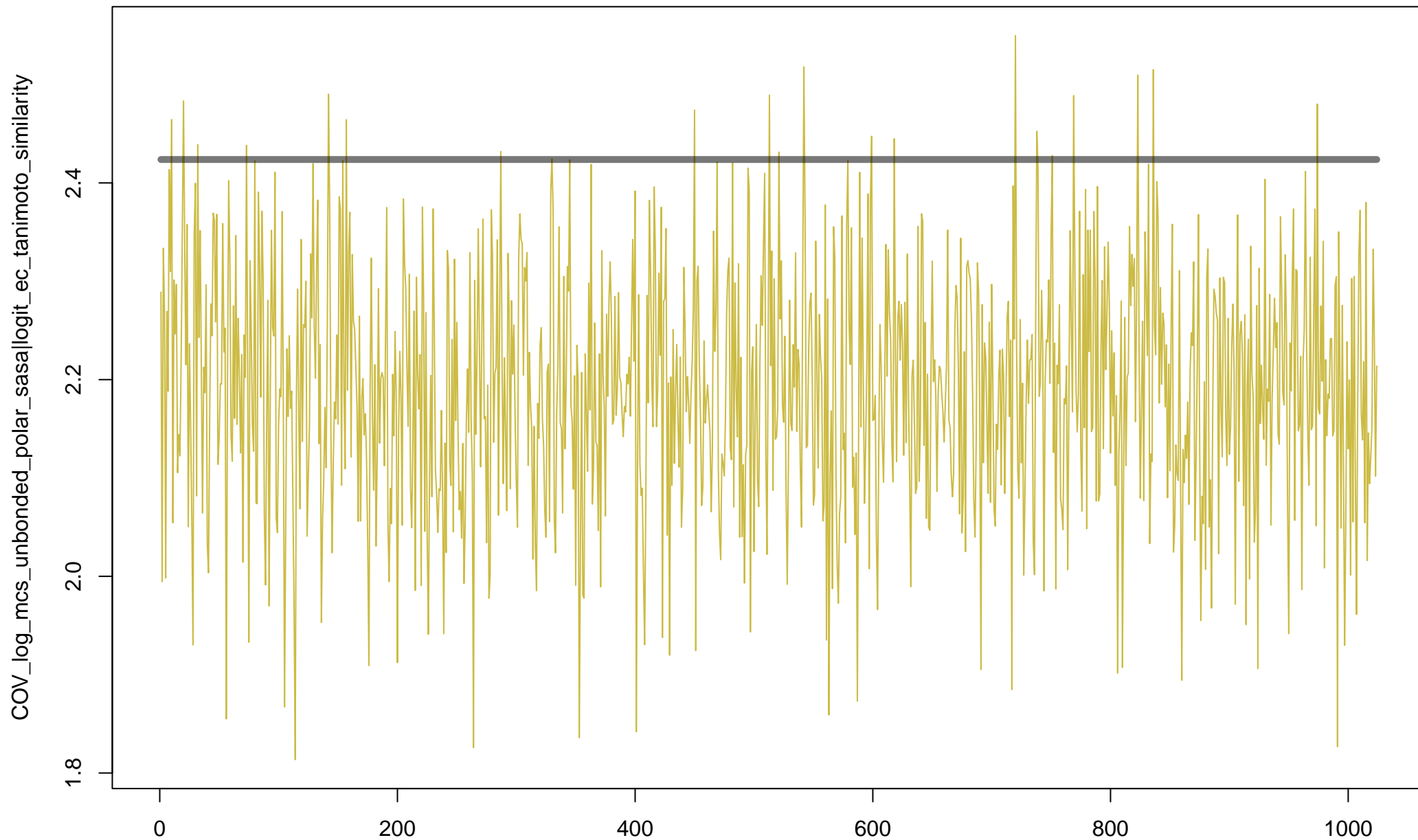
**COV\_log\_RMSD|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0421 | MCSE(6.27) = 3.6 | stat: TRUE | burn: 0 | percentile: 91.1**



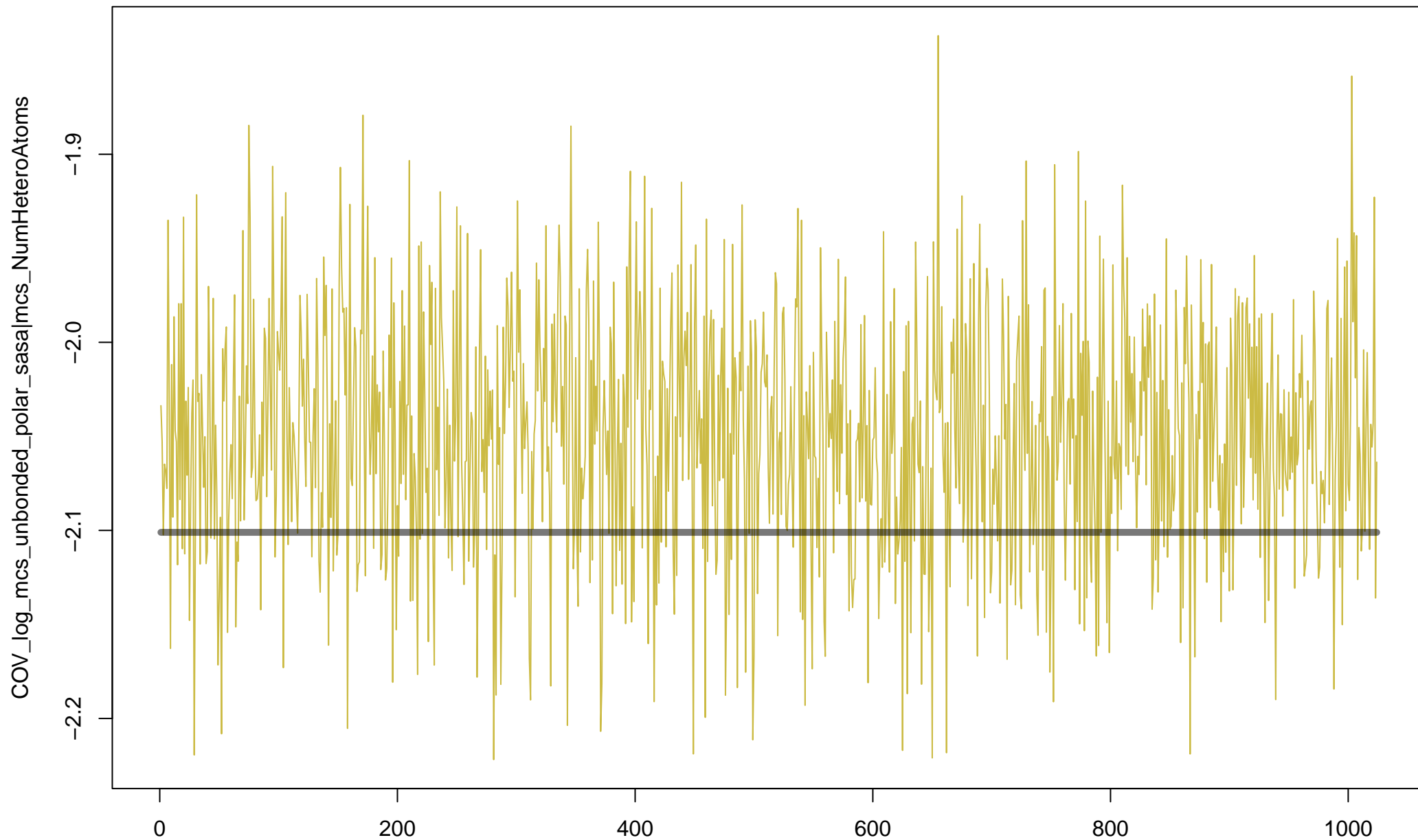
**COV\_log\_RMSD|mcs\_NOCount**  
**ESS = 875 | BMK = 0.031 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0 | percentile: 97.9**



**COV\_log\_mcs\_unbonded\_polar\_sasa|logit\_ec\_tanimoto\_similarity**  
**ESS = 913 | BMK = 0.0502 | MCSE(6.27) = 3.5 | stat: TRUE | burn: 0 | percentile: 97.9**

