

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.526327998034051

max MCSE = 11.778998711036

all stationary: FALSE

burn: 1224

-- STATS 2D --

min ESS = 801.53745656884

max BMK = 0.091532126893689

max MCSE = 3.44757224953281

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.517210613073053

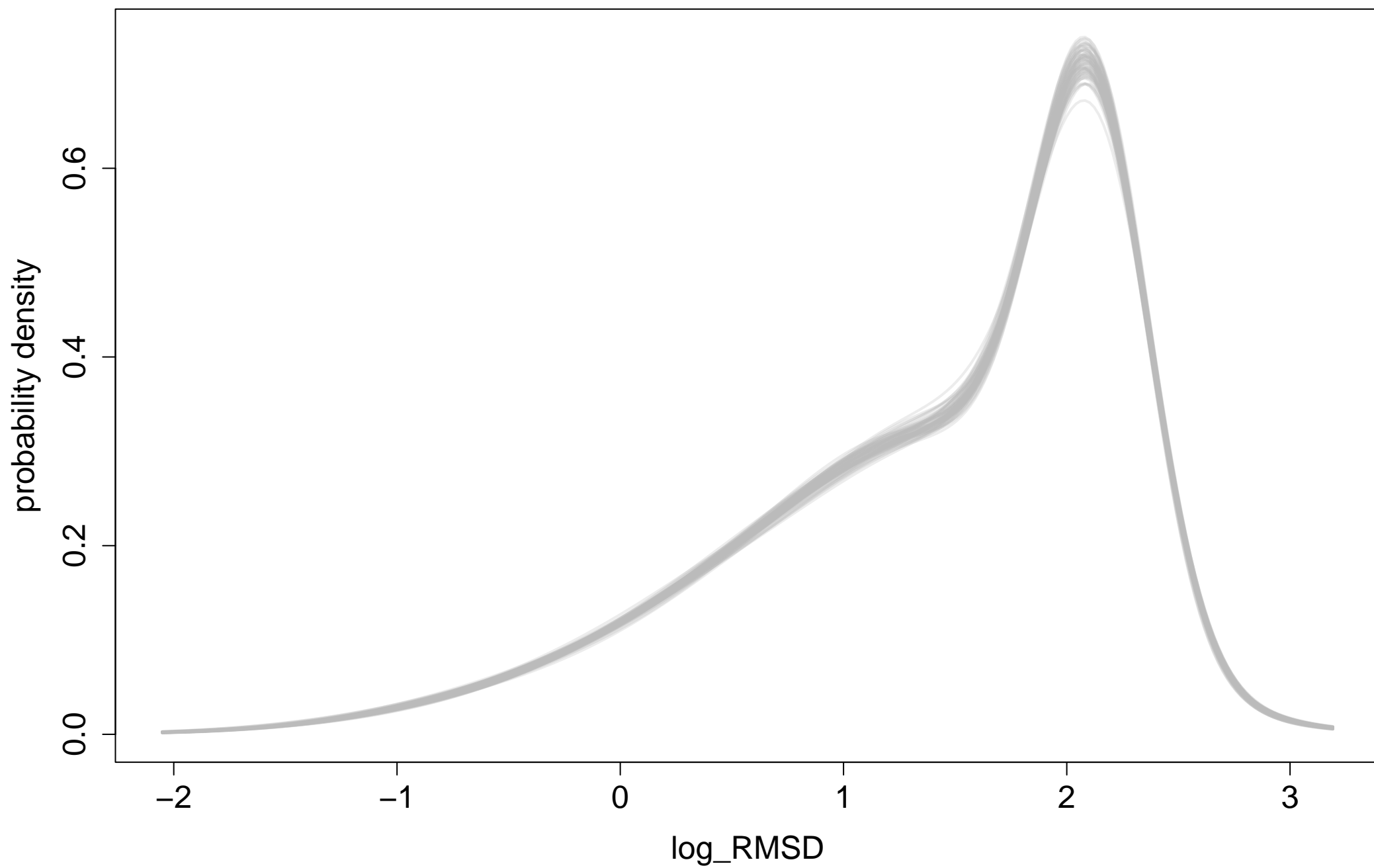
max MCSE = NaN

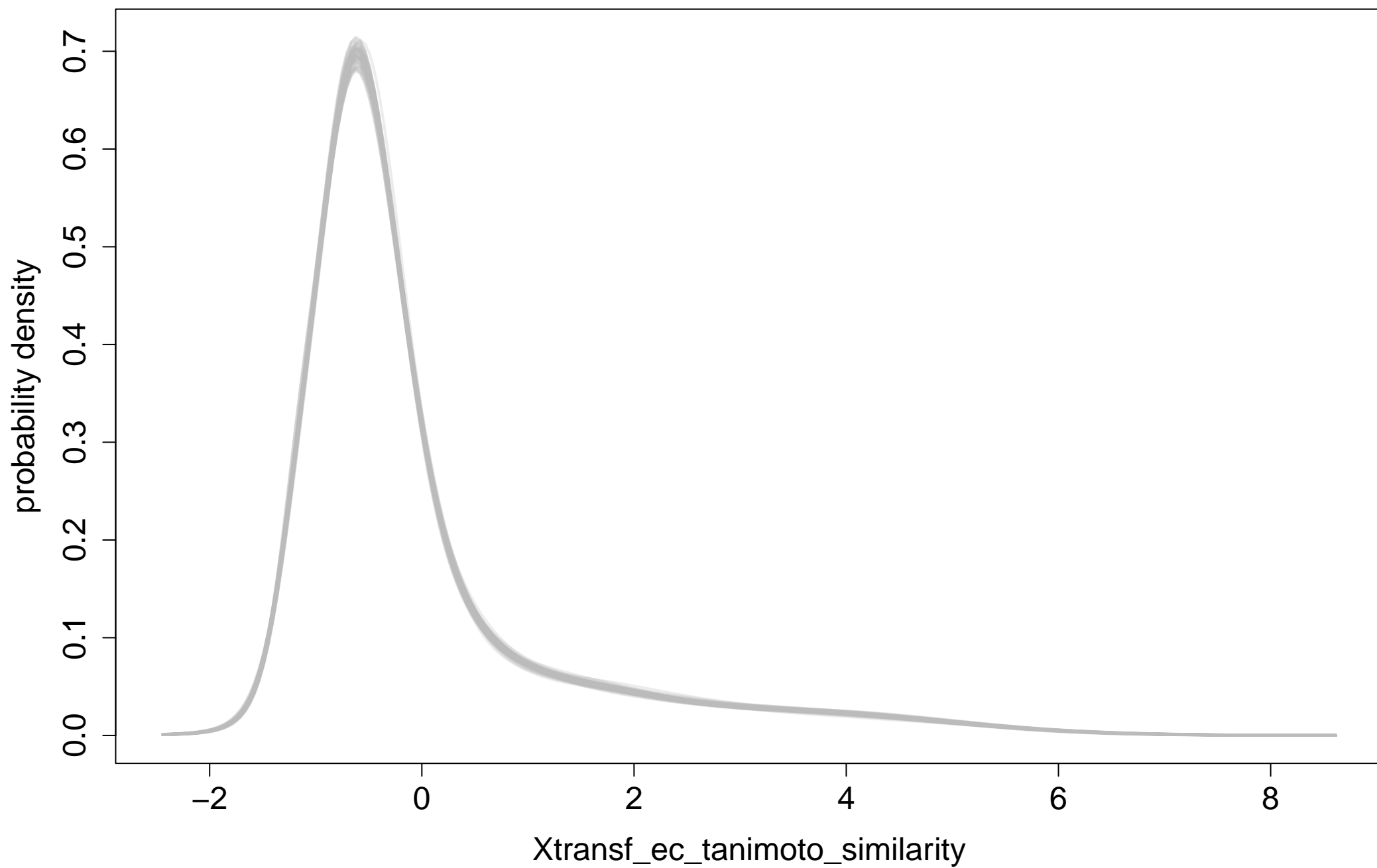
all stationary: FALSE

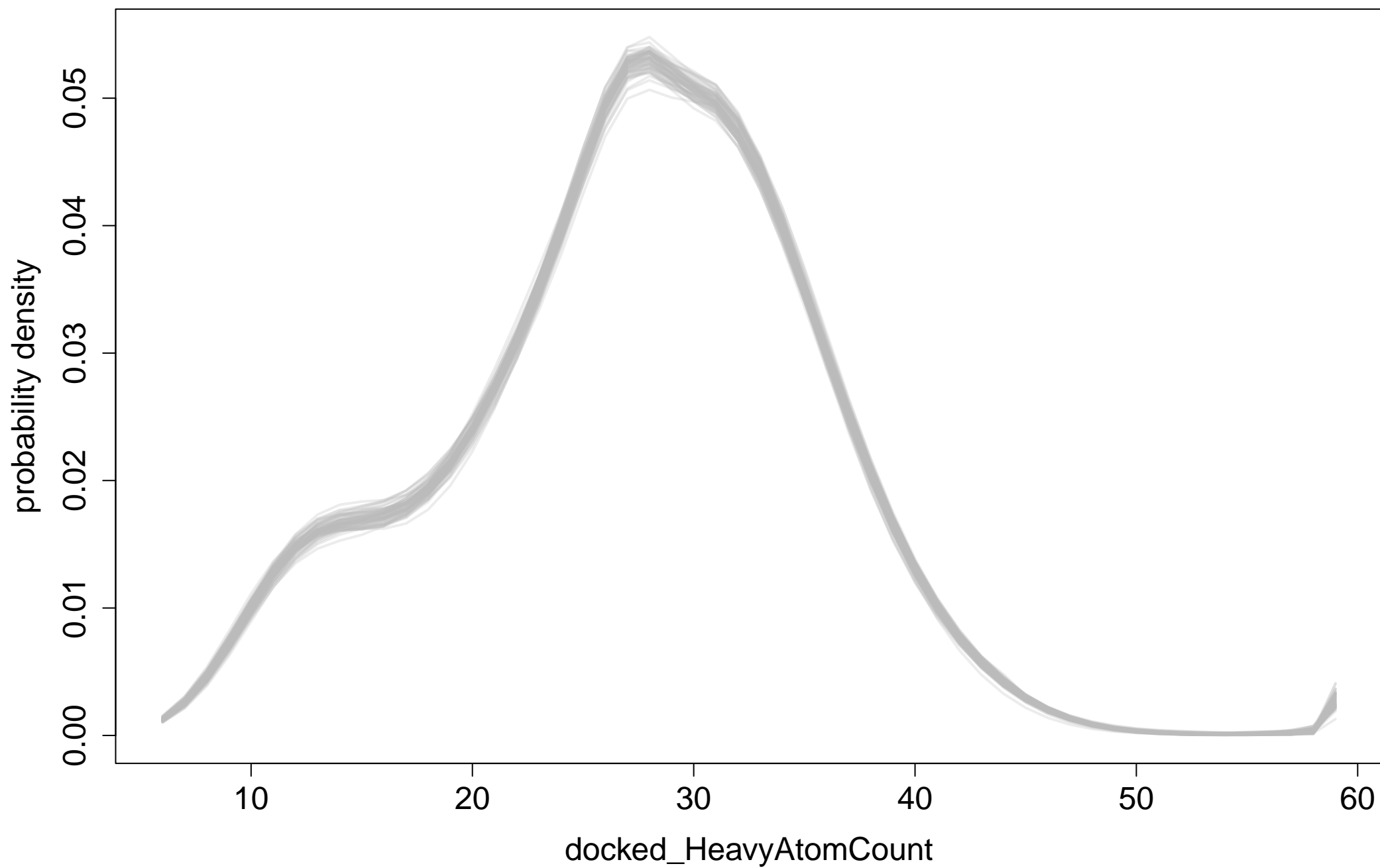
burn: 2040

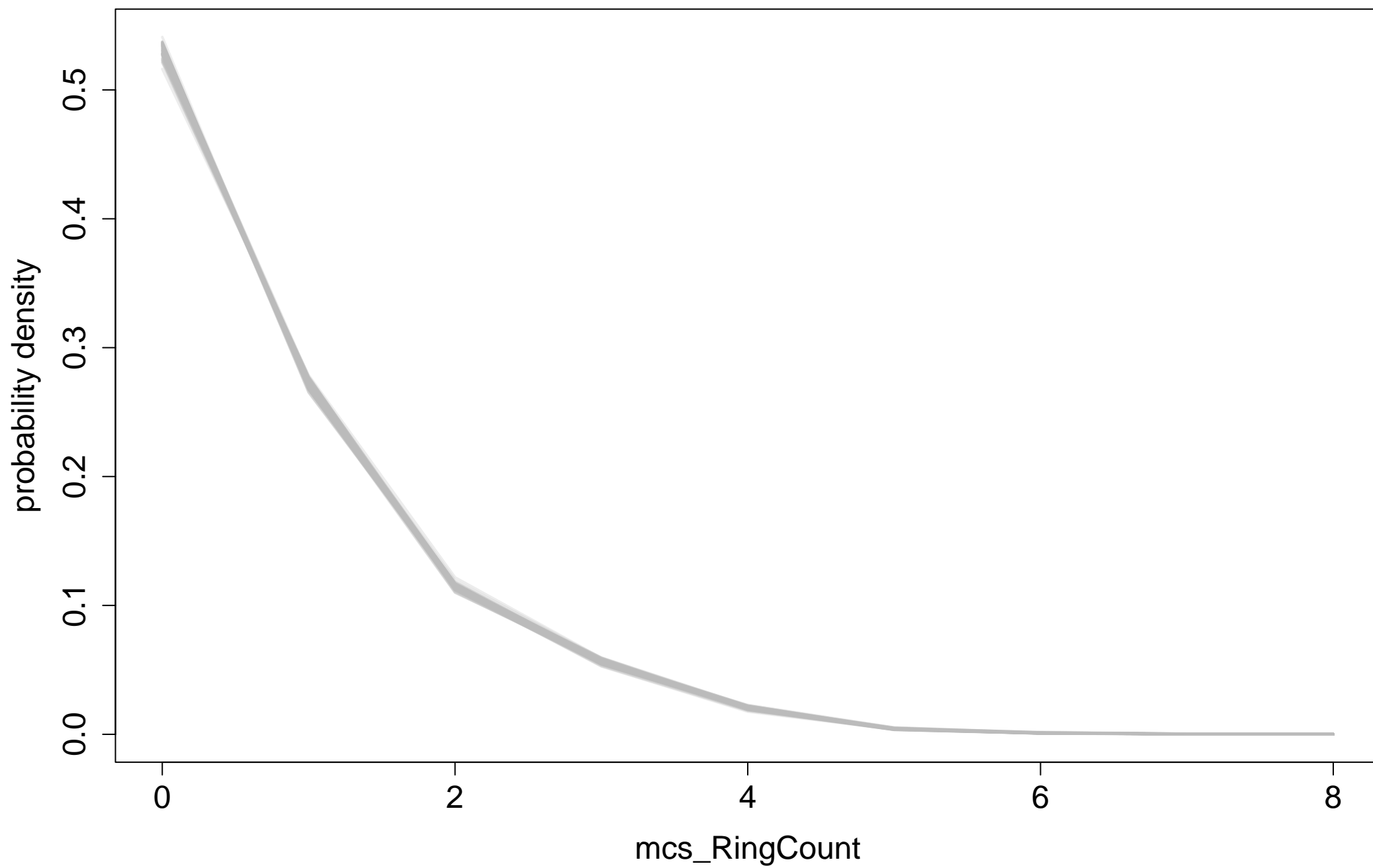
Occupied clusters: 48 of 91

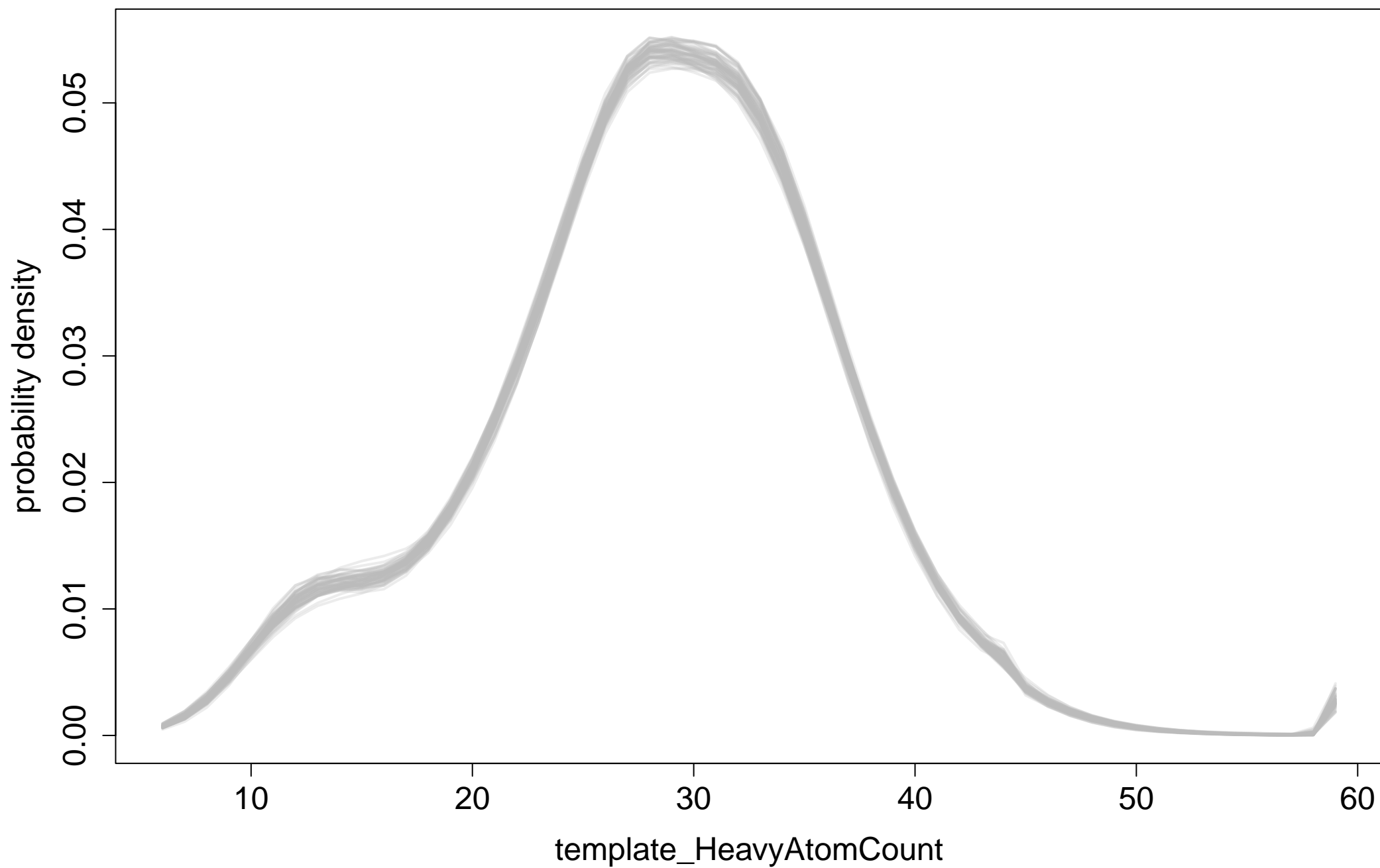
LL: -112000 +- 31.6

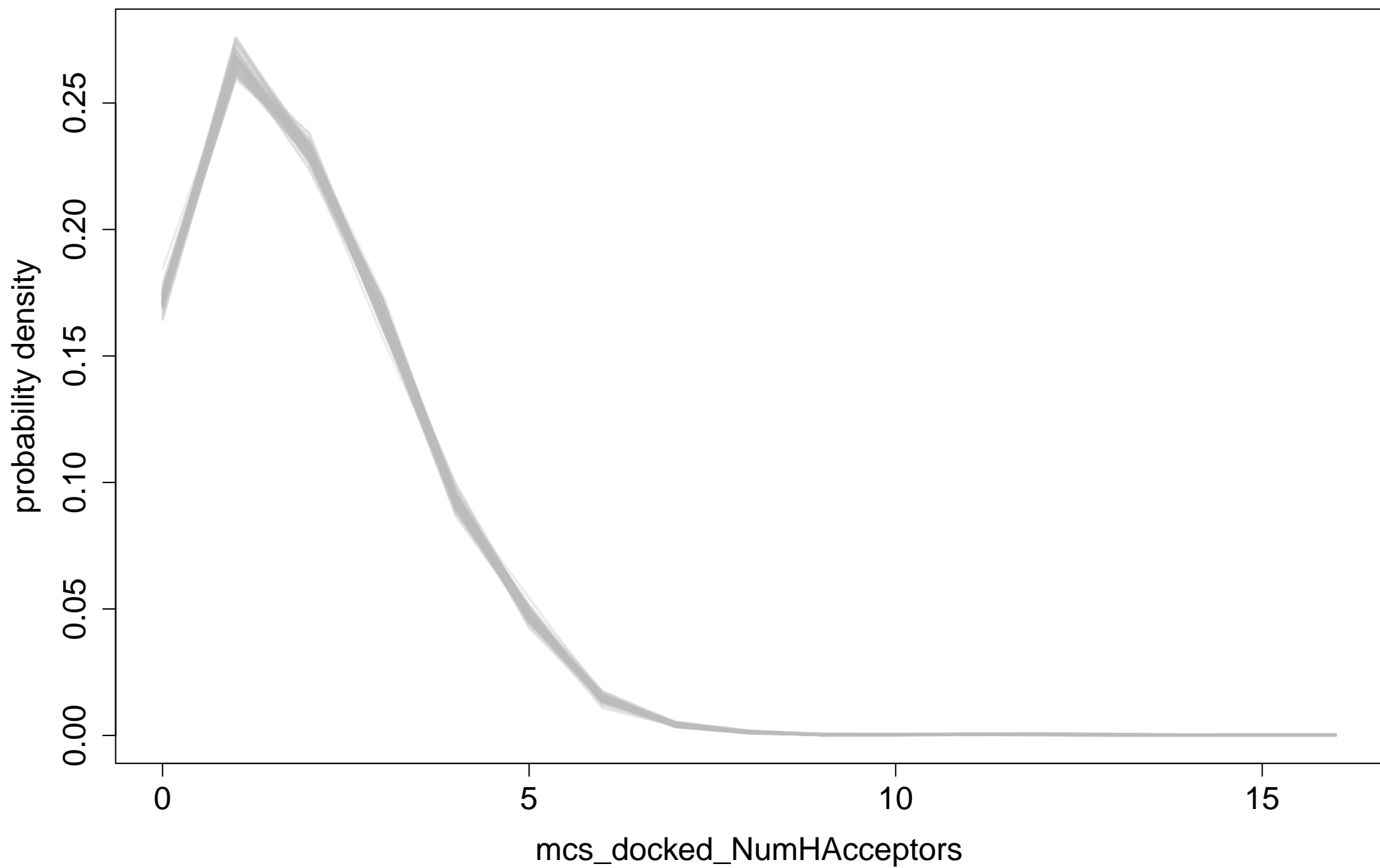


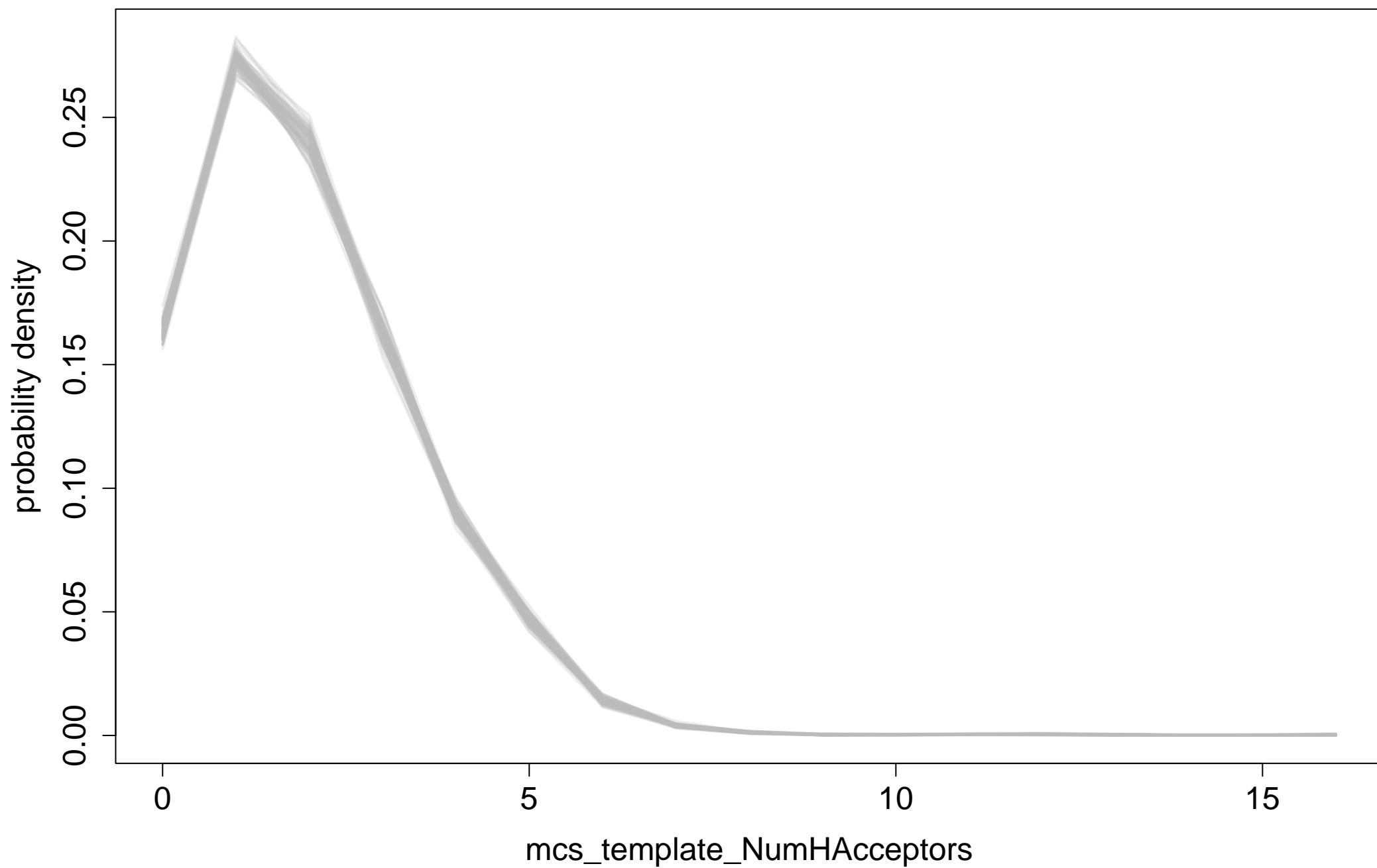




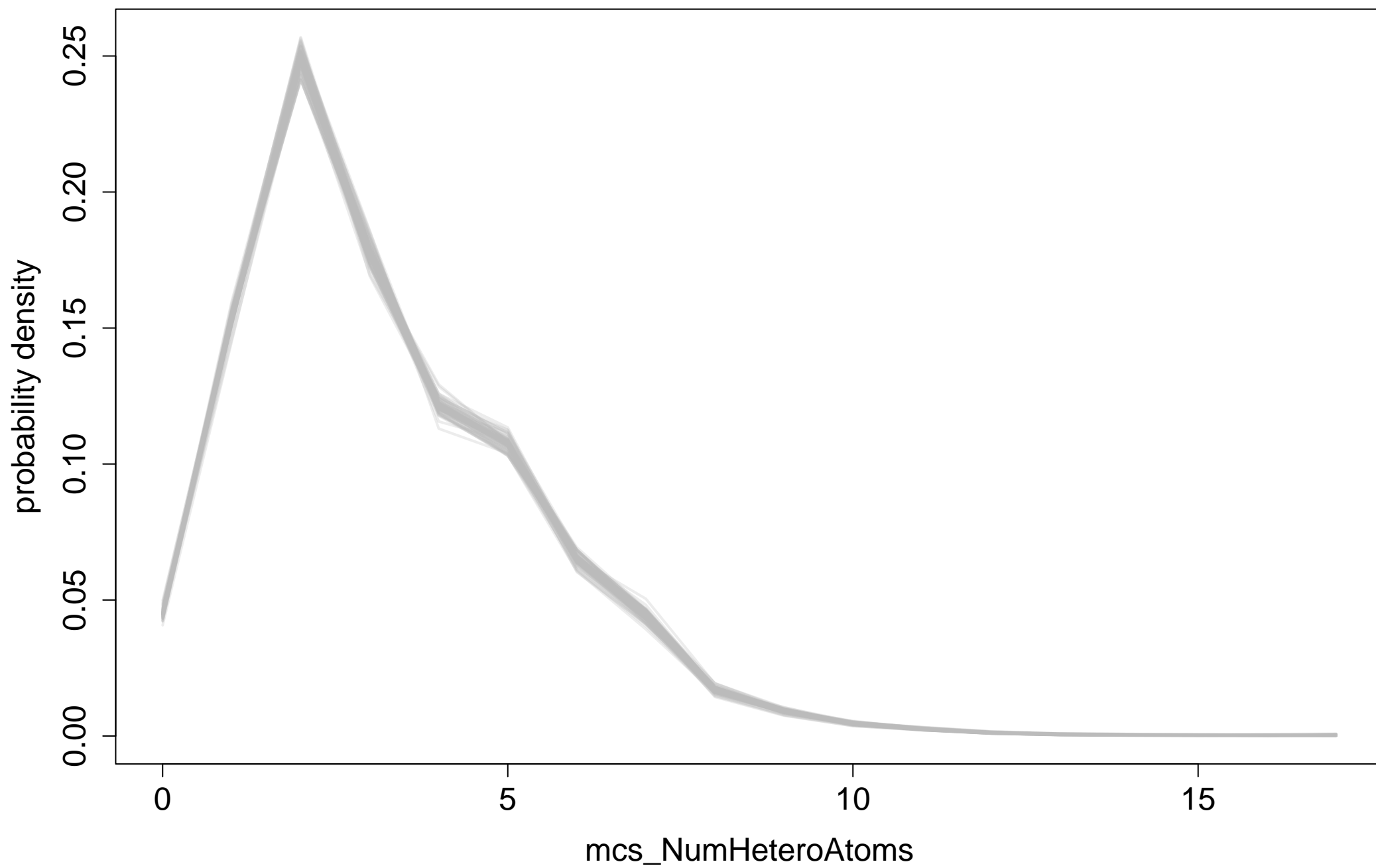


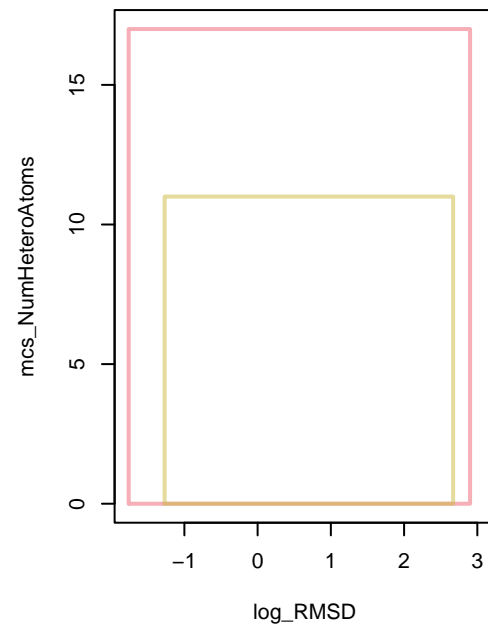
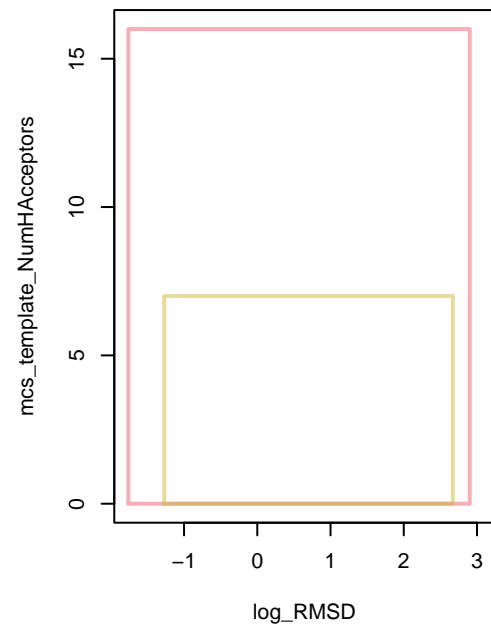
