

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 1

max MCSE = 15.5240293705988

all stationary: FALSE

burn: 1020

min percent.: 0

-- STATS 2D --

min ESS = 733.357336113444

max BMK = 0.235691190594886

max MCSE = 3.72490186409727

all stationary: FALSE

burn: 0

min percent.: 0

-- STATS 1D --

min ESS = 759.395836244138

max BMK = 0.867796195932841

max MCSE = 4.34181770847443

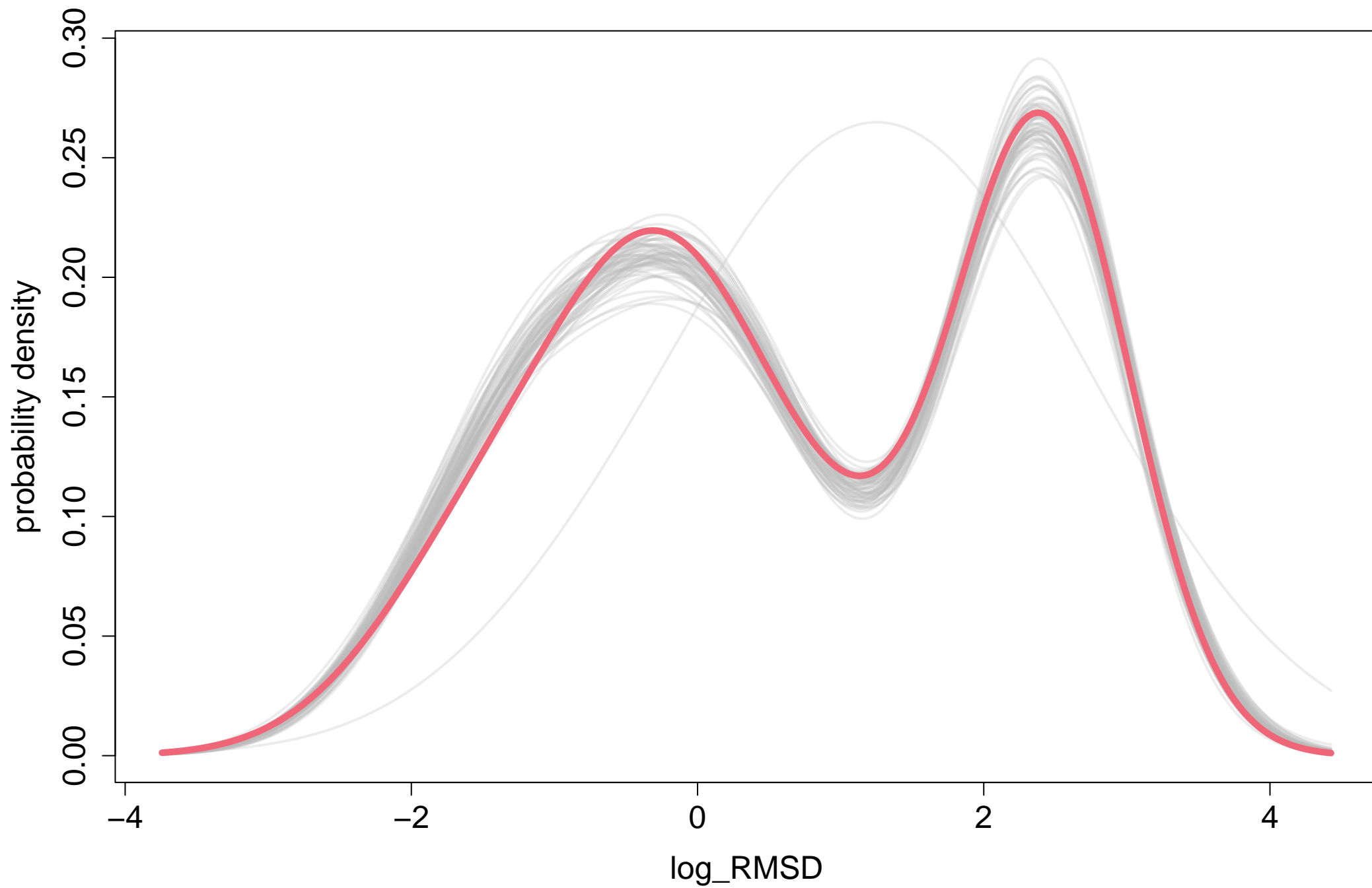
all stationary: FALSE

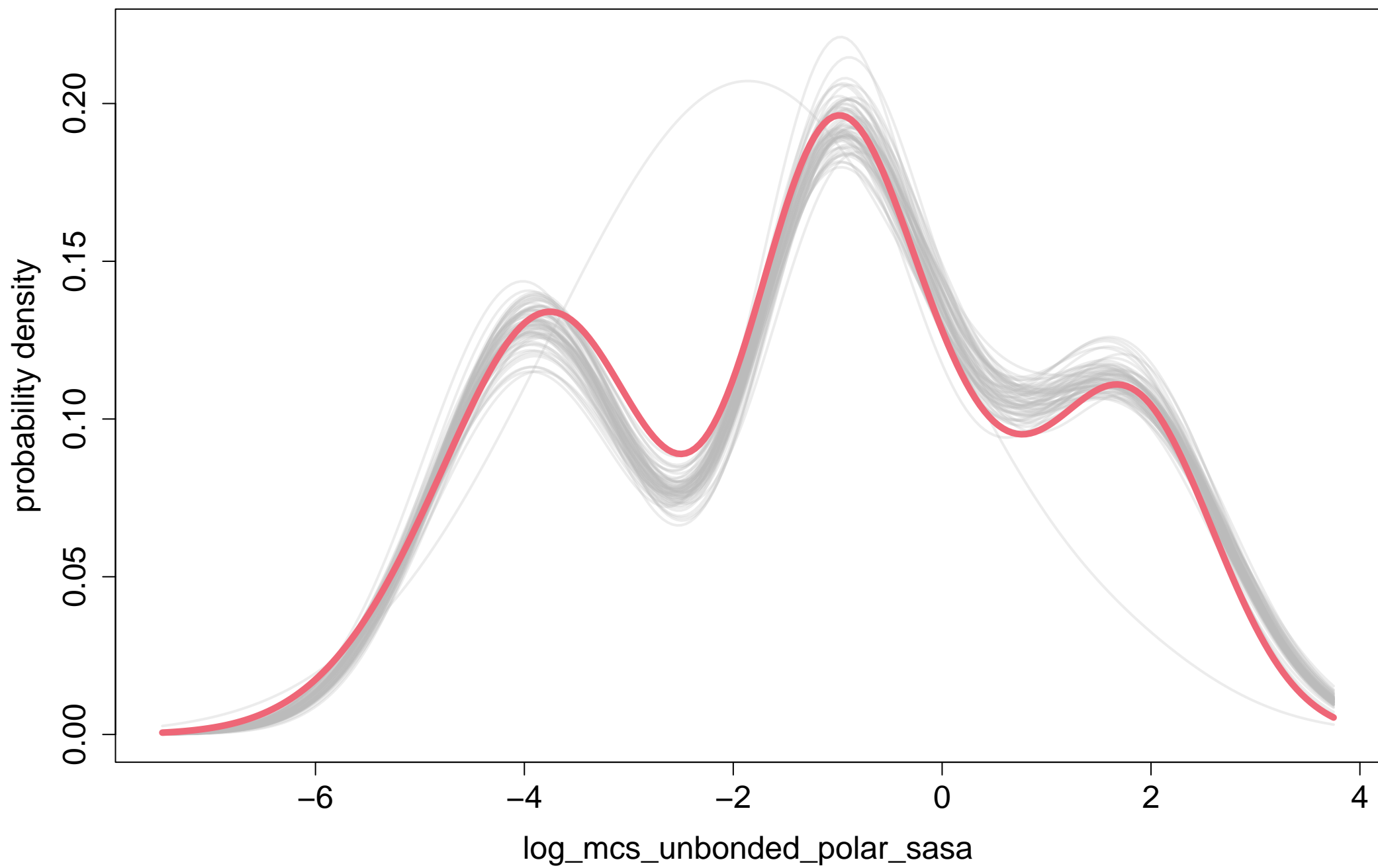
burn: 1020

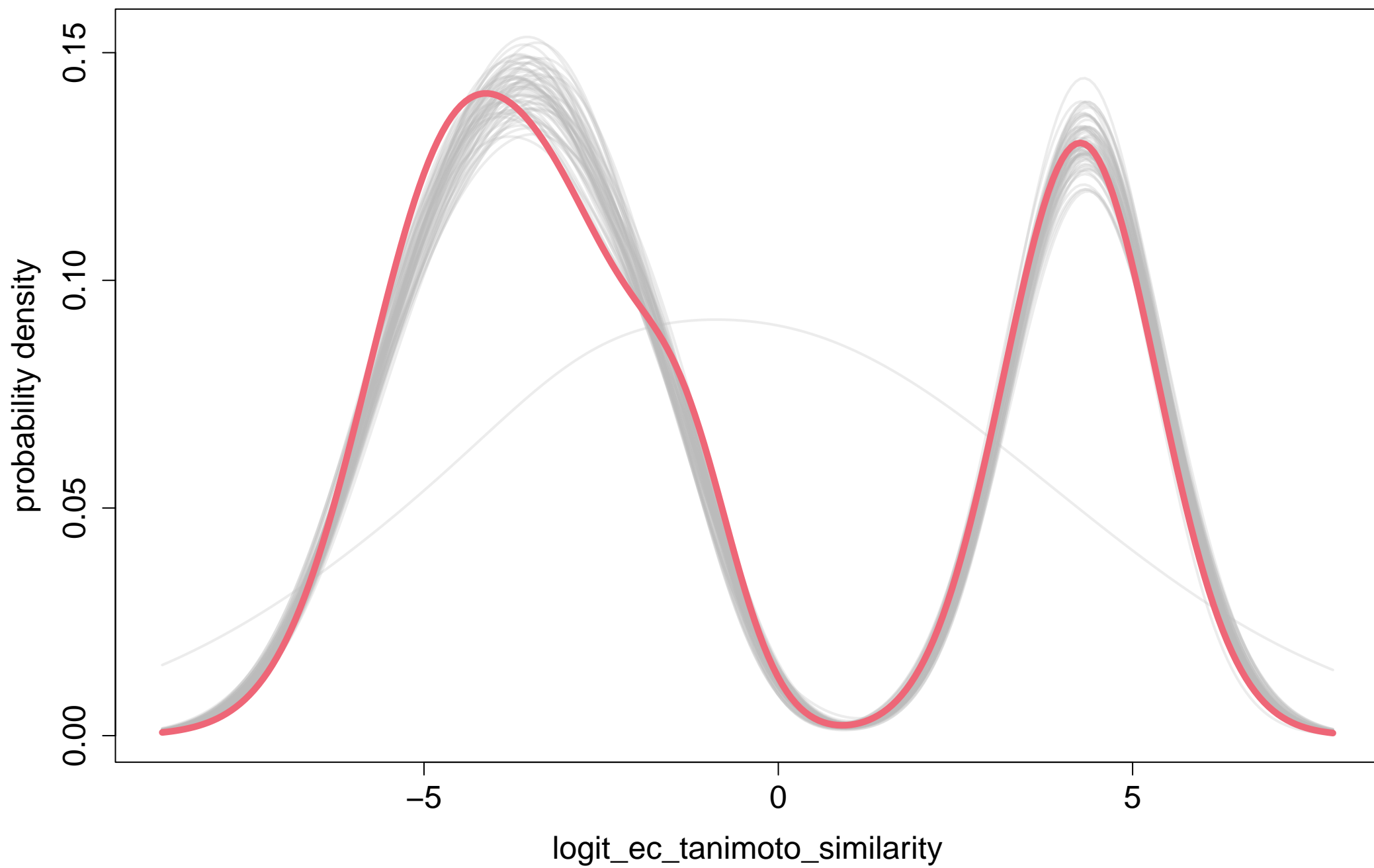
min percent.: 0

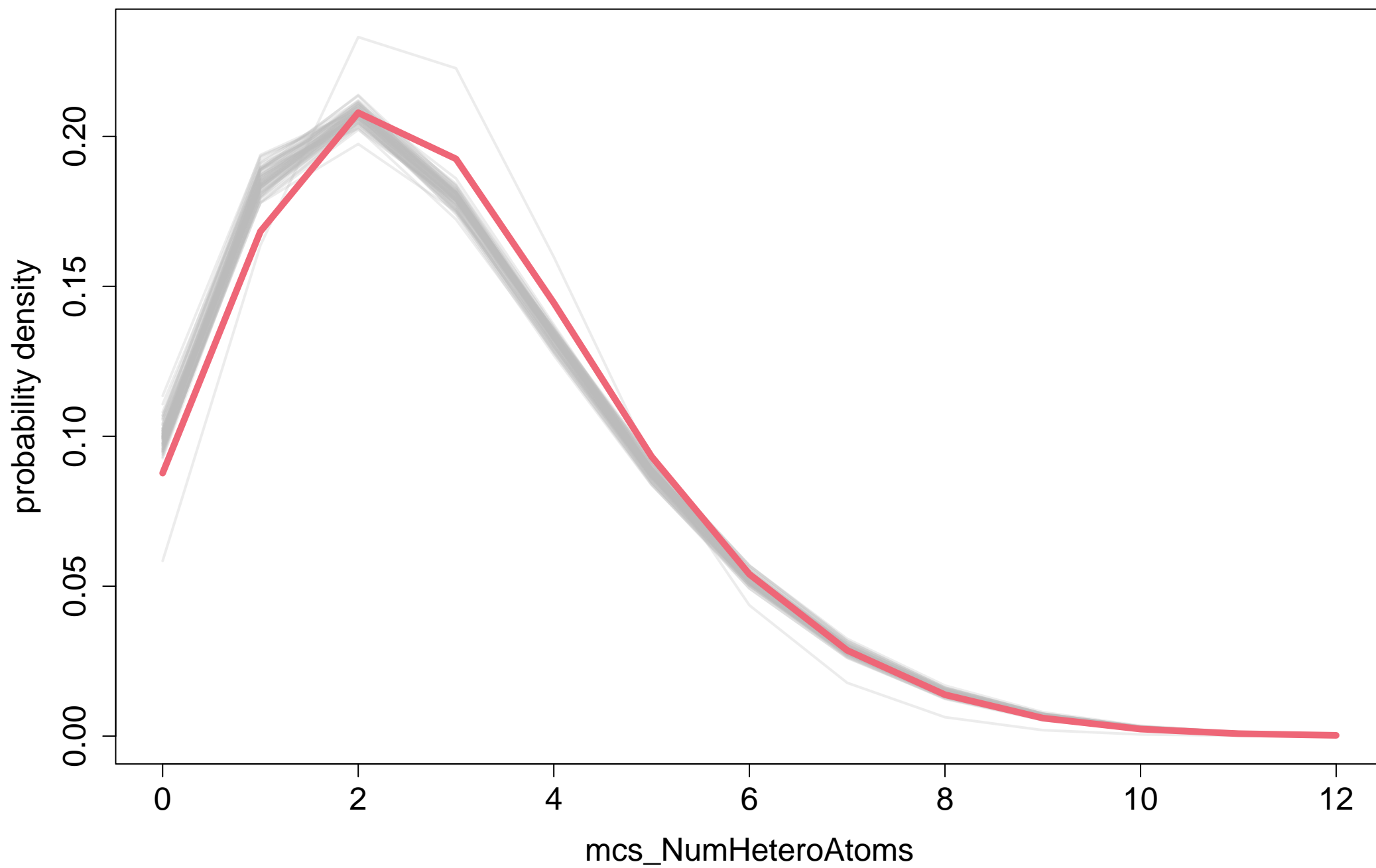
Occupied clusters: 5 of 64

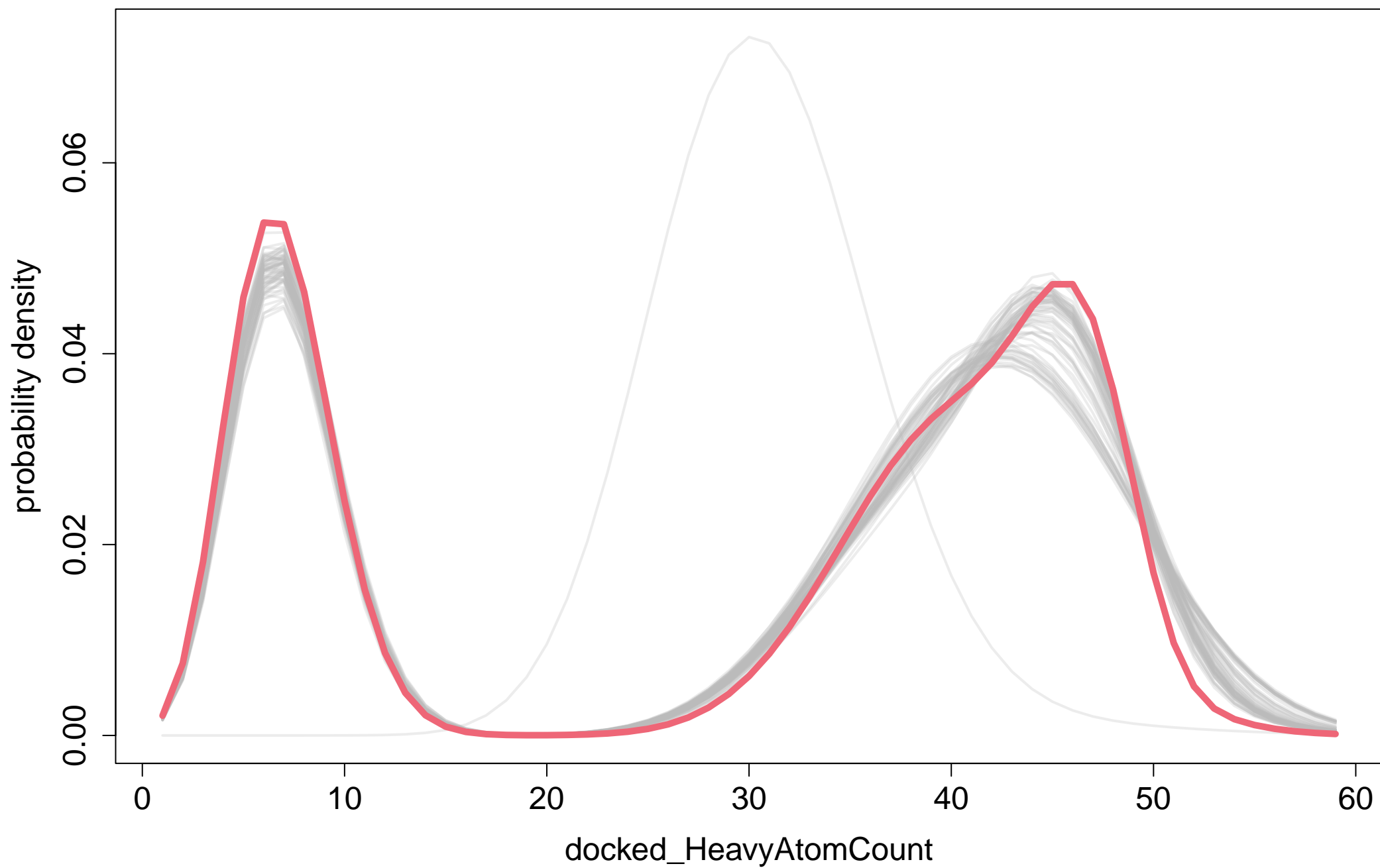
LL: -34200 +- 731

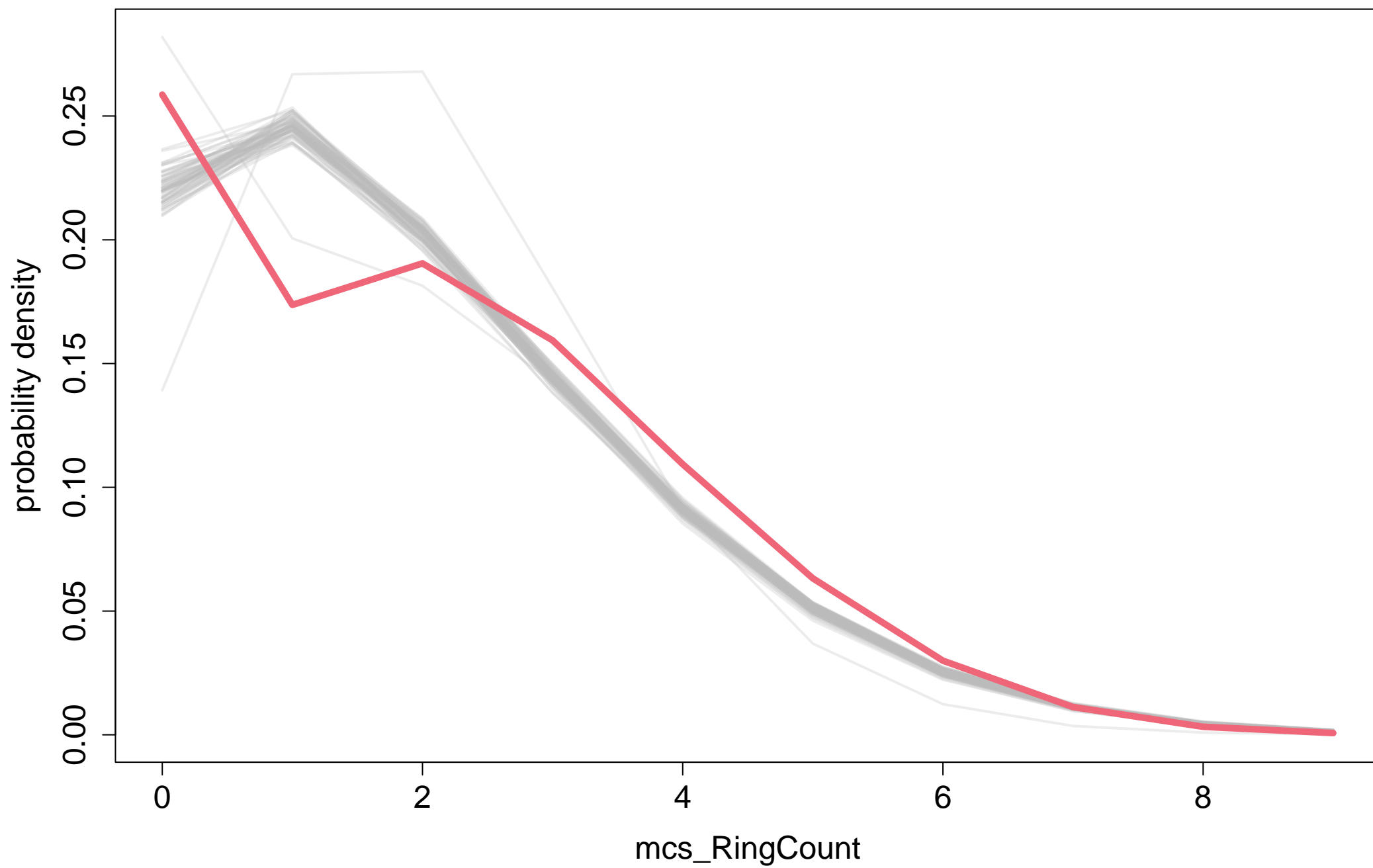


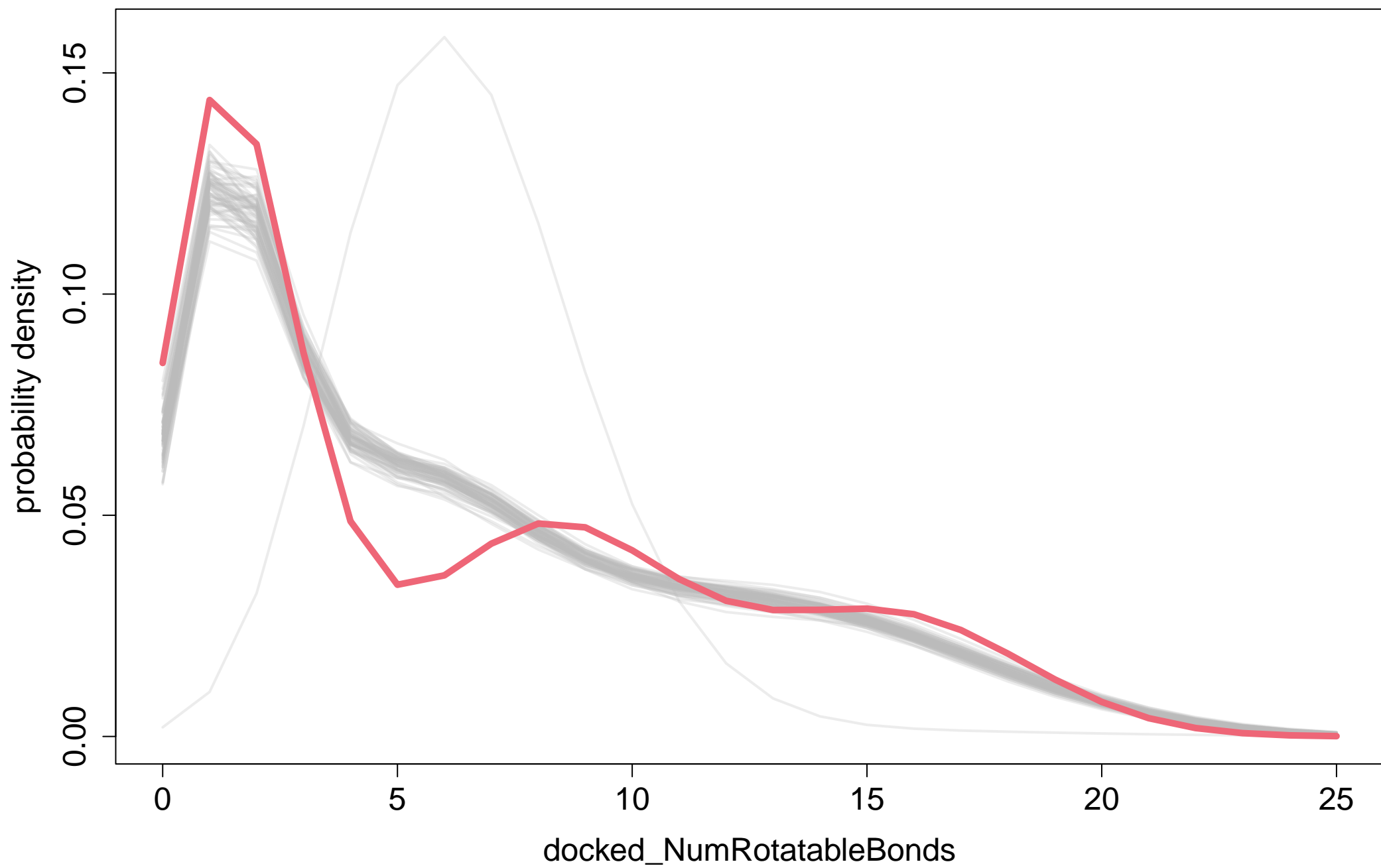




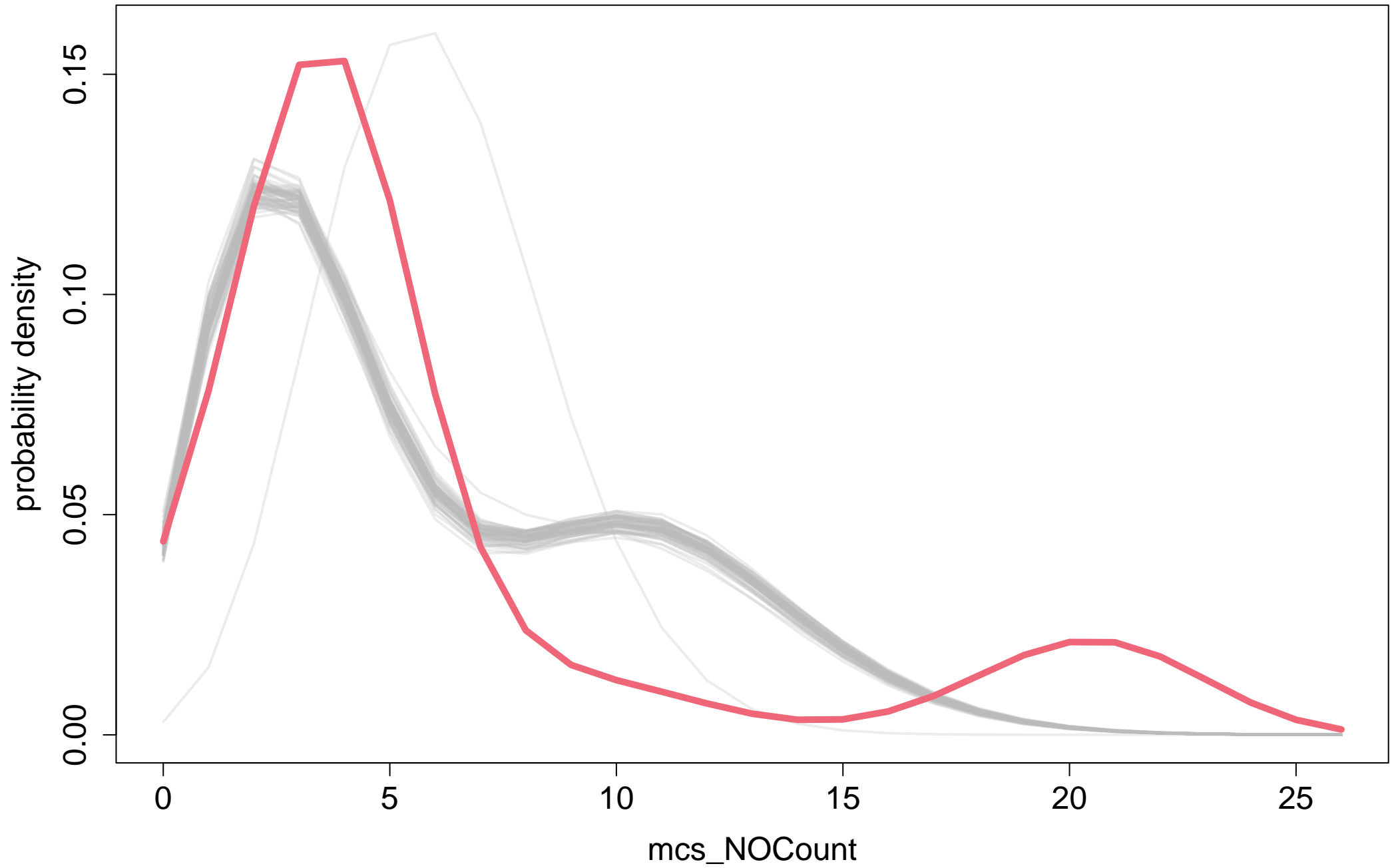


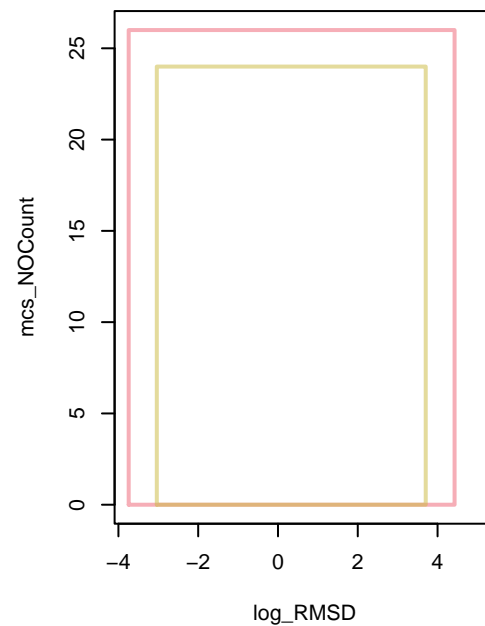
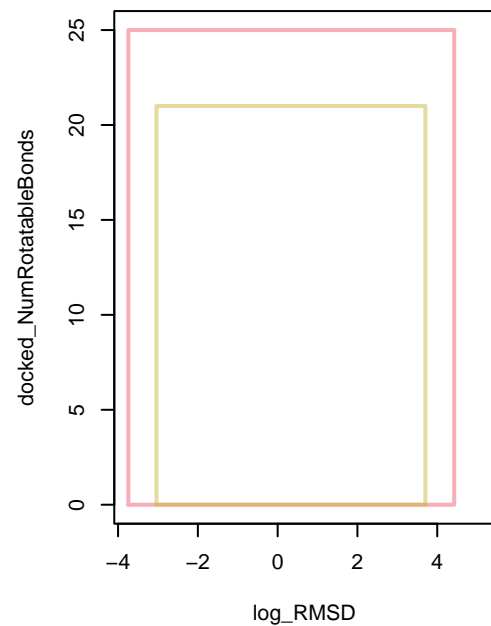
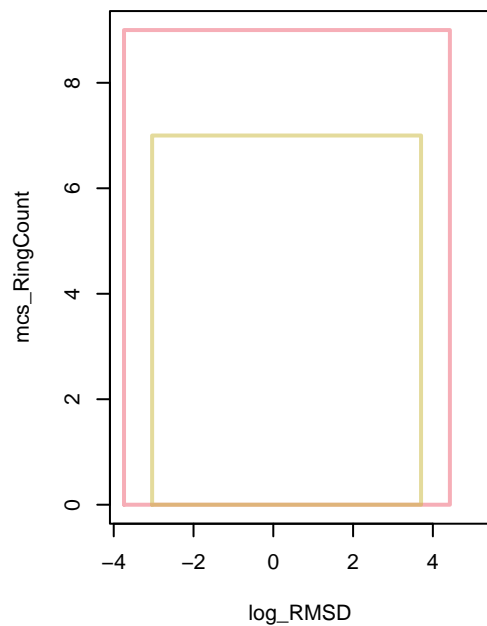
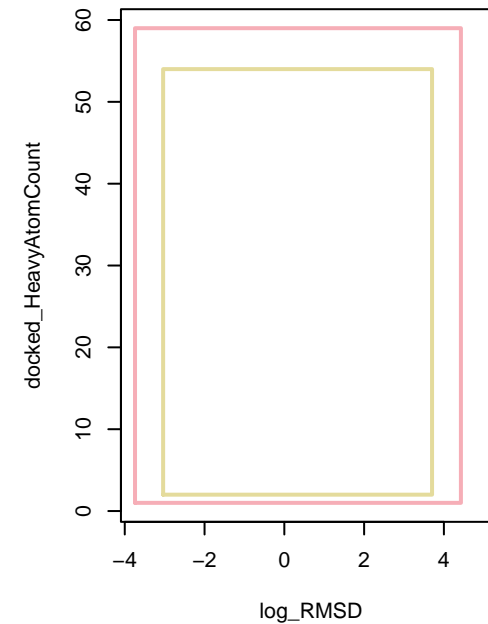
