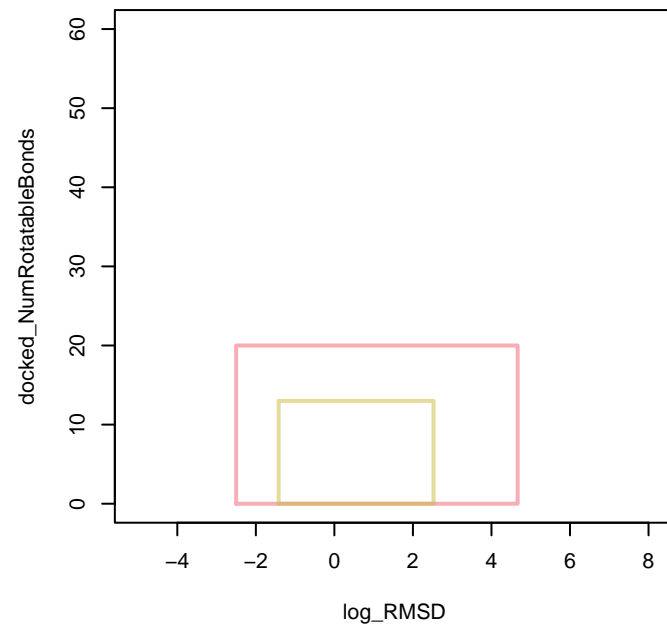
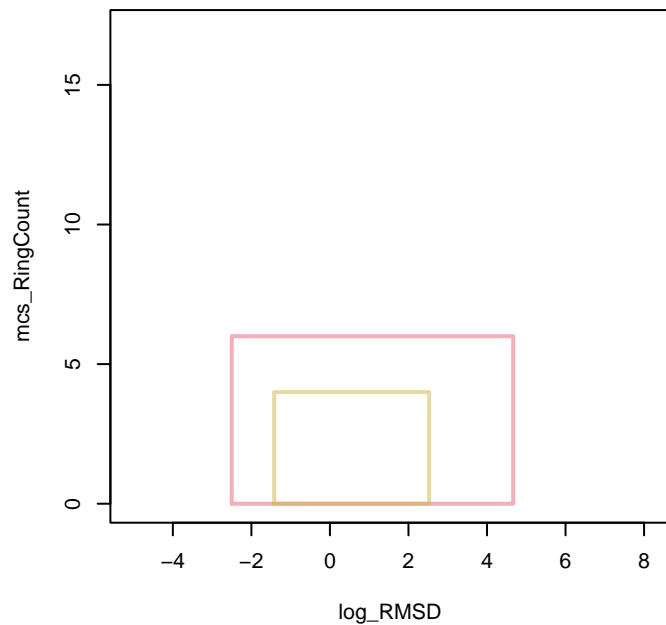
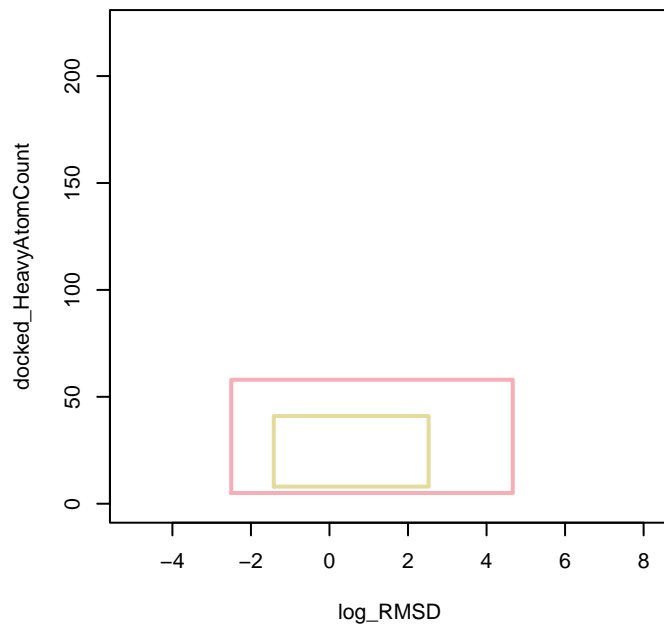
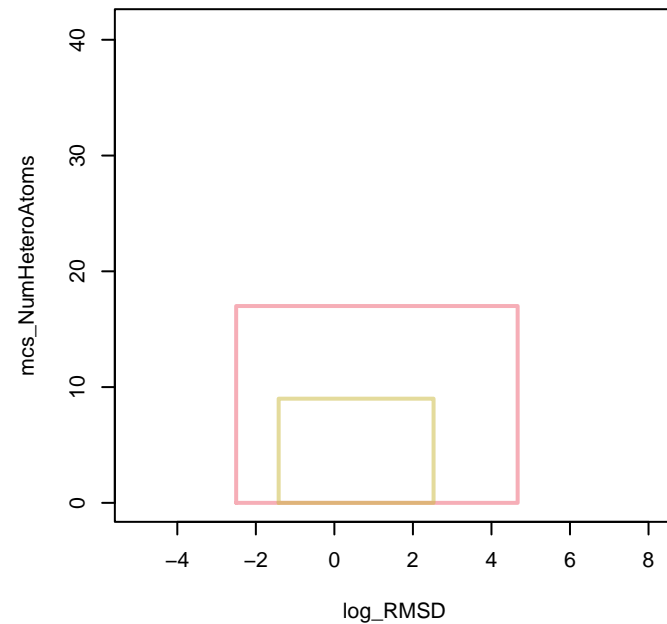
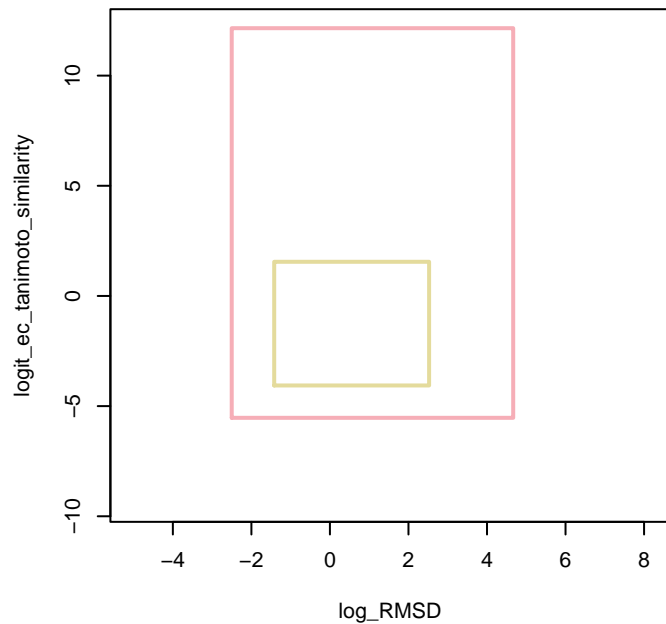
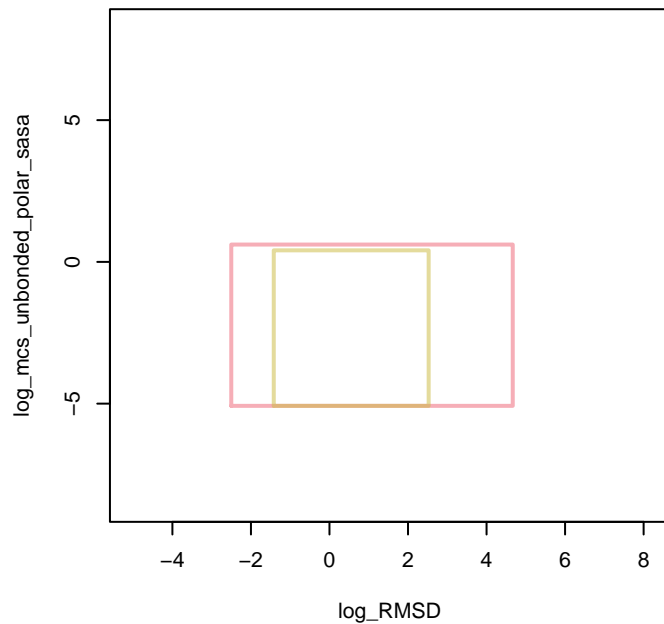


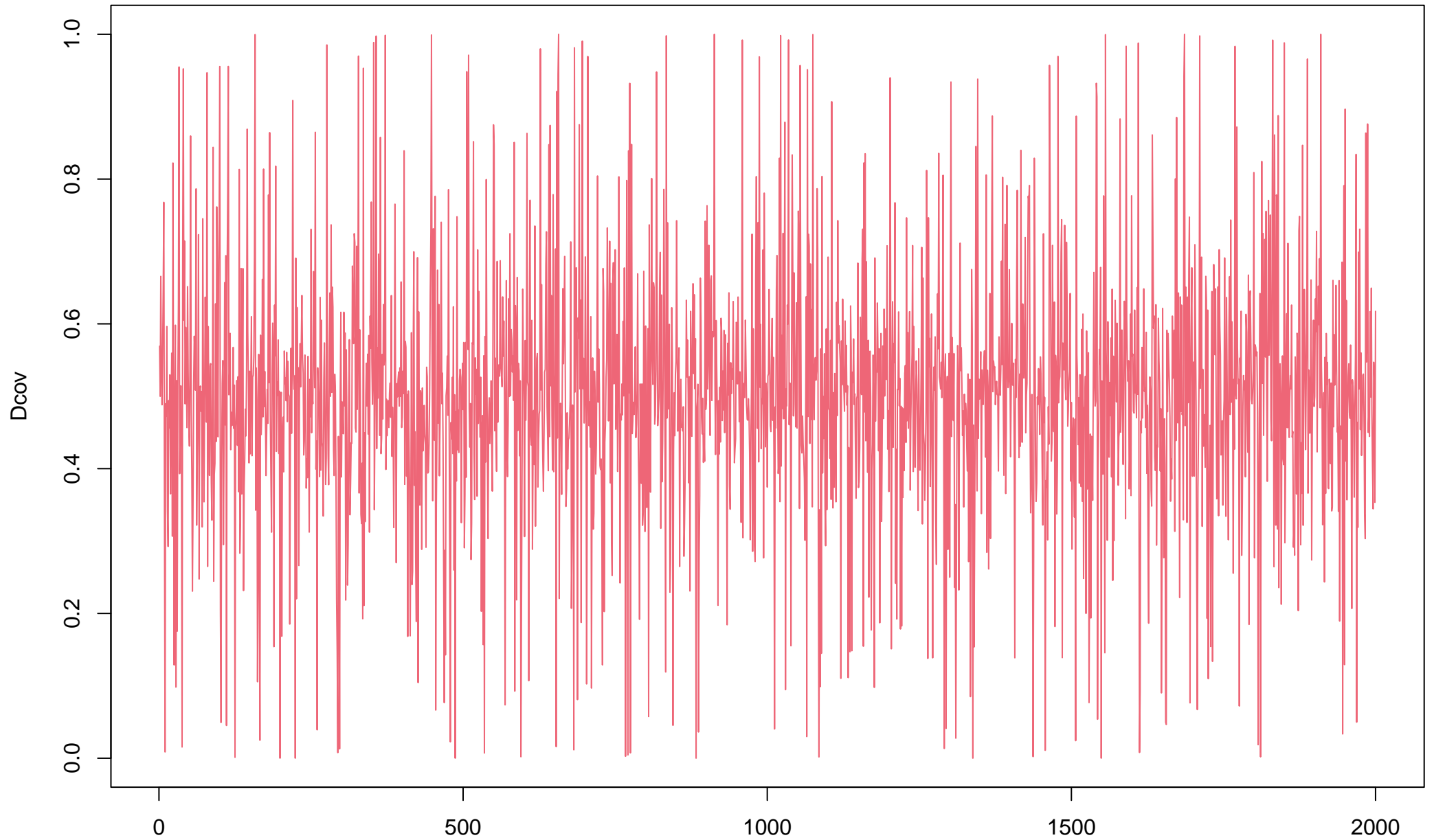
## Stats

min ESS = 1435.61509222742  
max BMK = 0.104333623331125  
max MCSE = 0.361275723189575  
all stationary: TRUE  
burn: 0

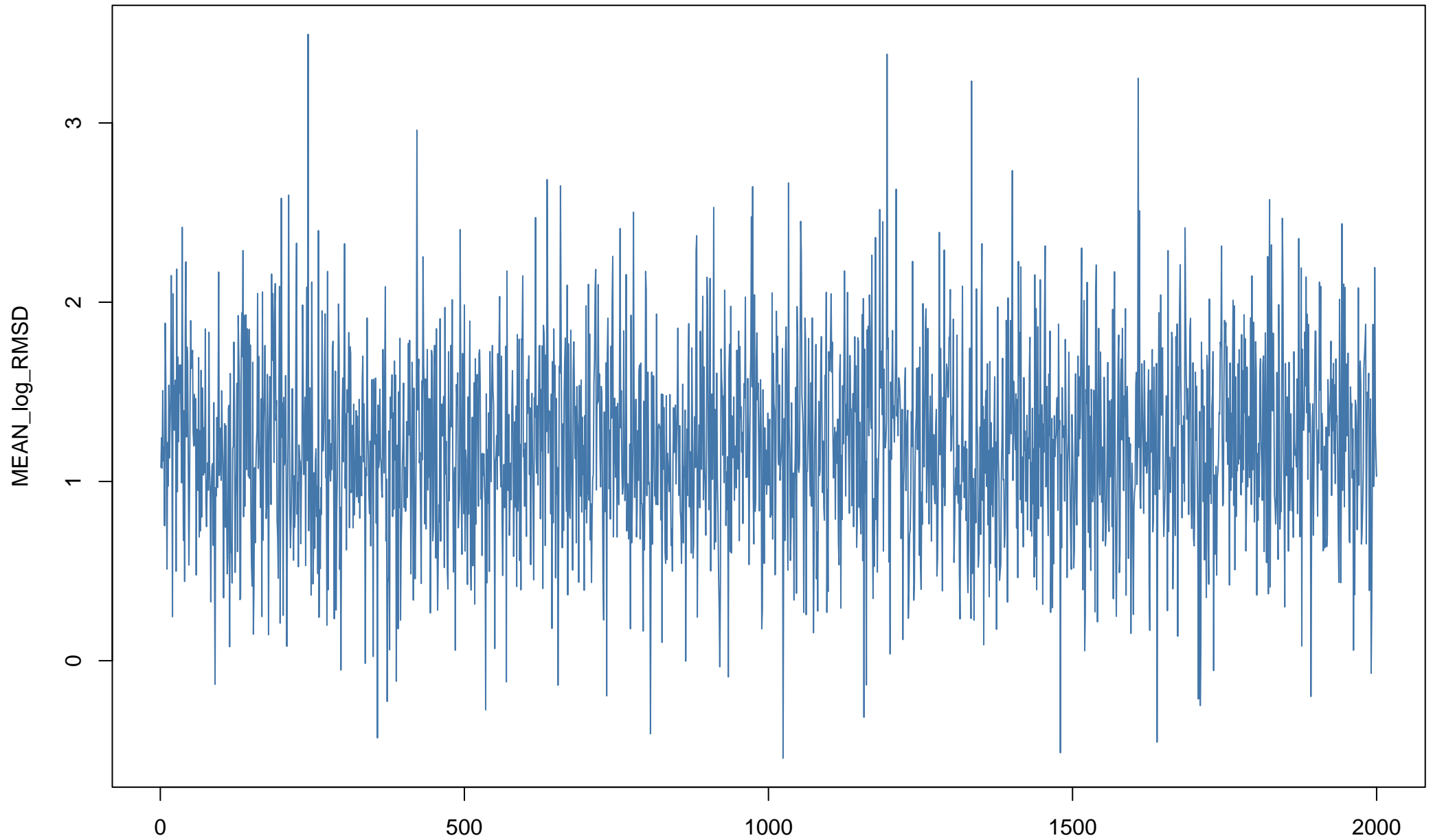
1:2



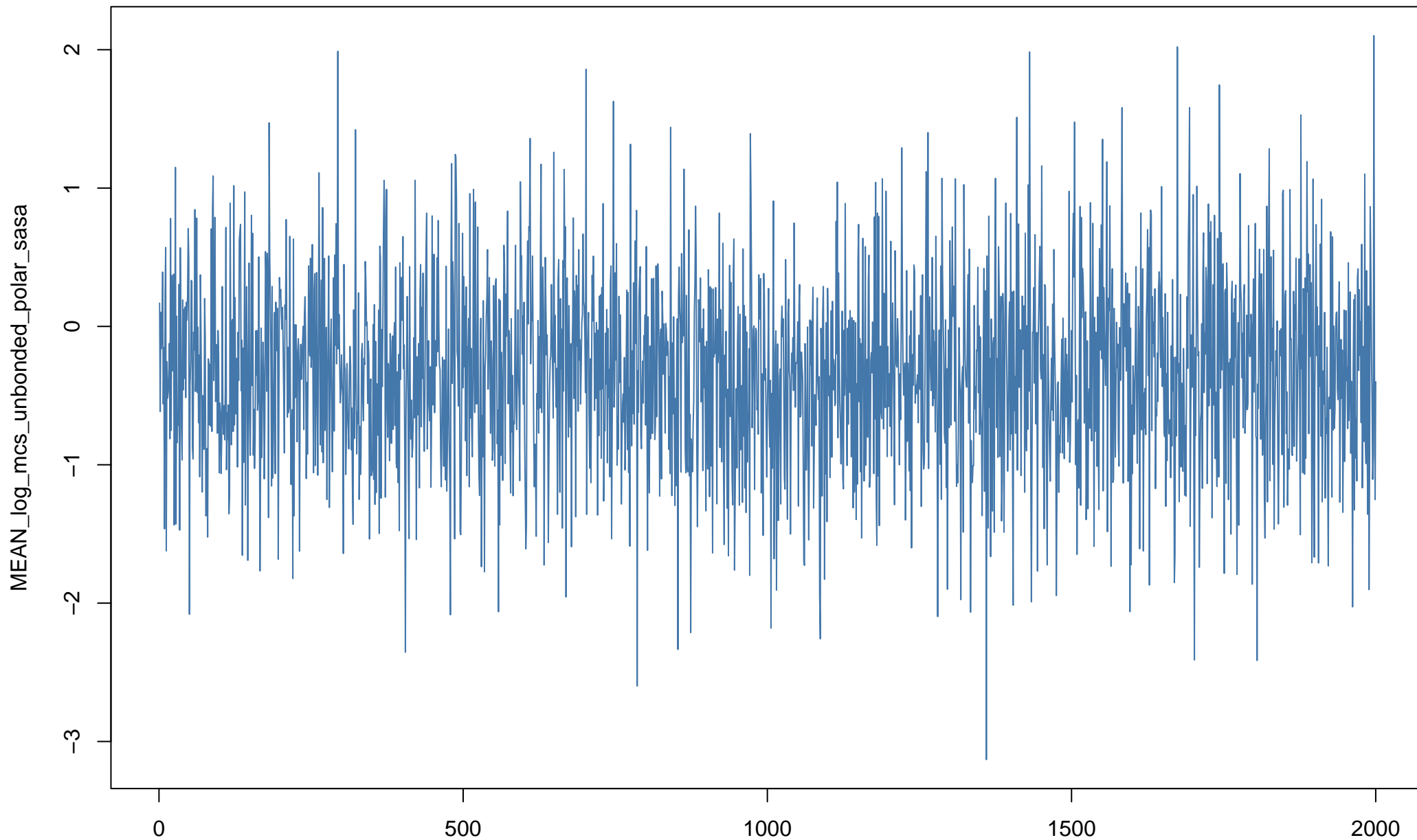
**Dcov**  
**ESS = 2000 | BMK = 0.0446 | MCSE(6.27) = 0.361 | stat: TRUE | burn: 0**