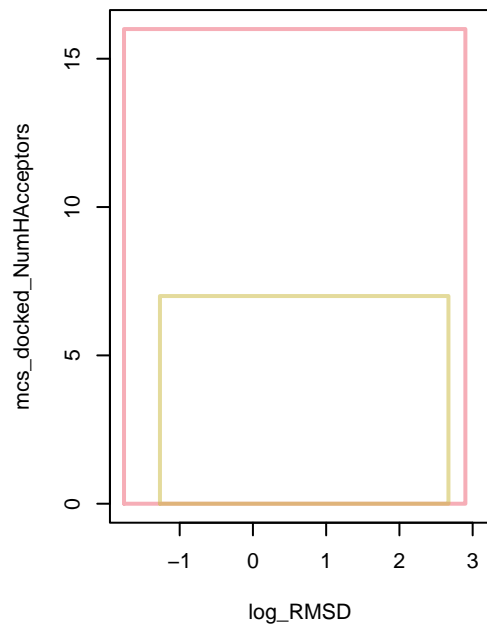
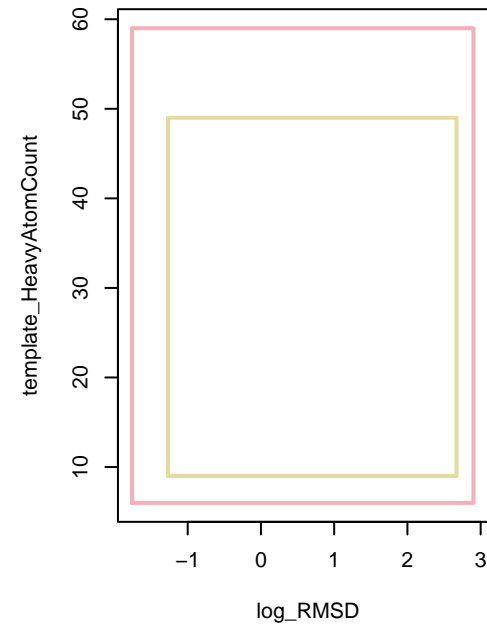
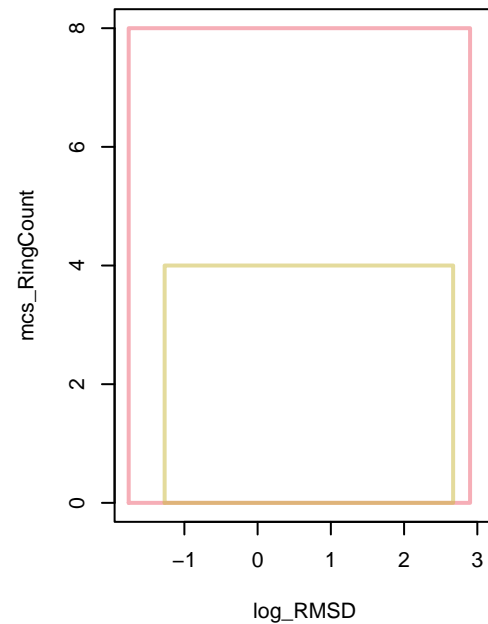
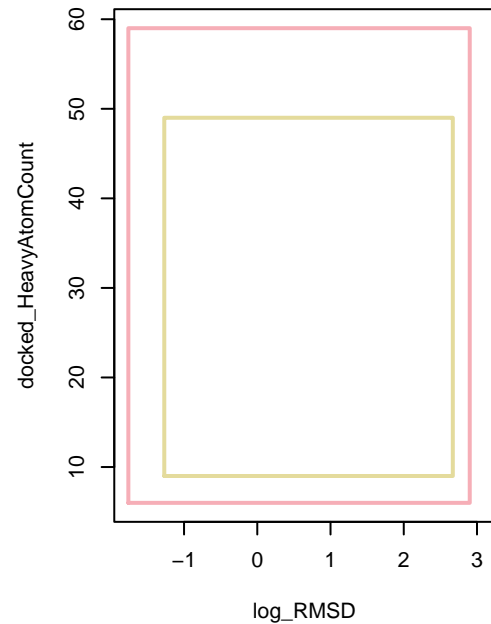
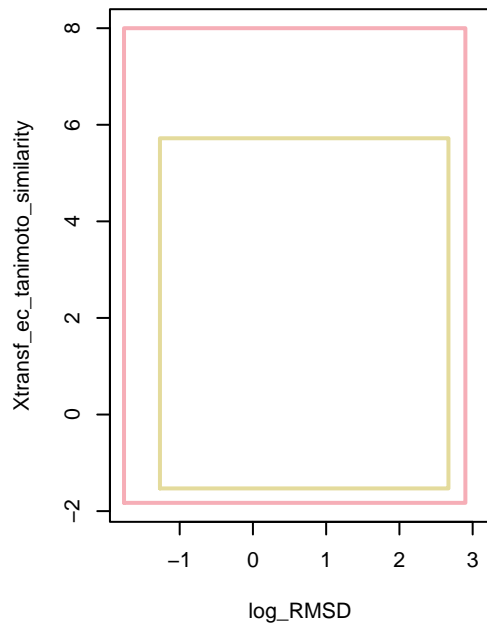




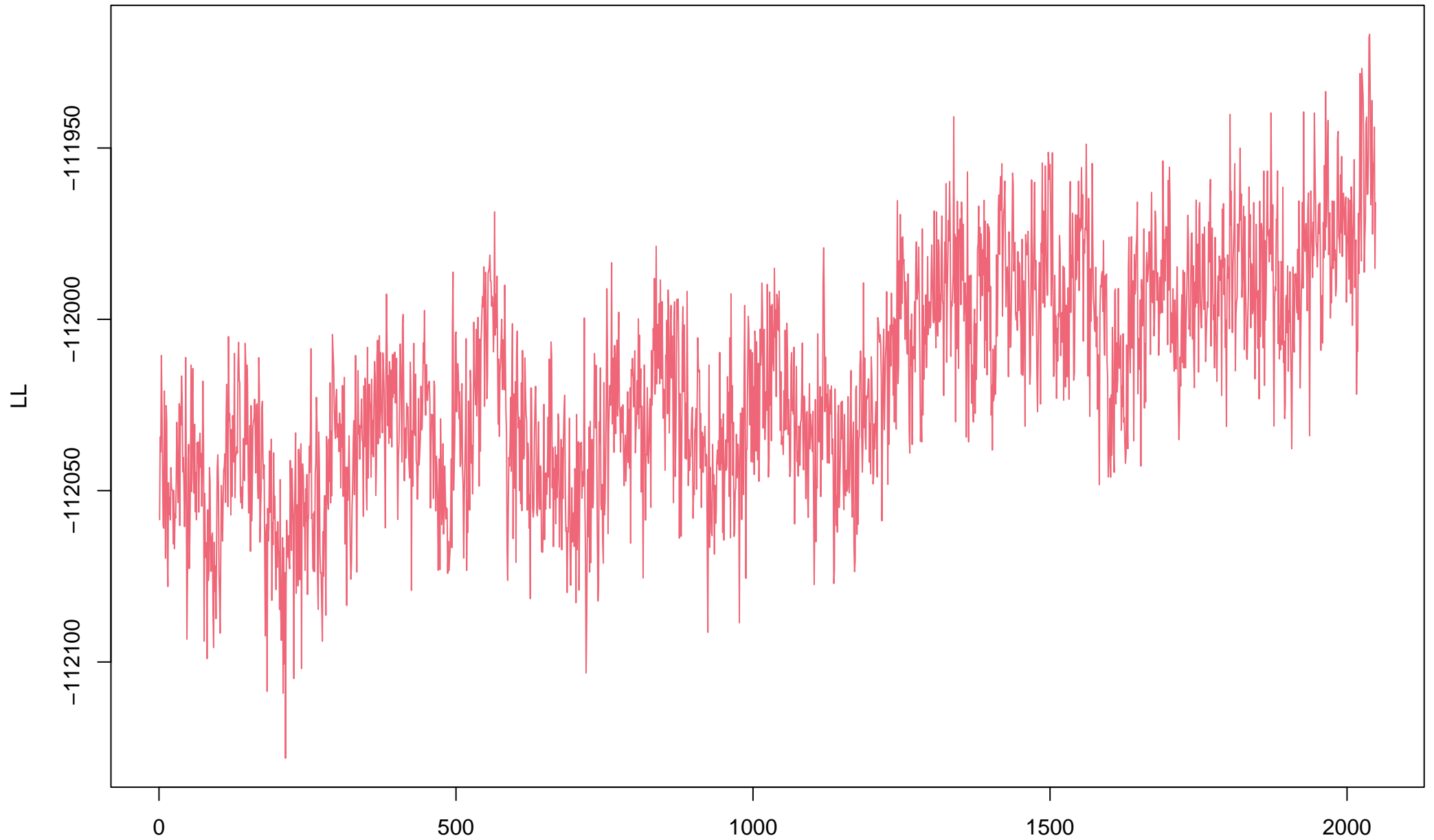




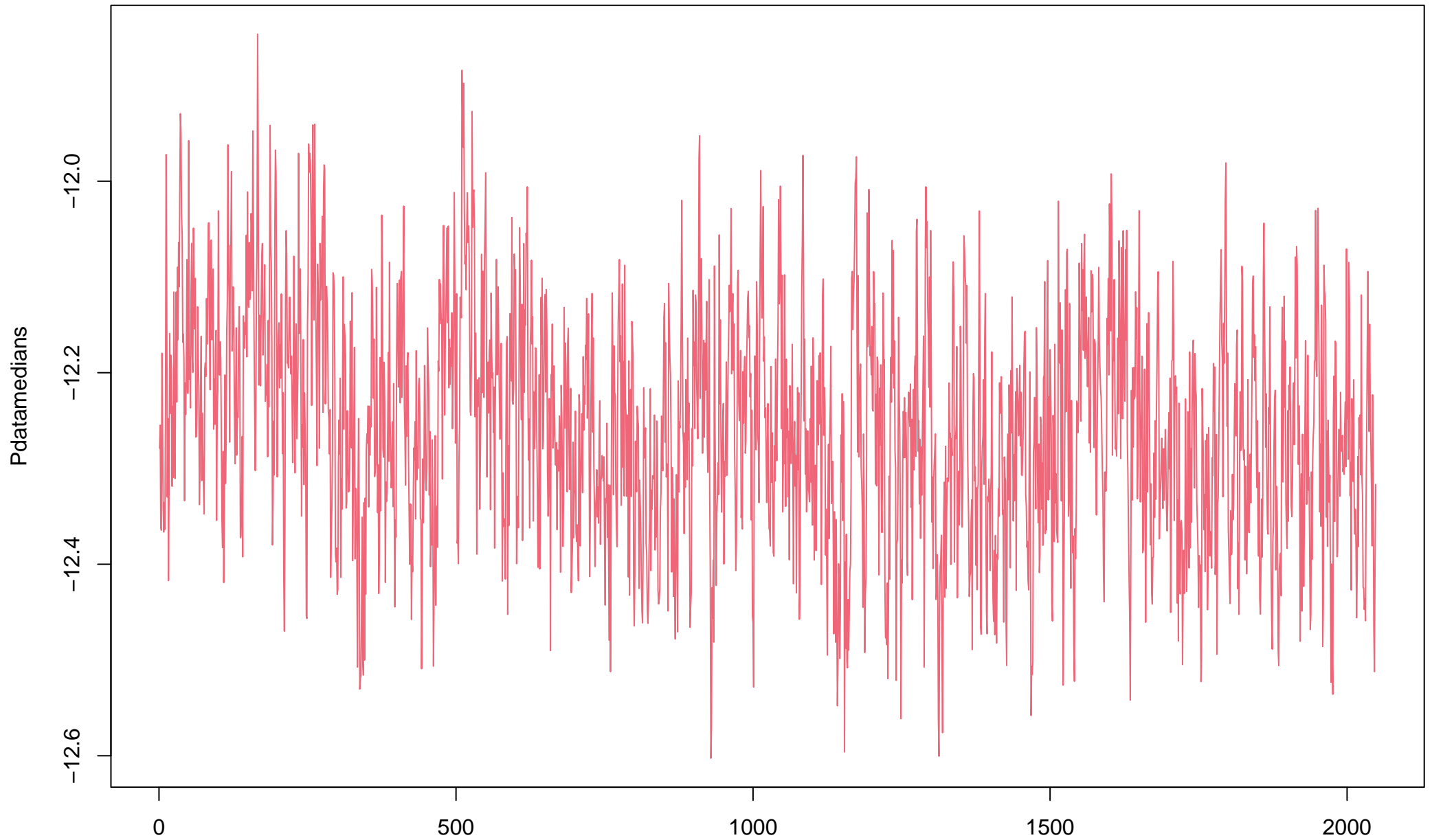




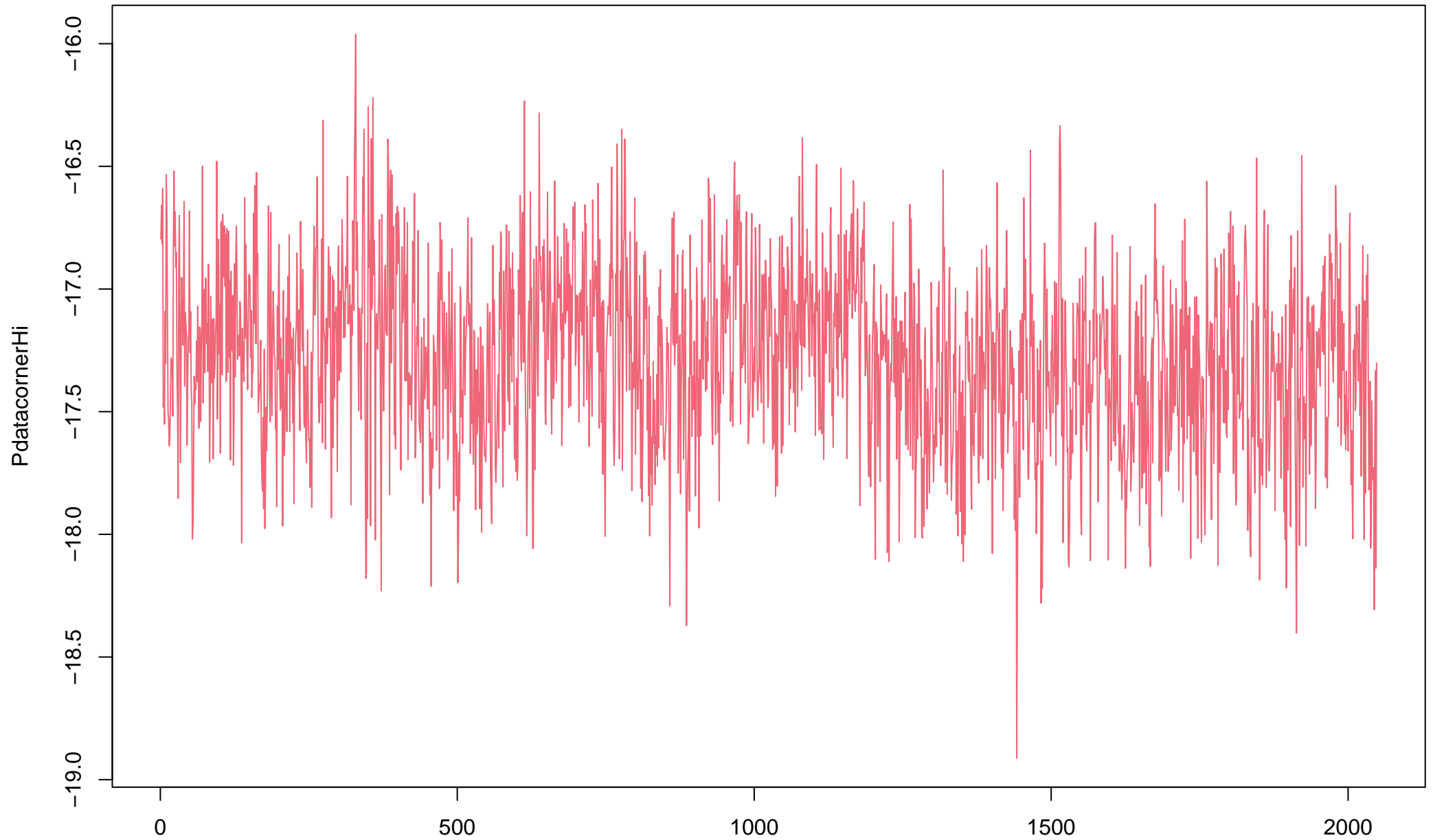
LL  
ESS = 17.2 | BMK = 0.526 | MCSE(6.27) = 11.8 | stat: FALSE | burn: 1224



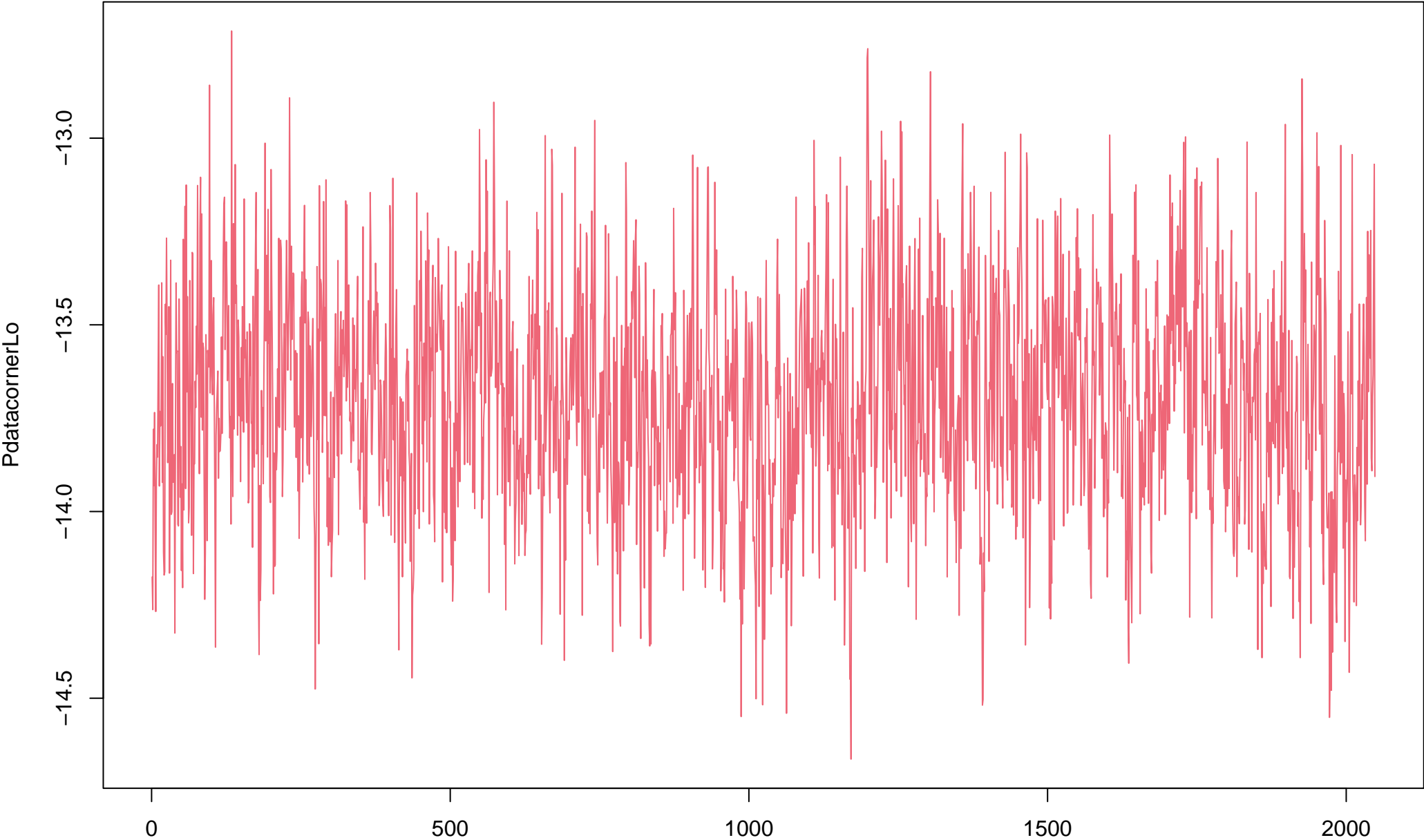
**Pdatamedians**  
**ESS = 322 | BMK = 0.15 | MCSE(6.27) = 6.45 | stat: FALSE | burn: 0**



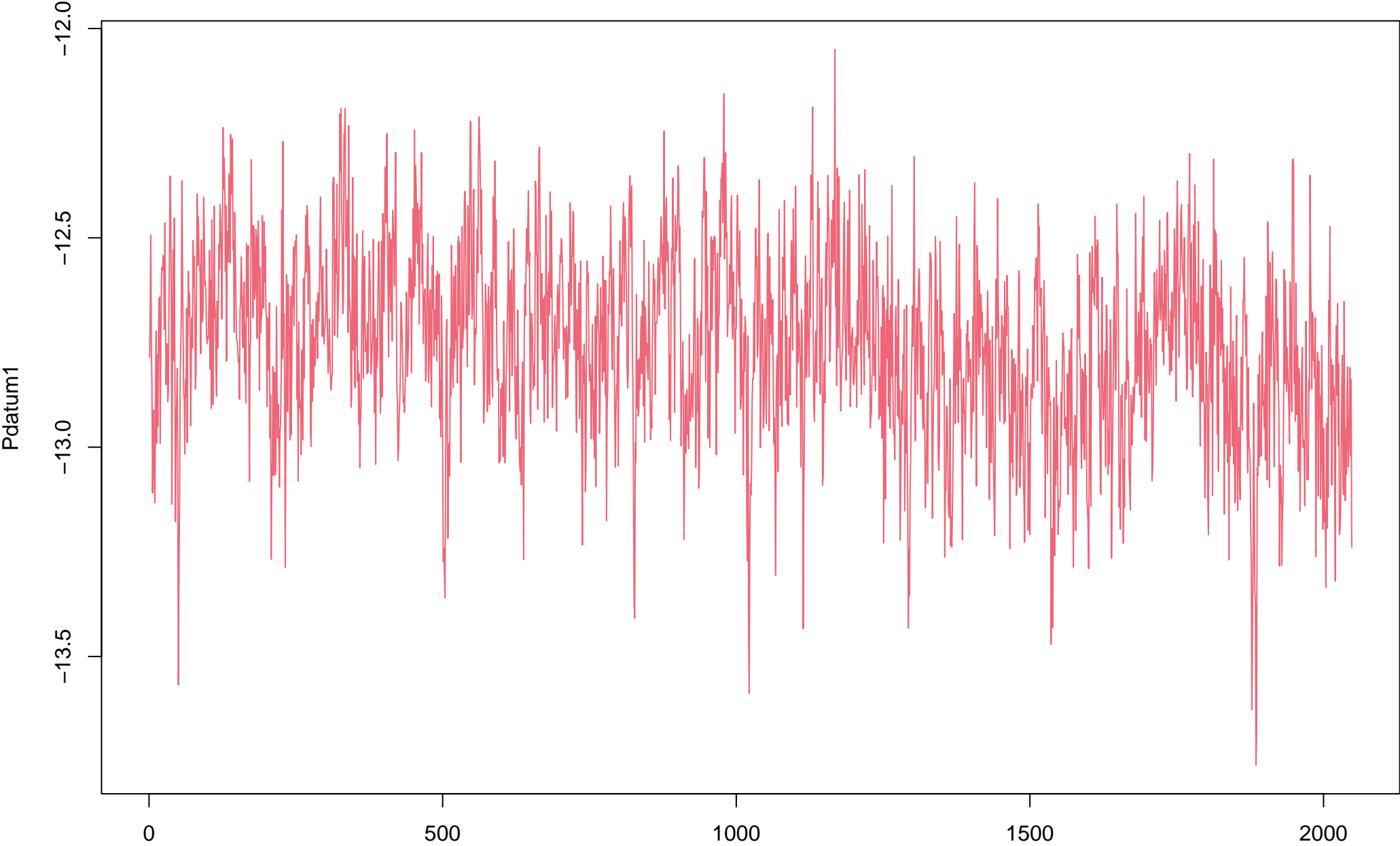
**PdatacornerHi**  
**ESS = 2.22e-16 | BMK = 0.129 | MCSE(6.27) = 5.33 | stat: FALSE | burn: 0**



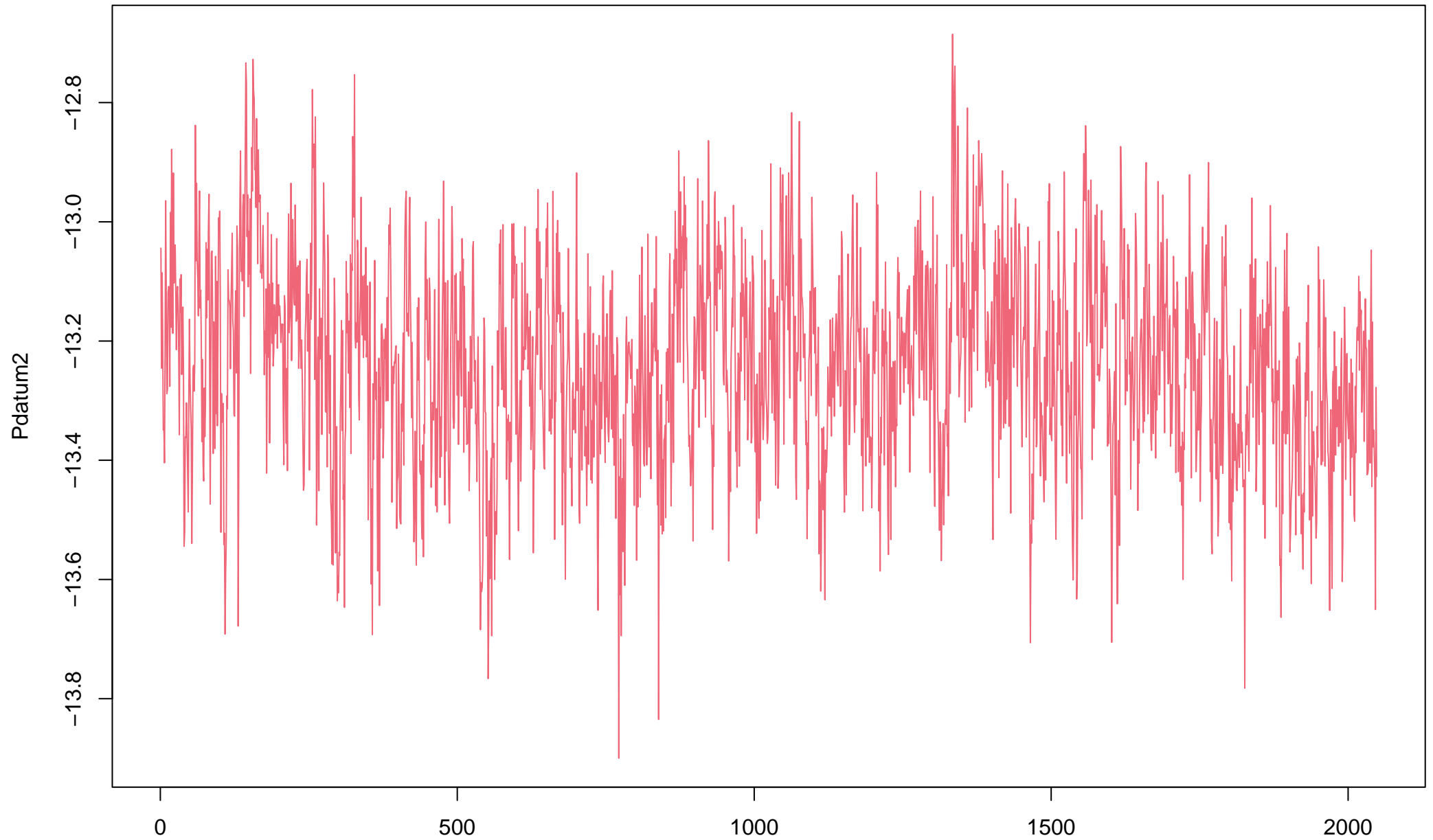
**PdatacornerLo**  
**ESS = 676 | BMK = 0.0521 | MCSE(6.27) = 4.22 | stat: TRUE | burn: 0**



