

-- STATS maxD --

min ESS = 9.9080767694803

max BMK = 0.465709874883969

max MCSE = 15.991870148243

all stationary: FALSE

burn: 306

-- STATS 2D --

min ESS = 10.6168323462166

max BMK = 0.328426258107277

max MCSE = 15.3535627515438

all stationary: FALSE

burn: 102

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.6761665872193

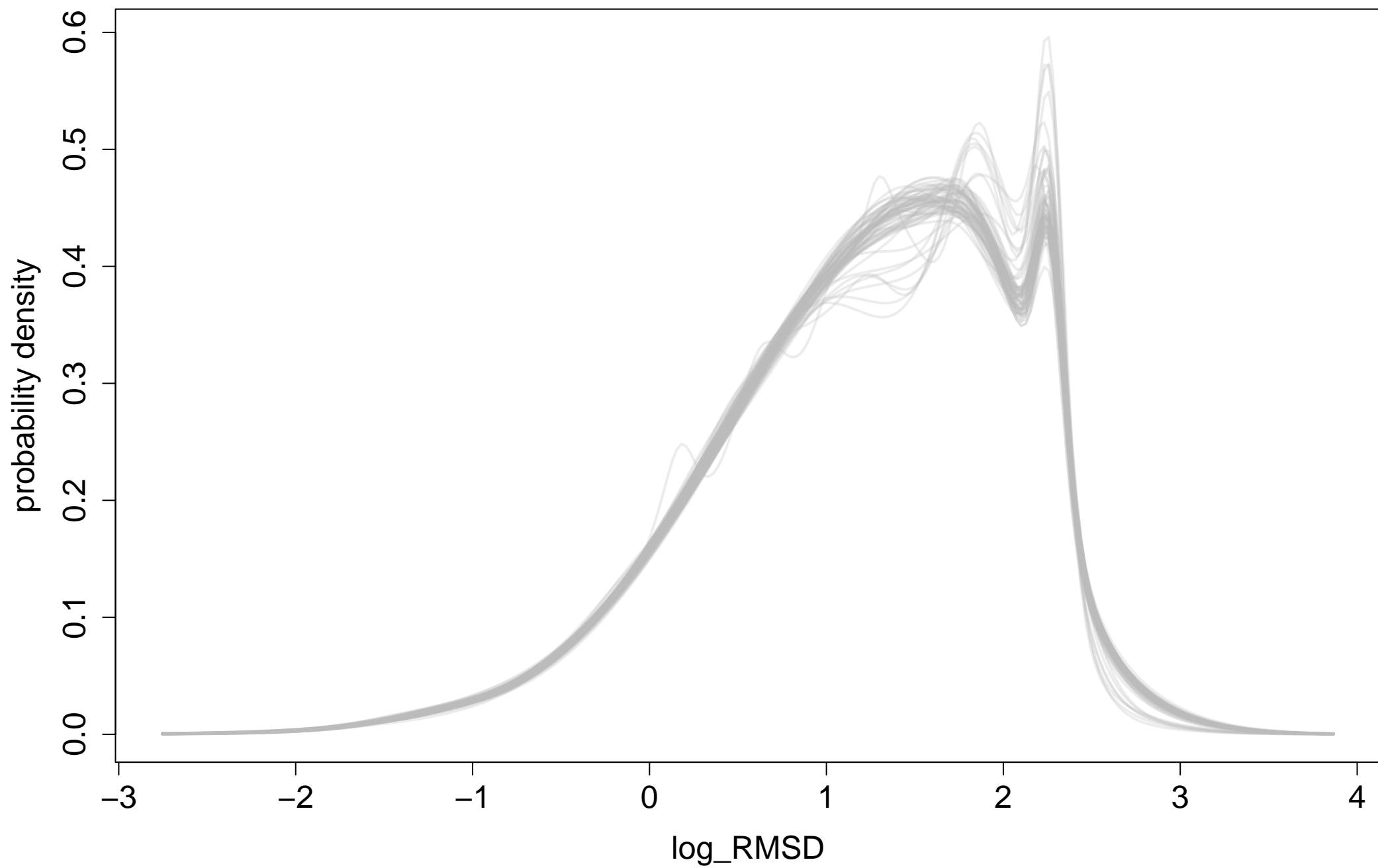
max MCSE = NaN

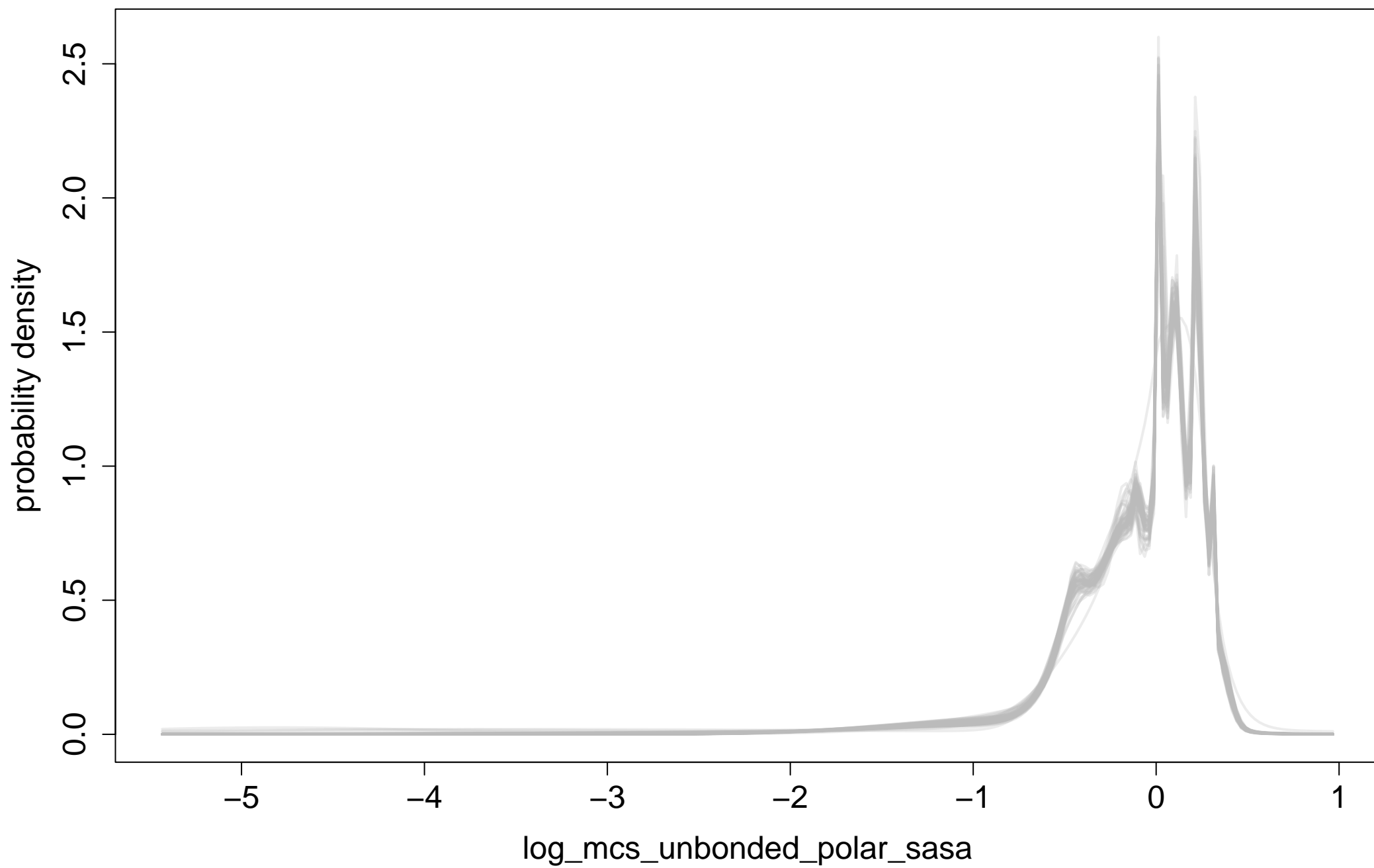
all stationary: FALSE

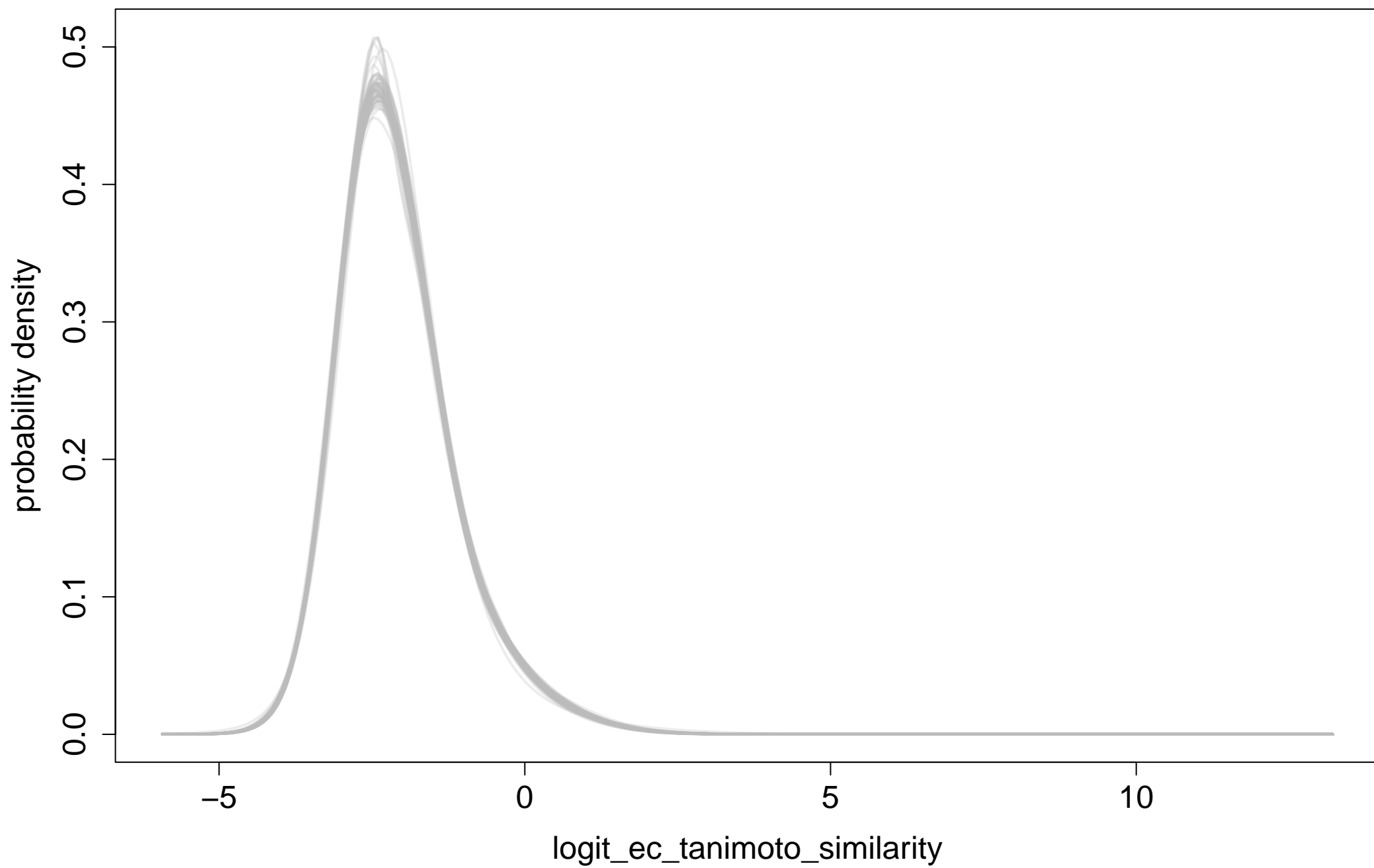
burn: 1020

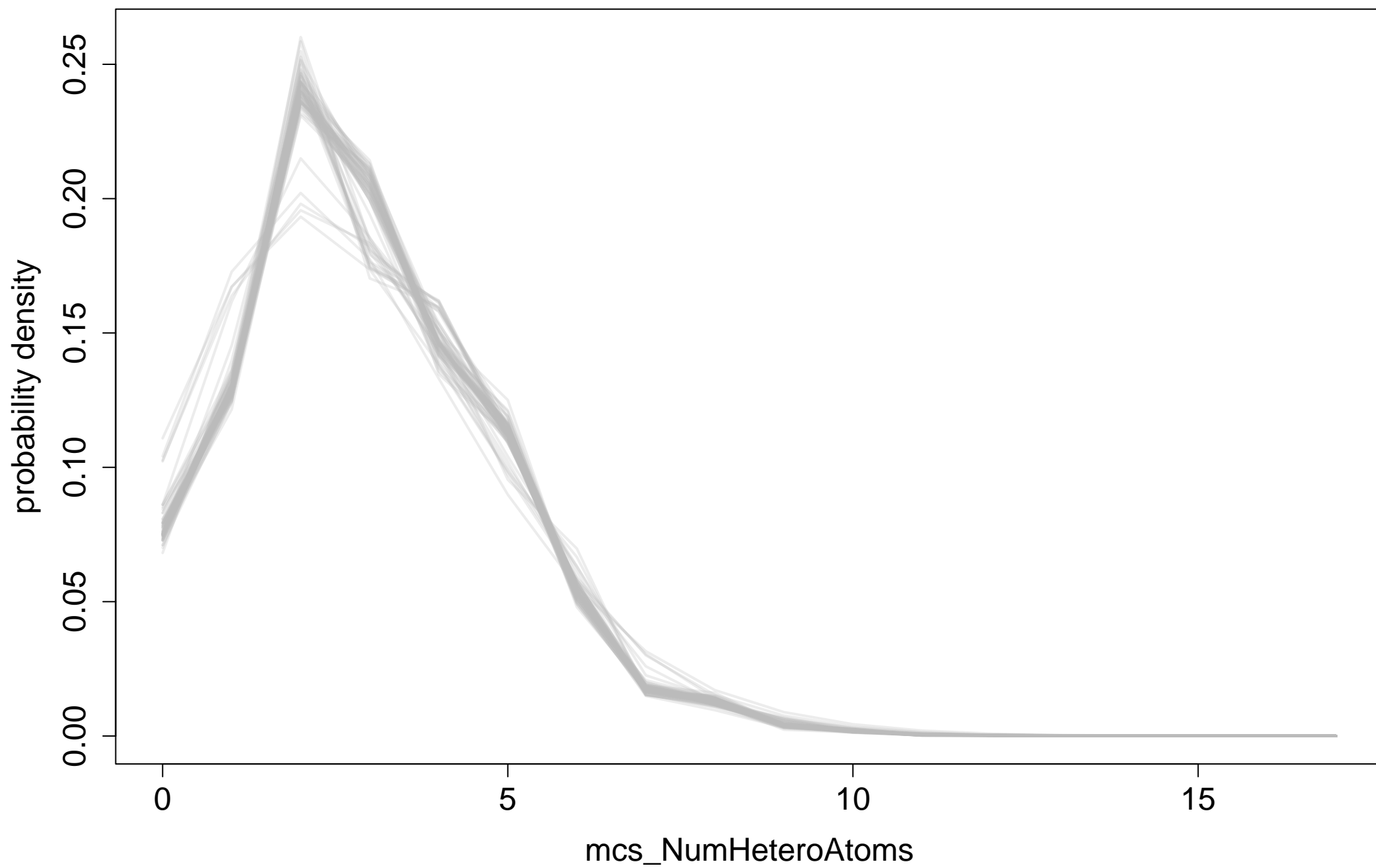
Occupied clusters: 52 of 64

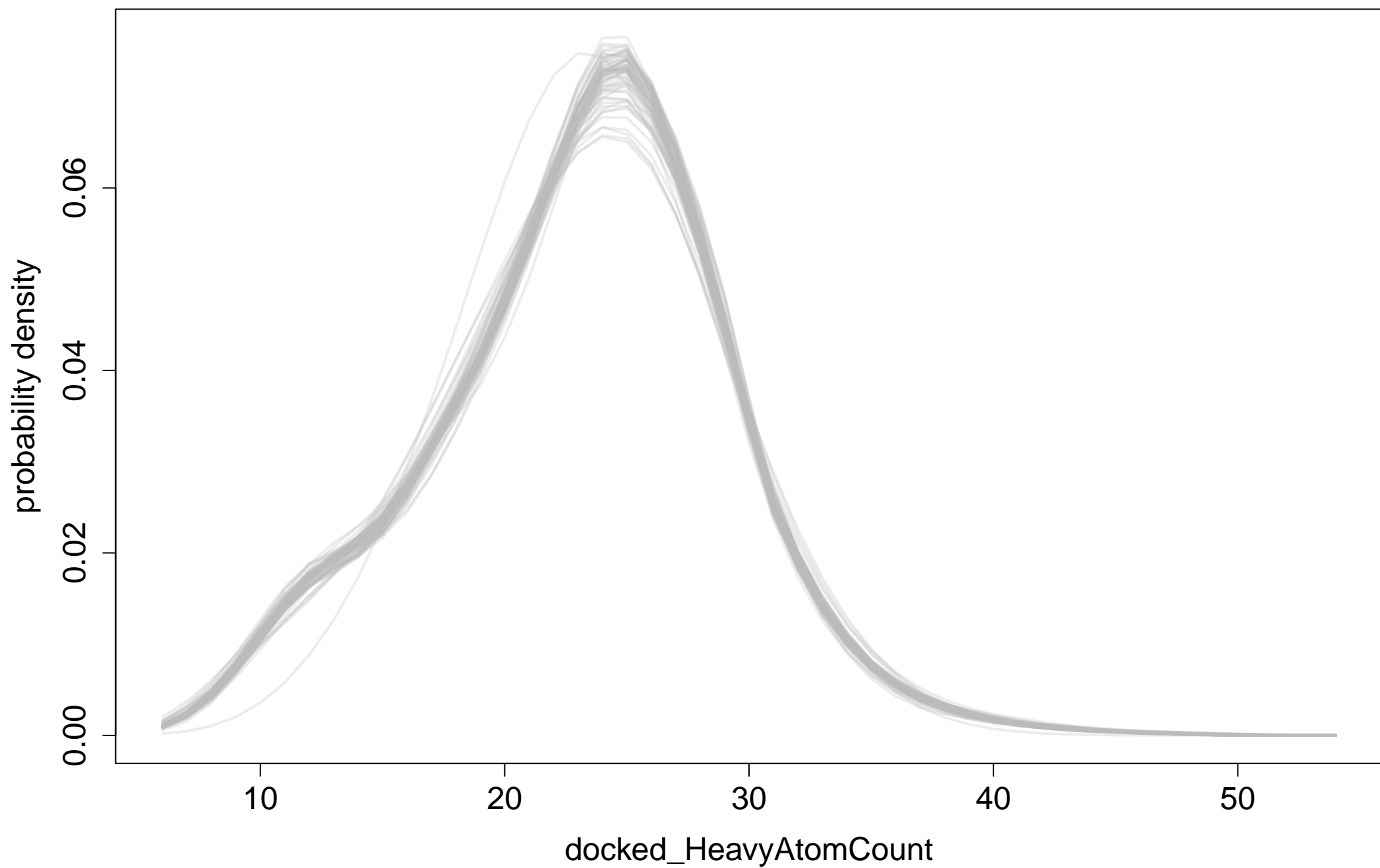
LL: -74600 +- 4630

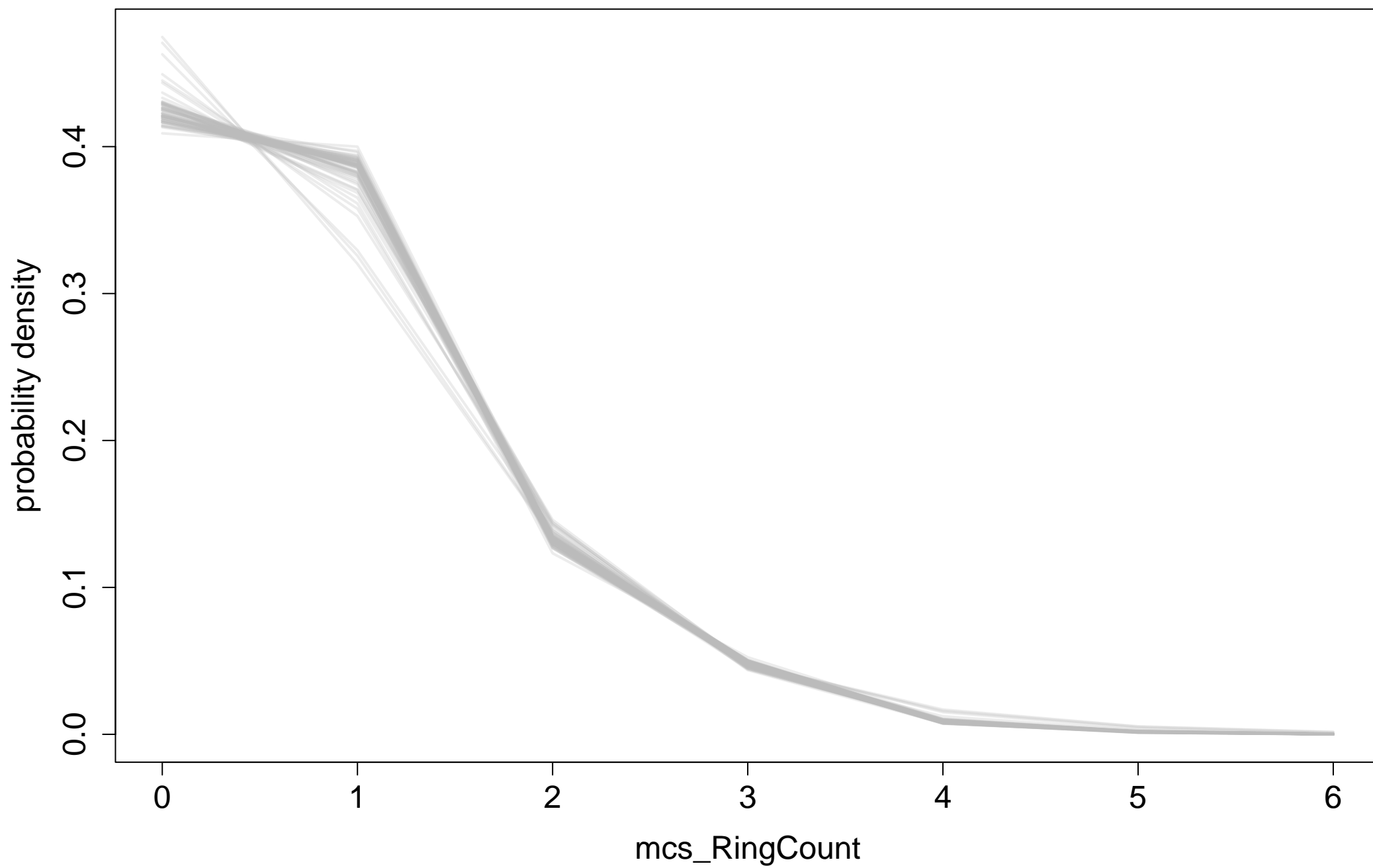


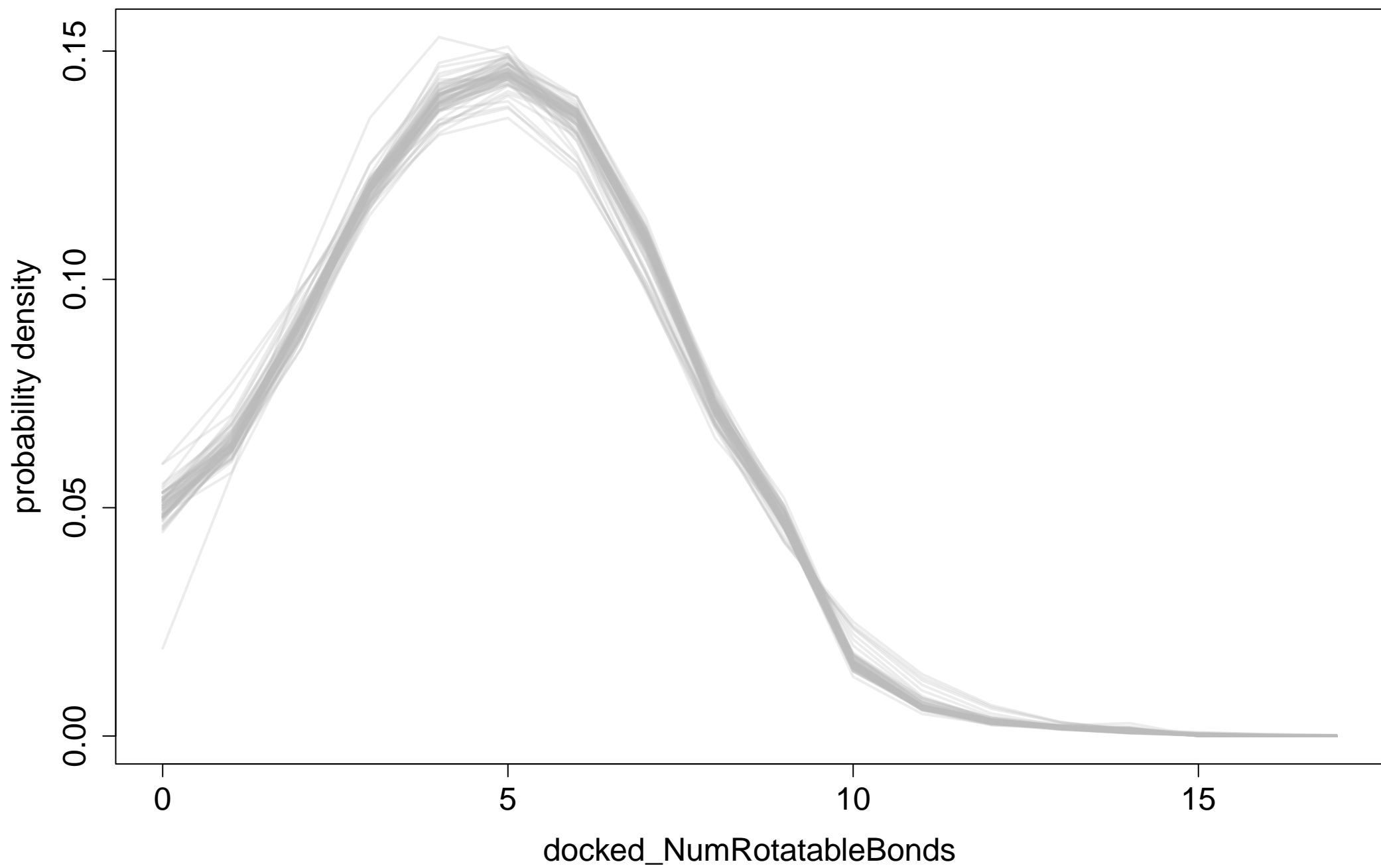




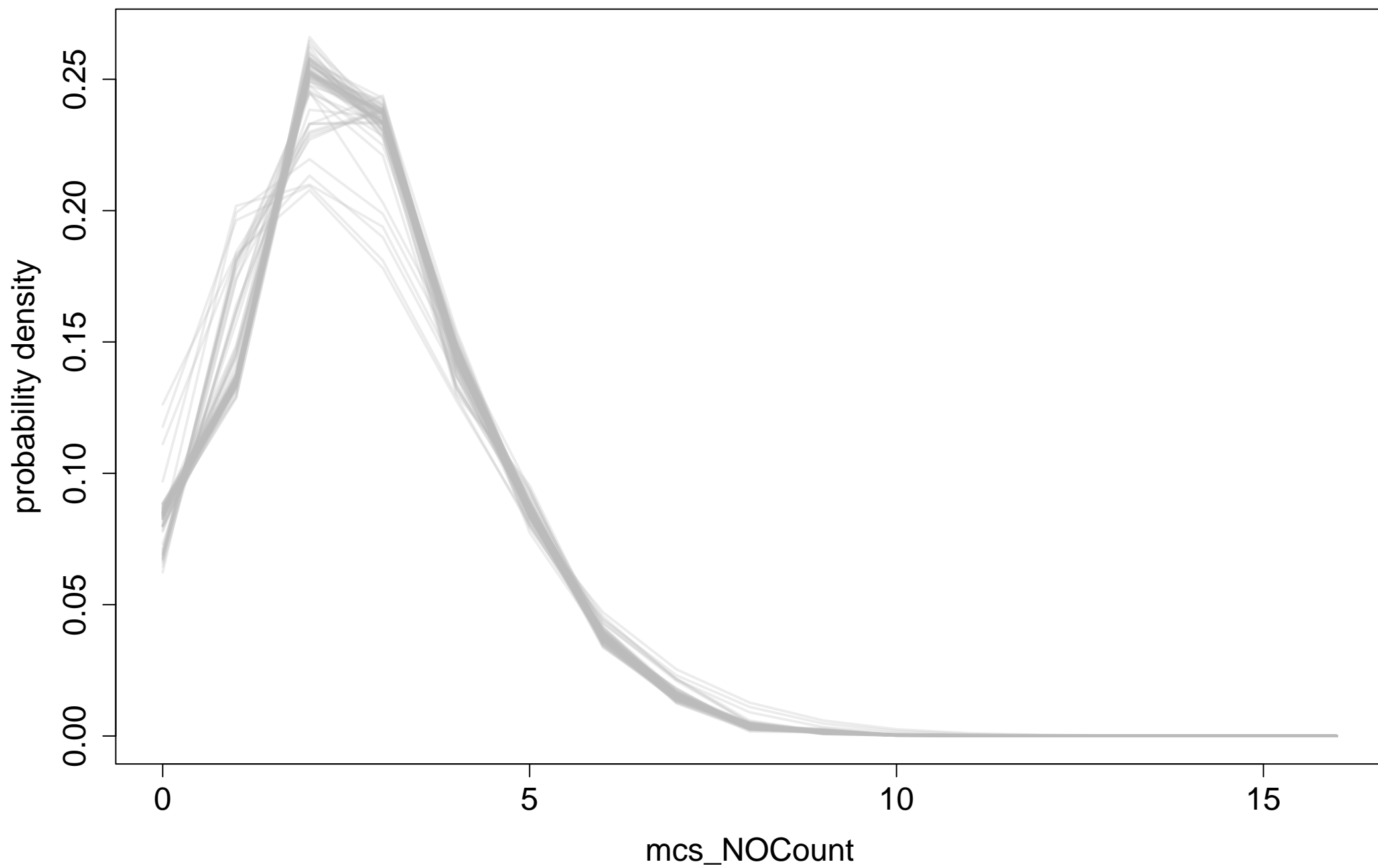


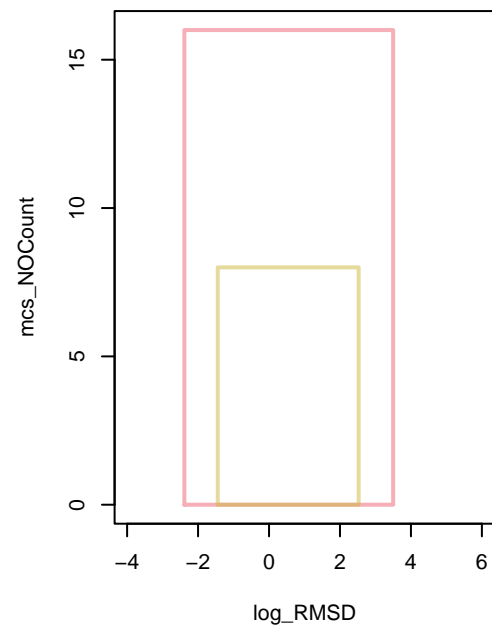
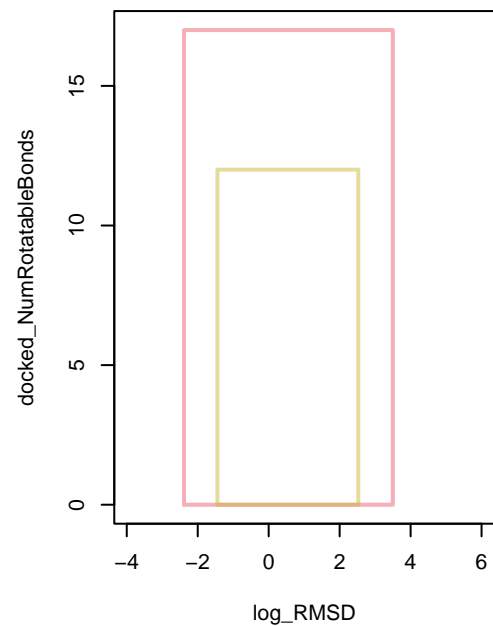
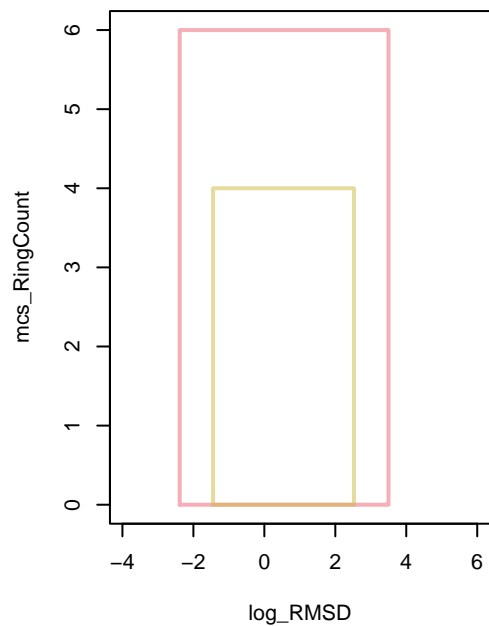
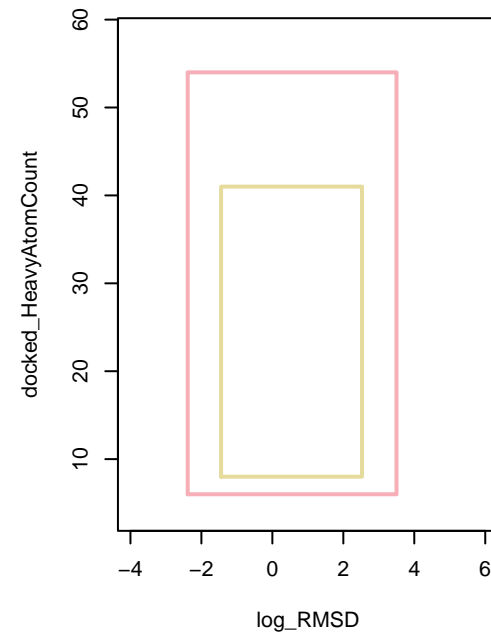
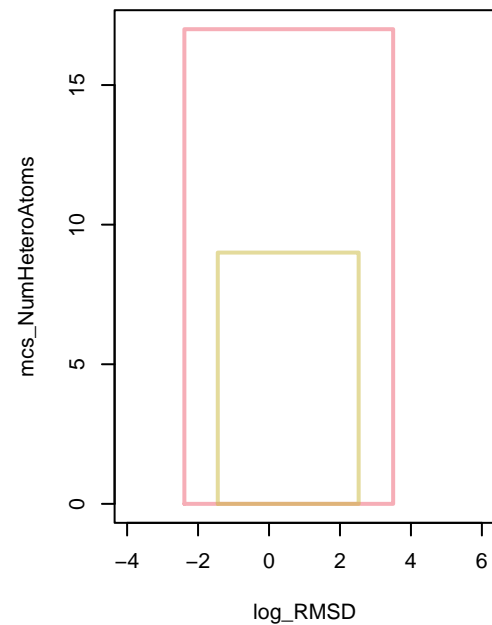
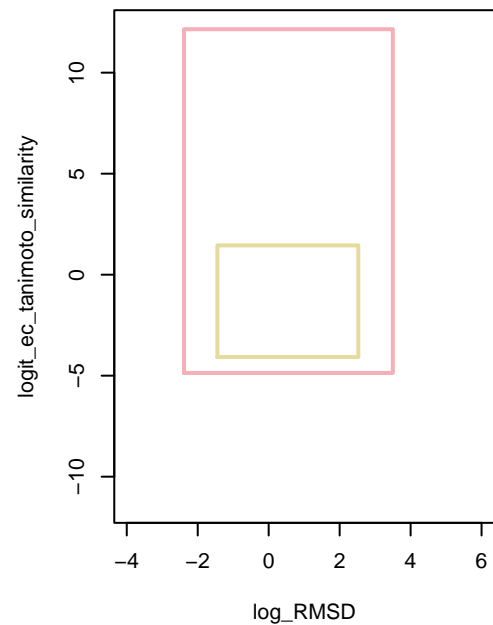
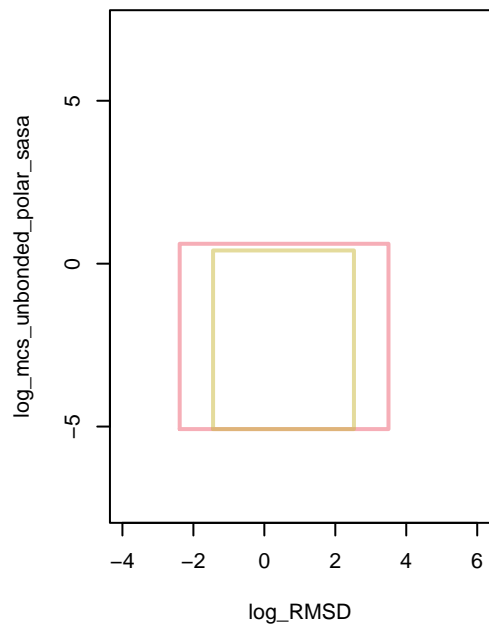




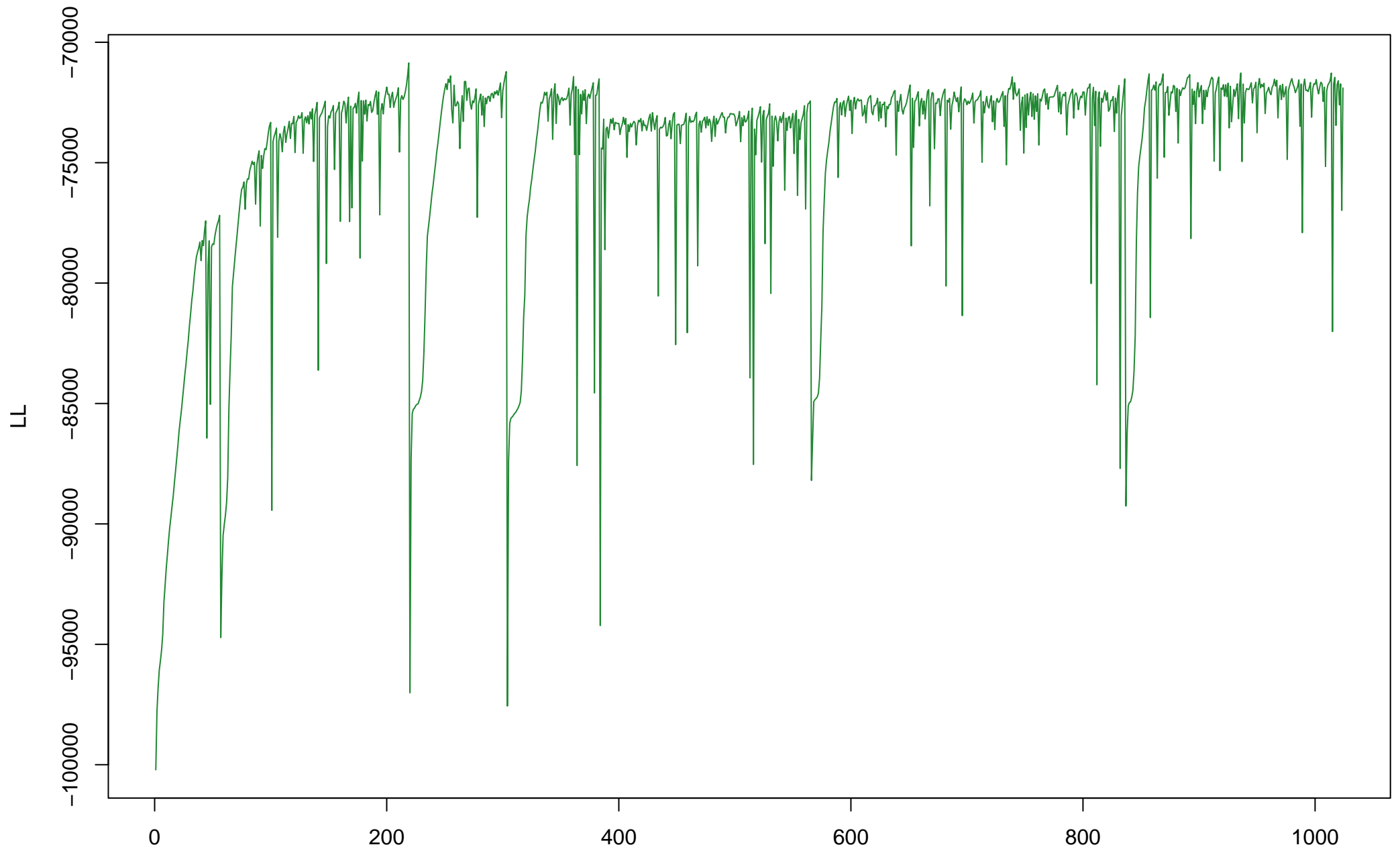




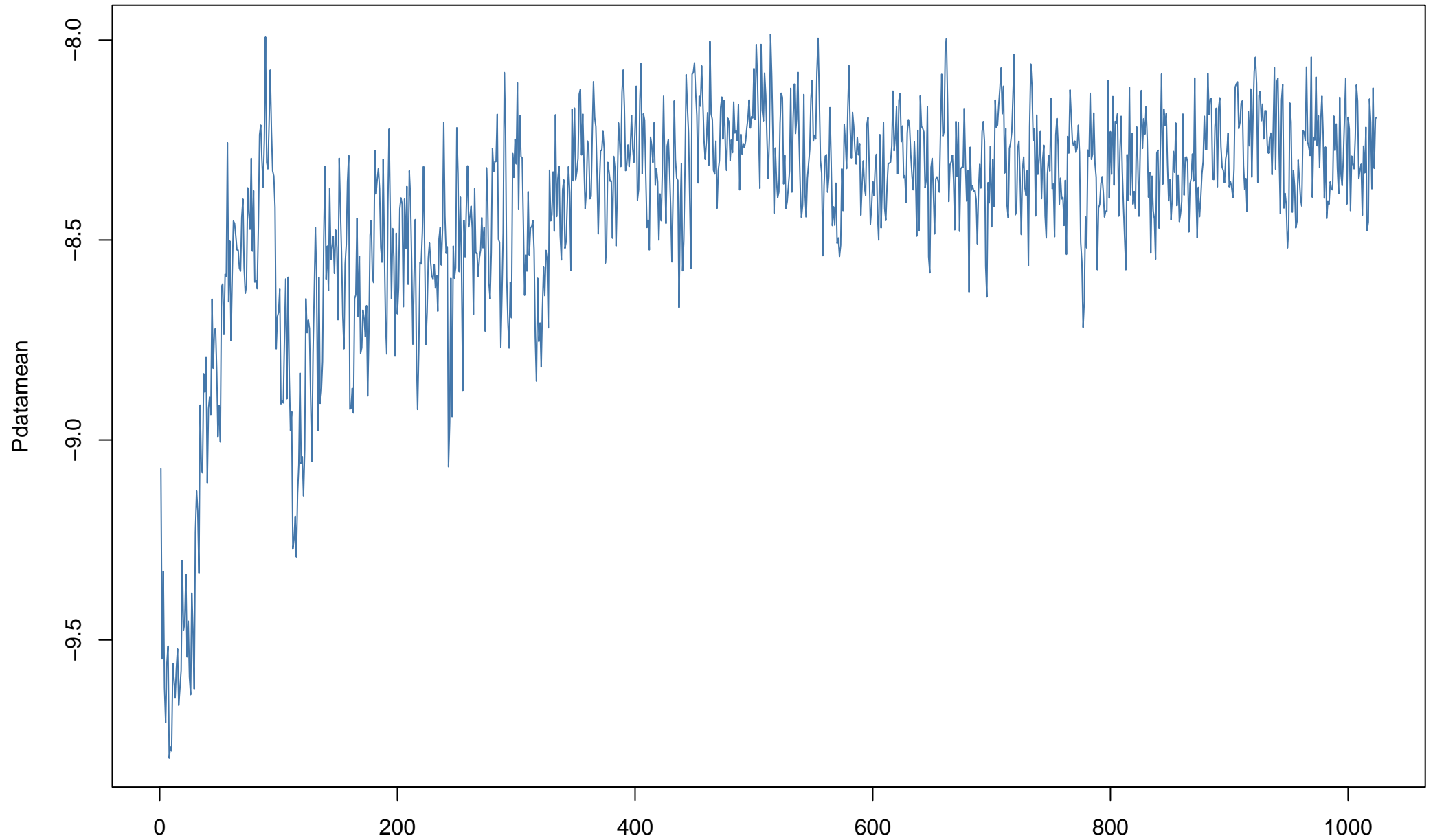




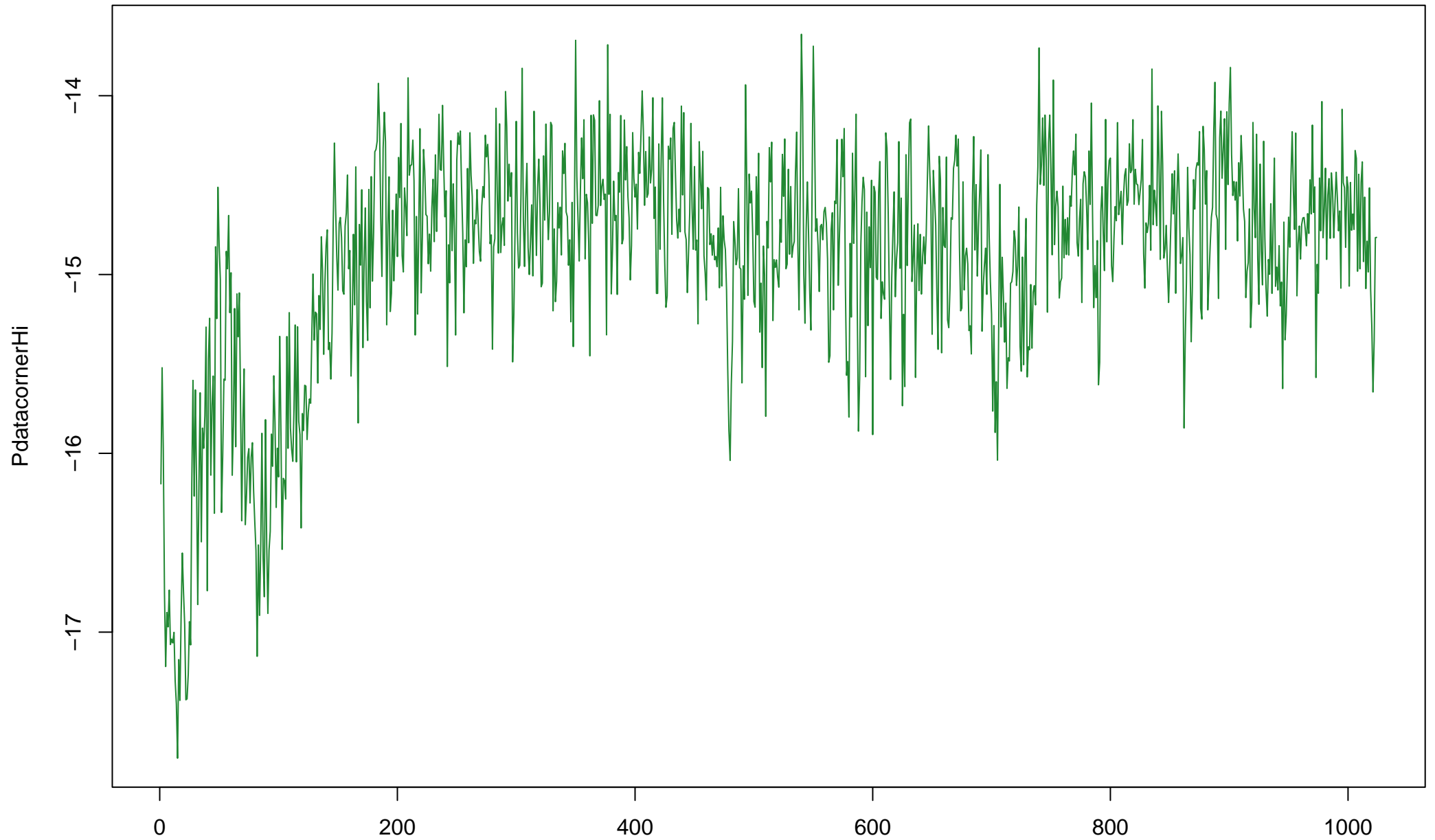
LL



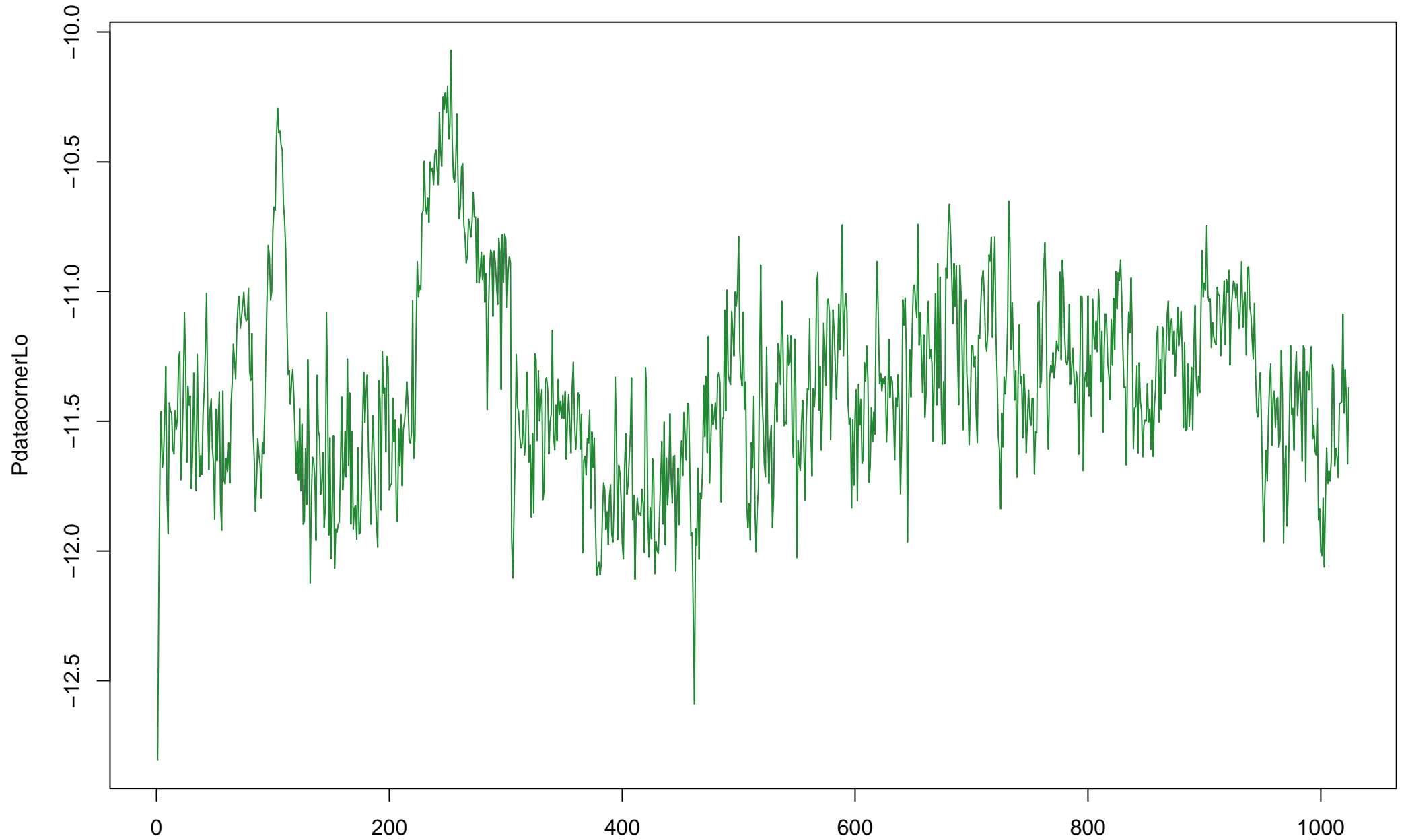
**Pdatamean**  
**ESS = 23.6 | BMK = 0.412 | MCSE(6.27) = 14.5 | stat: FALSE | burn: 0**