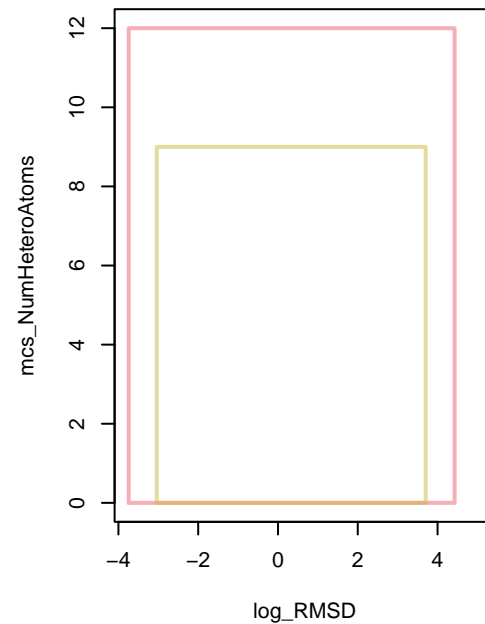
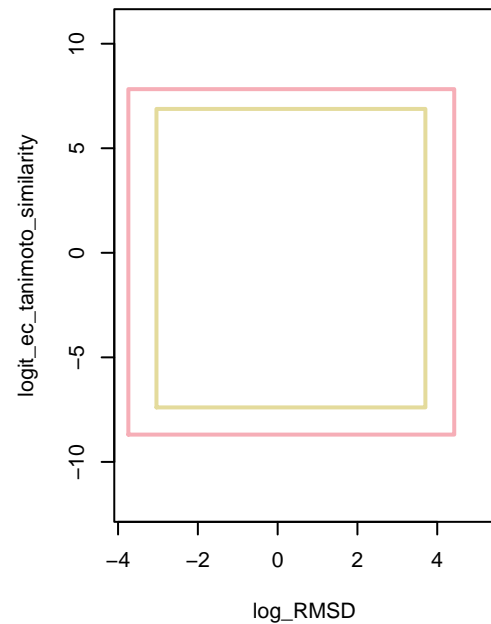
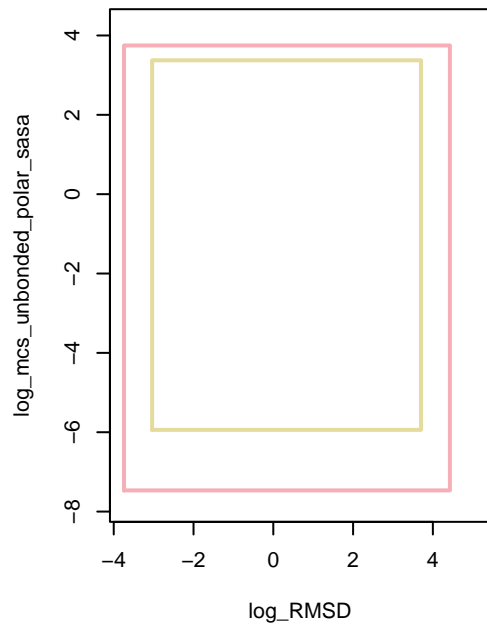




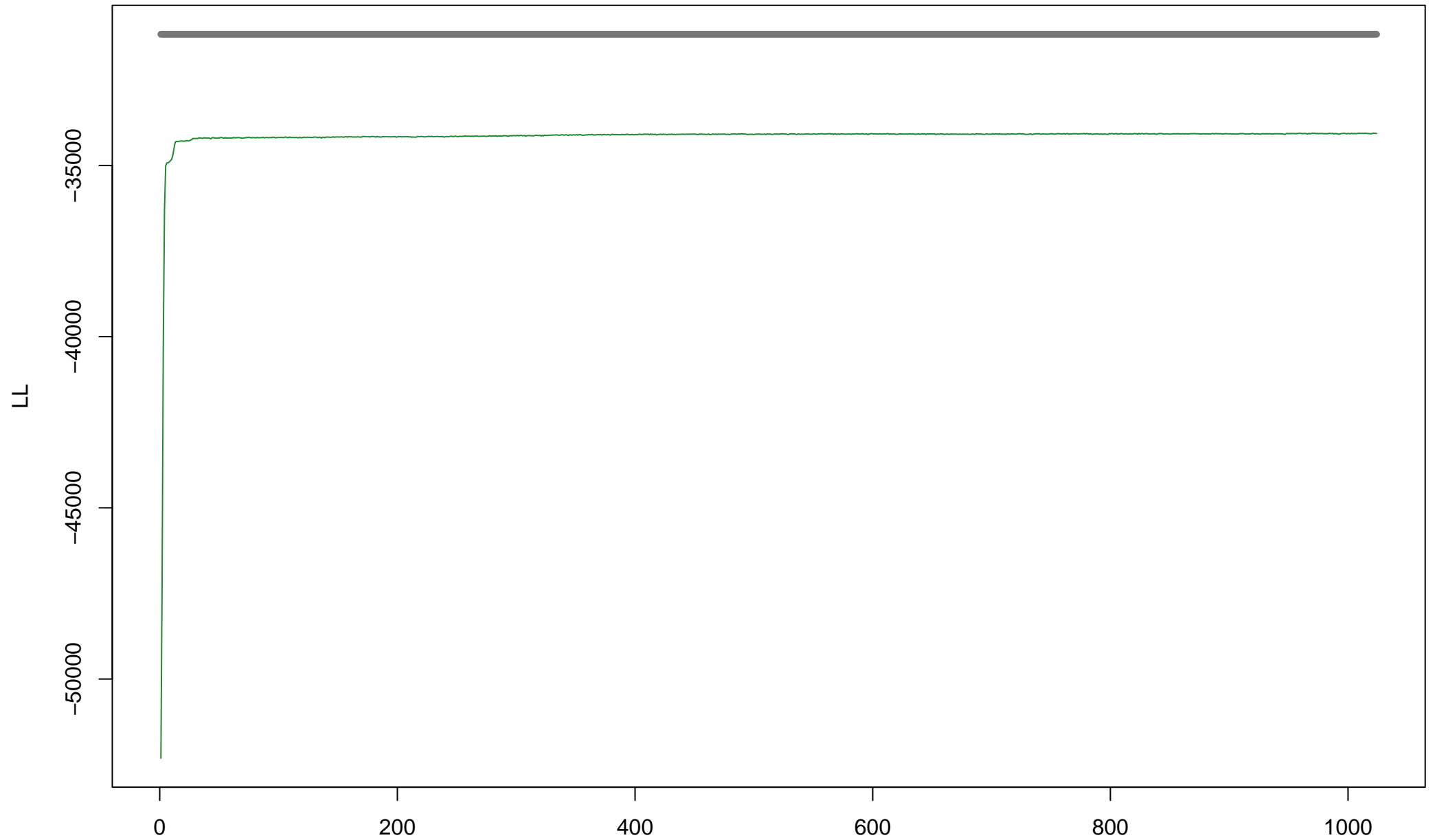






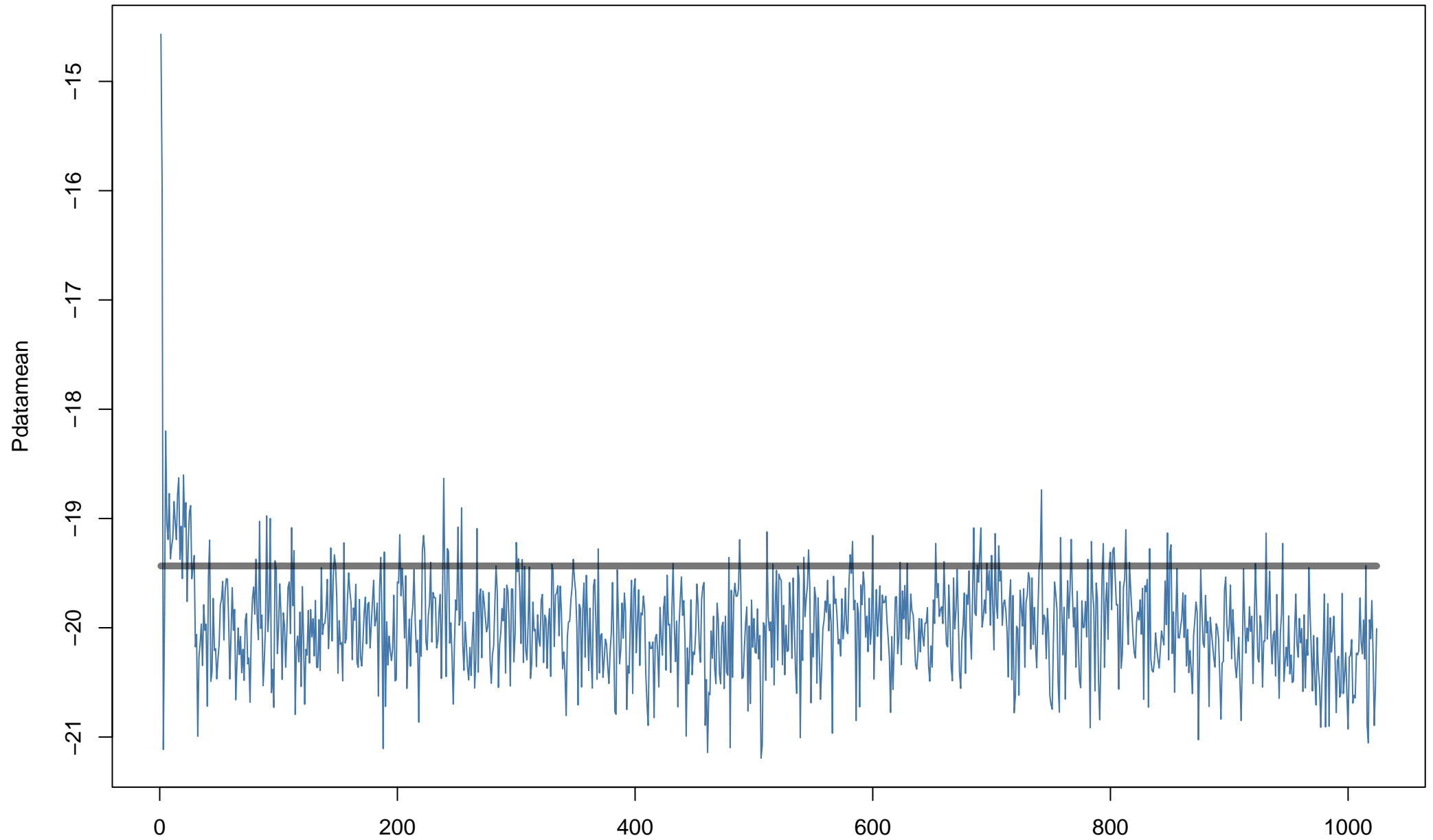


LL



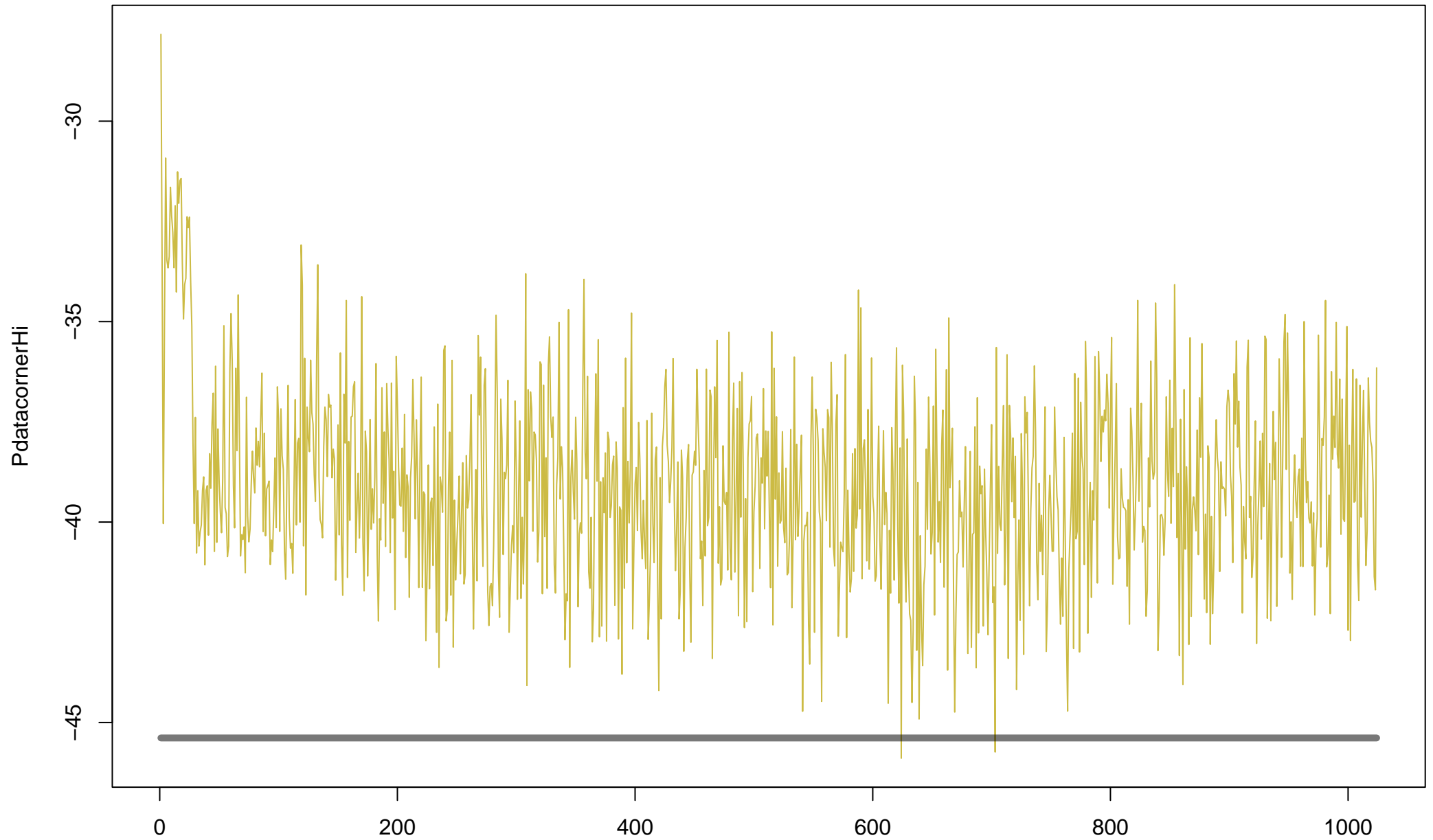
**Pdatamean**

**ESS = 717 | BMK = 0.128 | MCSE(6.27) = 4.29 | stat: TRUE | burn: 0 | percentile: 90.4**



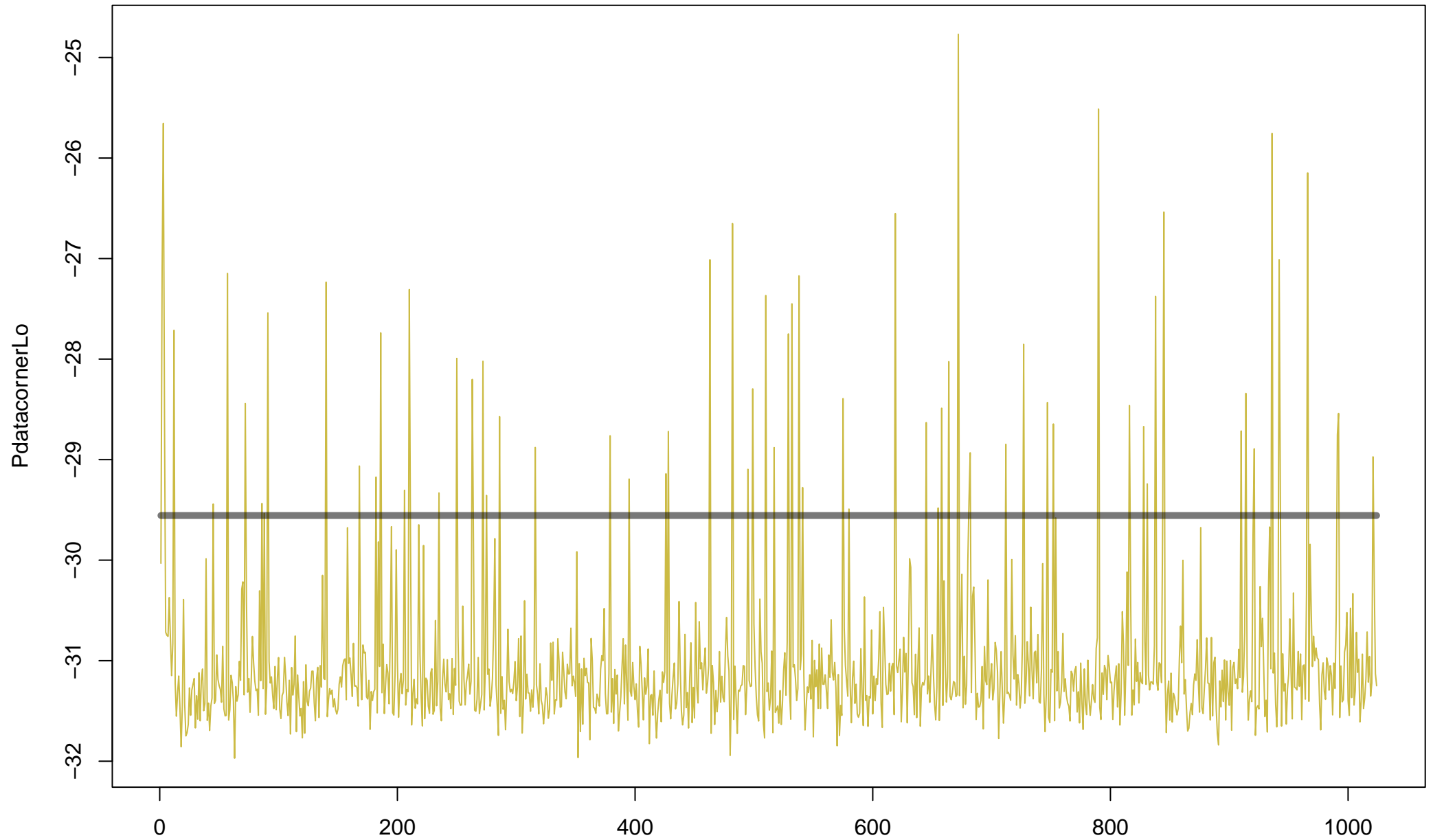
# PdatacornerHi

ESS = 2.22e-16 | BMK = 1 | MCSE(6.27) = 3.92 | stat: TRUE | burn: 102 | percentile: 0.195

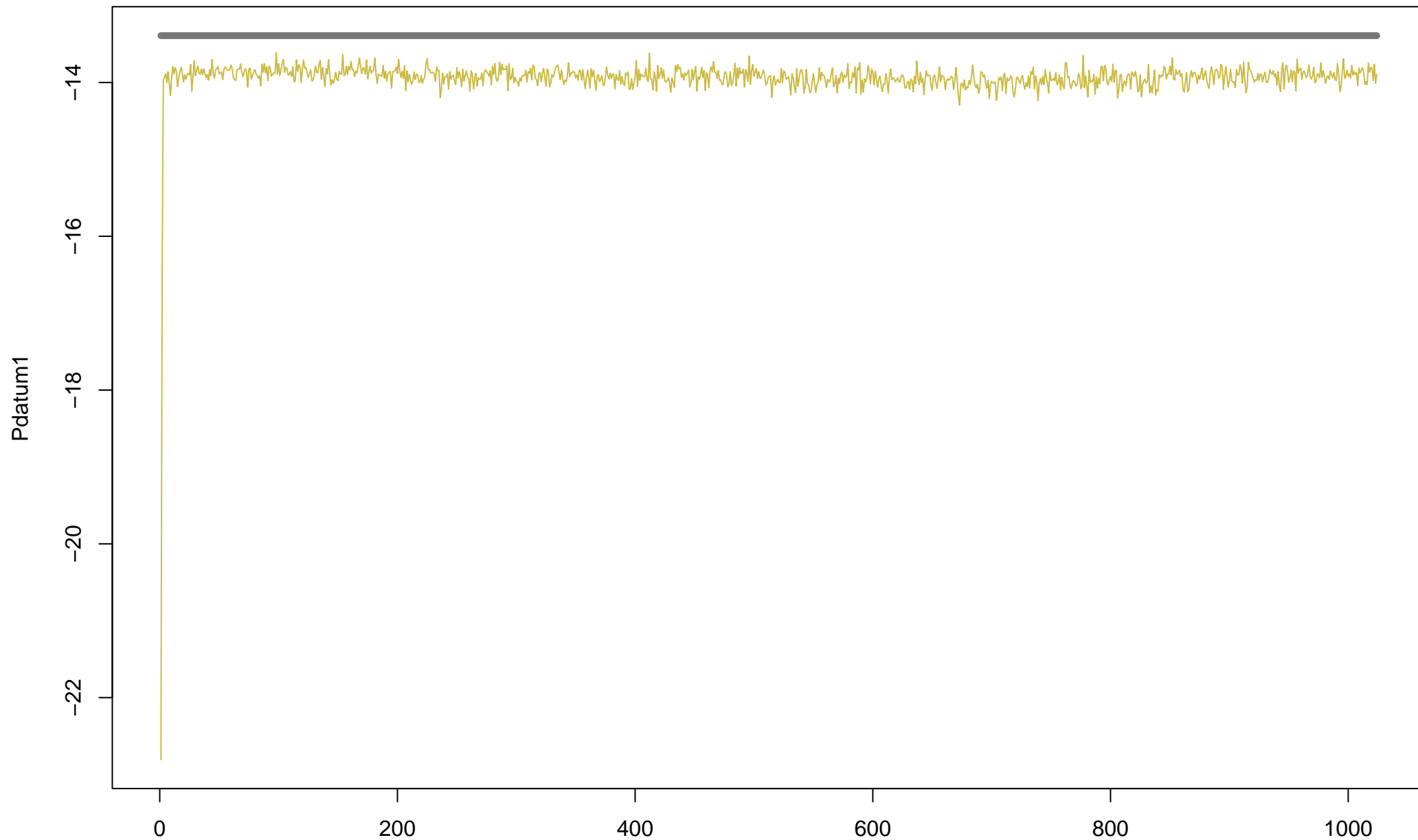


# PdatacornerLo

ESS = 2.22e-16 | BMK = 0.371 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 714 | percentile: 93.4

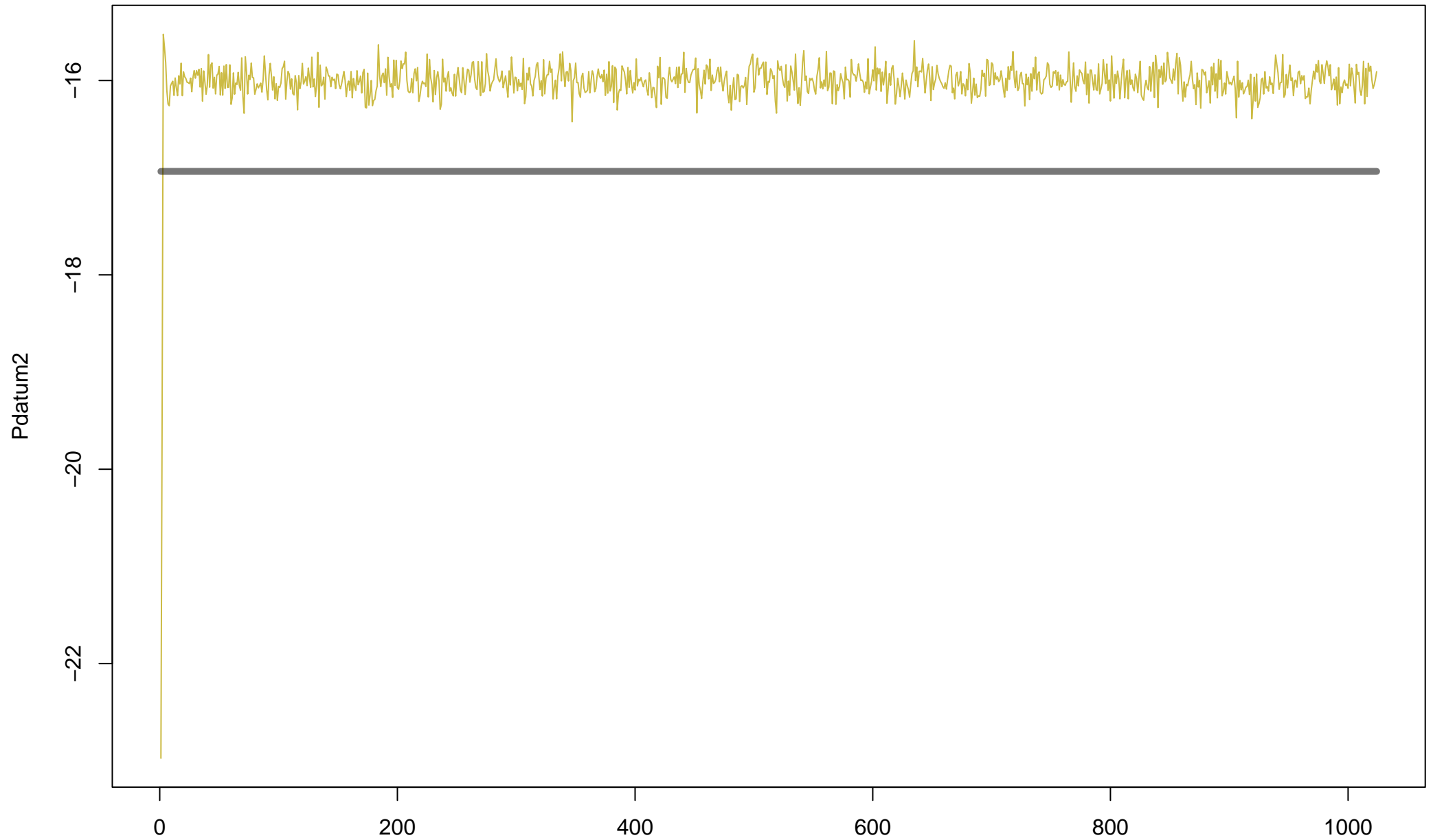


**Pdatum1**  
**ESS = 93 | BMK = 0.195 | MCSE(6.27) = 6.61 | stat: FALSE | burn: 0 | percentile: 100**



**Pdatum2**

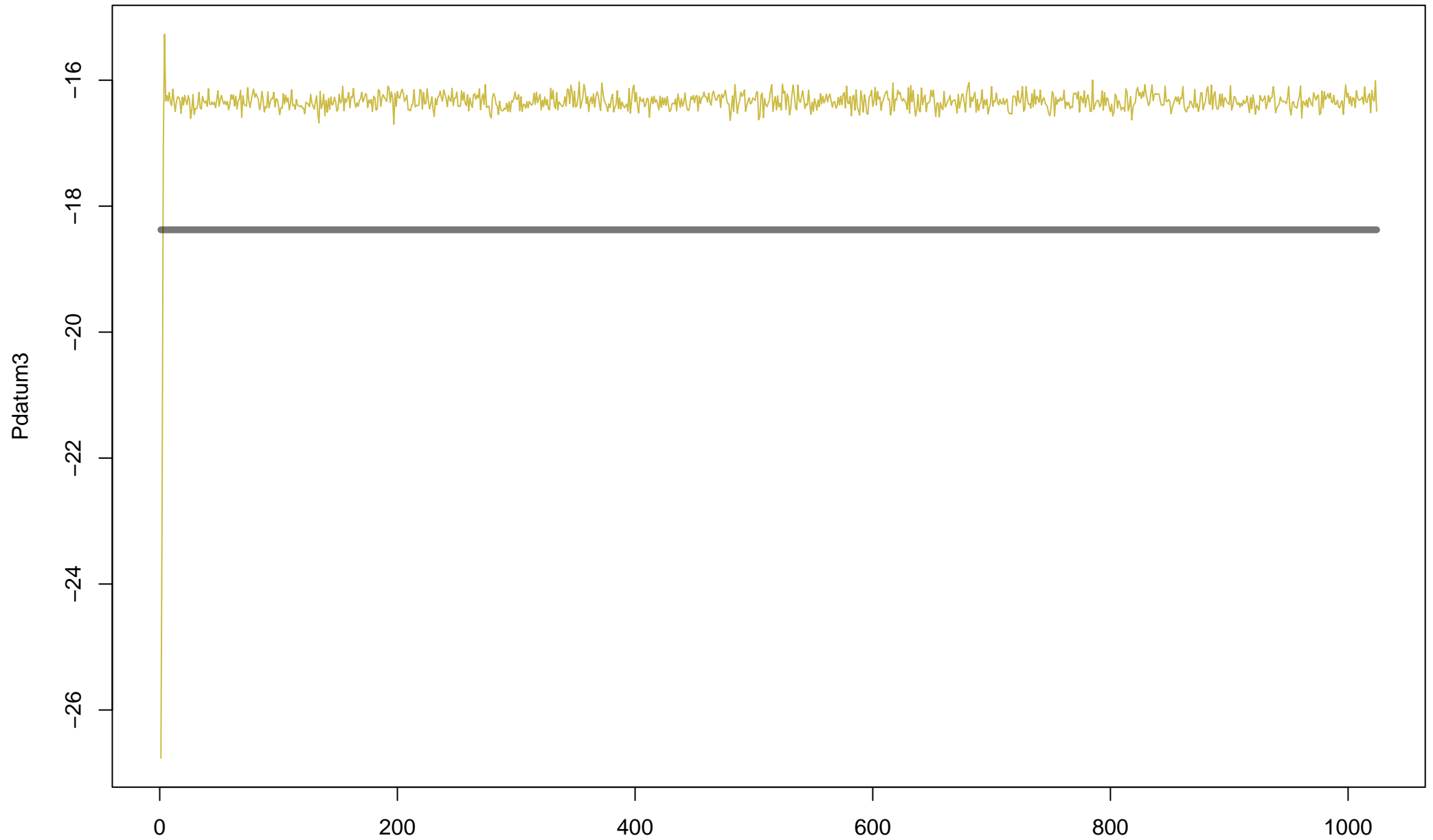
**ESS = 1020 | BMK = 0.0492 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0 | percentile: 0.195**





