

-- STATS maxD --

min ESS = 1.51819374972057

max BMK = 0.815809744750633

max MCSE = 17.6140373732861

all stationary: FALSE

burn: 1020

-- STATS 2D --

min ESS = 9.92114680322367

max BMK = 0.446877392257239

max MCSE = 14.5955334431816

all stationary: FALSE

burn: 816

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 1

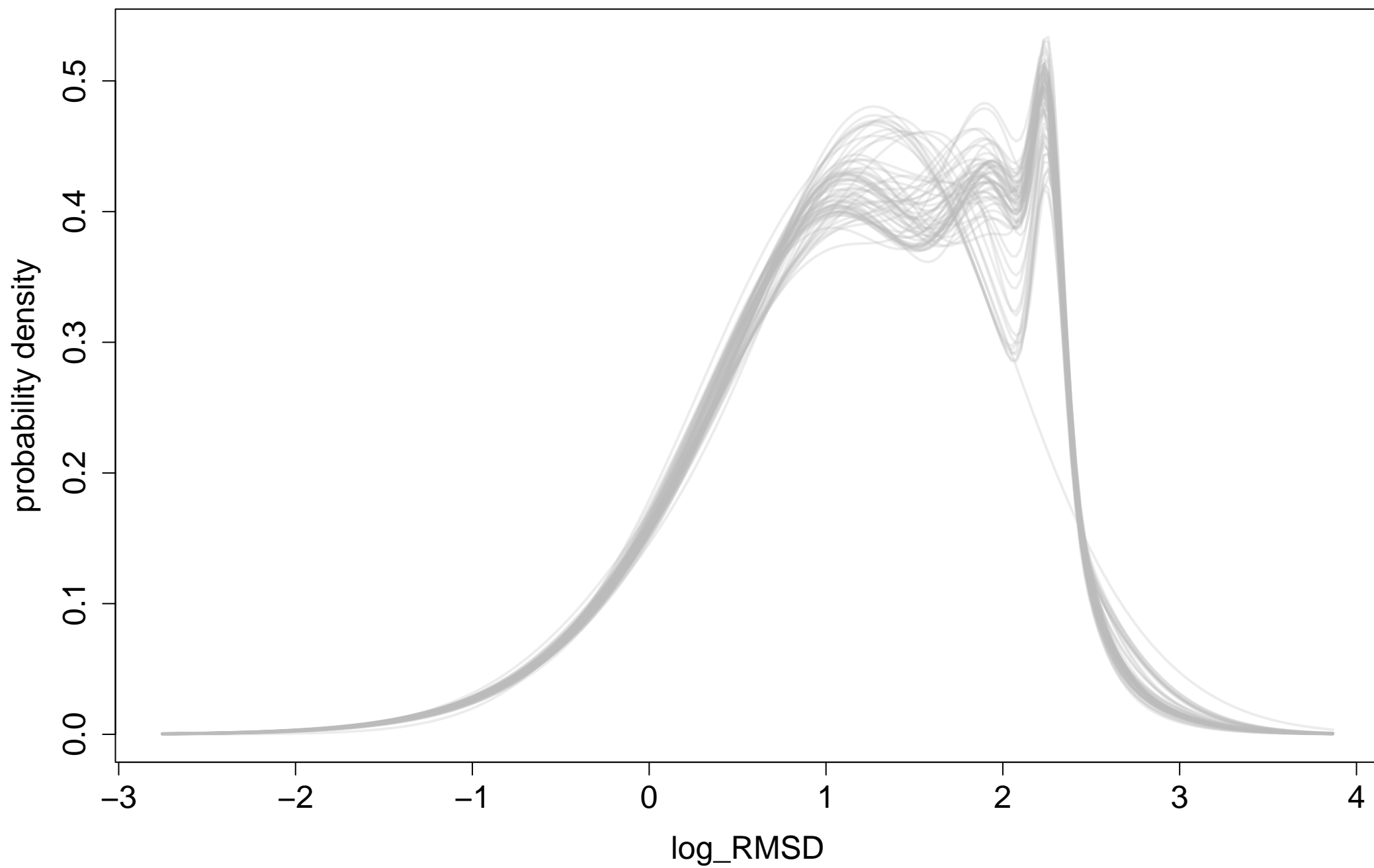
max MCSE = NaN

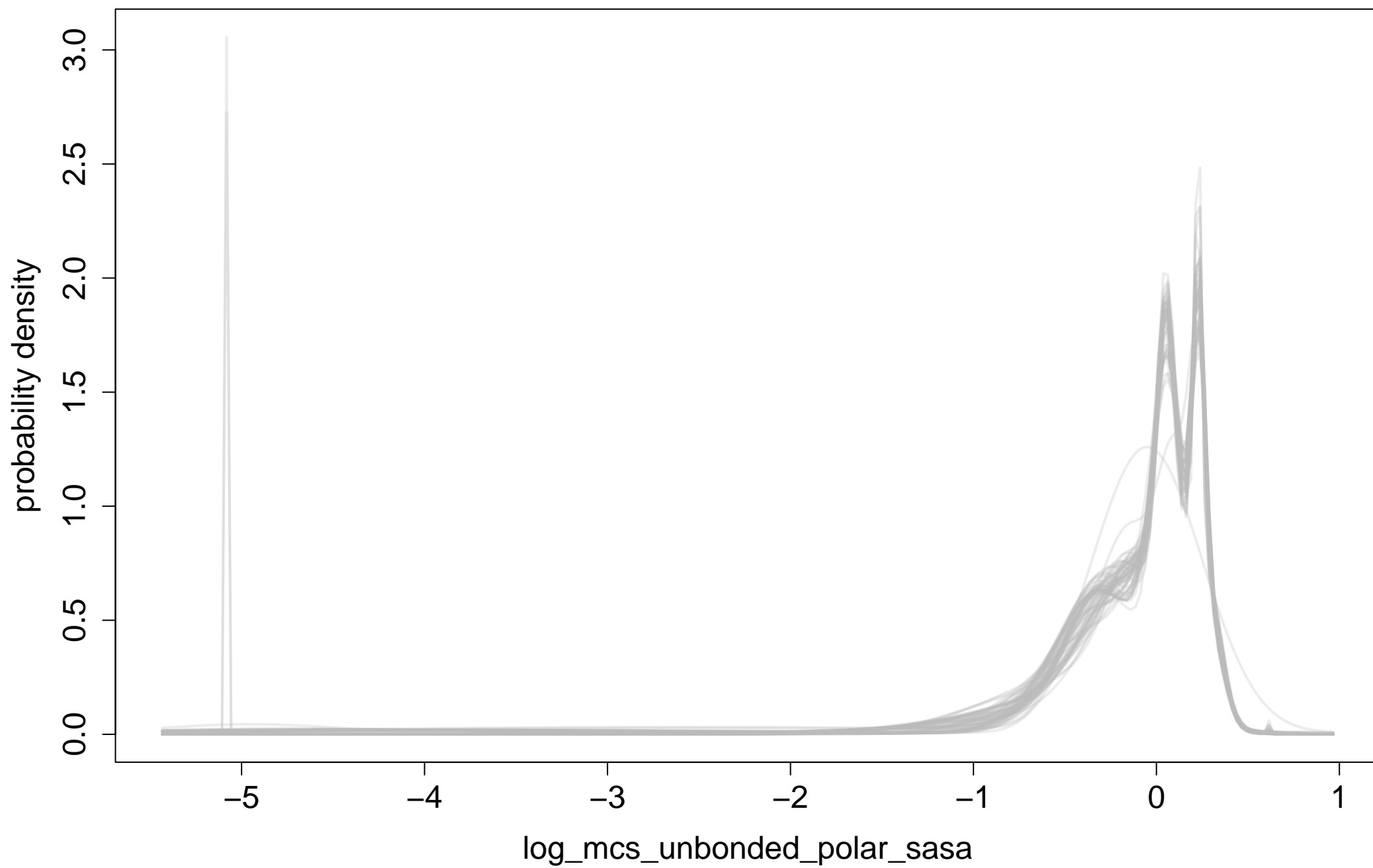
all stationary: FALSE

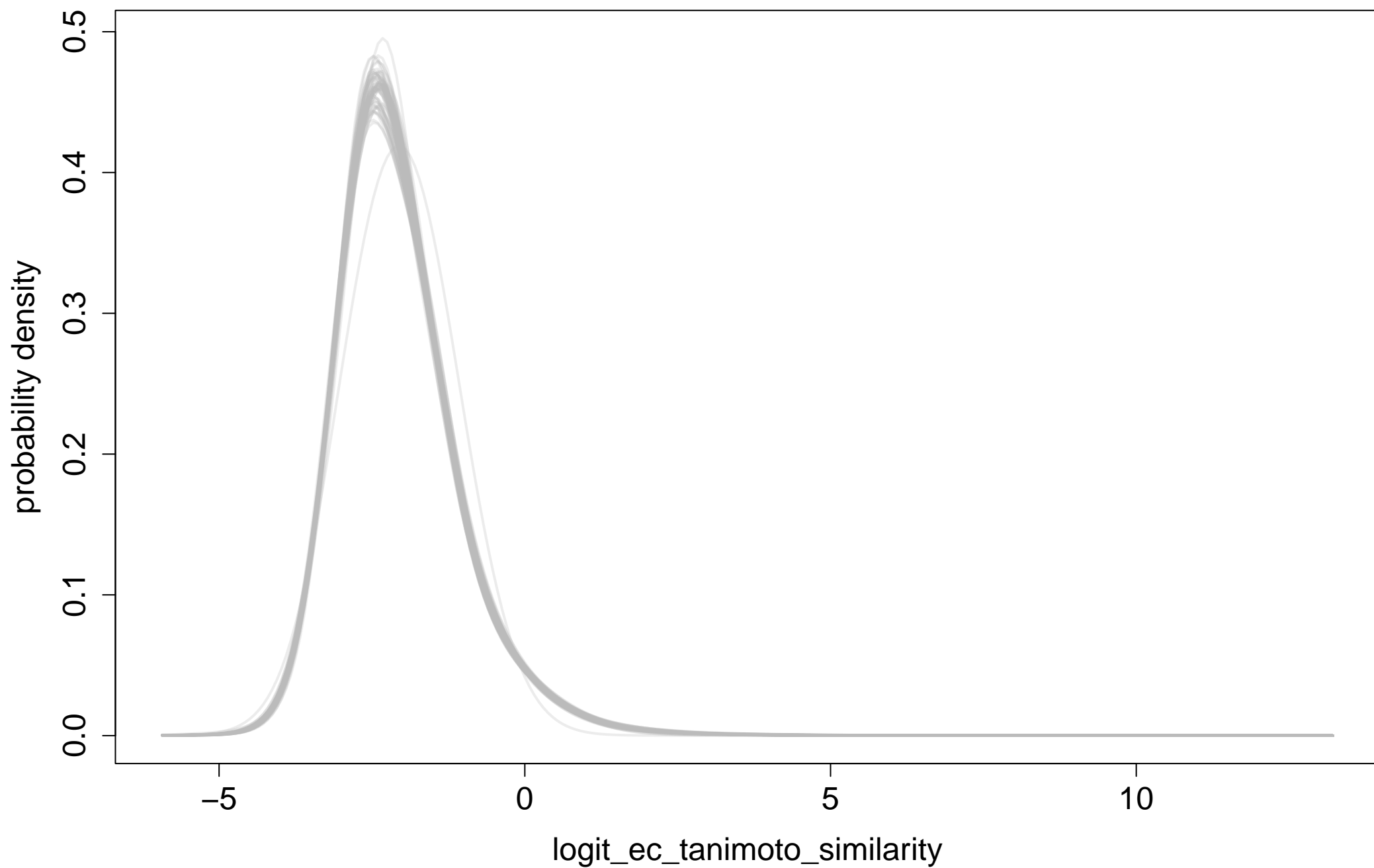
burn: 1020

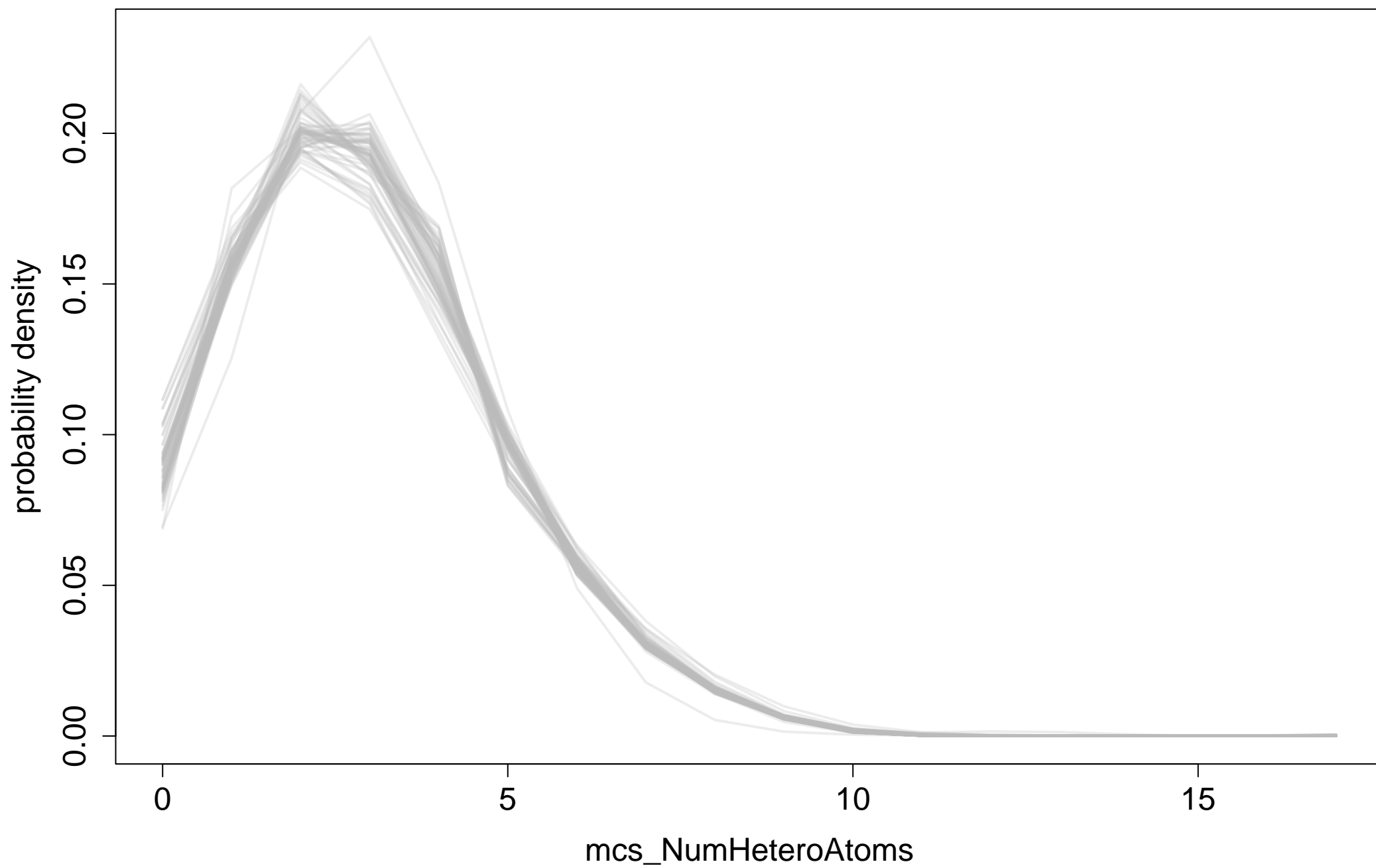
Occupied clusters: 14 of 64

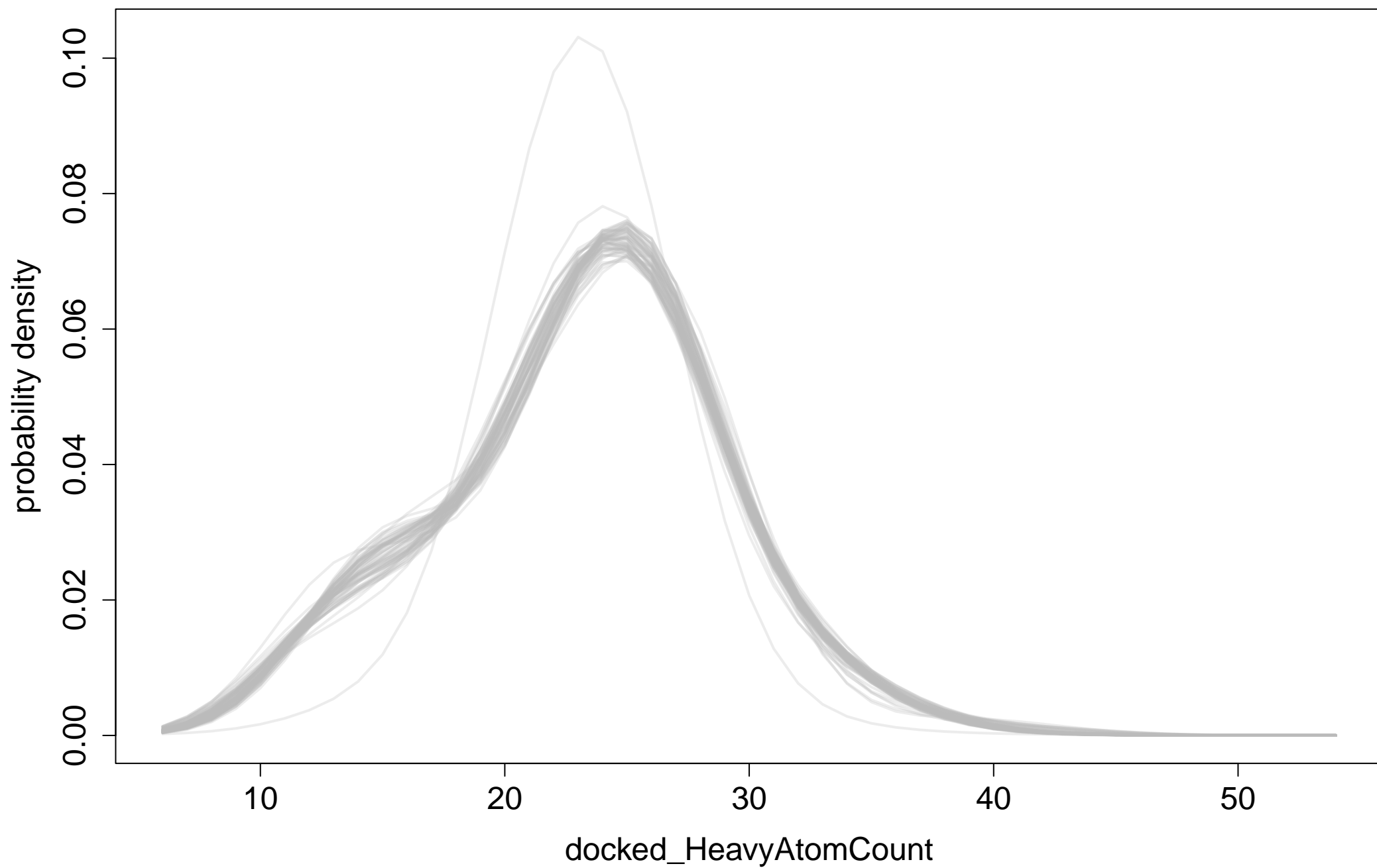
LL: -89900 +- 6780

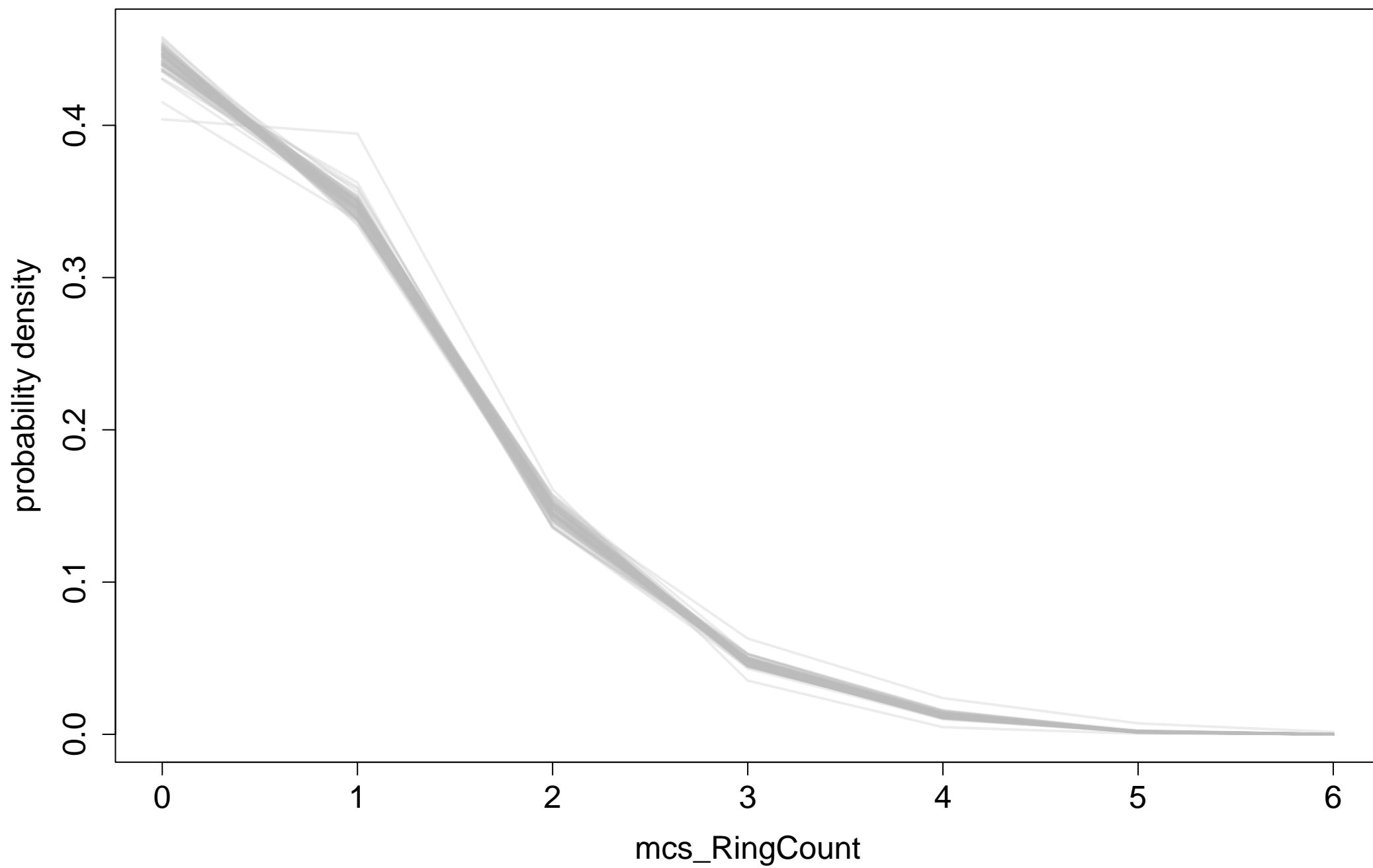


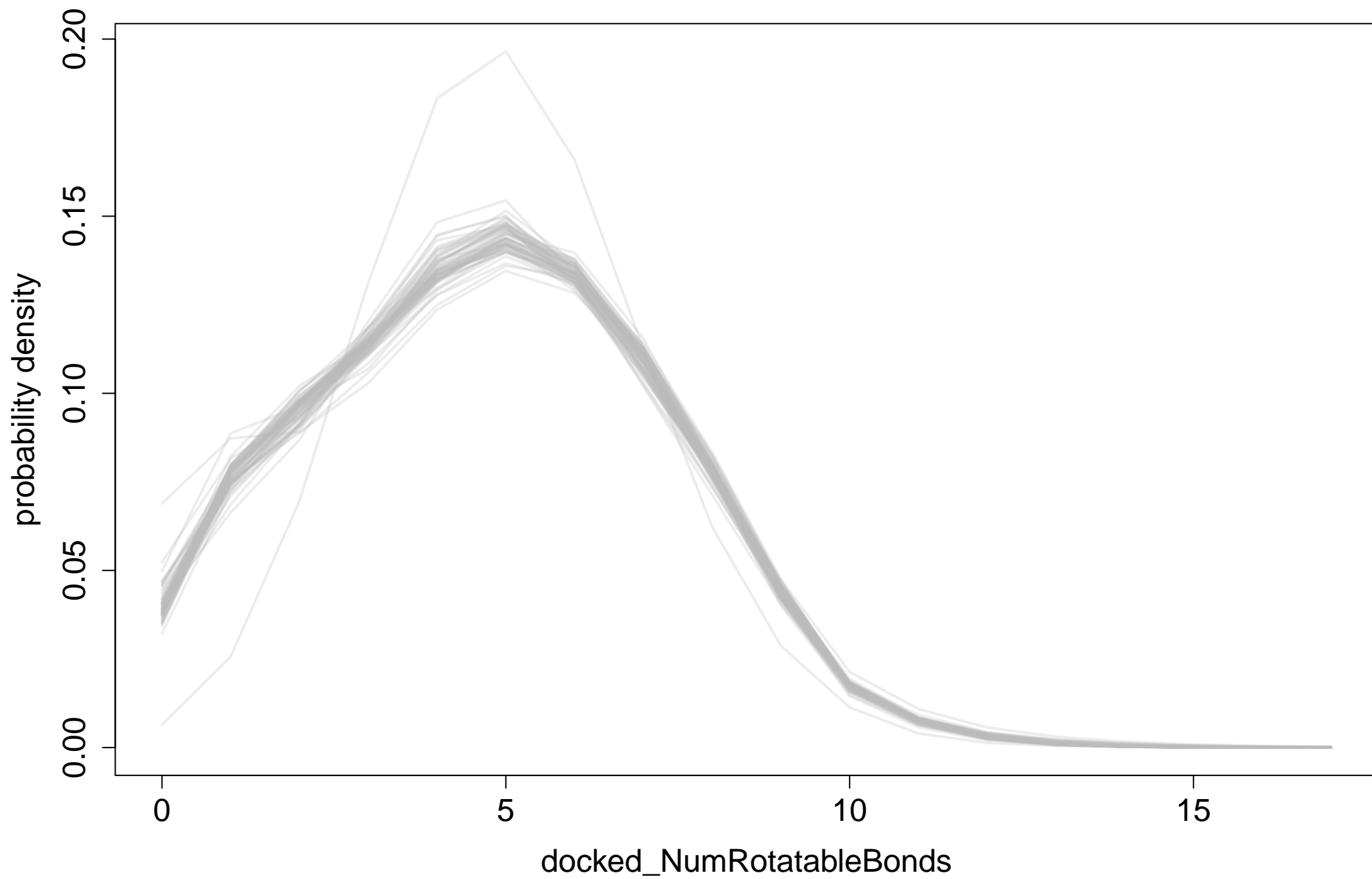




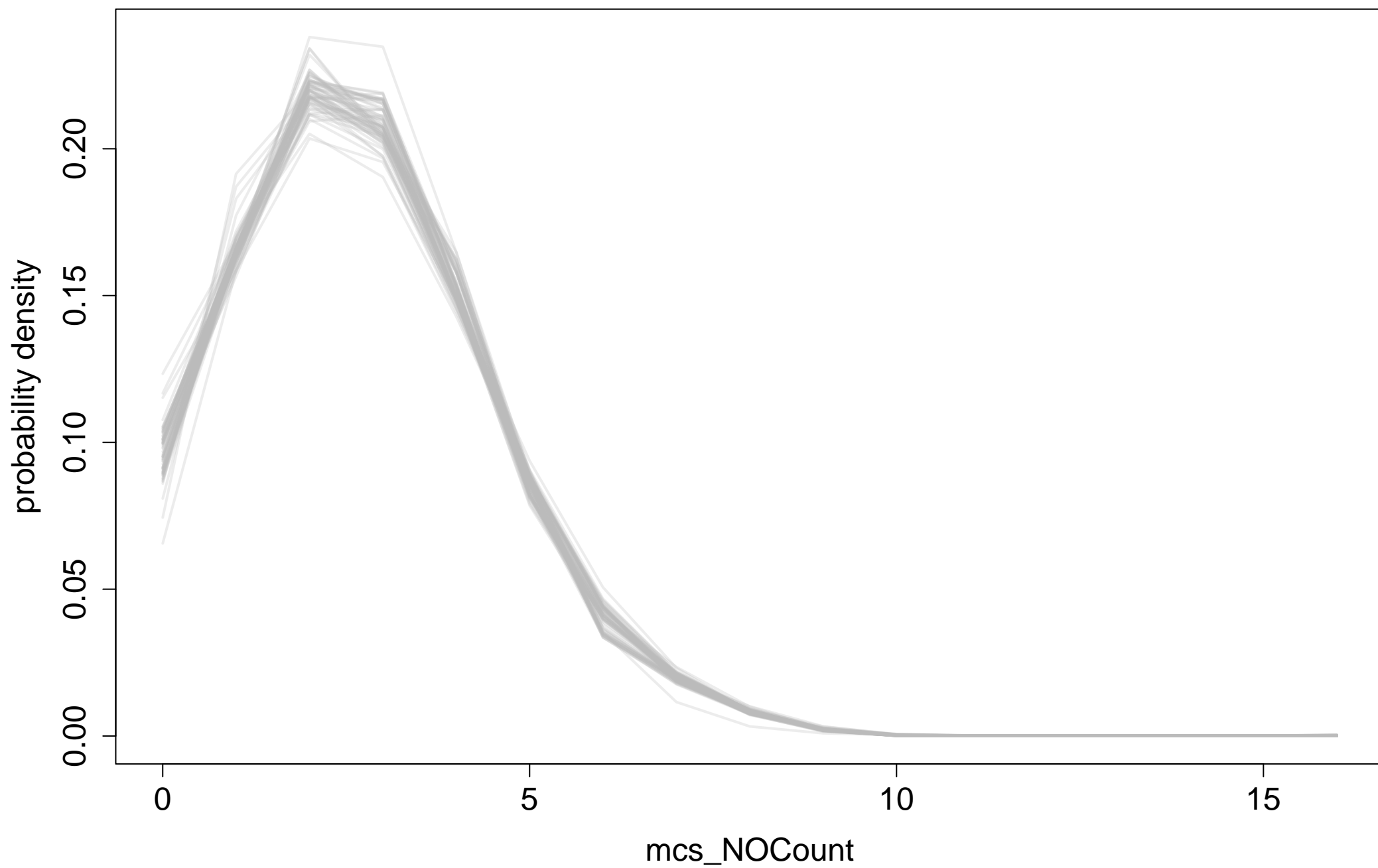


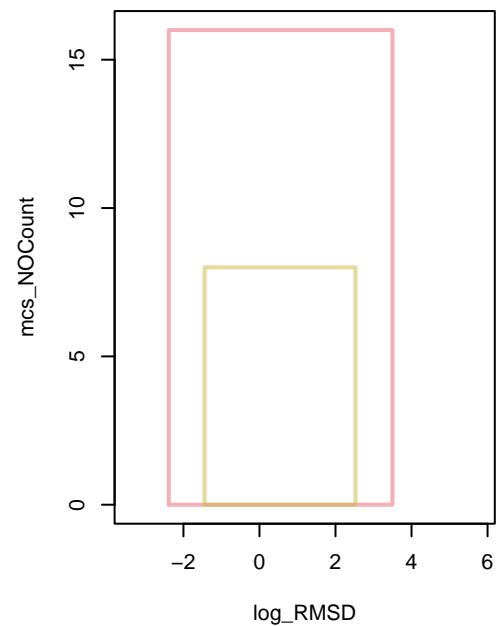
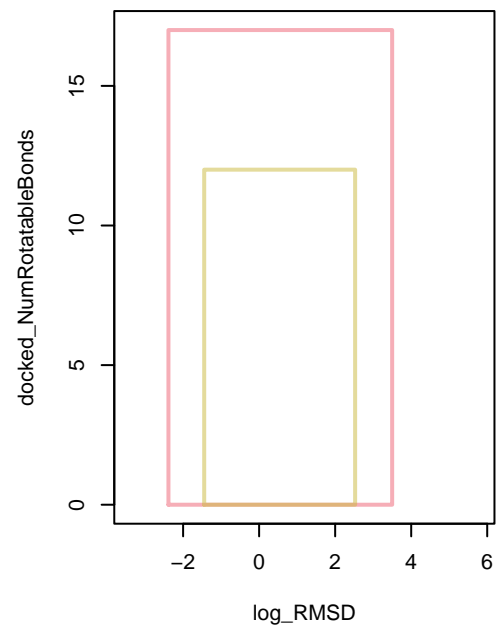
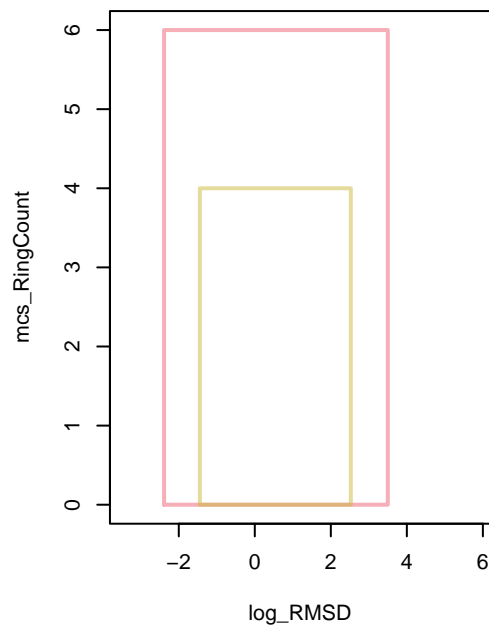
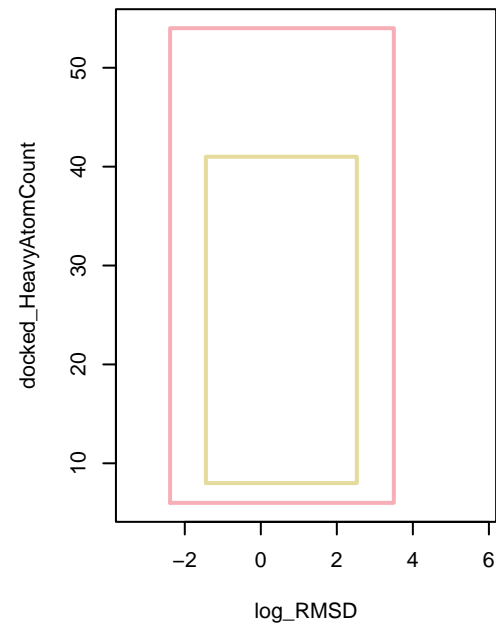
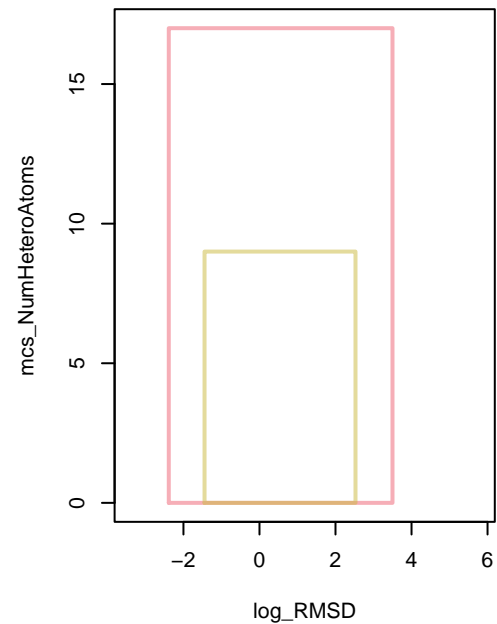
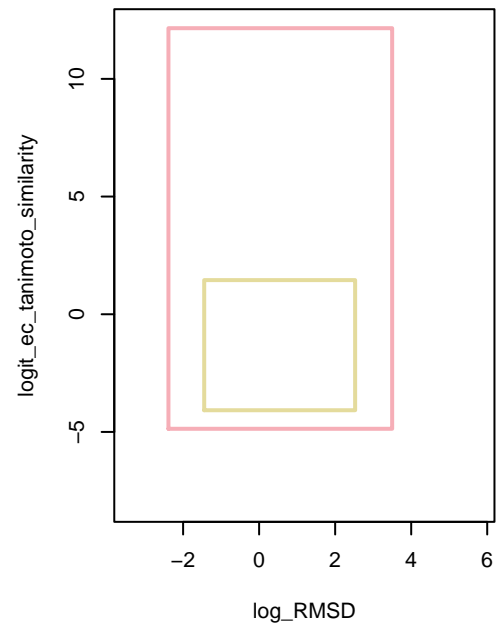
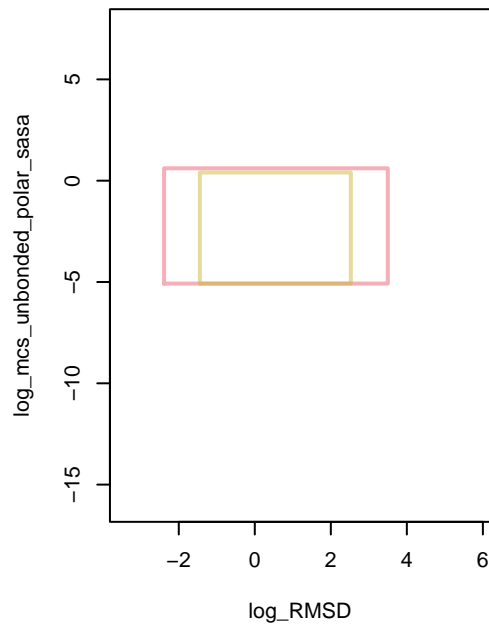




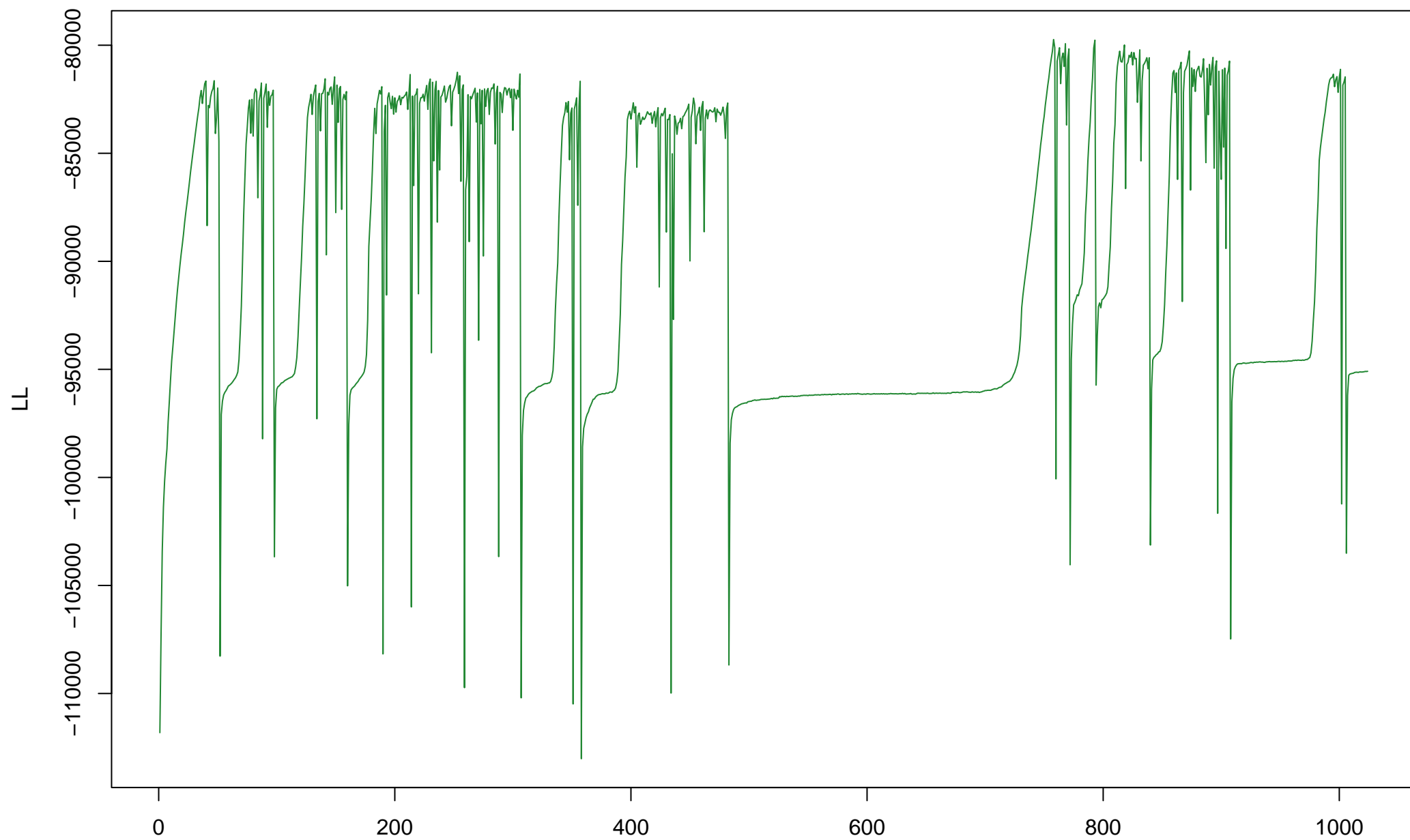




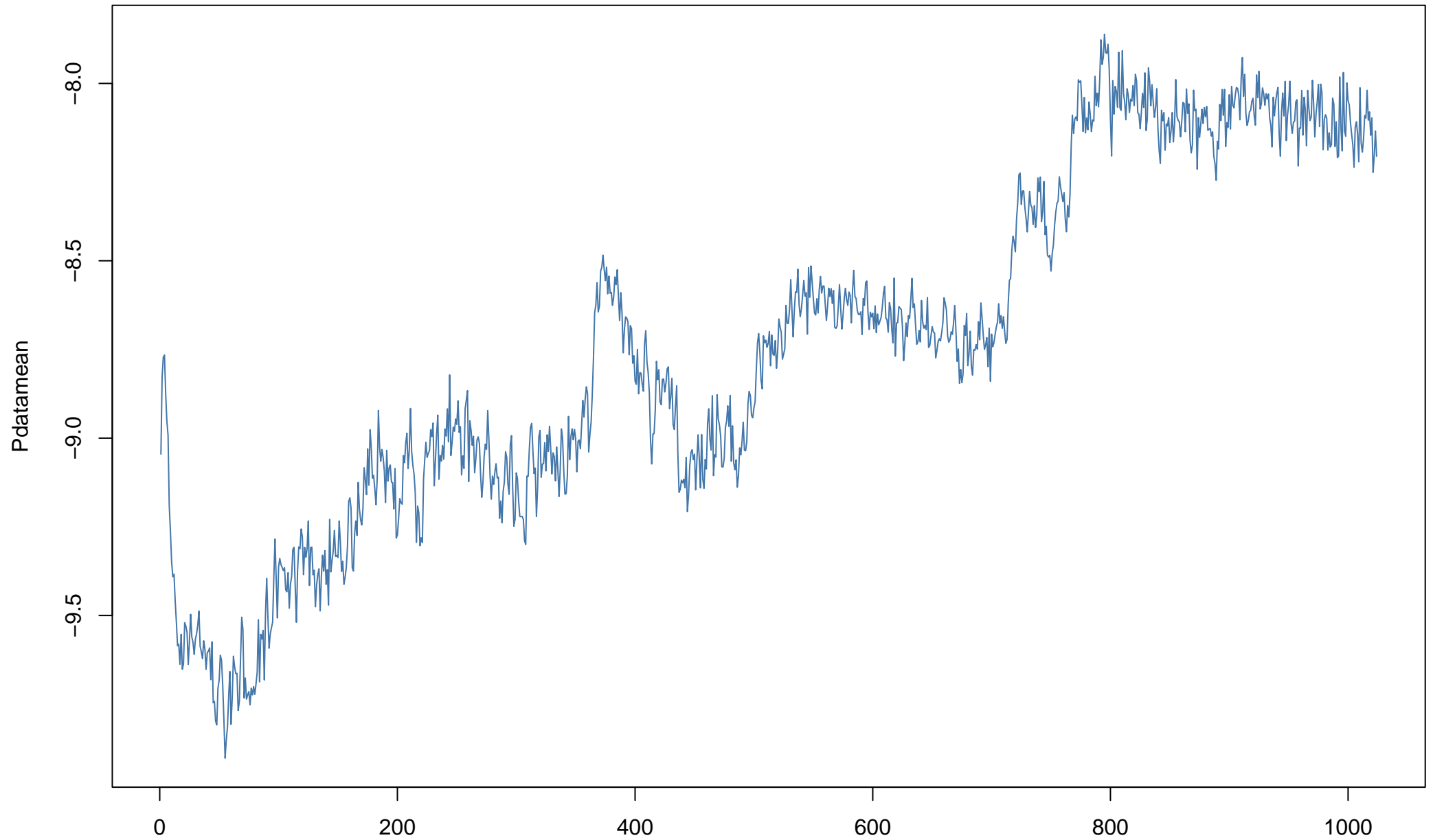




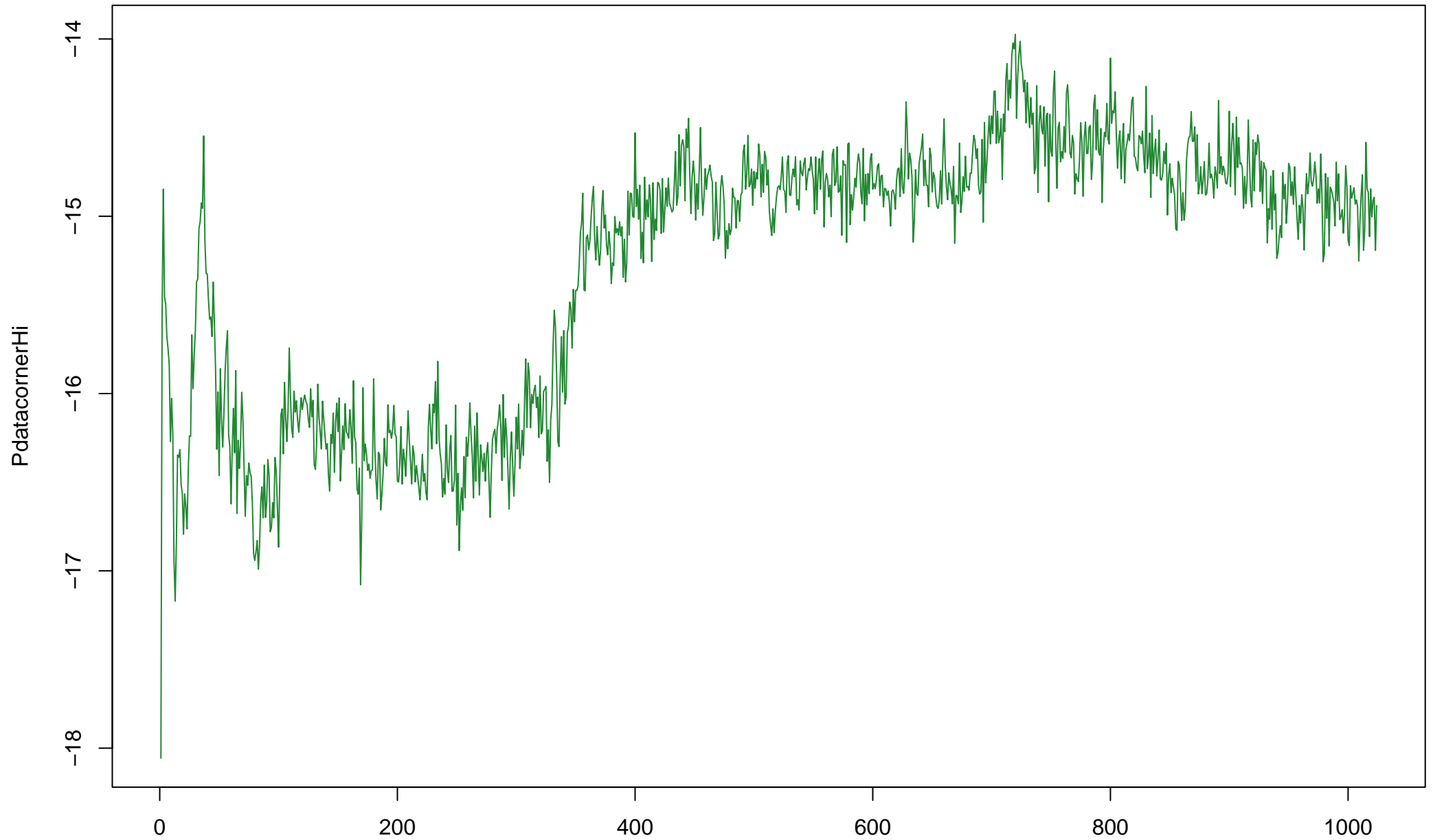
LL



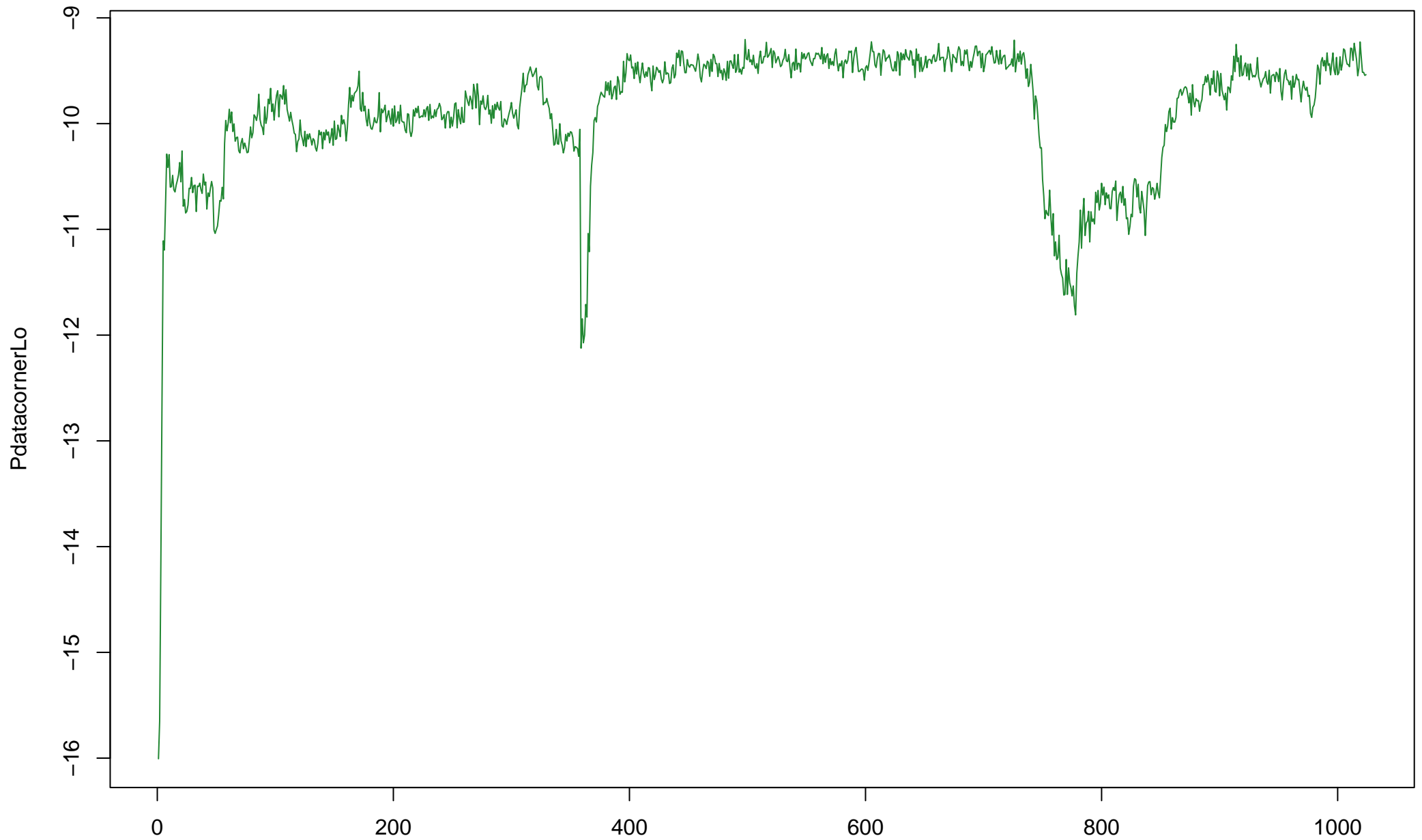
**Pdatamean**  
**ESS = 1.52 | BMK = 0.816 | MCSE(6.27) = 17.6 | stat: FALSE | burn: 816**



