

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.688248186919269

max MCSE = 14.3437941391713

all stationary: FALSE

burn: 2040

-- STATS 2D --

min ESS = 323.546835312983

max BMK = 0.116910030050631

max MCSE = 4.01652082271779

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.5247026486506

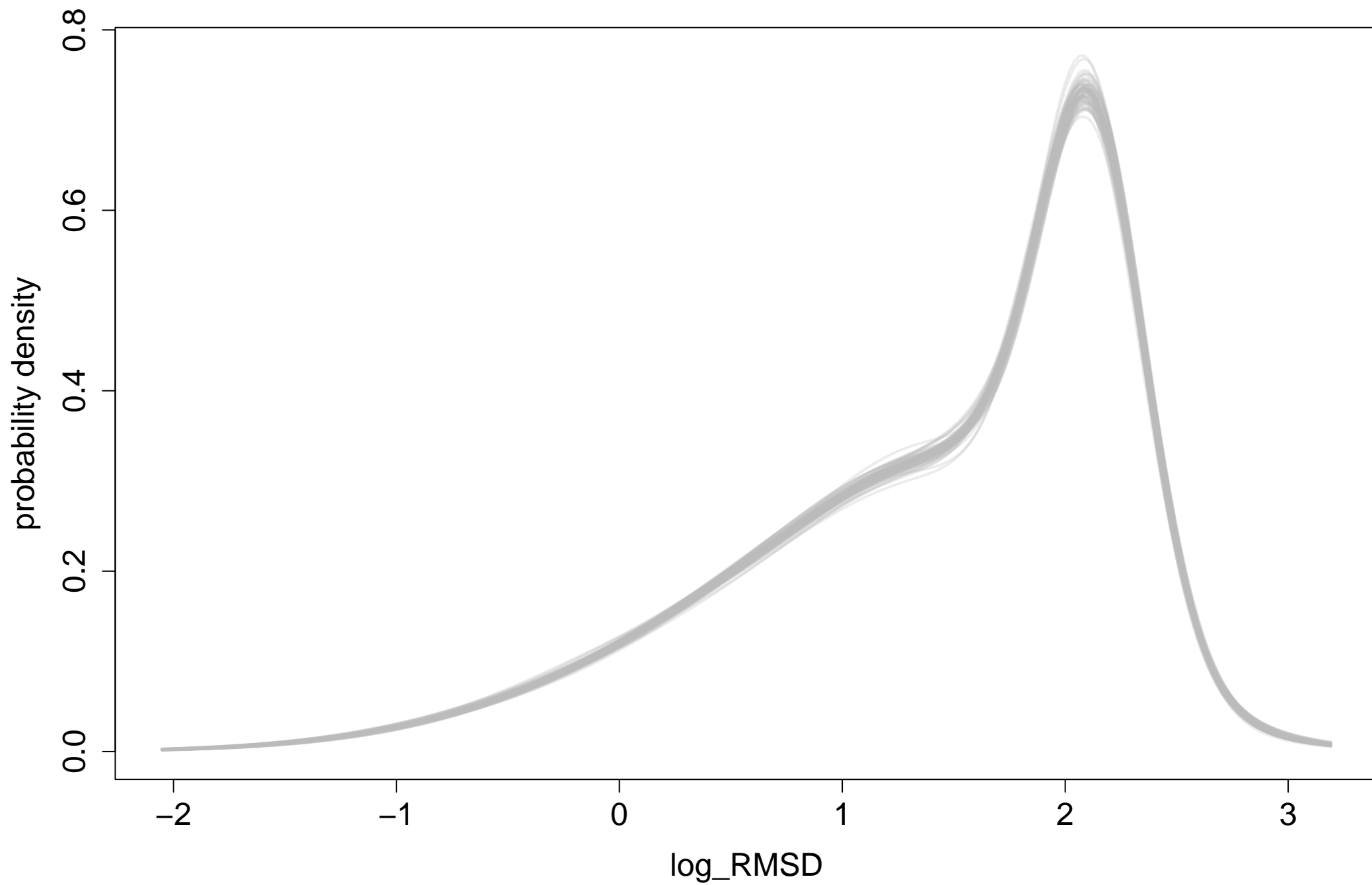
max MCSE = NaN

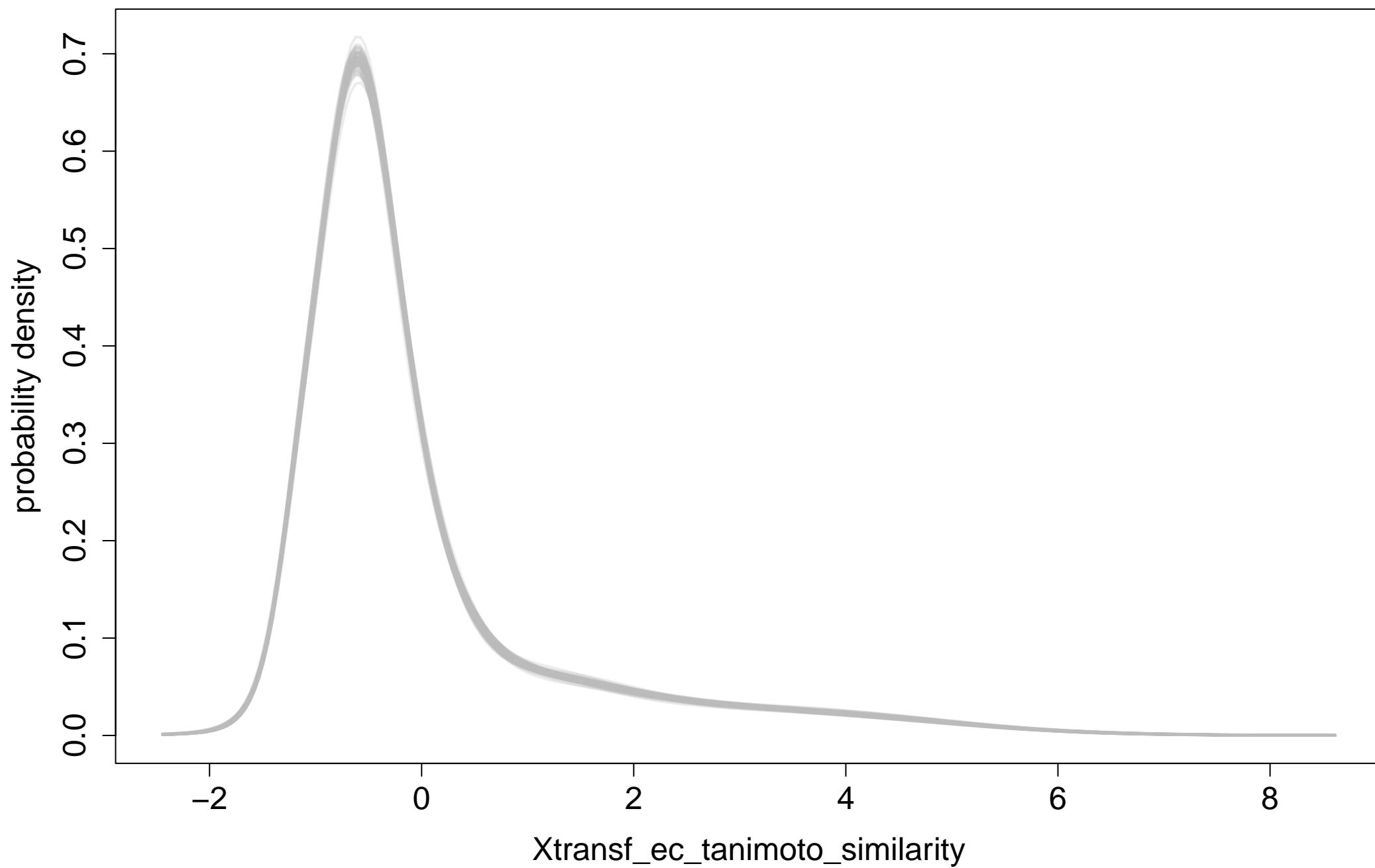
all stationary: FALSE

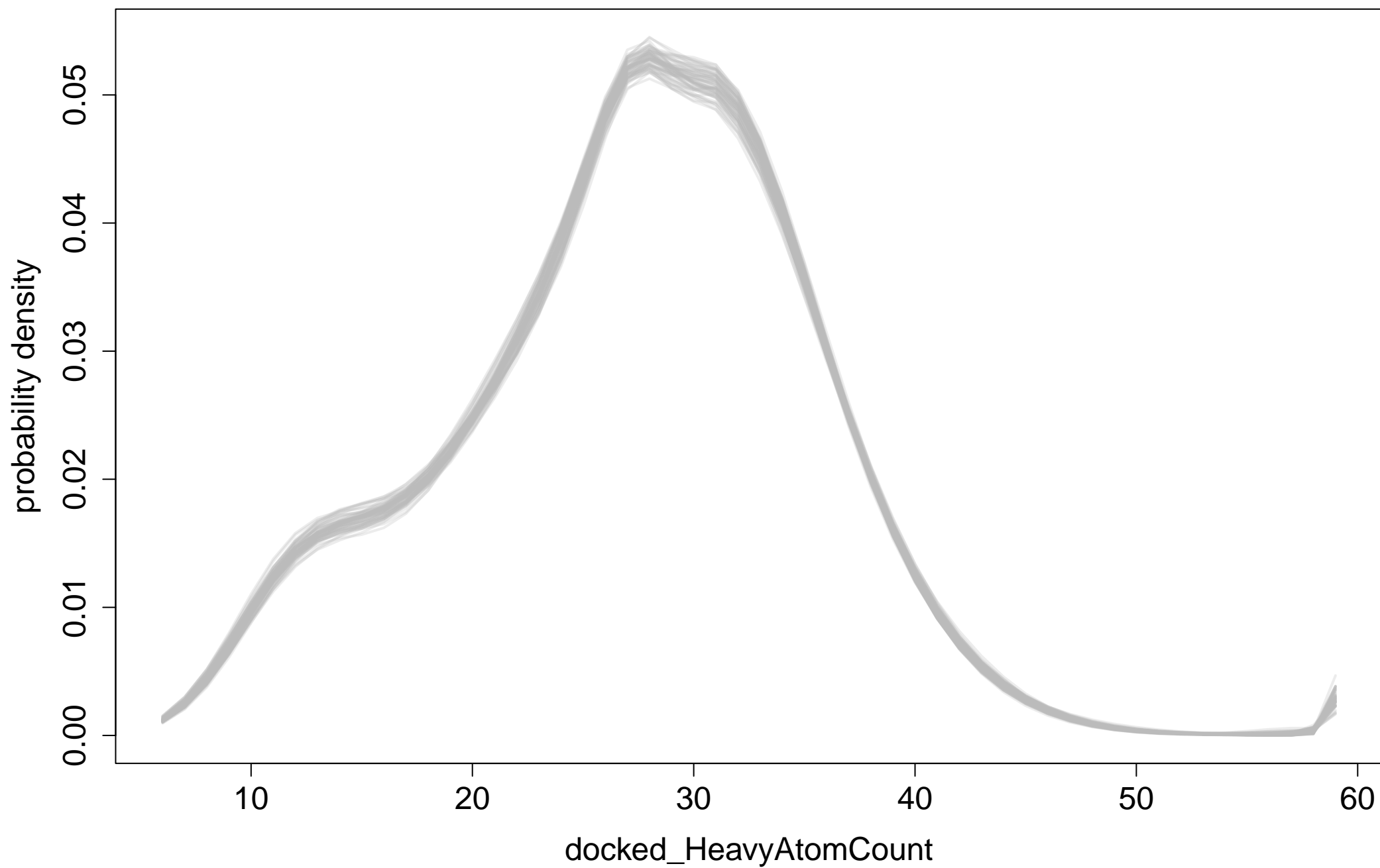
burn: 1428

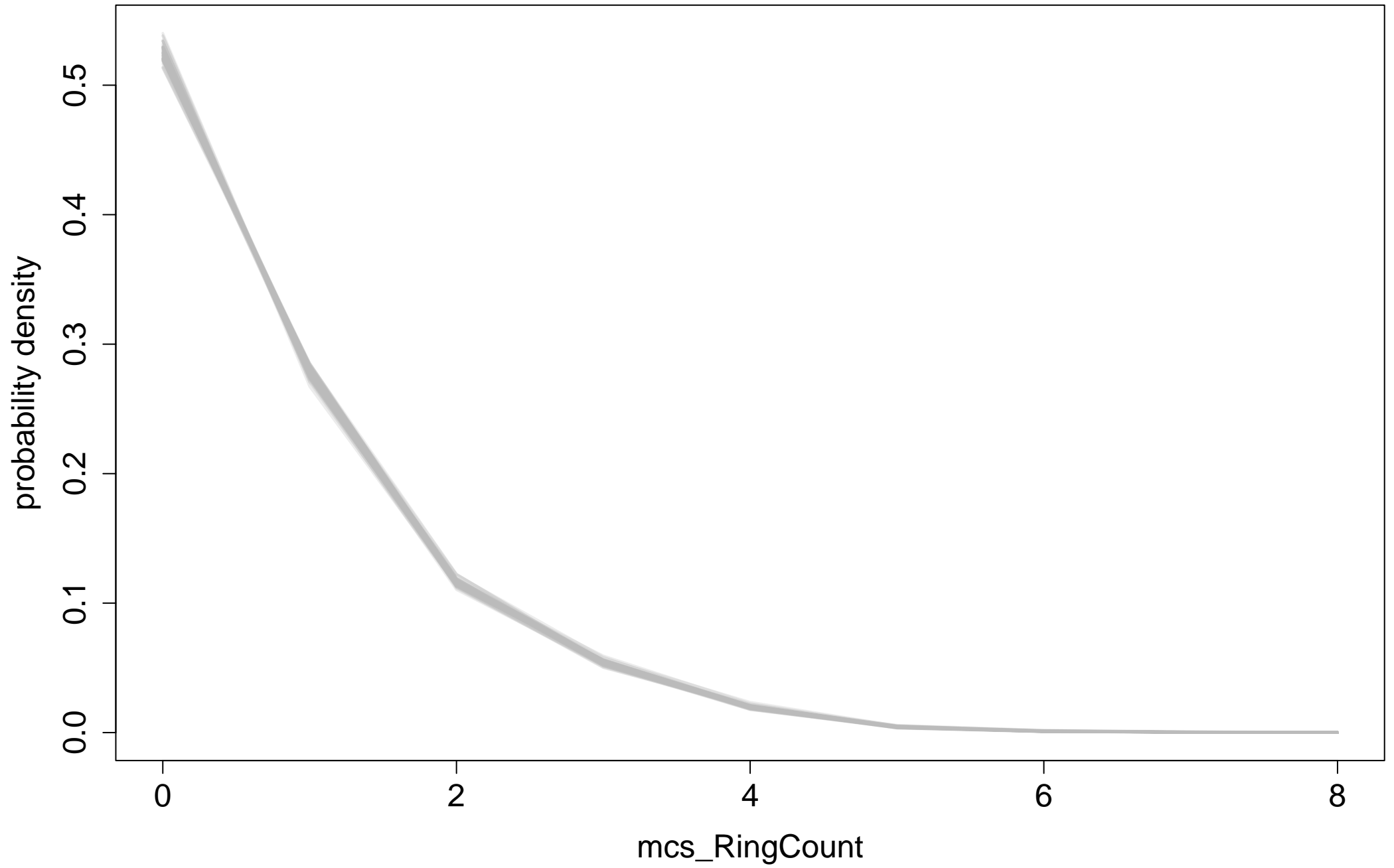
Occupied clusters: 43 of 91

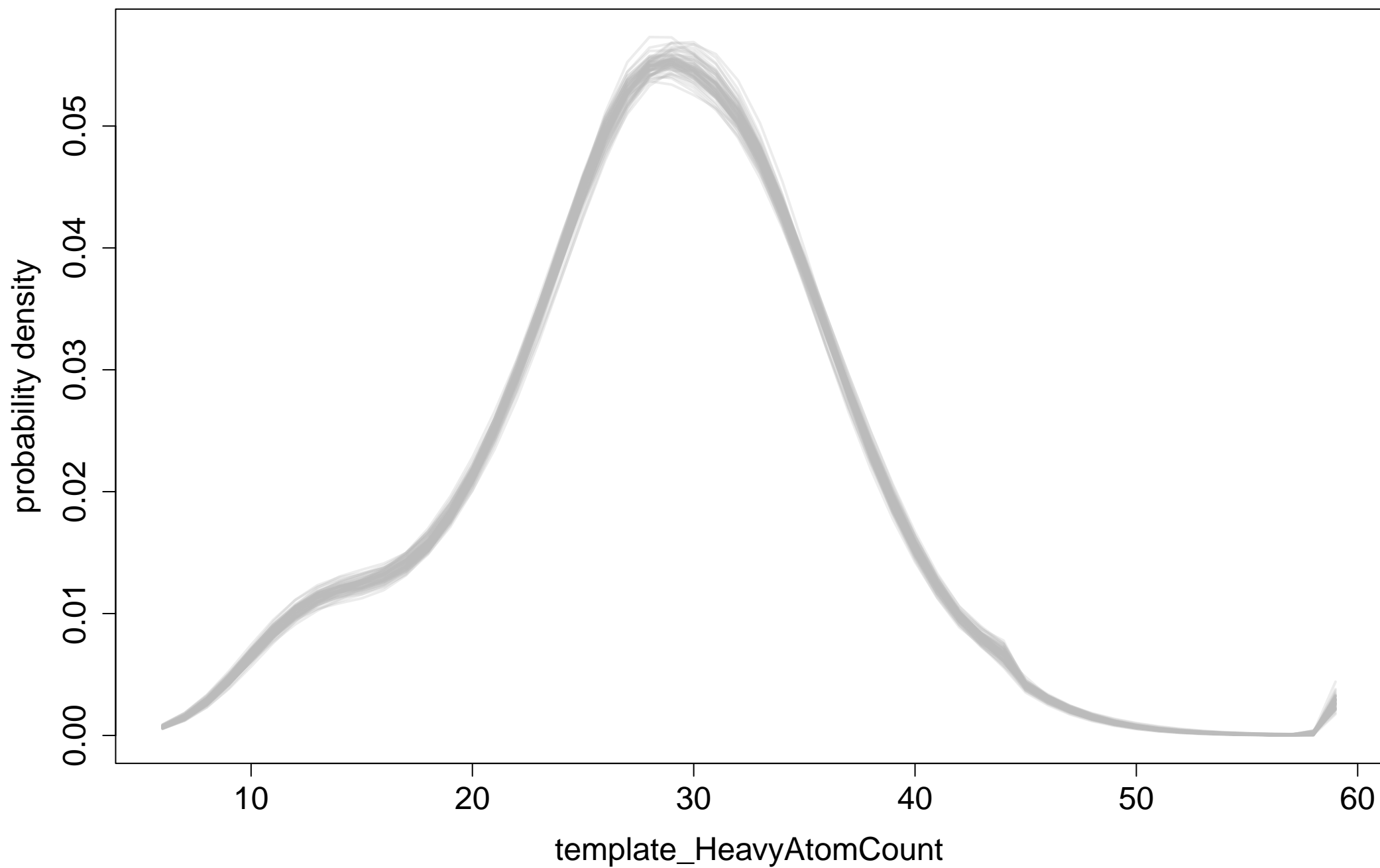
LL: -113000 +- 152

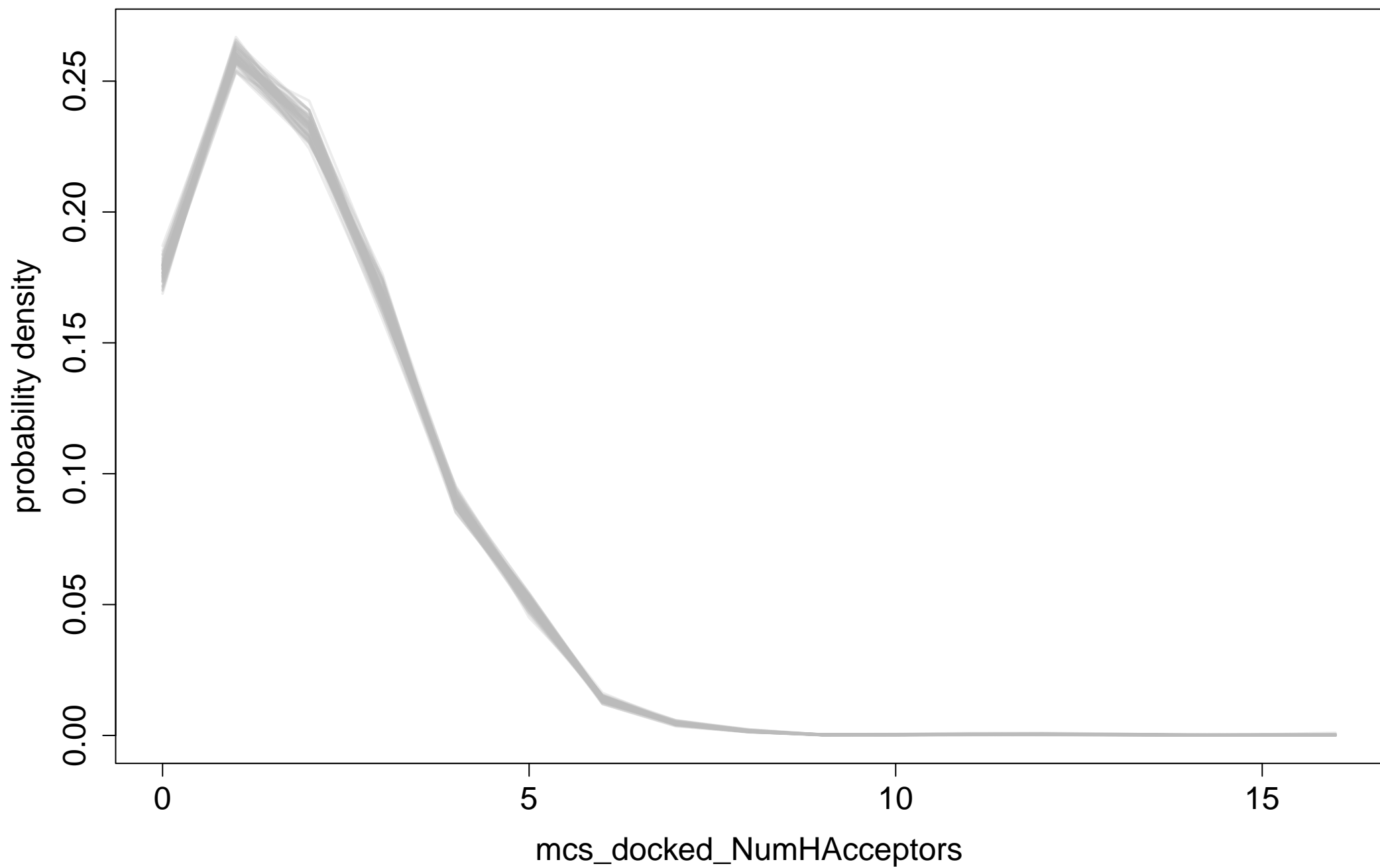


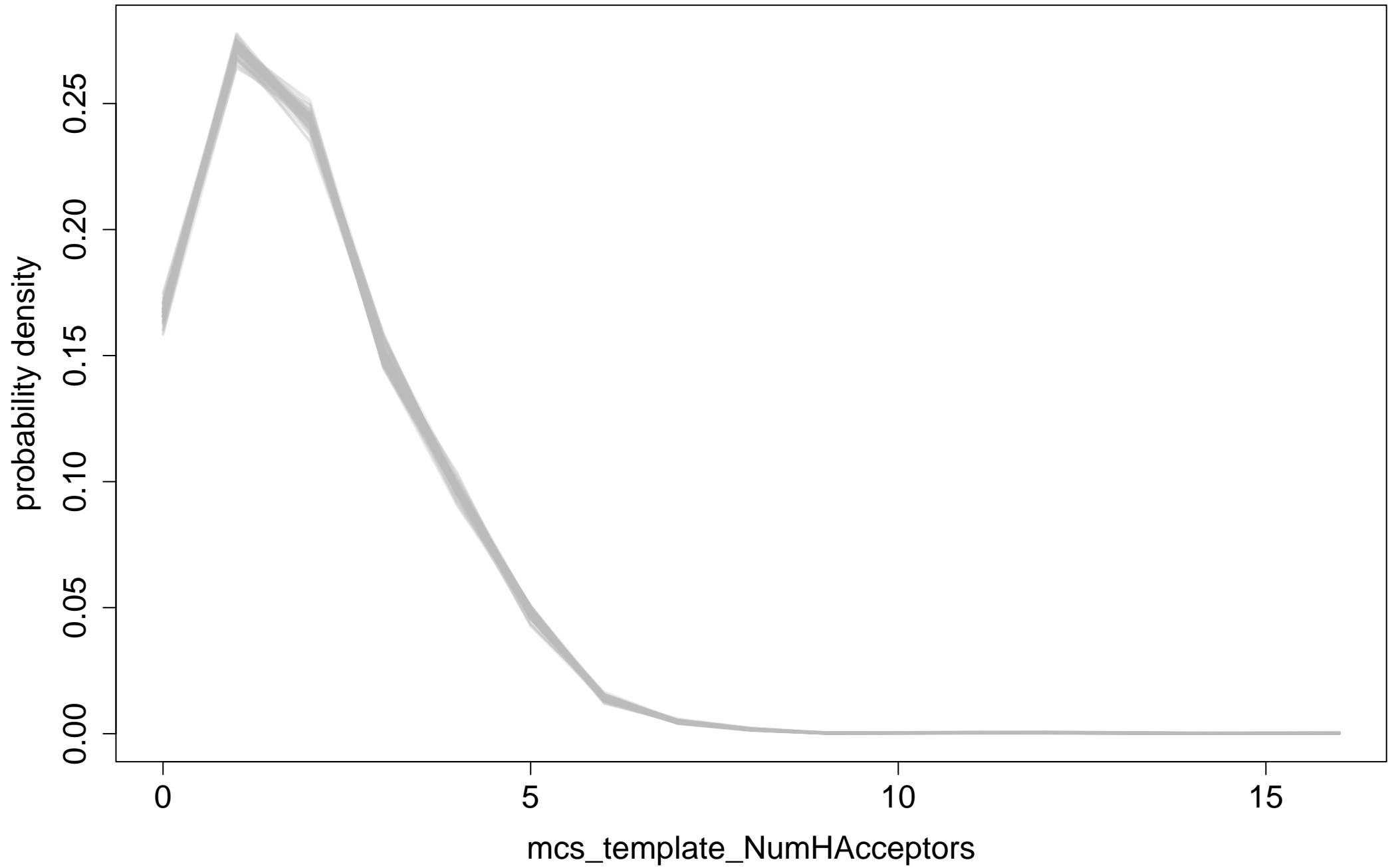




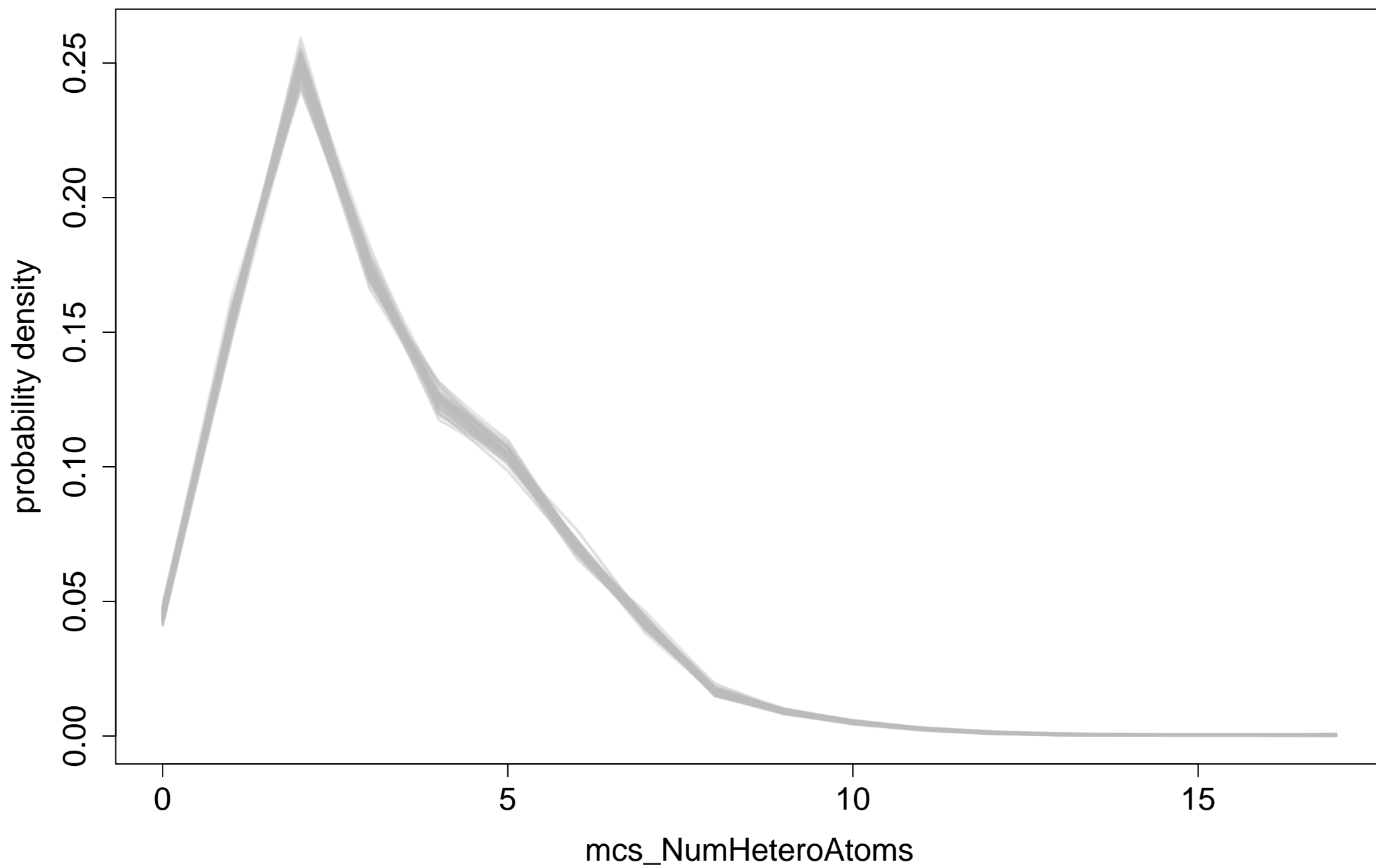


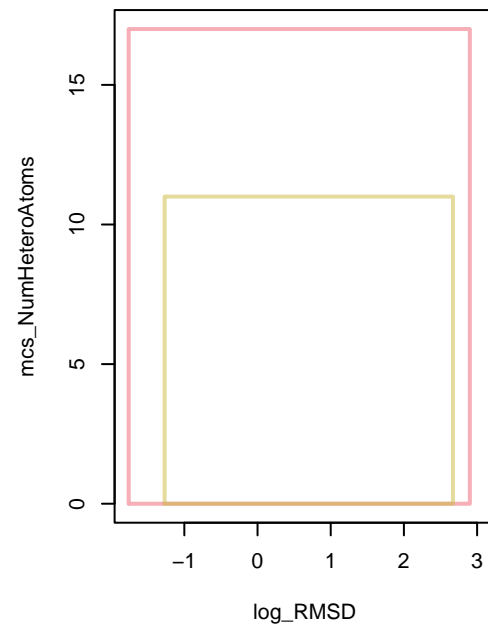
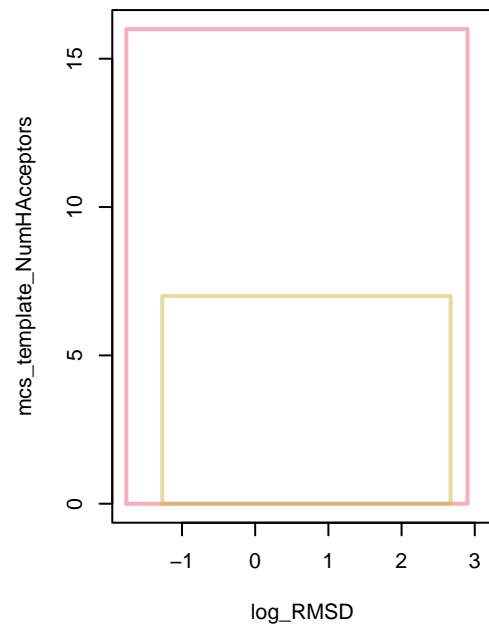
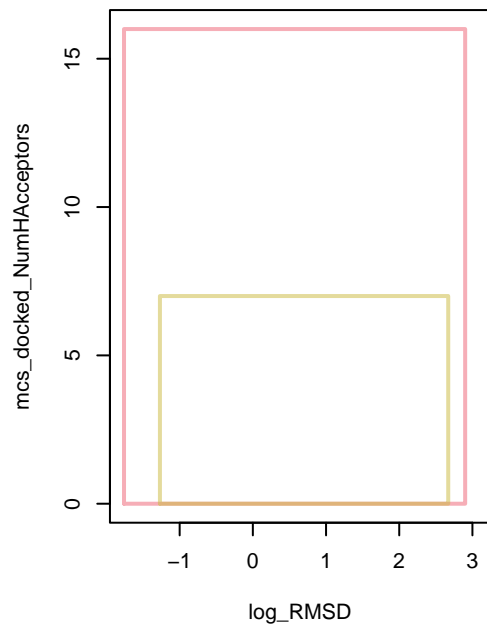
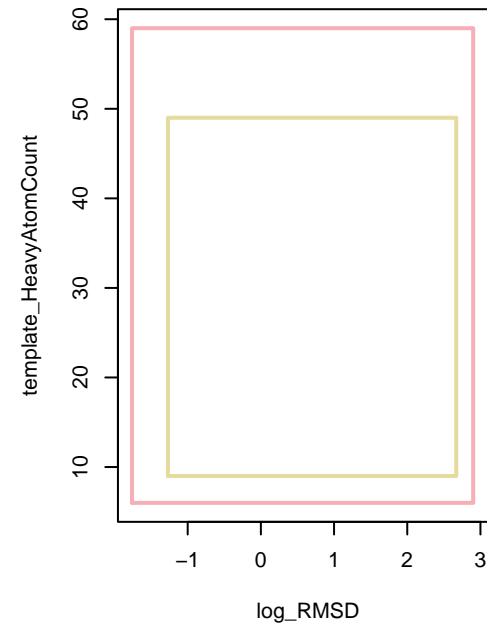
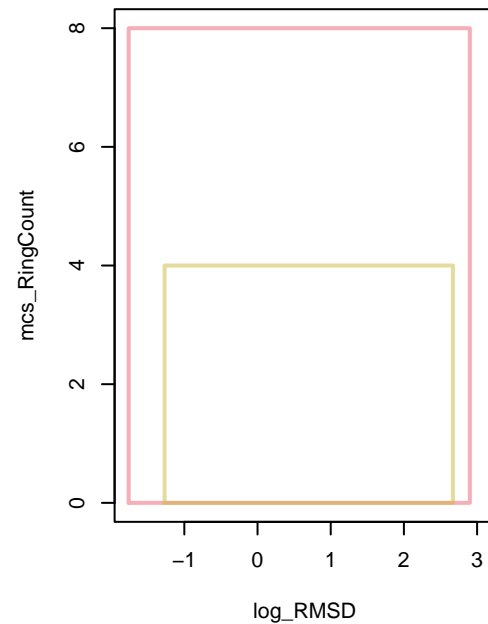
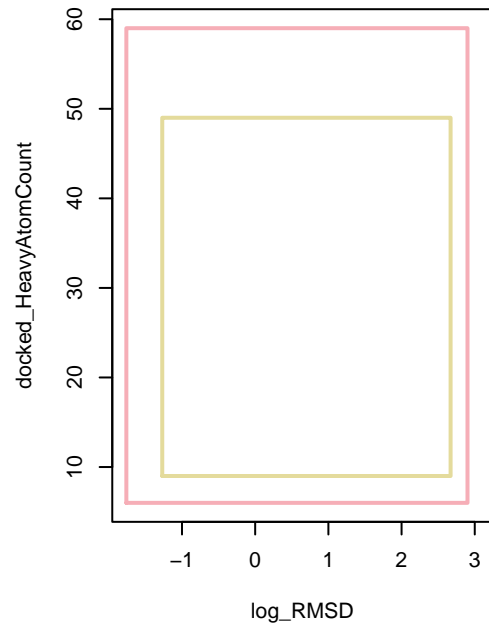
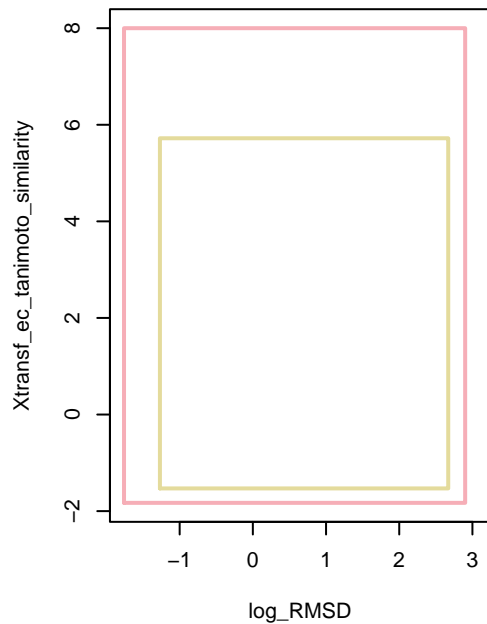




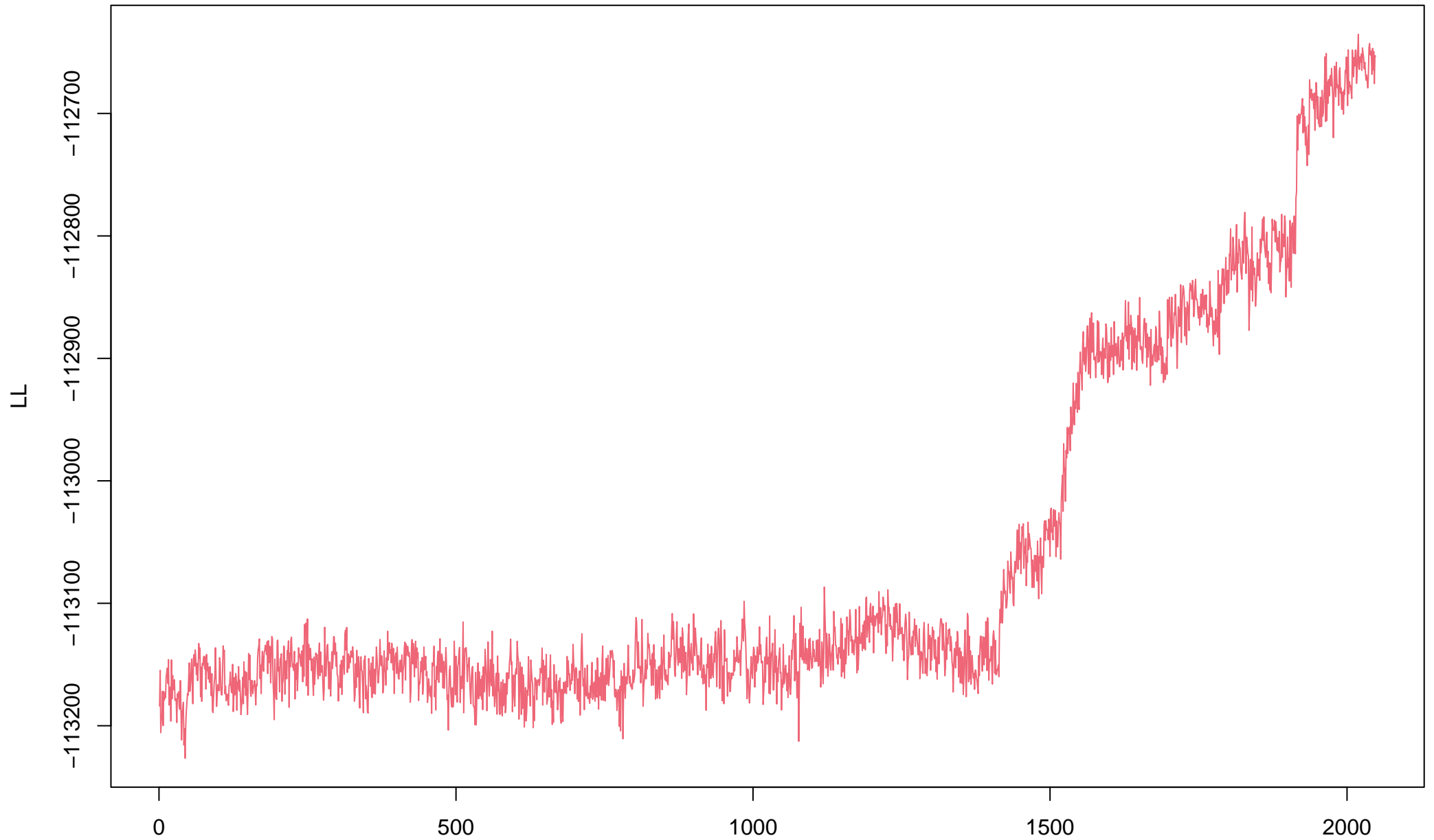




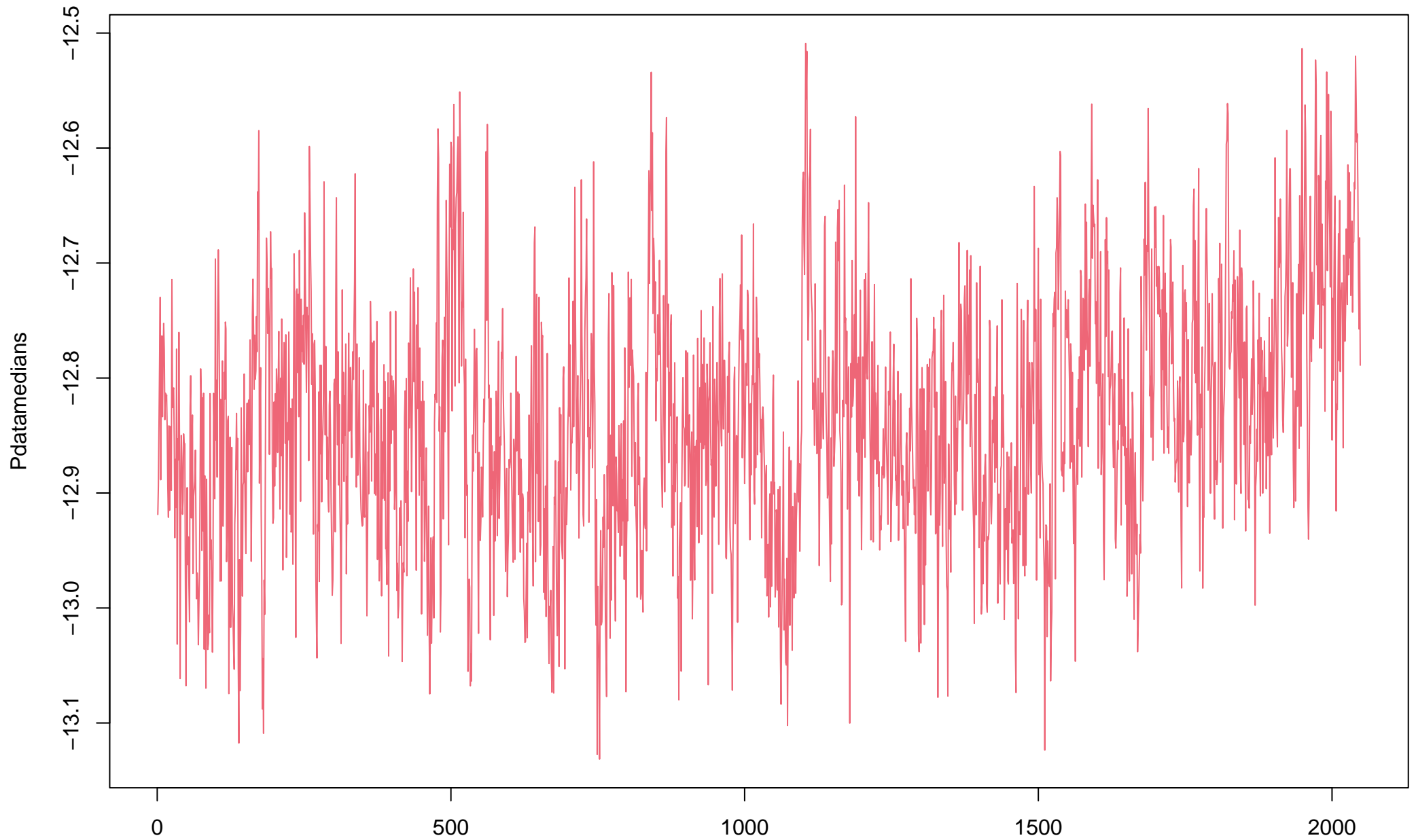




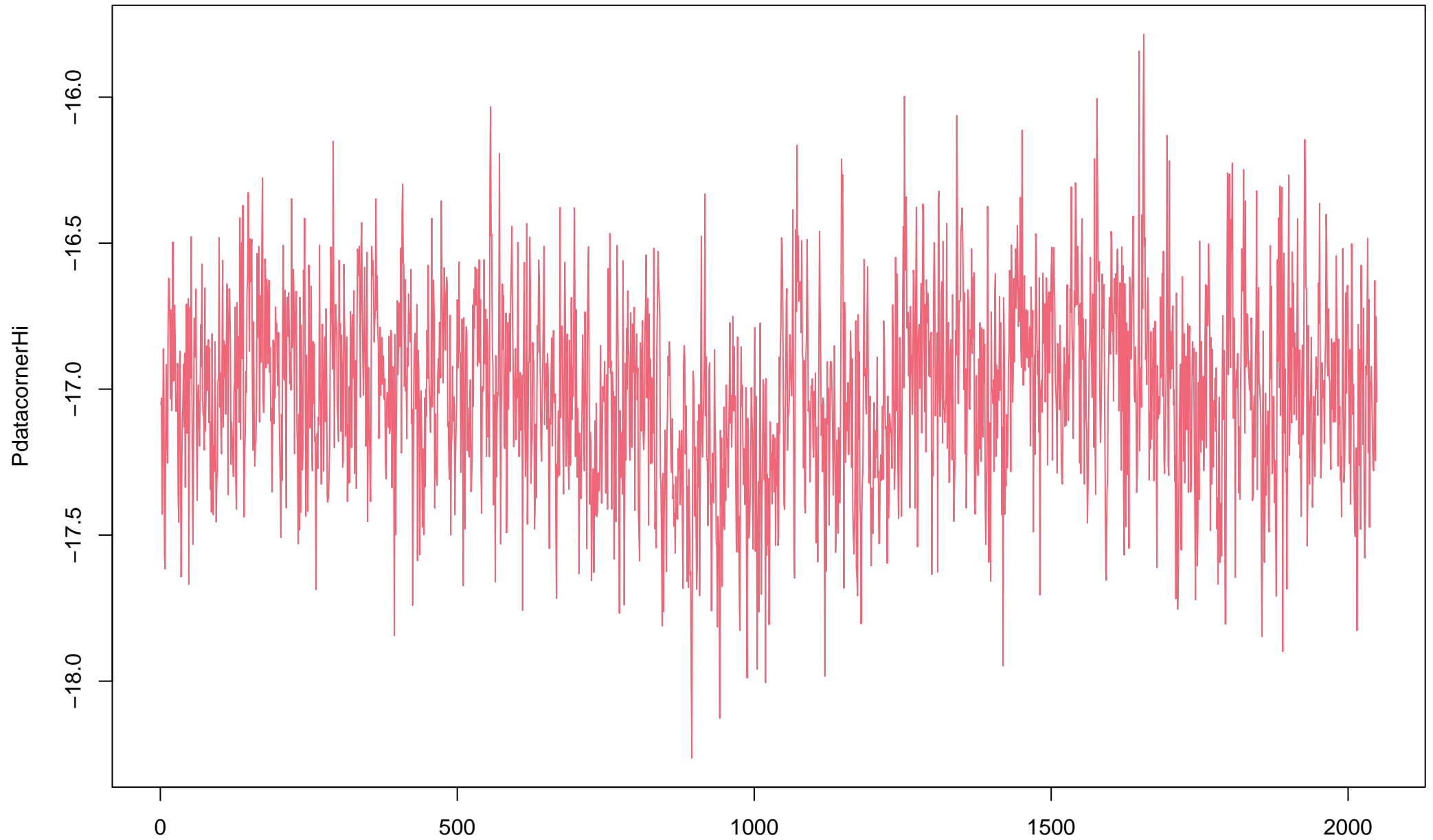
LL  
ESS = 2.74 | BMK = 0.688 | MCSE(6.27) = 14.3 | stat: FALSE | burn: 2040