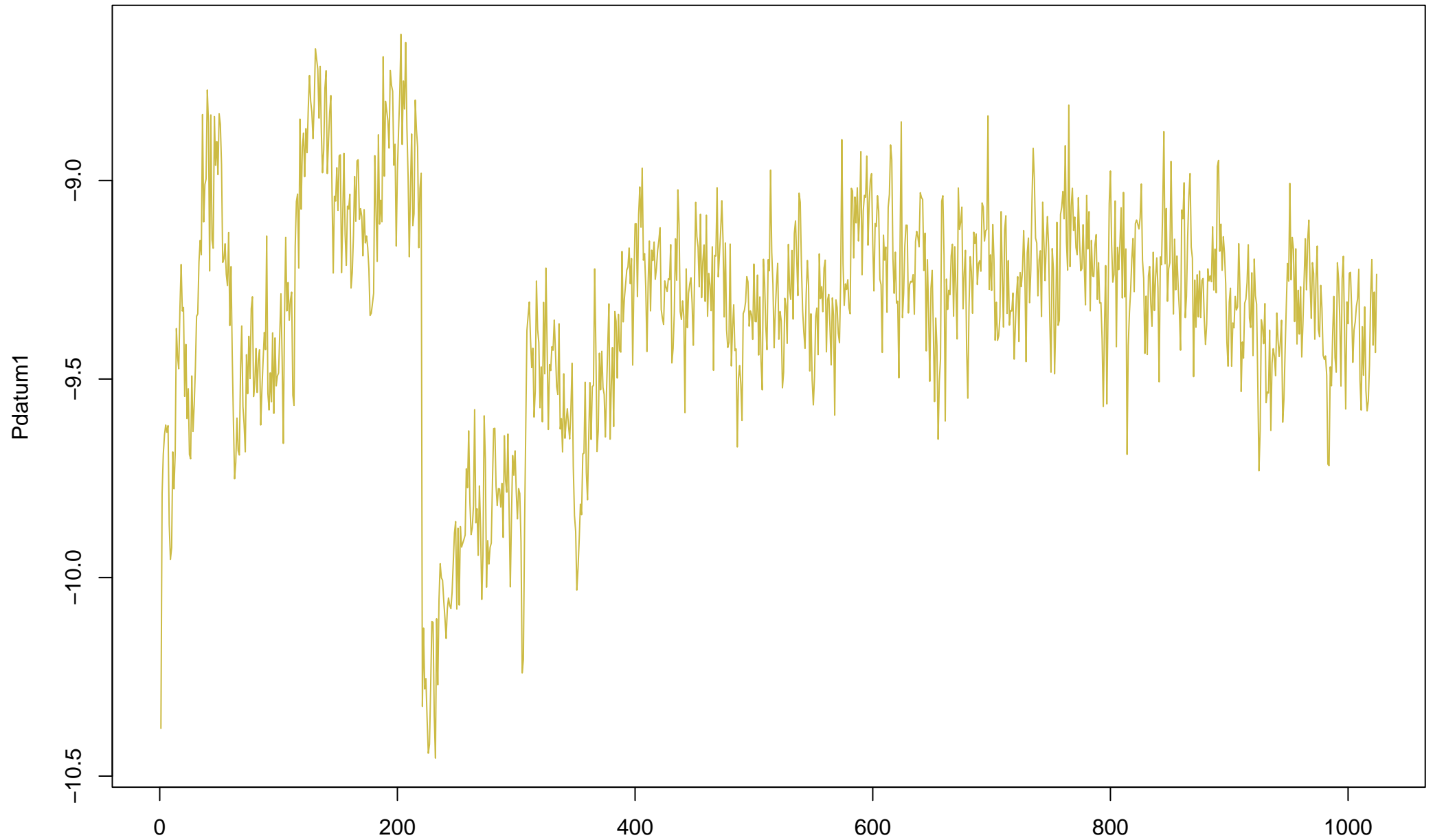
**PdatacornerHi**  
**ESS = 24 | BMK = 0.2 | MCSE(6.27) = 11.2 | stat: FALSE | burn: 0**



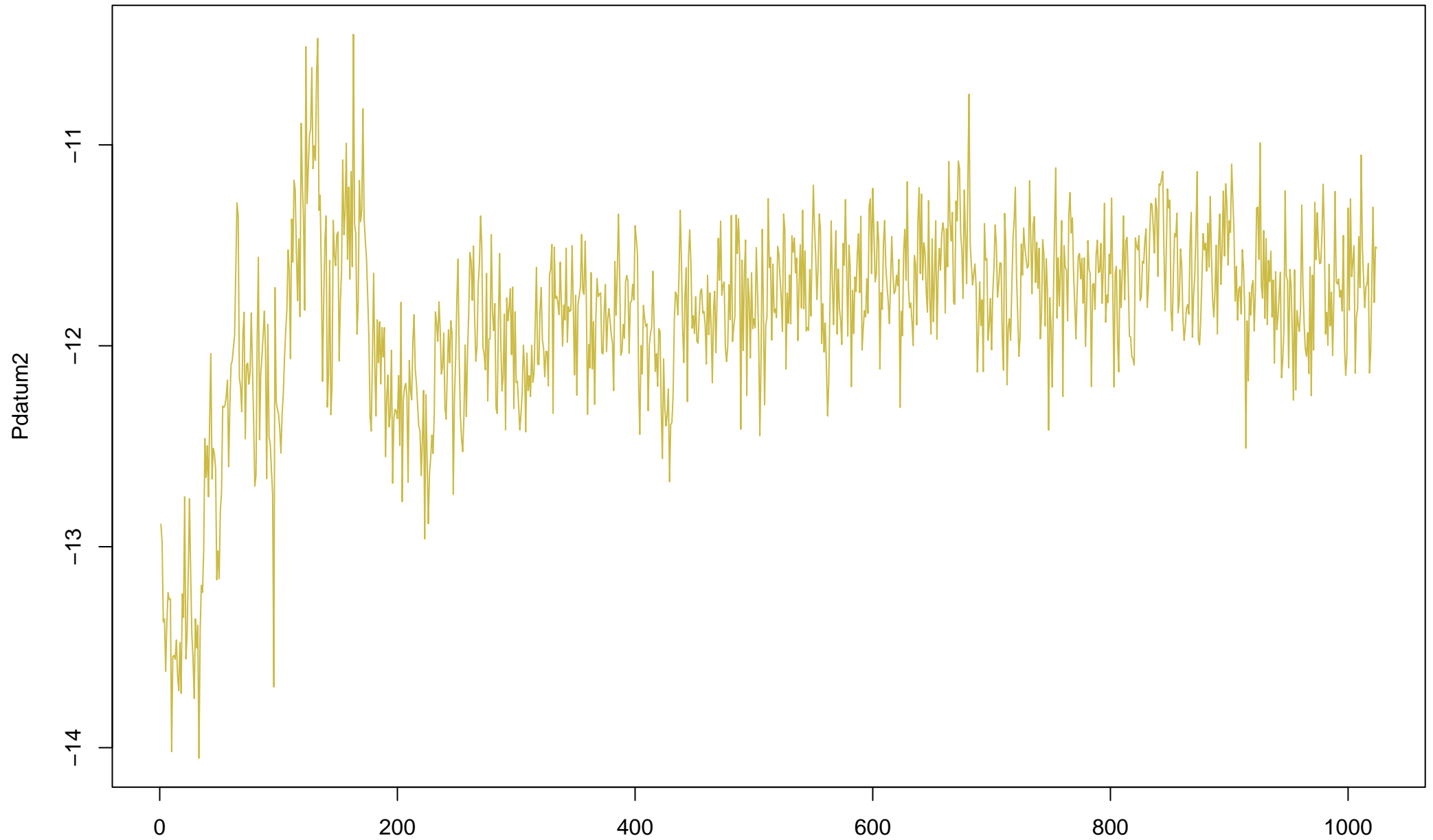
**PdatacornerLo**  
**ESS = 25.1 | BMK = 0.336 | MCSE(6.27) = 13.9 | stat: TRUE | burn: 306**



**Pdatum1**  
**ESS = 24.8 | BMK = 0.385 | MCSE(6.27) = 13.8 | stat: FALSE | burn: 306**

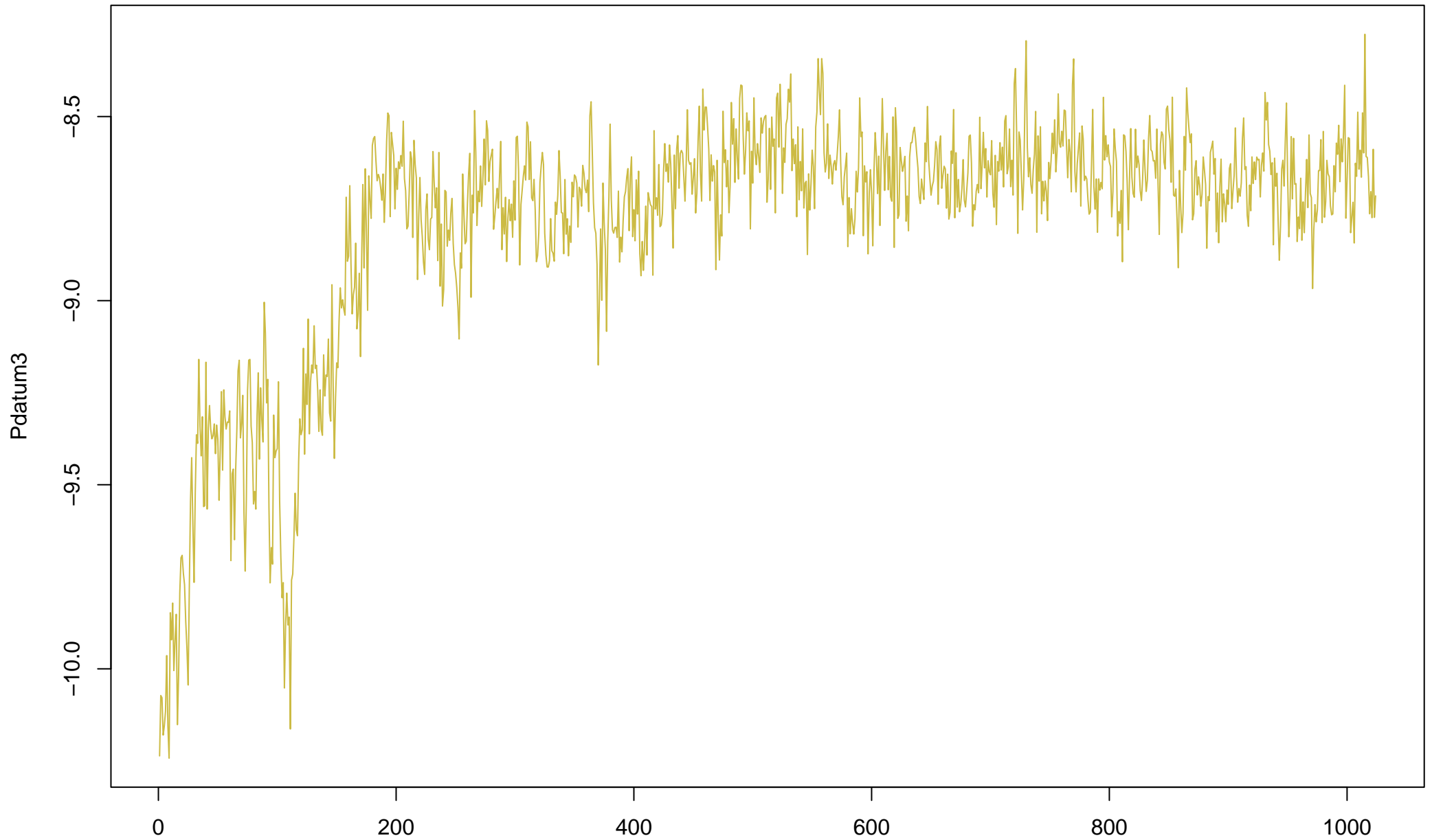


**Pdatum2**  
**ESS = 36.3 | BMK = 0.382 | MCSE(6.27) = 11.1 | stat: FALSE | burn: 102**

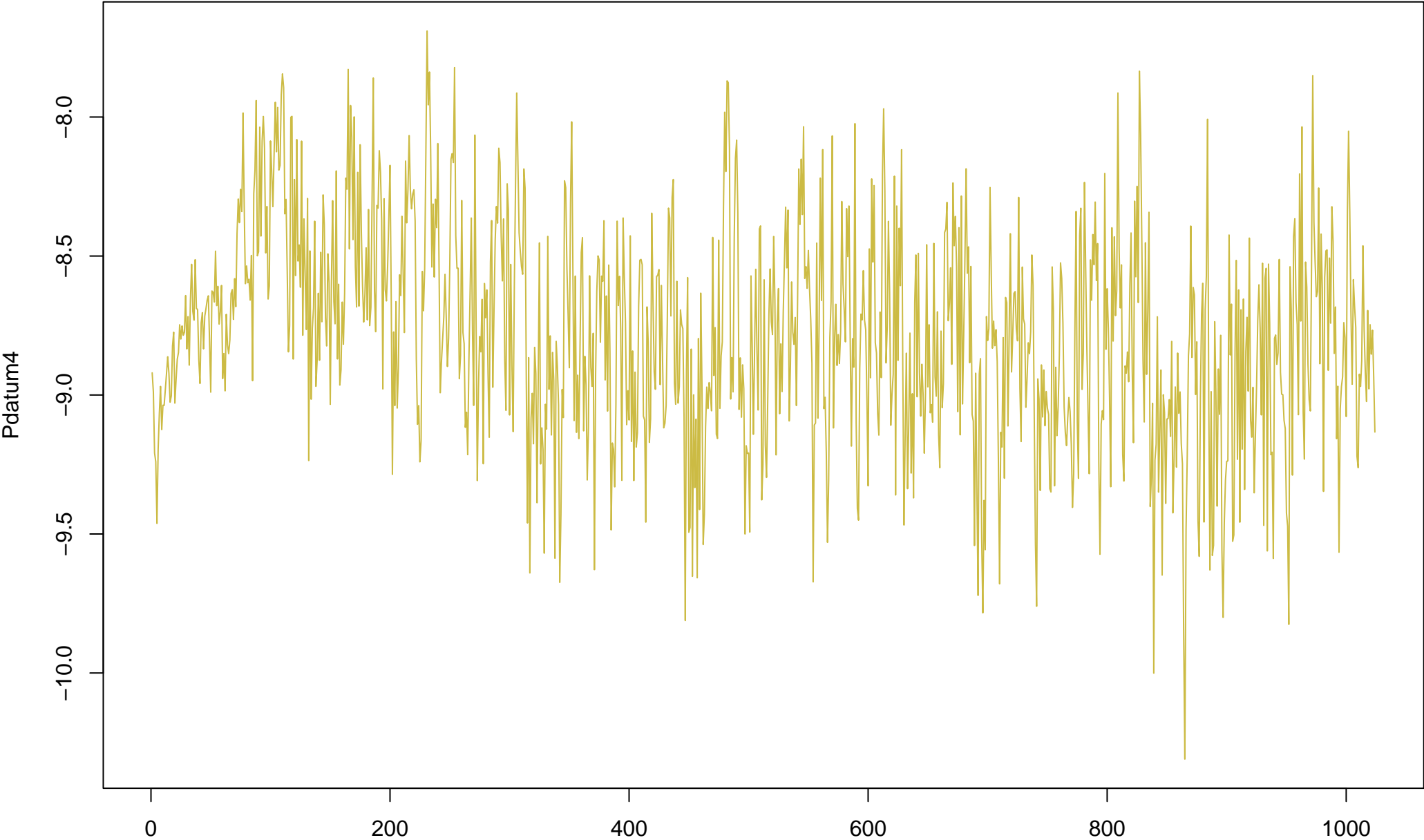




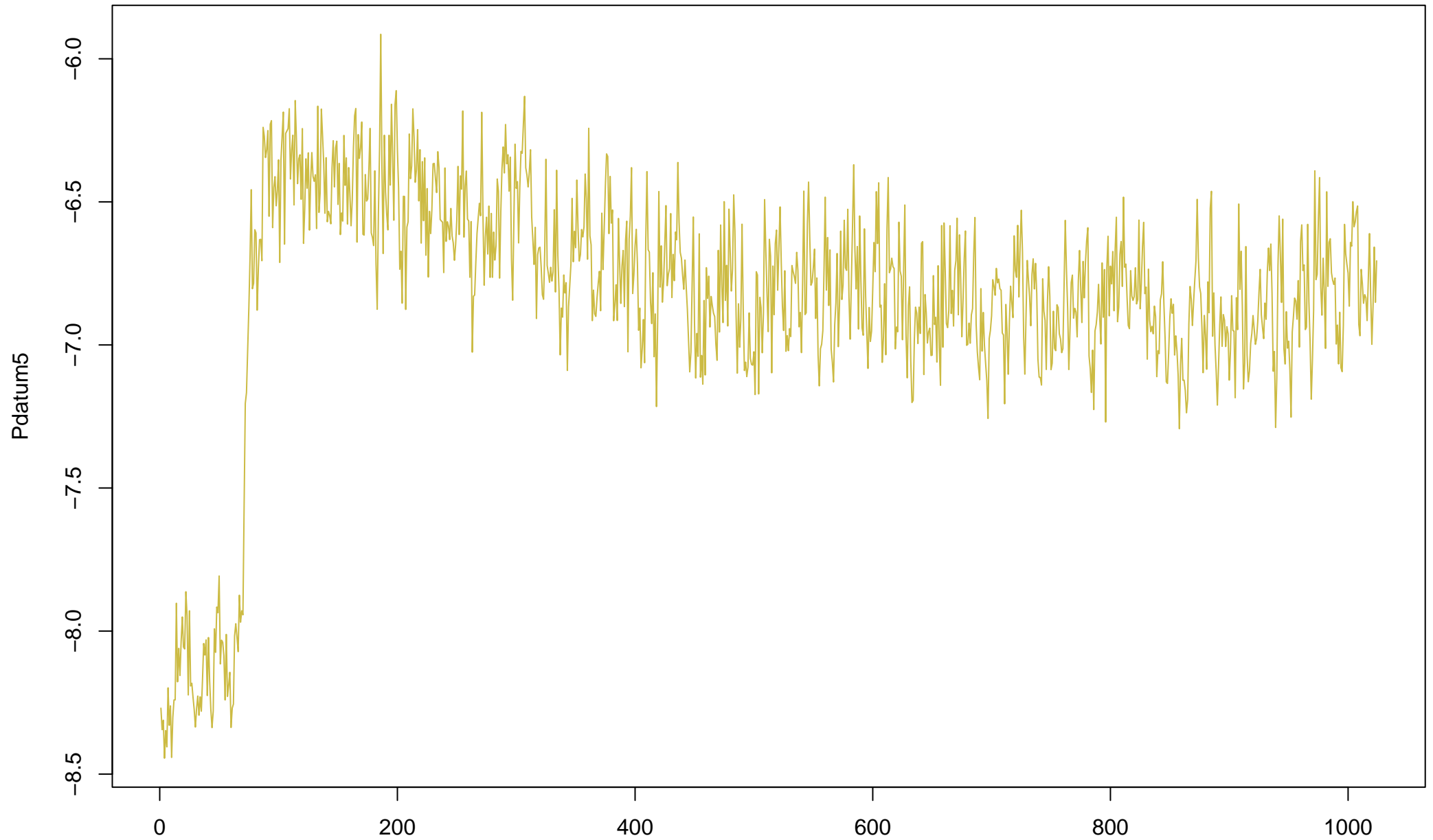
**Pdatum3**  
**ESS = 9.91 | BMK = 0.462 | MCSE(6.27) = 16 | stat: FALSE | burn: 204**



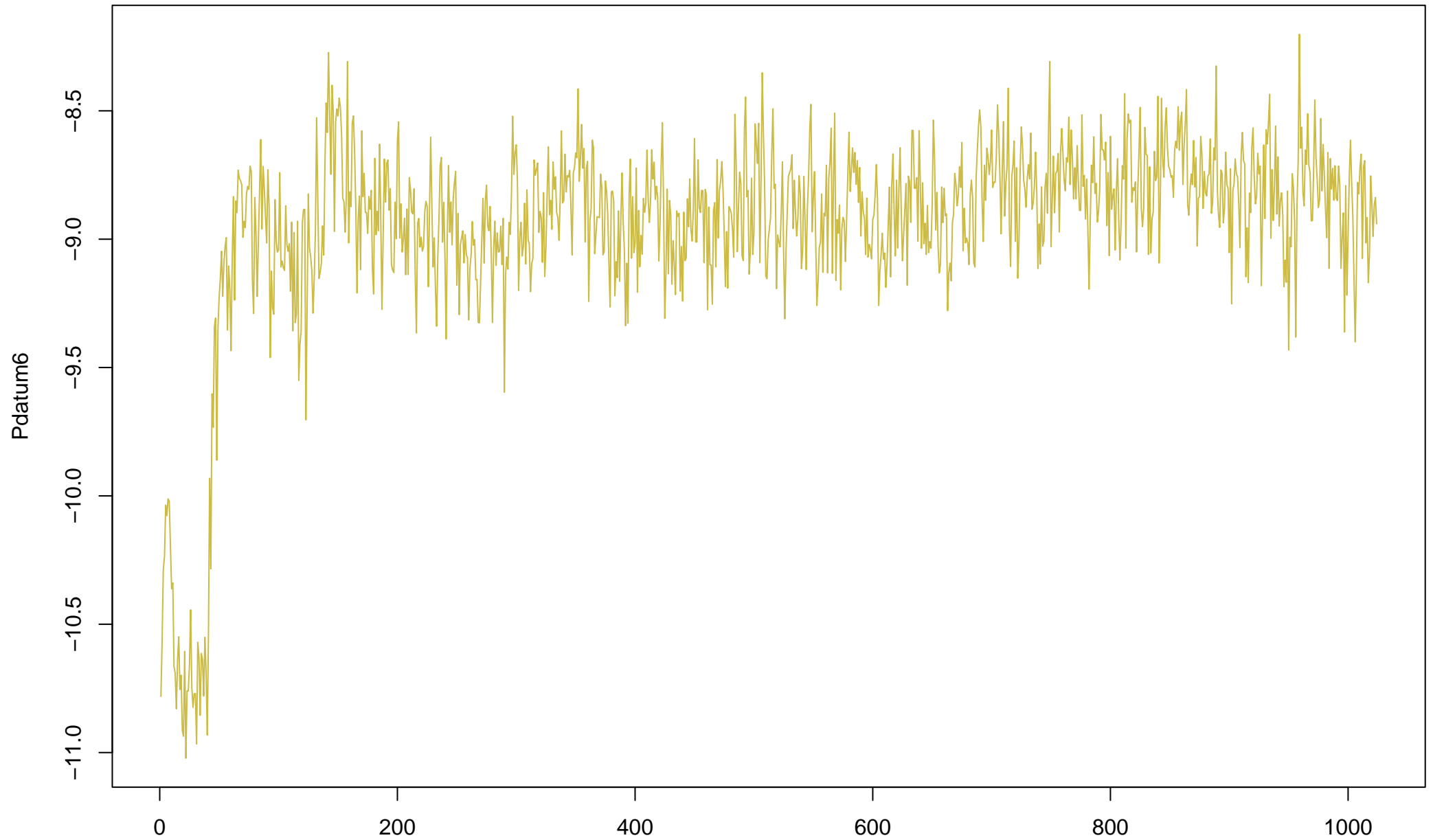
**Pdatum4**  
**ESS = 63.3 | BMK = 0.147 | MCSE(6.27) = 9.06 | stat: FALSE | burn: 0**



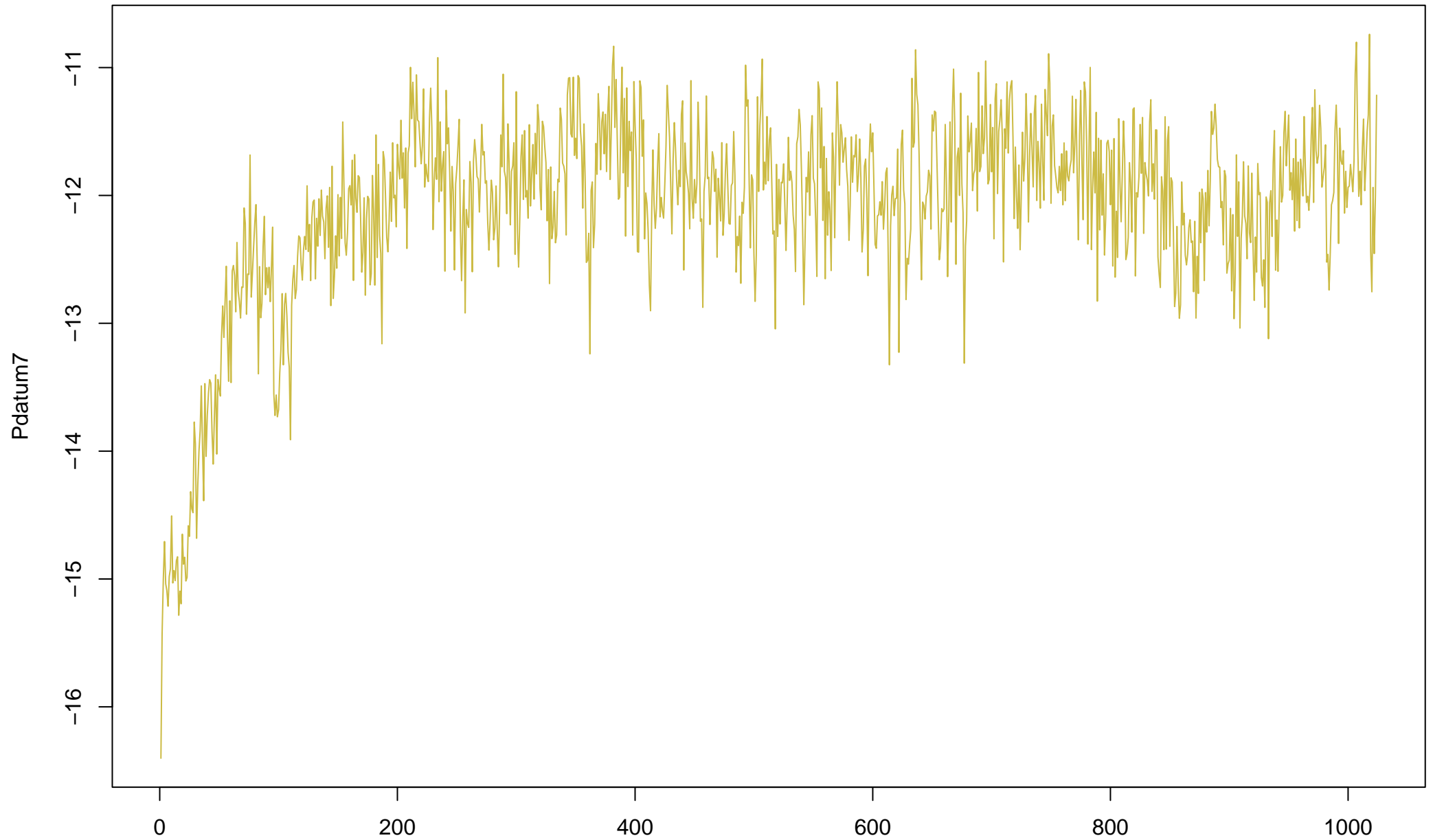
**Pdatum5**  
**ESS = 10.3 | BMK = 0.466 | MCSE(6.27) = 14.6 | stat: FALSE | burn: 102**



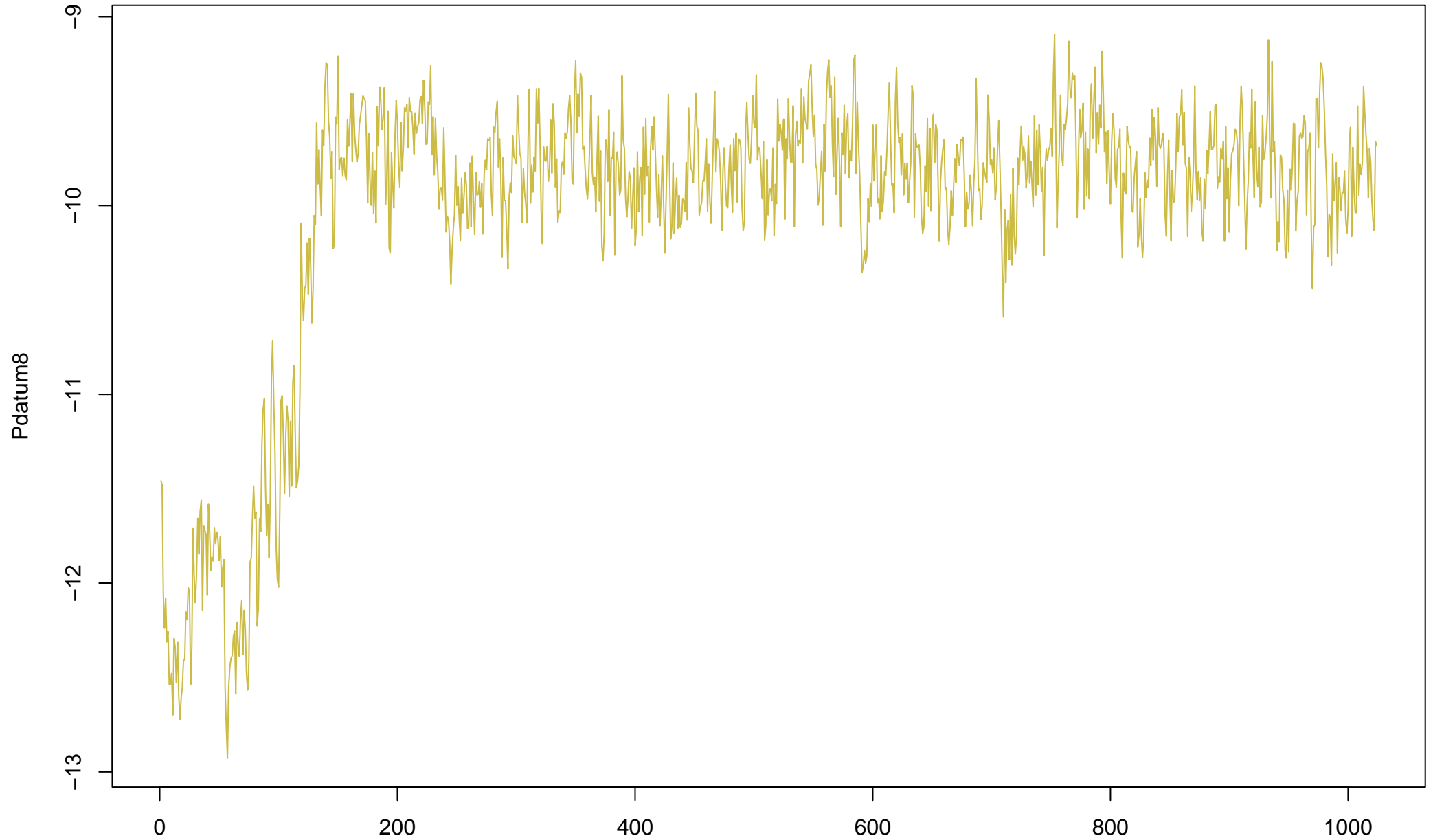
**Pdatum6**  
**ESS = 23.1 | BMK = 0.272 | MCSE(6.27) = 12.7 | stat: FALSE | burn: 0**



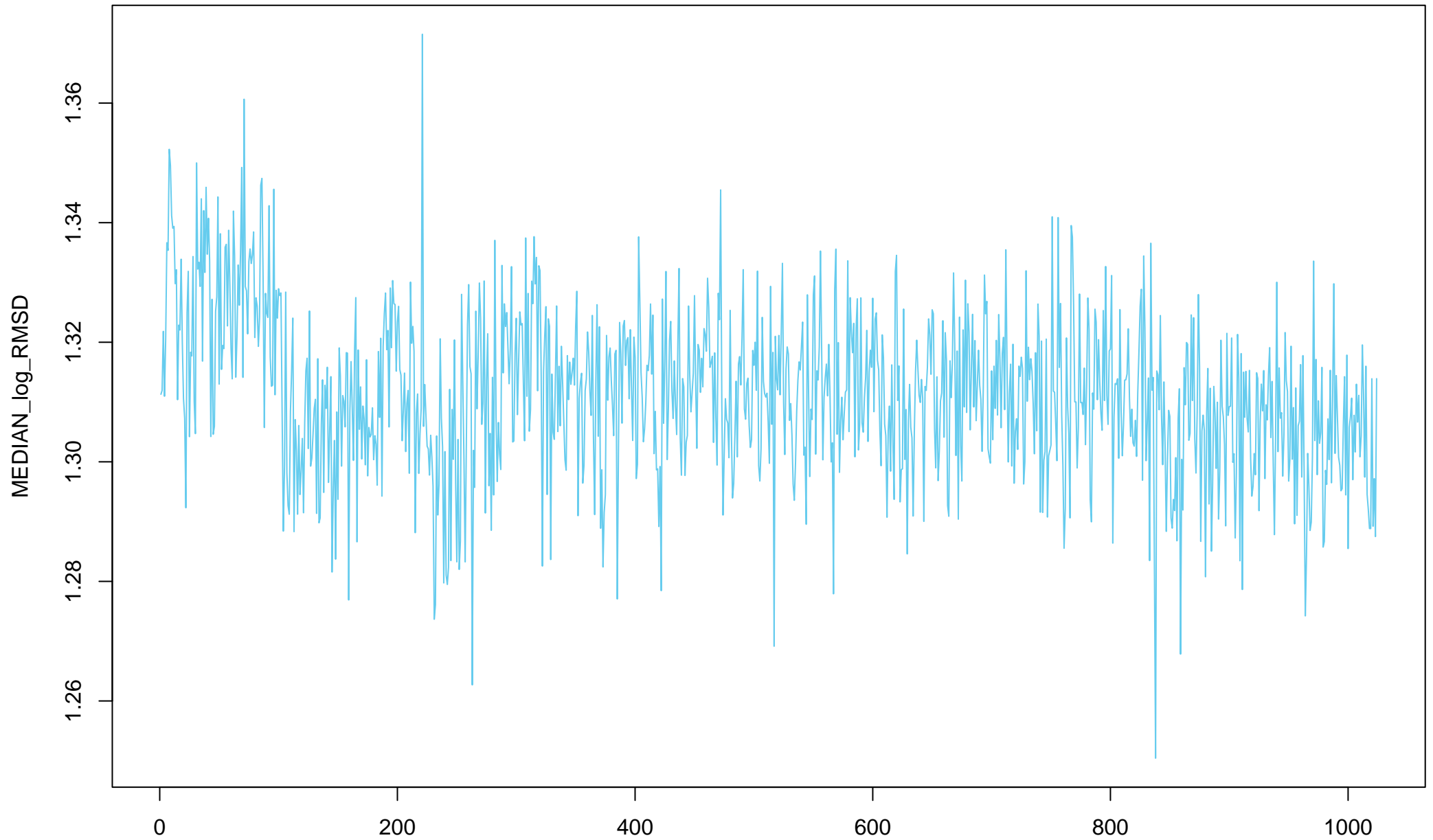
**Pdatum7**  
**ESS = 40.5 | BMK = 0.179 | MCSE(6.27) = 10.7 | stat: FALSE | burn: 102**



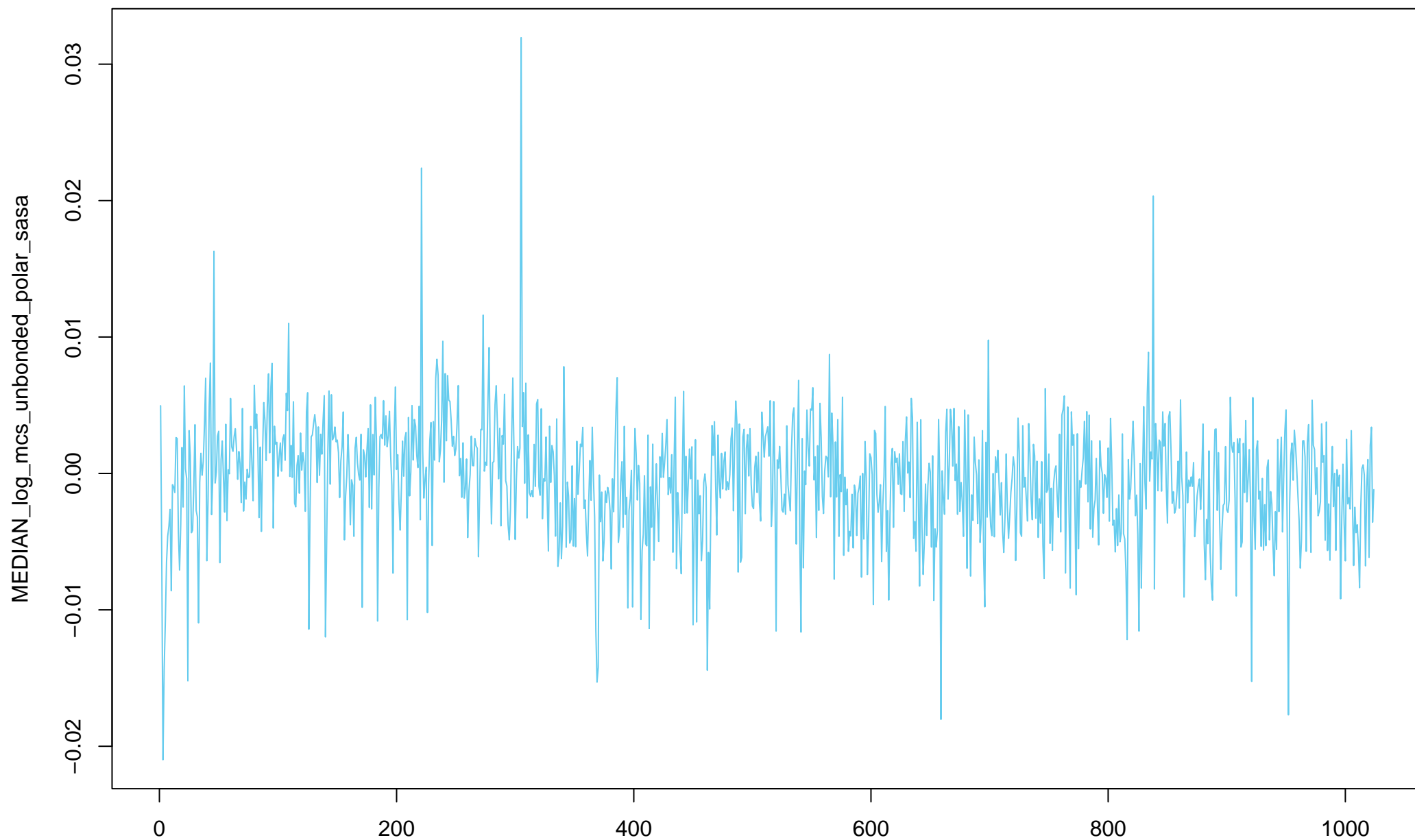
**Pdatum8**  
**ESS = 12.3 | BMK = 0.311 | MCSE(6.27) = 14.3 | stat: FALSE | burn: 102**



**MEDIAN\_log\_RMSD**  
**ESS = 74.1 | BMK = 0.16 | MCSE(6.27) = 9.06 | stat: FALSE | burn: 102**

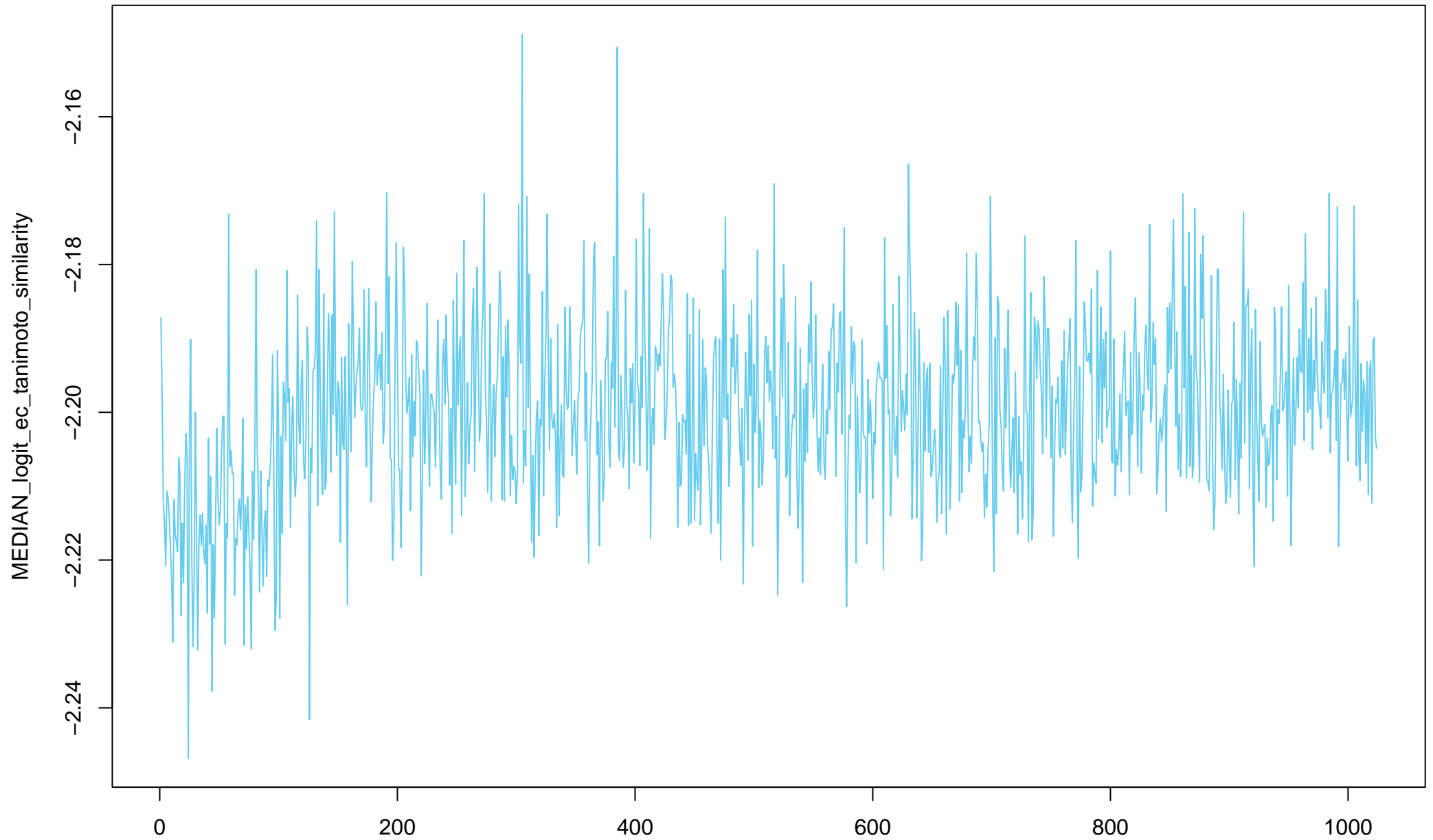


**MEDIAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 266 | BMK = 0.154 | MCSE(6.27) = 6.43 | stat: TRUE | burn: 0**

