

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.181470817927167

max MCSE = 9.16447878707828

all stationary: FALSE

burn: 0

-- STATS 2D --

min ESS = 1571.81926731234

max BMK = 0.0774622834026406

max MCSE = 2.74949624018538

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.627852113064889

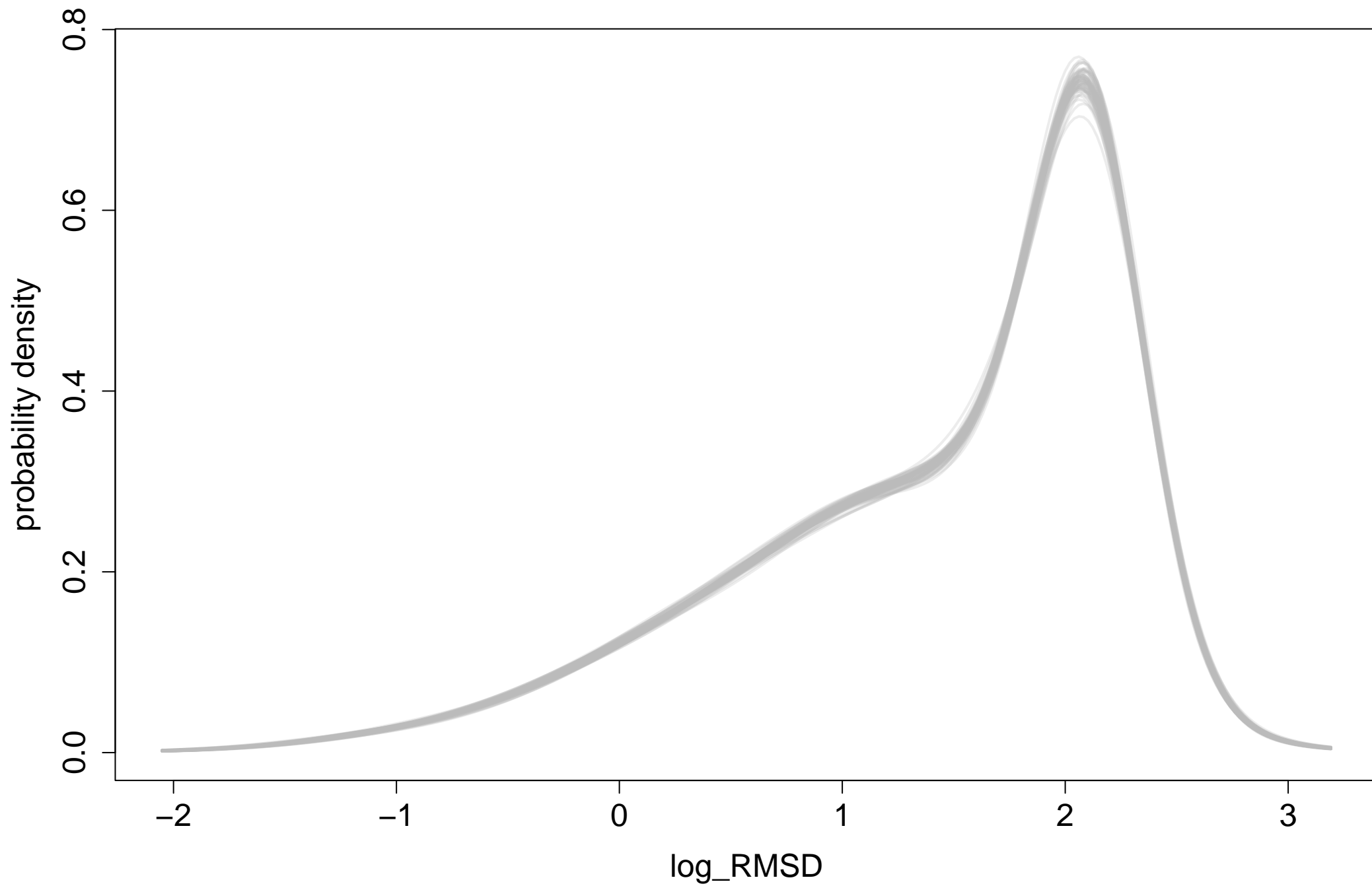
max MCSE = NaN

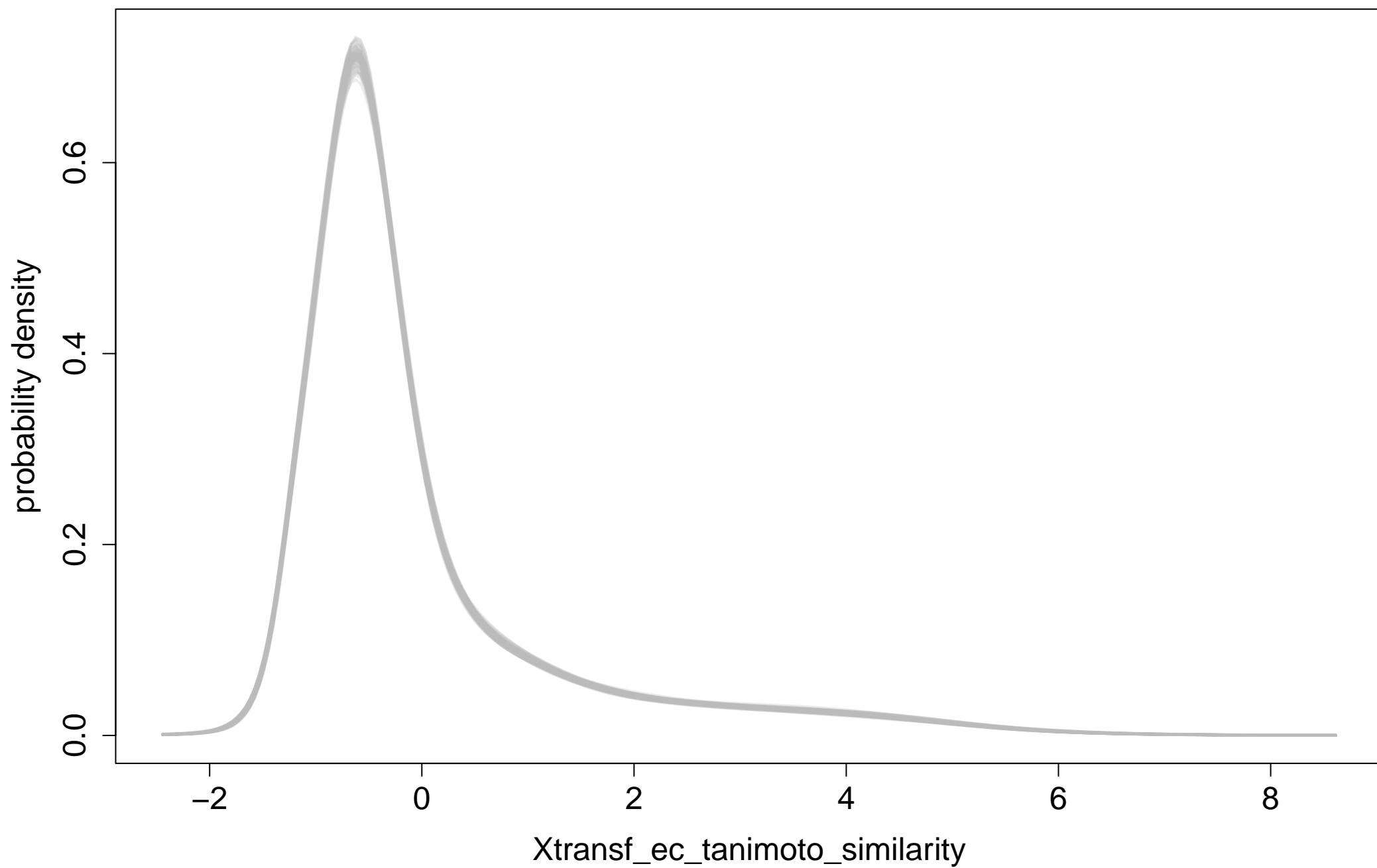
all stationary: FALSE

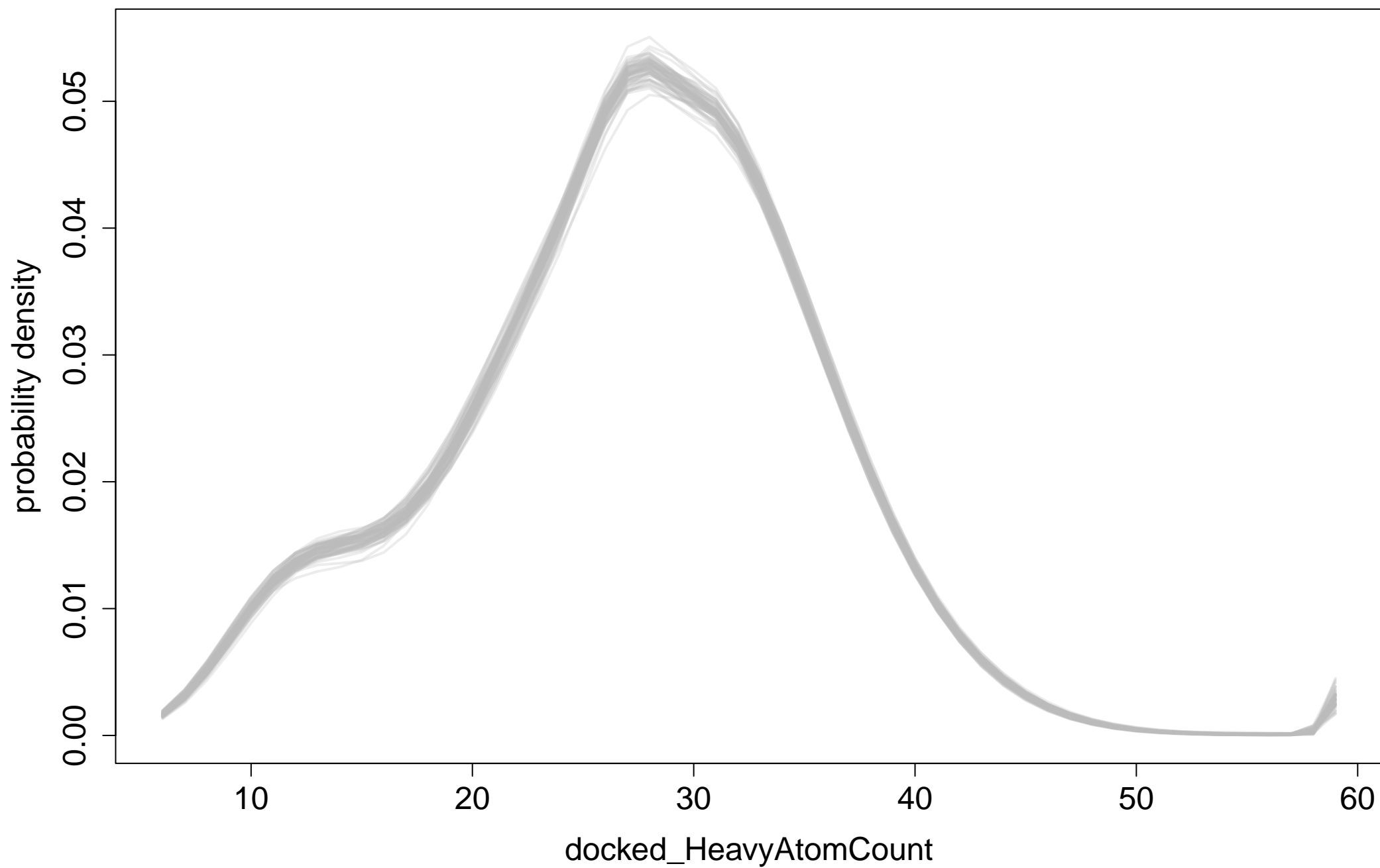
burn: 2040

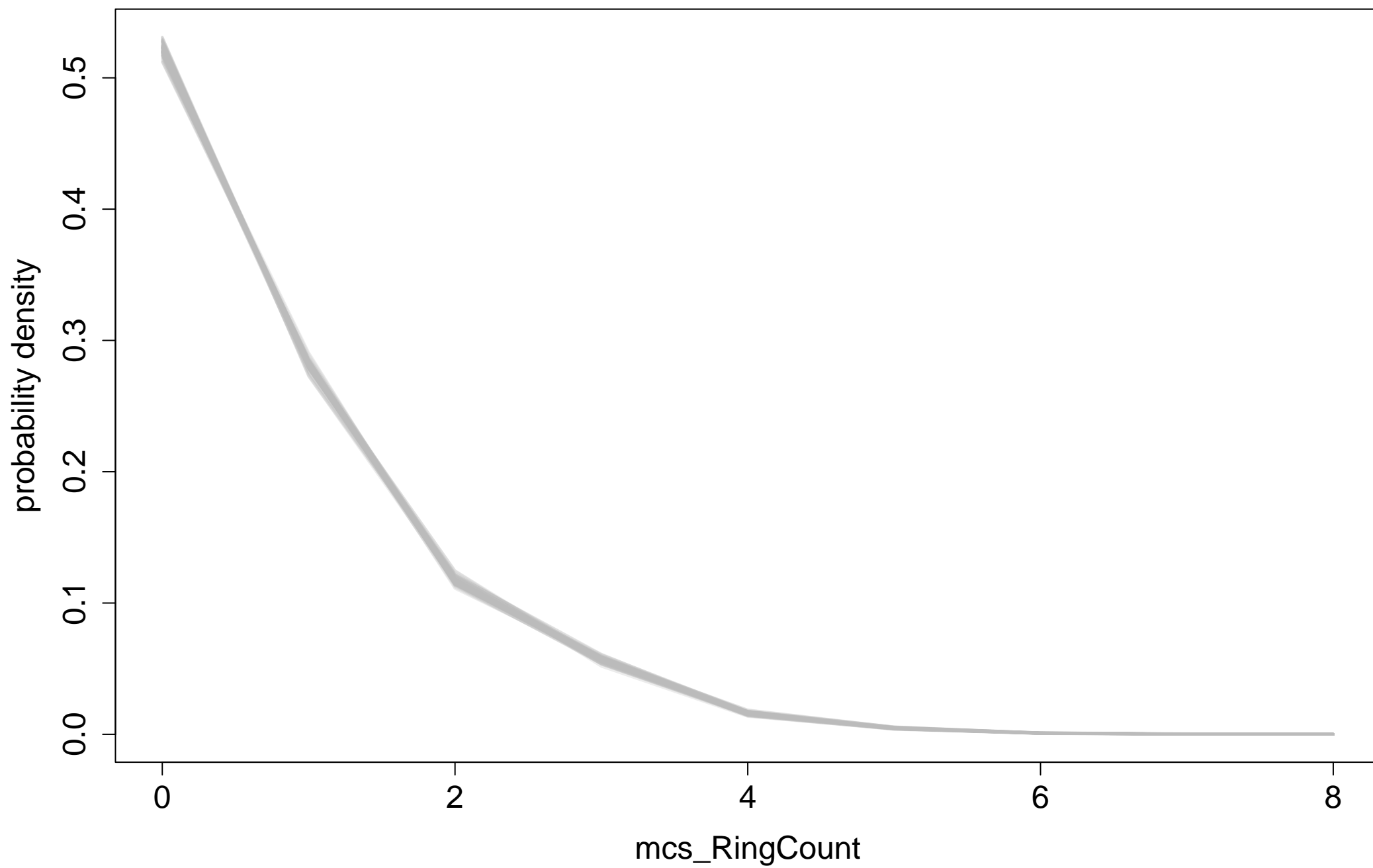
Occupied clusters: 62 of 64

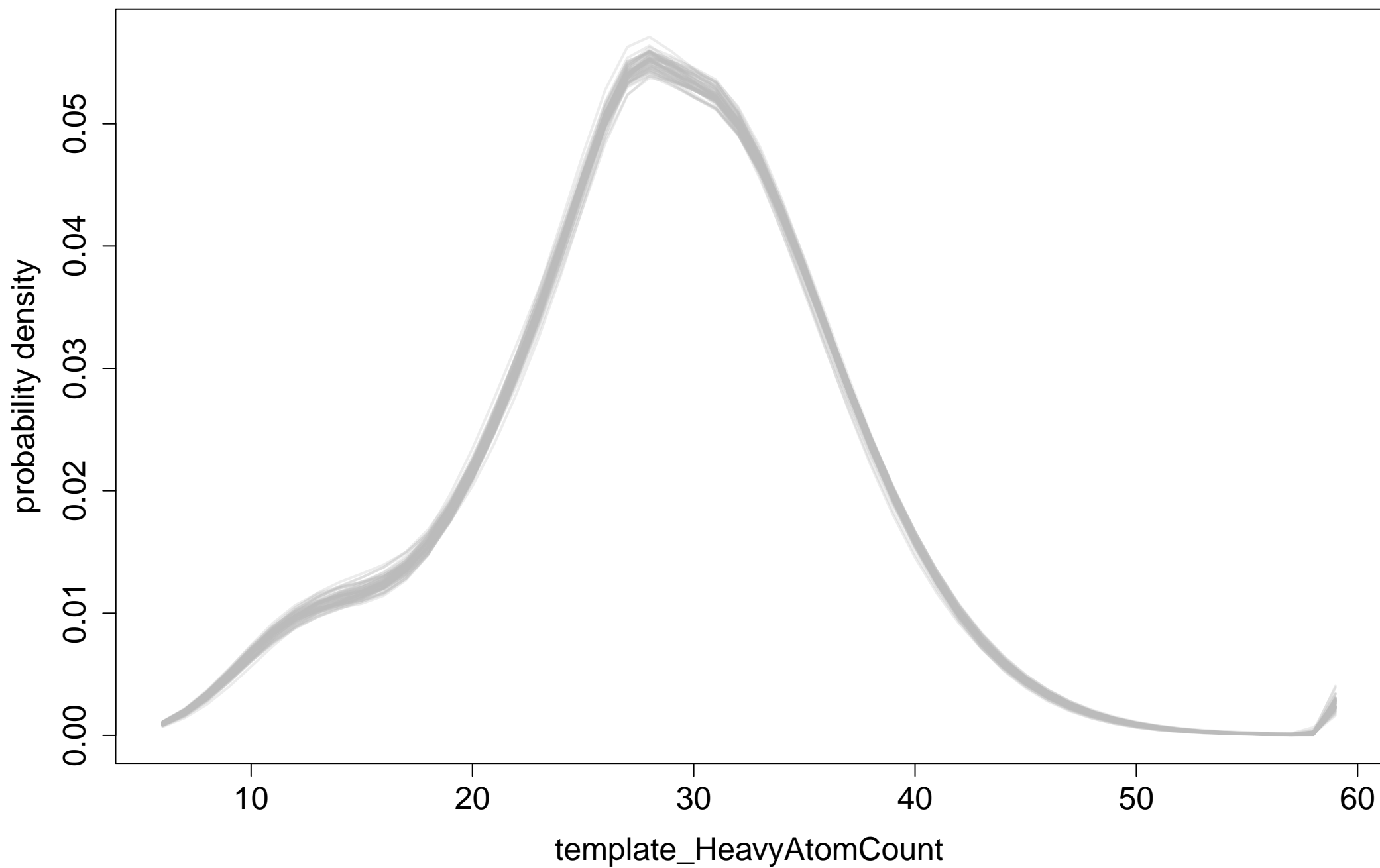
LL: -110000 +- 21.5

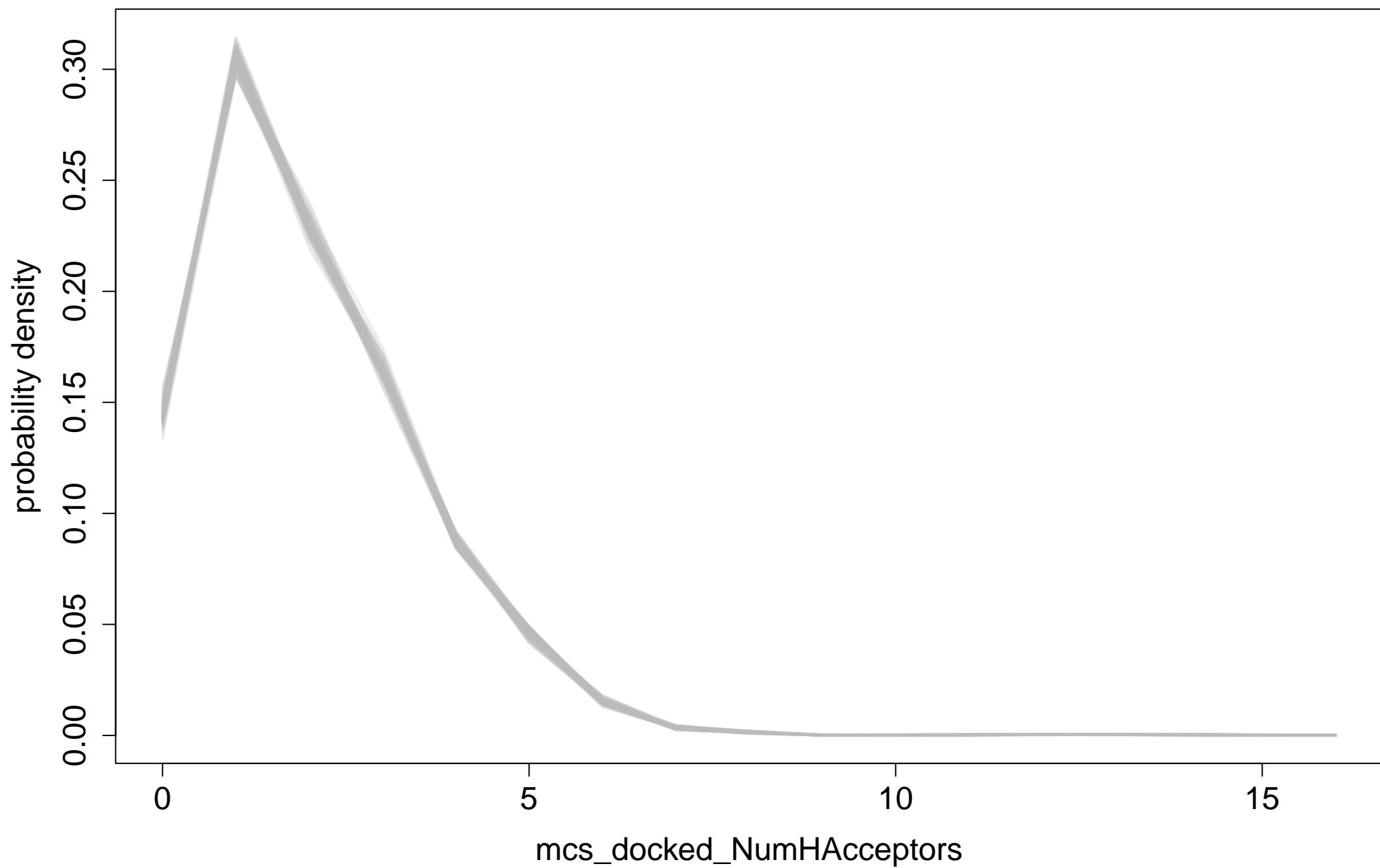


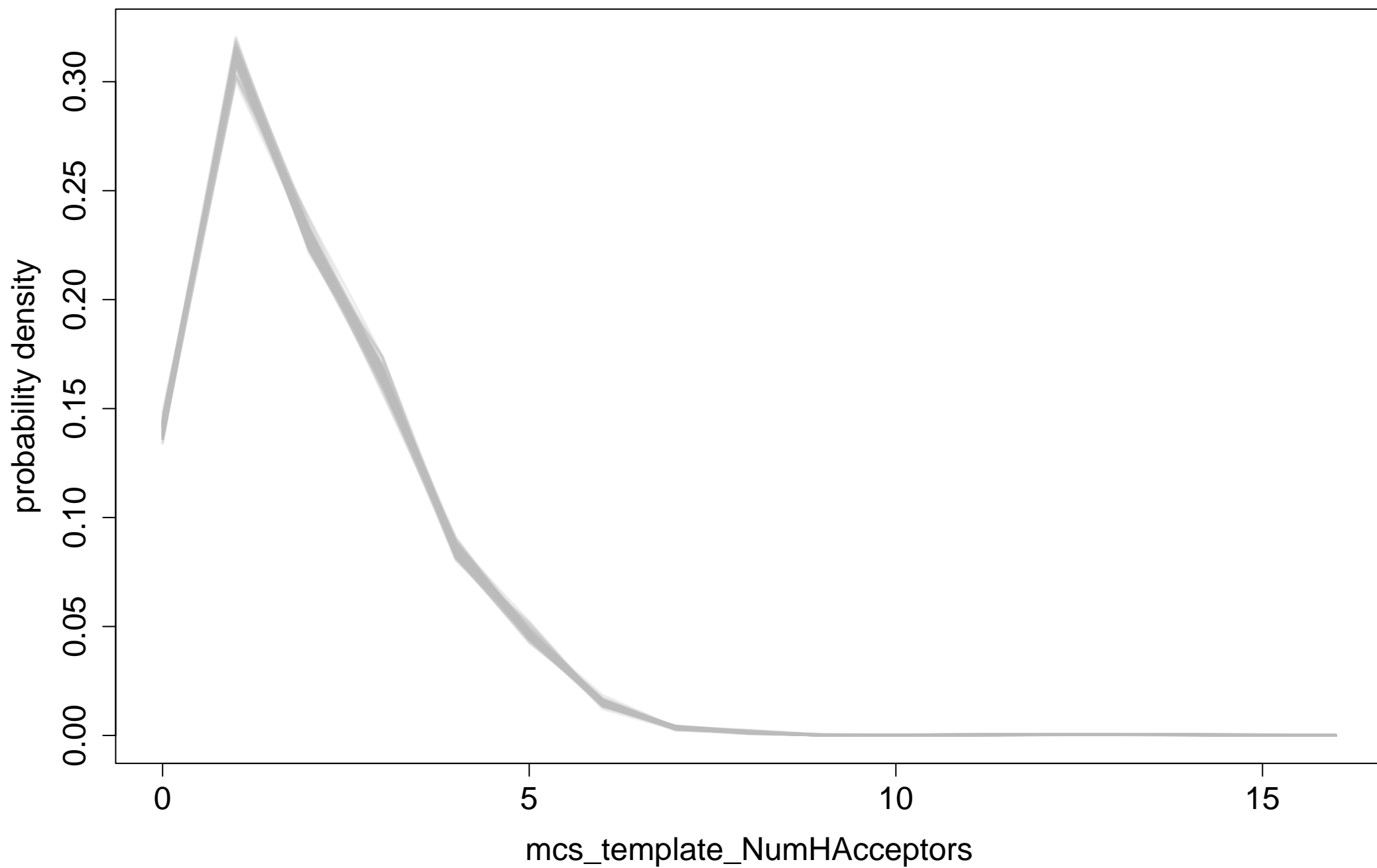




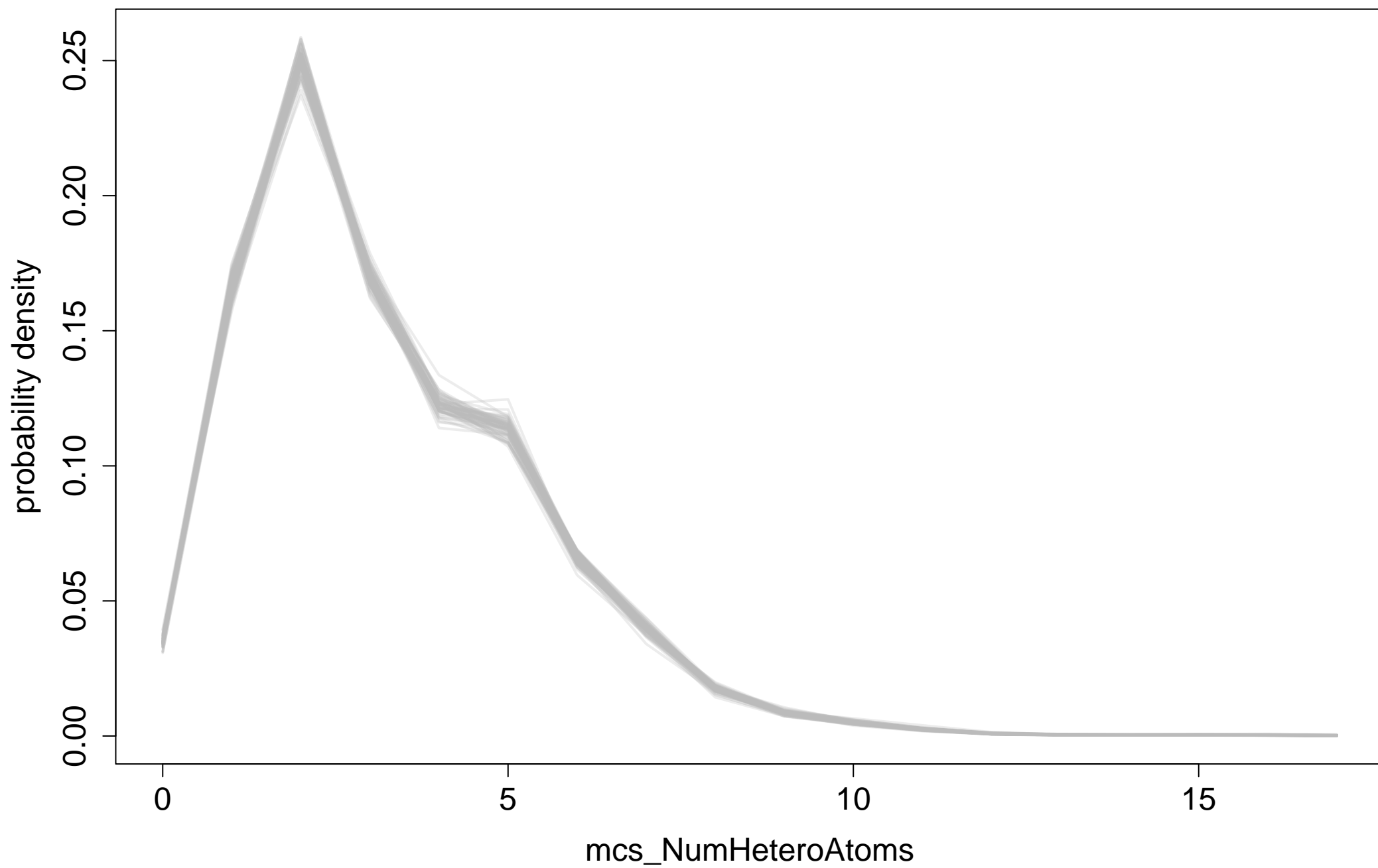


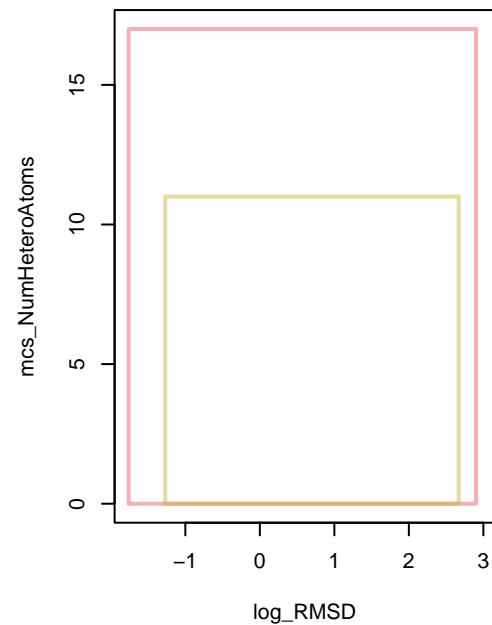
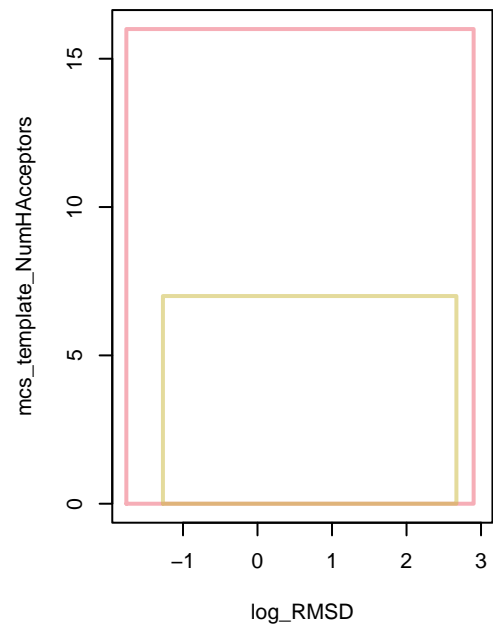
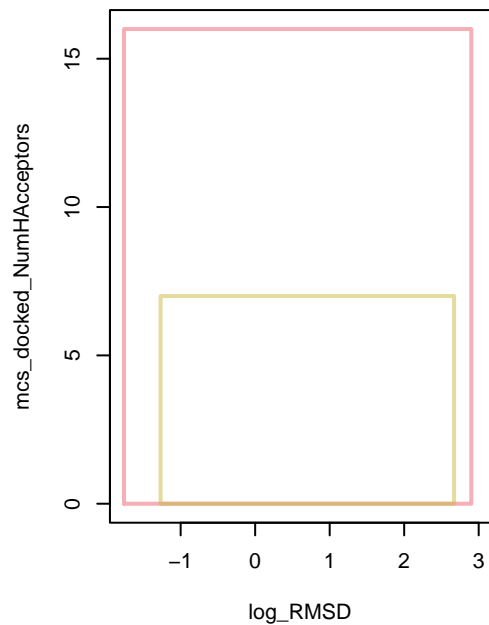
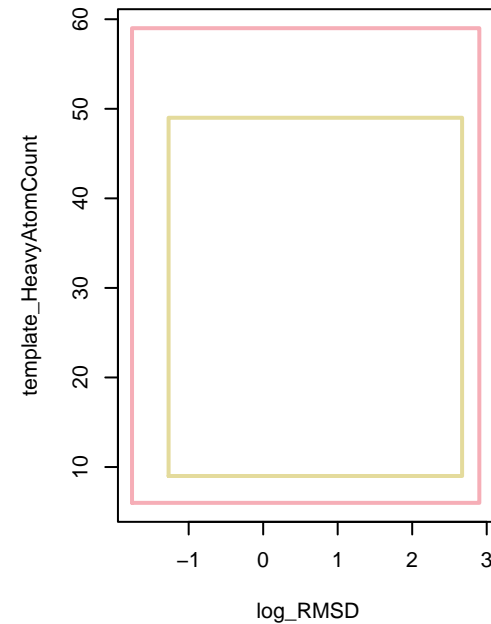
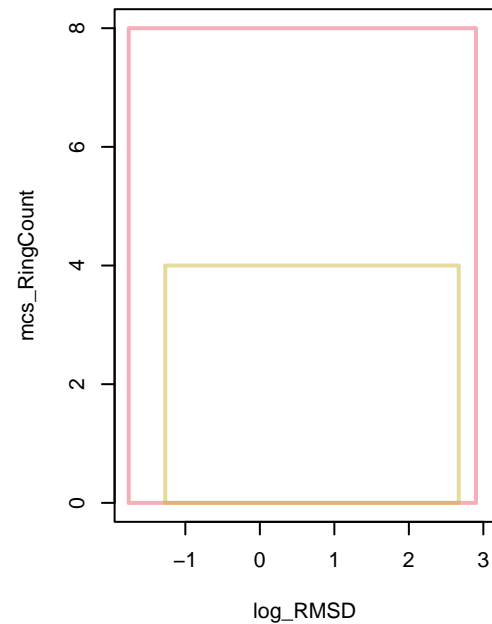
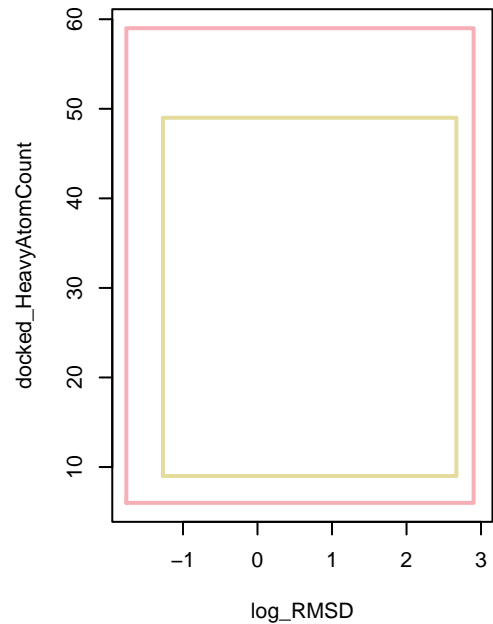
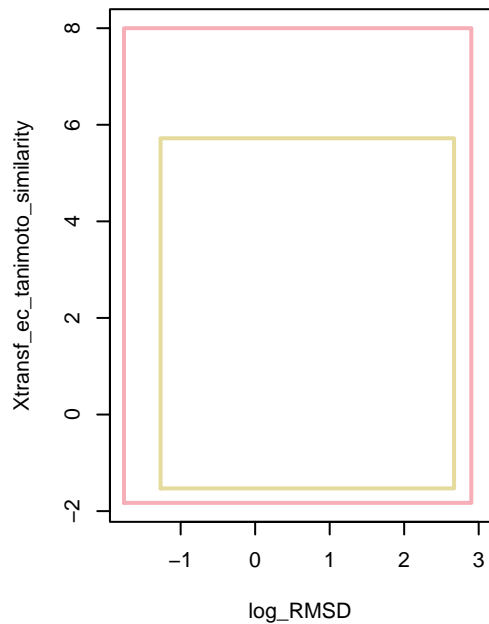




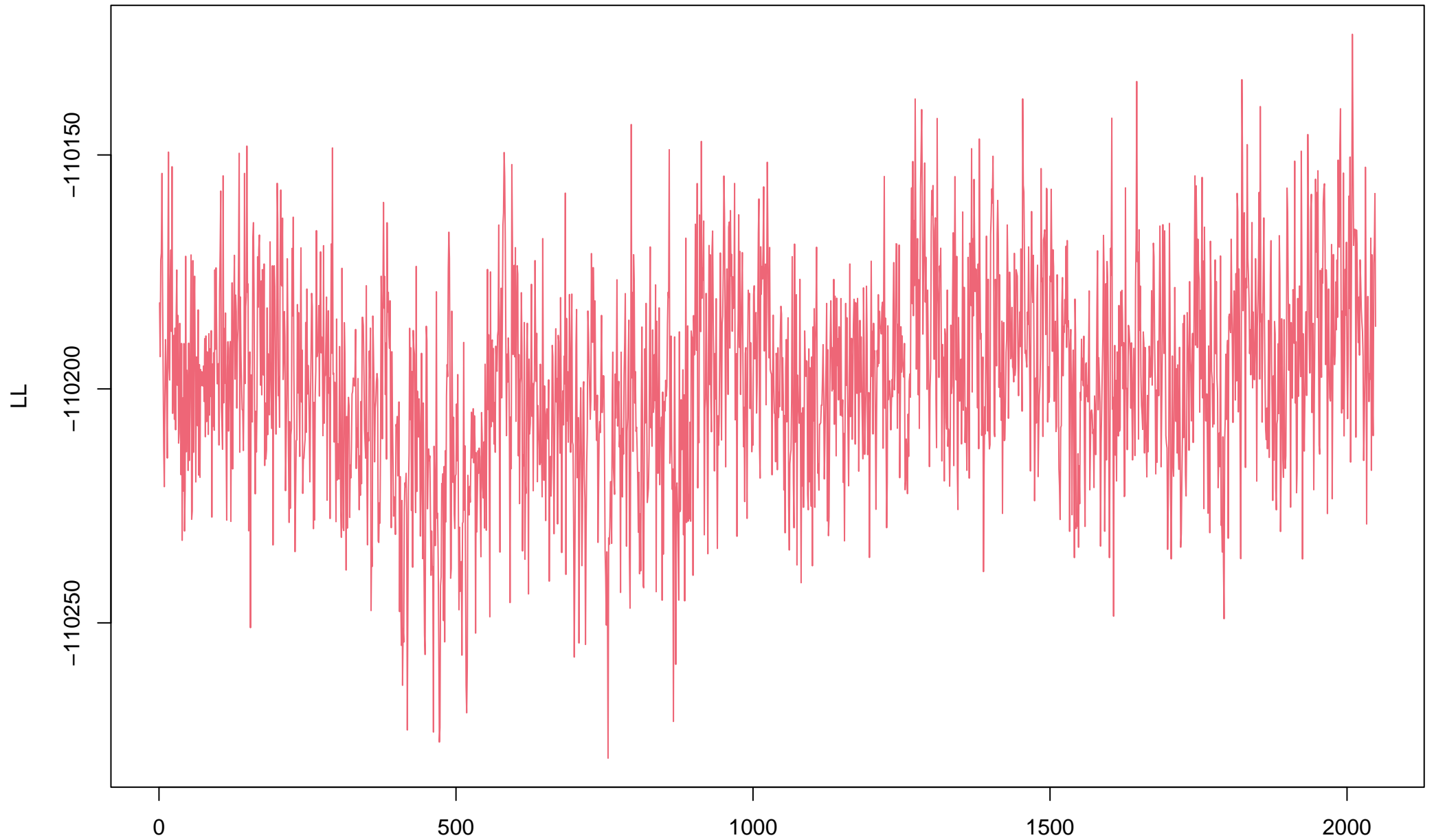




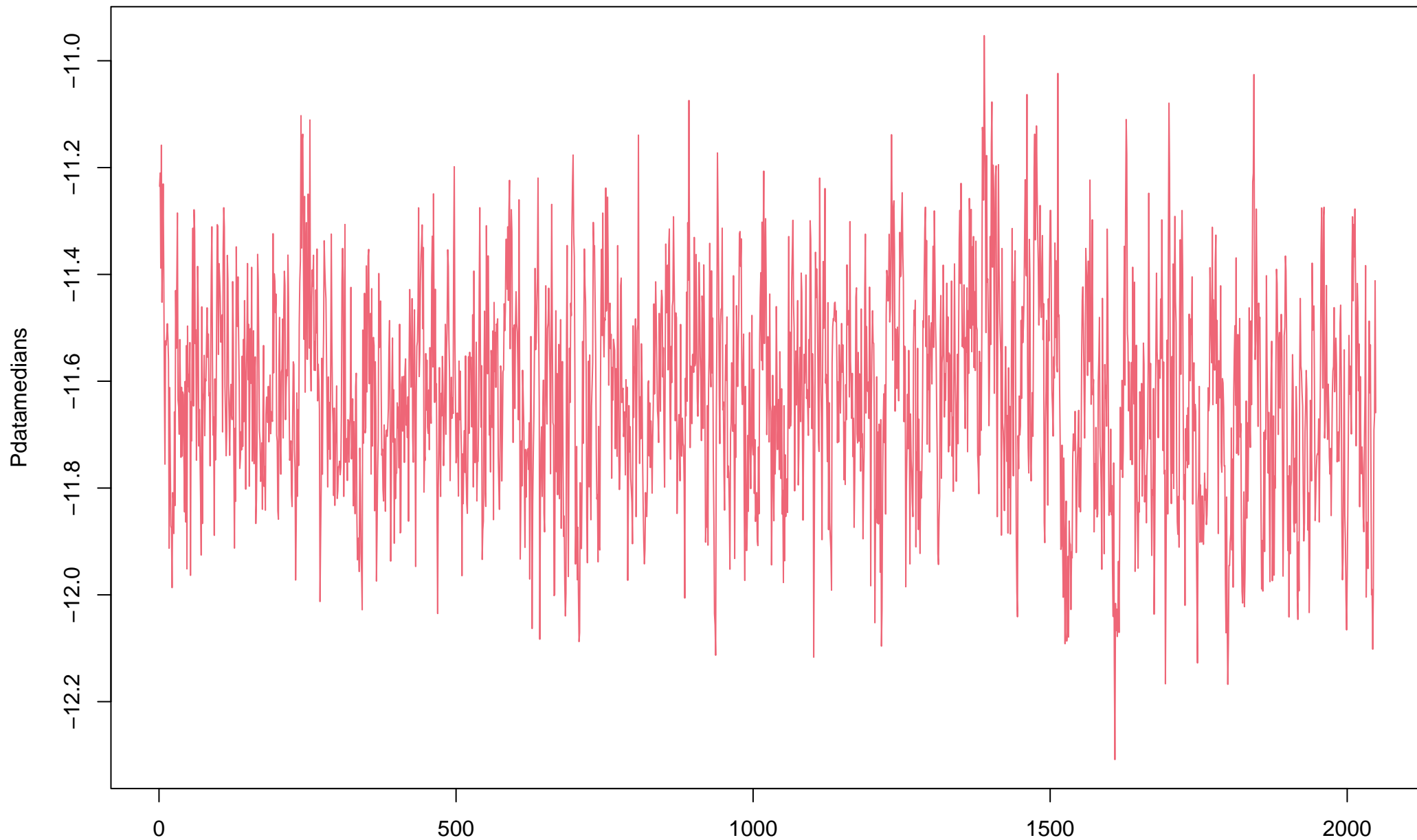




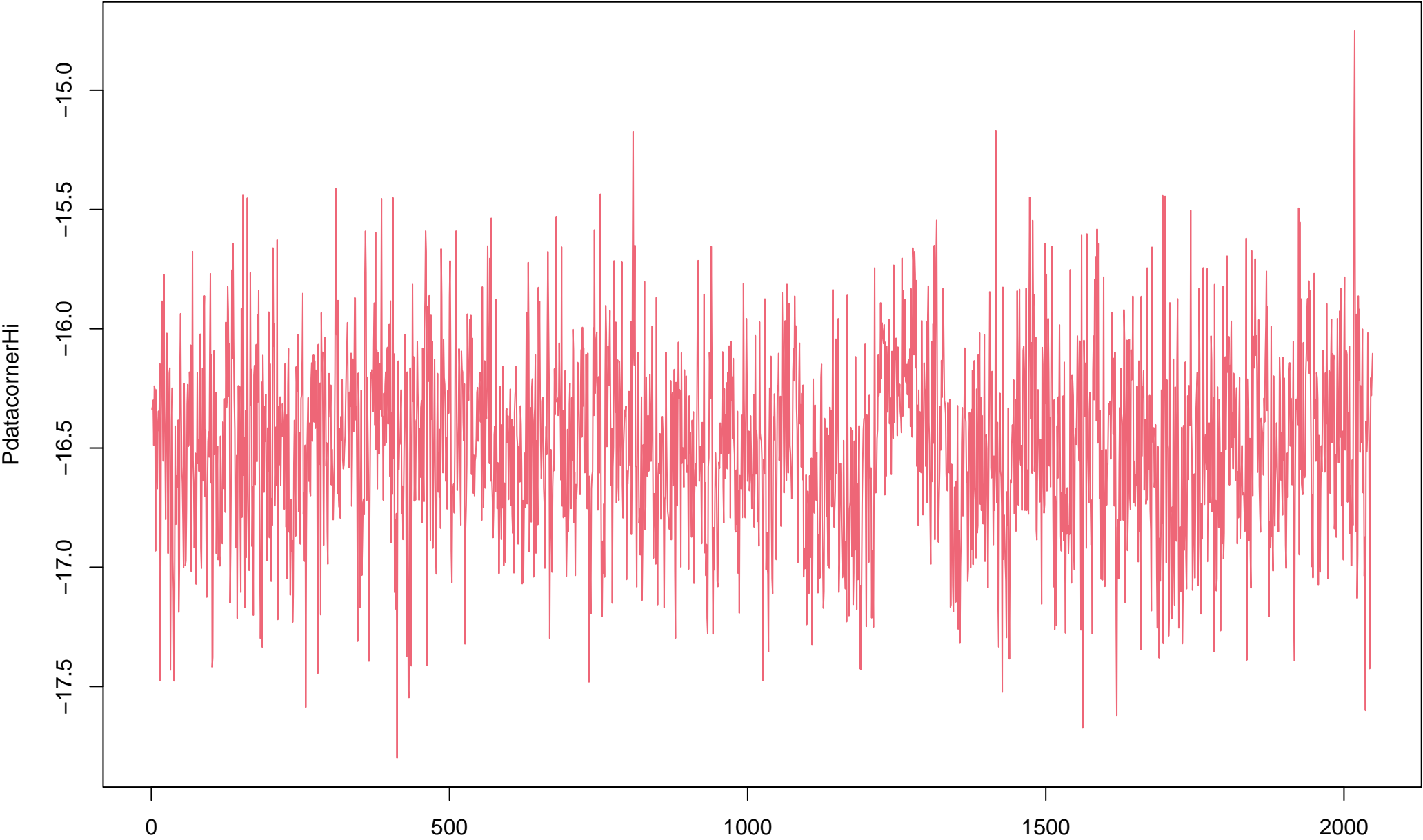
LL  
ESS = 175 | BMK = 0.181 | MCSE(6.27) = 7.22 | stat: TRUE | burn: 0