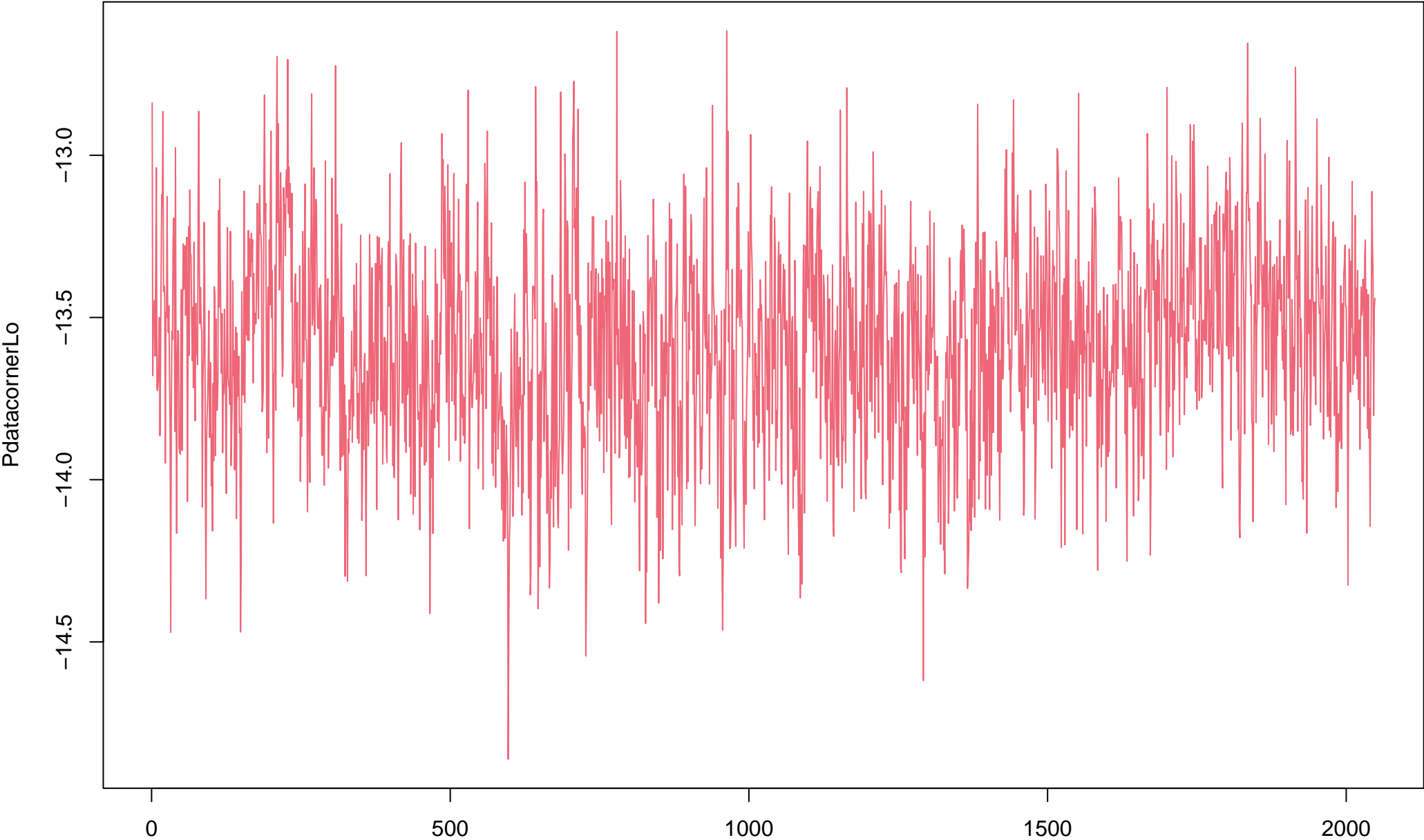
**Pdatamedians**  
**ESS = 179 | BMK = 0.138 | MCSE(6.27) = 7.1 | stat: FALSE | burn: 0**



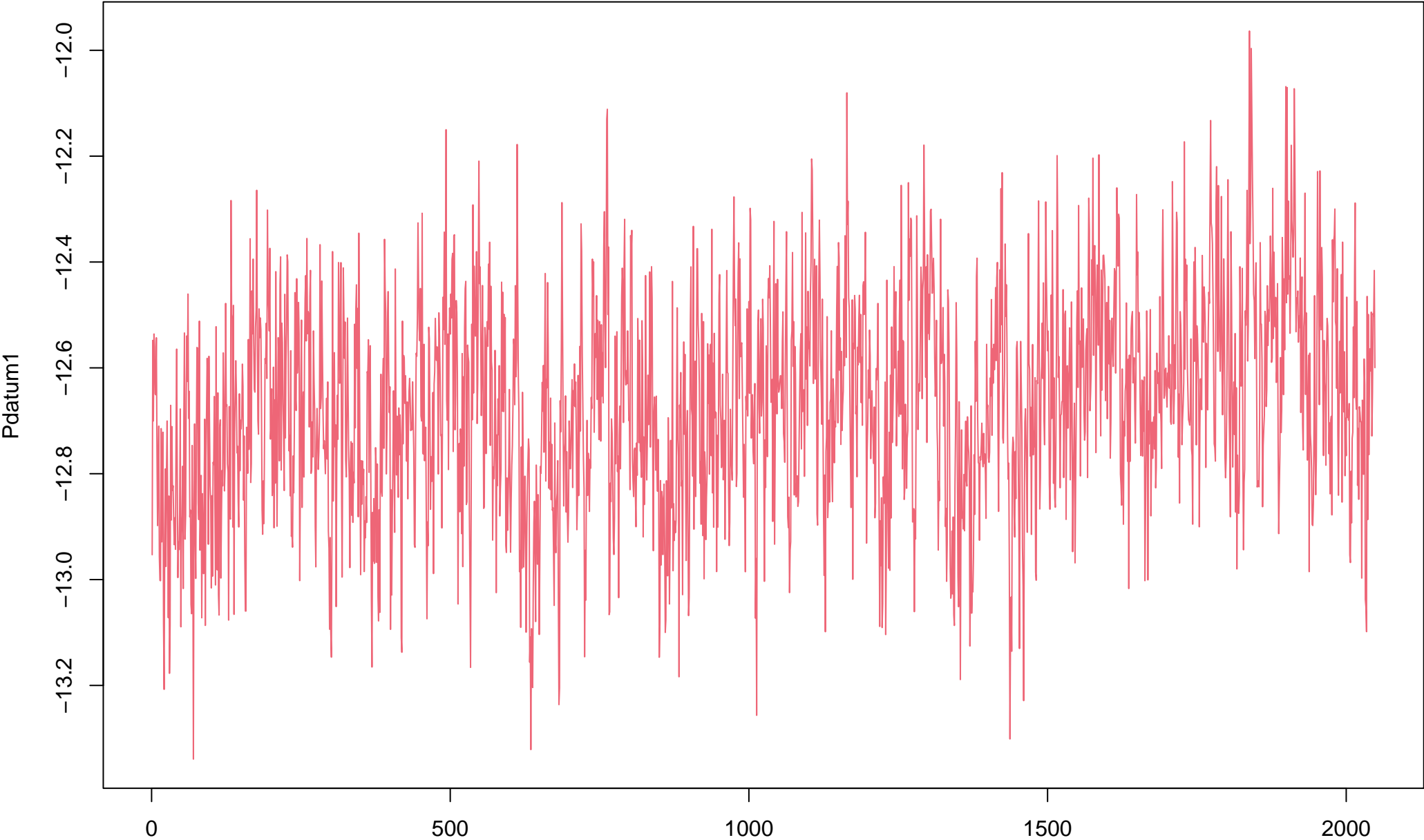
**PdatacornerHi**  
**ESS = 2.22e-16 | BMK = 0.0816 | MCSE(6.27) = 5.38 | stat: TRUE | burn: 0**



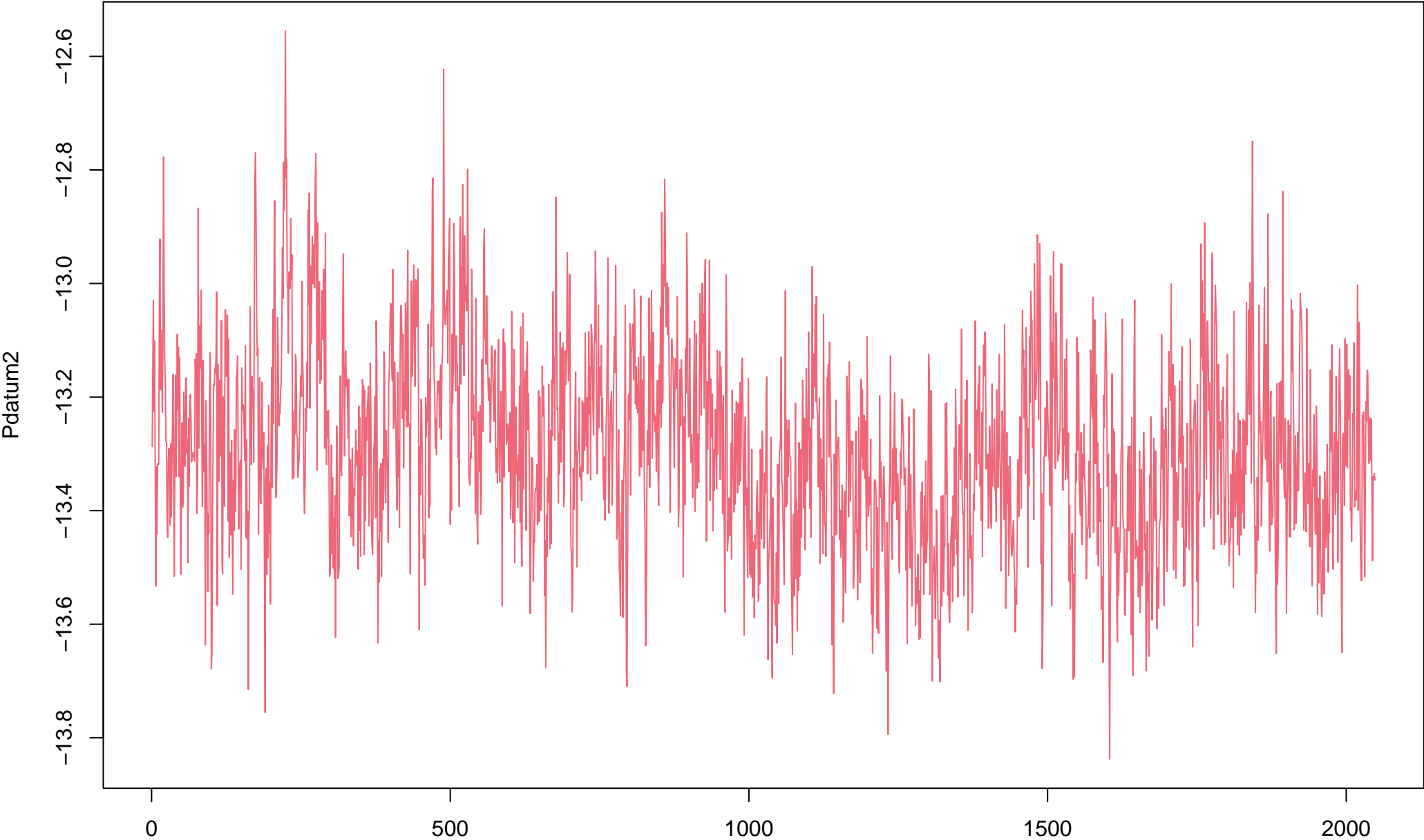
**PdatacornerLo**  
**ESS = 643 | BMK = 0.0765 | MCSE(6.27) = 4.59 | stat: TRUE | burn: 0**



**Pdatum1**  
**ESS = 177 | BMK = 0.168 | MCSE(6.27) = 6.55 | stat: FALSE | burn: 0**

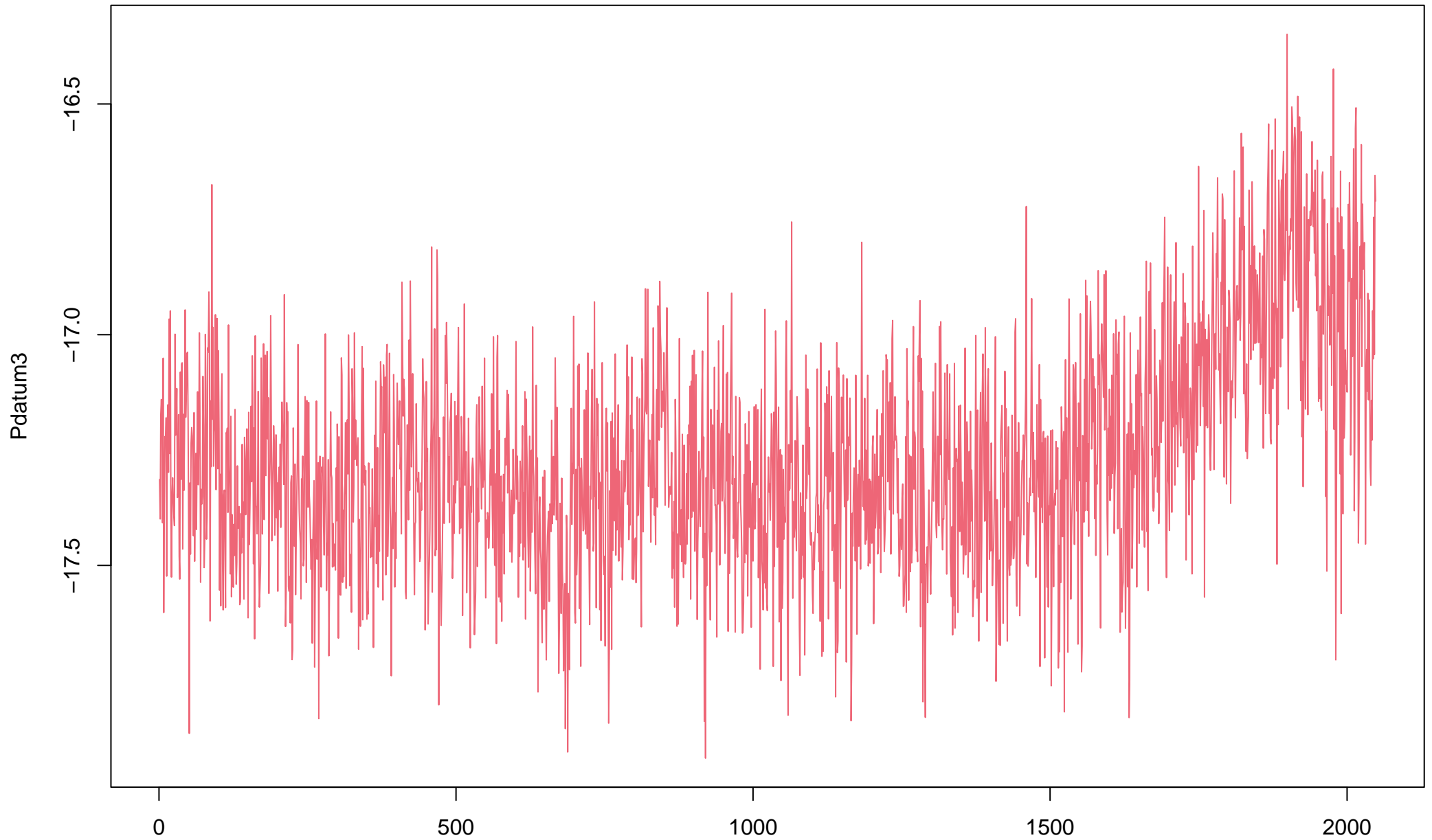


**Pdatum2**  
**ESS = 162 | BMK = 0.223 | MCSE(6.27) = 7.17 | stat: FALSE | burn: 0**

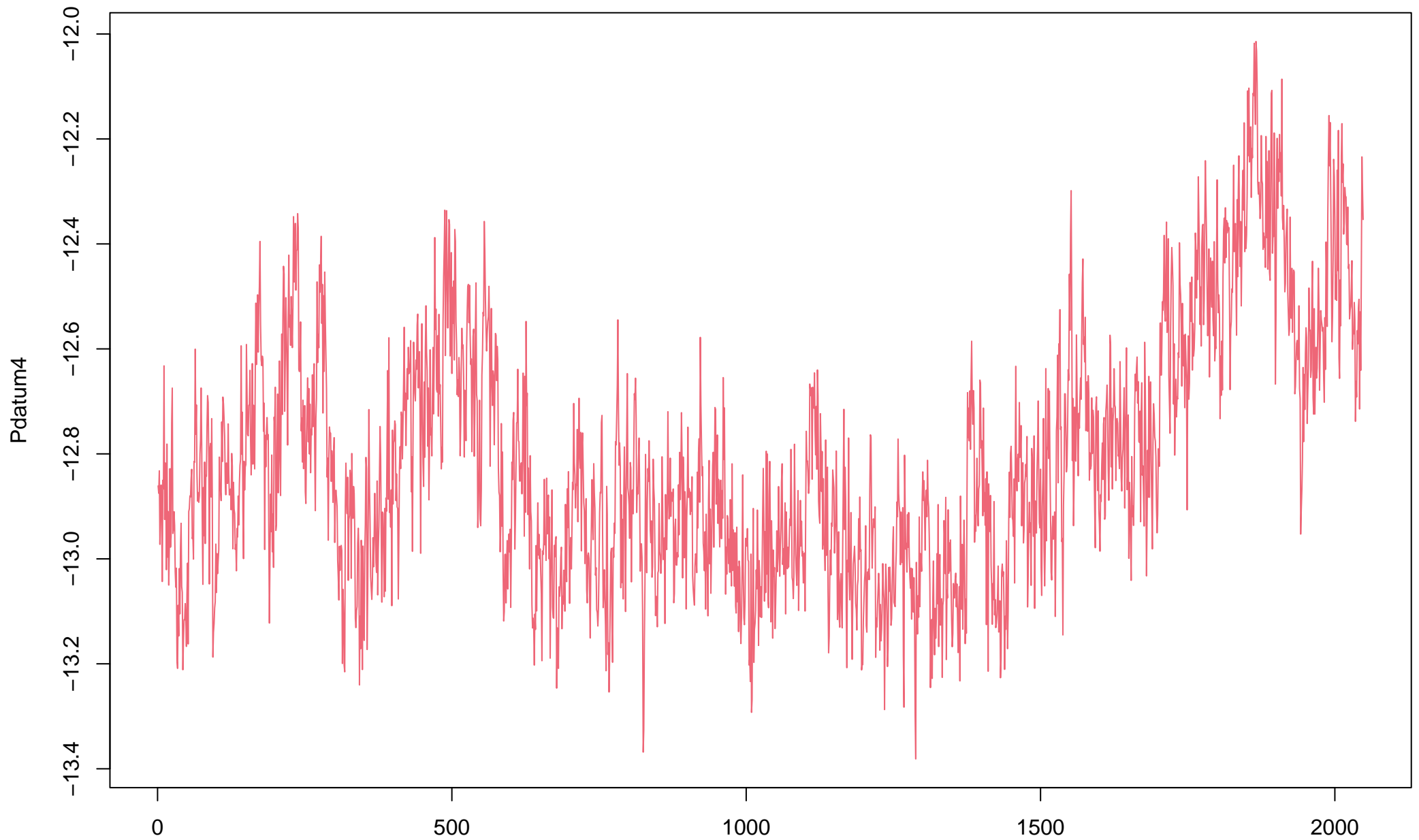




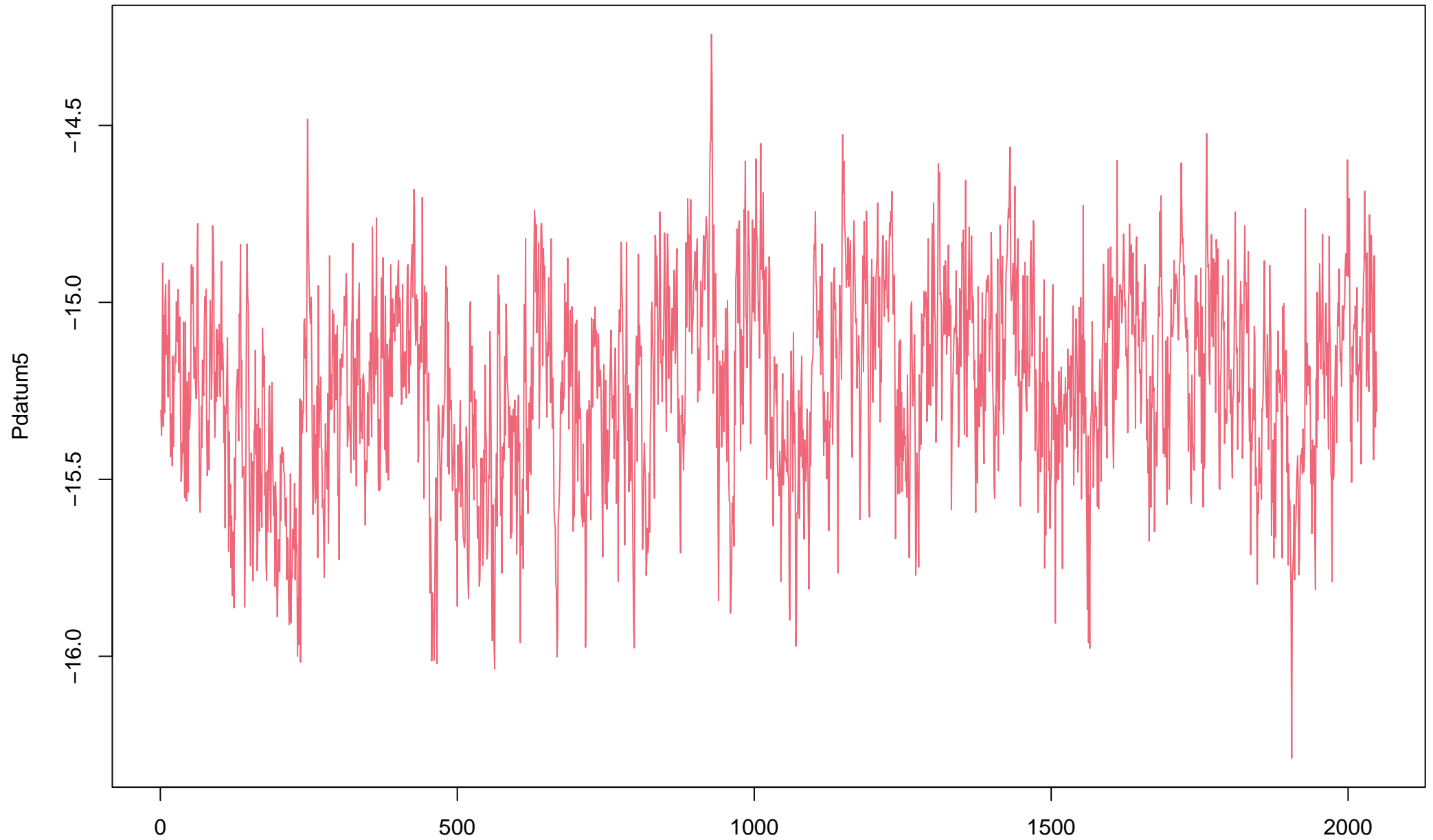
**Pdatum3**  
**ESS = 2.22e-16 | BMK = 0.257 | MCSE(6.27) = 9.68 | stat: TRUE | burn: 0**



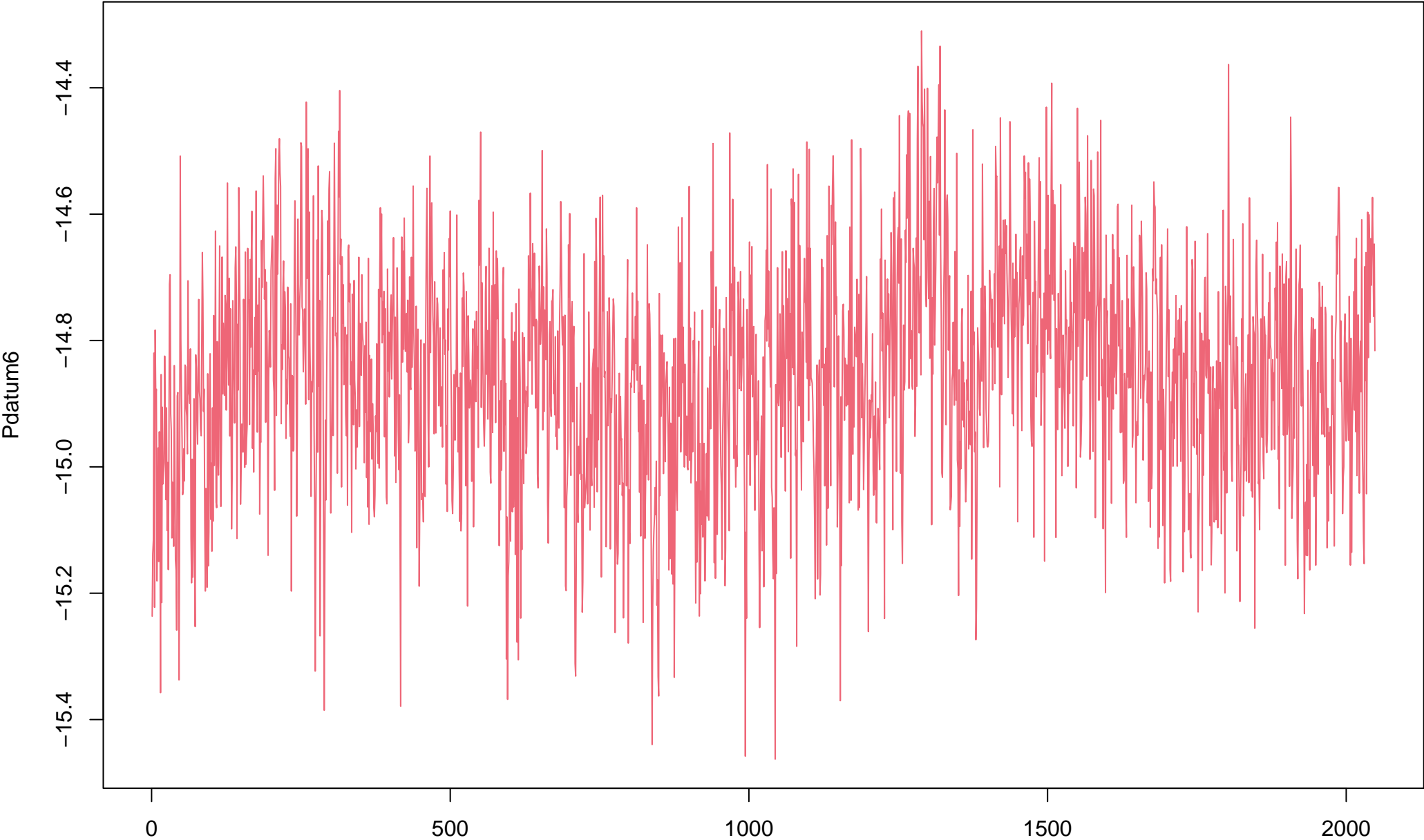
**Pdatum4**  
**ESS = 16 | BMK = 0.227 | MCSE(6.27) = 12.6 | stat: FALSE | burn: 612**



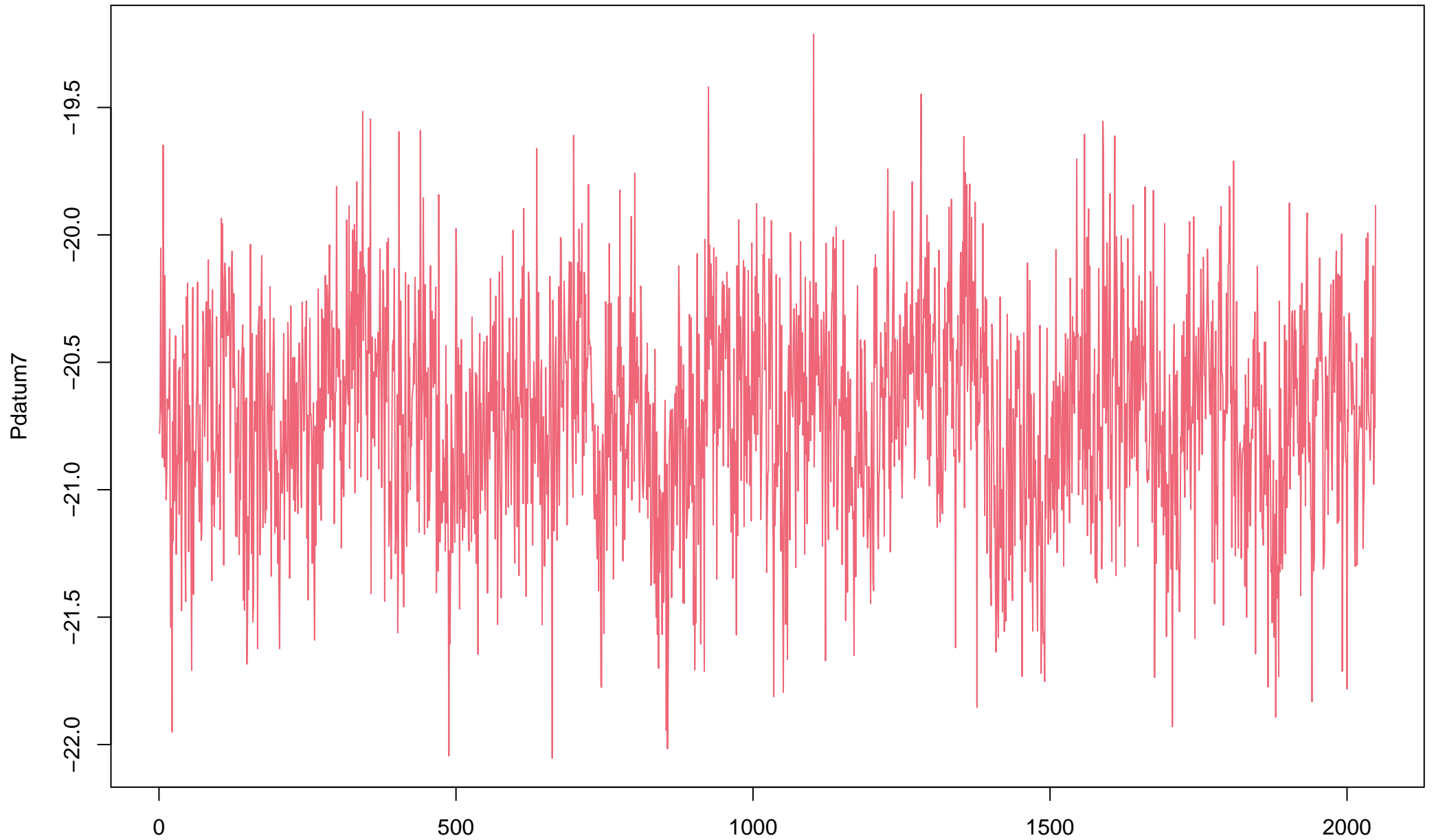
**Pdatum5**  
**ESS = 121 | BMK = 0.128 | MCSE(6.27) = 7.5 | stat: FALSE | burn: 0**



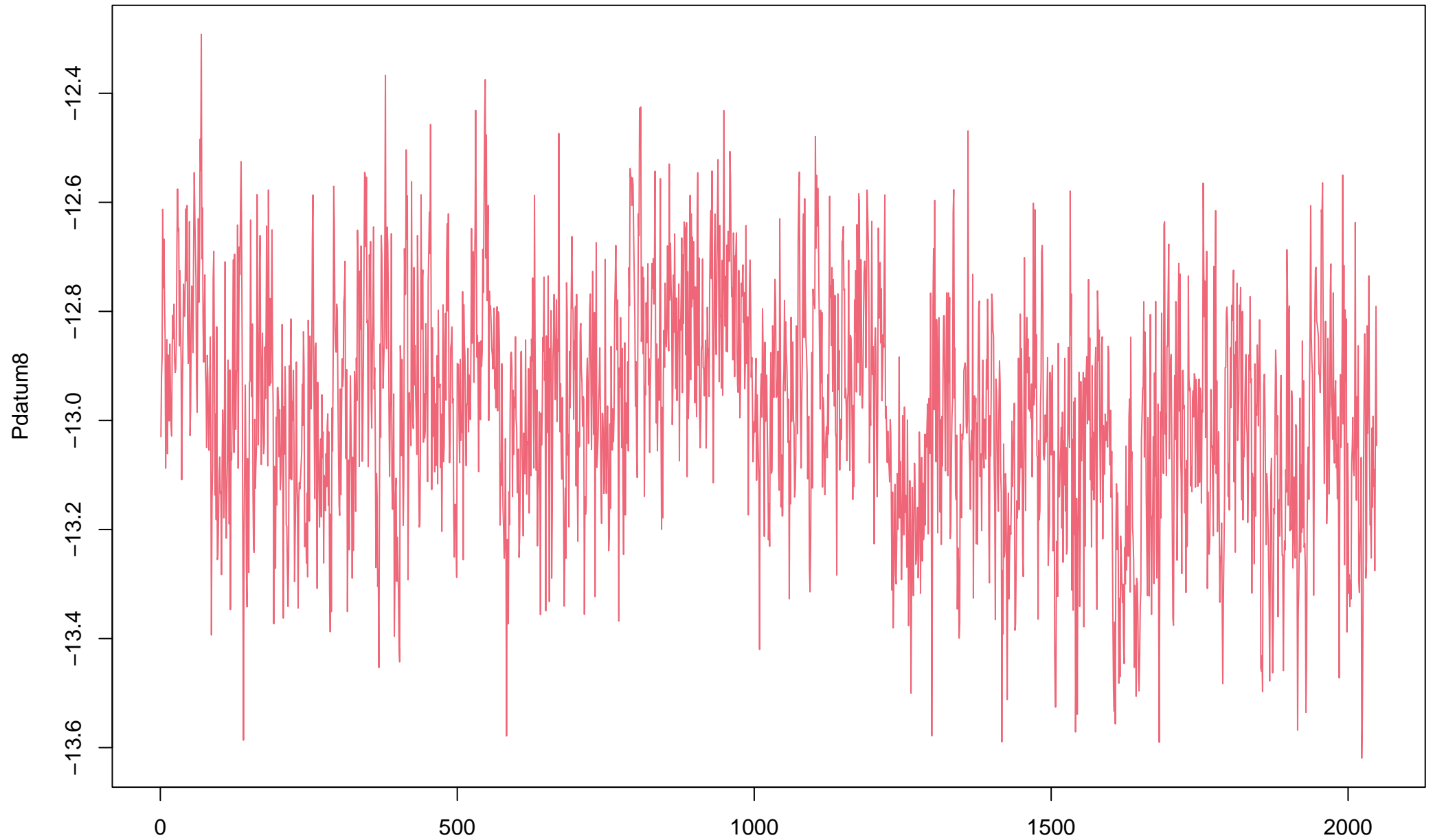
**Pdatum6**  
**ESS = 284 | BMK = 0.115 | MCSE(6.27) = 6.24 | stat: FALSE | burn: 0**



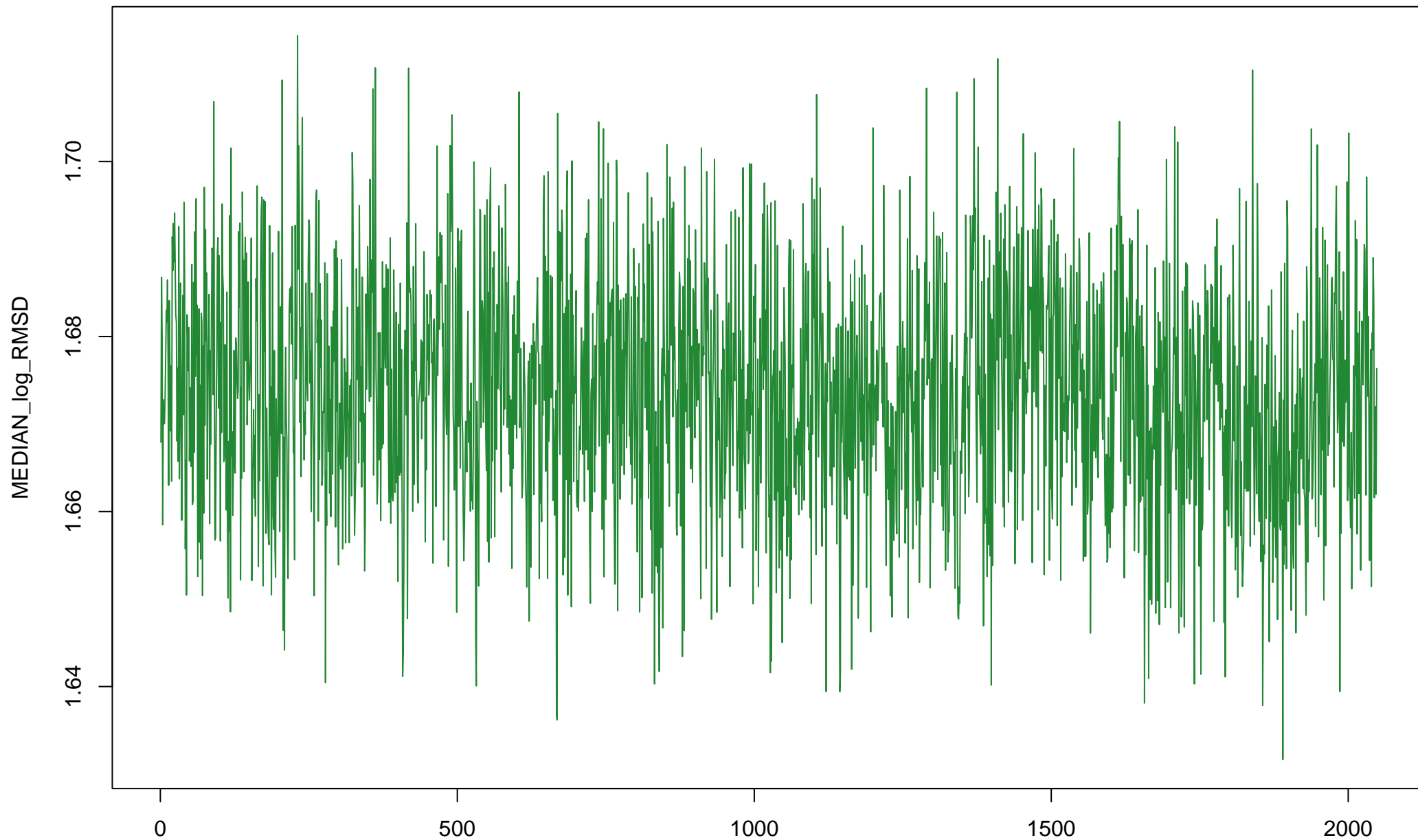
**Pdatum7**  
**ESS = 2.22e-16 | BMK = 0.0451 | MCSE(6.27) = 5.37 | stat: TRUE | burn: 0**