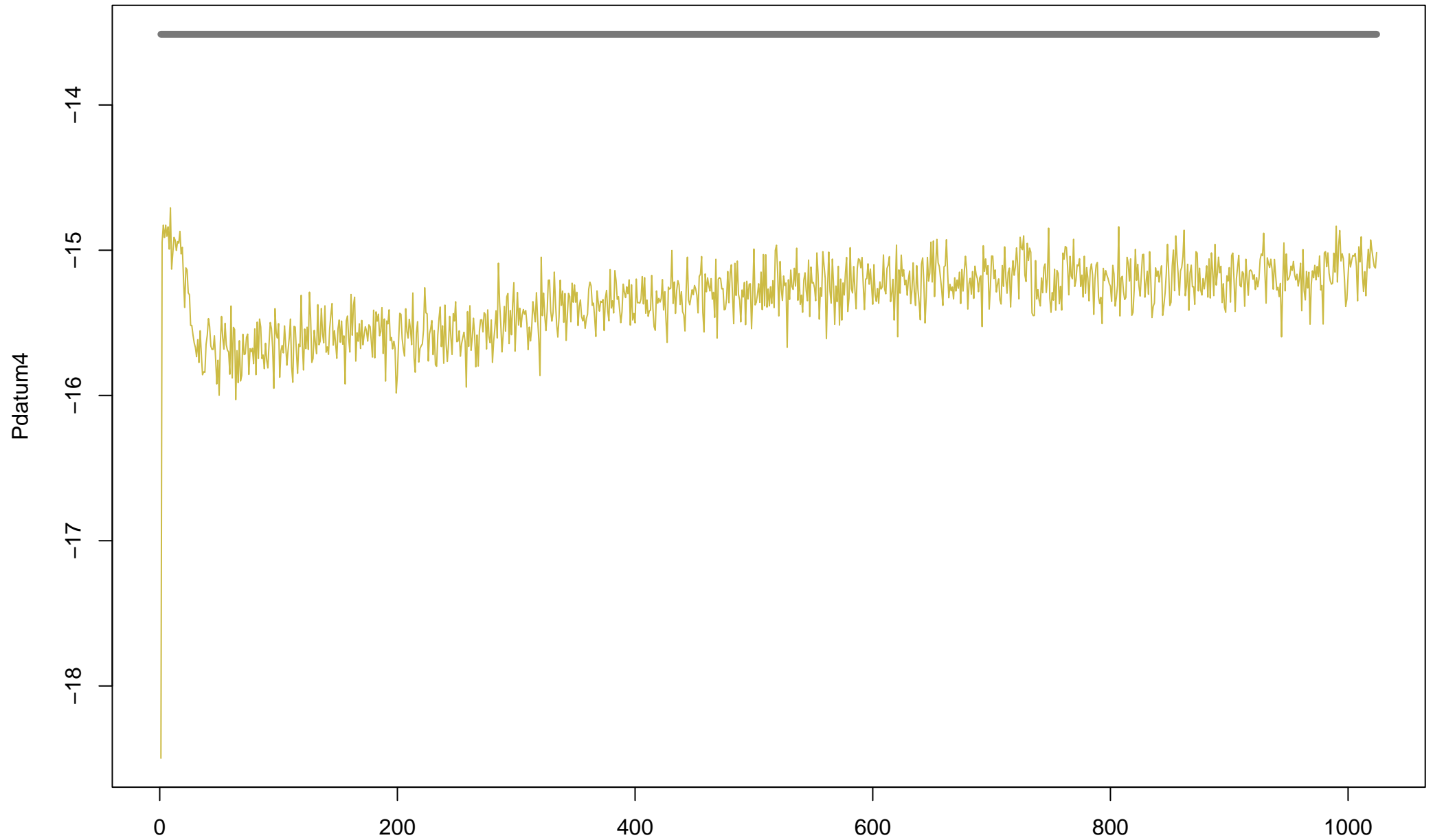
Pdatum3

ESS = 2.22e-16 | BMK = 0.0859 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | percentile: 0.195



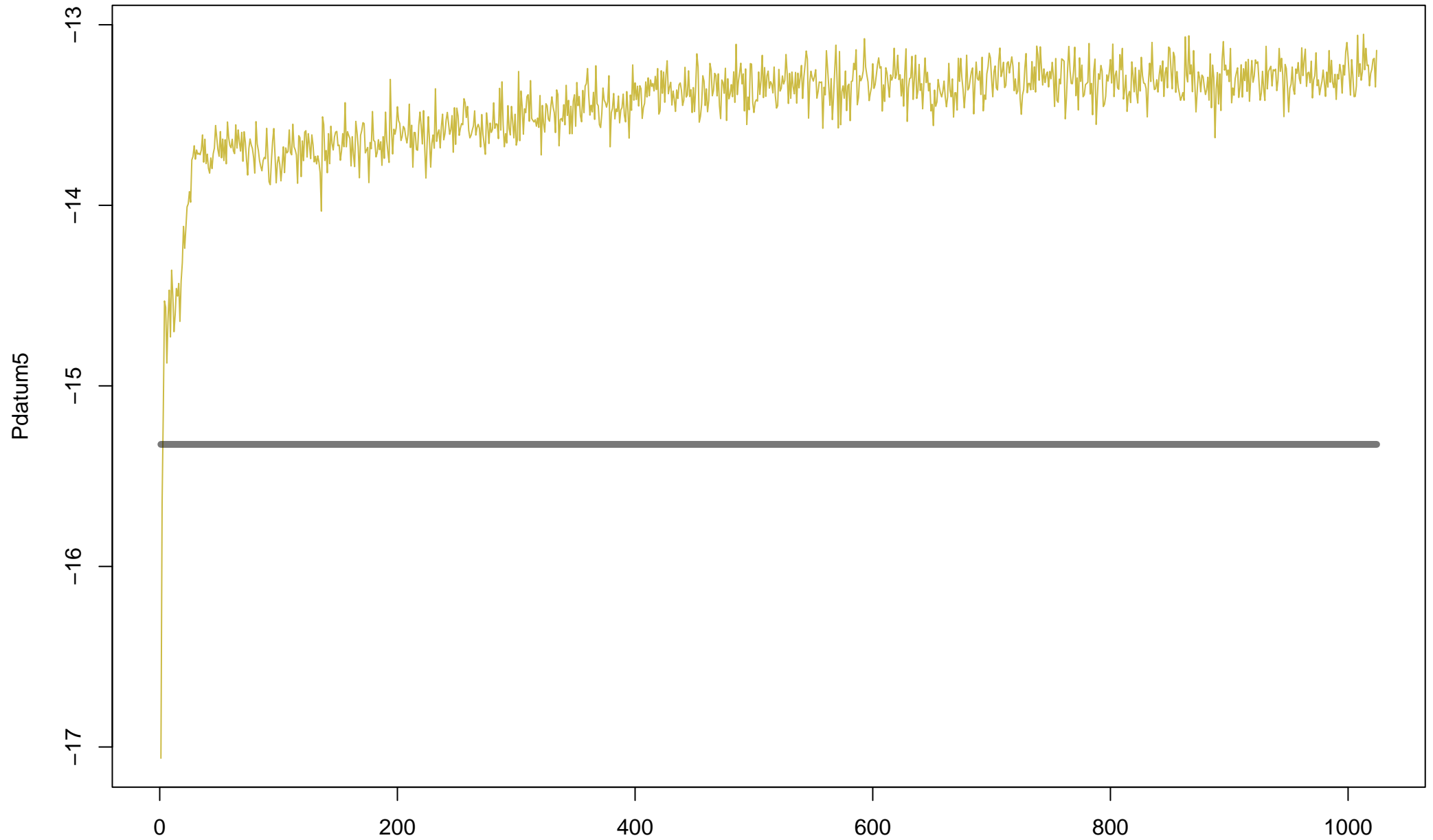
**Pdatum4**

**ESS = 15.5 | BMK = 0.522 | MCSE(6.27) = 13.4 | stat: FALSE | burn: 0 | percentile: 100**



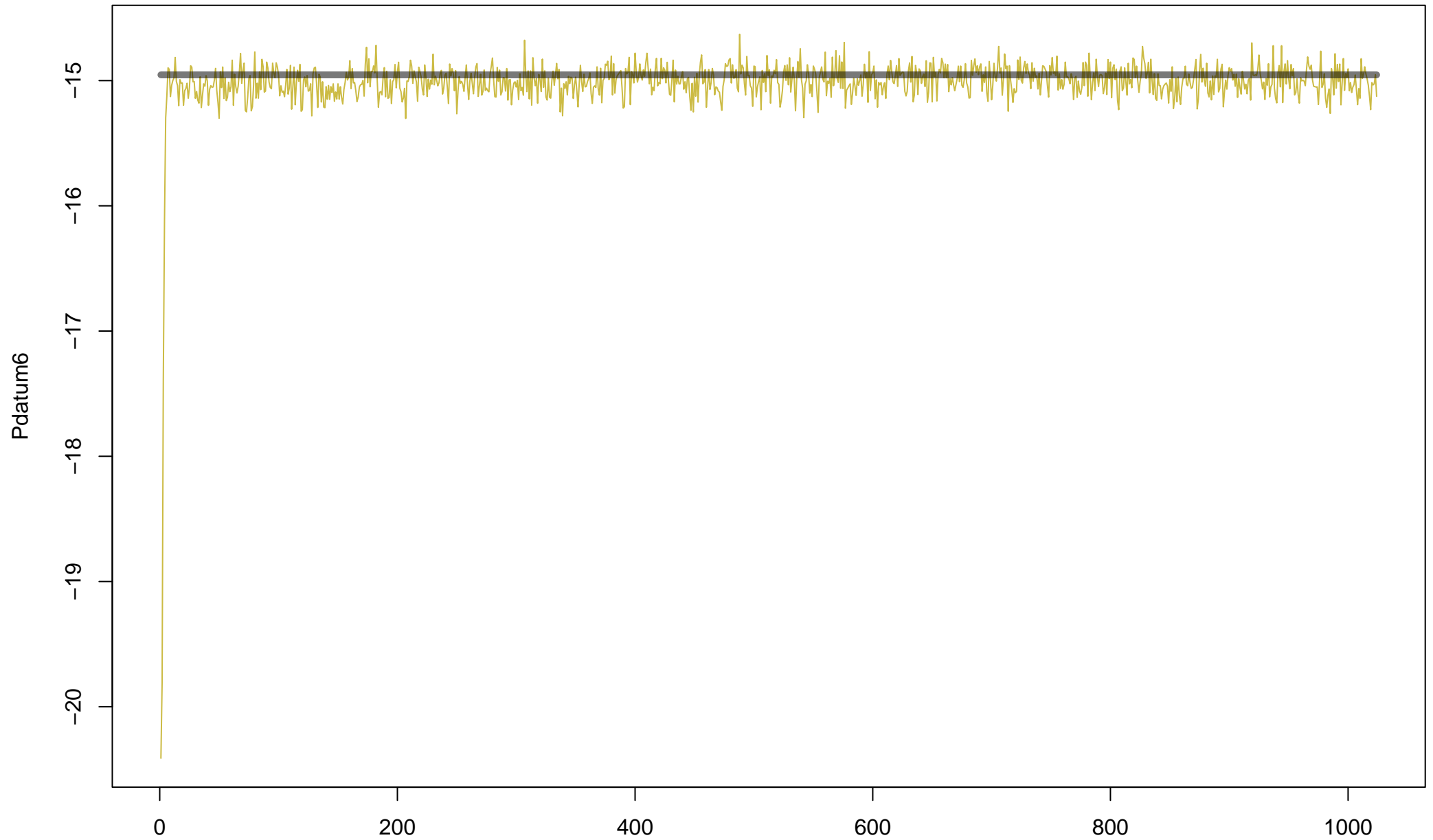
# Pdatum5

ESS = 10.6 | BMK = 0.595 | MCSE(6.27) = 15.5 | stat: FALSE | burn: 0 | percentile: 0.195



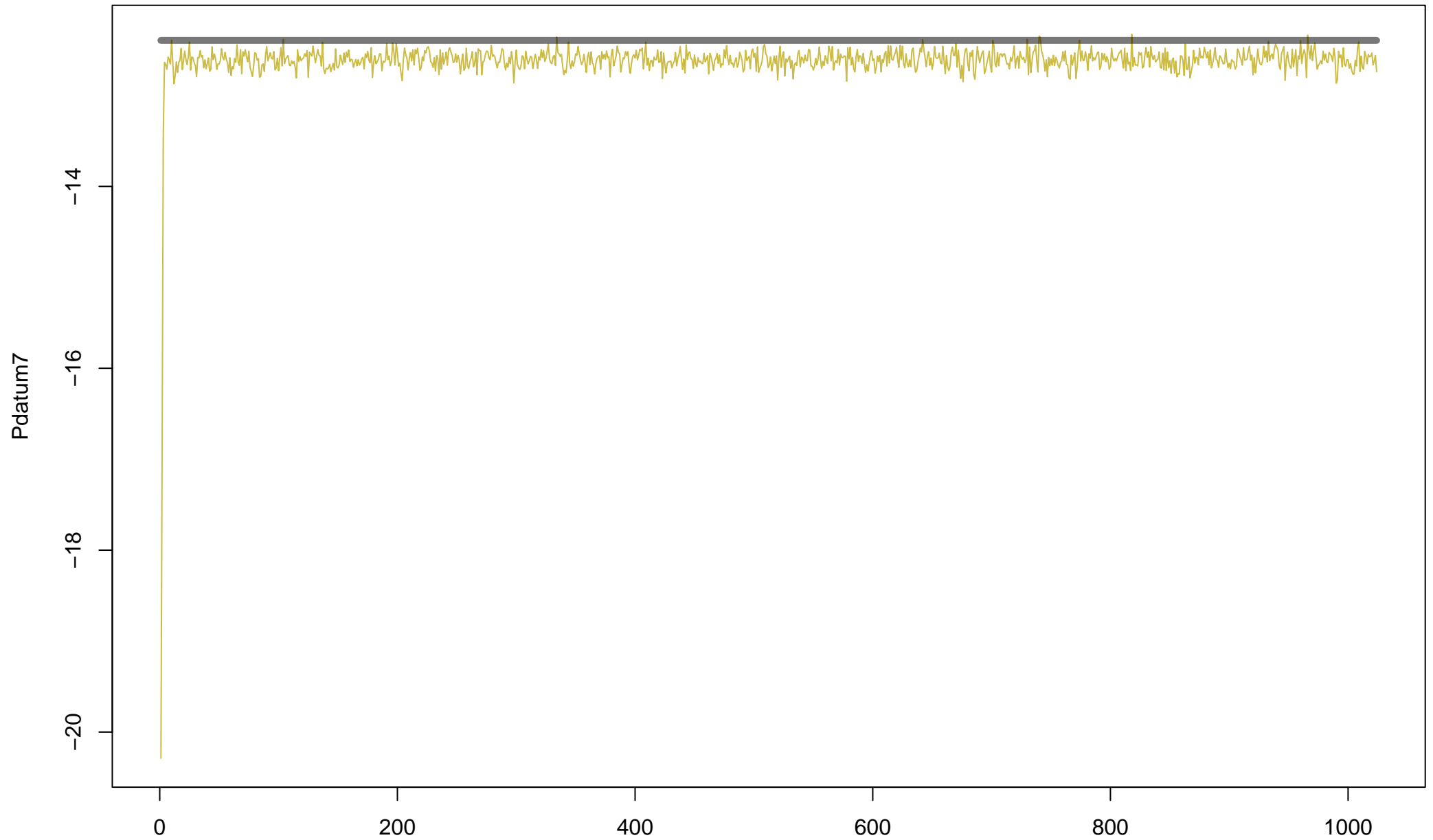
**Pdatum6**

**ESS = 508 | BMK = 0.101 | MCSE(6.27) = 5.34 | stat: FALSE | burn: 0 | percentile: 67.6**



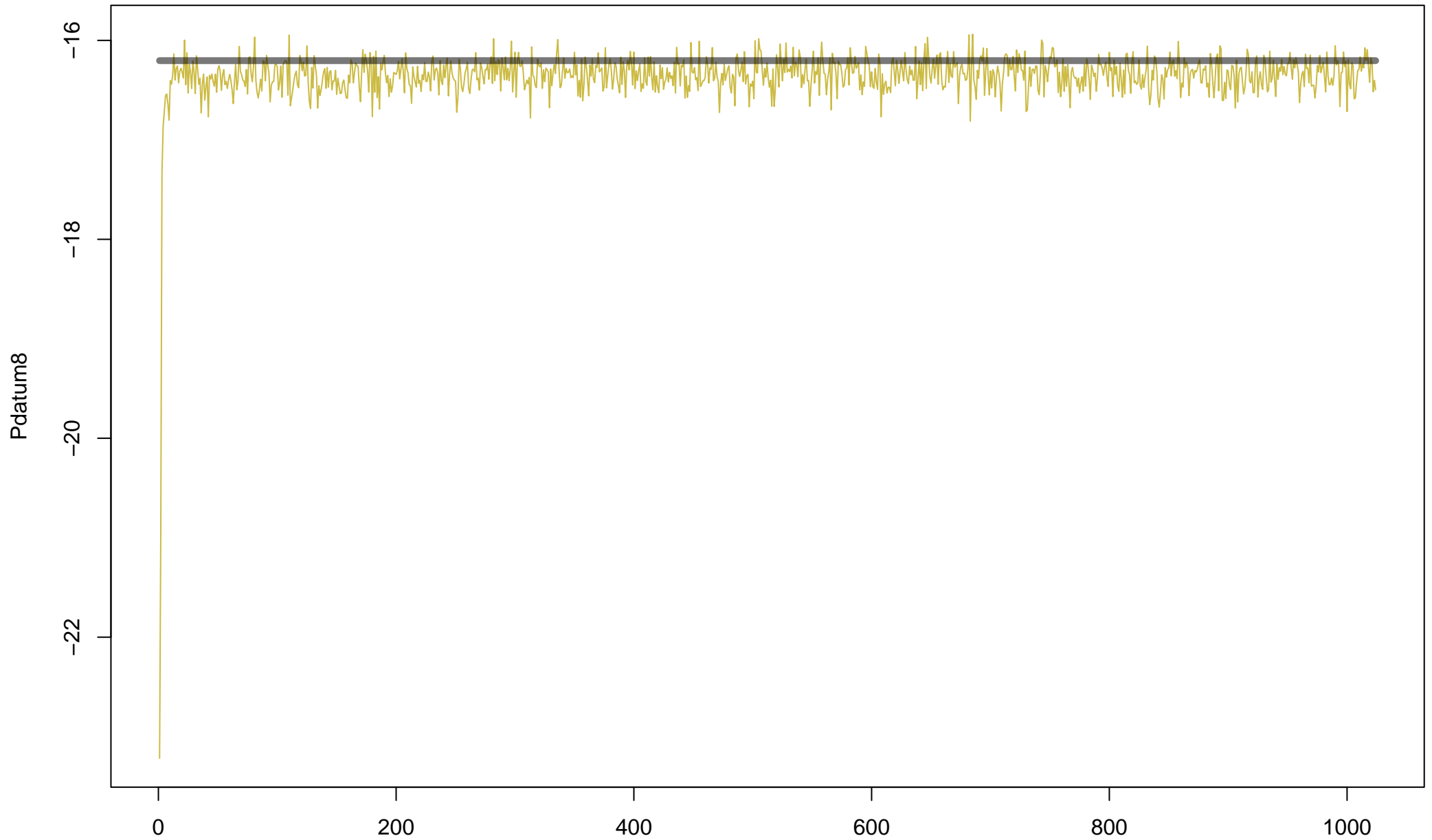
**Pdatum7**

**ESS = 723 | BMK = 0.0731 | MCSE(6.27) = 4.14 | stat: TRUE | burn: 0 | percentile: 99**



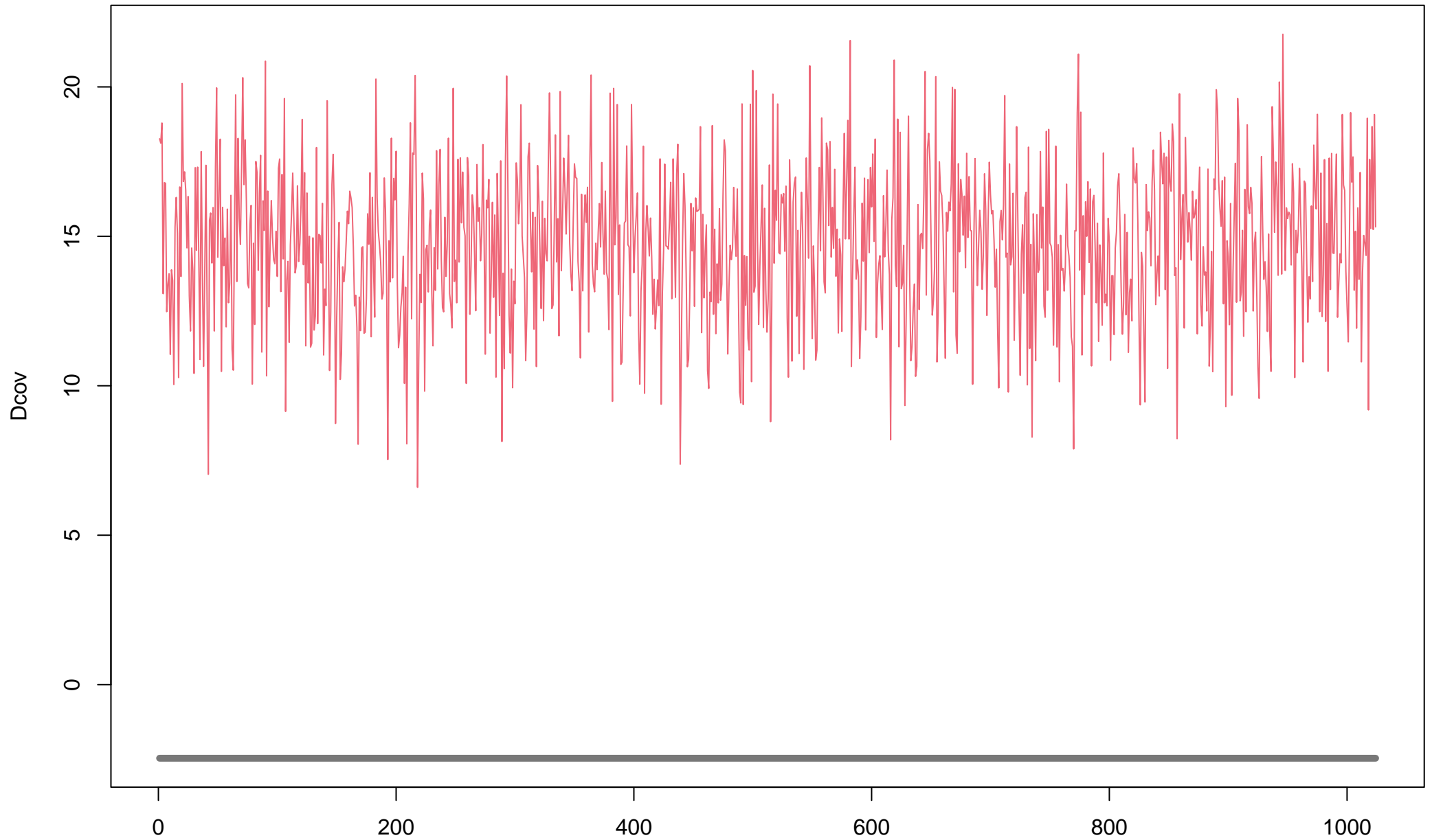
**Pdatum8**

**ESS = 2.22e-16 | BMK = 0.0859 | MCSE(6.27) = 4.05 | stat: TRUE | burn: 0 | percentile: 83.4**



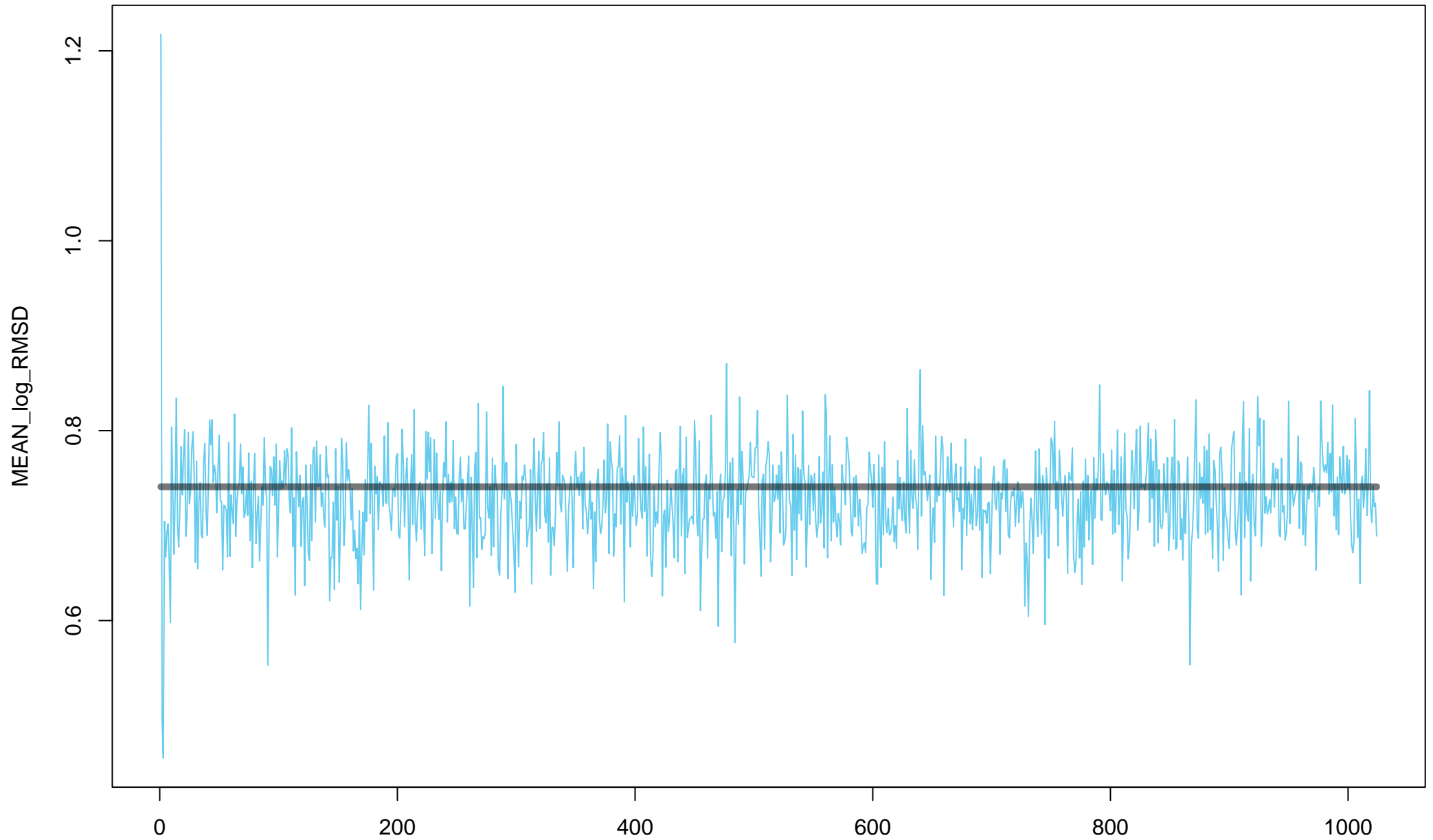
**Dcov**

**ESS = 1020 | BMK = 0.47 | MCSE(6.27) = 3.35 | stat: FALSE | burn: 1020 | percentile: 47.3**



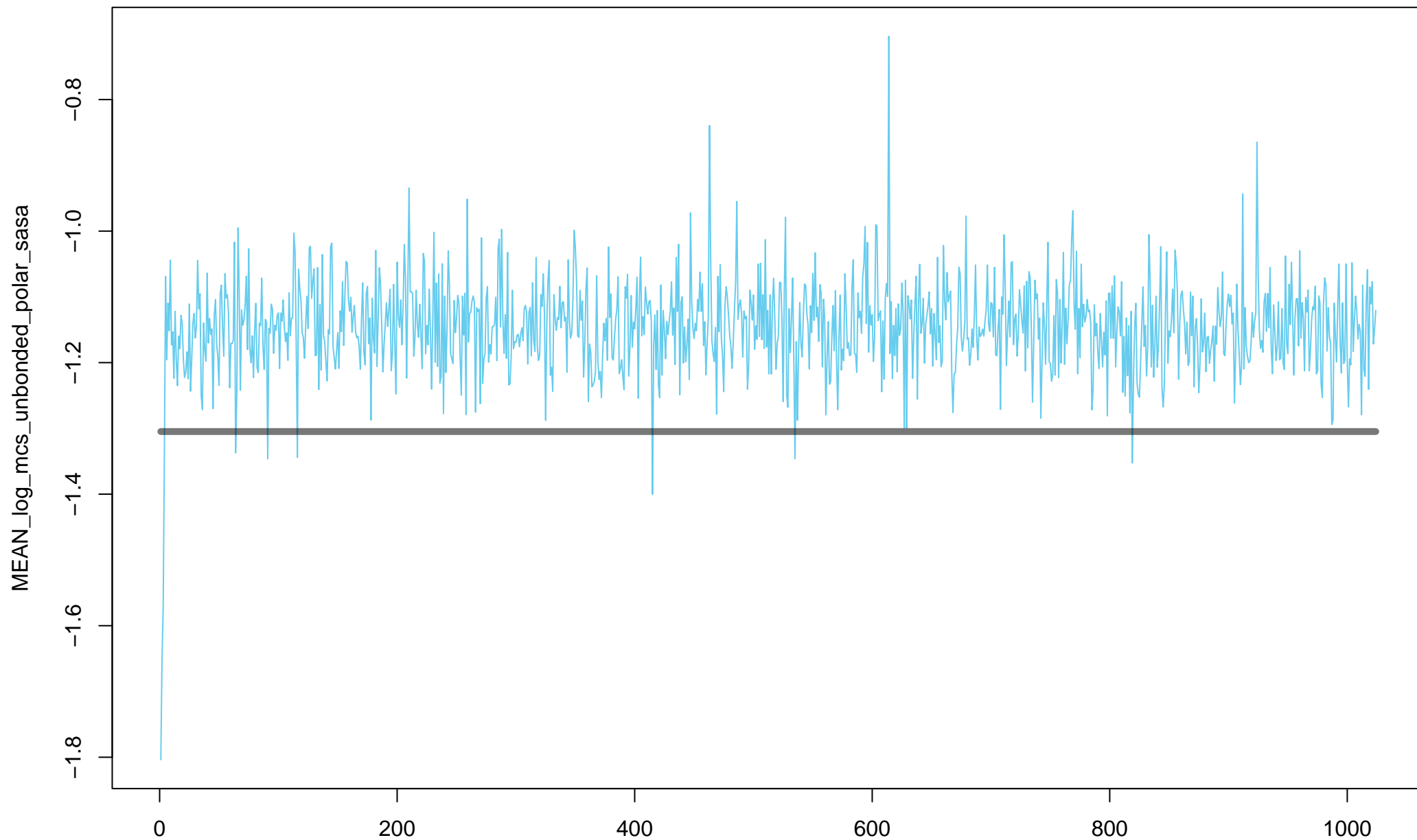
# MEAN\_log\_RMSD

ESS = 1020 | BMK = 0.0757 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0 | percentile: 59.4