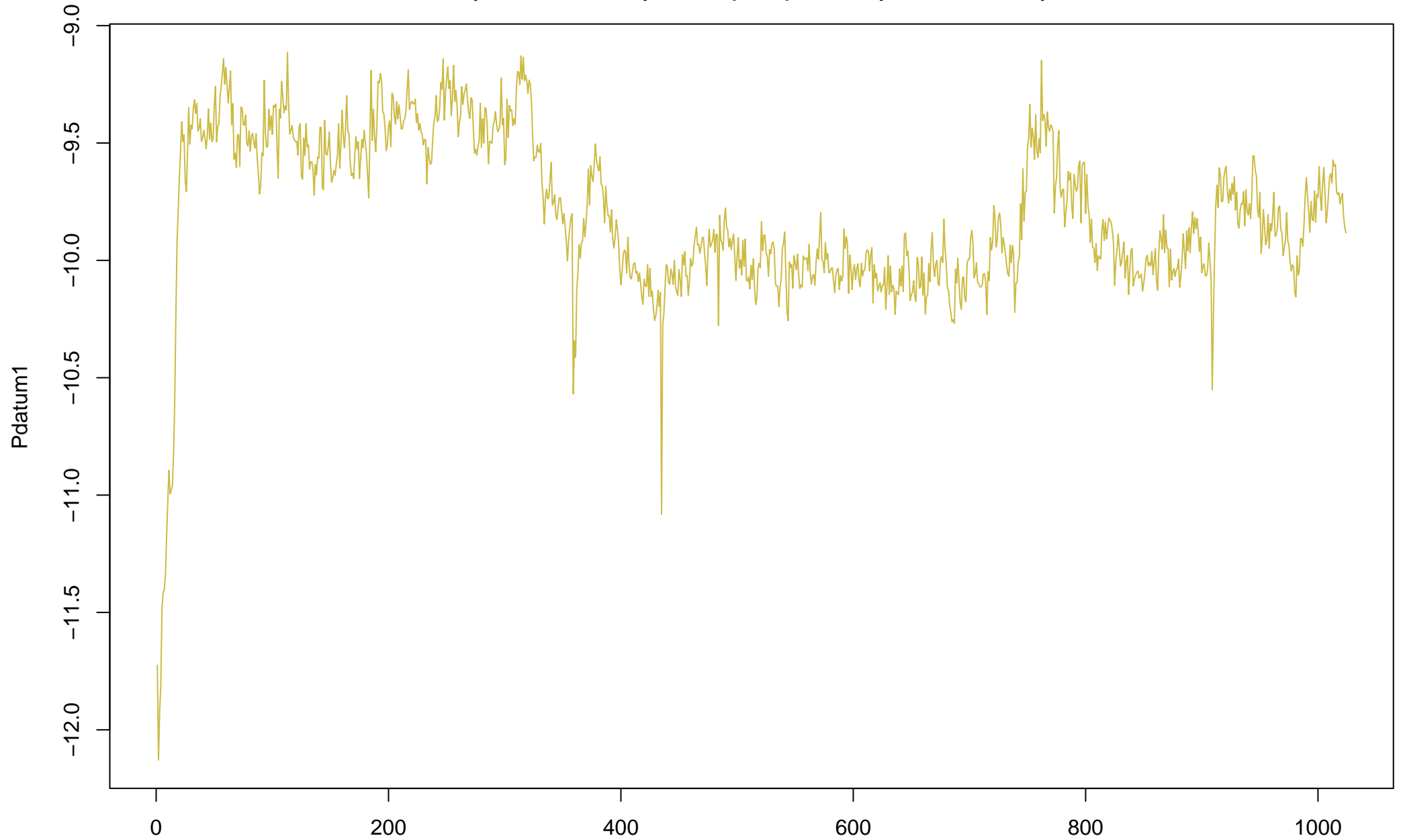
**PdatacornerHi**  
**ESS = 3.41 | BMK = 0.69 | MCSE(6.27) = 16.8 | stat: FALSE | burn: 408**



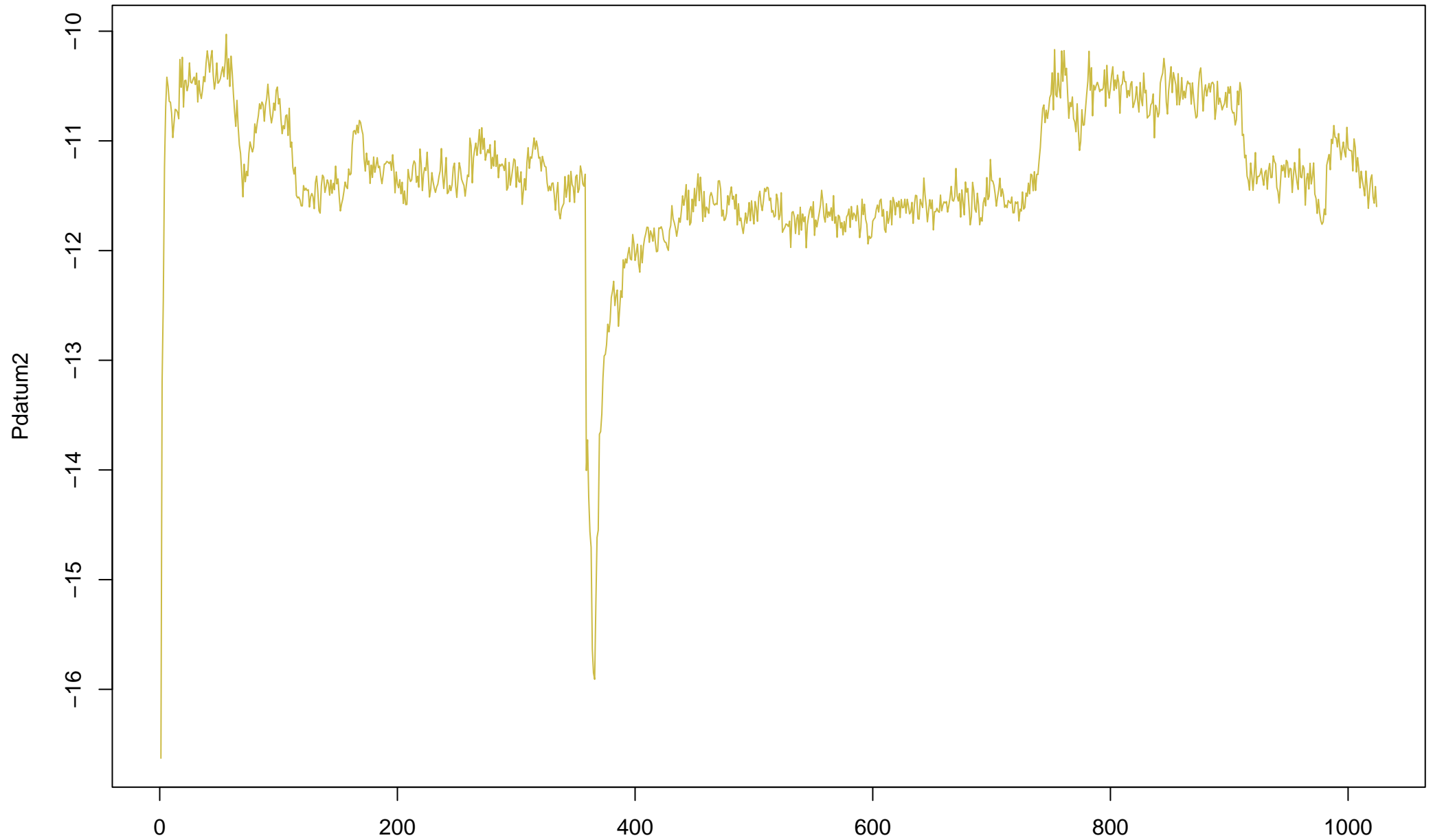
**PdatacornerLo**  
**ESS = 7.43 | BMK = 0.391 | MCSE(6.27) = 16.6 | stat: FALSE | burn: 1020**



**Pdatum1**  
**ESS = 12.1 | BMK = 0.469 | MCSE(6.27) = 15.6 | stat: FALSE | burn: 714**

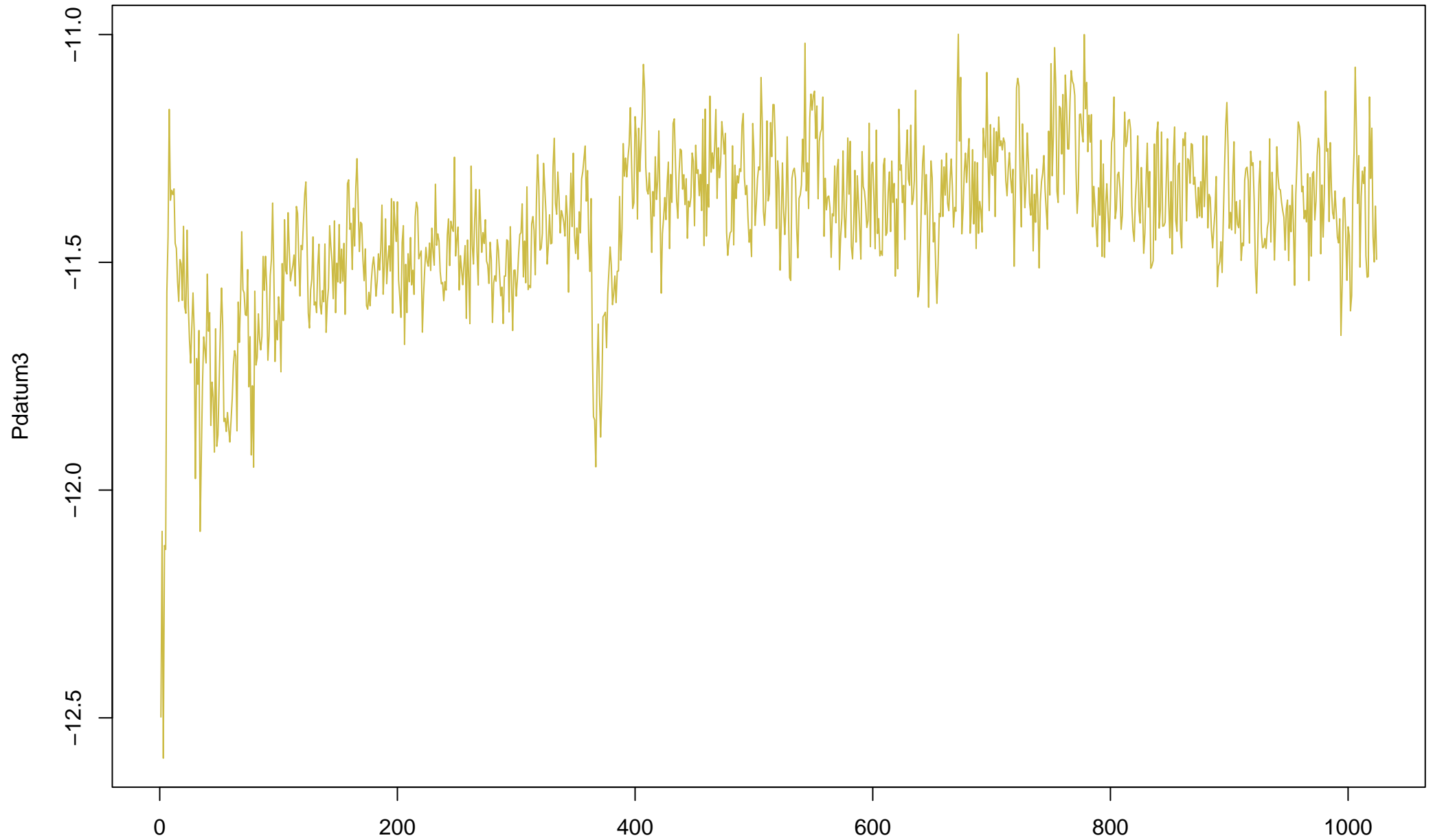


**Pdatum2**  
**ESS = 8.32 | BMK = 0.191 | MCSE(6.27) = 16.1 | stat: FALSE | burn: 1020**

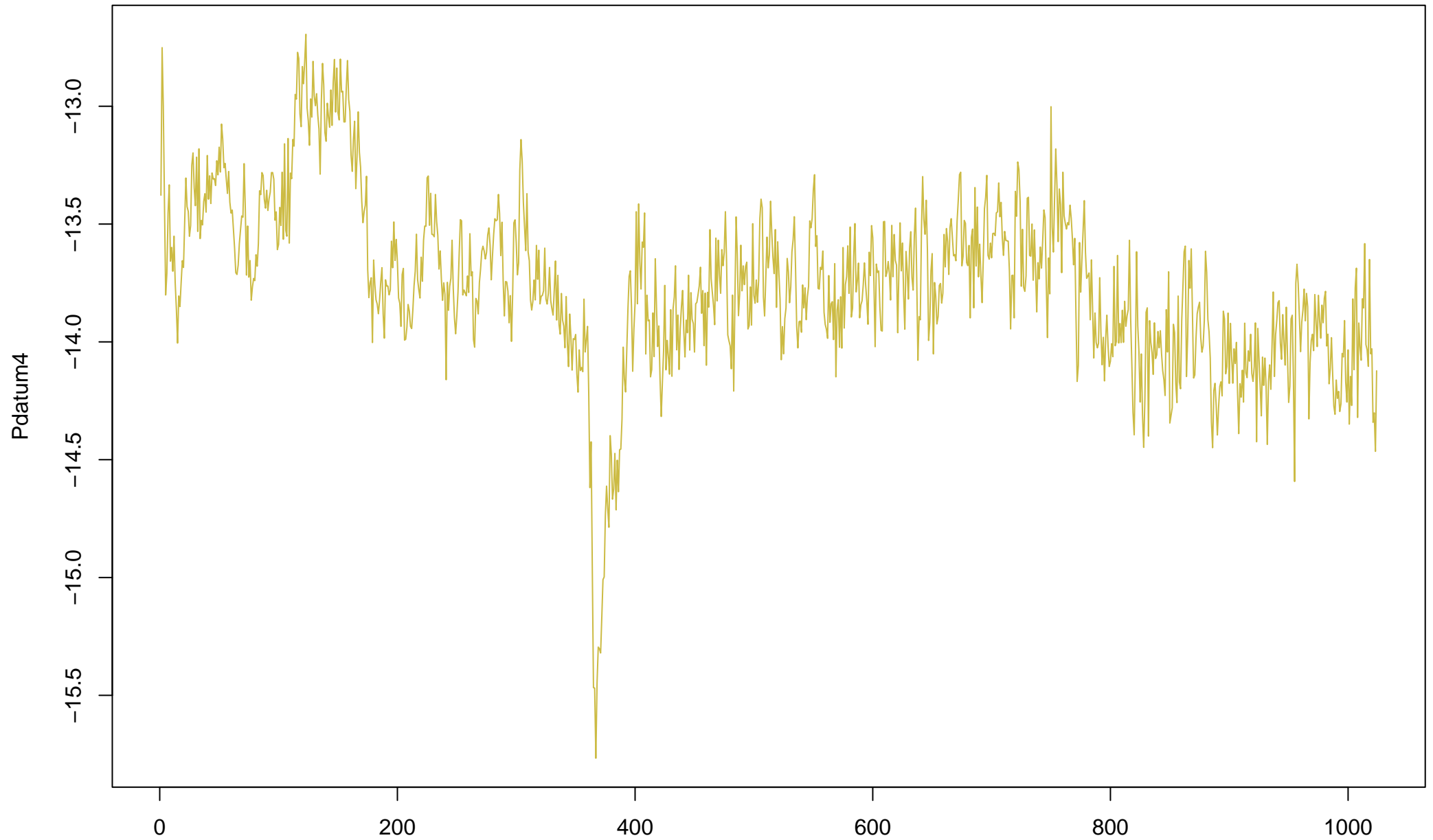




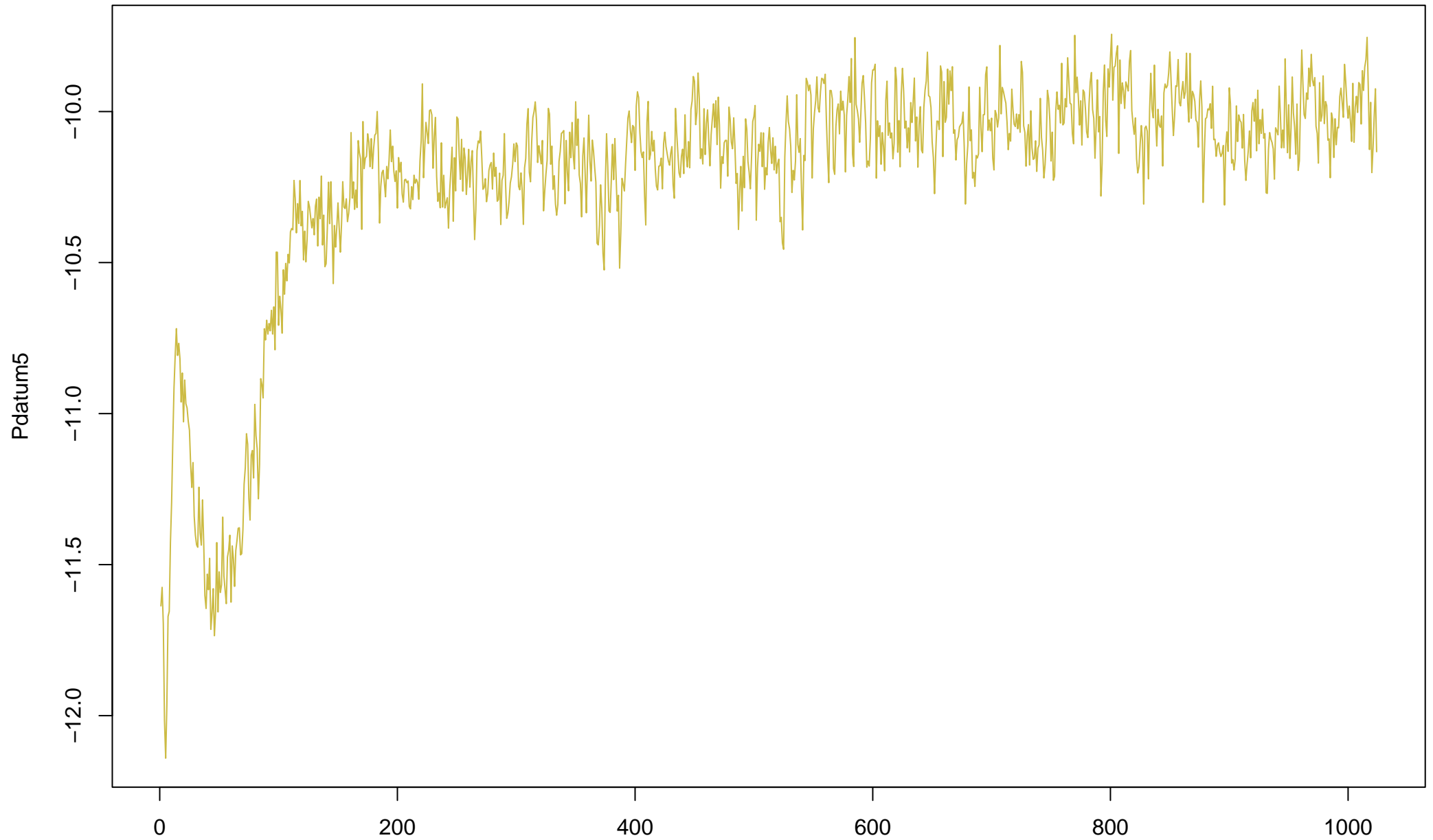
**Pdatum3**  
**ESS = 20.9 | BMK = 0.377 | MCSE(6.27) = 12.6 | stat: FALSE | burn: 102**



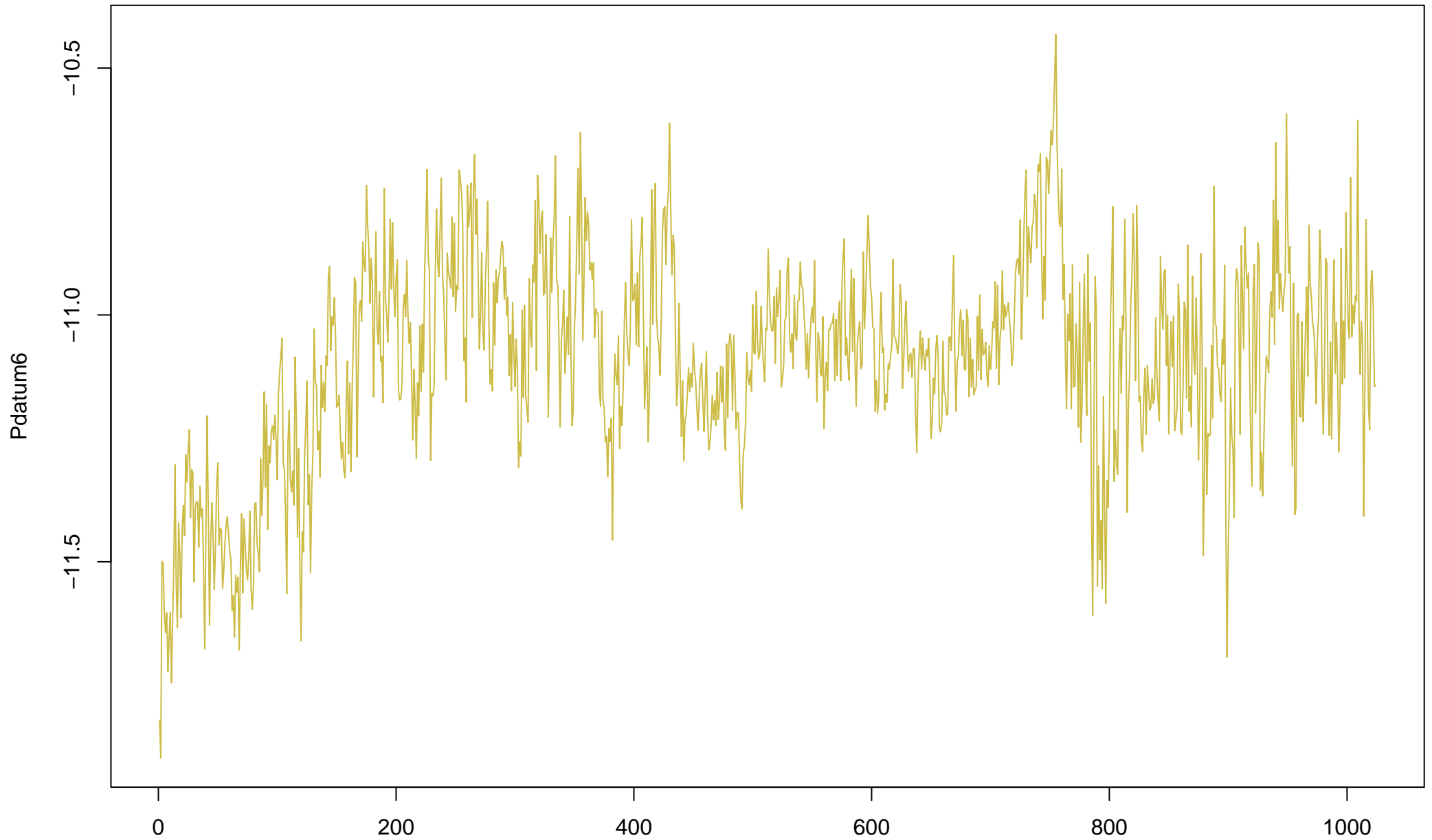
**Pdatum4**  
**ESS = 15.3 | BMK = 0.296 | MCSE(6.27) = 14.9 | stat: FALSE | burn: 204**



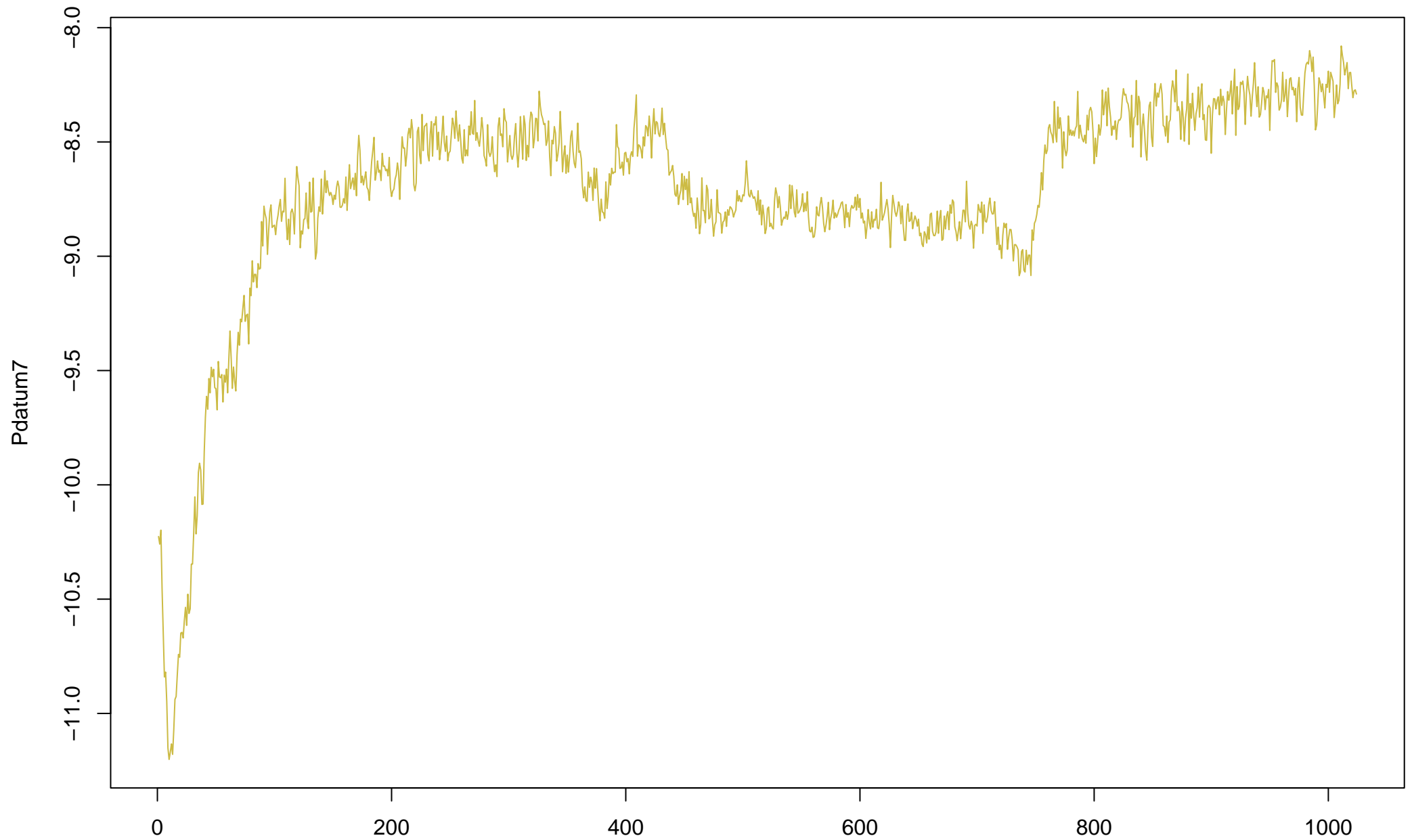
**Pdatum5**  
**ESS = 8.75 | BMK = 0.524 | MCSE(6.27) = 16.3 | stat: FALSE | burn: 102**



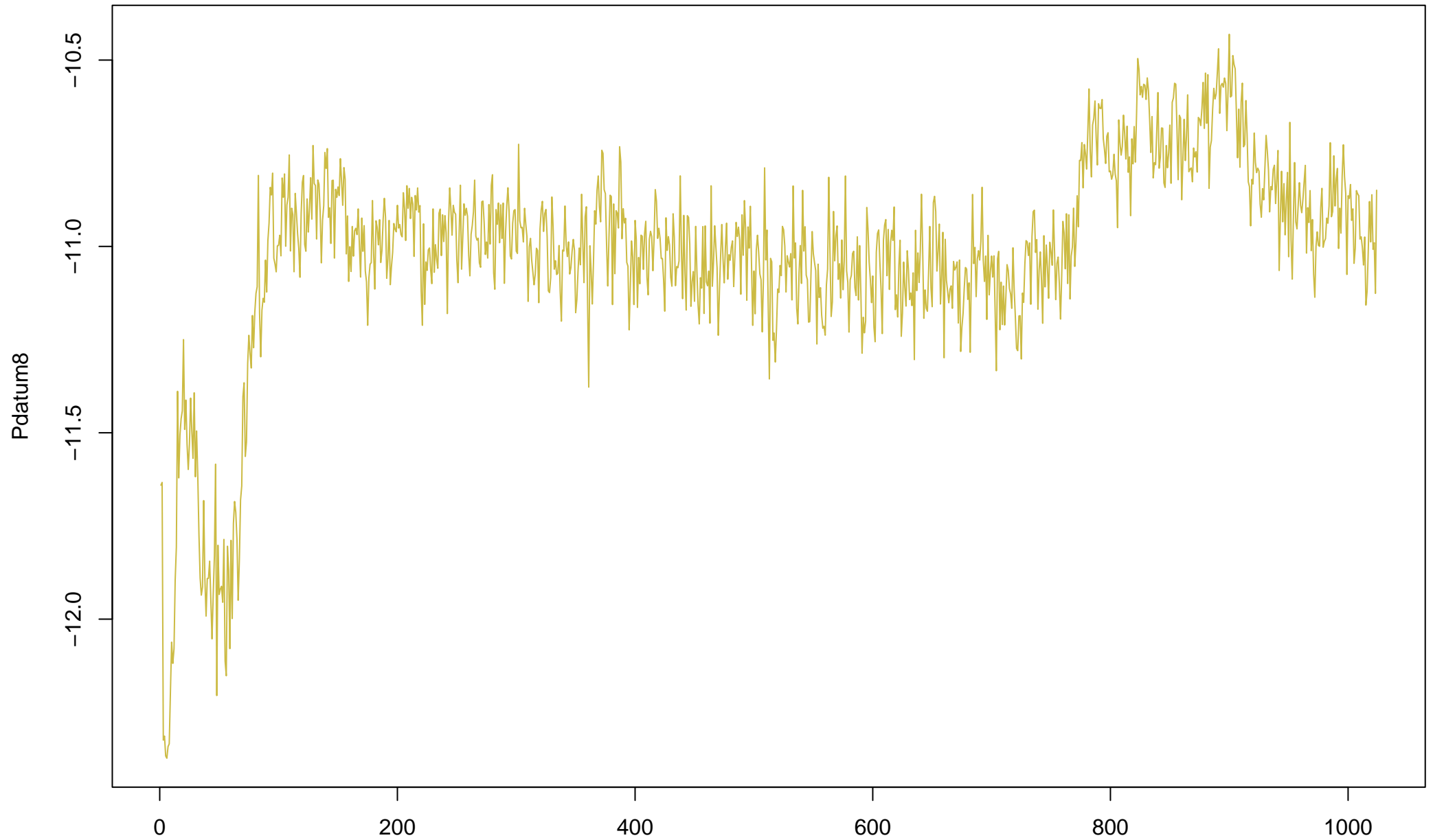
**Pdatum6**  
**ESS = 31.4 | BMK = 0.215 | MCSE(6.27) = 12.6 | stat: FALSE | burn: 714**



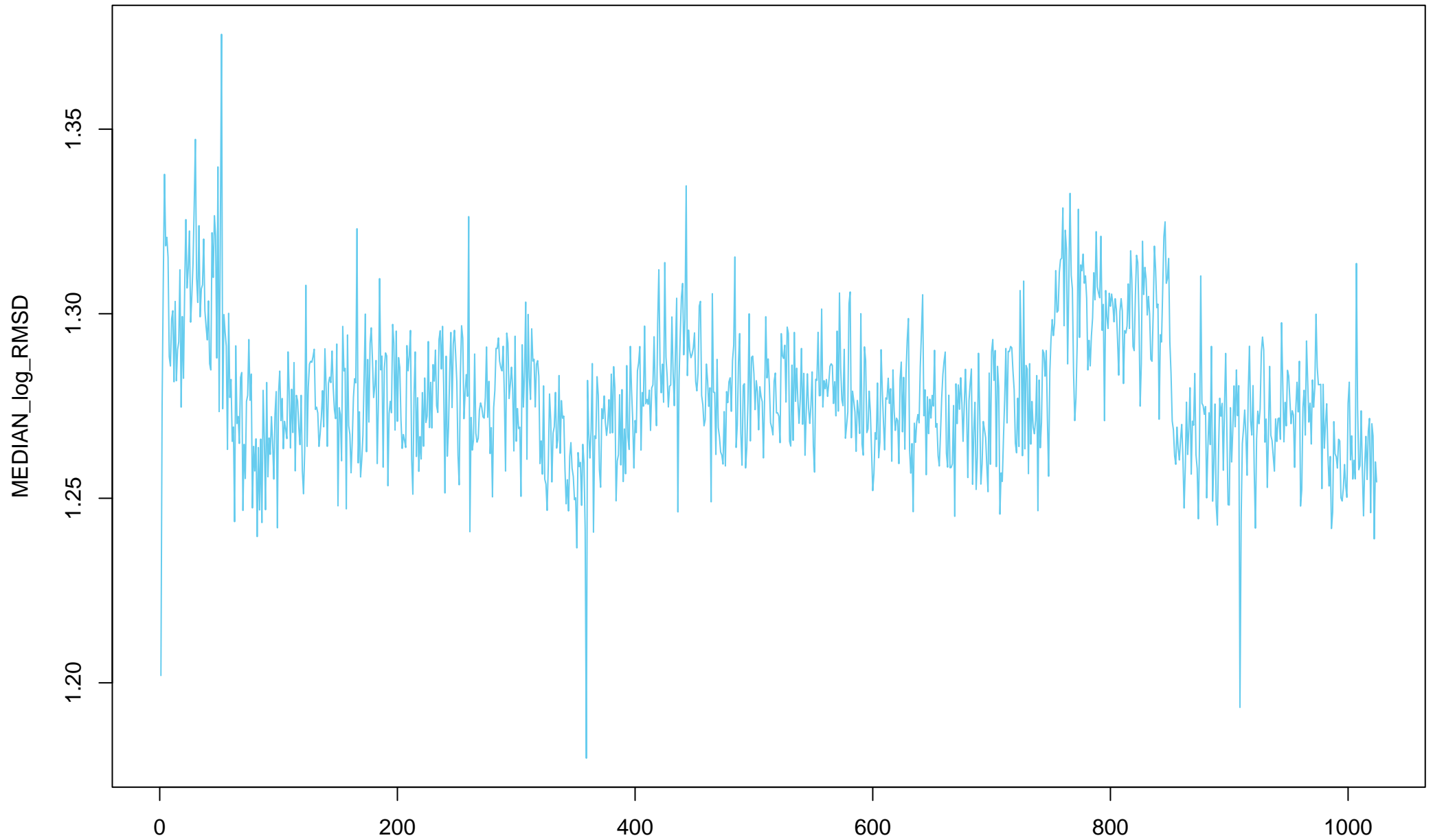
**Pdatum7**  
**ESS = 6.29 | BMK = 0.45 | MCSE(6.27) = 17.1 | stat: FALSE | burn: 816**



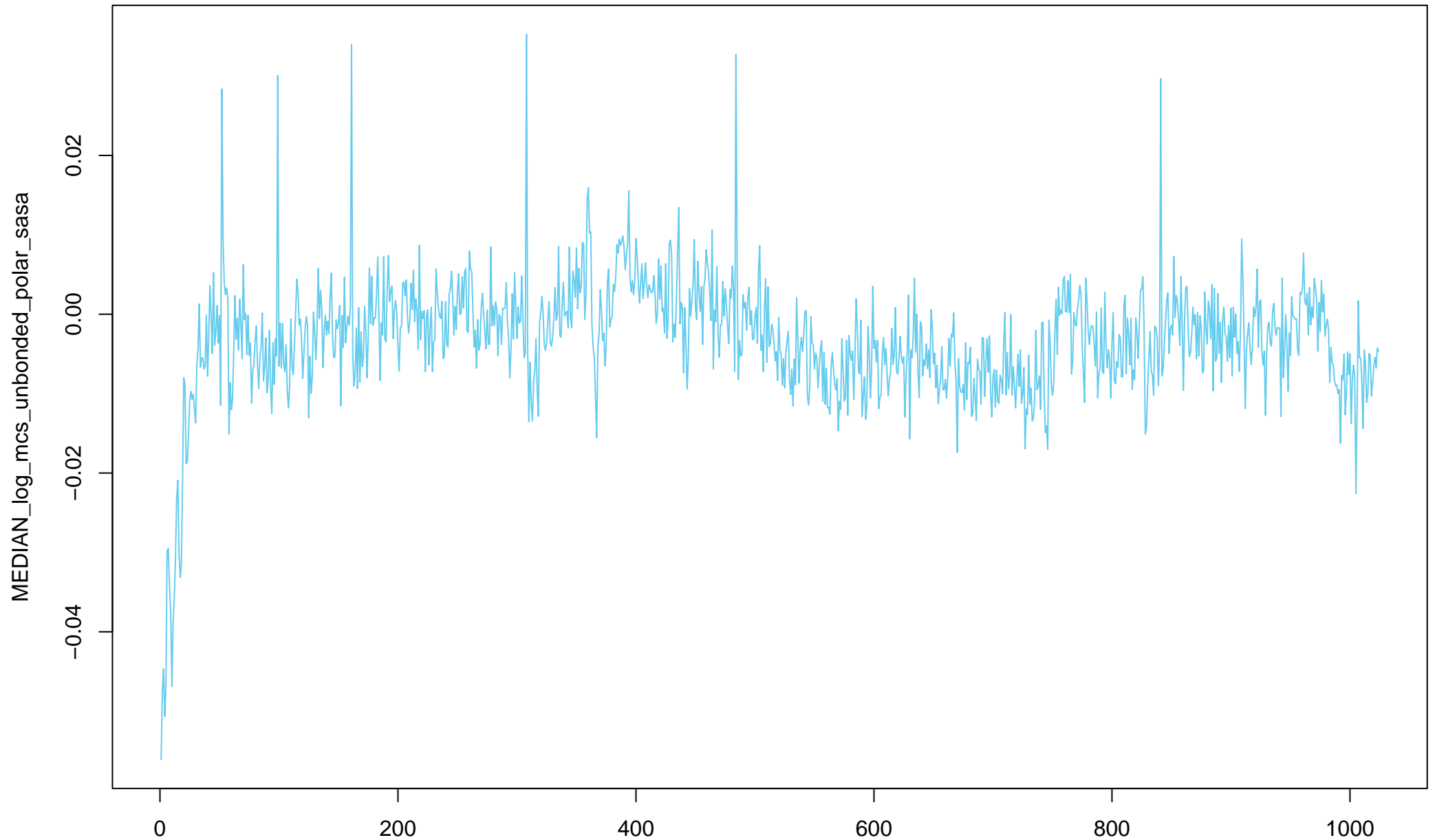
**Pdatum8**  
**ESS = 11.5 | BMK = 0.398 | MCSE(6.27) = 15.8 | stat: FALSE | burn: 1020**



**MEDIAN\_log\_RMSD**  
**ESS = 34.4 | BMK = 0.0921 | MCSE(6.27) = 10.6 | stat: FALSE | burn: 0**

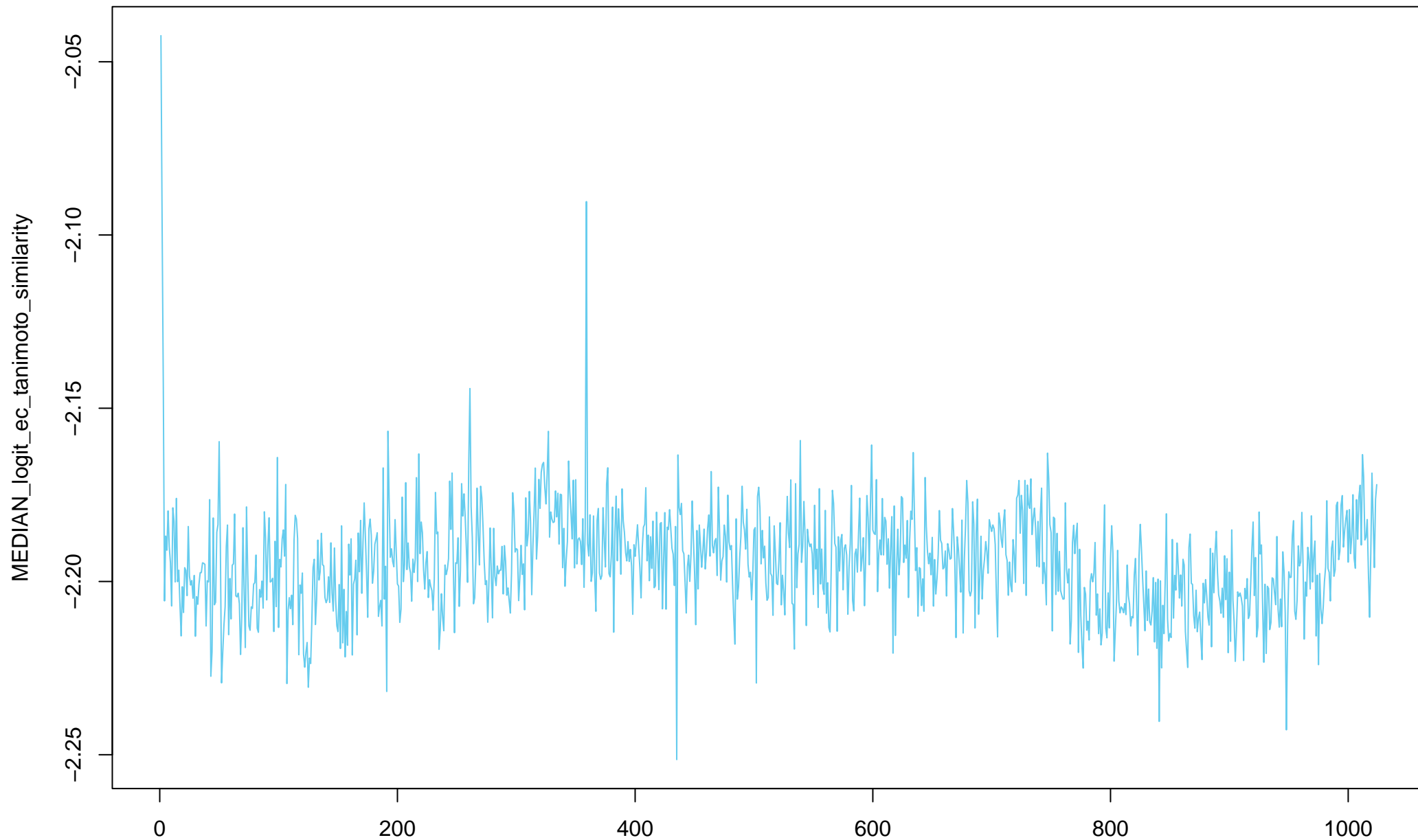


**MEDIAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 46.3 | BMK = 0.31 | MCSE(6.27) = 12.3 | stat: FALSE | burn: 510**