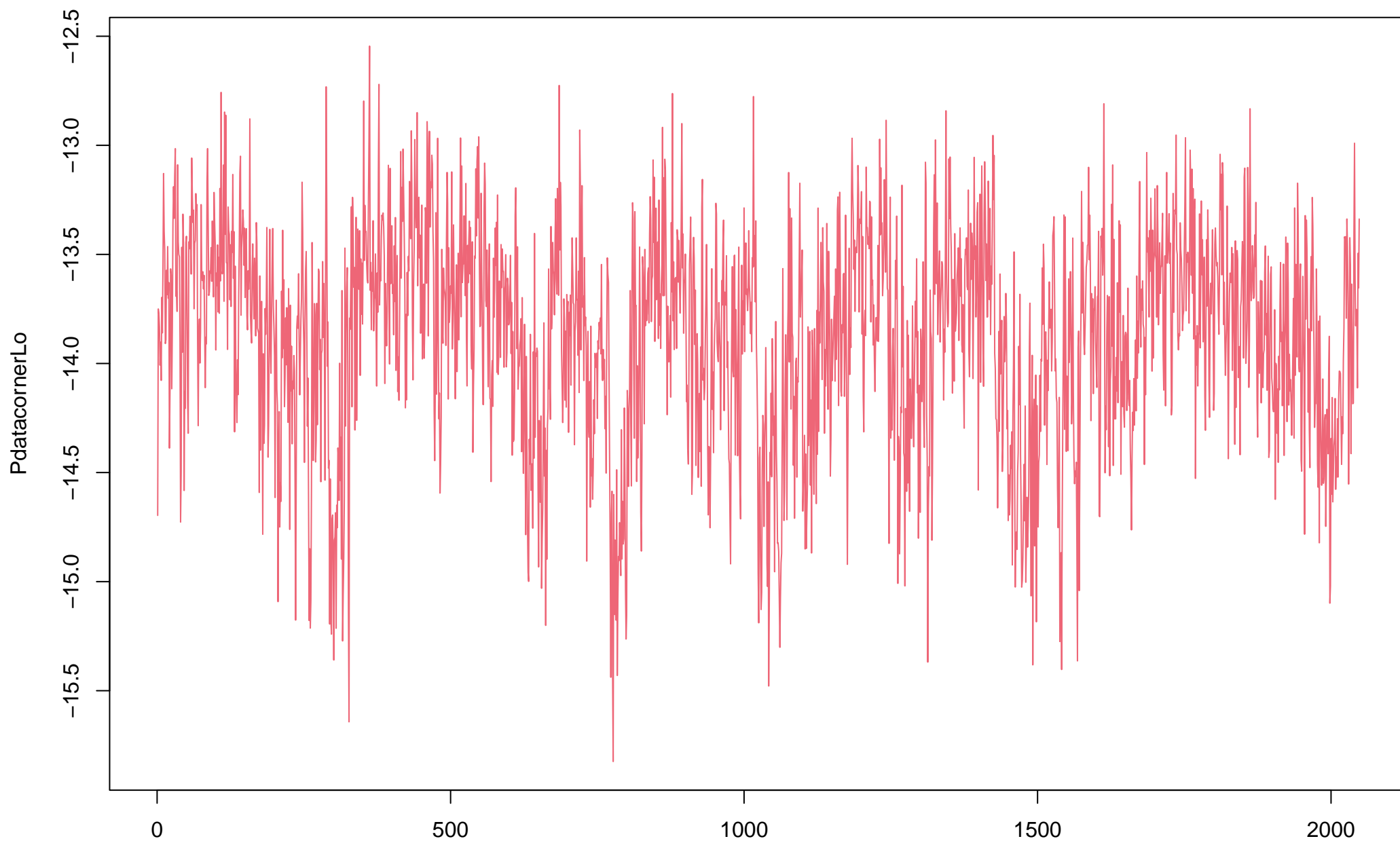
**Pdatamedians**  
**ESS = 393 | BMK = 0.0877 | MCSE(6.27) = 4.7 | stat: TRUE | burn: 0**



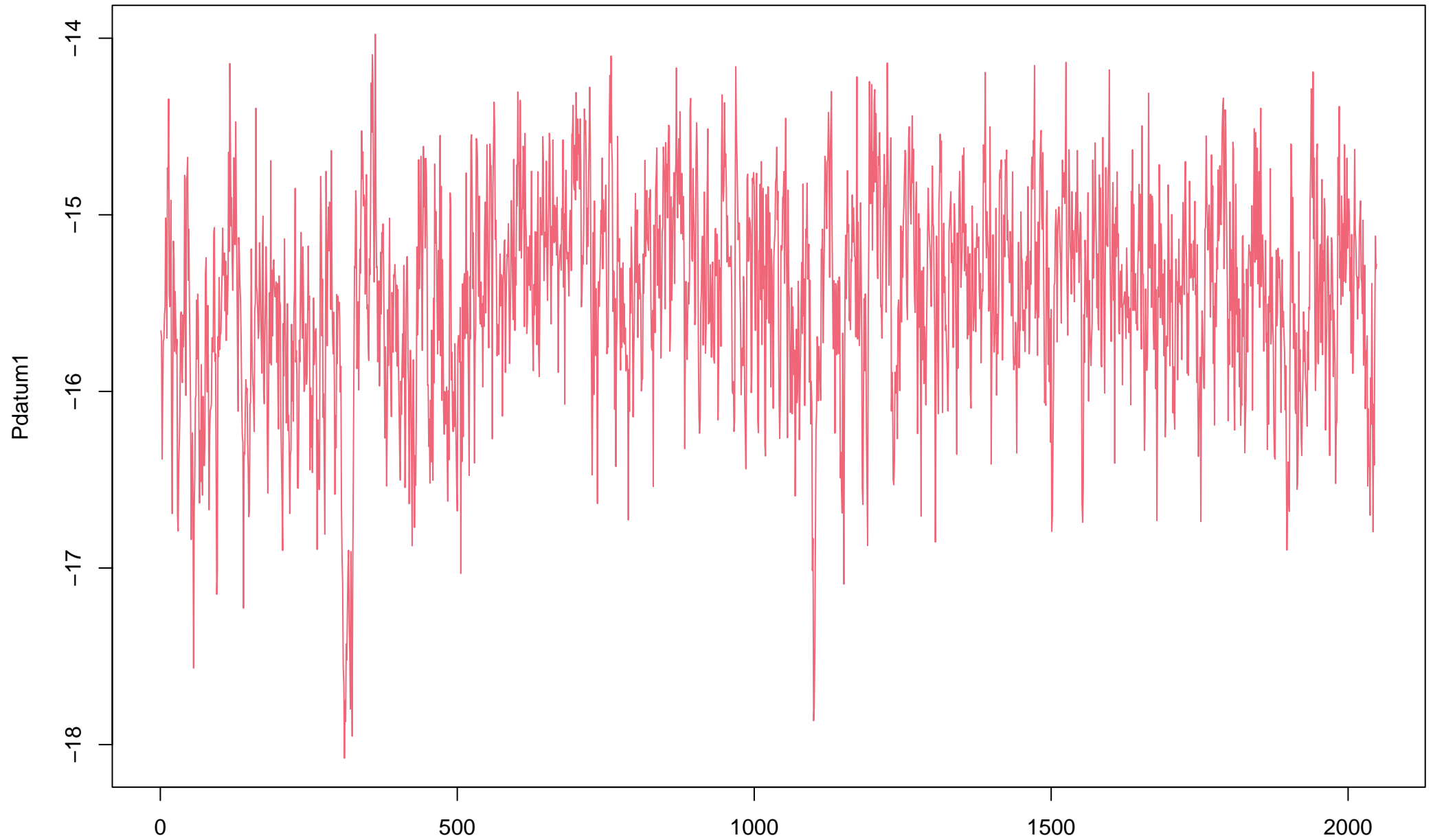
**PdatacornerHi**  
**ESS = 840 | BMK = 0.0681 | MCSE(6.27) = 4.04 | stat: TRUE | burn: 0**



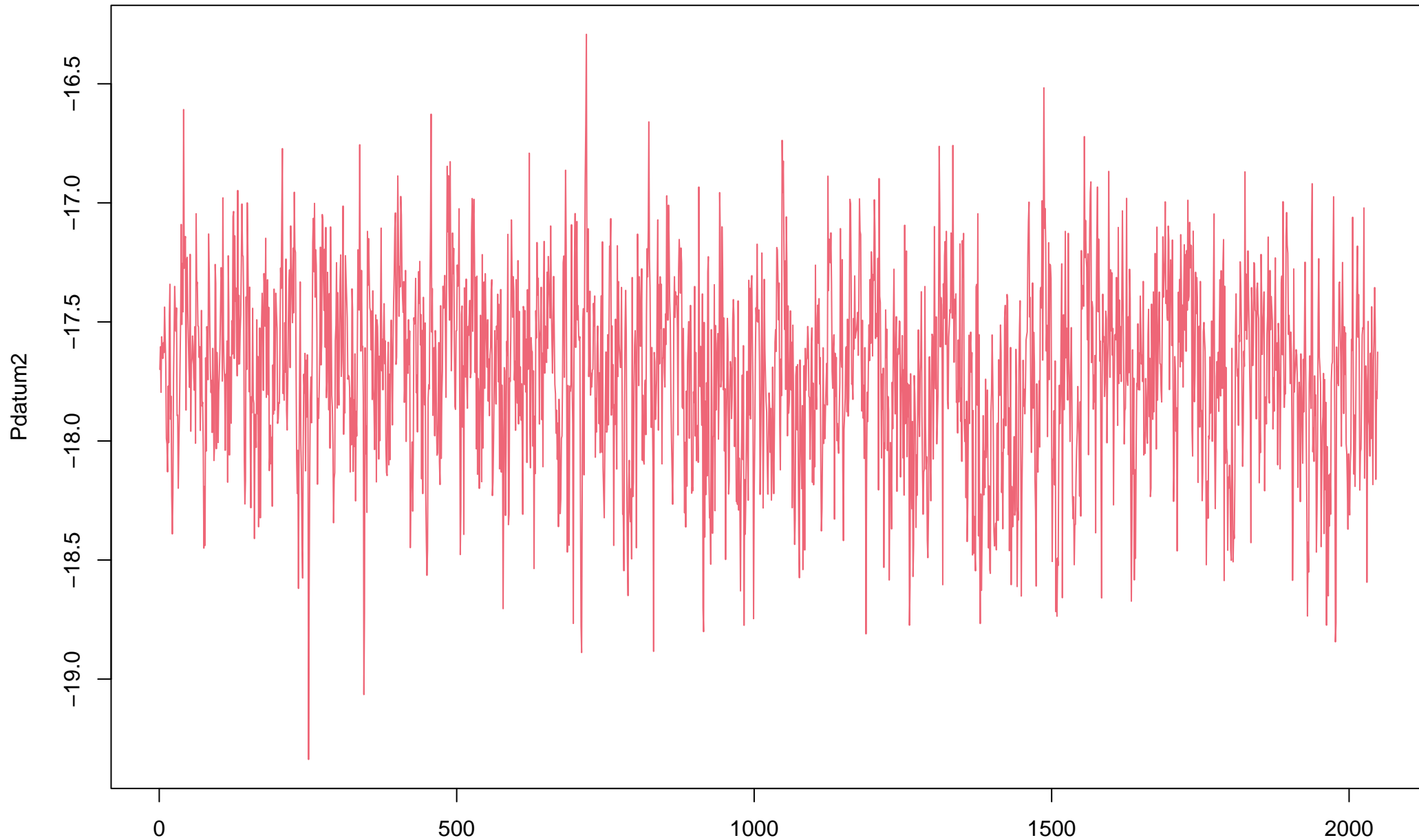
**PdatacornerLo**  
**ESS = 105 | BMK = 0.0858 | MCSE(6.27) = 7.65 | stat: FALSE | burn: 0**



**Pdatum1**  
**ESS = 295 | BMK = 0.0744 | MCSE(6.27) = 5.82 | stat: FALSE | burn: 0**

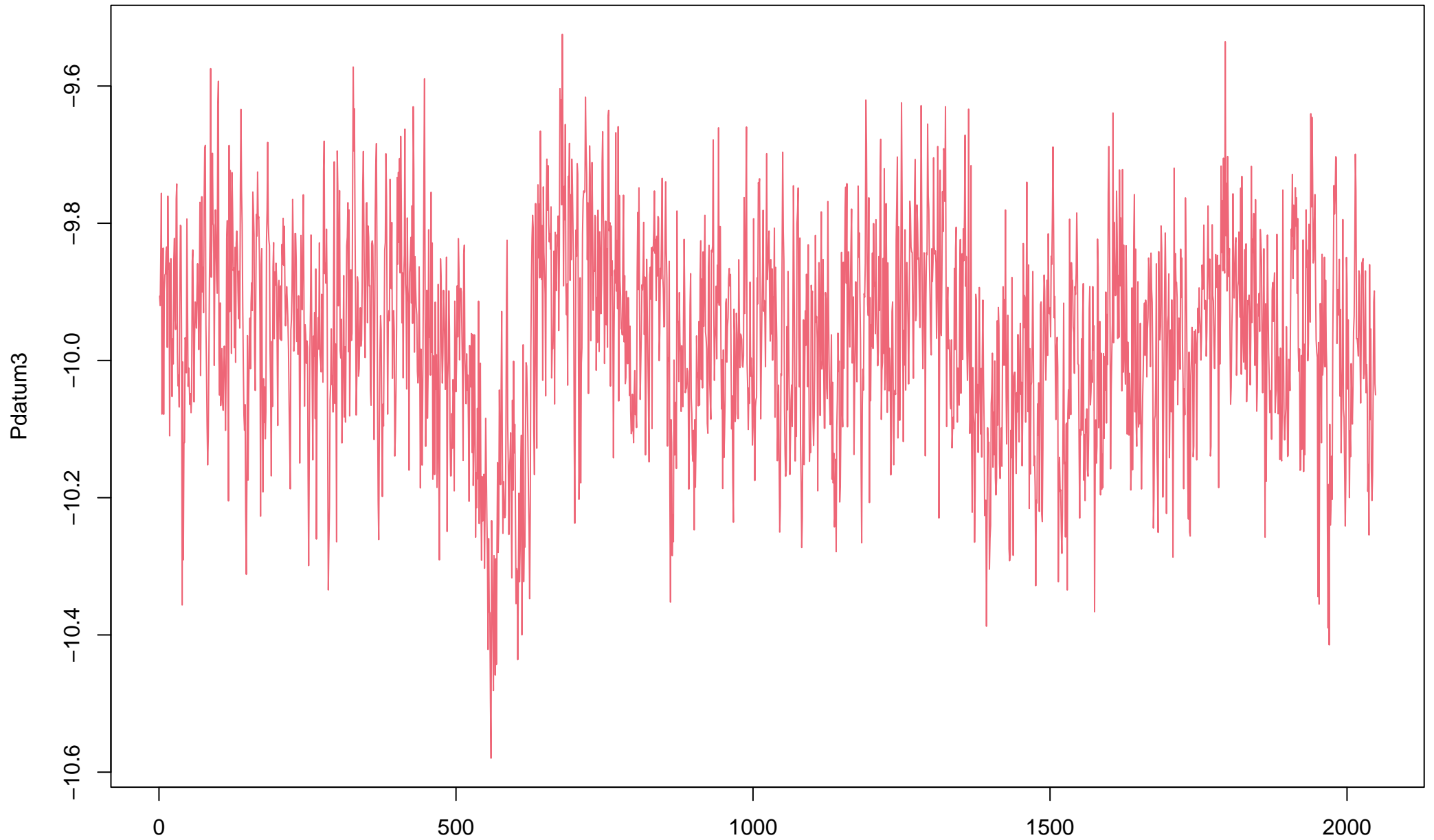


**Pdatum2**  
**ESS = 2.22e-16 | BMK = 0.0763 | MCSE(6.27) = 4.46 | stat: TRUE | burn: 0**

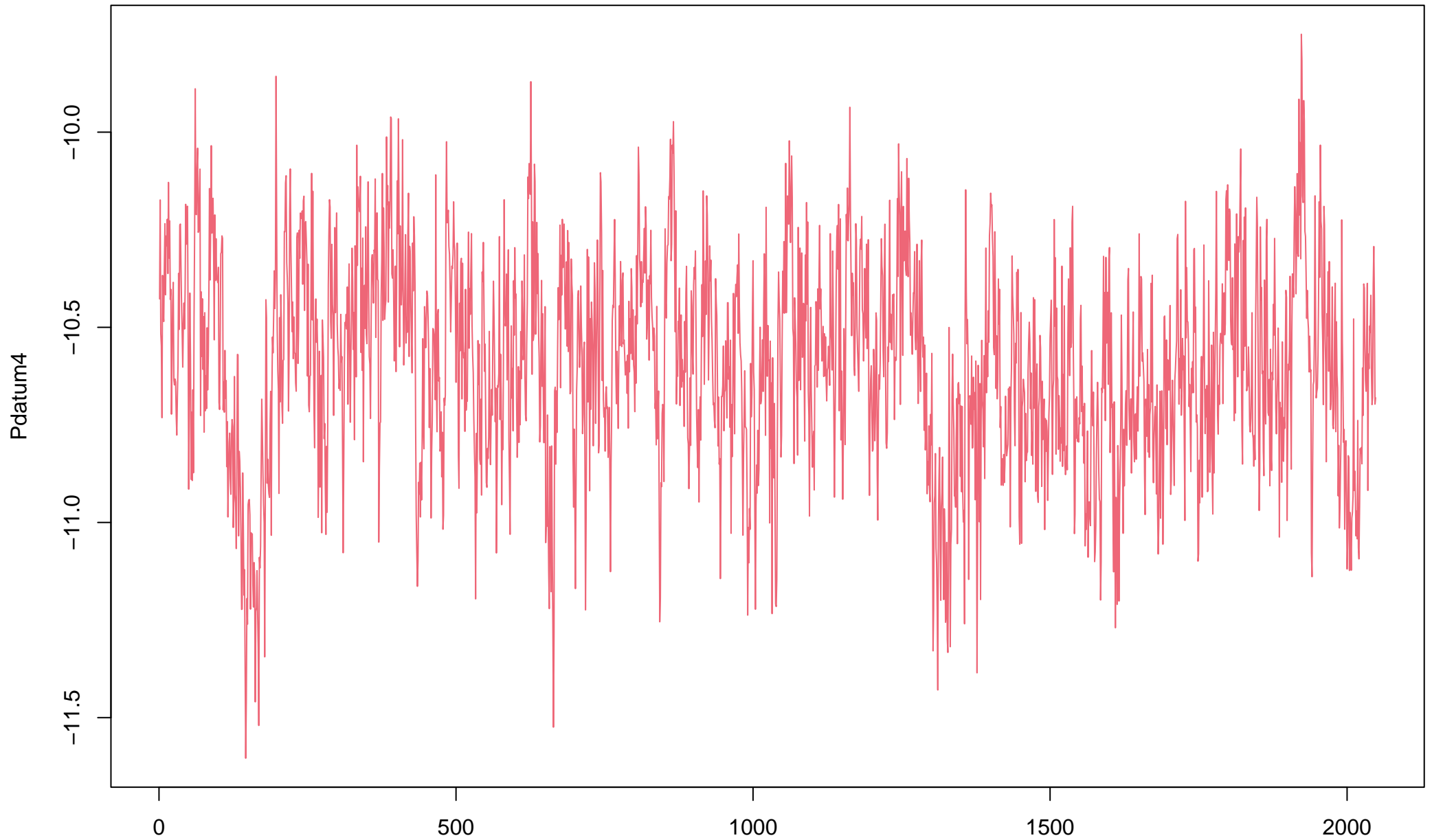




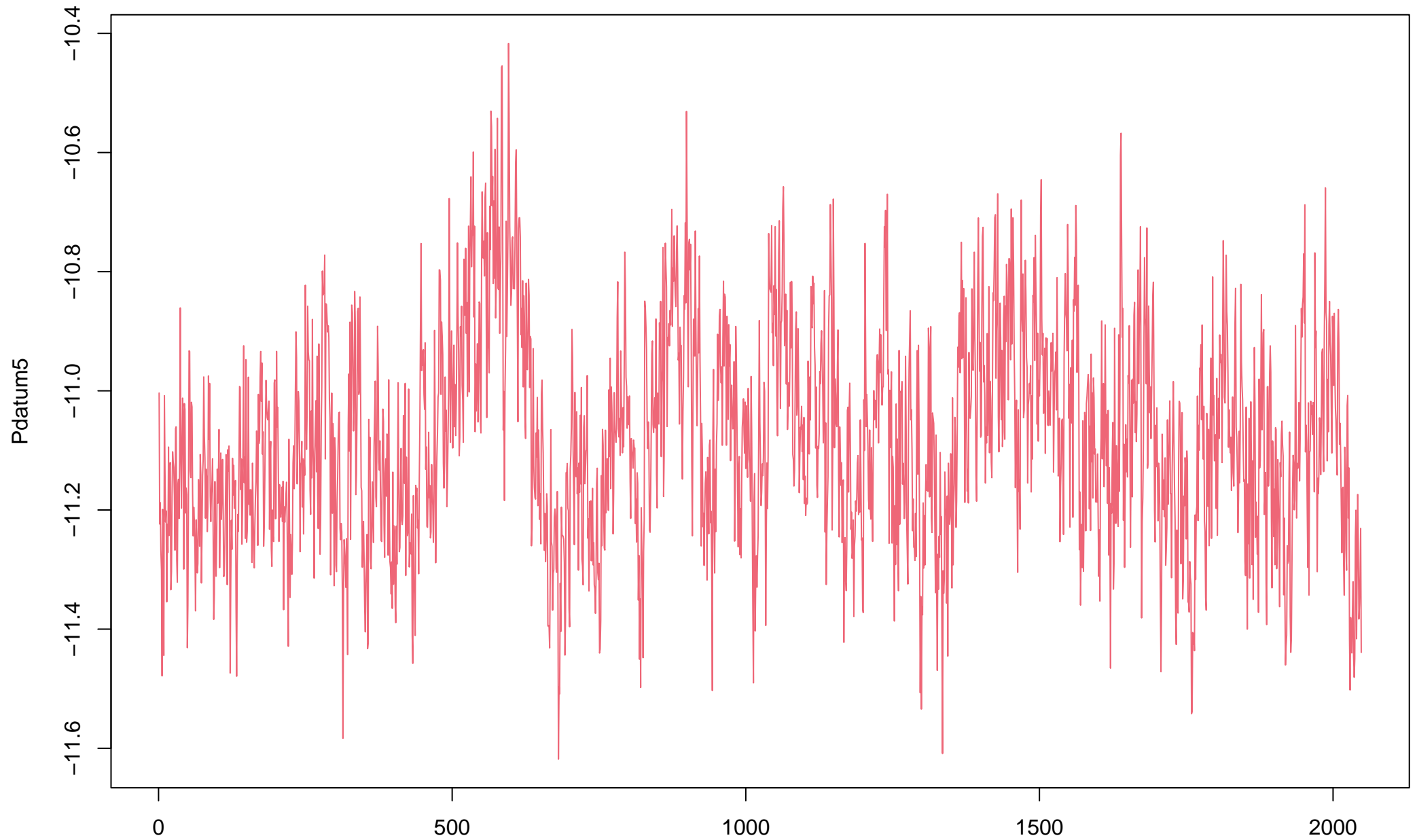
**Pdatum3**  
**ESS = 190 | BMK = 0.0862 | MCSE(6.27) = 7.23 | stat: FALSE | burn: 0**



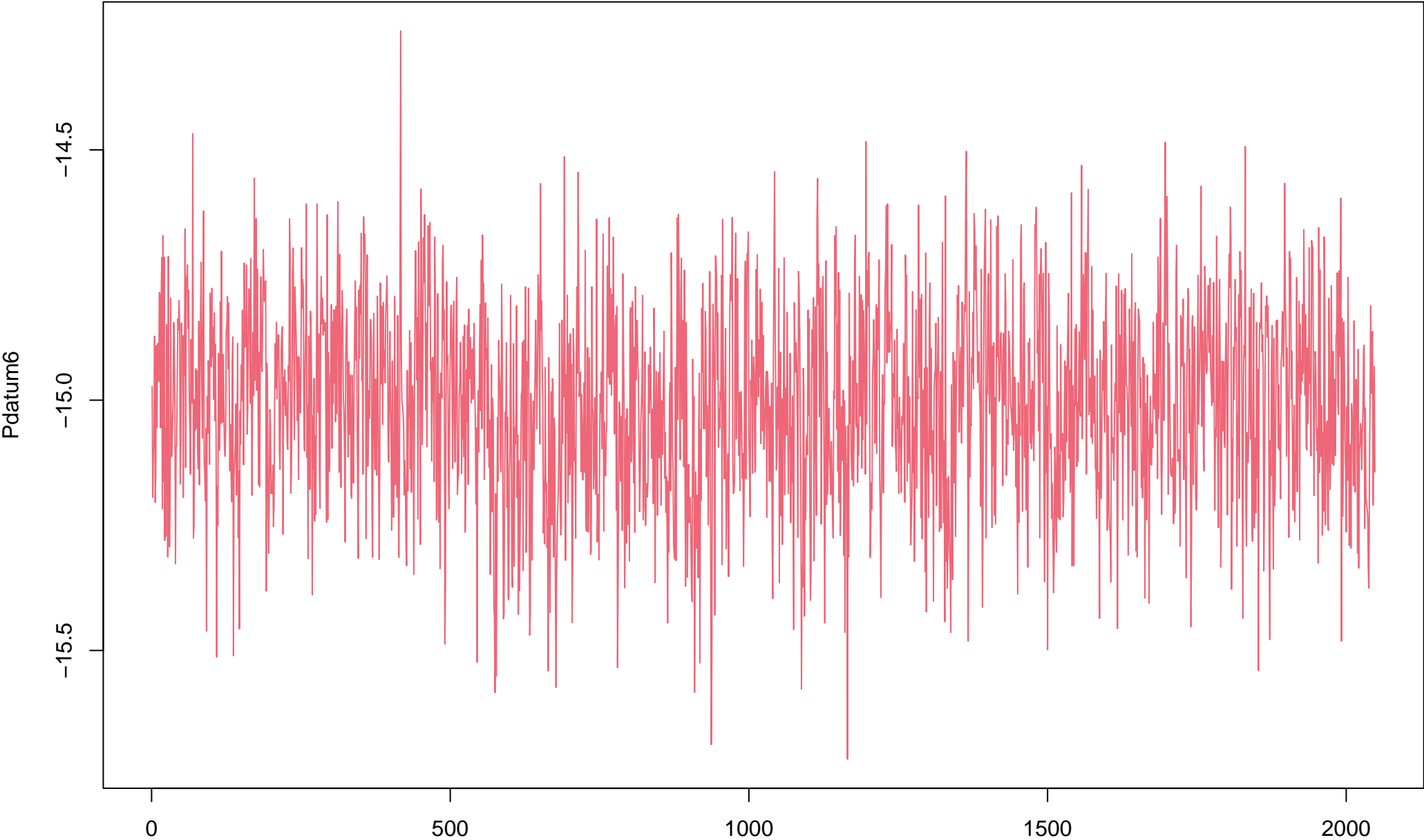
**Pdatum4**  
**ESS = 165 | BMK = 0.112 | MCSE(6.27) = 7.62 | stat: TRUE | burn: 0**



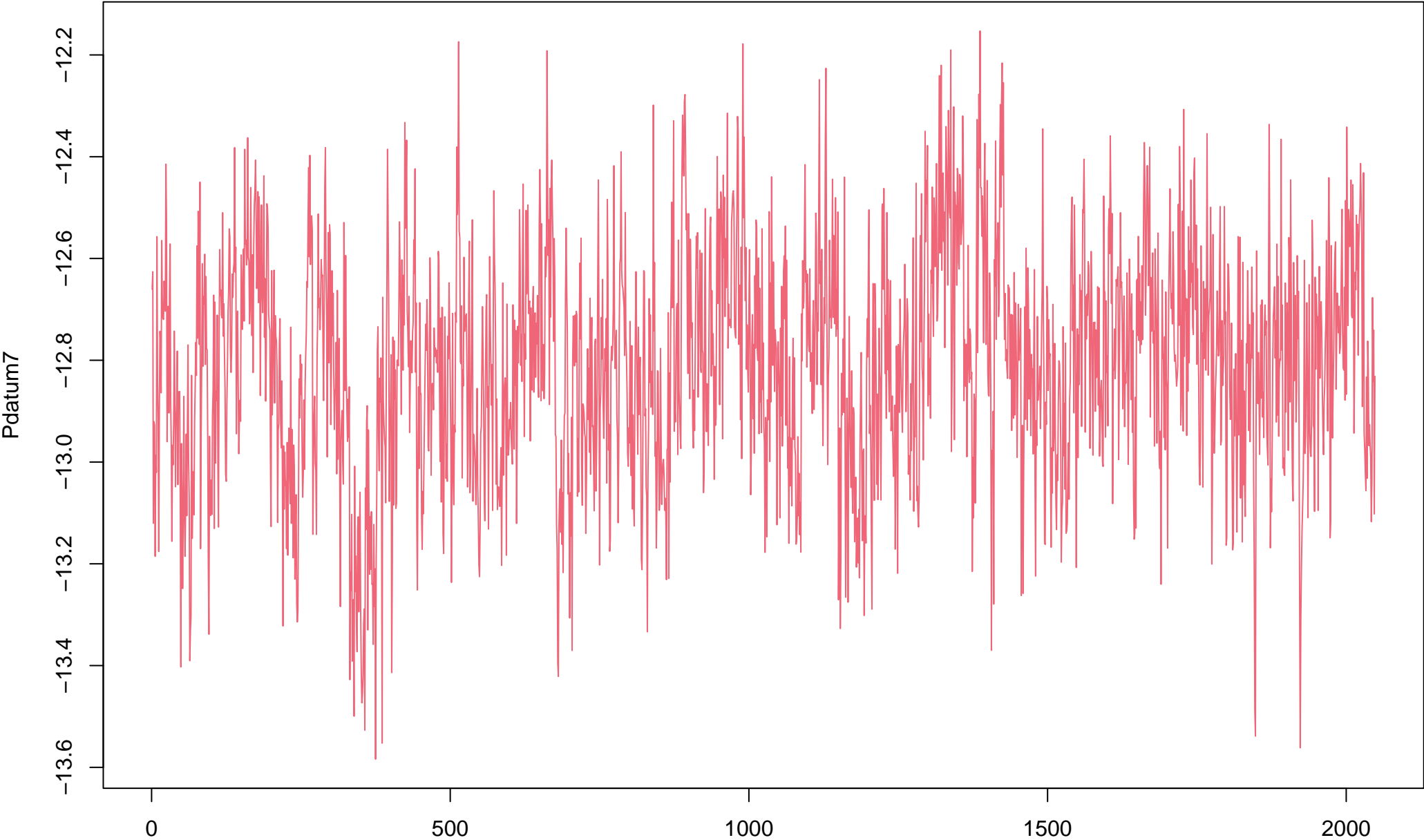
**Pdatum5**  
**ESS = 64.1 | BMK = 0.0898 | MCSE(6.27) = 9.16 | stat: FALSE | burn: 0**



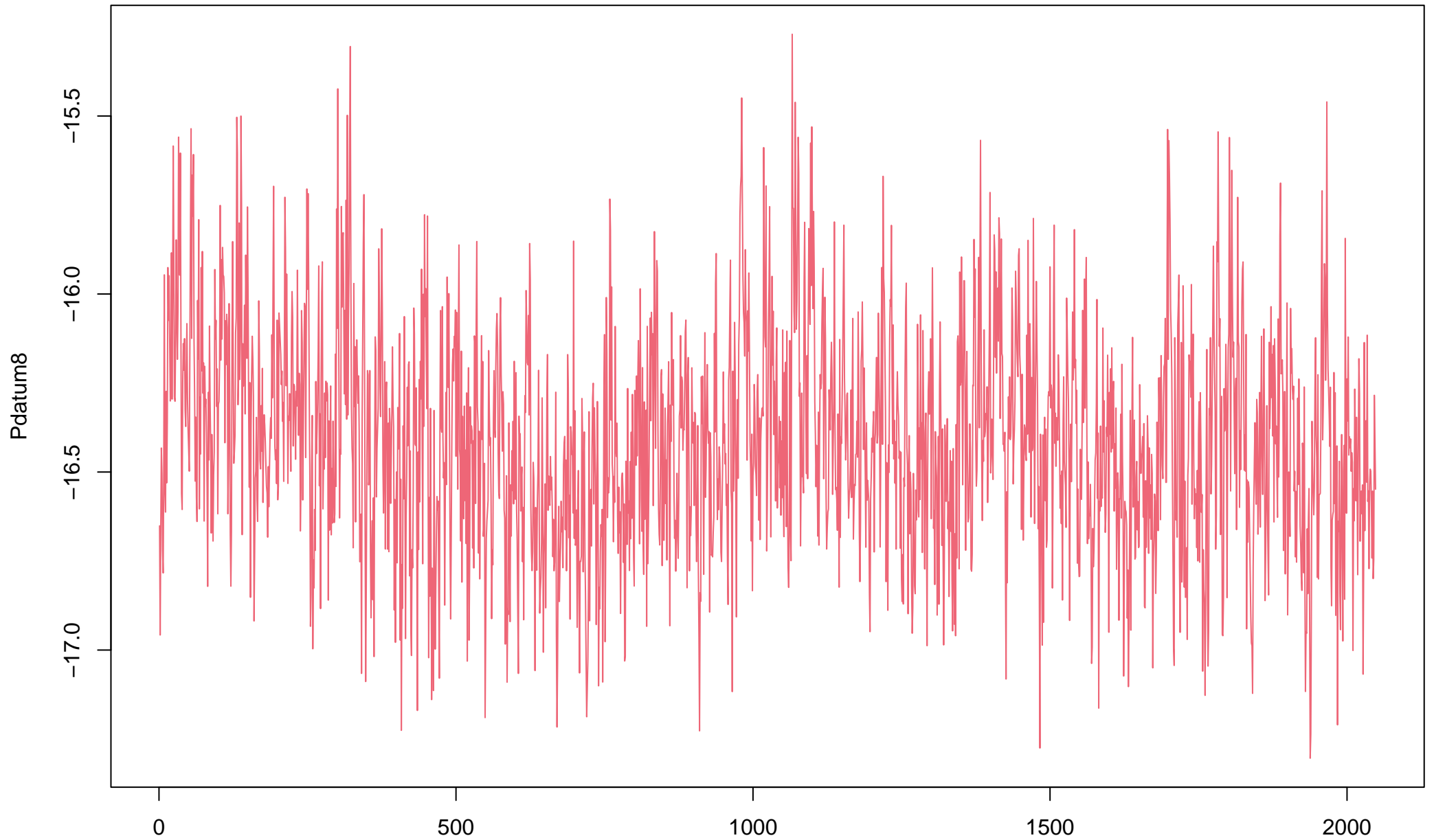
**Pdatum6**  
**ESS = 781 | BMK = 0.0403 | MCSE(6.27) = 3.67 | stat: TRUE | burn: 0**



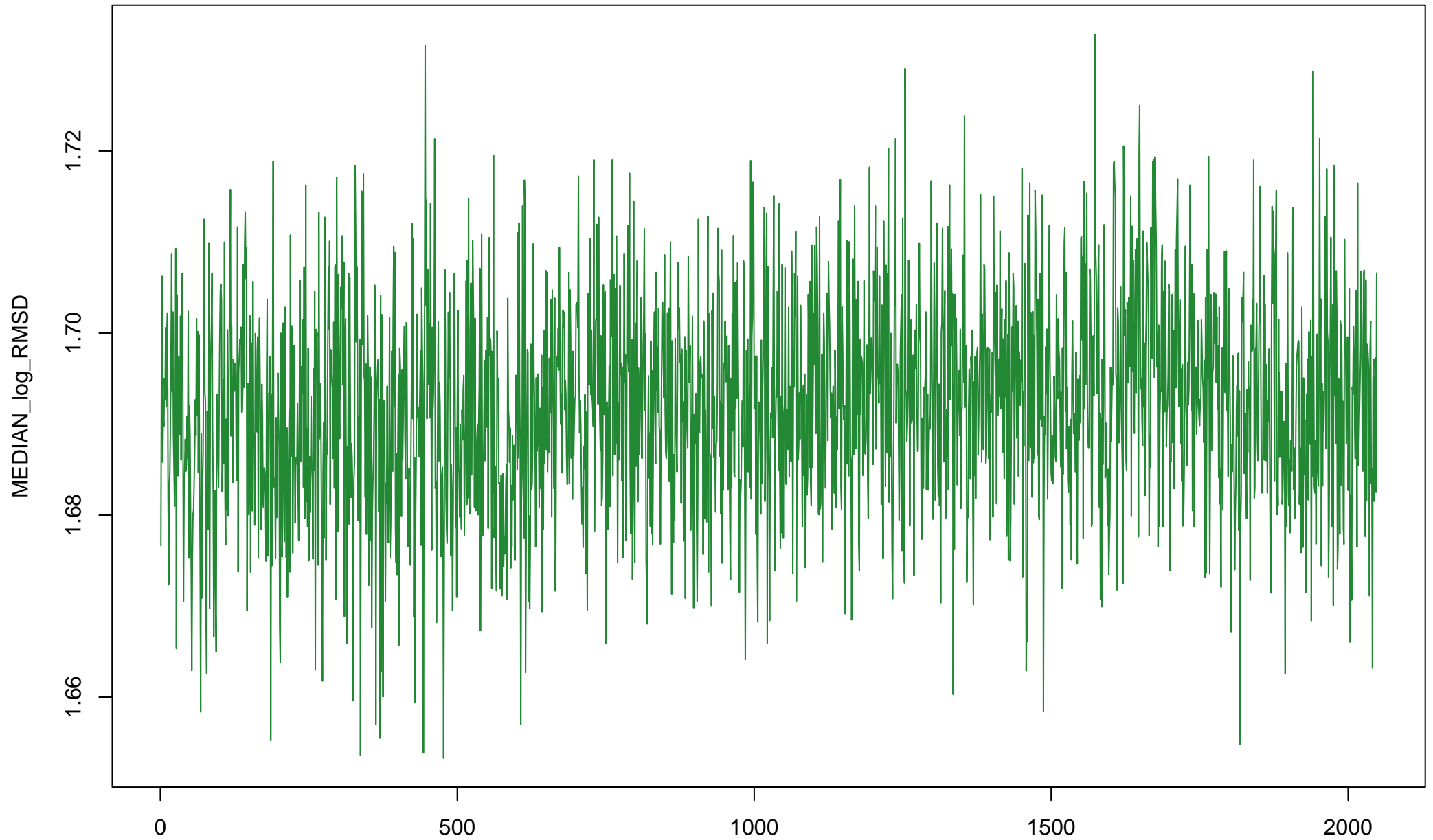
**Pdatum7**  
**ESS = 160 | BMK = 0.0863 | MCSE(6.27) = 7.21 | stat: TRUE | burn: 0**