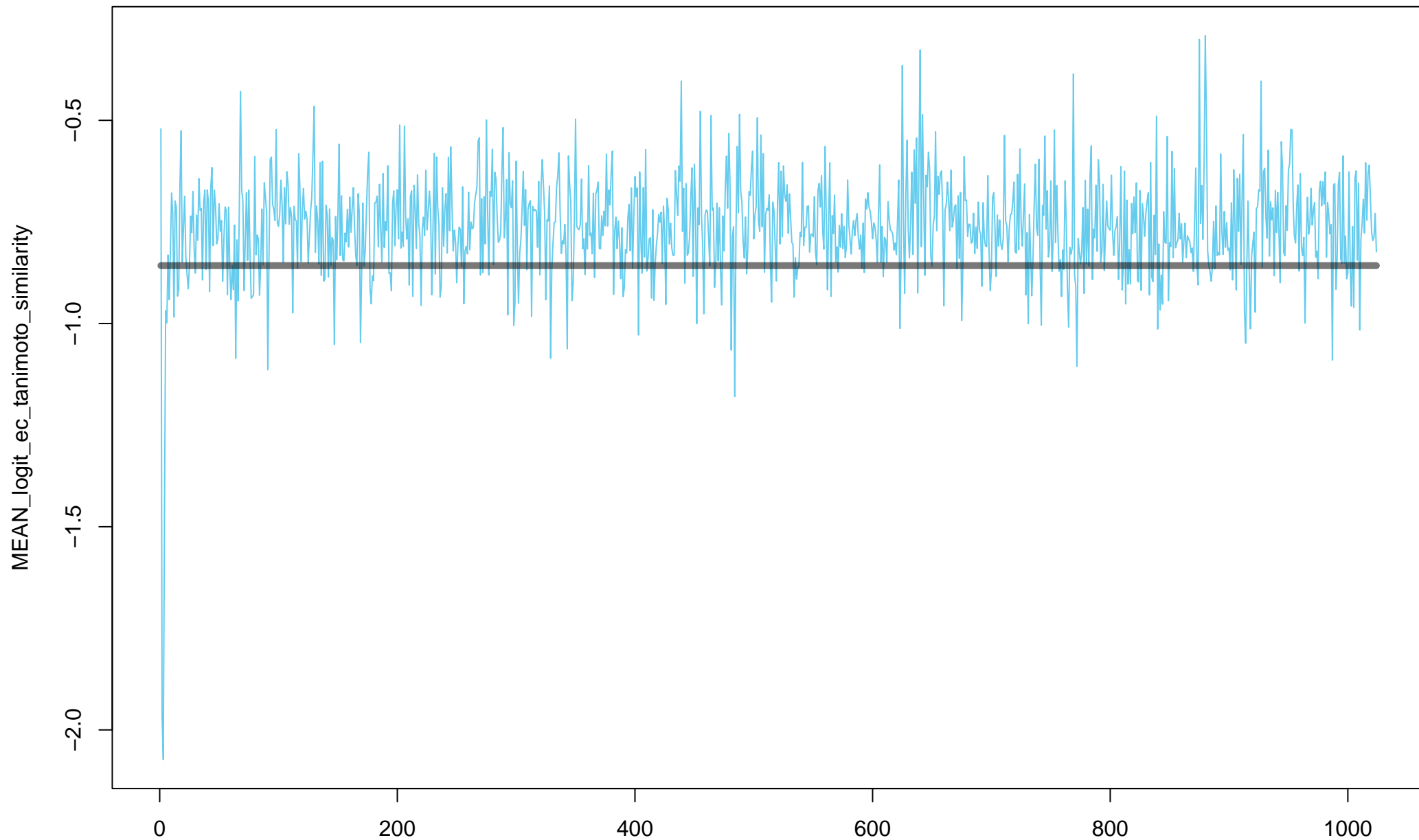




**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 774 | BMK = 0.0823 | MCSE(6.27) = 4.32 | stat: TRUE | burn: 0 | percentile: 0.977**

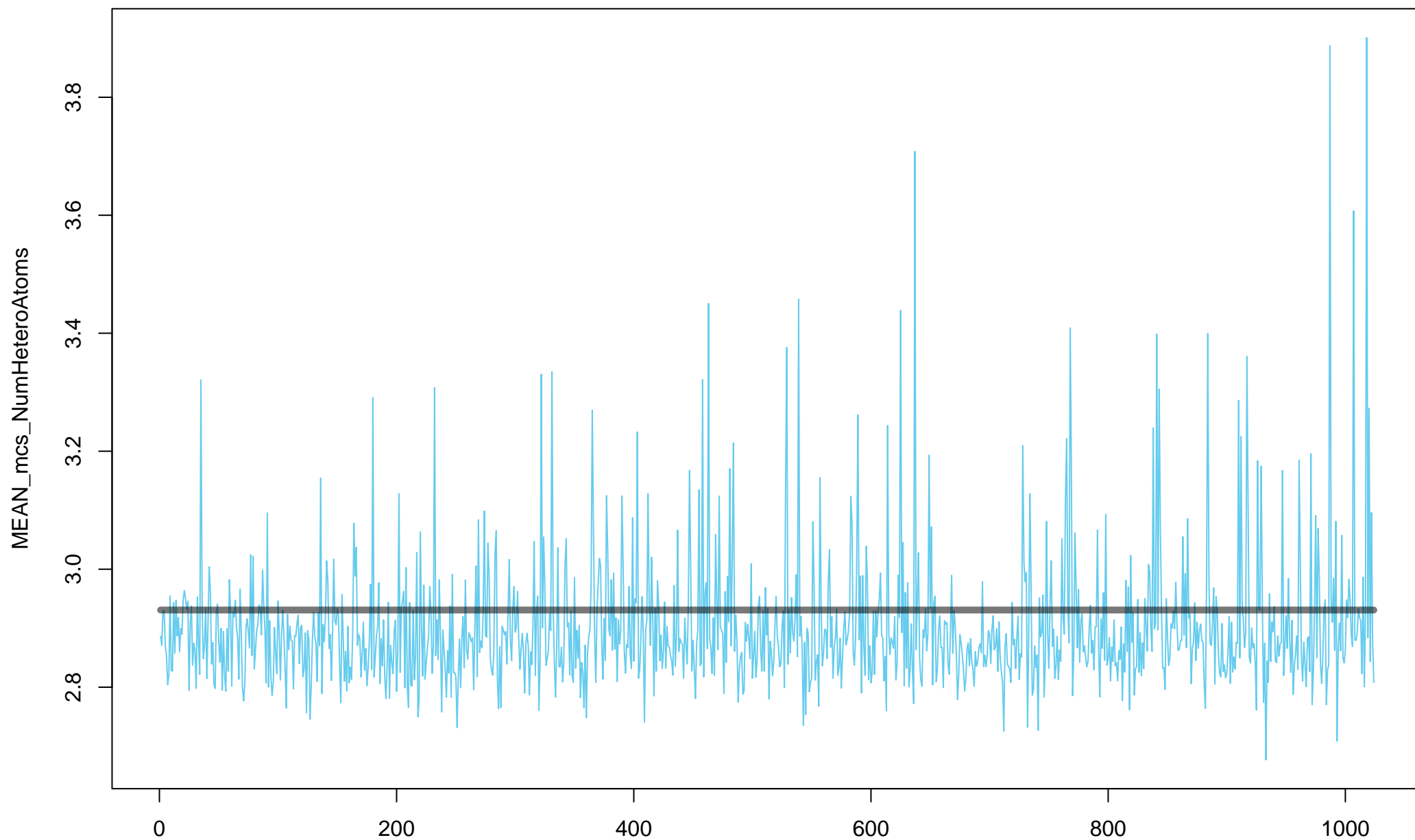


**MEAN\_logit\_ec\_tanimoto\_similarity**  
**ESS = 759 | BMK = 0.11 | MCSE(6.27) = 4.34 | stat: TRUE | burn: 0 | percentile: 18.1**

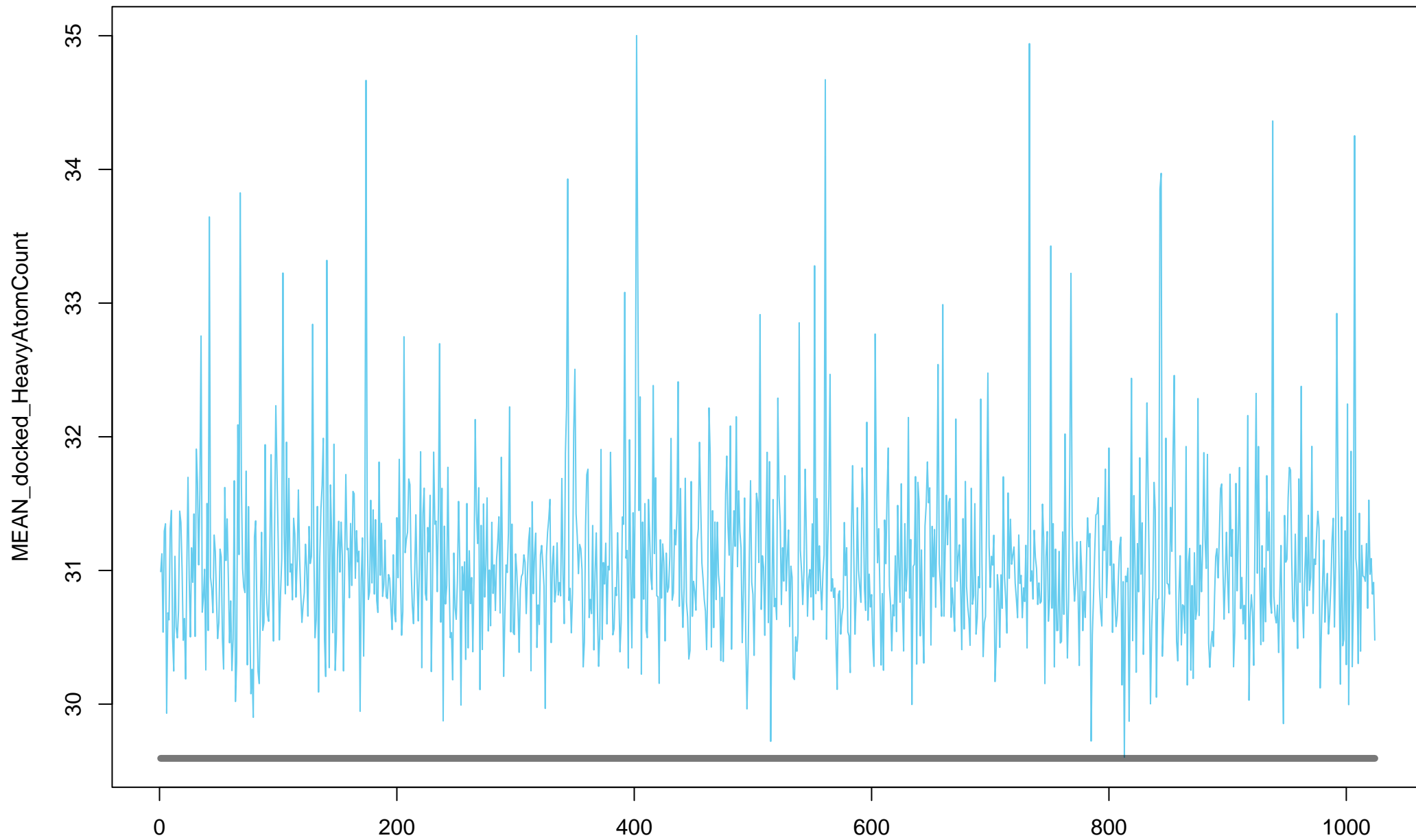


# MEAN\_mcs\_NumHeteroAtoms

ESS = 1020 | BMK = 0.115 | MCSE(6.27) = 3.75 | stat: TRUE | burn: 0 | percentile: 75.7

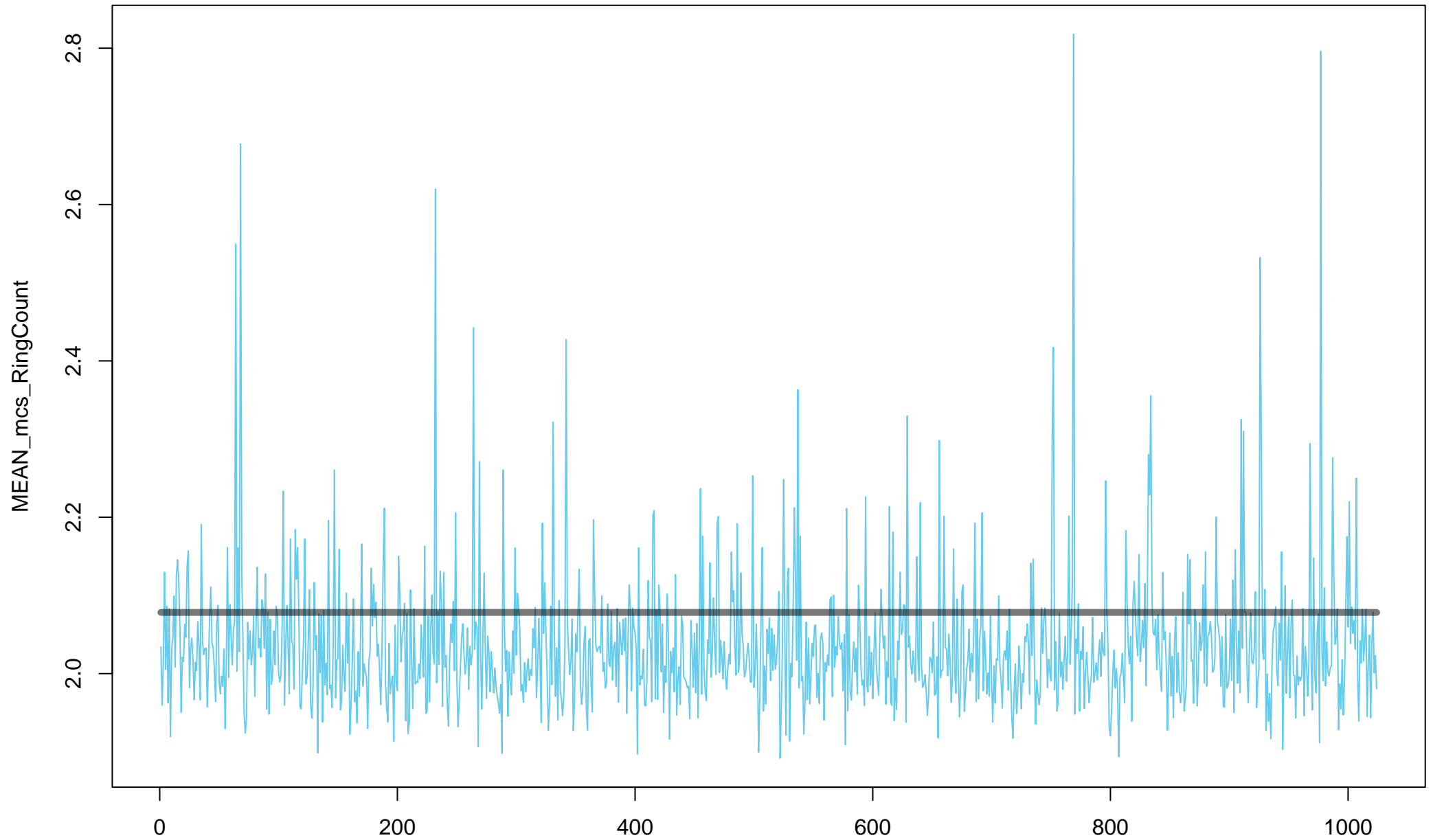


**MEAN\_docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.0672 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | percentile: 0**

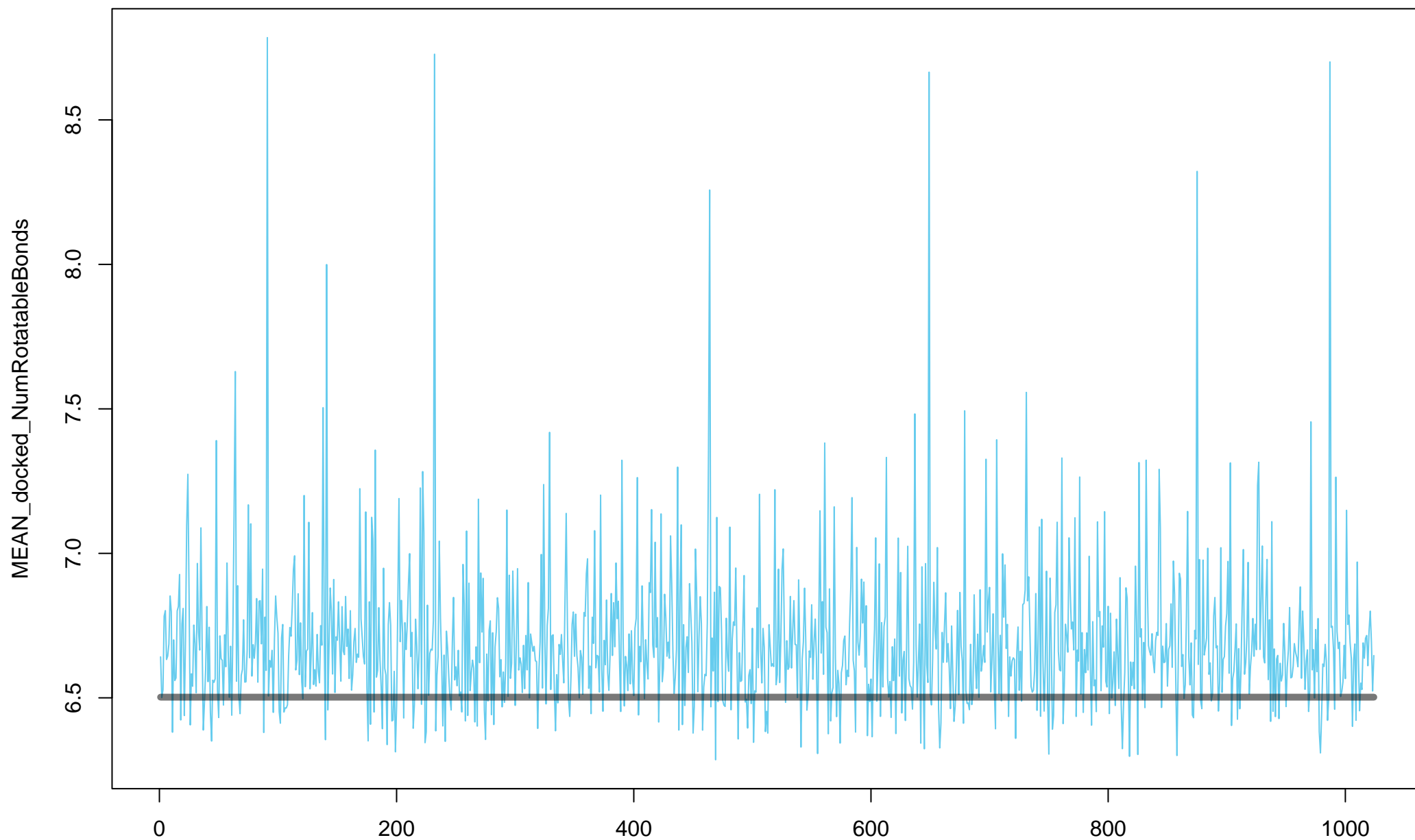


# MEAN\_mcs\_RingCount

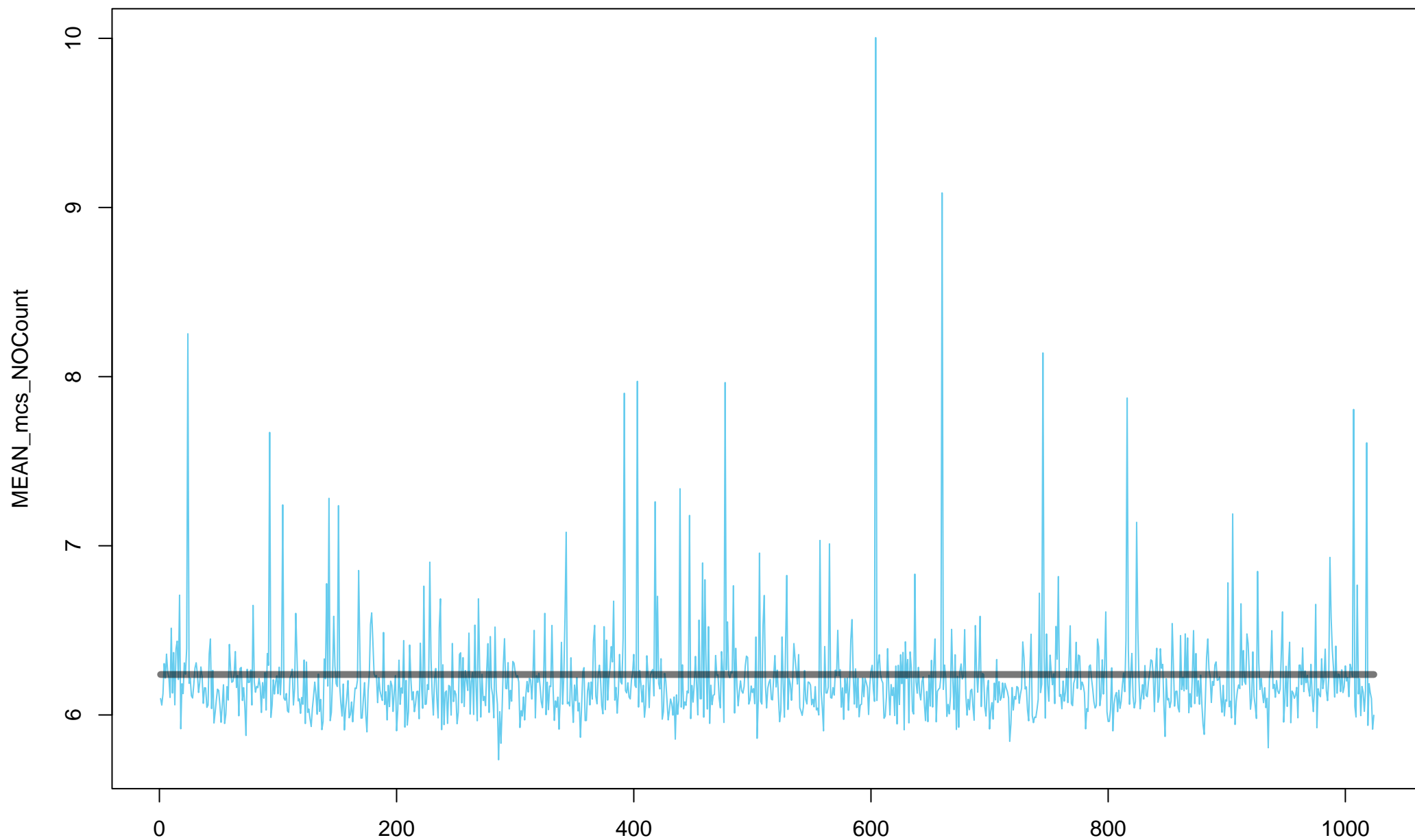
ESS = 1020 | BMK = 0.101 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0 | percentile: 80.4



**MEAN\_docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.073 | MCSE(6.27) = 1.86 | stat: TRUE | burn: 0 | percentile: 18.1**

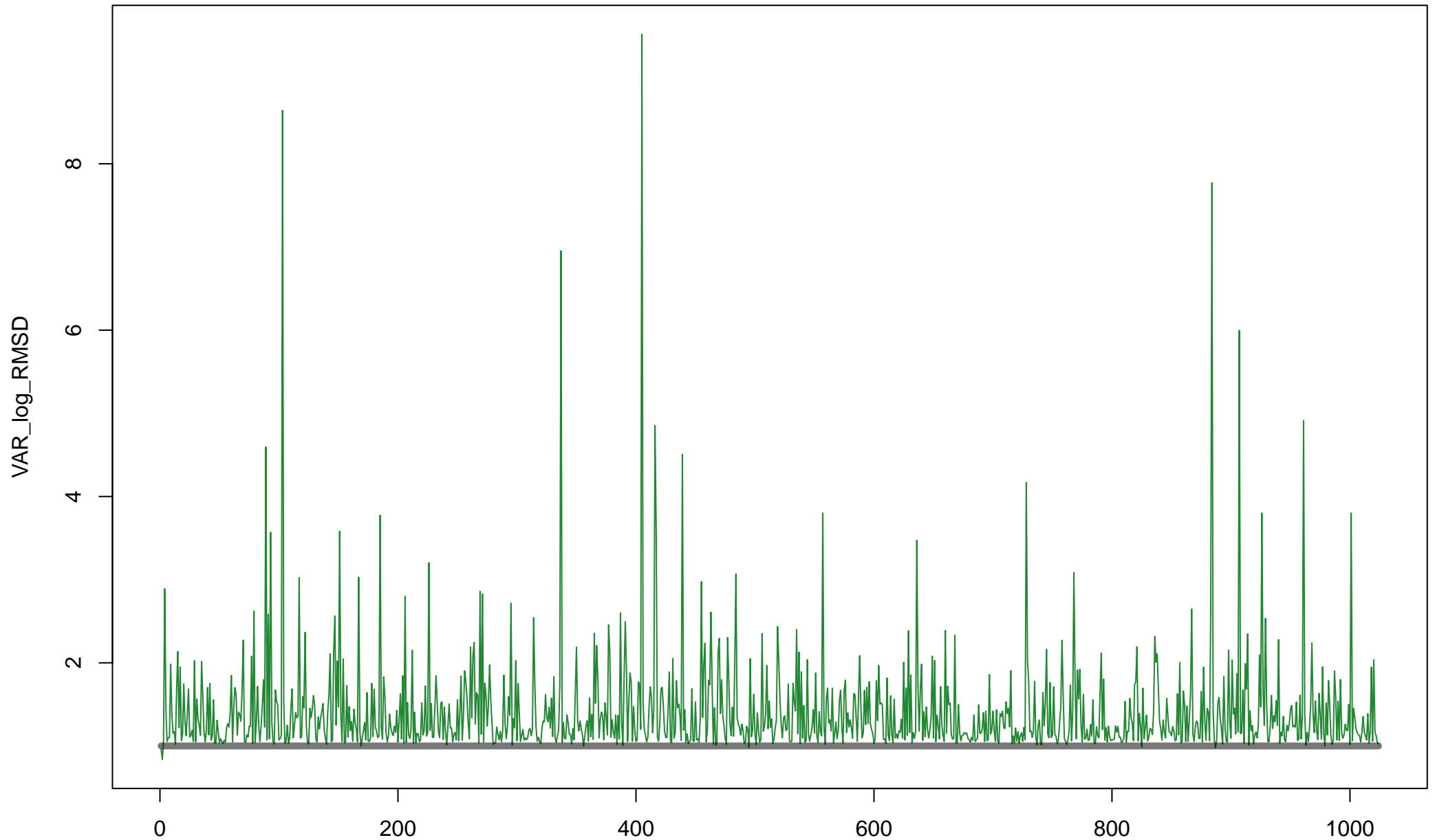


**MEAN\_mcs\_NOCount**  
**ESS = 1020 | BMK = 0.105 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0 | percentile: 71.4**



# VAR\_log\_RMSD

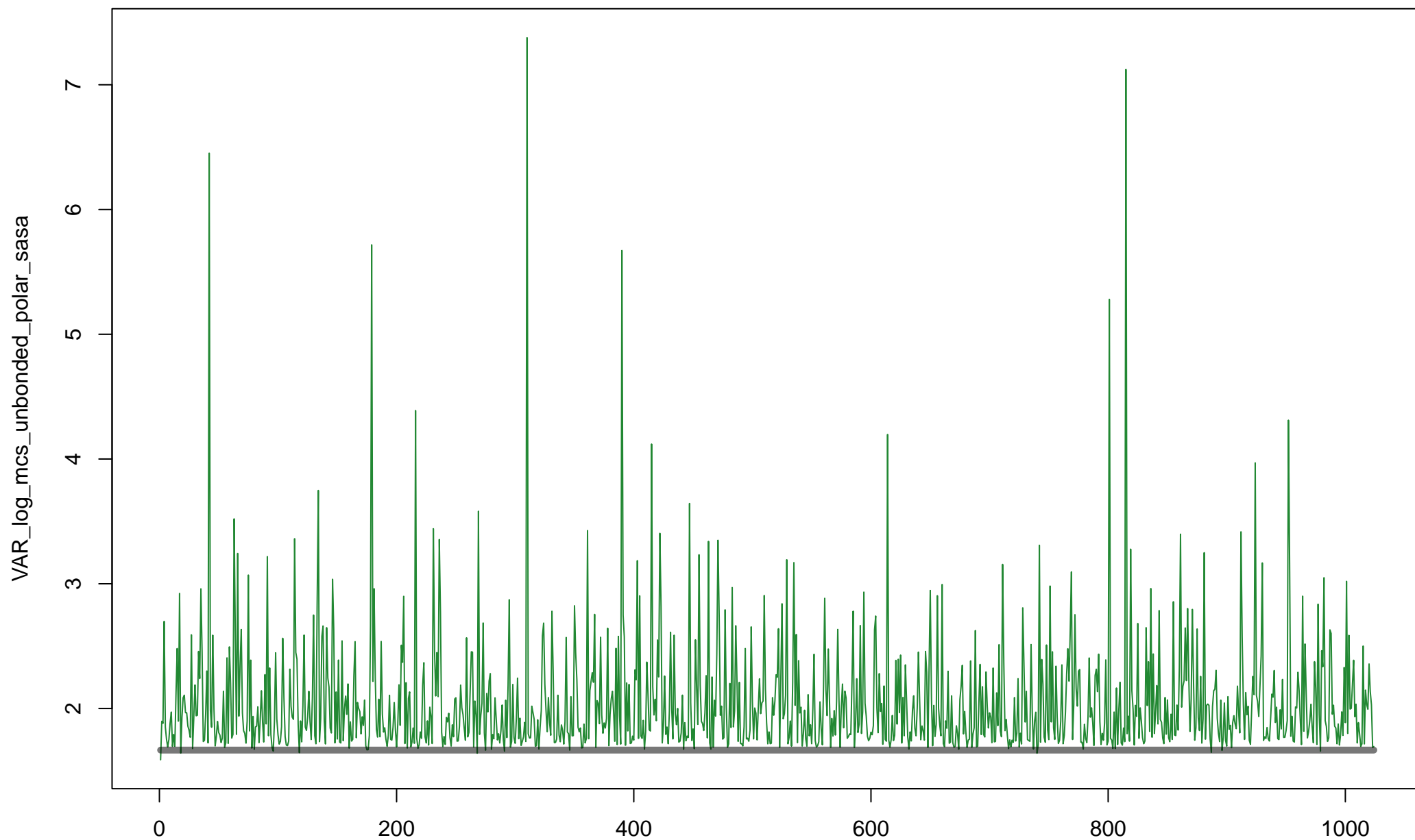
ESS = 1020 | BMK = 0.546 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 1020 | percentile: 0.684