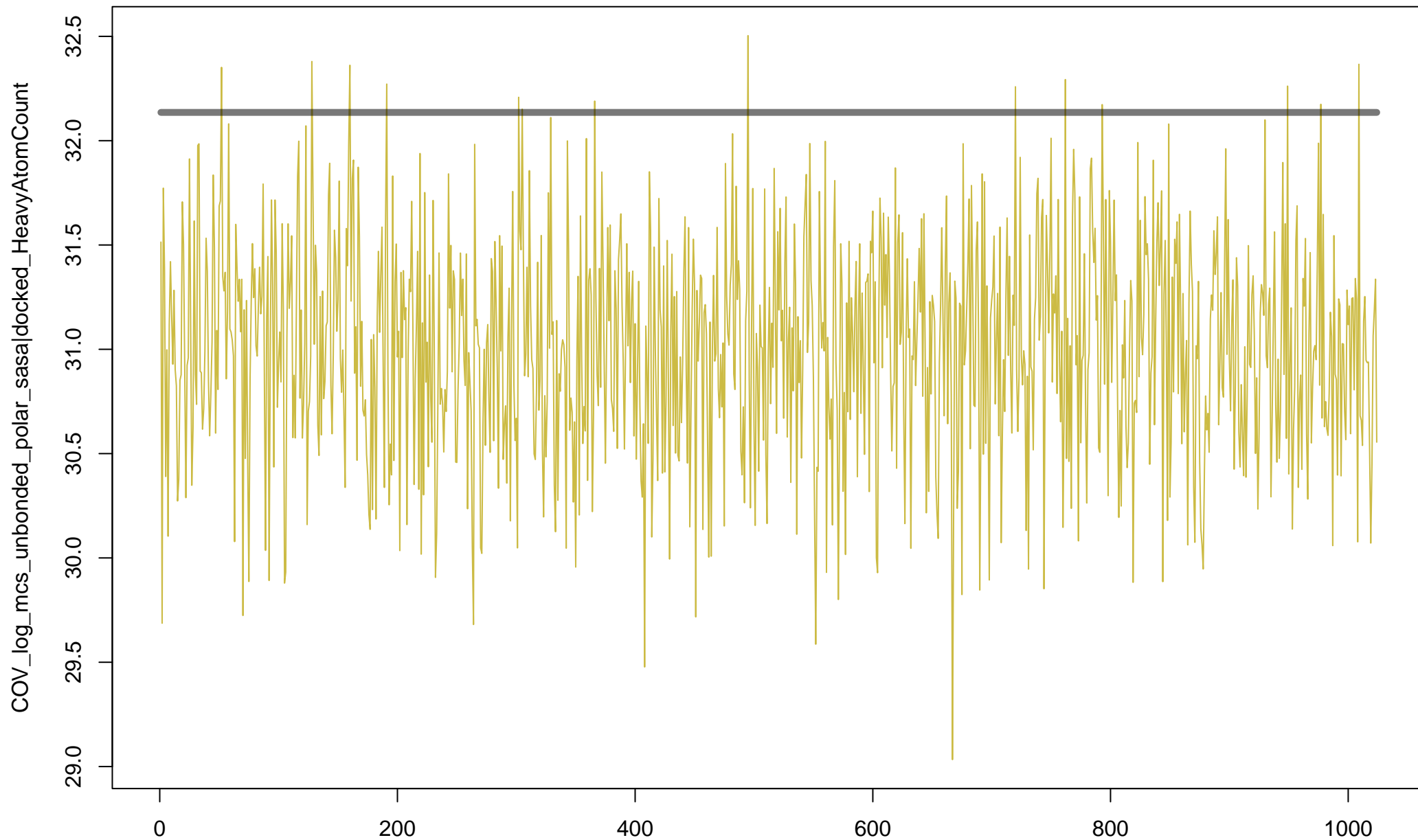


COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms  
ESS = 1020 | BMK = 0.0683 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0 | percentile: 21.9

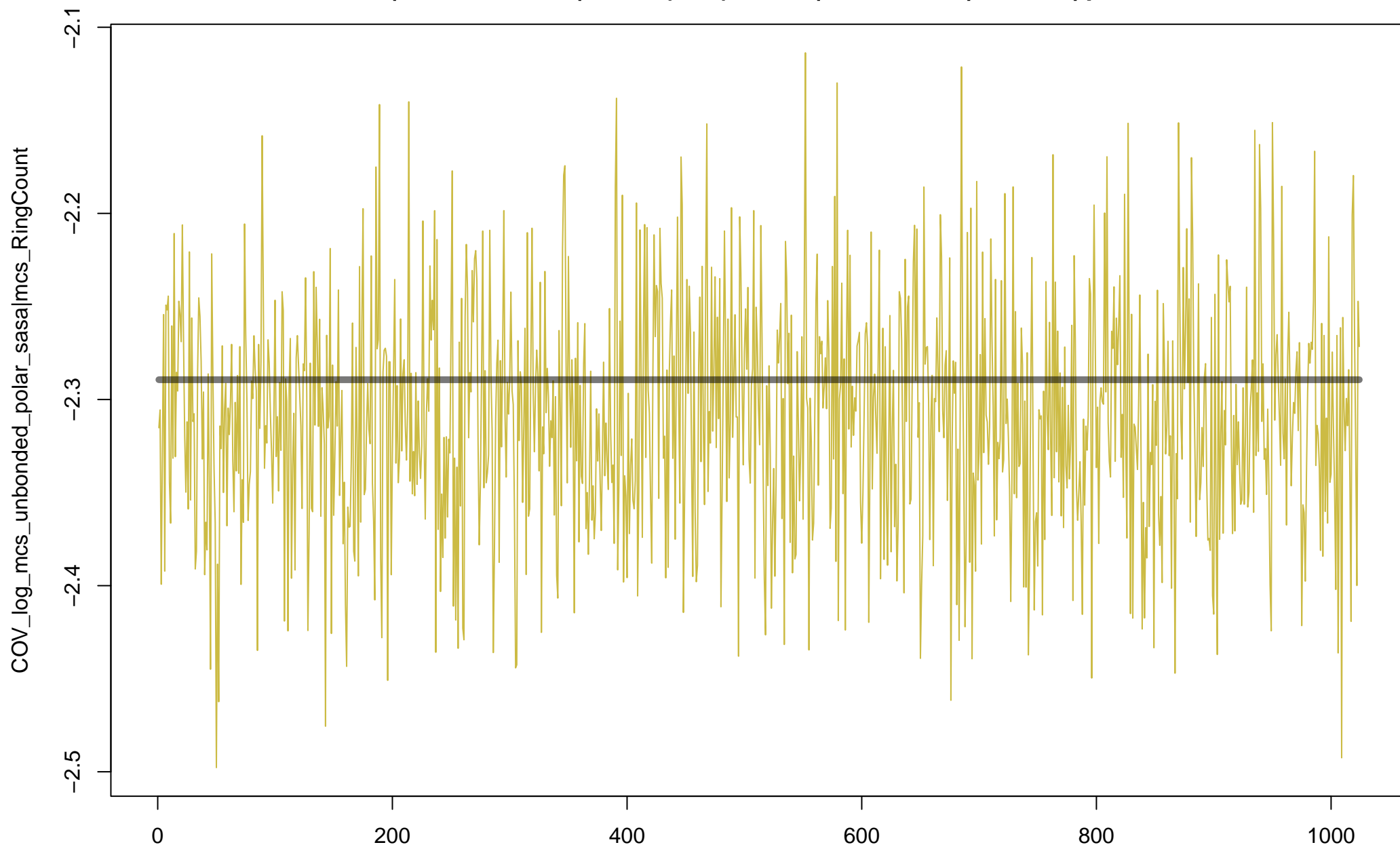




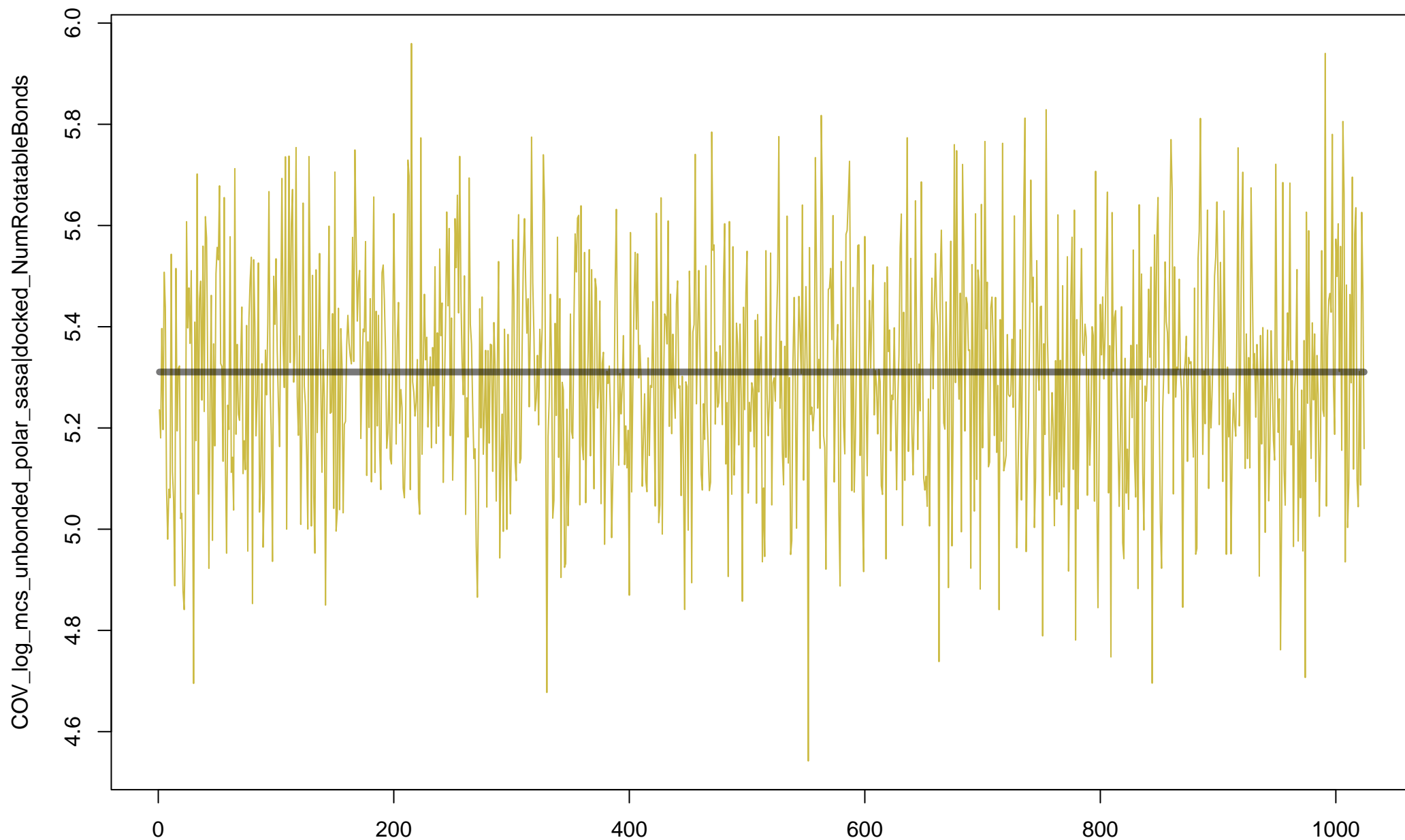
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 898 | BMK = 0.0409 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | percentile: 98.6**