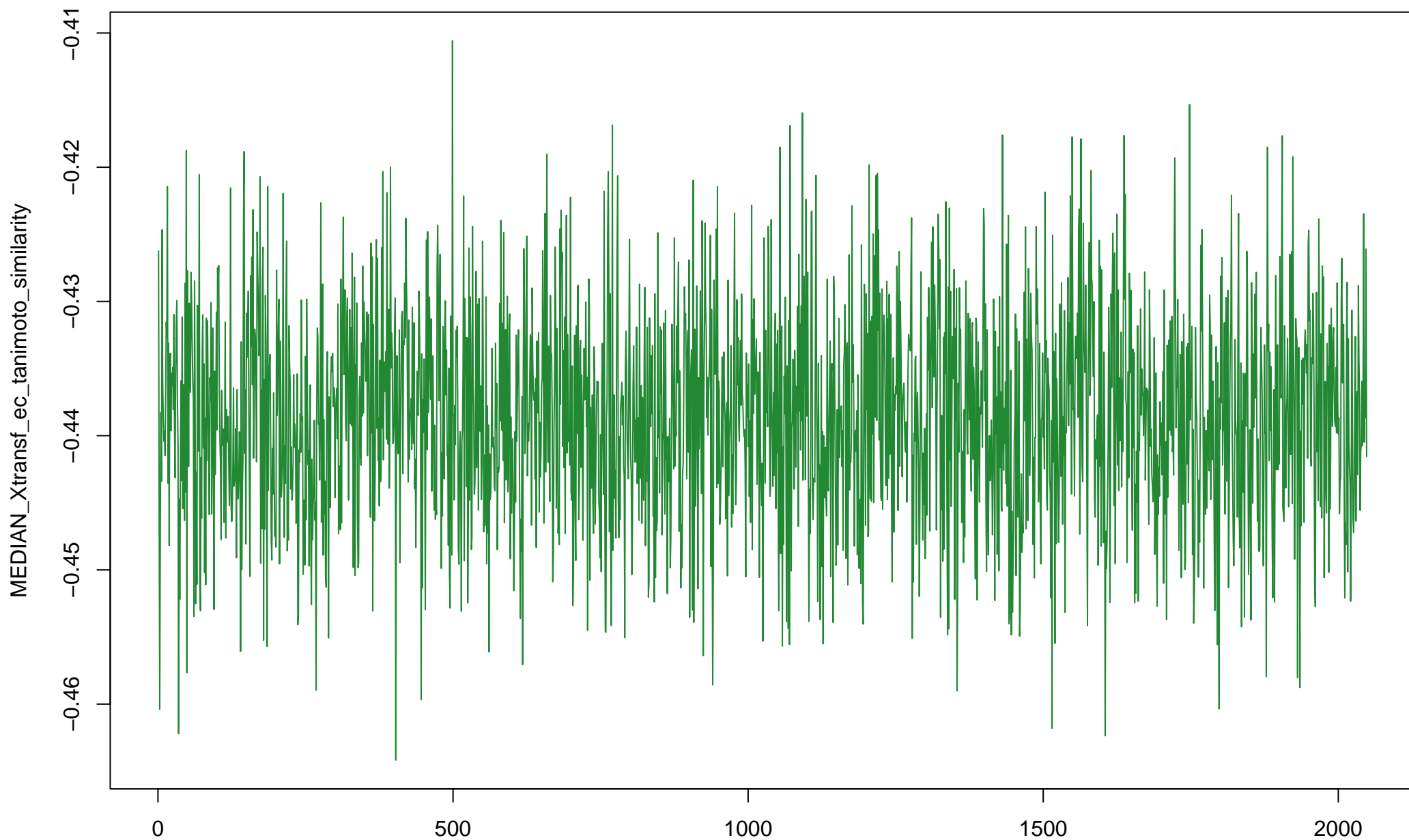
**Pdatum8**  
**ESS = 329 | BMK = 0.0414 | MCSE(6.27) = 5.33 | stat: FALSE | burn: 0**



**MEDIAN\_log\_RMSD**  
**ESS = 1430 | BMK = 0.0977 | MCSE(6.27) = 3.54 | stat: FALSE | burn: 0**

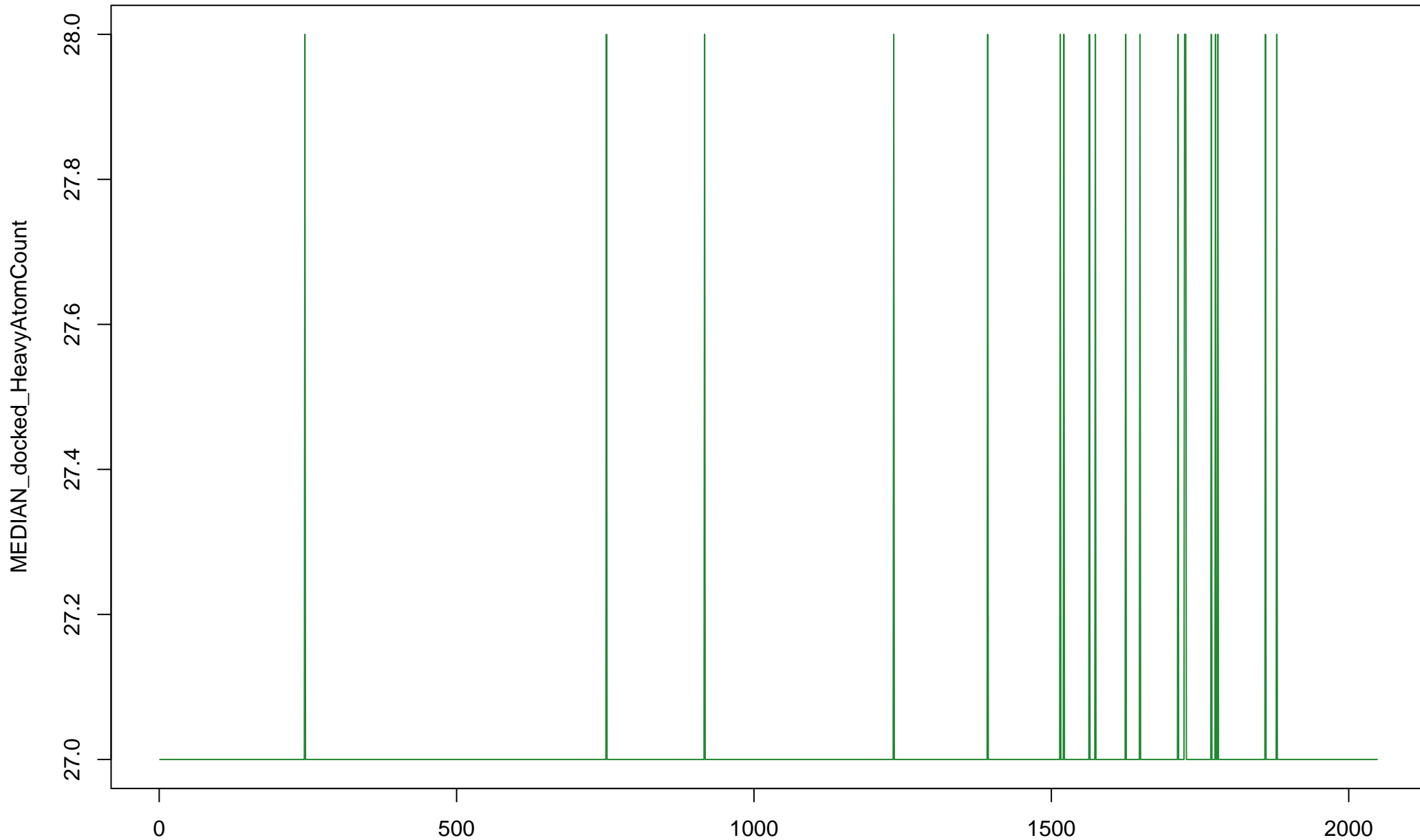


**MEDIAN\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1750 | BMK = 0.0423 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0**

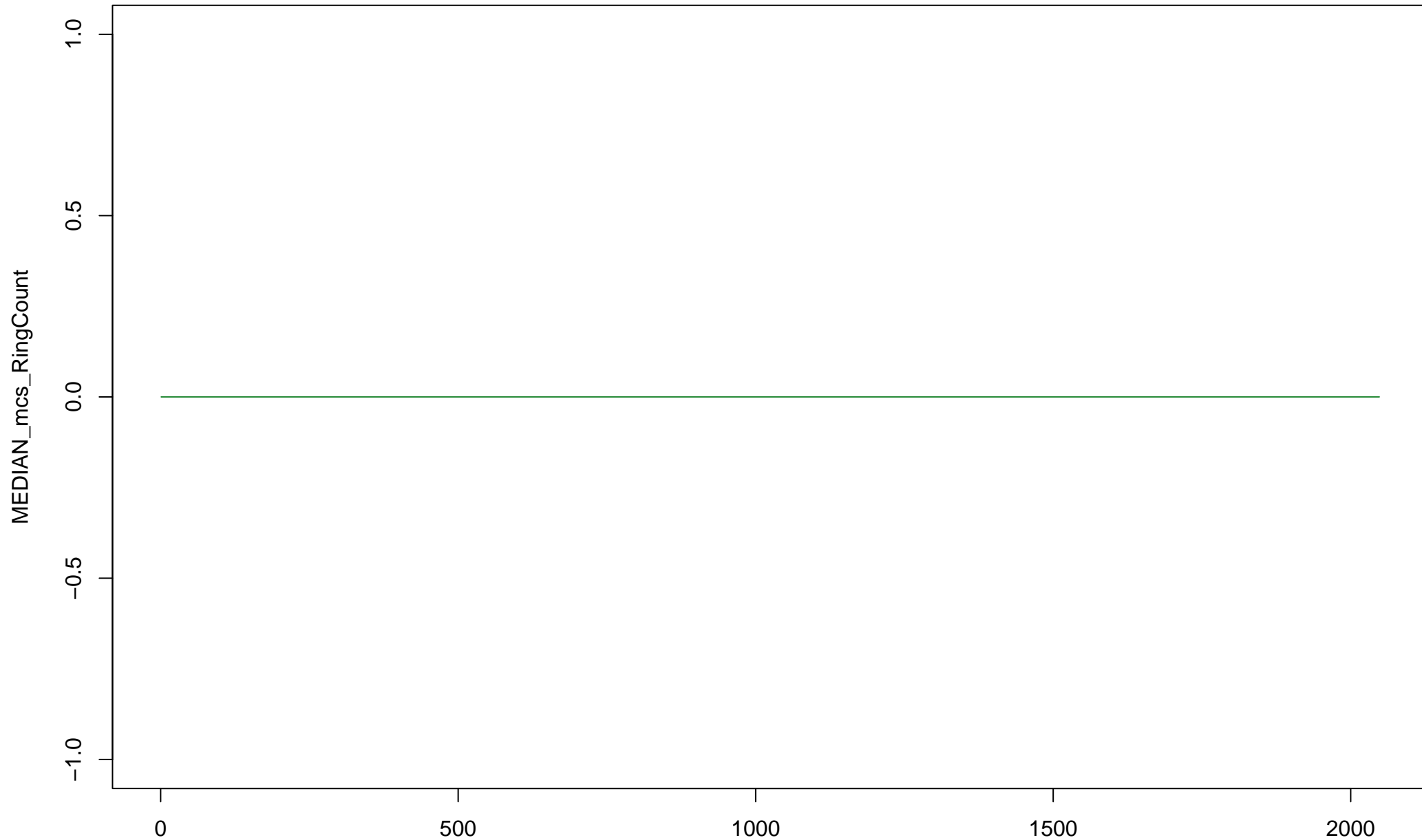




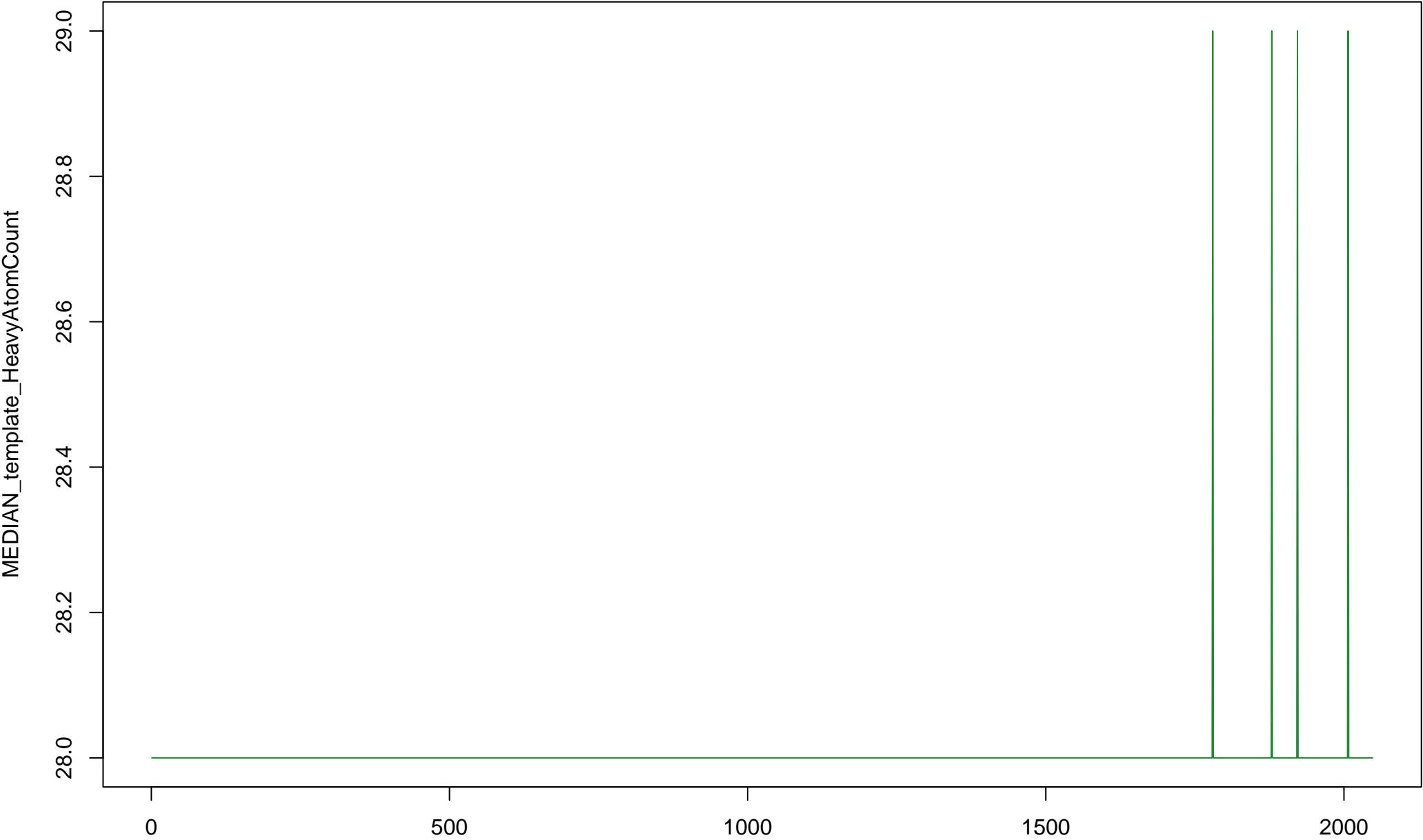
**MEDIAN\_docked\_HeavyAtomCount**  
**ESS = 1110 | BMK = 0.28 | MCSE(6.27) = 3.08 | stat: FALSE | burn: 1020**



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



MEDIAN\_template\_HeavyAtomCount  
ESS = 2050 | BMK = 0.502 | MCSE(6.27) = 2.15 | stat: FALSE | burn: 1632



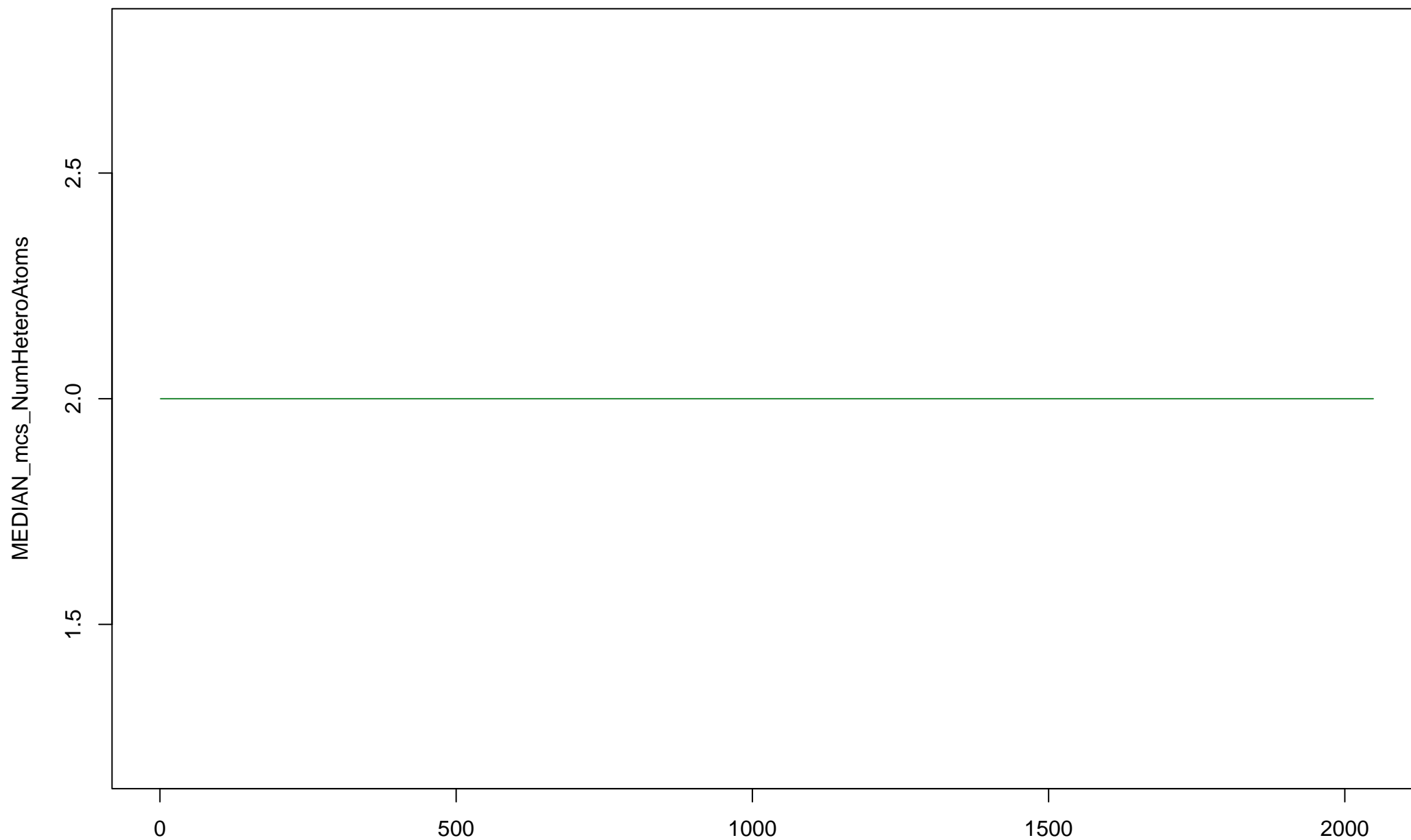
**MEDIAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



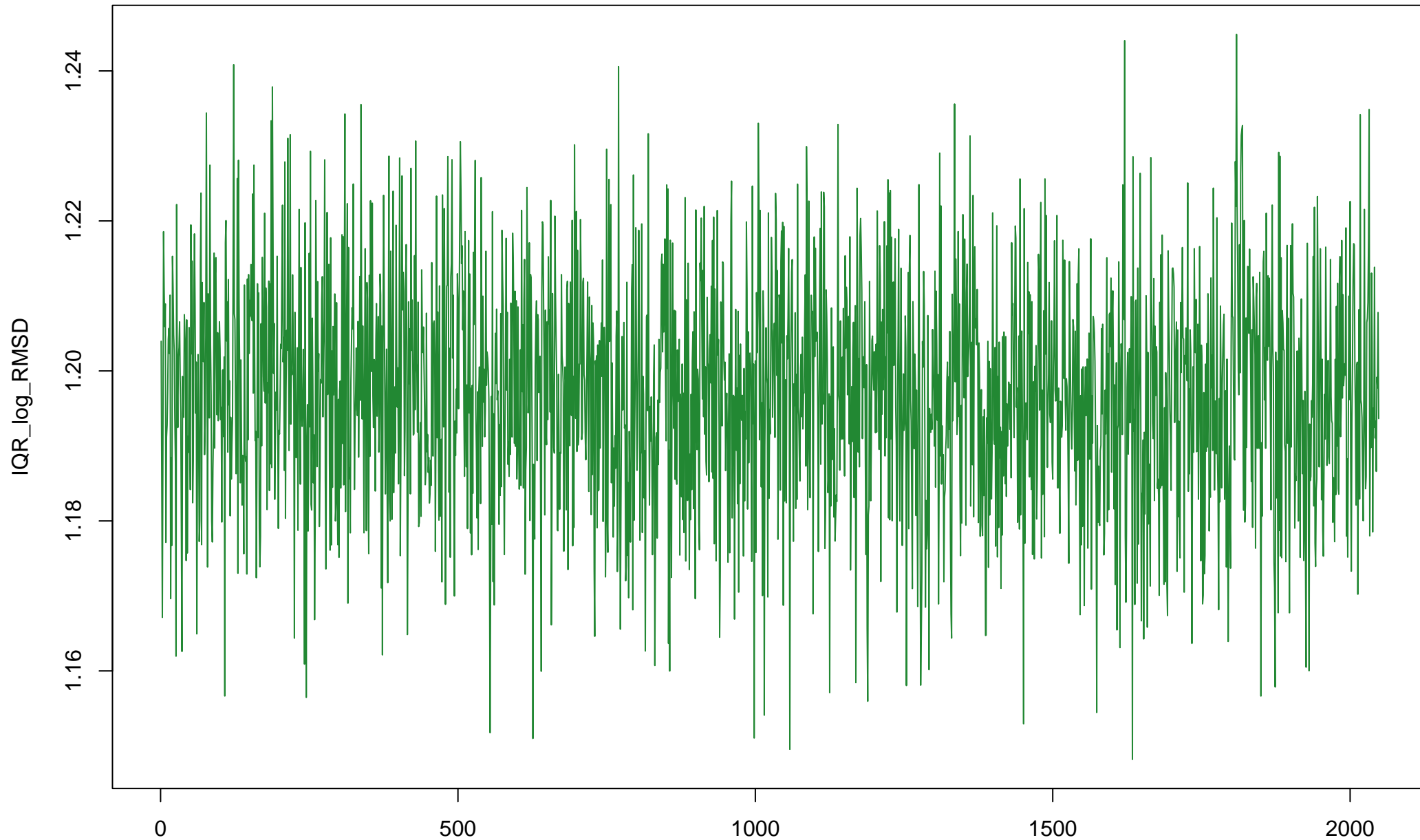
**MEDIAN\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



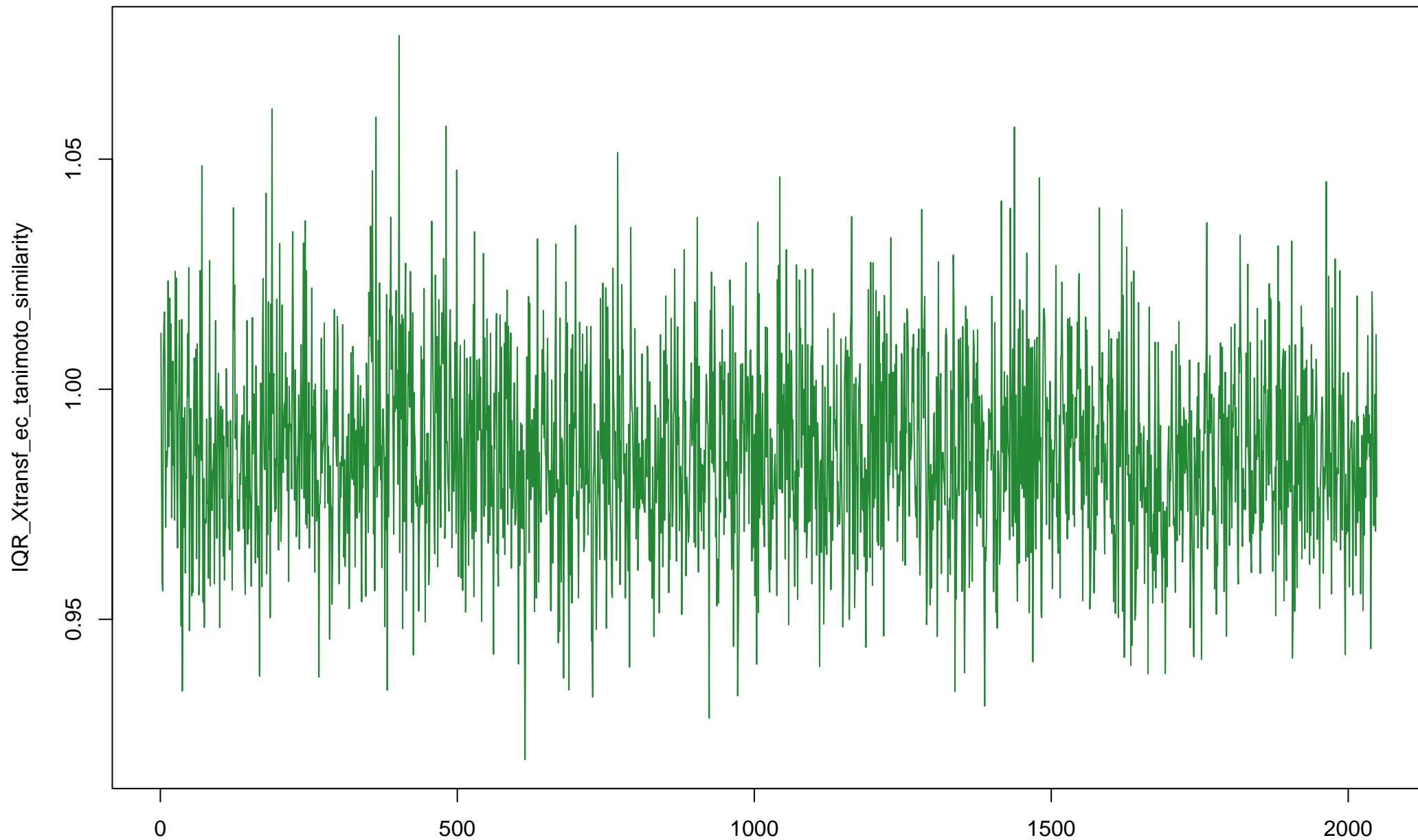
**MEDIAN\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**IQR\_log\_RMSD**  
**ESS = 1860 | BMK = 0.0348 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0**

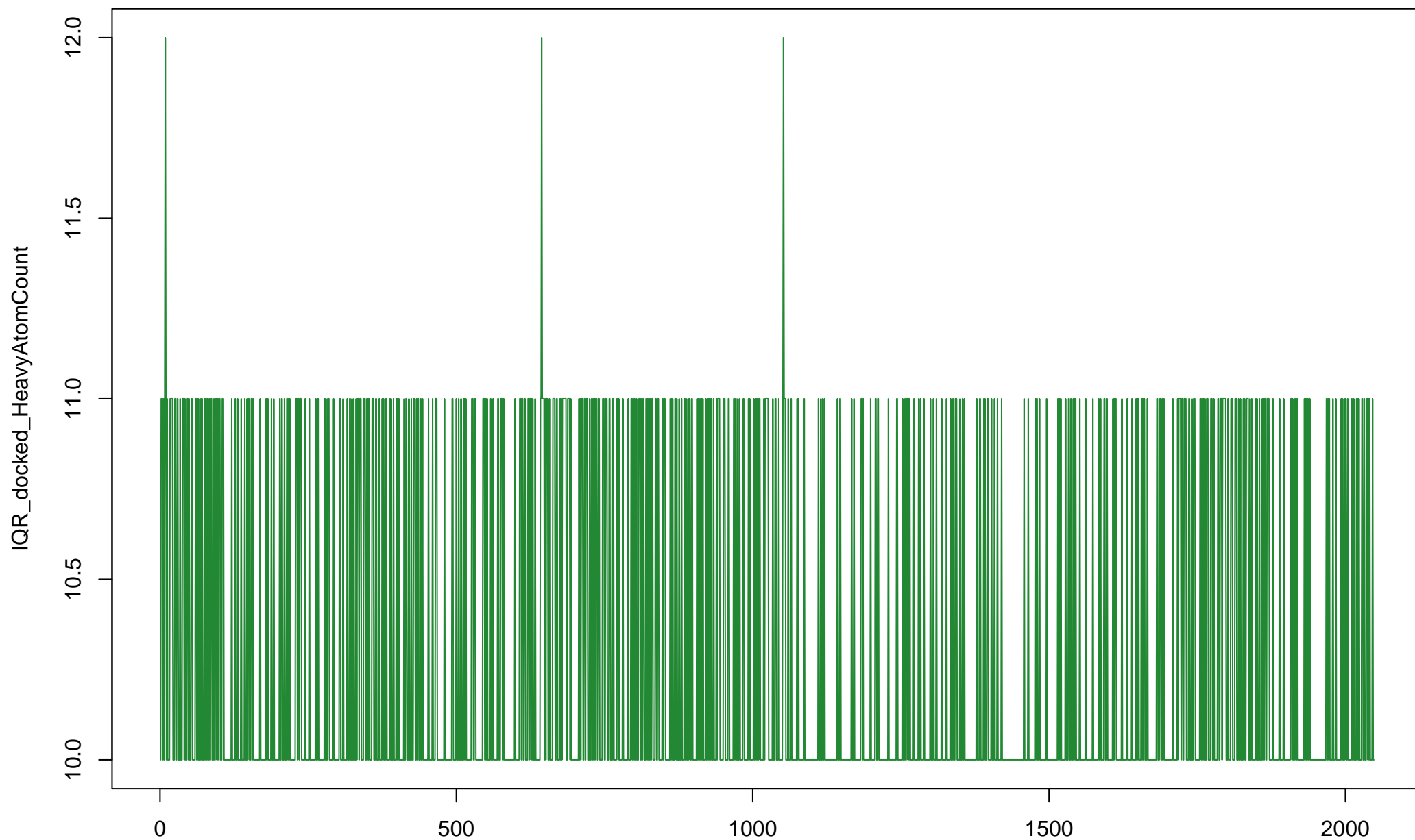


**IQR\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1650 | BMK = 0.0425 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0**

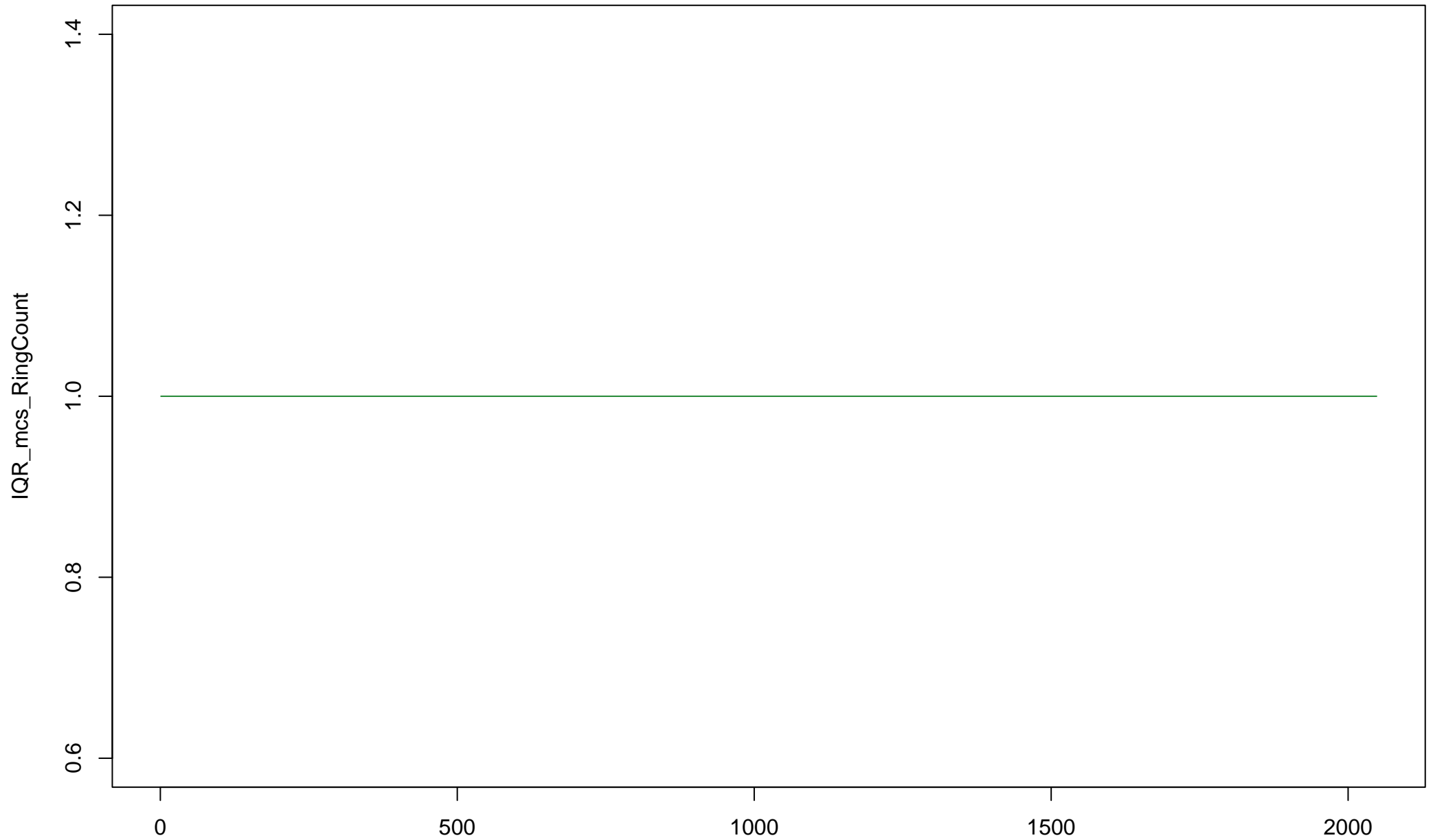




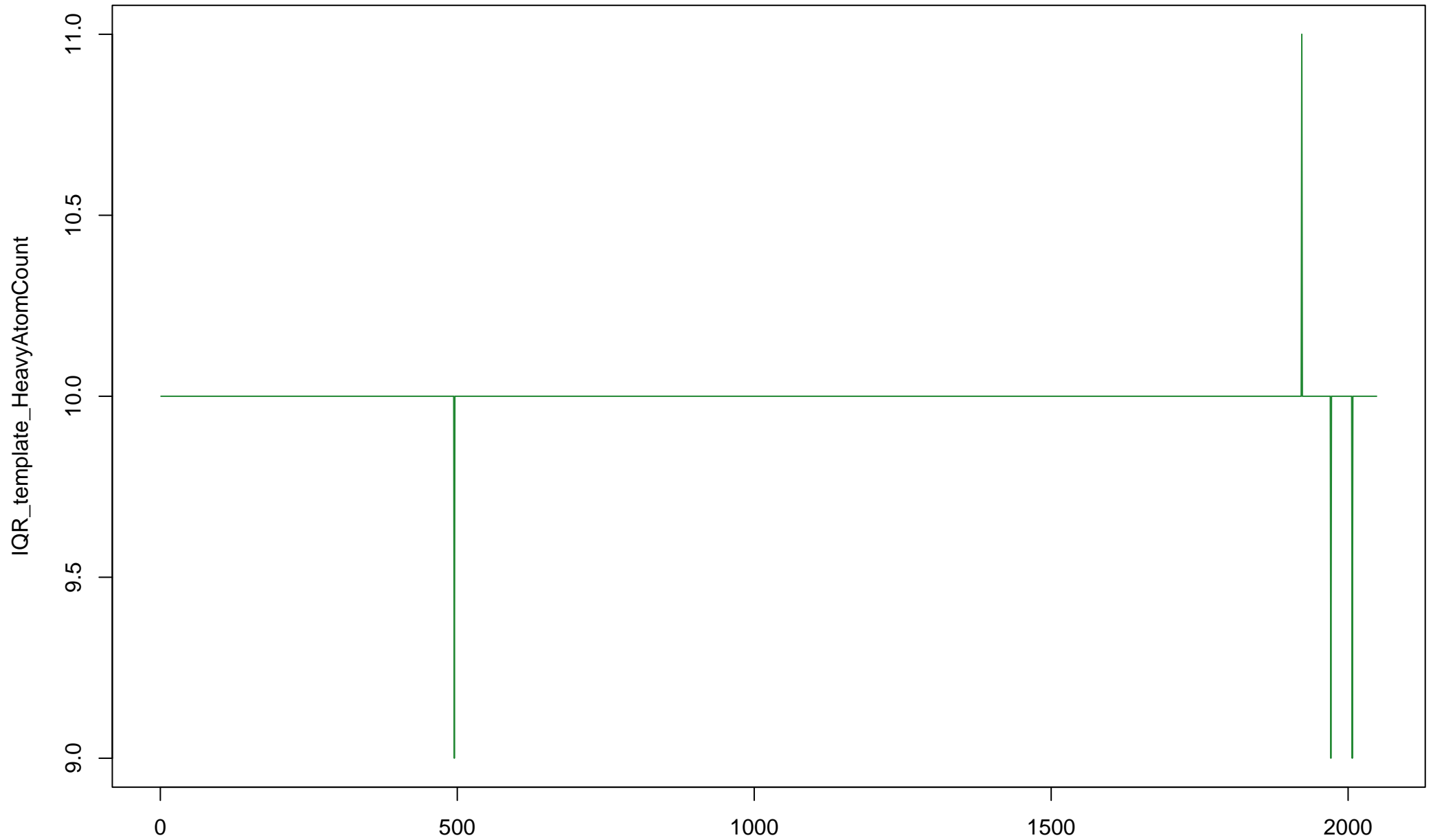
IQR\_docked\_HeavyAtomCount  
ESS = 1130 | BMK = 0.0974 | MCSE(6.27) = 3.78 | stat: FALSE | burn: 0



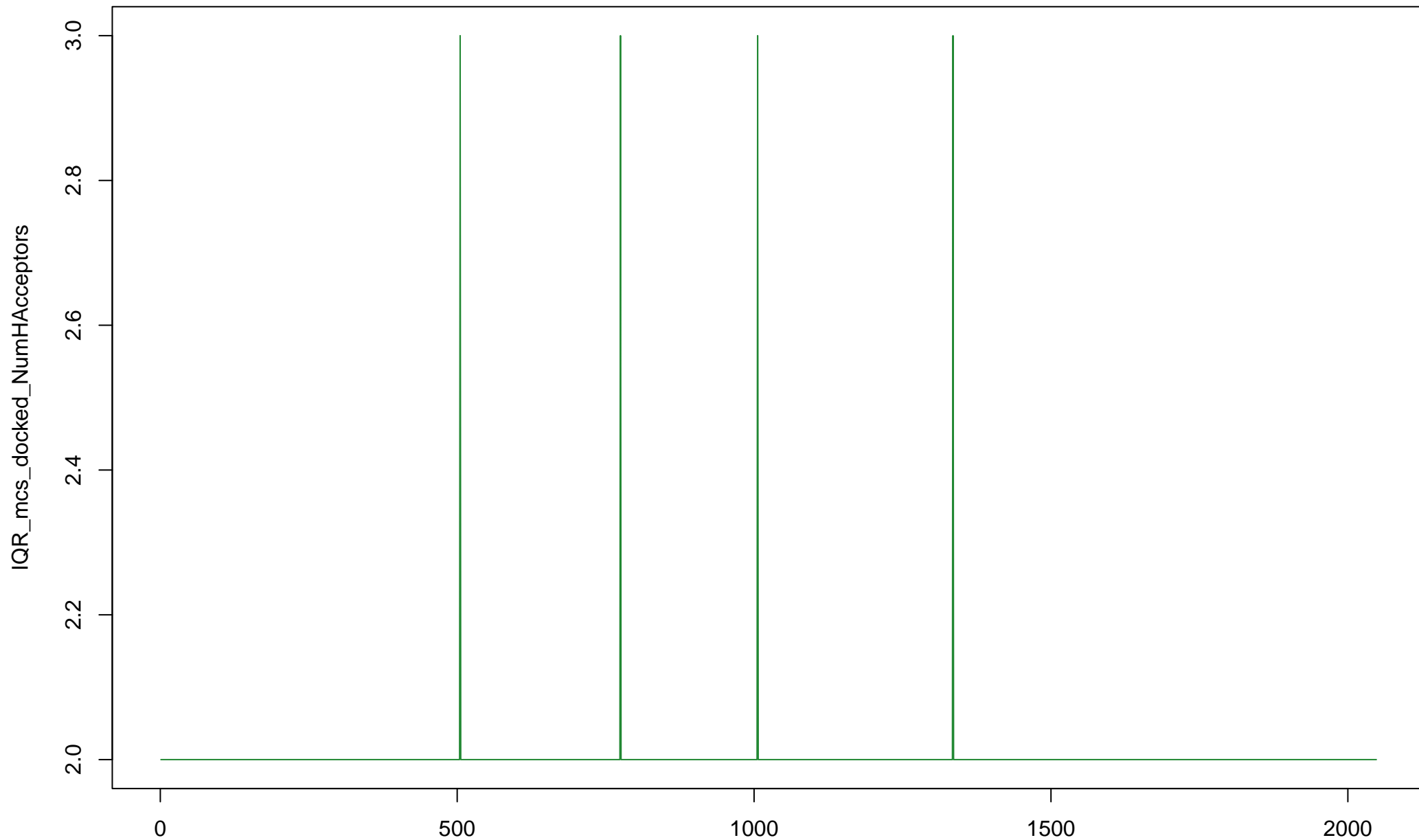
**IQR\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