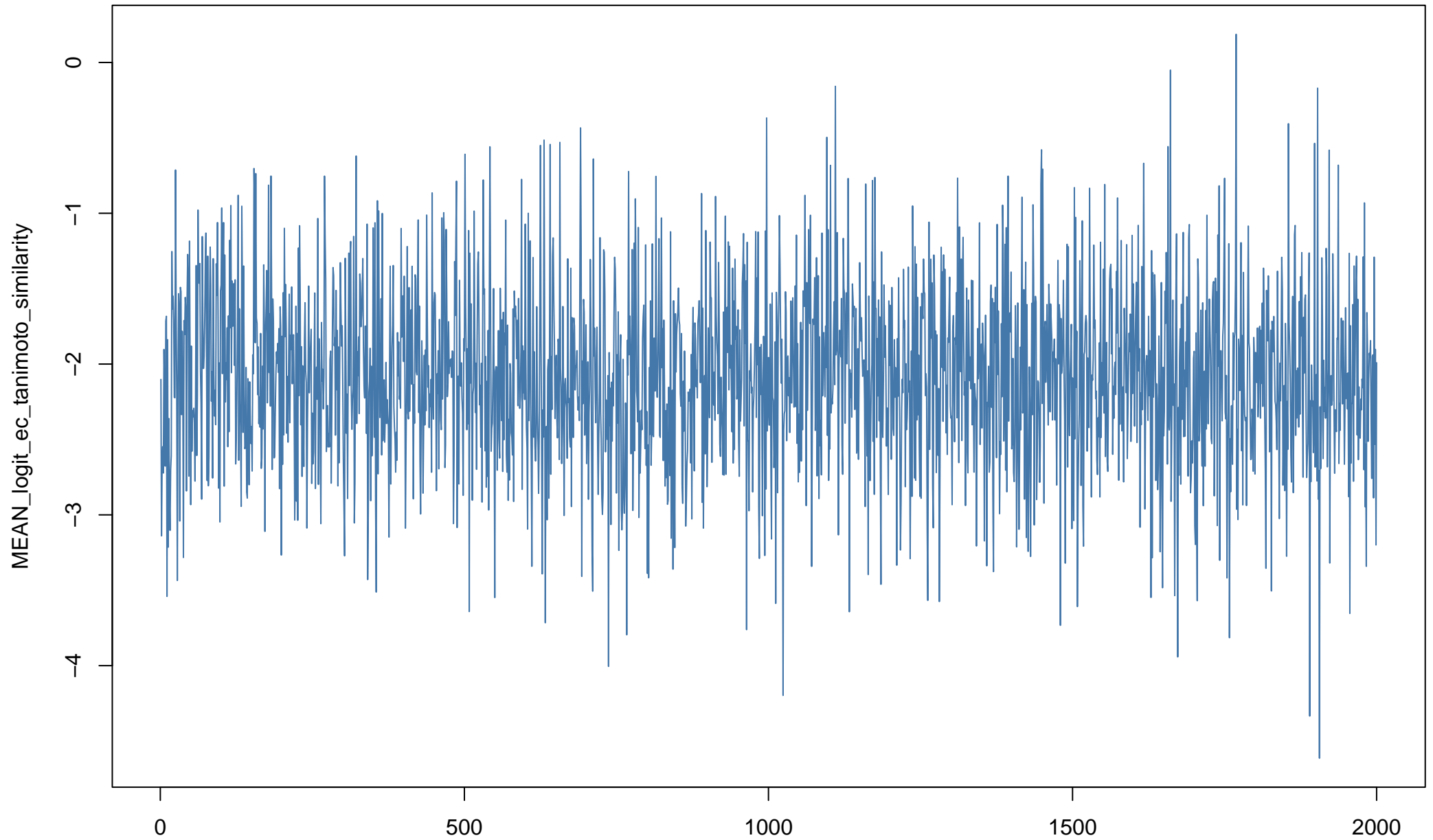
**MEAN\_log\_RMSD**  
**ESS = 2000 | BMK = 0.0475 | MCSE(6.27) = 0.121 | stat: TRUE | burn: 0**



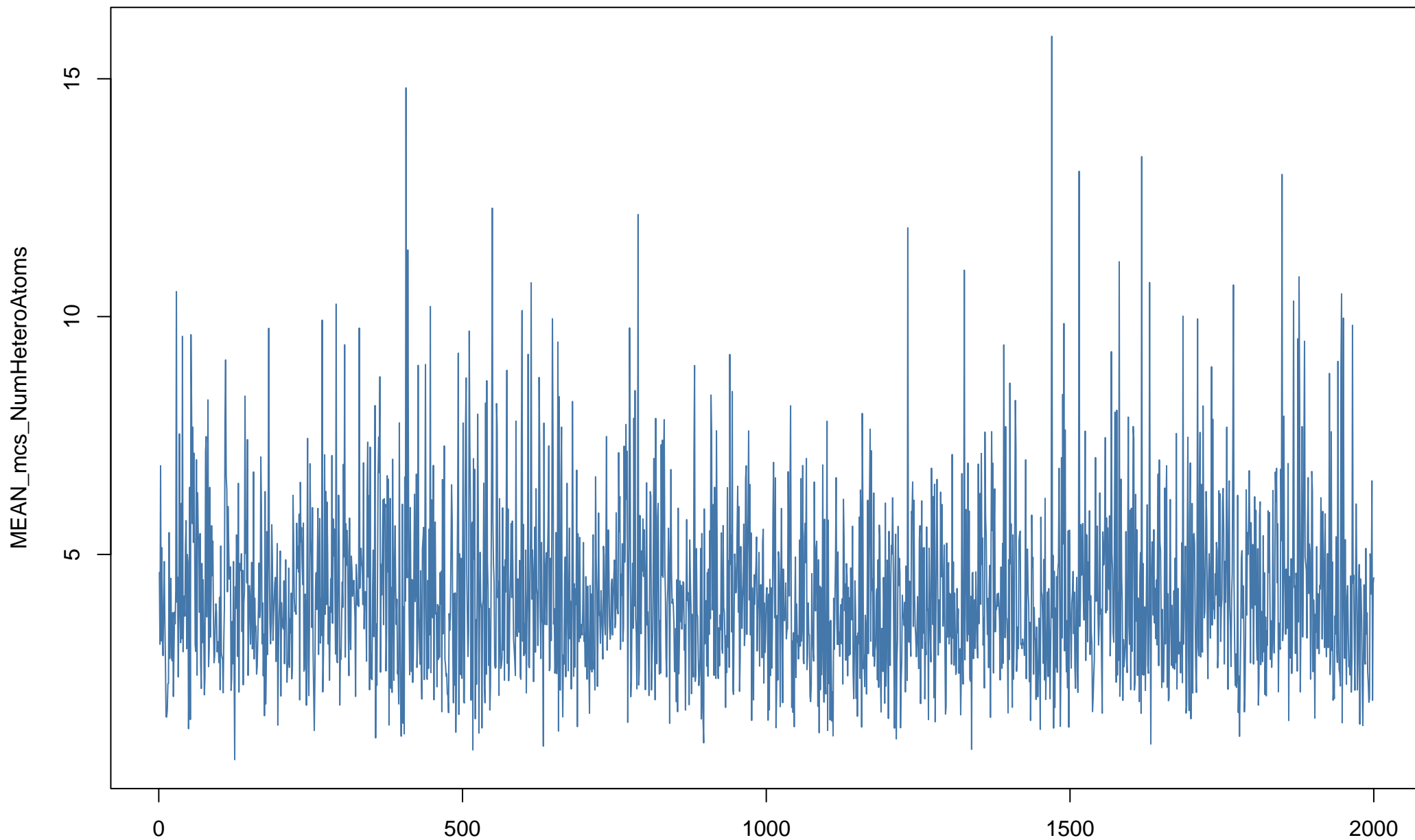
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2000 | BMK = 0.0459 | MCSE(6.27) = 0.0927 | stat: TRUE | burn: 0**



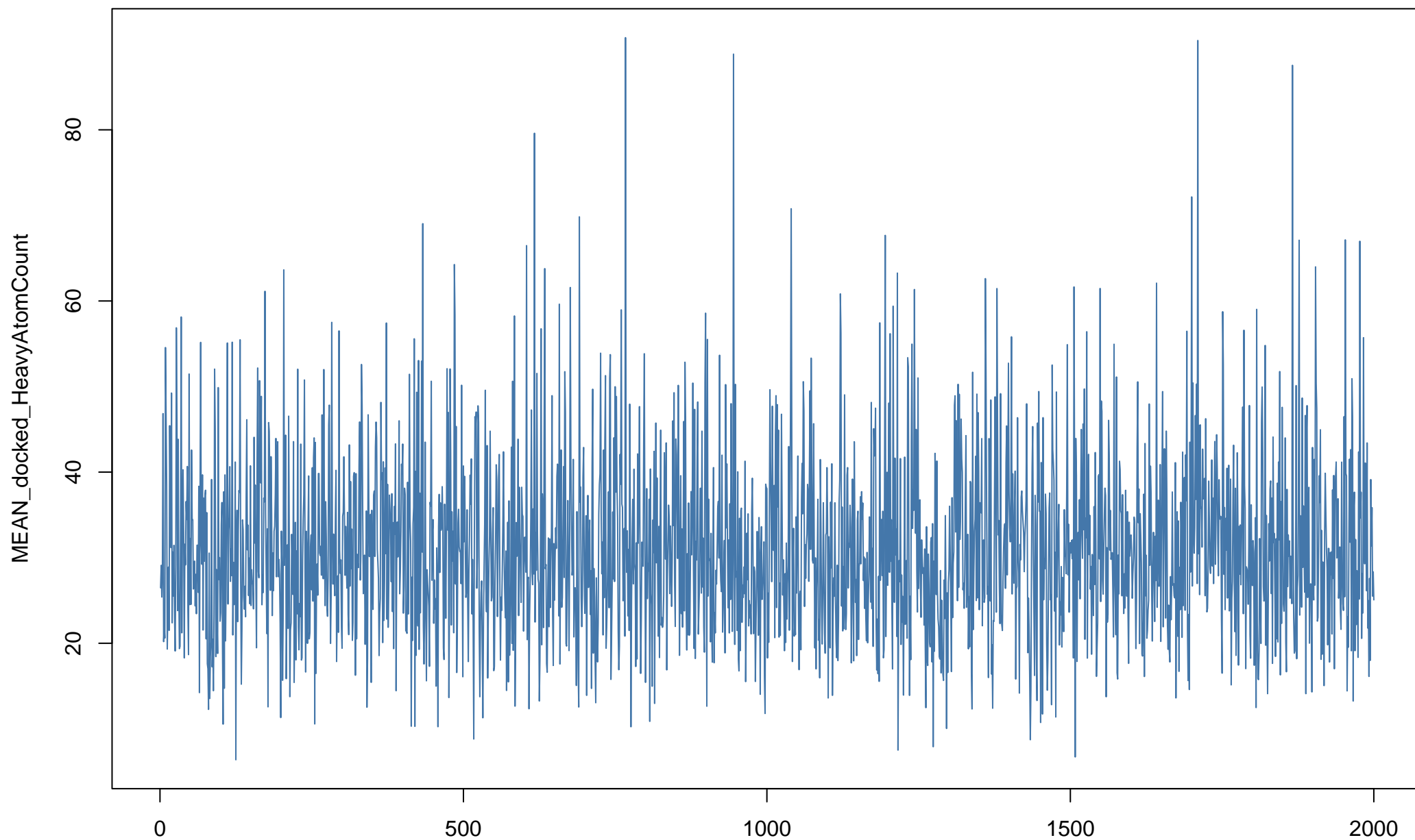
**MEAN\_logit\_ec\_tanimoto\_similarity**  
**ESS = 2000 | BMK = 0.056 | MCSE(6.27) = 0.106 | stat: TRUE | burn: 0**



**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 2000 | BMK = 0.062 | MCSE(6.27) = 0.0341 | stat: TRUE | burn: 0**