**Pdatum1**  
**ESS = 247 | BMK = 0.198 | MCSE(6.27) = 6.83 | stat: FALSE | burn: 0**

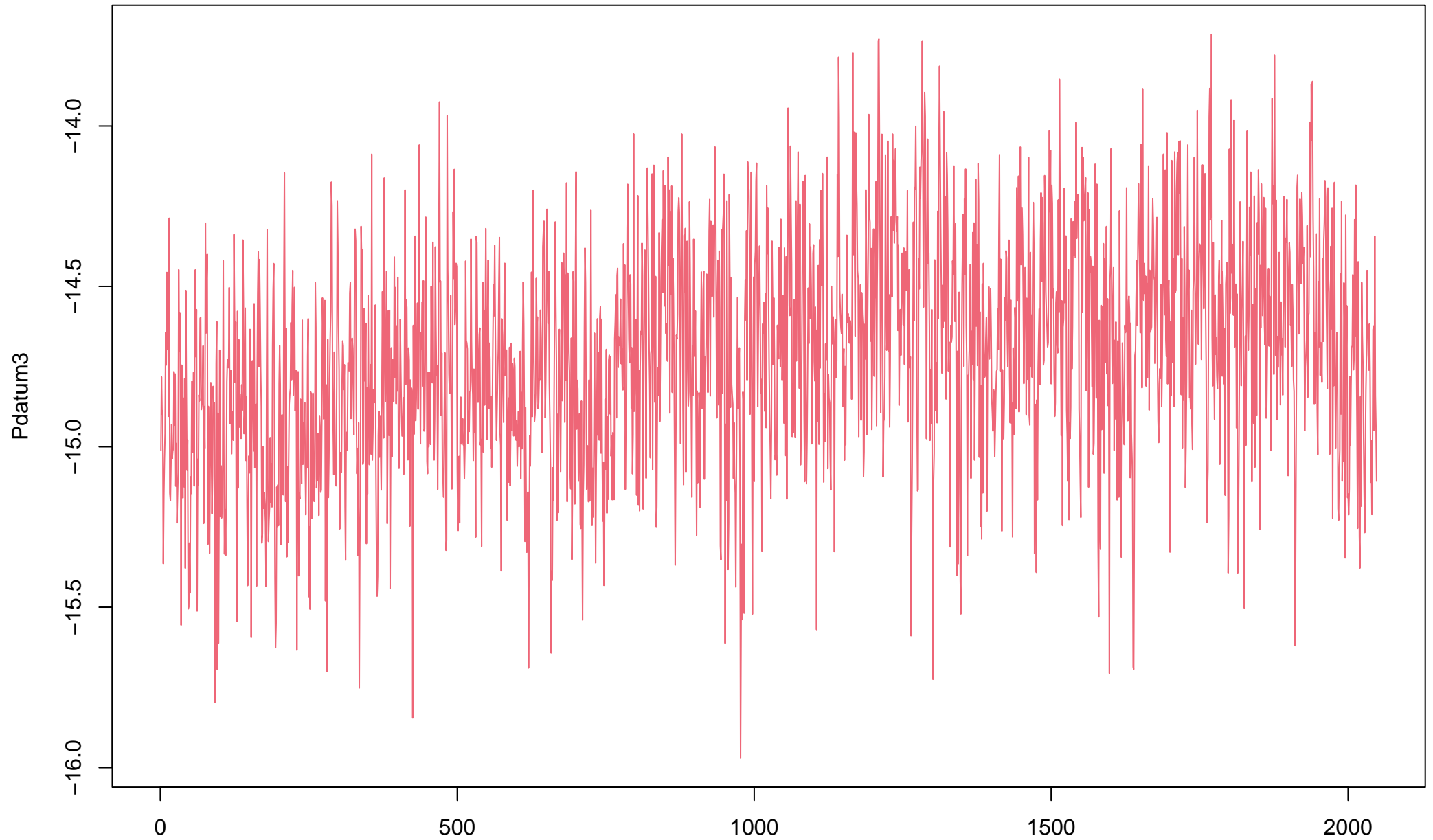


**Pdatum2**  
**ESS = 307 | BMK = 0.052 | MCSE(6.27) = 6.4 | stat: FALSE | burn: 0**

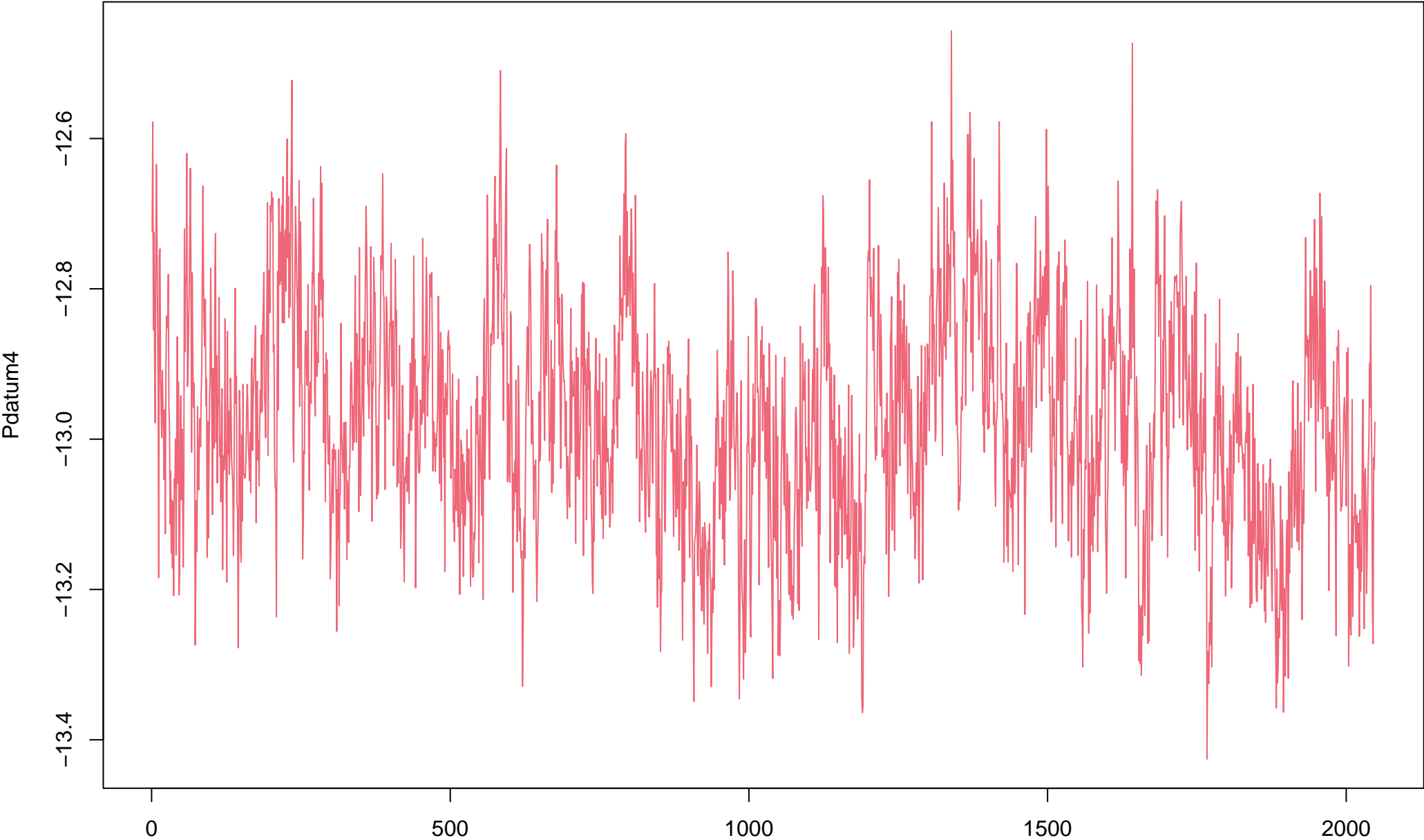




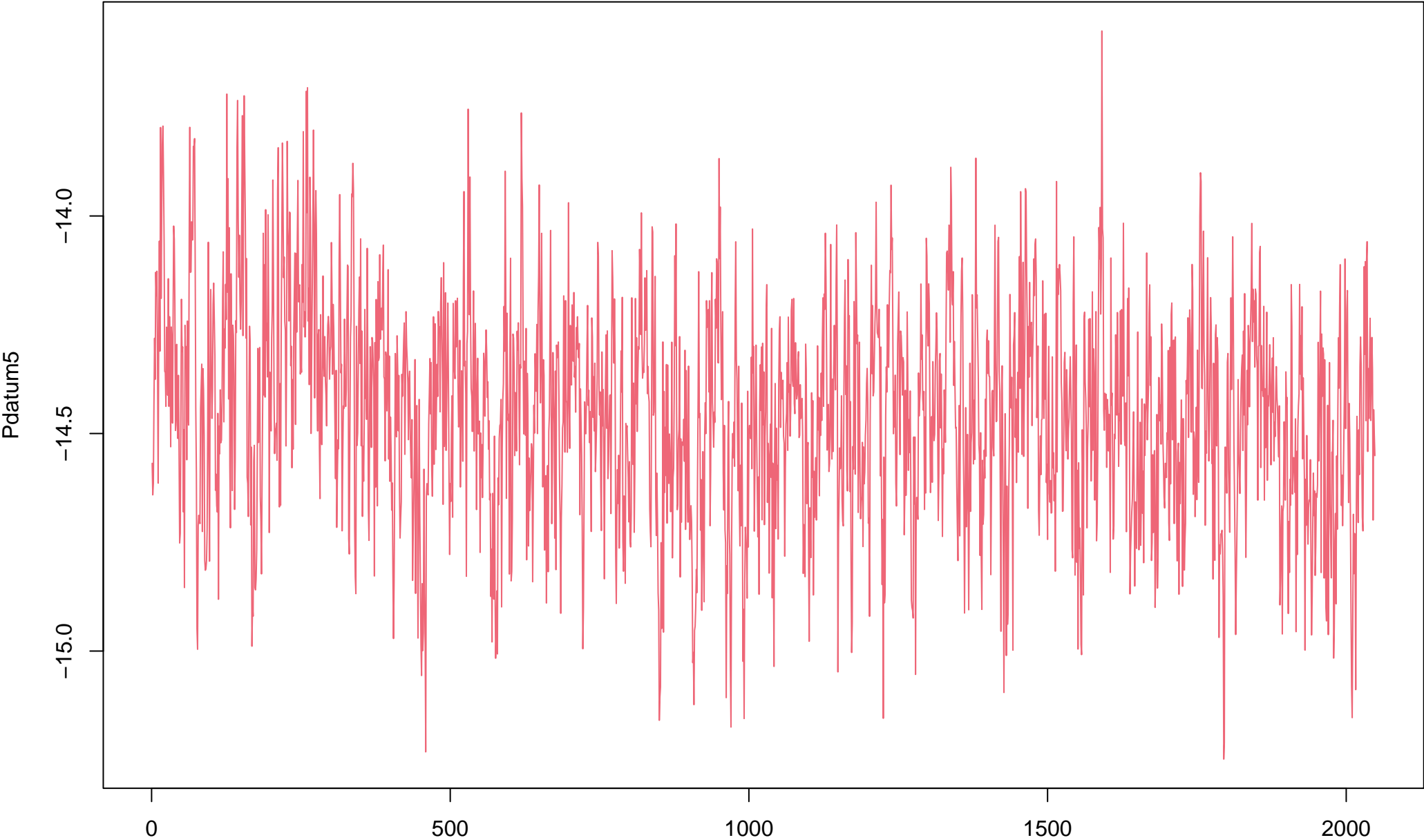
**Pdatum3**  
**ESS = 94.8 | BMK = 0.227 | MCSE(6.27) = 6.37 | stat: FALSE | burn: 0**



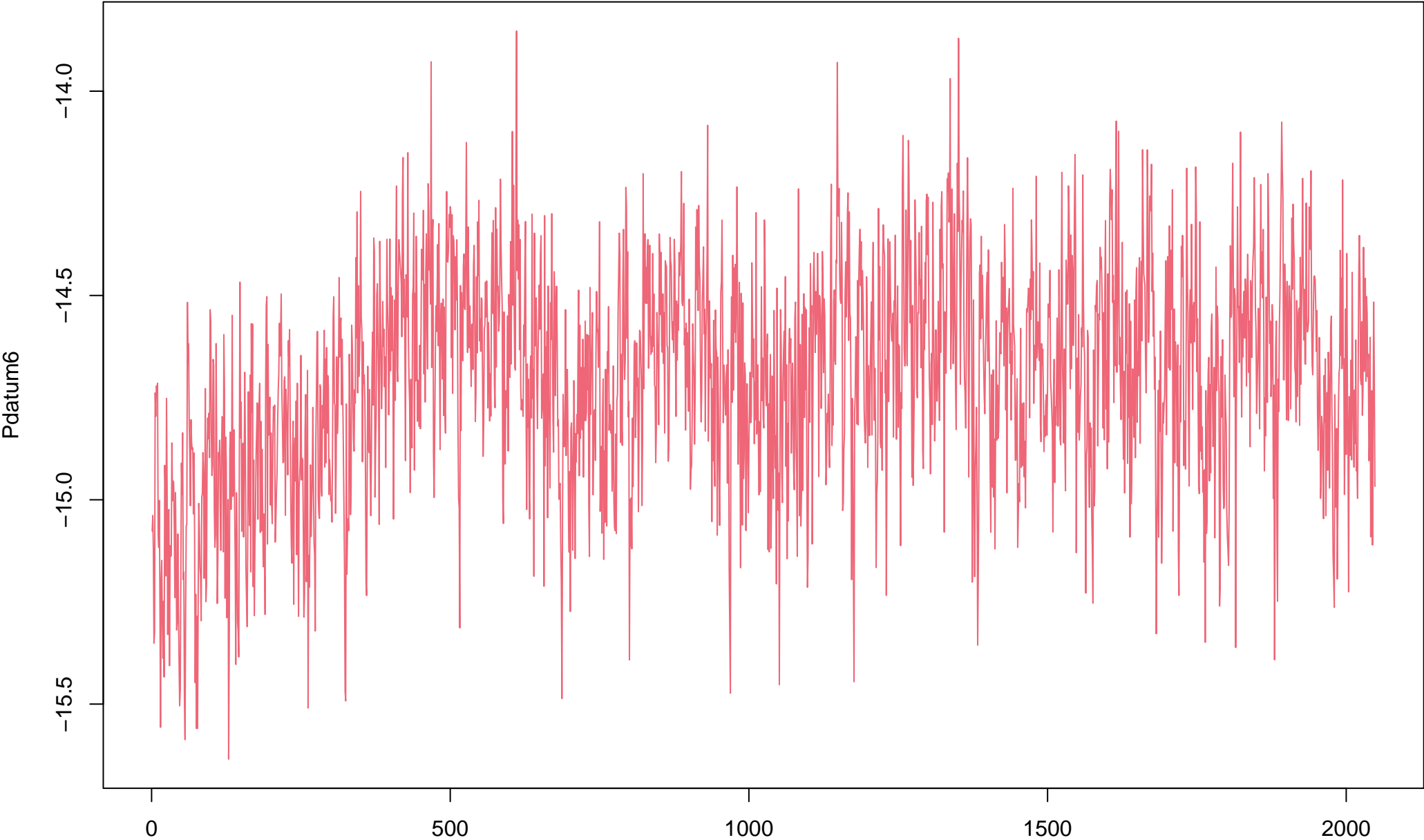
**Pdatum4**  
**ESS = 127 | BMK = 0.0884 | MCSE(6.27) = 7.97 | stat: TRUE | burn: 0**



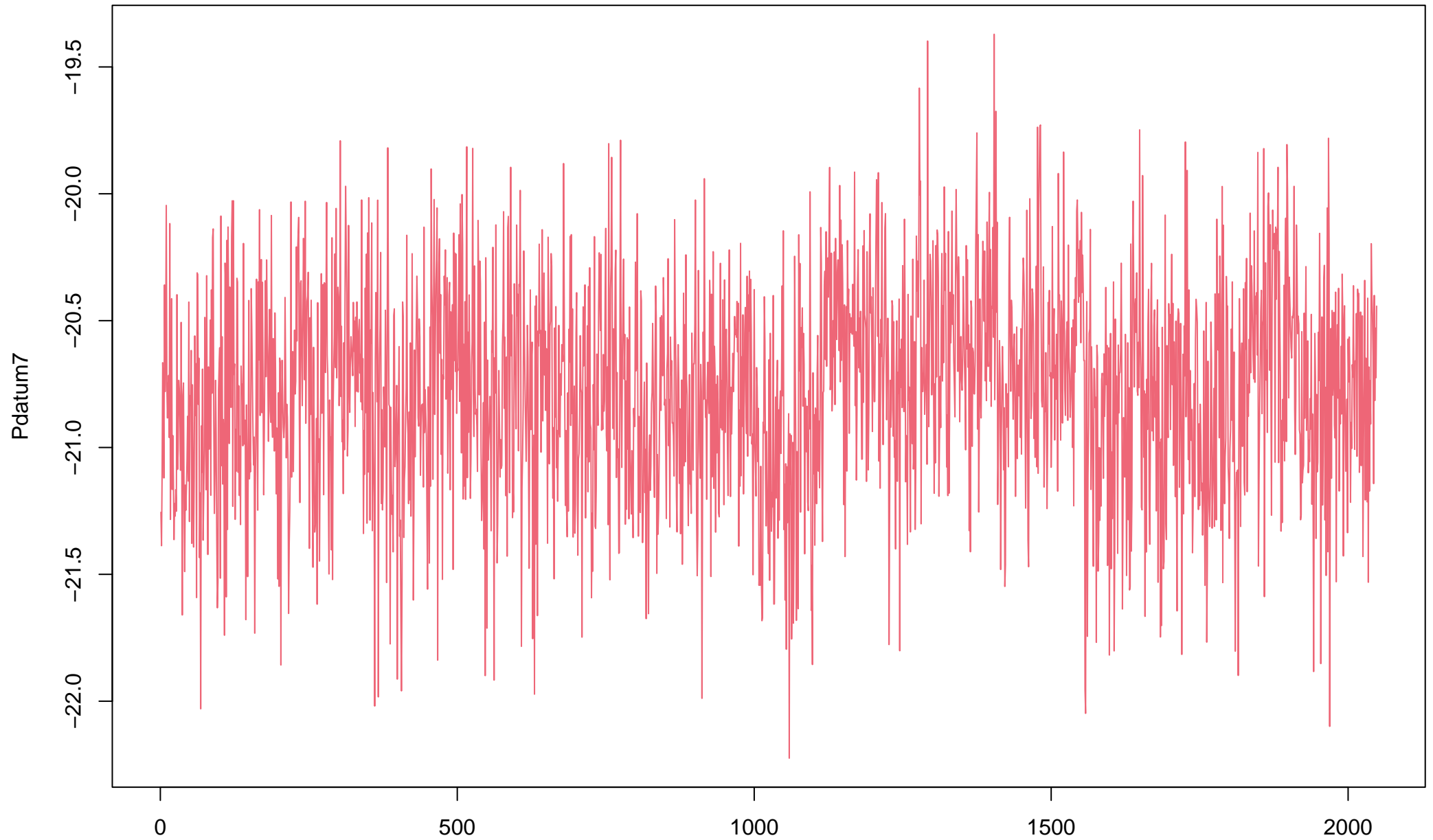
**Pdatum5**  
**ESS = 316 | BMK = 0.118 | MCSE(6.27) = 5.67 | stat: FALSE | burn: 0**



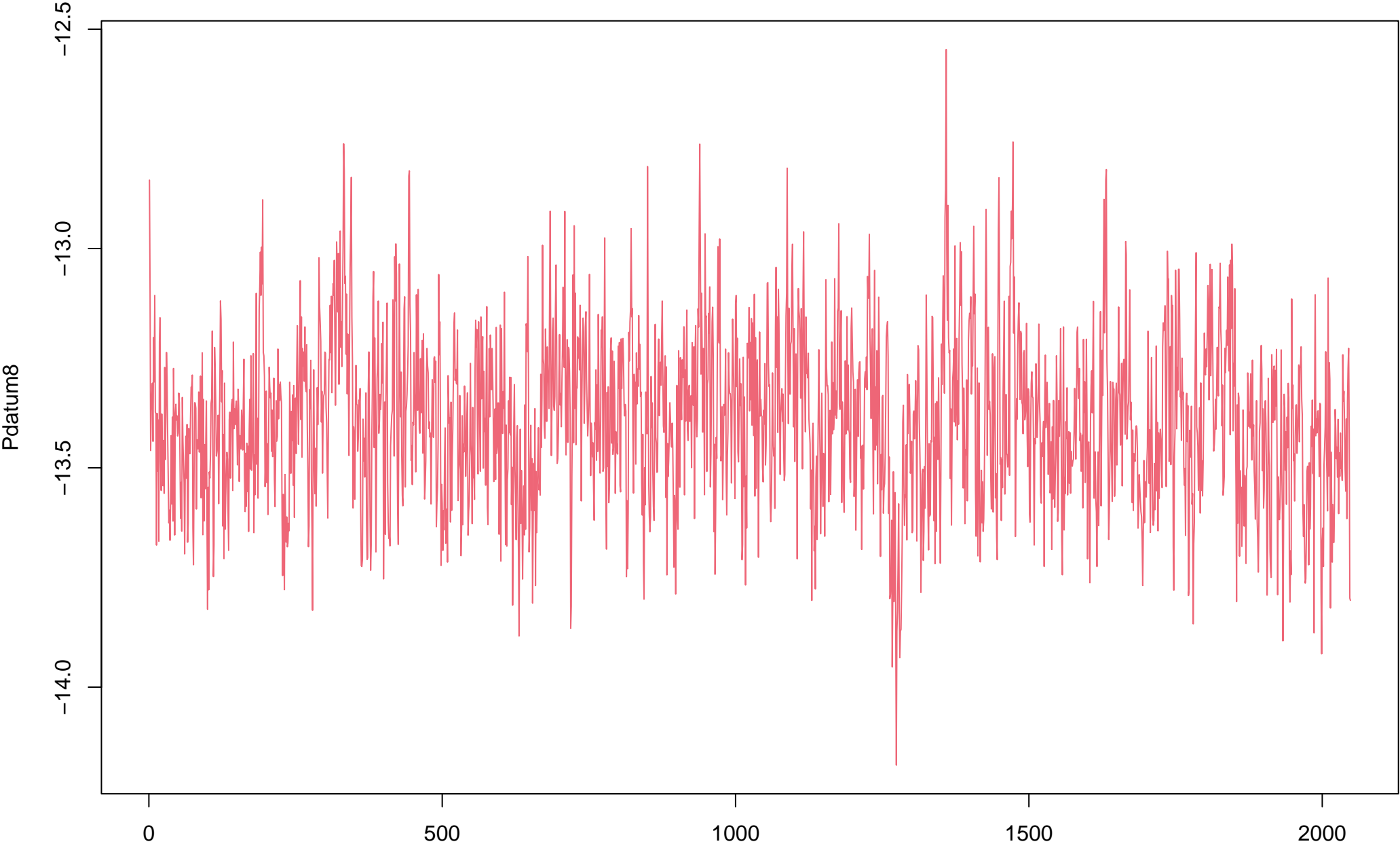
**Pdatum6**  
**ESS = 126 | BMK = 0.136 | MCSE(6.27) = 7.79 | stat: FALSE | burn: 0**



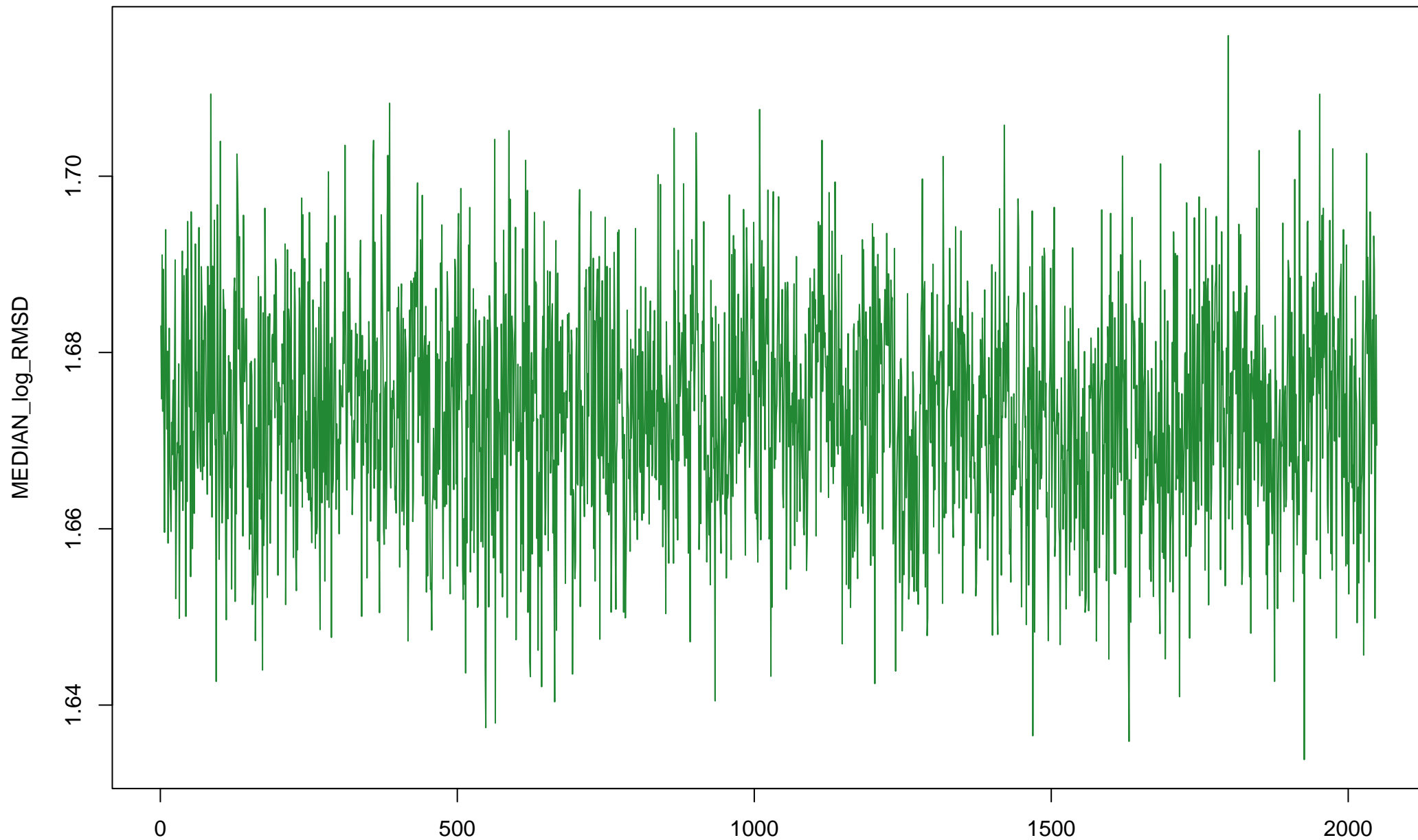
**Pdatum7**  
**ESS = 2.22e-16 | BMK = 0.088 | MCSE(6.27) = 4.61 | stat: TRUE | burn: 0**



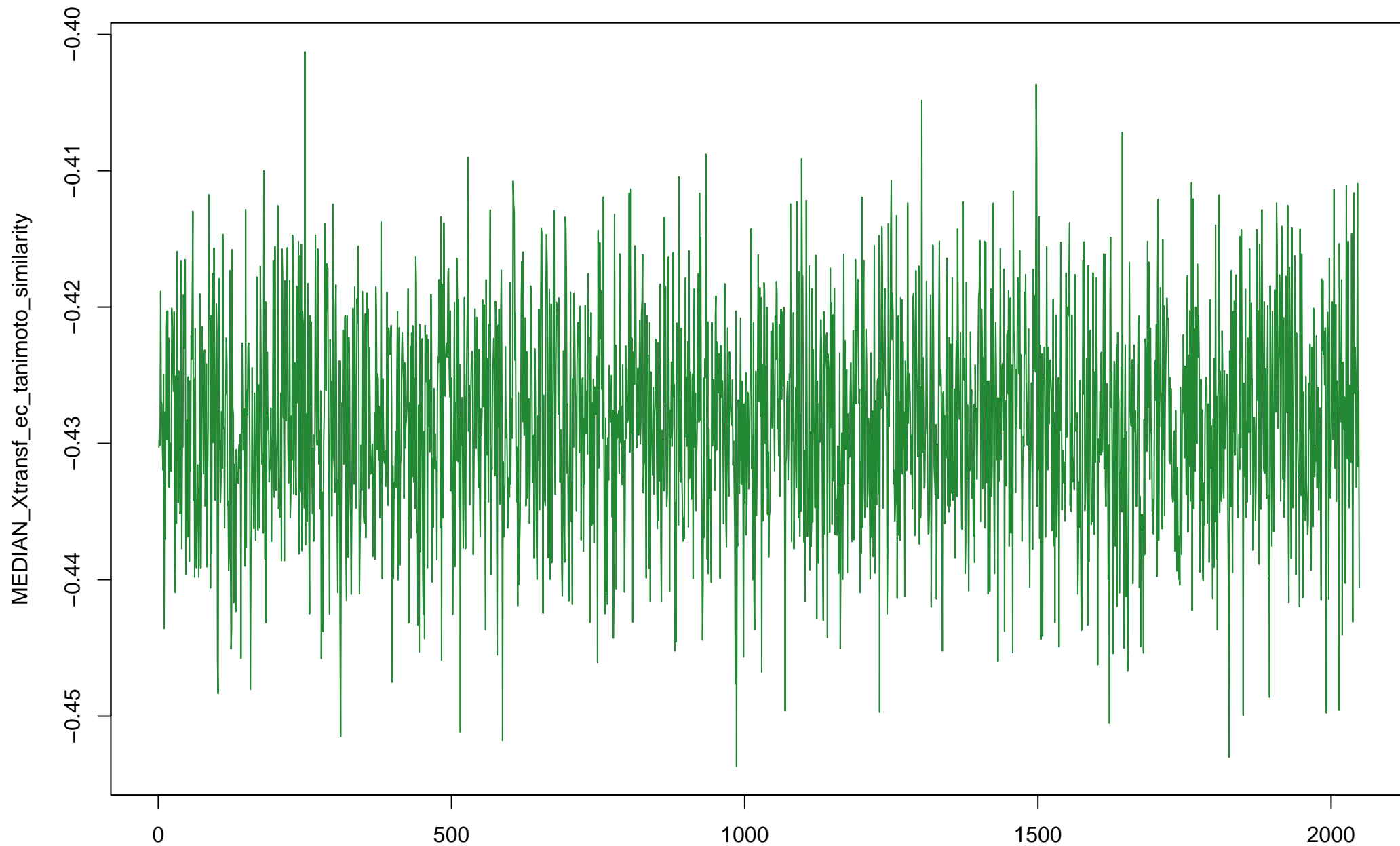
**Pdatum8**  
**ESS = 328 | BMK = 0.0653 | MCSE(6.27) = 6.24 | stat: TRUE | burn: 0**



