

-- STATS maxD --

min ESS = 3.23812205843075

max BMK = 0.913160858849009

max MCSE = 14.7165578393178

all stationary: FALSE

burn: 2040

-- STATS 2D --

min ESS = 262.267754309019

max BMK = 0.144958033825794

max MCSE = 4.02909600930449

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.644167081150378

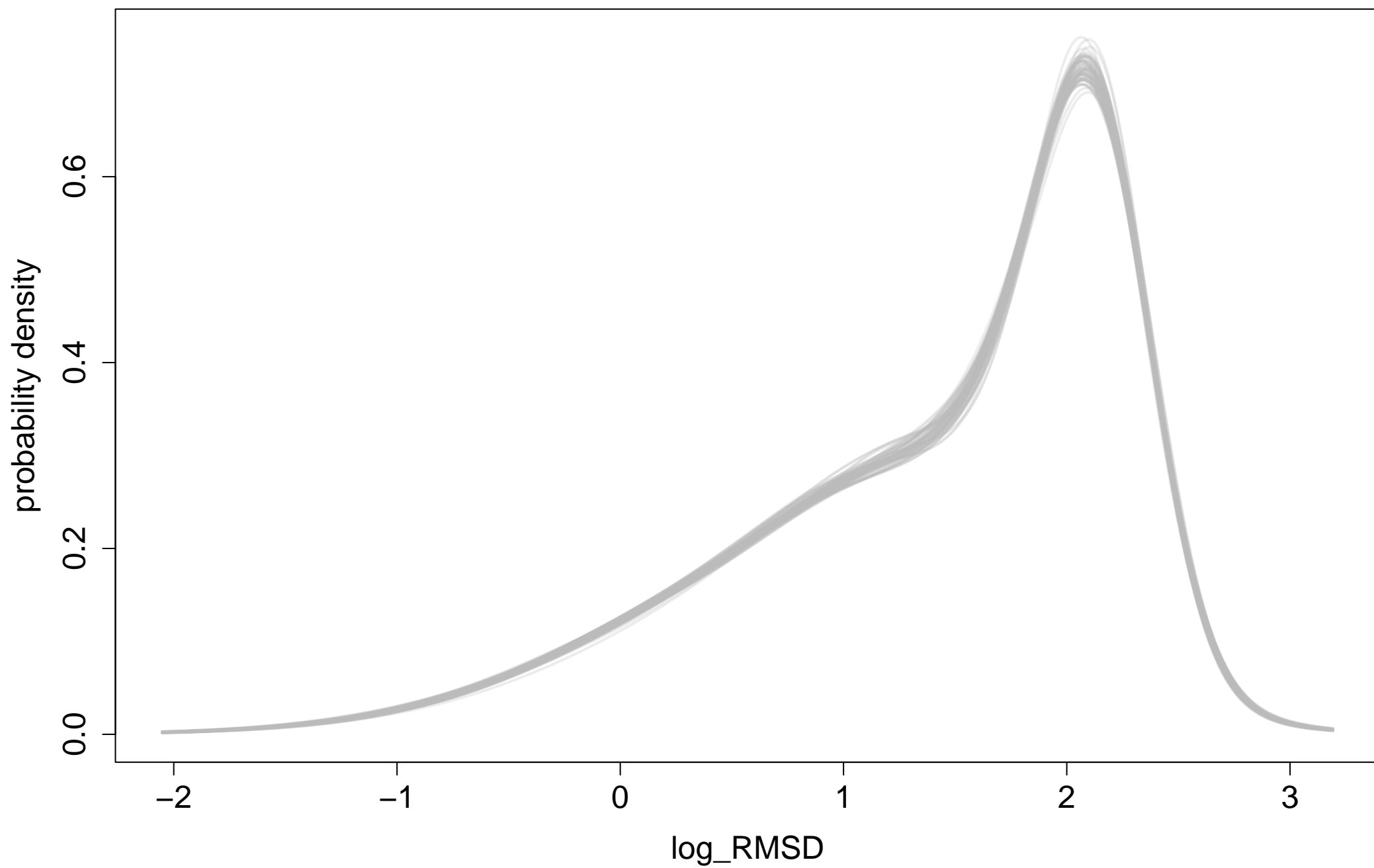
max MCSE = NaN

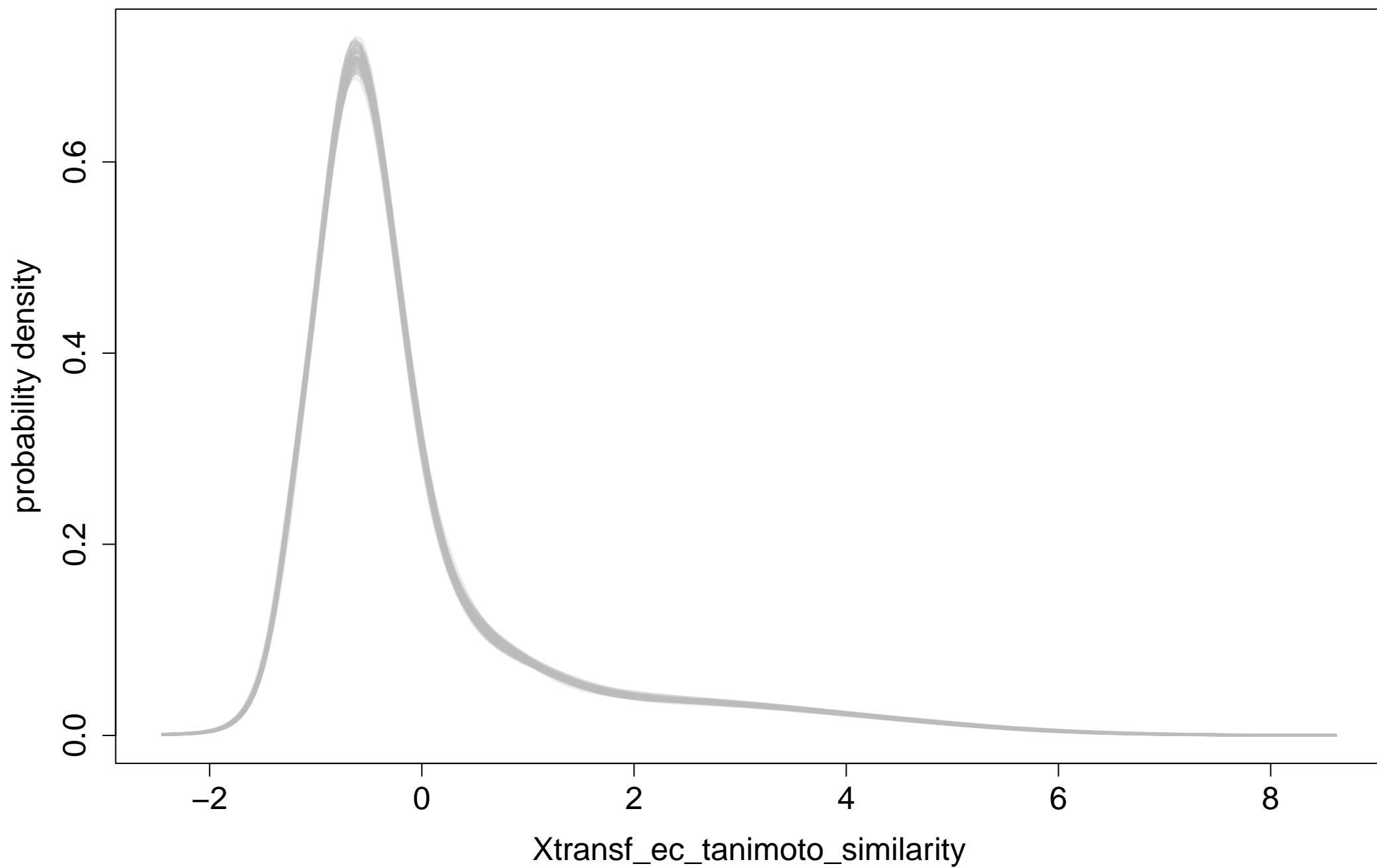
all stationary: FALSE

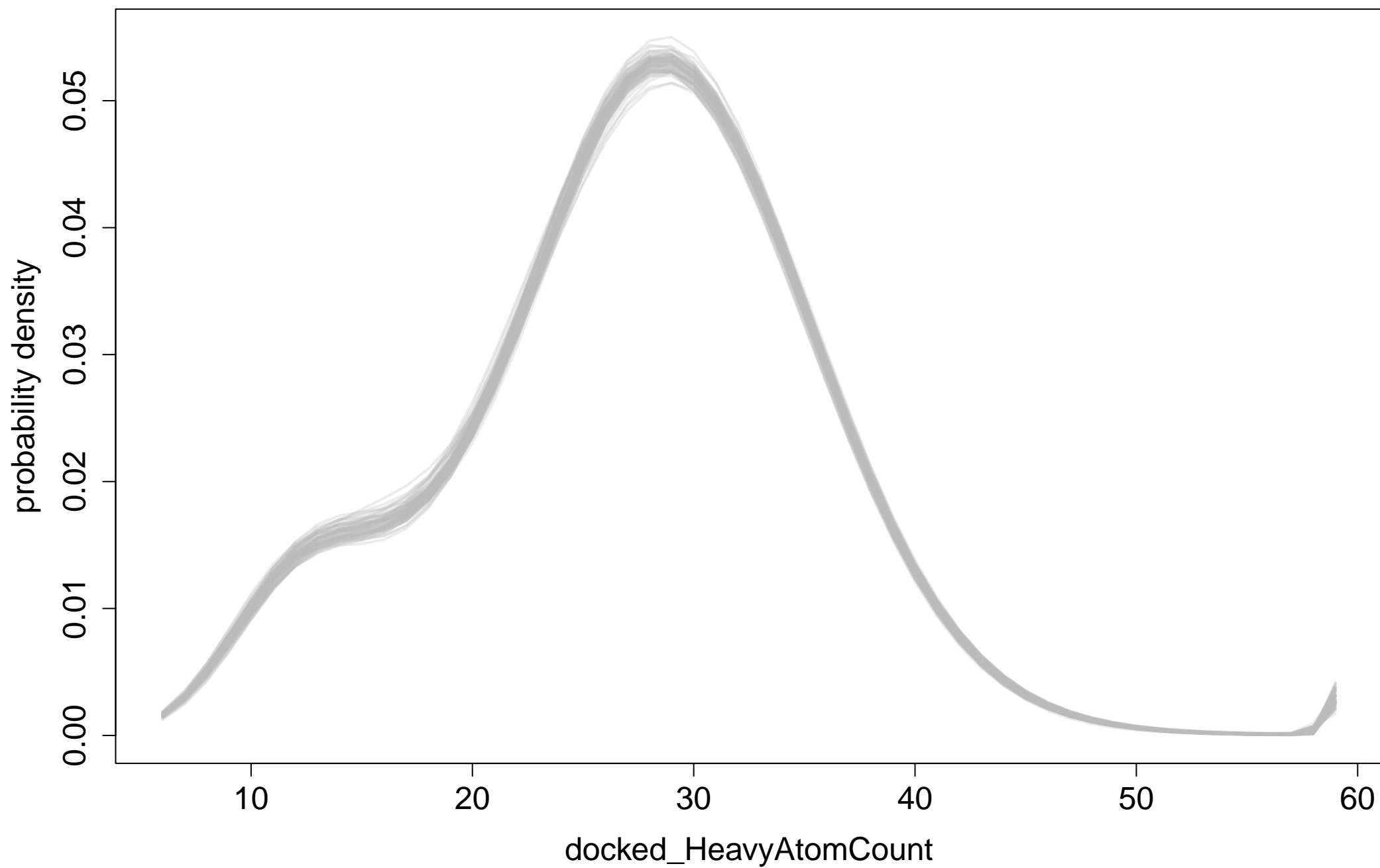
burn: 2040

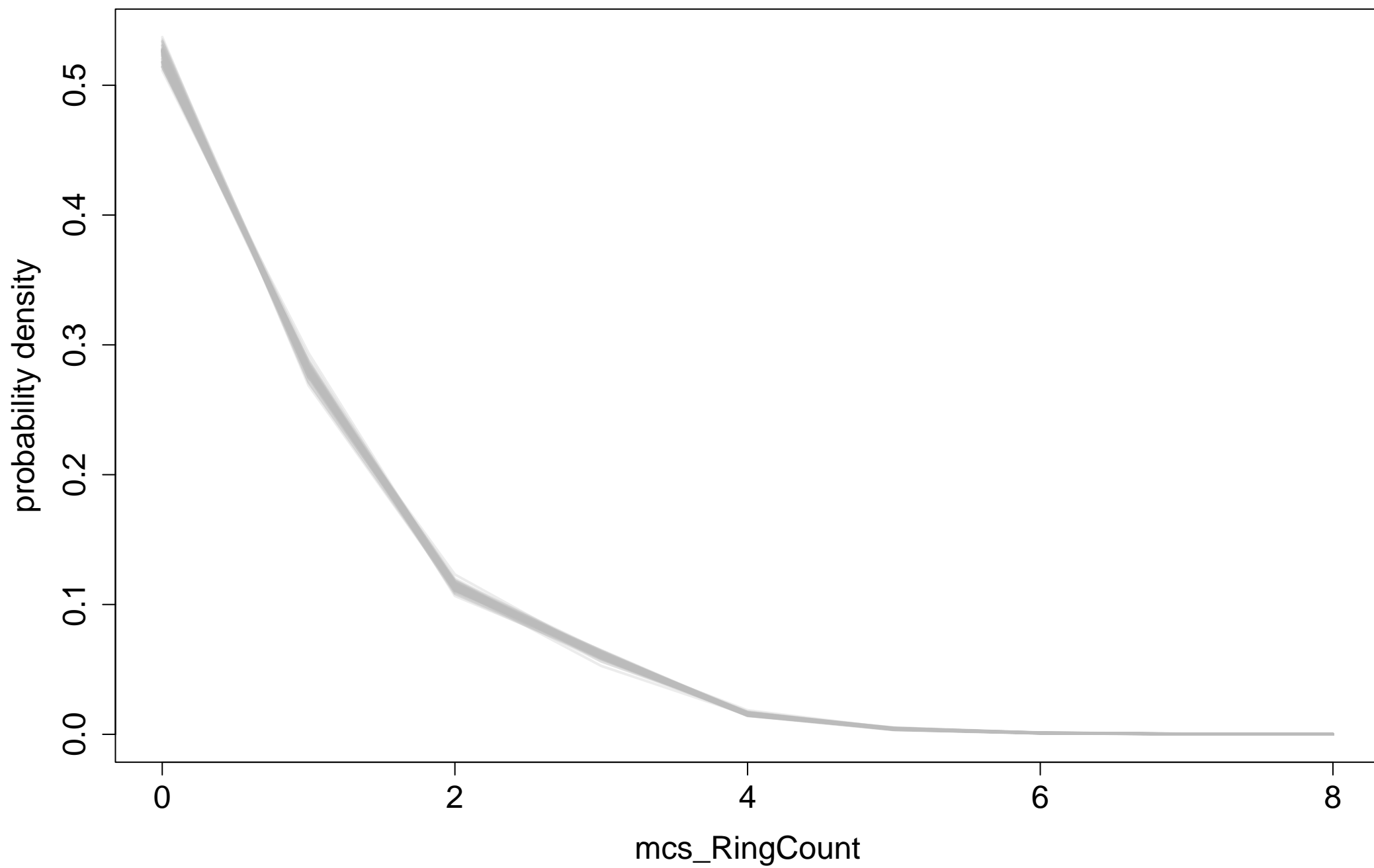
Occupied clusters: 56 of 91

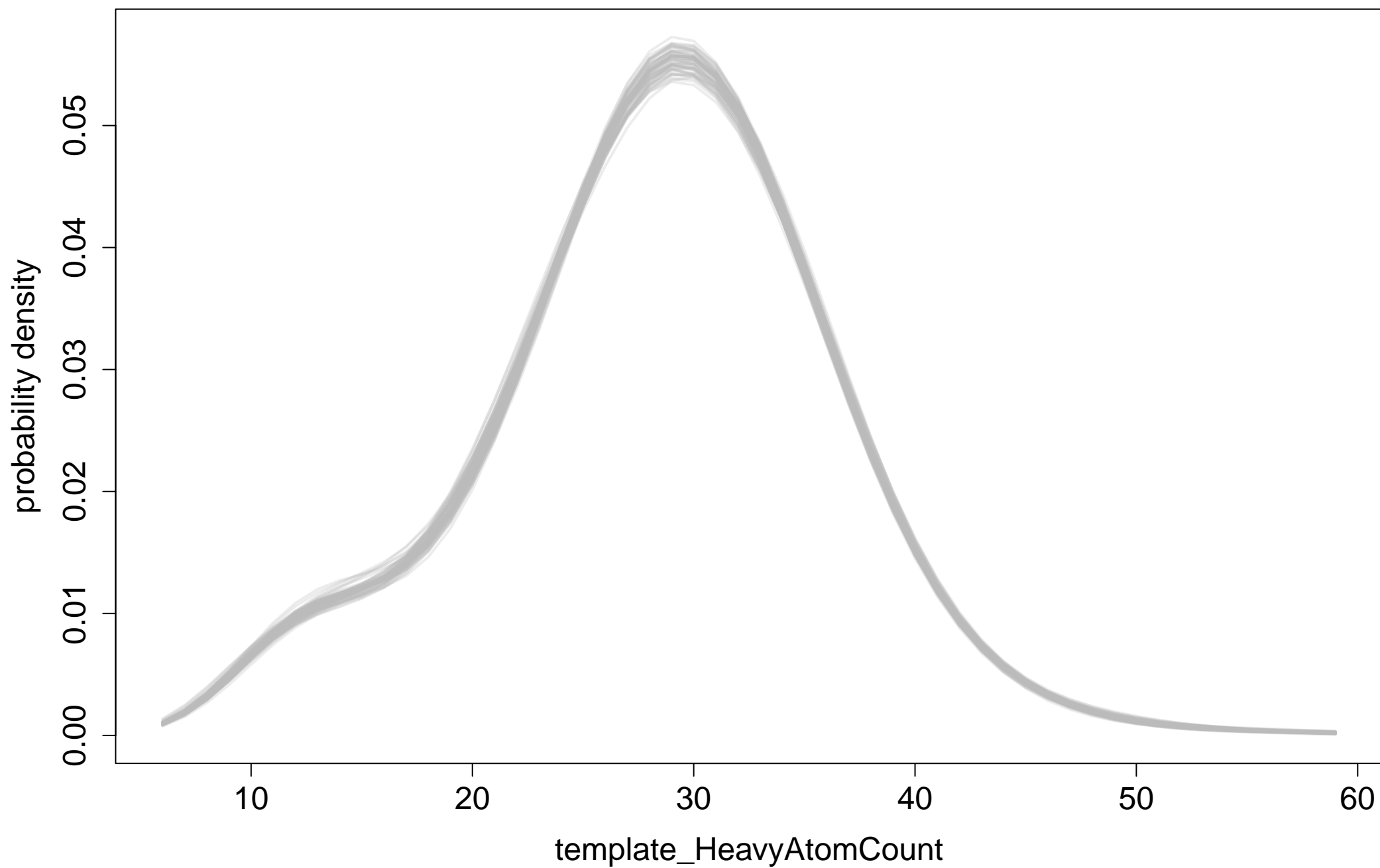
LL: -111000 +- 198

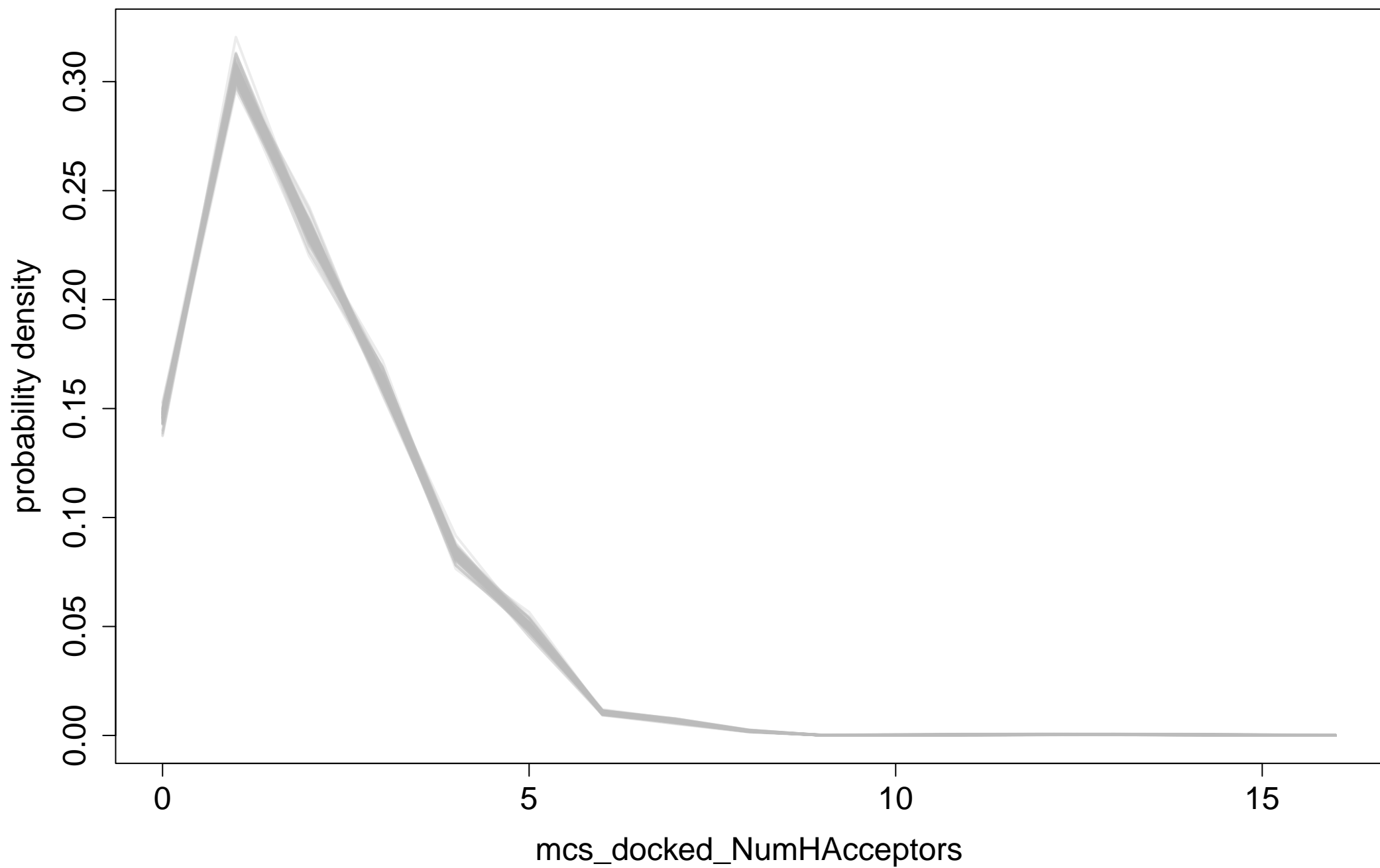


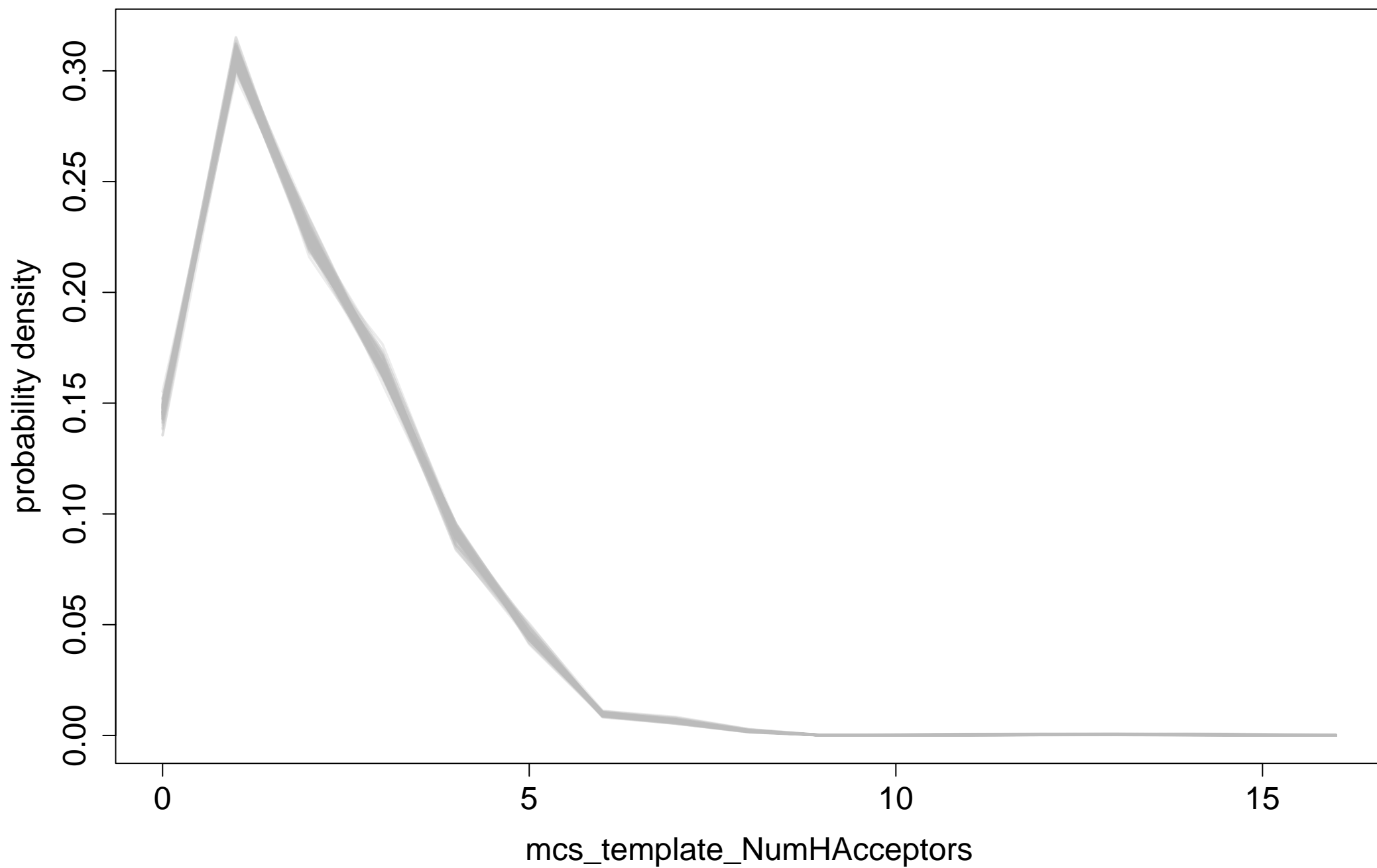




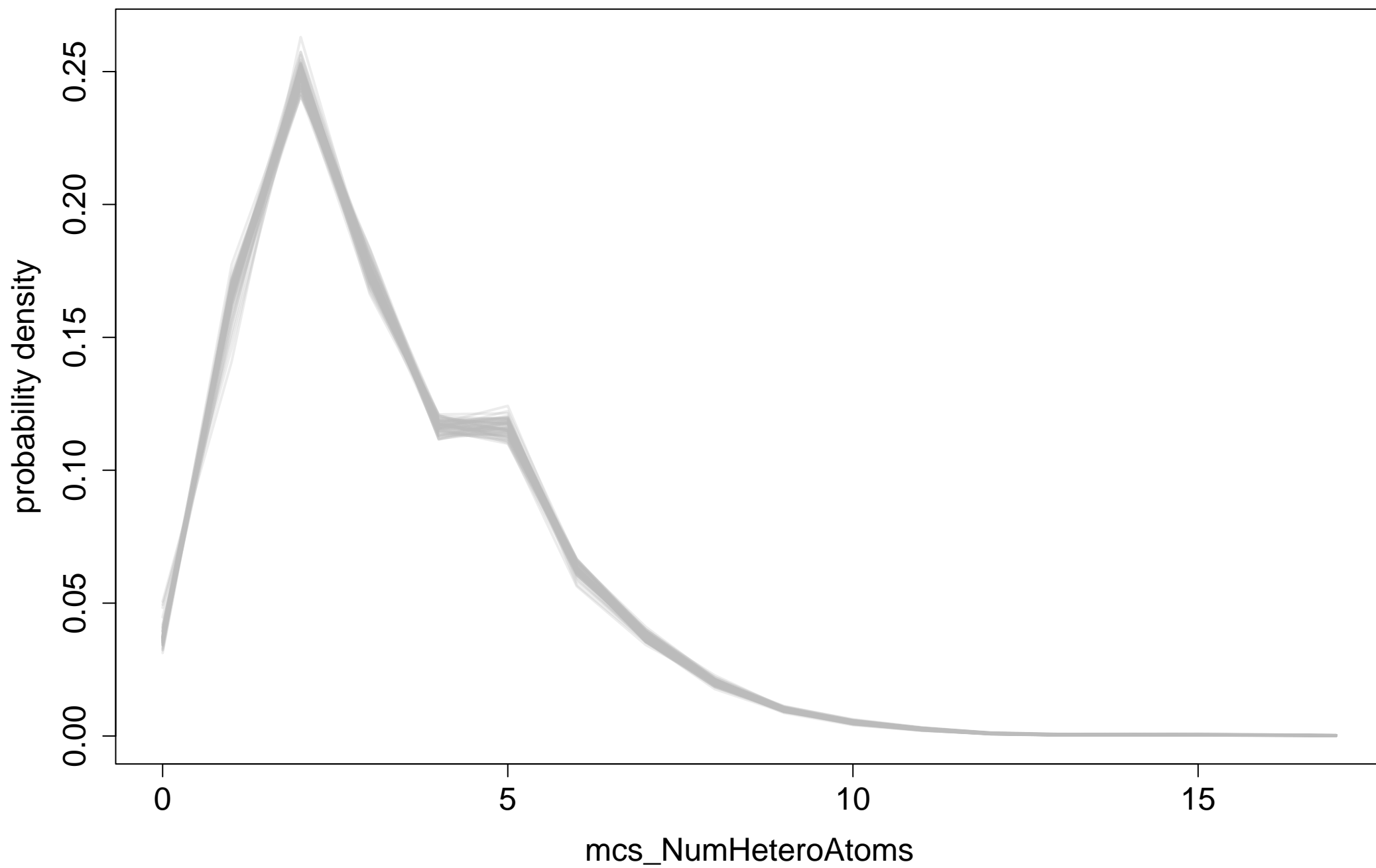


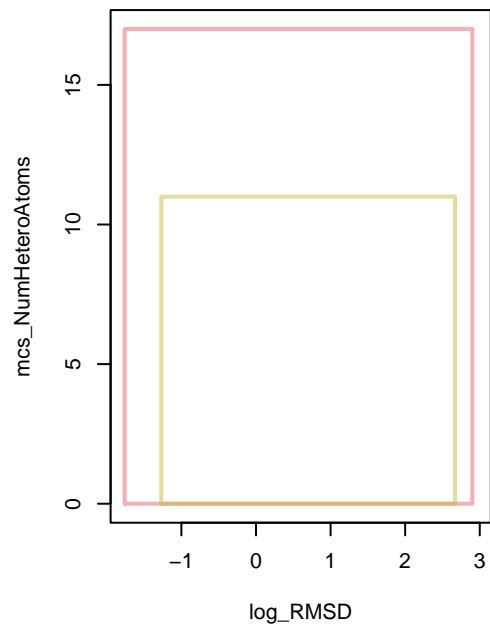
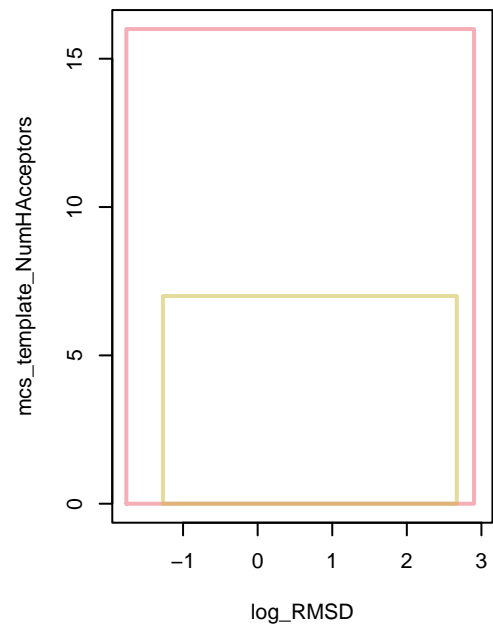
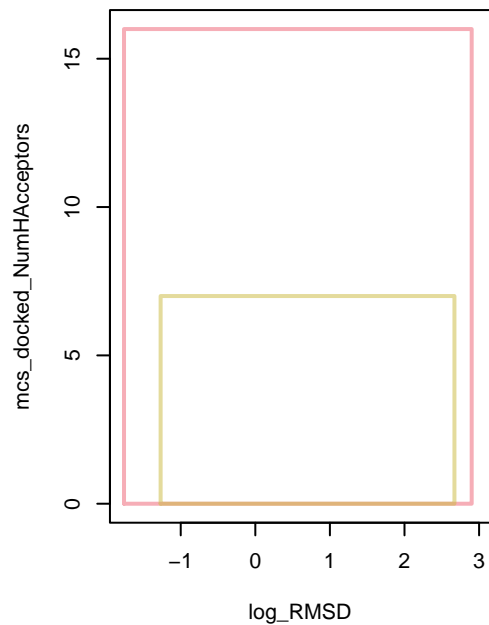
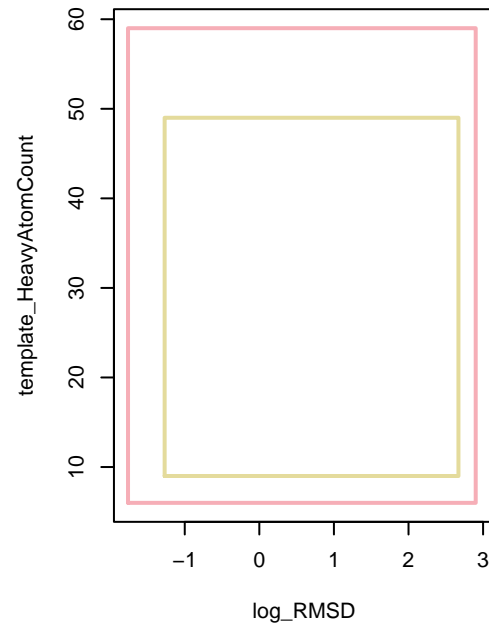
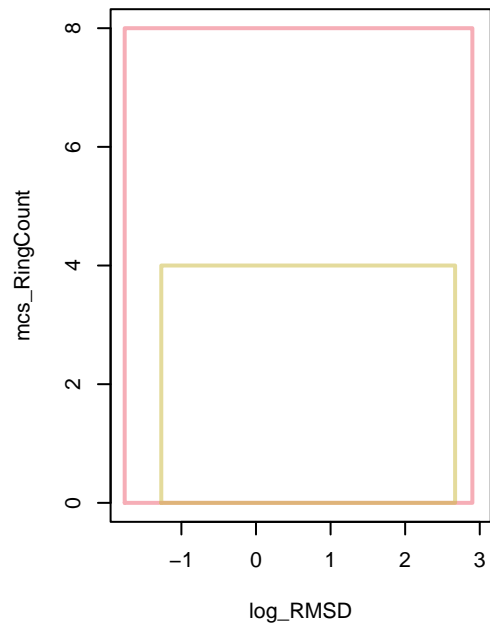
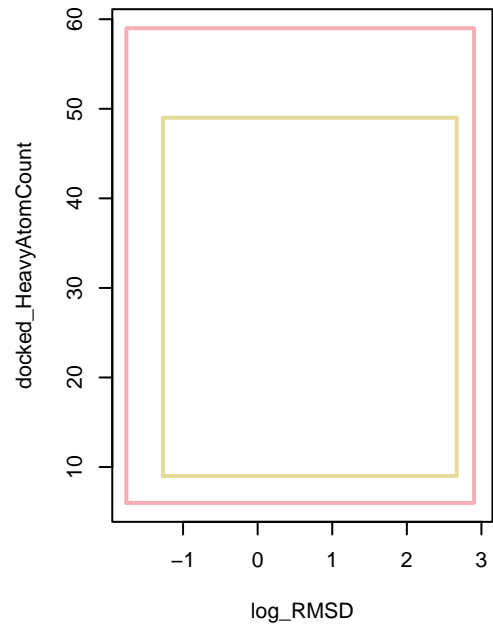
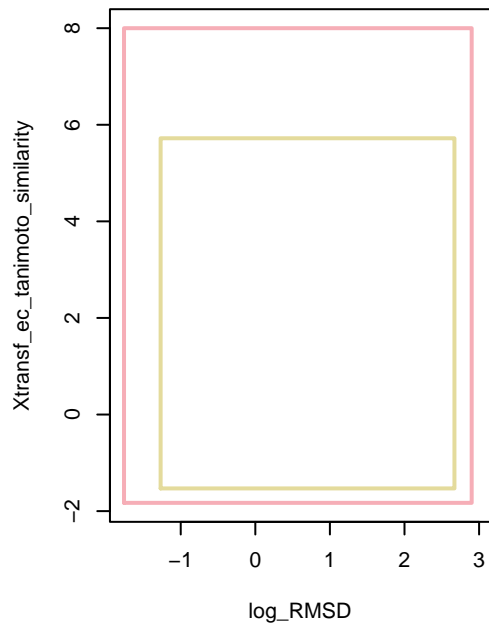