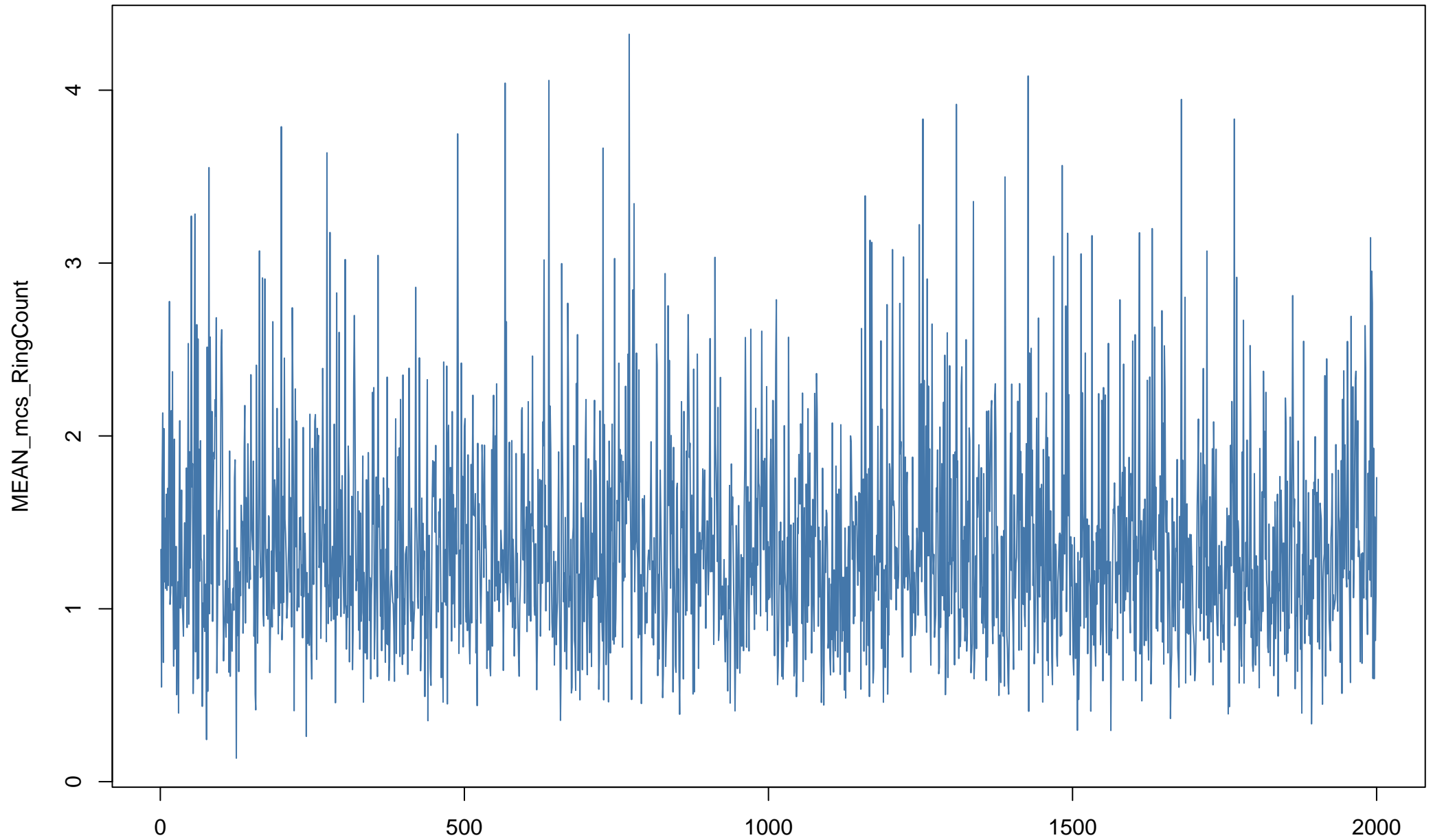


**MEAN\_docked\_HeavyAtomCount**  
**ESS = 2000 | BMK = 0.0366 | MCSE(6.27) = 0.00585 | stat: TRUE | burn: 0**

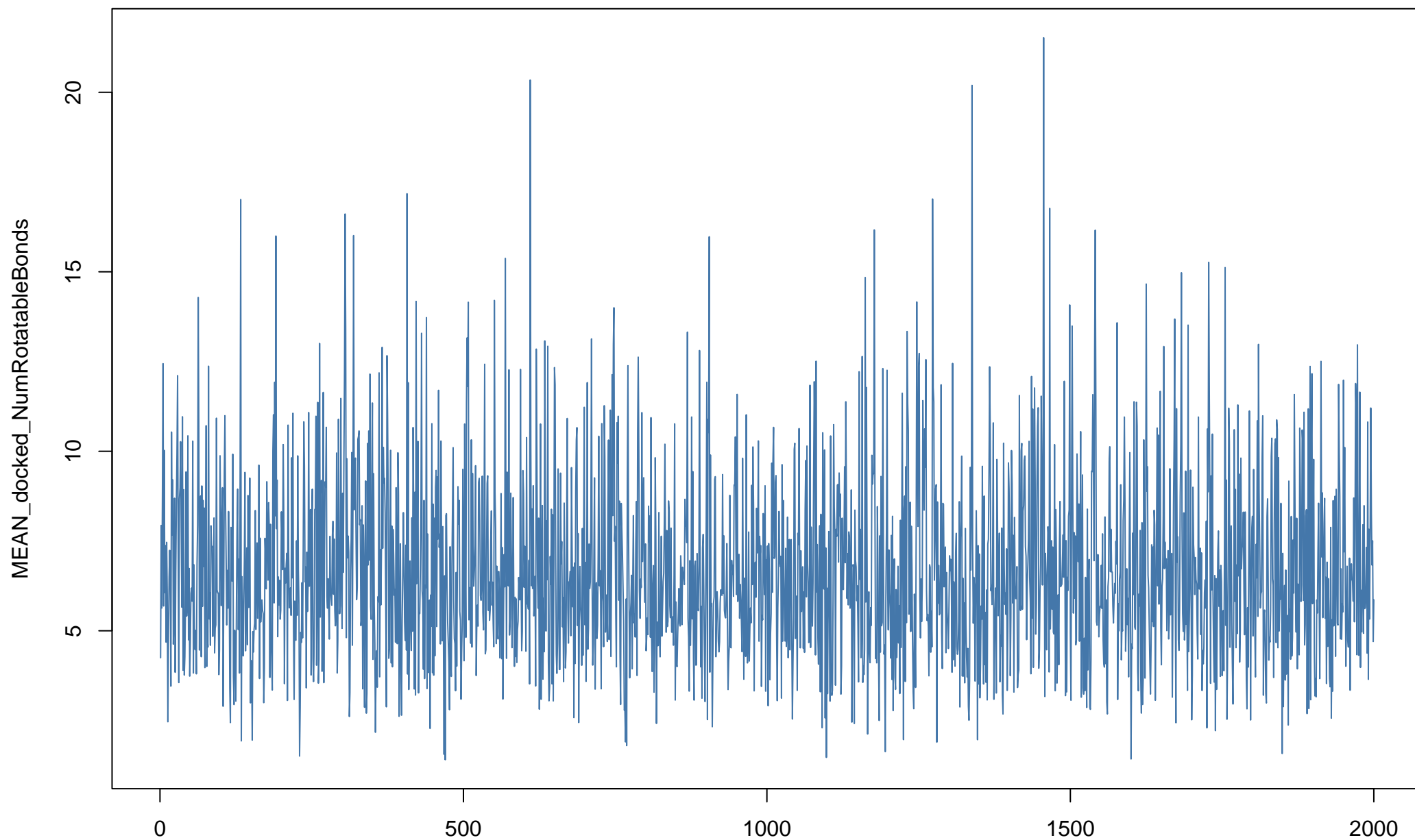




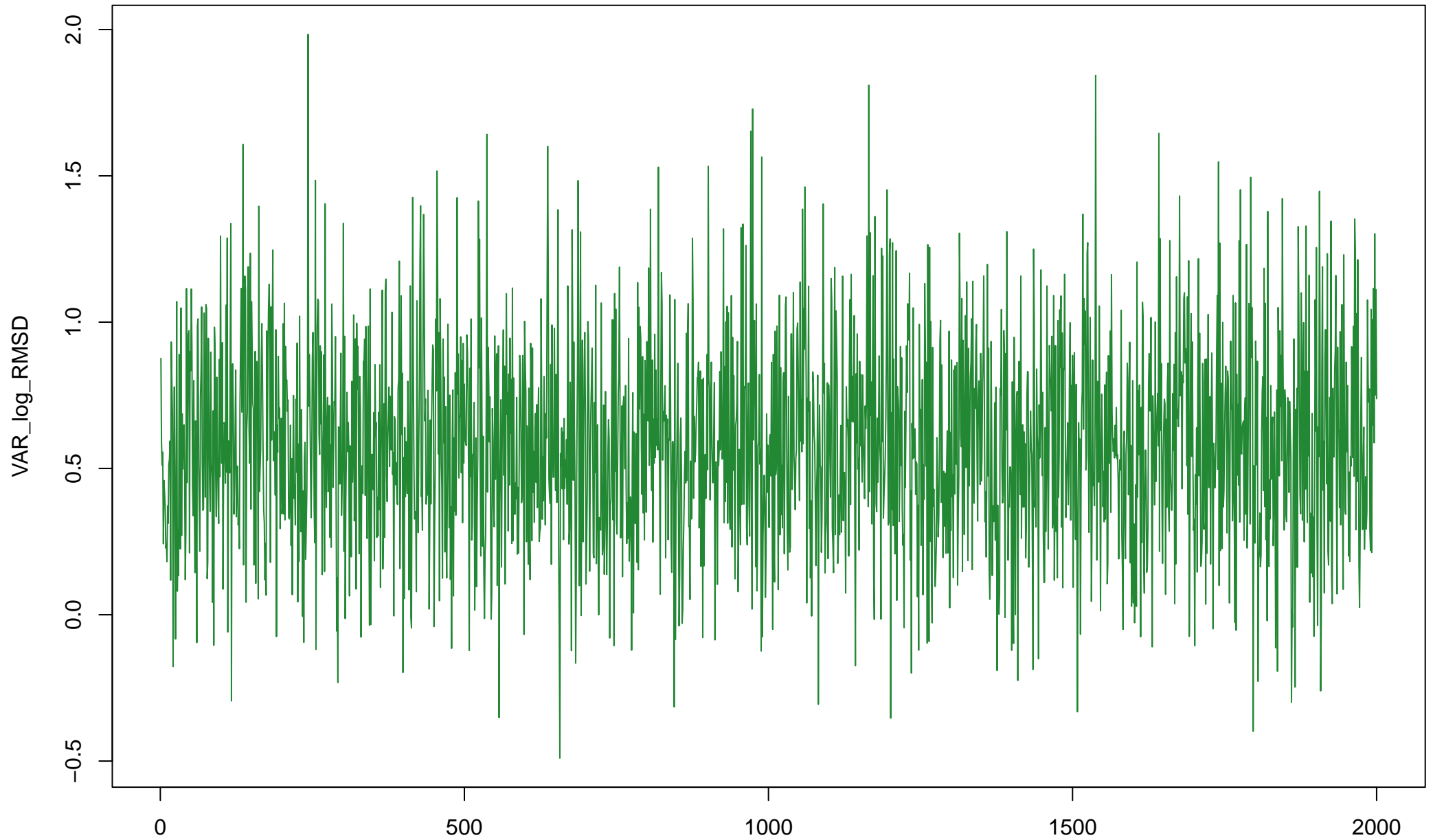
**MEAN\_mcs\_RingCount**  
**ESS = 2000 | BMK = 0.0396 | MCSE(6.27) = 0.105 | stat: TRUE | burn: 0**



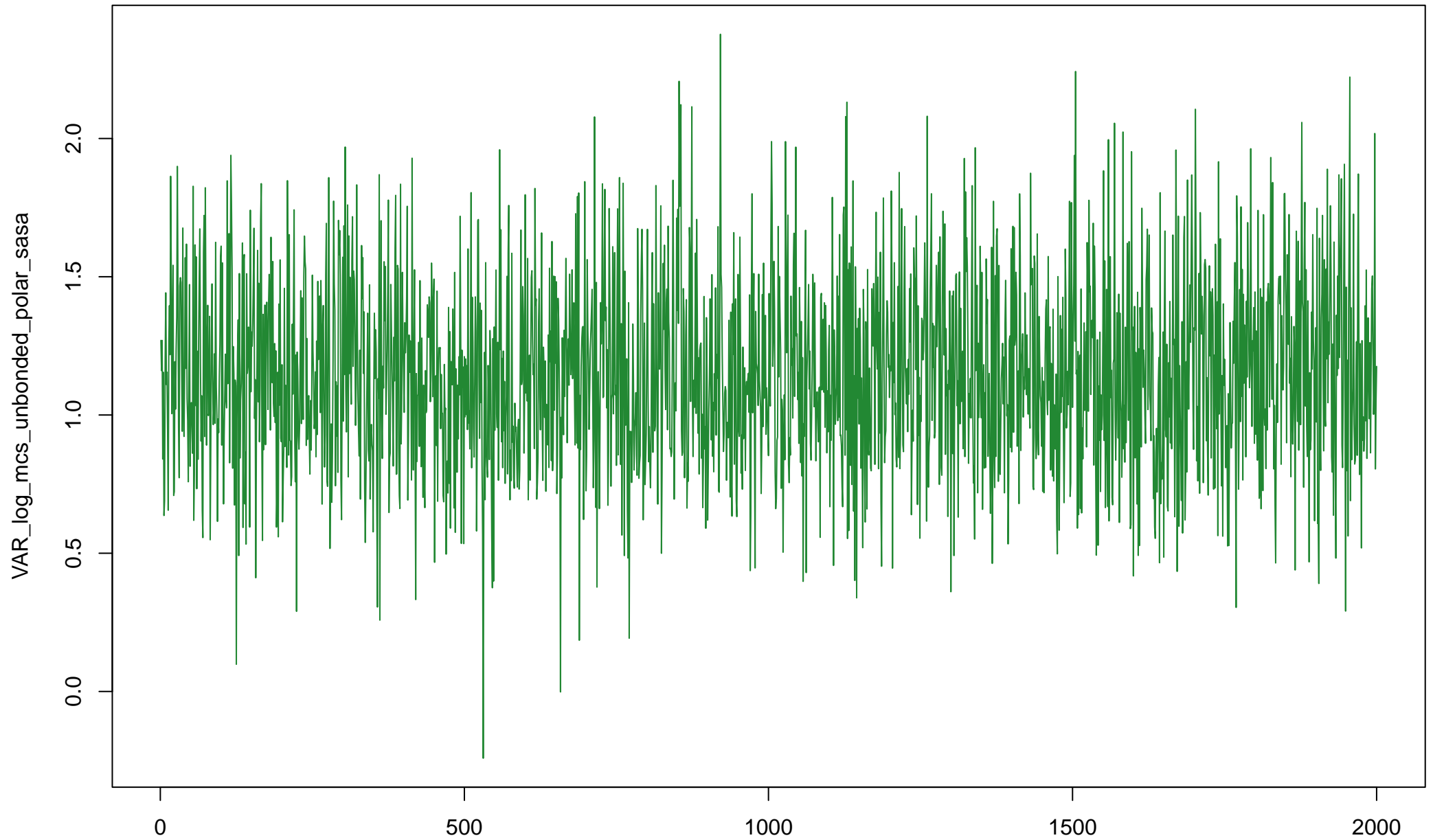
**MEAN\_docked\_NumRotatableBonds**  
**ESS = 1710 | BMK = 0.0398 | MCSE(6.27) = 0.0239 | stat: TRUE | burn: 0**



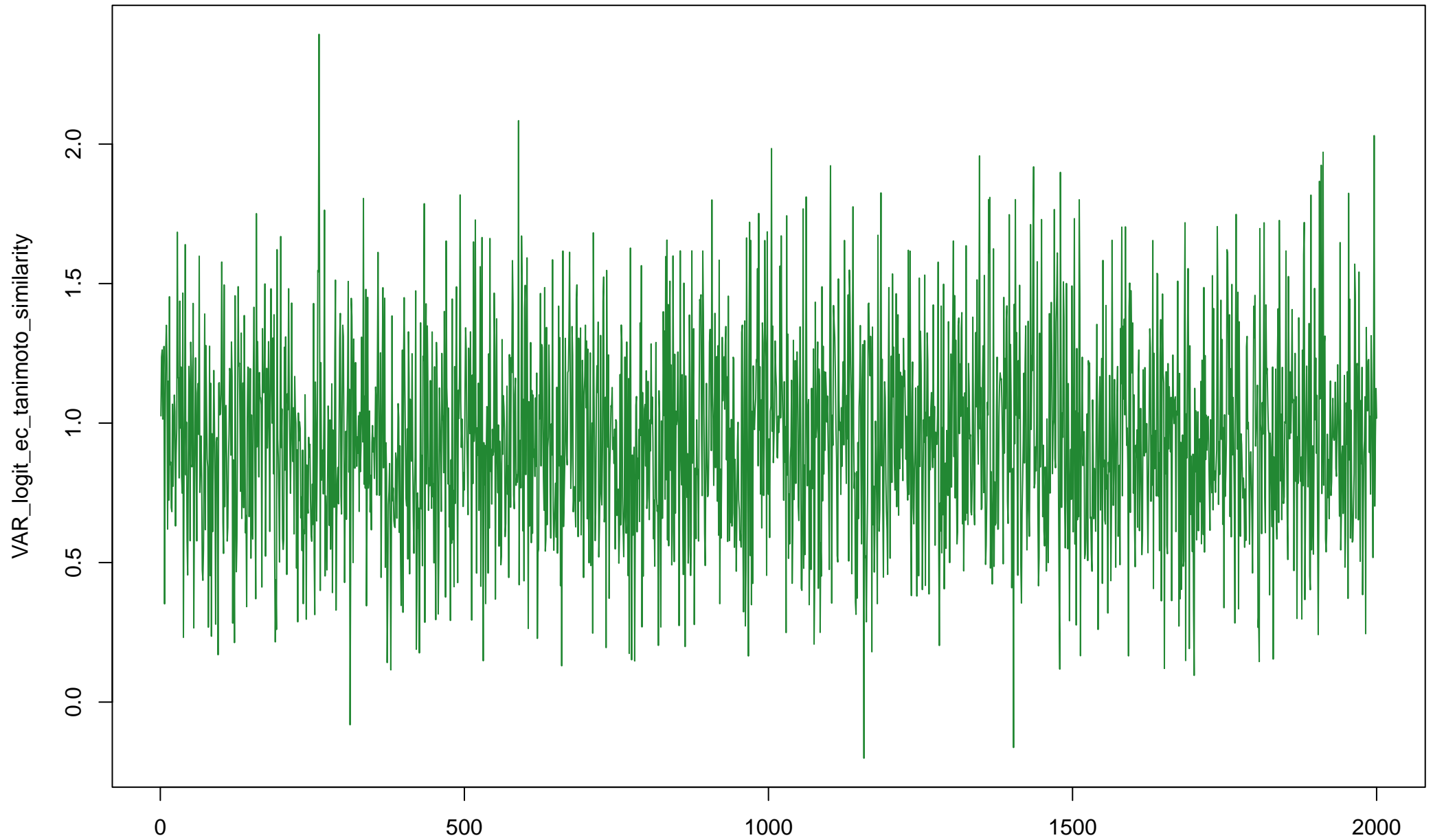
**VAR\_log\_RMSD**  
**ESS = 2000 | BMK = 0.0505 | MCSE(6.27) = 0.181 | stat: TRUE | burn: 0**



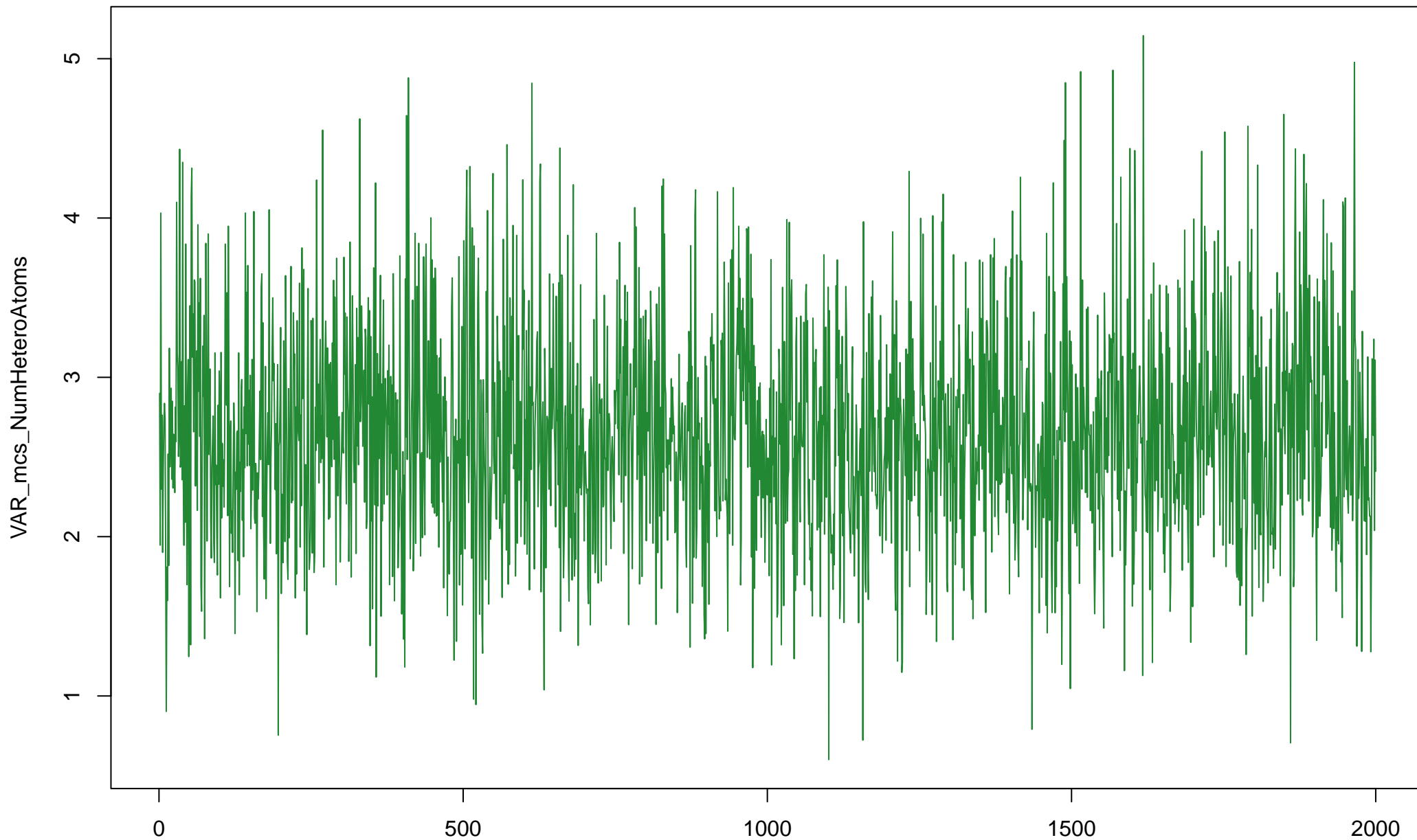
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2000 | BMK = 0.0666 | MCSE(6.27) = 0.182 | stat: TRUE | burn: 0**



