

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.323193006782206

max MCSE = 11.0265310114355

all stationary: FALSE

burn: 0

-- STATS 2D --

min ESS = 1465.66637917878

max BMK = 0.0658451453186946

max MCSE = 3.30415688388226

all stationary: TRUE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.121424818674845

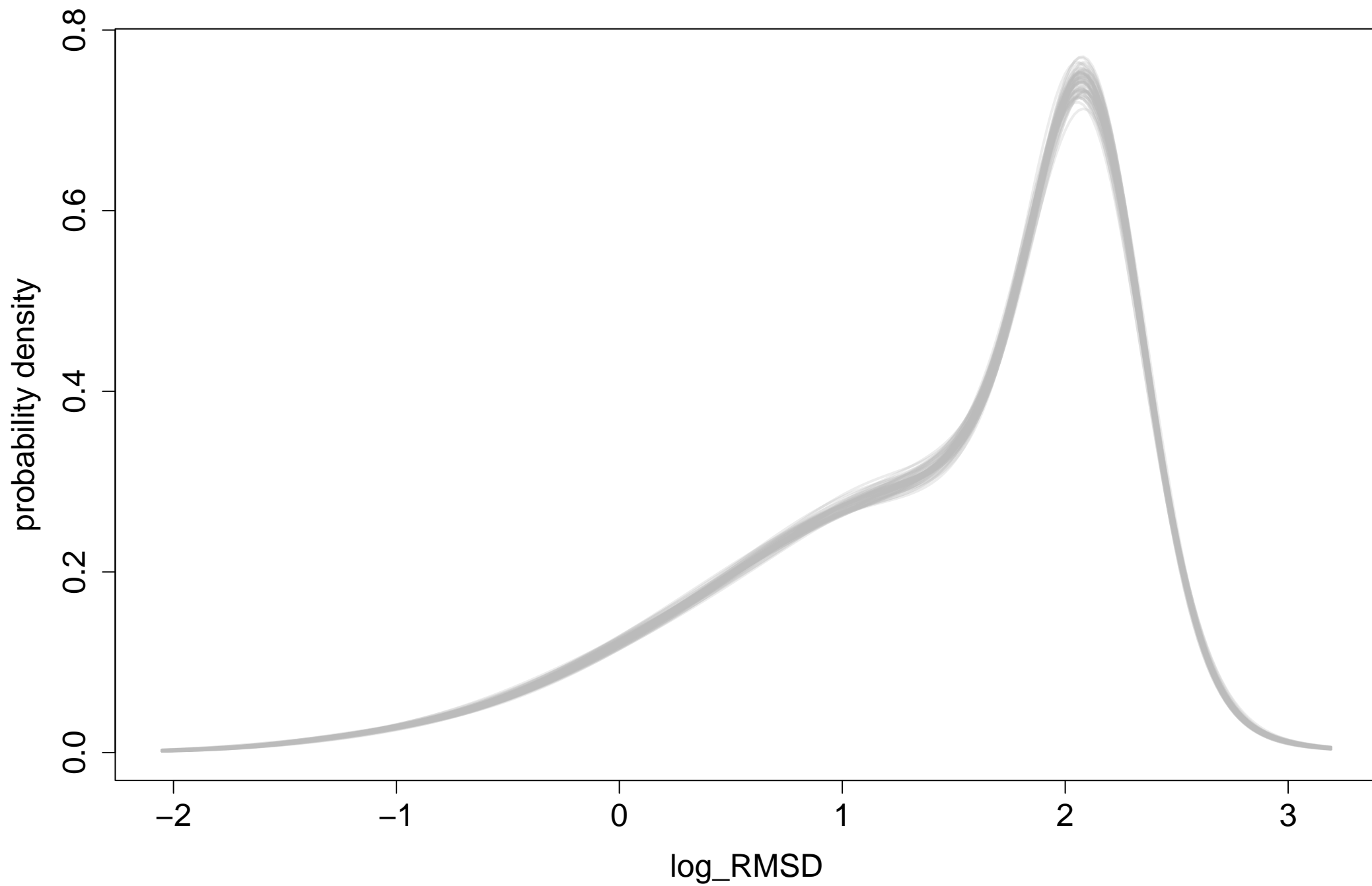
max MCSE = NaN

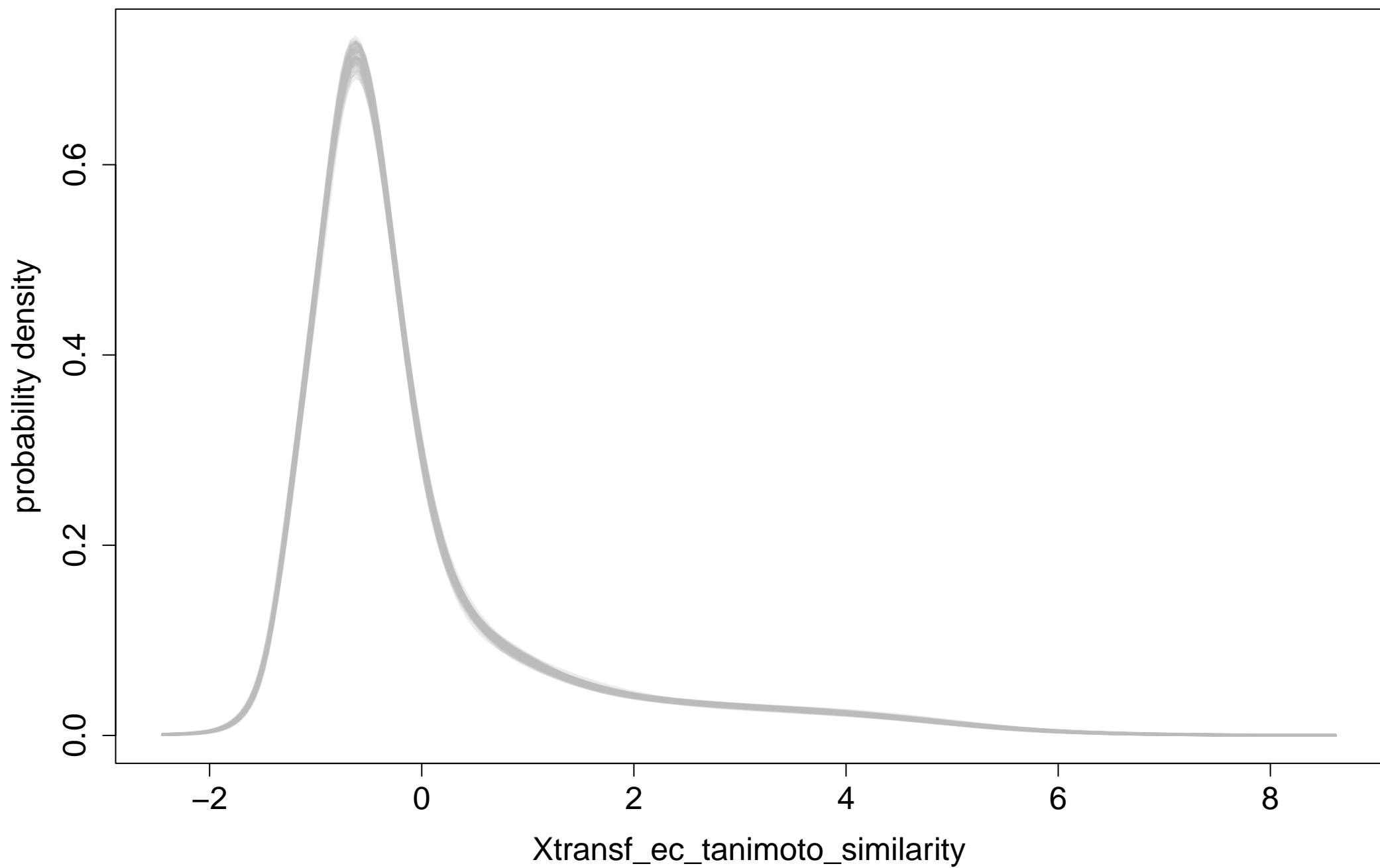
all stationary: FALSE

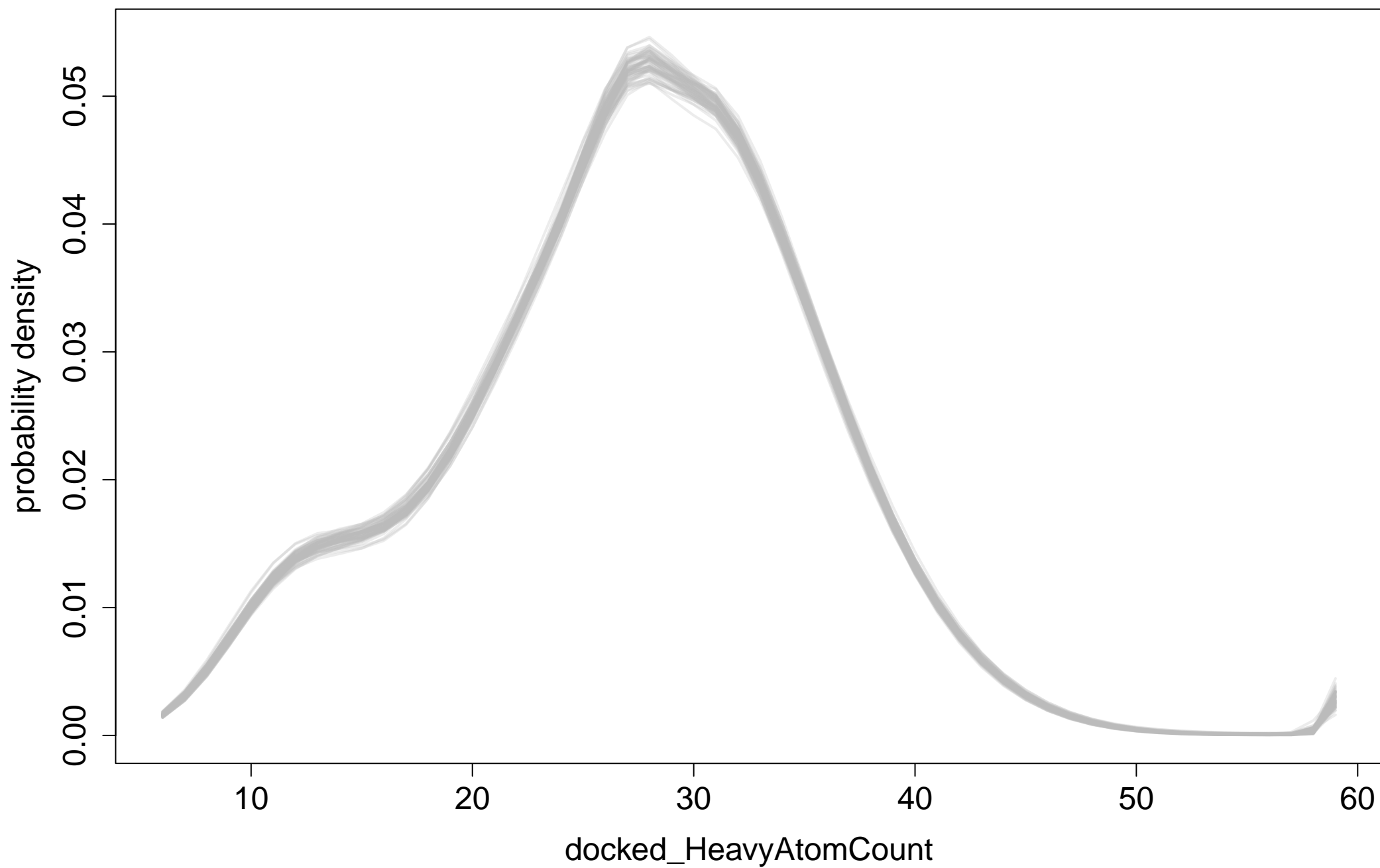
burn: 2040

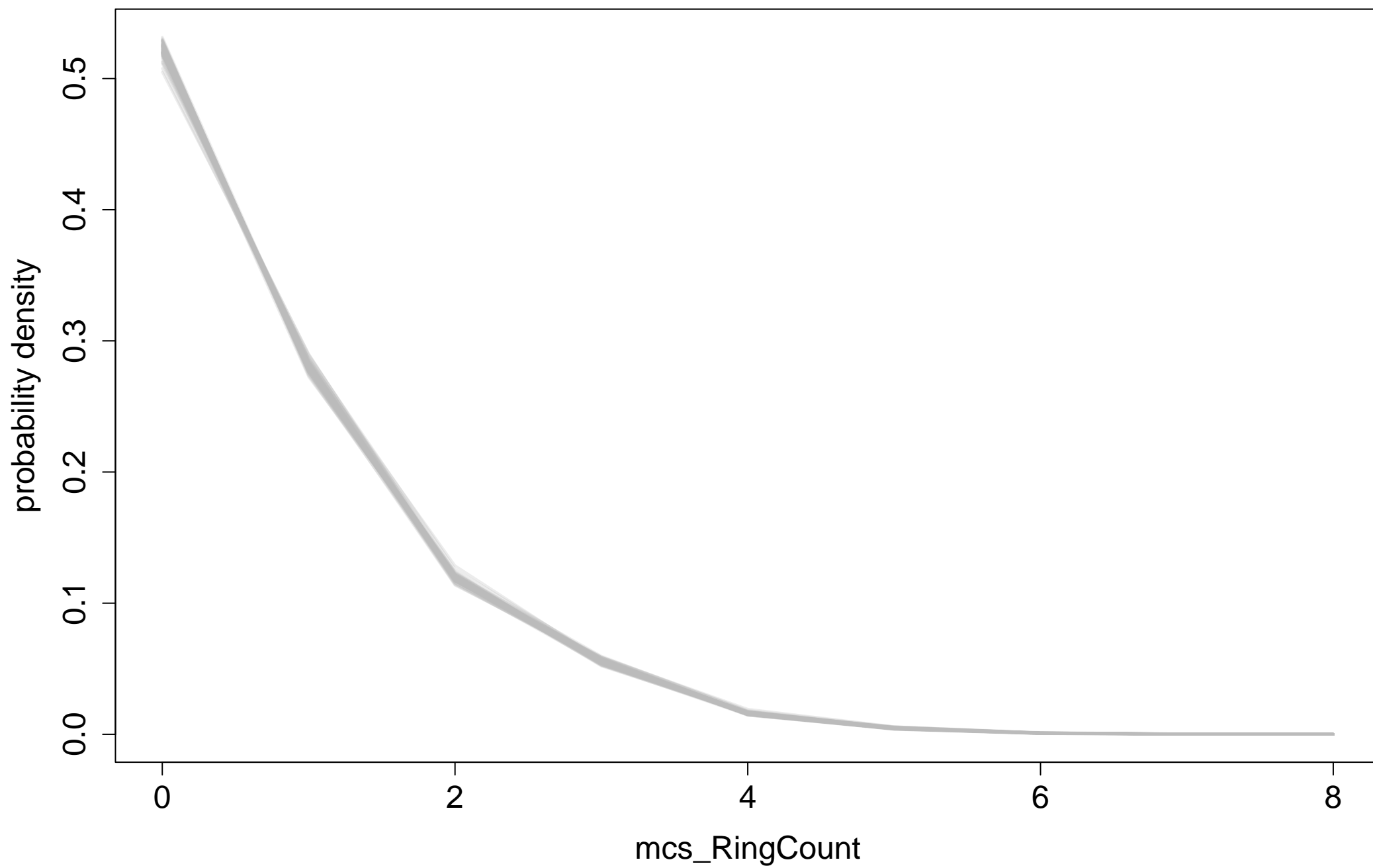
Occupied clusters: 62 of 64

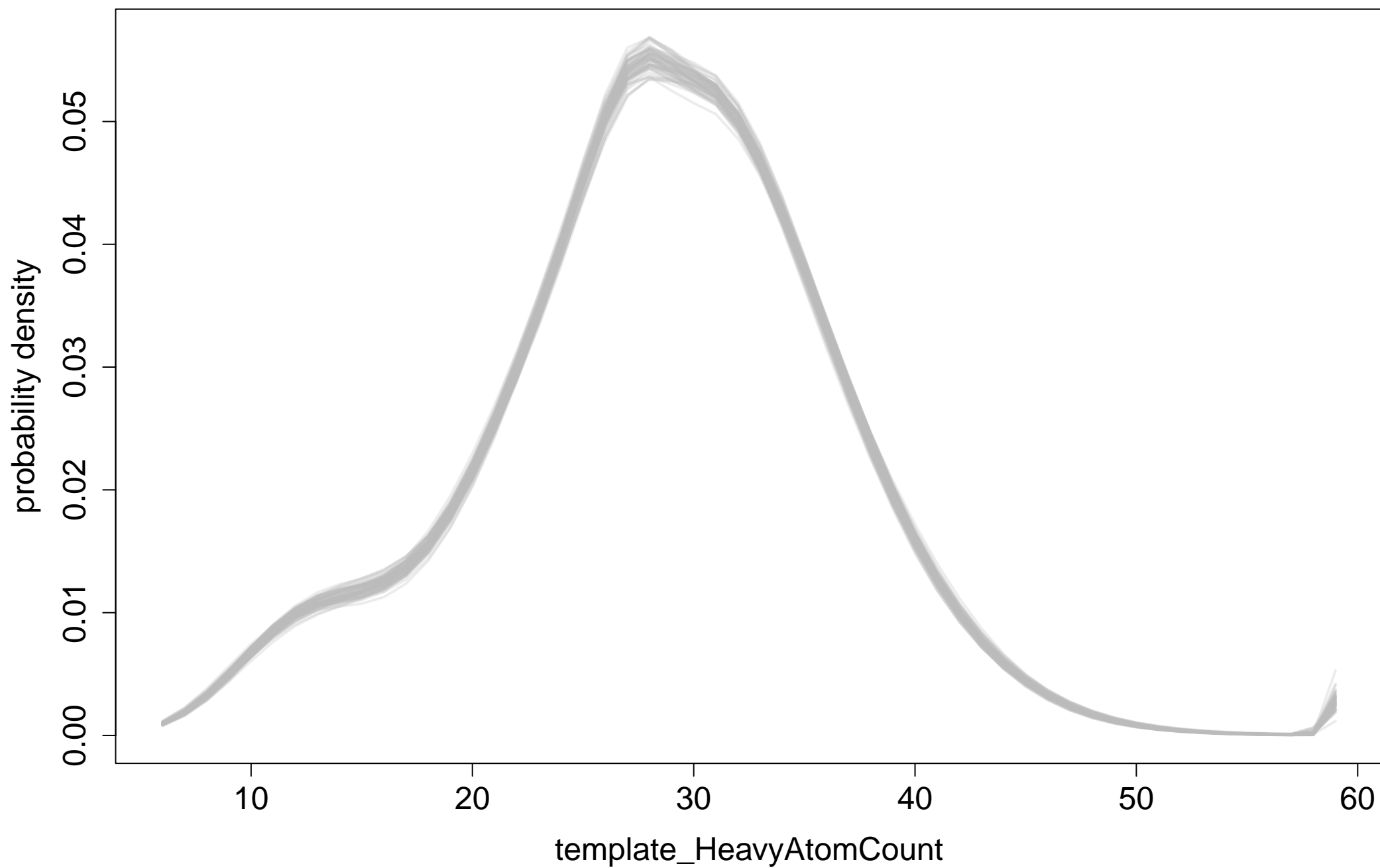
LL: -110000 +- 22.2

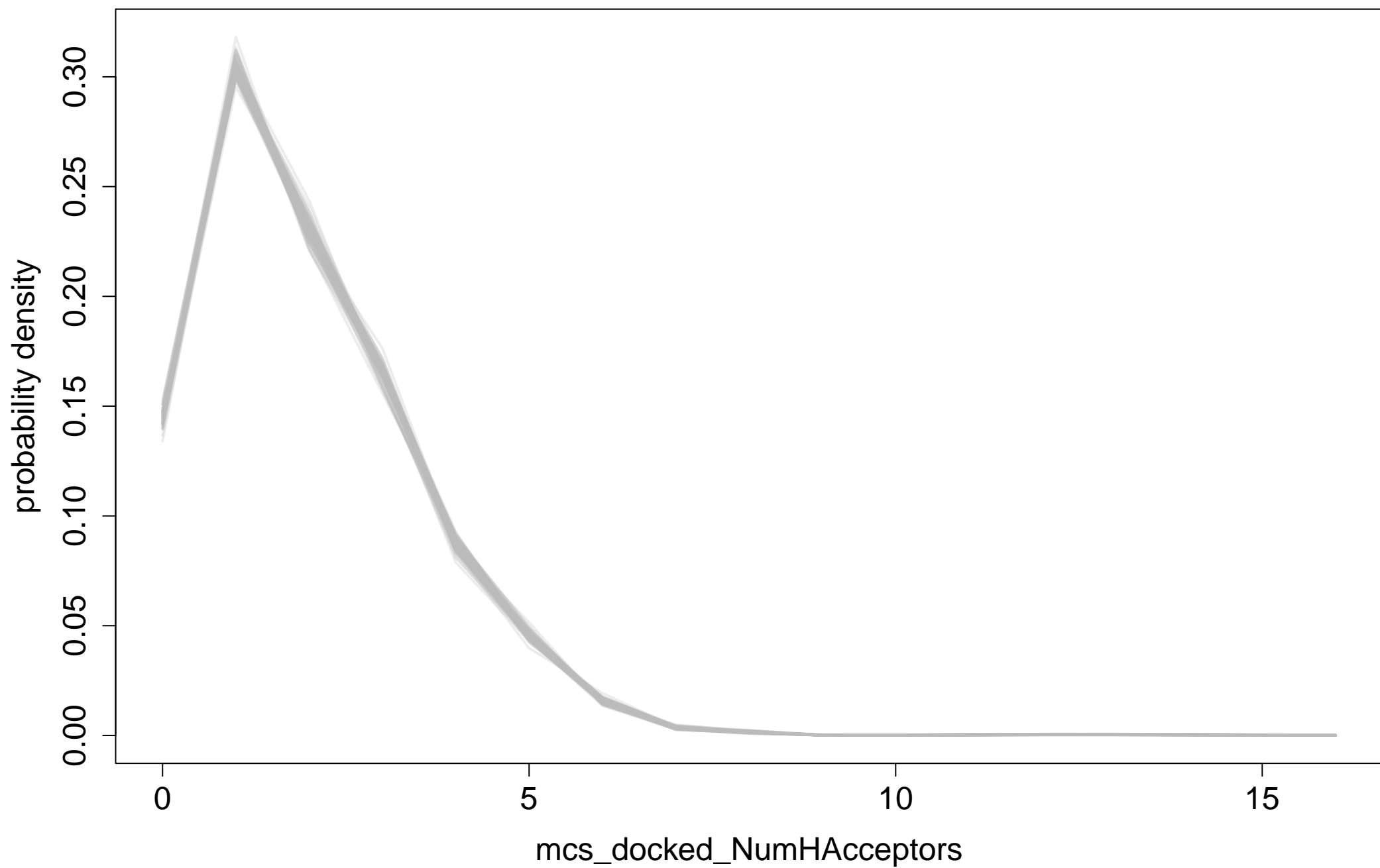


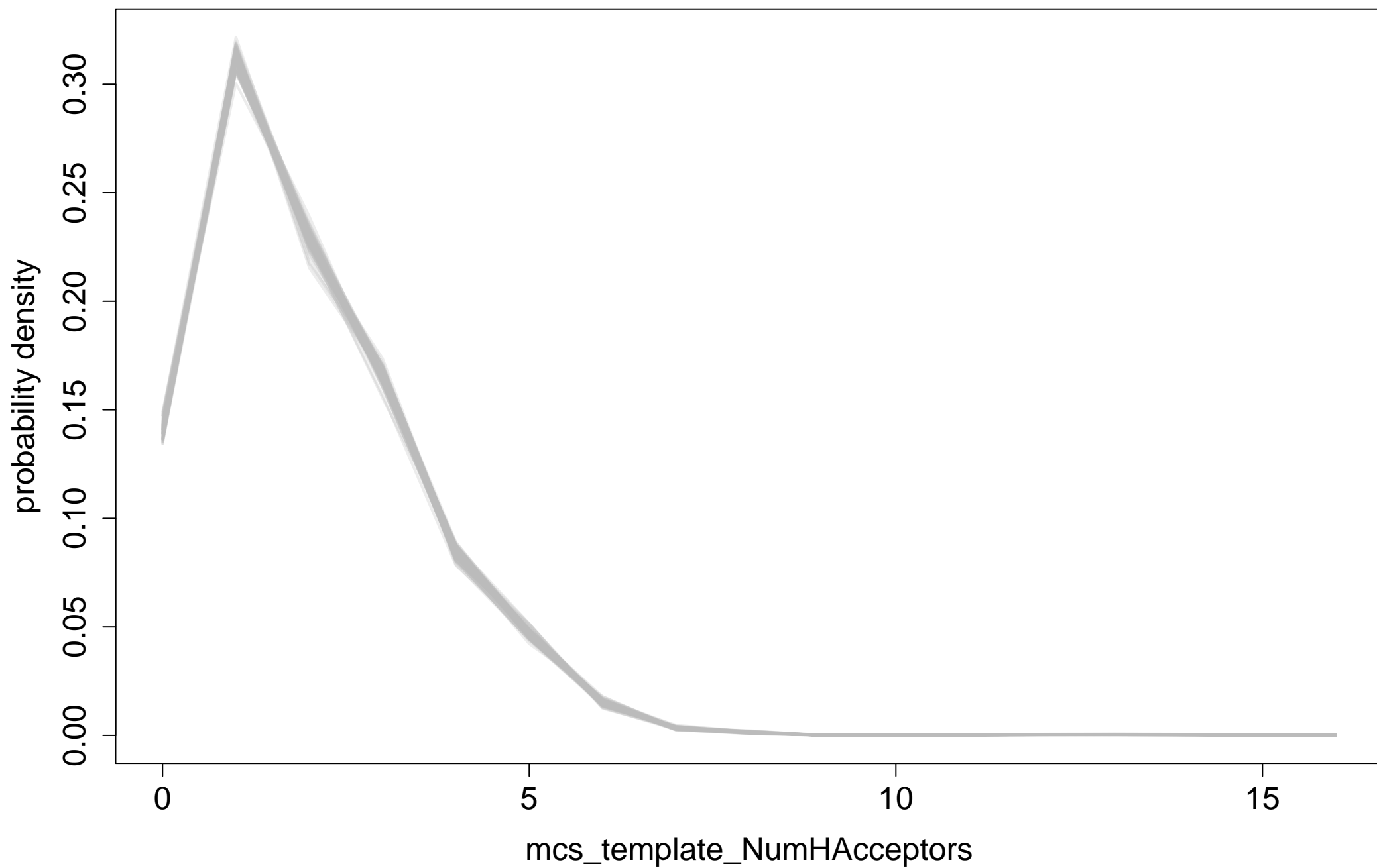




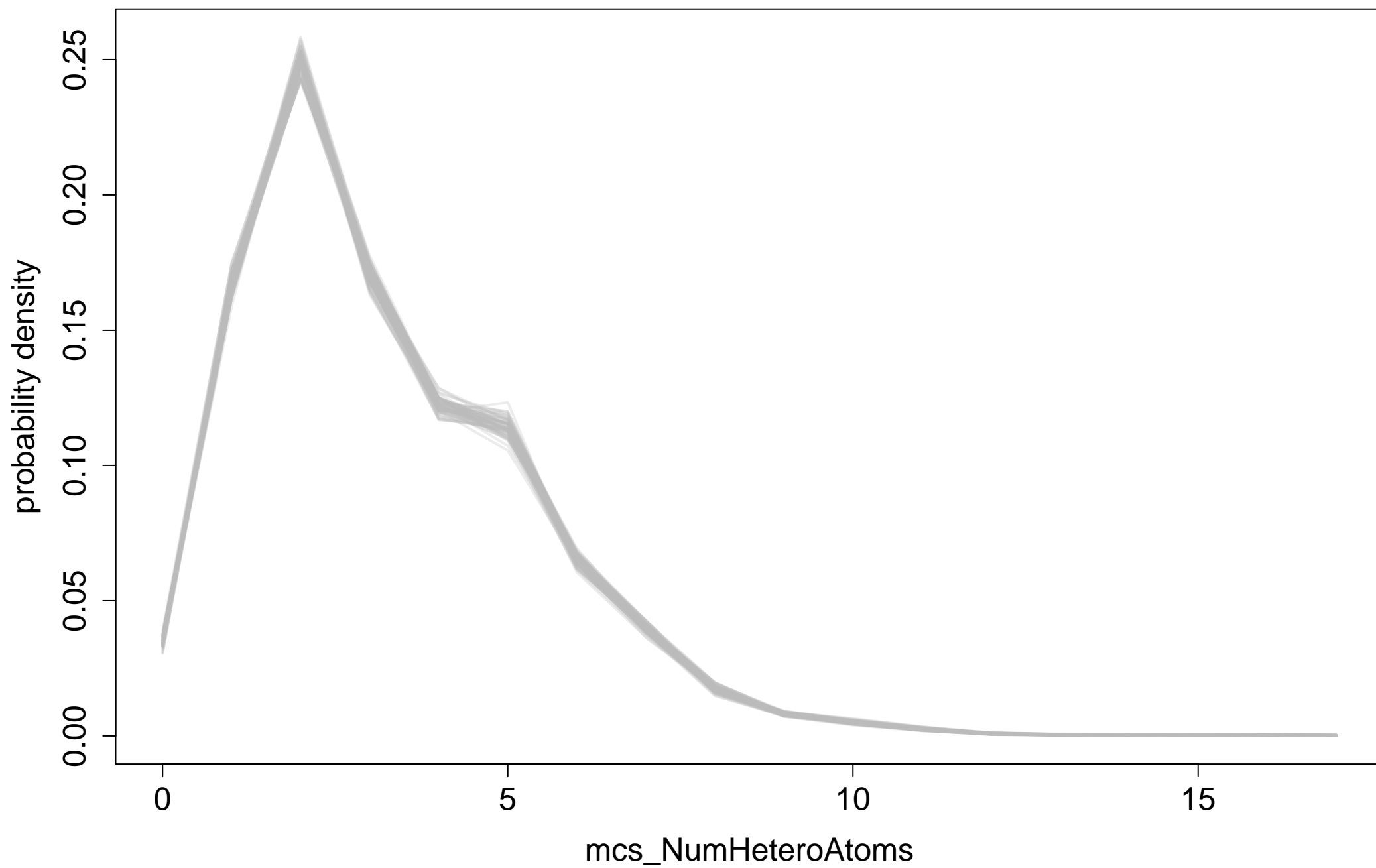


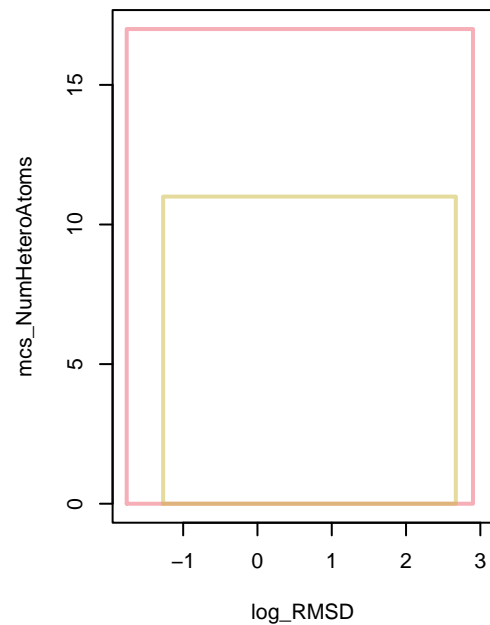
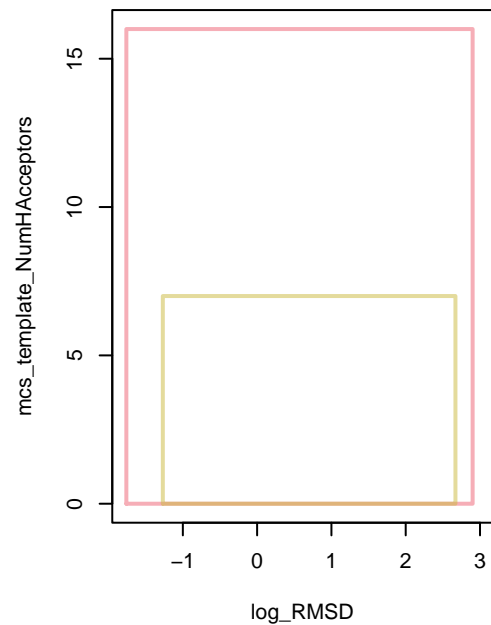
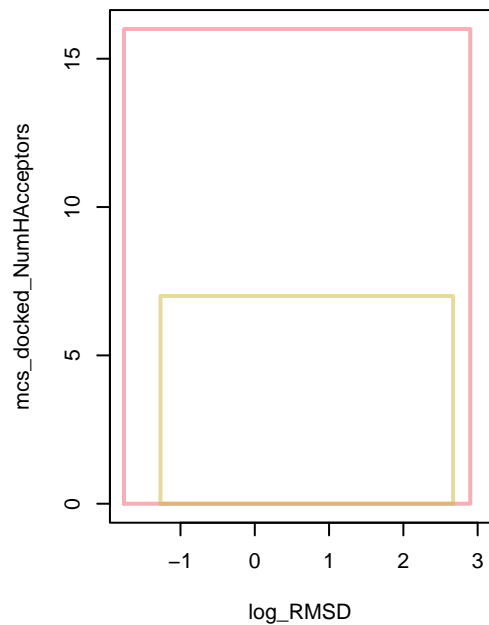
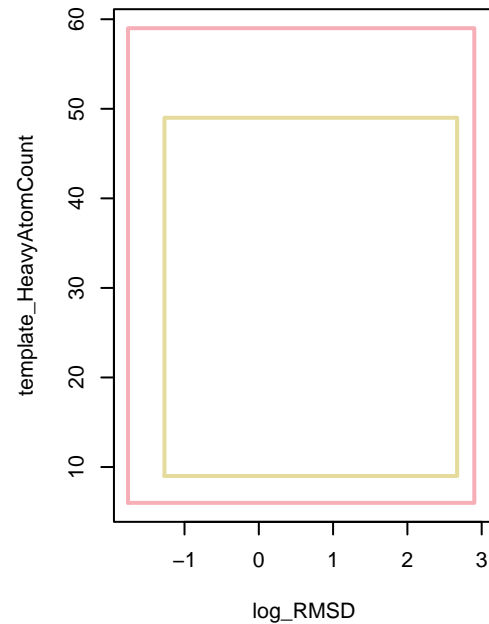
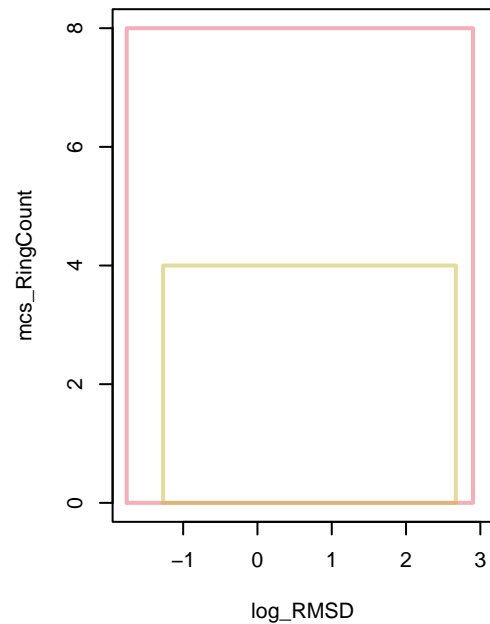
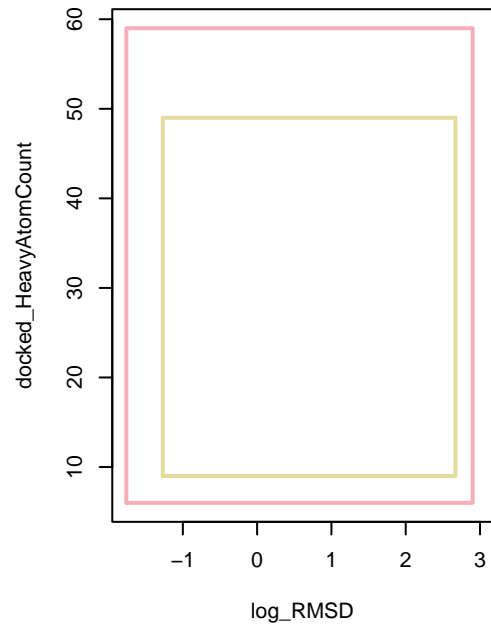
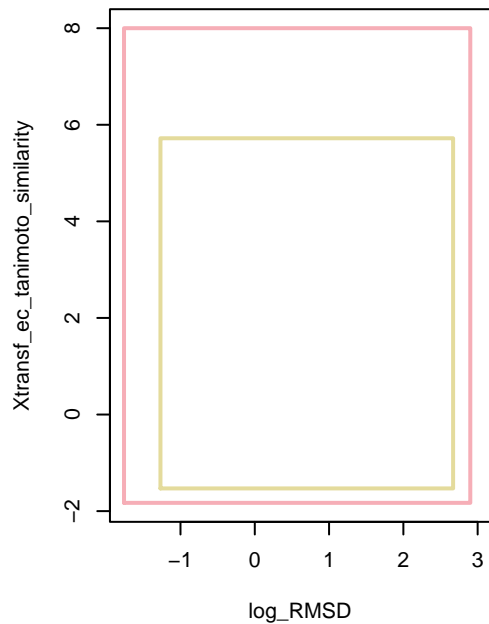




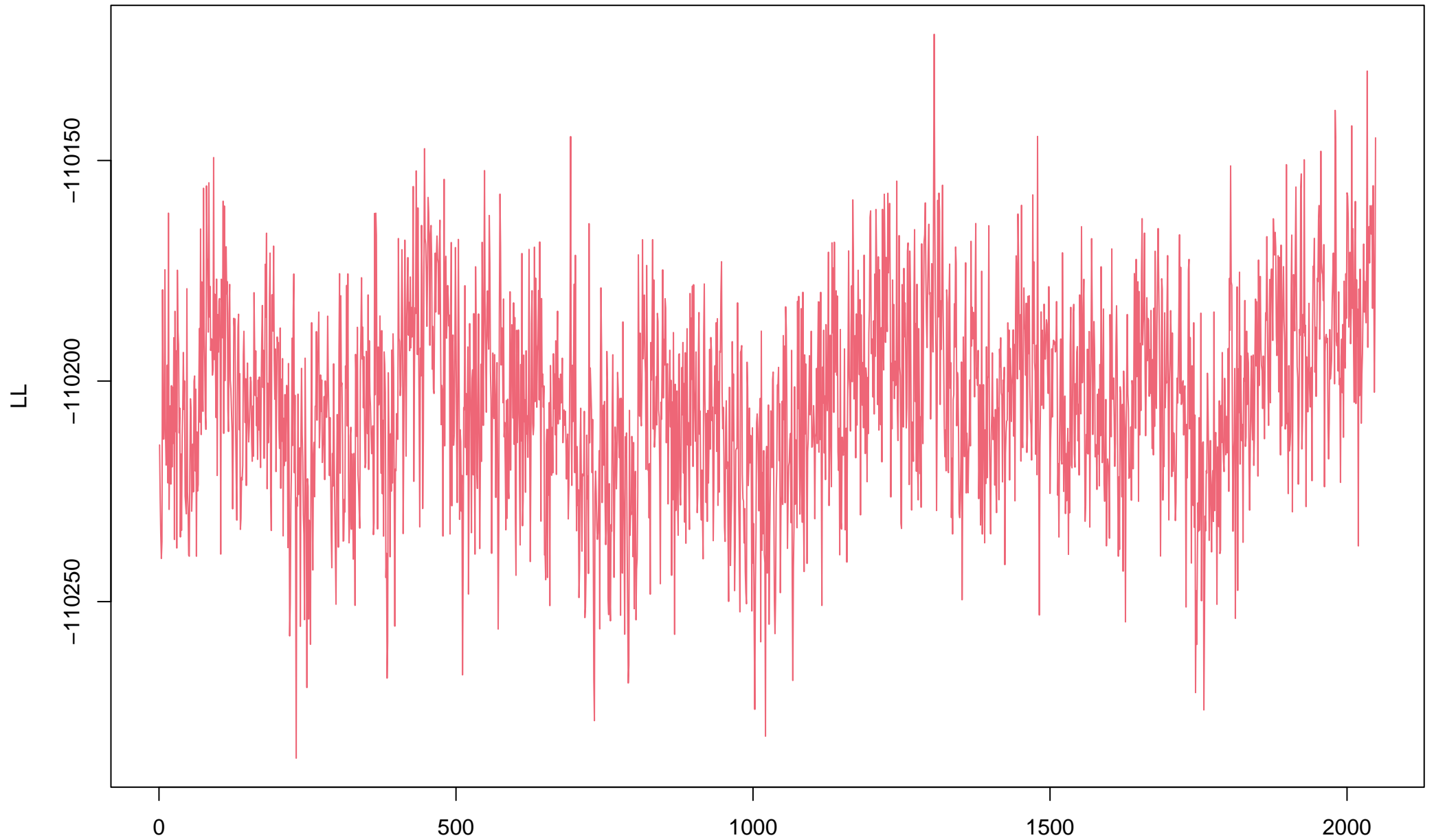




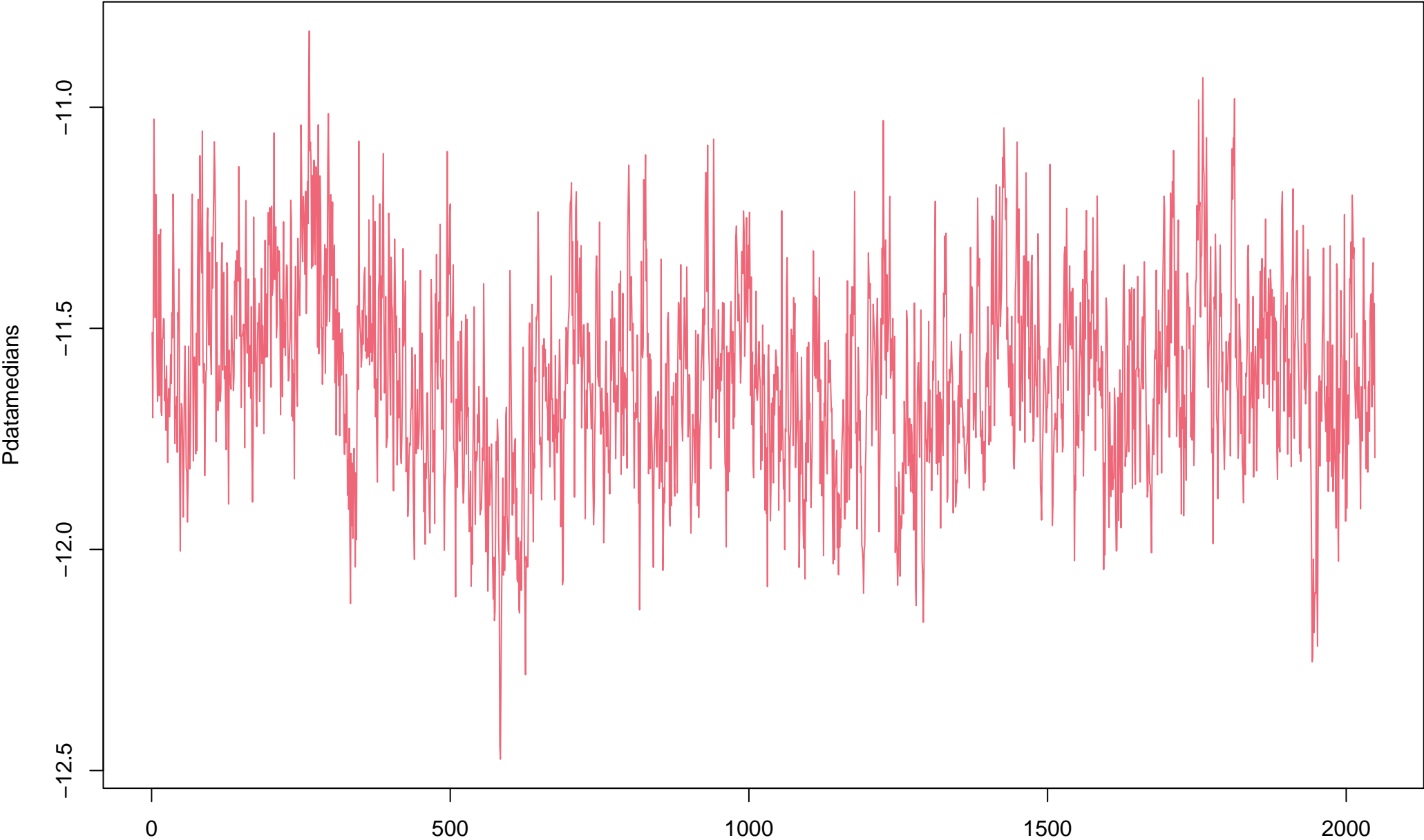




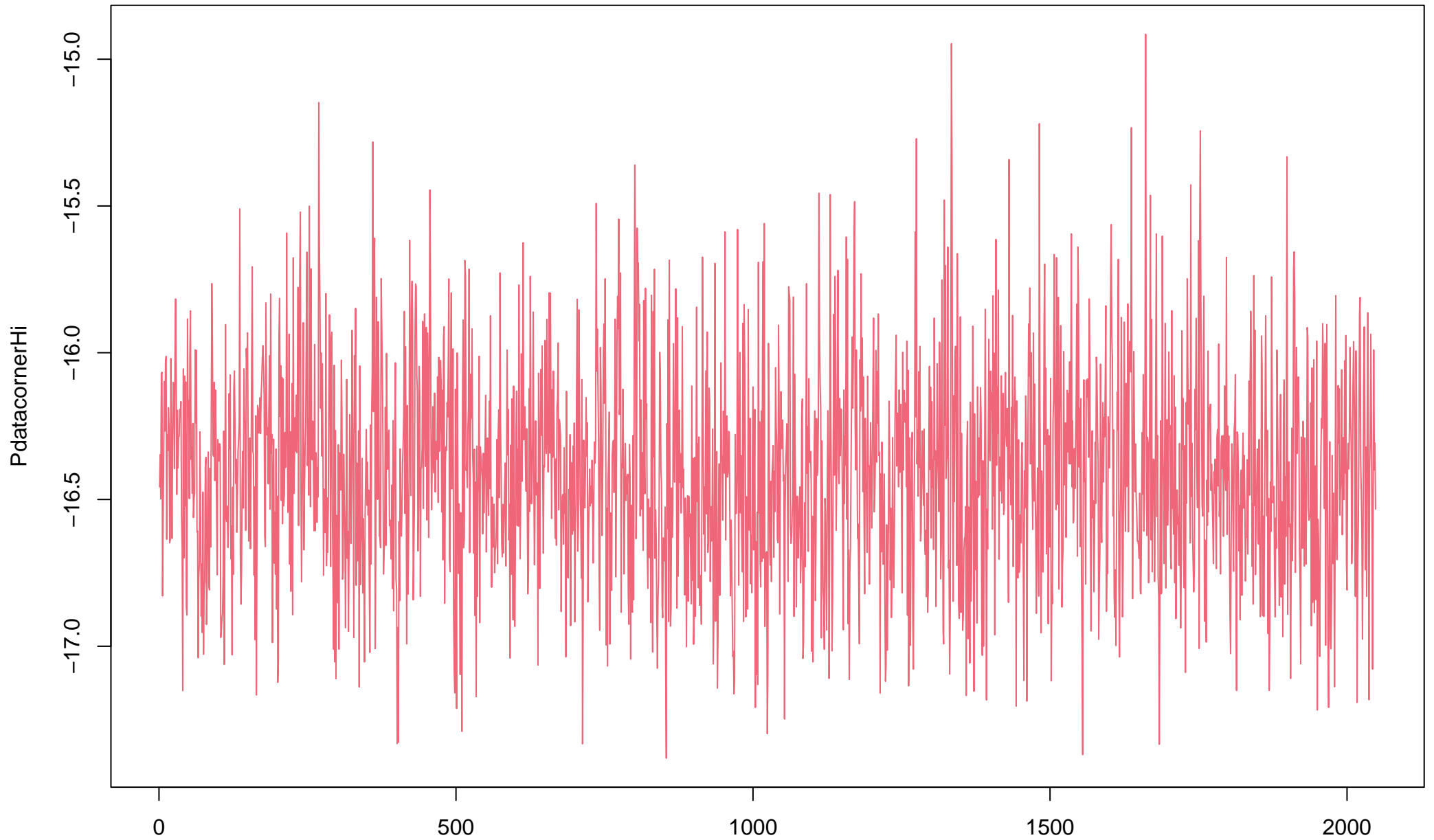
LL  
ESS = 111 | BMK = 0.129 | MCSE(6.27) = 7.11 | stat: TRUE | burn: 0