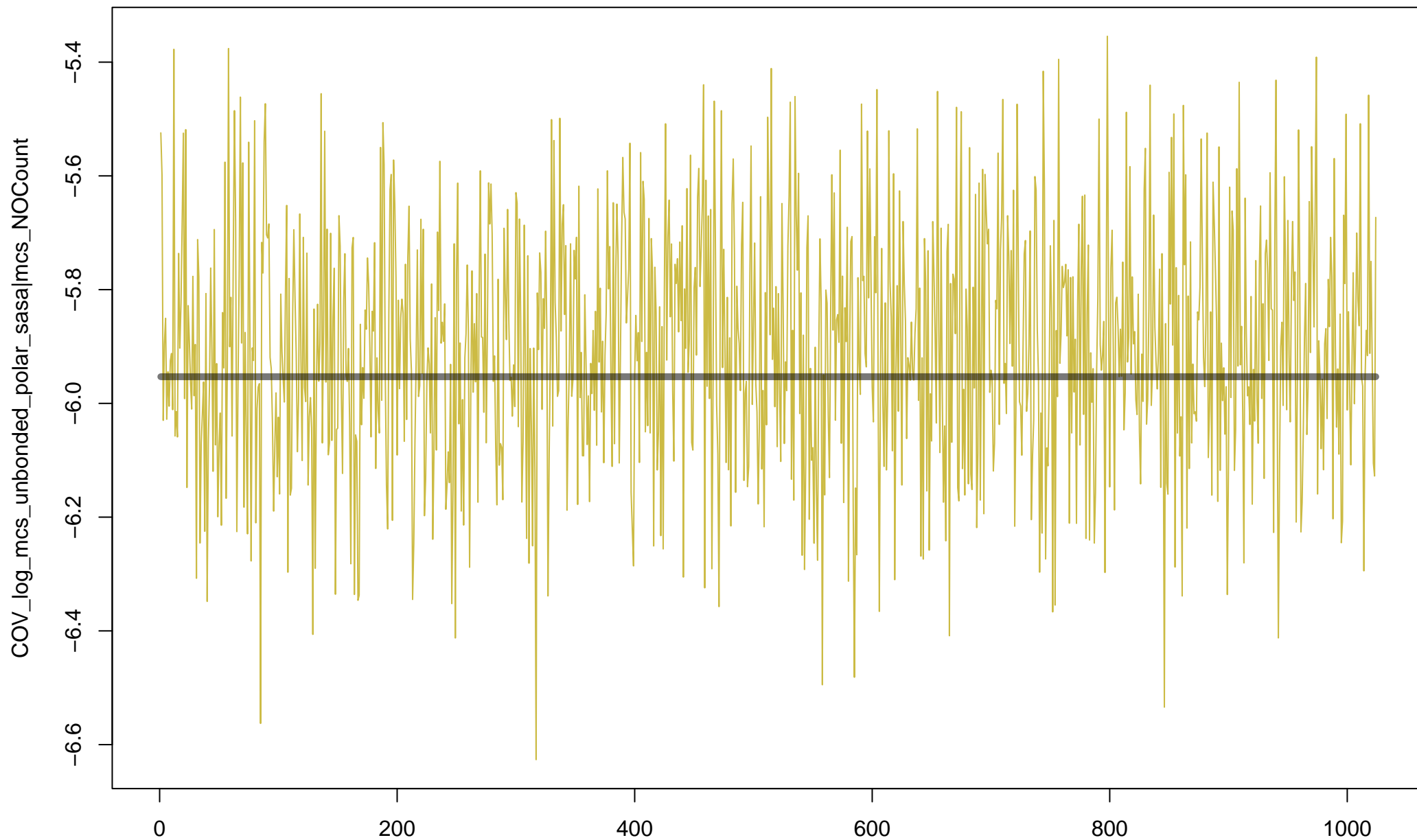
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.0339 | MCSE(6.27) = 3.52 | stat: TRUE | burn: 0 | percentile: 63.4**



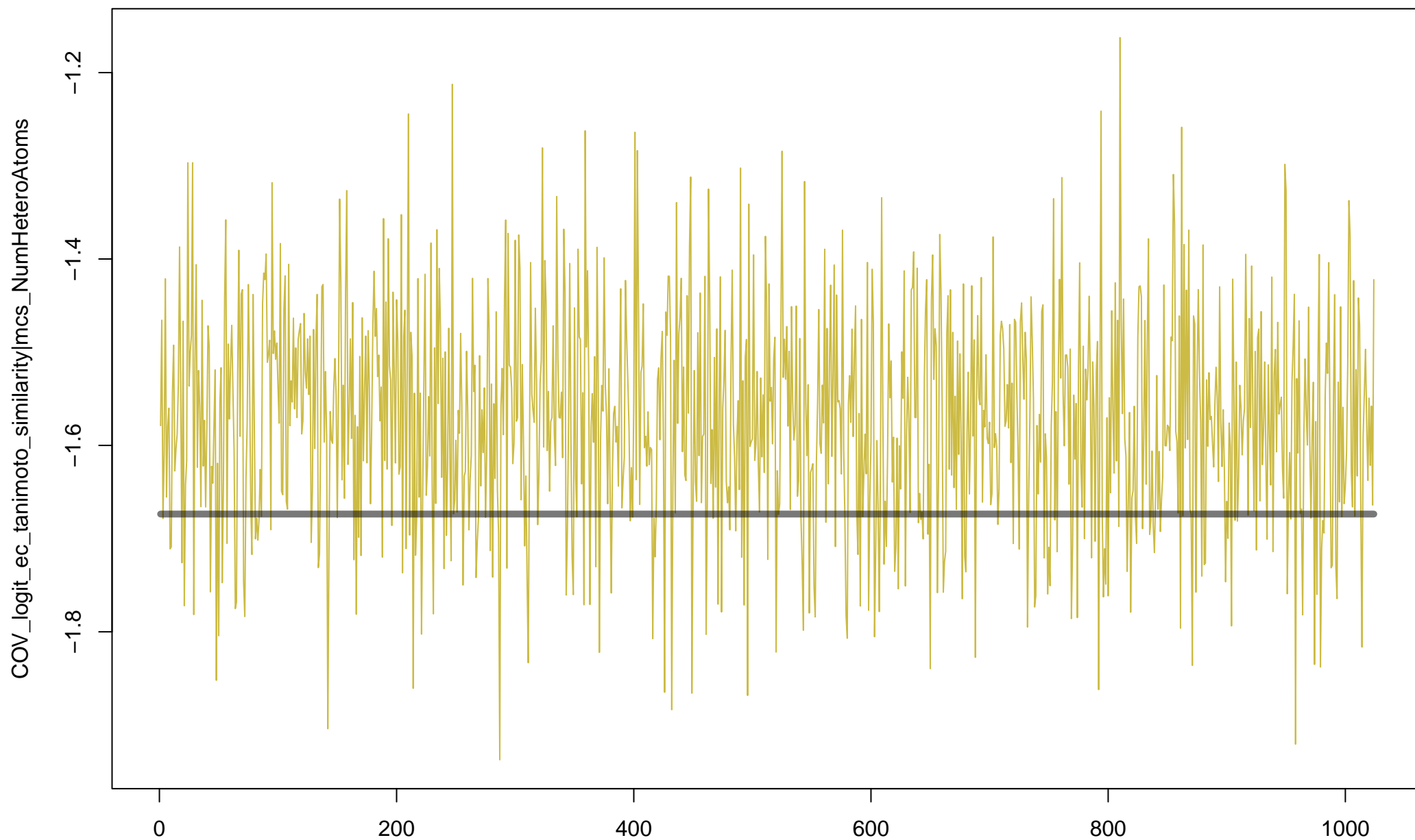
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0524 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 0 | percentile: 51.2**