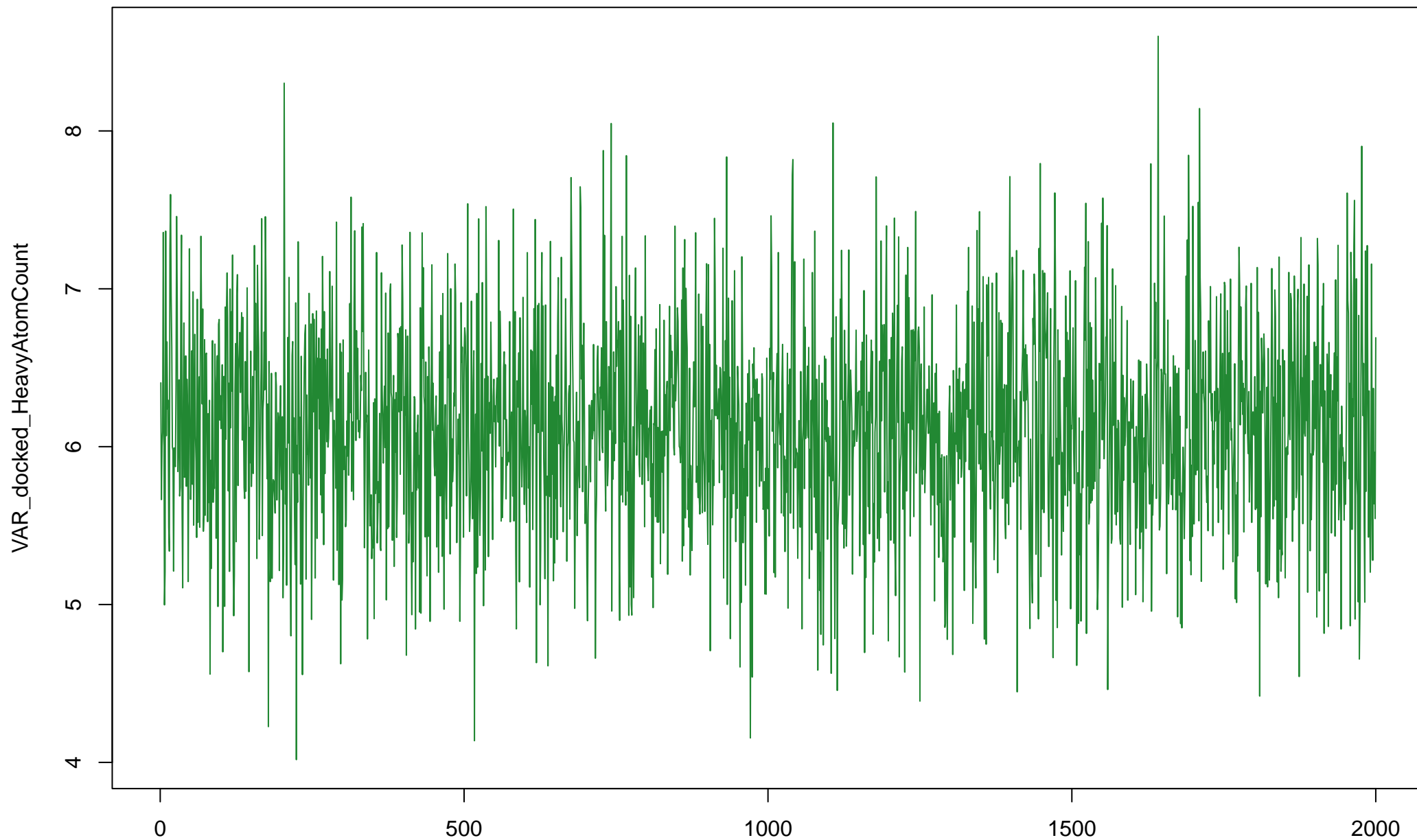
**VAR\_logit\_ec\_tanimoto\_similarity**  
**ESS = 2000 | BMK = 0.0586 | MCSE(6.27) = 0.179 | stat: TRUE | burn: 0**



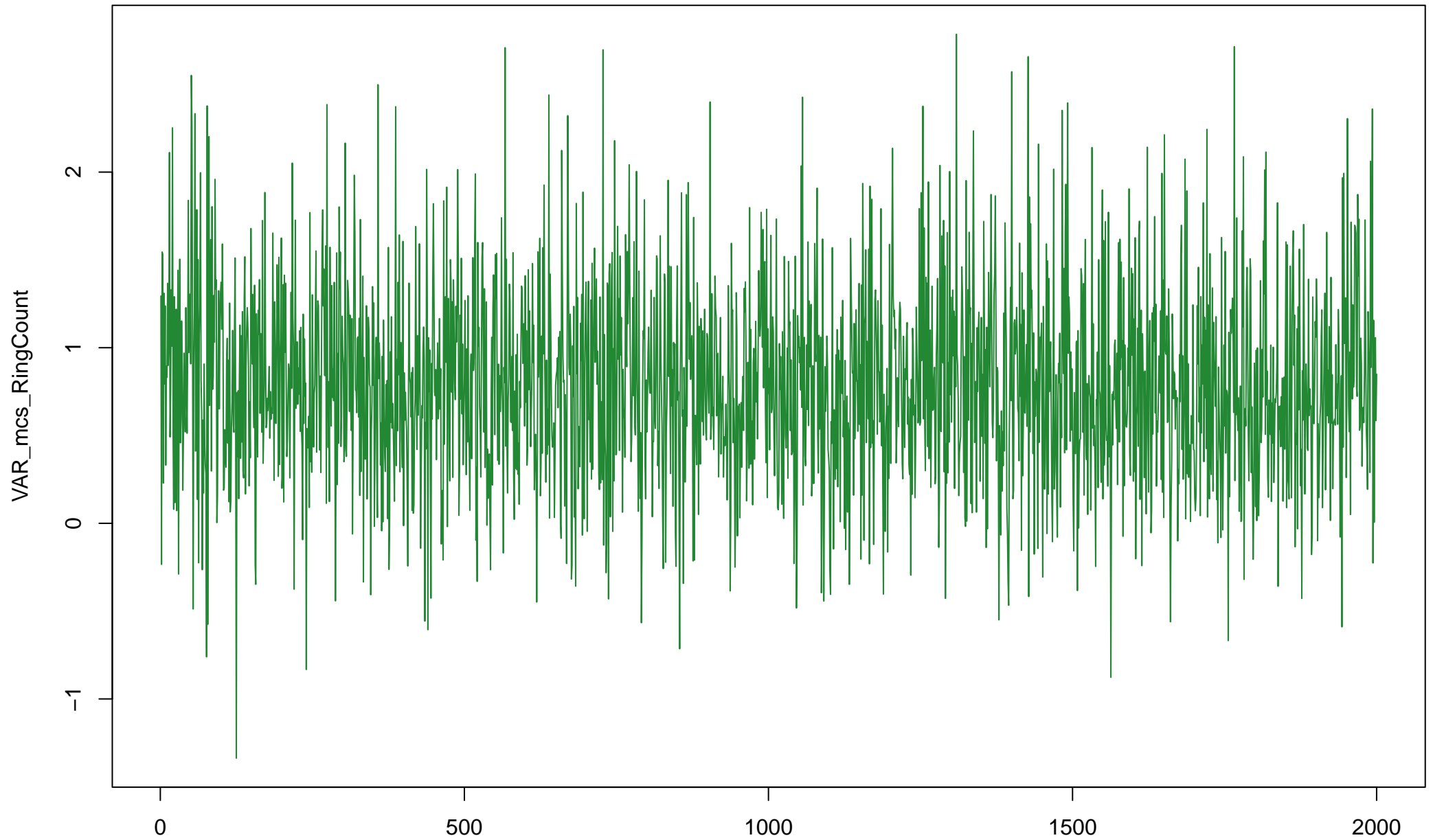
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 2000 | BMK = 0.0387 | MCSE(6.27) = 0.0937 | stat: TRUE | burn: 0**



**VAR\_docked\_HeavyAtomCount**  
**ESS = 2000 | BMK = 0.0404 | MCSE(6.27) = 0.0989 | stat: TRUE | burn: 0**

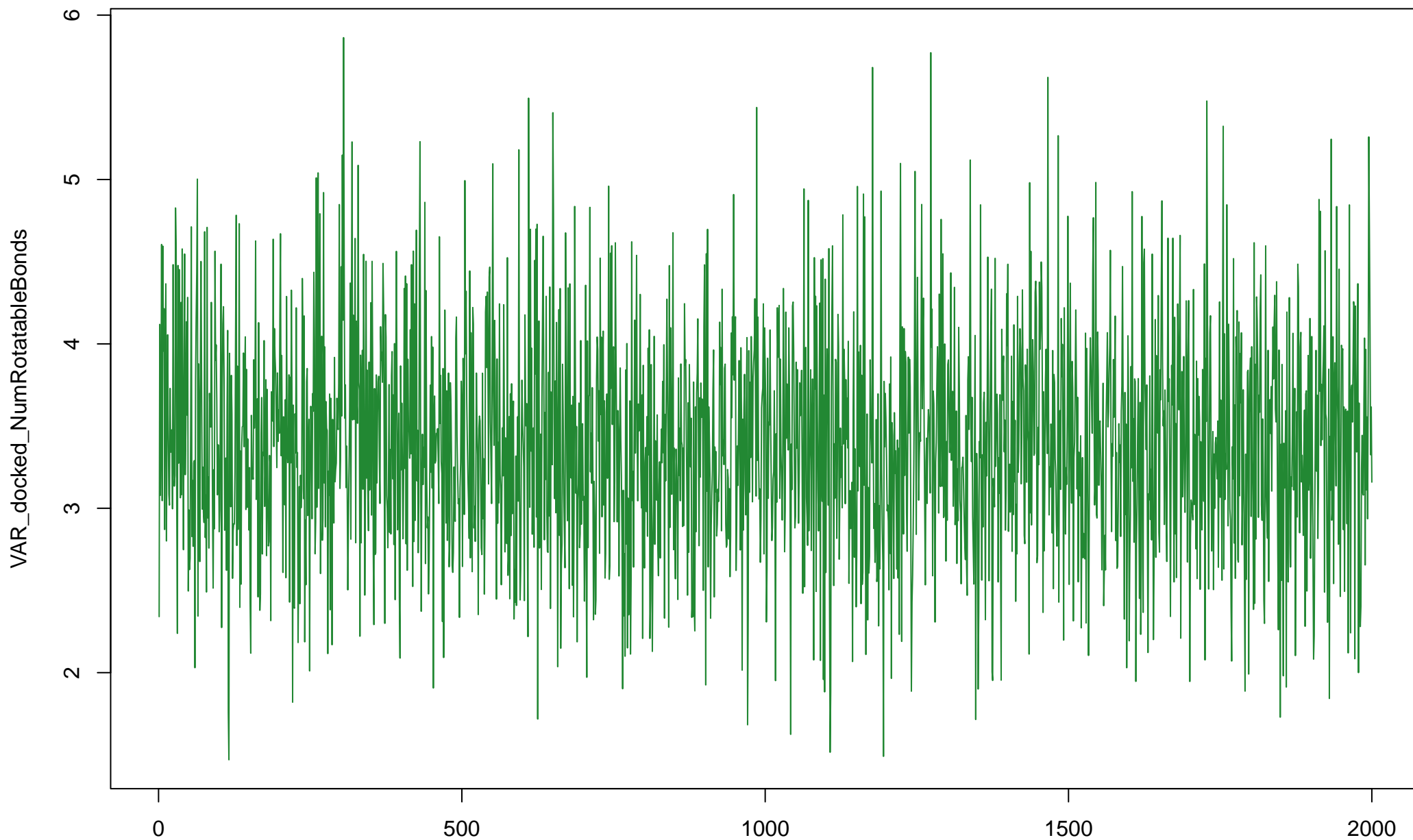


**VAR\_mcs\_RingCount**  
**ESS = 2000 | BMK = 0.0499 | MCSE(6.27) = 0.113 | stat: TRUE | burn: 0**

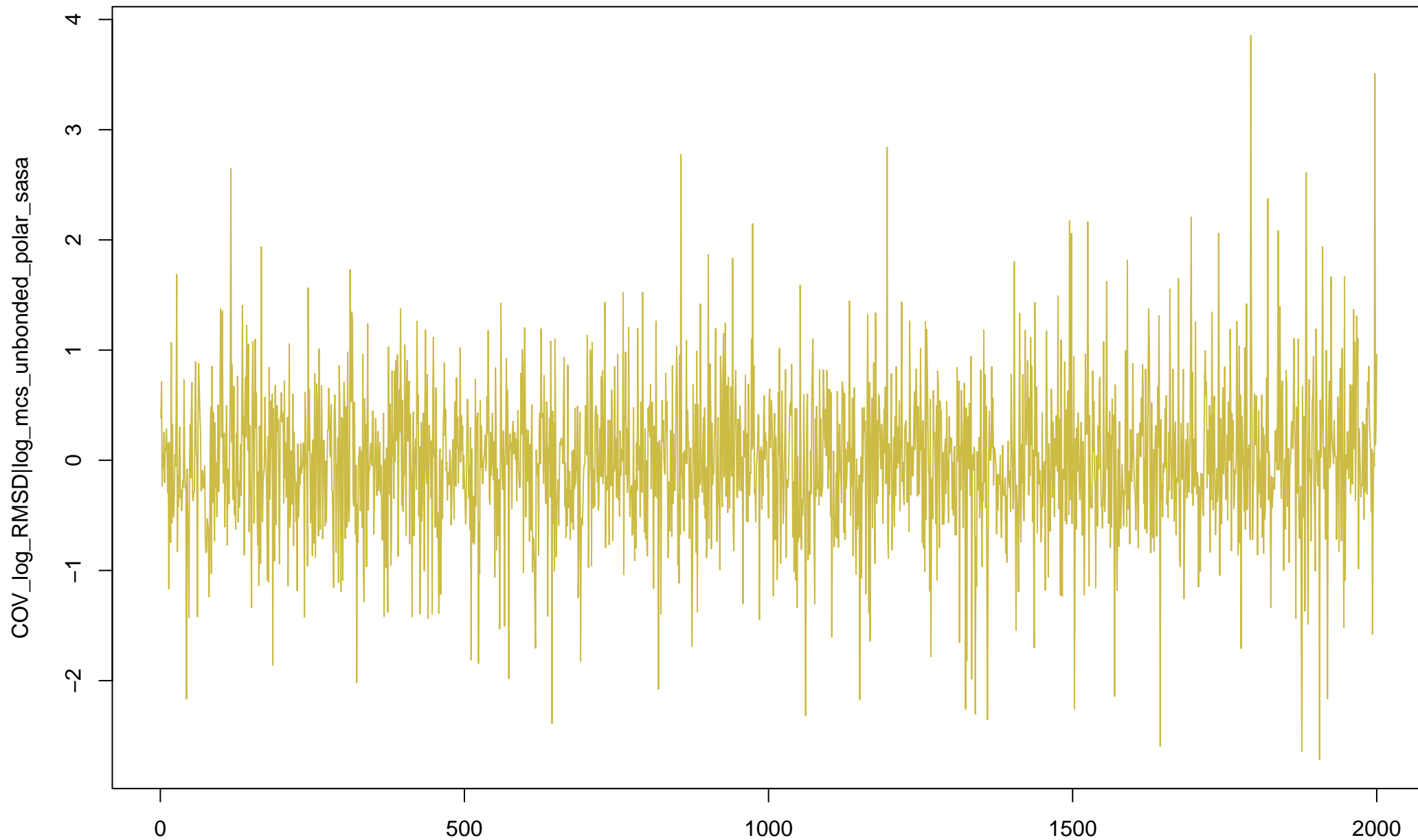




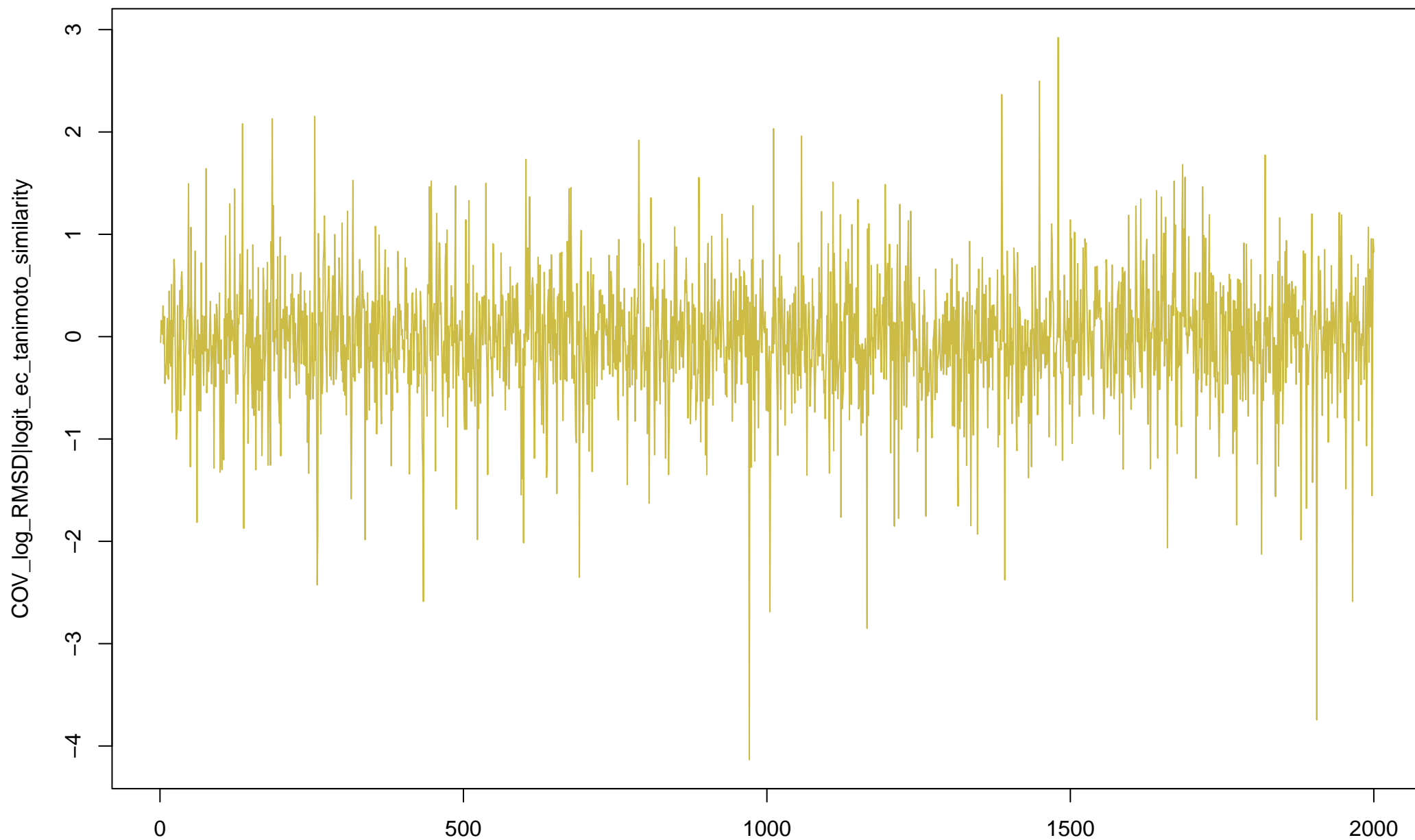
**VAR\_docked\_NumRotatableBonds**  
**ESS = 2000 | BMK = 0.0392 | MCSE(6.27) = 0.0942 | stat: TRUE | burn: 0**