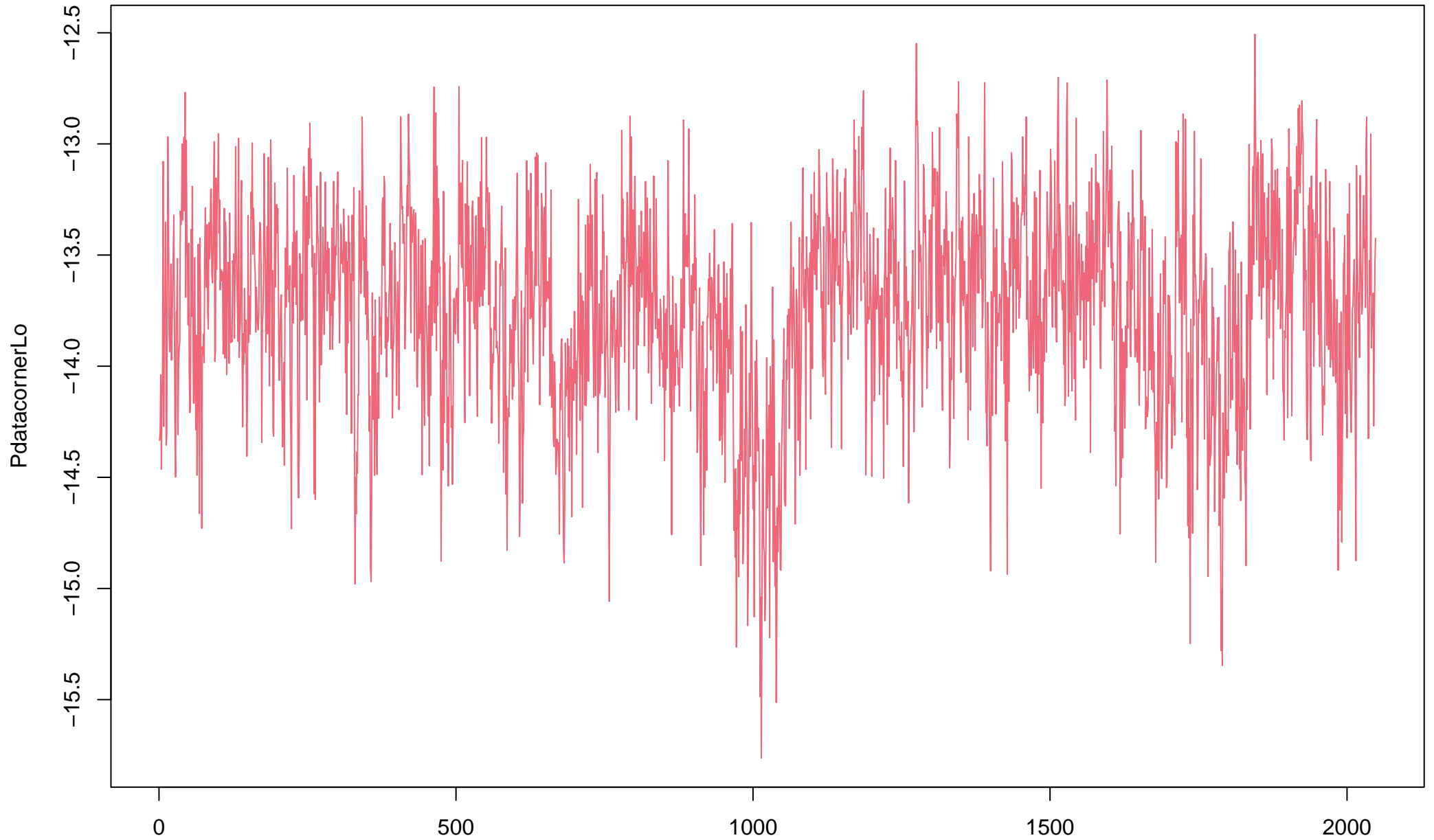
**Pdatamedians**  
**ESS = 148 | BMK = 0.0563 | MCSE(6.27) = 7.3 | stat: FALSE | burn: 0**



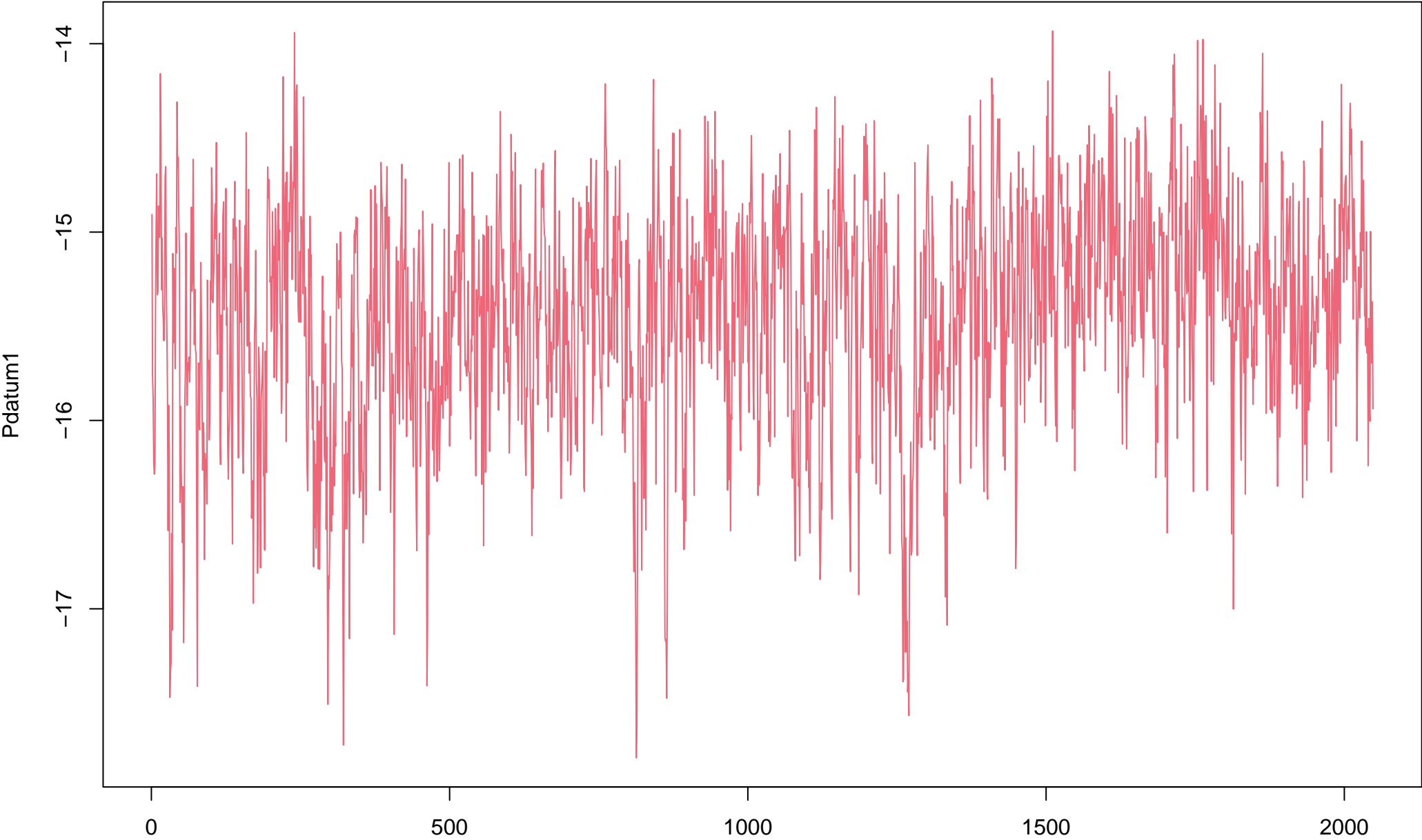
**PdatacornerHi**  
**ESS = 1220 | BMK = 0.0586 | MCSE(6.27) = 3.42 | stat: TRUE | burn: 0**



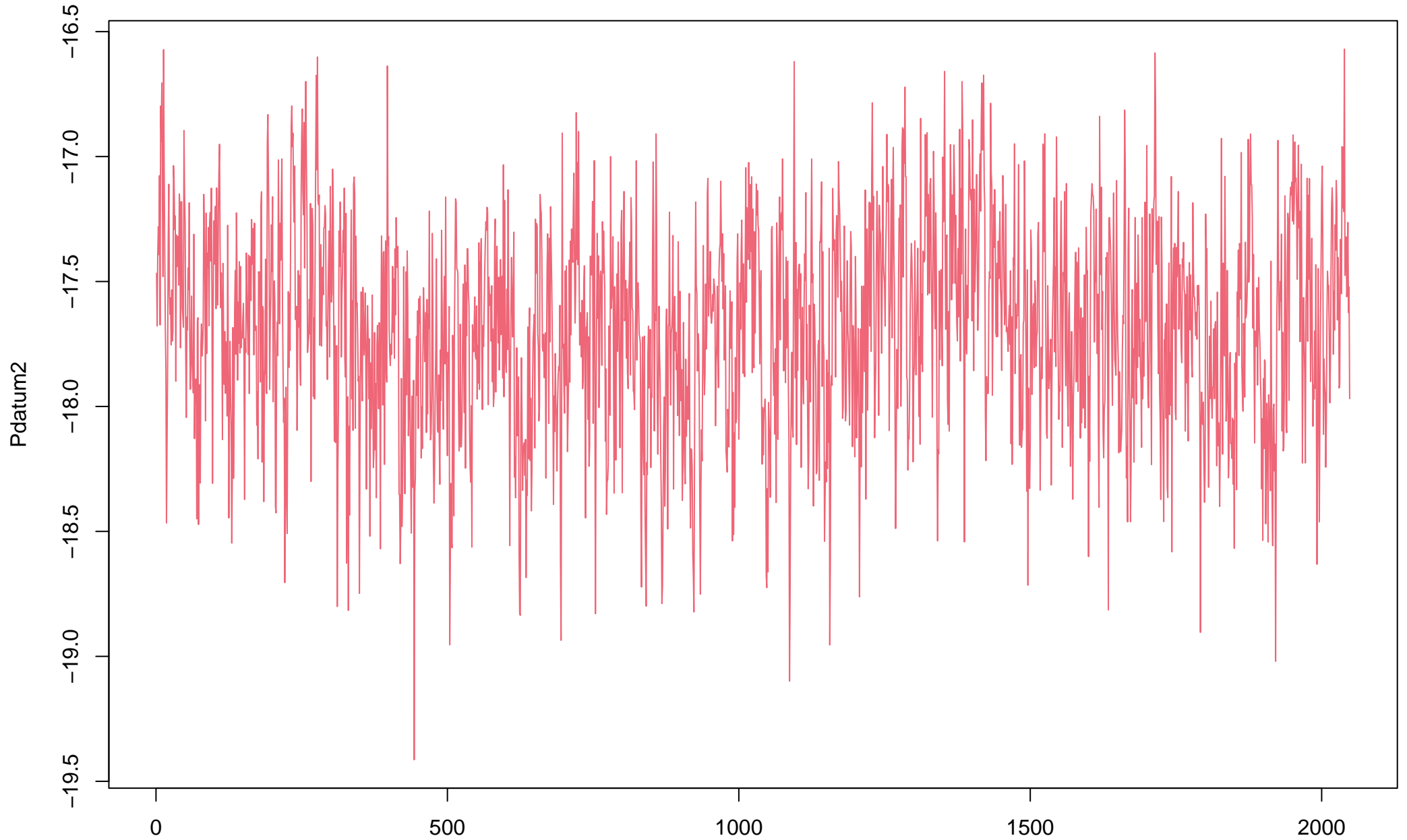
**PdatacornerLo**  
**ESS = 285 | BMK = 0.08 | MCSE(6.27) = 6.46 | stat: TRUE | burn: 0**



**Pdatum1**  
**ESS = 316 | BMK = 0.135 | MCSE(6.27) = 6.01 | stat: FALSE | burn: 0**

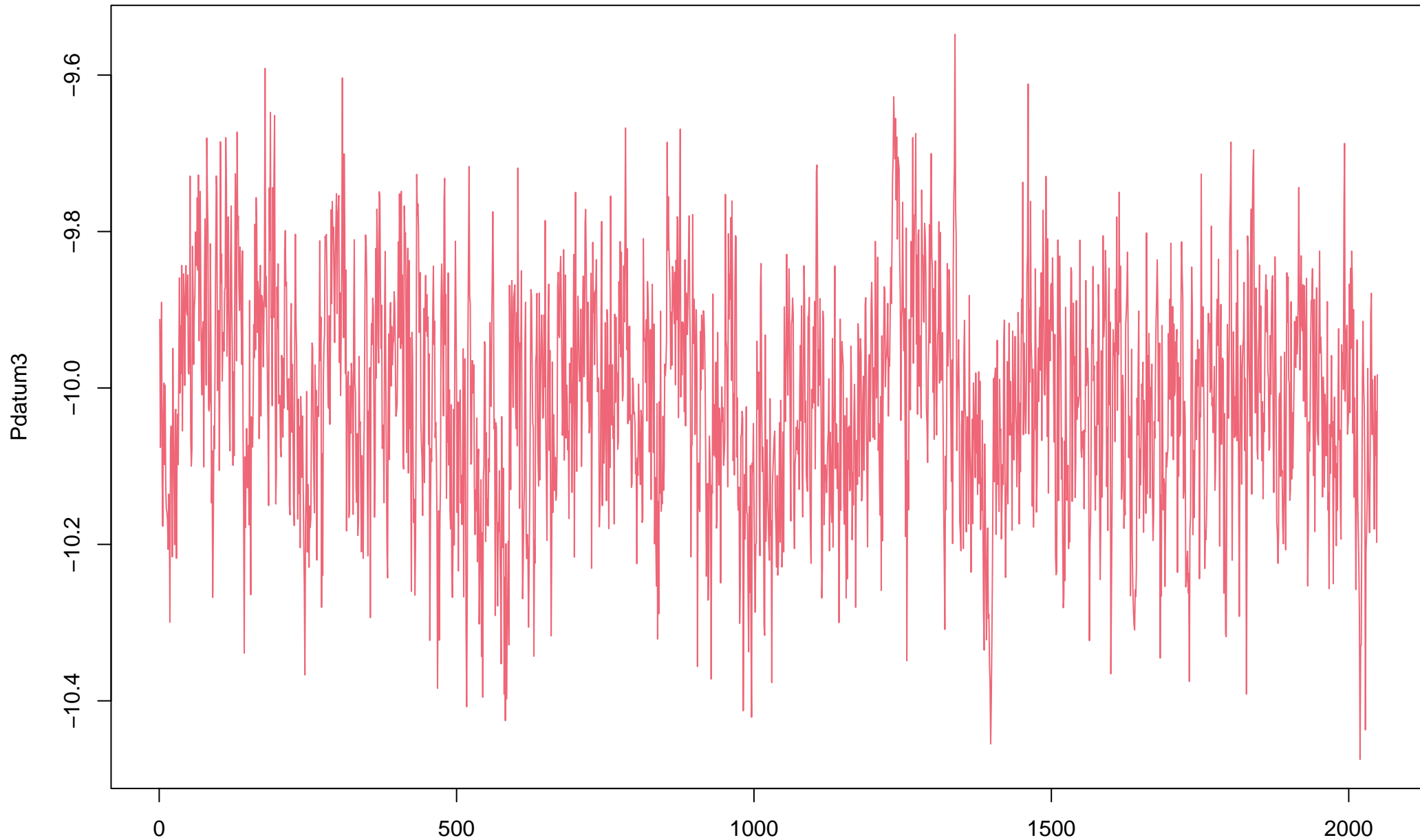


**Pdatum2**  
**ESS = 2.22e-16 | BMK = 0.0751 | MCSE(6.27) = 5.78 | stat: TRUE | burn: 0**

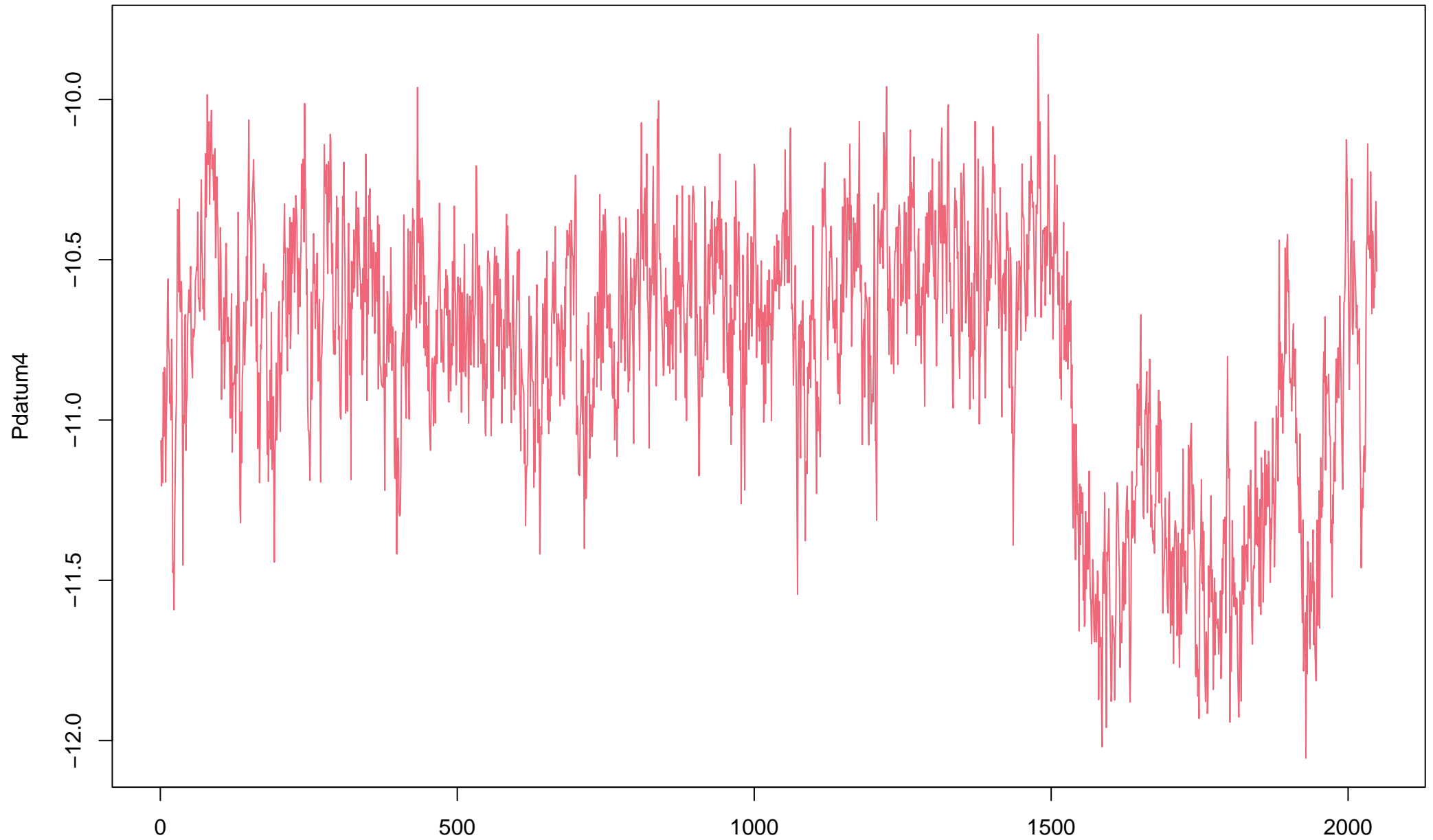




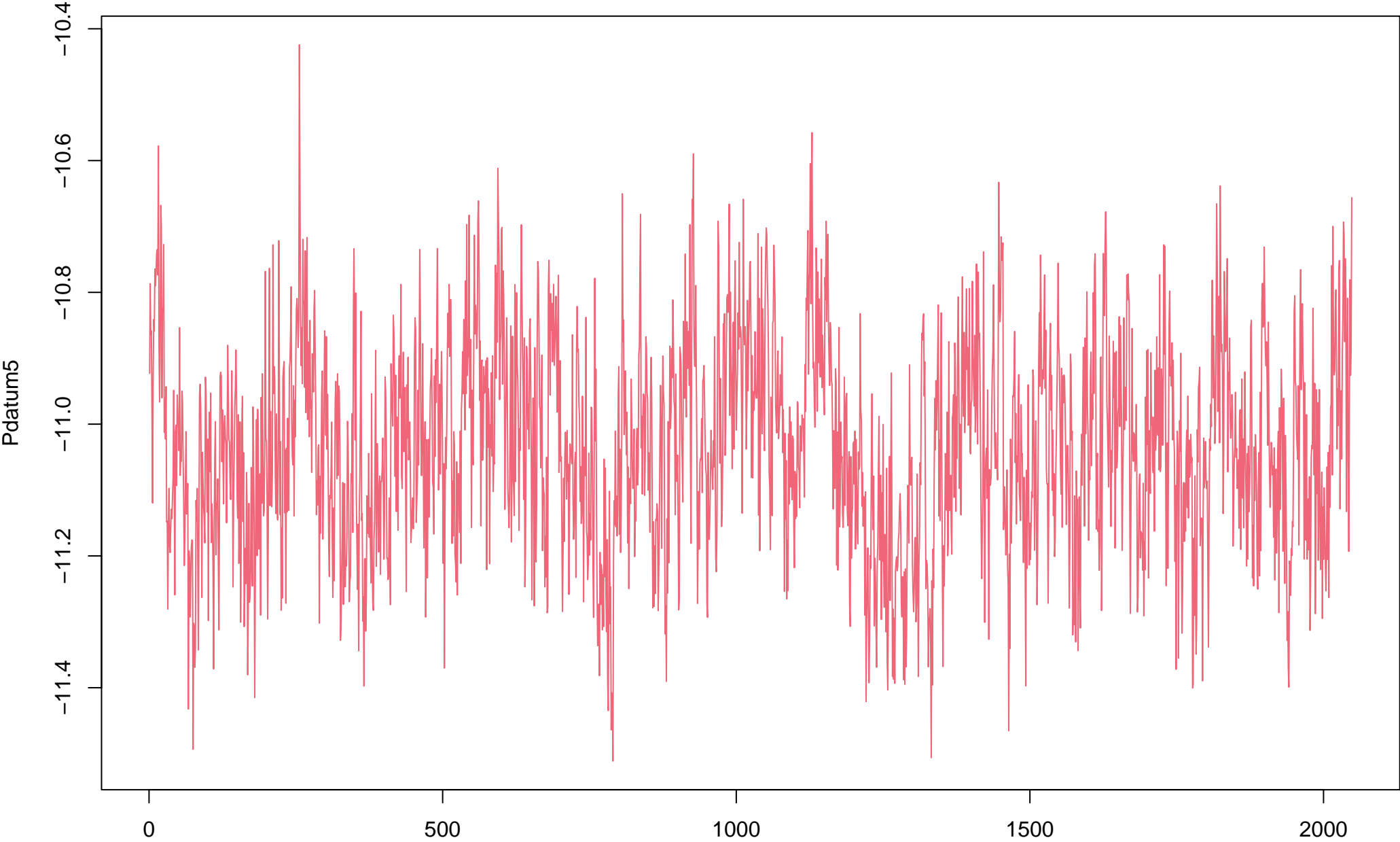
**Pdatum3**  
**ESS = 206 | BMK = 0.0651 | MCSE(6.27) = 6.57 | stat: FALSE | burn: 0**



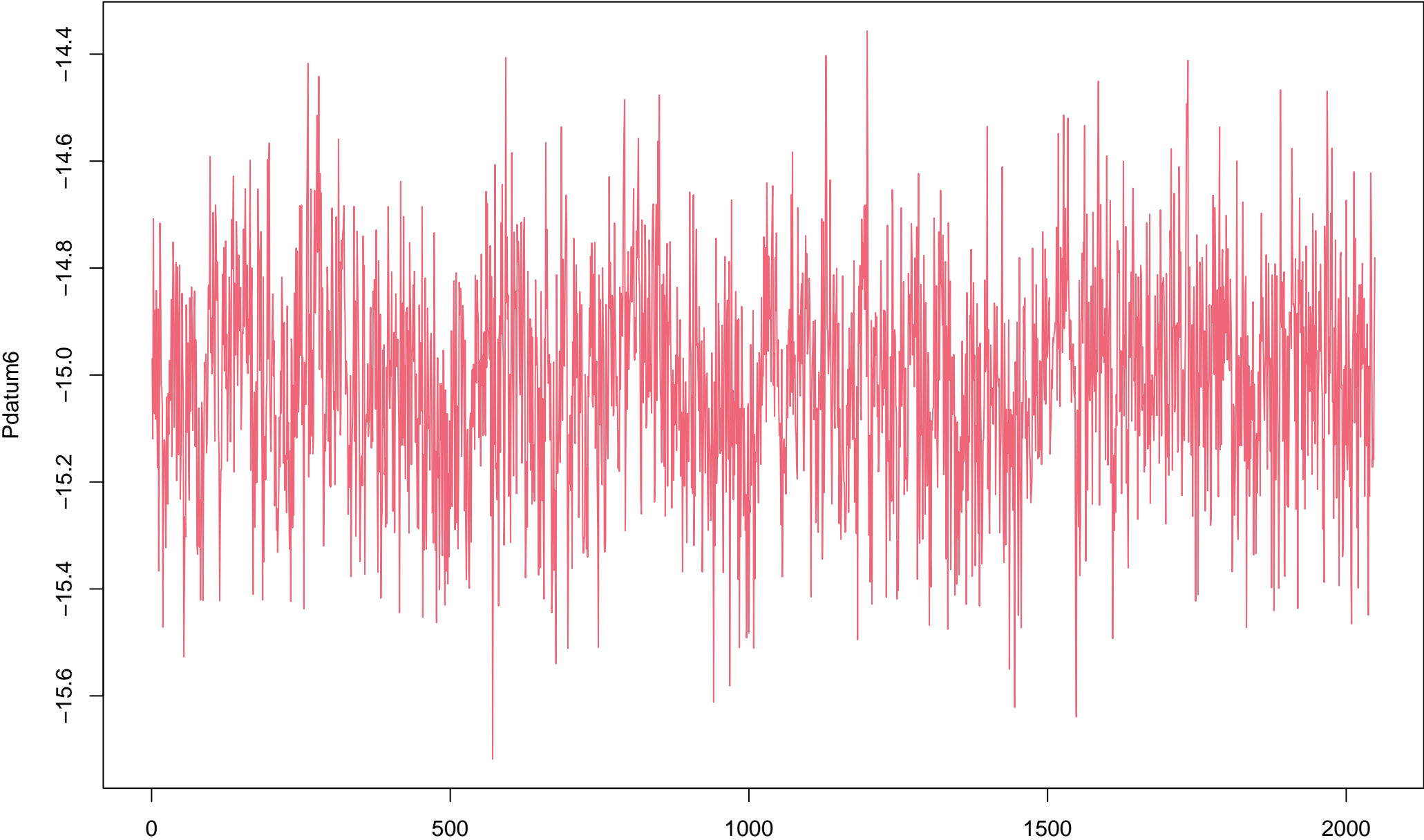
**Pdatum4**  
**ESS = 37.5 | BMK = 0.323 | MCSE(6.27) = 11 | stat: FALSE | burn: 0**



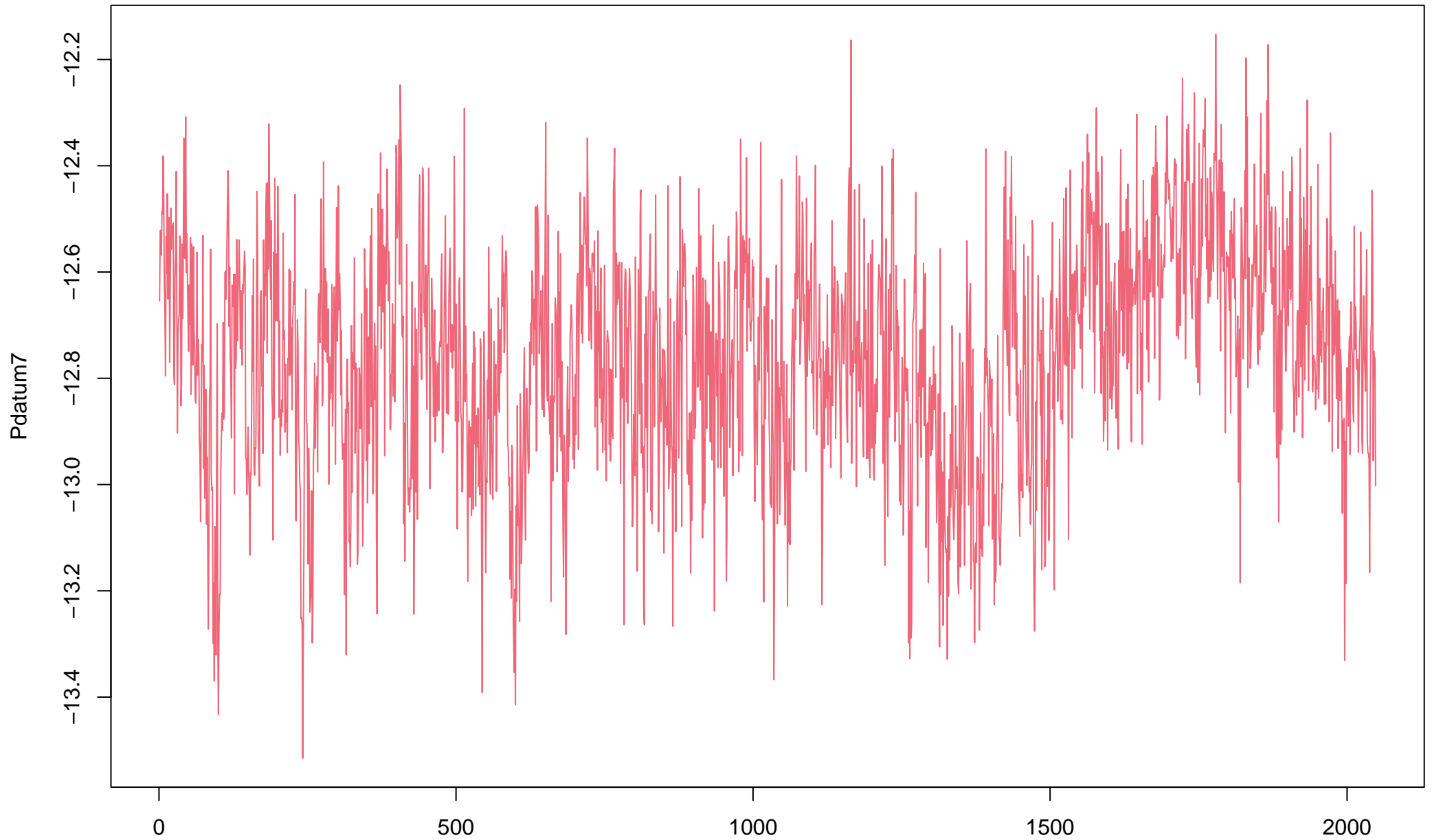
**Pdatum5**  
**ESS = 186 | BMK = 0.0454 | MCSE(6.27) = 7.07 | stat: TRUE | burn: 0**



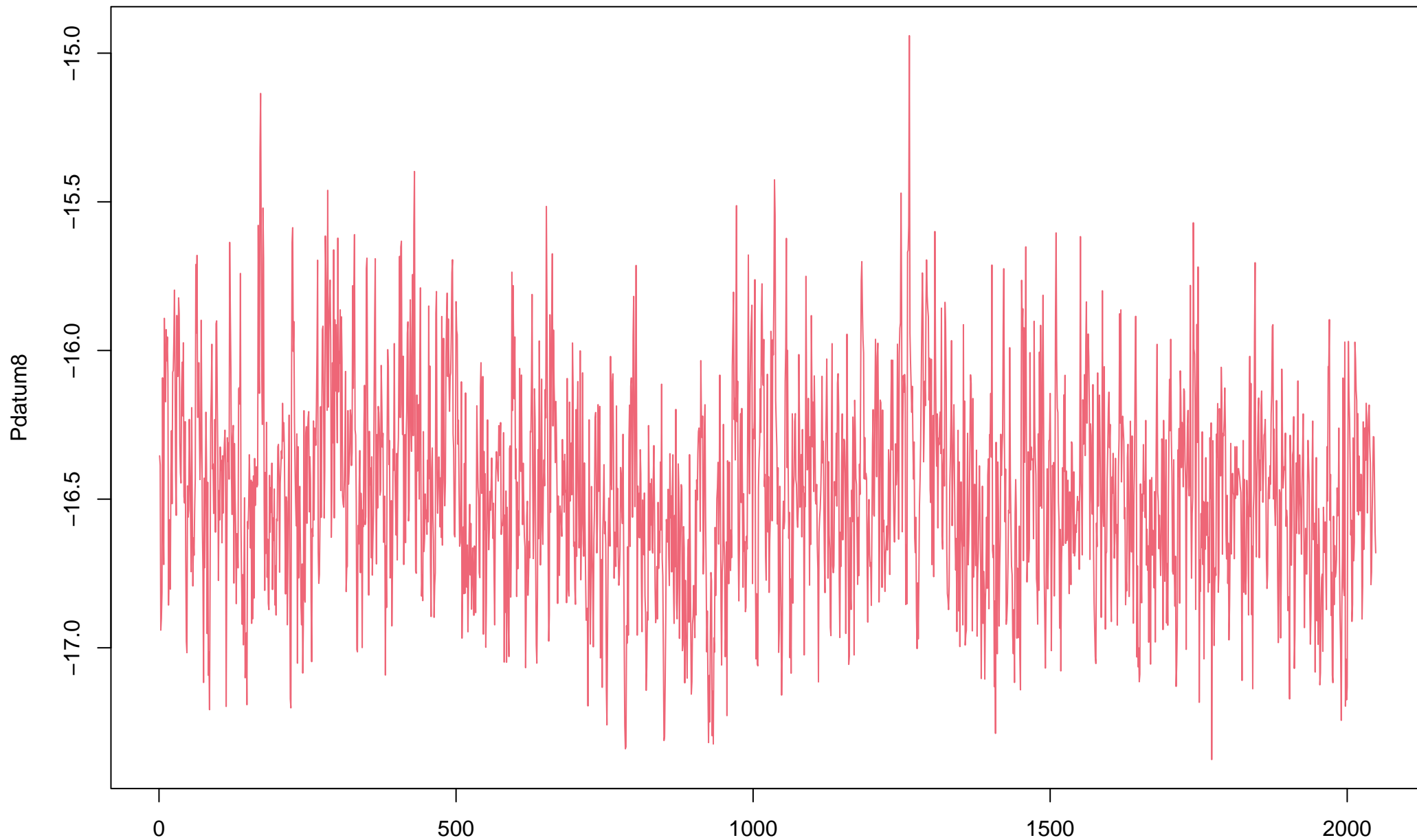
**Pdatum6**  
**ESS = 613 | BMK = 0.0488 | MCSE(6.27) = 4.51 | stat: TRUE | burn: 0**



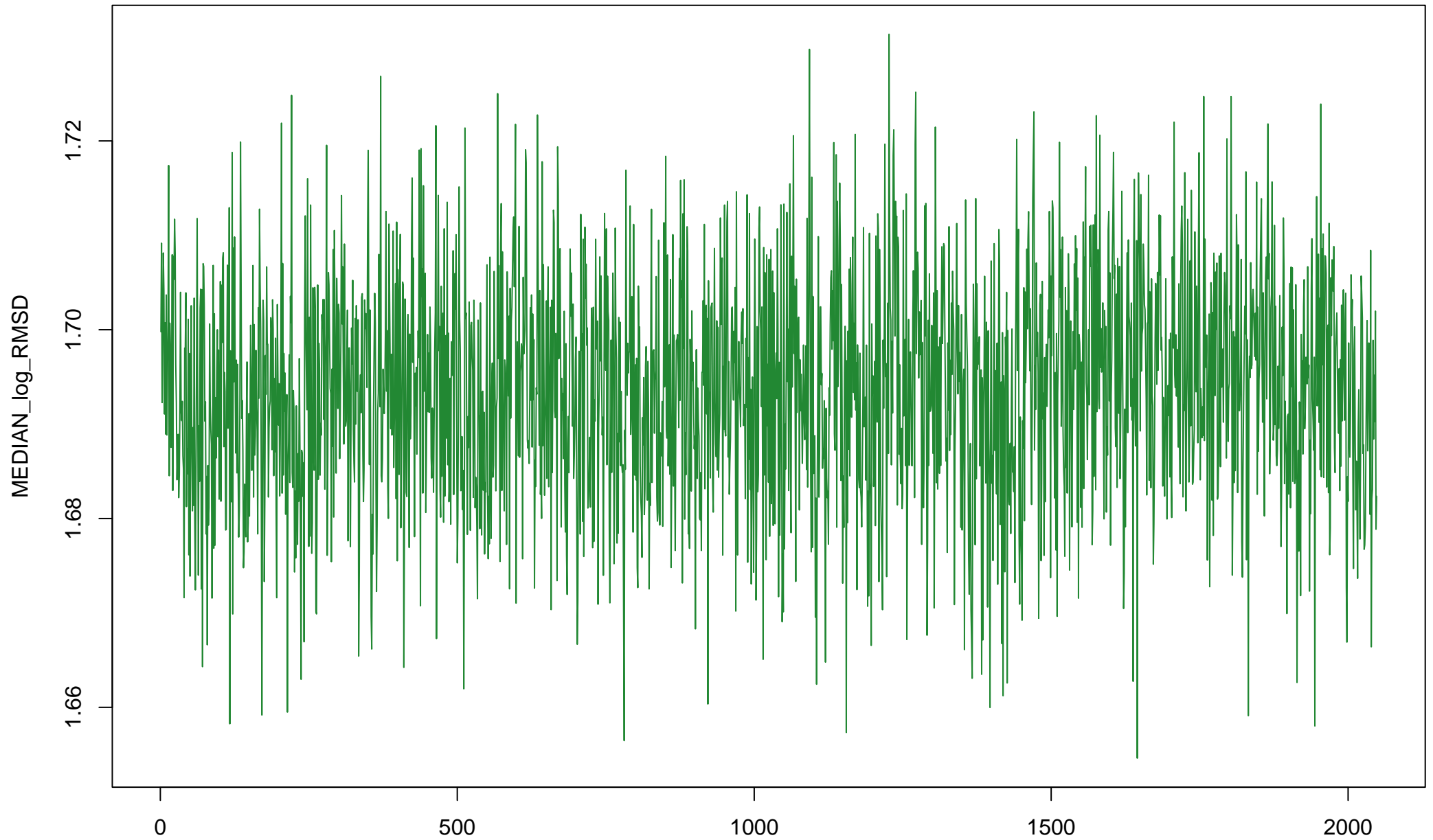
**Pdatum7**  
**ESS = 134 | BMK = 0.104 | MCSE(6.27) = 7.93 | stat: TRUE | burn: 0**



