

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.896207751935795

max MCSE = 14.8884503341565

all stationary: FALSE

burn: 2040

-- STATS 2D --

min ESS = 99.9343278636941

max BMK = 0.235116810223668

max MCSE = 5.77103491867434

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.609283558405166

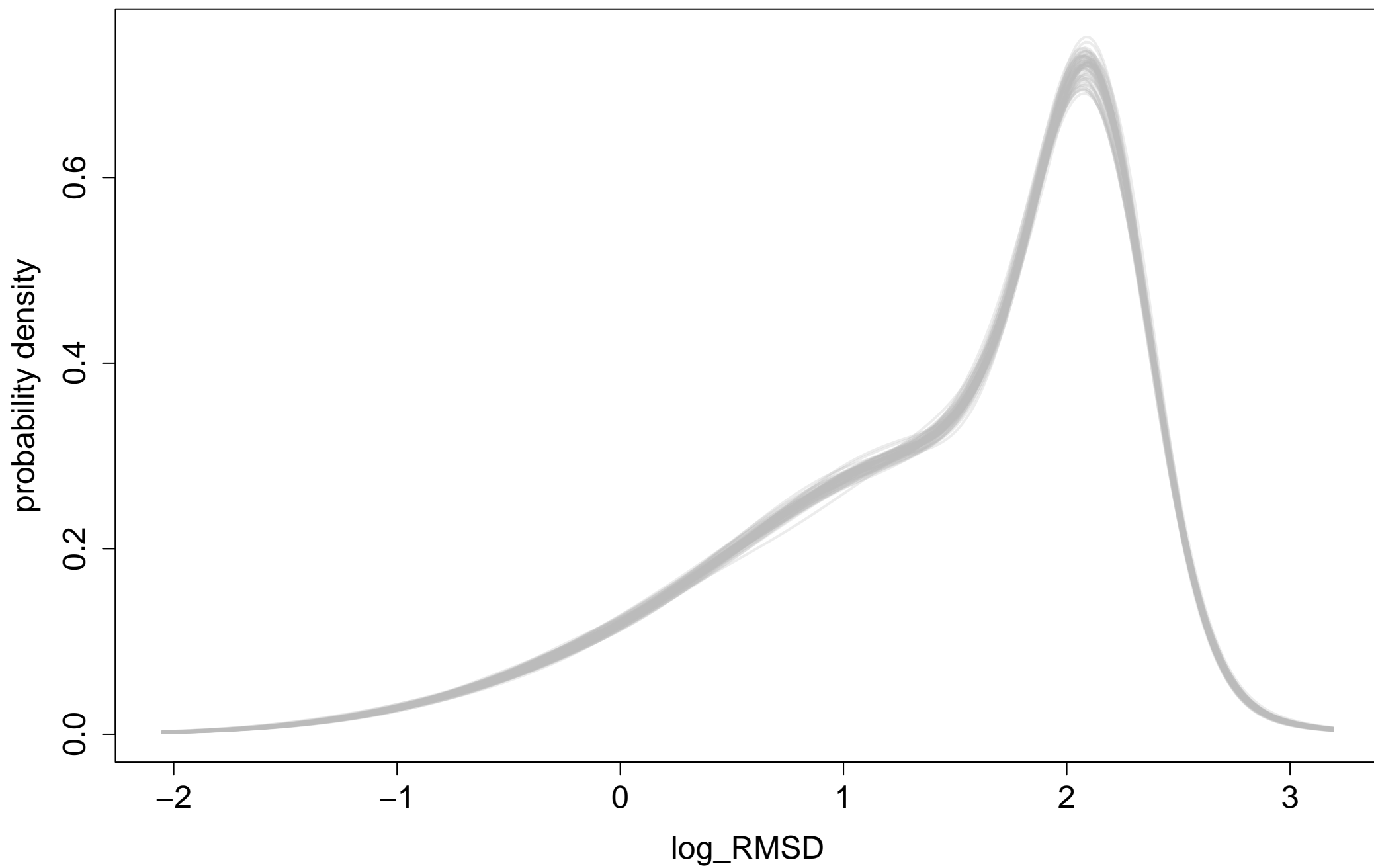
max MCSE = NaN

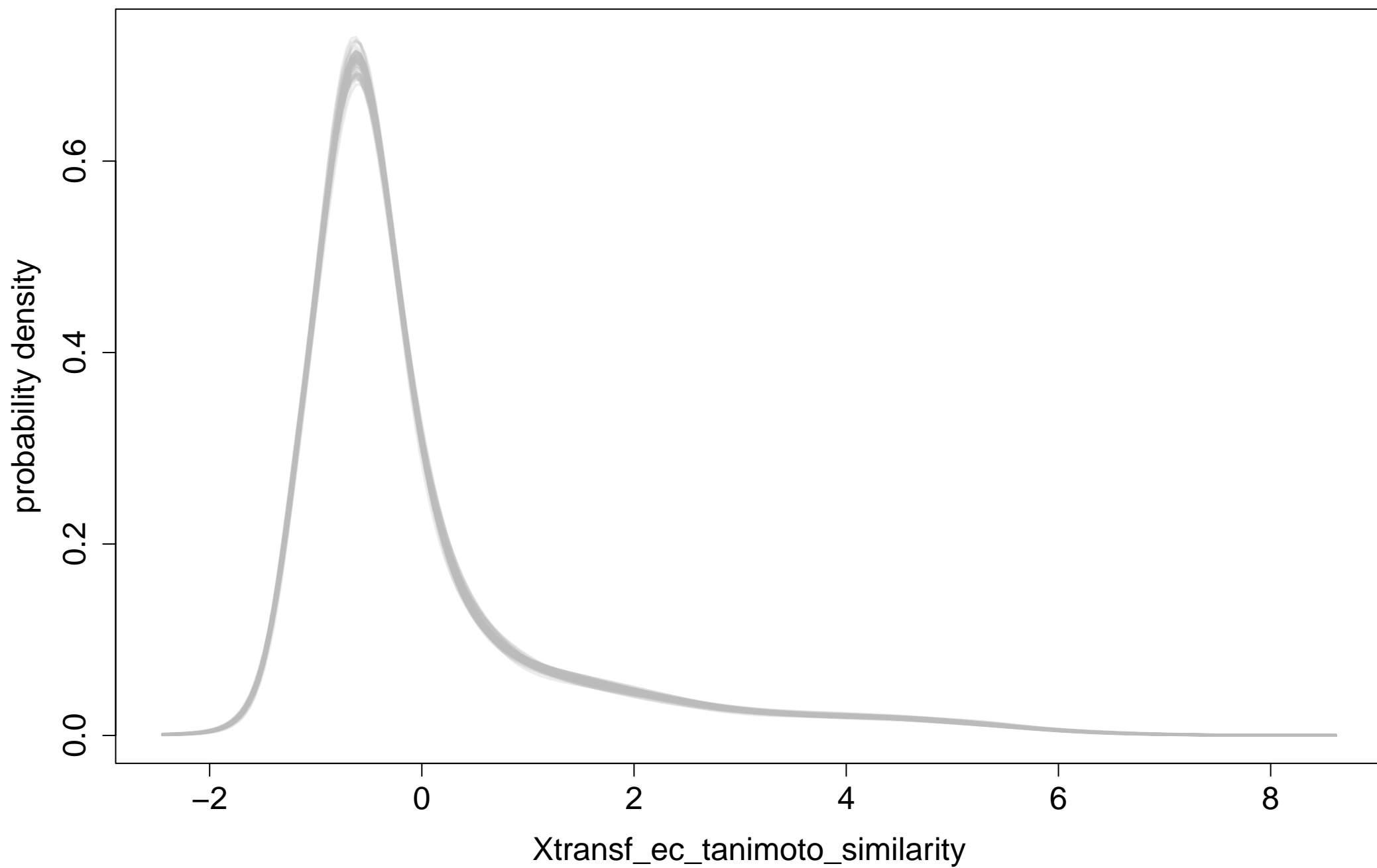
all stationary: FALSE

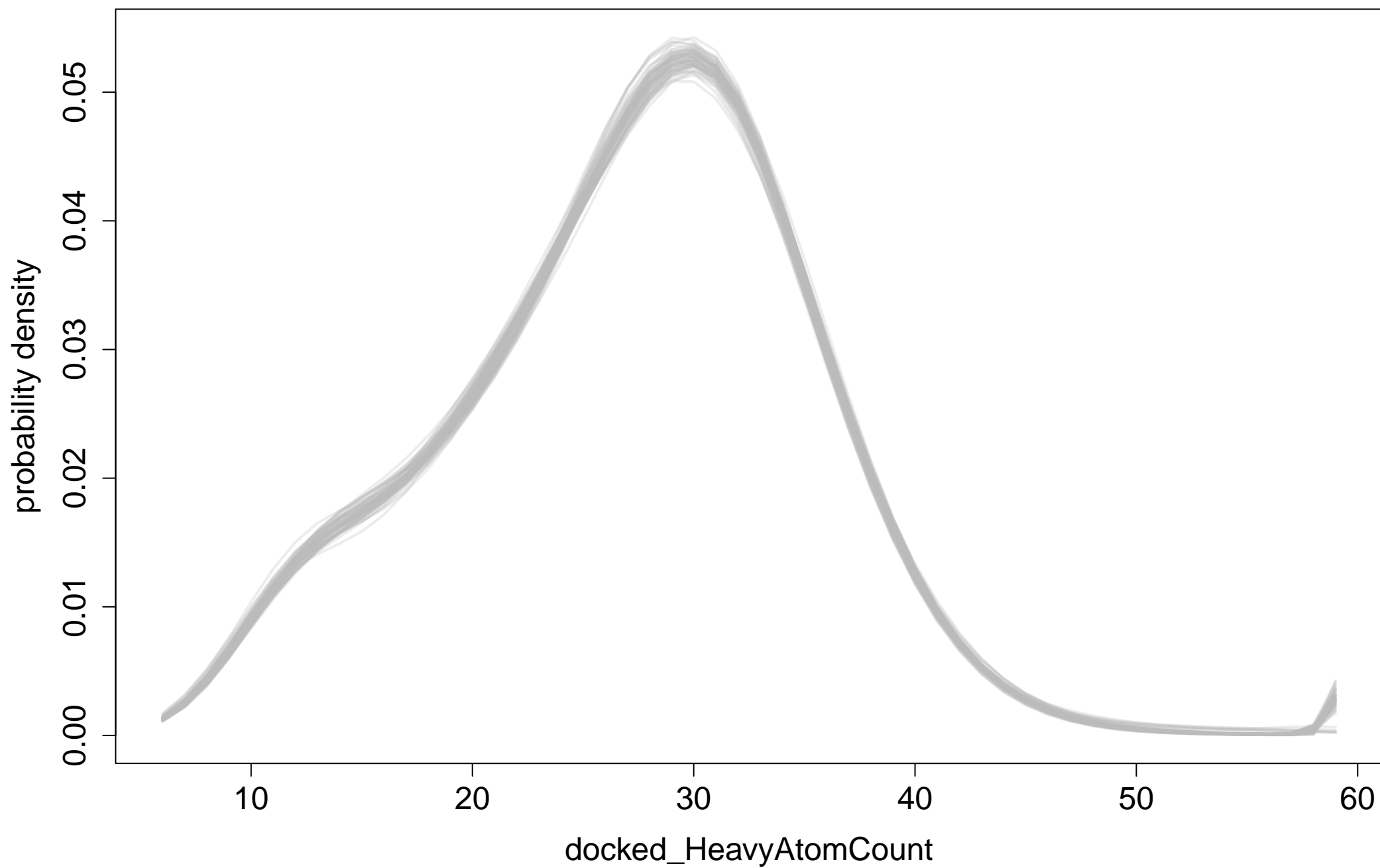
burn: 2040

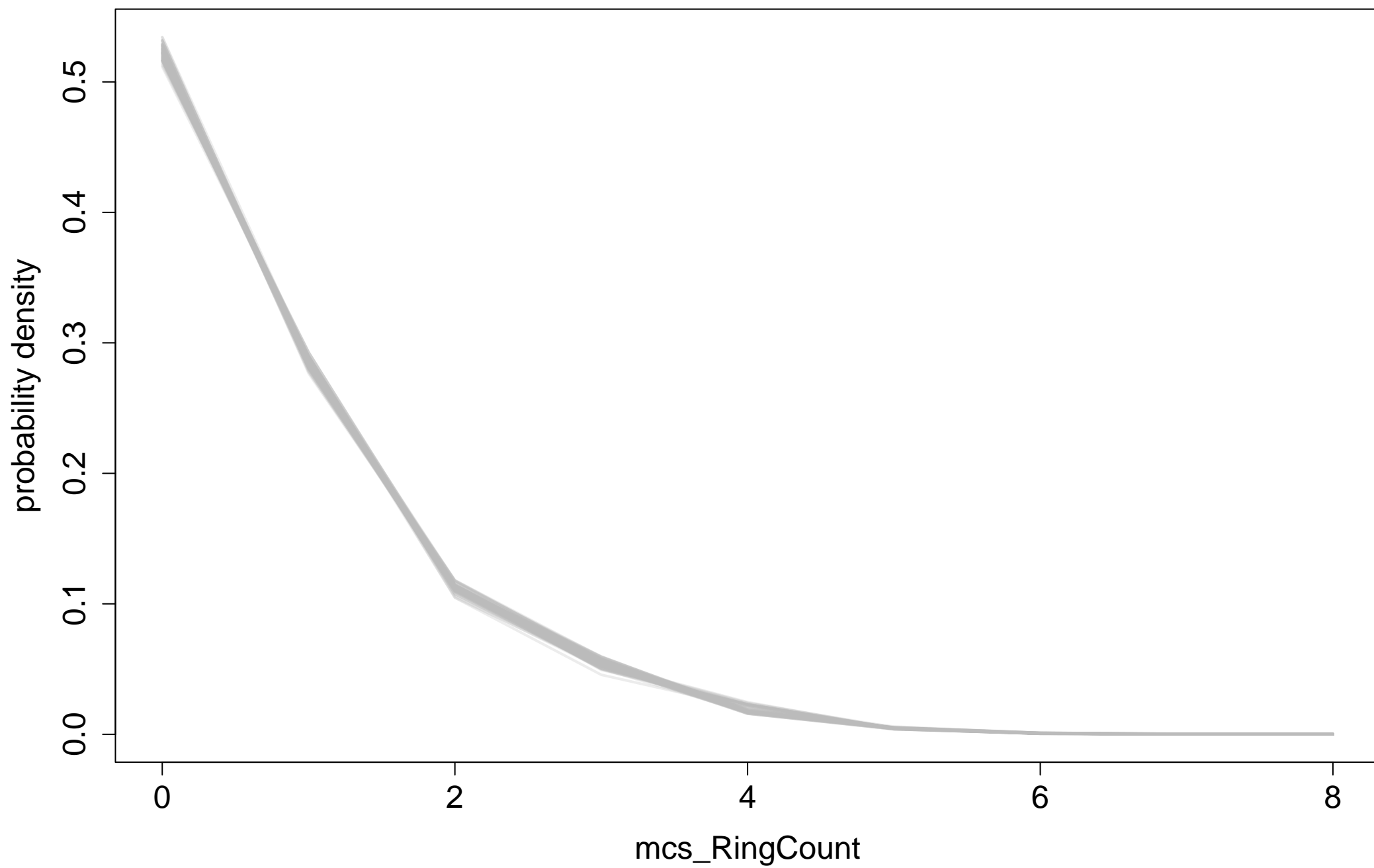
Occupied clusters: 47 of 64

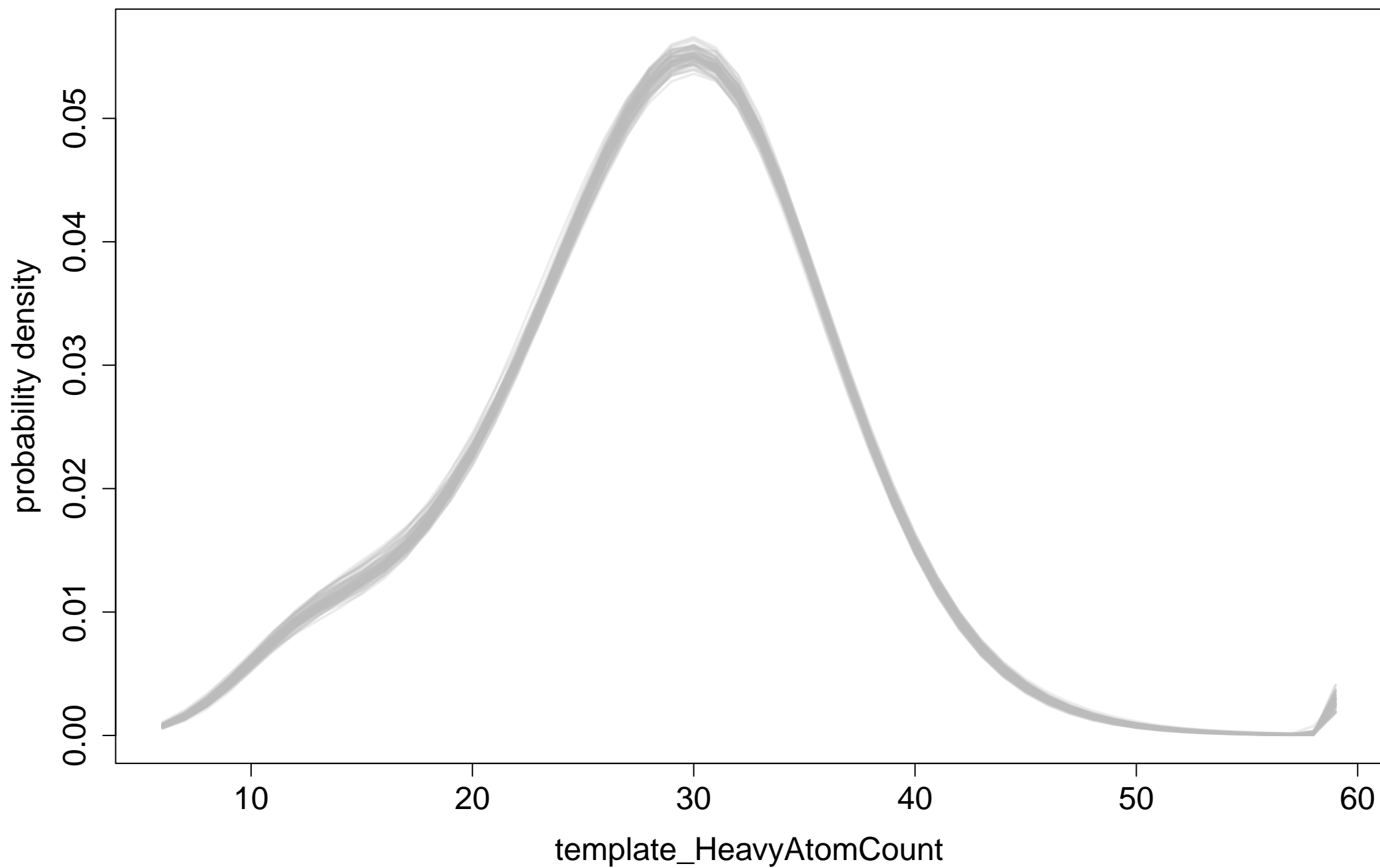
LL: -113000 +- 342

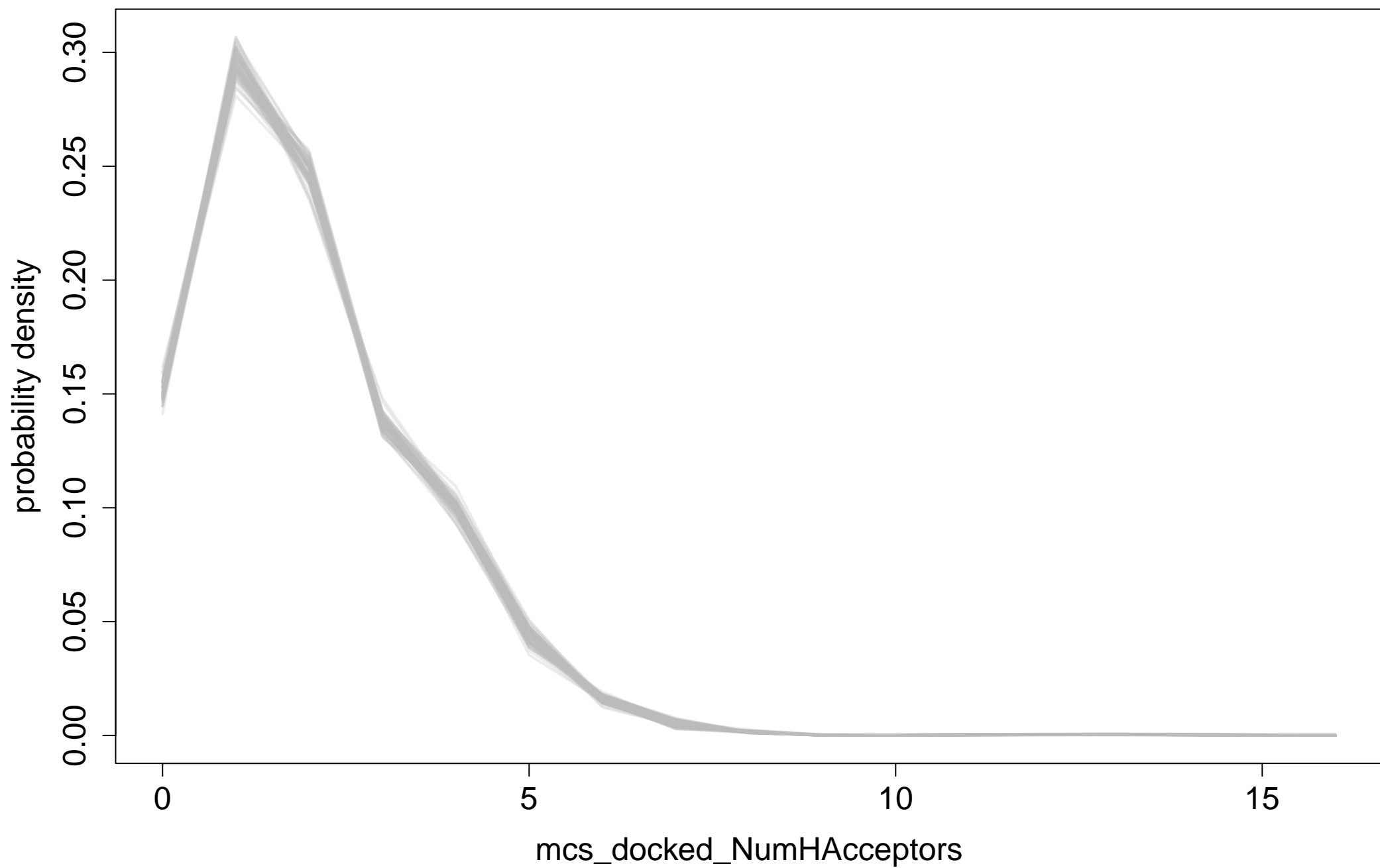


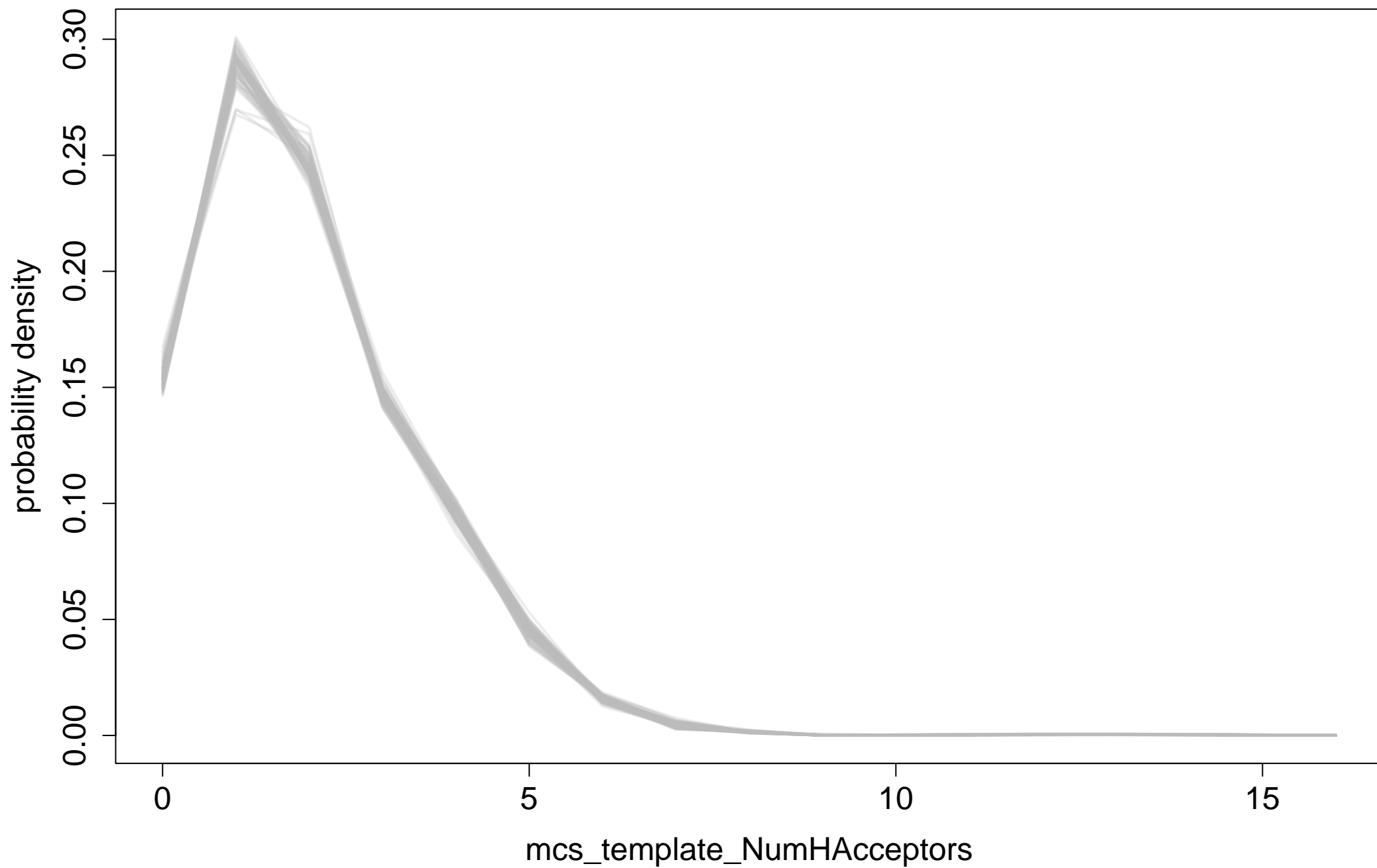




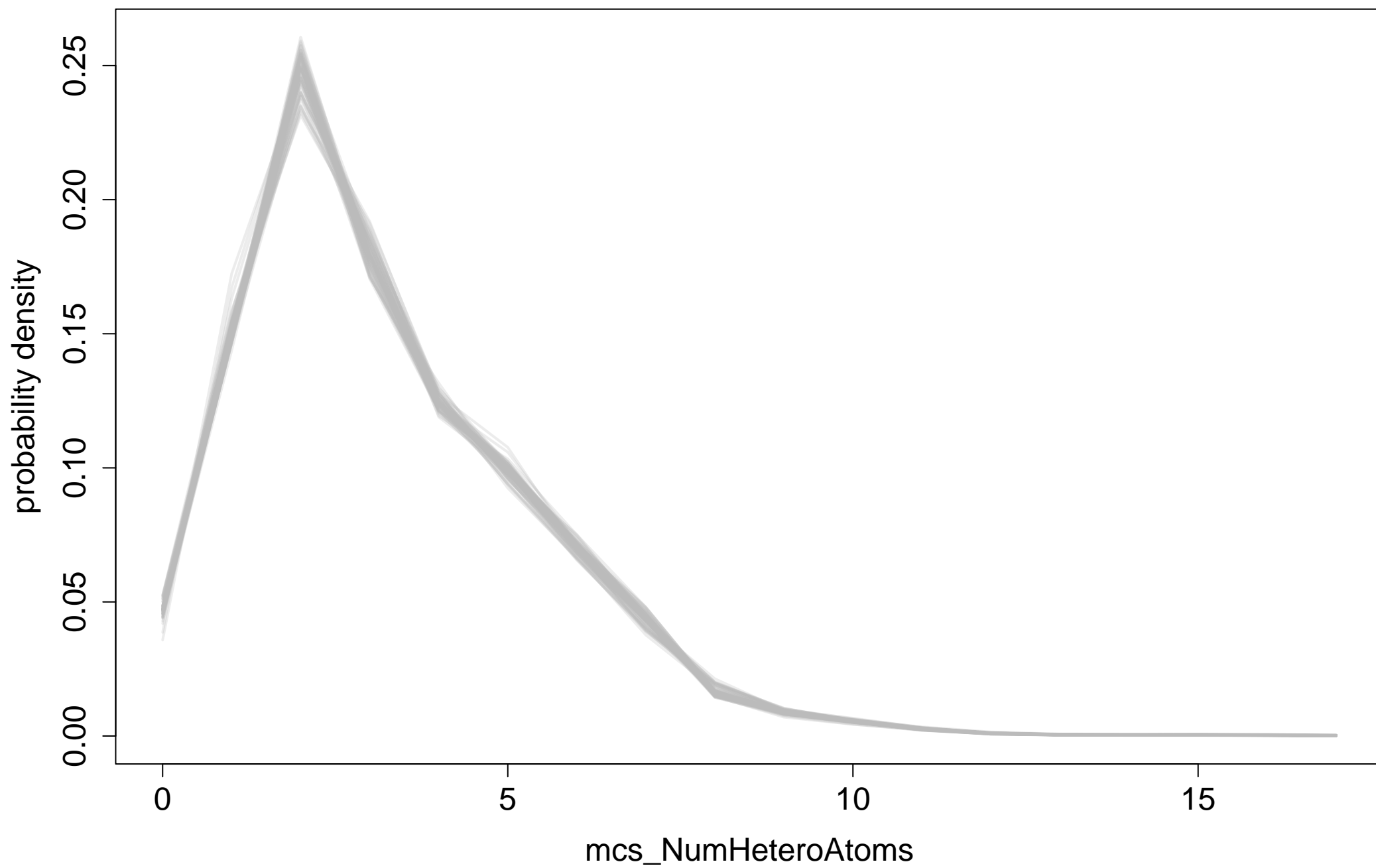


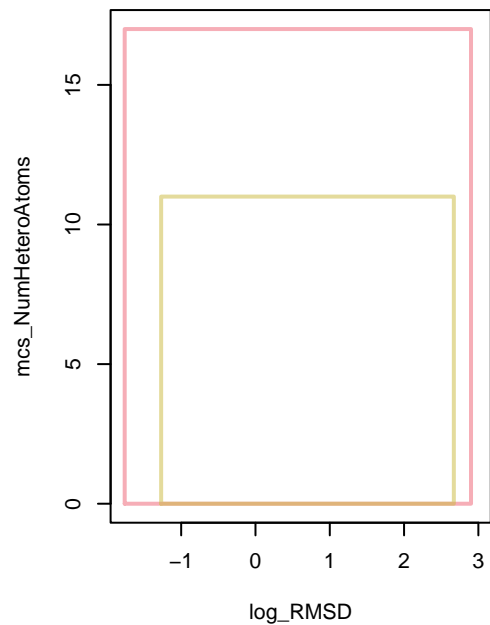
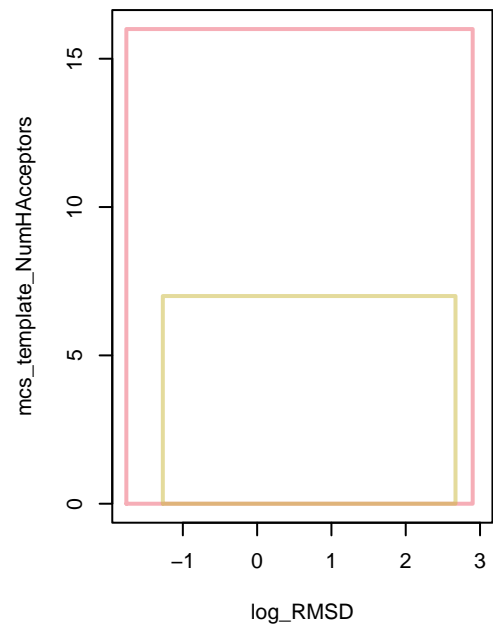
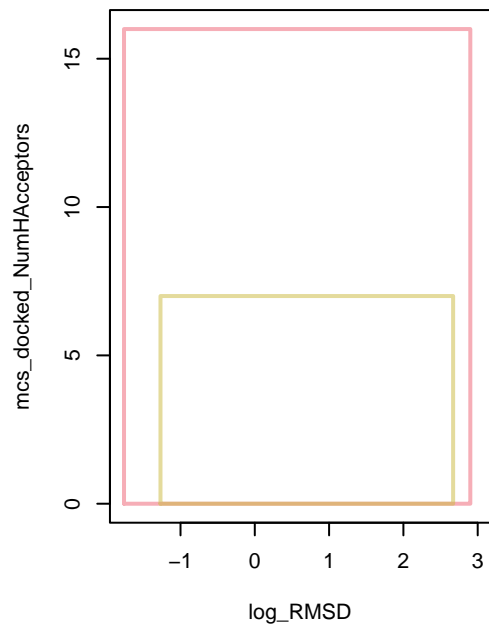
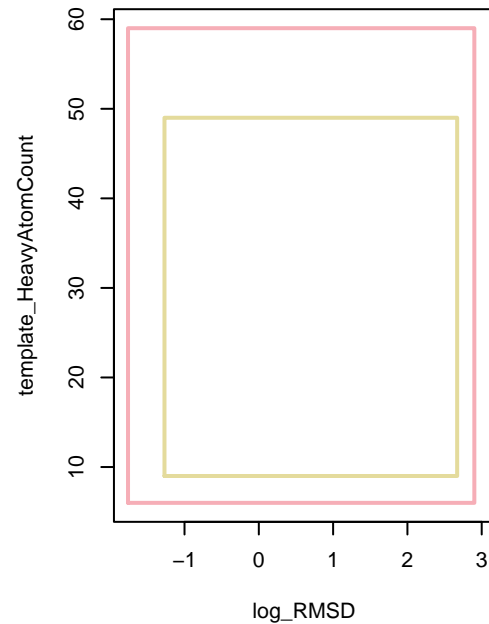
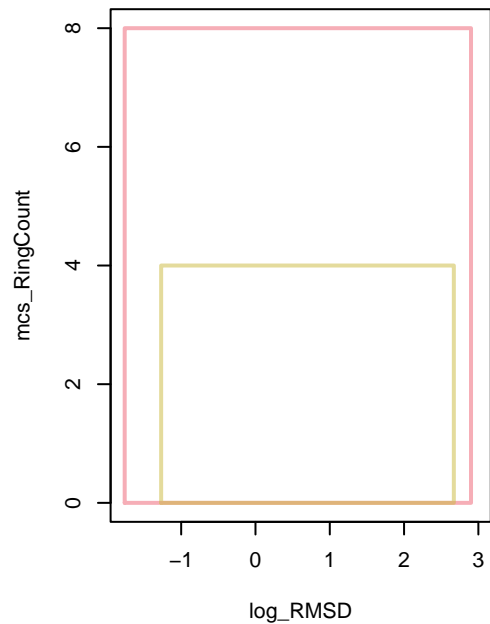
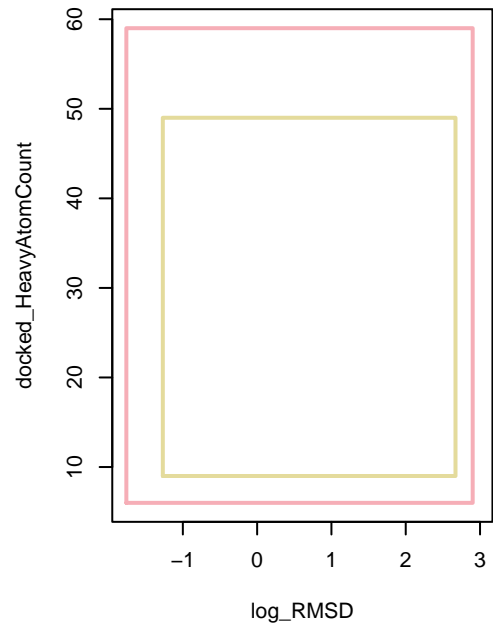
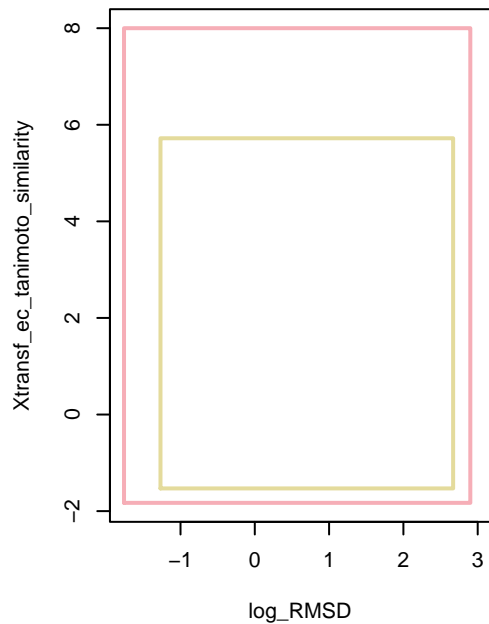




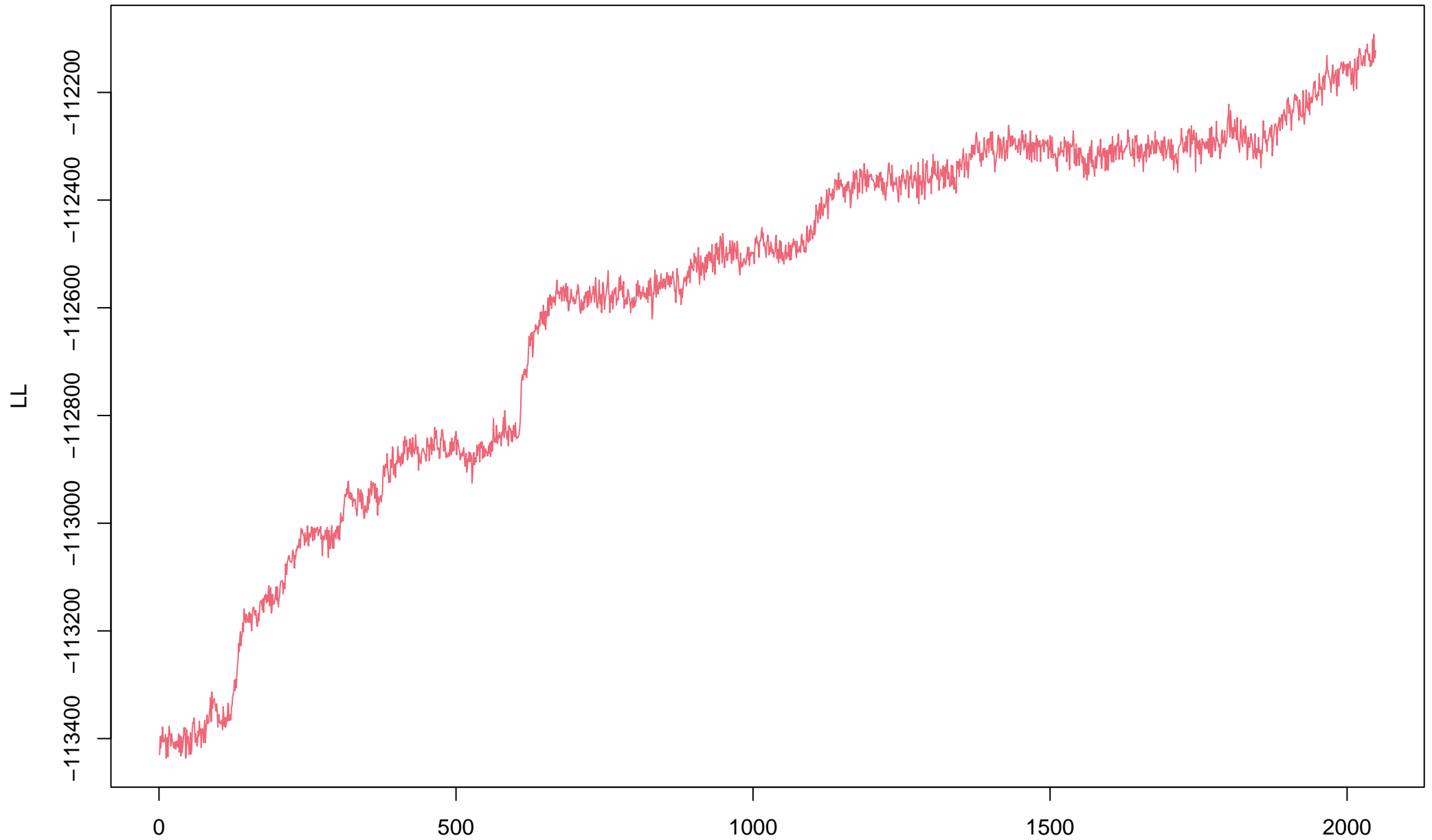




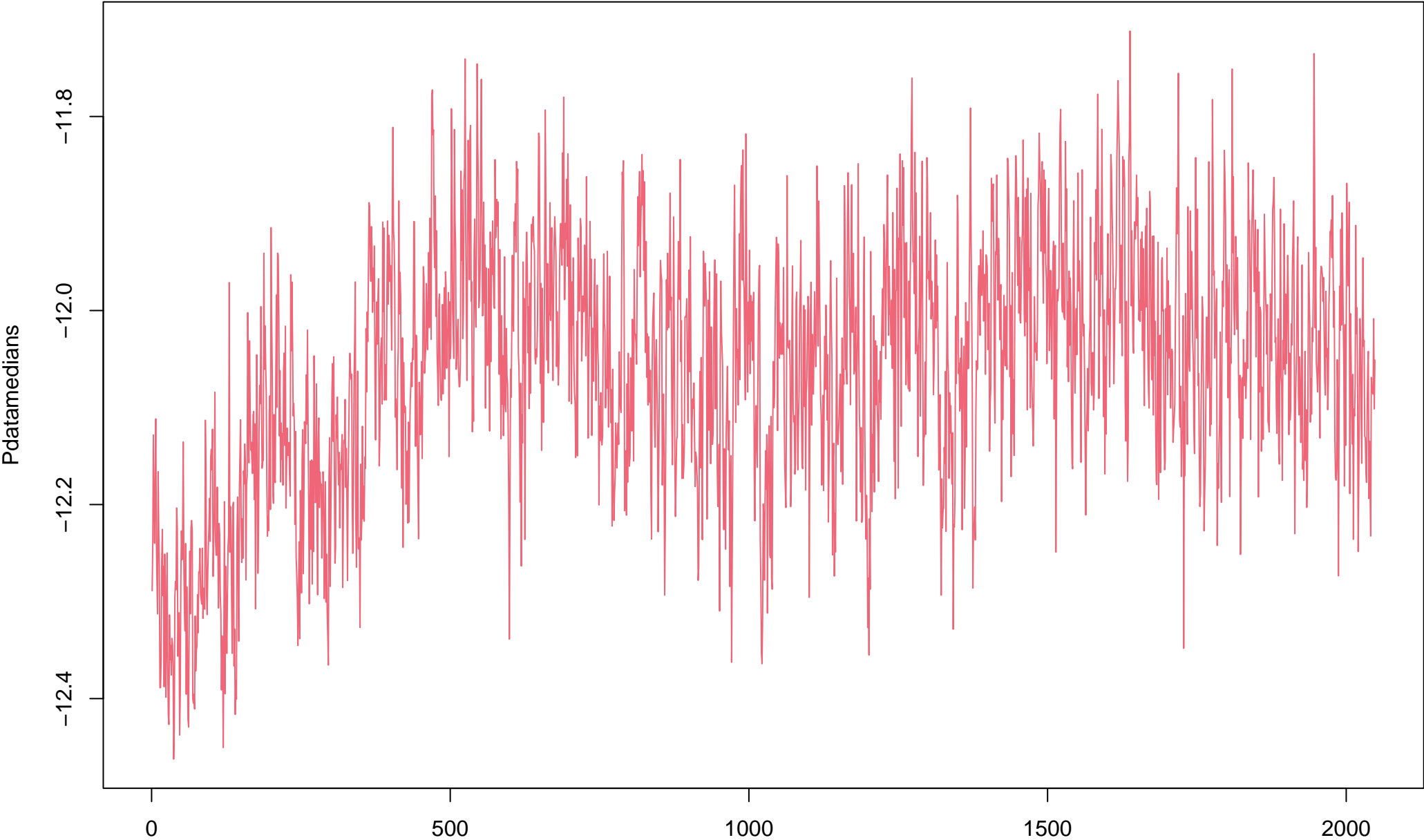




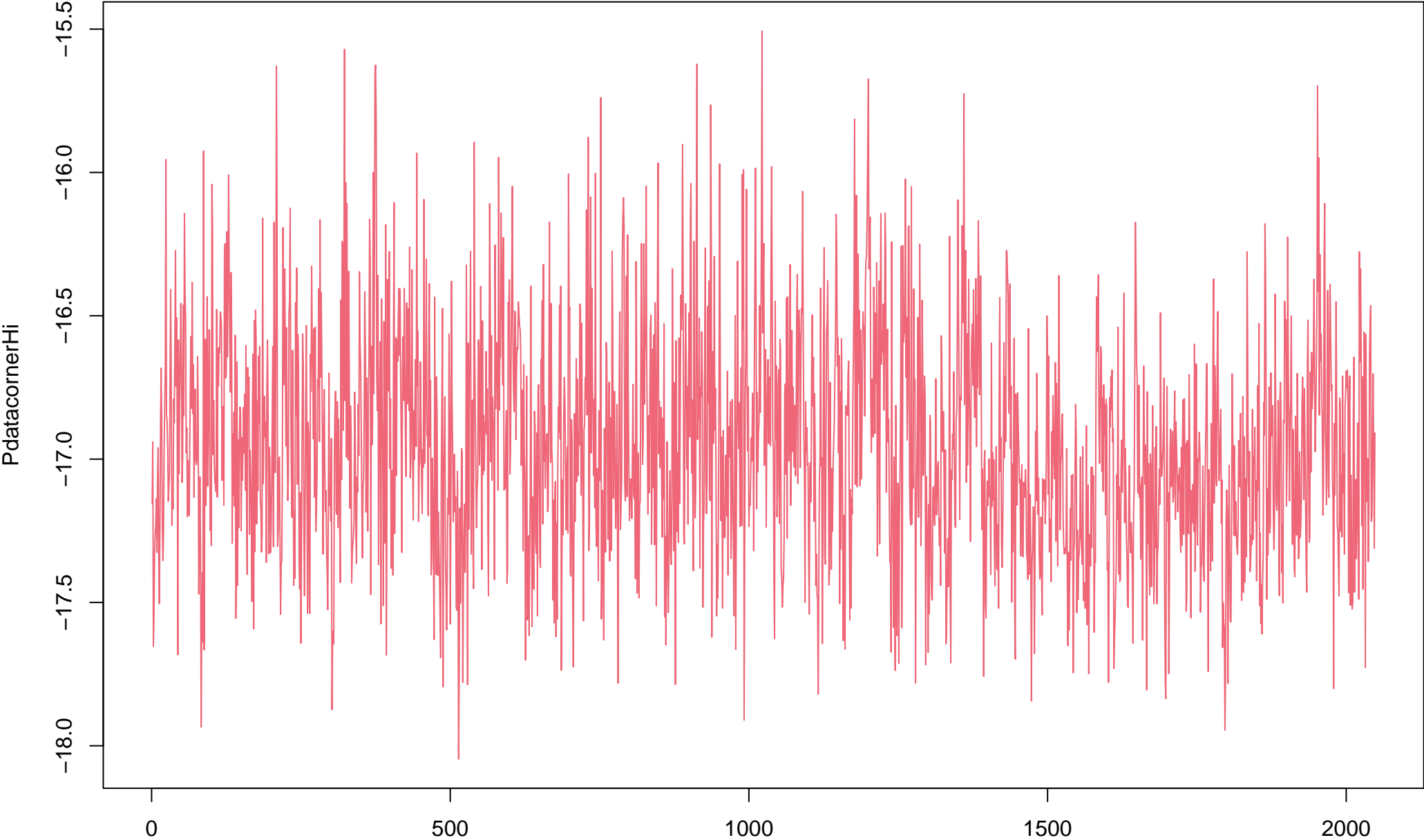
LL  
ESS = 2.17 | BMK = 0.896 | MCSE(6.27) = 14.9 | stat: FALSE | burn: 2040