**MEDIAN\_log\_RMSD**  
**ESS = 1220 | BMK = 0.0419 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0**

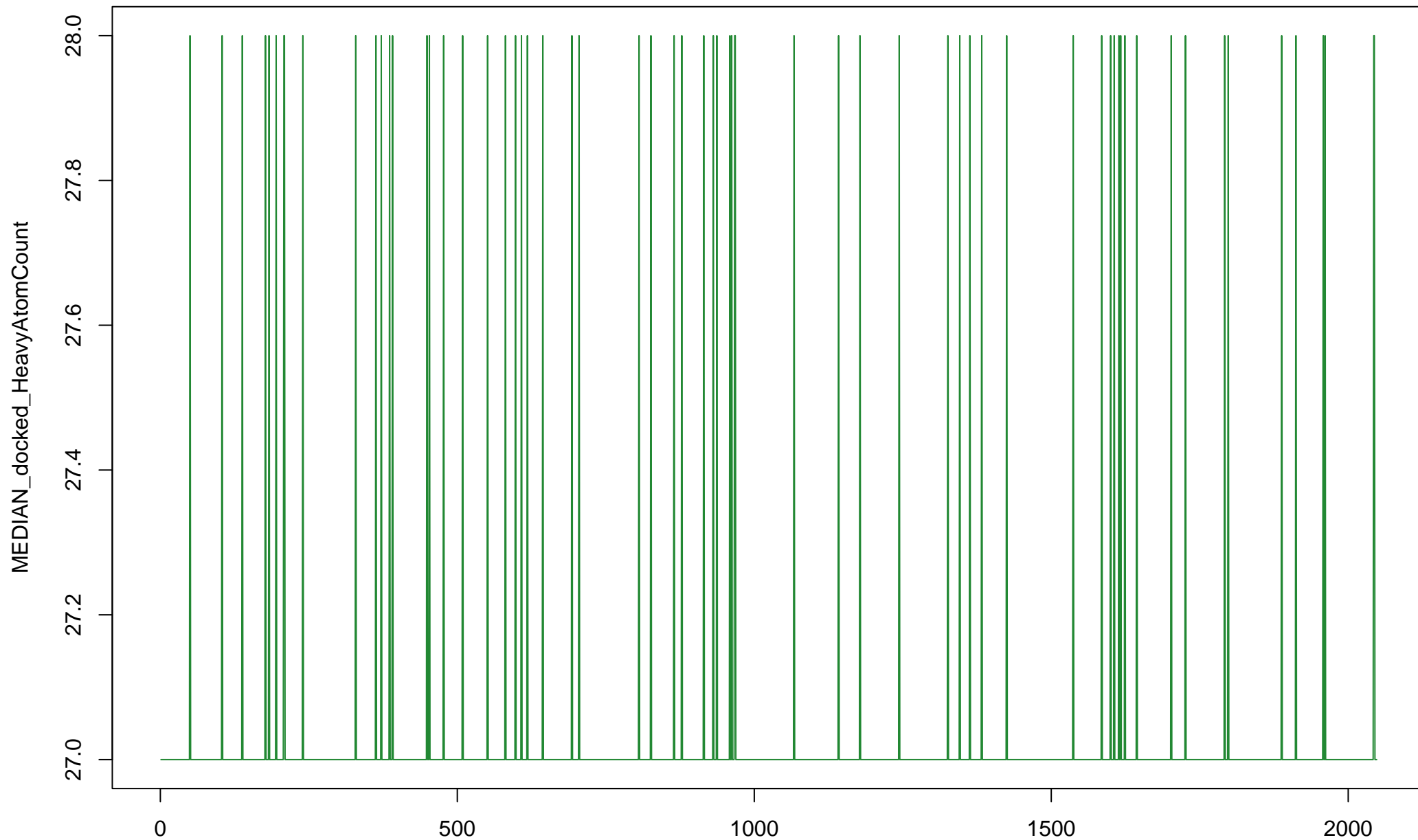


**MEDIAN\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0344 | MCSE(6.27) = 1.86 | stat: TRUE | burn: 0**

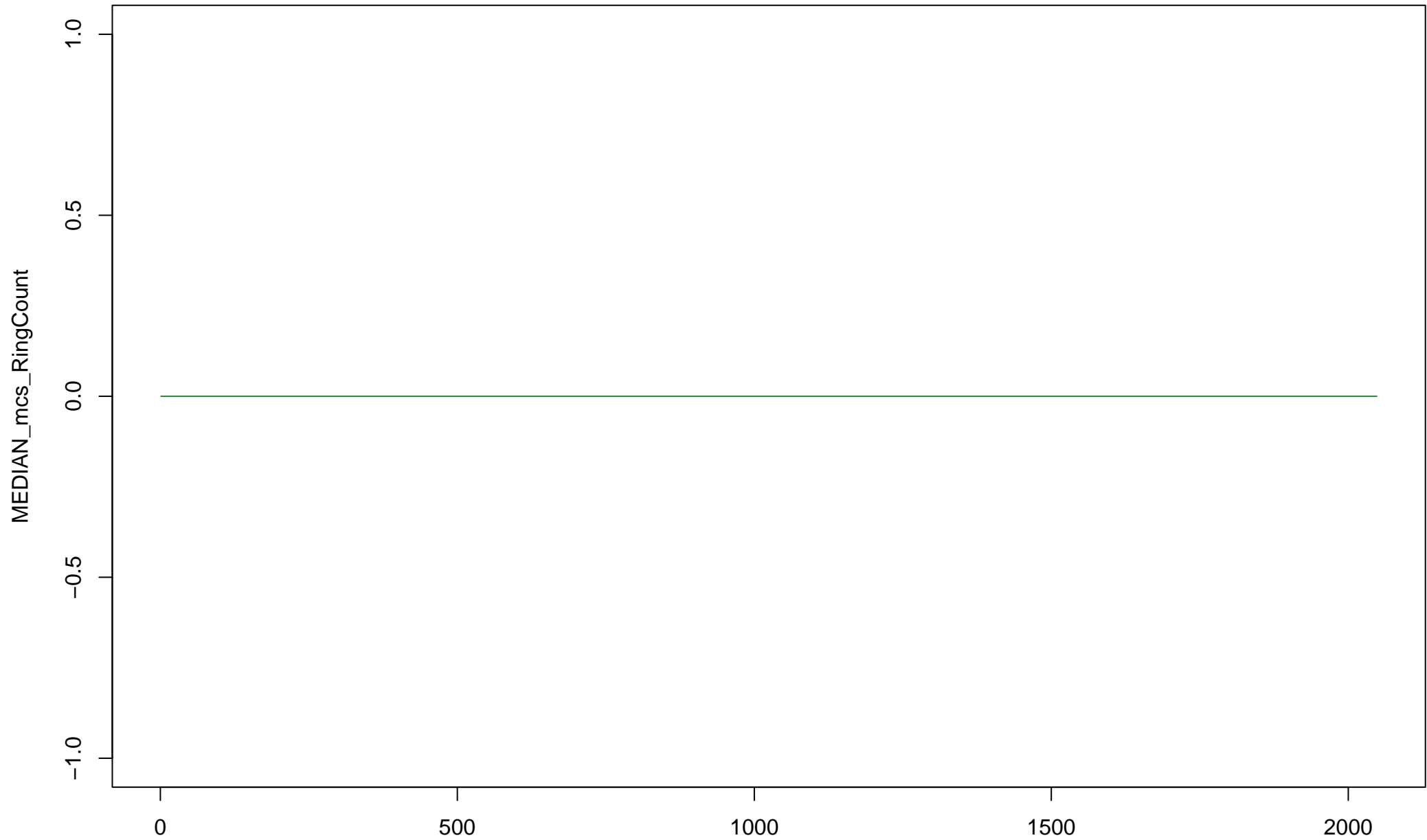




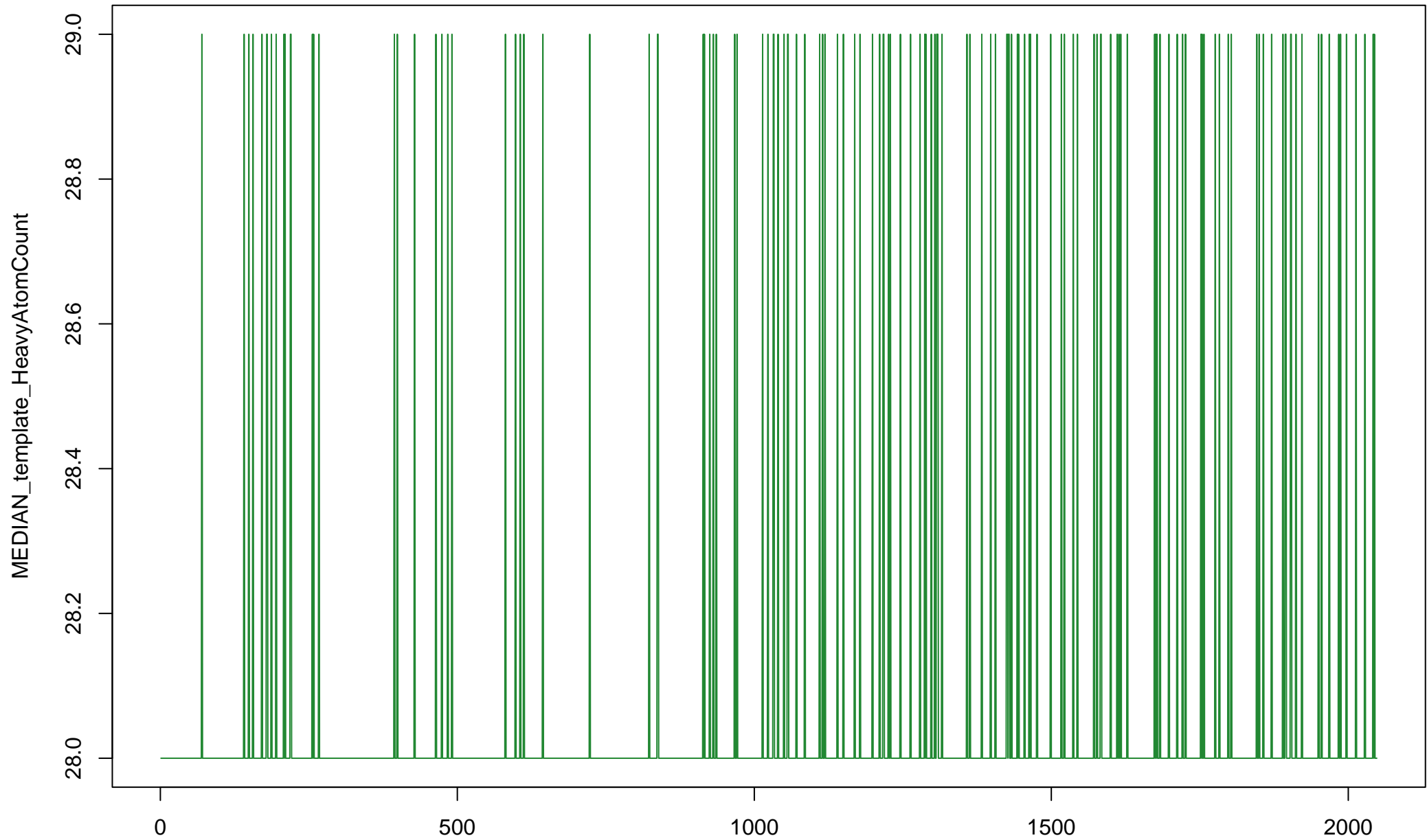
**MEDIAN\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0557 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0**



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



**MEDIAN\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.151 | MCSE(6.27) = 2.85 | stat: FALSE | burn: 0**



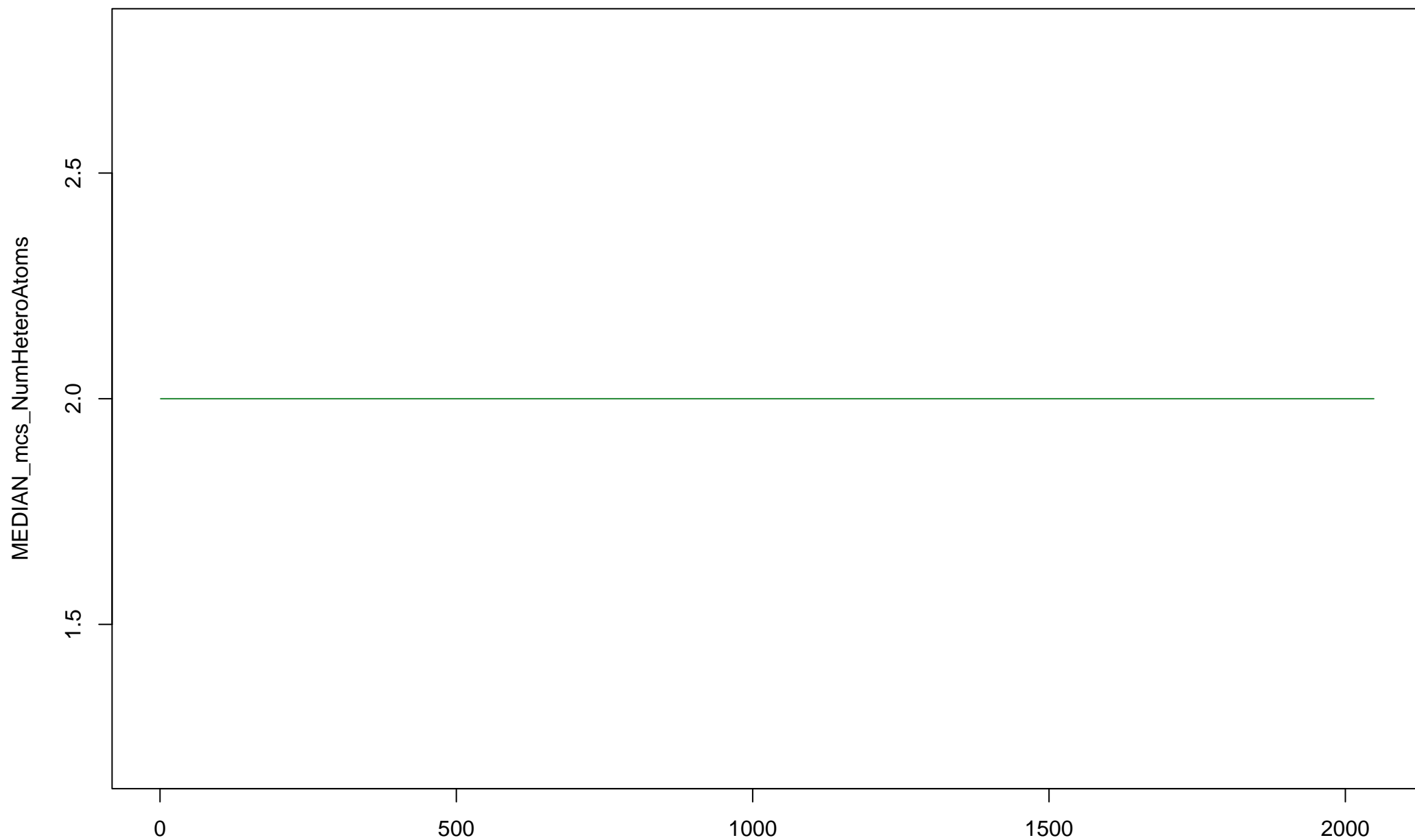
**MEDIAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



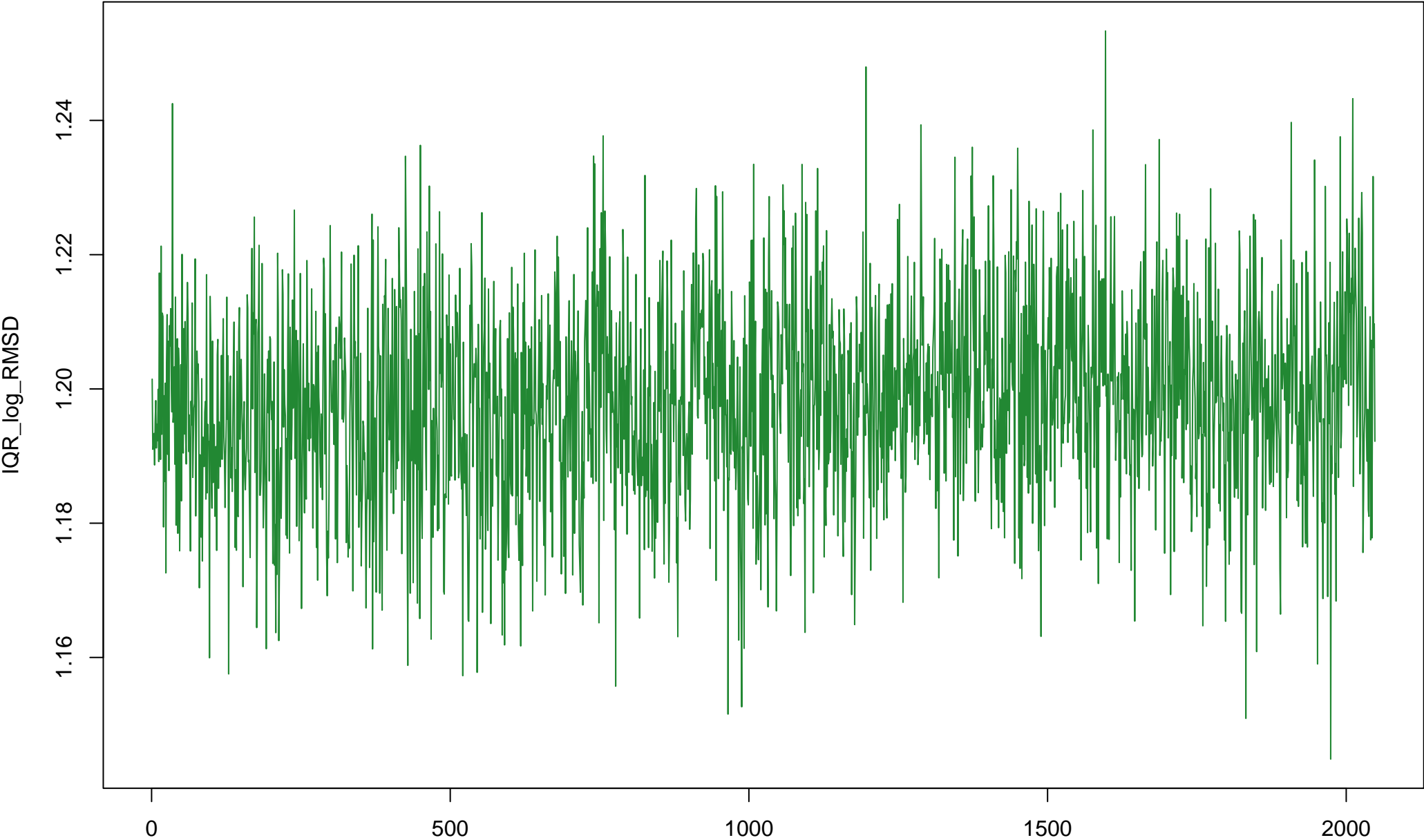
**MEDIAN\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



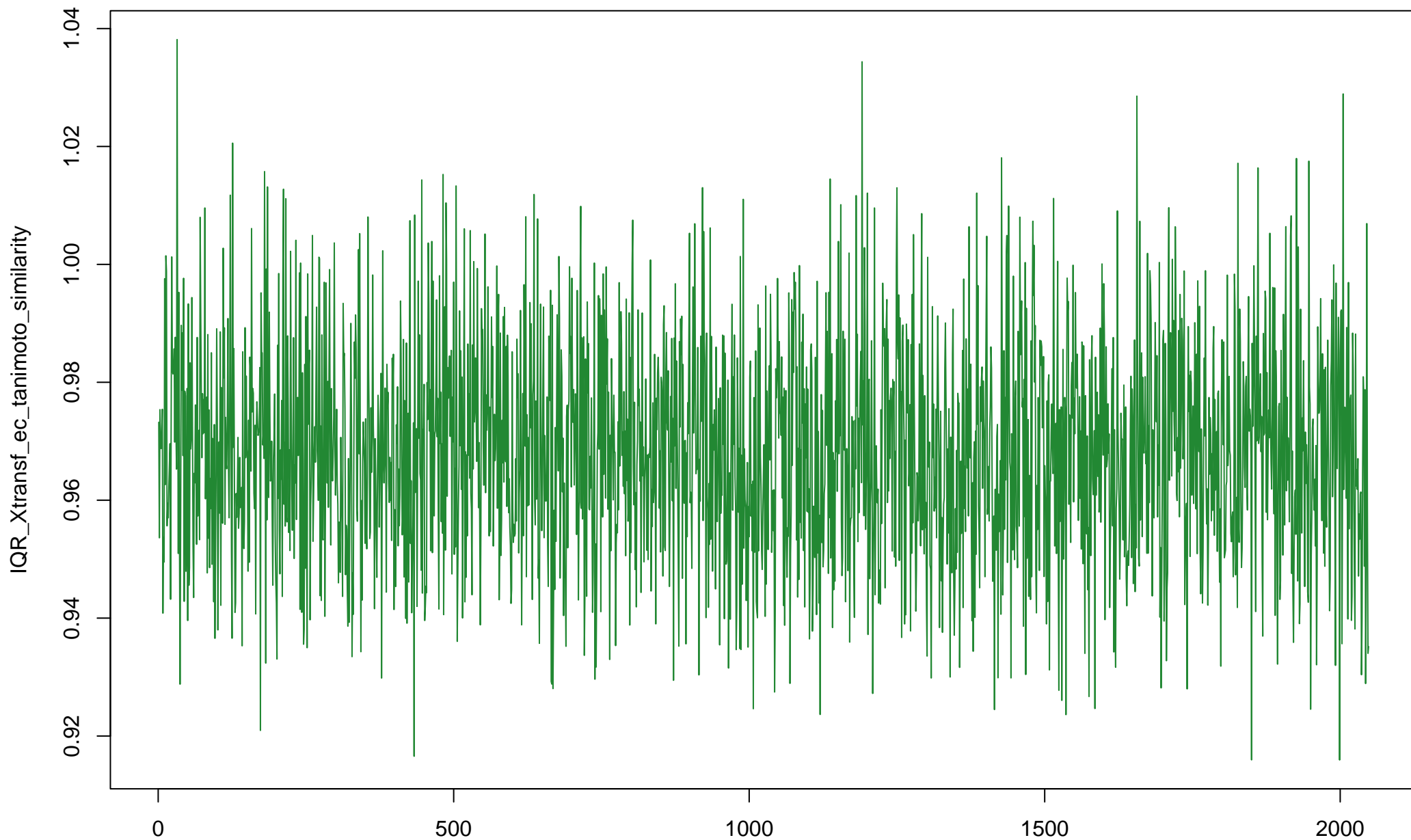
**MEDIAN\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



IQR\_log\_RMSD  
ESS = 813 | BMK = 0.118 | MCSE(6.27) = 3.74 | stat: FALSE | burn: 0

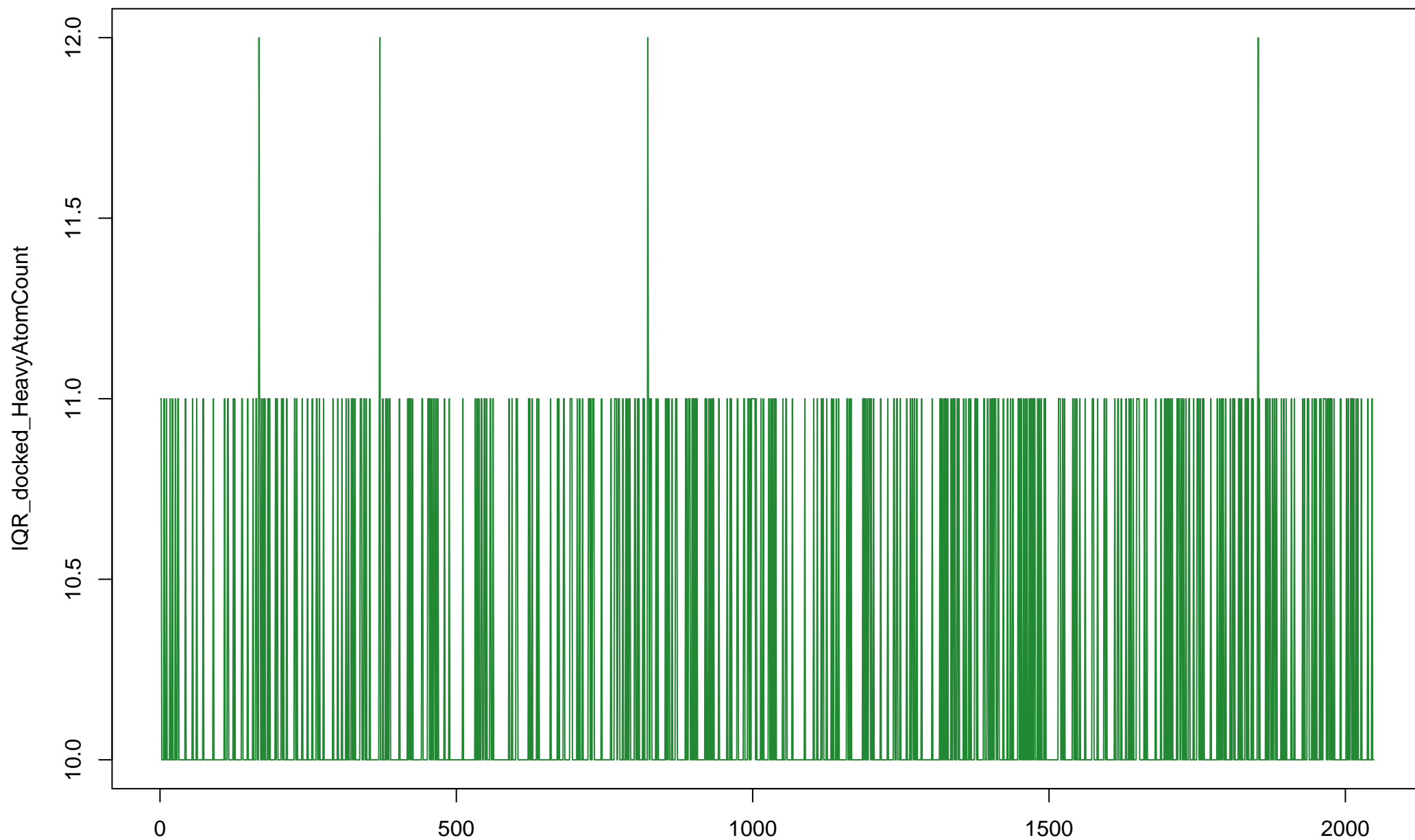


IQR\_Xtransf\_ec\_tanimoto\_similarity  
ESS = 2050 | BMK = 0.0497 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0

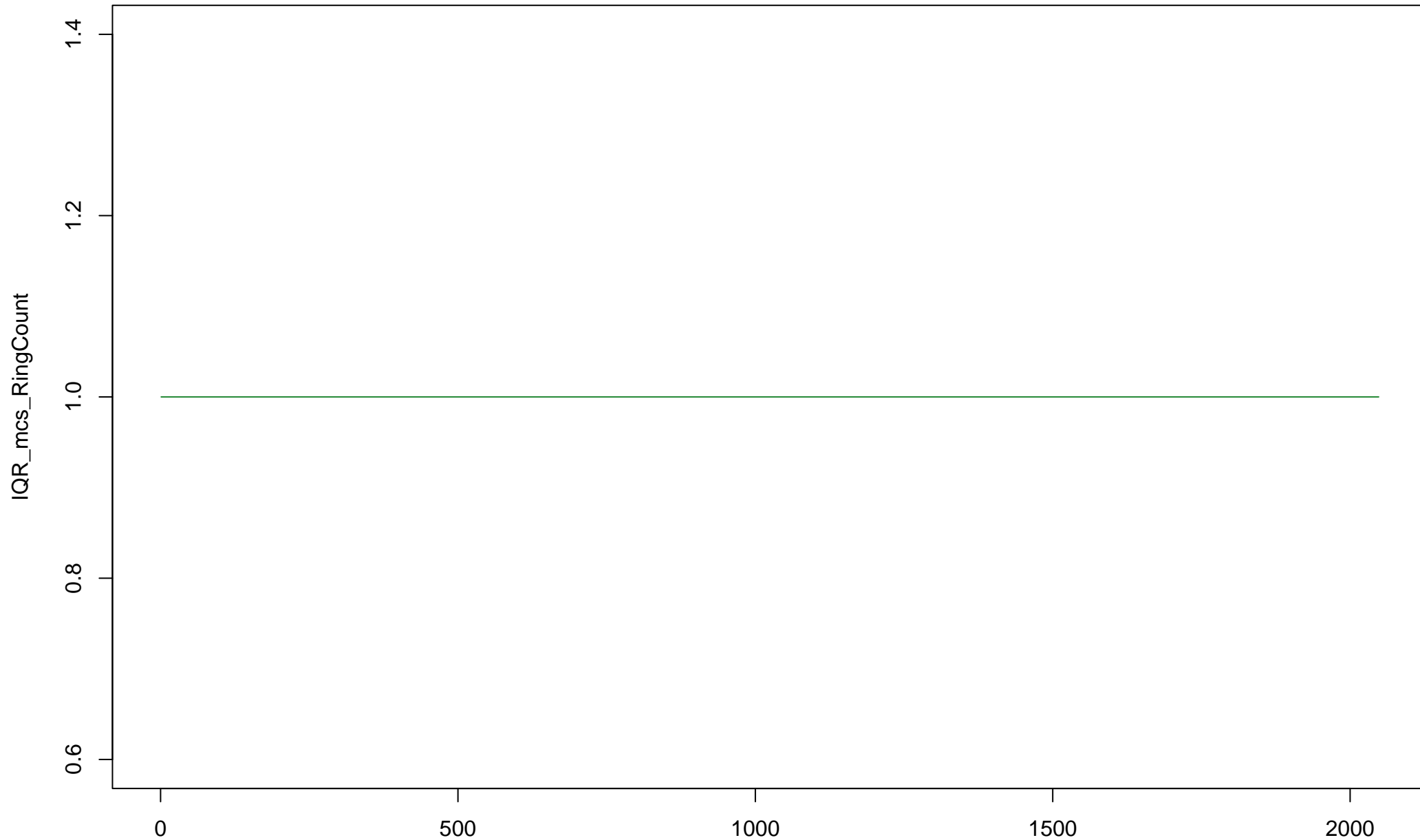




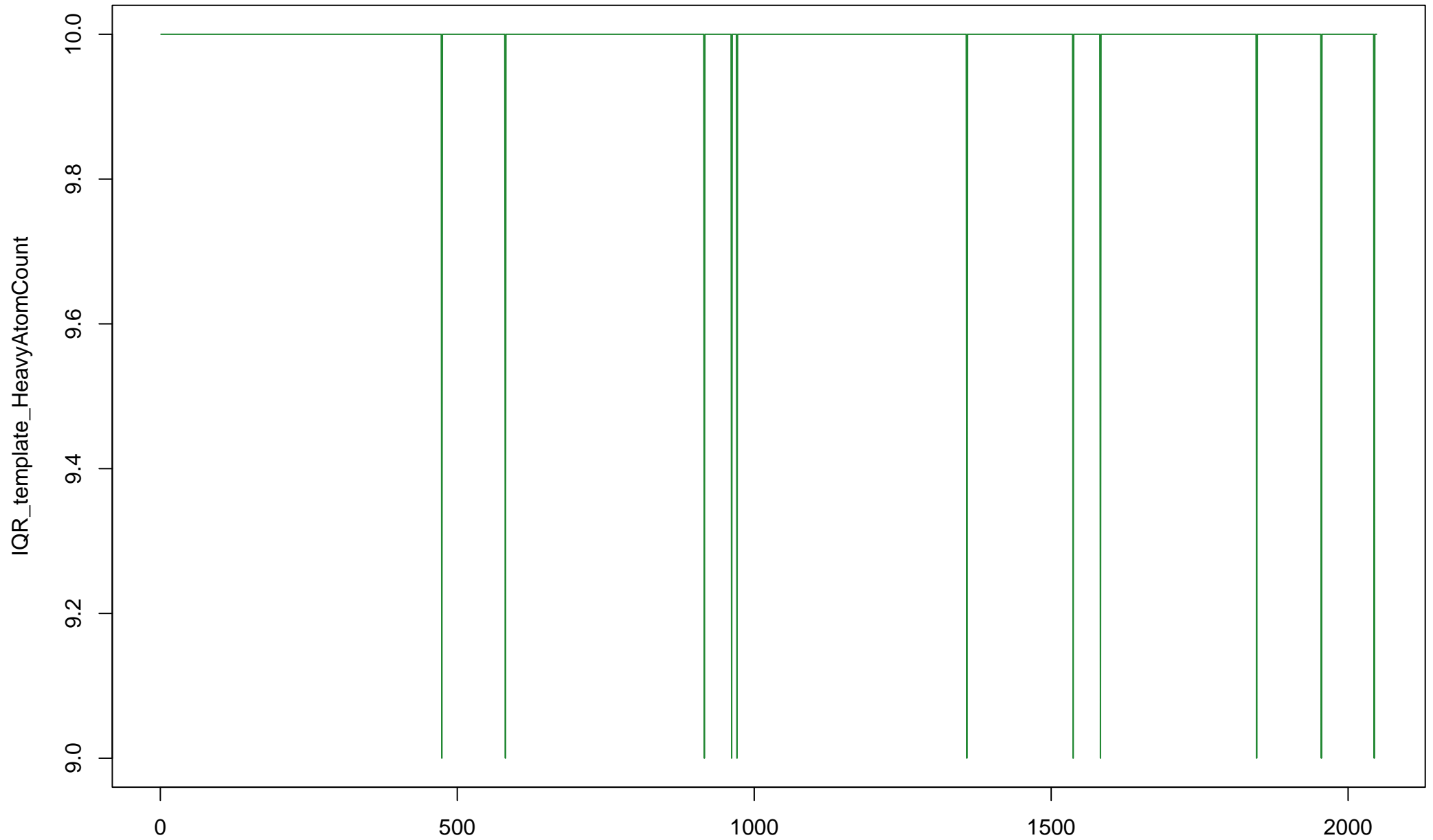
IQR\_docked\_HeavyAtomCount  
ESS = 1810 | BMK = 0.0253 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0