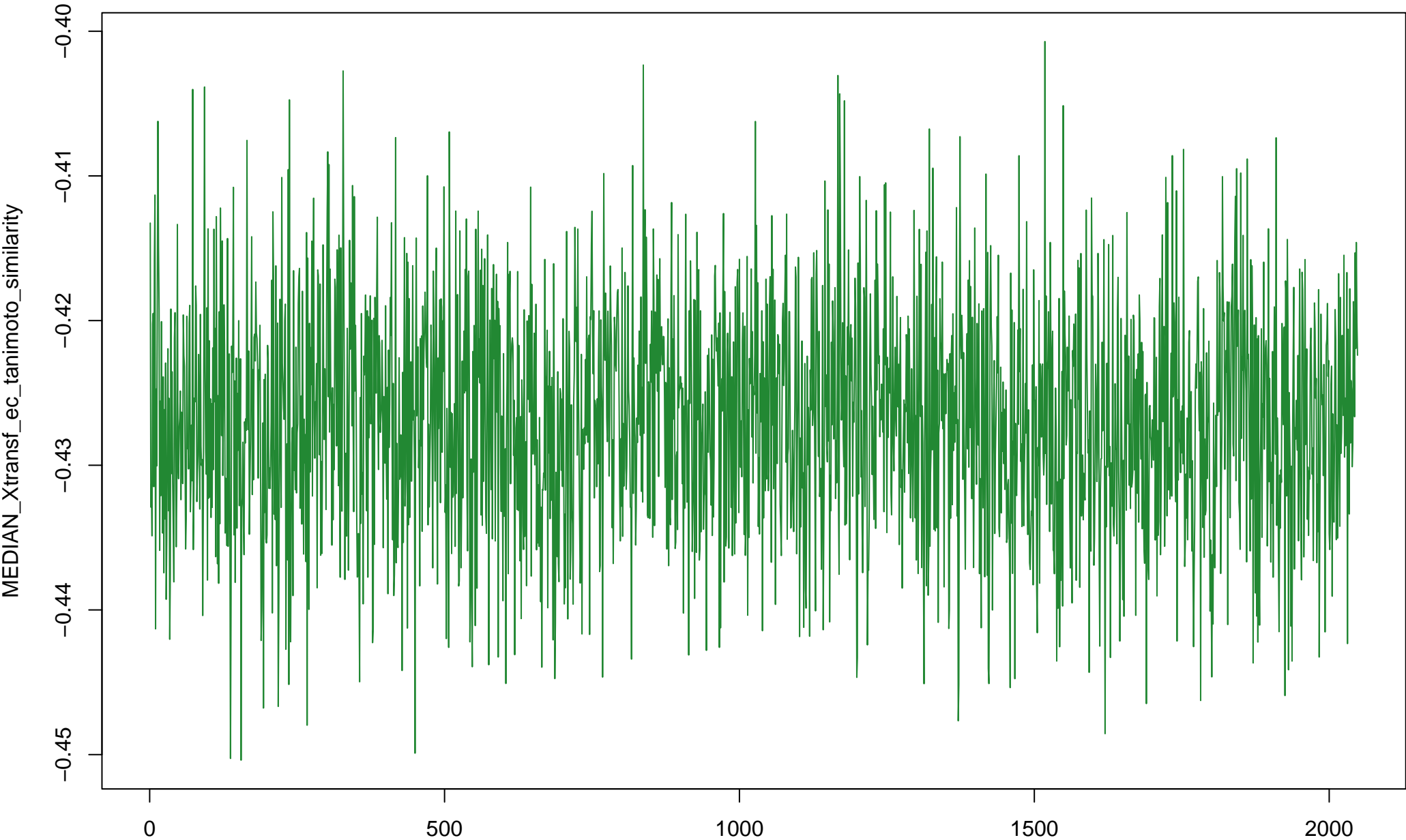
**Pdatum8**  
**ESS = 97.8 | BMK = 0.187 | MCSE(6.27) = 7.39 | stat: FALSE | burn: 0**



**MEDIAN\_log\_RMSD**  
**ESS = 1100 | BMK = 0.0611 | MCSE(6.27) = 3.82 | stat: TRUE | burn: 0**

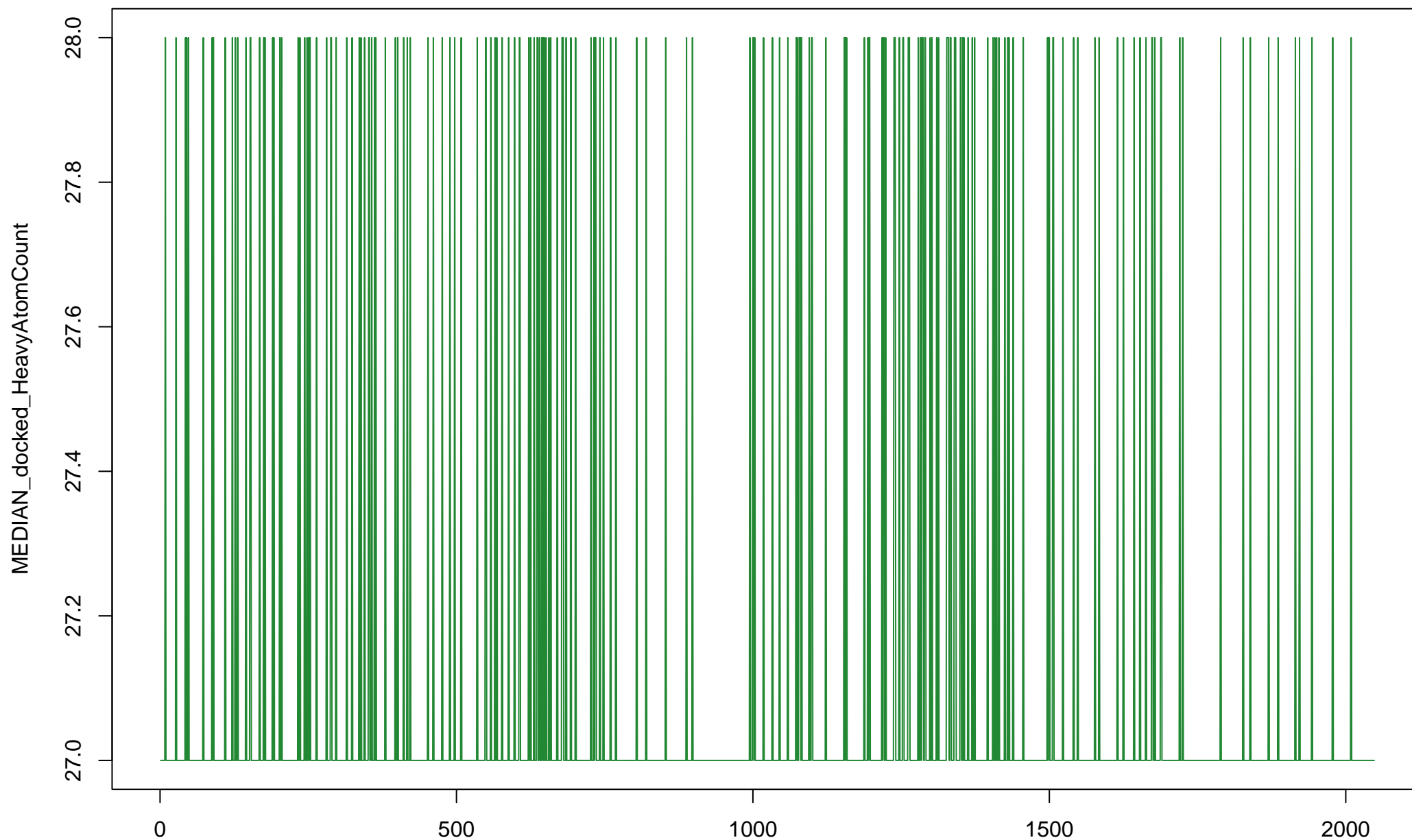


**MEDIAN\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0358 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0**

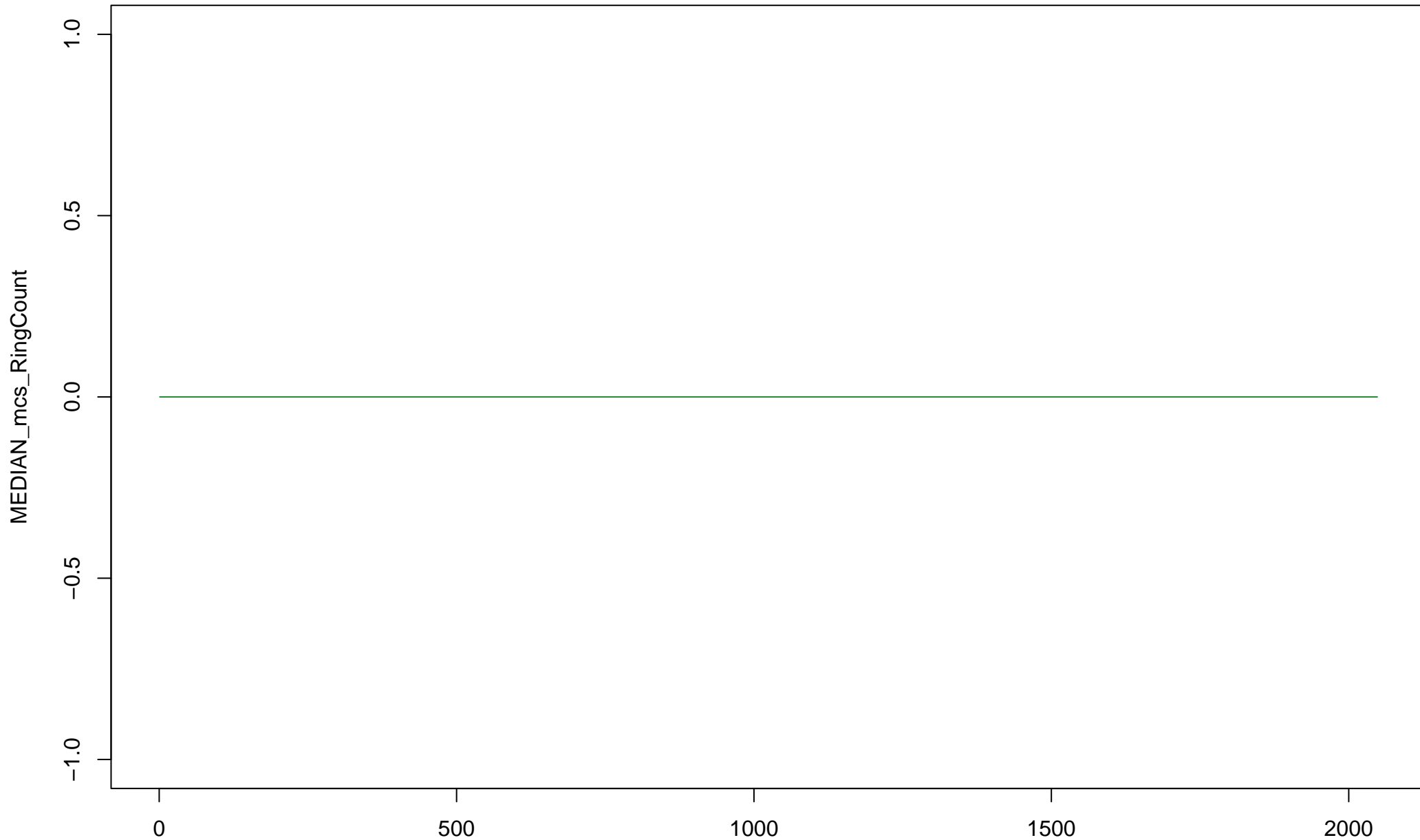




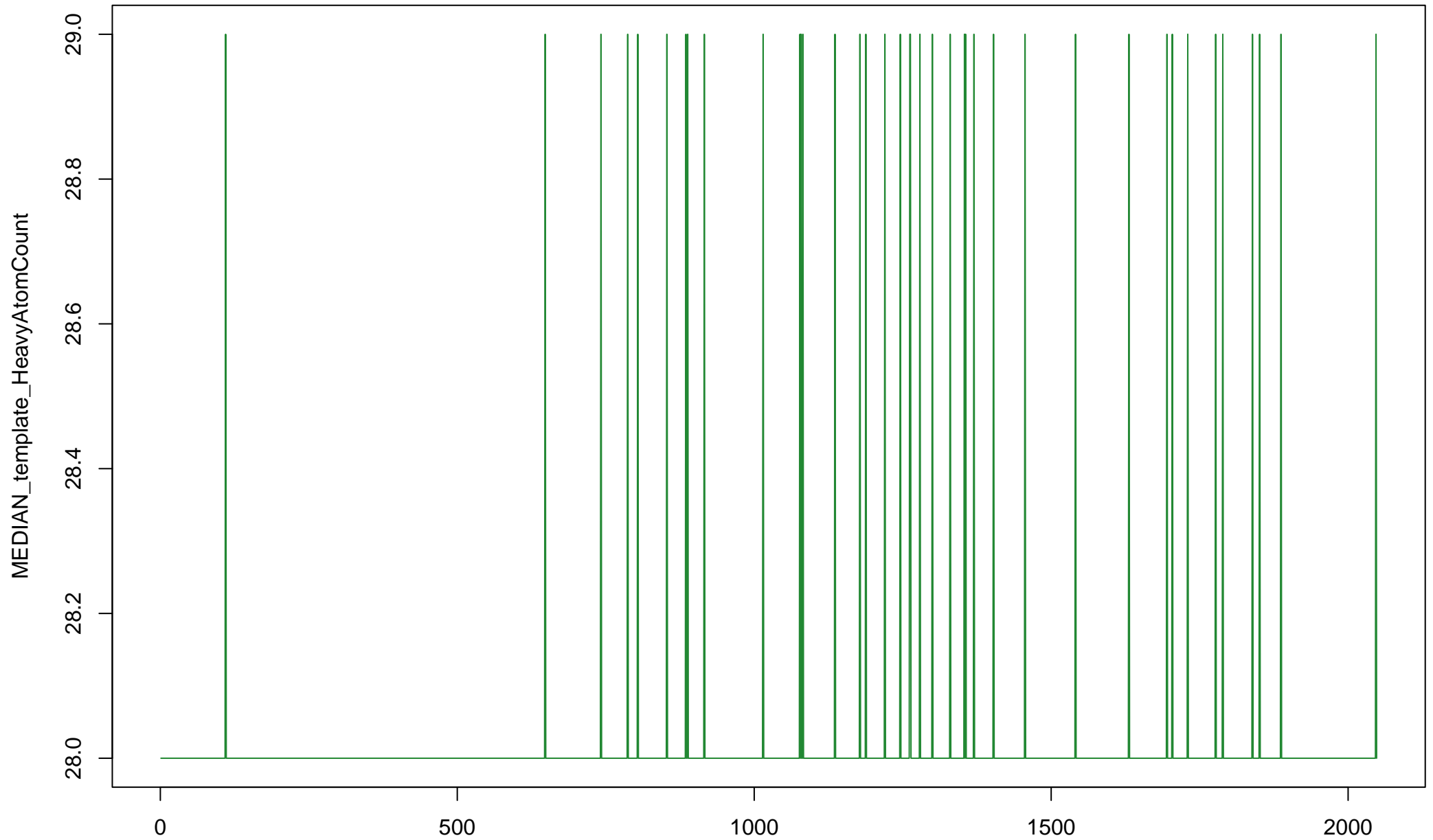
**MEDIAN\_docked\_HeavyAtomCount**  
**ESS = 975 | BMK = 0.00174 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0**



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



**MEDIAN\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.182 | MCSE(6.27) = 2.29 | stat: FALSE | burn: 204**



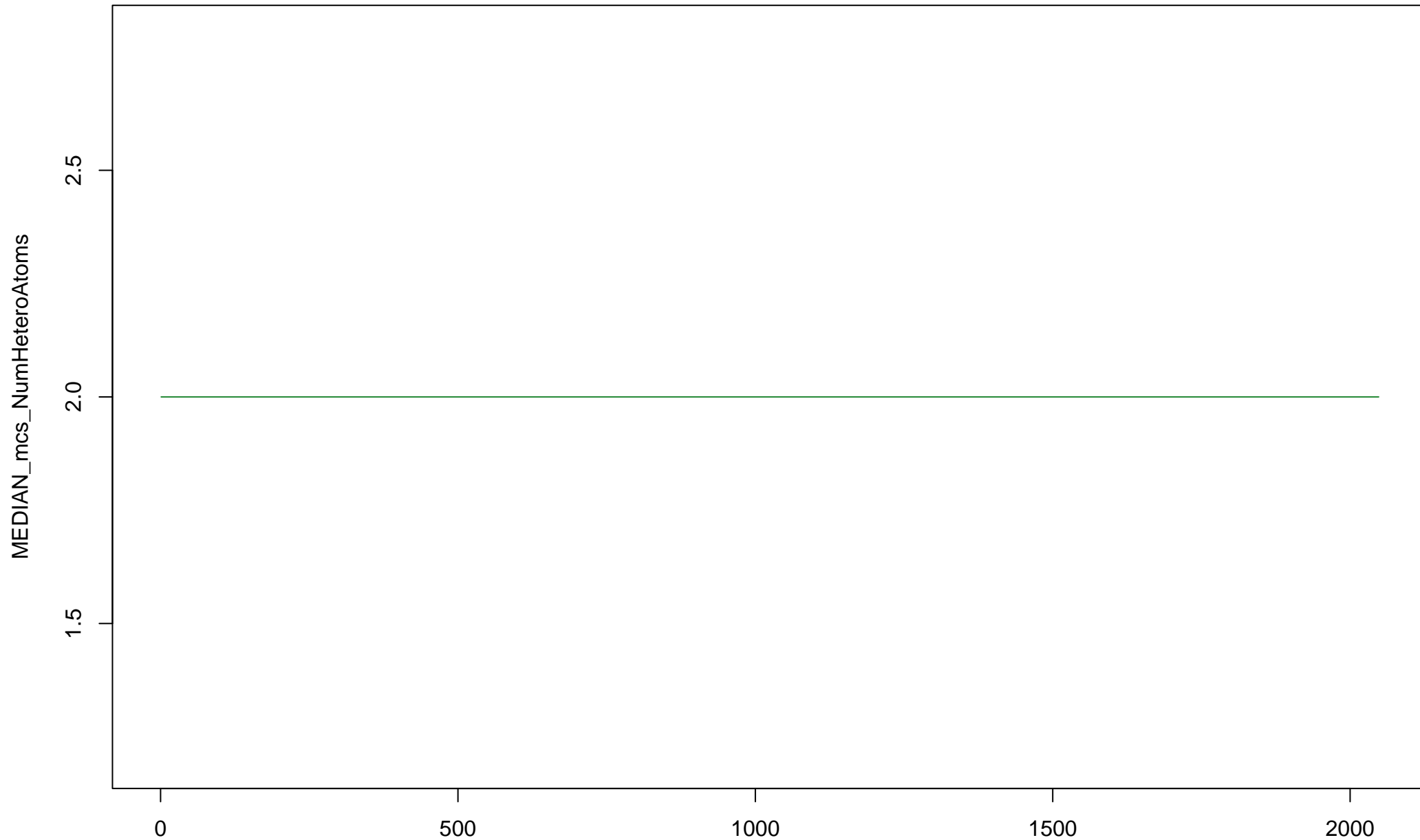
**MEDIAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



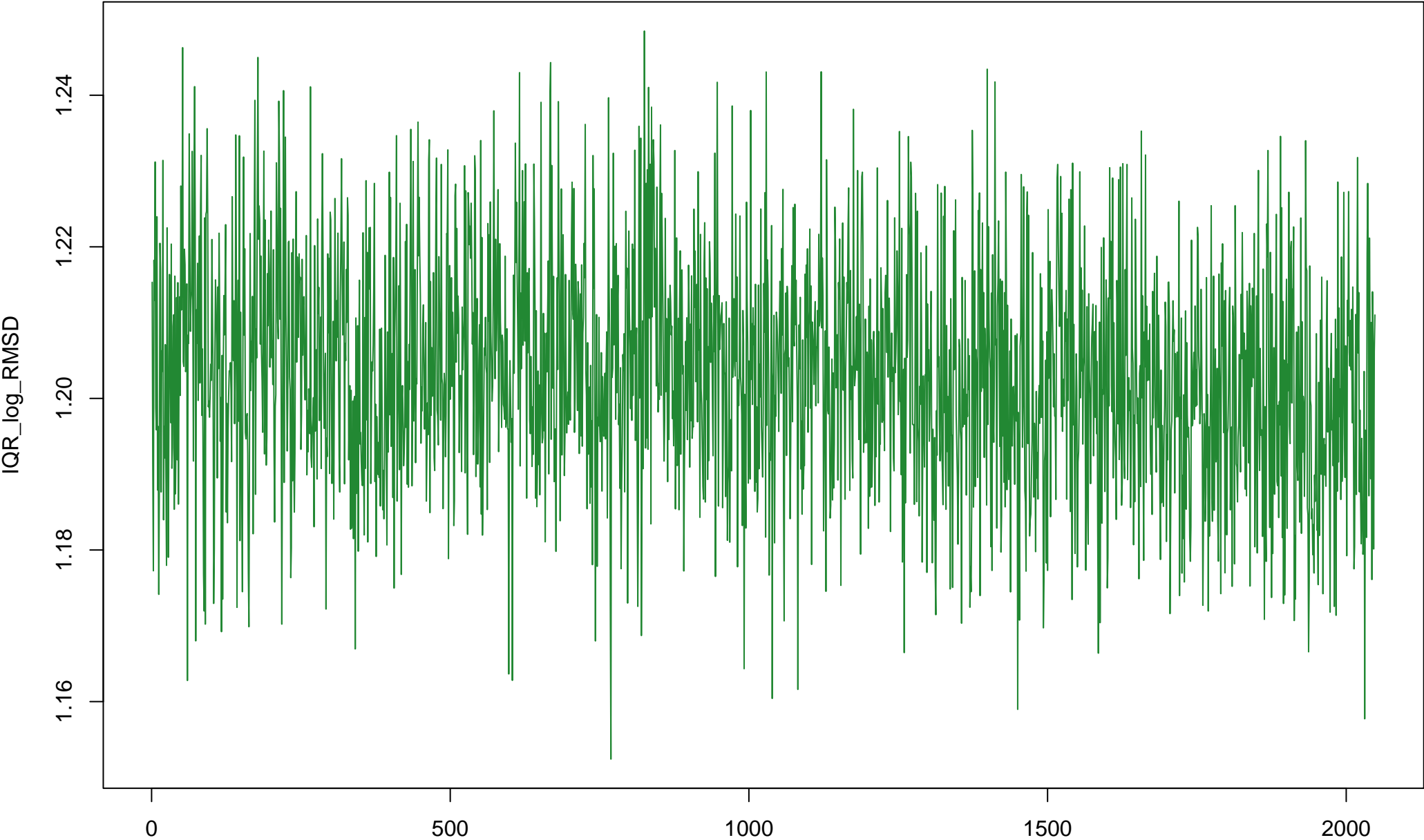
**MEDIAN\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



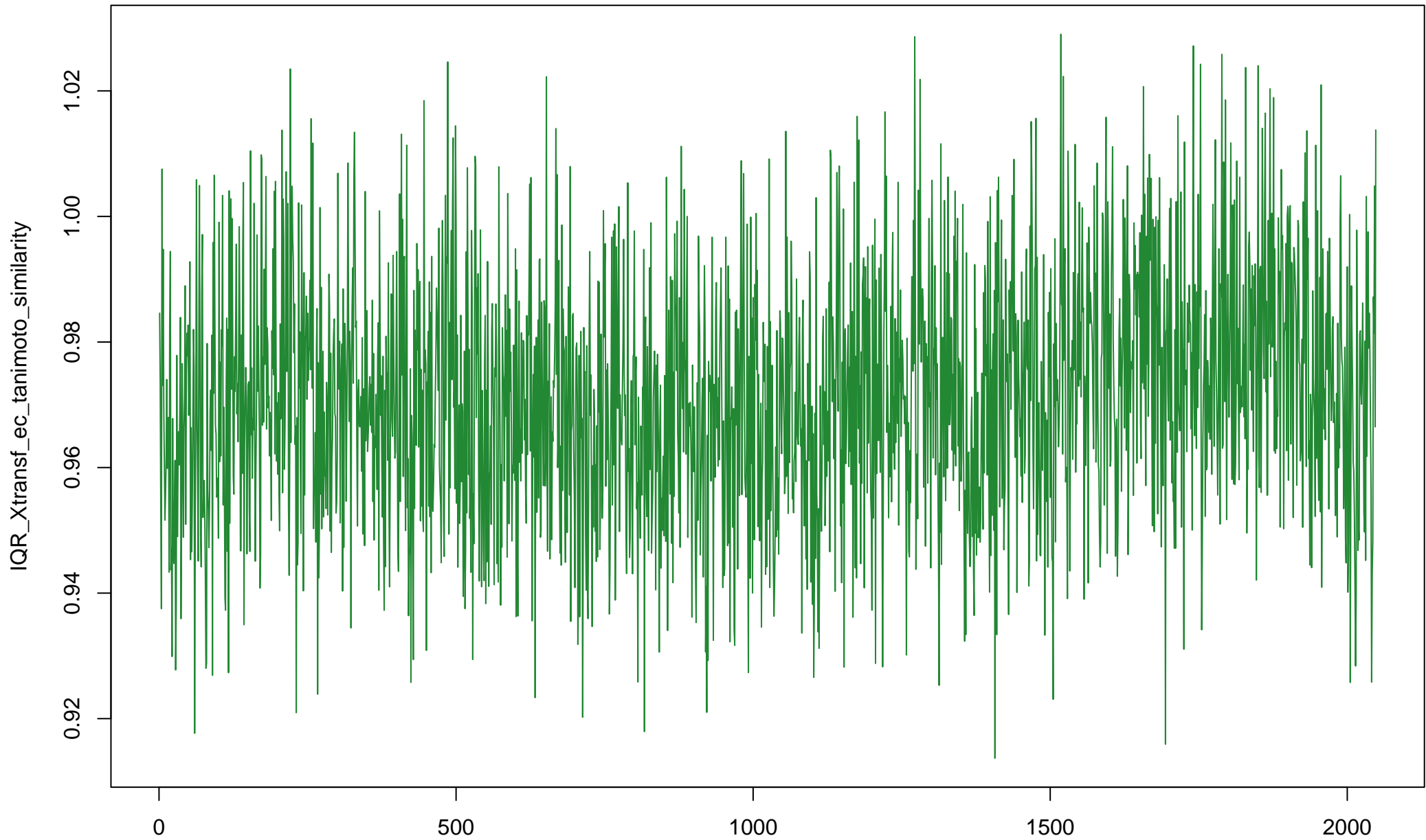
**MEDIAN\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



IQR\_log\_RMSD  
ESS = 947 | BMK = 0.107 | MCSE(6.27) = 3.63 | stat: FALSE | burn: 0

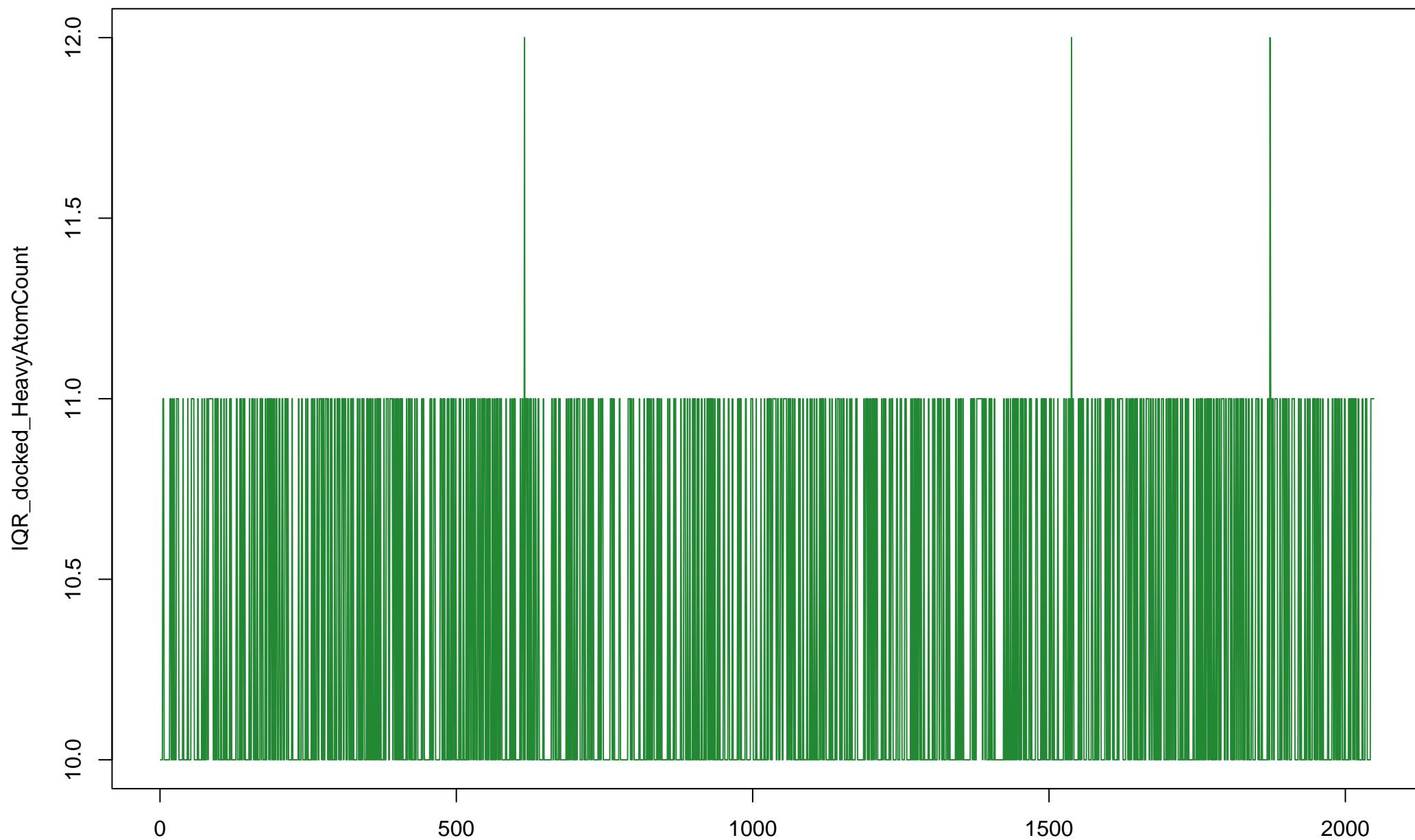


IQR\_Xtransf\_ec\_tanimoto\_similarity  
ESS = 464 | BMK = 0.0972 | MCSE(6.27) = 4.24 | stat: FALSE | burn: 0

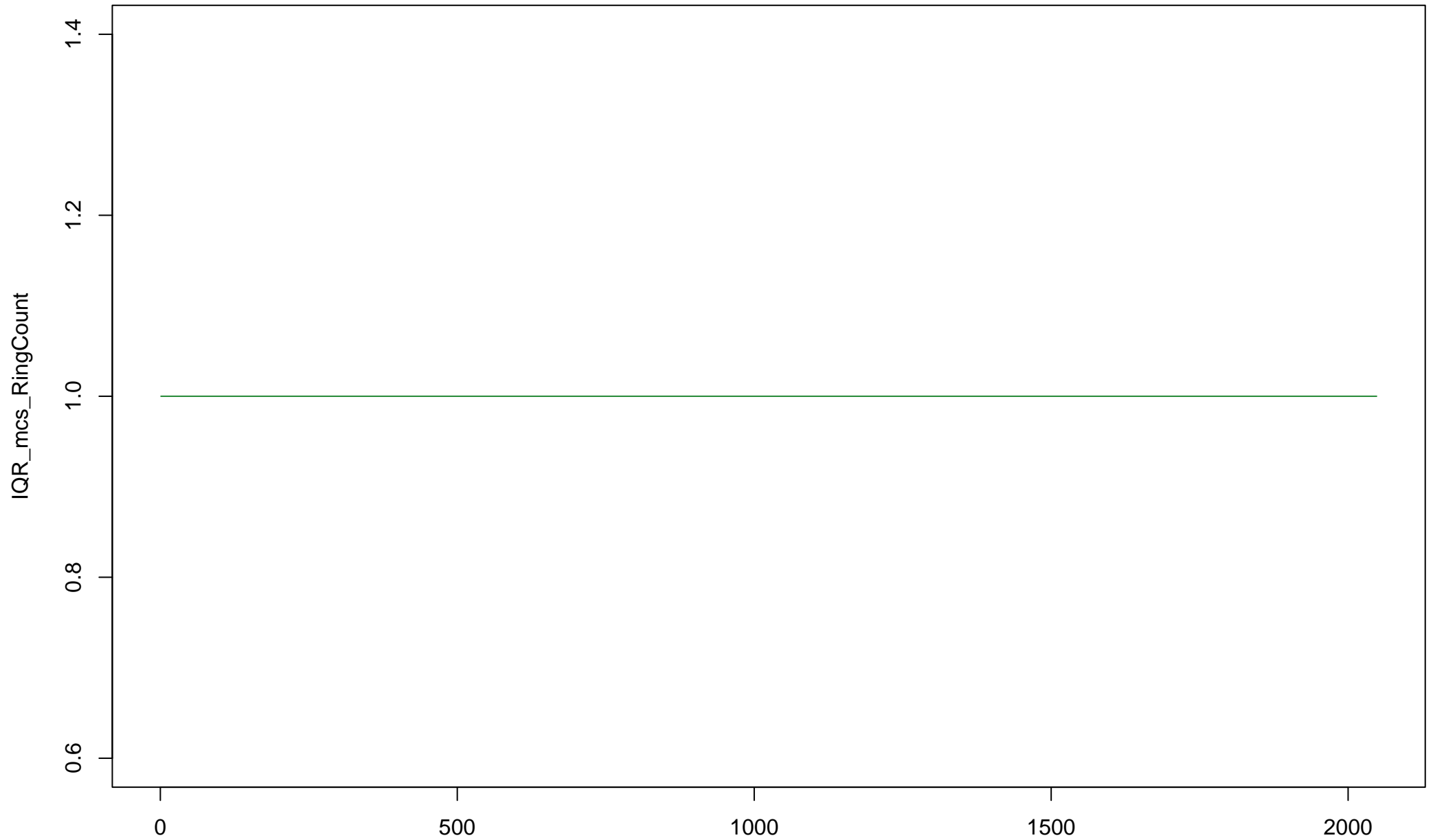




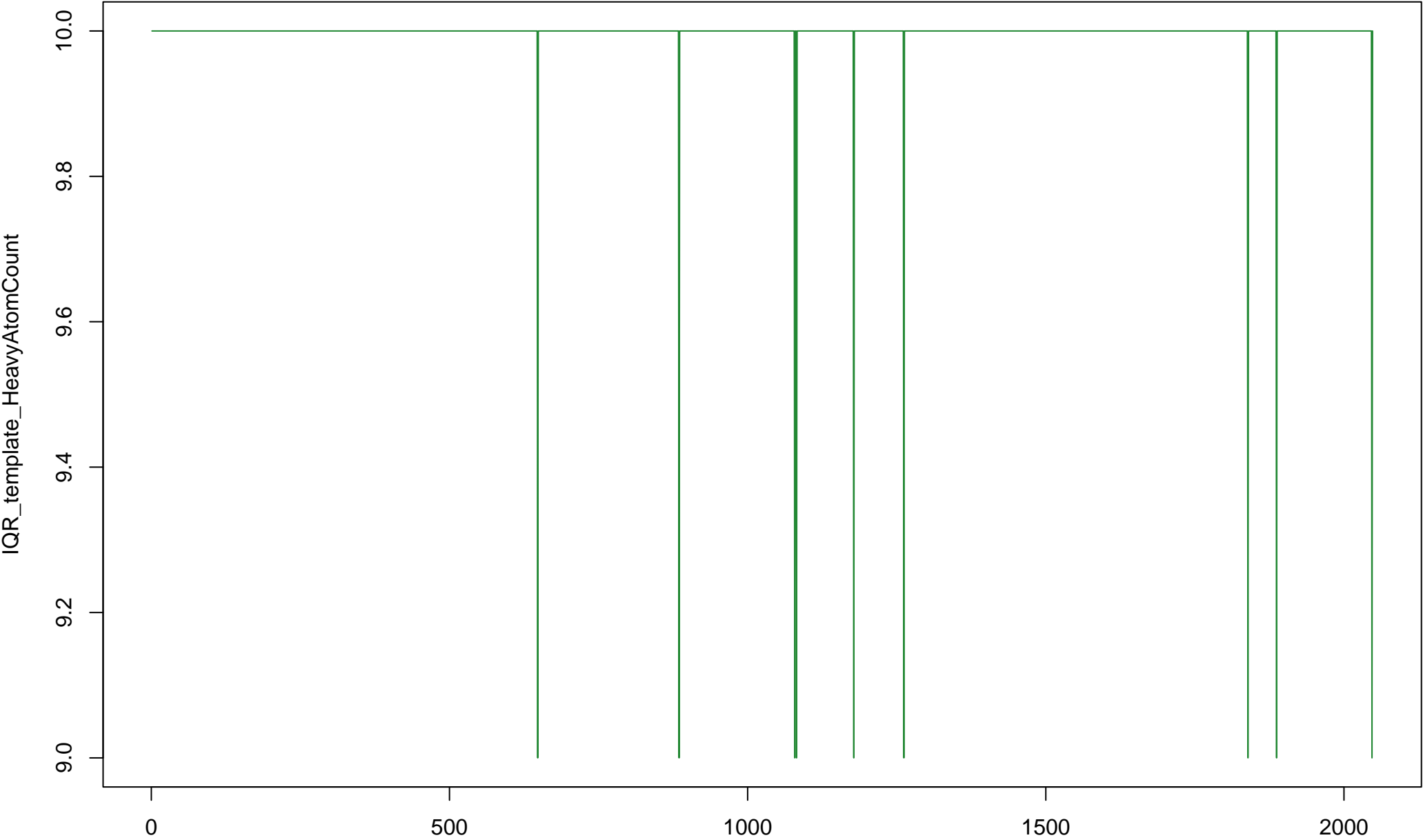
IQR\_docked\_HeavyAtomCount  
ESS = 1920 | BMK = 0.0362 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0



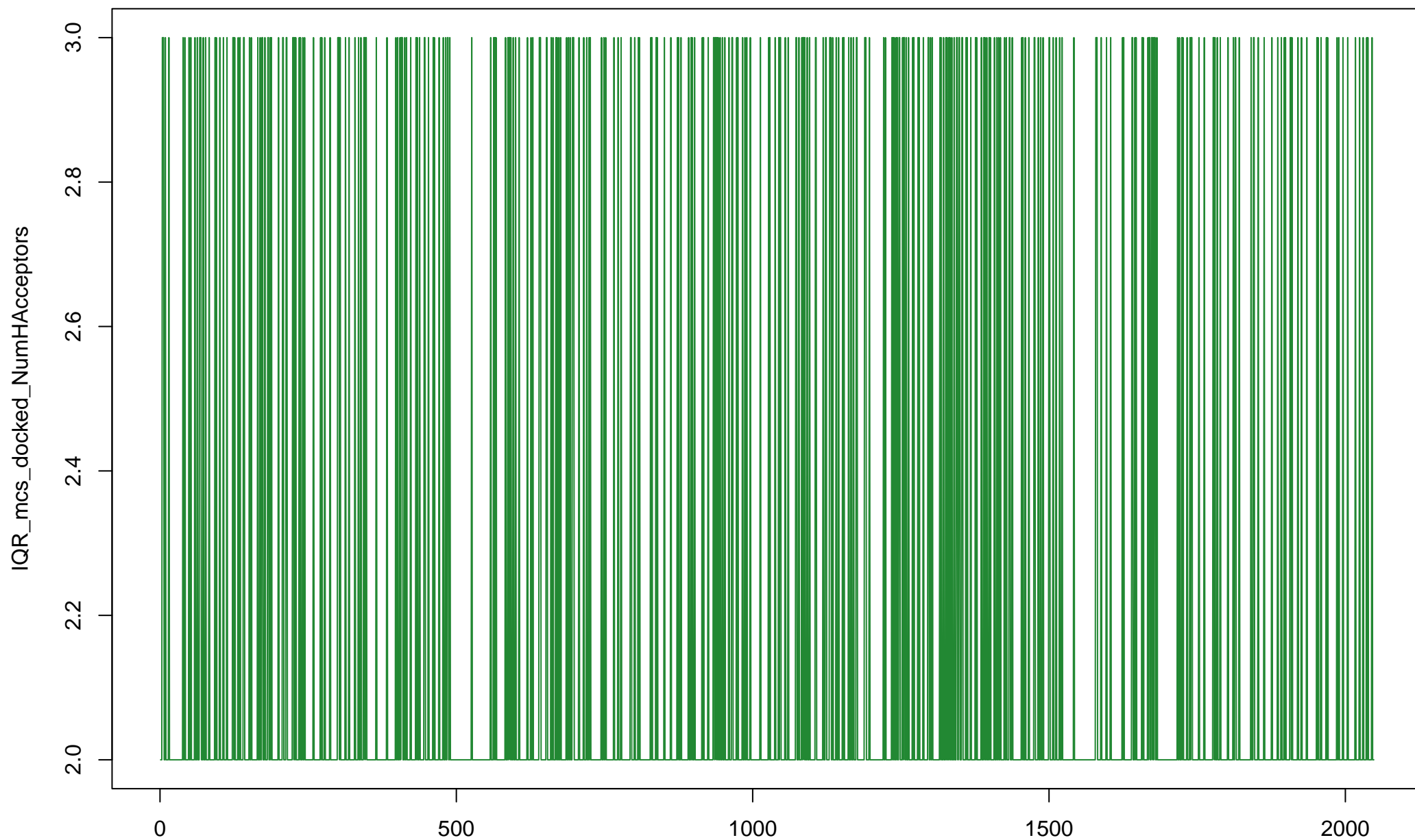
**IQR\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