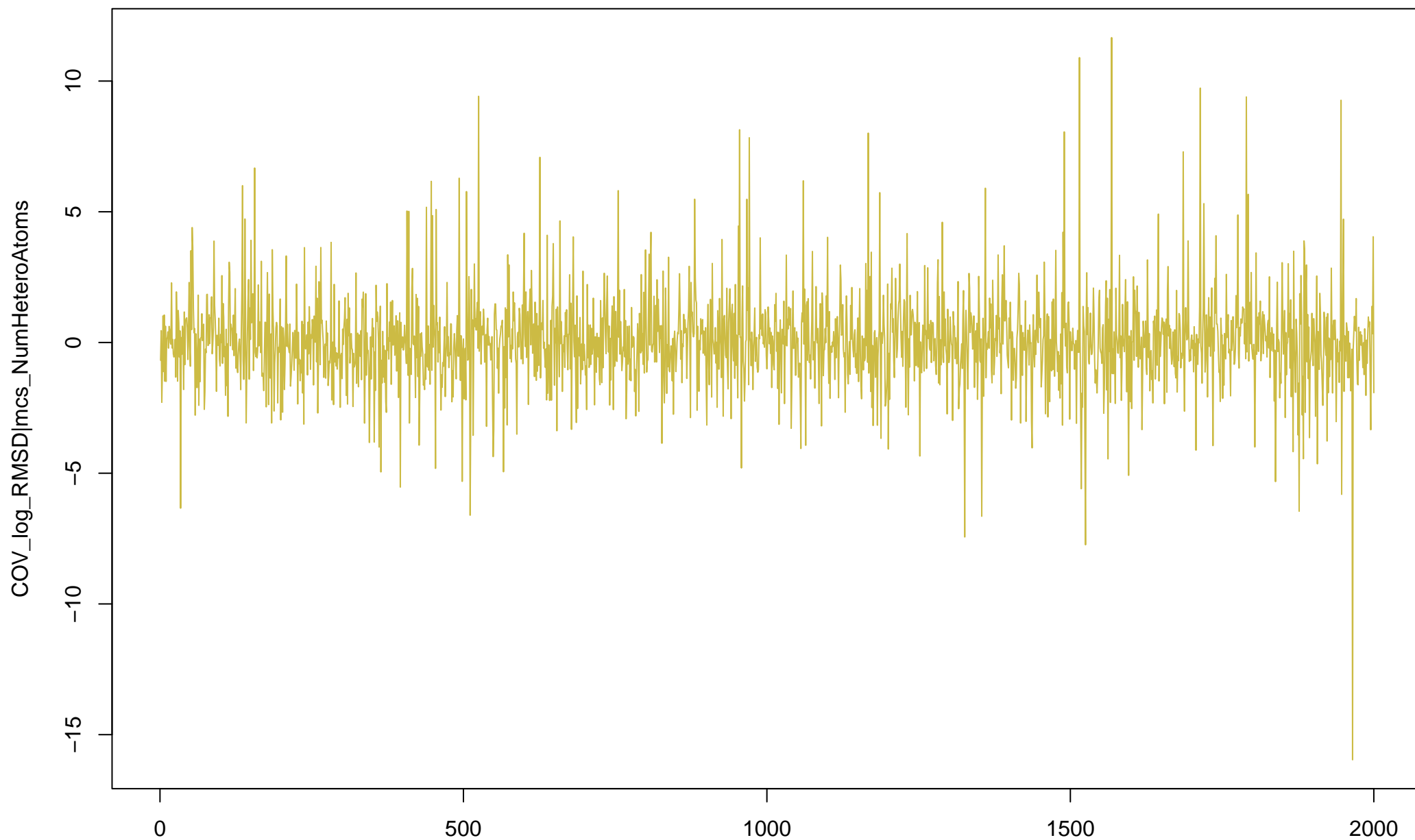
**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2000 | BMK = 0.0642 | MCSE(6.27) = 0.0955 | stat: TRUE | burn: 0**



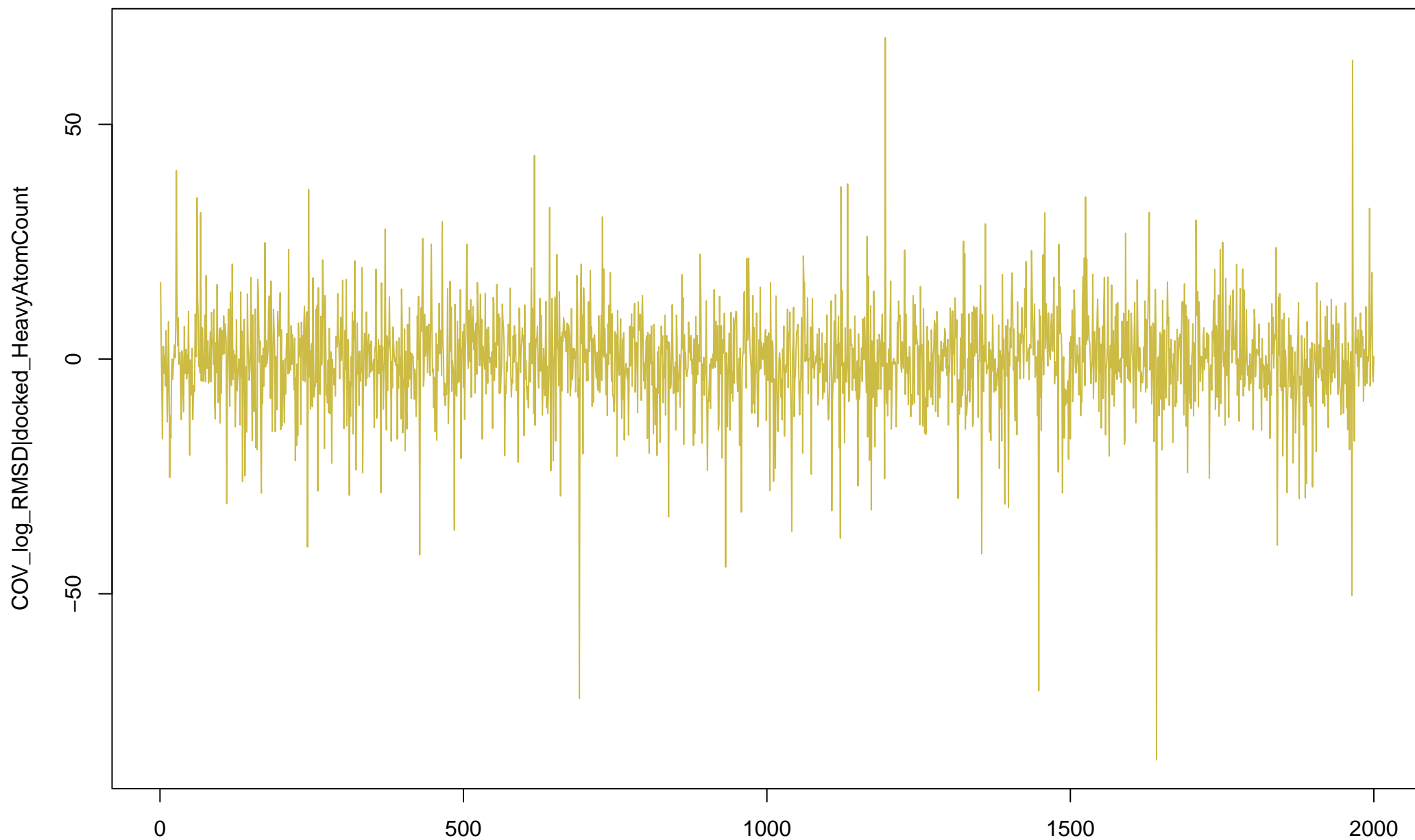
**COV\_log\_RMSD|logit\_ec\_tanimoto\_similarity**  
**ESS = 2000 | BMK = 0.0624 | MCSE(6.27) = 0.104 | stat: TRUE | burn: 0**



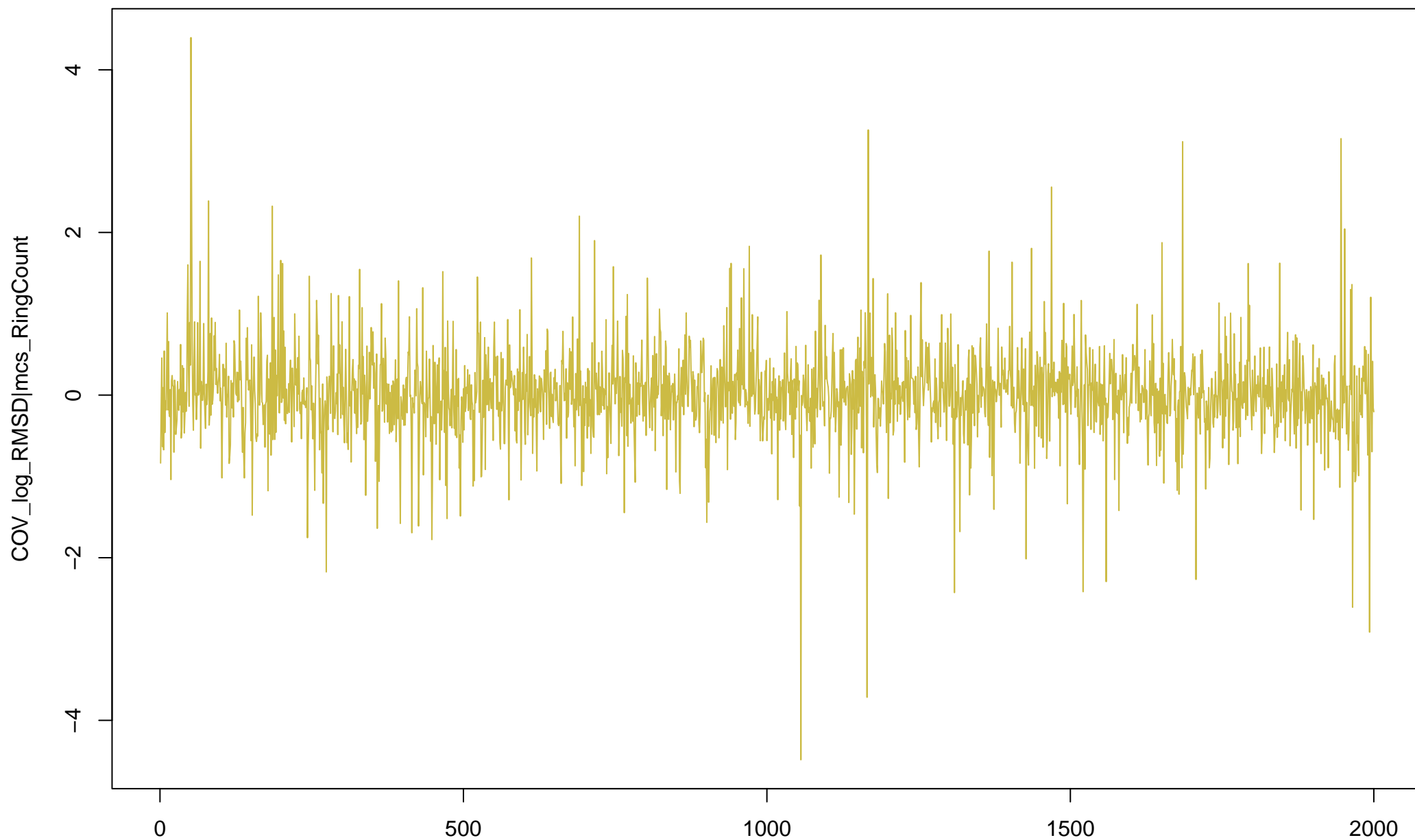
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 2000 | BMK = 0.0654 | MCSE(6.27) = 0.0355 | stat: TRUE | burn: 0**



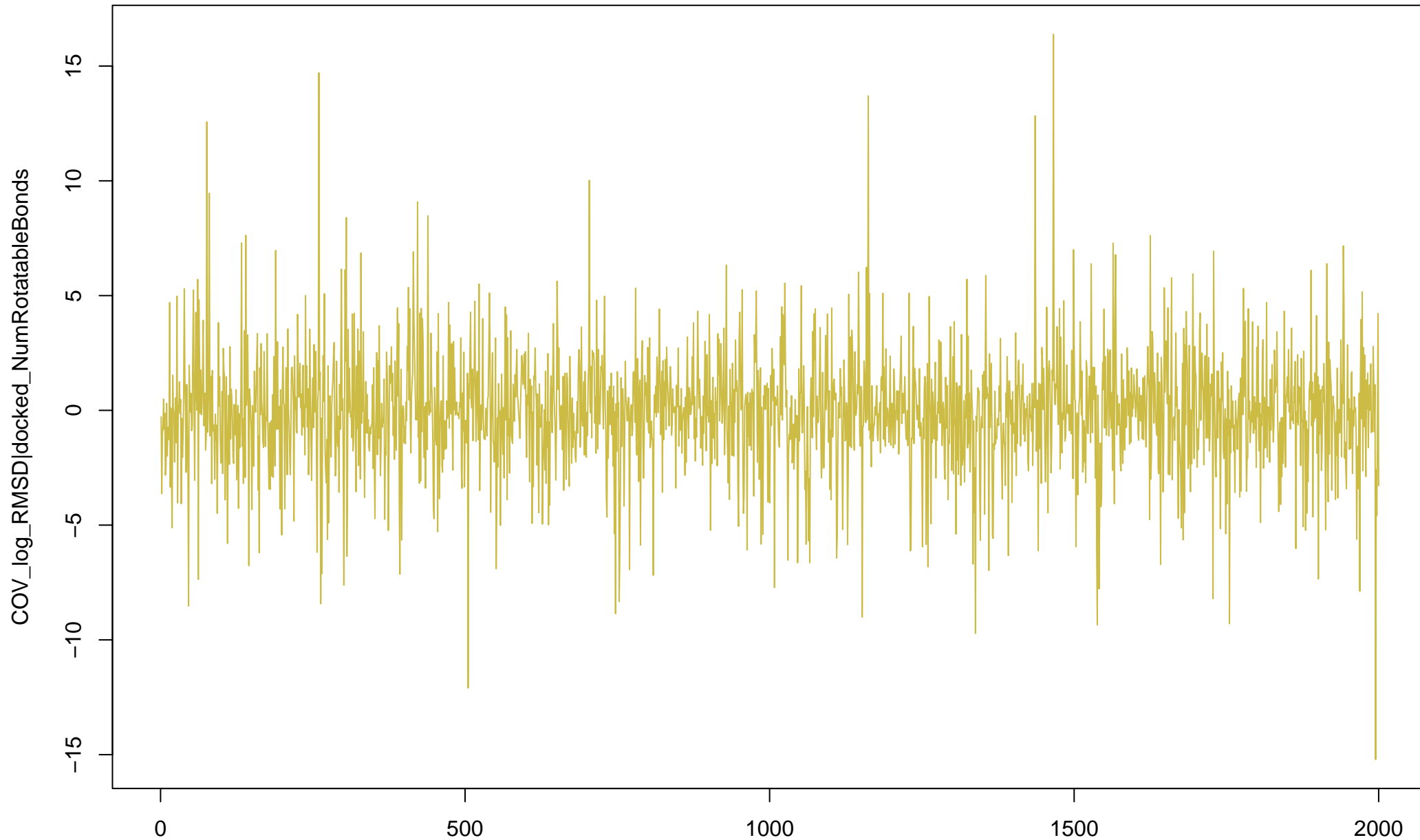
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 2000 | BMK = 0.0619 | MCSE(6.27) = 0.00595 | stat: TRUE | burn: 0**