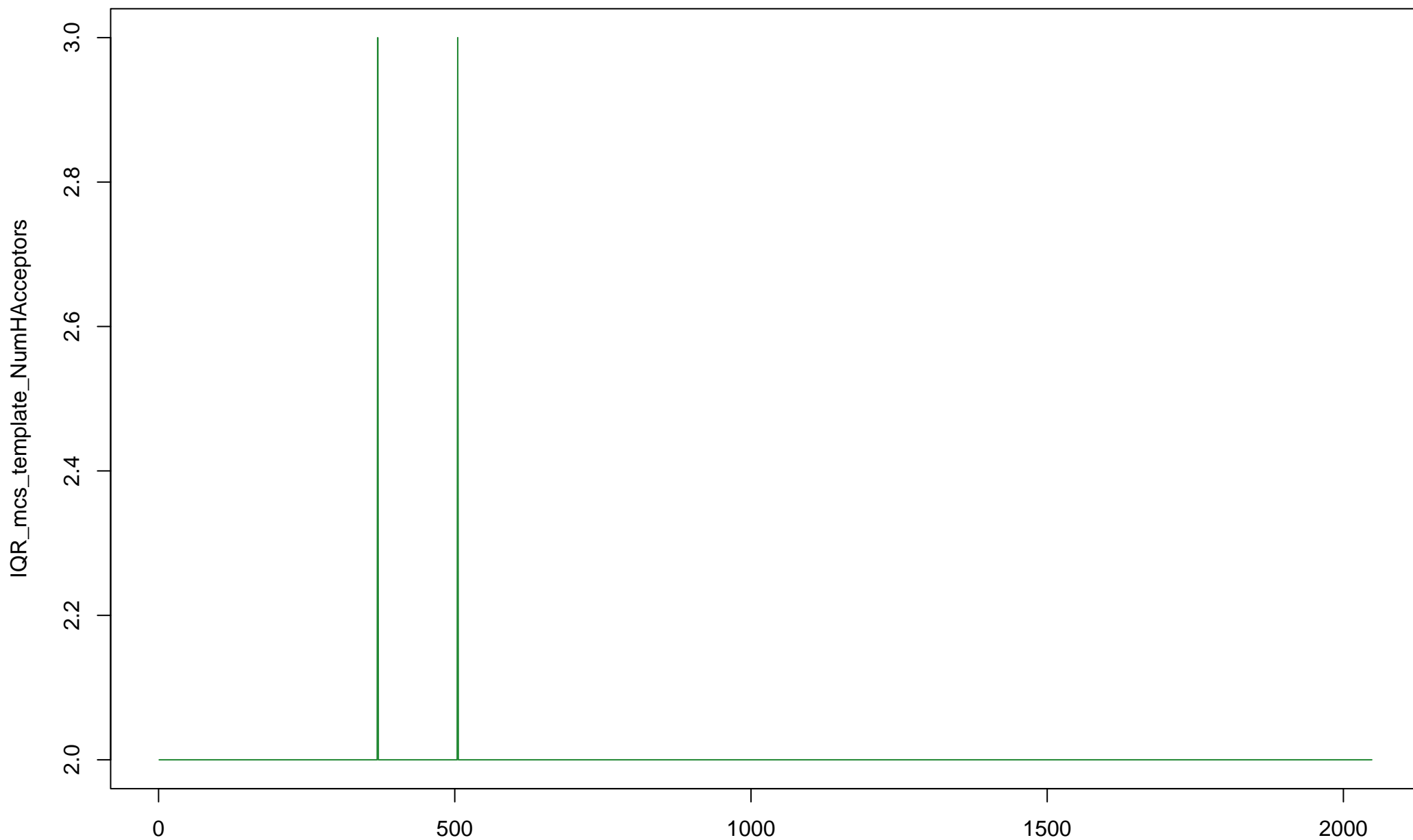
IQR\_template\_HeavyAtomCount  
ESS = 2050 | BMK = 0.259 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 2040



**IQR\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.188 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 1428**



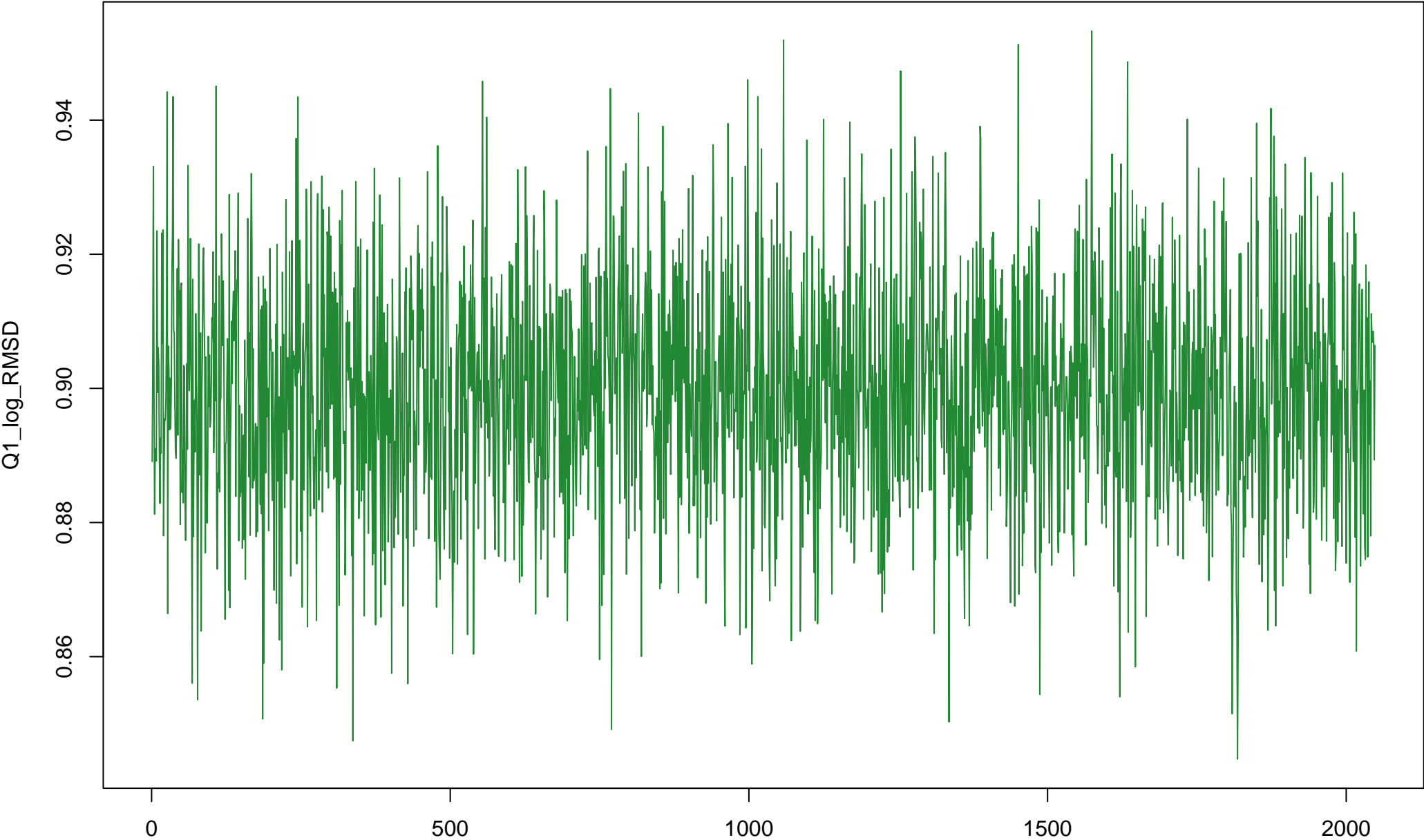
IQR\_mcs\_template\_NumHAcceptors  
ESS = 2050 | BMK = 0.628 | MCSE(6.27) = 2.2 | stat: FALSE | burn: 612



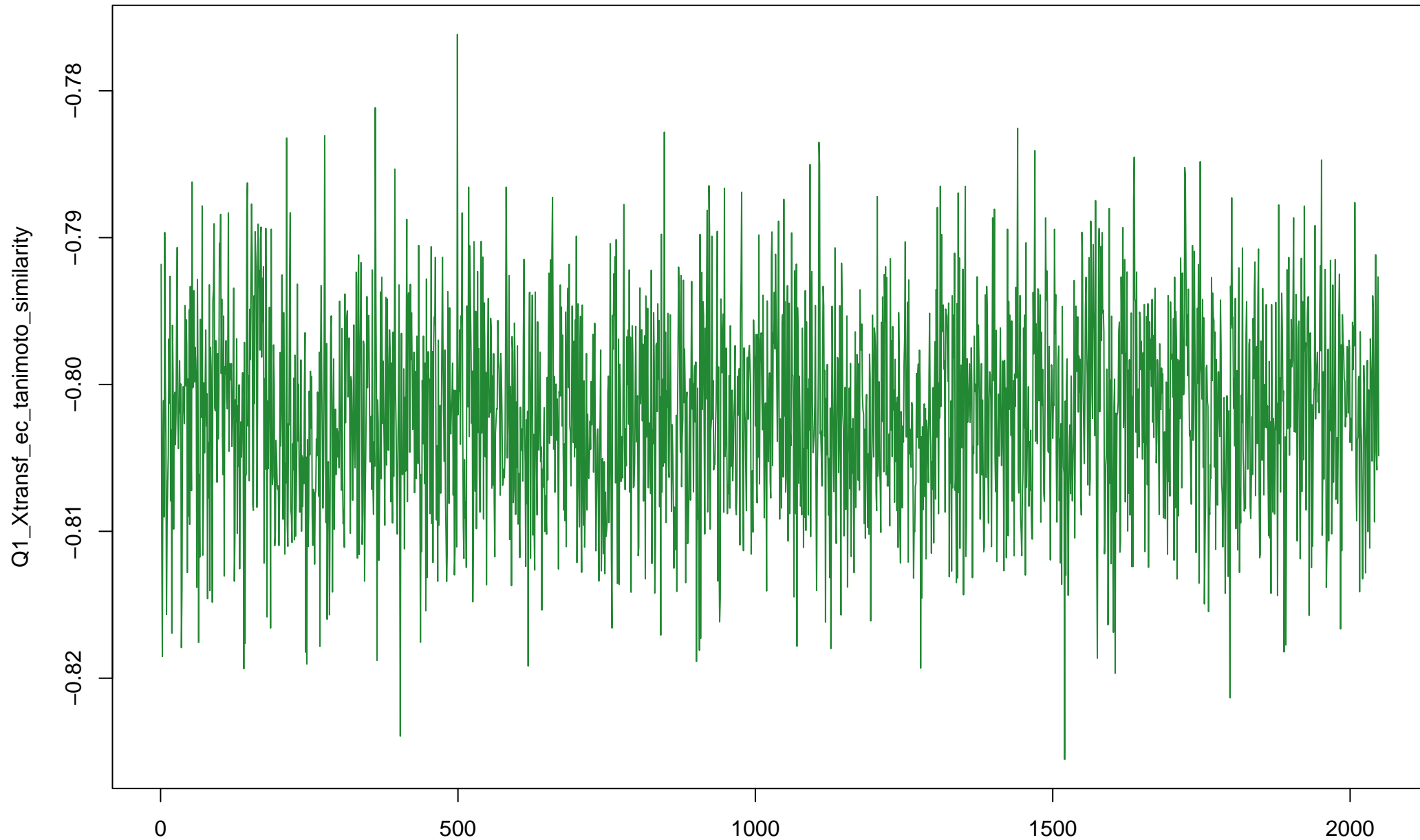
IQR\_mcs\_NumHeteroAtoms  
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



**Q1\_log\_RMSD**  
**ESS = 2050 | BMK = 0.039 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0**

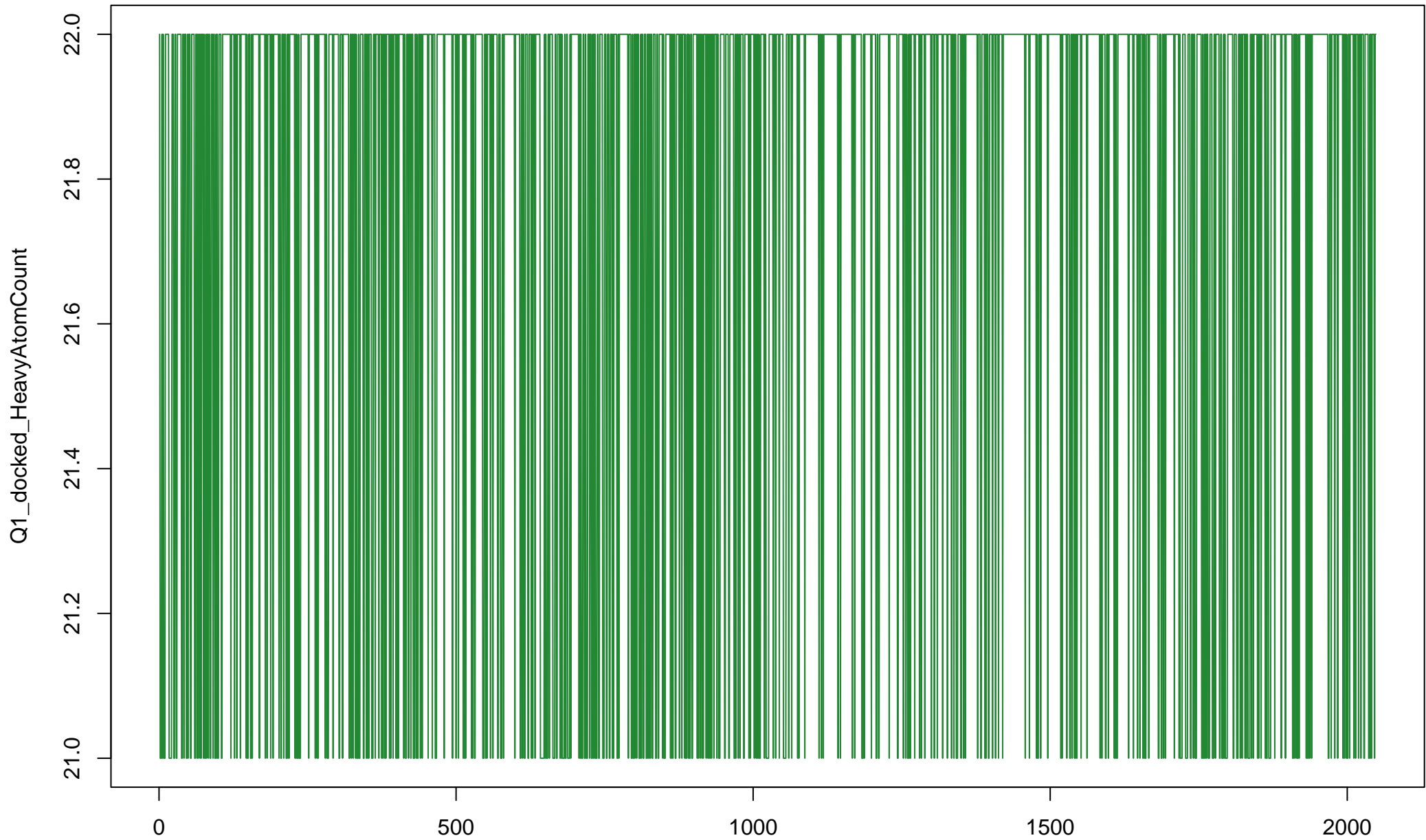


**Q1\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1520 | BMK = 0.0486 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0**





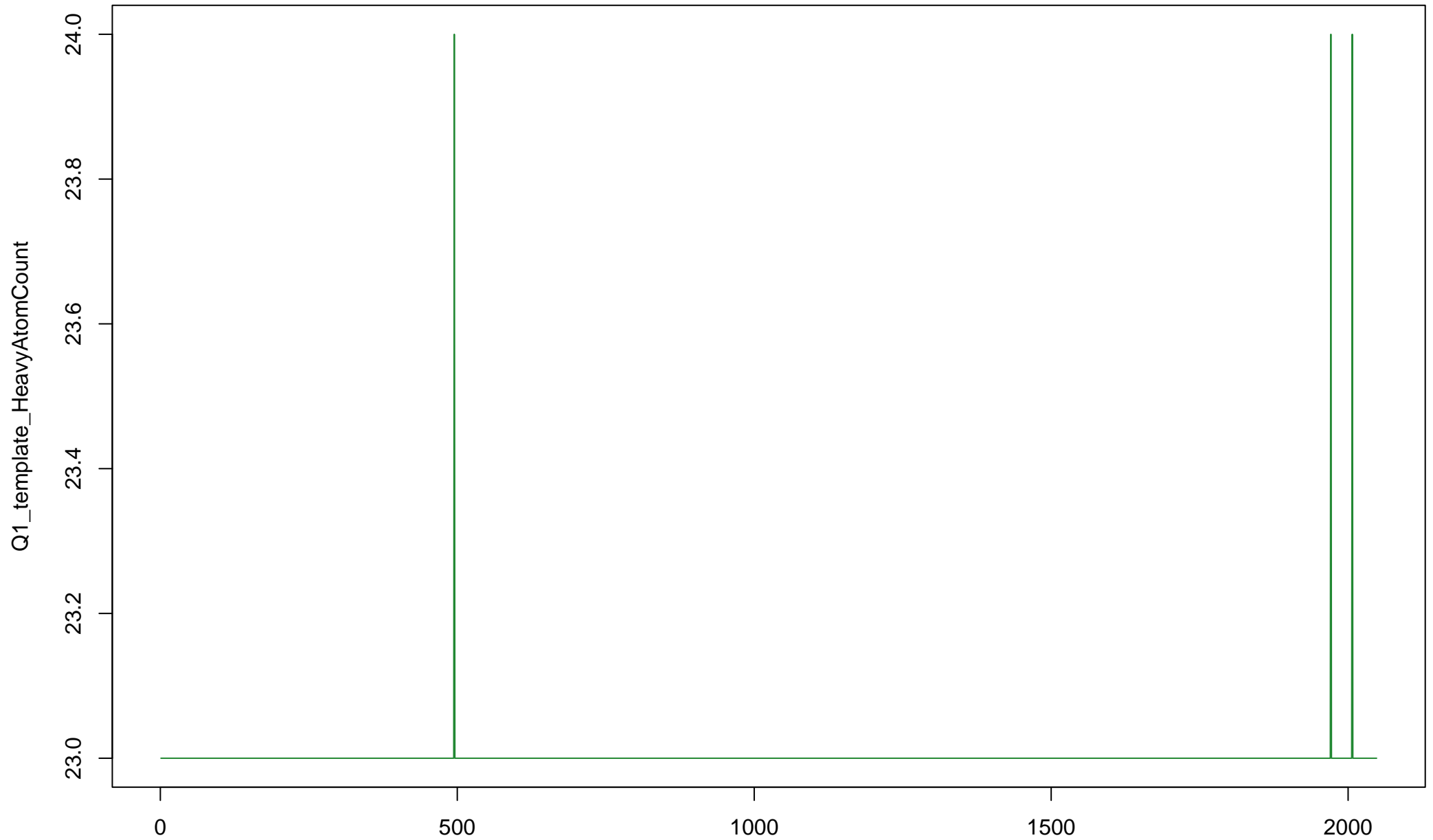
**Q1\_docked\_HeavyAtomCount**  
**ESS = 1250 | BMK = 0.074 | MCSE(6.27) = 3.66 | stat: FALSE | burn: 0**



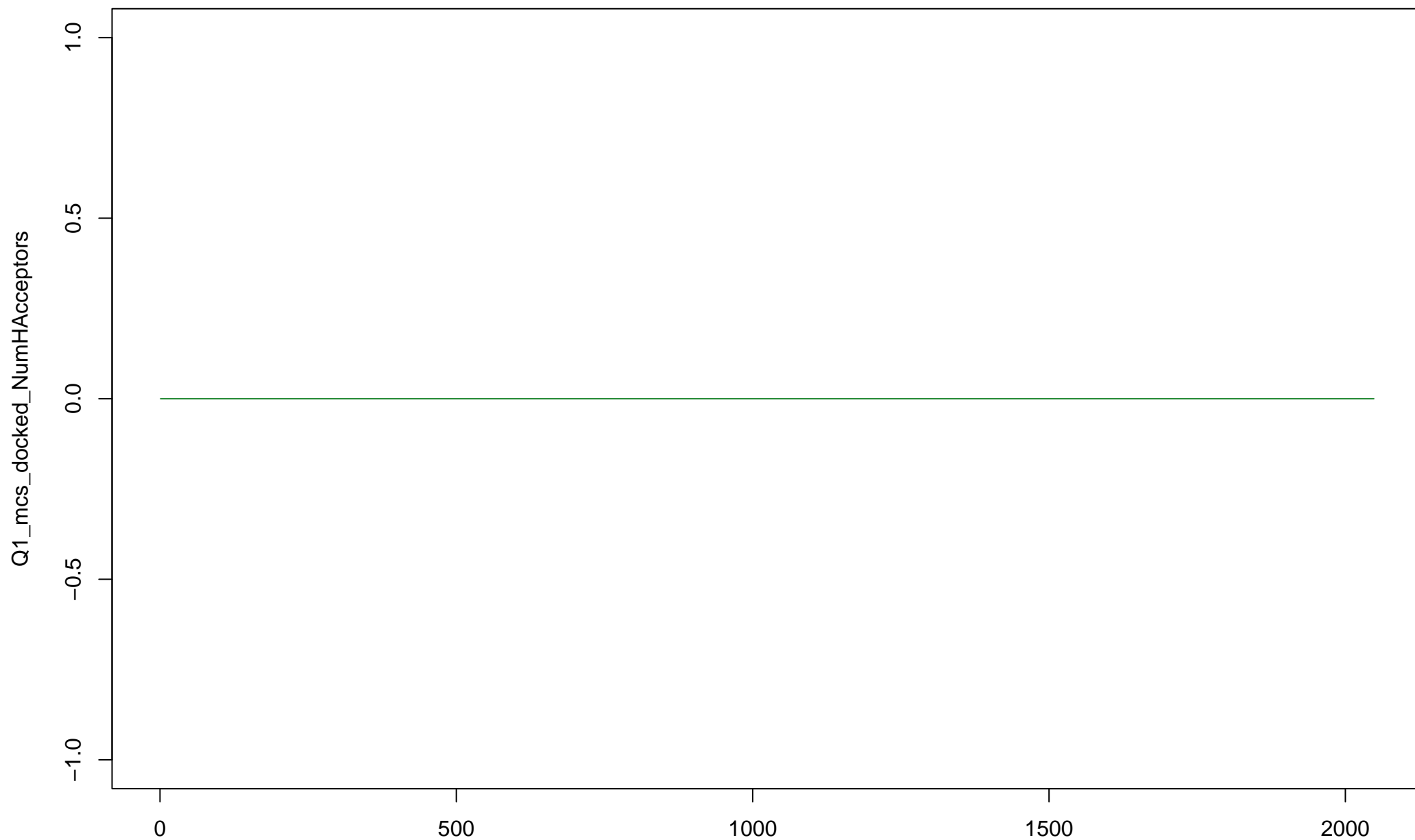
**Q1\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q1\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.121 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 612**



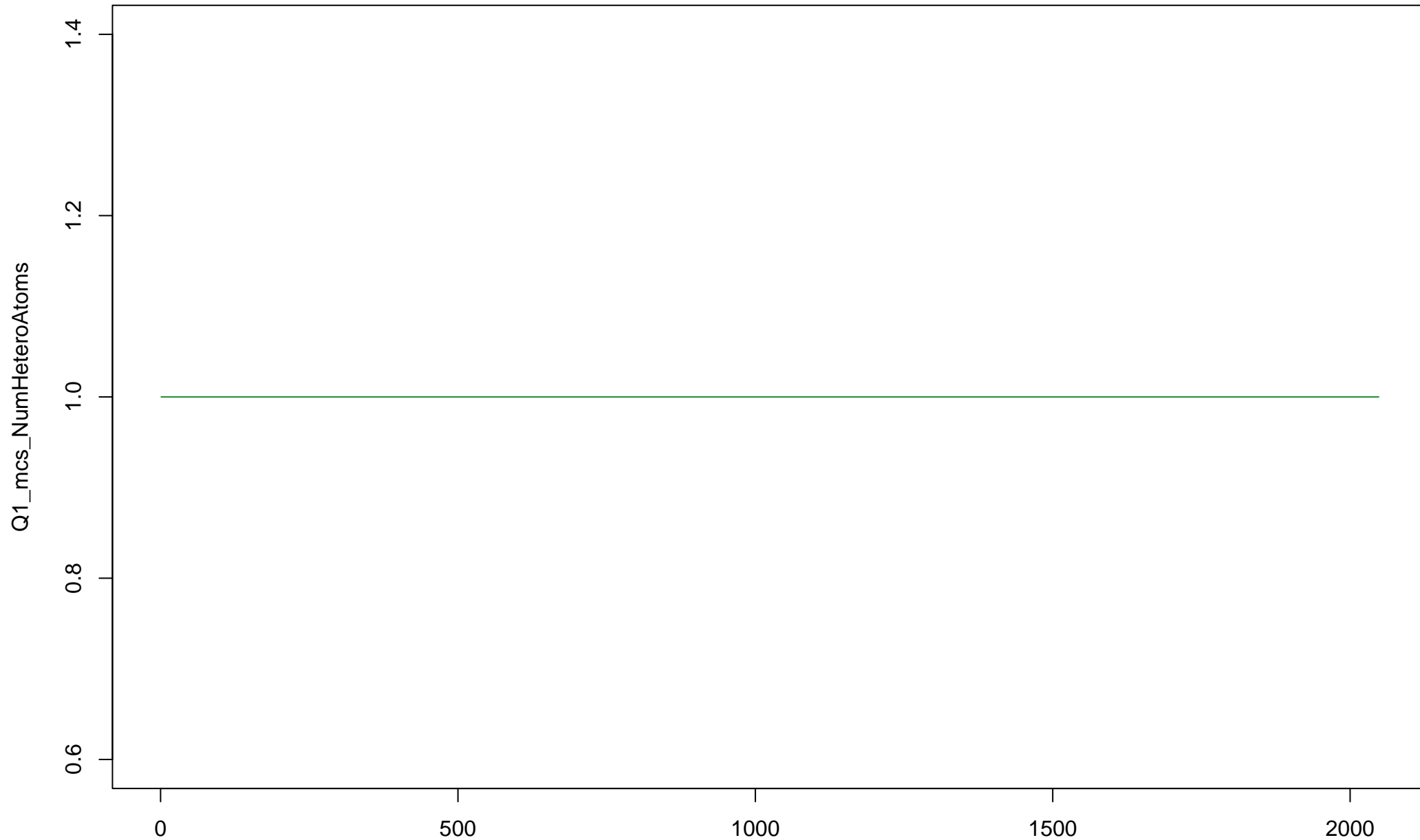
**Q1\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



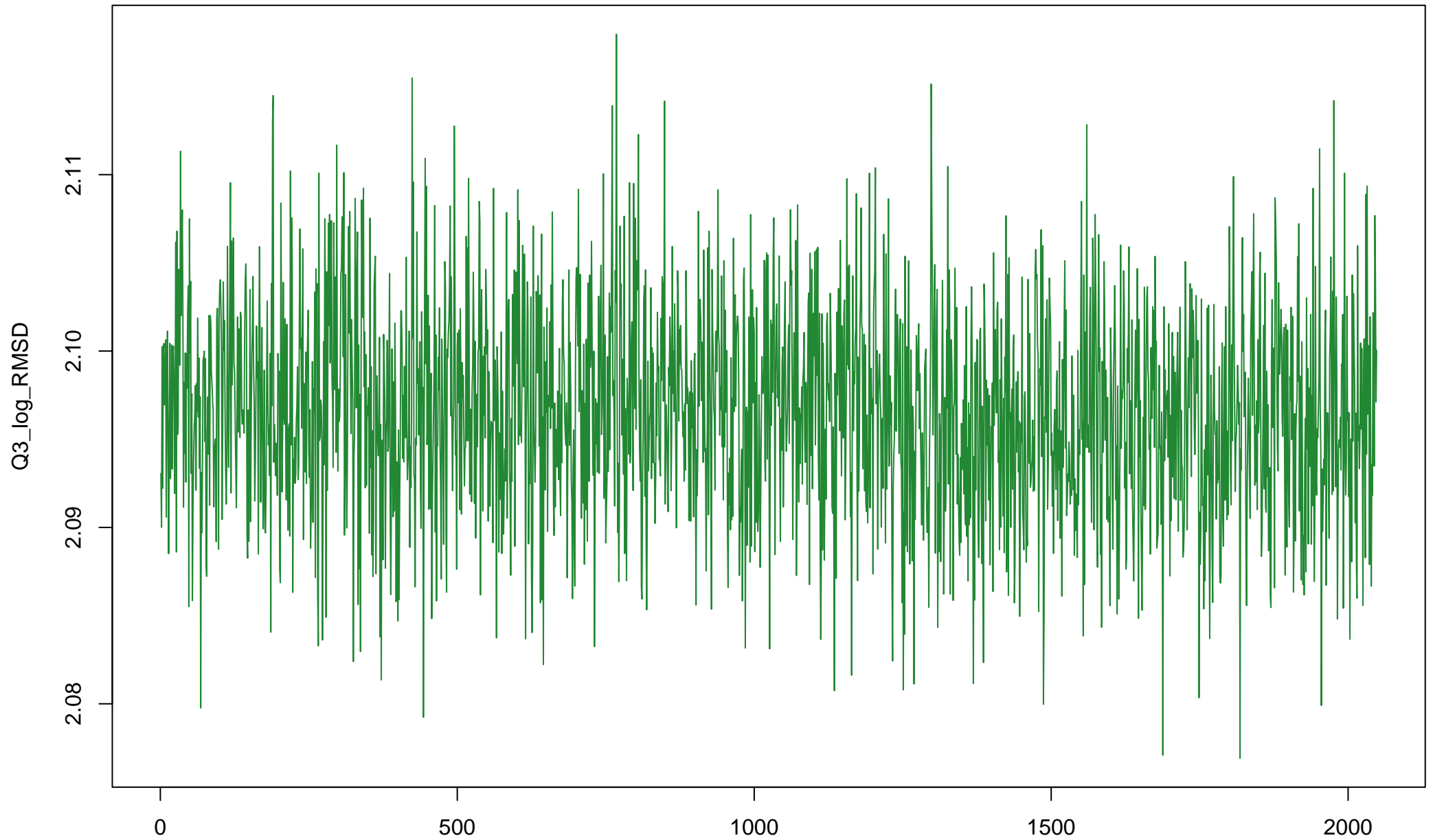
**Q1\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



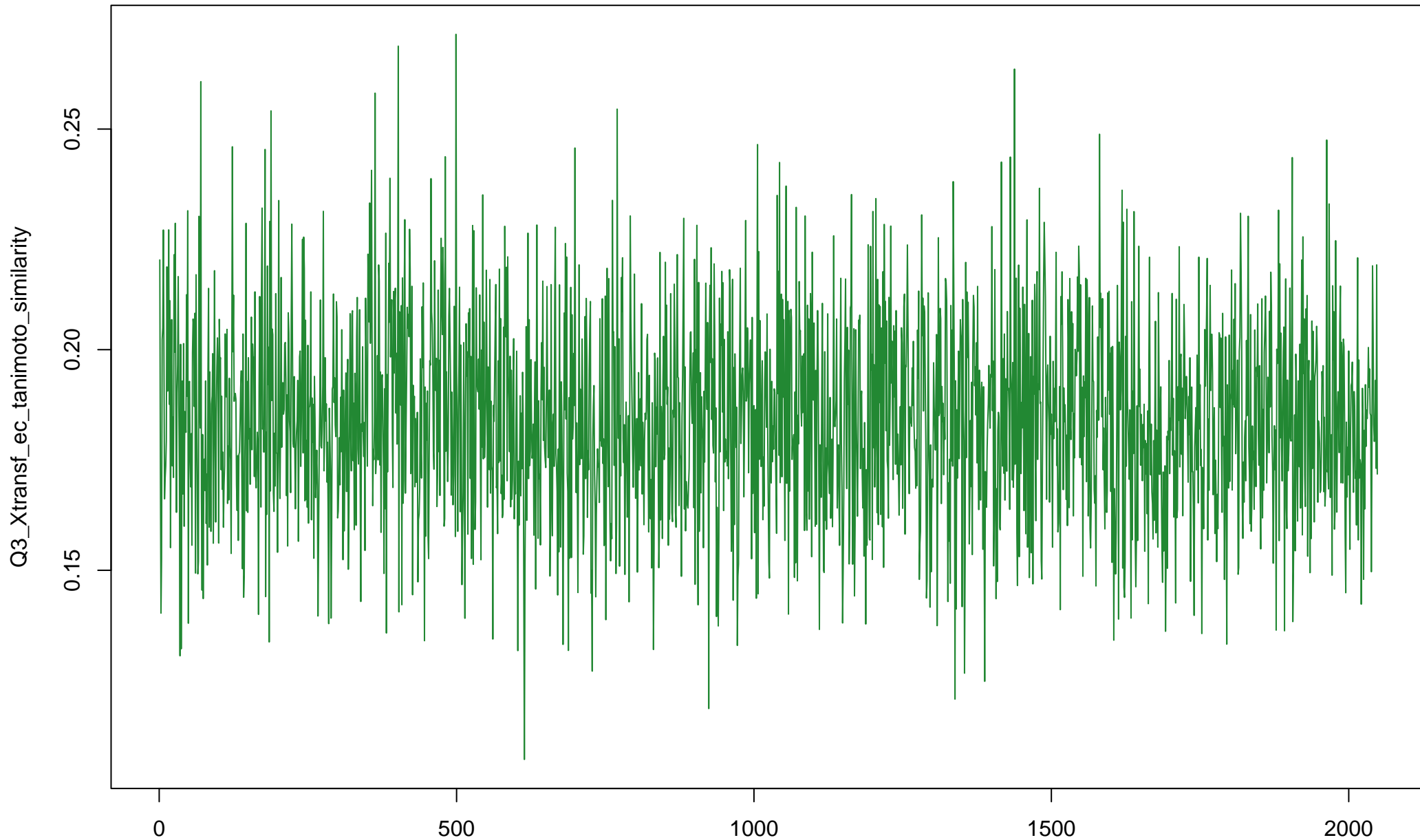
**Q1\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q3\_log\_RMSD**  
**ESS = 1660 | BMK = 0.0683 | MCSE(6.27) = 2.91 | stat: FALSE | burn: 0**

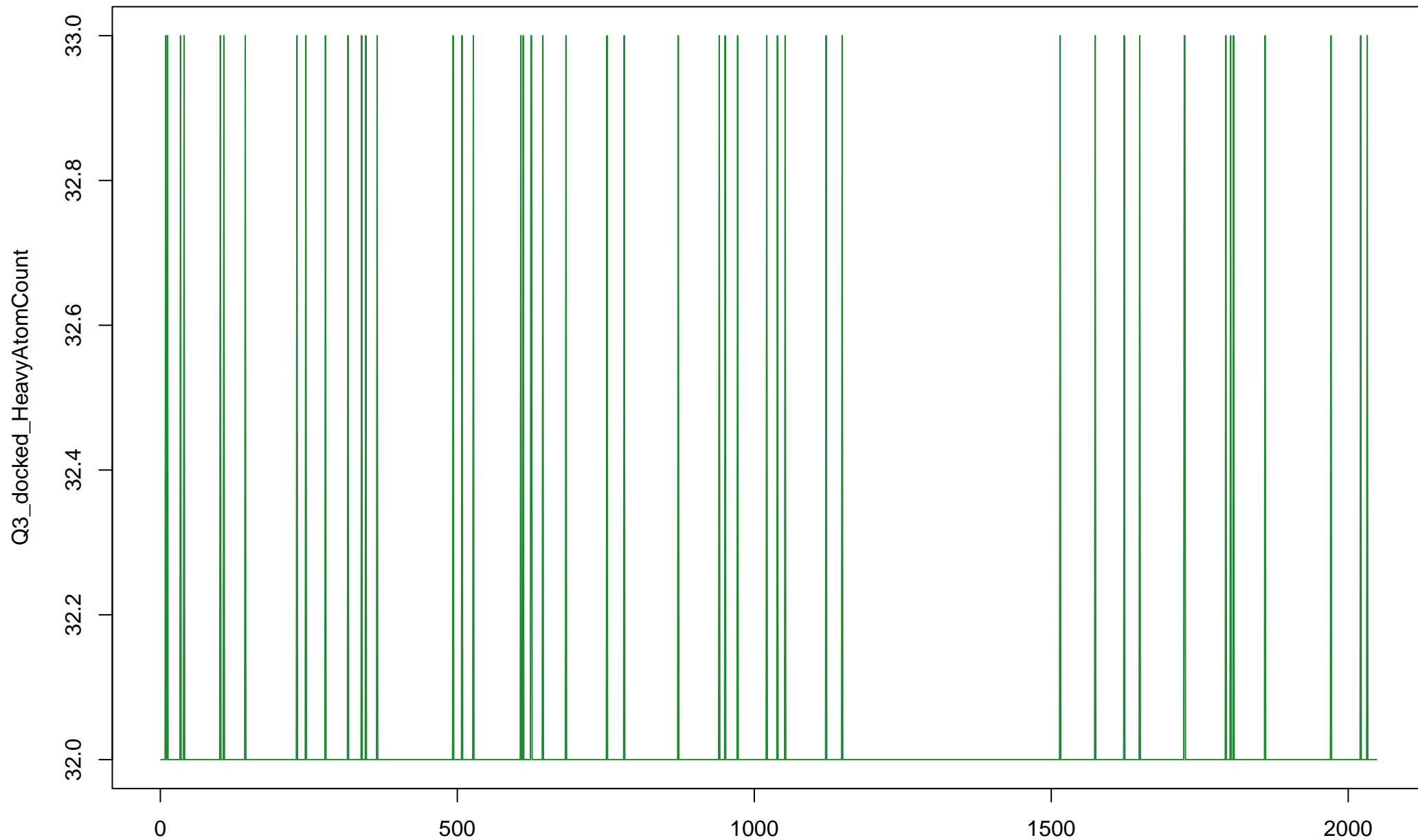


**Q3\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1900 | BMK = 0.0362 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0**





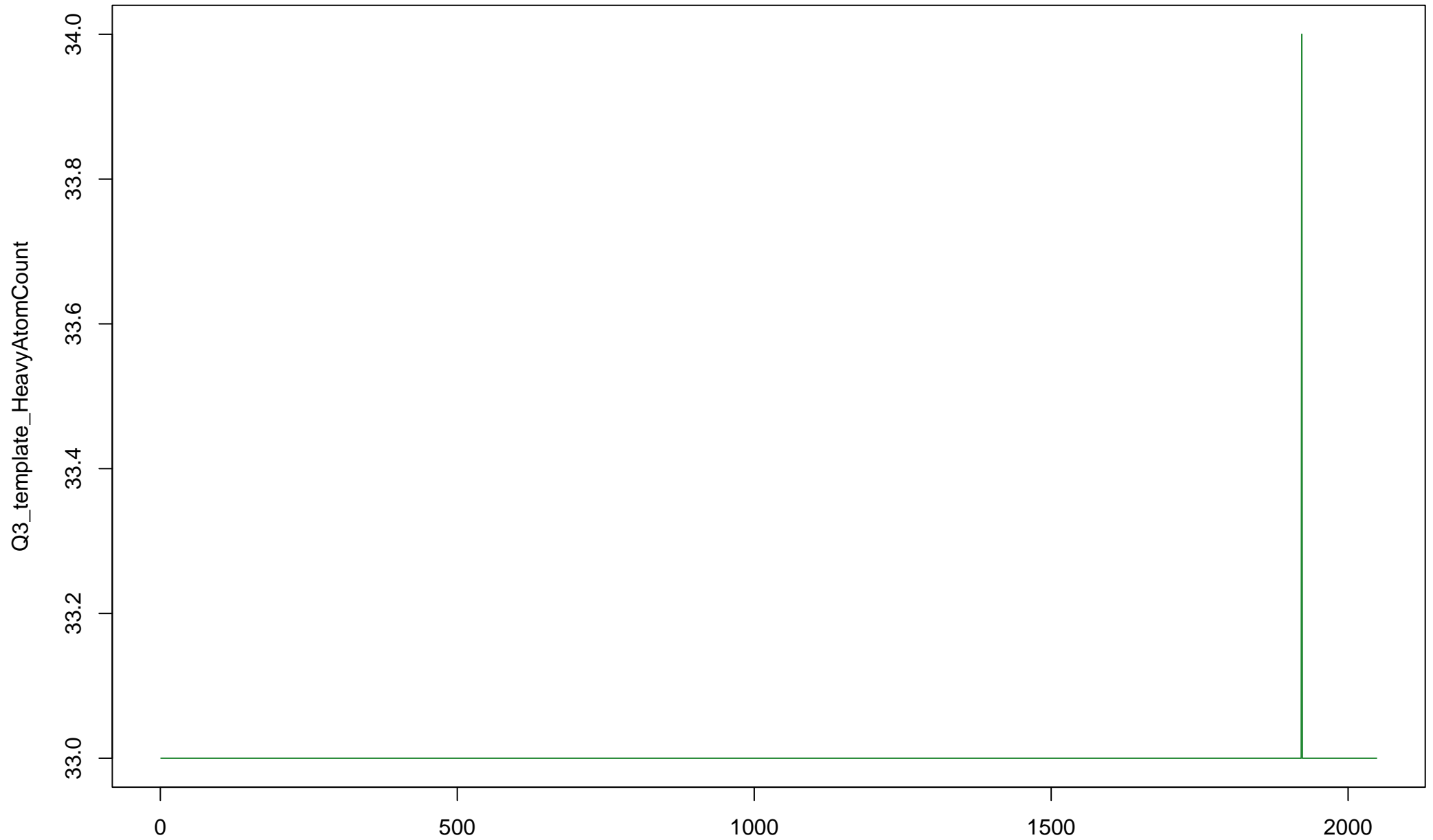
**Q3\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0996 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0**