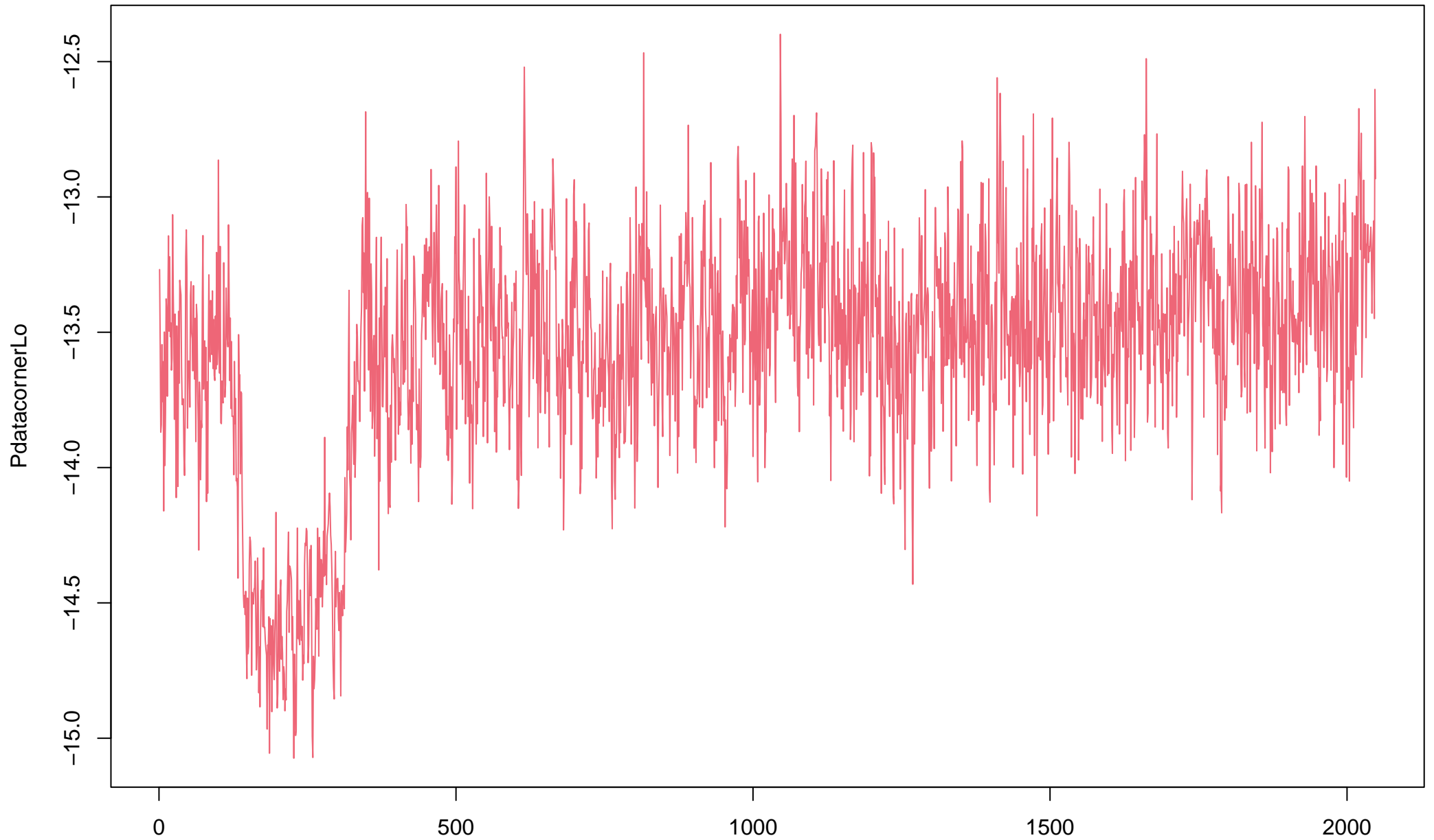
**Pdatamedians**  
**ESS = 30.5 | BMK = 0.208 | MCSE(6.27) = 9.82 | stat: FALSE | burn: 0**



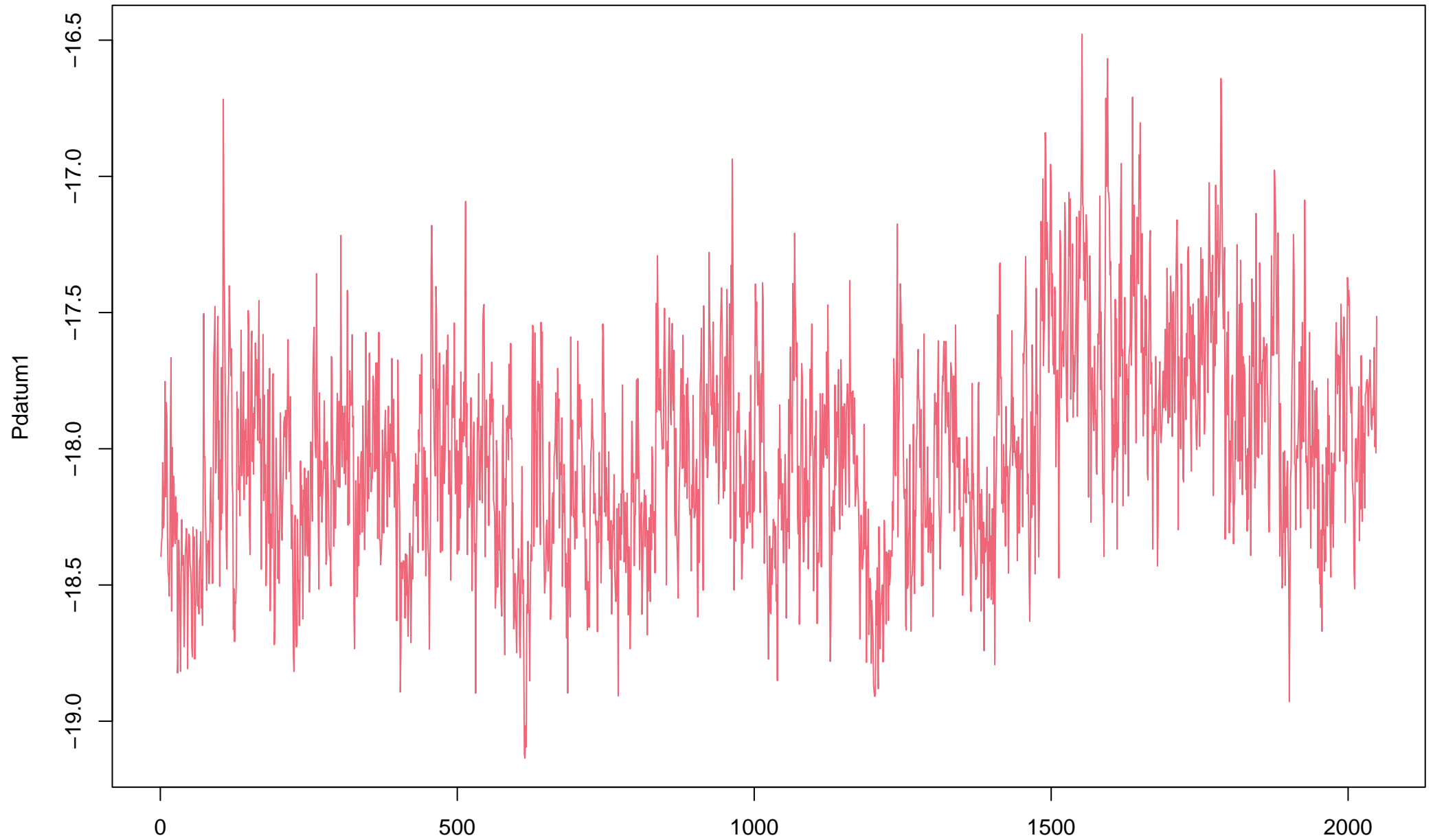
**PdatacornerHi**  
**ESS = 328 | BMK = 0.0984 | MCSE(6.27) = 5.29 | stat: TRUE | burn: 0**



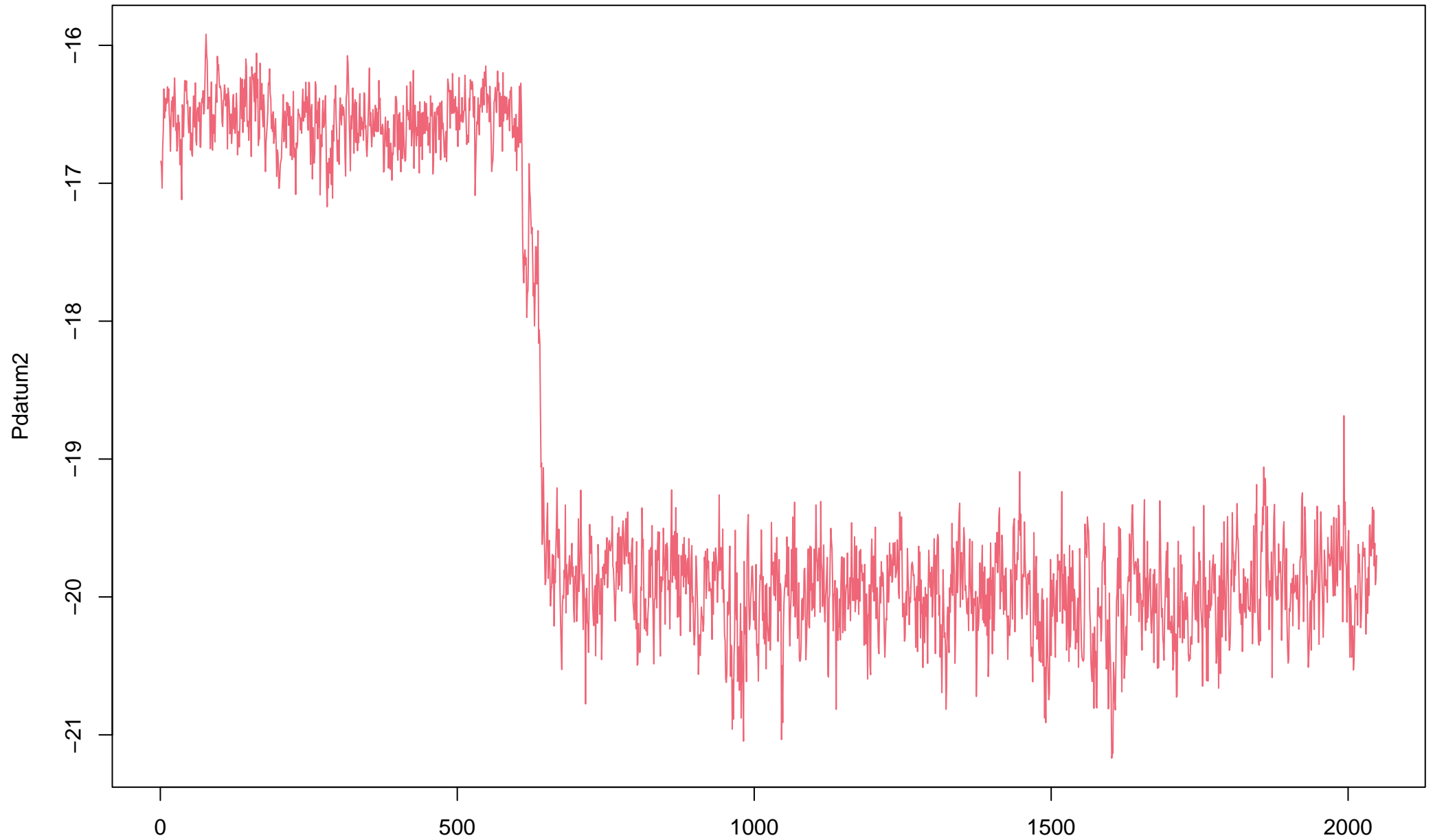
**PdatacornerLo**  
**ESS = 42.8 | BMK = 0.285 | MCSE(6.27) = 8.96 | stat: FALSE | burn: 0**



**Pdatum1**  
**ESS = 2.22e-16 | BMK = 0.22 | MCSE(6.27) = 9.07 | stat: FALSE | burn: 0**

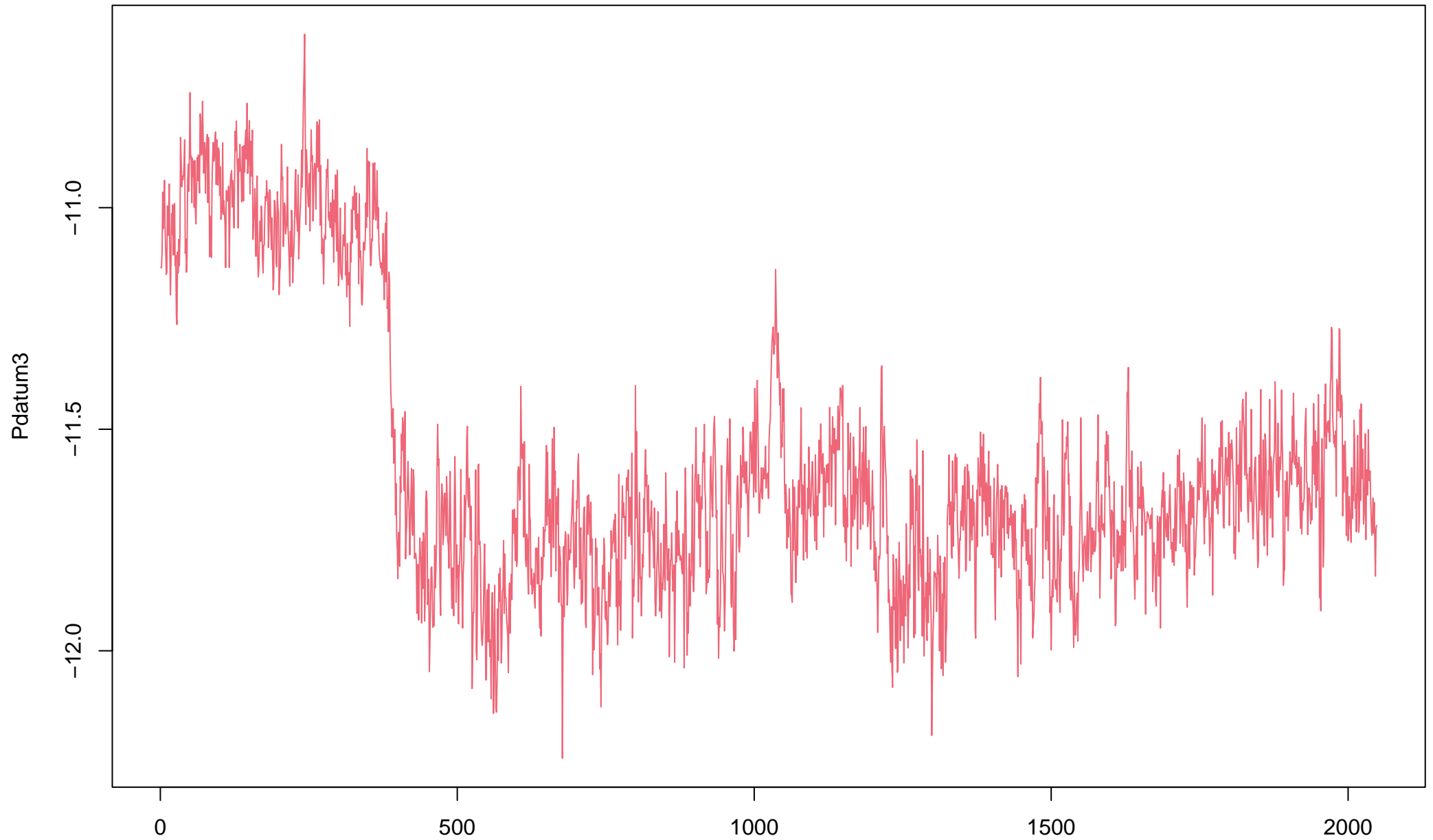


**Pdatum2**  
**ESS = 1.61 | BMK = 0.81 | MCSE(6.27) = 14.6 | stat: FALSE | burn: 612**

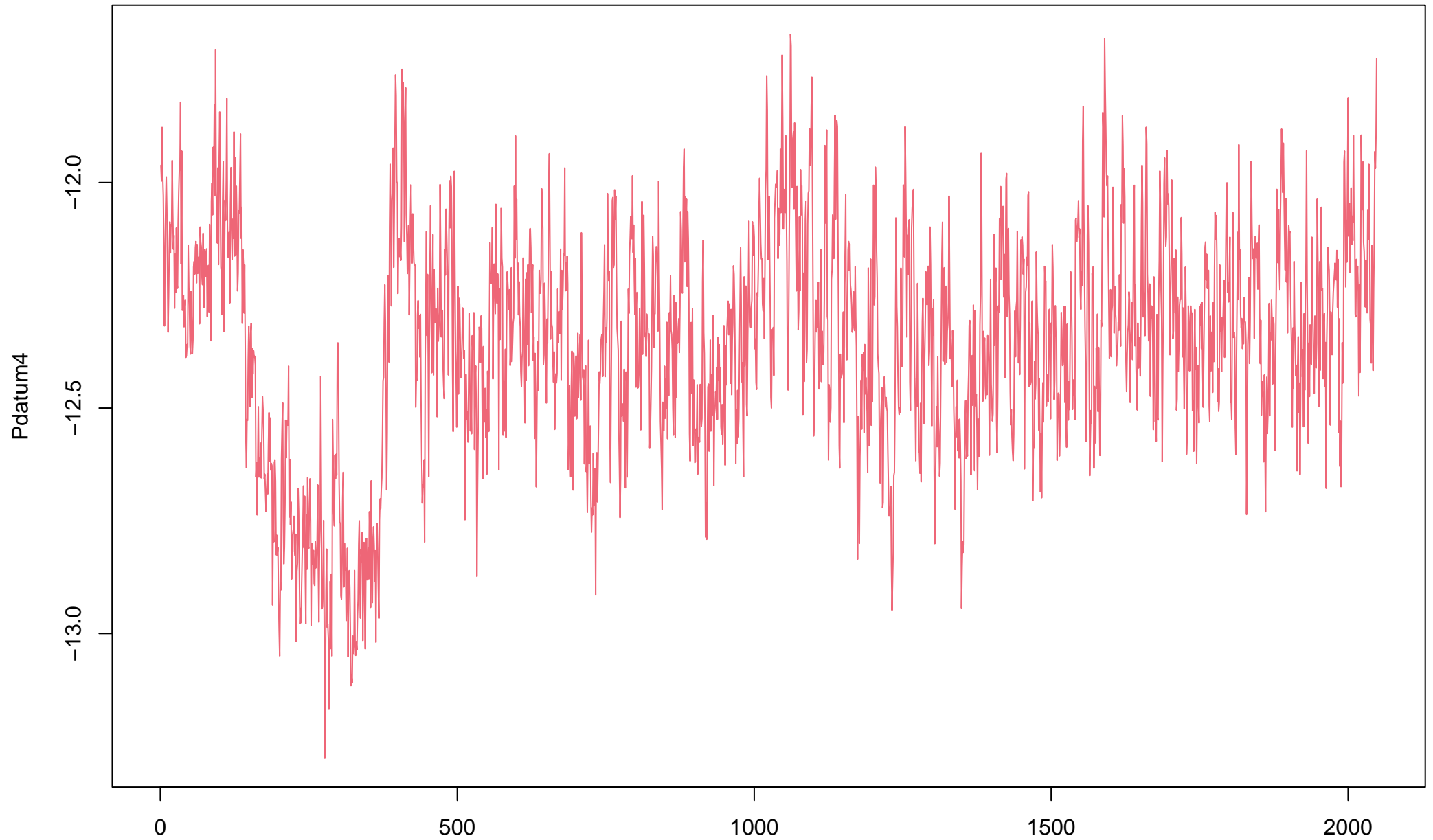




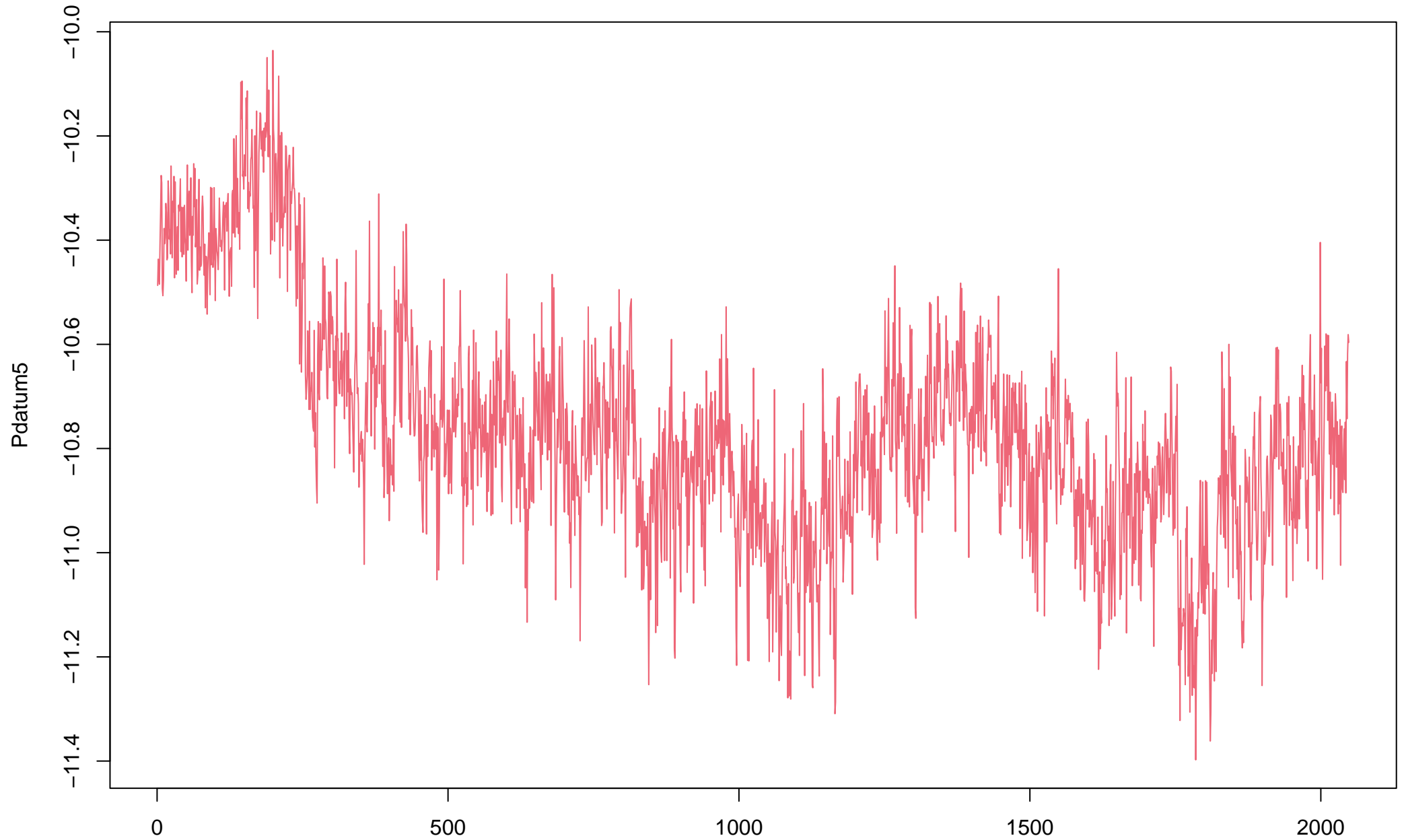
**Pdatum3**  
**ESS = 3.98 | BMK = 0.476 | MCSE(6.27) = 14.2 | stat: FALSE | burn: 408**



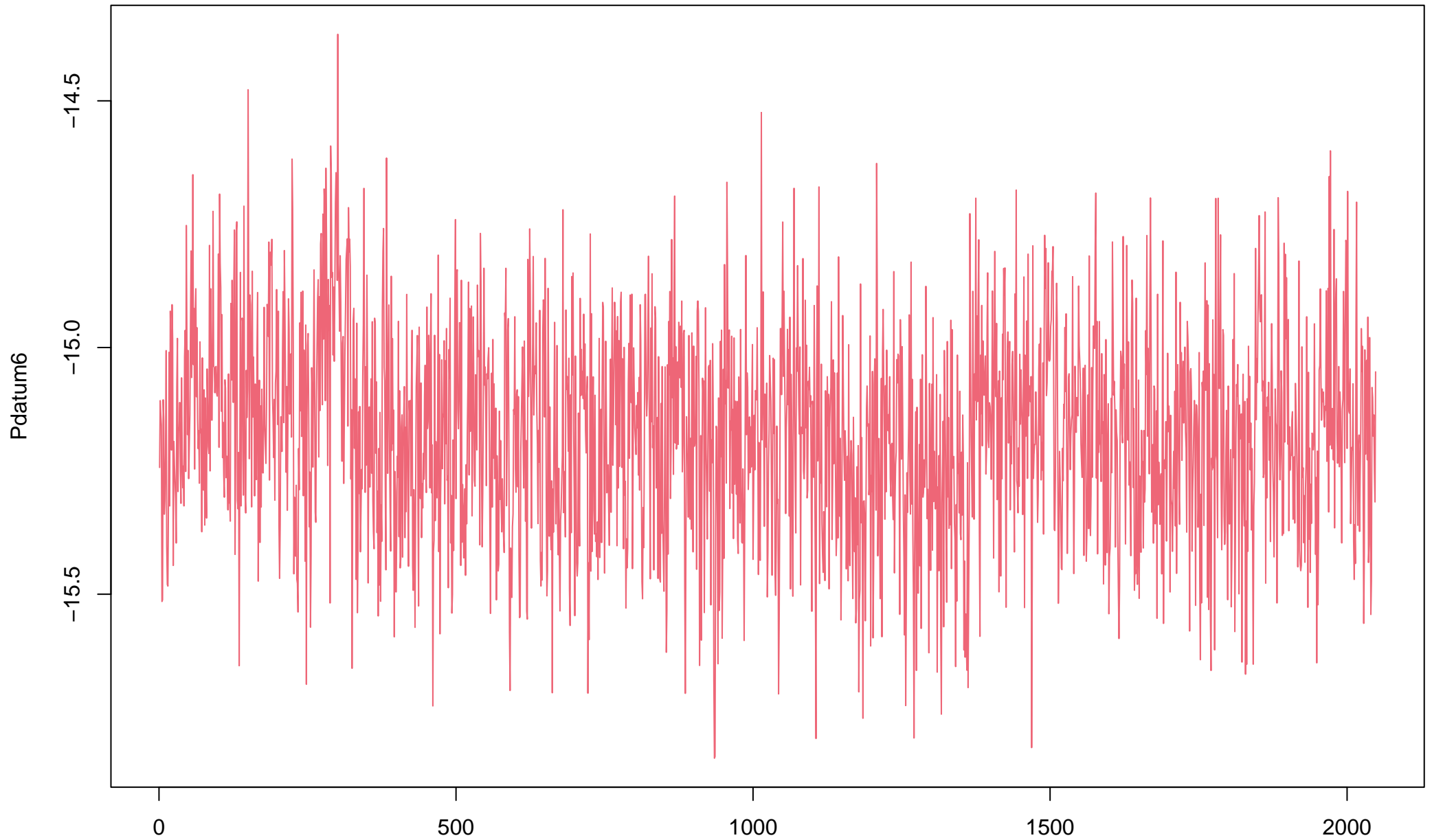
**Pdatum4**  
**ESS = 58.6 | BMK = 0.203 | MCSE(6.27) = 9.78 | stat: TRUE | burn: 408**



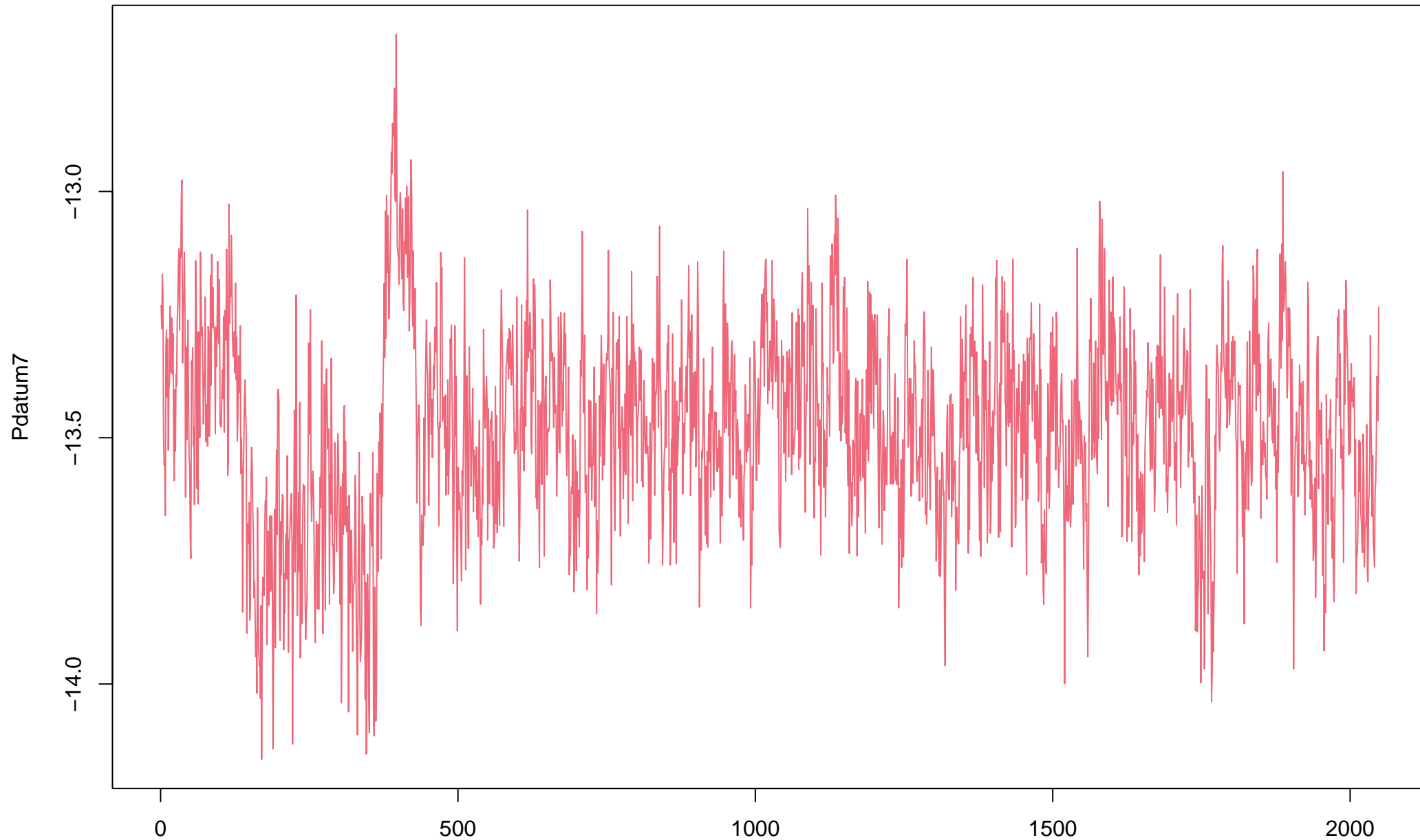
**Pdatum5**  
**ESS = 9.48 | BMK = 0.389 | MCSE(6.27) = 13.2 | stat: FALSE | burn: 1224**



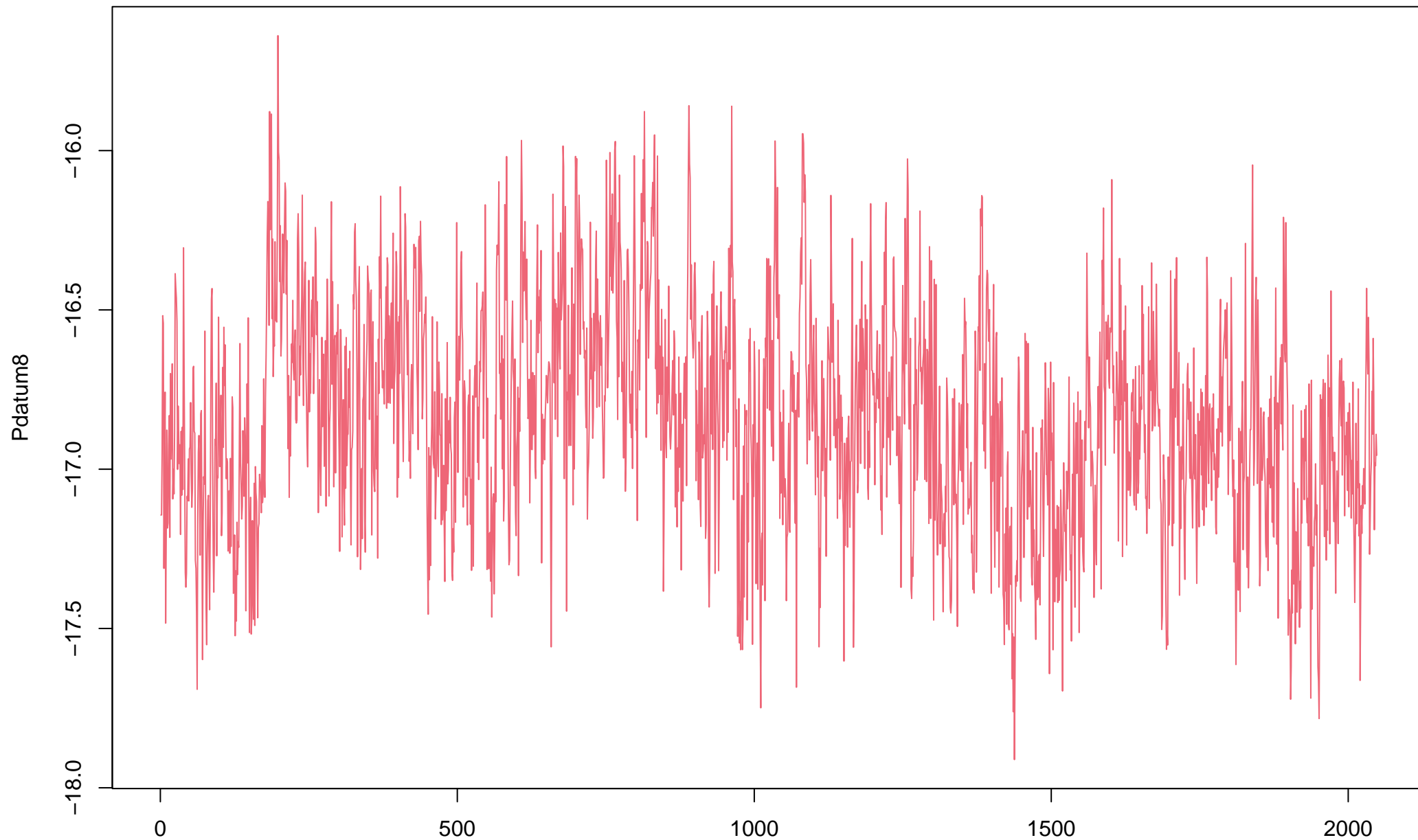
**Pdatum6**  
**ESS = 442 | BMK = 0.0774 | MCSE(6.27) = 4.94 | stat: FALSE | burn: 0**



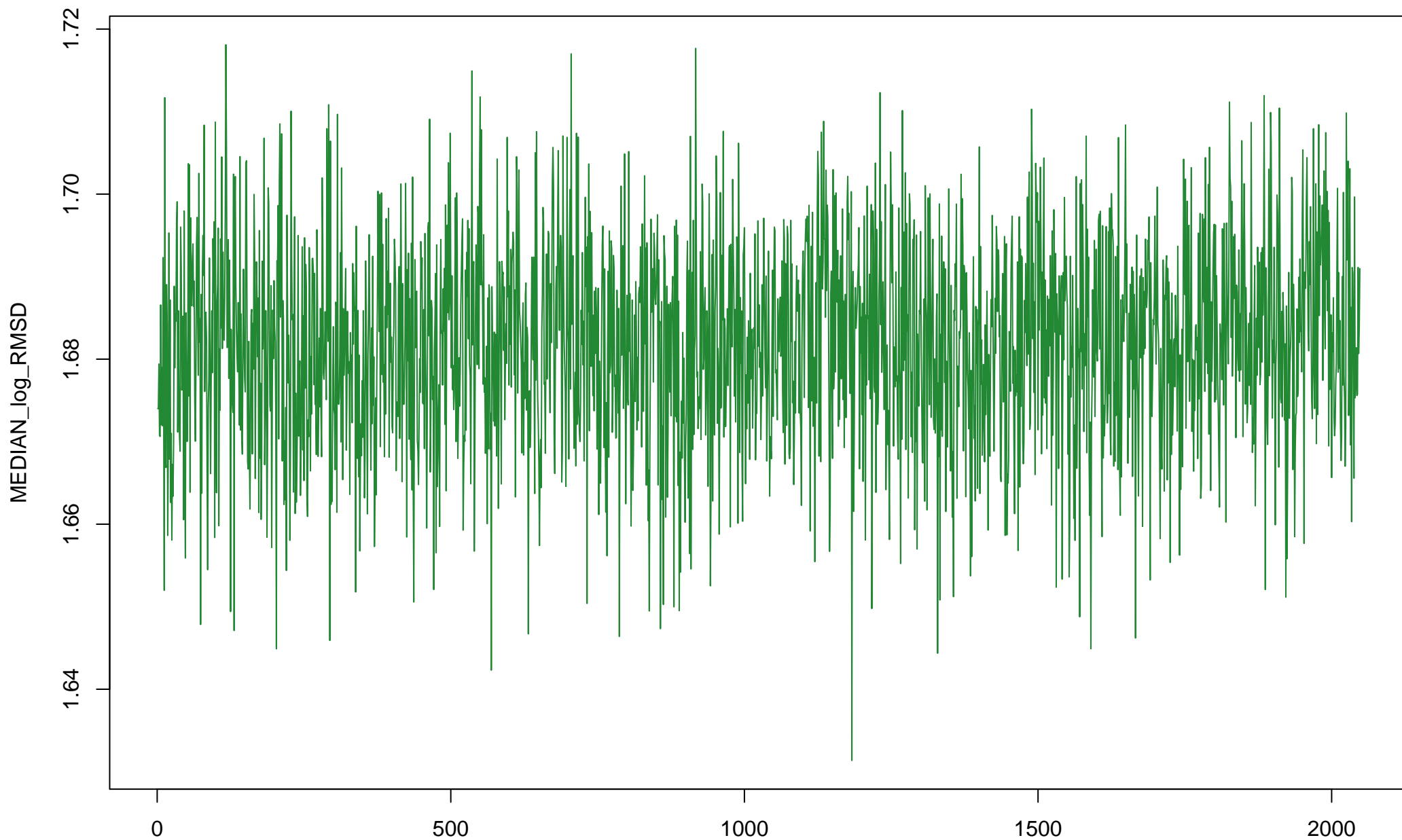
**Pdatum7**  
**ESS = 105 | BMK = 0.122 | MCSE(6.27) = 8.3 | stat: TRUE | burn: 0**