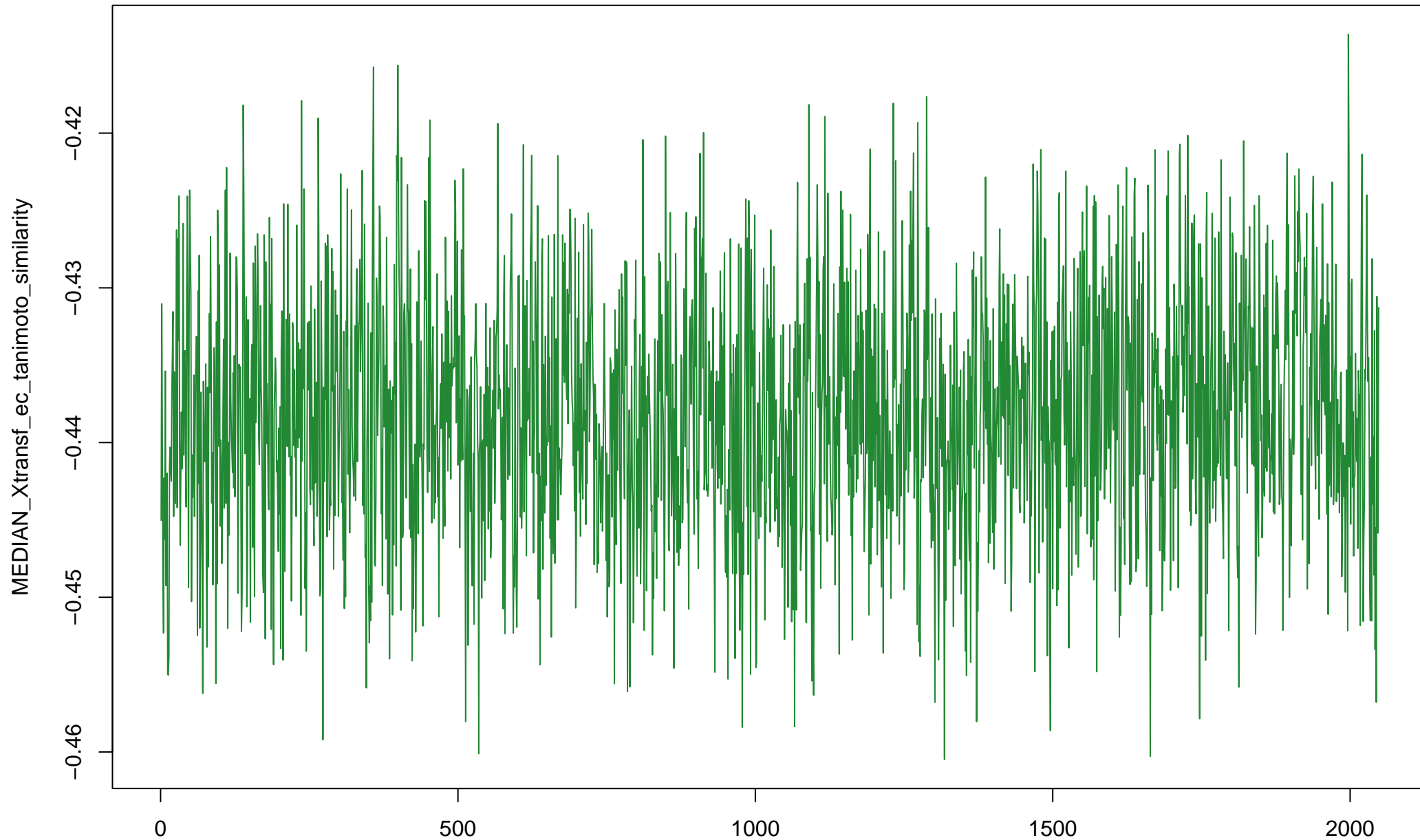
**Pdatum8**  
**ESS = 508 | BMK = 0.0609 | MCSE(6.27) = 5.3 | stat: TRUE | burn: 0**



**MEDIAN\_log\_RMSD**  
**ESS = 1530 | BMK = 0.0572 | MCSE(6.27) = 3.48 | stat: FALSE | burn: 0**

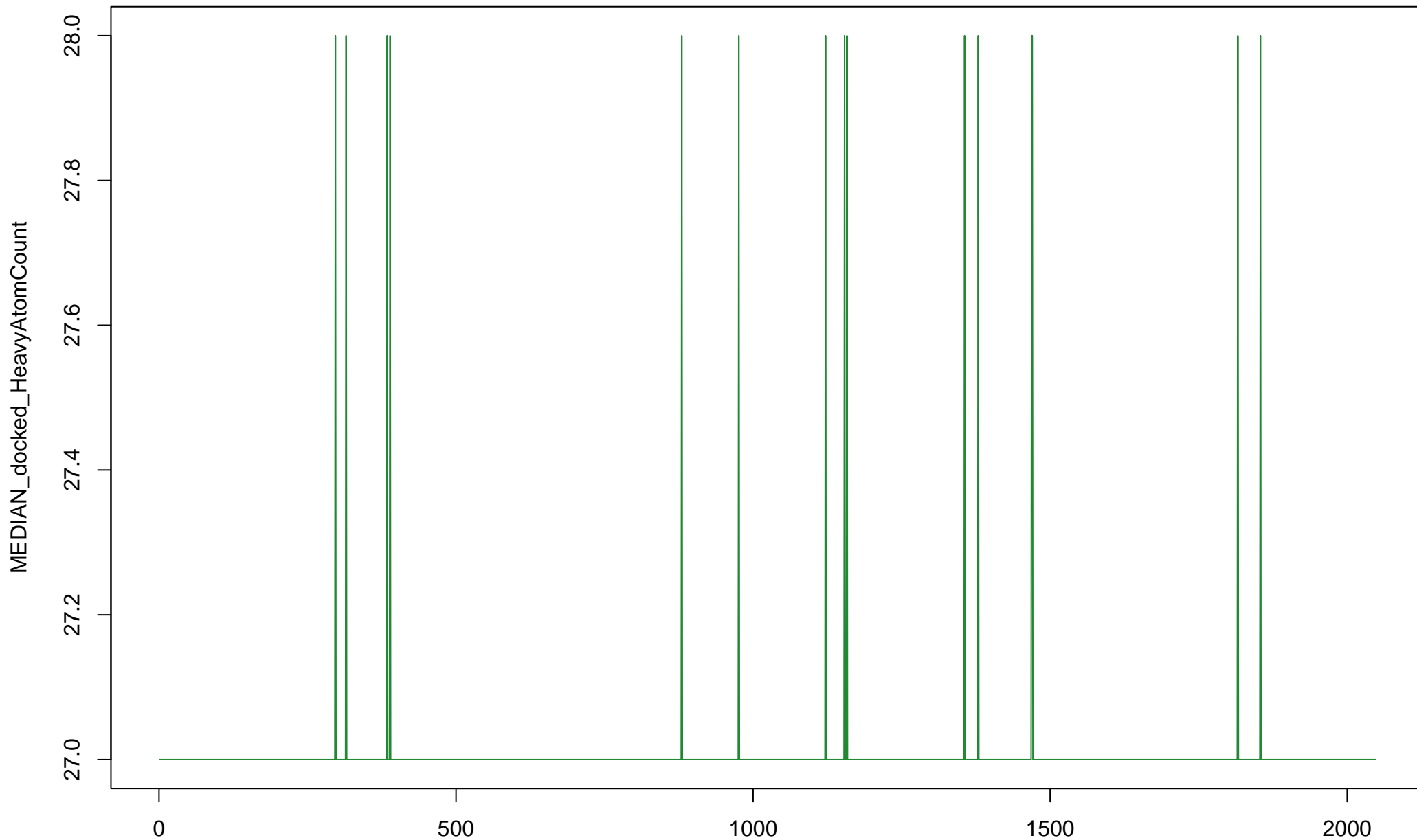


**MEDIAN\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1410 | BMK = 0.0367 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0**

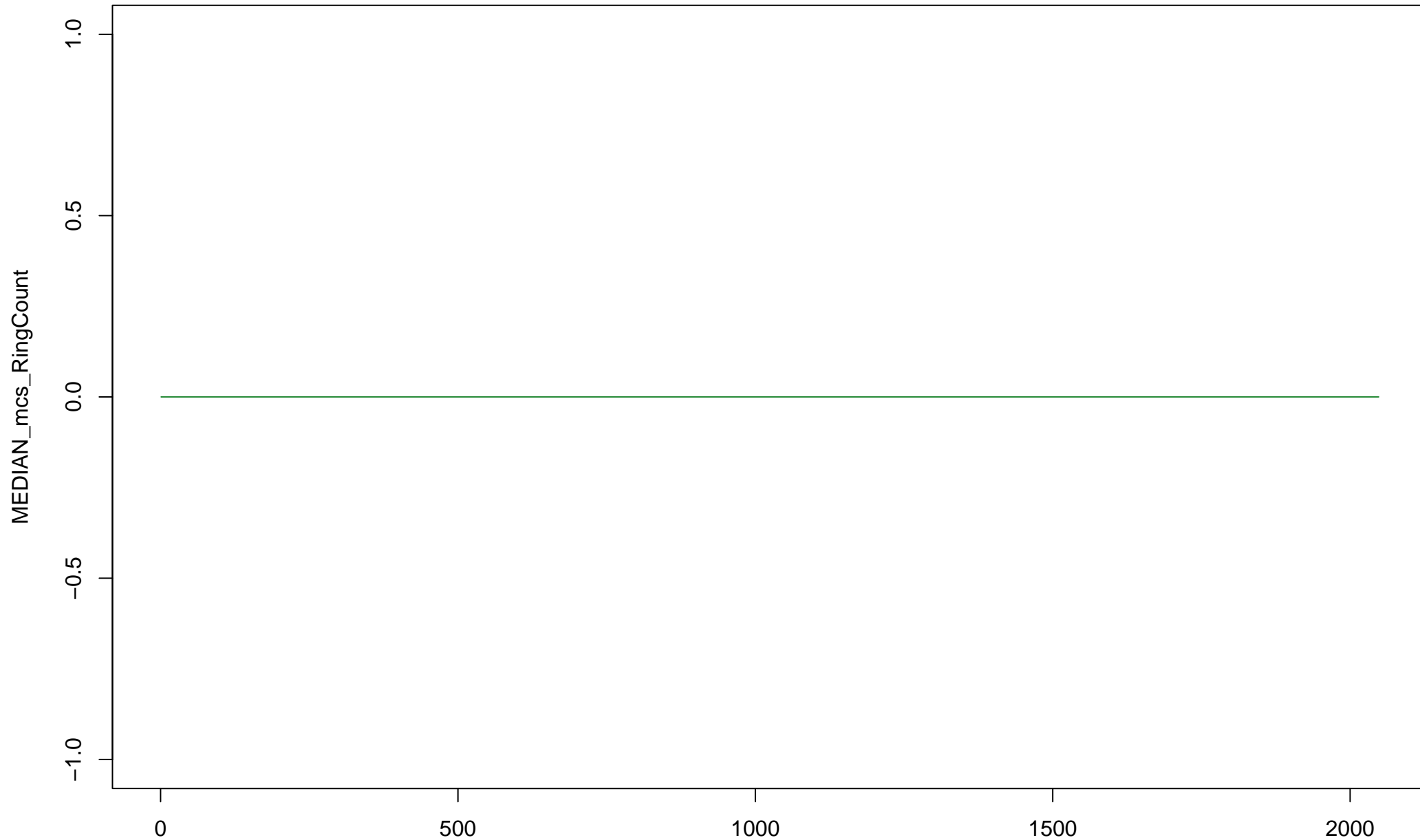




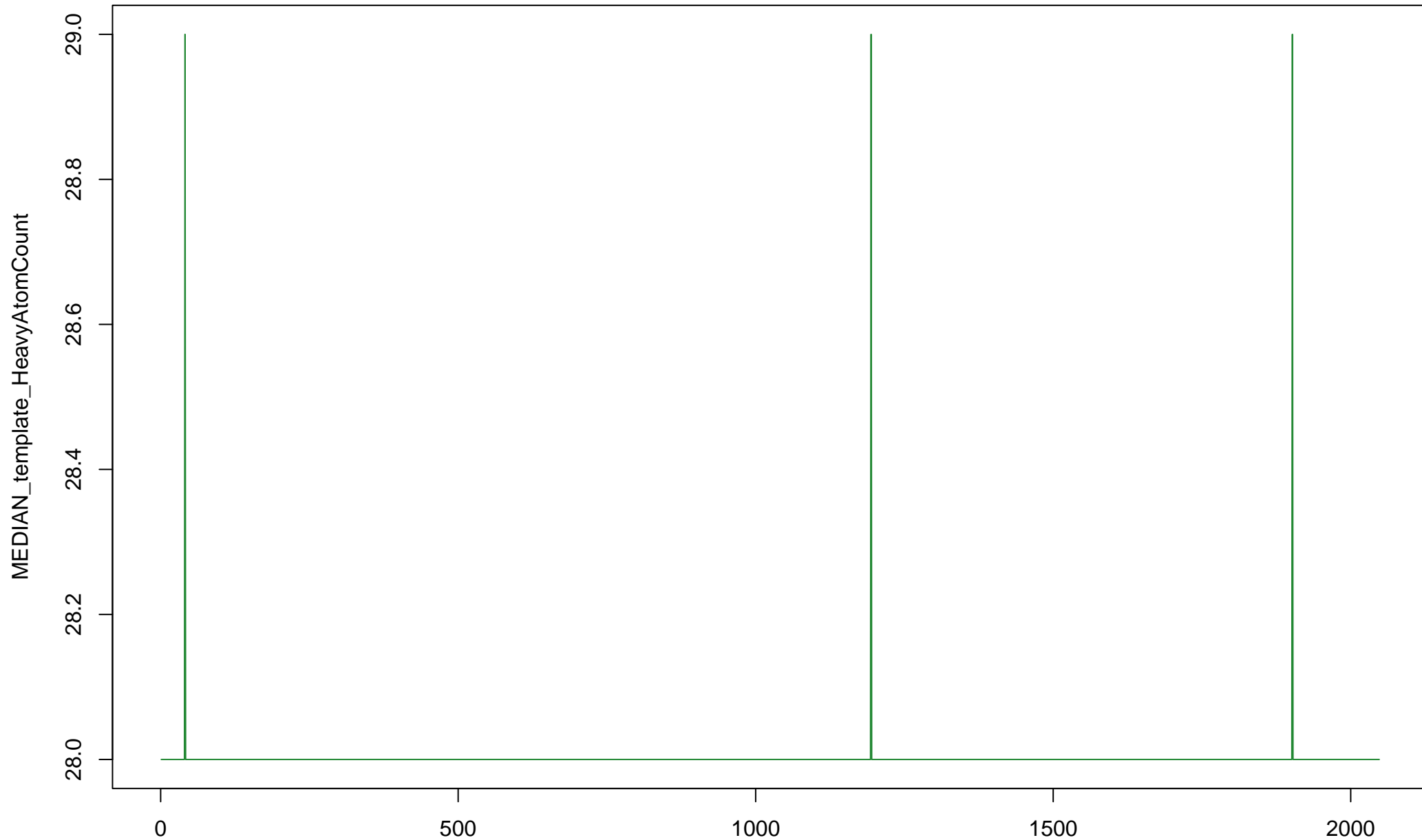
**MEDIAN\_docked\_HeavyAtomCount**  
**ESS = 1490 | BMK = 0.0716 | MCSE(6.27) = 2.6 | stat: FALSE | burn: 0**



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



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



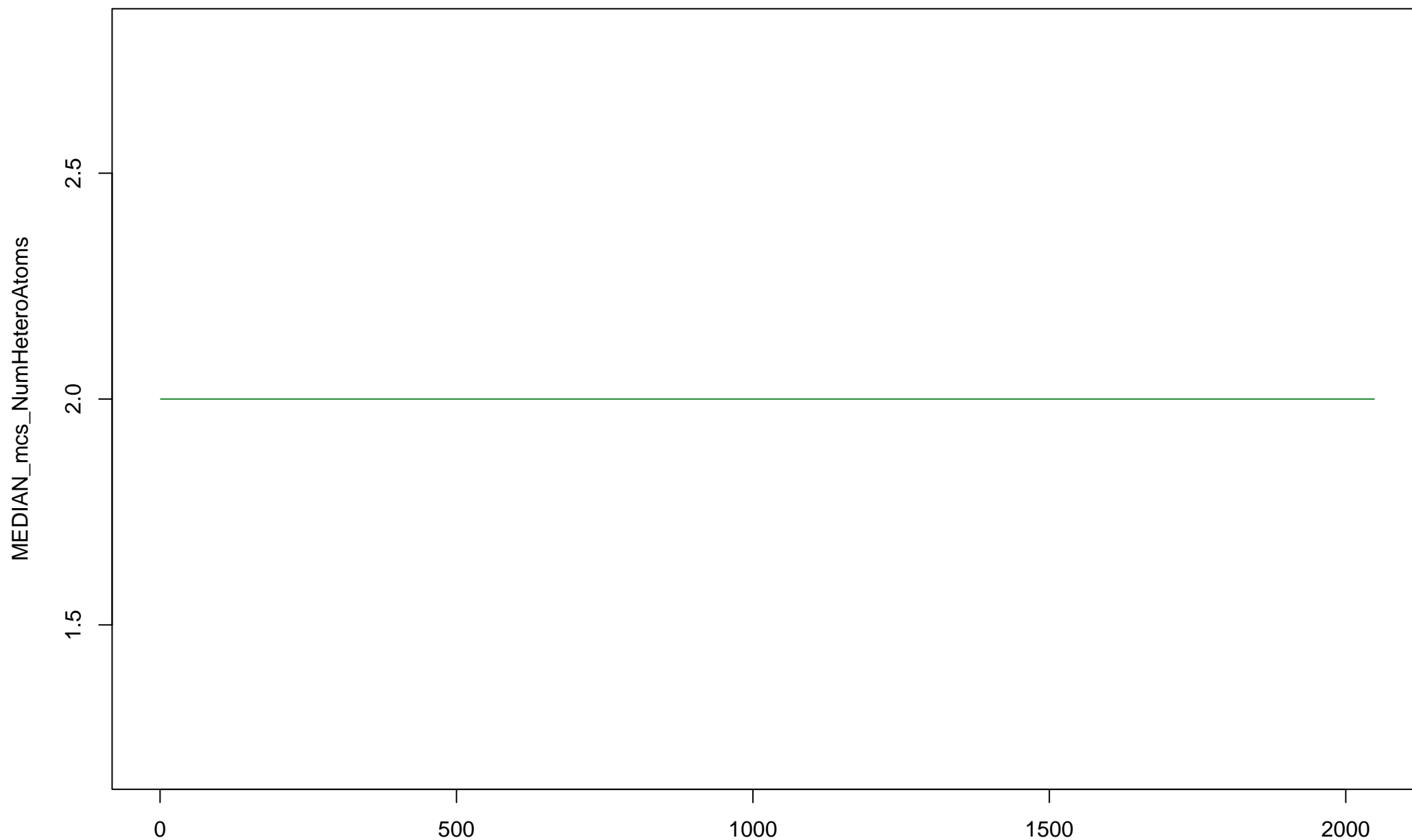
**MEDIAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



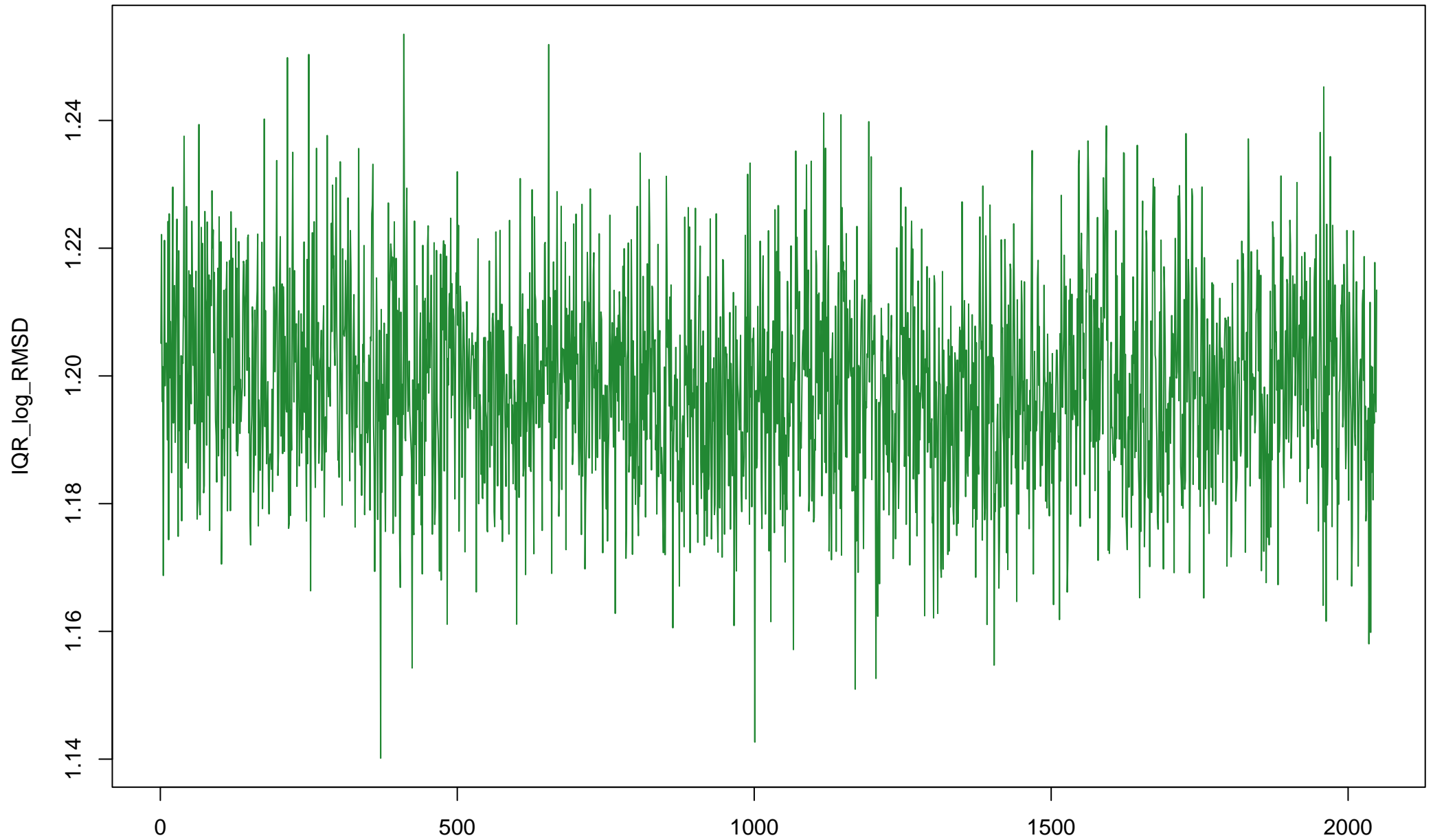
**MEDIAN\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



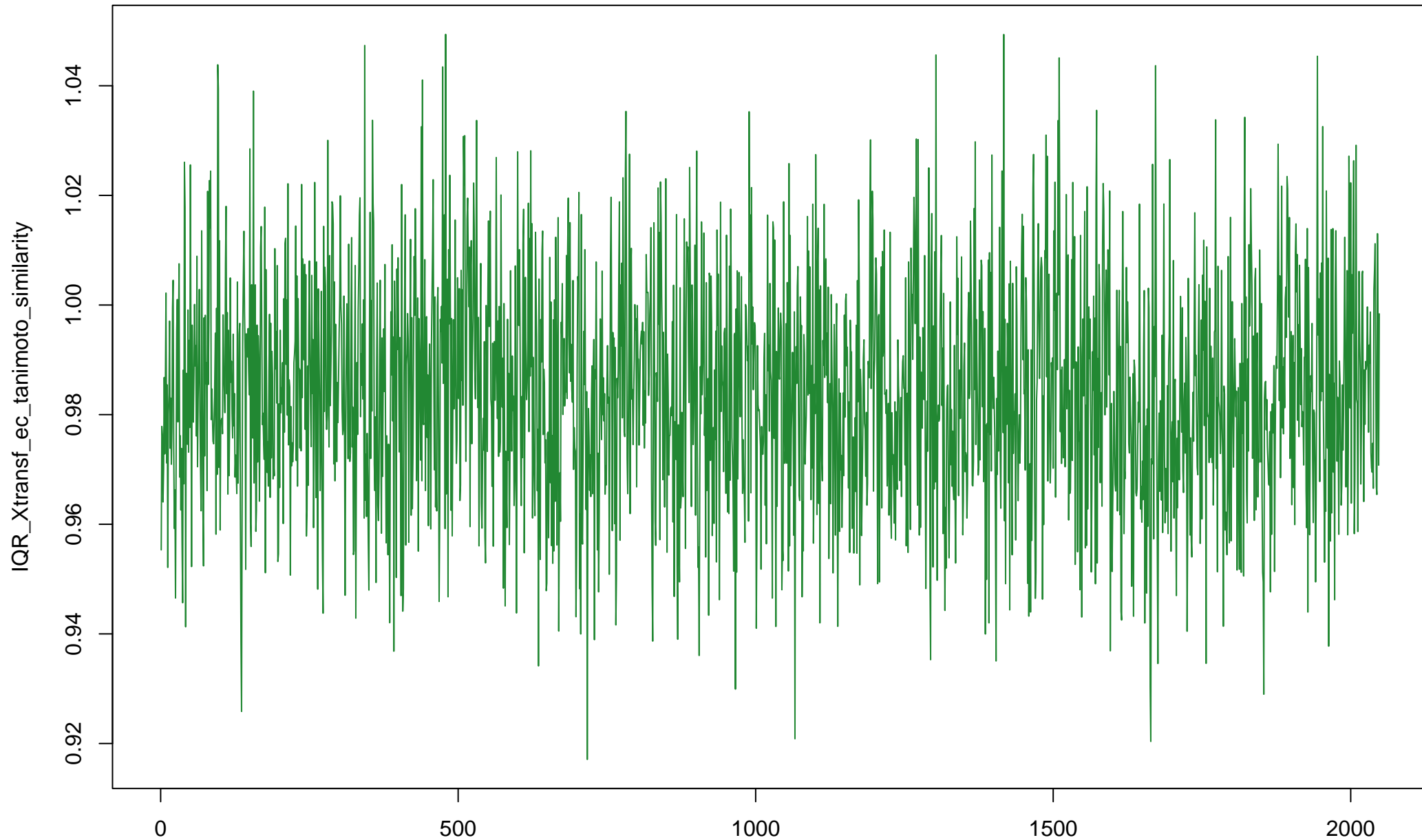
**MEDIAN\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**IQR\_log\_RMSD**  
**ESS = 1610 | BMK = 0.0632 | MCSE(6.27) = 2.91 | stat: FALSE | burn: 0**

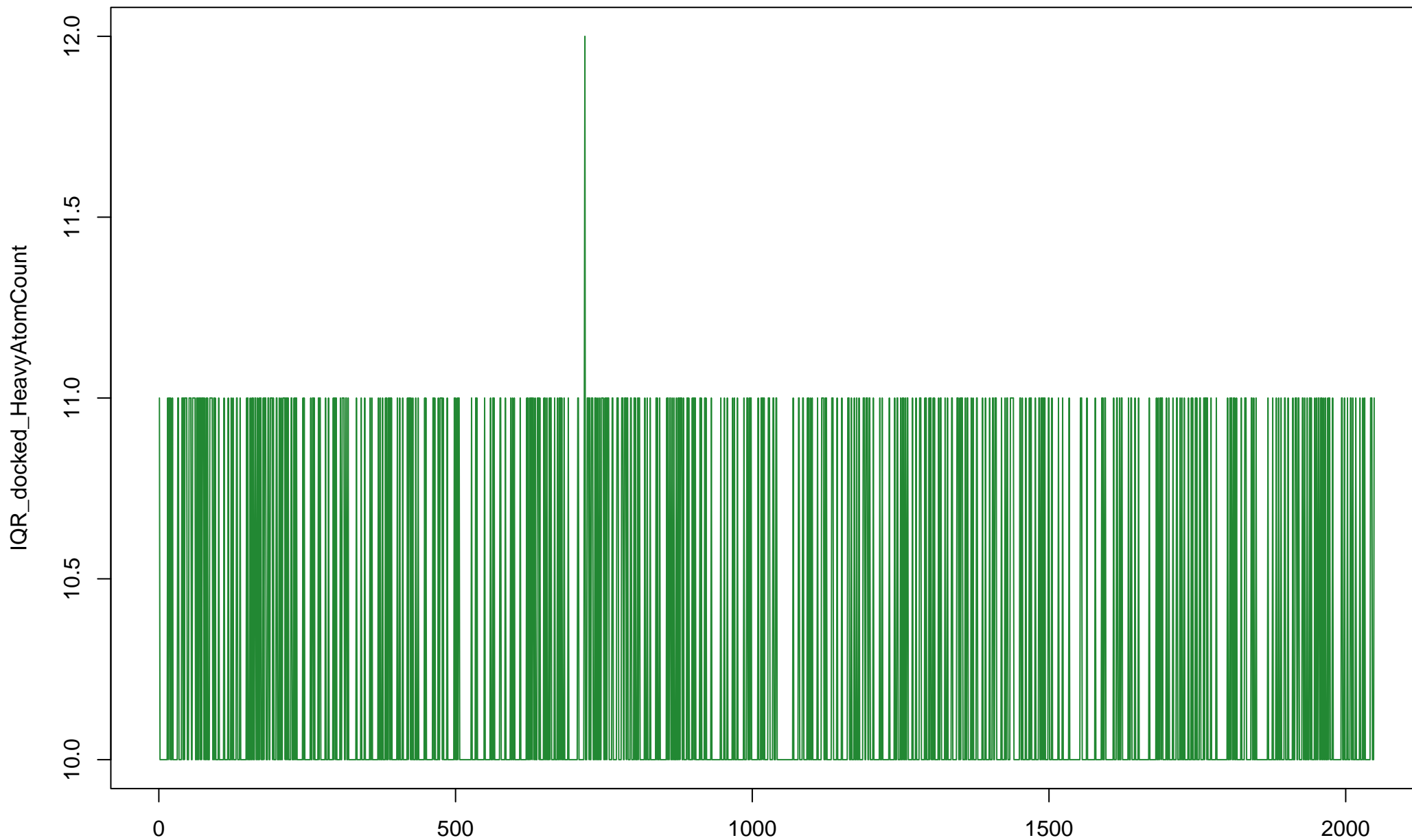


IQR\_Xtransf\_ec\_tanimoto\_similarity  
ESS = 1580 | BMK = 0.0379 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0

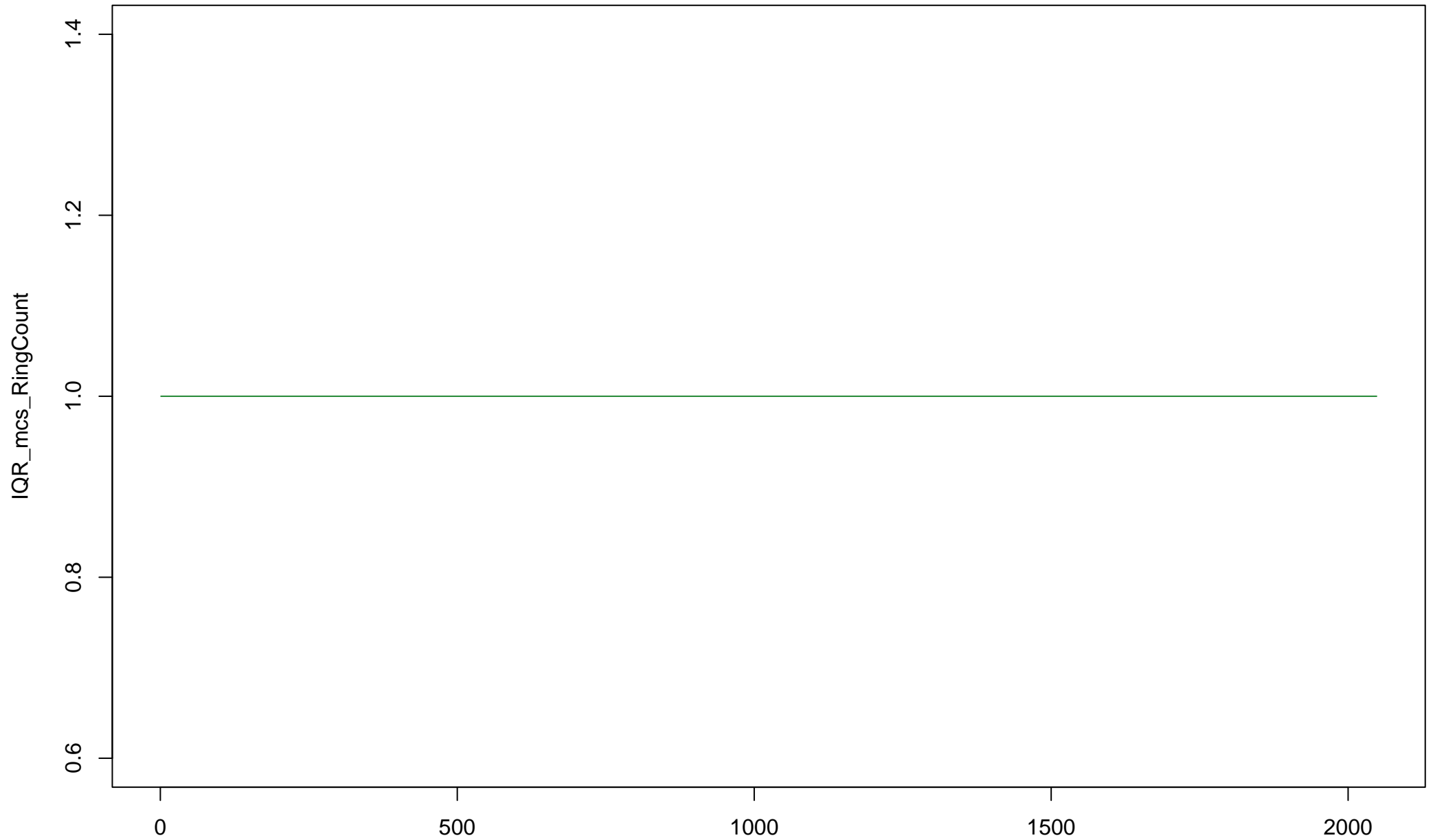




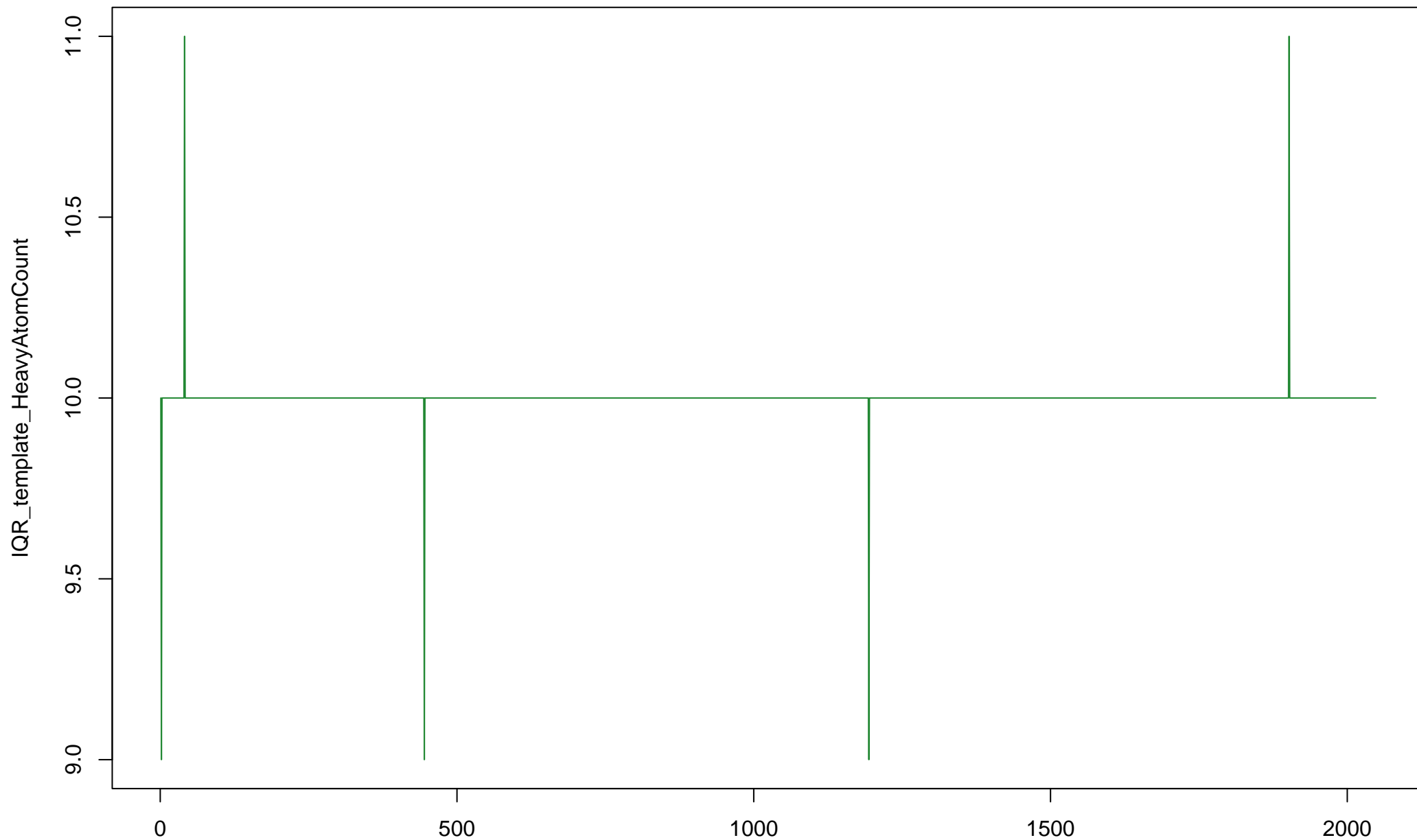
IQR\_docked\_HeavyAtomCount  
ESS = 1100 | BMK = 0.044 | MCSE(6.27) = 3.45 | stat: FALSE | burn: 0



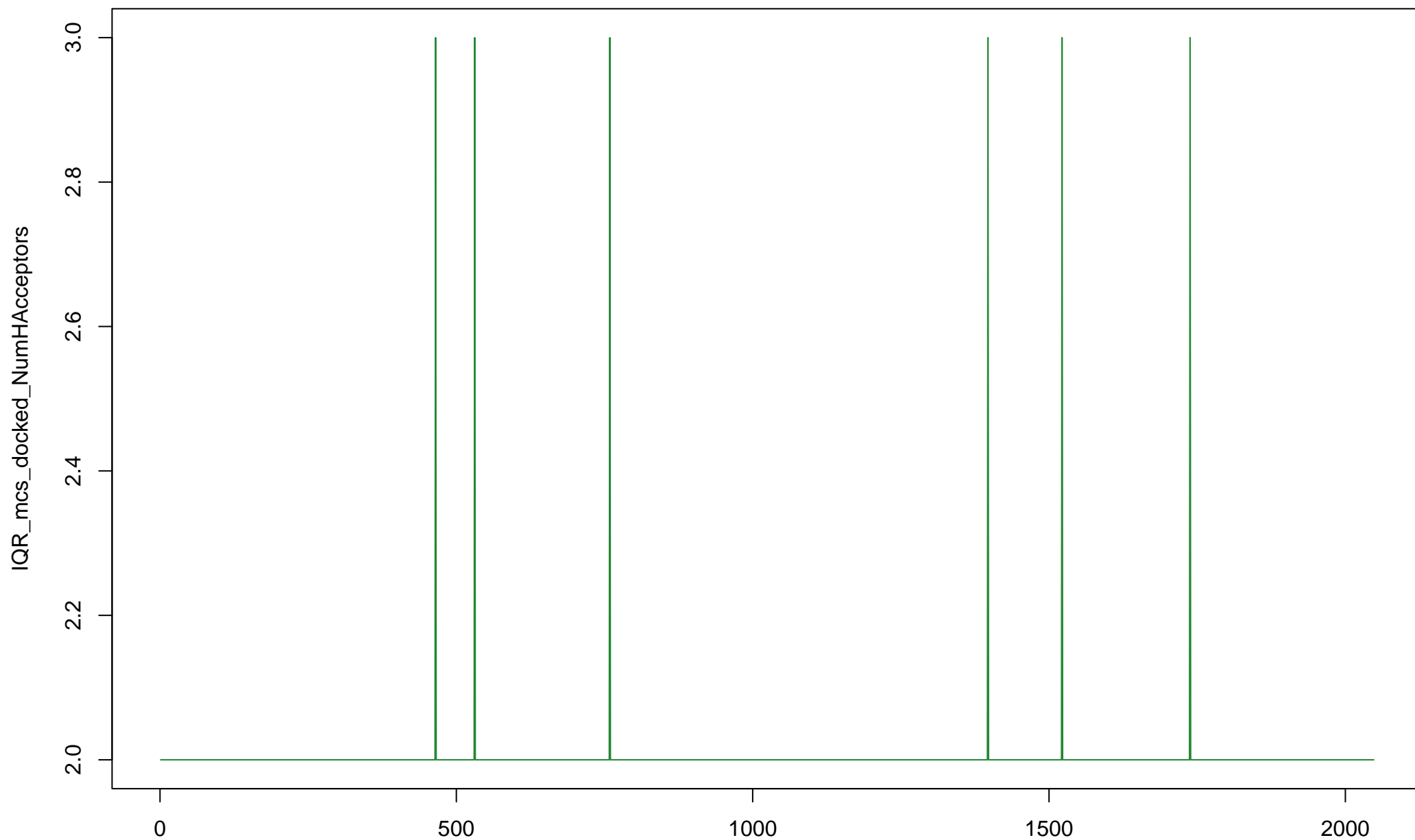
**IQR\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



