

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.190620143516965

max MCSE = 8.85998170261972

all stationary: FALSE

burn: 2040

-- STATS 2D --

min ESS = 1375.0114758339

max BMK = 0.0892866026334967

max MCSE = 3.22294180381656

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.627852113064889

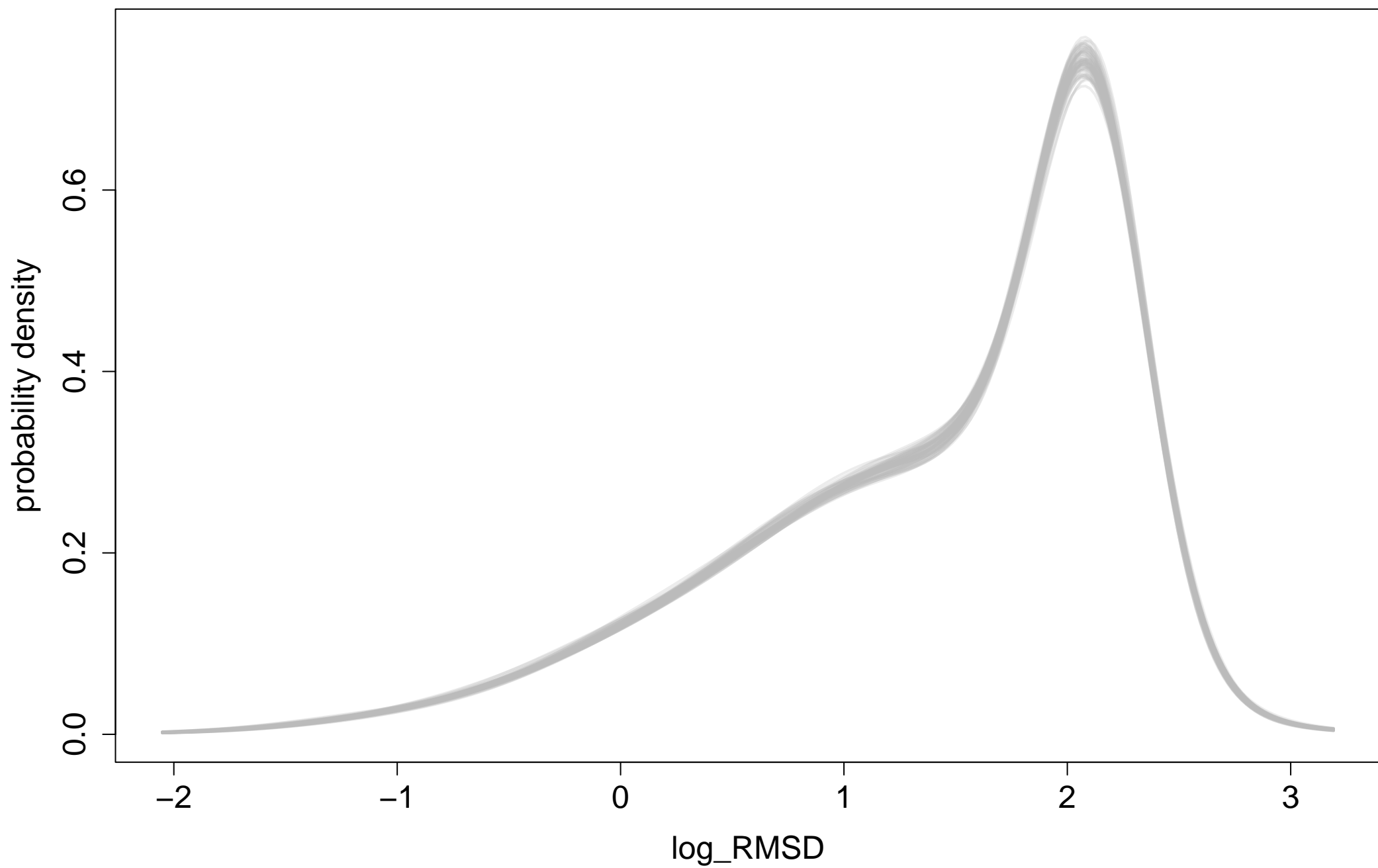
max MCSE = NaN

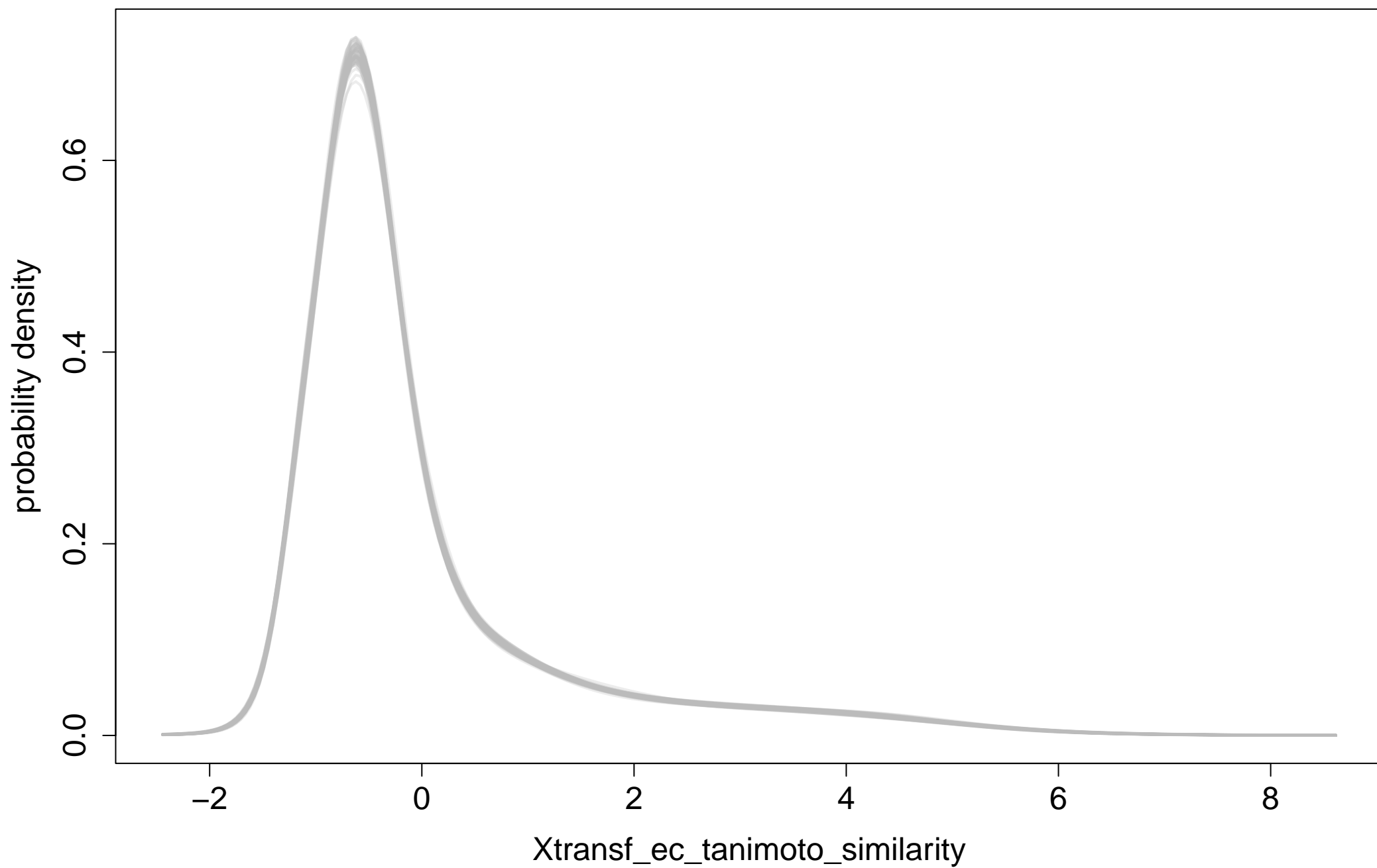
all stationary: FALSE

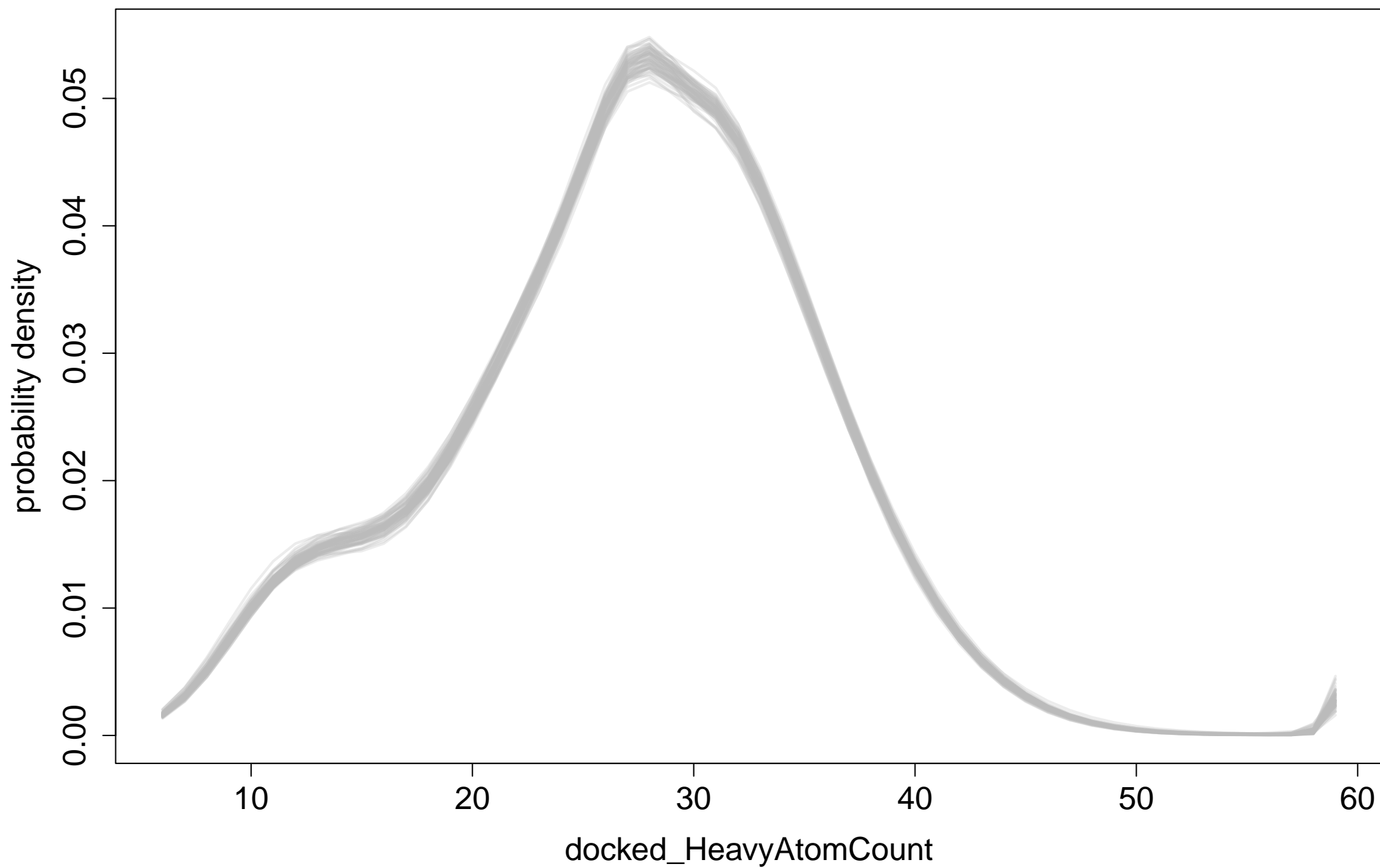
burn: 2040

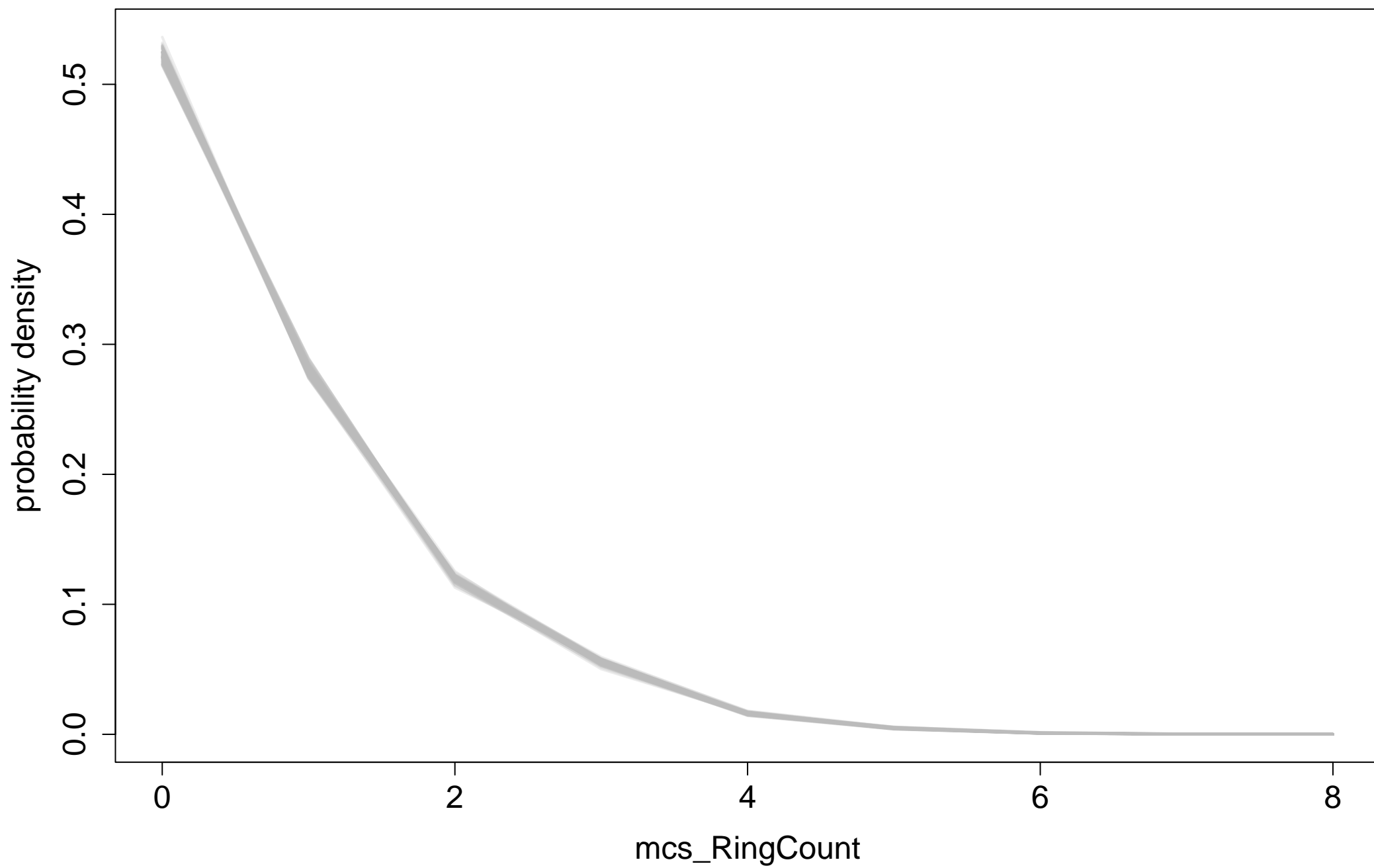
Occupied clusters: 62 of 64

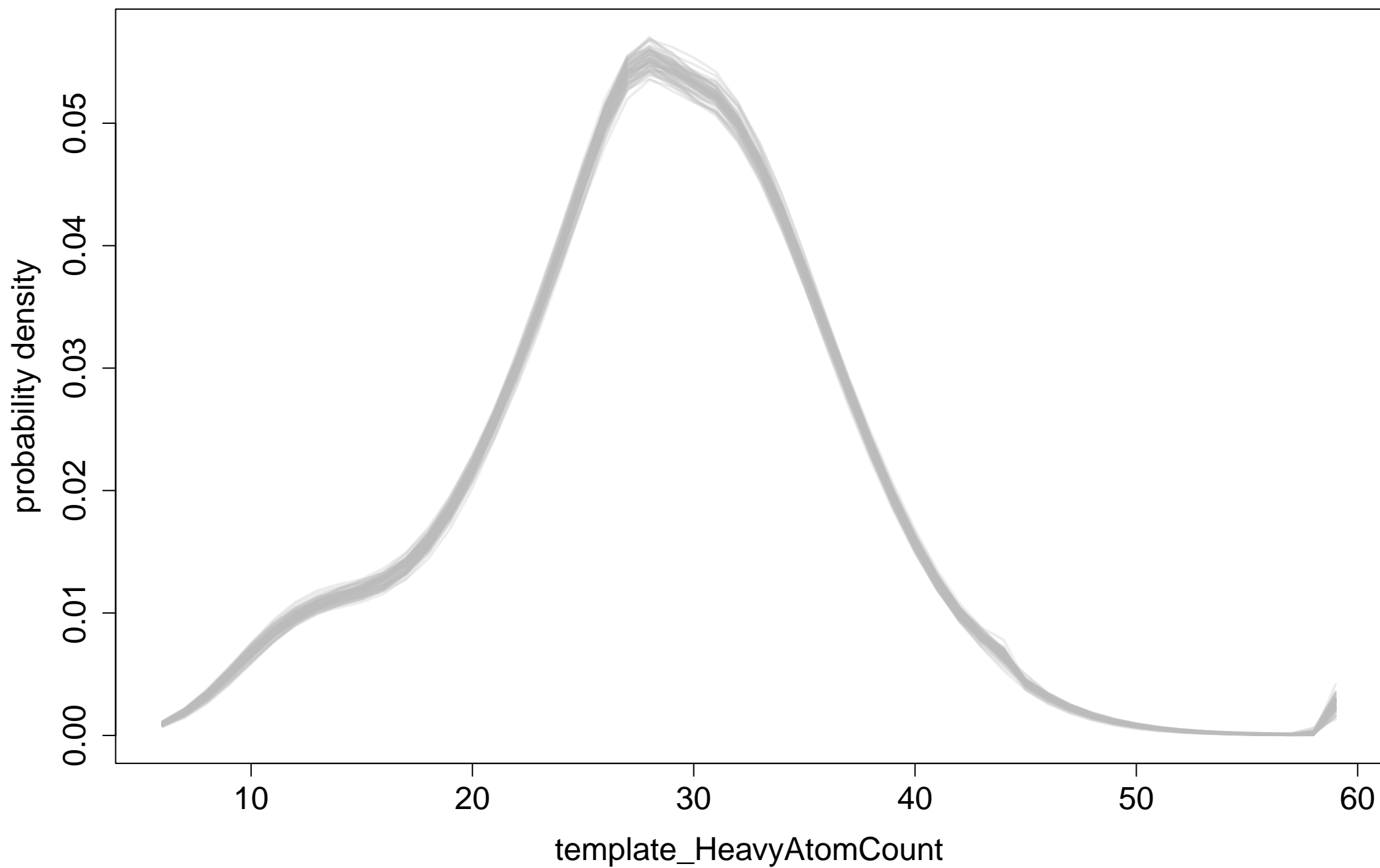
LL: -110000 +- 22.9

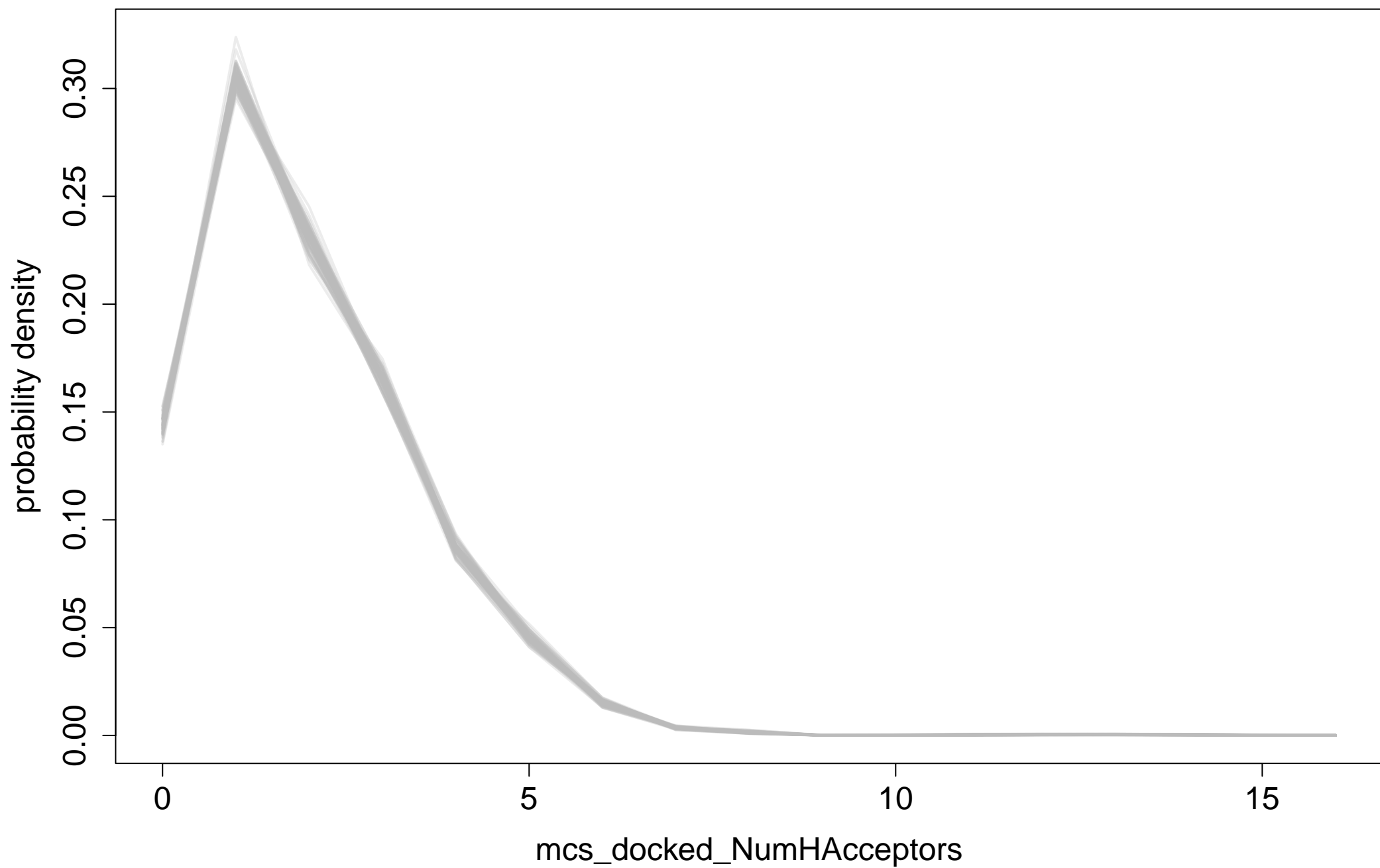


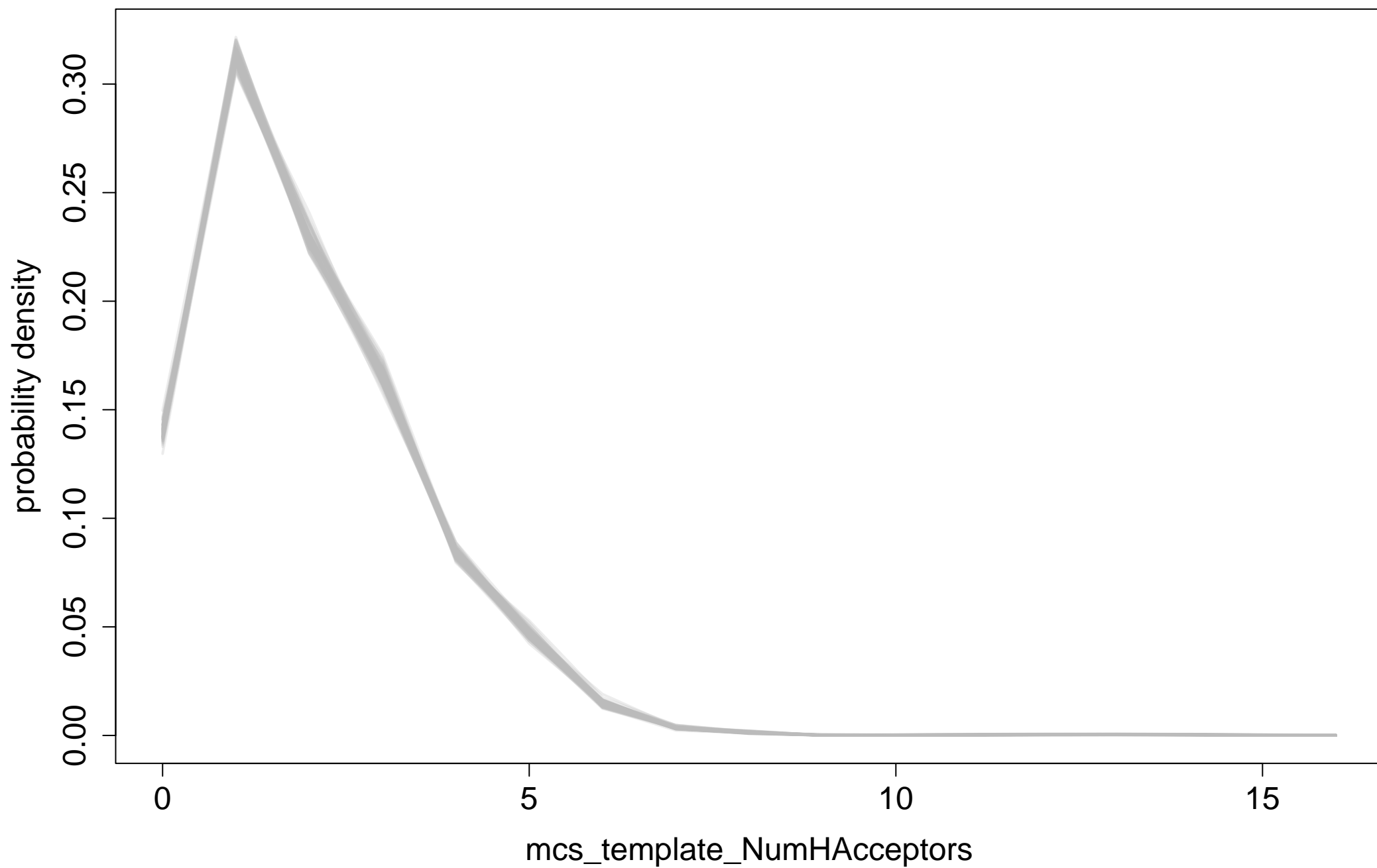




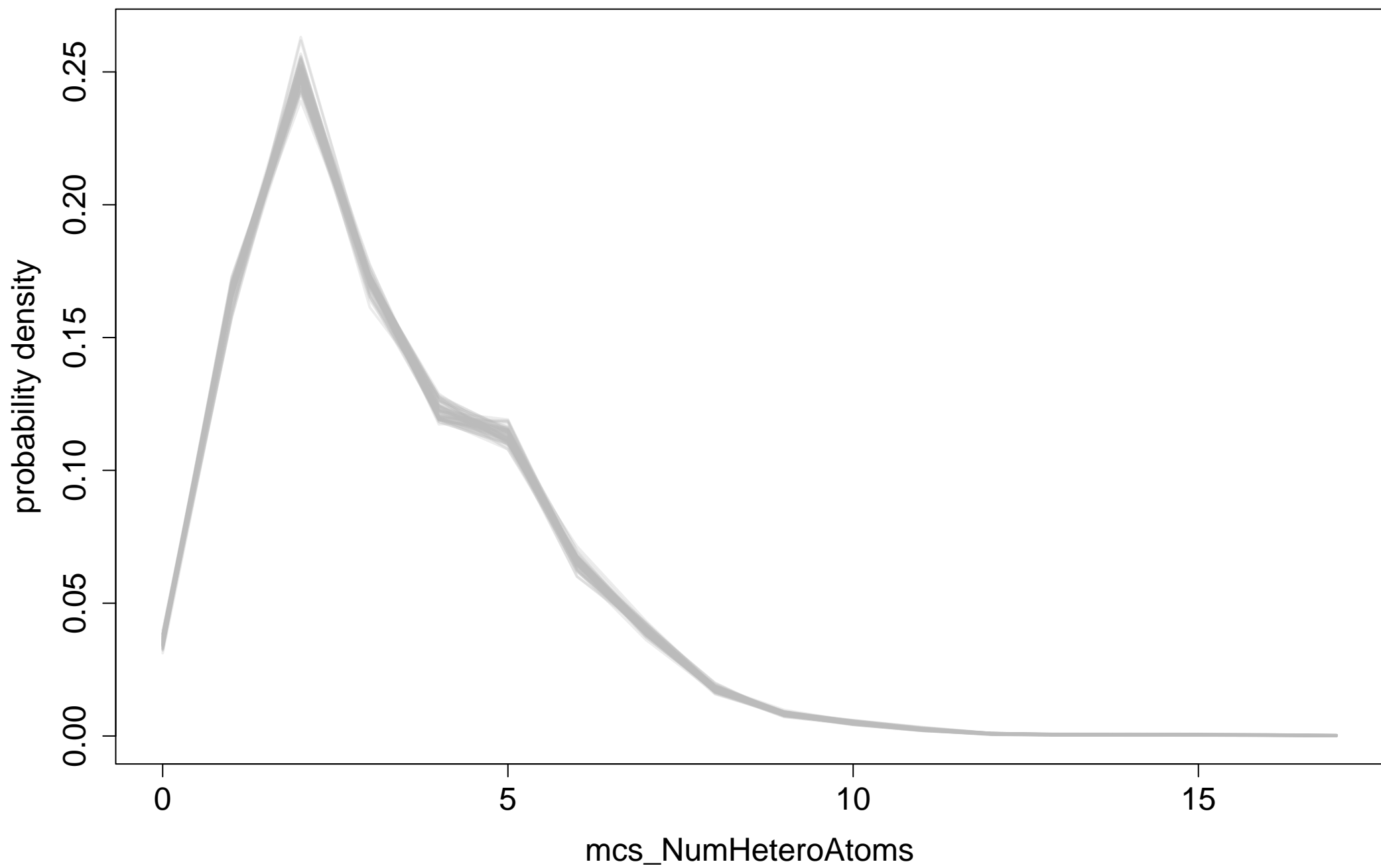


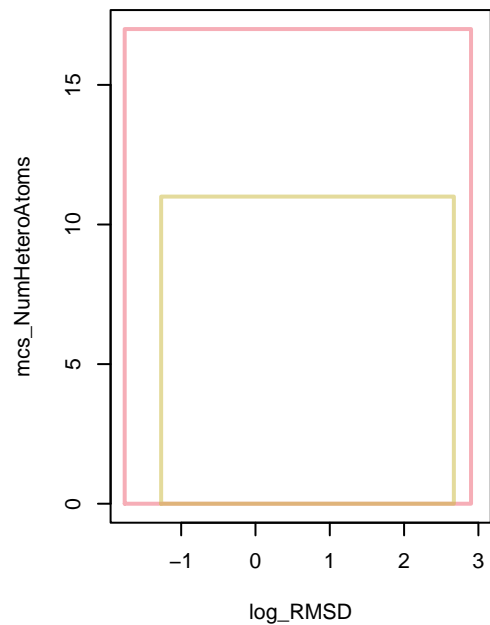
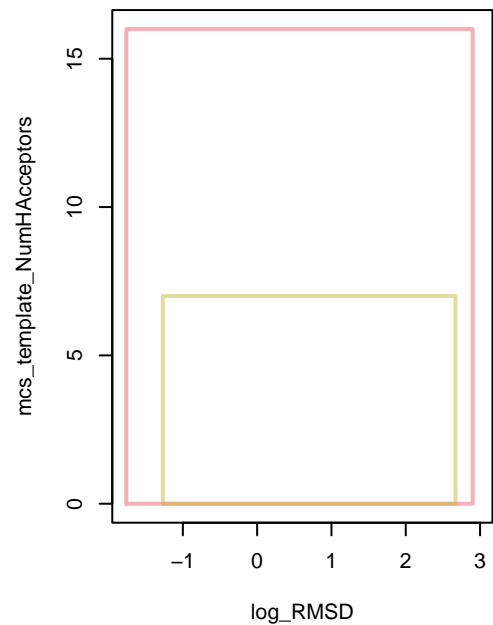
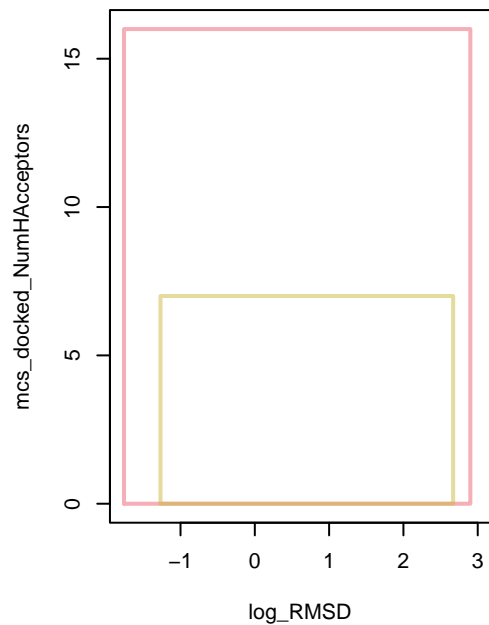
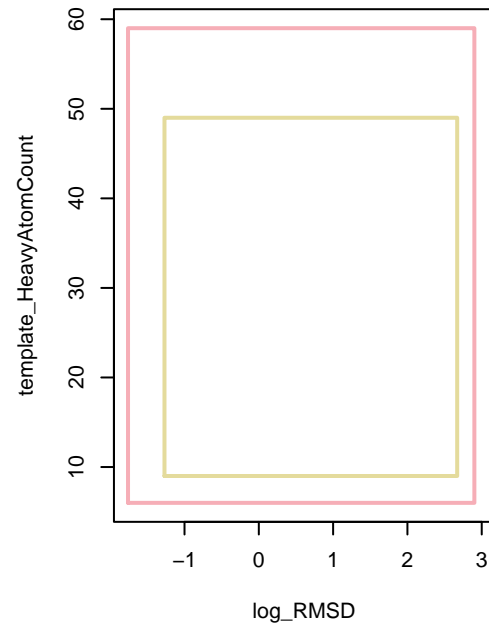
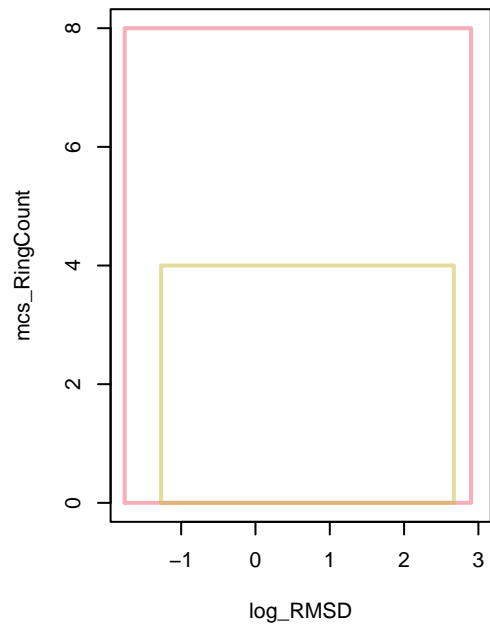
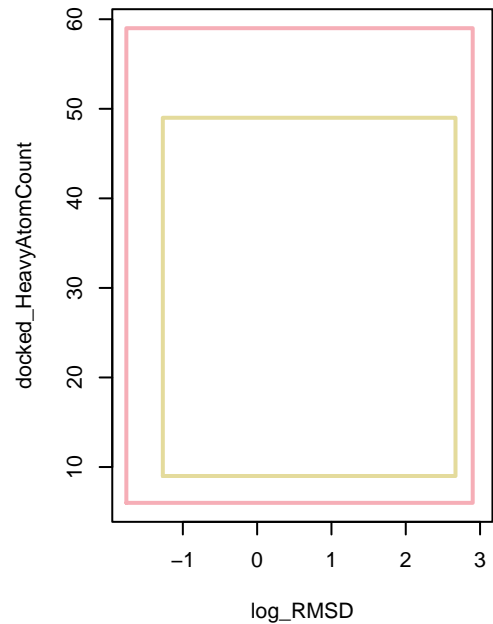
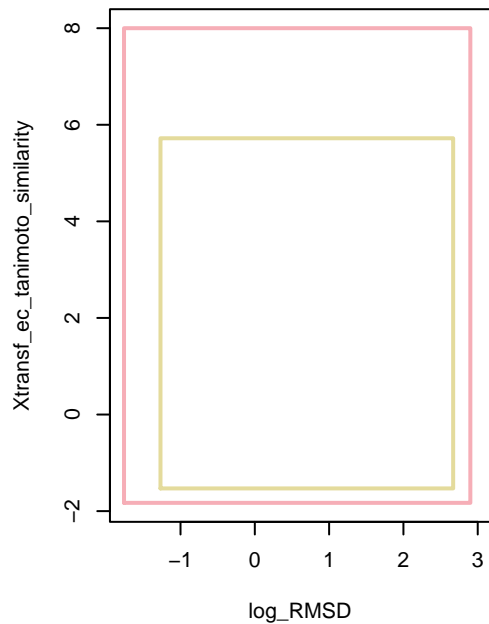