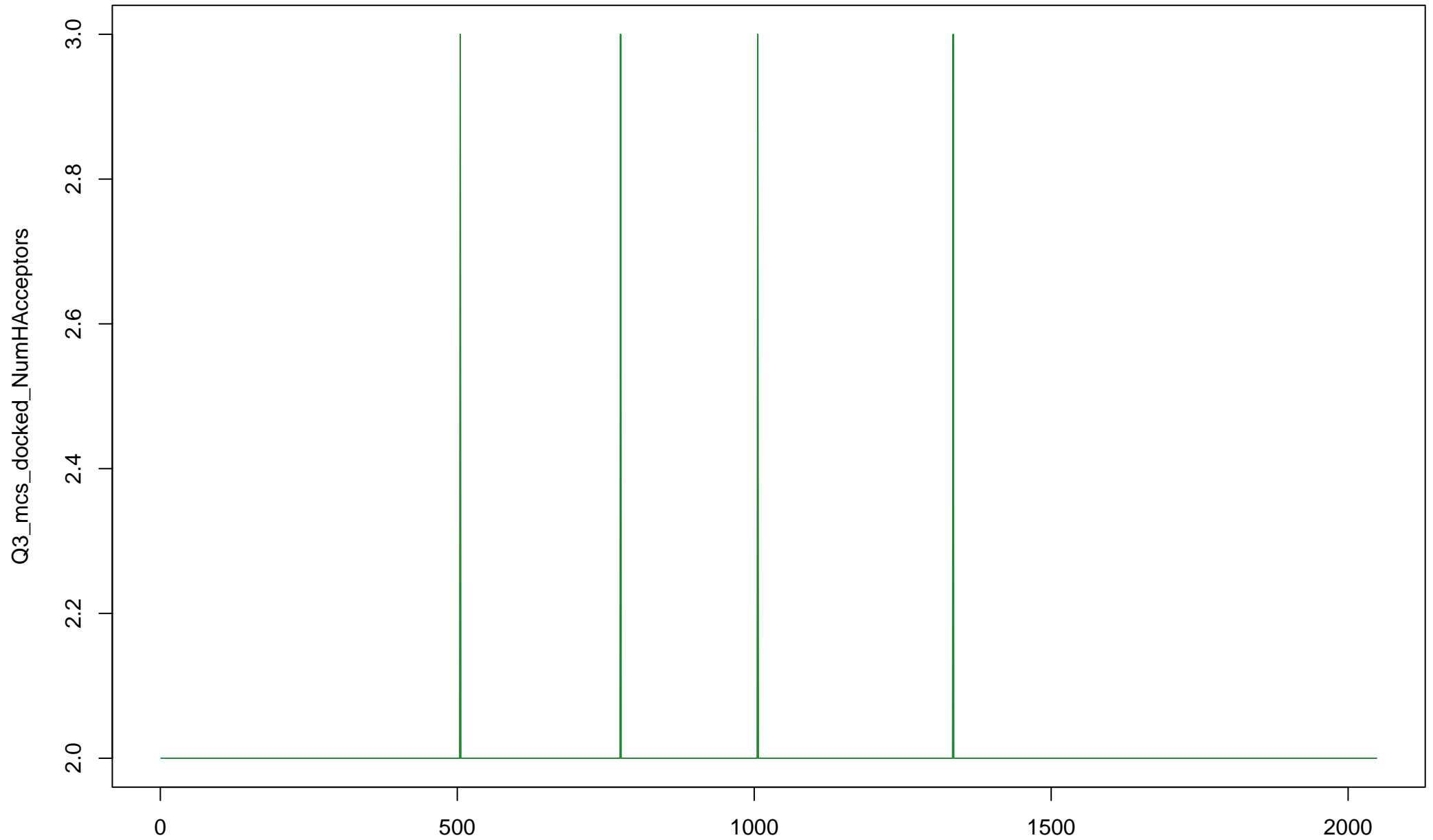
**Q3\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



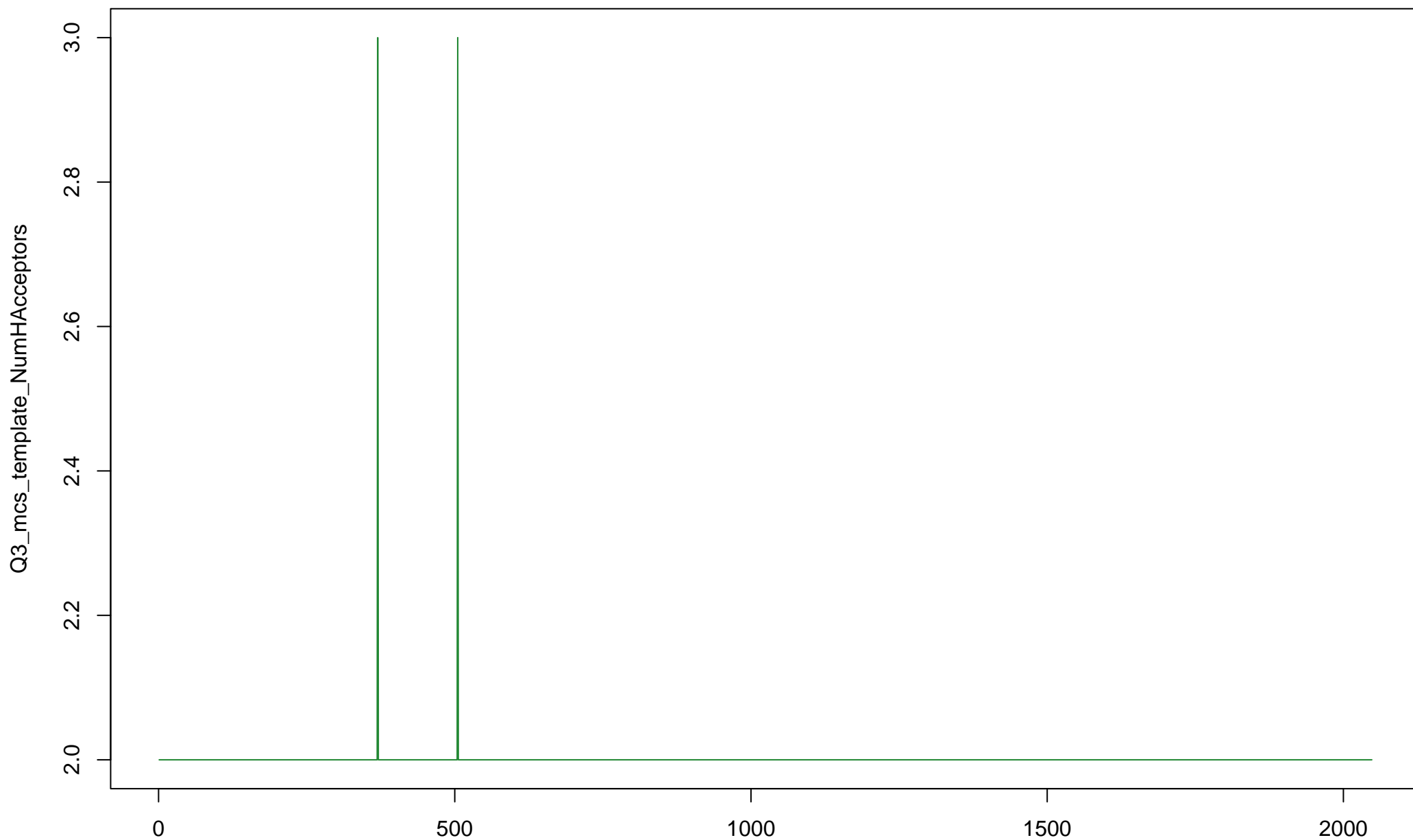
**Q3\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.517 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 2040**



**Q3\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.188 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 1428**



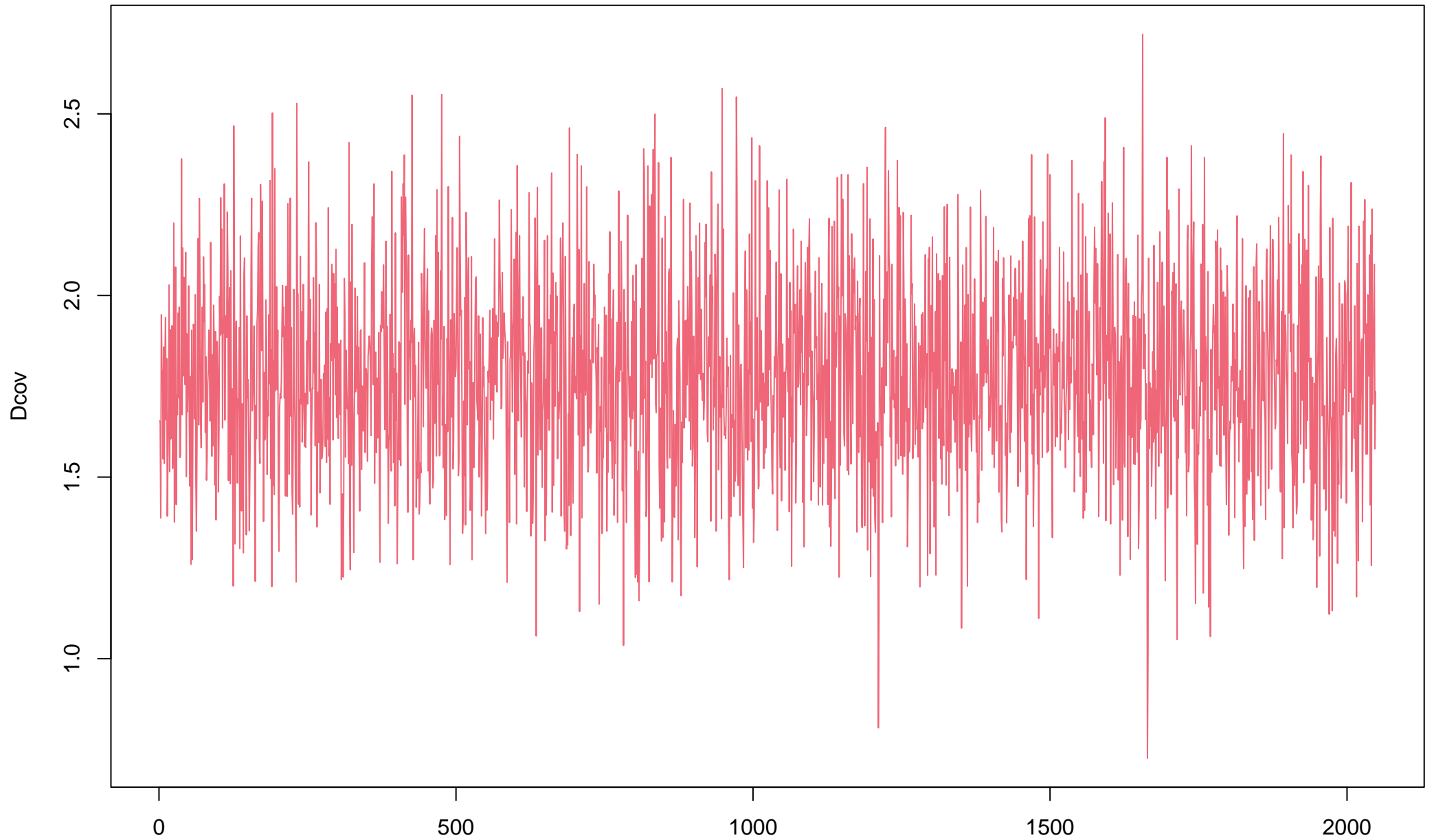
**Q3\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.628 | MCSE(6.27) = 2.2 | stat: FALSE | burn: 612**



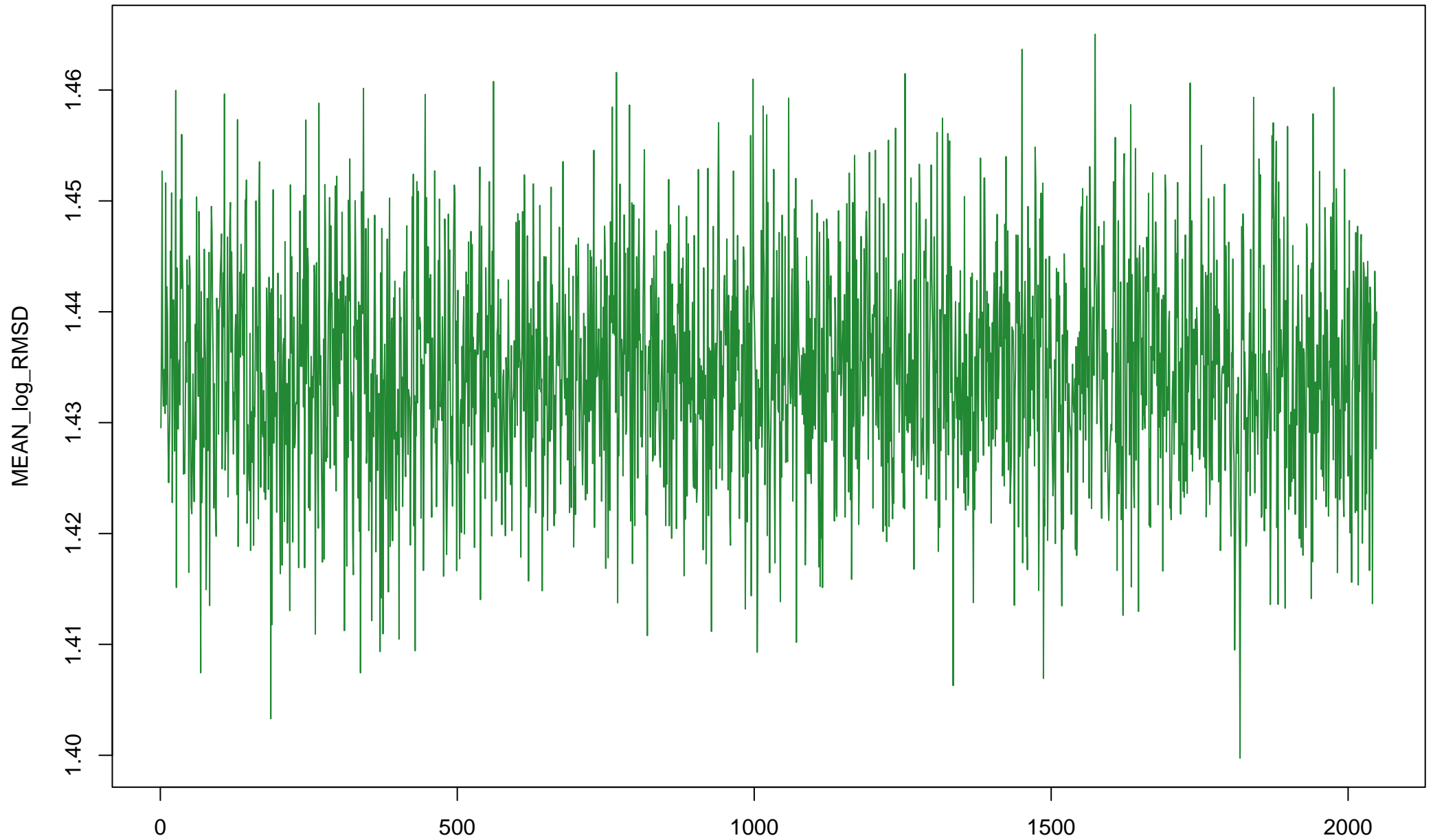
**Q3\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Dcov**  
**ESS = 2050 | BMK = 0.0652 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0**

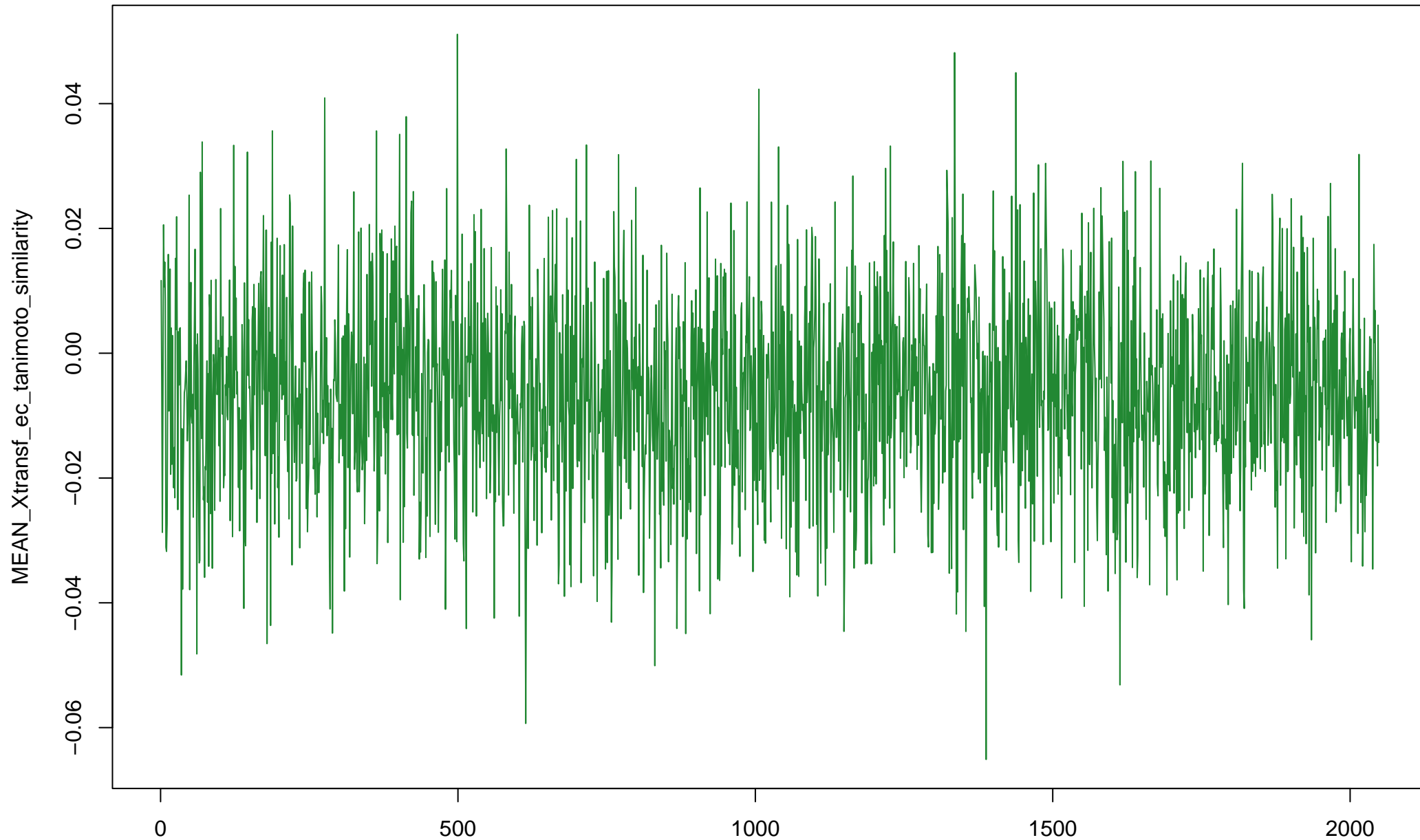


**MEAN\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0346 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0**

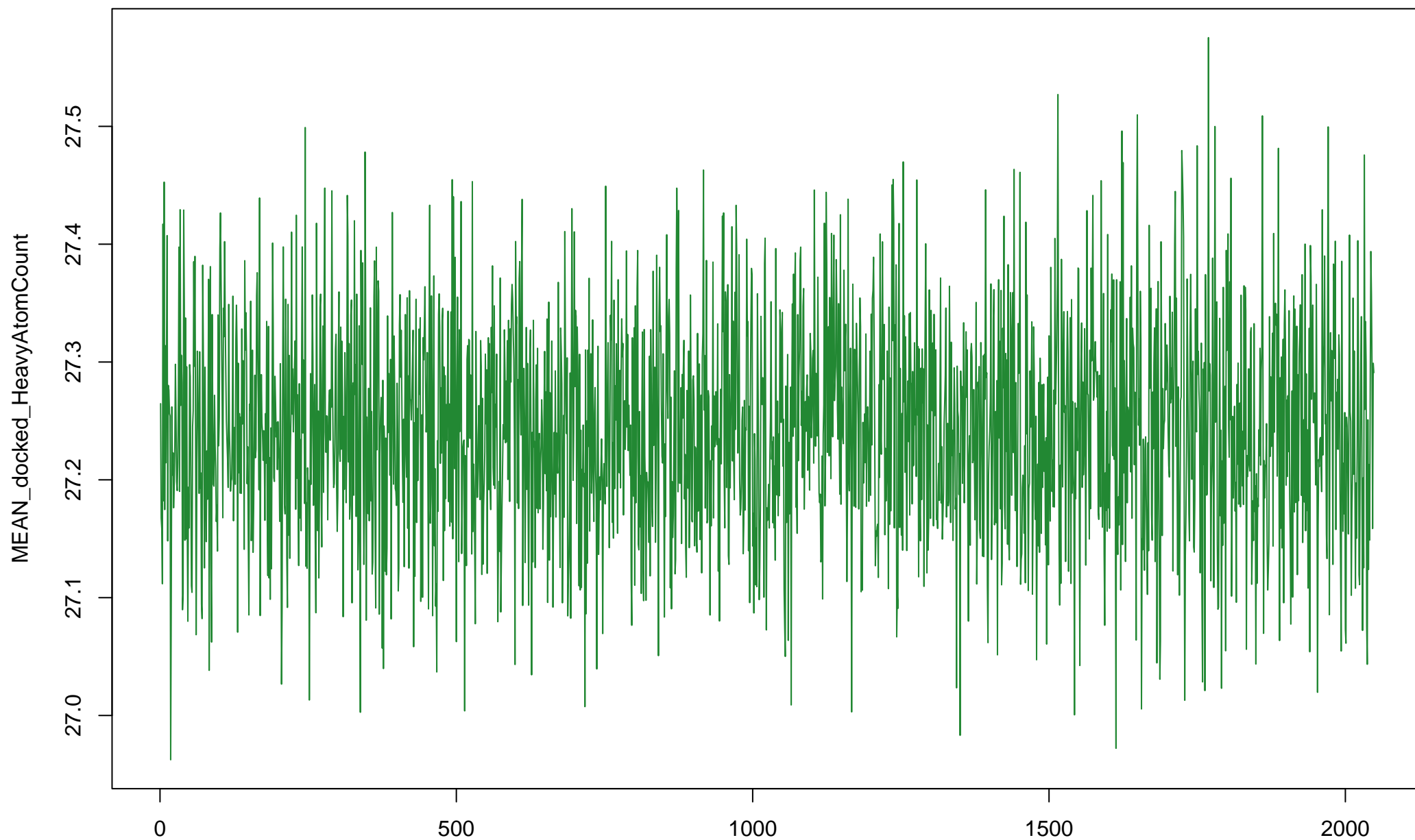




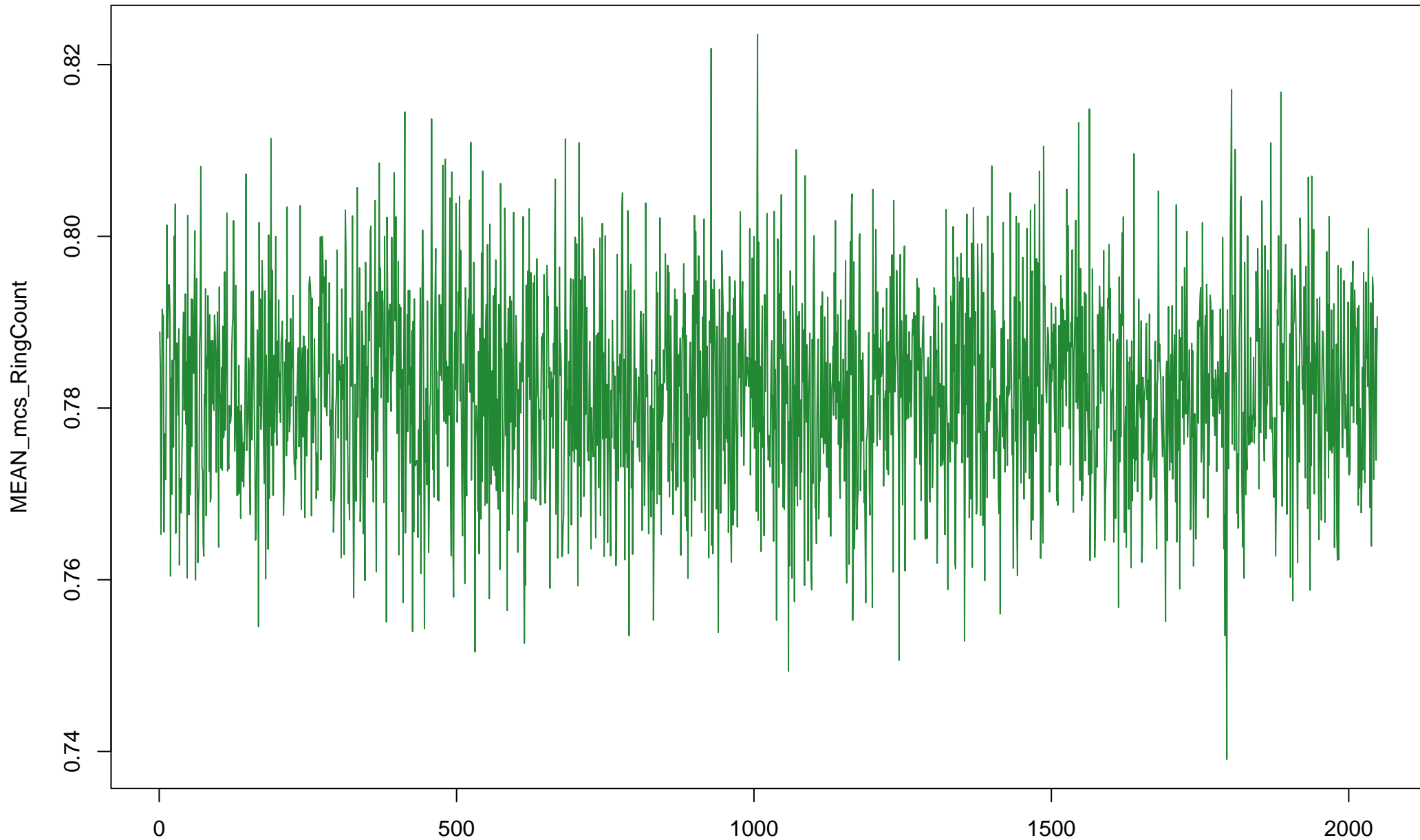
**MEAN\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0419 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0**



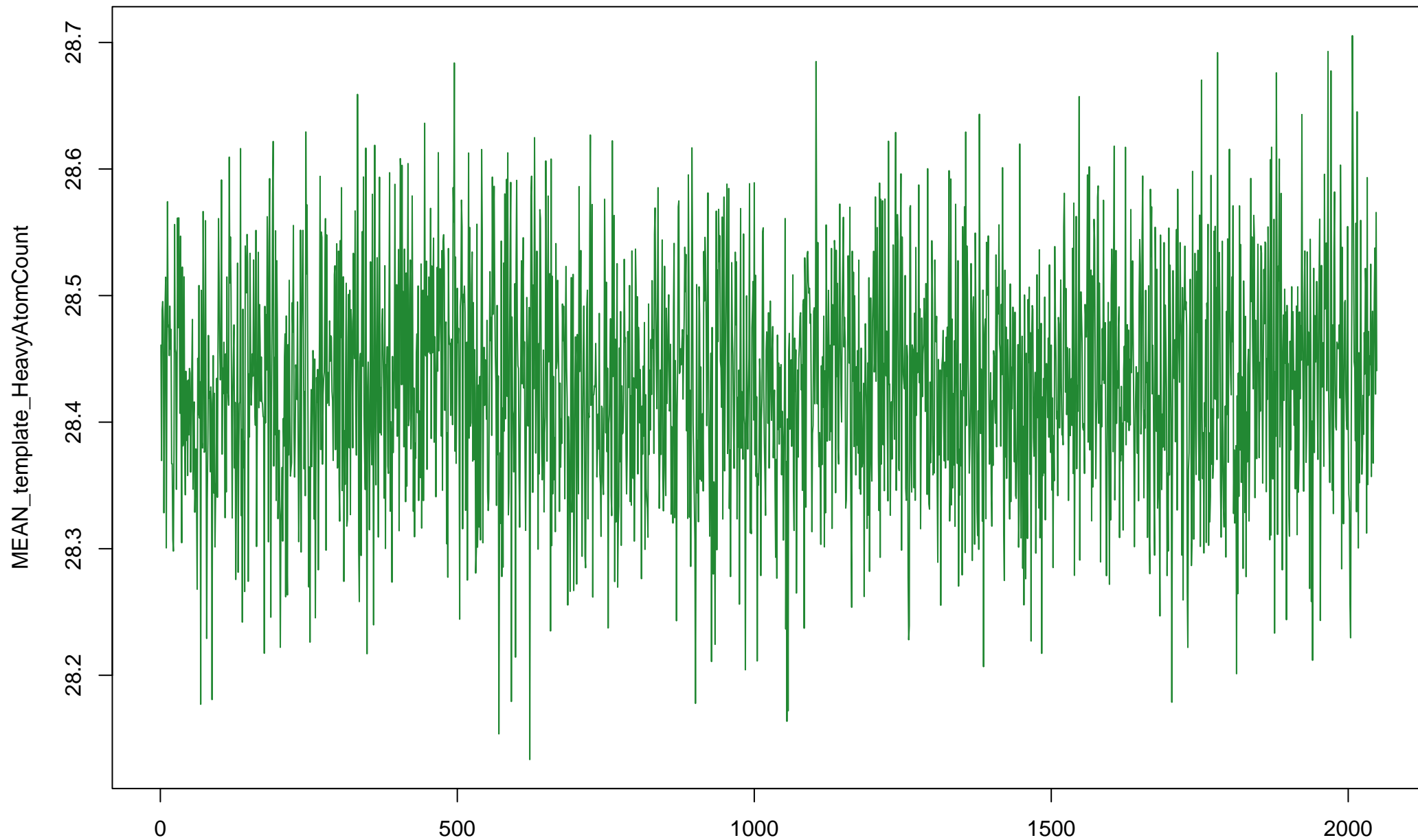
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 1860 | BMK = 0.0555 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0**



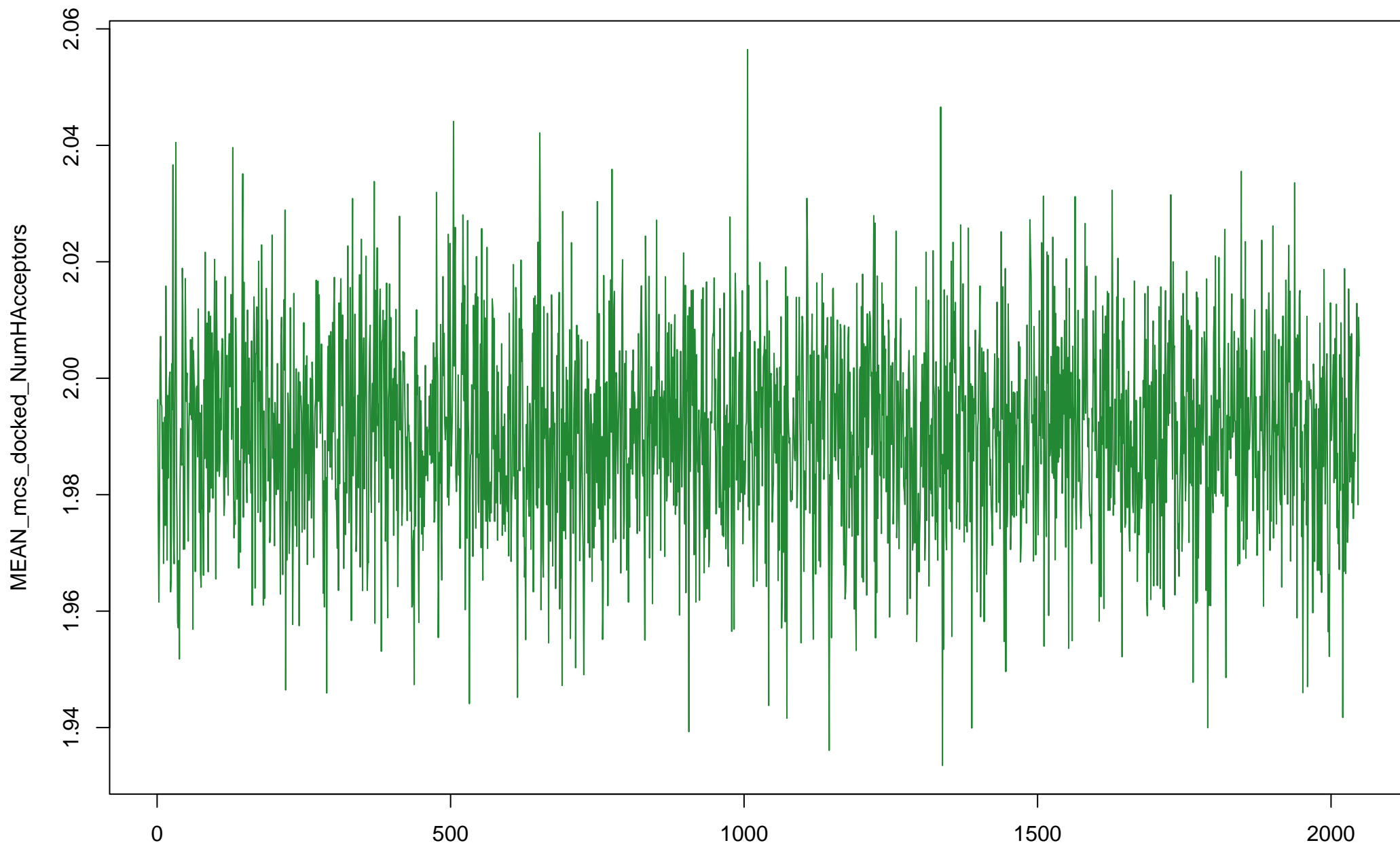
**MEAN\_mcs\_RingCount**  
**ESS = 2050 | BMK = 0.0386 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0**



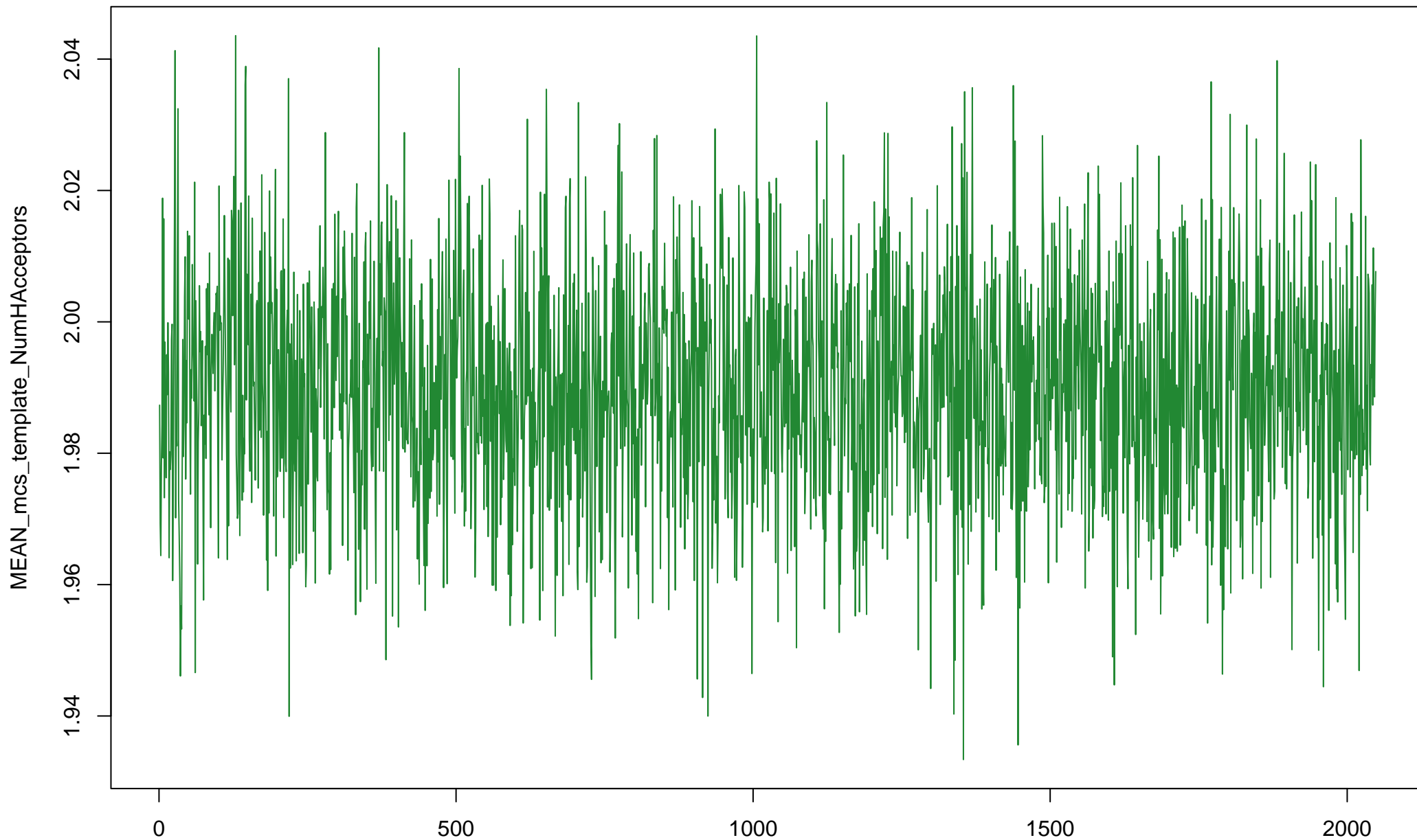
**MEAN\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0408 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0**



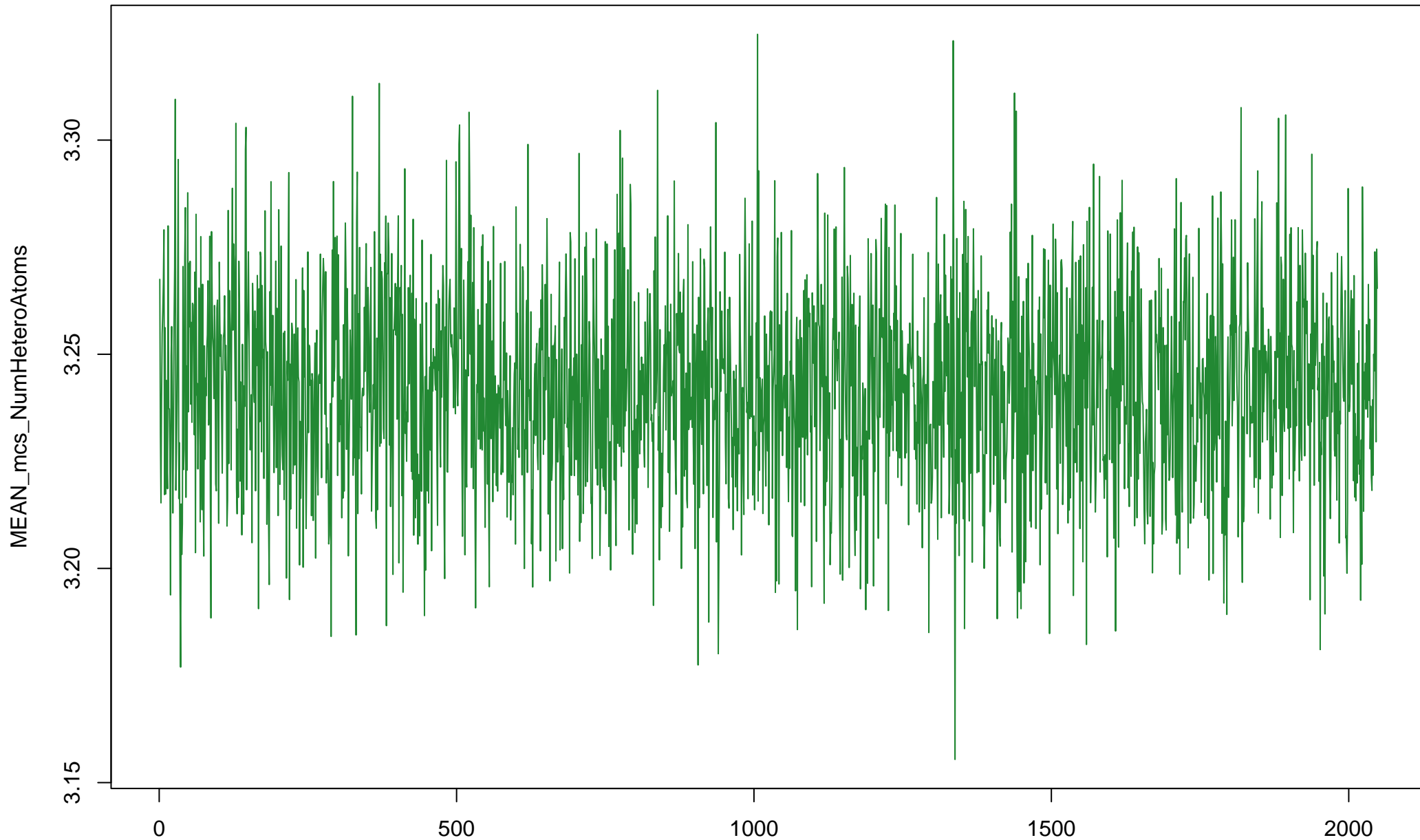
**MEAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0366 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0**



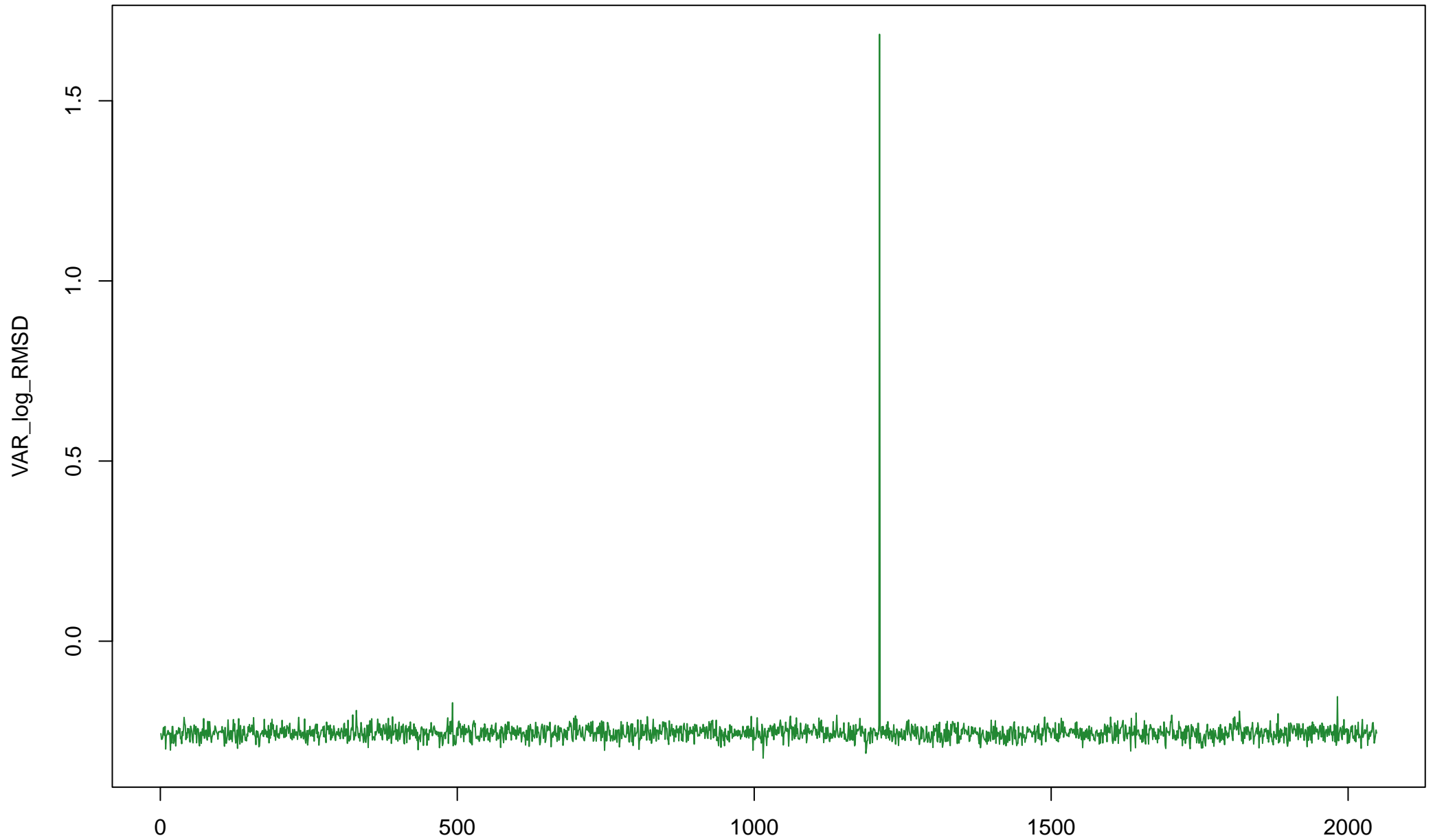
**MEAN\_mcs\_template\_NumHAcceptors**  
**ESS = 1890 | BMK = 0.0341 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0**