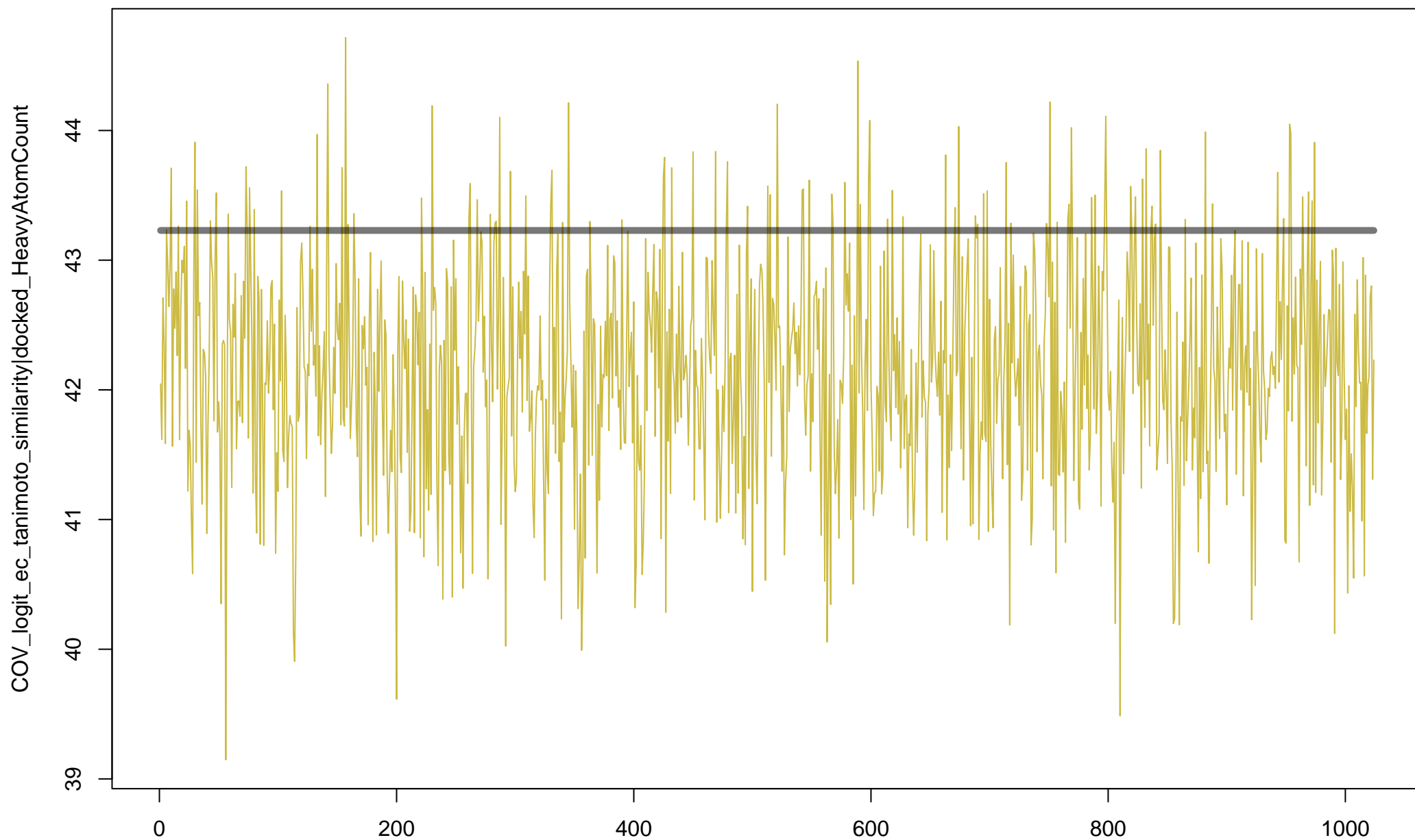
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0443 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0 | percentile: 40.7**



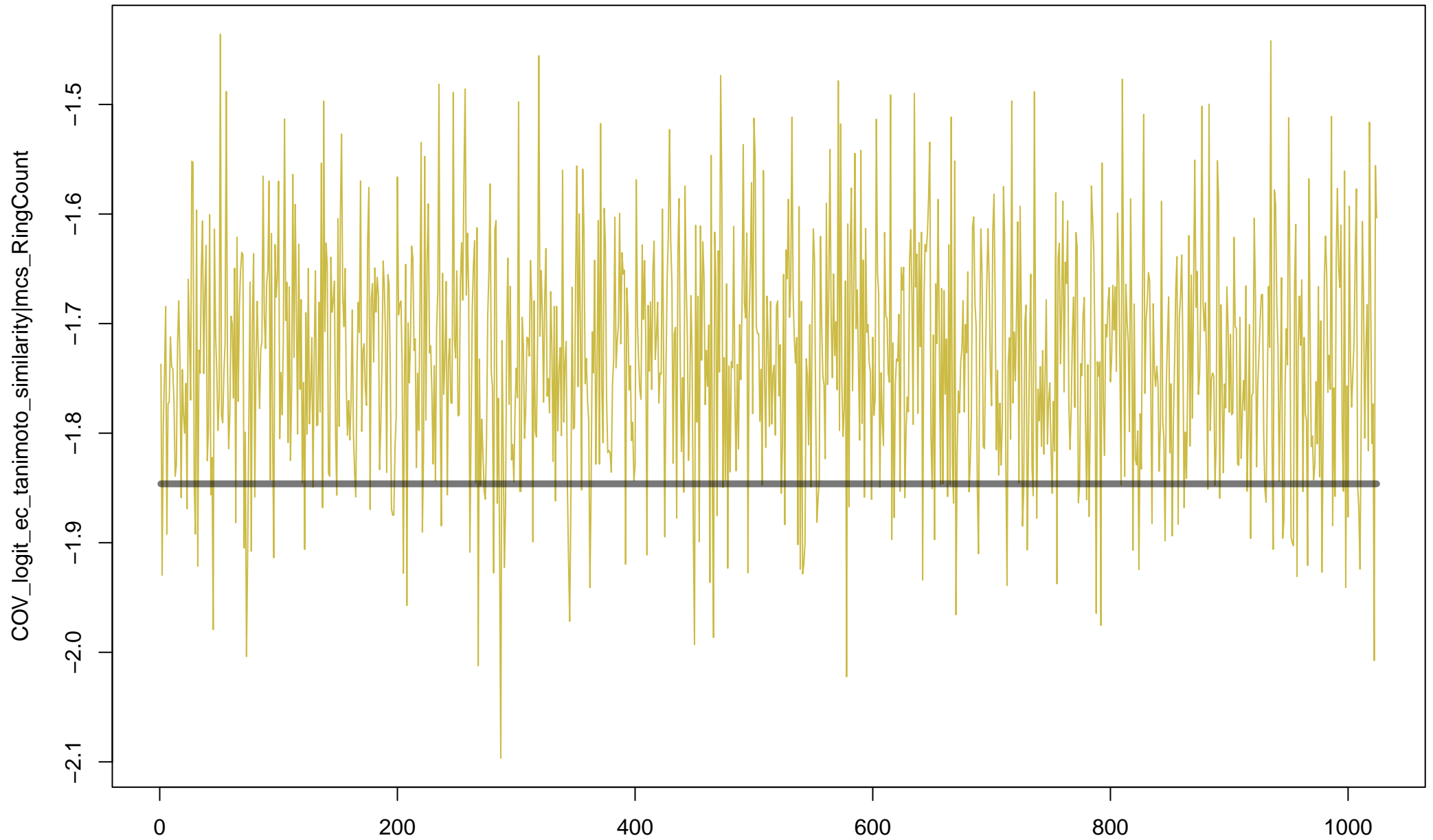
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms**  
**ESS = 1020 | BMK = 0.0605 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0 | percentile: 19.2**



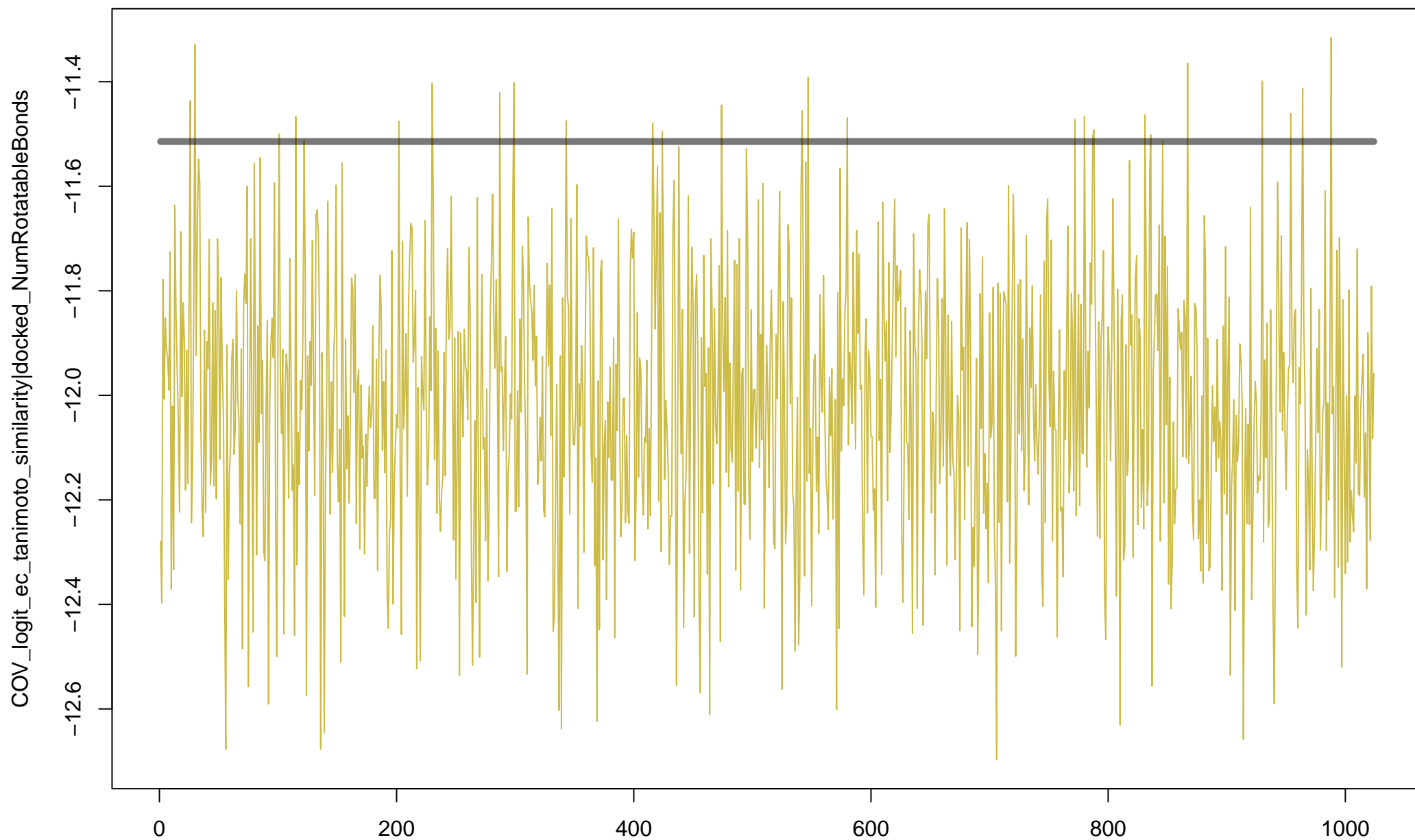
**COV\_logit\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount**  
**ESS = 826 | BMK = 0.0498 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0 | percentile: 90.3**