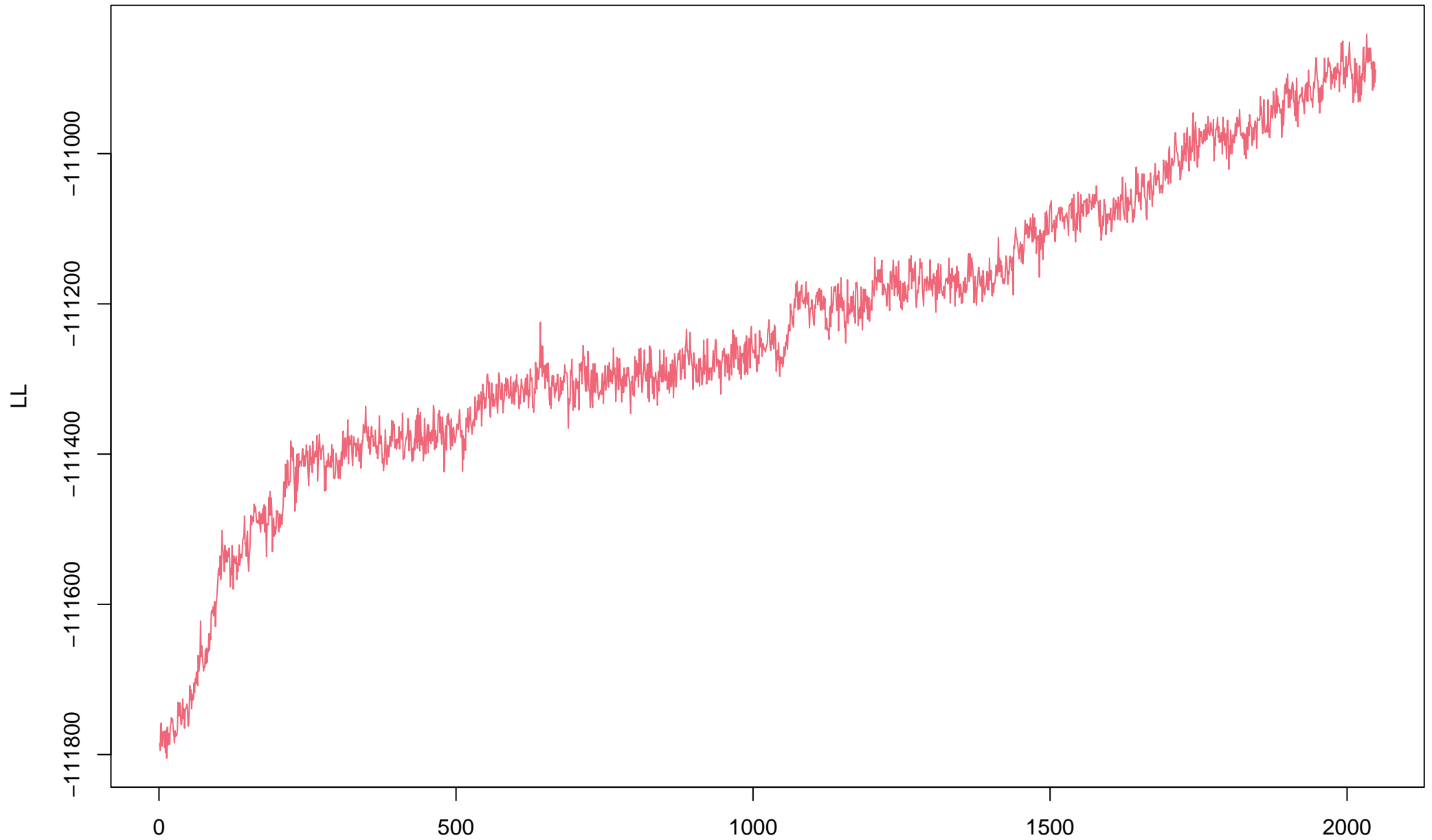




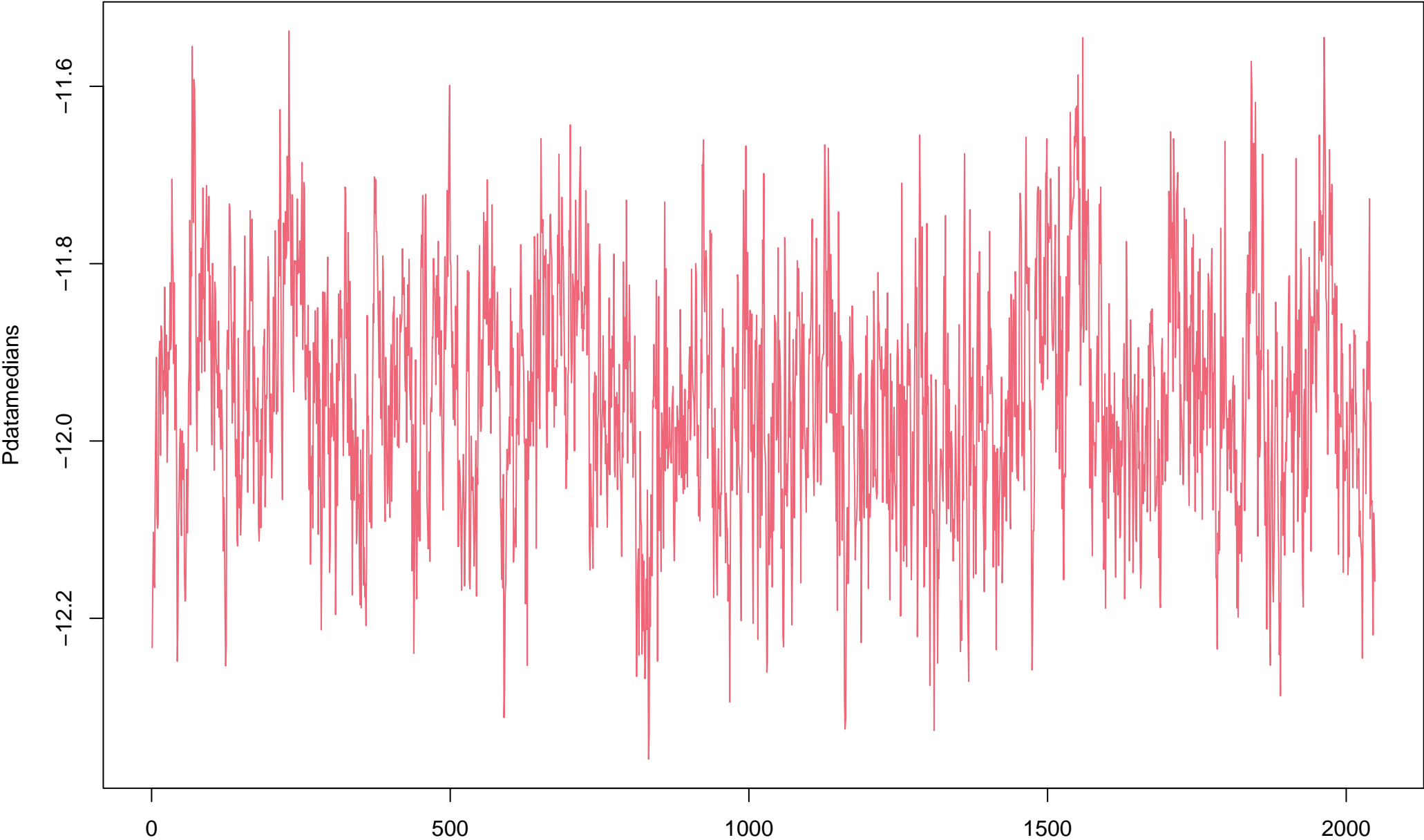




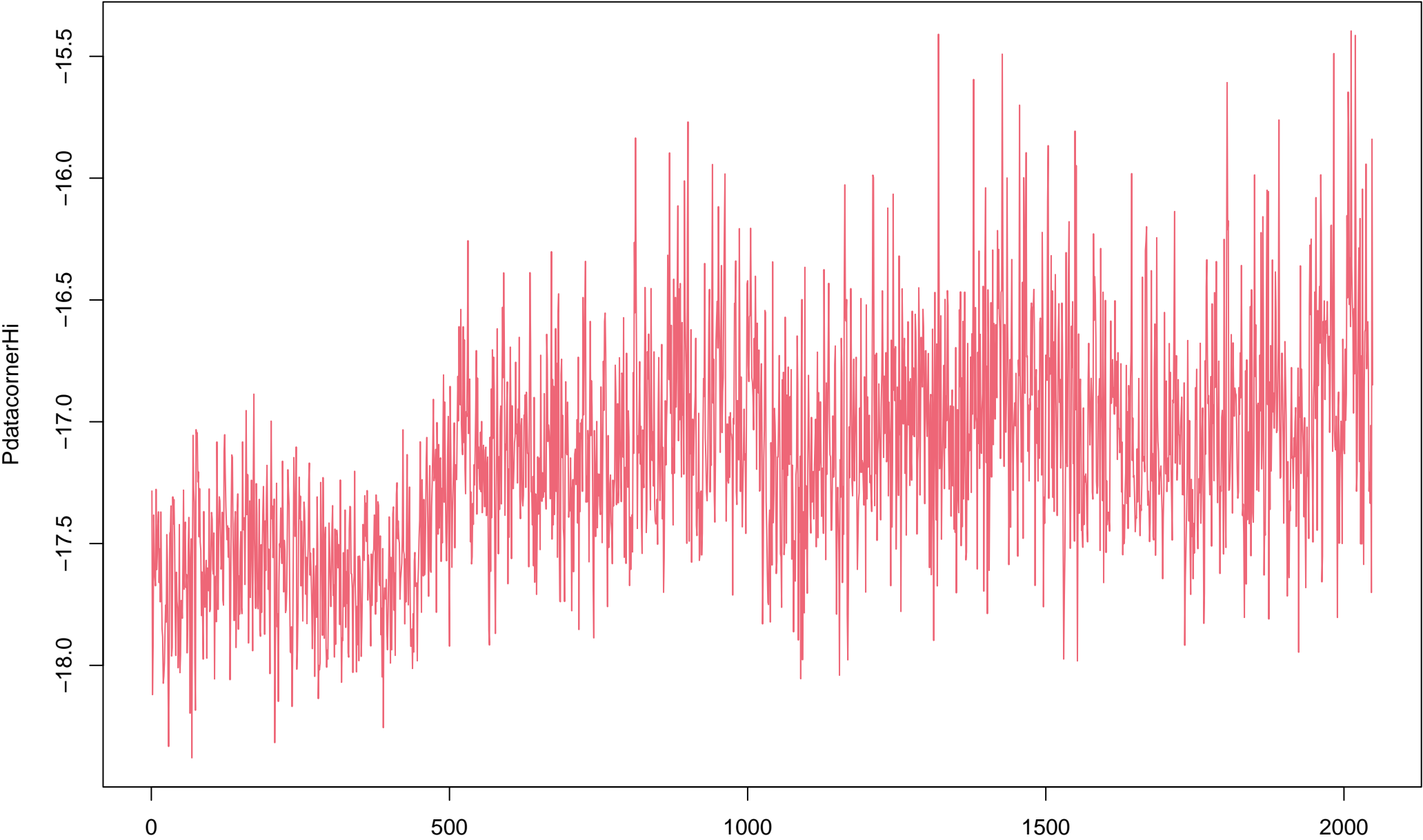
LL  
ESS = 3.24 | BMK = 0.913 | MCSE(6.27) = 14.7 | stat: FALSE | burn: 2040



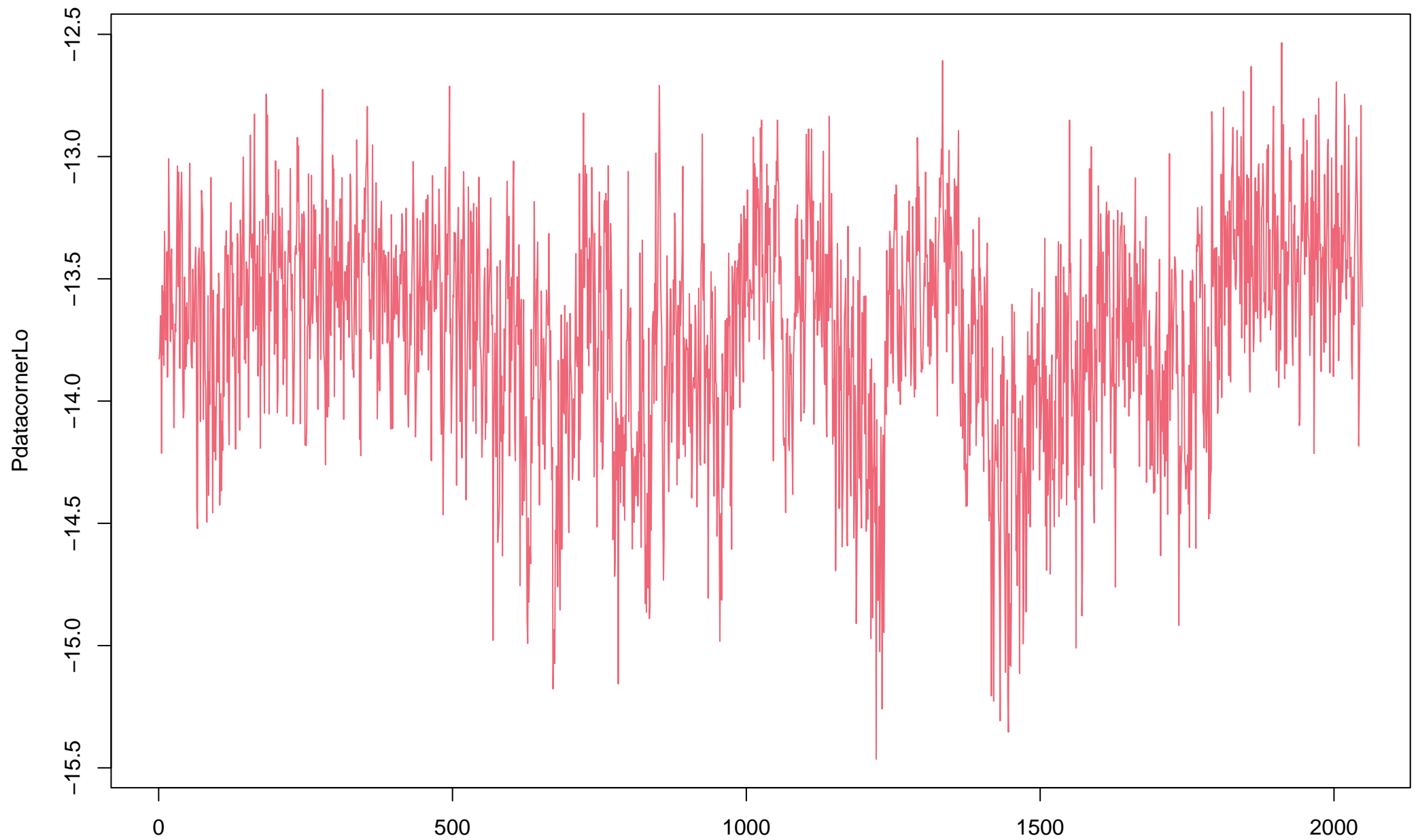
**Pdatamedians**  
**ESS = 260 | BMK = 0.0676 | MCSE(6.27) = 6.82 | stat: TRUE | burn: 0**



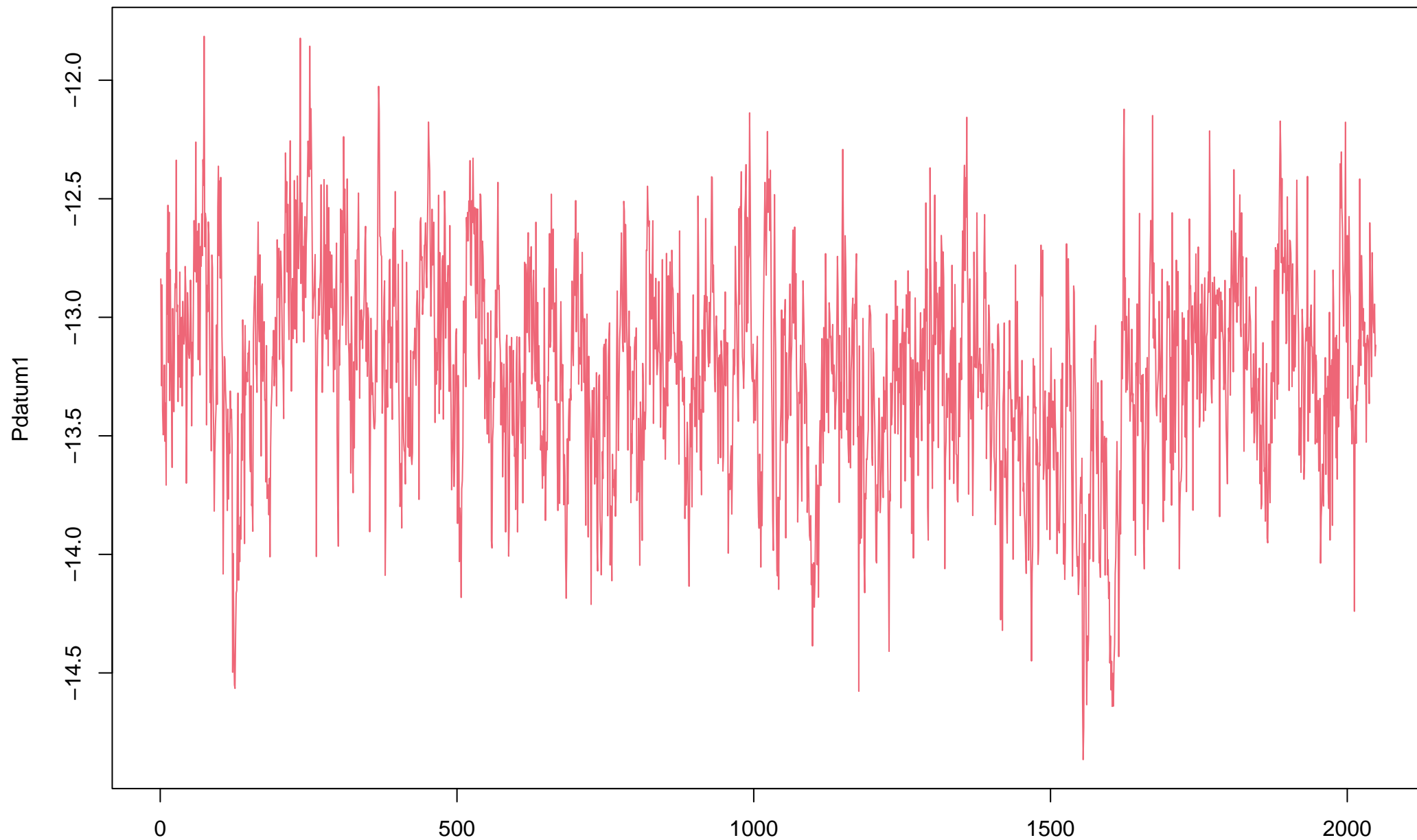
**PdatacornerHi**  
**ESS = 43.8 | BMK = 0.262 | MCSE(6.27) = 7.66 | stat: FALSE | burn: 0**



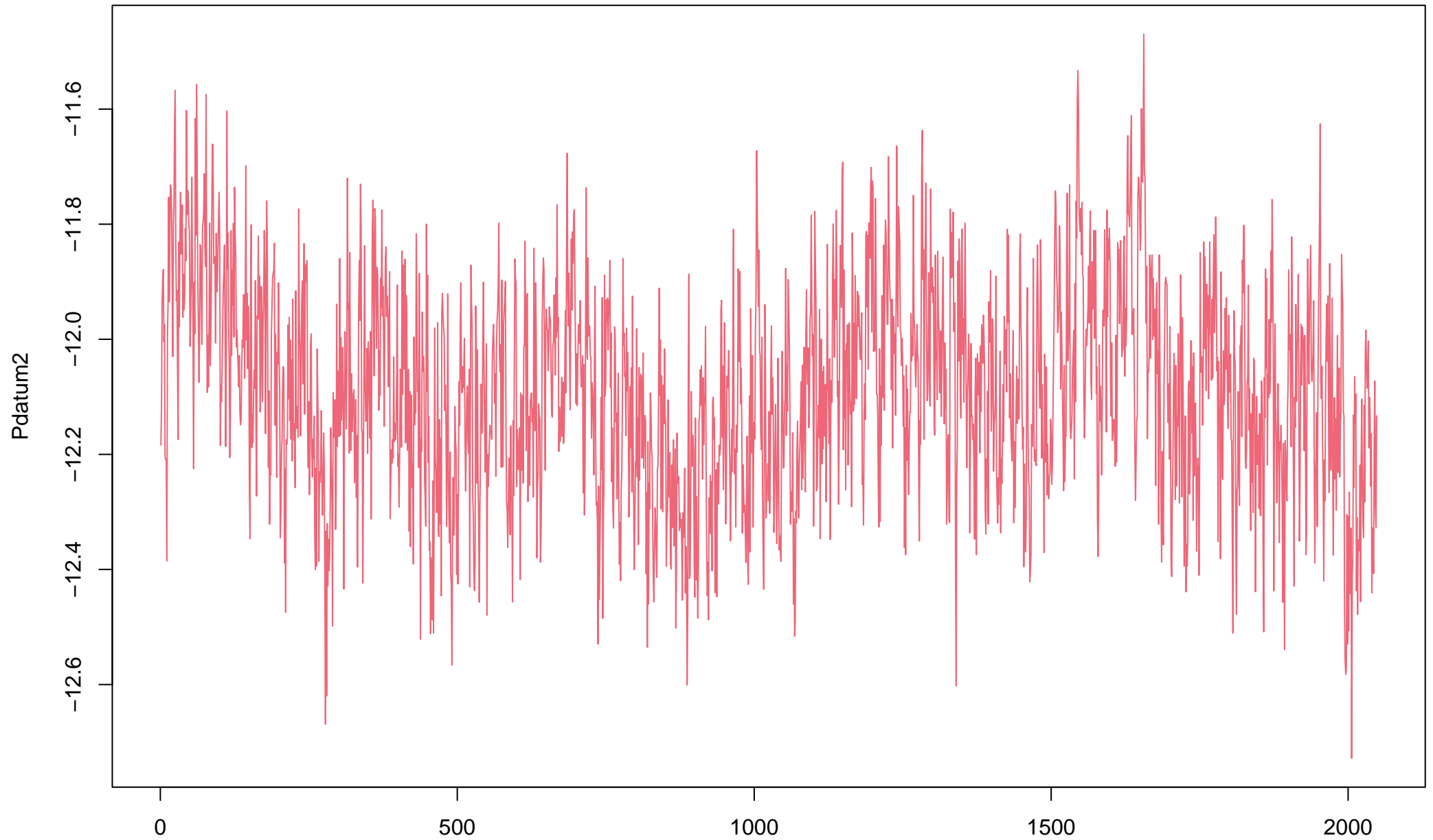
**PdatacornerLo**  
**ESS = 51.1 | BMK = 0.0687 | MCSE(6.27) = 7.92 | stat: TRUE | burn: 0**



**Pdatum1**  
**ESS = 199 | BMK = 0.142 | MCSE(6.27) = 7.24 | stat: TRUE | burn: 0**

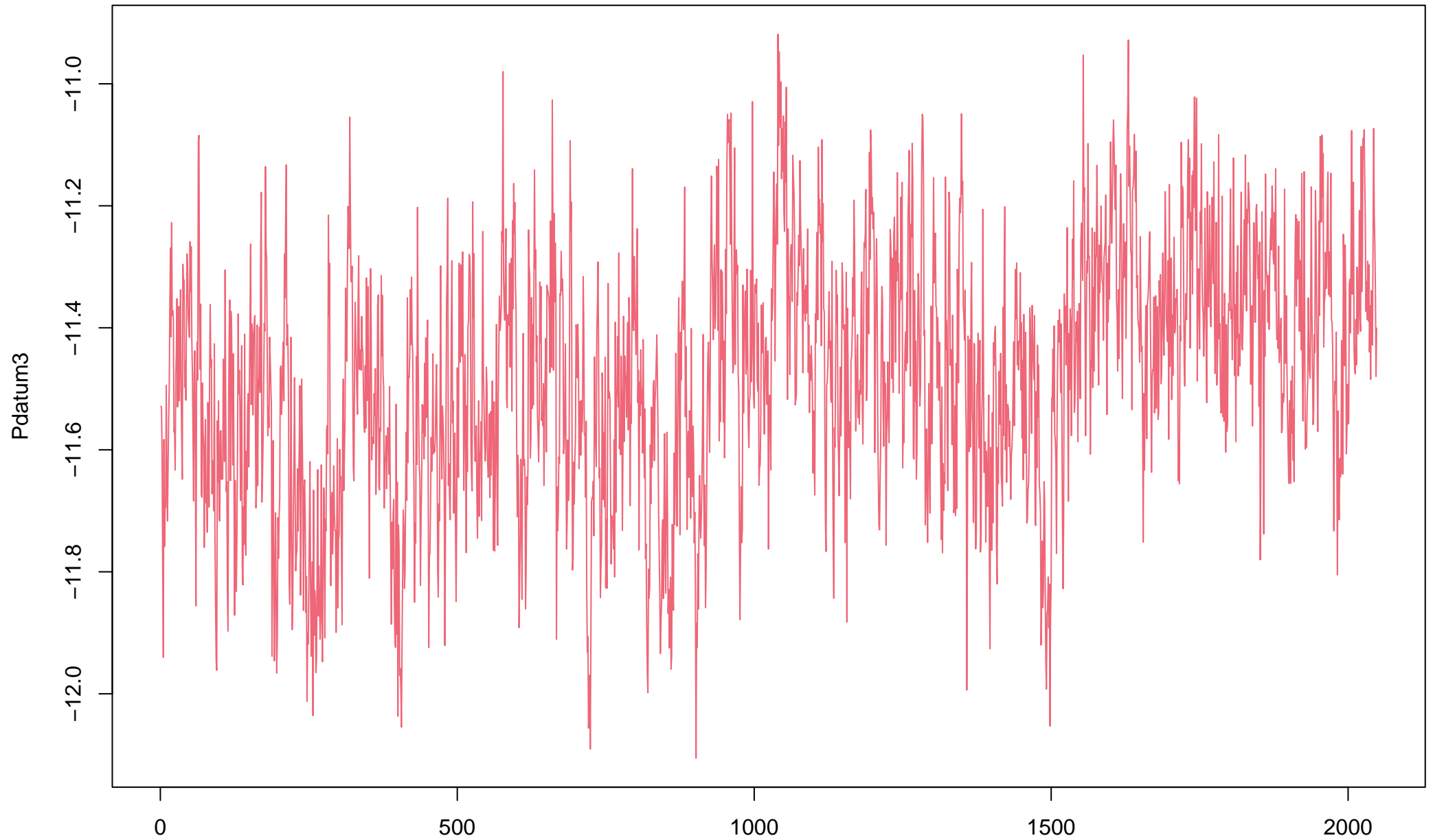


**Pdatum2**  
**ESS = 77.9 | BMK = 0.0644 | MCSE(6.27) = 8.12 | stat: FALSE | burn: 0**

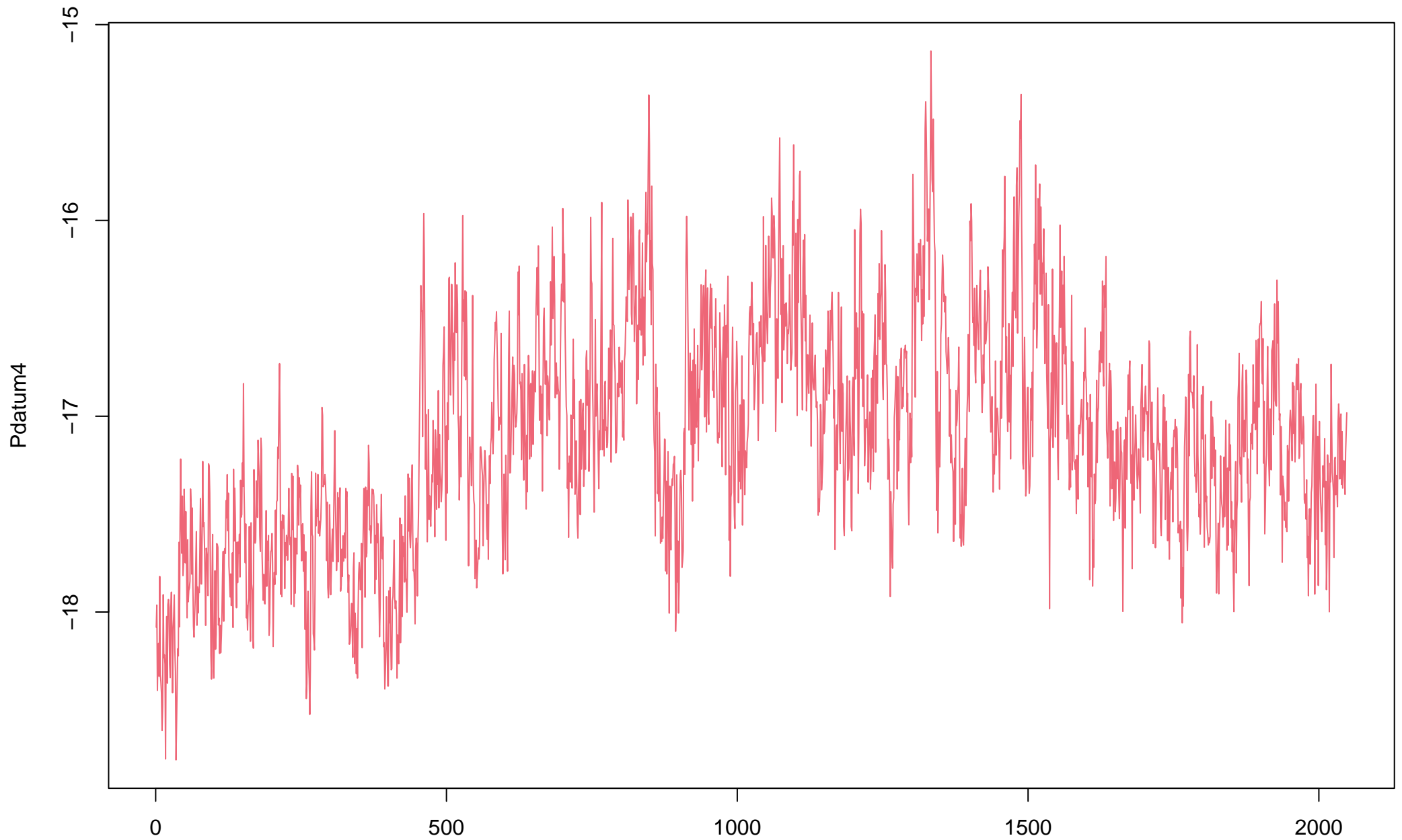




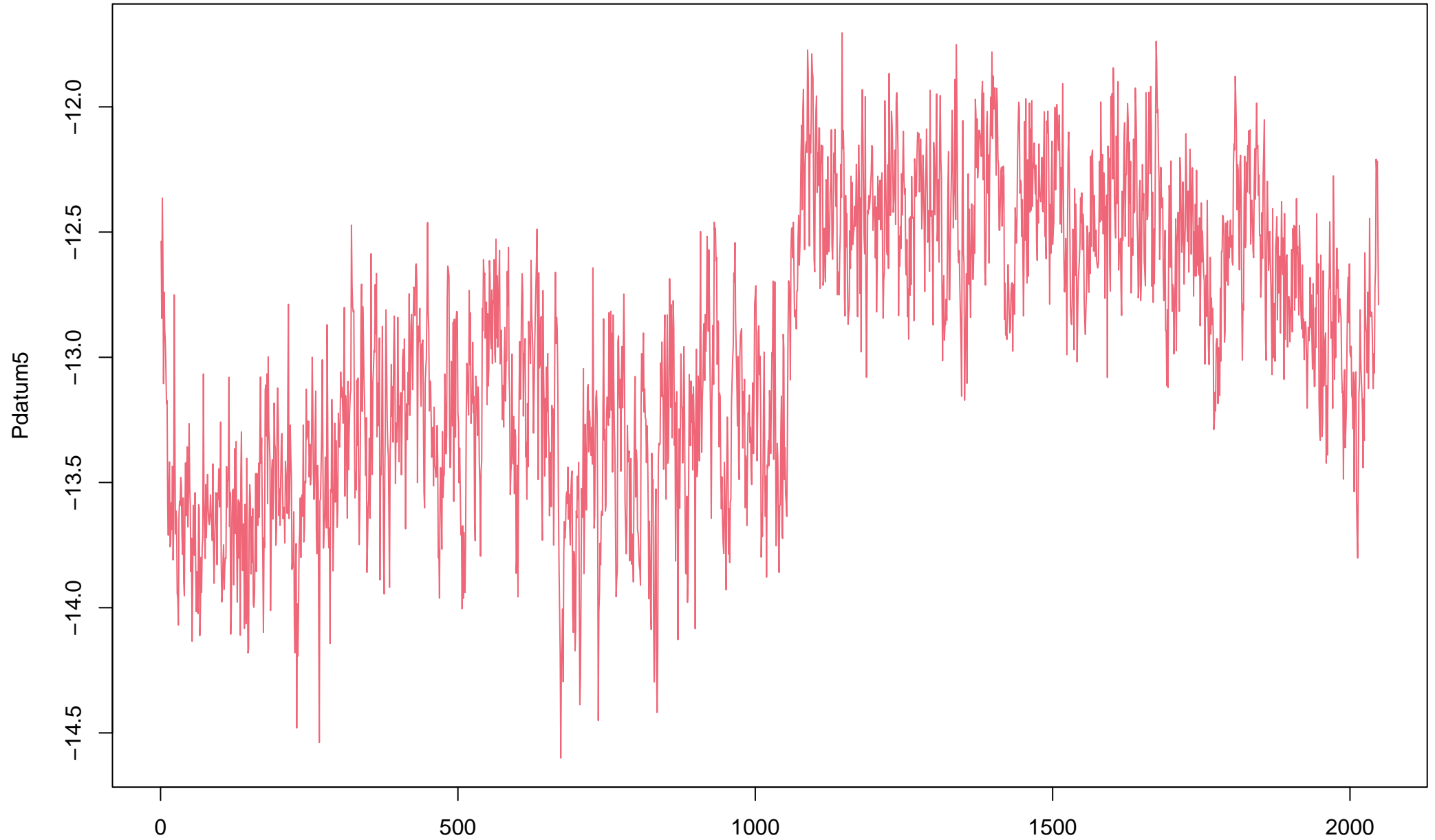
**Pdatum3**  
**ESS = 72.6 | BMK = 0.275 | MCSE(6.27) = 8.73 | stat: FALSE | burn: 0**



**Pdatum4**  
**ESS = 60.2 | BMK = 0.262 | MCSE(6.27) = 10.7 | stat: TRUE | burn: 0**



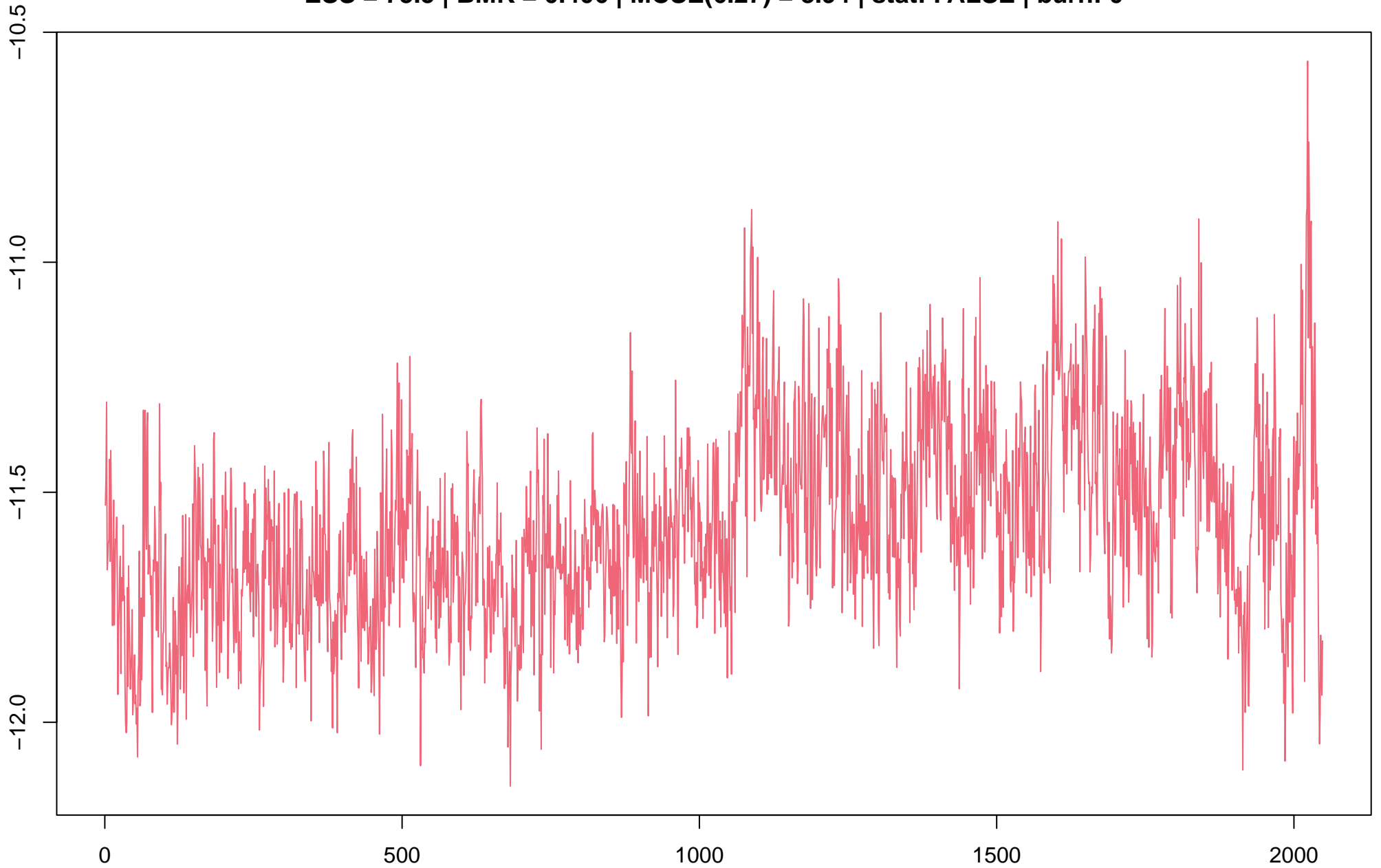
**Pdatum5**  
**ESS = 12.2 | BMK = 0.661 | MCSE(6.27) = 12.5 | stat: FALSE | burn: 1020**



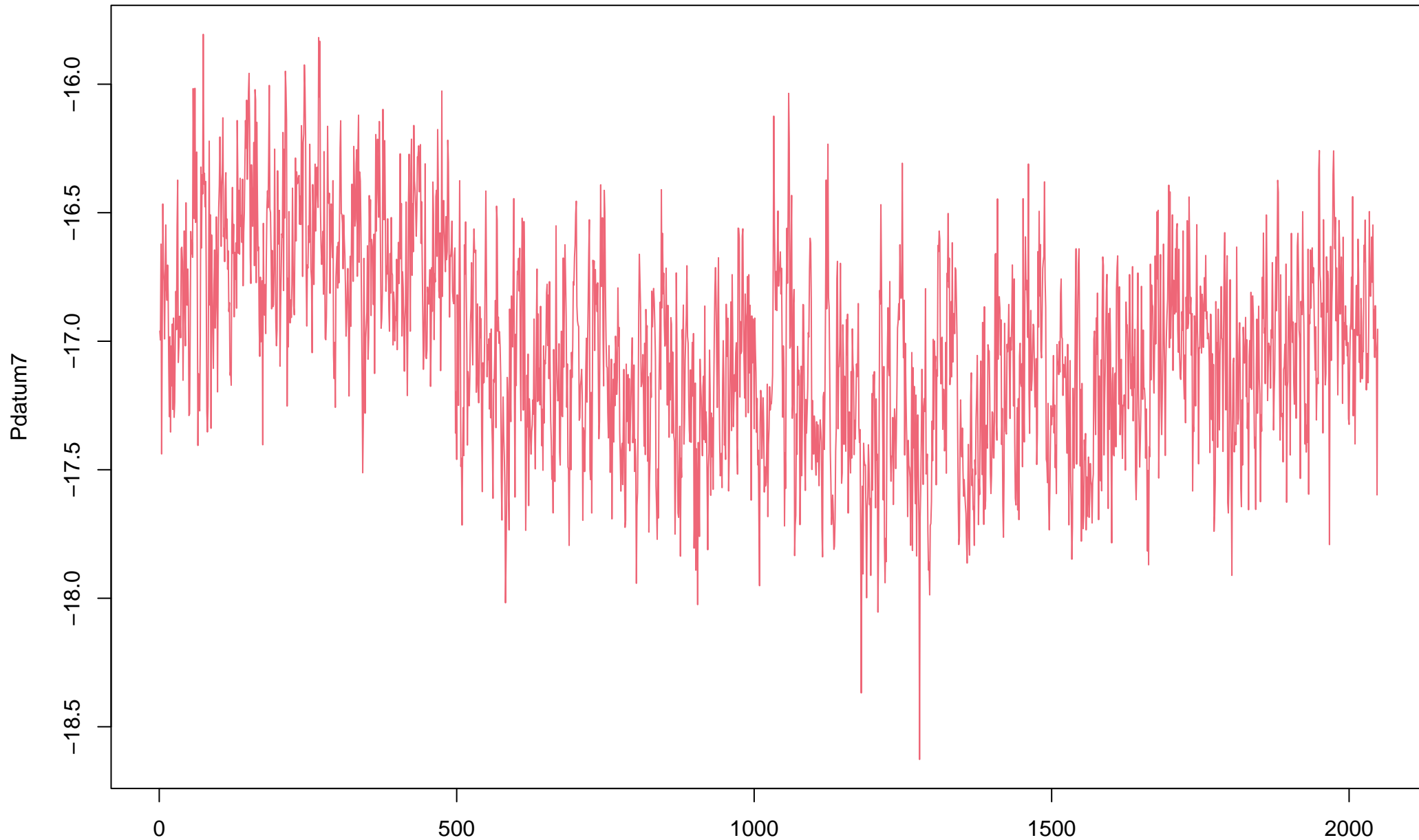
Pdatum6

Pdatum6

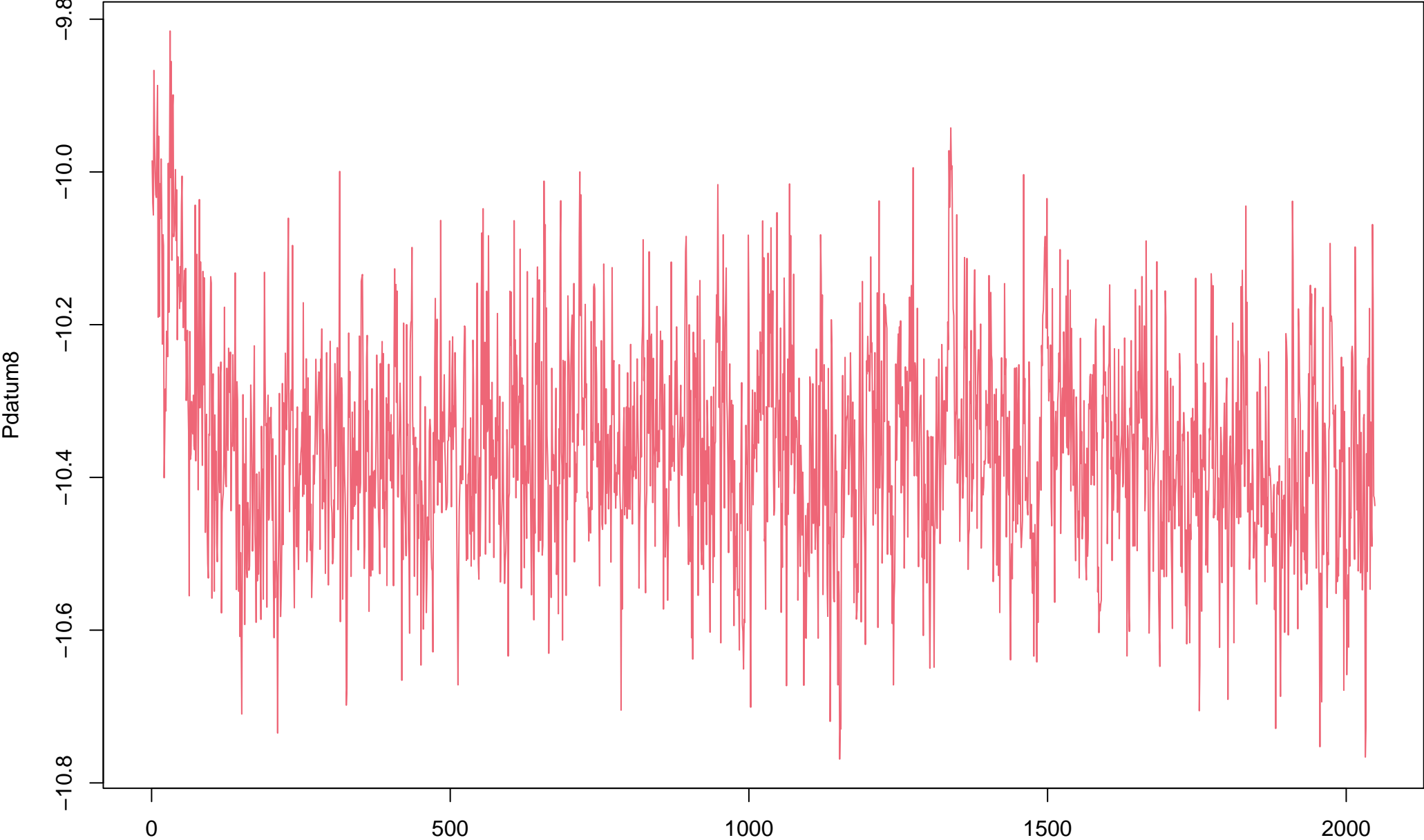
ESS = 75.5 | BMK = 0.406 | MCSE(6.27) = 8.94 | stat: FALSE | burn: 0



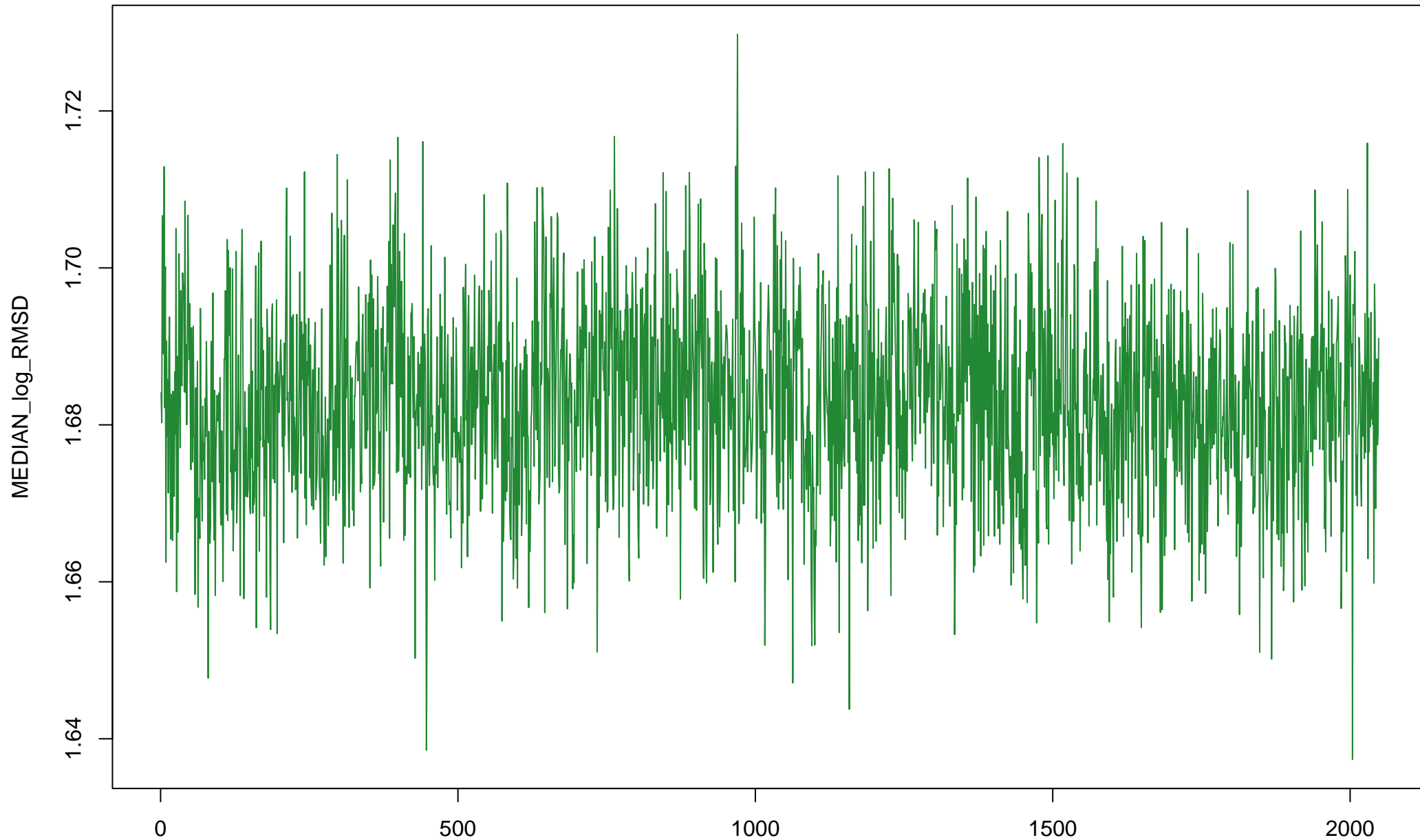
**Pdatum7**  
**ESS = 29 | BMK = 0.228 | MCSE(6.27) = 9.75 | stat: TRUE | burn: 0**