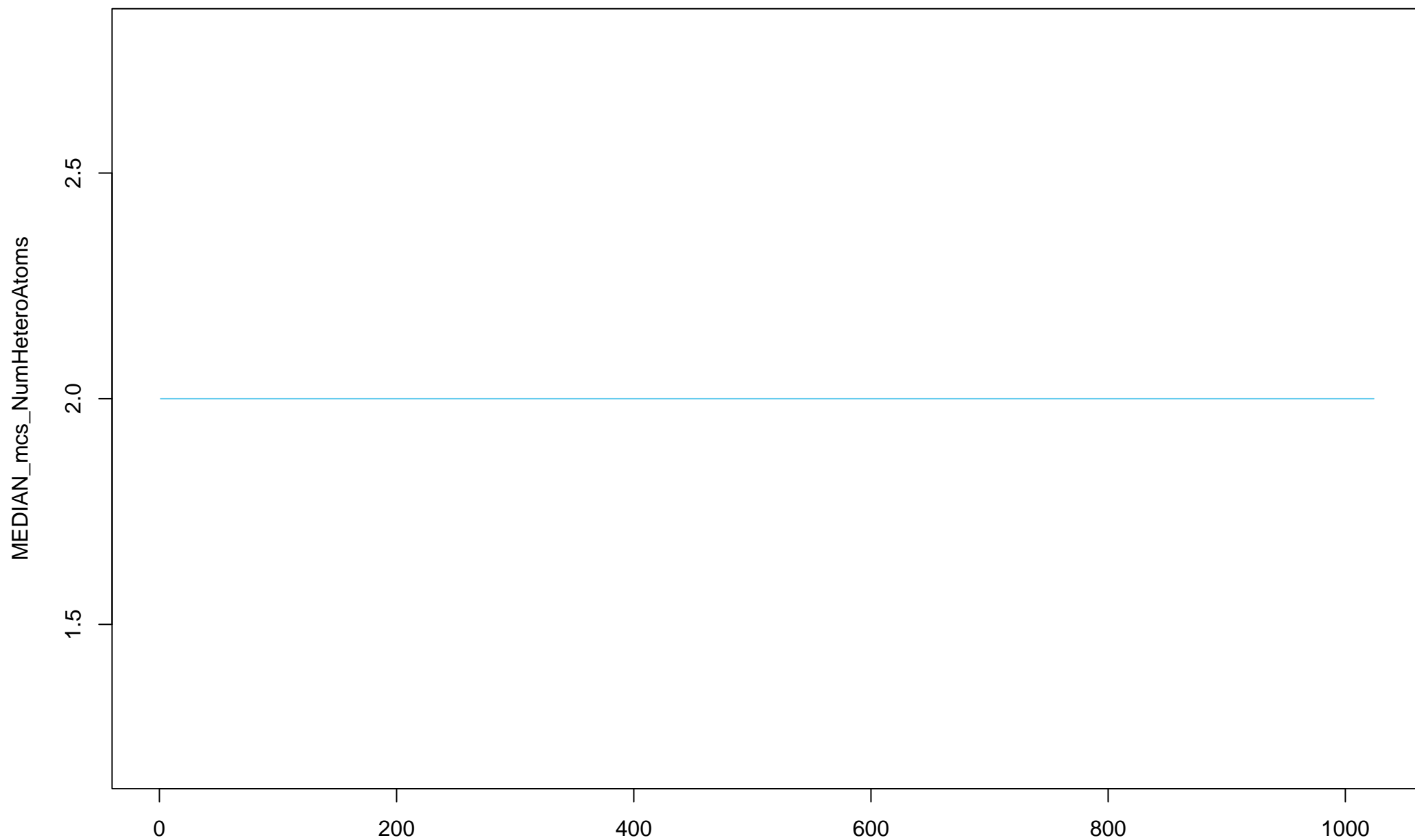




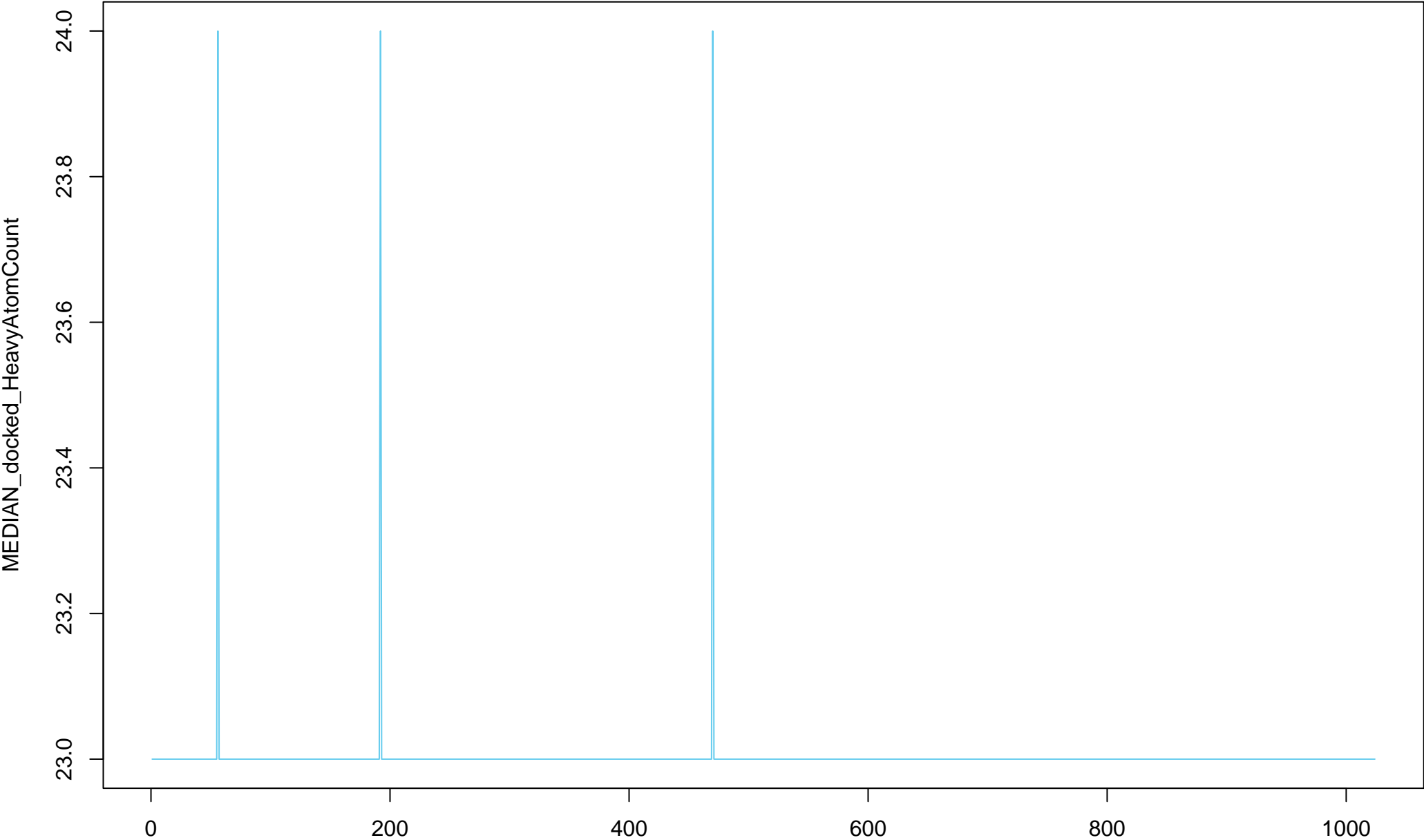
**MEDIAN\_logit\_ec\_tanimoto\_similarity**  
**ESS = 83.6 | BMK = 0.111 | MCSE(6.27) = 7.98 | stat: TRUE | burn: 0**



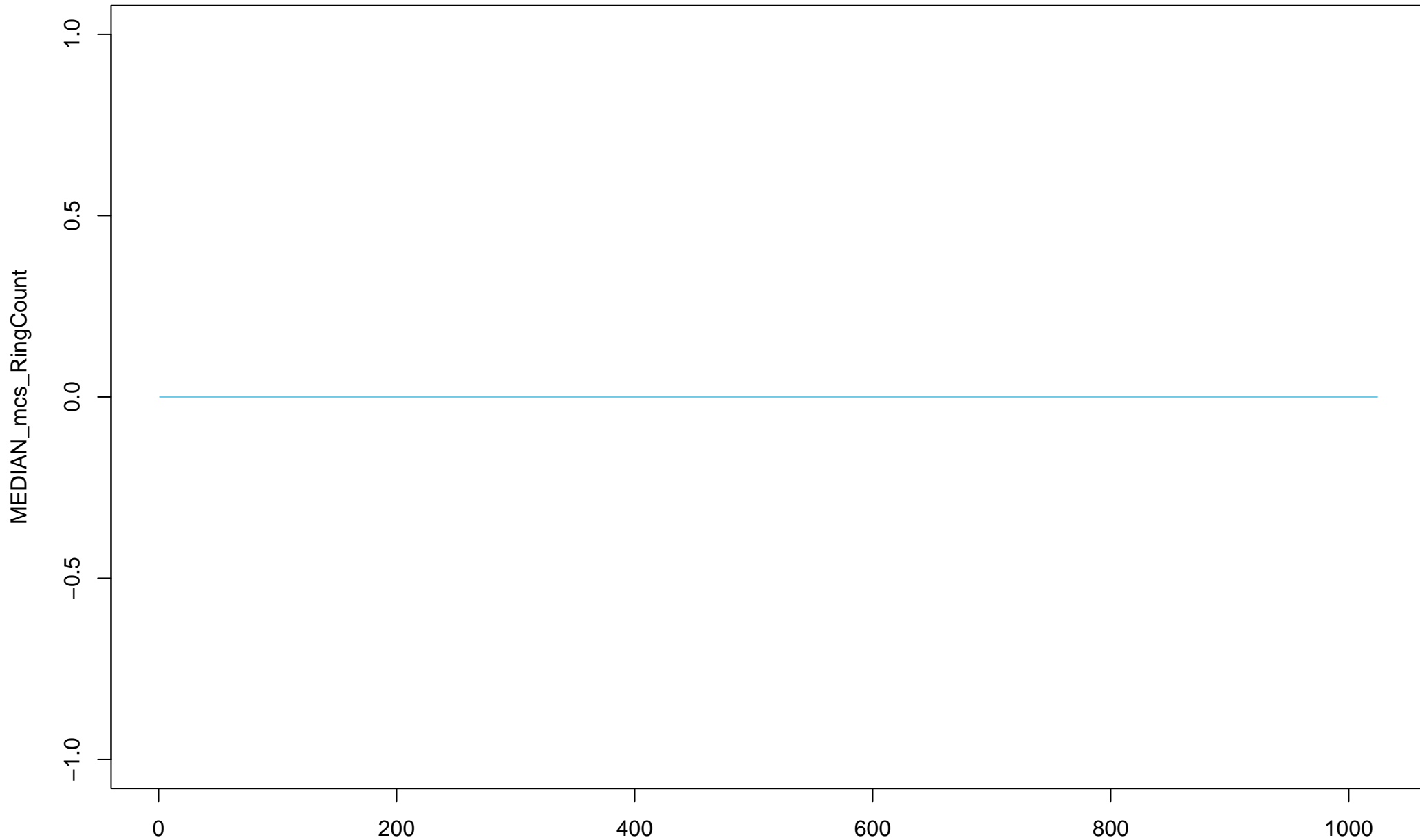
**MEDIAN\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



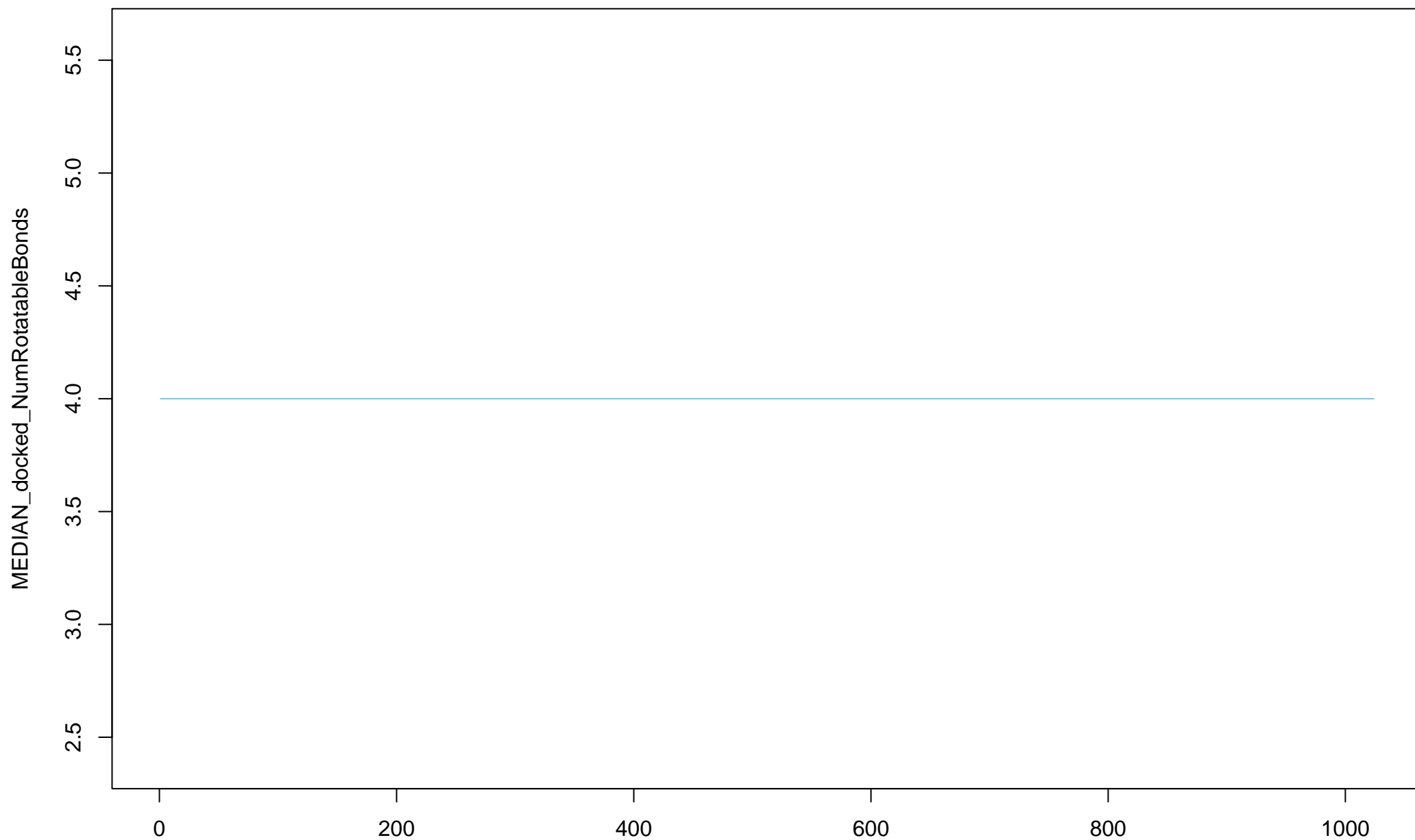
**MEDIAN\_docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.499 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0**



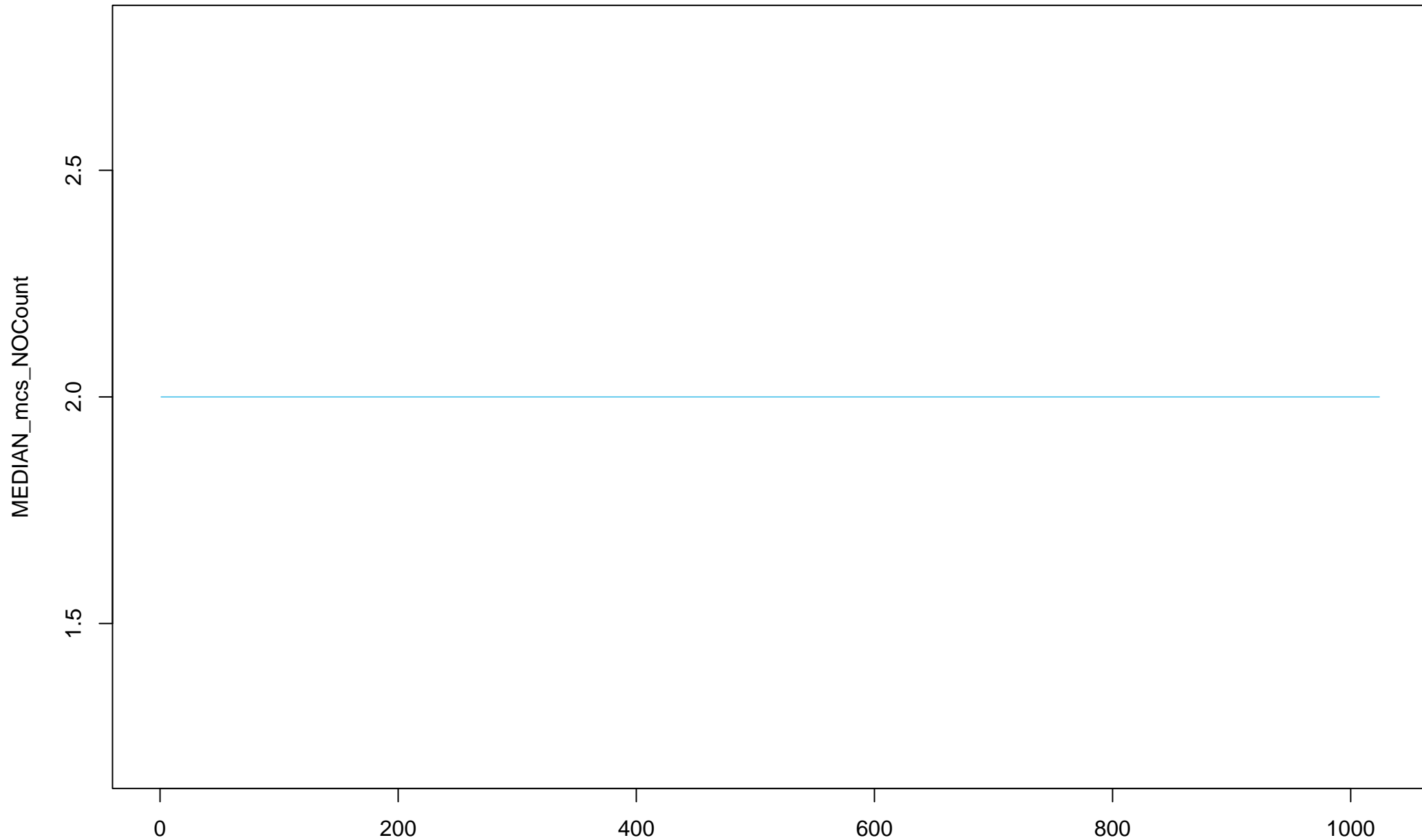
**MEDIAN\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



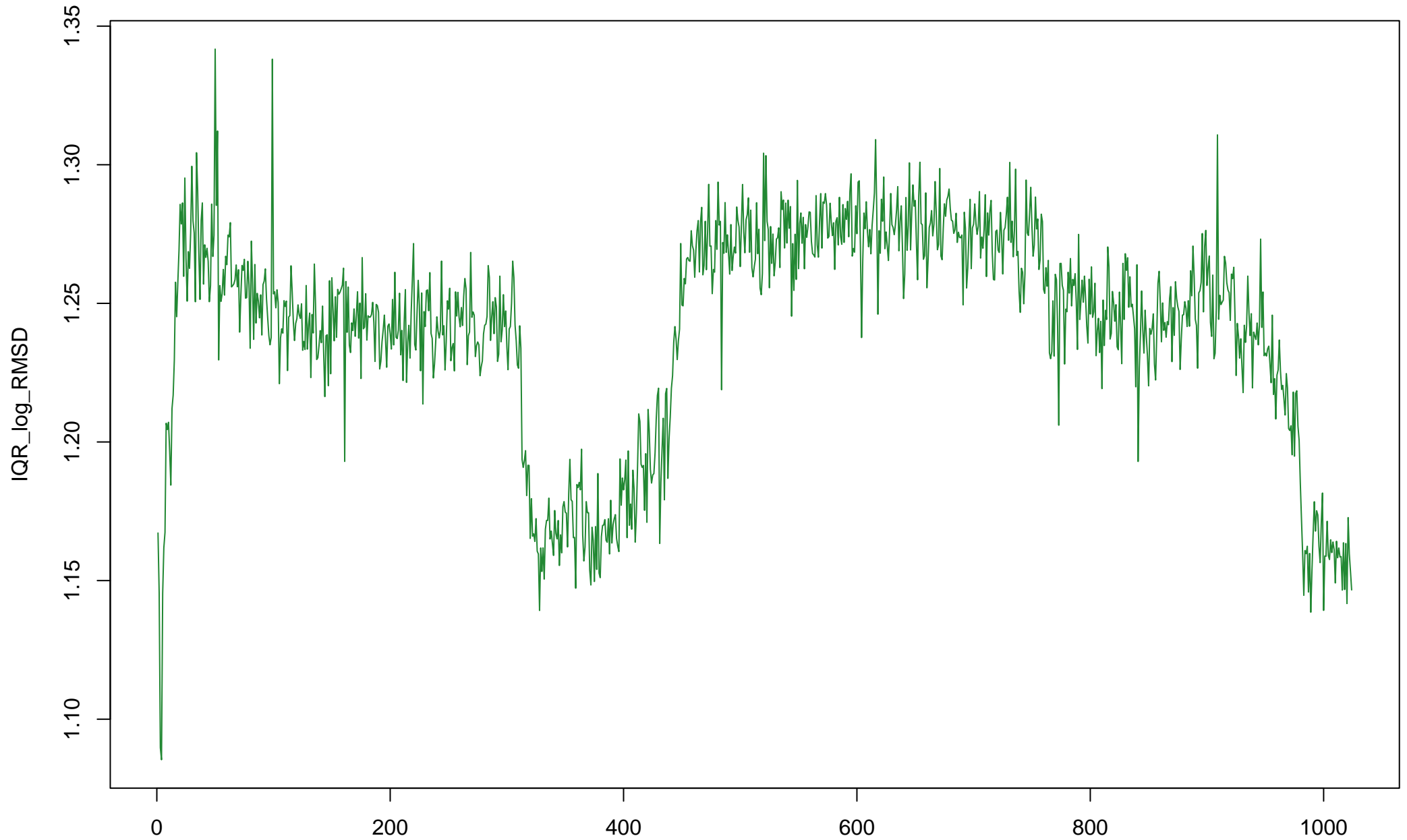
**MEDIAN\_docked\_NumRotatableBonds**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



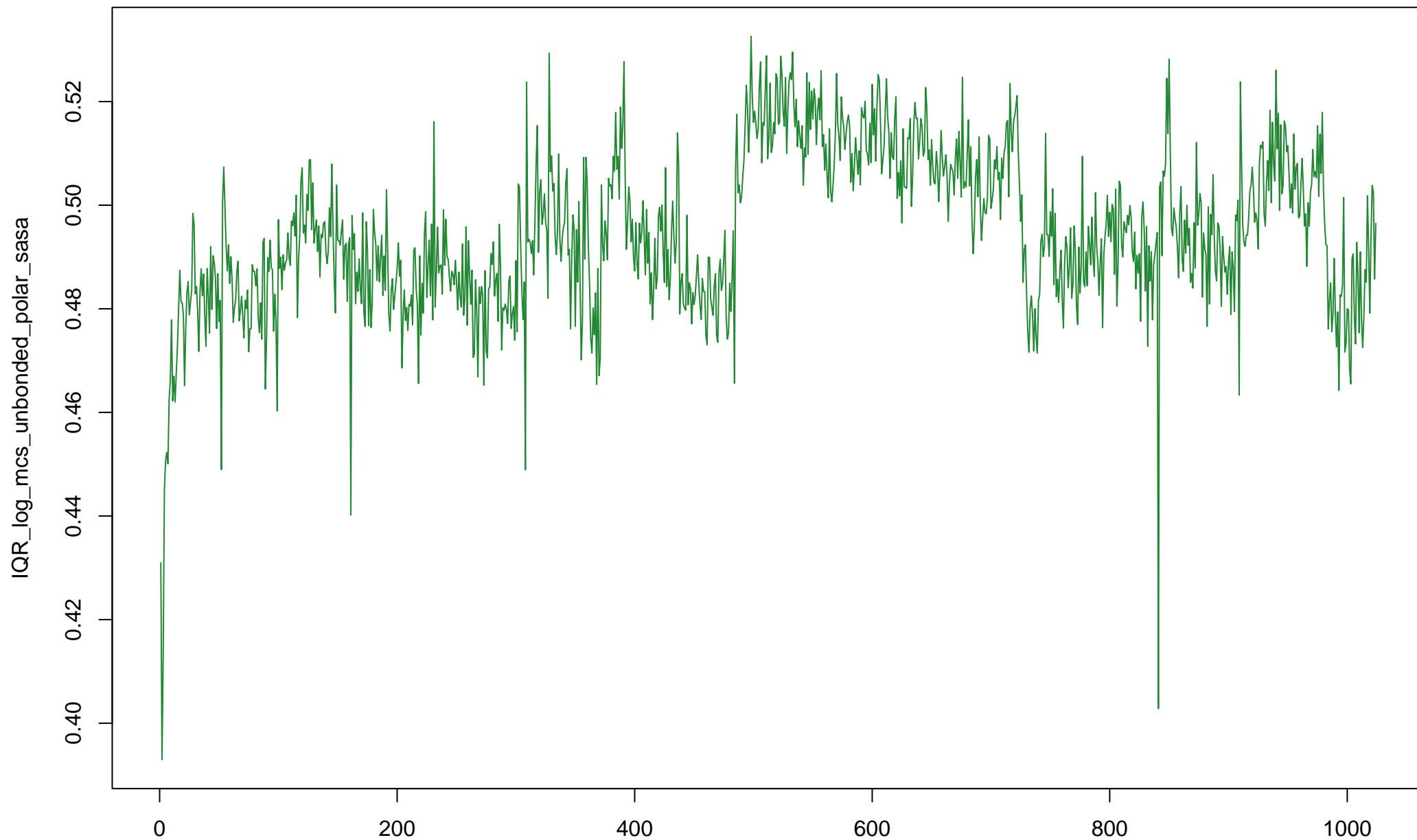
**MEDIAN\_mcs\_NOCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**IQR\_log\_RMSD**  
**ESS = 8.76 | BMK = 0.248 | MCSE(6.27) = 16 | stat: TRUE | burn: 1020**

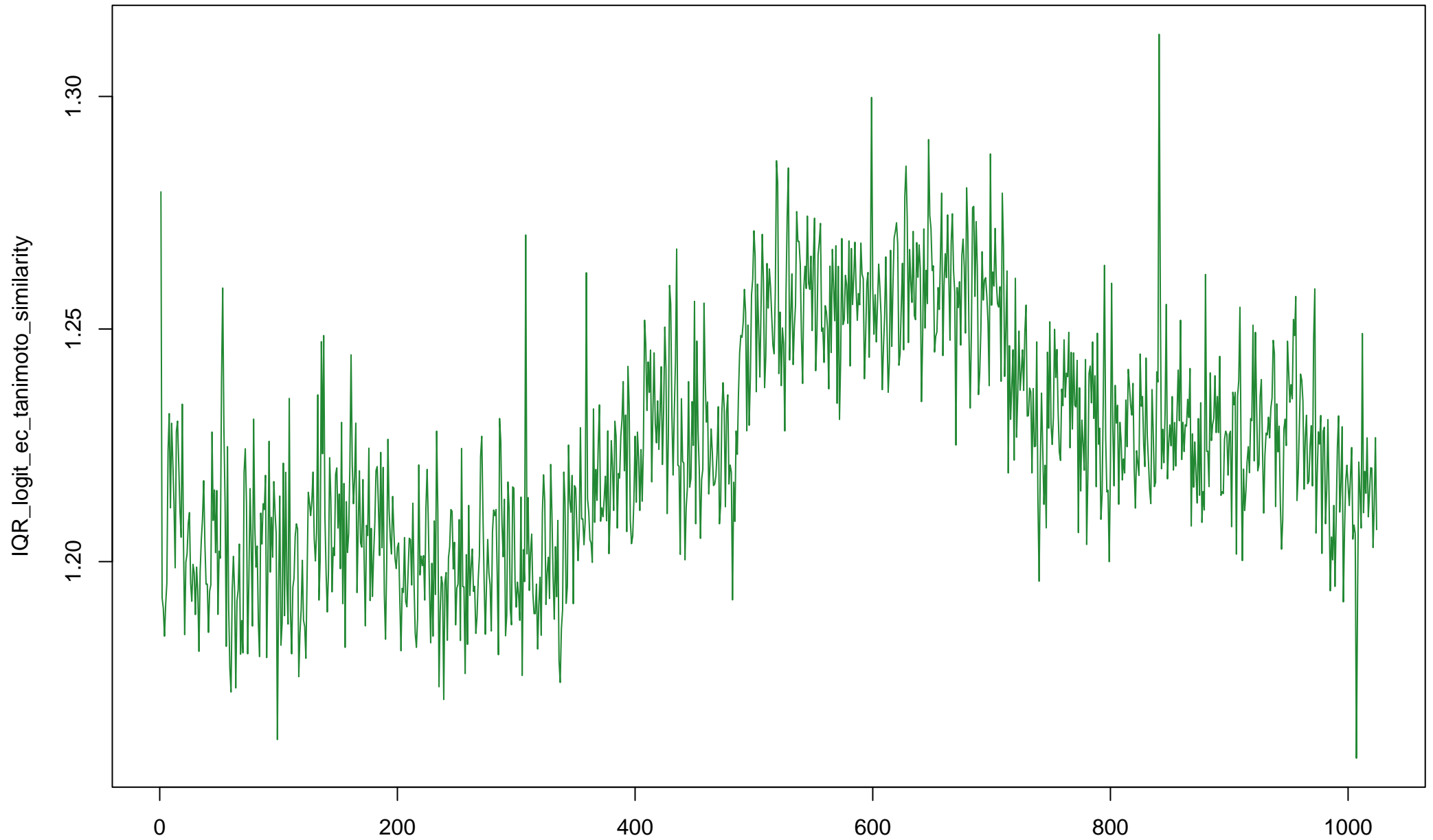


**IQR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 31.7 | BMK = 0.327 | MCSE(6.27) = 13.1 | stat: FALSE | burn: 714**

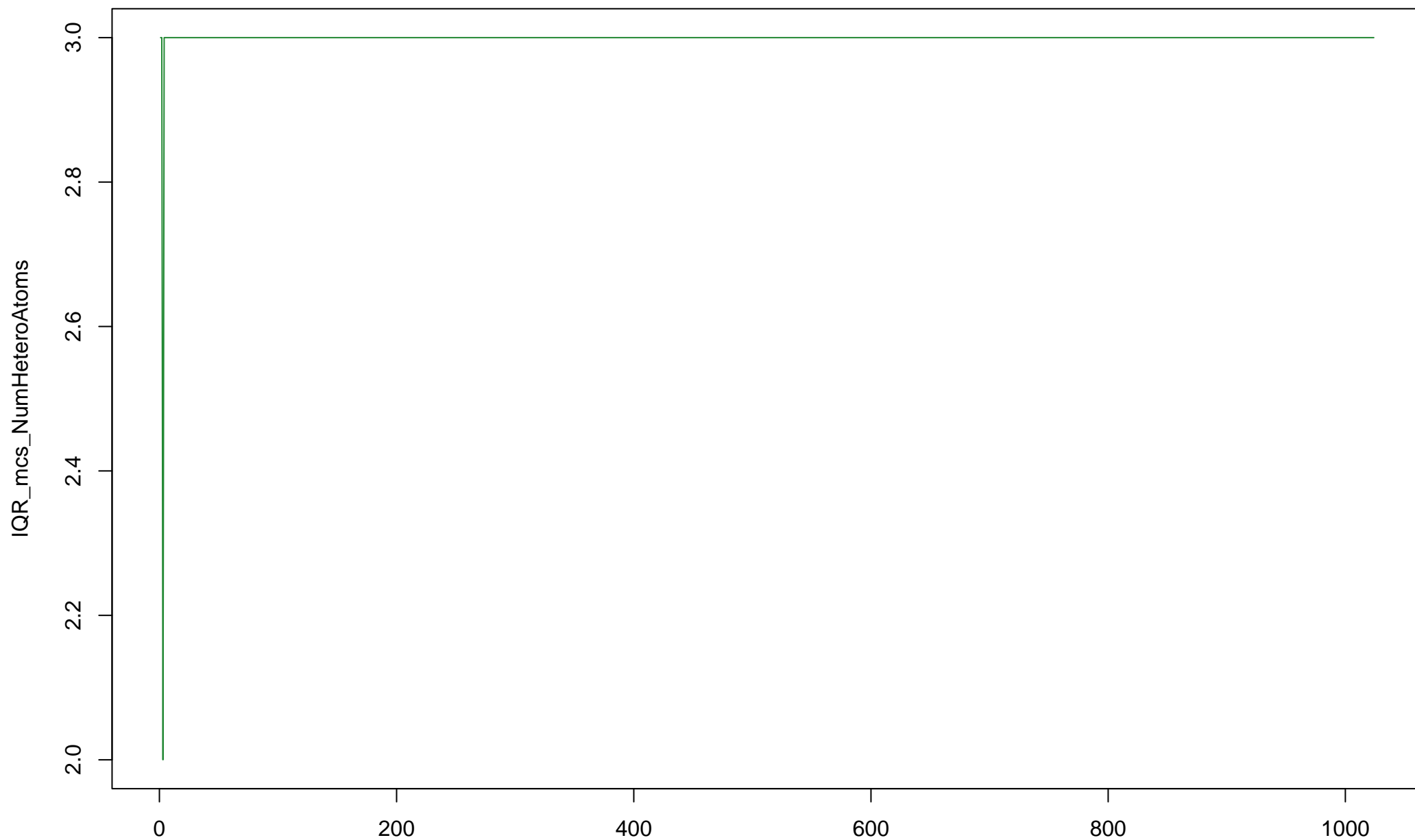




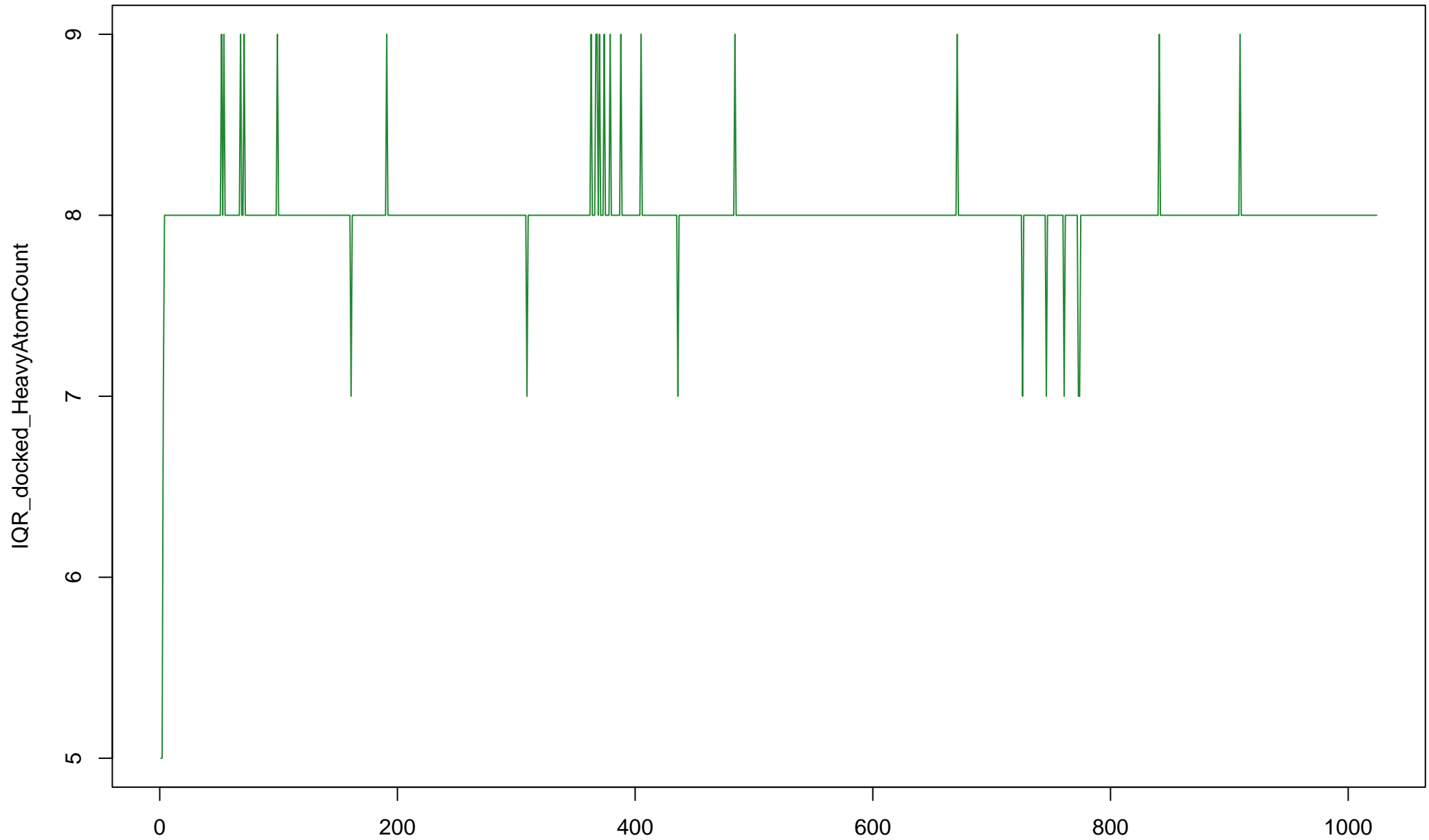
**IQR\_logit\_ec\_tanimoto\_similarity**  
**ESS = 3.22 | BMK = 0.47 | MCSE(6.27) = 14.7 | stat: FALSE | burn: 714**



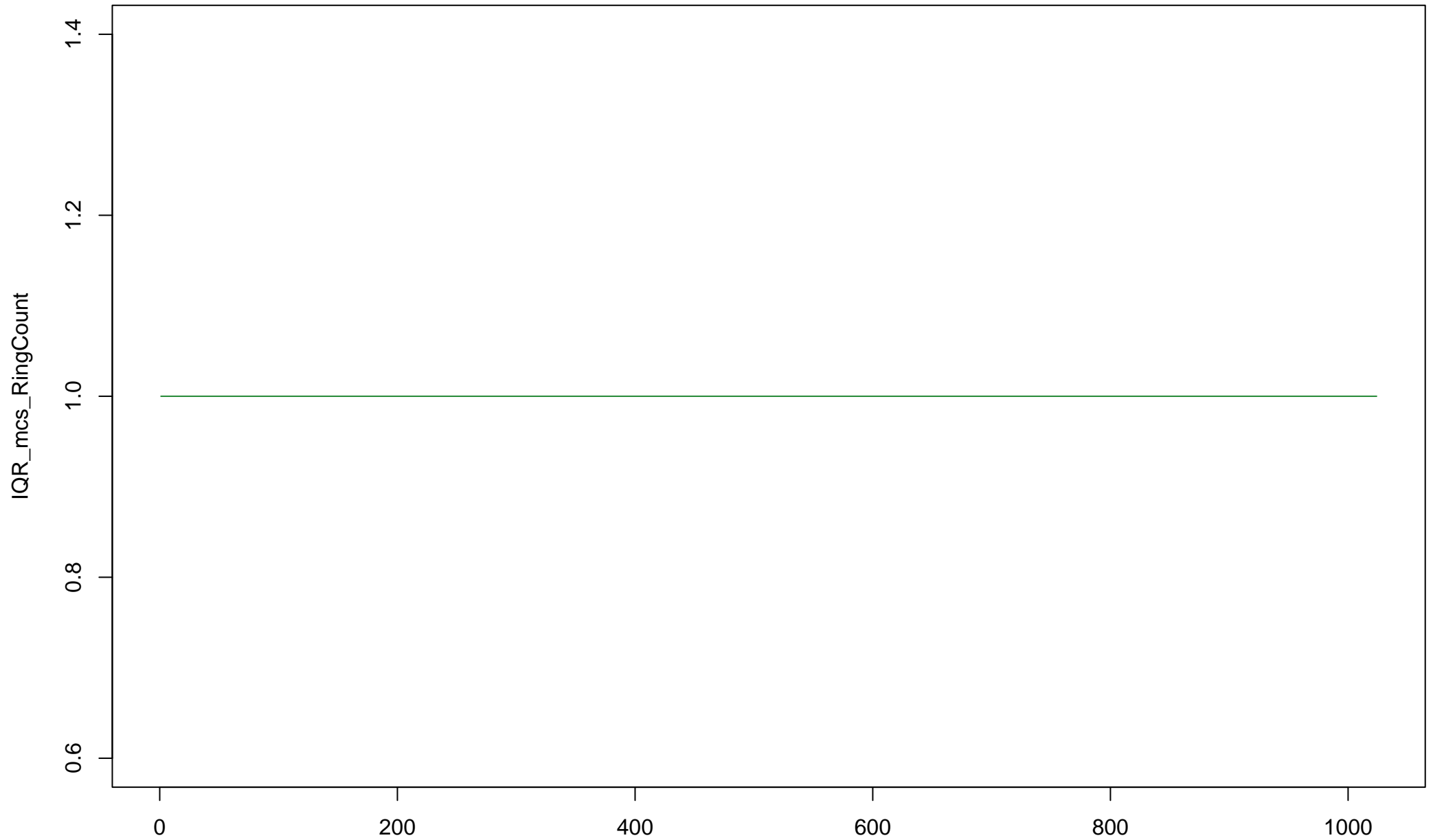
**IQR\_mcs\_NumHeteroAtoms**  
**ESS = 1020 | BMK = 0.613 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102**



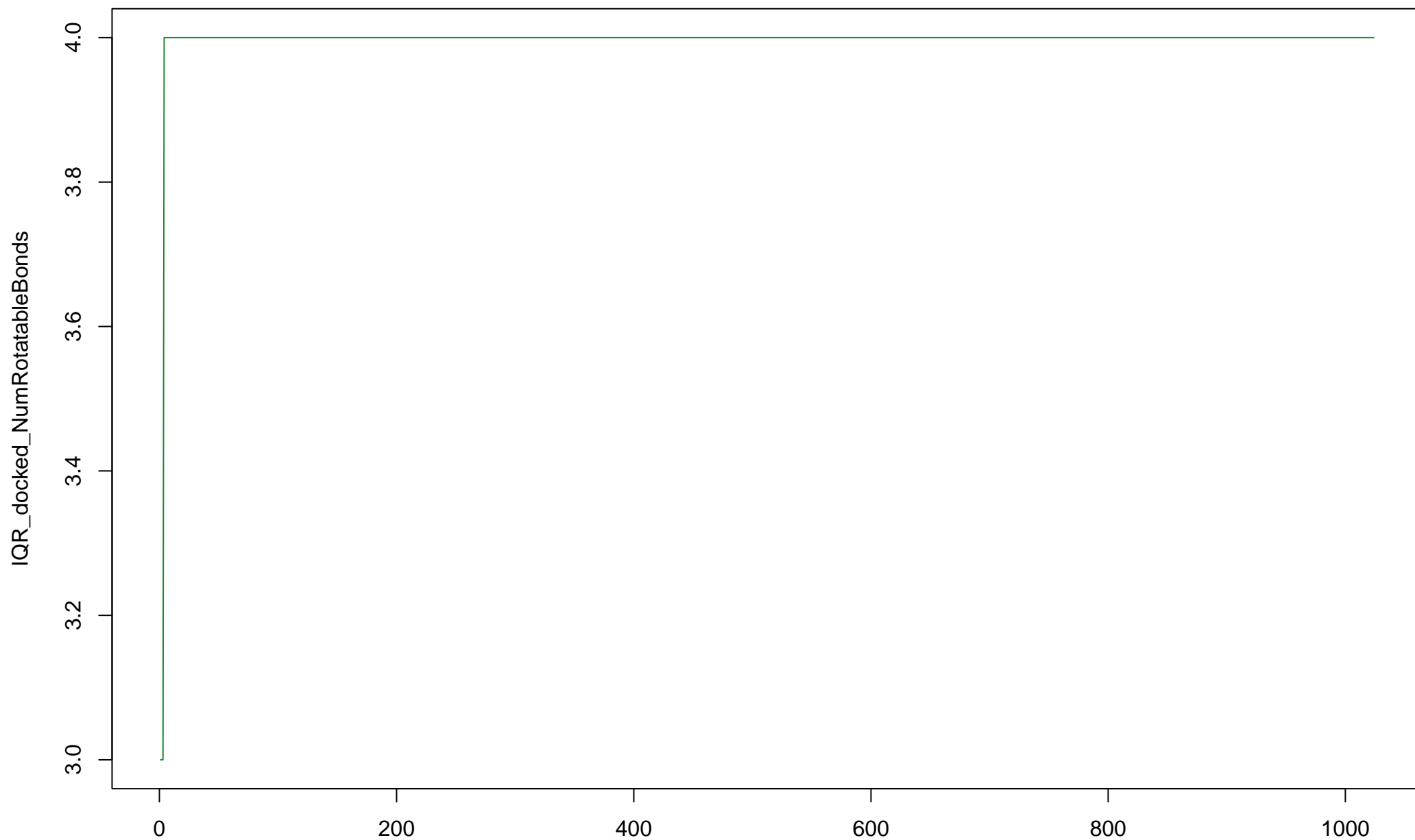
**IQR\_docked\_HeavyAtomCount**  
**ESS = 538 | BMK = 0.353 | MCSE(6.27) = 5.02 | stat: TRUE | burn: 612**