**COV\_logit\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.0318 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0 | percentile: 14**

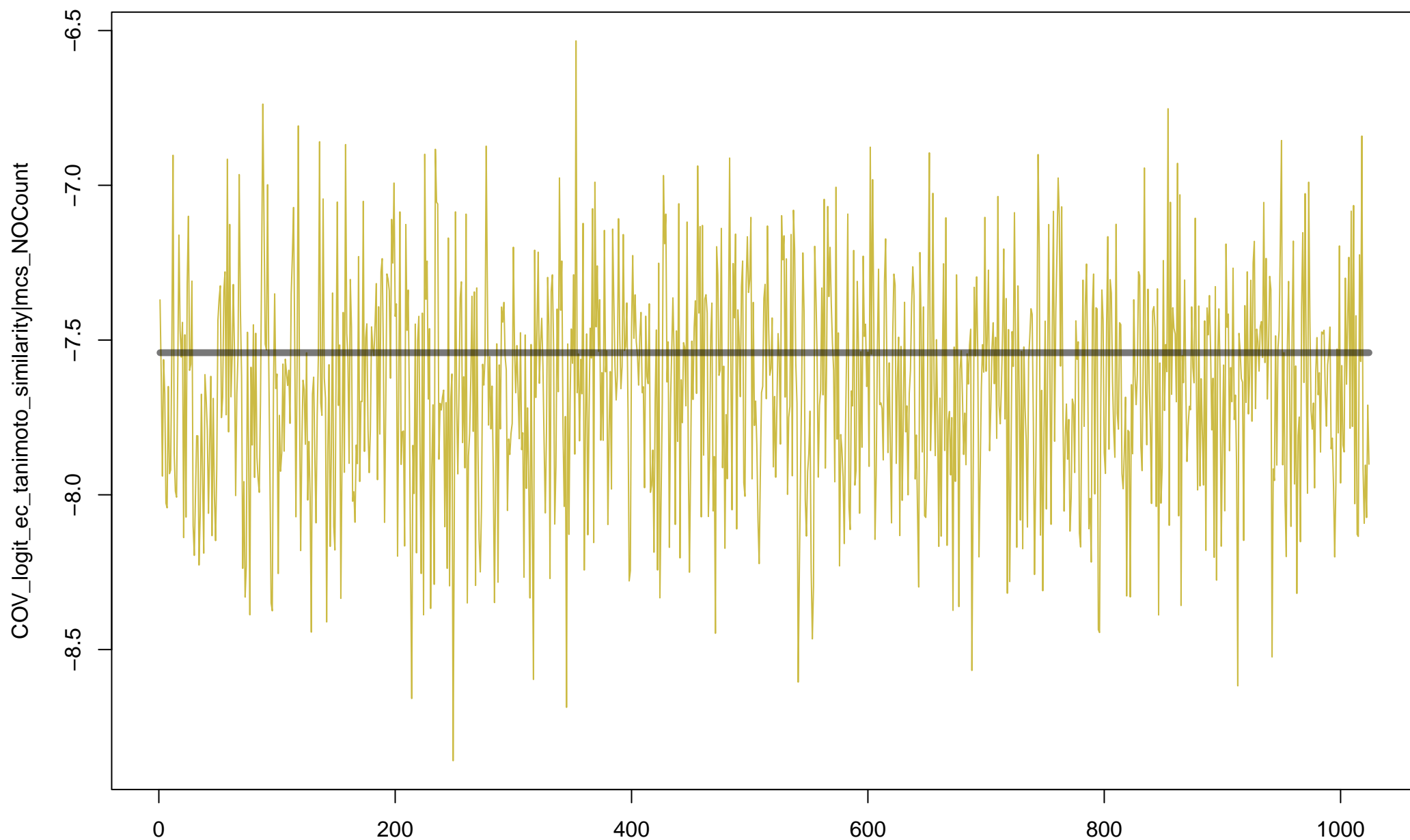


**COV\_logit\_ec\_tanimoto\_similarity|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0557 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0 | percentile: 97.3**

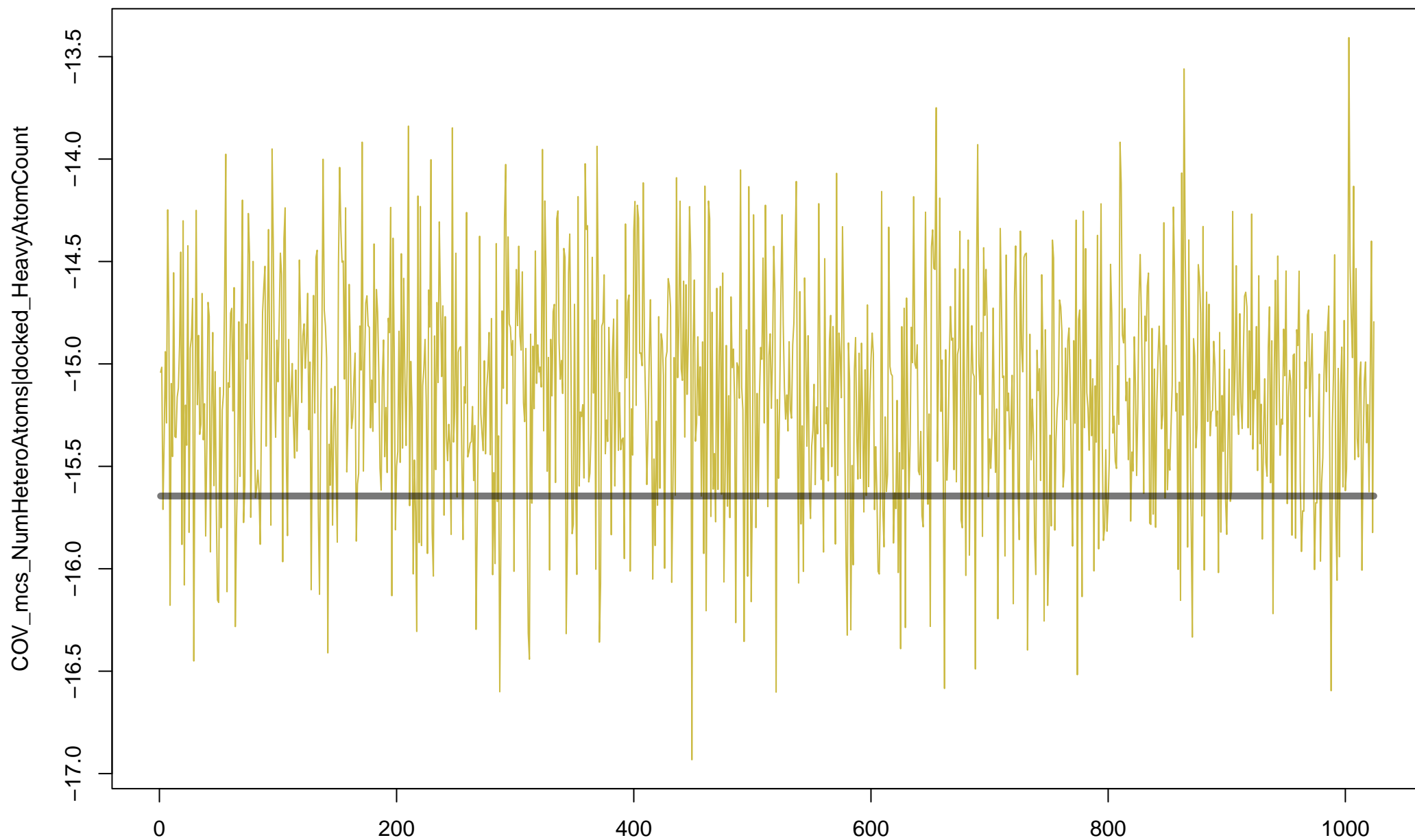




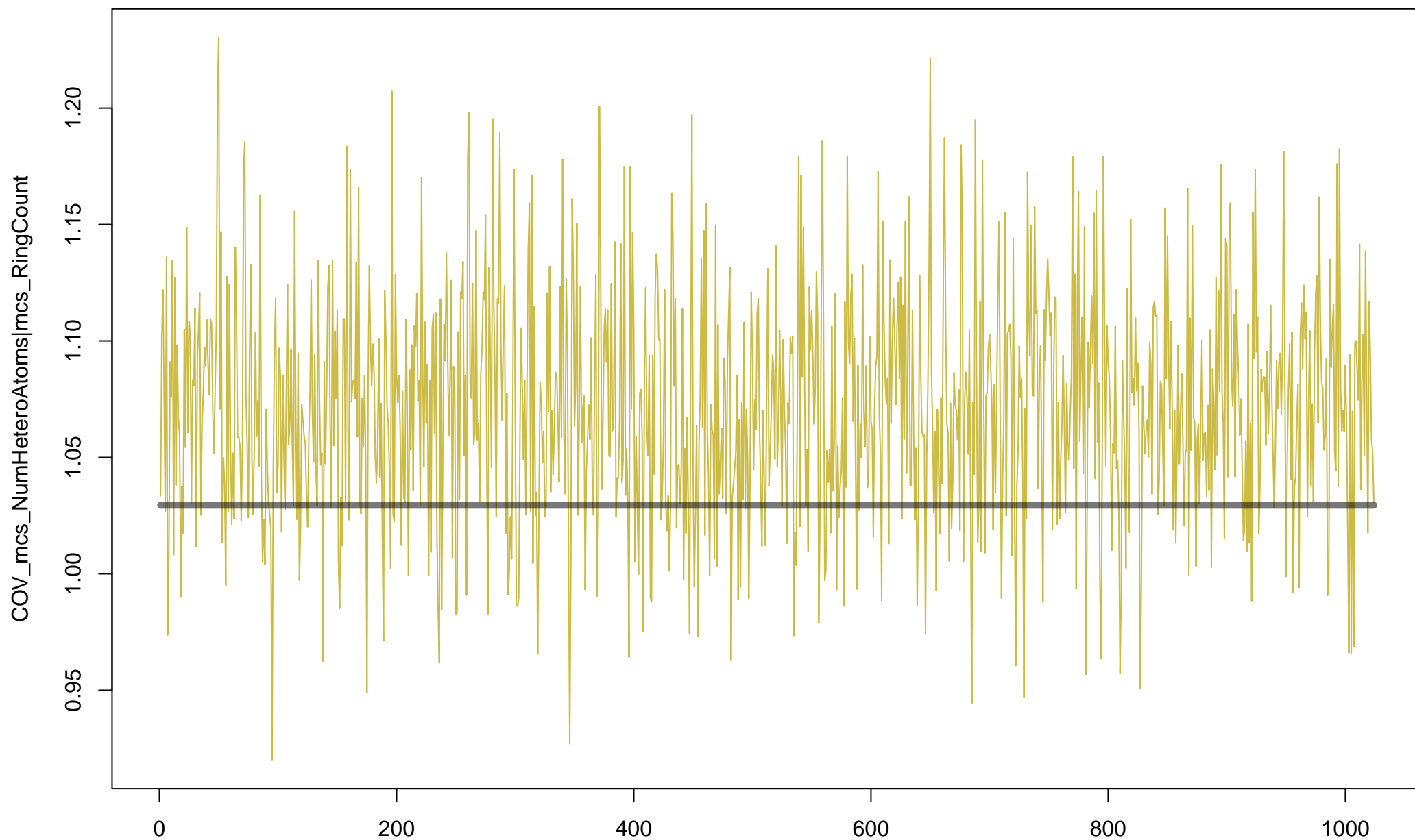
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NOCount**  
**ESS = 889 | BMK = 0.0433 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0 | percentile: 62.1**