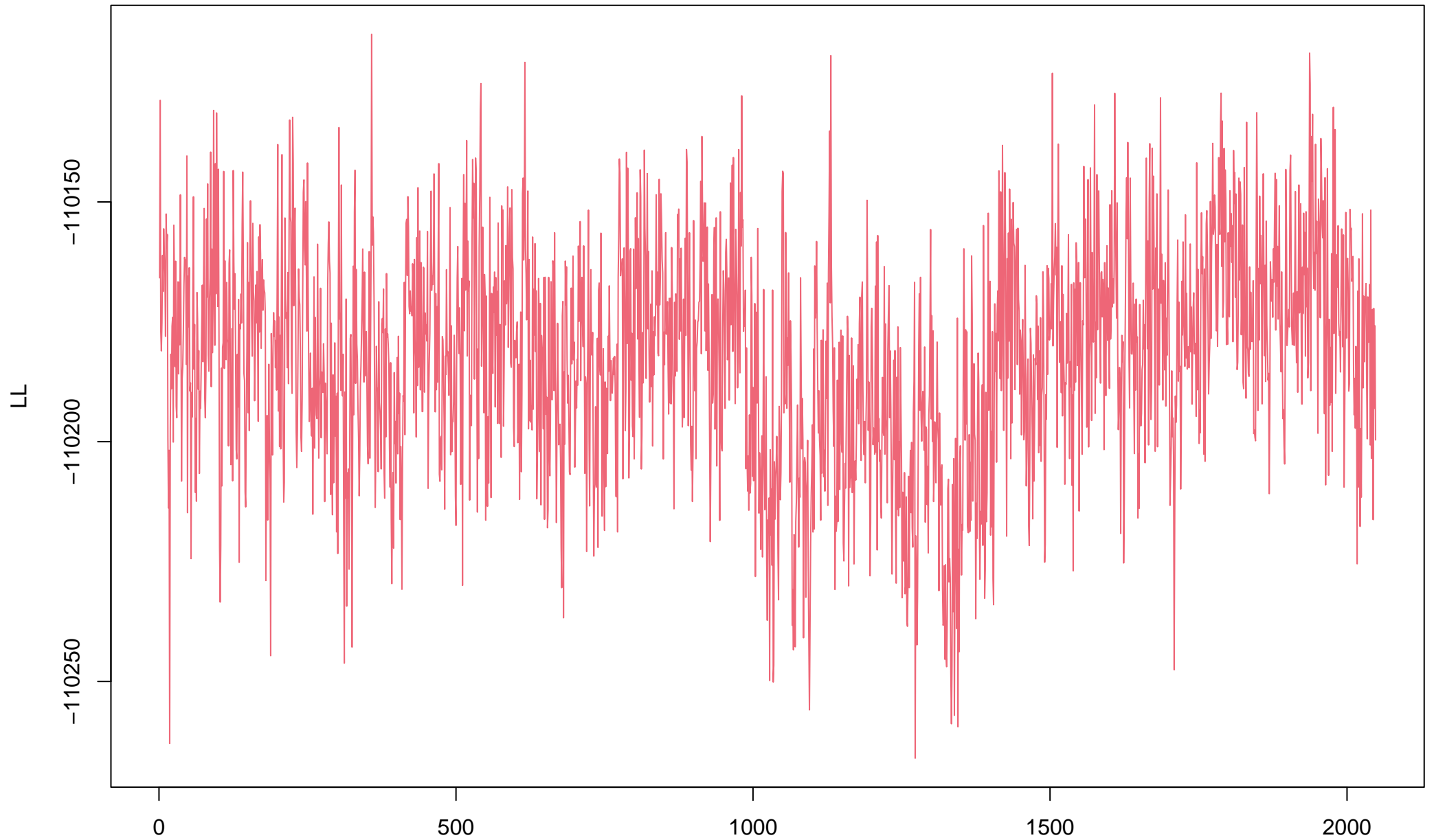




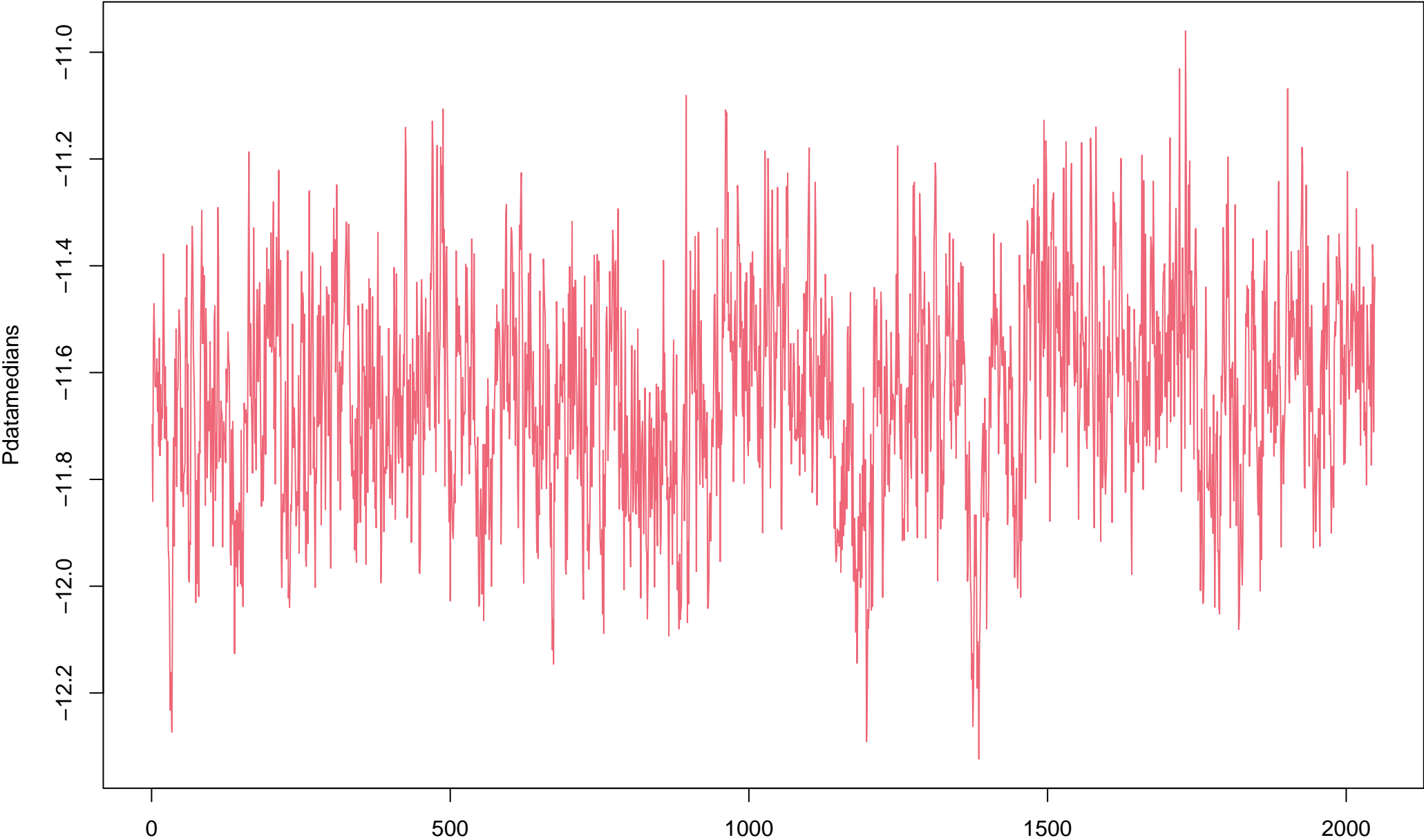




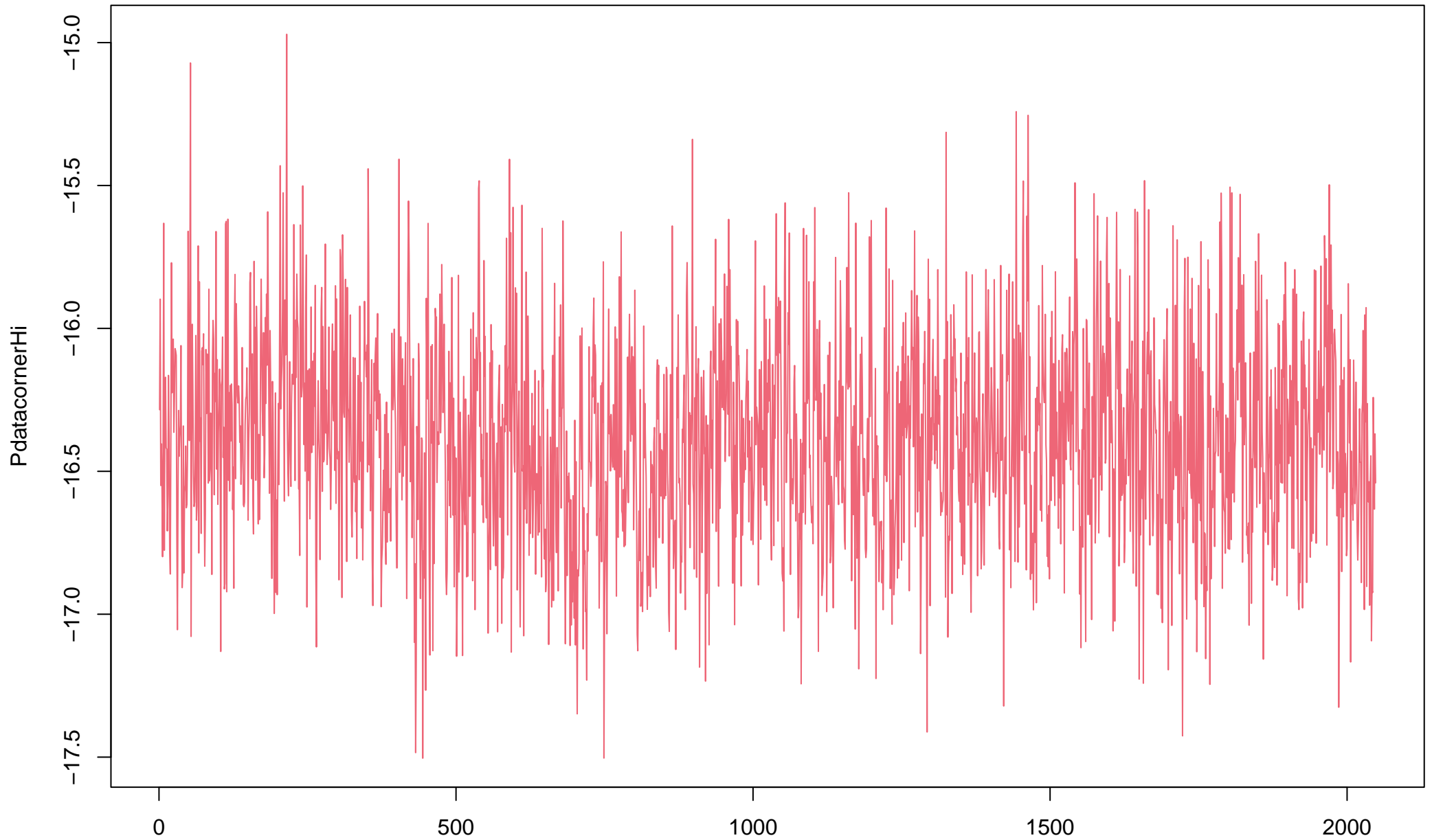
LL  
ESS = 61.6 | BMK = 0.105 | MCSE(6.27) = 7.74 | stat: TRUE | burn: 0



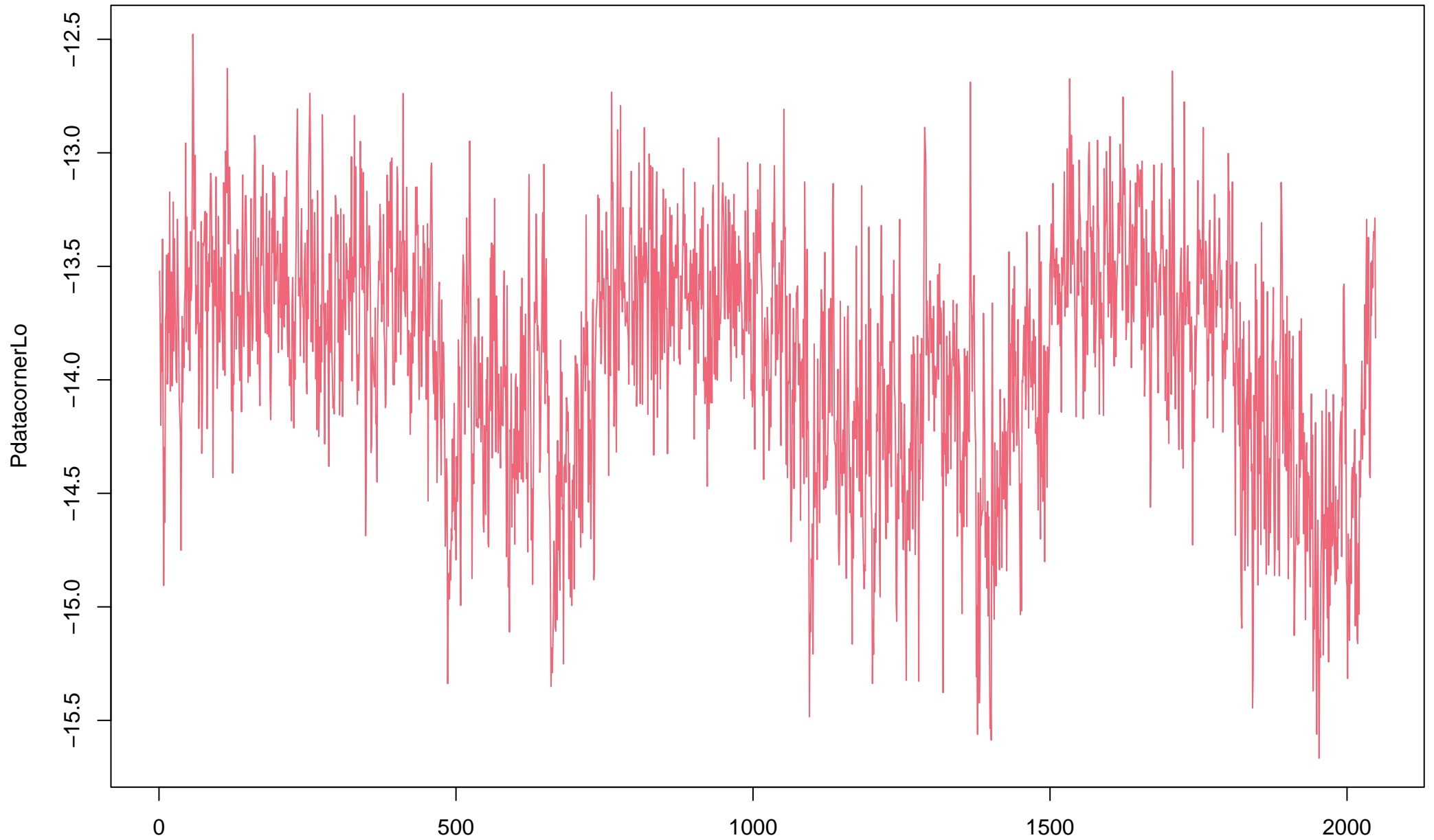
**Pdatamedians**  
**ESS = 235 | BMK = 0.108 | MCSE(6.27) = 6.74 | stat: FALSE | burn: 0**



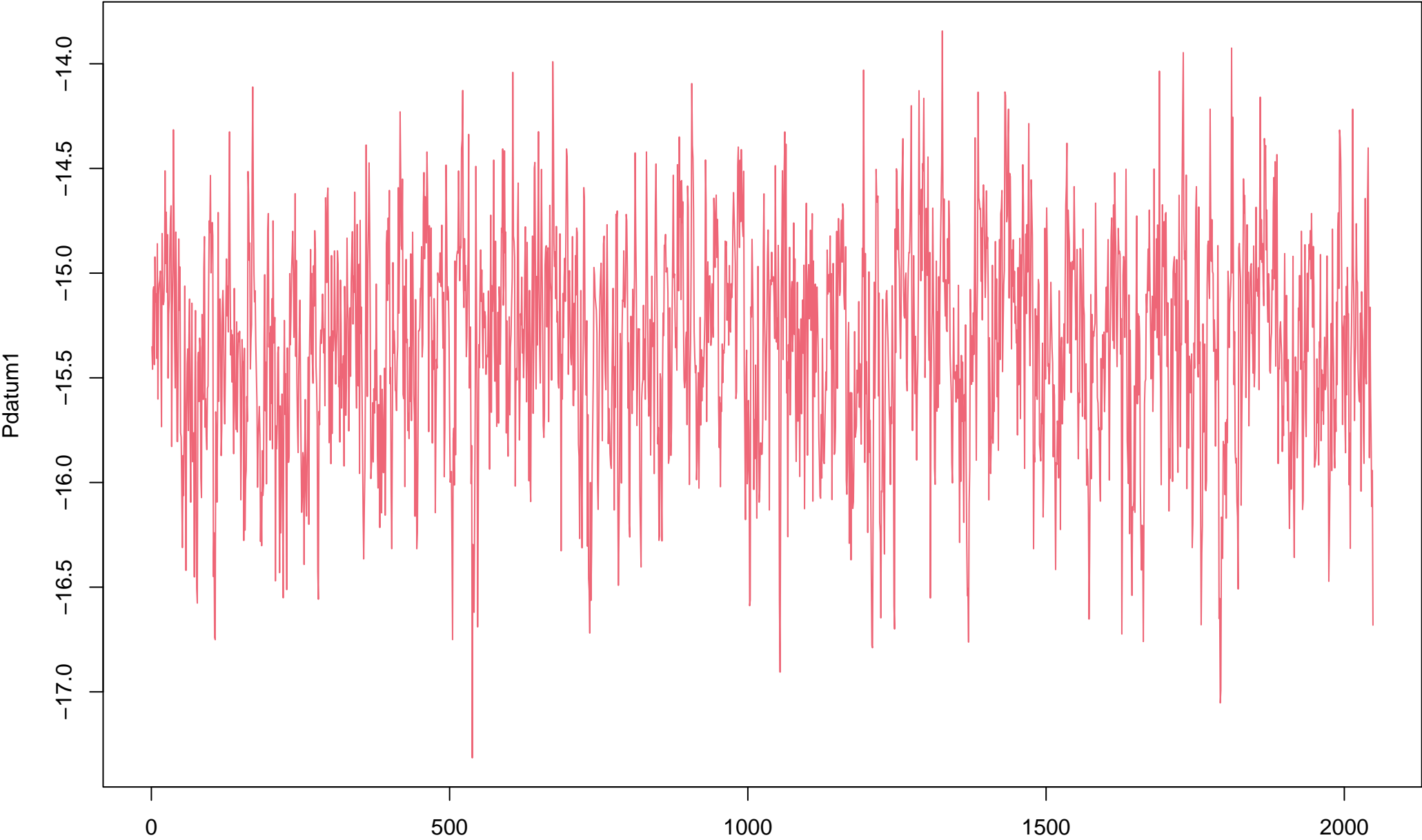
**PdatacornerHi**  
**ESS = 1120 | BMK = 0.0637 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0**



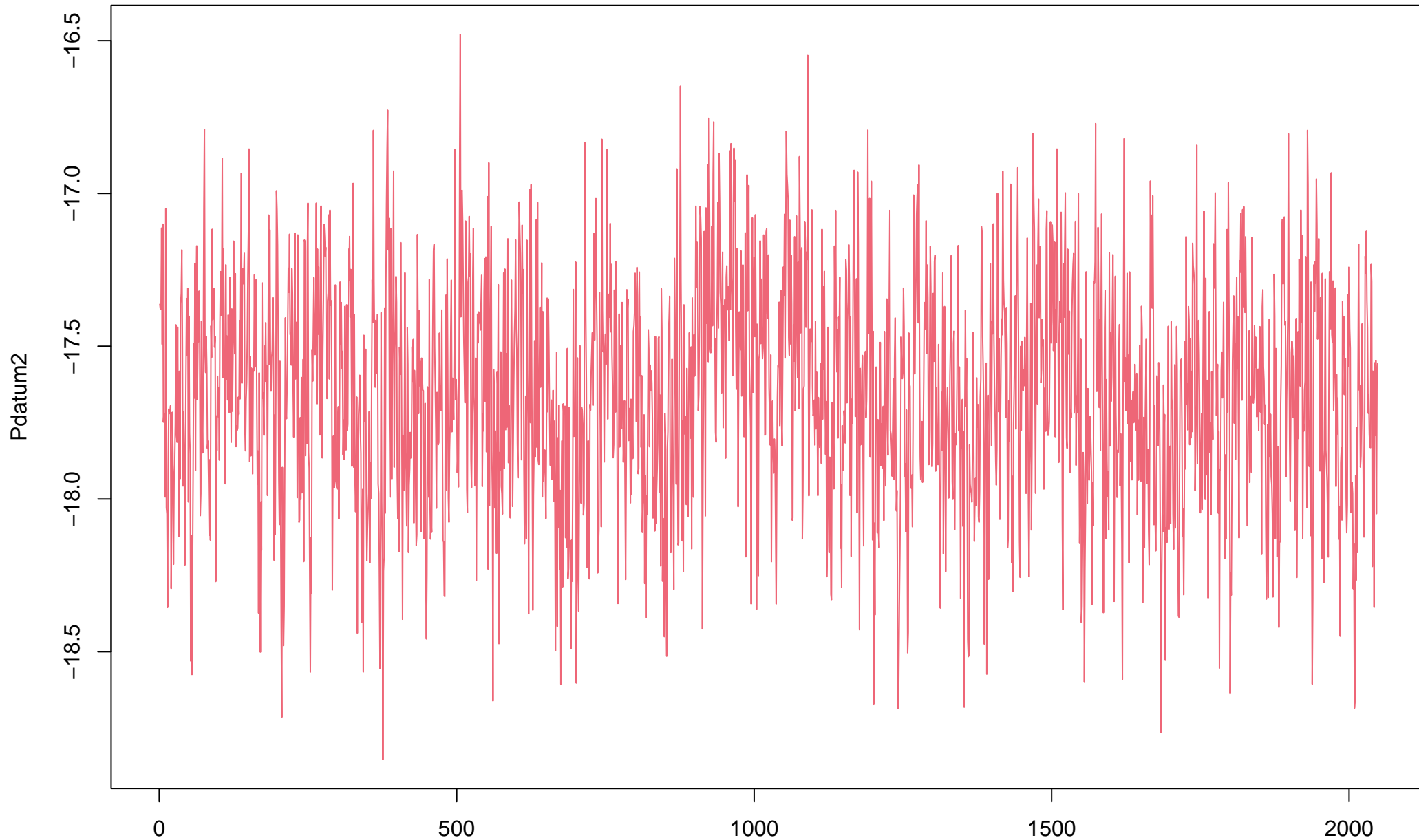
**PdatacornerLo**  
**ESS = 44.7 | BMK = 0.175 | MCSE(6.27) = 8.86 | stat: FALSE | burn: 2040**



**Pdatum1**  
**ESS = 467 | BMK = 0.0573 | MCSE(6.27) = 4.78 | stat: TRUE | burn: 0**

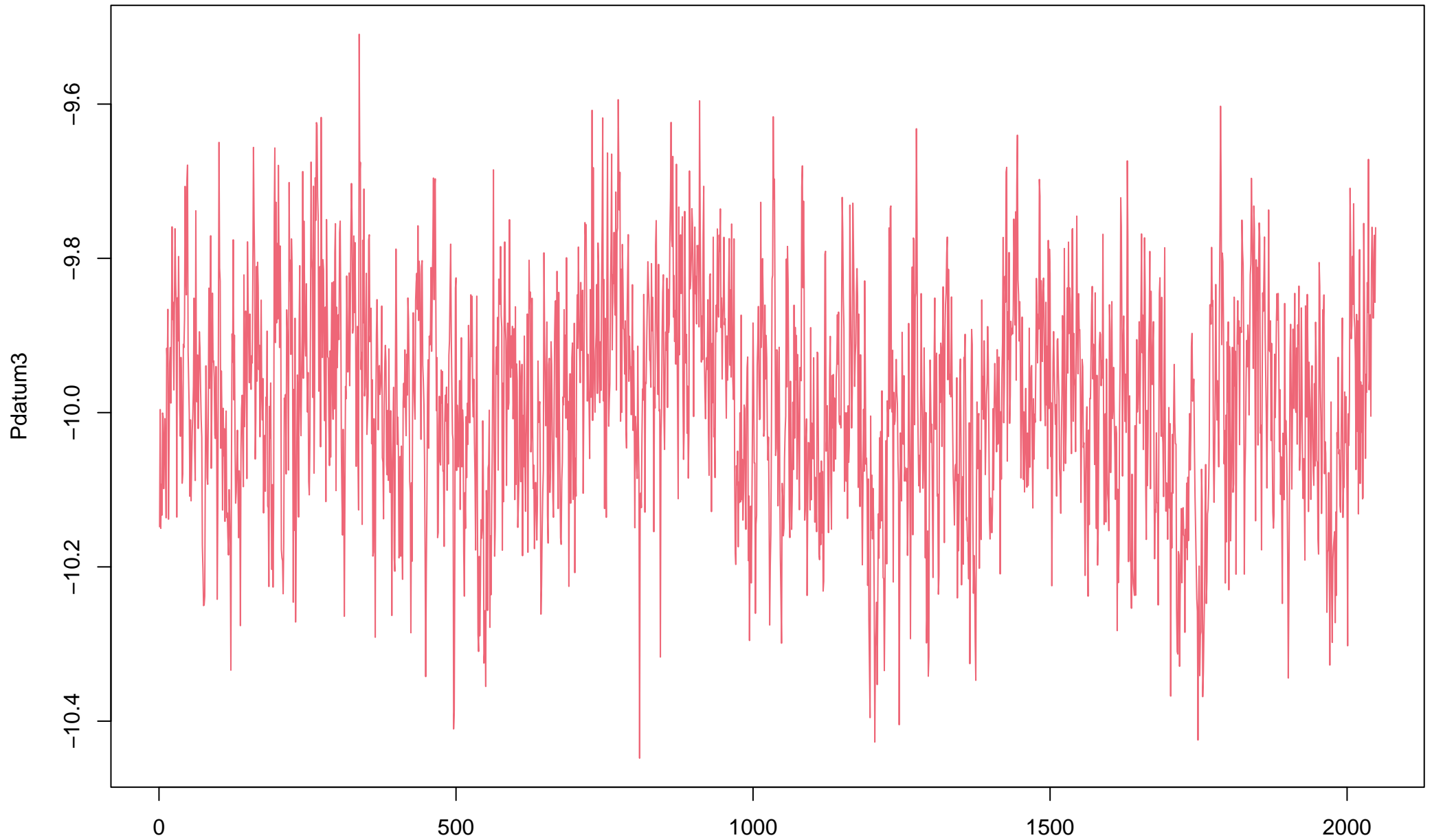


**Pdatum2**  
**ESS = 2.22e-16 | BMK = 0.0509 | MCSE(6.27) = 5.06 | stat: TRUE | burn: 0**

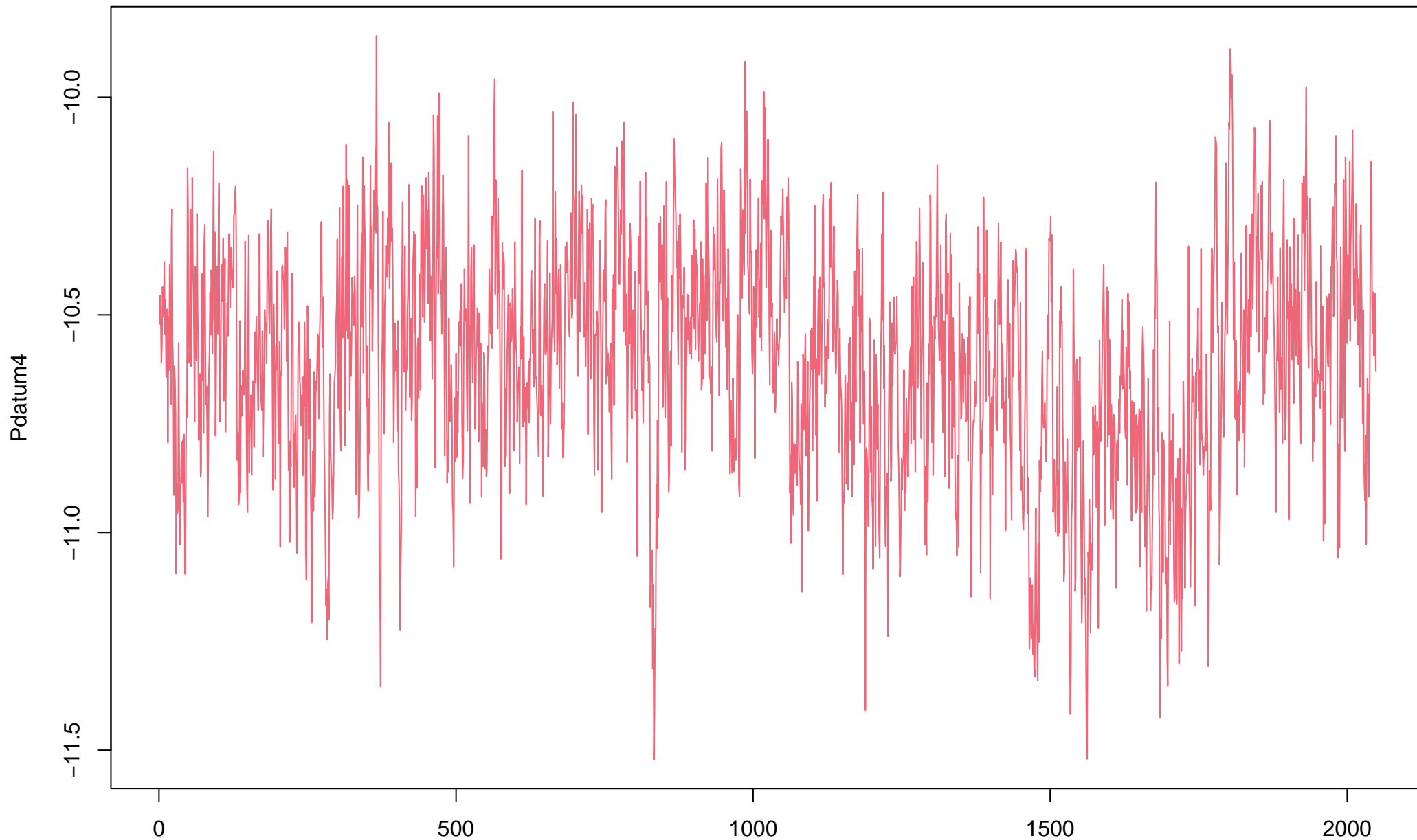




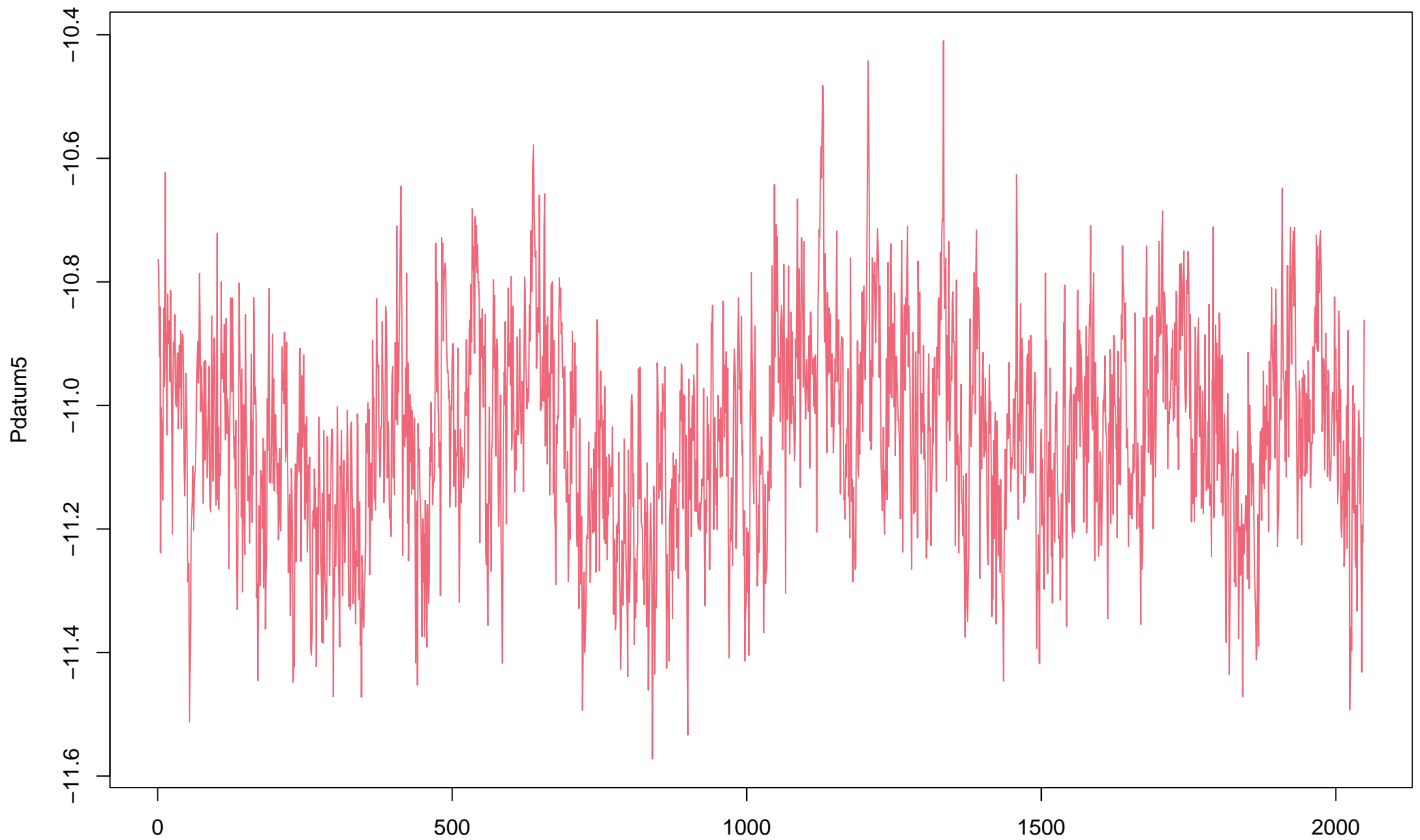
**Pdatum3**  
**ESS = 237 | BMK = 0.113 | MCSE(6.27) = 6.05 | stat: TRUE | burn: 0**



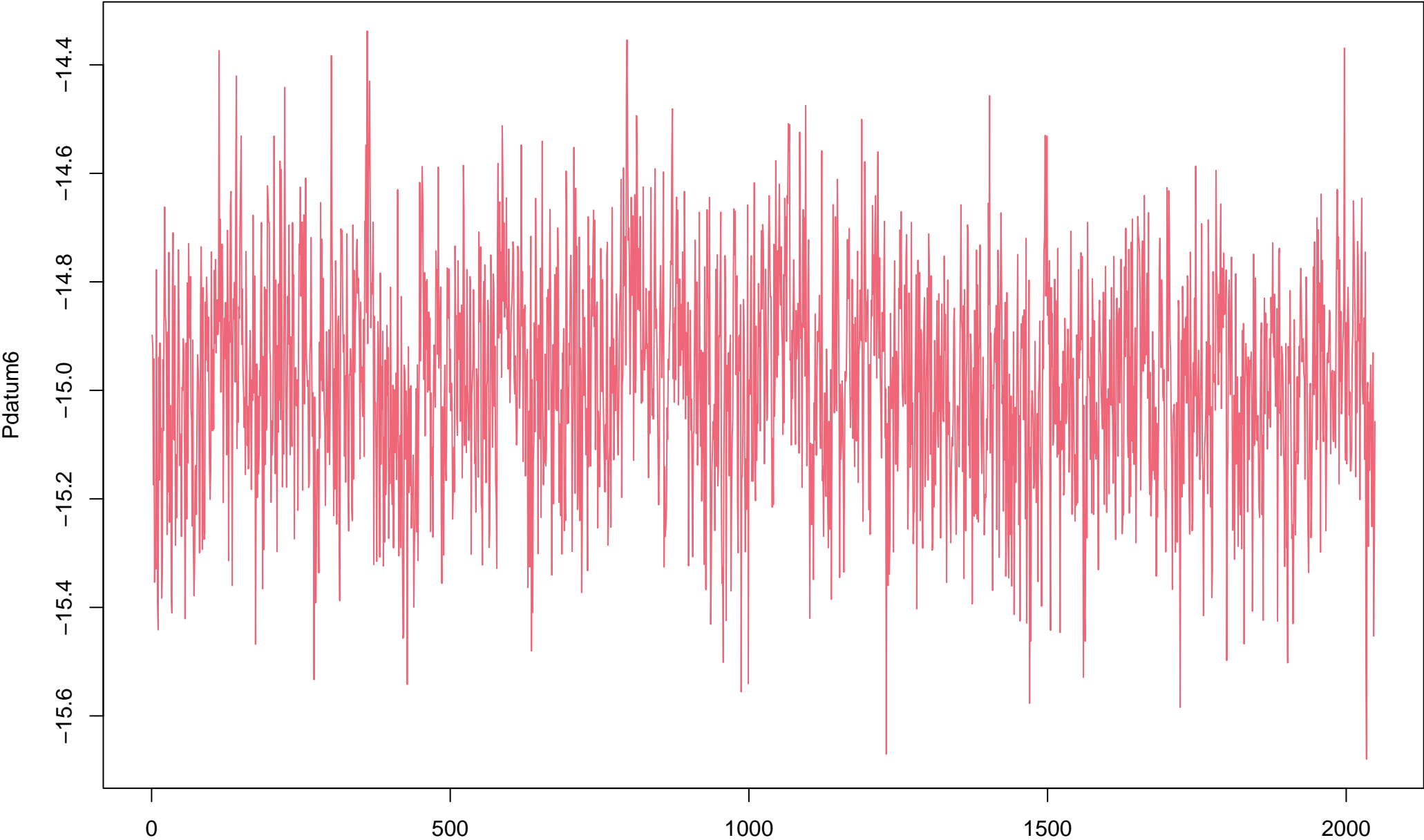
**Pdatum4**  
**ESS = 106 | BMK = 0.158 | MCSE(6.27) = 7.4 | stat: TRUE | burn: 0**



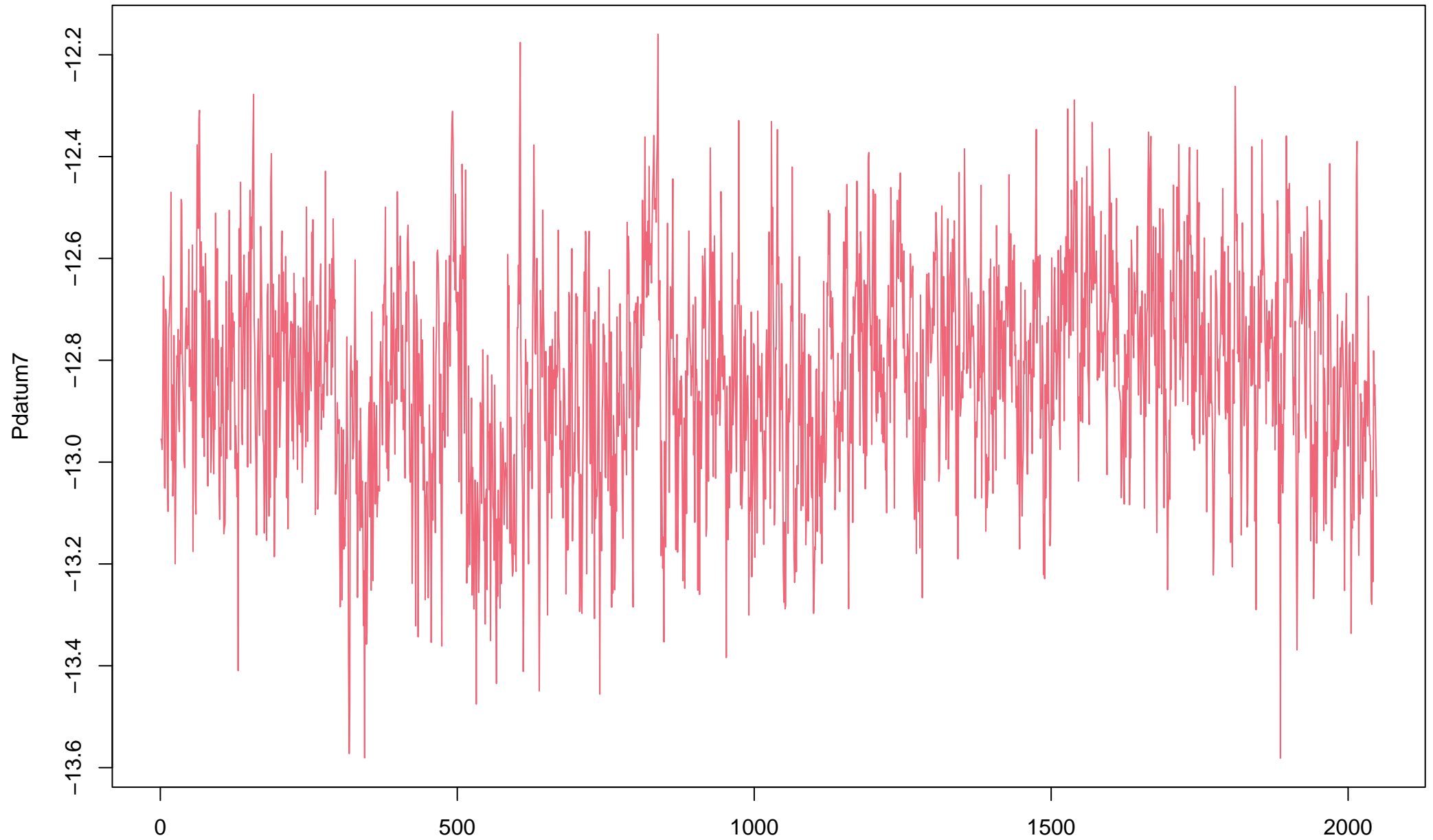
**Pdatum5**  
**ESS = 132 | BMK = 0.141 | MCSE(6.27) = 7.99 | stat: TRUE | burn: 0**



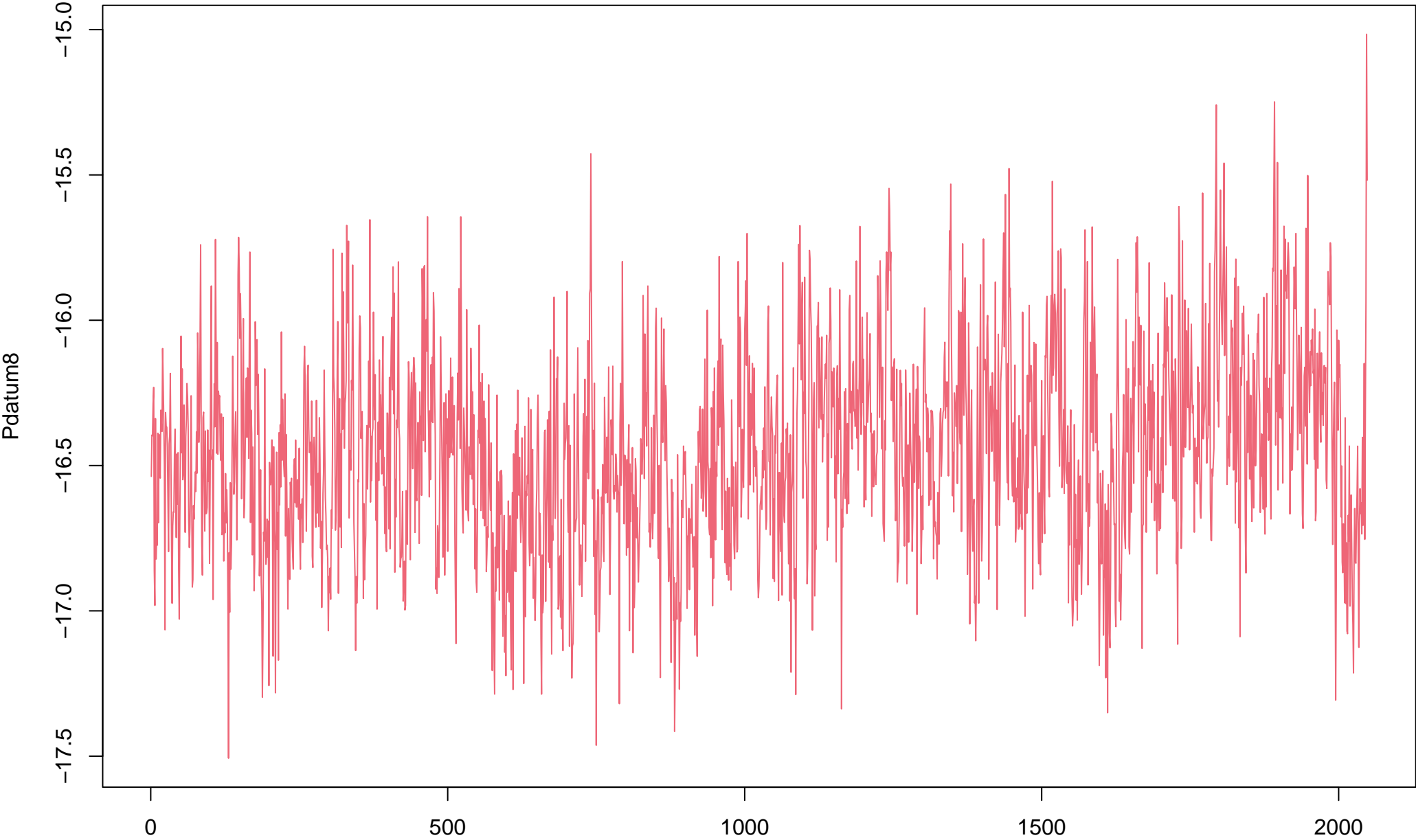
**Pdatum6**  
**ESS = 555 | BMK = 0.0648 | MCSE(6.27) = 4.37 | stat: TRUE | burn: 0**