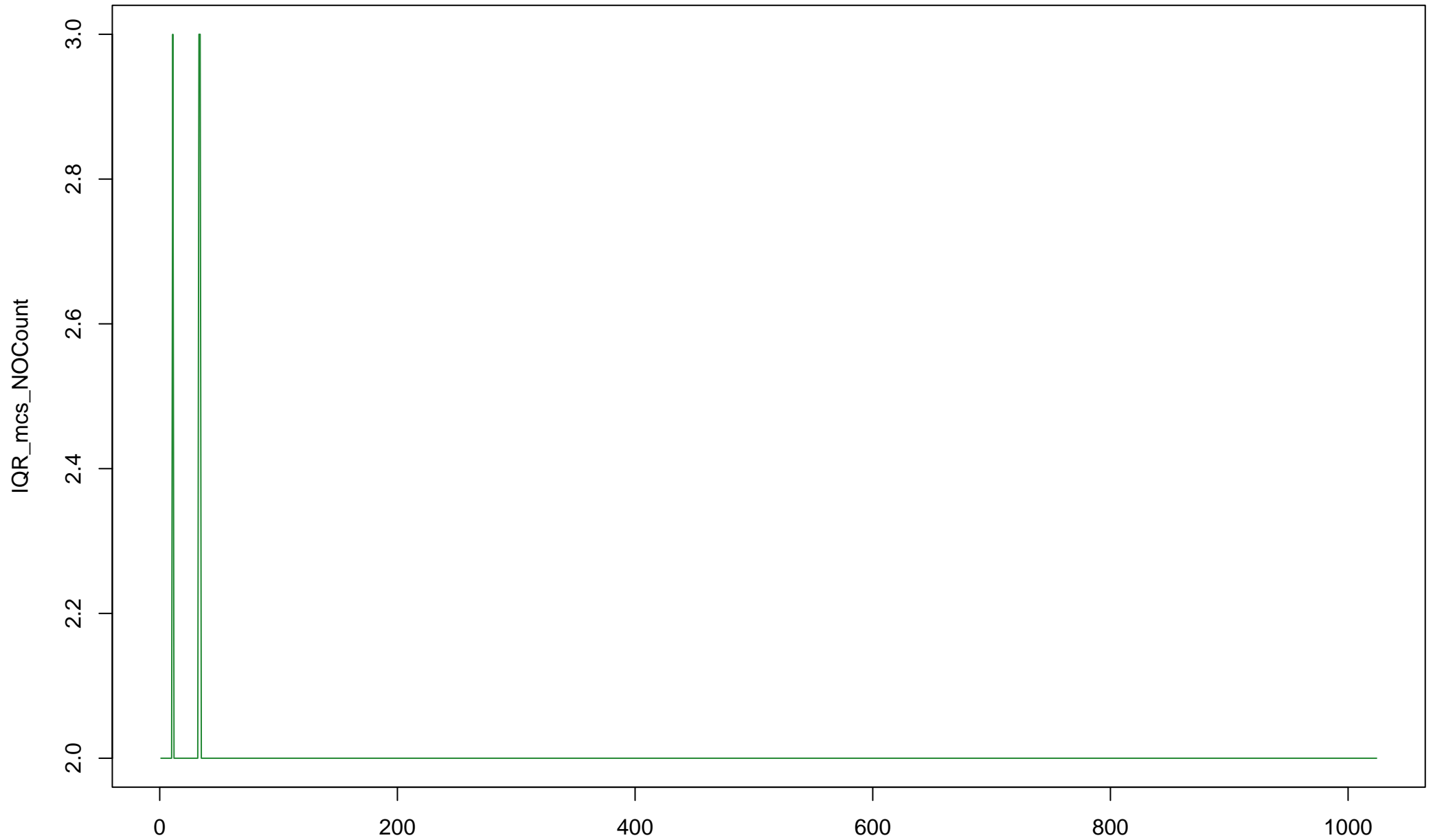
**IQR\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



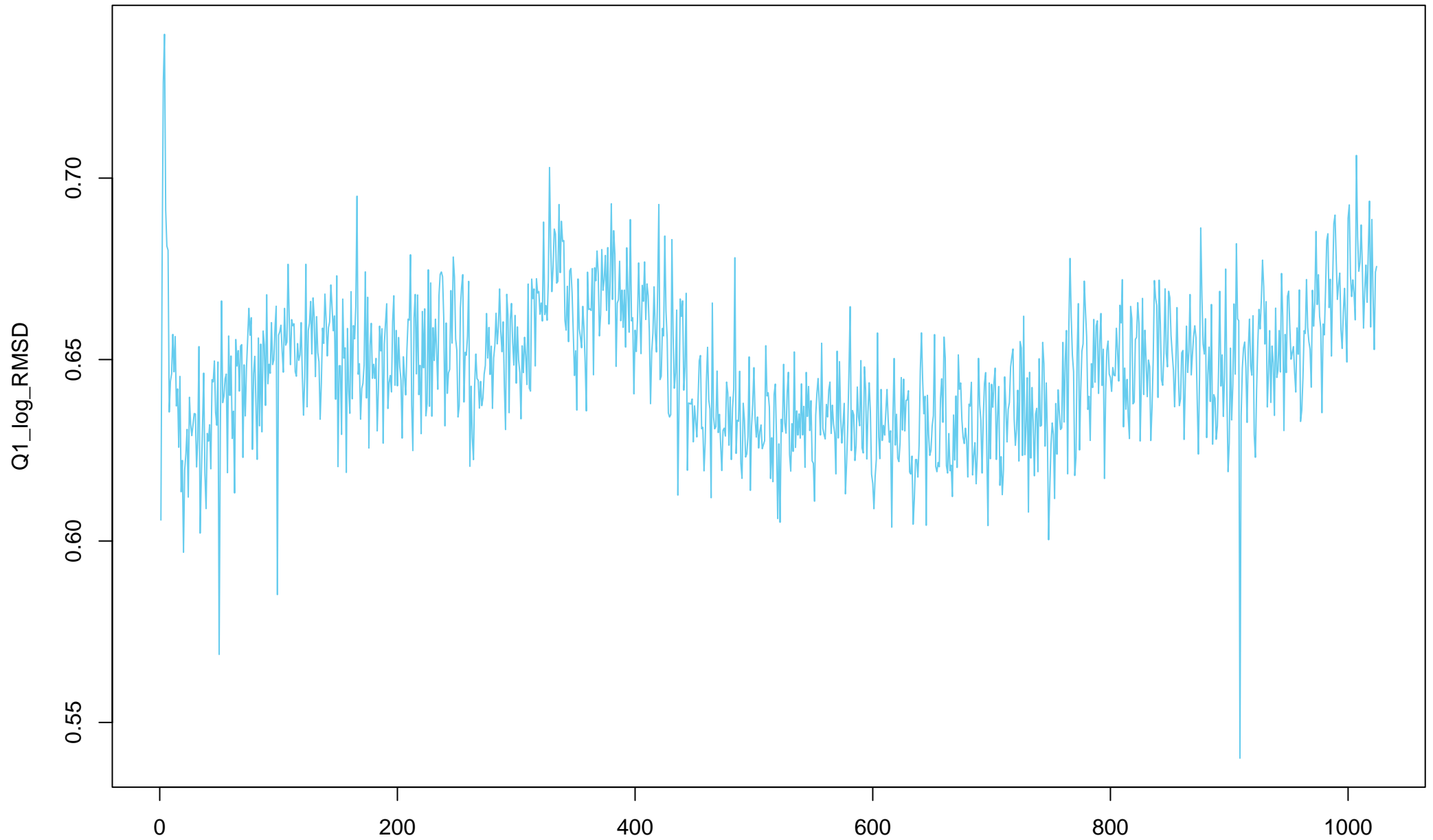
**IQR\_docked\_NumRotatableBonds**  
**ESS = 312 | BMK = 0.566 | MCSE(6.27) = 5.42 | stat: TRUE | burn: 0**



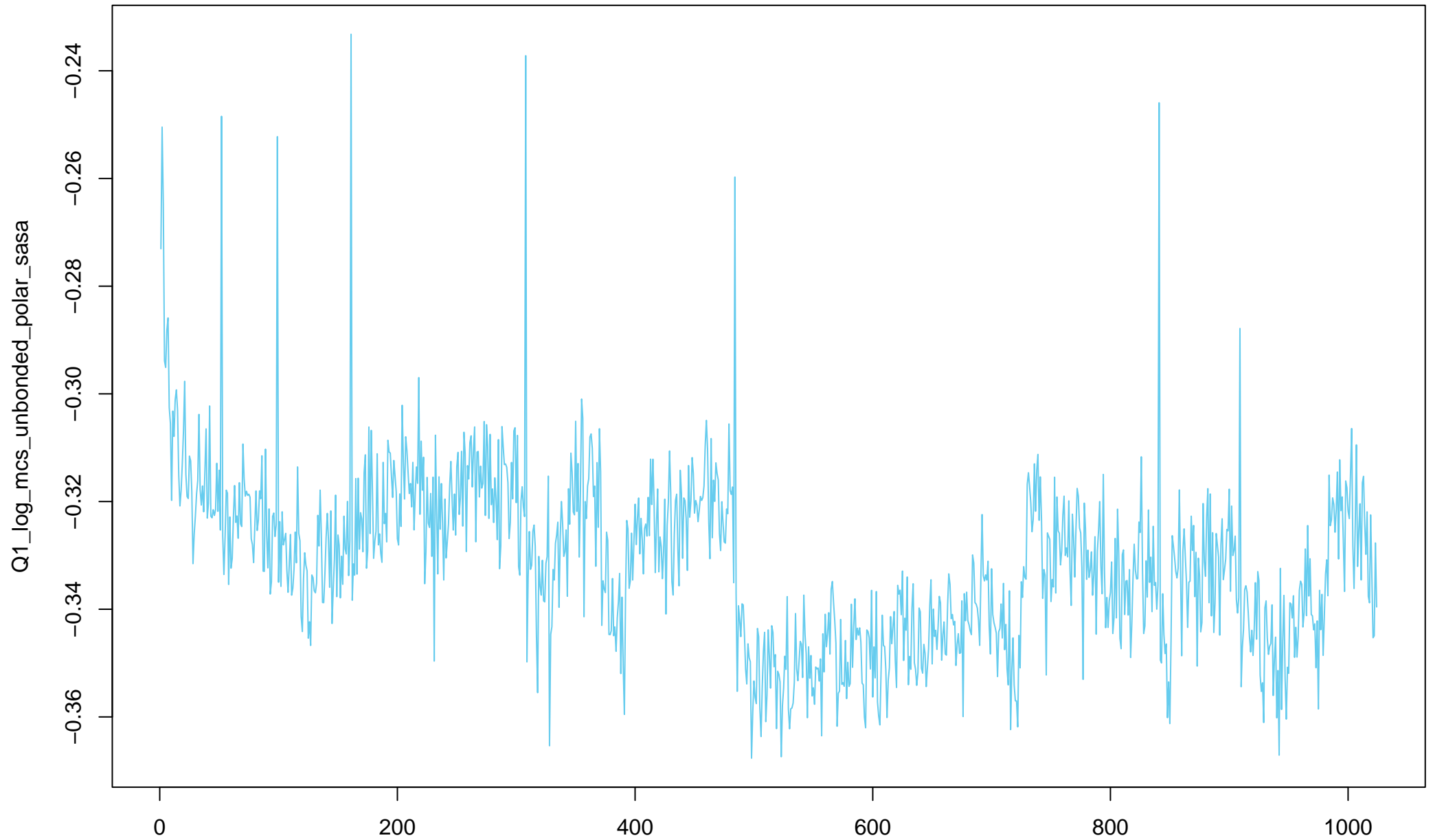
**IQR\_mcs\_NOCCount**  
**ESS = 258 | BMK = 0.593 | MCSE(6.27) = 3.99 | stat: TRUE | burn: 0**



**Q1\_log\_RMSD**  
**ESS = 23.8 | BMK = 0.158 | MCSE(6.27) = 11.5 | stat: TRUE | burn: 408**

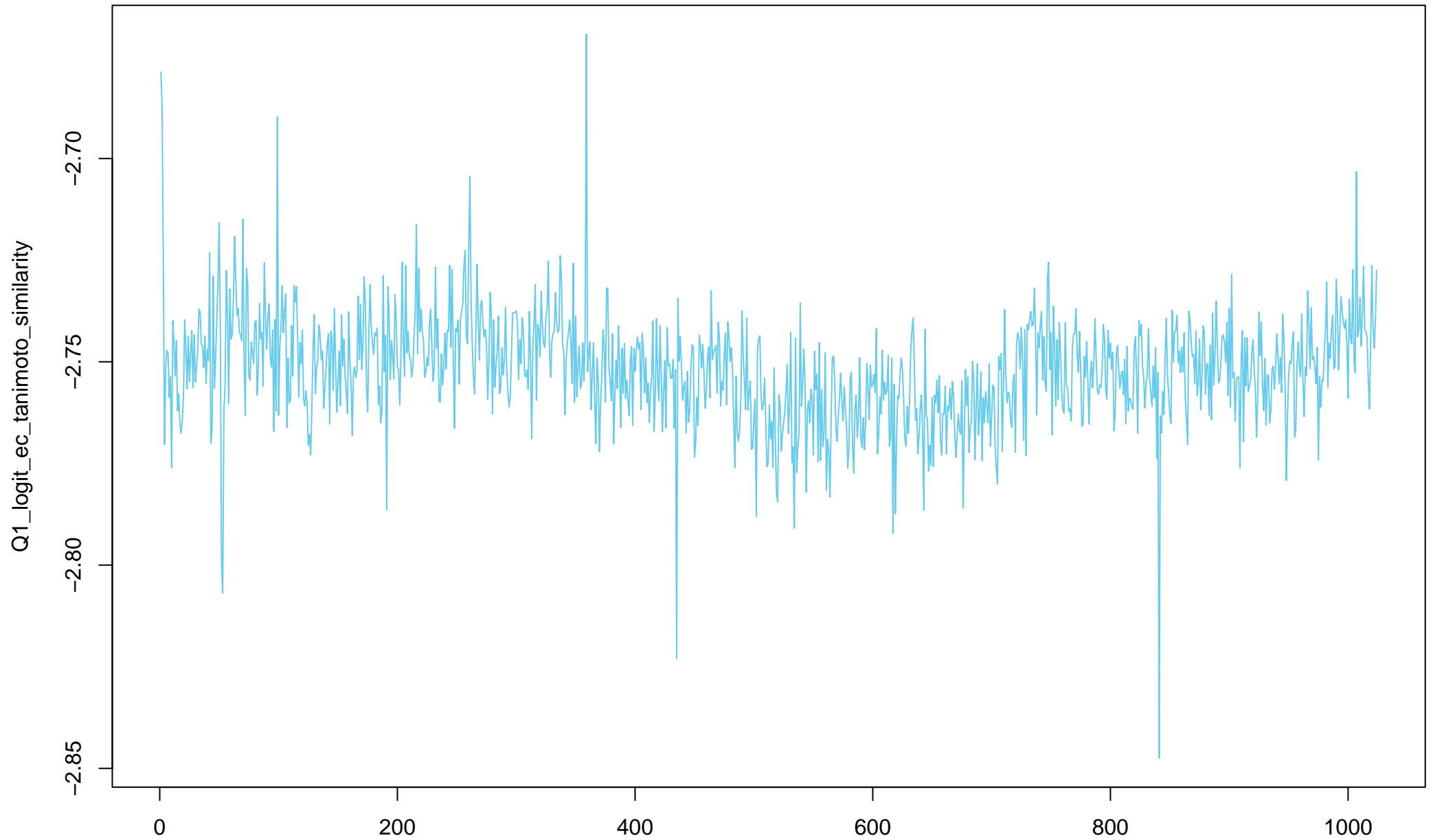


**Q1\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 29.8 | BMK = 0.41 | MCSE(6.27) = 12.5 | stat: FALSE | burn: 510**

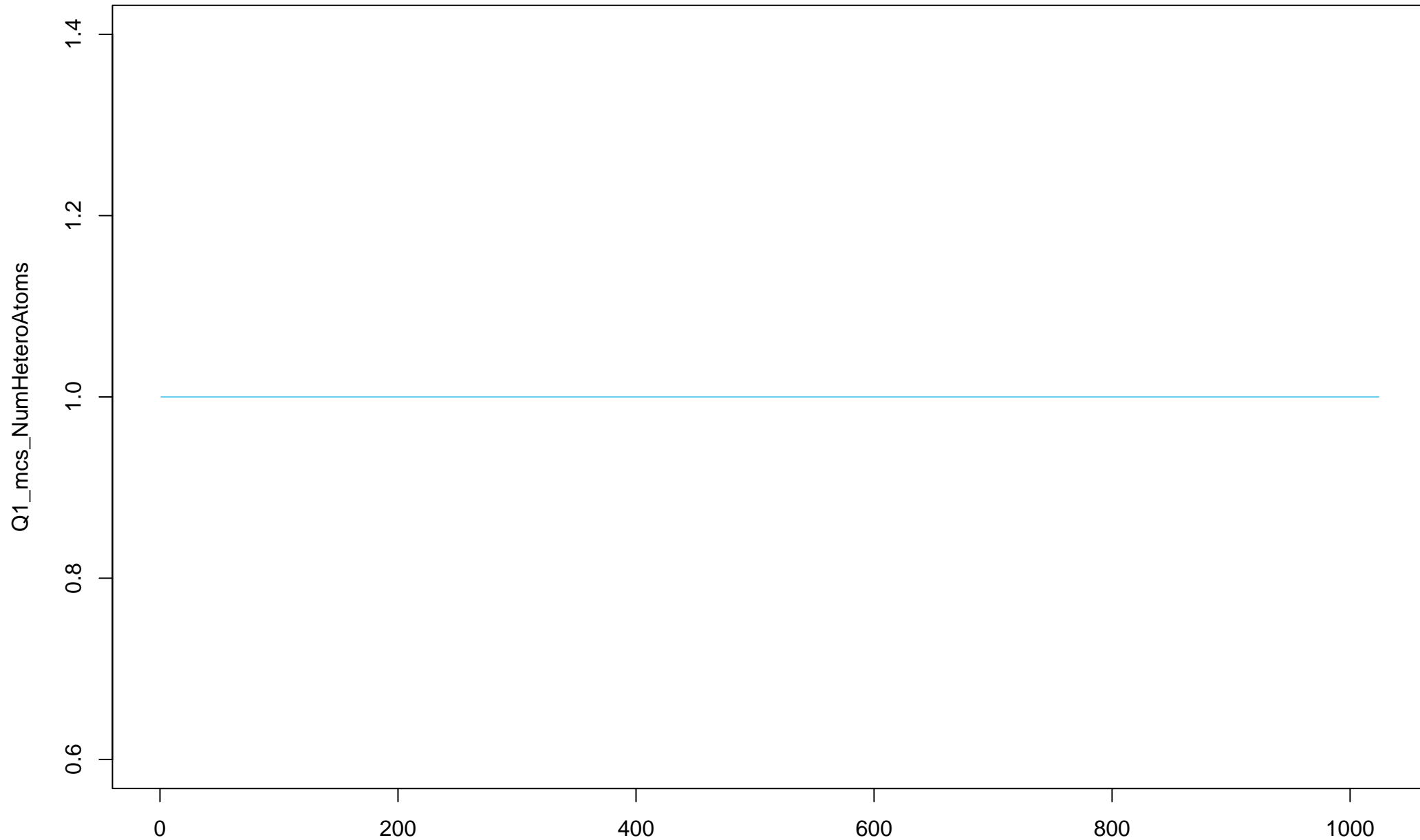




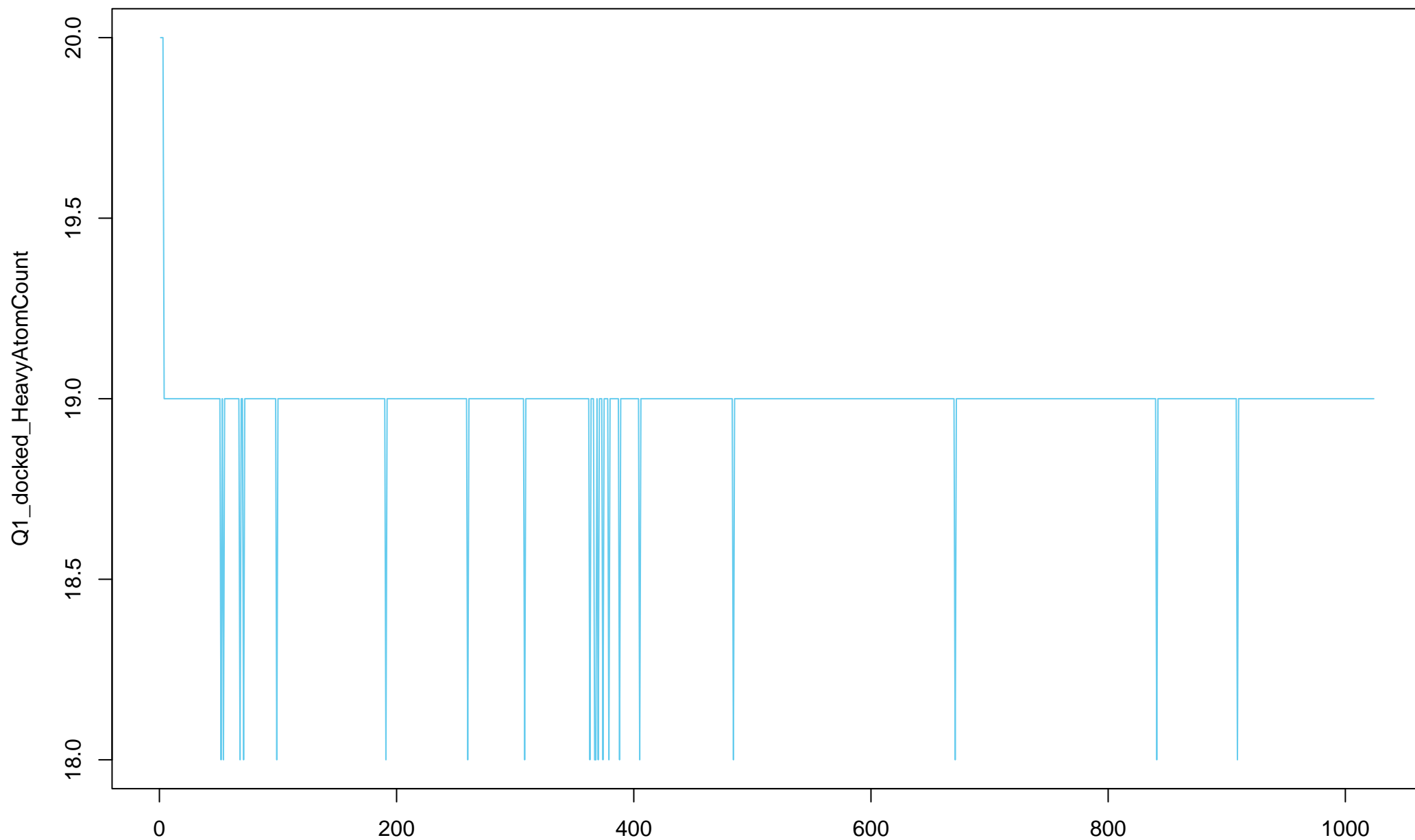
**Q1\_logit\_ec\_tanimoto\_similarity**  
**ESS = 56.8 | BMK = 0.207 | MCSE(6.27) = 8.72 | stat: FALSE | burn: 0**



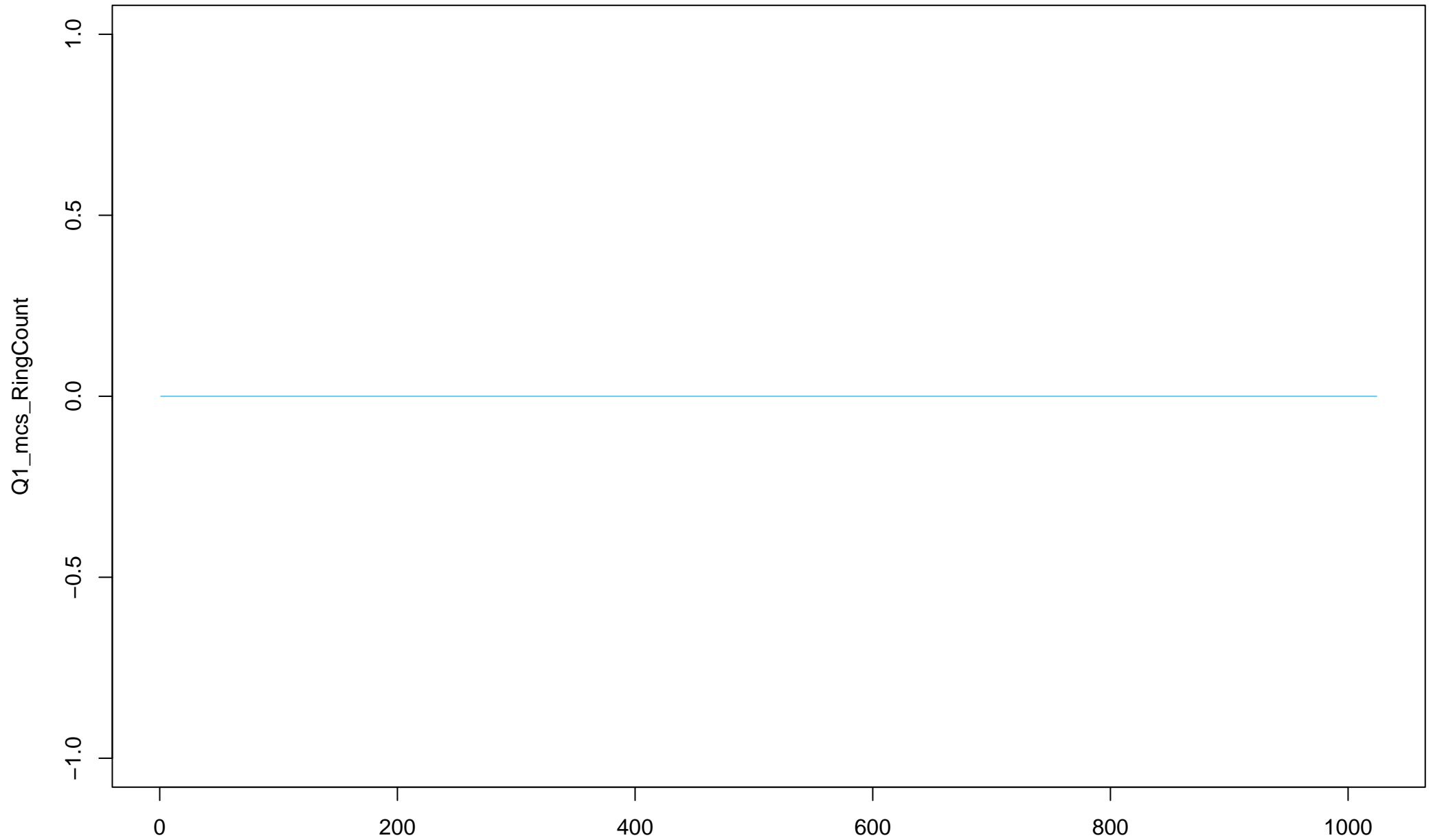
**Q1\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



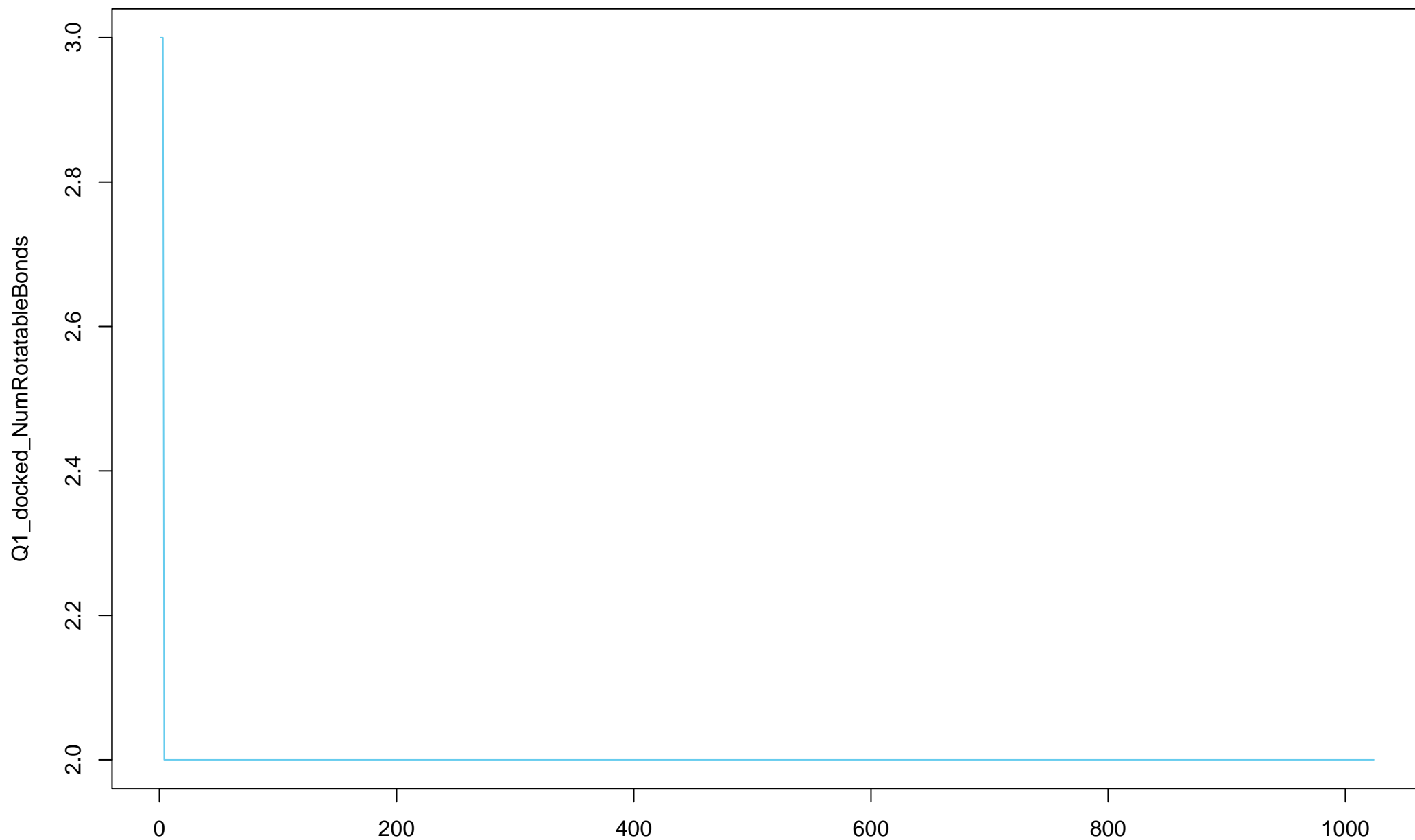
**Q1\_docked\_HeavyAtomCount**  
**ESS = 297 | BMK = 0.421 | MCSE(6.27) = 4.98 | stat: TRUE | burn: 0**



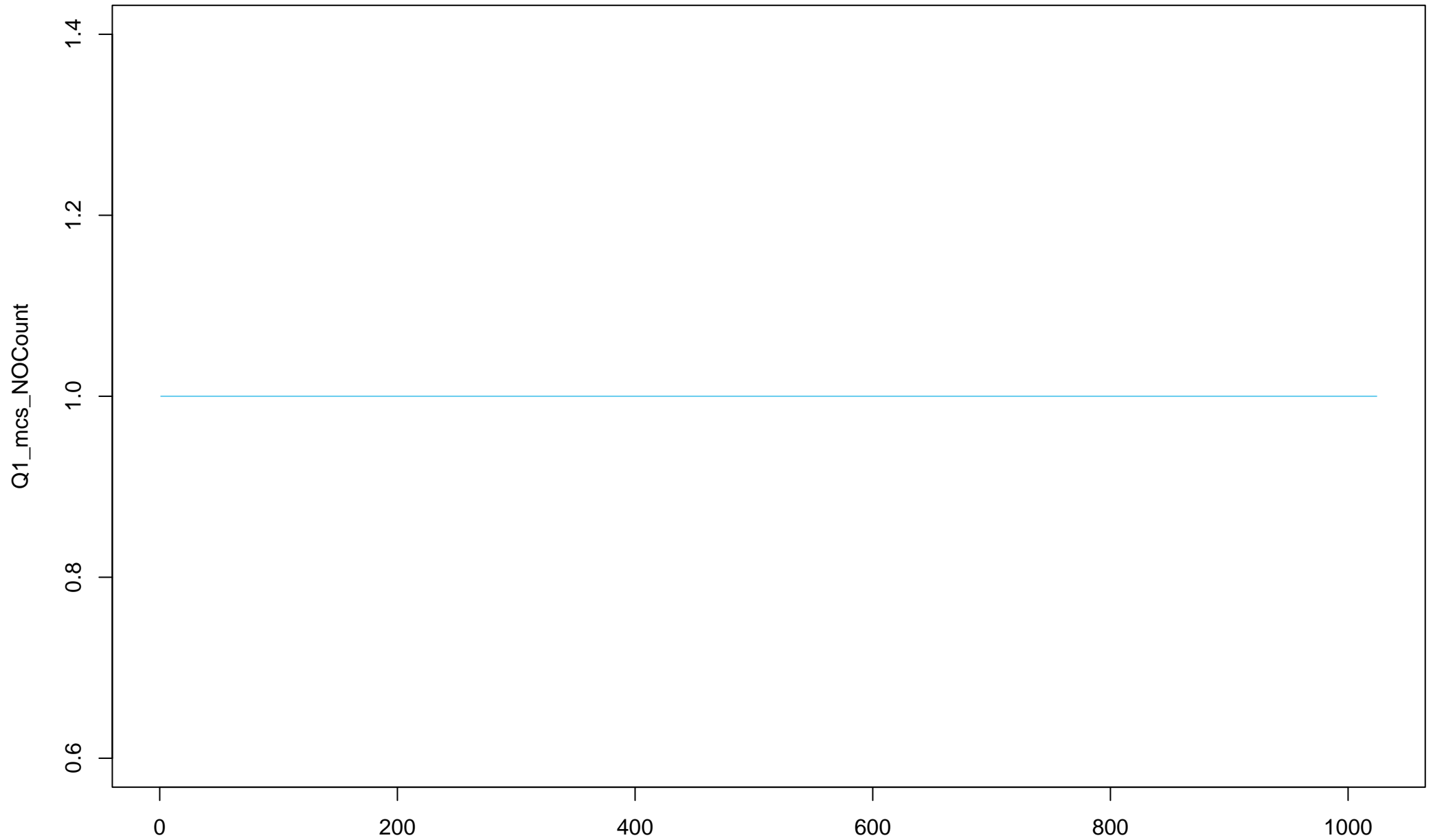
**Q1\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



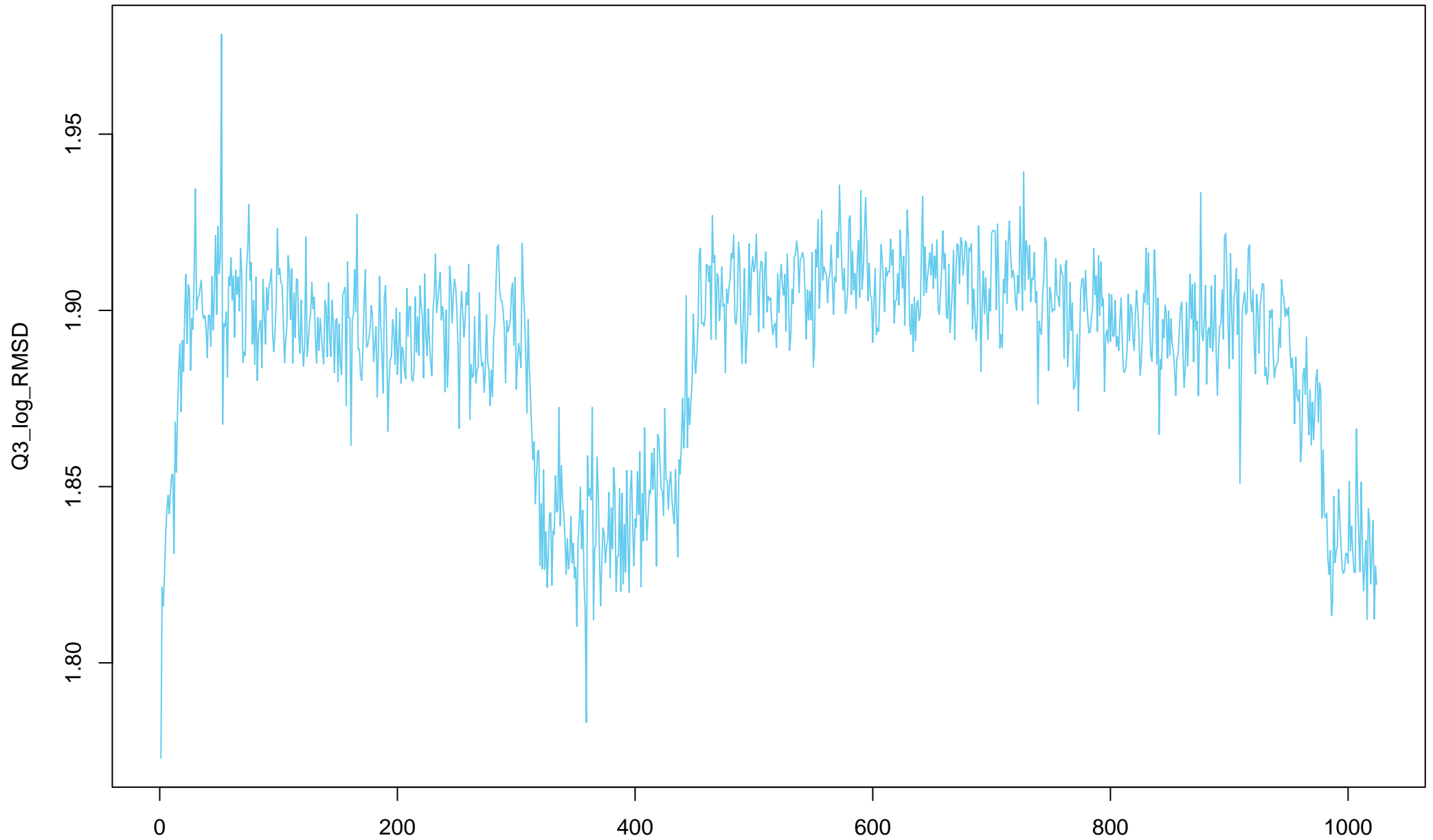
**Q1\_docked\_NumRotatableBonds**  
**ESS = 312 | BMK = 0.593 | MCSE(6.27) = 5.42 | stat: TRUE | burn: 0**



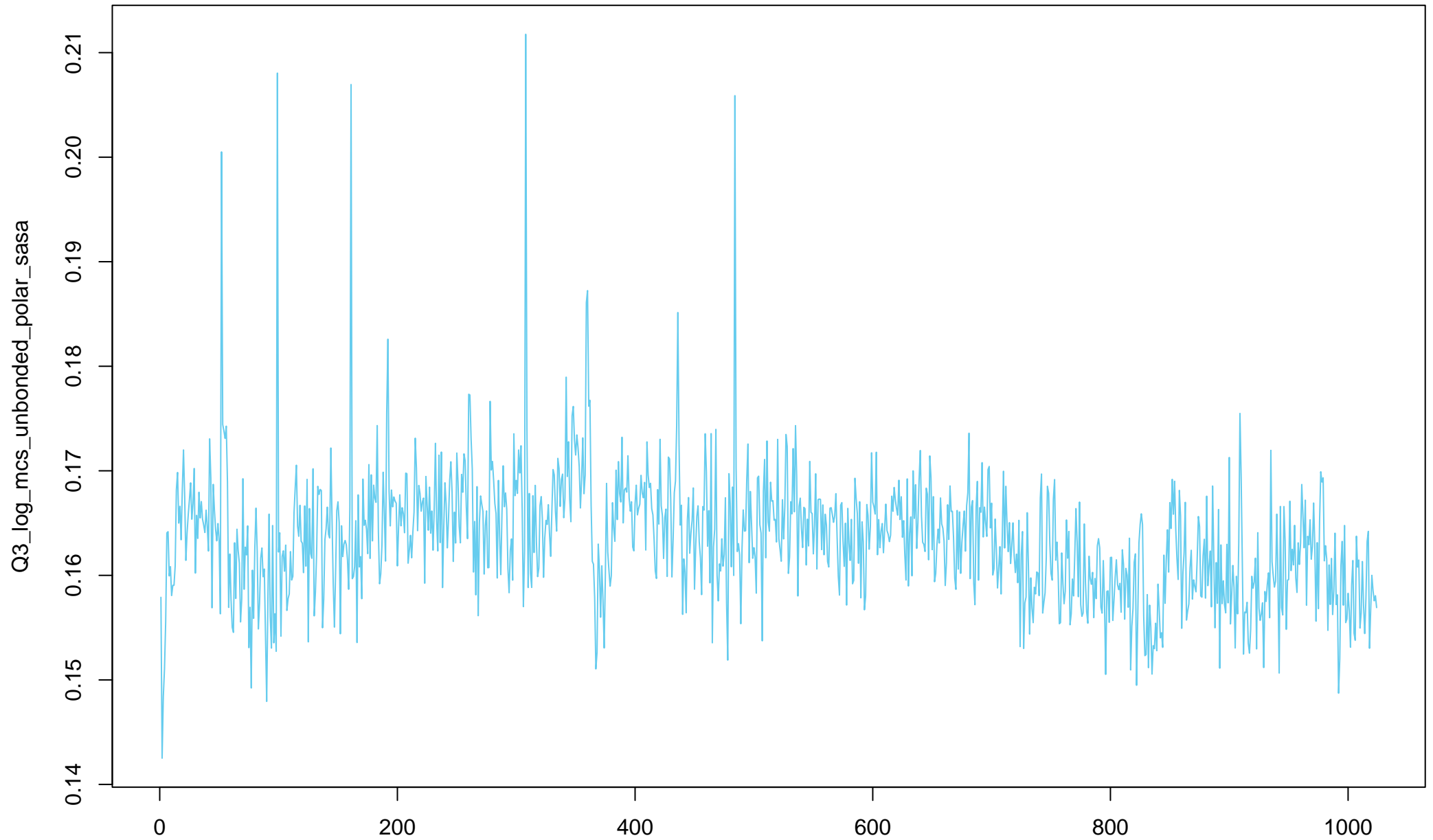
**Q1\_mcs\_NOCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q3\_log\_RMSD**  
**ESS = 9.44 | BMK = 0.207 | MCSE(6.27) = 15.5 | stat: TRUE | burn: 1020**

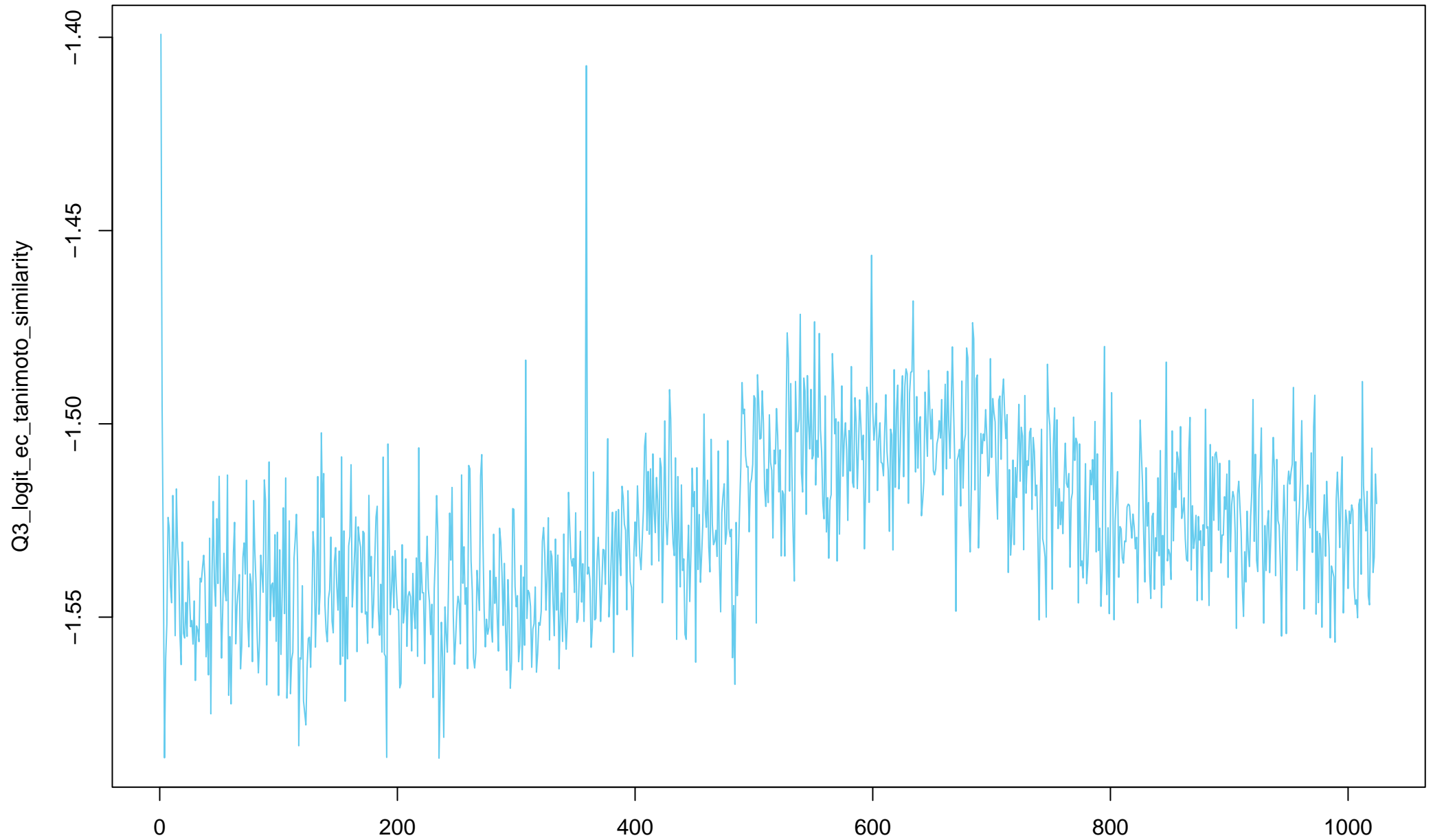


**Q3\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 70.6 | BMK = 0.223 | MCSE(6.27) = 8.47 | stat: TRUE | burn: 0**