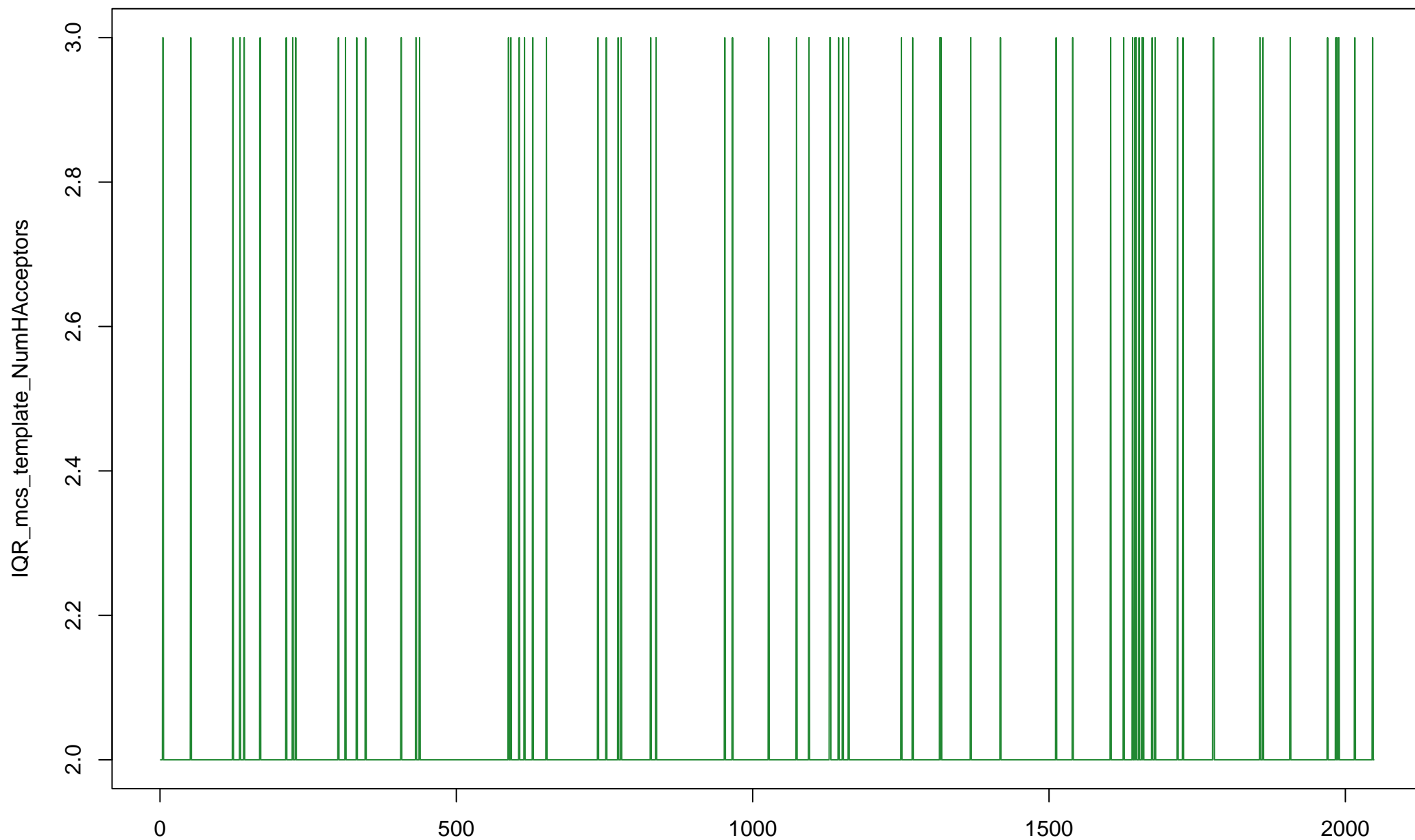
IQR\_template\_HeavyAtomCount  
ESS = 1680 | BMK = 0.211 | MCSE(6.27) = 1.93 | stat: FALSE | burn: 1428



**IQR\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.00692 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0**



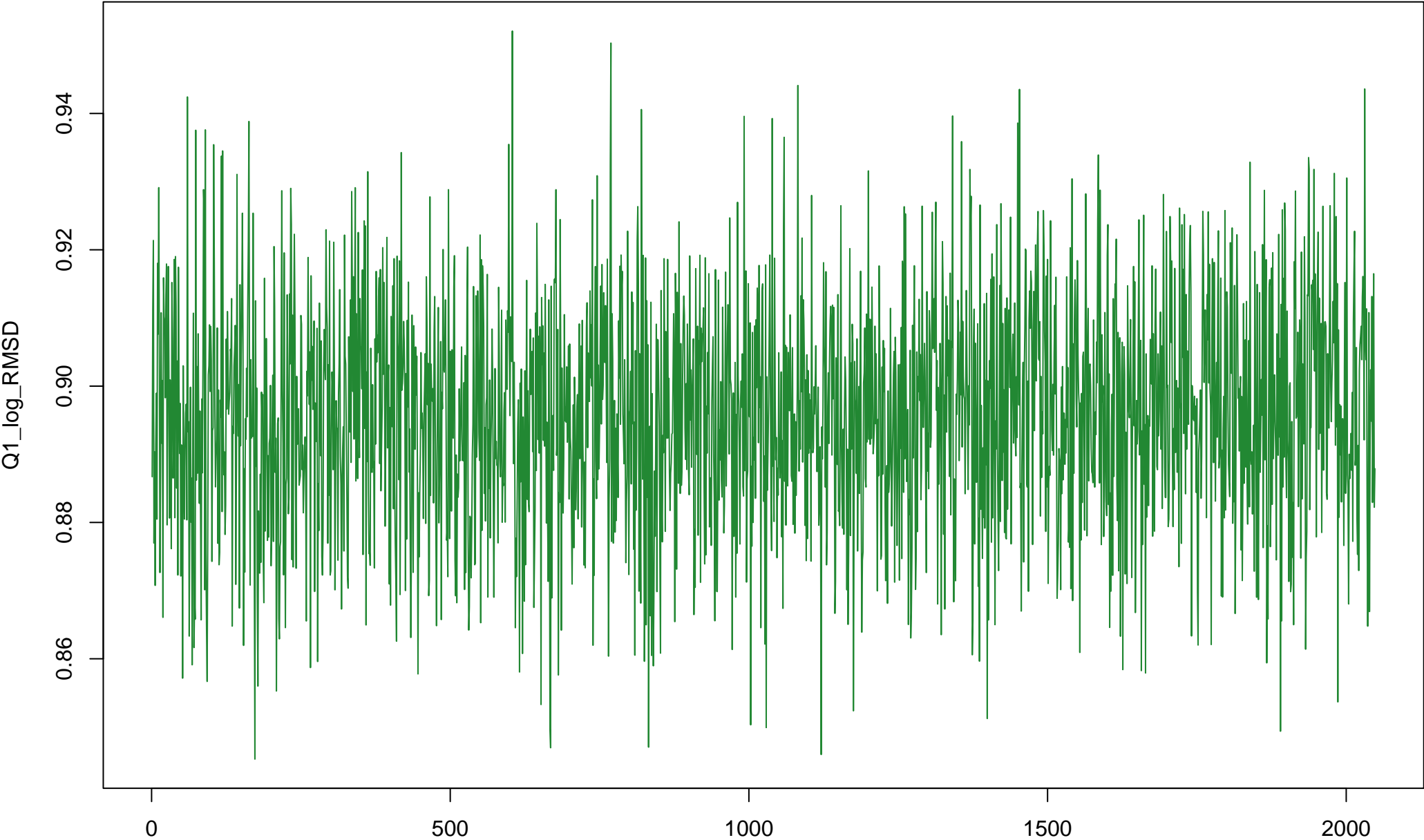
**IQR\_mcs\_template\_NumHAcceptors**  
**ESS = 1780 | BMK = 0.0464 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0**



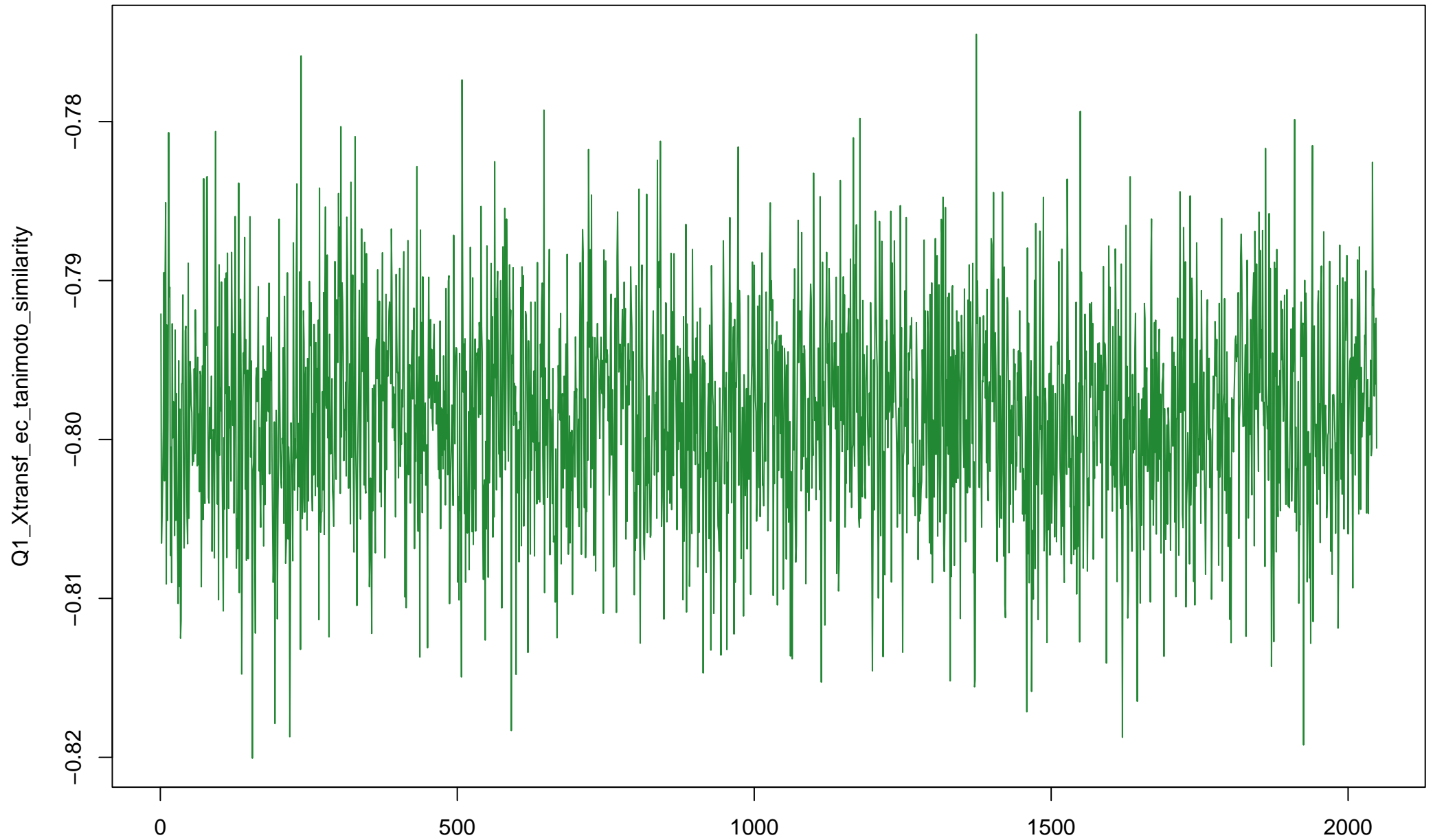
IQR\_mcs\_NumHeteroAtoms  
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



**Q1\_log\_RMSD**  
**ESS = 1740 | BMK = 0.0544 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0**

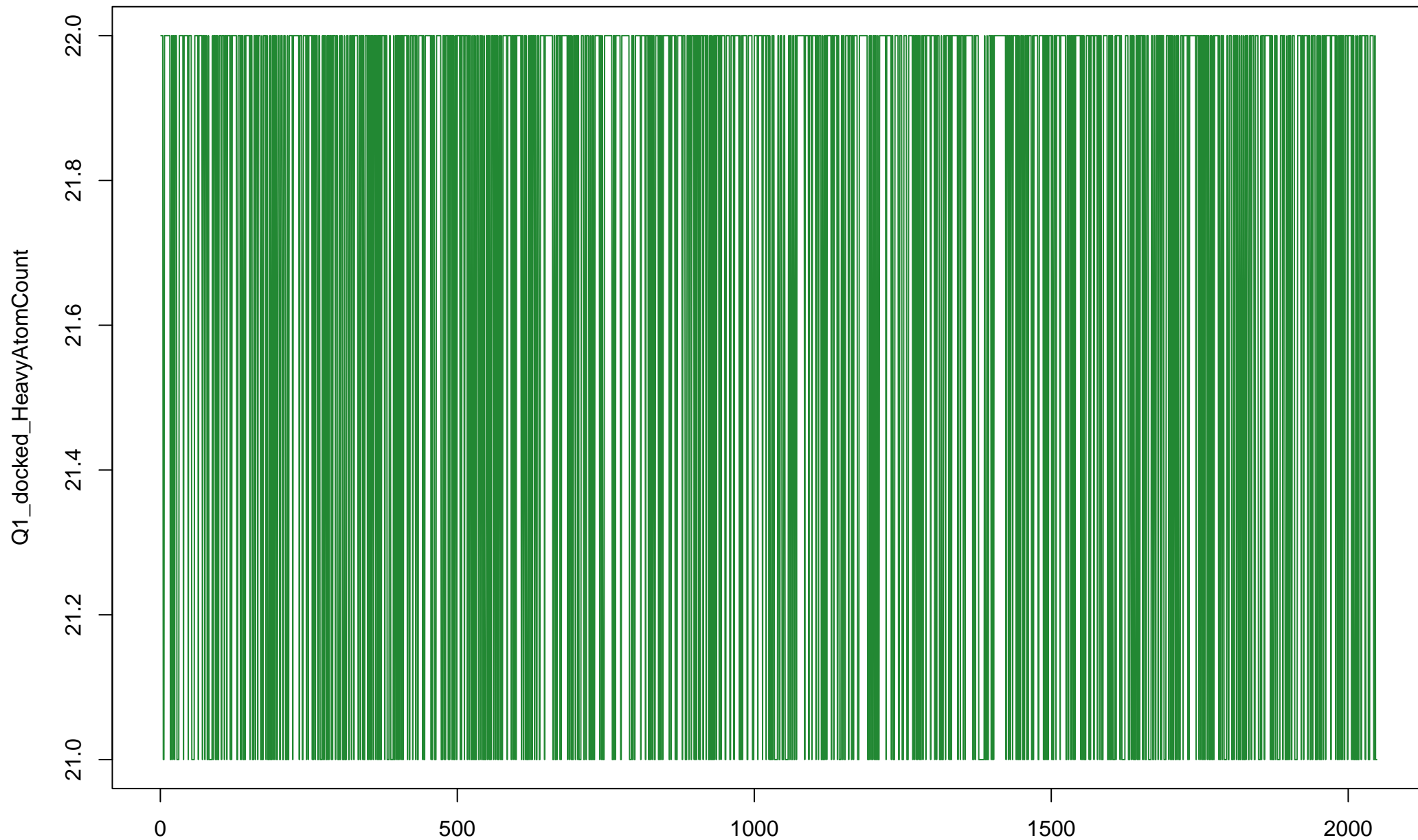


**Q1\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0284 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0**





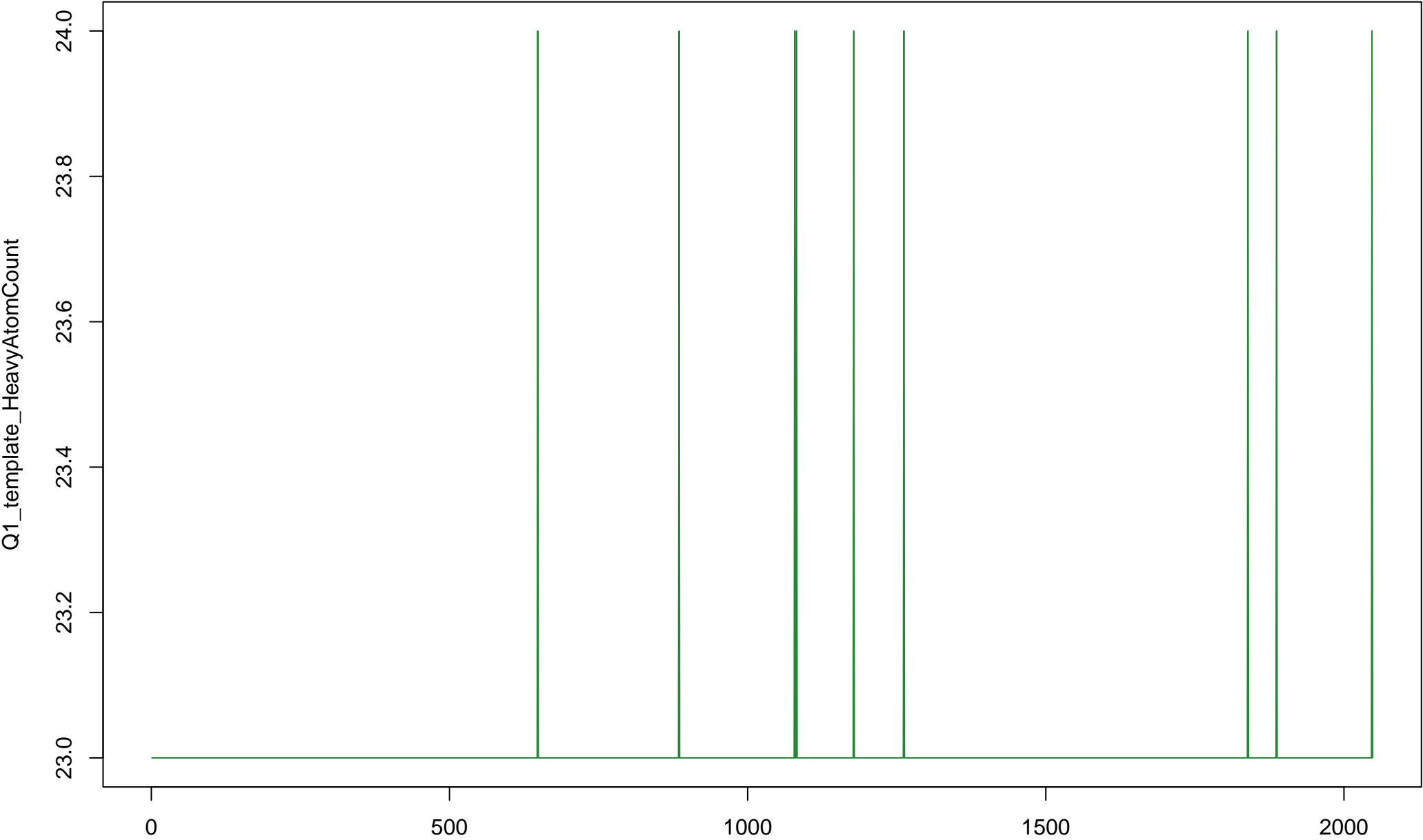
**Q1\_docked\_HeavyAtomCount**  
**ESS = 1900 | BMK = 0.0156 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0**



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



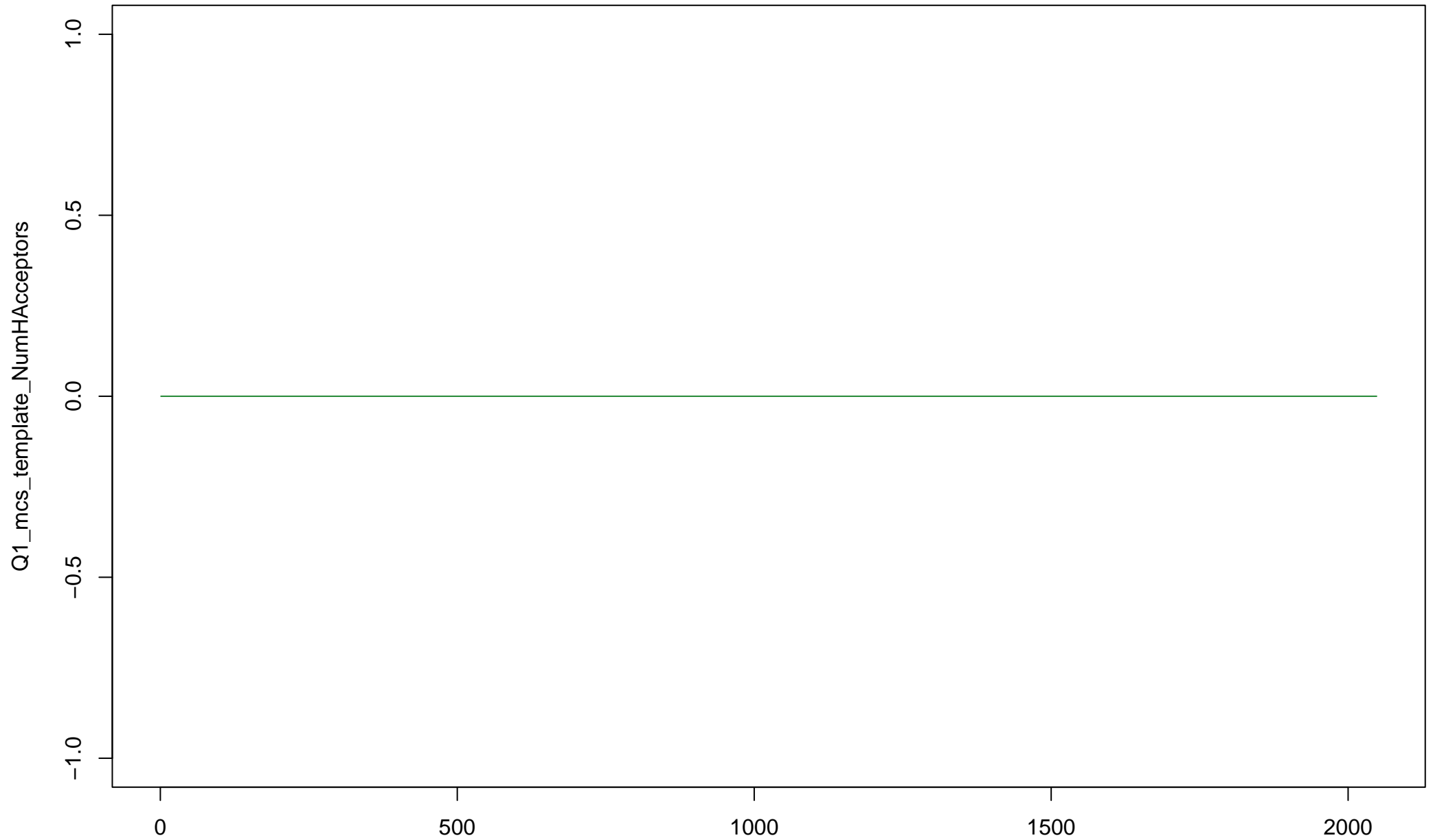
Q1\_template\_HeavyAtomCount  
ESS = 1680 | BMK = 0.211 | MCSE(6.27) = 1.93 | stat: FALSE | burn: 1428



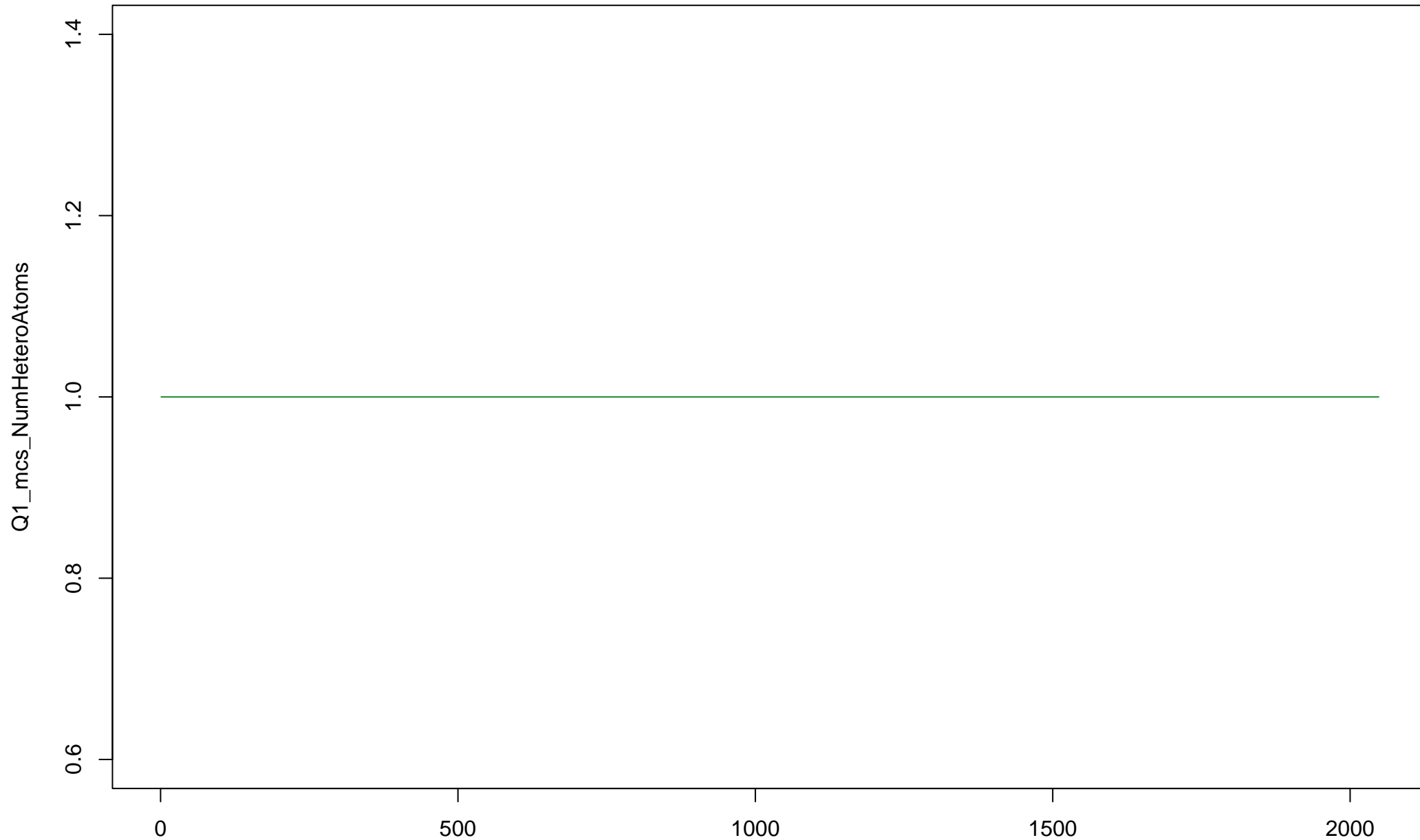
**Q1\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



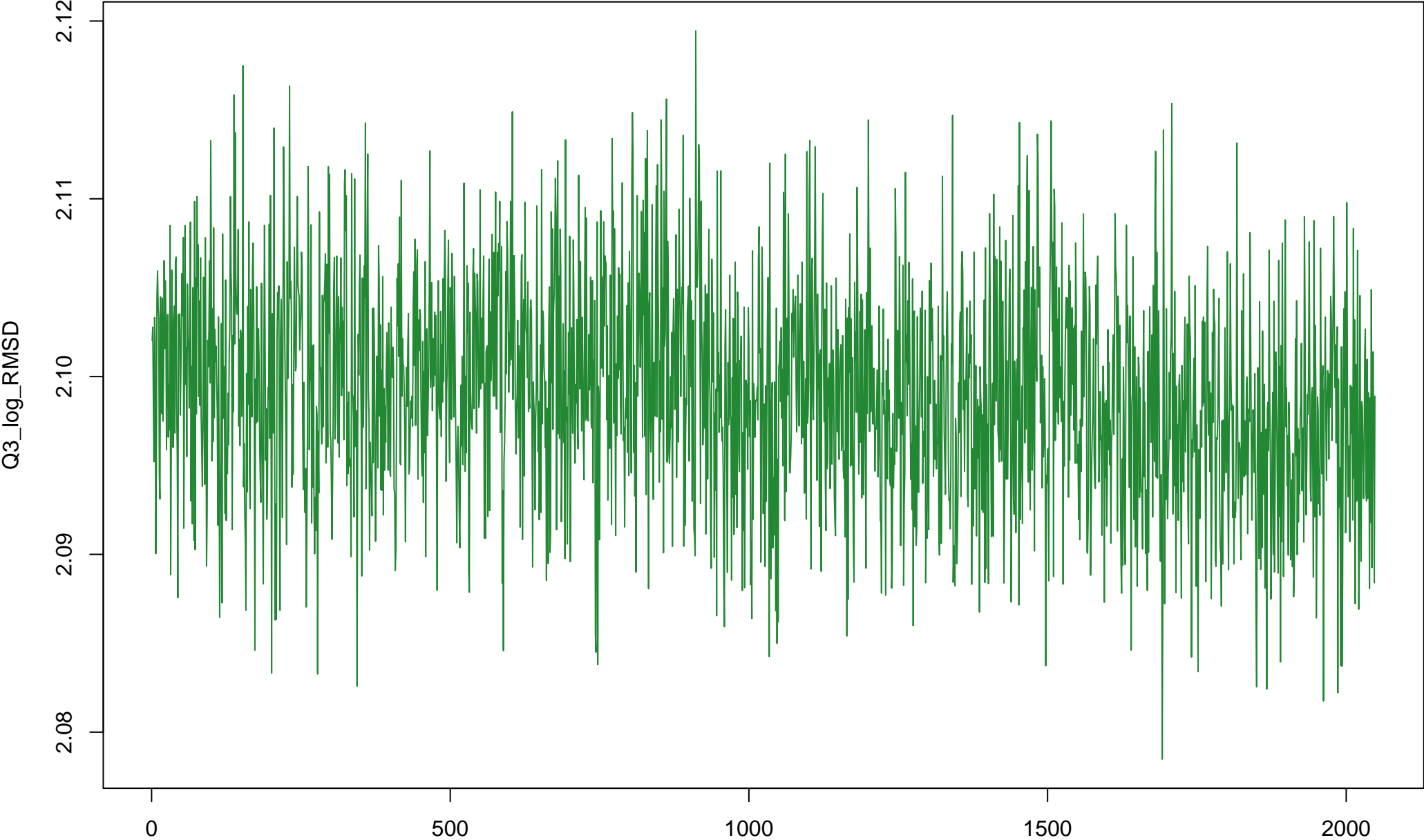
**Q1\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



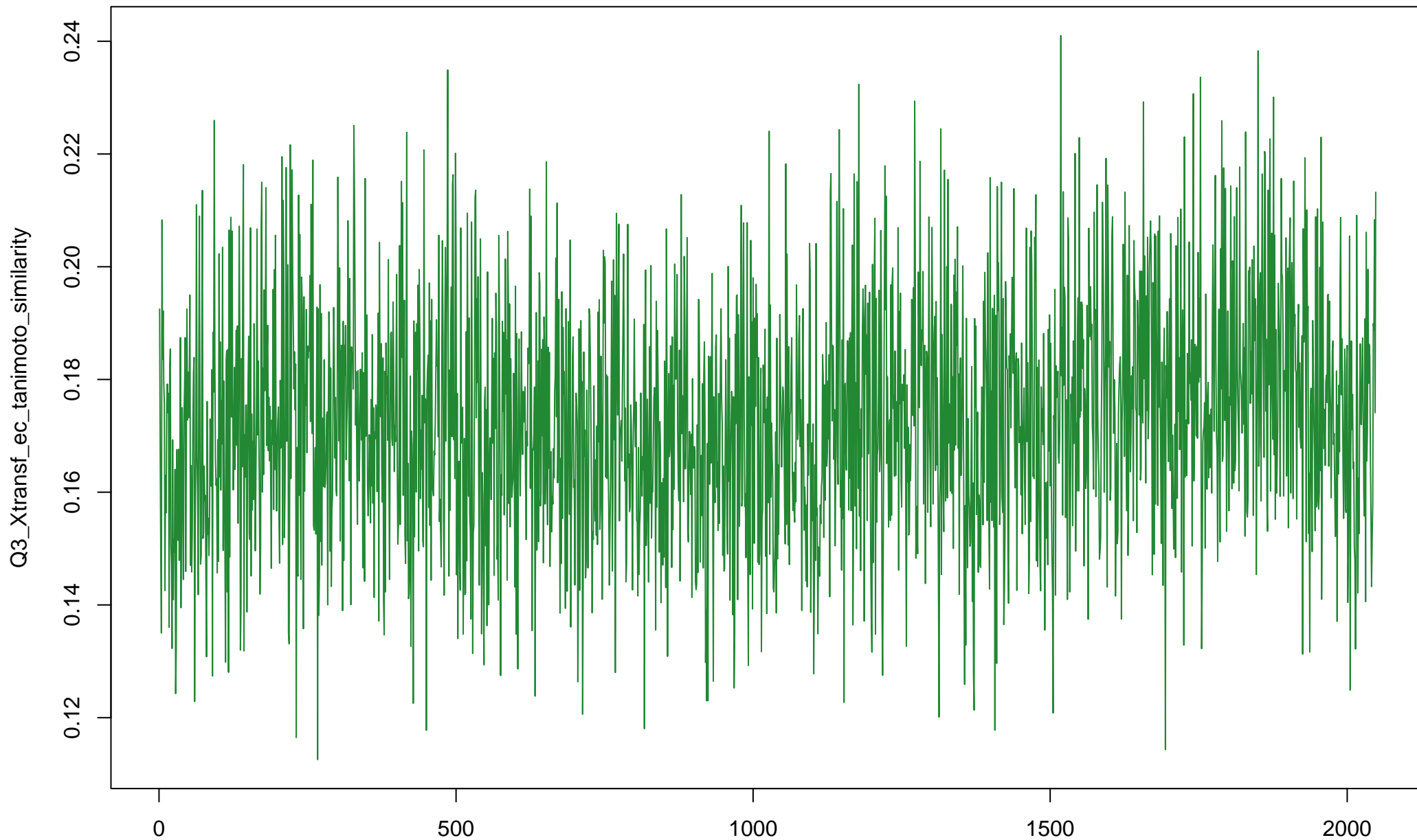
**Q1\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q3\_log\_RMSD**  
**ESS = 933 | BMK = 0.133 | MCSE(6.27) = 4.27 | stat: FALSE | burn: 0**

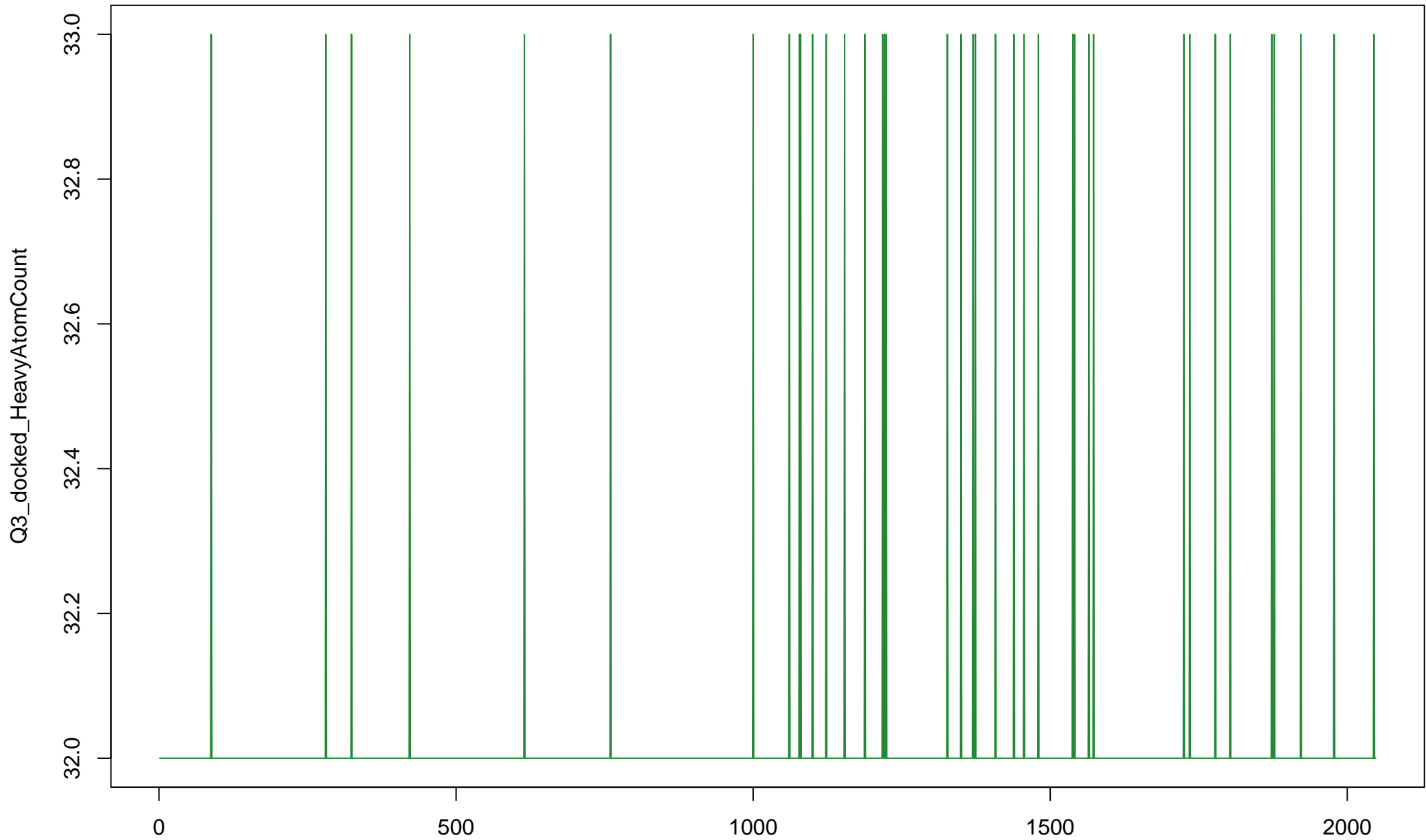


**Q3\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 629 | BMK = 0.0885 | MCSE(6.27) = 3.87 | stat: FALSE | burn: 0**





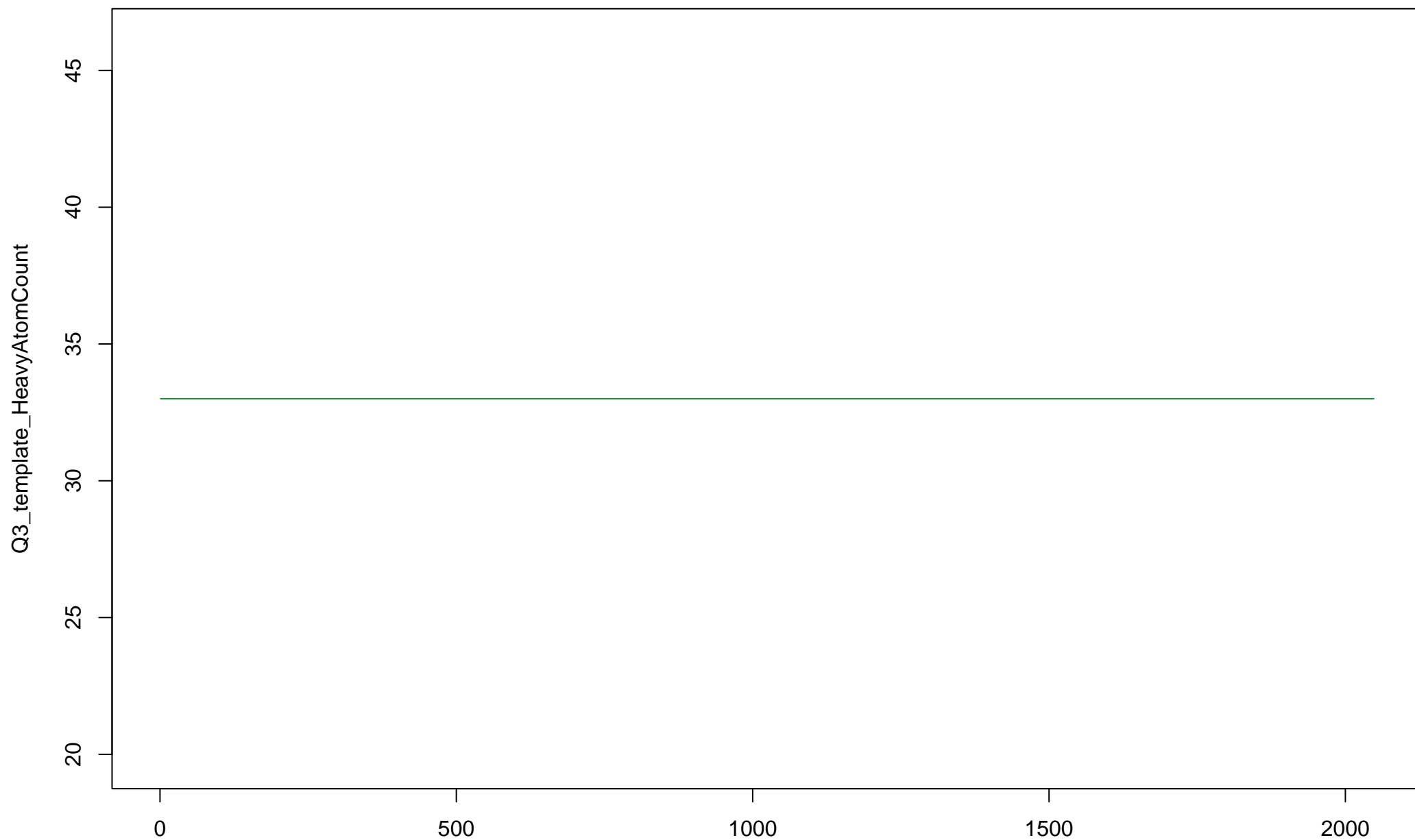
**Q3\_docked\_HeavyAtomCount**  
**ESS = 1710 | BMK = 0.246 | MCSE(6.27) = 2.46 | stat: FALSE | burn: 0**



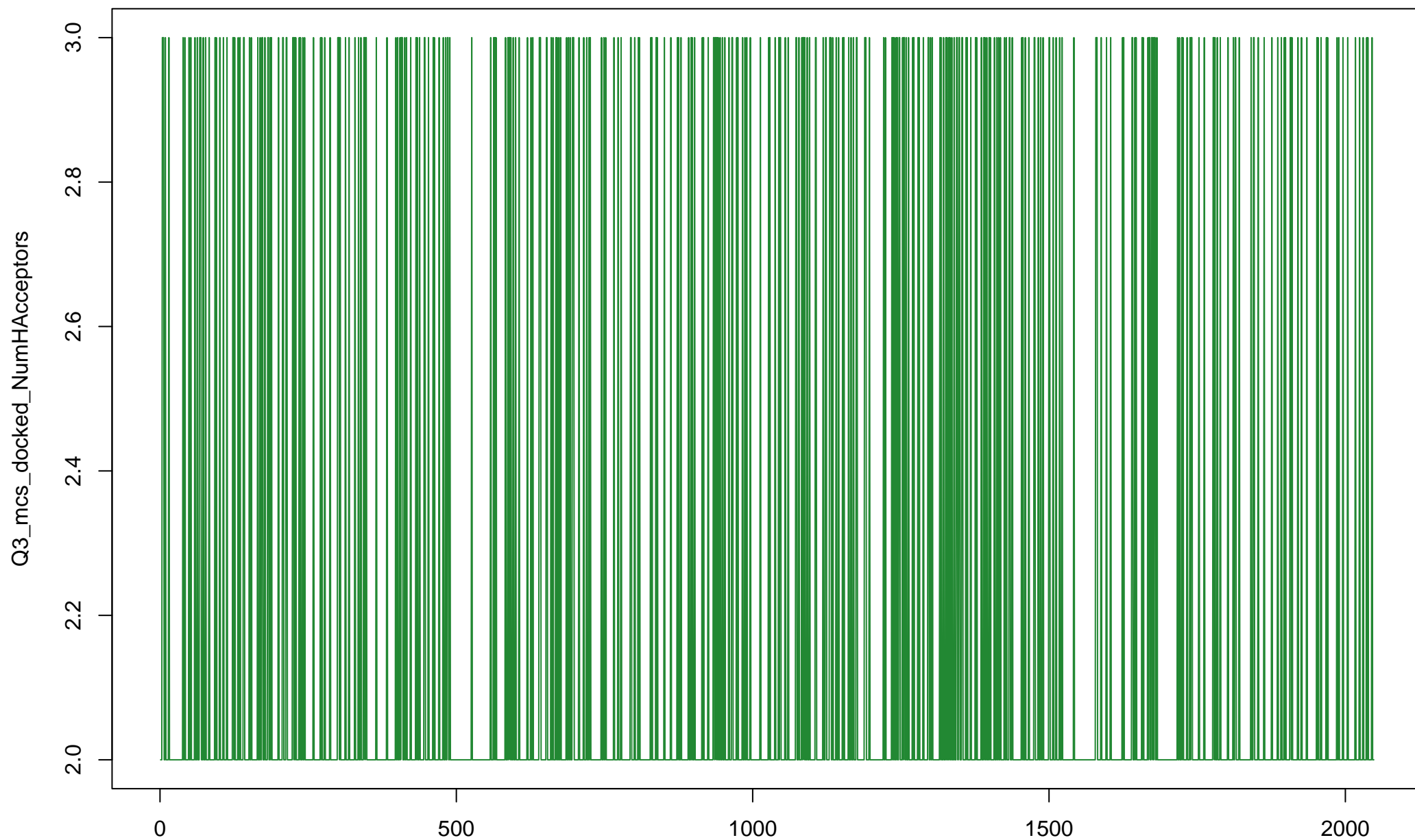
**Q3\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