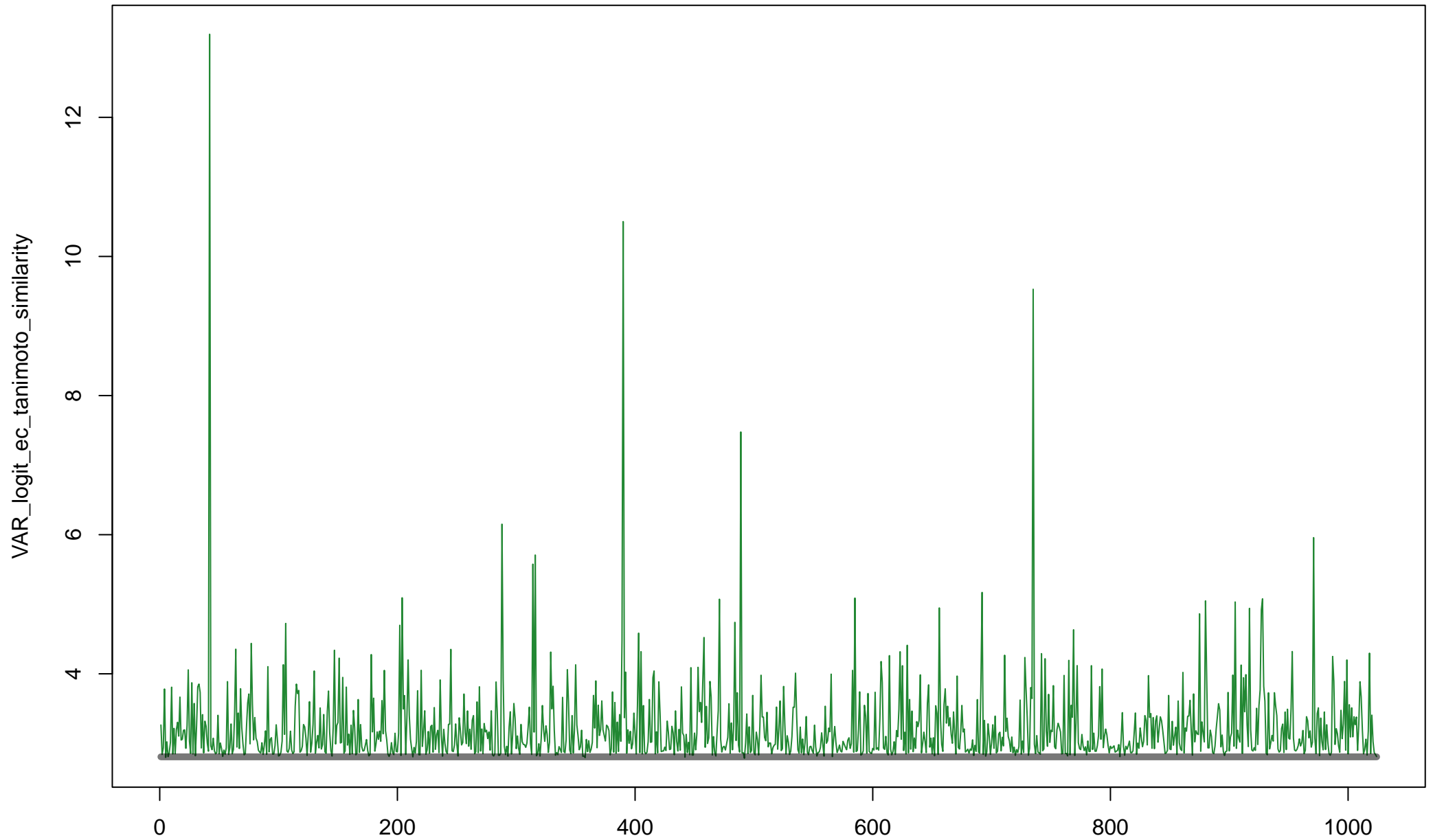
VAR\_log\_mcs\_unbonded\_polar\_sasa

ESS = 1020 | BMK = 0.176 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | percentile: 1.17

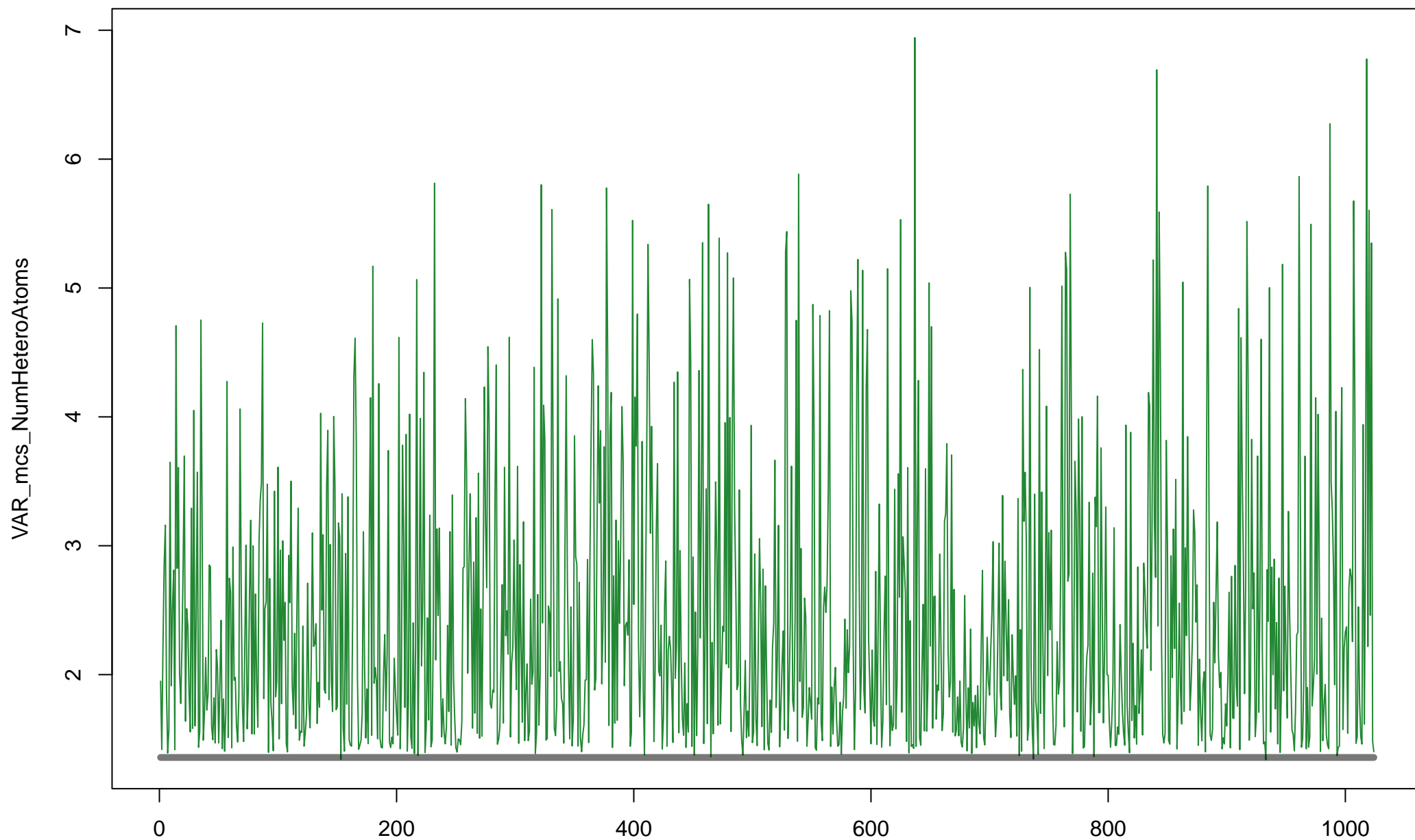


# VAR\_logit\_ec\_tanimoto\_similarity

ESS = 1020 | BMK = 0.868 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 816 | percentile: 0.391

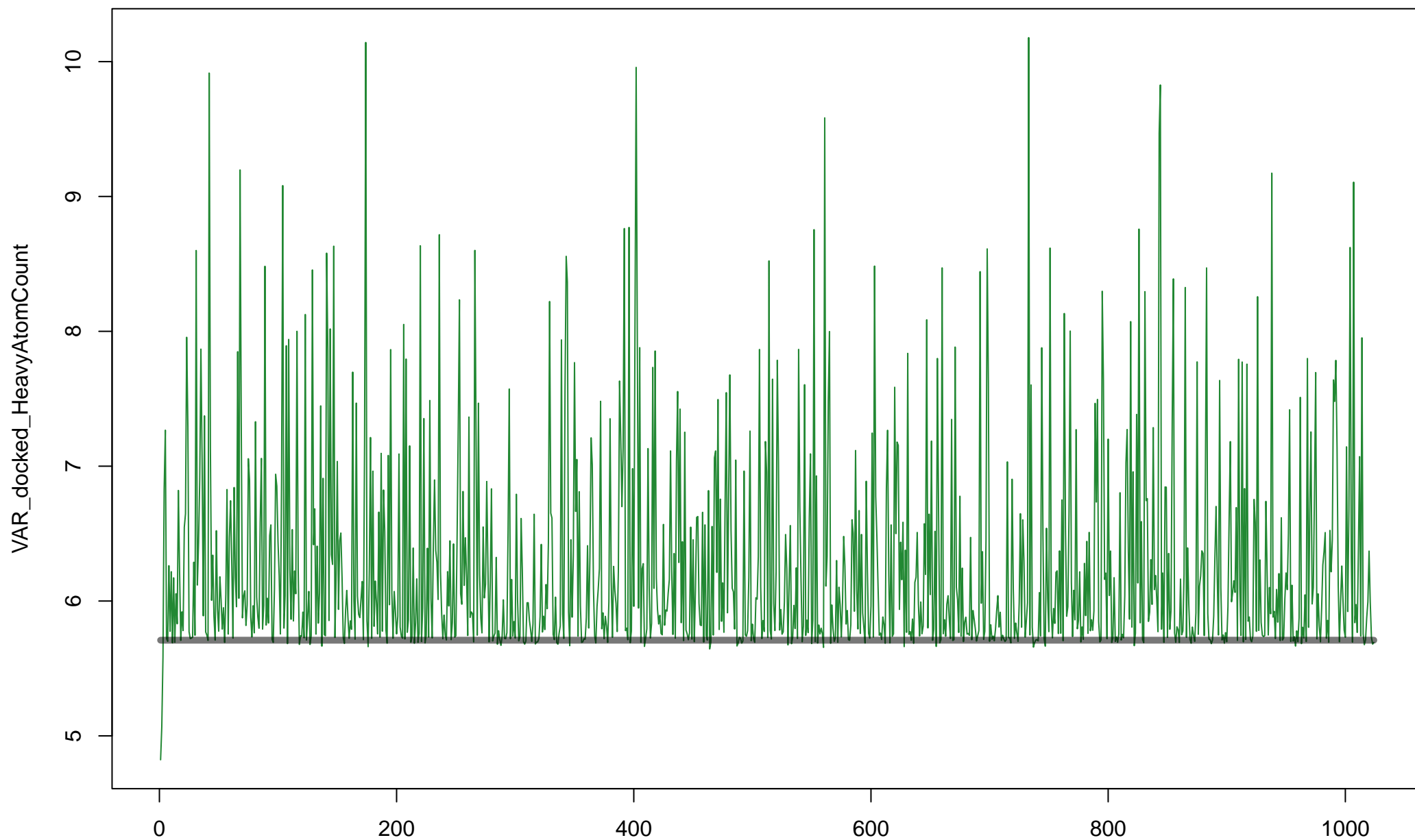


**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 896 | BMK = 0.162 | MCSE(6.27) = 3.81 | stat: FALSE | burn: 0 | percentile: 0.293**

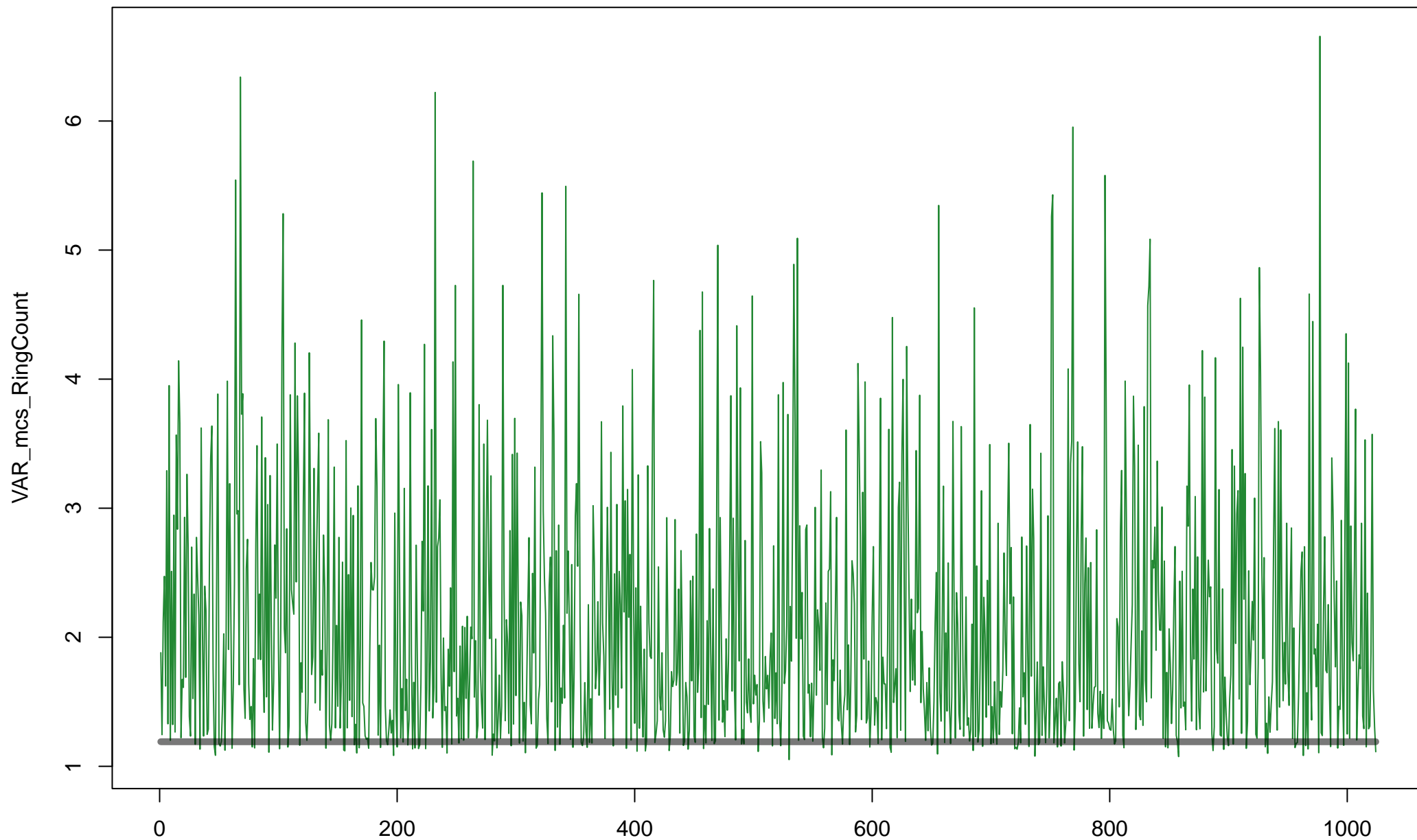


# VAR\_docked\_HeavyAtomCount

ESS = 913 | BMK = 0.151 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0 | percentile: 11.9

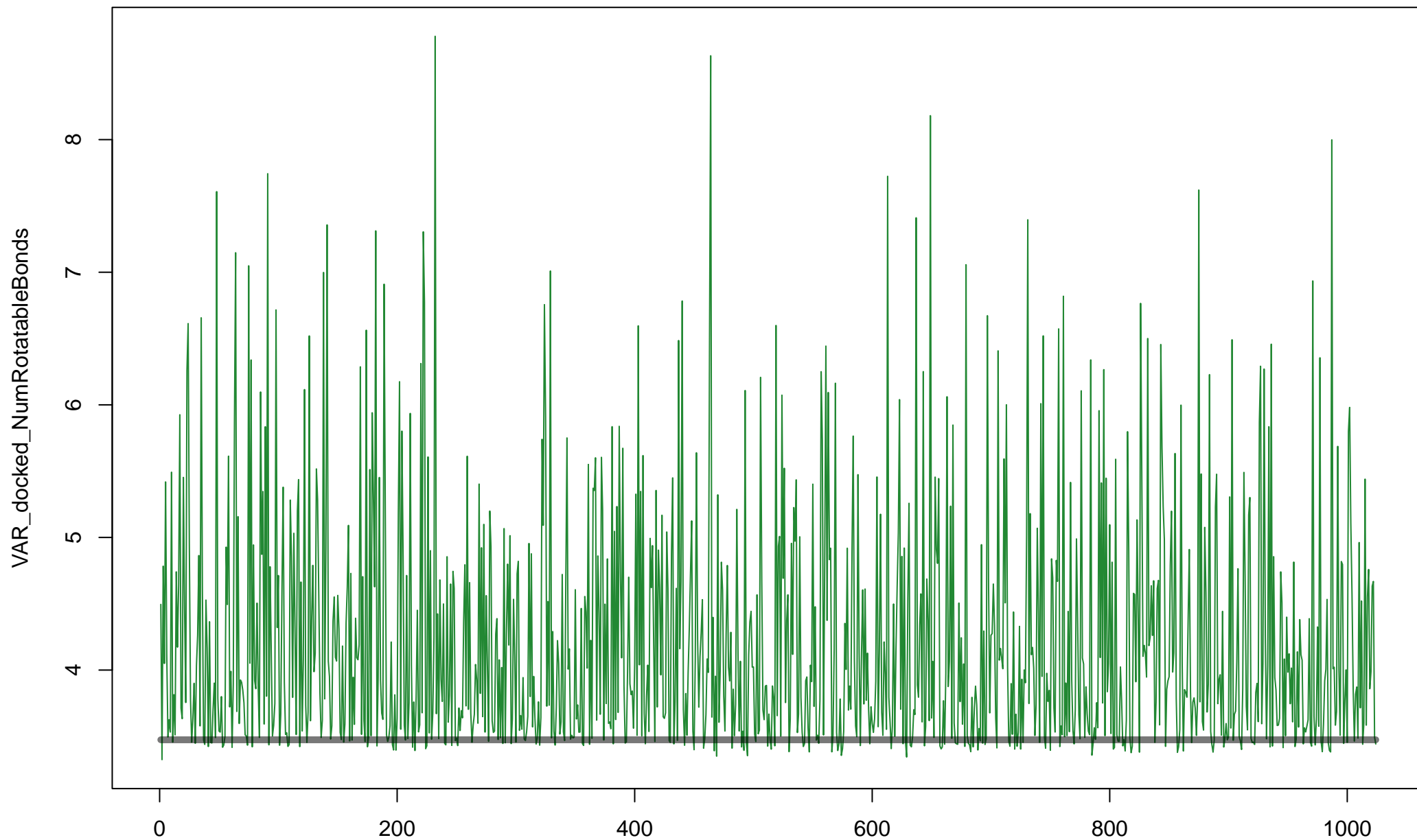


**VAR\_mcs\_RingCount**  
**ESS = 1020 | BMK = 0.142 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0 | percentile: 12.5**



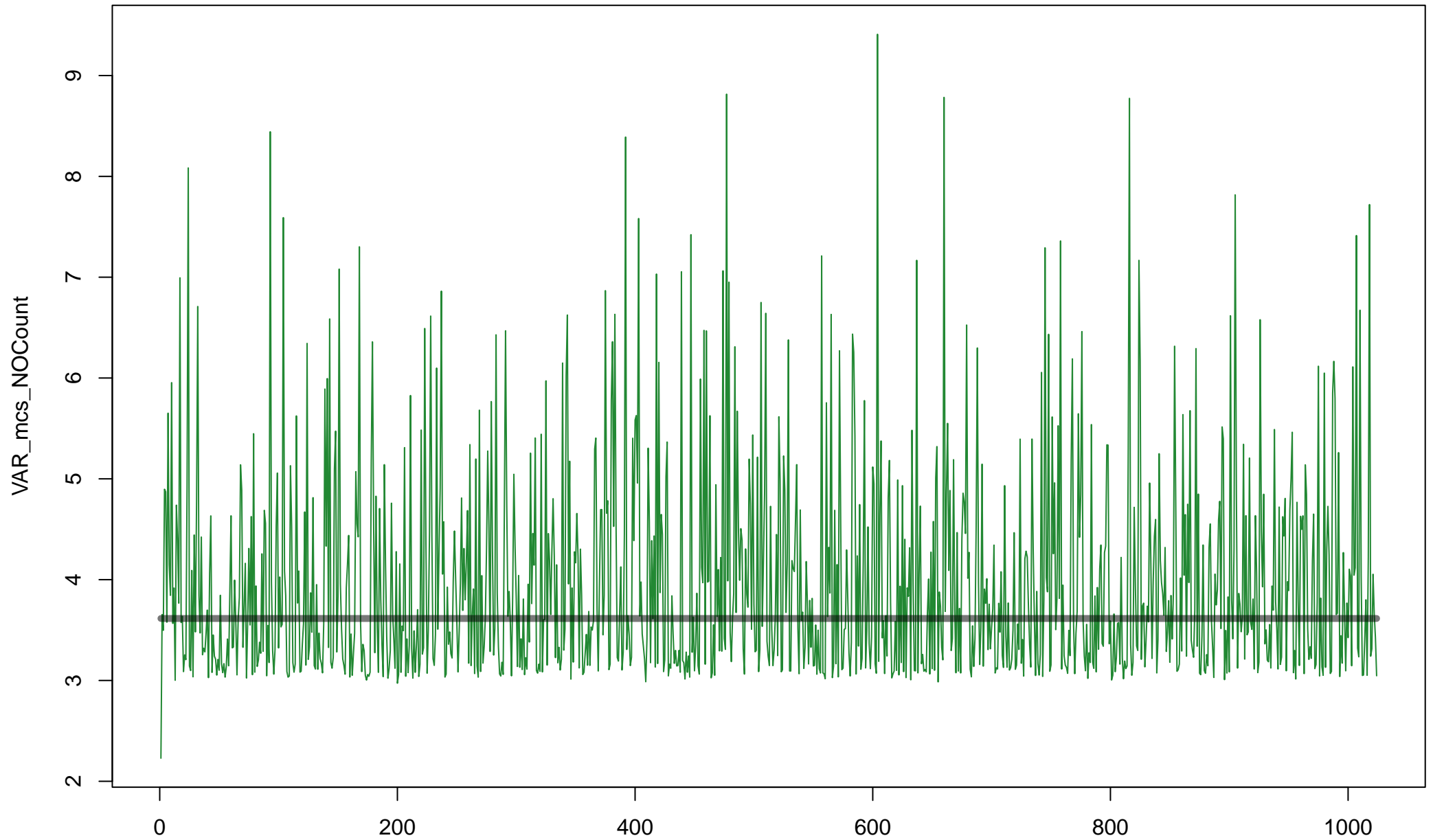
# VAR\_docked\_NumRotatableBonds

ESS = 1020 | BMK = 0.144 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0 | percentile: 16.9

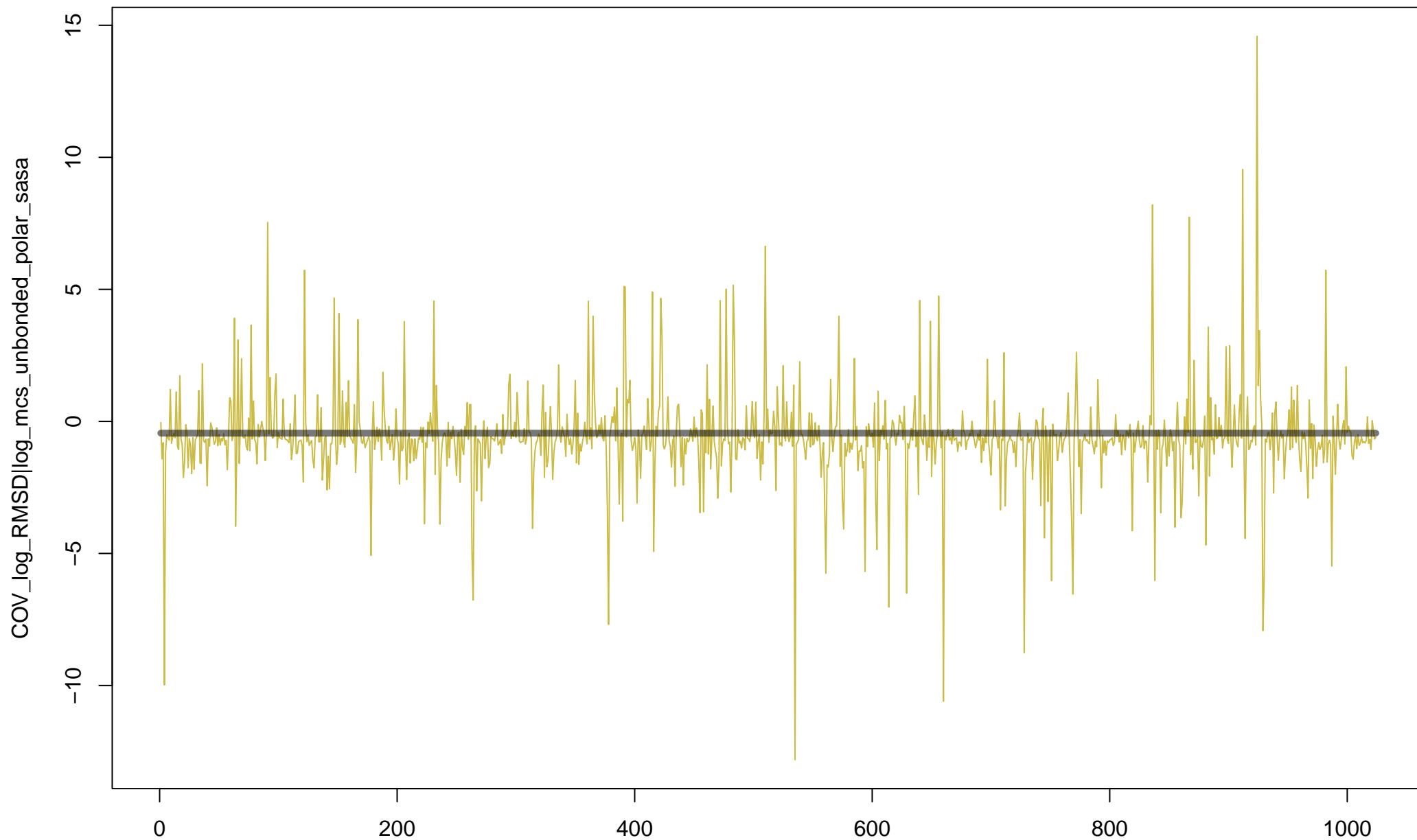


# VAR\_mcs\_NOCount

ESS = 1020 | BMK = 0.172 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0 | percentile: 50.9

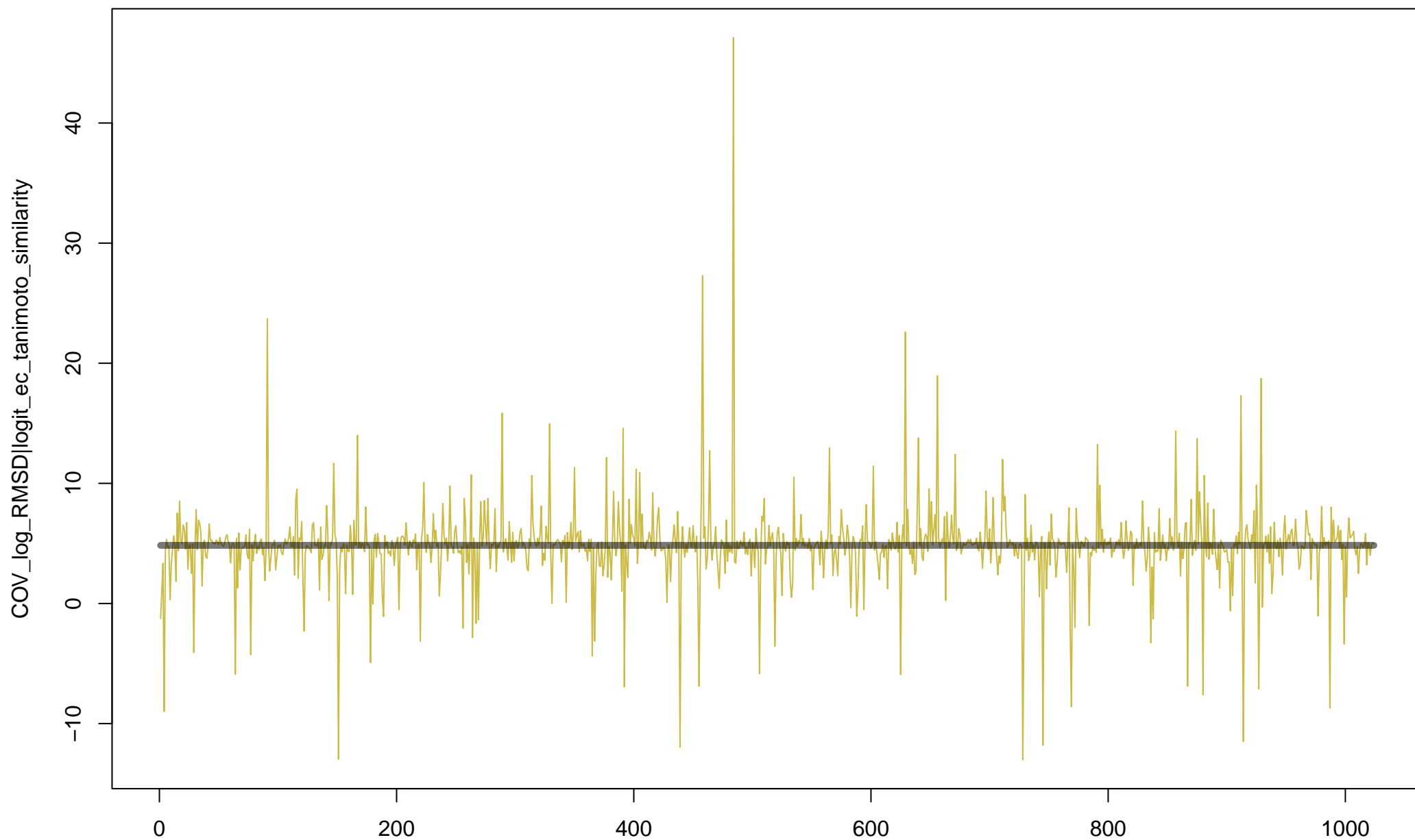


**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1020 | BMK = 0.179 | MCSE(6.27) = 3.7 | stat: TRUE | burn: 0 | percentile: 69.3**