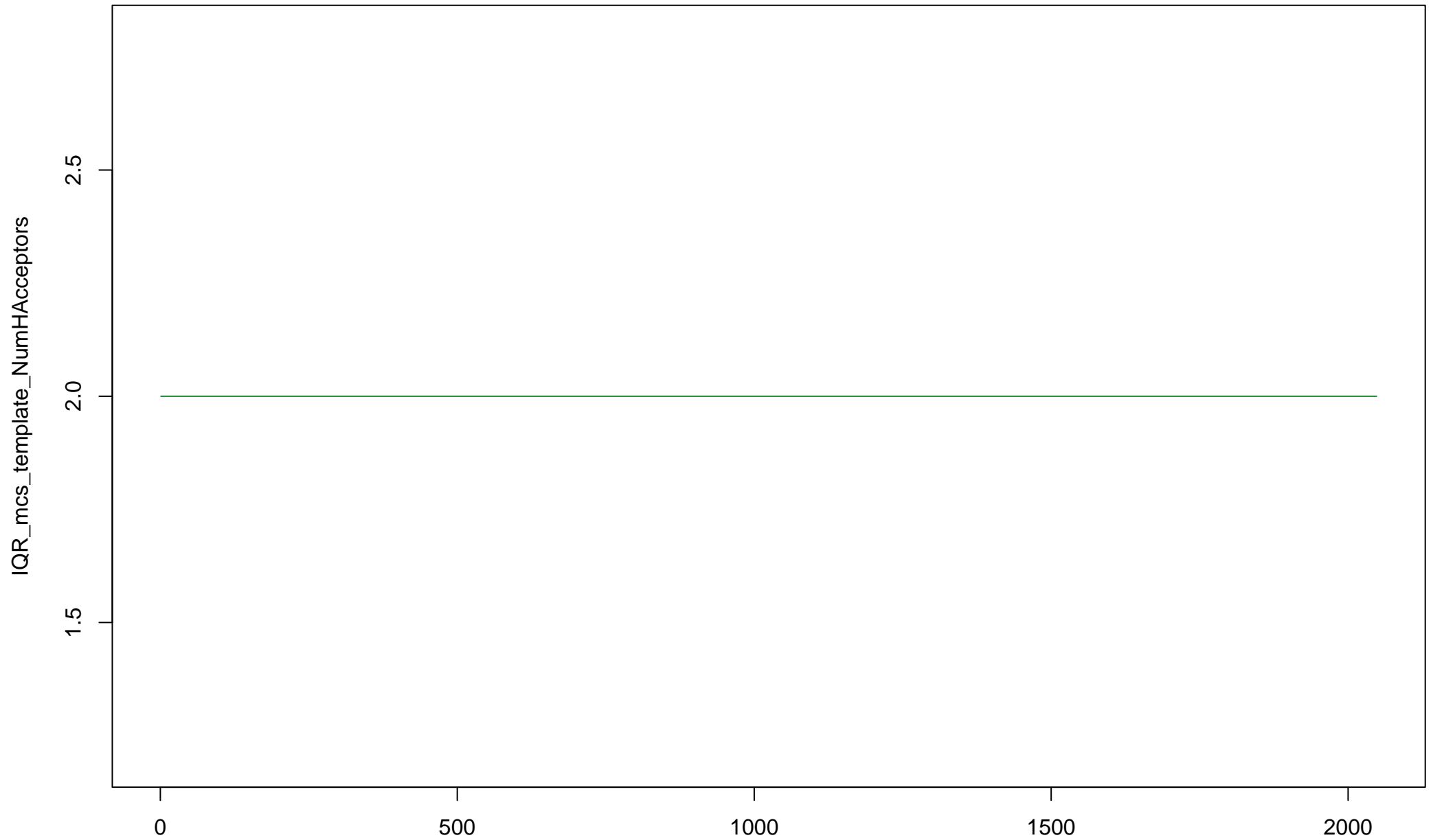
IQR\_template\_HeavyAtomCount  
ESS = 2050 | BMK = 0.0993 | MCSE(6.27) = 1.73 | stat: FALSE | burn: 2040



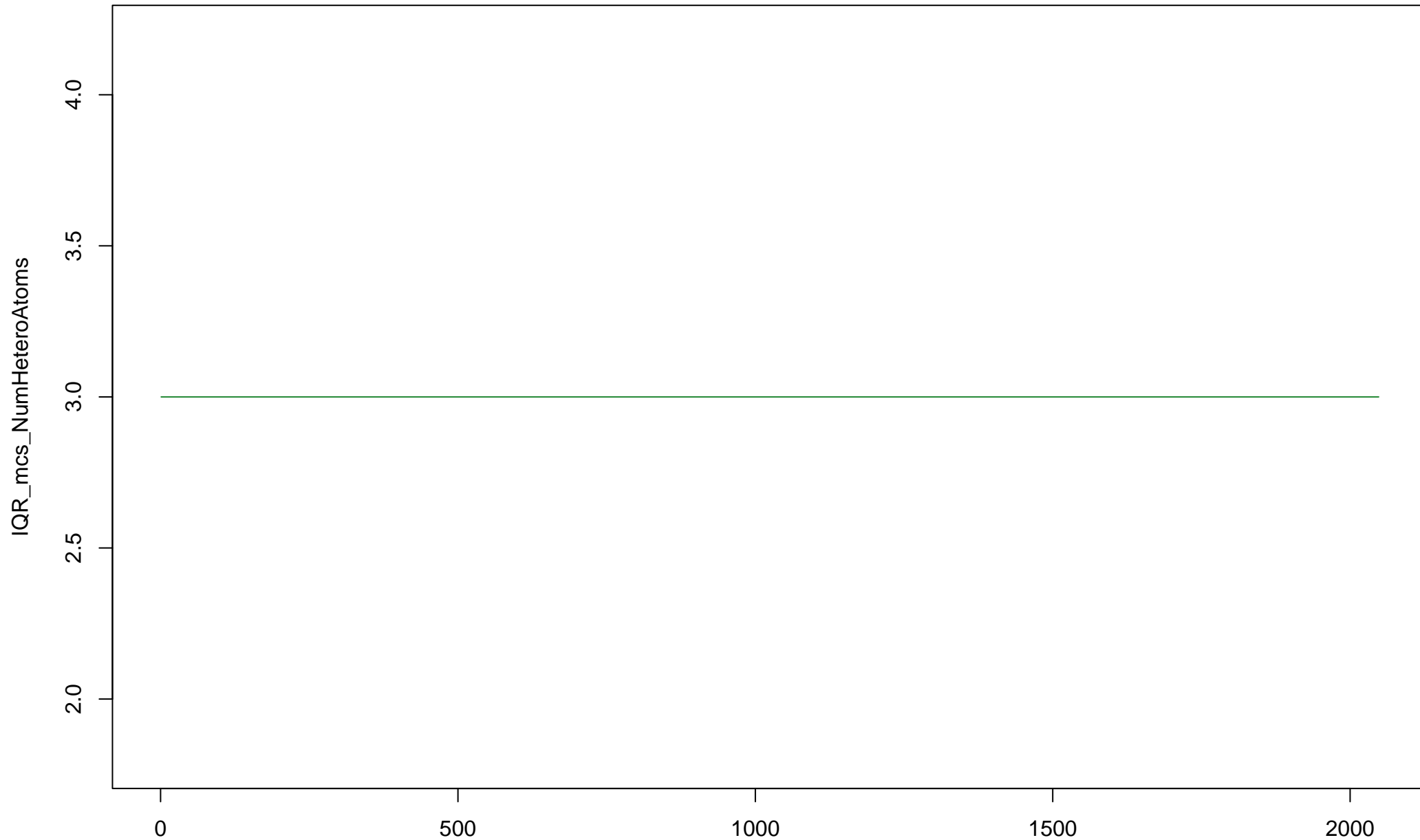
**IQR\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 2040**



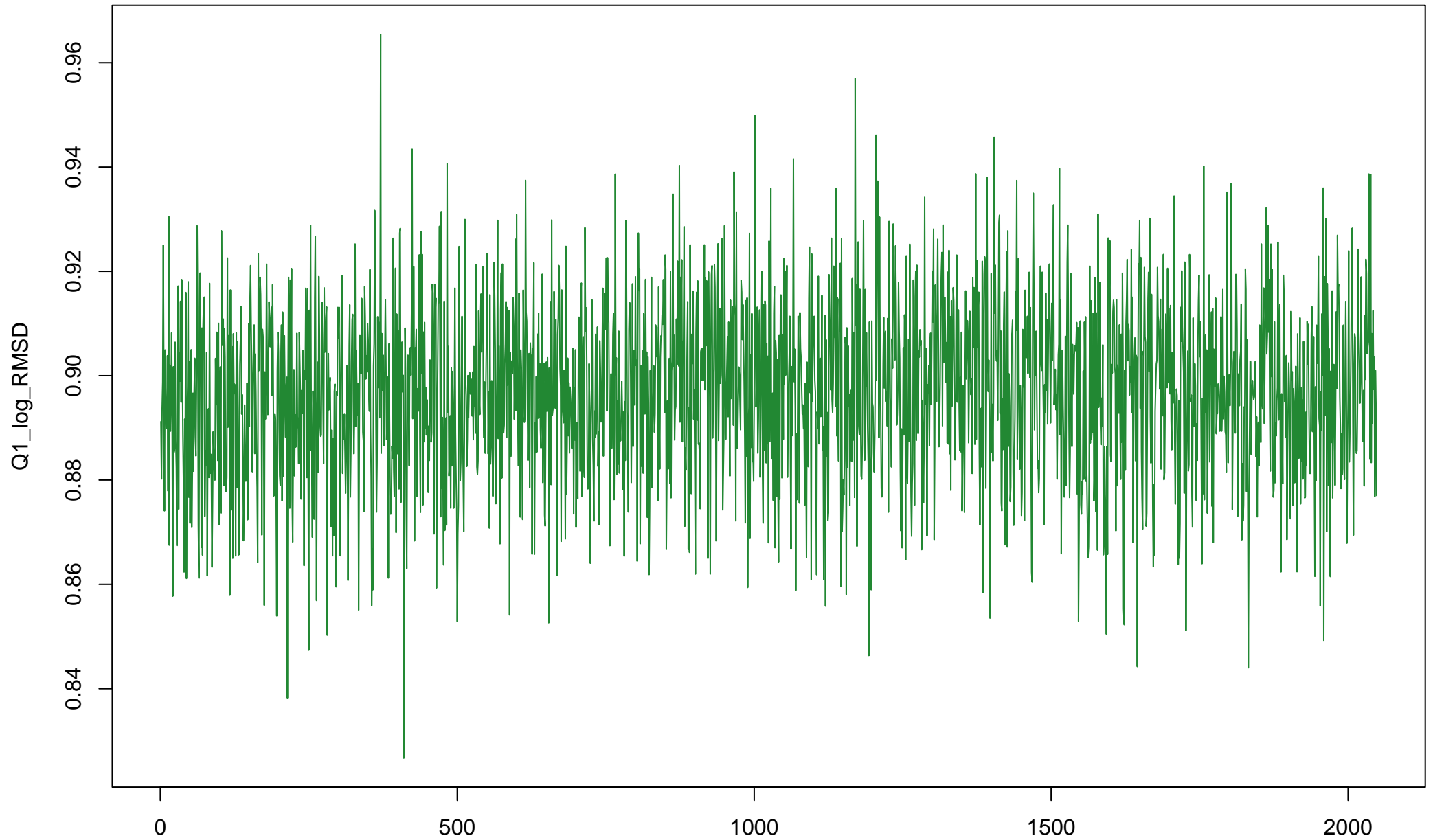
**IQR\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



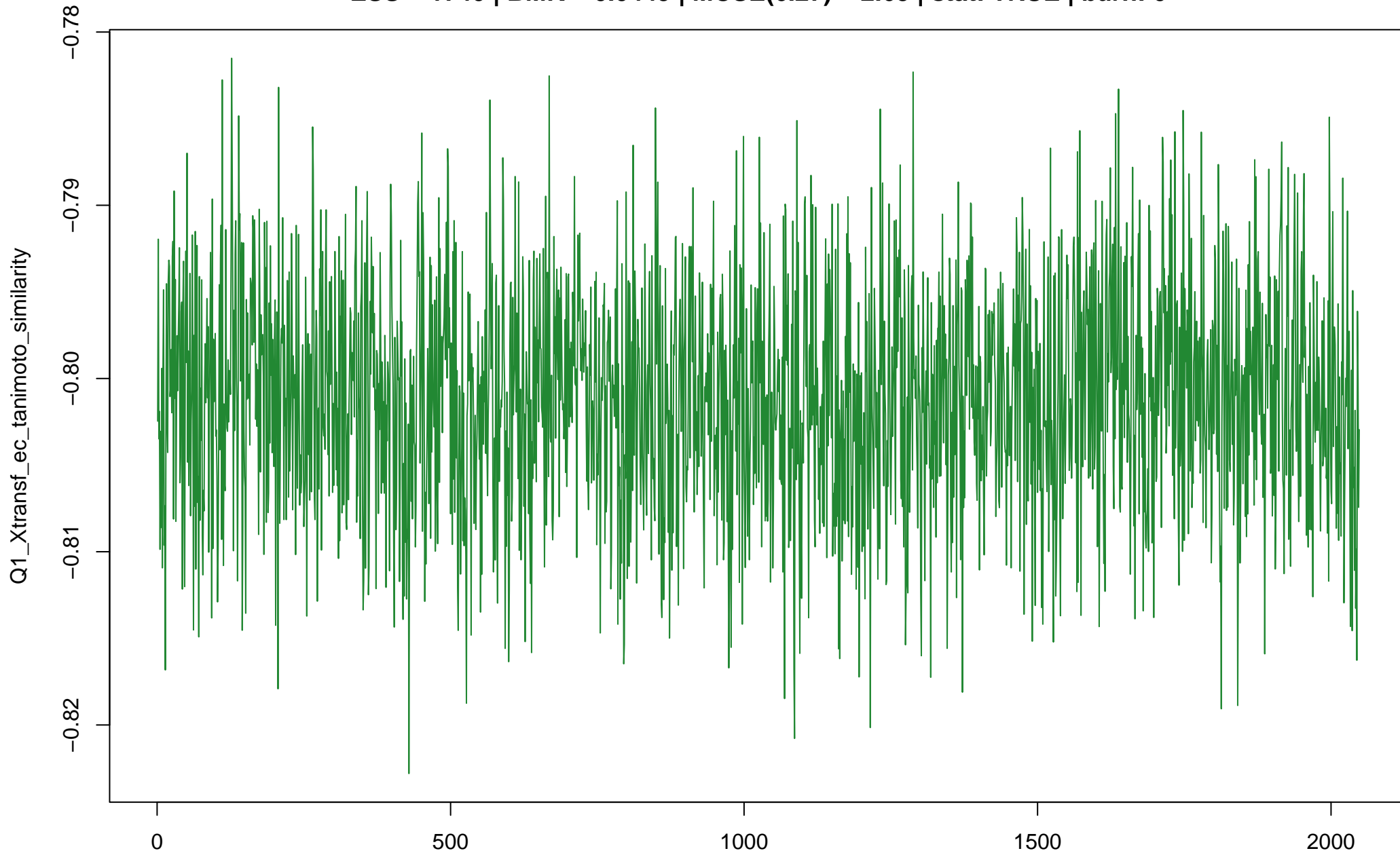
IQR\_mcs\_NumHeteroAtoms  
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



**Q1\_log\_RMSD**  
**ESS = 1840 | BMK = 0.0491 | MCSE(6.27) = 2.47 | stat: FALSE | burn: 0**

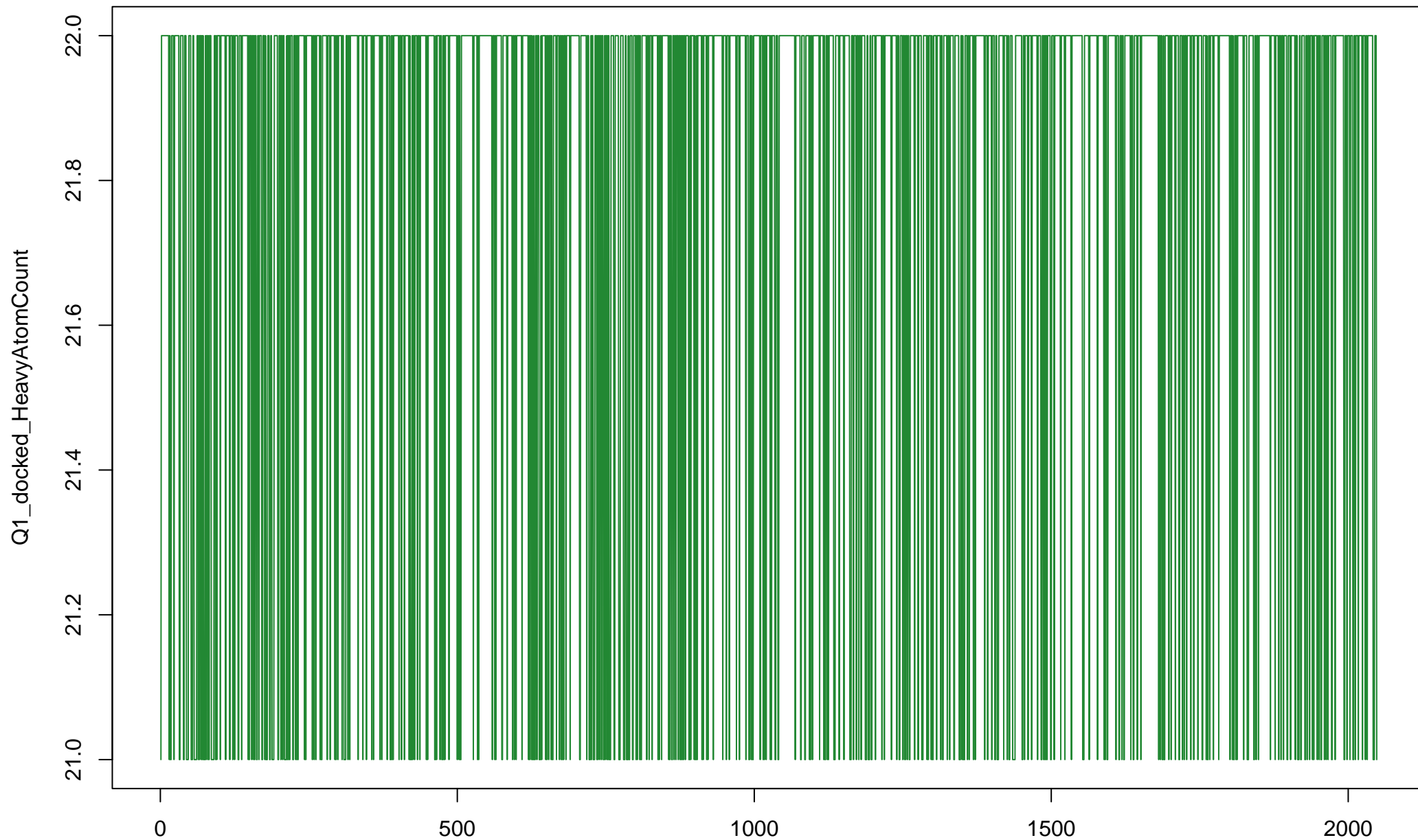


**Q1\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1740 | BMK = 0.0449 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0**





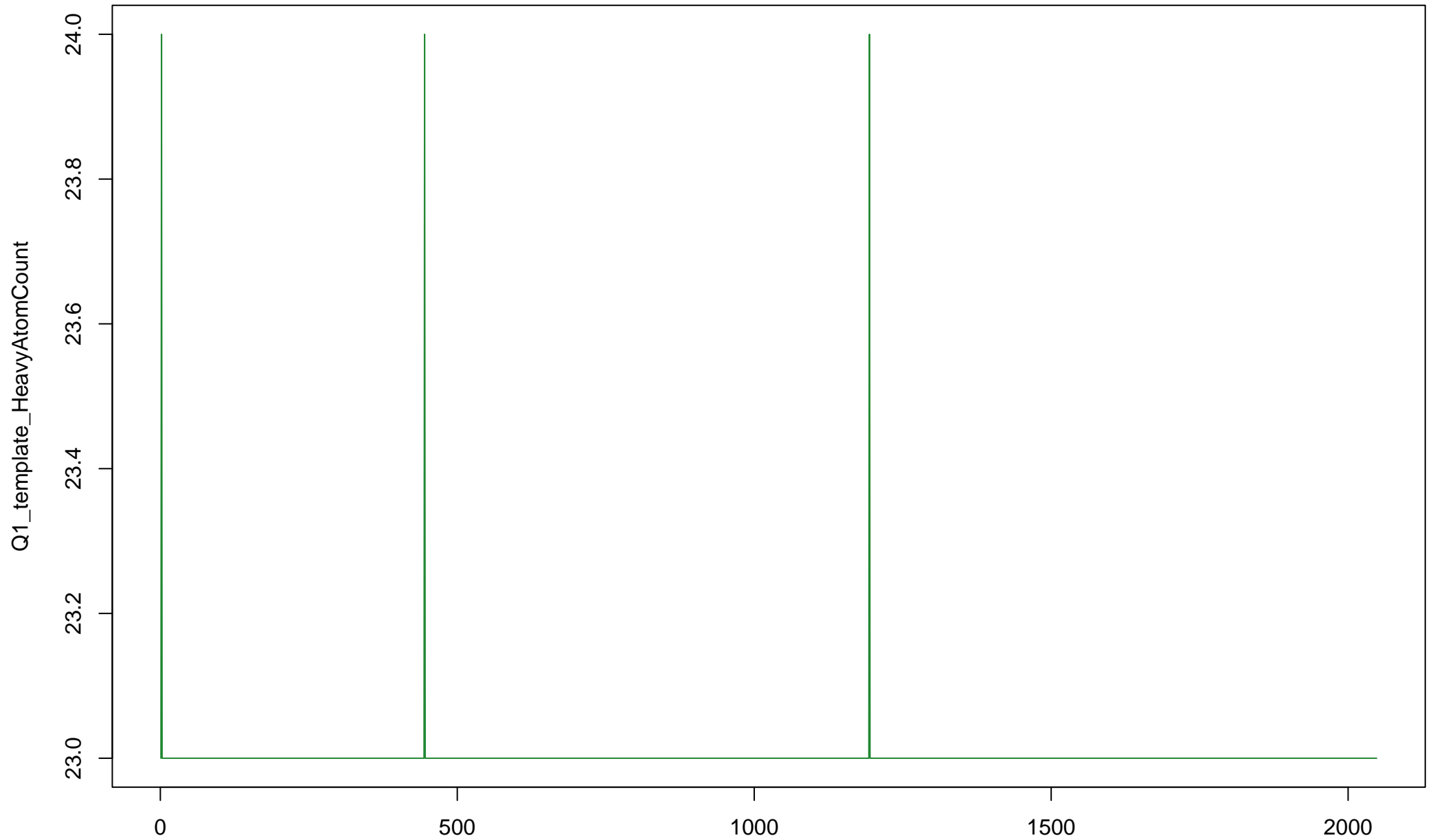
**Q1\_docked\_HeavyAtomCount**  
**ESS = 1300 | BMK = 0.0336 | MCSE(6.27) = 3.36 | stat: FALSE | burn: 0**



**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: 1224**



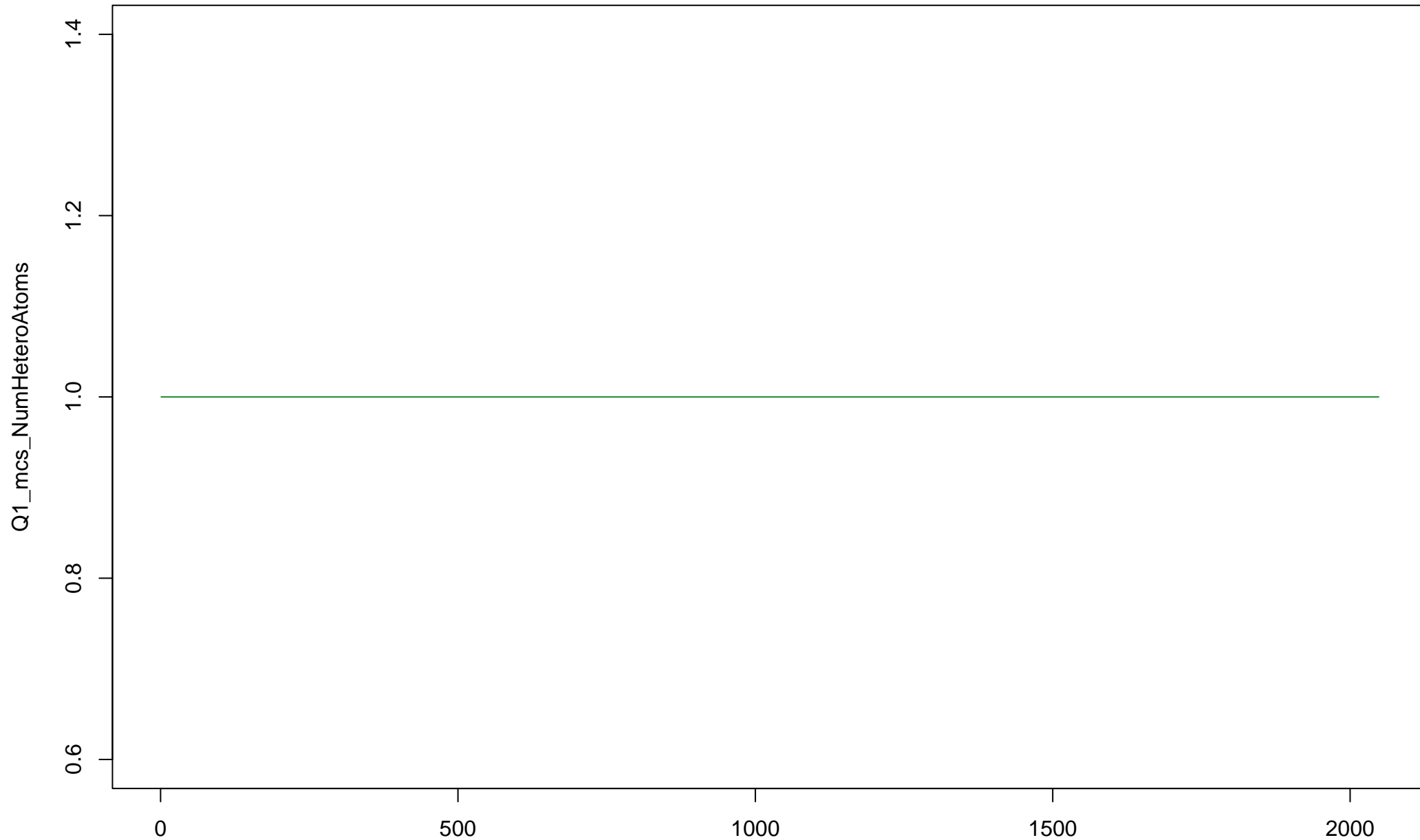
**Q1\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



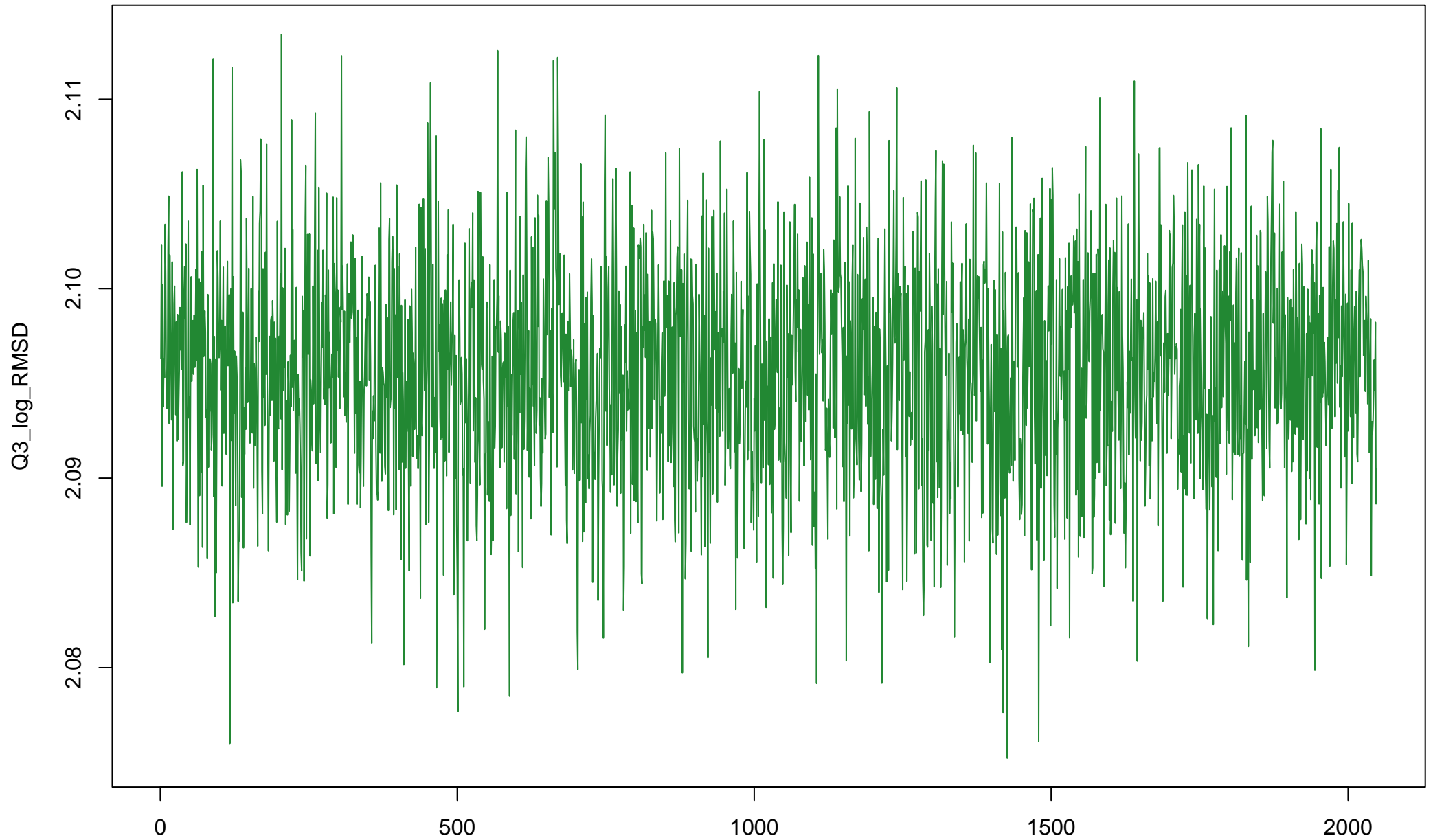
**Q1\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



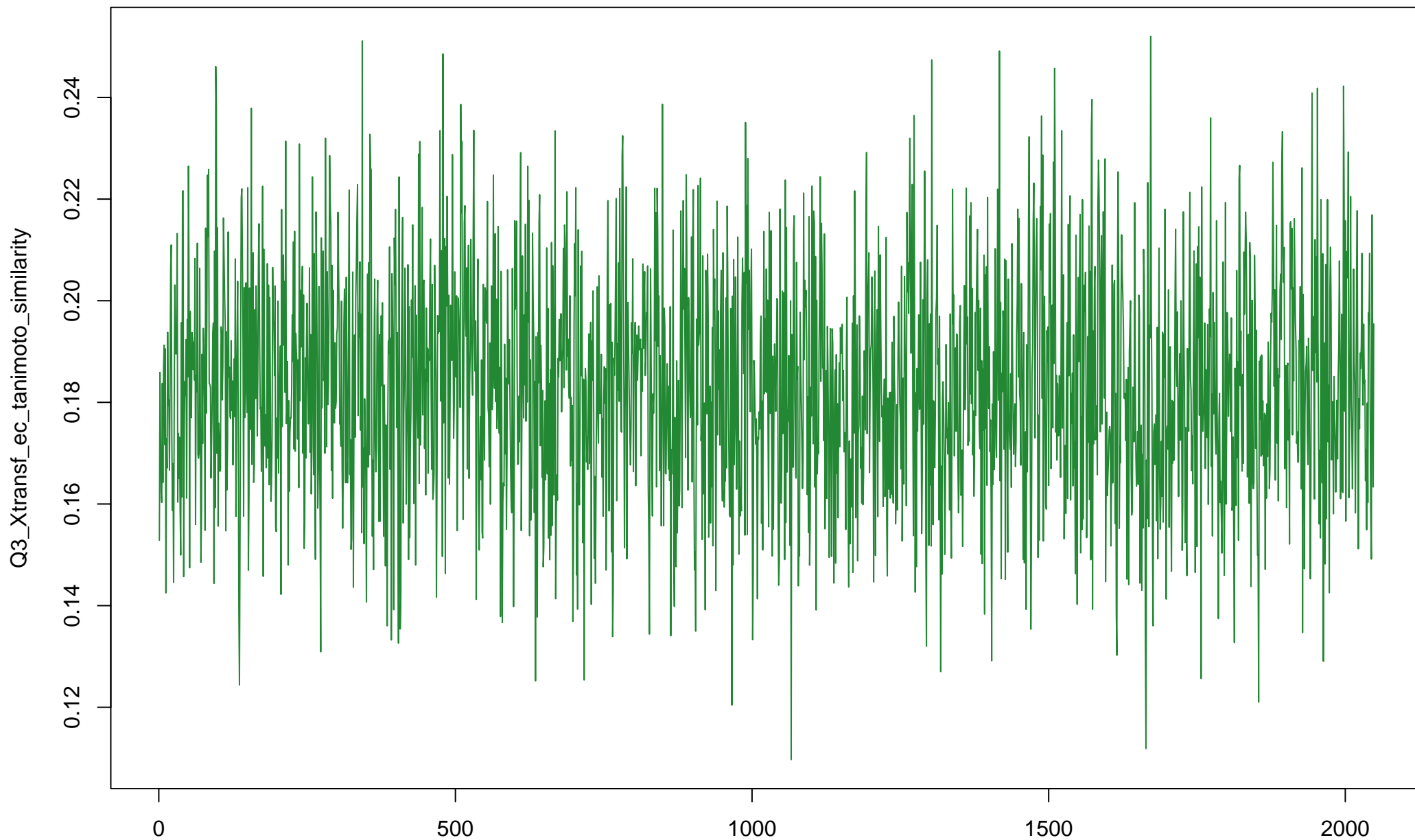
**Q1\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q3\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0387 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0**

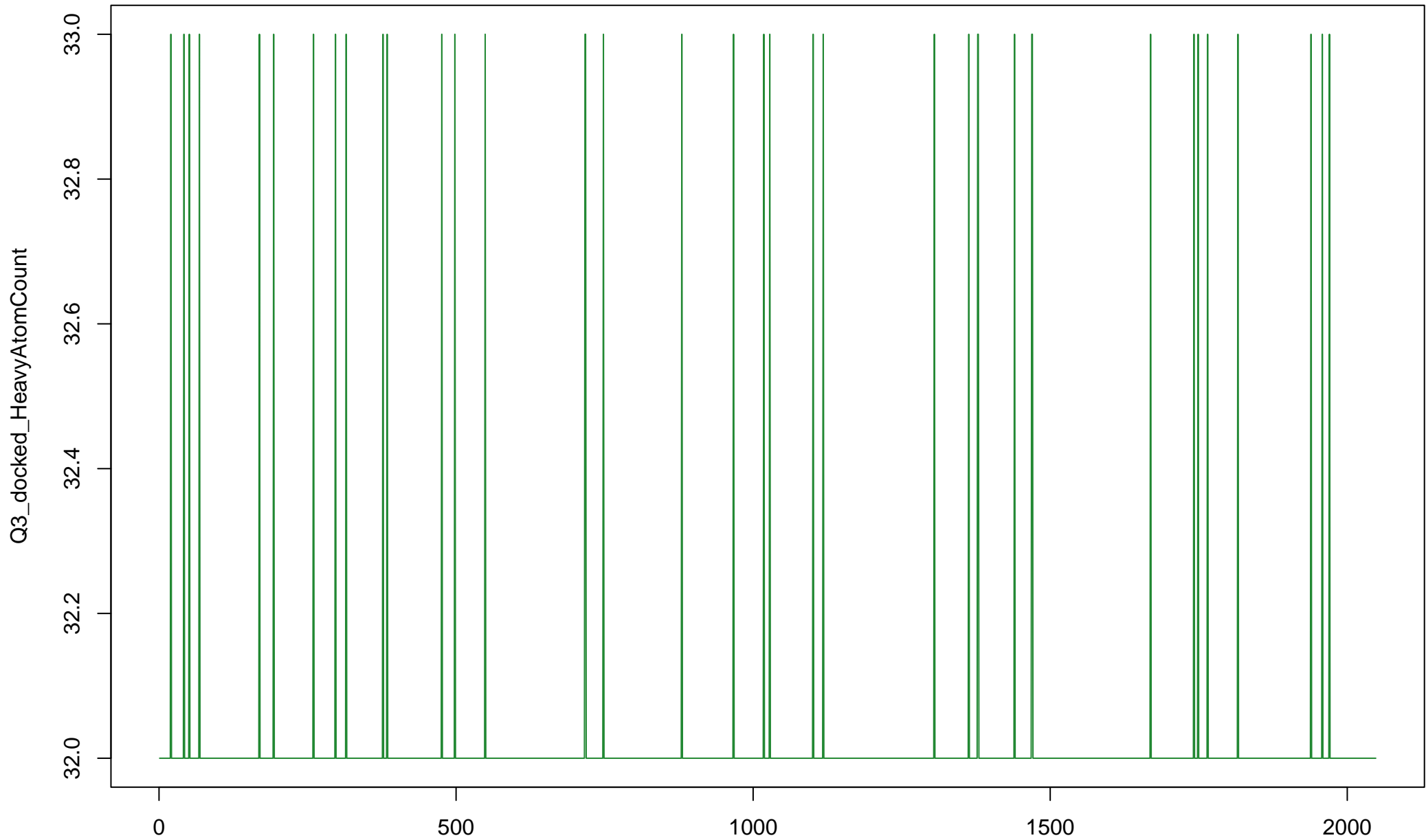


**Q3\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1620 | BMK = 0.0432 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0**





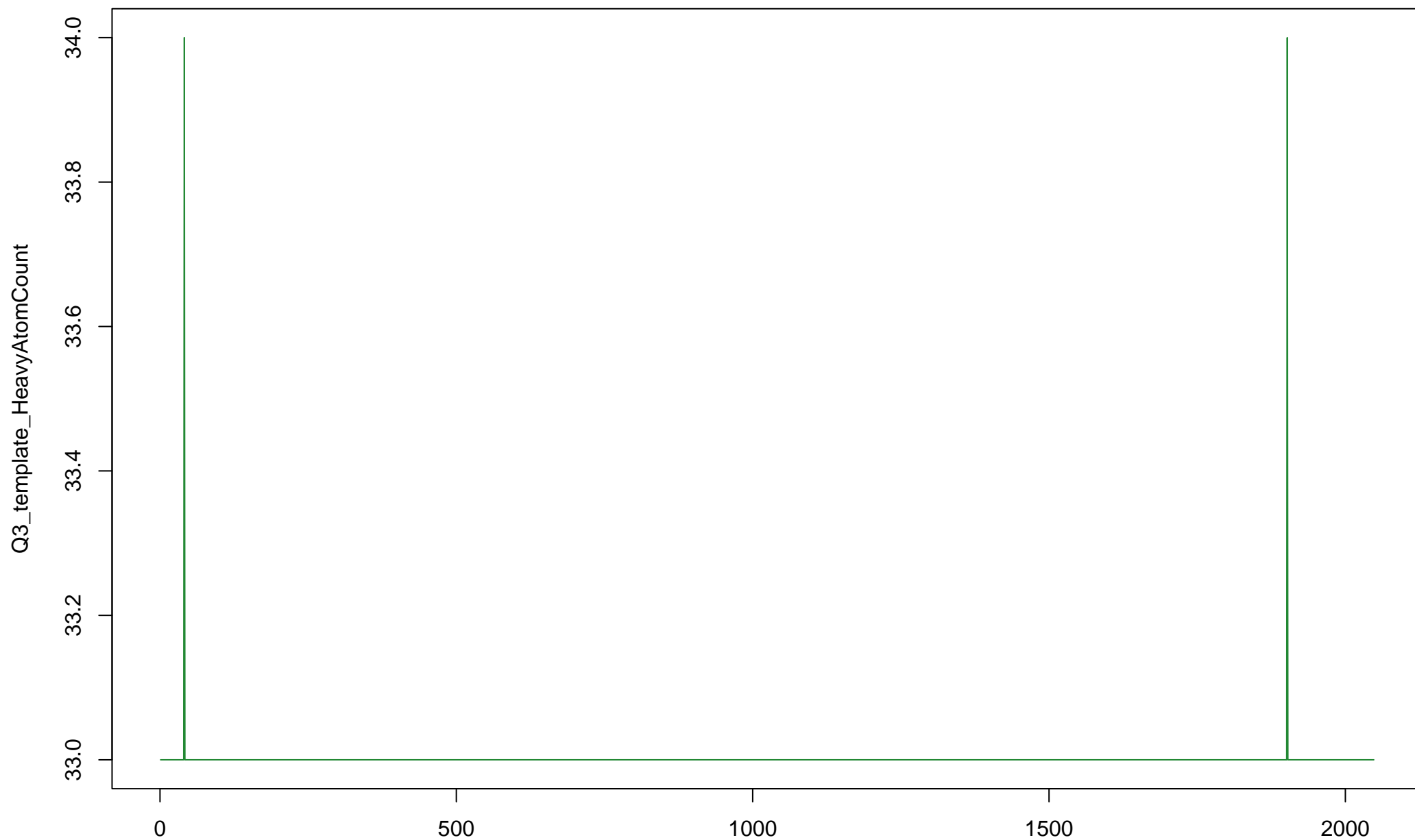
**Q3\_docked\_HeavyAtomCount**  
**ESS = 1810 | BMK = 0.0187 | MCSE(6.27) = 2.2 | stat: FALSE | burn: 0**