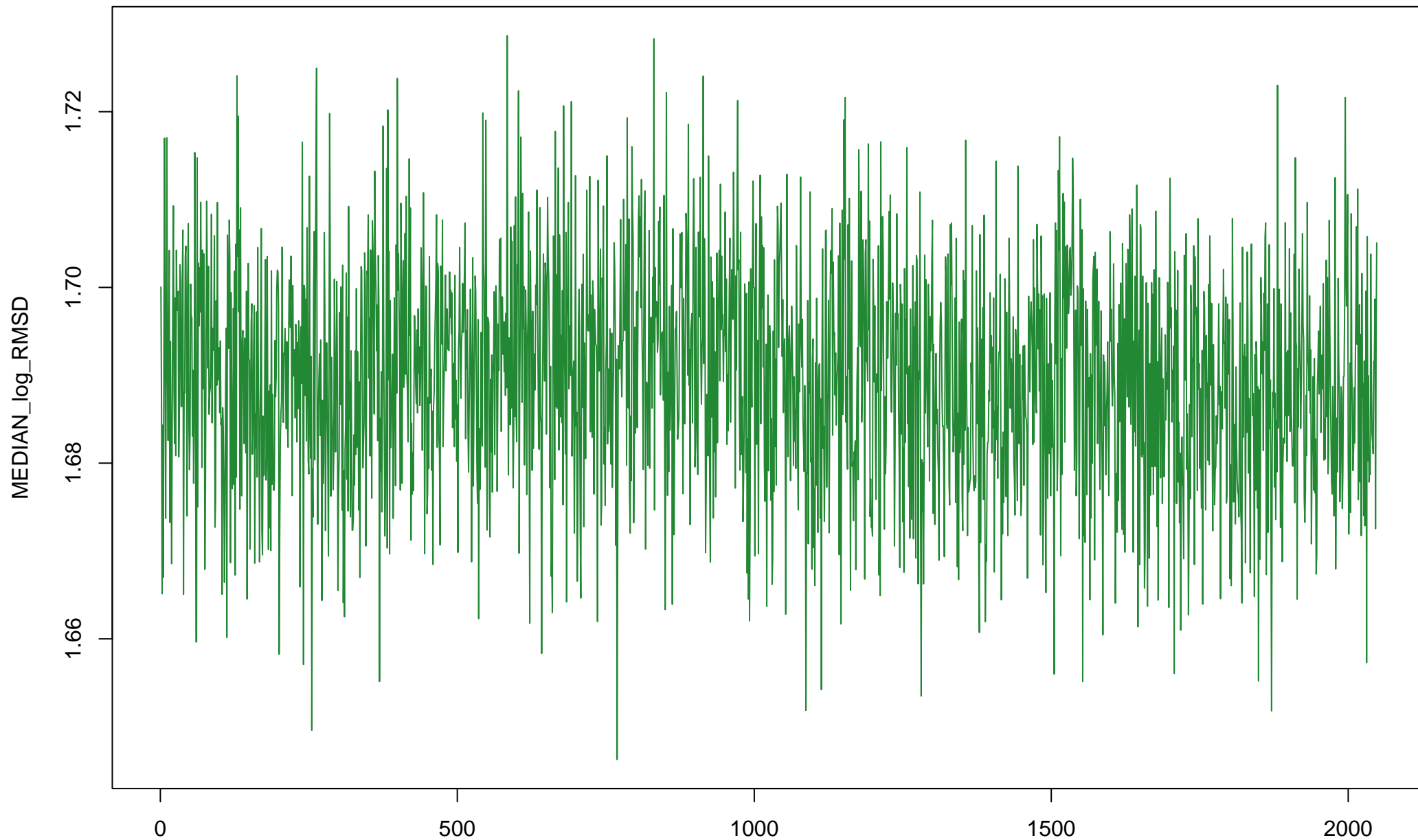
**Pdatum7**  
**ESS = 363 | BMK = 0.131 | MCSE(6.27) = 5.95 | stat: TRUE | burn: 0**



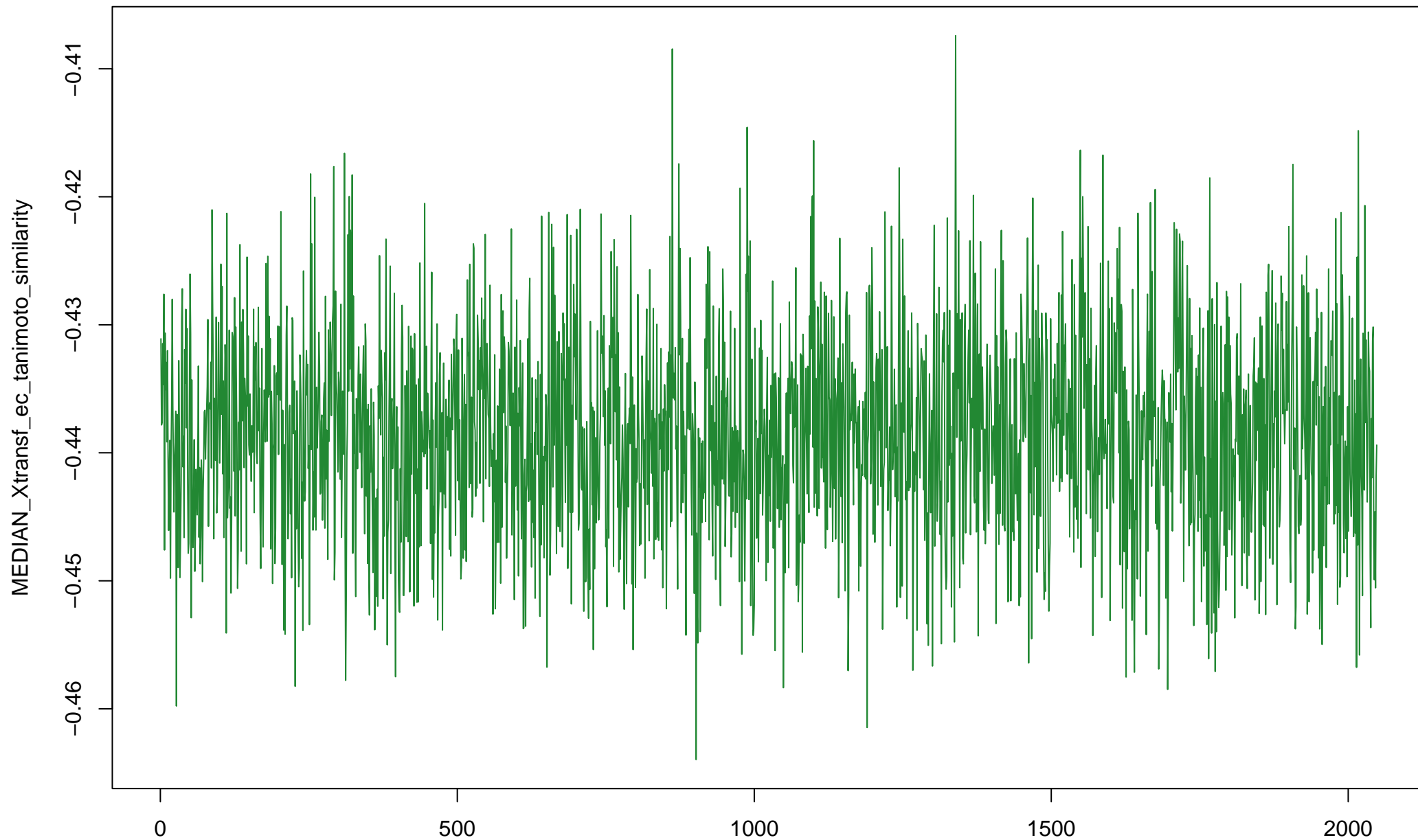
**Pdatum8**  
**ESS = 196 | BMK = 0.191 | MCSE(6.27) = 6.12 | stat: FALSE | burn: 0**



**MEDIAN\_log\_RMSD**  
**ESS = 1410 | BMK = 0.0923 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0**

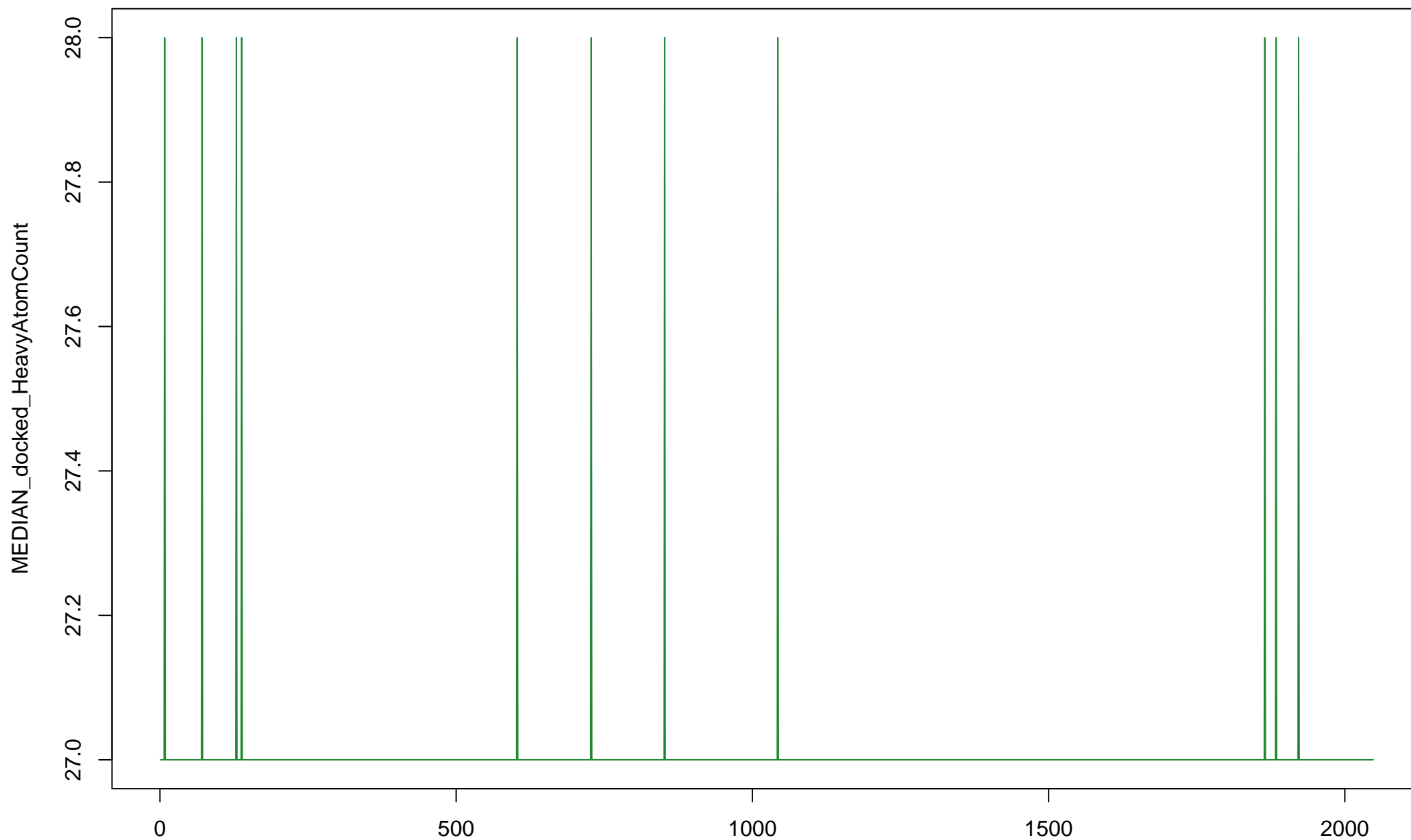


**MEDIAN\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1320 | BMK = 0.0519 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0**

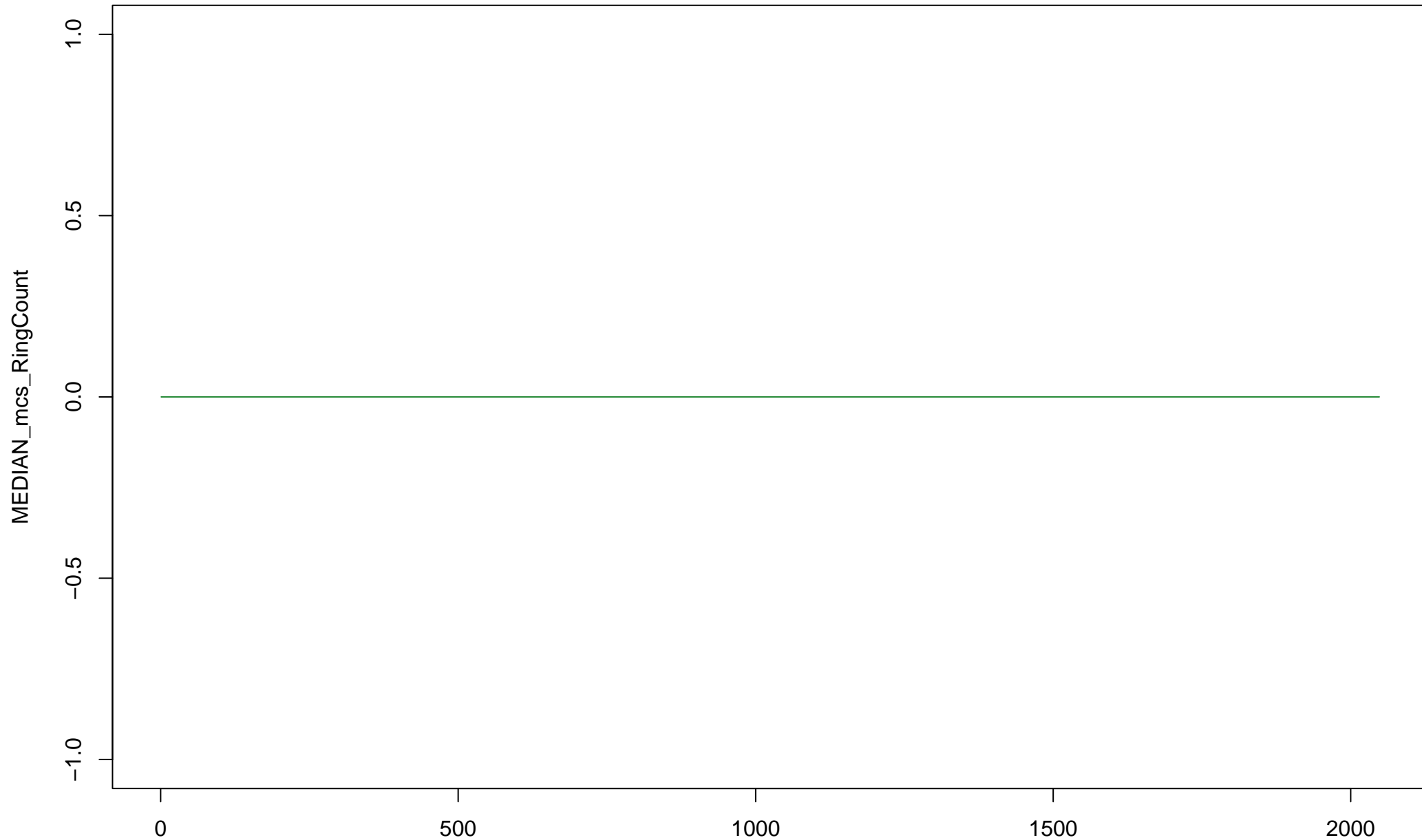




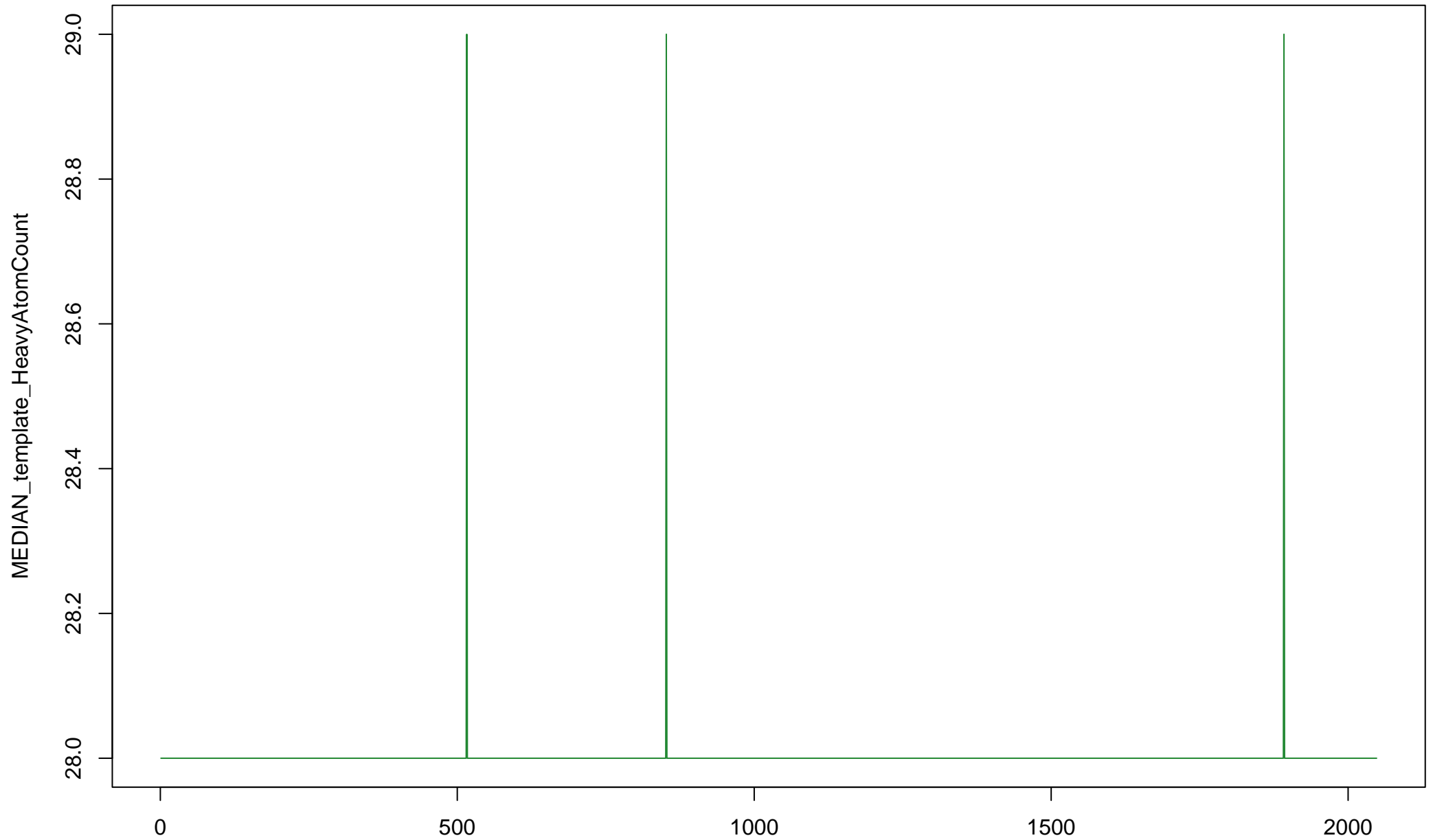
**MEDIAN\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0982 | MCSE(6.27) = 2.18 | stat: FALSE | burn: 1224**



**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**



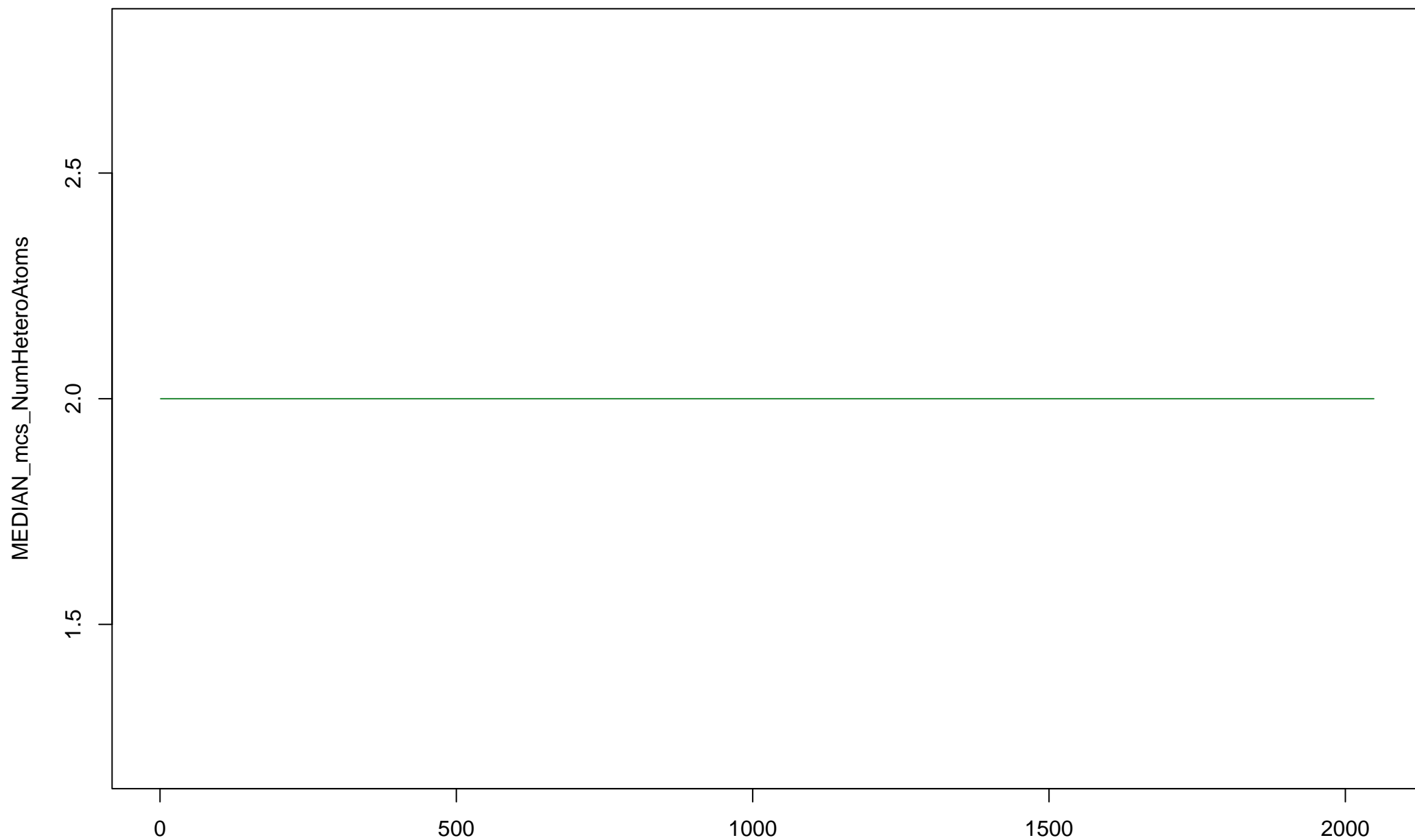
**MEDIAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



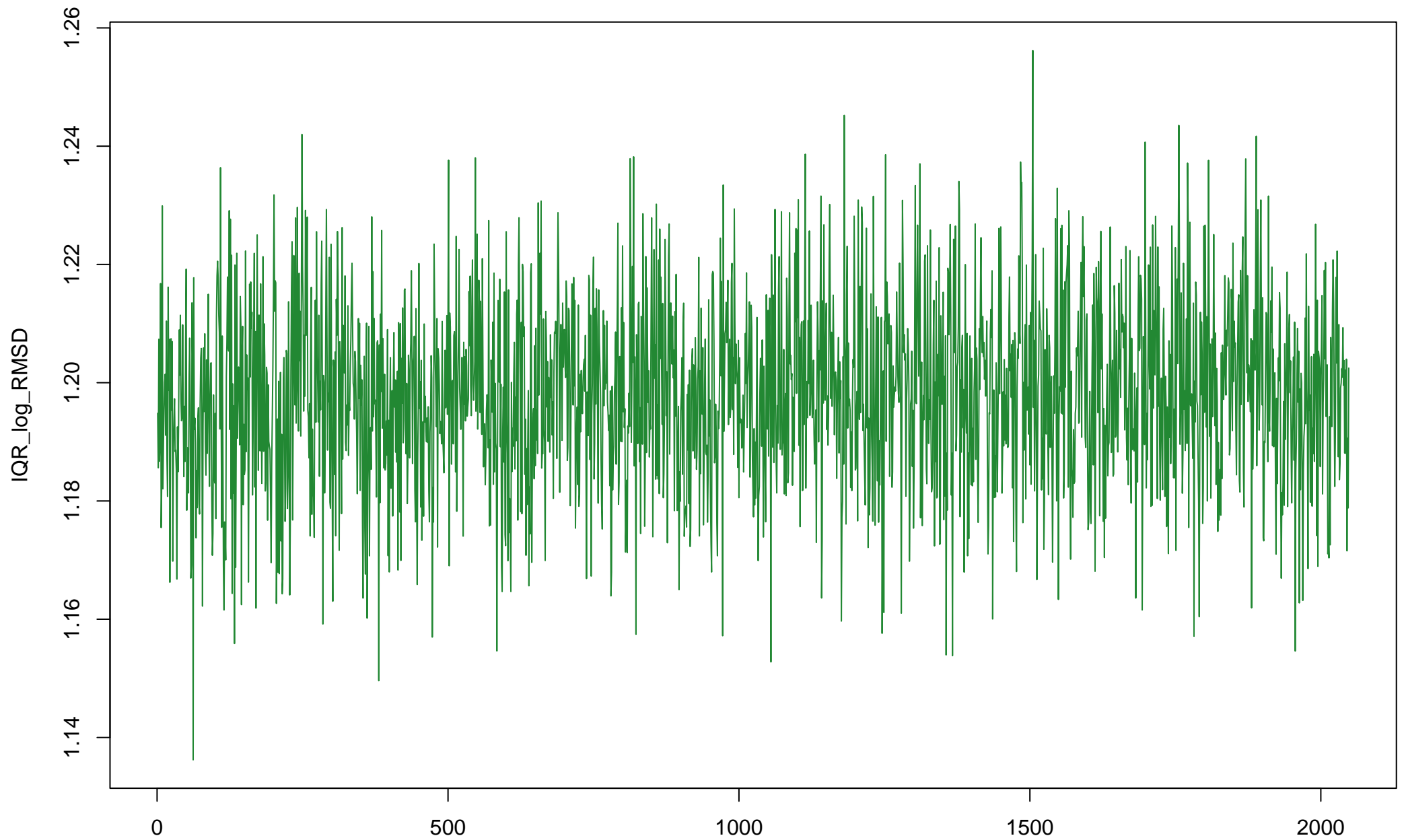
**MEDIAN\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



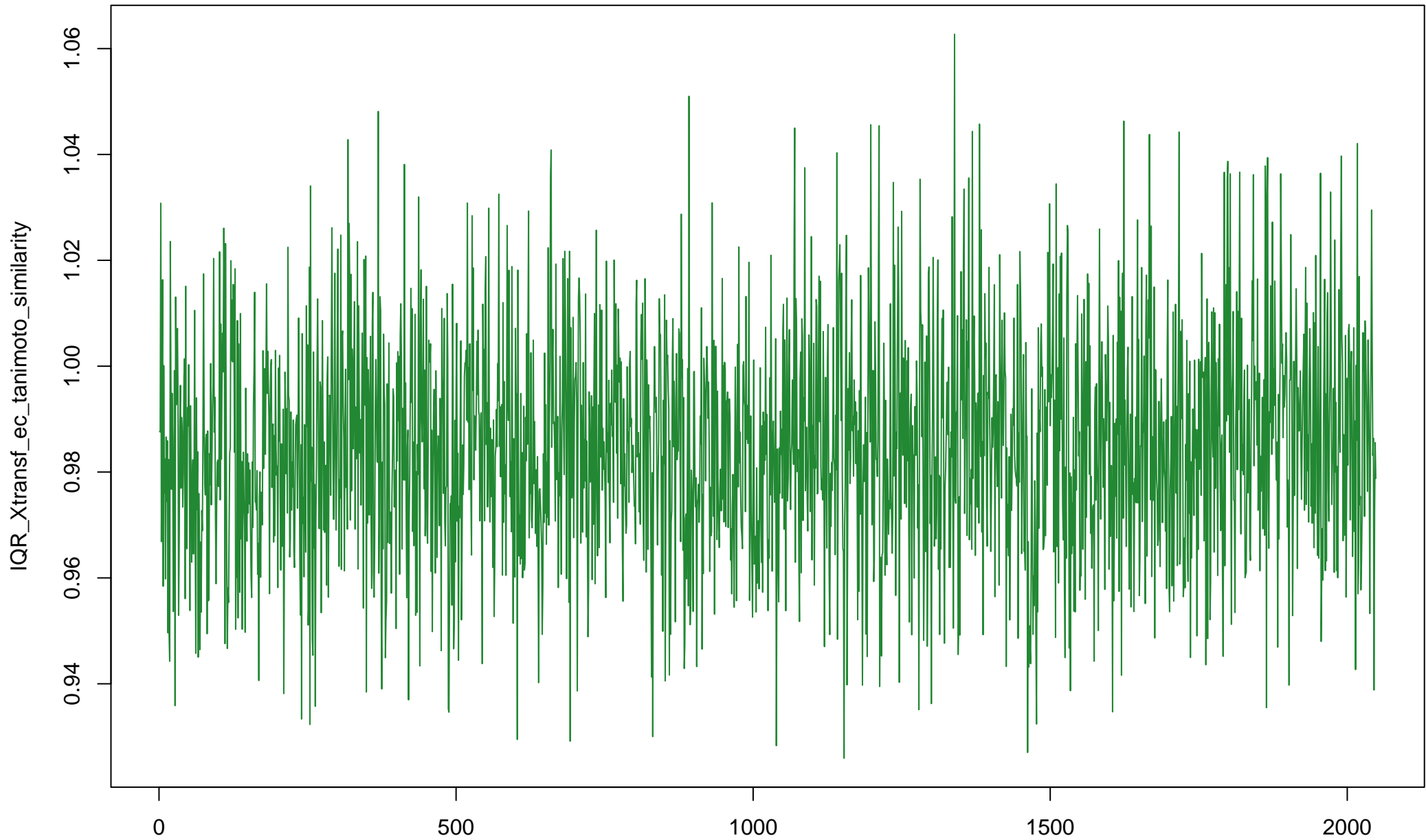
**MEDIAN\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**IQR\_log\_RMSD**  
**ESS = 1370 | BMK = 0.0627 | MCSE(6.27) = 2.84 | stat: FALSE | burn: 0**

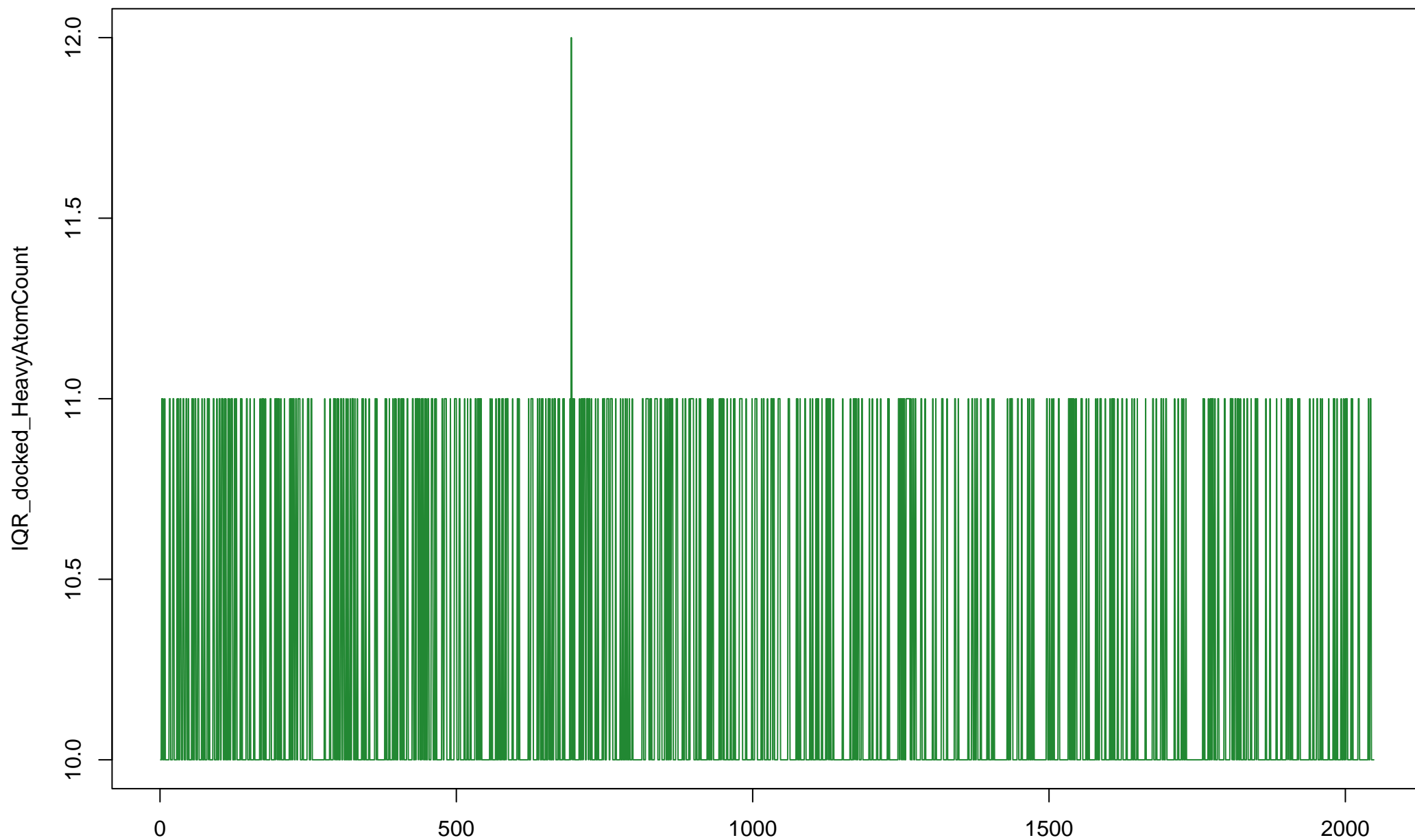


IQR\_Xtransf\_ec\_tanimoto\_similarity  
ESS = 1680 | BMK = 0.063 | MCSE(6.27) = 3.02 | stat: FALSE | burn: 0

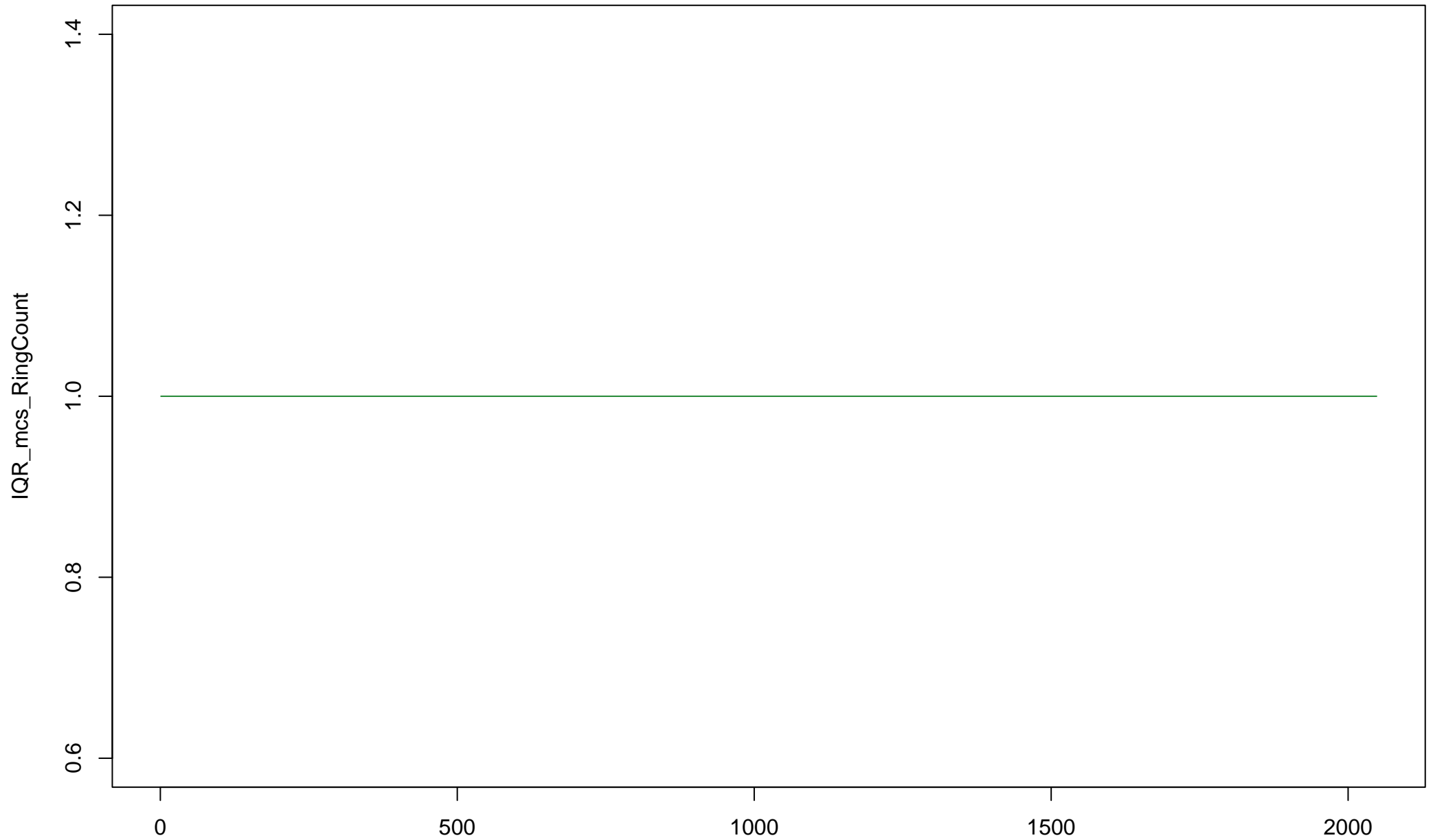




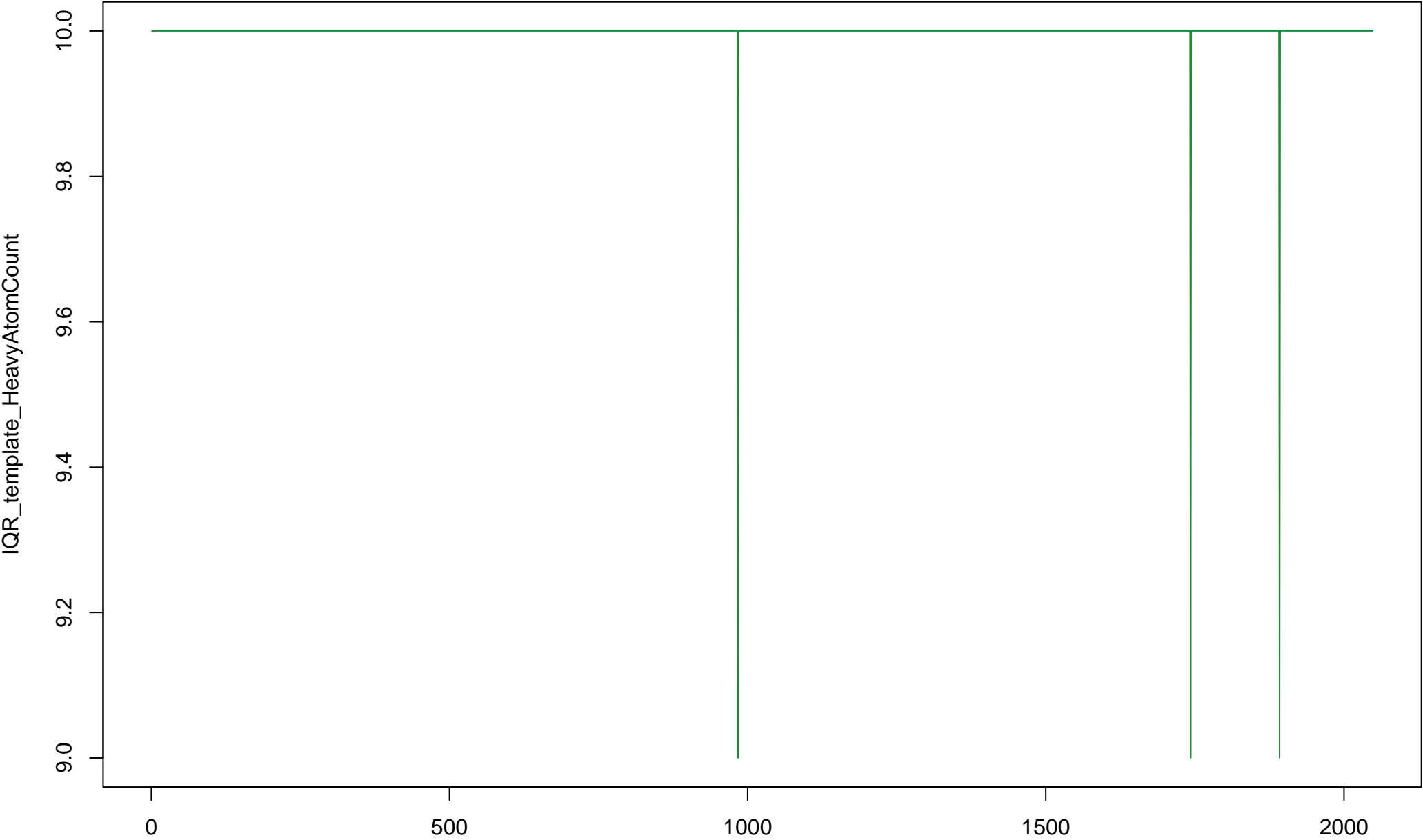
**IQR\_docked\_HeavyAtomCount**  
**ESS = 1710 | BMK = 0.0849 | MCSE(6.27) = 2.65 | stat: FALSE | burn: 0**



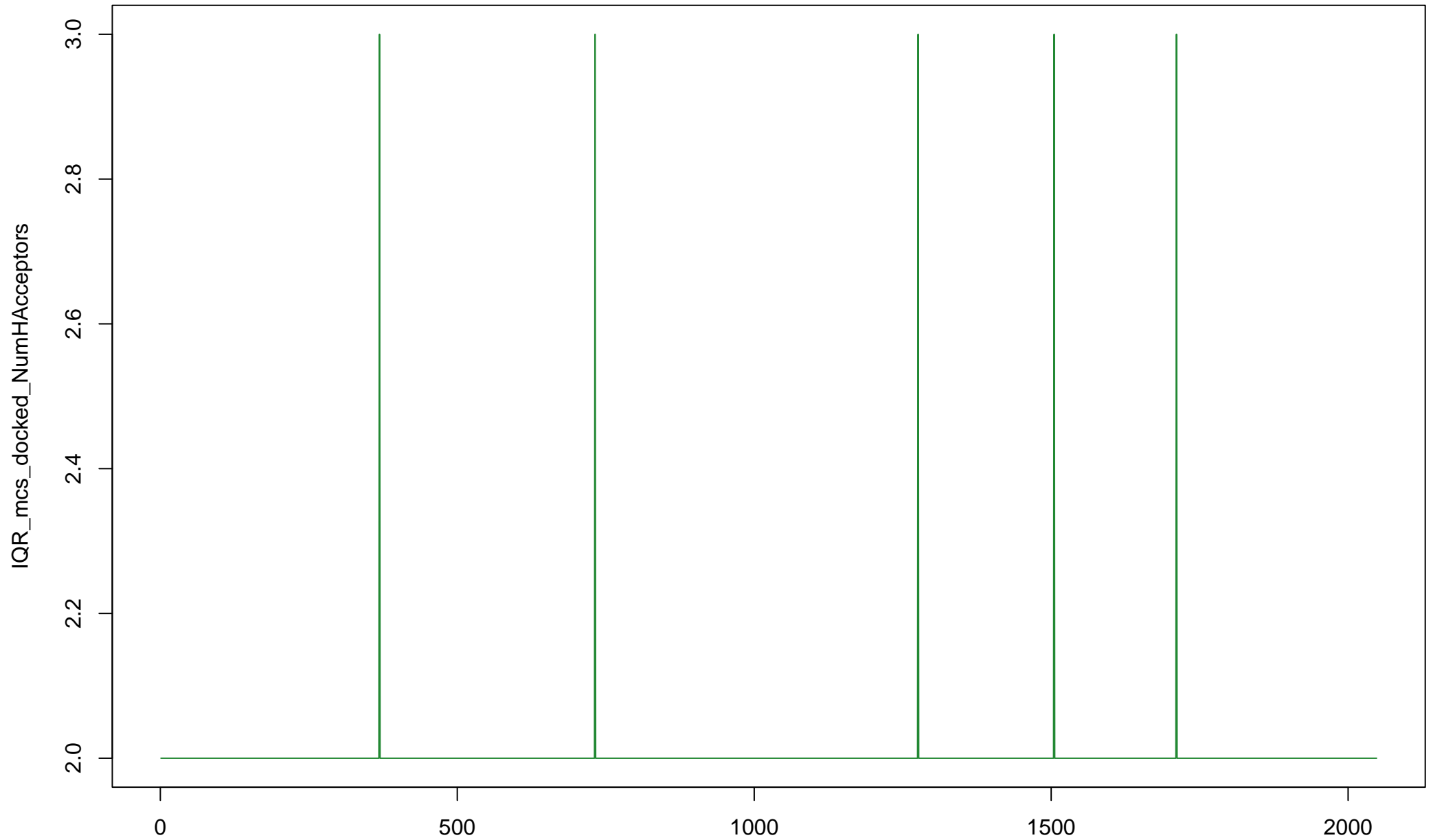
**IQR\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