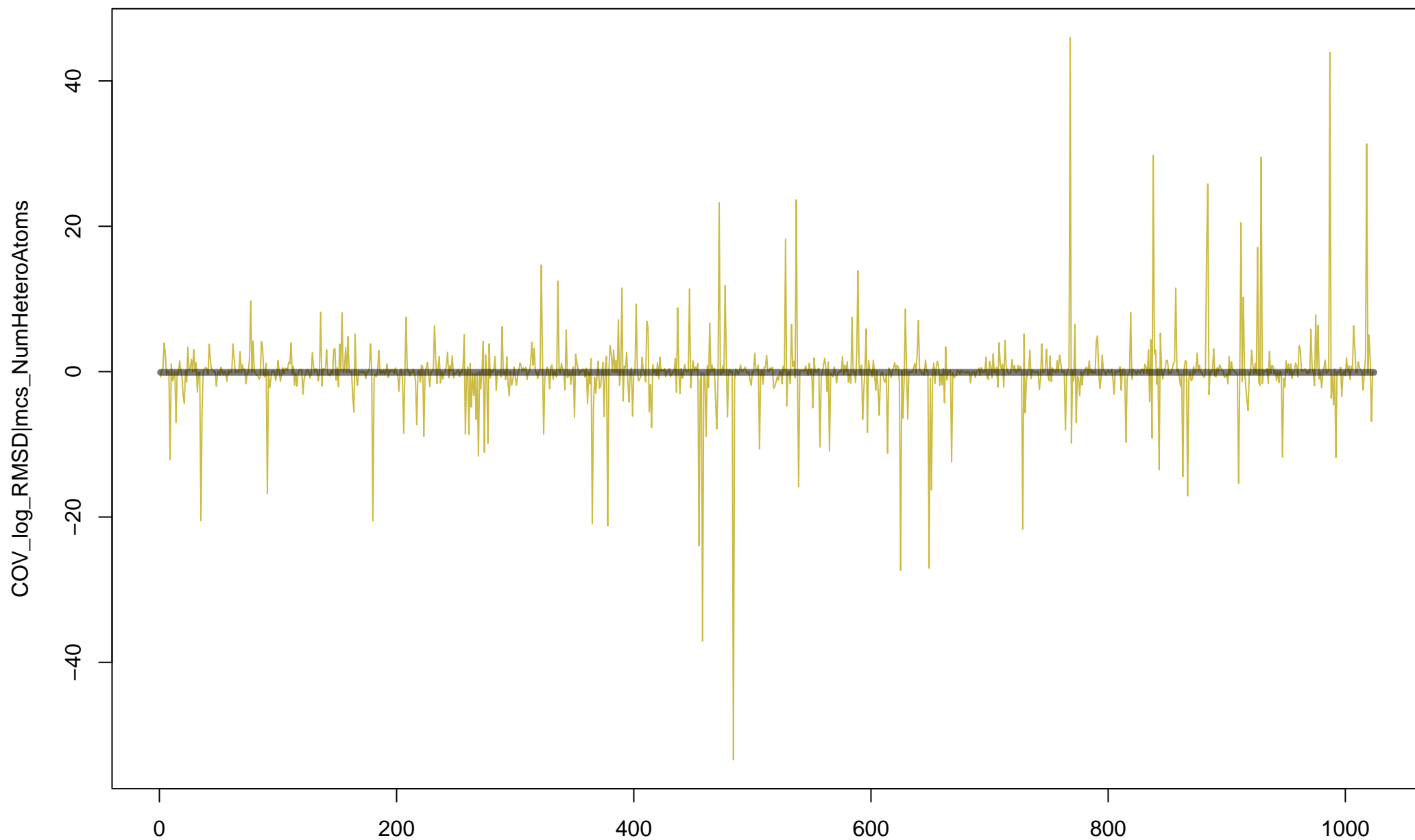




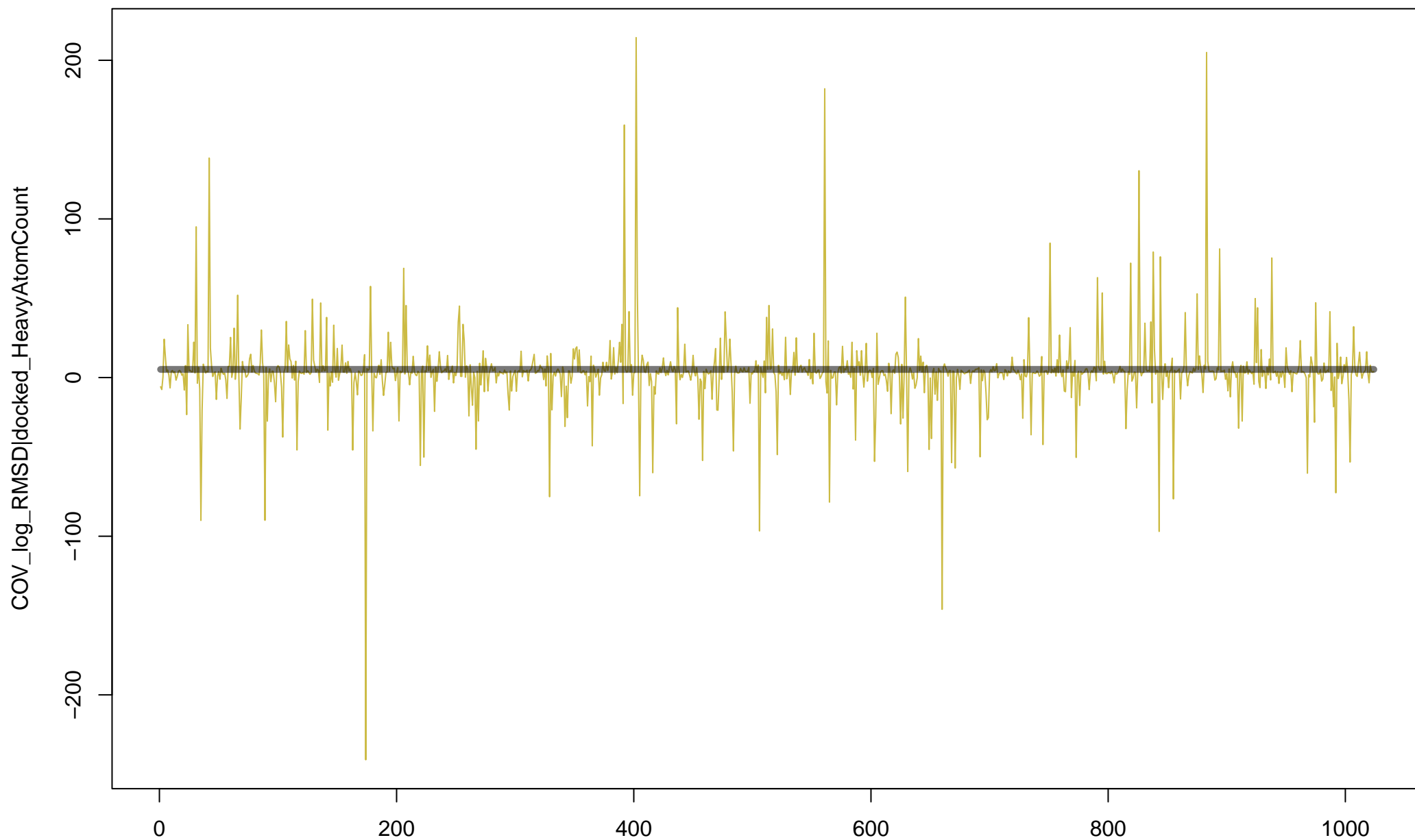
**COV\_log\_RMSD|logit\_ec\_tanimoto\_similarity**  
**ESS = 1020 | BMK = 0.145 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0 | percentile: 45.9**



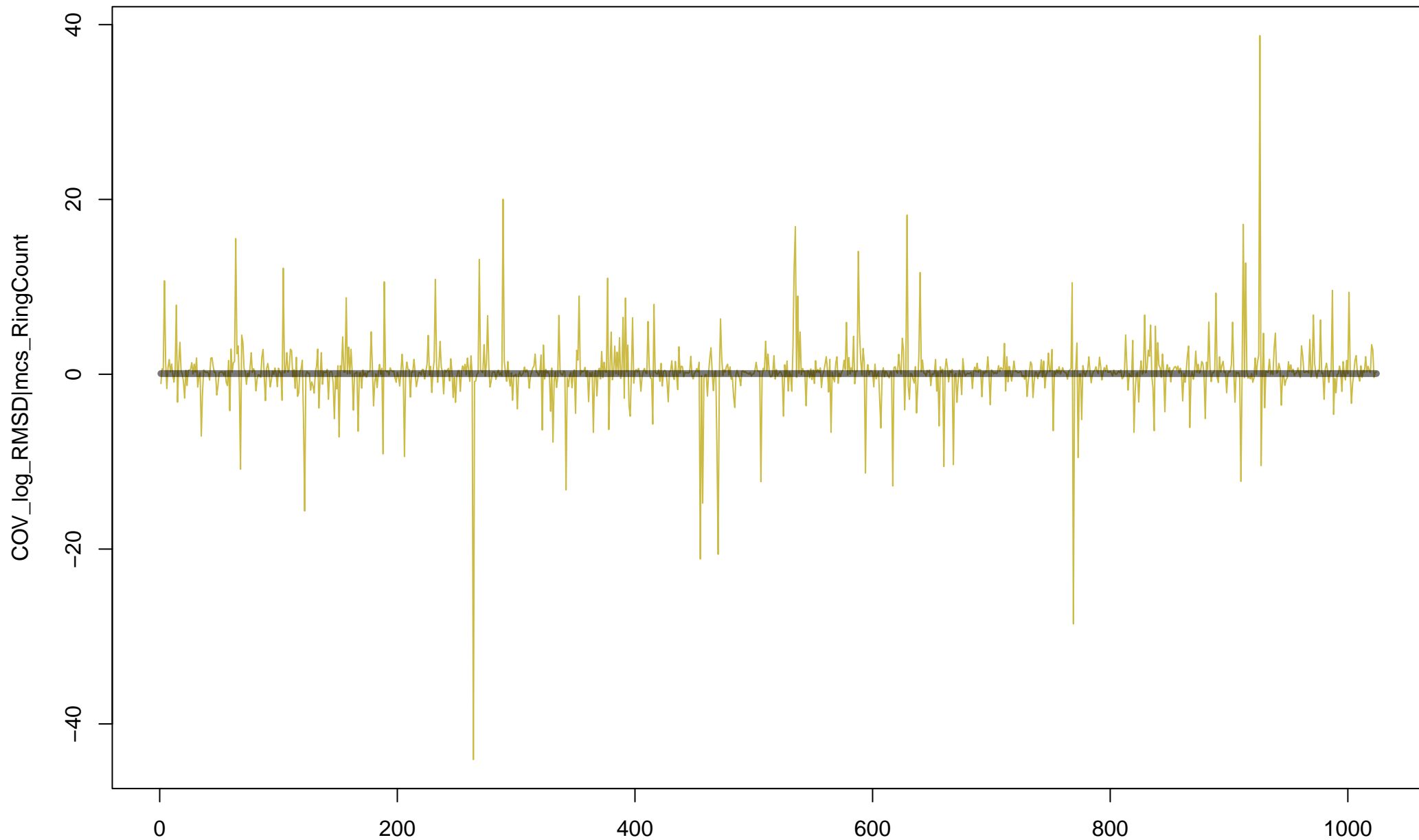
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 1020 | BMK = 0.182 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0 | percentile: 39.8**



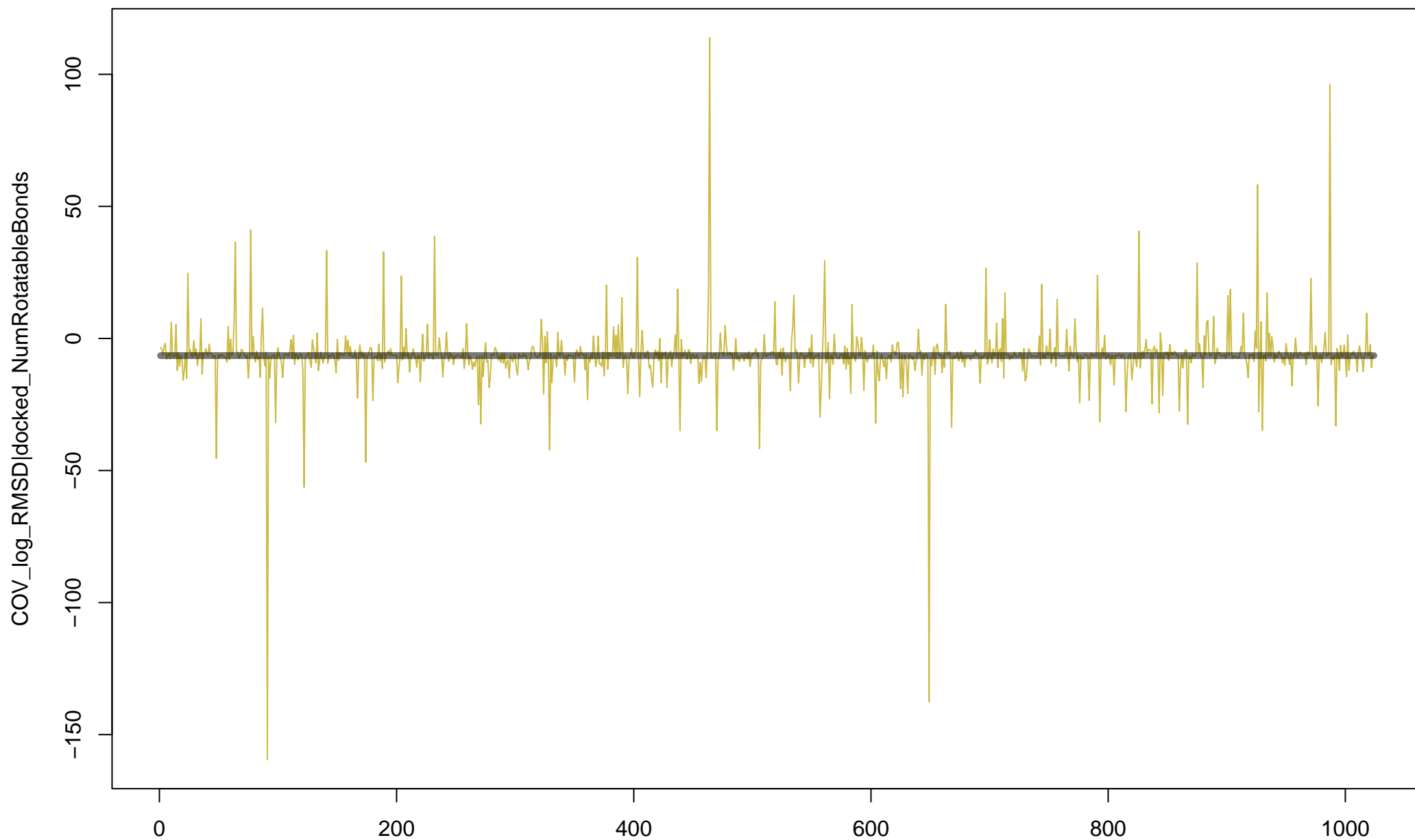
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.179 | MCSE(6.27) = 3.52 | stat: TRUE | burn: 0 | percentile: 70.9**



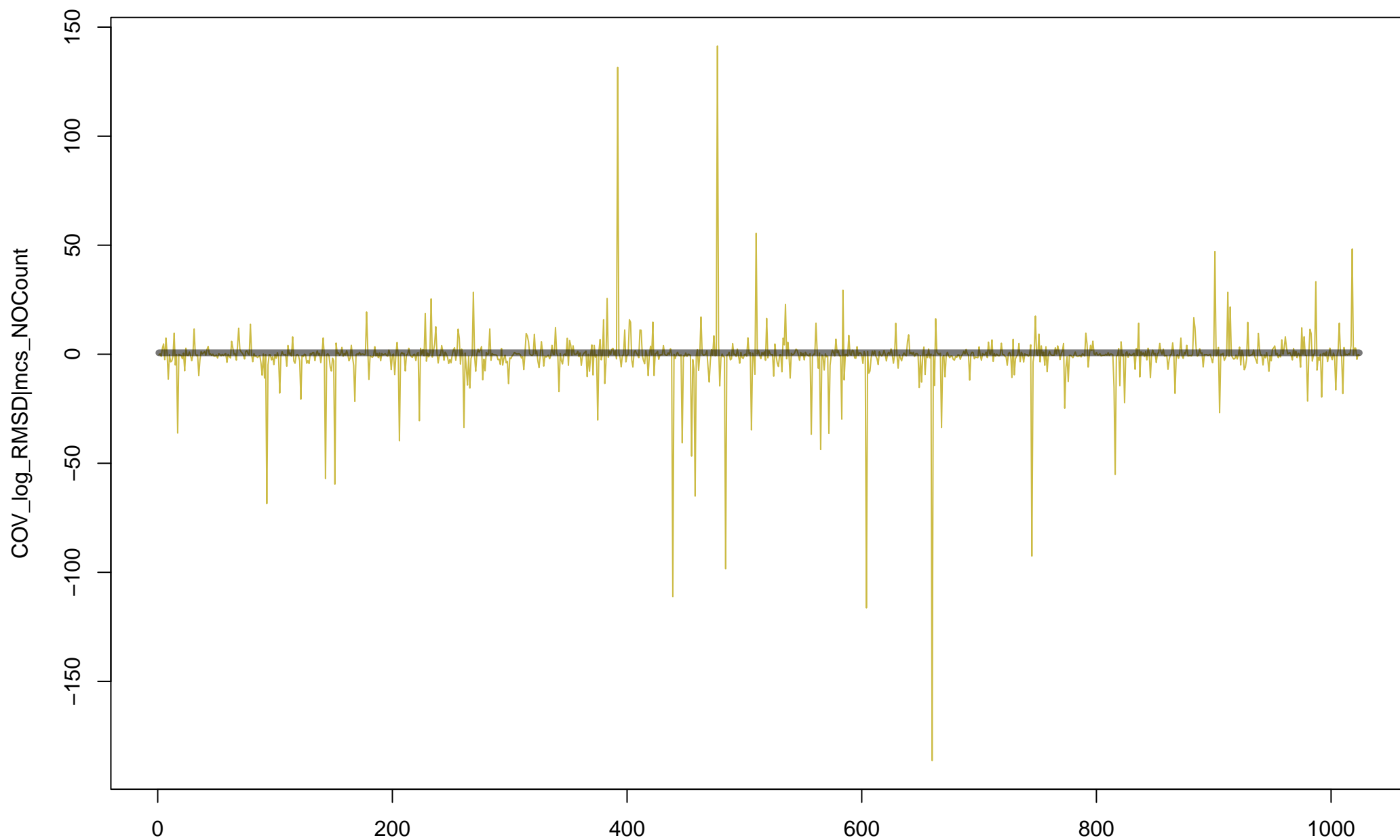
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.18 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | percentile: 36.7**



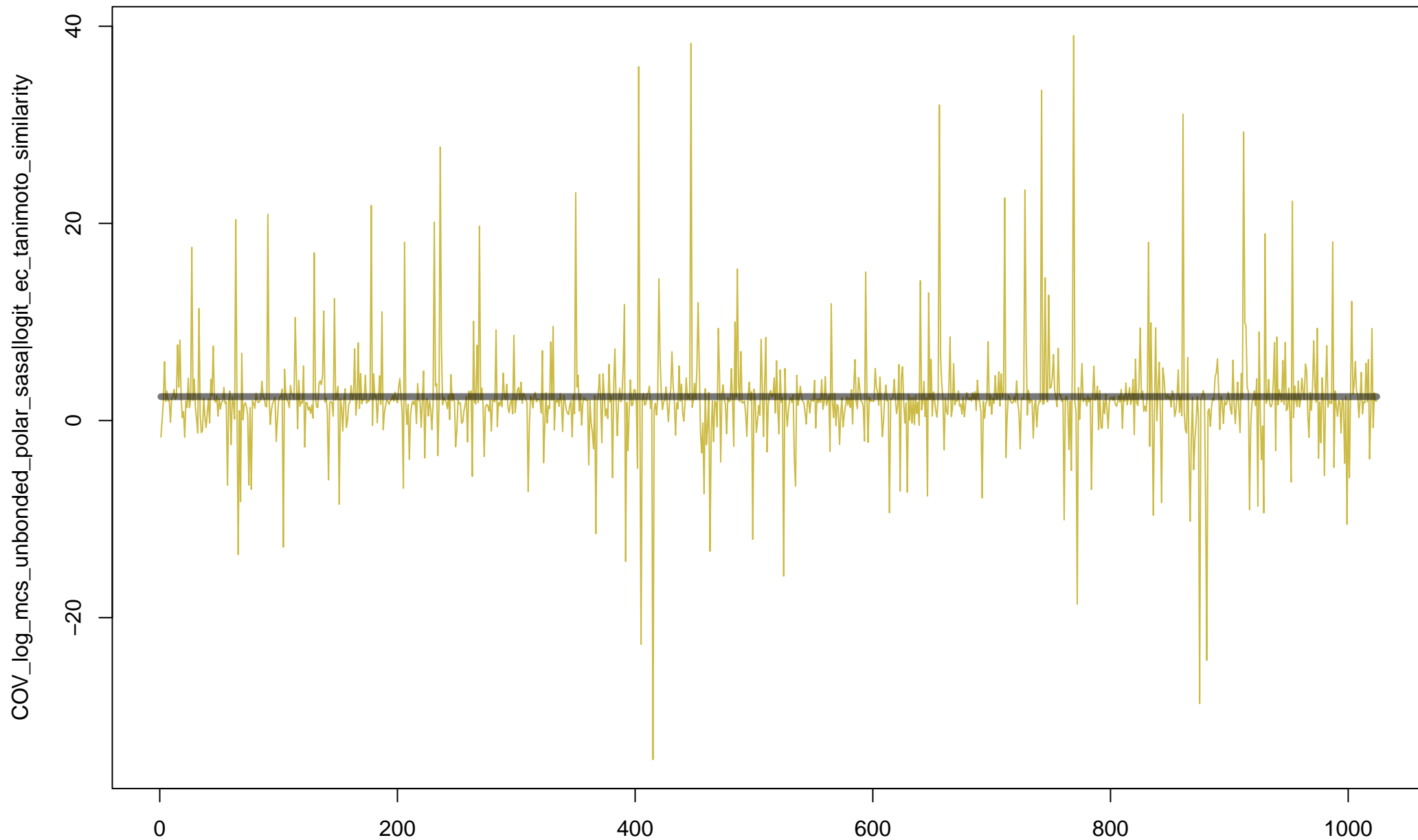
**COV\_log\_RMSD|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.191 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | percentile: 48.9**



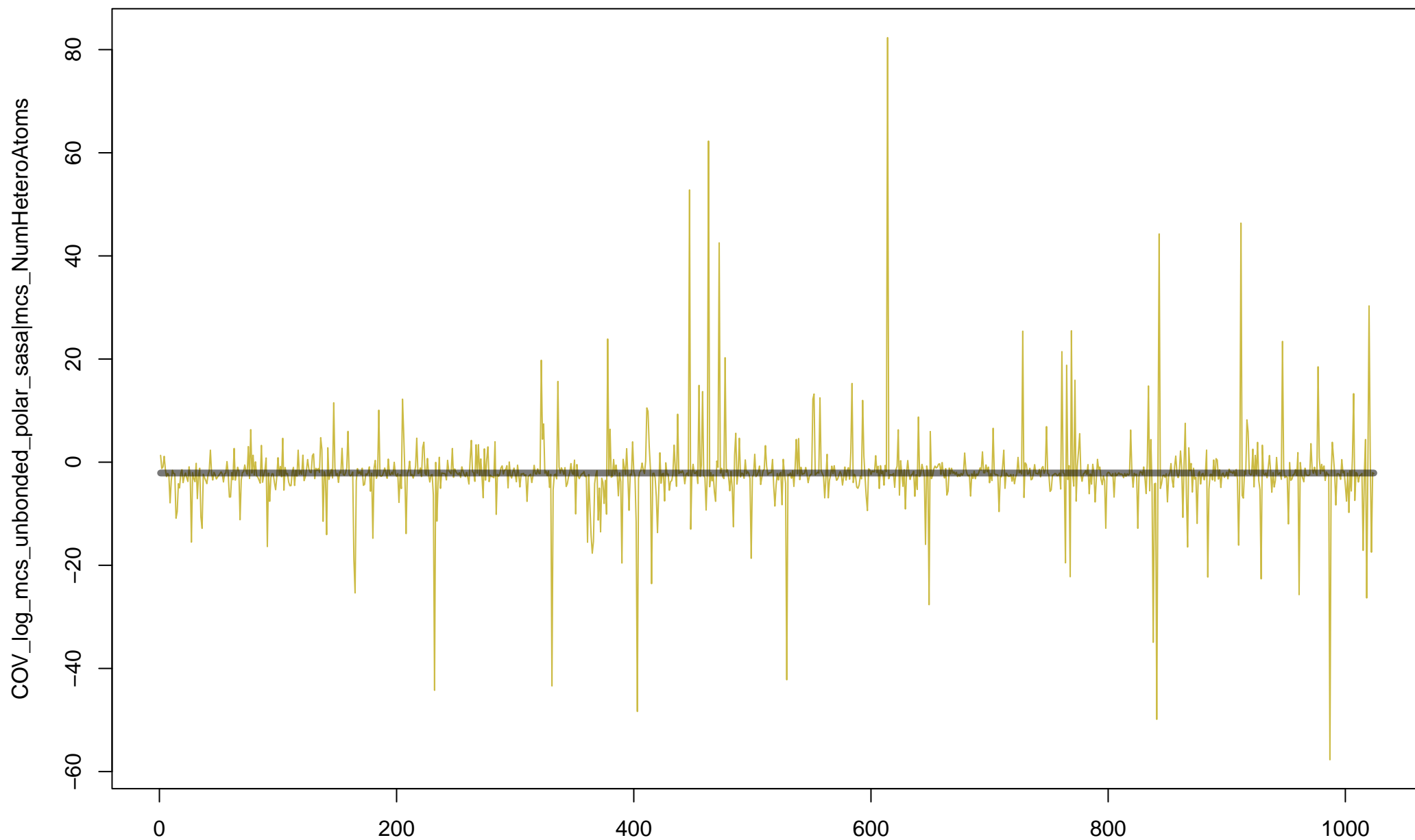
**COV\_log\_RMSD|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.182 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | percentile: 74.7**



**COV\_log\_mcs\_unbonded\_polar\_sasa|logit\_ec\_tanimoto\_similarity**  
**ESS = 1020 | BMK = 0.189 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0 | percentile: 67.9**

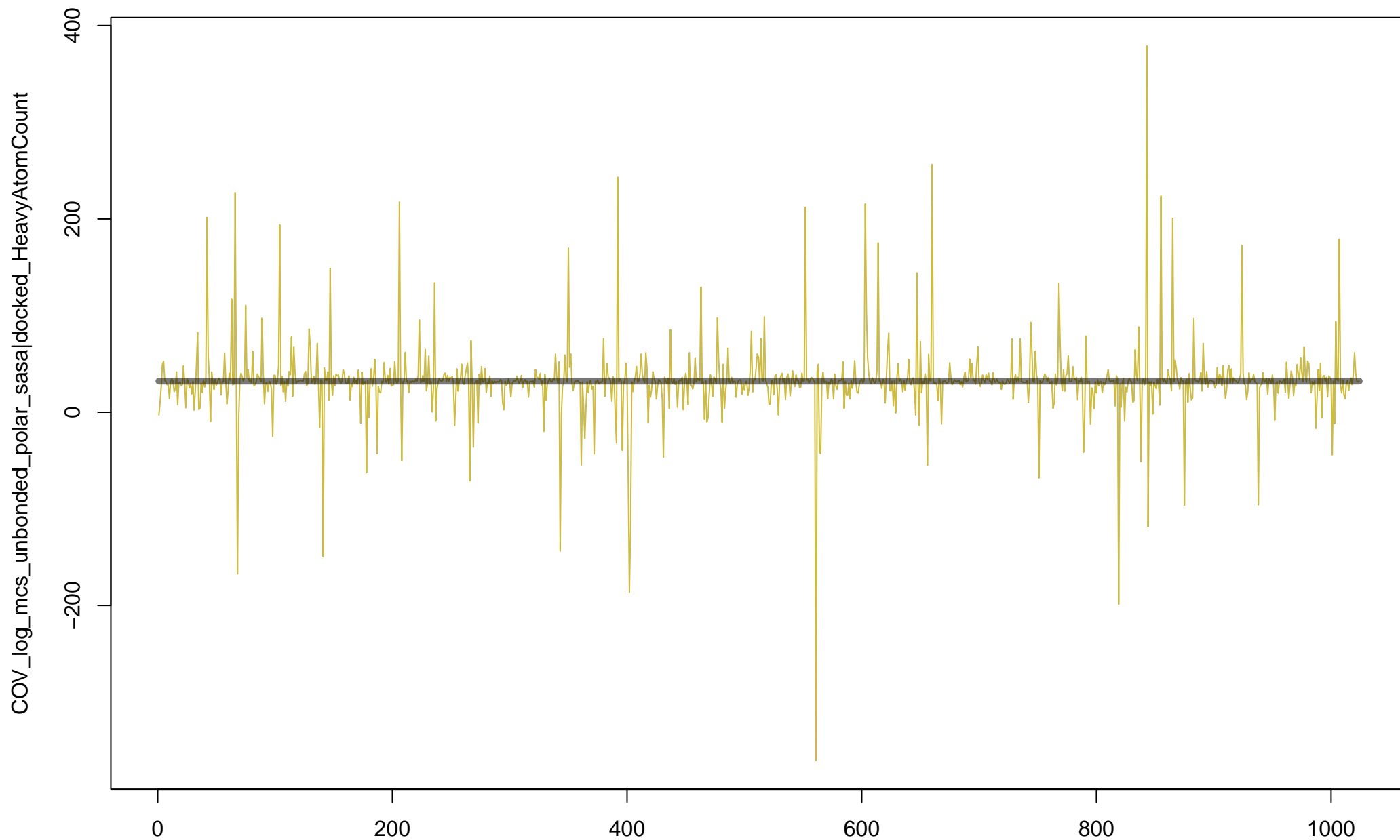


**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 1020 | BMK = 0.202 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0 | percentile: 61**