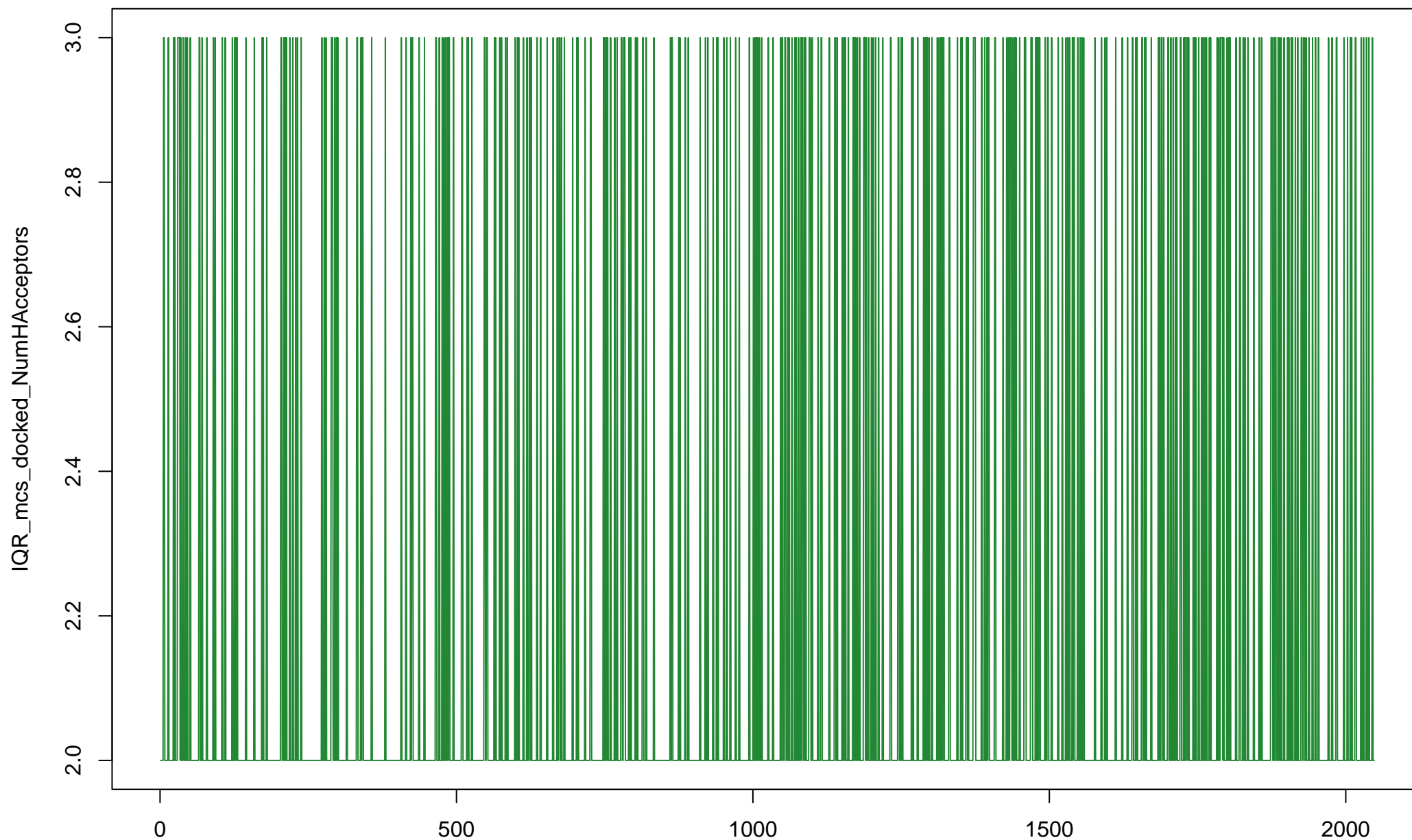
**IQR\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



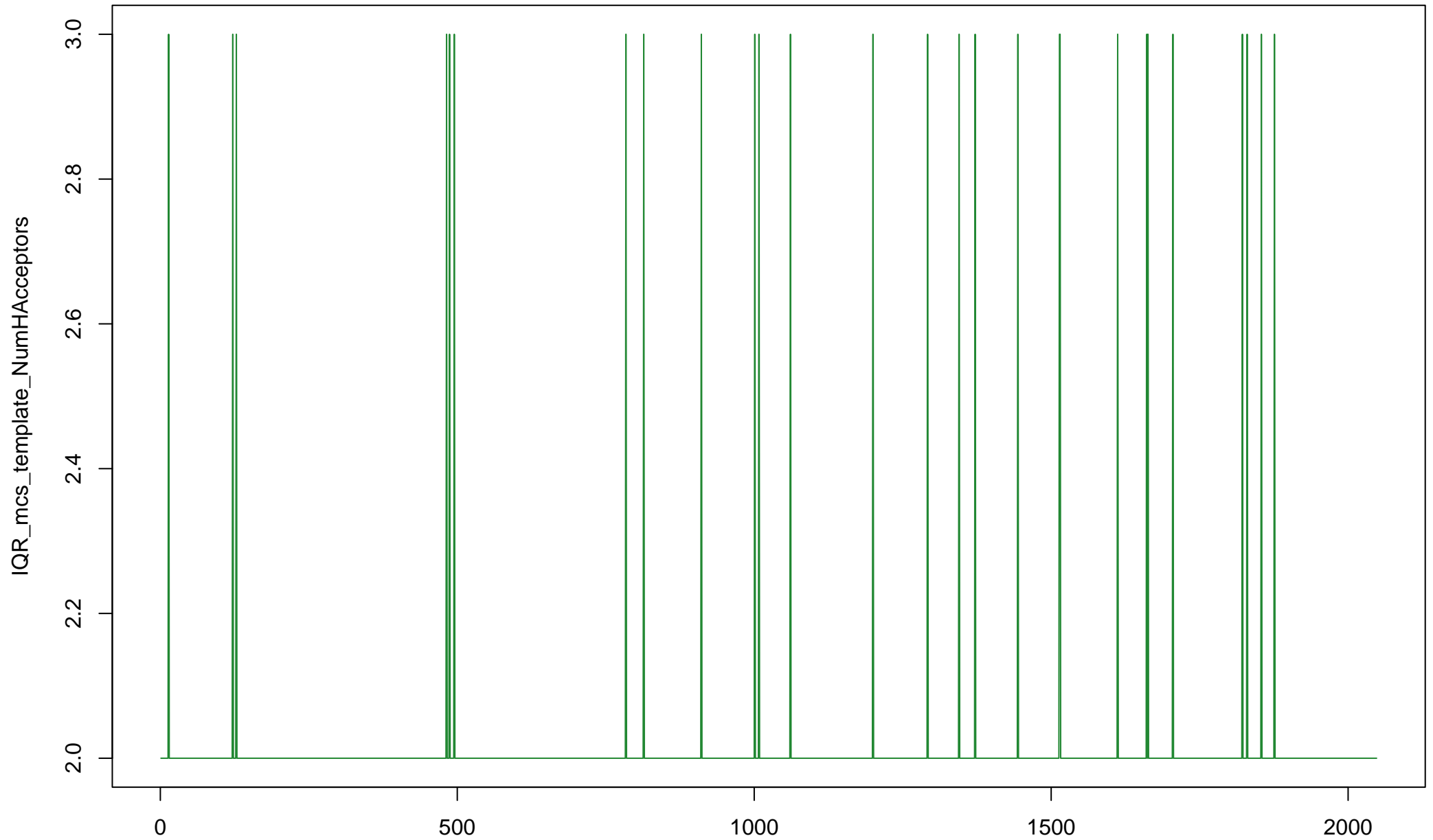
**IQR\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0324 | MCSE(6.27) = 2.12 | stat: FALSE | burn: 1224**



IQR\_mcs\_docked\_NumHAcceptors  
ESS = 2050 | BMK = 0.0664 | MCSE(6.27) = 2.51 | stat: FALSE | burn: 0



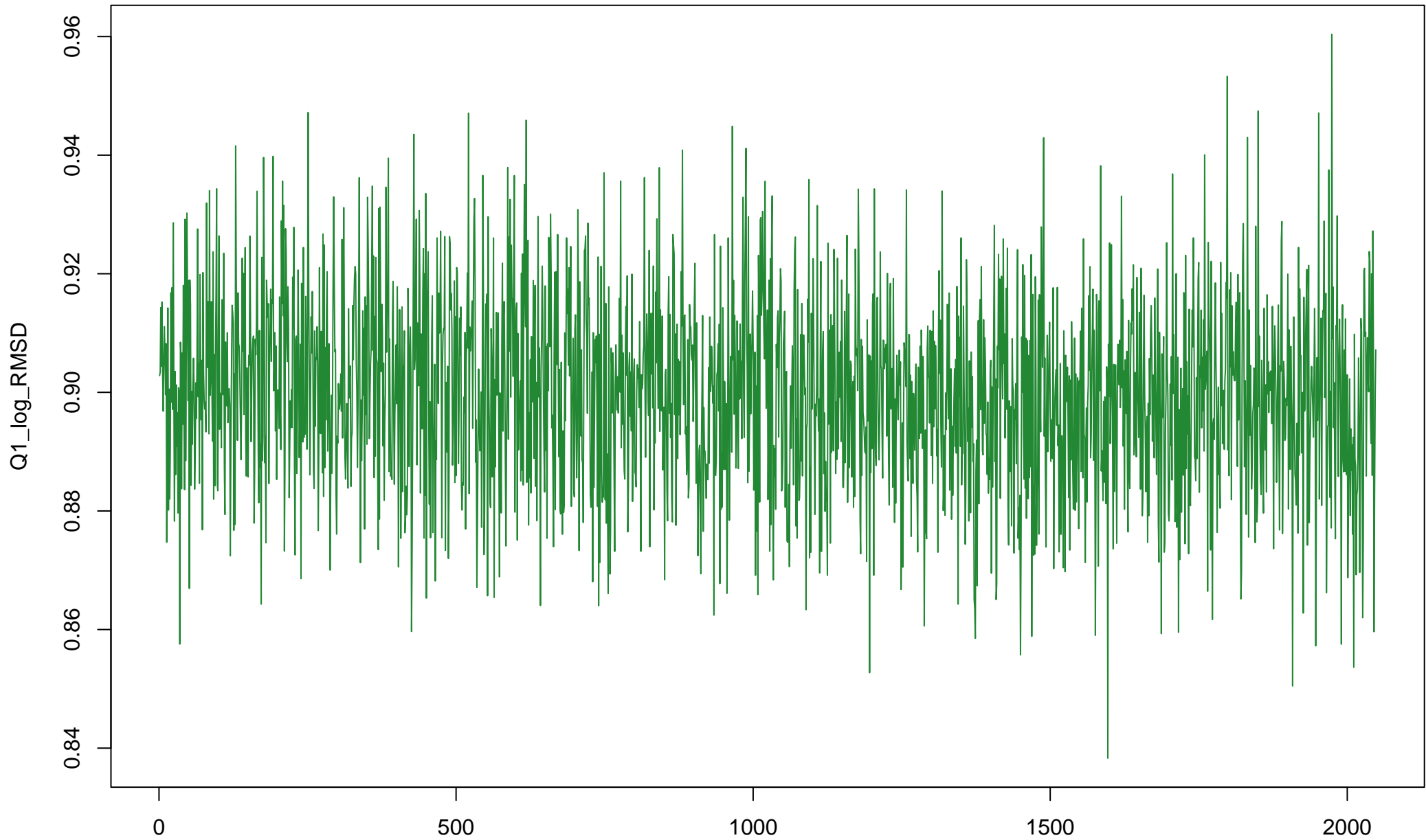
**IQR\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0662 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 408**



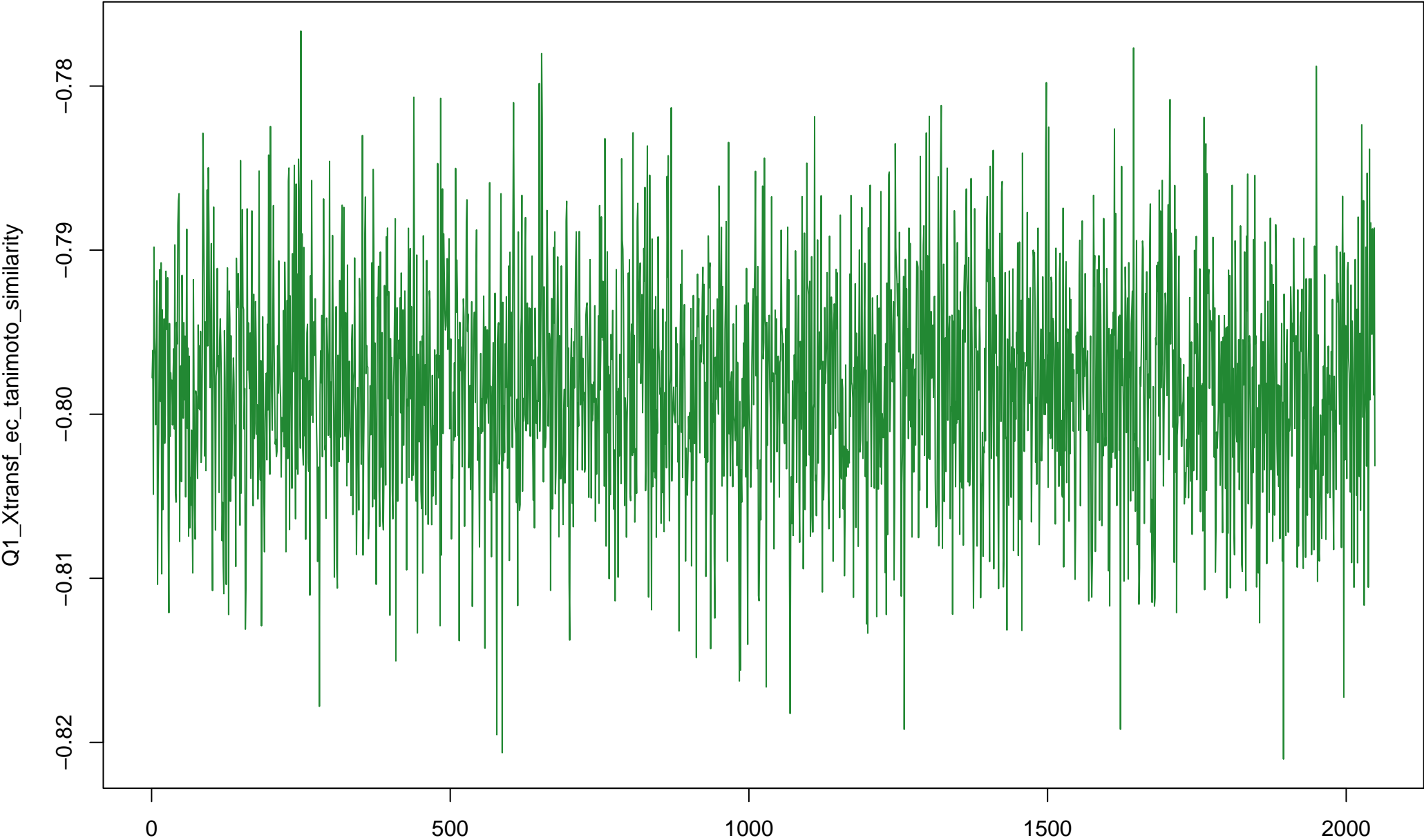
IQR\_mcs\_NumHeteroAtoms  
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



**Q1\_log\_RMSD**  
**ESS = 1740 | BMK = 0.104 | MCSE(6.27) = 3.01 | stat: FALSE | burn: 0**

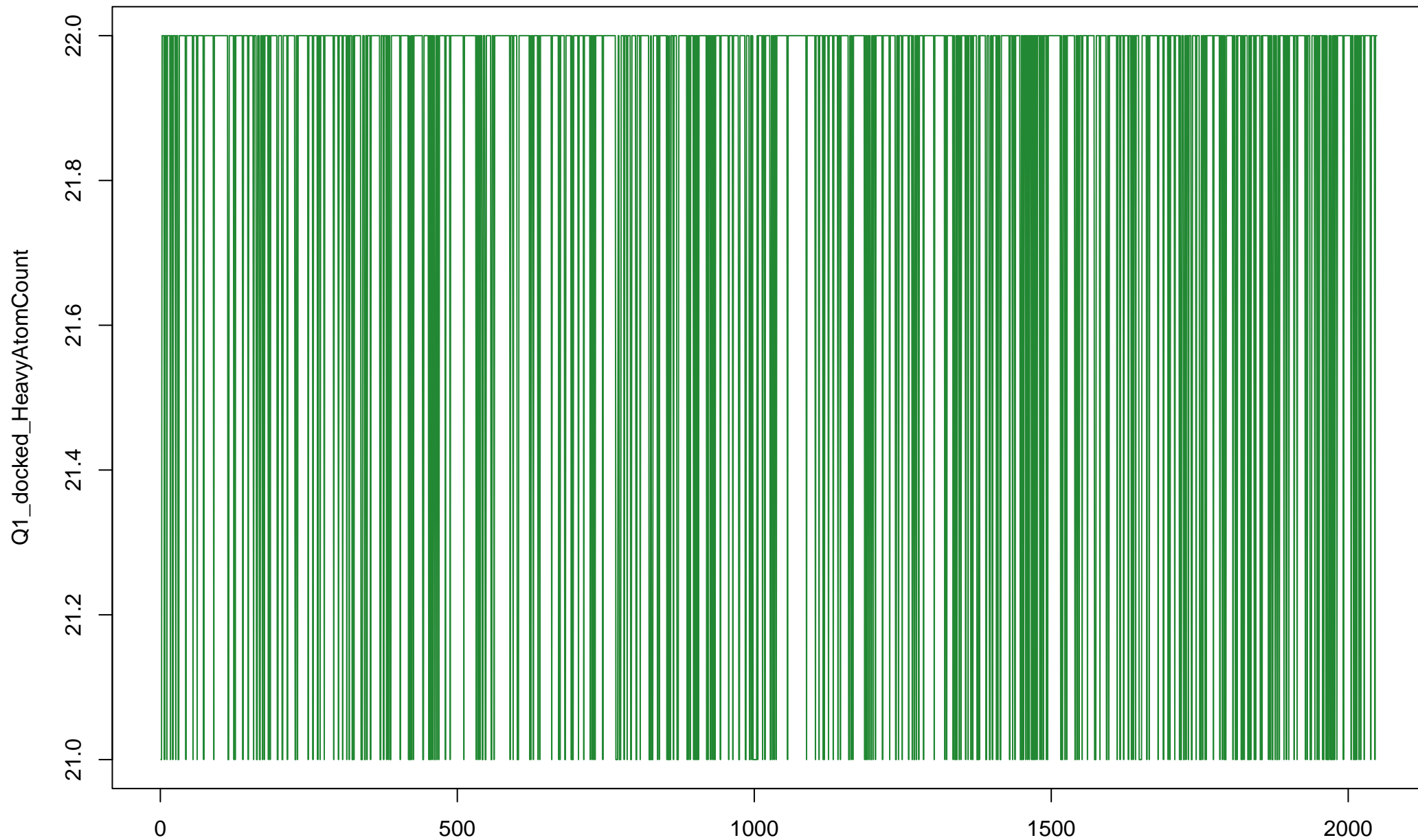


Q1\_Xtransf\_ec\_tanimoto\_similarity  
ESS = 2050 | BMK = 0.049 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0





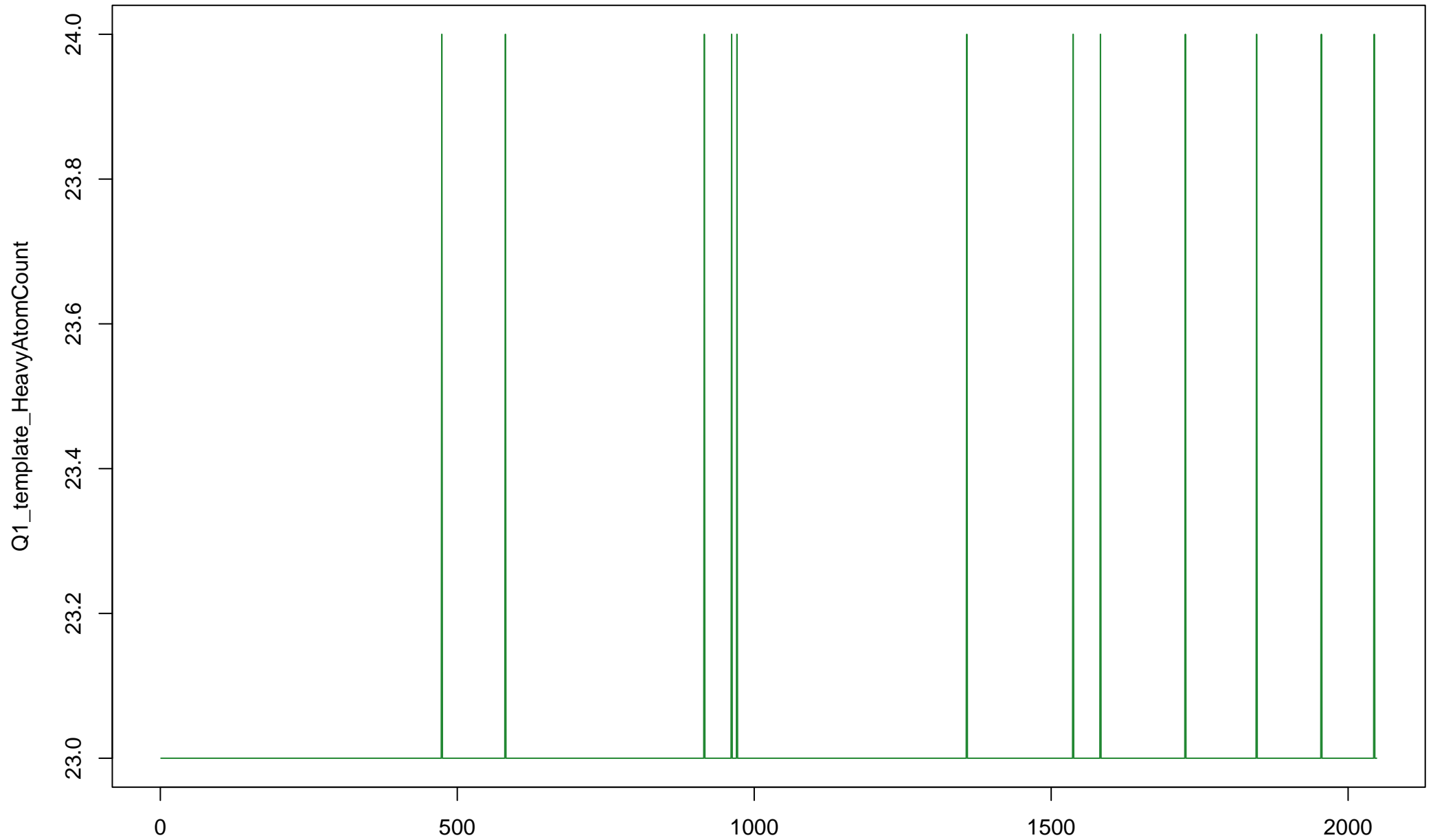
**Q1\_docked\_HeavyAtomCount**  
**ESS = 1580 | BMK = 0.0206 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0**



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



**Q1\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0596 | MCSE(6.27) = 2.09 | stat: FALSE | burn: 1224**



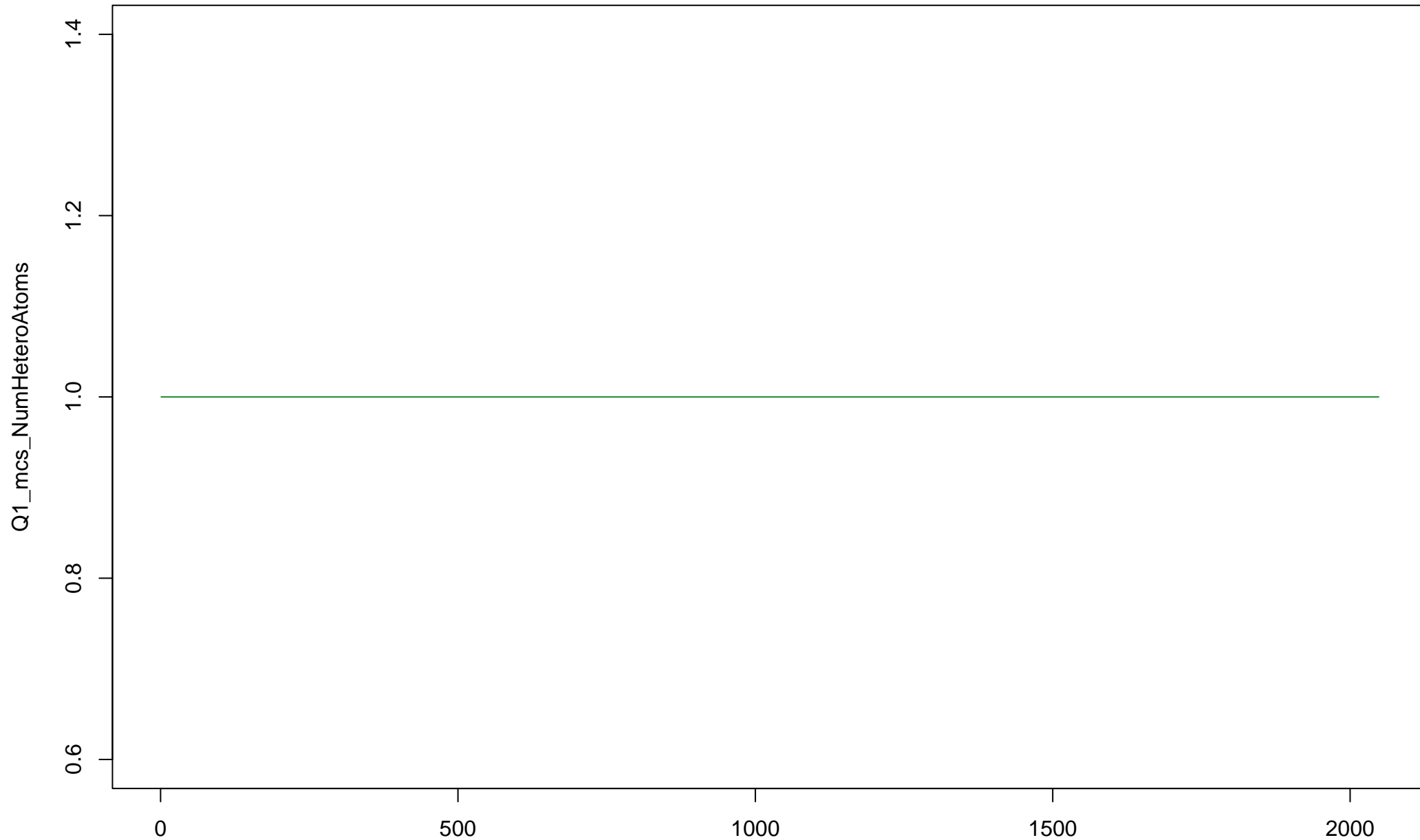
**Q1\_mcs\_docked\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