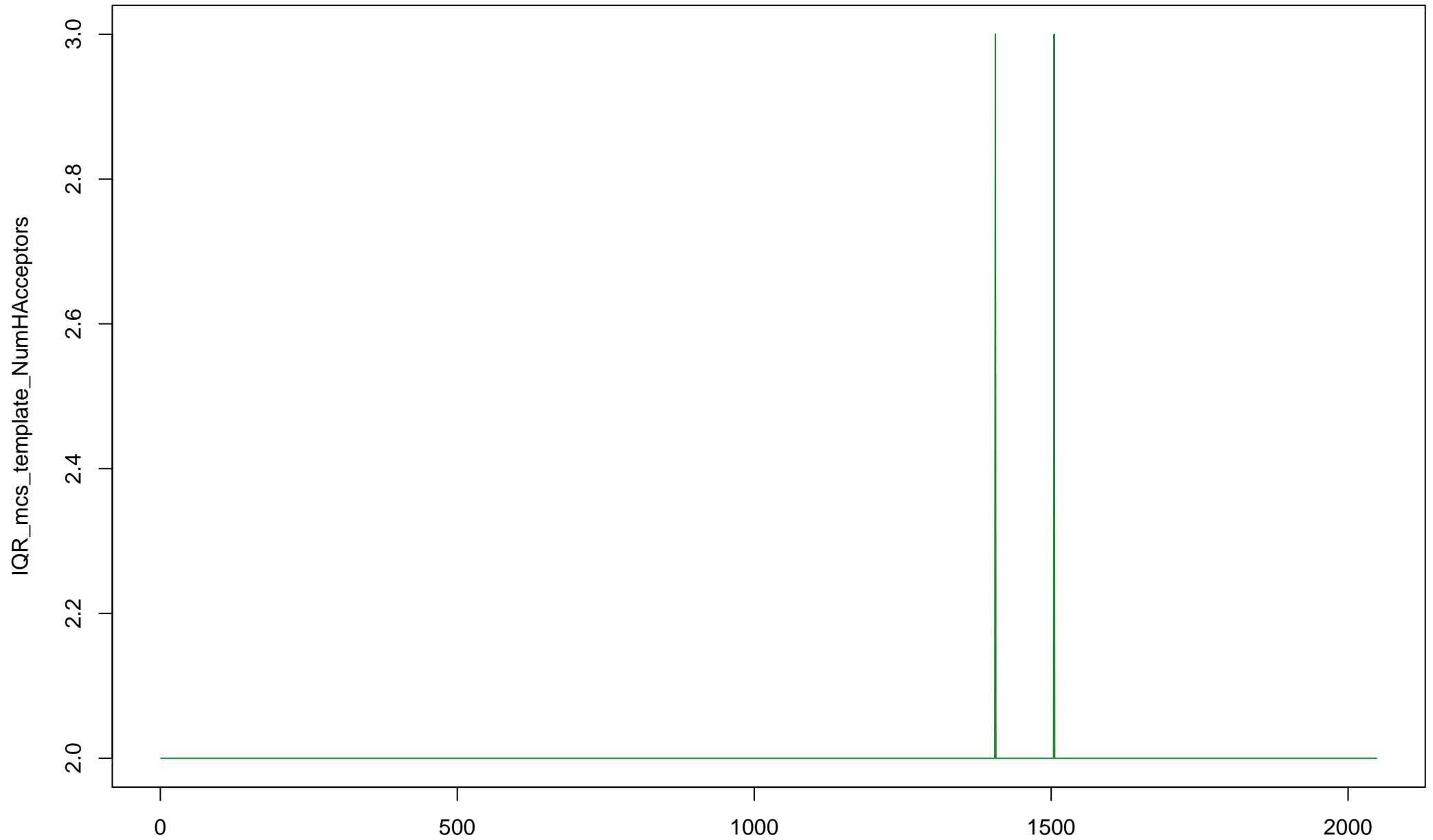
IQR\_template\_HeavyAtomCount  
ESS = 2050 | BMK = 0.121 | MCSE(6.27) = 2.17 | stat: FALSE | burn: 1632



**IQR\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0717 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 2040**



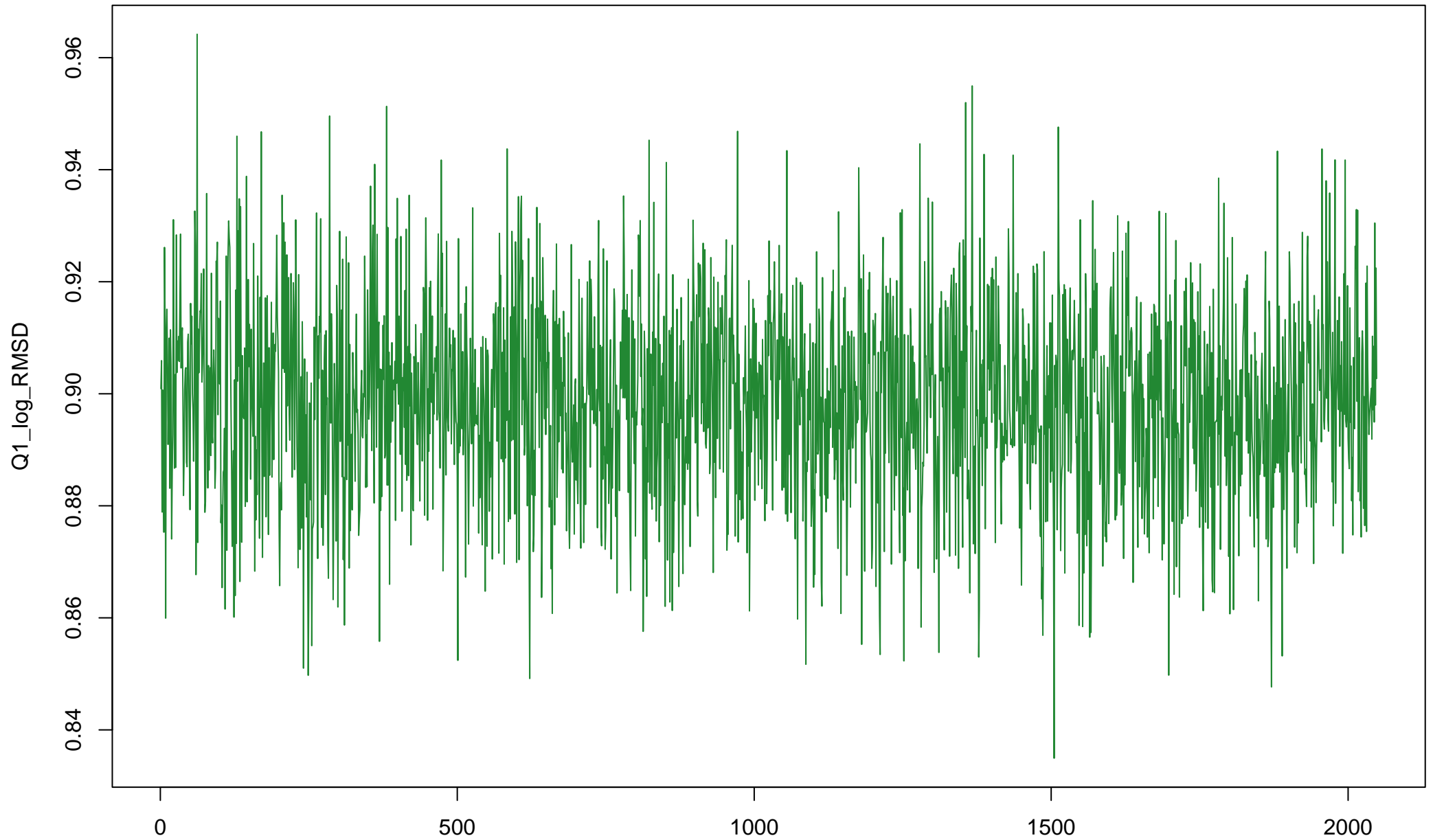
**IQR\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.628 | MCSE(6.27) = 2.2 | stat: FALSE | burn: 1632**



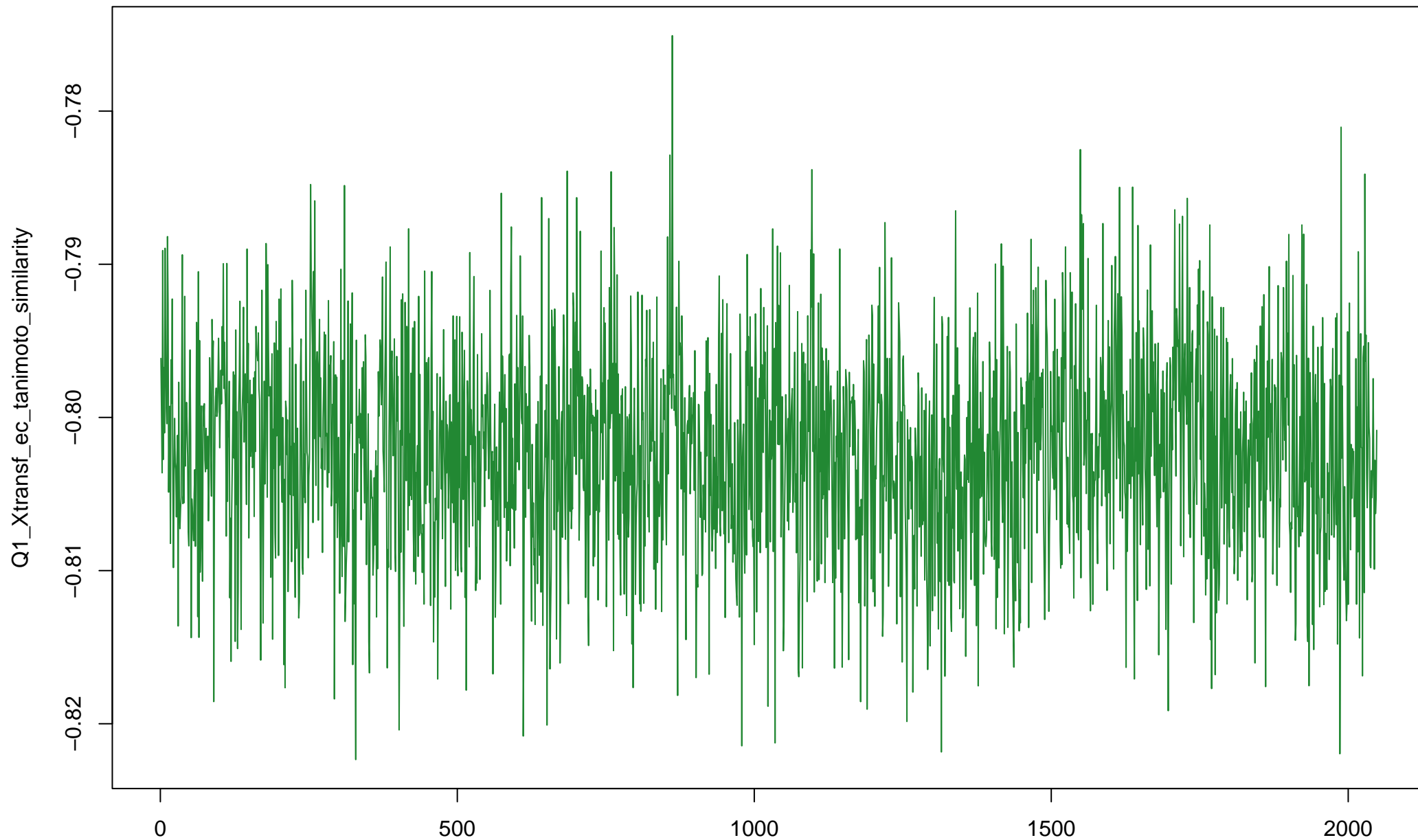
IQR\_mcs\_NumHeteroAtoms  
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



**Q1\_log\_RMSD**  
**ESS = 1770 | BMK = 0.0483 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0**

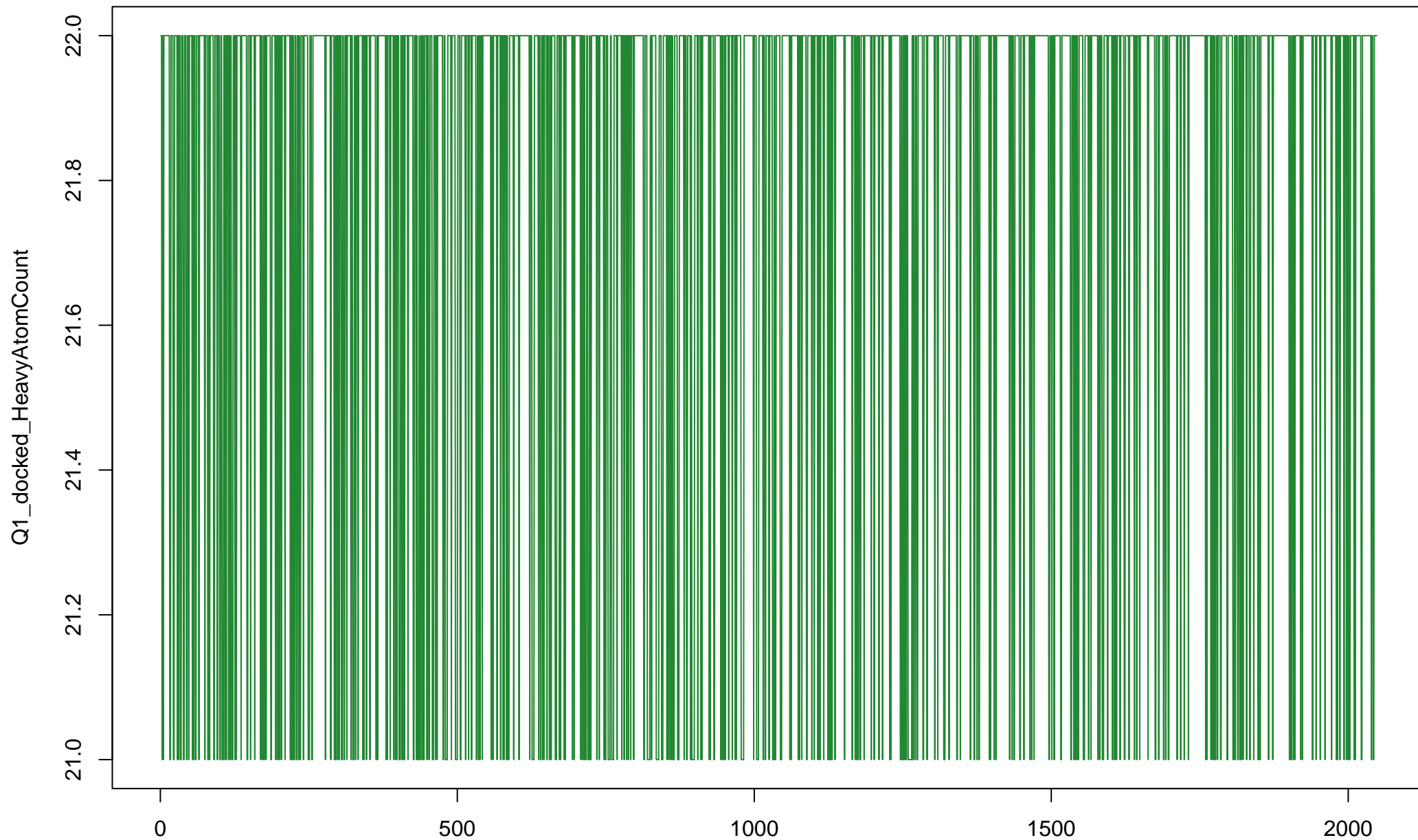


**Q1\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1200 | BMK = 0.0352 | MCSE(6.27) = 3.28 | stat: FALSE | burn: 0**





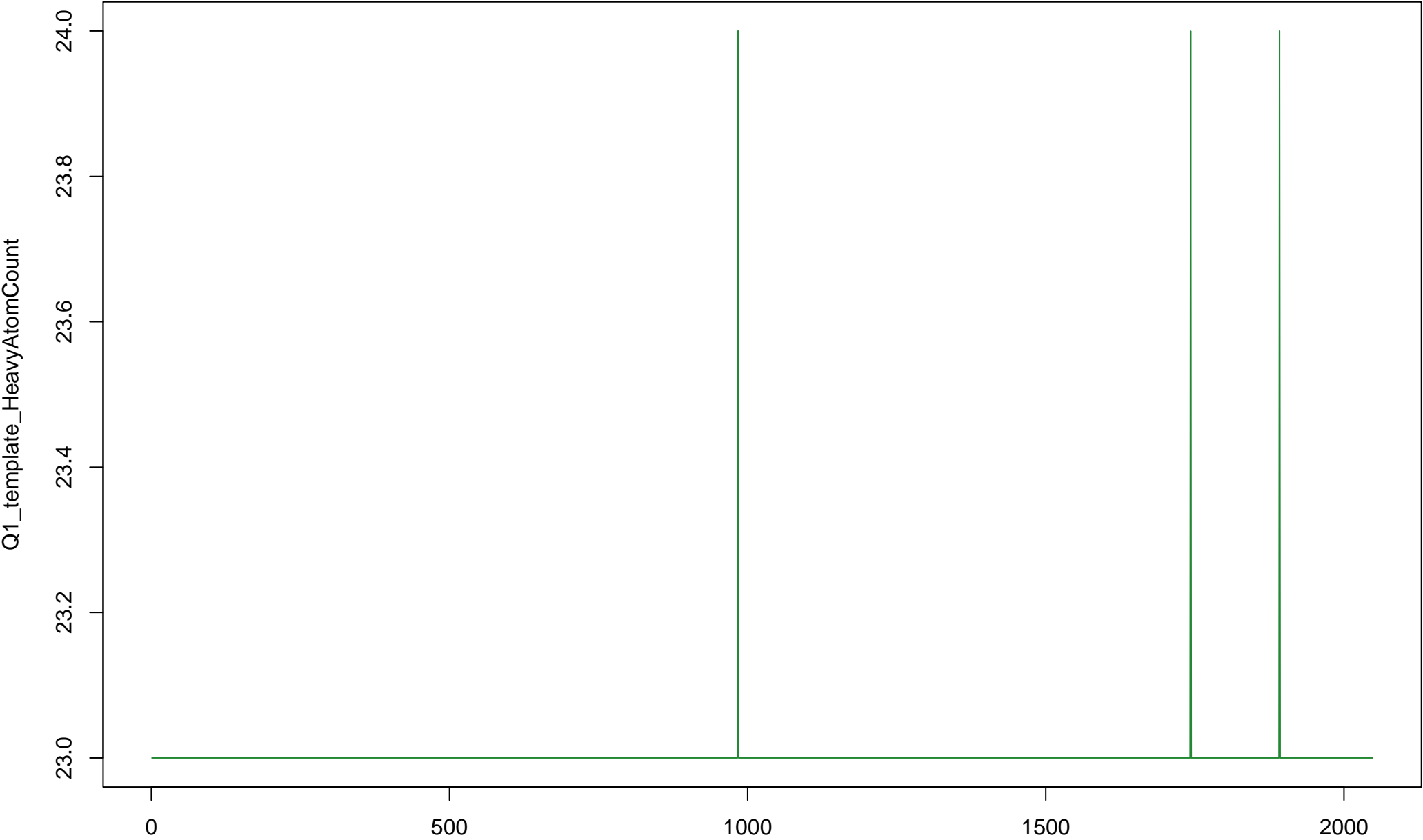
**Q1\_docked\_HeavyAtomCount**  
**ESS = 1680 | BMK = 0.0632 | MCSE(6.27) = 2.63 | stat: FALSE | burn: 0**



**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: FALSE | burn: 1632



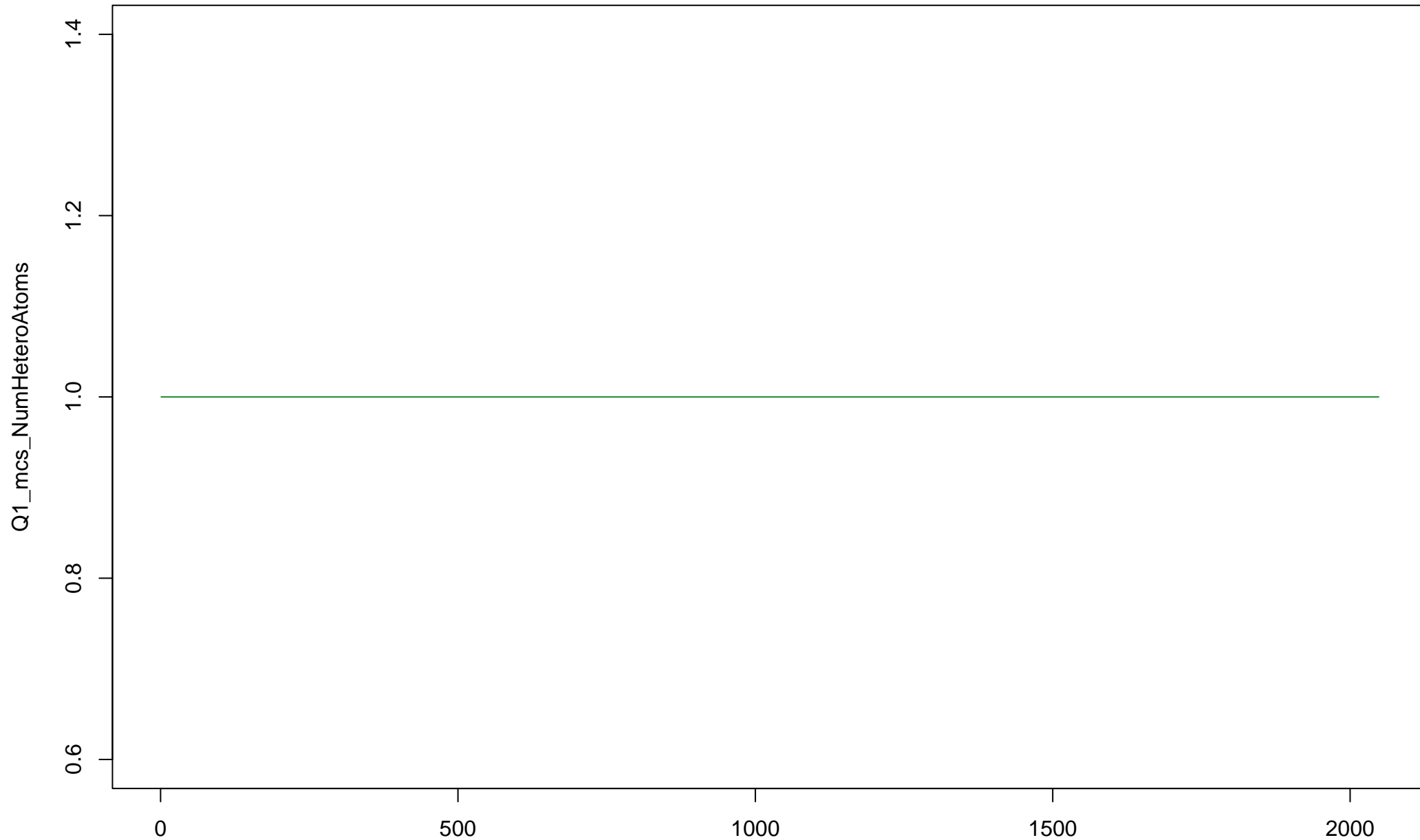
**Q1\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



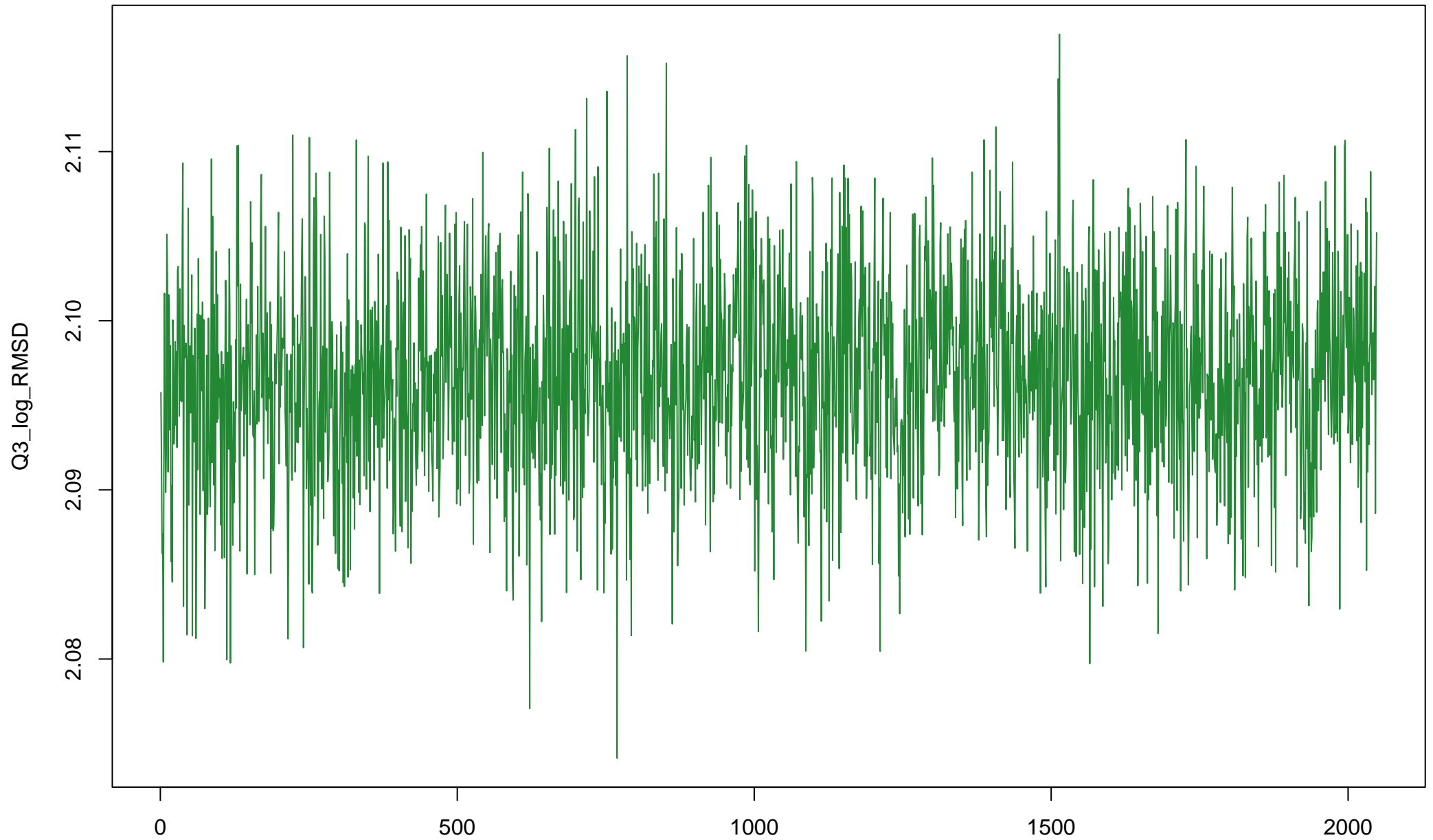
**Q1\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



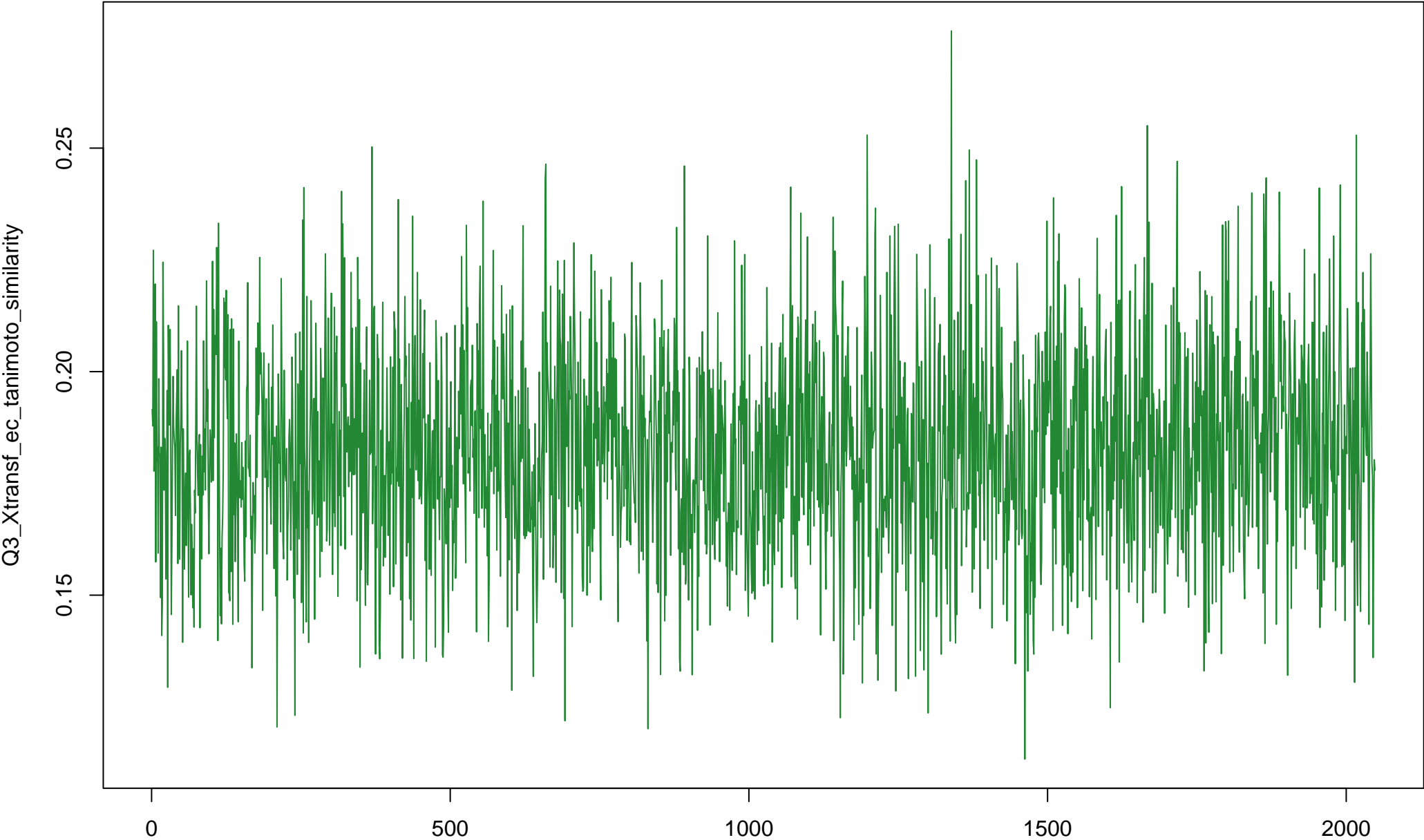
**Q1\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q3\_log\_RMSD**  
**ESS = 1520 | BMK = 0.0614 | MCSE(6.27) = 2.43 | stat: FALSE | burn: 0**

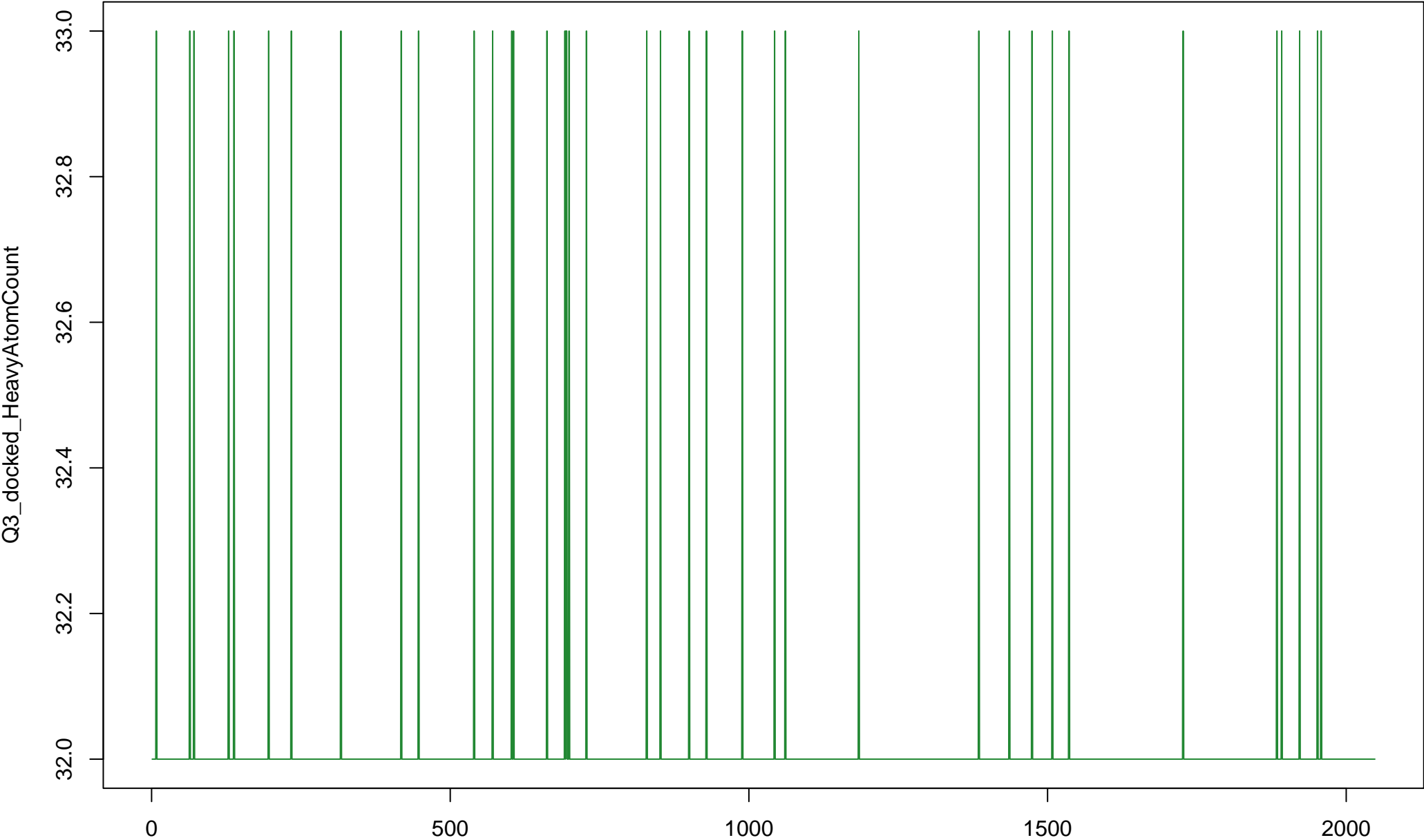


**Q3\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1840 | BMK = 0.0552 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0**





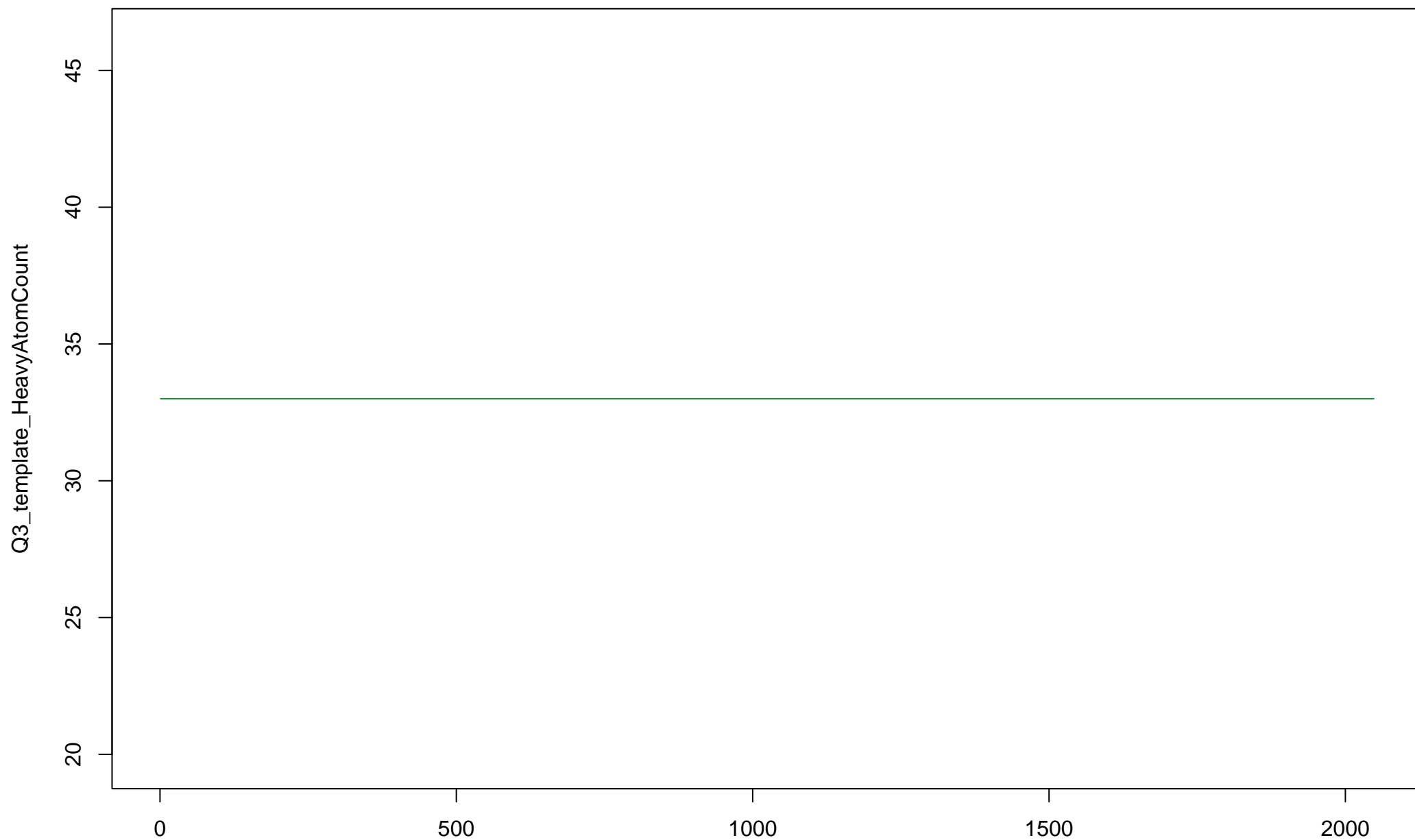
Q3\_docked\_HeavyAtomCount  
ESS = 2050 | BMK = 0.102 | MCSE(6.27) = 2.03 | stat: TRUE | burn: 0



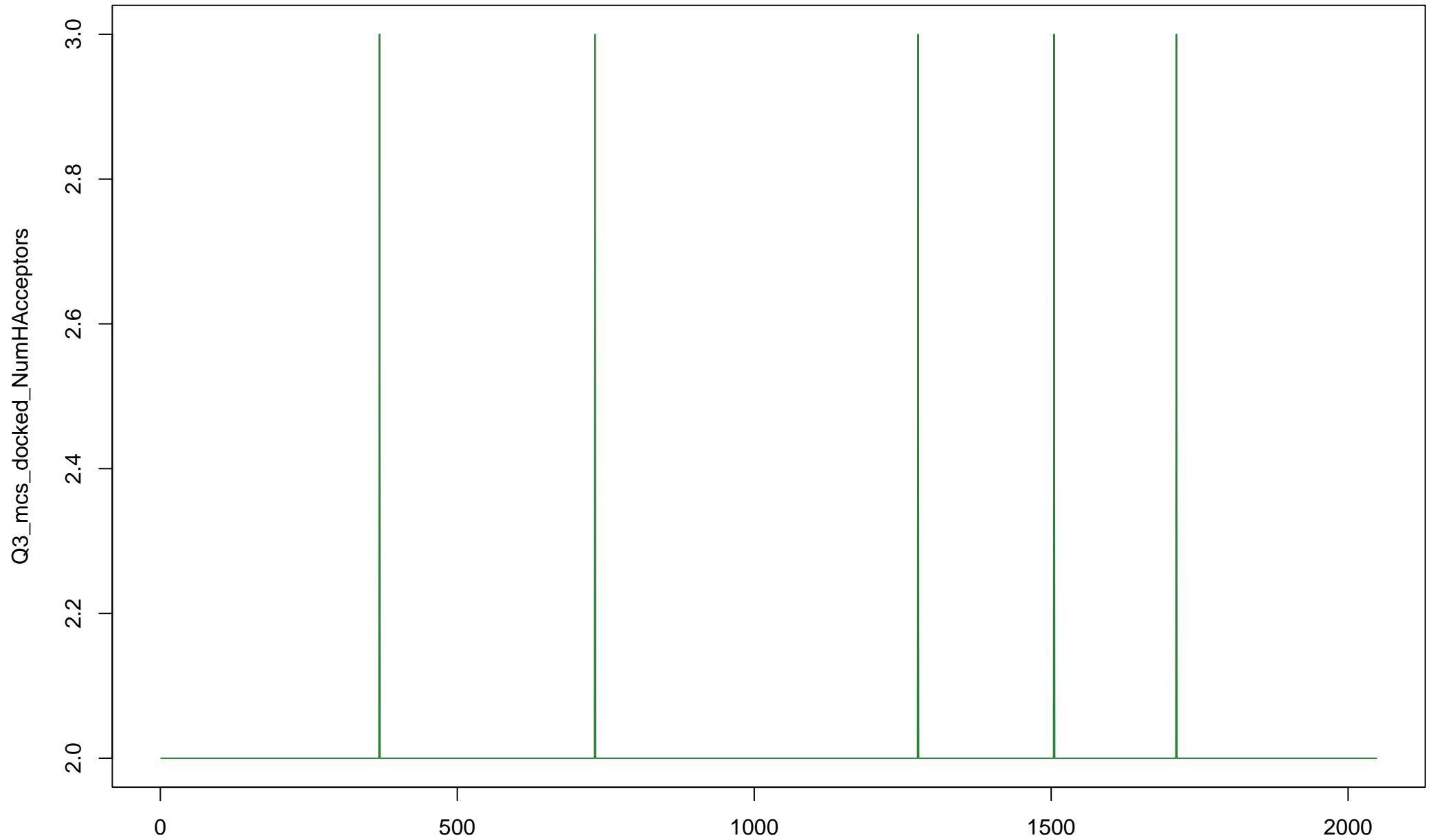
**Q3\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