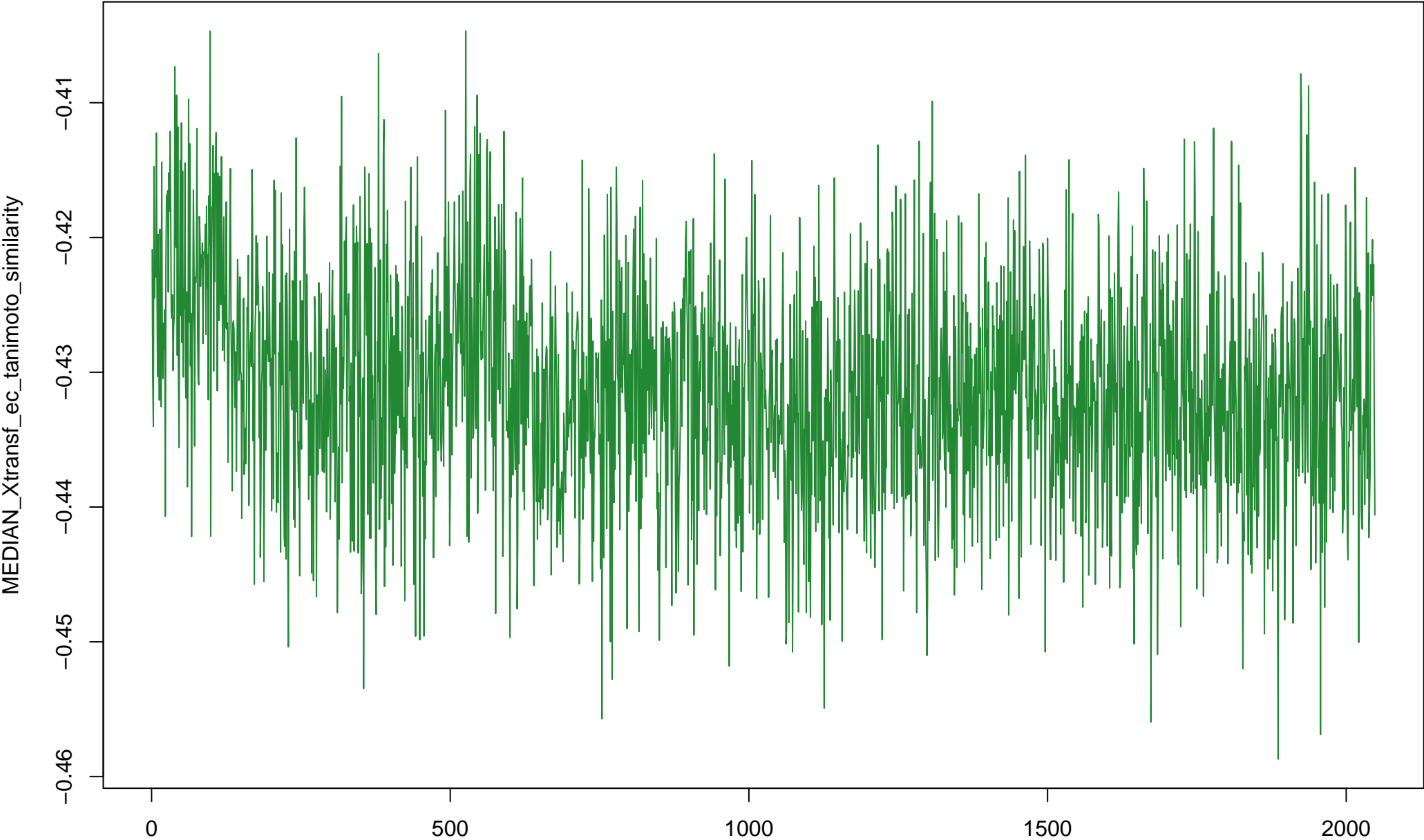
**Pdatum8**  
**ESS = 175 | BMK = 0.185 | MCSE(6.27) = 7.78 | stat: TRUE | burn: 0**



**MEDIAN\_log\_RMSD**  
**ESS = 1170 | BMK = 0.0611 | MCSE(6.27) = 2.79 | stat: TRUE | burn: 0**

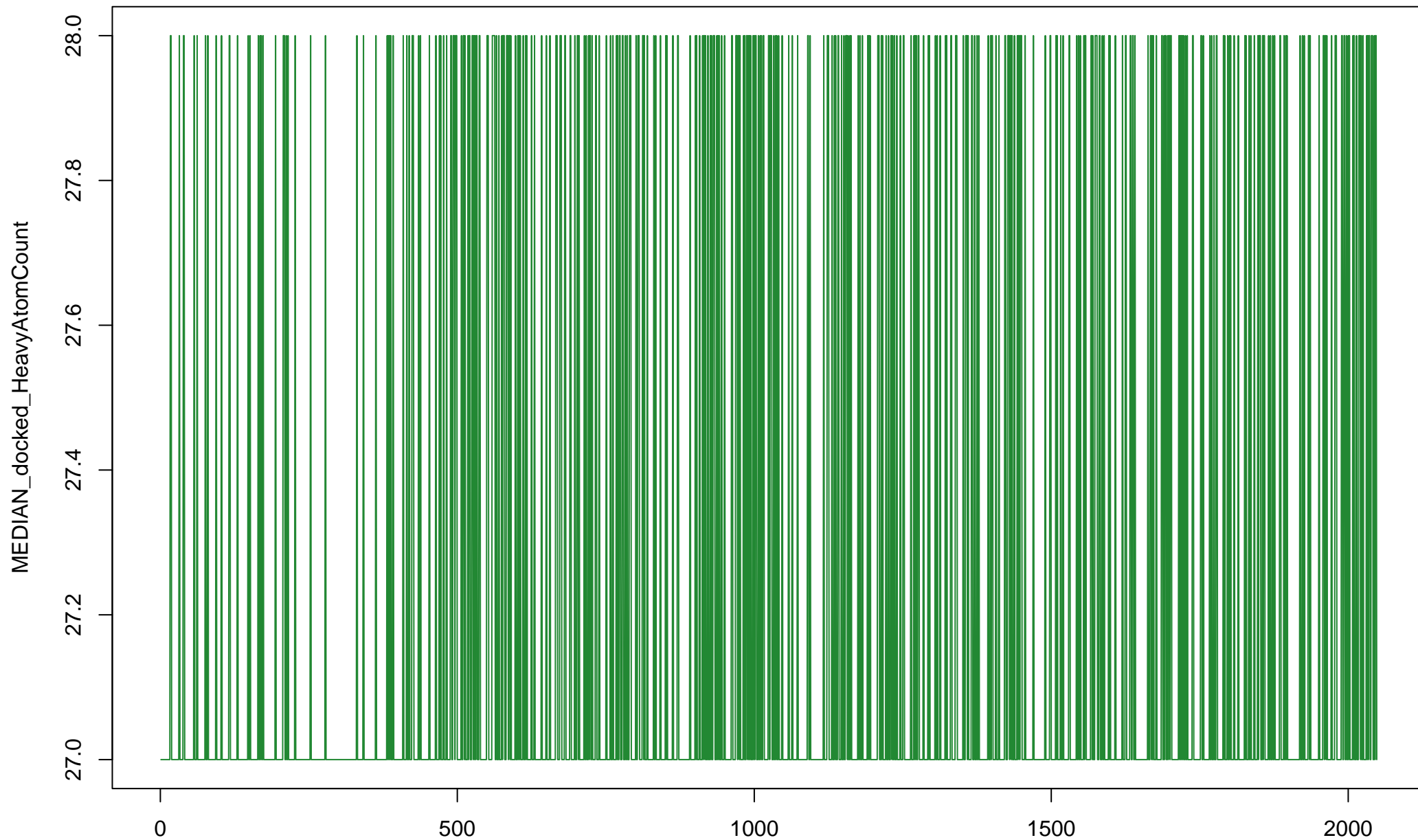


**MEDIAN\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 144 | BMK = 0.119 | MCSE(6.27) = 5.02 | stat: FALSE | burn: 0**

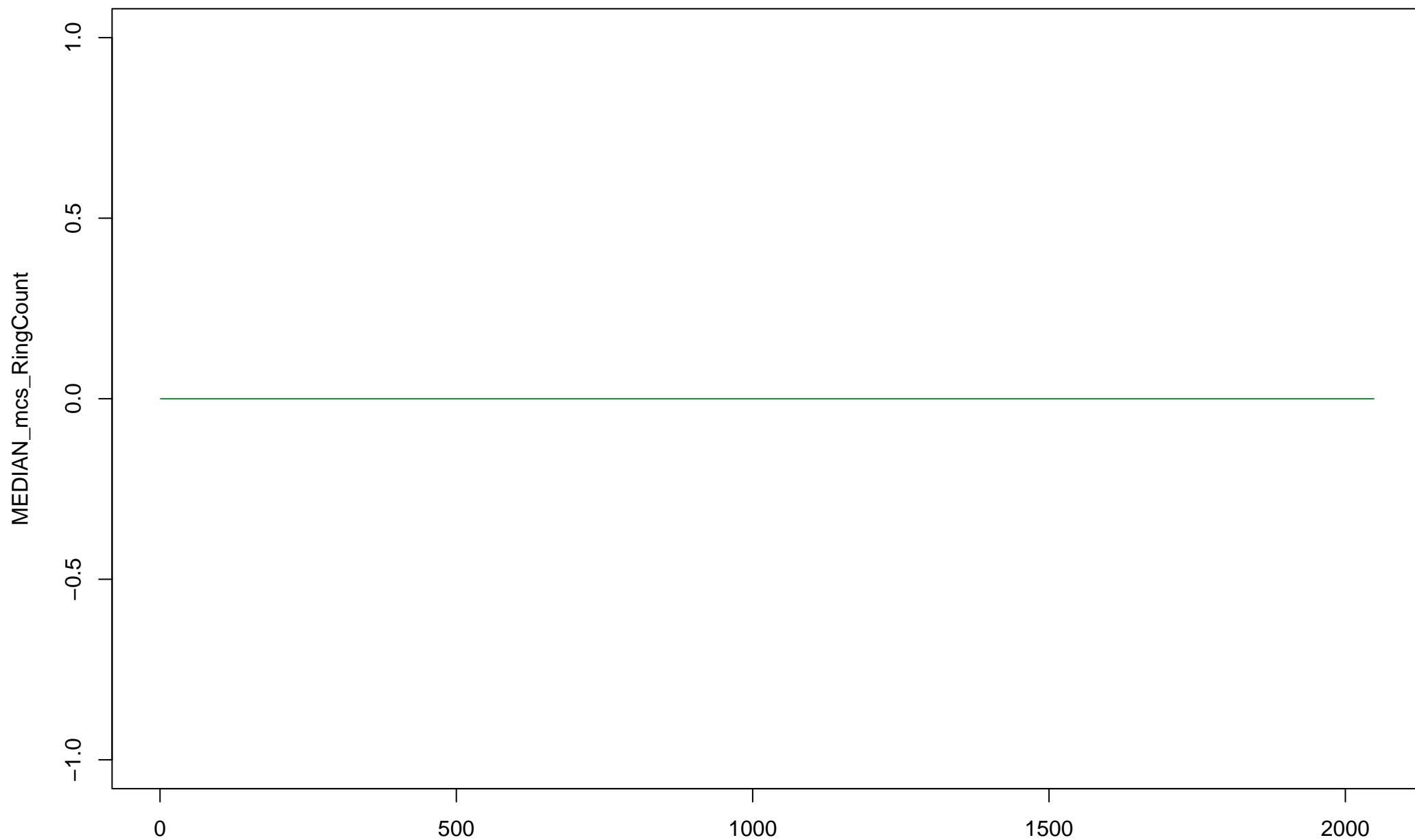




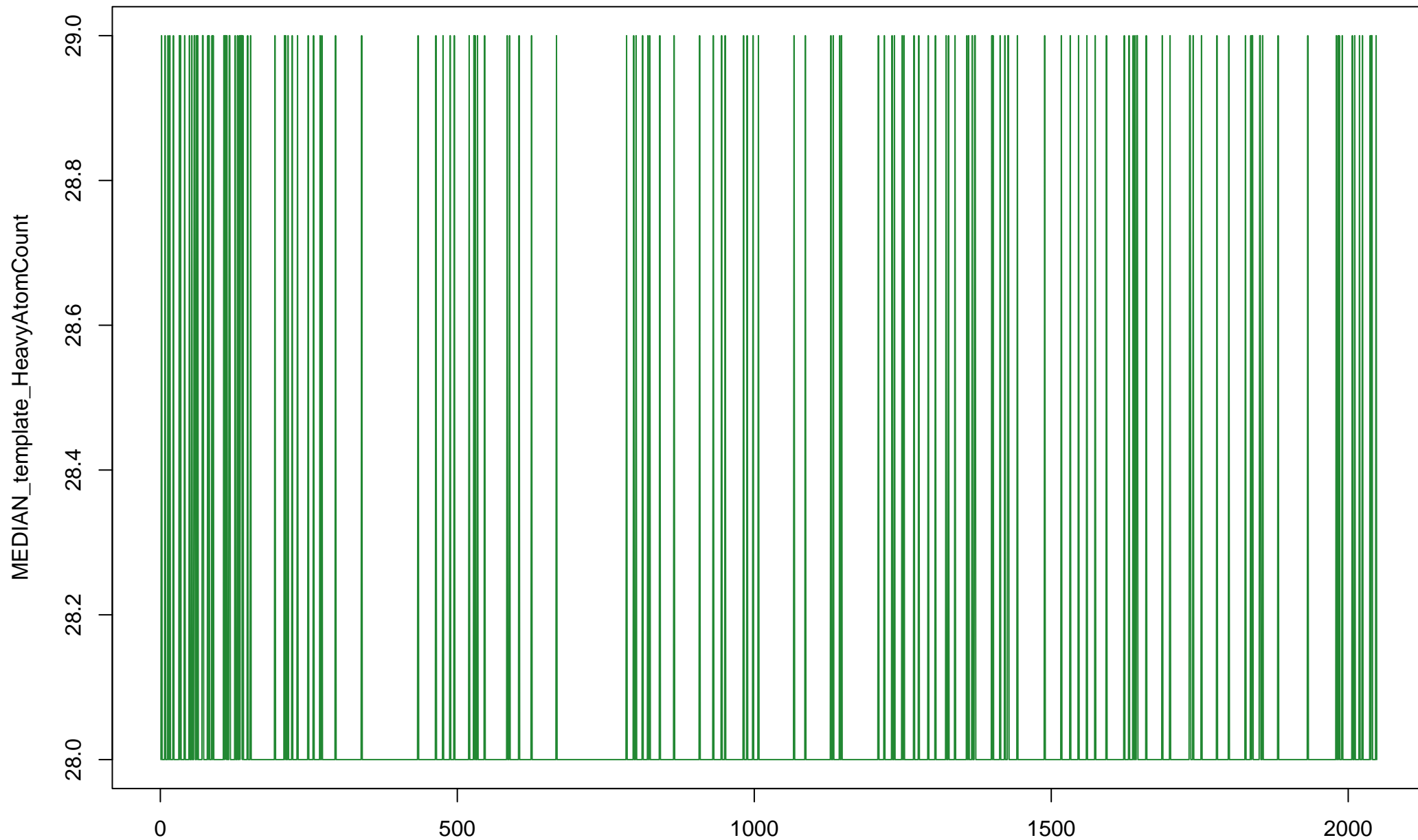
**MEDIAN\_docked\_HeavyAtomCount**  
**ESS = 1170 | BMK = 0.0338 | MCSE(6.27) = 3.33 | stat: FALSE | burn: 0**



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



**MEDIAN\_template\_HeavyAtomCount**  
**ESS = 1580 | BMK = 0.00935 | MCSE(6.27) = 3.25 | stat: FALSE | burn: 0**



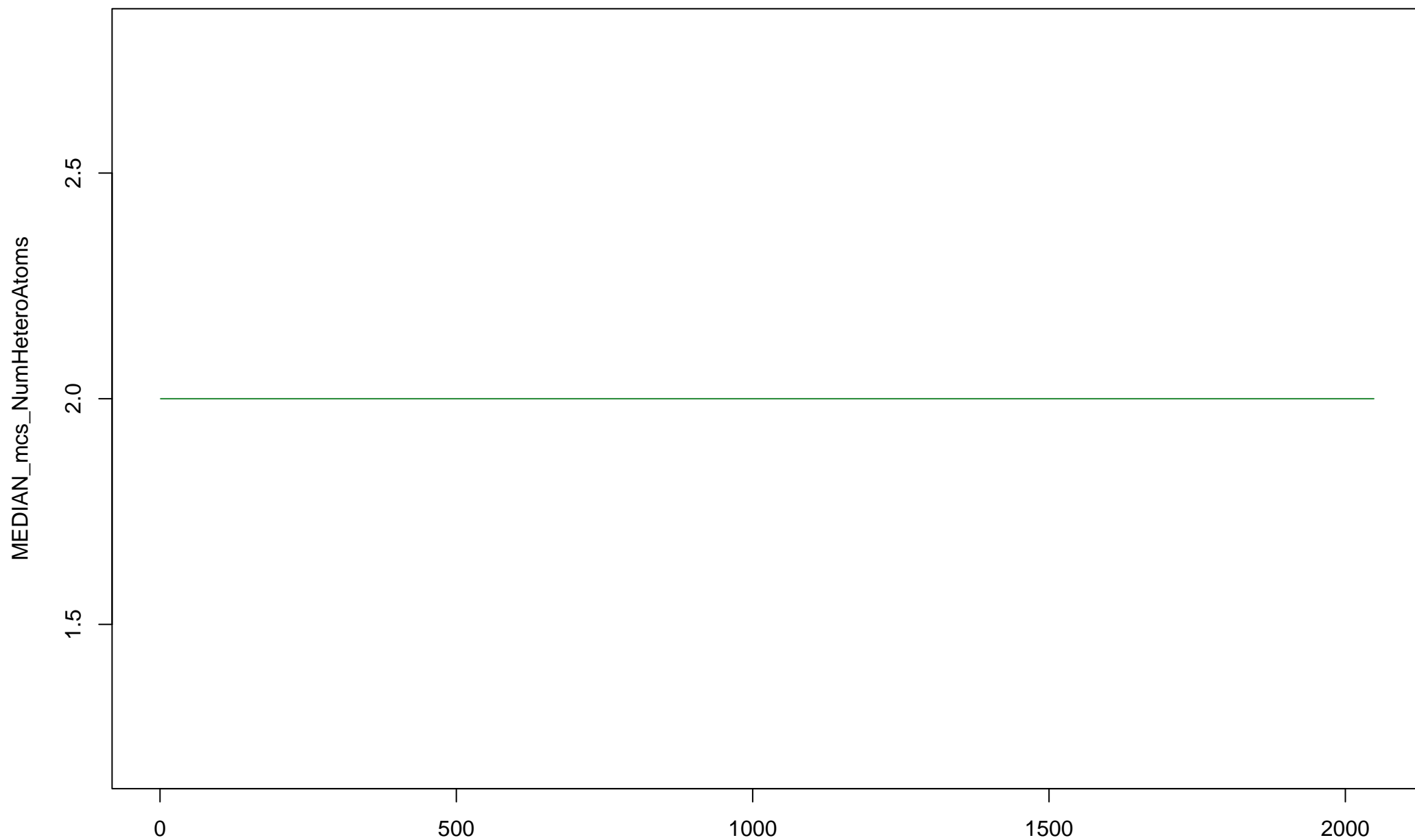
**MEDIAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



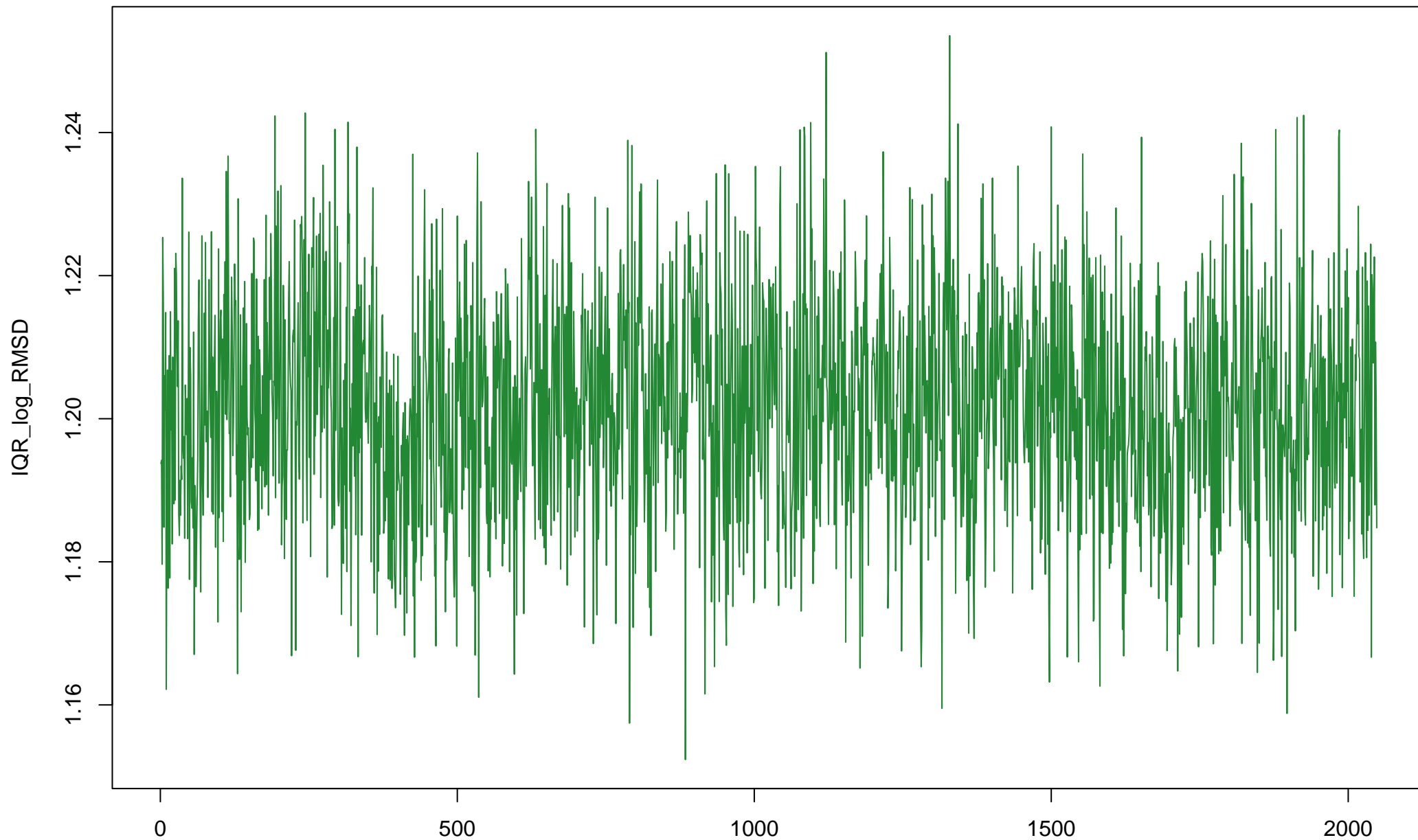
**MEDIAN\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



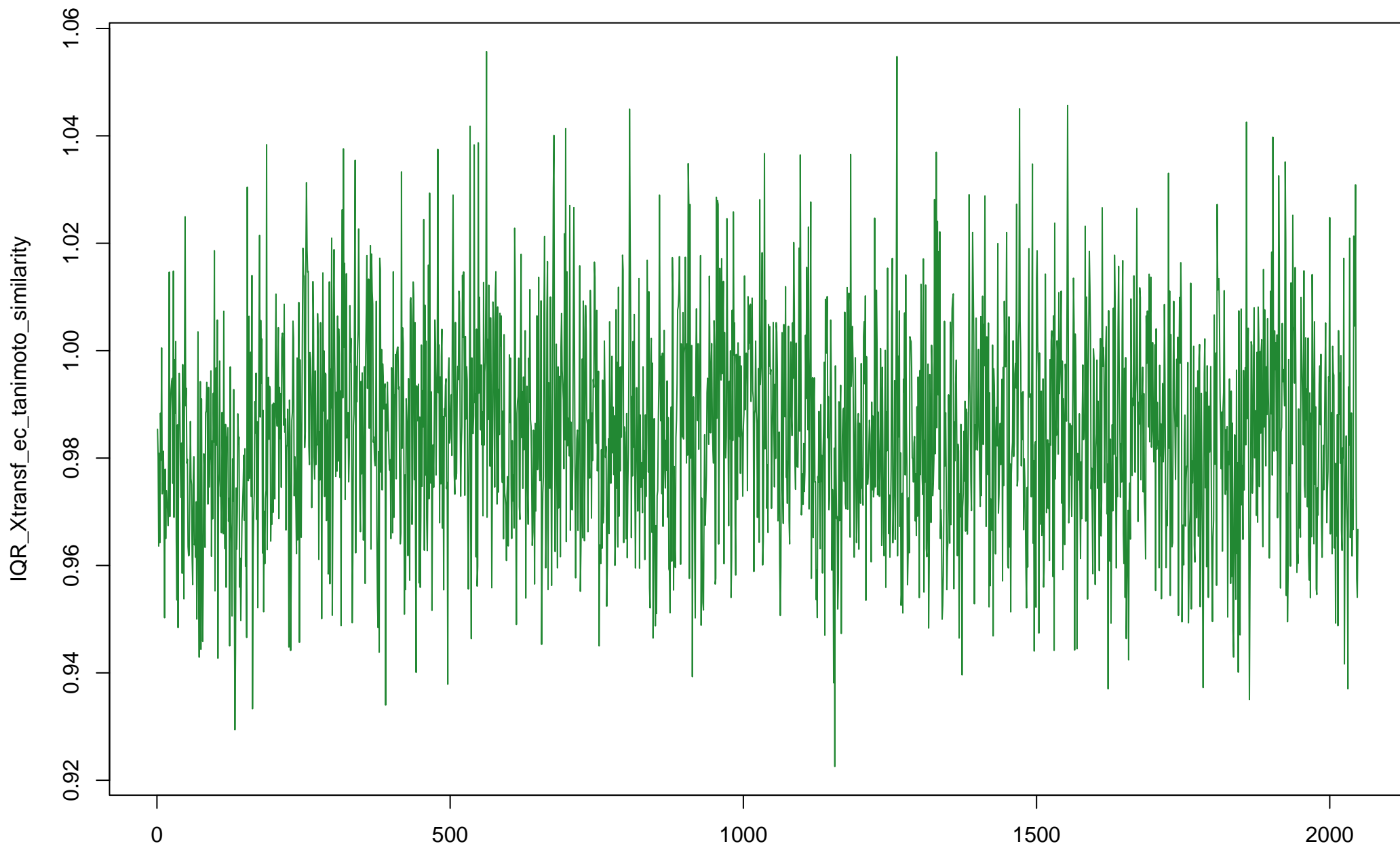
**MEDIAN\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



IQR\_log\_RMSD  
ESS = 1030 | BMK = 0.0439 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0

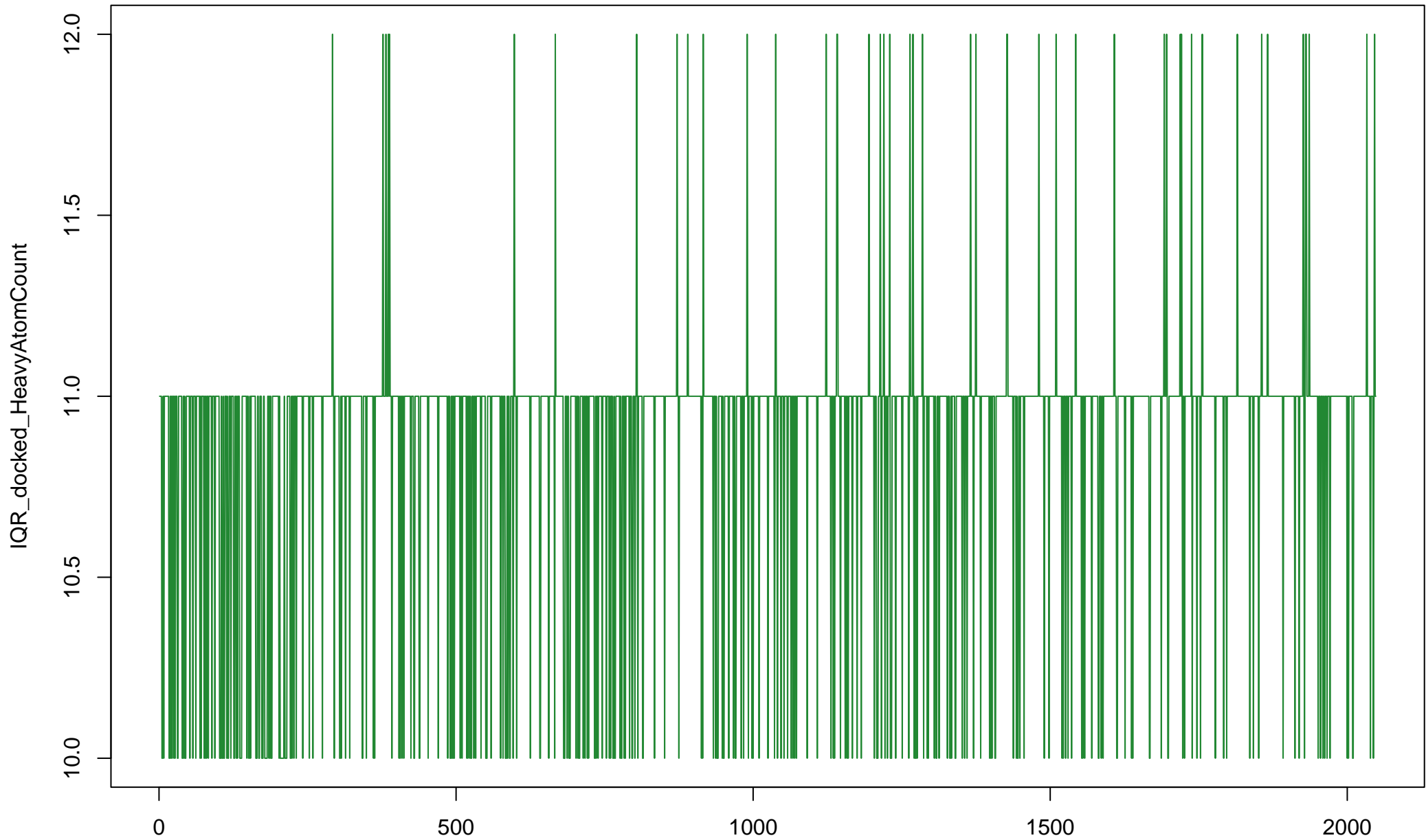


IQR\_Xtransf\_ec\_tanimoto\_similarity  
ESS = 996 | BMK = 0.0327 | MCSE(6.27) = 3.51 | stat: FALSE | burn: 0

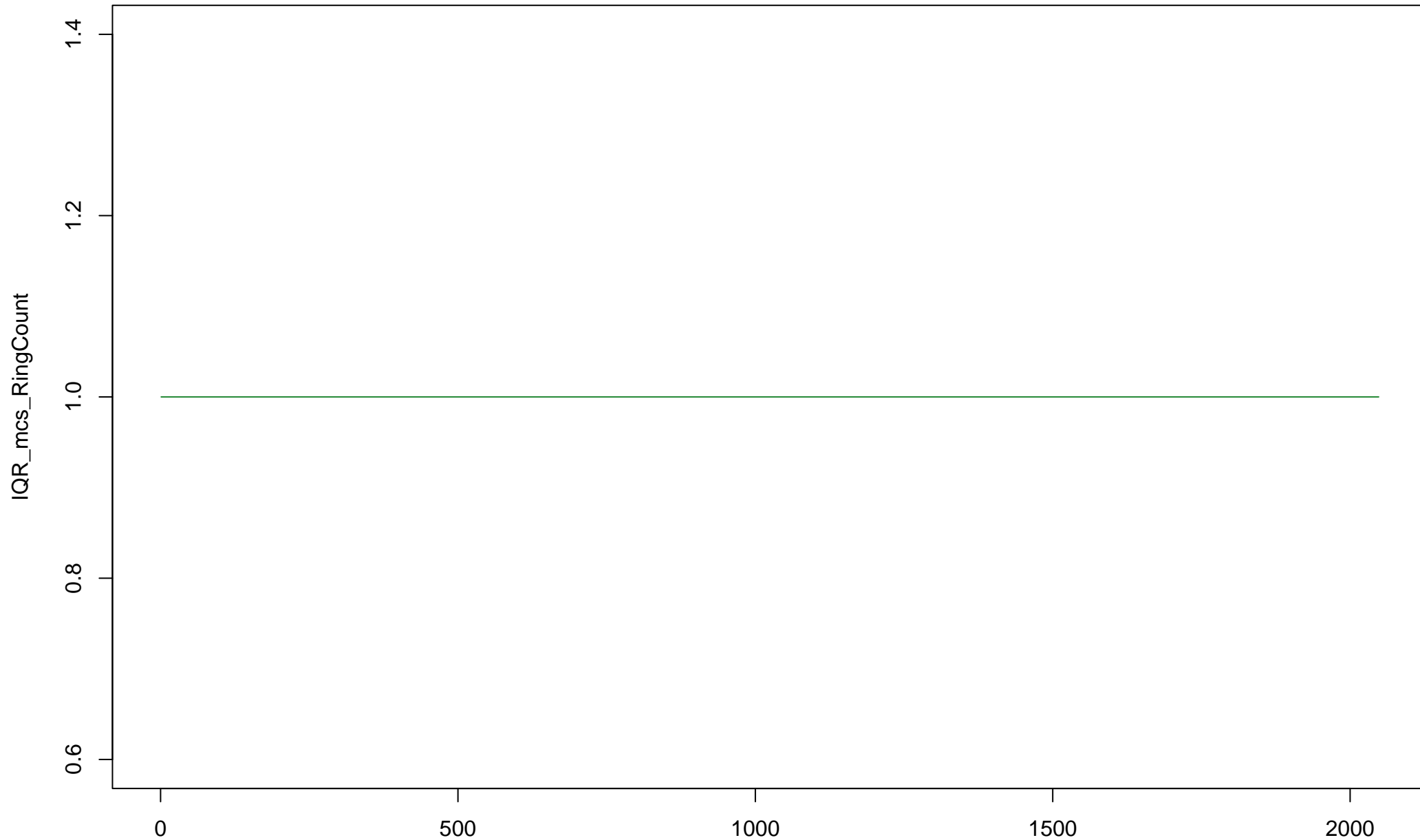




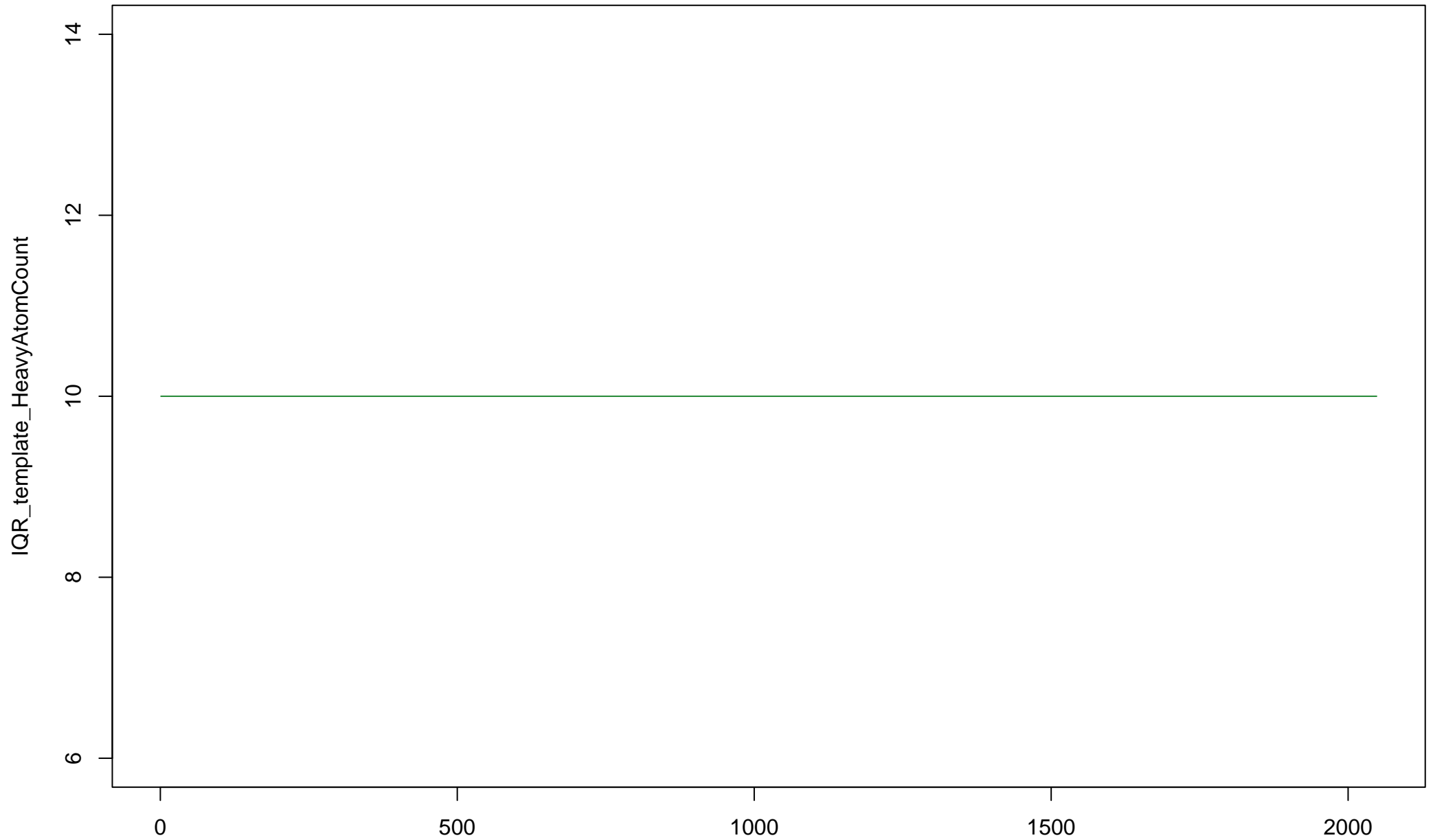
IQR\_docked\_HeavyAtomCount  
ESS = 798 | BMK = 0.0874 | MCSE(6.27) = 4.04 | stat: FALSE | burn: 0



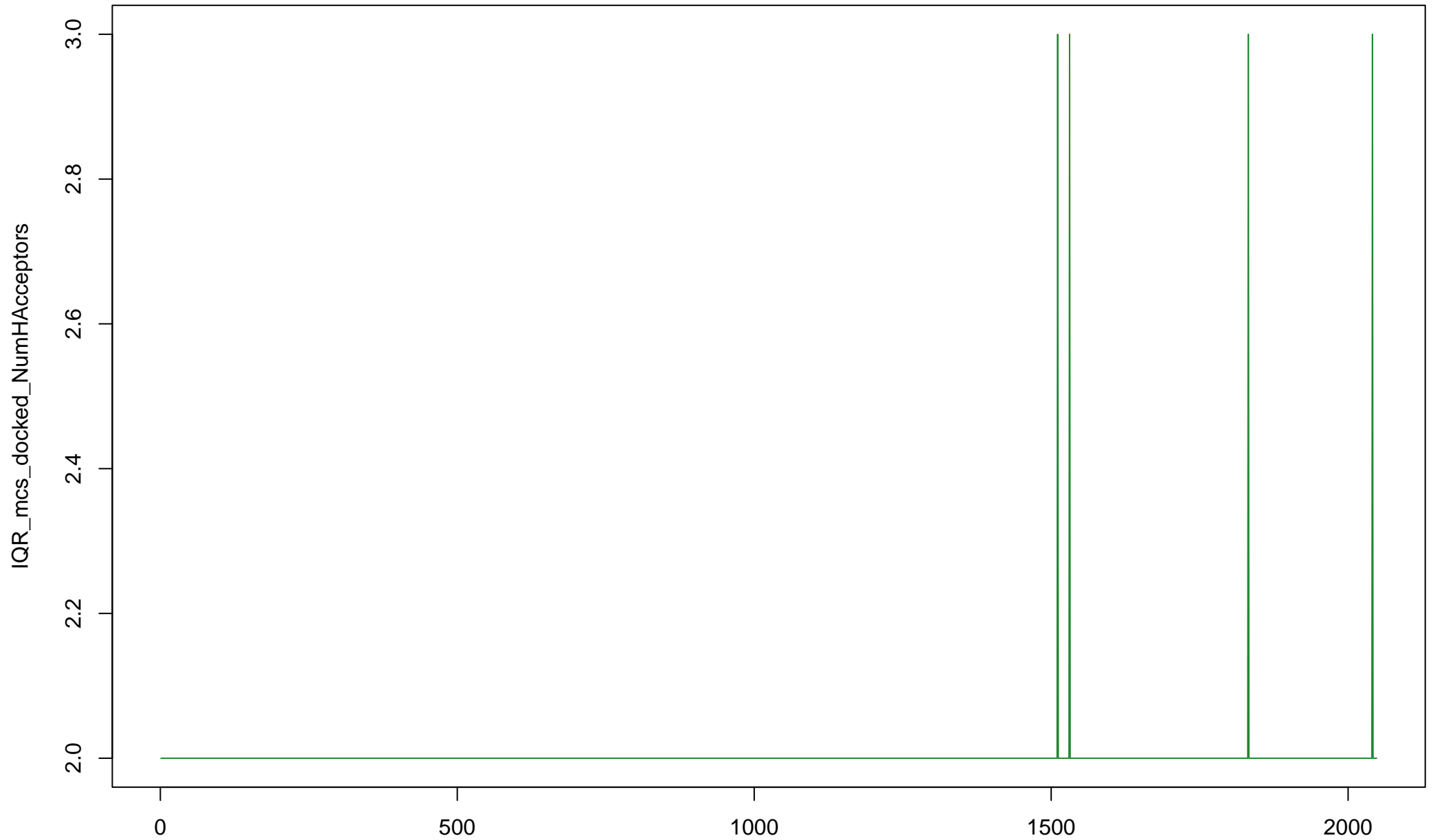
**IQR\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