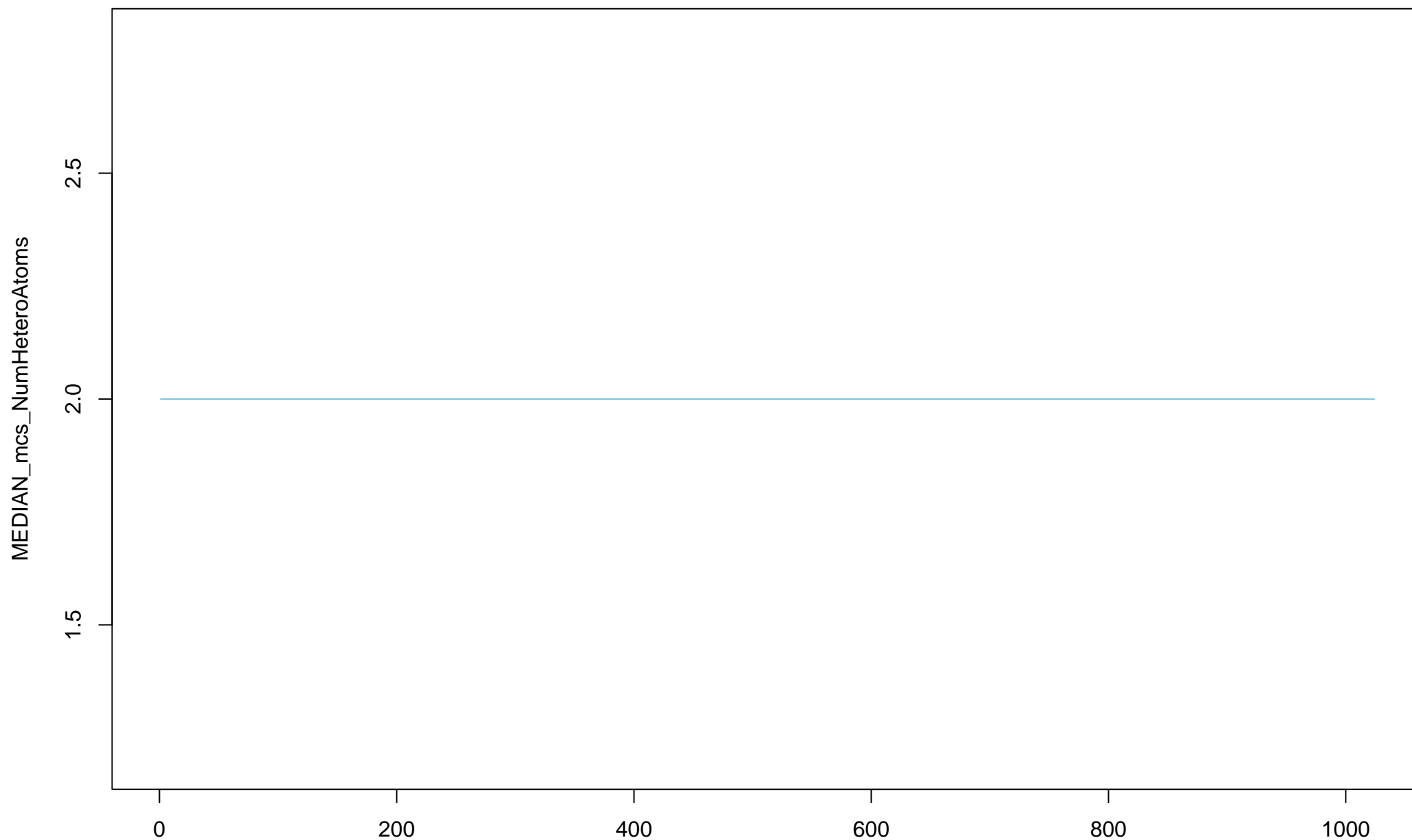




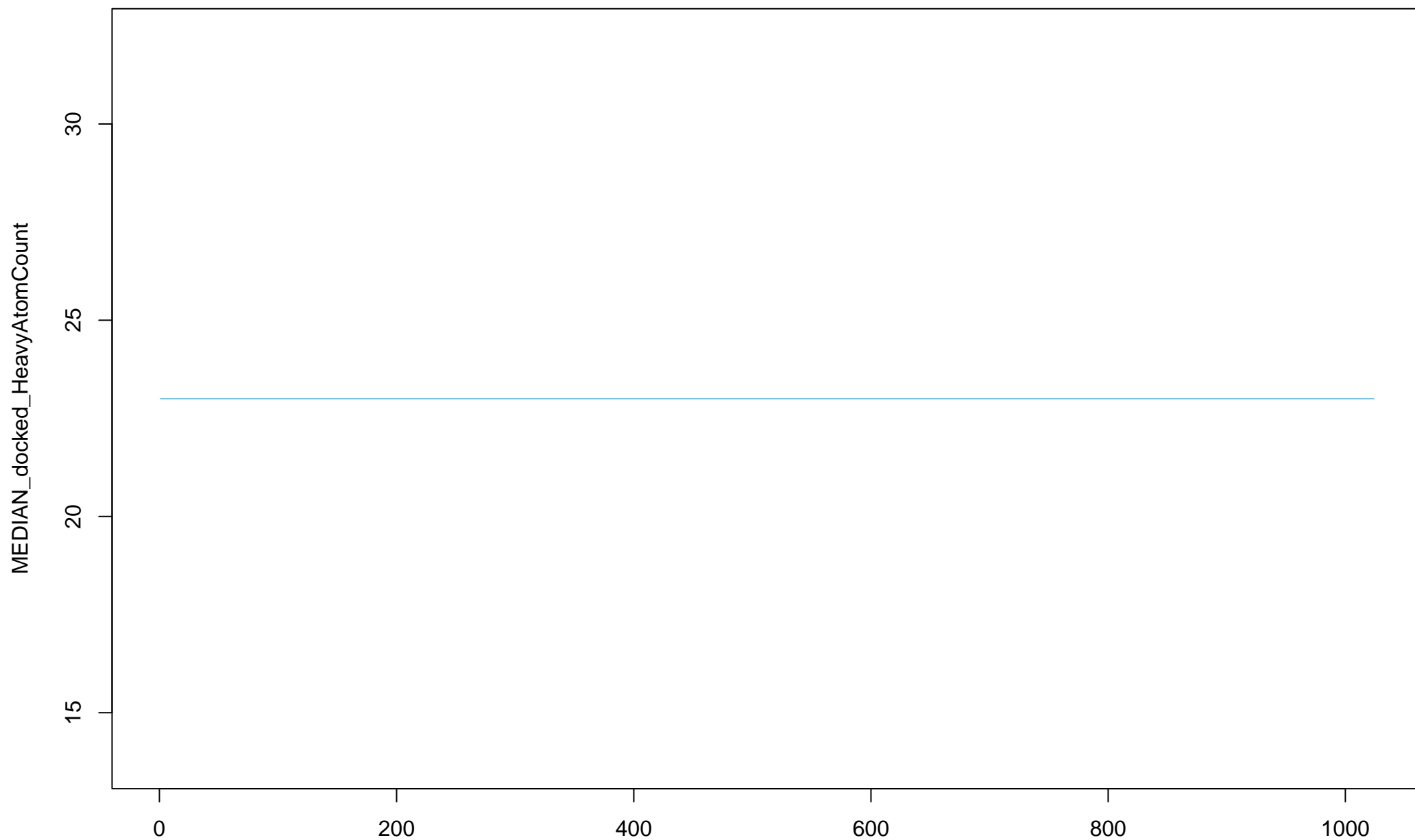
**MEDIAN\_logit\_ec\_tanimoto\_similarity**  
**ESS = 81.2 | BMK = 0.141 | MCSE(6.27) = 7.5 | stat: FALSE | burn: 0**



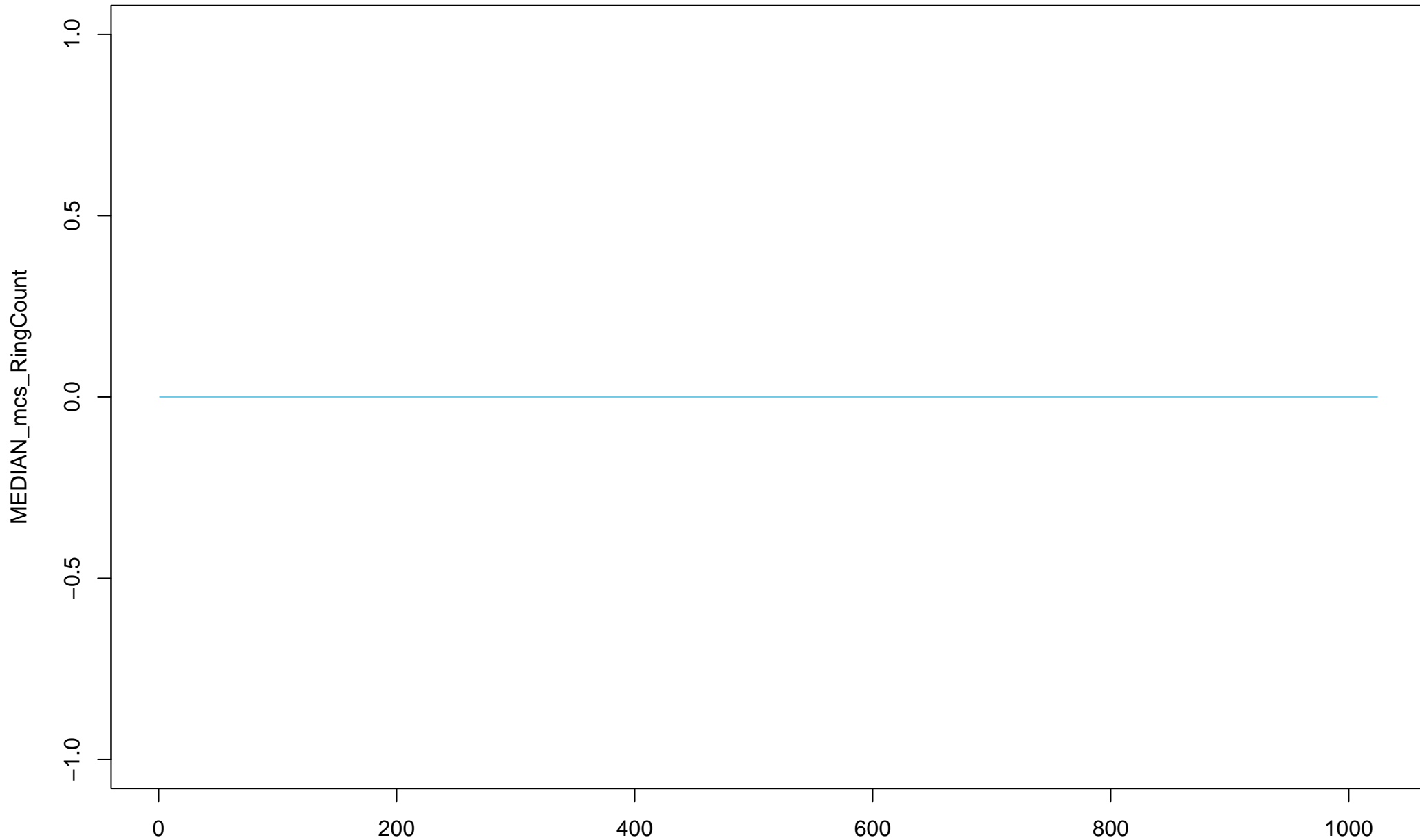
**MEDIAN\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



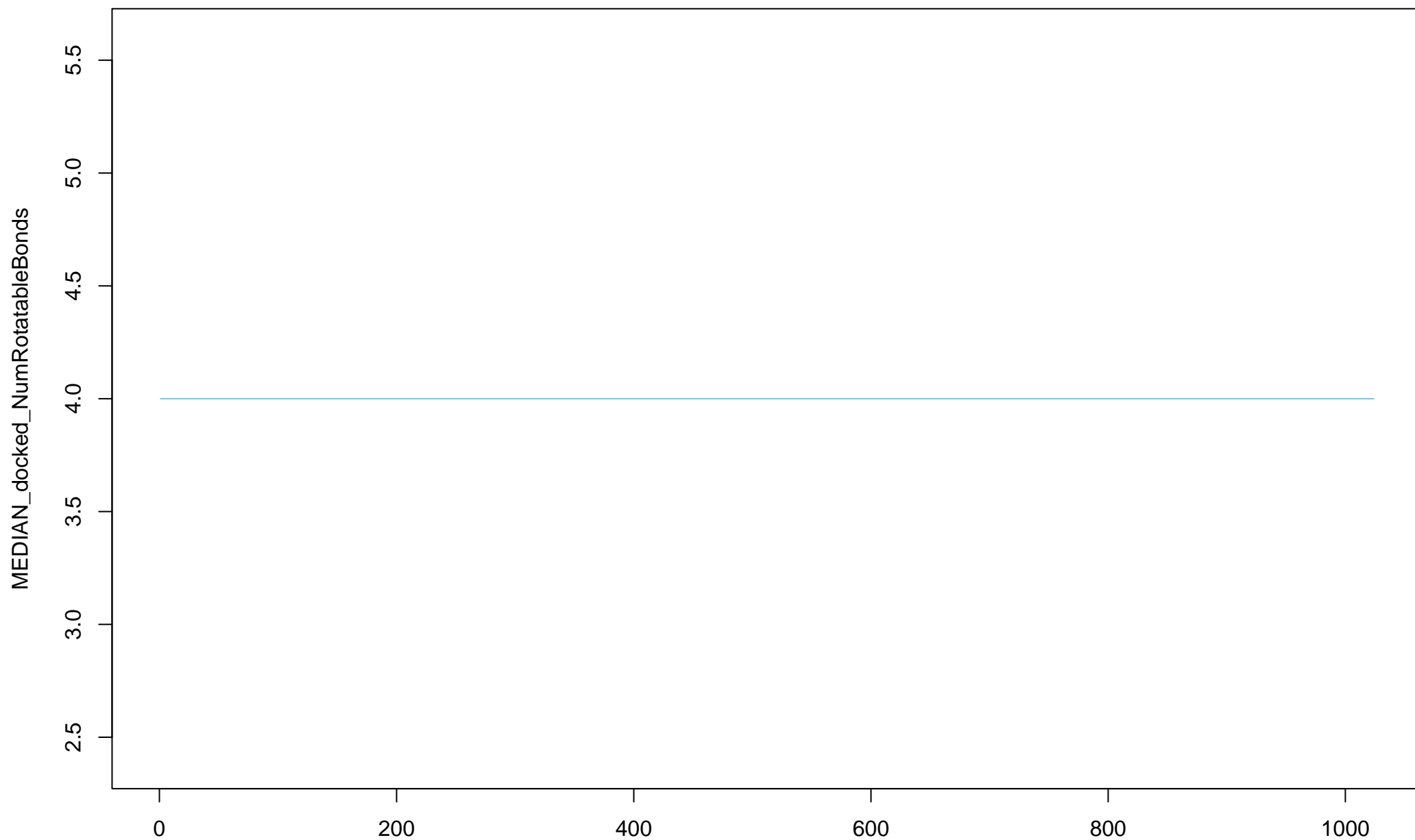
**MEDIAN\_docked\_HeavyAtomCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



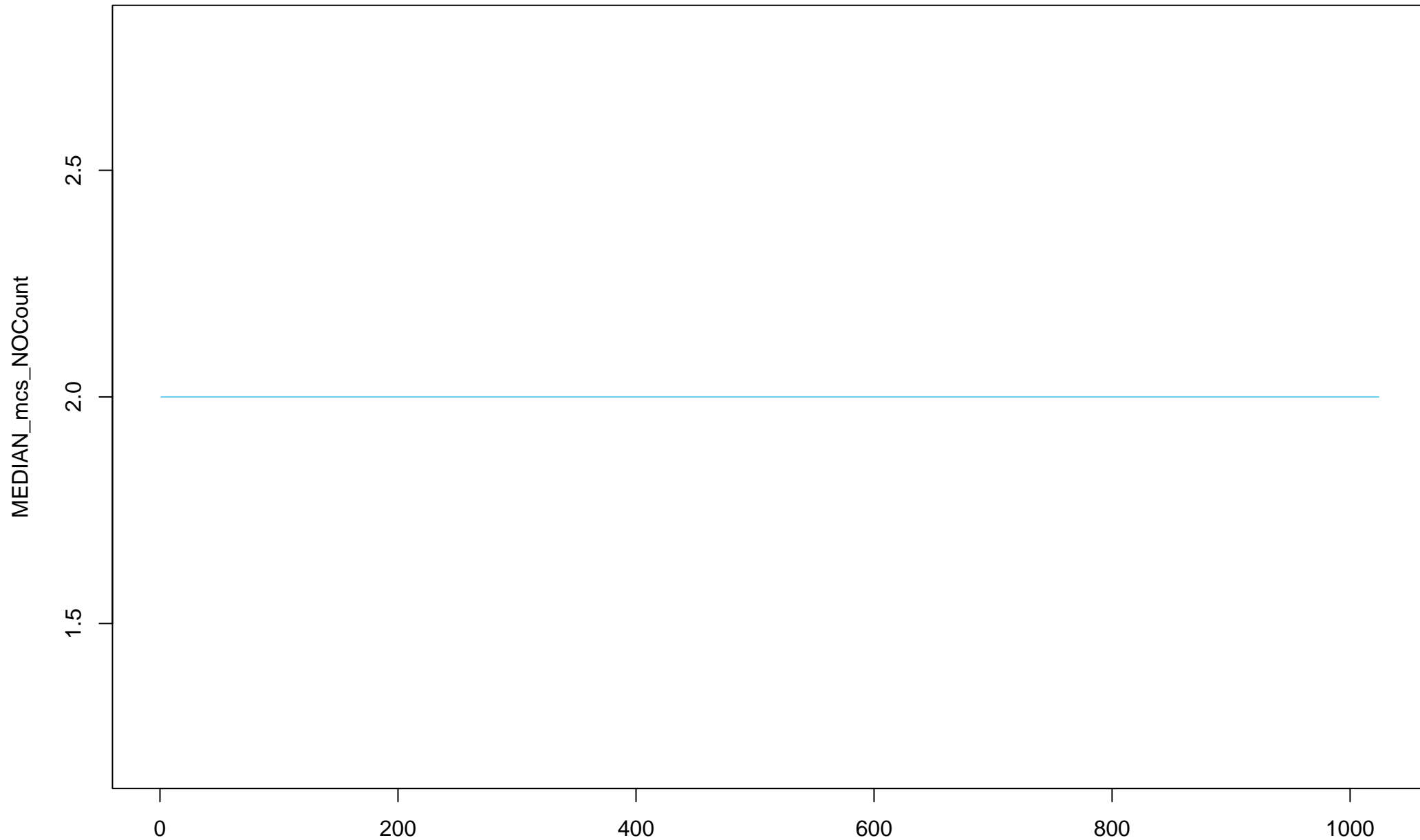
**MEDIAN\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



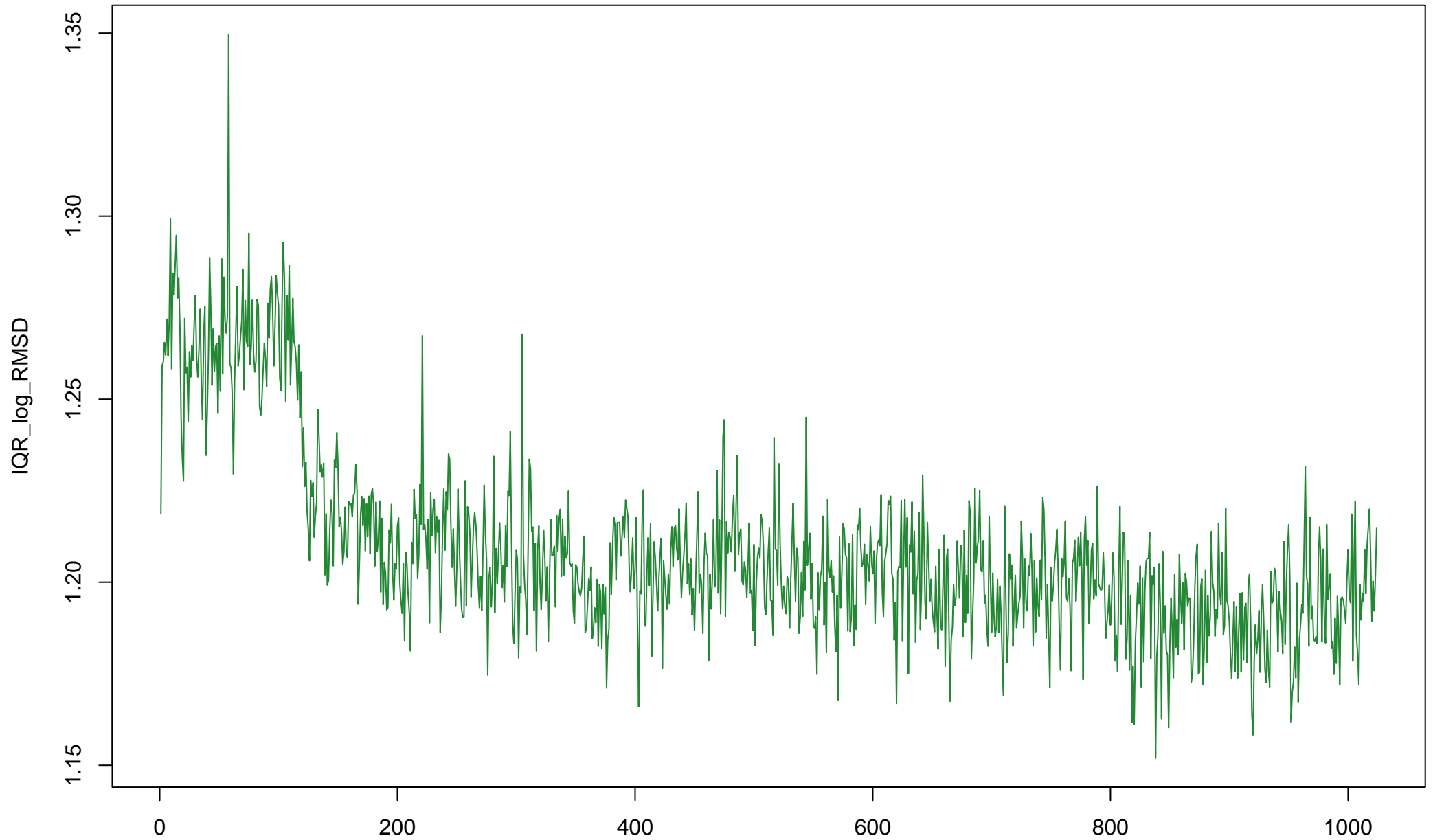
**MEDIAN\_docked\_NumRotatableBonds**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



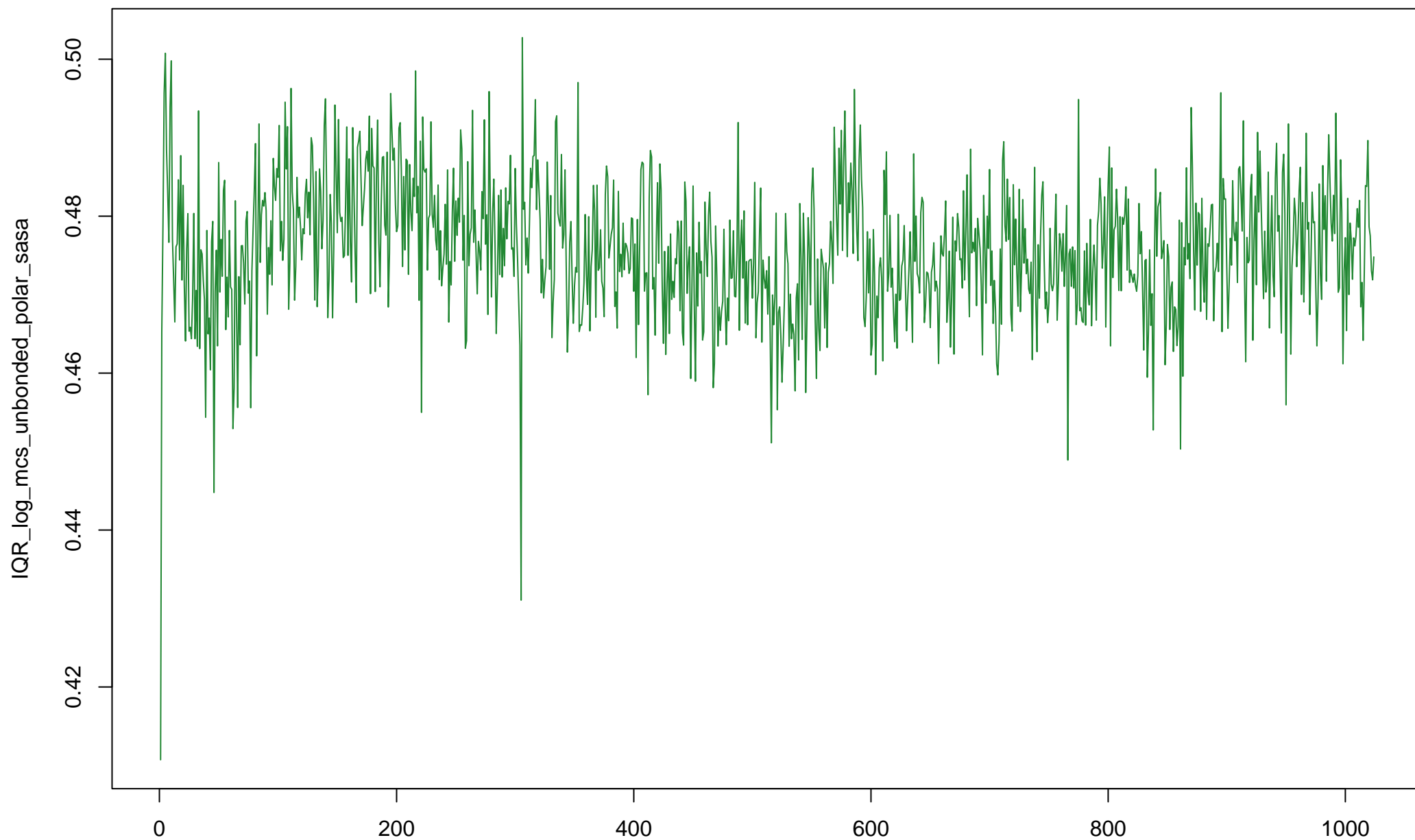
**MEDIAN\_mcs\_NOCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**IQR\_log\_RMSD**  
**ESS = 6.13 | BMK = 0.423 | MCSE(6.27) = 15.2 | stat: FALSE | burn: 102**

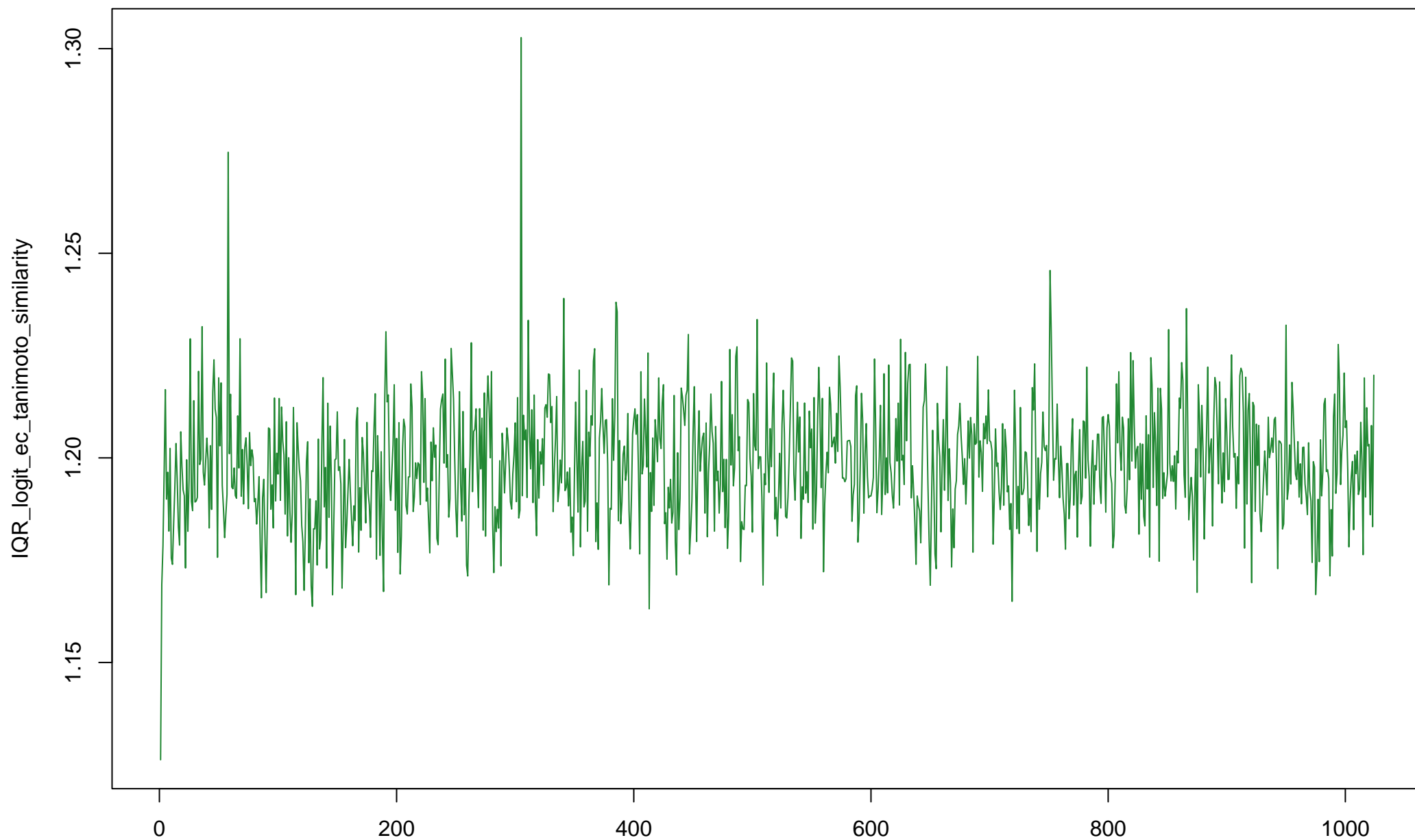


**IQR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 130 | BMK = 0.121 | MCSE(6.27) = 7.01 | stat: TRUE | burn: 0**

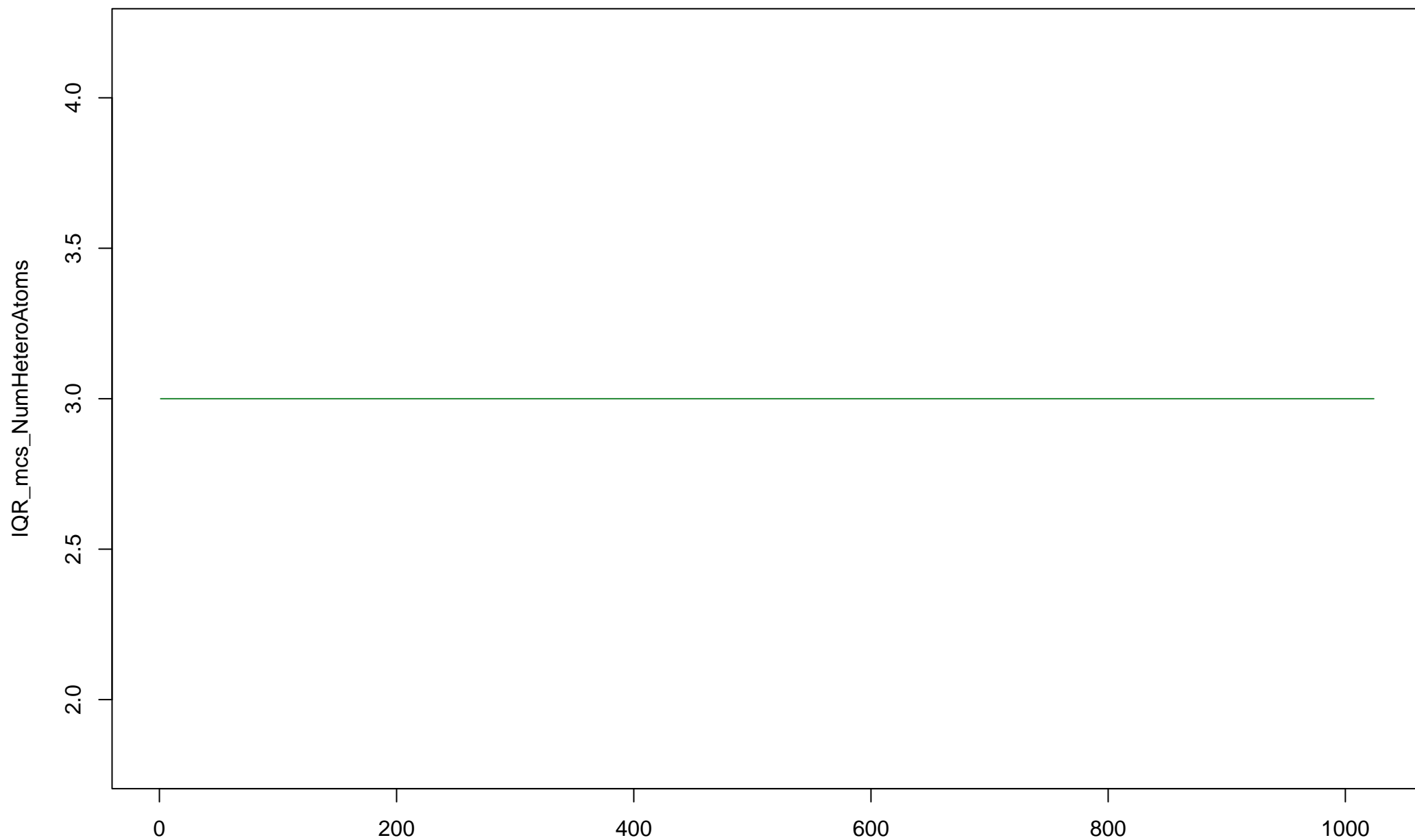




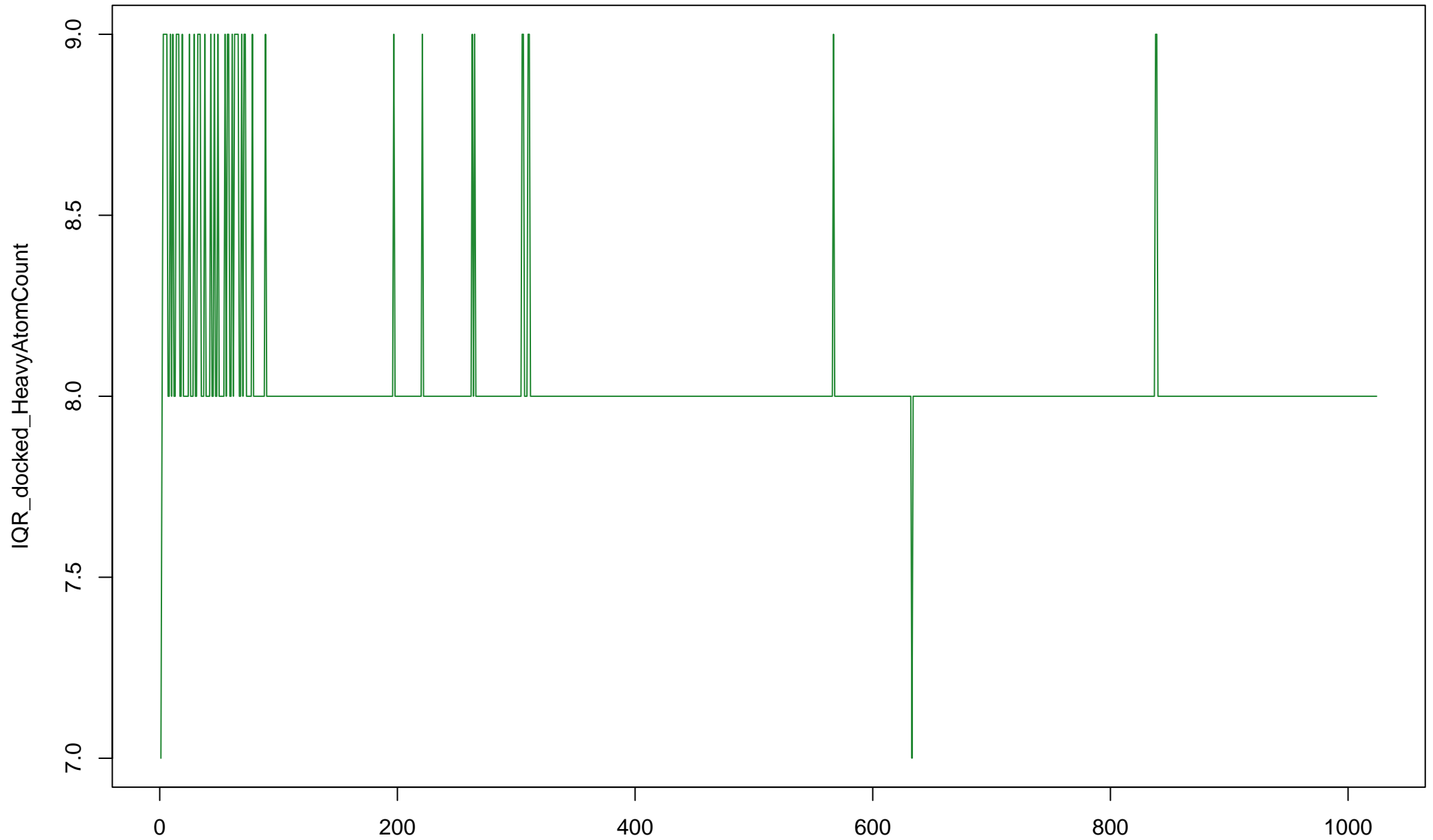
**IQR\_logit\_ec\_tanimoto\_similarity**  
**ESS = 760 | BMK = 0.107 | MCSE(6.27) = 4.55 | stat: TRUE | burn: 0**



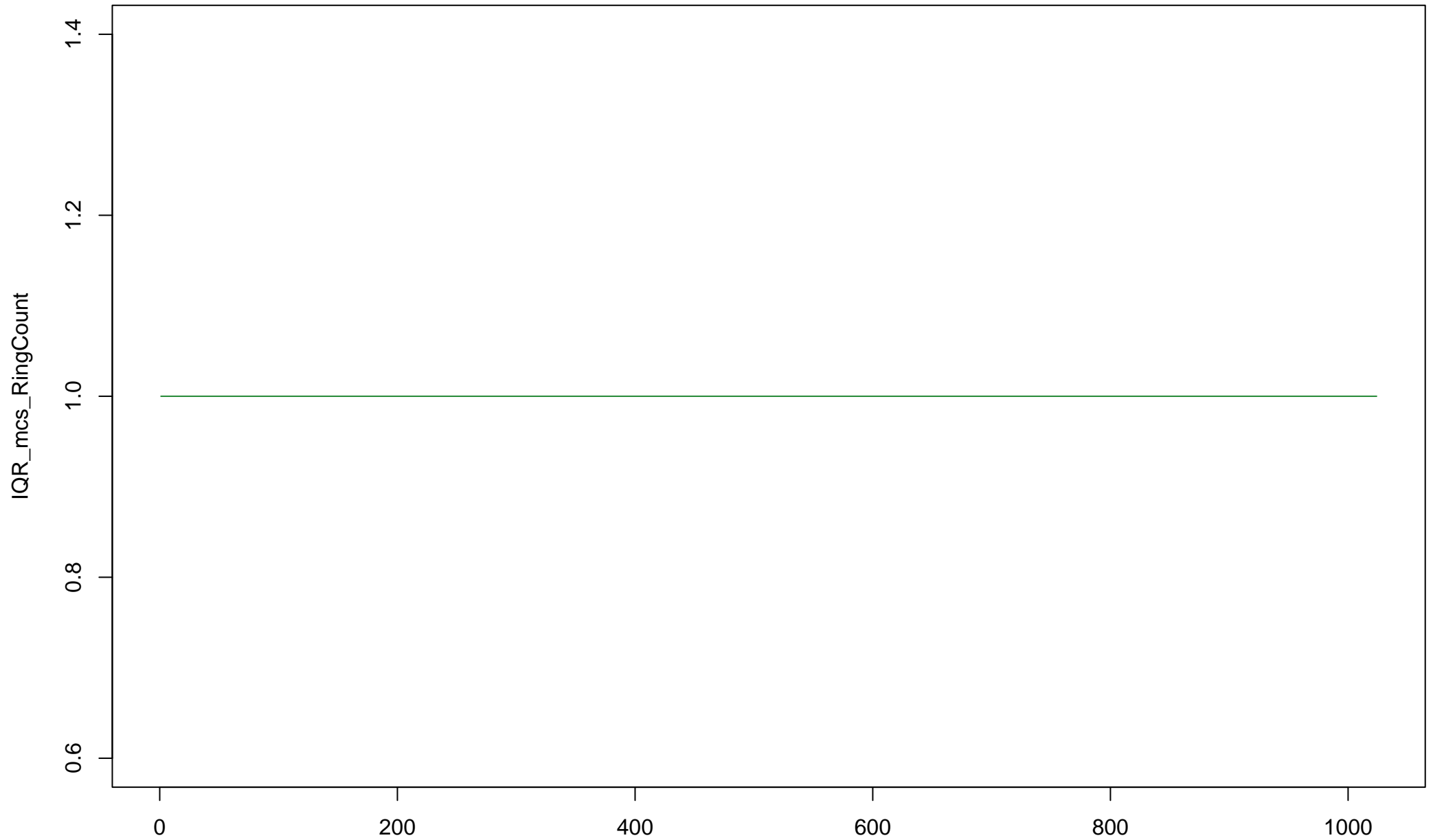
IQR\_mcs\_NumHeteroAtoms  
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



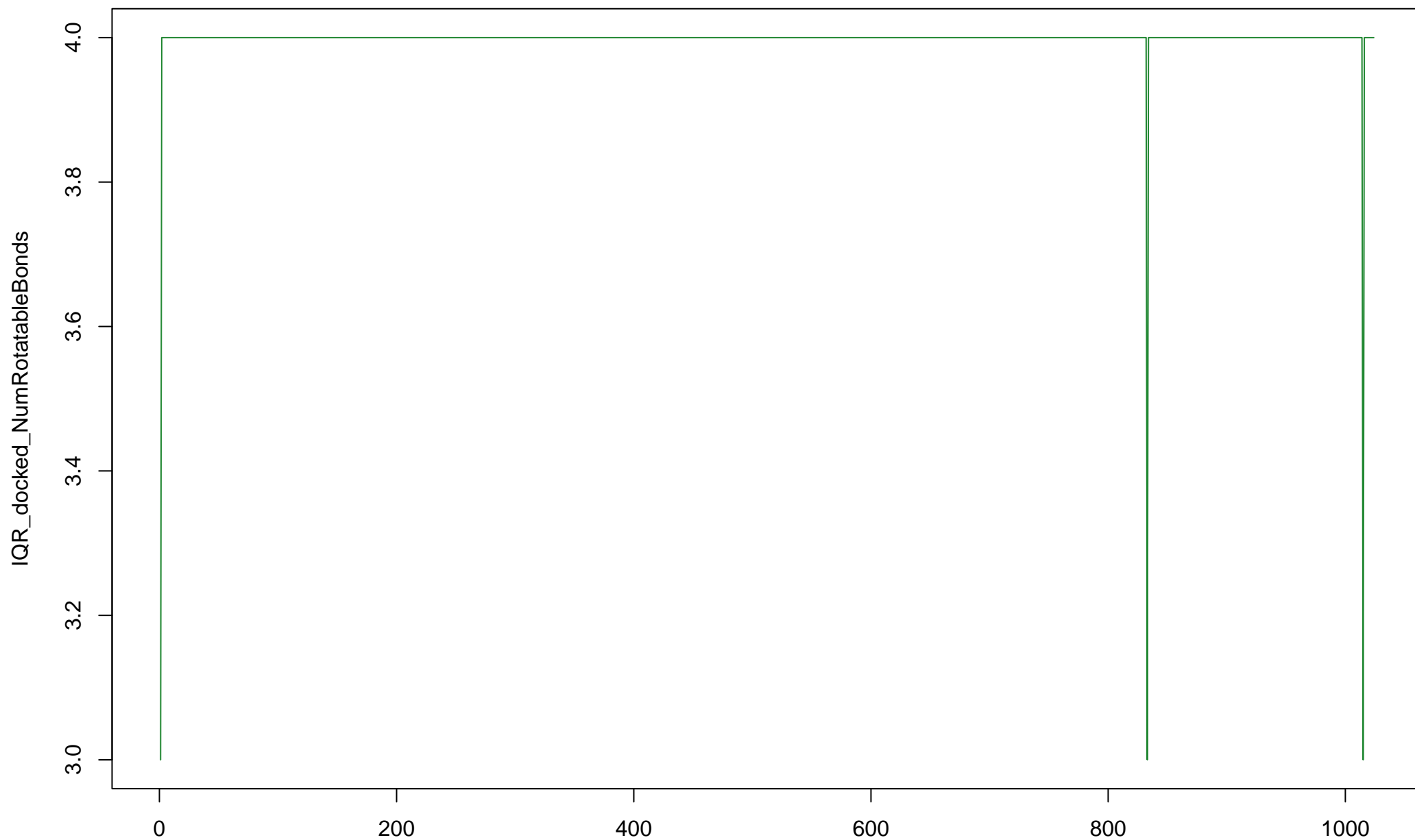
**IQR\_docked\_HeavyAtomCount**  
**ESS = 49.7 | BMK = 0.486 | MCSE(6.27) = 8.55 | stat: FALSE | burn: 714**