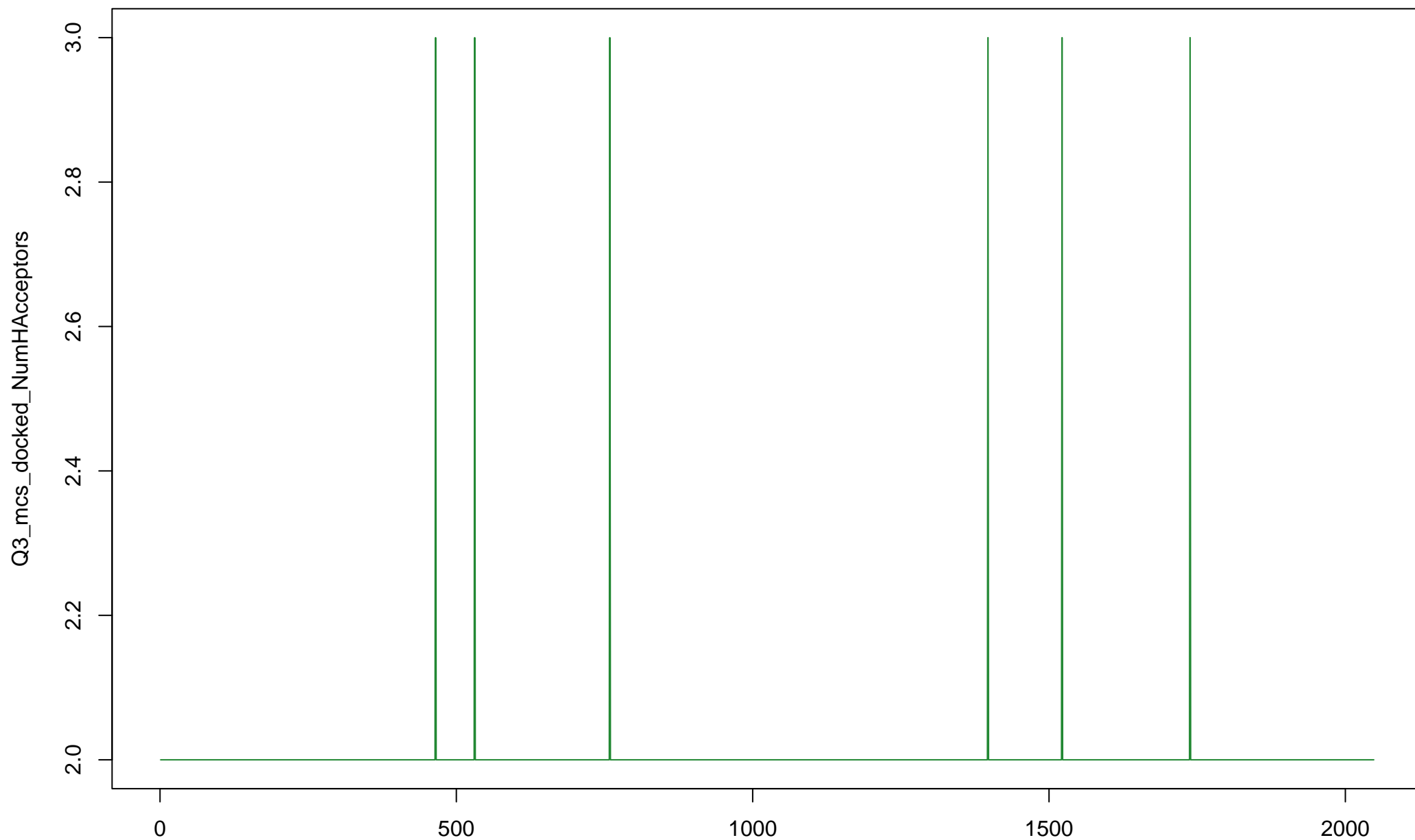
**Q3\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



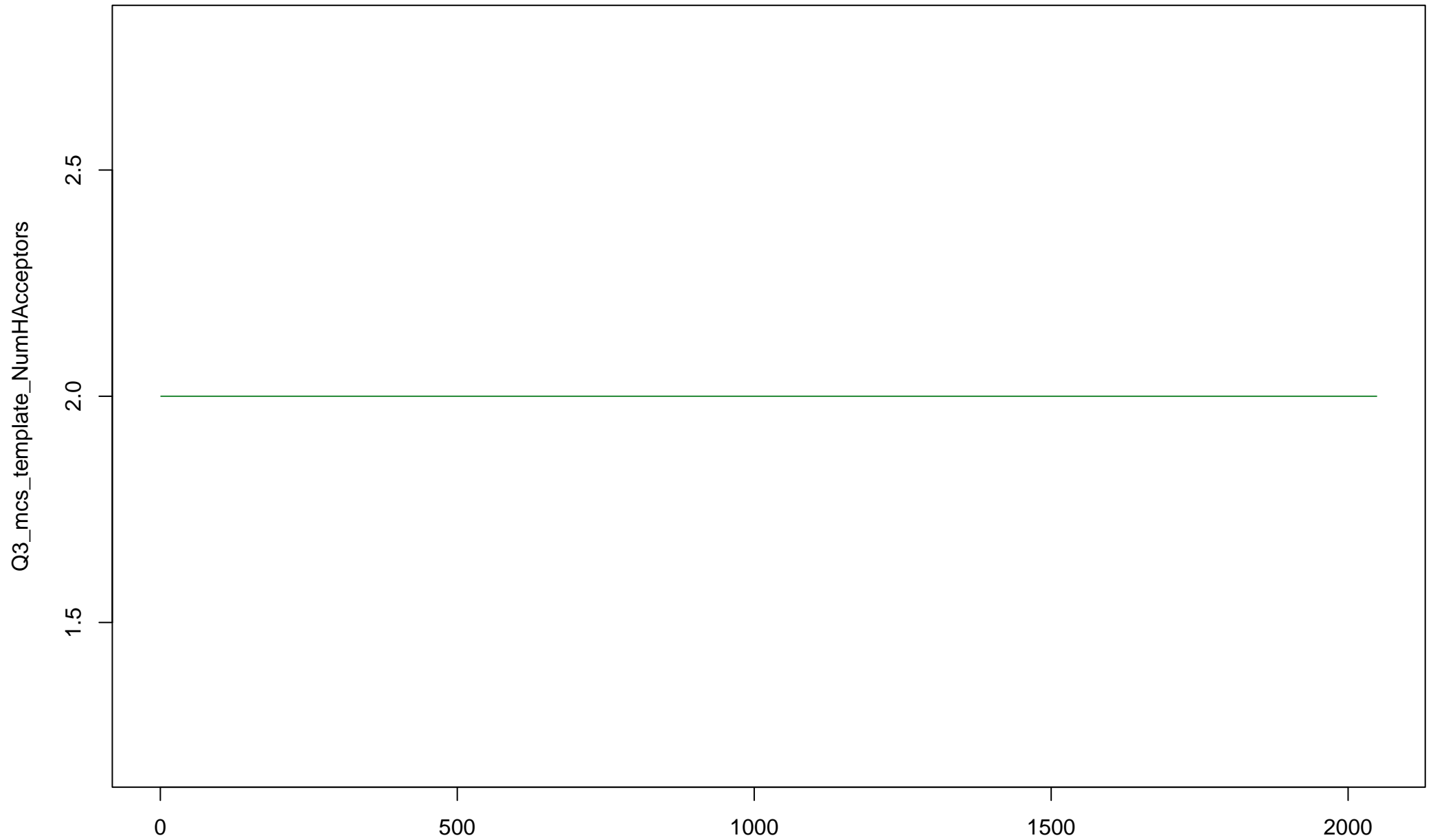
**Q3\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 2040**



**Q3\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 2040**



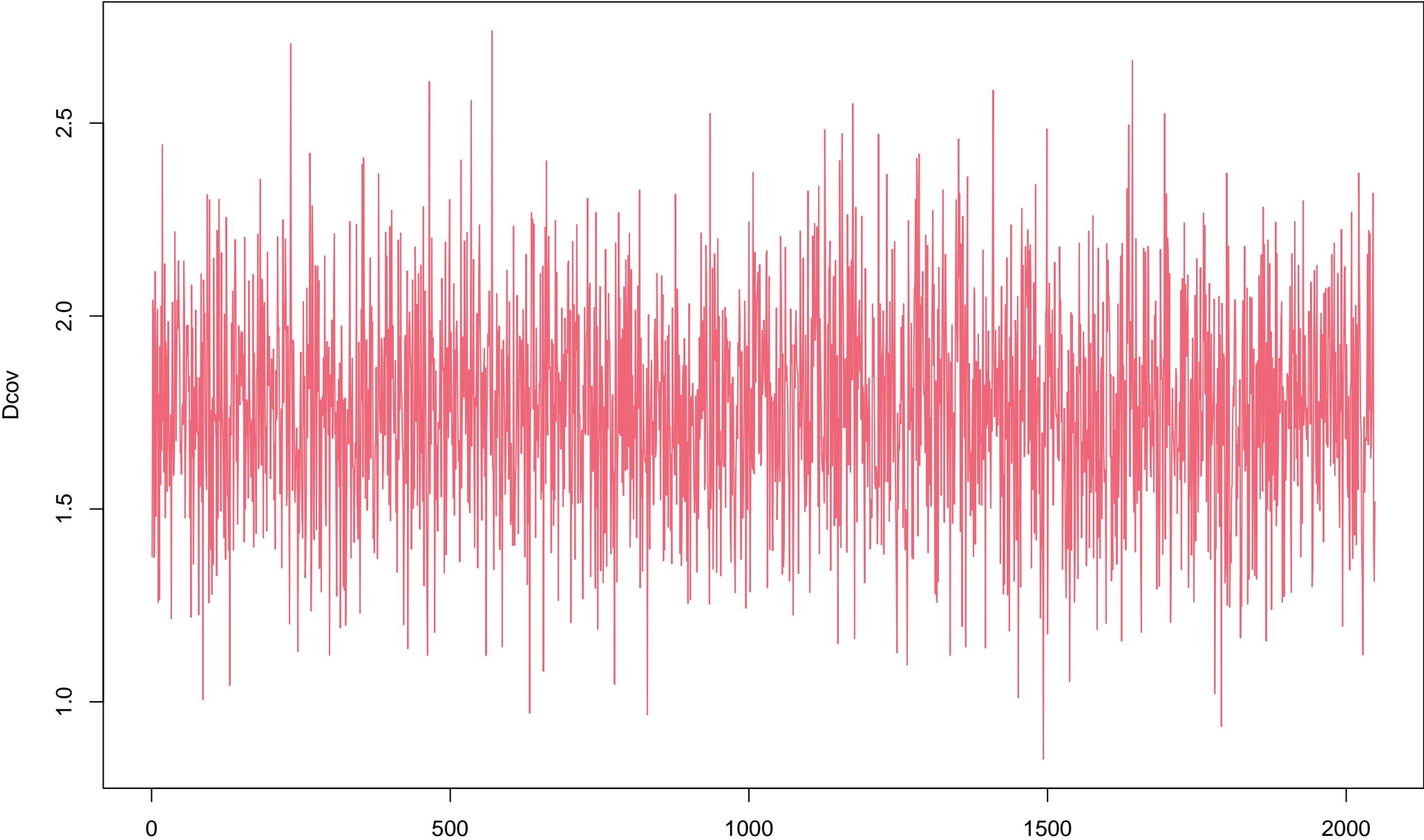
**Q3\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



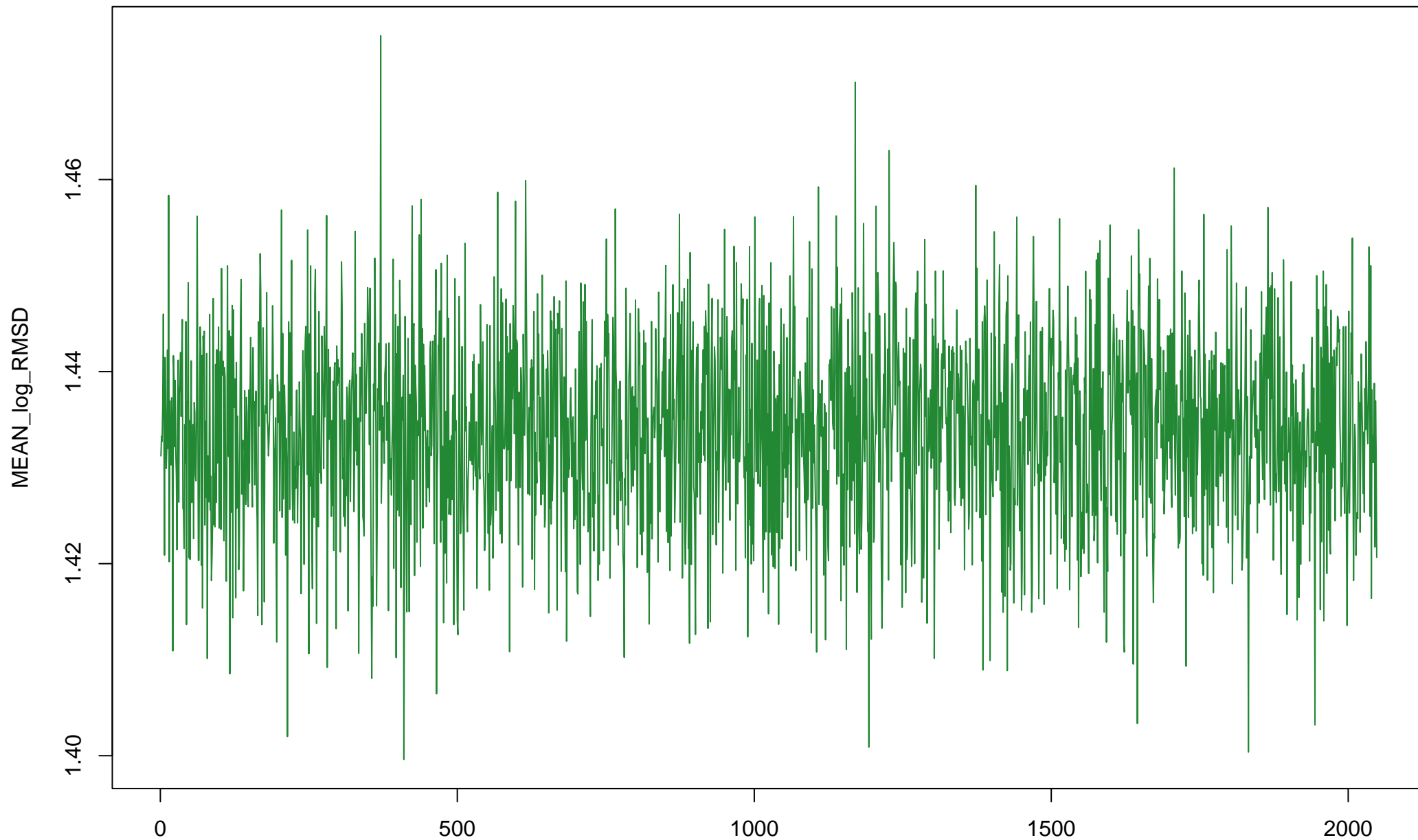
**Q3\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Dcov**  
**ESS = 2050 | BMK = 0.0499 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0**

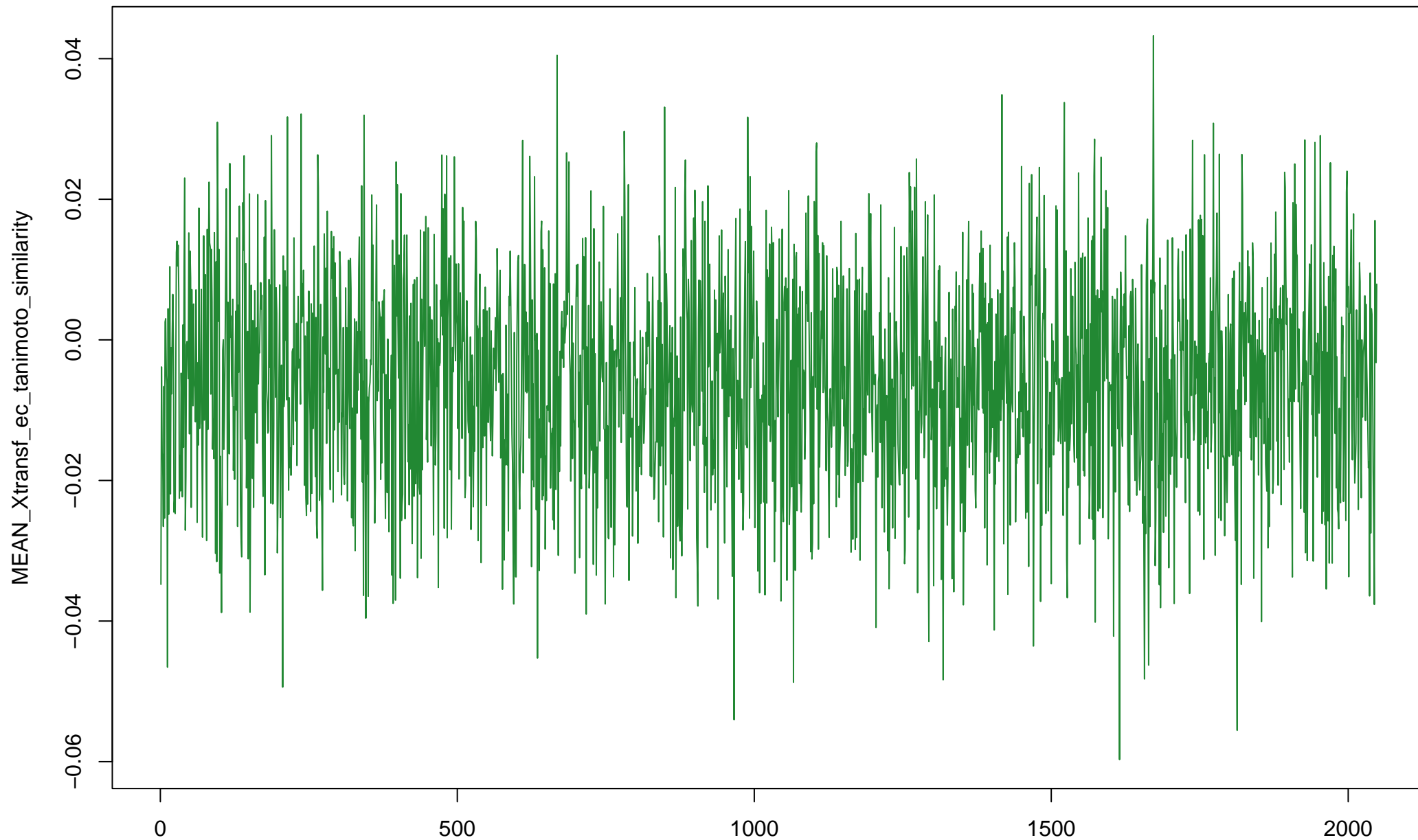


**MEAN\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0361 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0**

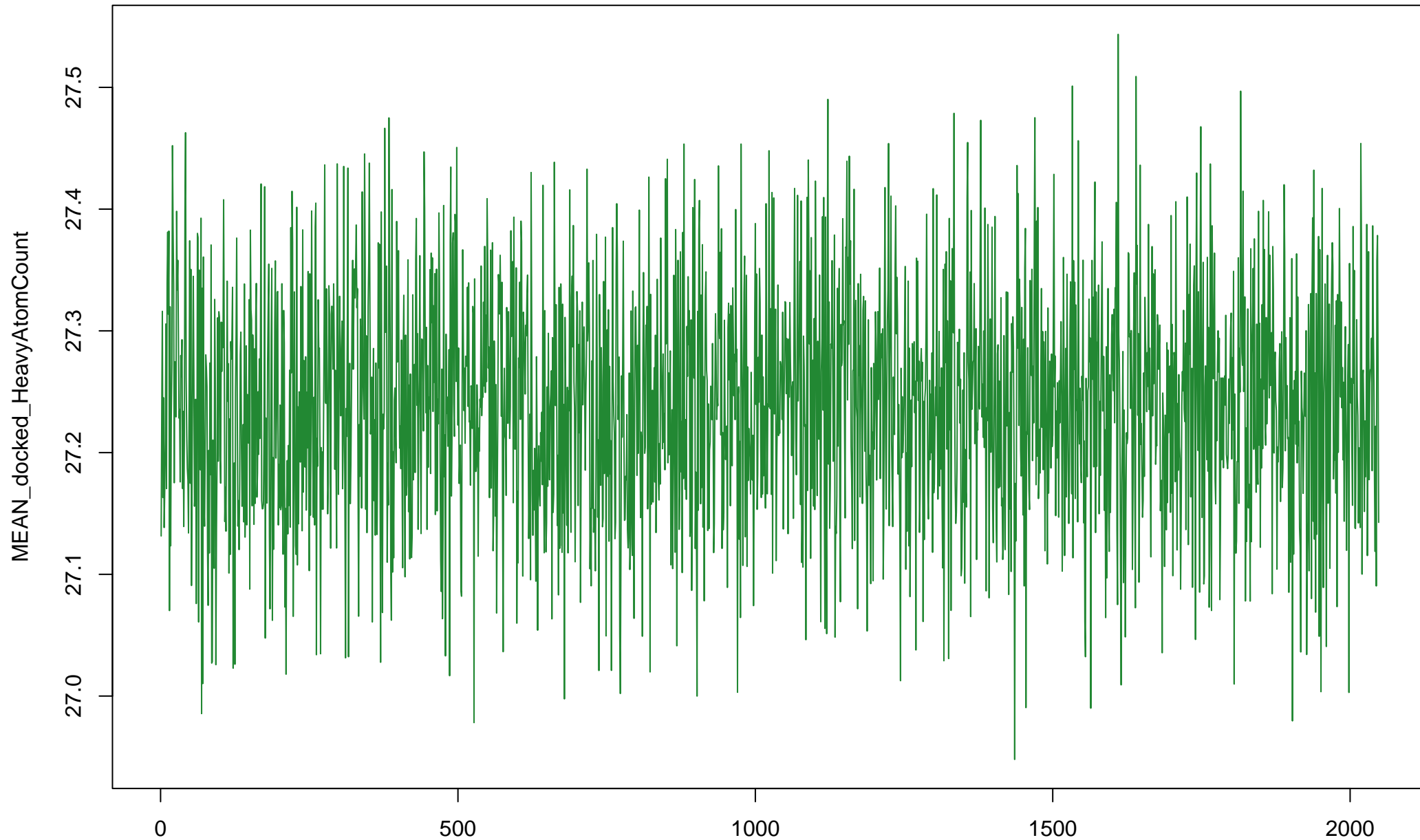




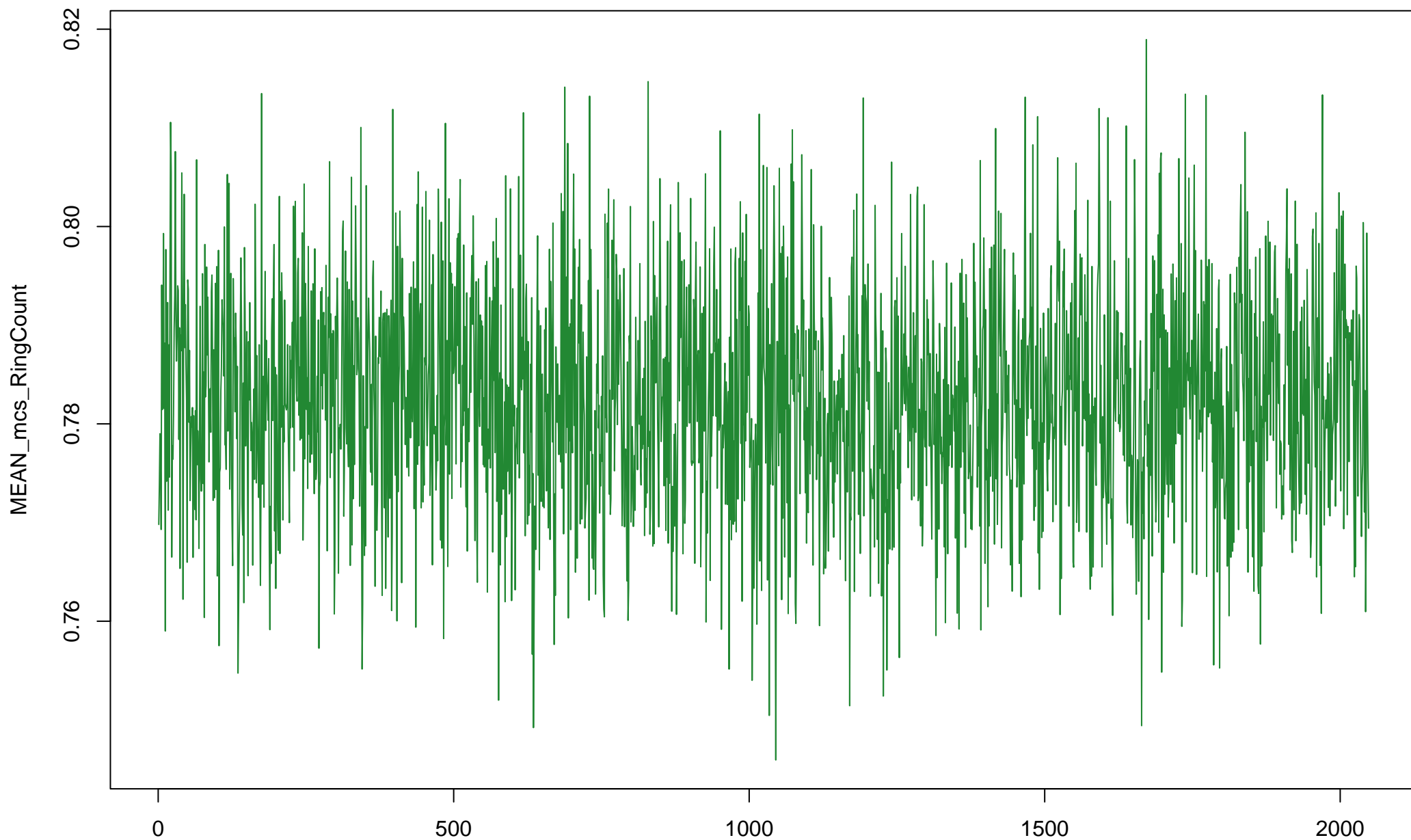
**MEAN\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0278 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0**



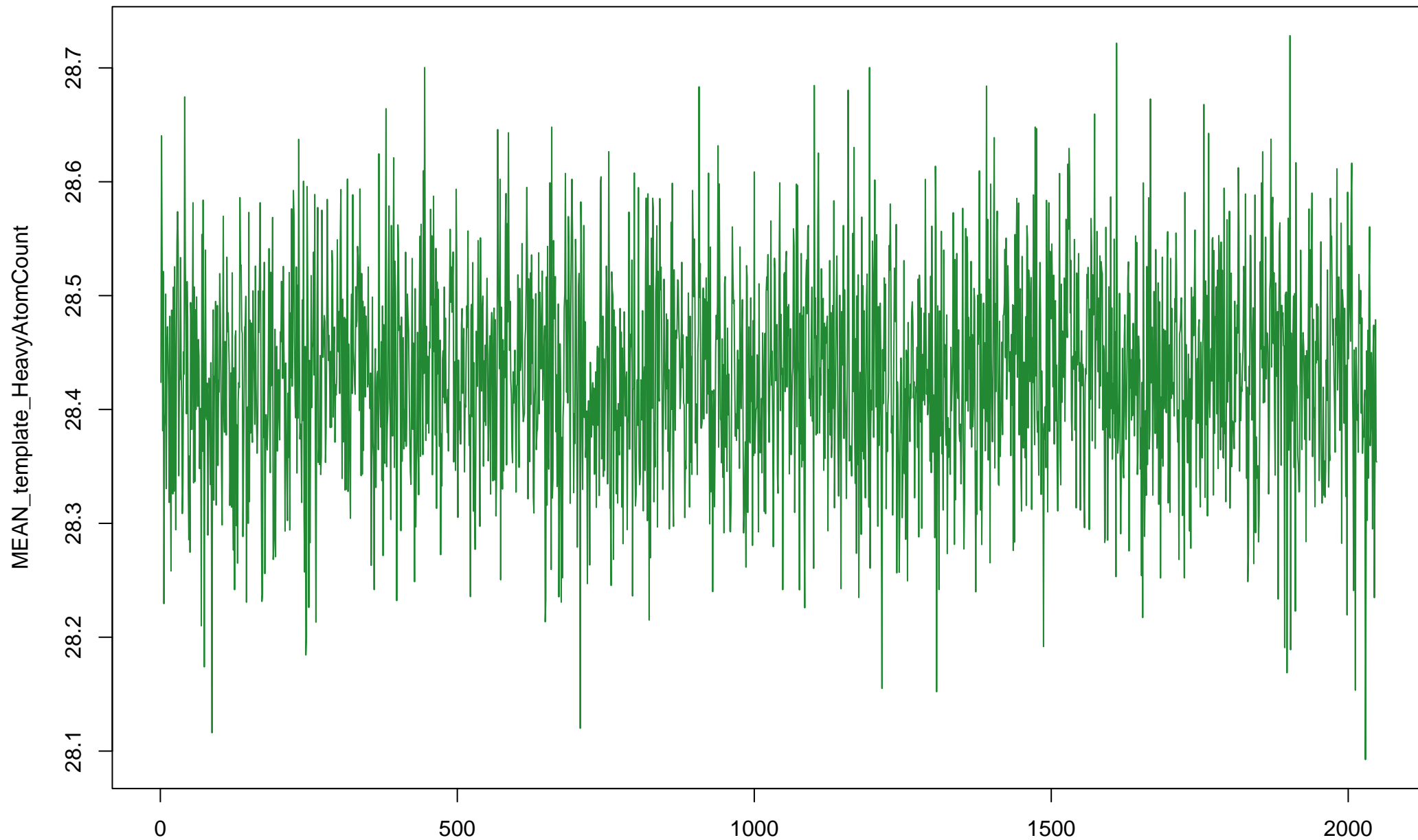
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0544 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0**



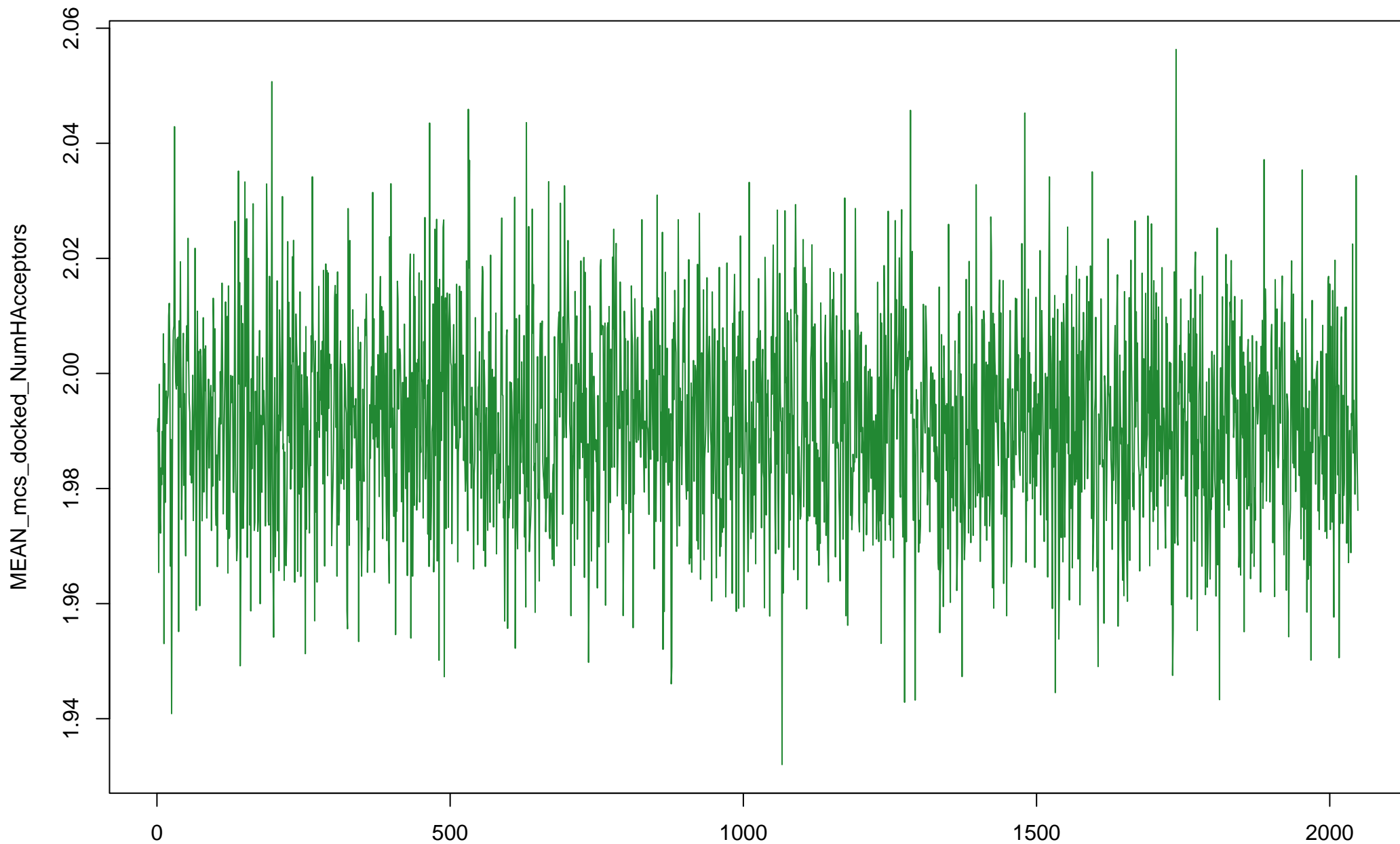
**MEAN\_mcs\_RingCount**  
**ESS = 1920 | BMK = 0.0367 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0**



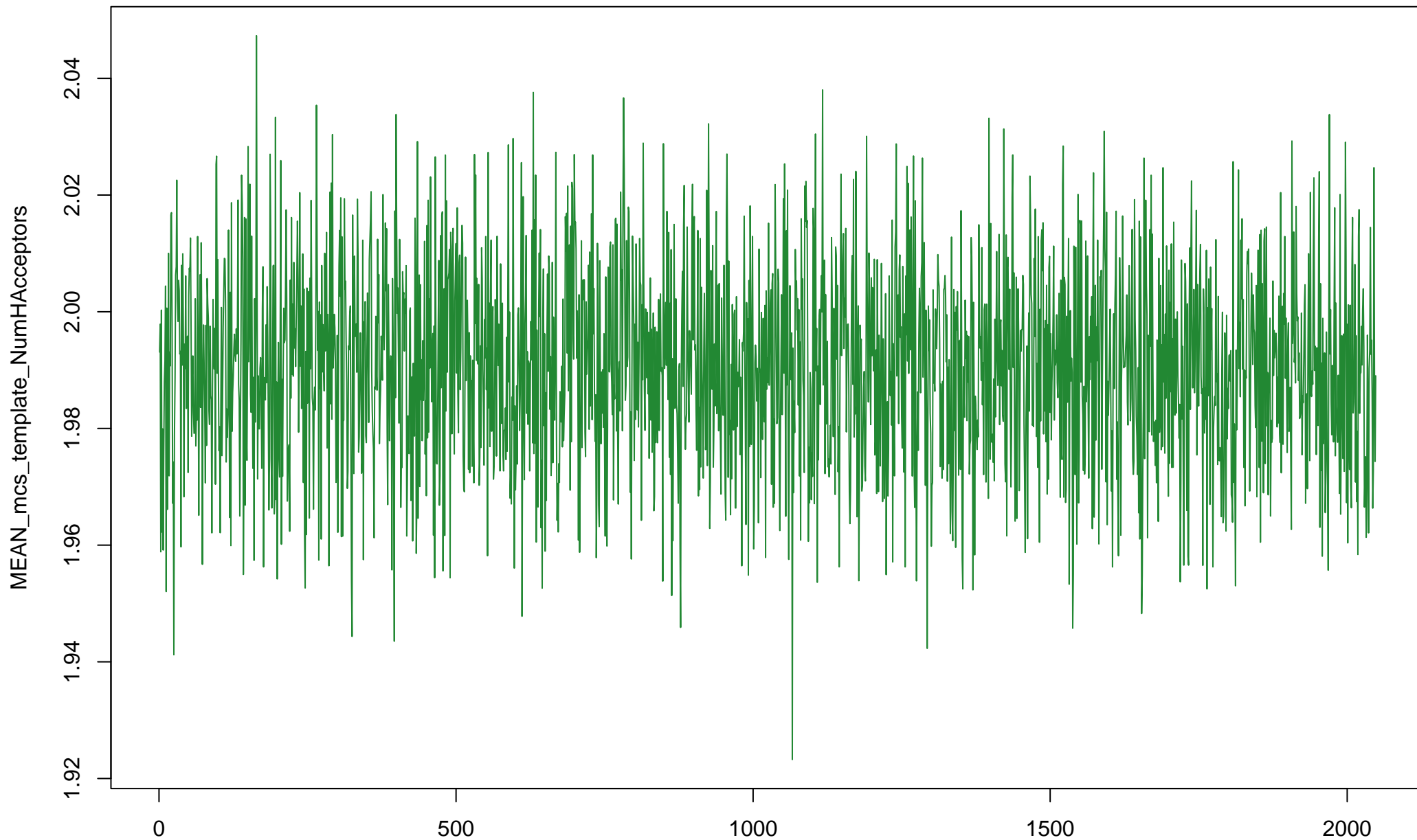
**MEAN\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0388 | MCSE(6.27) = 2.37 | stat: FALSE | burn: 0**



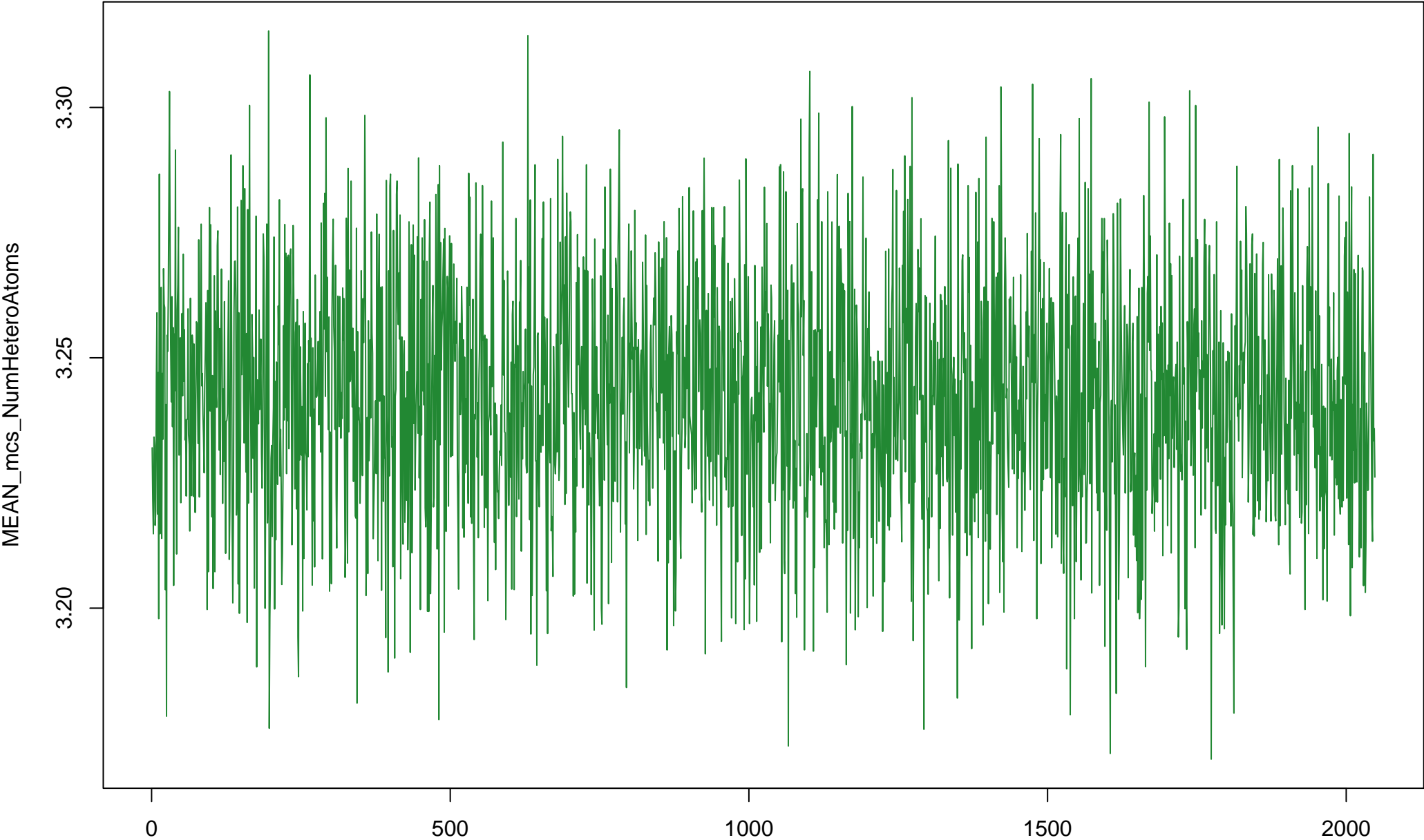
**MEAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0382 | MCSE(6.27) = 1.82 | stat: TRUE | burn: 0**



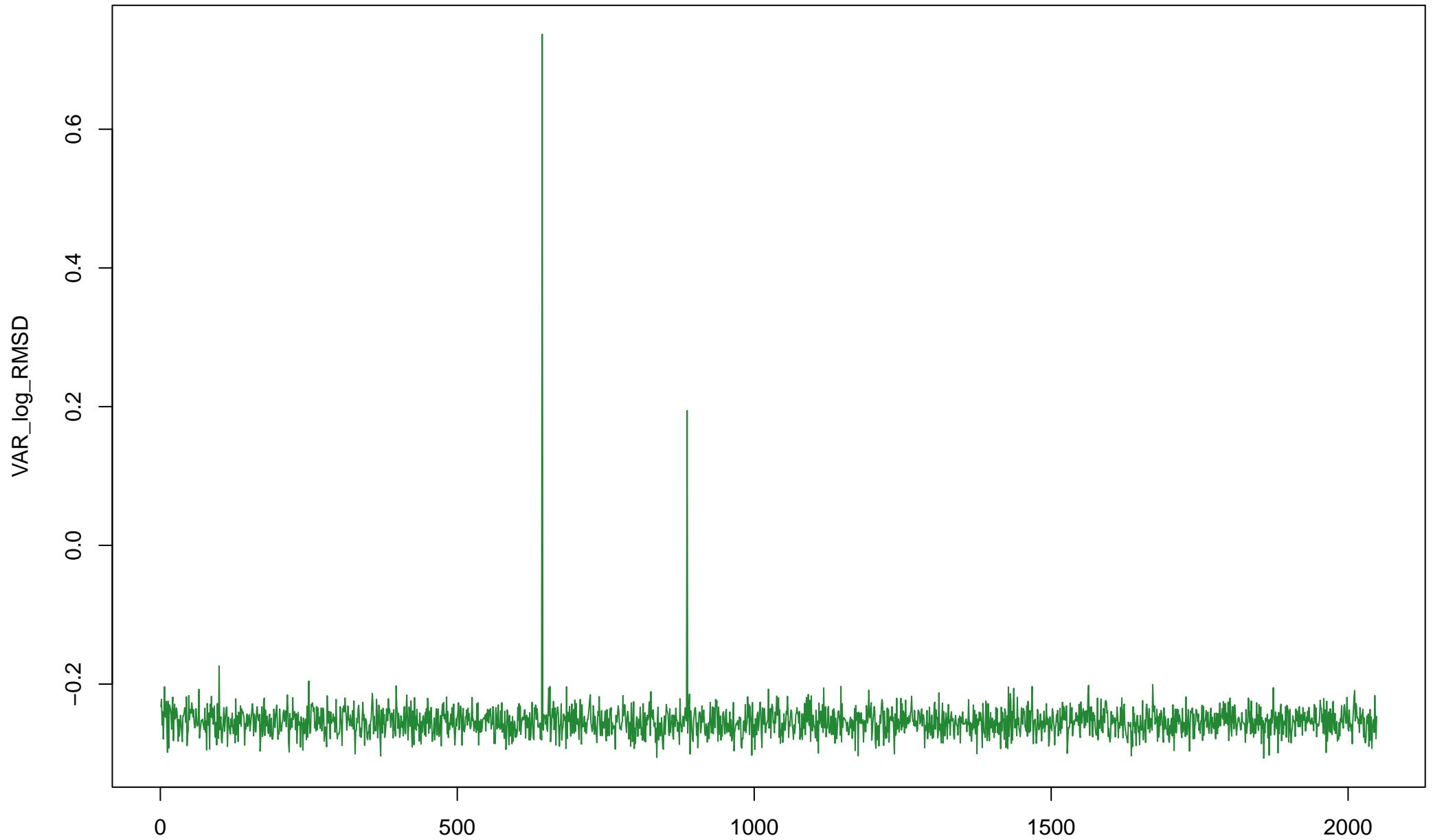
**MEAN\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0381 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0**