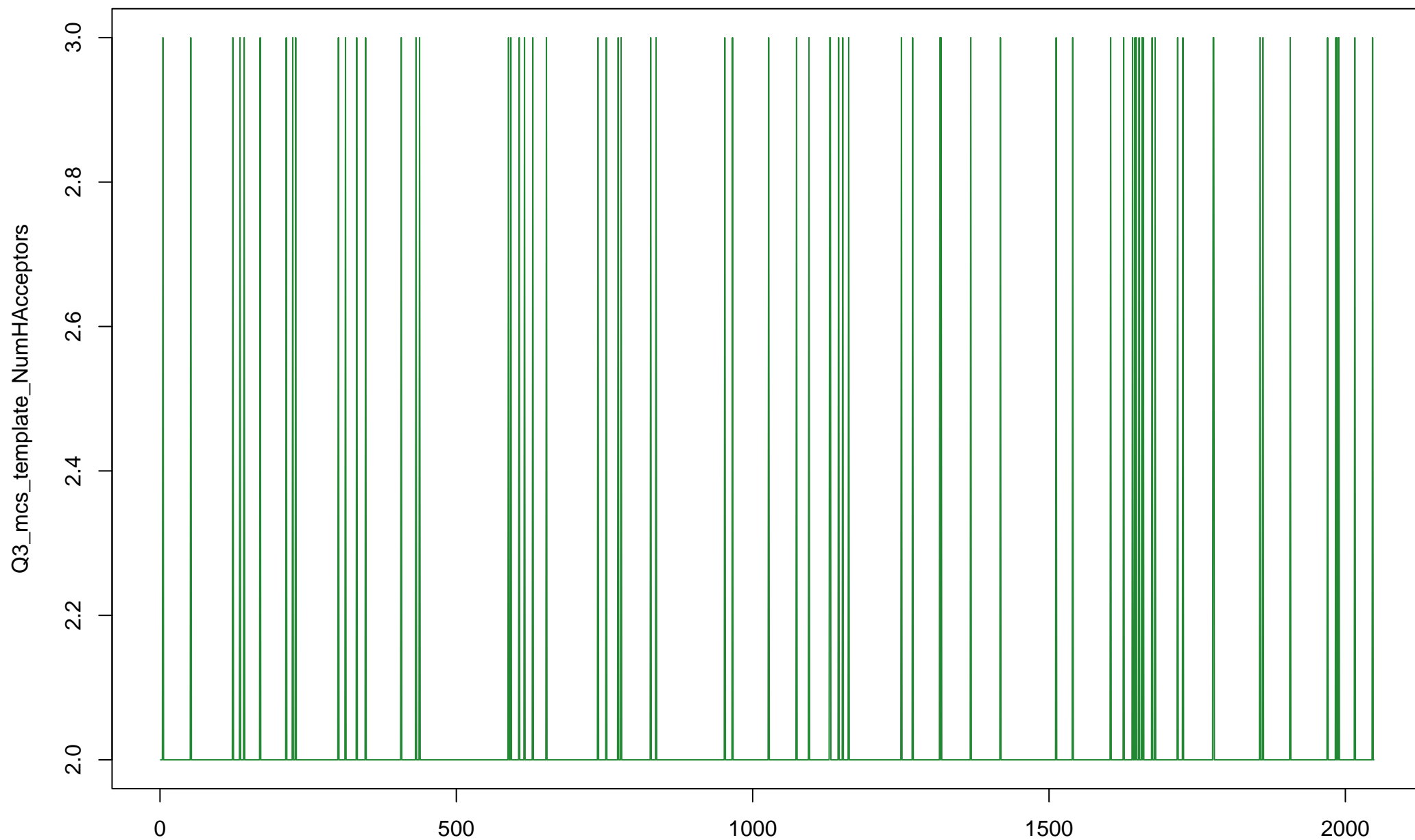
**Q3\_template\_HeavyAtomCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q3\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.00692 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0**



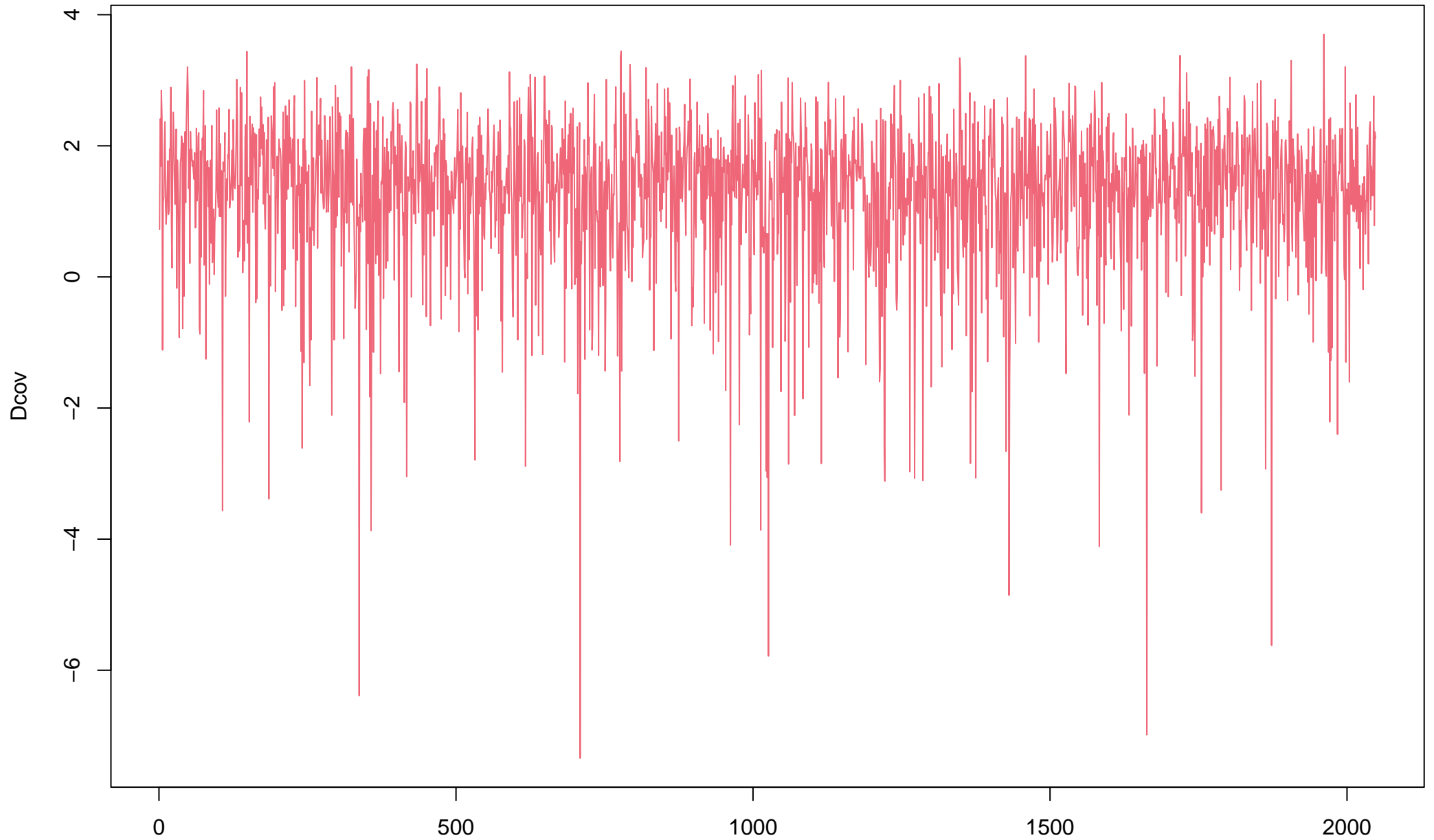
**Q3\_mcs\_template\_NumHAcceptors**  
**ESS = 1780 | BMK = 0.0464 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0**



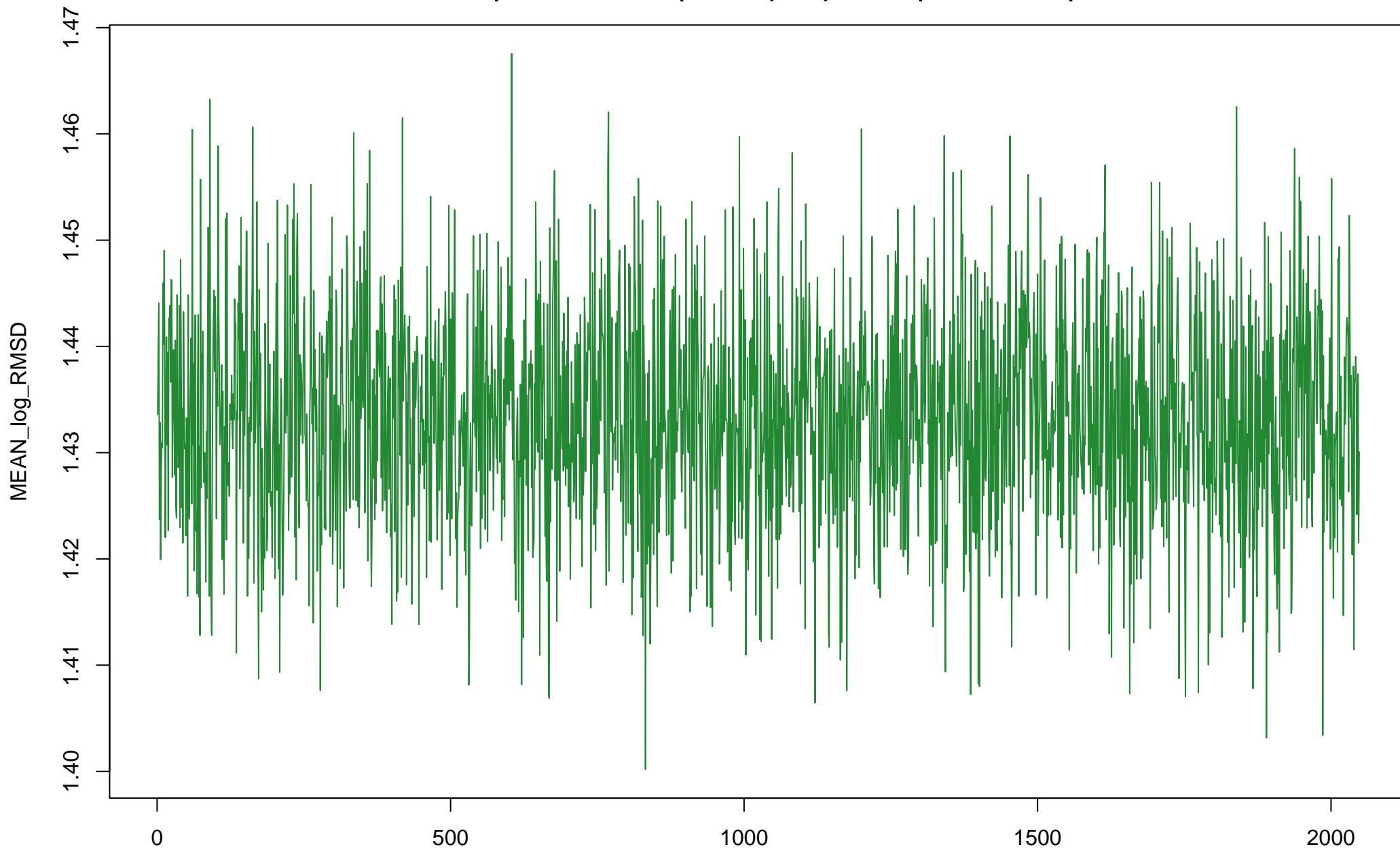
**Q3\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Dcov**  
**ESS = 1870 | BMK = 0.0742 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0**

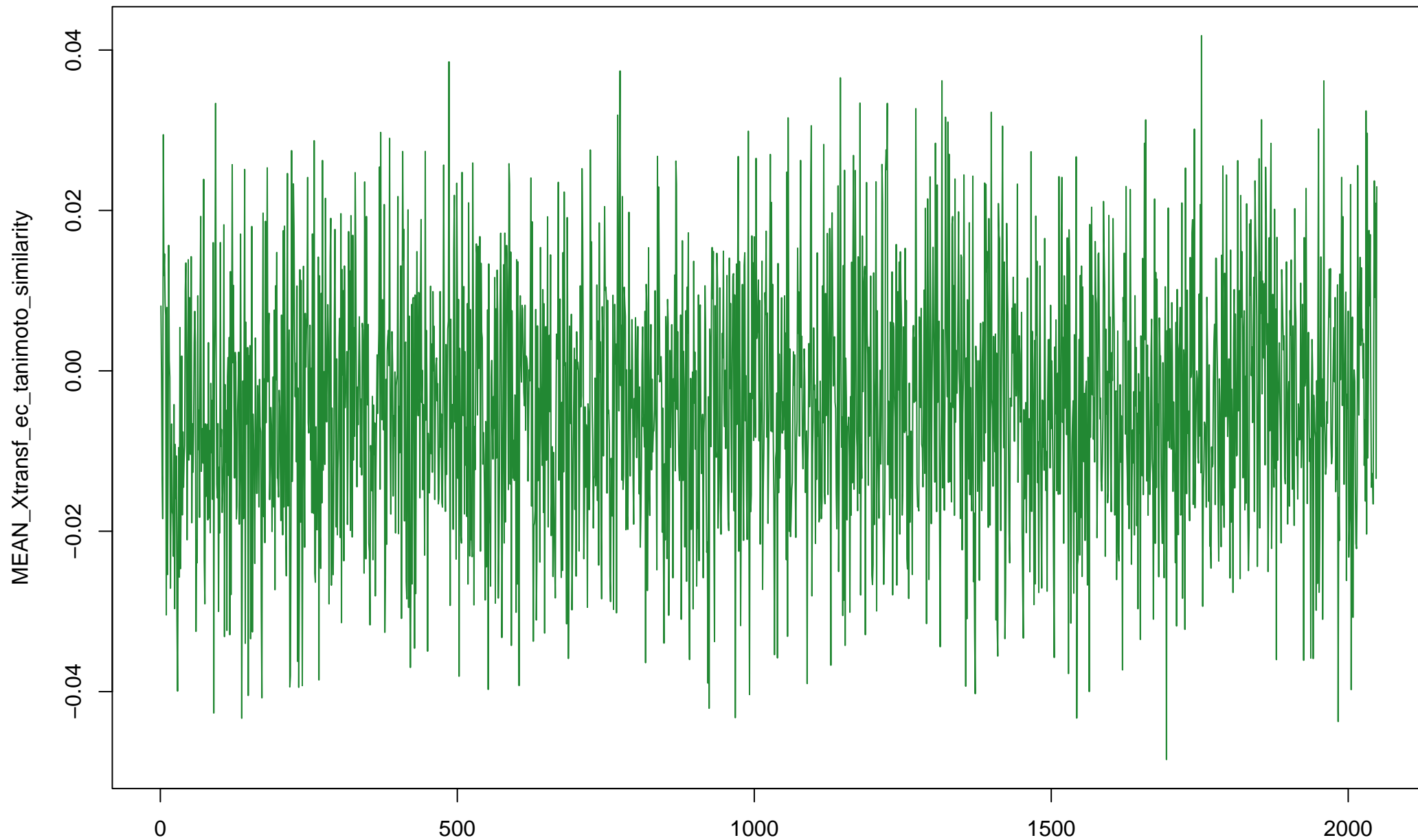


**MEAN\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0442 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0**

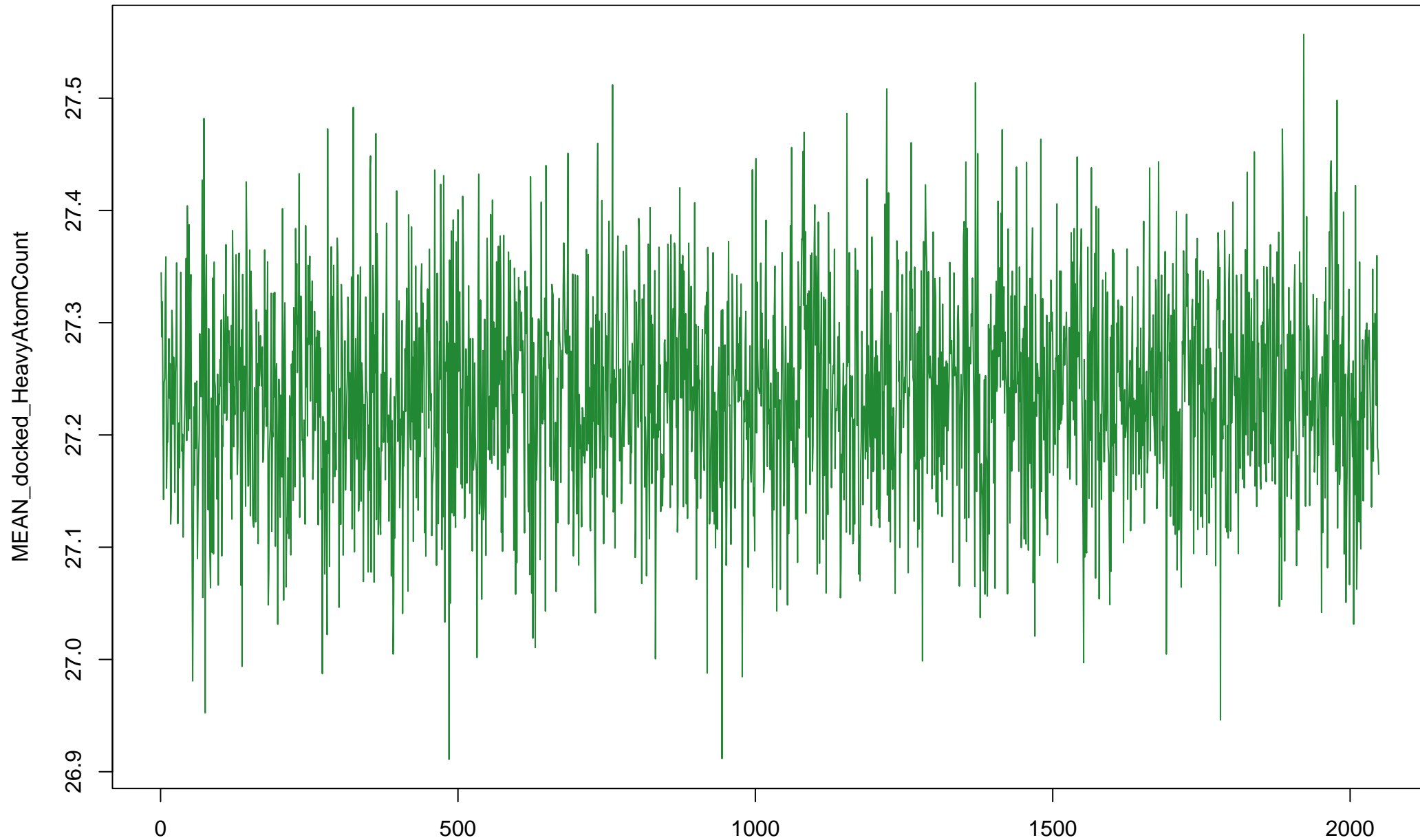




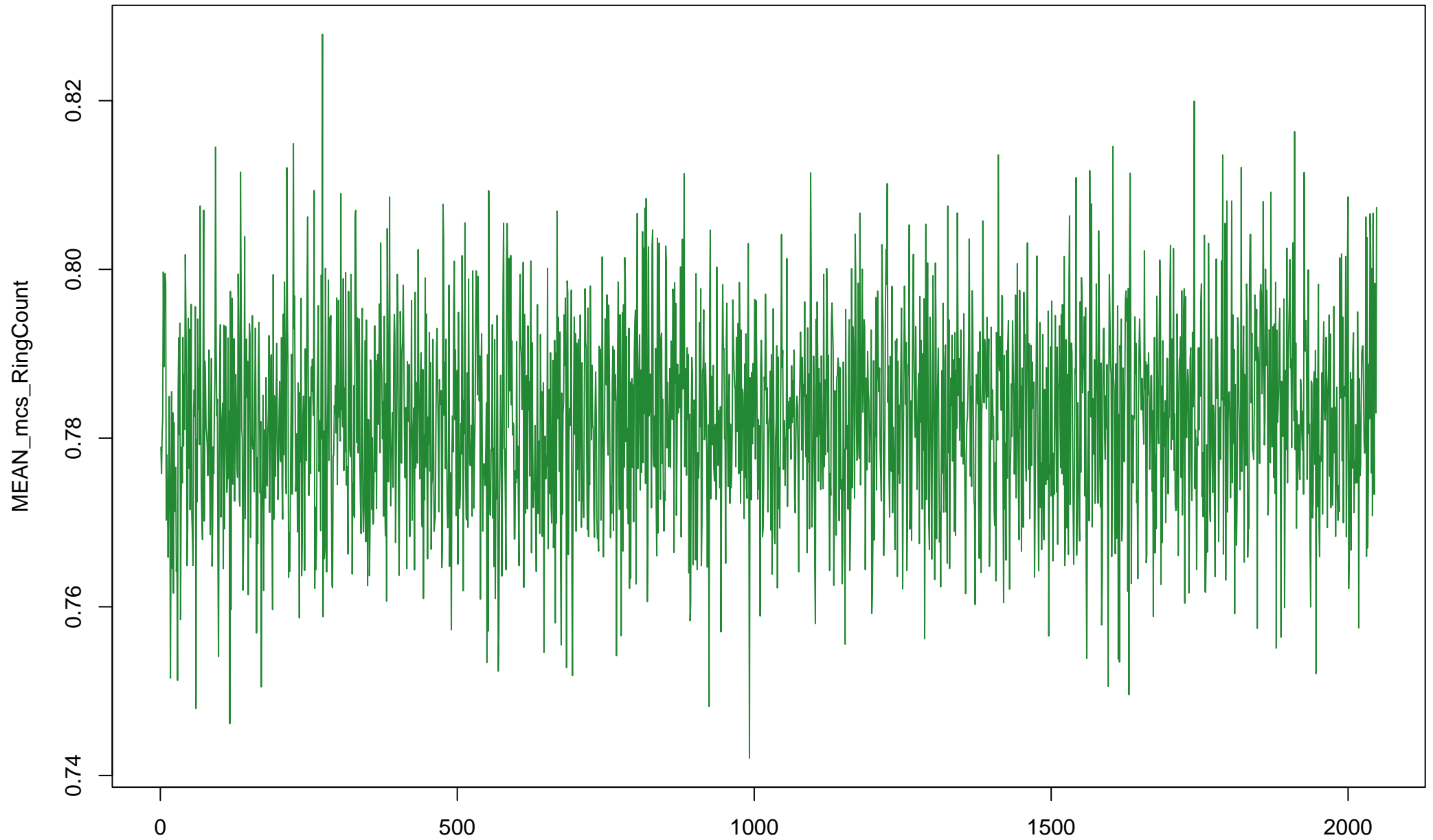
**MEAN\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0582 | MCSE(6.27) = 2.15 | stat: FALSE | burn: 0**



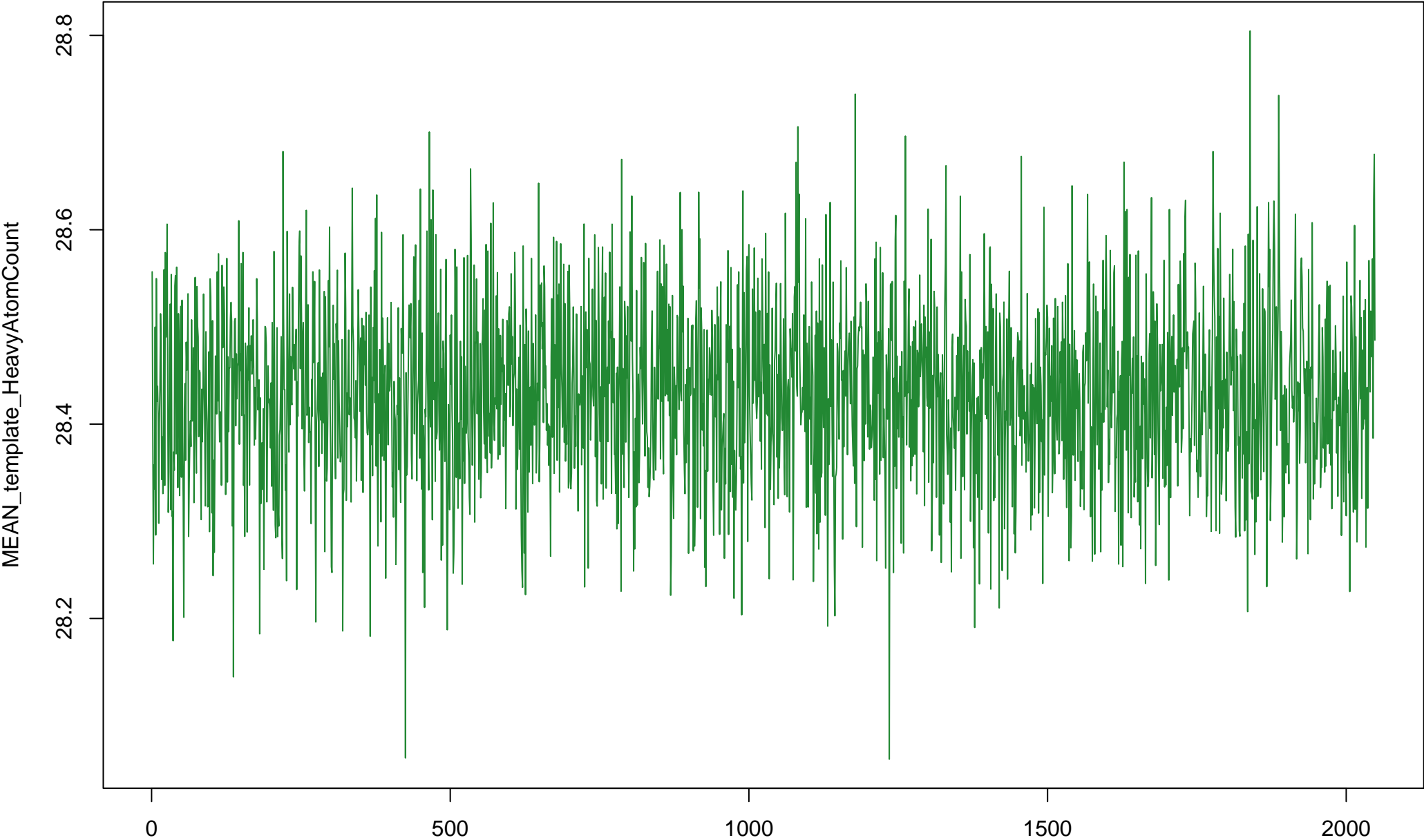
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0456 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0**



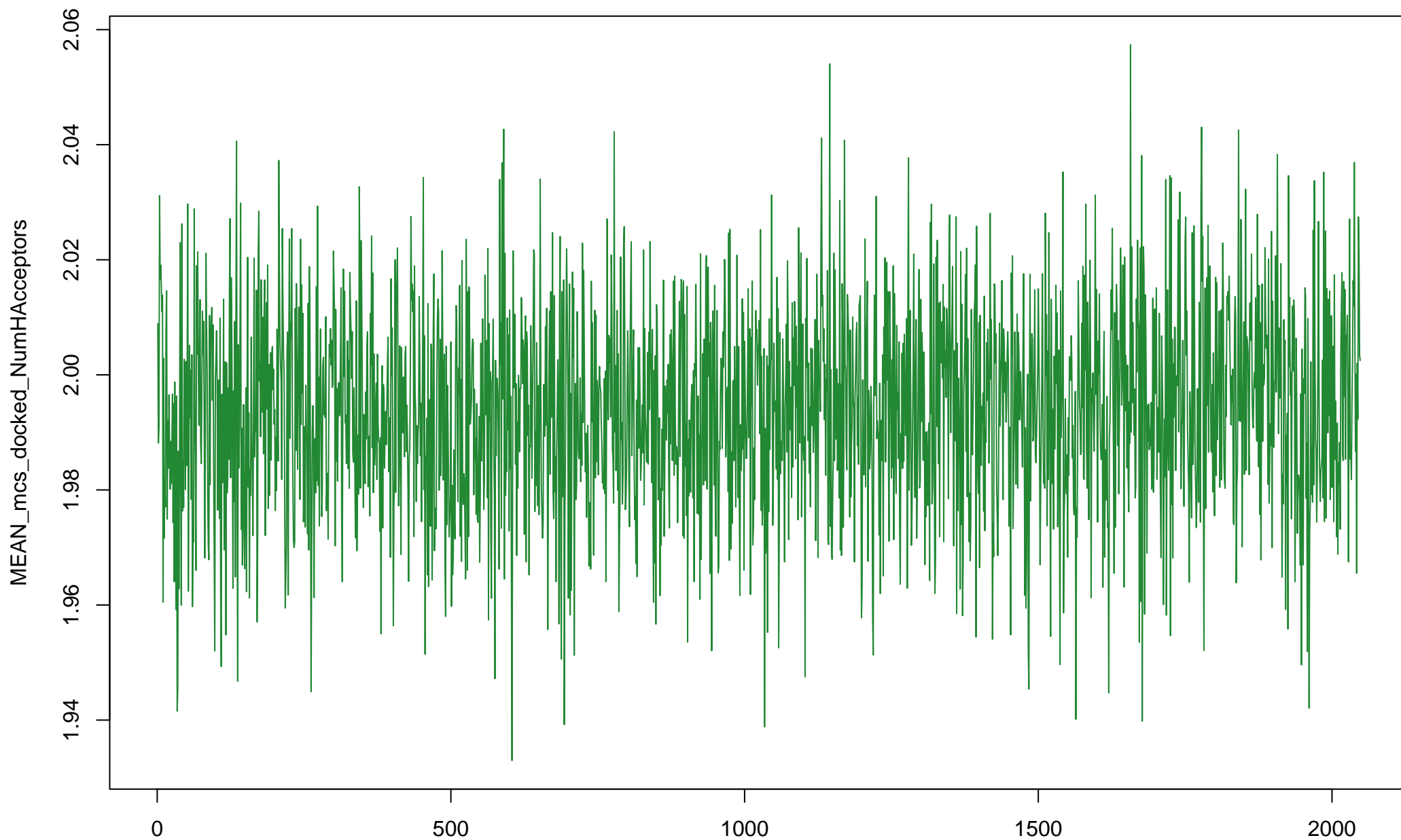
**MEAN\_mcs\_RingCount**  
**ESS = 2050 | BMK = 0.0545 | MCSE(6.27) = 2.37 | stat: FALSE | burn: 0**



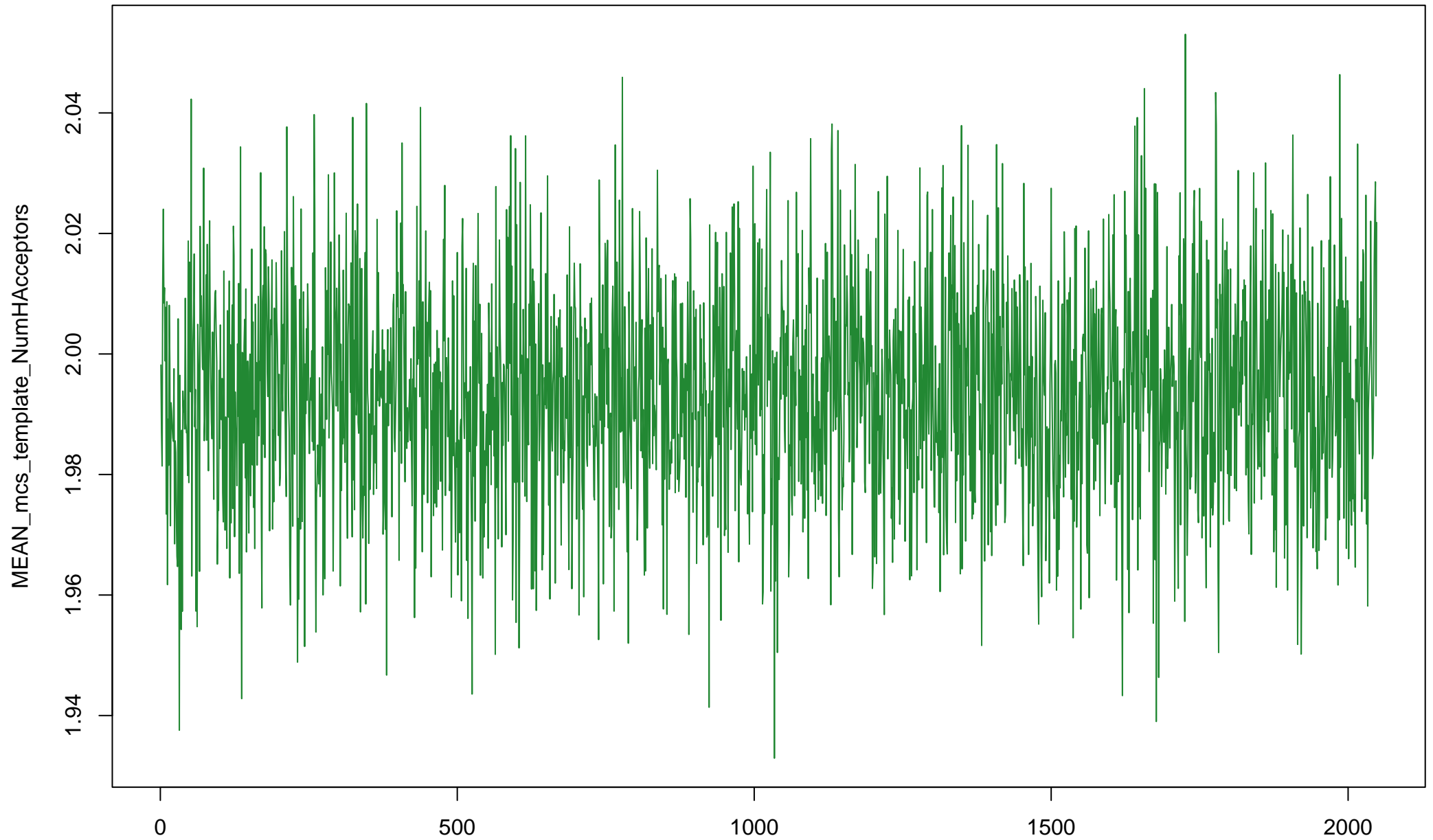
MEAN\_template\_HeavyAtomCount  
ESS = 2050 | BMK = 0.056 | MCSE(6.27) = 2.03 | stat: TRUE | burn: 0



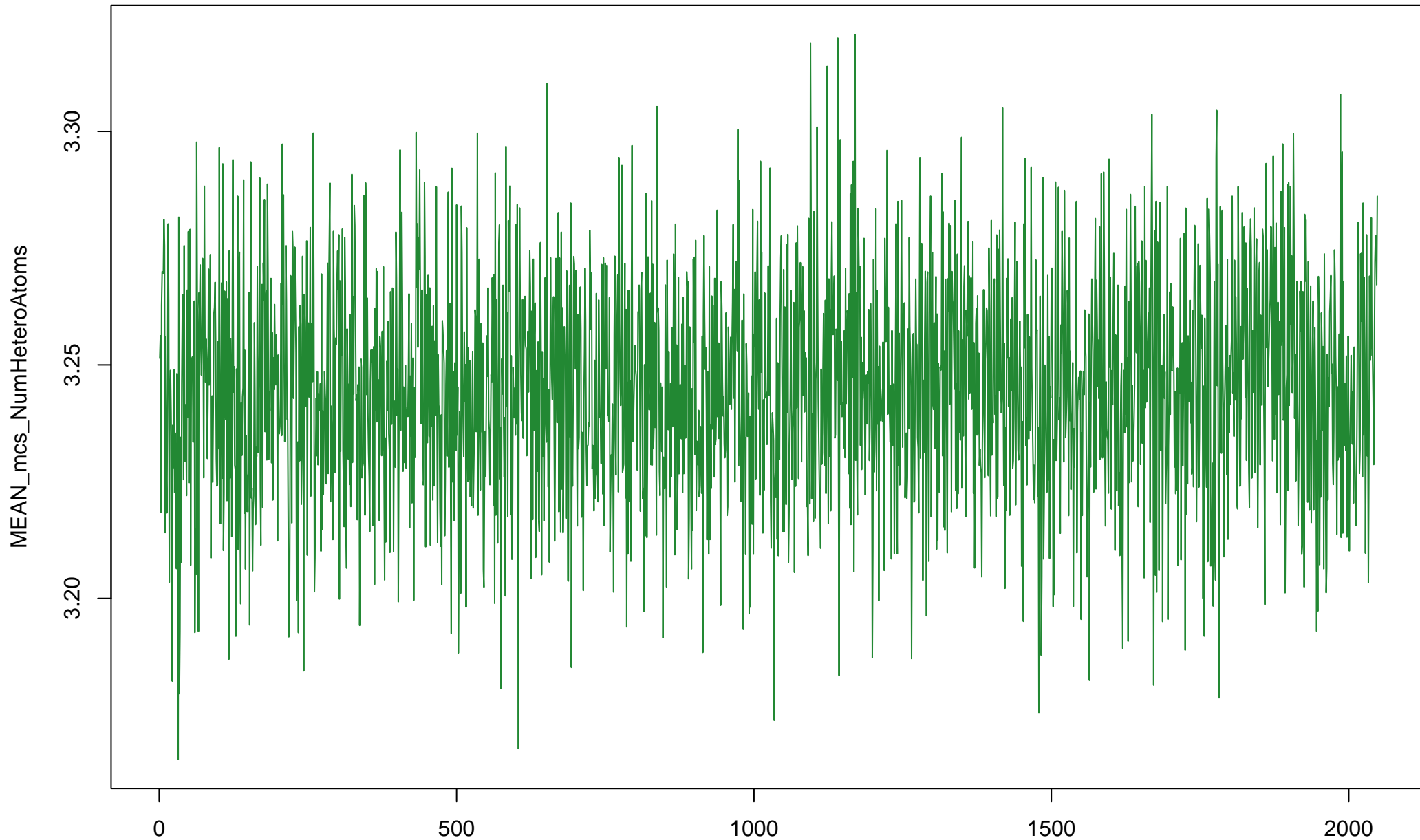
**MEAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0564 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0**



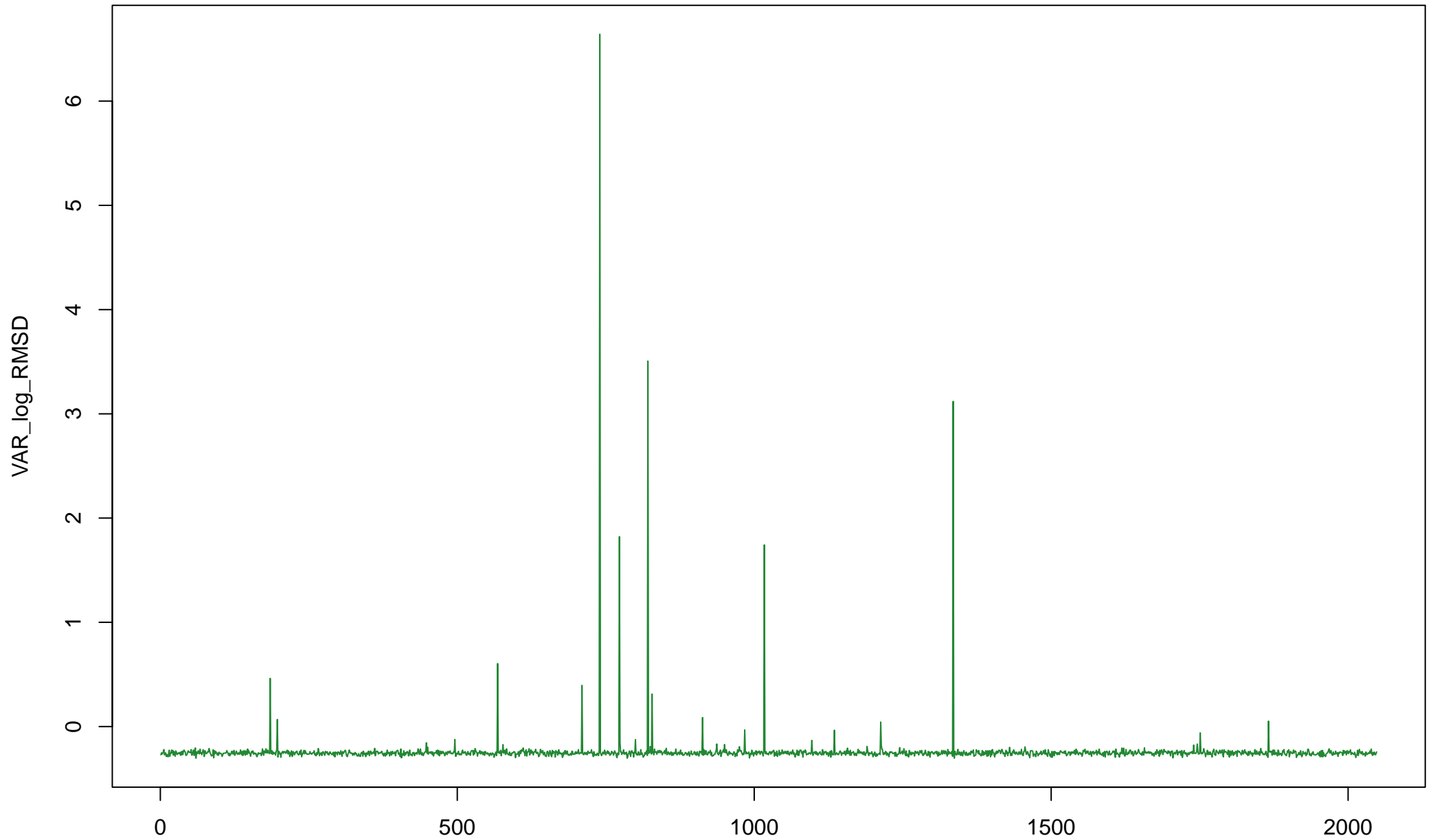
**MEAN\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0431 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0**