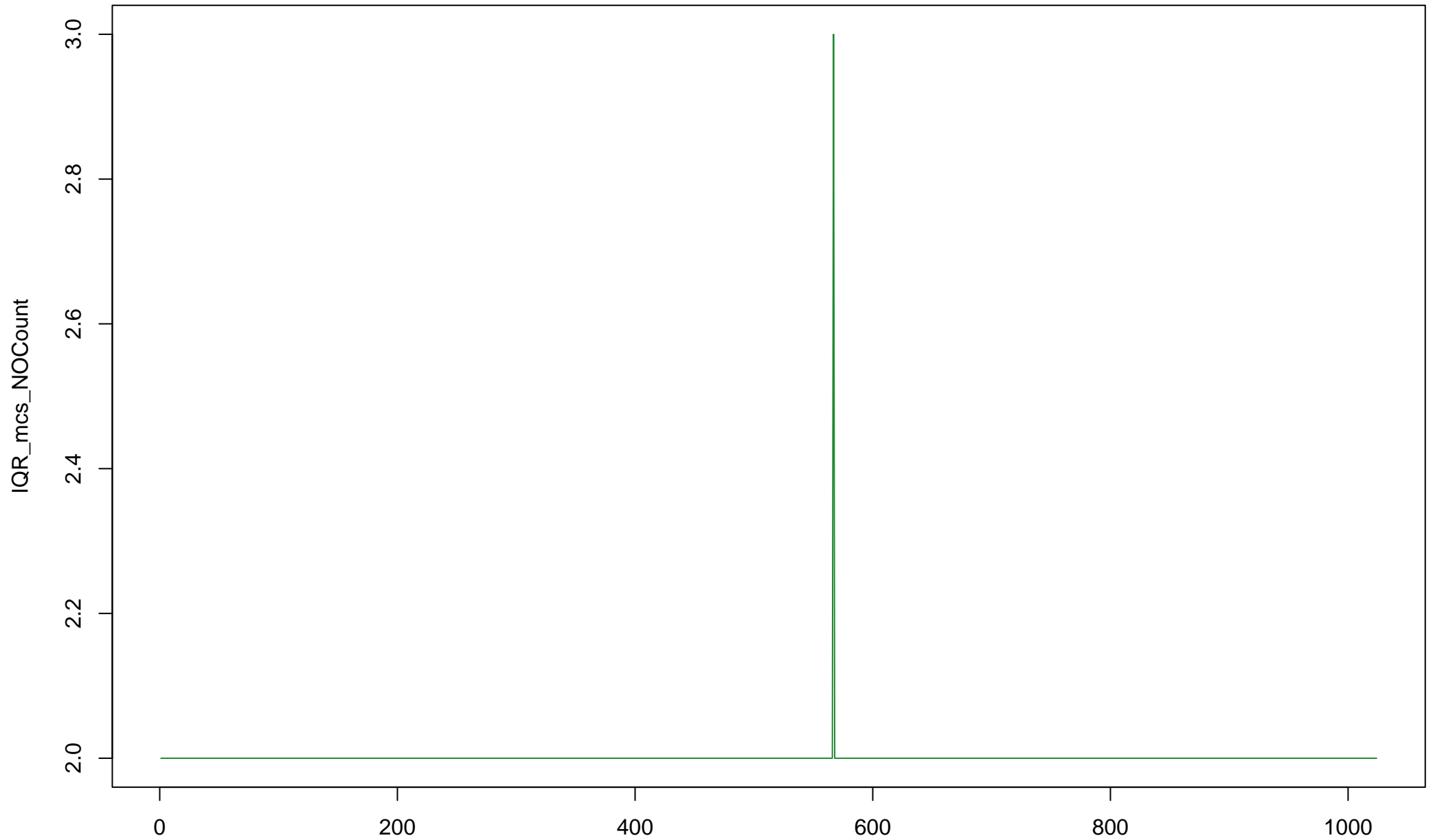
**IQR\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



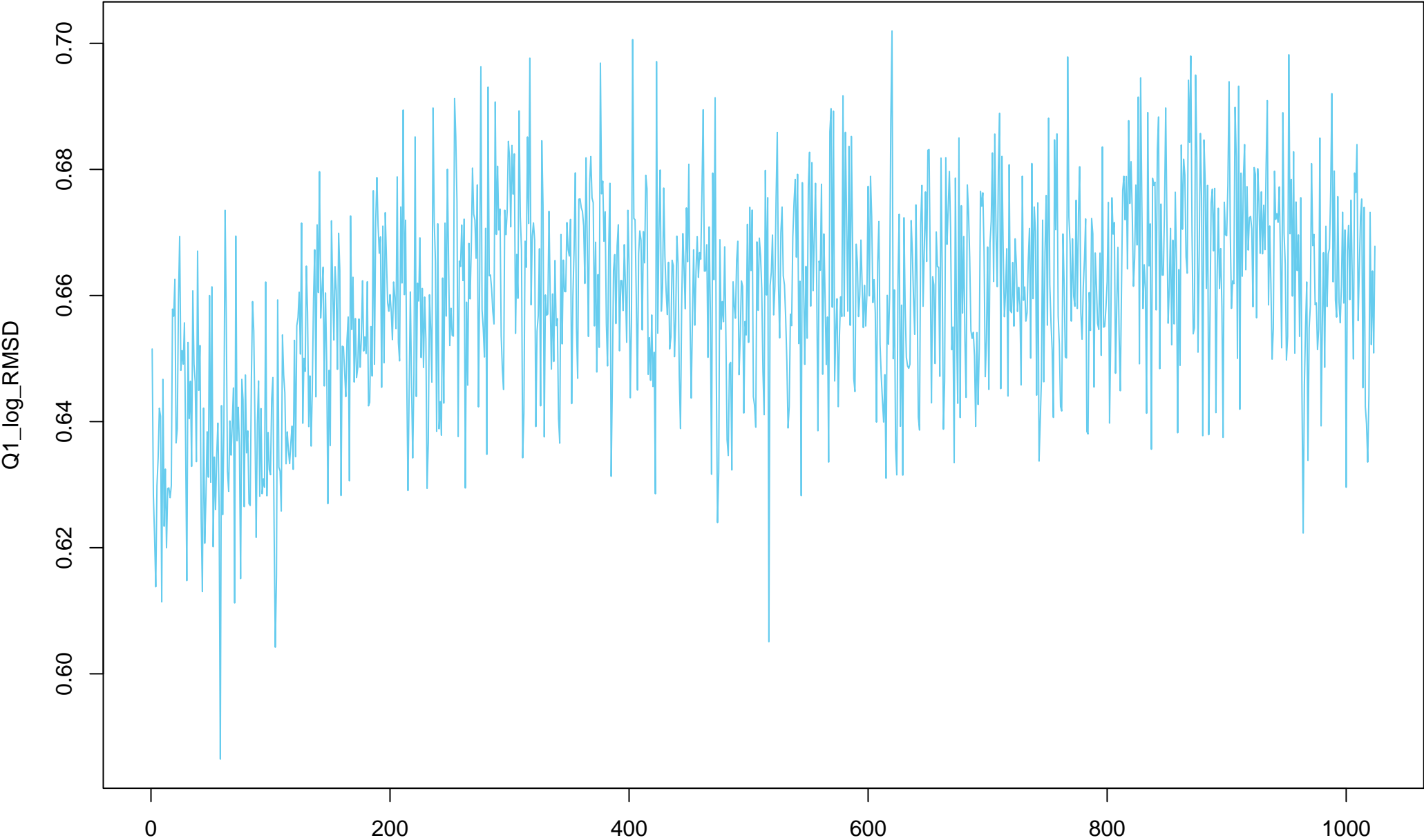
**IQR\_docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.121 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 816**



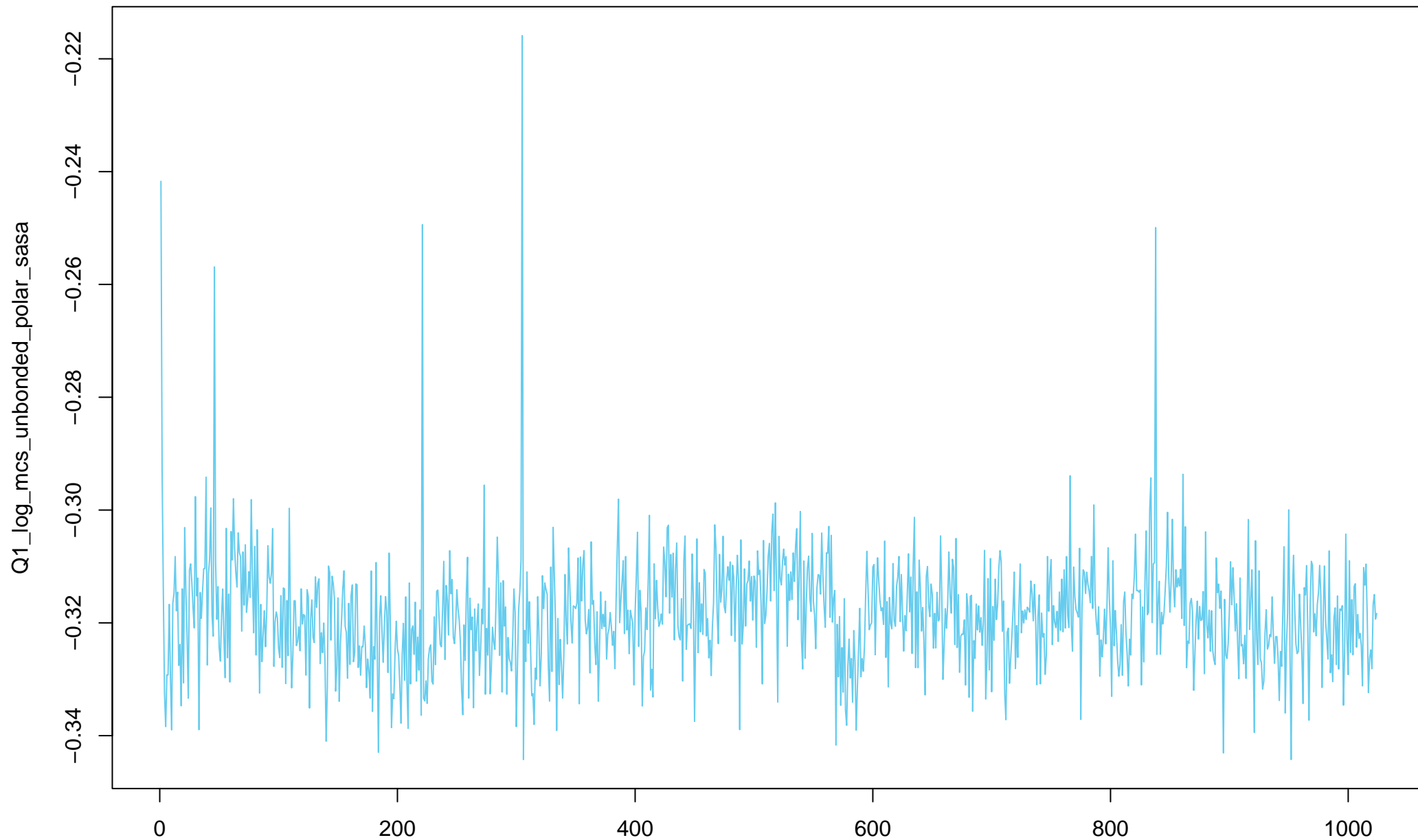
**IQR\_mcs\_NOCOUNT**  
**ESS = 1020 | BMK = 0.626 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 612**



**Q1\_log\_RMSD**  
**ESS = 35.7 | BMK = 0.208 | MCSE(6.27) = 9.74 | stat: FALSE | burn: 0**

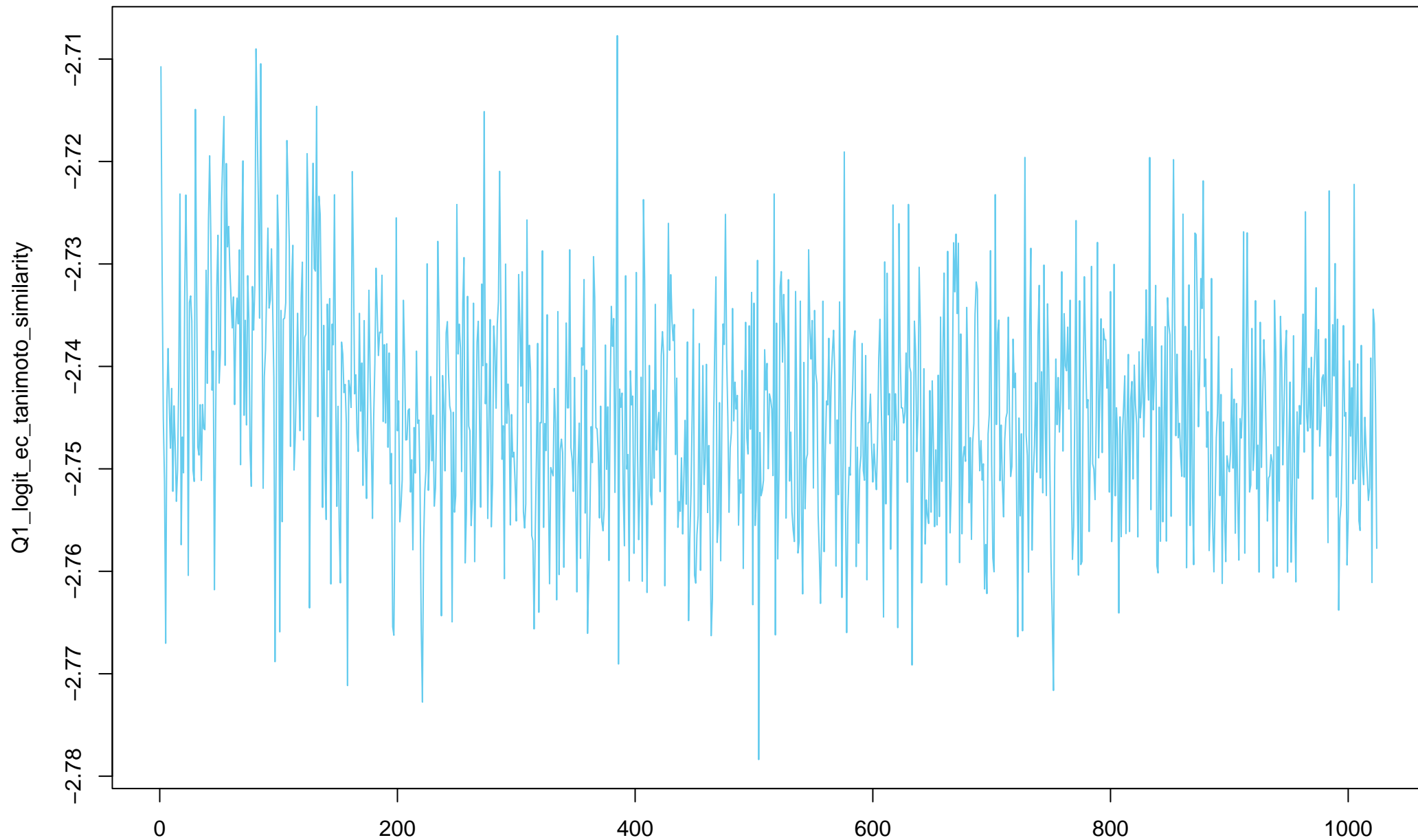


**Q1\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 379 | BMK = 0.076 | MCSE(6.27) = 5.56 | stat: TRUE | burn: 0**

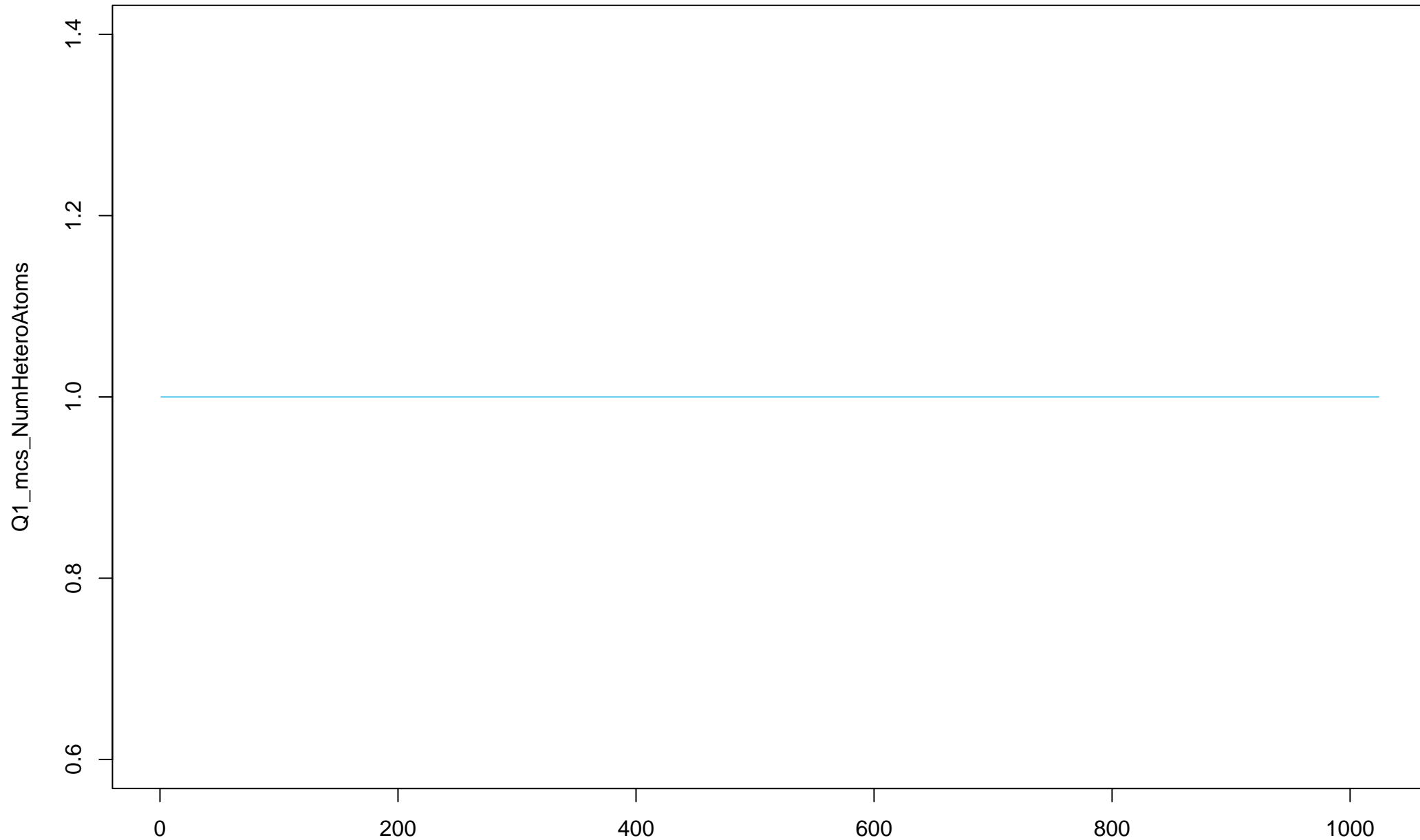




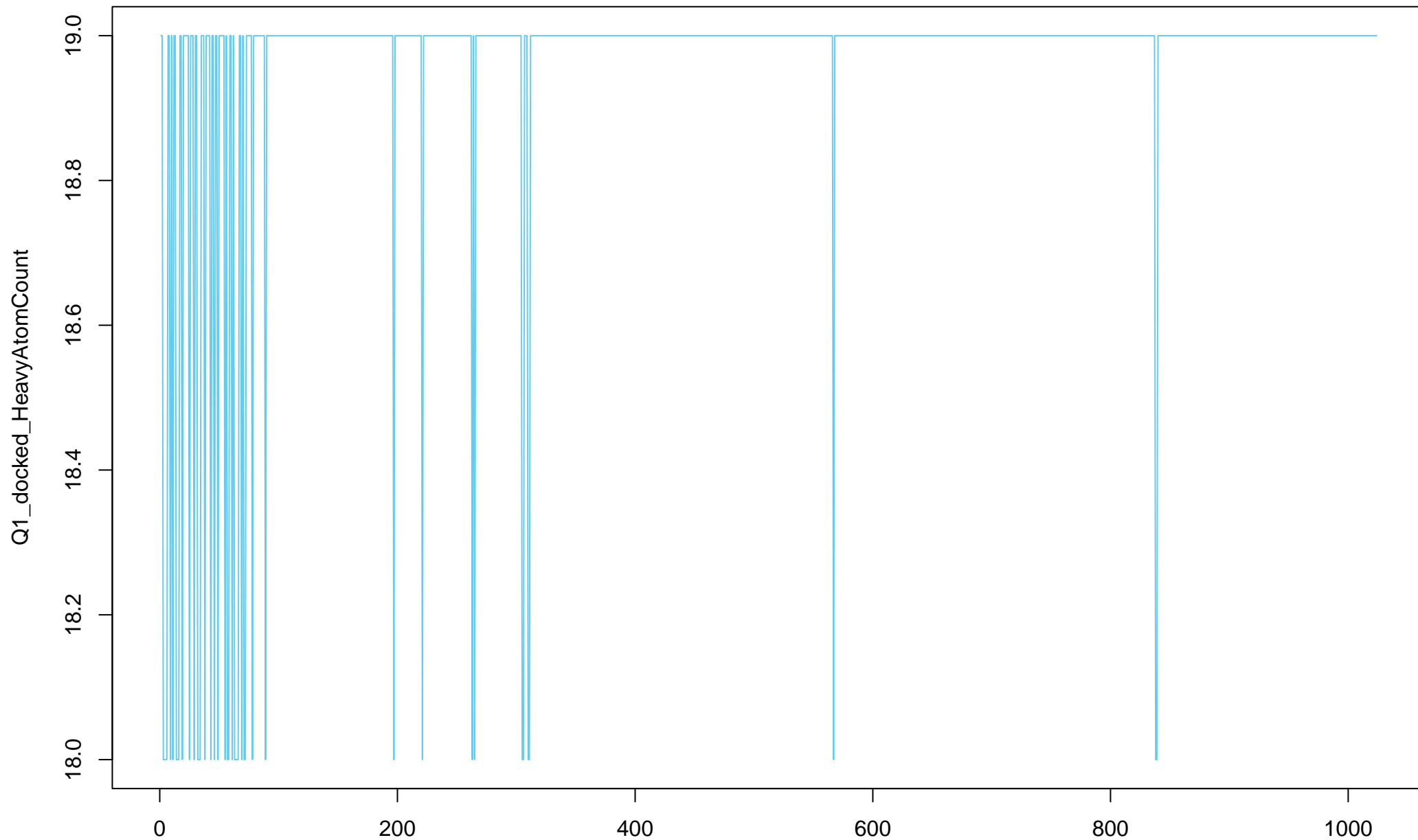
**Q1\_logit\_ec\_tanimoto\_similarity**  
**ESS = 309 | BMK = 0.107 | MCSE(6.27) = 6 | stat: FALSE | burn: 0**



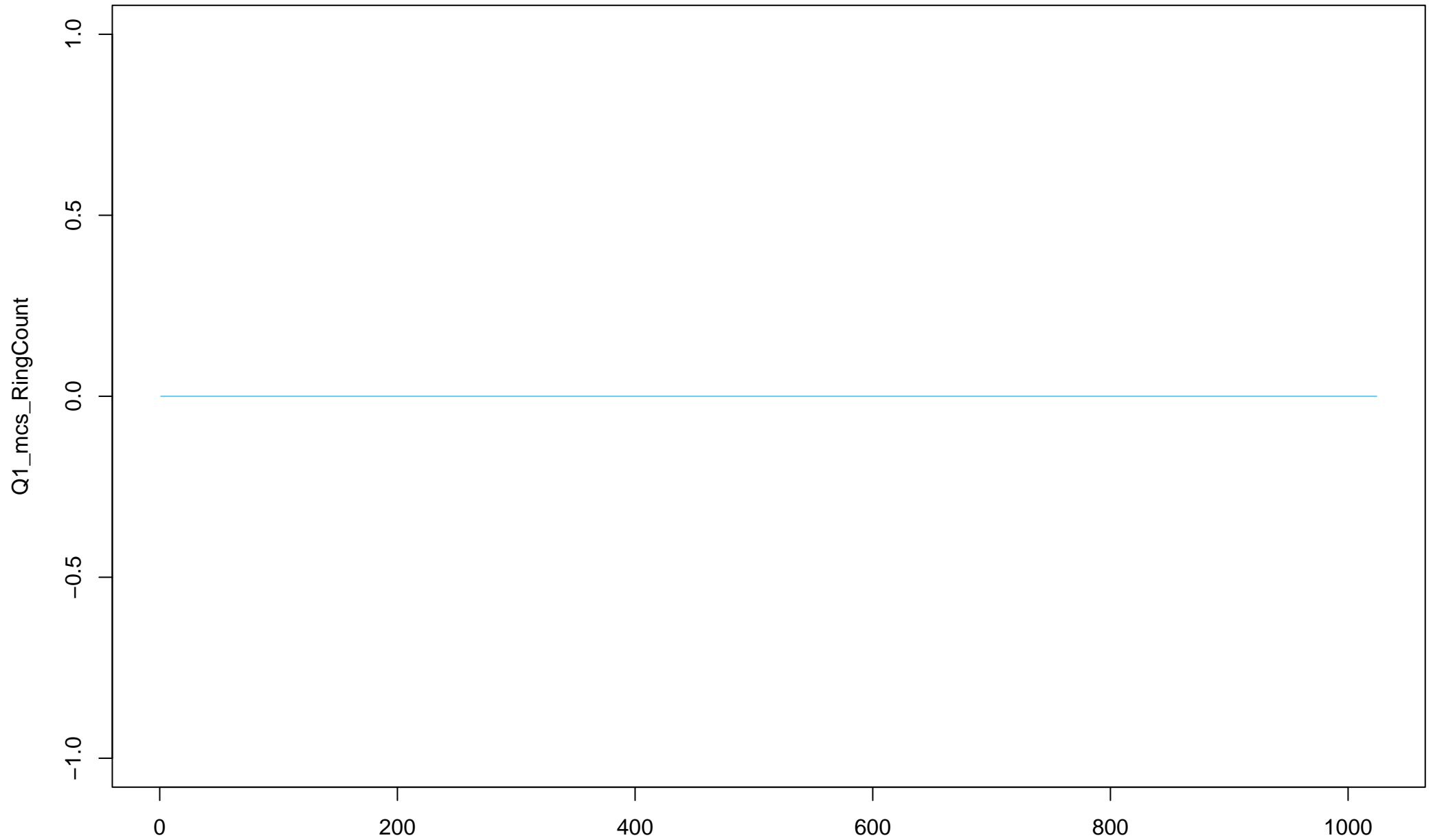
**Q1\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



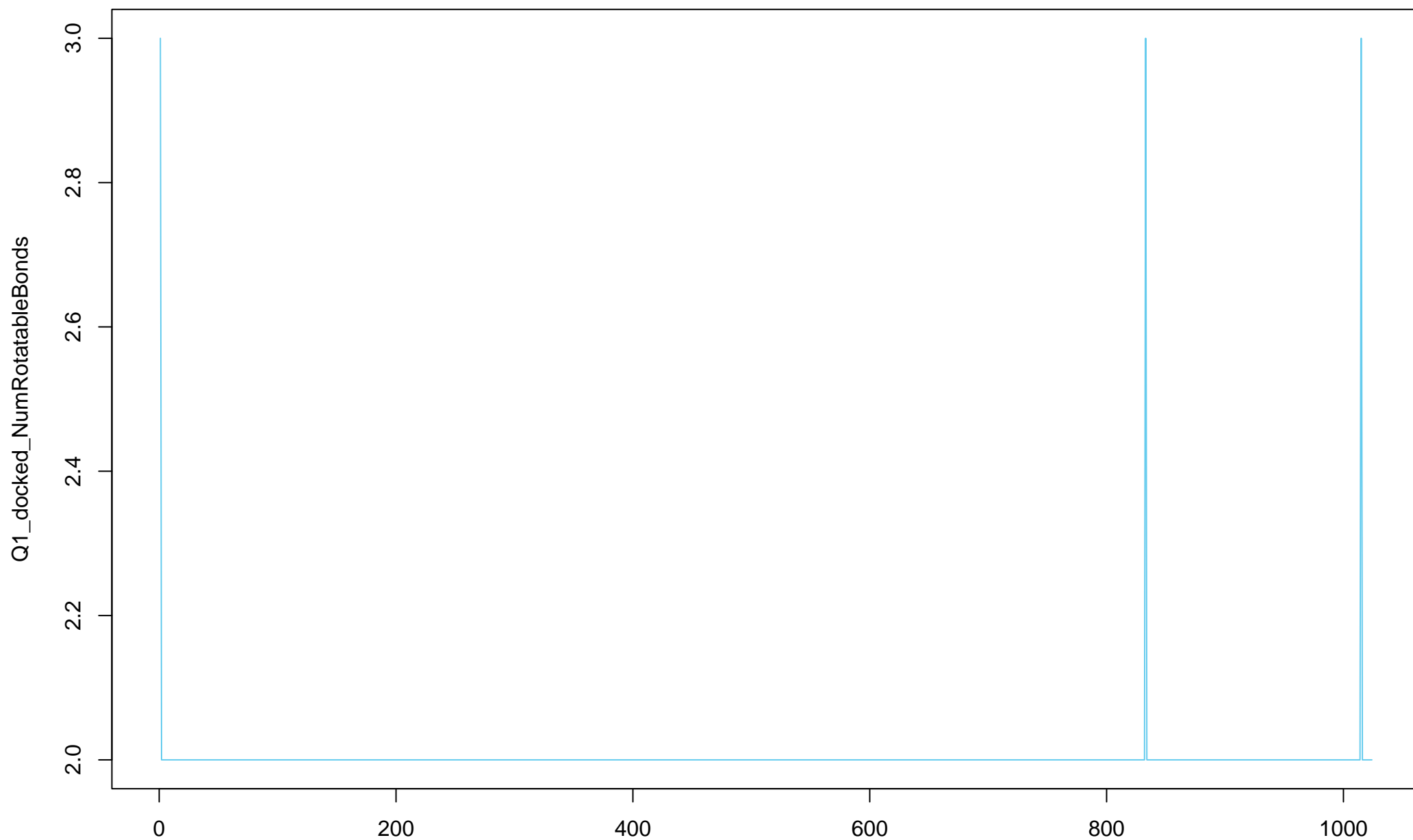
**Q1\_docked\_HeavyAtomCount**  
**ESS = 42 | BMK = 0.384 | MCSE(6.27) = 9.03 | stat: FALSE | burn: 0**



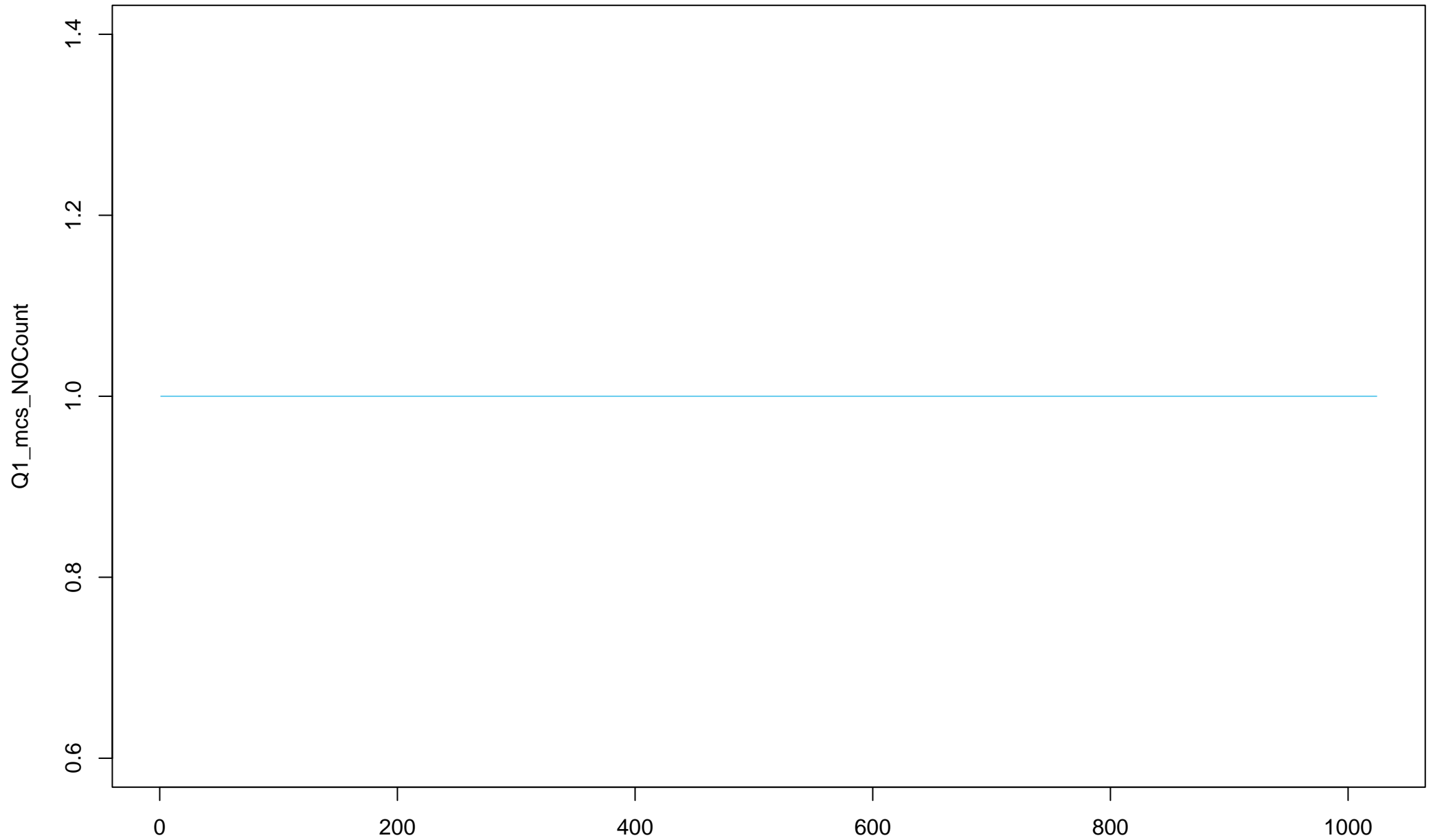
**Q1\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



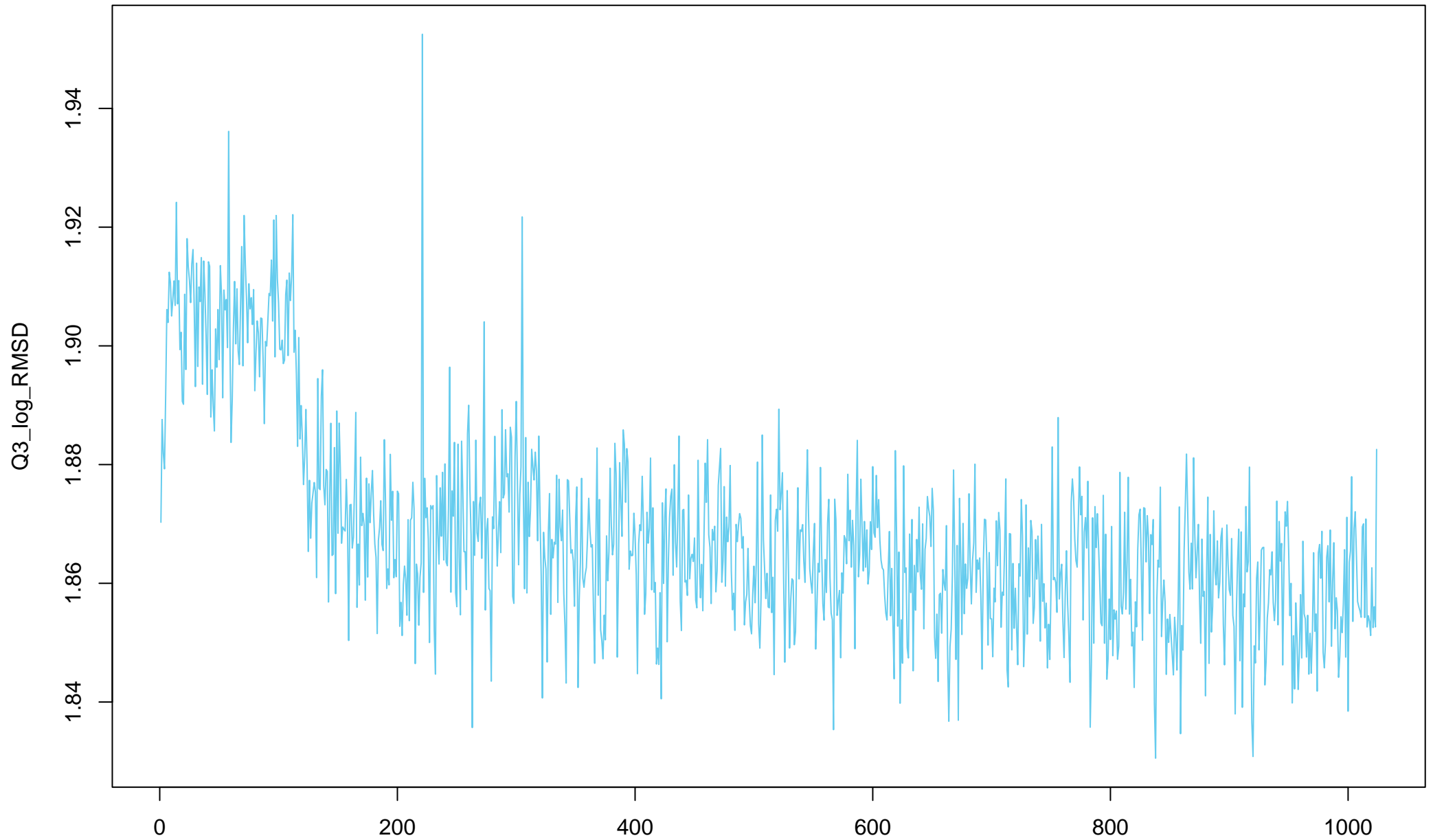
**Q1\_docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.121 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 816**



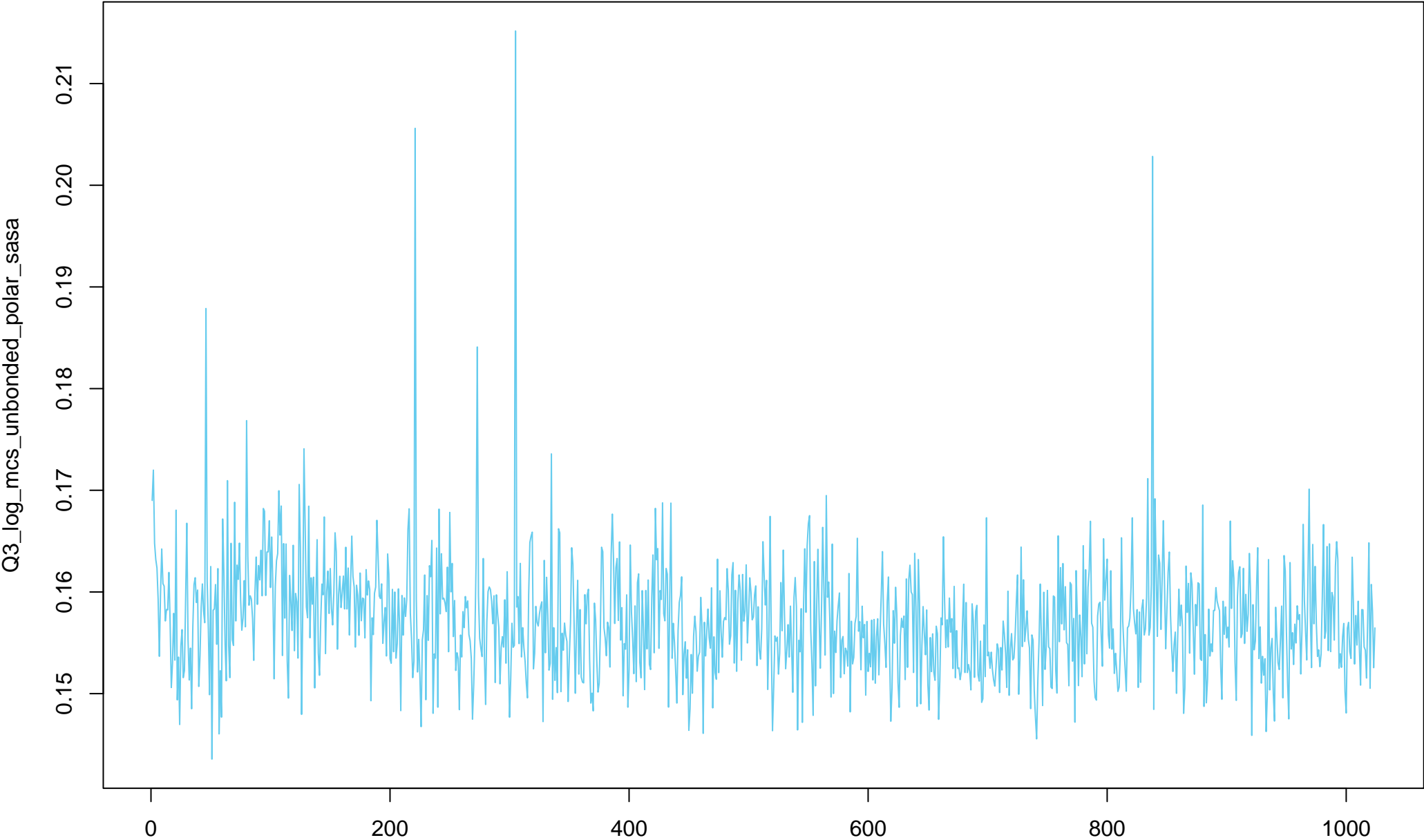
**Q1\_mcs\_NOCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q3\_log\_RMSD**  
**ESS = 8.12 | BMK = 0.412 | MCSE(6.27) = 14.2 | stat: FALSE | burn: 102**

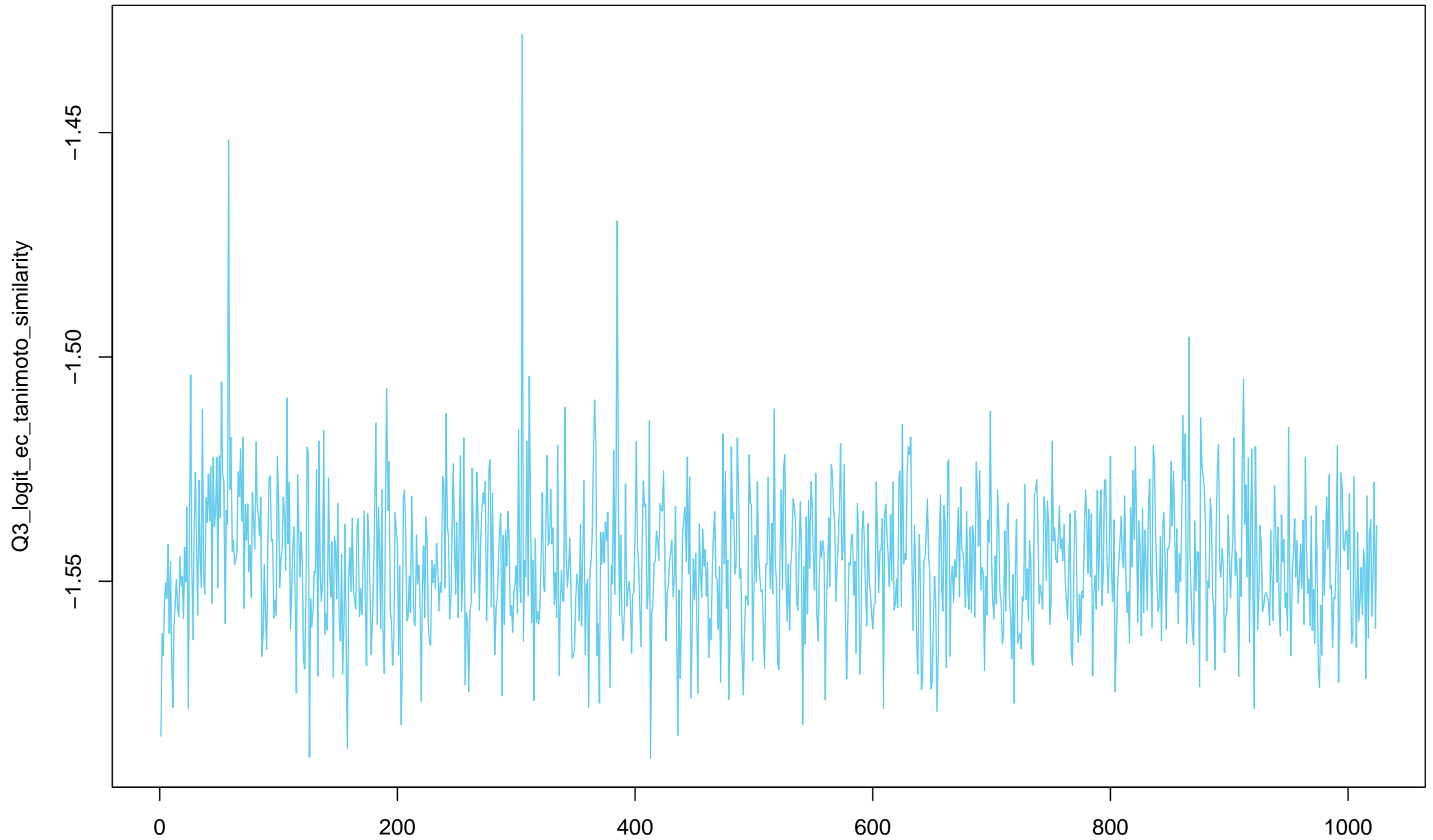


**Q3\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 471 | BMK = 0.132 | MCSE(6.27) = 5.58 | stat: FALSE | burn: 0**