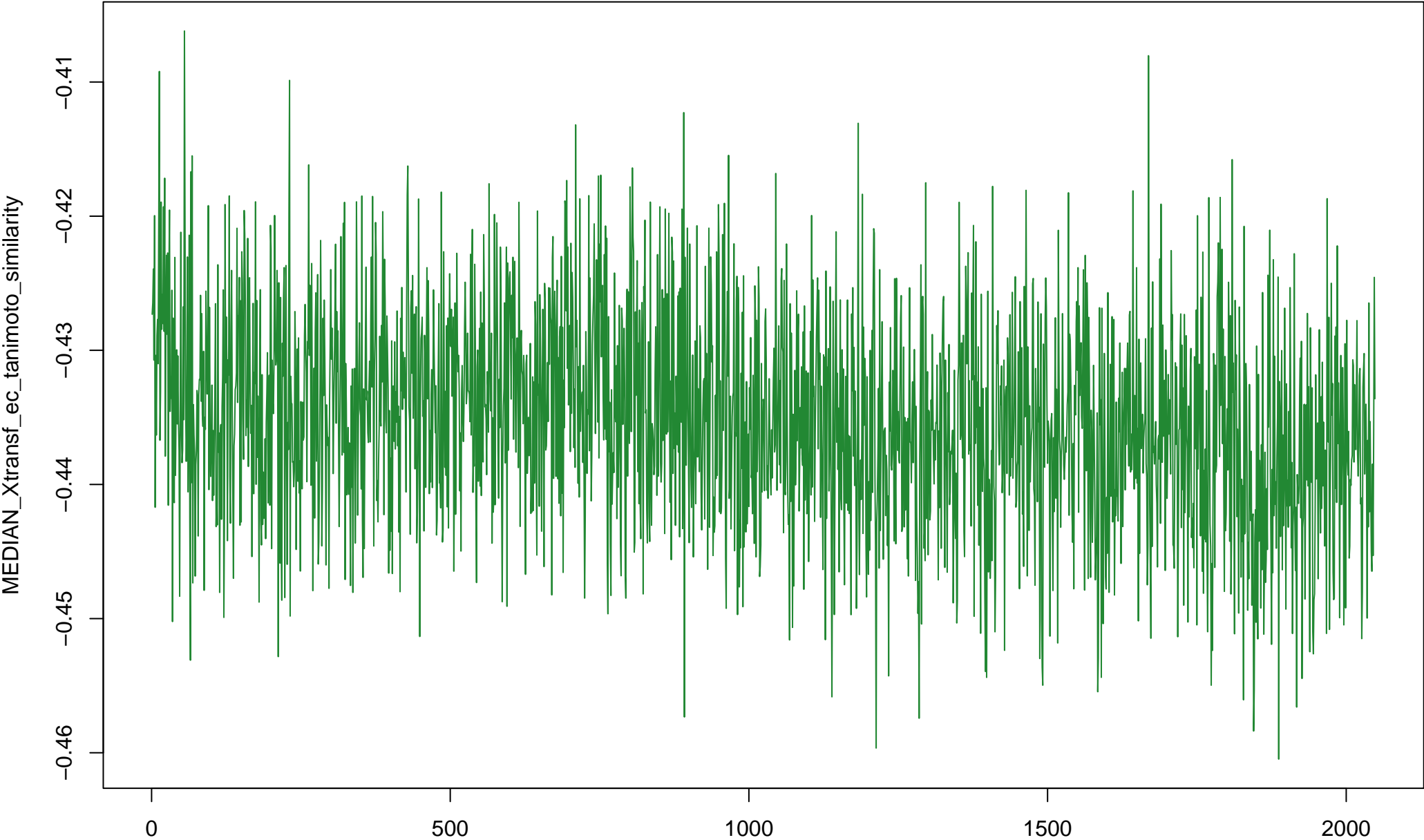
**Pdatum8**  
**ESS = 280 | BMK = 0.0808 | MCSE(6.27) = 6.9 | stat: FALSE | burn: 0**



**MEDIAN\_log\_RMSD**  
**ESS = 1040 | BMK = 0.0343 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0**

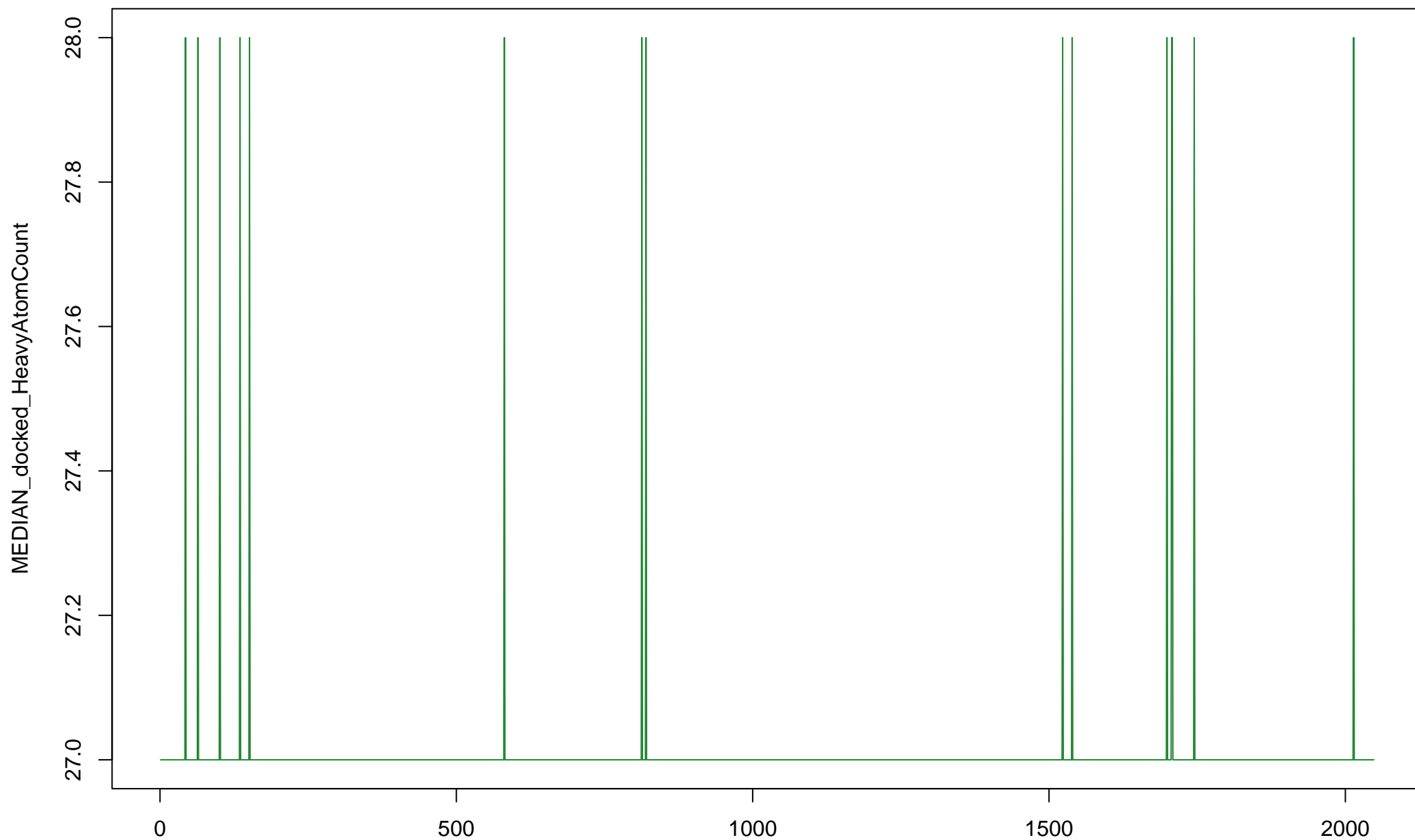


**MEDIAN\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 461 | BMK = 0.171 | MCSE(6.27) = 4.49 | stat: FALSE | burn: 0**

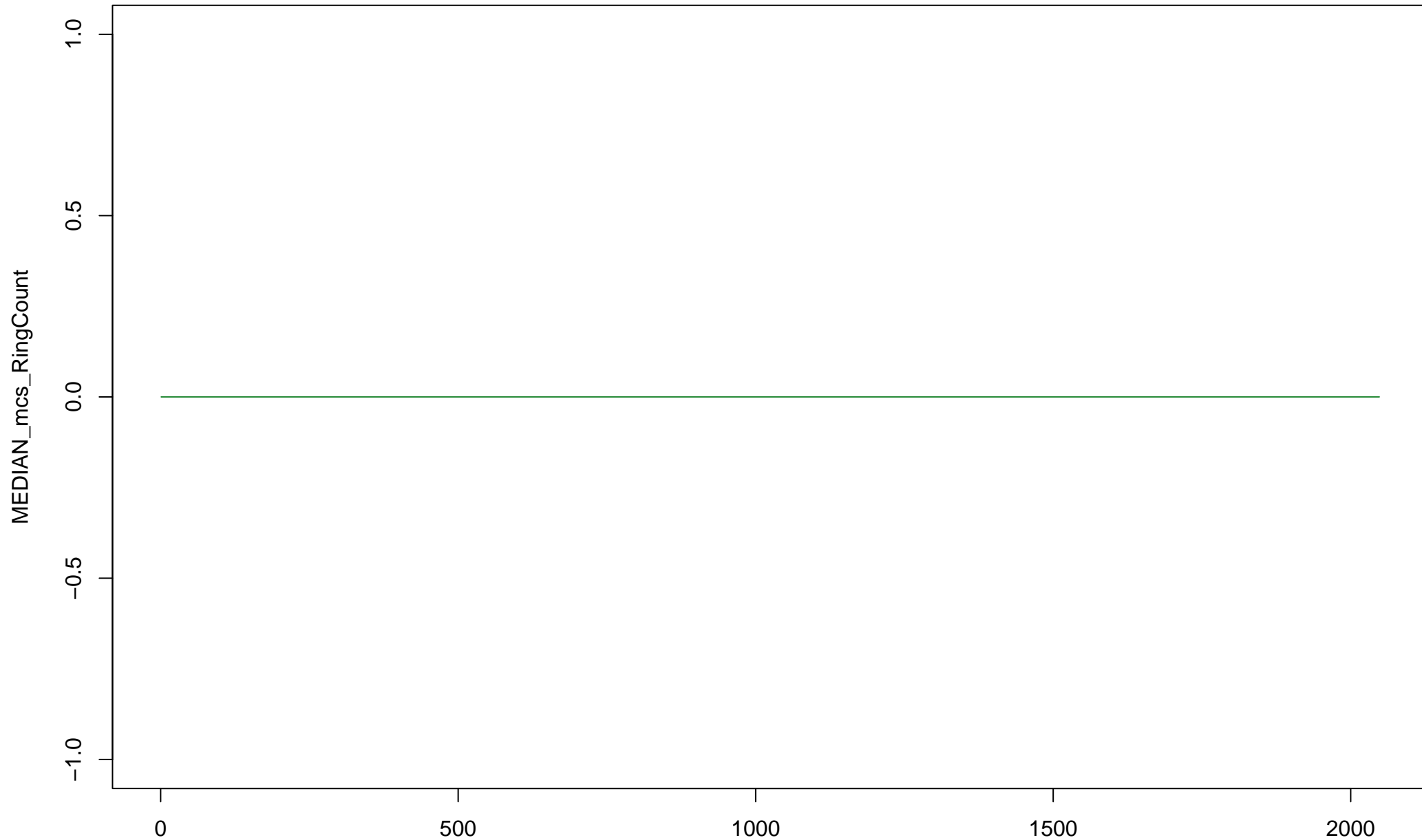




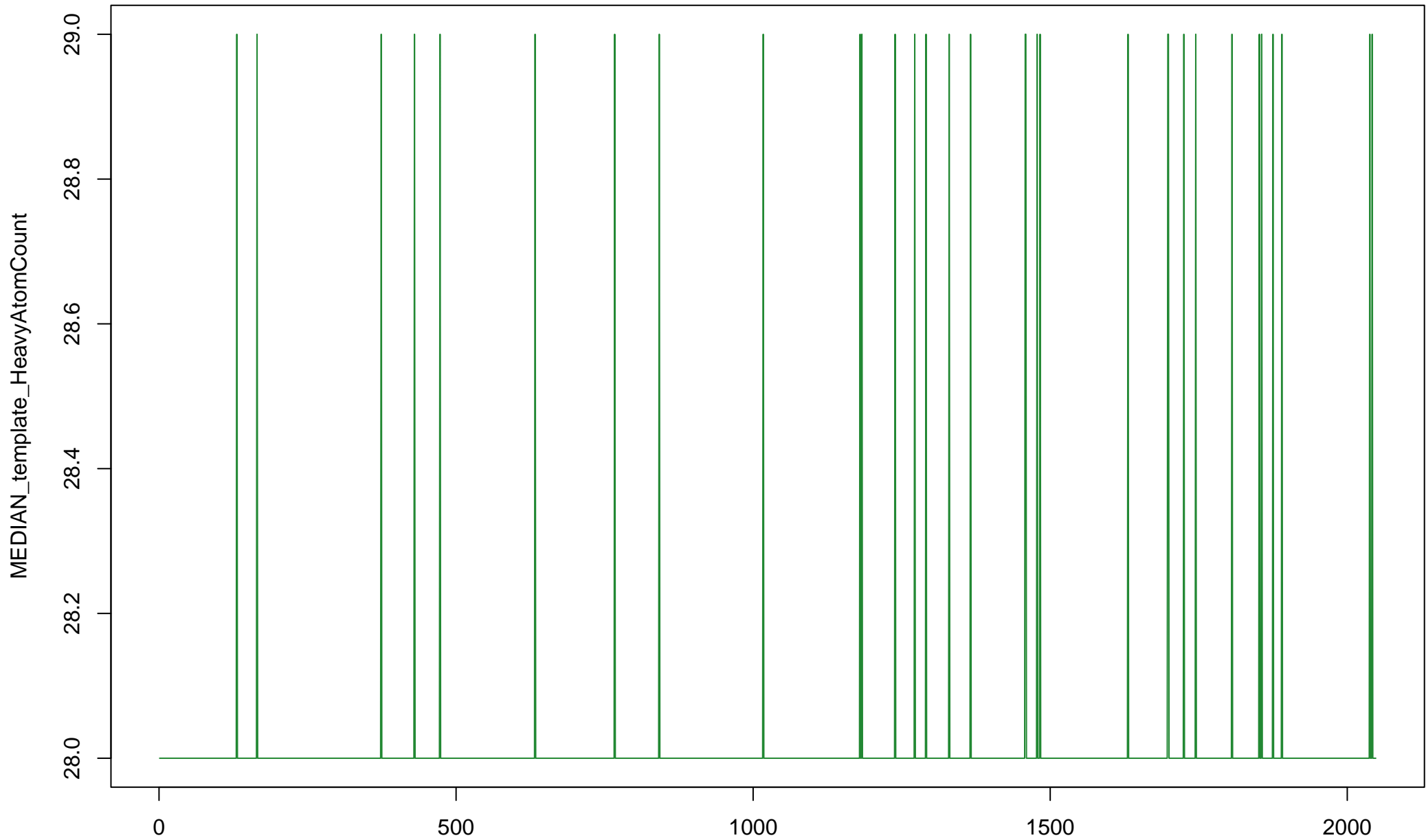
**MEDIAN\_docked\_HeavyAtomCount**  
**ESS = 1140 | BMK = 0.0237 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 1020**



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



**MEDIAN\_template\_HeavyAtomCount**  
**ESS = 1860 | BMK = 0.162 | MCSE(6.27) = 2.59 | stat: FALSE | burn: 0**



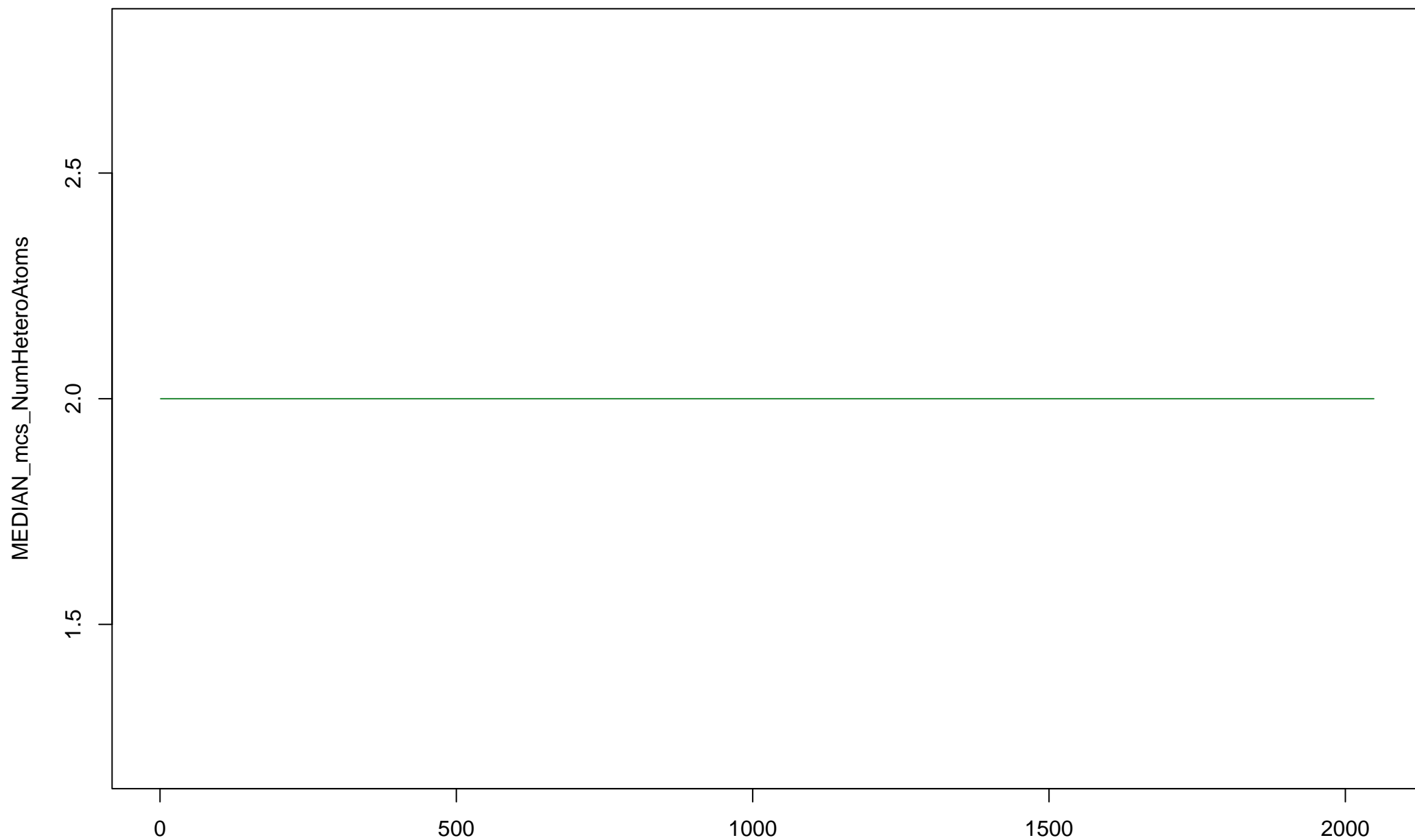
**MEDIAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



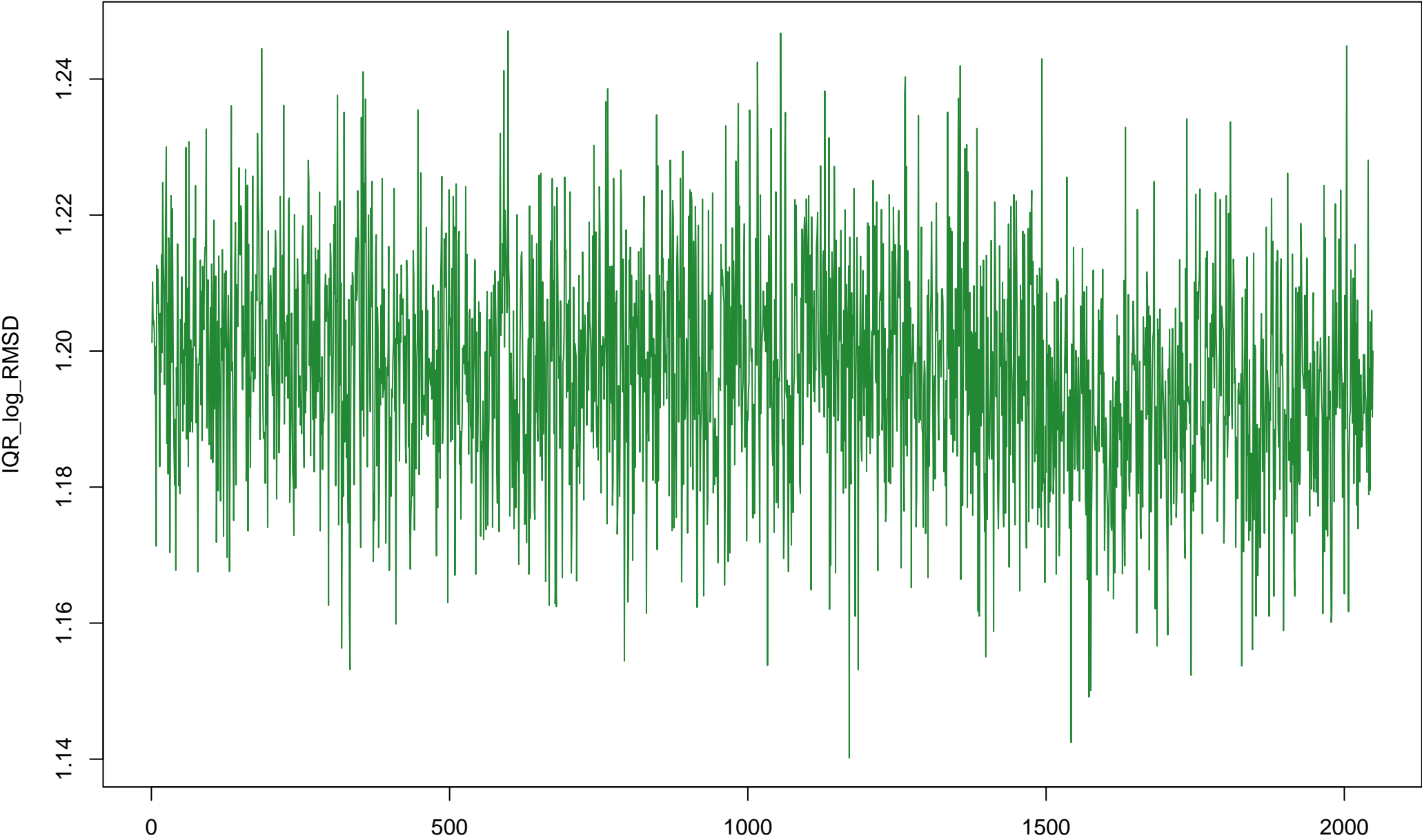
**MEDIAN\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



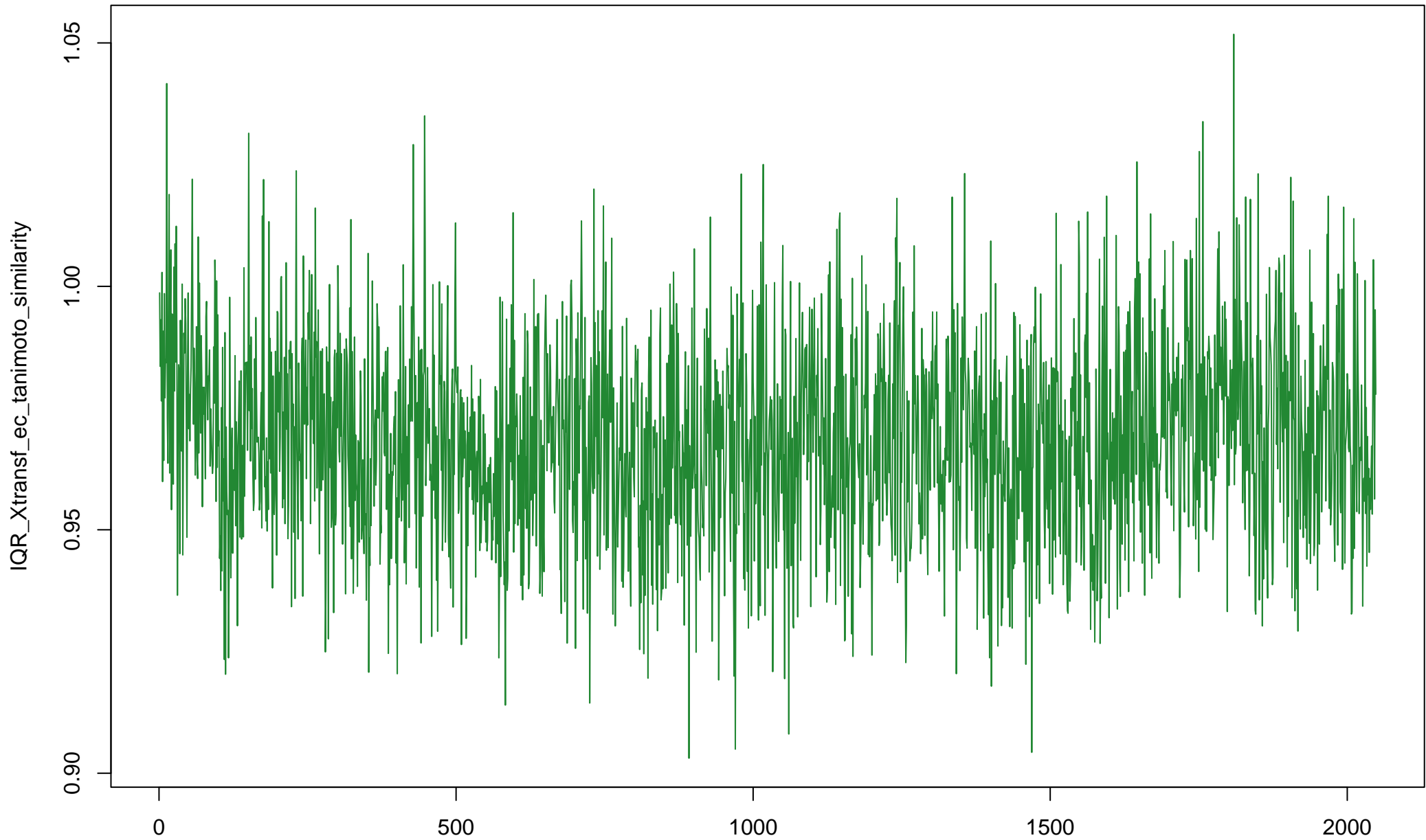
**MEDIAN\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



IQR\_log\_RMSD  
ESS = 736 | BMK = 0.091 | MCSE(6.27) = 3.77 | stat: FALSE | burn: 0

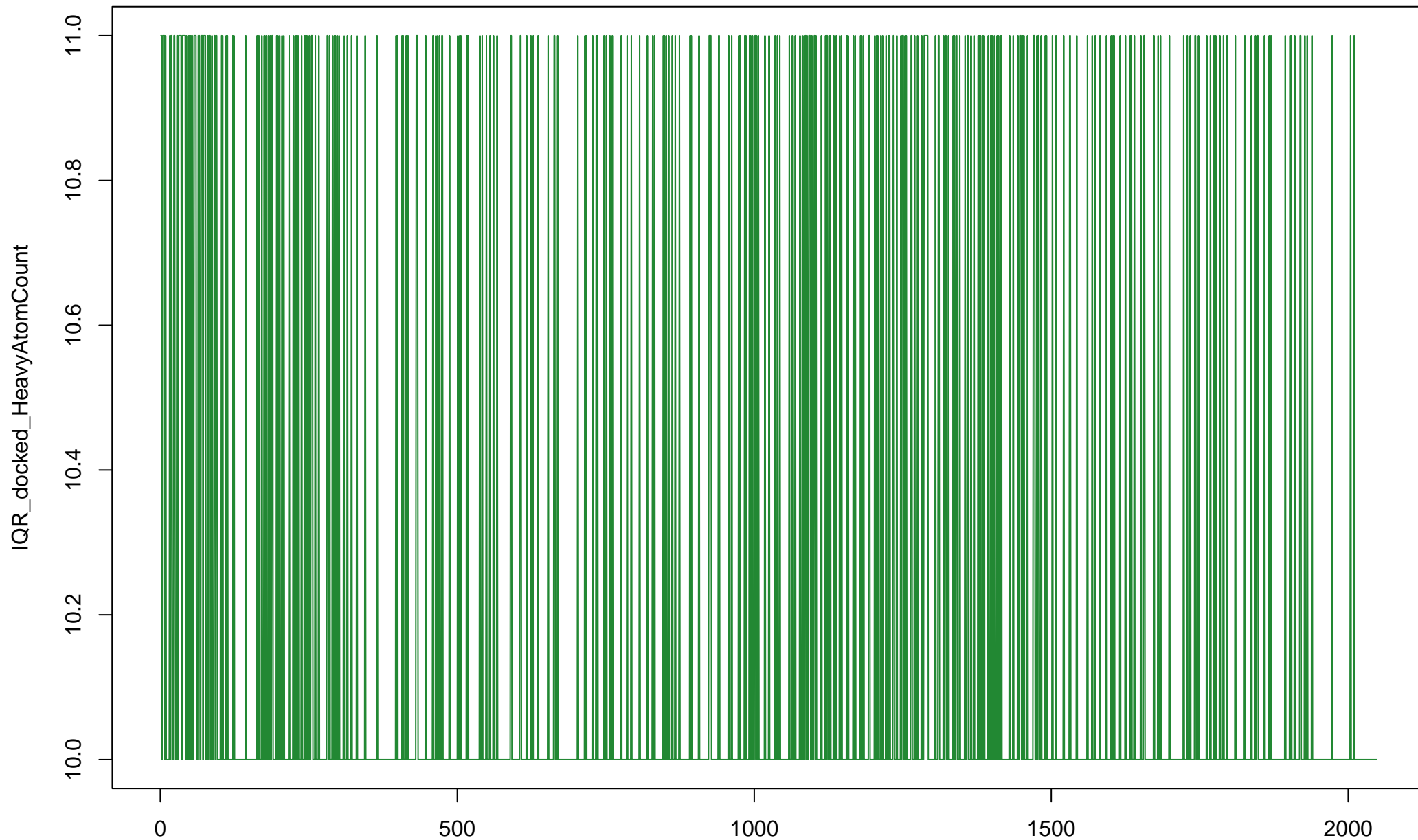


IQR\_Xtransf\_ec\_tanimoto\_similarity  
ESS = 945 | BMK = 0.0388 | MCSE(6.27) = 3.89 | stat: FALSE | burn: 0

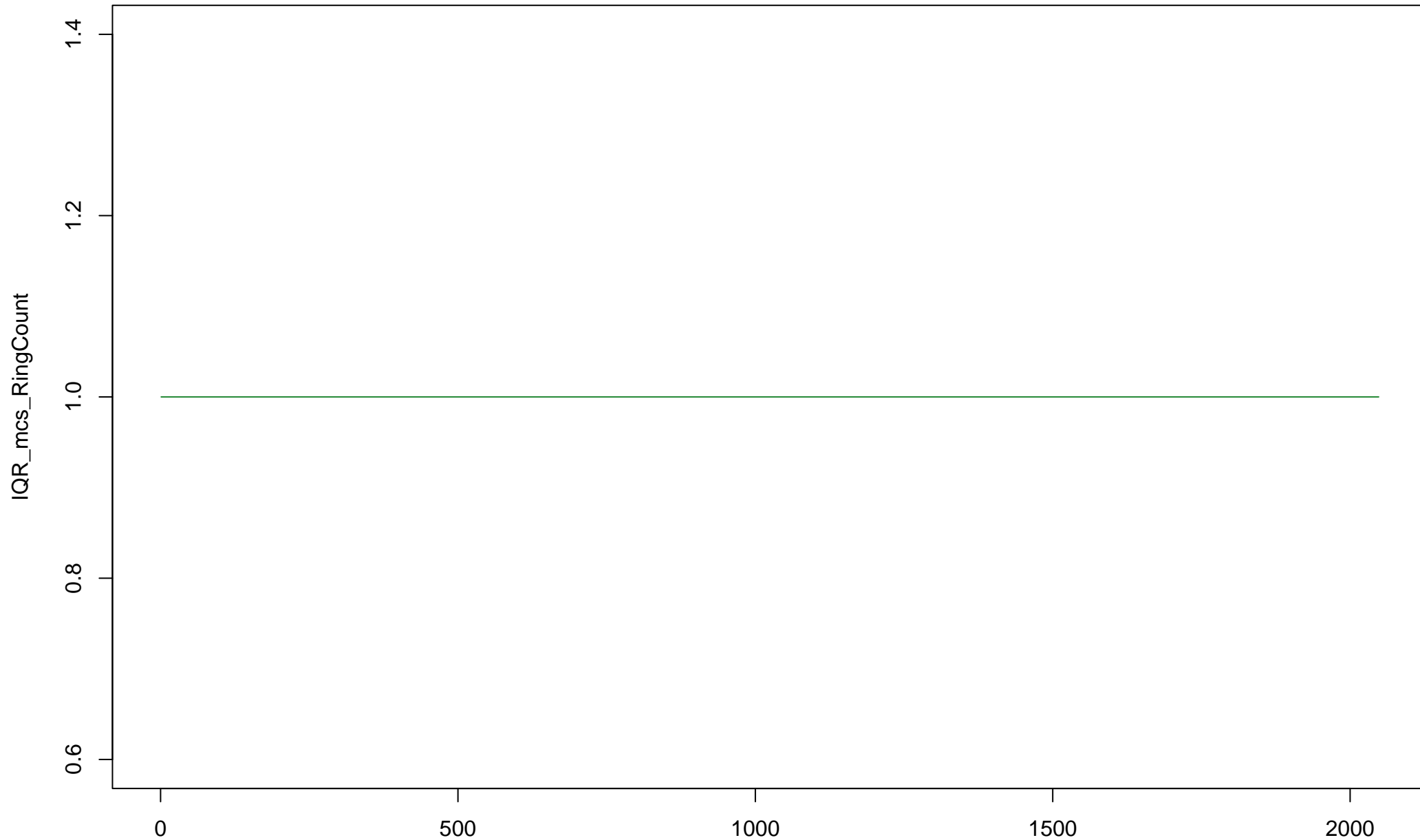




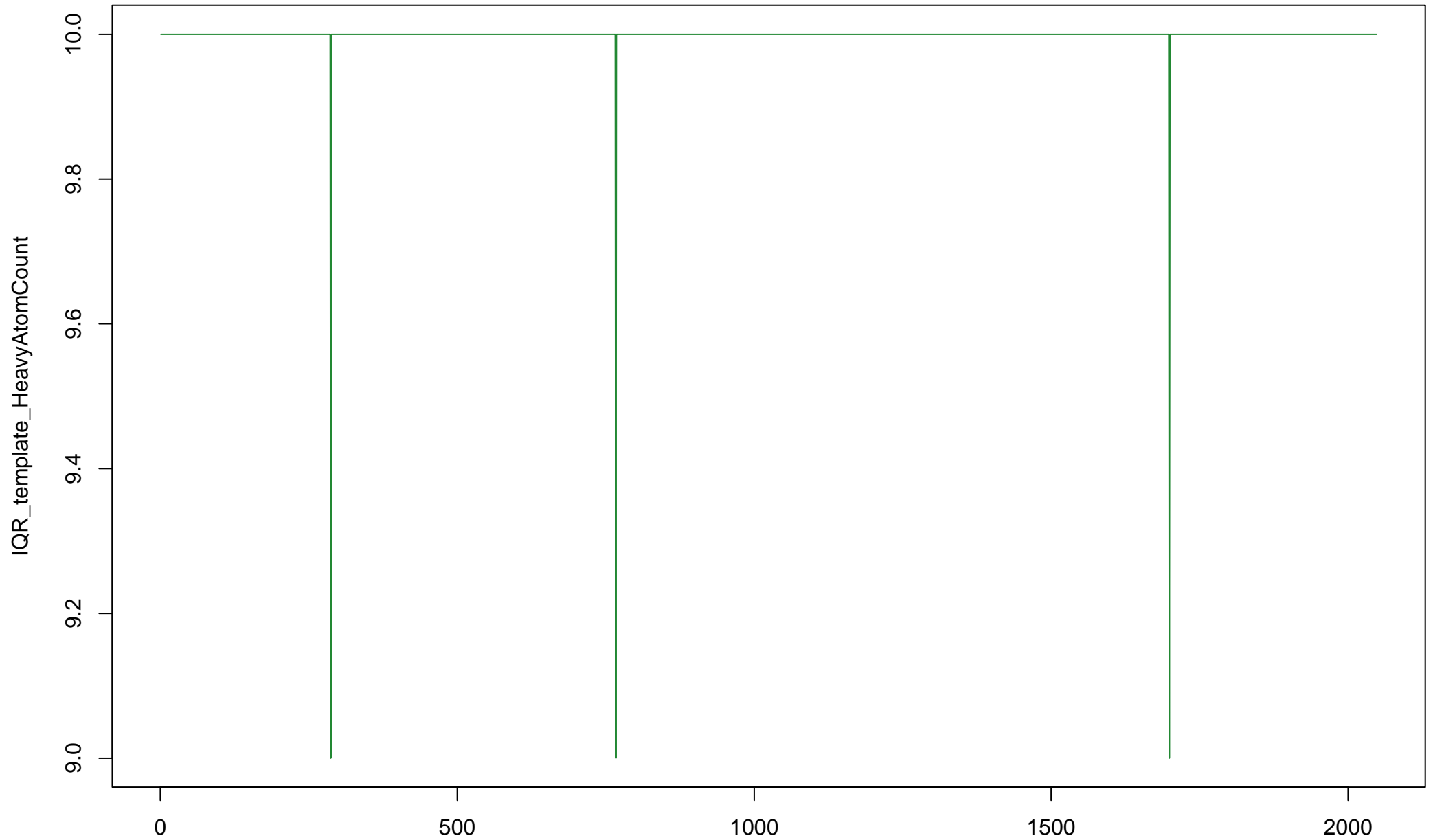
IQR\_docked\_HeavyAtomCount  
ESS = 330 | BMK = 0.0147 | MCSE(6.27) = 4.24 | stat: FALSE | burn: 0



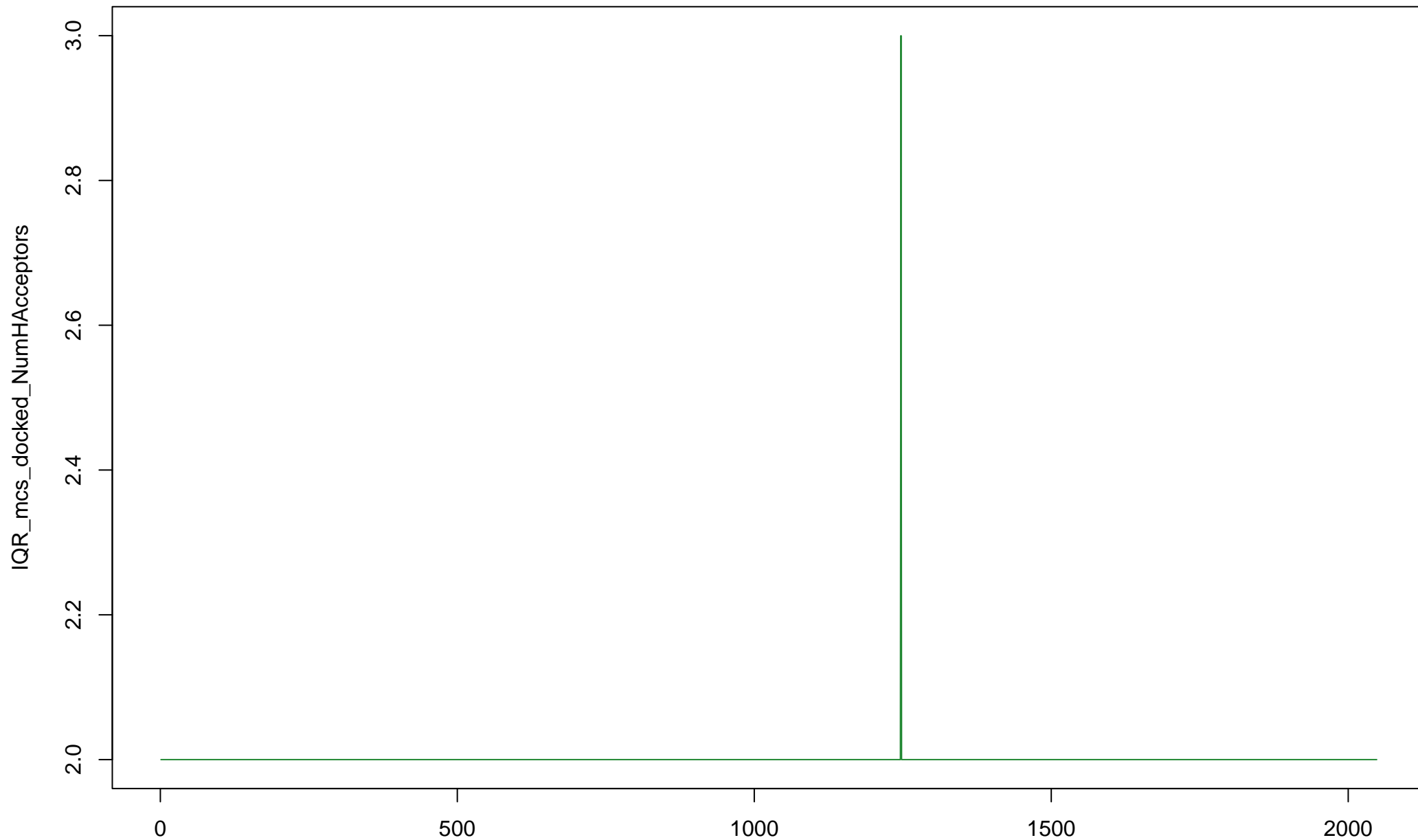
**IQR\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