**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0506 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0**

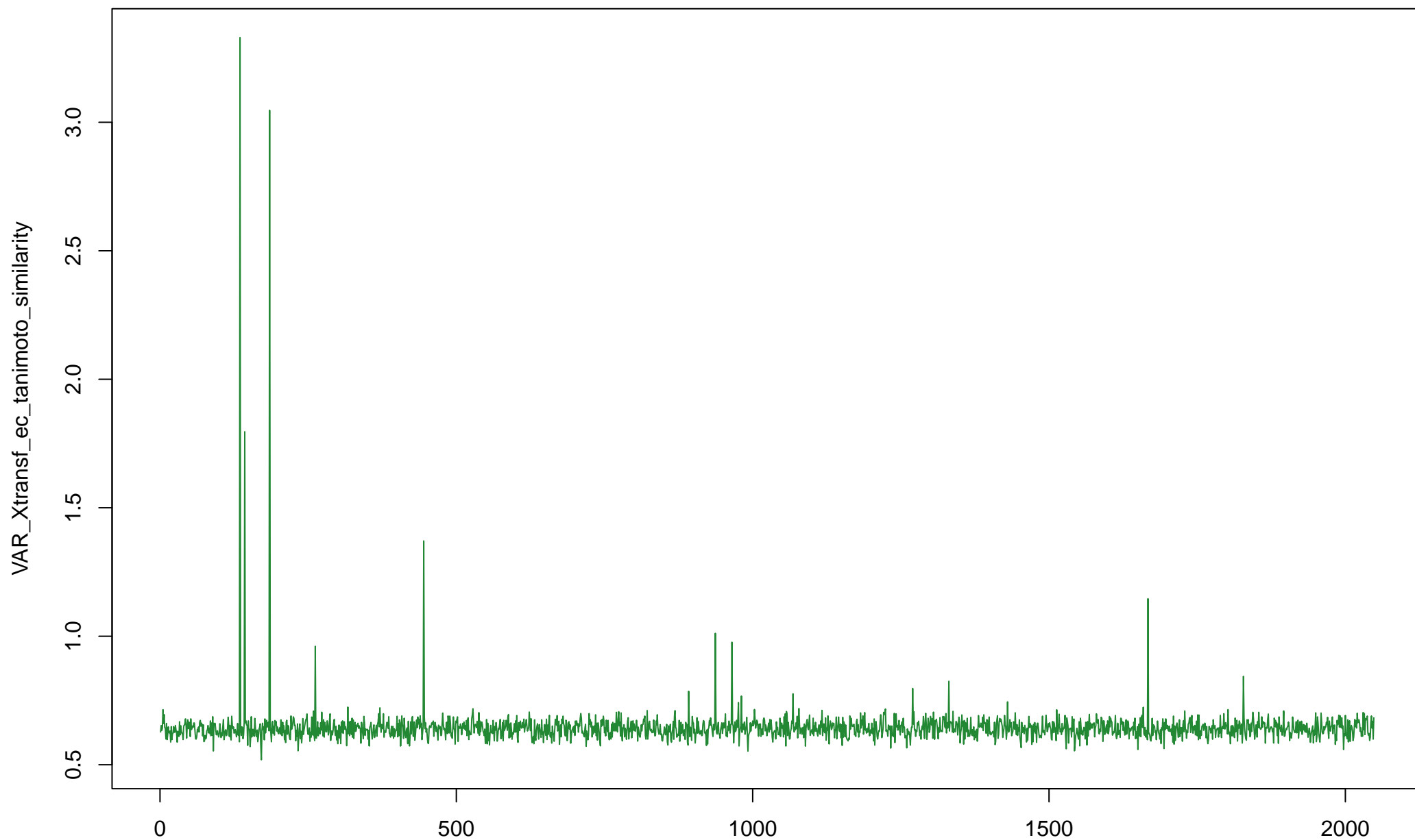


**VAR\_log\_RMSD**  
**ESS = 2050 | BMK = 0.525 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 816**

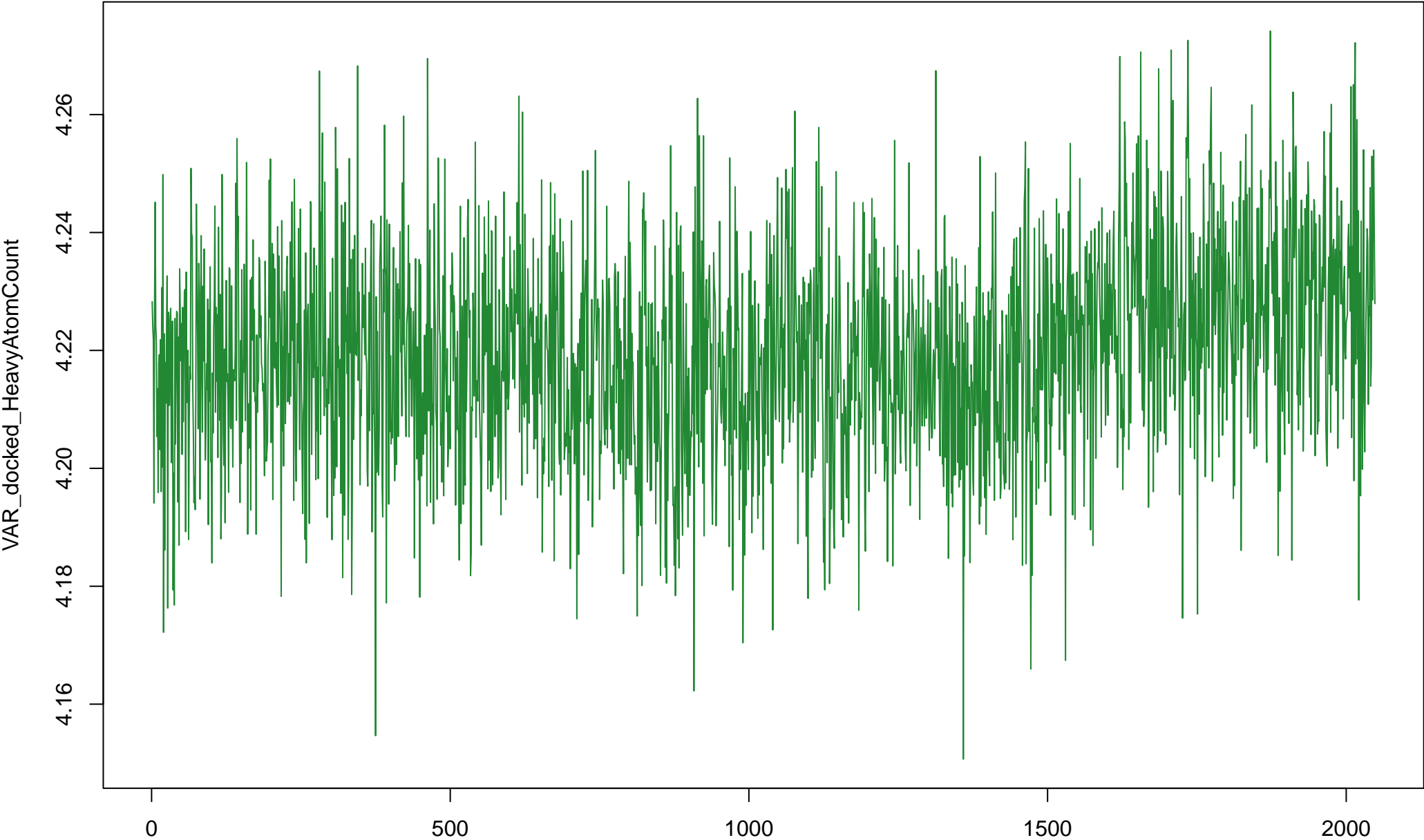




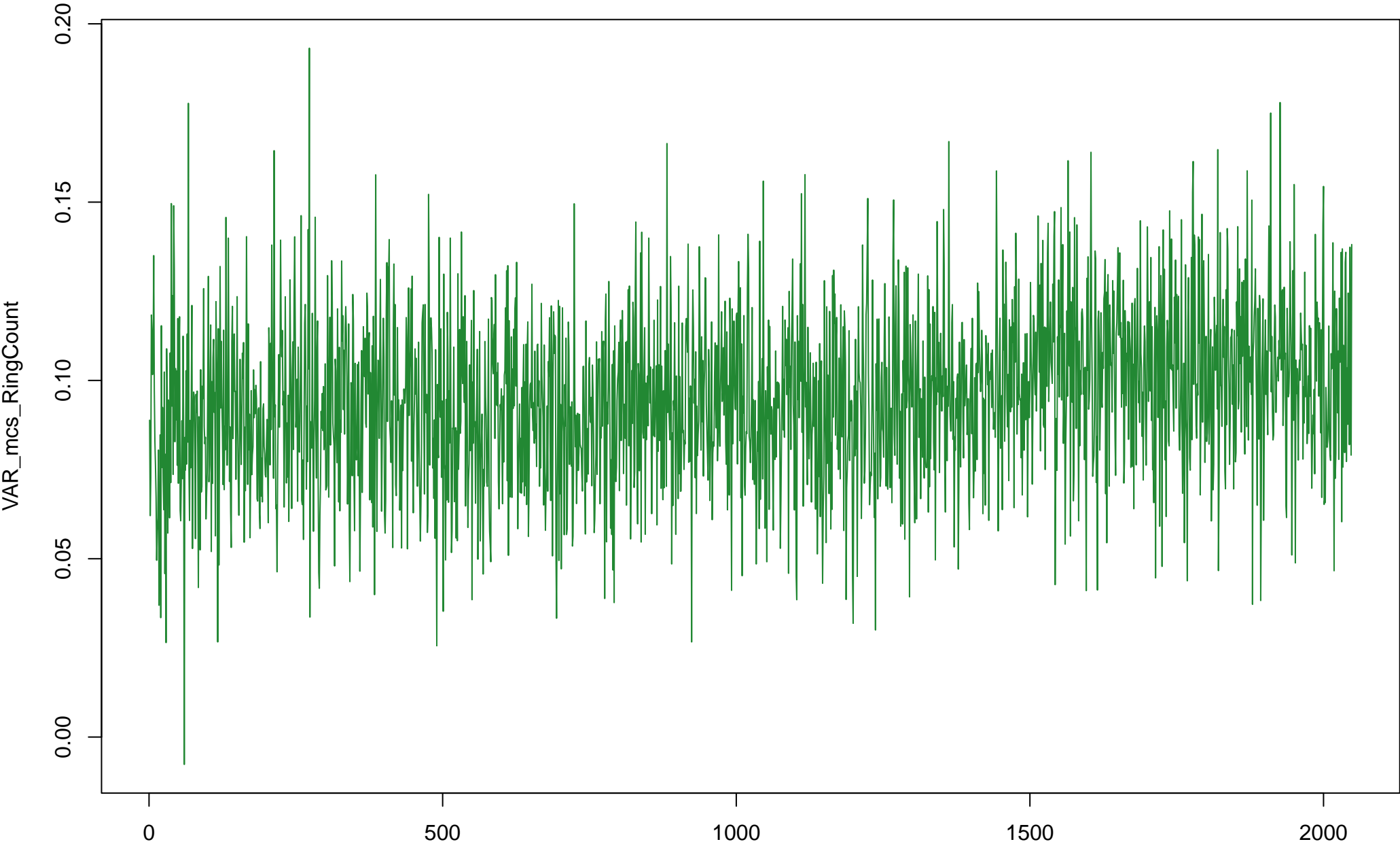
**VAR\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1730 | BMK = 0.0882 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0**



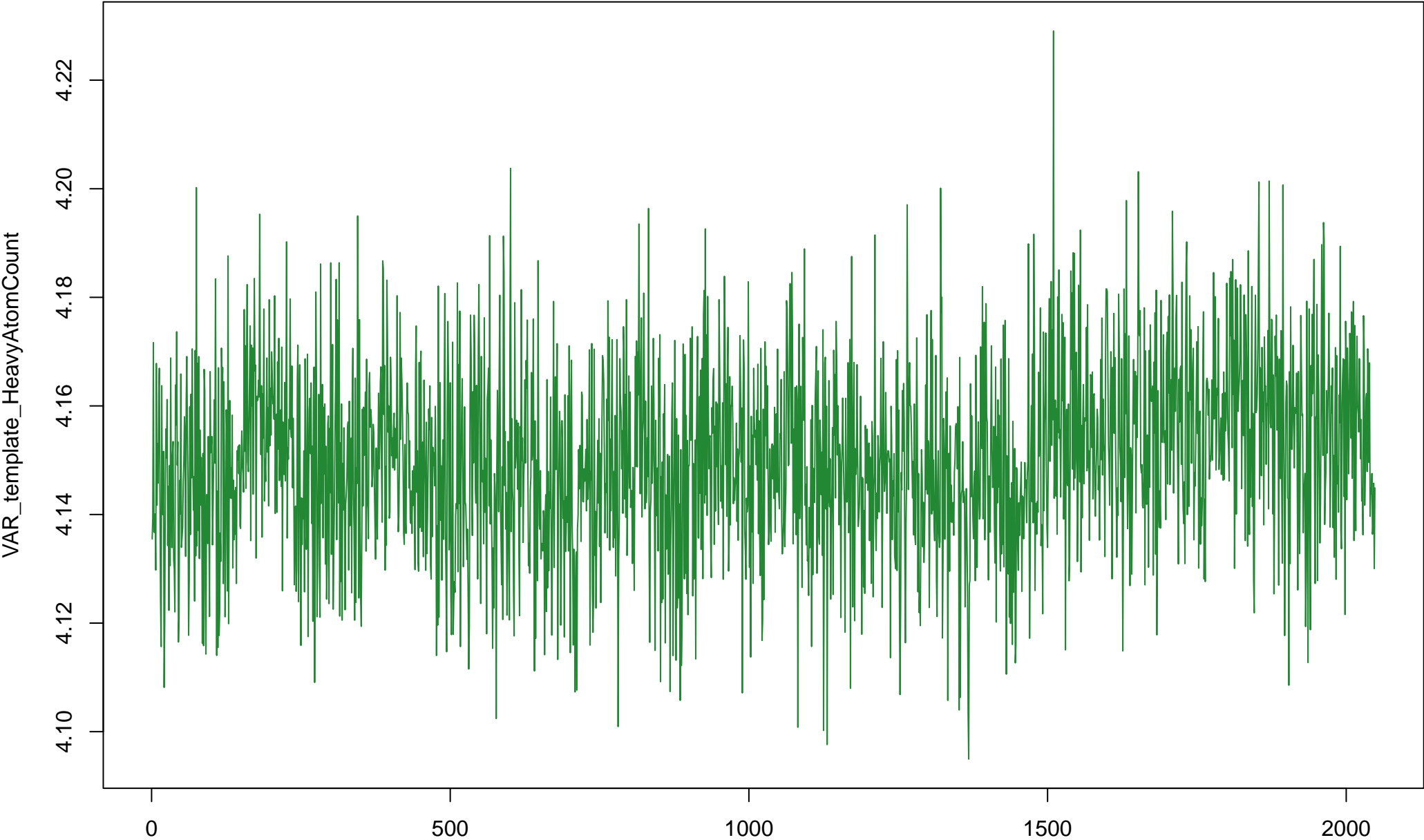
**VAR\_docked\_HeavyAtomCount**  
**ESS = 213 | BMK = 0.105 | MCSE(6.27) = 4.78 | stat: FALSE | burn: 0**



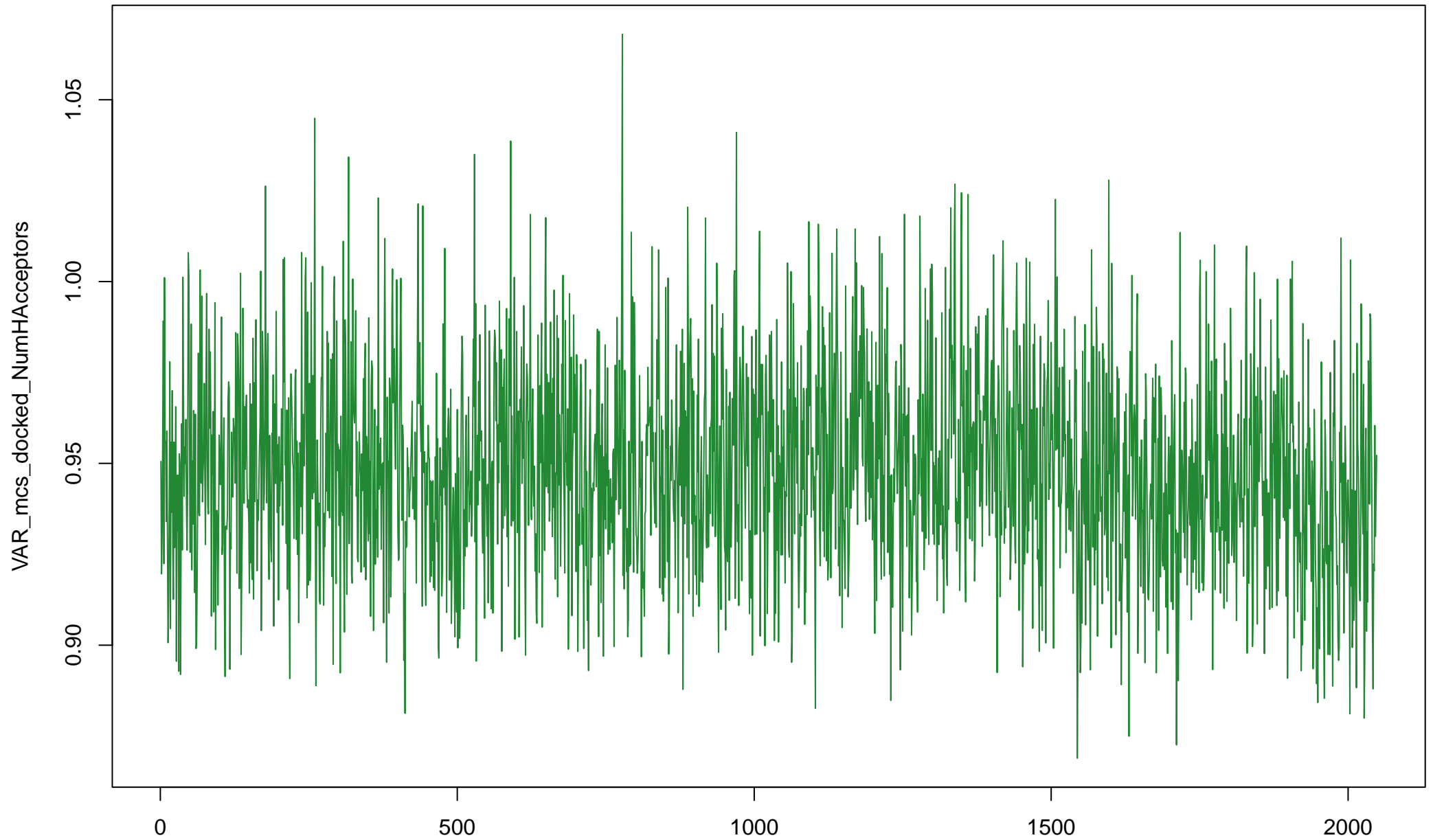
**VAR\_mcs\_RingCount**  
**ESS = 585 | BMK = 0.129 | MCSE(6.27) = 4.04 | stat: FALSE | burn: 0**



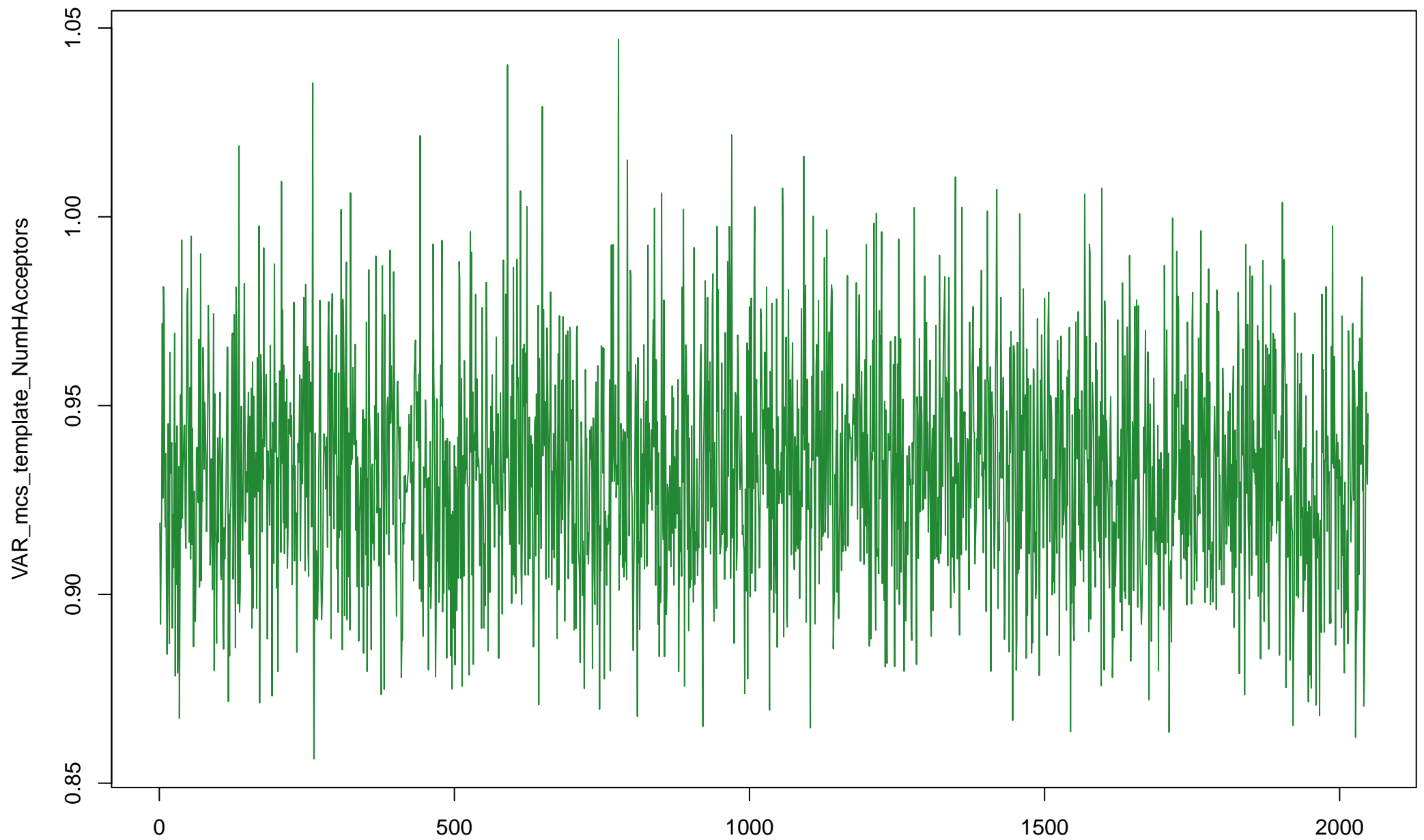
**VAR\_template\_HeavyAtomCount**  
**ESS = 228 | BMK = 0.0939 | MCSE(6.27) = 4.65 | stat: TRUE | burn: 0**



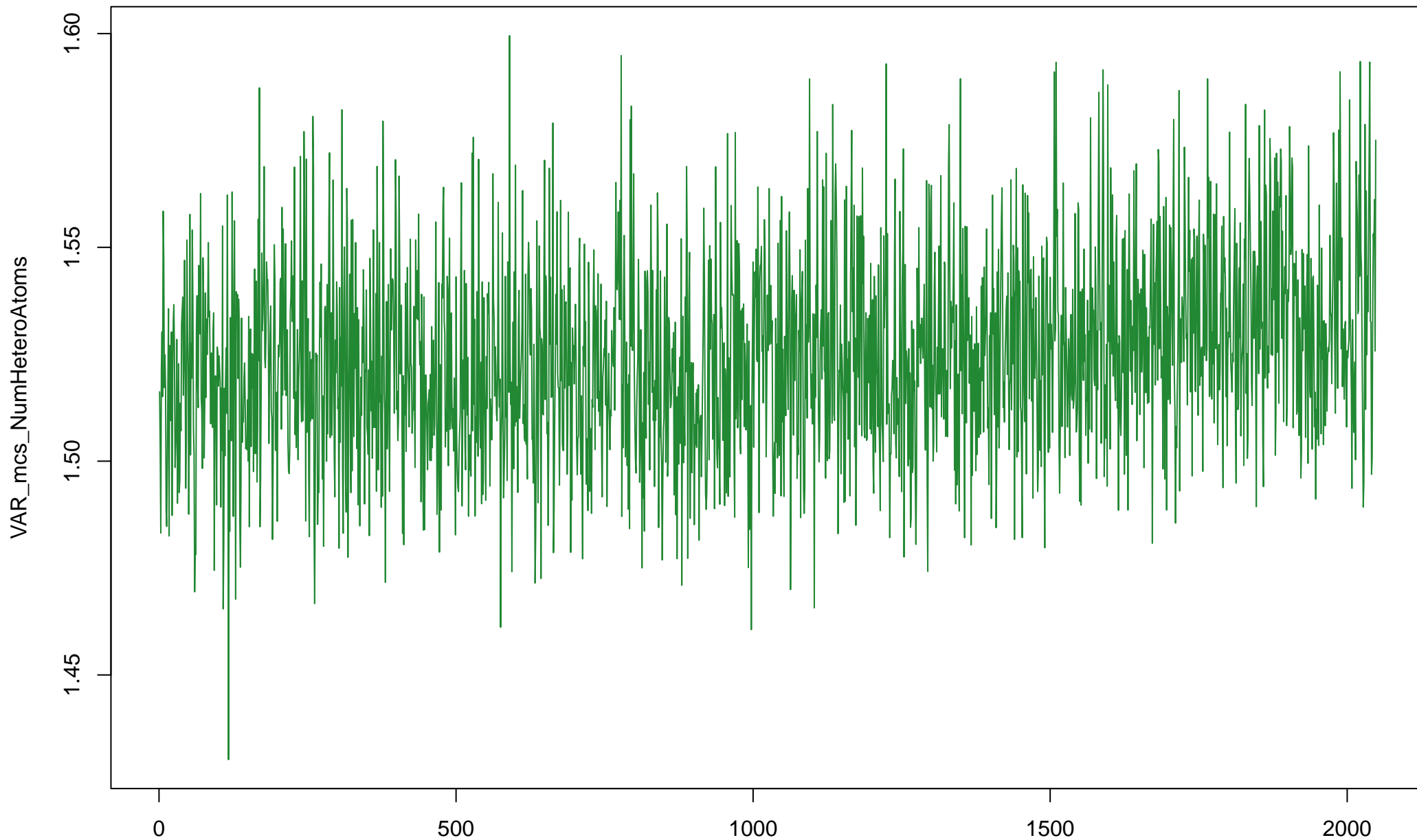
**VAR\_mcs\_docked\_NumHAcceptors**  
**ESS = 1680 | BMK = 0.0562 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0**



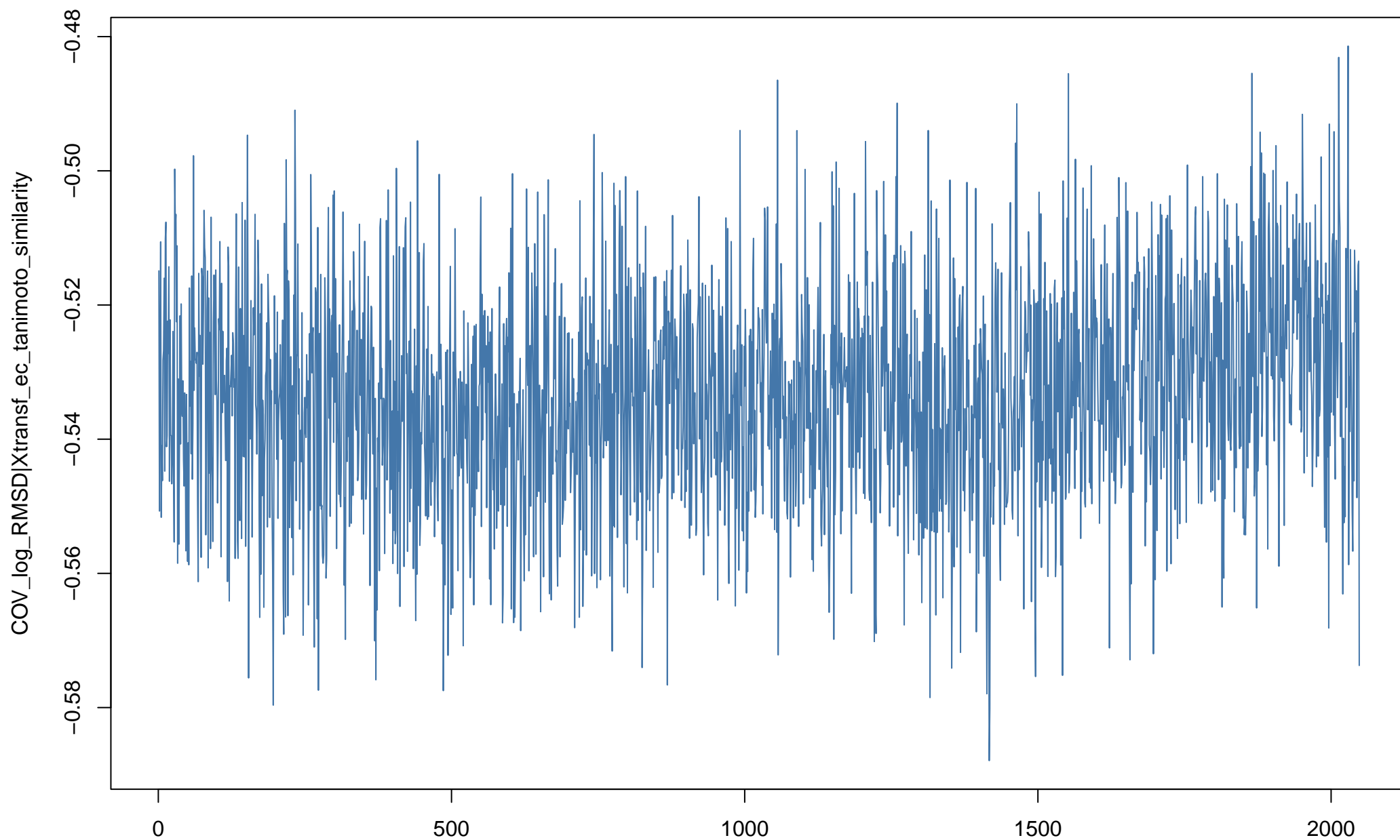
**VAR\_mcs\_template\_NumHAcceptors**  
**ESS = 1840 | BMK = 0.0539 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0**



**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 455 | BMK = 0.142 | MCSE(6.27) = 4.08 | stat: FALSE | burn: 0**

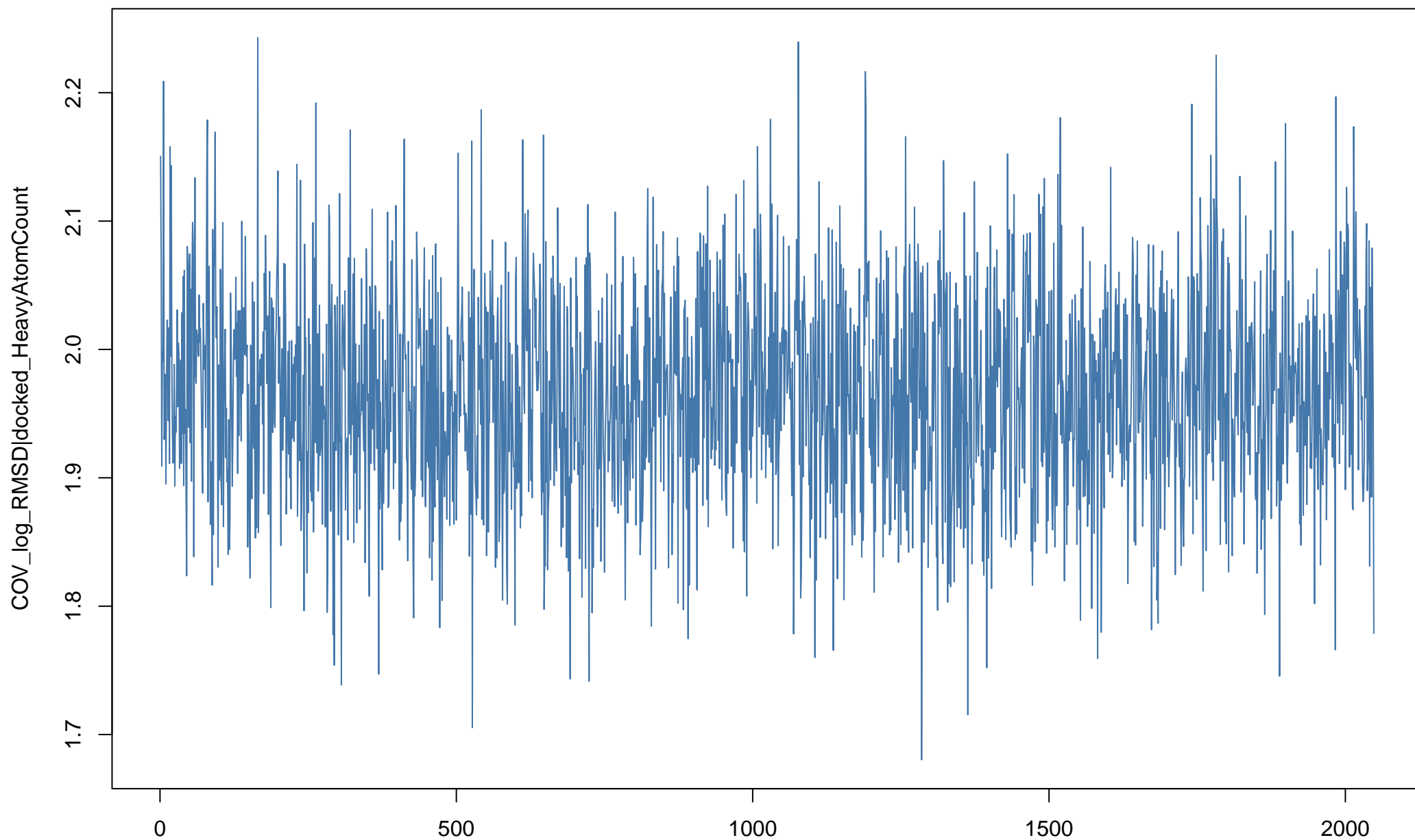


**COV\_log\_RMSD|Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 324 | BMK = 0.093 | MCSE(6.27) = 3.56 | stat: TRUE | burn: 0**

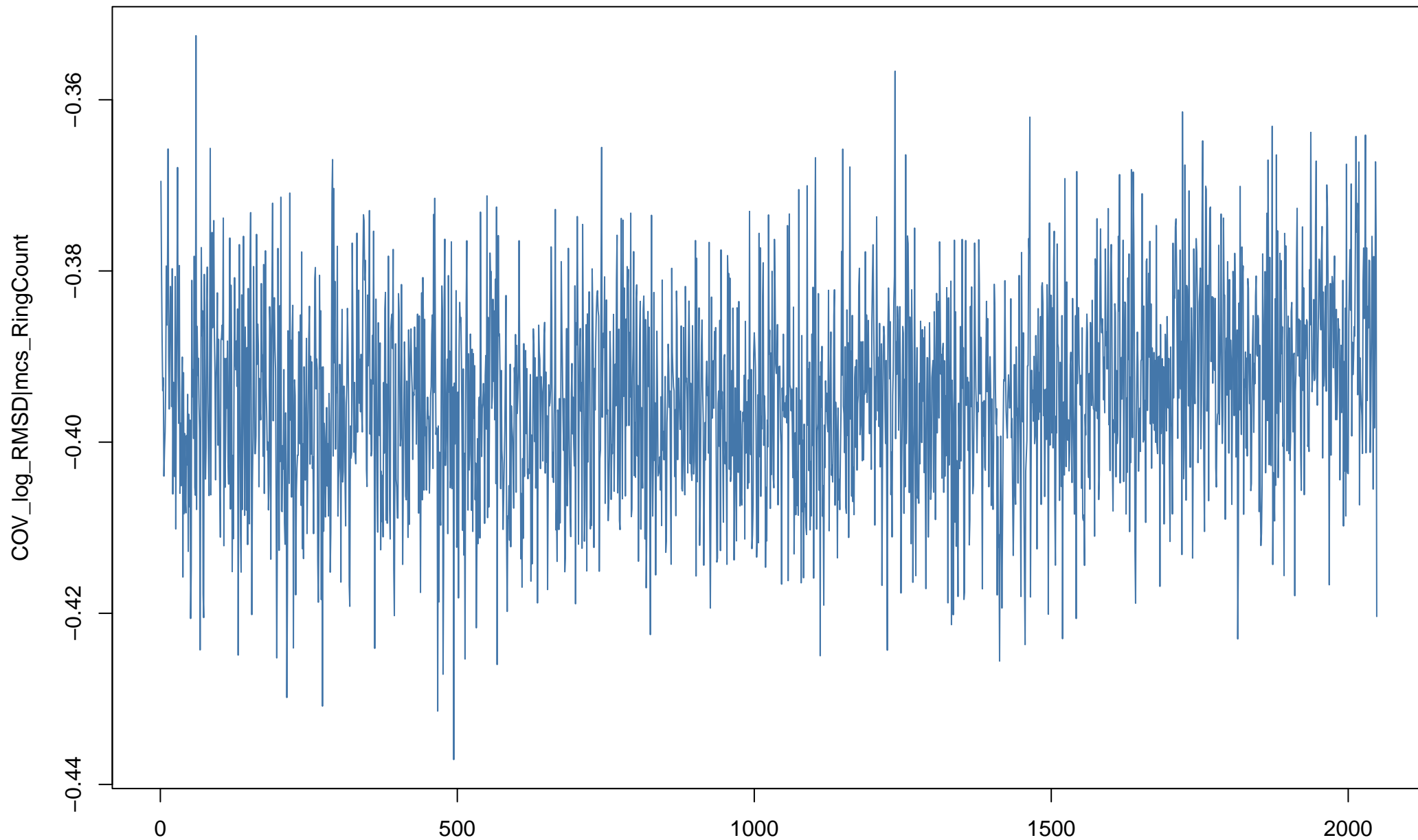




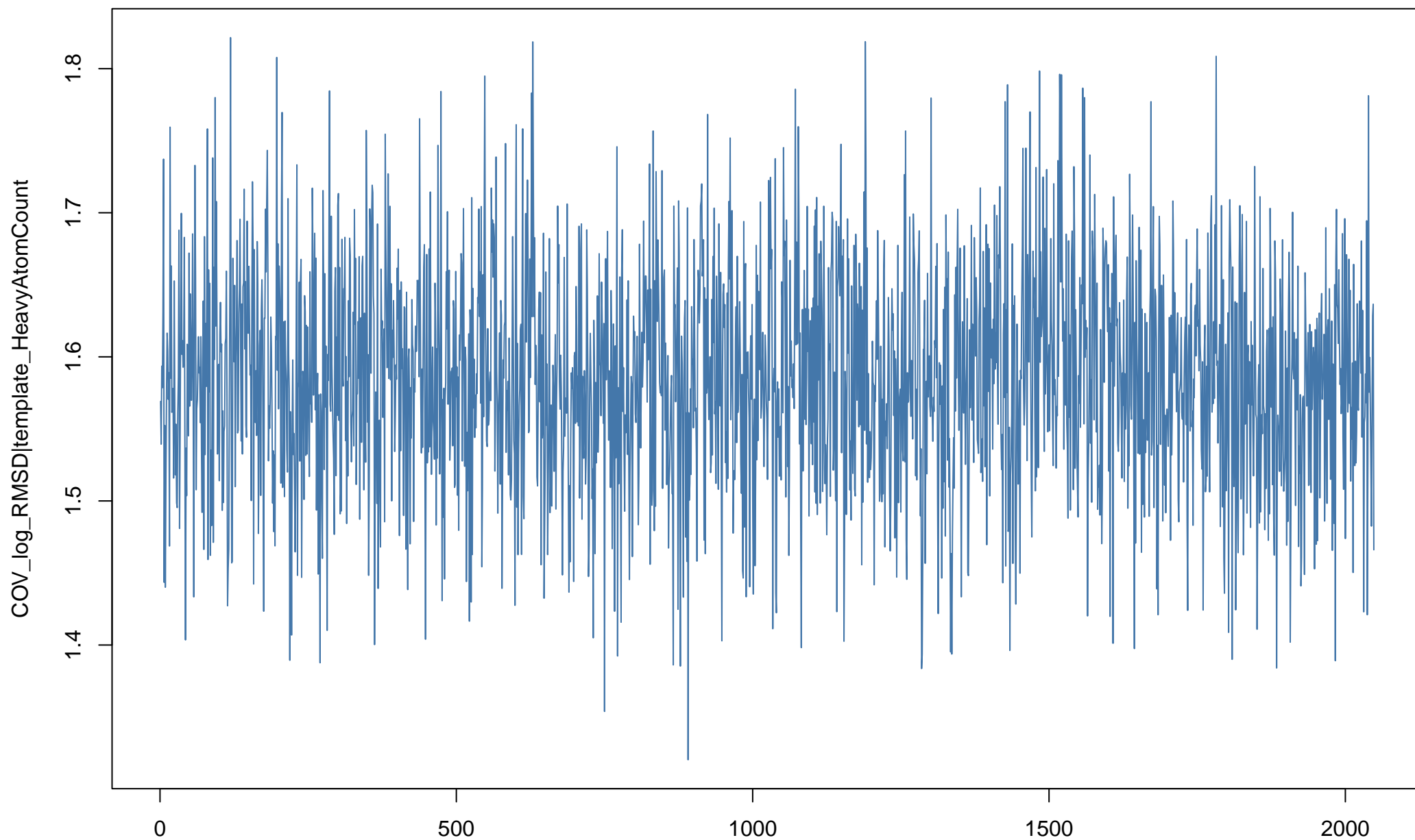
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 1820 | BMK = 0.0282 | MCSE(6.27) = 2.74 | stat: FALSE | burn: 0**