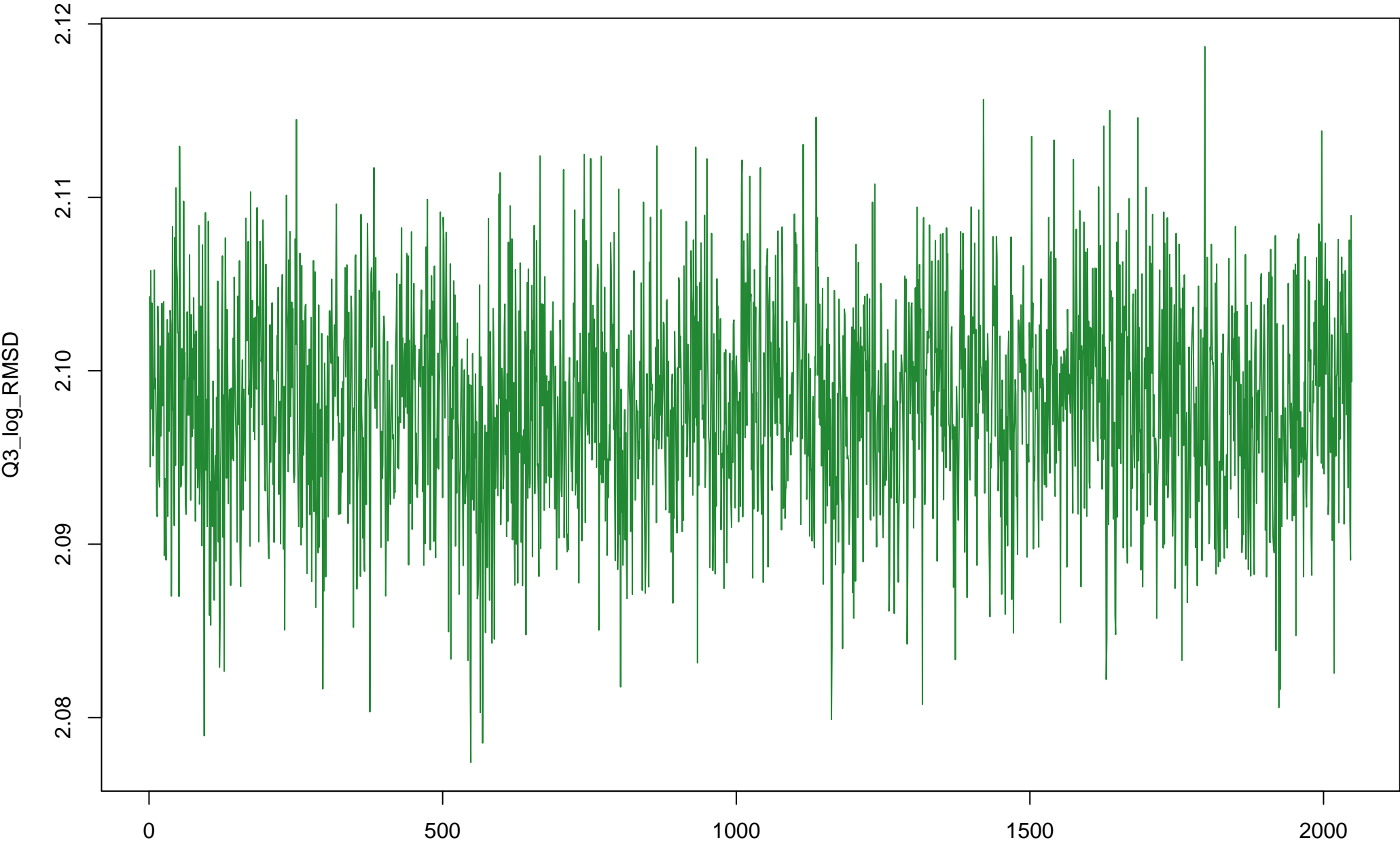
**Q1\_mcs\_template\_NumHAcceptors**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



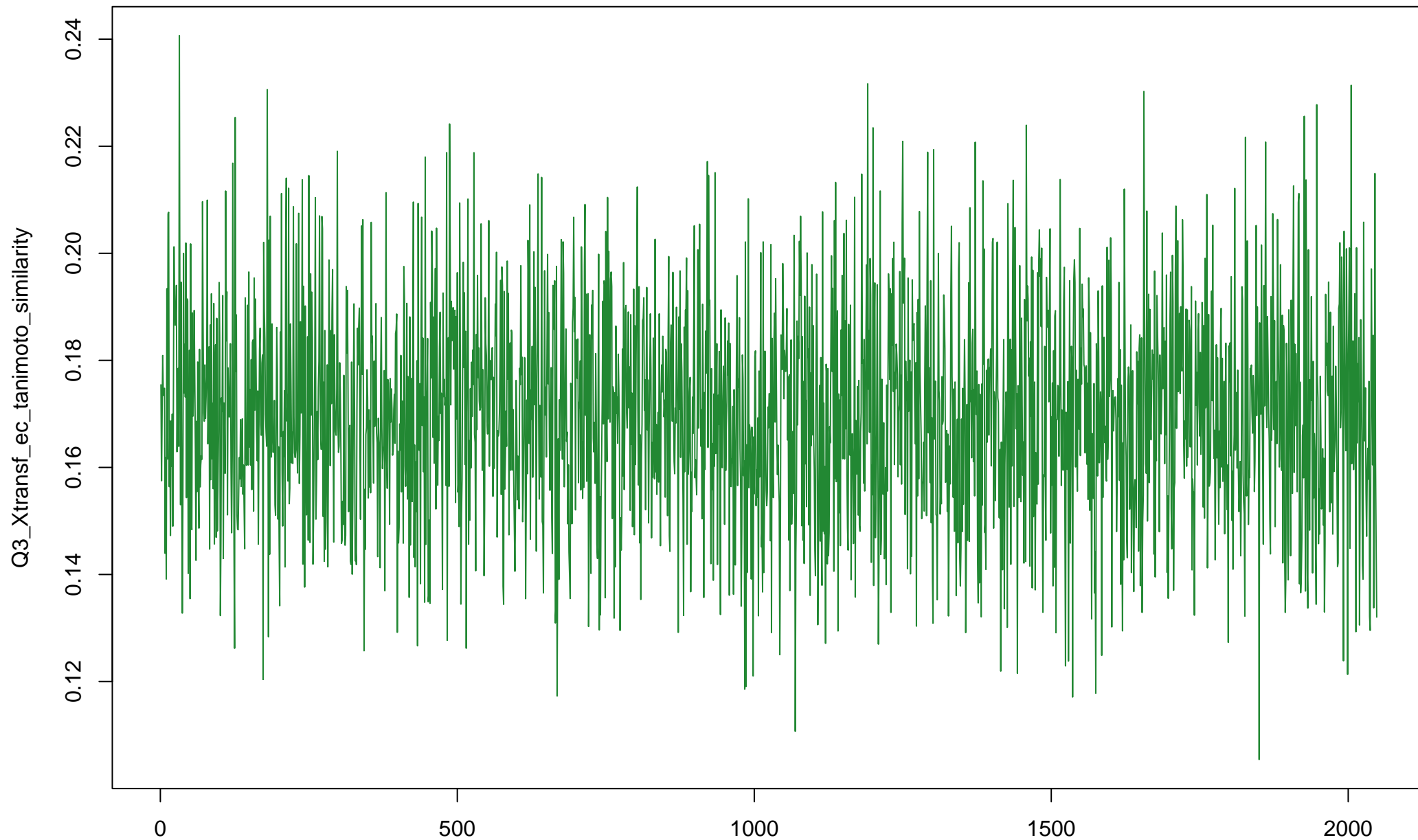
**Q1\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Q3\_log\_RMSD**  
**ESS = 895 | BMK = 0.0478 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0**

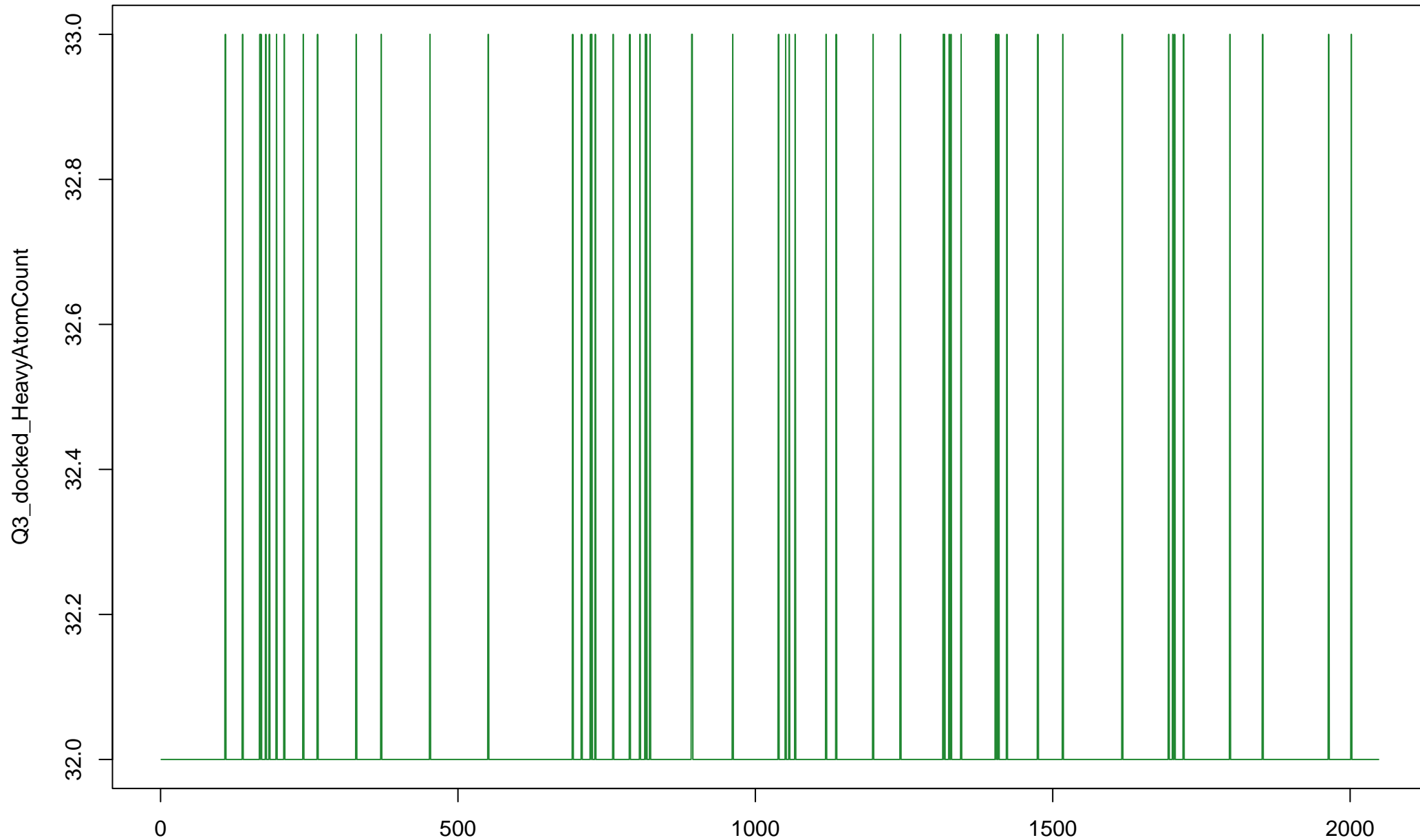


**Q3\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0459 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0**





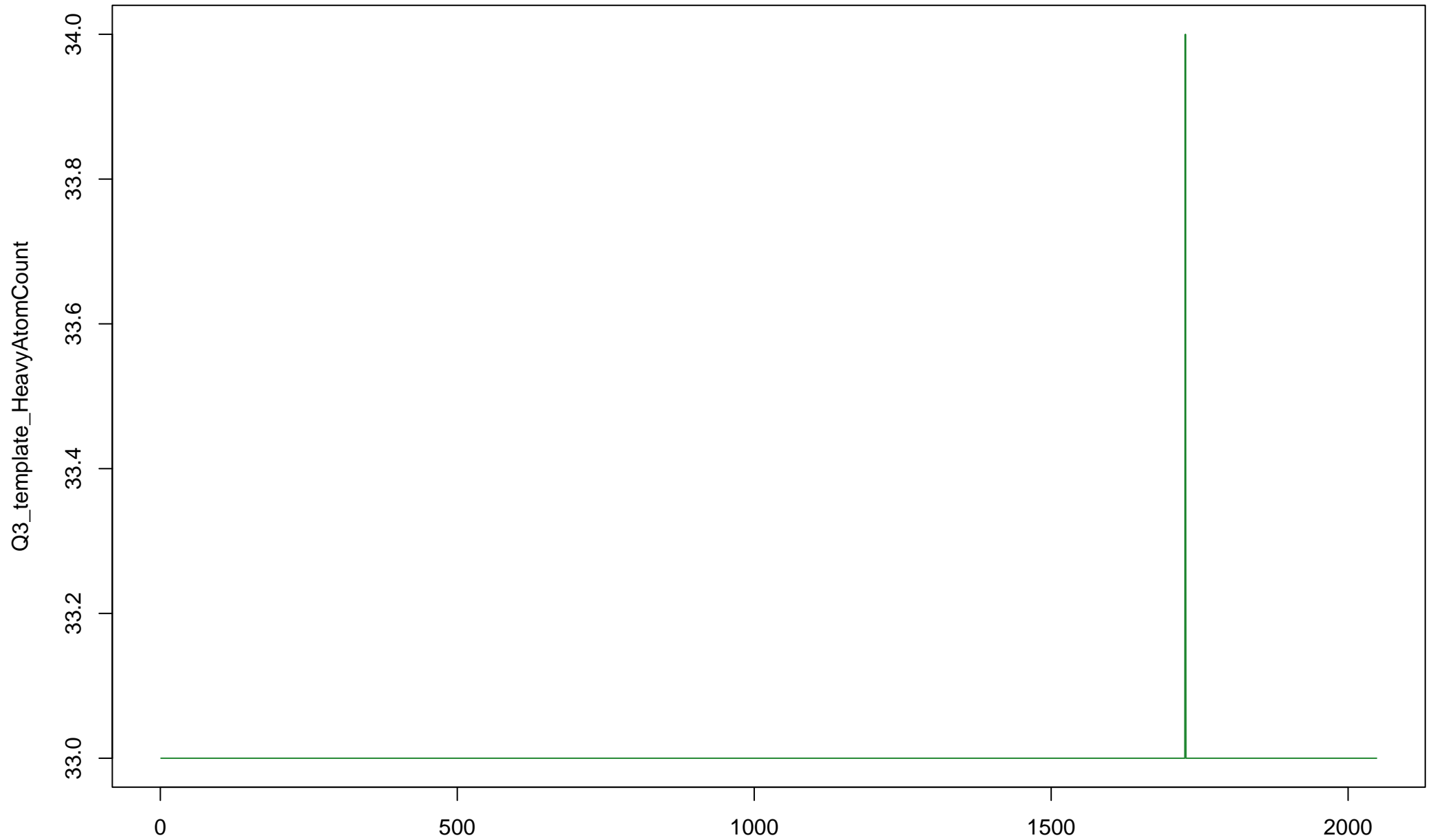
**Q3\_docked\_HeavyAtomCount**  
**ESS = 1140 | BMK = 0 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0**



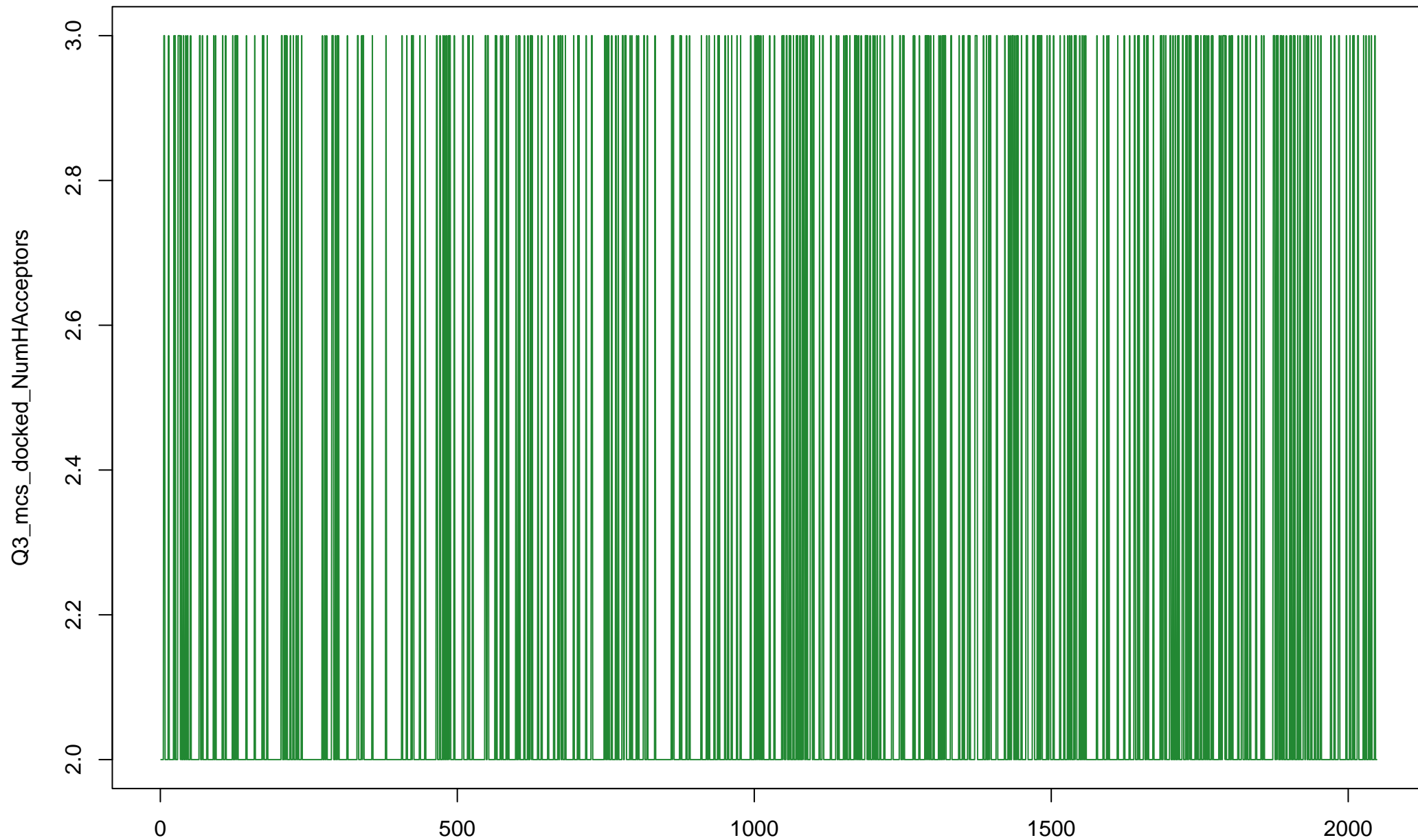
**Q3\_mcs\_RingCount**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



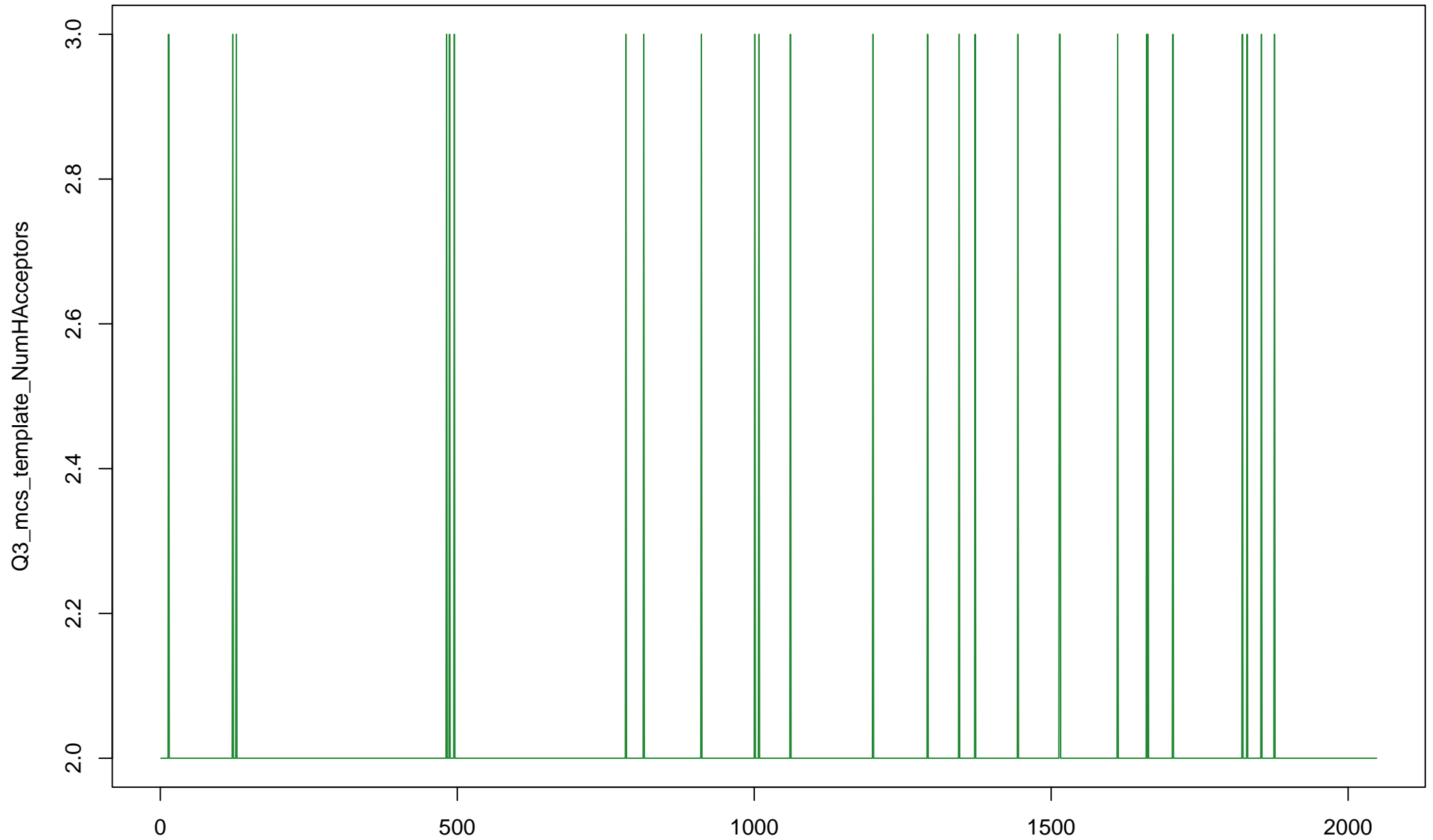
**Q3\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.517 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 2040**



**Q3\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0664 | MCSE(6.27) = 2.51 | stat: FALSE | burn: 0**



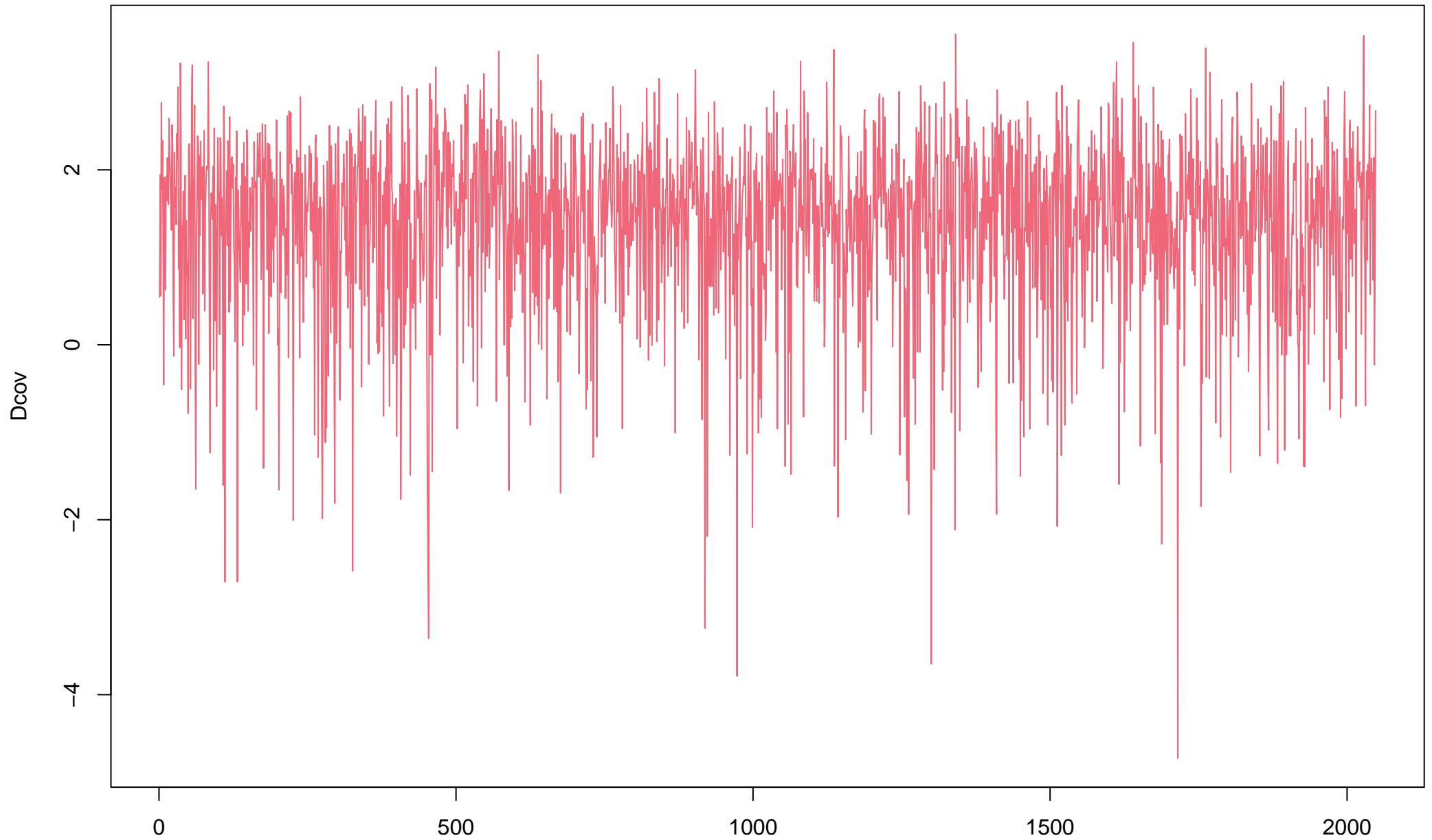
**Q3\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0662 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 408**



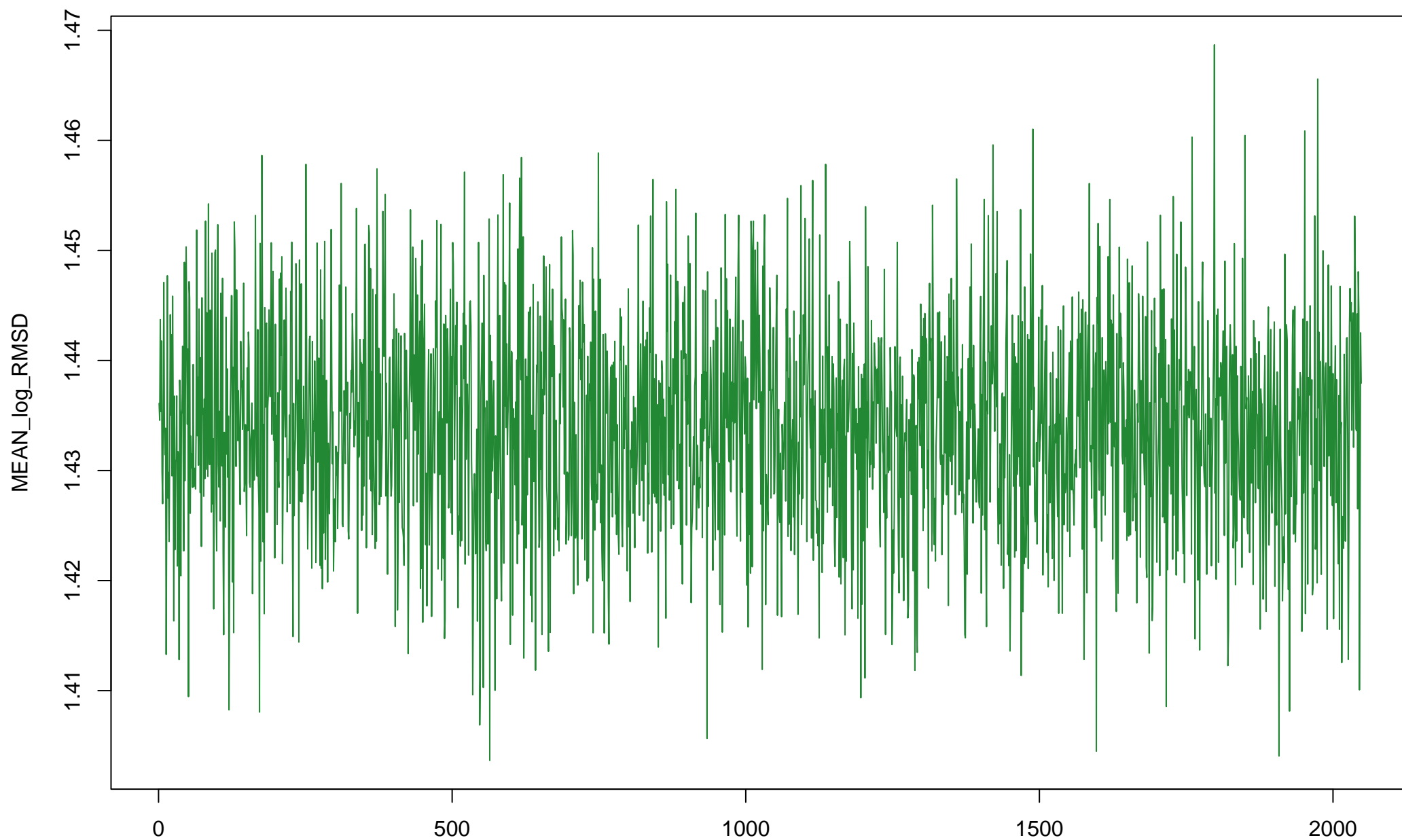
**Q3\_mcs\_NumHeteroAtoms**  
**ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0**