**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0504 | MCSE(6.27) = 1.7 | stat: TRUE | burn: 0**

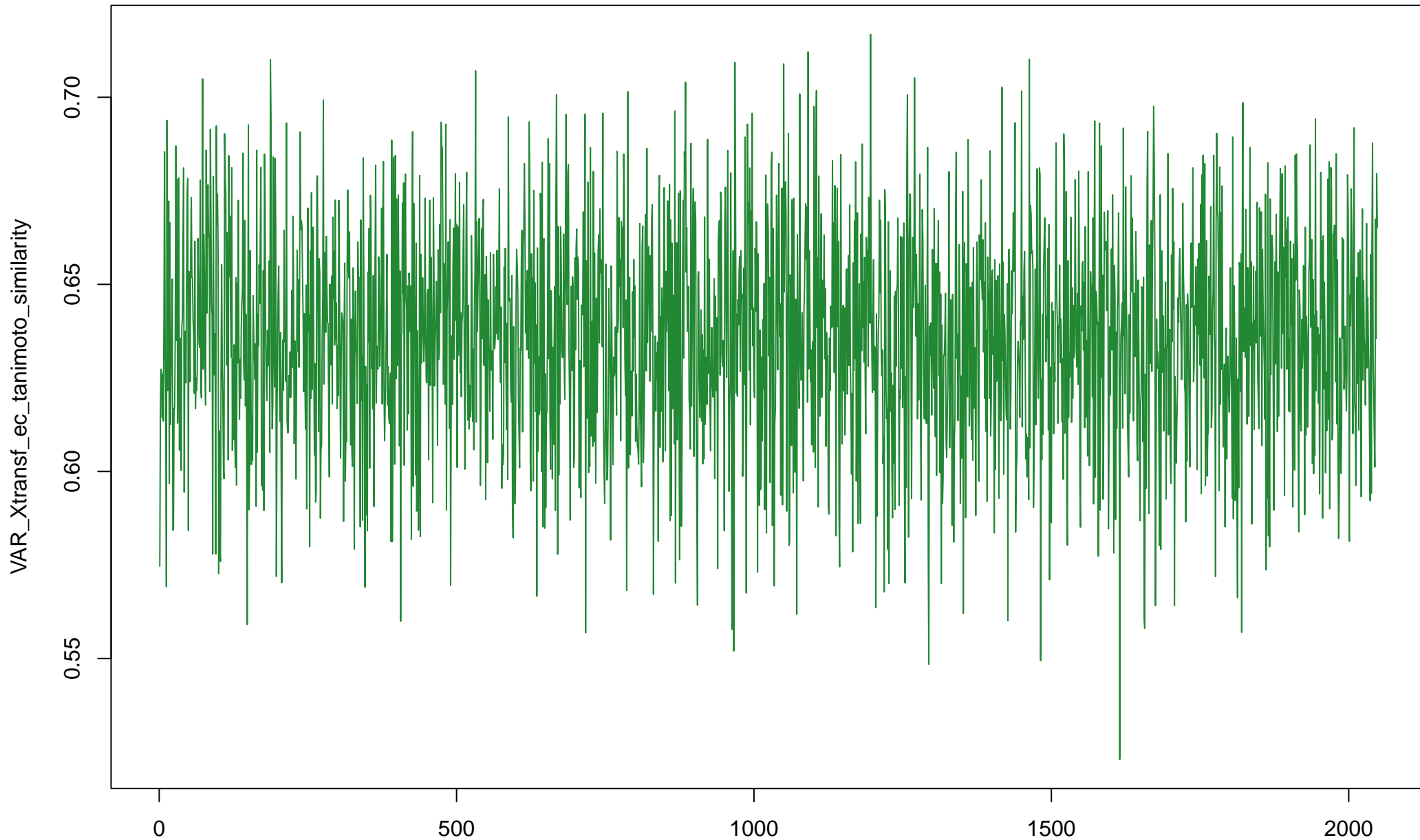


**VAR\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0516 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0**

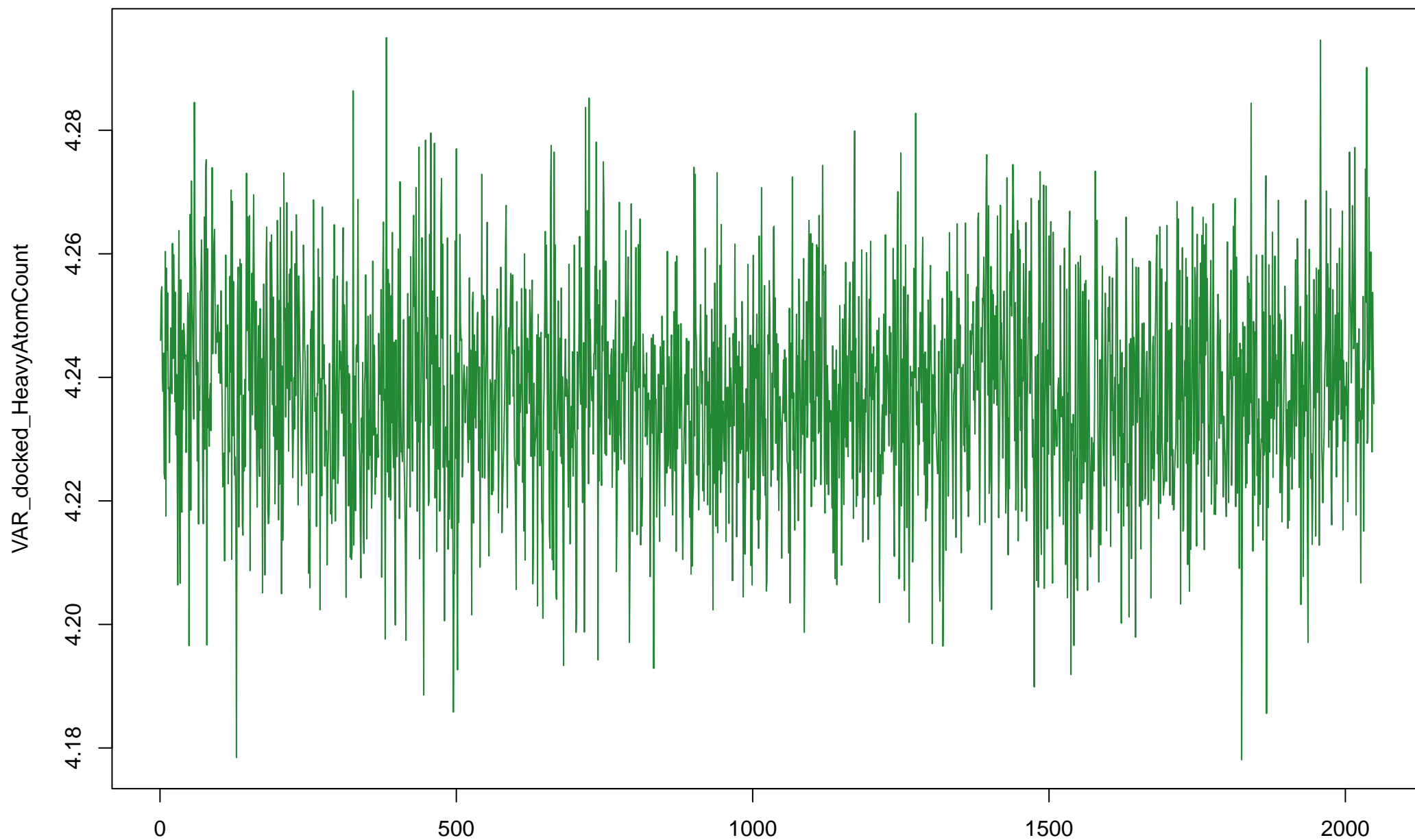




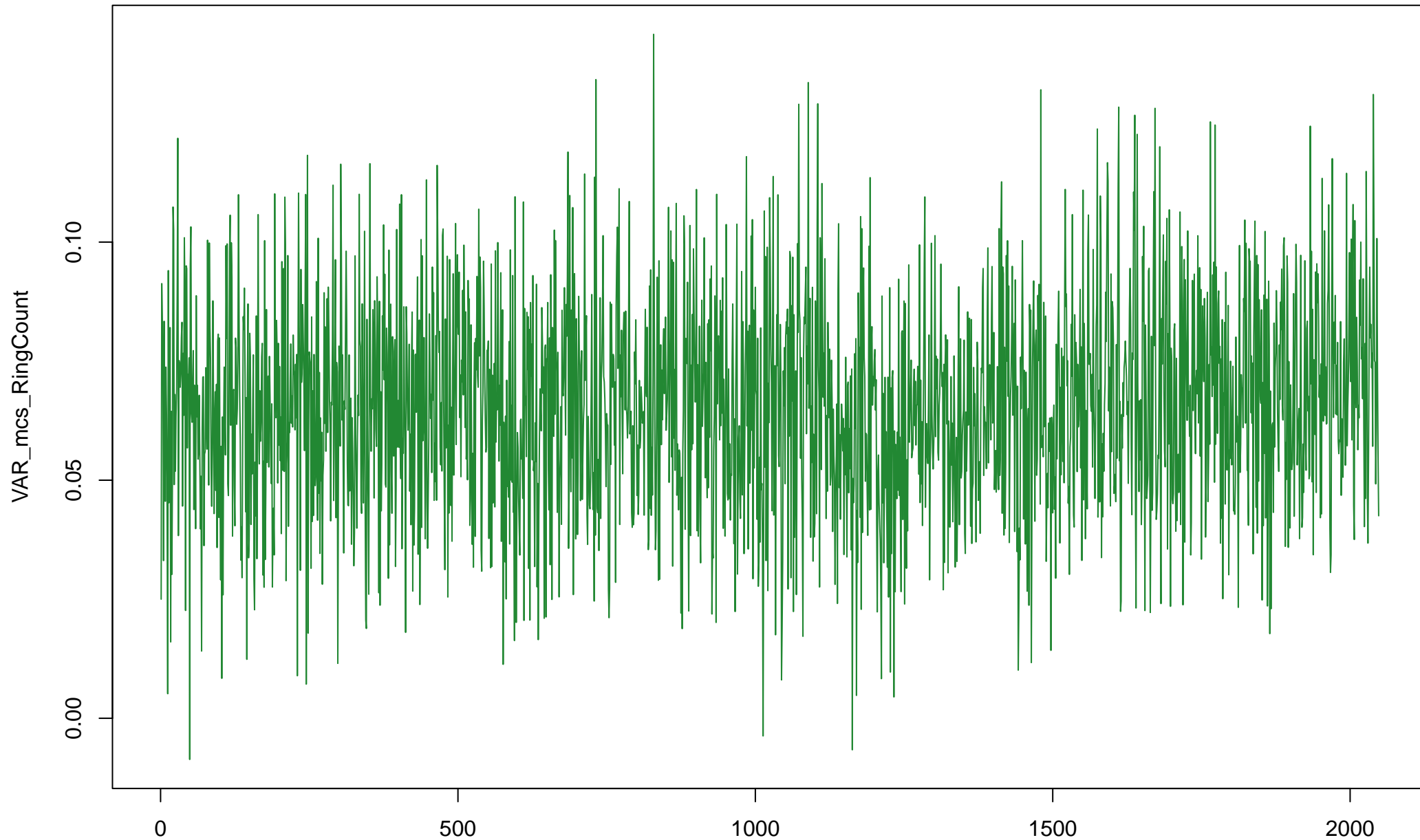
**VAR\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0377 | MCSE(6.27) = 1.93 | stat: TRUE | burn: 0**



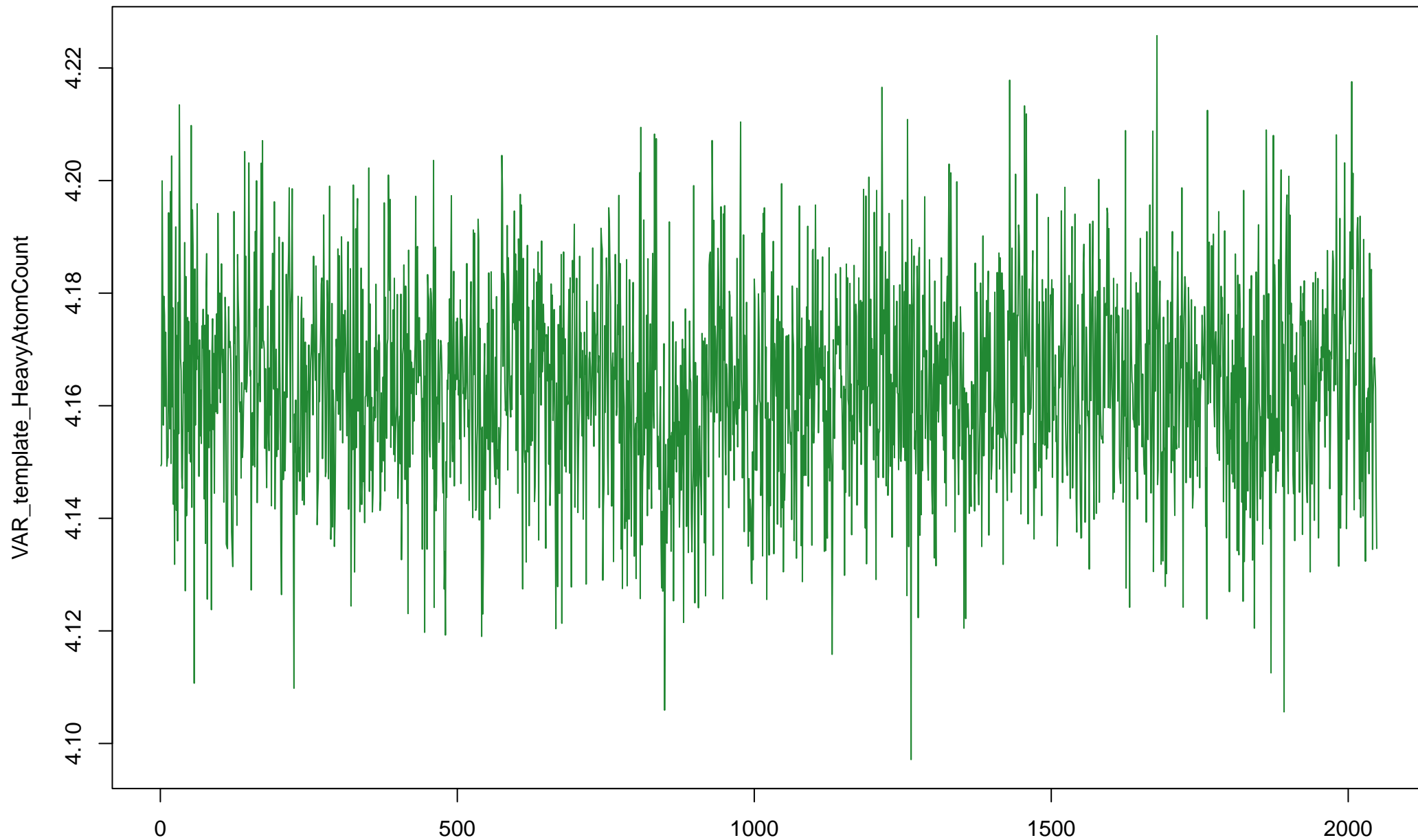
**VAR\_docked\_HeavyAtomCount**  
**ESS = 1890 | BMK = 0.0328 | MCSE(6.27) = 2.69 | stat: FALSE | burn: 0**



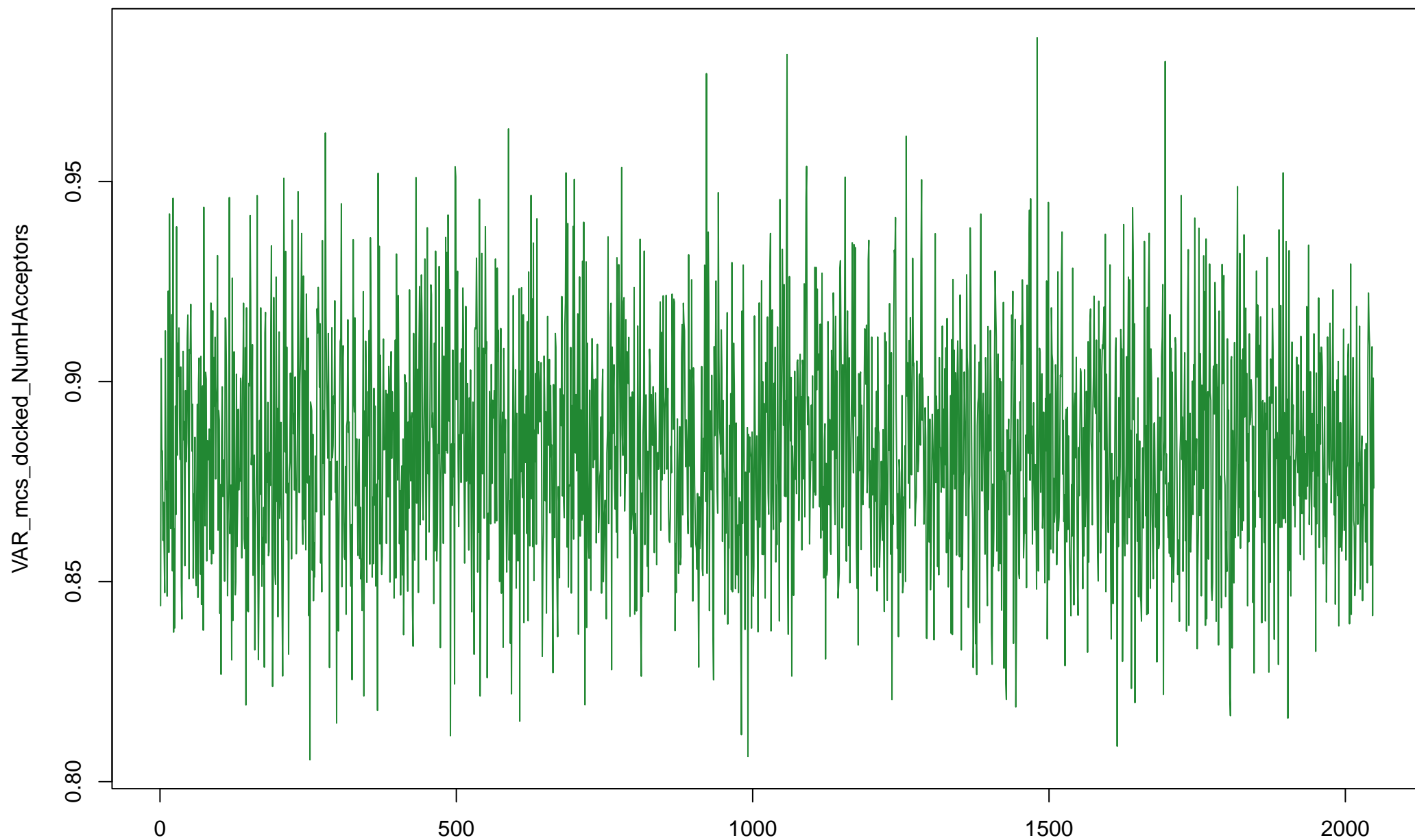
**VAR\_mcs\_RingCount**  
**ESS = 2050 | BMK = 0.0537 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0**



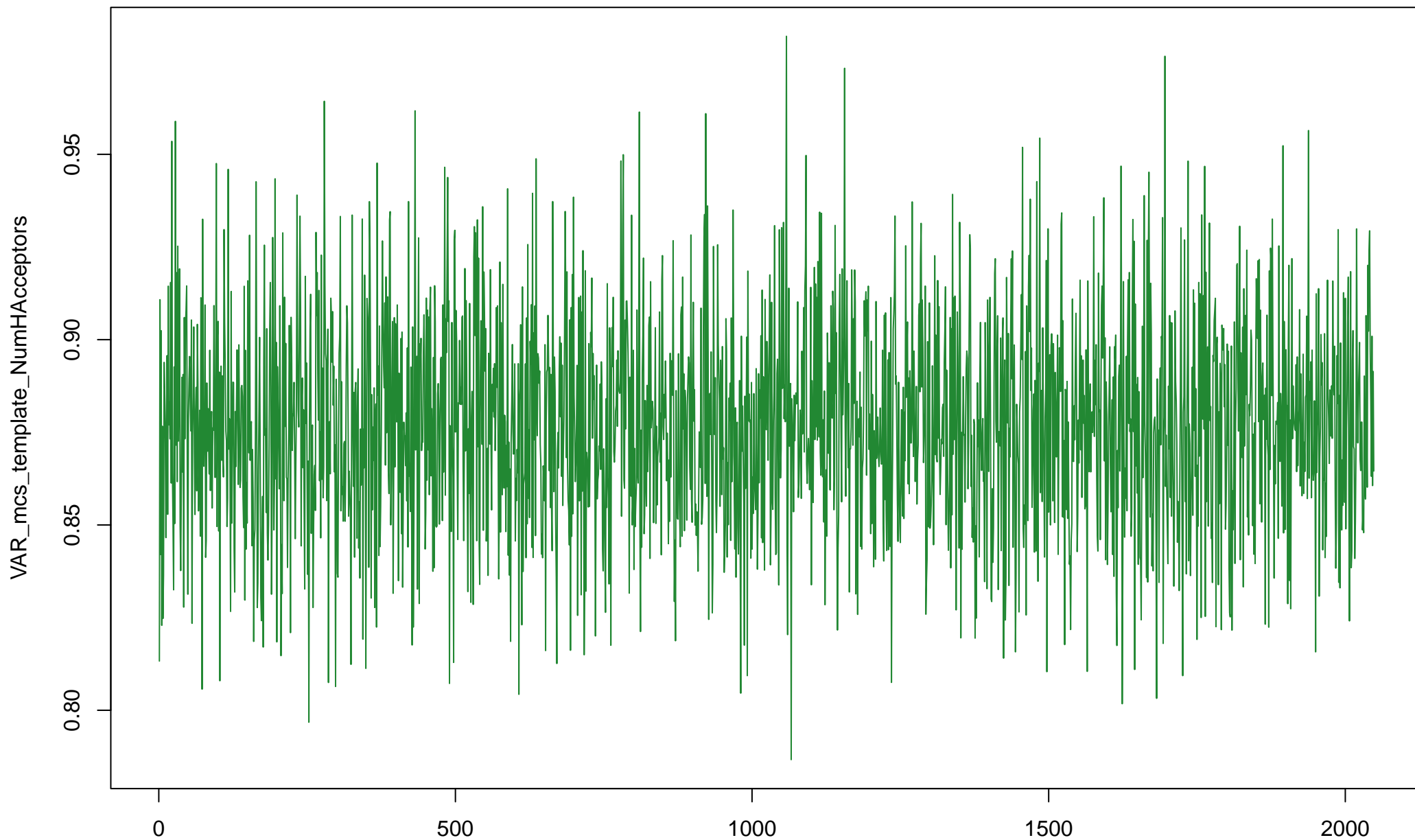
**VAR\_template\_HeavyAtomCount**  
**ESS = 1560 | BMK = 0.0512 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0**



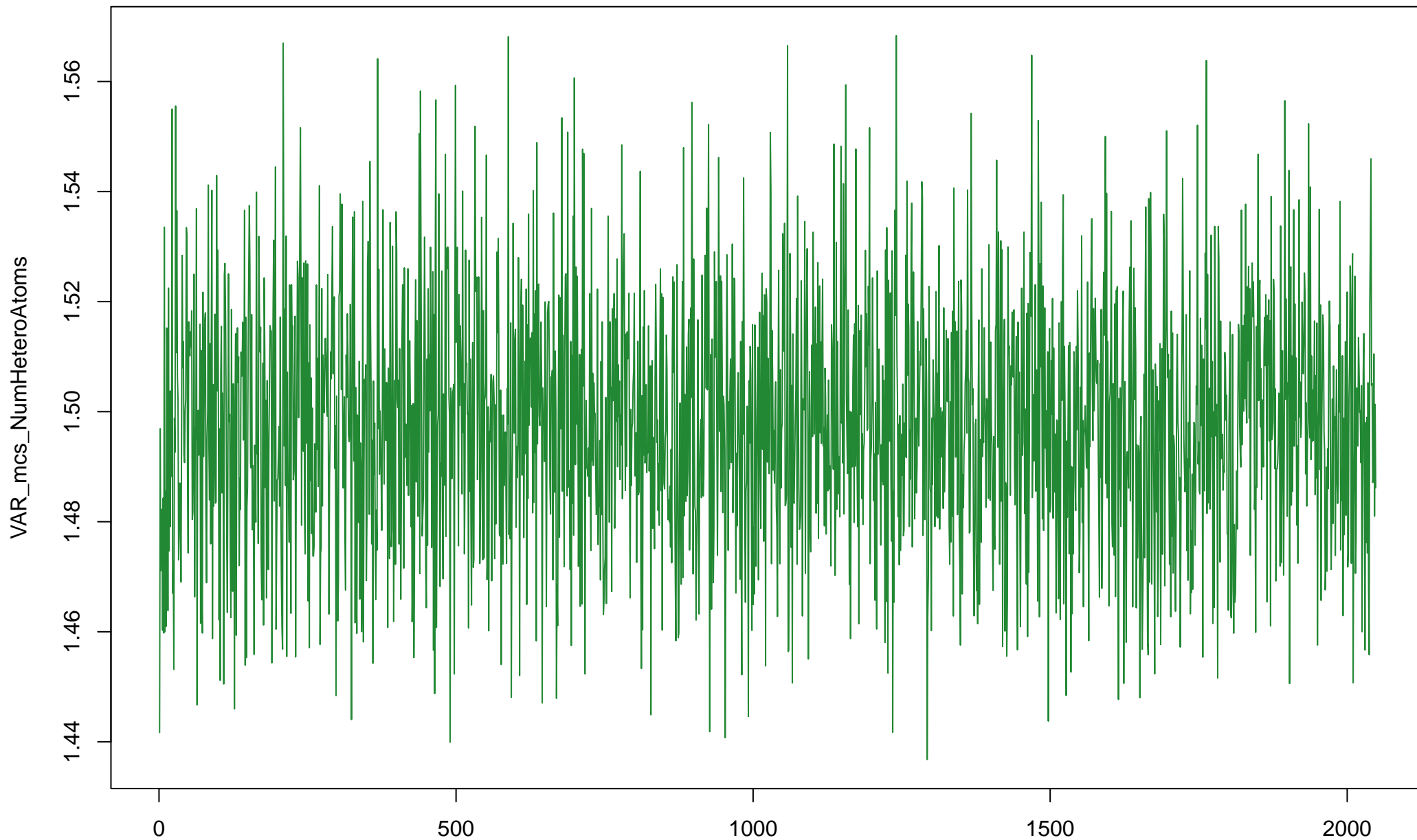
**VAR\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0369 | MCSE(6.27) = 1.95 | stat: TRUE | burn: 0**



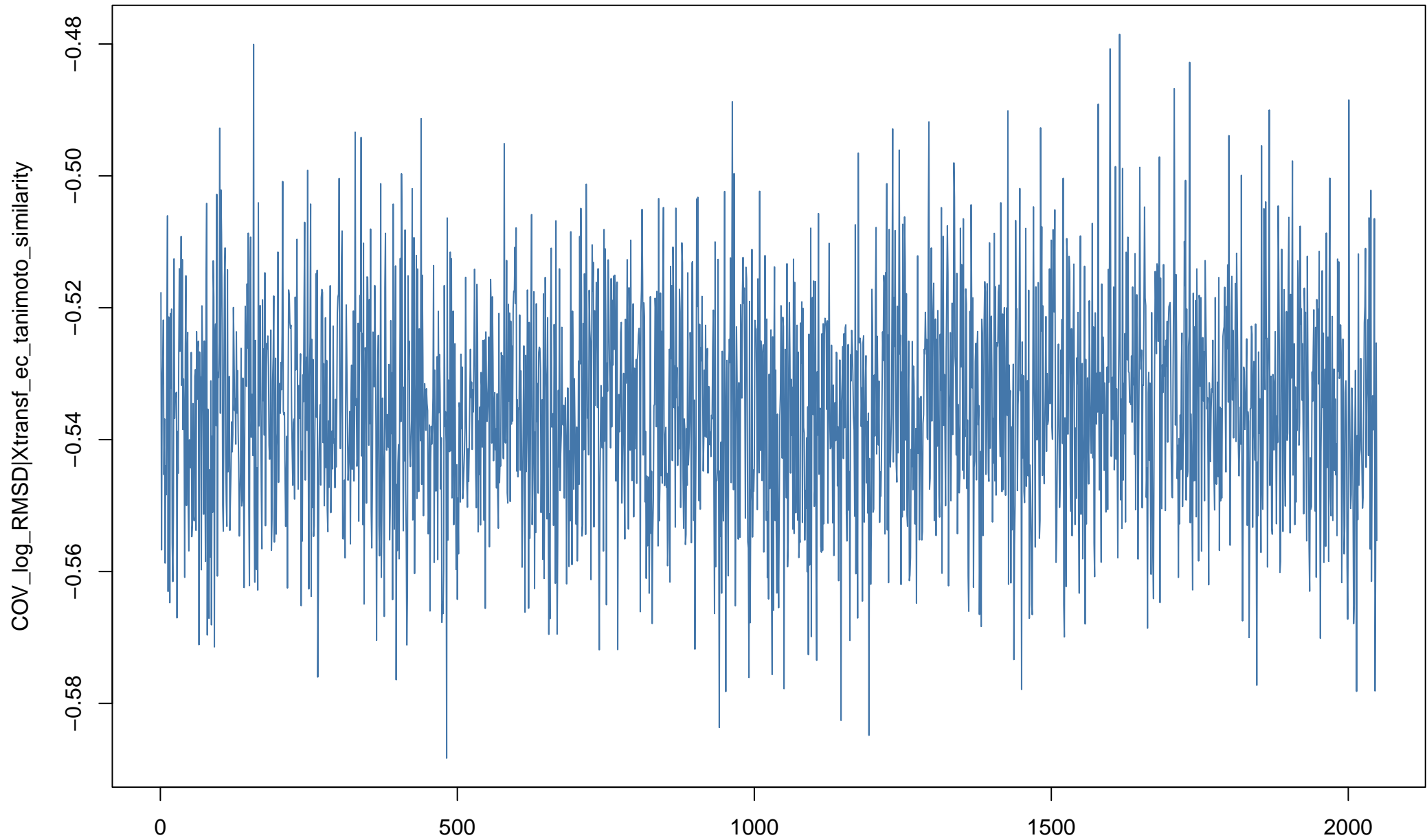
**VAR\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0487 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0**



**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0396 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0**

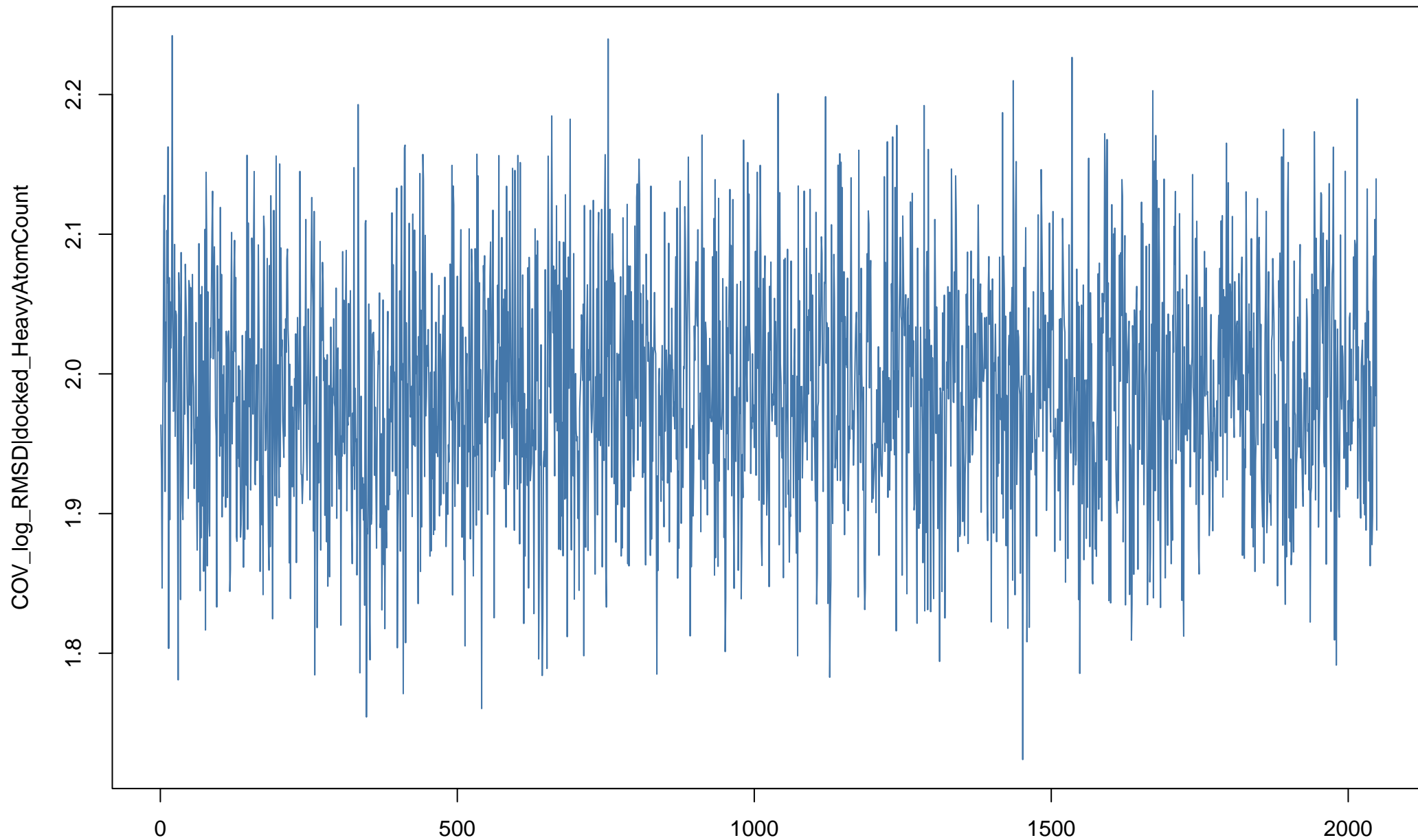


**COV\_log\_RMSD|Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0417 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0**

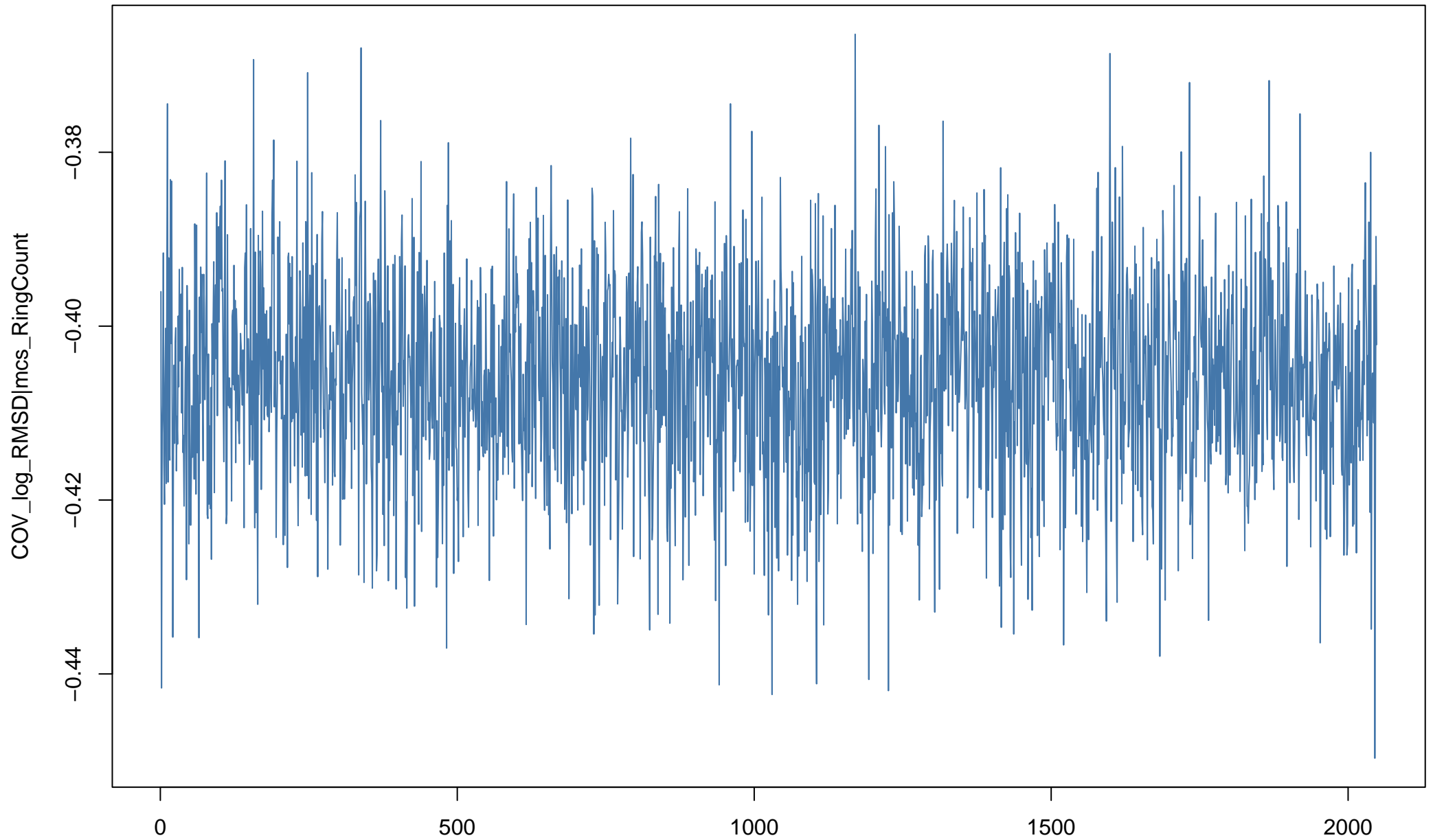




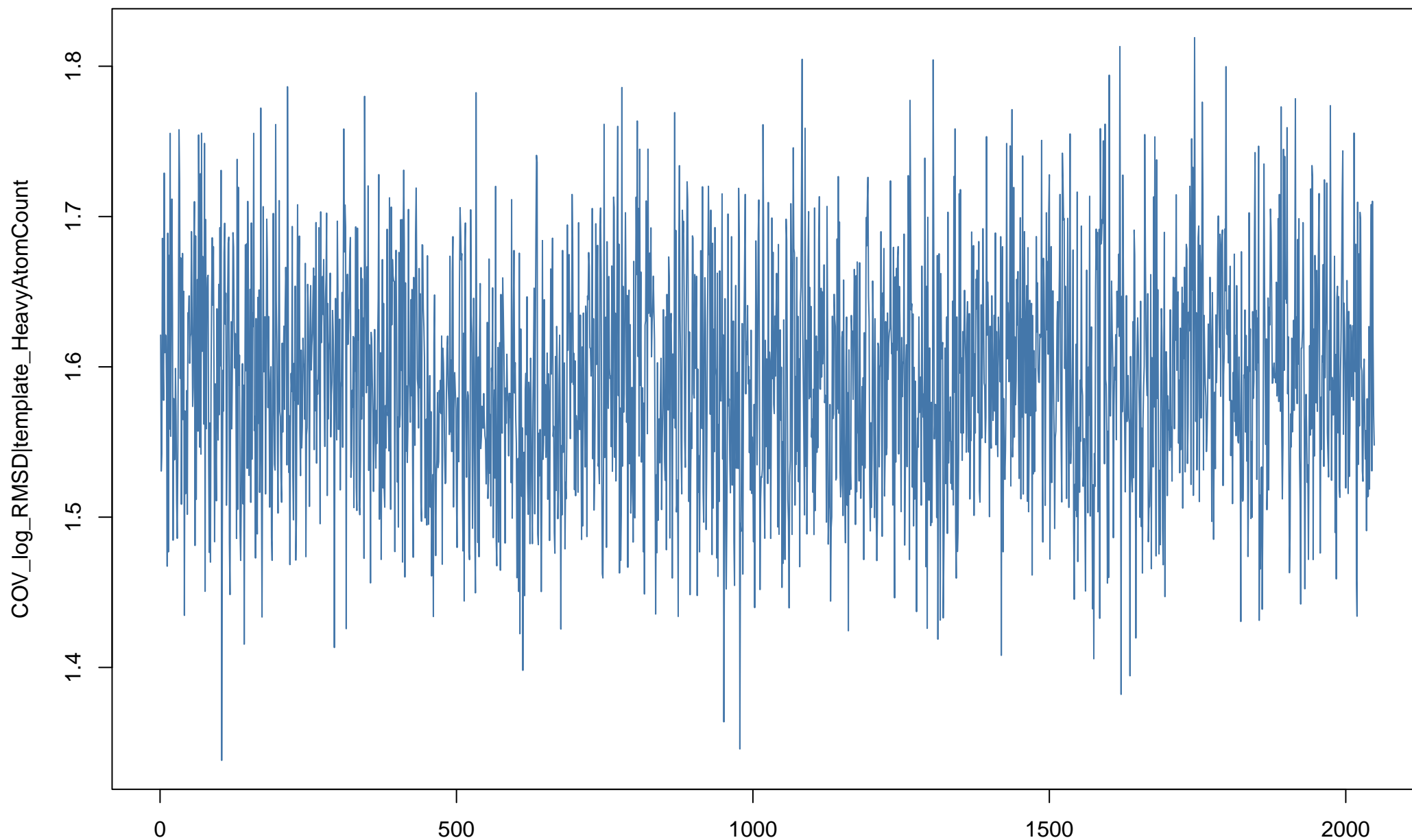
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 1820 | BMK = 0.0496 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0**