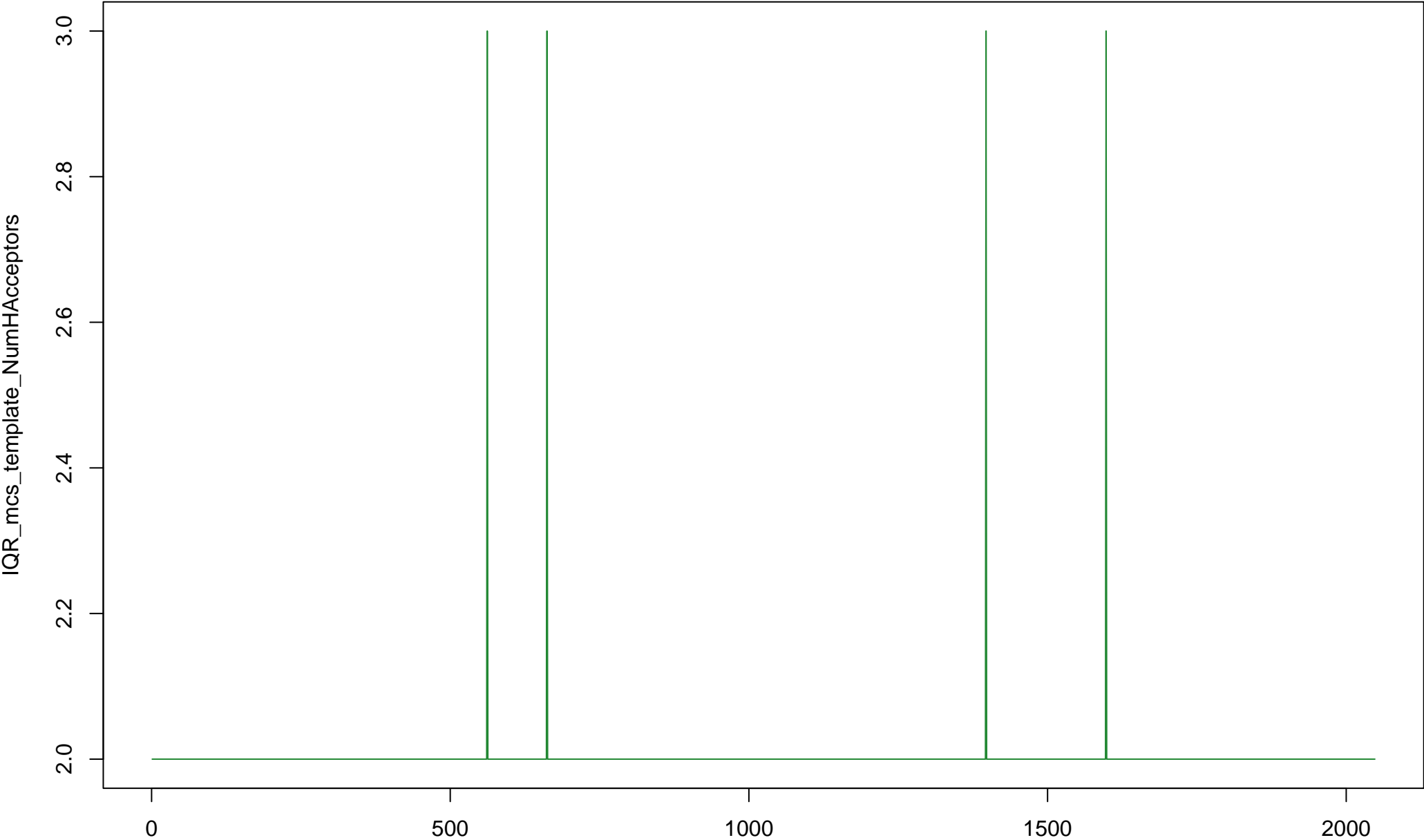
IQR\_template\_HeavyAtomCount  
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



**IQR\_mcs\_docked\_NumHAcceptors**  
**ESS = 1300 | BMK = 0.609 | MCSE(6.27) = 1.88 | stat: TRUE | burn: 2040**



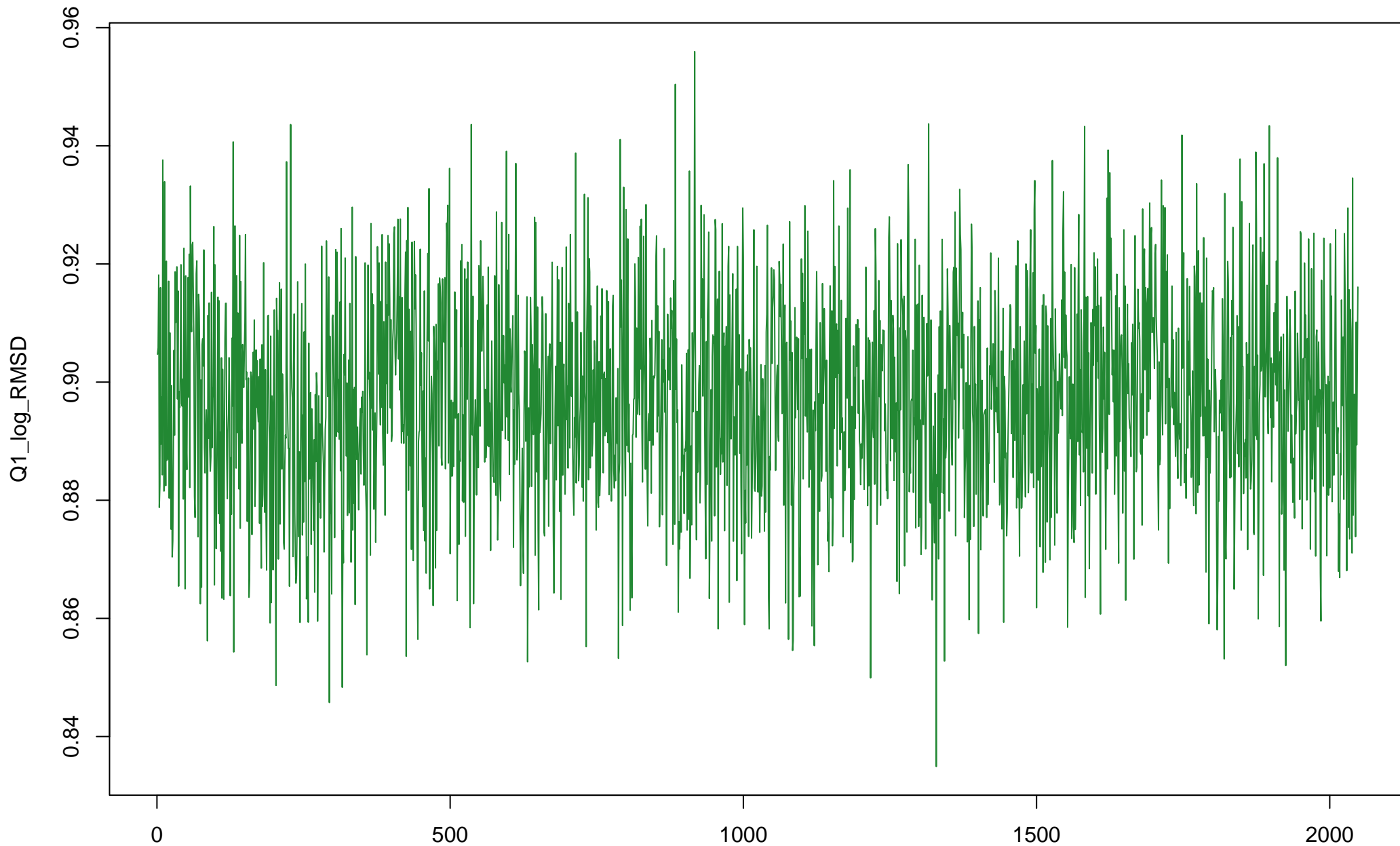
IQR\_mcs\_template\_NumHAcceptors  
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.15 | stat: FALSE | burn: 1632



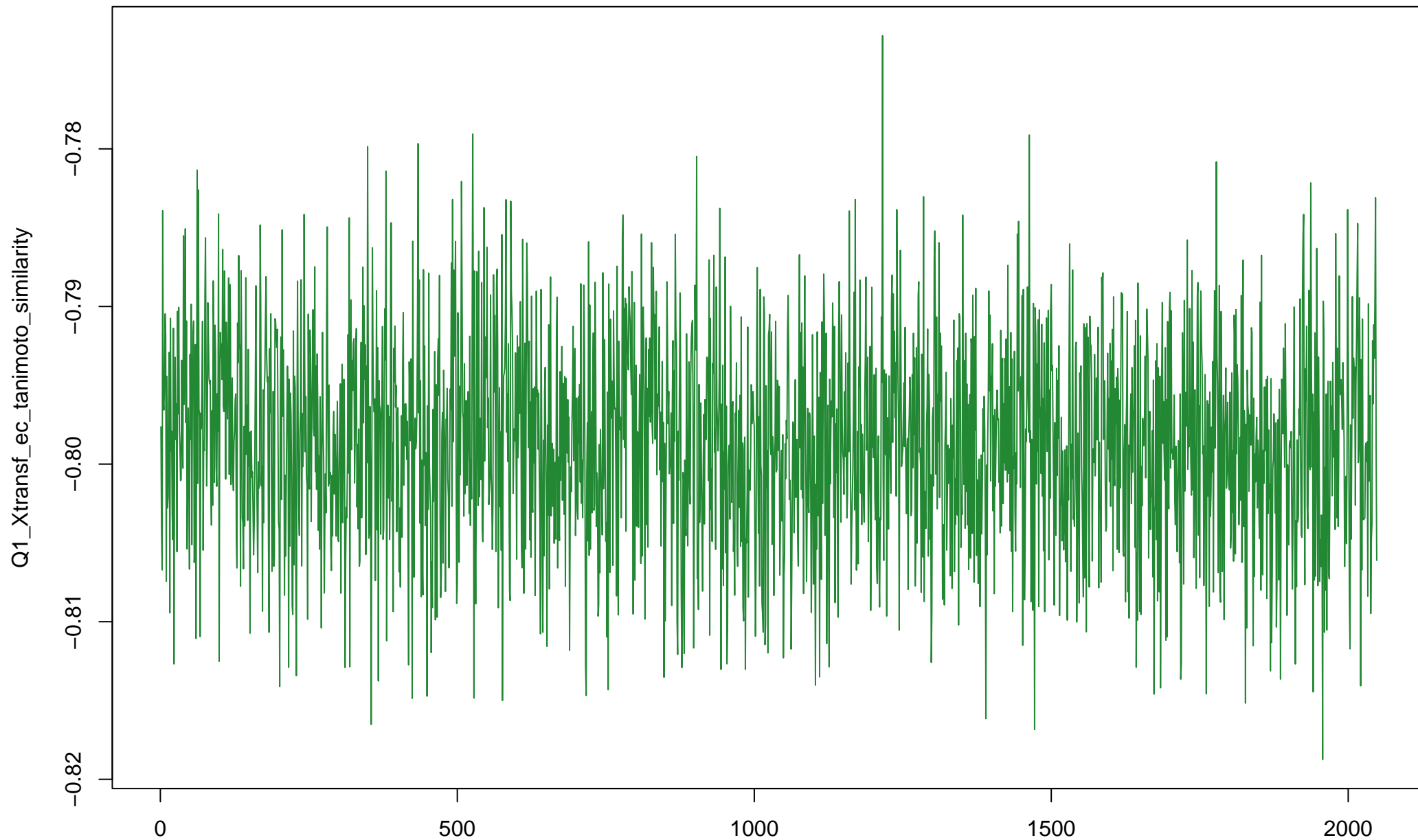
IQR\_mcs\_NumHeteroAtoms  
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



**Q1\_log\_RMSD**  
**ESS = 1100 | BMK = 0.0454 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0**

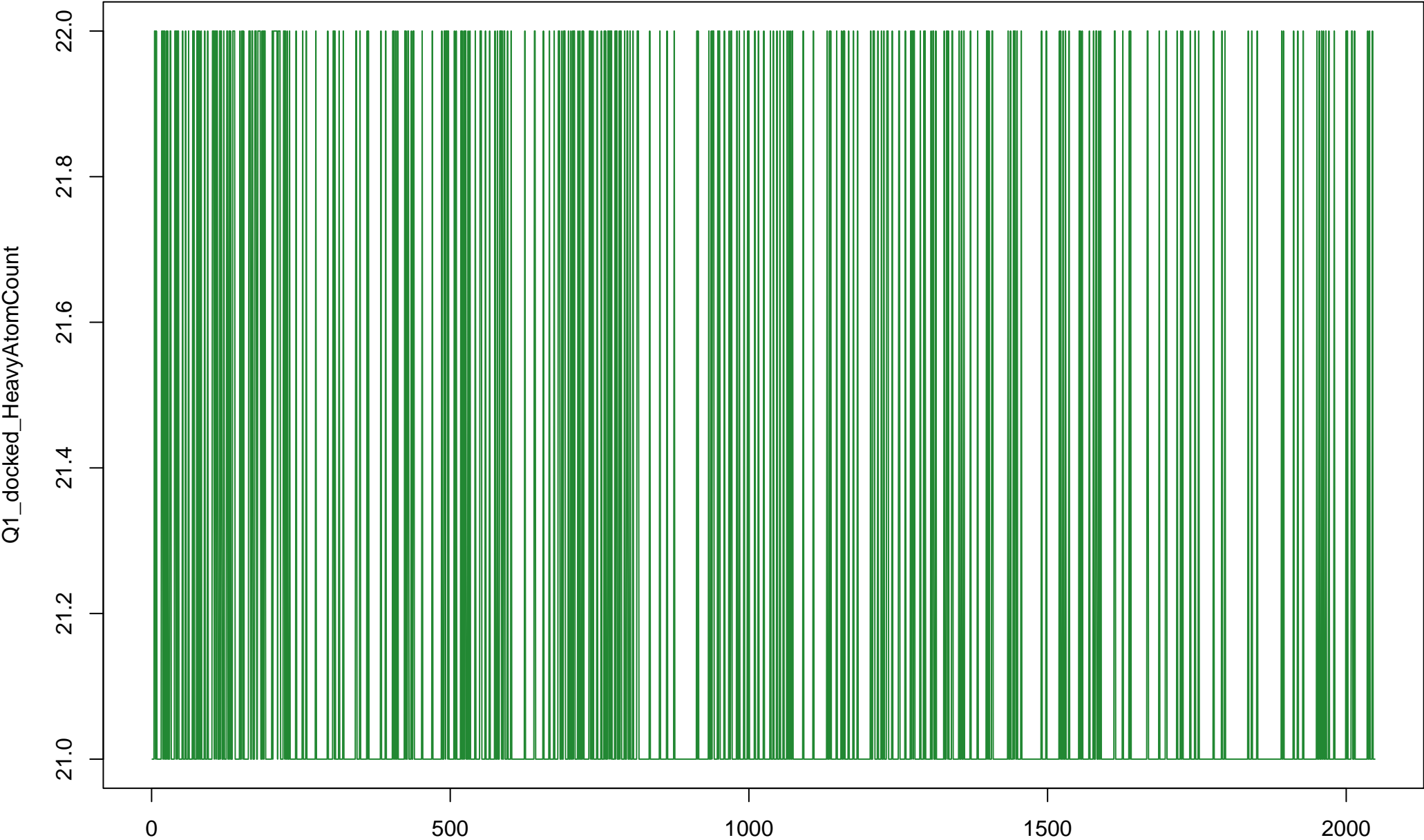


**Q1\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0579 | MCSE(6.27) = 2.93 | stat: FALSE | burn: 0**





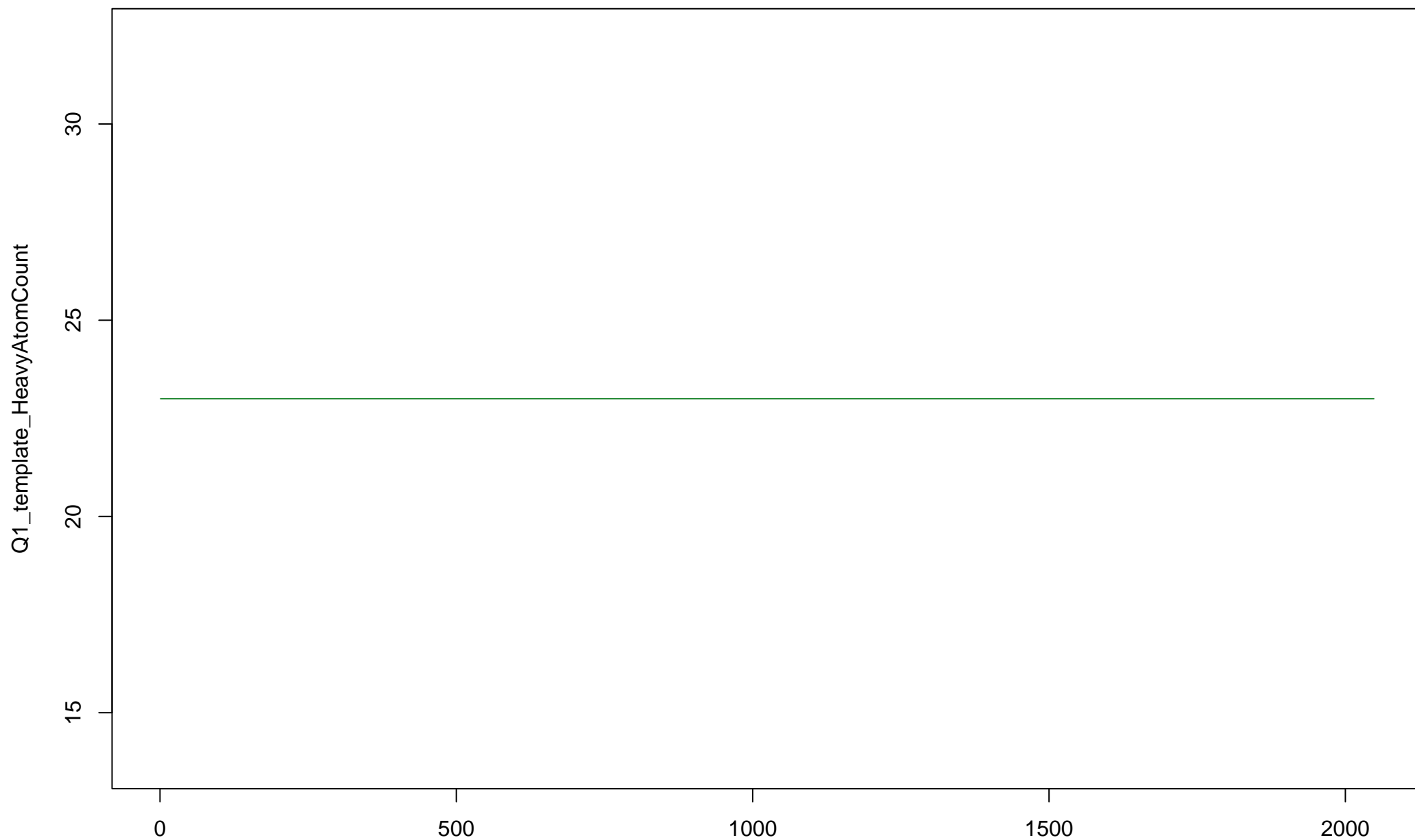
**Q1\_docked\_HeavyAtomCount**  
**ESS = 738 | BMK = 0.0957 | MCSE(6.27) = 3.9 | stat: FALSE | burn: 0**



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



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



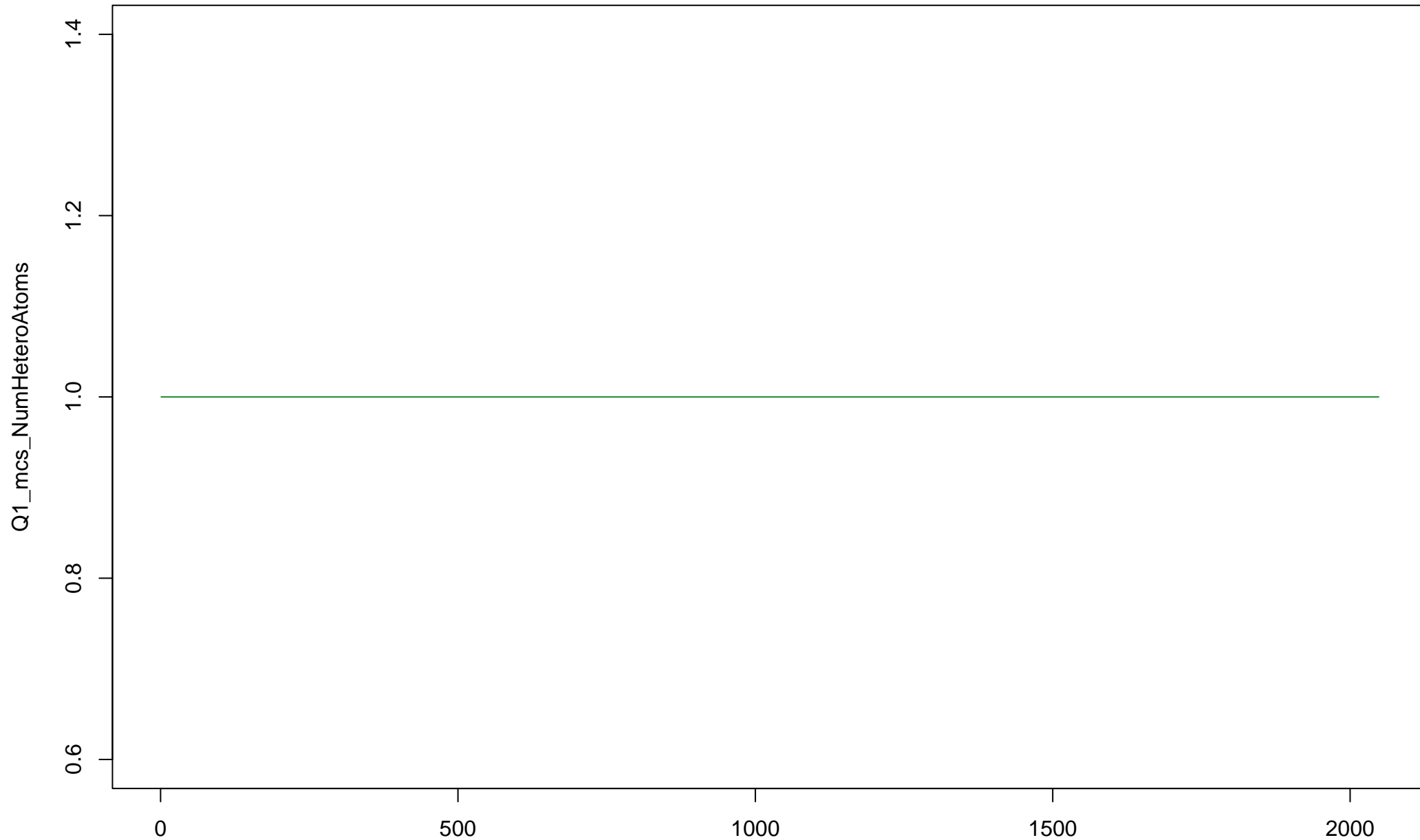
**Q1\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



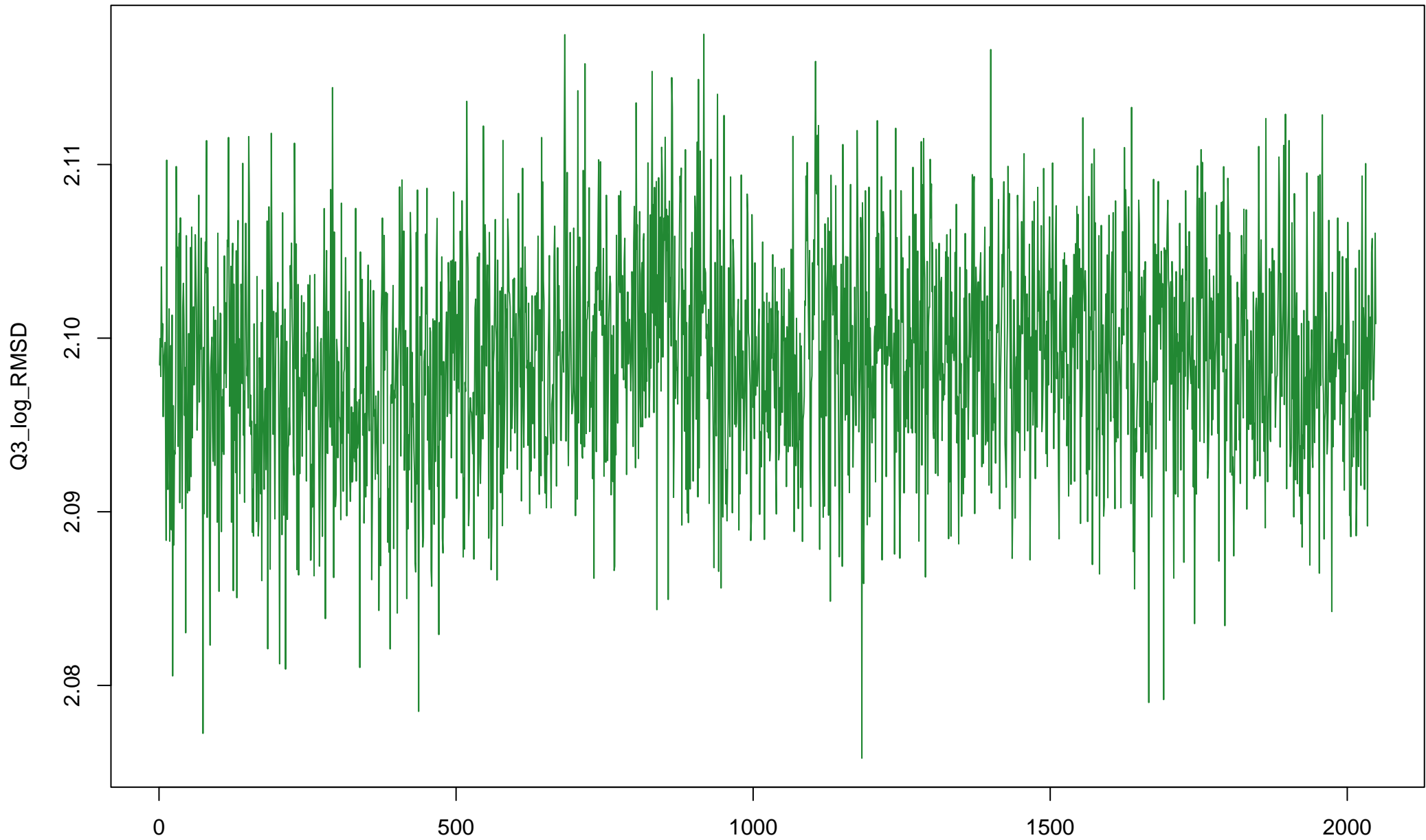
**Q1\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



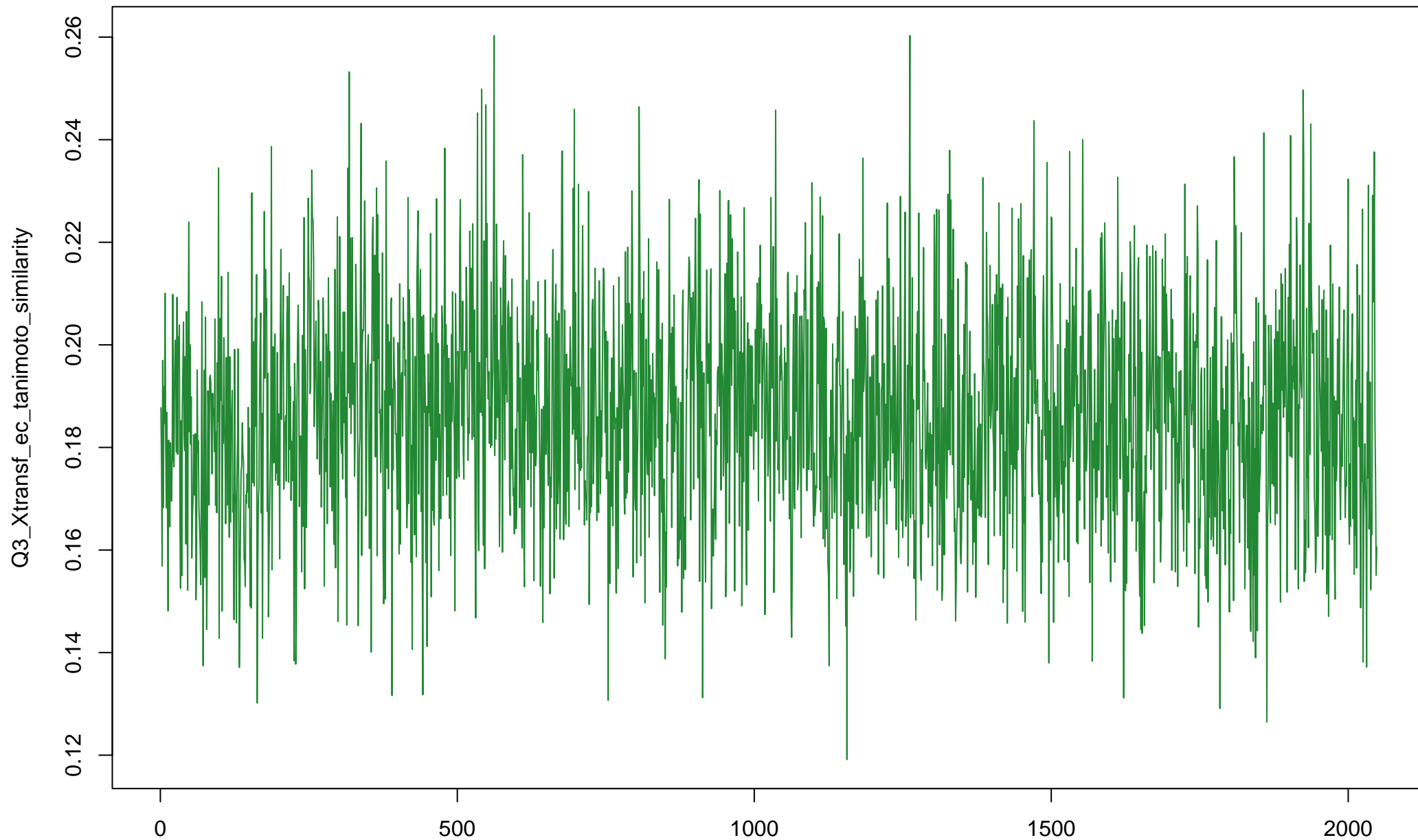
**Q1\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q3\_log\_RMSD**  
**ESS = 891 | BMK = 0.0741 | MCSE(6.27) = 3.51 | stat: FALSE | burn: 0**

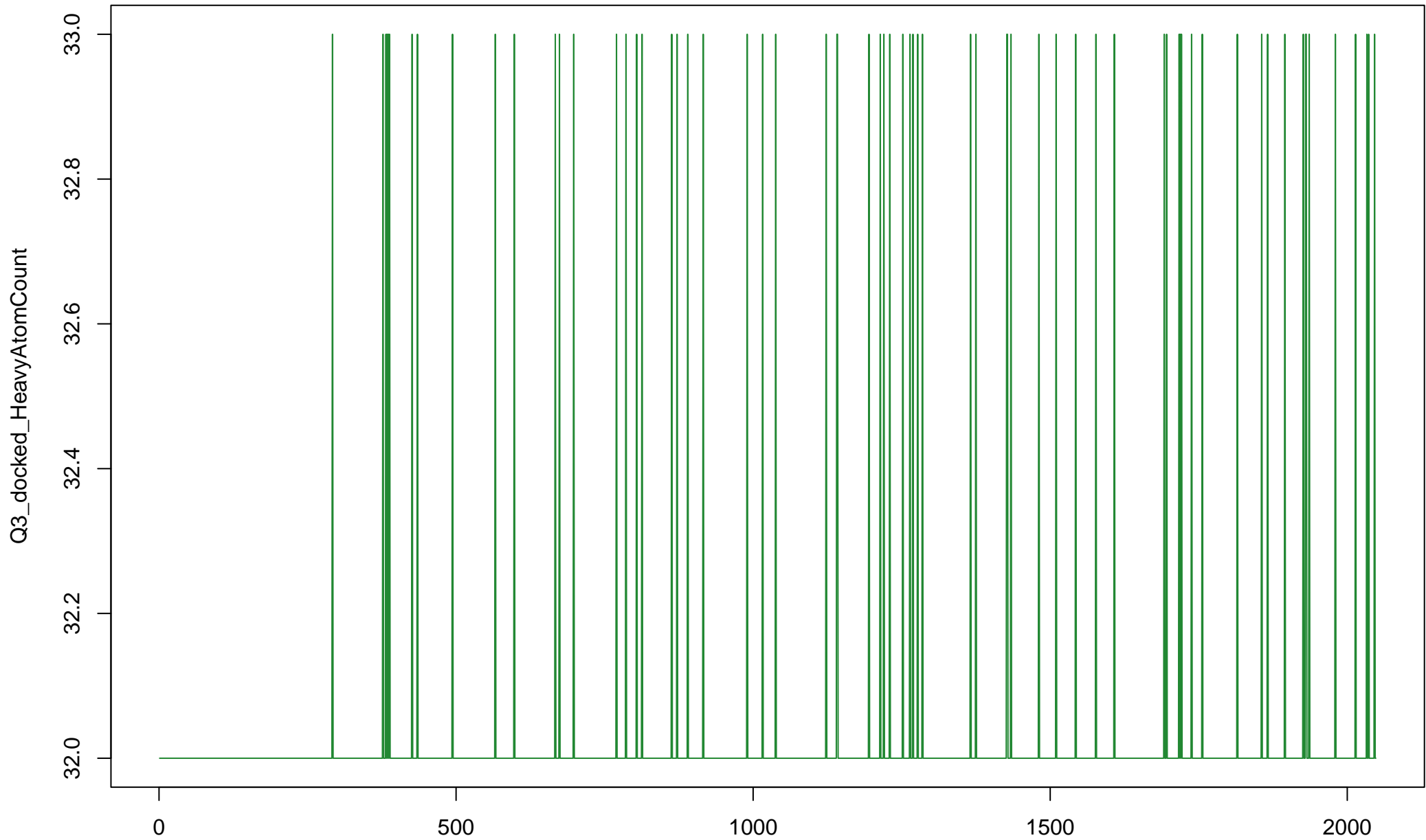


**Q3\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1540 | BMK = 0.0458 | MCSE(6.27) = 3.11 | stat: FALSE | burn: 0**





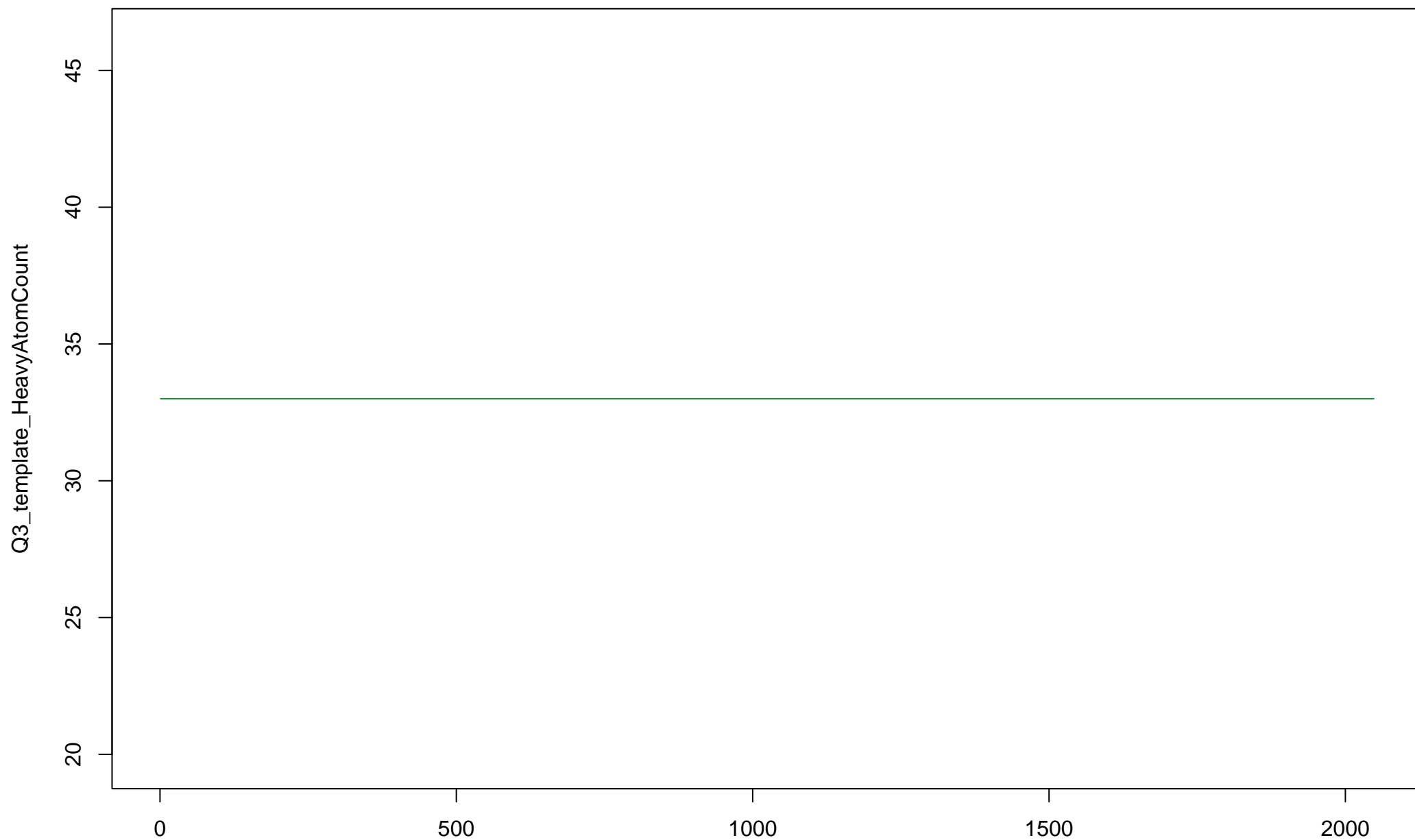
**Q3\_docked\_HeavyAtomCount**  
**ESS = 1740 | BMK = 0.102 | MCSE(6.27) = 2.35 | stat: FALSE | burn: 0**



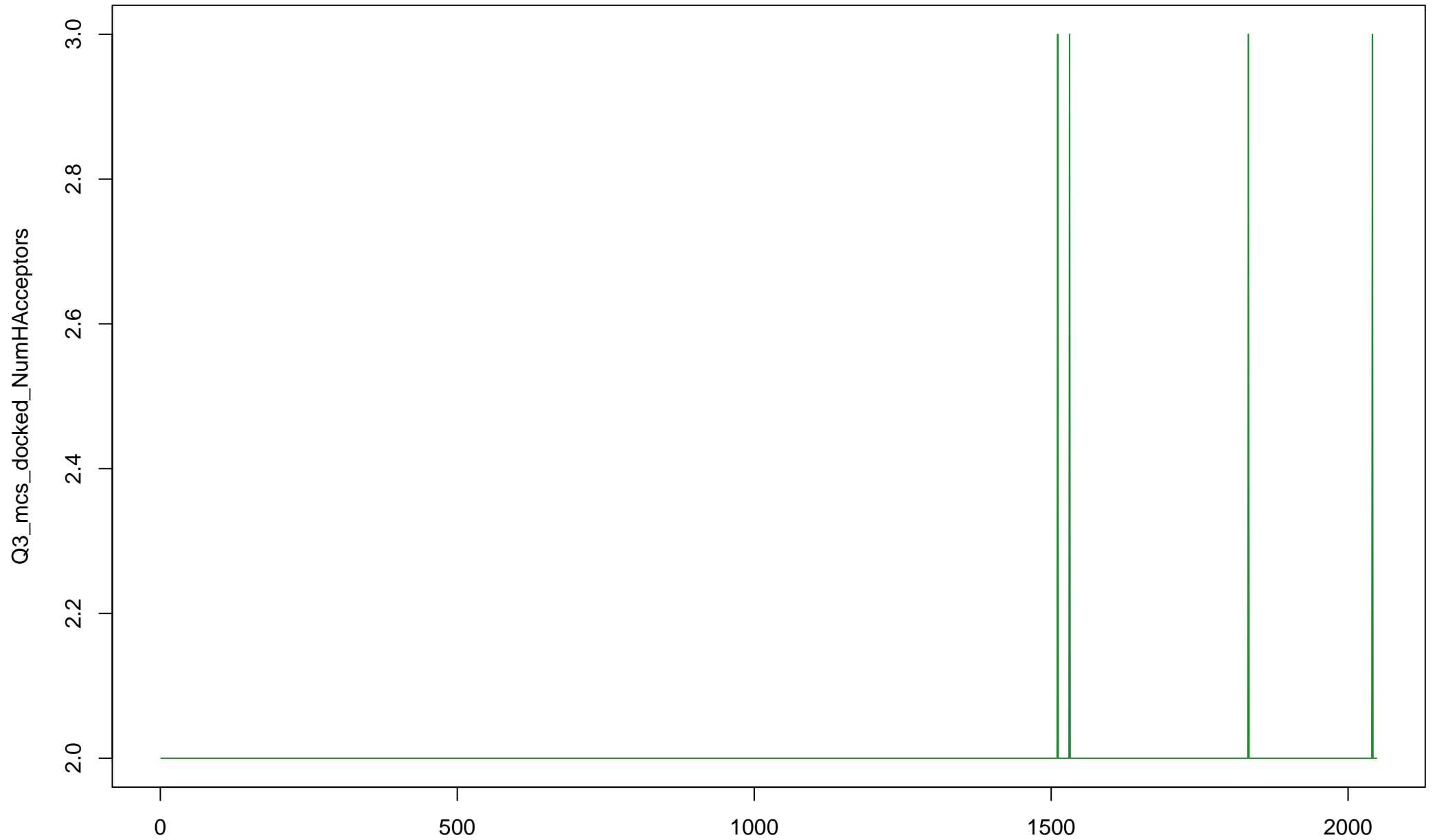
**Q3\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