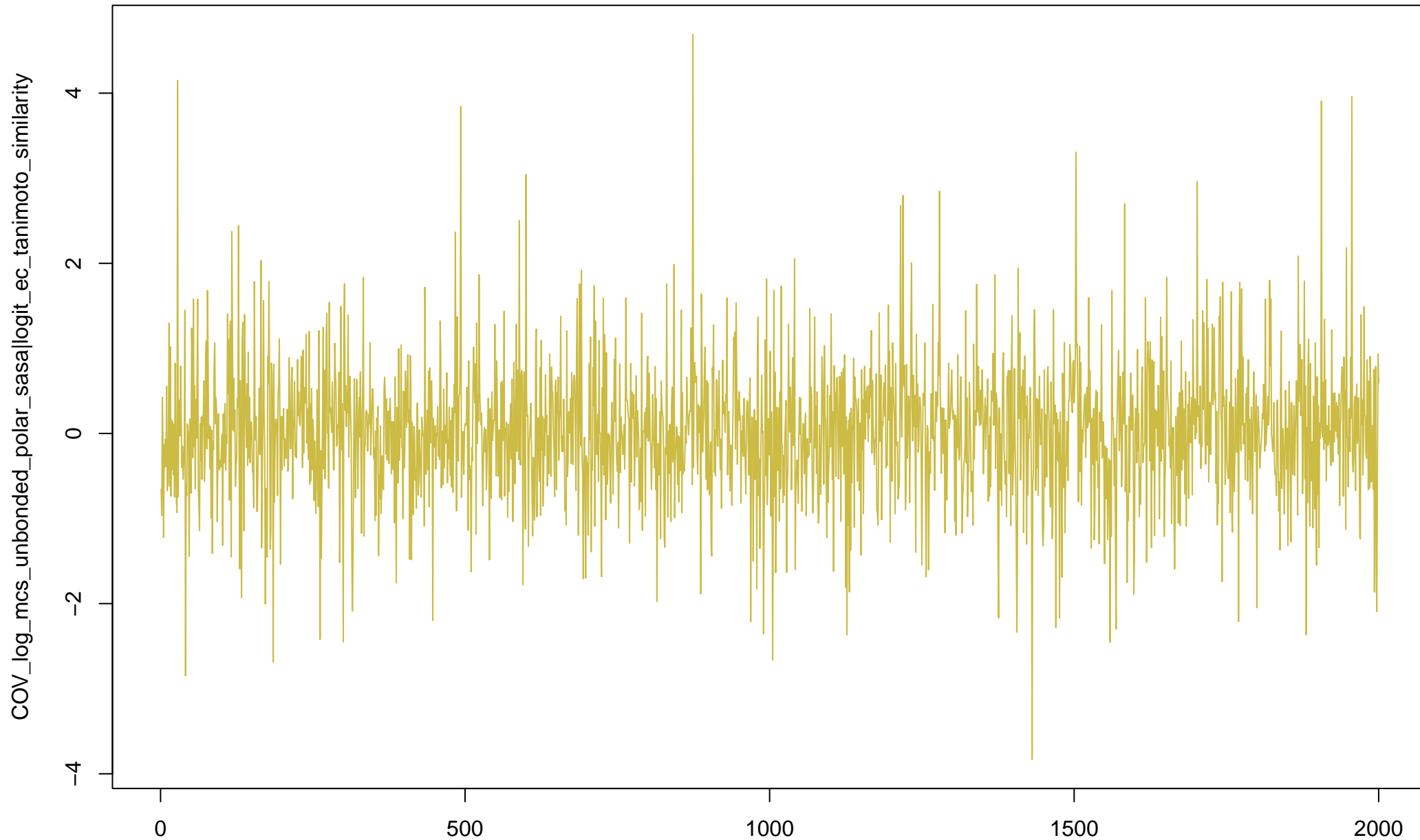
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 1790 | BMK = 0.101 | MCSE(6.27) = 0.111 | stat: TRUE | burn: 0**



**COV\_log\_RMSD|docked\_NumRotatableBonds**  
**ESS = 2000 | BMK = 0.0742 | MCSE(6.27) = 0.0246 | stat: TRUE | burn: 0**

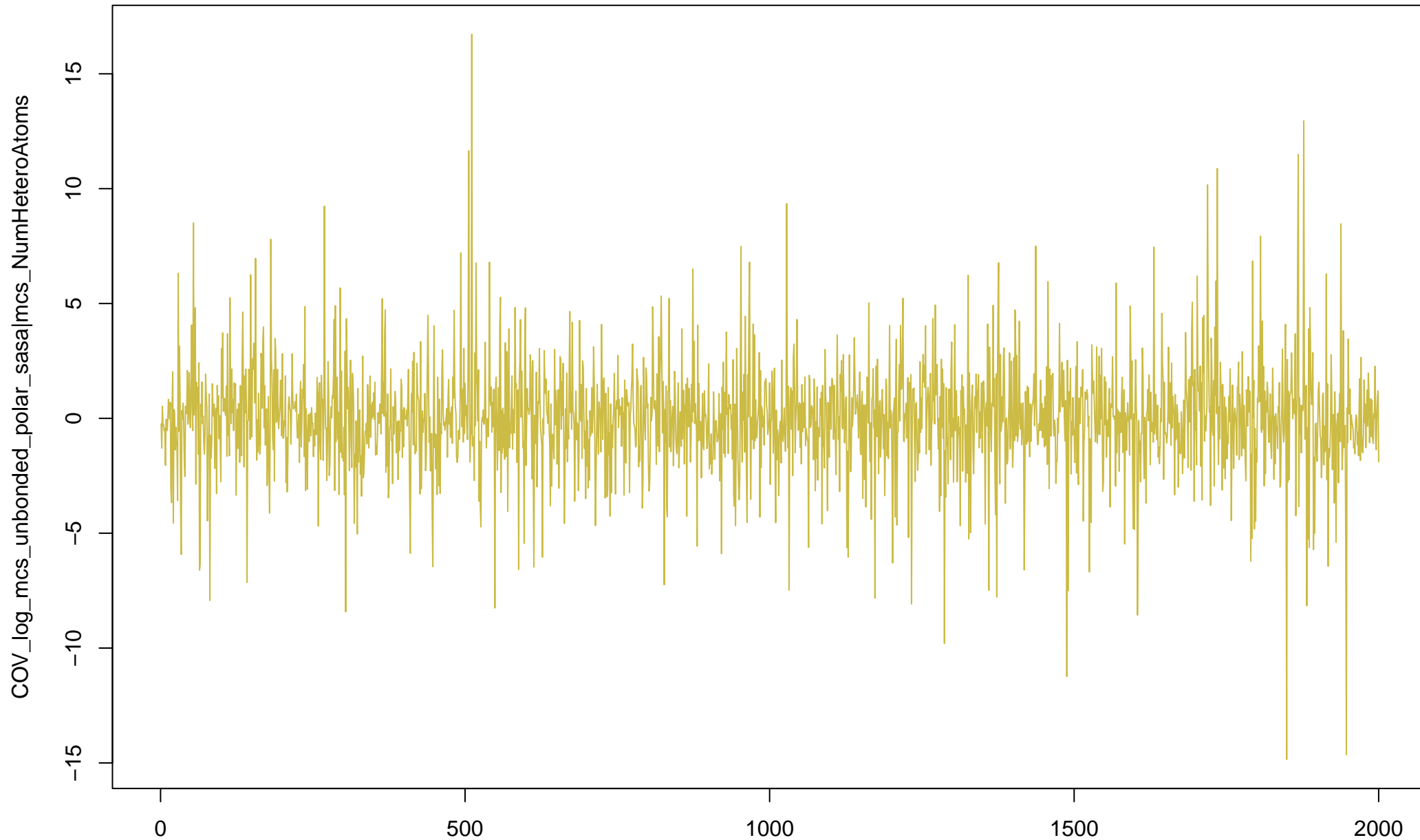


**COV\_log\_mcs\_unbonded\_polar\_sasa|logit\_ec\_tanimoto\_similarity**  
**ESS = 2000 | BMK = 0.0707 | MCSE(6.27) = 0.0806 | stat: TRUE | burn: 0**

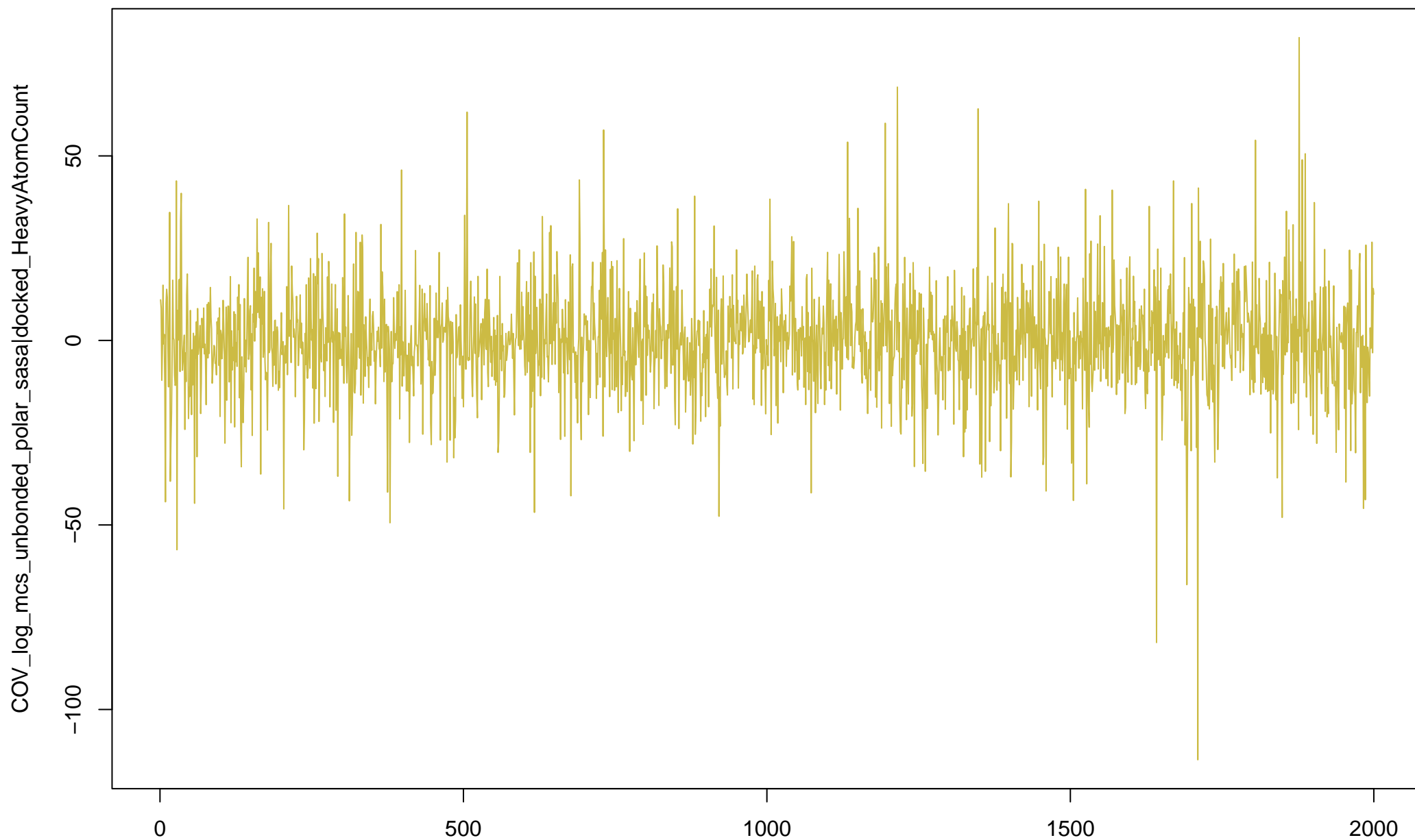




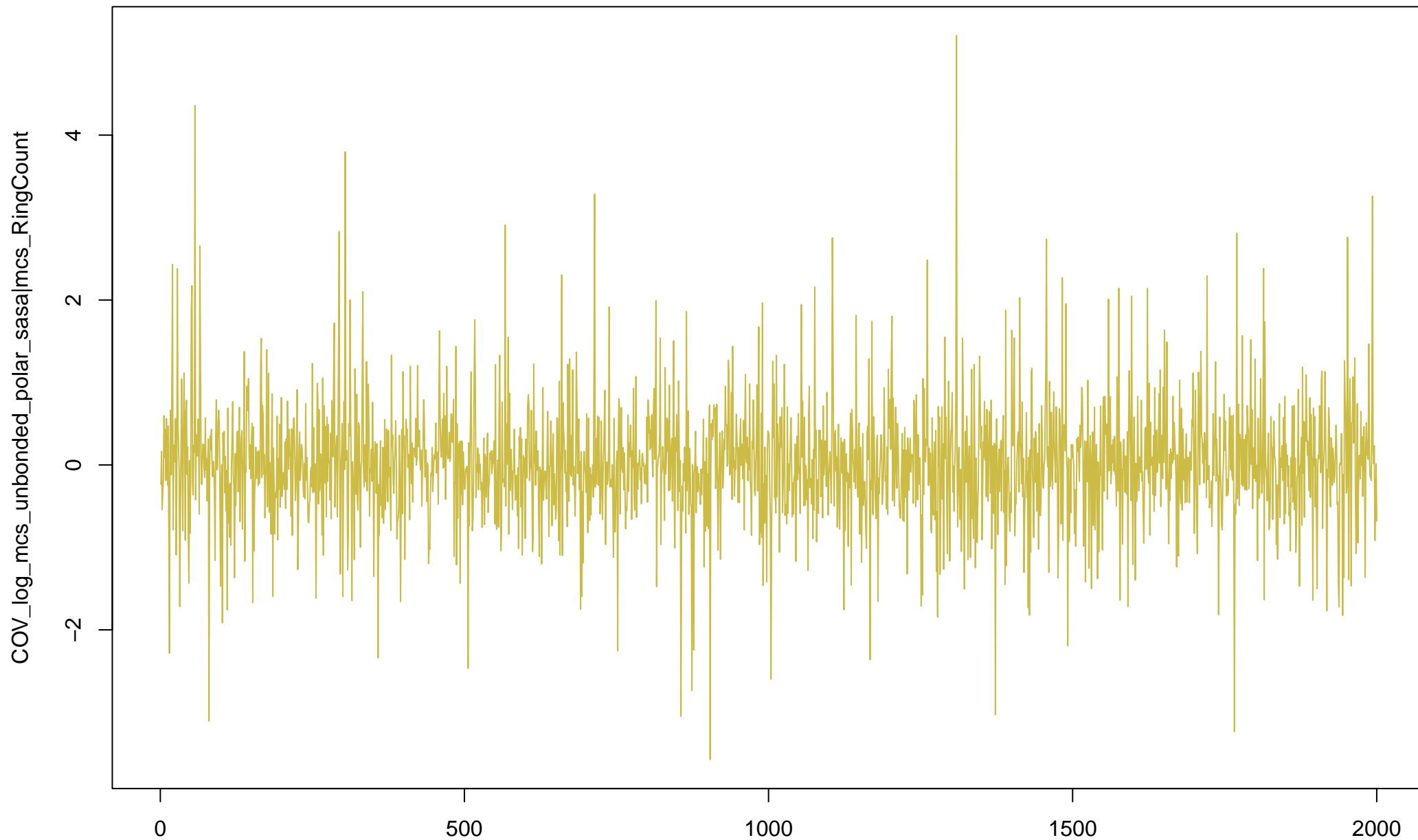
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 2000 | BMK = 0.0749 | MCSE(6.27) = 0.0269 | stat: TRUE | burn: 0**



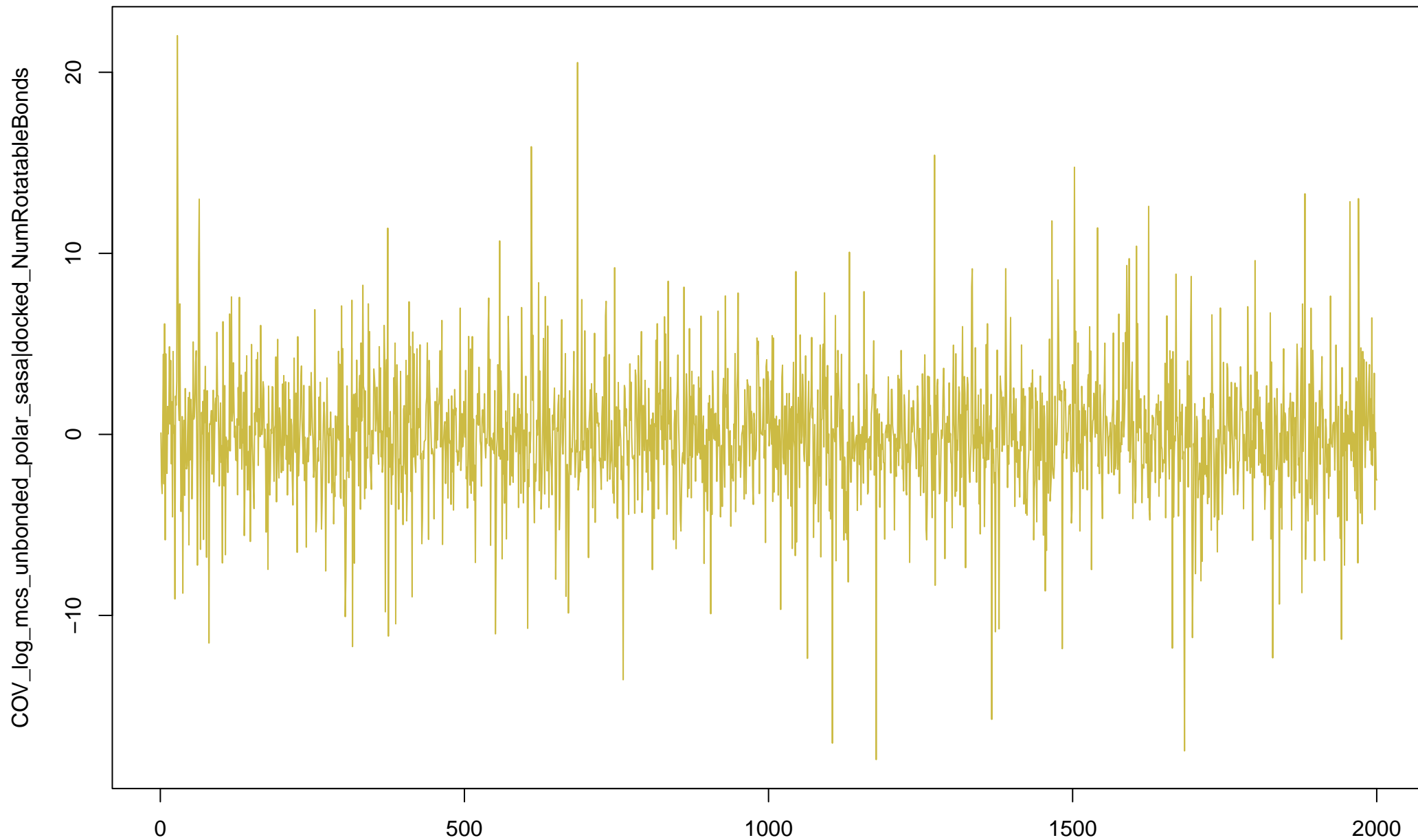
COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount  
ESS = 2000 | BMK = 0.08 | MCSE(6.27) = 0.00439 | stat: TRUE | burn: 0