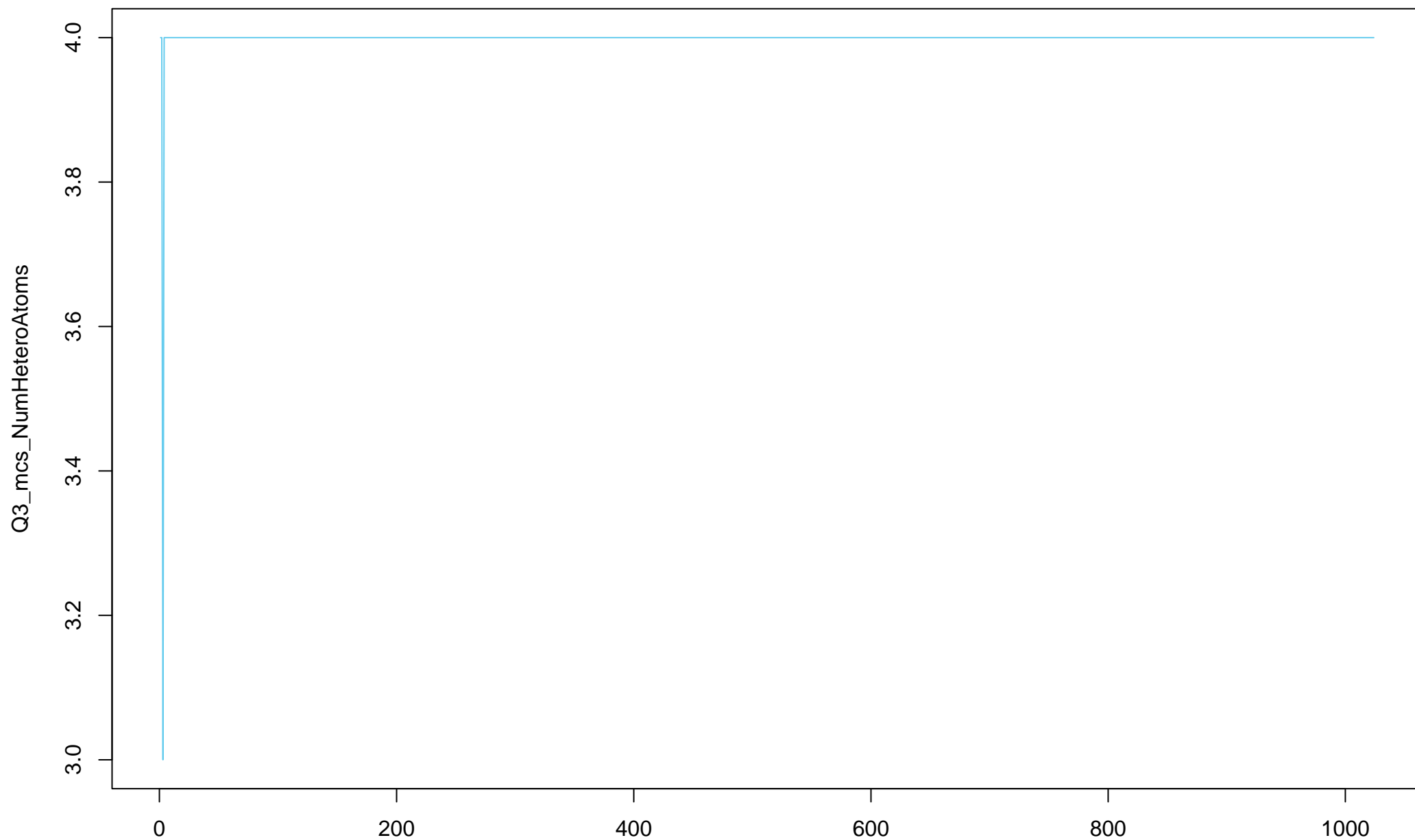




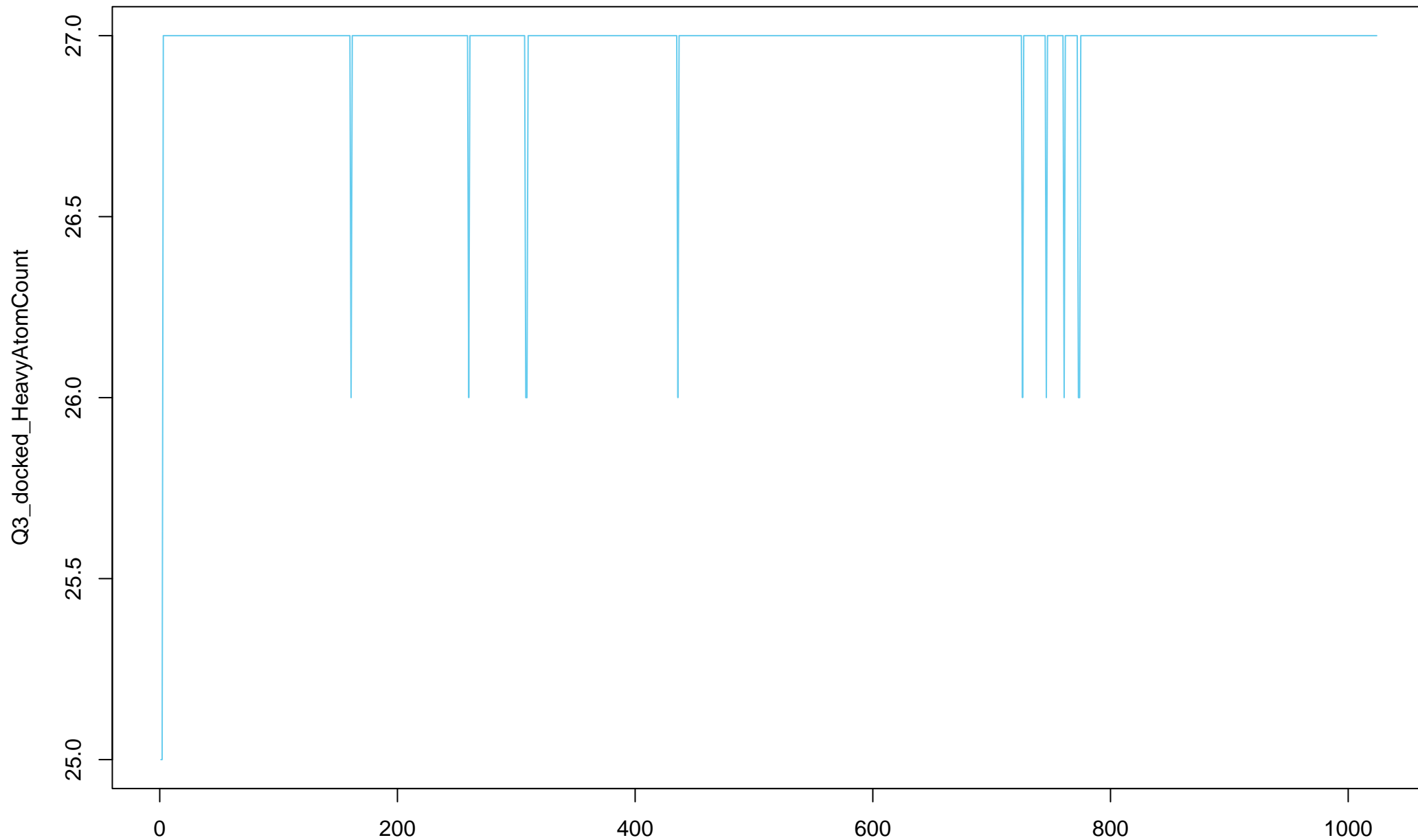
**Q3\_logit\_ec\_tanimoto\_similarity**  
**ESS = 10.4 | BMK = 0.423 | MCSE(6.27) = 12 | stat: FALSE | burn: 0**



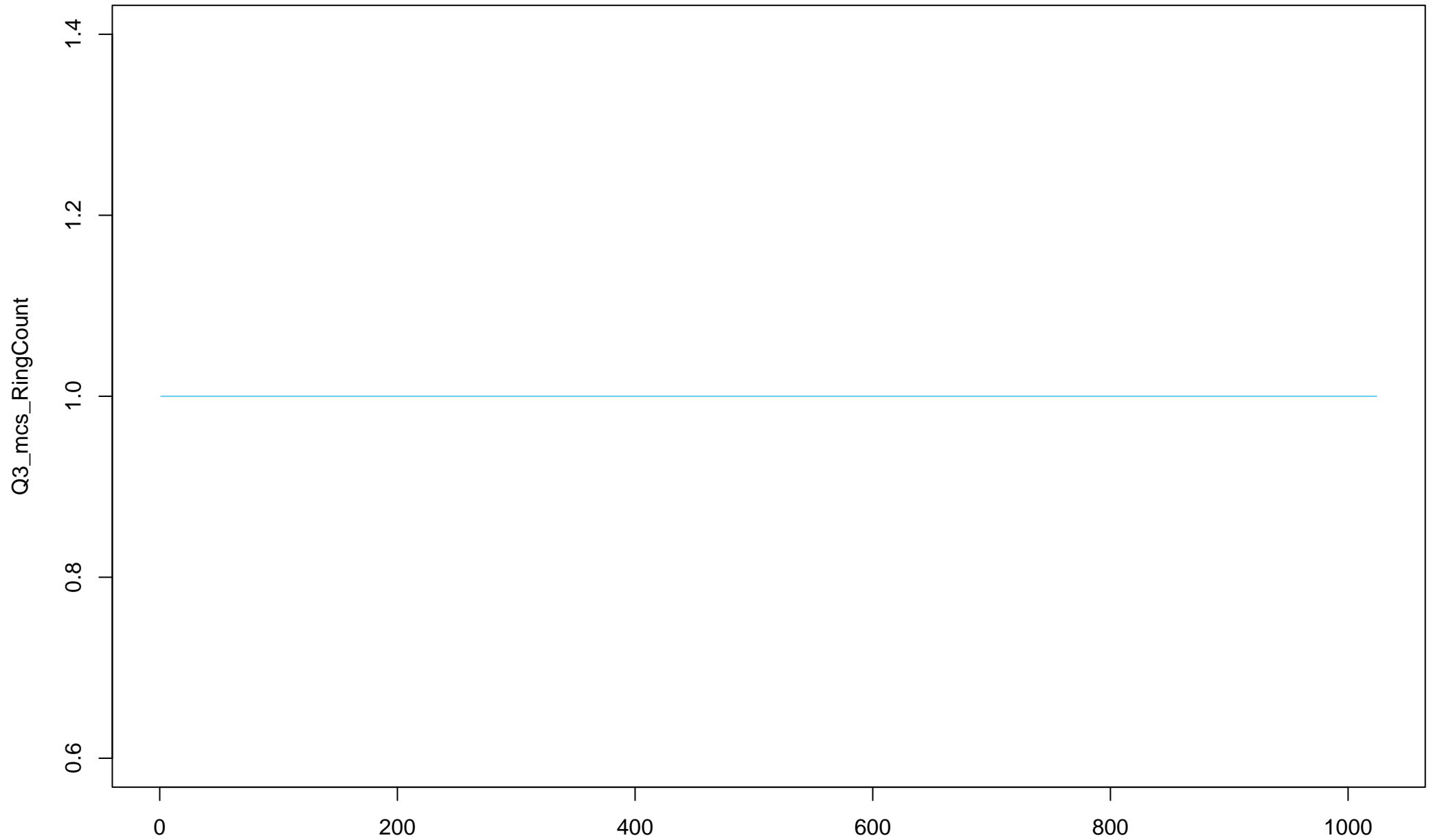
**Q3\_mcs\_NumHeteroAtoms**  
**ESS = 1020 | BMK = 0.594 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102**



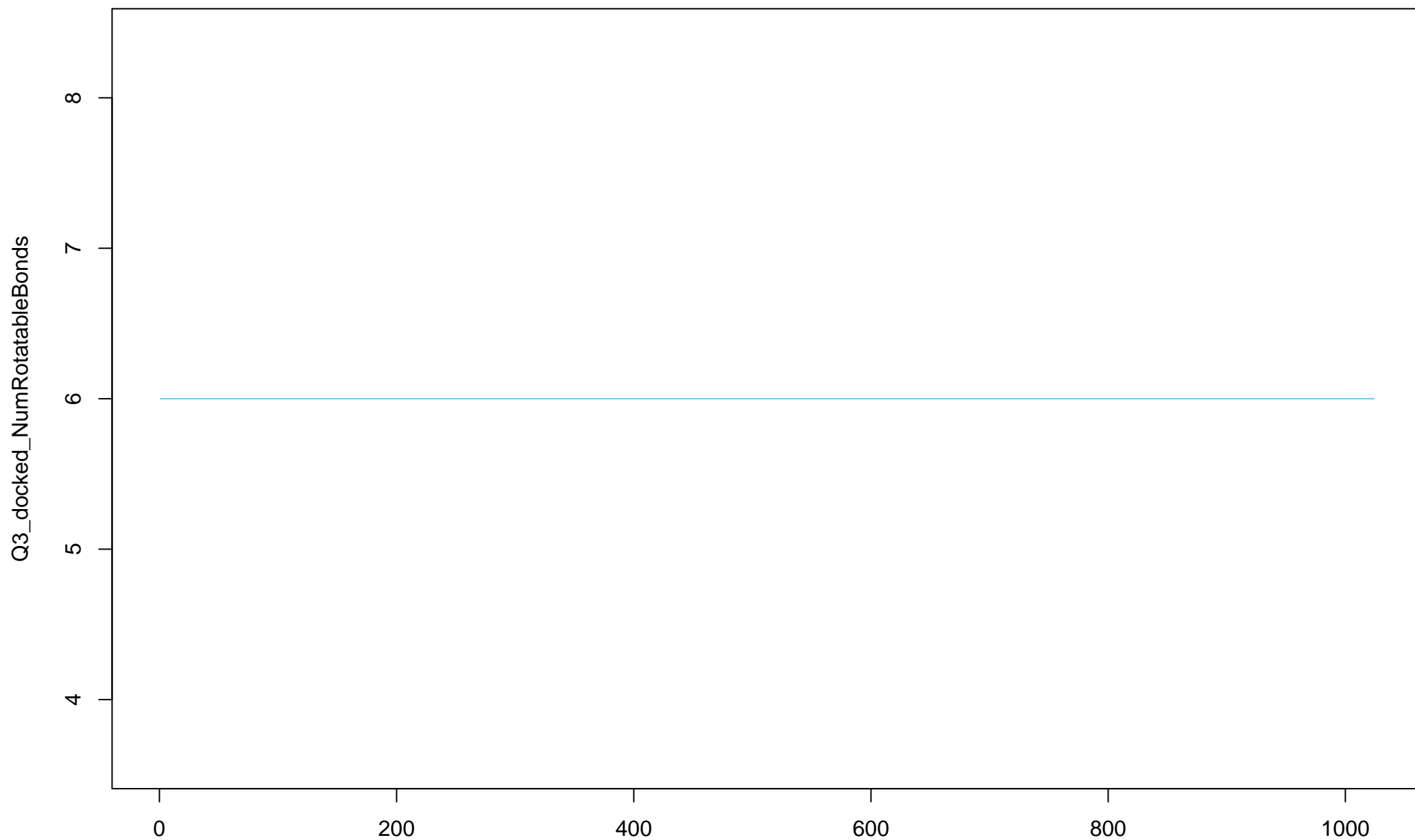
**Q3\_docked\_HeavyAtomCount**  
**ESS = 671 | BMK = 0.168 | MCSE(6.27) = 3.83 | stat: TRUE | burn: 0**



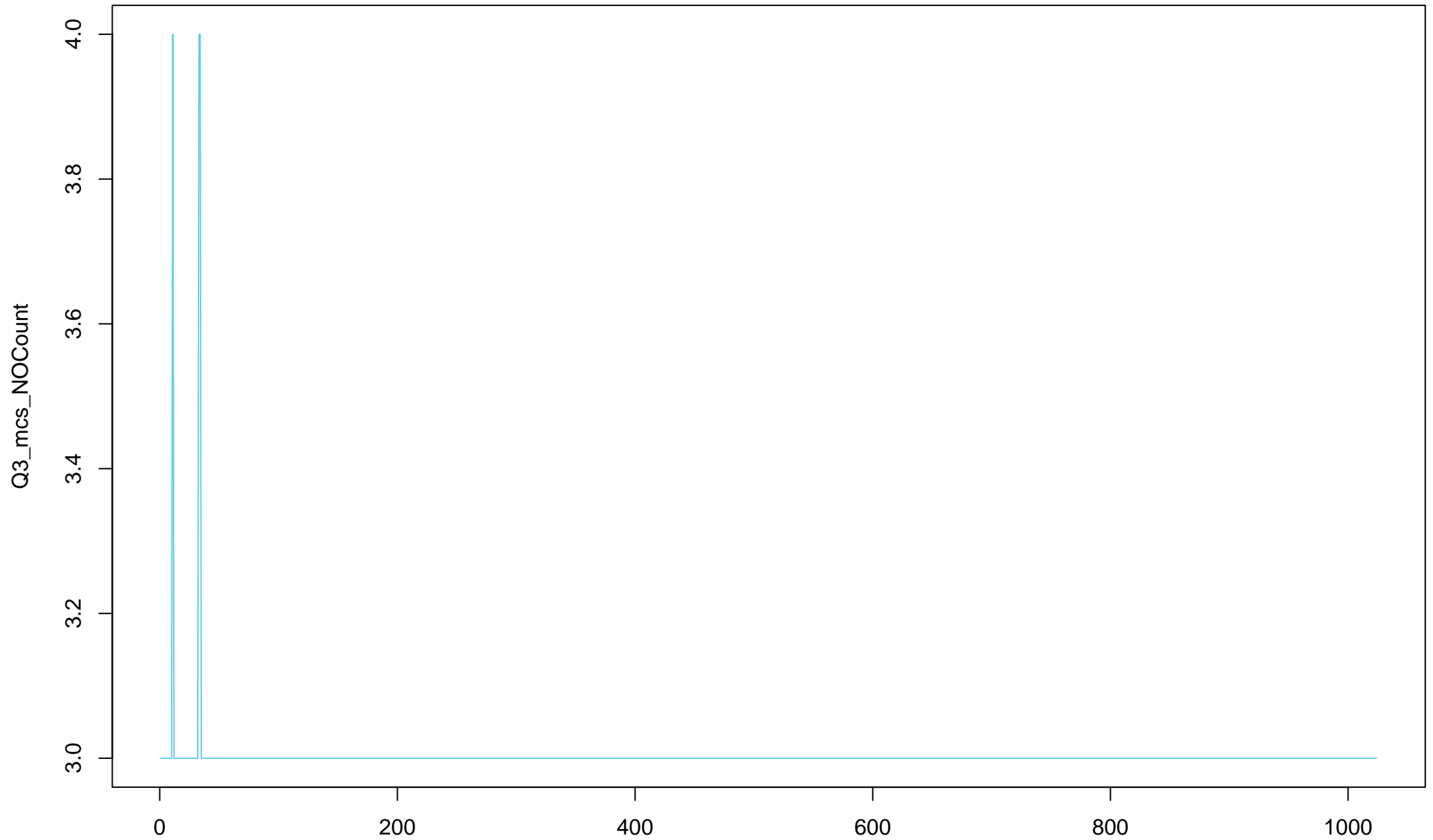
**Q3\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



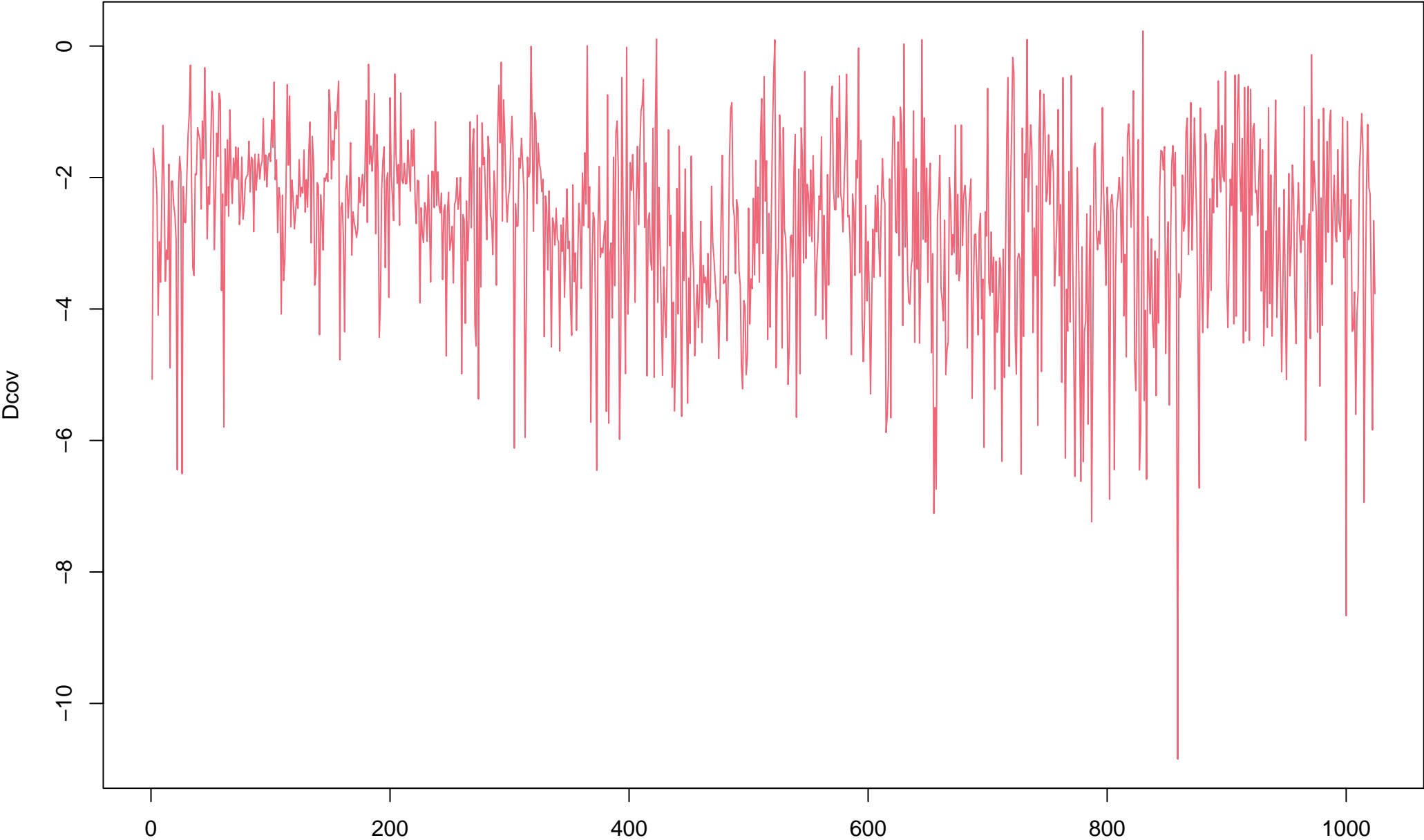
**Q3\_docked\_NumRotatableBonds**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



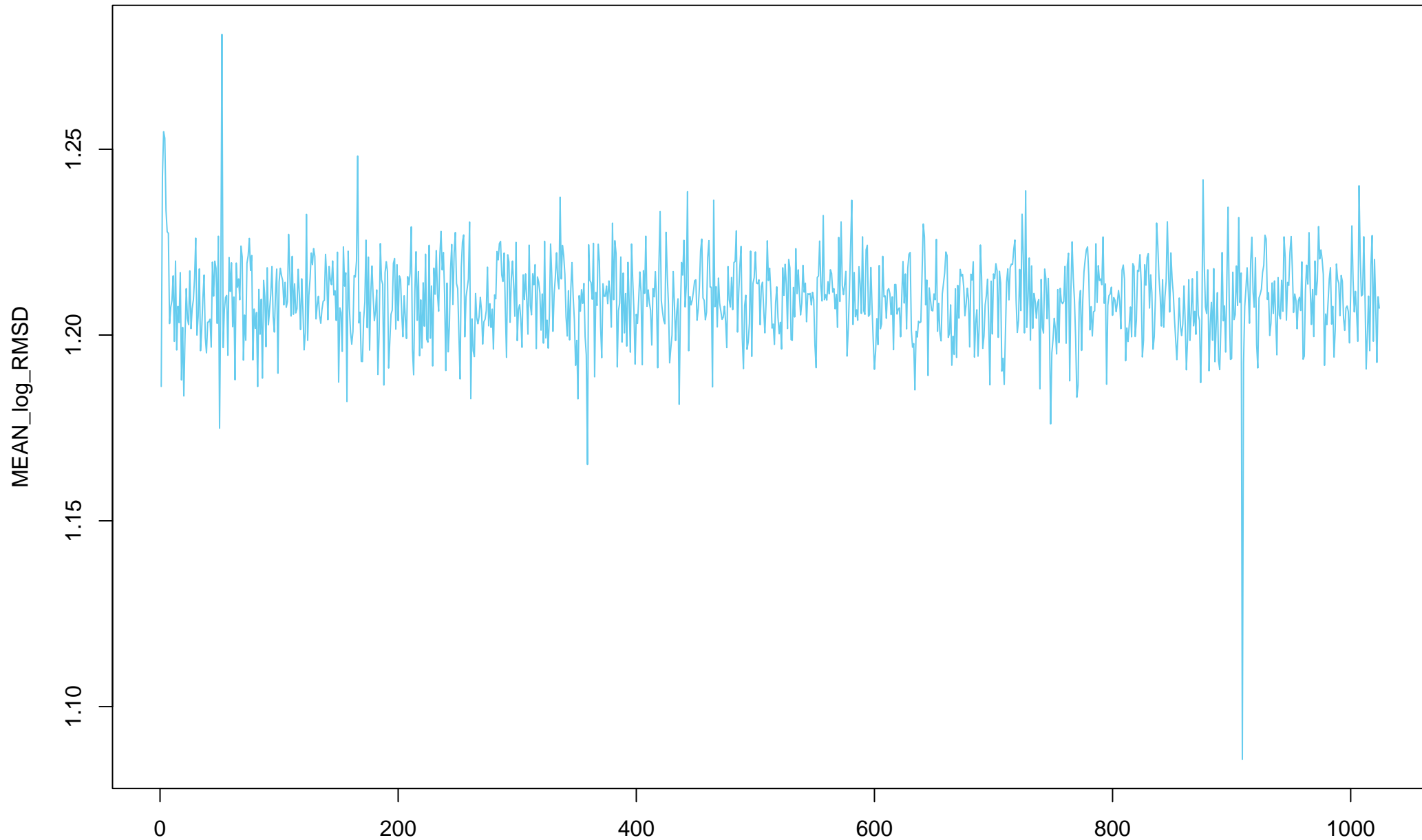
**Q3\_mcs\_NOCount**  
**ESS = 258 | BMK = 0.583 | MCSE(6.27) = 3.99 | stat: TRUE | burn: 0**



**Dcov**  
**ESS = 449 | BMK = 0.205 | MCSE(6.27) = 4.67 | stat: FALSE | burn: 0**

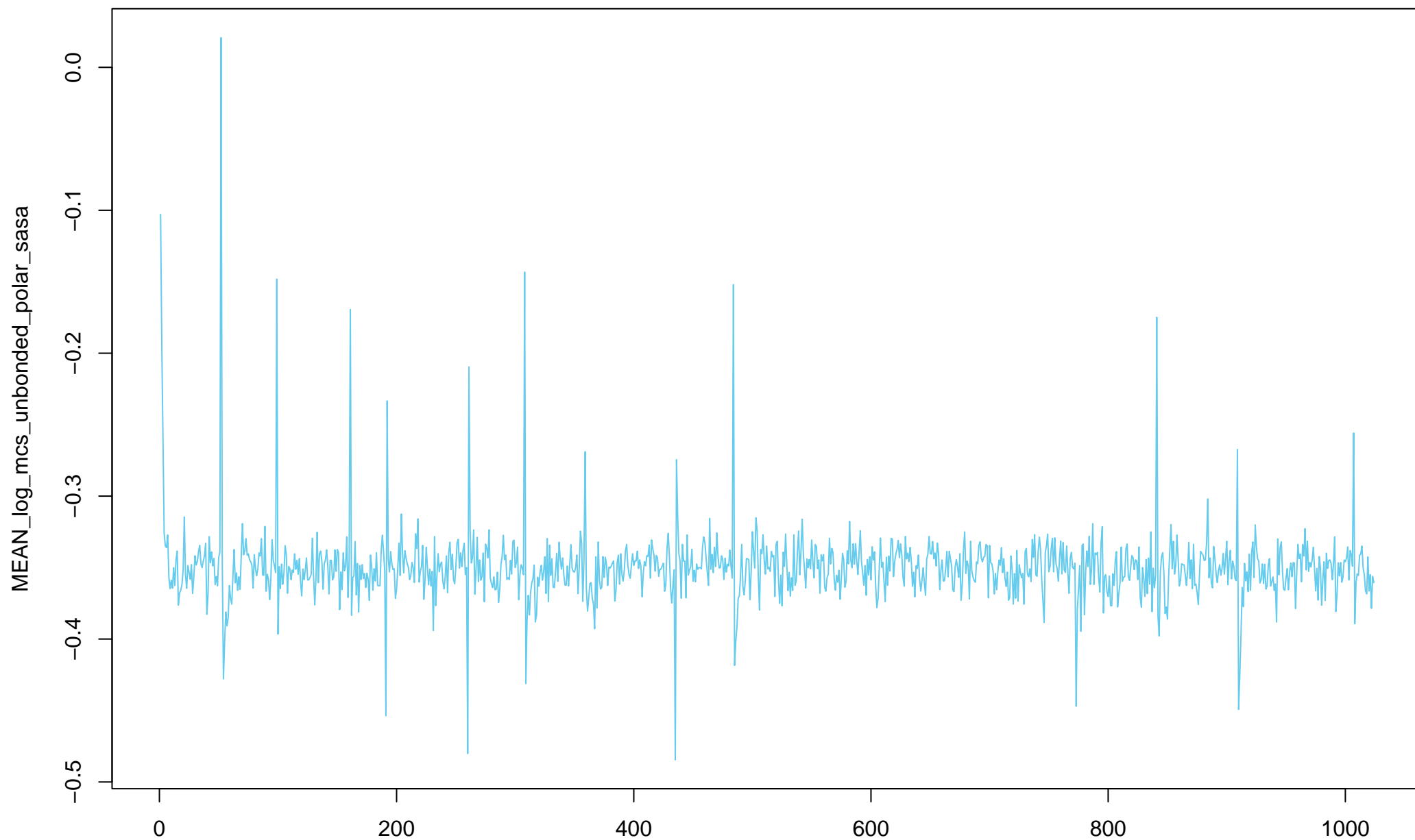


**MEAN\_log\_RMSD**  
**ESS = 822 | BMK = 0.081 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0**

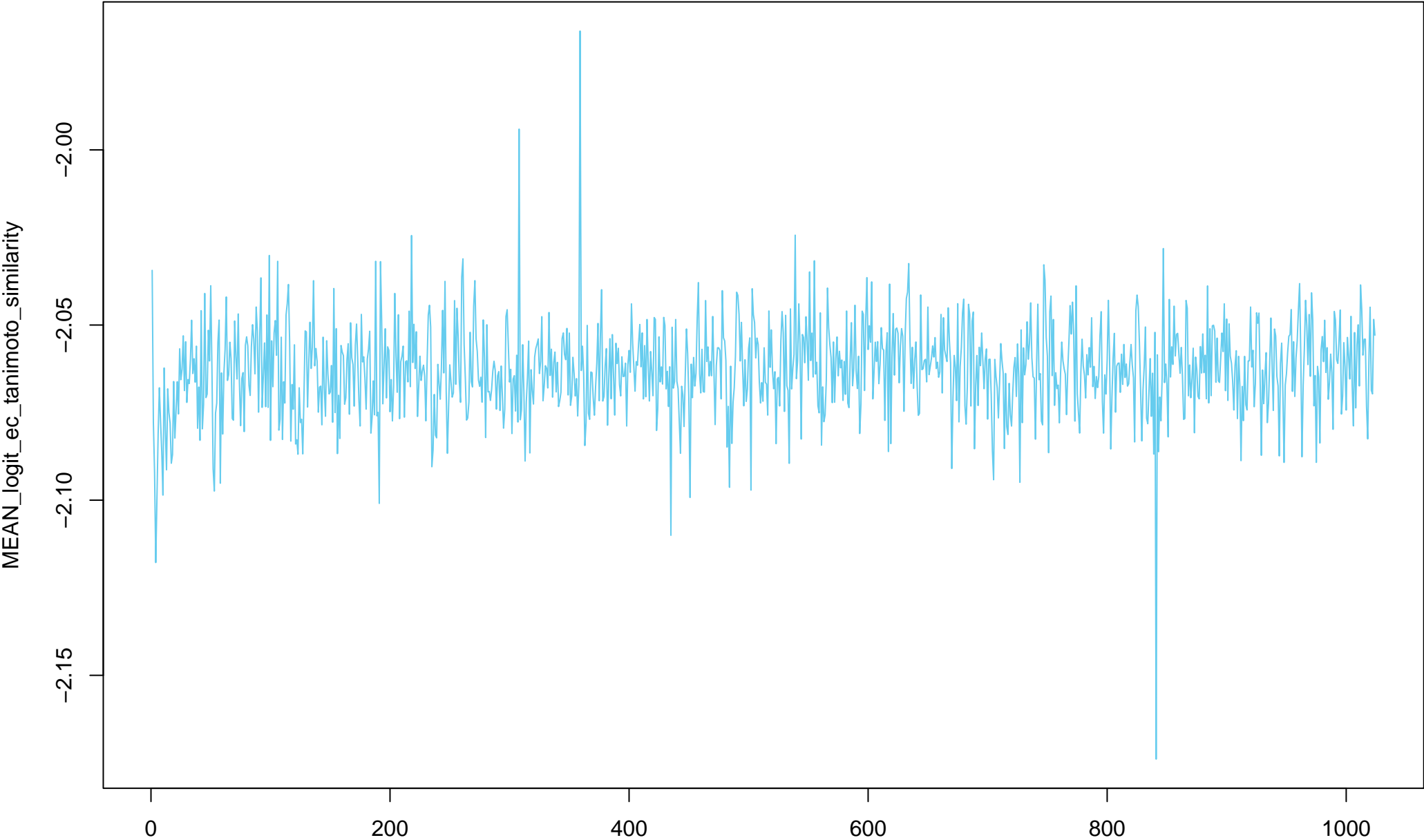




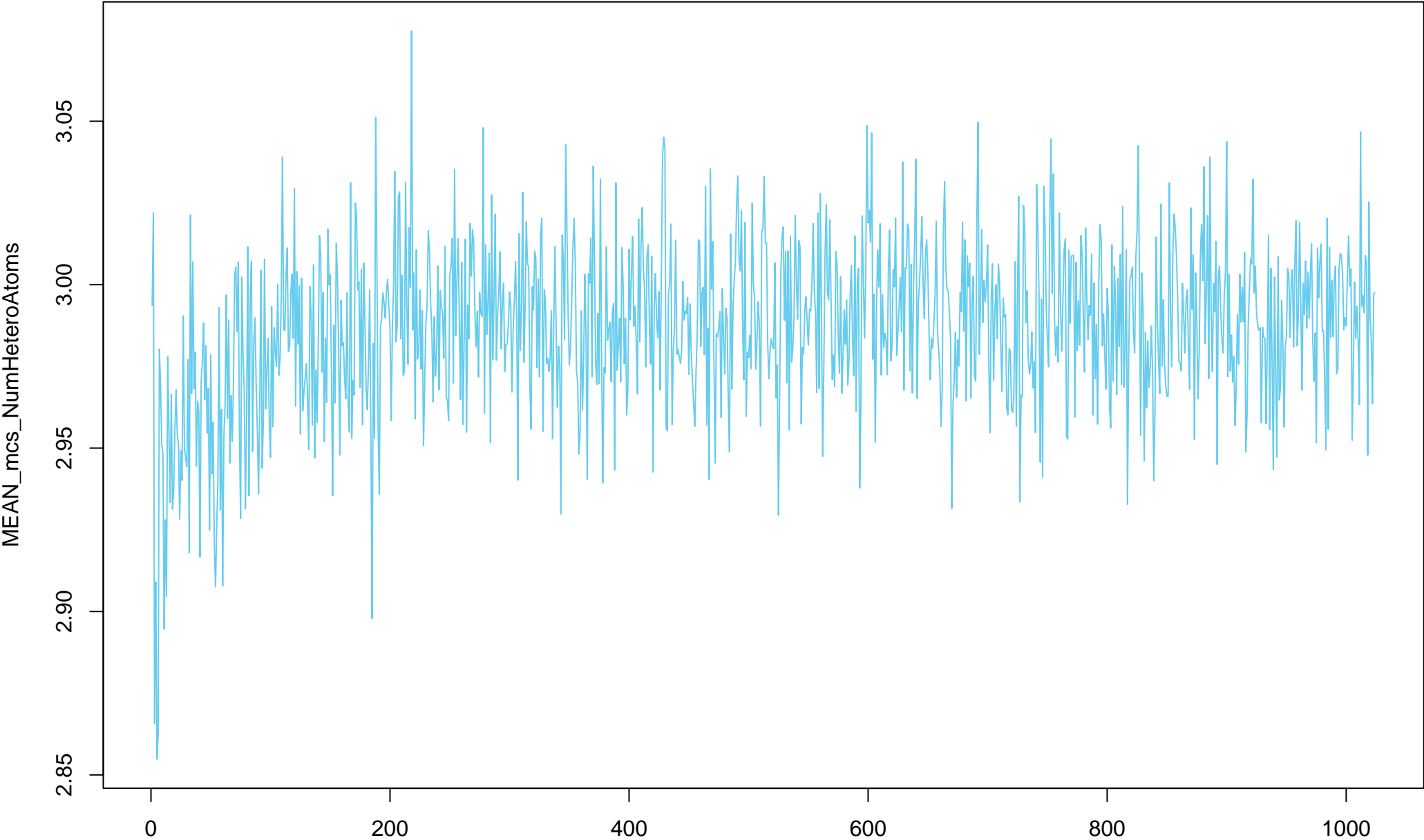
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1020 | BMK = 0.12 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0**



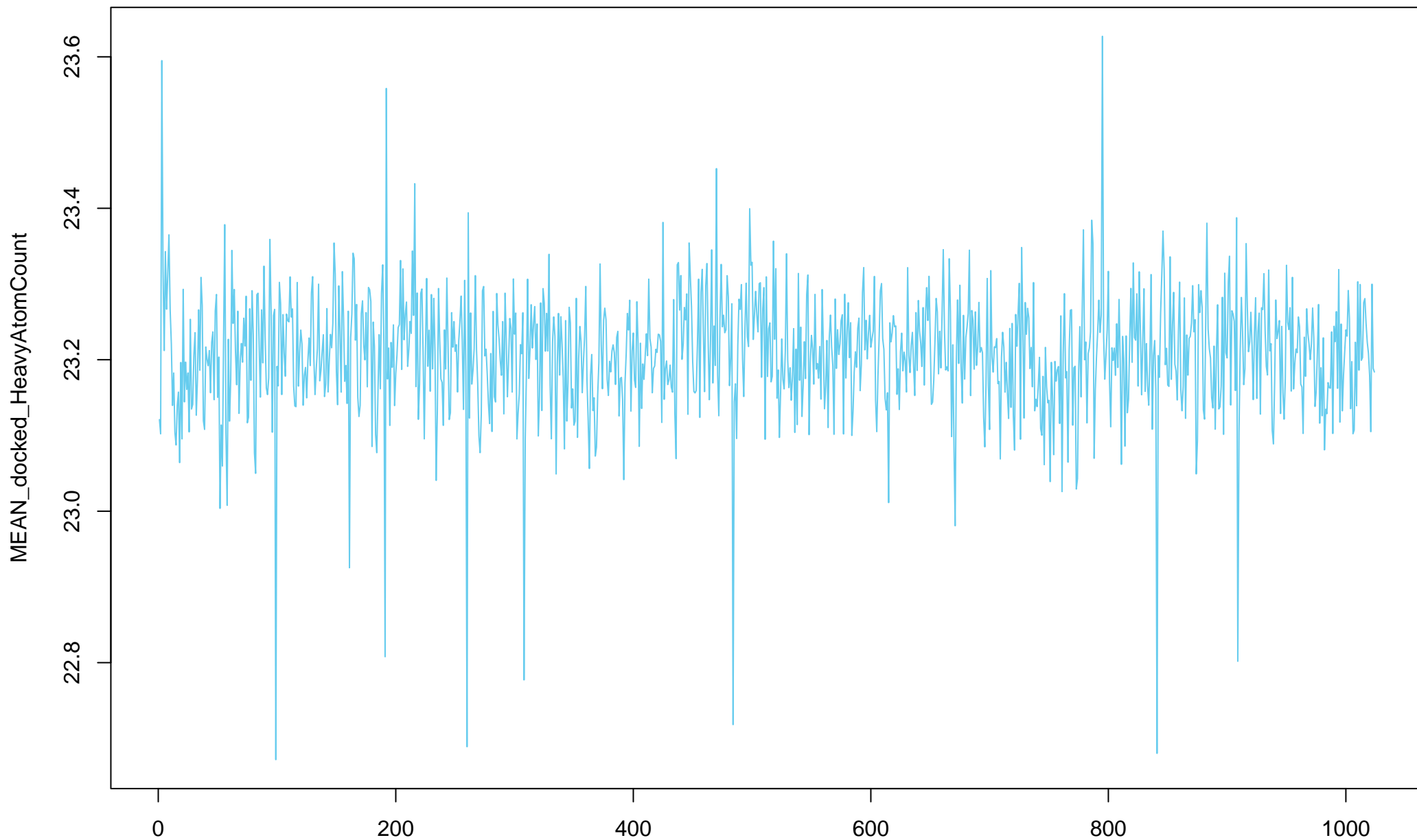
**MEAN\_logit\_ec\_tanimoto\_similarity**  
**ESS = 789 | BMK = 0.116 | MCSE(6.27) = 4.14 | stat: FALSE | burn: 0**



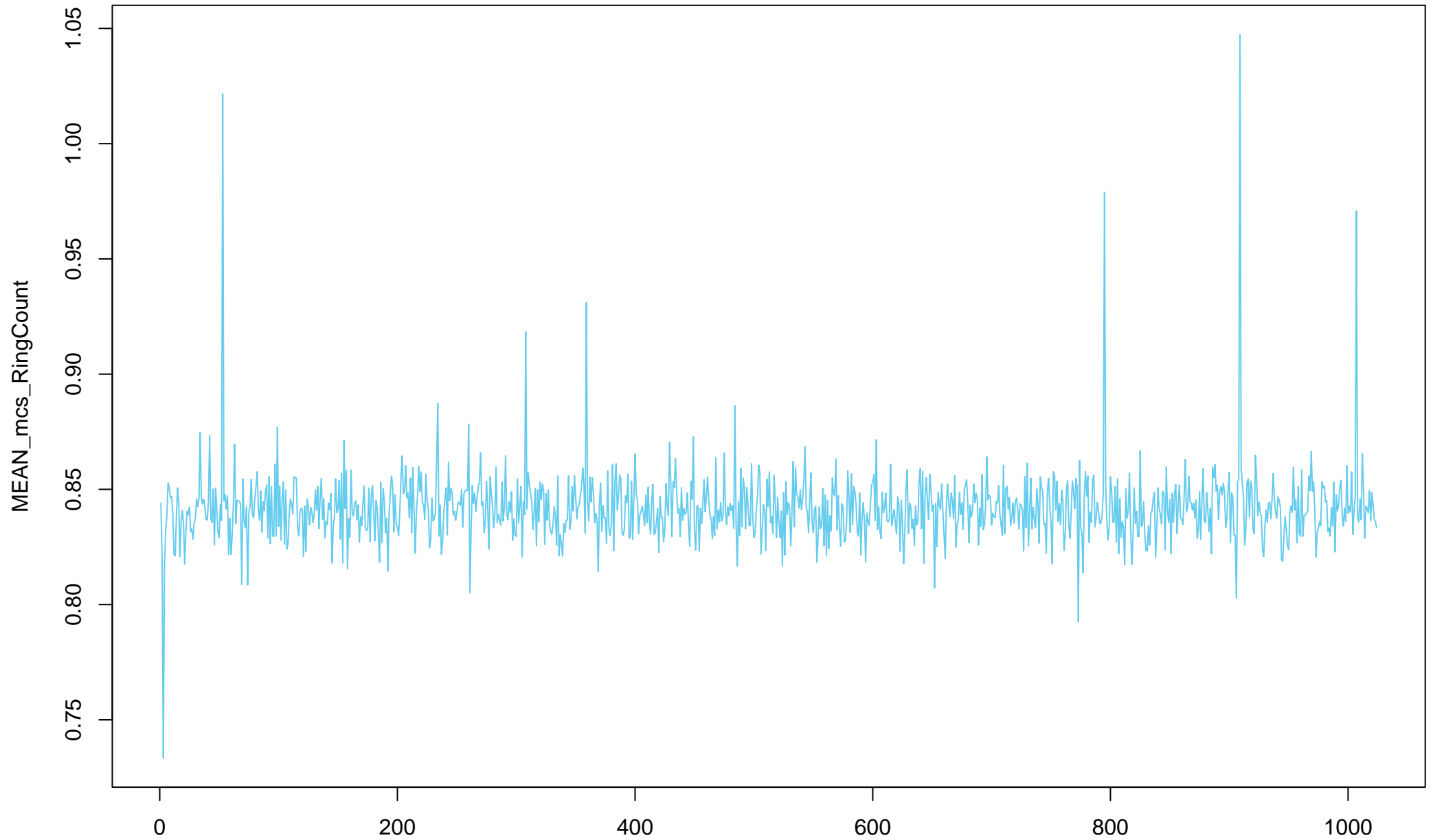
**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 104 | BMK = 0.151 | MCSE(6.27) = 7.73 | stat: FALSE | burn: 0**



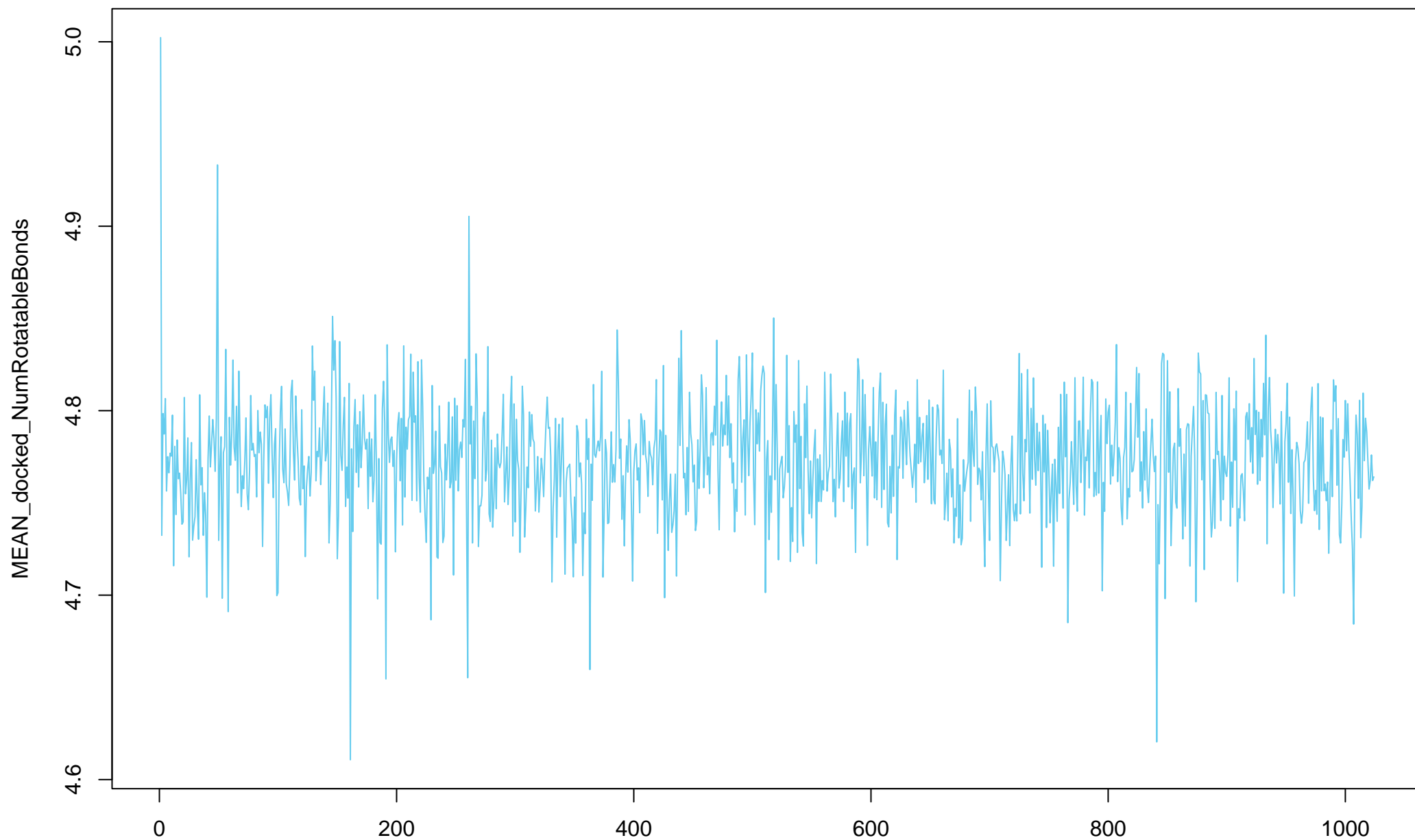
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0.0844 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0**