**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0456 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0**

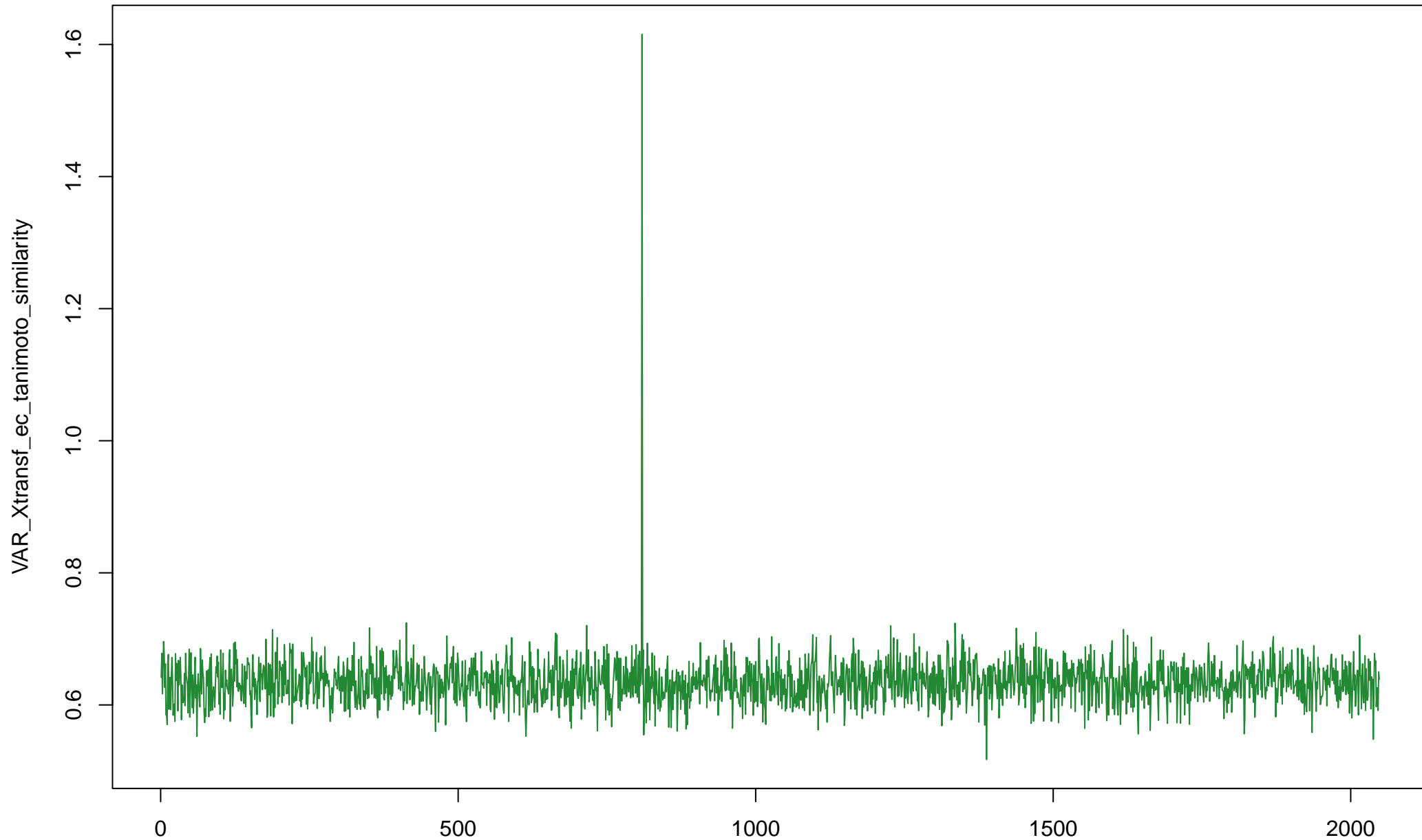


**VAR\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0448 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0**

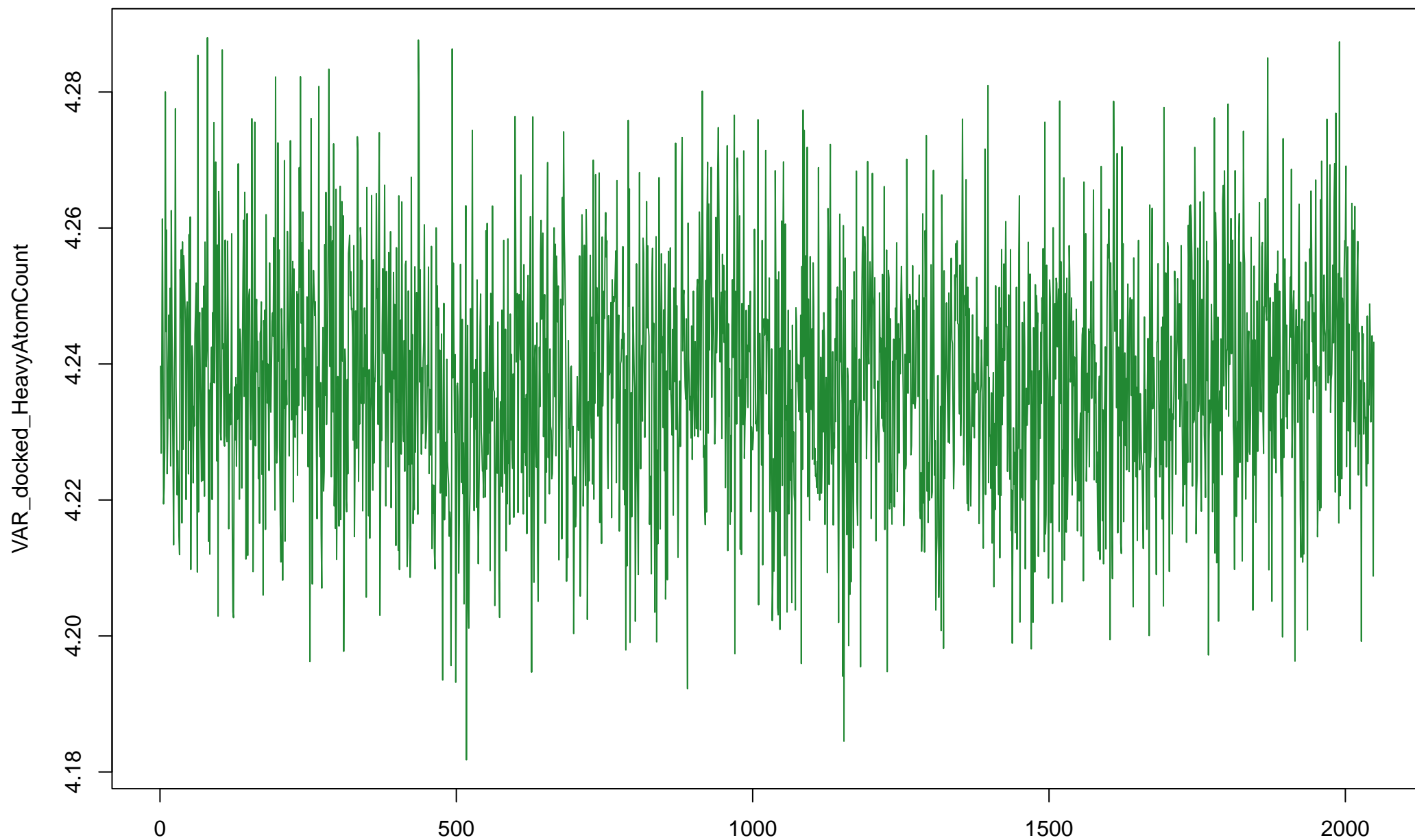




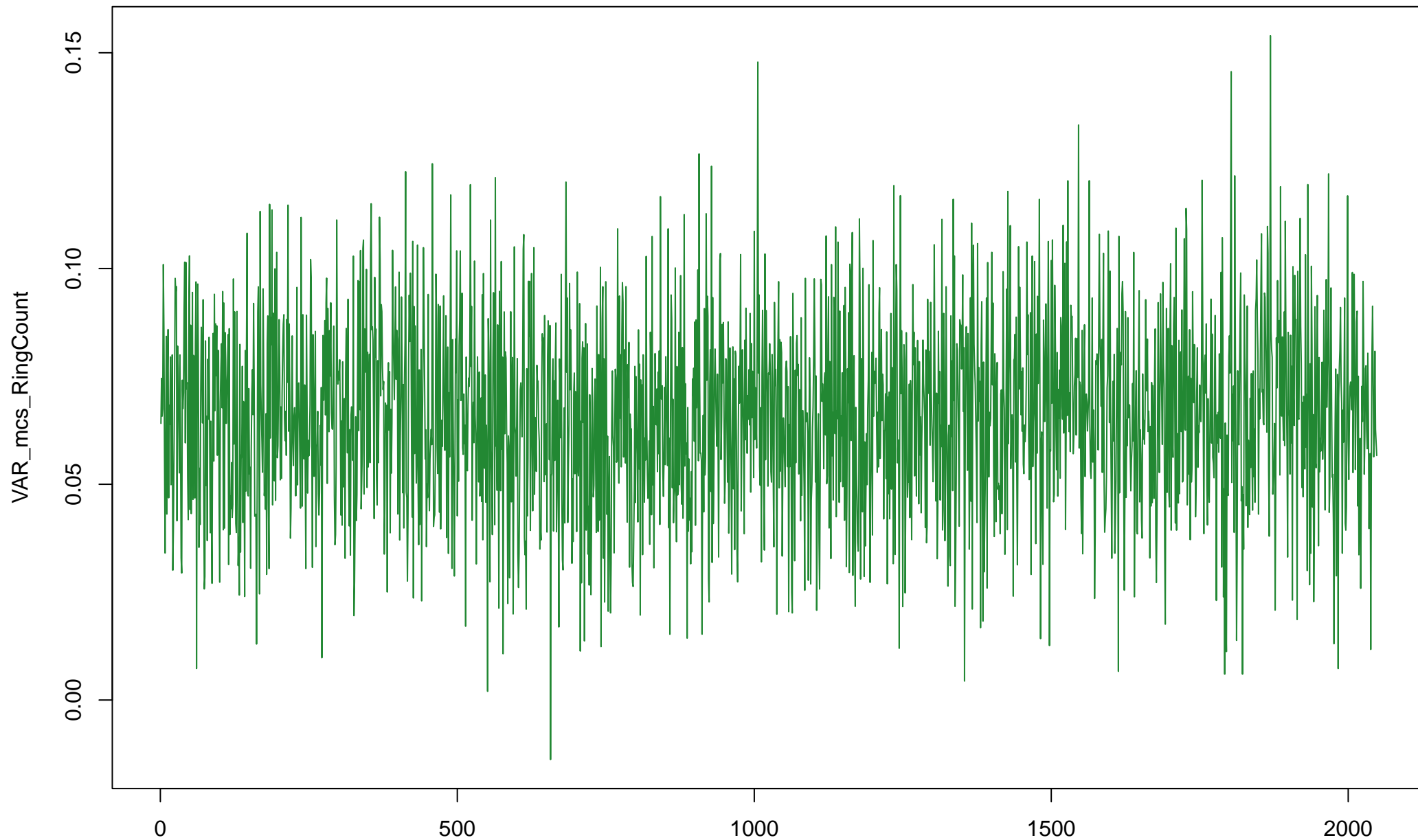
**VAR\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0446 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0**



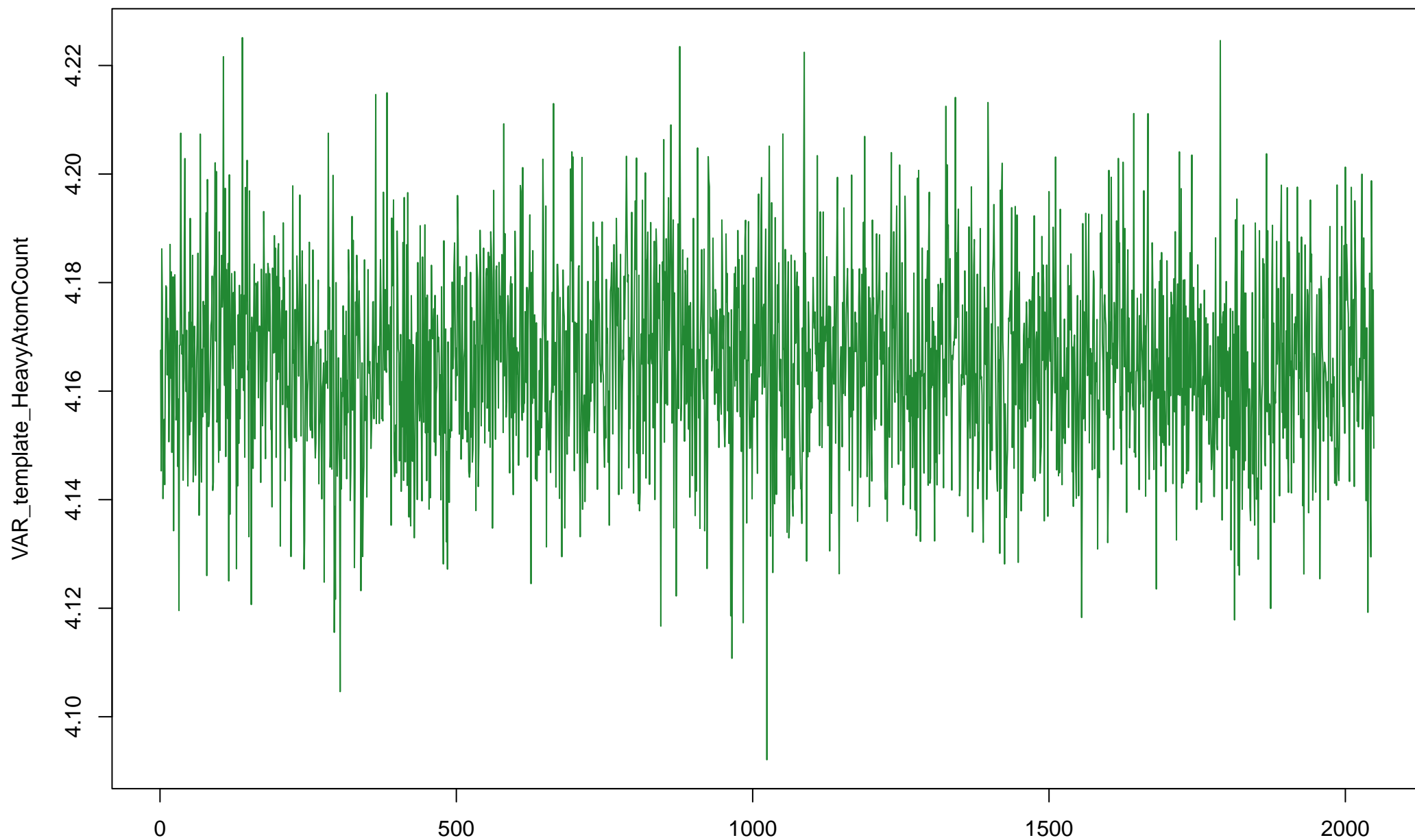
**VAR\_docked\_HeavyAtomCount**  
**ESS = 1470 | BMK = 0.0357 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0**



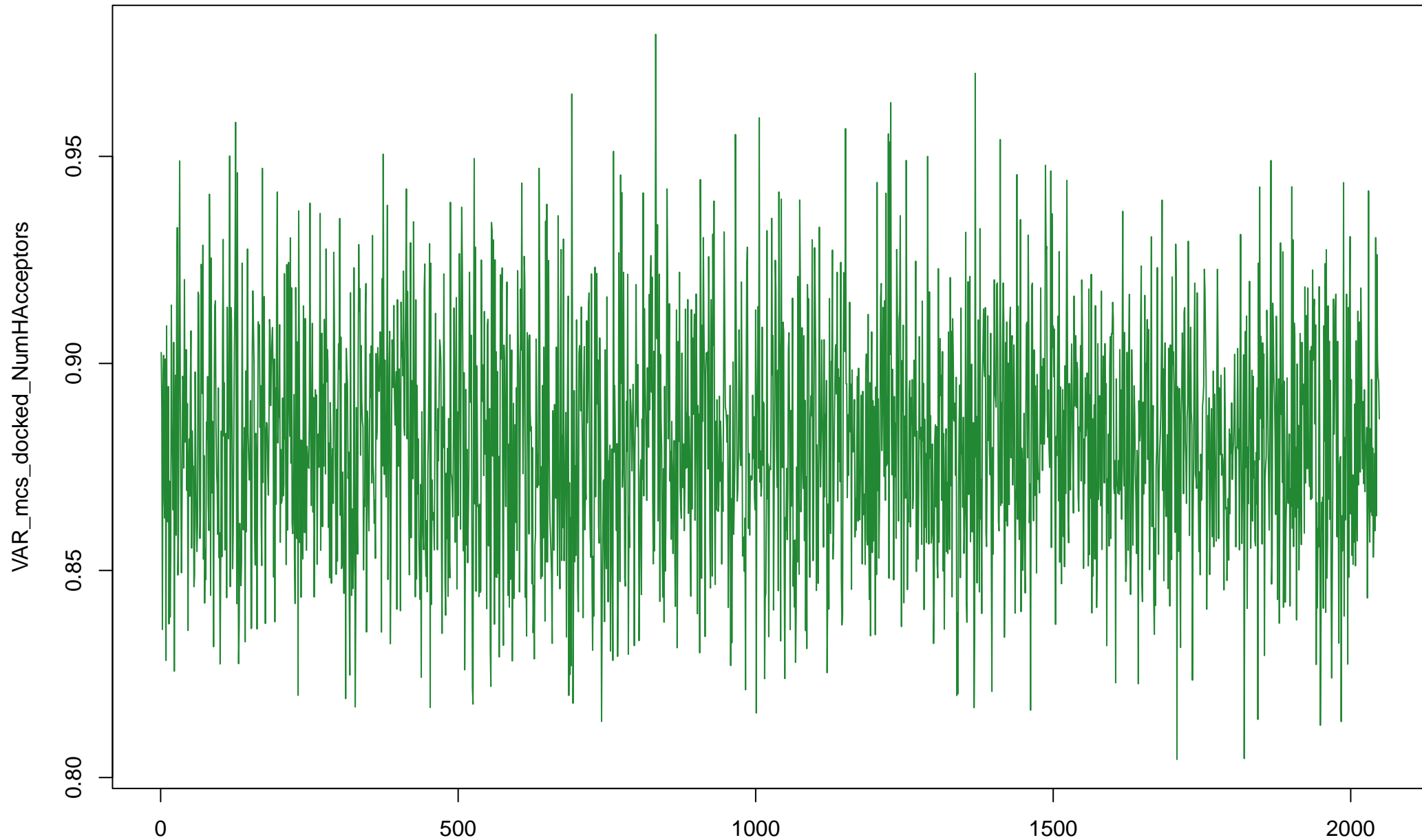
**VAR\_mcs\_RingCount**  
**ESS = 2050 | BMK = 0.0429 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0**



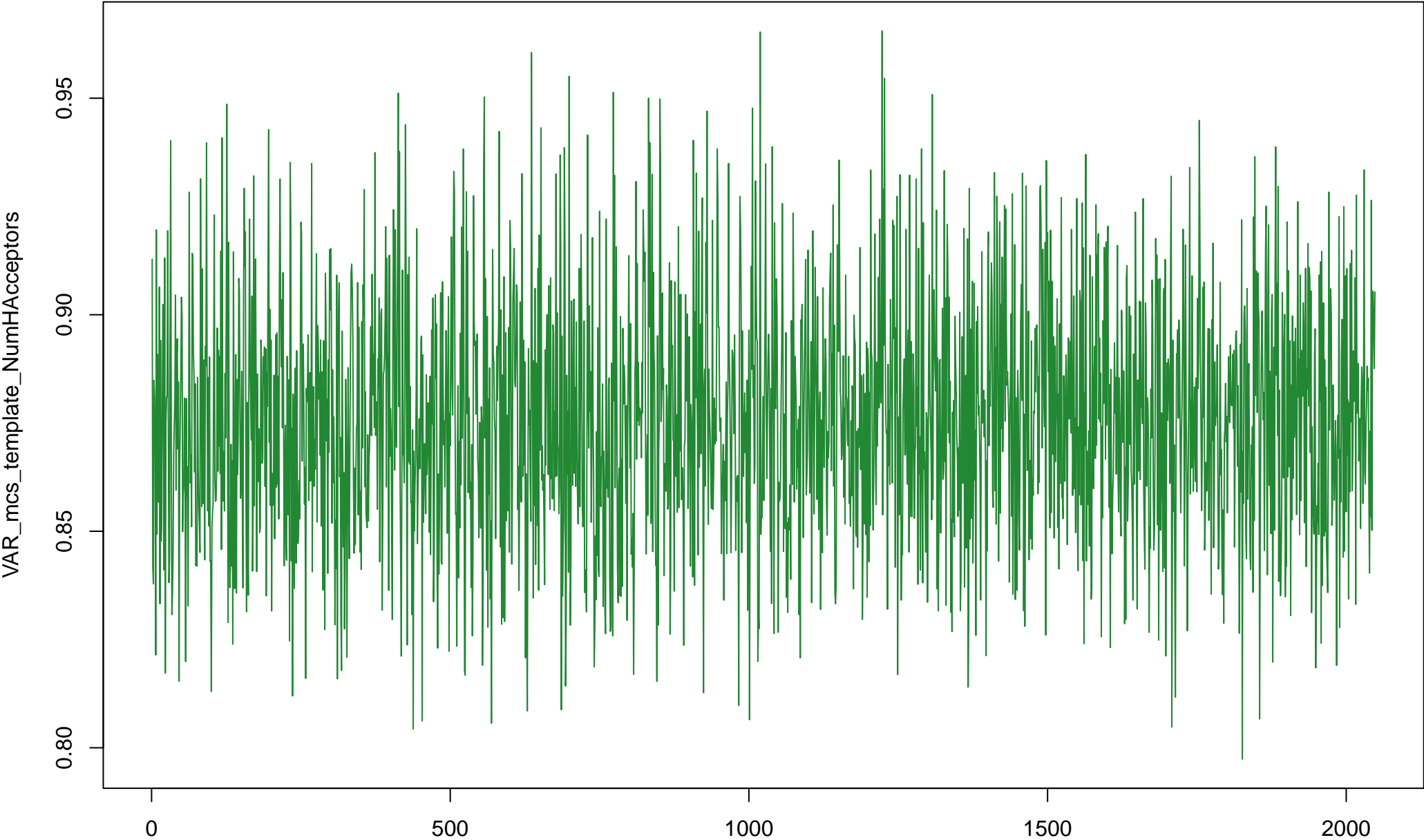
**VAR\_template\_HeavyAtomCount**  
**ESS = 2030 | BMK = 0.0589 | MCSE(6.27) = 2.62 | stat: FALSE | burn: 0**



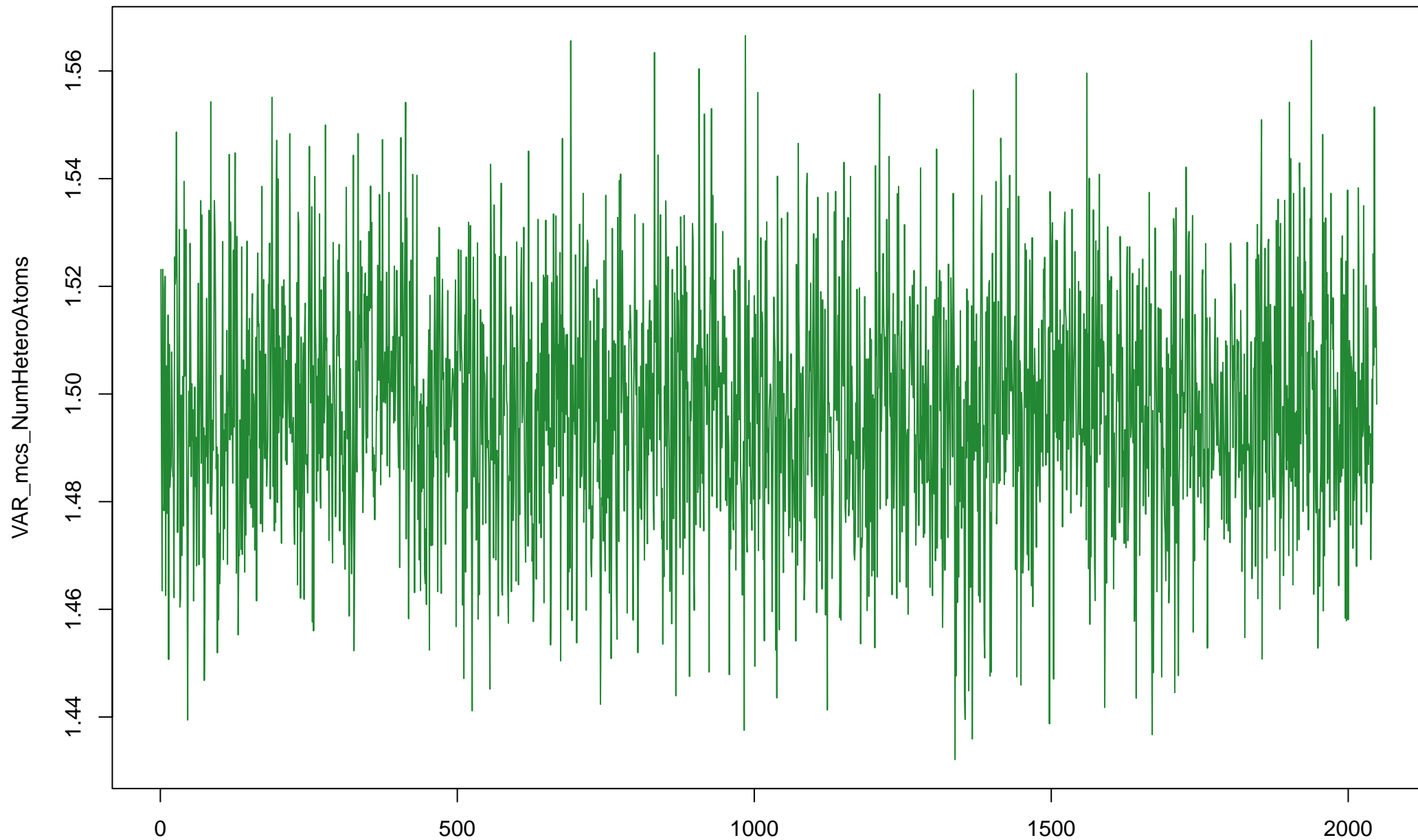
**VAR\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0551 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0**



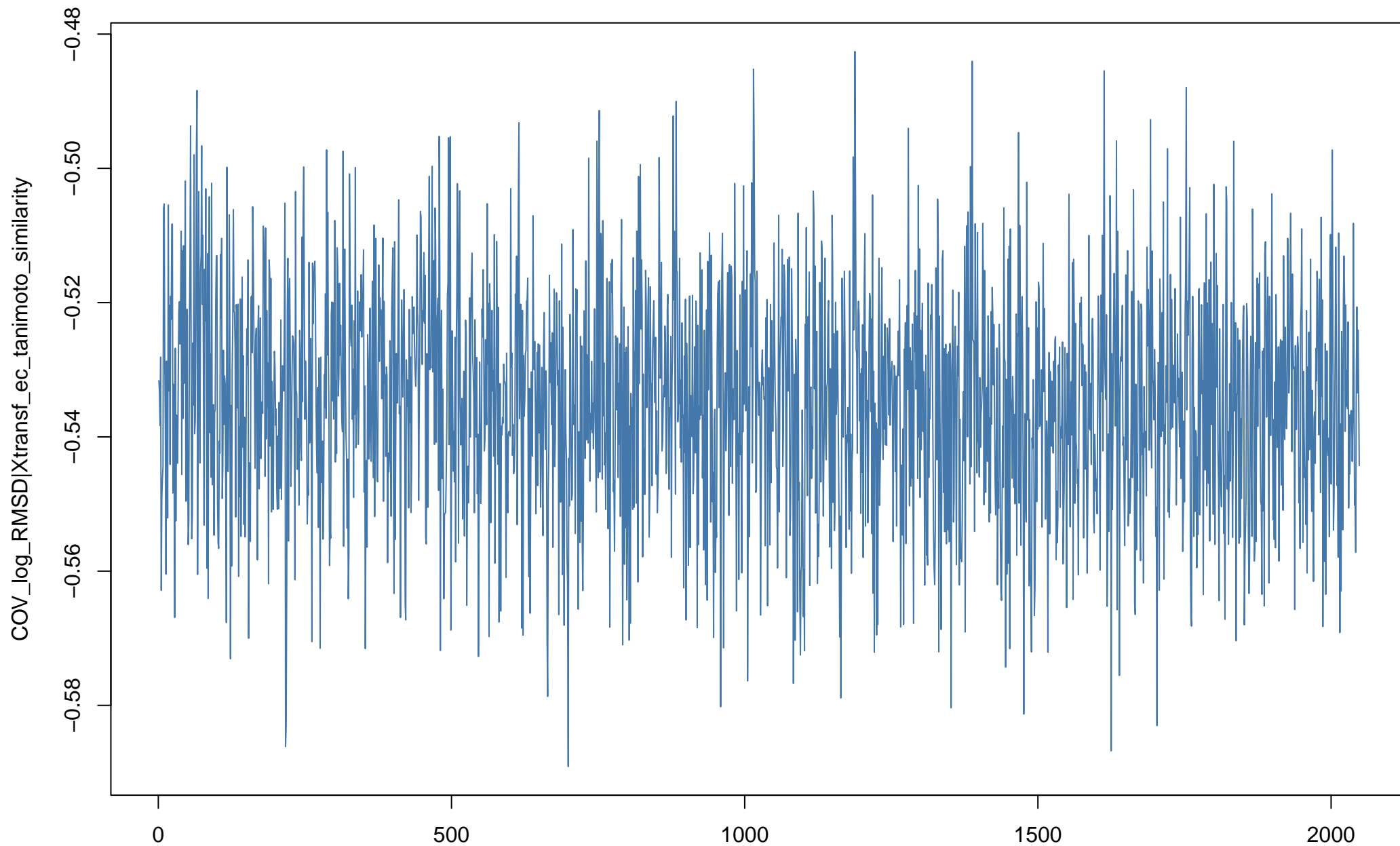
**VAR\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0711 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0**



**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0322 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0**

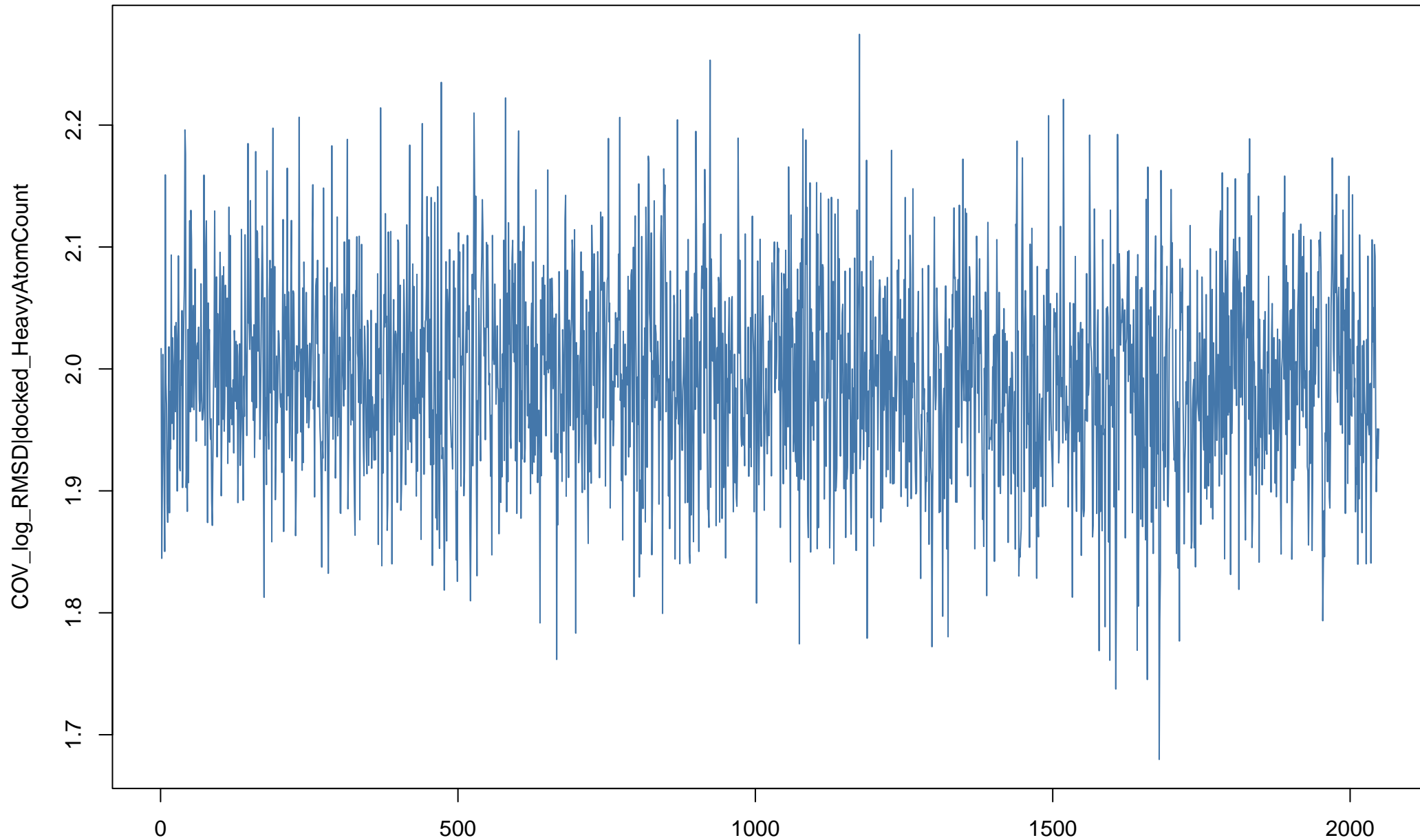


**COV\_log\_RMSD|Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1720 | BMK = 0.0677 | MCSE(6.27) = 2.61 | stat: FALSE | burn: 0**

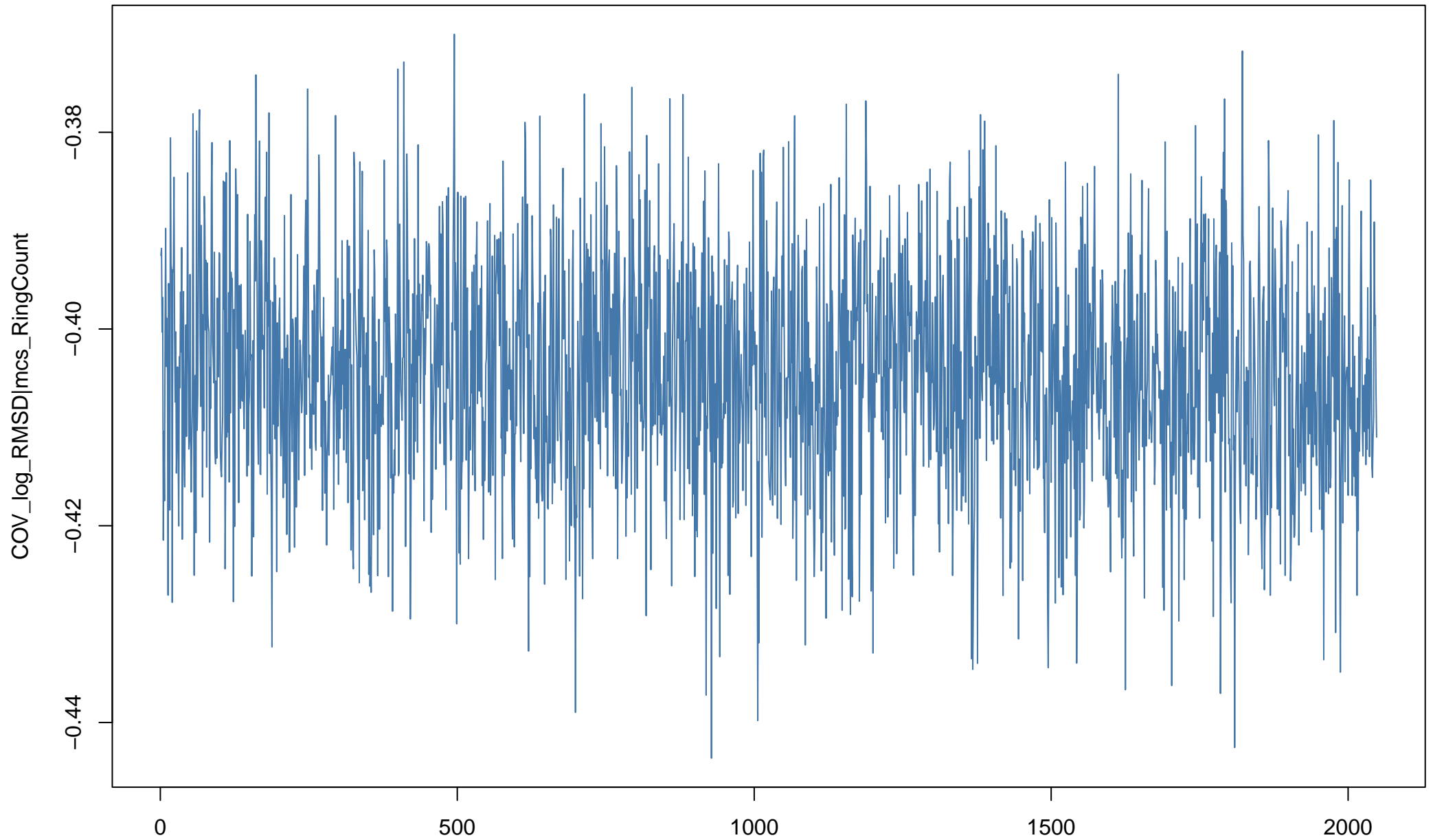




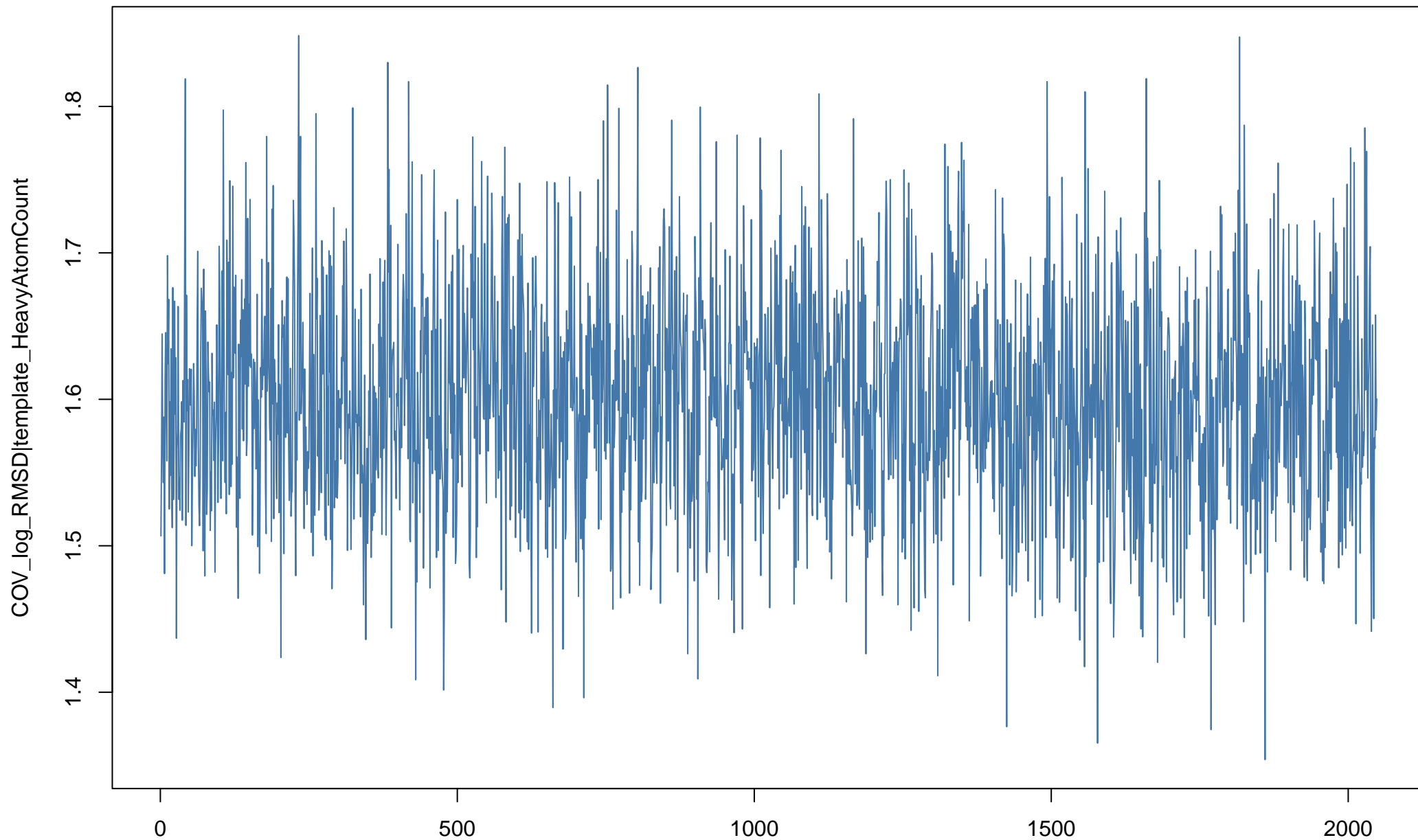
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 1810 | BMK = 0.0656 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0**