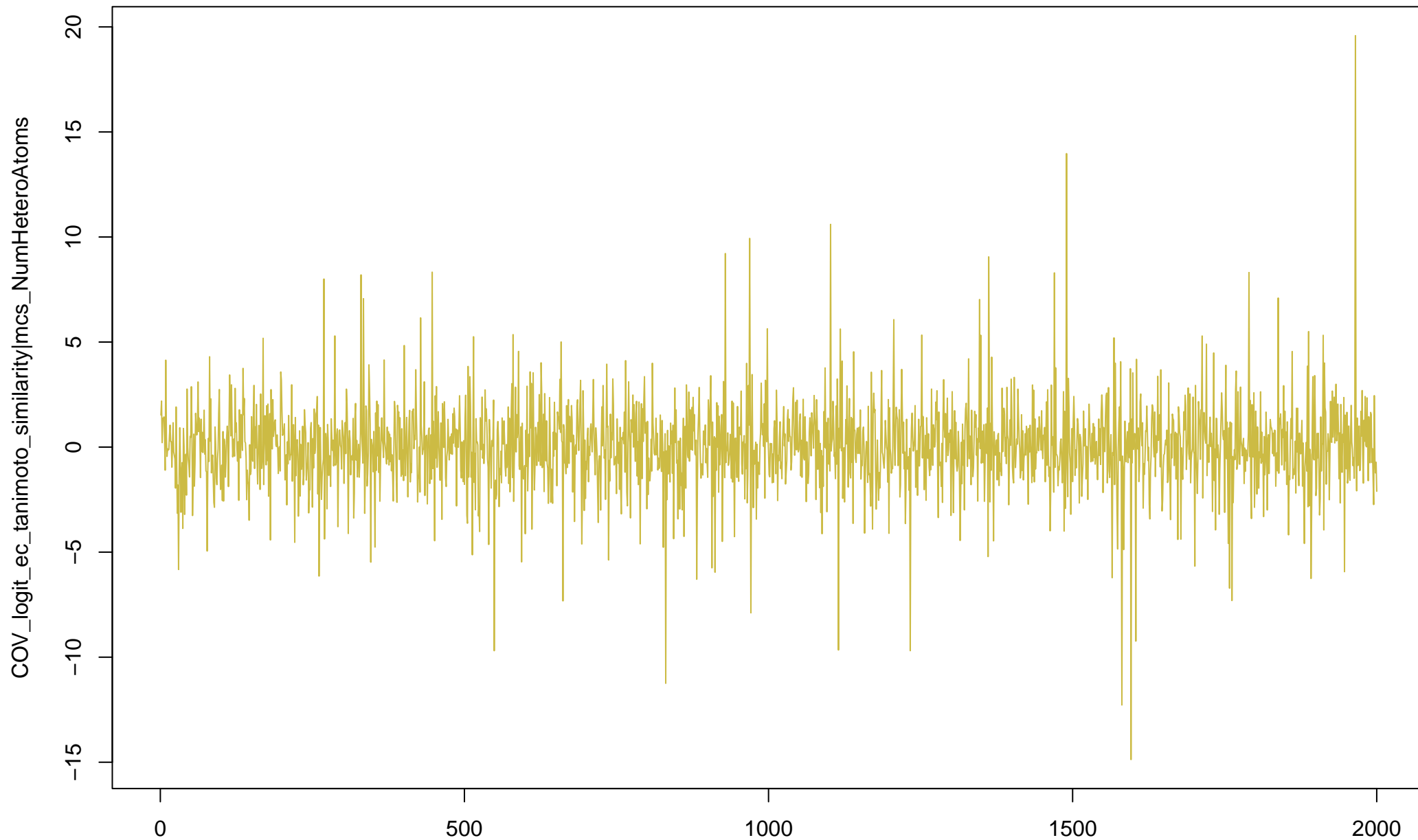
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_RingCount**  
**ESS = 2000 | BMK = 0.0666 | MCSE(6.27) = 0.0876 | stat: TRUE | burn: 0**



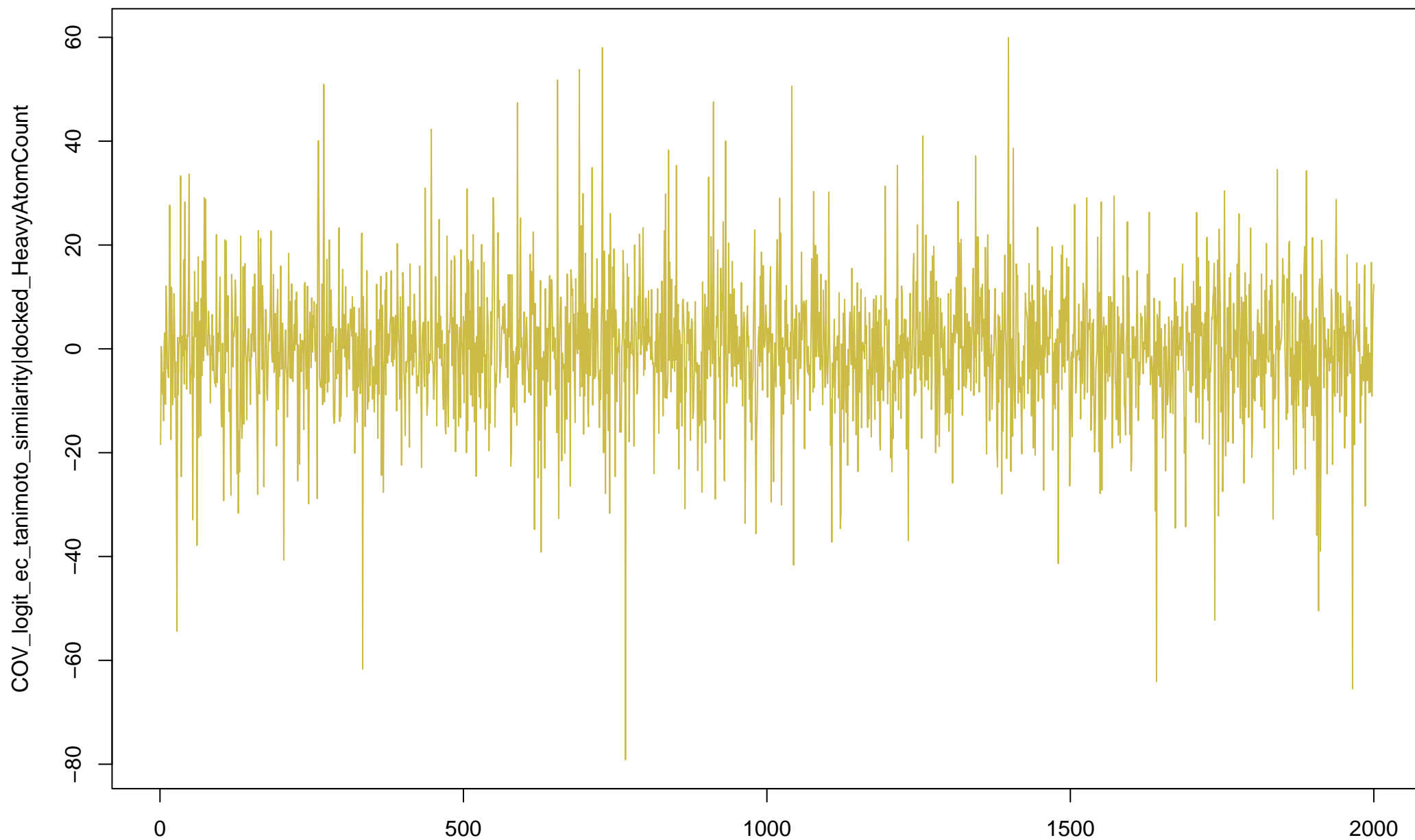
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_NumRotatableBonds**  
**ESS = 2000 | BMK = 0.0747 | MCSE(6.27) = 0.0182 | stat: TRUE | burn: 0**



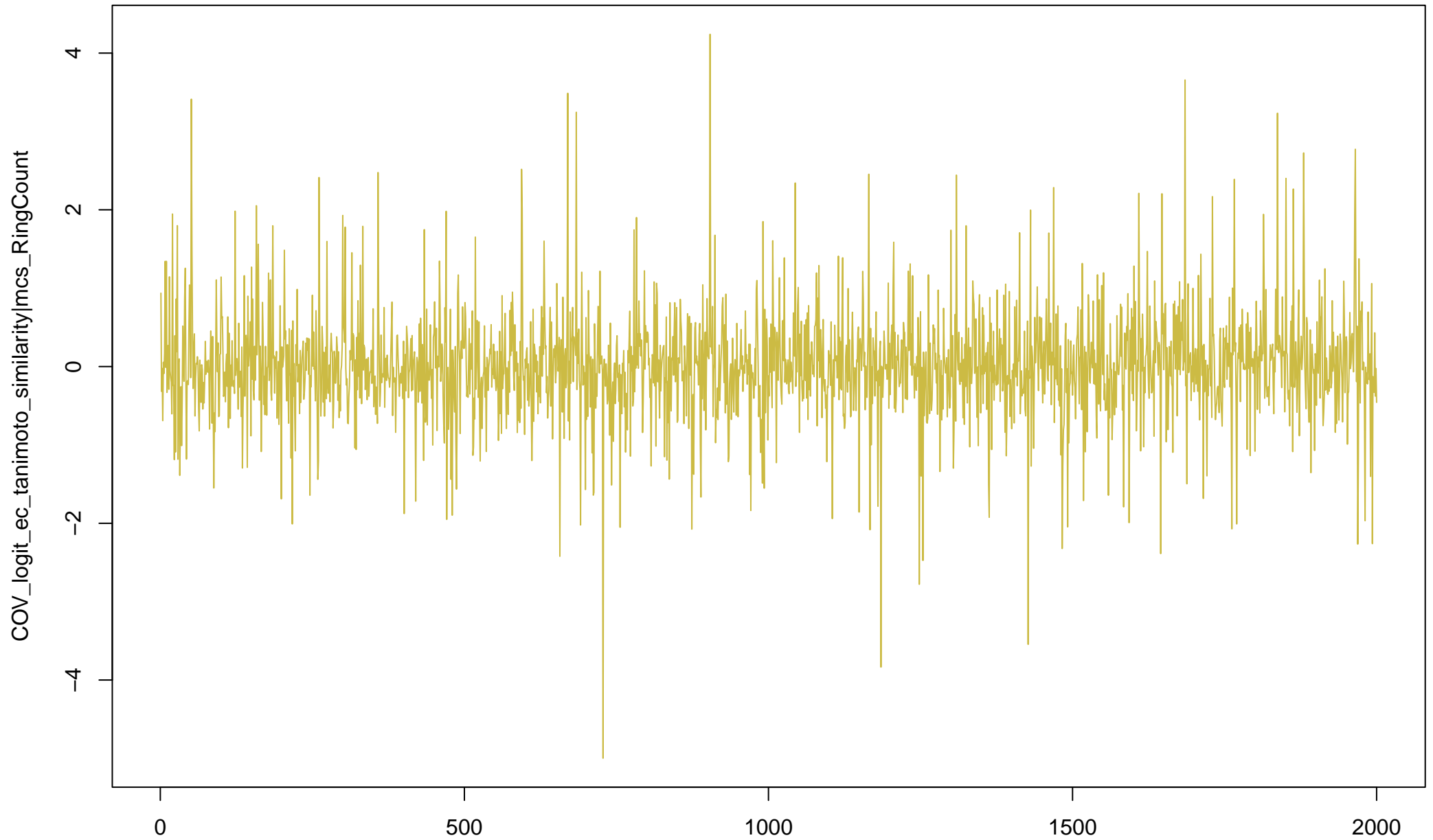
COV\_logit\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms  
ESS = 2000 | BMK = 0.0621 | MCSE(6.27) = 0.0304 | stat: TRUE | burn: 0



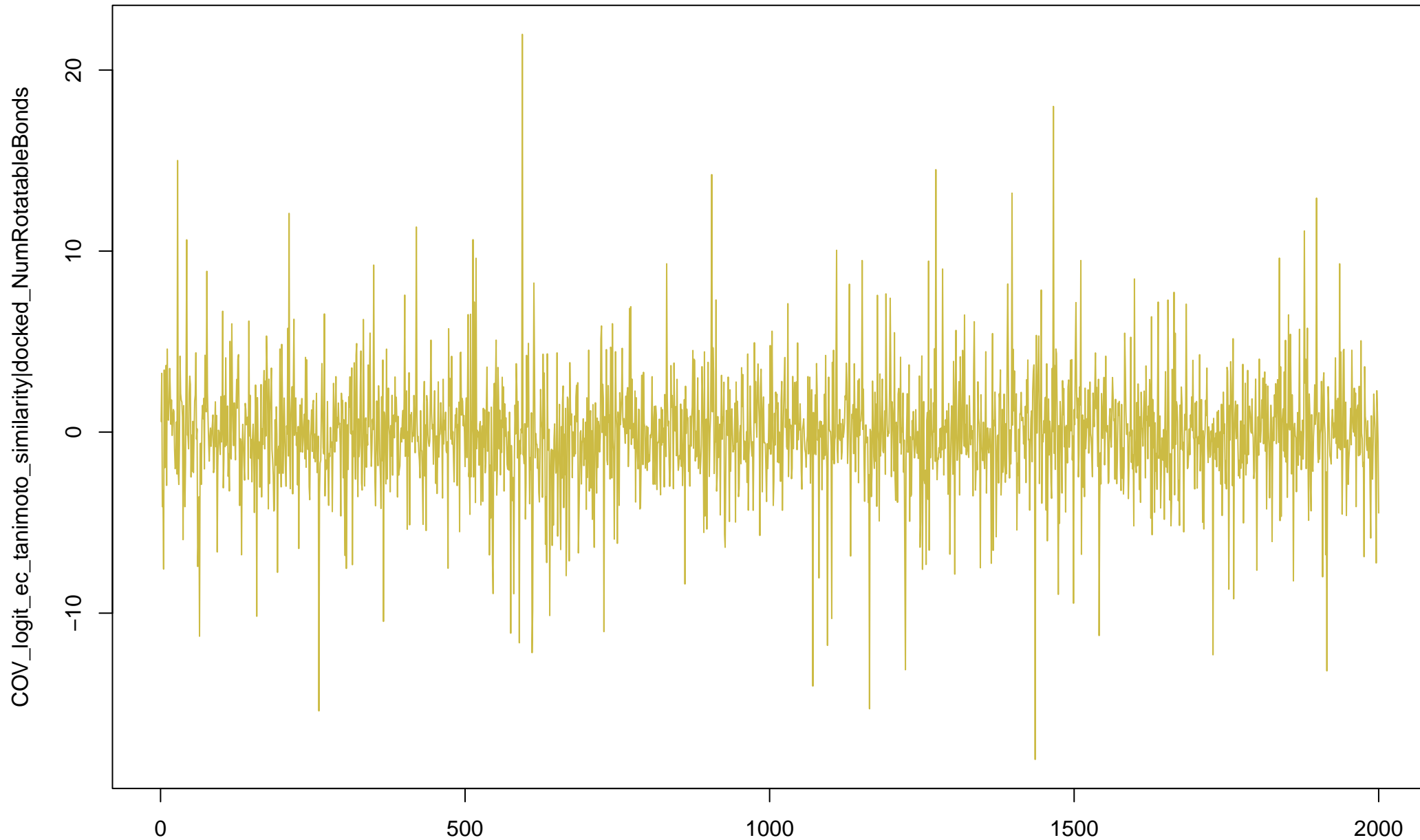
COV\_logit\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount  
ESS = 2000 | BMK = 0.0555 | MCSE(6.27) = 0.00499 | stat: TRUE | burn: 0



**COV\_logit\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 2000 | BMK = 0.0904 | MCSE(6.27) = 0.0918 | stat: TRUE | burn: 0**