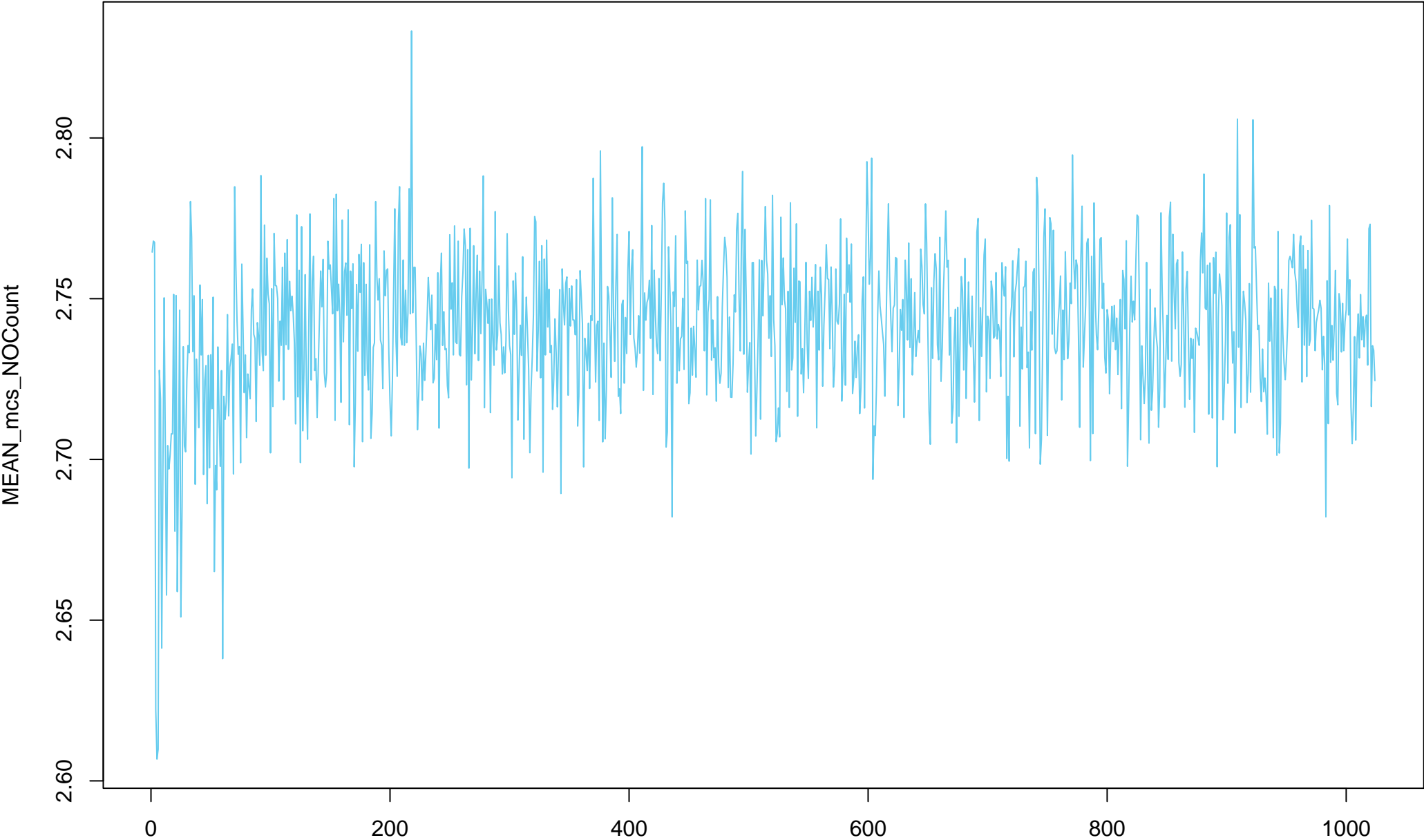
**MEAN\_mcs\_RingCount**  
**ESS = 1020 | BMK = 0.11 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0**



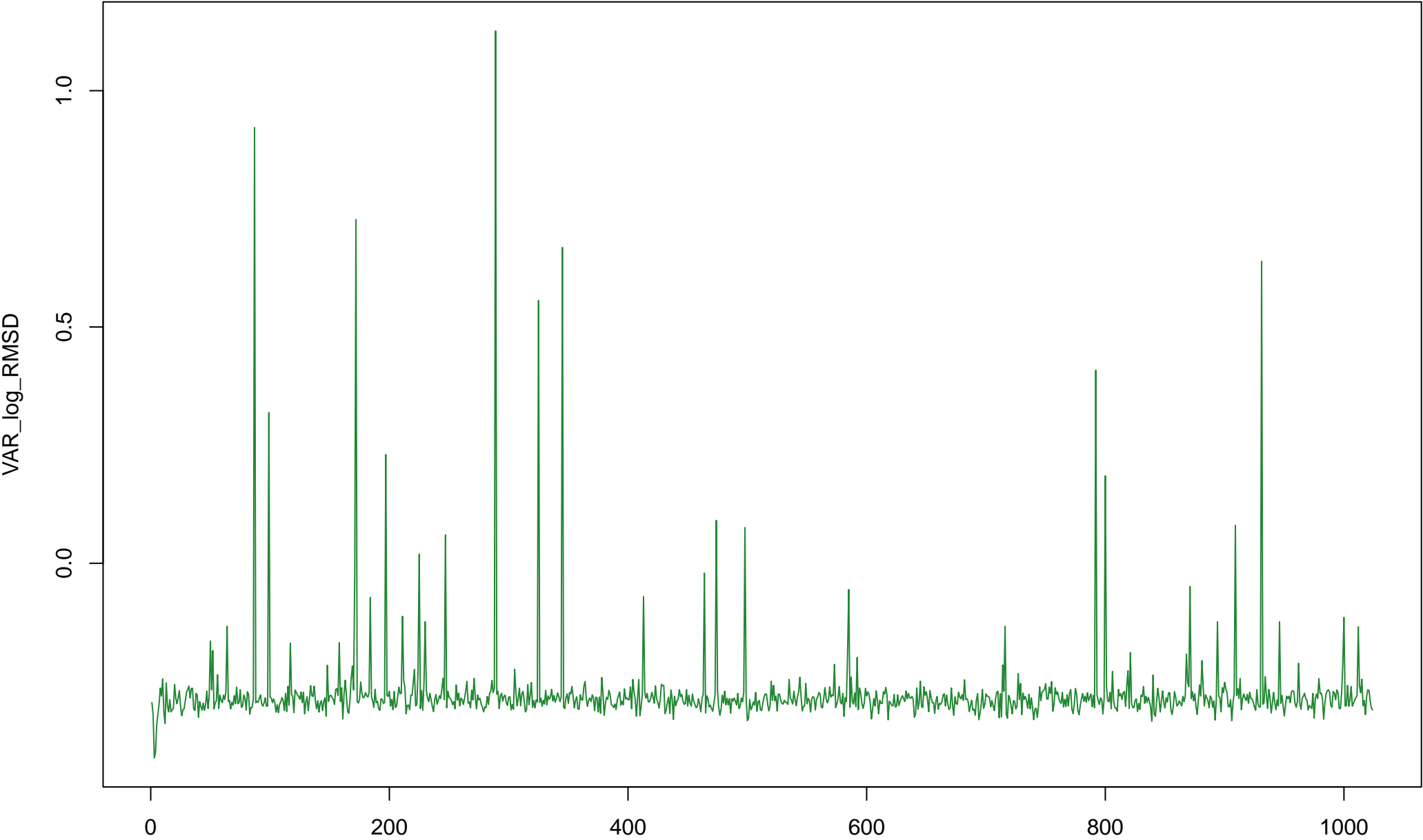
**MEAN\_docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0886 | MCSE(6.27) = 3.32 | stat: TRUE | burn: 0**



**MEAN\_mcs\_NOCount**  
**ESS = 180 | BMK = 0.123 | MCSE(6.27) = 6.51 | stat: FALSE | burn: 0**

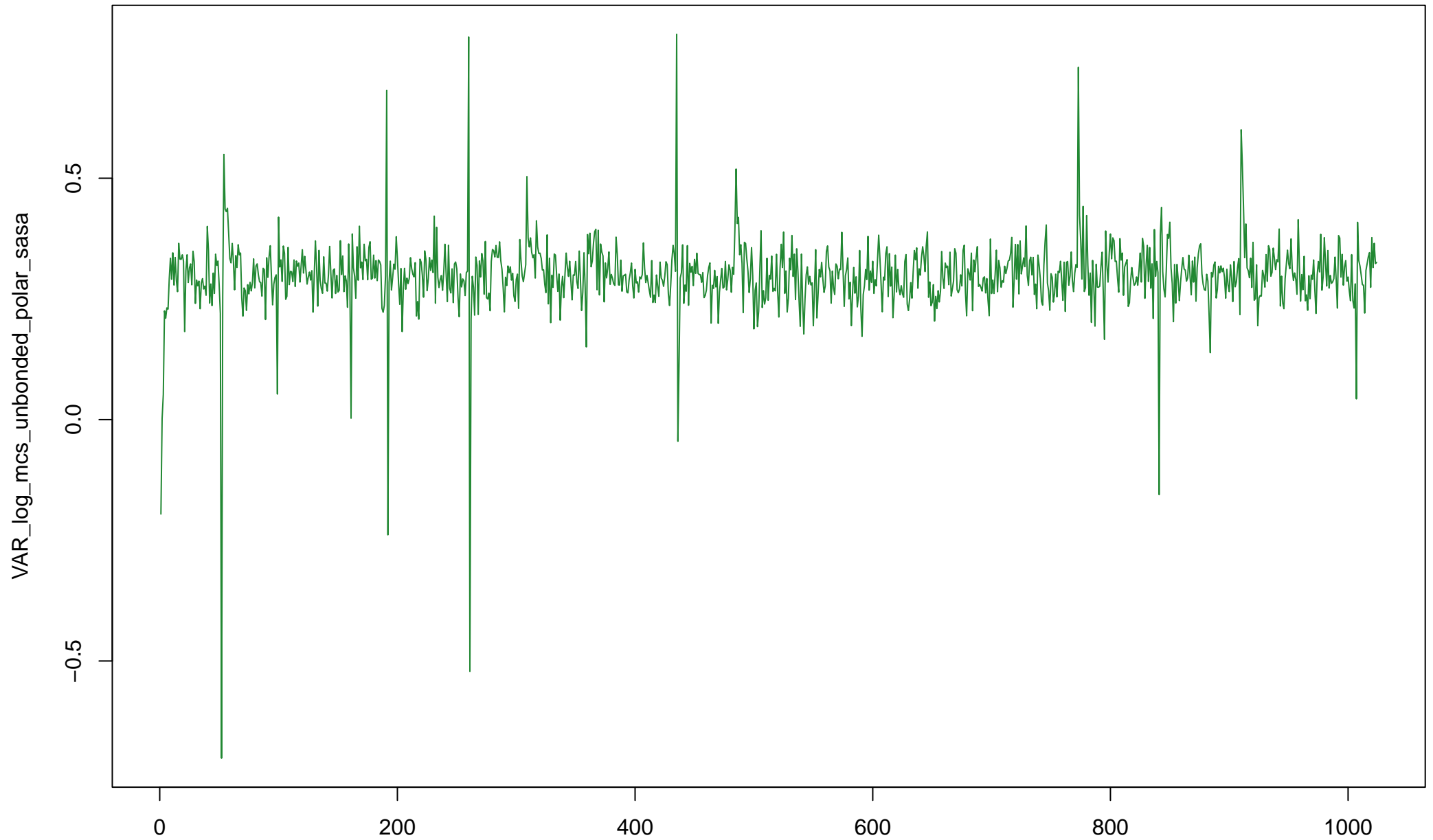


**VAR\_log\_RMSD**  
**ESS = 1020 | BMK = 0.161 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0**

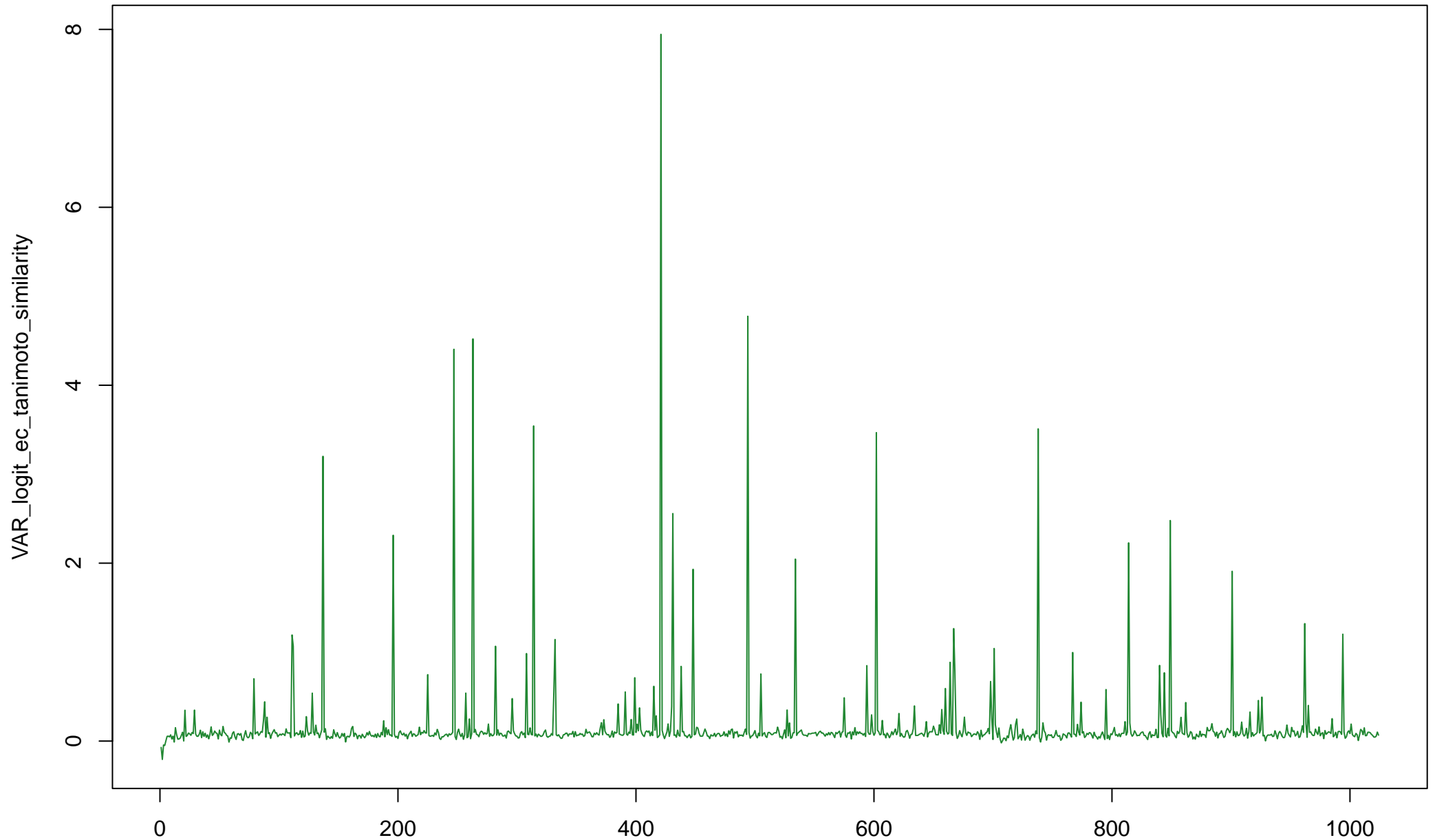




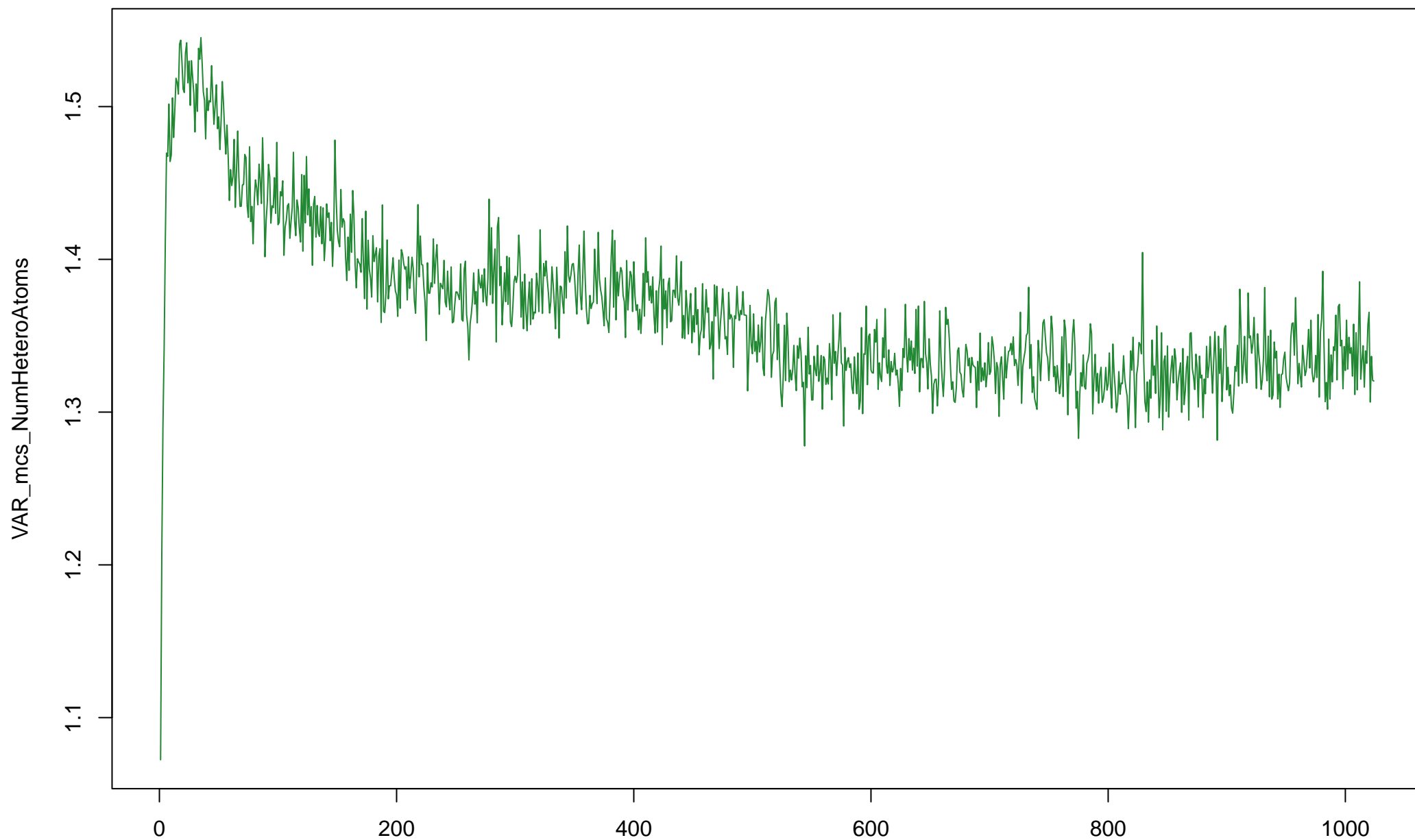
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1020 | BMK = 0.113 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0**



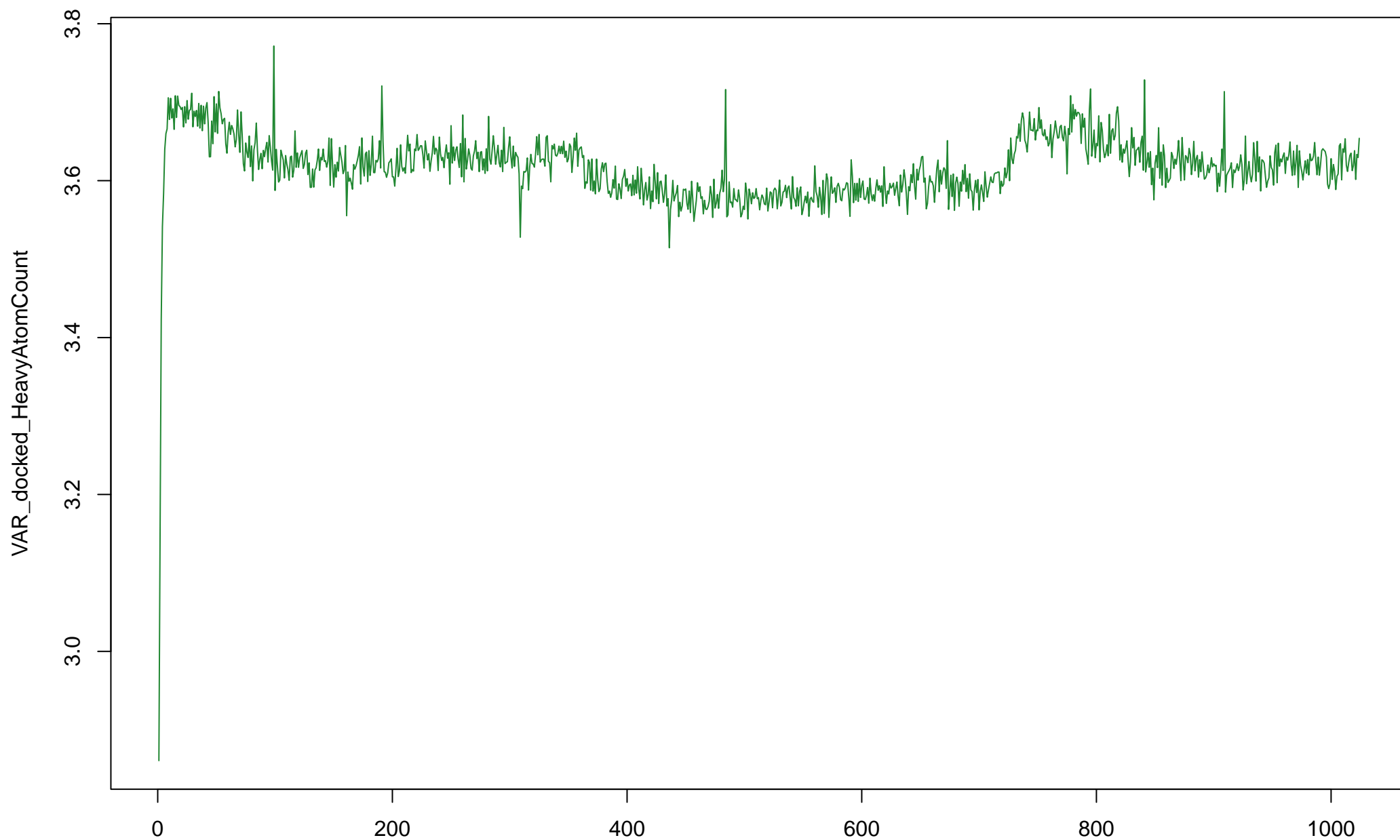
**VAR\_logit\_ec\_tanimoto\_similarity**  
**ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.13 | stat: FALSE | burn: 510**



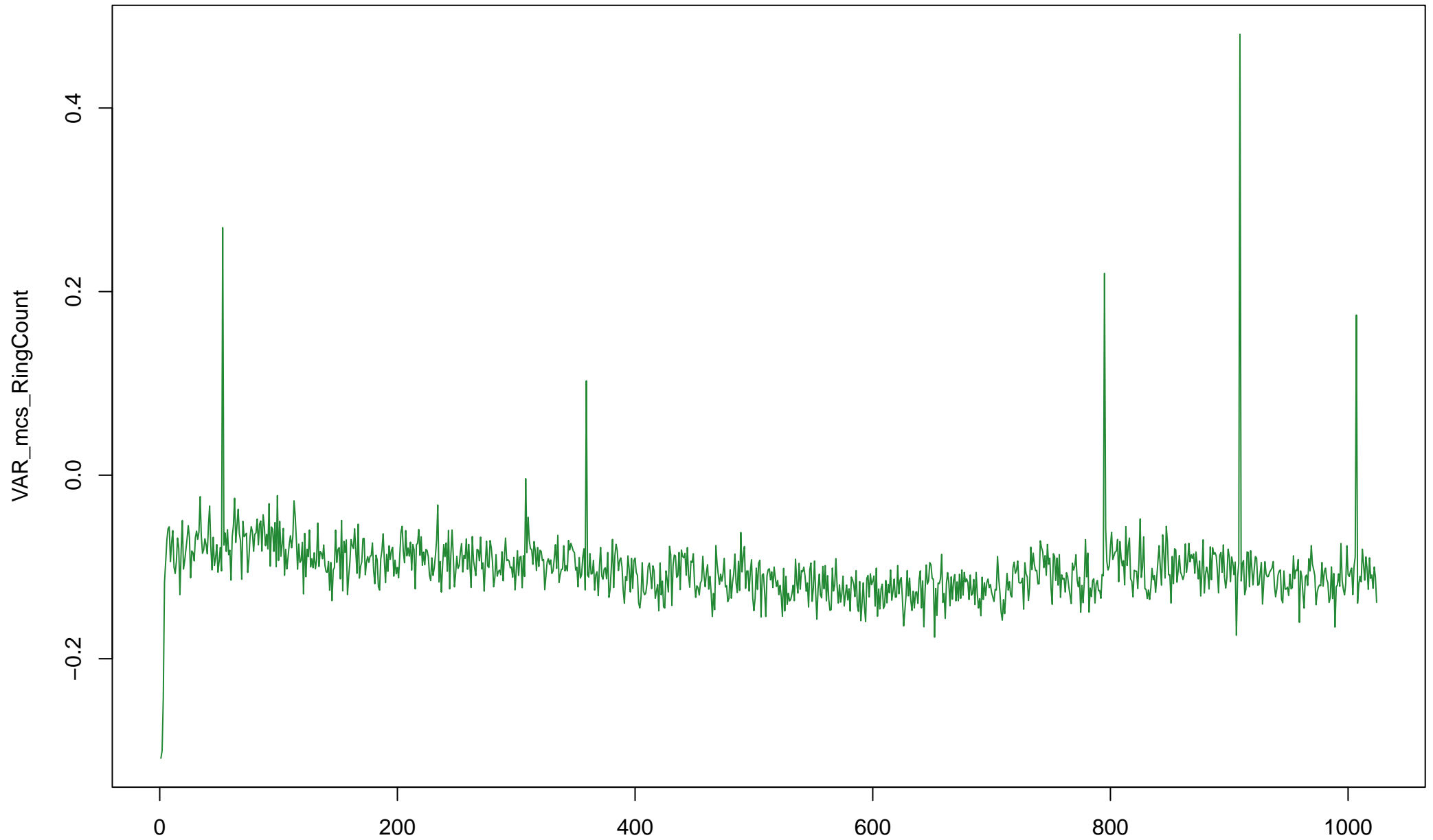
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 6.55 | BMK = 0.717 | MCSE(6.27) = 15.7 | stat: FALSE | burn: 102**



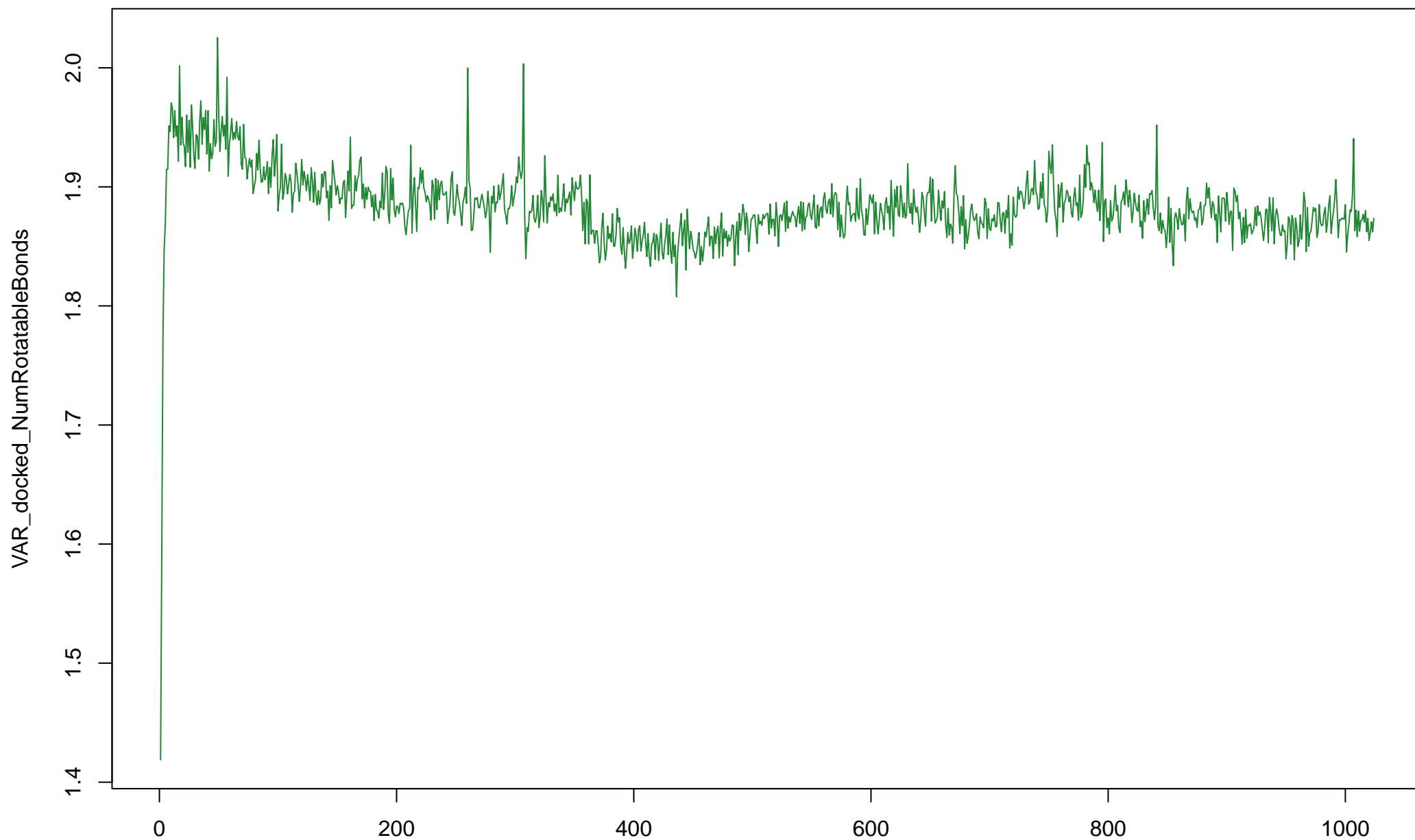
**VAR\_docked\_HeavyAtomCount**  
**ESS = 30.4 | BMK = 0.126 | MCSE(6.27) = 11.5 | stat: FALSE | burn: 714**



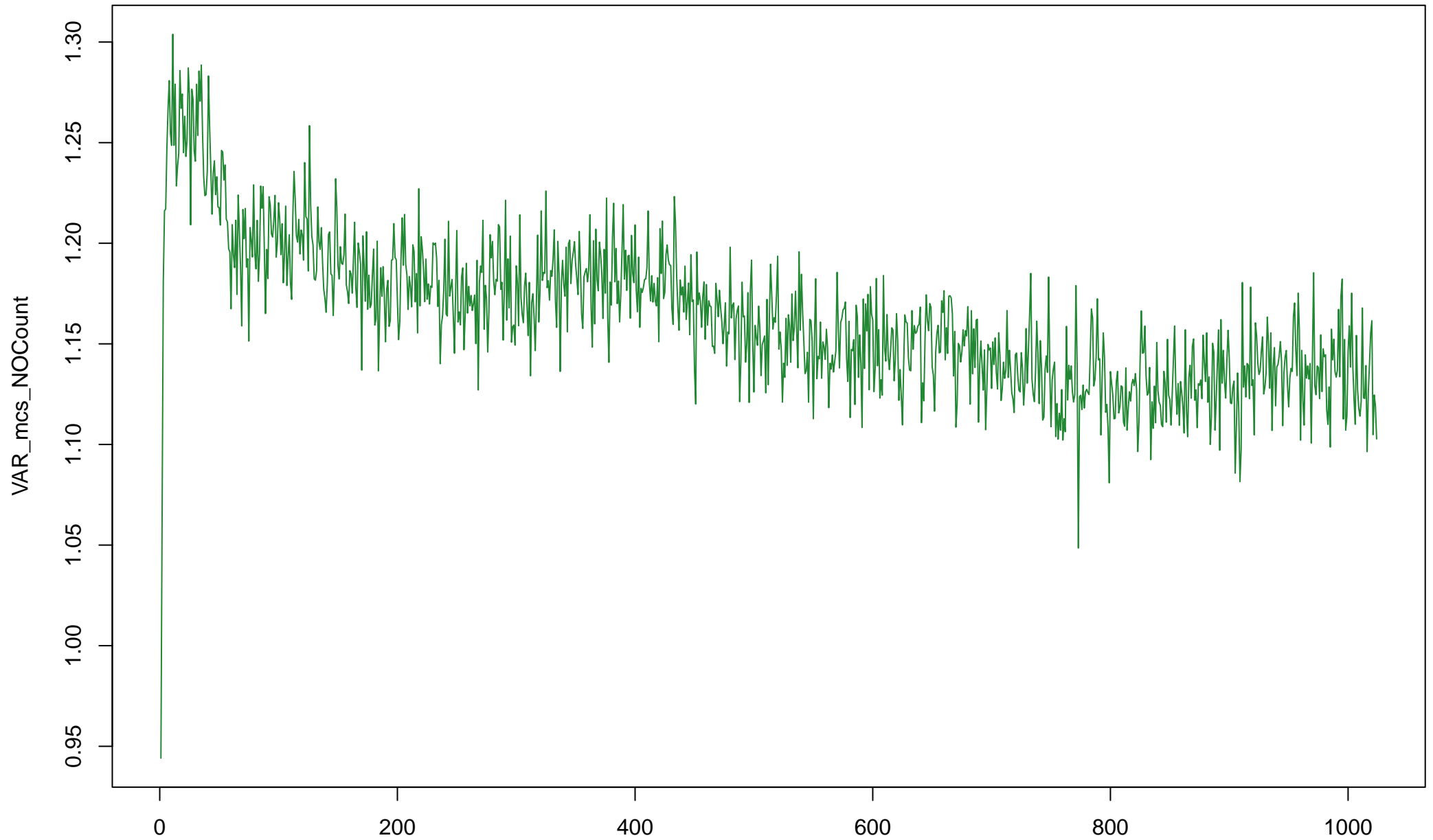
**VAR\_mcs\_RingCount**  
**ESS = 92.1 | BMK = 0.328 | MCSE(6.27) = 7.06 | stat: FALSE | burn: 0**



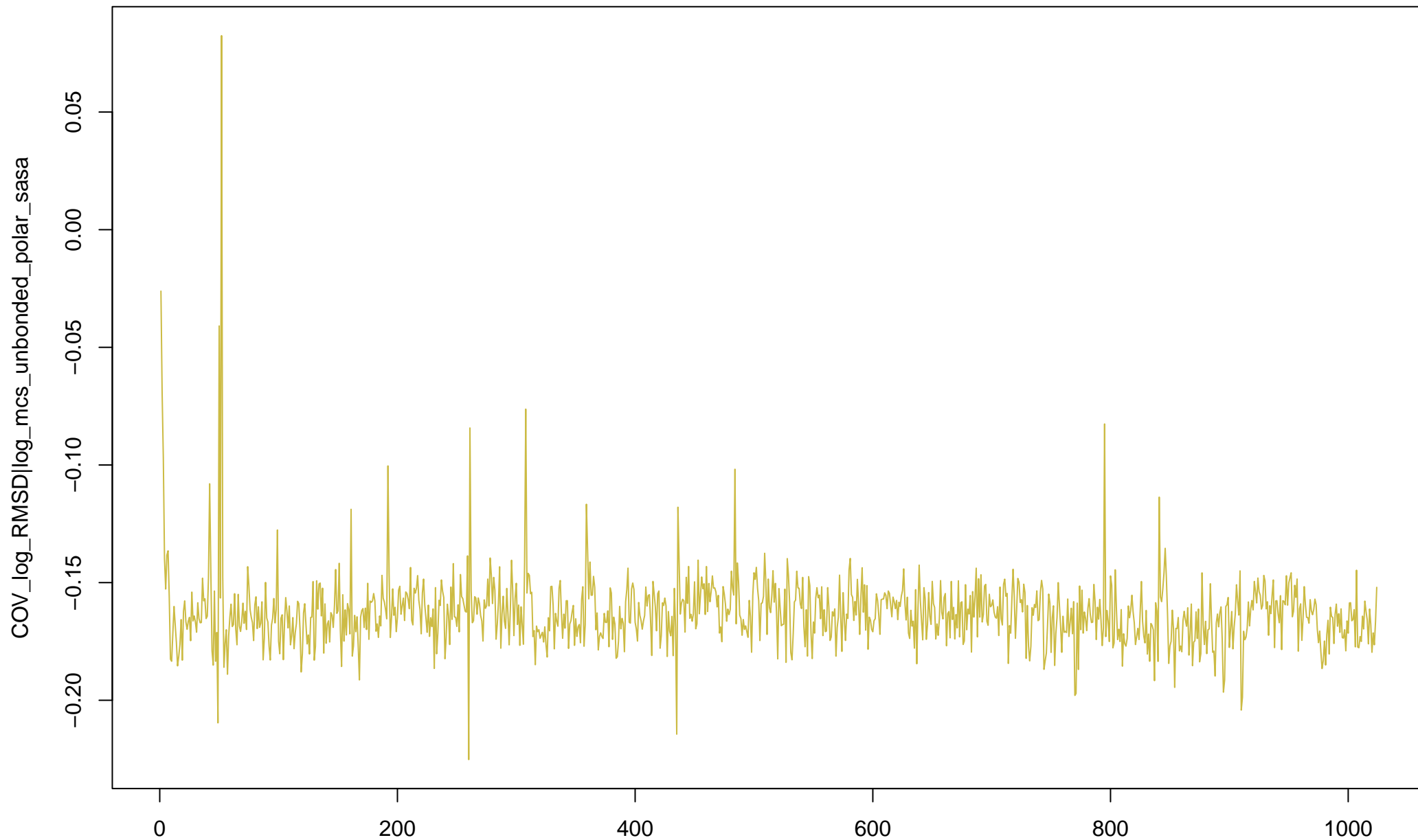
**VAR\_docked\_NumRotatableBonds**  
**ESS = 20.6 | BMK = 0.324 | MCSE(6.27) = 11.4 | stat: FALSE | burn: 510**



**VAR\_mcs\_NOCount**  
**ESS = 8.11 | BMK = 0.646 | MCSE(6.27) = 14.6 | stat: FALSE | burn: 0**

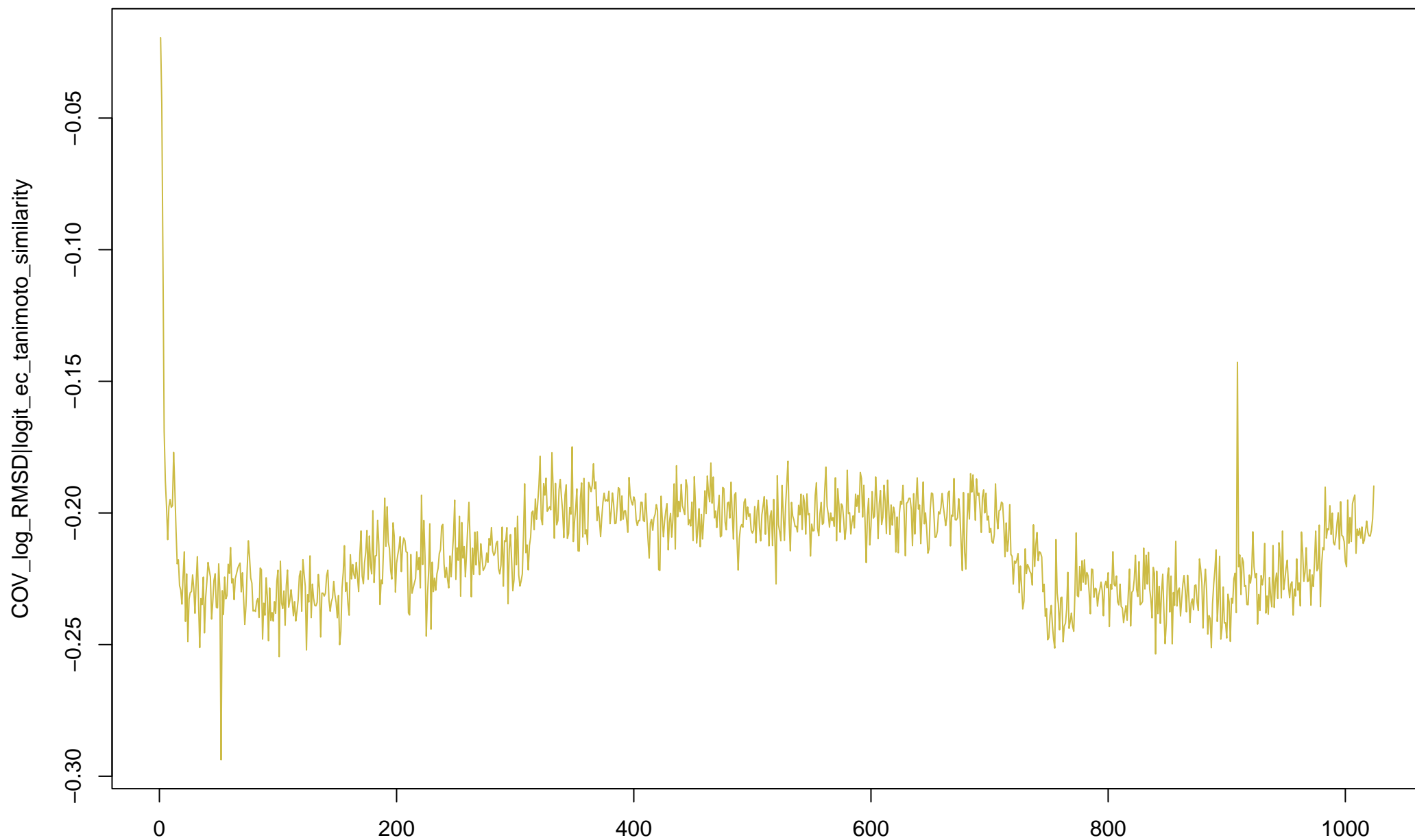


**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 540 | BMK = 0.135 | MCSE(6.27) = 4.38 | stat: TRUE | burn: 0**

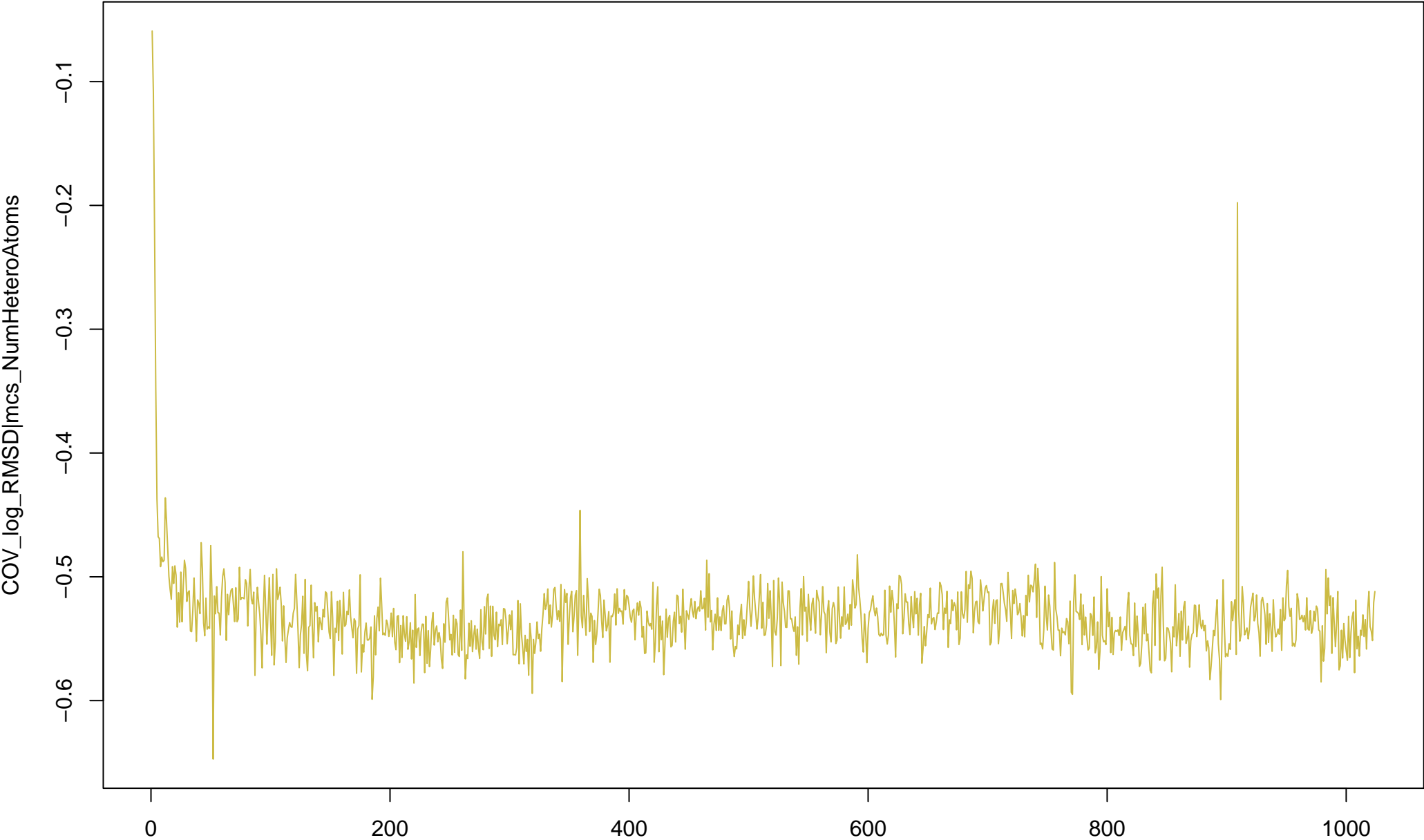




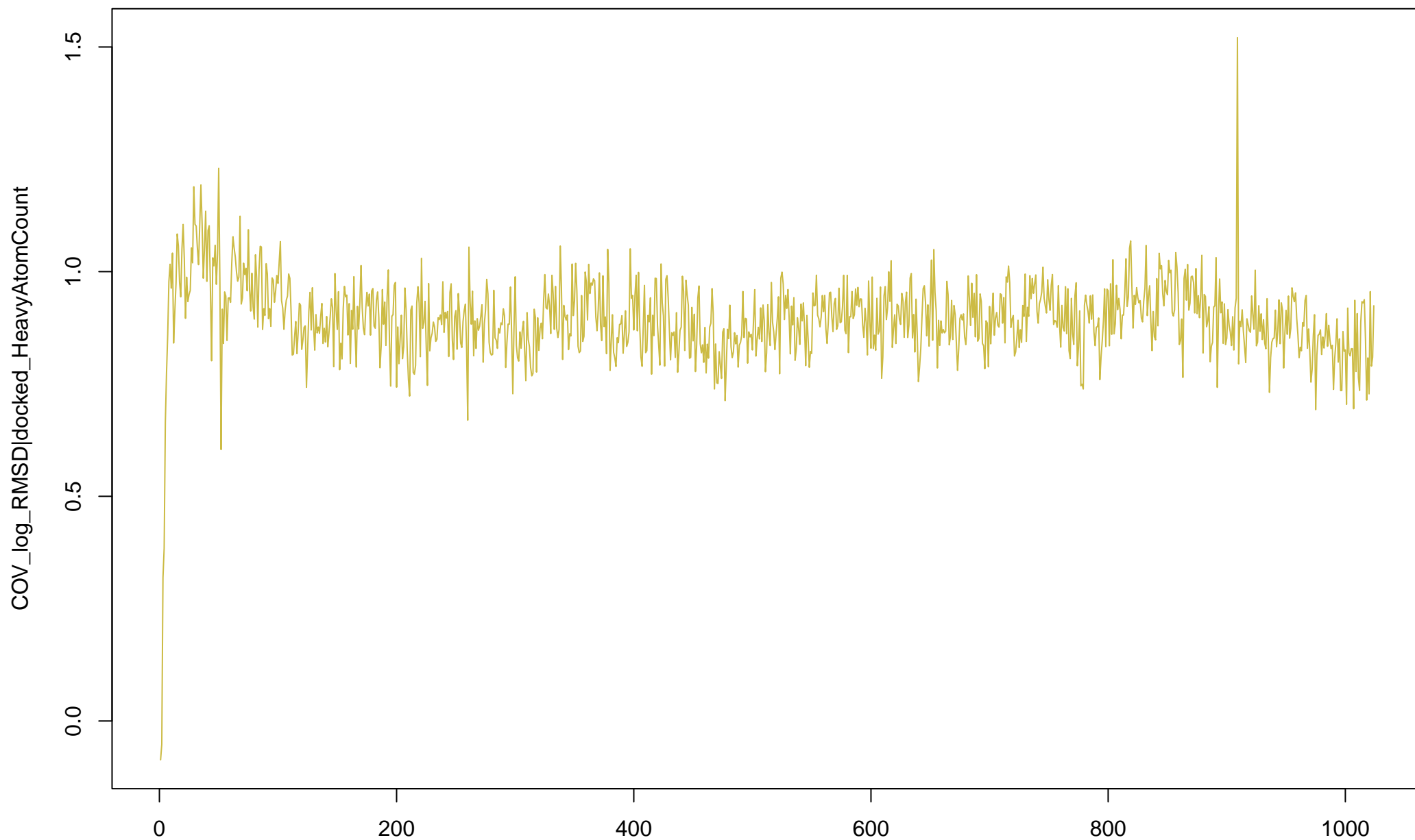
**COV\_log\_RMSD|logit\_ec\_tanimoto\_similarity**  
**ESS = 19.6 | BMK = 0.0928 | MCSE(6.27) = 12.8 | stat: TRUE | burn: 714**