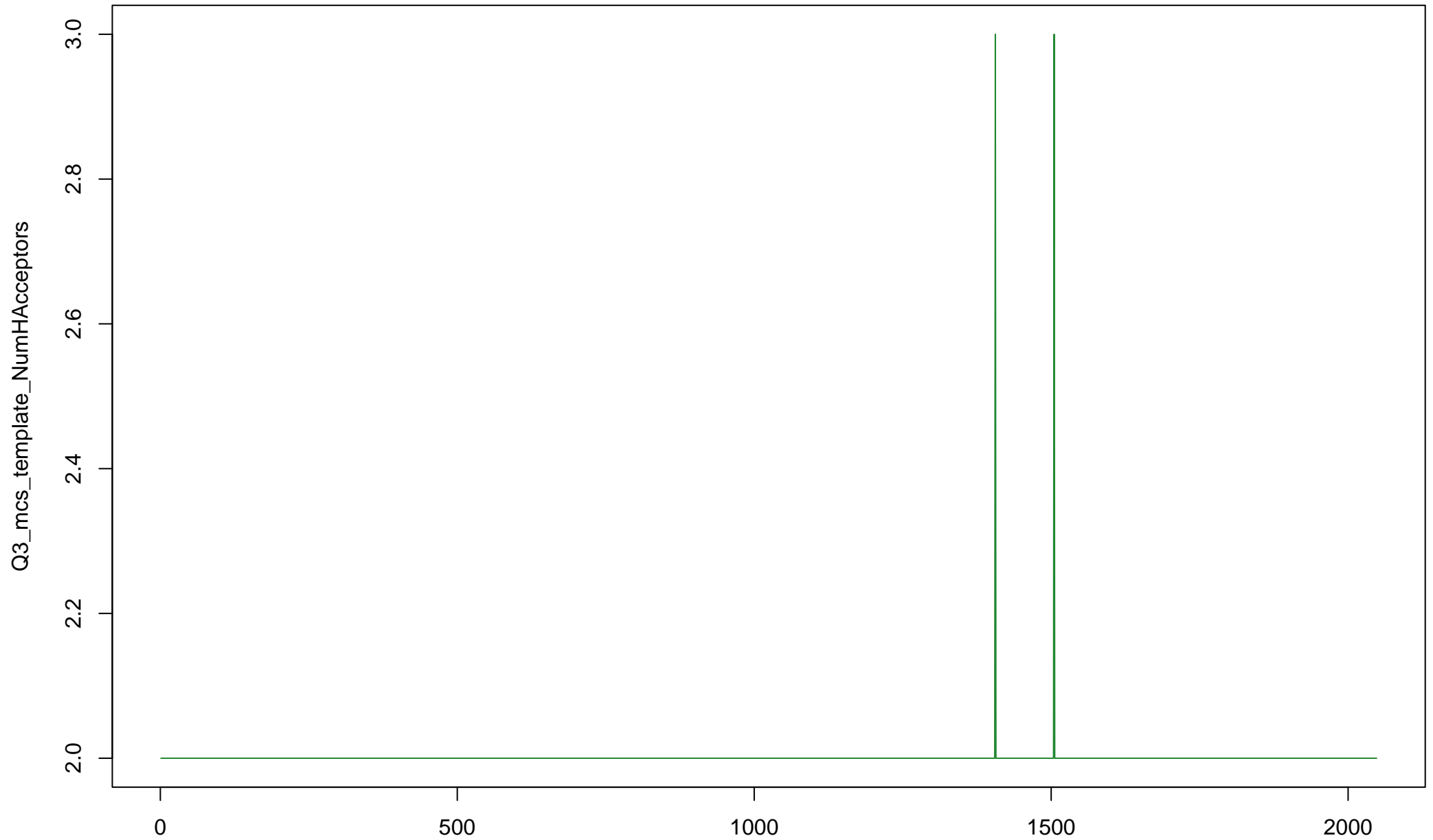
**Q3\_template\_HeavyAtomCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q3\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0717 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 2040**



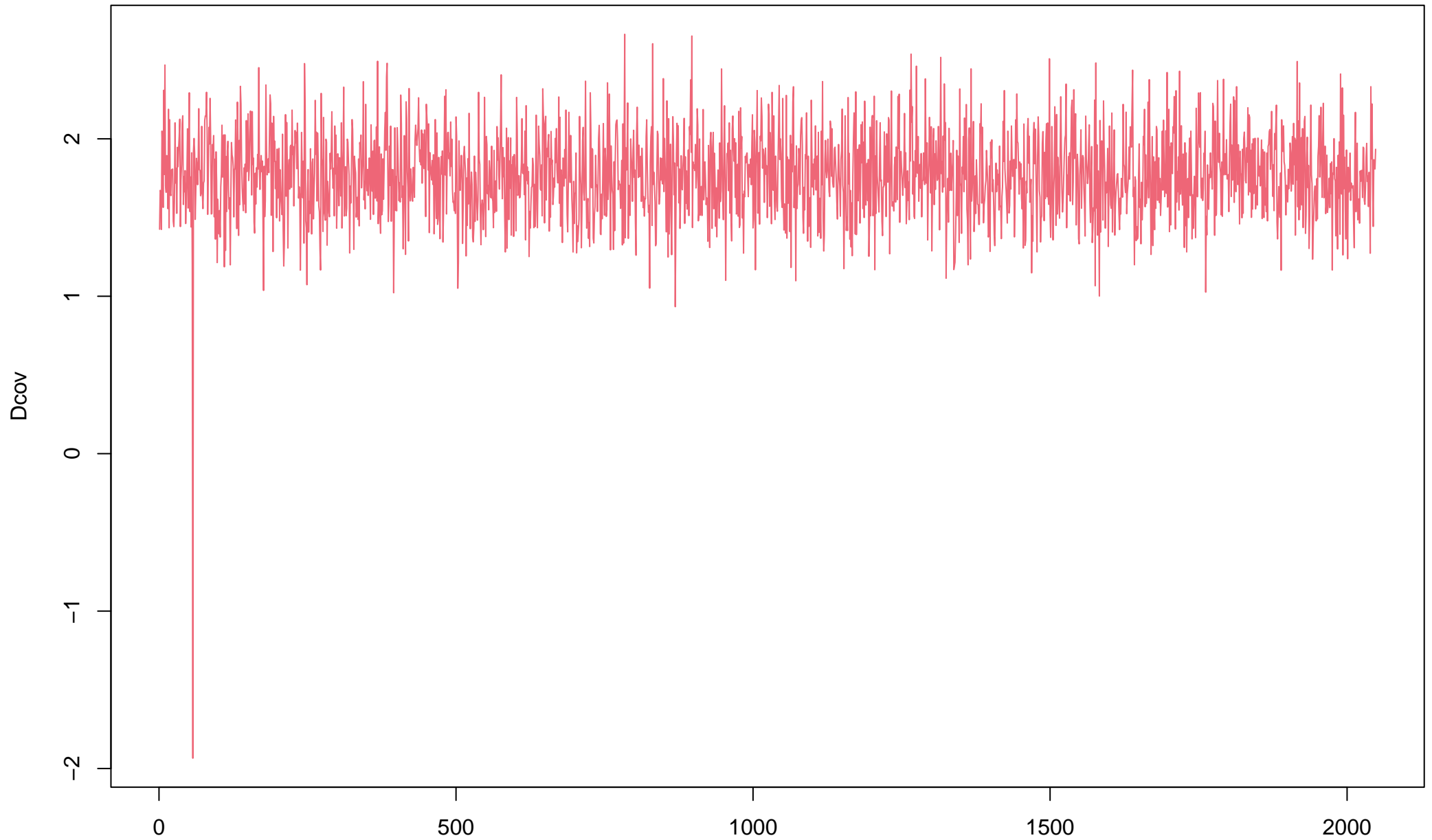
**Q3\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.628 | MCSE(6.27) = 2.2 | stat: FALSE | burn: 1632**



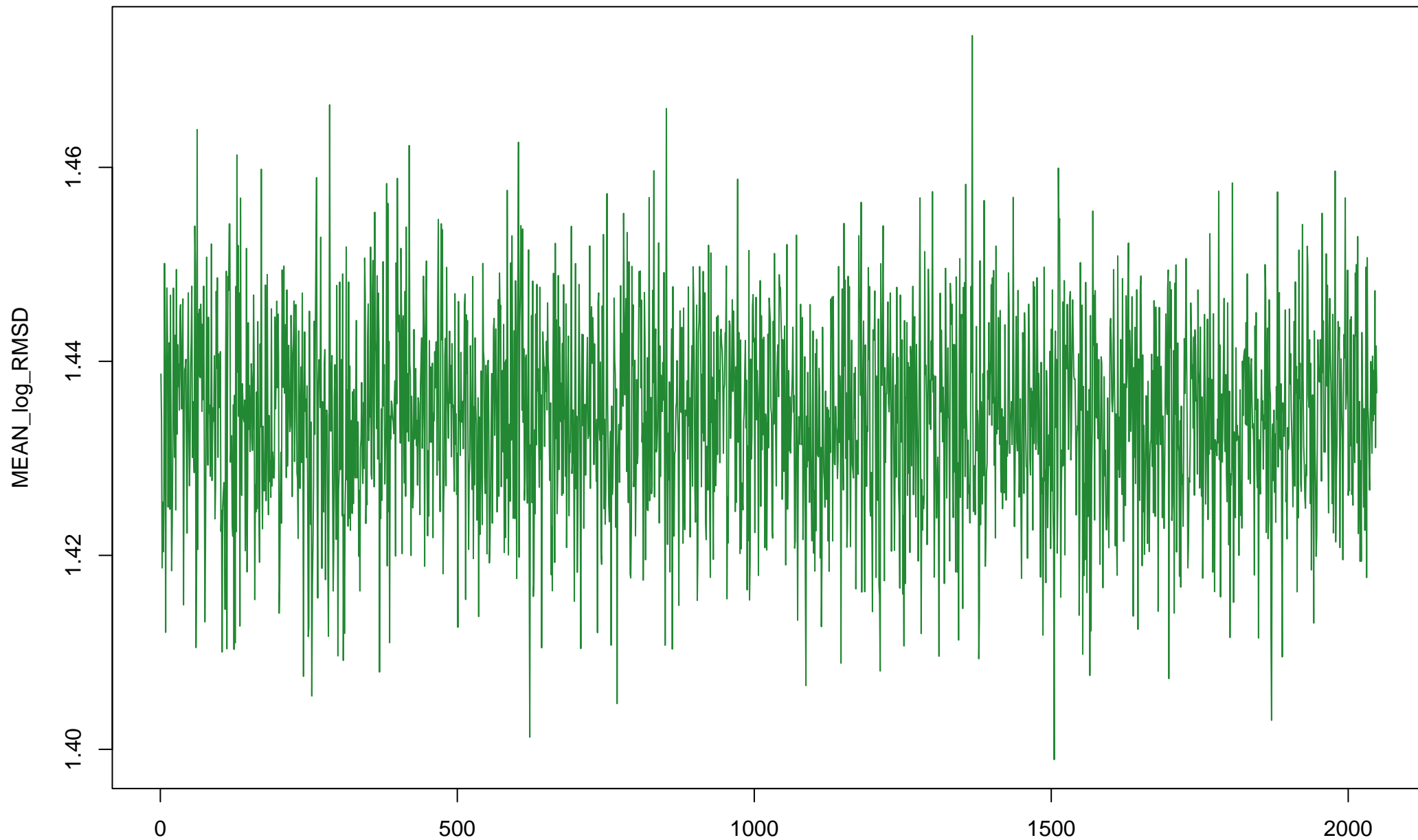
**Q3\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Dcov**  
**ESS = 2050 | BMK = 0.0481 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0**

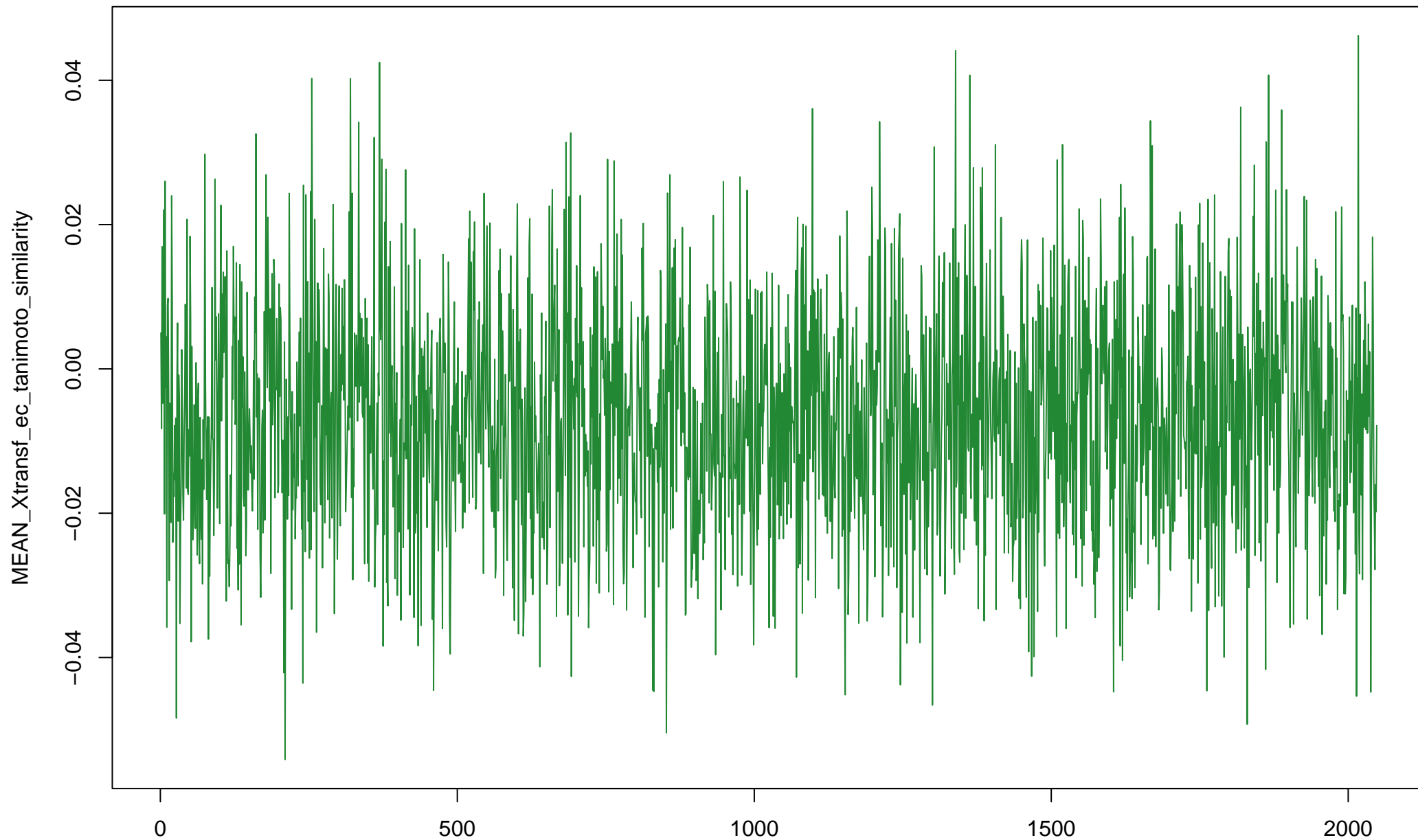


**MEAN\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0509 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0**

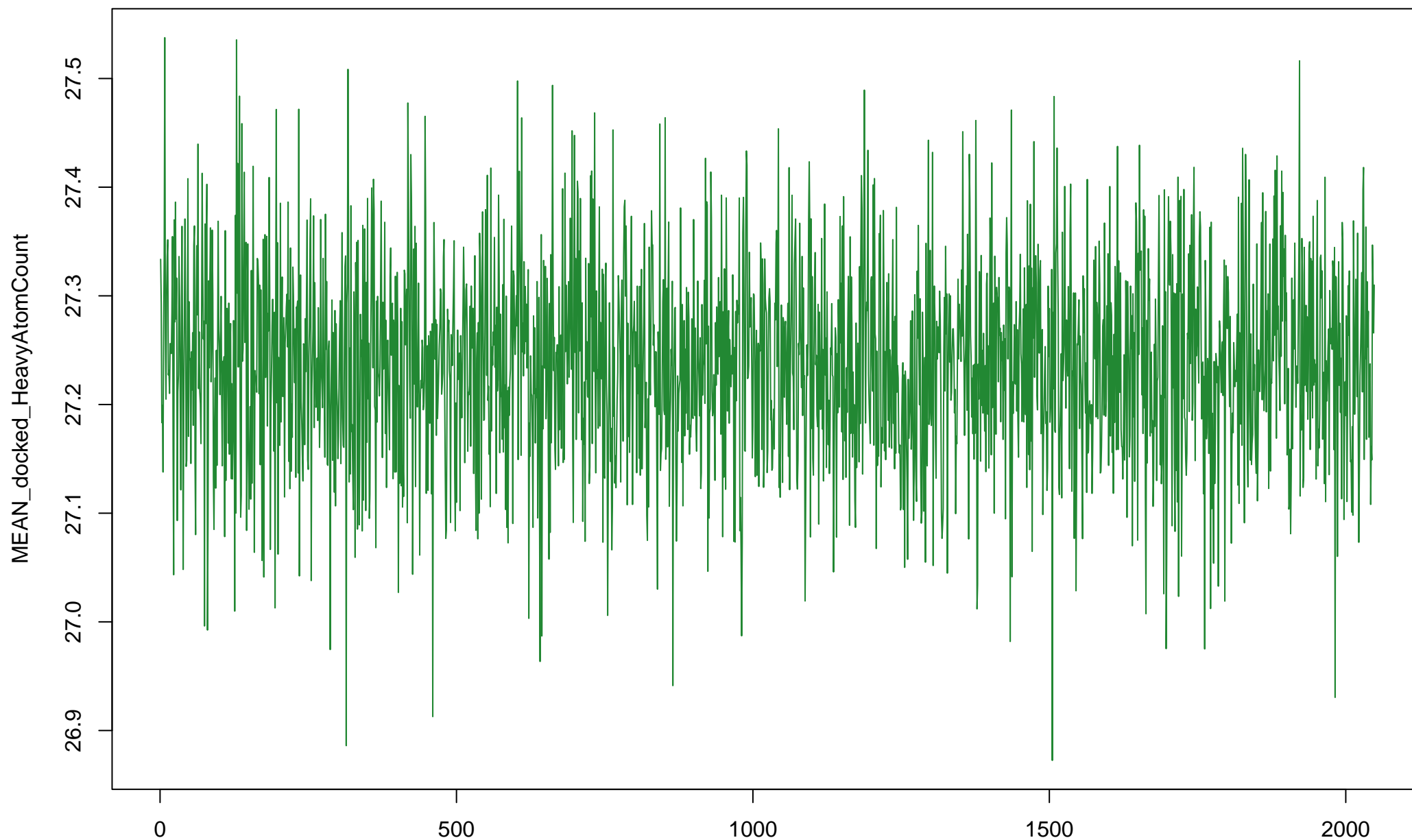




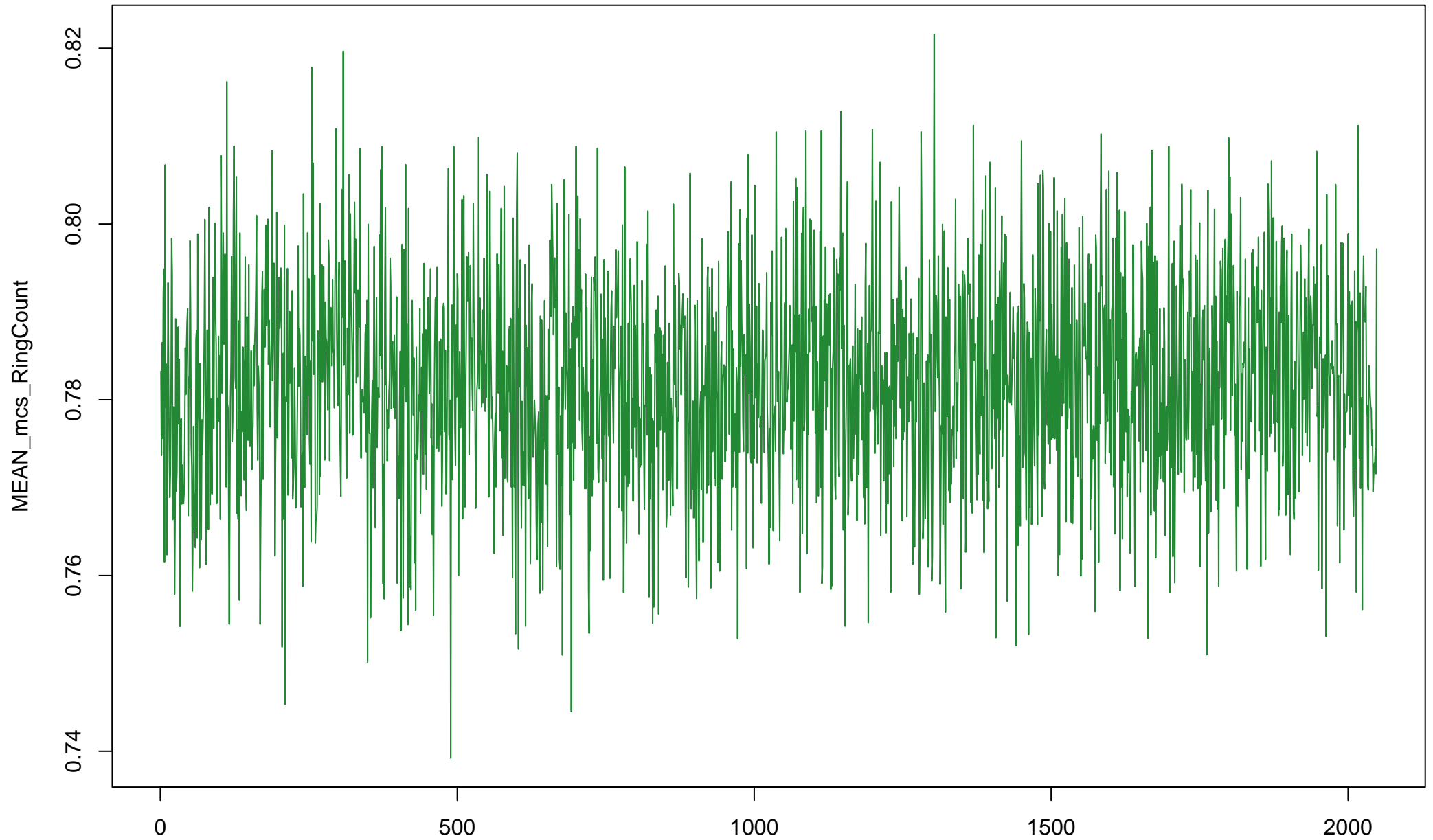
**MEAN\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1920 | BMK = 0.0335 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0**



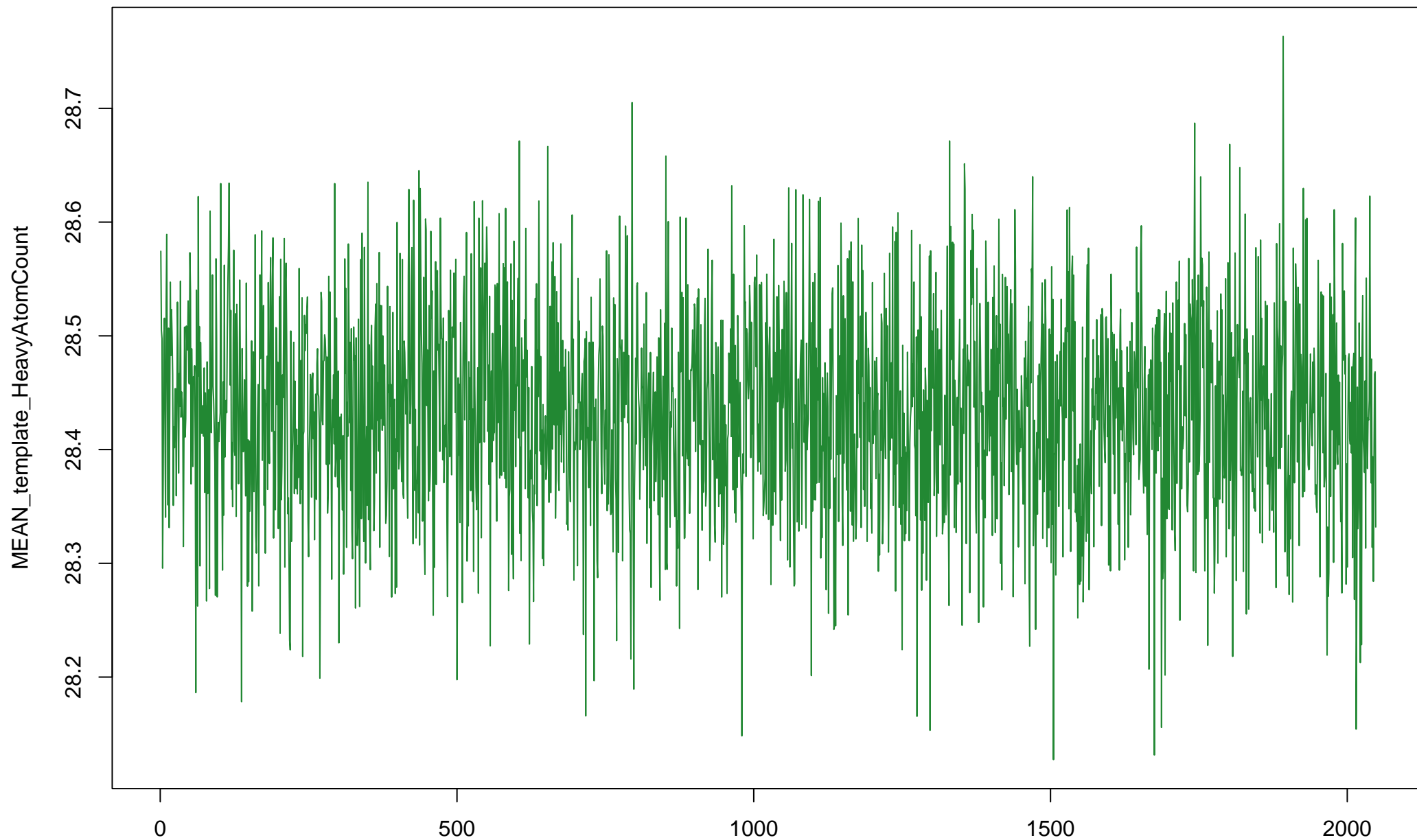
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0456 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0**



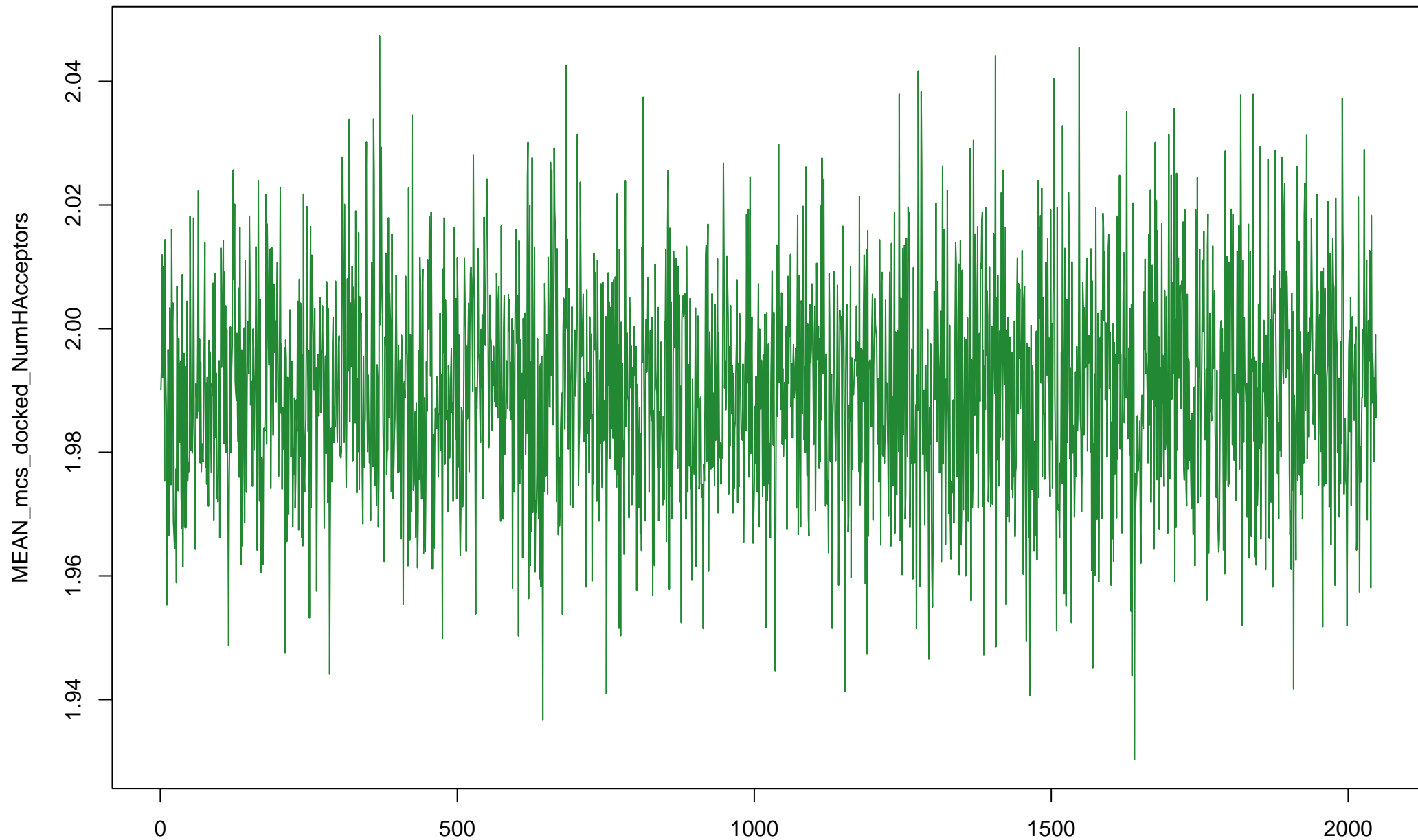
**MEAN\_mcs\_RingCount**  
**ESS = 1840 | BMK = 0.0516 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0**



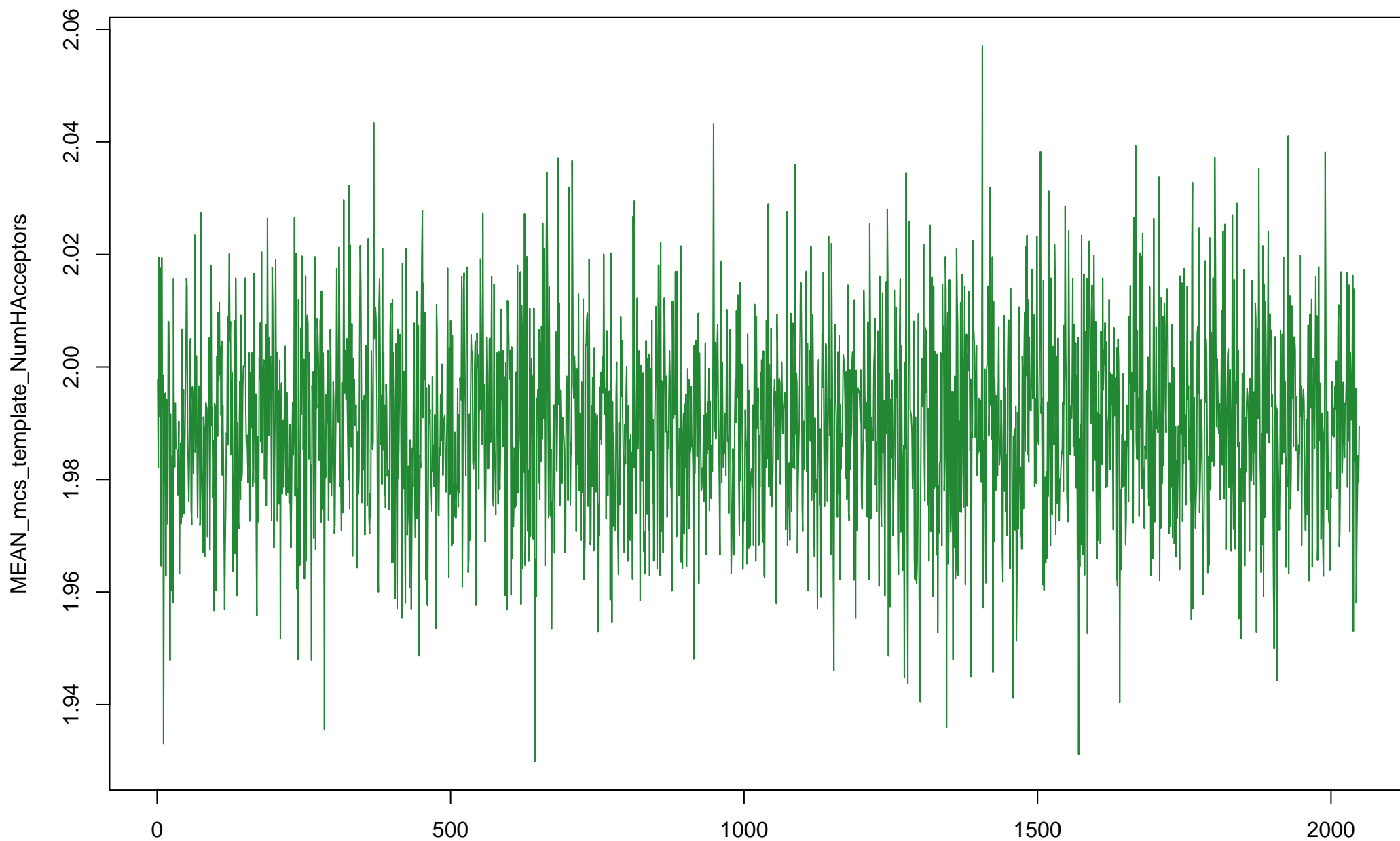
**MEAN\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0303 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0**



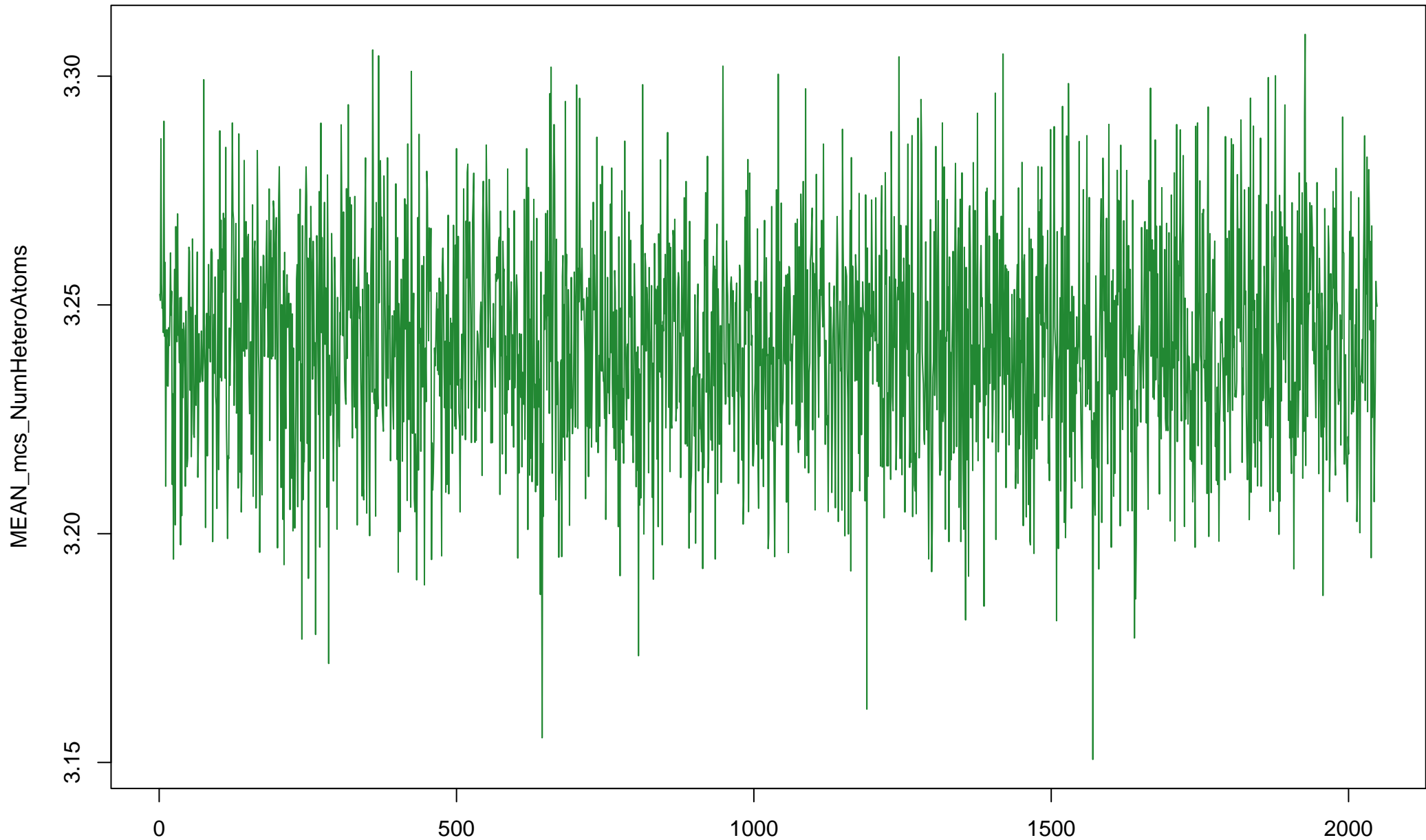
**MEAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 1700 | BMK = 0.0557 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0**



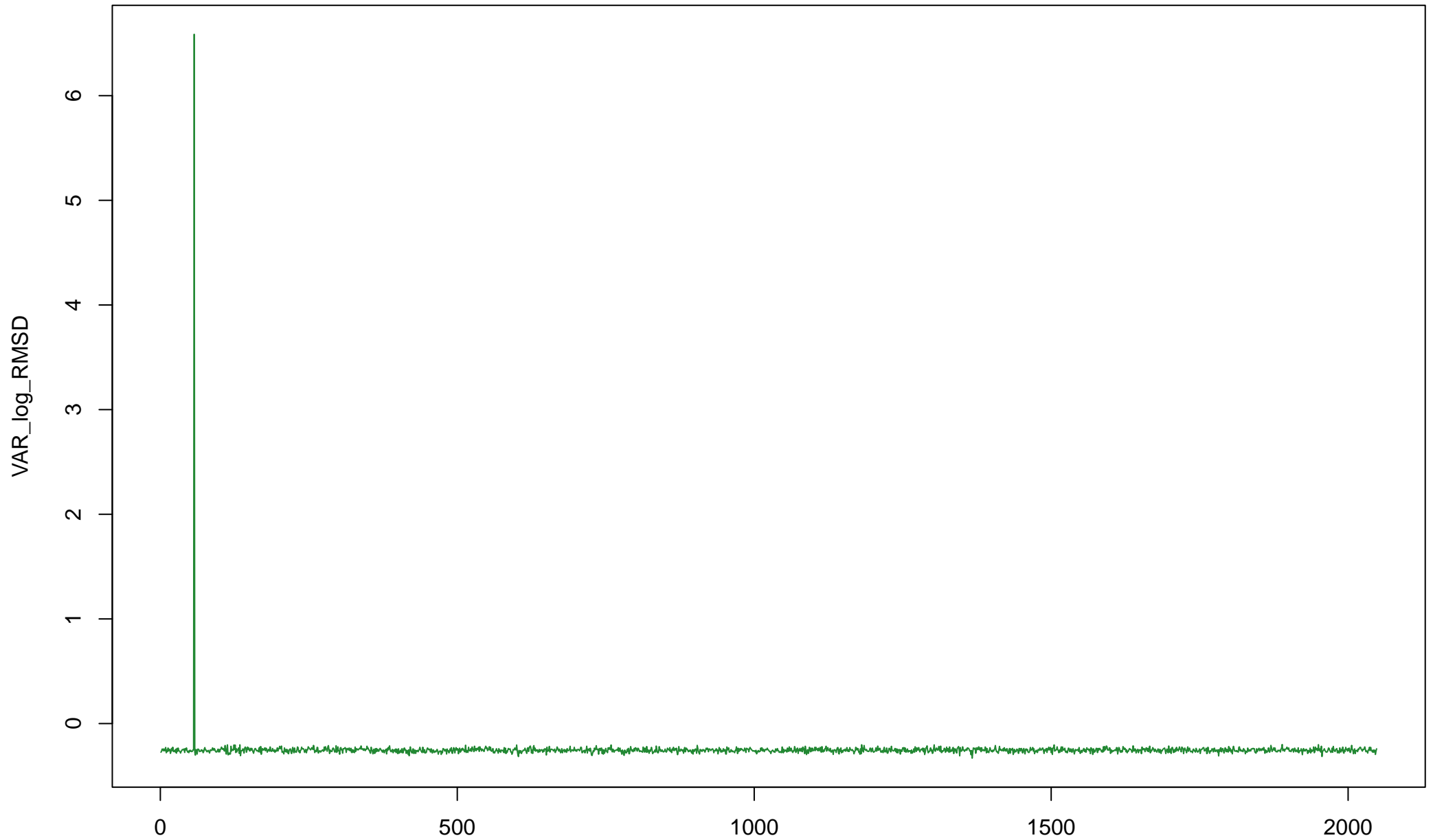
**MEAN\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0525 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0**