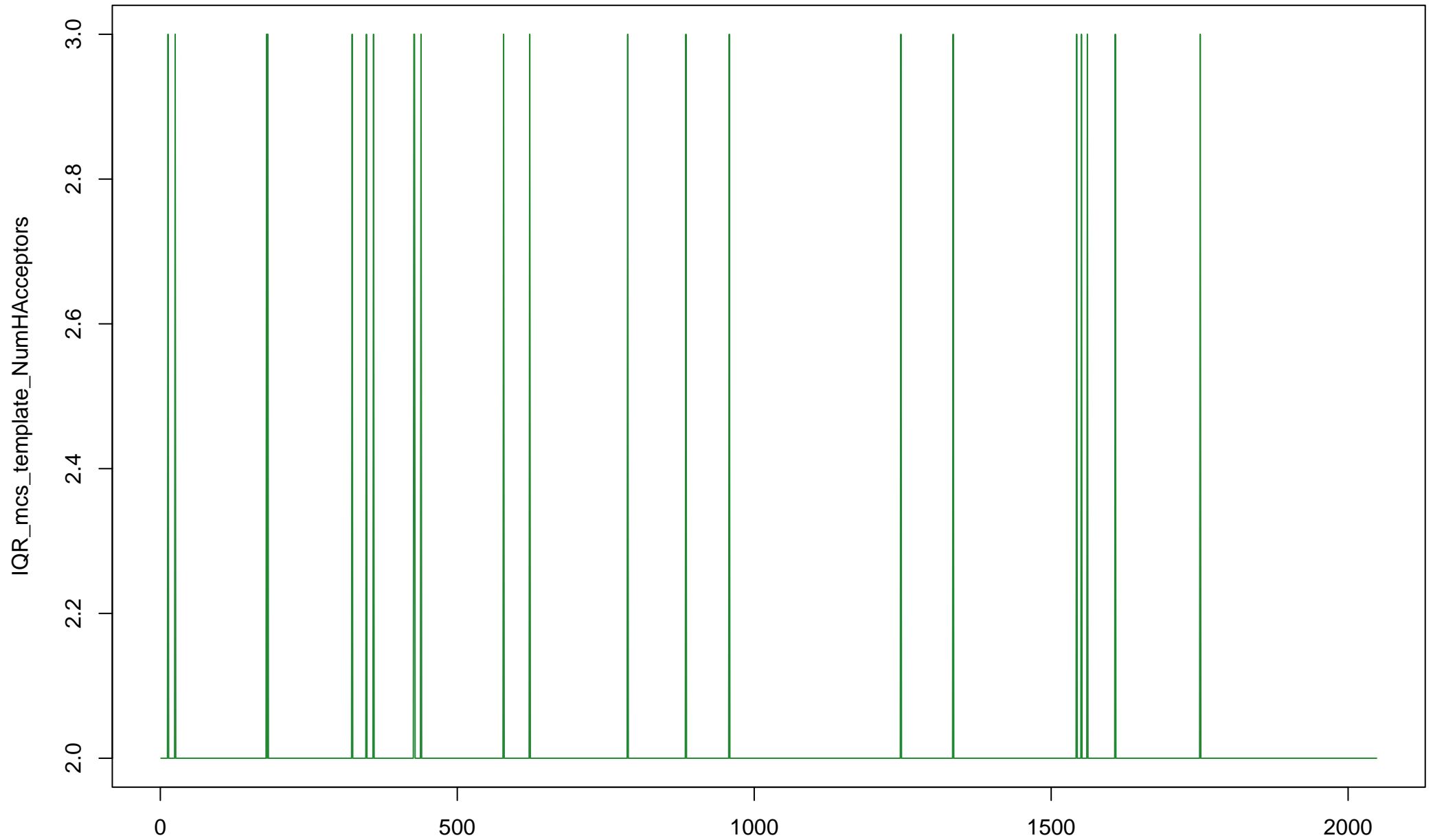
**IQR\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.121 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 2040**



**IQR\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.644 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 1428**



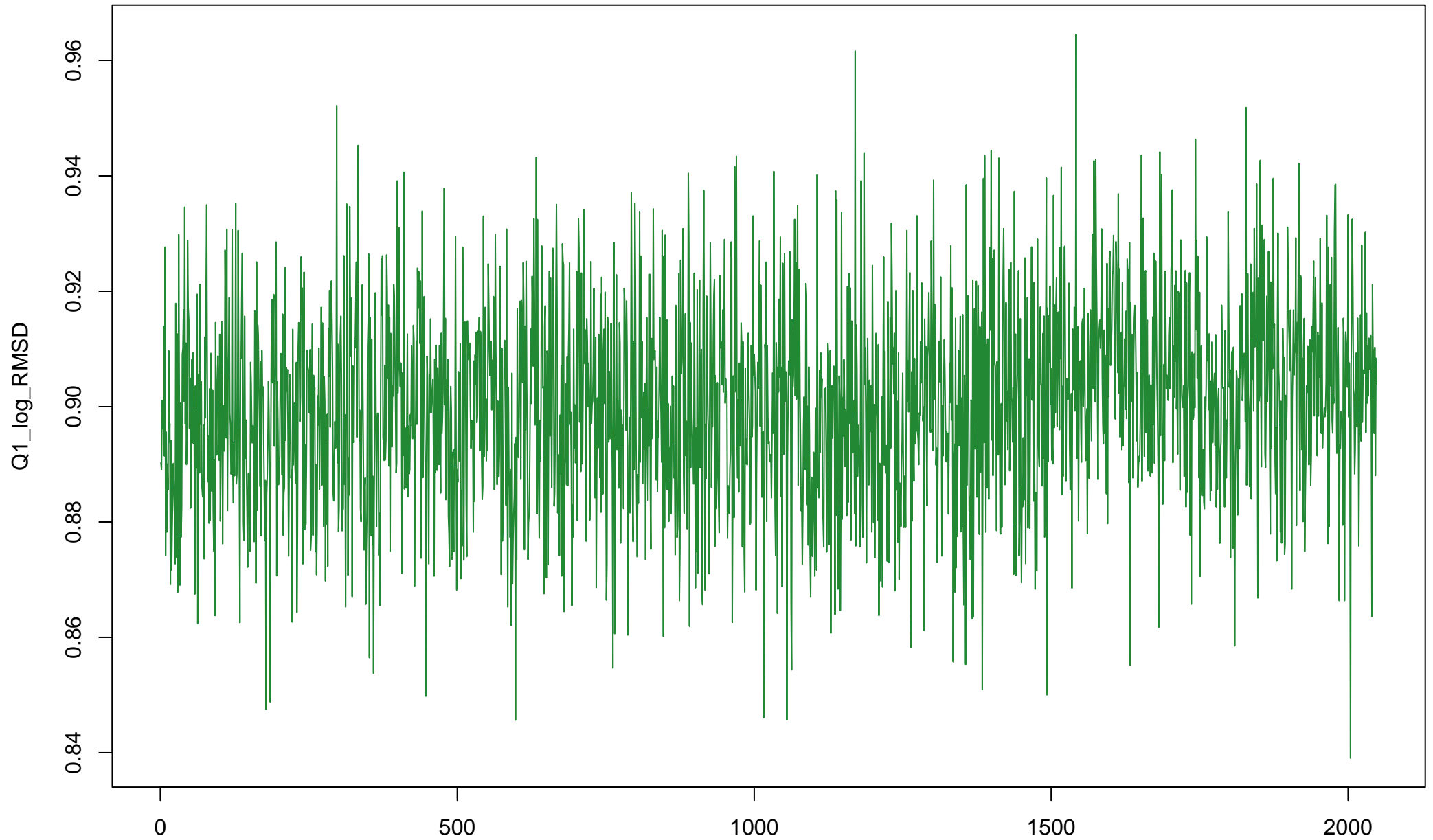
**IQR\_mcs\_template\_NumHAcceptors**  
**ESS = 1290 | BMK = 0.133 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 2040**



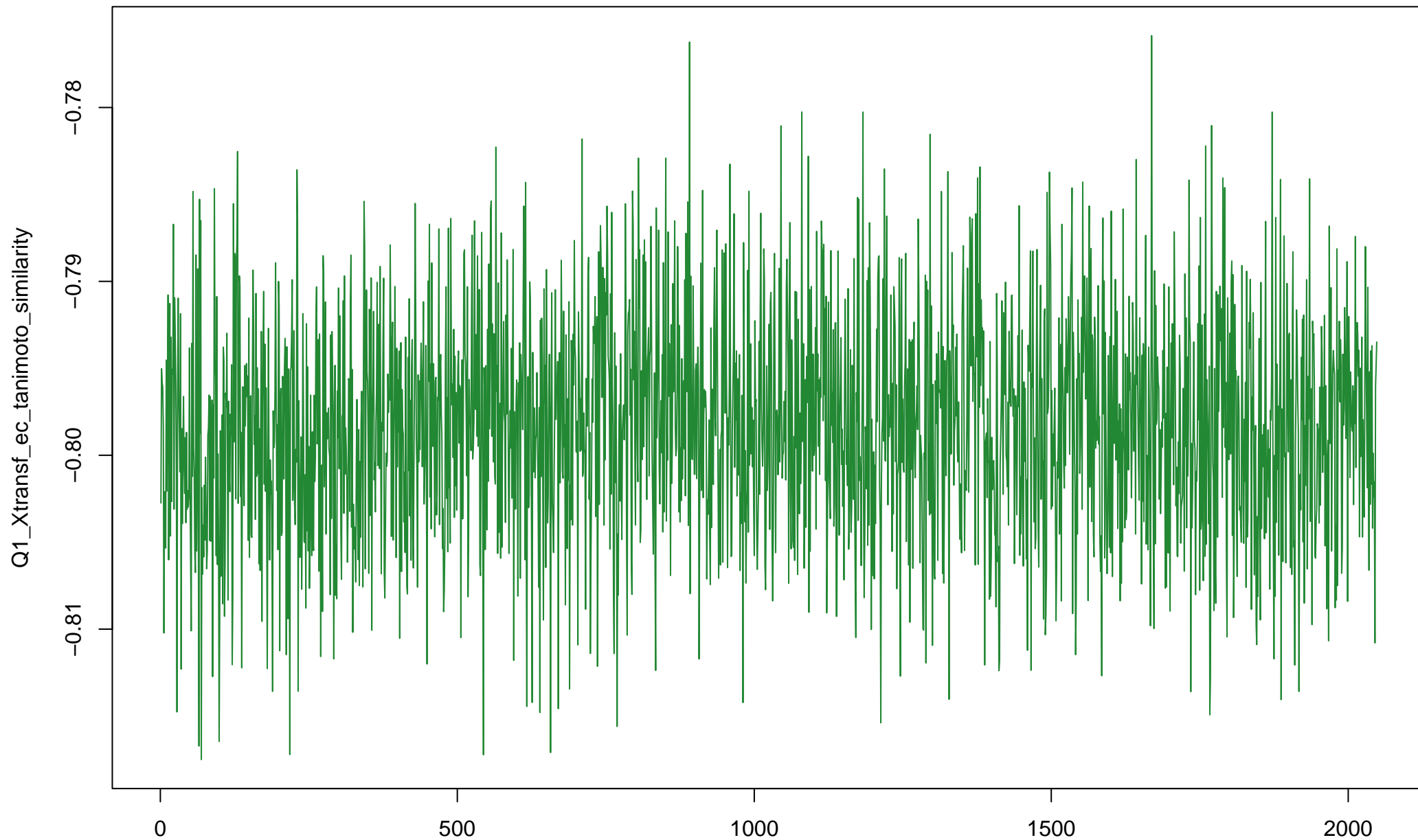
IQR\_mcs\_NumHeteroAtoms  
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



**Q1\_log\_RMSD**  
**ESS = 878 | BMK = 0.0827 | MCSE(6.27) = 3.46 | stat: FALSE | burn: 0**

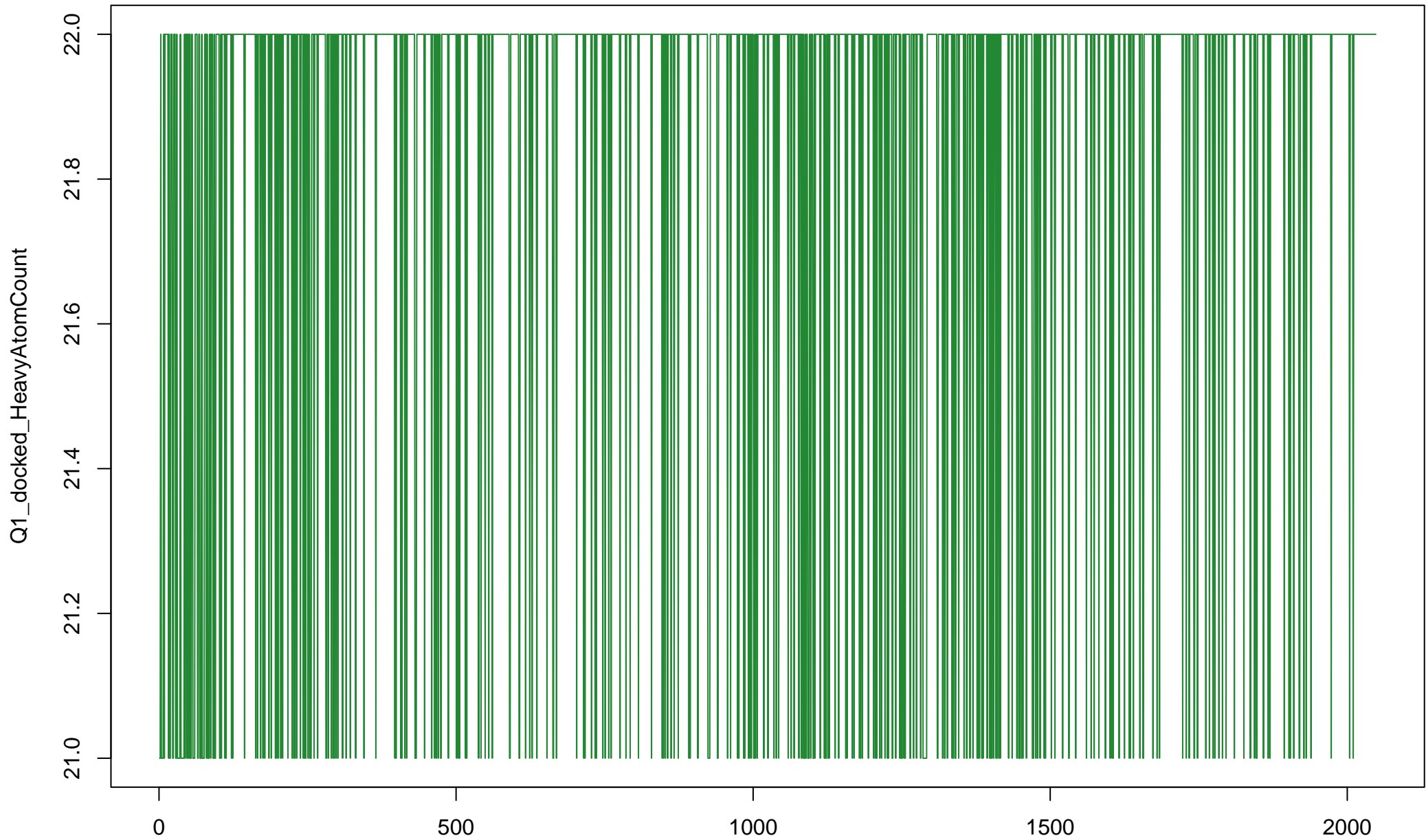


**Q1\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0508 | MCSE(6.27) = 2.79 | stat: FALSE | burn: 0**





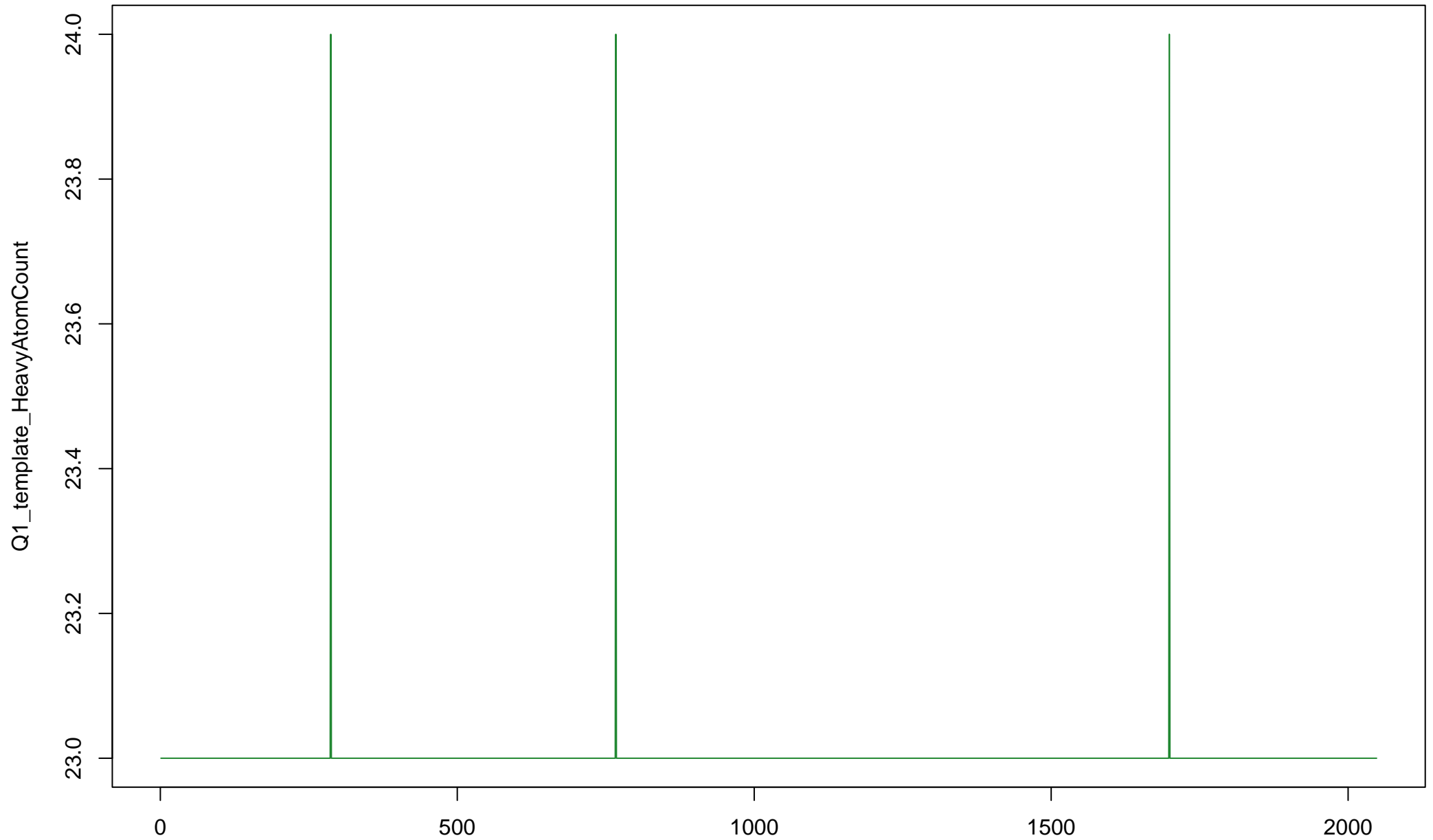
**Q1\_docked\_HeavyAtomCount**  
**ESS = 340 | BMK = 0.0152 | MCSE(6.27) = 4.23 | stat: FALSE | burn: 0**



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



**Q1\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.121 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 2040**



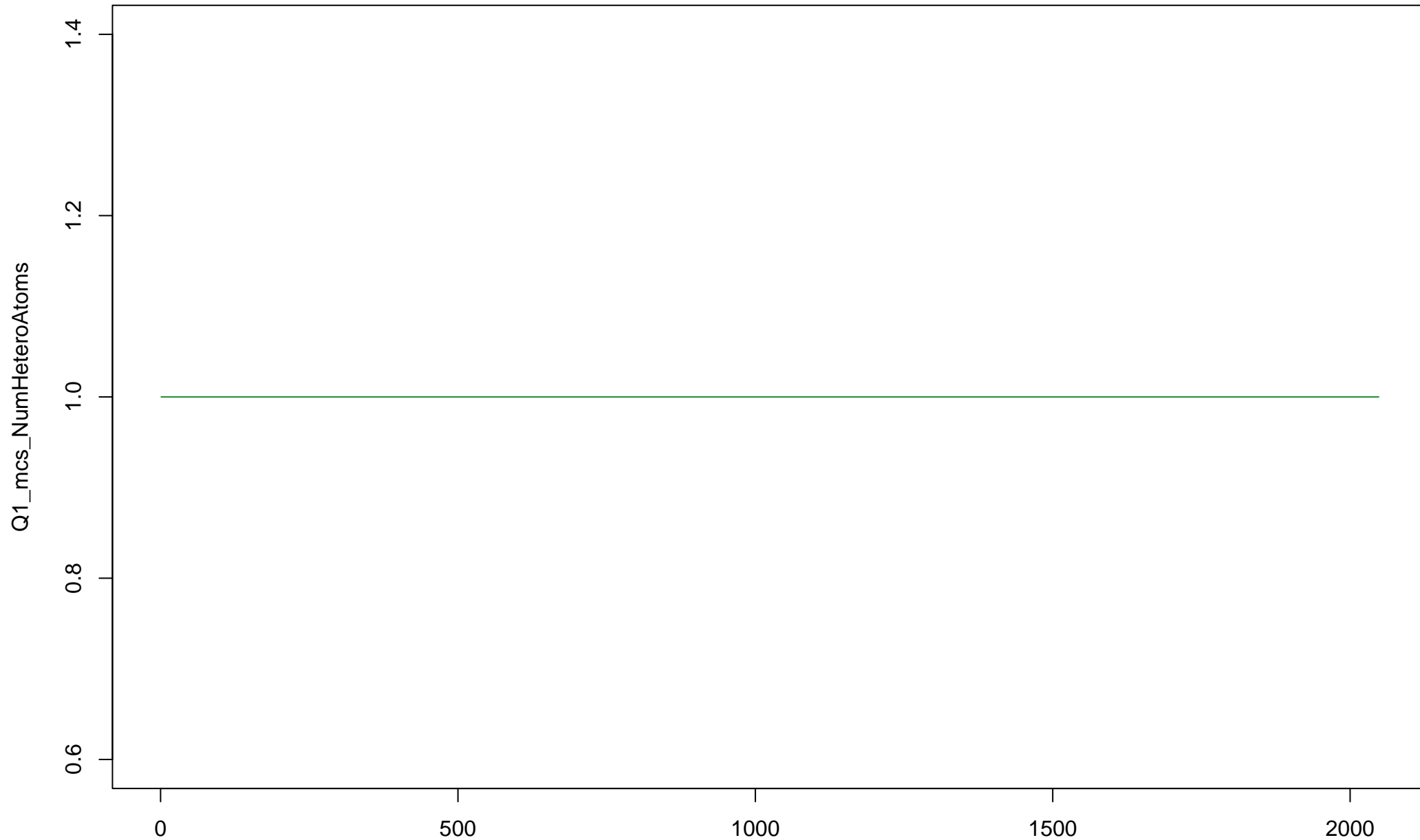
**Q1\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



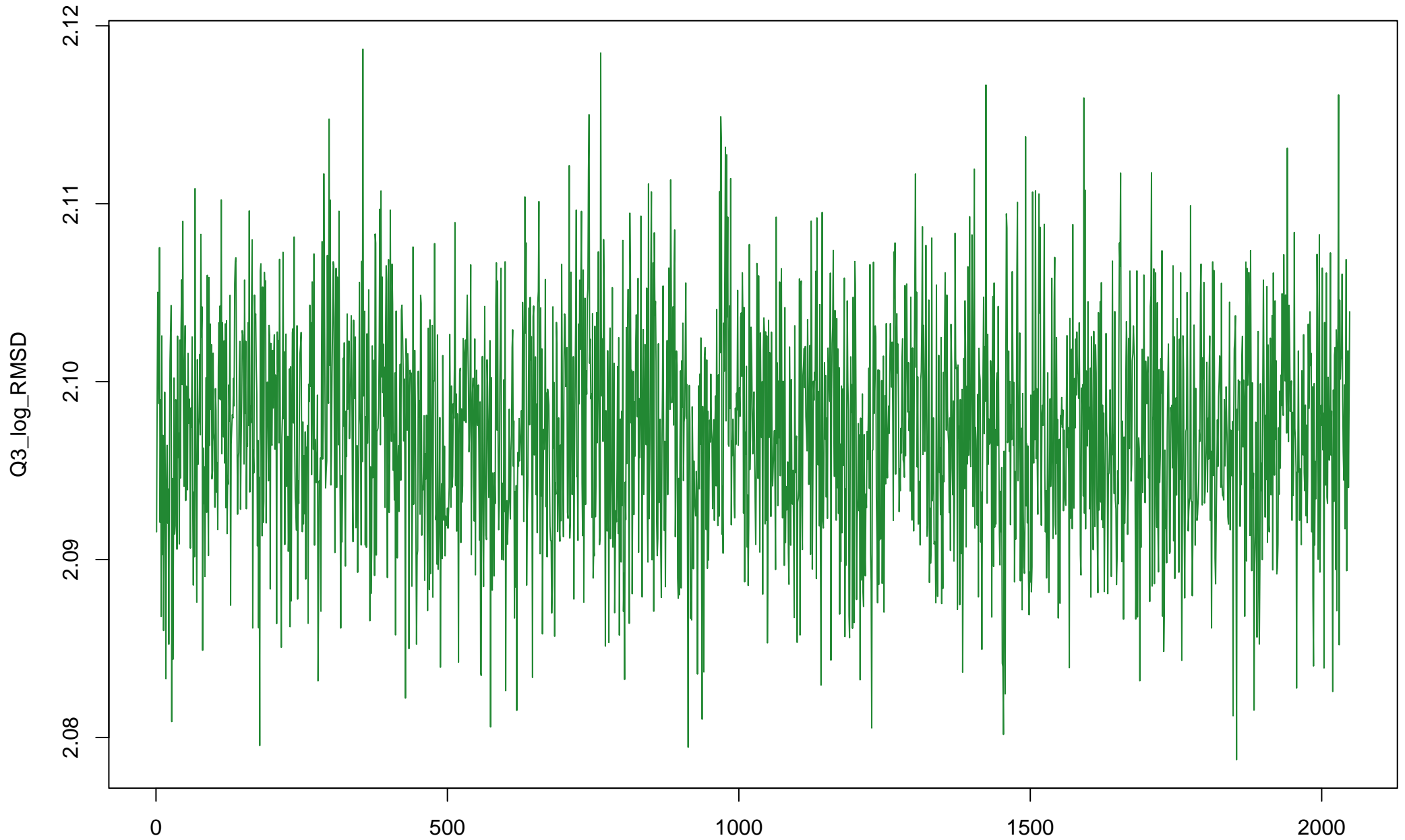
**Q1\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



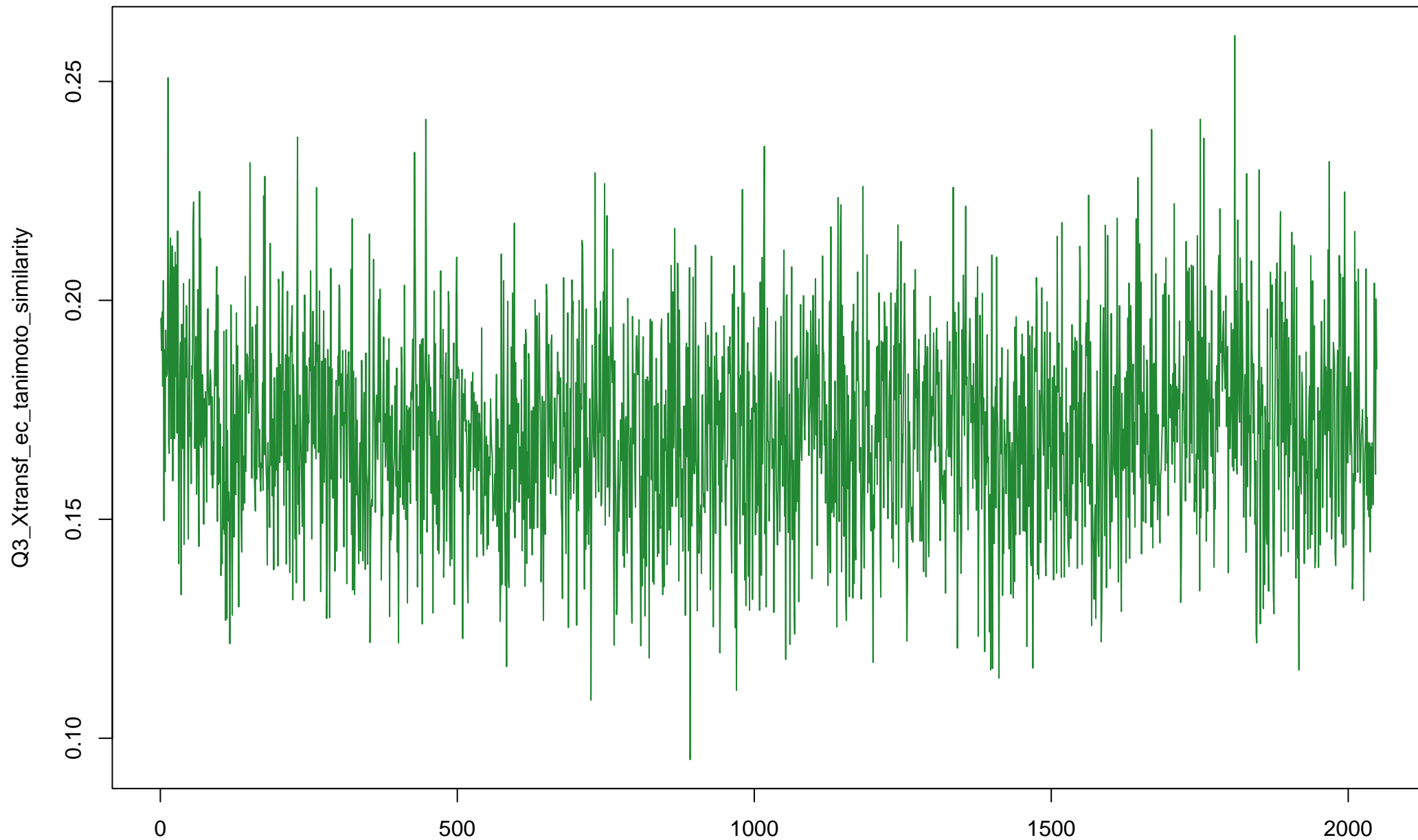
**Q1\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q3\_log\_RMSD**  
**ESS = 1430 | BMK = 0.0346 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0**

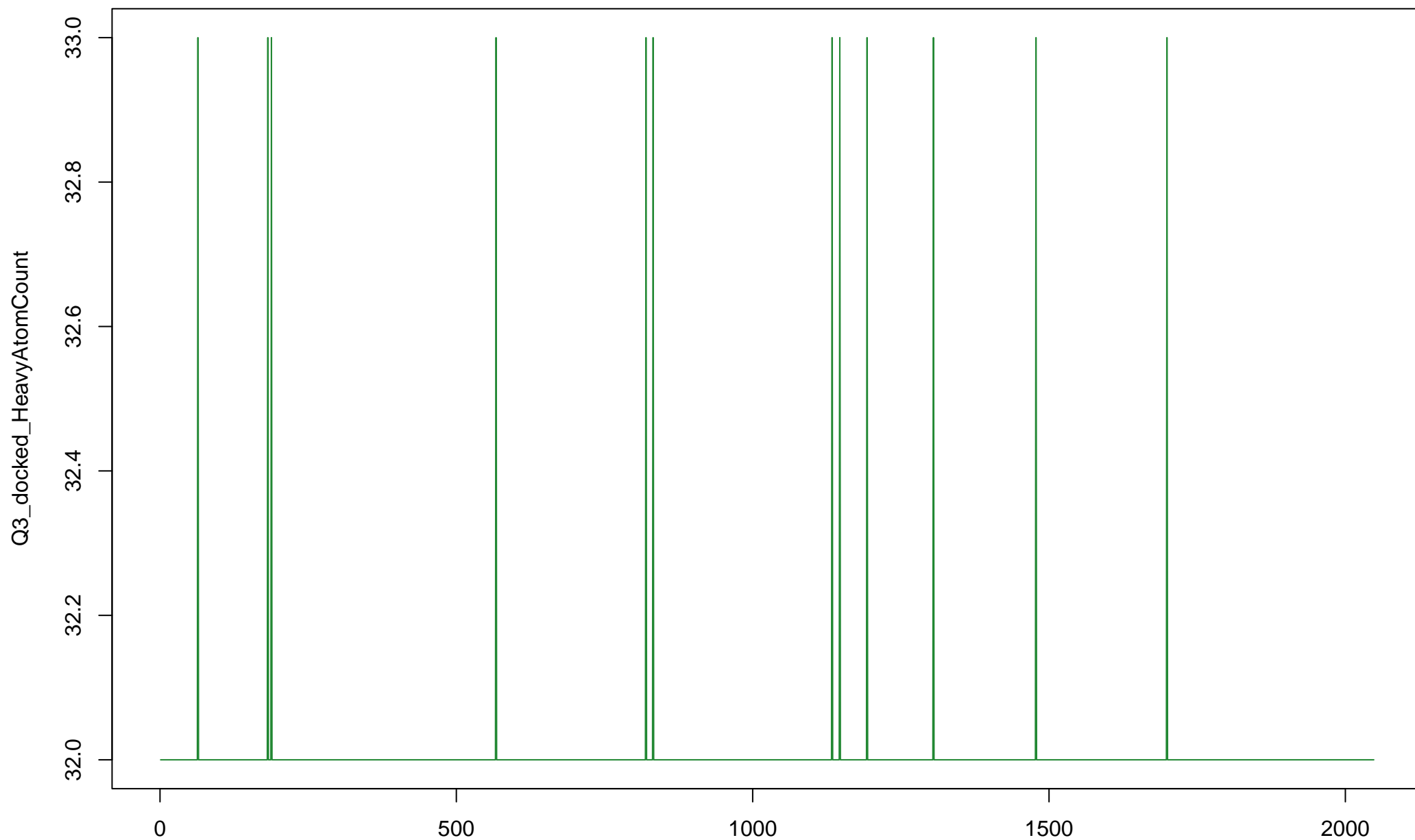


**Q3\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1330 | BMK = 0.0403 | MCSE(6.27) = 3.41 | stat: TRUE | burn: 0**





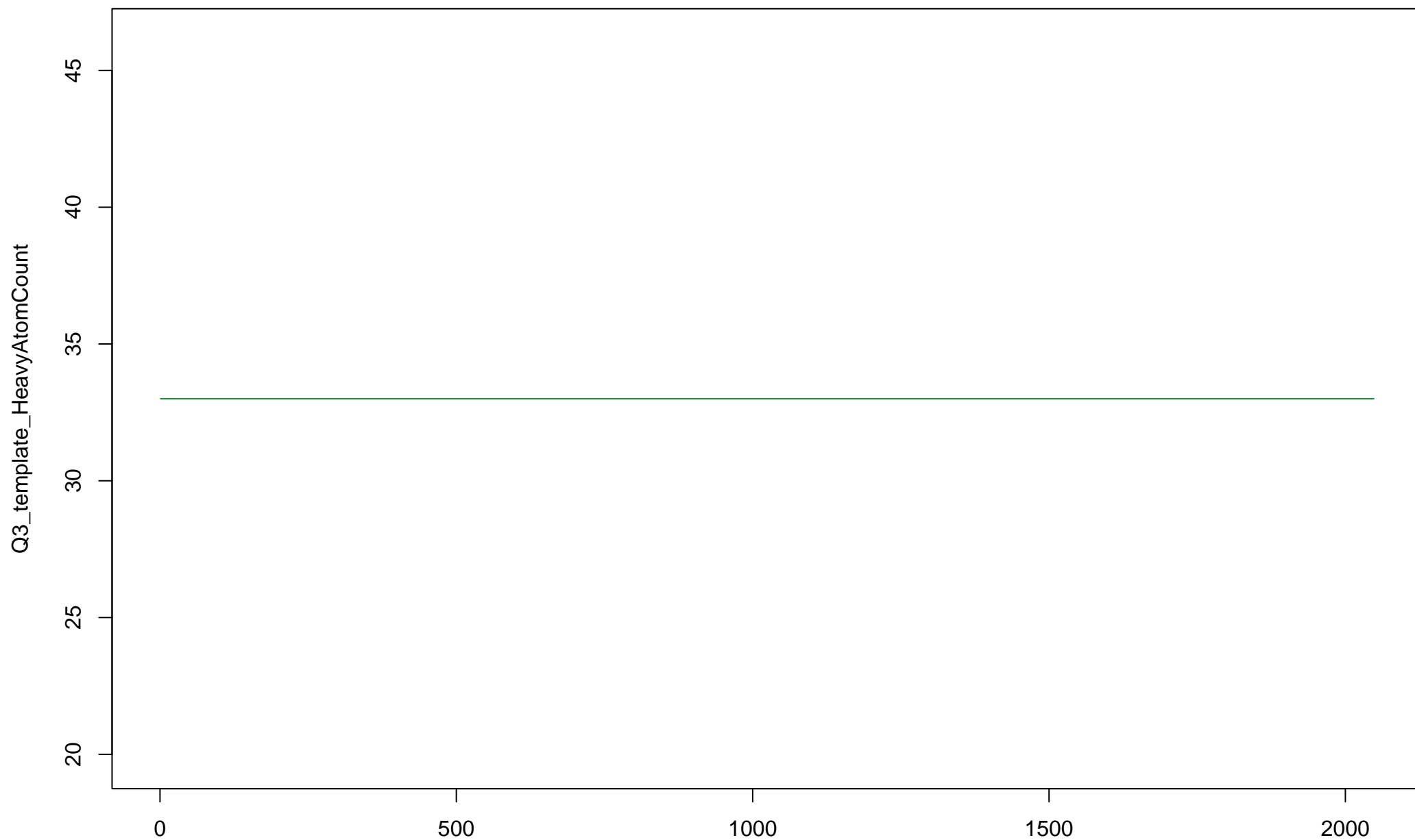
**Q3\_docked\_HeavyAtomCount**  
**ESS = 1440 | BMK = 0 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 2040**



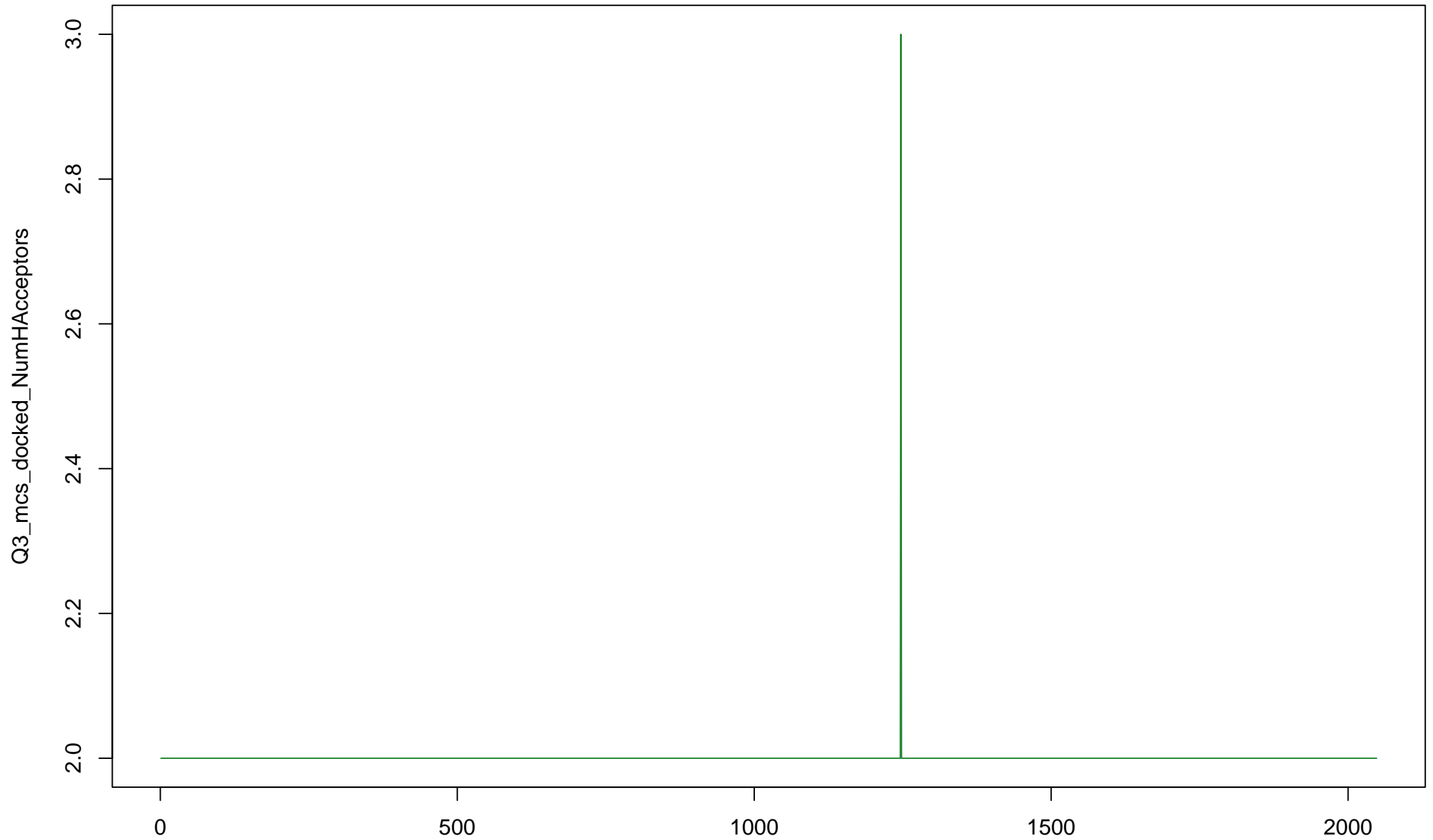
**Q3\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