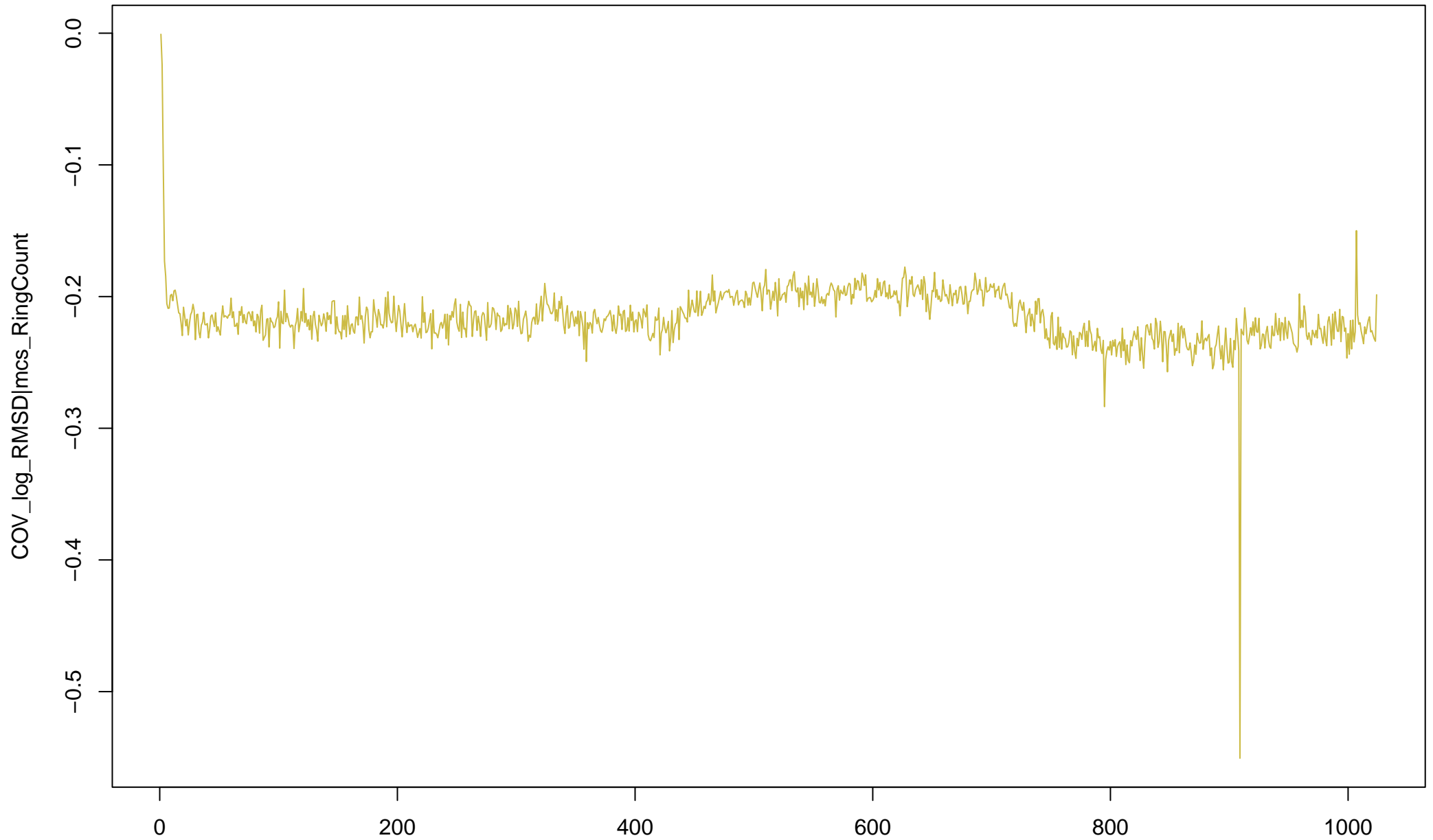
COV\_log\_RMSD|mcs\_NumHeteroAtoms  
ESS = 253 | BMK = 0.123 | MCSE(6.27) = 8.51 | stat: FALSE | burn: 0



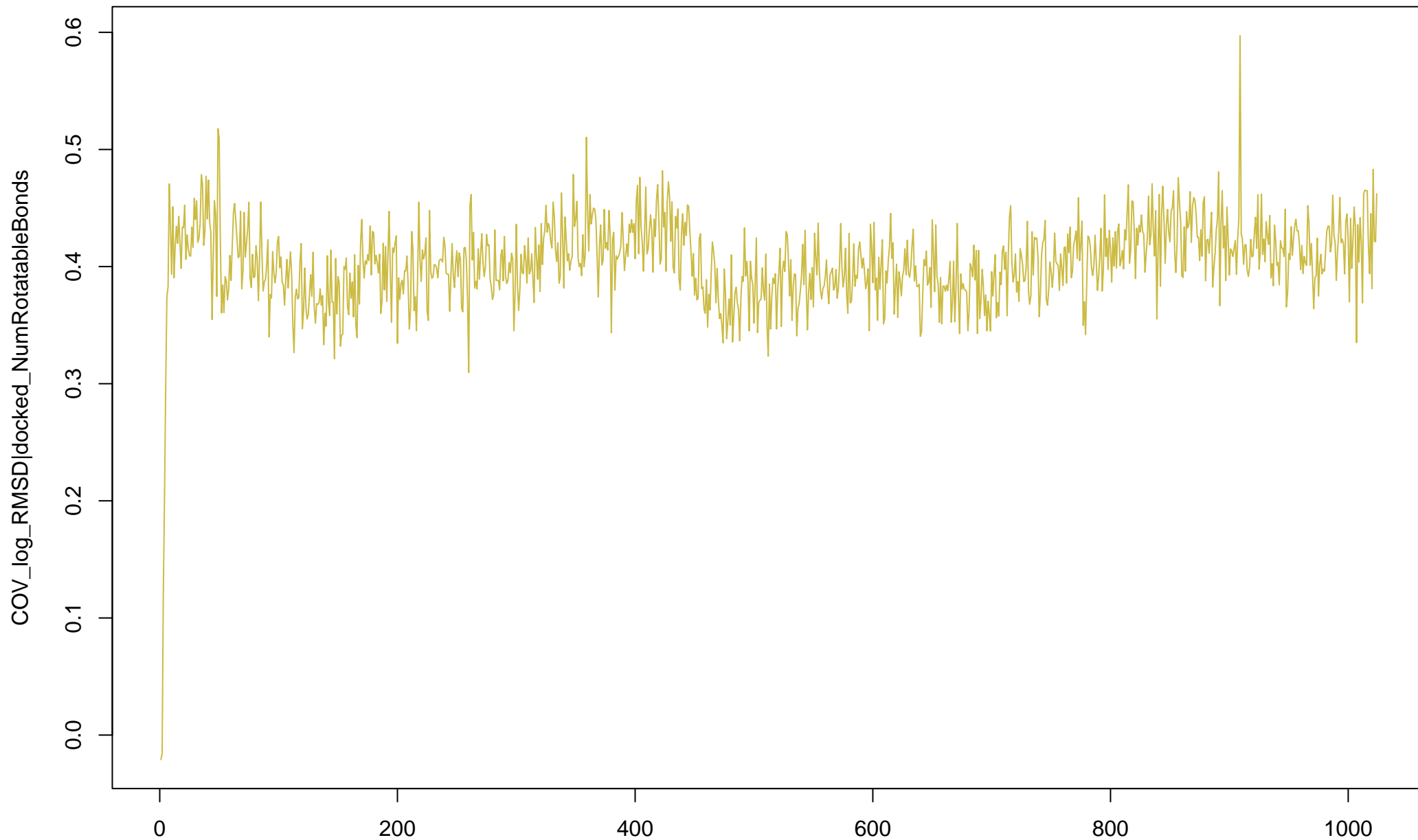
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 187 | BMK = 0.158 | MCSE(6.27) = 6.8 | stat: TRUE | burn: 102**



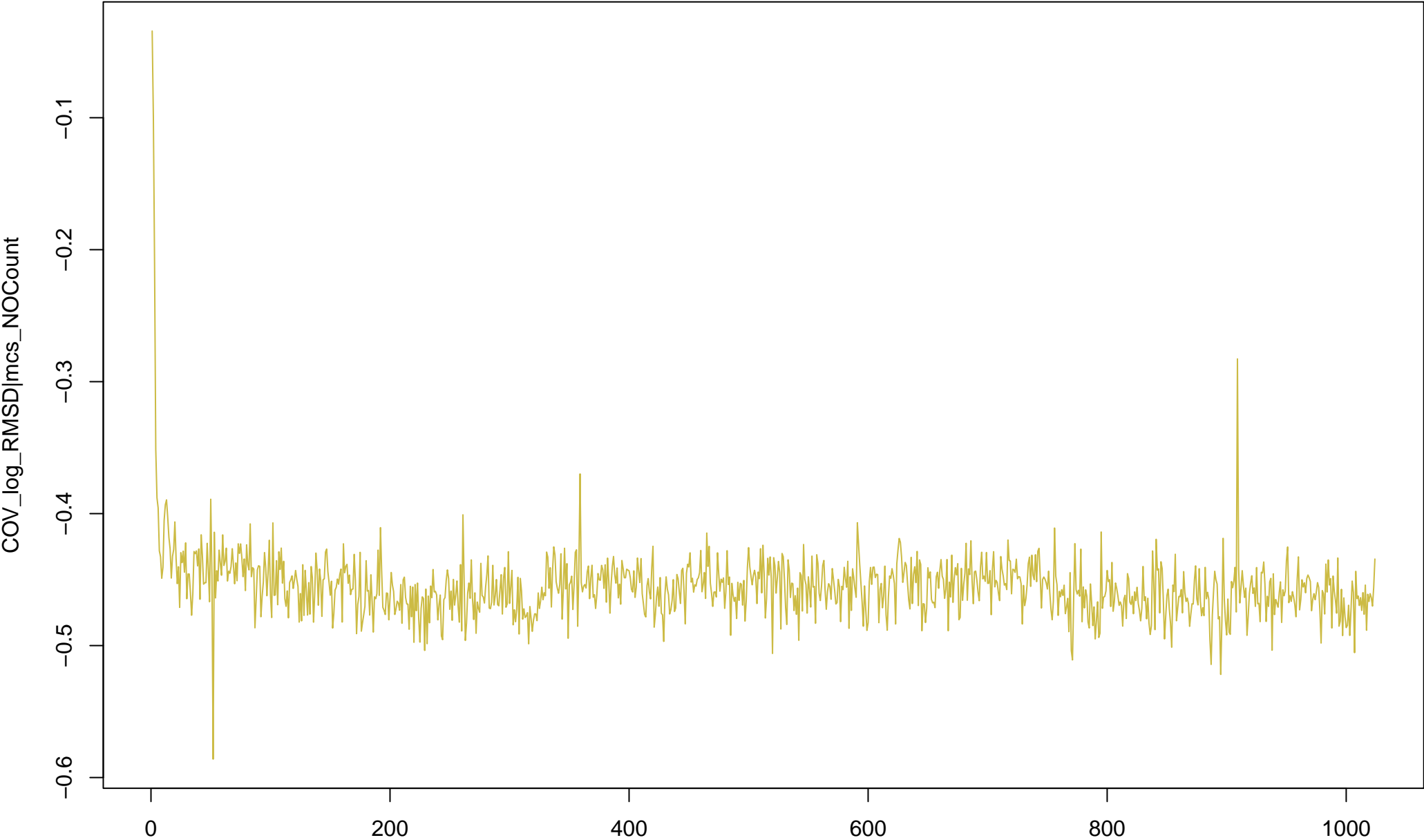
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 22.7 | BMK = 0.356 | MCSE(6.27) = 11.6 | stat: TRUE | burn: 714**



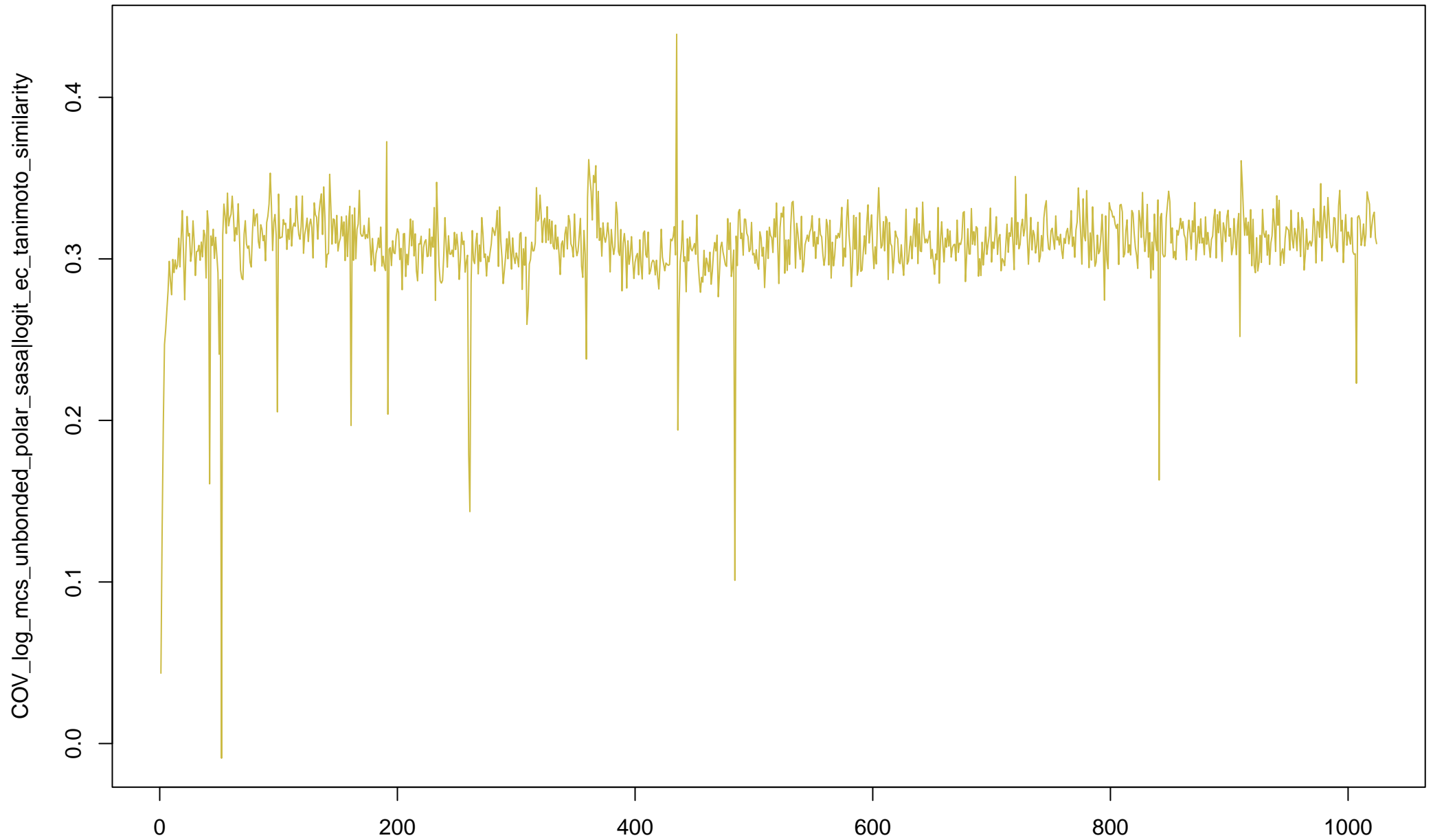
**COV\_log\_RMSD|docked\_NumRotatableBonds**  
**ESS = 94.7 | BMK = 0.119 | MCSE(6.27) = 8.63 | stat: TRUE | burn: 0**



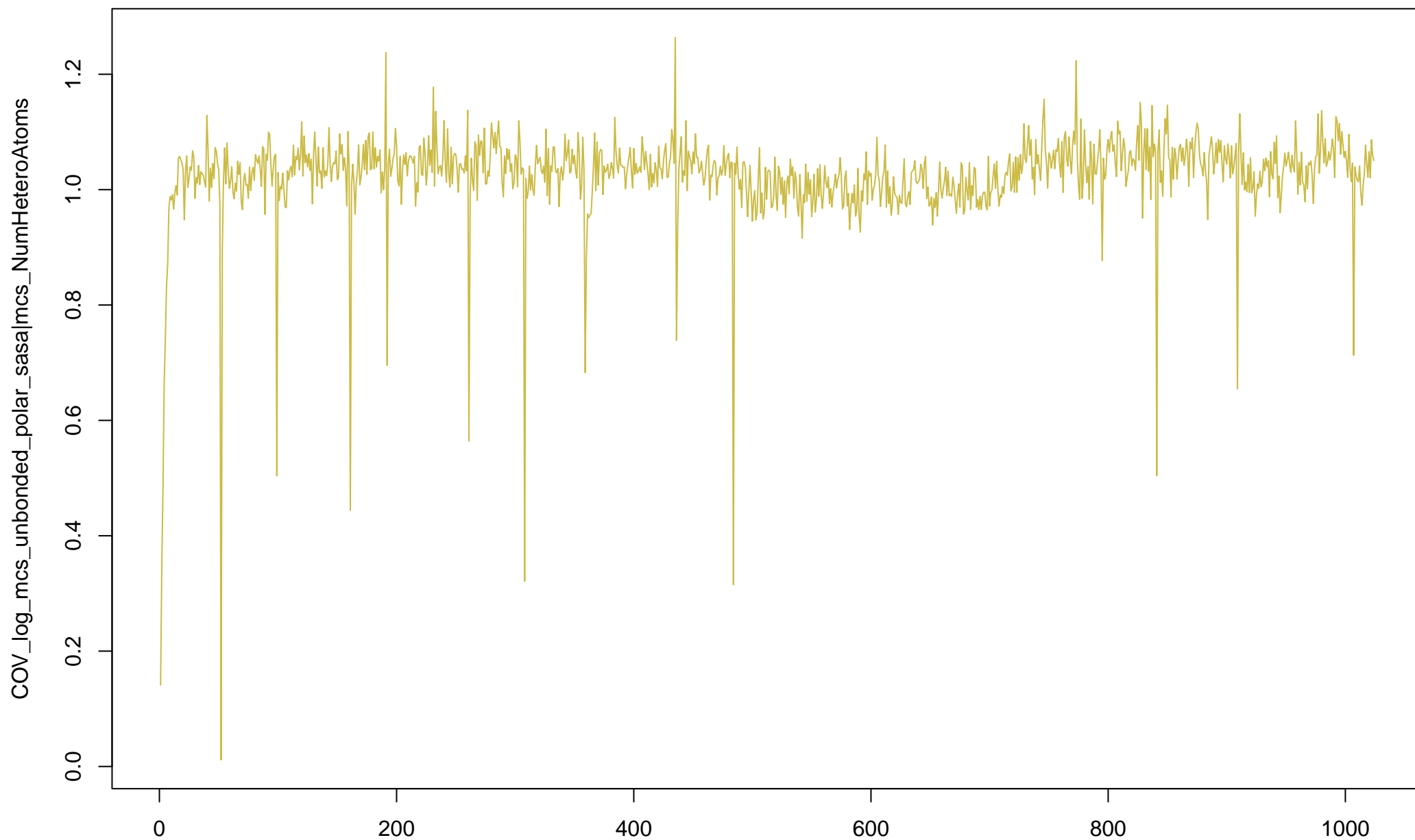
COV\_log\_RMSD|mcs\_NOCount  
ESS = 134 | BMK = 0.139 | MCSE(6.27) = 8.13 | stat: FALSE | burn: 0



**COV\_log\_mcs\_unbonded\_polar\_sasa|logit\_ec\_tanimoto\_similarity**  
**ESS = 463 | BMK = 0.181 | MCSE(6.27) = 5.65 | stat: FALSE | burn: 0**

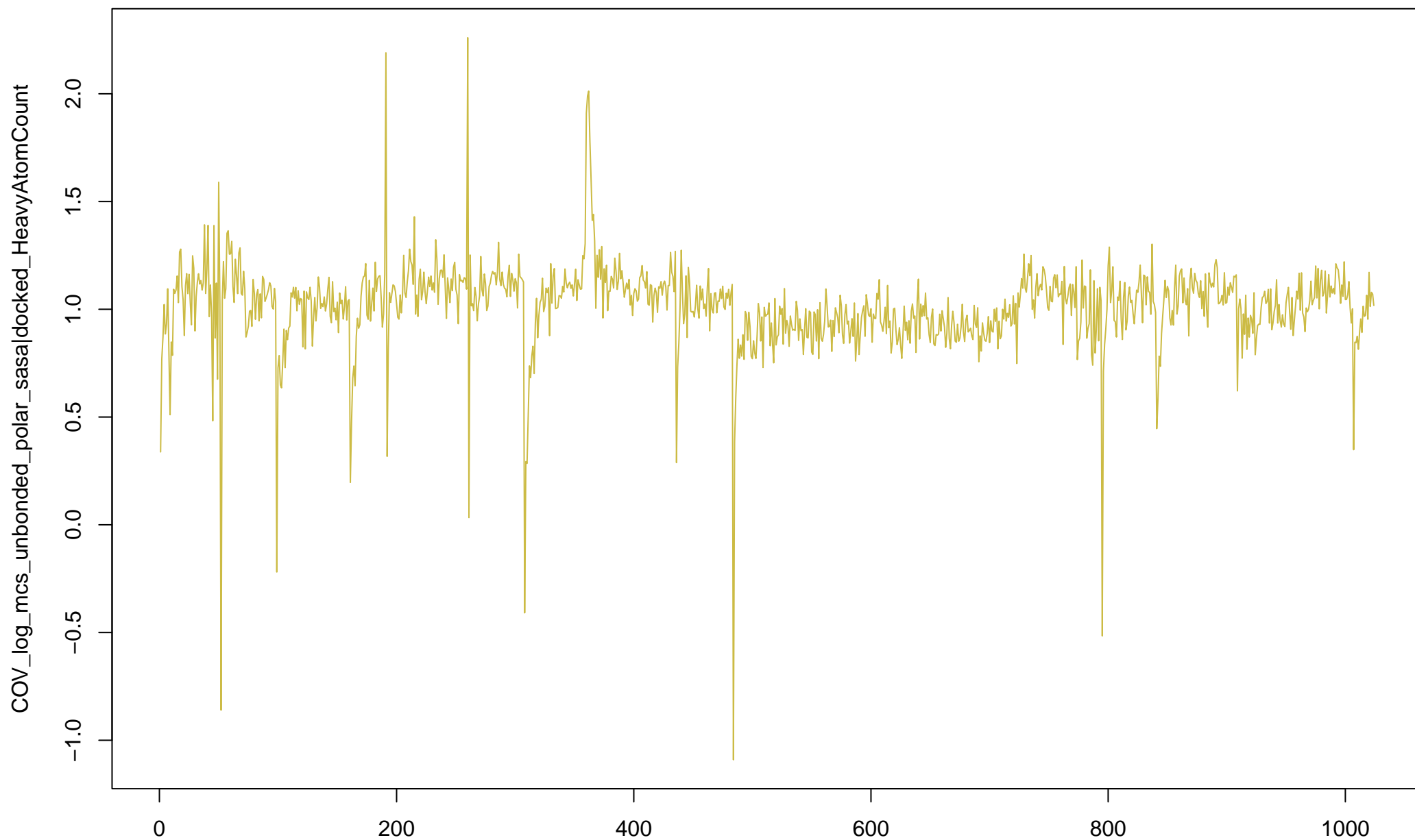


COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms  
ESS = 345 | BMK = 0.163 | MCSE(6.27) = 6.01 | stat: TRUE | burn: 714

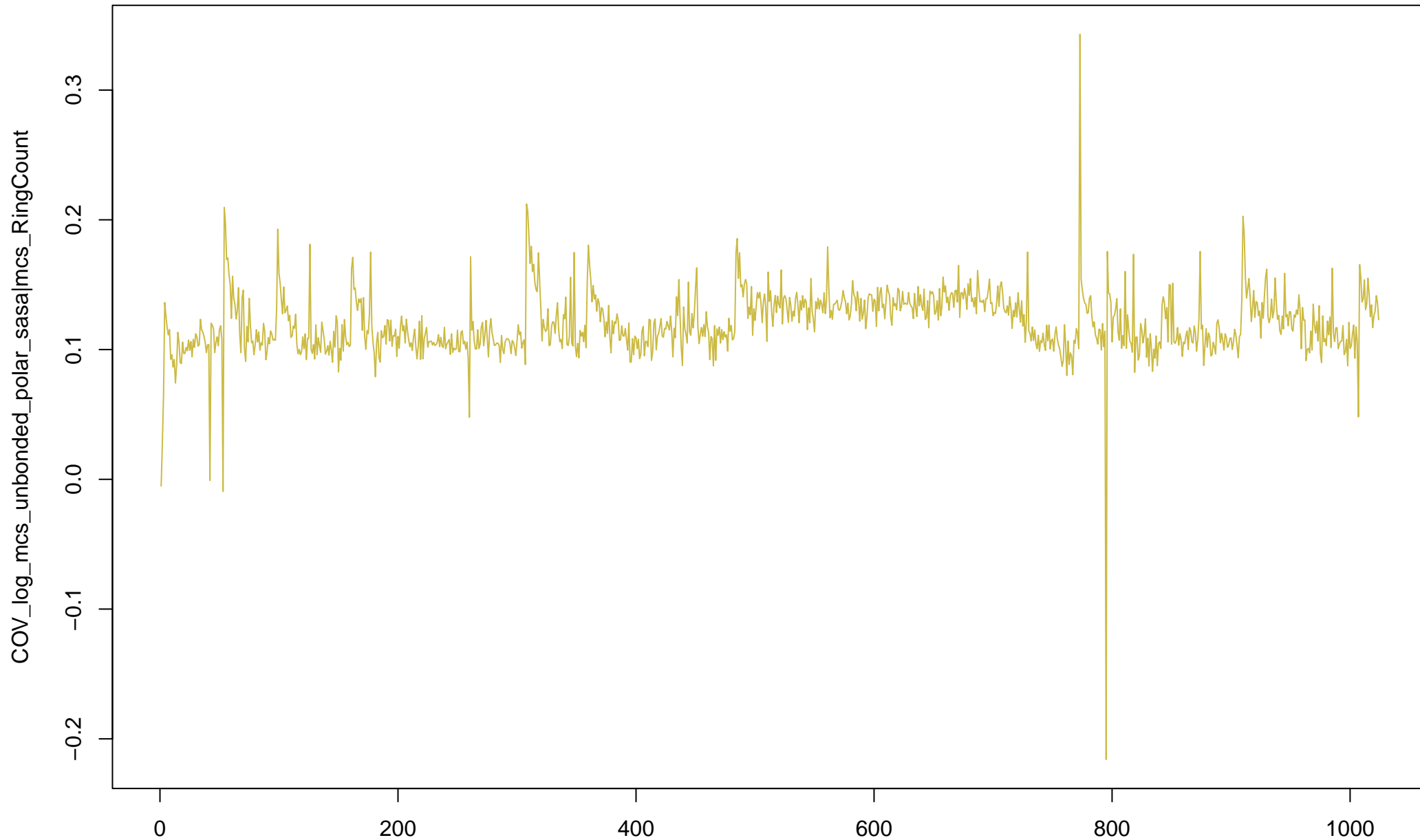




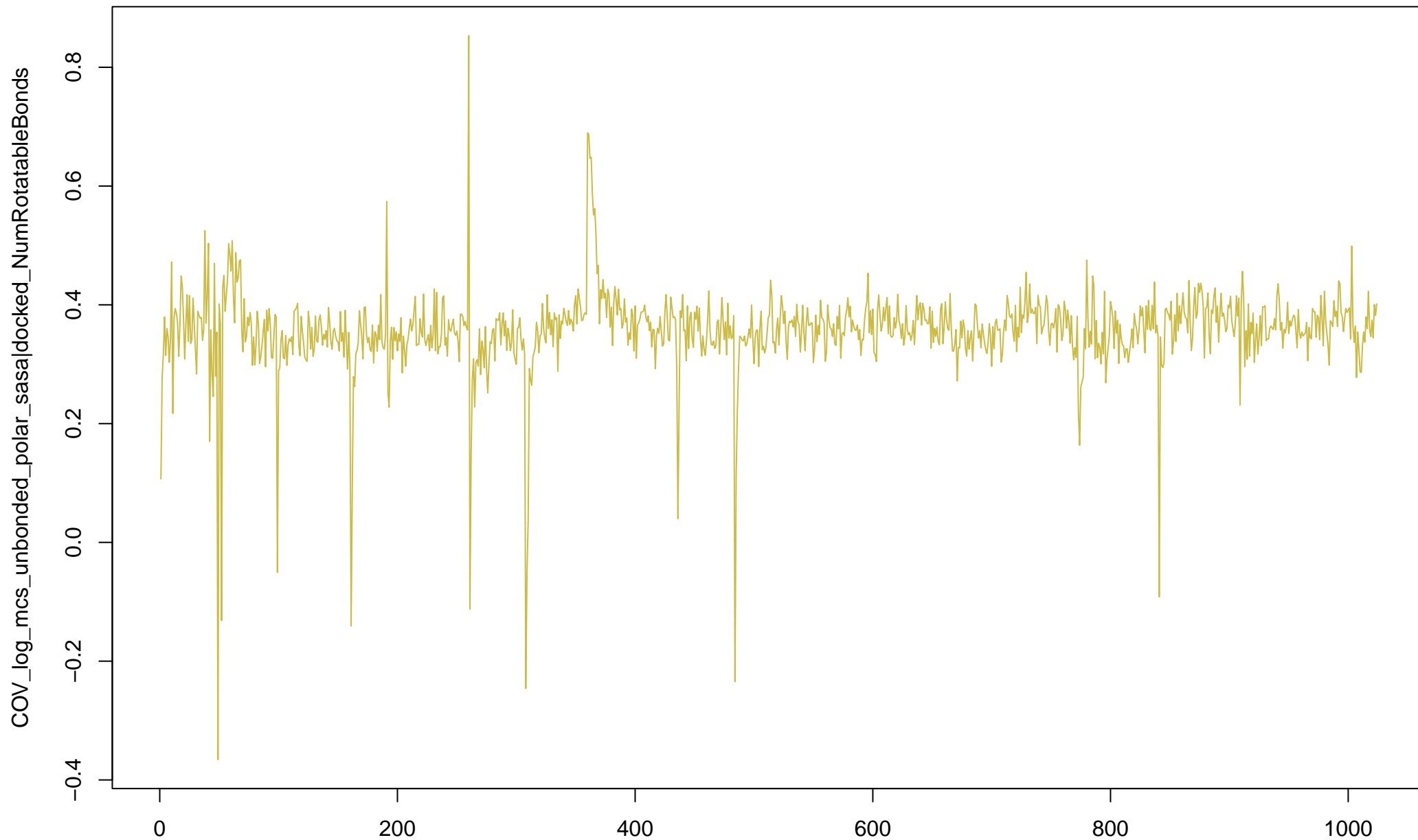
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 169 | BMK = 0.275 | MCSE(6.27) = 7.71 | stat: TRUE | burn: 0**



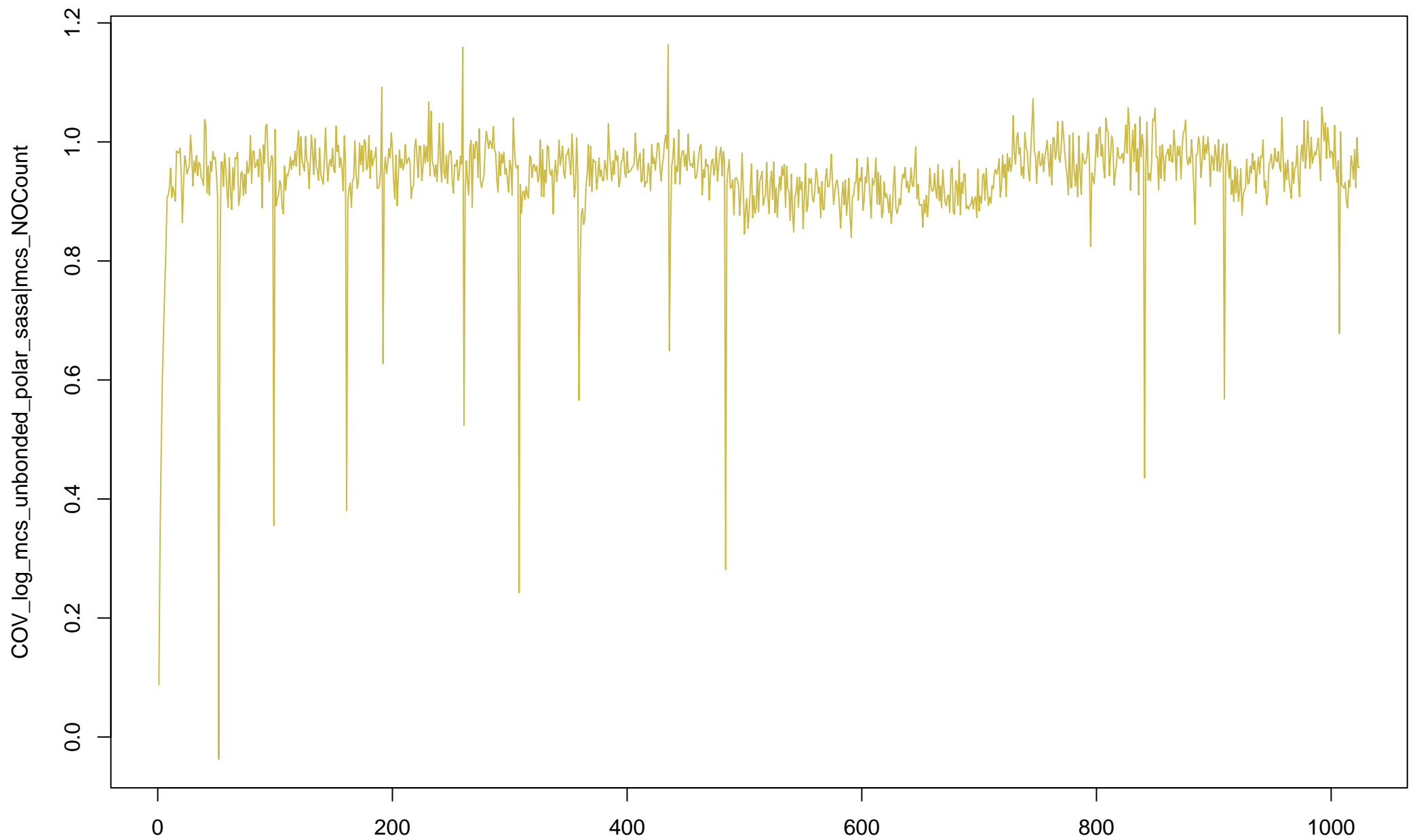
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_RingCount**  
**ESS = 83.6 | BMK = 0.269 | MCSE(6.27) = 8.45 | stat: FALSE | burn: 714**



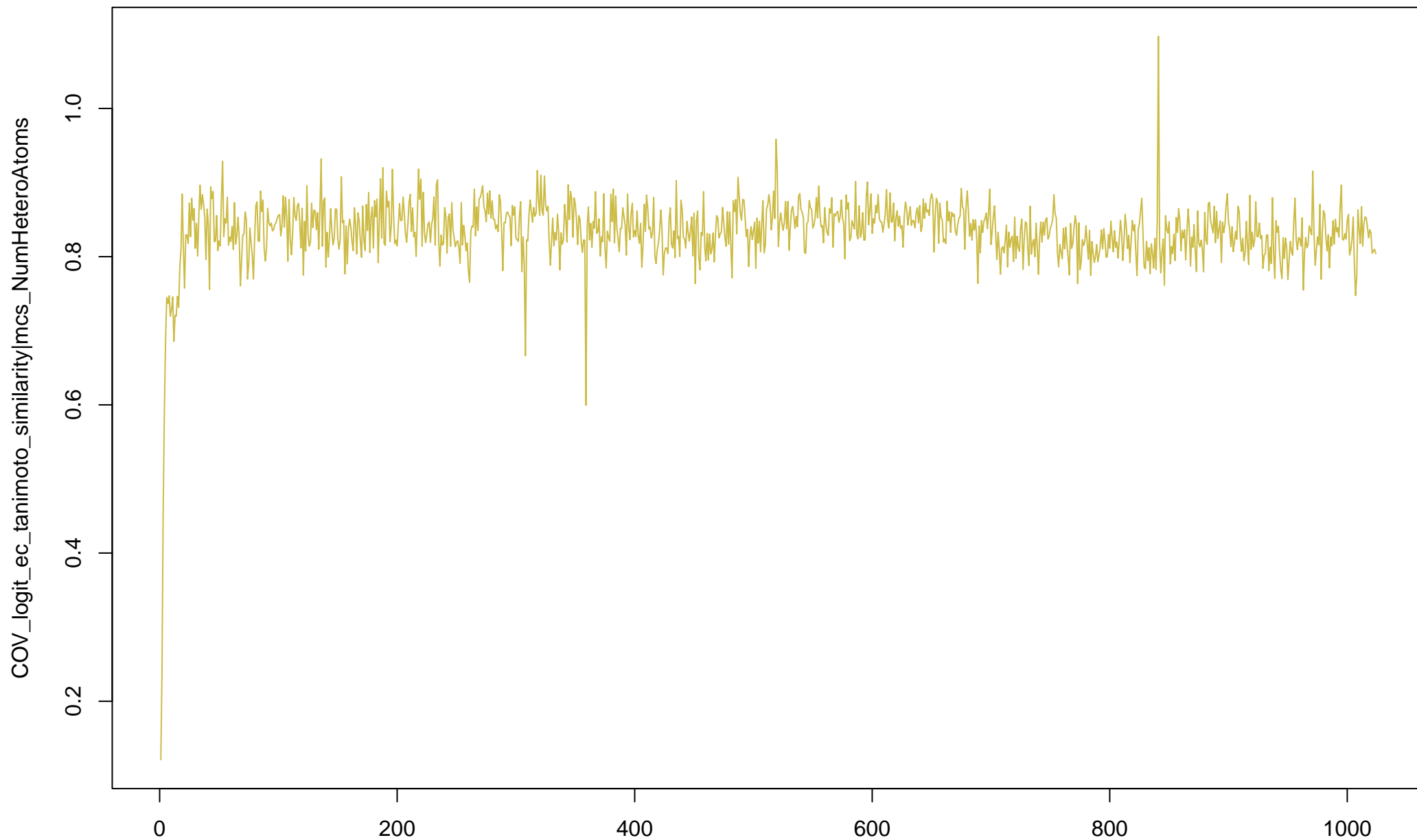
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_NumRotatableBonds**  
**ESS = 295 | BMK = 0.192 | MCSE(6.27) = 6.42 | stat: TRUE | burn: 0**



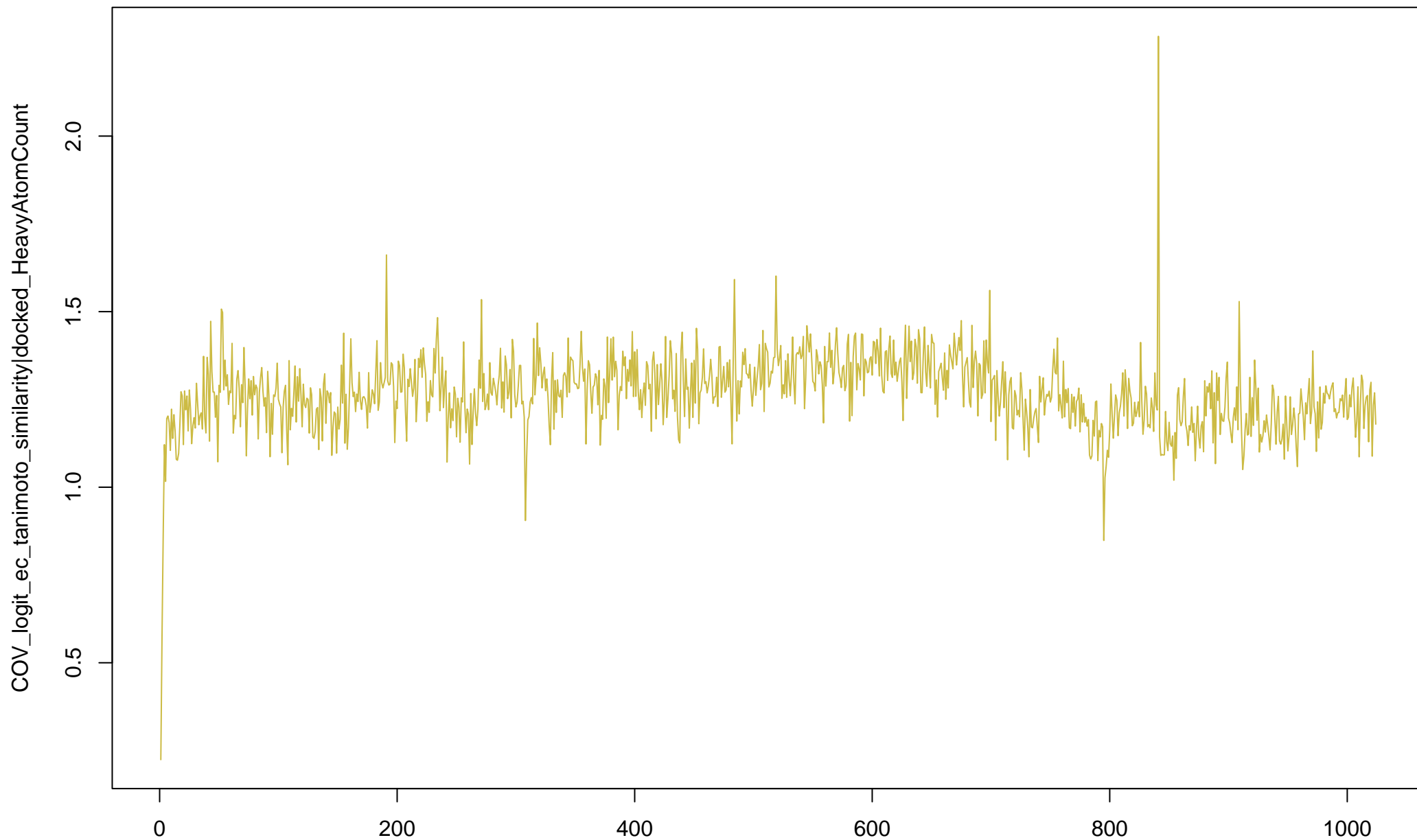
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NOCount**  
**ESS = 334 | BMK = 0.18 | MCSE(6.27) = 6.13 | stat: TRUE | burn: 714**