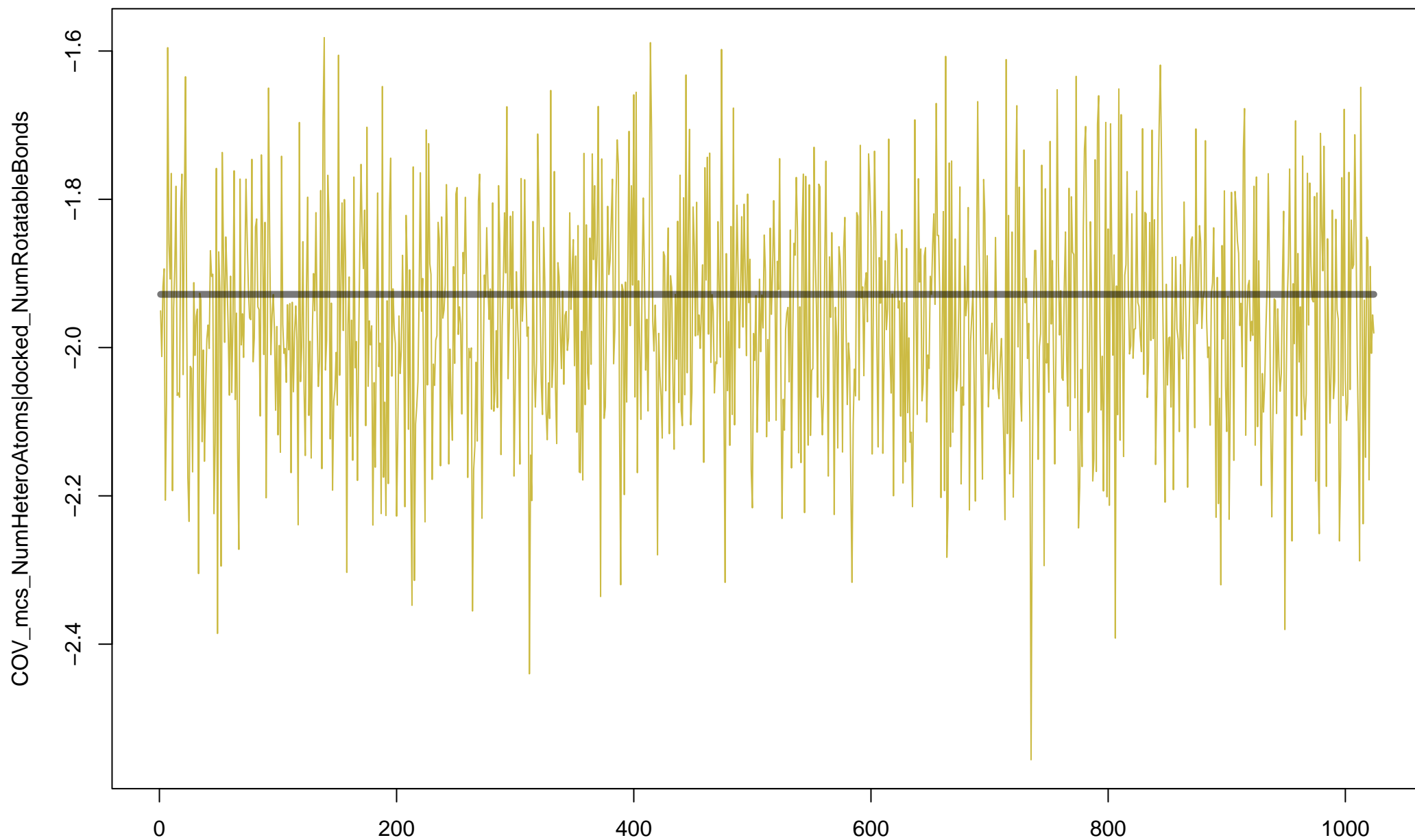
**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.0719 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0 | percentile: 17.7**



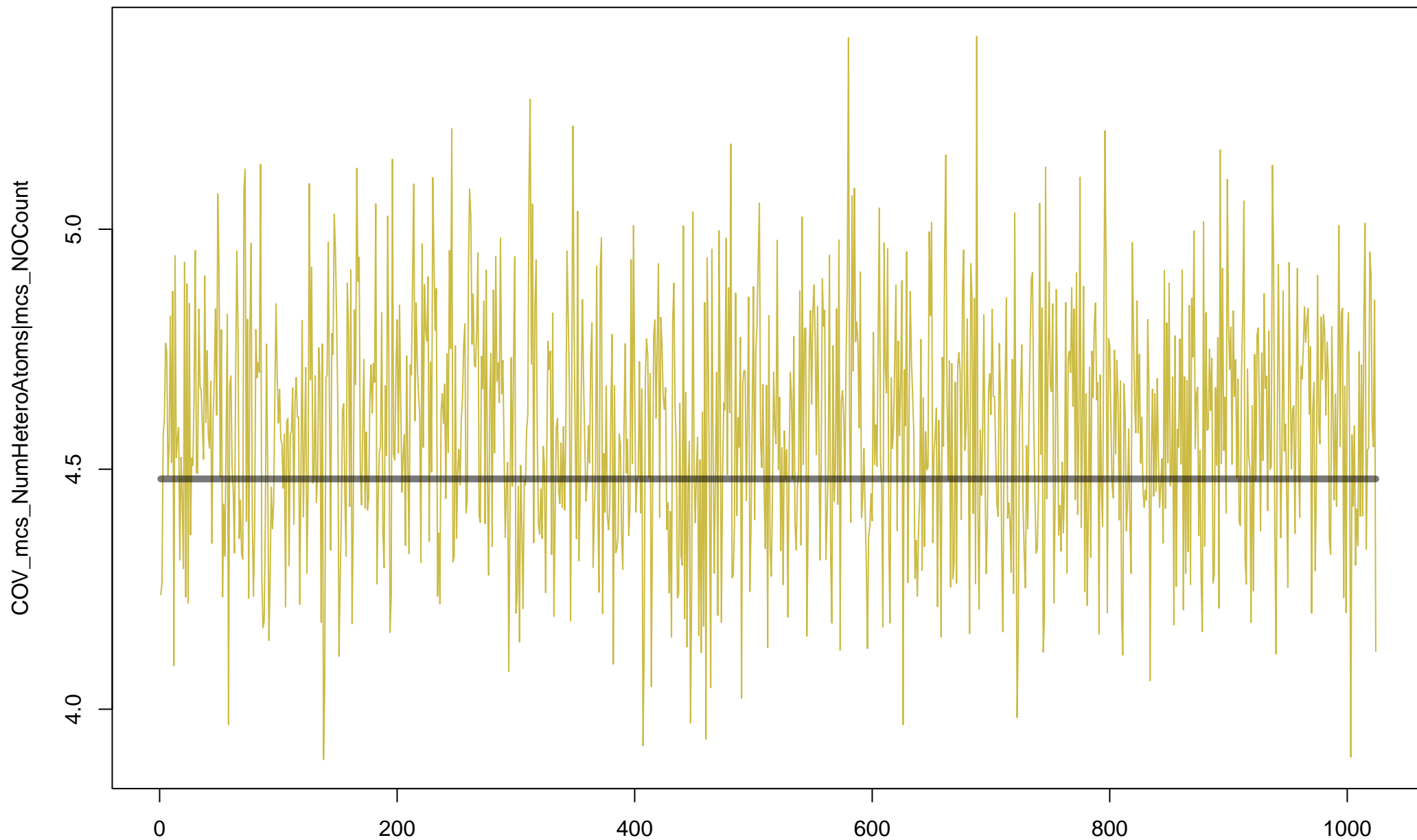
**COV\_mcs\_NumHeteroAtoms|mcs\_RingCount**  
**ESS = 936 | BMK = 0.0731 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | percentile: 19.6**