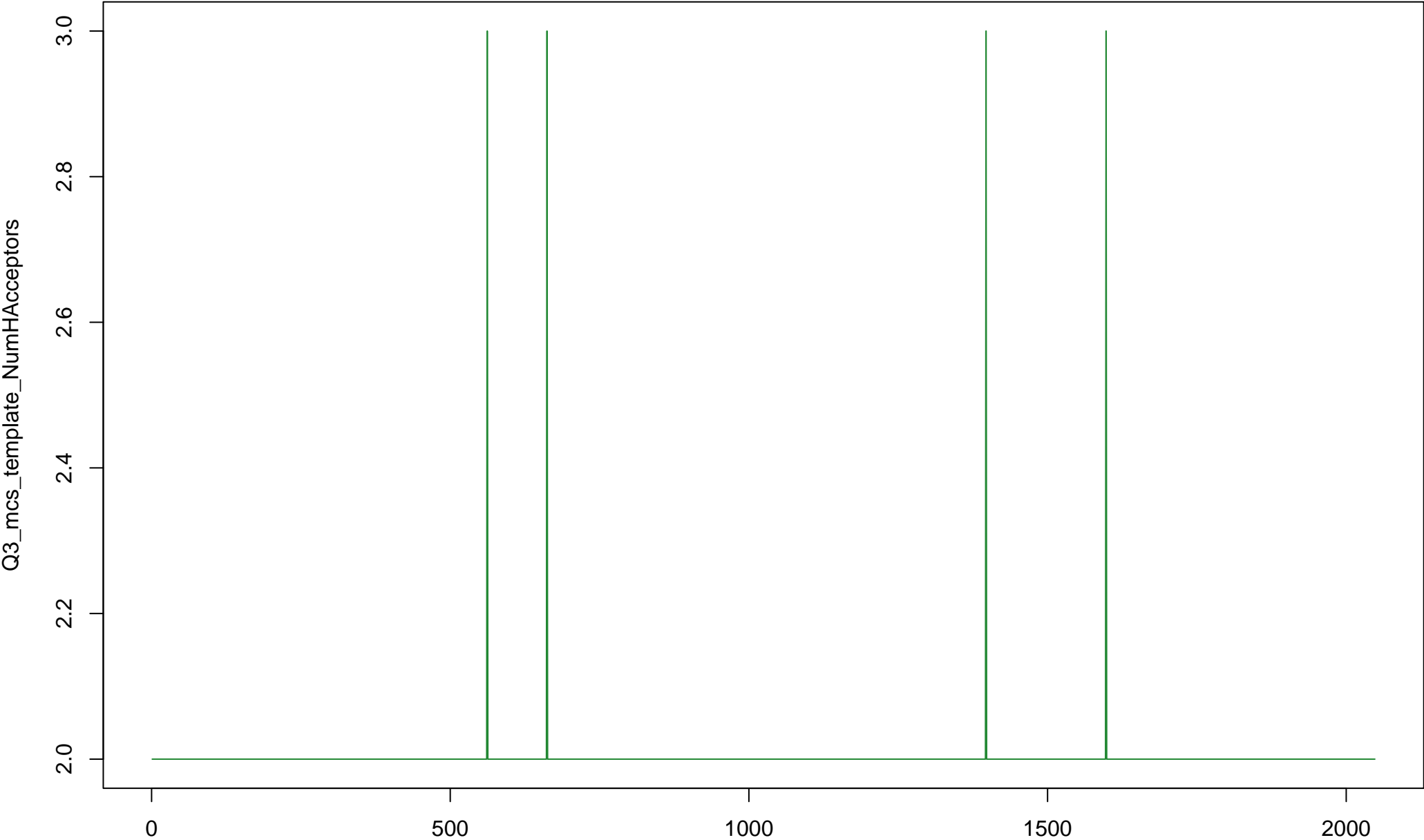
**Q3\_template\_HeavyAtomCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q3\_mcs\_docked\_NumHAcceptors**  
**ESS = 1300 | BMK = 0.609 | MCSE(6.27) = 1.88 | stat: TRUE | burn: 2040**



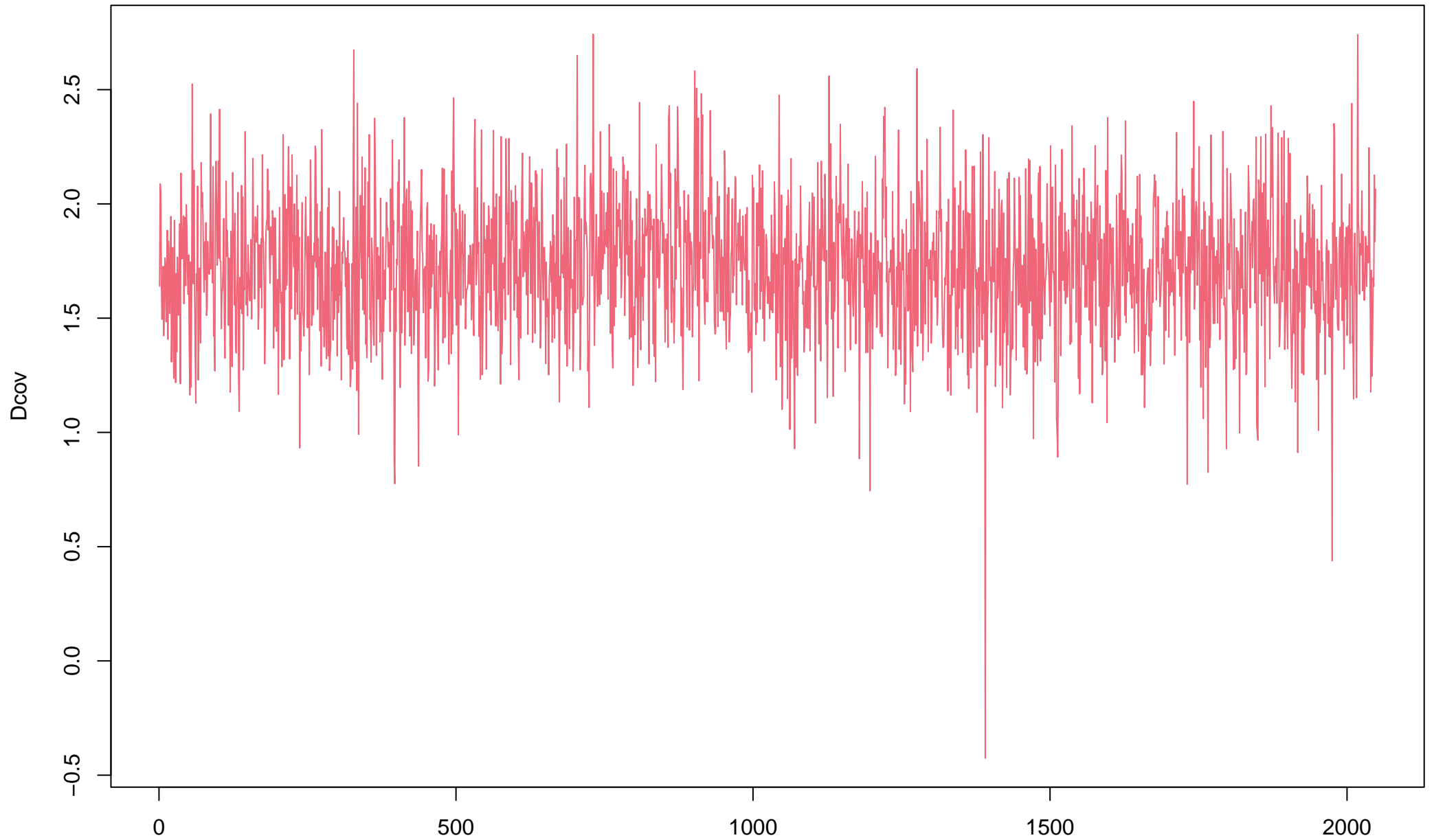
**Q3\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.15 | stat: FALSE | burn: 1632**



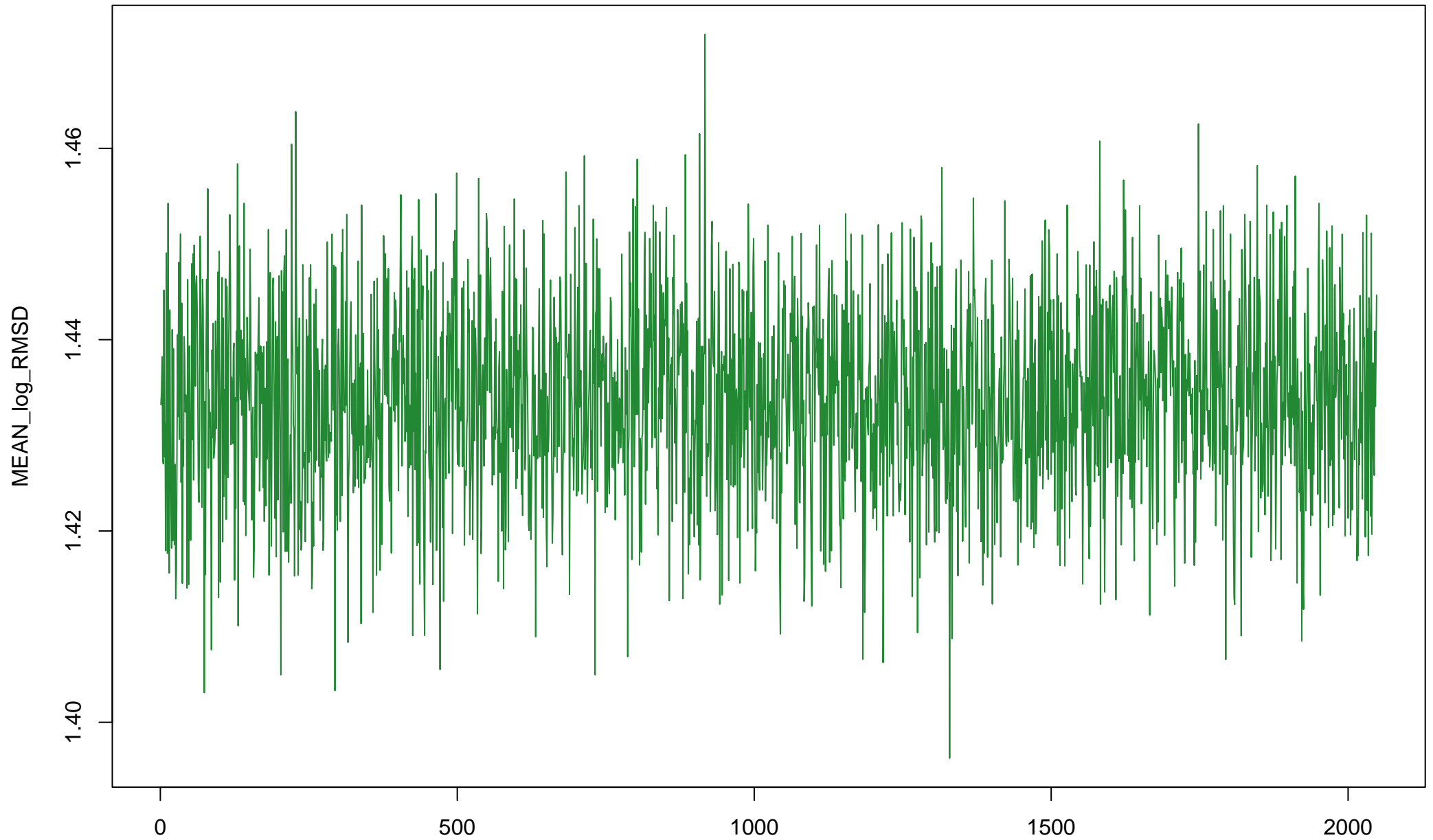
**Q3\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Dcov**  
**ESS = 1710 | BMK = 0.0651 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0**

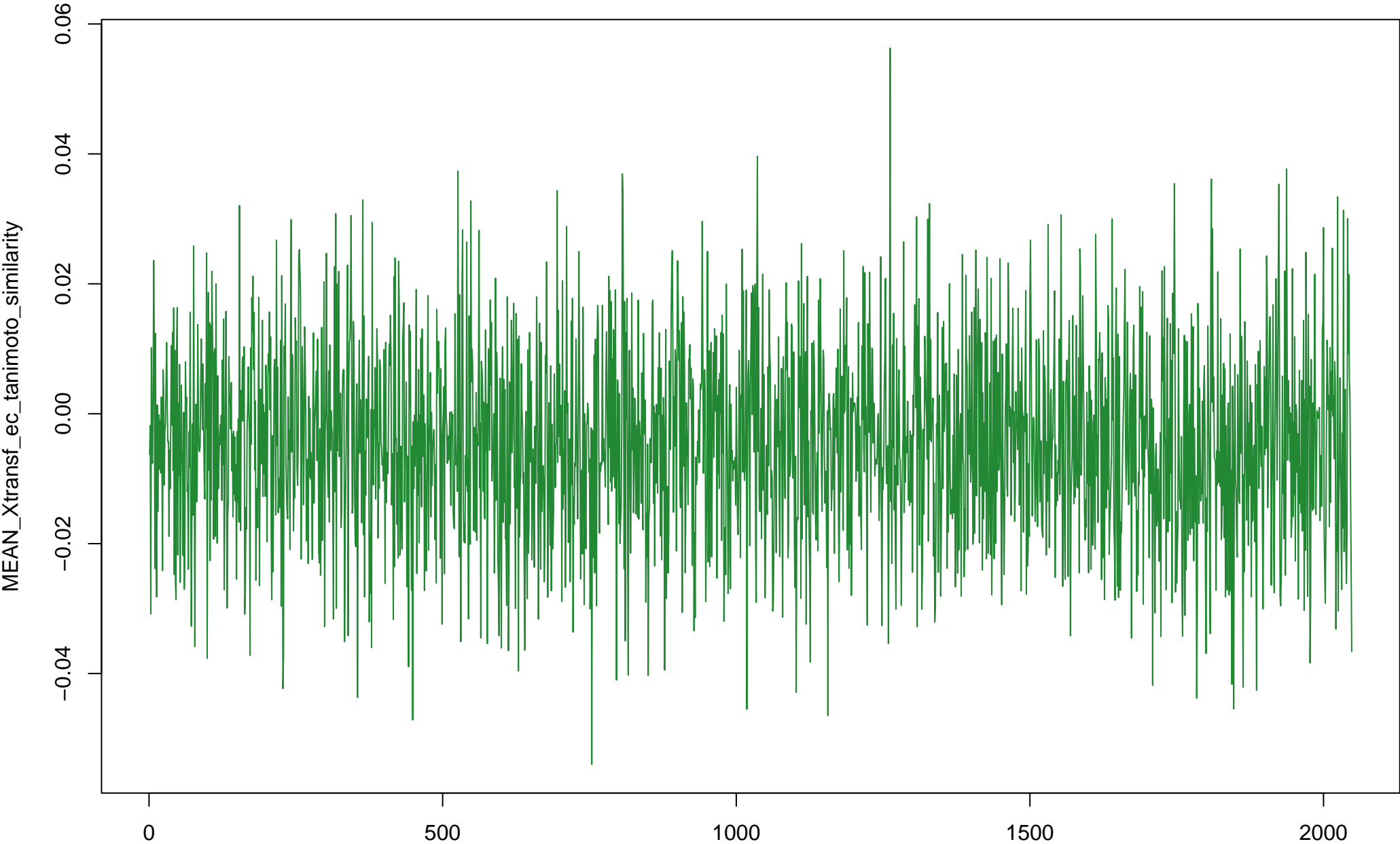


**MEAN\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0444 | MCSE(6.27) = 2 | stat: TRUE | burn: 0**

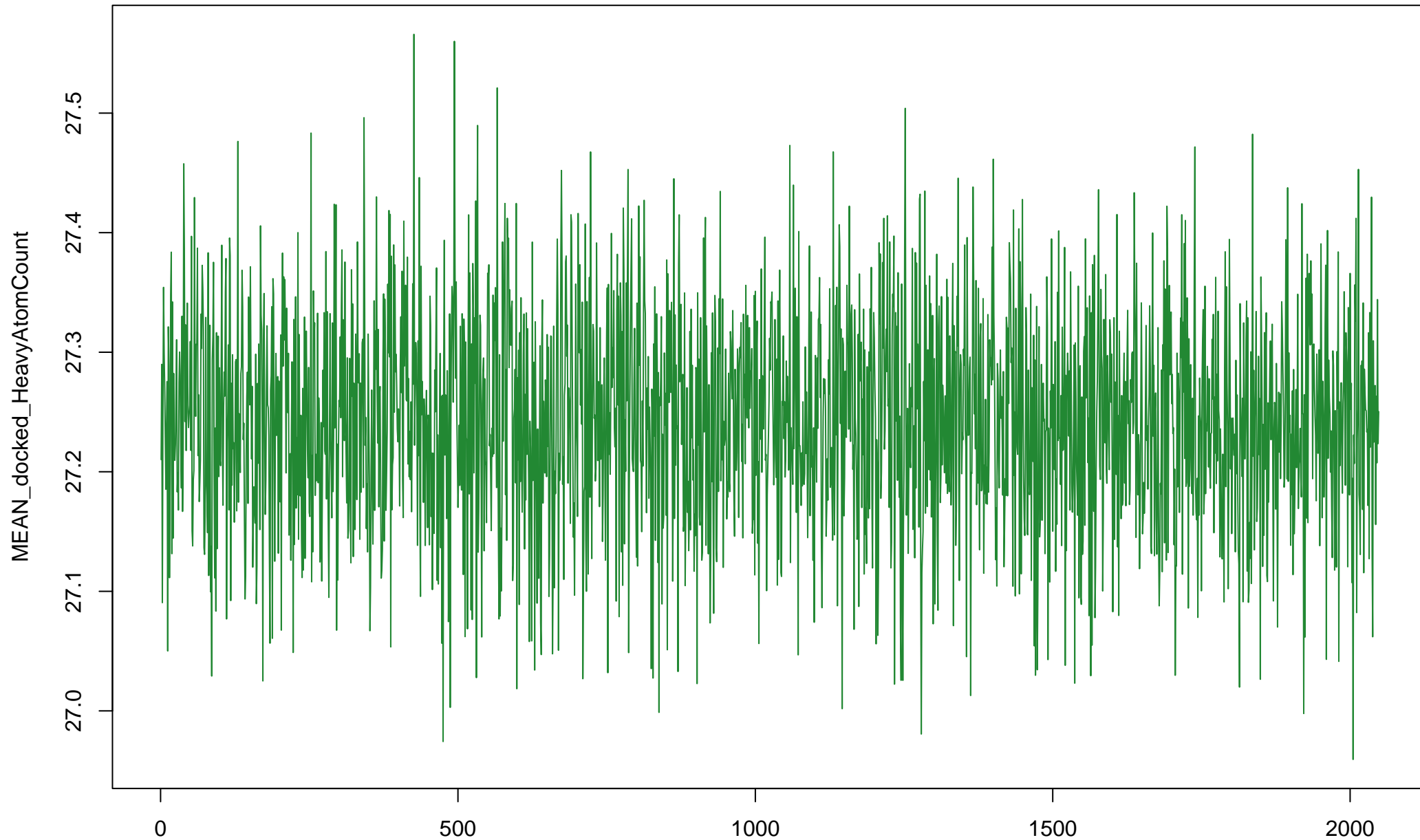




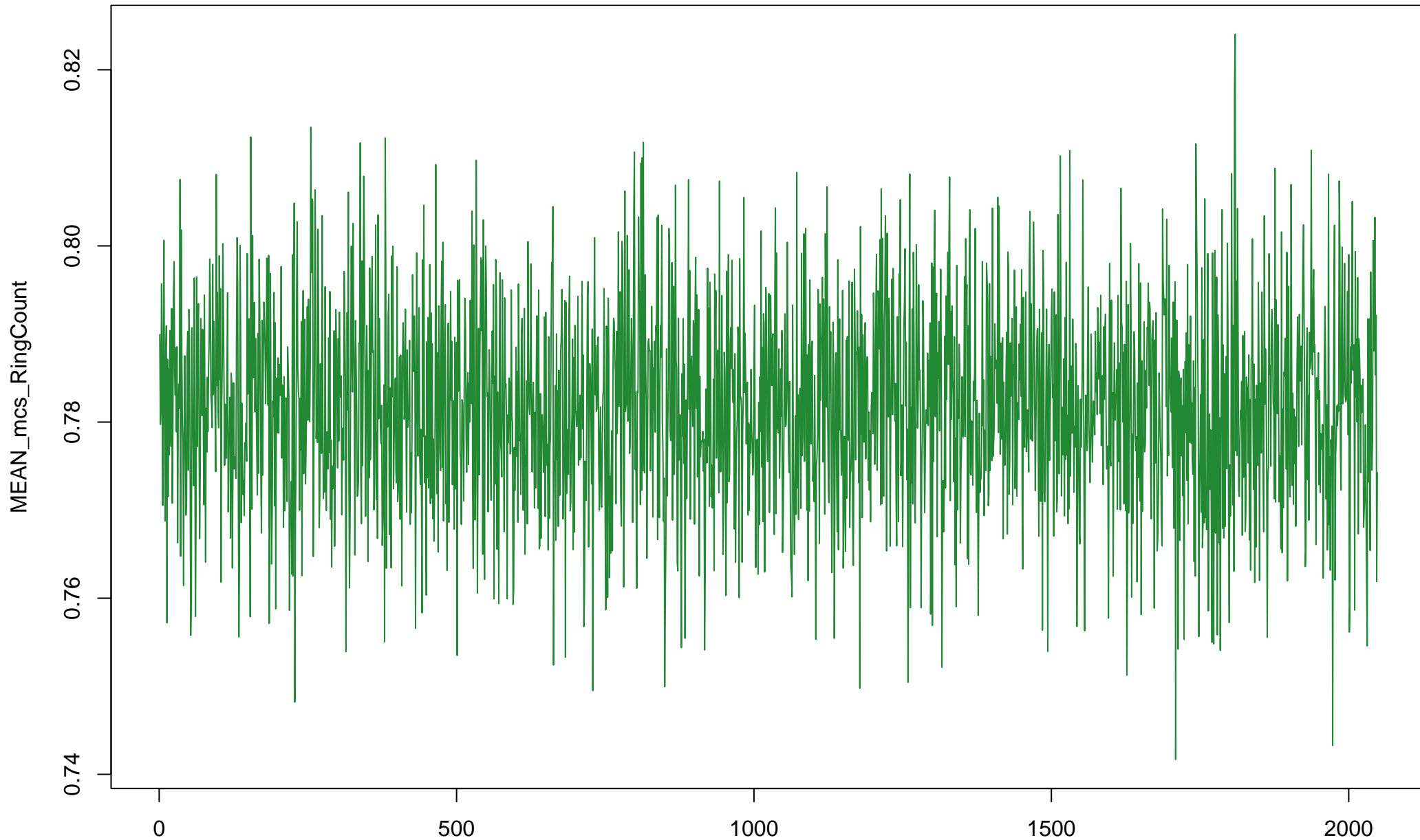
MEAN\_Xtransf\_ec\_tanimoto\_similarity  
ESS = 2050 | BMK = 0.042 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 0



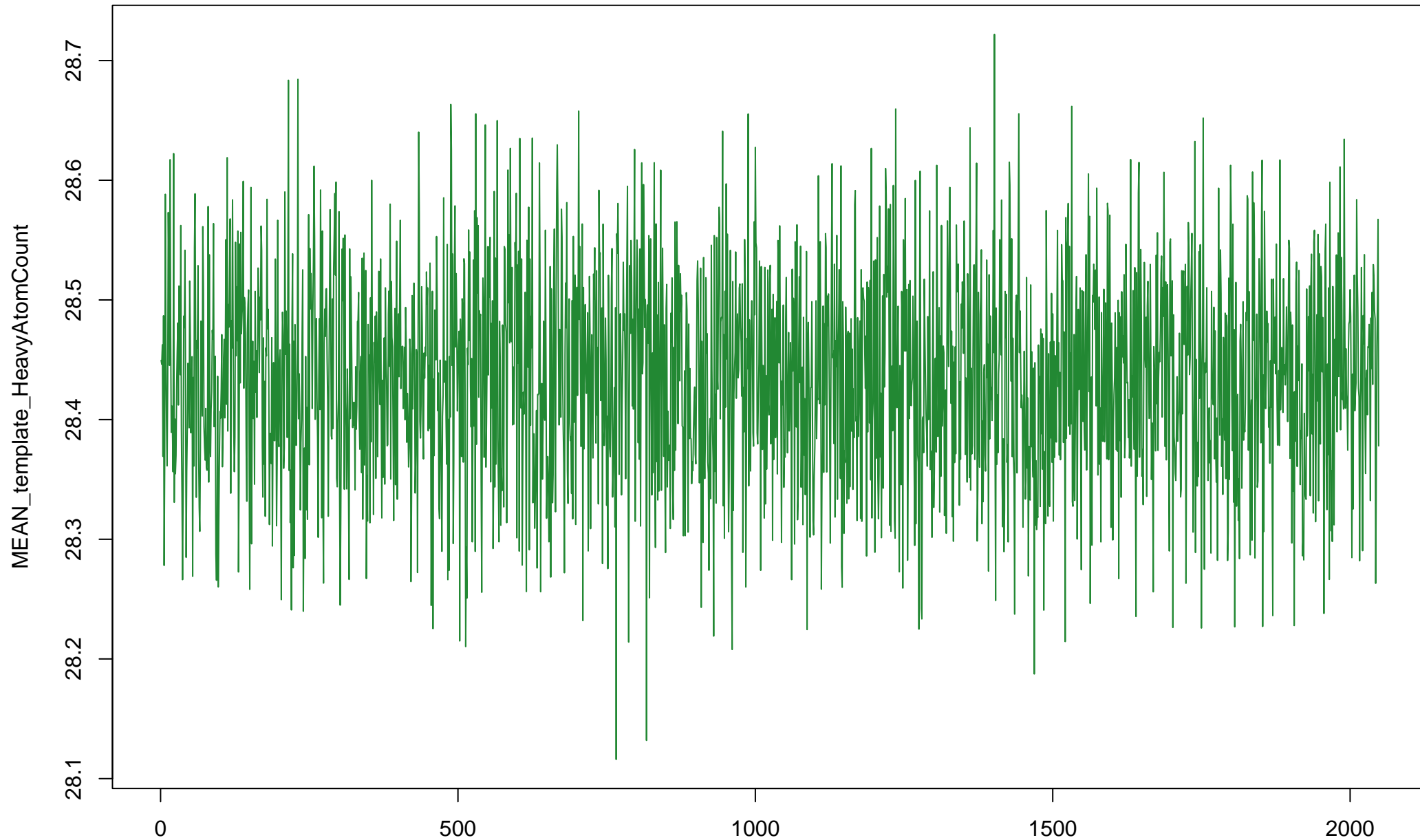
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0375 | MCSE(6.27) = 1.78 | stat: TRUE | burn: 0**



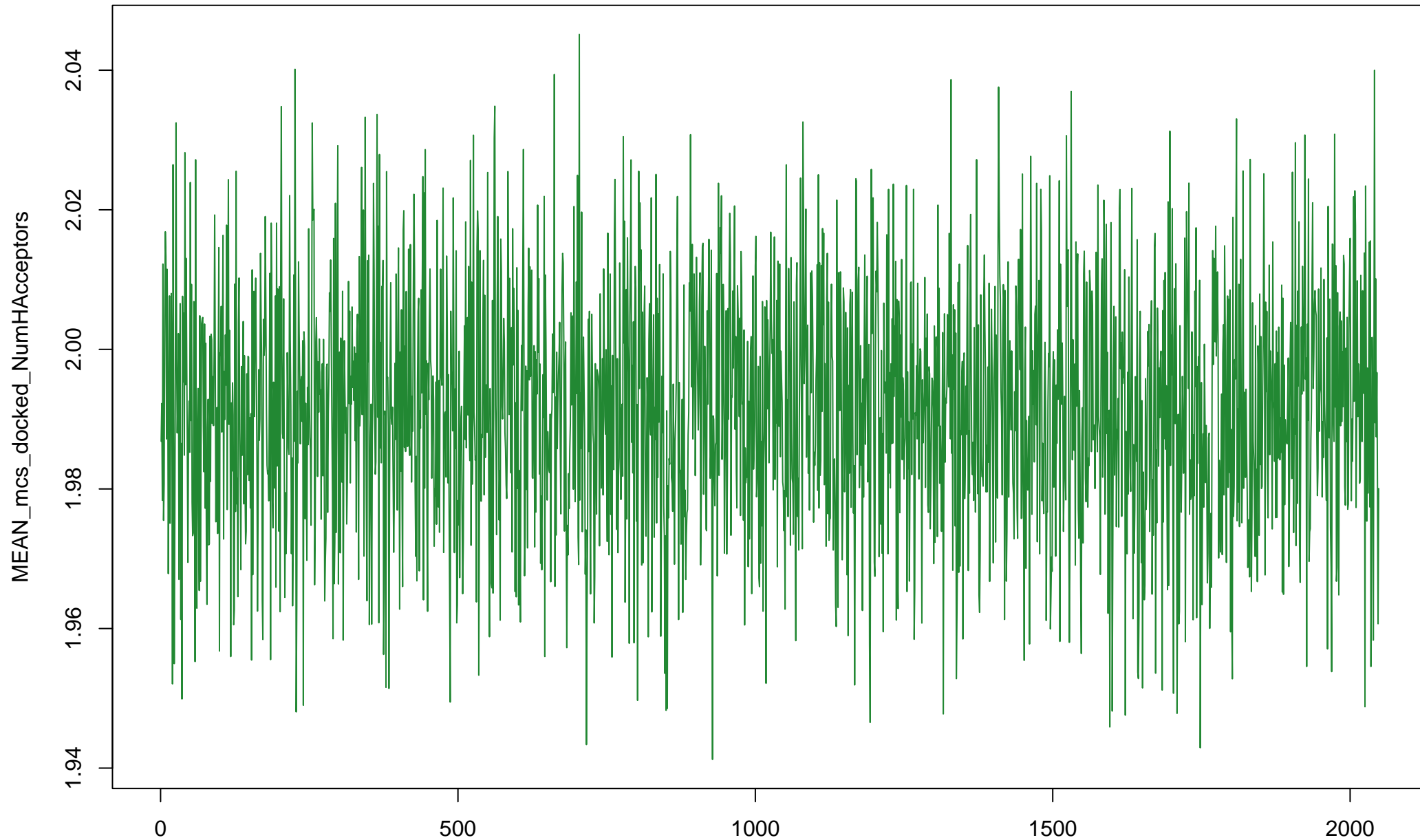
**MEAN\_mcs\_RingCount**  
**ESS = 2050 | BMK = 0.0334 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0**



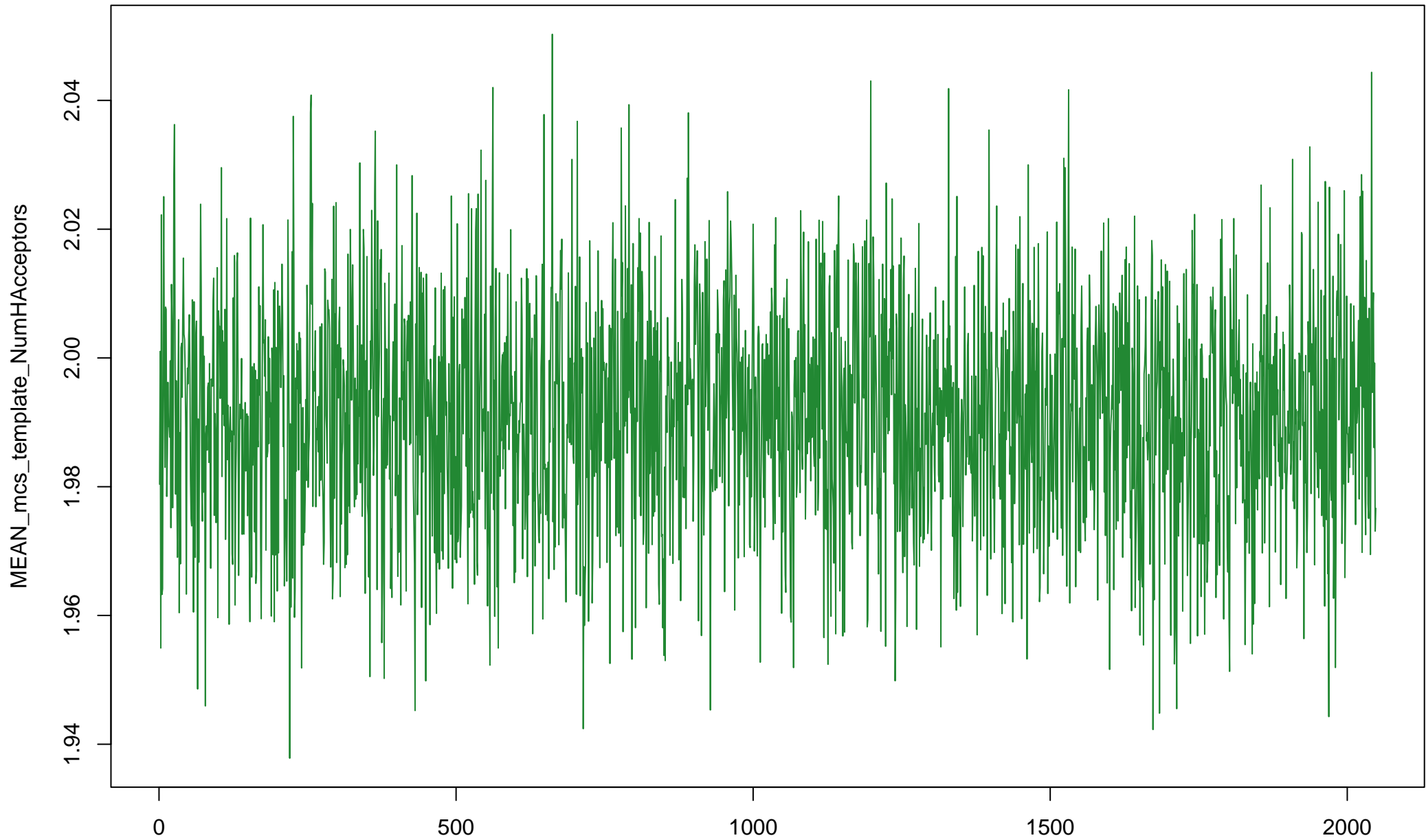
**MEAN\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0392 | MCSE(6.27) = 1.91 | stat: TRUE | burn: 0**



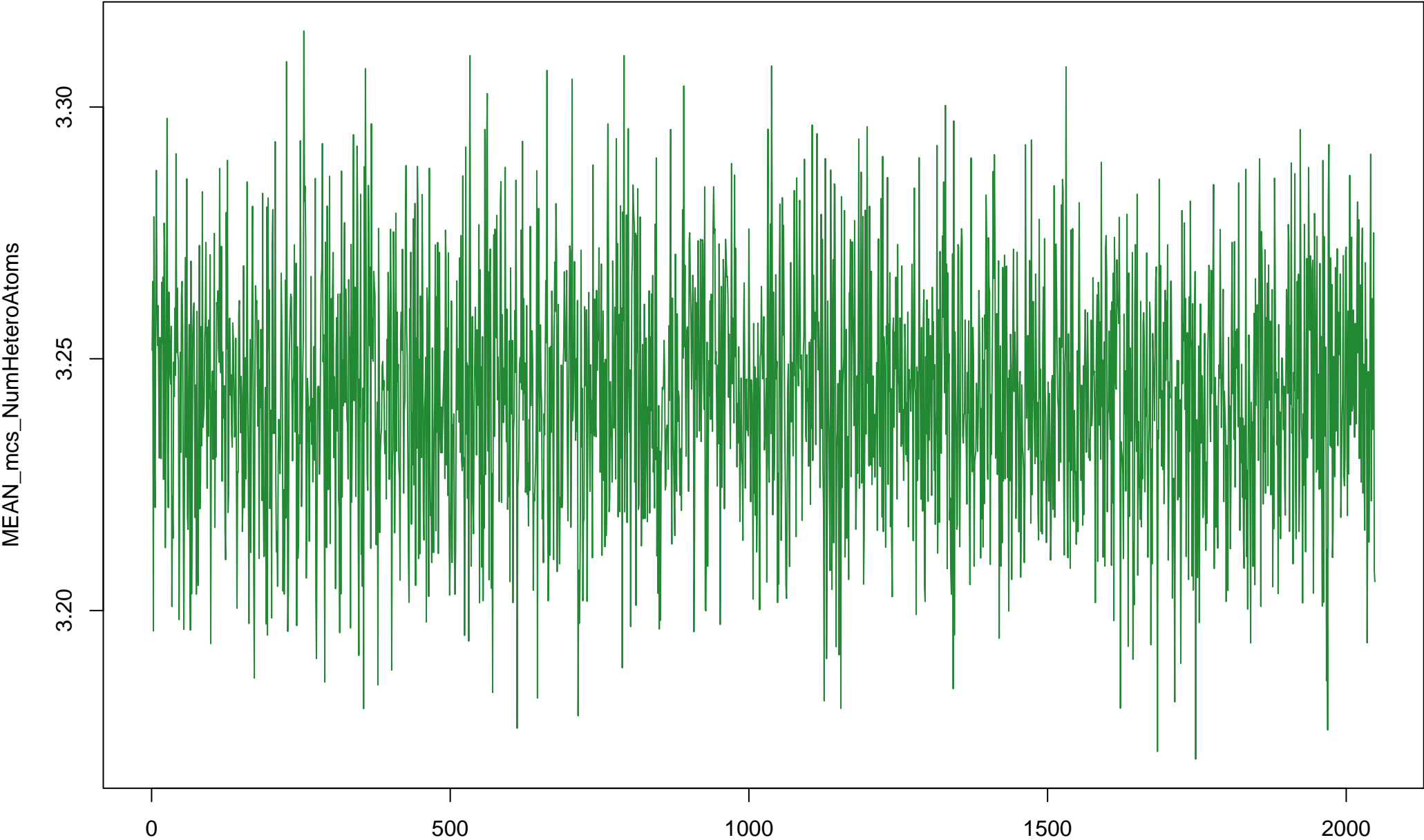
**MEAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0258 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0**



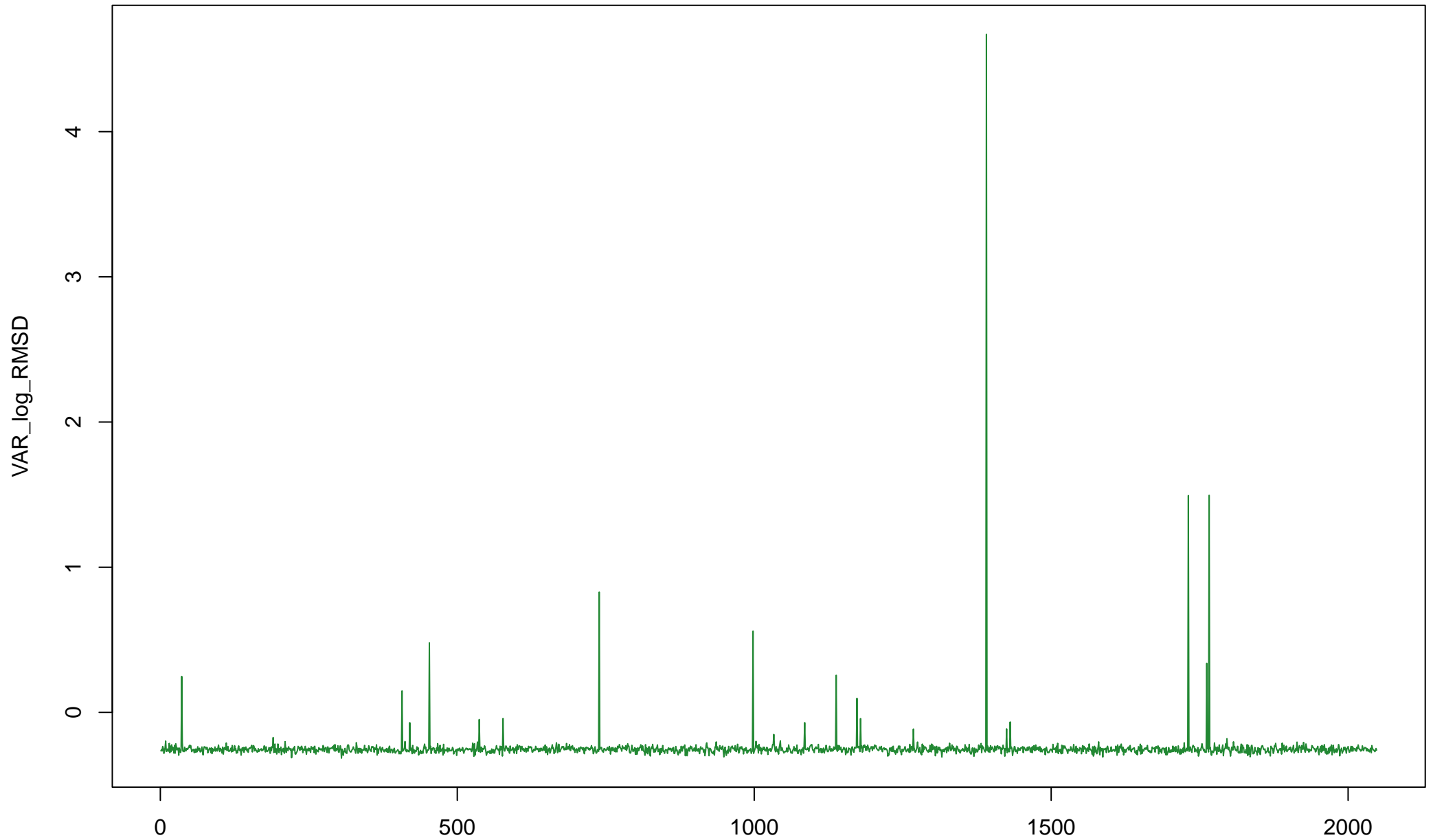
**MEAN\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0398 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0**