**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0413 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0**

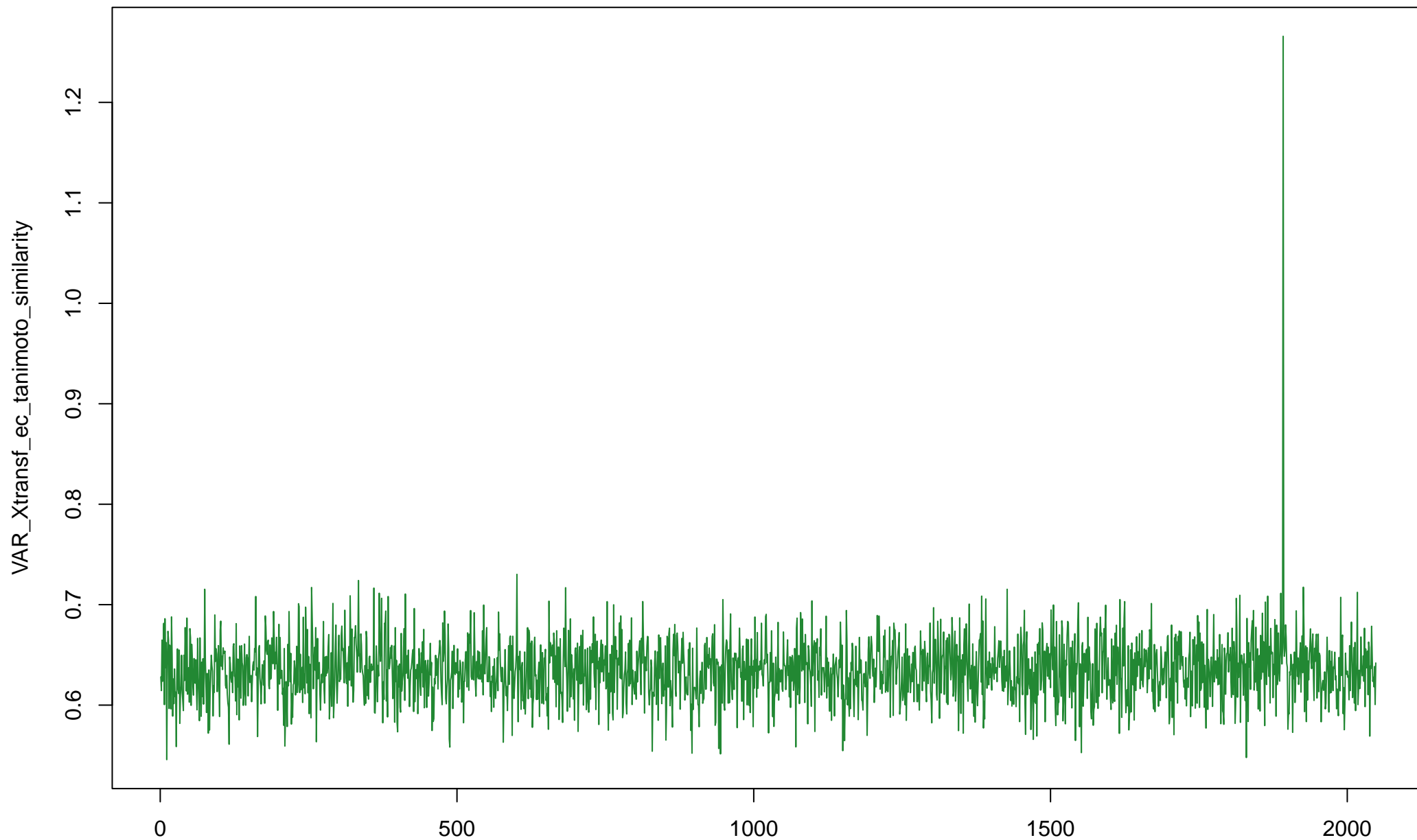


**VAR\_log\_RMSD**  
**ESS = 2050 | BMK = 0.243 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 204**

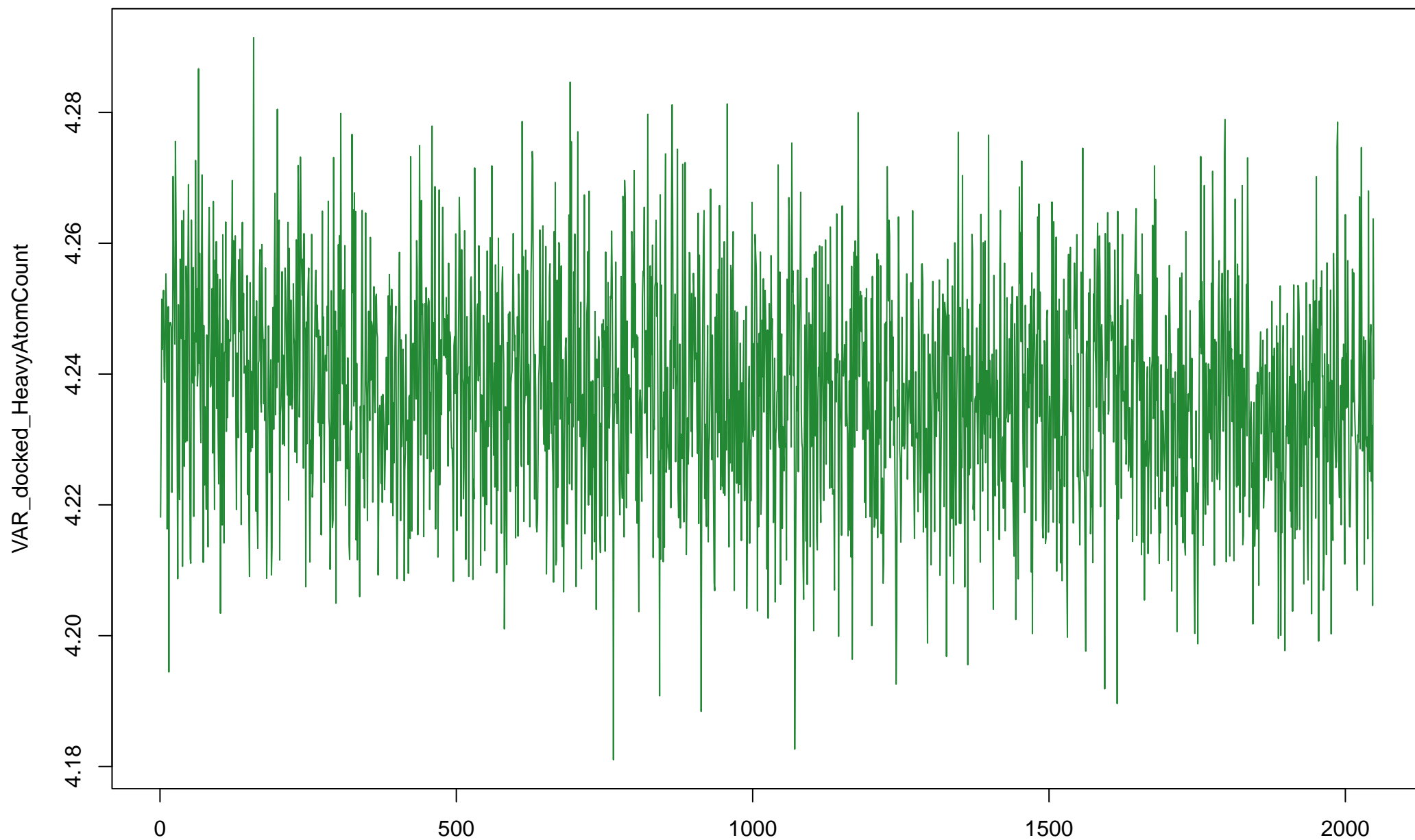




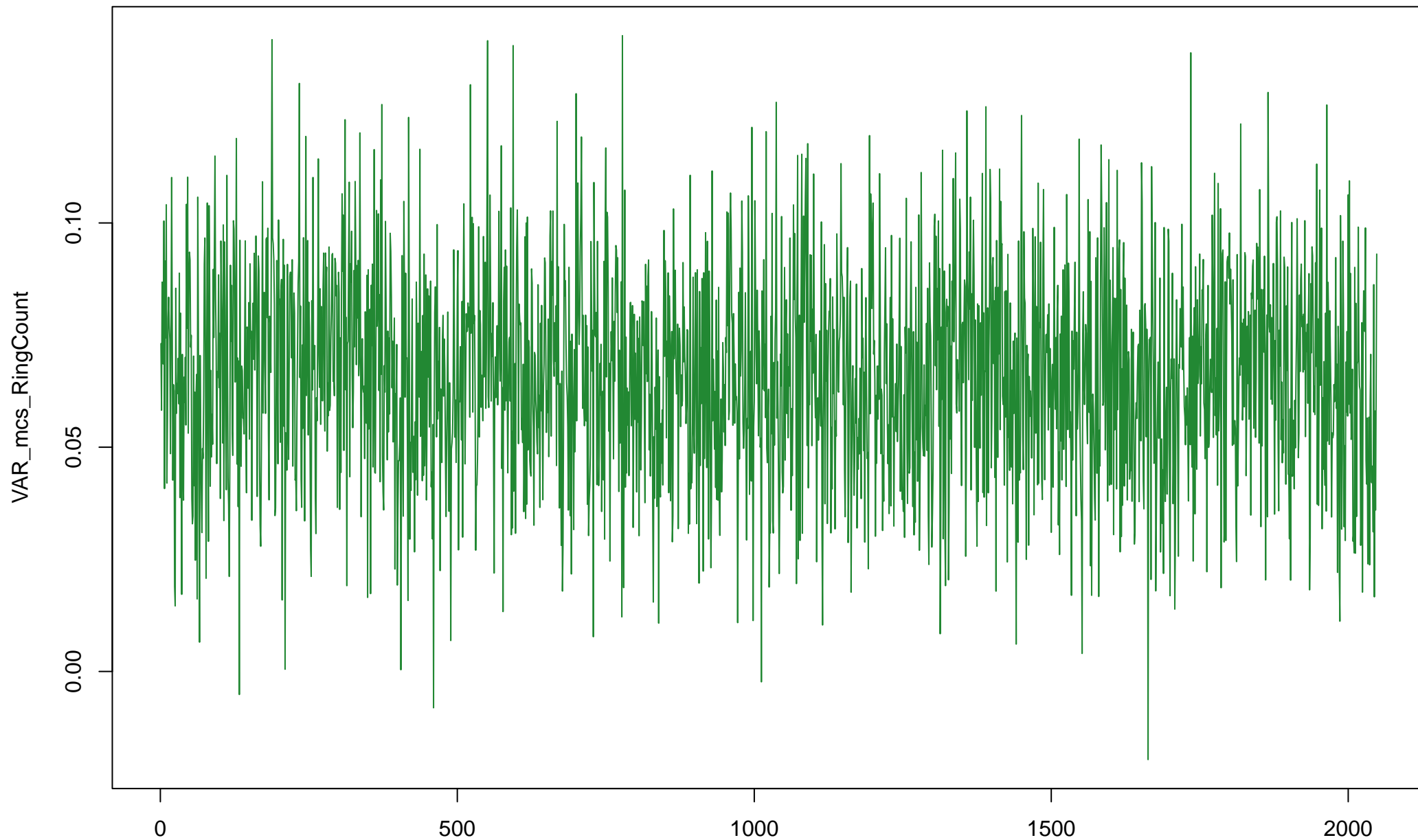
**VAR\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0374 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0**



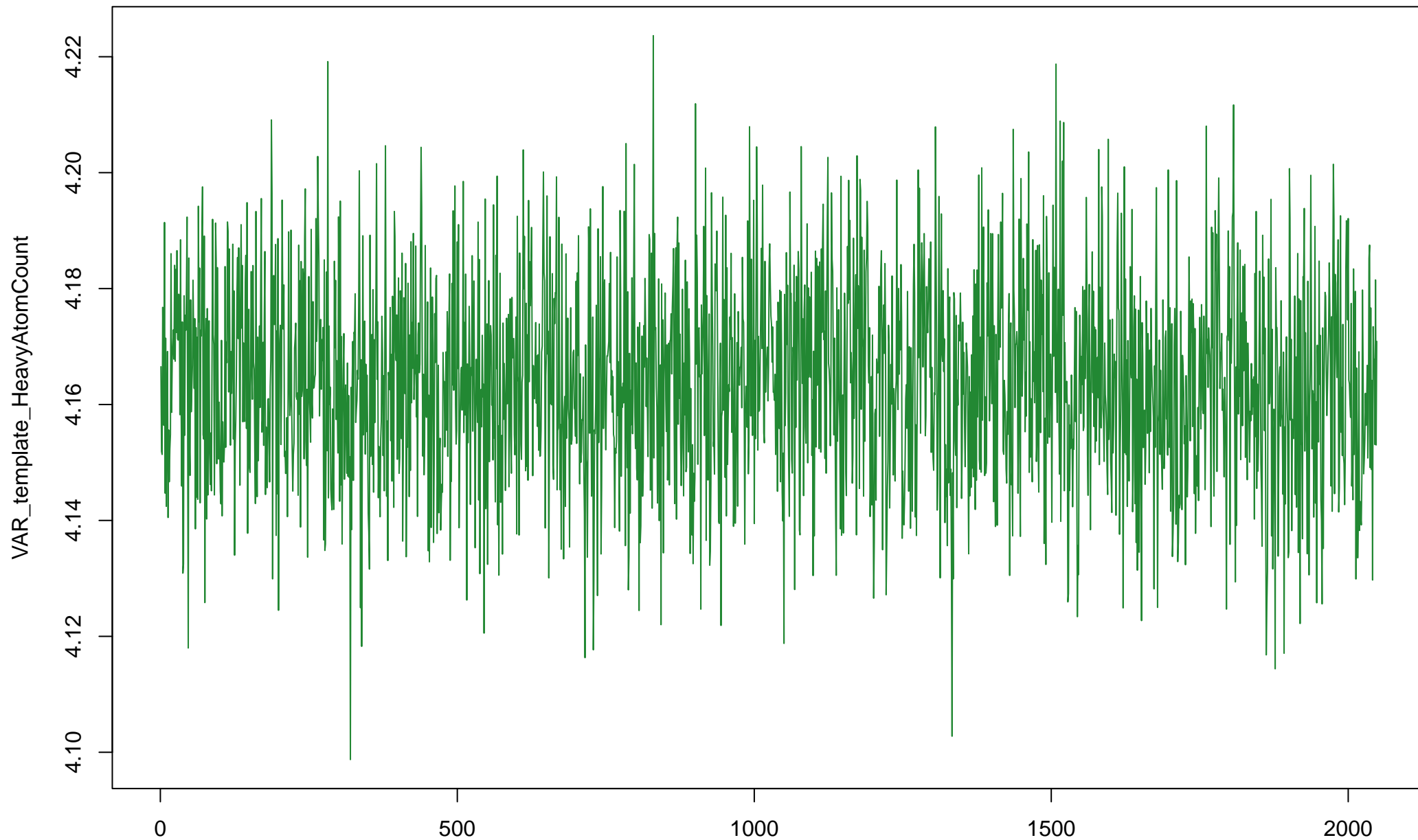
**VAR\_docked\_HeavyAtomCount**  
**ESS = 1700 | BMK = 0.089 | MCSE(6.27) = 3 | stat: FALSE | burn: 0**



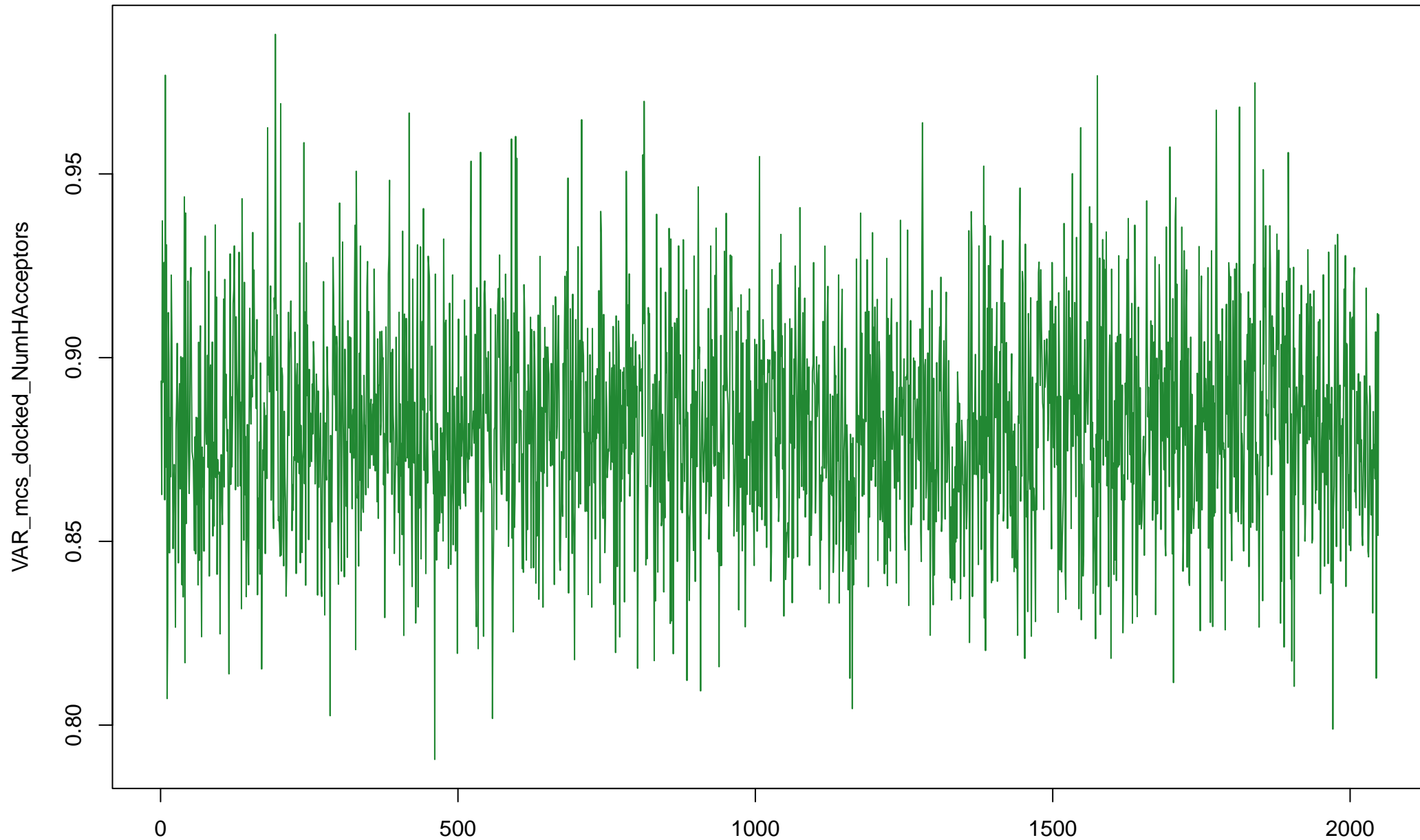
**VAR\_mcs\_RingCount**  
**ESS = 1900 | BMK = 0.0522 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0**



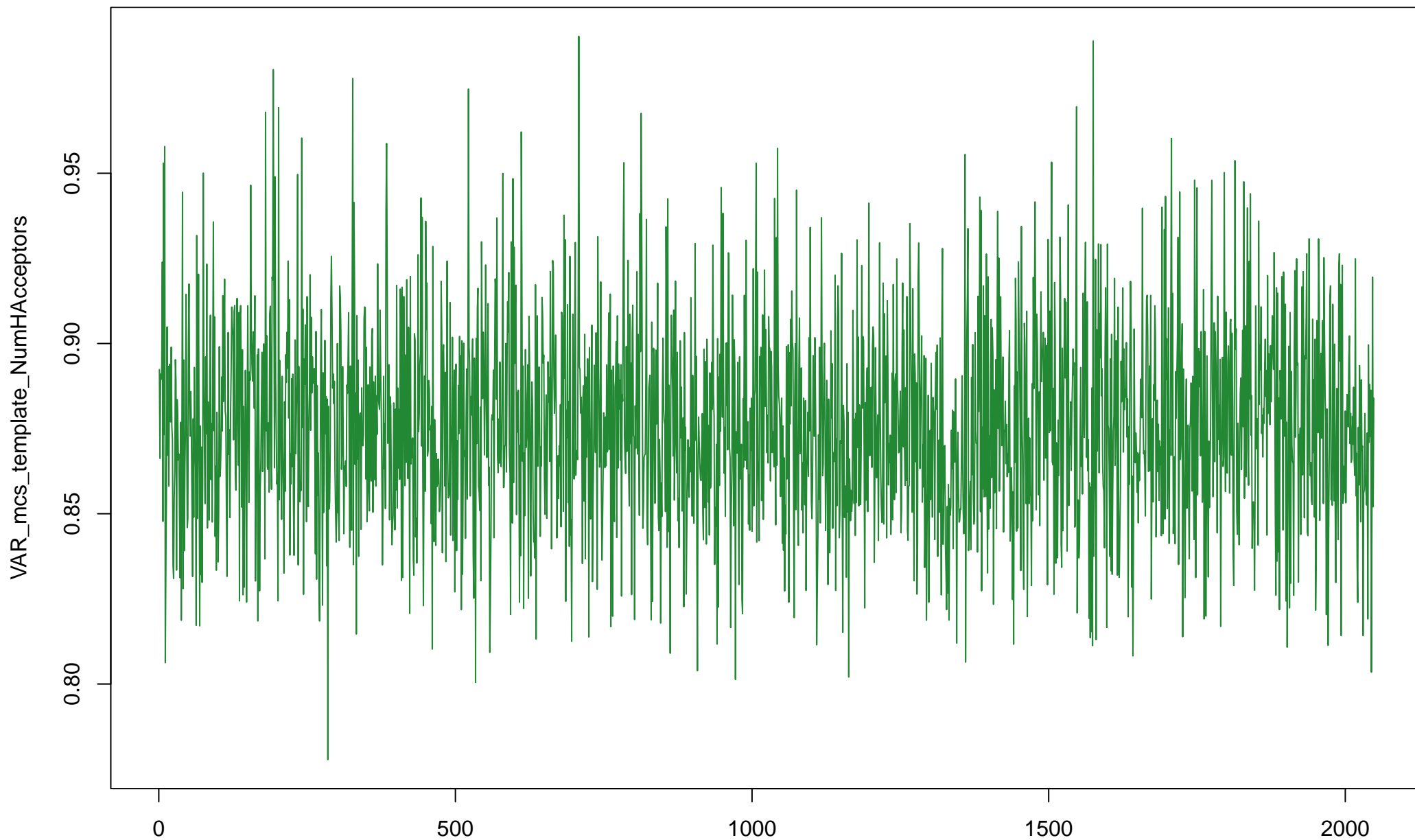
**VAR\_template\_HeavyAtomCount**  
**ESS = 1500 | BMK = 0.0372 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0**



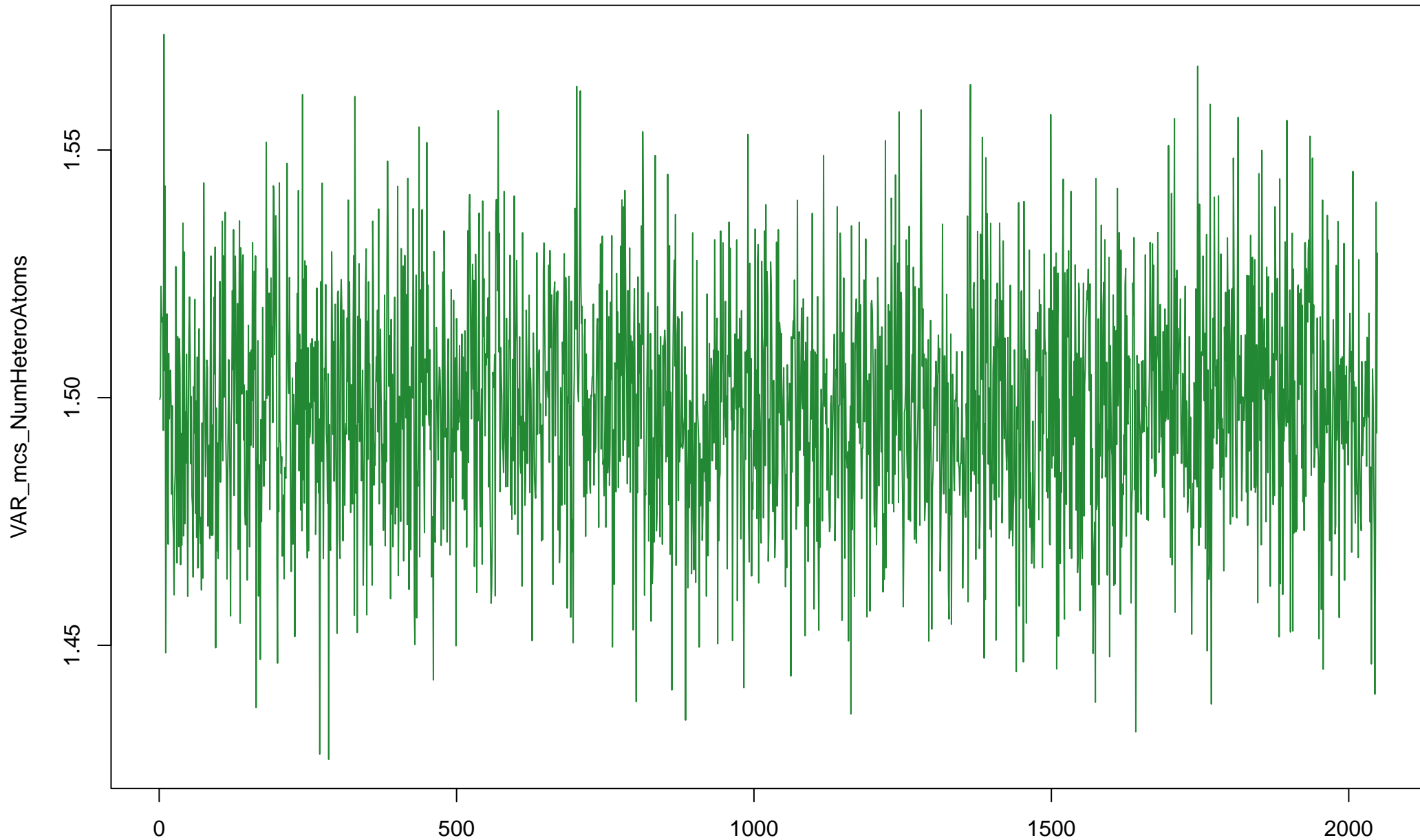
**VAR\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0447 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0**



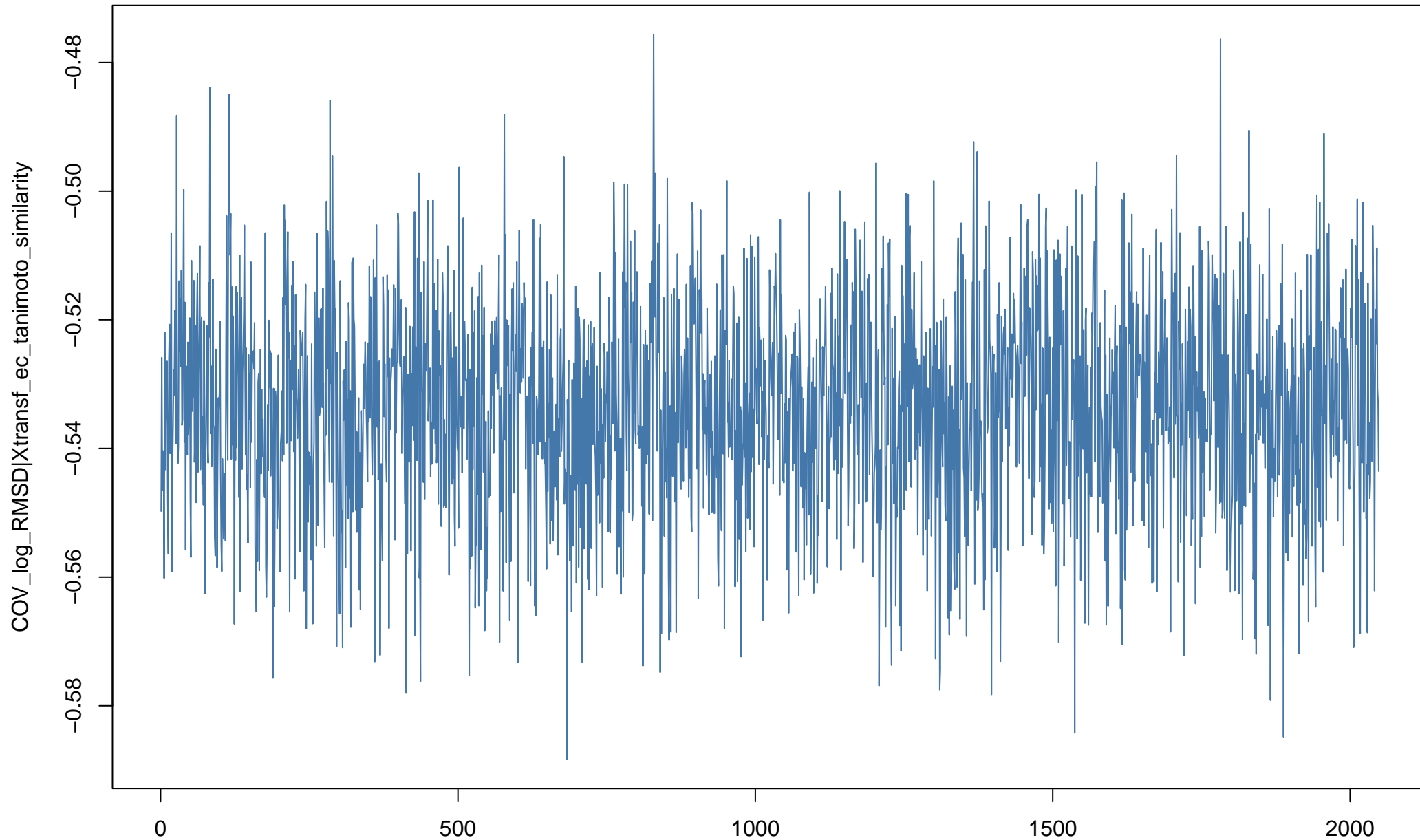
**VAR\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0427 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0**



**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 1640 | BMK = 0.0292 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0**

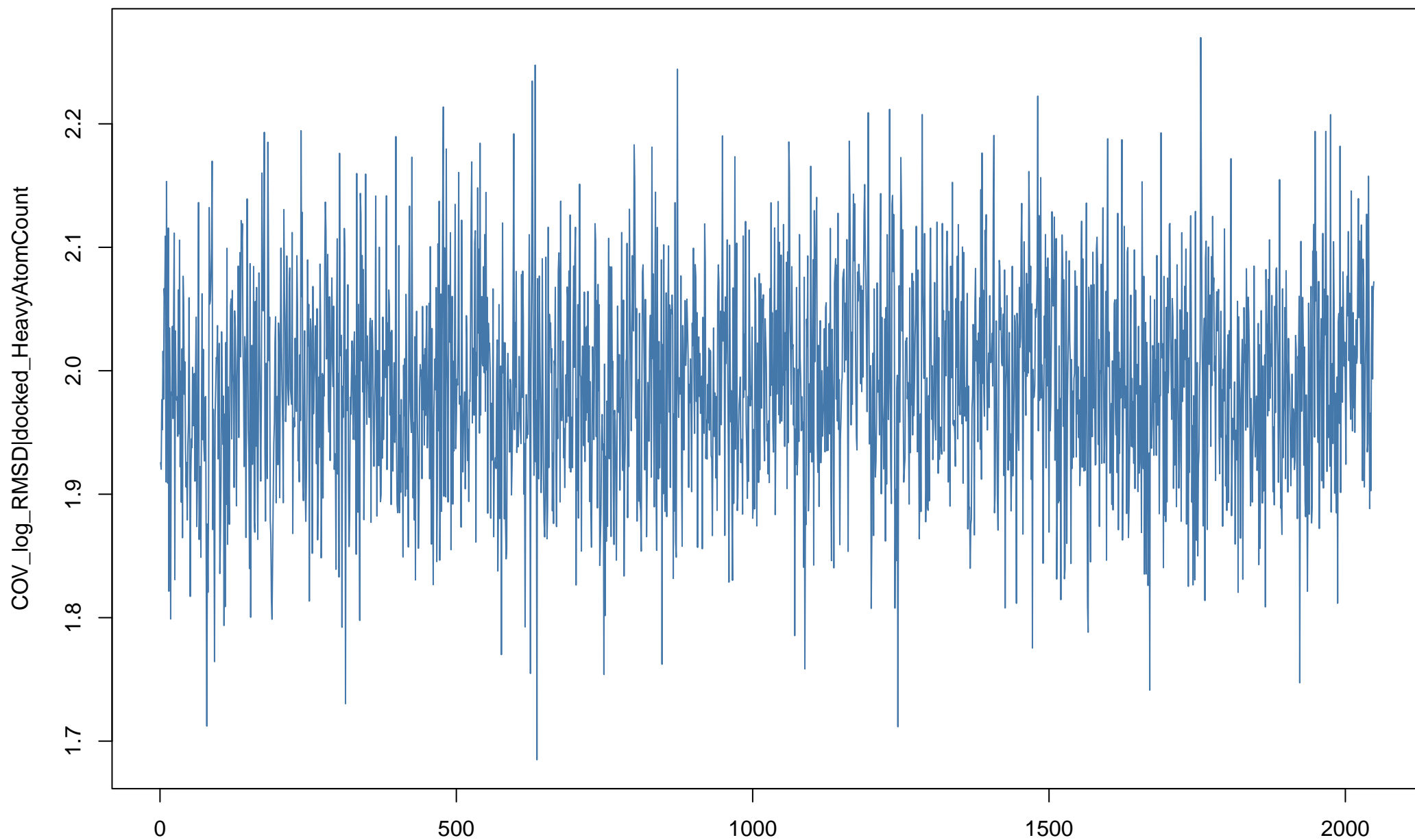


**COV\_log\_RMSD|Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1510 | BMK = 0.0403 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0**

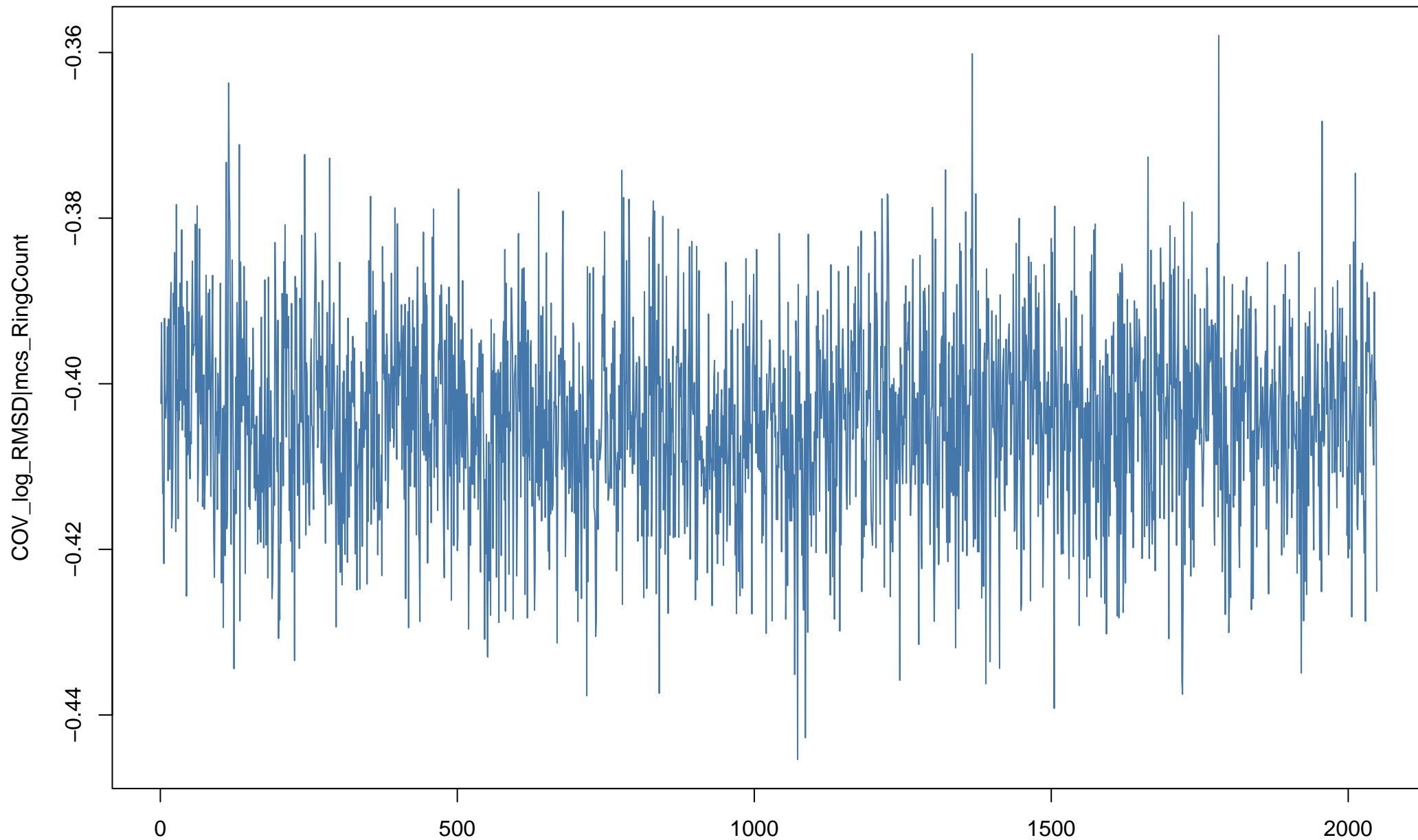




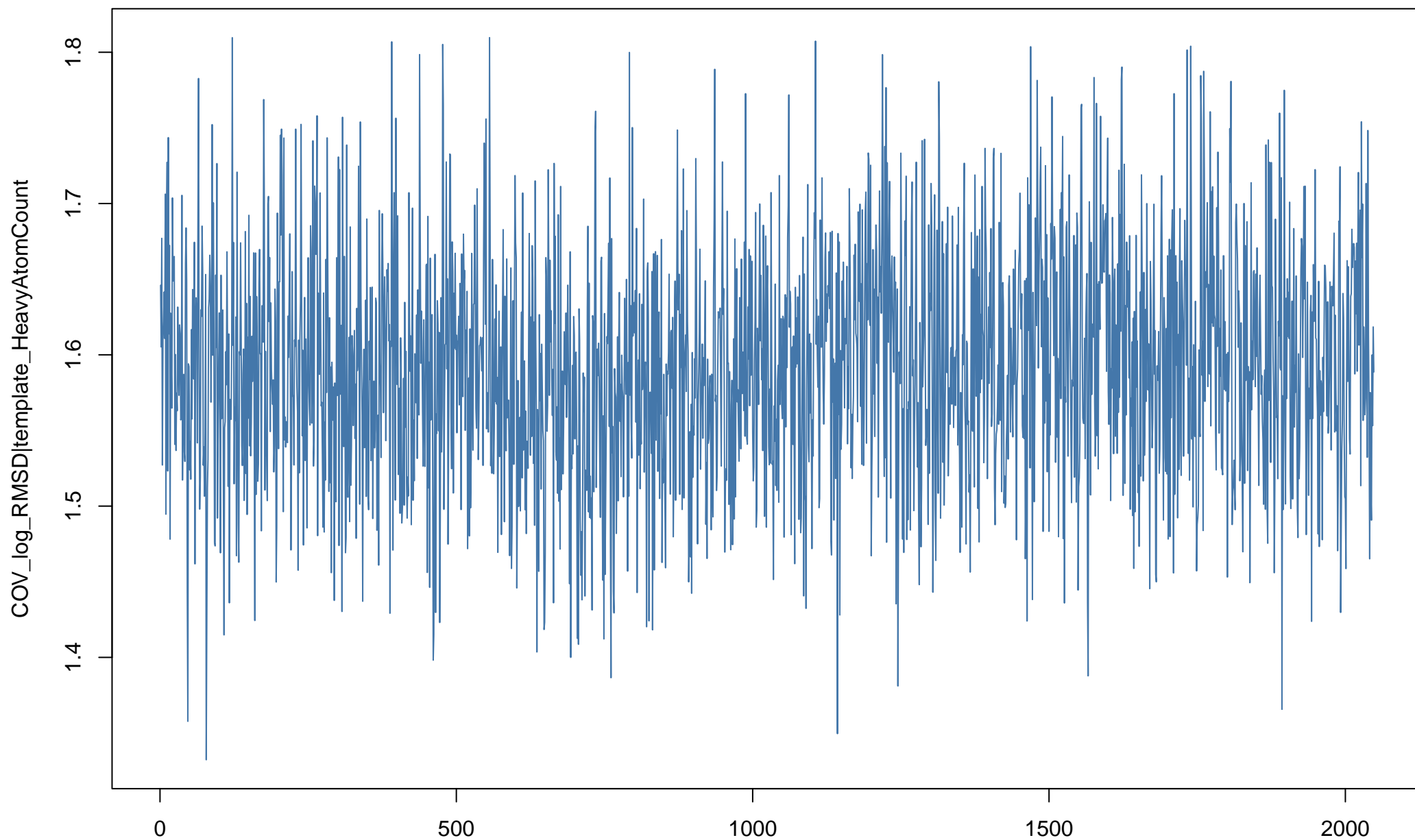
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 1720 | BMK = 0.0574 | MCSE(6.27) = 2.62 | stat: FALSE | burn: 0**