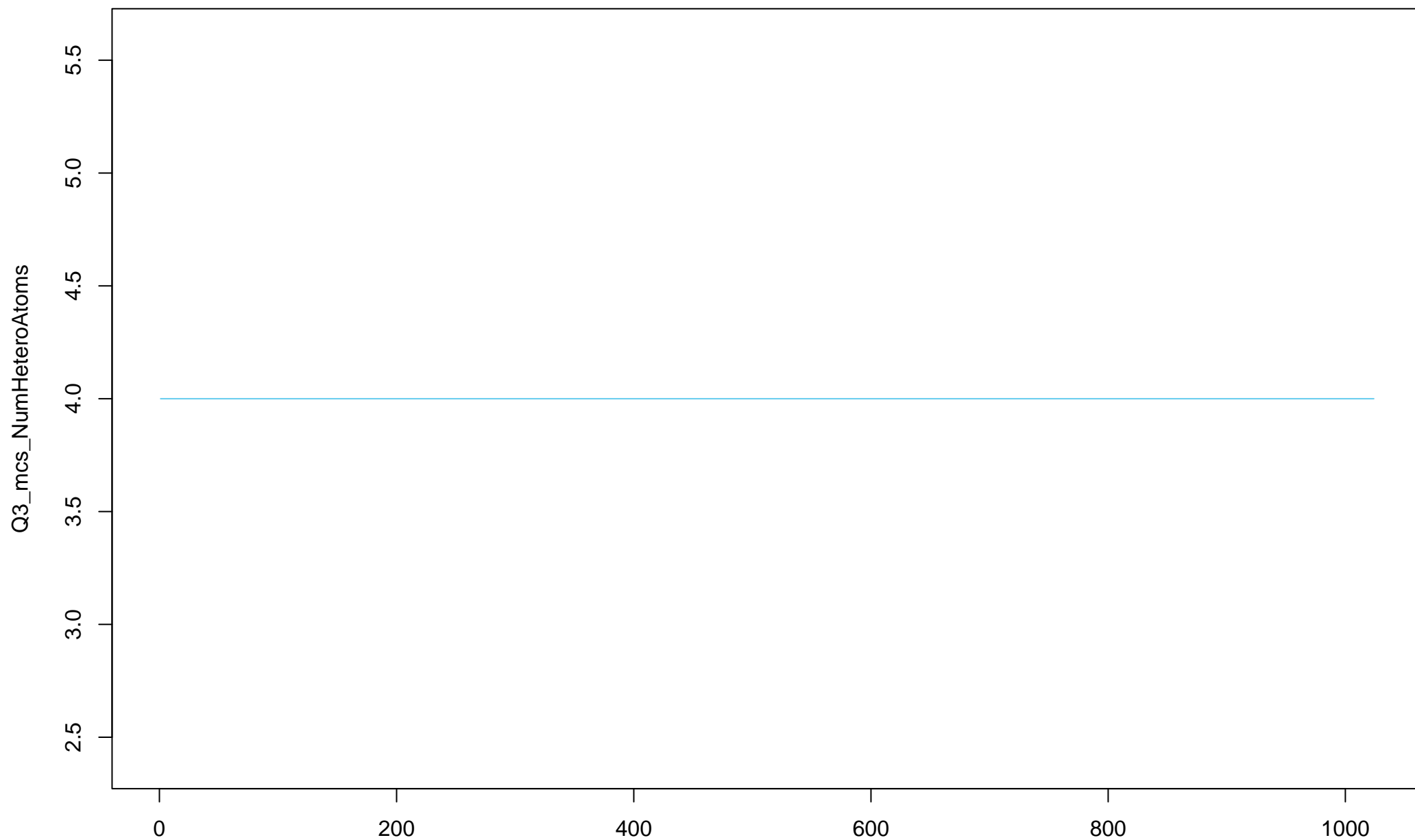




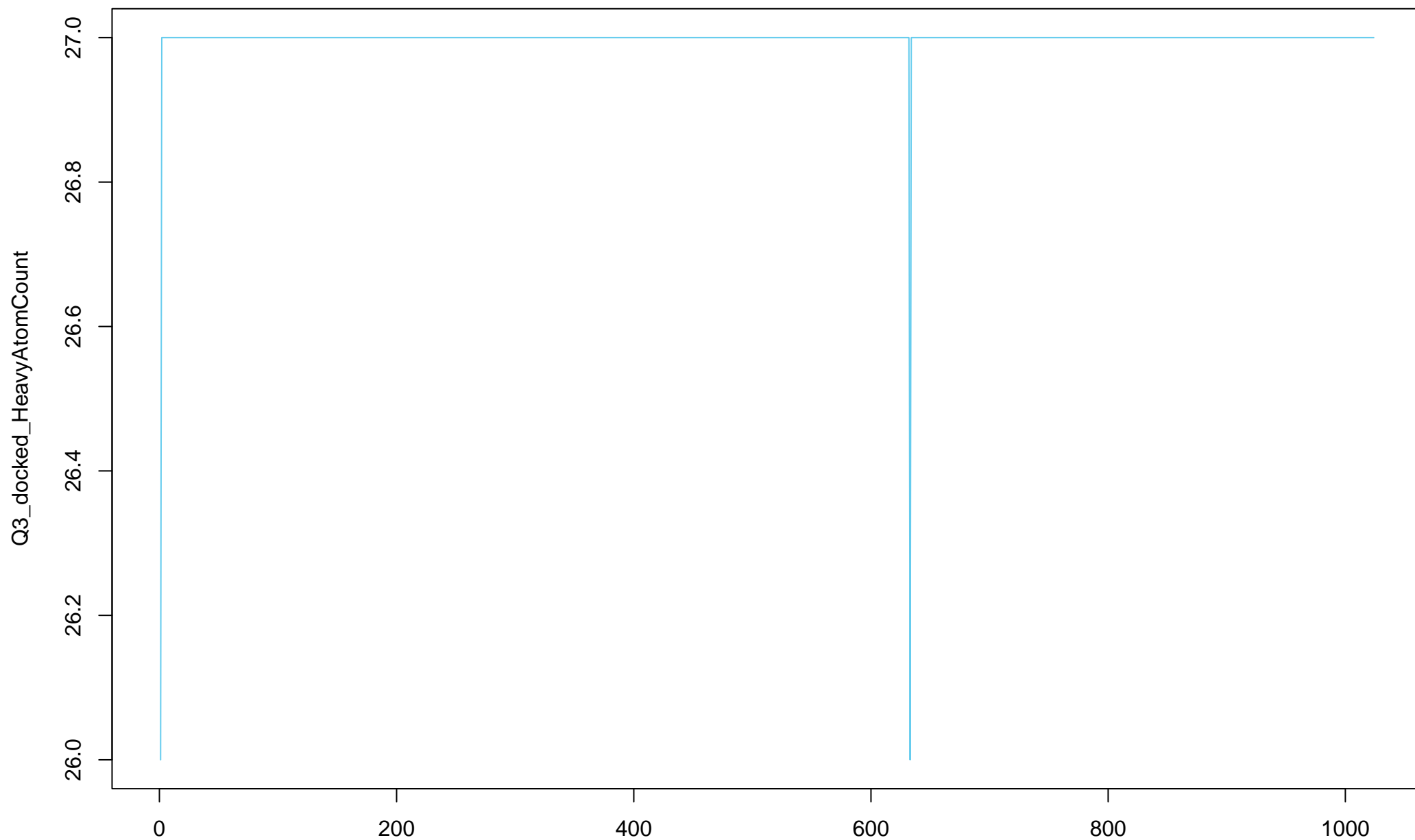
**Q3\_logit\_ec\_tanimoto\_similarity**  
**ESS = 797 | BMK = 0.0815 | MCSE(6.27) = 4.44 | stat: TRUE | burn: 0**



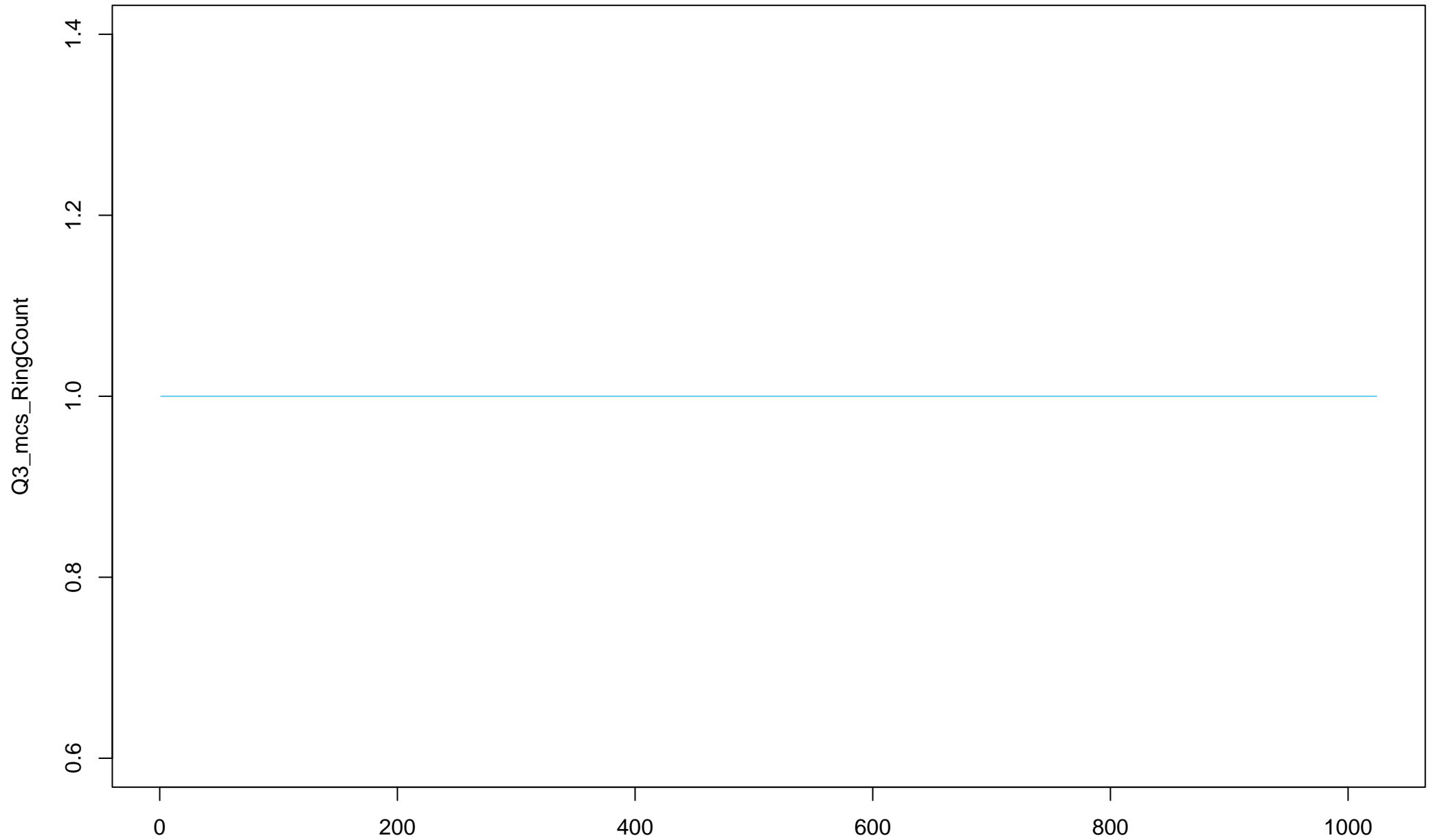
**Q3\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



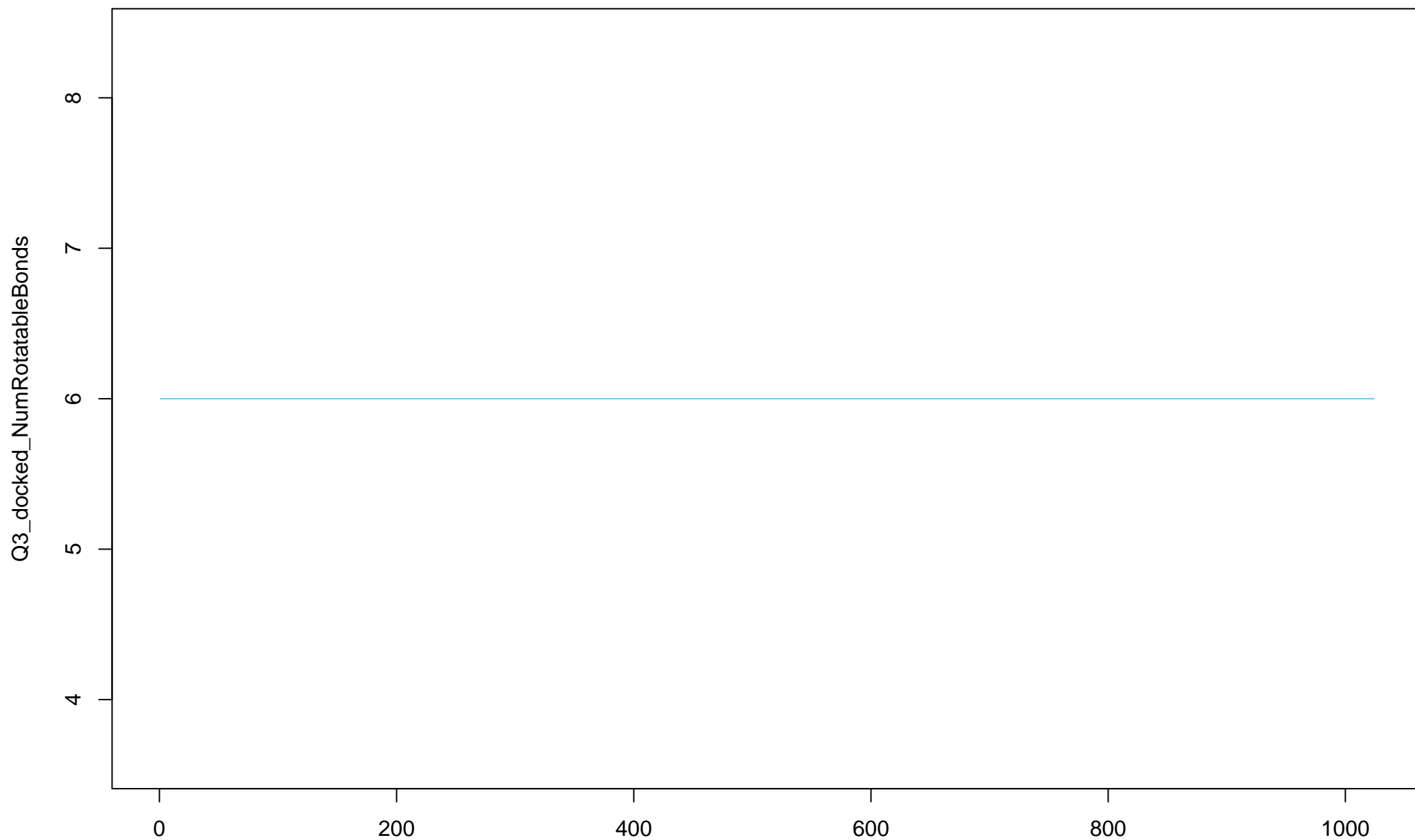
**Q3\_docked\_HeavyAtomCount**  
**ESS = 1020 | BMK = 0 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0**



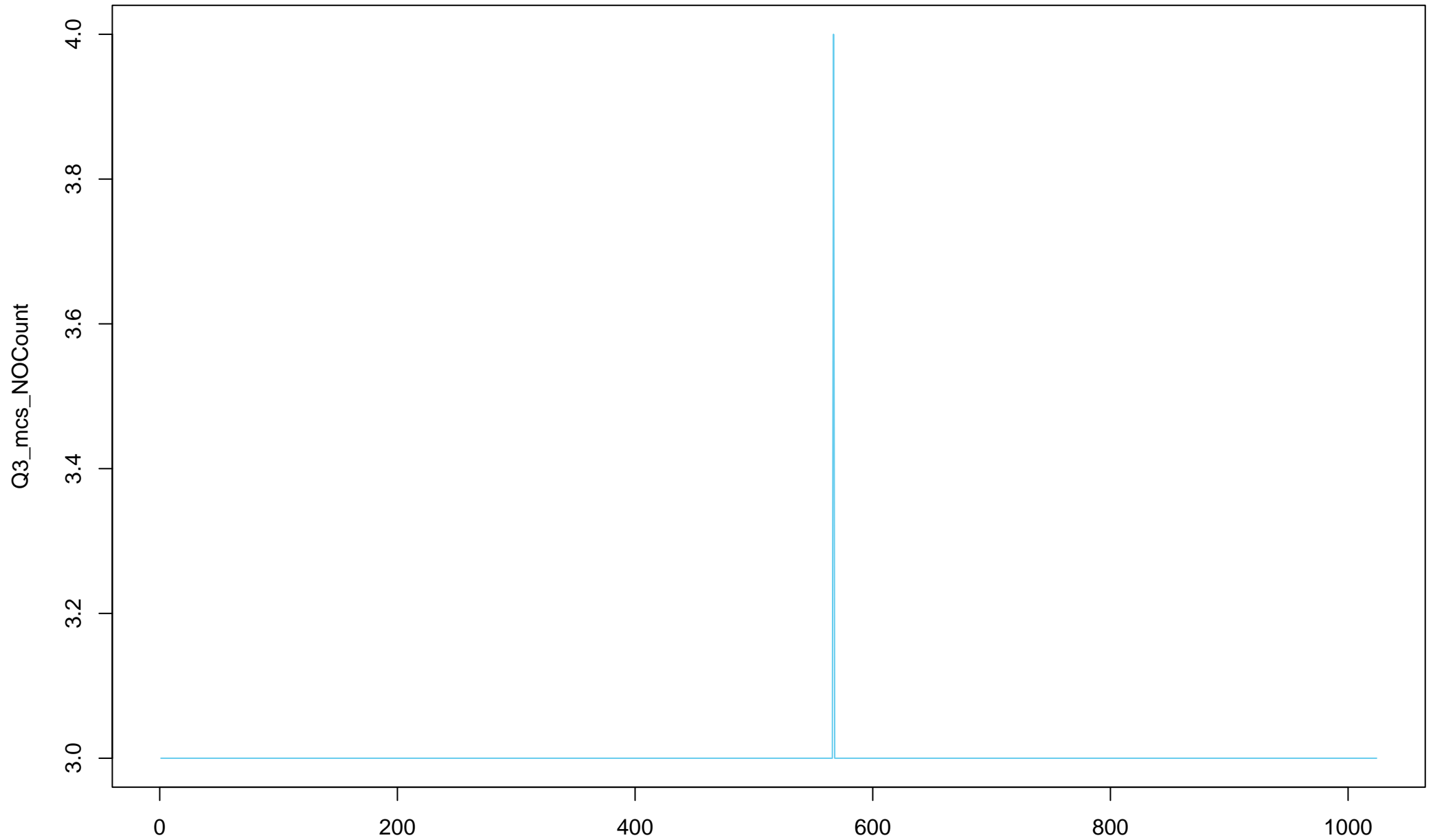
**Q3\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



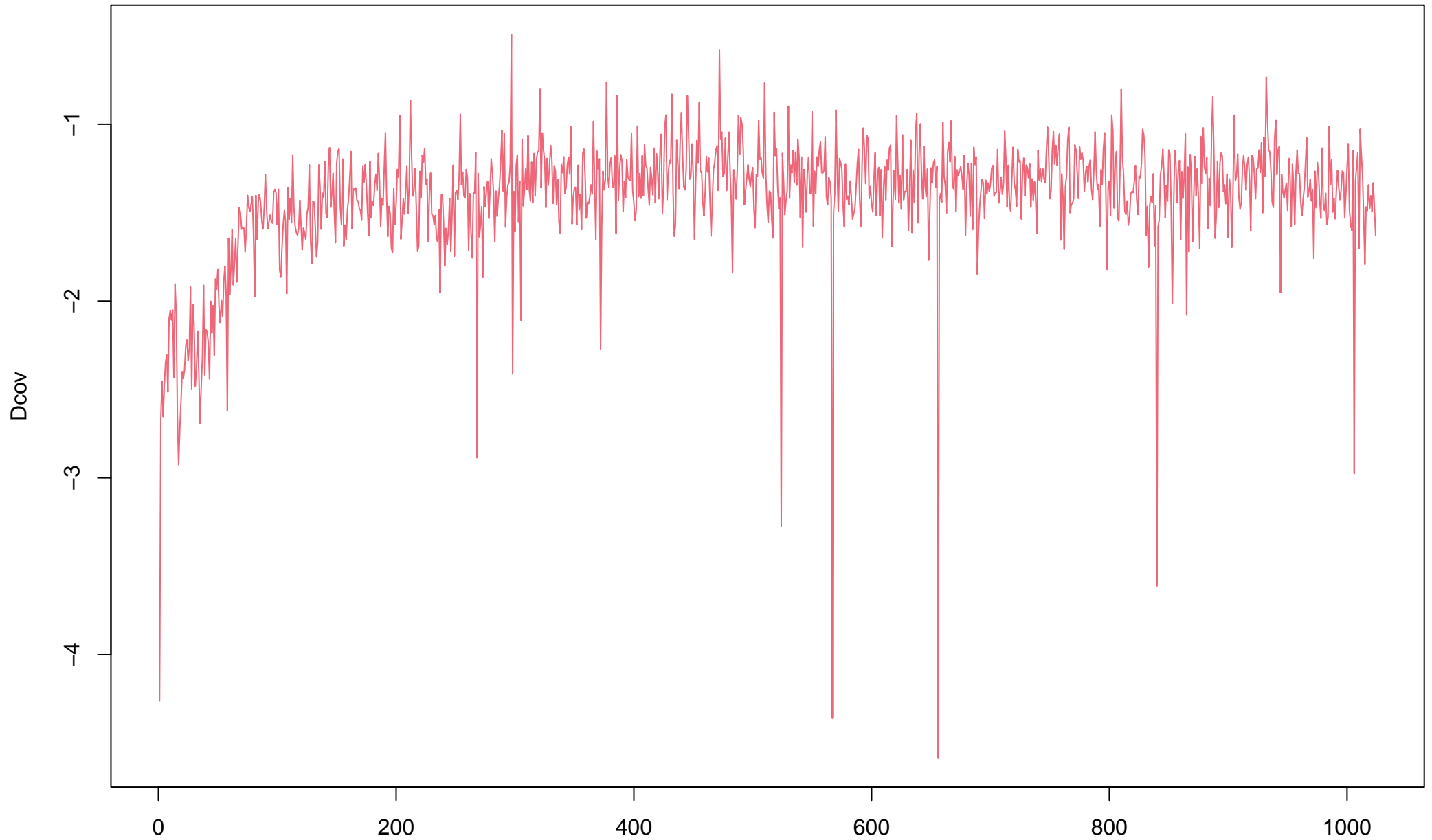
**Q3\_docked\_NumRotatableBonds**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



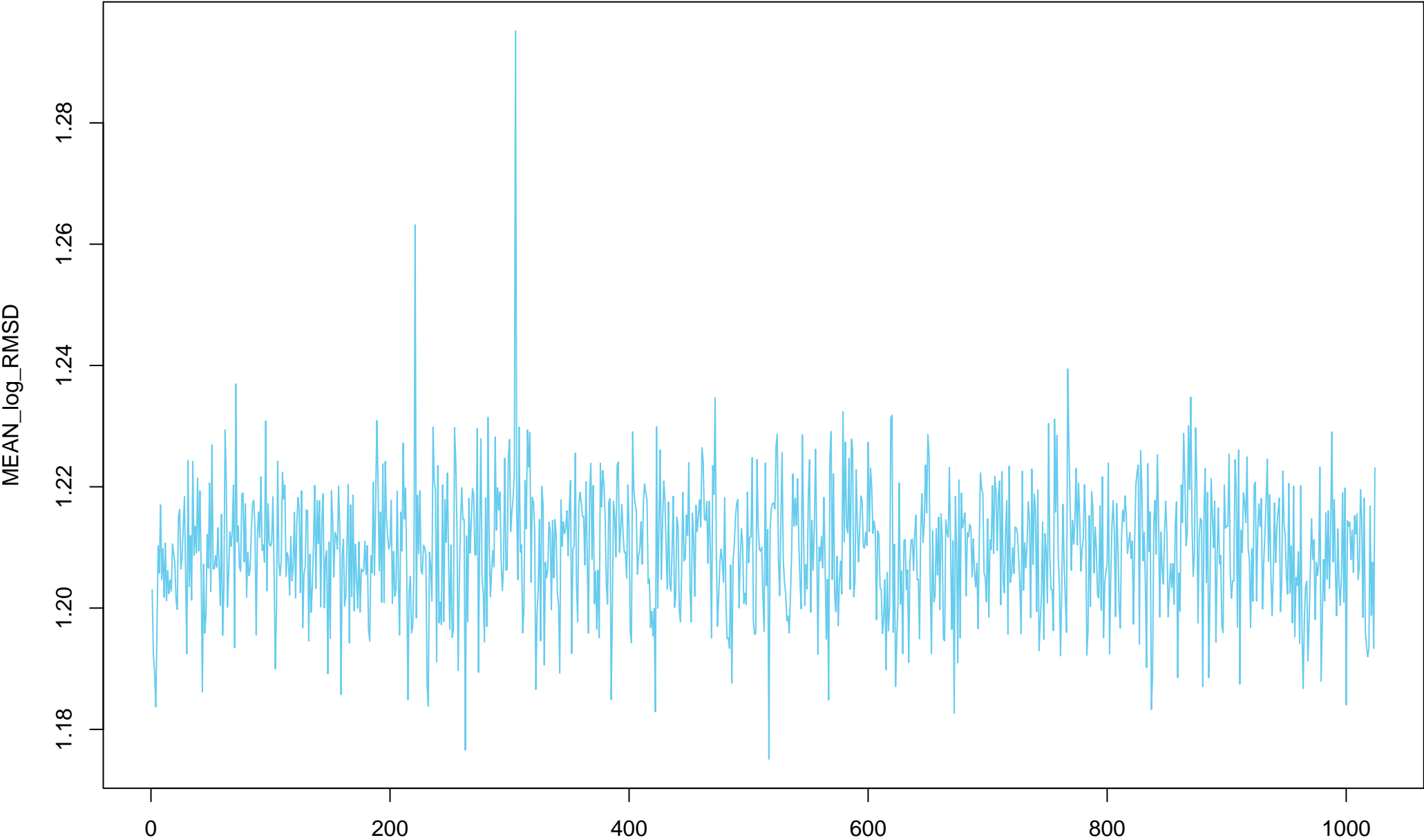
**Q3\_mcs\_NOCount**  
**ESS = 1020 | BMK = 0.613 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 612**



**Dcov**  
**ESS = 41.2 | BMK = 0.237 | MCSE(6.27) = 11.2 | stat: FALSE | burn: 102**

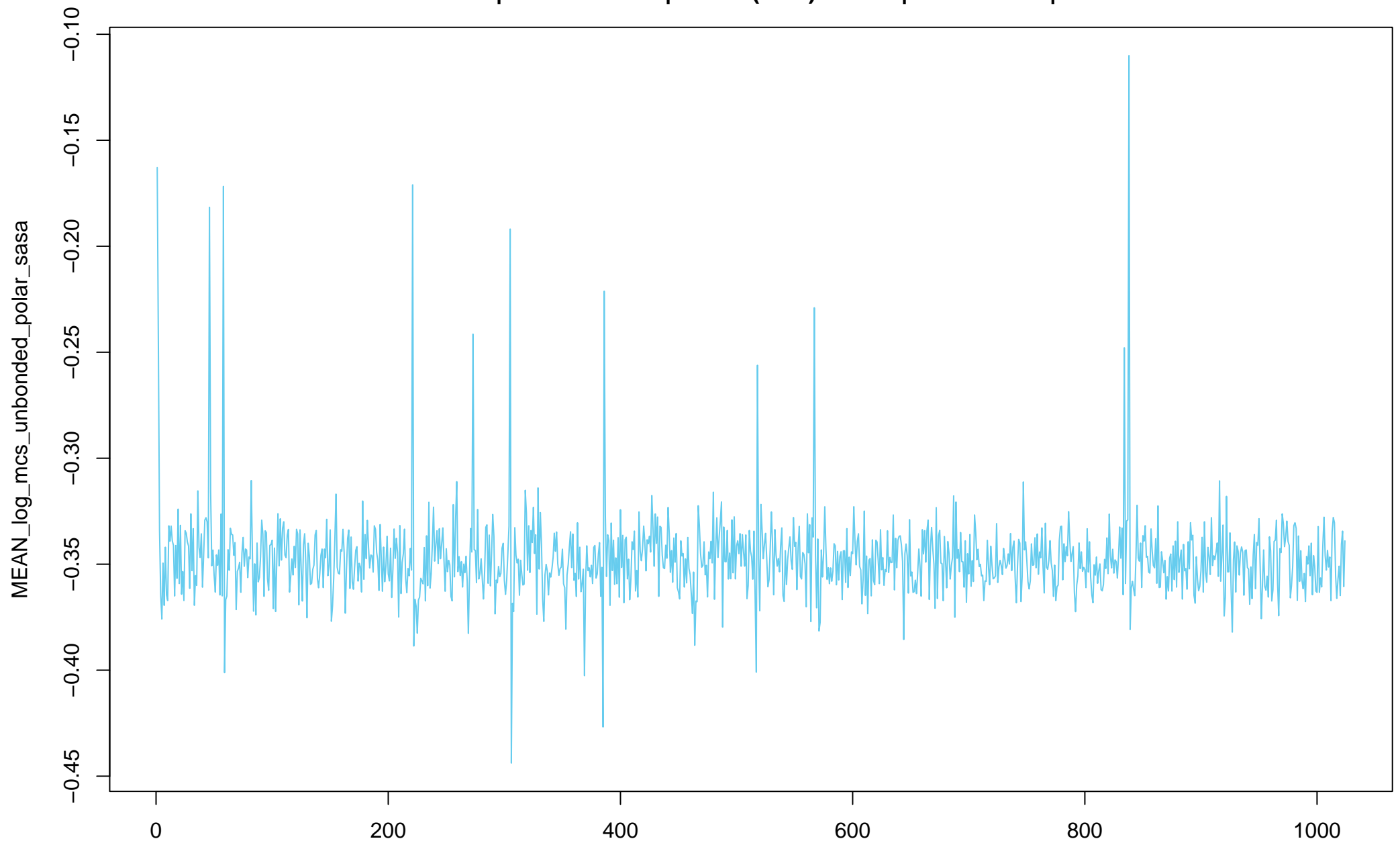


**MEAN\_log\_RMSD**  
**ESS = 851 | BMK = 0.0526 | MCSE(6.27) = 4.36 | stat: TRUE | burn: 0**

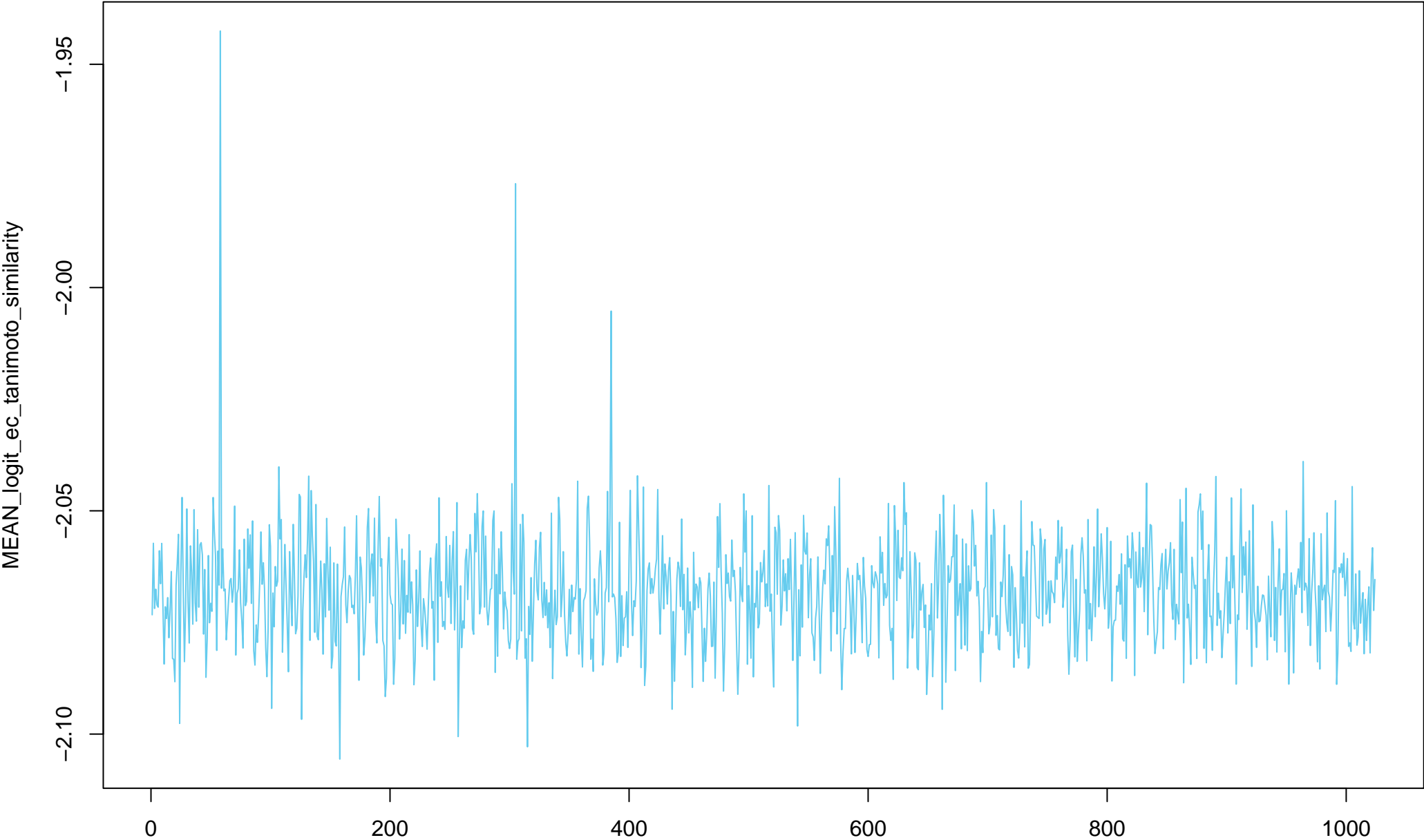




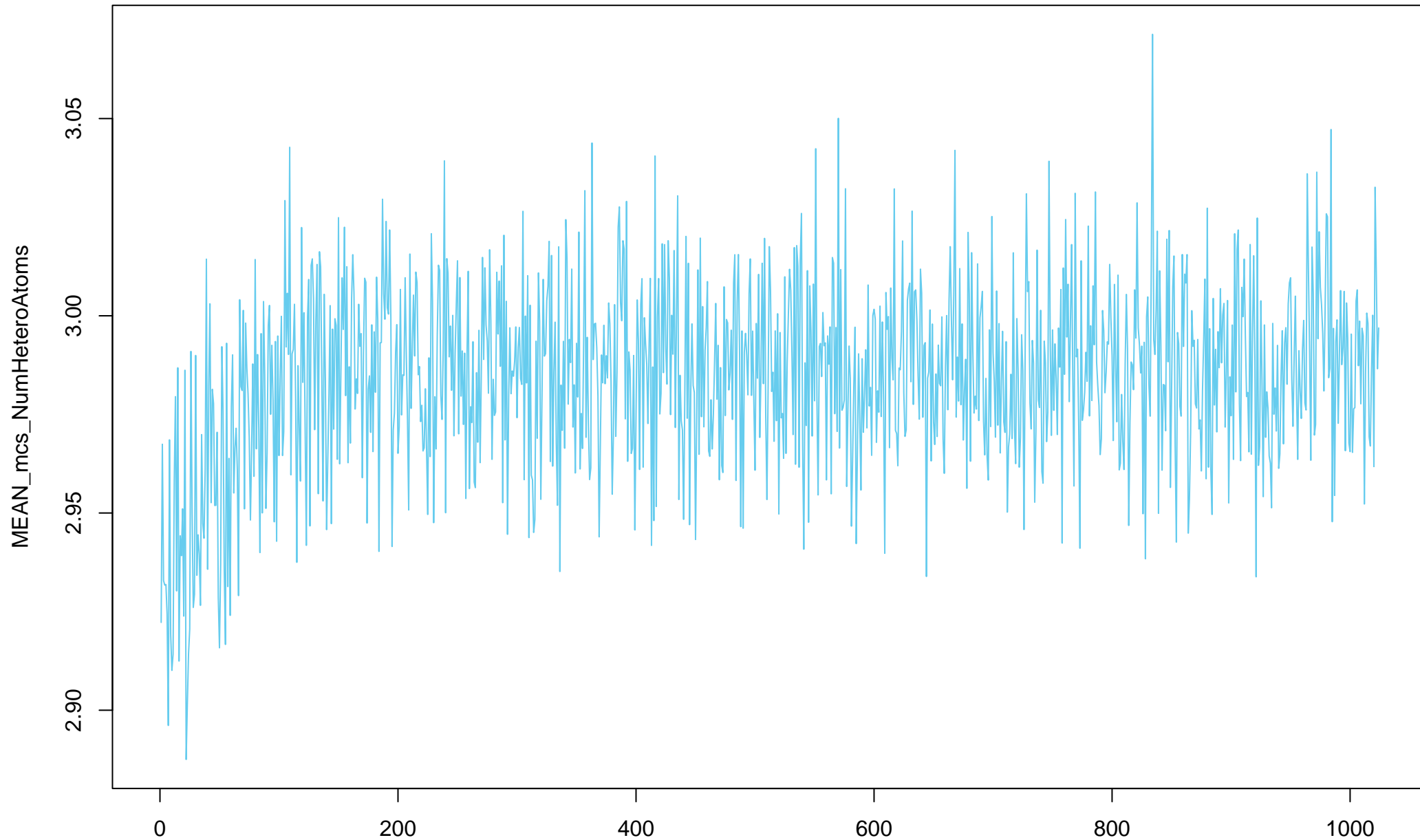
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1020 | BMK = 0.112 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 0**



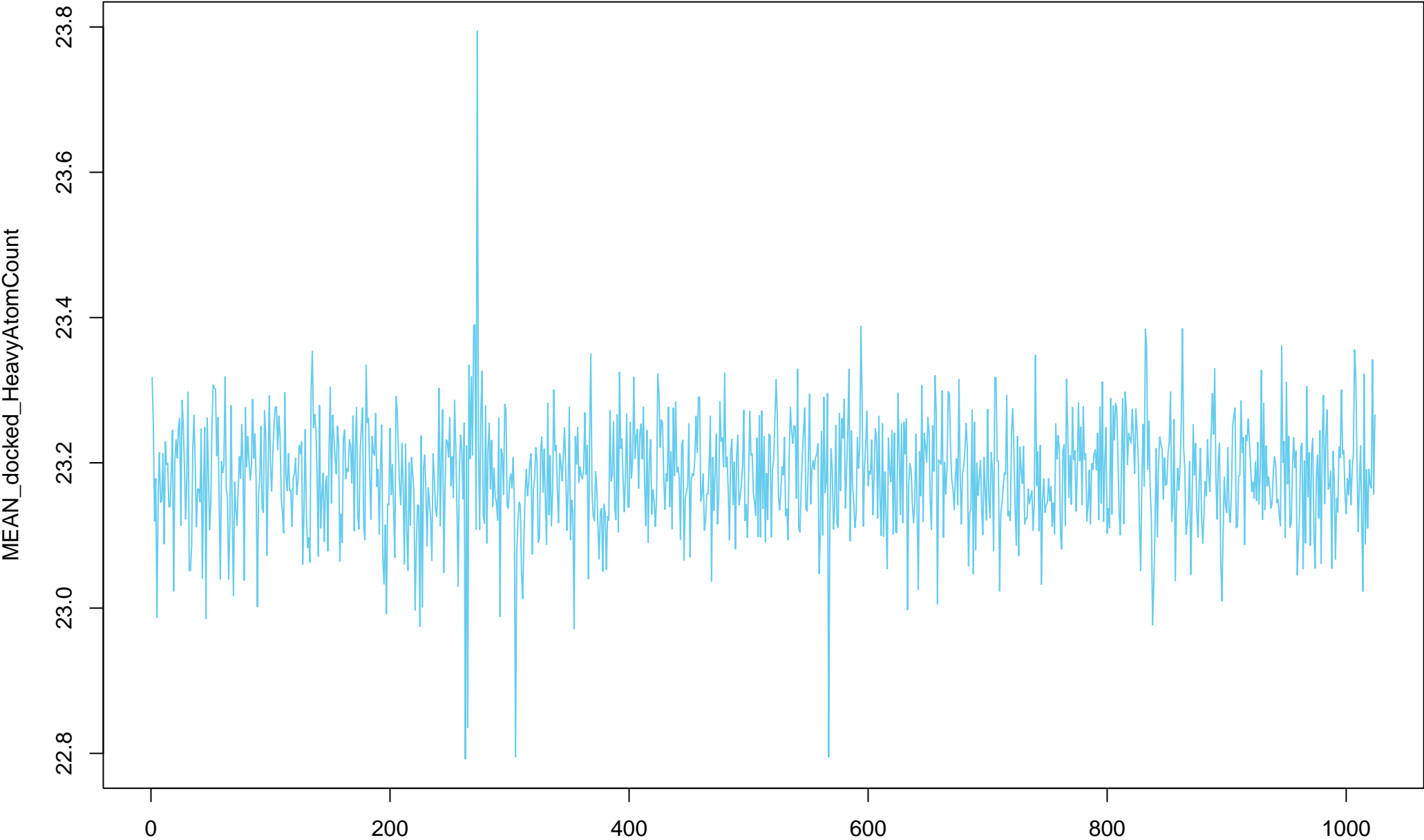
**MEAN\_logit\_ec\_tanimoto\_similarity**  
**ESS = 917 | BMK = 0.0736 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0**



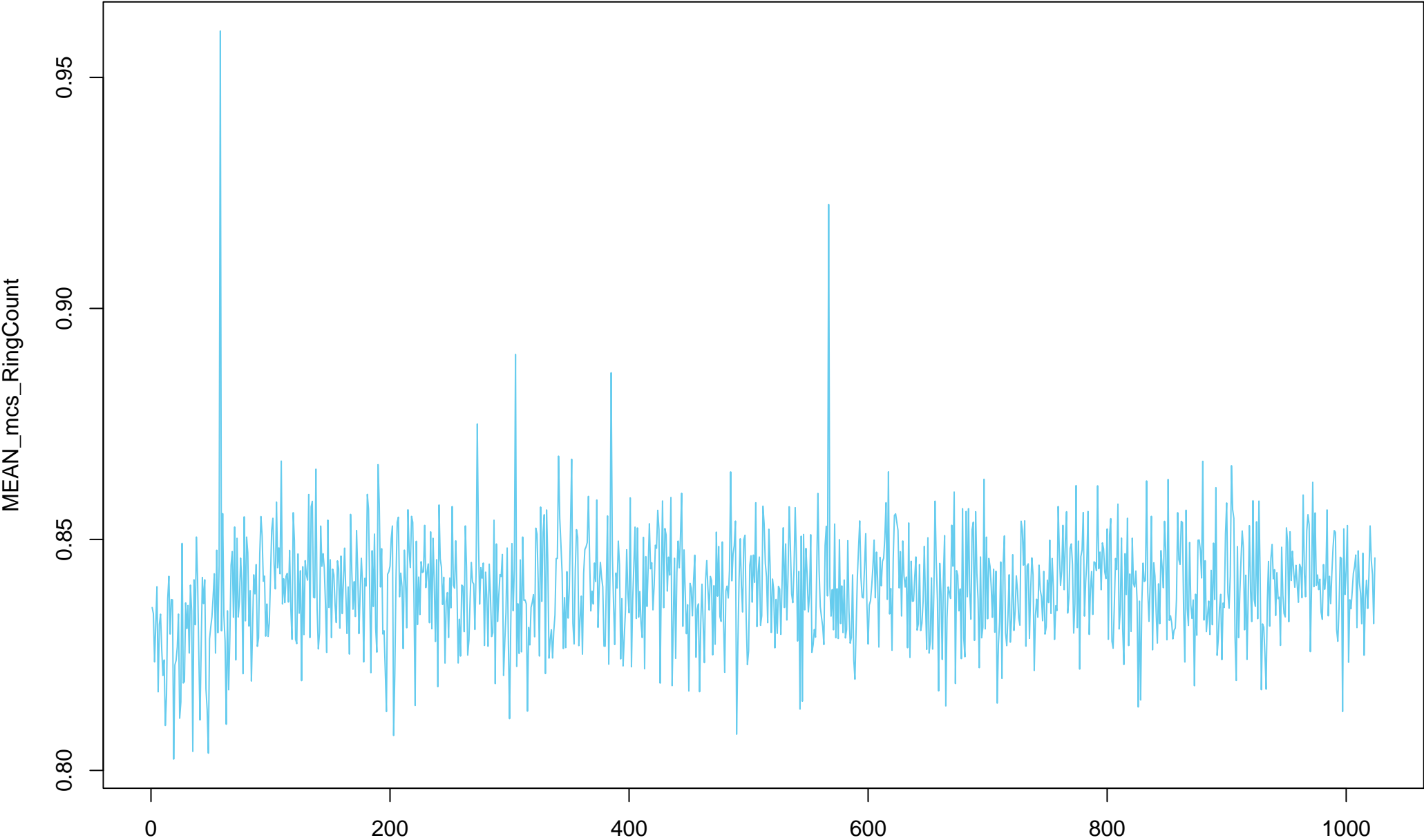
**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 149 | BMK = 0.159 | MCSE(6.27) = 7.9 | stat: FALSE | burn: 0**



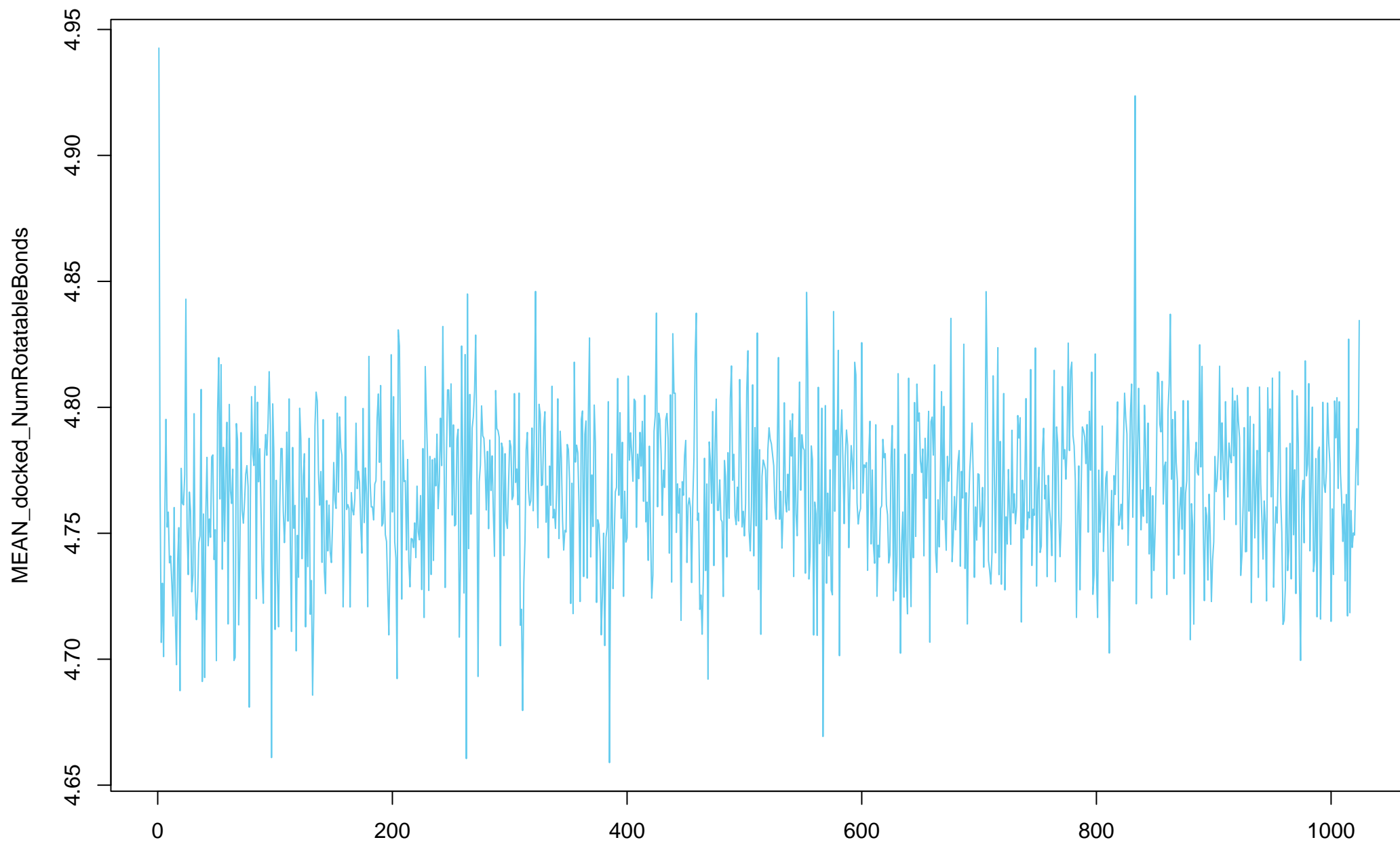
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 863 | BMK = 0.0691 | MCSE(6.27) = 3.66 | stat: TRUE | burn: 0**