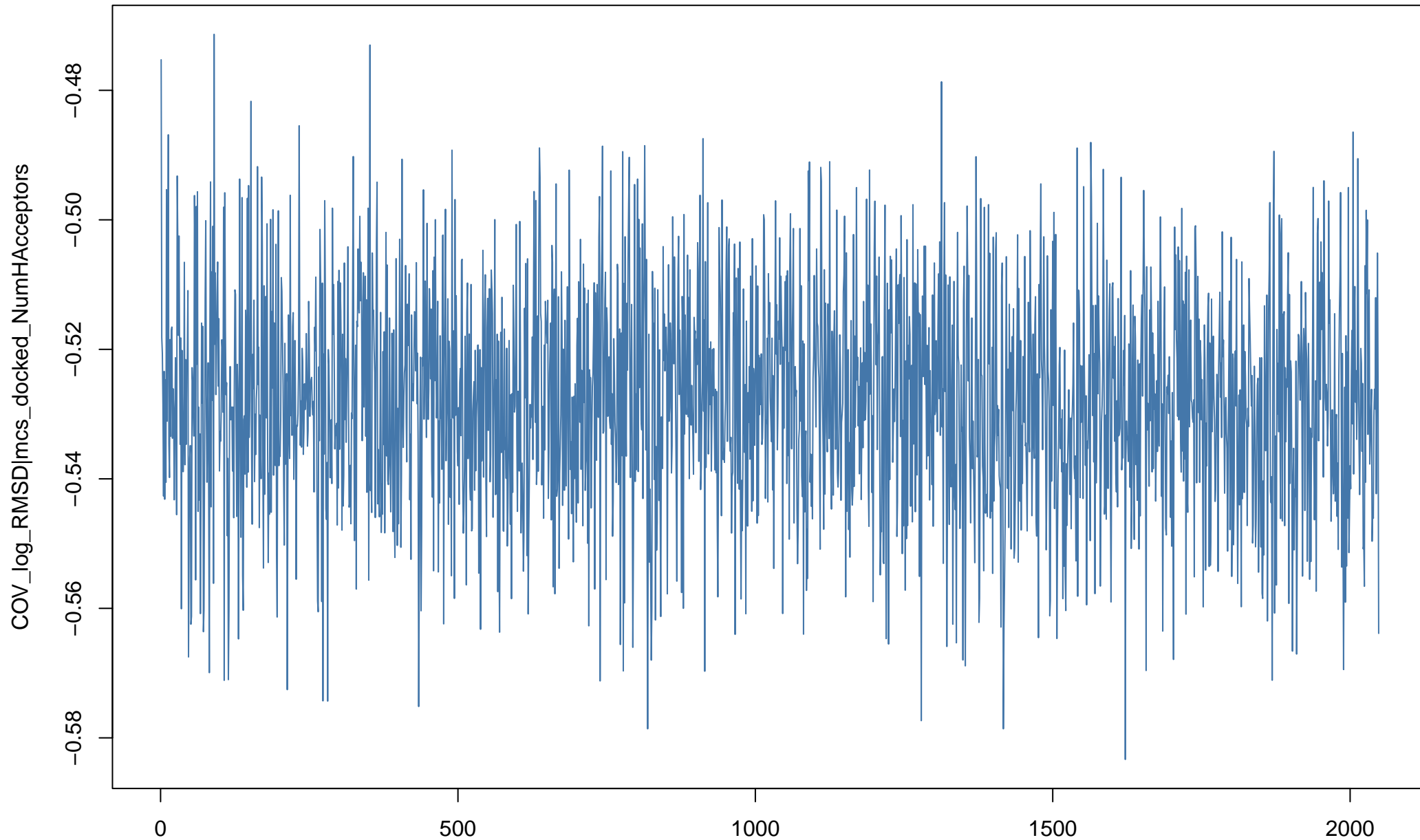
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 438 | BMK = 0.104 | MCSE(6.27) = 4.02 | stat: TRUE | burn: 0**



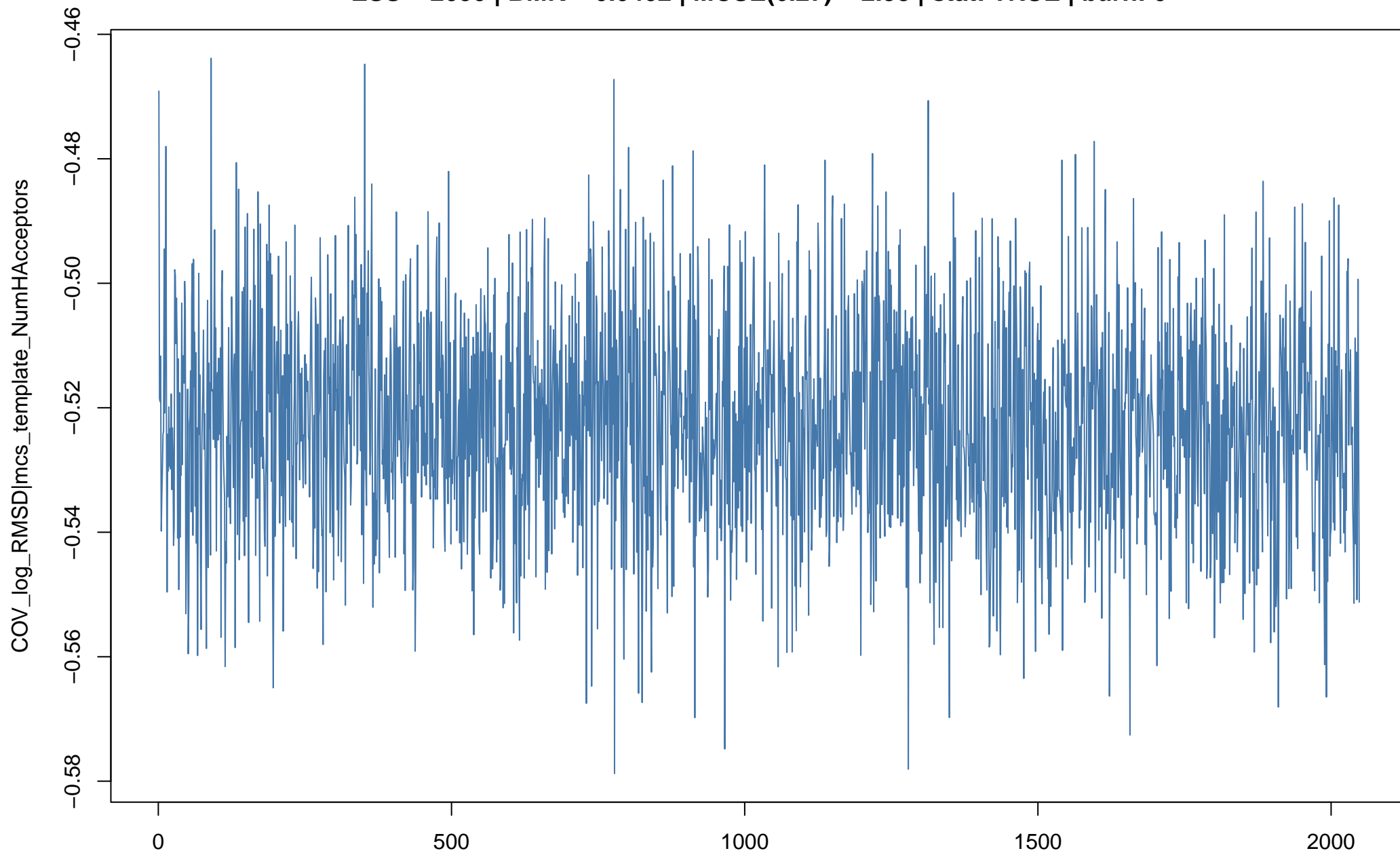
**COV\_log\_RMSD|template\_HeavyAtomCount**  
**ESS = 1740 | BMK = 0.0351 | MCSE(6.27) = 2.79 | stat: TRUE | burn: 0**



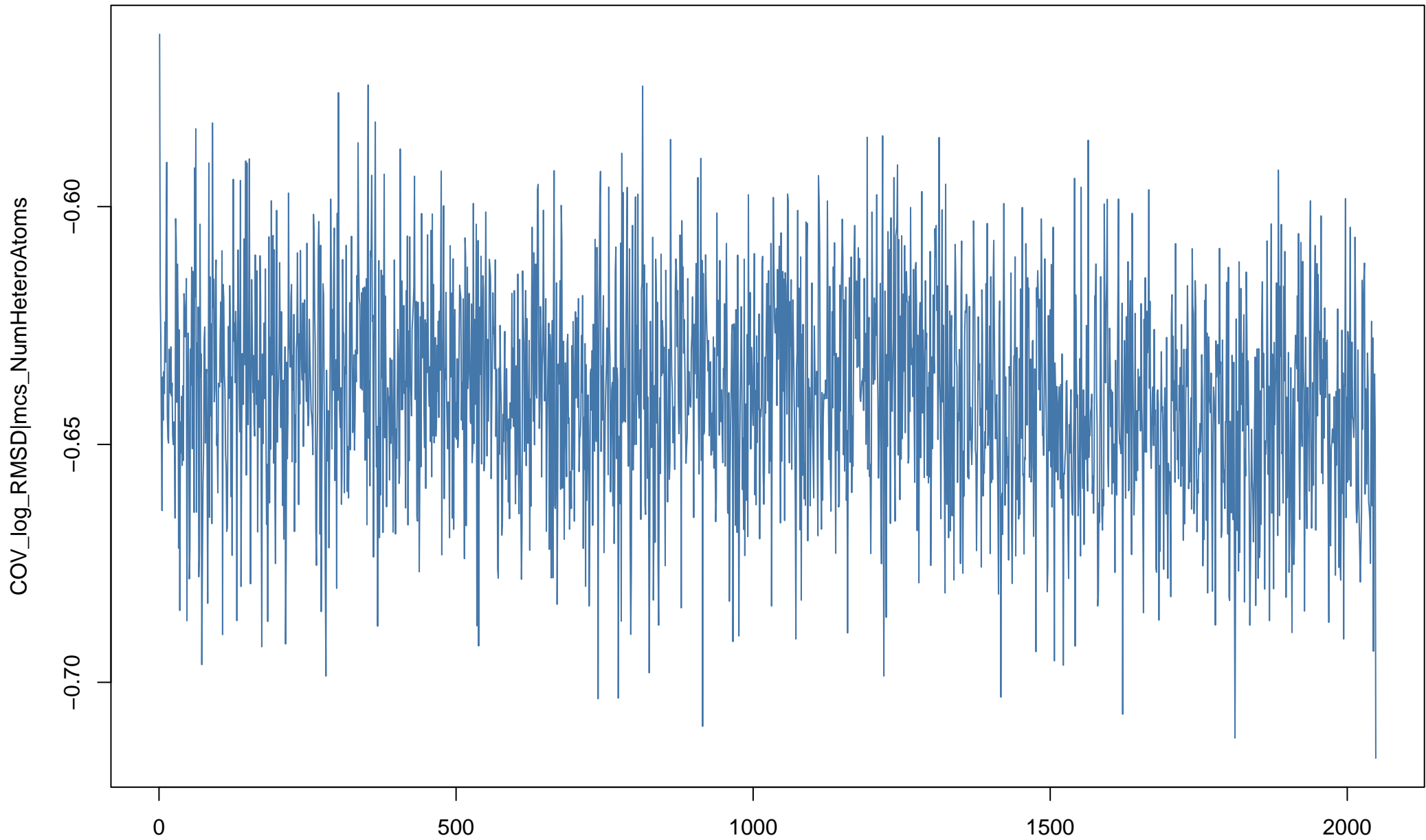
COV\_log\_RMSD|mcs\_docked\_NumHAcceptors  
ESS = 2050 | BMK = 0.0428 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0



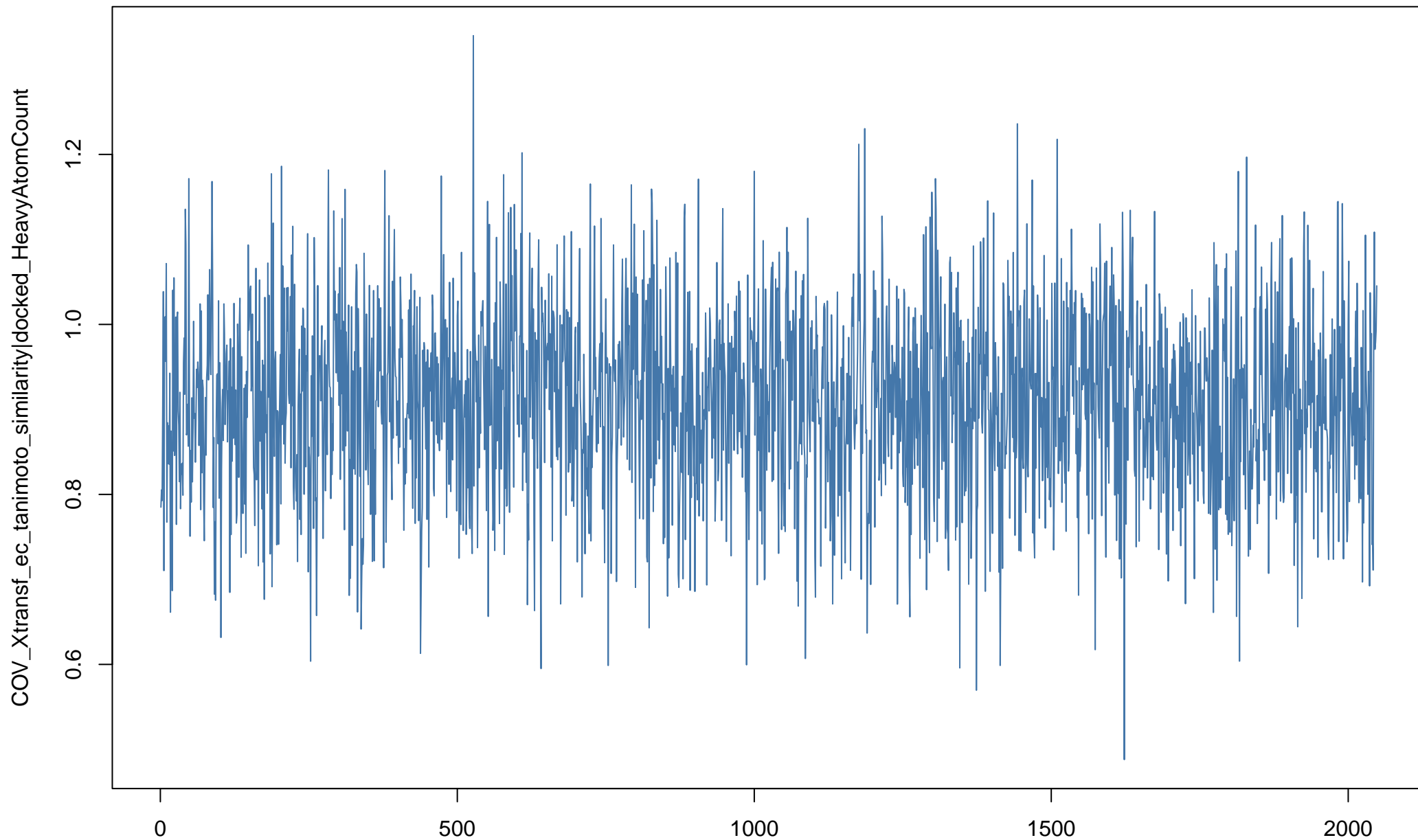
**COV\_log\_RMSD|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0402 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0**



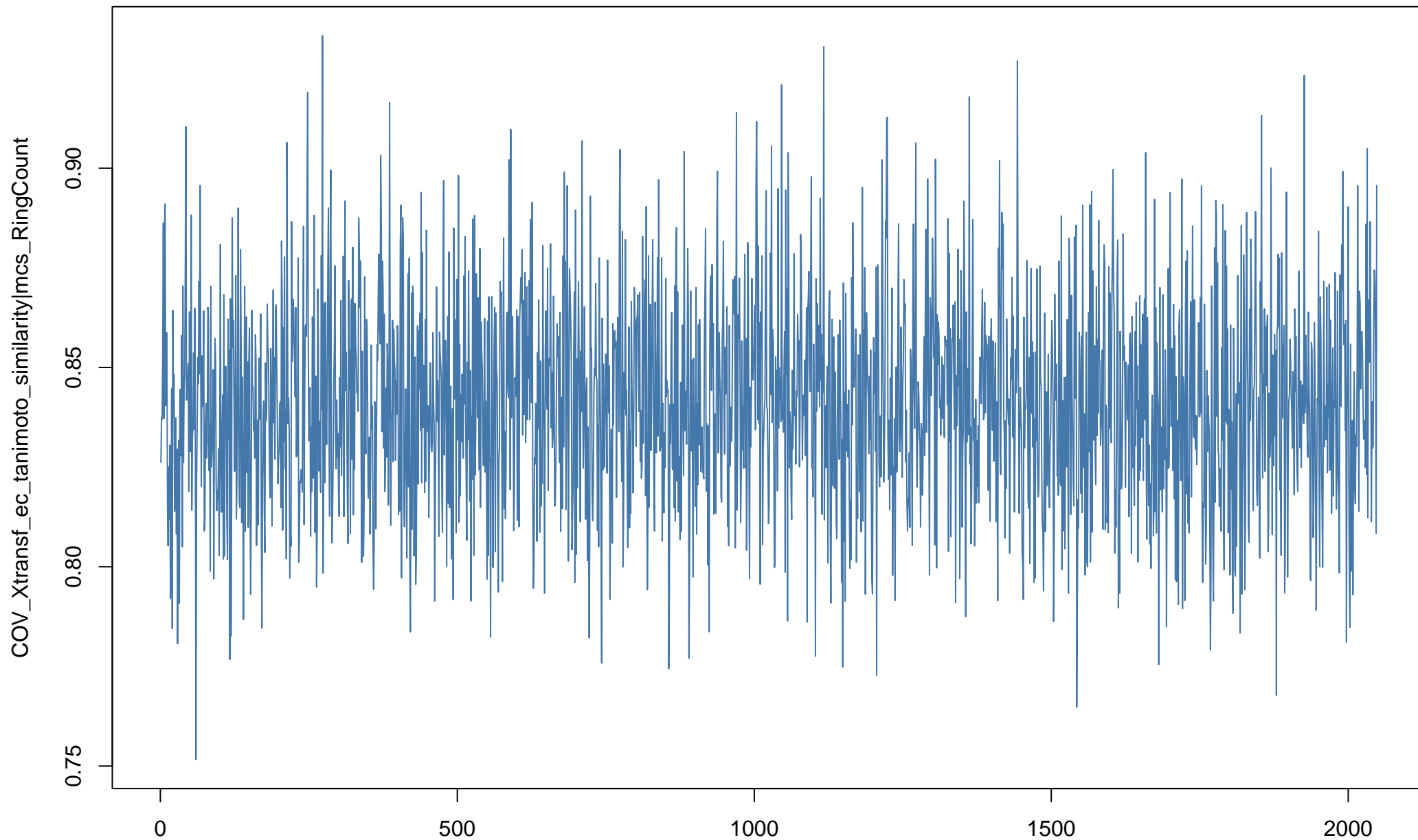
COV\_log\_RMSD|mcs\_NumHeteroAtoms  
ESS = 731 | BMK = 0.0869 | MCSE(6.27) = 3.52 | stat: FALSE | burn: 0



**COV\_Xtransf\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount**  
**ESS = 1870 | BMK = 0.0468 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0**

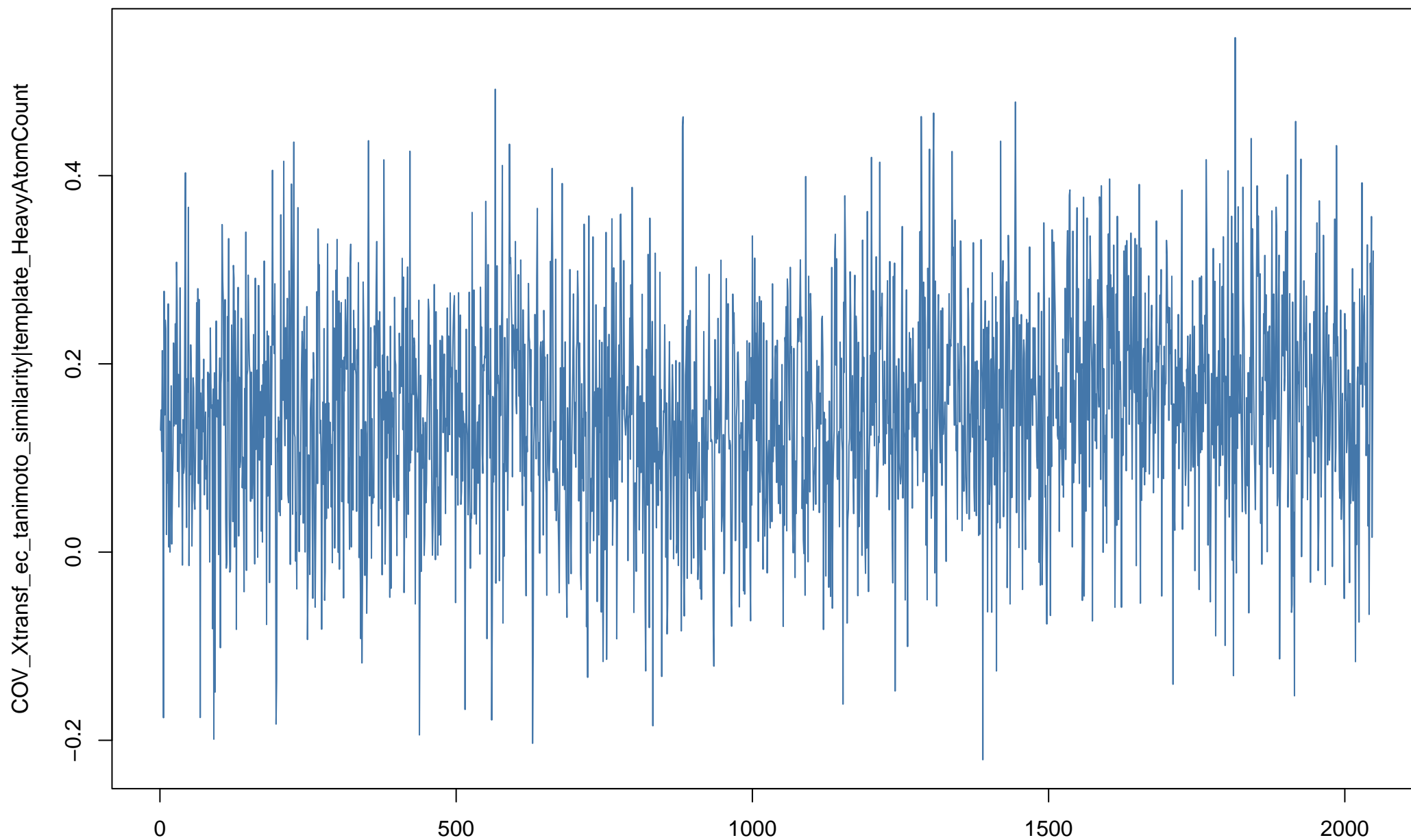


**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 1900 | BMK = 0.0442 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0**

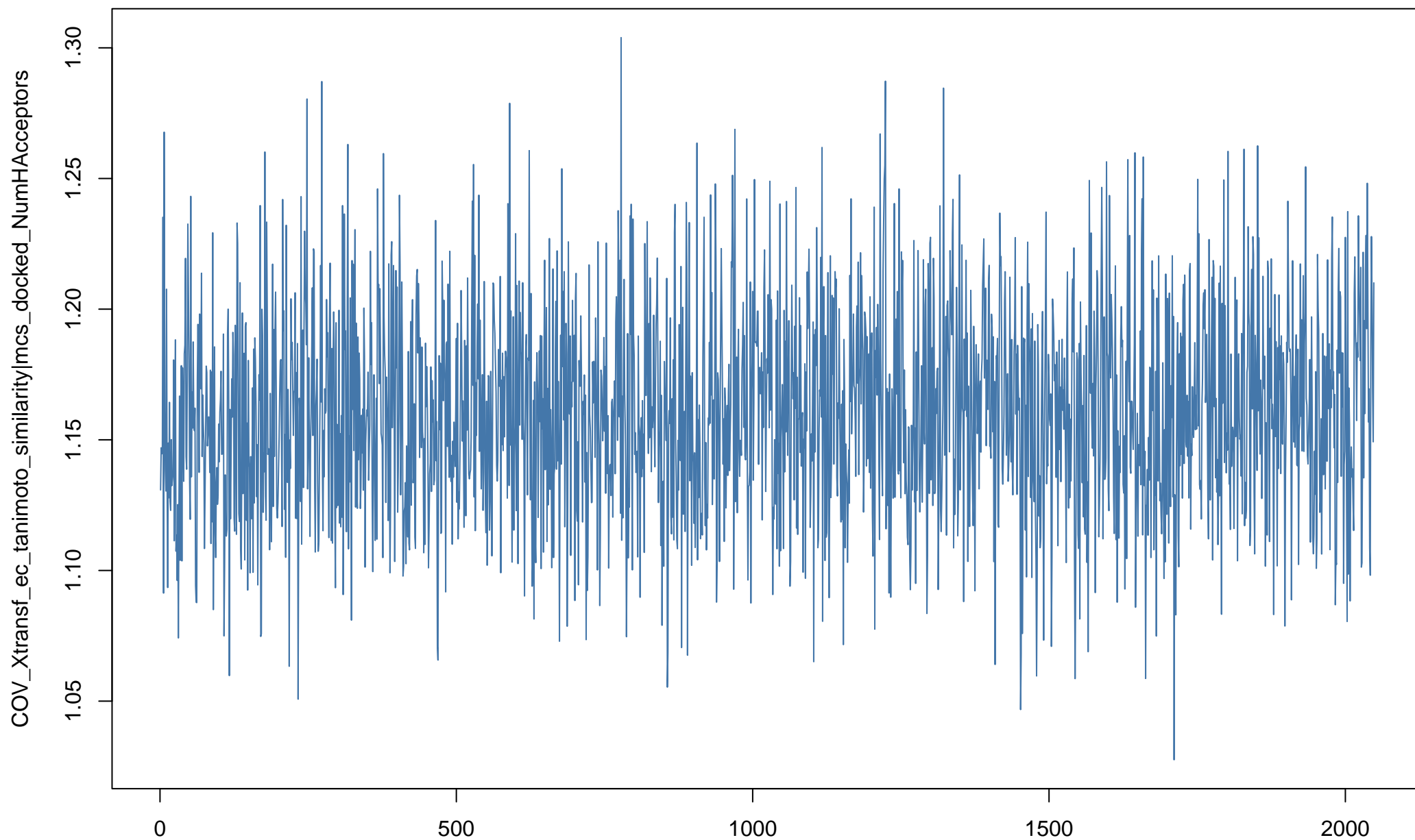




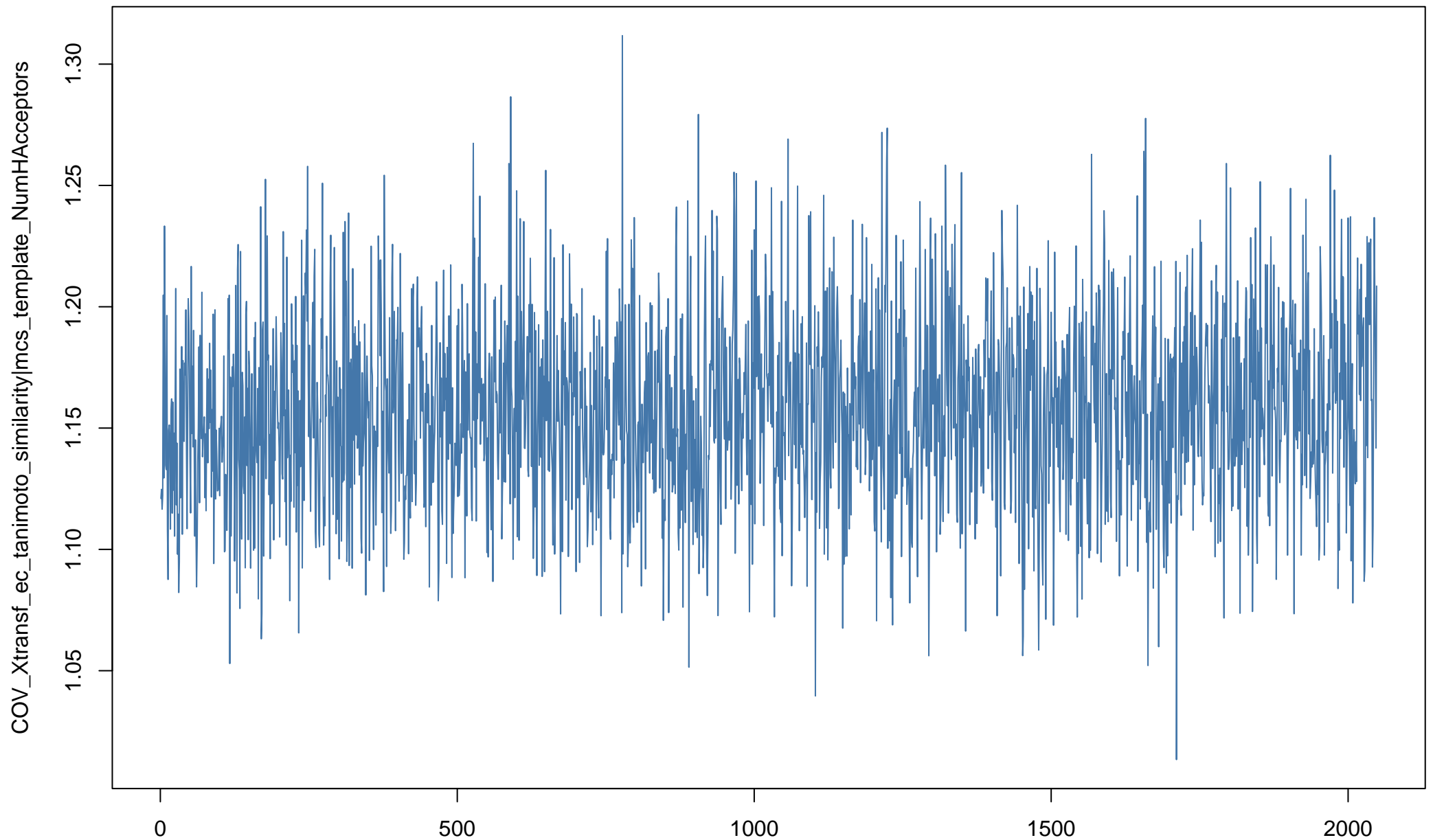
COV\_Xtransf\_ec\_tanimoto\_similarity|template\_HeavyAtomCount  
ESS = 1750 | BMK = 0.0928 | MCSE(6.27) = 3.03 | stat: FALSE | burn: 0



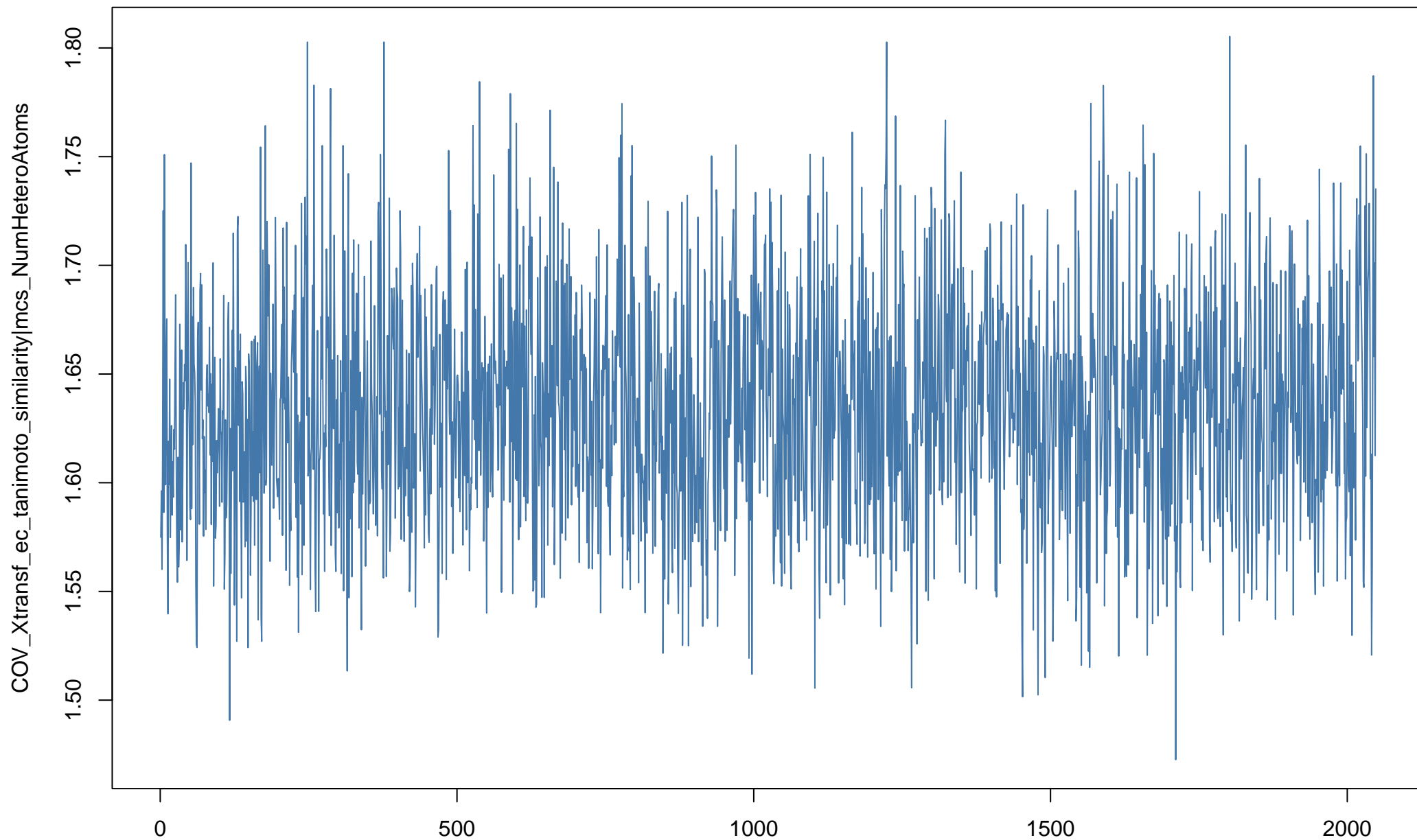
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_docked\_NumHAcceptors**  
**ESS = 1770 | BMK = 0.0517 | MCSE(6.27) = 2.42 | stat: FALSE | burn: 0**



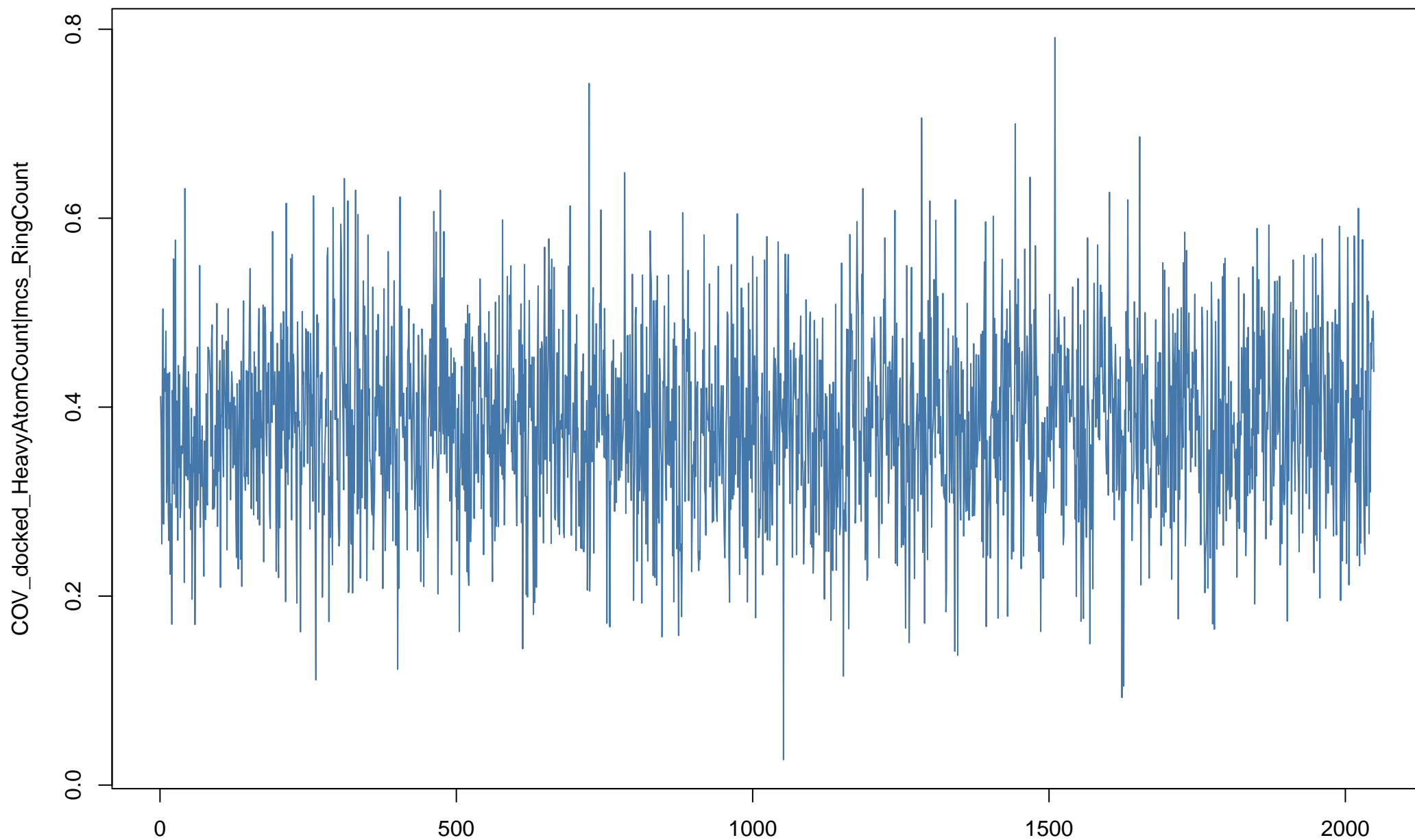
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_template\_NumHAcceptors**  
**ESS = 1780 | BMK = 0.0607 | MCSE(6.27) = 2.24 | stat: FALSE | burn: 0**



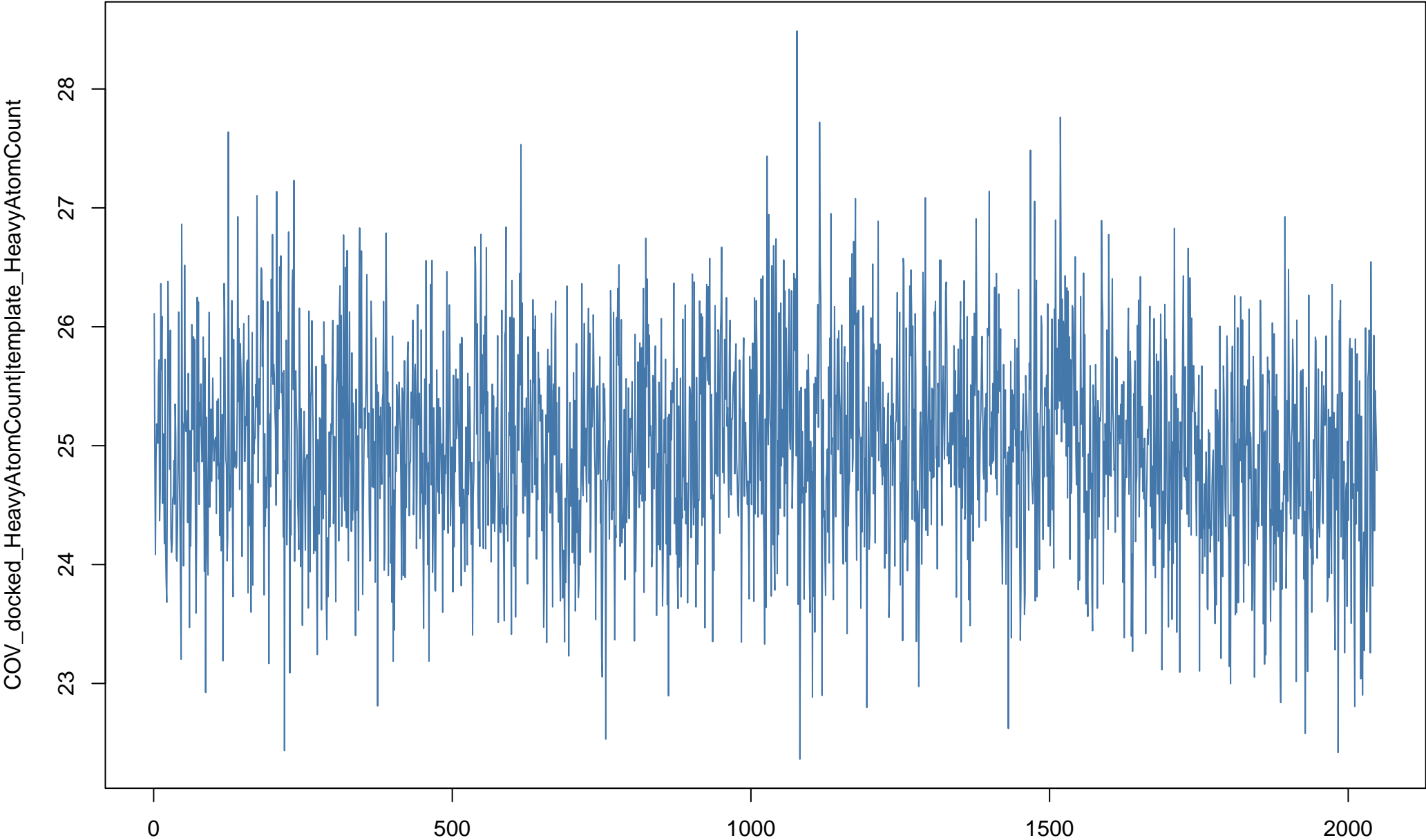
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms**  
**ESS = 1740 | BMK = 0.0417 | MCSE(6.27) = 2.29 | stat: FALSE | burn: 0**



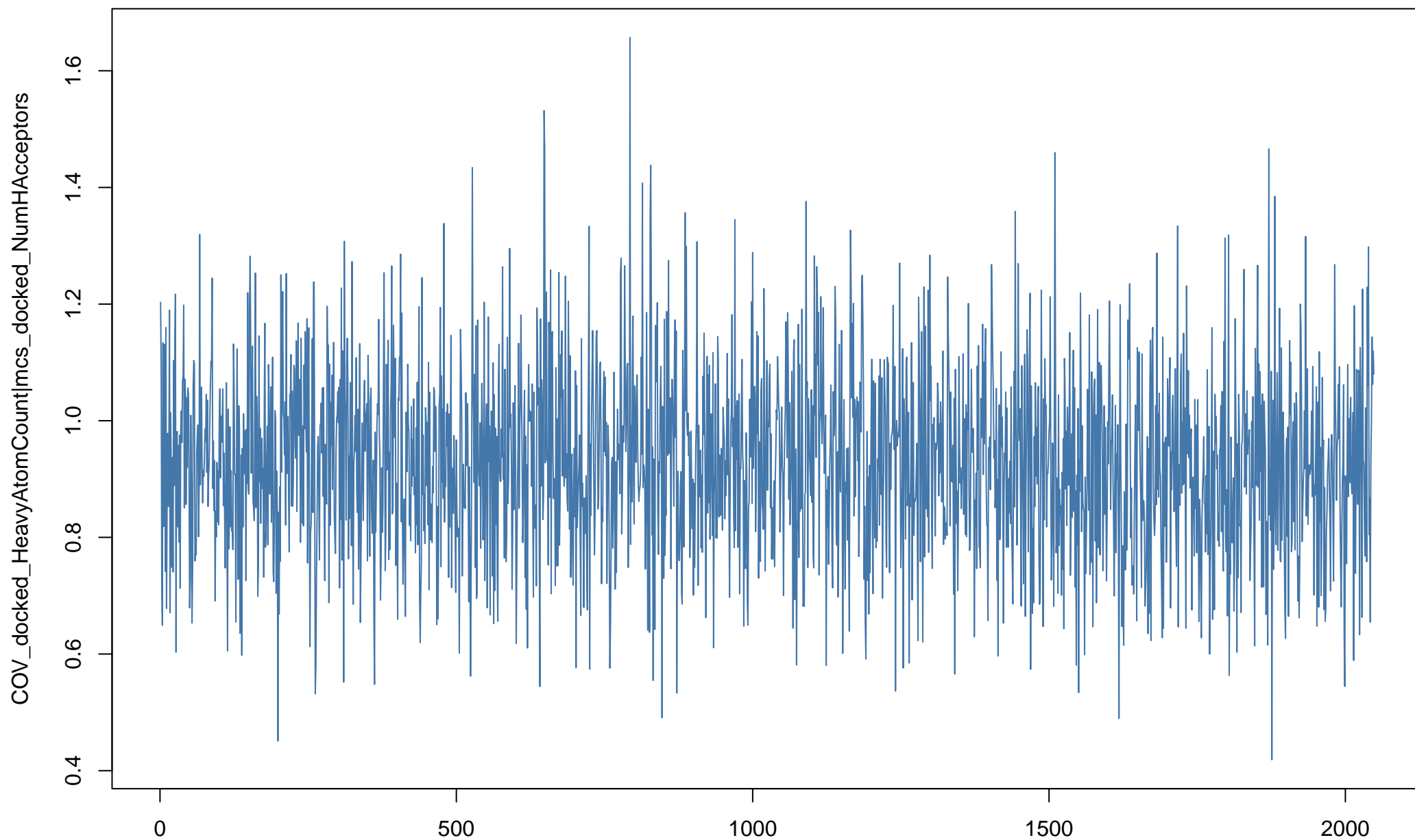
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 2050 | BMK = 0.0437 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0**