**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0381 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0**

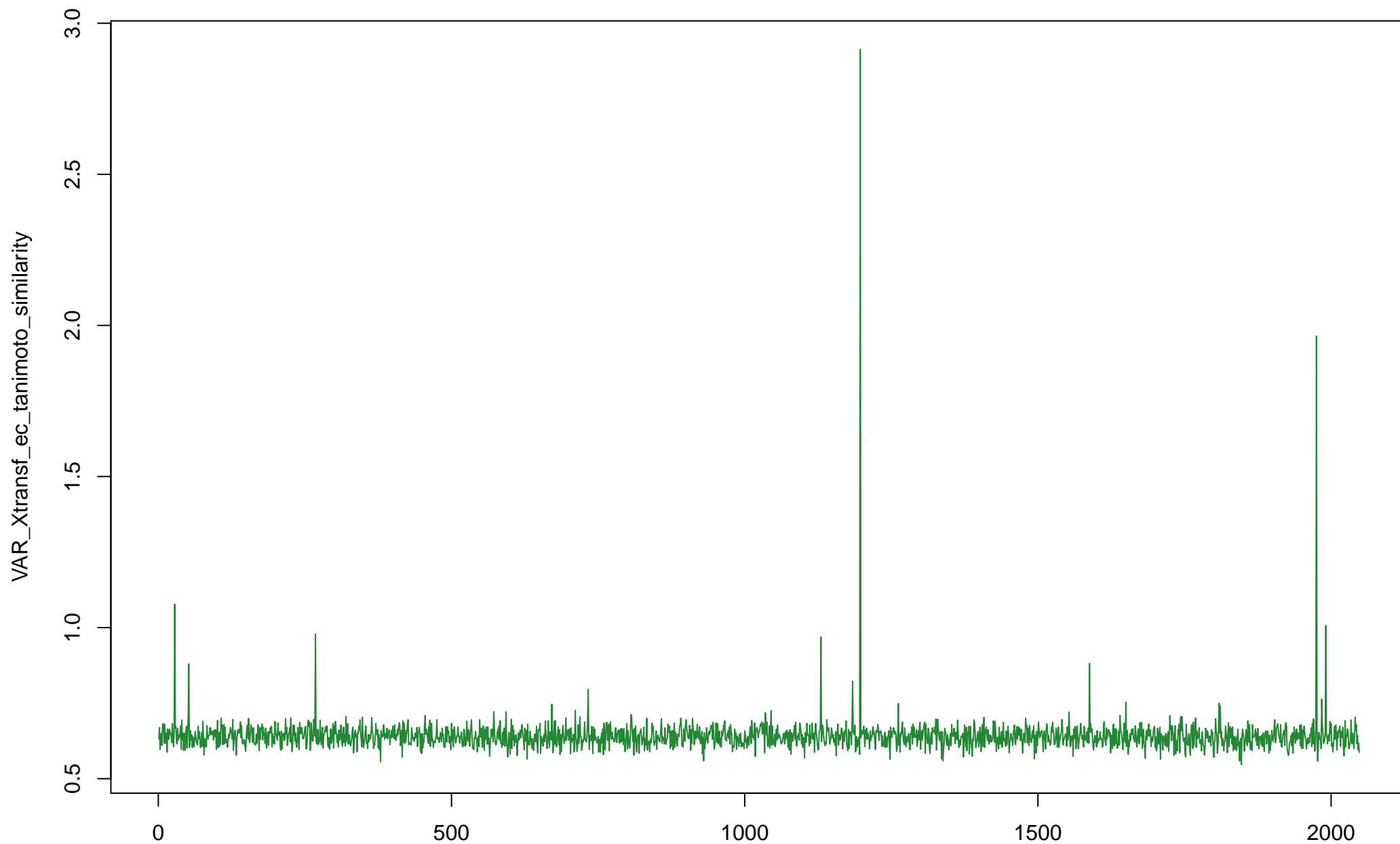


**VAR\_log\_RMSD**  
**ESS = 2050 | BMK = 0.231 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 1224**

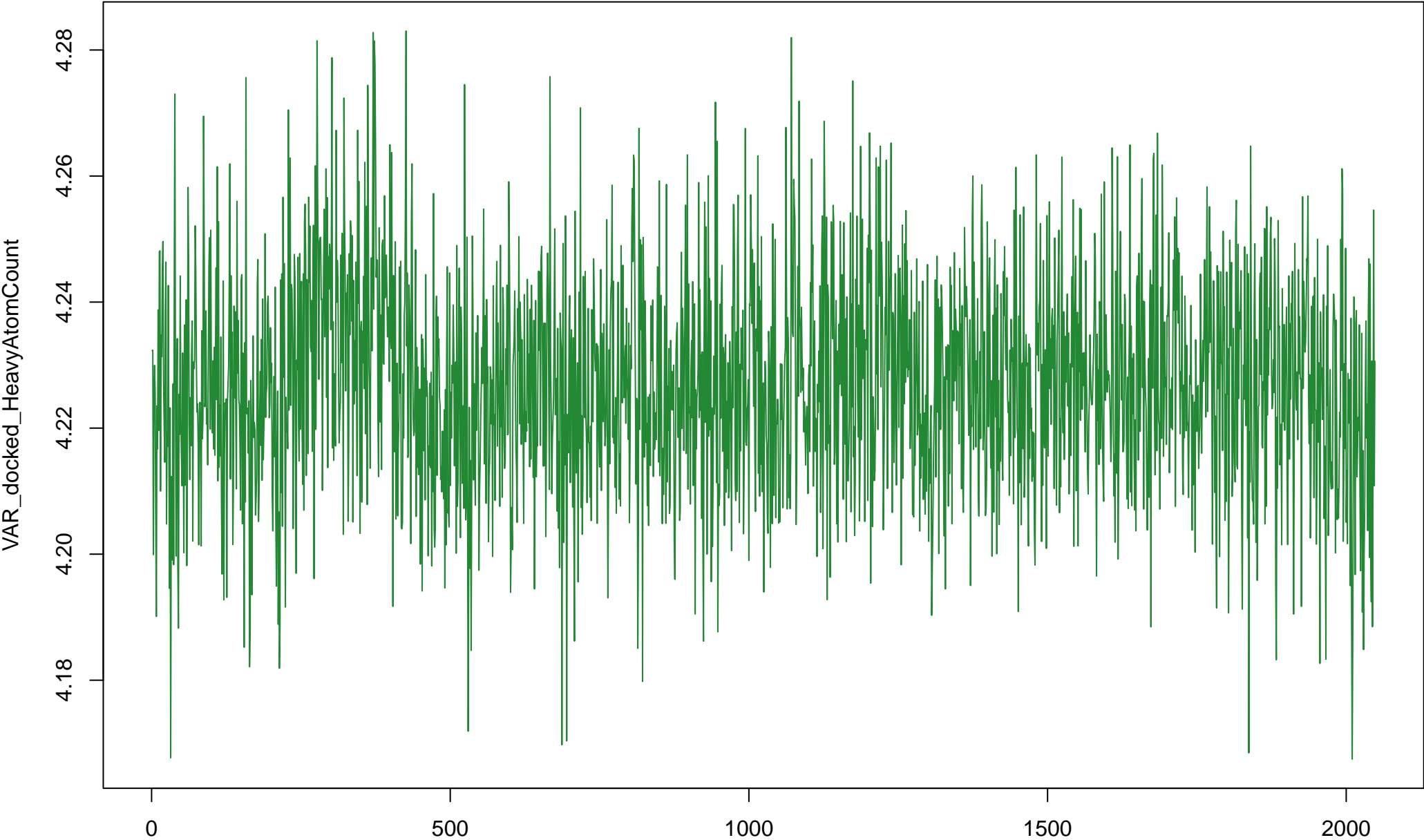




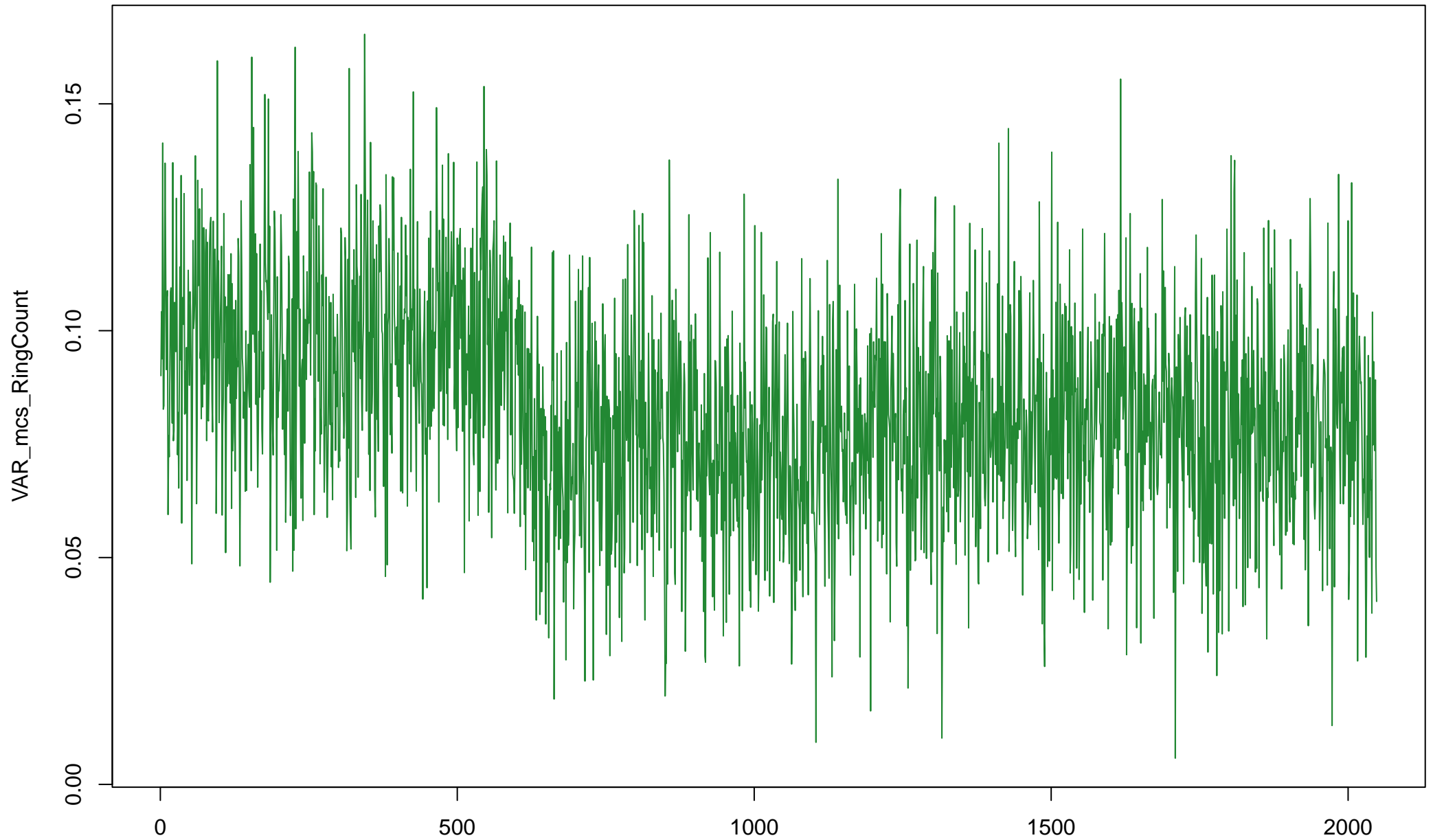
**VAR\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0752 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0**



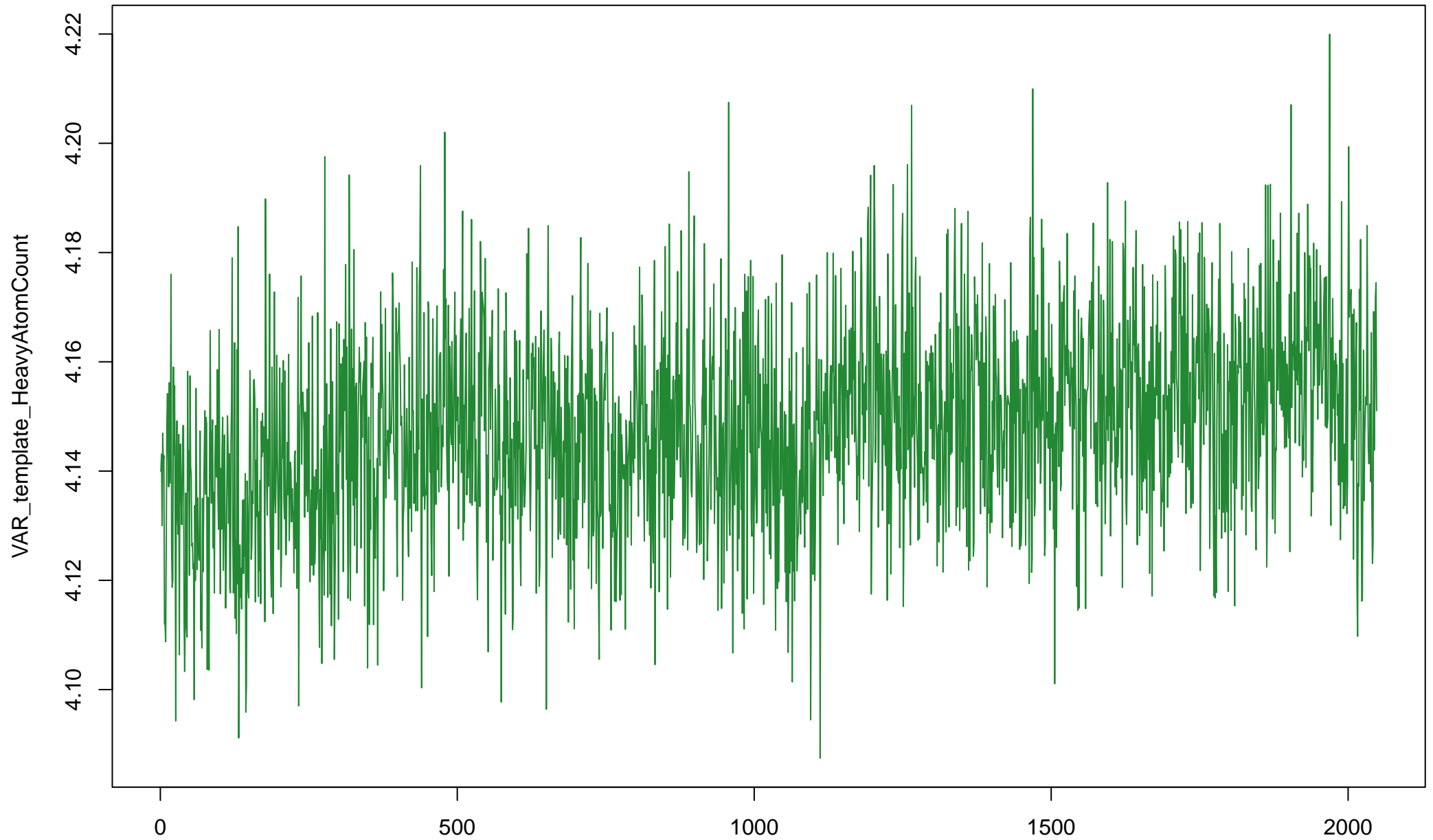
**VAR\_docked\_HeavyAtomCount**  
**ESS = 477 | BMK = 0.048 | MCSE(6.27) = 3.91 | stat: FALSE | burn: 0**



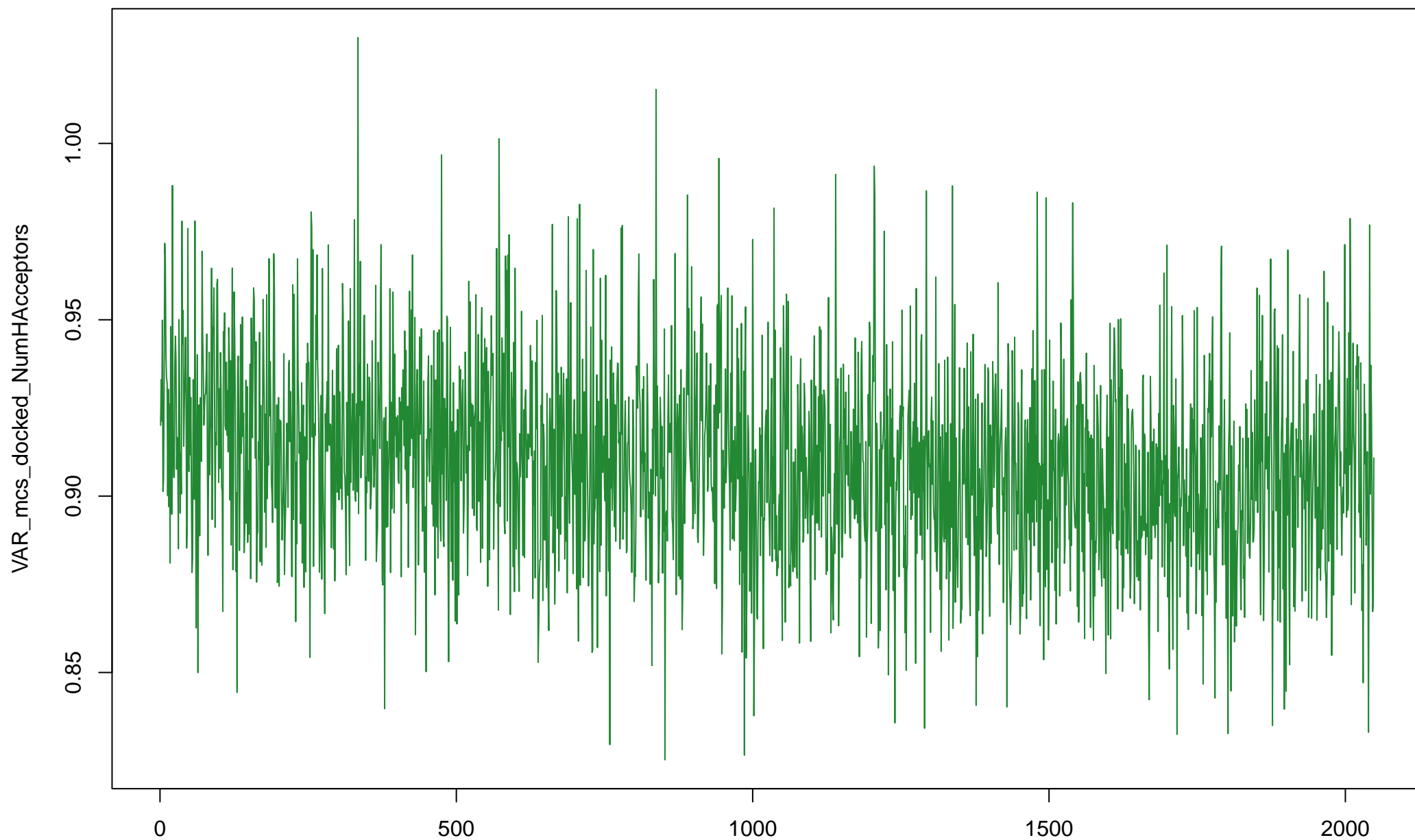
**VAR\_mcs\_RingCount**  
**ESS = 61 | BMK = 0.157 | MCSE(6.27) = 6.34 | stat: FALSE | burn: 0**



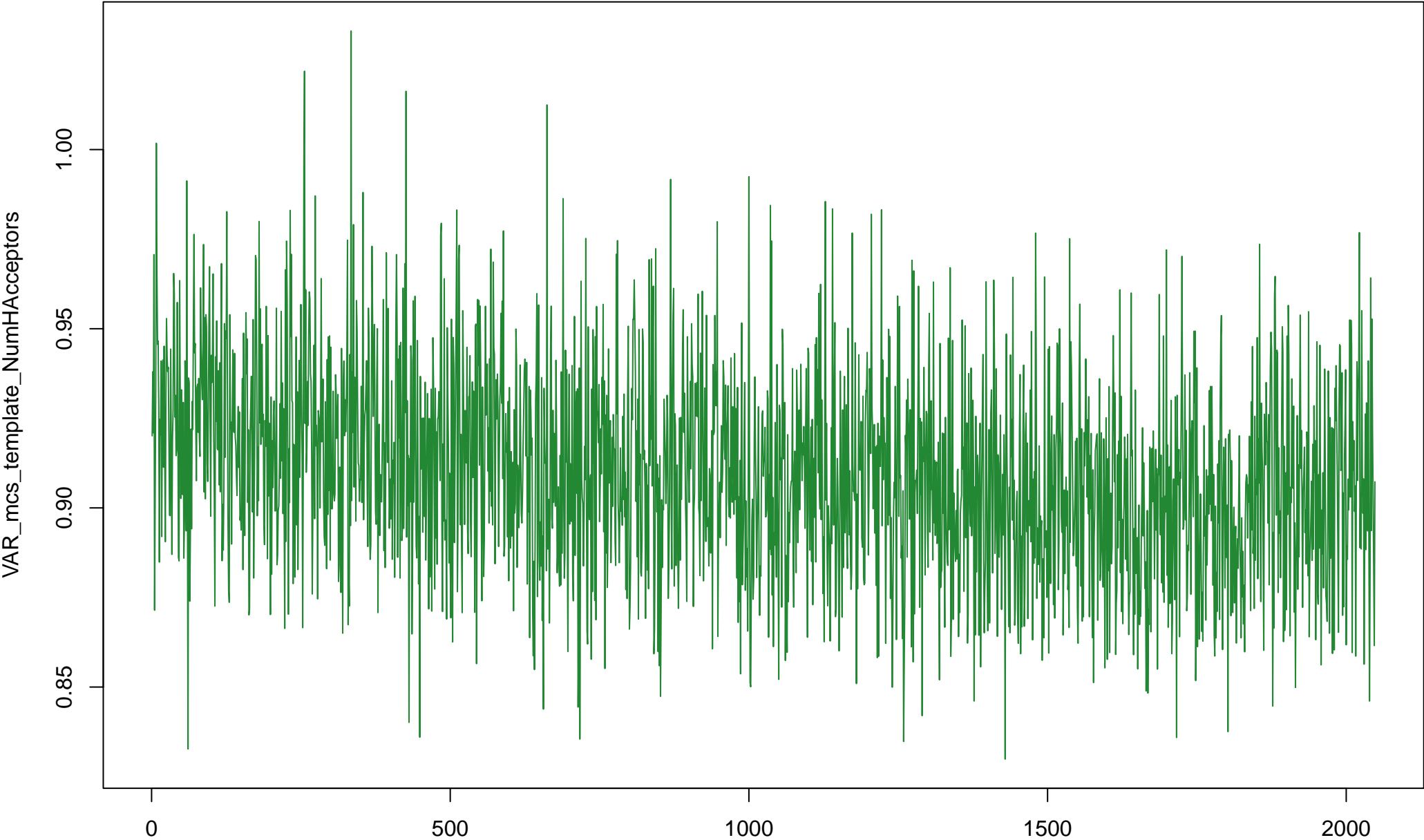
**VAR\_template\_HeavyAtomCount**  
**ESS = 82.4 | BMK = 0.18 | MCSE(6.27) = 5.61 | stat: FALSE | burn: 0**



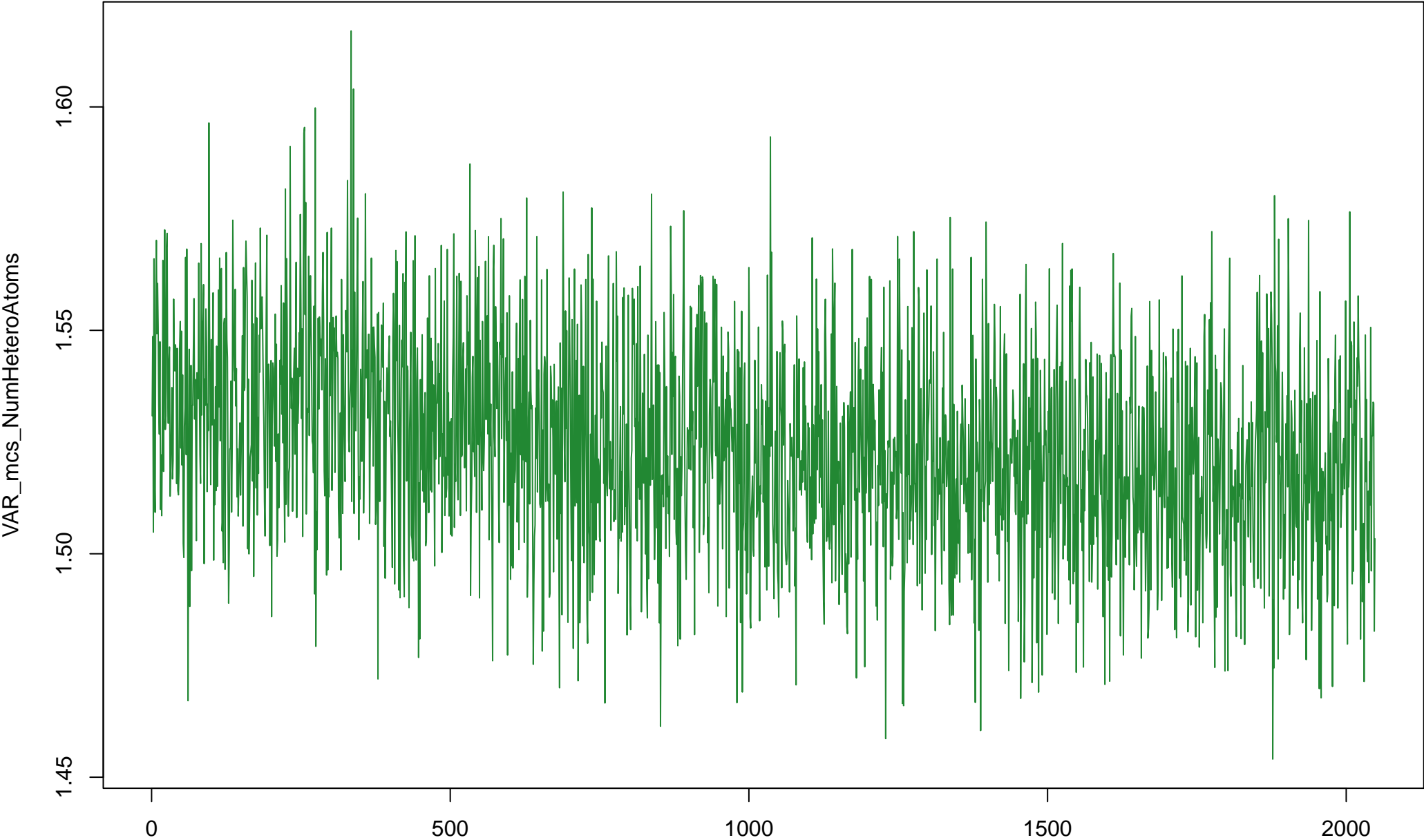
**VAR\_mcs\_docked\_NumHAcceptors**  
**ESS = 302 | BMK = 0.139 | MCSE(6.27) = 3.93 | stat: FALSE | burn: 0**



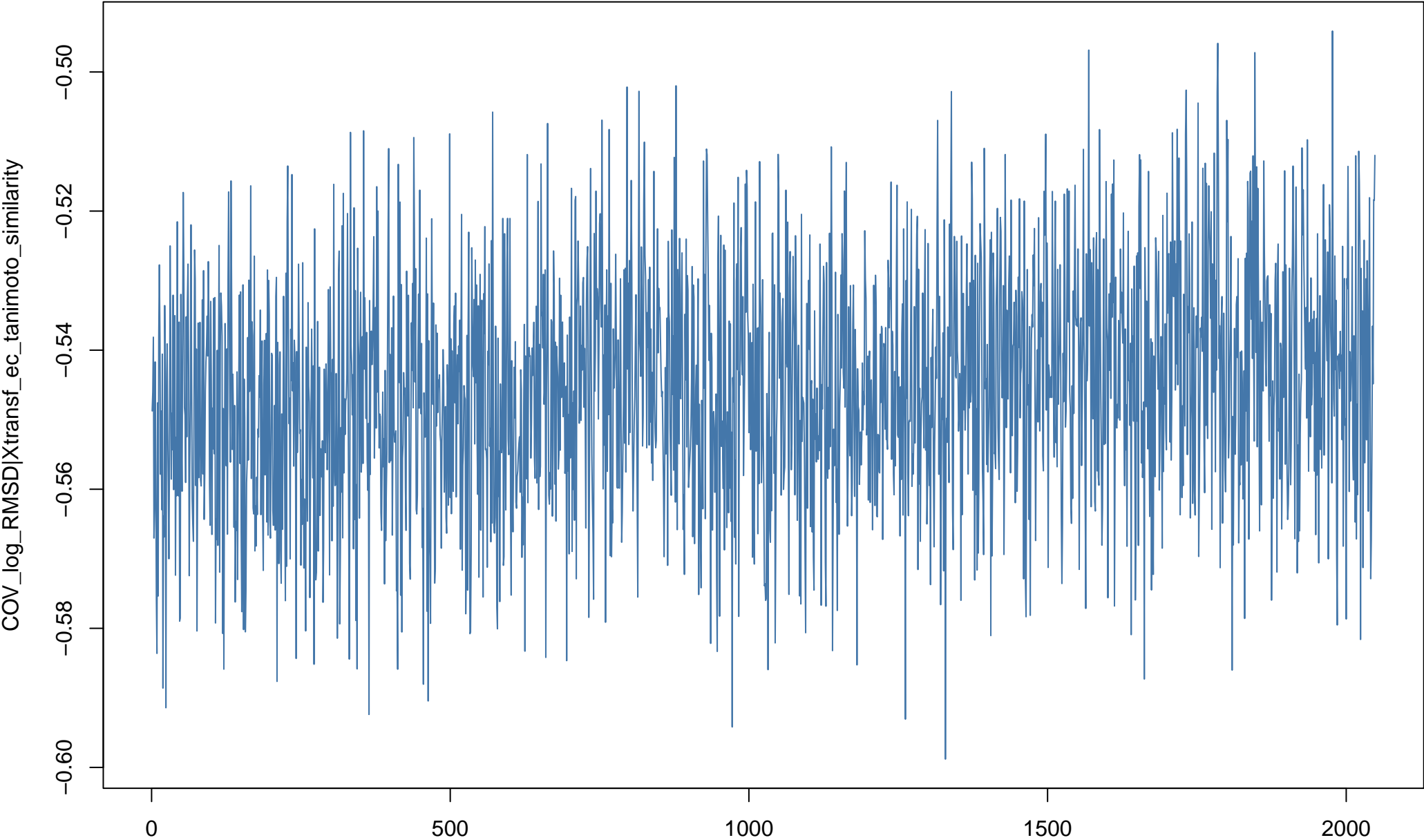
**VAR\_mcs\_template\_NumHAcceptors**  
**ESS = 156 | BMK = 0.166 | MCSE(6.27) = 4.72 | stat: FALSE | burn: 0**



**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 118 | BMK = 0.165 | MCSE(6.27) = 4.77 | stat: FALSE | burn: 0**

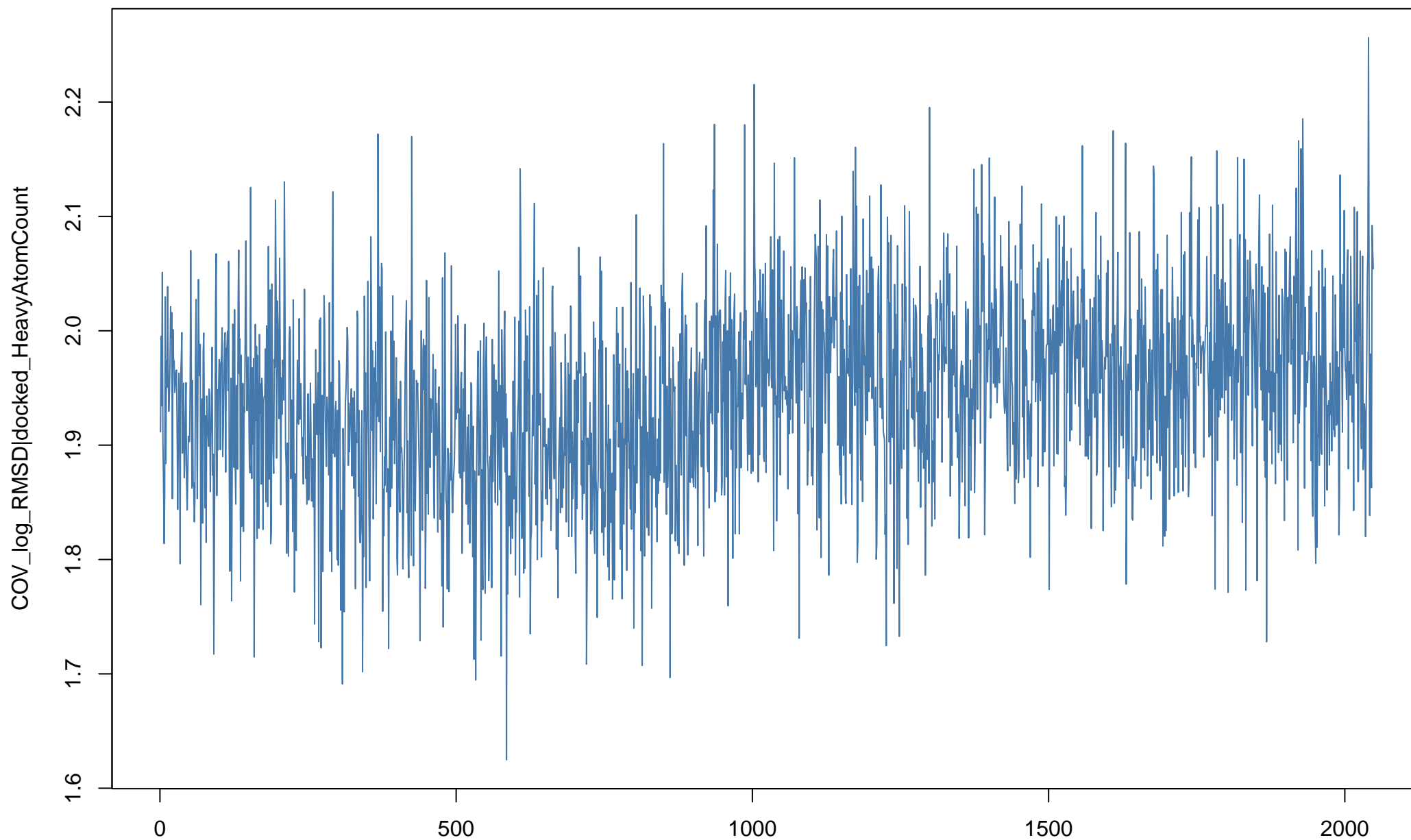


COV\_log\_RMSD|Xtransf\_ec\_tanimoto\_similarity  
ESS = 549 | BMK = 0.101 | MCSE(6.27) = 3.79 | stat: FALSE | burn: 0

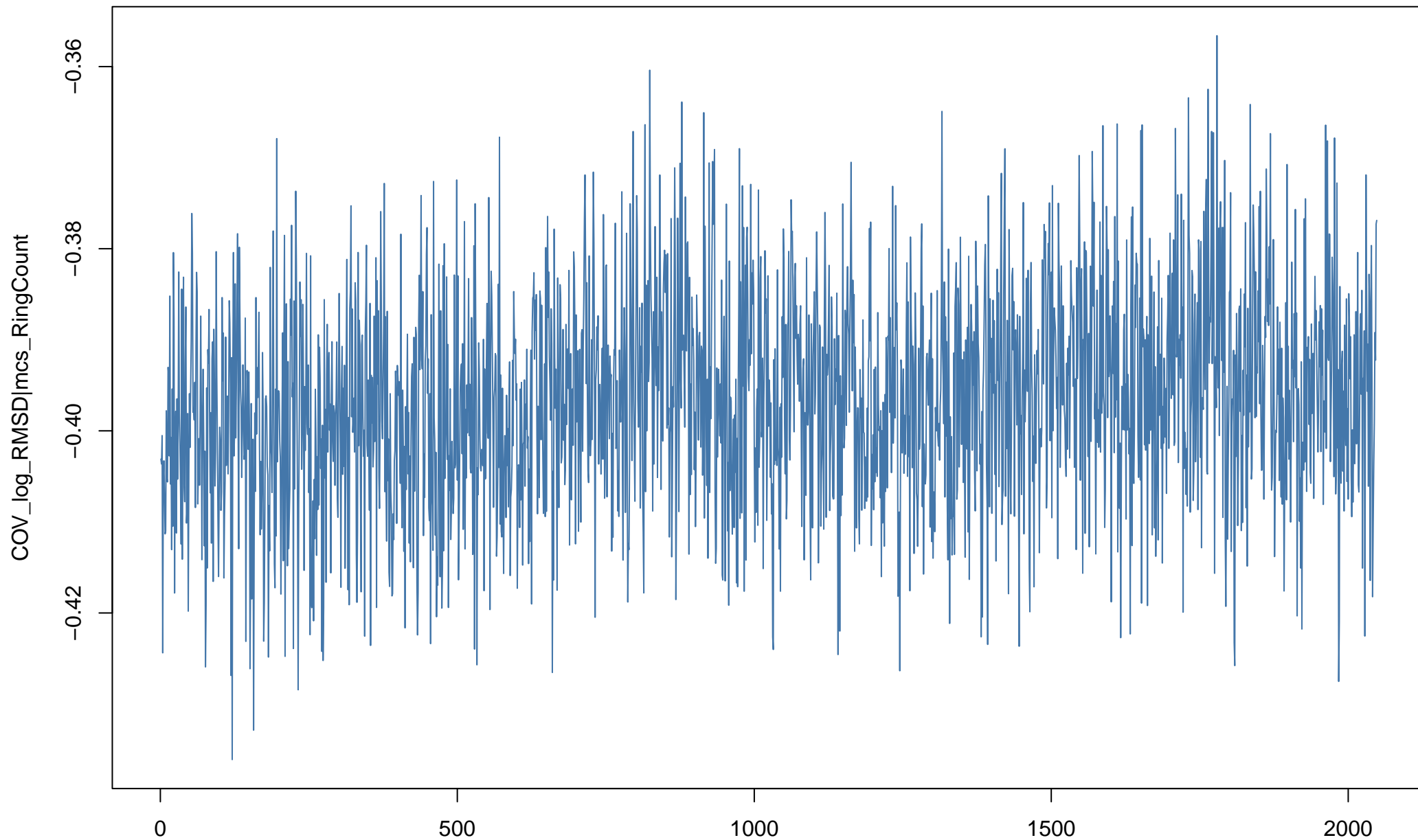




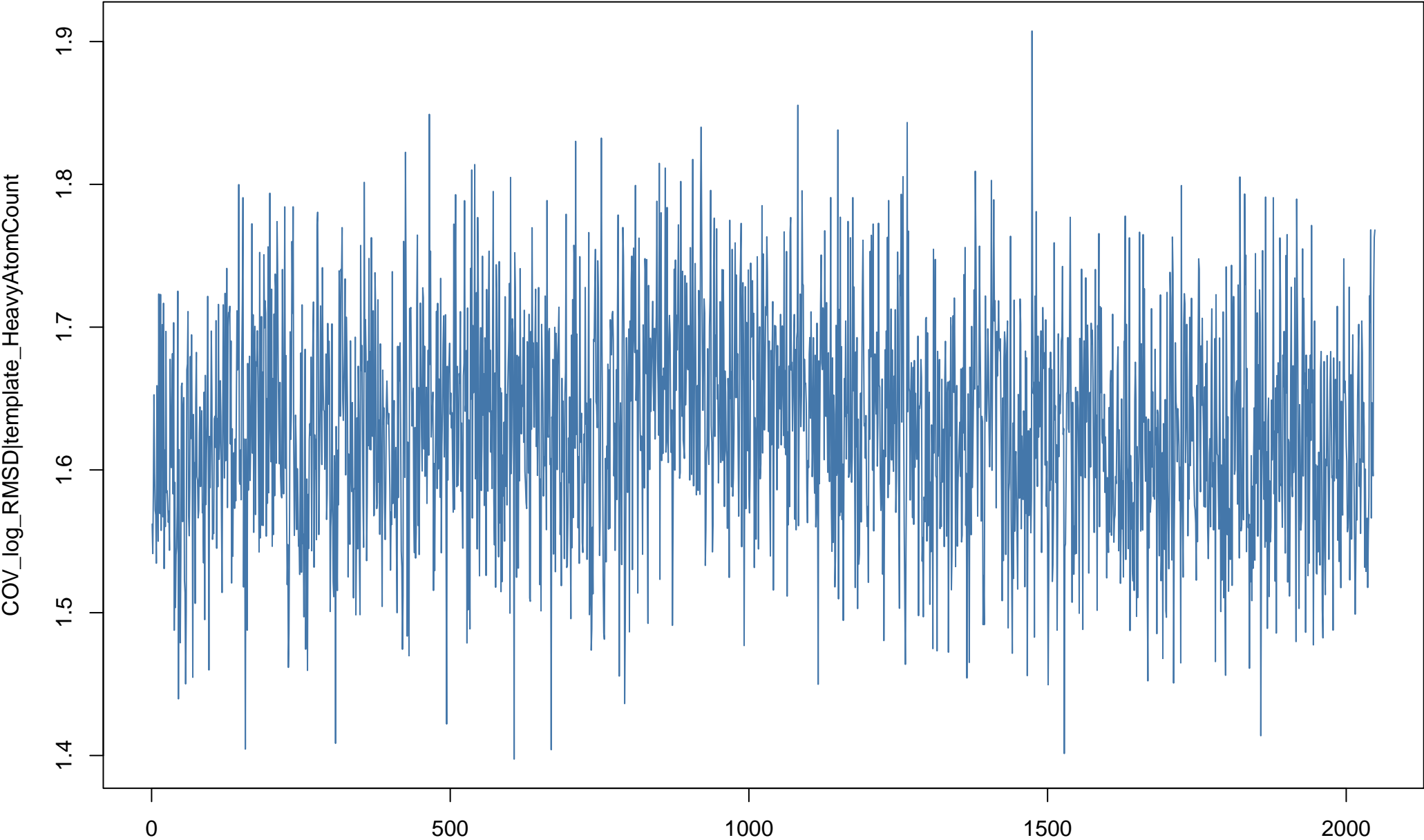
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 99.9 | BMK = 0.235 | MCSE(6.27) = 5.77 | stat: FALSE | burn: 0**



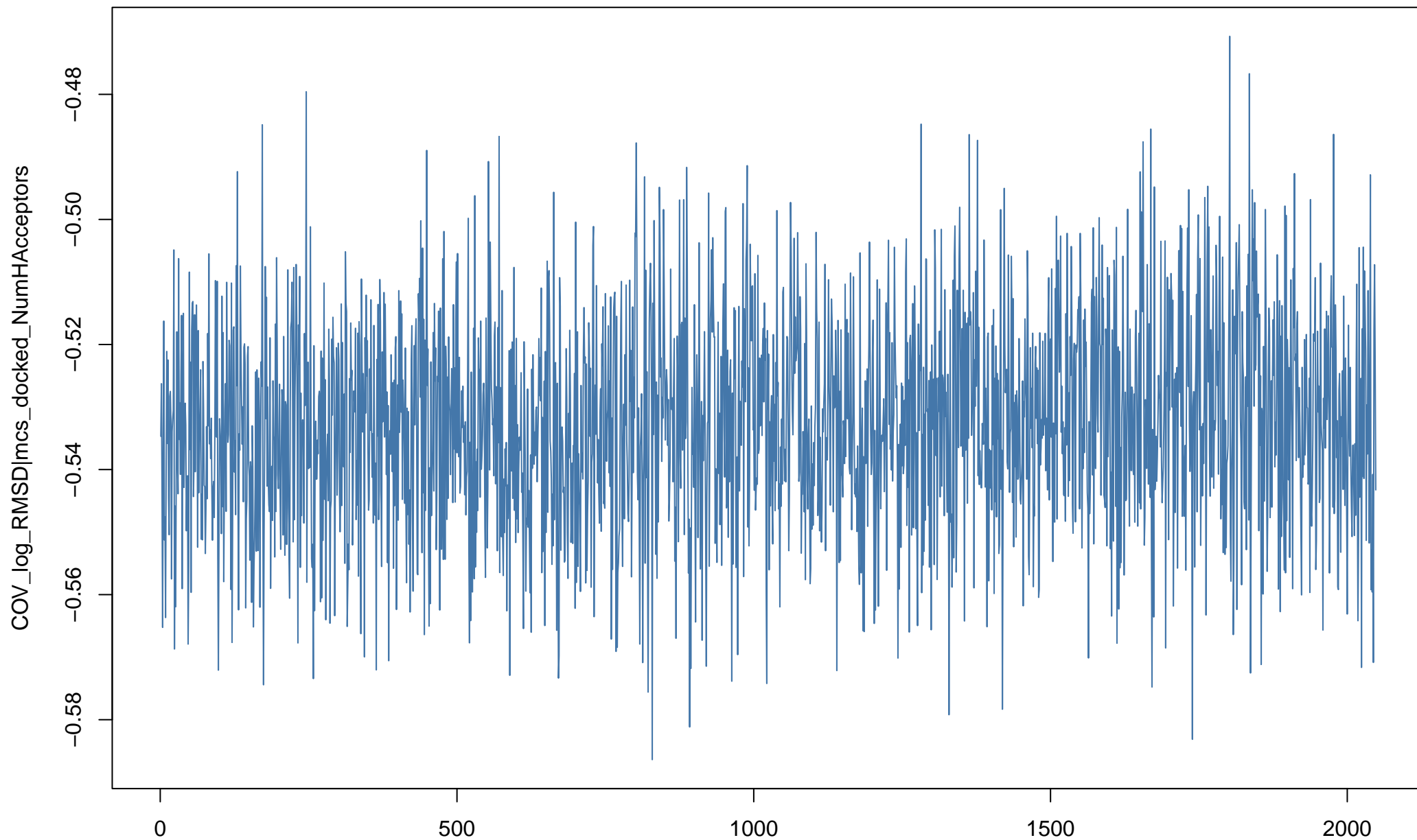
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 564 | BMK = 0.0902 | MCSE(6.27) = 4.11 | stat: FALSE | burn: 0**