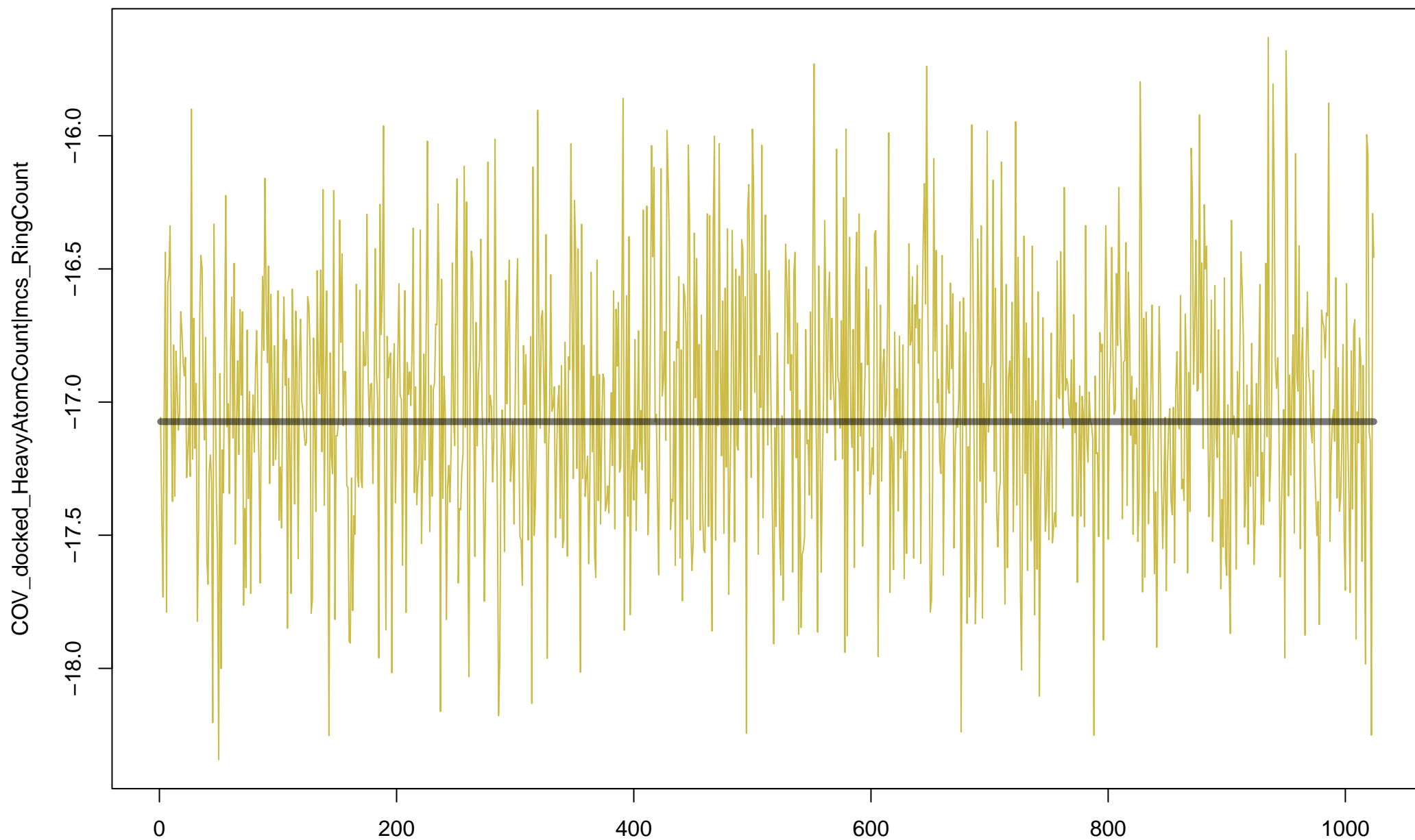
**COV\_mcs\_NumHeteroAtoms|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0497 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | percentile: 60.7**



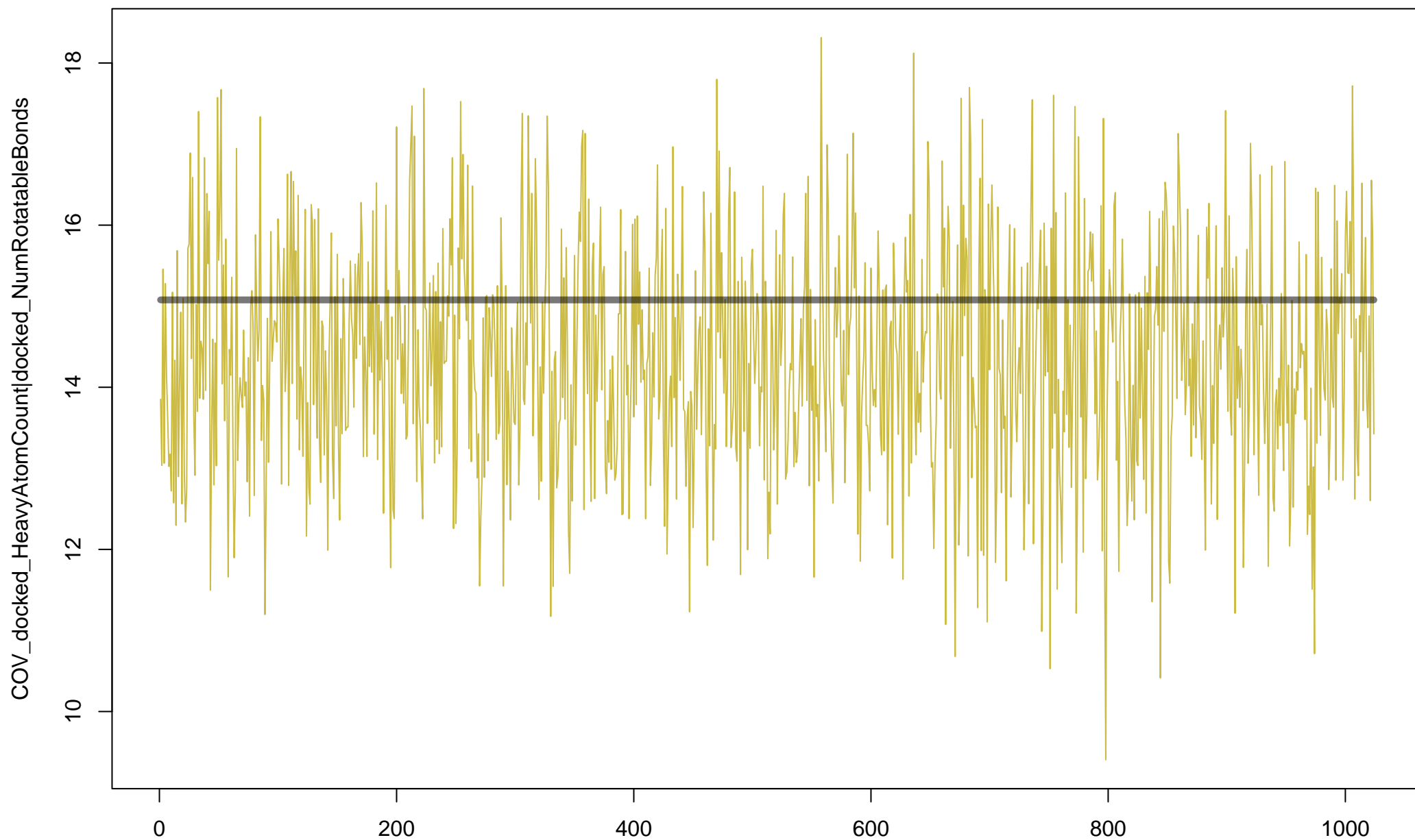
**COV\_mcs\_NumHeteroAtoms|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0504 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | percentile: 34.4**



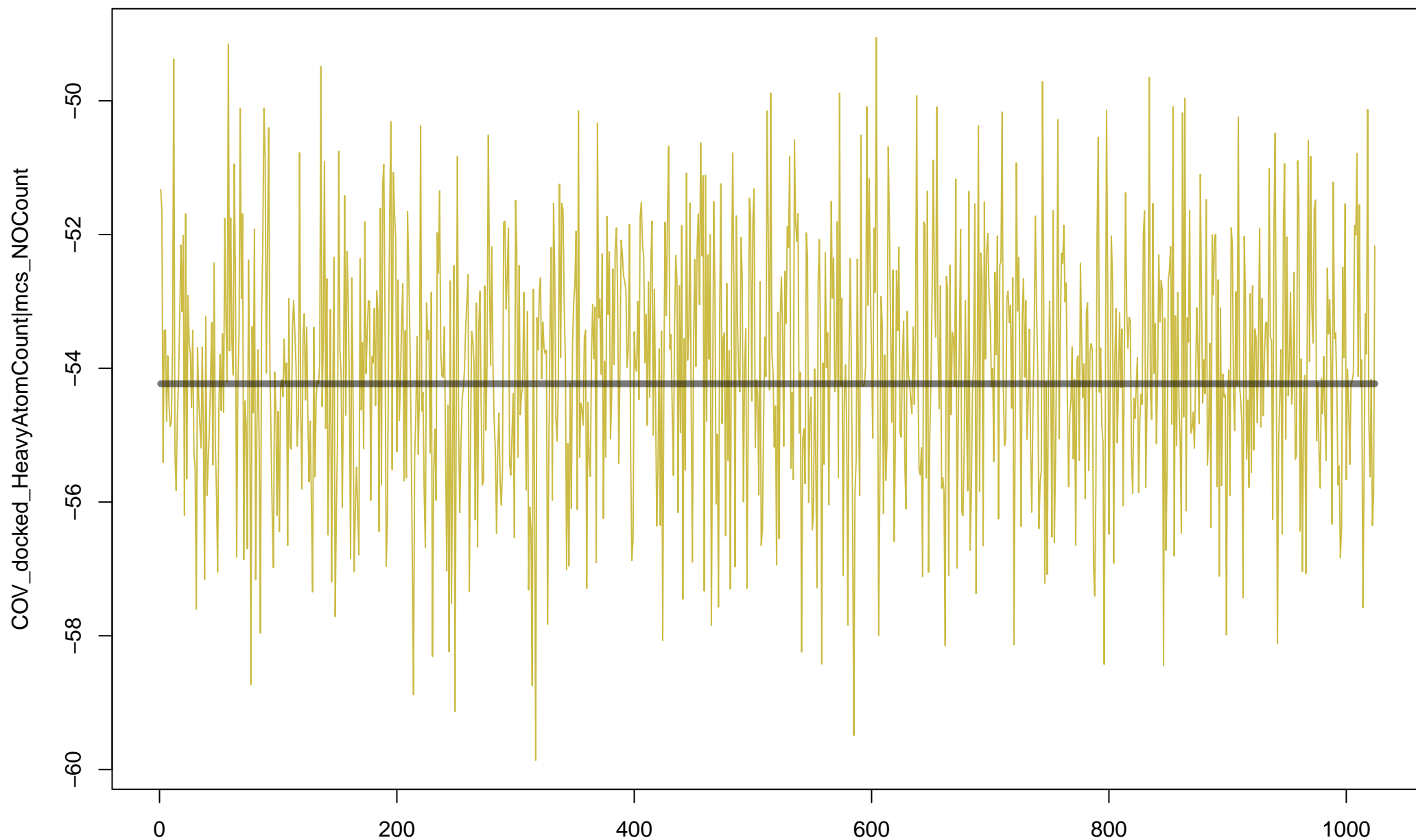
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.0519 | MCSE(6.27) = 3.39 | stat: TRUE | burn: 0 | percentile: 46**