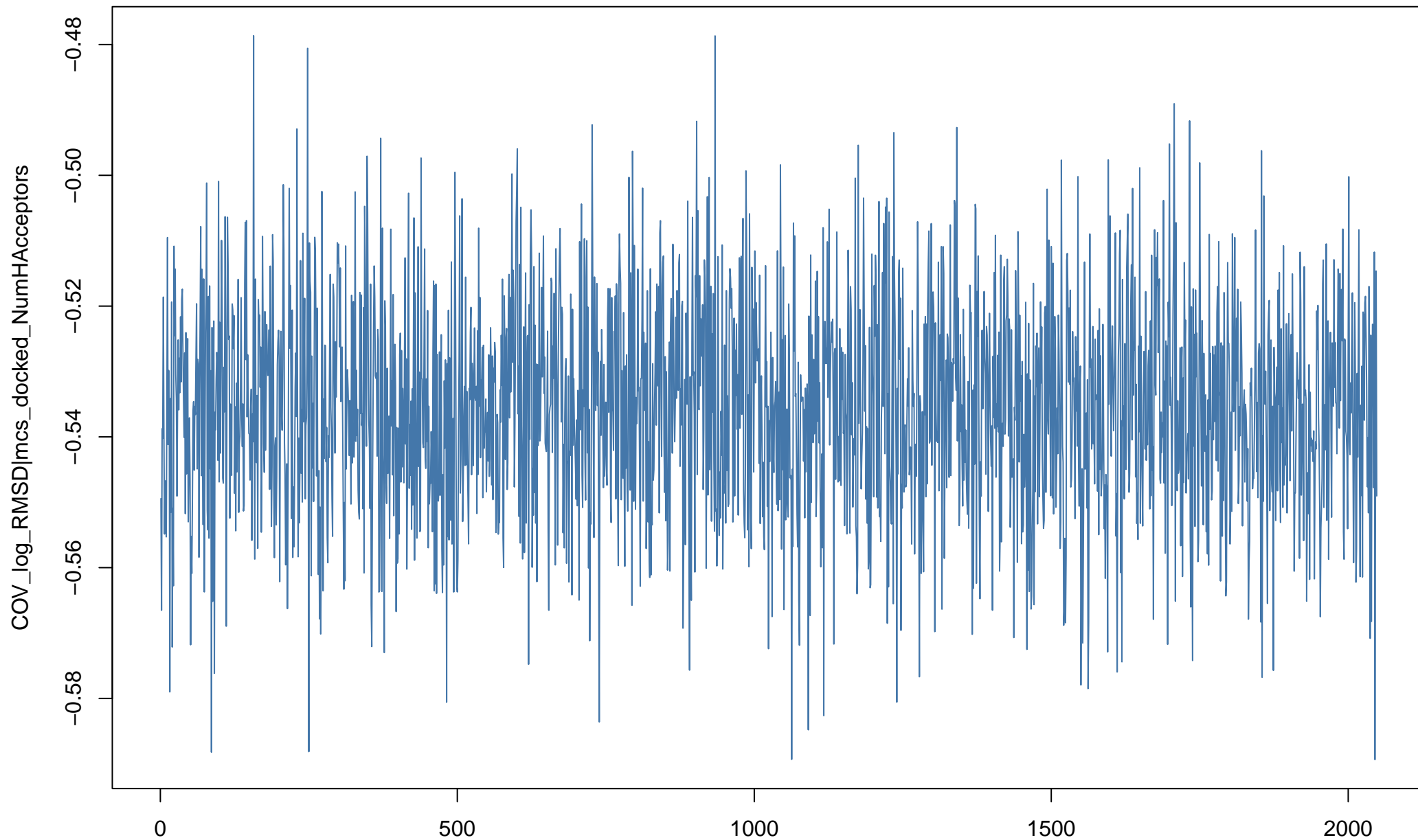
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 2050 | BMK = 0.0266 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0**



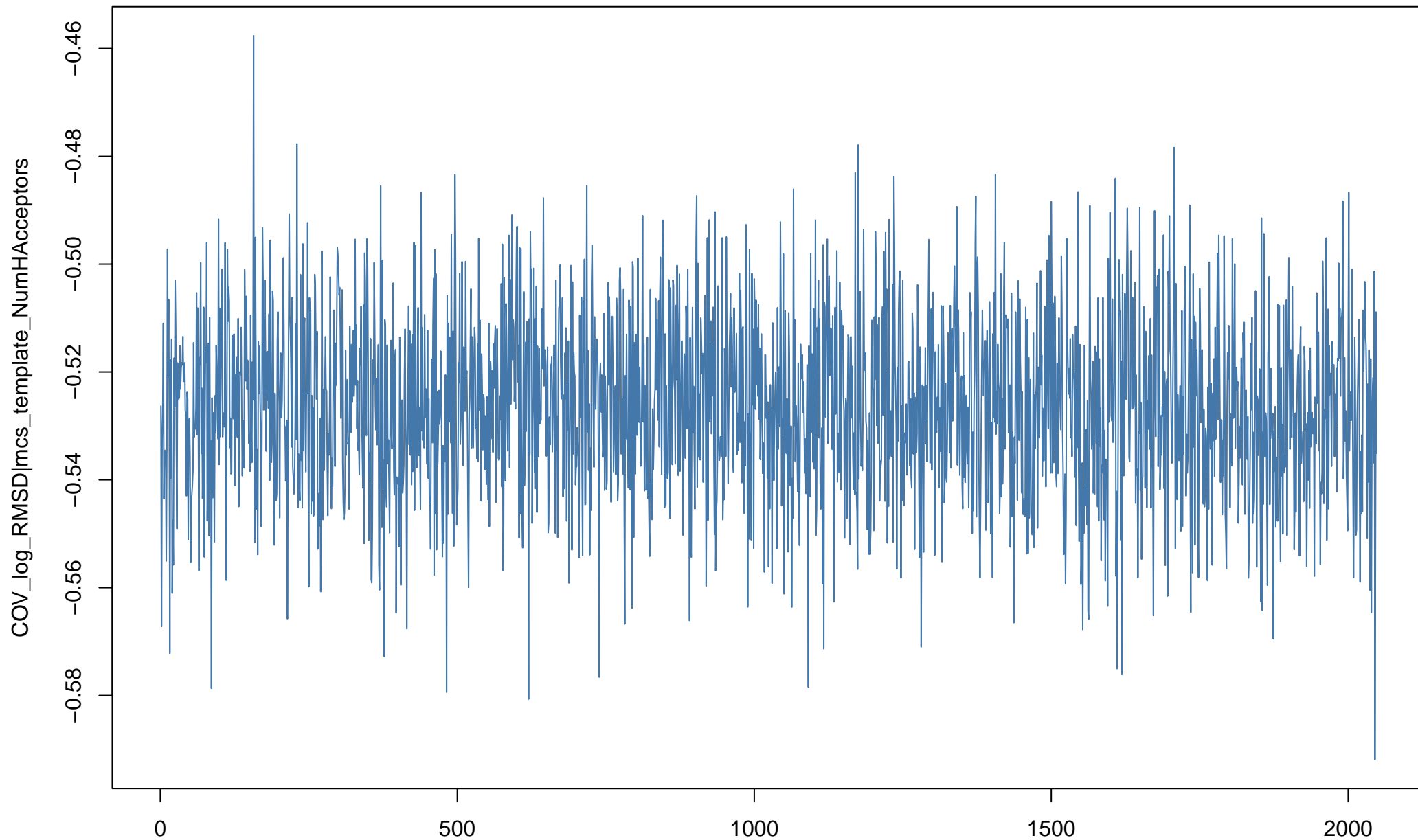
**COV\_log\_RMSD|template\_HeavyAtomCount**  
**ESS = 1630 | BMK = 0.0542 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0**



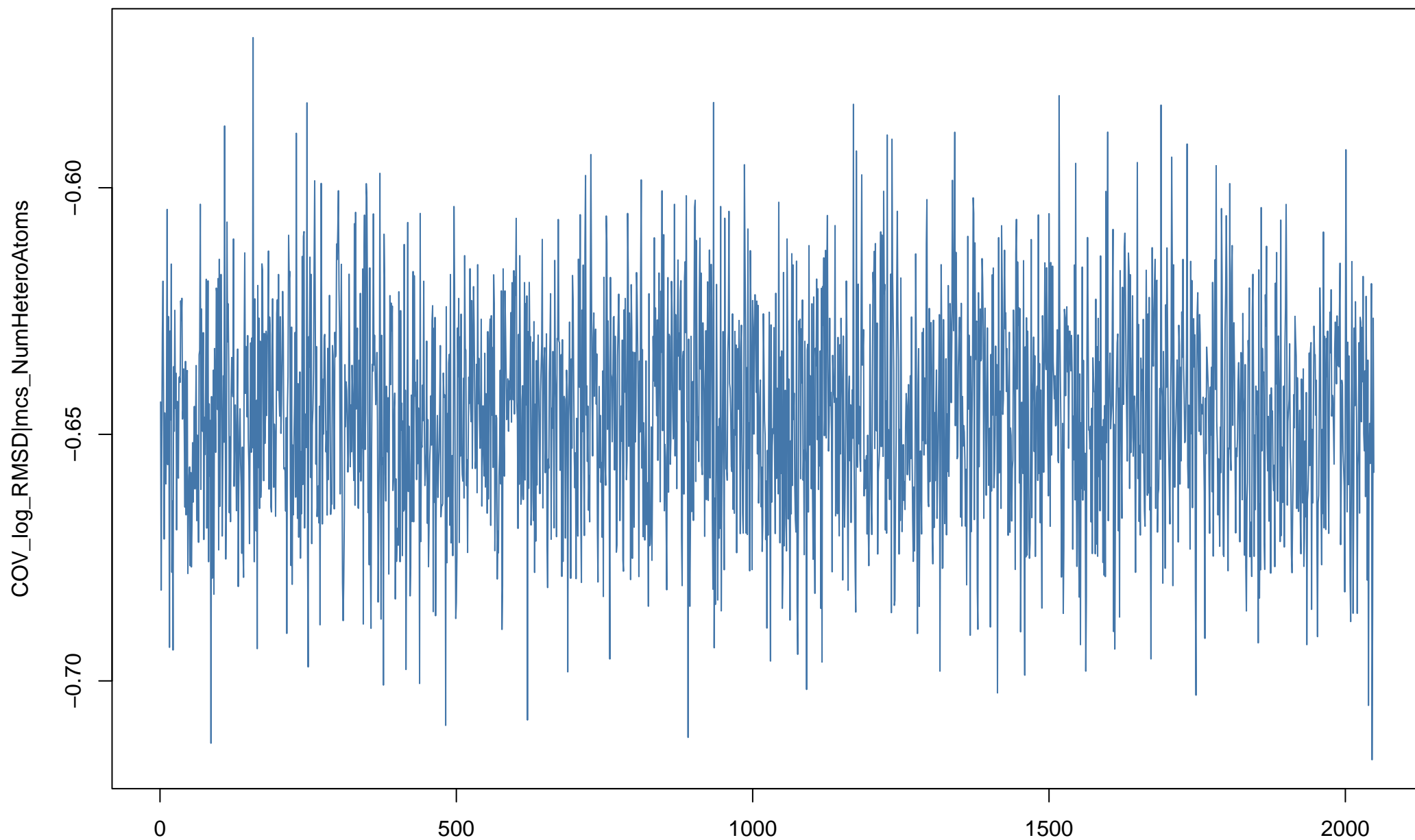
**COV\_log\_RMSD|mcs\_docked\_NumHAcceptors**  
**ESS = 1910 | BMK = 0.0501 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0**



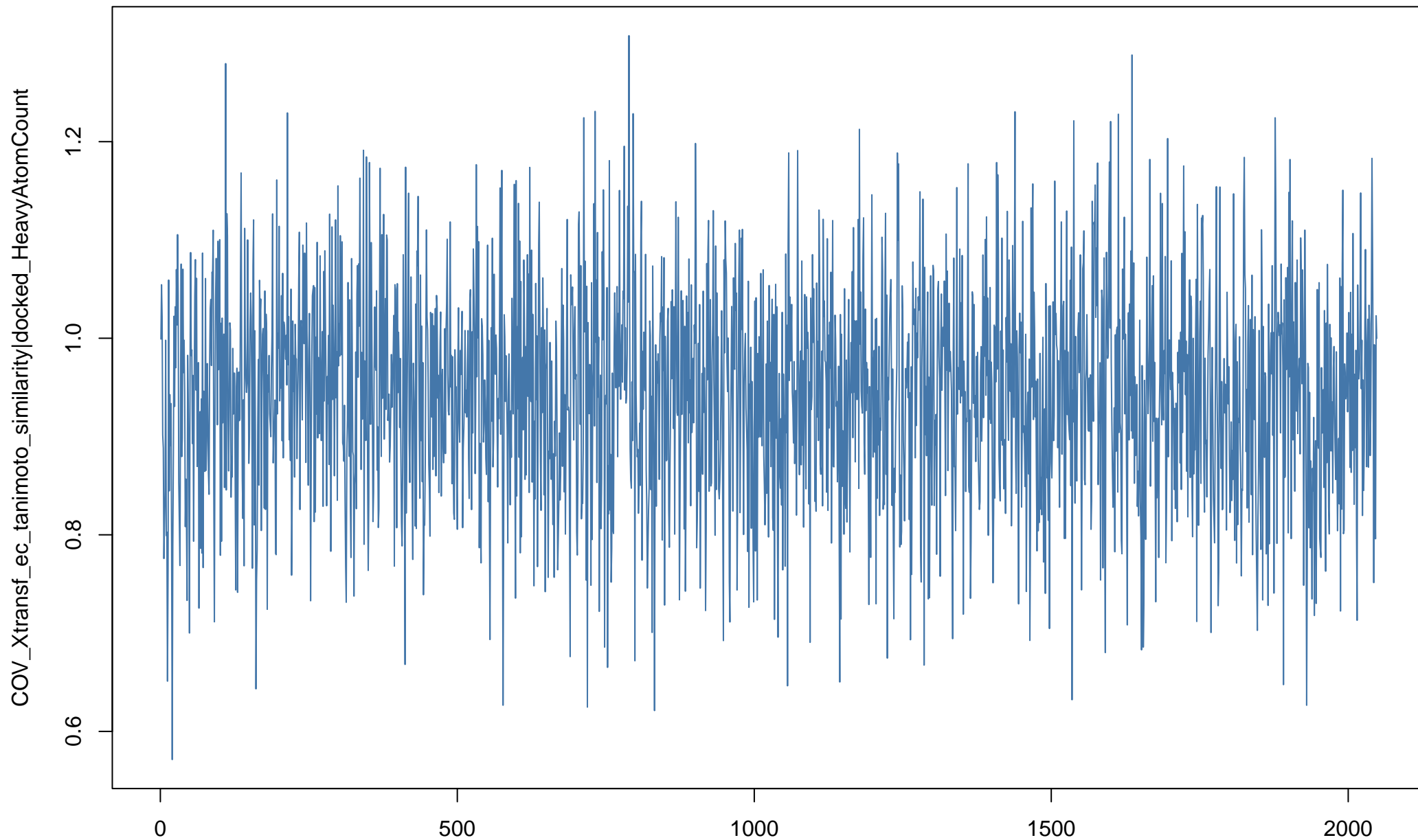
**COV\_log\_RMSD|mcs\_template\_NumHAcceptors**  
**ESS = 1920 | BMK = 0.0536 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0**



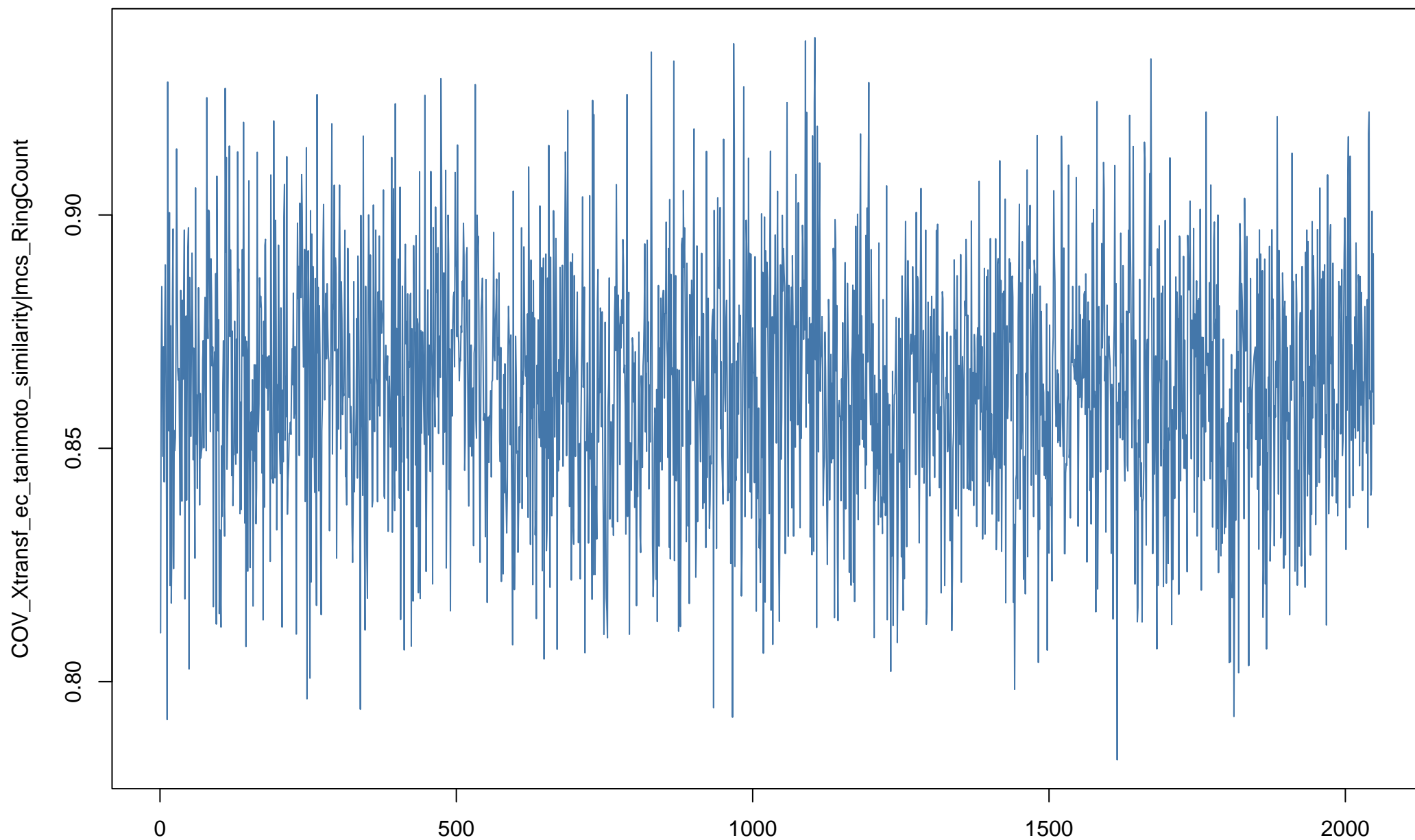
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 1800 | BMK = 0.0303 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0**



**COV\_Xtransf\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount**  
**ESS = 1800 | BMK = 0.0338 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0**

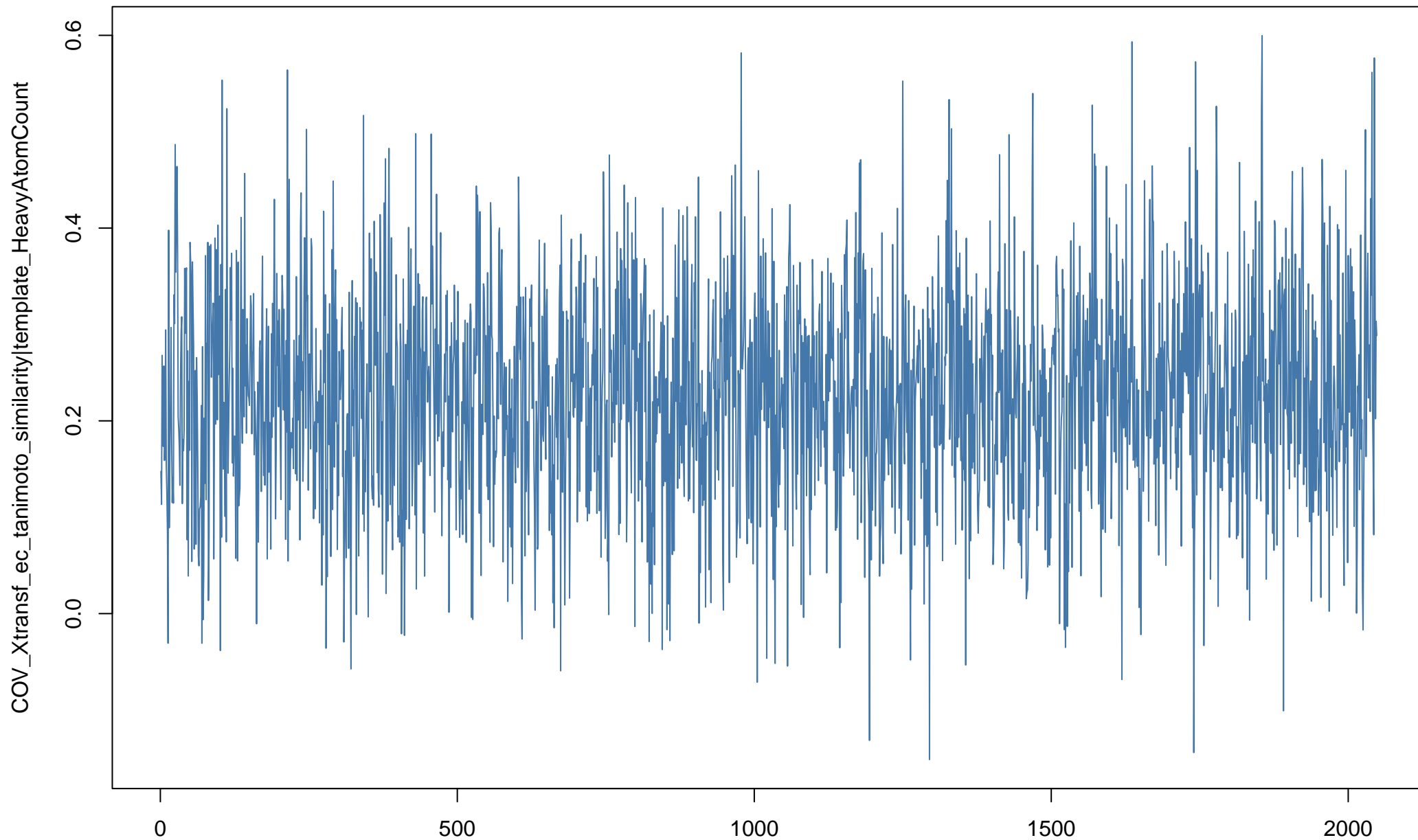


**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 1470 | BMK = 0.0298 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0**

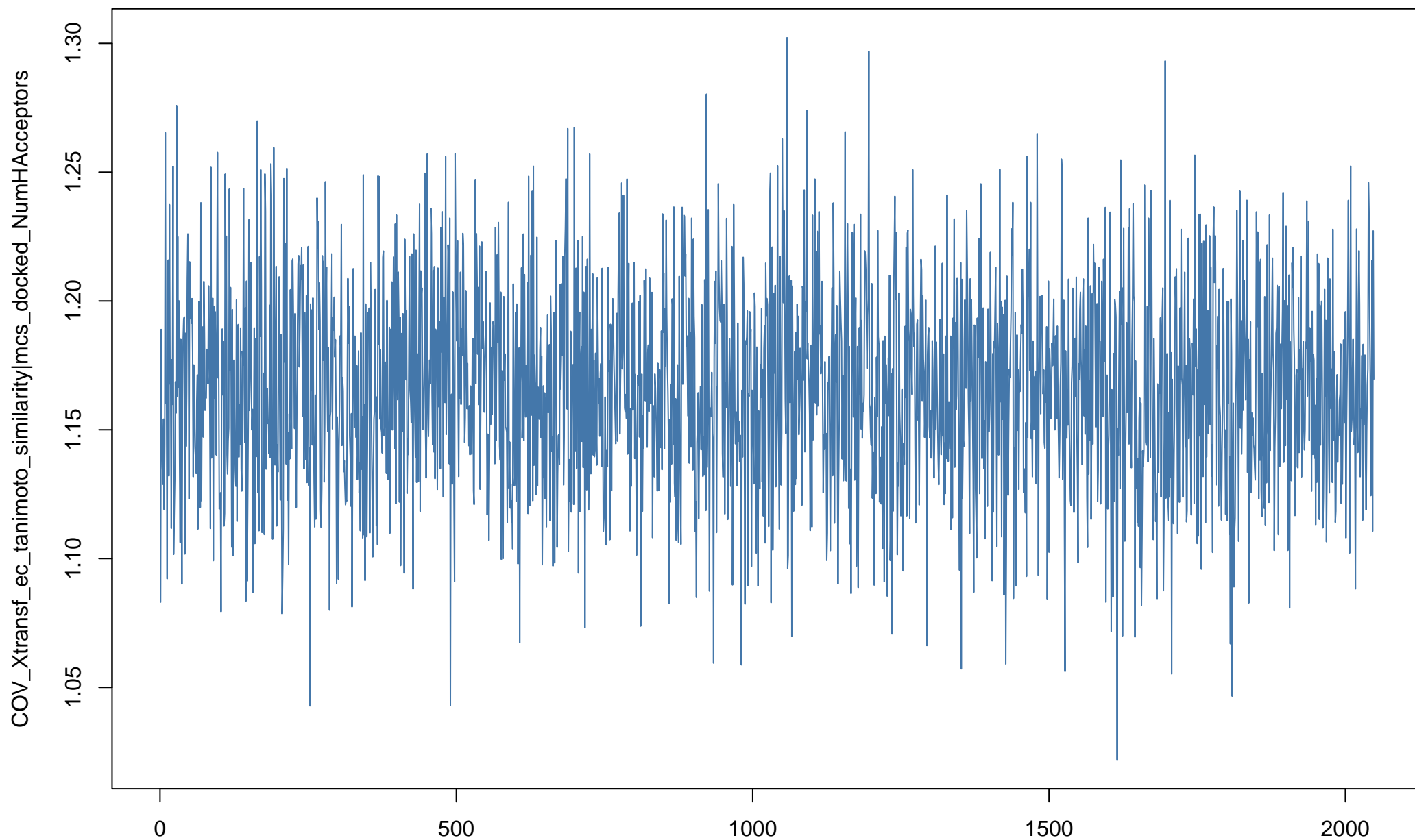




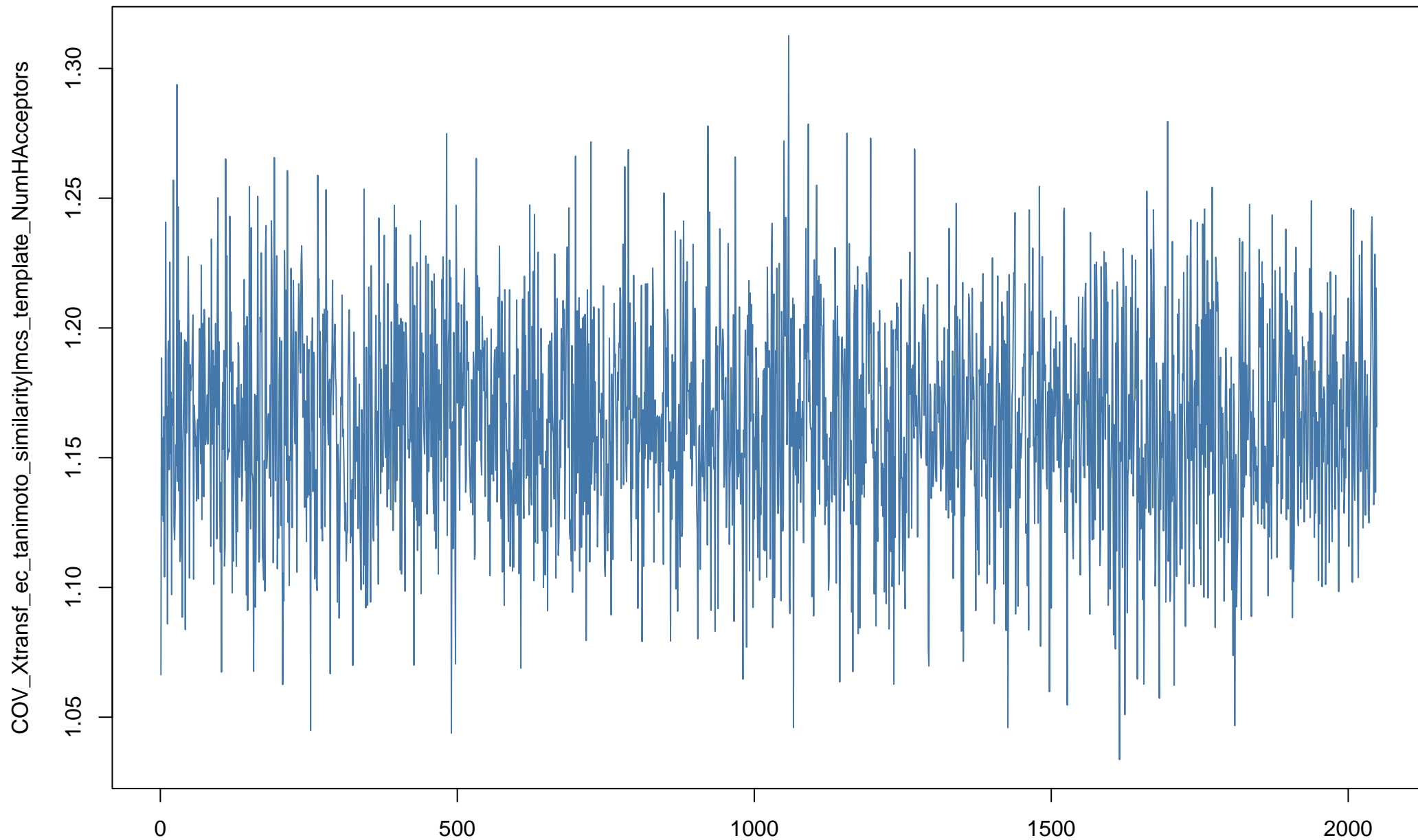
**COV\_Xtransf\_ec\_tanimoto\_similarity|template\_HeavyAtomCount**  
**ESS = 1620 | BMK = 0.0464 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0**



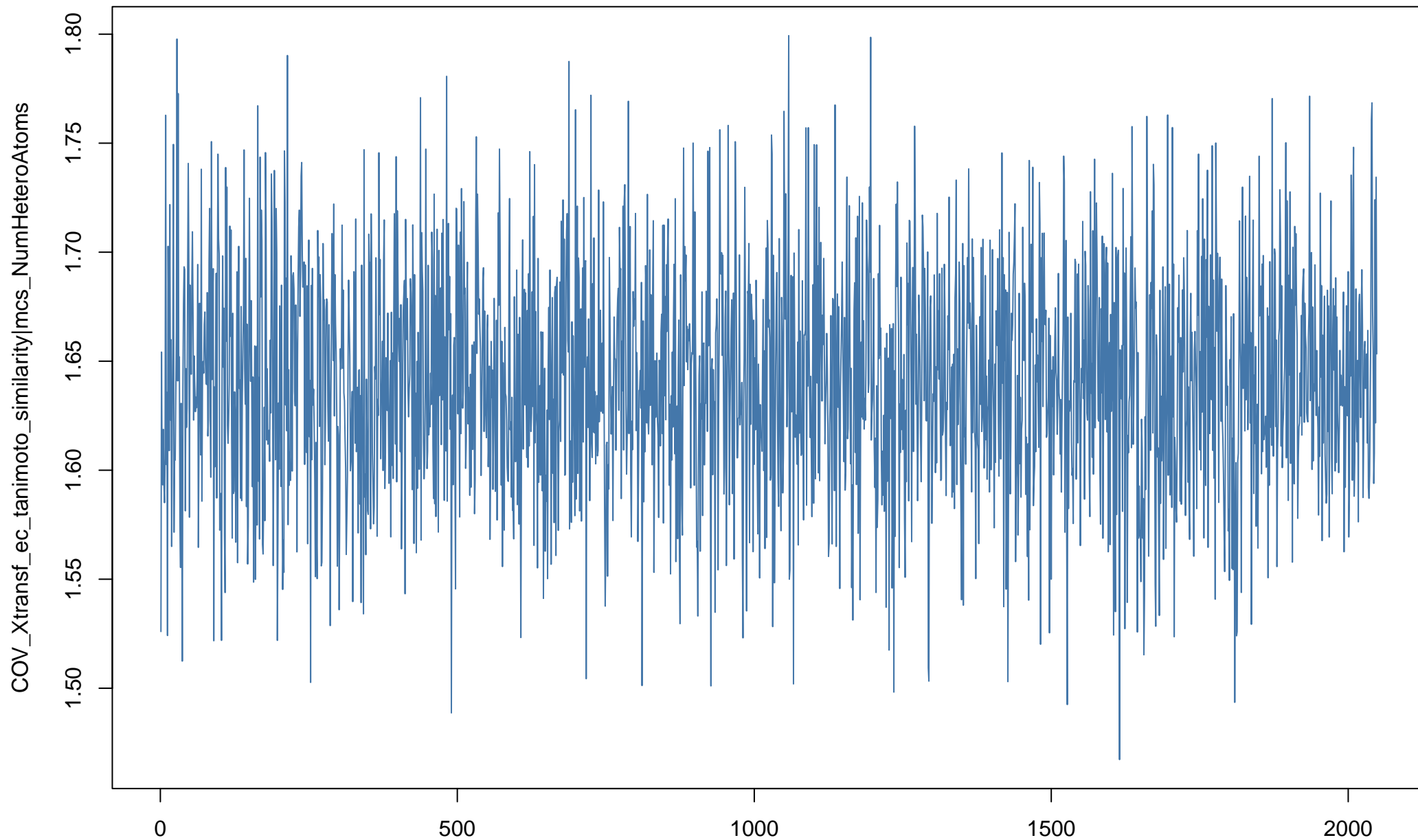
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0364 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0**



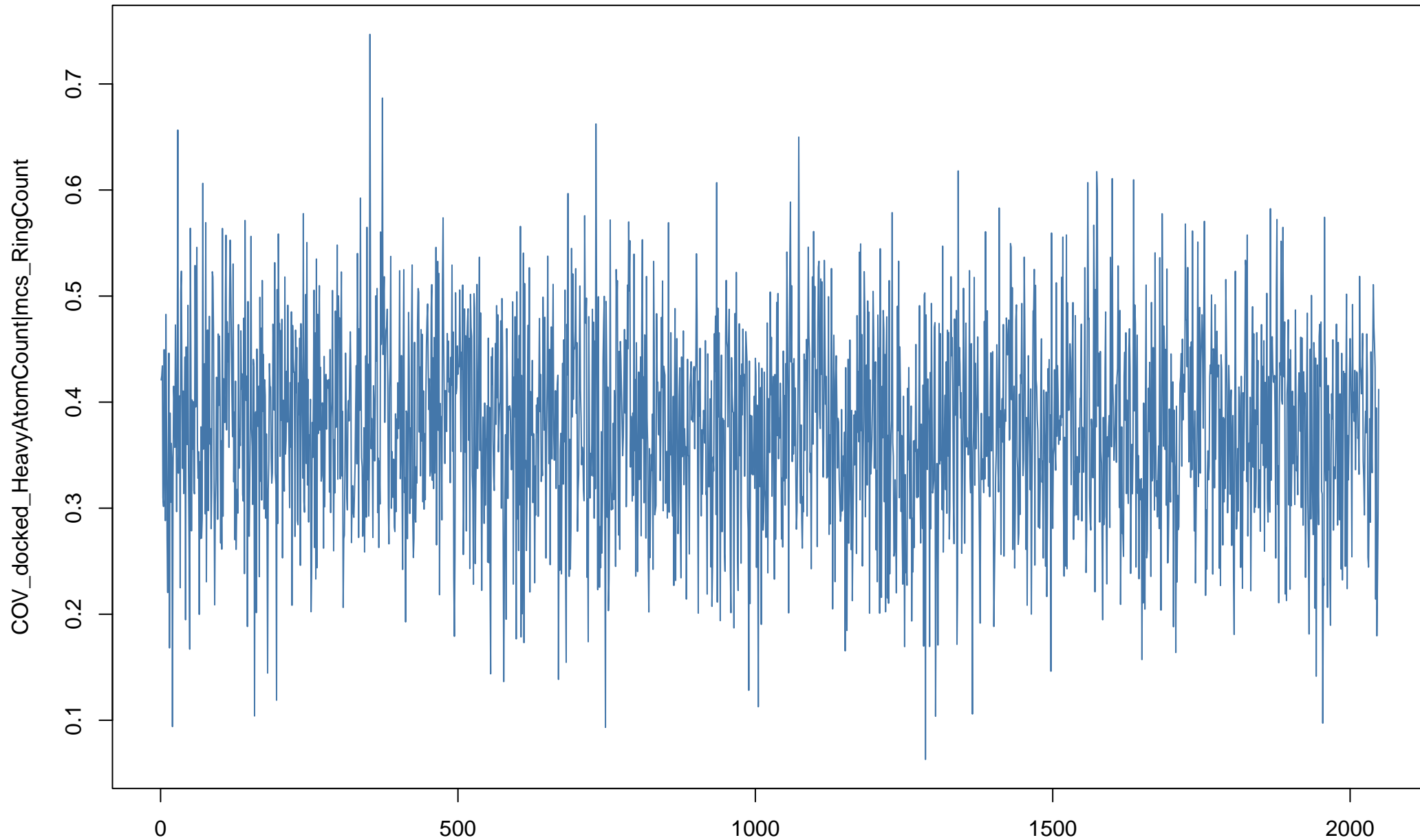
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.046 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0**



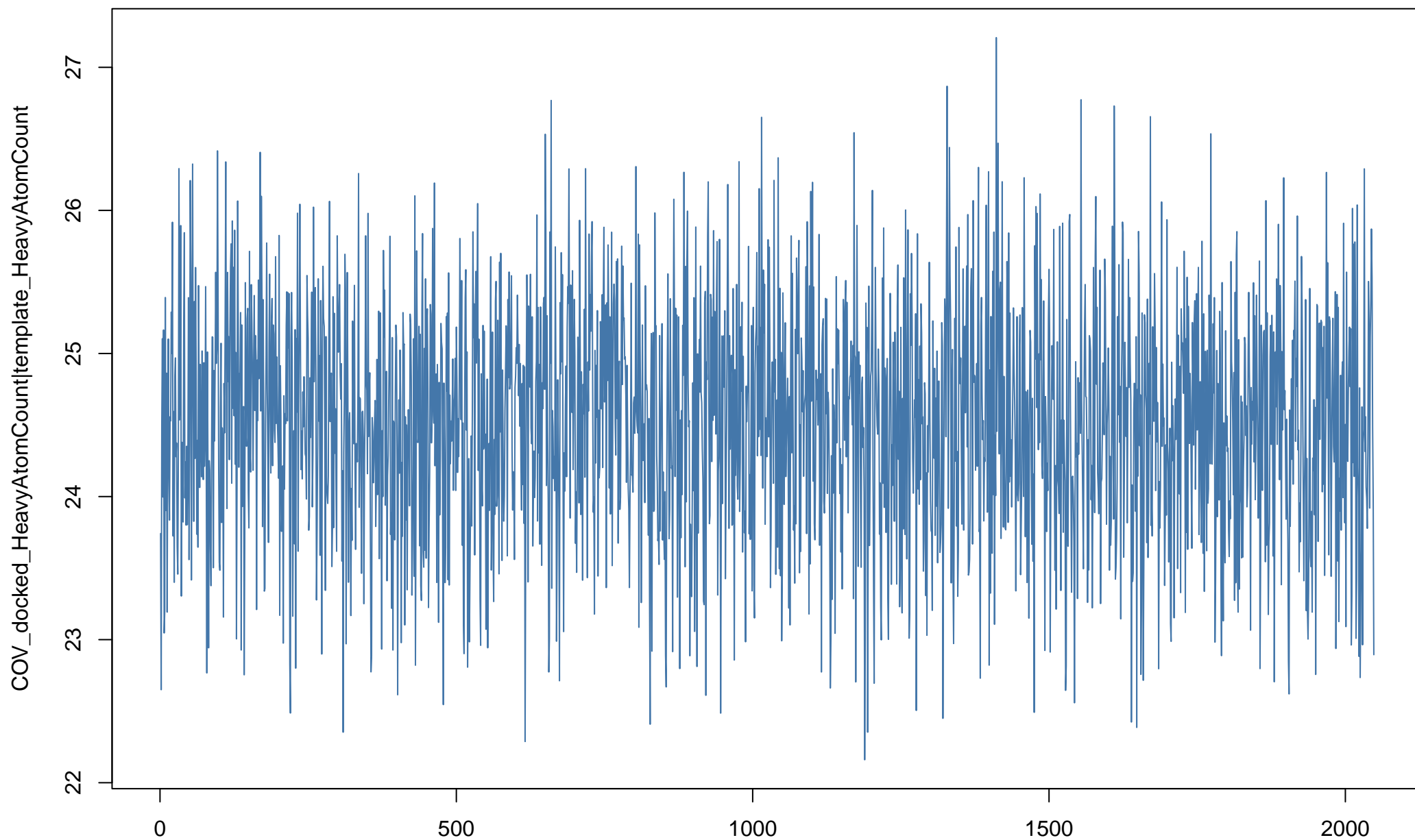
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms**  
**ESS = 1920 | BMK = 0.0287 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0**



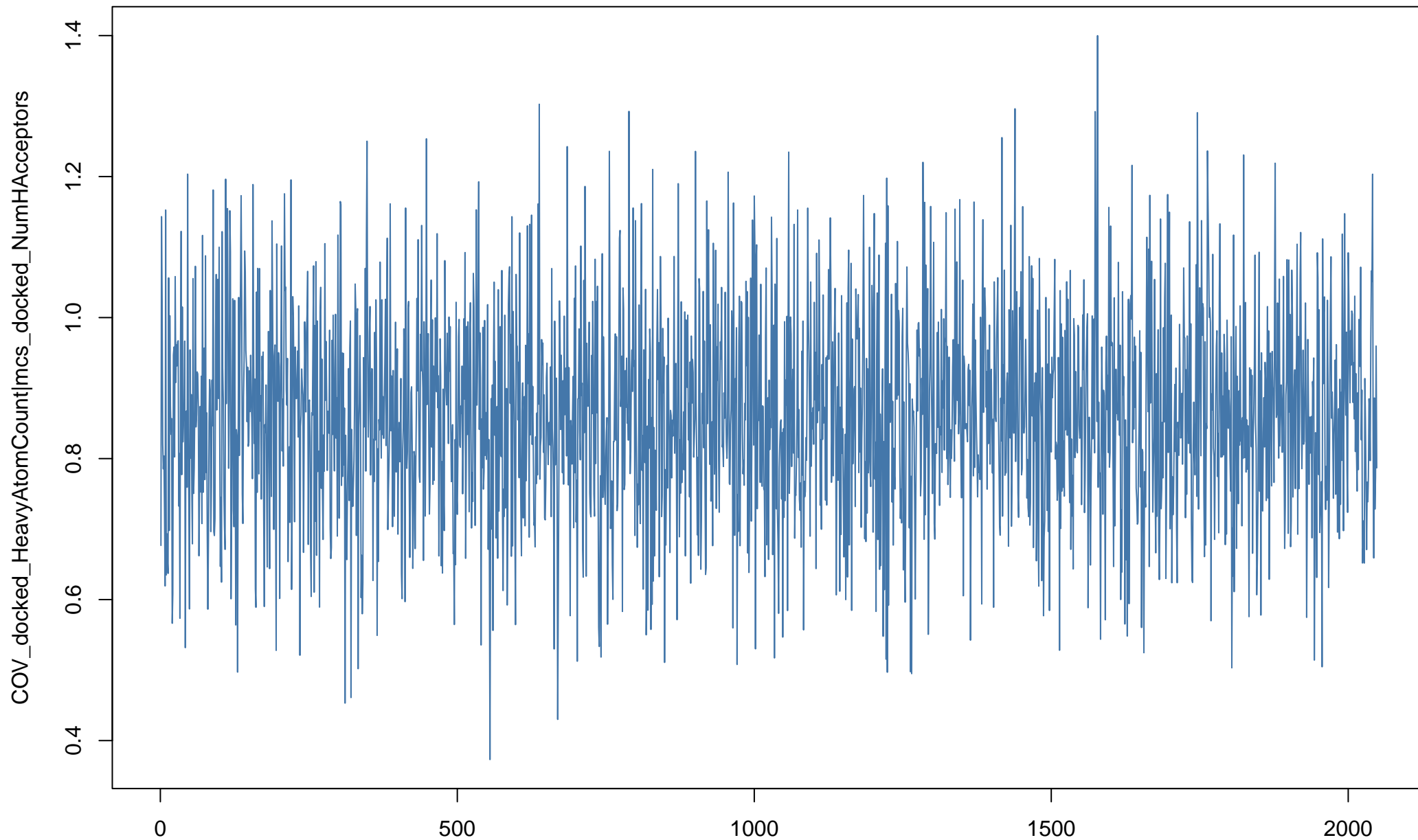
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 1740 | BMK = 0.045 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0**