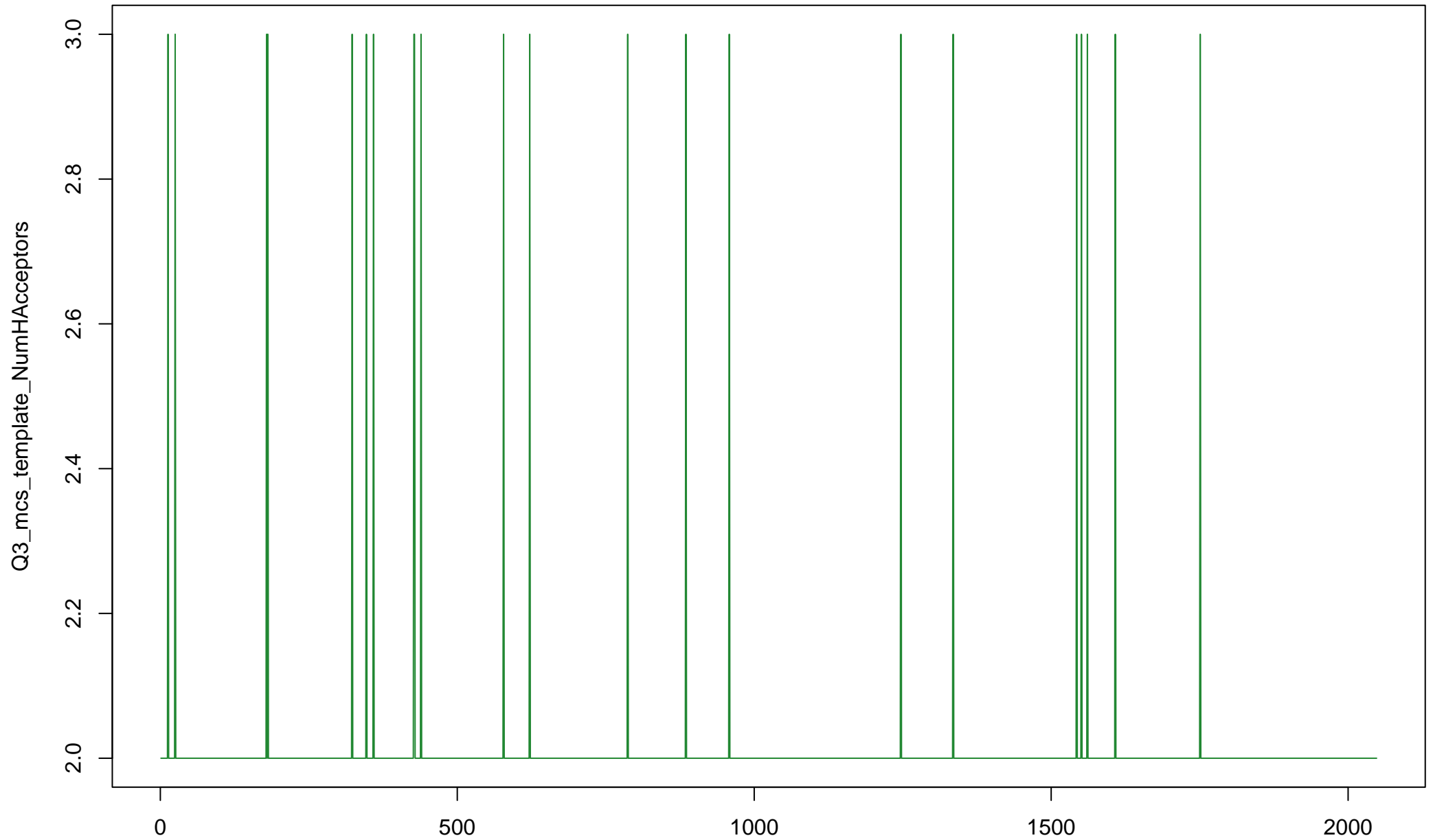
**Q3\_template\_HeavyAtomCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q3\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.644 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 1428**



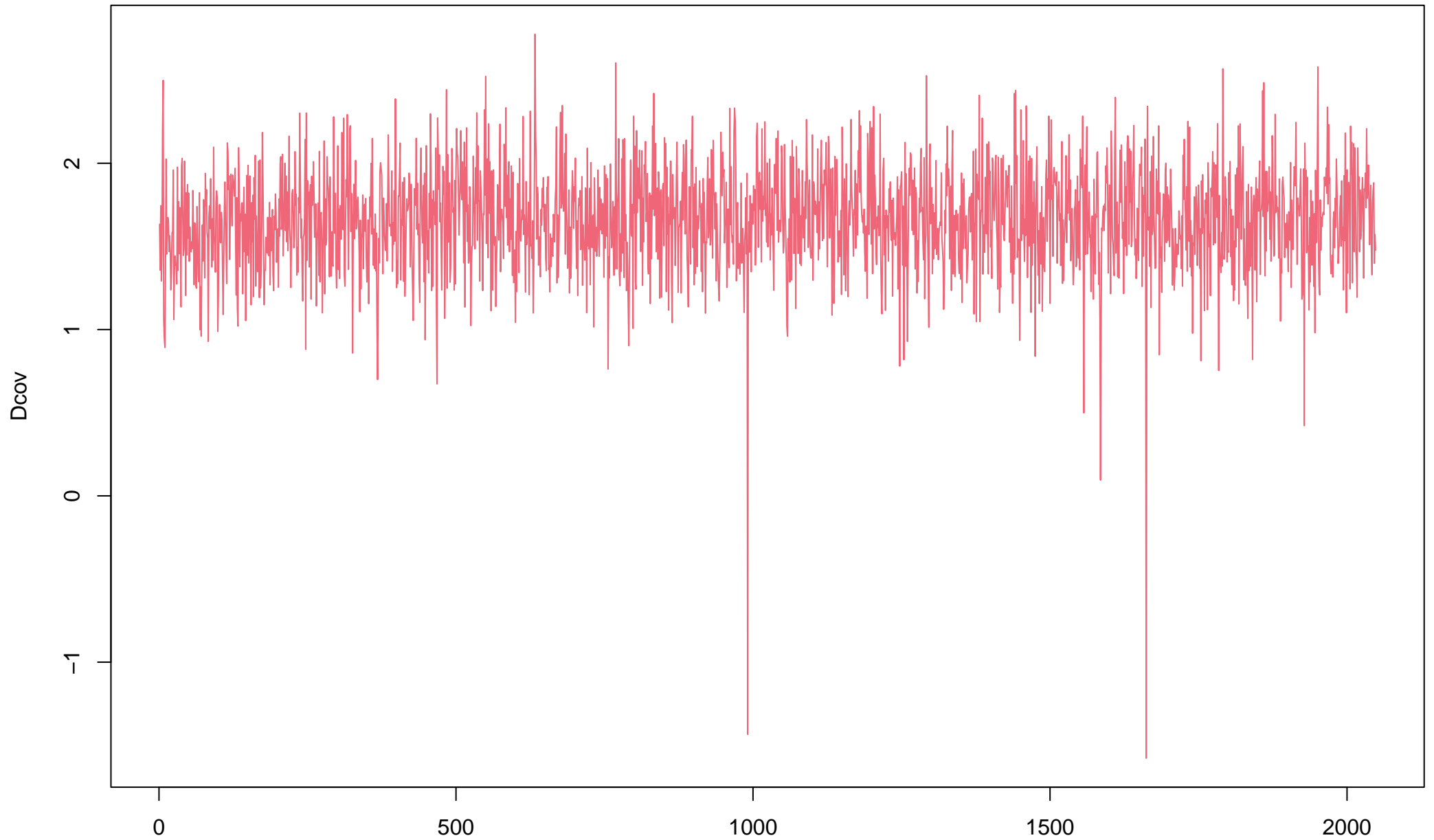
**Q3\_mcs\_template\_NumHAcceptors**  
**ESS = 1290 | BMK = 0.133 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 2040**



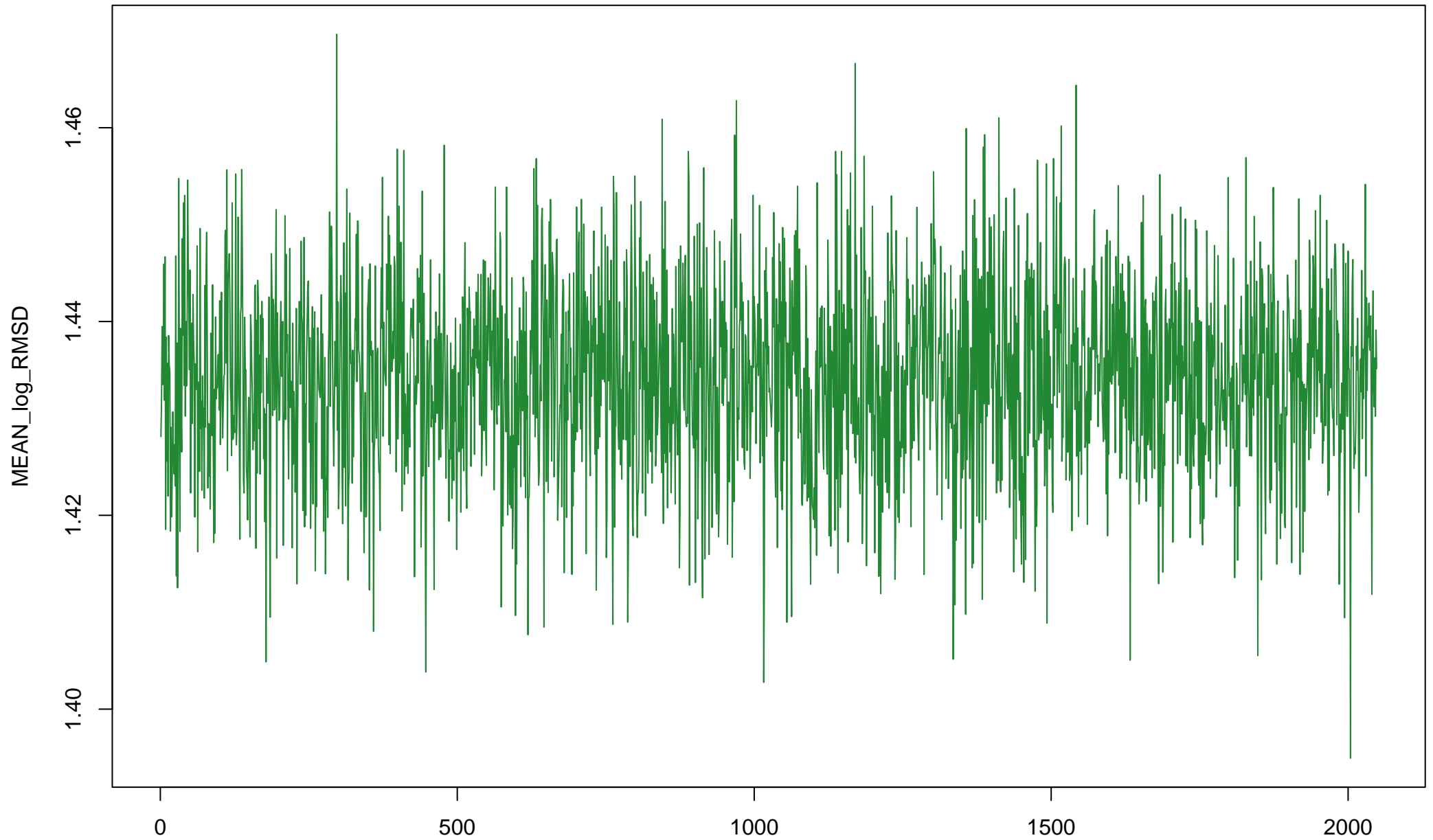
**Q3\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Dcov**  
**ESS = 1770 | BMK = 0.0511 | MCSE(6.27) = 2.43 | stat: FALSE | burn: 0**

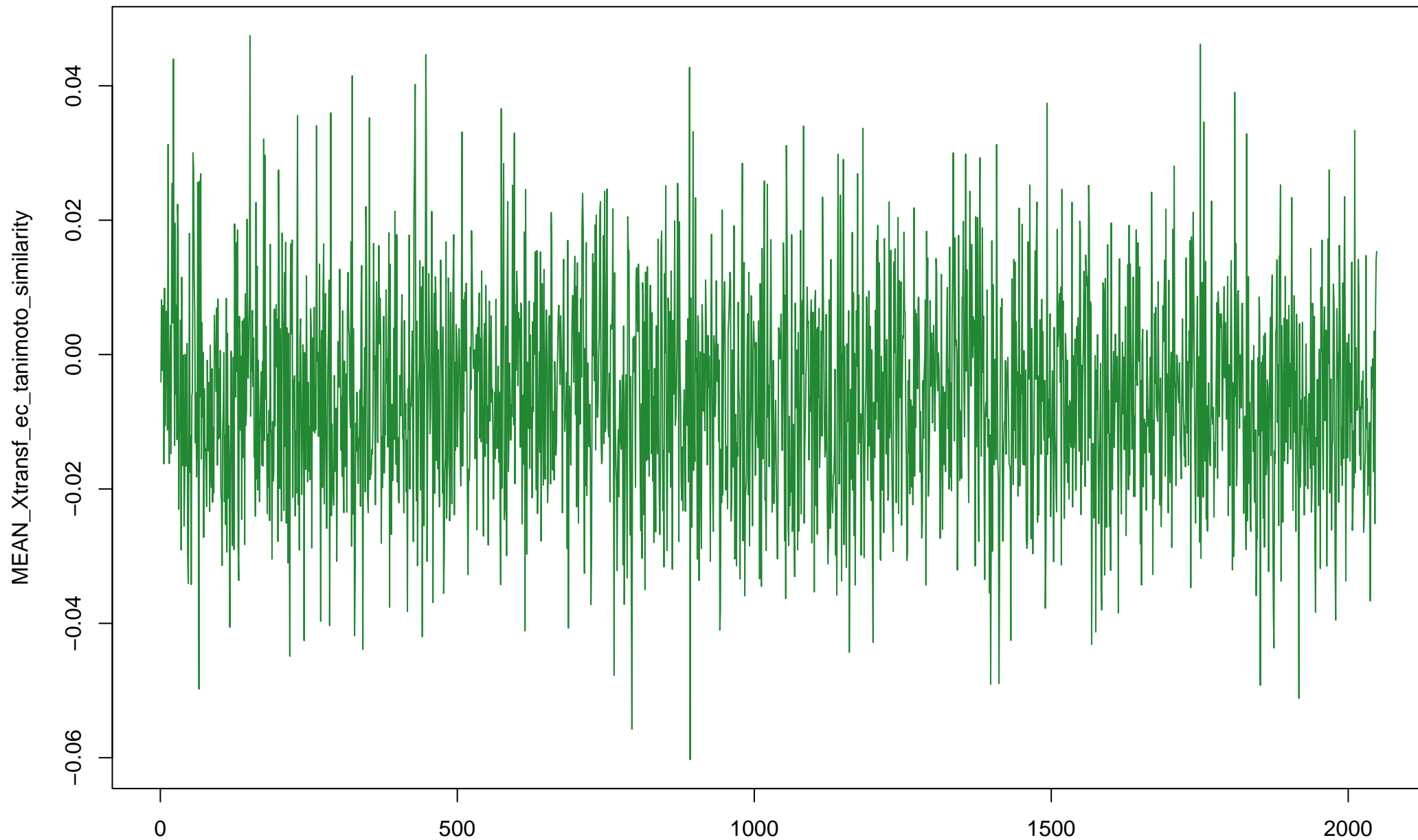


**MEAN\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0235 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0**

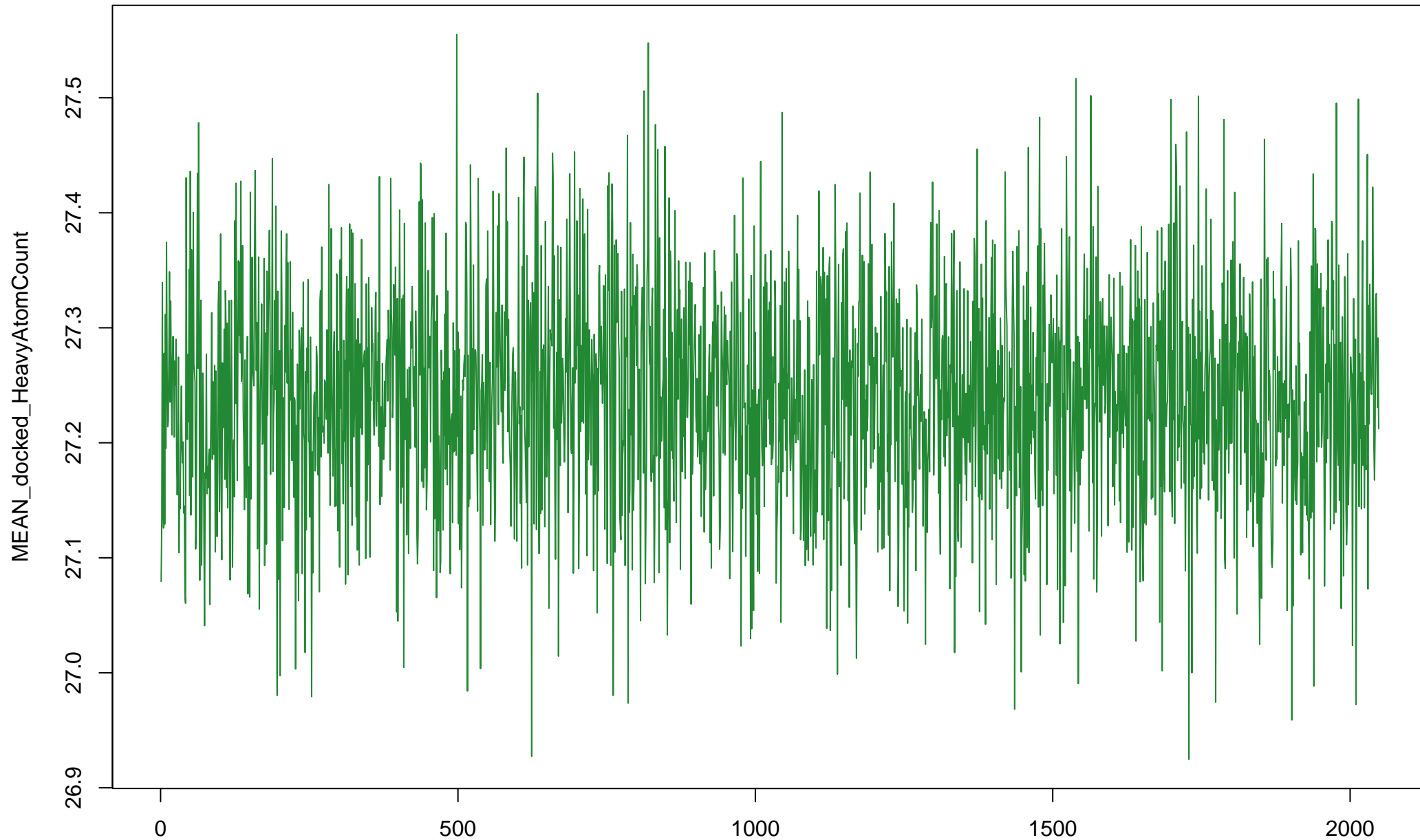




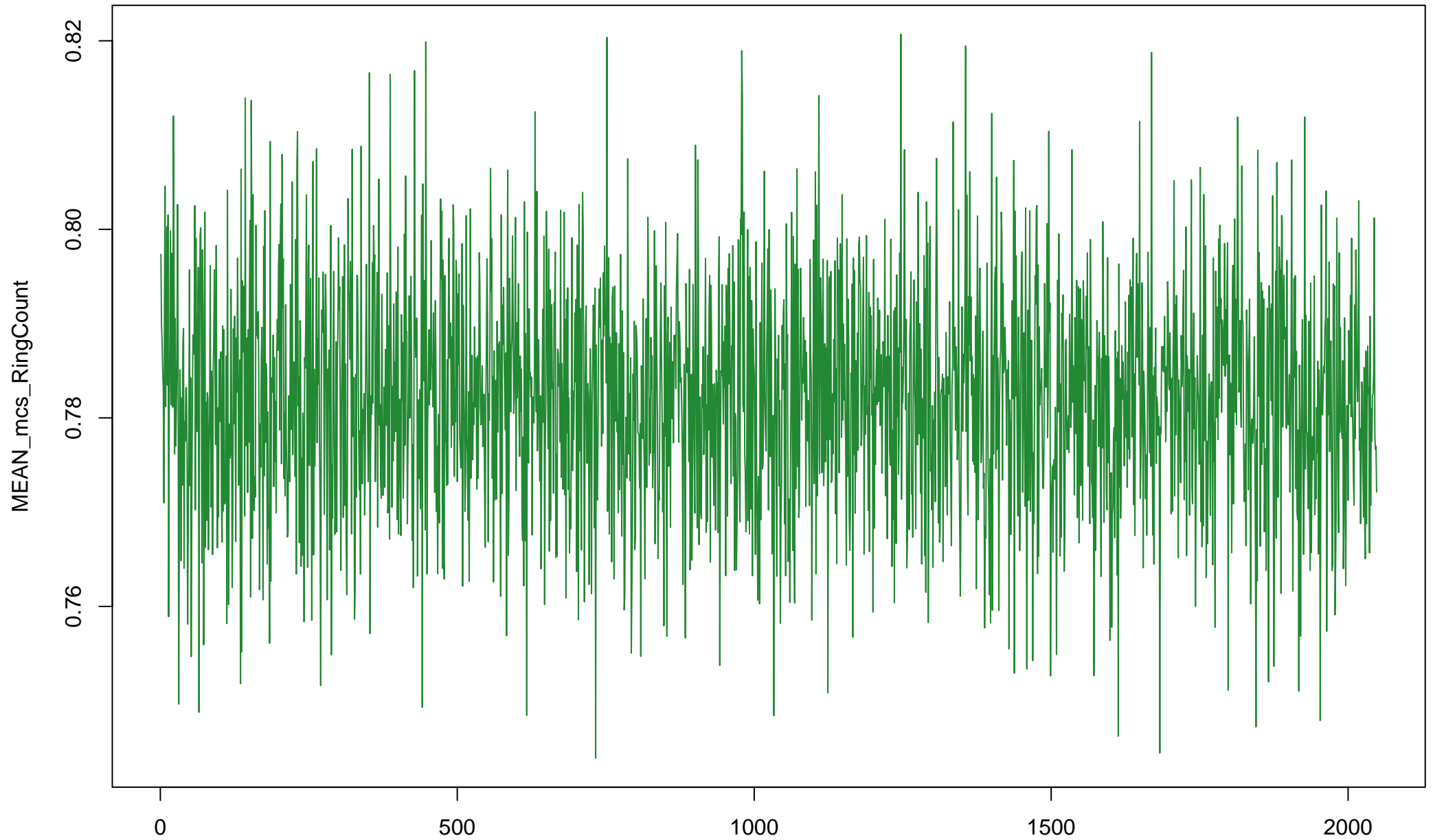
**MEAN\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0385 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0**



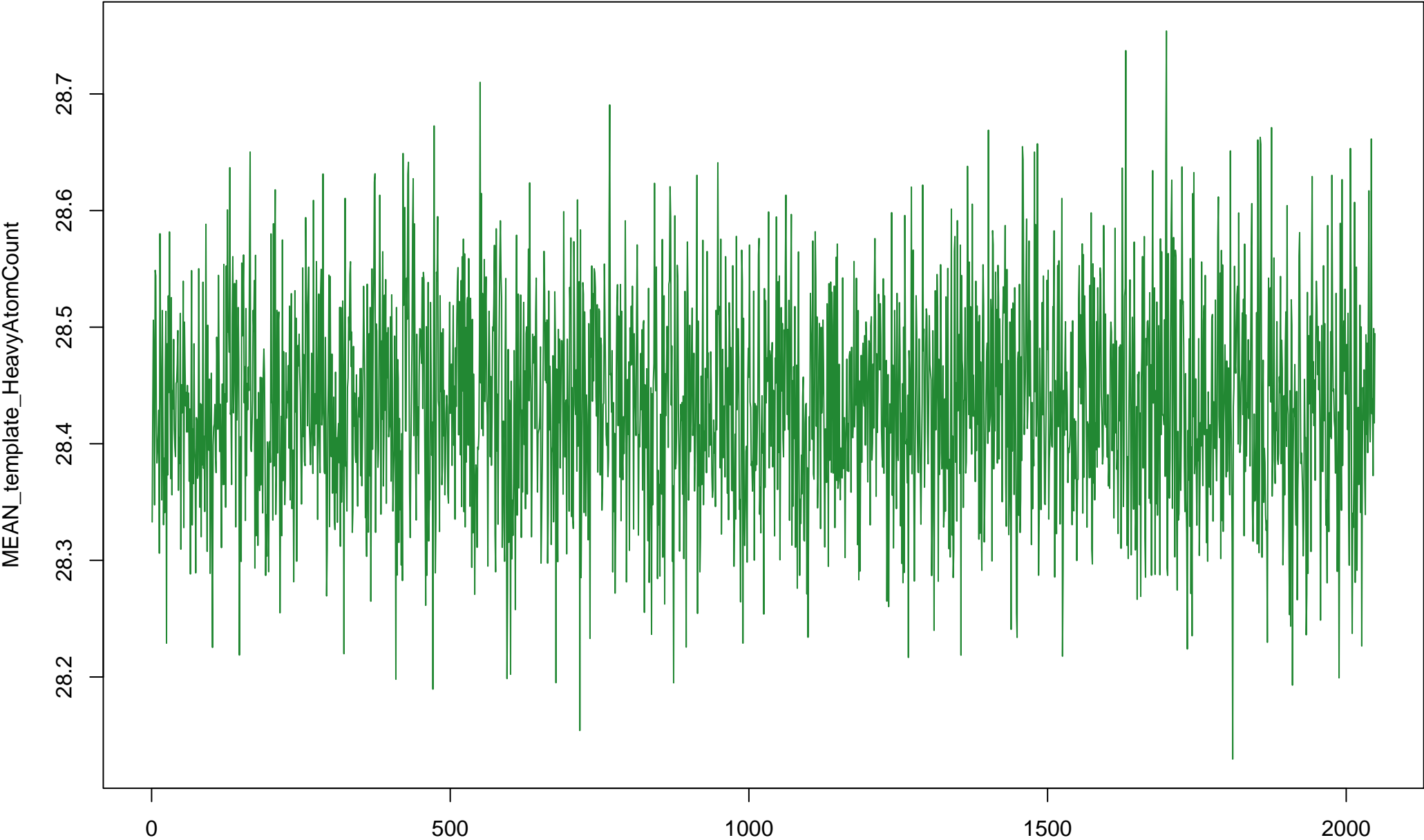
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0504 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0**



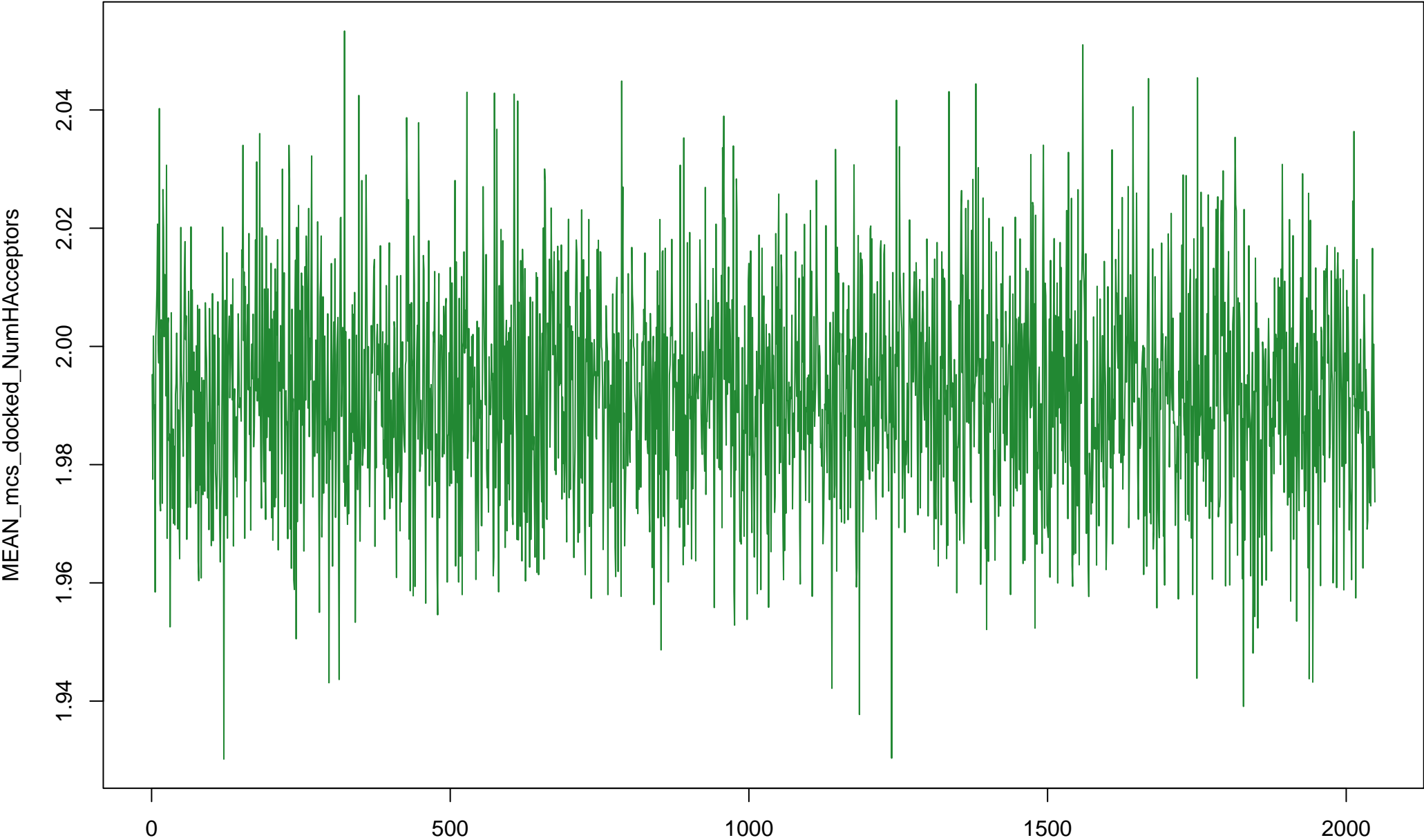
**MEAN\_mcs\_RingCount**  
**ESS = 2050 | BMK = 0.0364 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0**



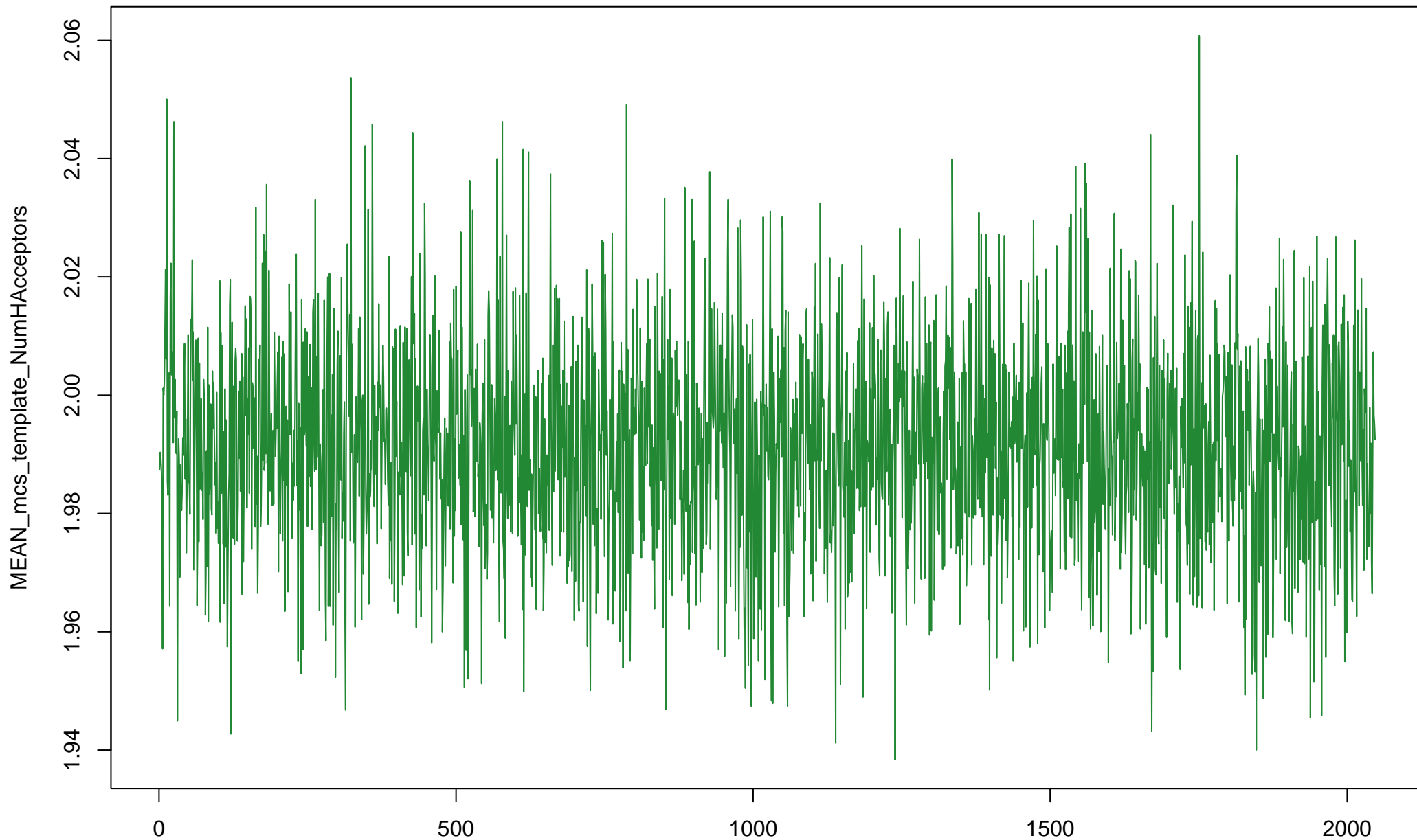
MEAN\_template\_HeavyAtomCount  
ESS = 2050 | BMK = 0.041 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0



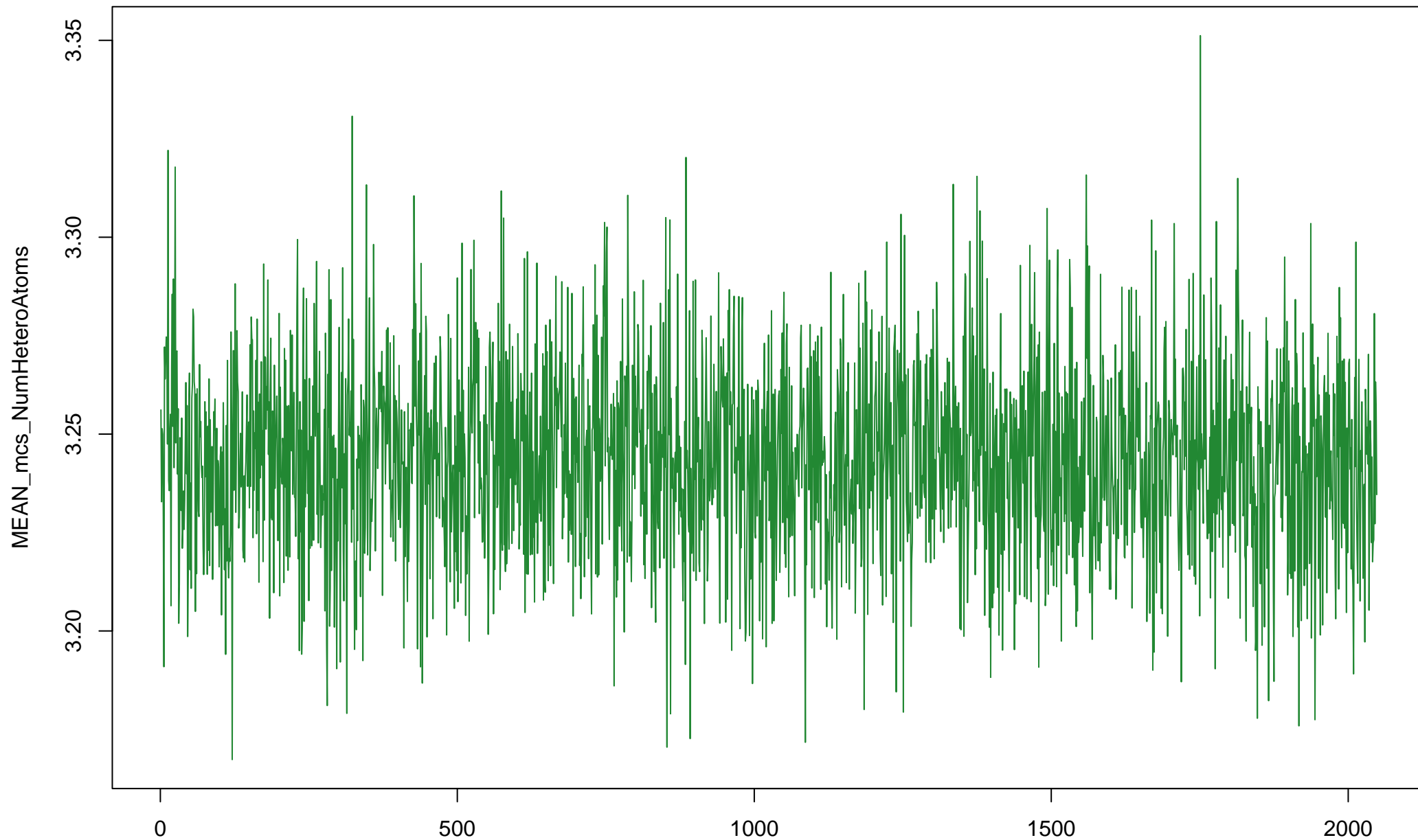
**MEAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.042 | MCSE(6.27) = 1.65 | stat: TRUE | burn: 0**



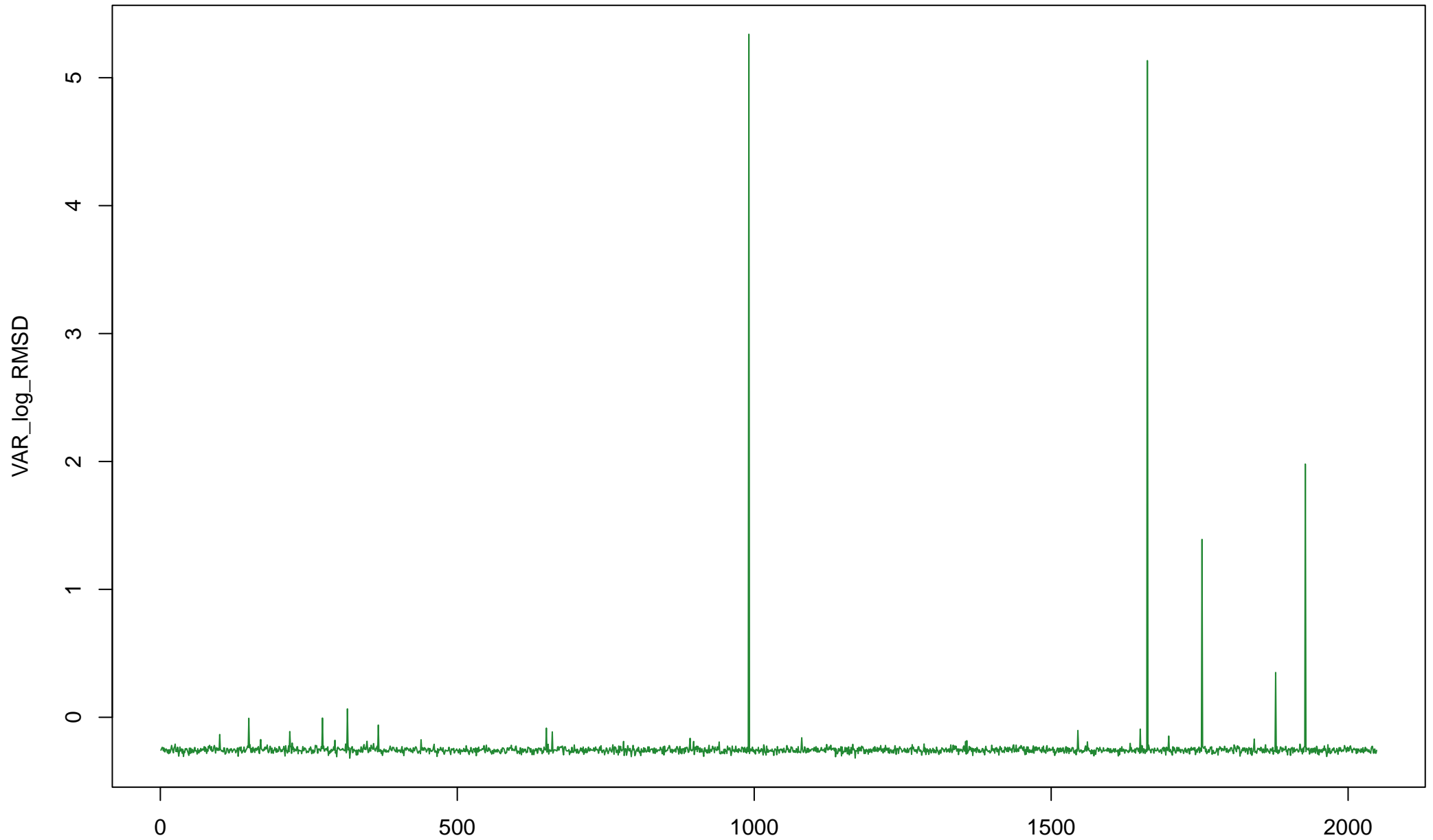
**MEAN\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0488 | MCSE(6.27) = 1.87 | stat: TRUE | burn: 0**