**COV\_docked\_HeavyAtomCount|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0708 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0 | percentile: 70.3**

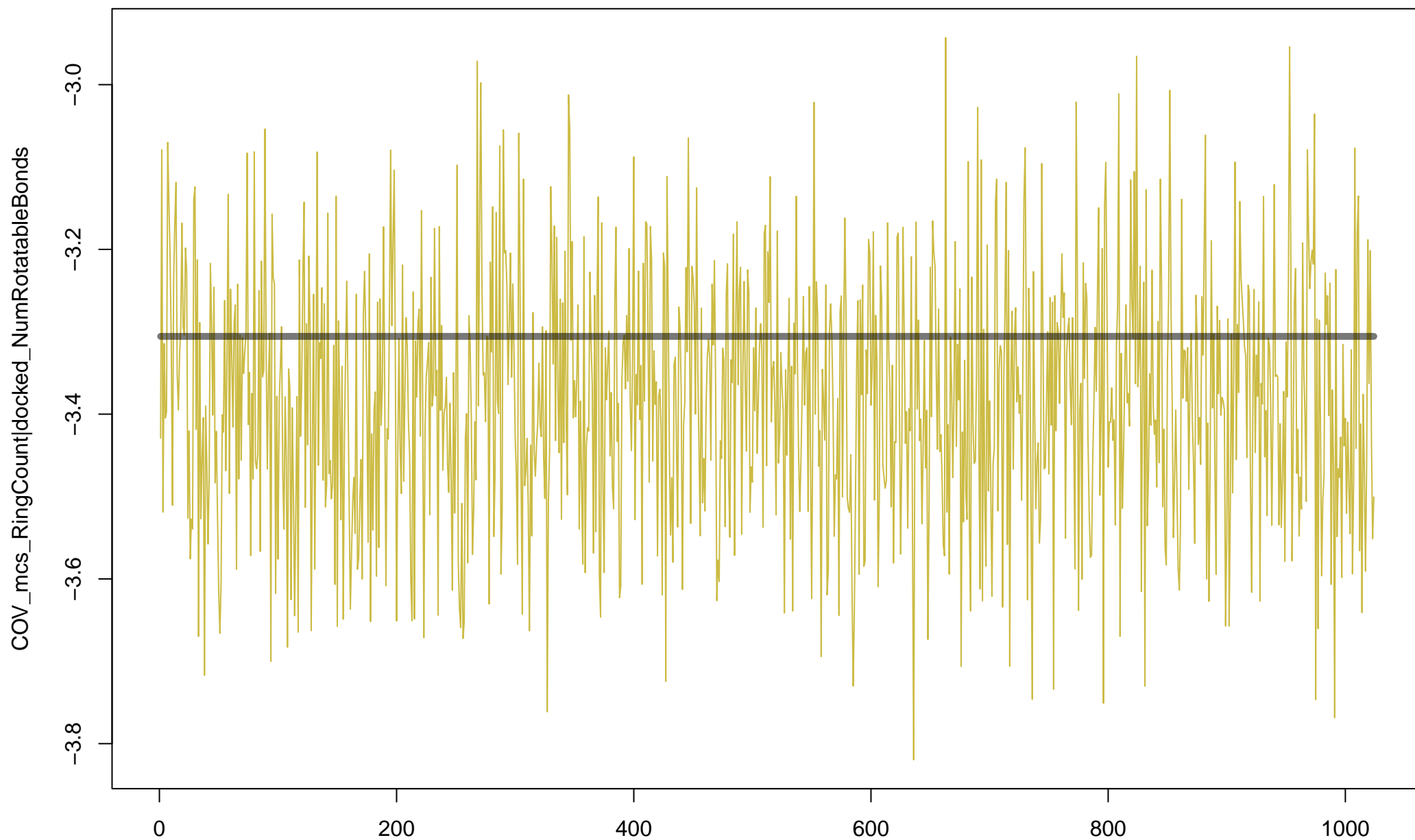


**COV\_docked\_HeavyAtomCount|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0419 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0 | percentile: 44.6**

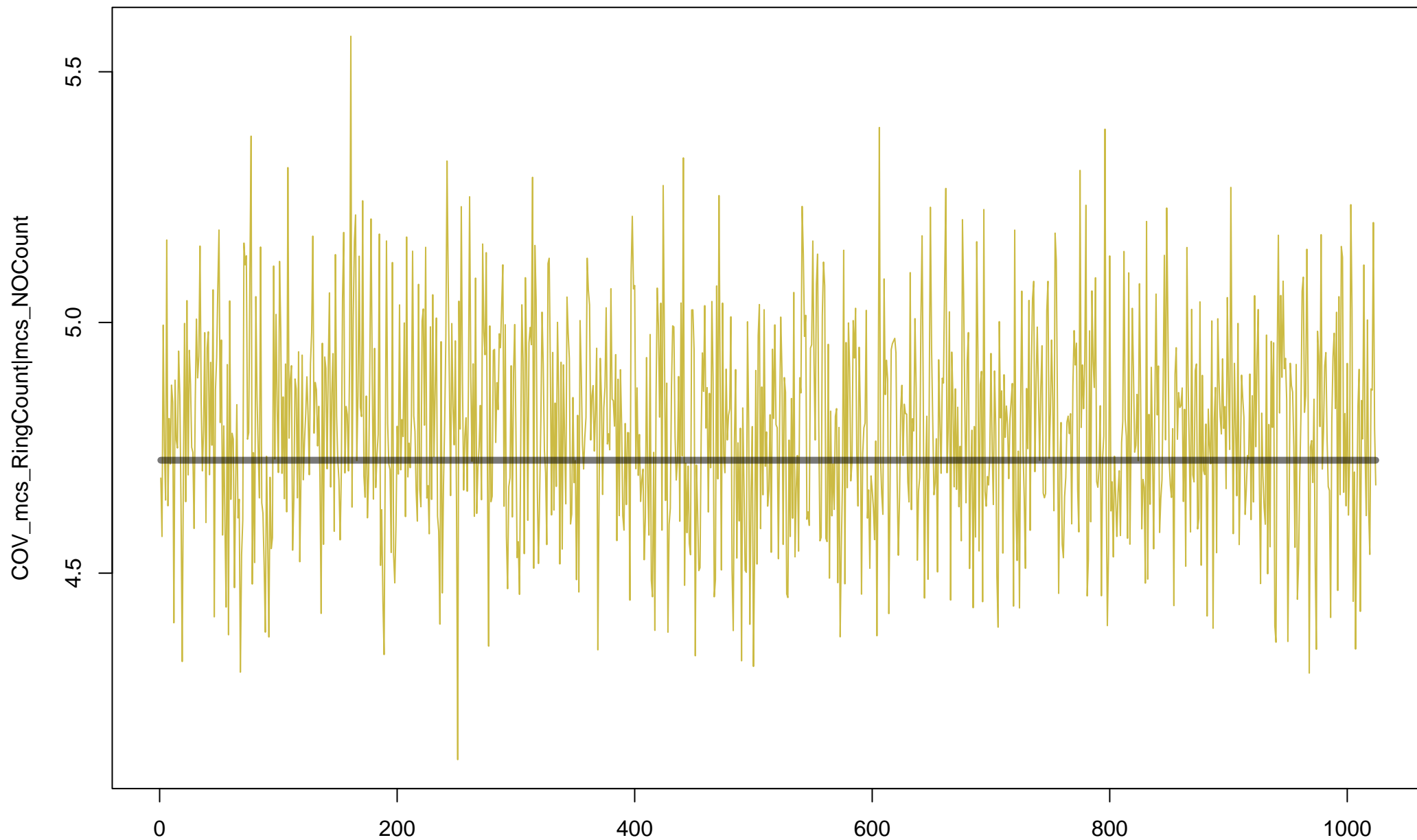




**COV\_mcs\_RingCount|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0412 | MCSE(6.27) = 3.39 | stat: TRUE | burn: 0 | percentile: 69.3**



**COV\_mcs\_RingCount|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0528 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0 | percentile: 39.4**



**COV\_docked\_NumRotatableBonds|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.0463 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0 | percentile: 16.1**