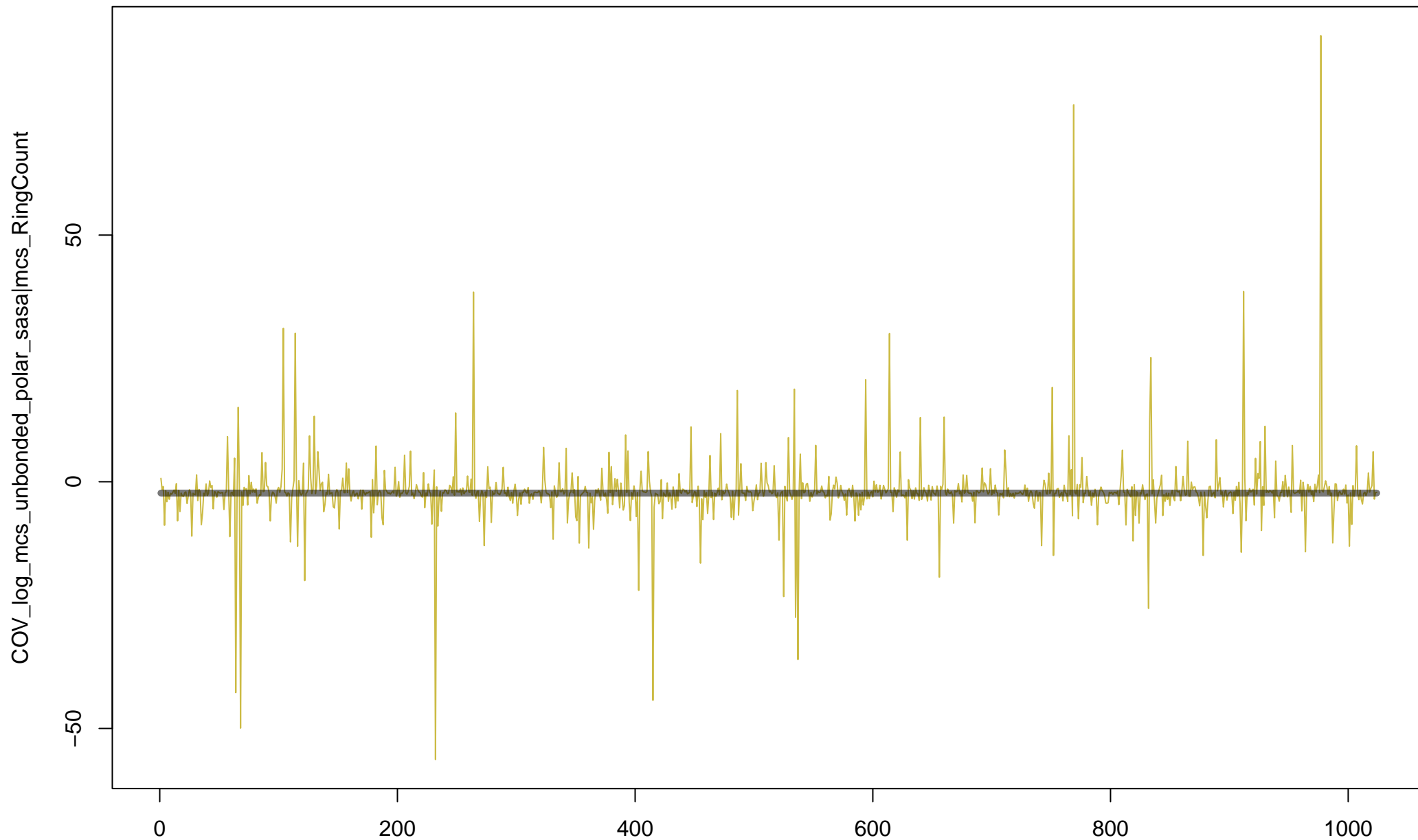




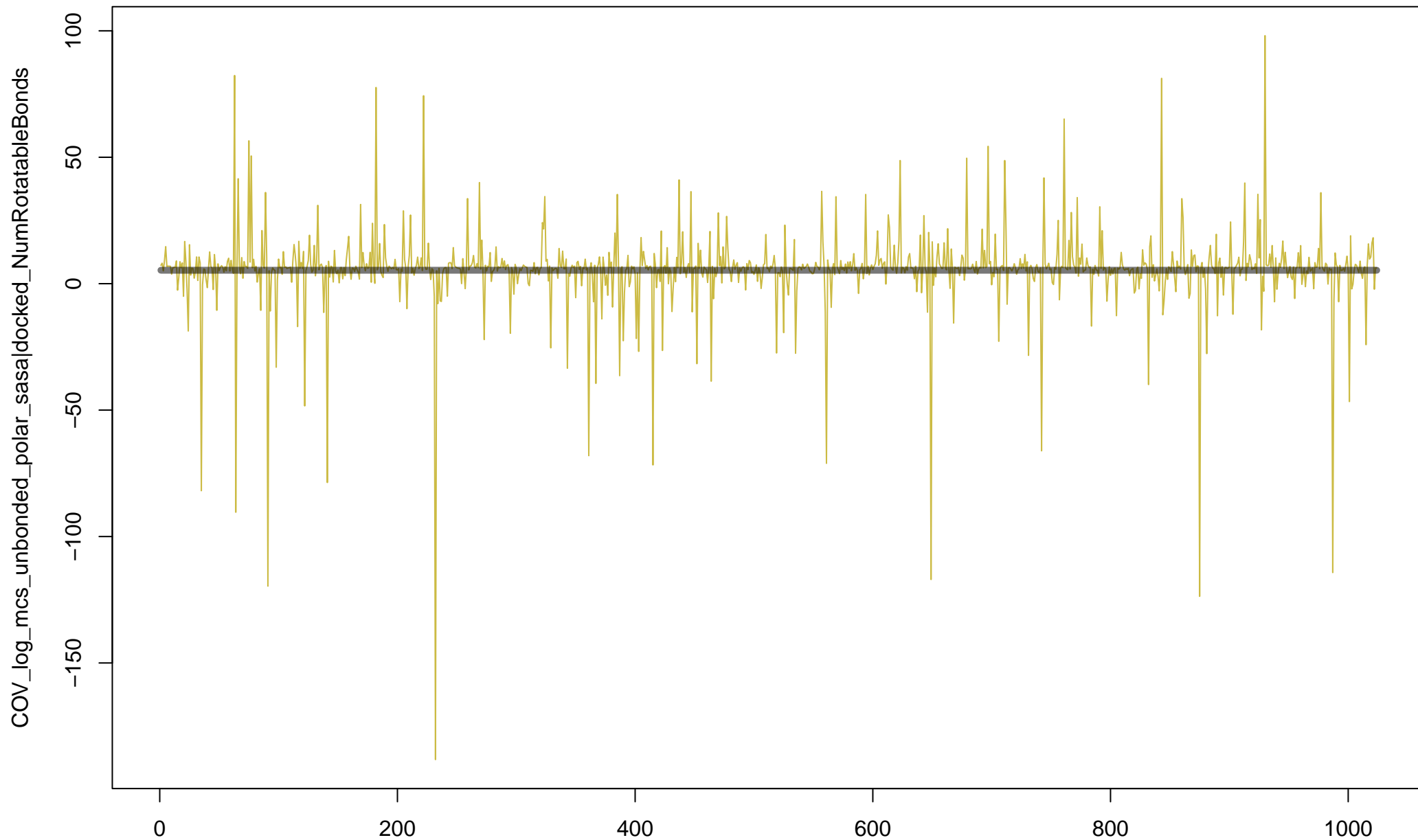
COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount  
ESS = 966 | BMK = 0.181 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0 | percentile: 54.8



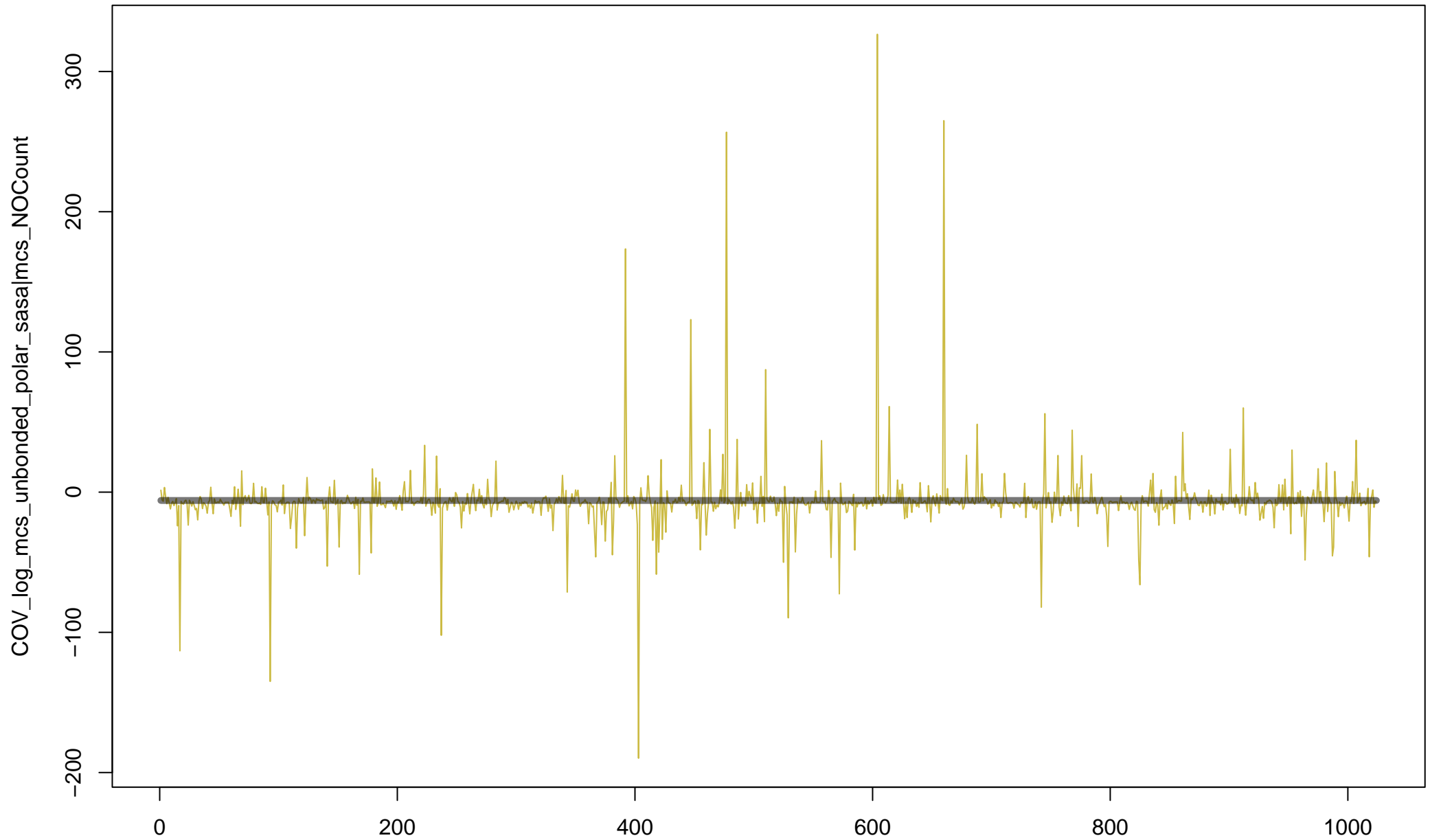
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.188 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0 | percentile: 43.8**



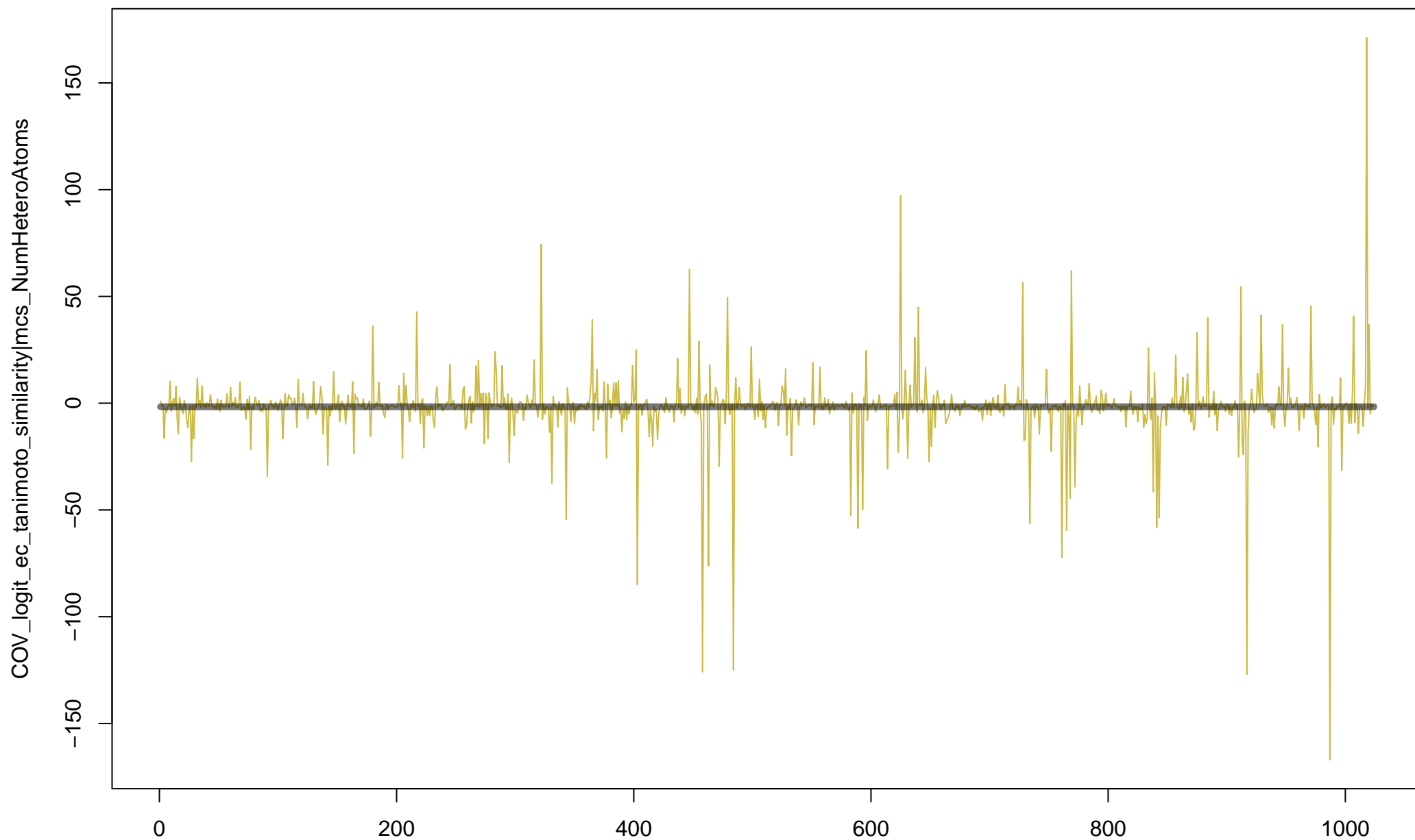
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.182 | MCSE(6.27) = 3.26 | stat: TRUE | burn: 0 | percentile: 32.1**



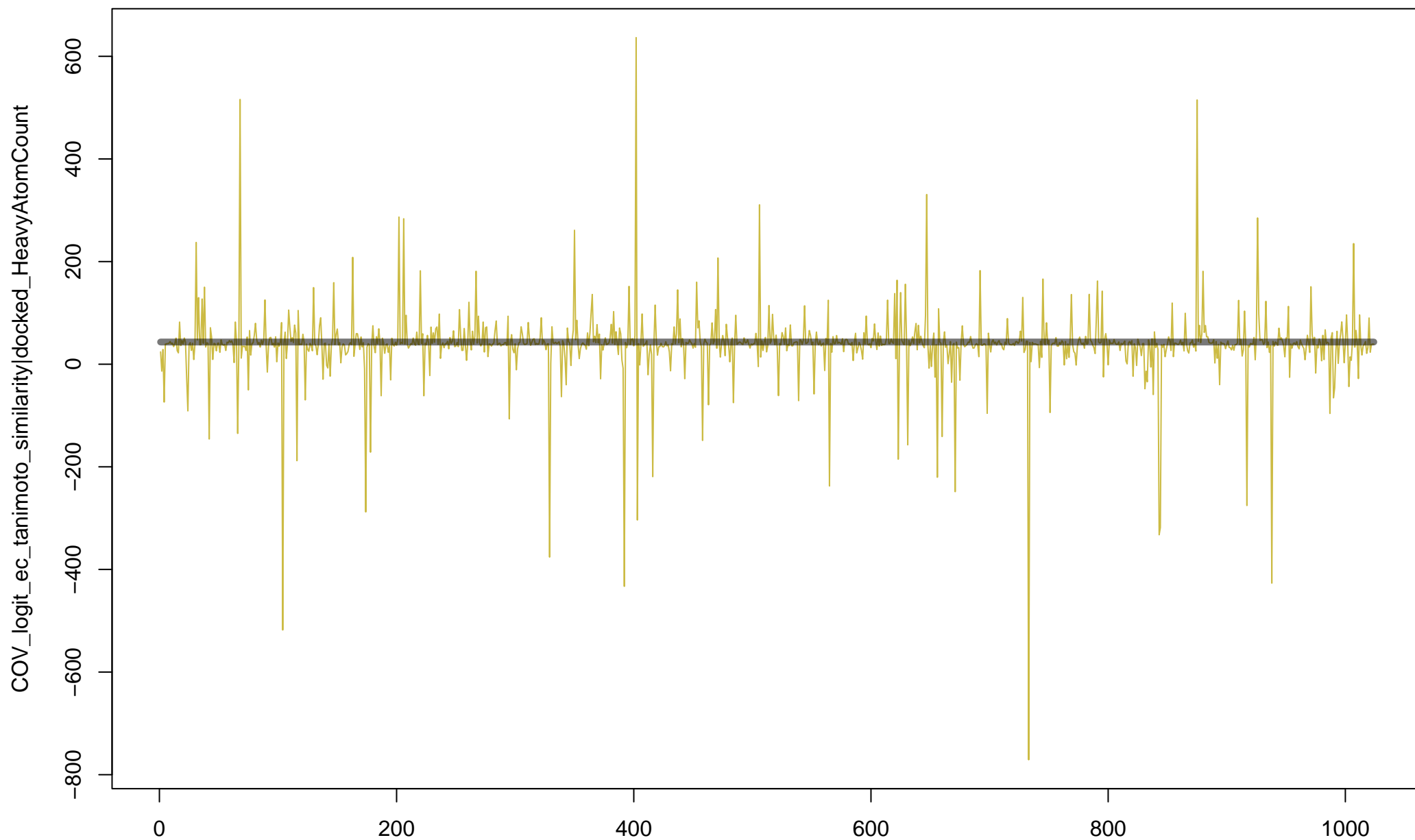
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.191 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | percentile: 72.6**



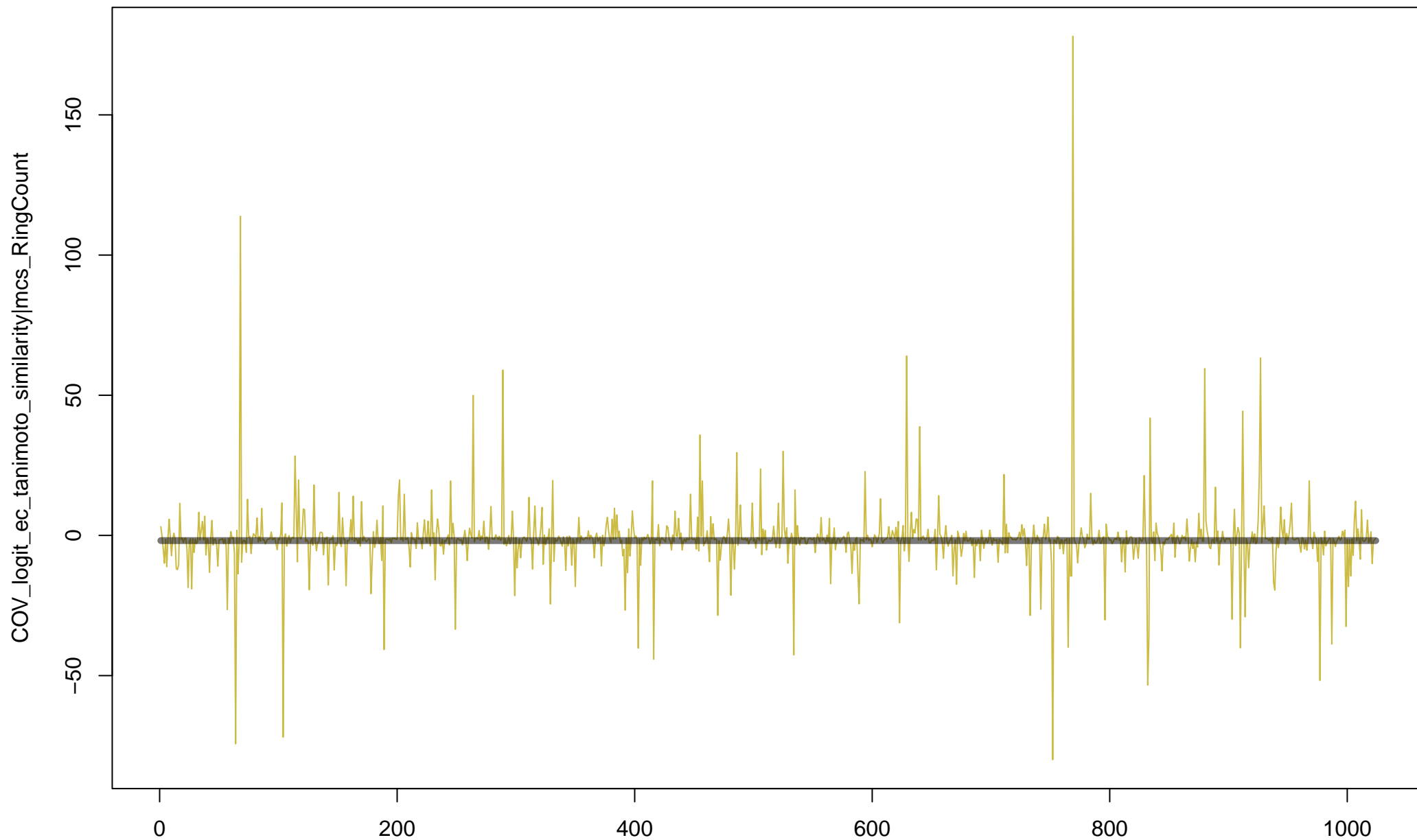
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms**  
**ESS = 1020 | BMK = 0.21 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | percentile: 40.3**



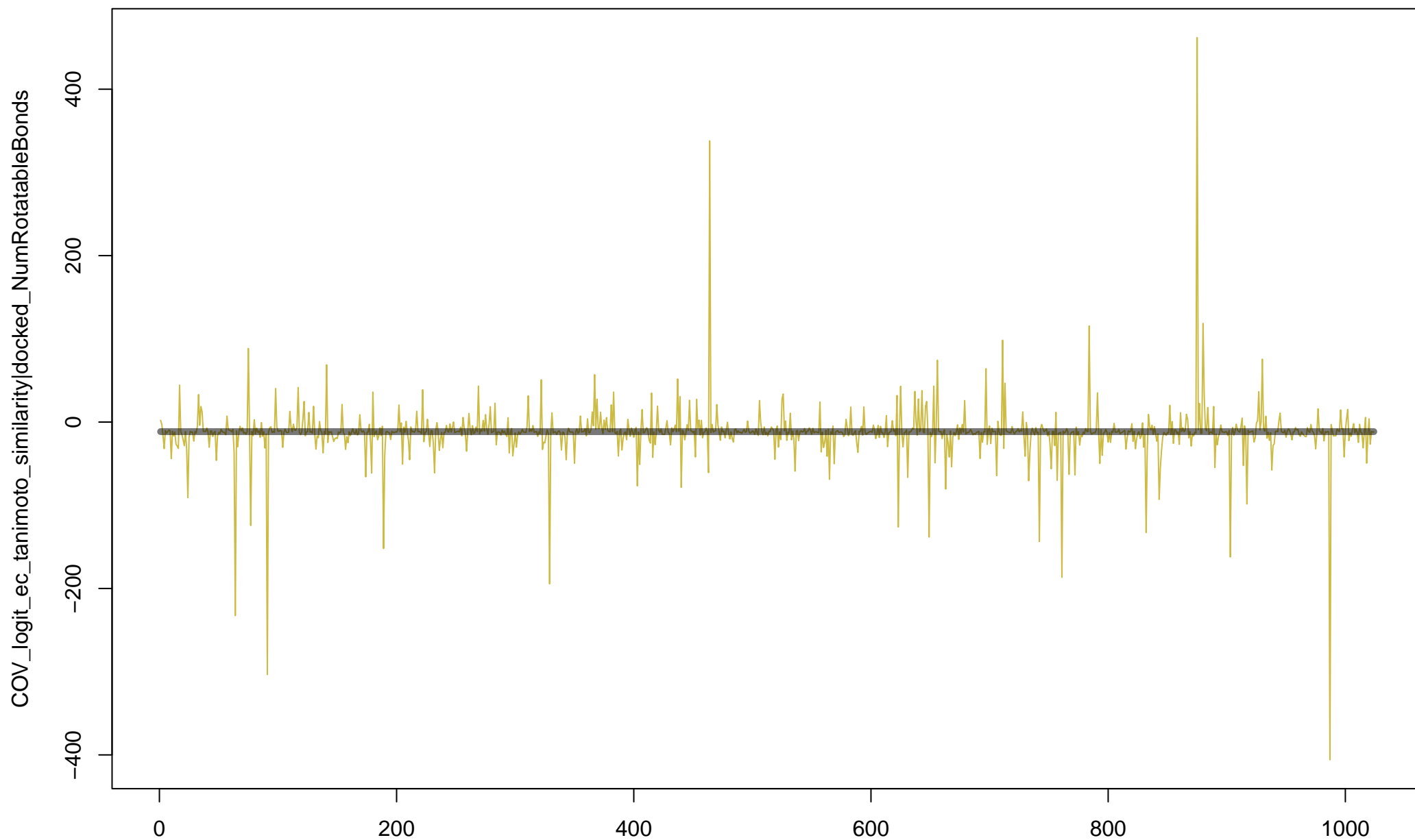
**COV\_logit\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.181 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | percentile: 68**



**COV\_logit\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.204 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | percentile: 34.9**

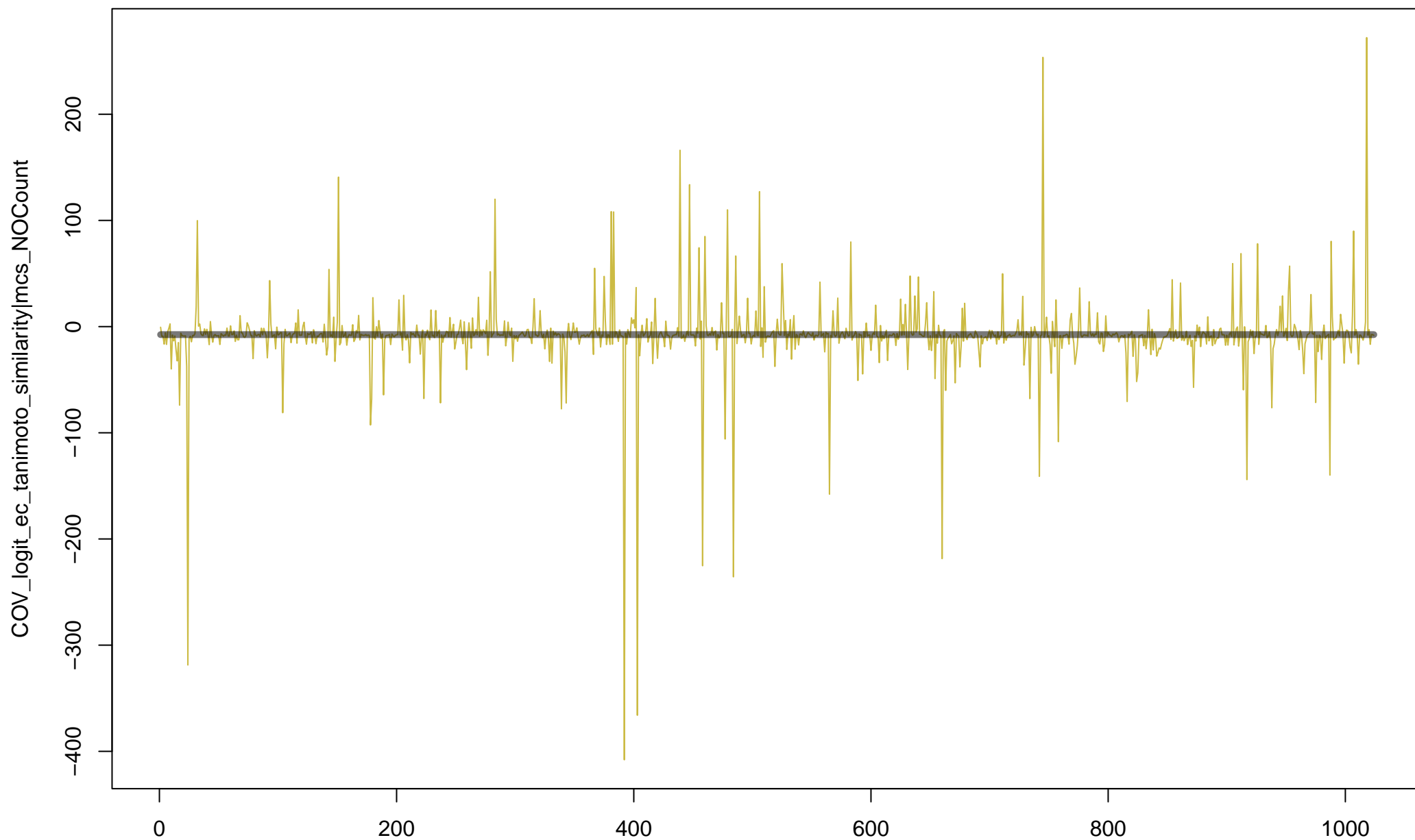


**COV\_logit\_ec\_tanimoto\_similarity|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.179 | MCSE(6.27) = 3.72 | stat: TRUE | burn: 0 | percentile: 57.4**