**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0449 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0**

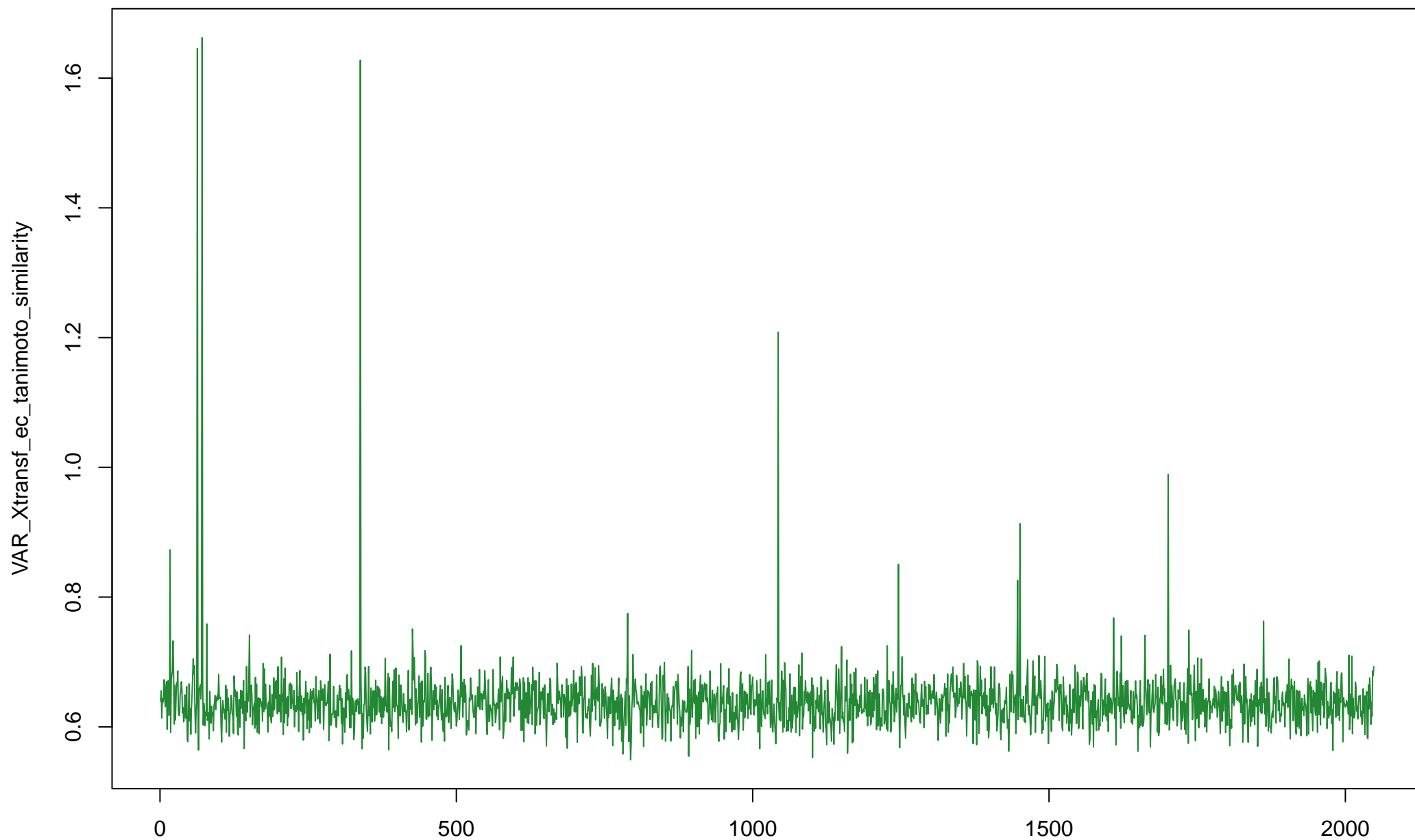


**VAR\_log\_RMSD**  
**ESS = 2050 | BMK = 0.278 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 2040**

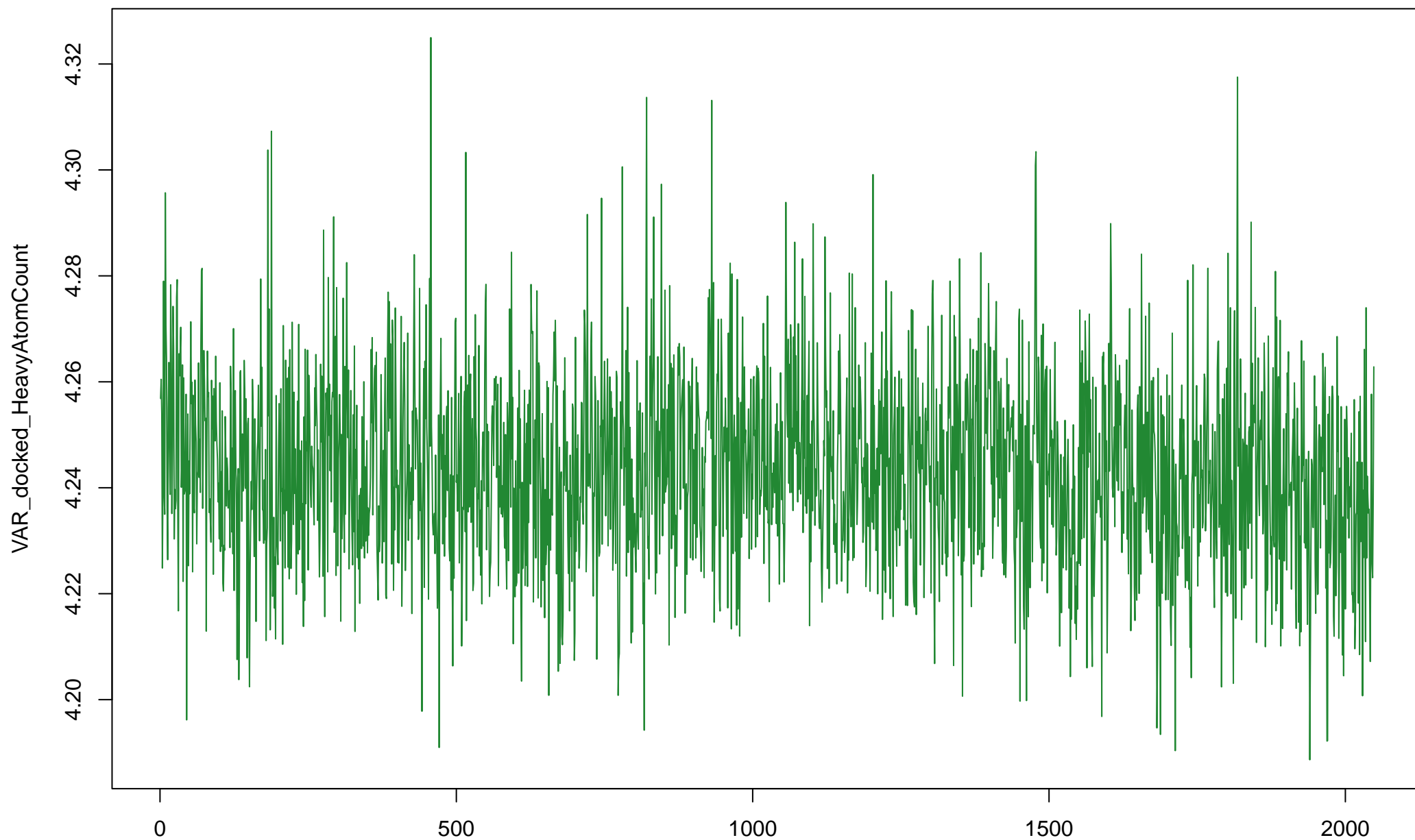




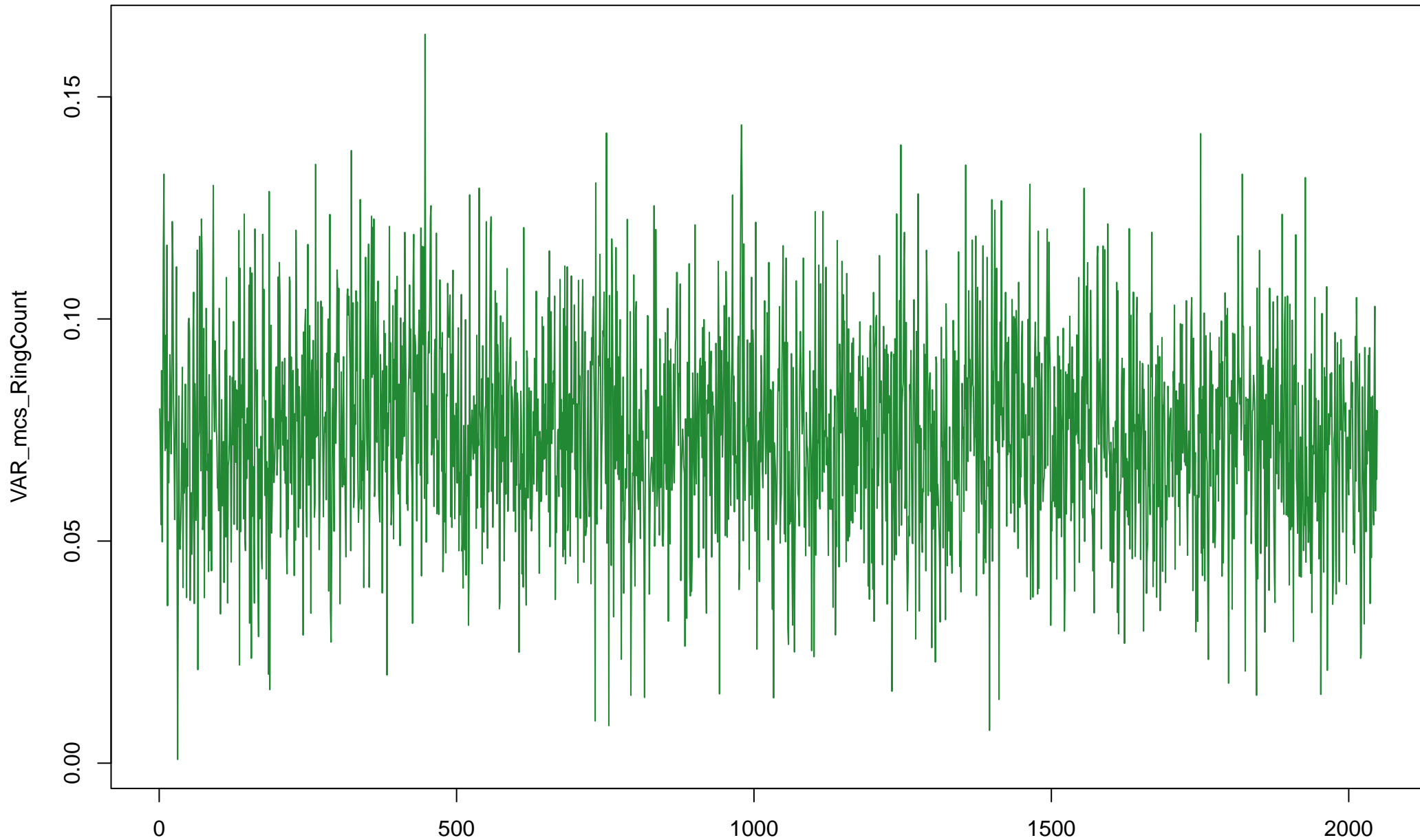
**VAR\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1550 | BMK = 0.0708 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0**



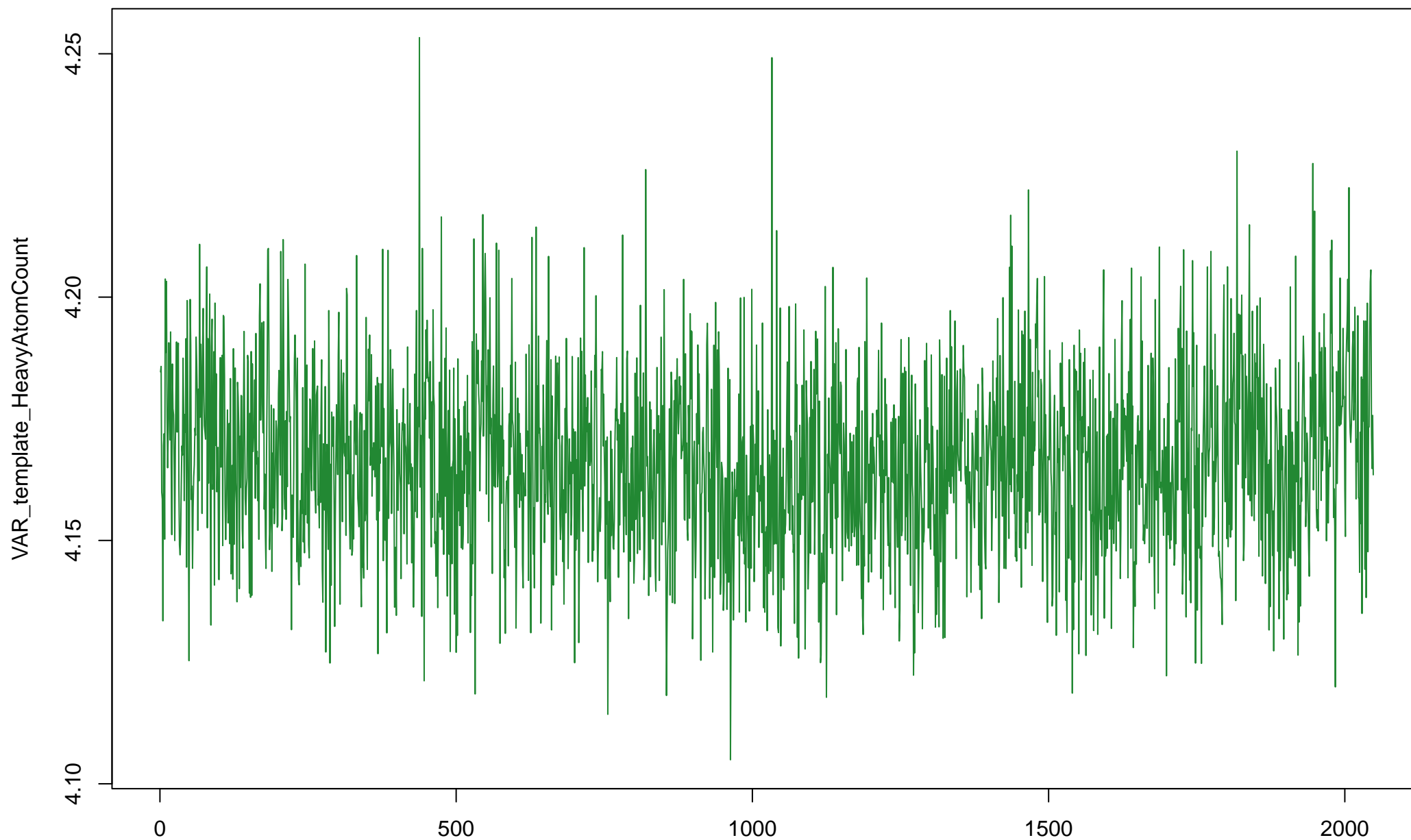
**VAR\_docked\_HeavyAtomCount**  
**ESS = 1520 | BMK = 0.0494 | MCSE(6.27) = 3.22 | stat: TRUE | burn: 0**



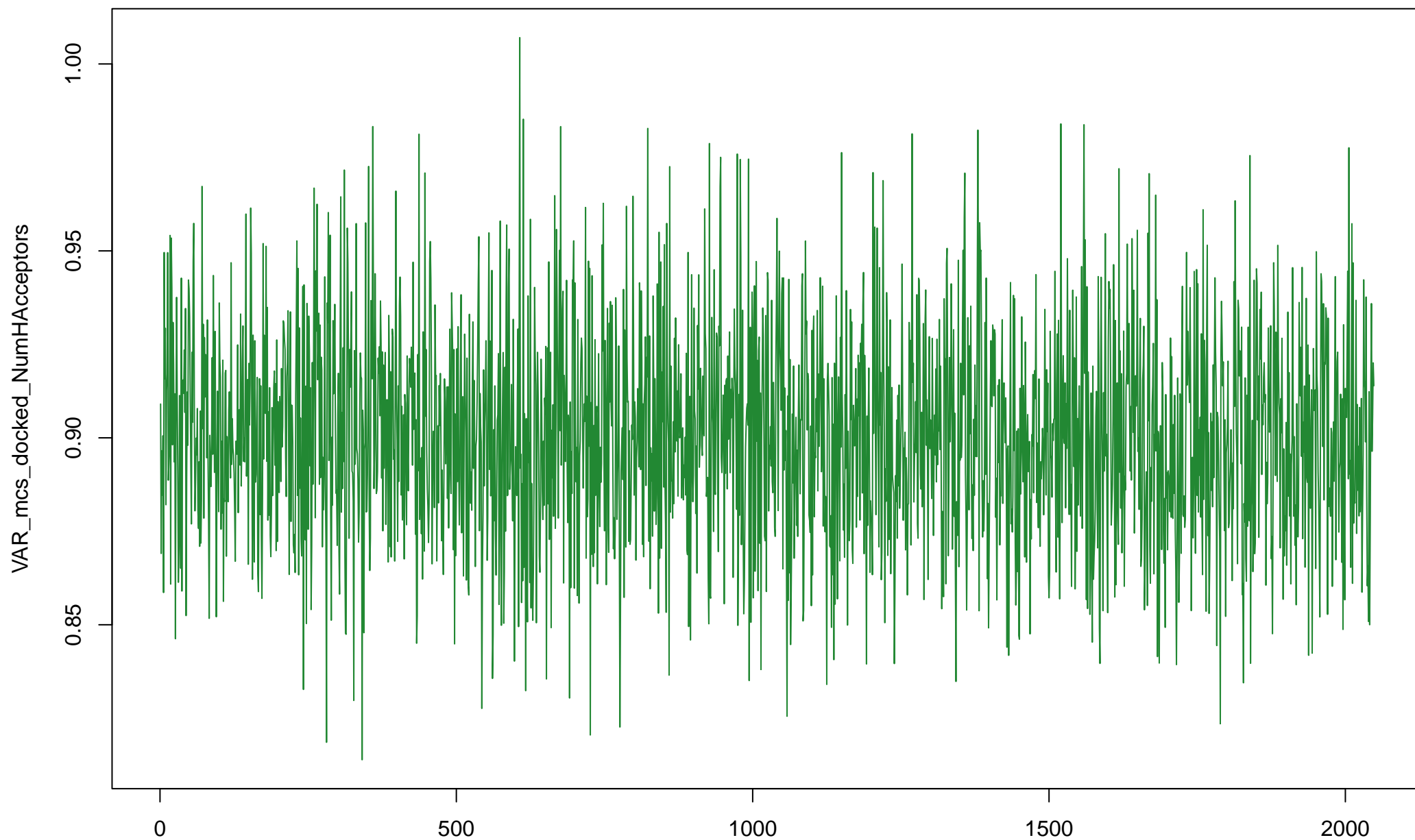
**VAR\_mcs\_RingCount**  
**ESS = 2050 | BMK = 0.0597 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0**



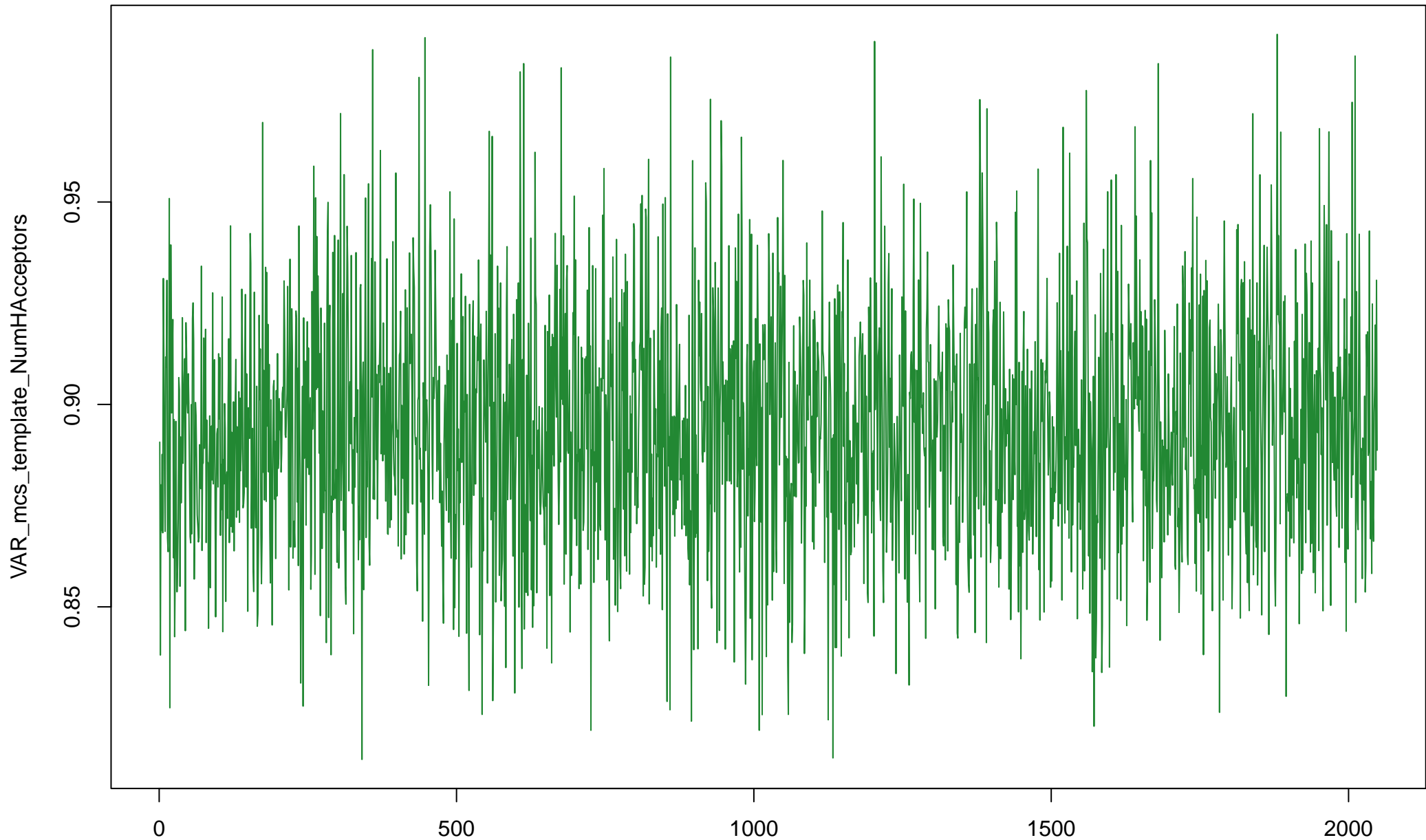
VAR\_template\_HeavyAtomCount  
ESS = 711 | BMK = 0.0374 | MCSE(6.27) = 3.51 | stat: FALSE | burn: 0



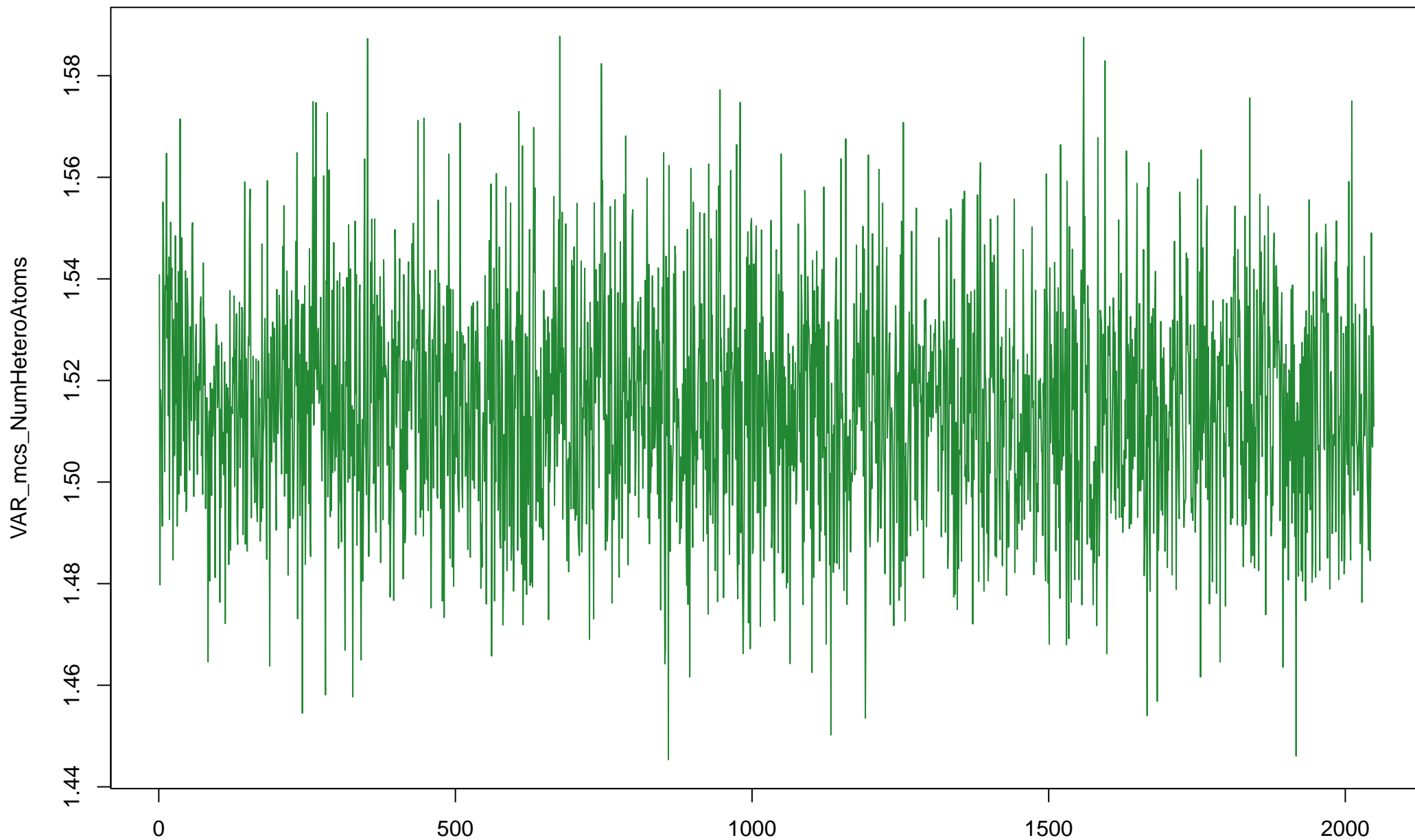
**VAR\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0506 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0**



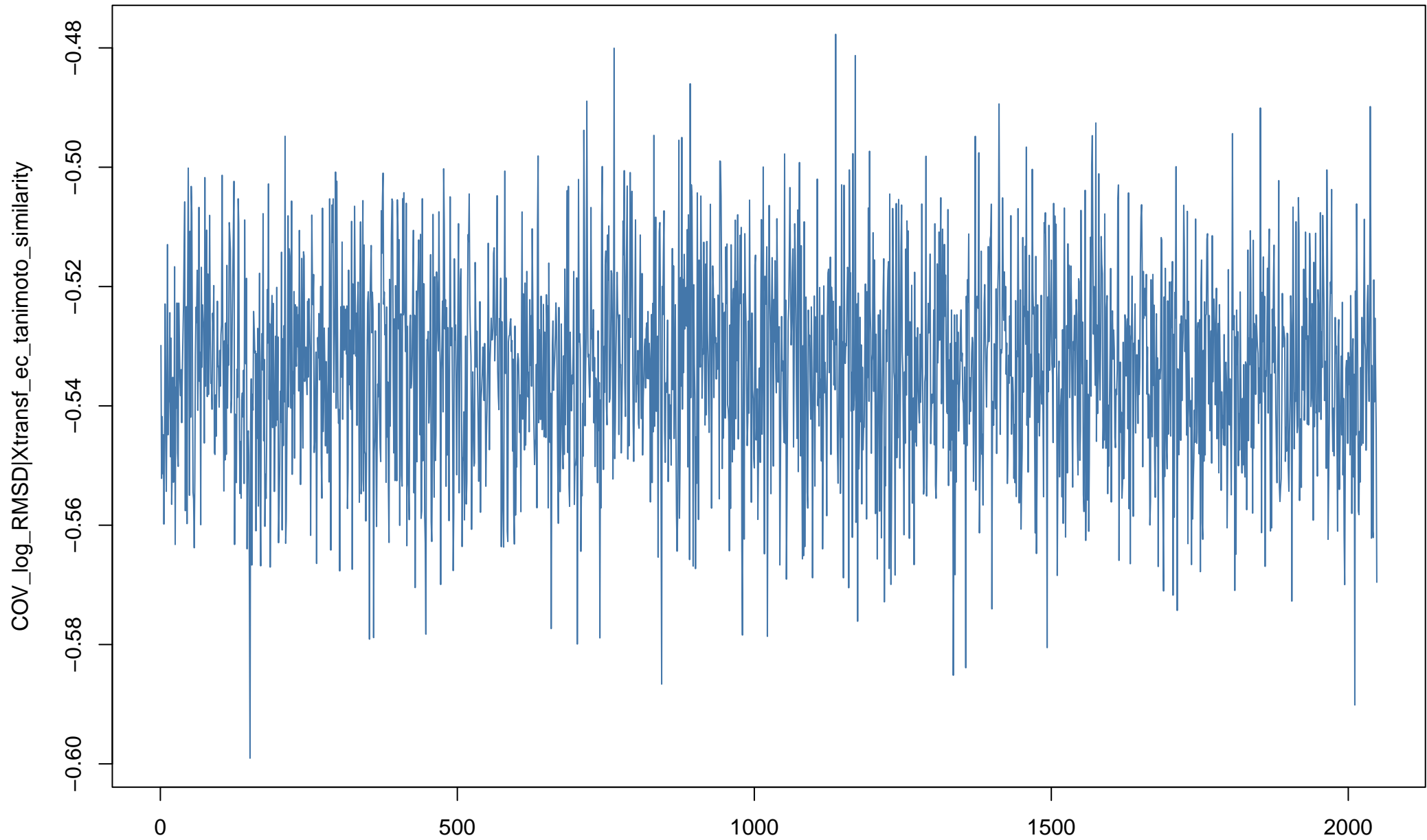
**VAR\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0372 | MCSE(6.27) = 2.1 | stat: FALSE | burn: 0**



**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0475 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0**

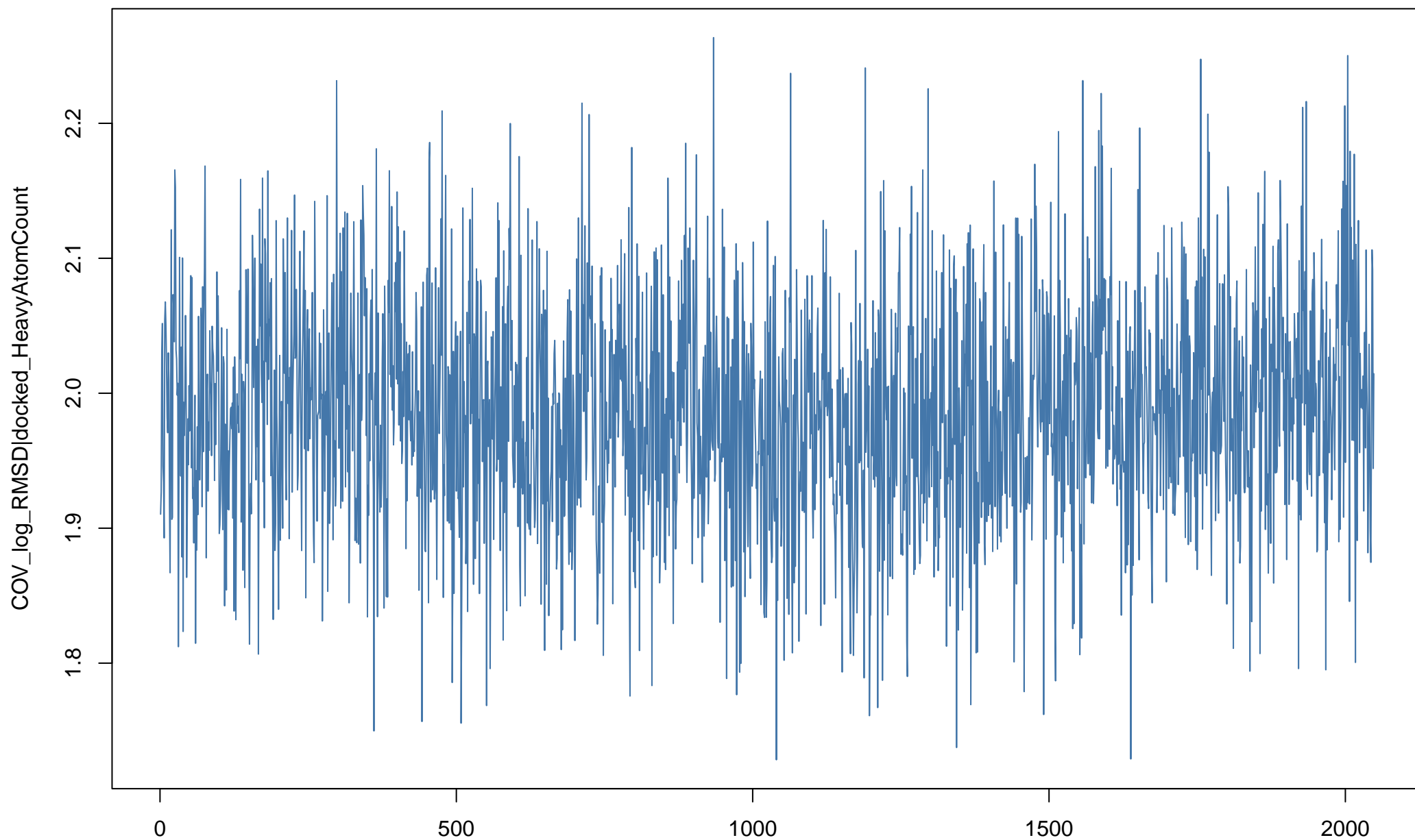


**COV\_log\_RMSD|Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1830 | BMK = 0.0404 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0**

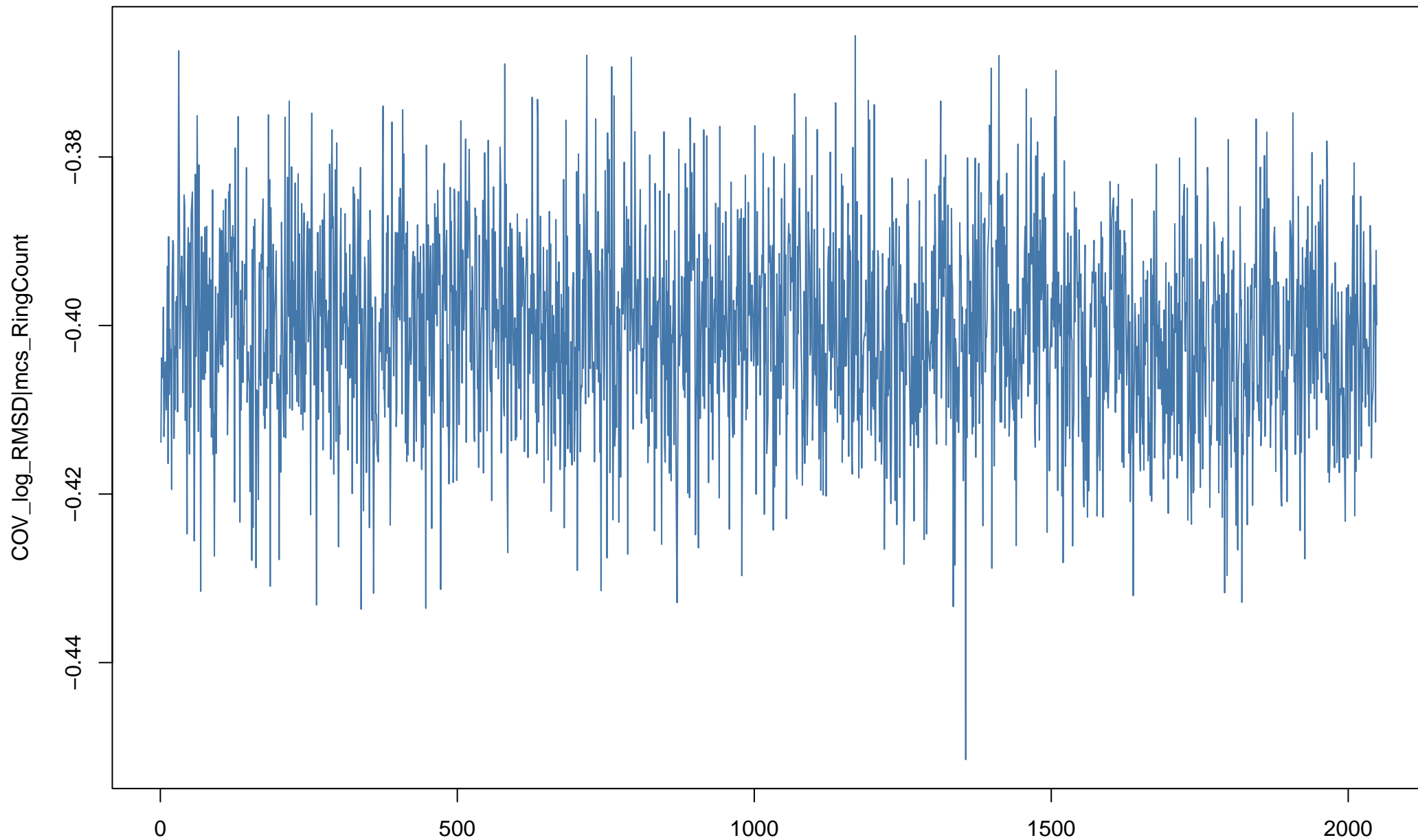




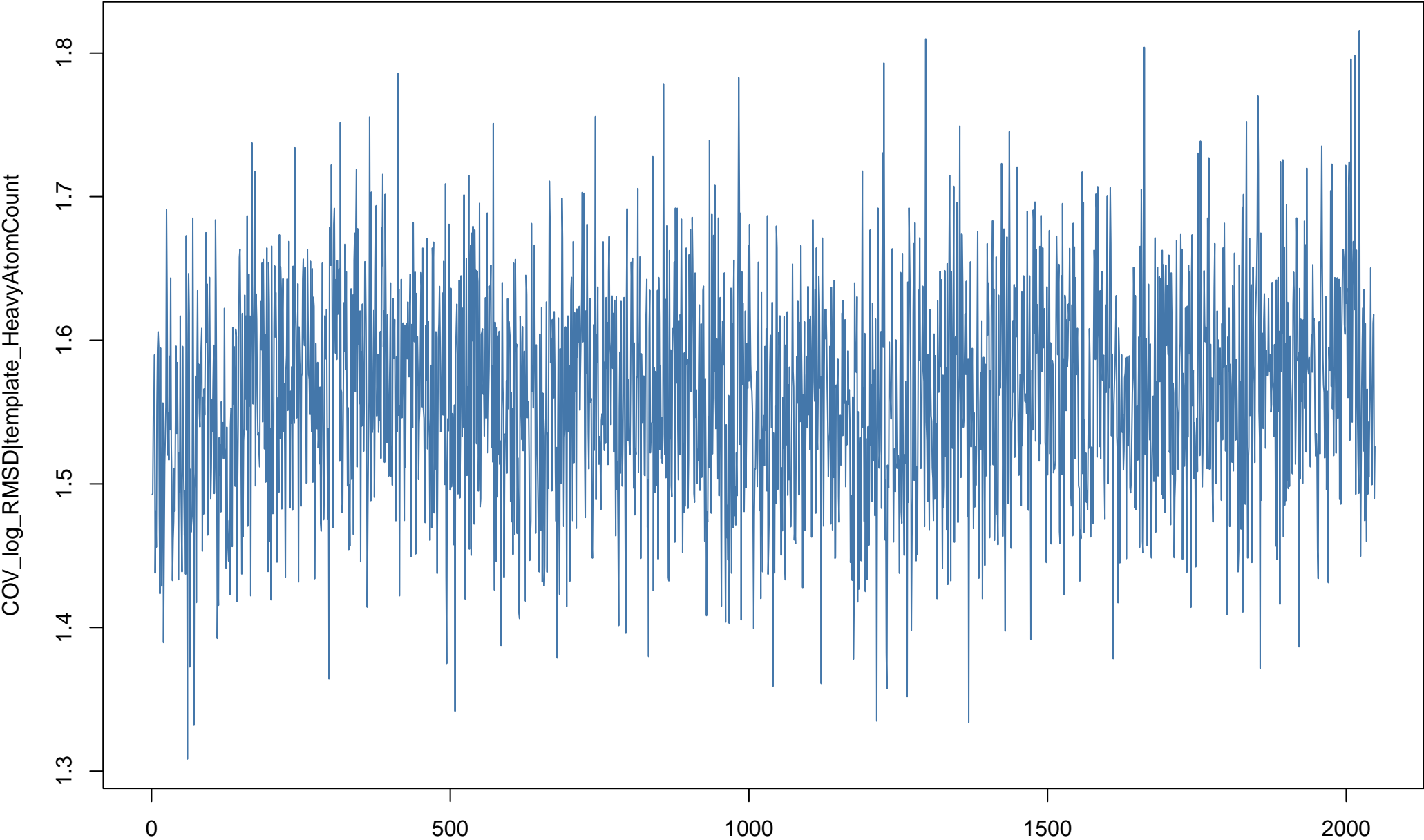
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 987 | BMK = 0.0362 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0**



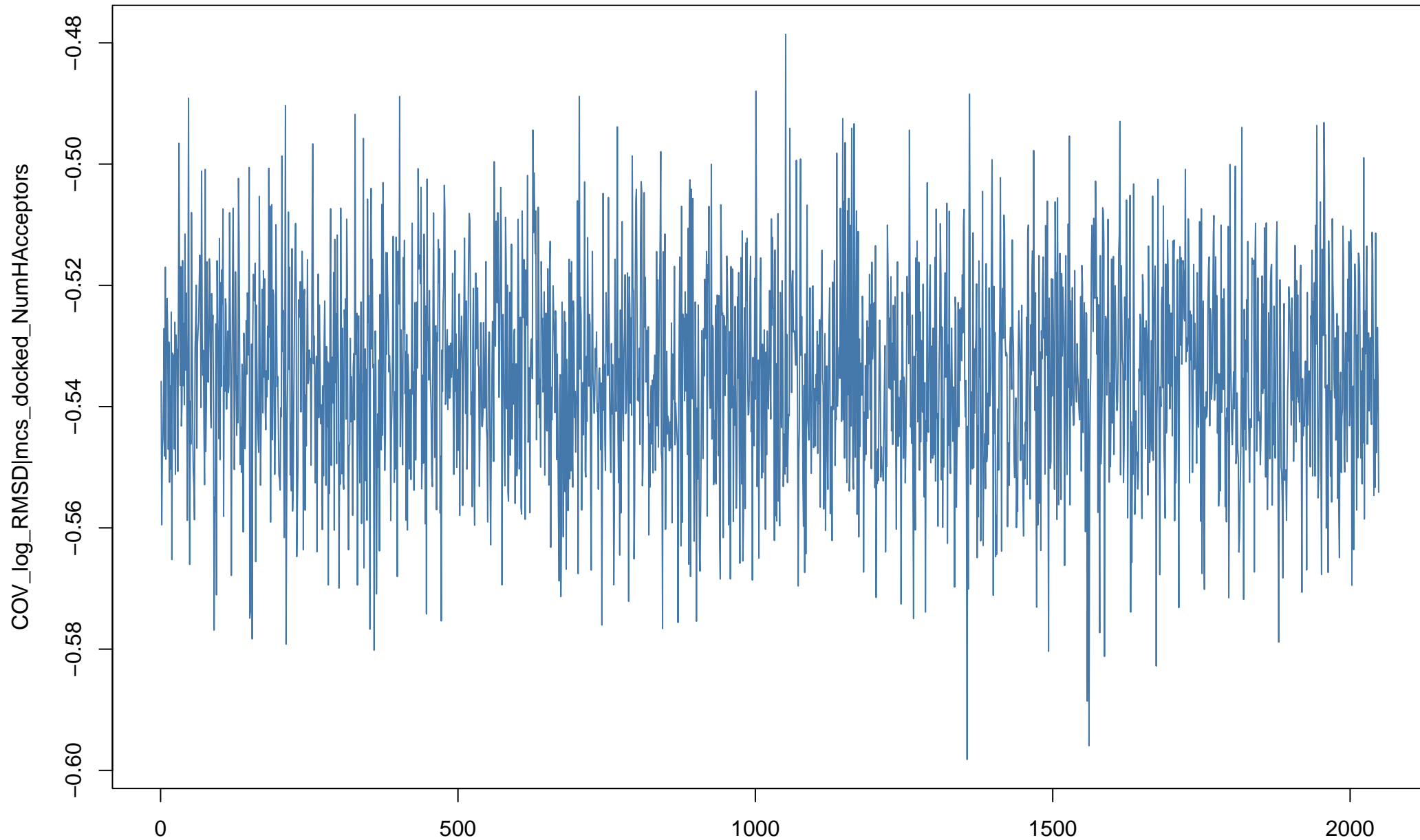
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 1620 | BMK = 0.0668 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0**