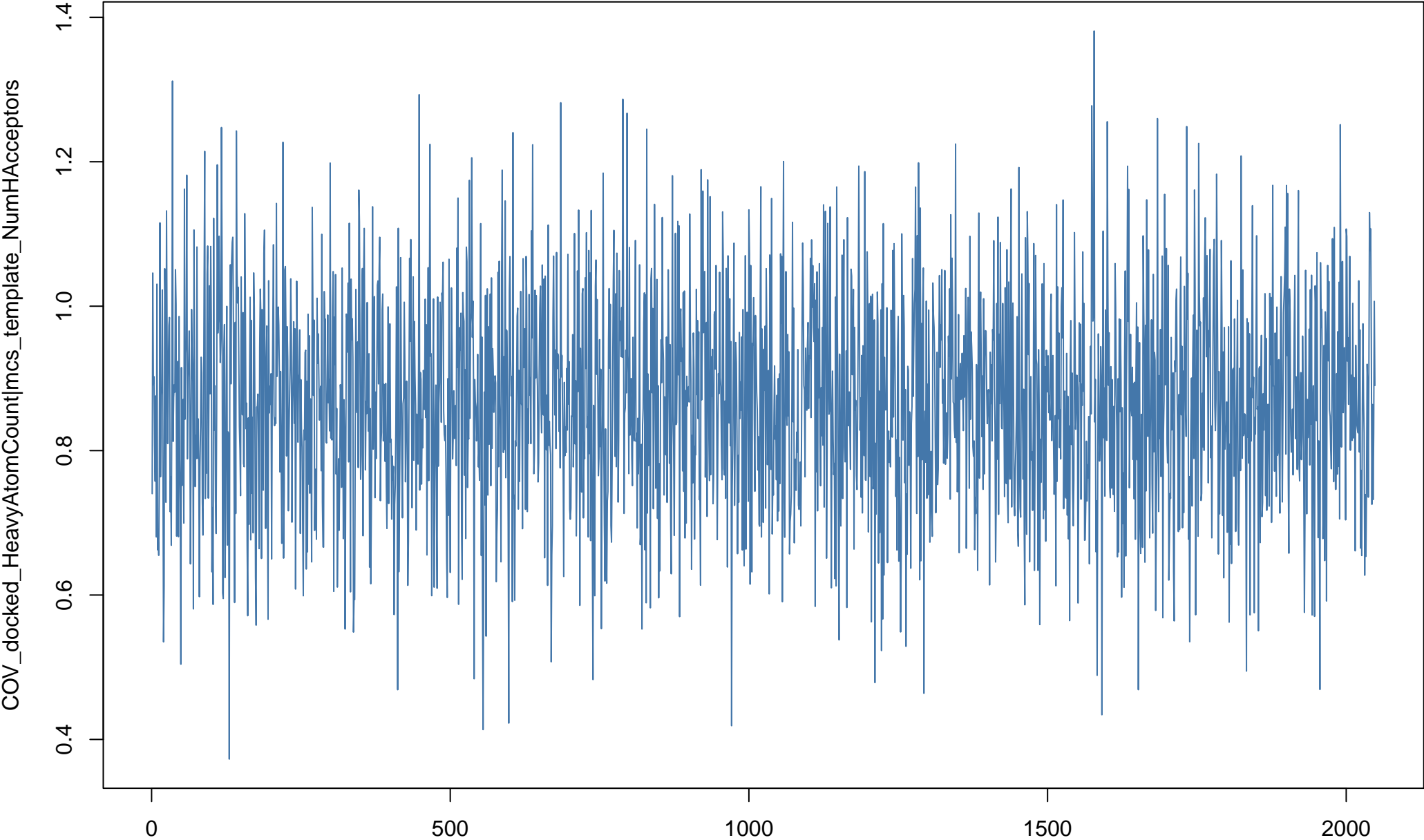
**COV\_docked\_HeavyAtomCount|template\_HeavyAtomCount**  
**ESS = 1960 | BMK = 0.0395 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0**



**COV\_docked\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0386 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0**

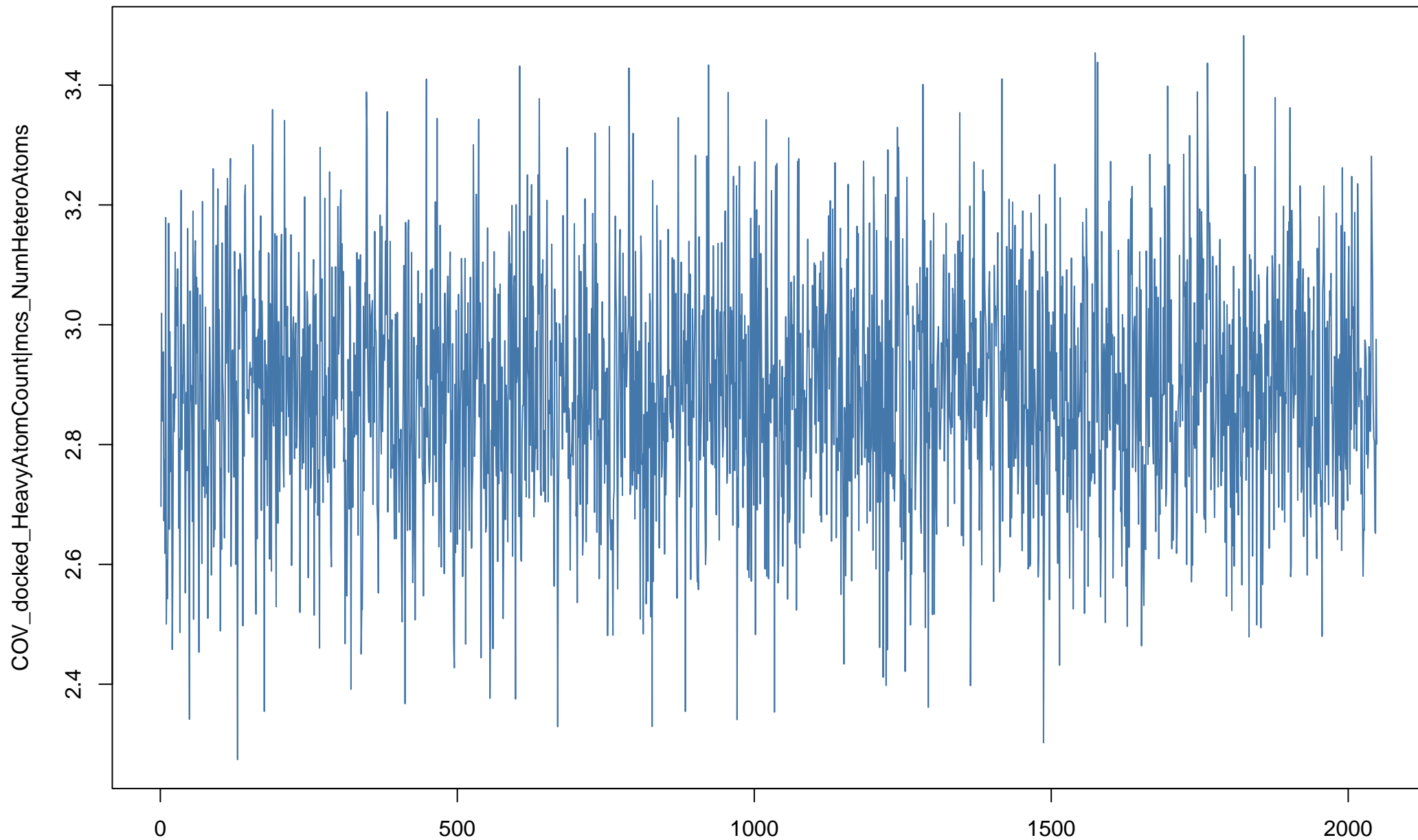


**COV\_docked\_HeavyAtomCount|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0374 | MCSE(6.27) = 1.9 | stat: TRUE | burn: 0**

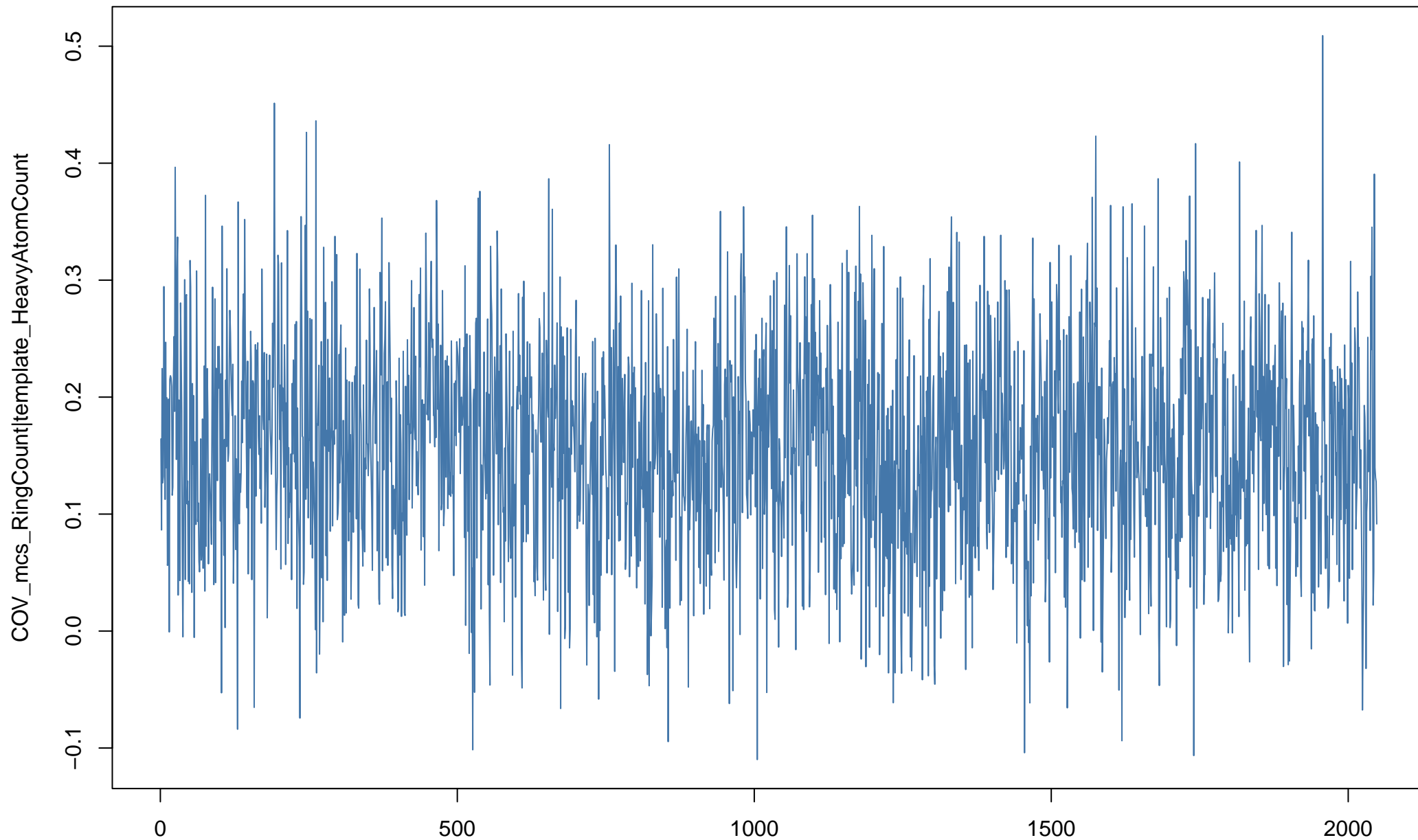




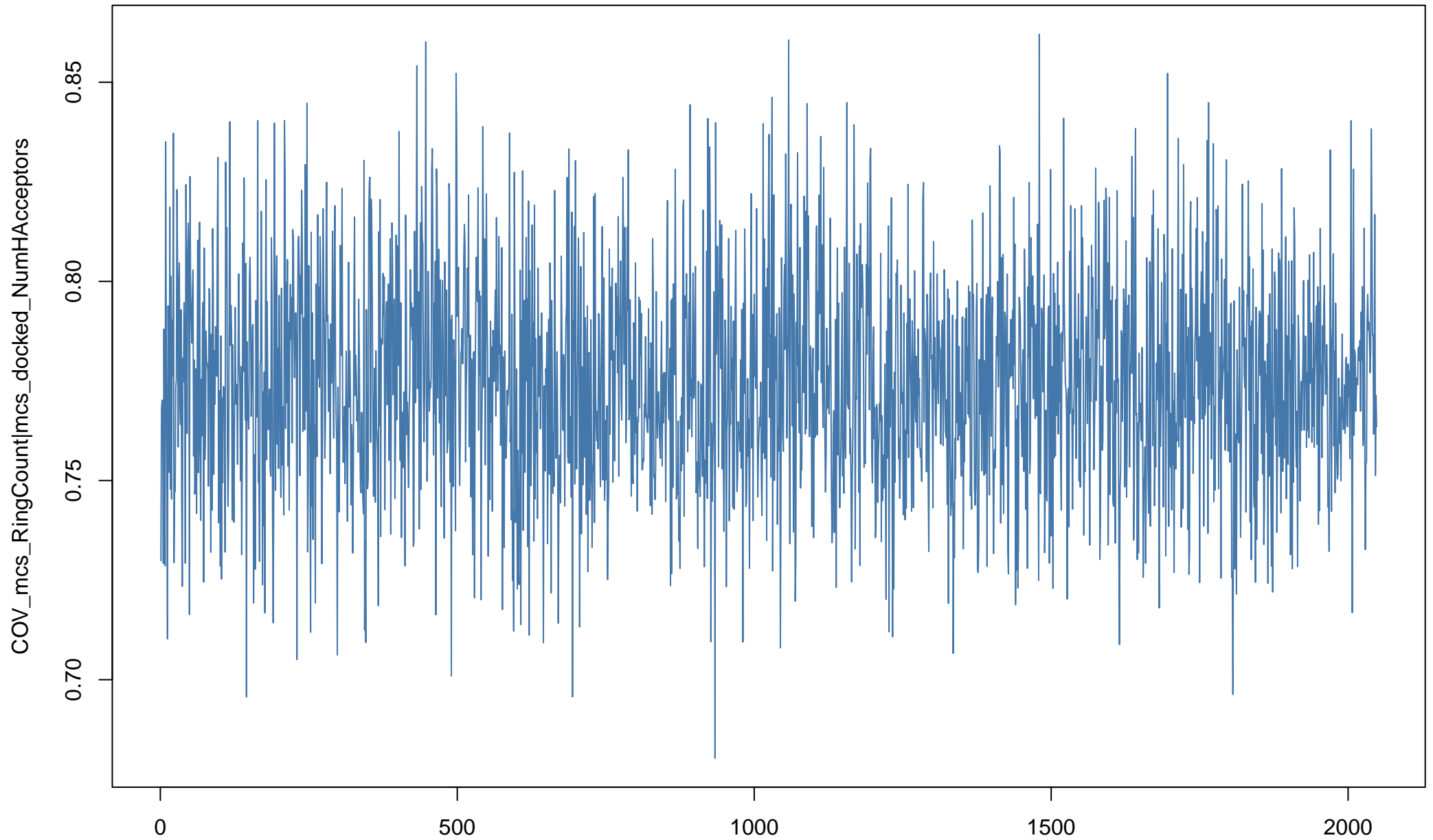
**COV\_docked\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0367 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0**



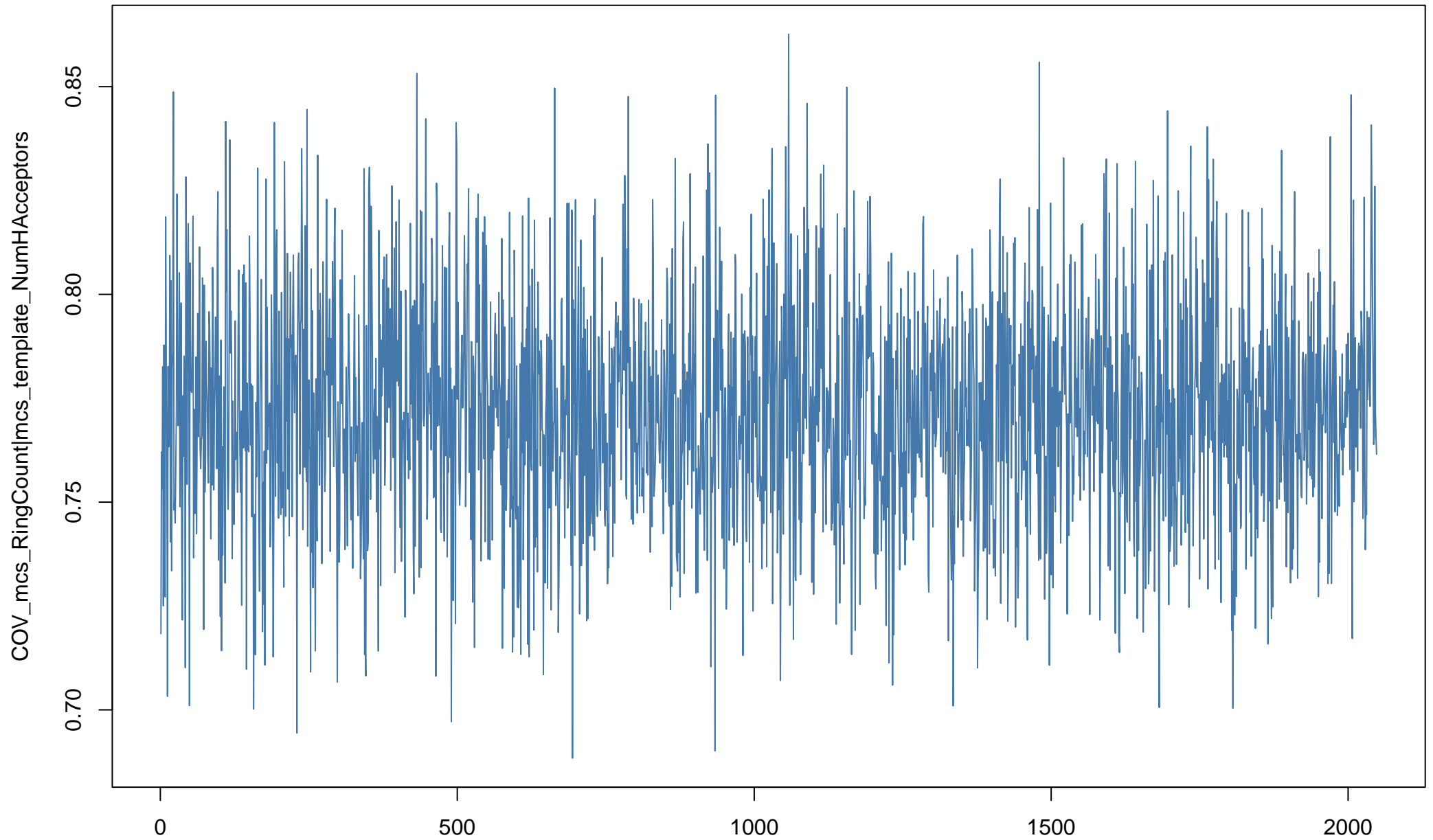
**COV\_mcs\_RingCount|template\_HeavyAtomCount**  
**ESS = 1660 | BMK = 0.0494 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0**



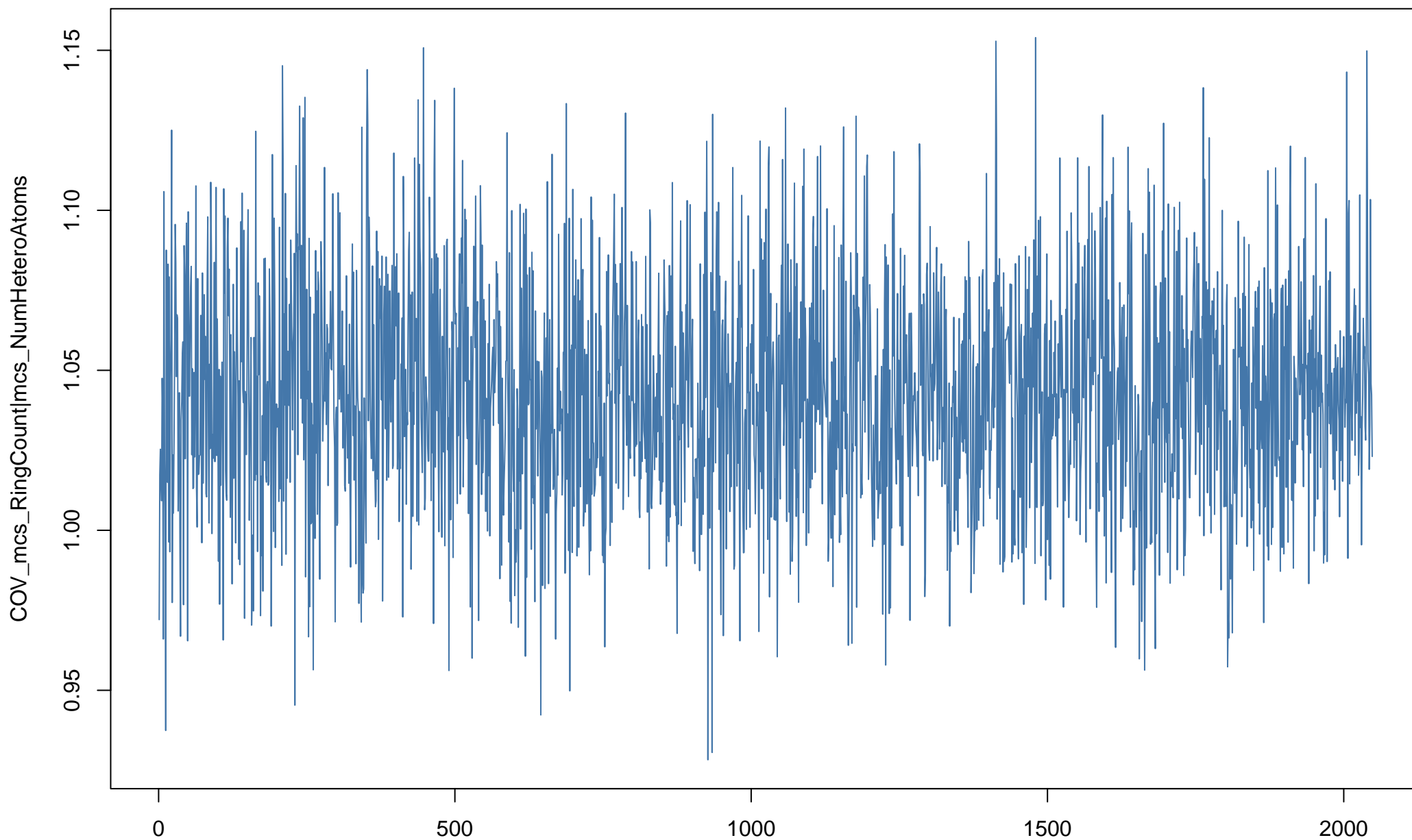
**COV\_mcs\_RingCount|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0513 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0**



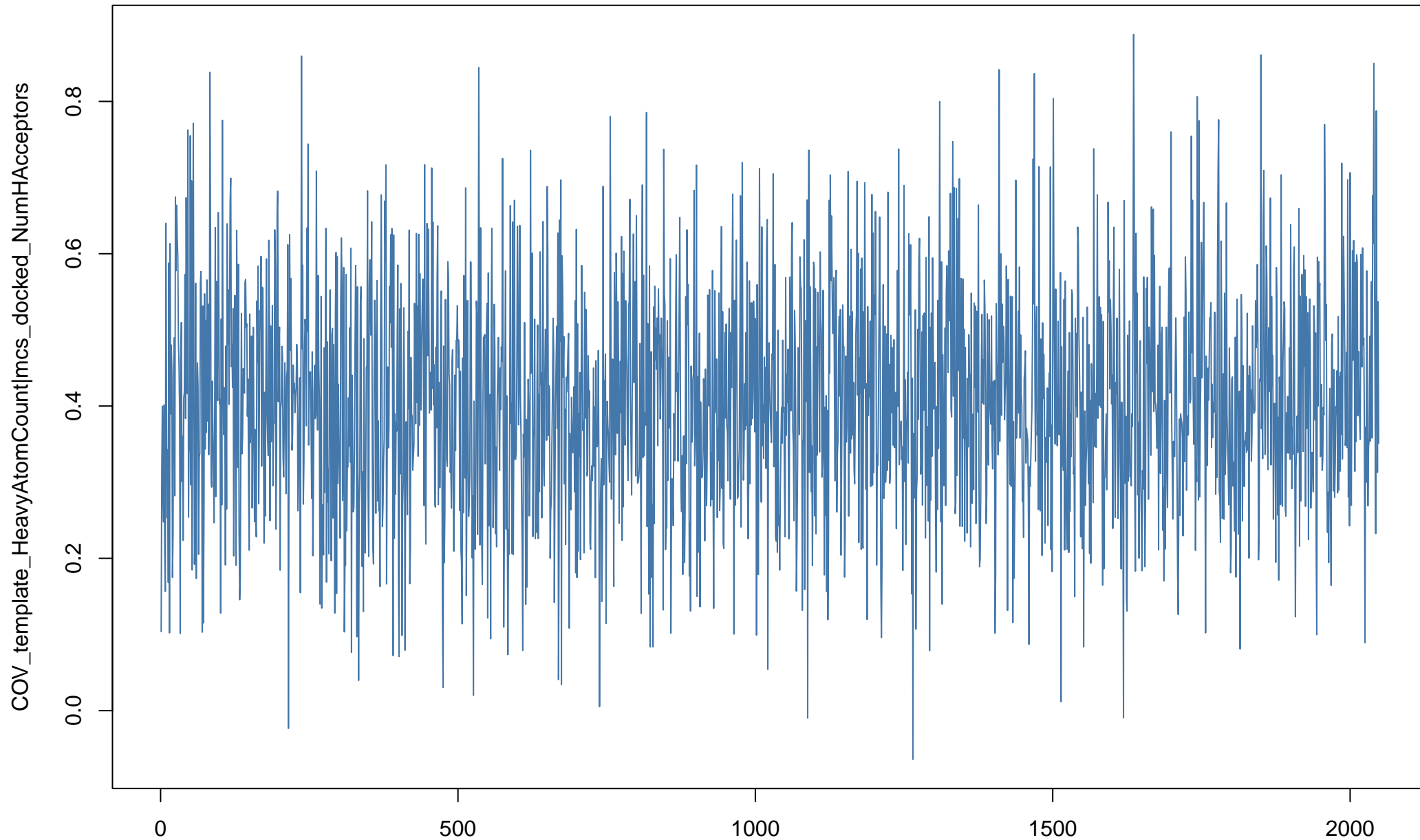
**COV\_mcs\_RingCount|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0413 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0**



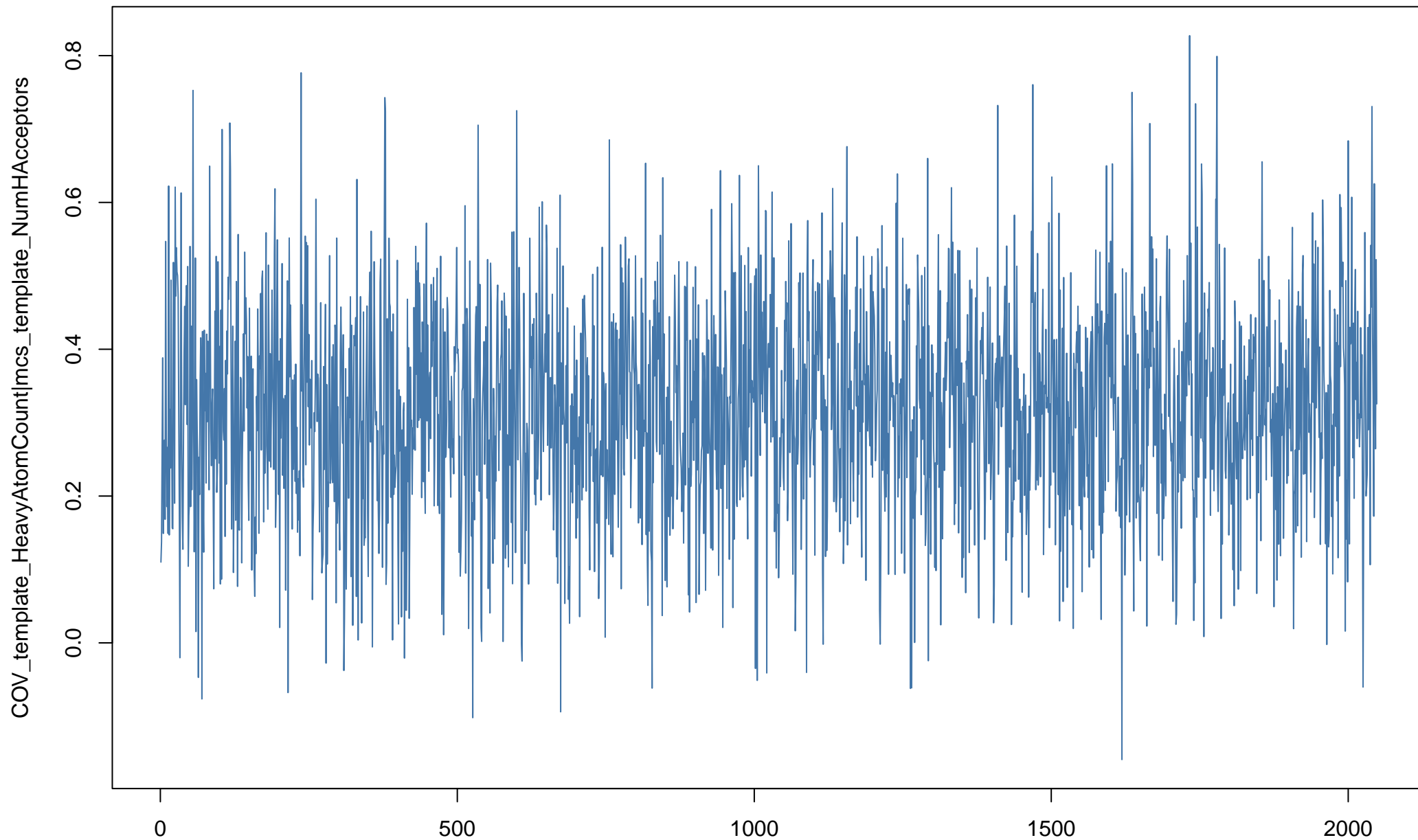
**COV\_mcs\_RingCount|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0658 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0**



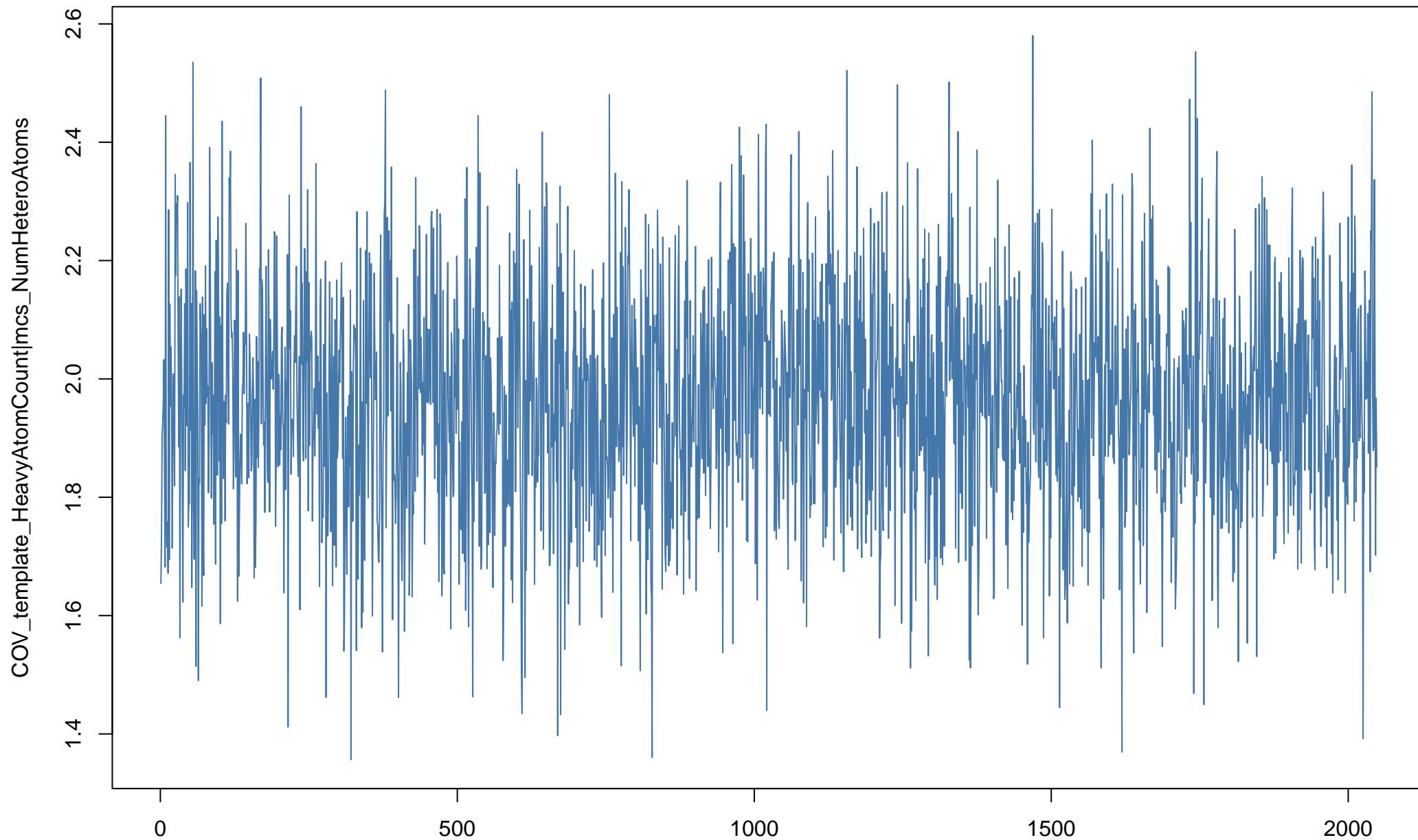
**COV\_template\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0615 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0**



**COV\_template\_HeavyAtomCount|mcs\_template\_NumHAcceptors**  
**ESS = 1830 | BMK = 0.0491 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0**

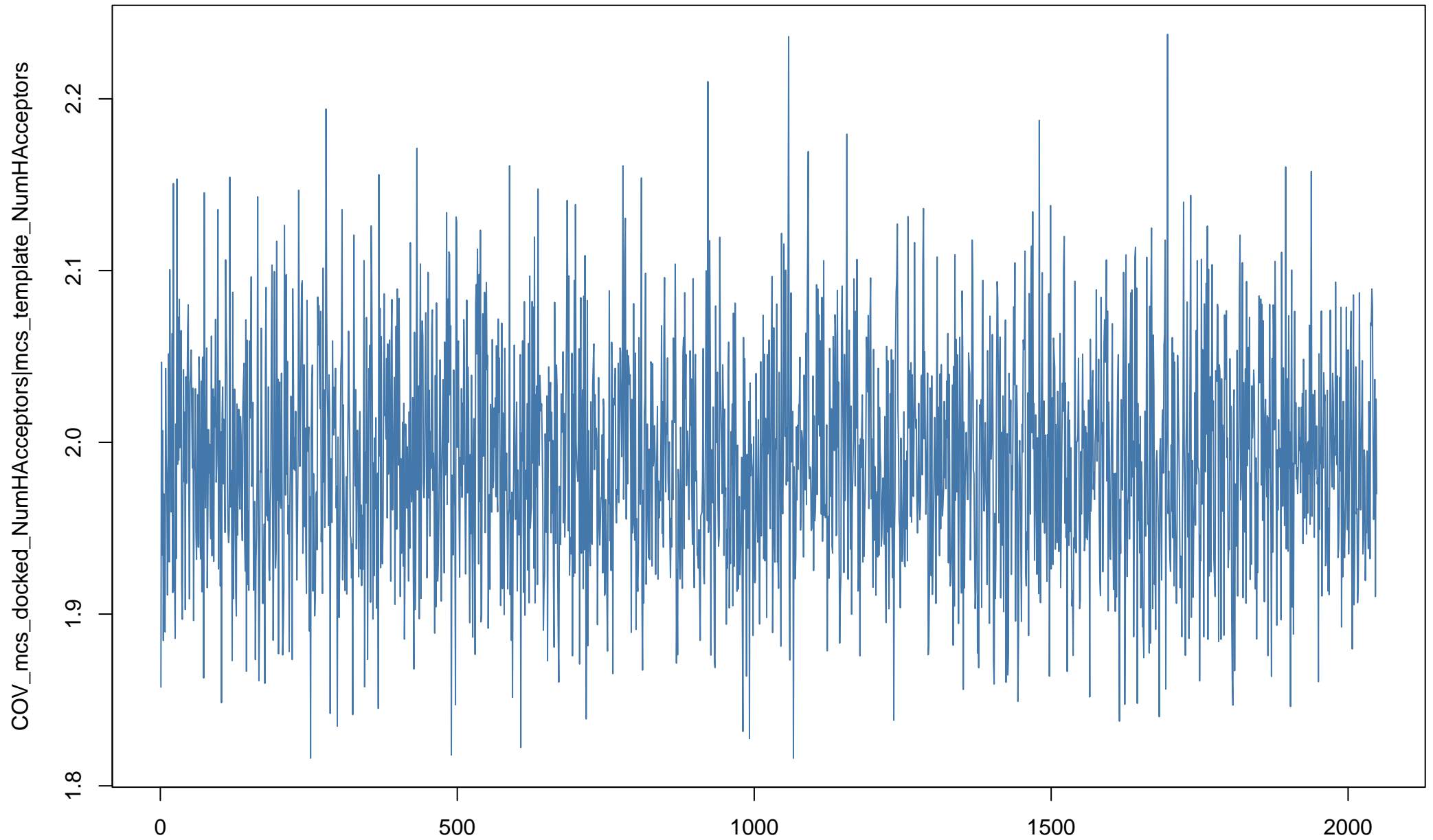


**COV\_template\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 1800 | BMK = 0.0368 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0**

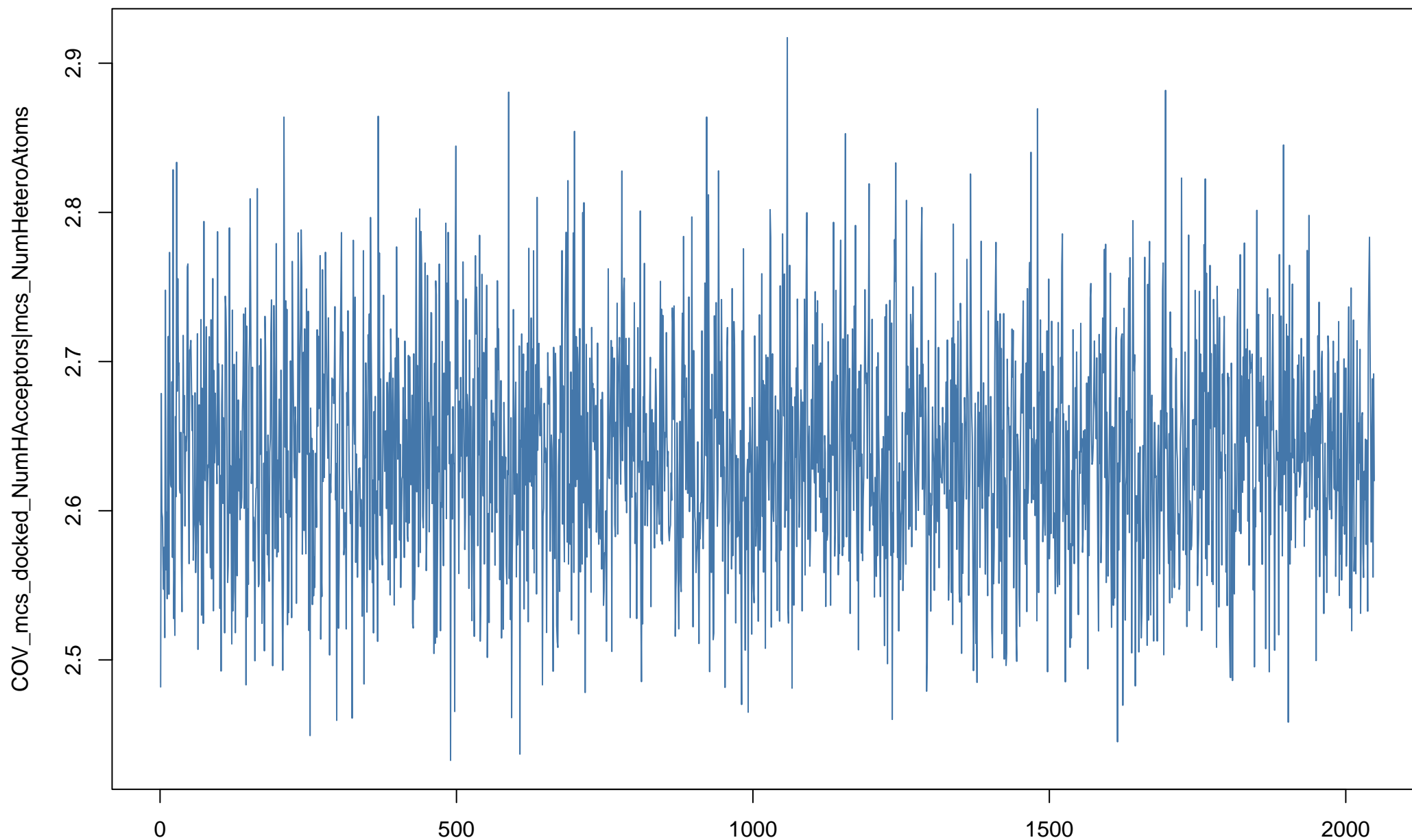




**COV\_mcs\_docked\_NumHAcceptors|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0431 | MCSE(6.27) = 1.85 | stat: TRUE | burn: 0**



**COV\_mcs\_docked\_NumHAcceptors|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.029 | MCSE(6.27) = 1.76 | stat: TRUE | burn: 0**



**COV\_mcs\_template\_NumHAcceptors|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0466 | MCSE(6.27) = 1.82 | stat: TRUE | burn: 0**