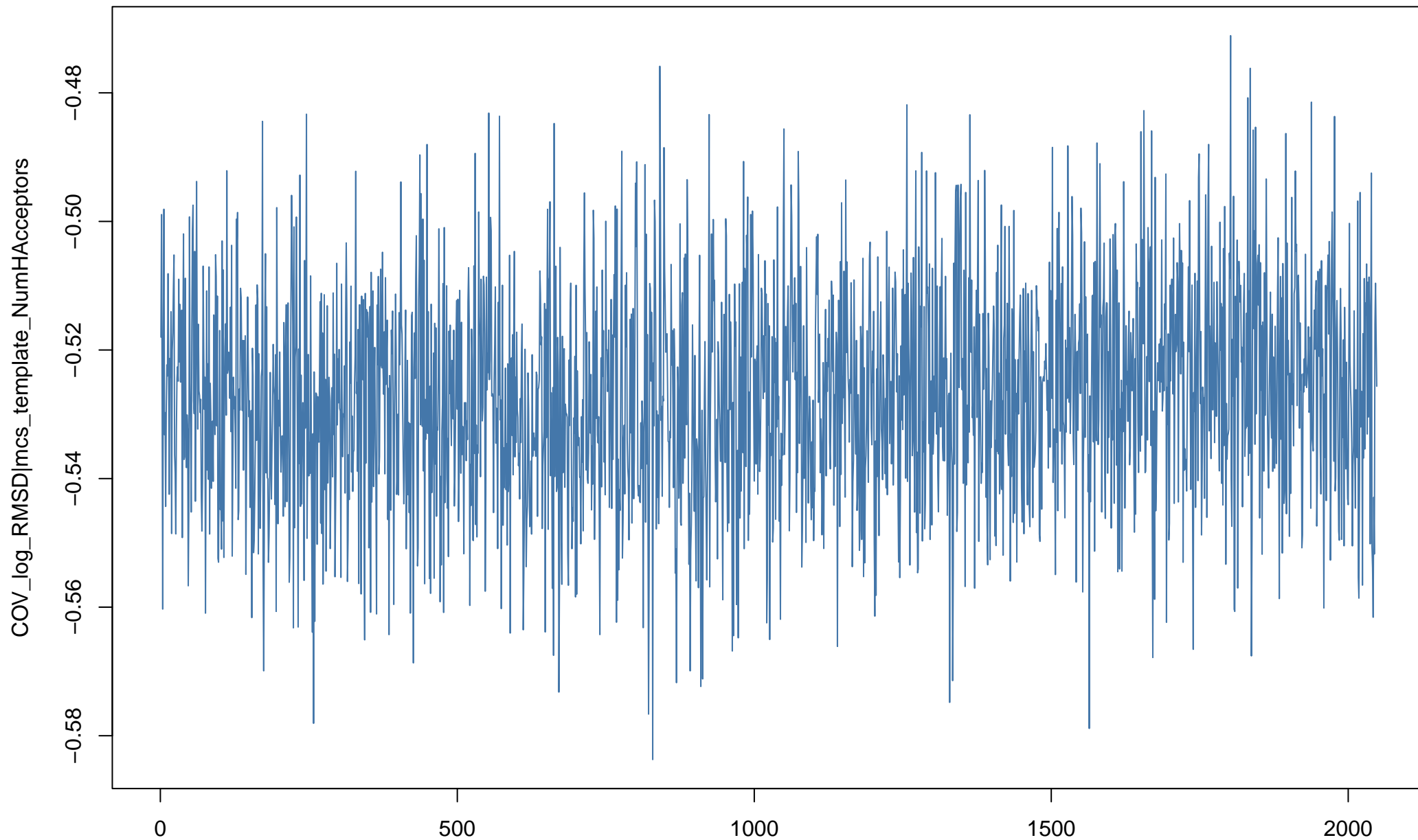
COV\_log\_RMSD|template\_HeavyAtomCount  
ESS = 603 | BMK = 0.0538 | MCSE(6.27) = 3.82 | stat: TRUE | burn: 0



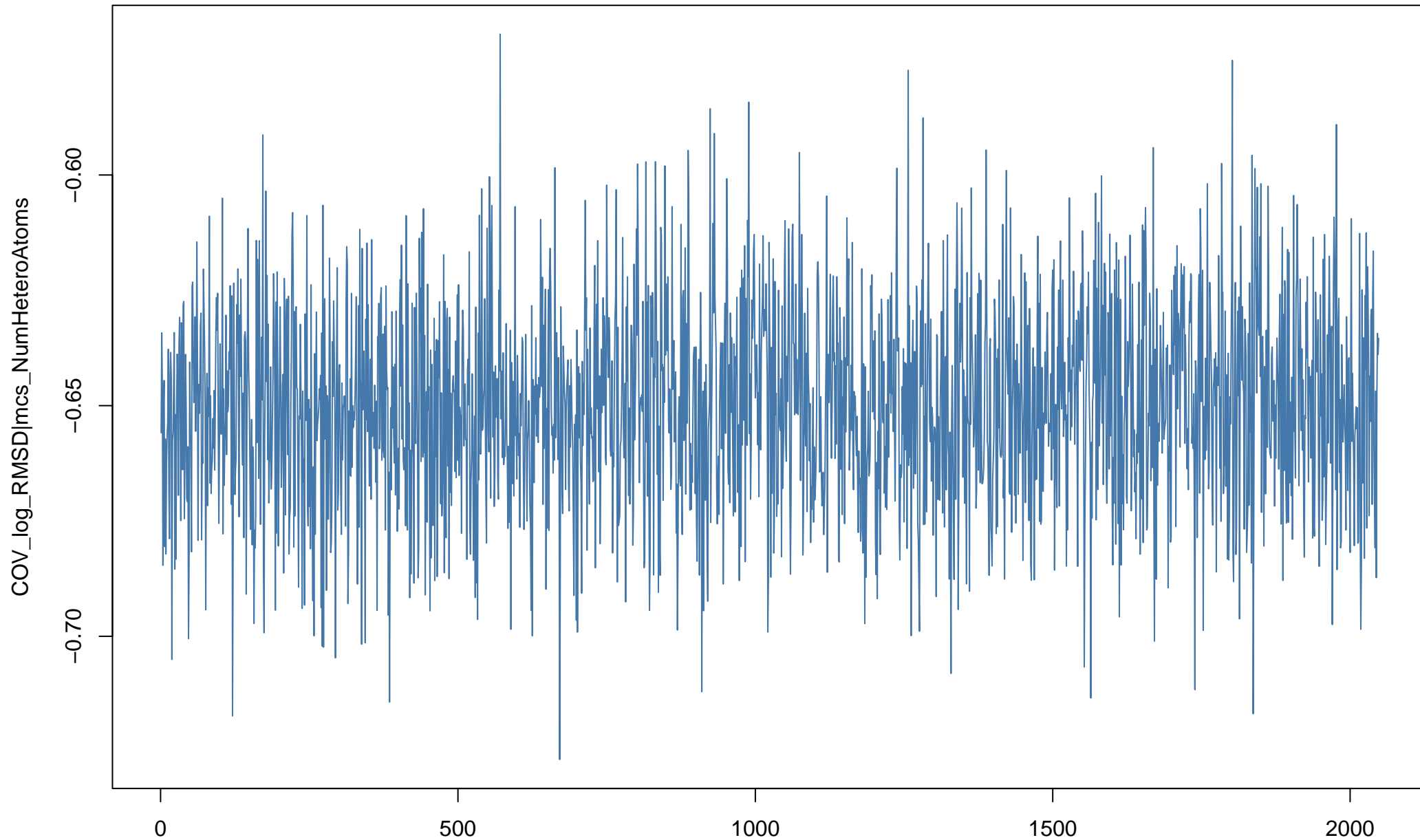
**COV\_log\_RMSD|mcs\_docked\_NumHAcceptors**  
**ESS = 1920 | BMK = 0.0693 | MCSE(6.27) = 2.75 | stat: FALSE | burn: 0**



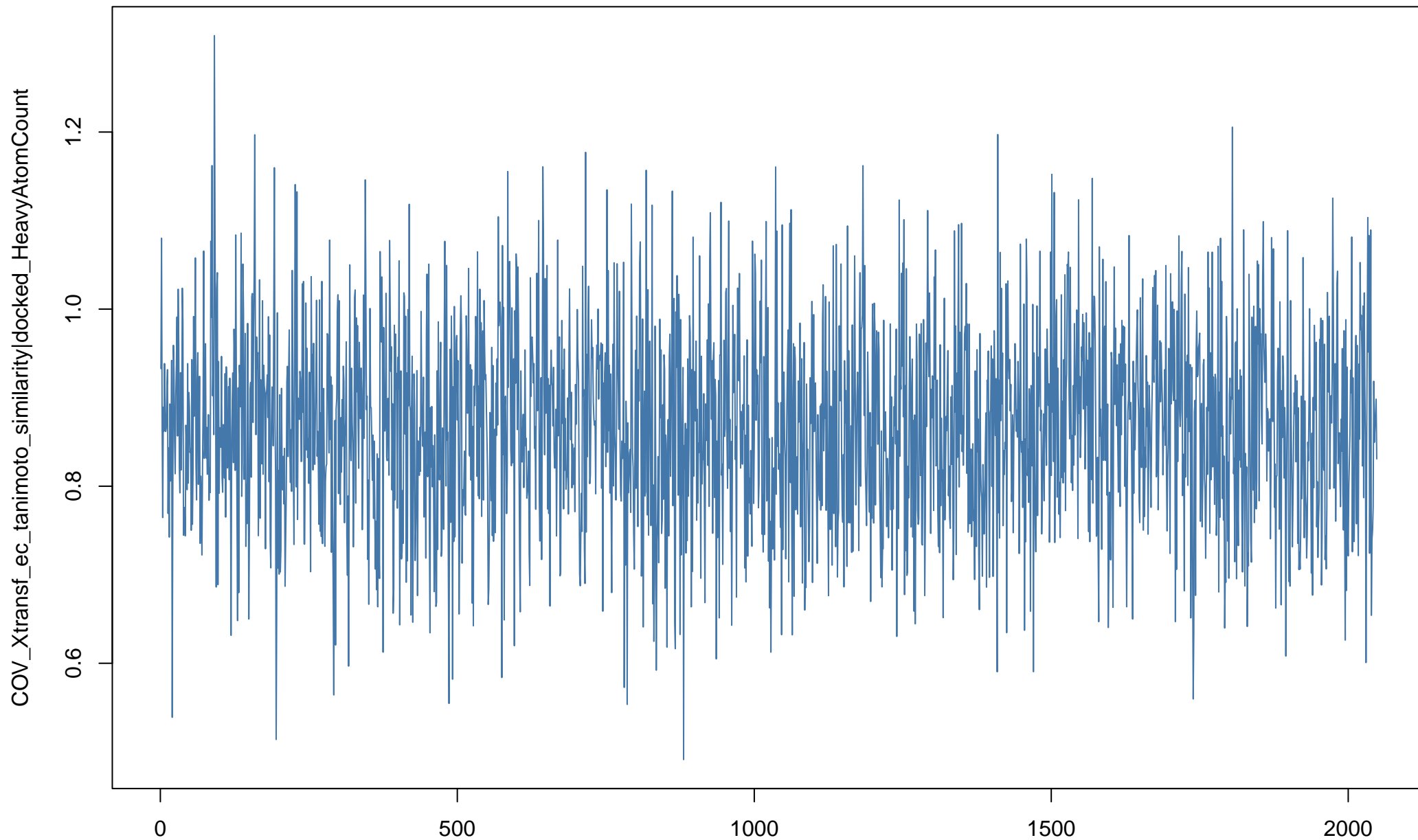
**COV\_log\_RMSD|mcs\_template\_NumHAcceptors**  
**ESS = 1040 | BMK = 0.0862 | MCSE(6.27) = 2.98 | stat: FALSE | burn: 0**



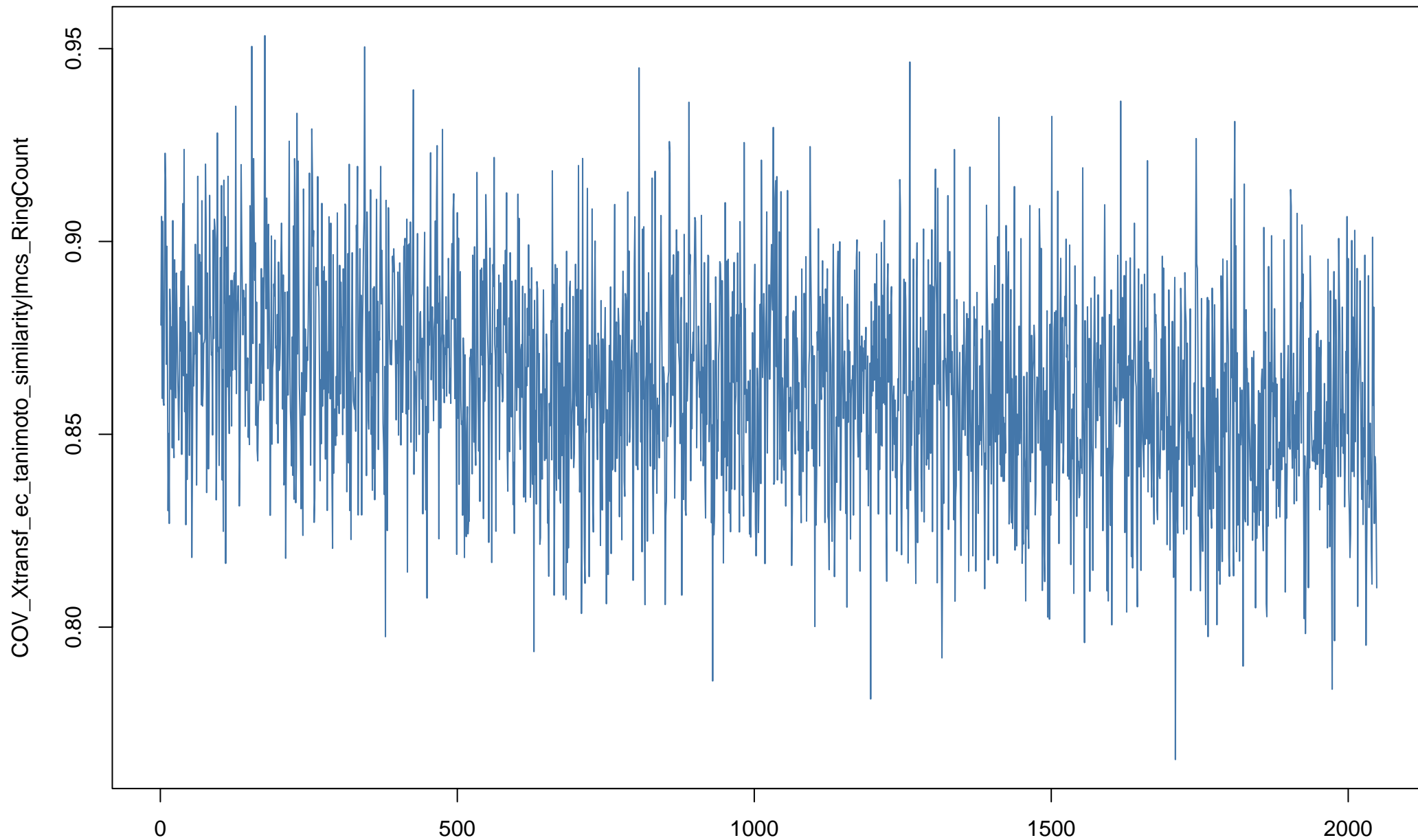
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 1790 | BMK = 0.0597 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0**



**COV\_Xtransf\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount**  
**ESS = 1570 | BMK = 0.0533 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0**

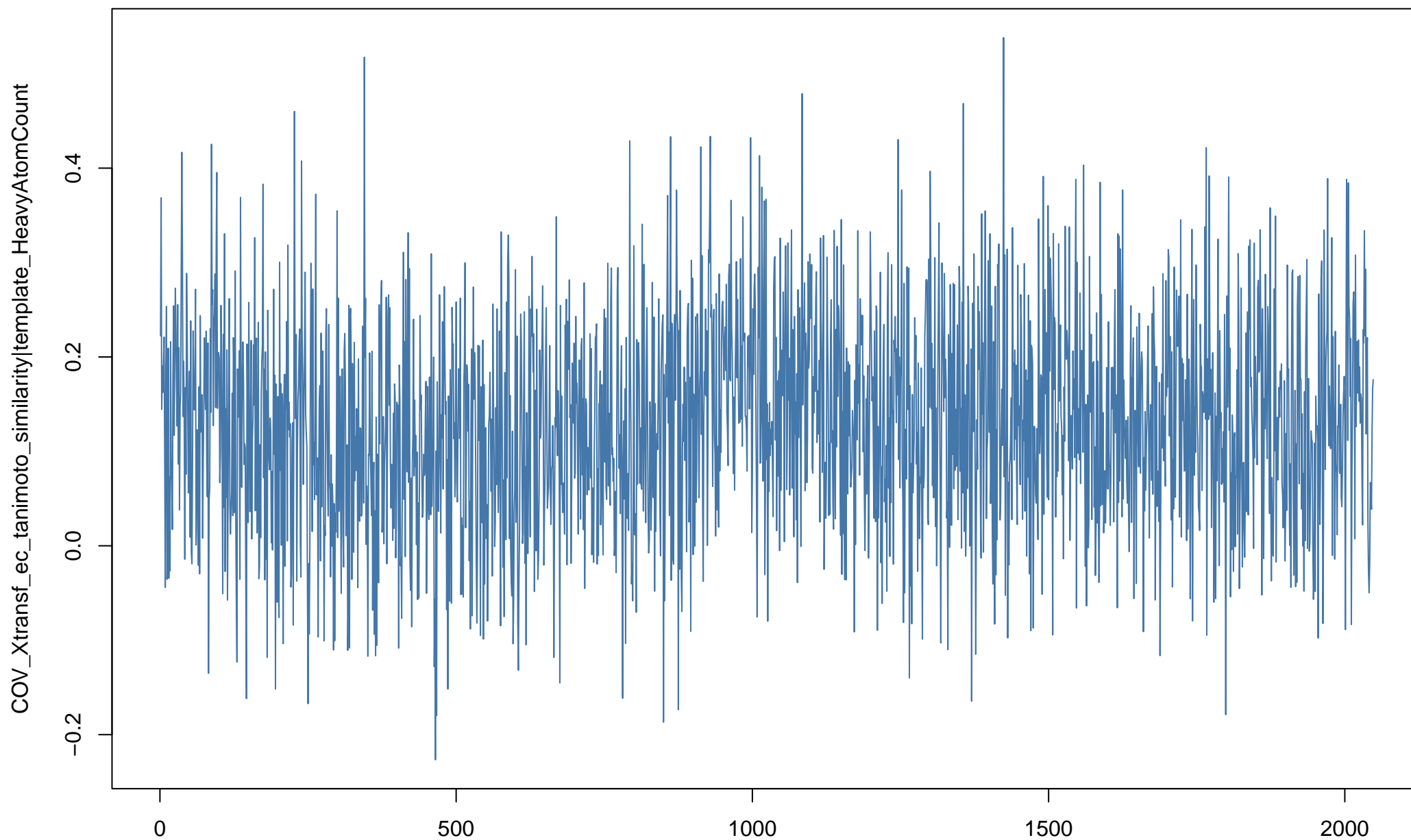


**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 274 | BMK = 0.145 | MCSE(6.27) = 4.54 | stat: FALSE | burn: 0**

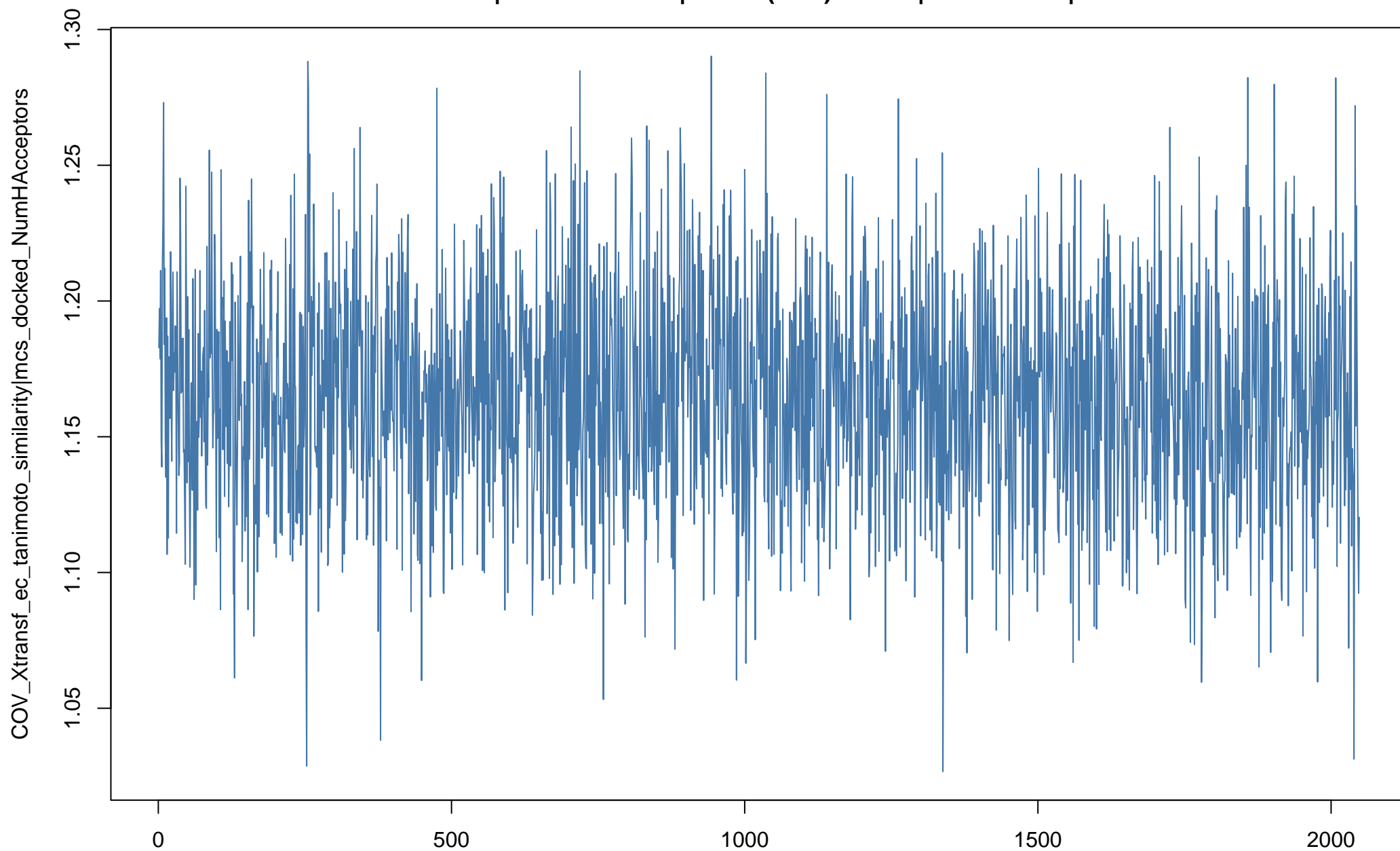




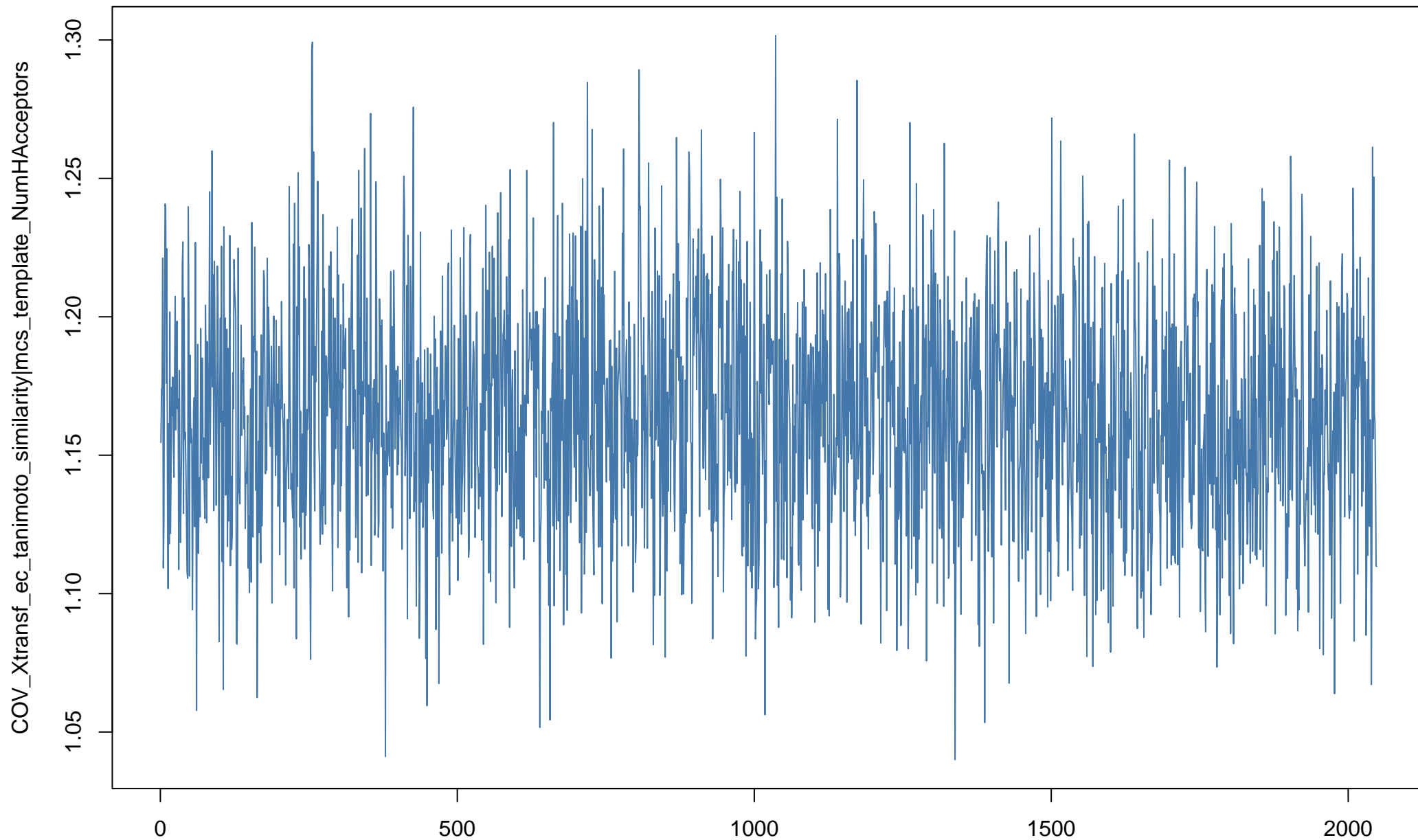
COV\_Xtransf\_ec\_tanimoto\_similarity|template\_HeavyAtomCount  
ESS = 840 | BMK = 0.08 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0



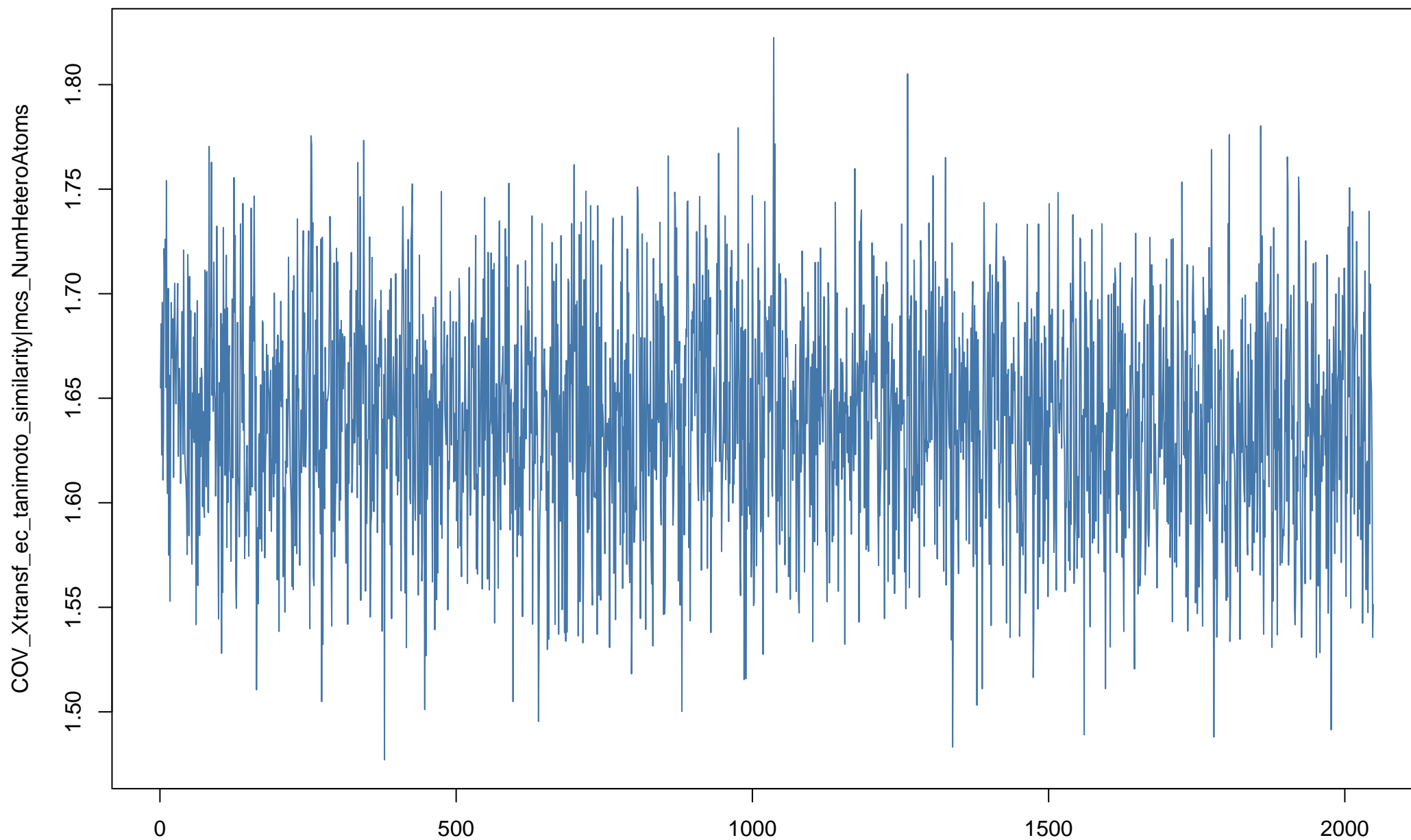
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0455 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0**



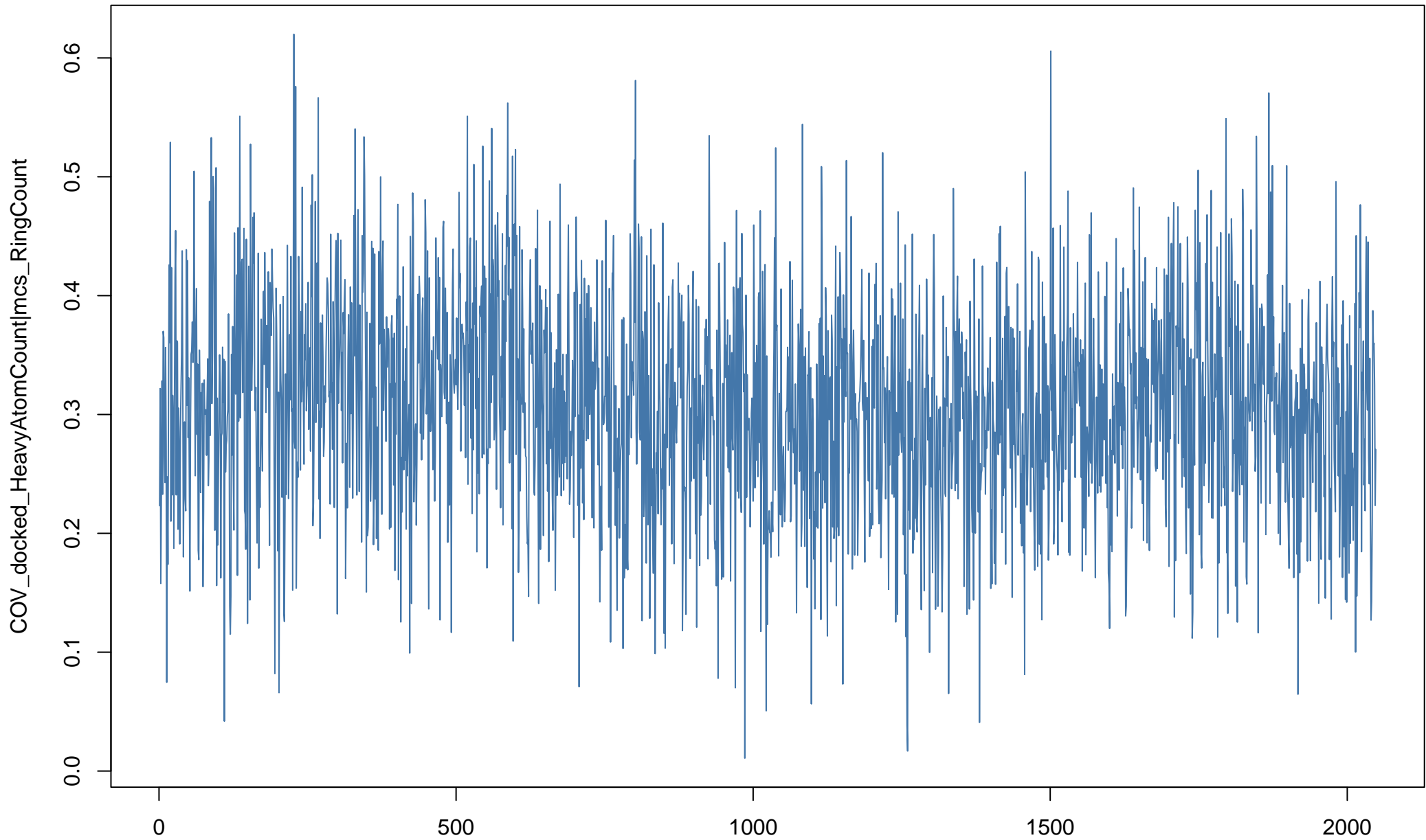
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0534 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0**



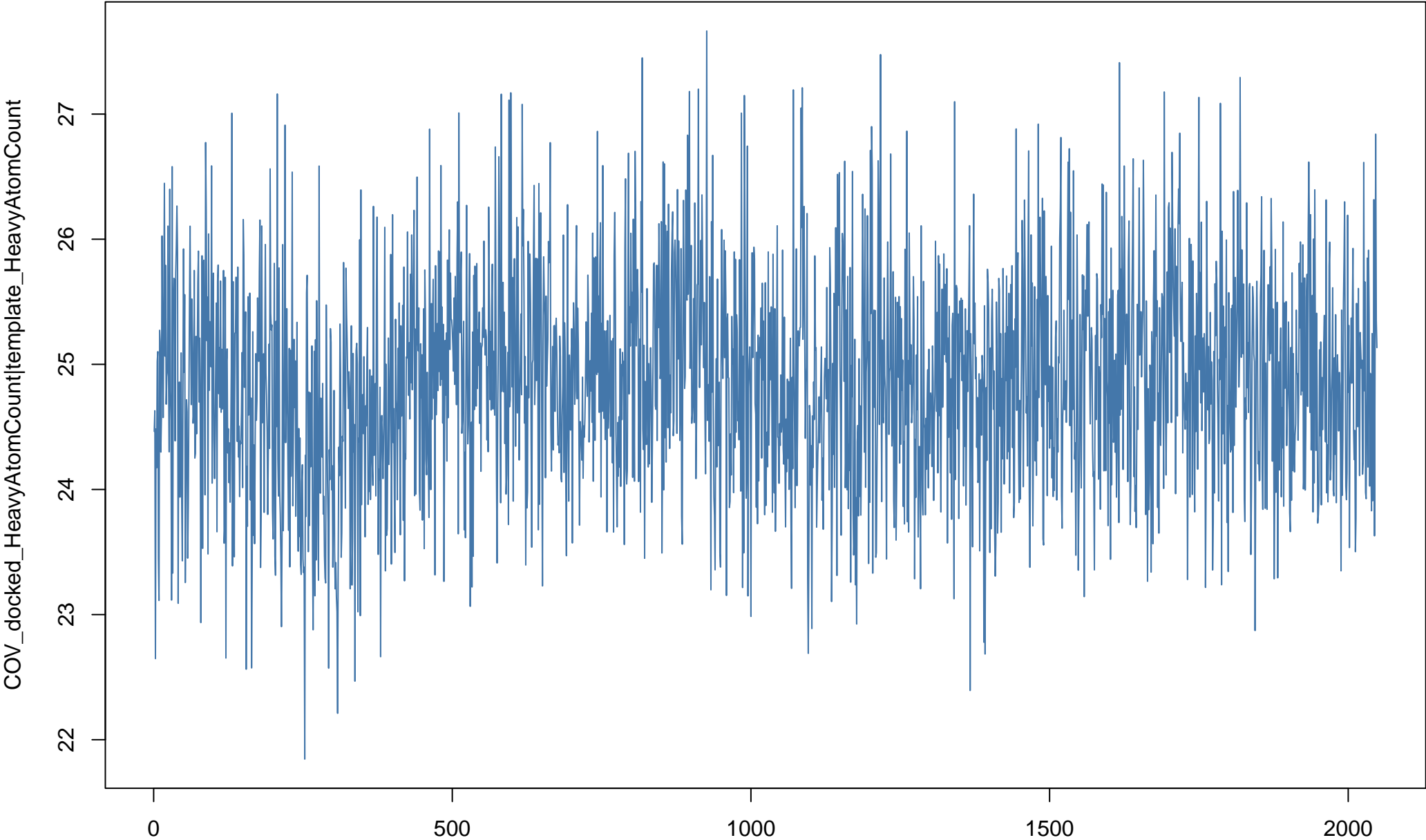
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0584 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0**



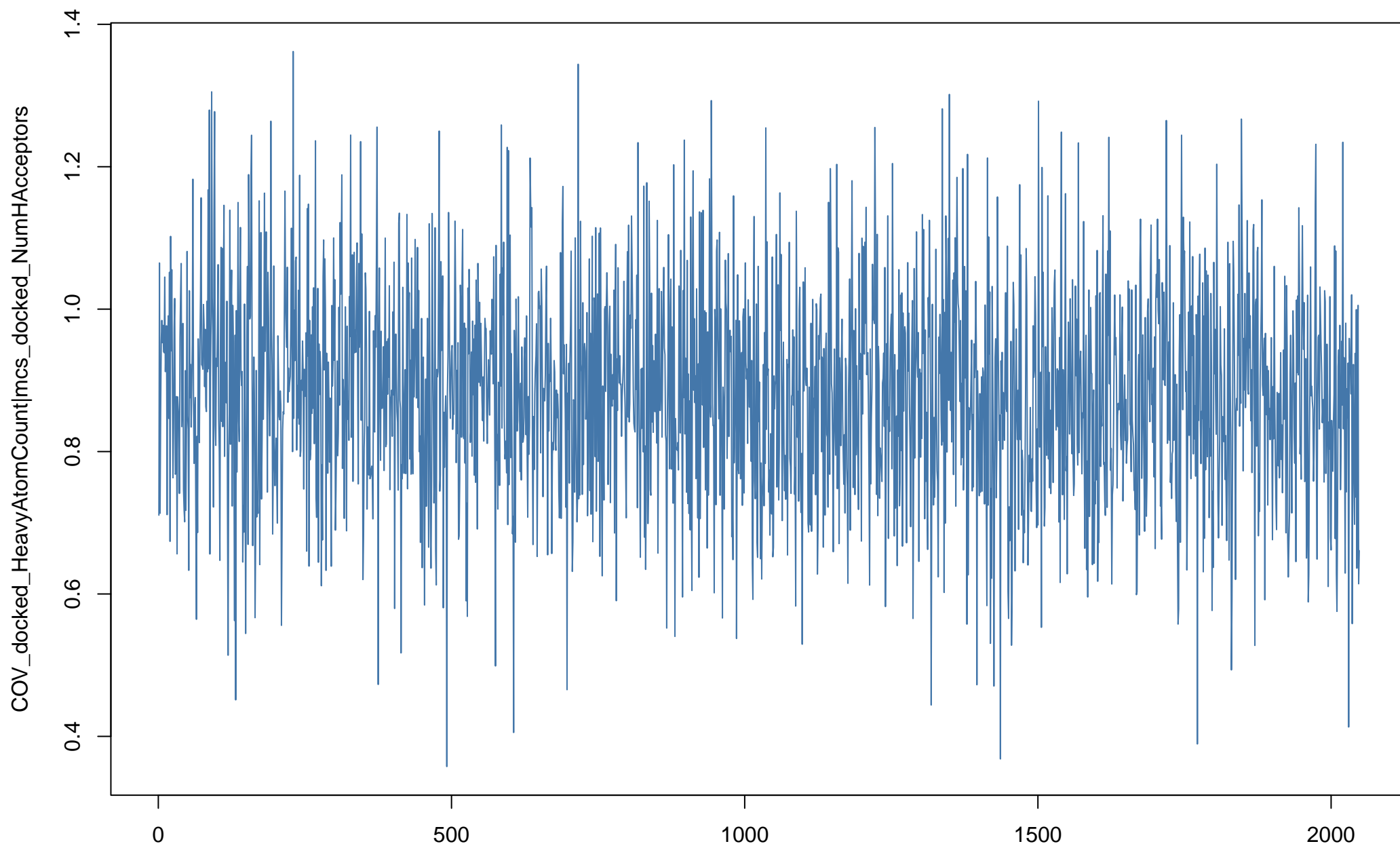
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 805 | BMK = 0.0877 | MCSE(6.27) = 3.52 | stat: TRUE | burn: 0**