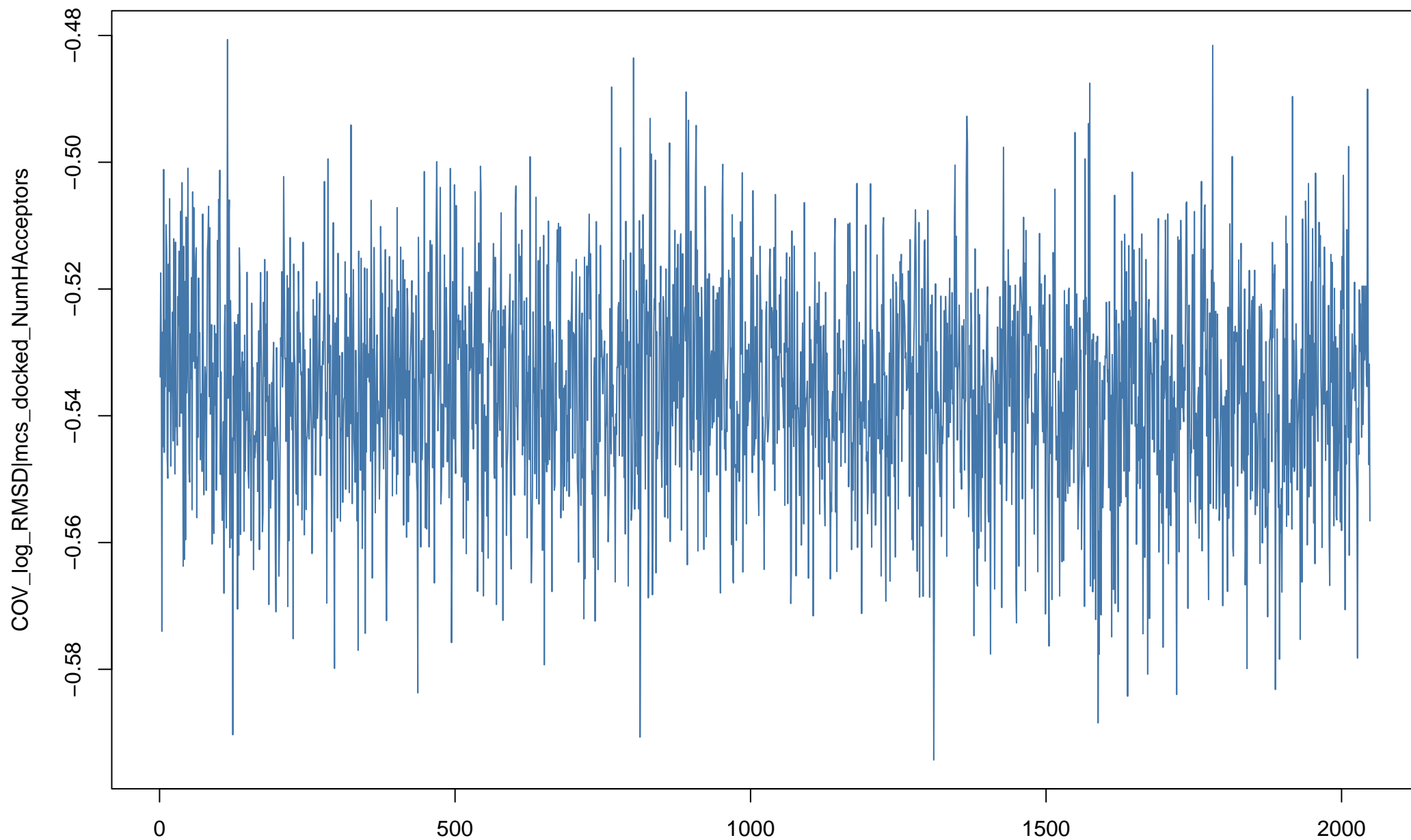
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 1380 | BMK = 0.0526 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0**



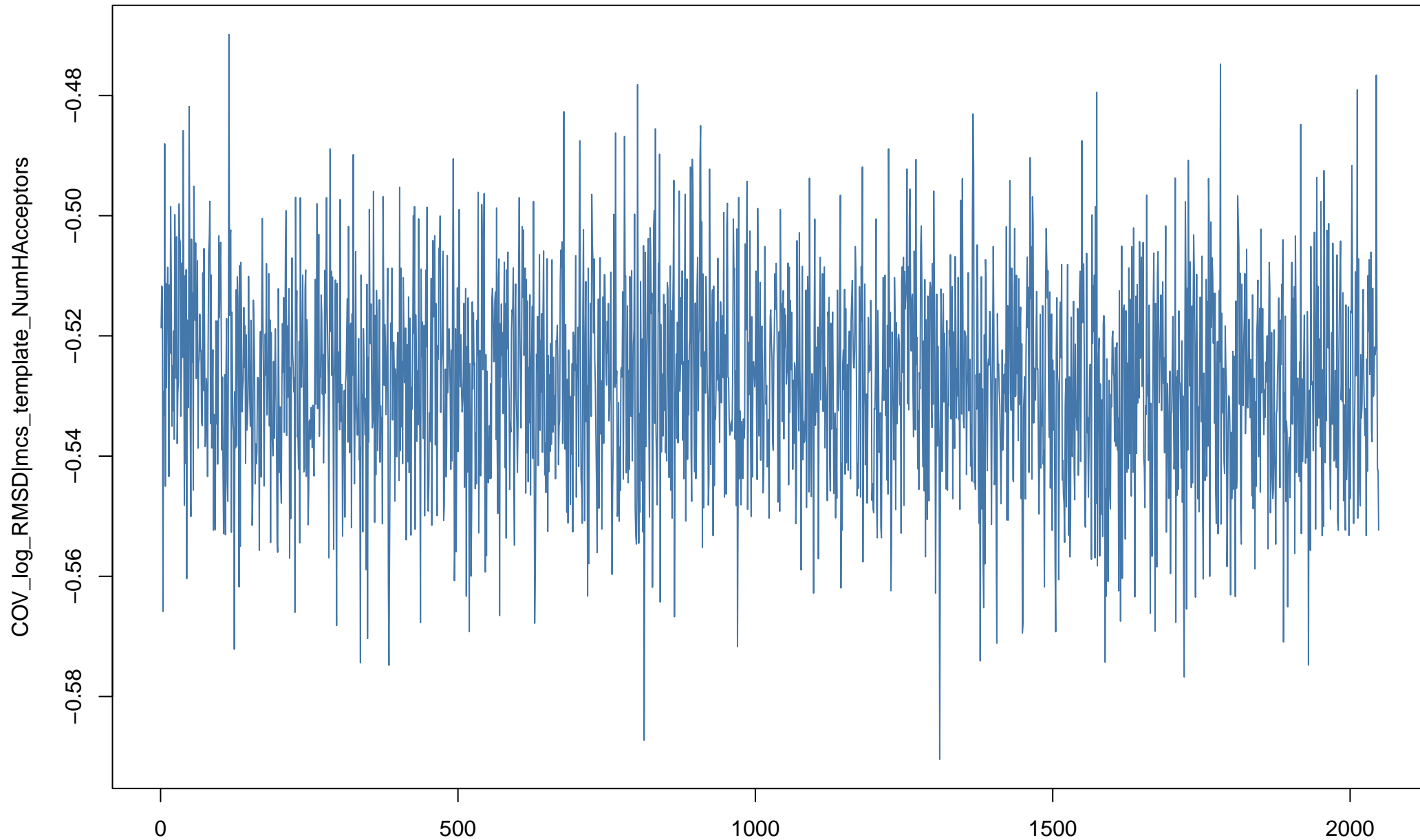
COV\_log\_RMSD|template\_HeavyAtomCount  
ESS = 1580 | BMK = 0.0893 | MCSE(6.27) = 3.22 | stat: TRUE | burn: 0



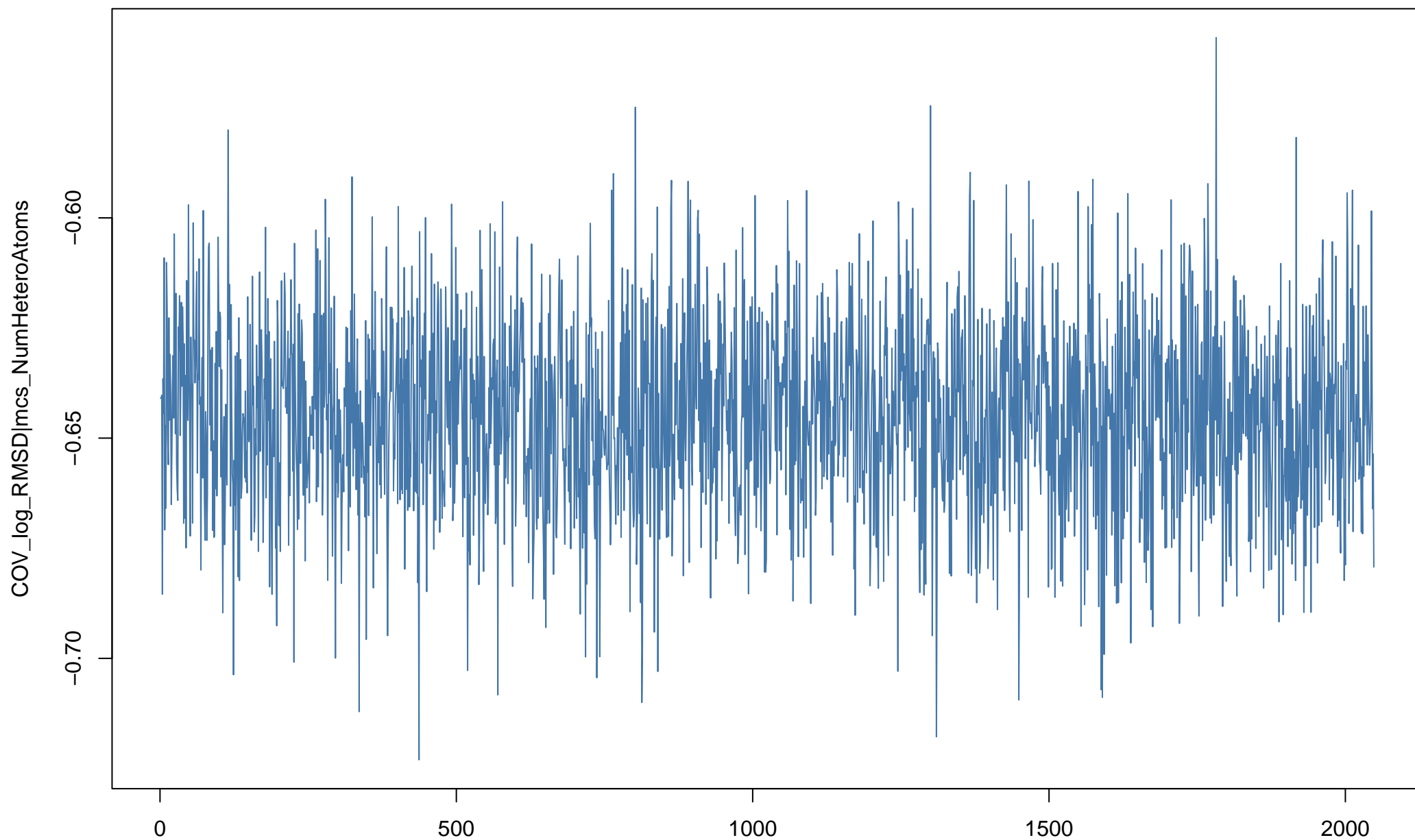
**COV\_log\_RMSD|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0532 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0**



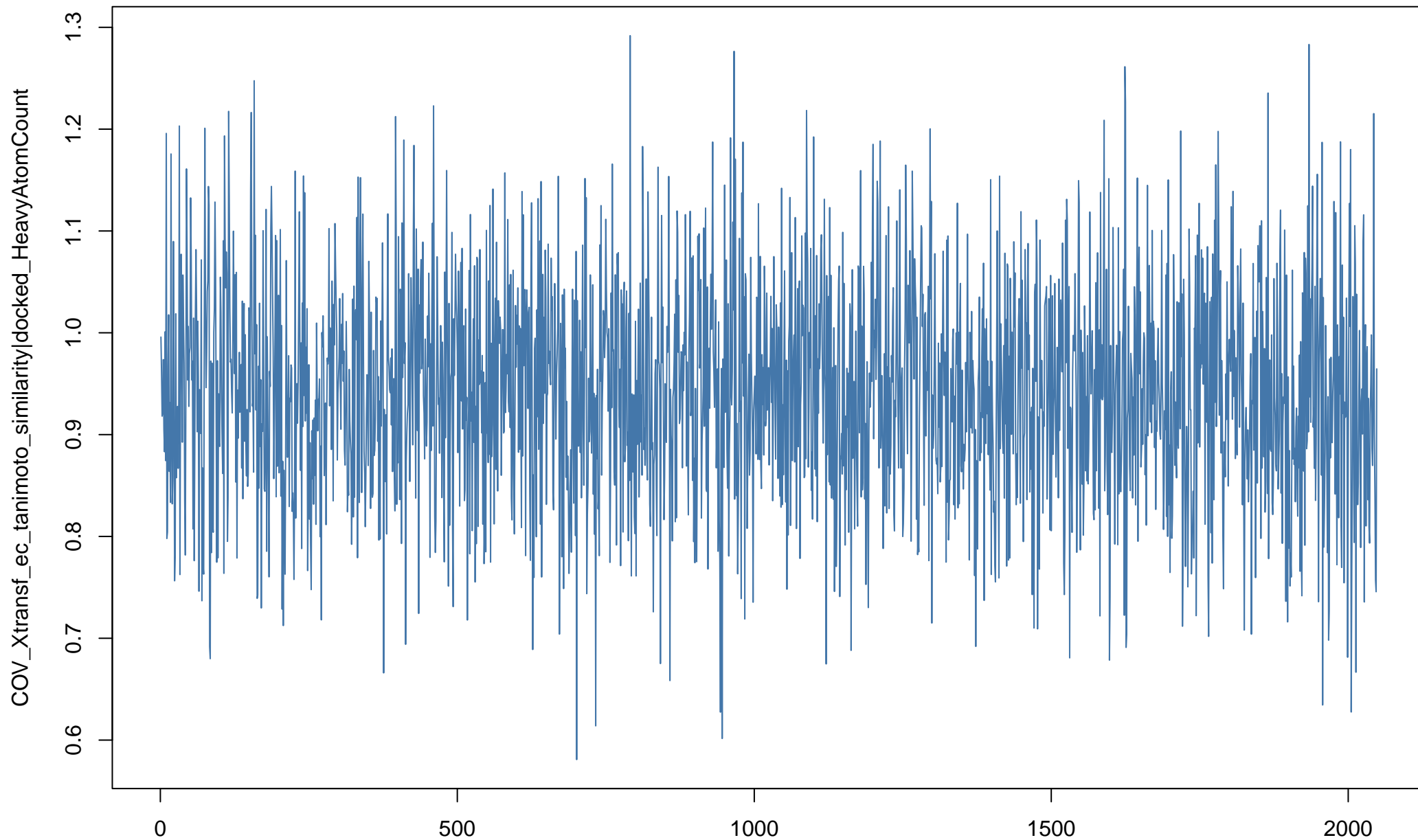
**COV\_log\_RMSD|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0474 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0**



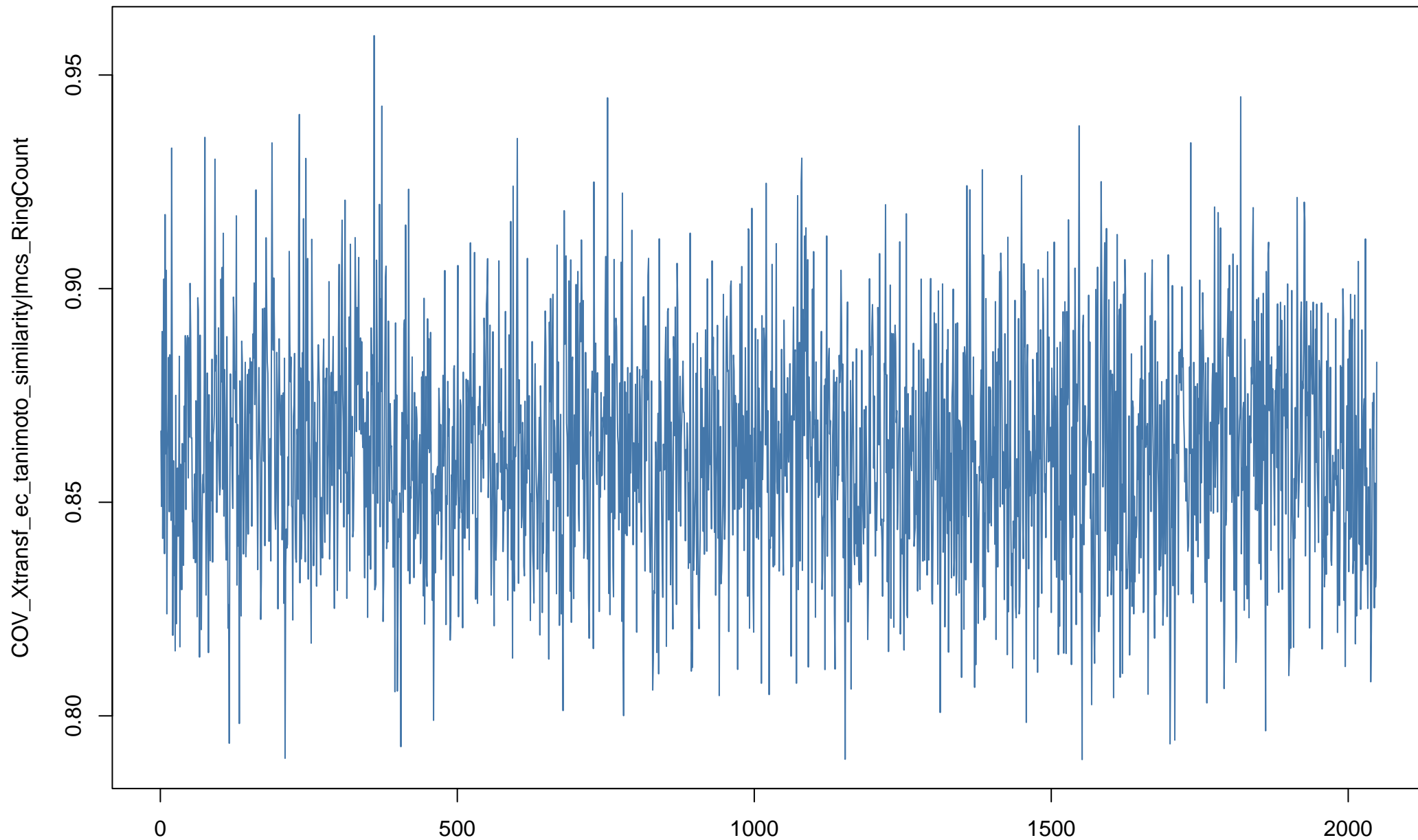
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.05 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0**



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

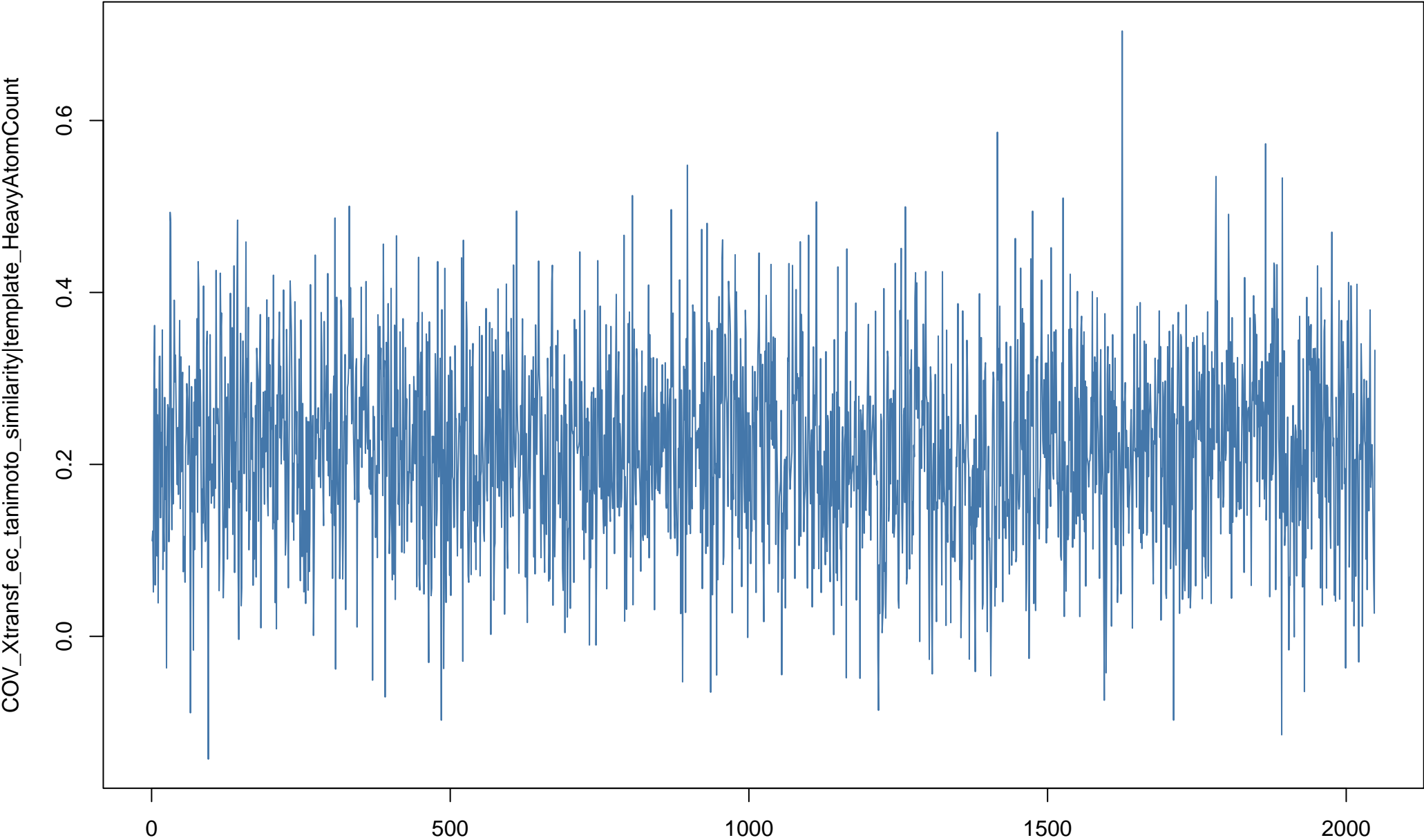


**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 1860 | BMK = 0.0525 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0**

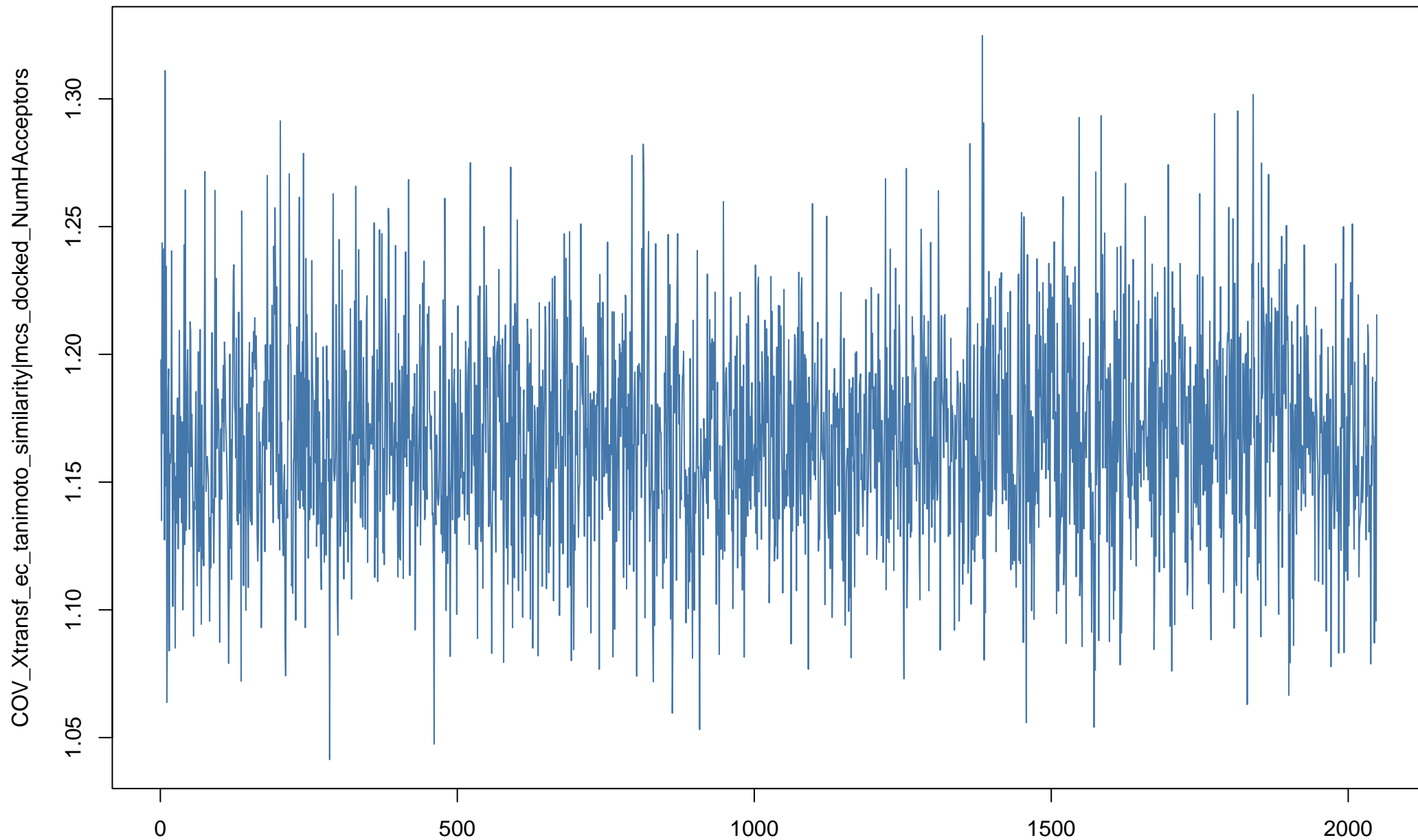




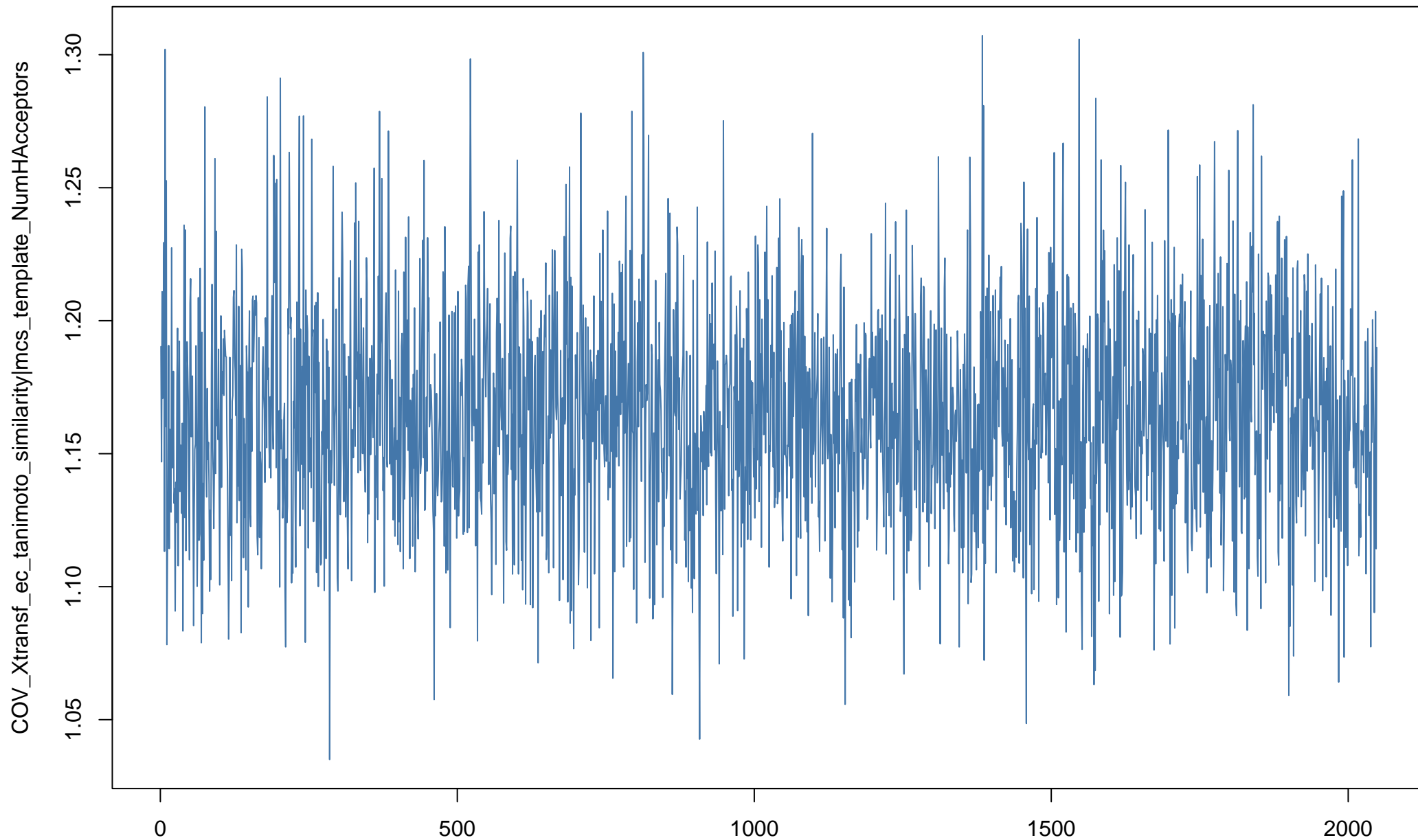
COV\_Xtransf\_ec\_tanimoto\_similarity|template\_HeavyAtomCount  
ESS = 2050 | BMK = 0.046 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0



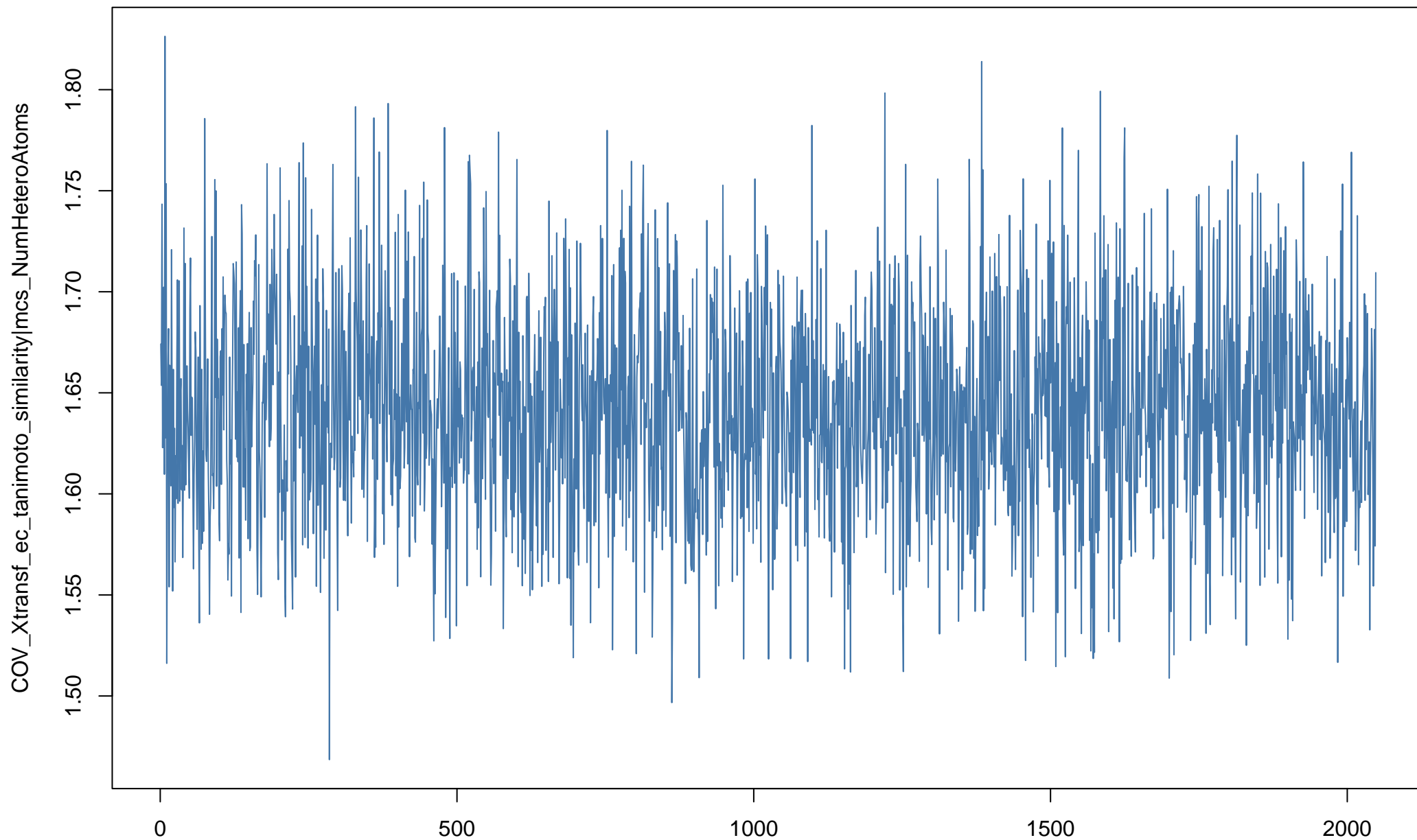
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0419 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0**



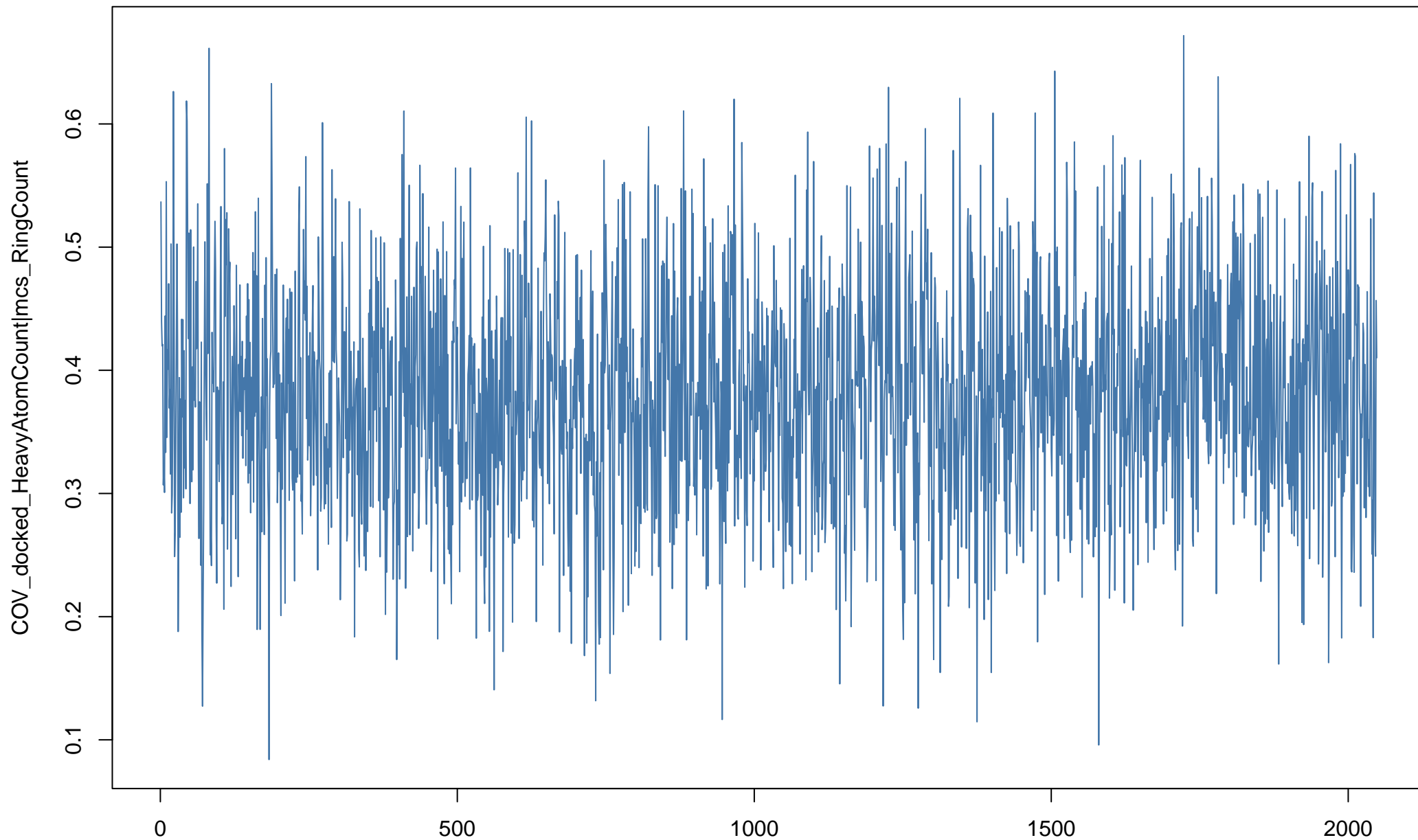
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0299 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0**



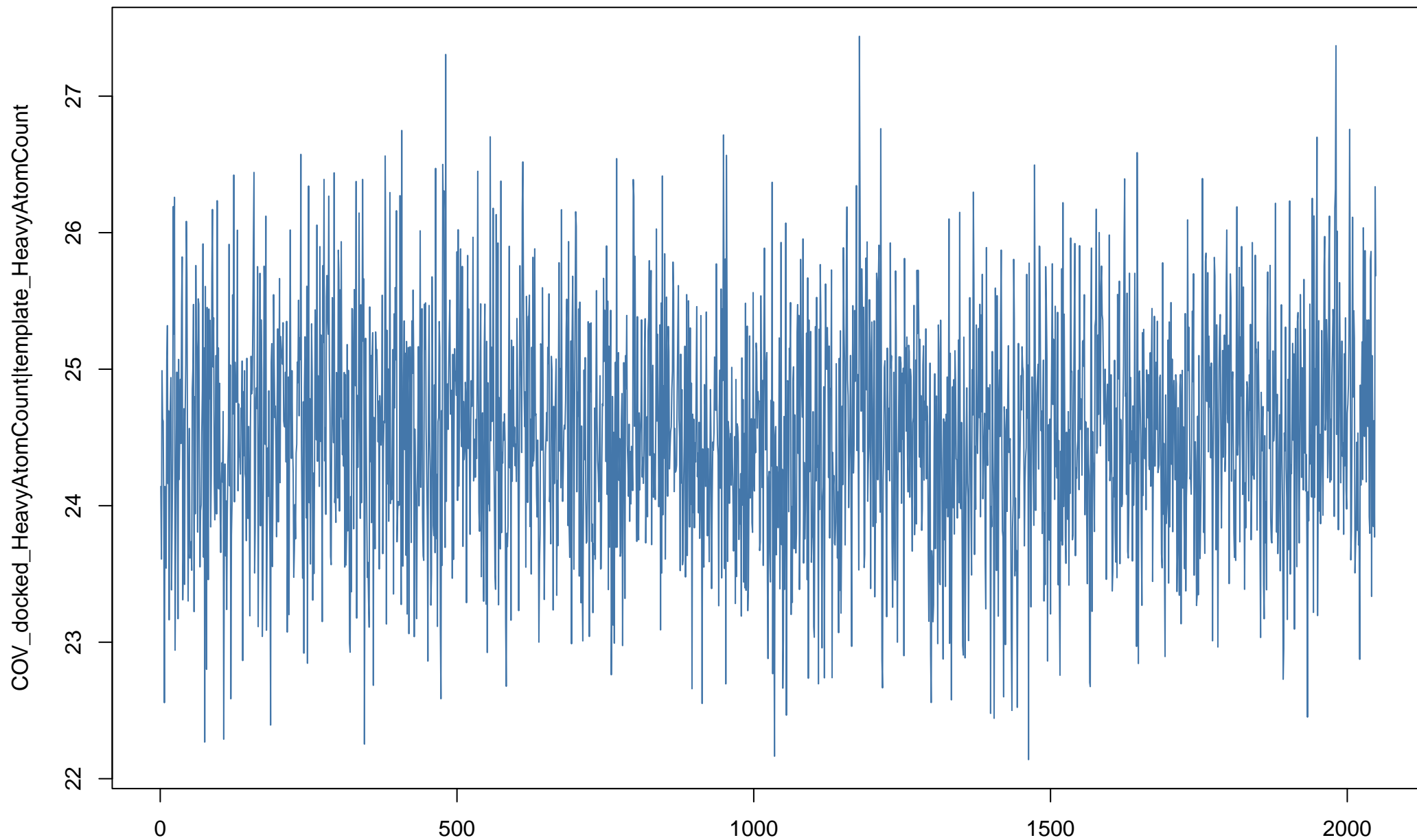
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0441 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0**



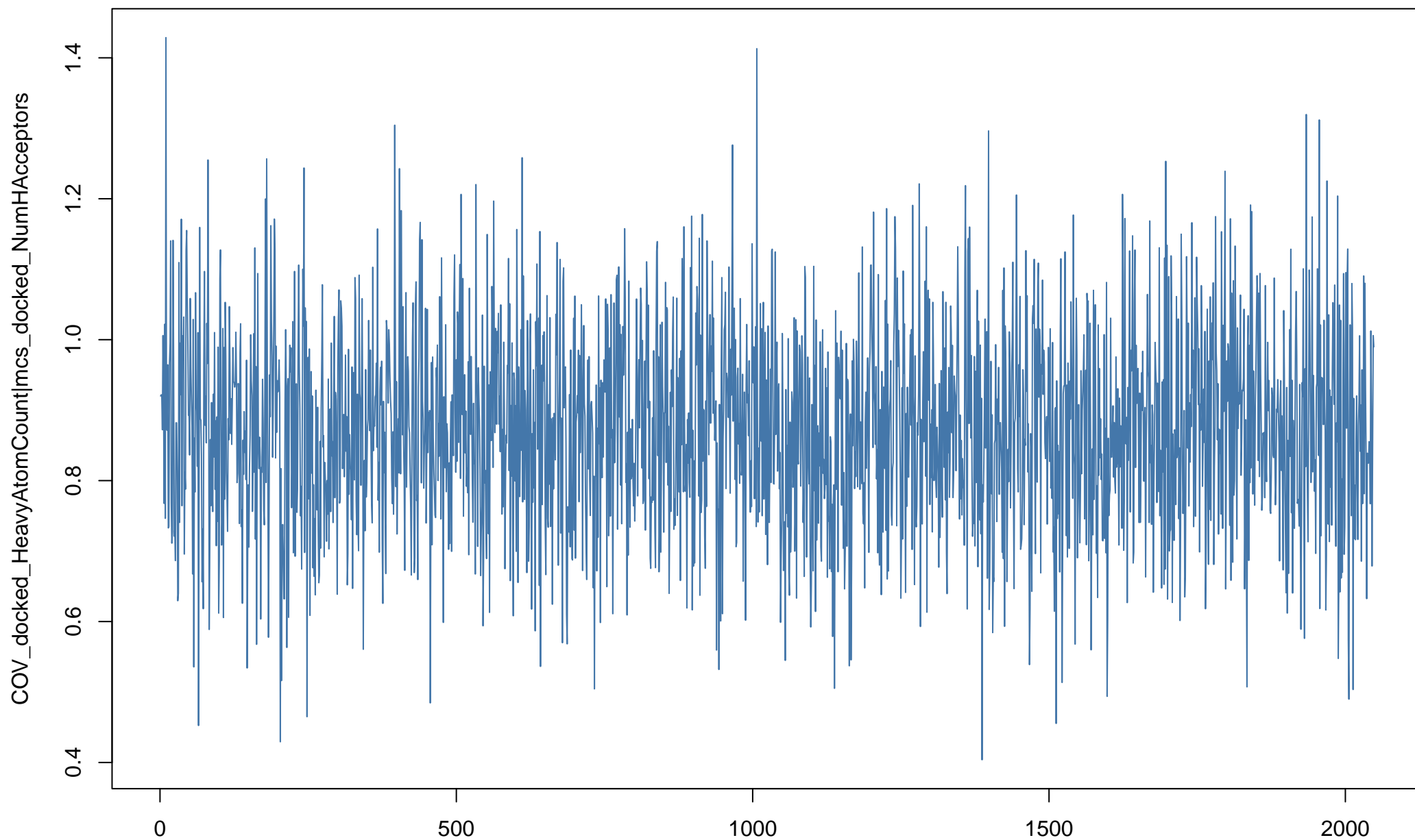
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 1810 | BMK = 0.0418 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0**