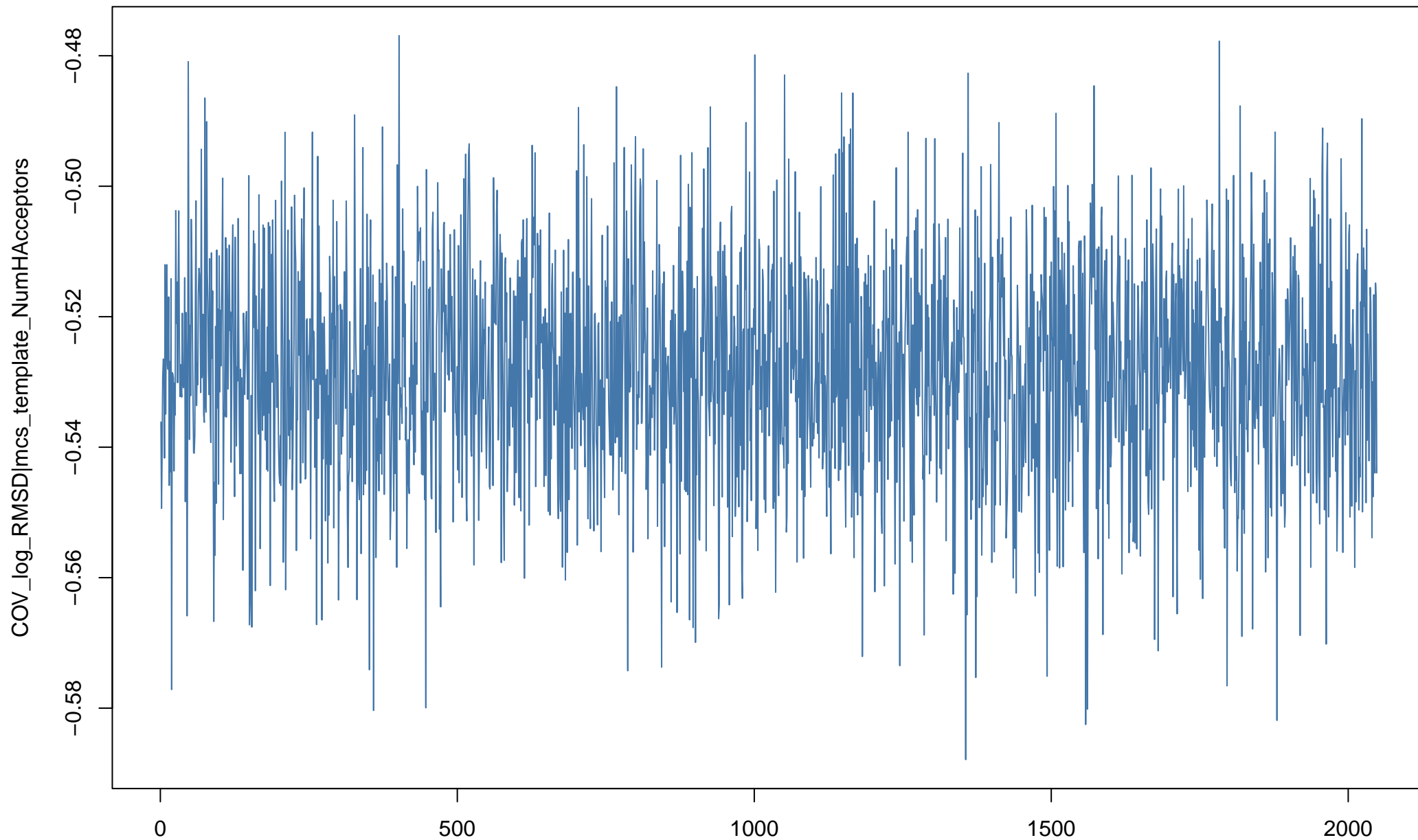
COV\_log\_RMSD|template\_HeavyAtomCount  
ESS = 731 | BMK = 0.044 | MCSE(6.27) = 3.49 | stat: FALSE | burn: 0



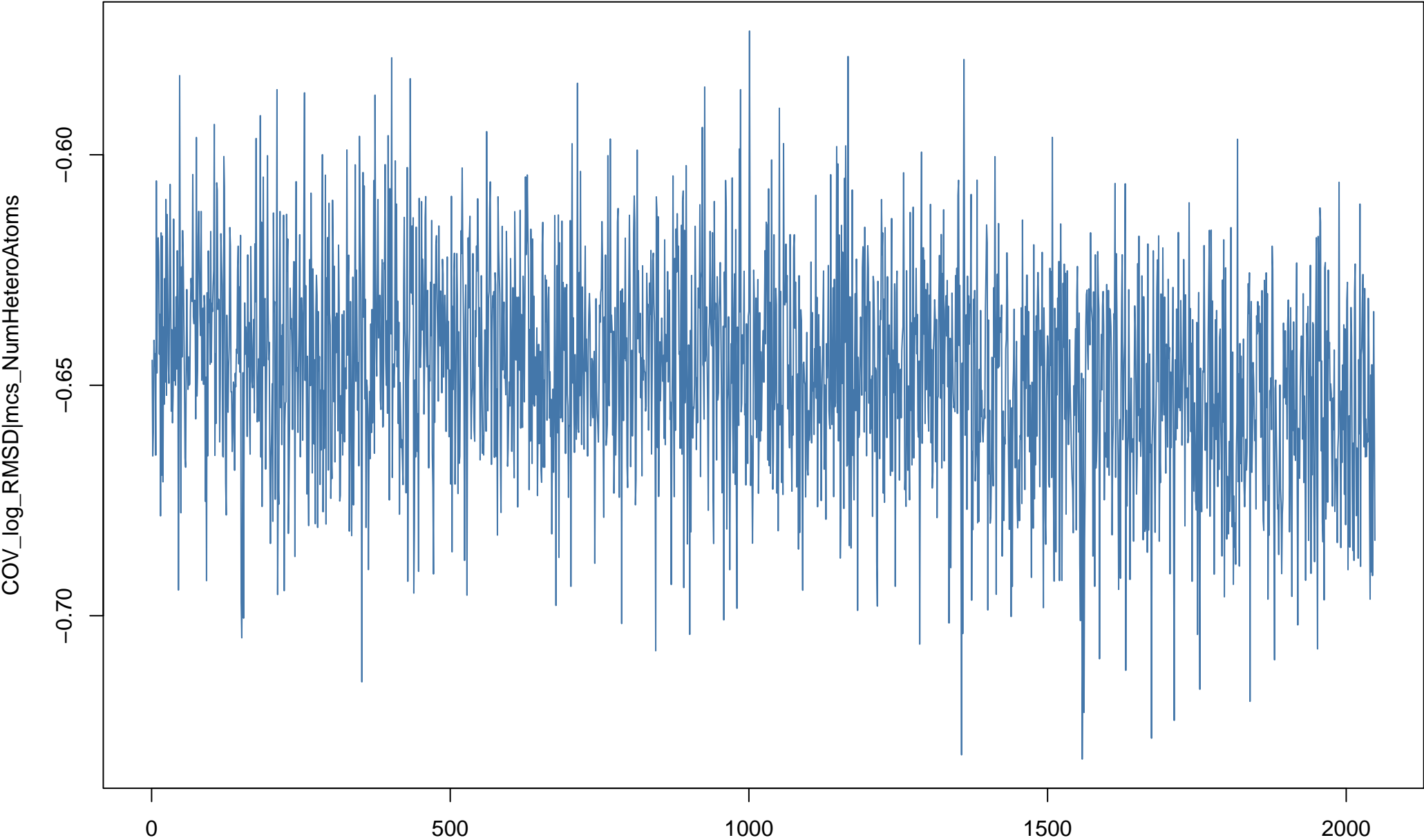
COV\_log\_RMSD|mcs\_docked\_NumHAcceptors  
ESS = 1900 | BMK = 0.0536 | MCSE(6.27) = 1.95 | stat: TRUE | burn: 0



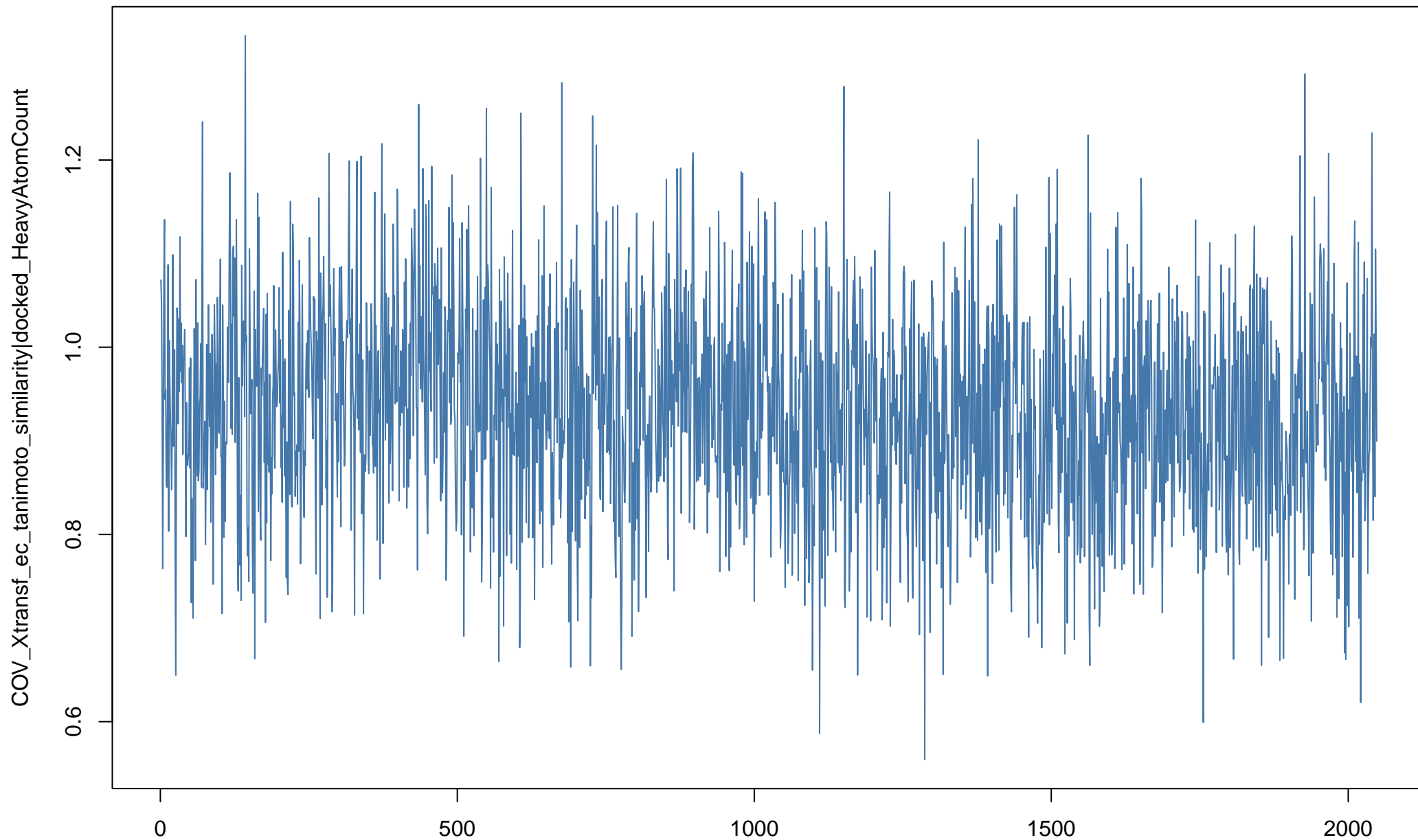
**COV\_log\_RMSD|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0281 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0**



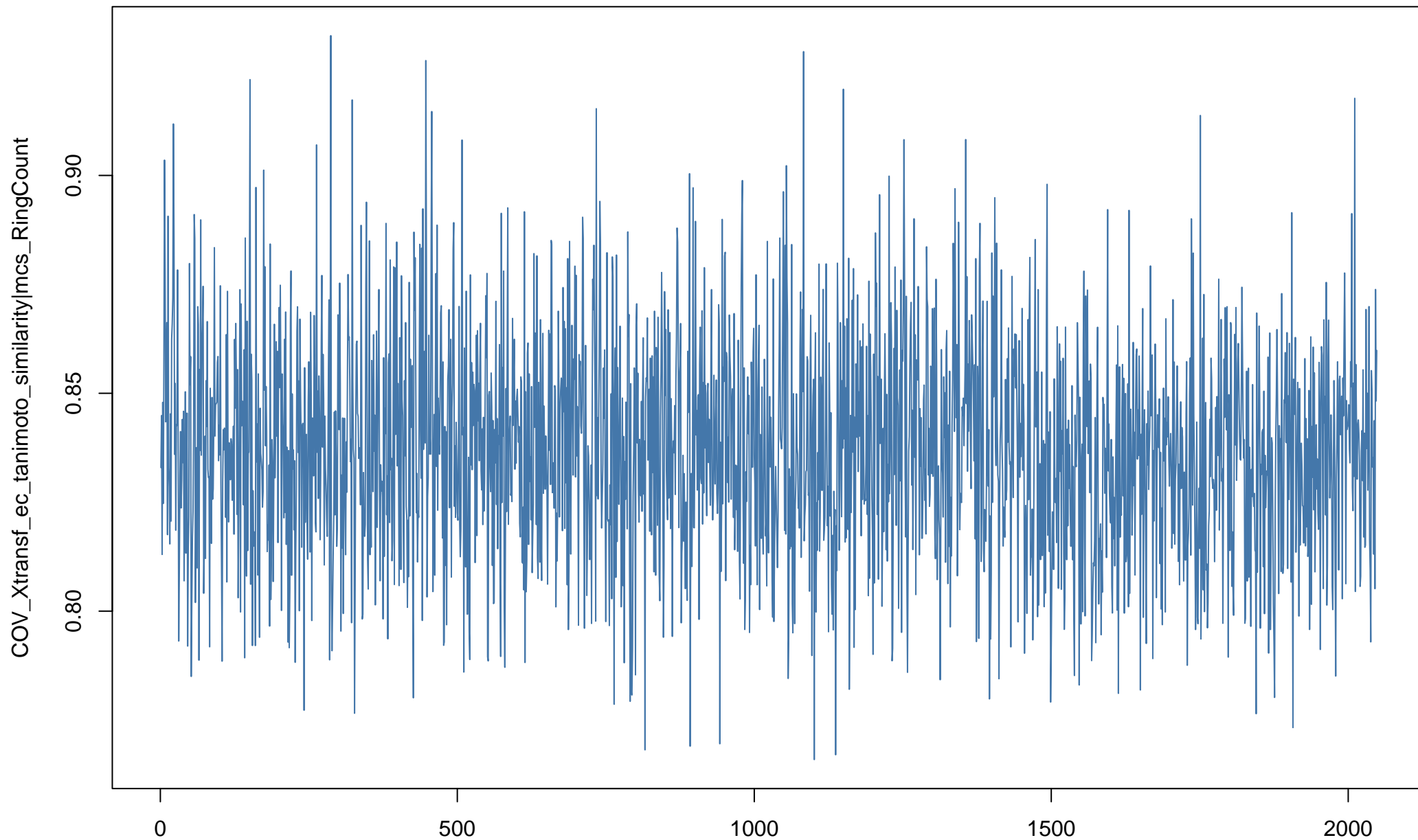
COV\_log\_RMSD|mcs\_NumHeteroAtoms  
ESS = 262 | BMK = 0.145 | MCSE(6.27) = 4.03 | stat: FALSE | burn: 0



**COV\_Xtransf\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount**  
**ESS = 1710 | BMK = 0.104 | MCSE(6.27) = 3.57 | stat: FALSE | burn: 0**

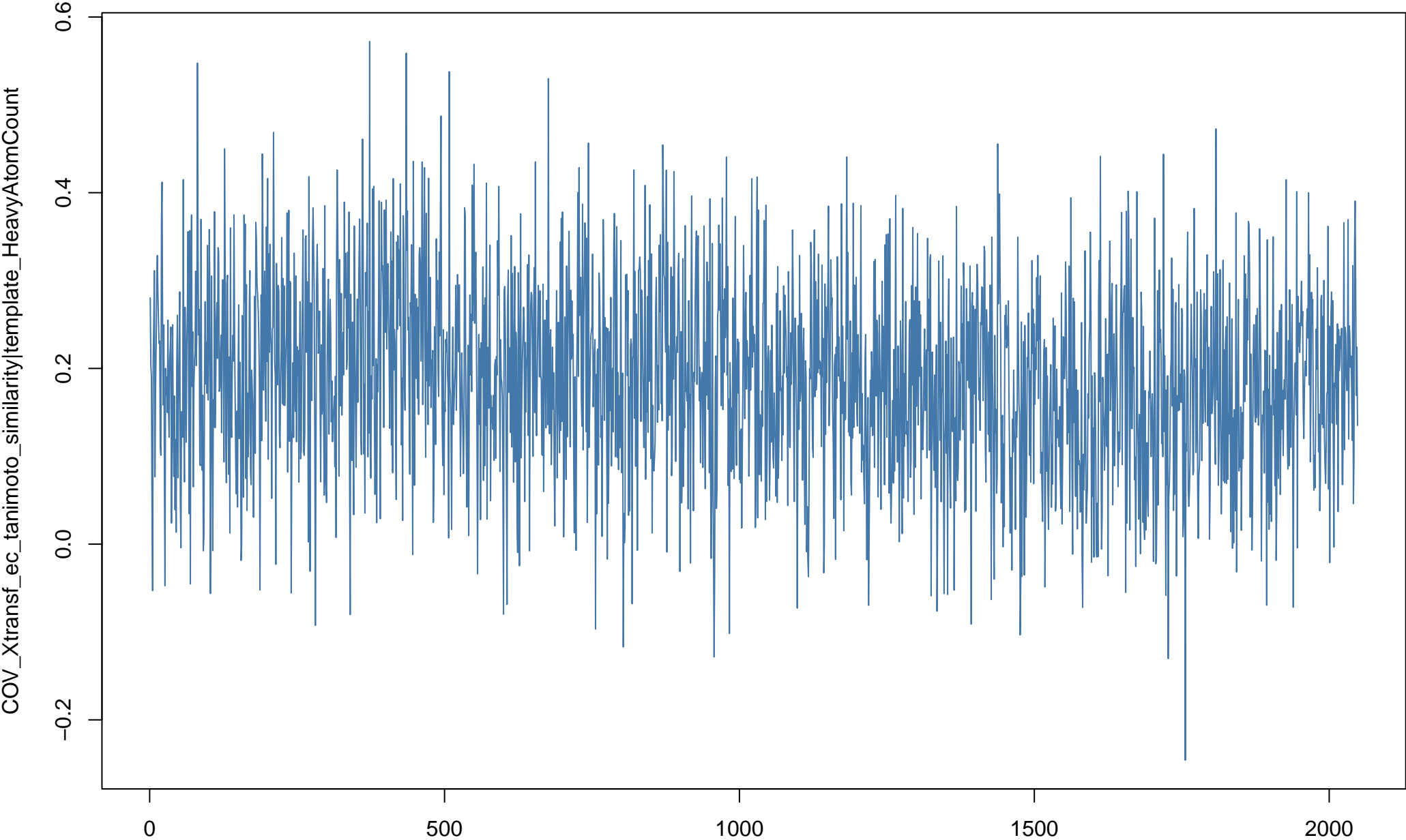


**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 1890 | BMK = 0.0523 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0**

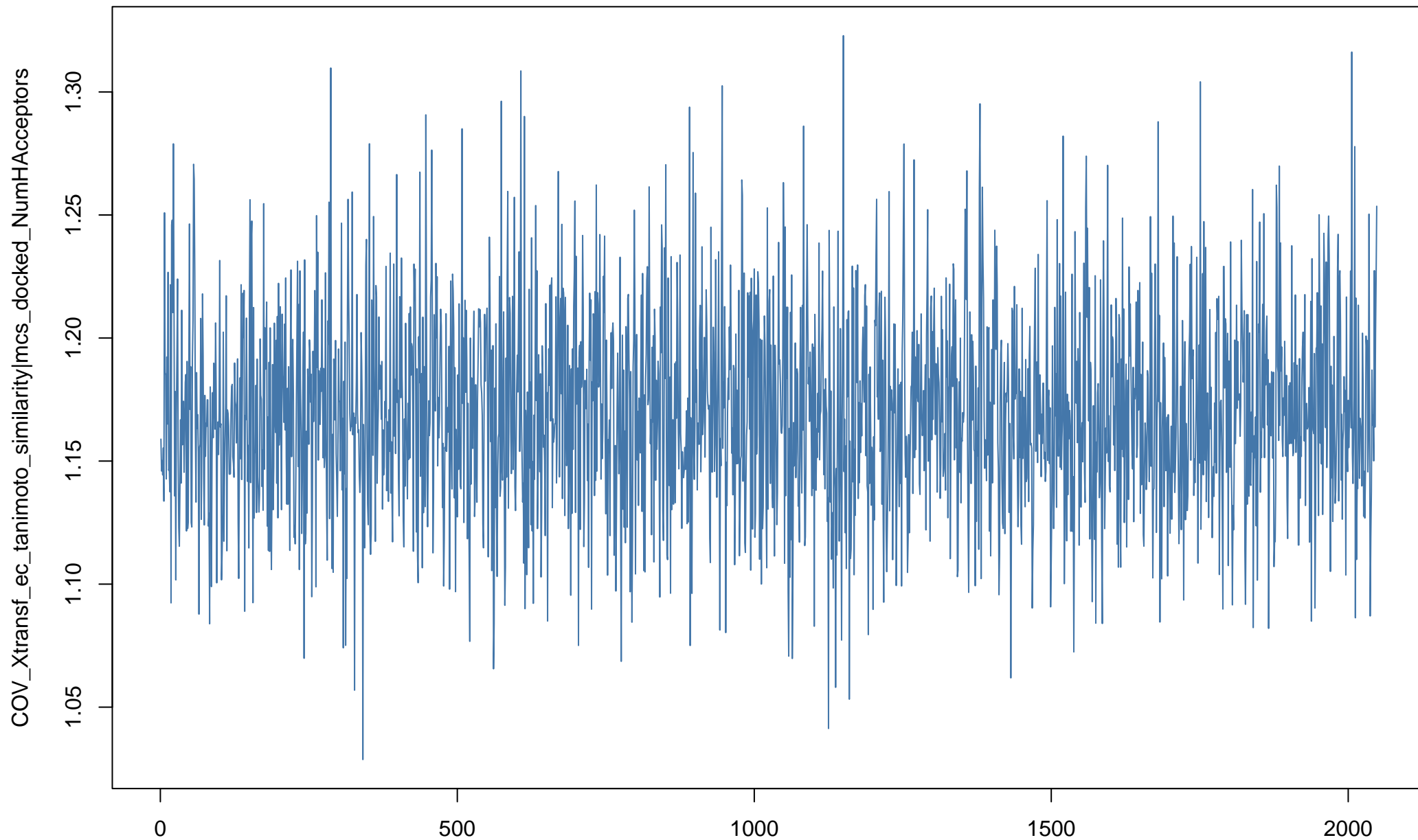




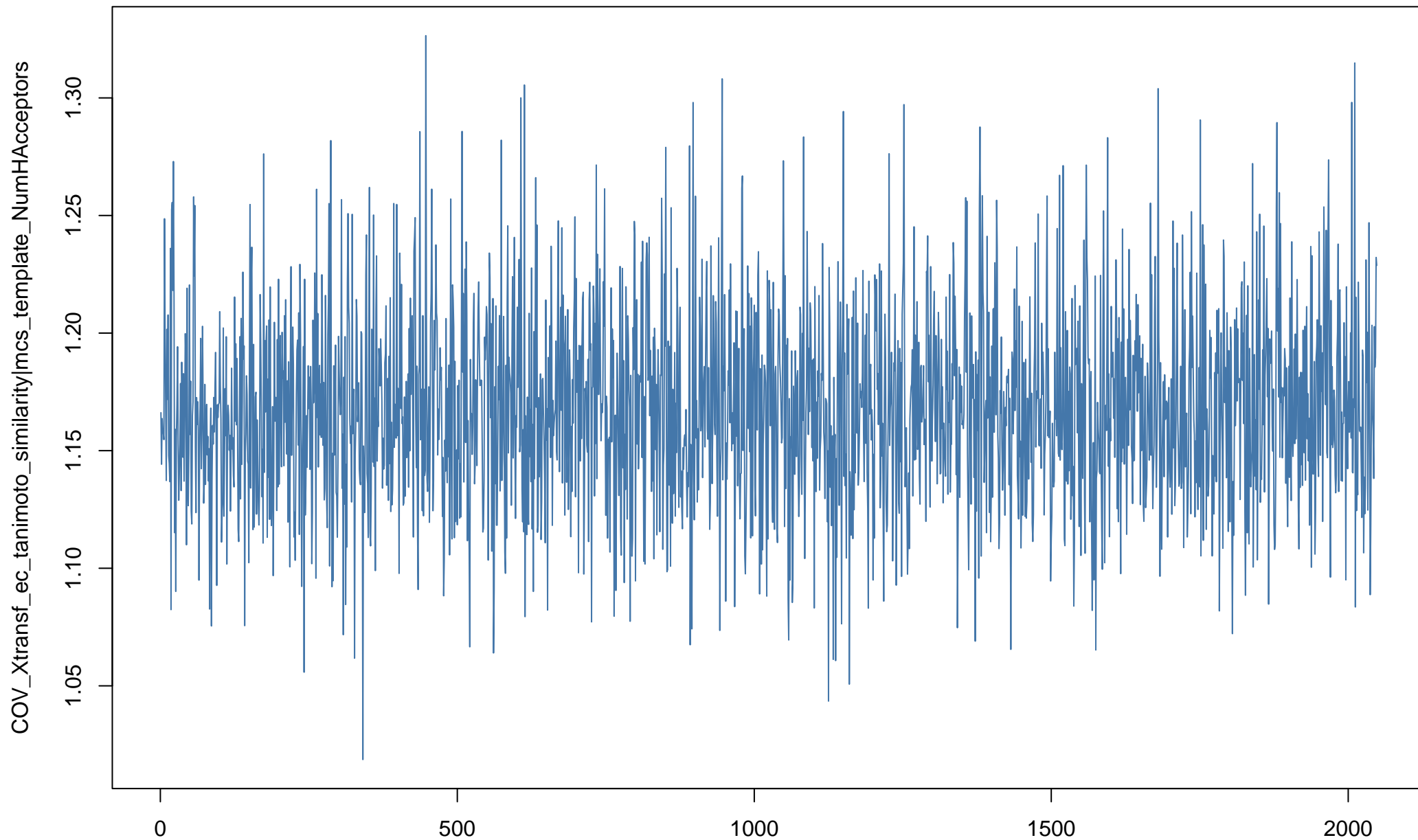
COV\_Xtransf\_ec\_tanimoto\_similarity|template\_HeavyAtomCount  
ESS = 604 | BMK = 0.122 | MCSE(6.27) = 3.86 | stat: FALSE | burn: 0



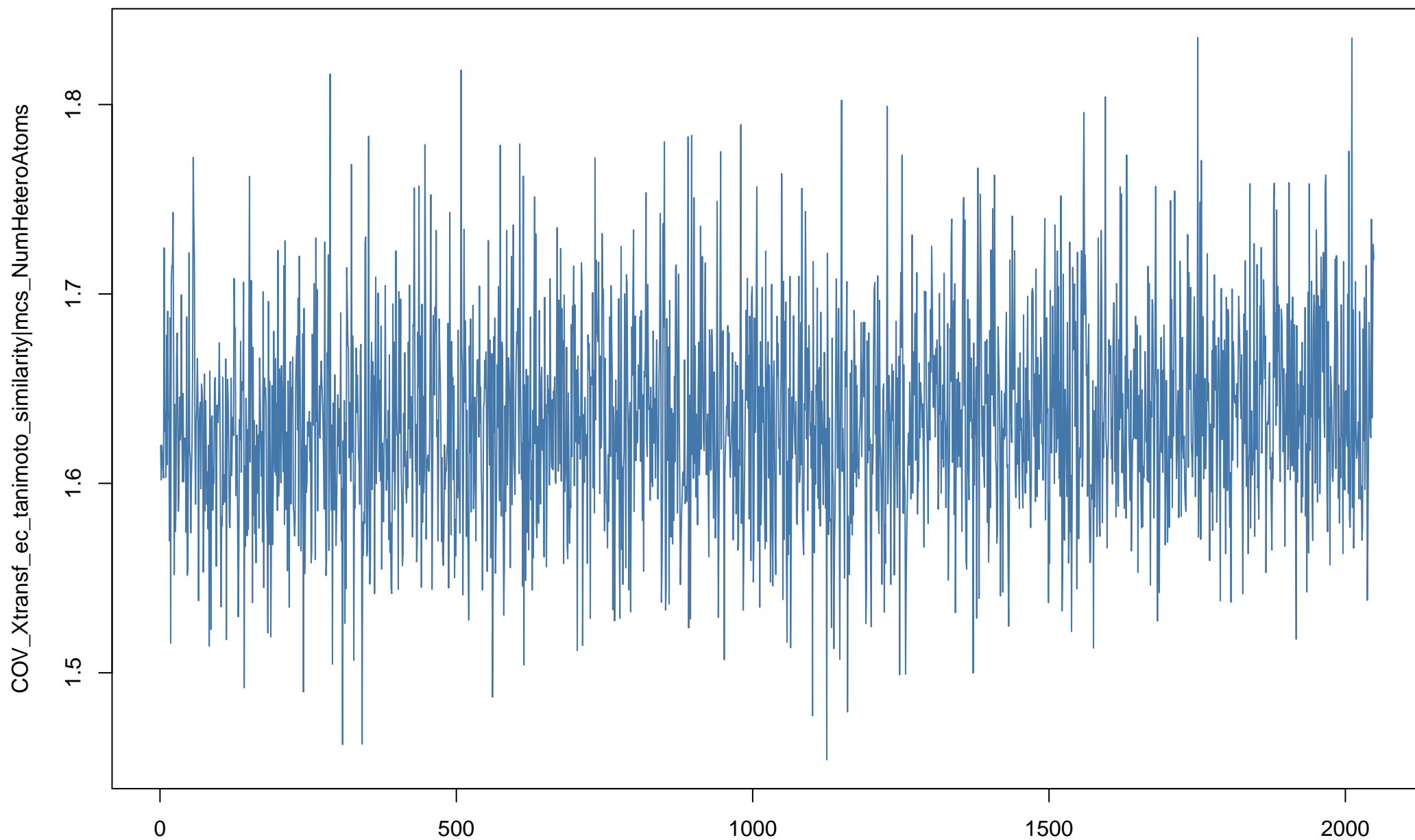
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0318 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0**



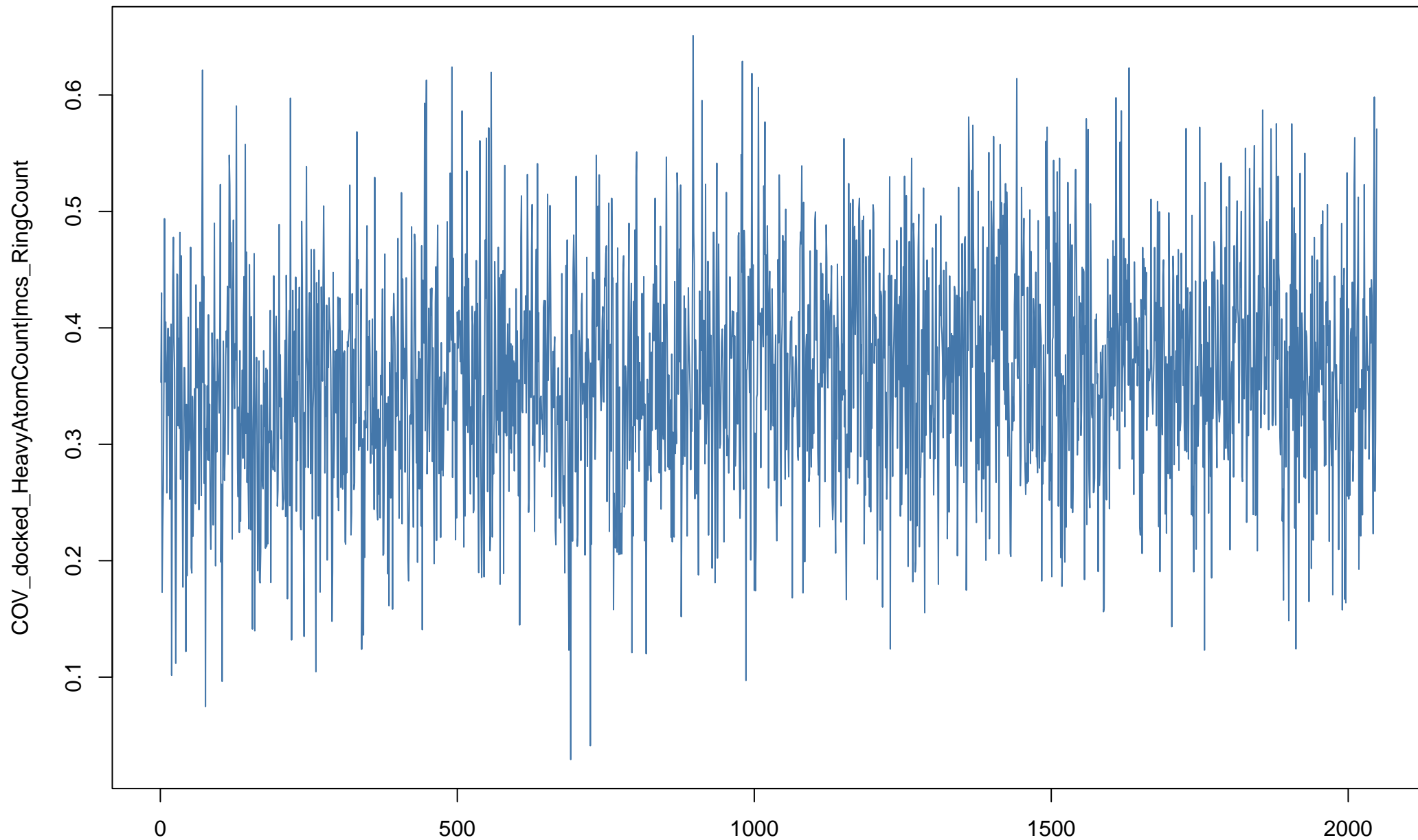
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0329 | MCSE(6.27) = 1.89 | stat: TRUE | burn: 0**



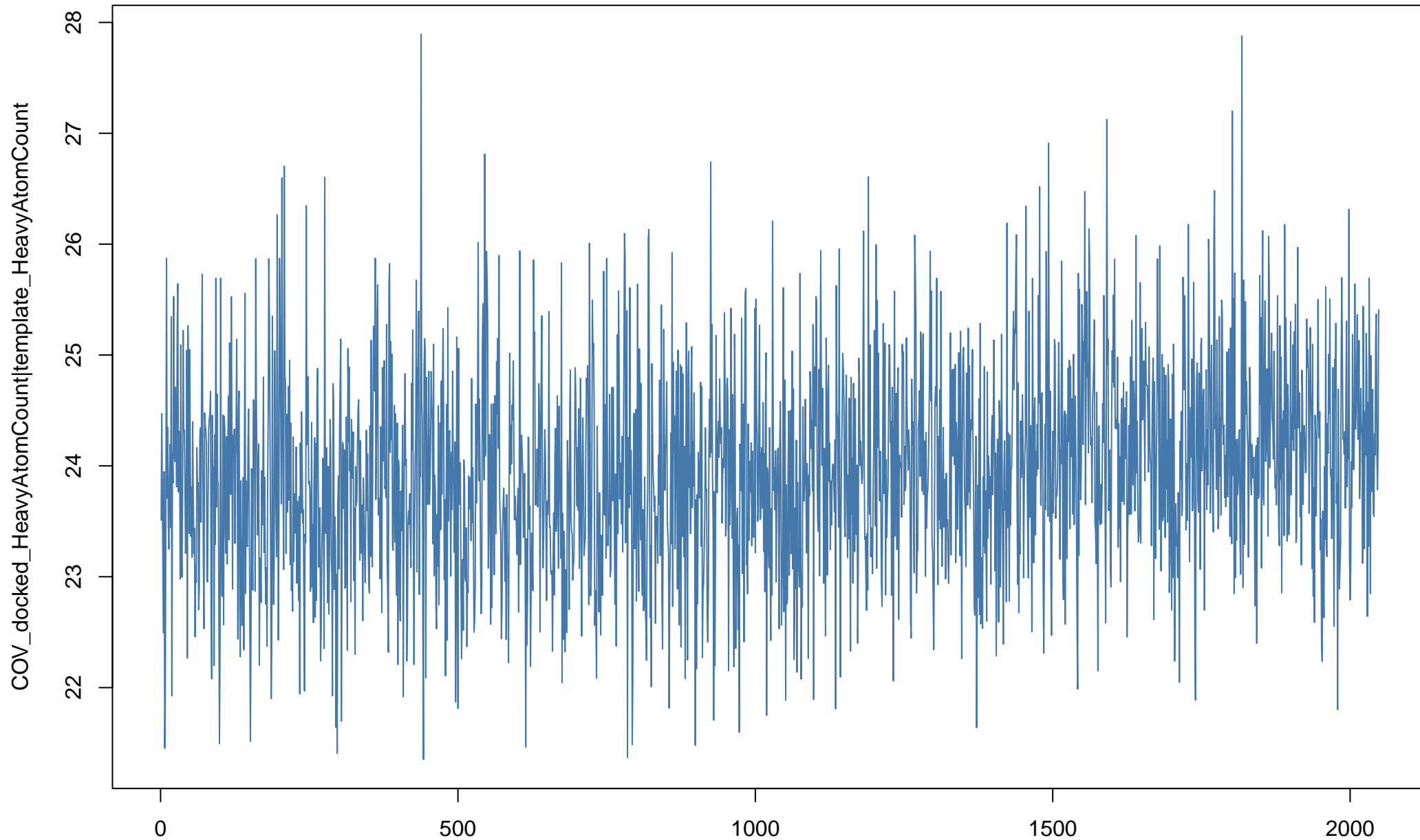
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms**  
**ESS = 1830 | BMK = 0.0632 | MCSE(6.27) = 2.45 | stat: FALSE | burn: 0**



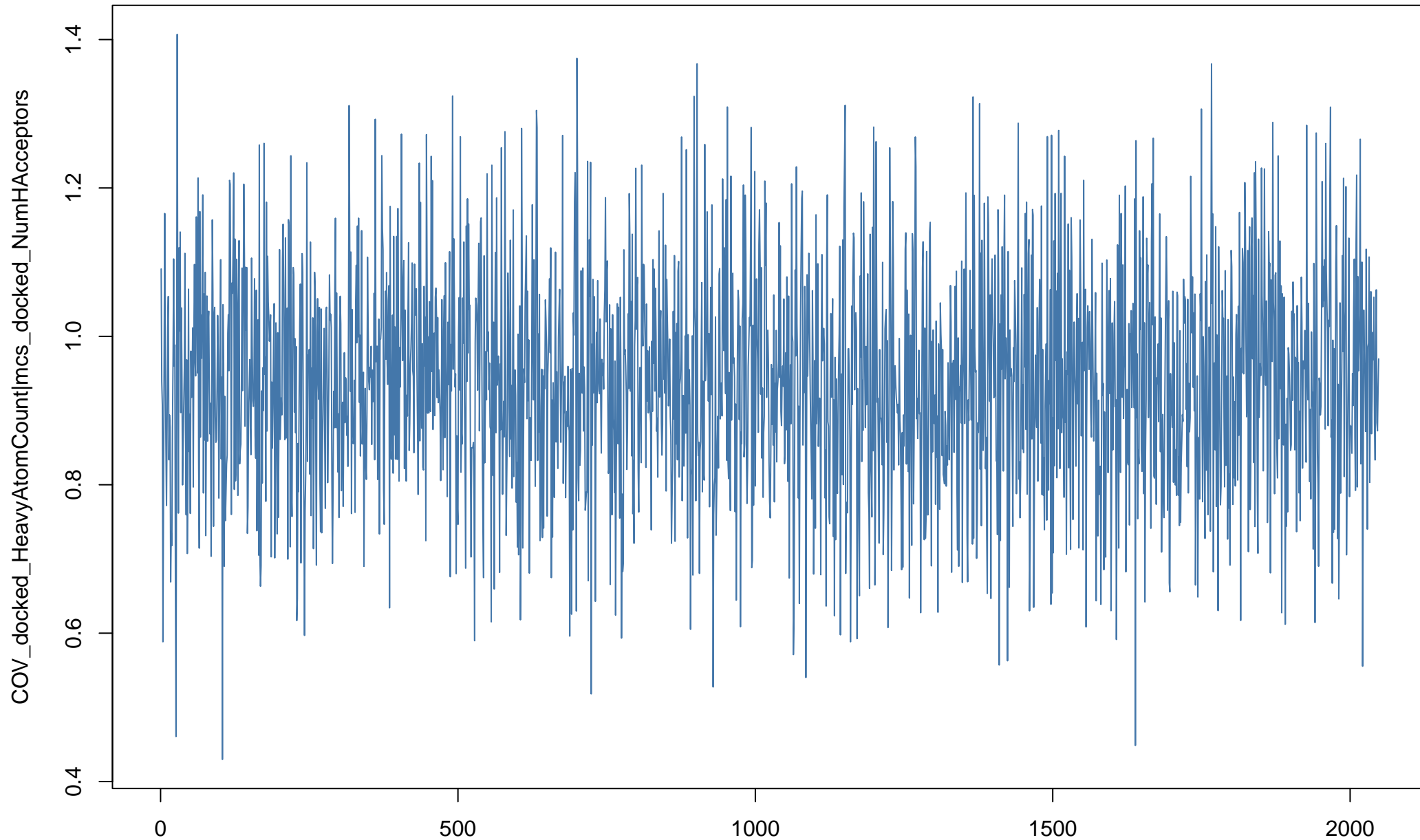
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 1710 | BMK = 0.101 | MCSE(6.27) = 2.98 | stat: FALSE | burn: 0**