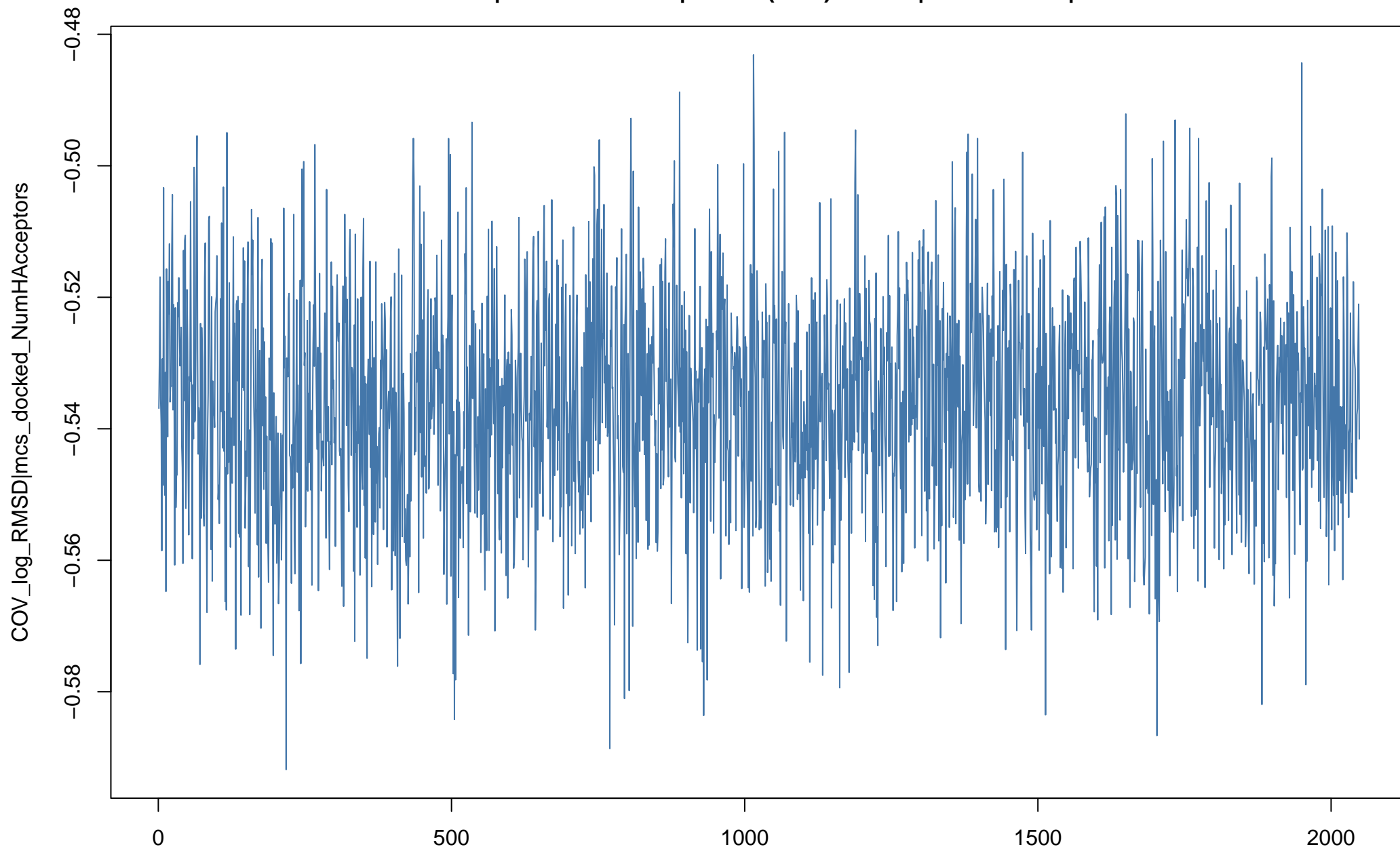
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 1770 | BMK = 0.0589 | MCSE(6.27) = 2.73 | stat: FALSE | burn: 0**



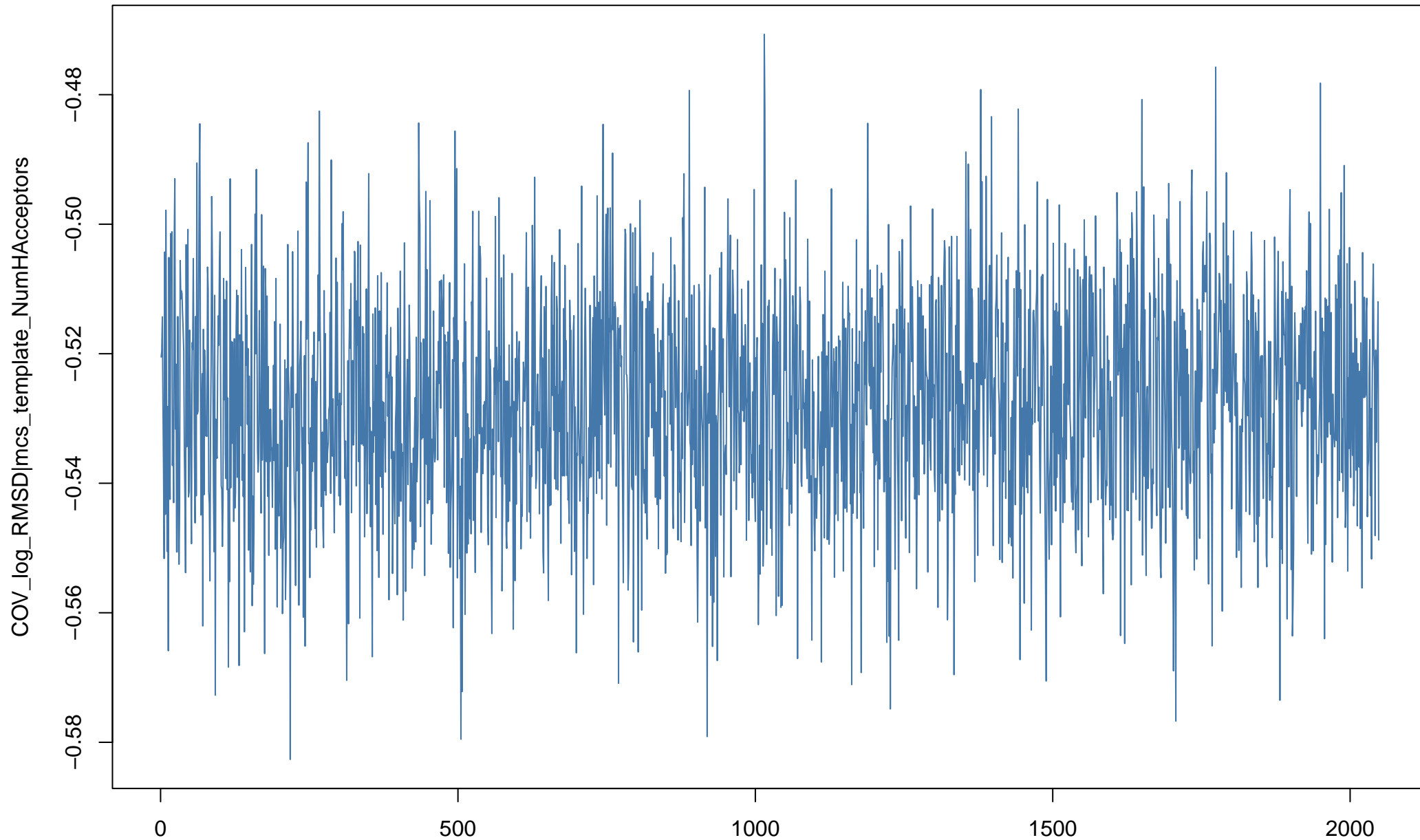
**COV\_log\_RMSD|template\_HeavyAtomCount**  
**ESS = 1570 | BMK = 0.0451 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0**



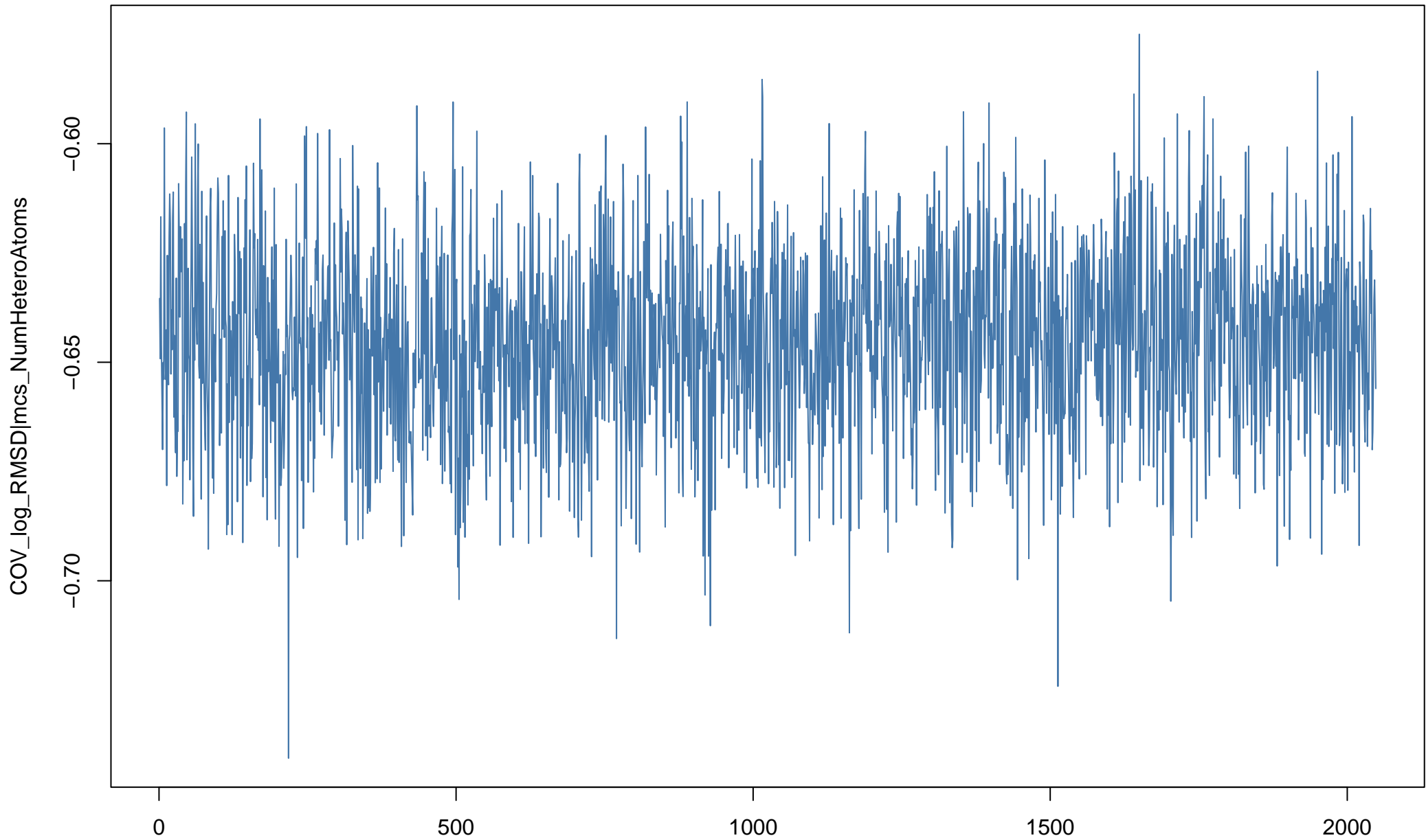
**COV\_log\_RMSD|mcs\_docked\_NumHAcceptors**  
**ESS = 1800 | BMK = 0.0408 | MCSE(6.27) = 2.67 | stat: TRUE | burn: 0**



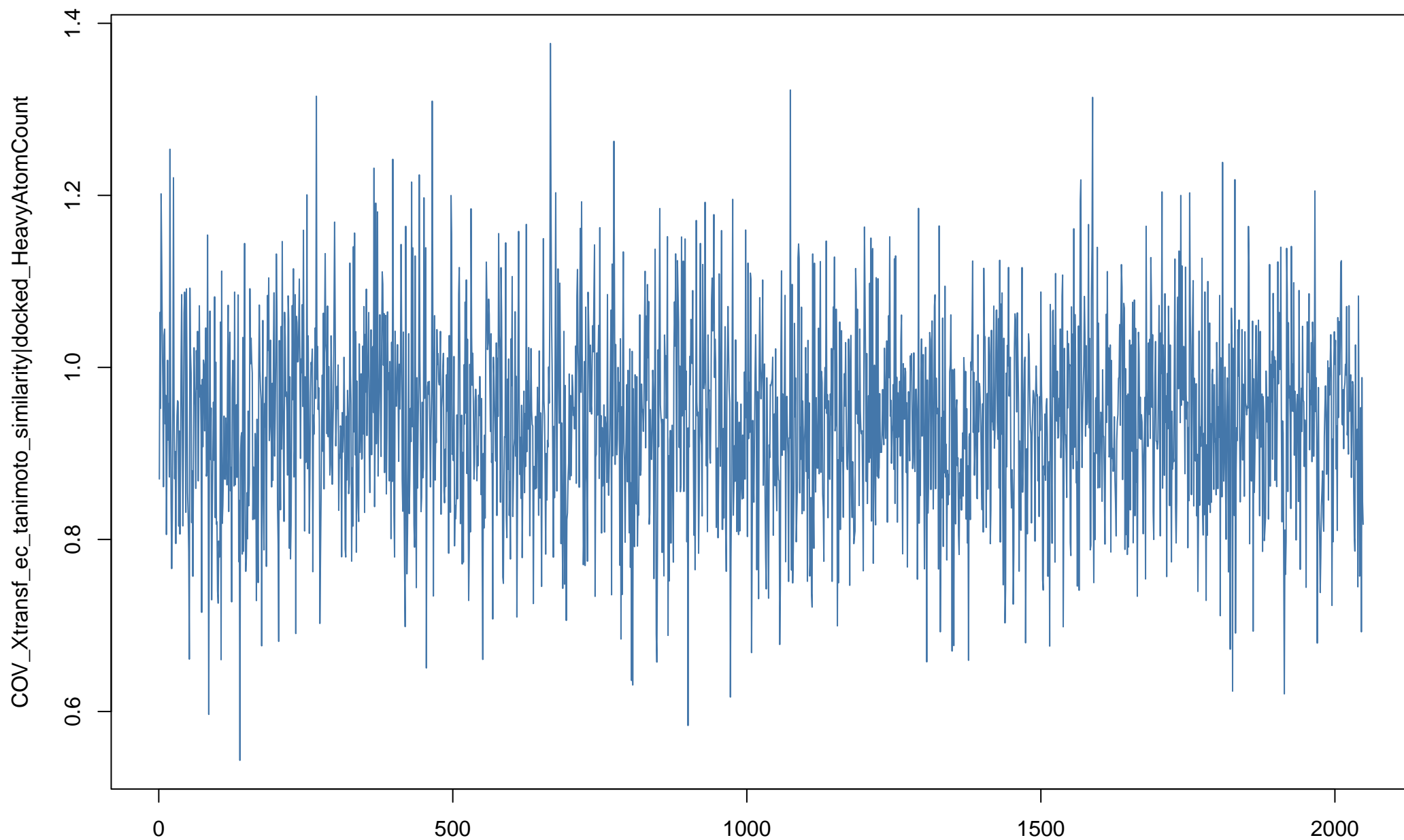
**COV\_log\_RMSD|mcs\_template\_NumHAcceptors**  
**ESS = 1940 | BMK = 0.0473 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0**



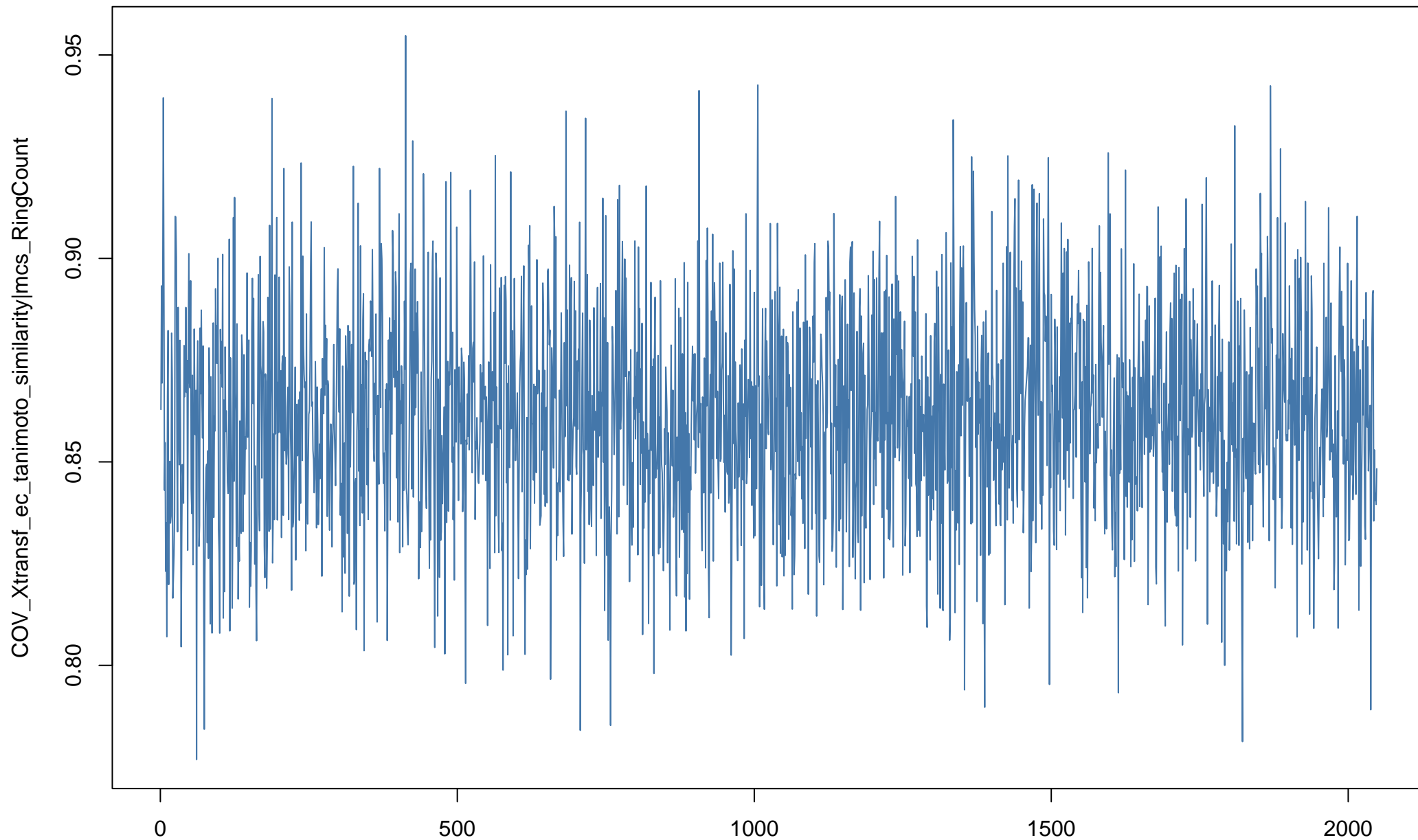
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 1820 | BMK = 0.0593 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0**



**COV\_Xtransf\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount**  
**ESS = 1740 | BMK = 0.0547 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0**

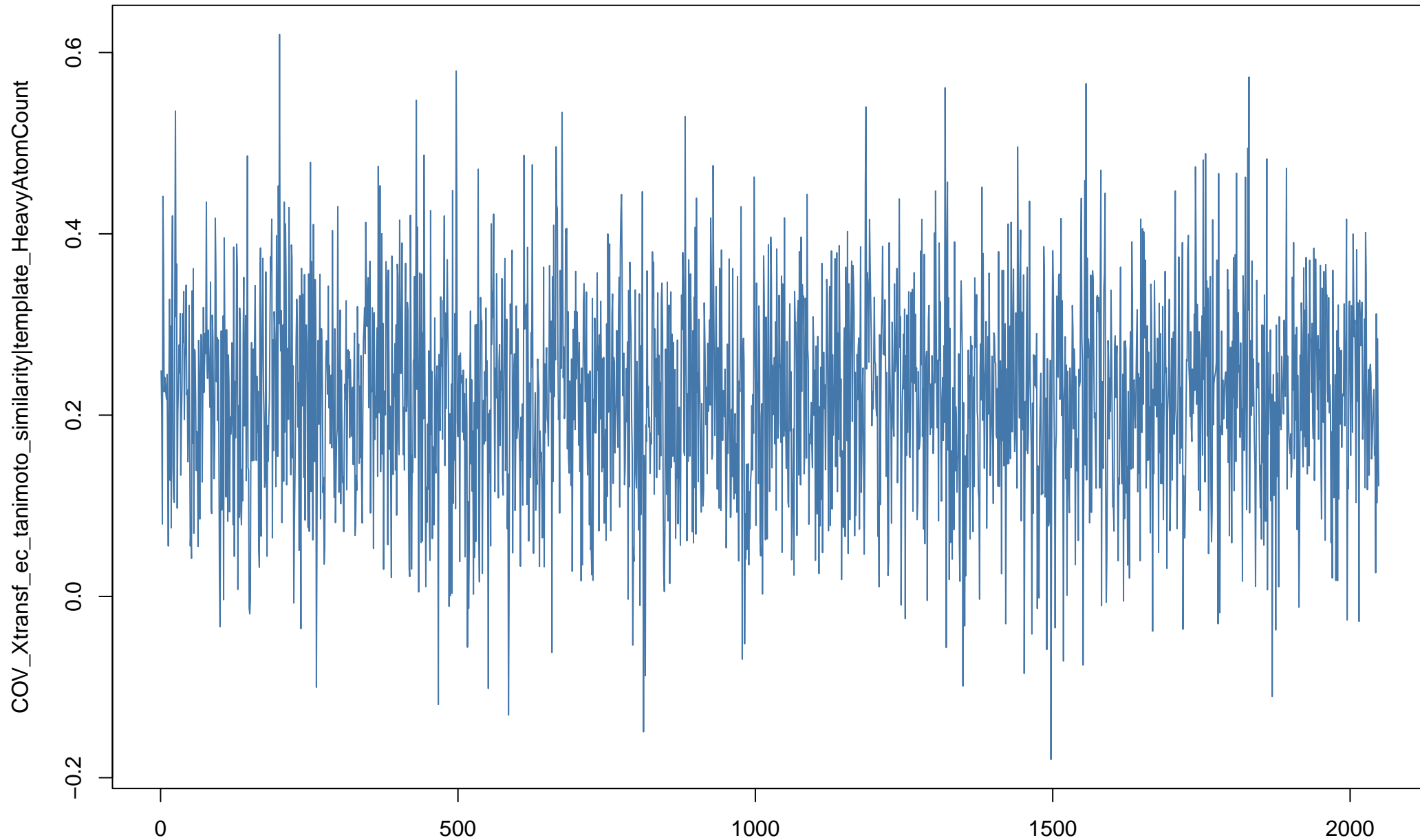


**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 1850 | BMK = 0.0494 | MCSE(6.27) = 2.39 | stat: FALSE | burn: 0**

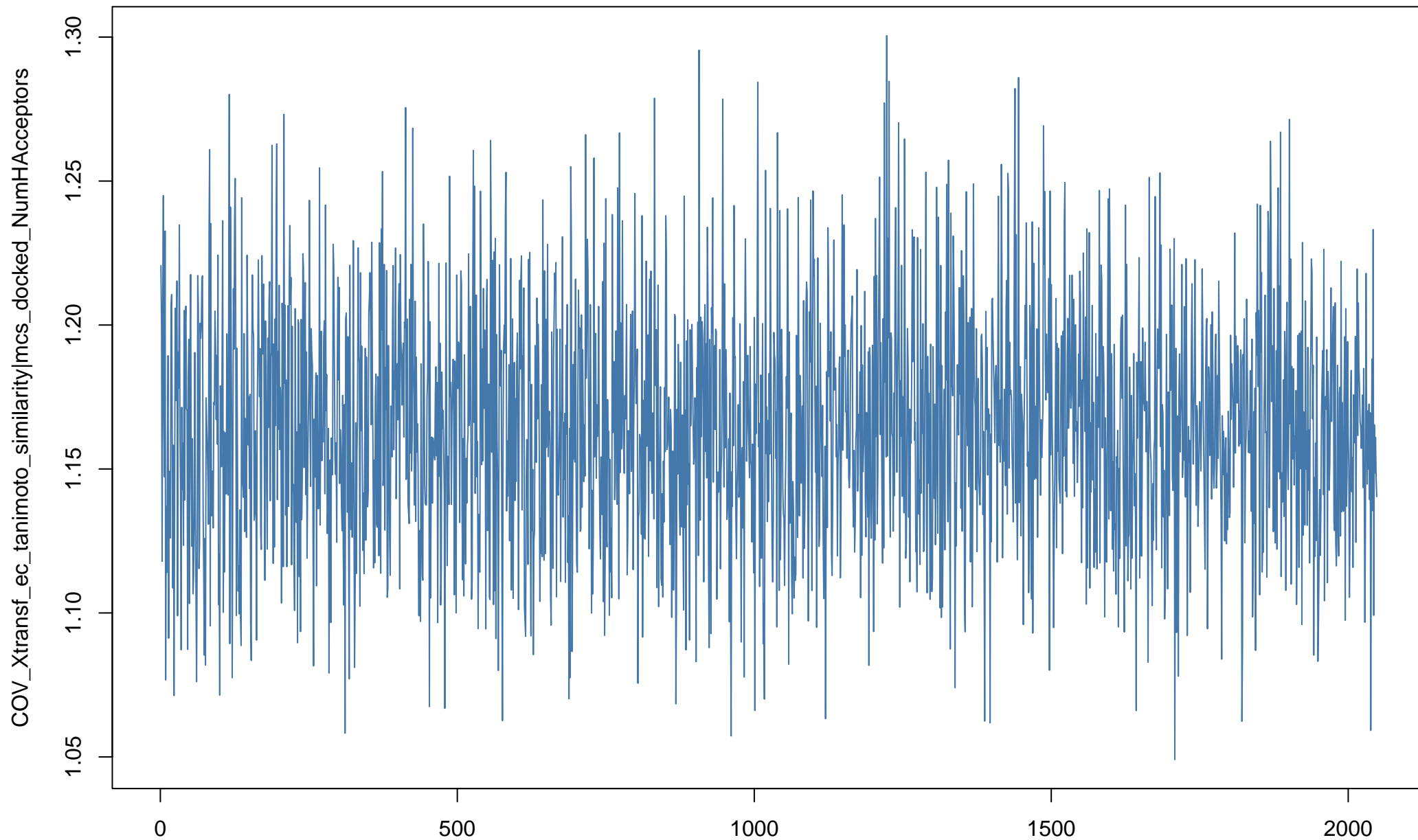




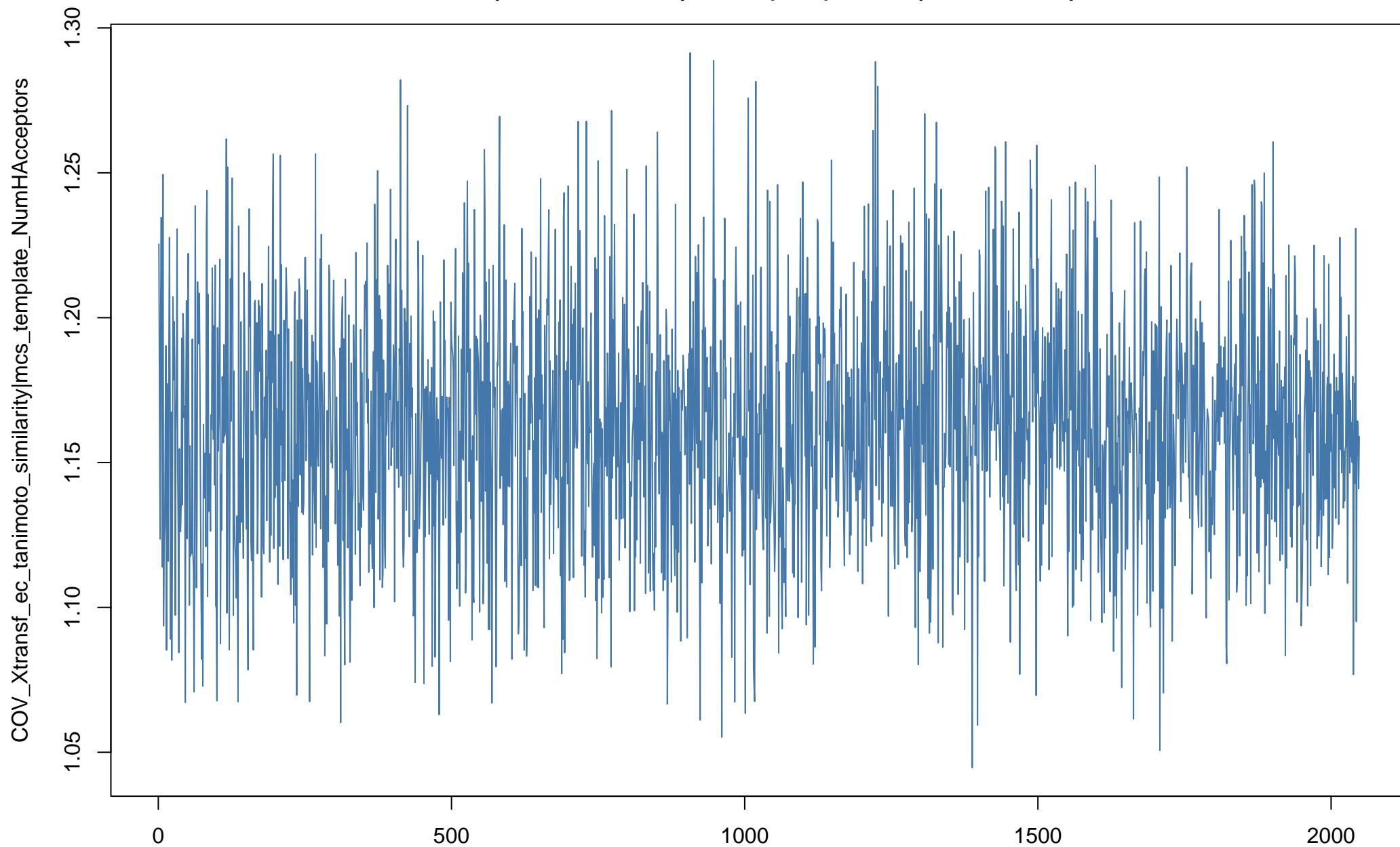
COV\_Xtransf\_ec\_tanimoto\_similarity|template\_HeavyAtomCount  
ESS = 1760 | BMK = 0.0456 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0



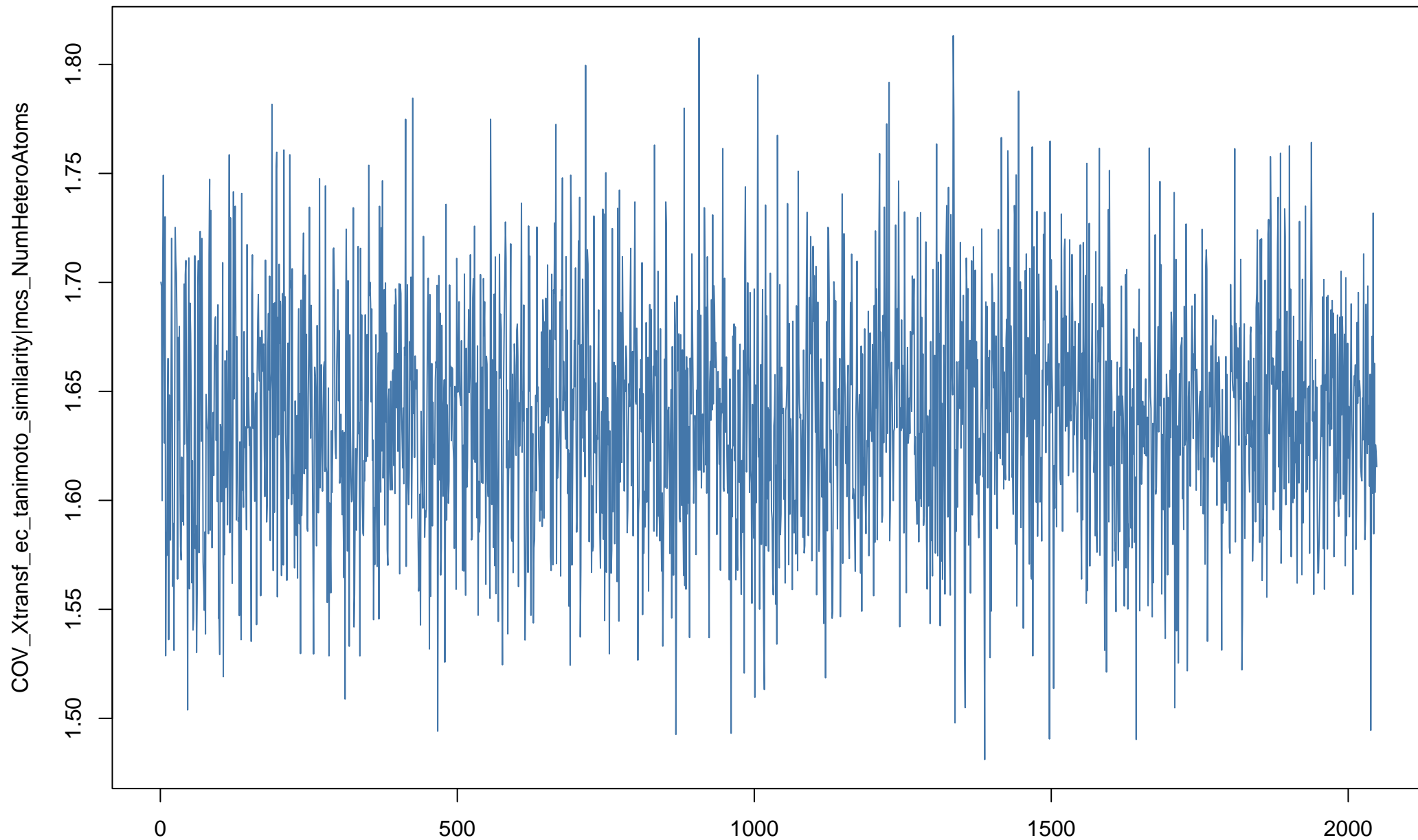
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0663 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0**



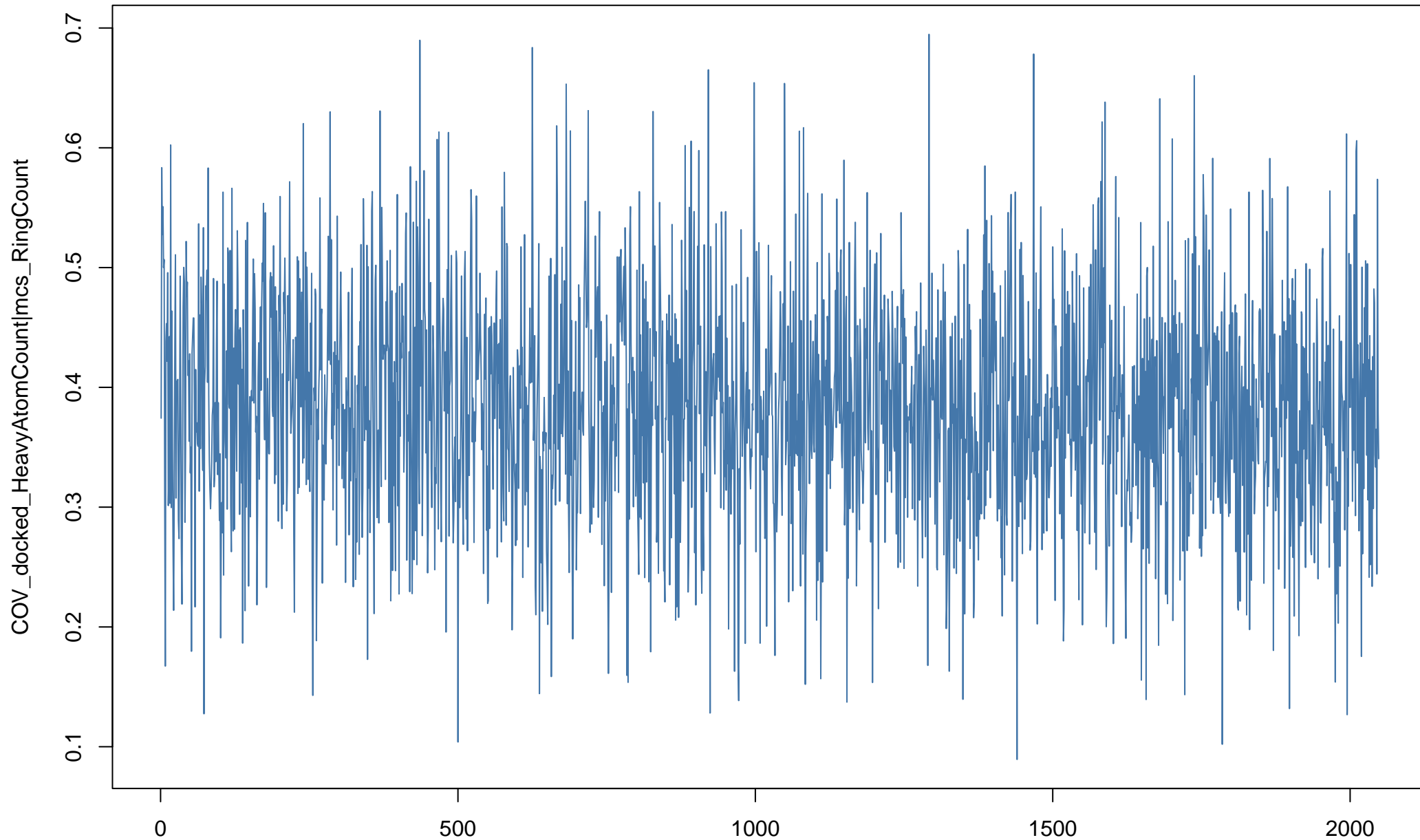
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0775 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0**



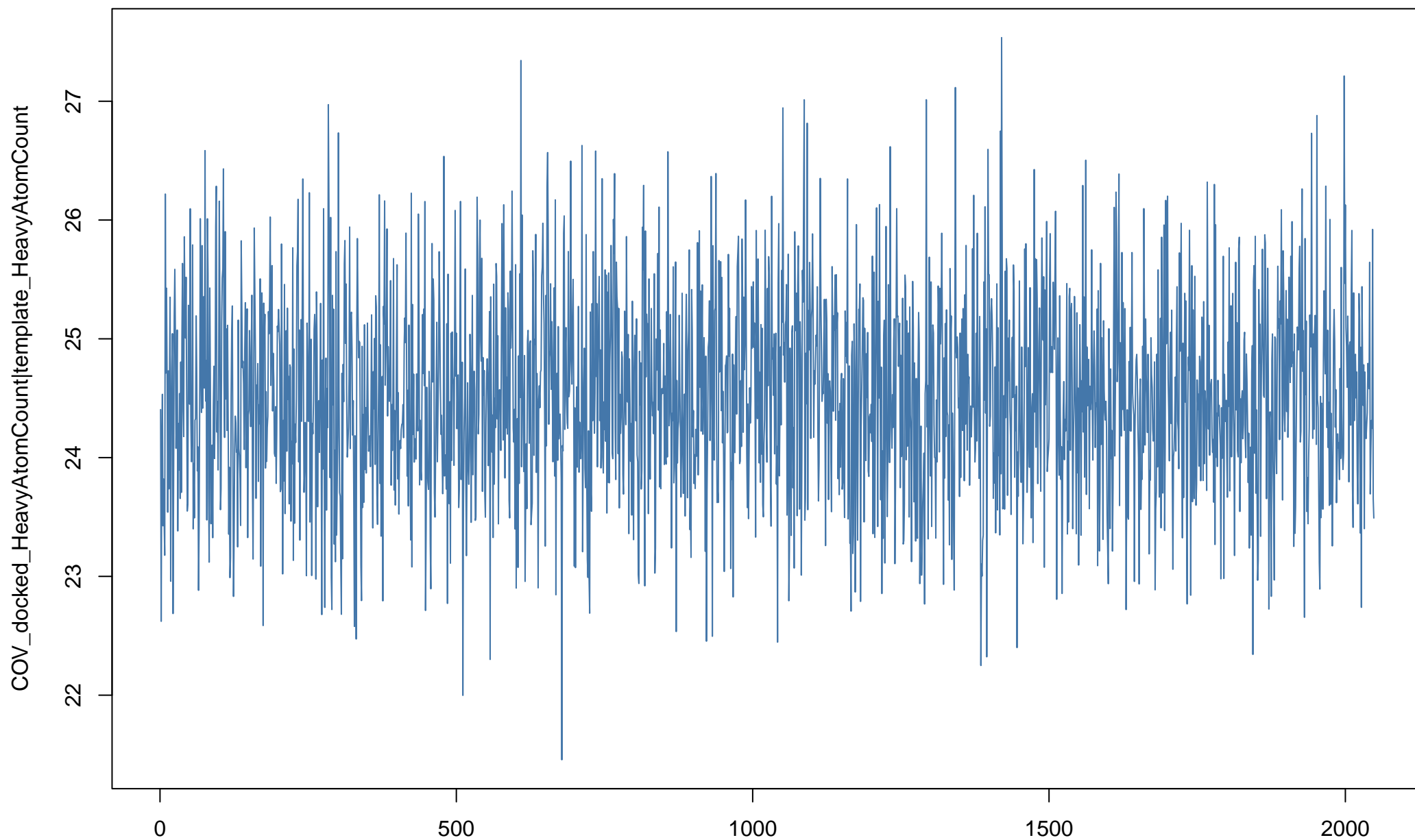
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0568 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0**



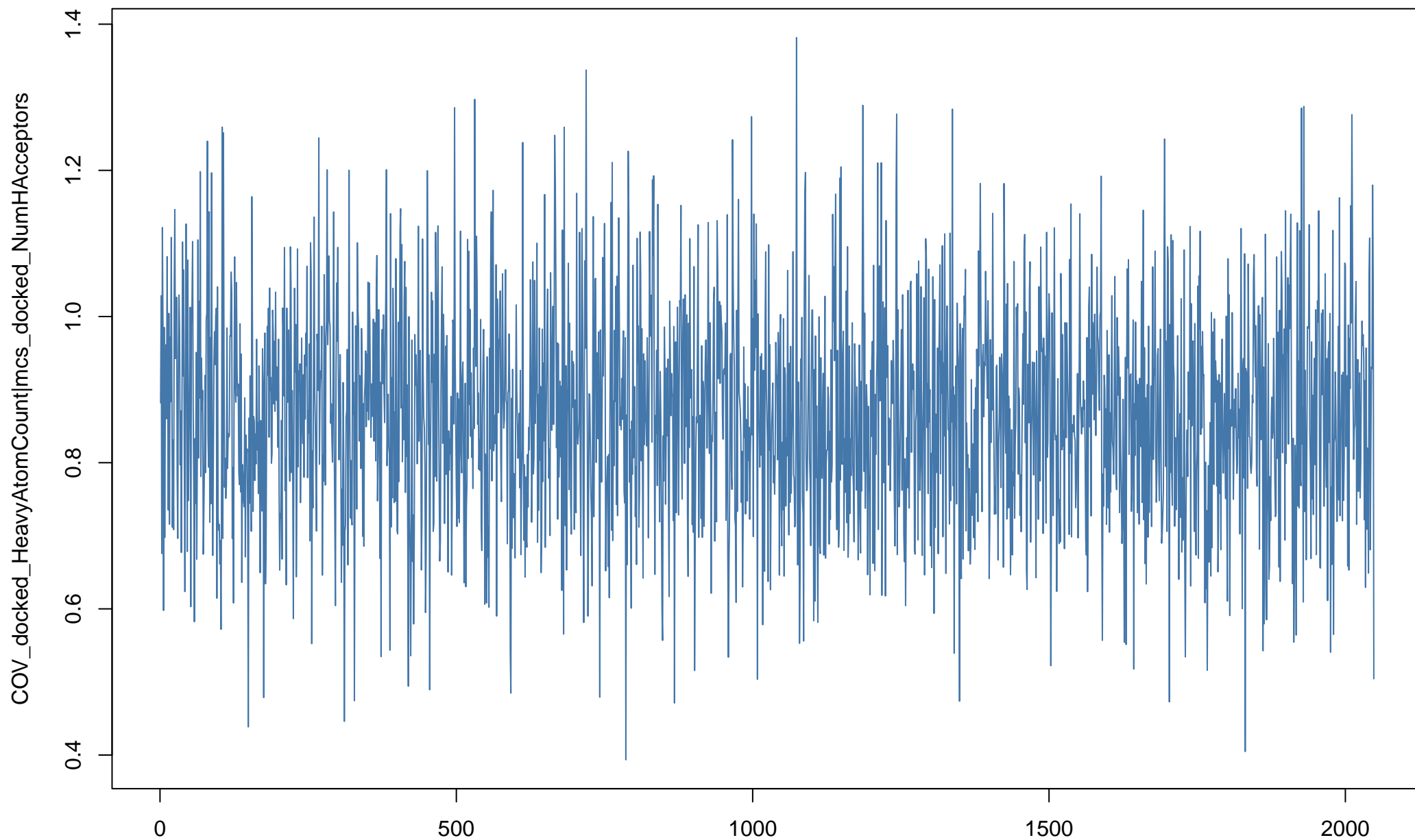
COV\_docked\_HeavyAtomCount|mcs\_RingCount  
ESS = 1860 | BMK = 0.0548 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0