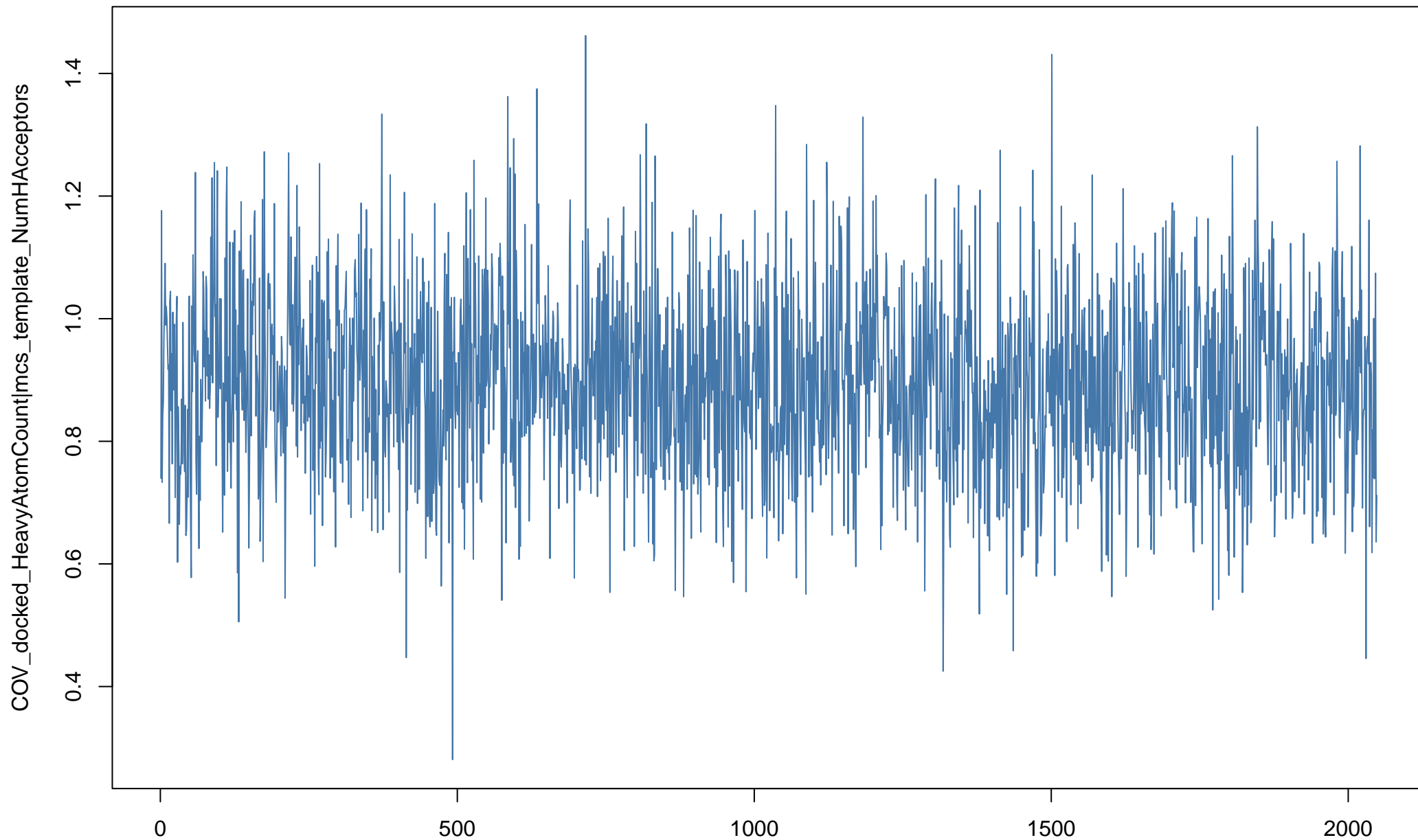
**COV\_docked\_HeavyAtomCount|template\_HeavyAtomCount**  
**ESS = 597 | BMK = 0.0577 | MCSE(6.27) = 4.06 | stat: TRUE | burn: 0**



**COV\_docked\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 1910 | BMK = 0.0547 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0**

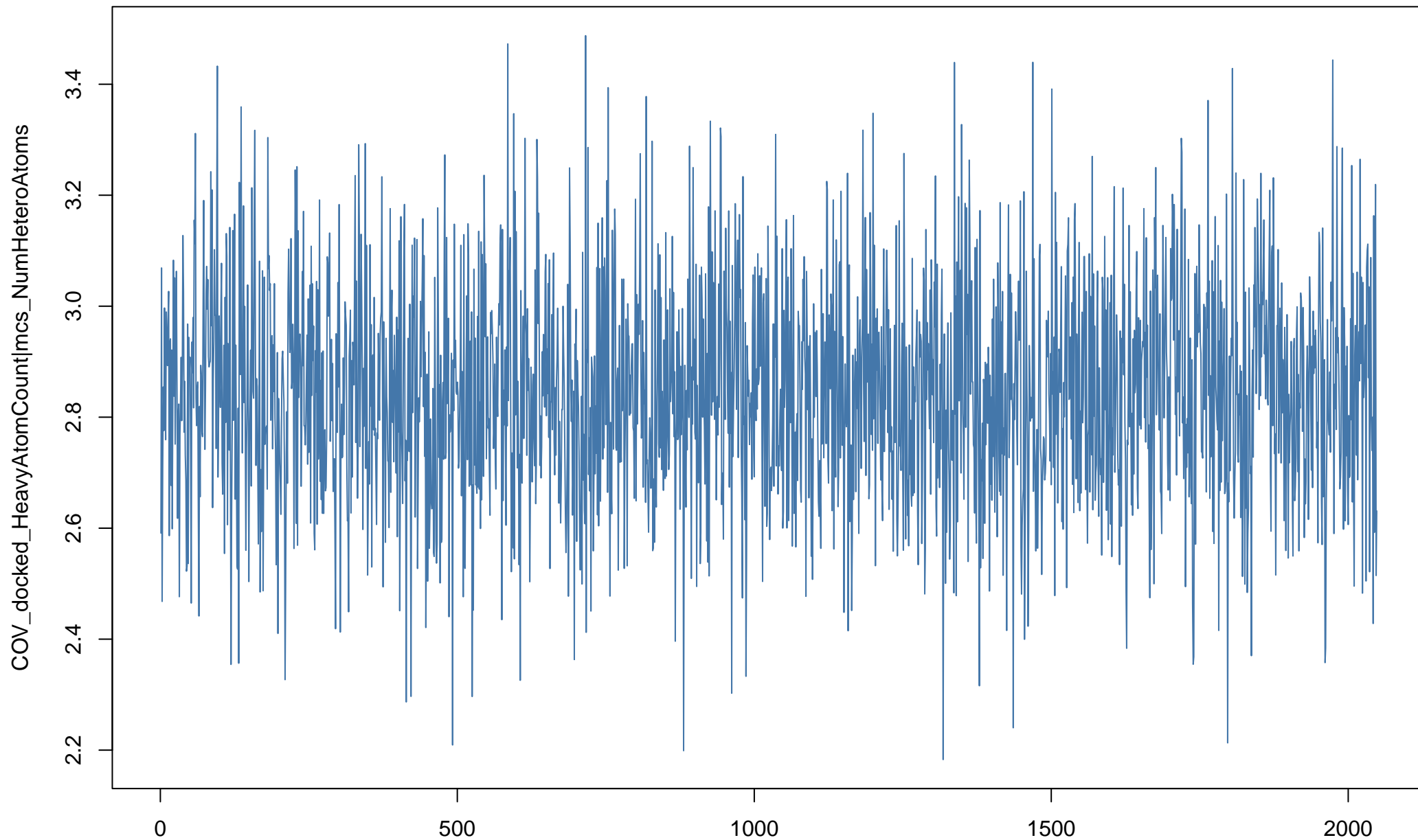


**COV\_docked\_HeavyAtomCount|mcs\_template\_NumHAcceptors**  
**ESS = 1900 | BMK = 0.0477 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0**

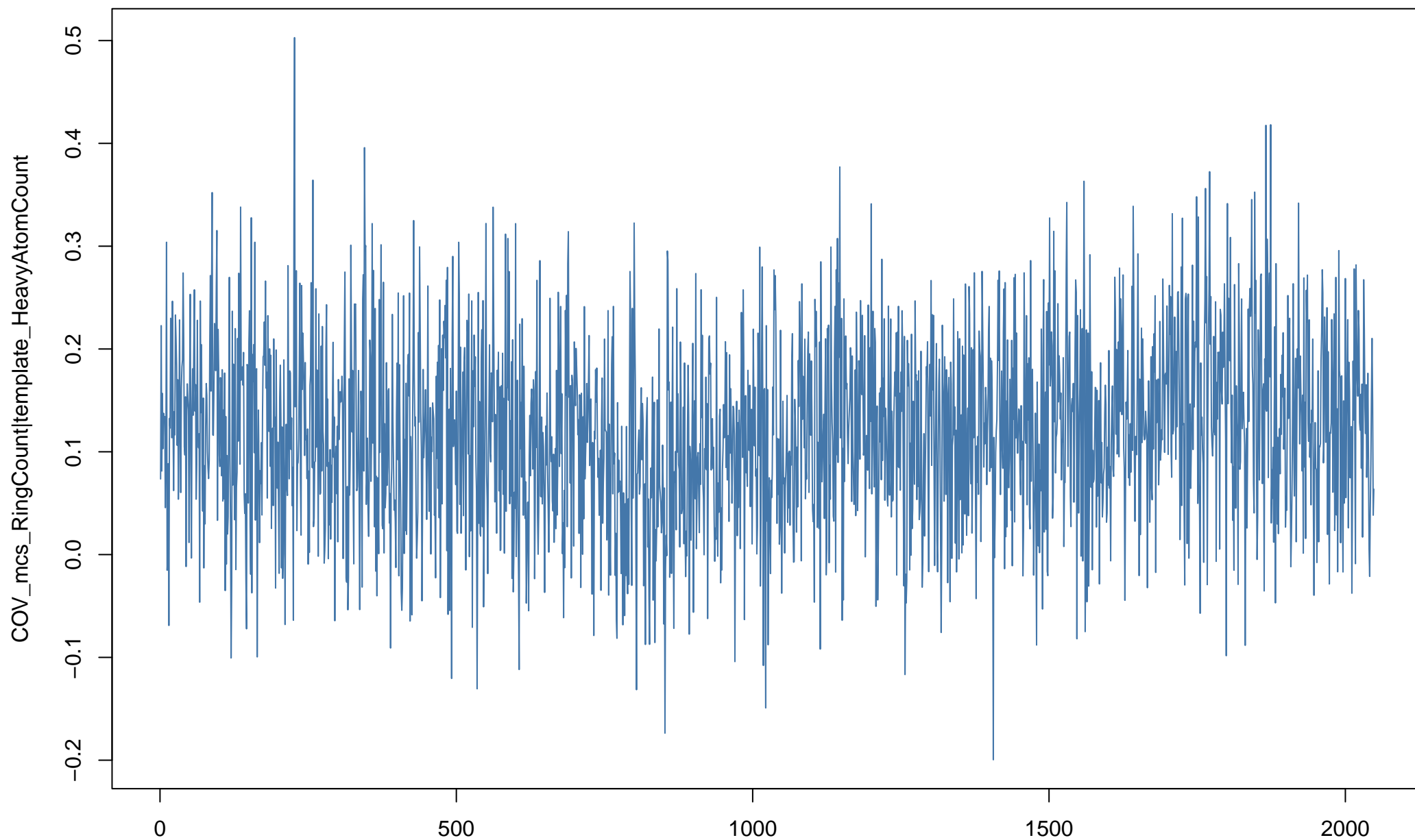




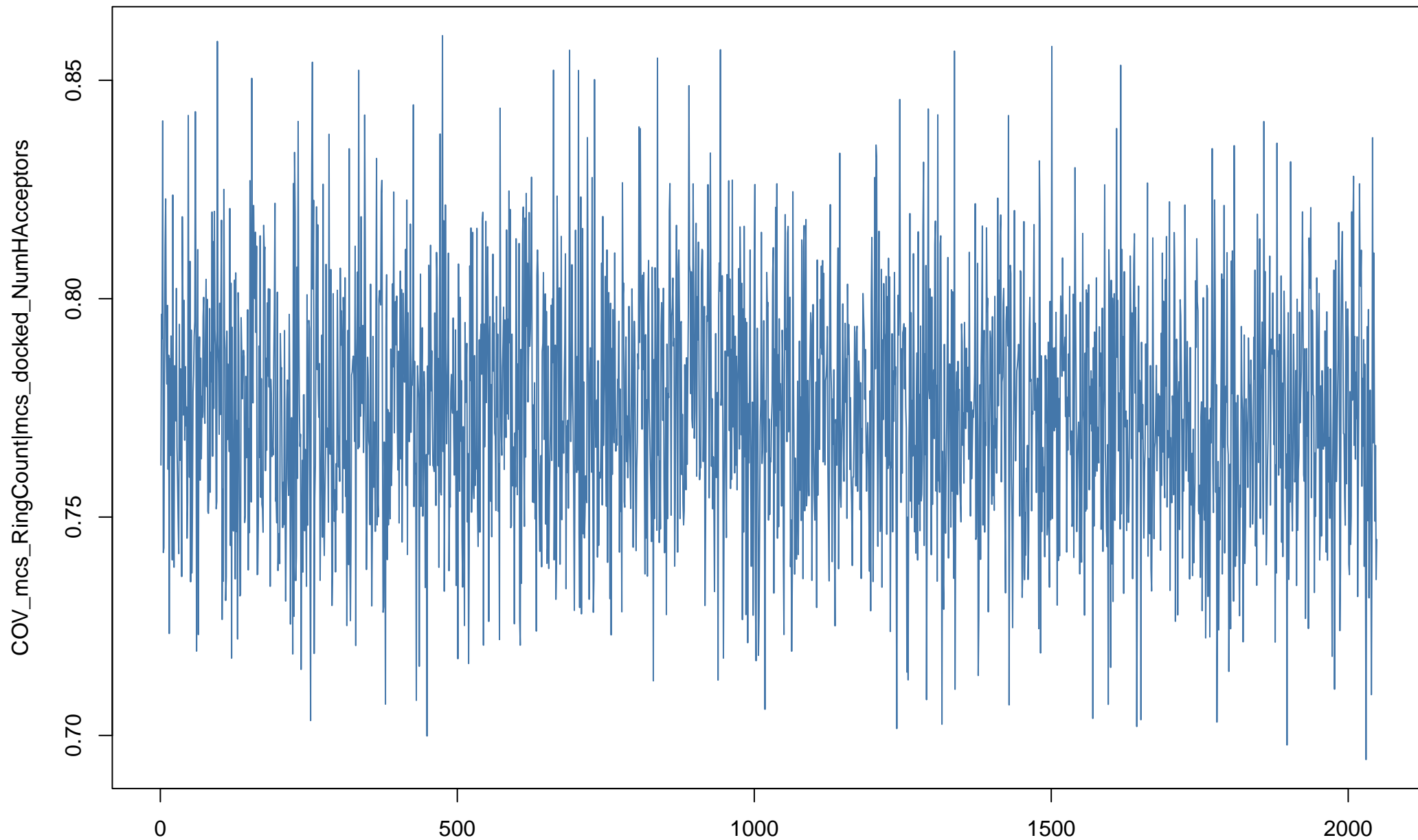
**COV\_docked\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0454 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0**



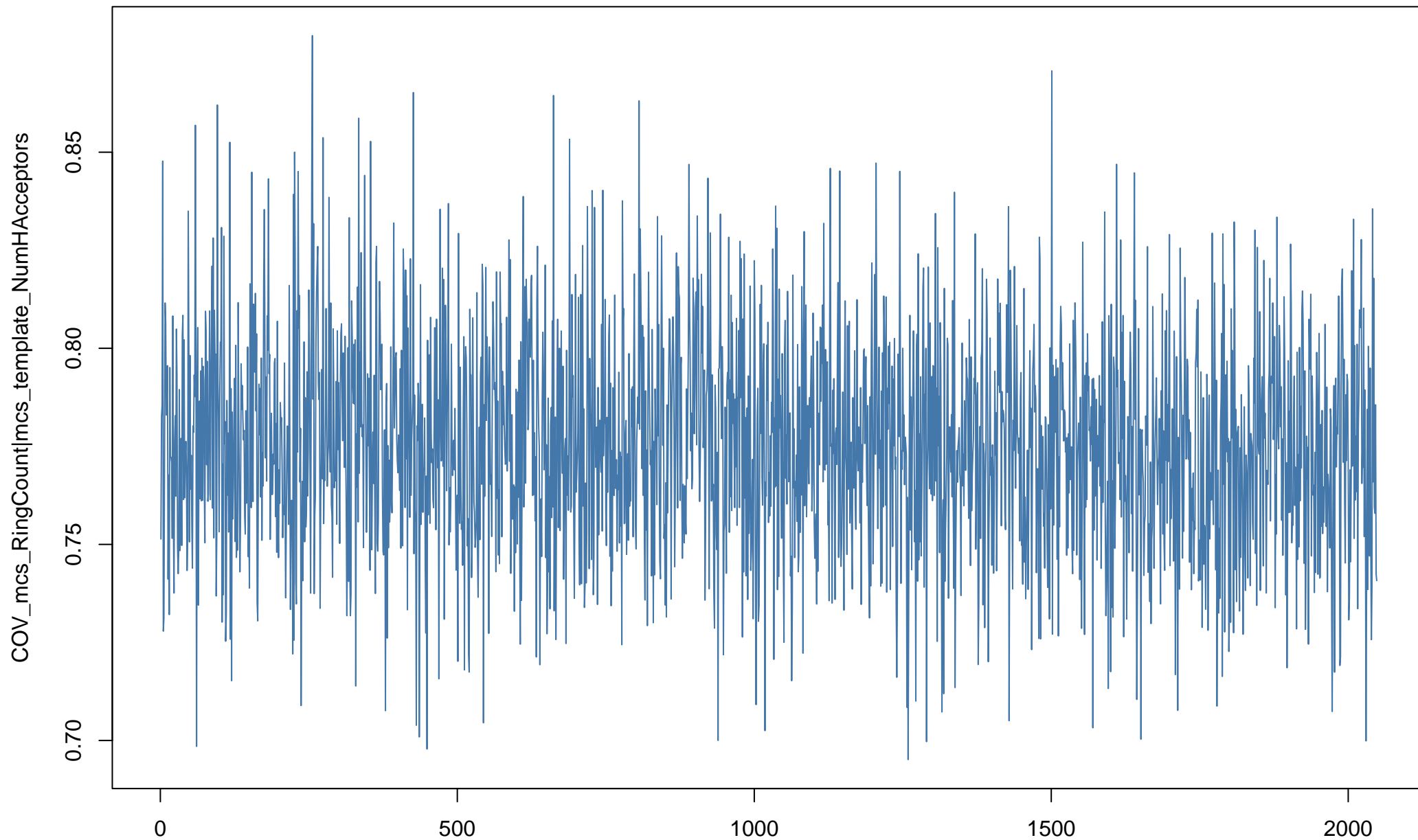
**COV\_mcs\_RingCount|template\_HeavyAtomCount**  
**ESS = 611 | BMK = 0.0948 | MCSE(6.27) = 3.8 | stat: TRUE | burn: 0**



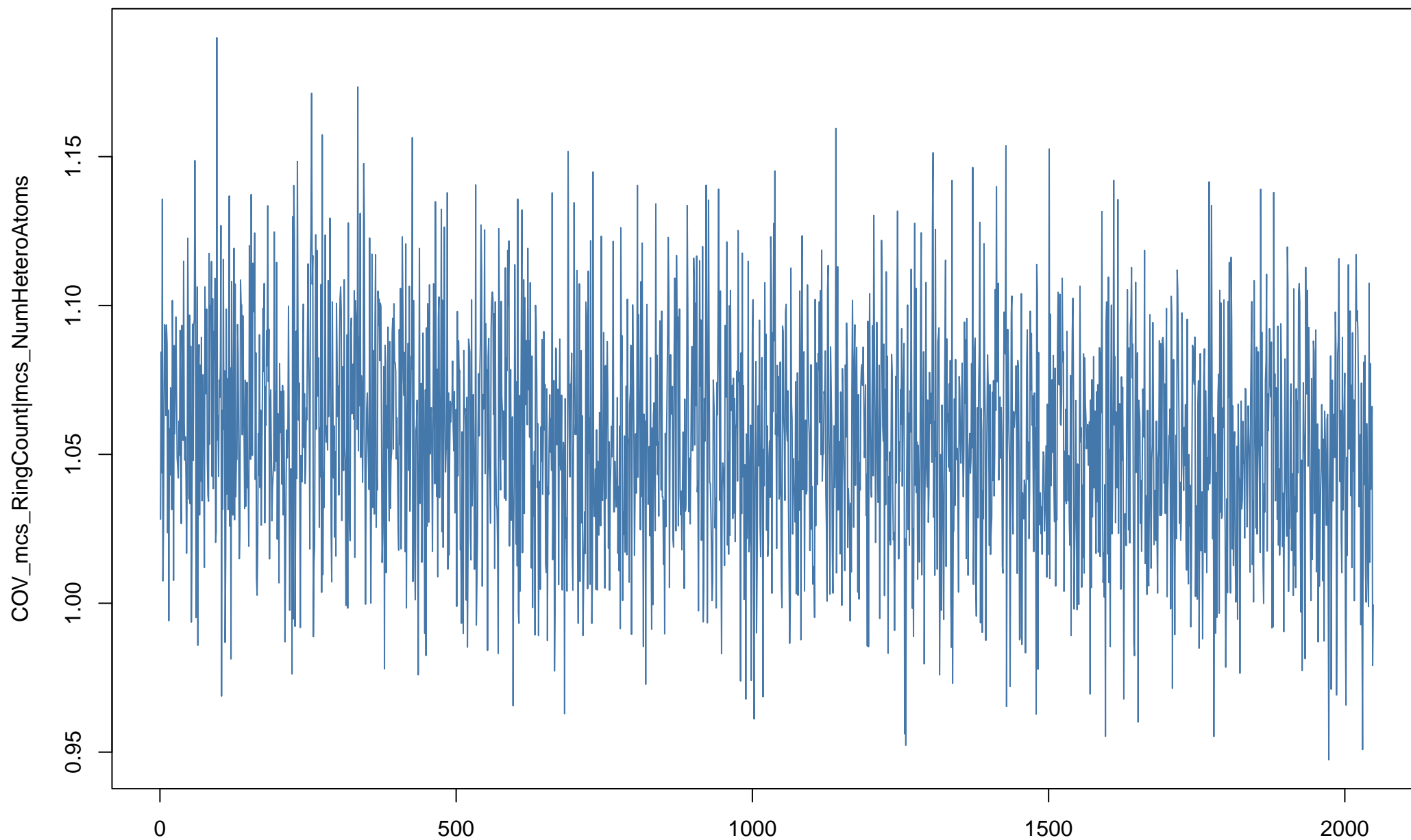
**COV\_mcs\_RingCount|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0579 | MCSE(6.27) = 2.26 | stat: FALSE | burn: 0**



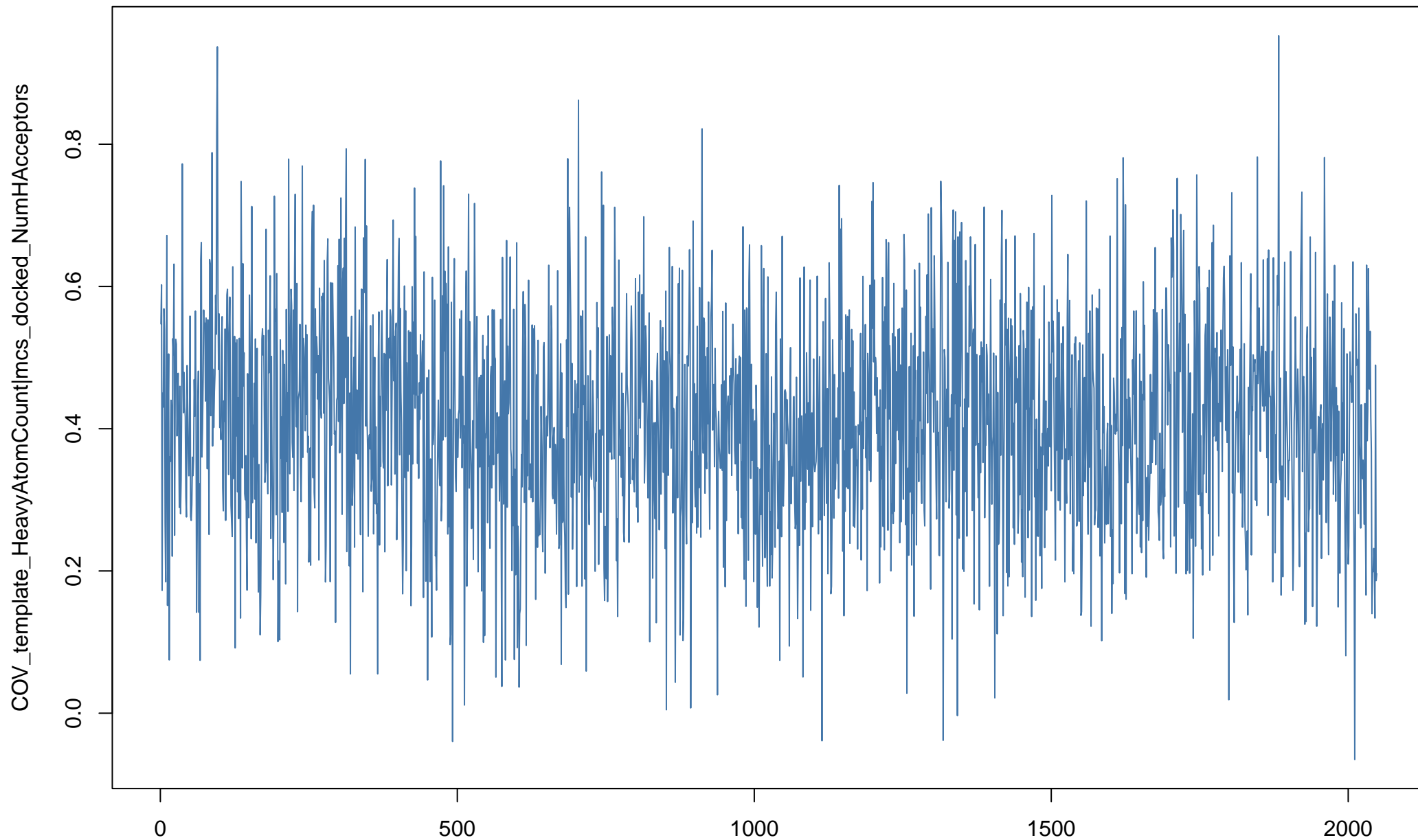
**COV\_mcs\_RingCount|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0716 | MCSE(6.27) = 2.57 | stat: FALSE | burn: 0**



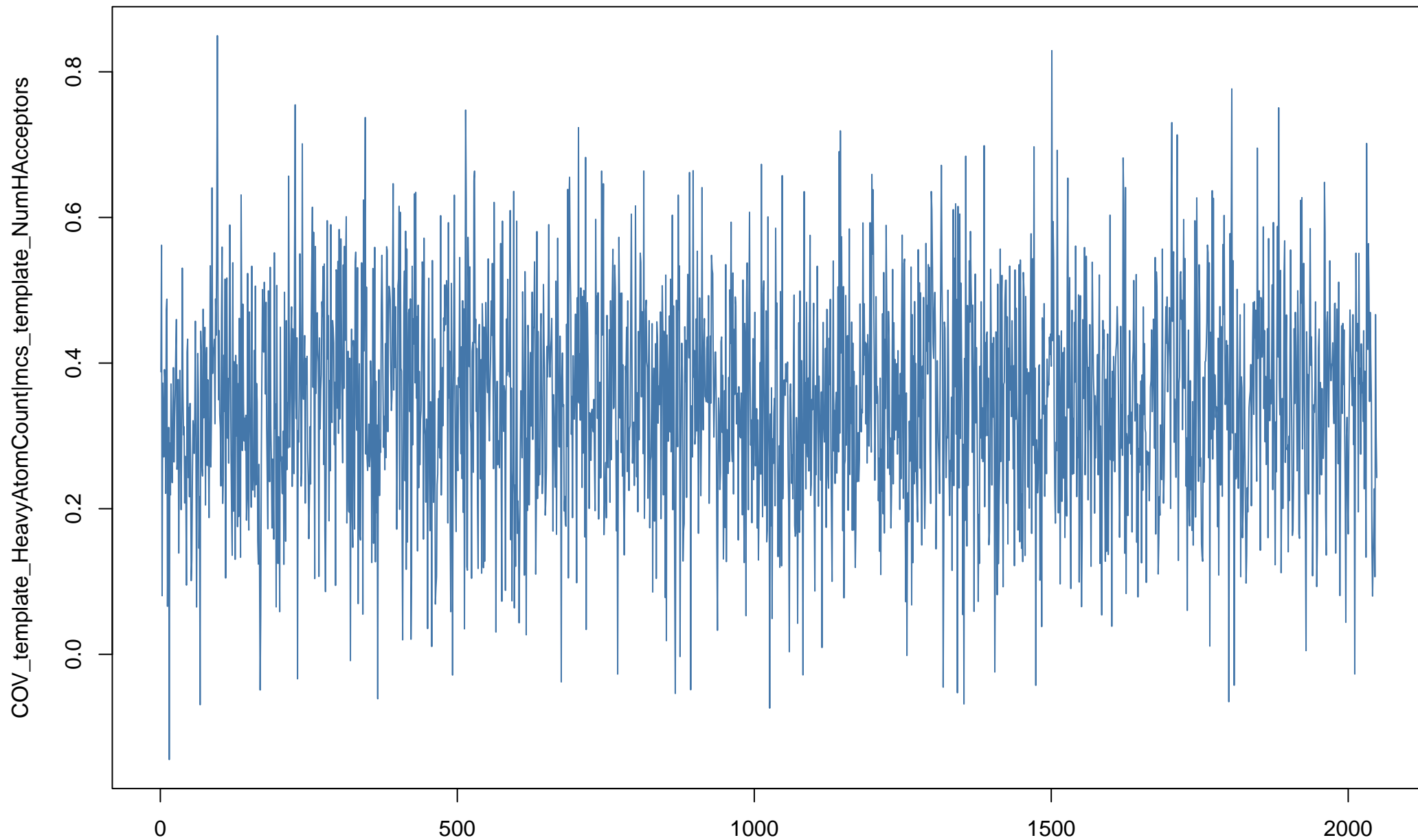
**COV\_mcs\_RingCount|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0828 | MCSE(6.27) = 2.97 | stat: FALSE | burn: 0**



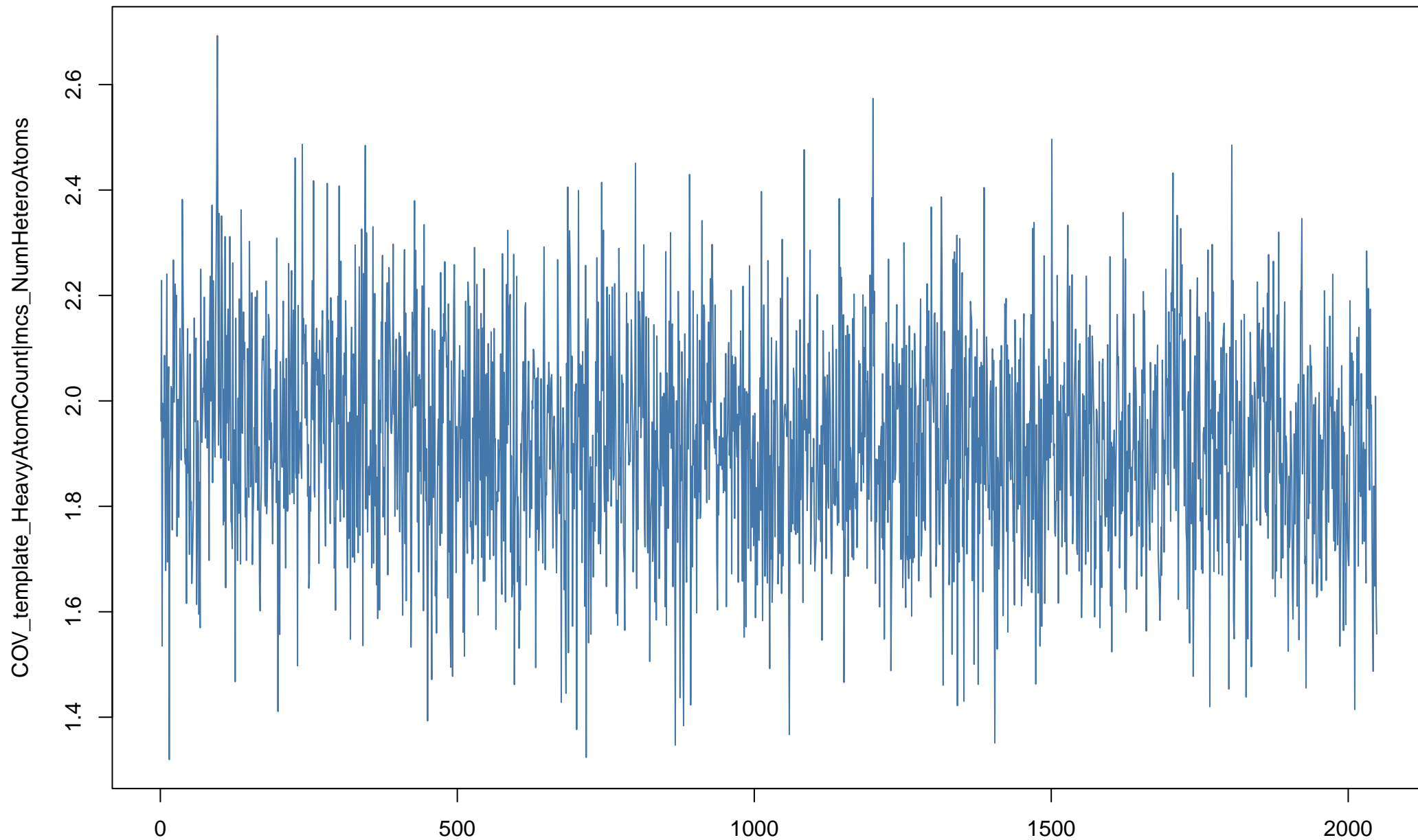
**COV\_template\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 1540 | BMK = 0.0581 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0**



**COV\_template\_HeavyAtomCount|mcs\_template\_NumHAcceptors**  
**ESS = 1610 | BMK = 0.0278 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0**

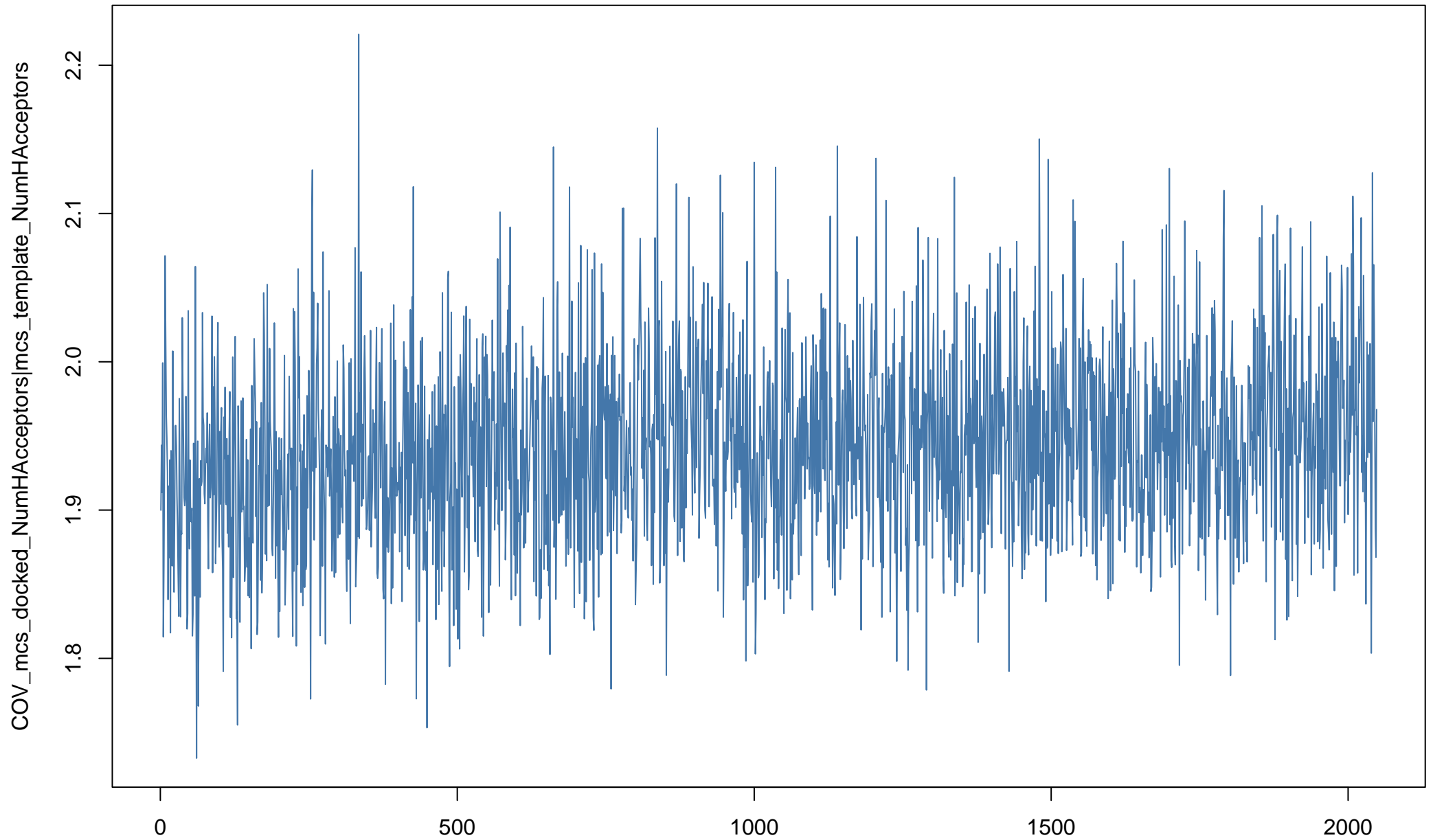


**COV\_template\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 1510 | BMK = 0.072 | MCSE(6.27) = 2.61 | stat: FALSE | burn: 0**

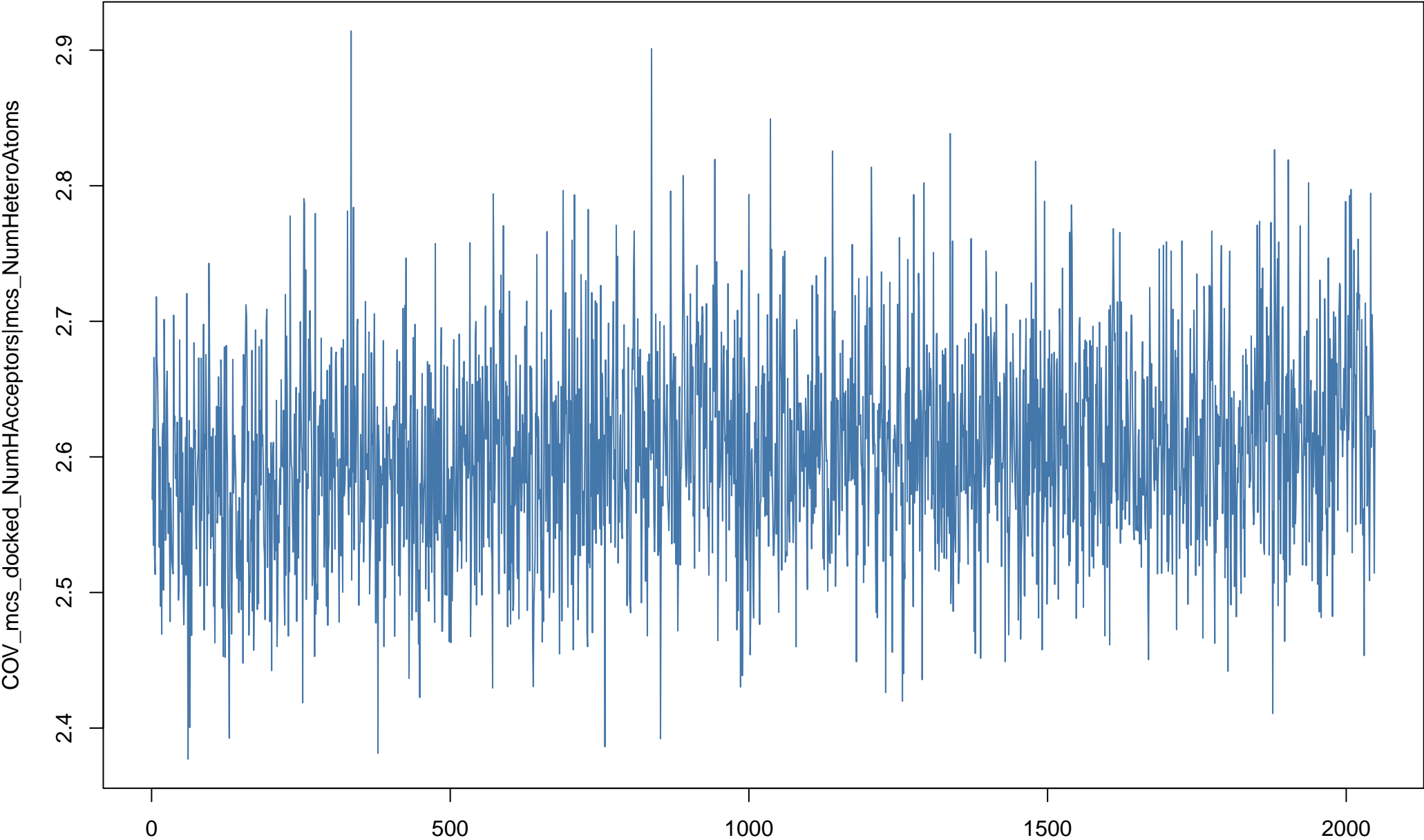




**COV\_mcs\_docked\_NumHAcceptors|mcs\_template\_NumHAcceptors**  
**ESS = 349 | BMK = 0.106 | MCSE(6.27) = 3.7 | stat: FALSE | burn: 0**



**COV\_mcs\_docked\_NumHAcceptors|mcs\_NumHeteroAtoms**  
**ESS = 445 | BMK = 0.107 | MCSE(6.27) = 3.65 | stat: FALSE | burn: 0**



**COV\_mcs\_template\_NumHAcceptors|mcs\_NumHeteroAtoms**  
**ESS = 481 | BMK = 0.103 | MCSE(6.27) = 3.89 | stat: FALSE | burn: 0**