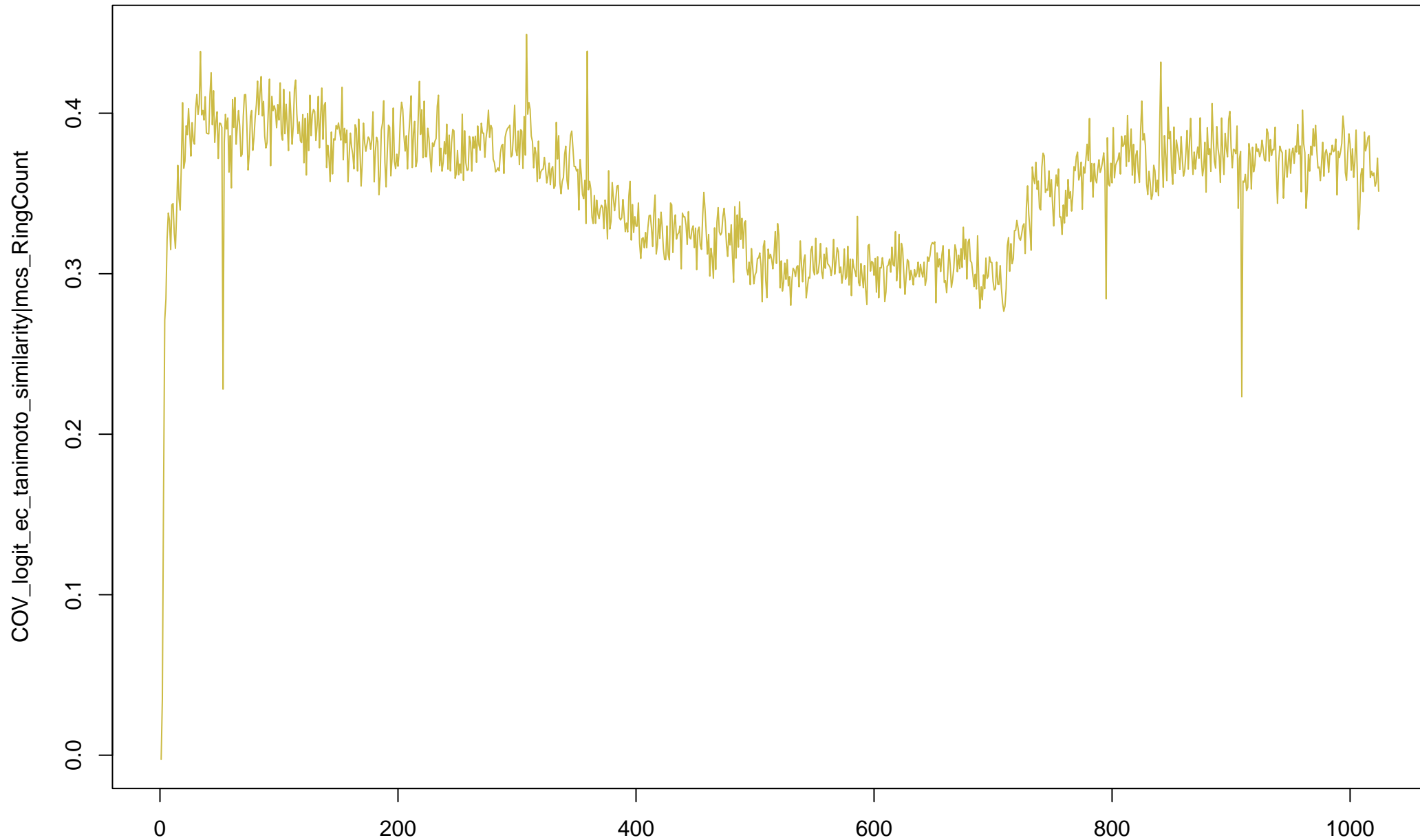
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms**  
**ESS = 134 | BMK = 0.157 | MCSE(6.27) = 8.33 | stat: TRUE | burn: 0**



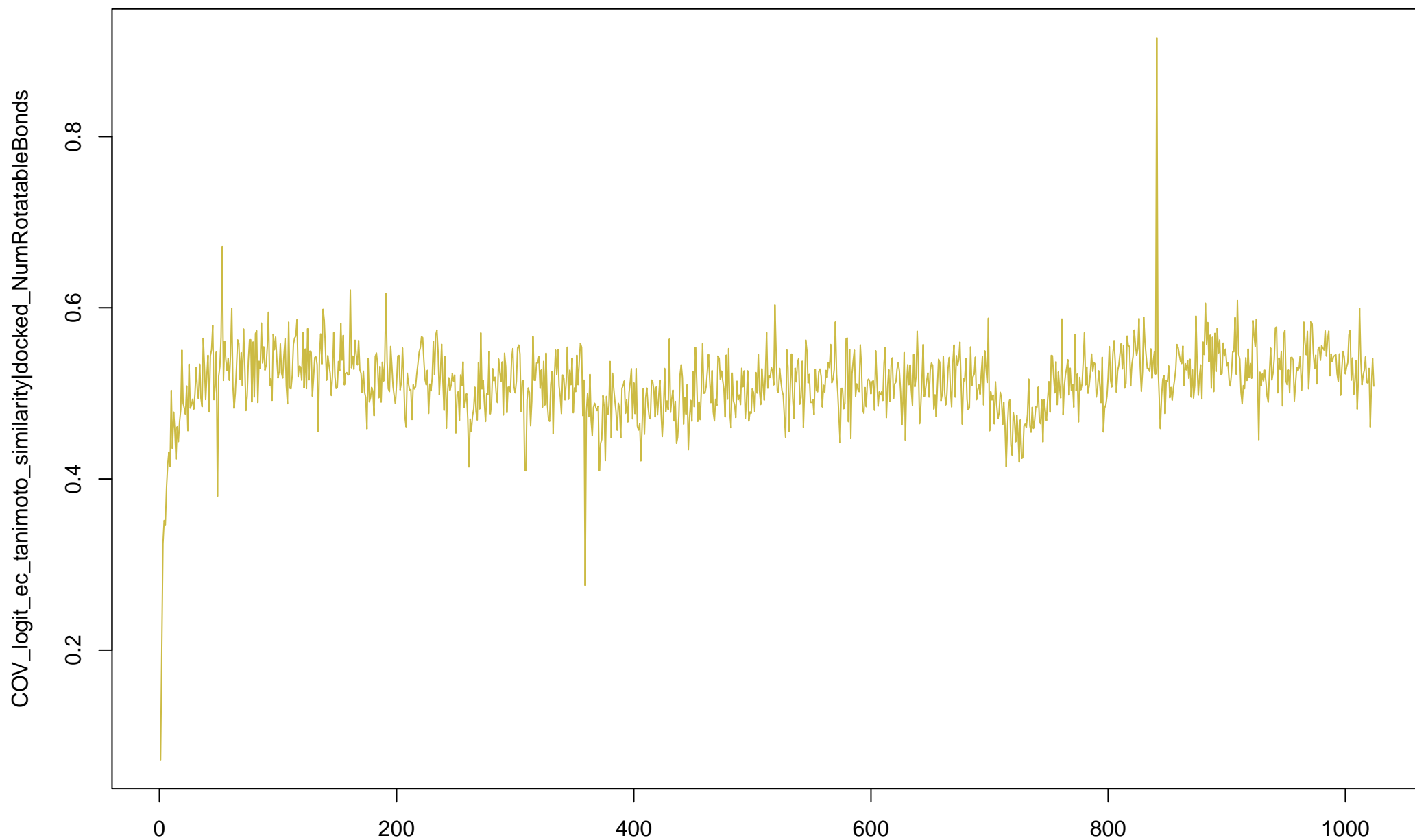
**COV\_logit\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount**  
**ESS = 44.9 | BMK = 0.124 | MCSE(6.27) = 9.72 | stat: TRUE | burn: 0**



**COV\_logit\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 9.92 | BMK = 0.292 | MCSE(6.27) = 14.6 | stat: FALSE | burn: 714**

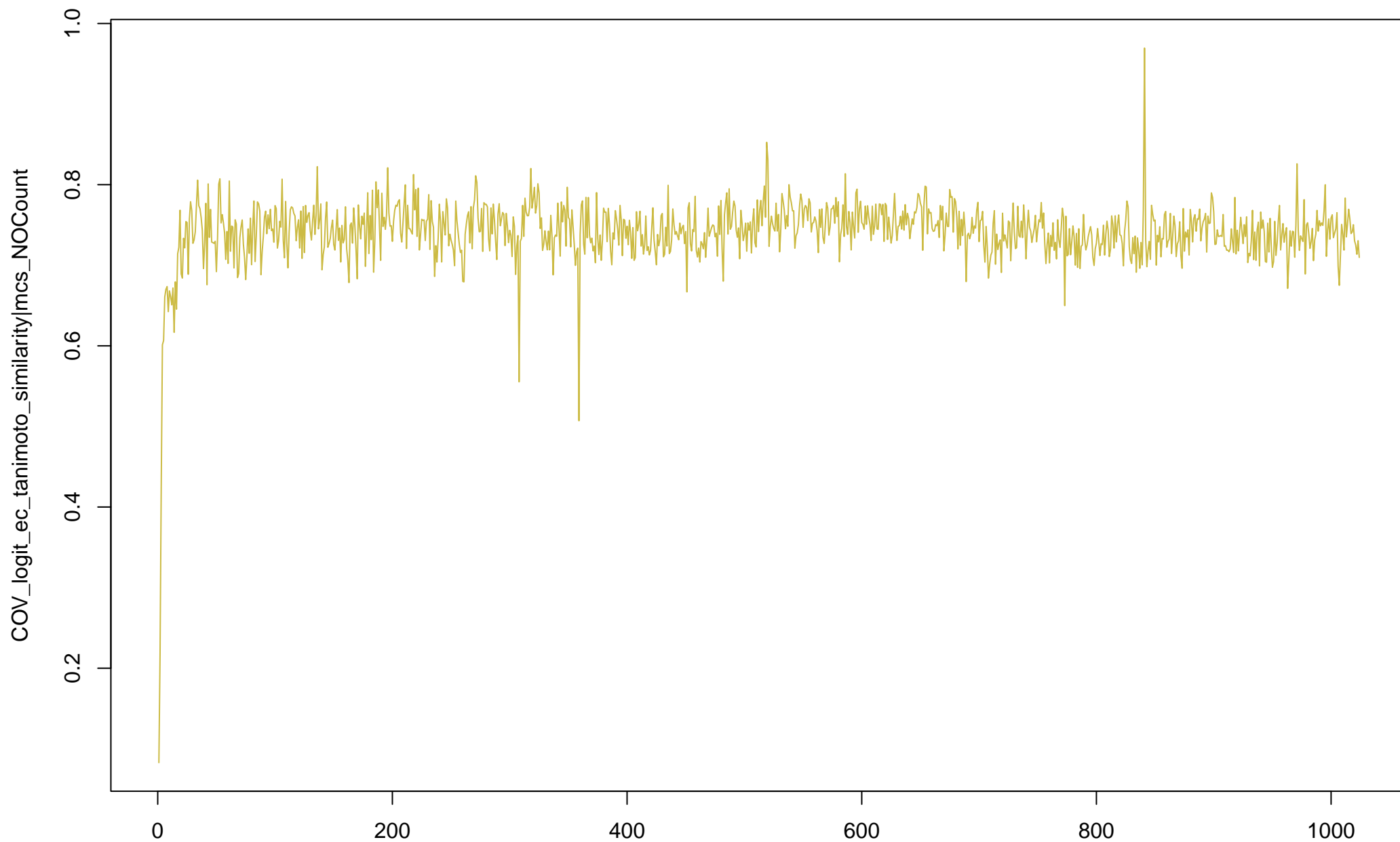


**COV\_logit\_ec\_tanimoto\_similarity|docked\_NumRotatableBonds**  
**ESS = 83.5 | BMK = 0.139 | MCSE(6.27) = 9.6 | stat: TRUE | burn: 0**

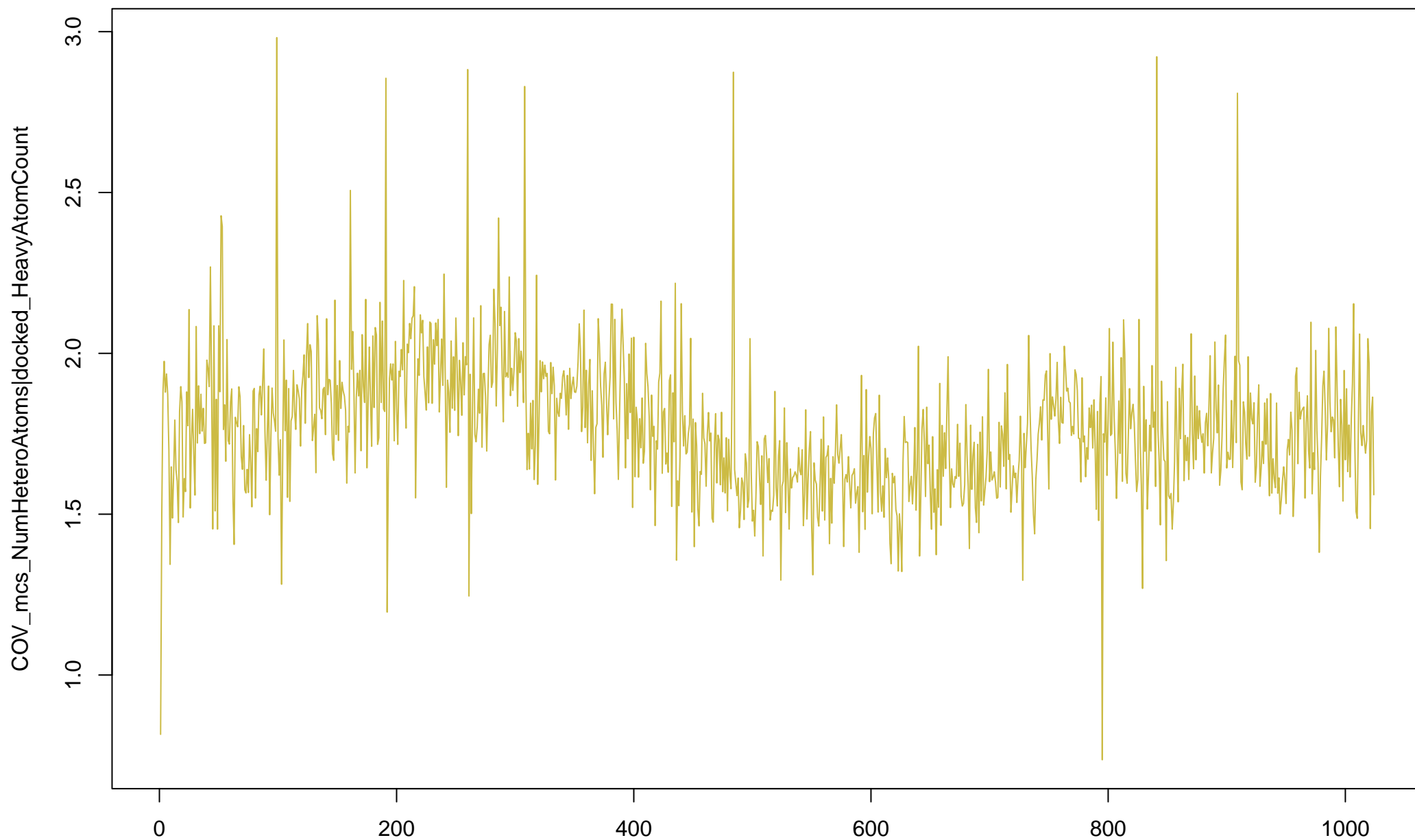




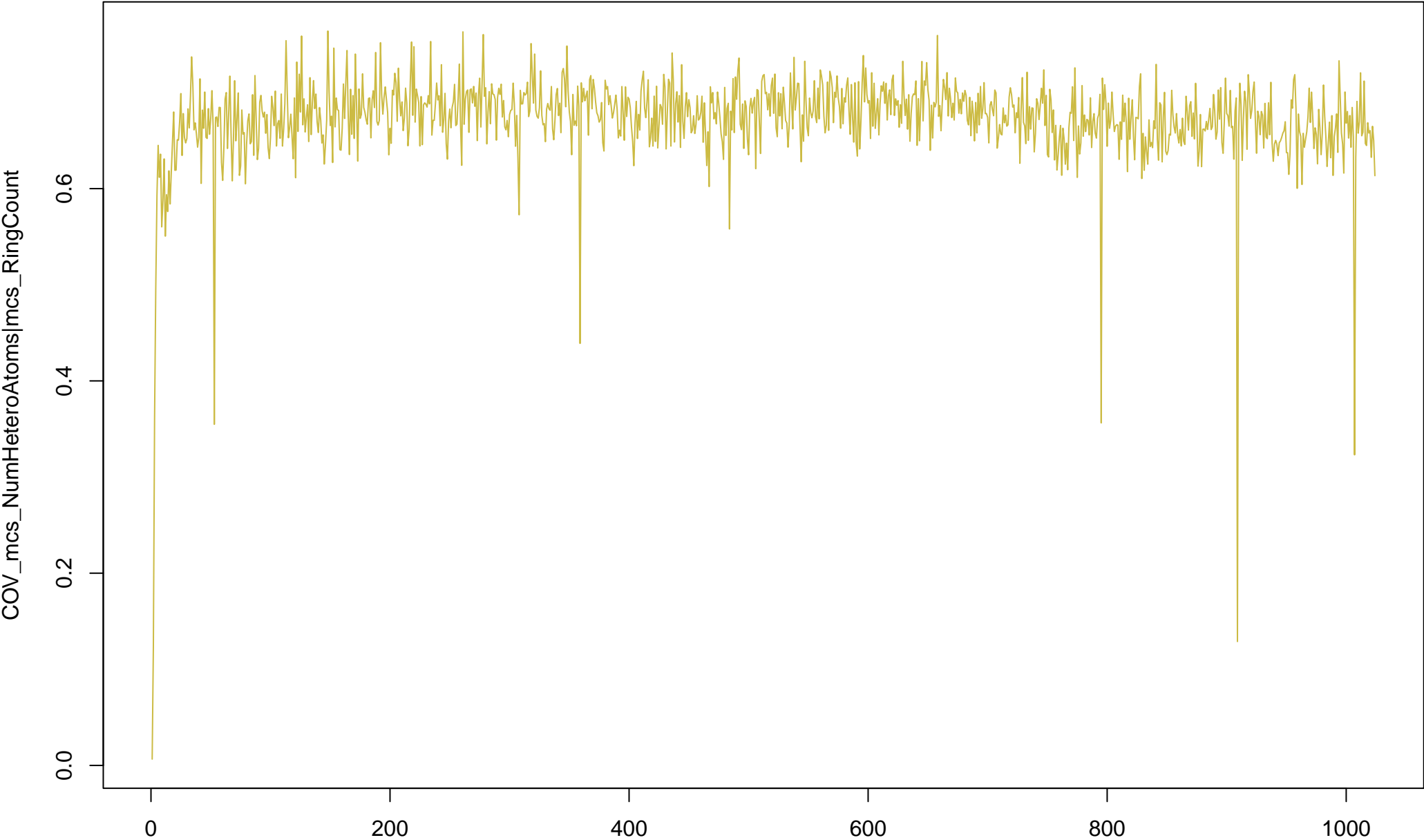
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NOCount**  
**ESS = 186 | BMK = 0.142 | MCSE(6.27) = 7.88 | stat: TRUE | burn: 0**



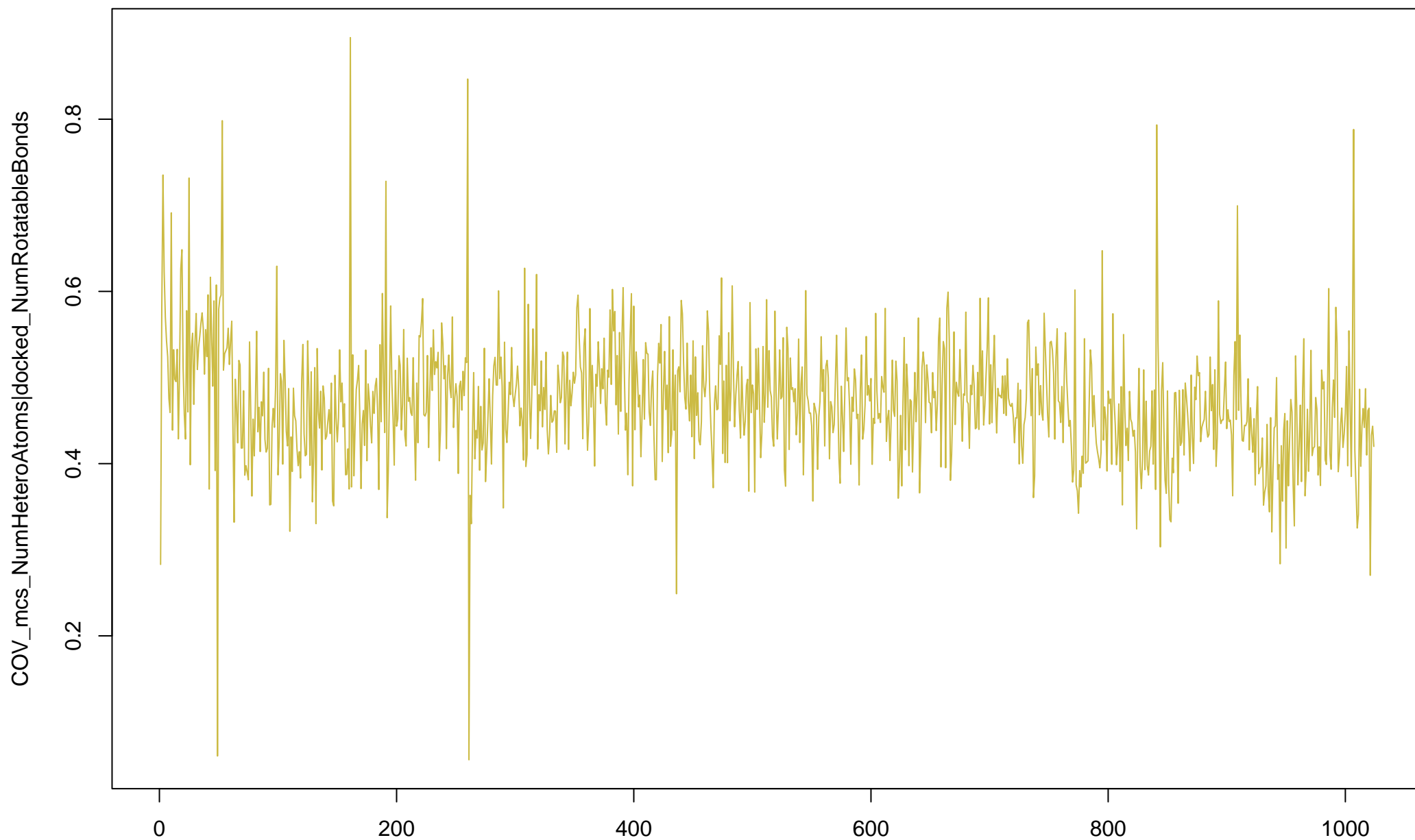
**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 33.5 | BMK = 0.272 | MCSE(6.27) = 9.22 | stat: TRUE | burn: 0**



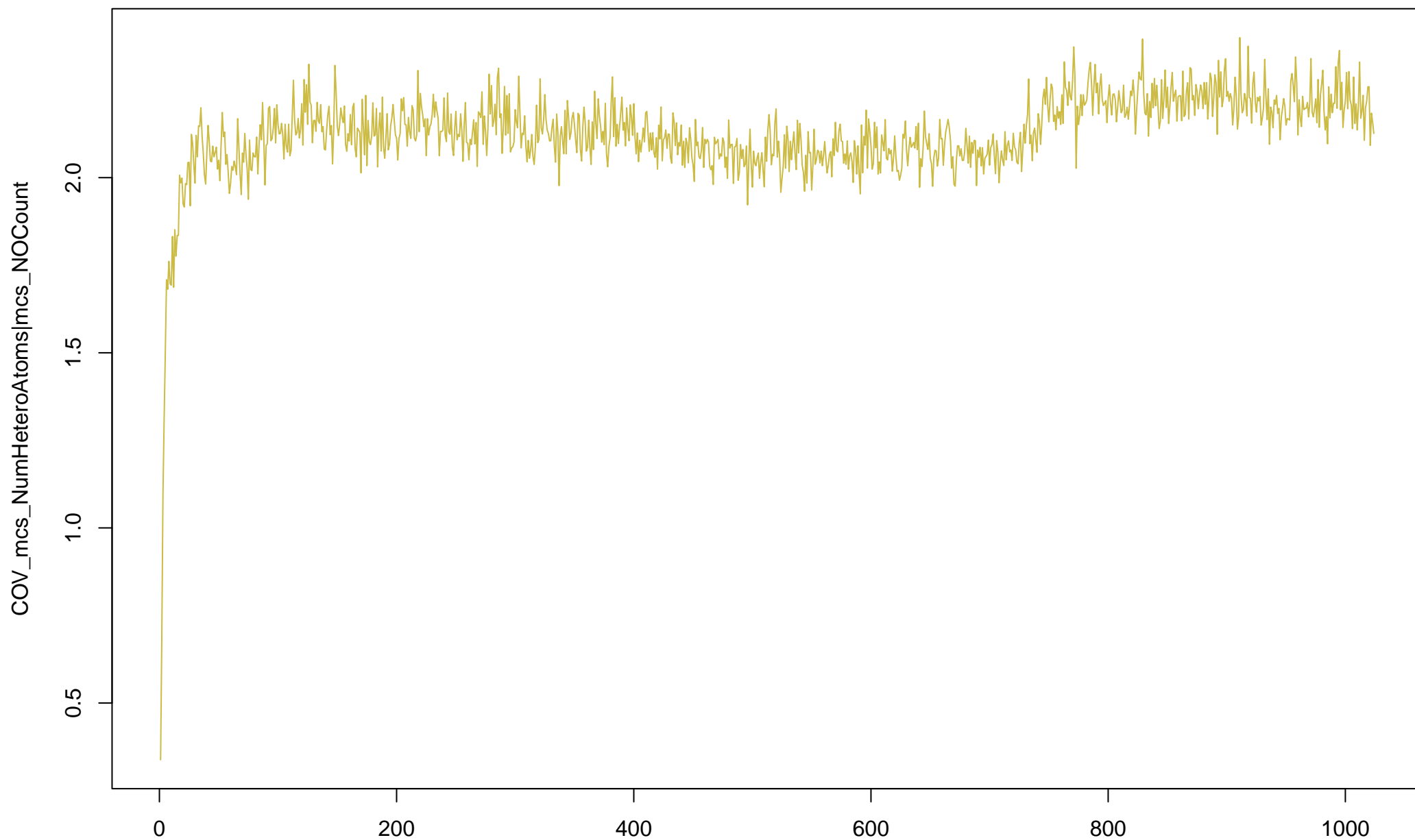
**COV\_mcs\_NumHeteroAtoms|mcs\_RingCount**  
**ESS = 186 | BMK = 0.134 | MCSE(6.27) = 7.29 | stat: FALSE | burn: 0**



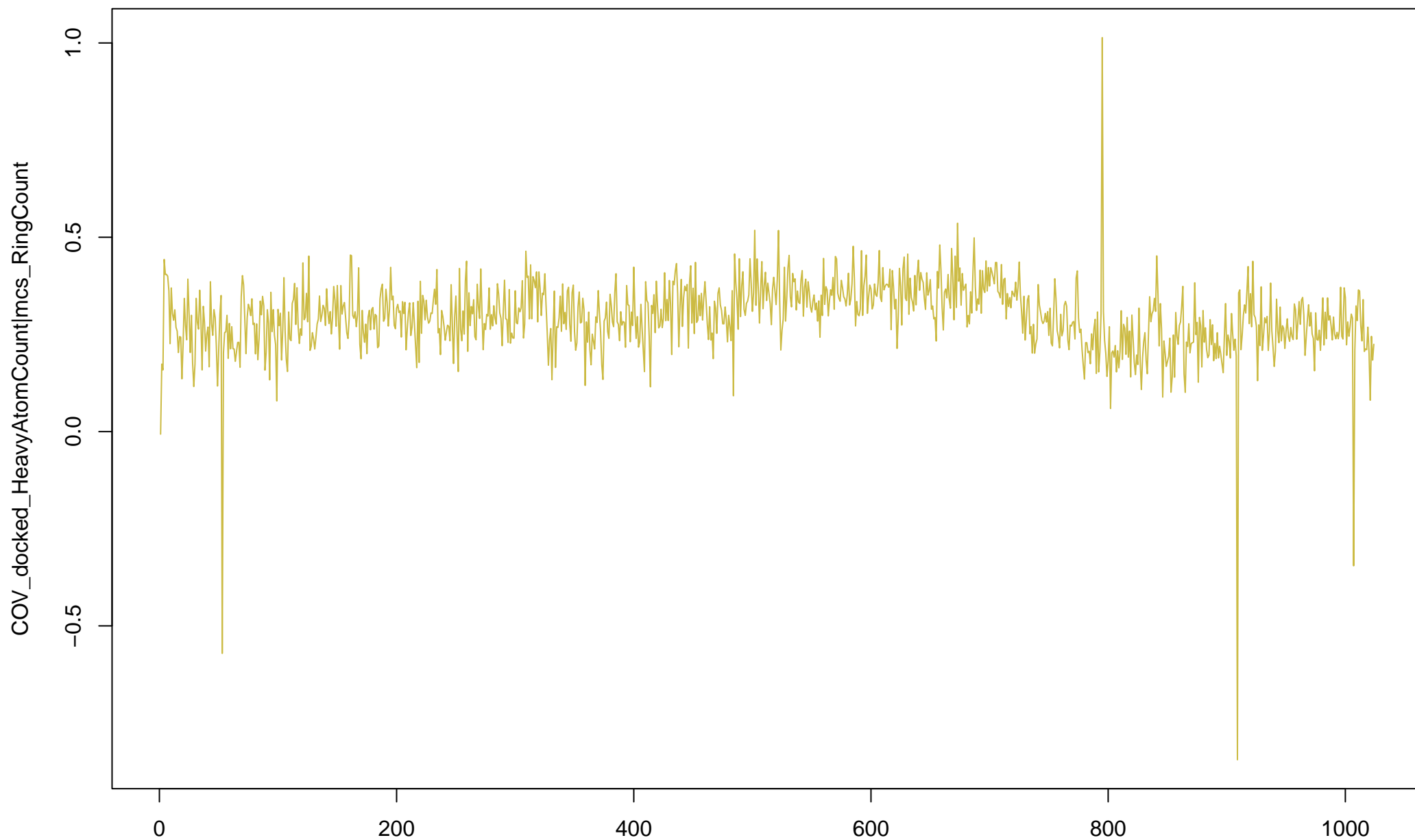
**COV\_mcs\_NumHeteroAtoms|docked\_NumRotatableBonds**  
**ESS = 131 | BMK = 0.151 | MCSE(6.27) = 6.53 | stat: FALSE | burn: 0**



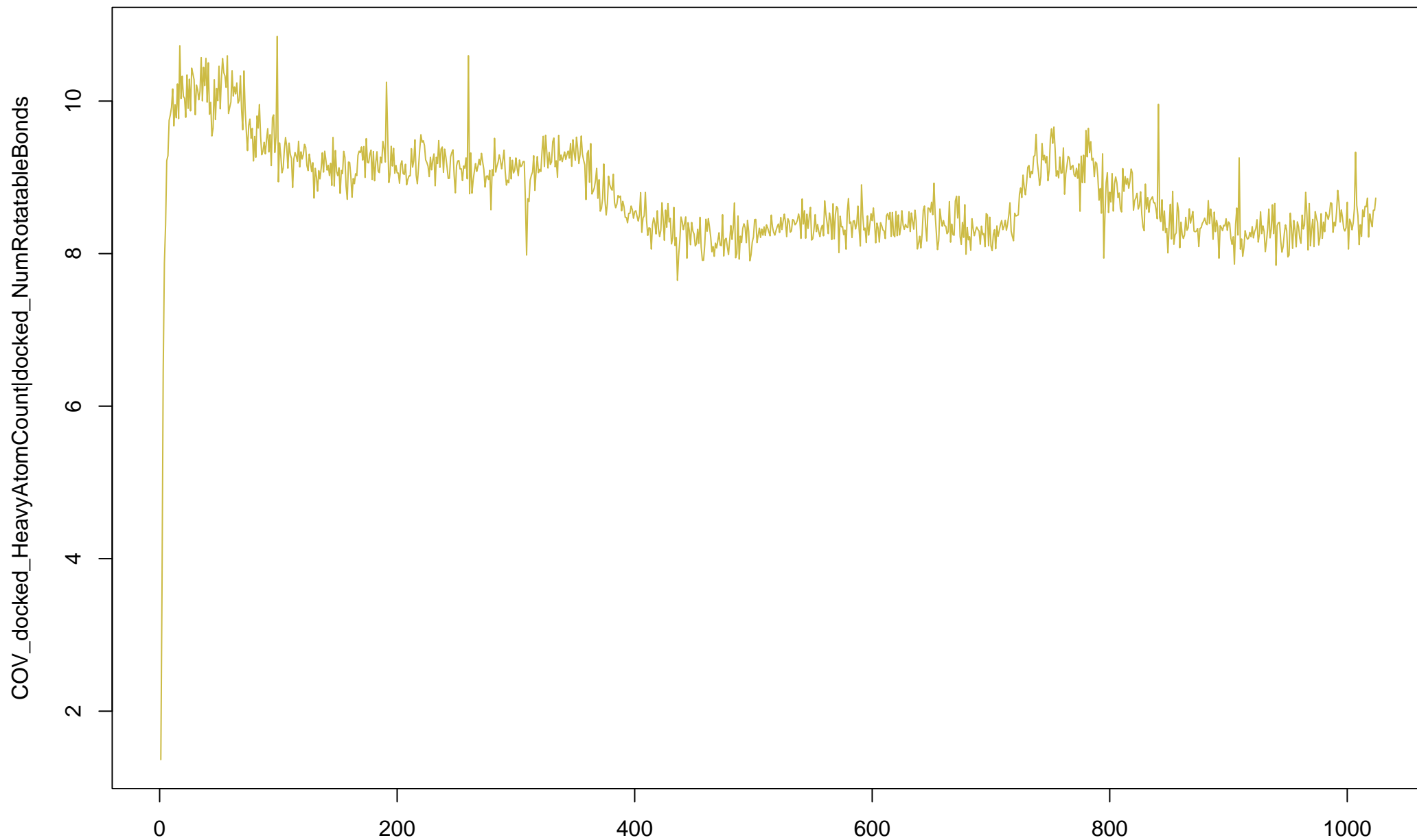
**COV\_mcs\_NumHeteroAtoms|mcs\_NOCount**  
**ESS = 45 | BMK = 0.257 | MCSE(6.27) = 12.6 | stat: FALSE | burn: 714**



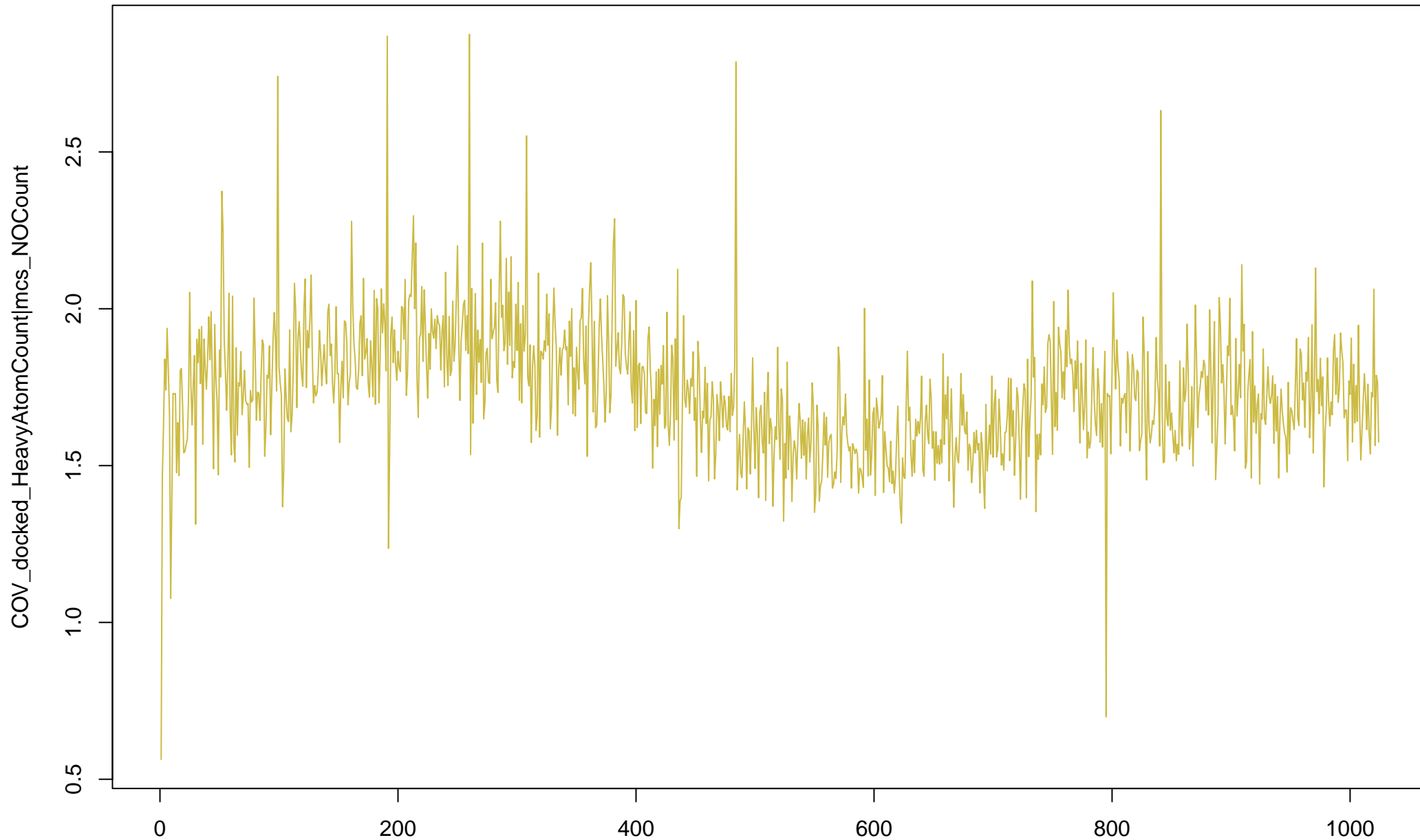
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 63.4 | BMK = 0.117 | MCSE(6.27) = 8.55 | stat: FALSE | burn: 0**



**COV\_docked\_HeavyAtomCount|docked\_NumRotatableBonds**  
**ESS = 15.3 | BMK = 0.447 | MCSE(6.27) = 13.7 | stat: FALSE | burn: 816**

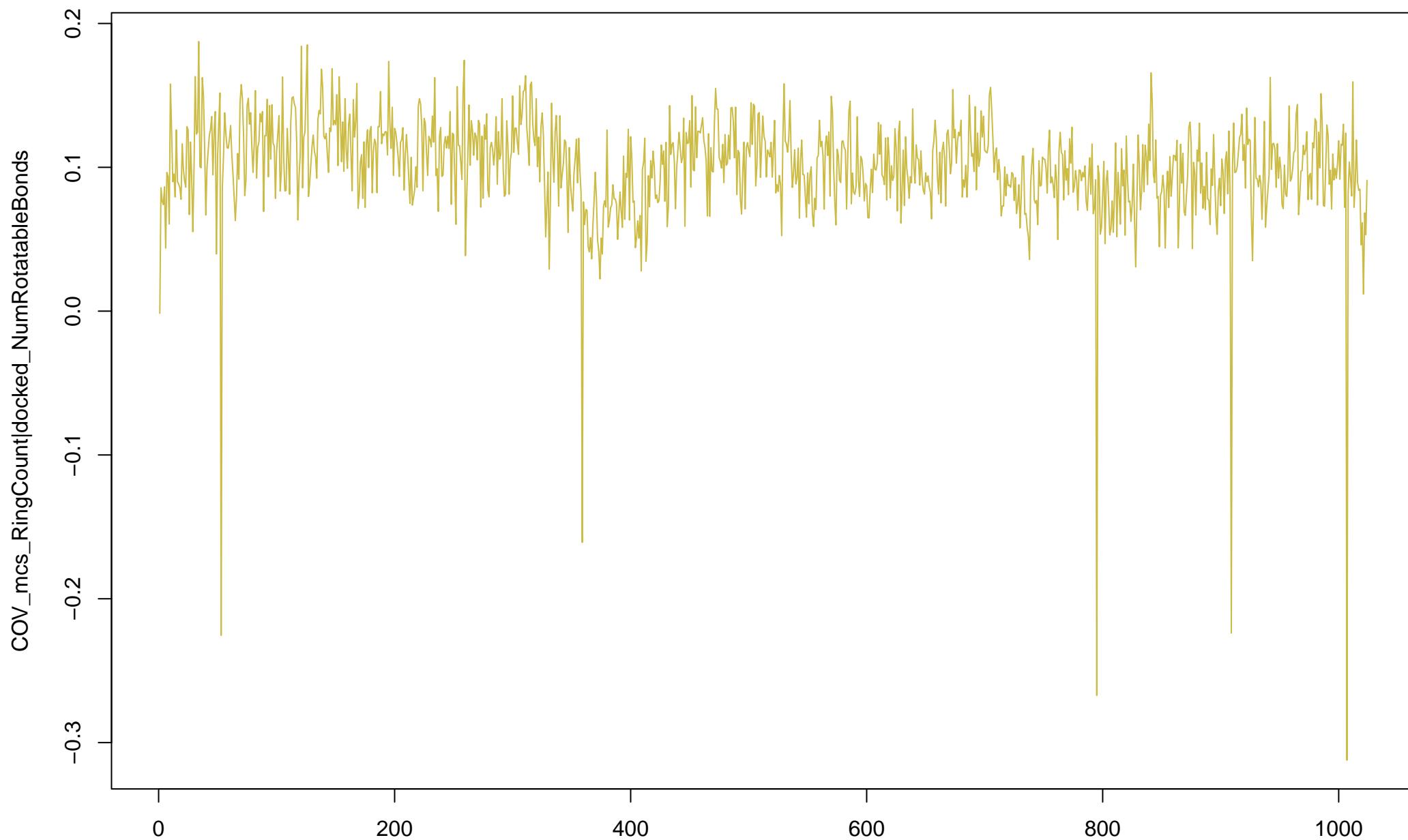


**COV\_docked\_HeavyAtomCount|mcs\_NOCount**  
**ESS = 15.7 | BMK = 0.316 | MCSE(6.27) = 10.2 | stat: FALSE | burn: 0**

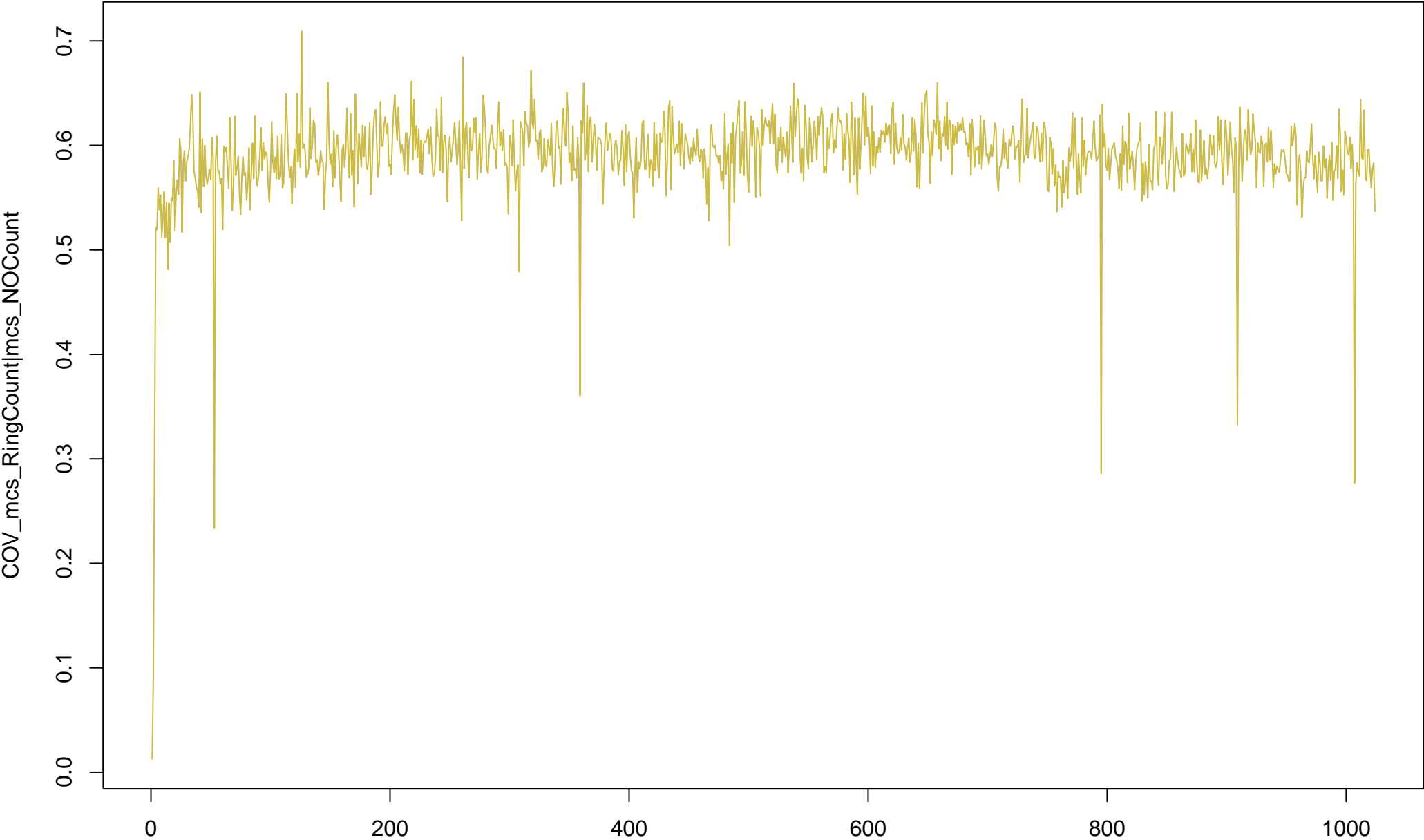




**COV\_mcs\_RingCount|docked\_NumRotatableBonds**  
**ESS = 101 | BMK = 0.196 | MCSE(6.27) = 7.3 | stat: FALSE | burn: 0**



**COV\_mcs\_RingCount|mcs\_NOCount**  
**ESS = 183 | BMK = 0.153 | MCSE(6.27) = 7.36 | stat: FALSE | burn: 0**



**COV\_docked\_NumRotatableBonds|mcs\_NOCount**  
**ESS = 231 | BMK = 0.224 | MCSE(6.27) = 6.85 | stat: FALSE | burn: 0**