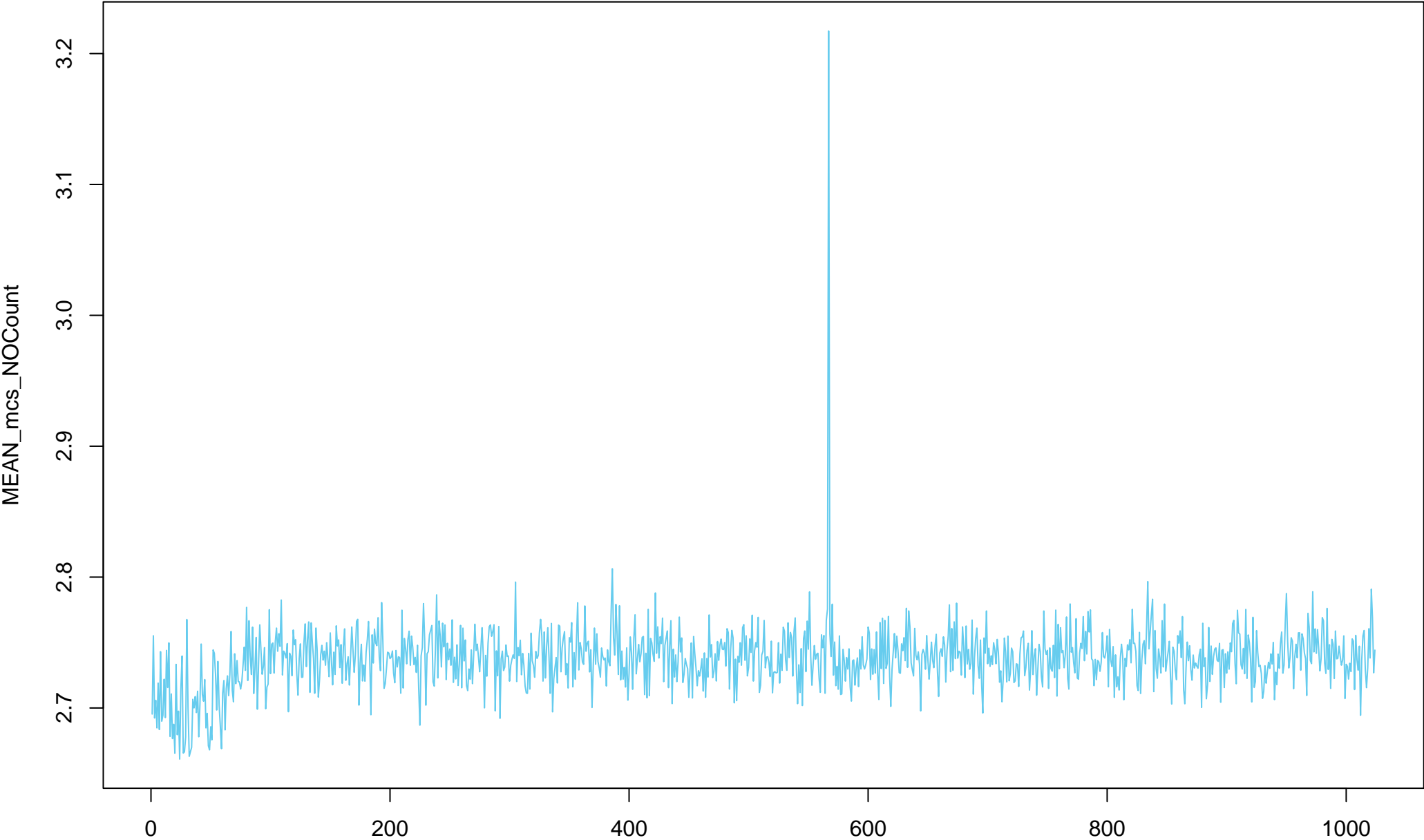
**MEAN\_mcs\_RingCount**  
**ESS = 754 | BMK = 0.113 | MCSE(6.27) = 4.63 | stat: FALSE | burn: 0**



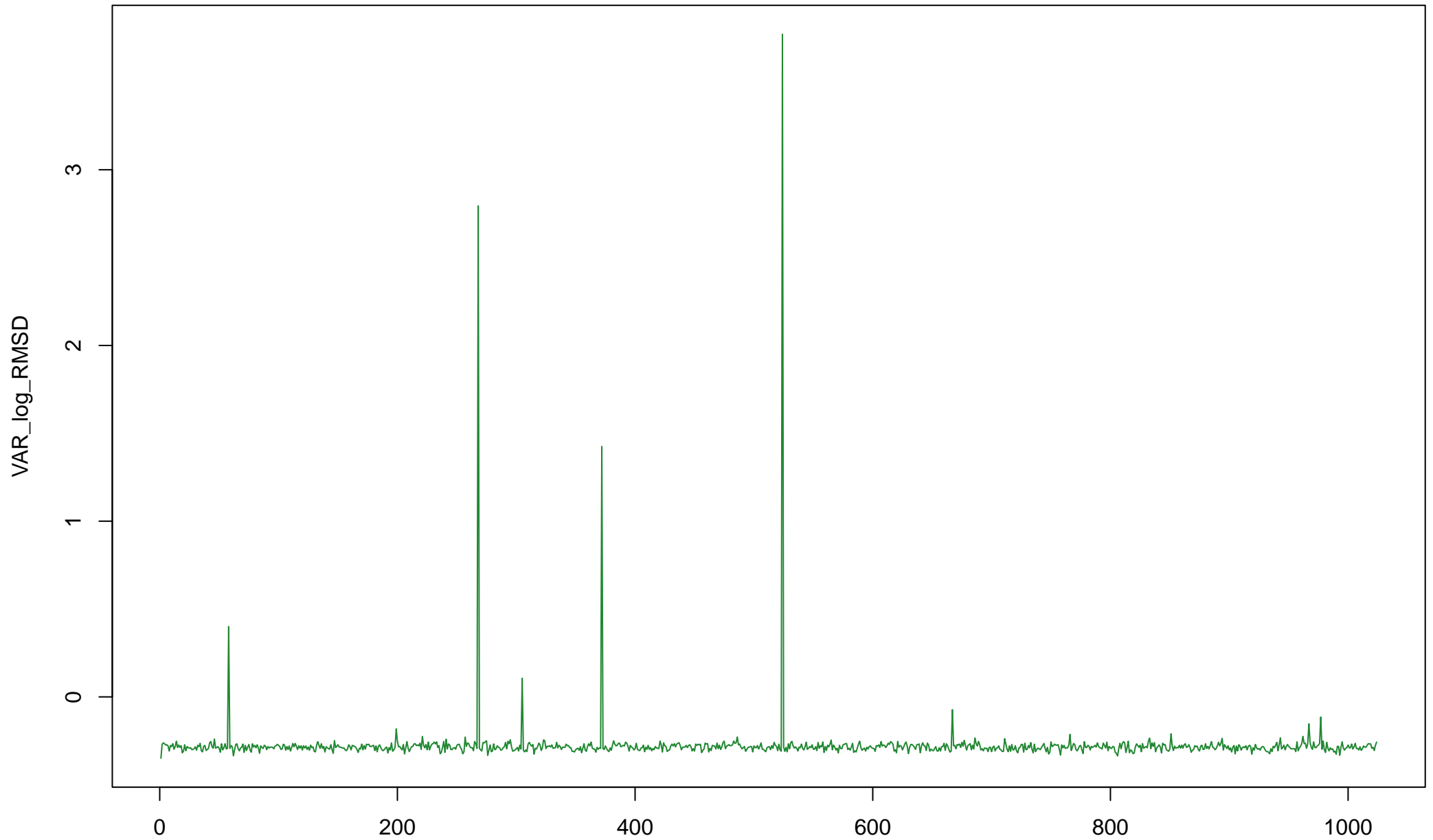
**MEAN\_docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0828 | MCSE(6.27) = 3.74 | stat: FALSE | burn: 0**



**MEAN\_mcs\_NOCount**  
**ESS = 108 | BMK = 0.171 | MCSE(6.27) = 7.12 | stat: FALSE | burn: 0**

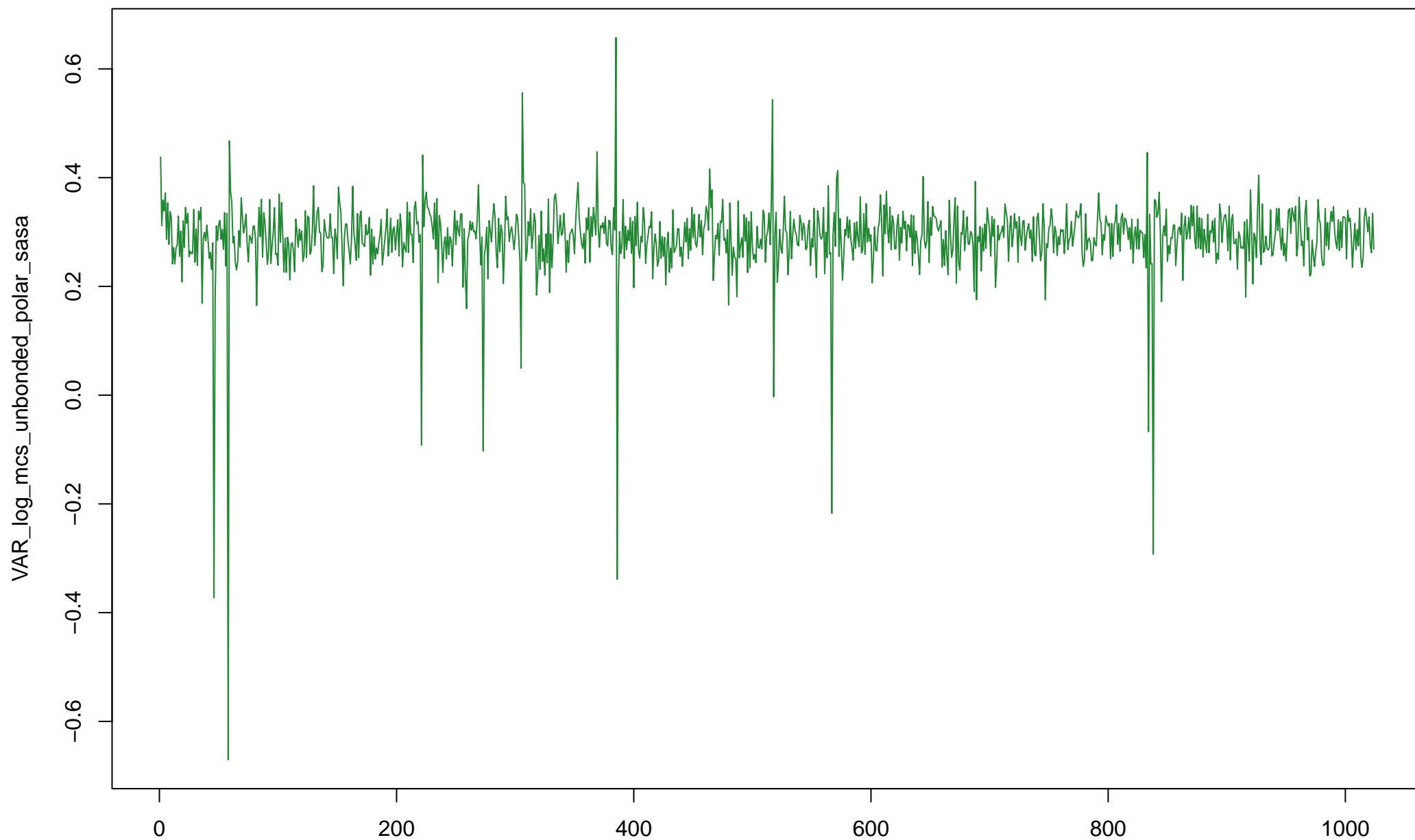


**VAR\_log\_RMSD**  
**ESS = 1020 | BMK = 0.245 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 612**

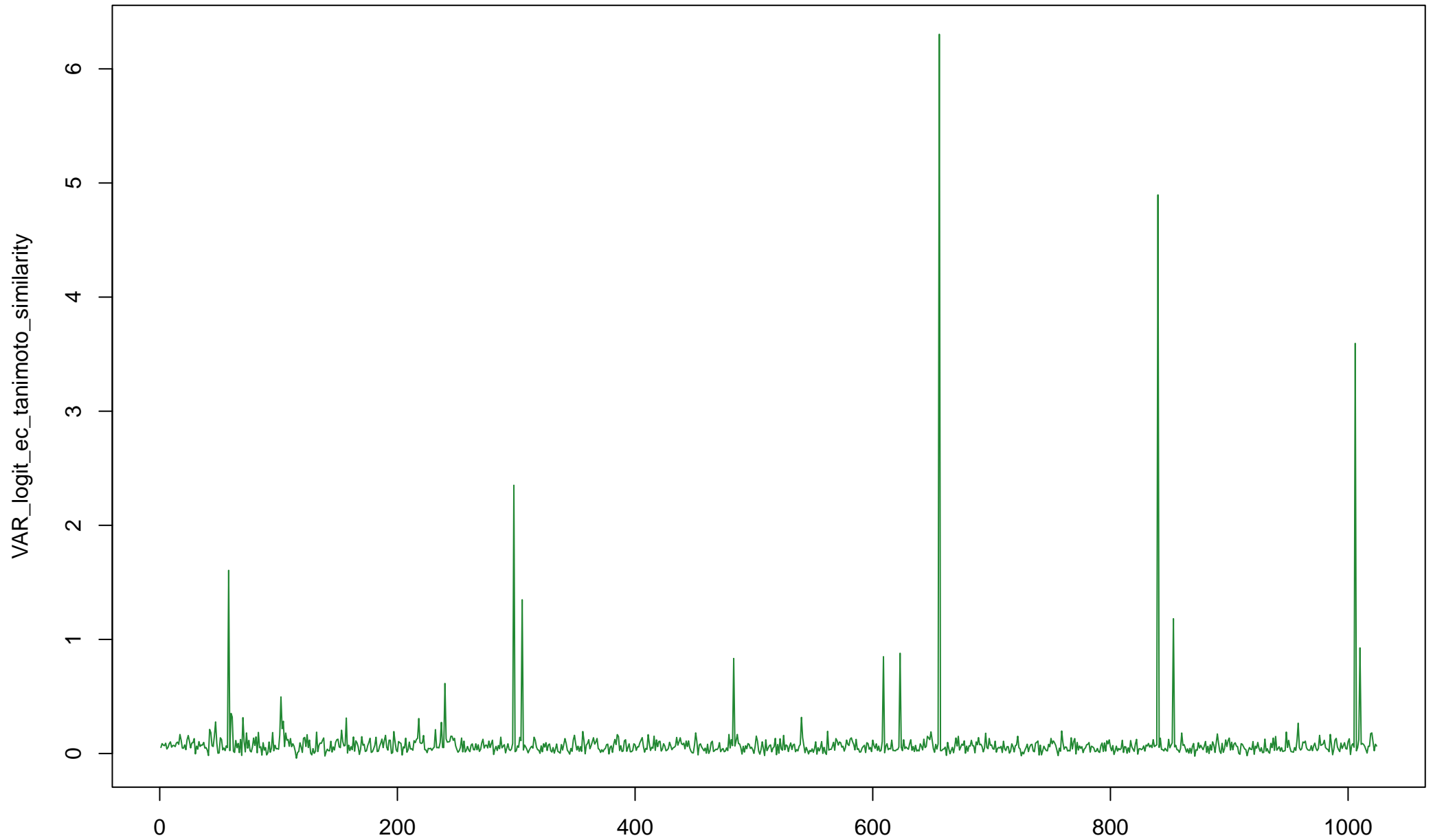




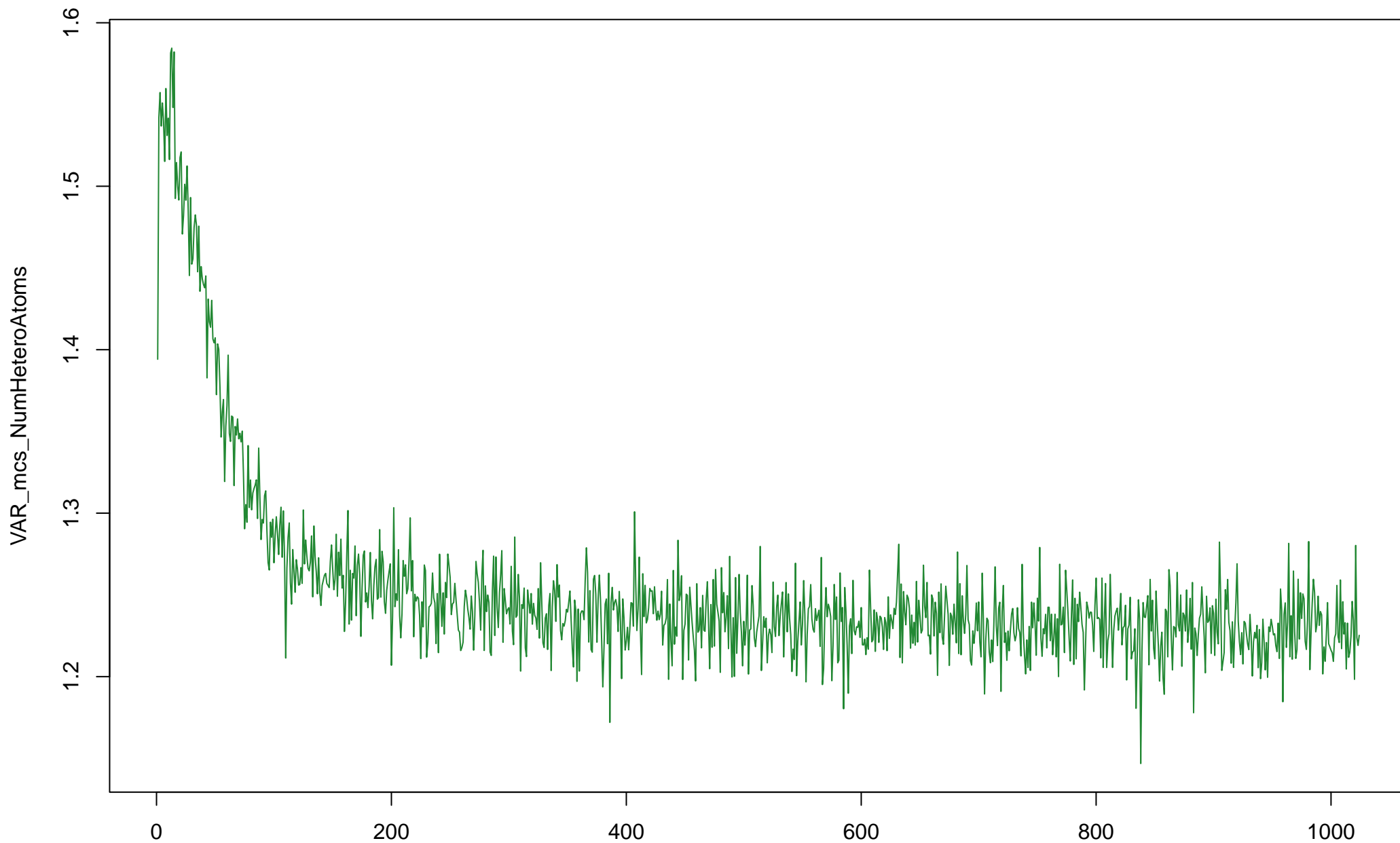
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1020 | BMK = 0.11 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0**



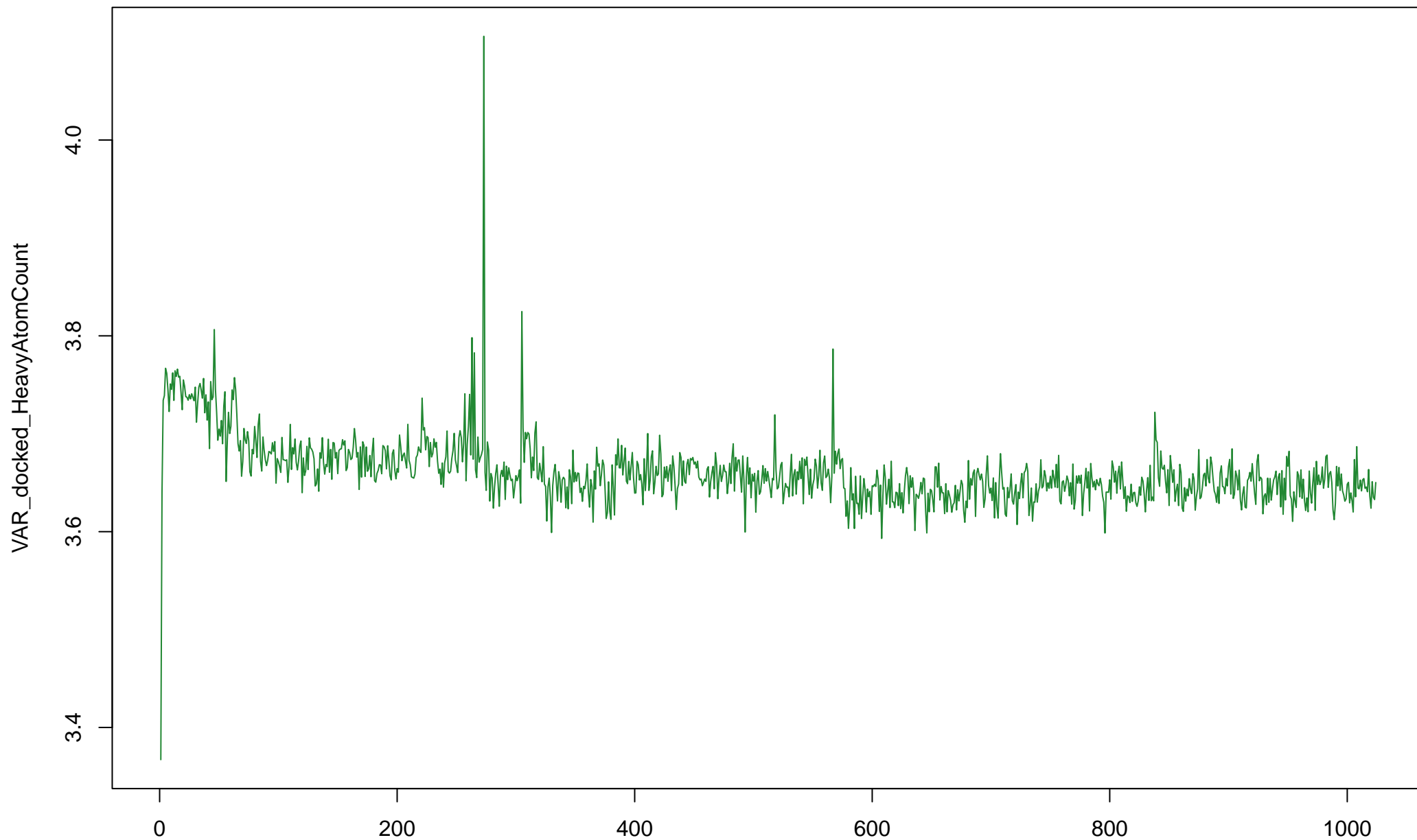
**VAR\_logit\_ec\_tanimoto\_similarity**  
**ESS = 1020 | BMK = 0.676 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 1020**



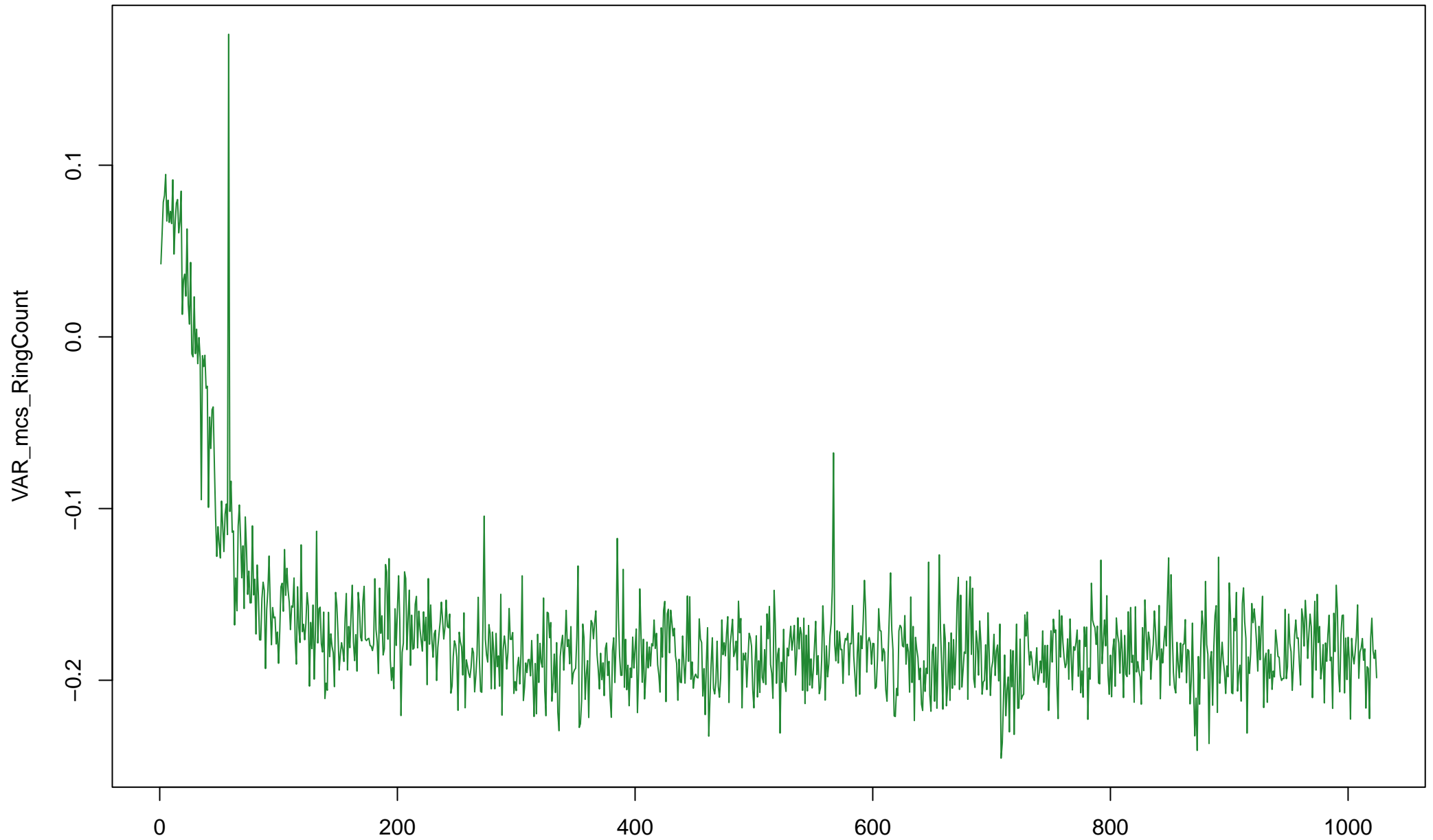
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 8.63 | BMK = 0.406 | MCSE(6.27) = 17 | stat: FALSE | burn: 102**



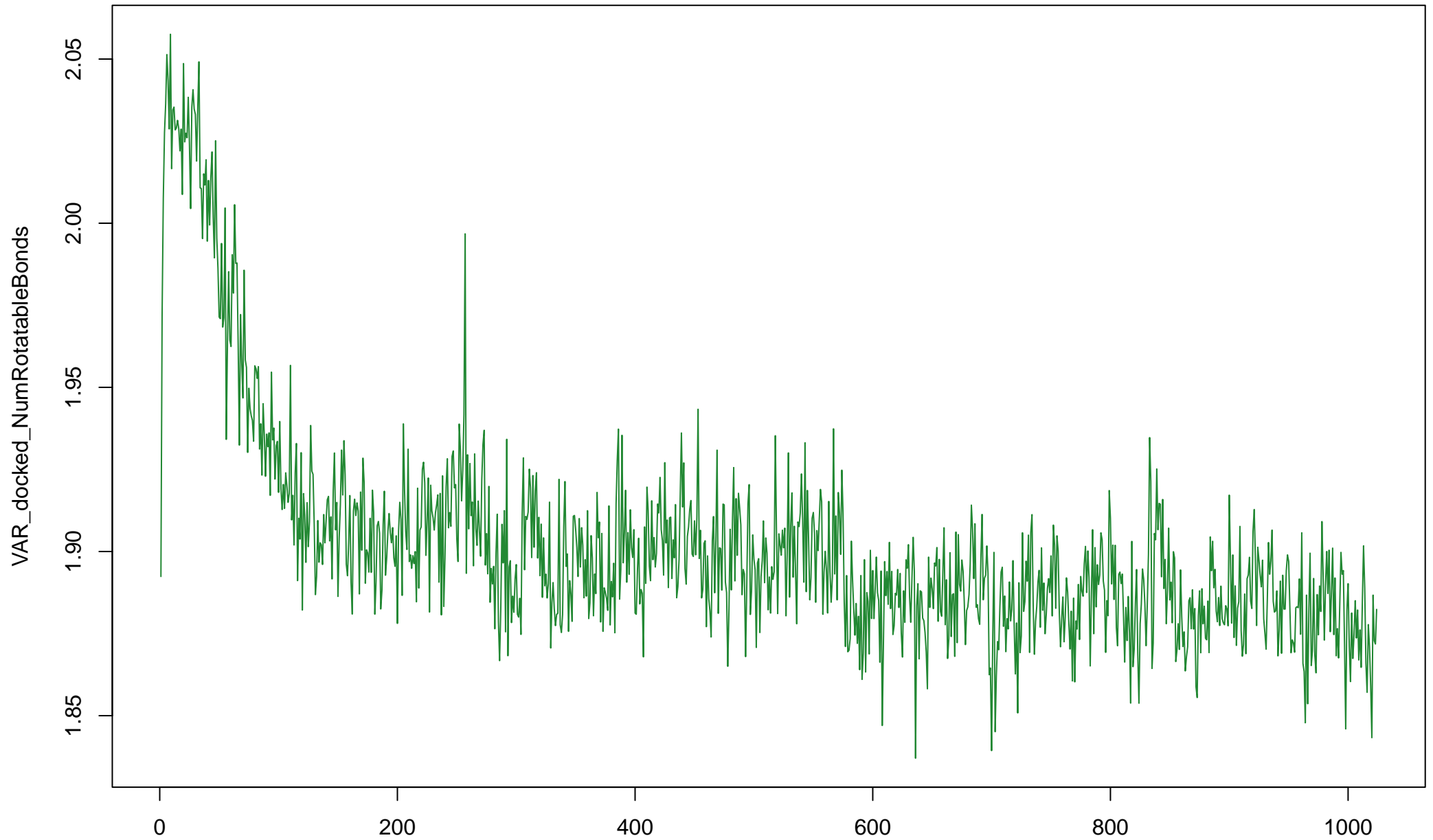
**VAR\_docked\_HeavyAtomCount**  
**ESS = 27.3 | BMK = 0.43 | MCSE(6.27) = 11.5 | stat: FALSE | burn: 102**



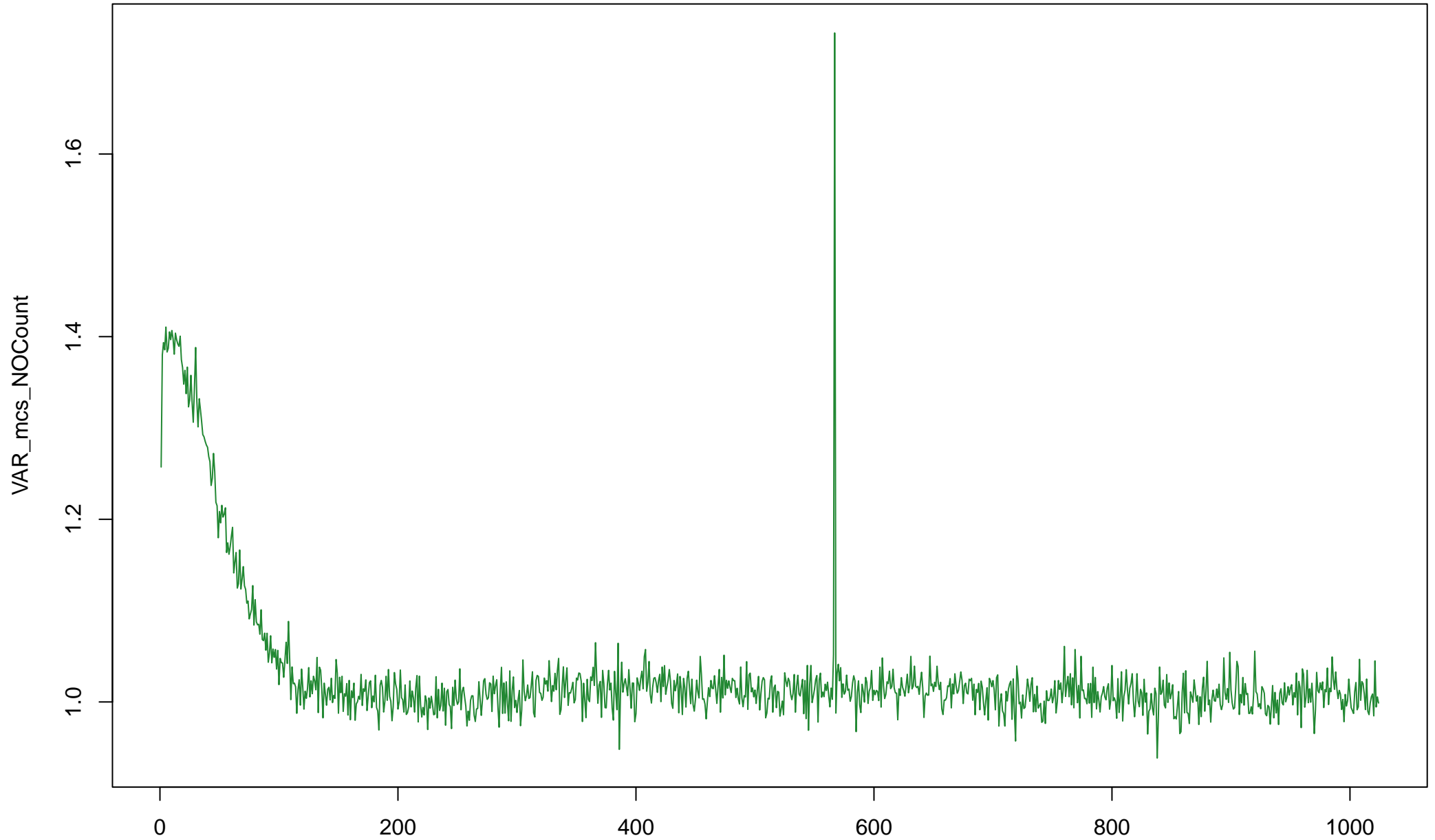
**VAR\_mcs\_RingCount**  
**ESS = 13 | BMK = 0.273 | MCSE(6.27) = 16.1 | stat: FALSE | burn: 102**



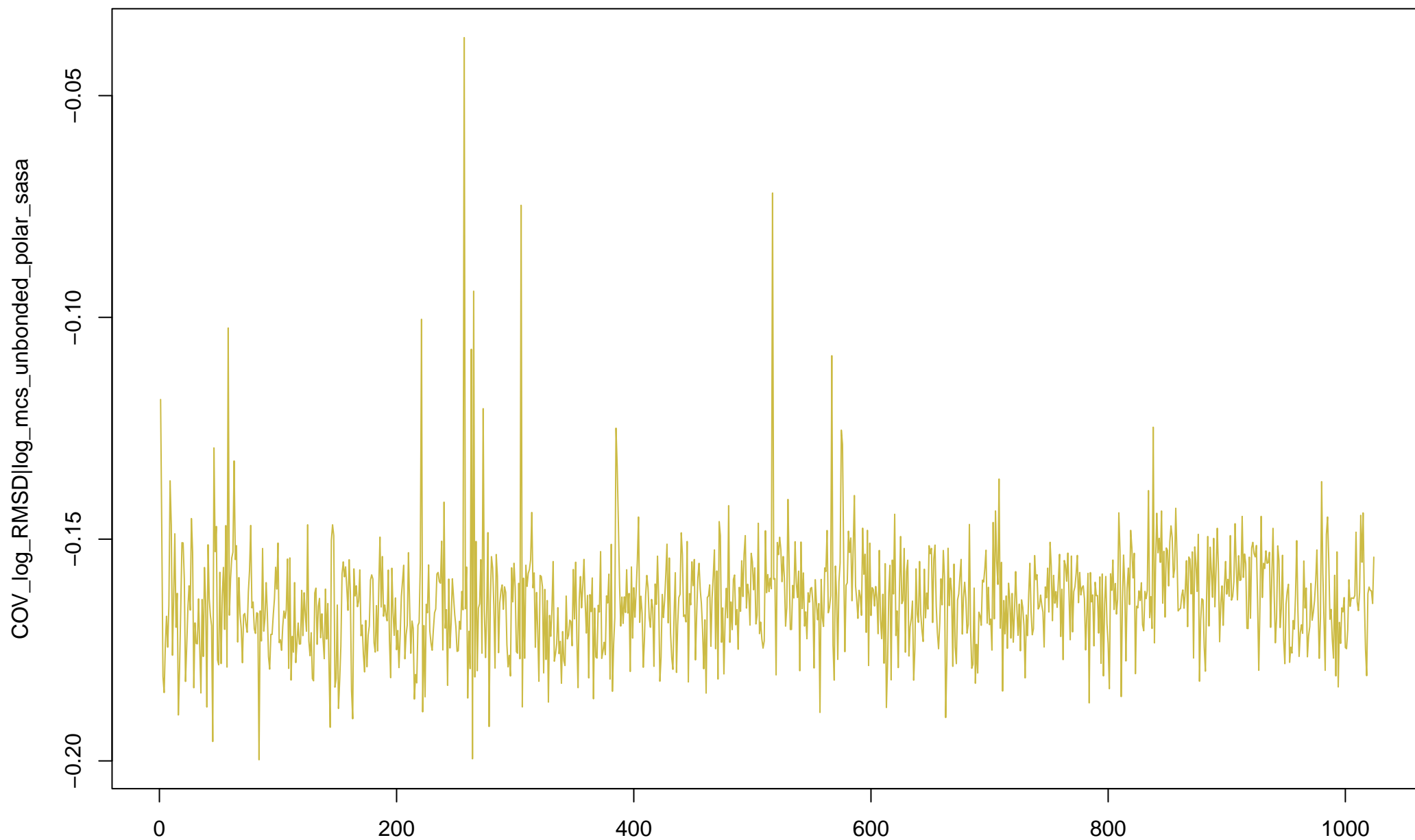
**VAR\_docked\_NumRotatableBonds**  
**ESS = 7.94 | BMK = 0.45 | MCSE(6.27) = 16.2 | stat: FALSE | burn: 102**



**VAR\_mcs\_NOCount**  
**ESS = 11.4 | BMK = 0.318 | MCSE(6.27) = 16.3 | stat: FALSE | burn: 102**

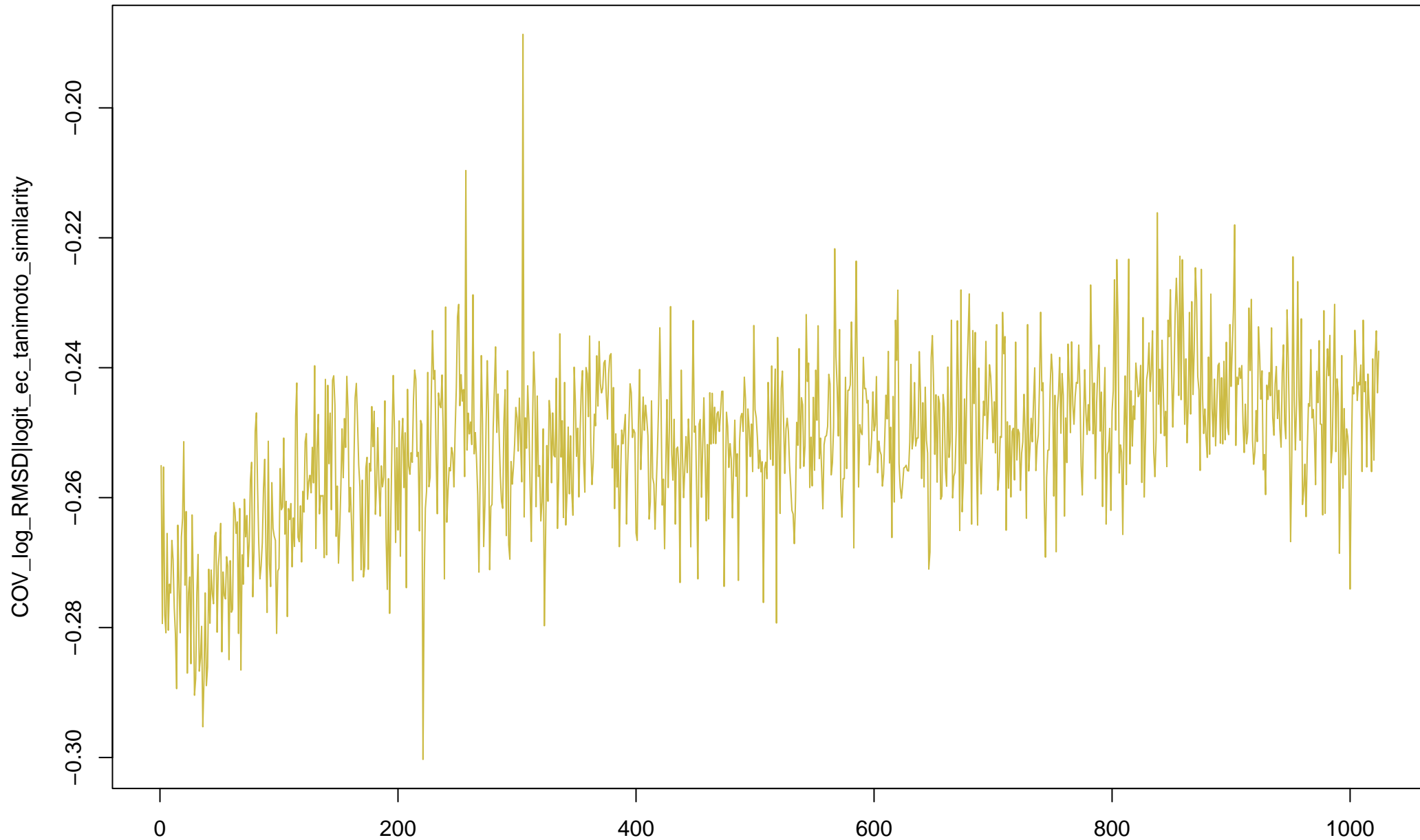


**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 514 | BMK = 0.158 | MCSE(6.27) = 4.68 | stat: TRUE | burn: 0**

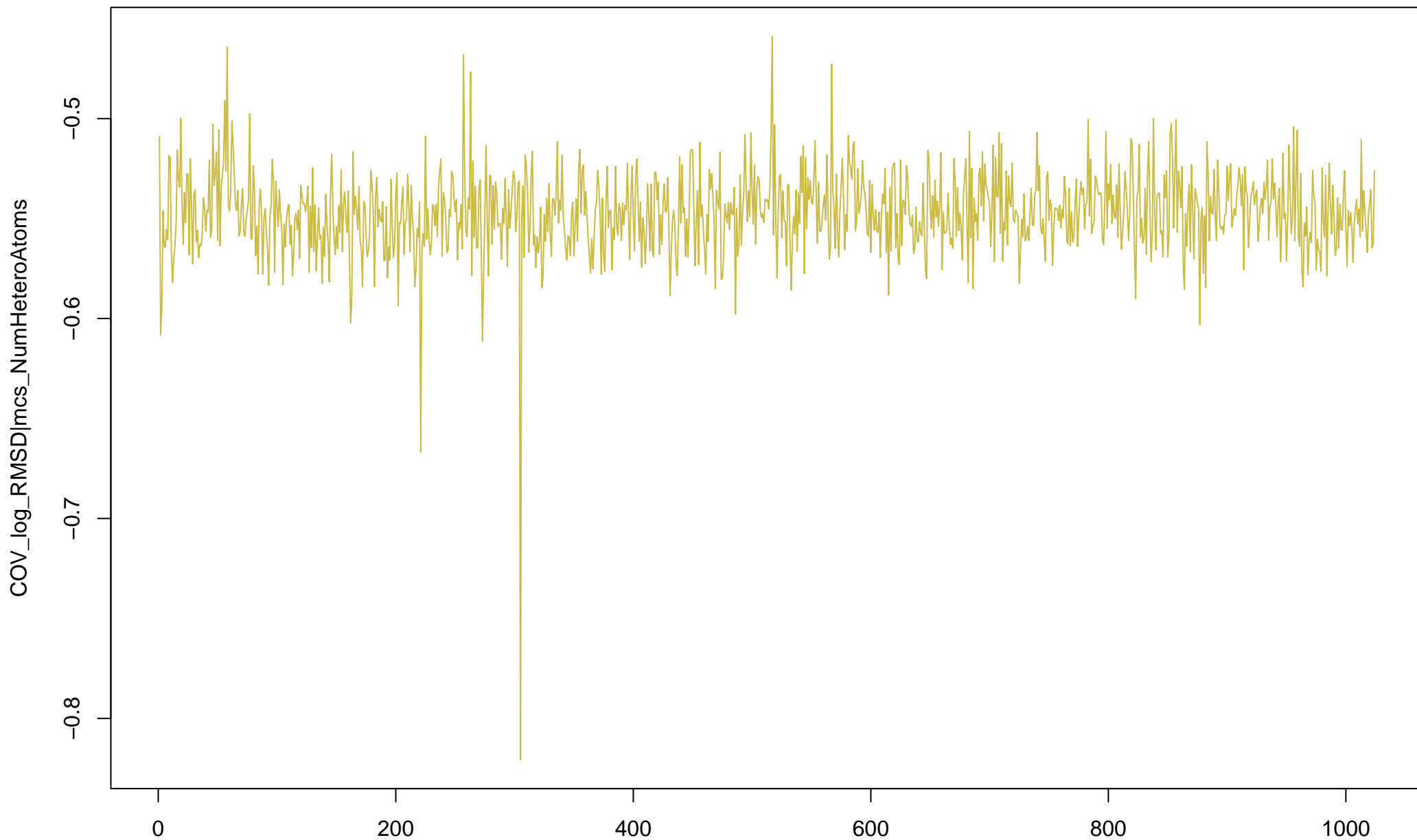




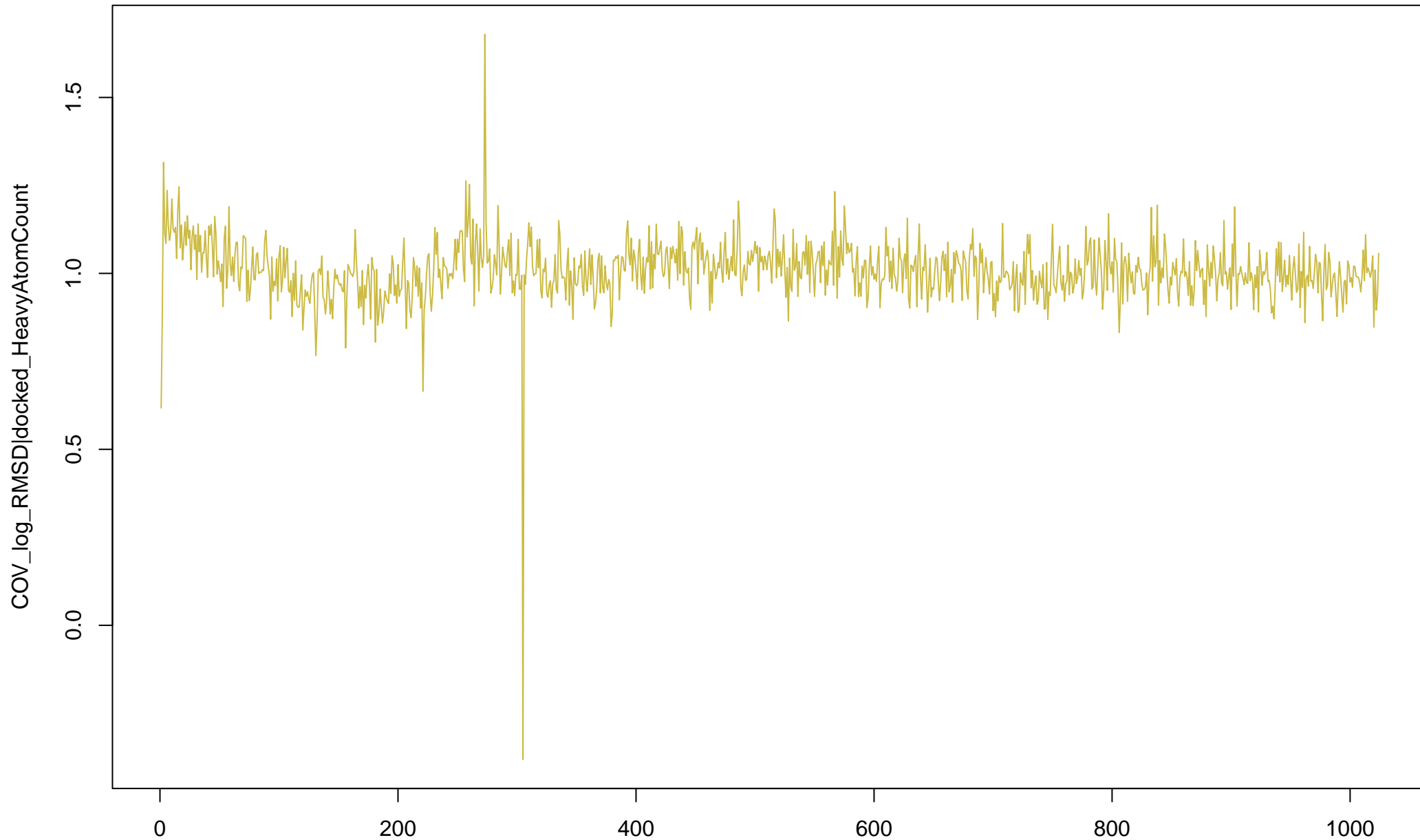
**COV\_log\_RMSD|logit\_ec\_tanimoto\_similarity**  
**ESS = 10.6 | BMK = 0.328 | MCSE(6.27) = 11.5 | stat: FALSE | burn: 0**