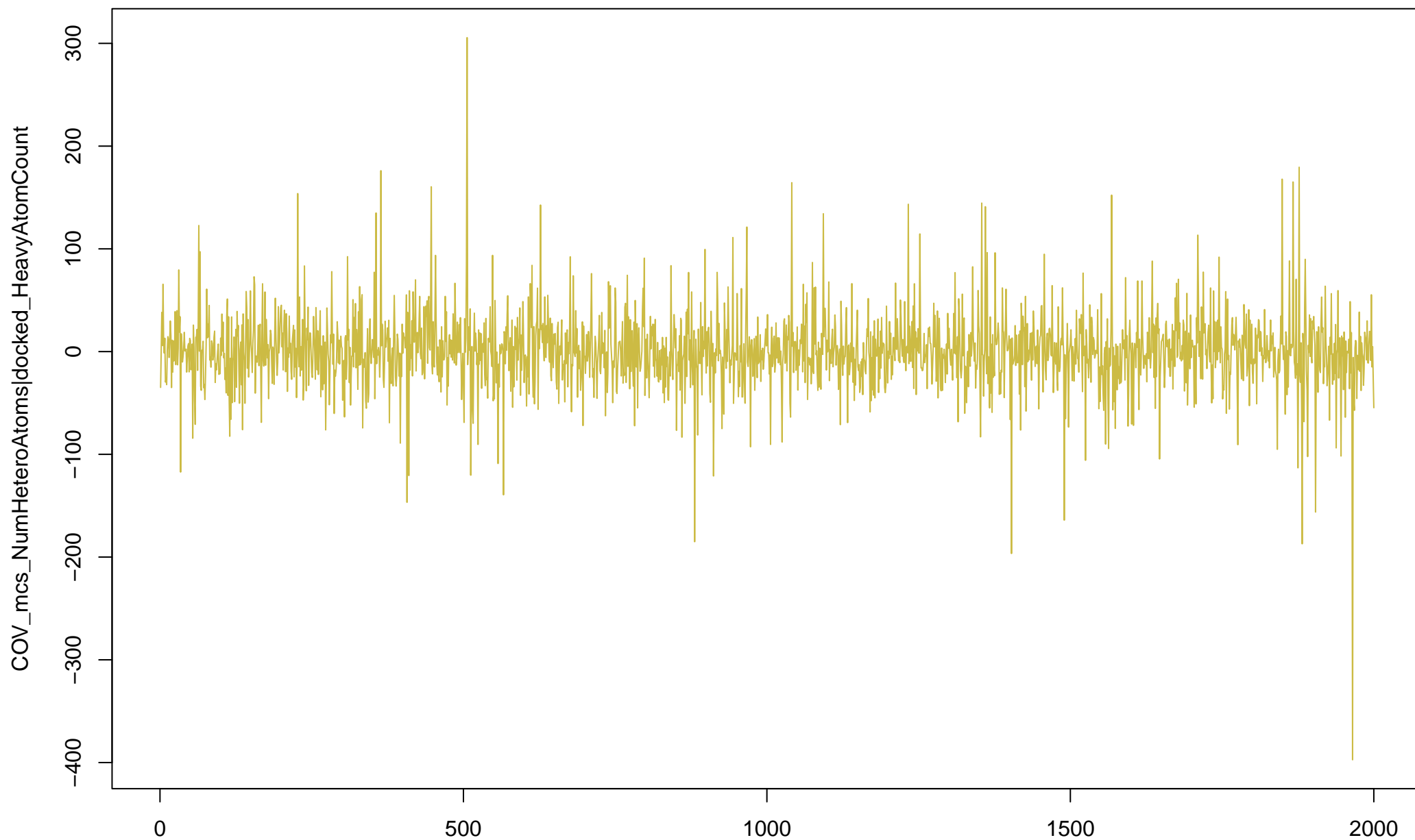


COV\_logit\_ec\_tanimoto\_similarity|docked\_NumRotatableBonds  
ESS = 2000 | BMK = 0.0684 | MCSE(6.27) = 0.02 | stat: TRUE | burn: 0

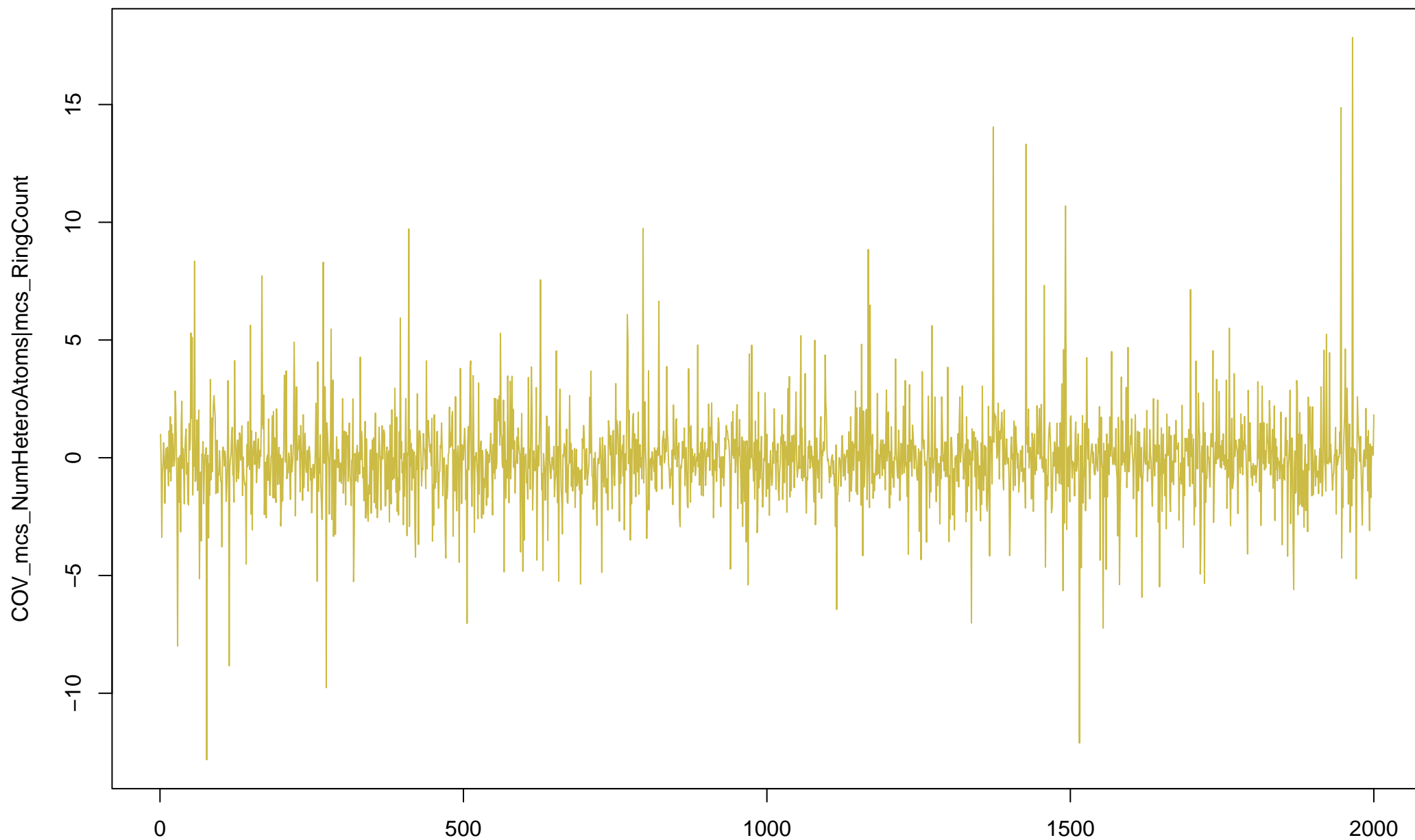




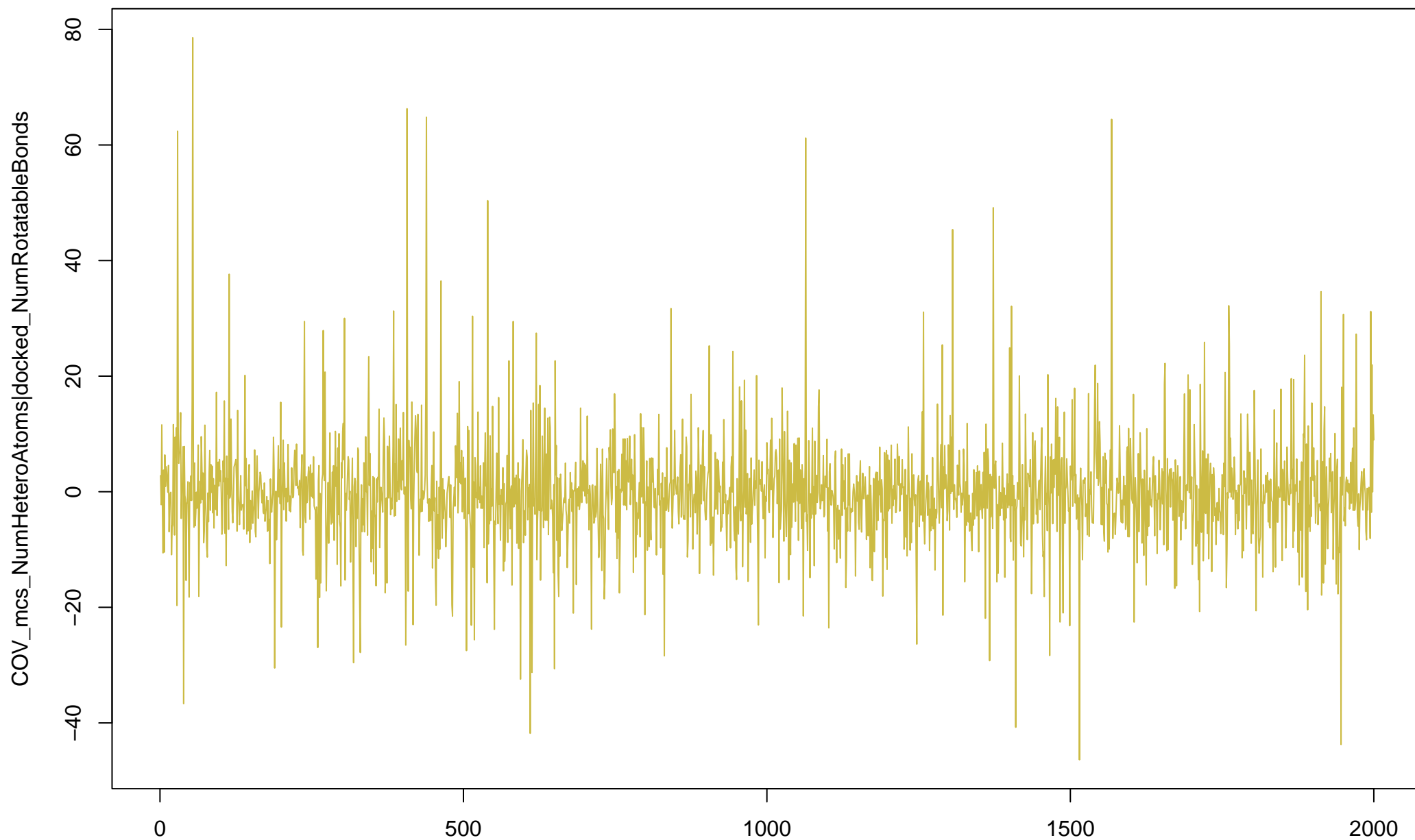
**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 2000 | BMK = 0.0776 | MCSE(6.27) = 0.00171 | stat: TRUE | burn: 0**



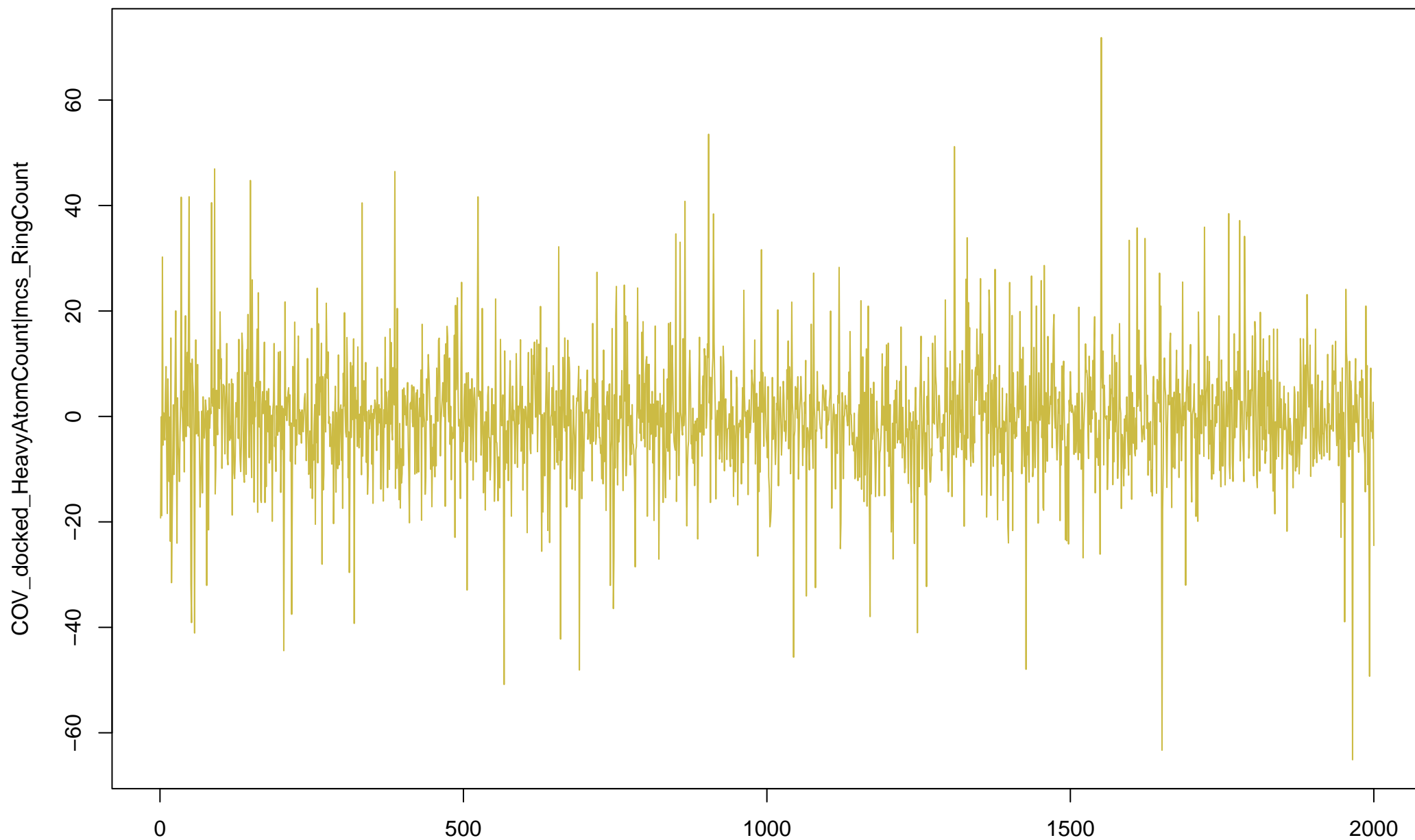
**COV\_mcs\_NumHeteroAtoms|mcs\_RingCount**  
**ESS = 2000 | BMK = 0.0949 | MCSE(6.27) = 0.0325 | stat: TRUE | burn: 0**



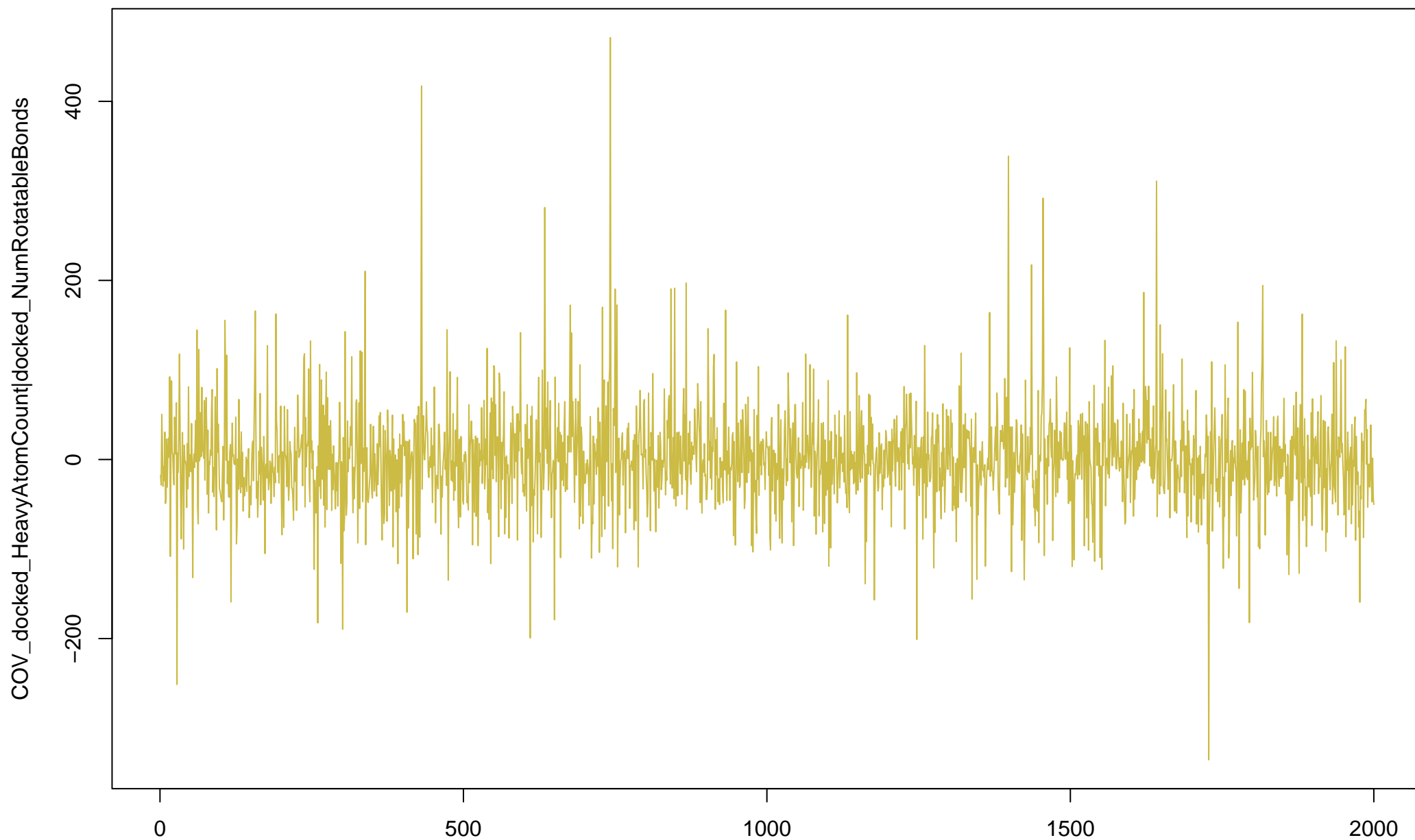
**COV\_mcs\_NumHeteroAtoms|docked\_NumRotatableBonds**  
**ESS = 2000 | BMK = 0.0801 | MCSE(6.27) = 0.00675 | stat: TRUE | burn: 0**



**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 2000 | BMK = 0.0781 | MCSE(6.27) = 0.00562 | stat: TRUE | burn: 0**



**COV\_docked\_HeavyAtomCount|docked\_NumRotatableBonds**  
**ESS = 1760 | BMK = 0.0796 | MCSE(6.27) = 0.00116 | stat: TRUE | burn: 0**



**COV\_mcs\_RingCount|docked\_NumRotatableBonds**  
**ESS = 1440 | BMK = 0.104 | MCSE(6.27) = 0.0201 | stat: TRUE | burn: 0**