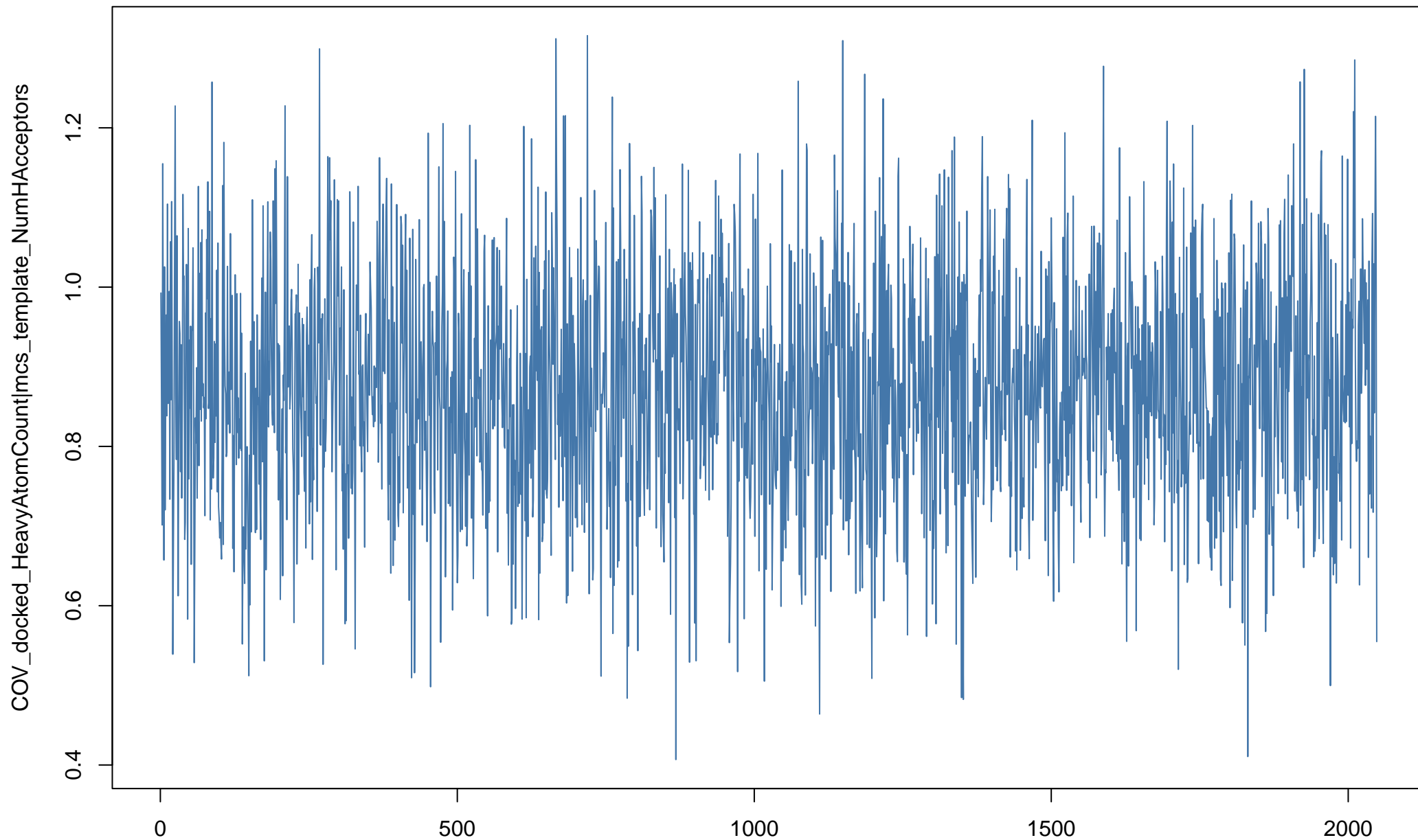
**COV\_docked\_HeavyAtomCount|template\_HeavyAtomCount**  
**ESS = 1820 | BMK = 0.0463 | MCSE(6.27) = 2 | stat: TRUE | burn: 0**



**COV\_docked\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0461 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0**

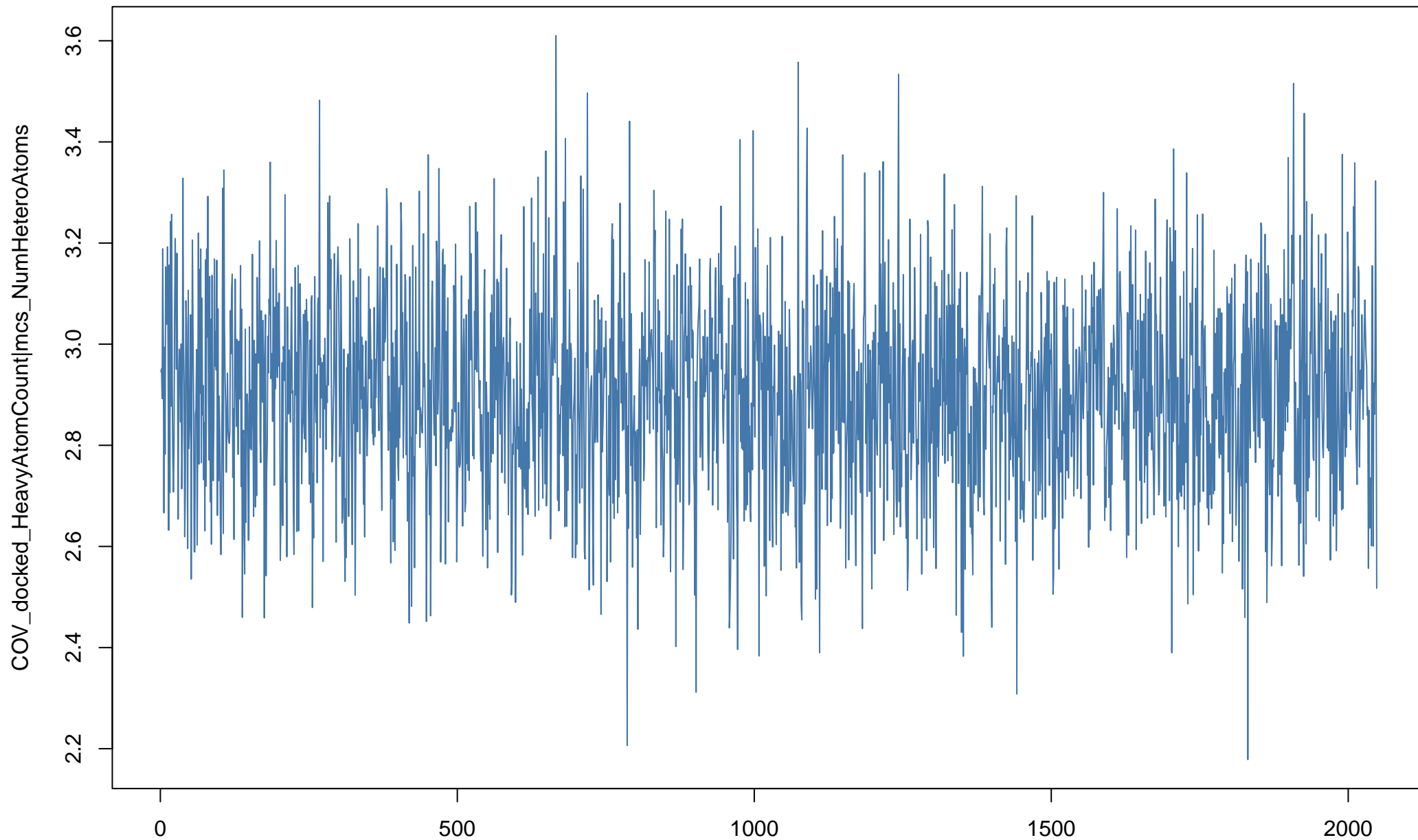


**COV\_docked\_HeavyAtomCount|mcs\_template\_NumHAcceptors**  
**ESS = 1880 | BMK = 0.0338 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0**

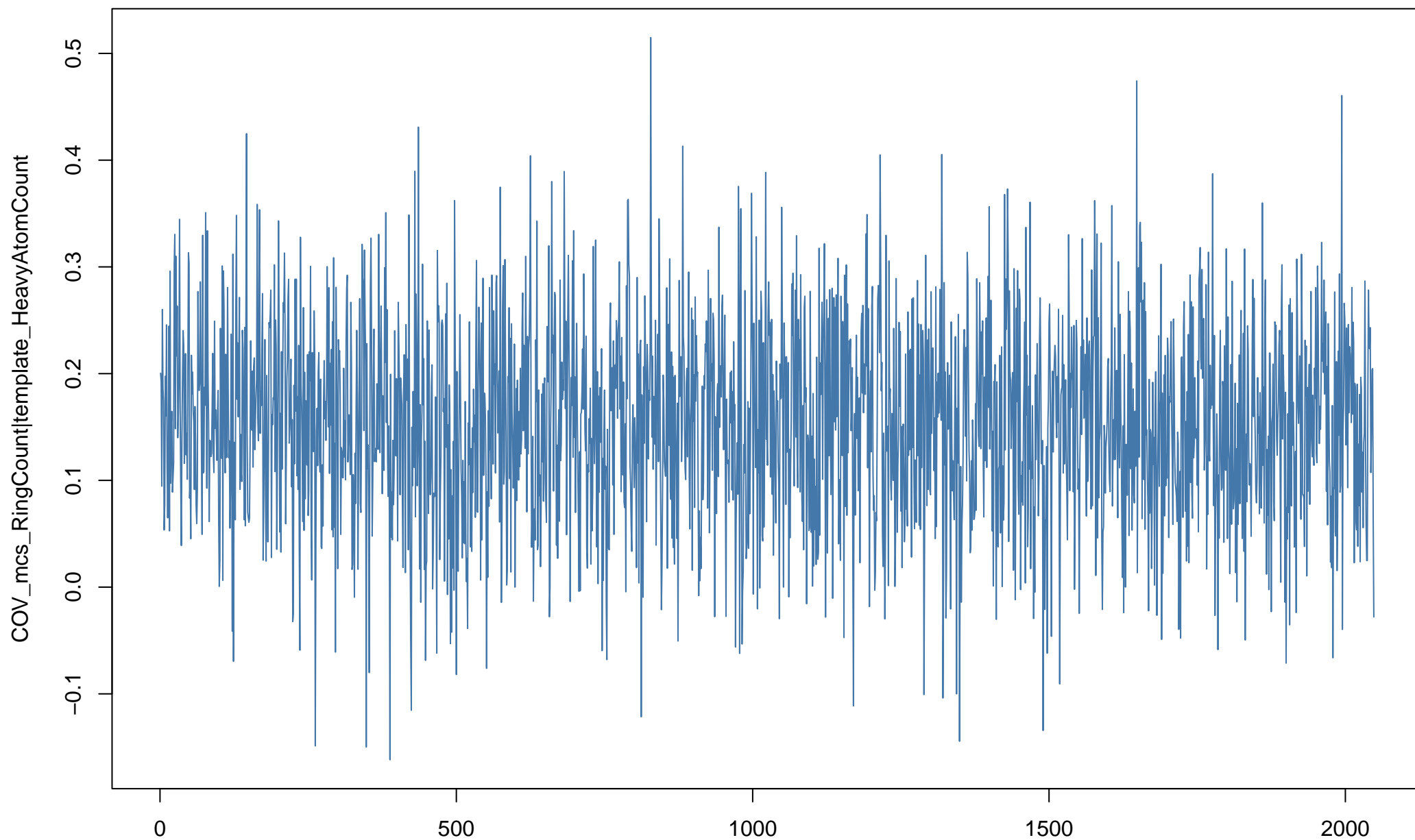




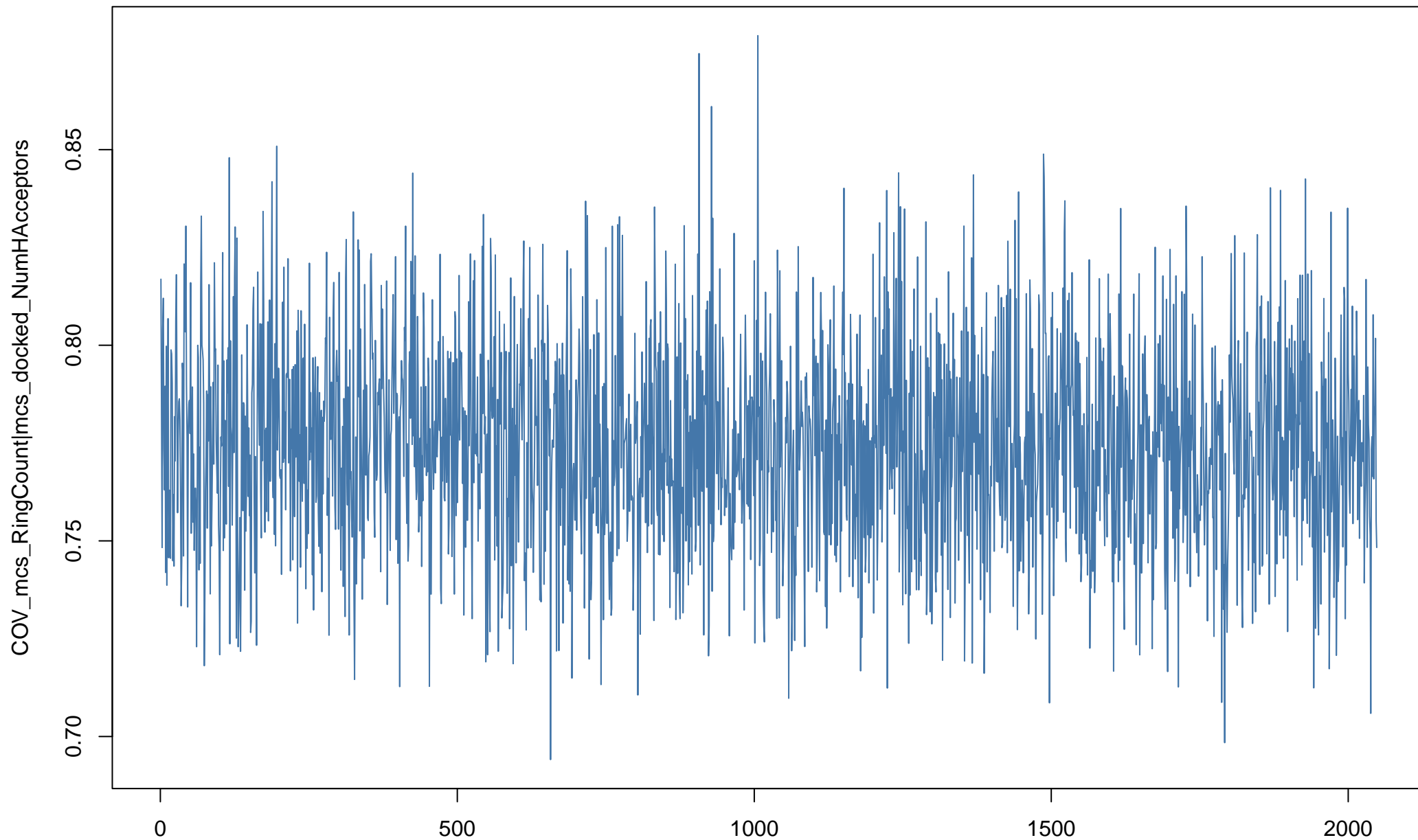
**COV\_docked\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 1890 | BMK = 0.0293 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0**



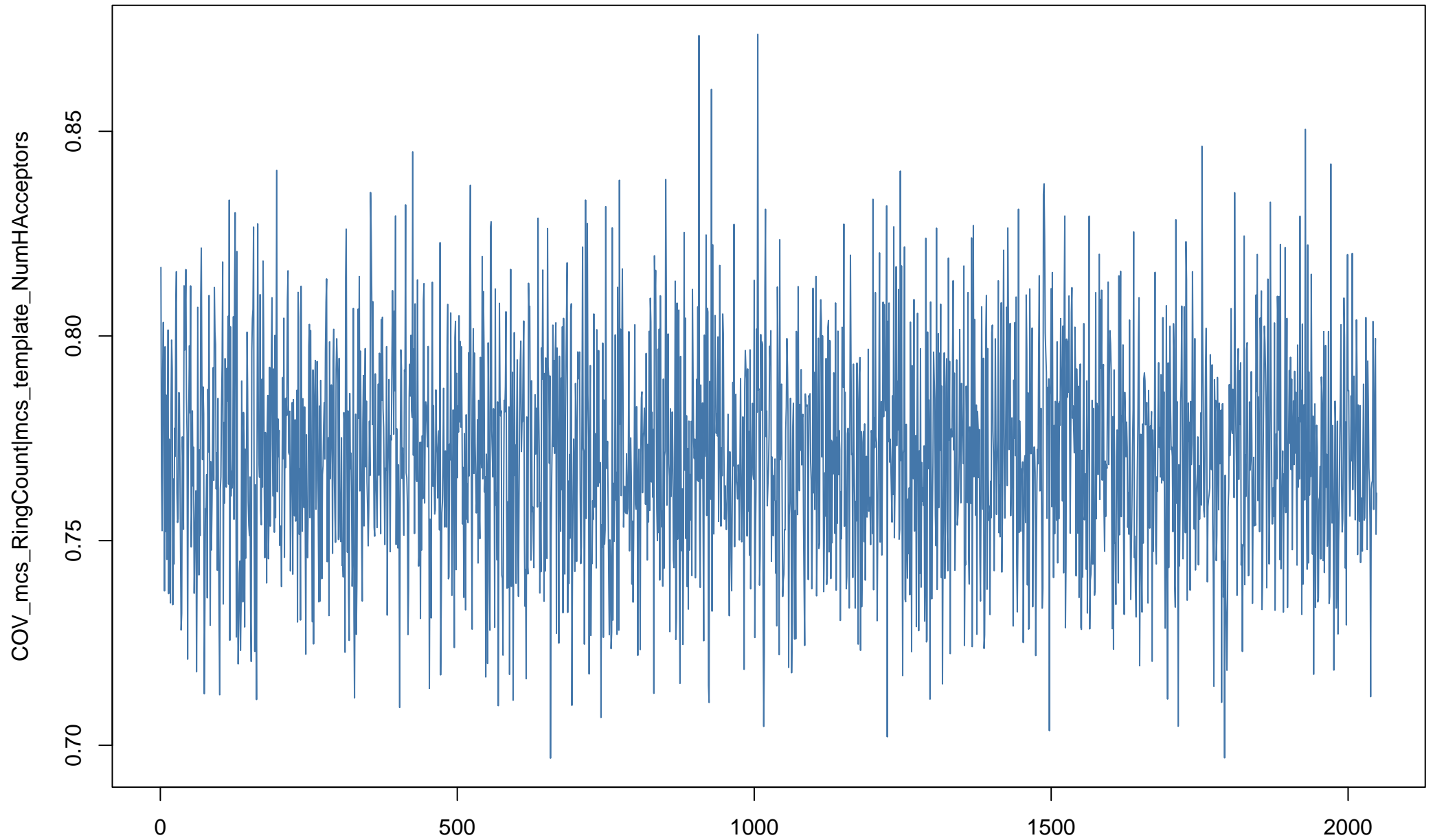
**COV\_mcs\_RingCount|template\_HeavyAtomCount**  
**ESS = 1640 | BMK = 0.0409 | MCSE(6.27) = 2.22 | stat: FALSE | burn: 0**



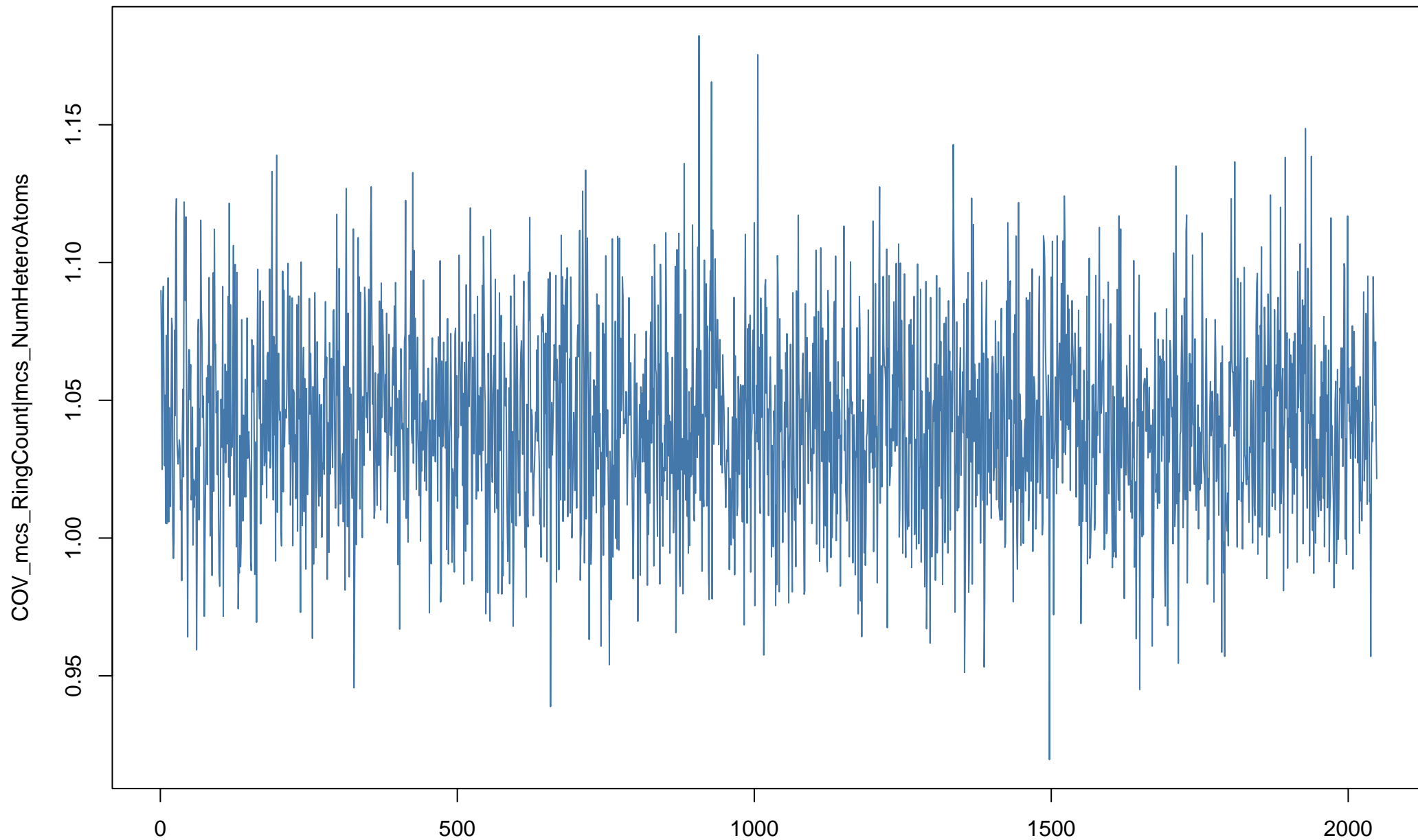
**COV\_mcs\_RingCount|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0525 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0**



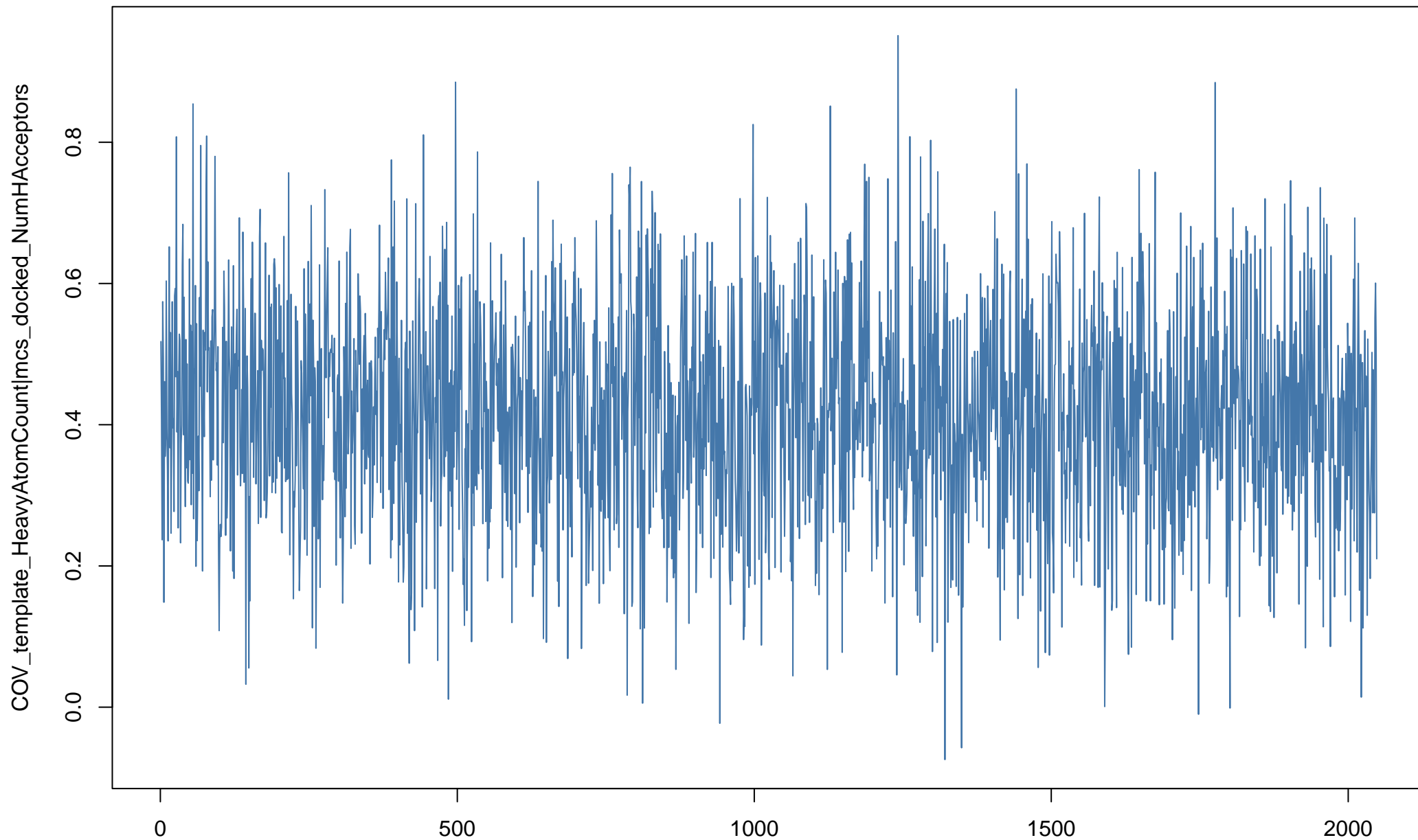
**COV\_mcs\_RingCount|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0399 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0**



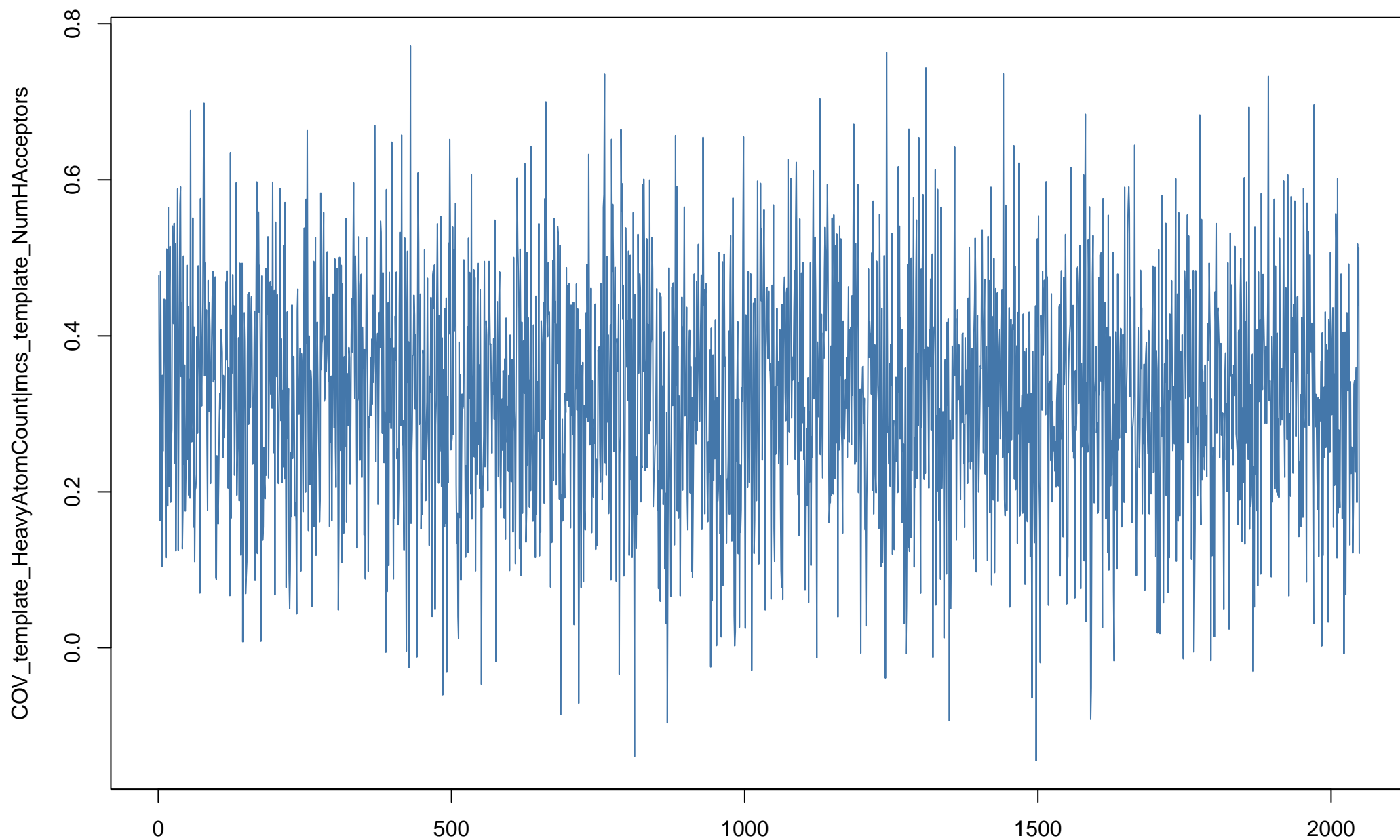
COV\_mcs\_RingCount|mcs\_NumHeteroAtoms  
ESS = 2050 | BMK = 0.0411 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0



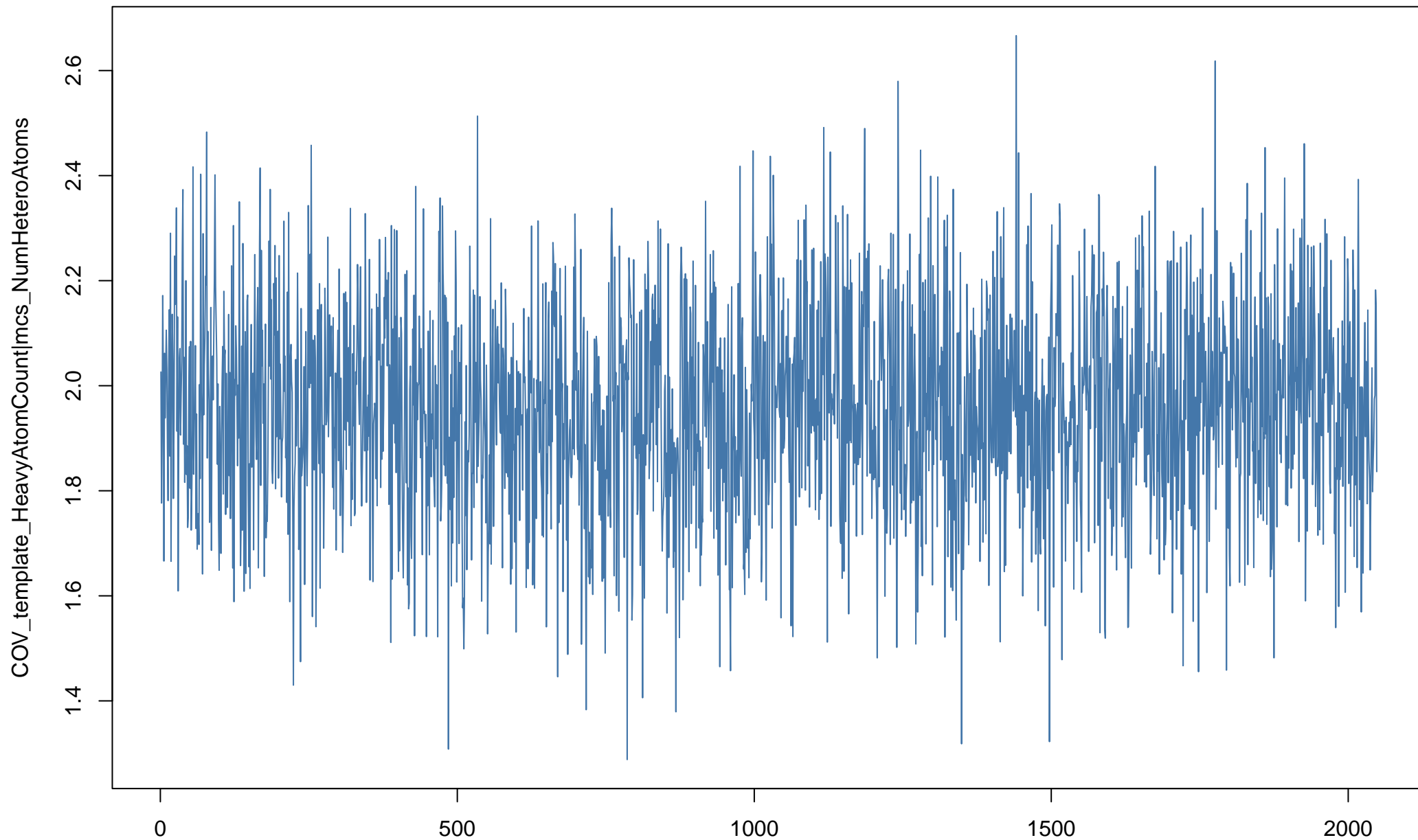
**COV\_template\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 1680 | BMK = 0.0446 | MCSE(6.27) = 2.2 | stat: FALSE | burn: 0**



**COV\_template\_HeavyAtomCount|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0439 | MCSE(6.27) = 1.93 | stat: TRUE | burn: 0**

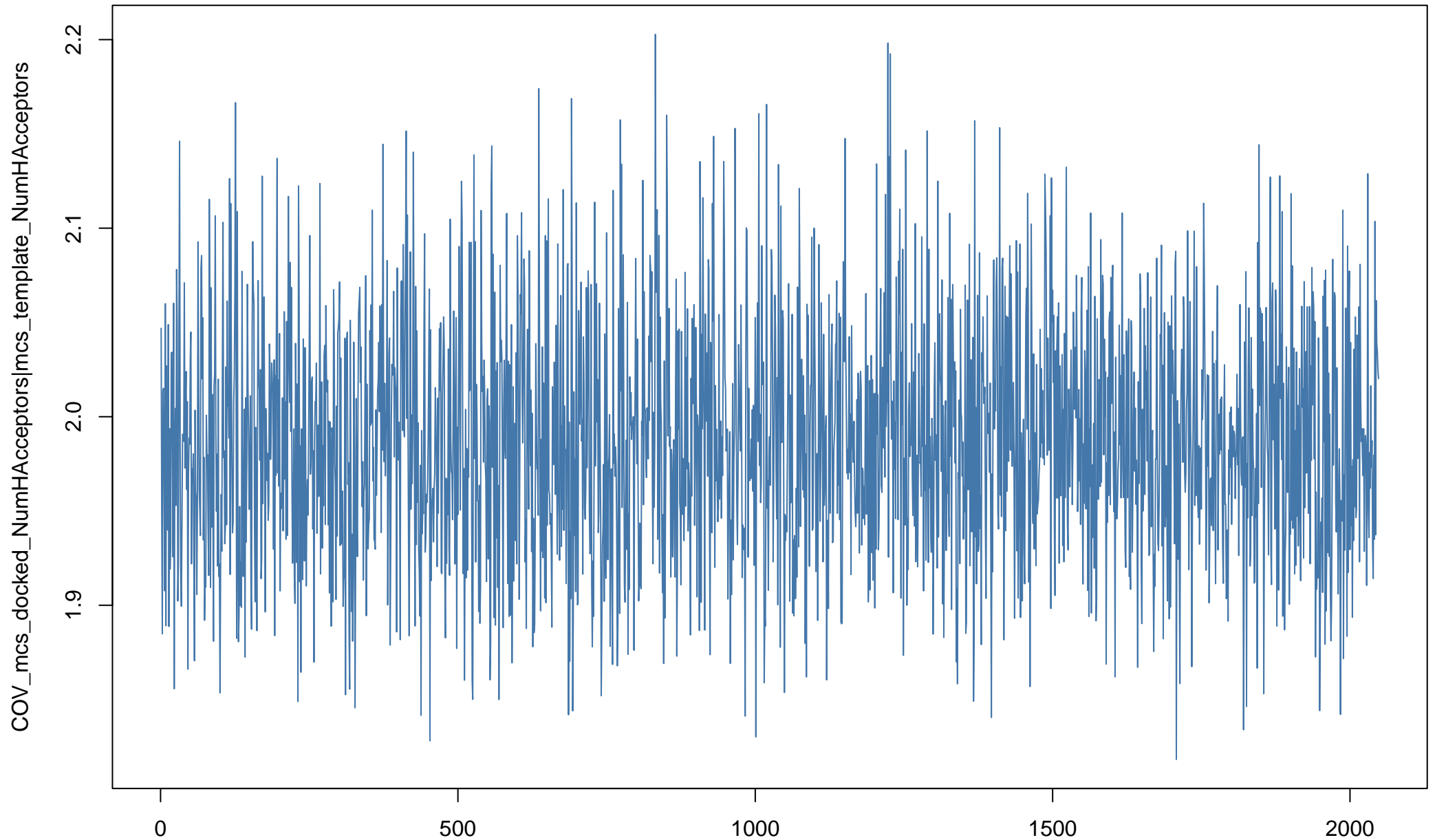


**COV\_template\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0608 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0**

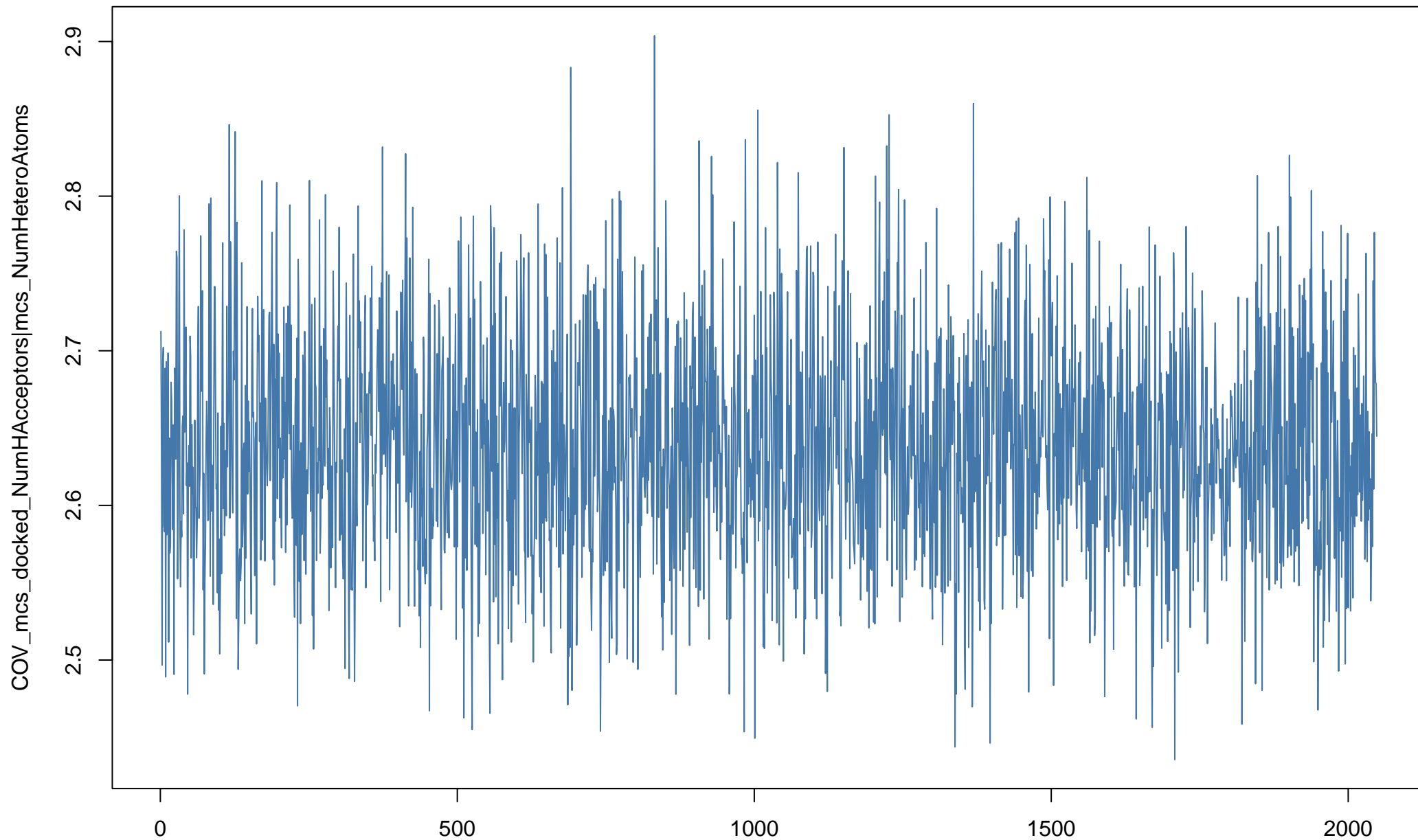




**COV\_mcs\_docked\_NumHAcceptors|mcs\_template\_NumHAcceptors**  
**ESS = 1920 | BMK = 0.0561 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0**



**COV\_mcs\_docked\_NumHAcceptors|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0351 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0**



**COV\_mcs\_template\_NumHAcceptors|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.048 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0**