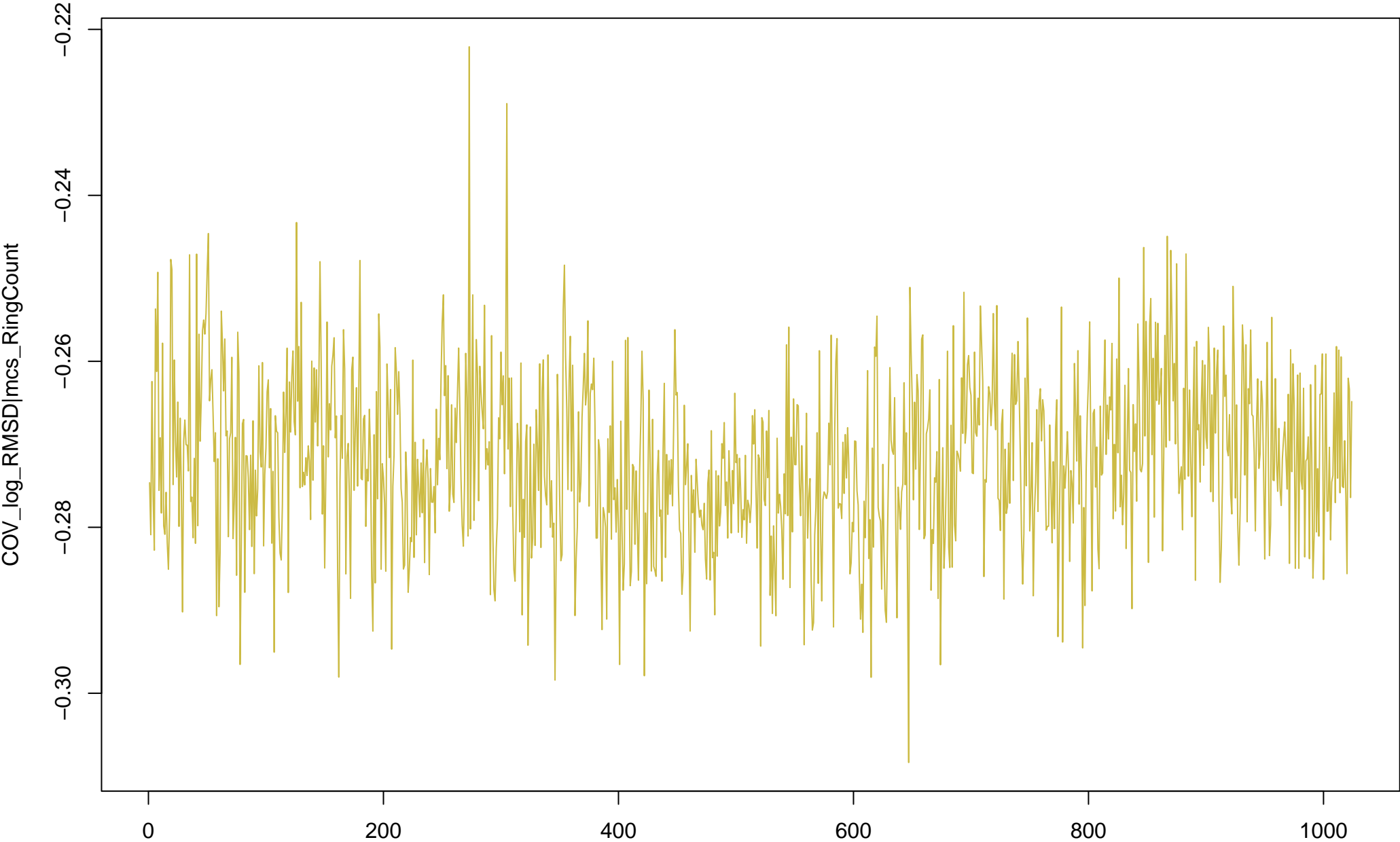
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 886 | BMK = 0.0948 | MCSE(6.27) = 4.31 | stat: TRUE | burn: 0**



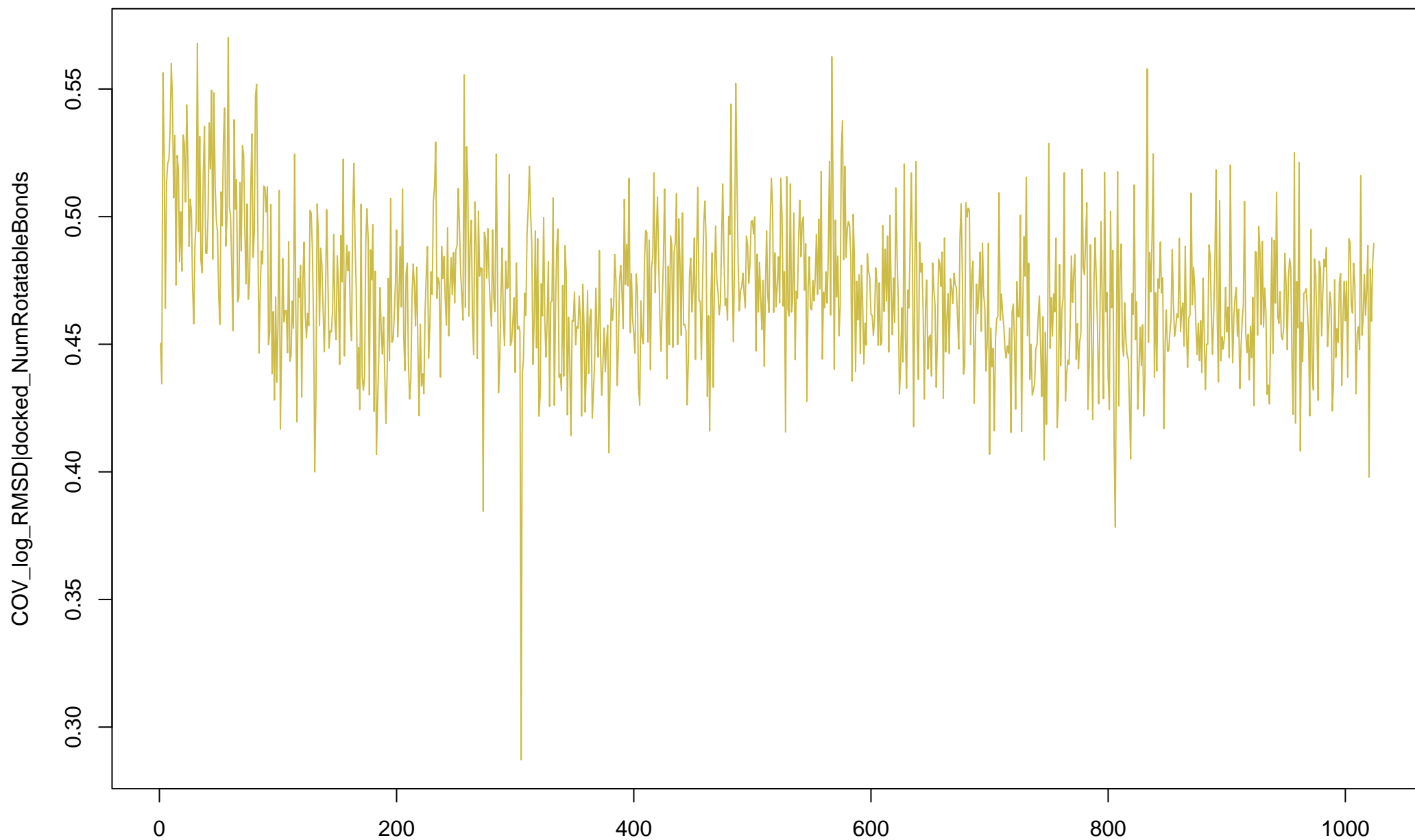
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 175 | BMK = 0.134 | MCSE(6.27) = 7 | stat: FALSE | burn: 0**



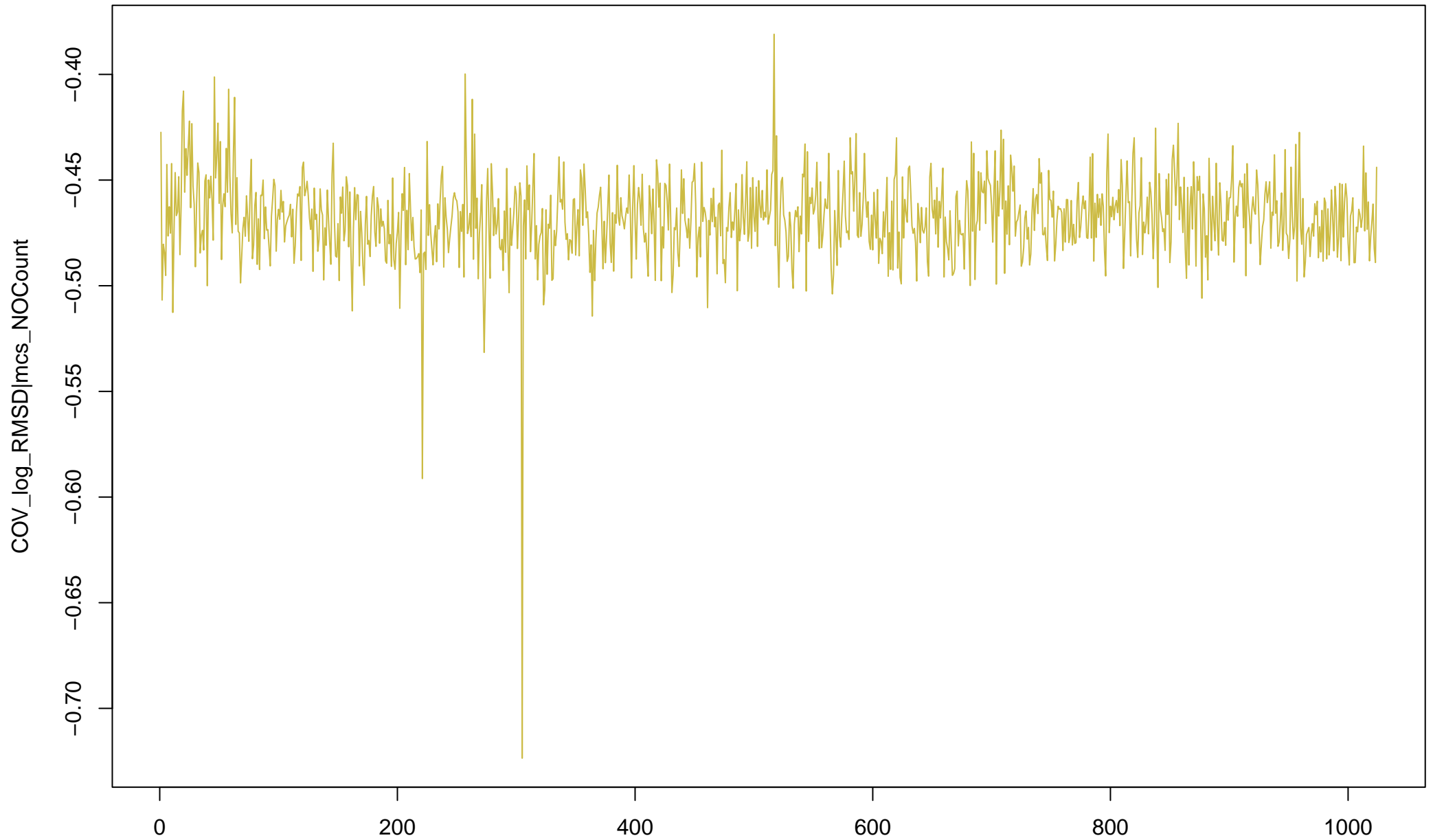
COV\_log\_RMSD|mcs\_RingCount  
ESS = 238 | BMK = 0.0664 | MCSE(6.27) = 6.11 | stat: TRUE | burn: 0



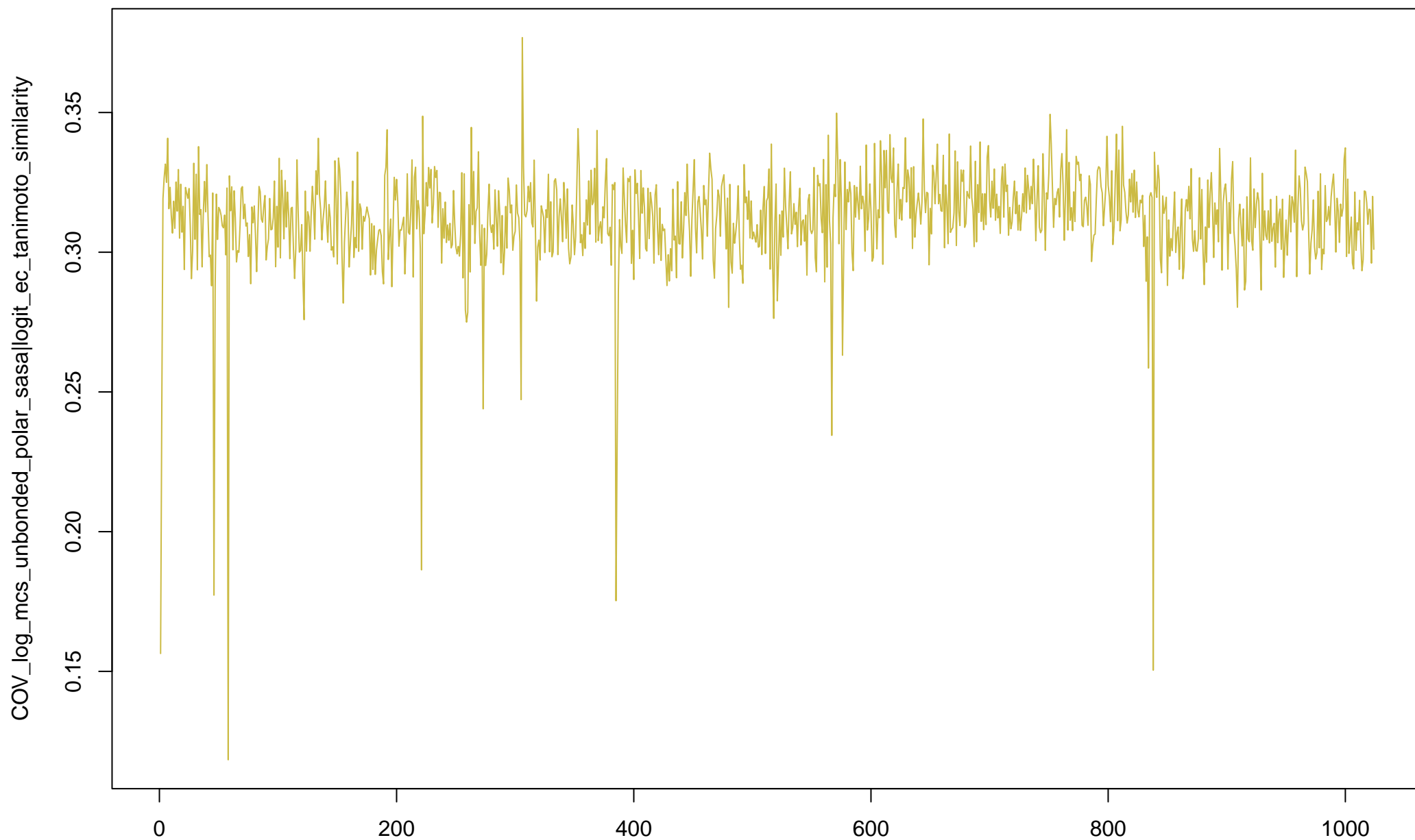
**COV\_log\_RMSD|docked\_NumRotatableBonds**  
**ESS = 83 | BMK = 0.138 | MCSE(6.27) = 8.32 | stat: FALSE | burn: 0**



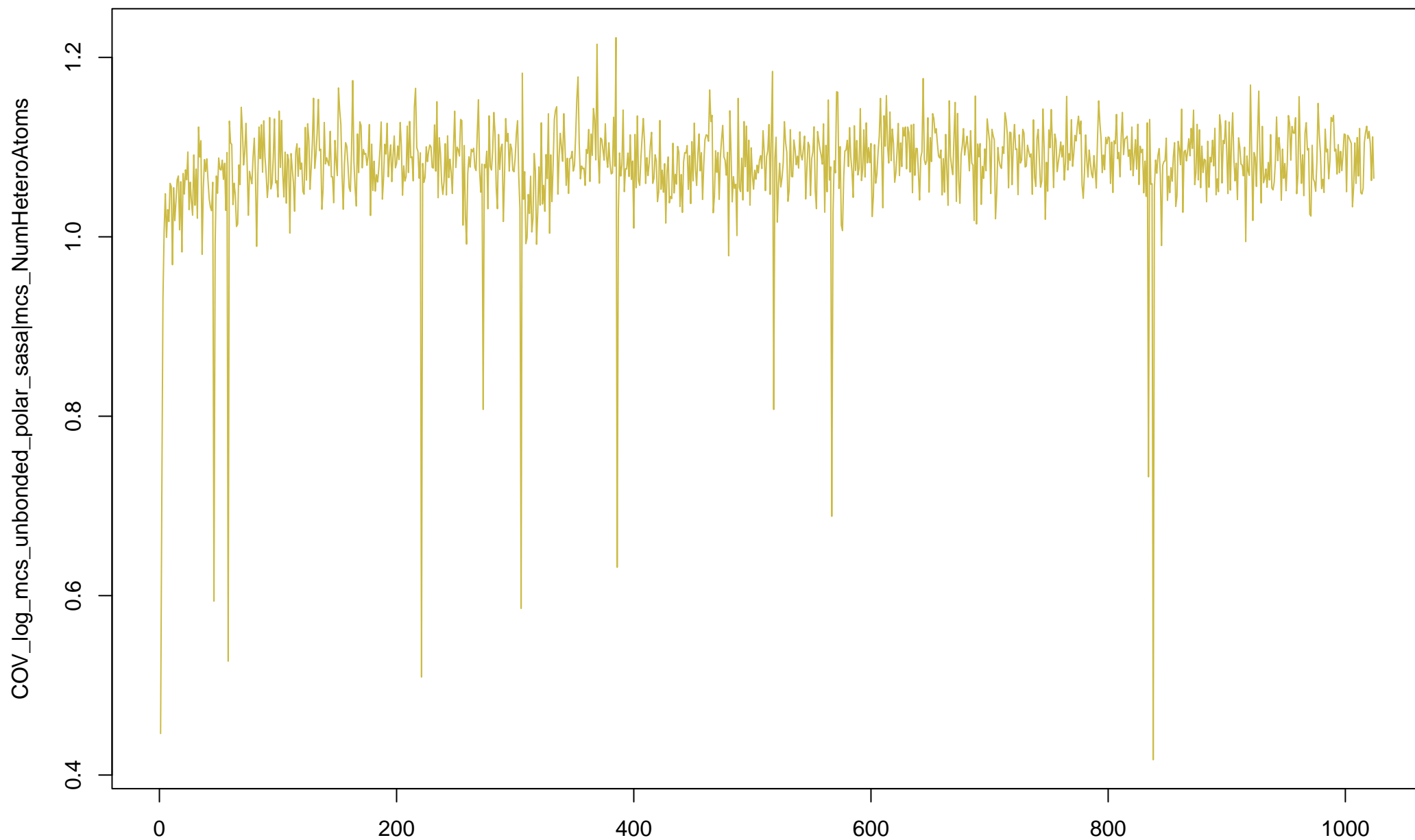
**COV\_log\_RMSD|mcs\_NOCount**  
**ESS = 805 | BMK = 0.117 | MCSE(6.27) = 4.62 | stat: TRUE | burn: 0**



**COV\_log\_mcs\_unbonded\_polar\_sasa|logit\_ec\_tanimoto\_similarity**  
**ESS = 795 | BMK = 0.14 | MCSE(6.27) = 4.84 | stat: FALSE | burn: 0**

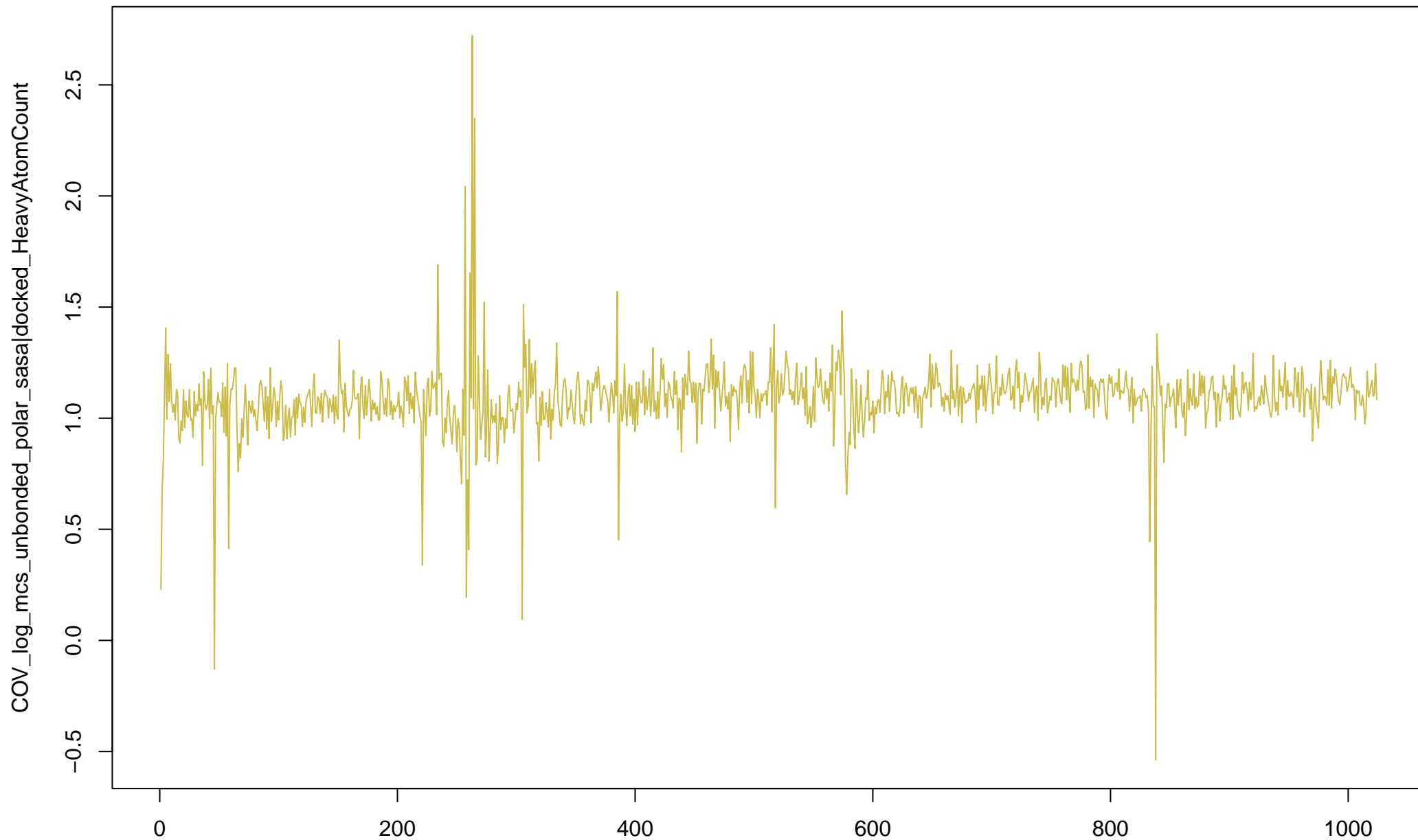


**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 340 | BMK = 0.16 | MCSE(6.27) = 5.54 | stat: FALSE | burn: 0**

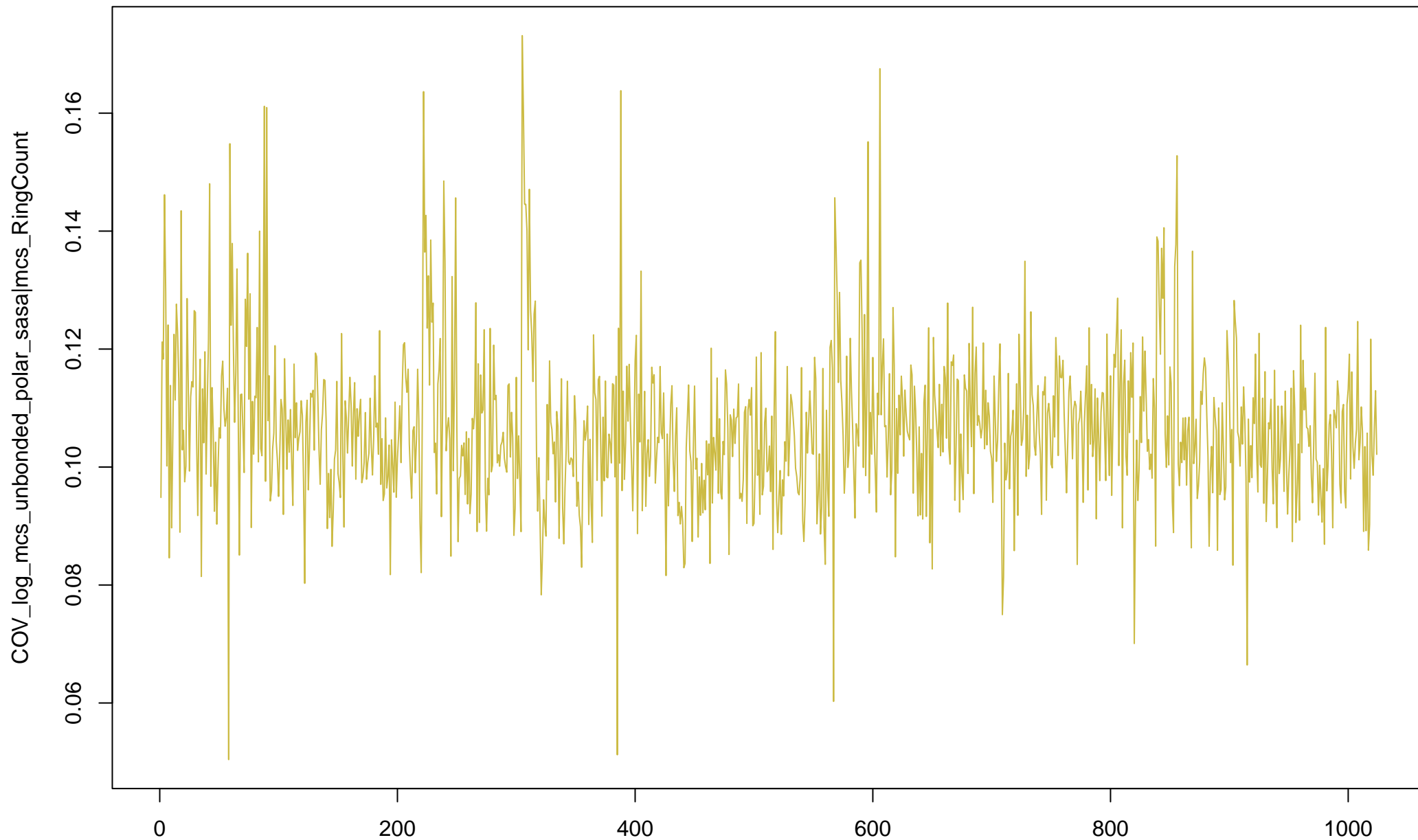




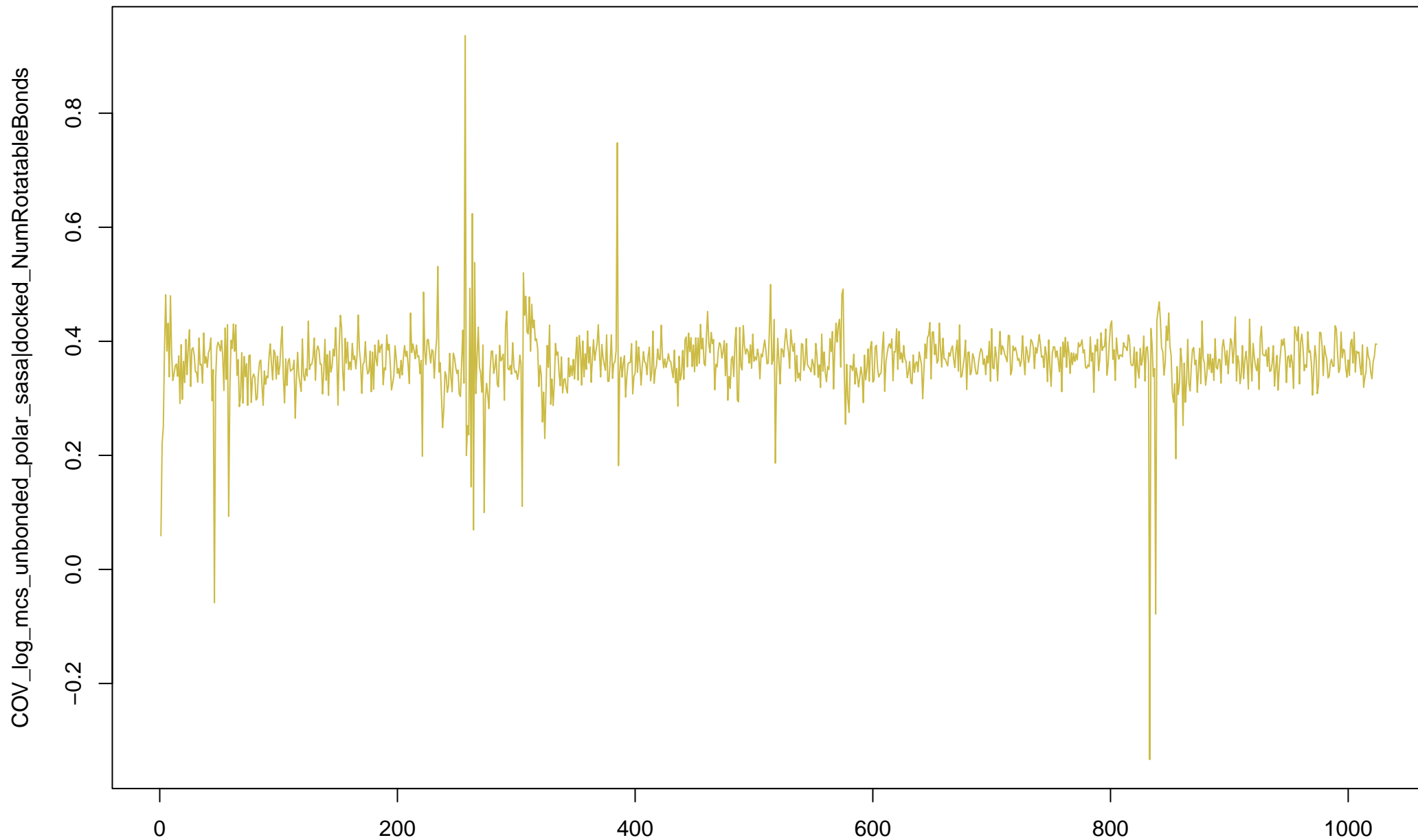
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 558 | BMK = 0.22 | MCSE(6.27) = 4.67 | stat: FALSE | burn: 0**



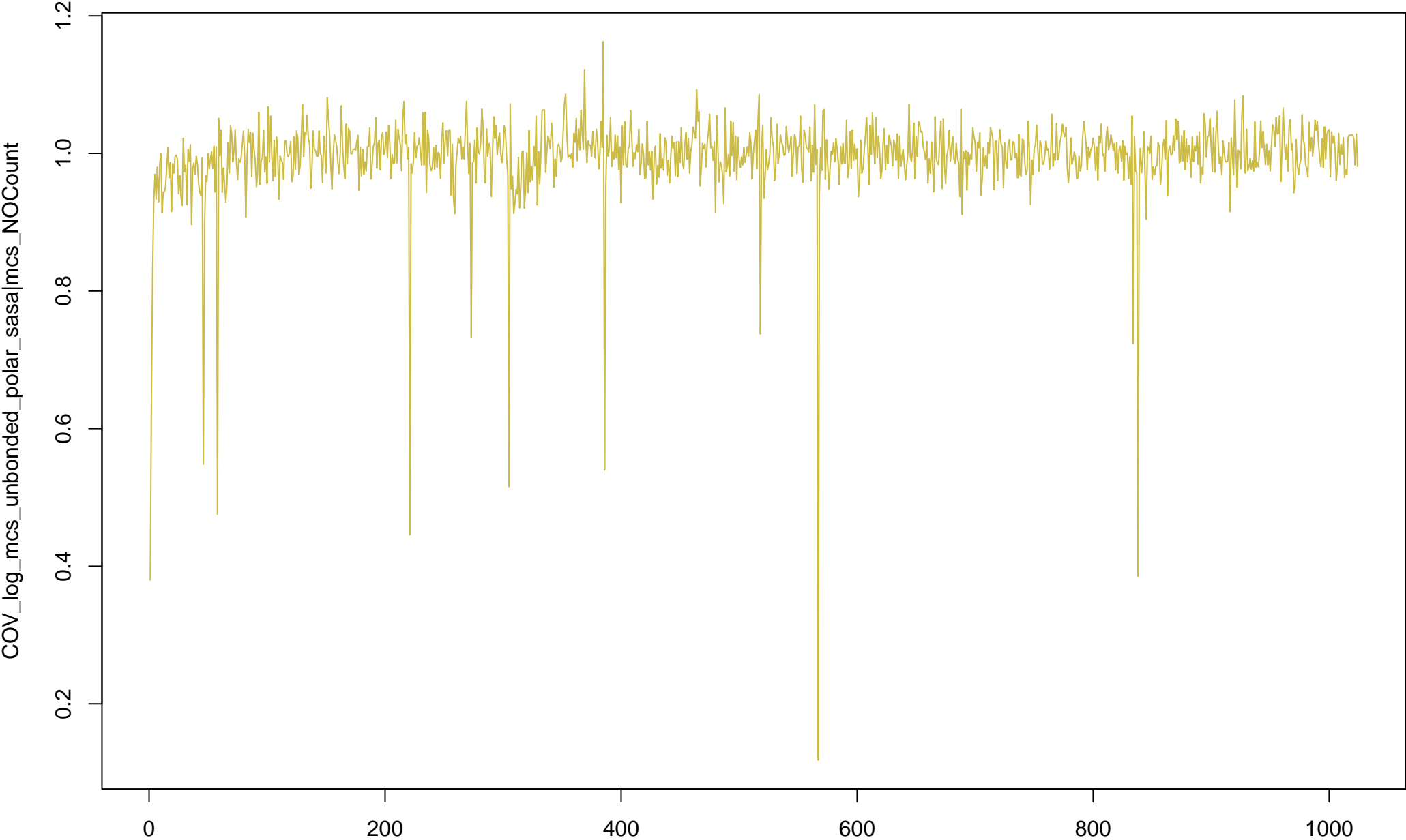
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_RingCount**  
**ESS = 435 | BMK = 0.0984 | MCSE(6.27) = 5.39 | stat: FALSE | burn: 0**



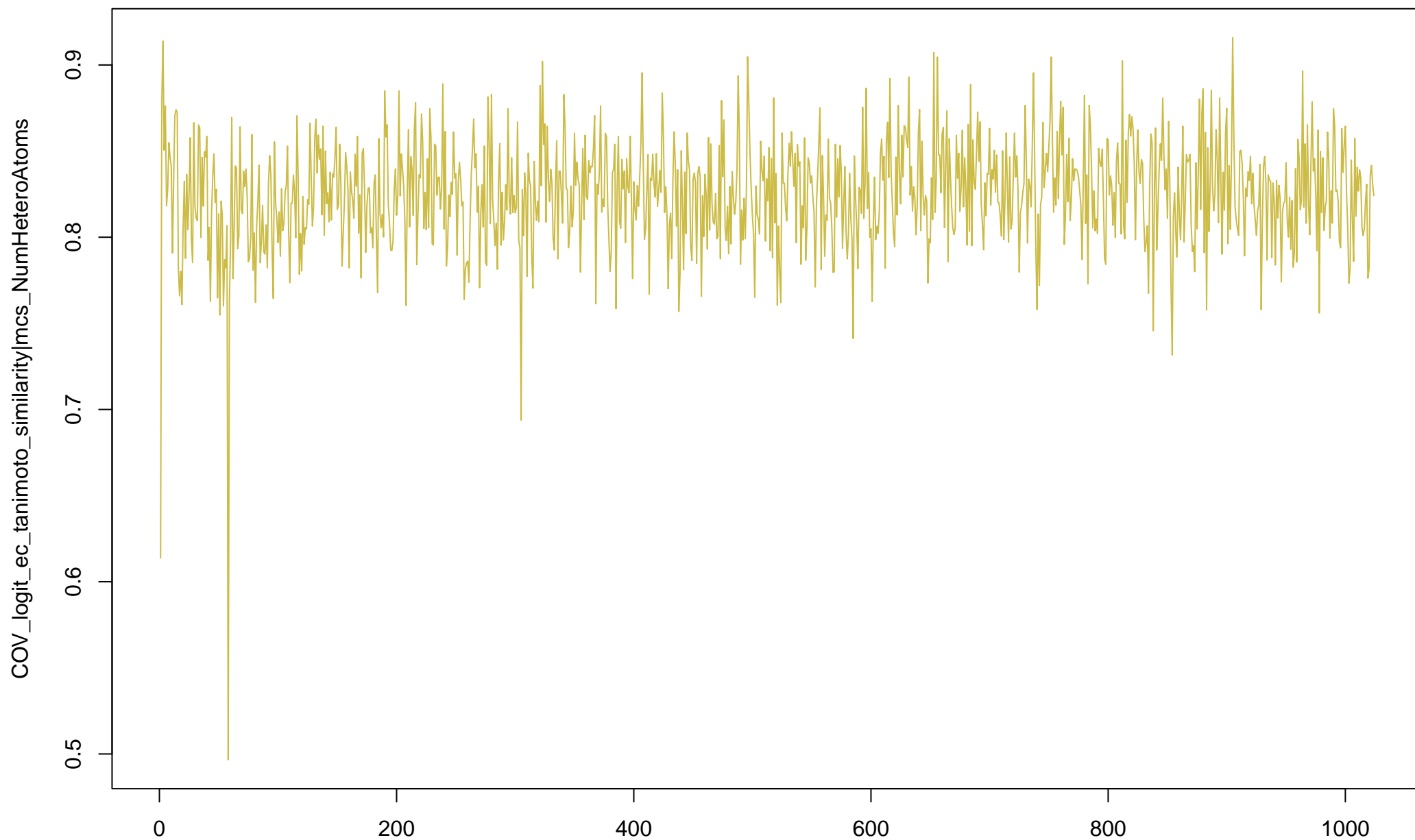
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_NumRotatableBonds**  
**ESS = 948 | BMK = 0.165 | MCSE(6.27) = 4.08 | stat: FALSE | burn: 0**



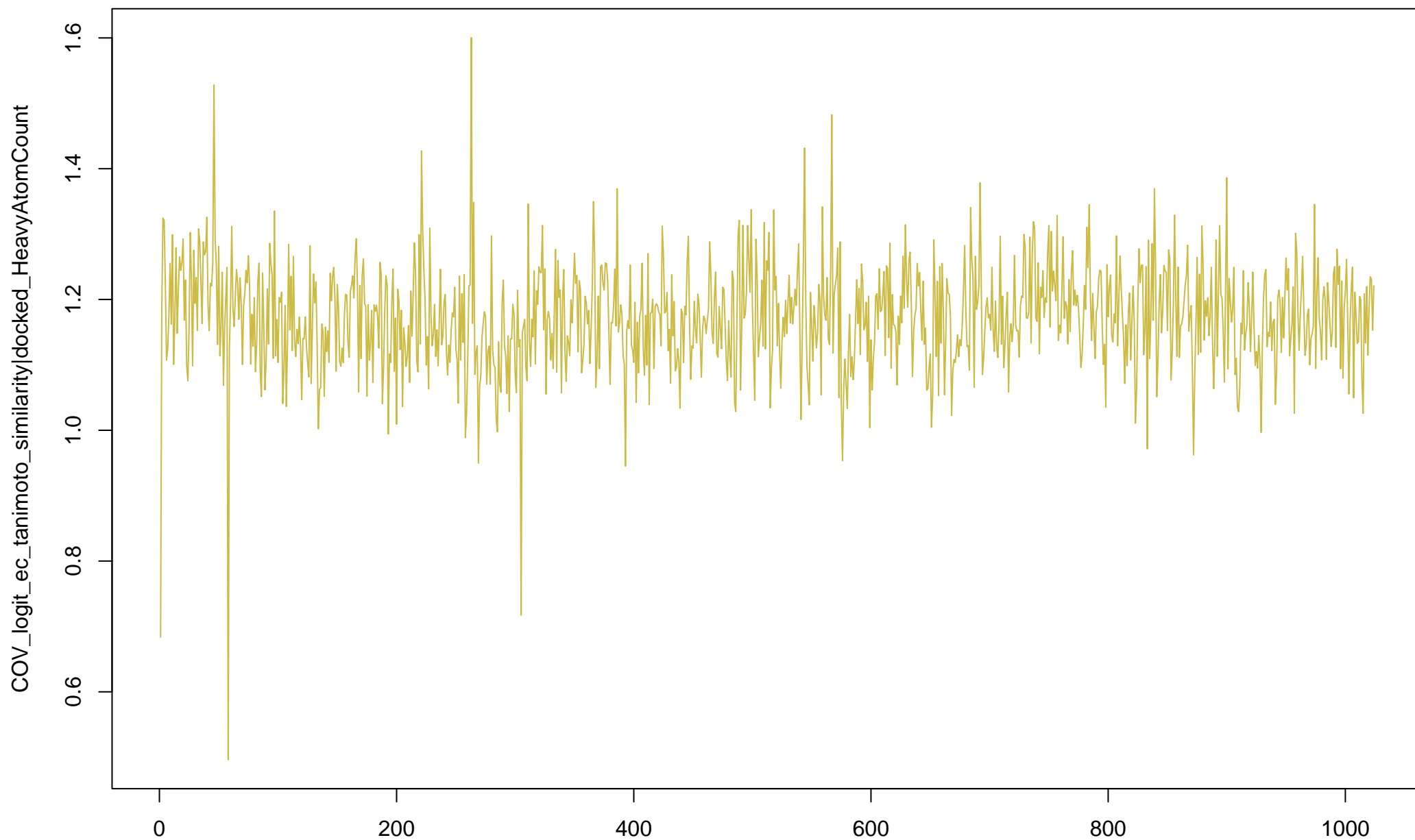
COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NOCount  
ESS = 649 | BMK = 0.135 | MCSE(6.27) = 5.04 | stat: FALSE | burn: 0