**Dcov**  
**ESS = 2050 | BMK = 0.0617 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0**

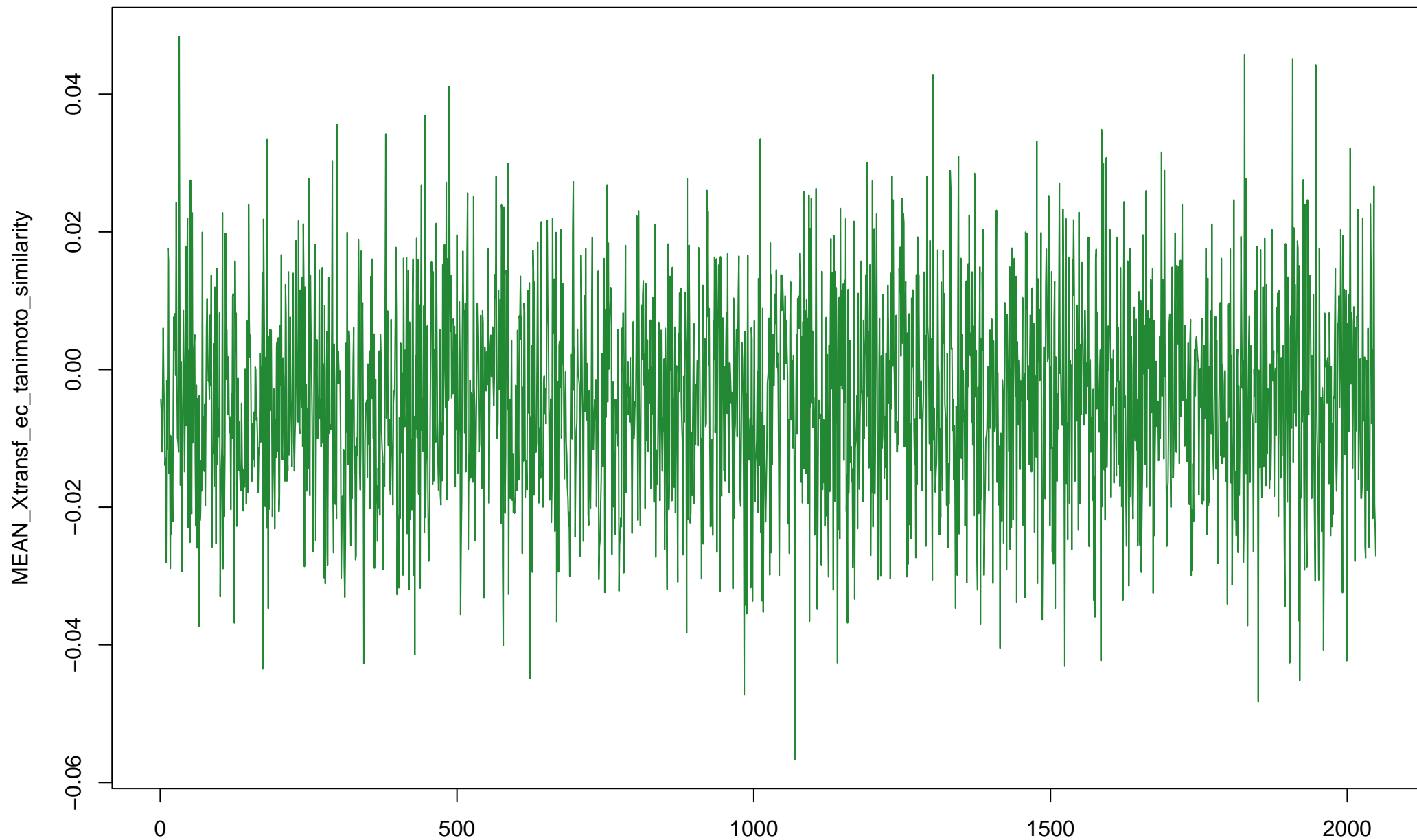


**MEAN\_log\_RMSD**  
**ESS = 2050 | BMK = 0.062 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0**

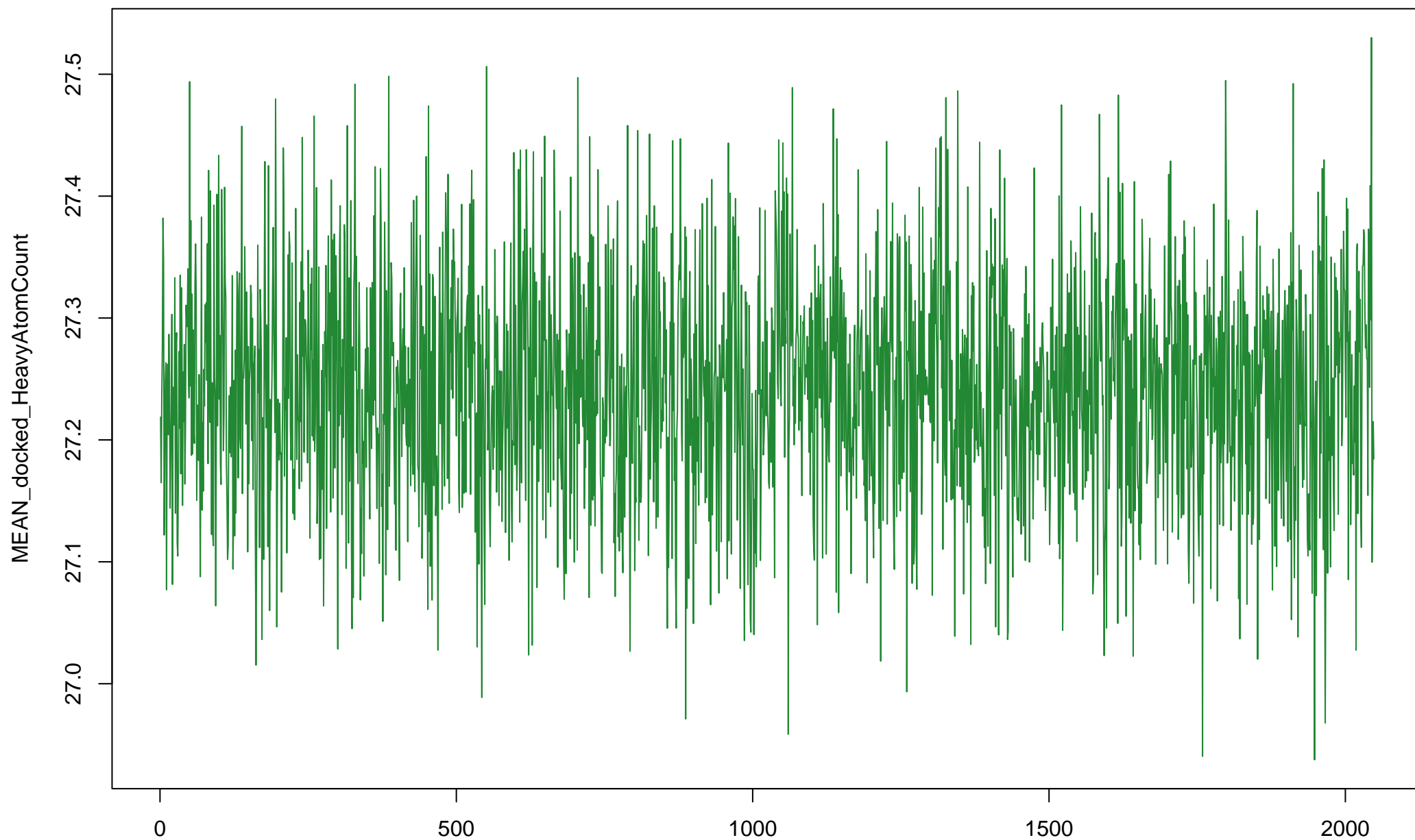




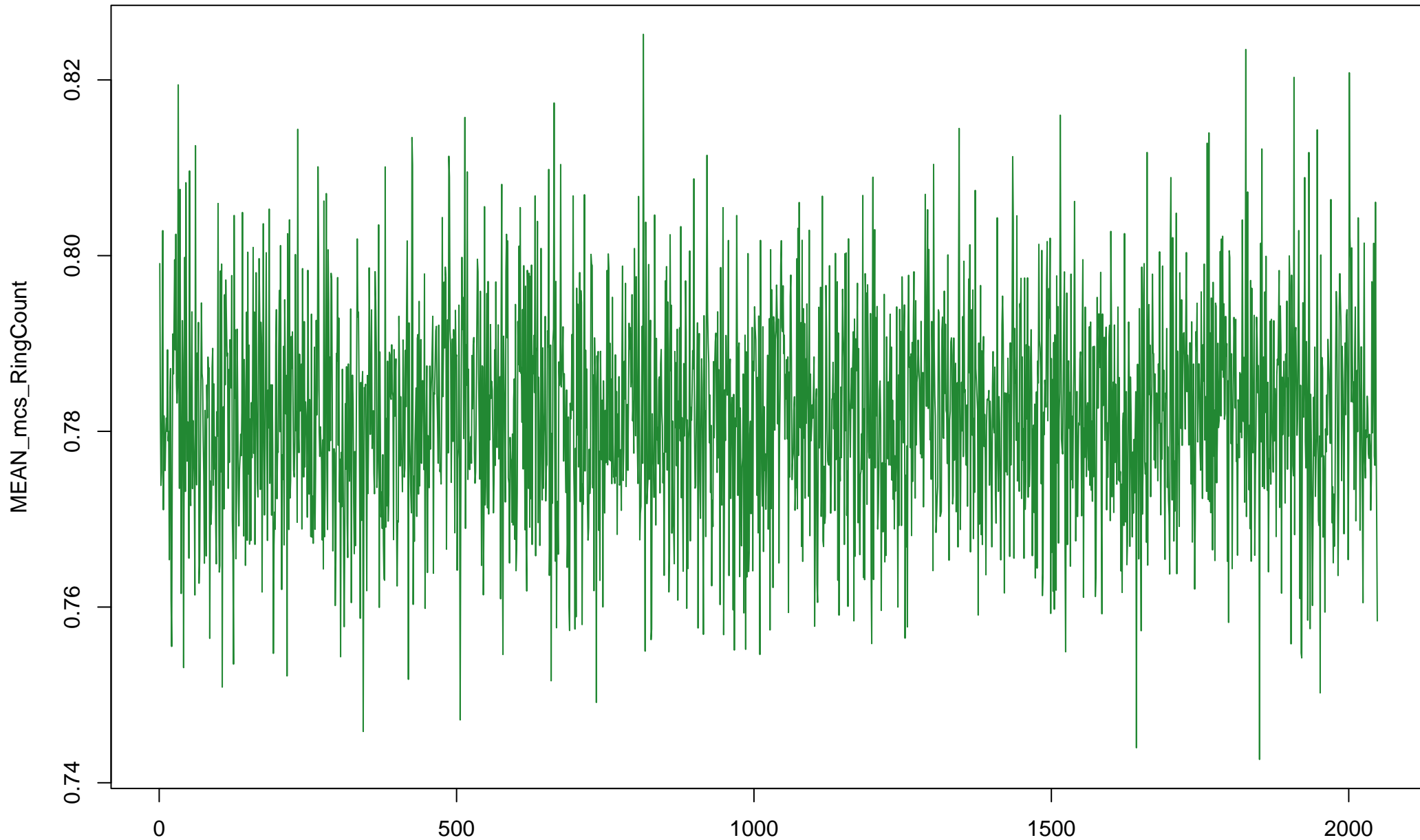
**MEAN\_Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 2050 | BMK = 0.0606 | MCSE(6.27) = 2.17 | stat: FALSE | burn: 0**



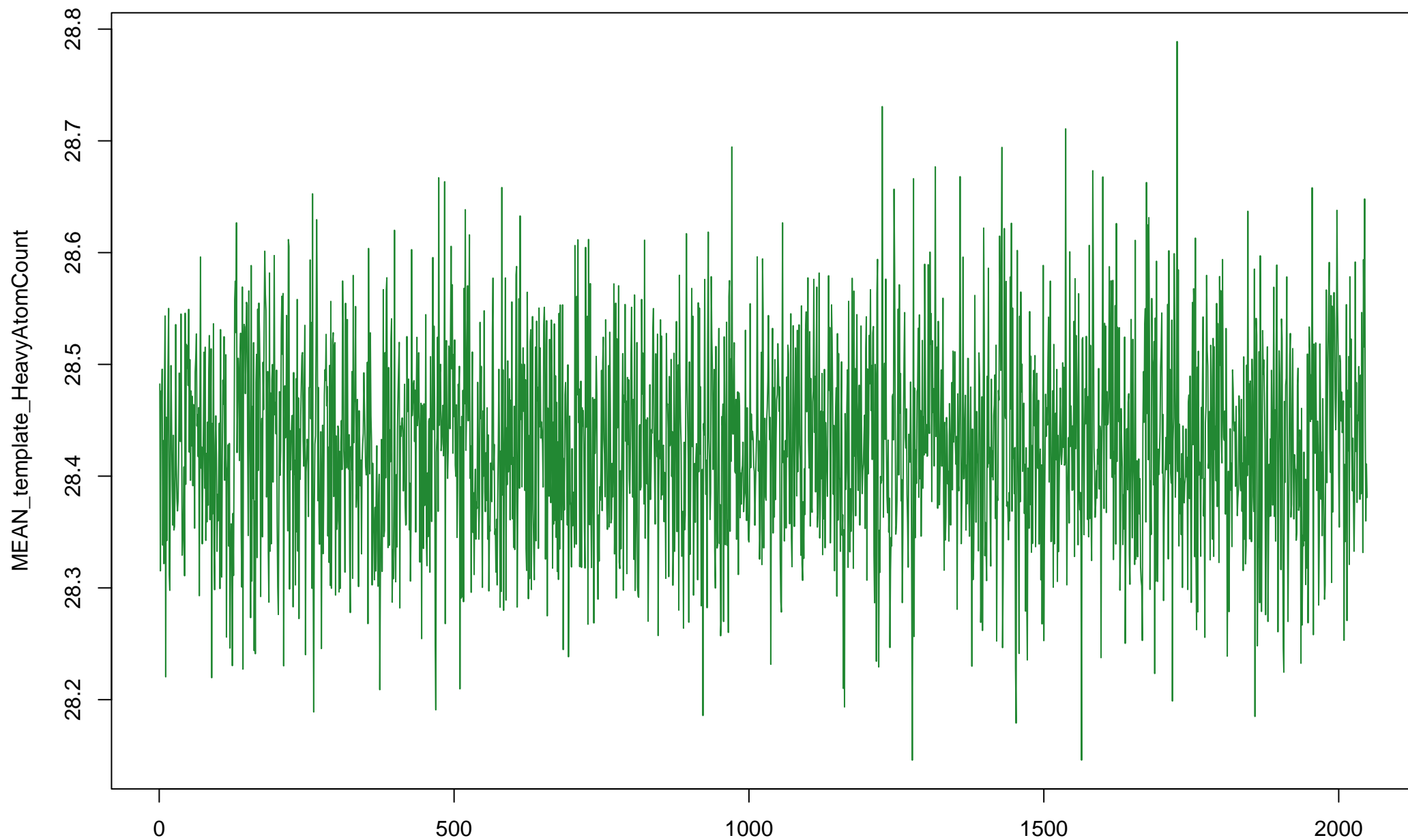
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0532 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0**



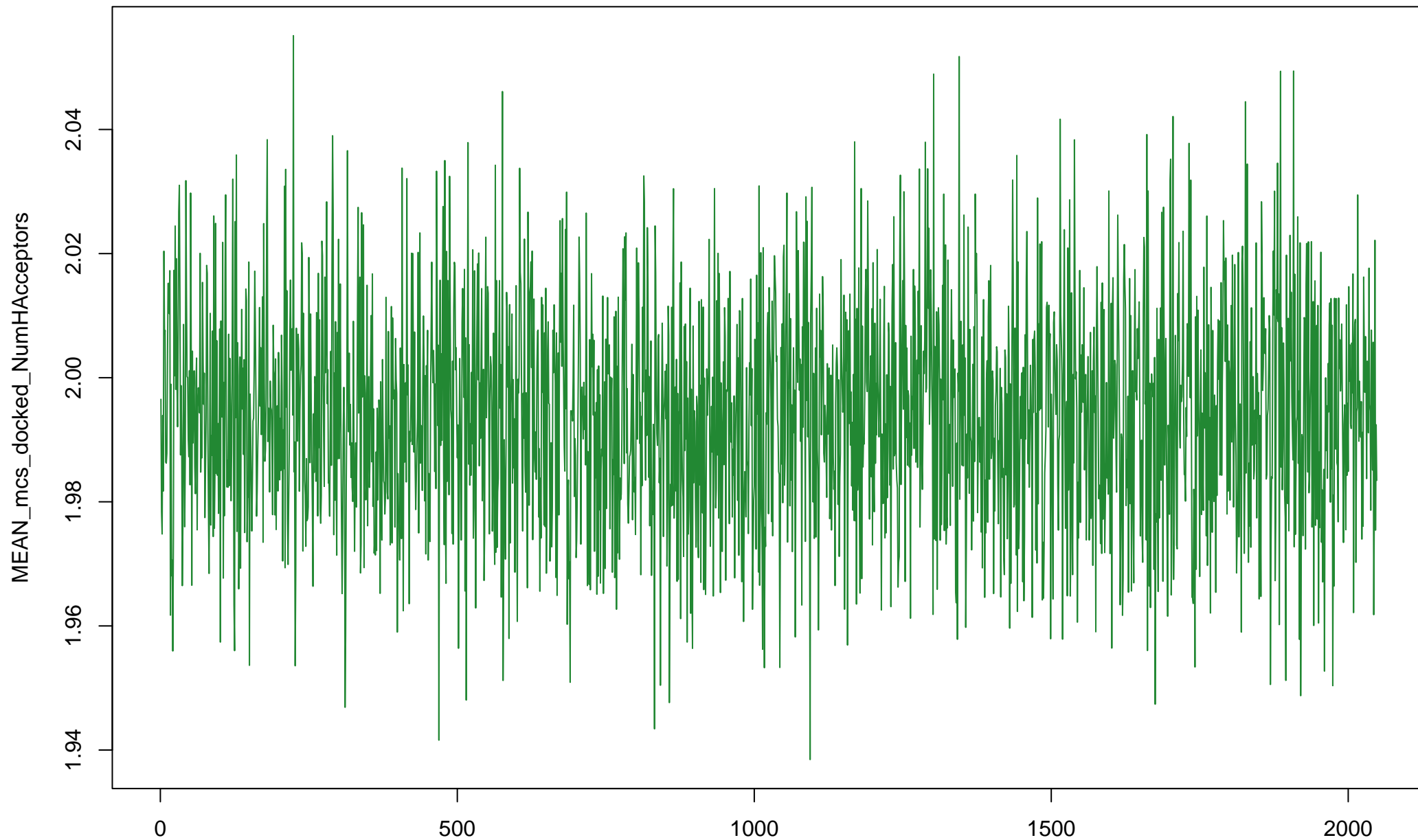
**MEAN\_mcs\_RingCount**  
**ESS = 2050 | BMK = 0.0542 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0**



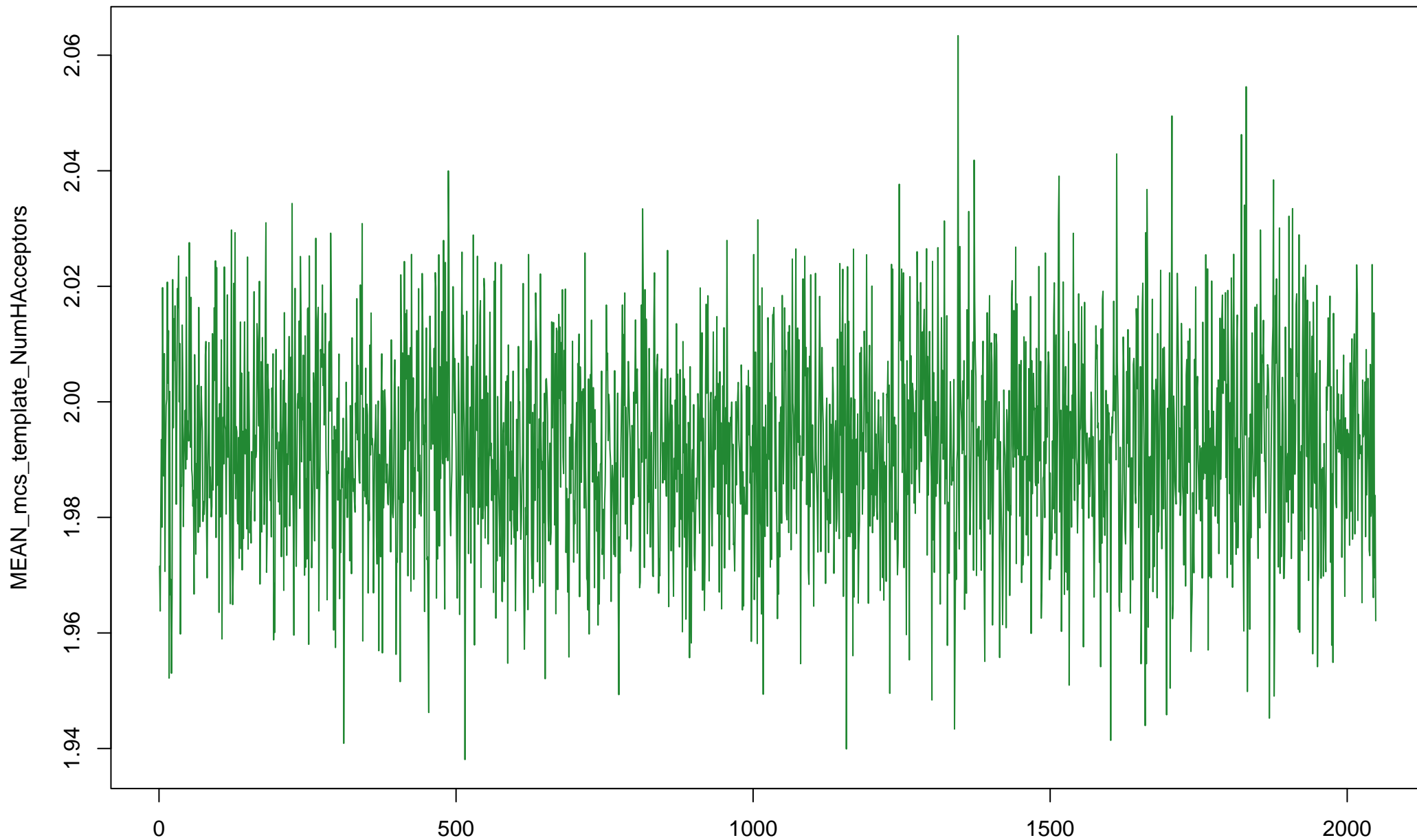
**MEAN\_template\_HeavyAtomCount**  
**ESS = 1850 | BMK = 0.0558 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0**



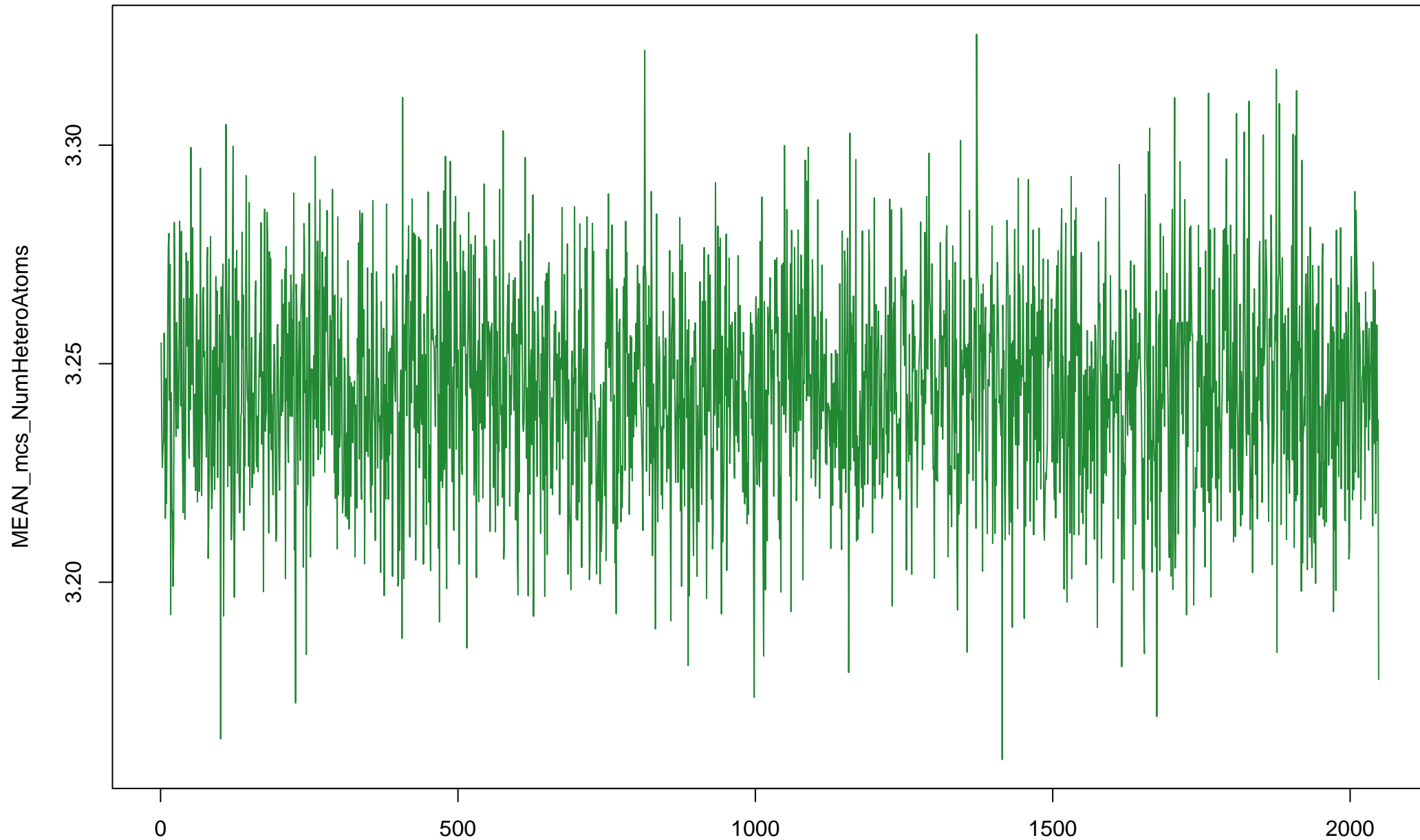
**MEAN\_mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0485 | MCSE(6.27) = 2 | stat: TRUE | burn: 0**



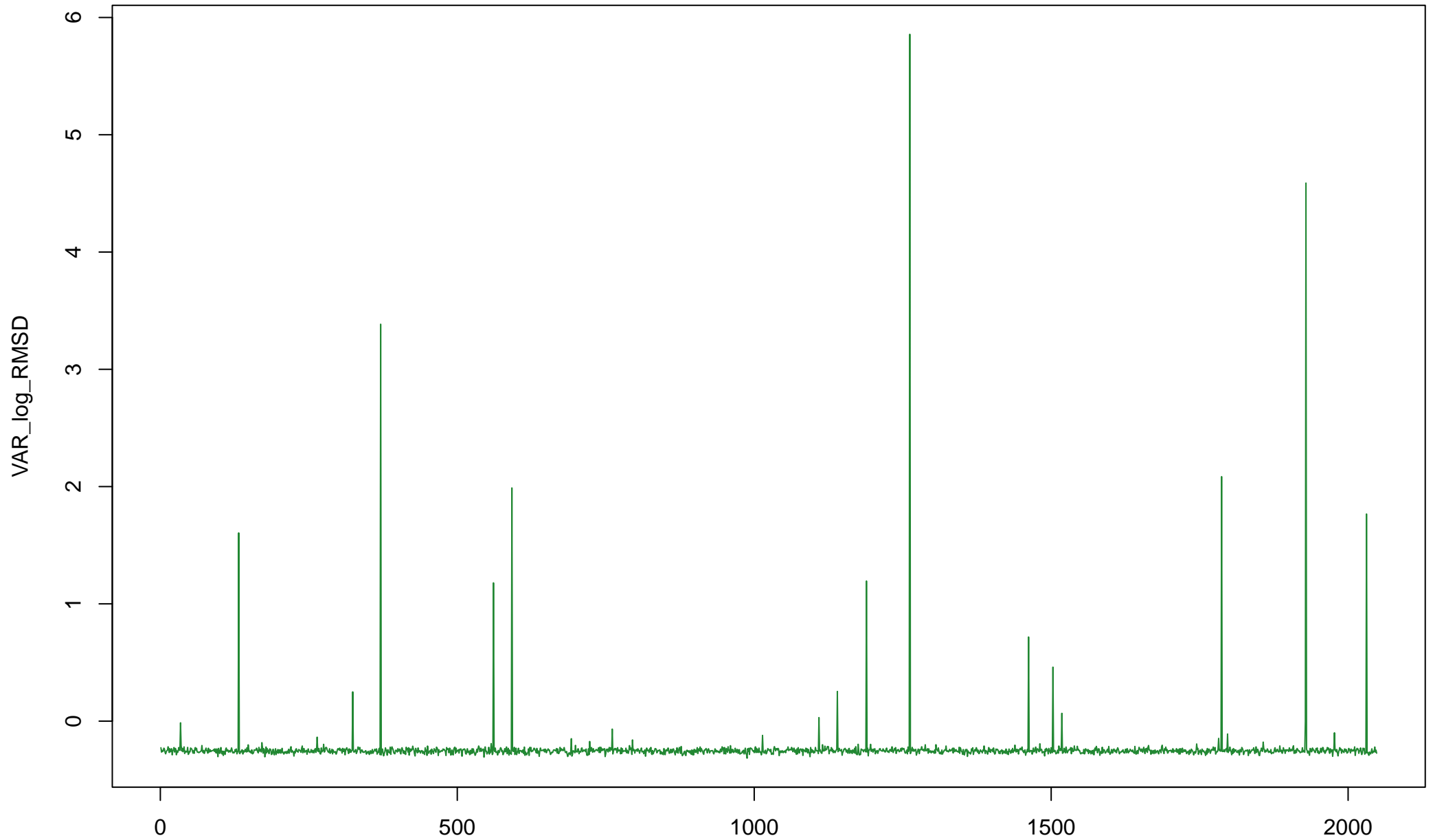
**MEAN\_mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0578 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0**