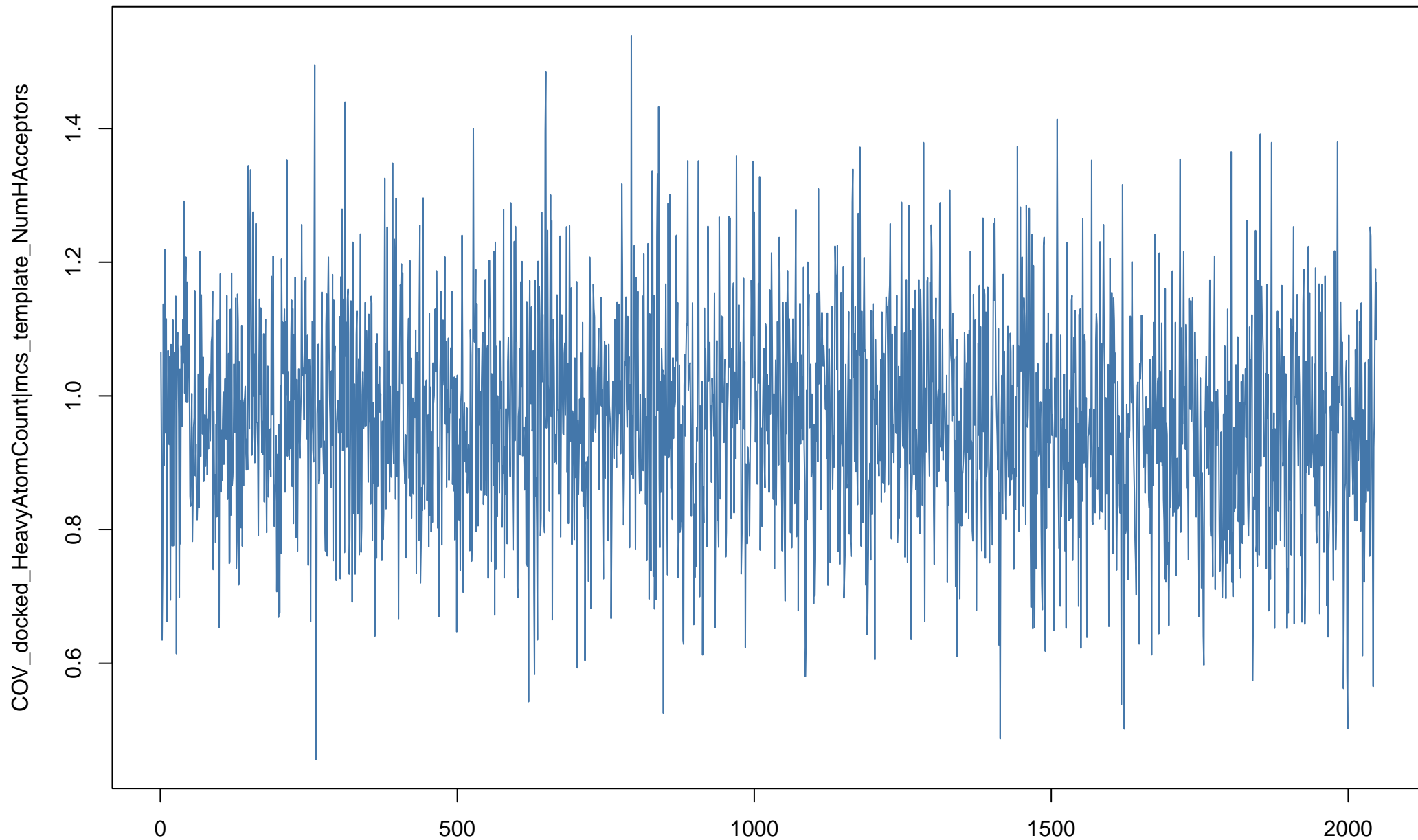
**COV\_docked\_HeavyAtomCount|template\_HeavyAtomCount**  
**ESS = 1340 | BMK = 0.0462 | MCSE(6.27) = 3.6 | stat: TRUE | burn: 0**



**COV\_docked\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 1830 | BMK = 0.0416 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0**

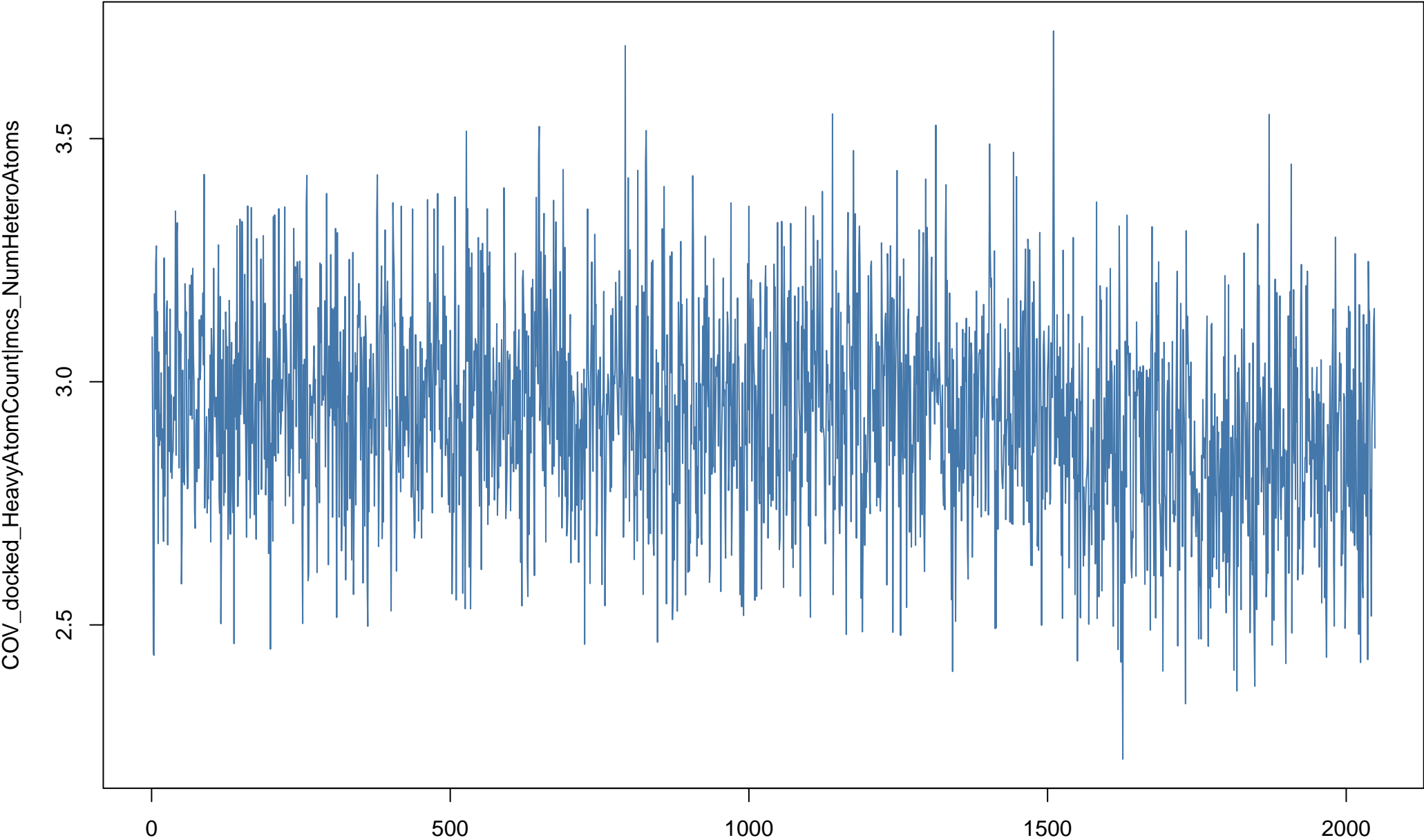


**COV\_docked\_HeavyAtomCount|mcs\_template\_NumHAcceptors**  
**ESS = 1830 | BMK = 0.0664 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0**

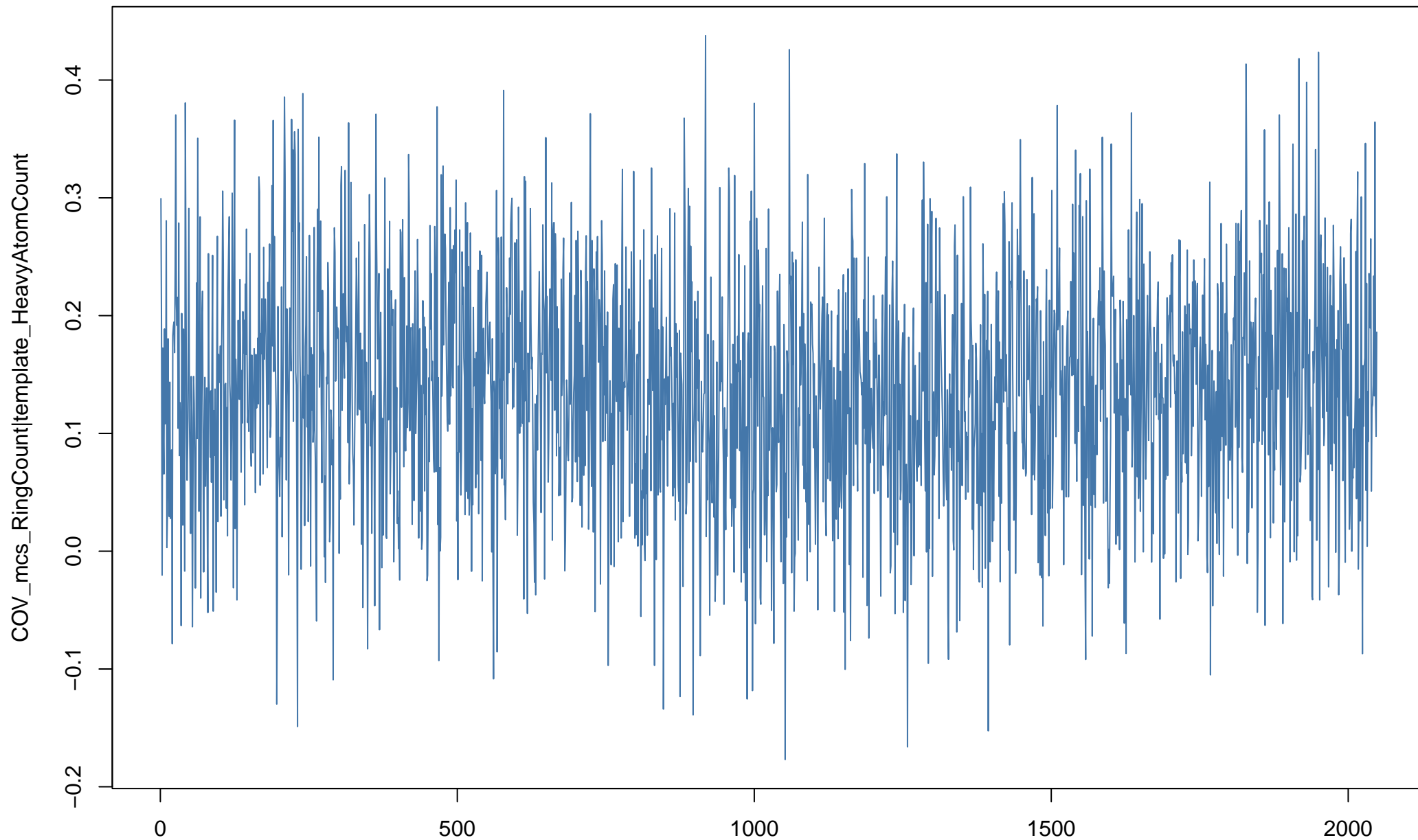




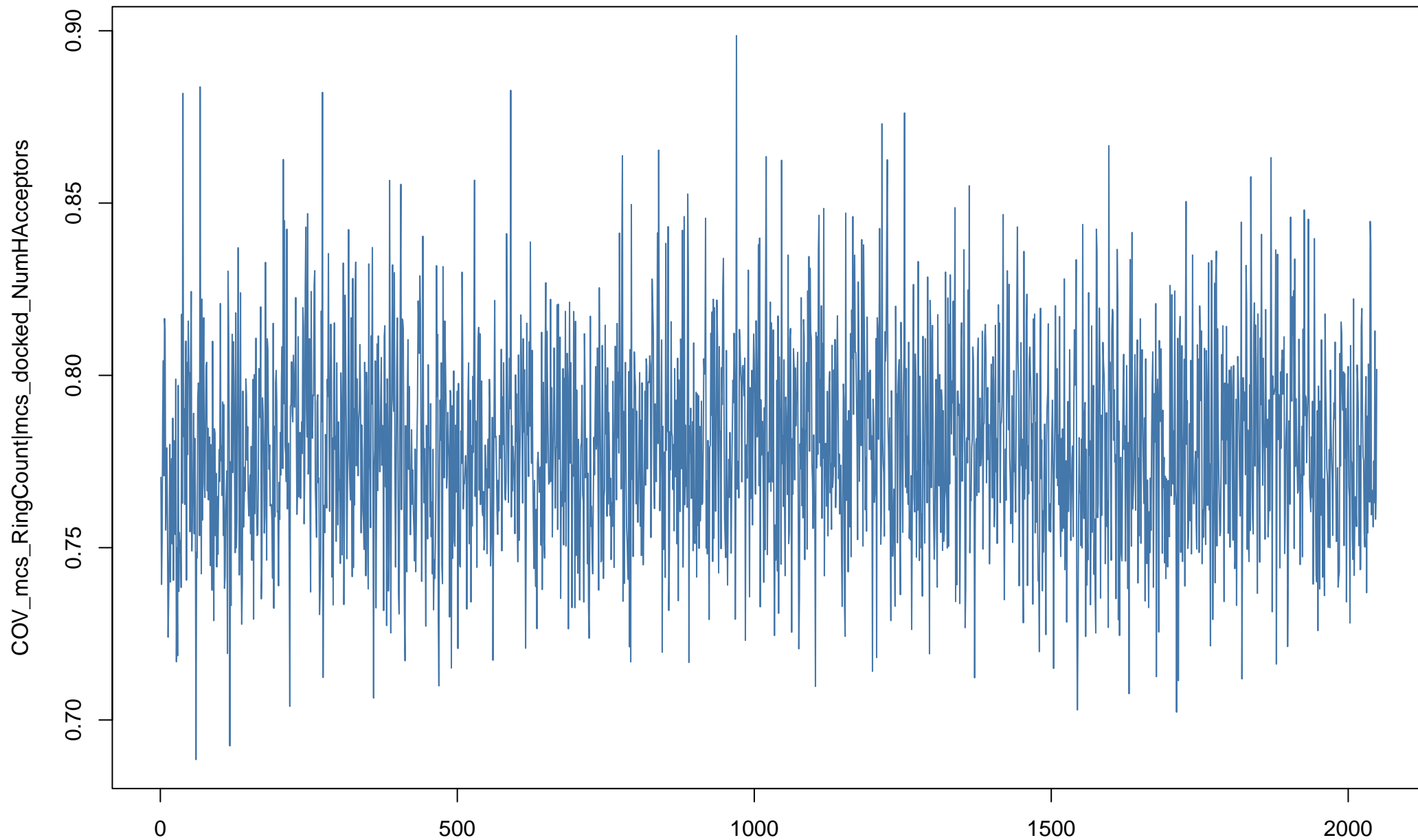
**COV\_docked\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 501 | BMK = 0.108 | MCSE(6.27) = 3.92 | stat: FALSE | burn: 0**



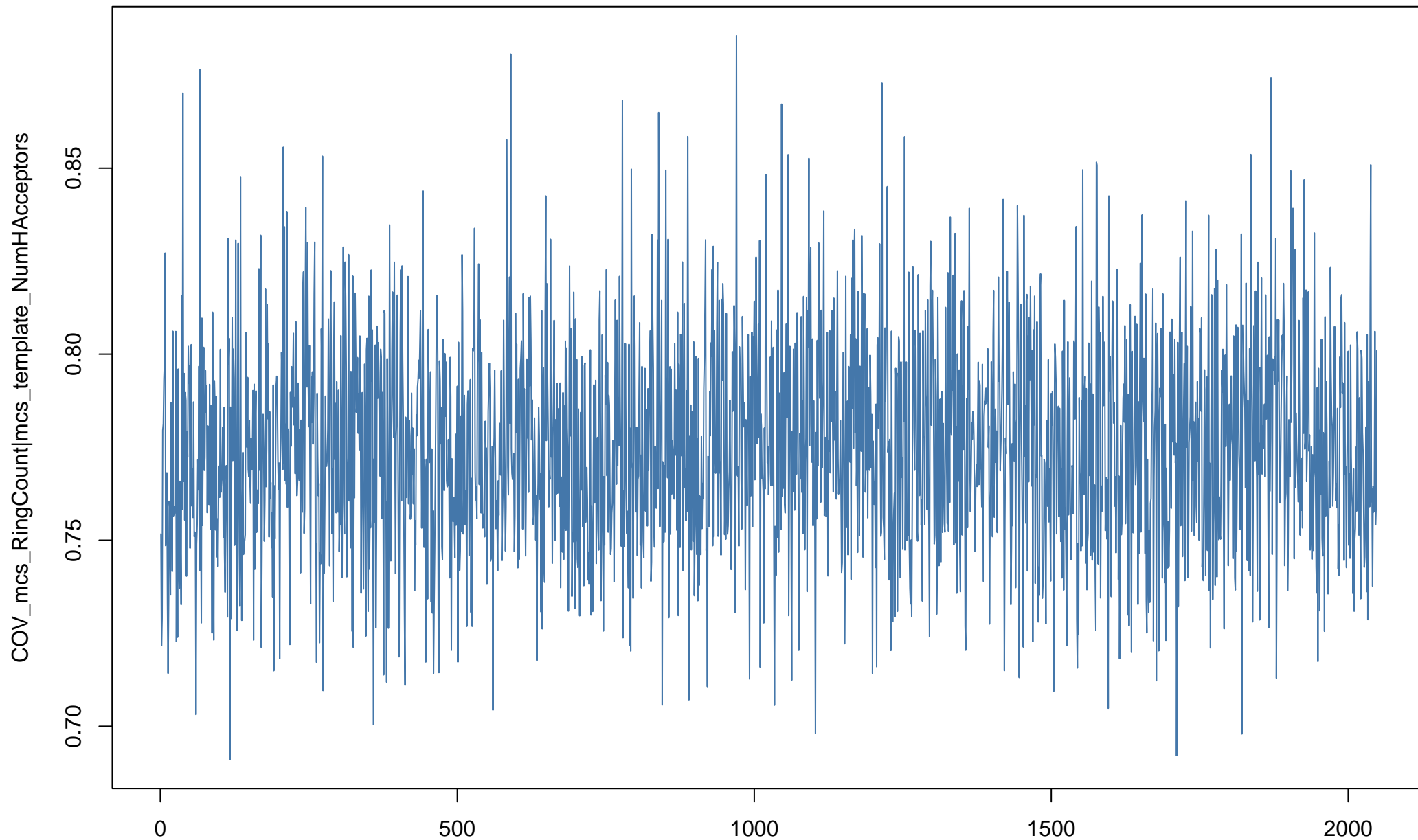
**COV\_mcs\_RingCount|template\_HeavyAtomCount**  
**ESS = 1840 | BMK = 0.0503 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0**



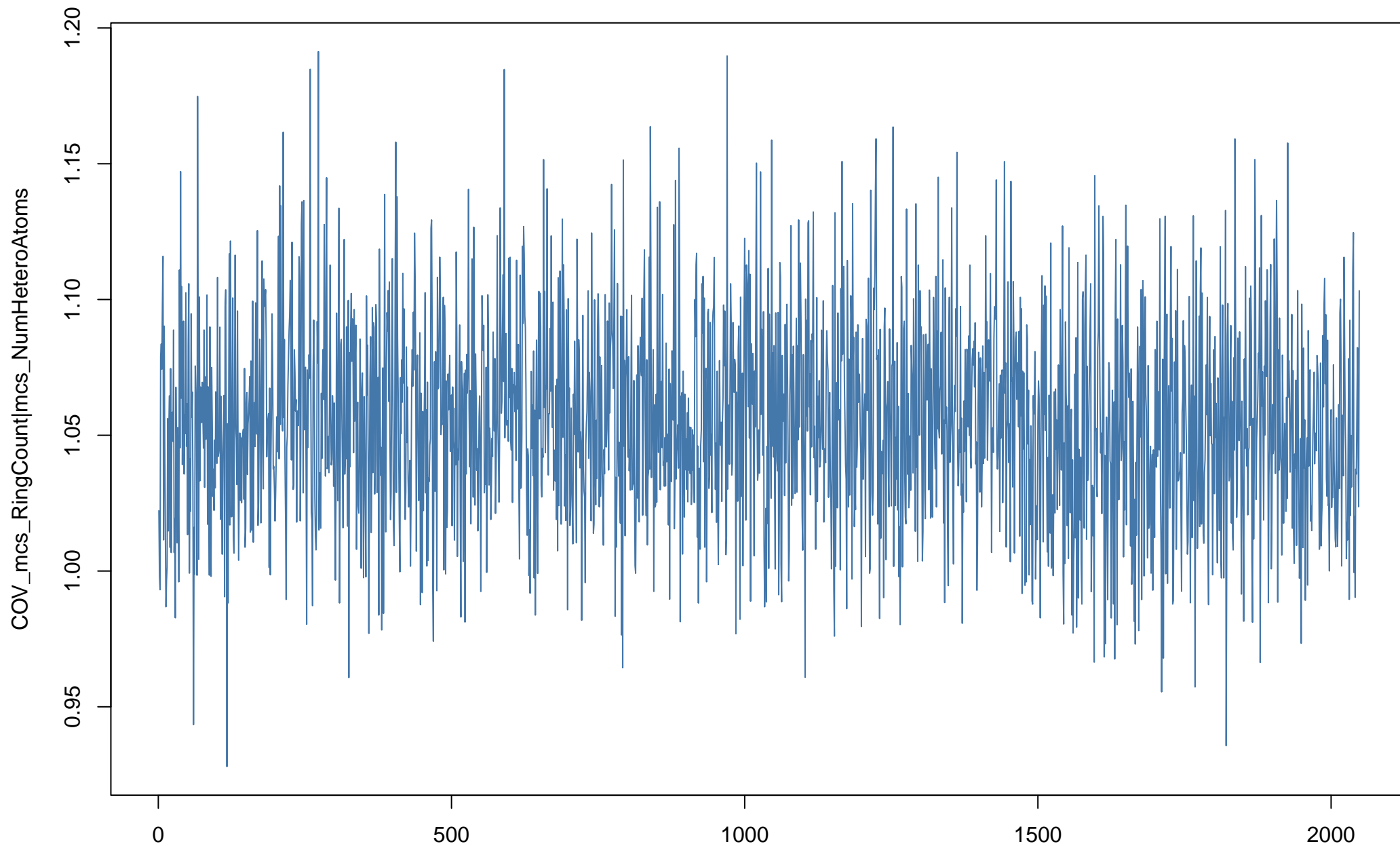
**COV\_mcs\_RingCount|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0454 | MCSE(6.27) = 2.59 | stat: FALSE | burn: 0**



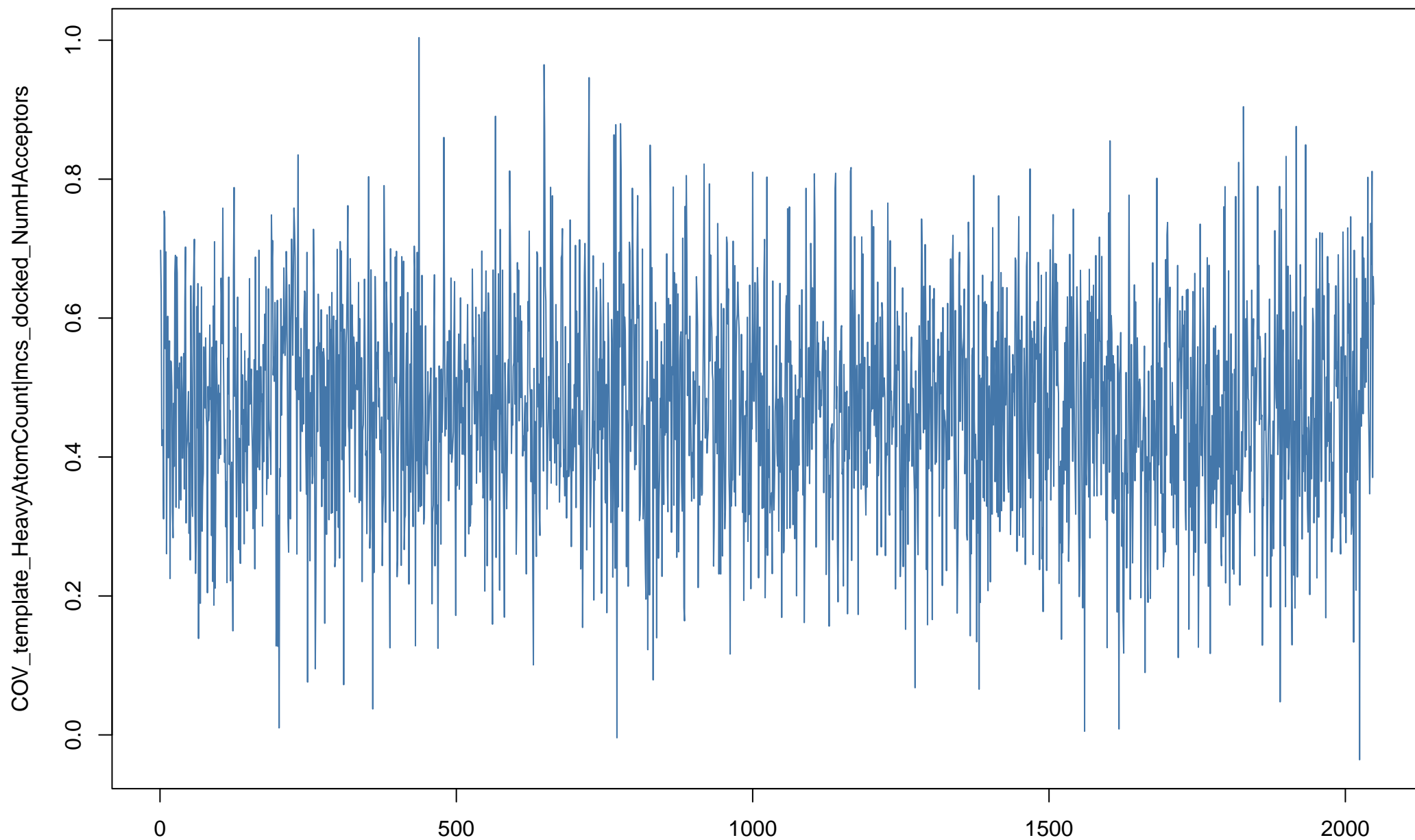
**COV\_mcs\_RingCount|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0513 | MCSE(6.27) = 2.43 | stat: FALSE | burn: 0**



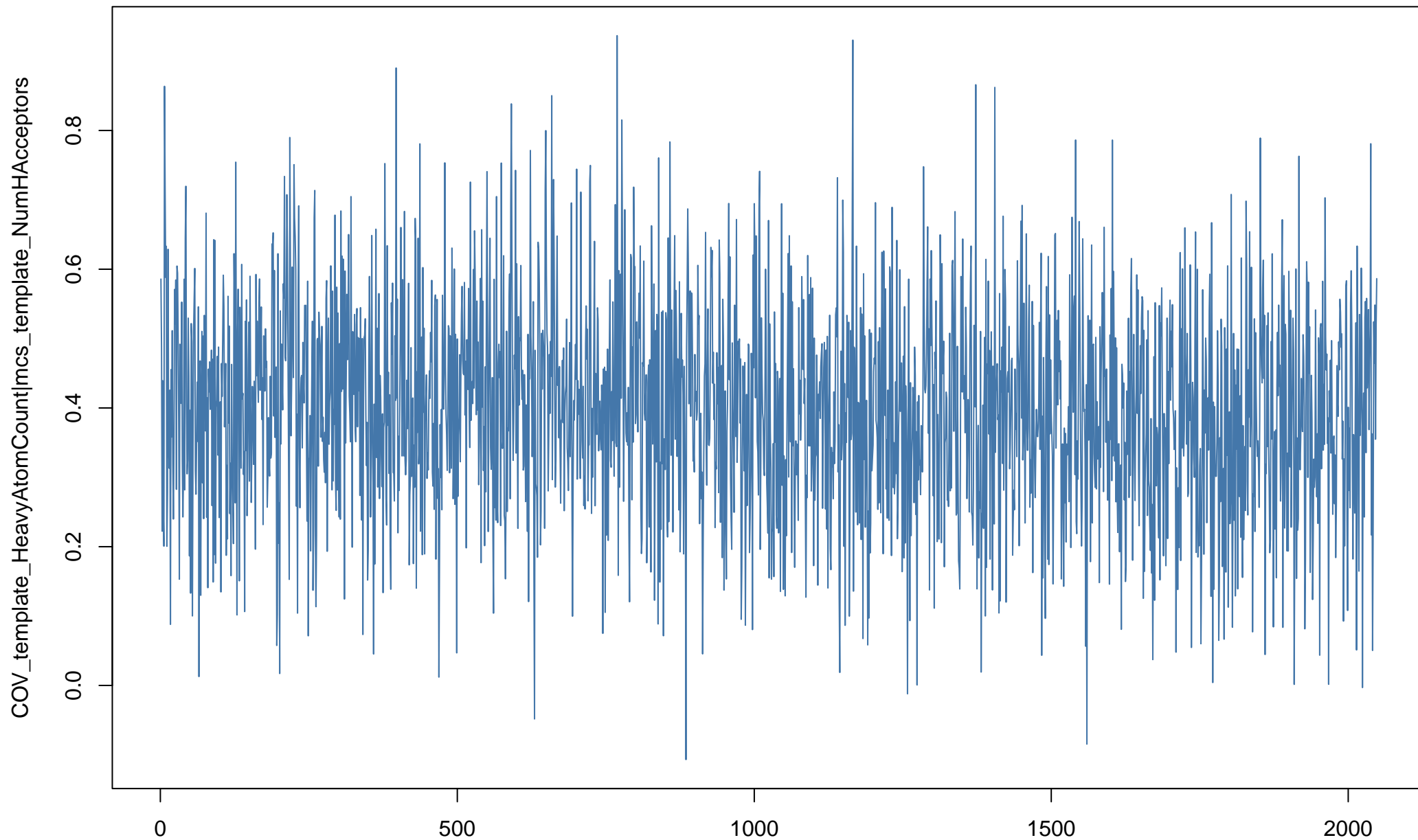
**COV\_mcs\_RingCount|mcs\_NumHeteroAtoms**  
**ESS = 1840 | BMK = 0.0632 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0**



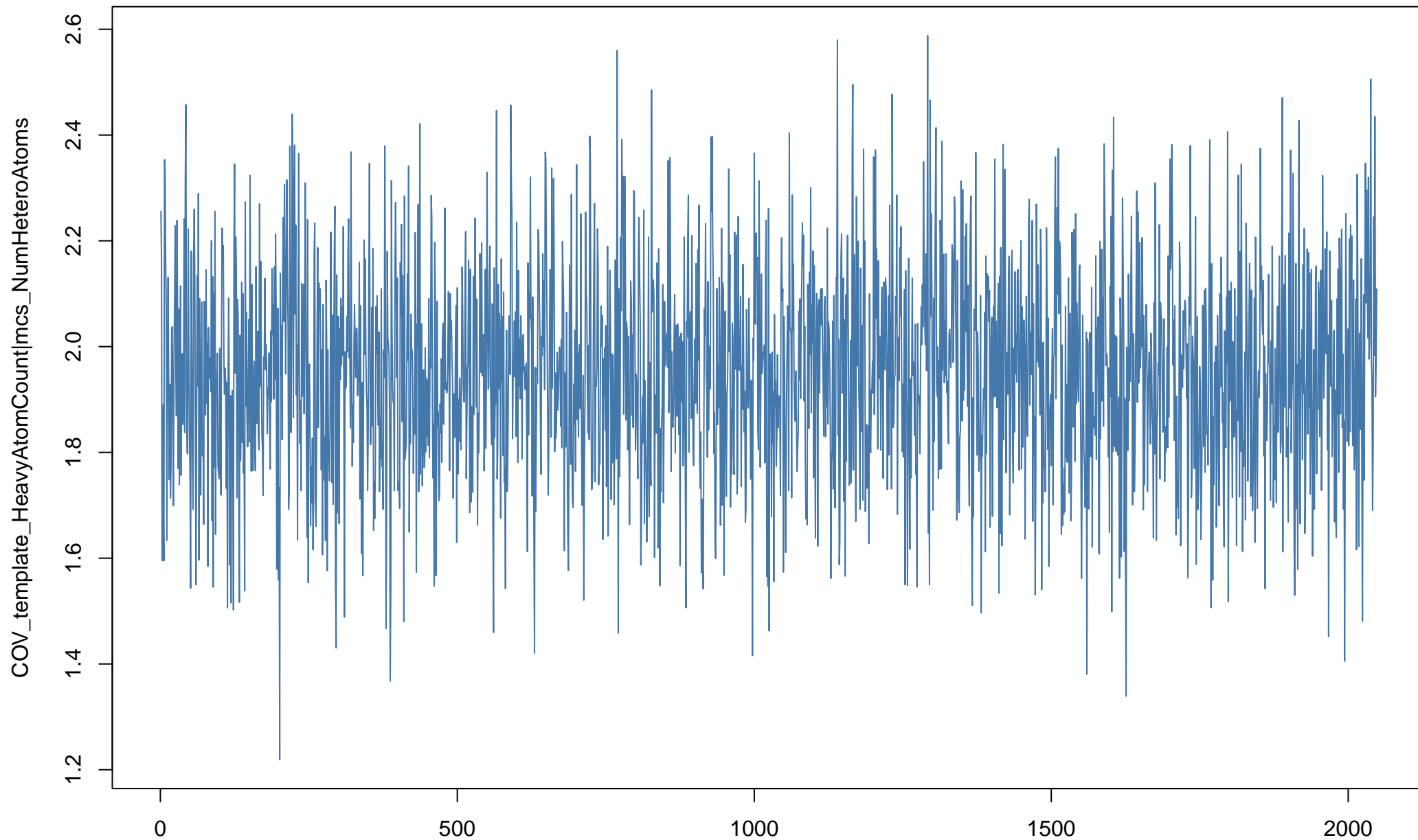
**COV\_template\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 1880 | BMK = 0.0427 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0**



**COV\_template\_HeavyAtomCount|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0868 | MCSE(6.27) = 2.57 | stat: FALSE | burn: 0**

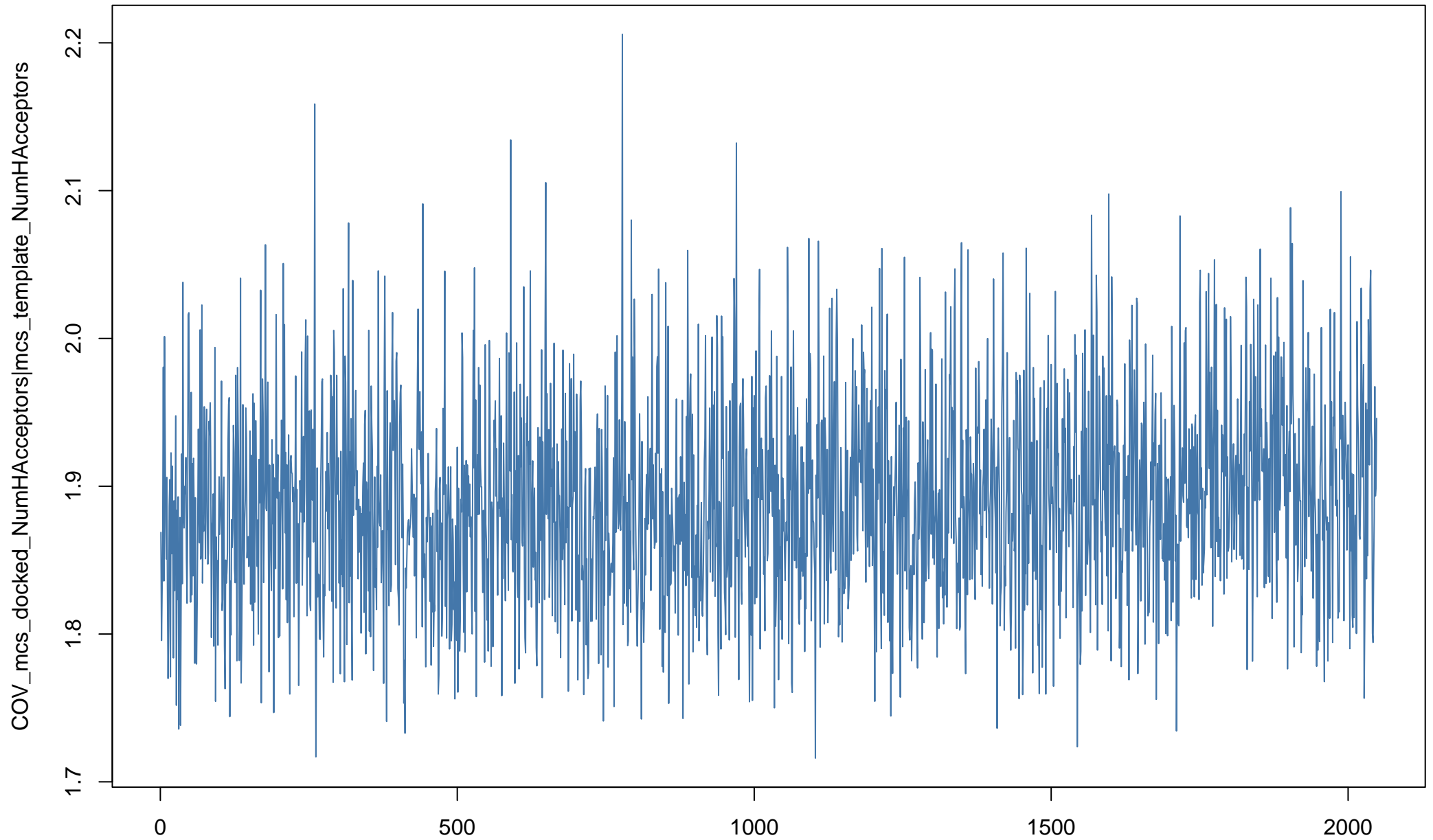


**COV\_template\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 1840 | BMK = 0.0409 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0**

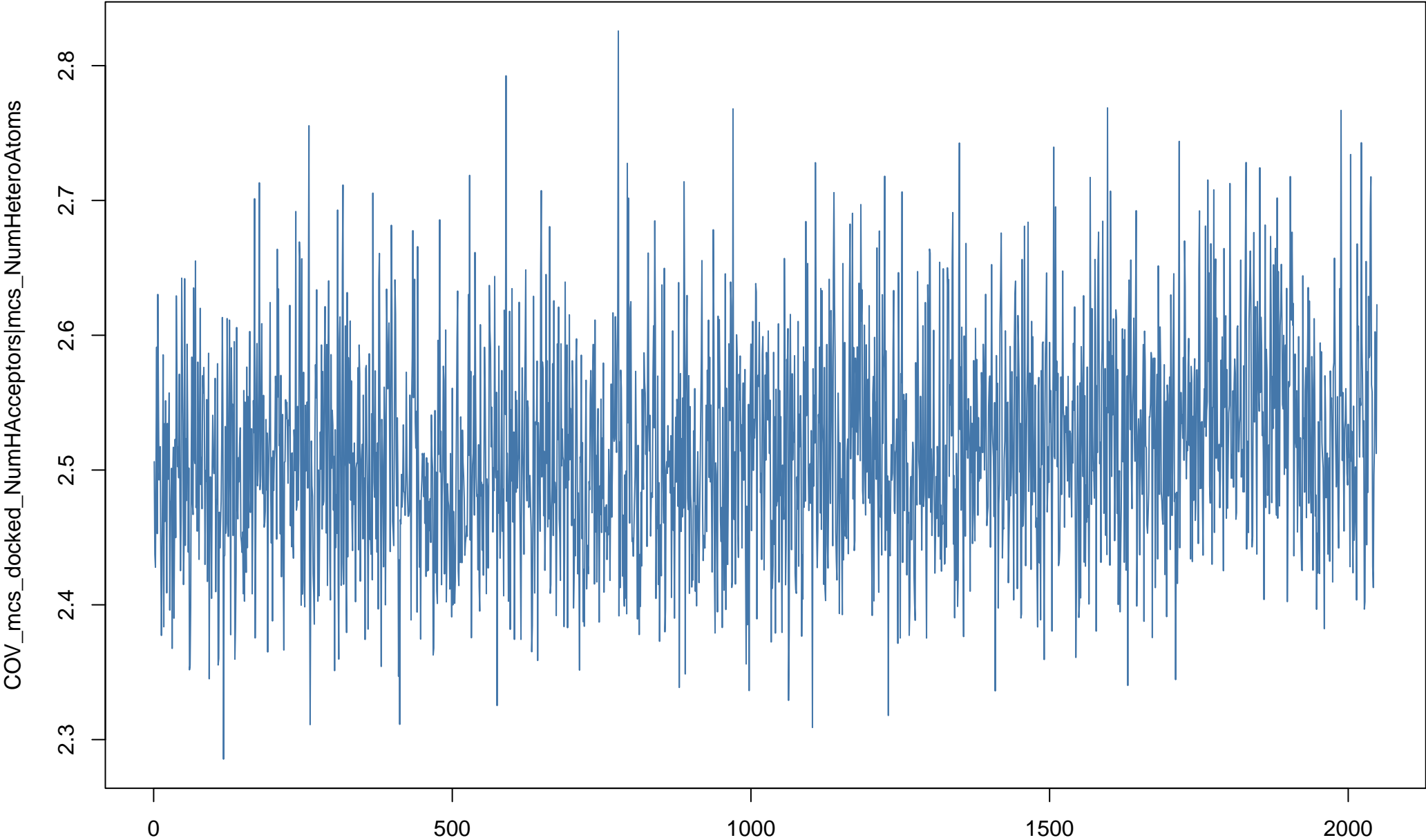




**COV\_mcs\_docked\_NumHAcceptors|mcs\_template\_NumHAcceptors**  
**ESS = 1750 | BMK = 0.091 | MCSE(6.27) = 2.85 | stat: FALSE | burn: 0**



**COV\_mcs\_docked\_NumHAcceptors|mcs\_NumHeteroAtoms**  
**ESS = 540 | BMK = 0.117 | MCSE(6.27) = 3.49 | stat: FALSE | burn: 0**



COV\_mcs\_template\_NumHAcceptors|mcs\_NumHeteroAtoms  
ESS = 861 | BMK = 0.116 | MCSE(6.27) = 3.56 | stat: FALSE | burn: 0