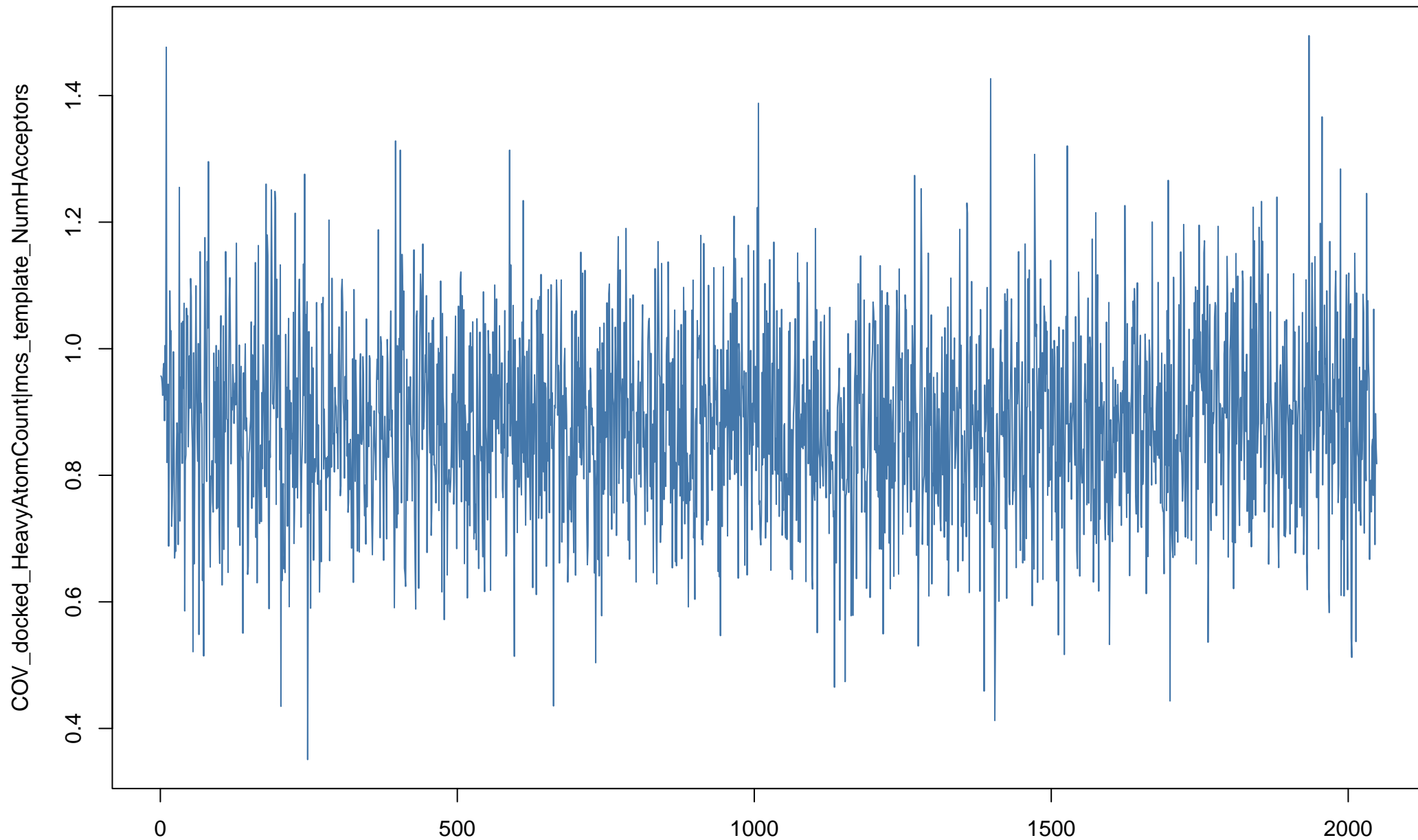
**COV\_docked\_HeavyAtomCount|template\_HeavyAtomCount**  
**ESS = 1870 | BMK = 0.0397 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0**



**COV\_docked\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0367 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0**

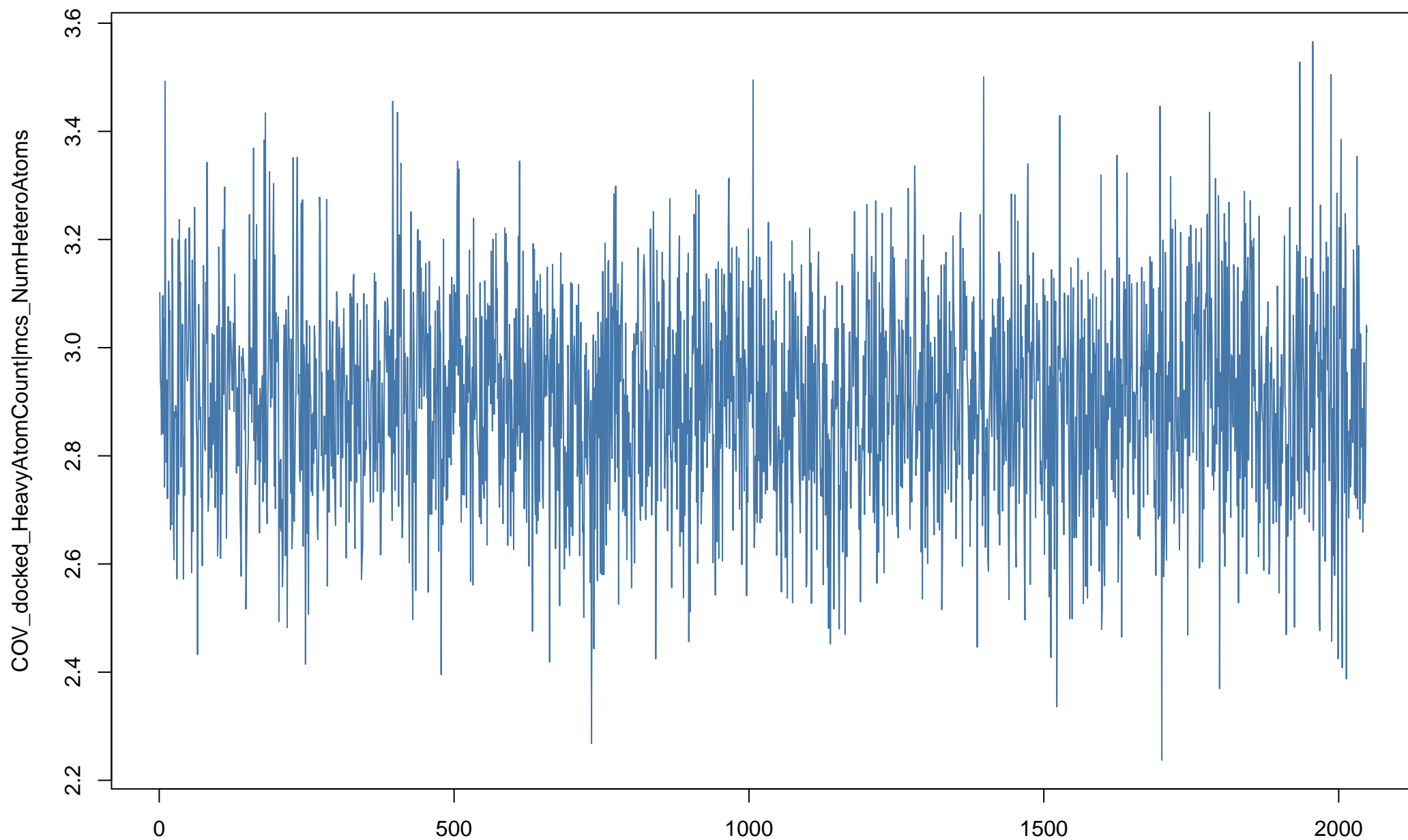


**COV\_docked\_HeavyAtomCount|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0324 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0**

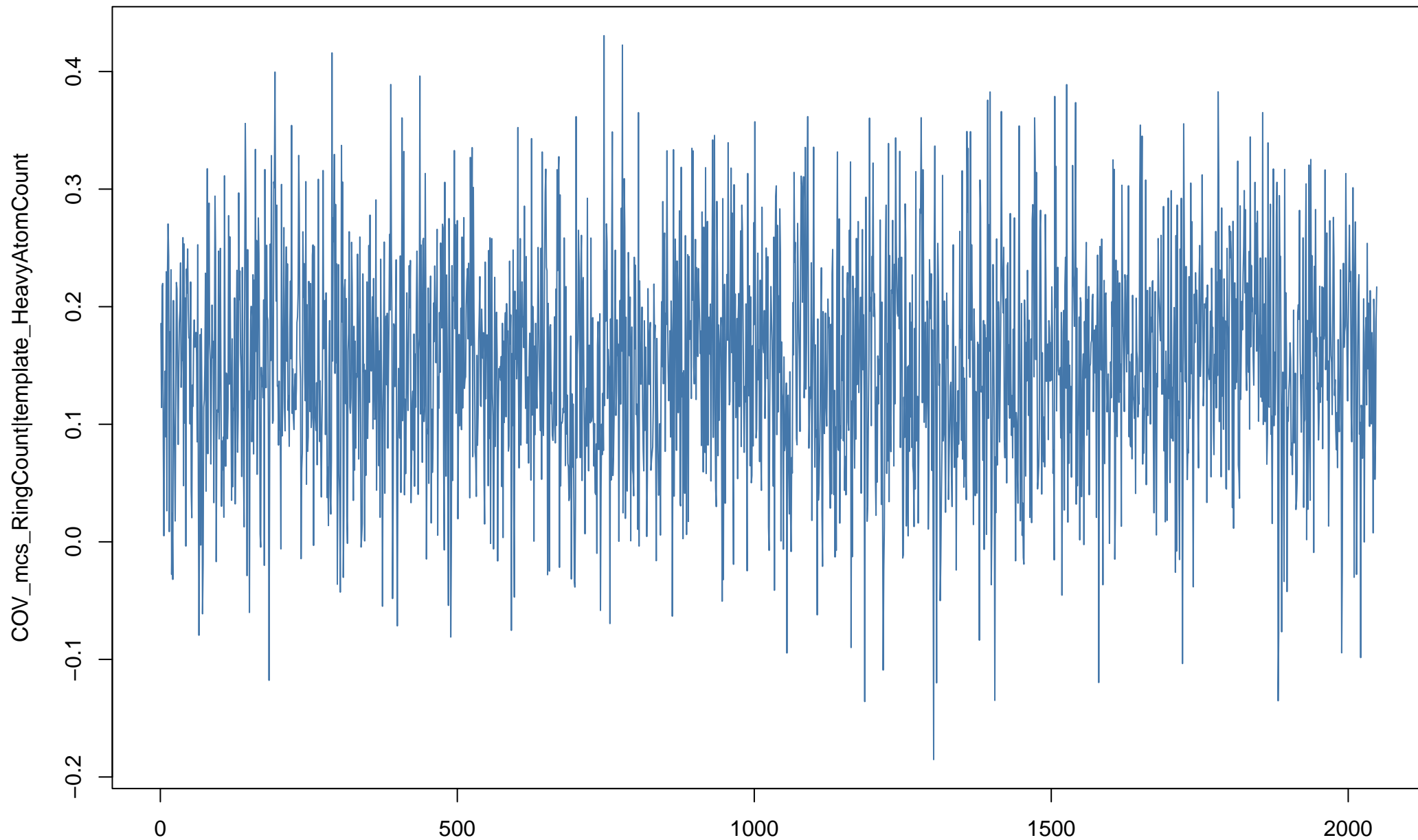




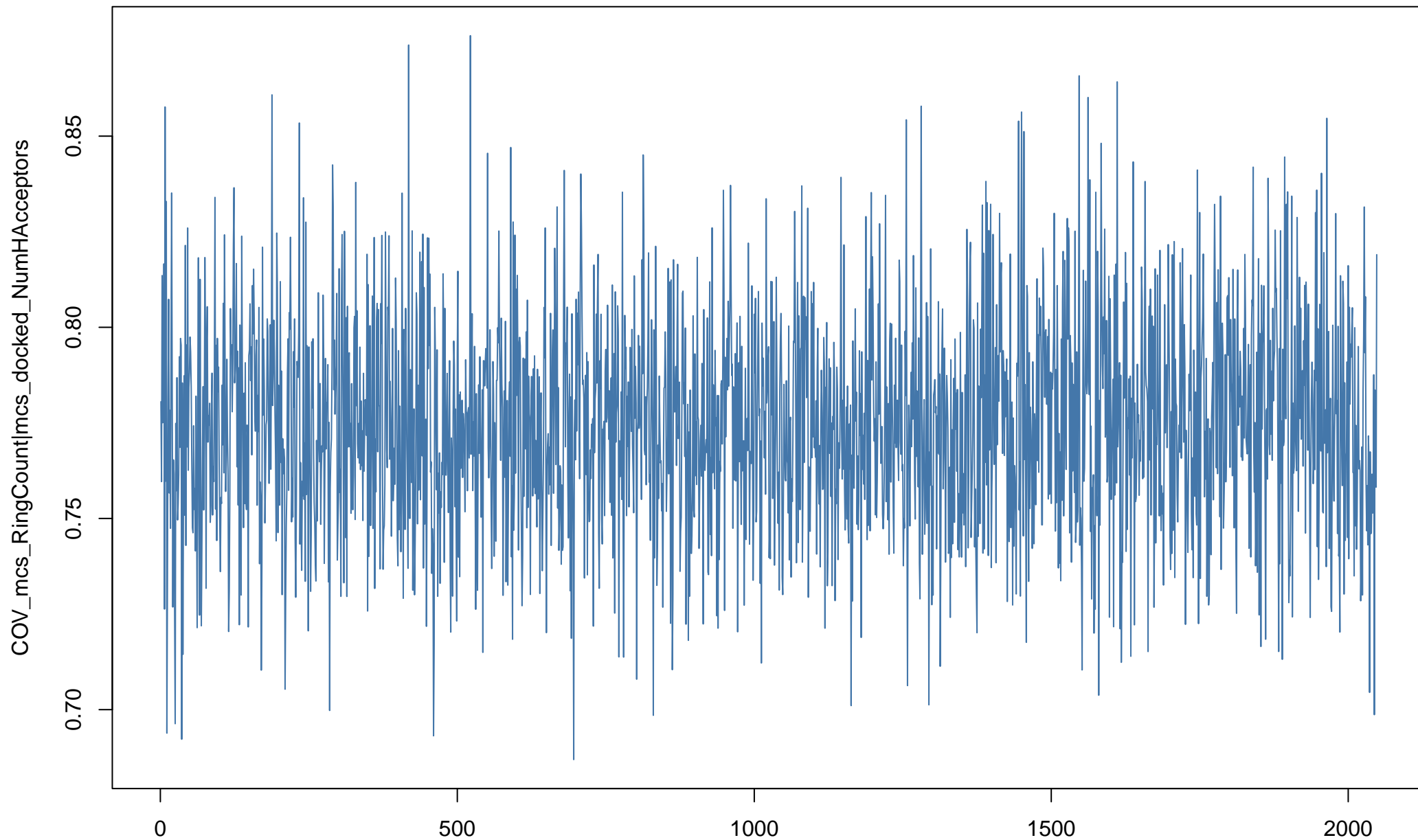
**COV\_docked\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0361 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0**



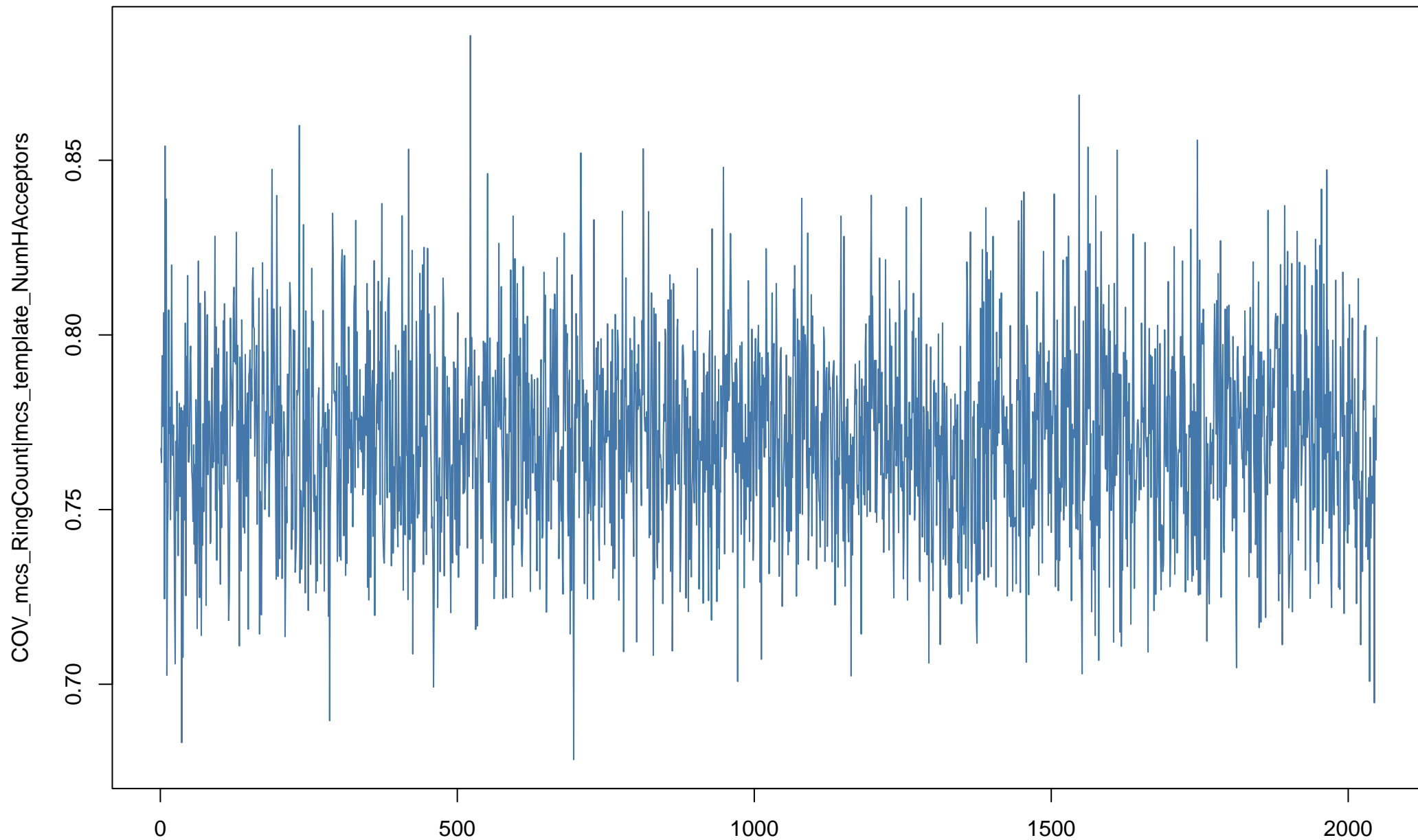
**COV\_mcs\_RingCount|template\_HeavyAtomCount**  
**ESS = 1830 | BMK = 0.0518 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0**



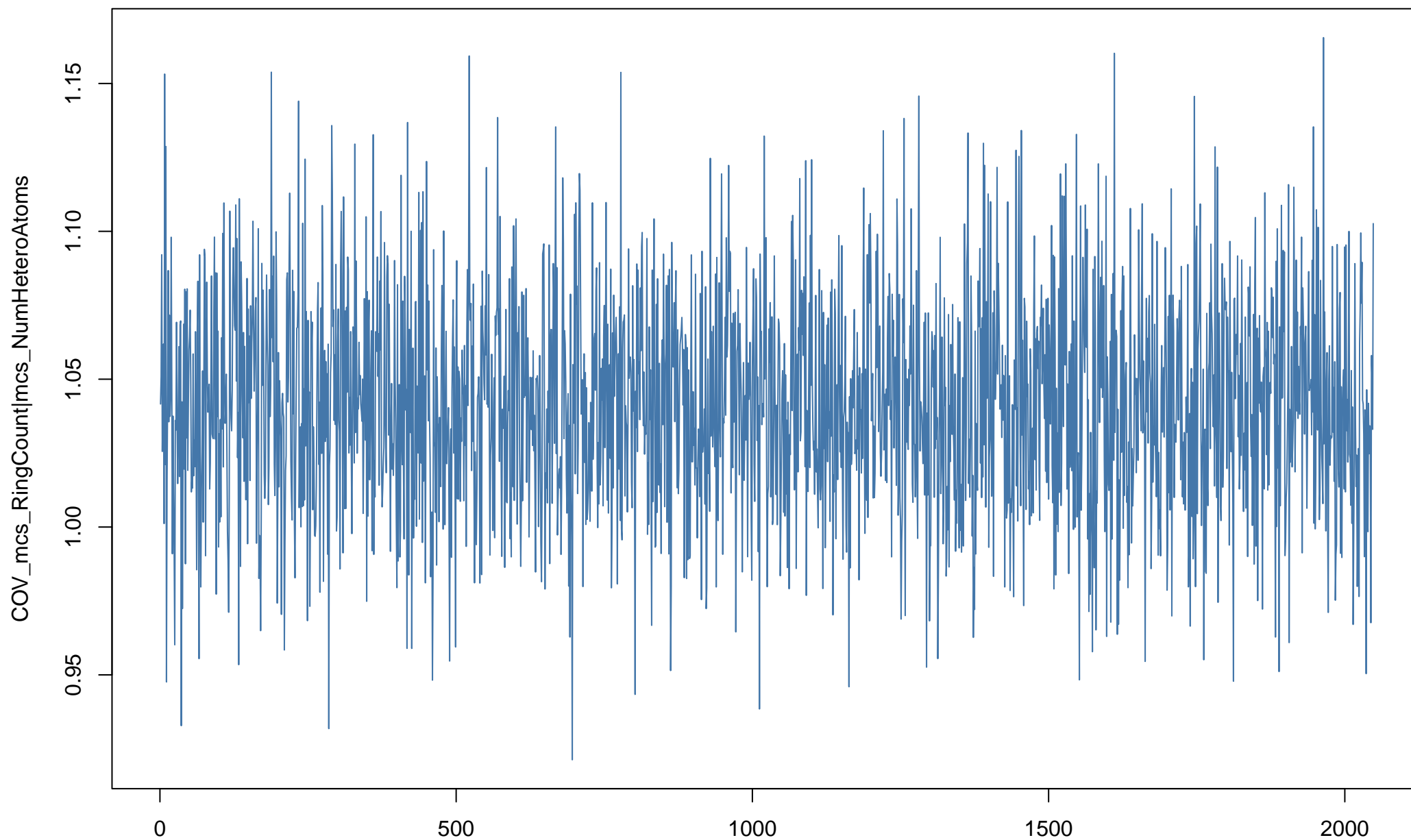
**COV\_mcs\_RingCount|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0468 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0**



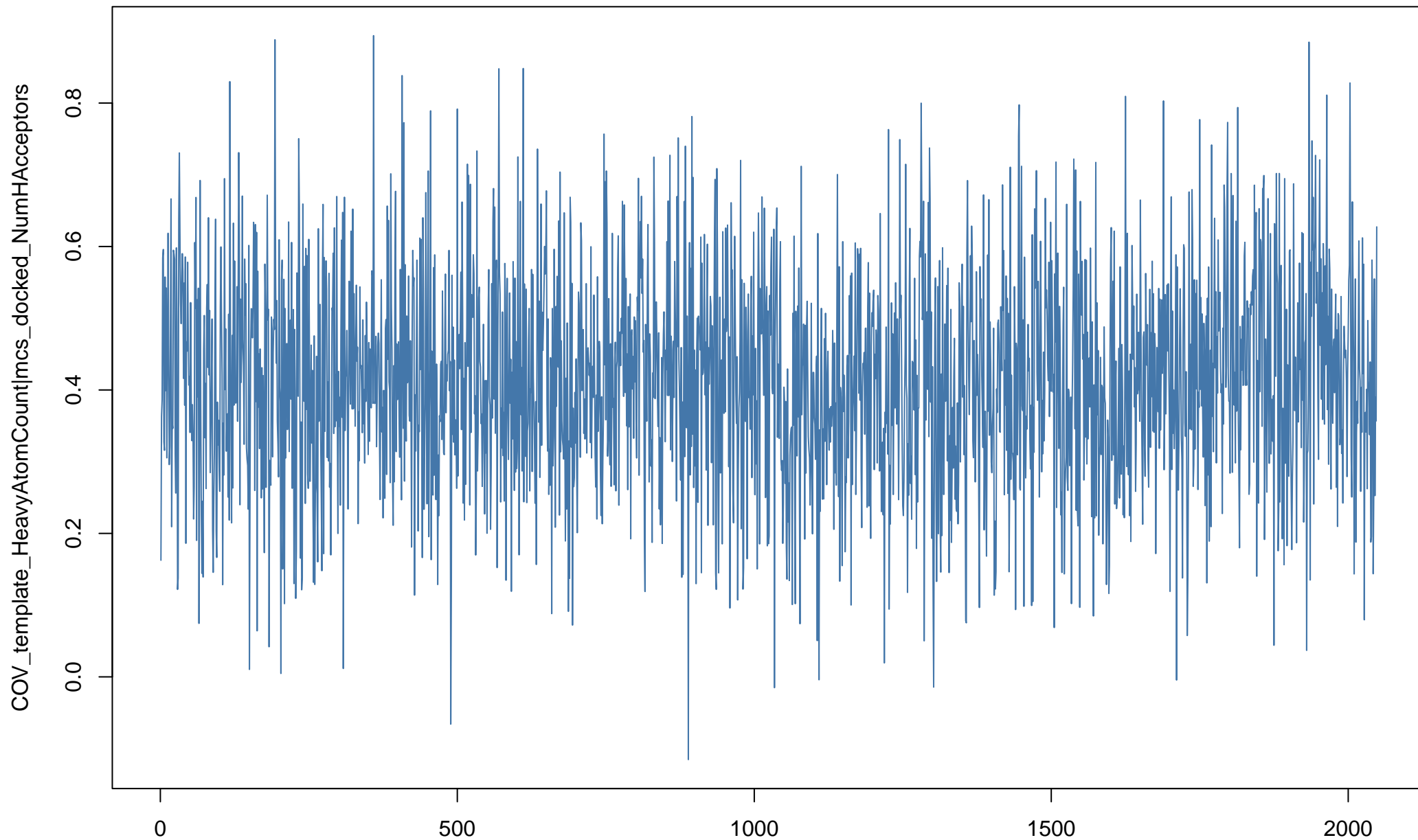
**COV\_mcs\_RingCount|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0333 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0**



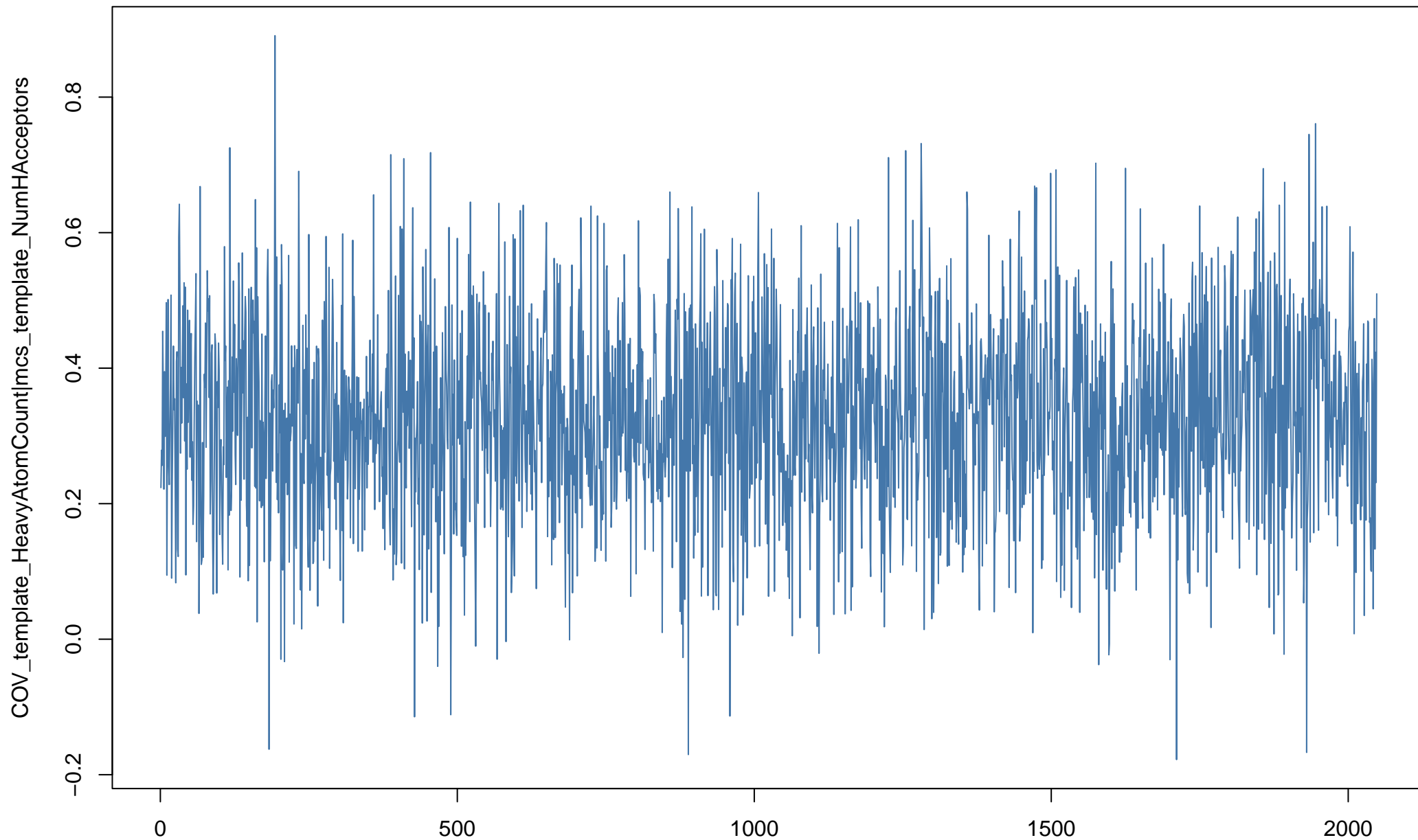
**COV\_mcs\_RingCount|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0395 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0**



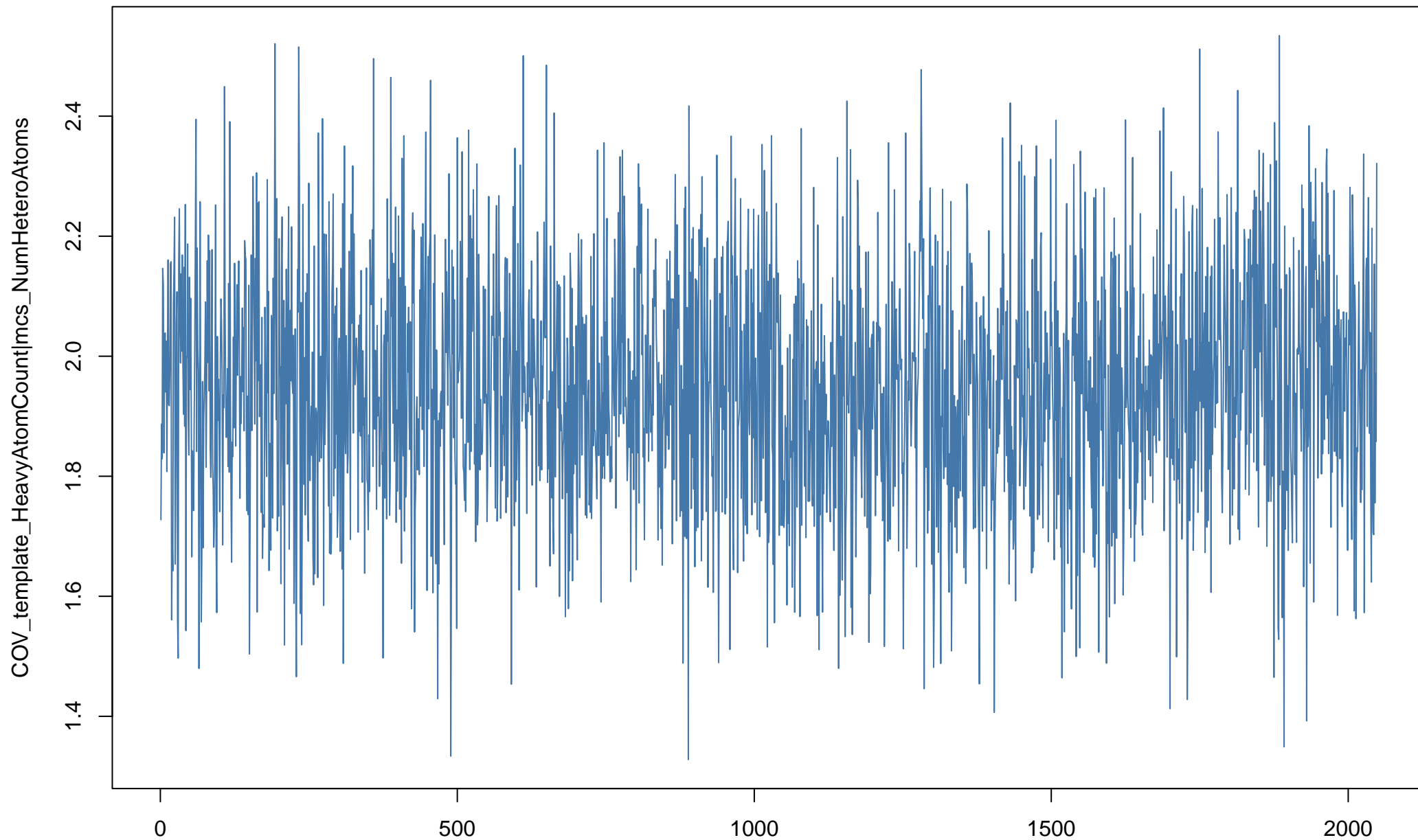
**COV\_template\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0384 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0**



**COV\_template\_HeavyAtomCount|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0437 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0**

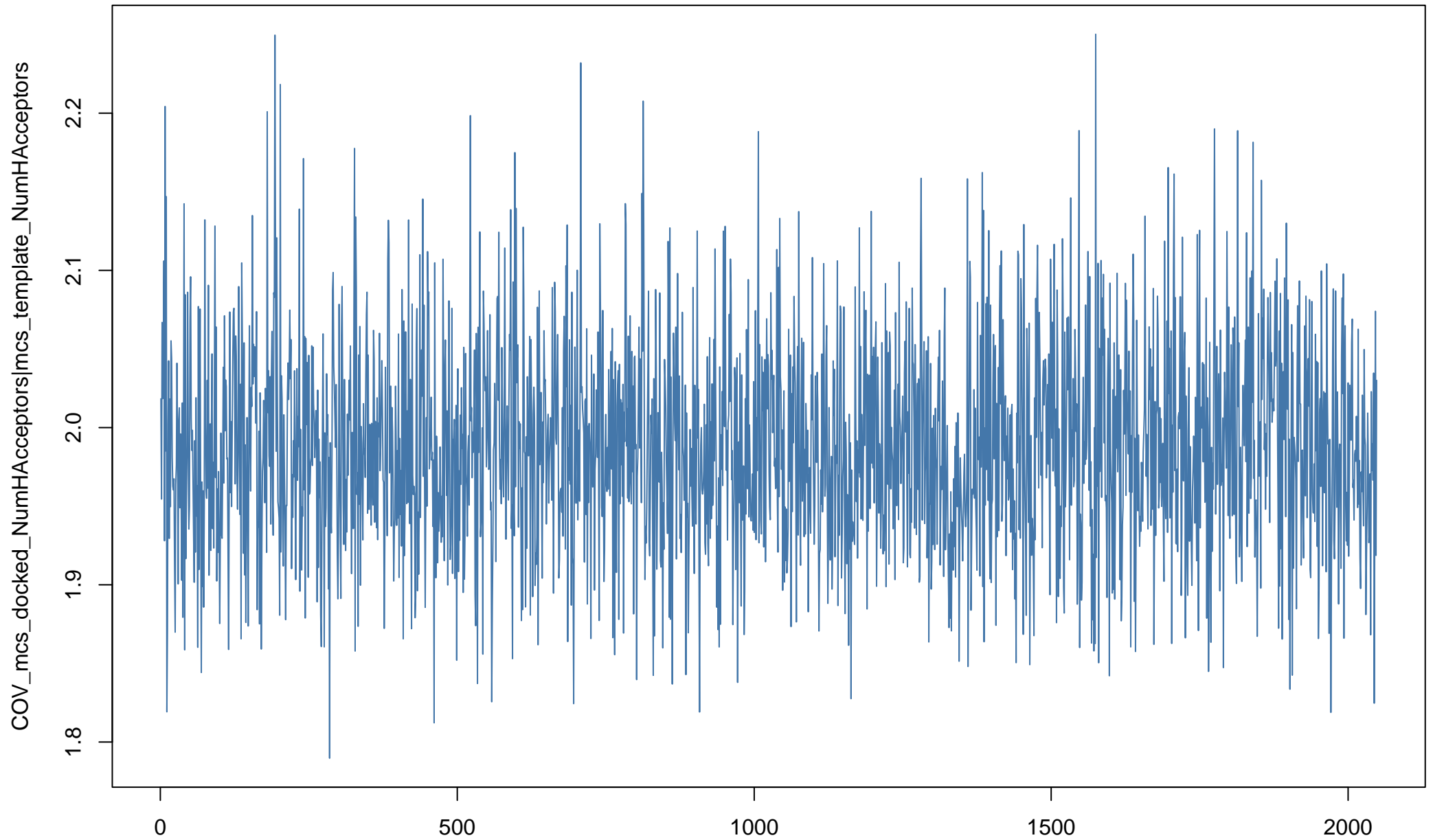


**COV\_template\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0514 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0**

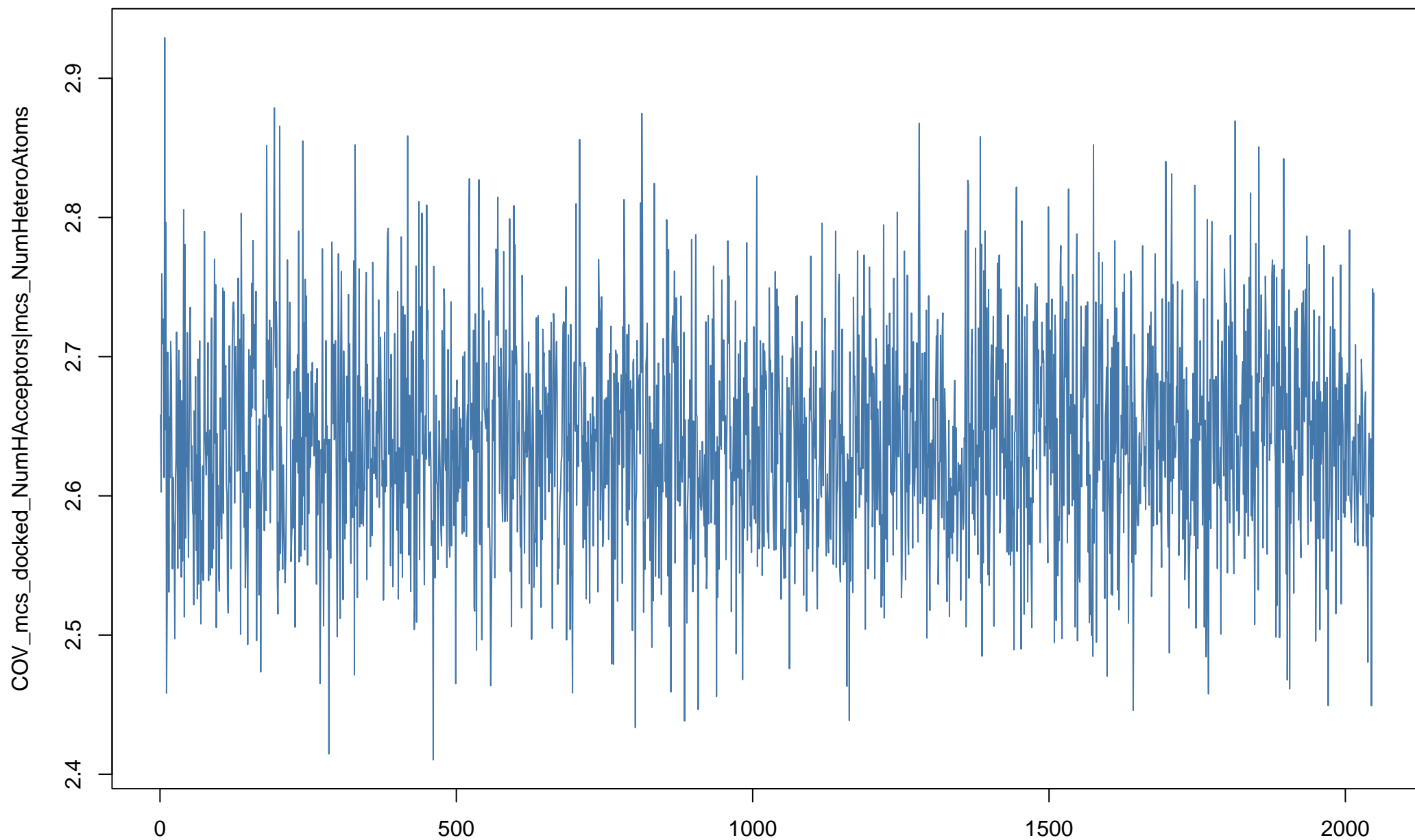




**COV\_mcs\_docked\_NumHAcceptors|mcs\_template\_NumHAcceptors**  
**ESS = 1770 | BMK = 0.0472 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0**



**COV\_mcs\_docked\_NumHAcceptors|mcs\_NumHeteroAtoms**  
**ESS = 1710 | BMK = 0.0422 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0**



**COV\_mcs\_template\_NumHAcceptors|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0458 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0**