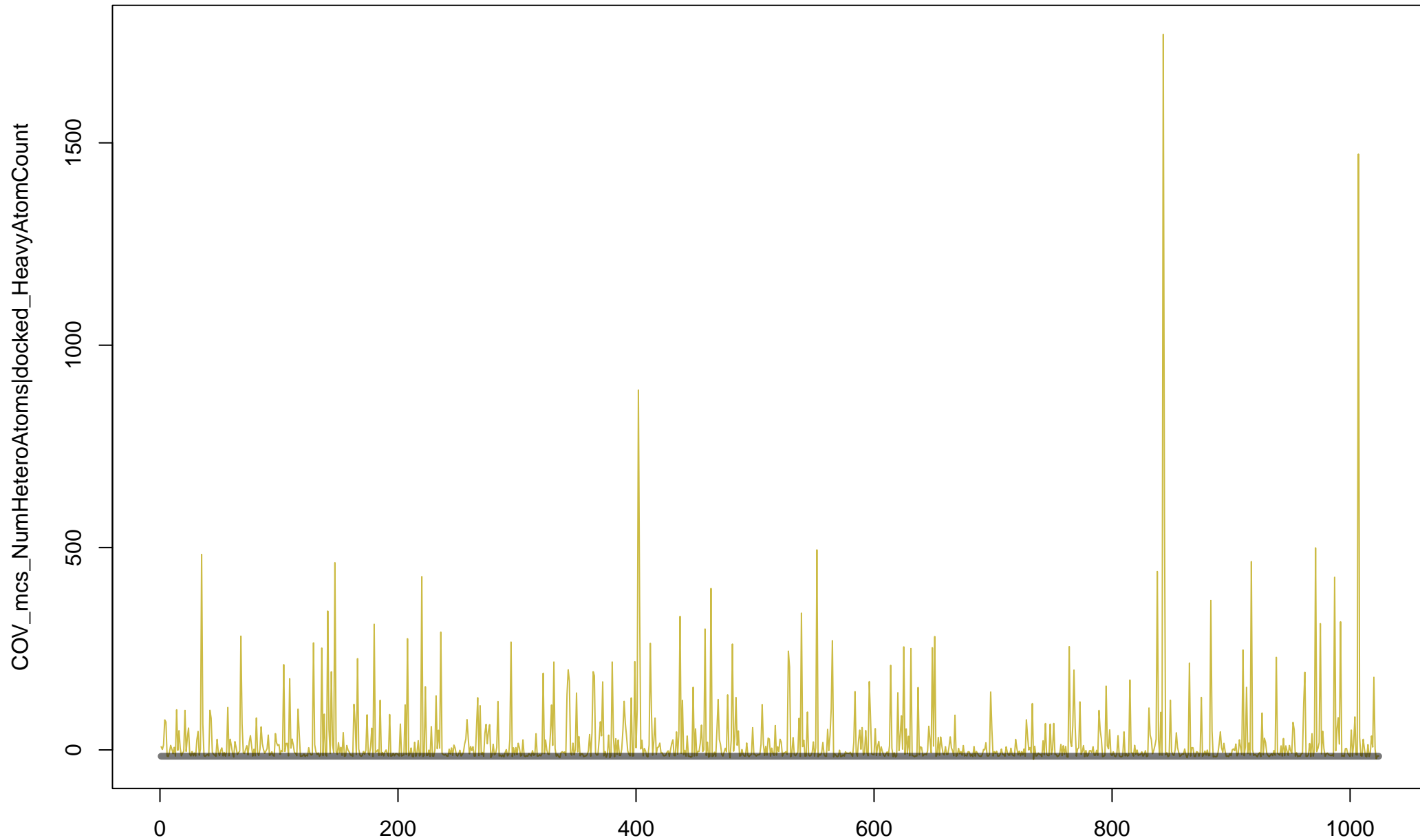




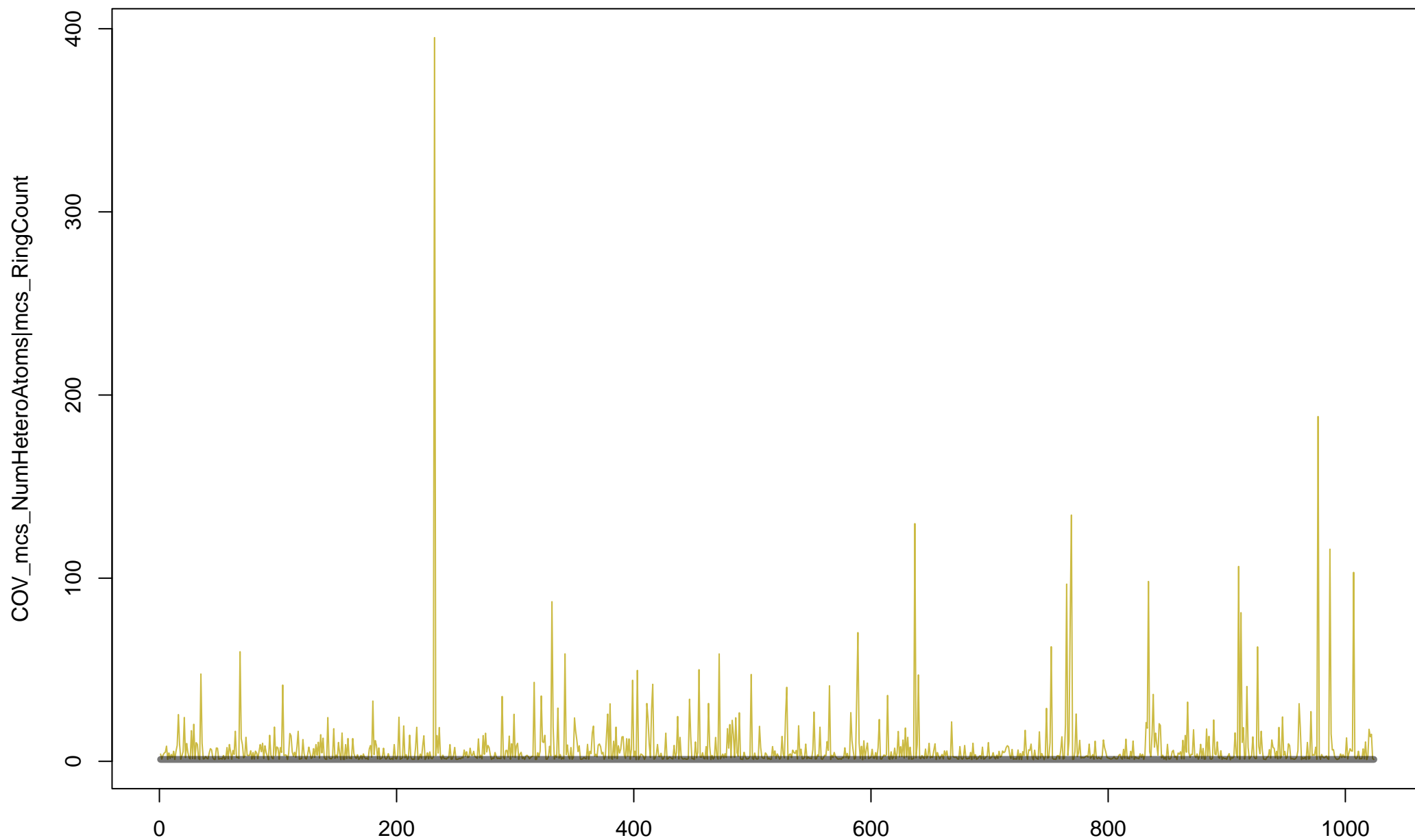
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.236 | MCSE(6.27) = 3.28 | stat: TRUE | burn: 0 | percentile: 60.4**



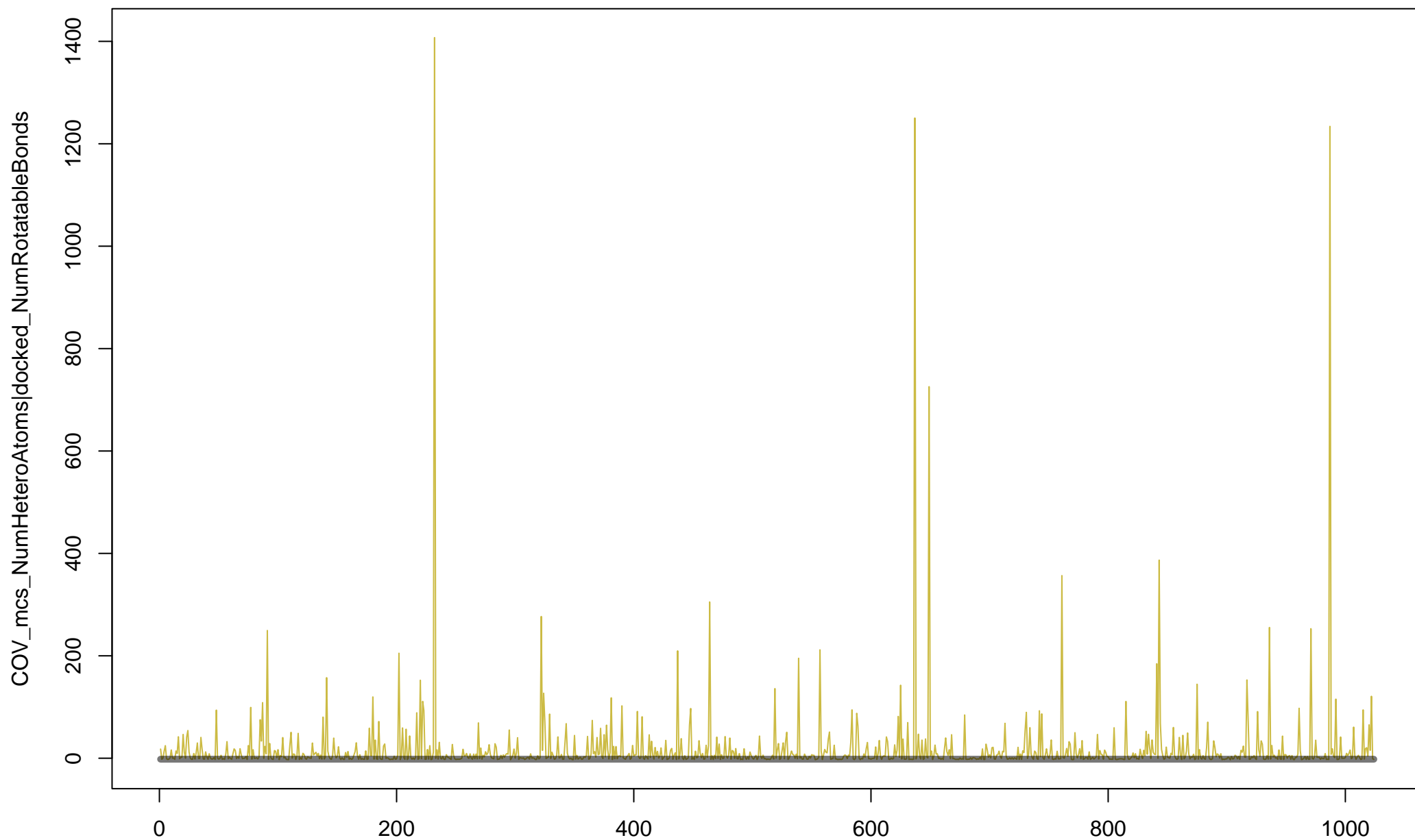
**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 846 | BMK = 0.132 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0 | percentile: 9.77**



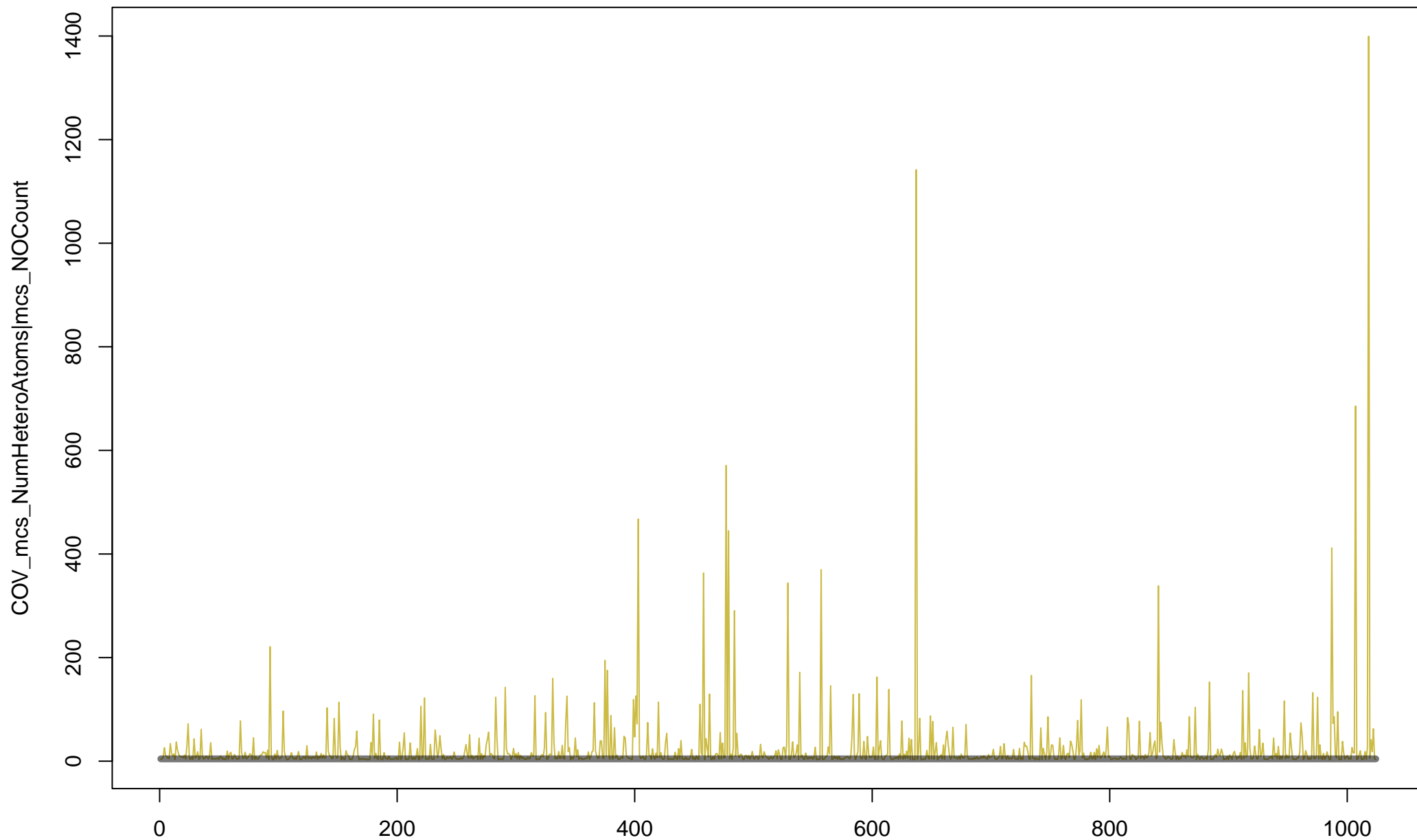
**COV\_mcs\_NumHeteroAtoms|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.152 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0 | percentile: 2.25**



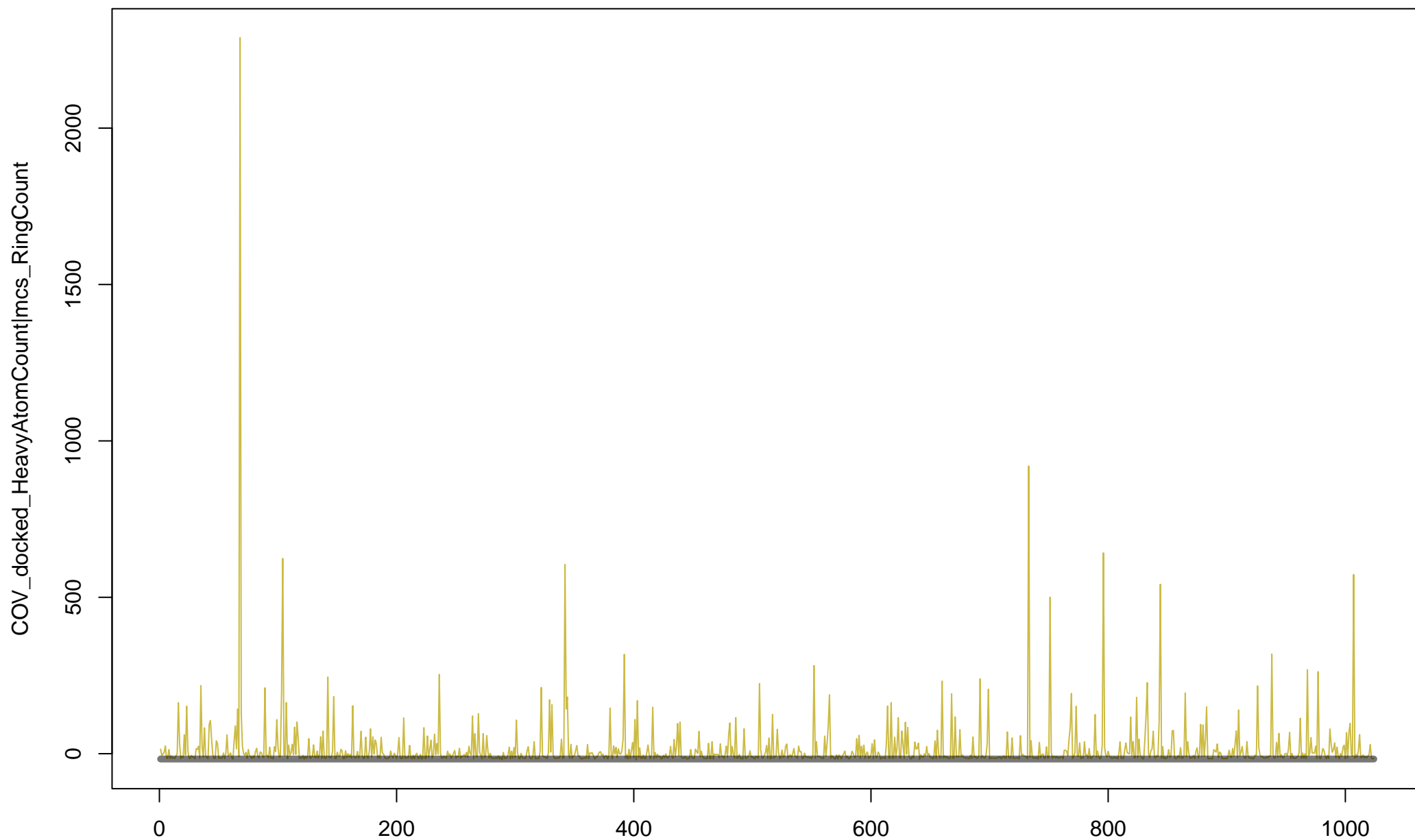
**COV\_mcs\_NumHeteroAtoms|docked\_NumRotatableBonds**  
**ESS = 840 | BMK = 0.127 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | percentile: 16.7**



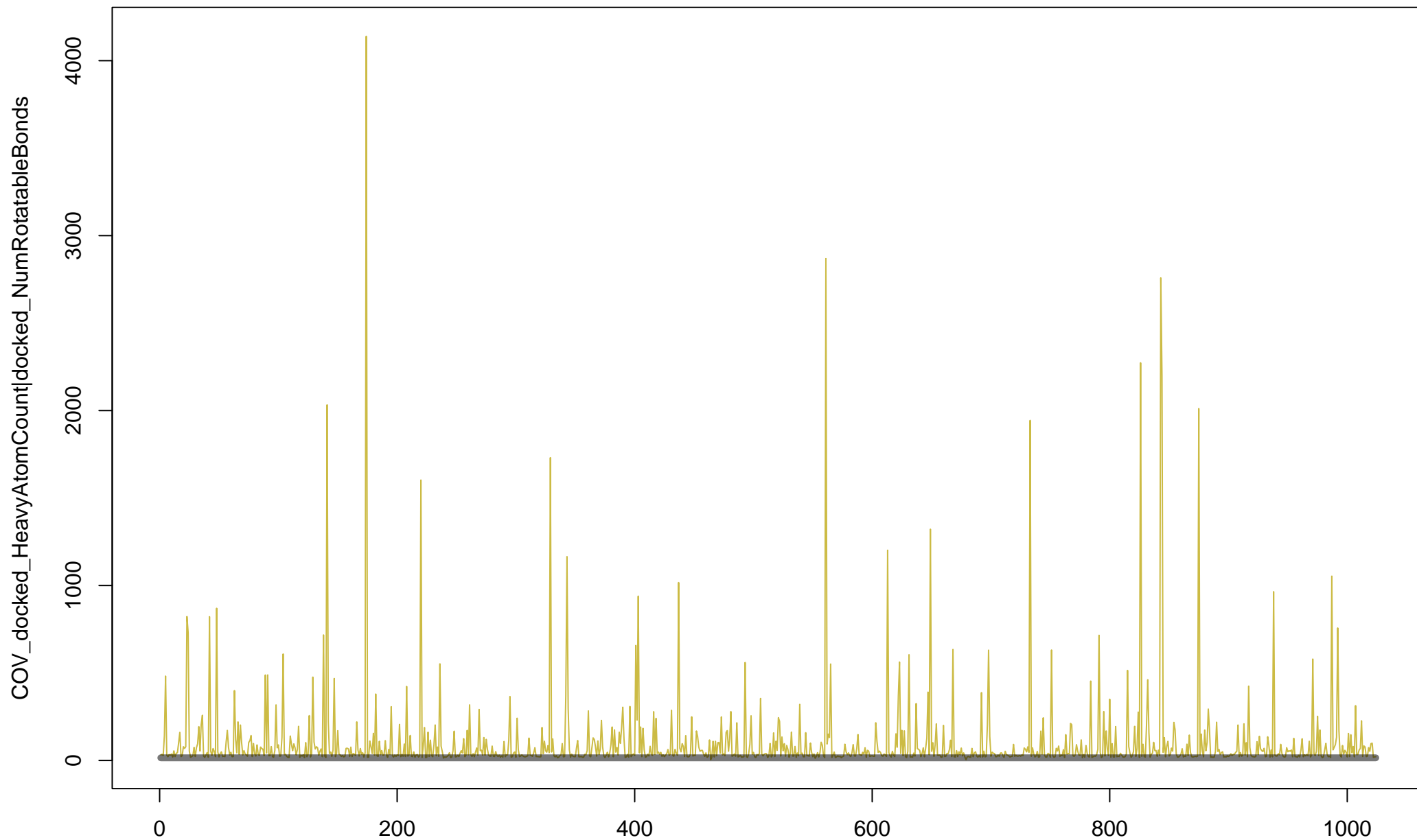
**COV\_mcs\_NumHeteroAtoms|mcs\_NOCount**  
**ESS = 733 | BMK = 0.149 | MCSE(6.27) = 3.6 | stat: FALSE | burn: 0 | percentile: 26.2**



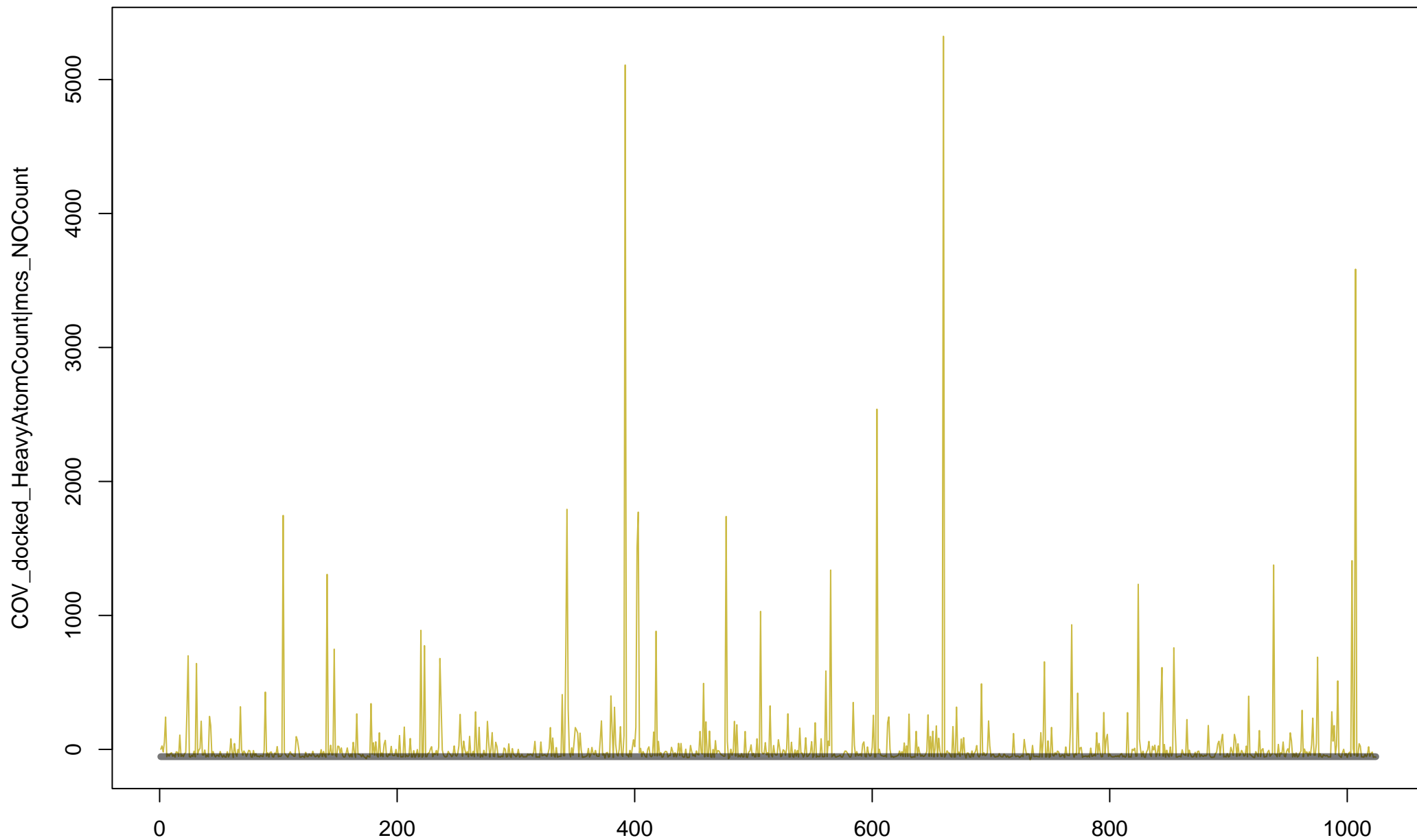
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 1020 | BMK = 0.125 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0 | percentile: 0.293**



**COV\_docked\_HeavyAtomCount|docked\_NumRotatableBonds**  
**ESS = 919 | BMK = 0.155 | MCSE(6.27) = 2.67 | stat: TRUE | burn: 0 | percentile: 0.391**

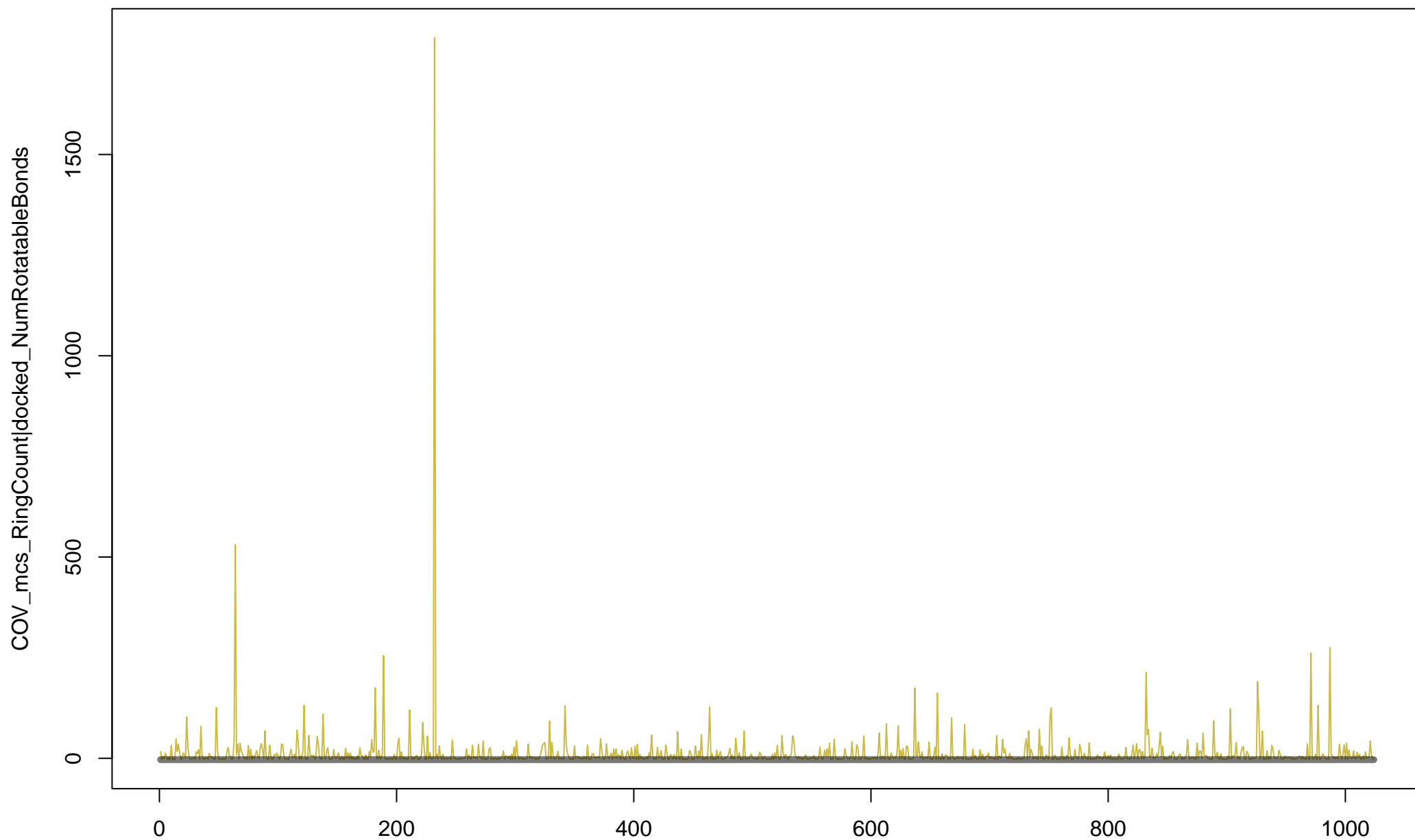


**COV\_docked\_HeavyAtomCount|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.145 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 0 | percentile: 22.3**

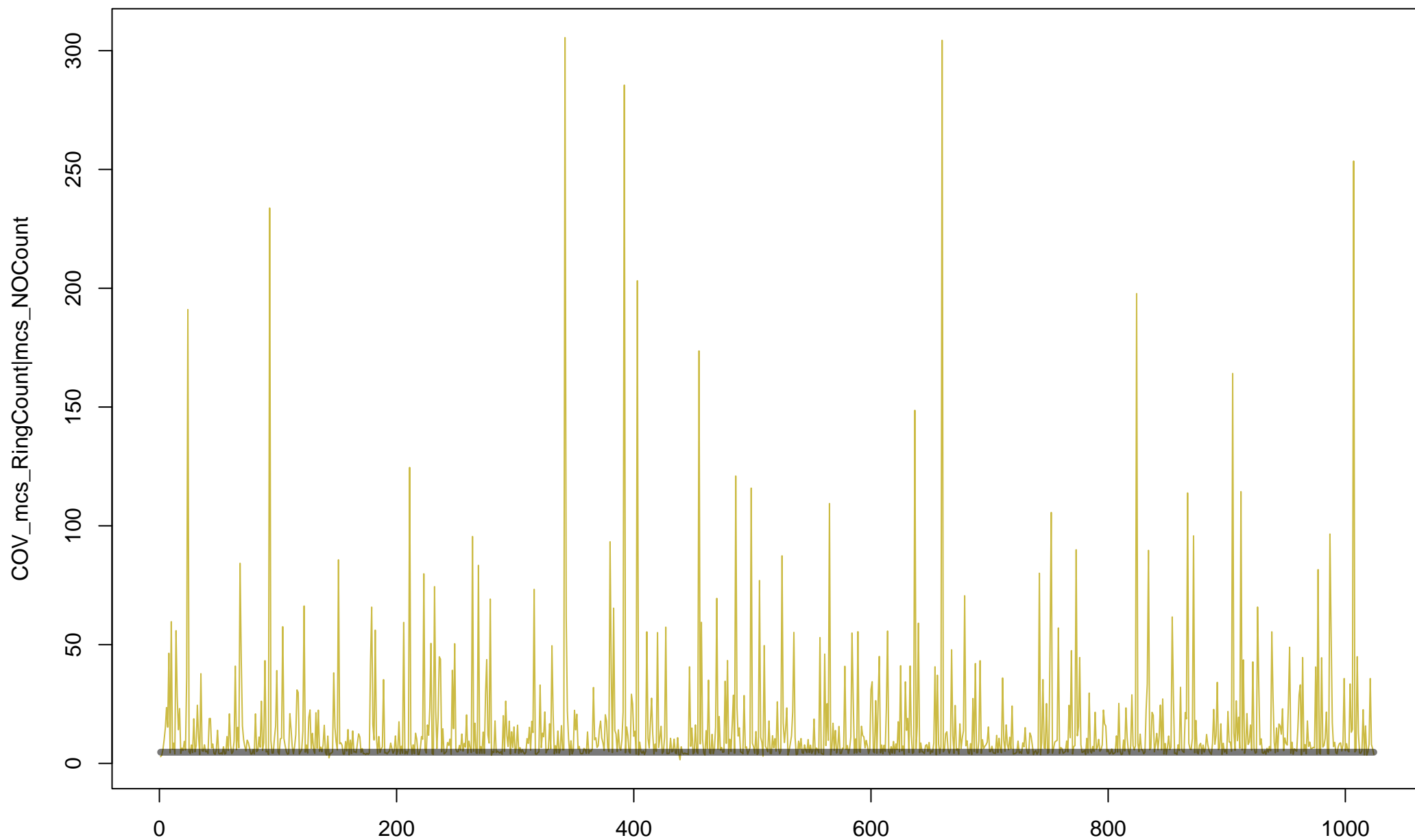




**COV\_mcs\_RingCount|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.108 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0 | percentile: 0.391**



**COV\_mcs\_RingCount|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.143 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0 | percentile: 26.2**



**COV\_docked\_NumRotatableBonds|mcs\_NOCount**  
**ESS = 1020 | BMK = 0.154 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0 | percentile: 0**