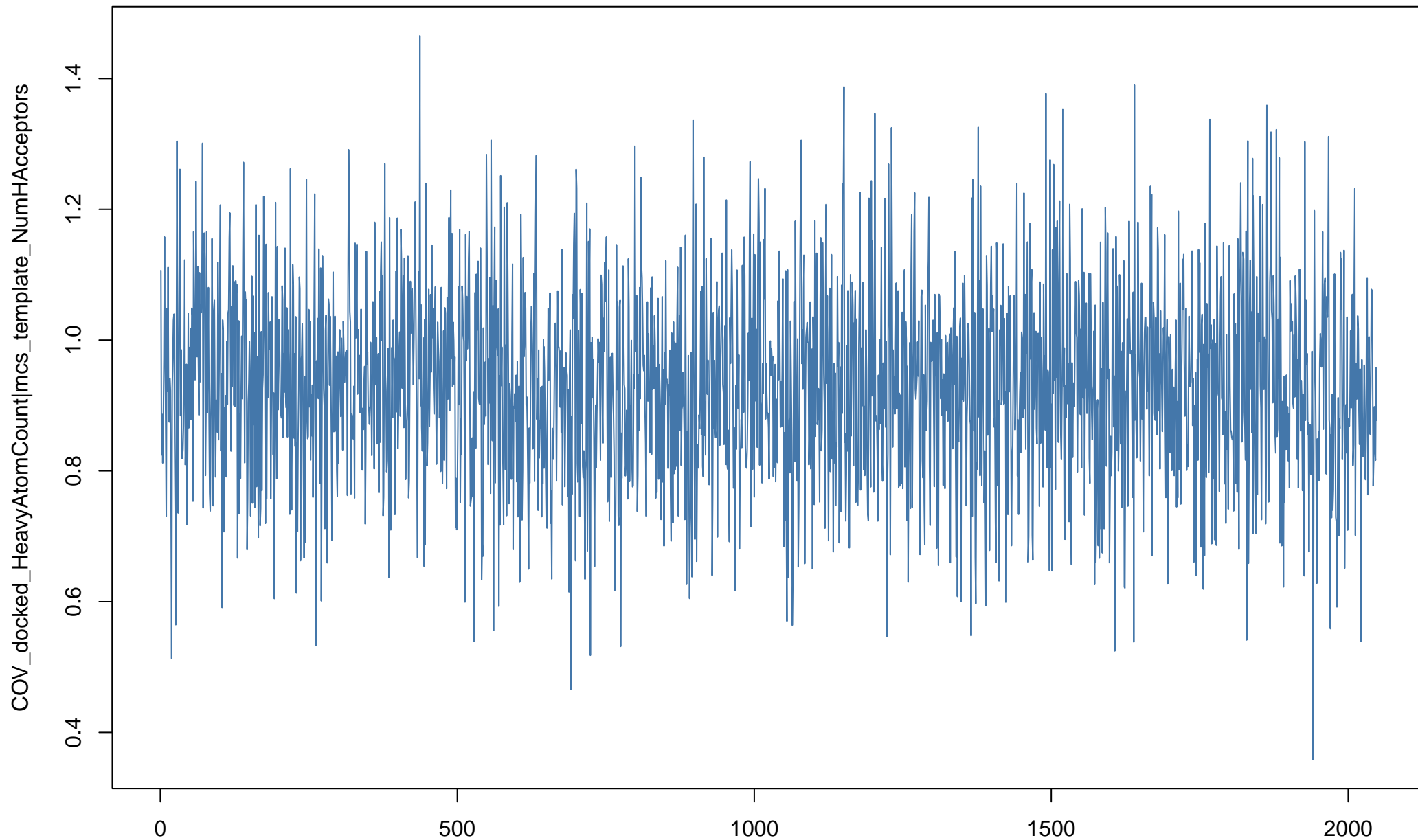
**COV\_docked\_HeavyAtomCount|template\_HeavyAtomCount**  
**ESS = 709 | BMK = 0.128 | MCSE(6.27) = 3.98 | stat: FALSE | burn: 0**



**COV\_docked\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0406 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0**

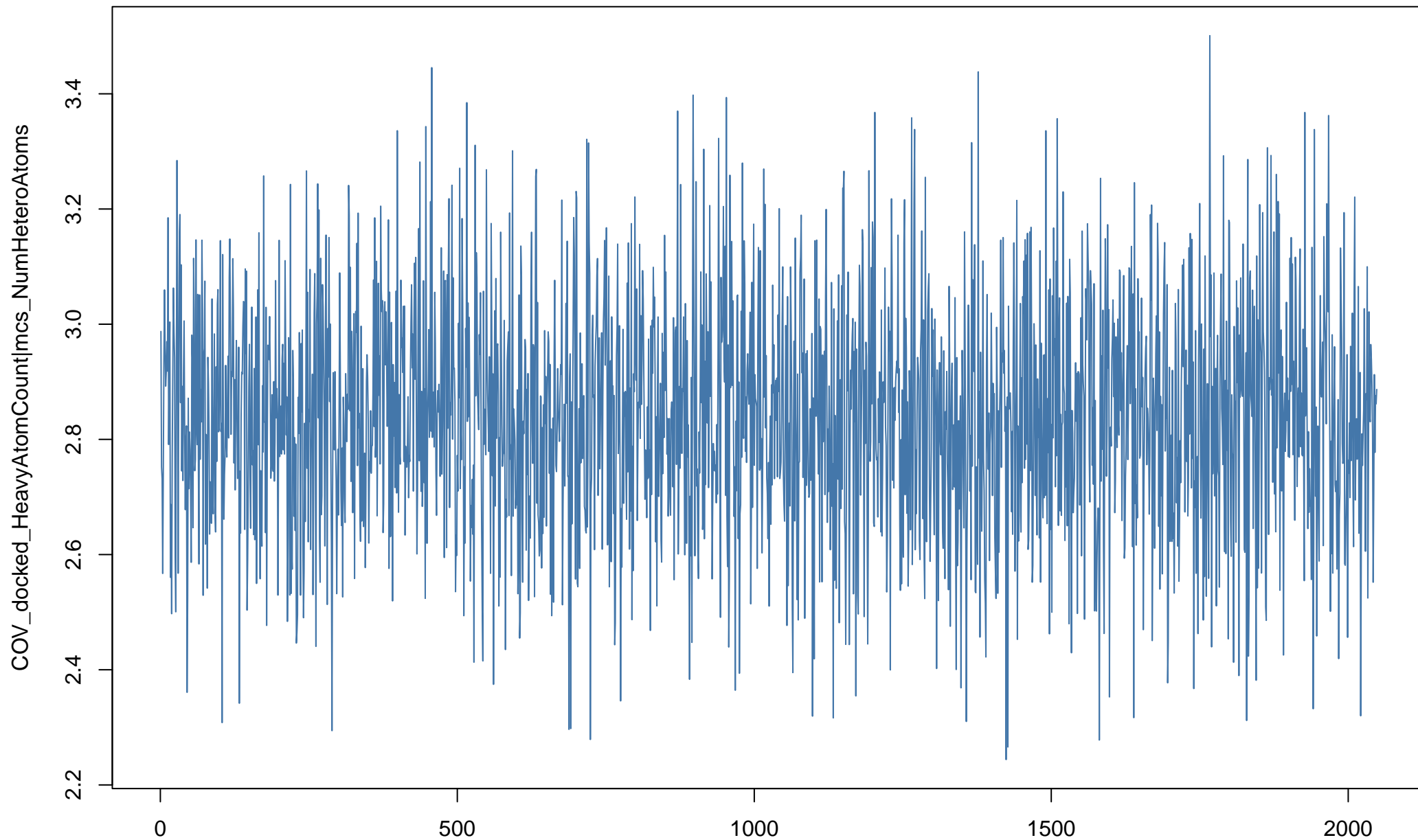


**COV\_docked\_HeavyAtomCount|mcs\_template\_NumHAcceptors**  
**ESS = 1920 | BMK = 0.0503 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0**

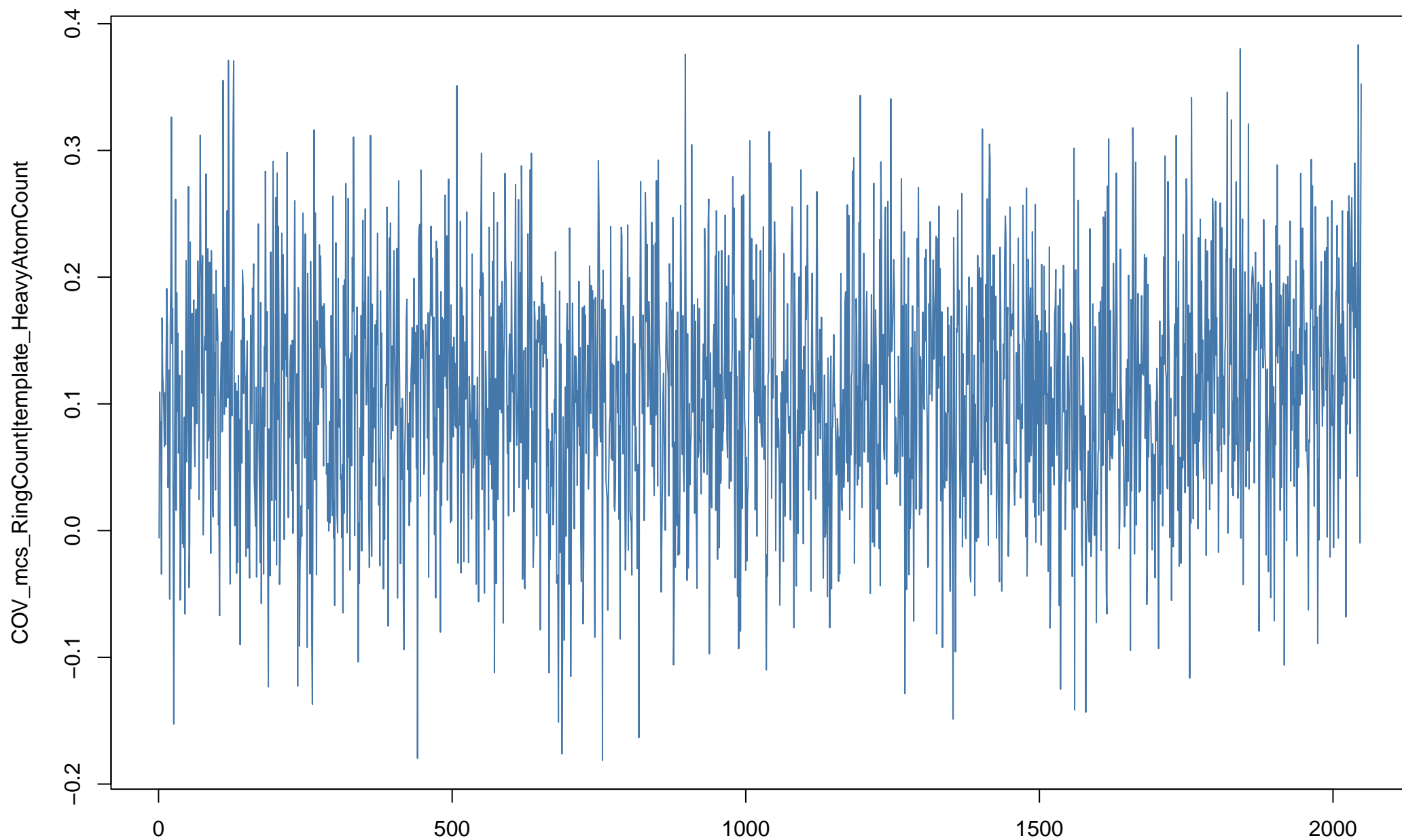




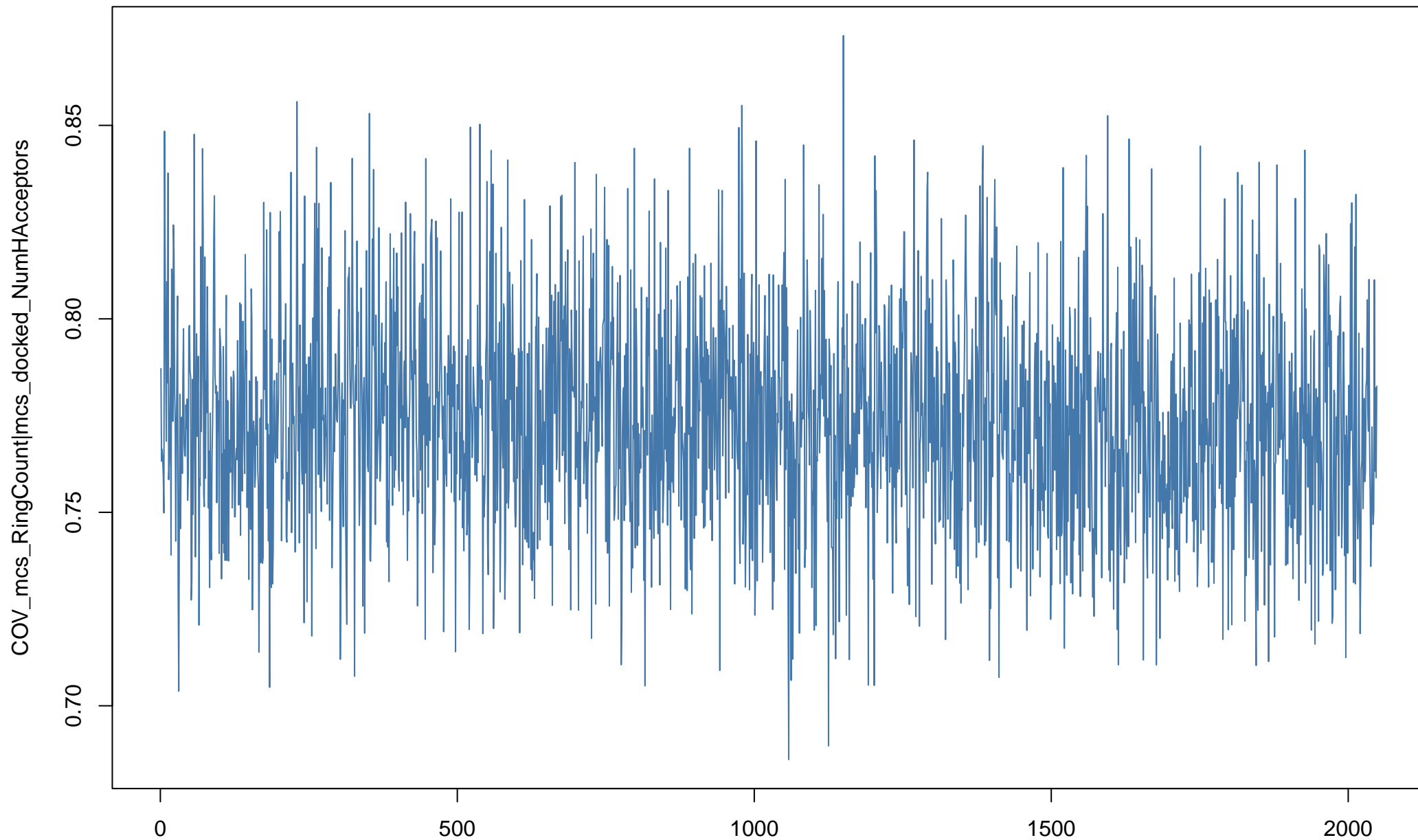
**COV\_docked\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 1920 | BMK = 0.0411 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0**



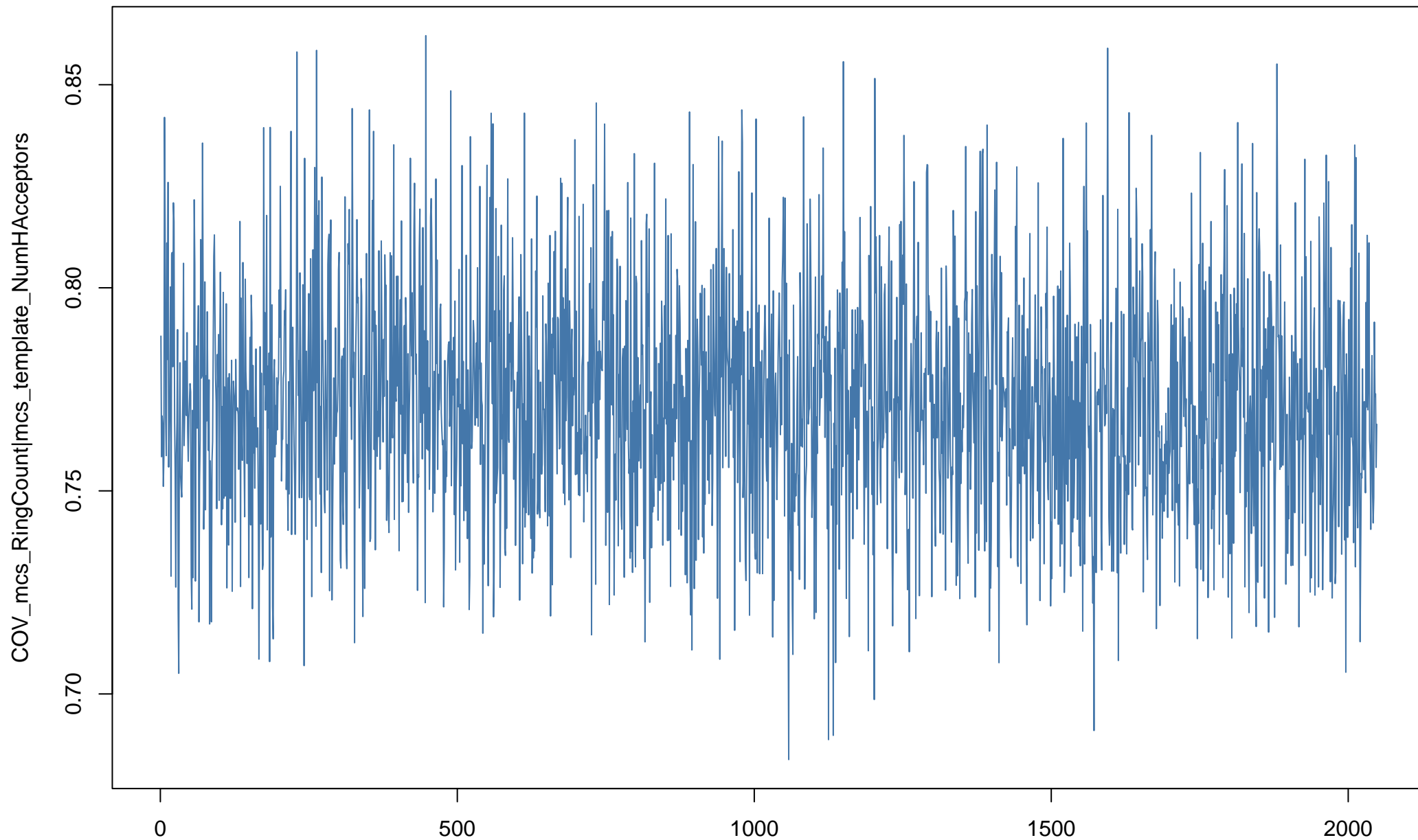
**COV\_mcs\_RingCount|template\_HeavyAtomCount**  
**ESS = 1660 | BMK = 0.0423 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0**



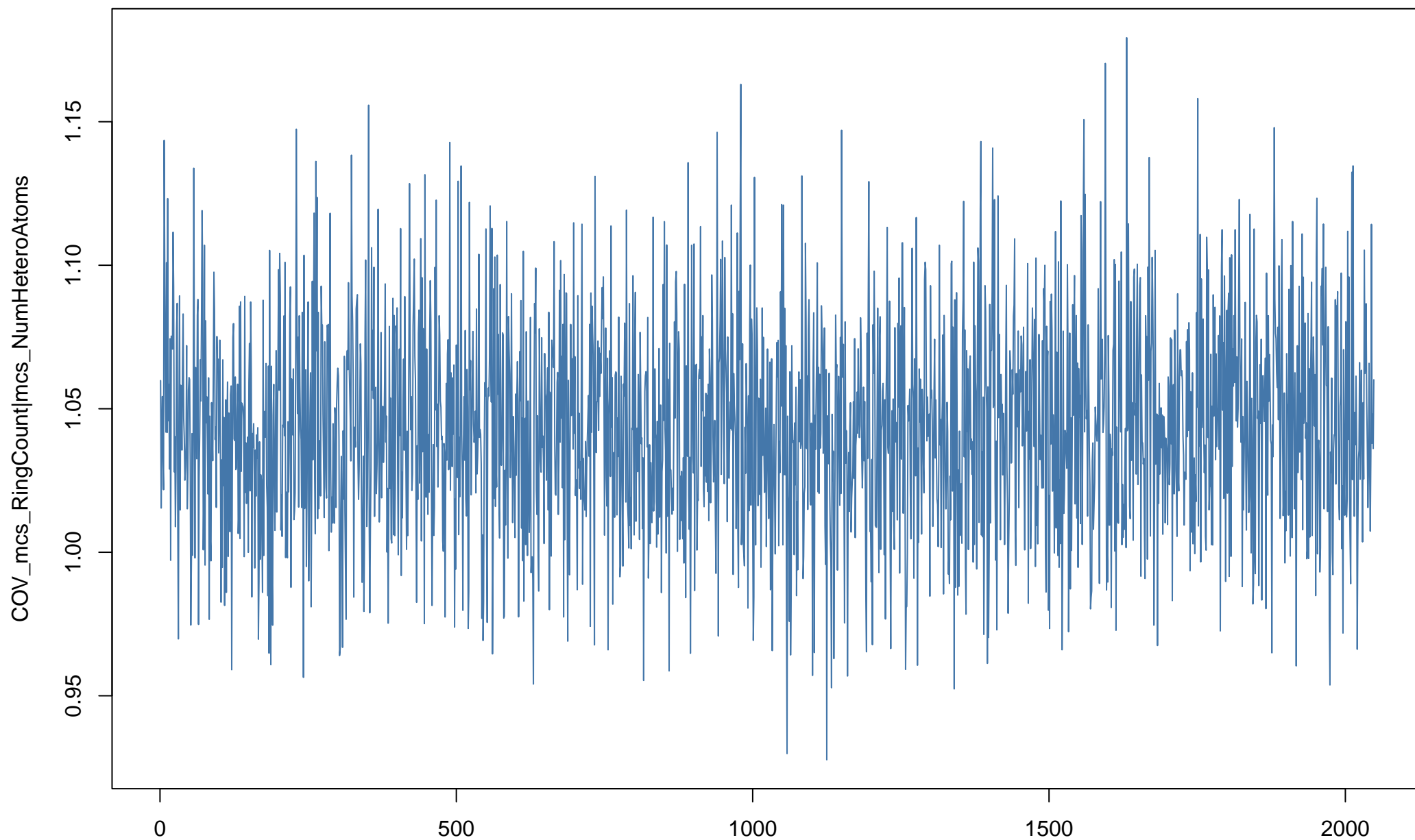
**COV\_mcs\_RingCount|mcs\_docked\_NumHAcceptors**  
**ESS = 1920 | BMK = 0.0661 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0**



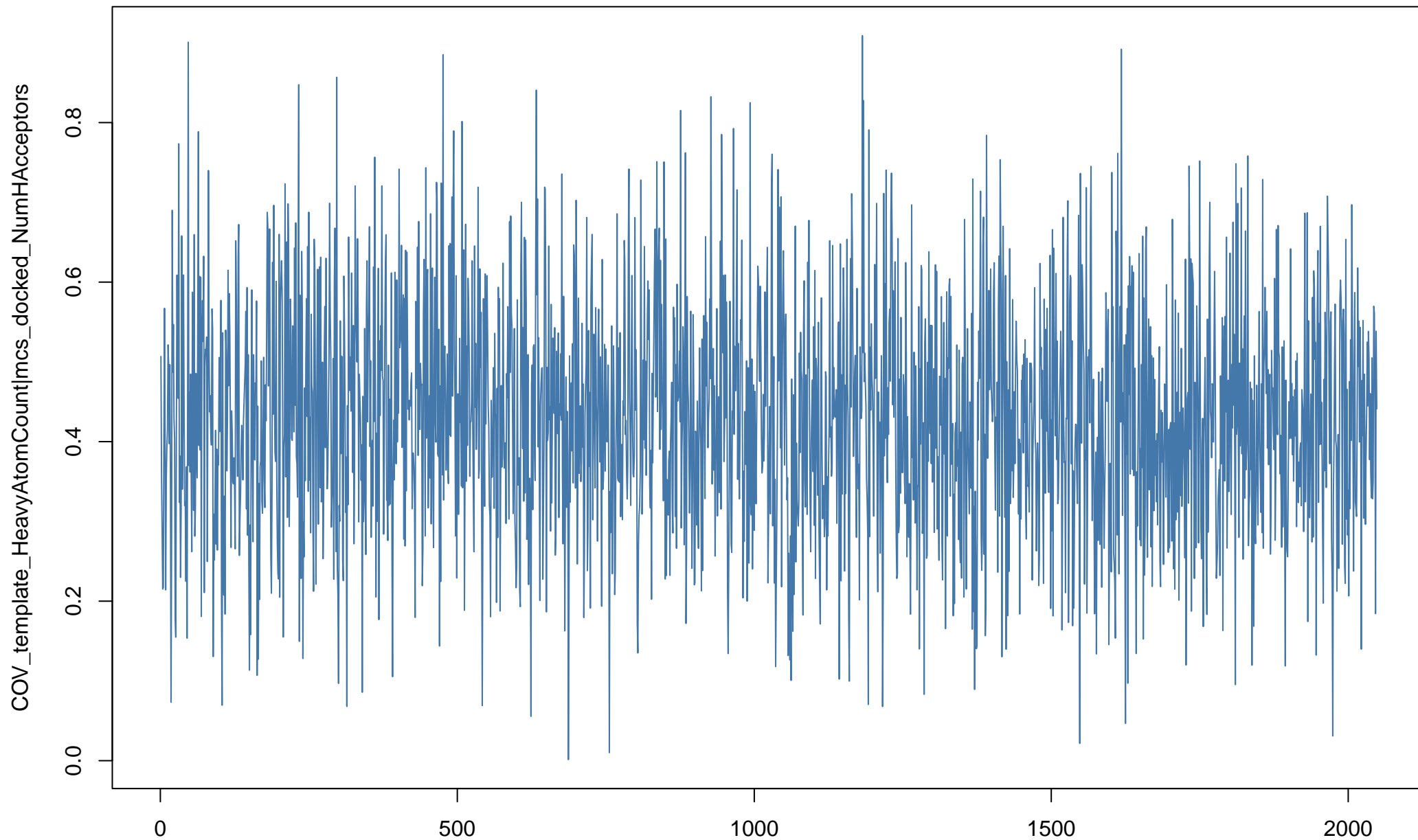
**COV\_mcs\_RingCount|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0549 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0**



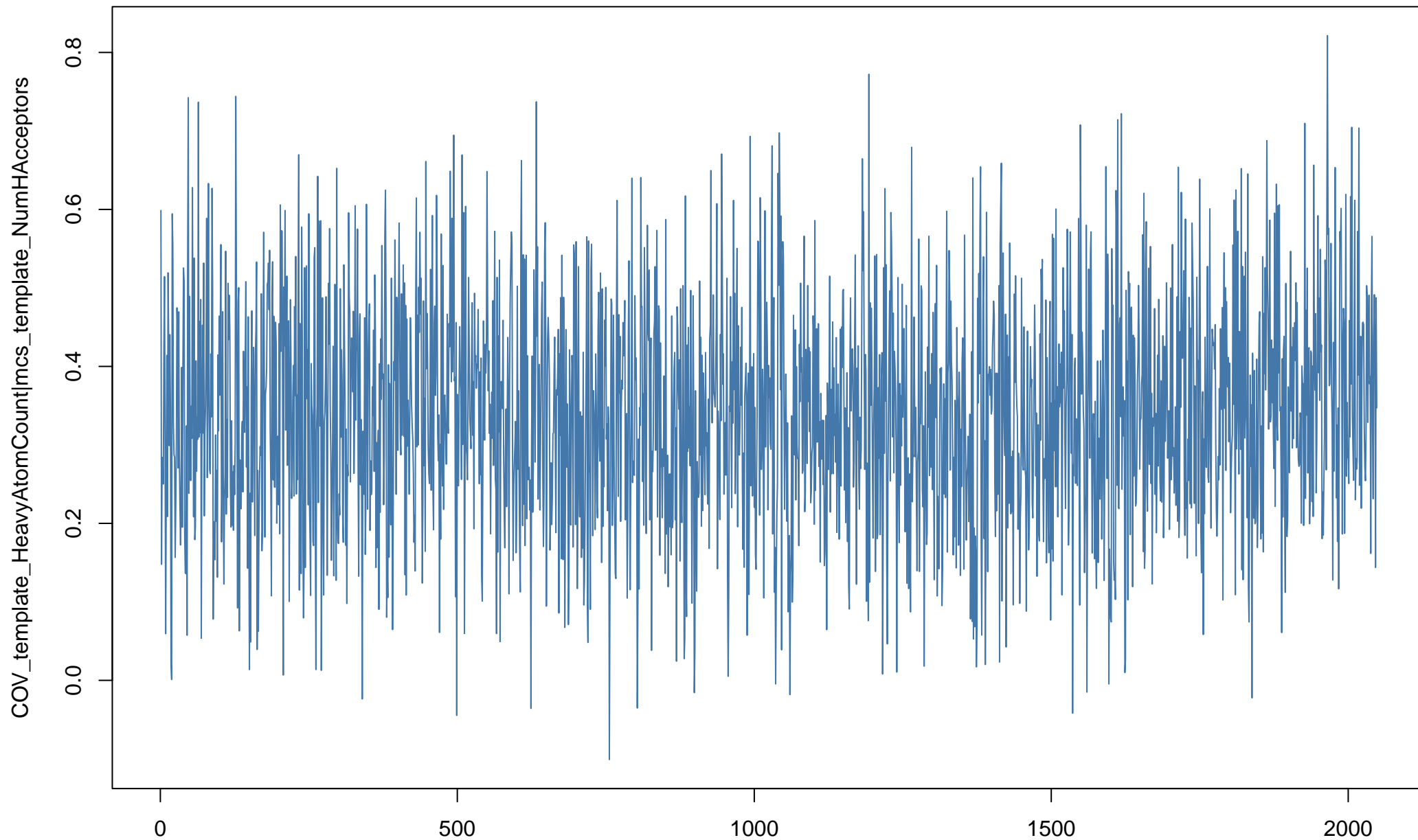
**COV\_mcs\_RingCount|mcs\_NumHeteroAtoms**  
**ESS = 1880 | BMK = 0.045 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0**



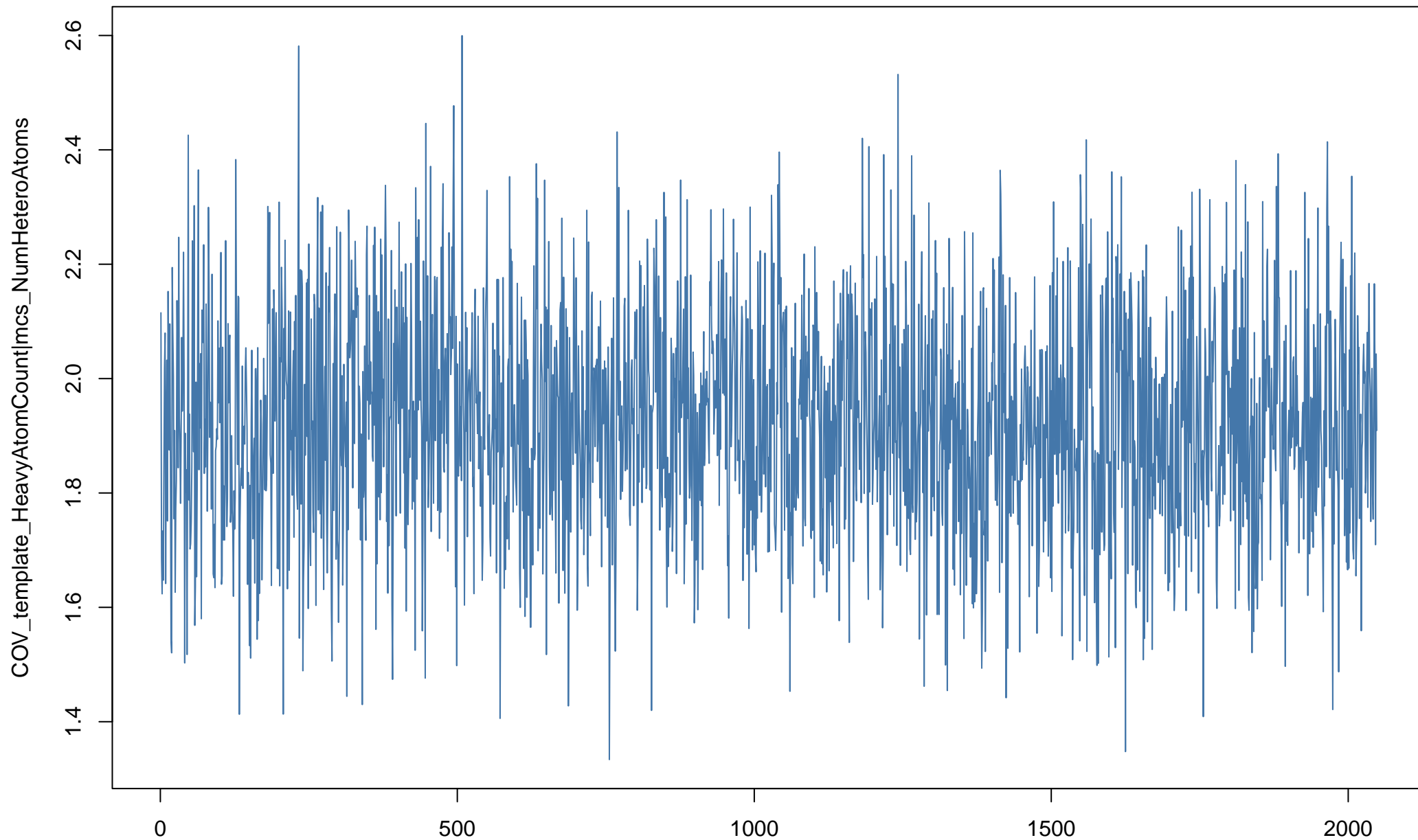
**COV\_template\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 1870 | BMK = 0.0528 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0**



**COV\_template\_HeavyAtomCount|mcs\_template\_NumHAcceptors**  
**ESS = 1820 | BMK = 0.0323 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0**

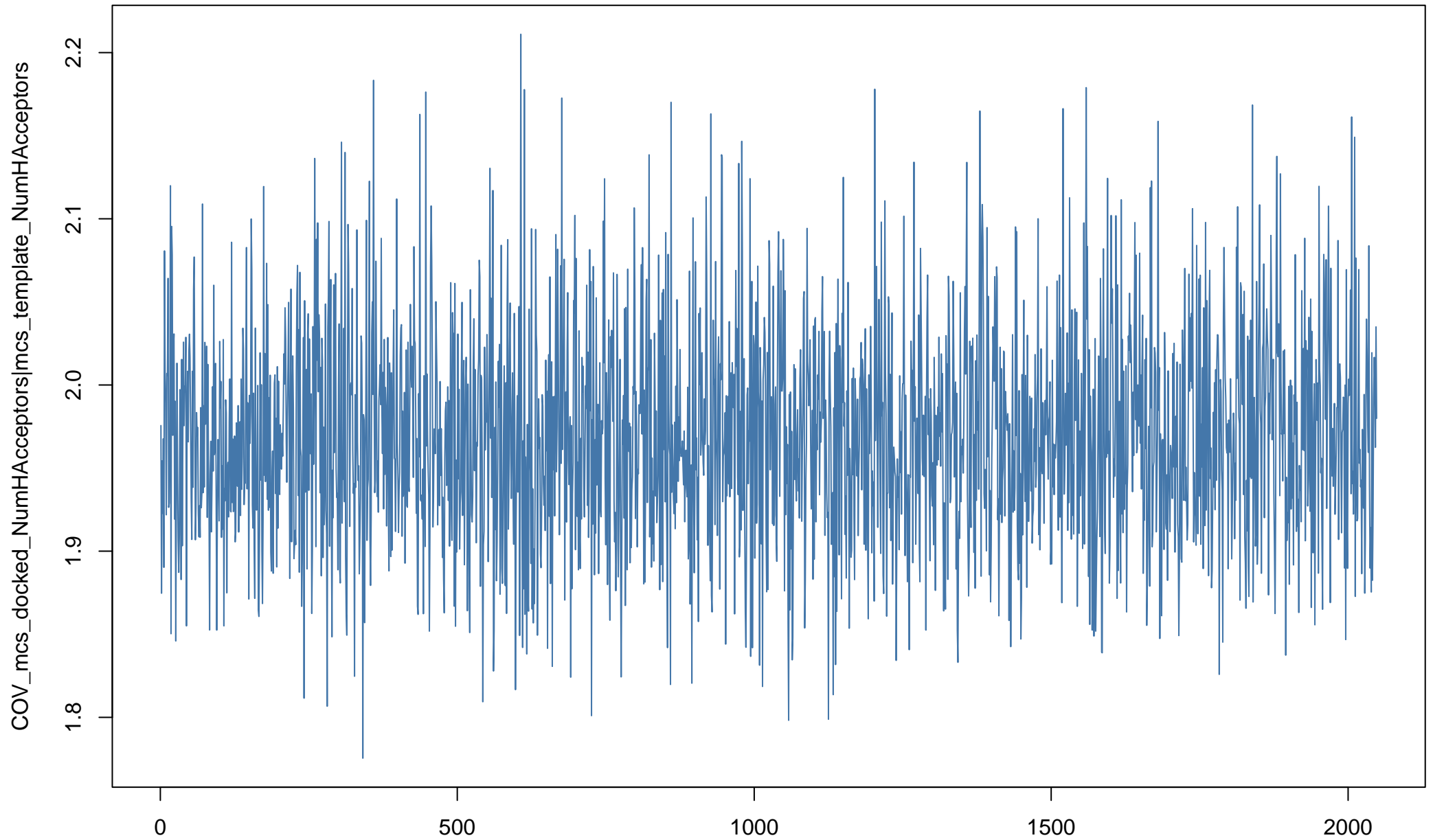


**COV\_template\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 1810 | BMK = 0.0364 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0**

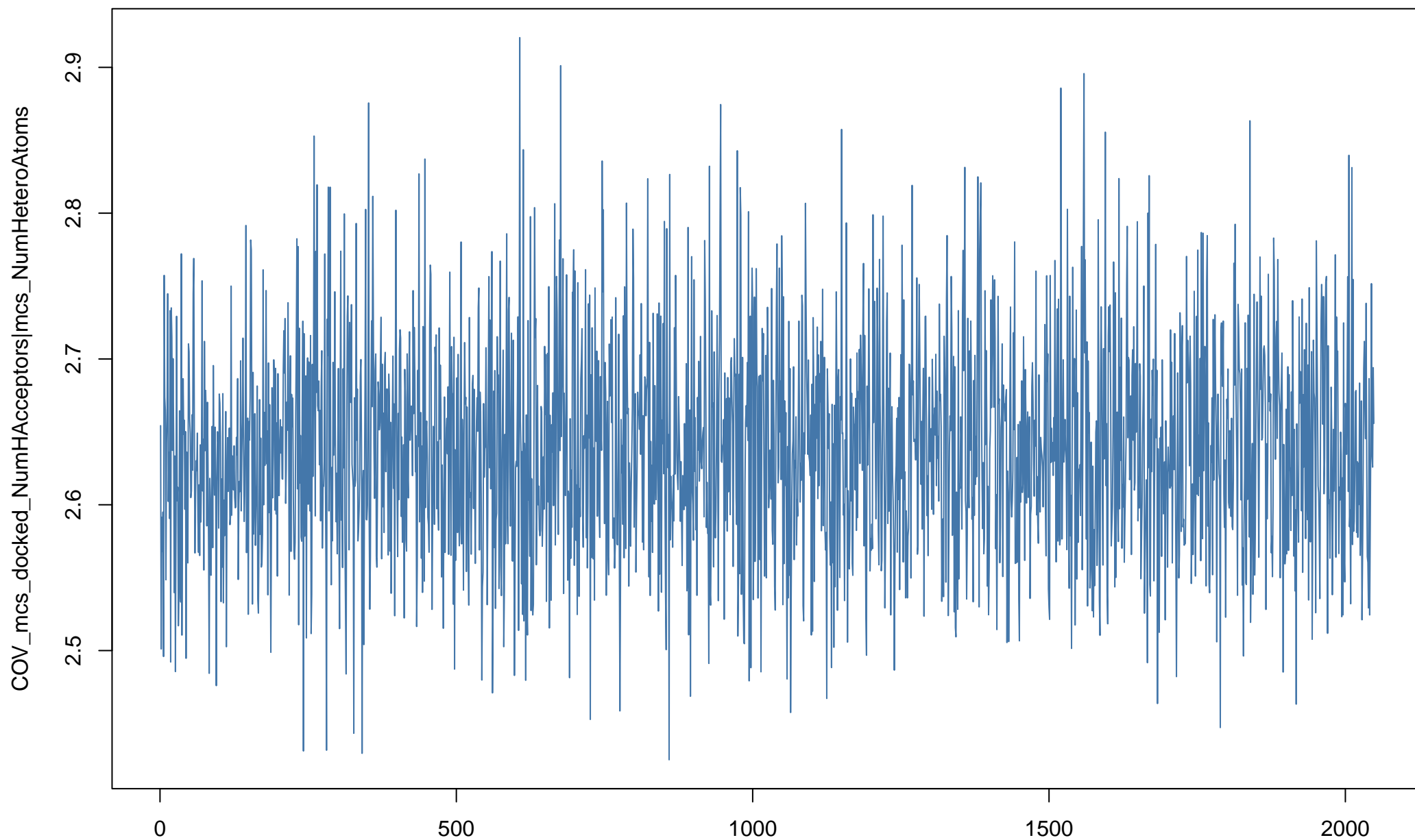




**COV\_mcs\_docked\_NumHAcceptors|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0329 | MCSE(6.27) = 2.03 | stat: TRUE | burn: 0**



**COV\_mcs\_docked\_NumHAcceptors|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0411 | MCSE(6.27) = 2.1 | stat: FALSE | burn: 0**



**COV\_mcs\_template\_NumHAcceptors|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0407 | MCSE(6.27) = 2.12 | stat: FALSE | burn: 0**