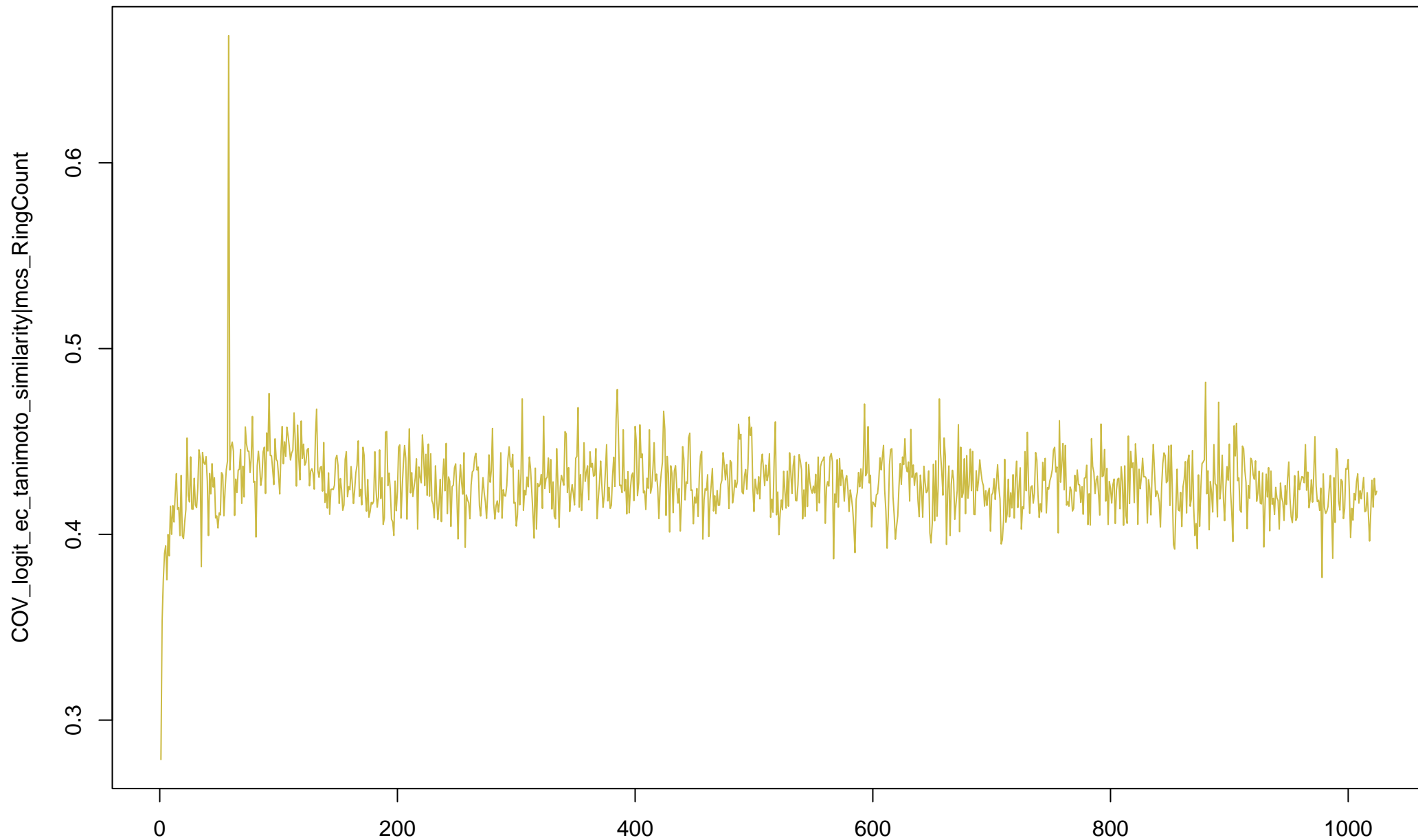
COV\_logit\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms  
ESS = 737 | BMK = 0.0888 | MCSE(6.27) = 4.56 | stat: FALSE | burn: 0



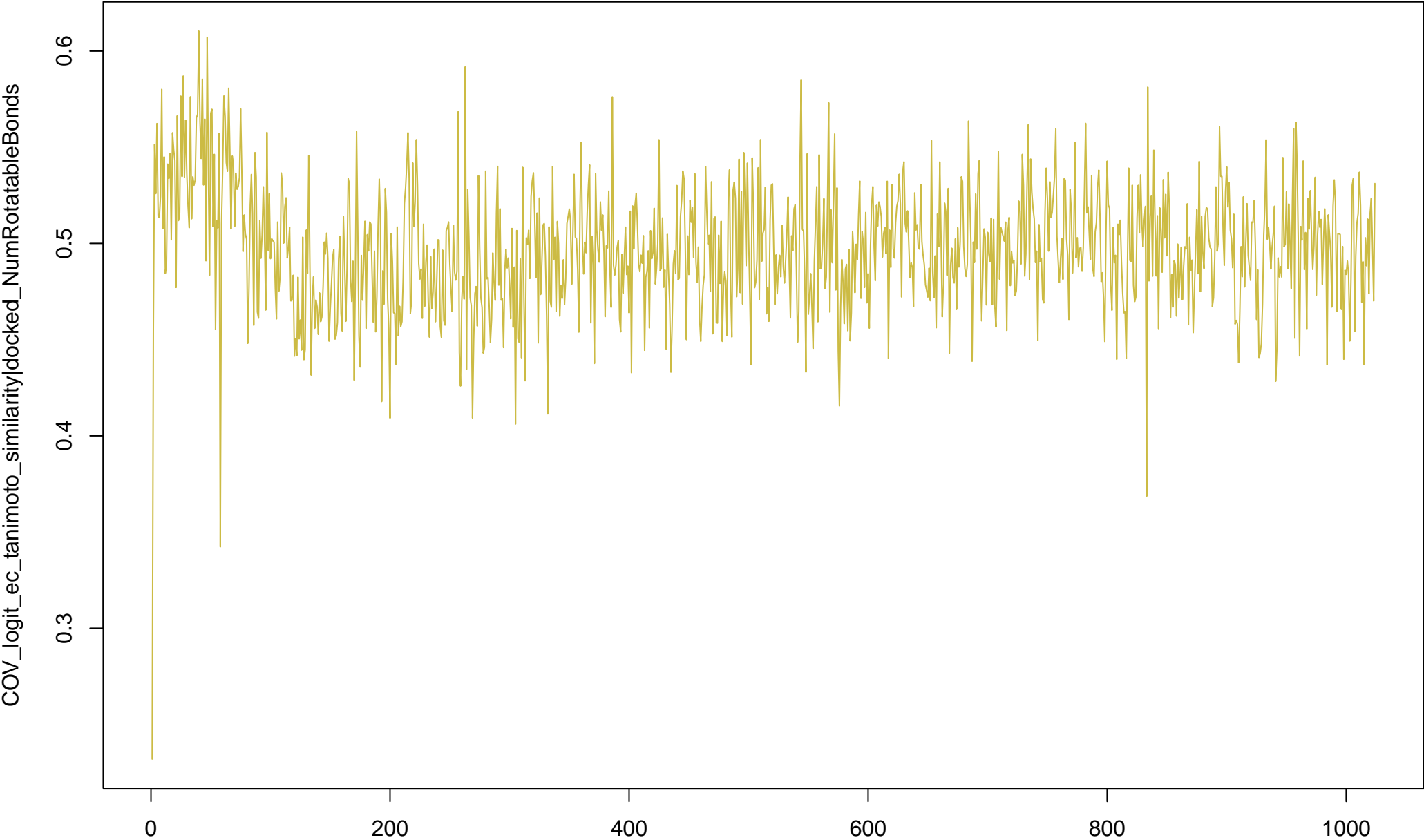
**COV\_logit\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount**  
**ESS = 654 | BMK = 0.0839 | MCSE(6.27) = 4.2 | stat: TRUE | burn: 0**



**COV\_logit\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 157 | BMK = 0.111 | MCSE(6.27) = 6.36 | stat: TRUE | burn: 0**

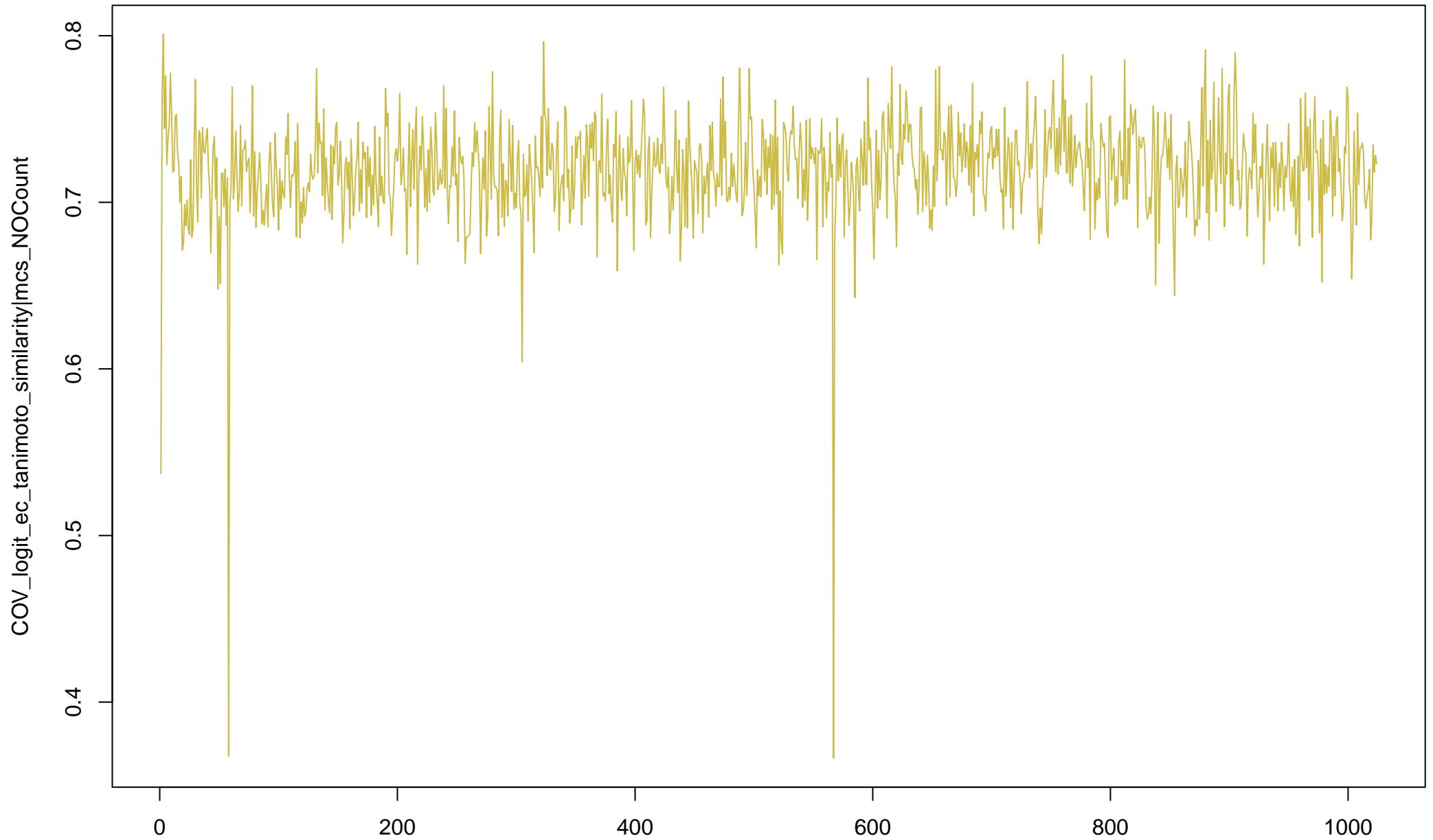


COV\_logit\_ec\_tanimoto\_similarity|docked\_NumRotatableBonds  
ESS = 163 | BMK = 0.143 | MCSE(6.27) = 6.41 | stat: FALSE | burn: 0

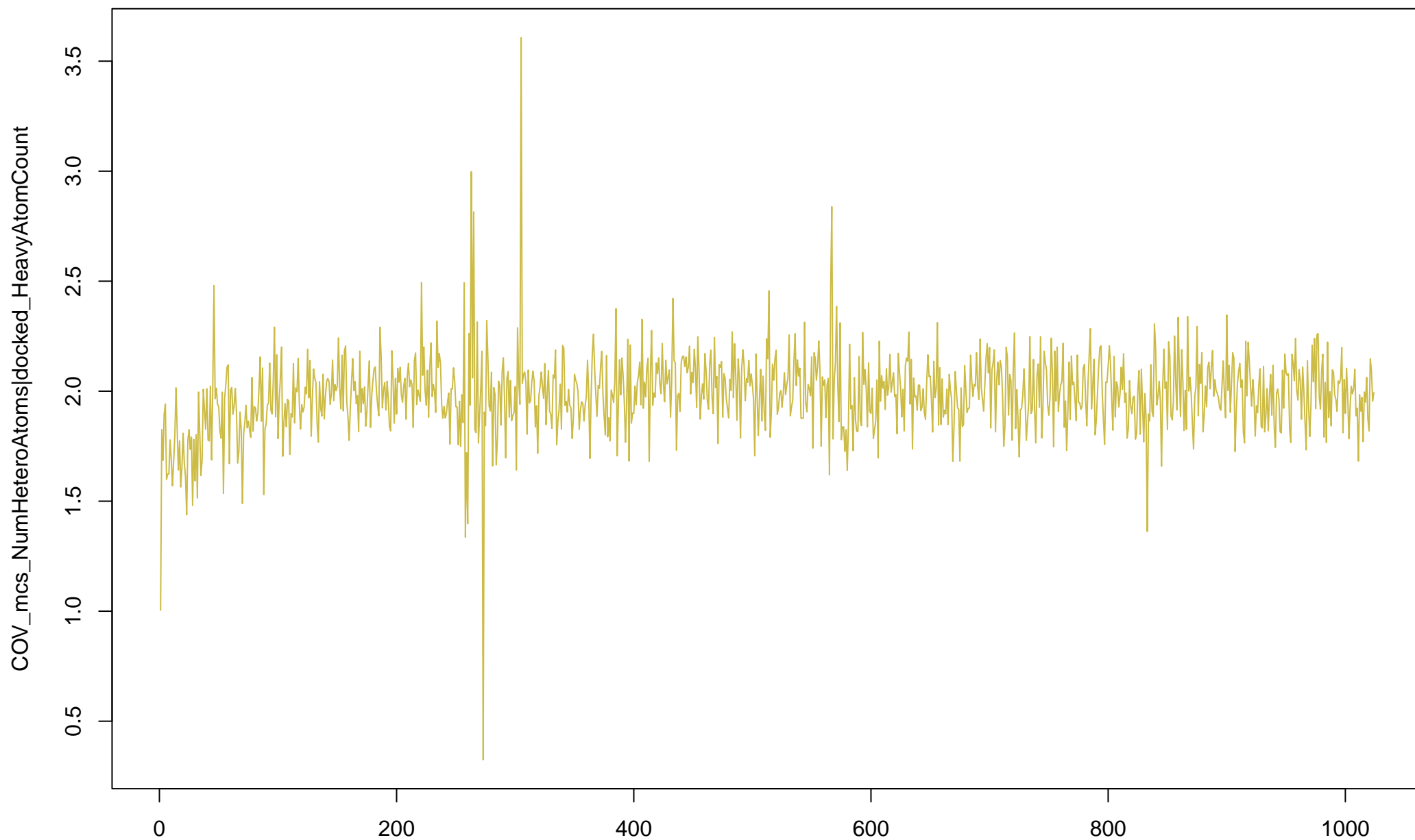




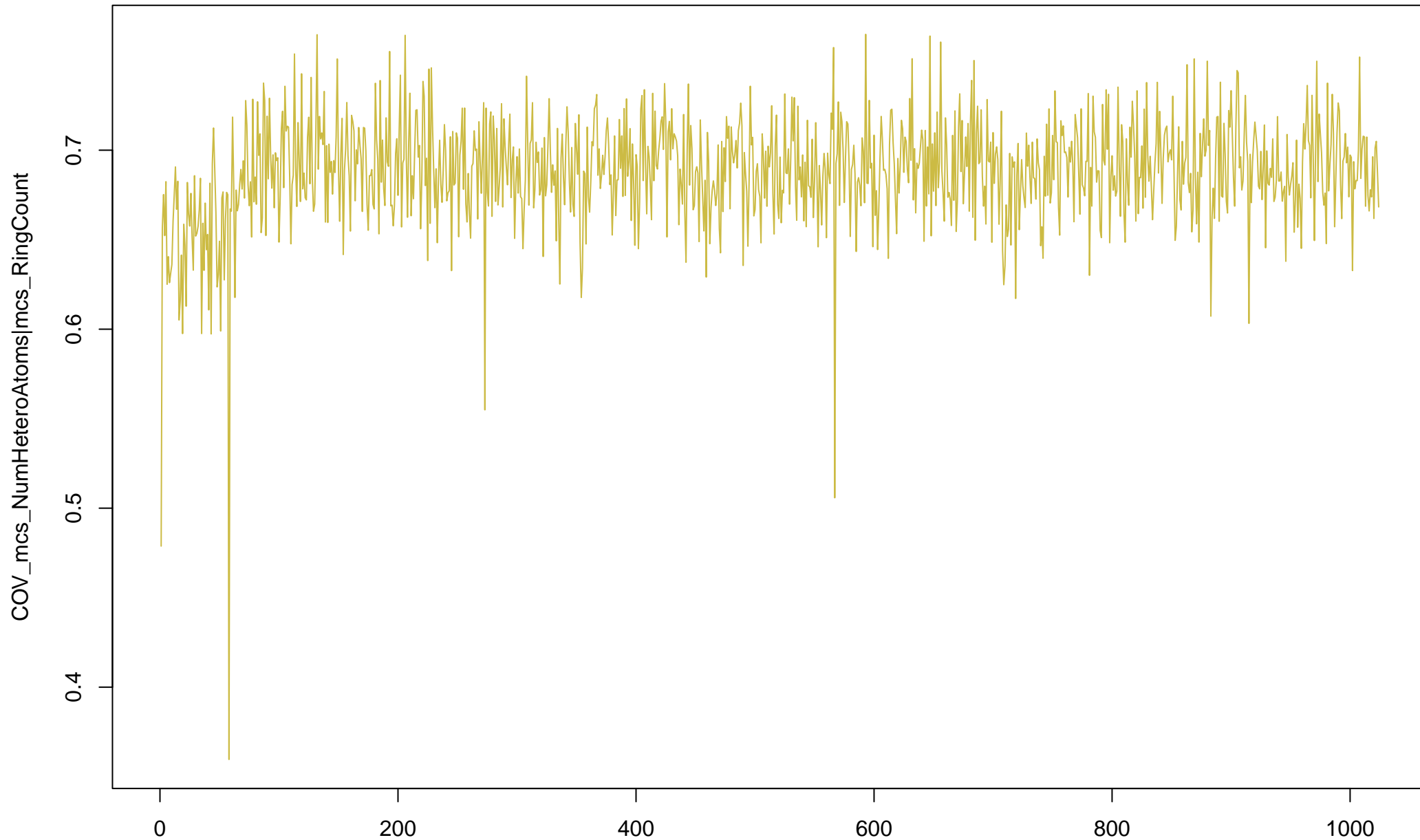
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NOCount**  
**ESS = 753 | BMK = 0.0926 | MCSE(6.27) = 3.85 | stat: TRUE | burn: 0**



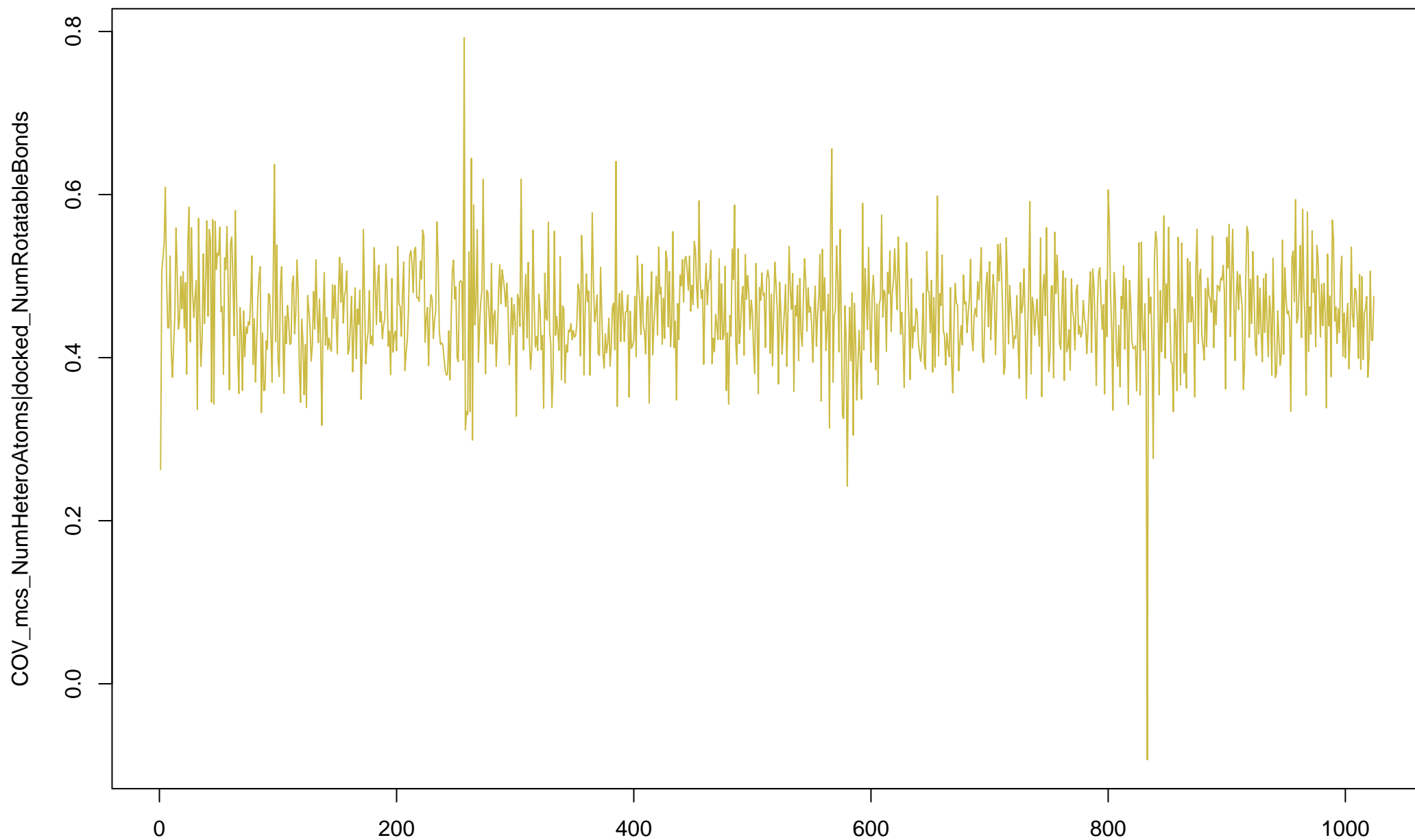
**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 165 | BMK = 0.122 | MCSE(6.27) = 6.56 | stat: FALSE | burn: 0**



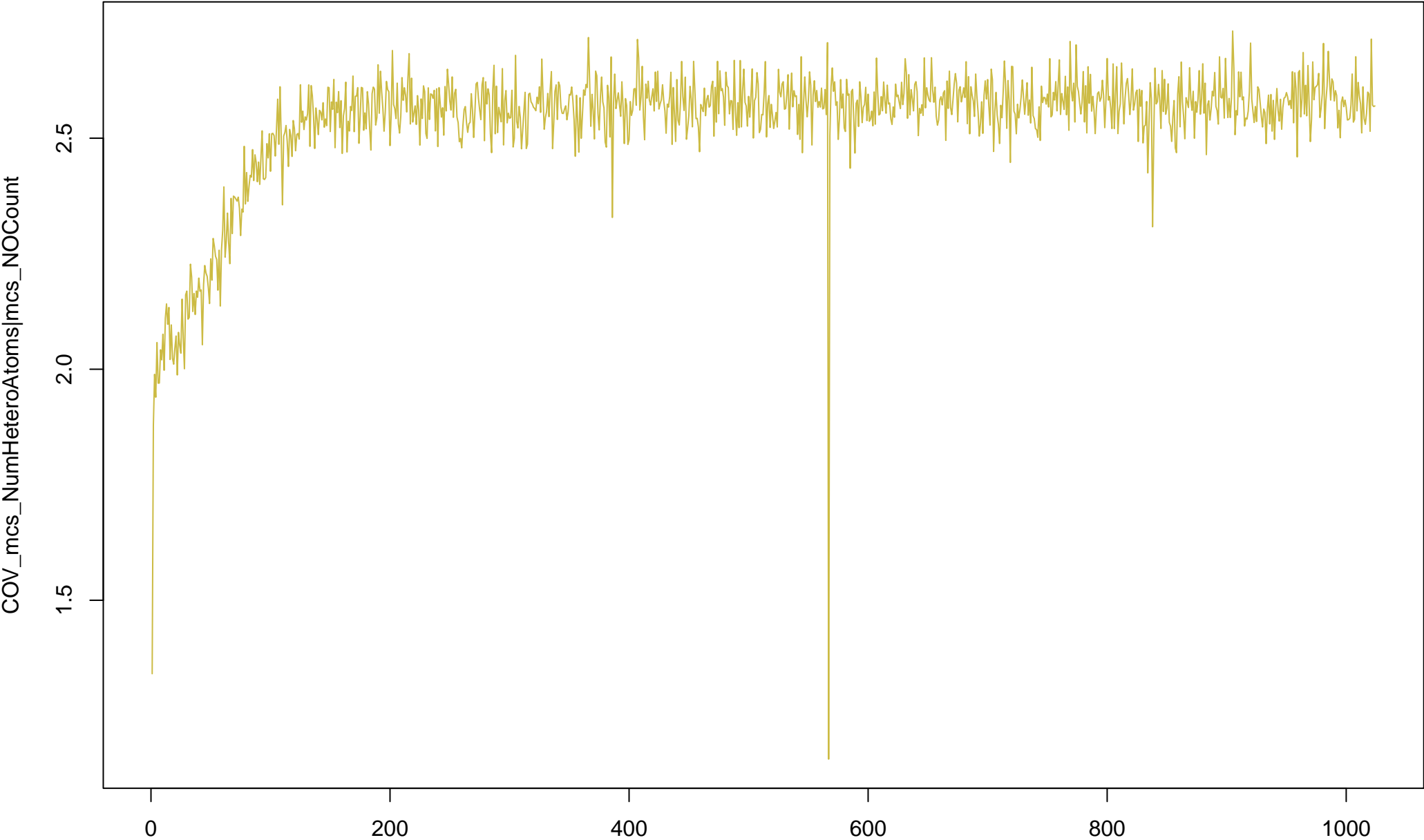
**COV\_mcs\_NumHeteroAtoms|mcs\_RingCount**  
**ESS = 181 | BMK = 0.1 | MCSE(6.27) = 7.02 | stat: FALSE | burn: 0**



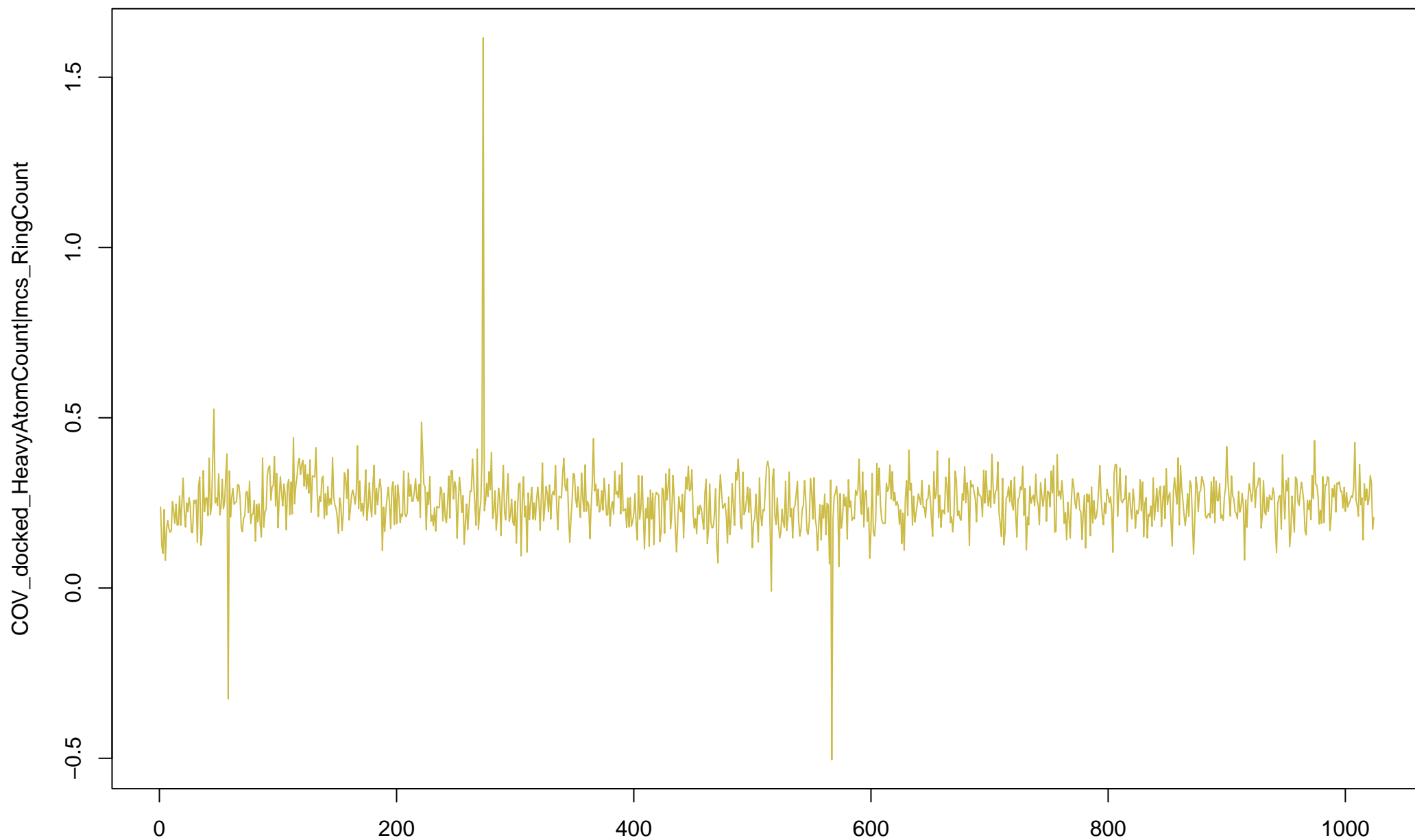
**COV\_mcs\_NumHeteroAtoms|docked\_NumRotatableBonds**  
**ESS = 1020 | BMK = 0.0657 | MCSE(6.27) = 4.11 | stat: TRUE | burn: 0**



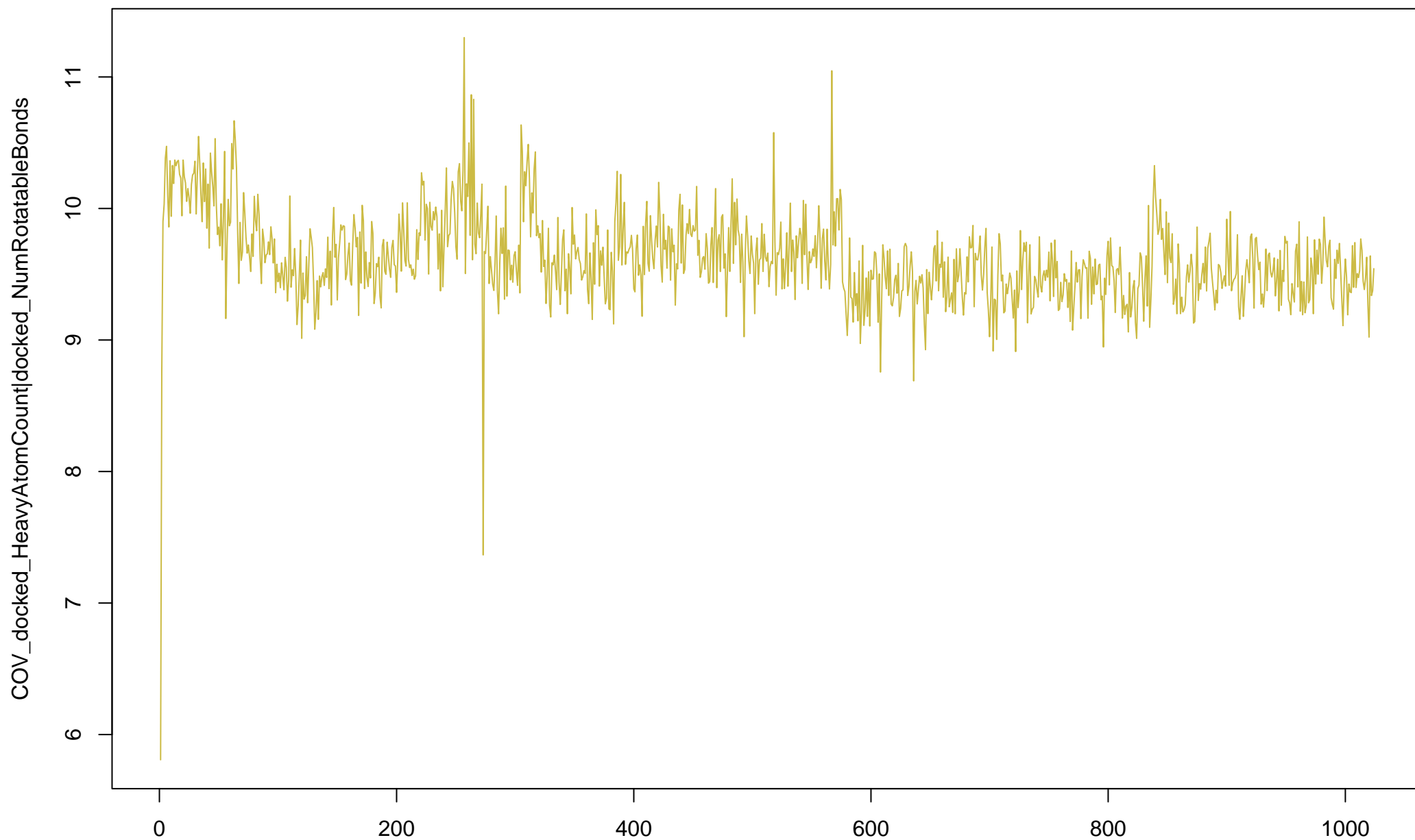
COV\_mcs\_NumHeteroAtoms|mcs\_NOCount  
ESS = 13 | BMK = 0.32 | MCSE(6.27) = 15.4 | stat: FALSE | burn: 102



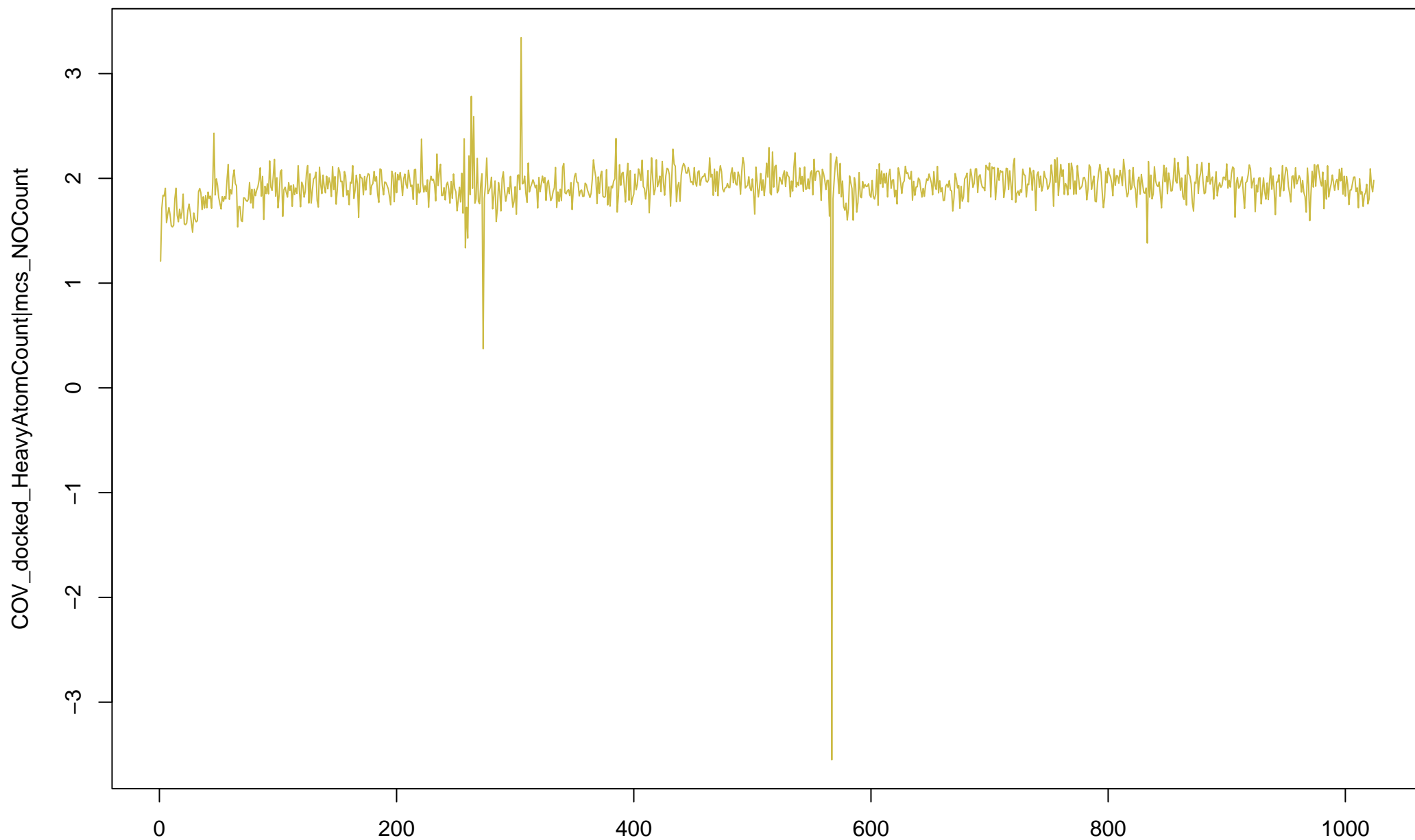
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 909 | BMK = 0.0844 | MCSE(6.27) = 4.62 | stat: TRUE | burn: 0**



**COV\_docked\_HeavyAtomCount|docked\_NumRotatableBonds**  
**ESS = 66.9 | BMK = 0.321 | MCSE(6.27) = 9.53 | stat: FALSE | burn: 102**

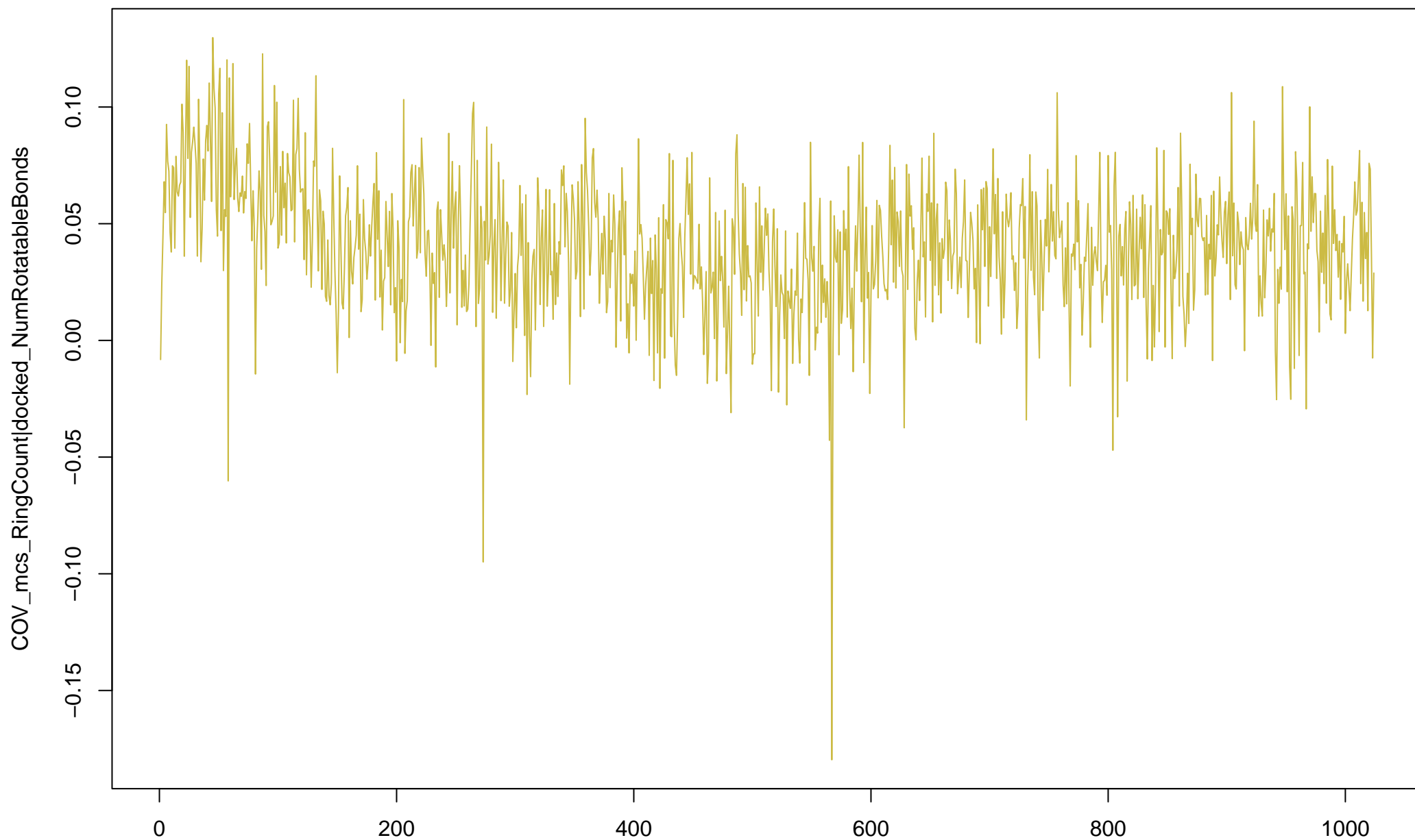


**COV\_docked\_HeavyAtomCount|mcs\_NOCount**  
**ESS = 791 | BMK = 0.164 | MCSE(6.27) = 5.1 | stat: FALSE | burn: 0**

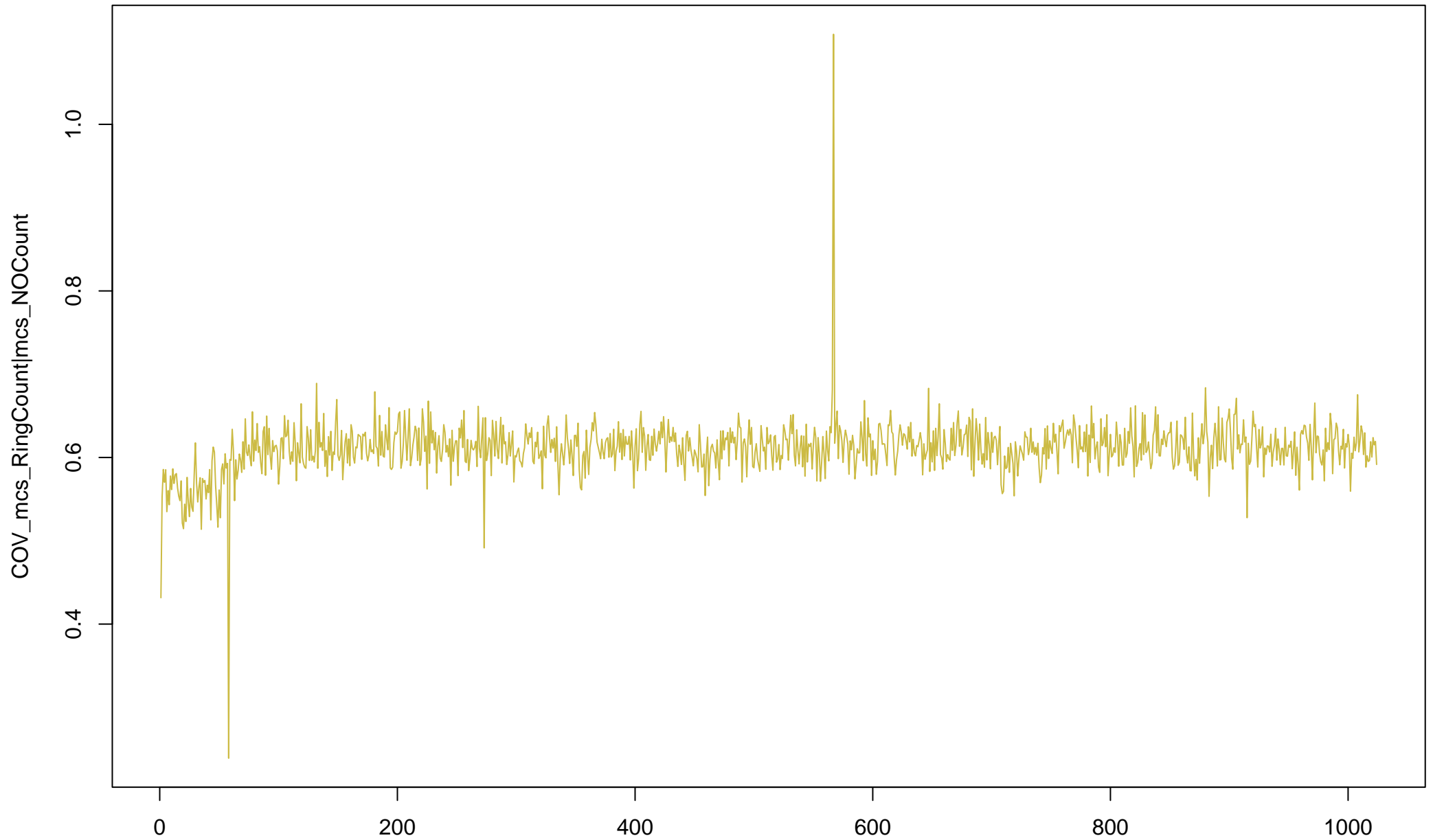




**COV\_mcs\_RingCount|docked\_NumRotatableBonds**  
**ESS = 59.9 | BMK = 0.151 | MCSE(6.27) = 7.71 | stat: FALSE | burn: 0**



**COV\_mcs\_RingCount|mcs\_NOCount**  
**ESS = 87.8 | BMK = 0.141 | MCSE(6.27) = 7.95 | stat: FALSE | burn: 0**



**COV\_docked\_NumRotatableBonds|mcs\_NOCount**  
**ESS = 903 | BMK = 0.0957 | MCSE(6.27) = 4.07 | stat: TRUE | burn: 0**