**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0443 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0**

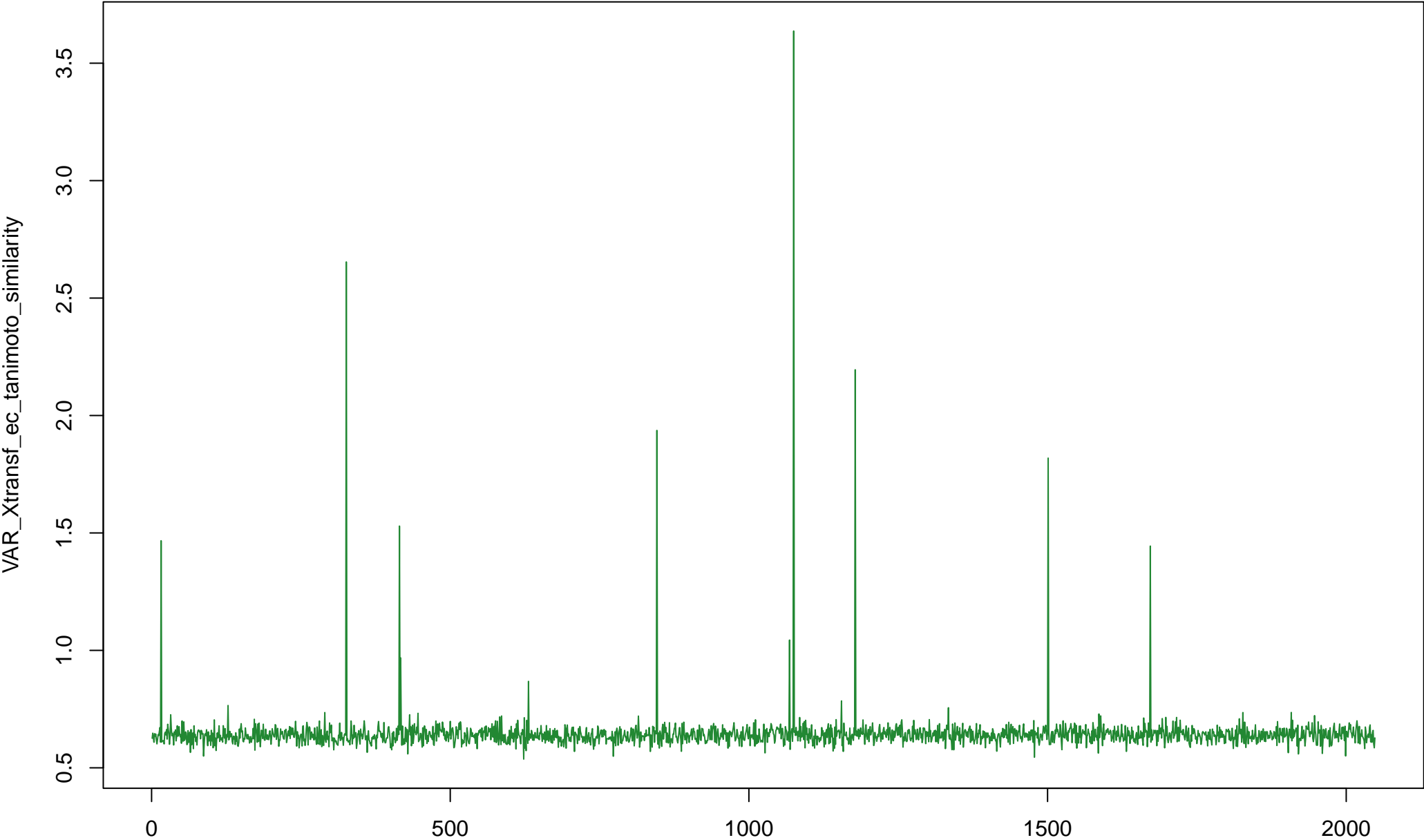


**VAR\_log\_RMSD**  
**ESS = 2050 | BMK = 0.483 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 2040**

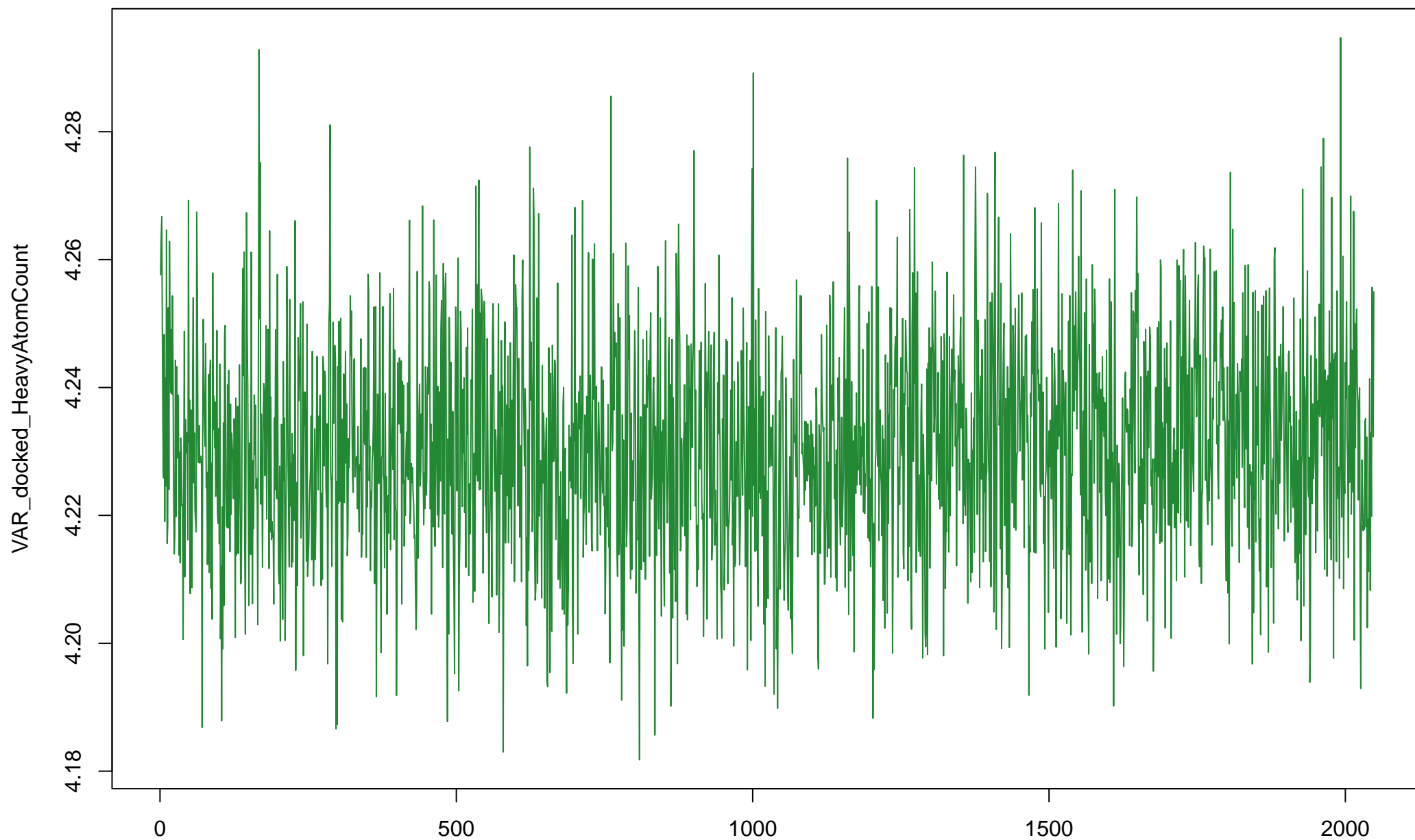




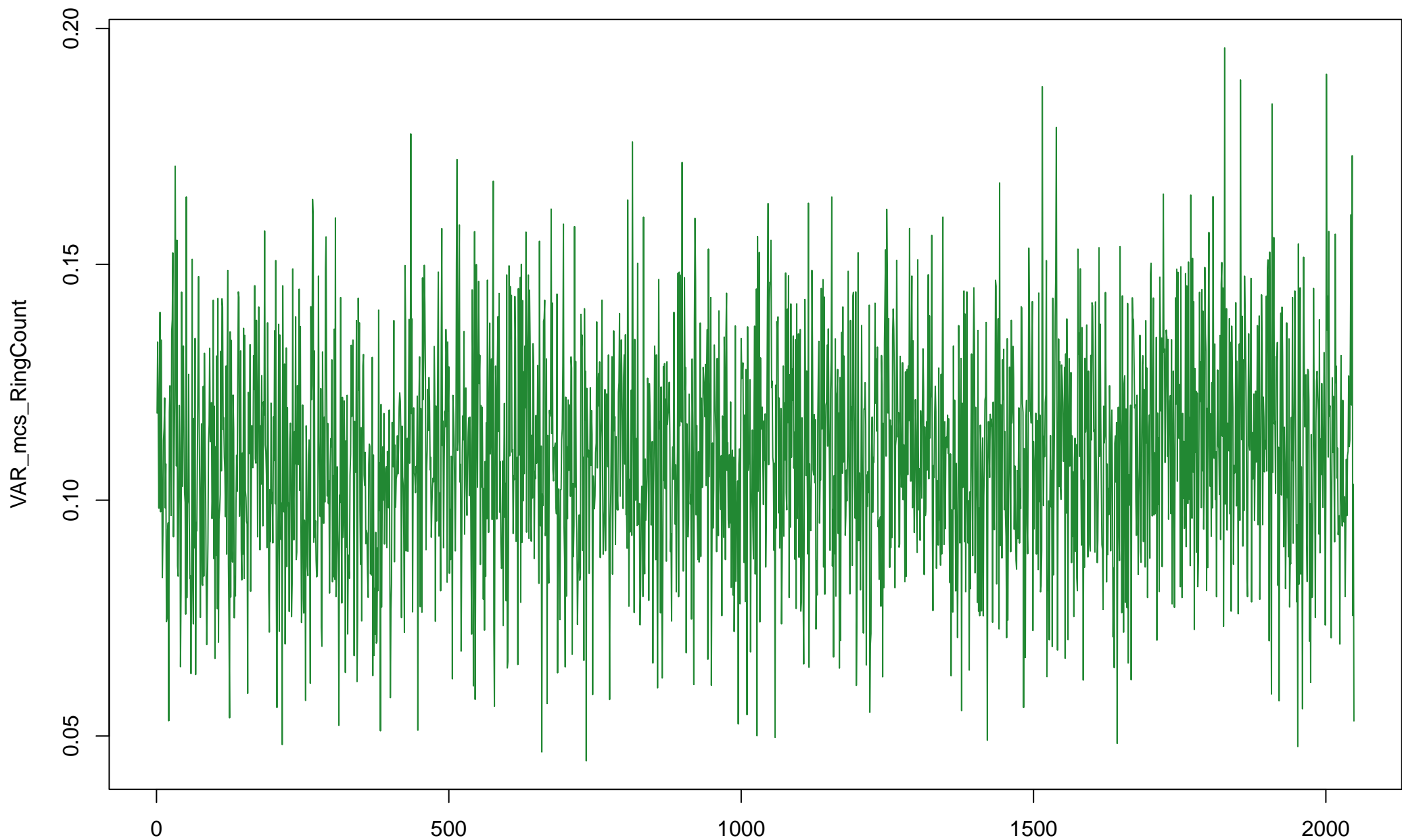
VAR\_Xtransf\_ec\_tanimoto\_similarity  
ESS = 2050 | BMK = 0.107 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0



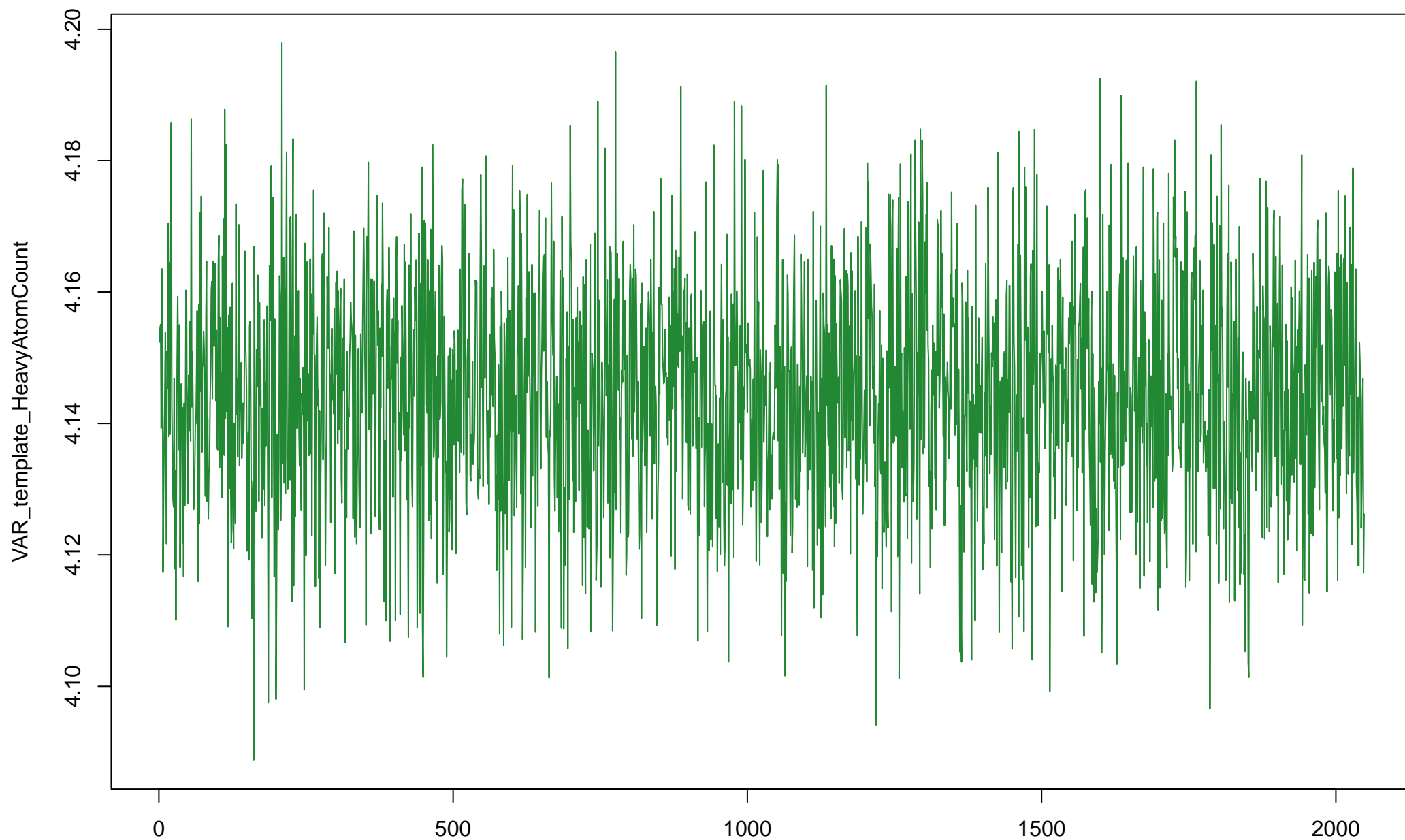
**VAR\_docked\_HeavyAtomCount**  
**ESS = 1800 | BMK = 0.0596 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0**



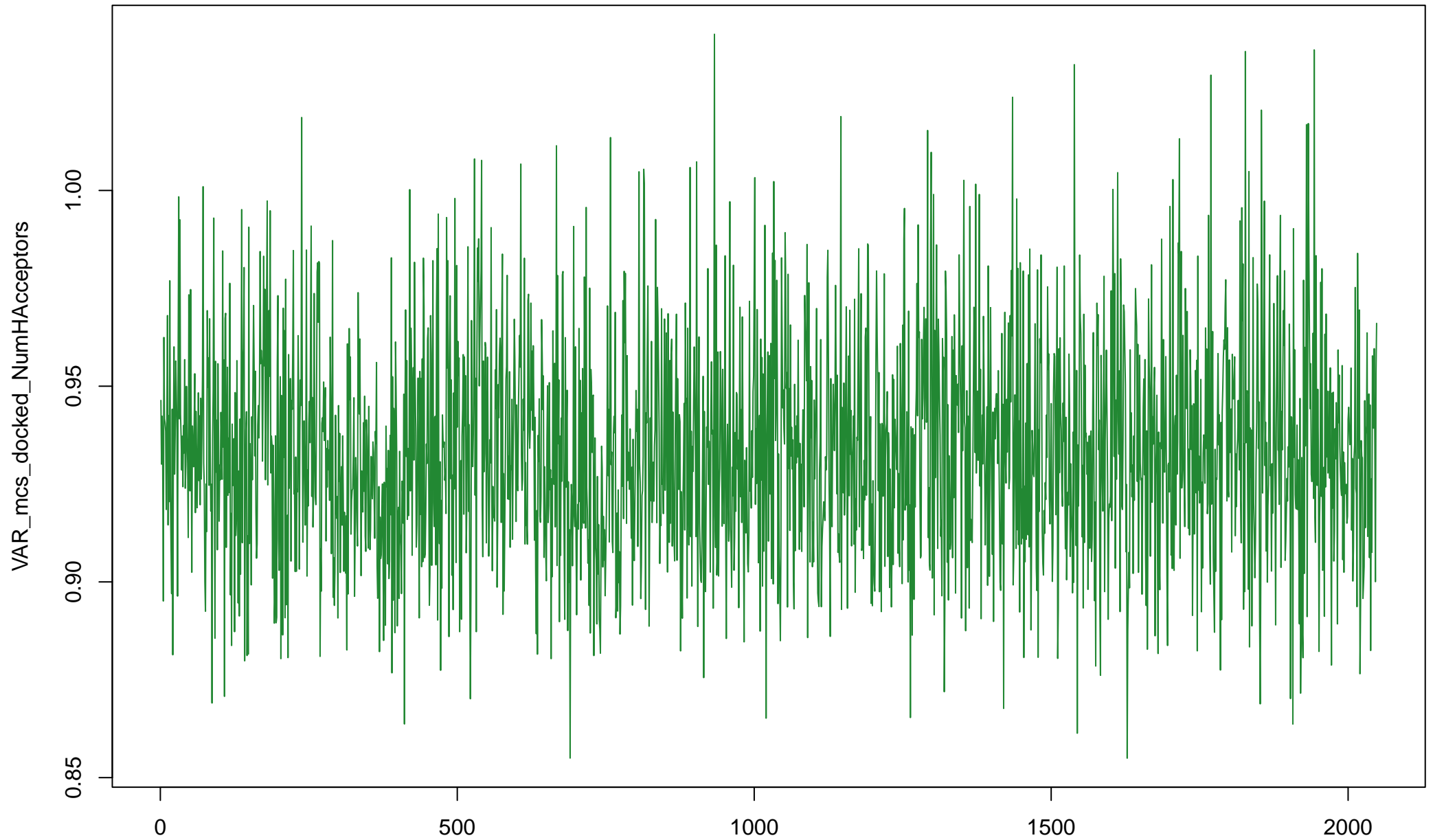
**VAR\_mcs\_RingCount**  
**ESS = 1830 | BMK = 0.0676 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0**



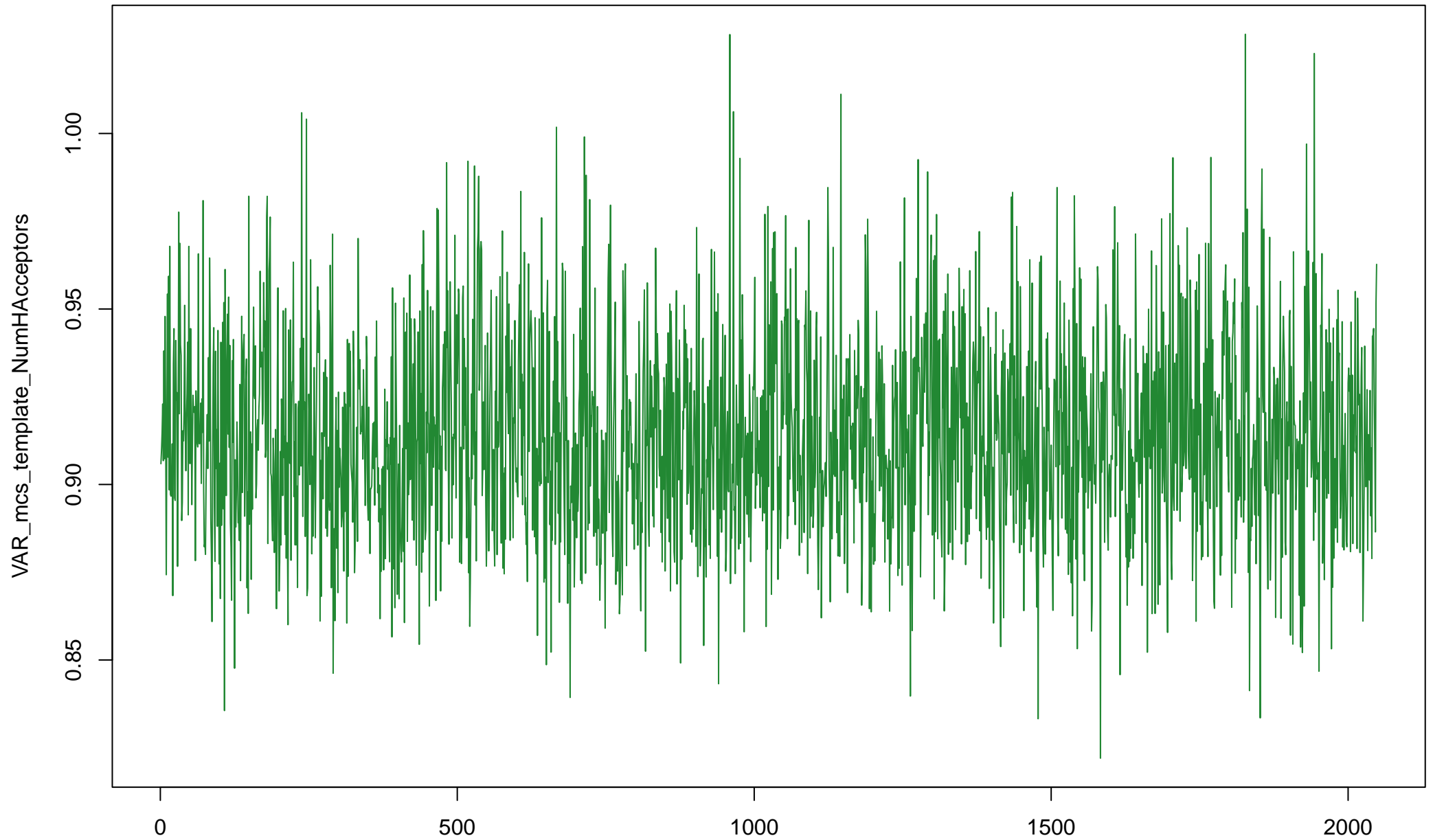
**VAR\_template\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.044 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0**



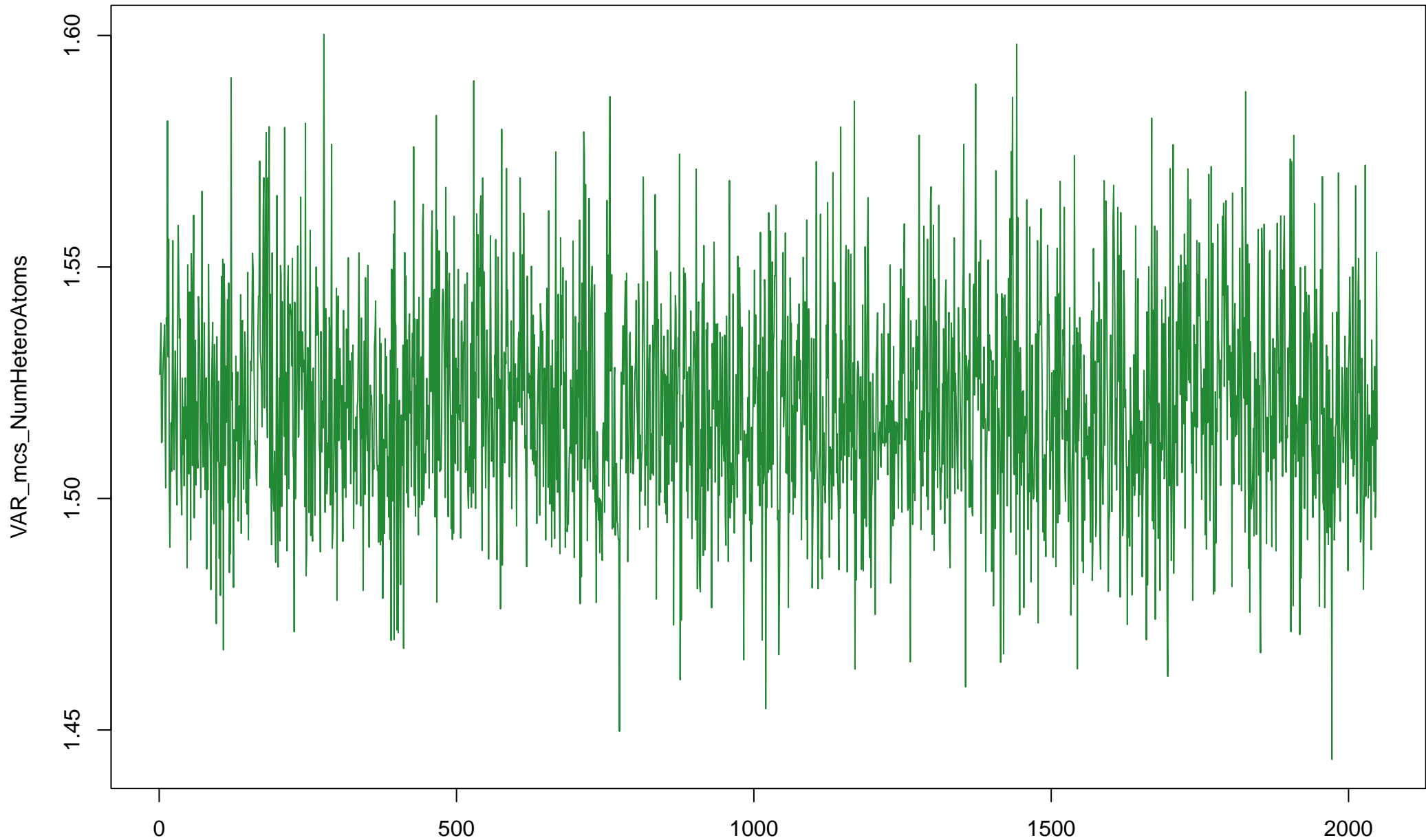
**VAR\_mcs\_docked\_NumHAcceptors**  
**ESS = 1710 | BMK = 0.0541 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0**



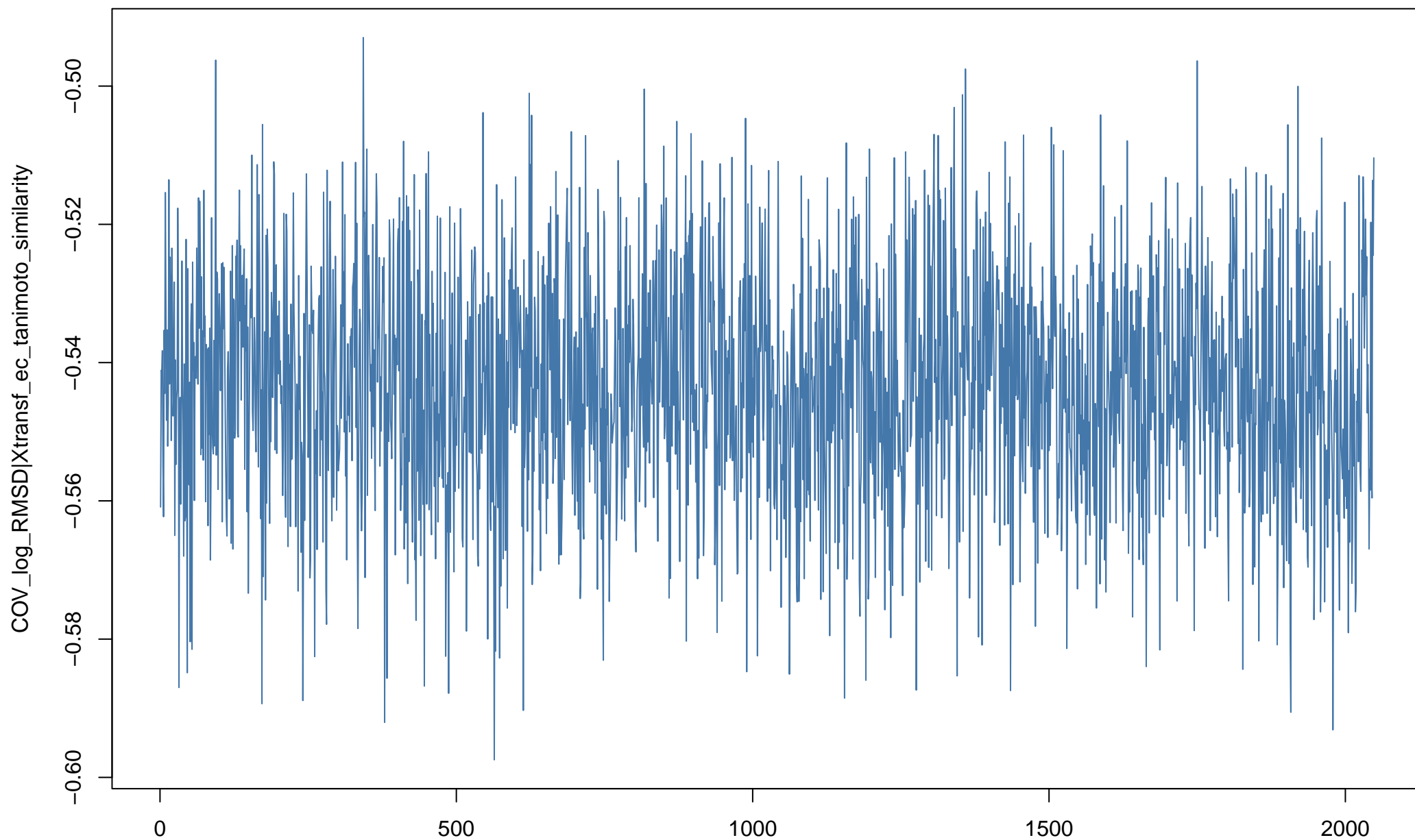
**VAR\_mcs\_template\_NumHAcceptors**  
**ESS = 1730 | BMK = 0.0402 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0**



**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 1800 | BMK = 0.0475 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0**

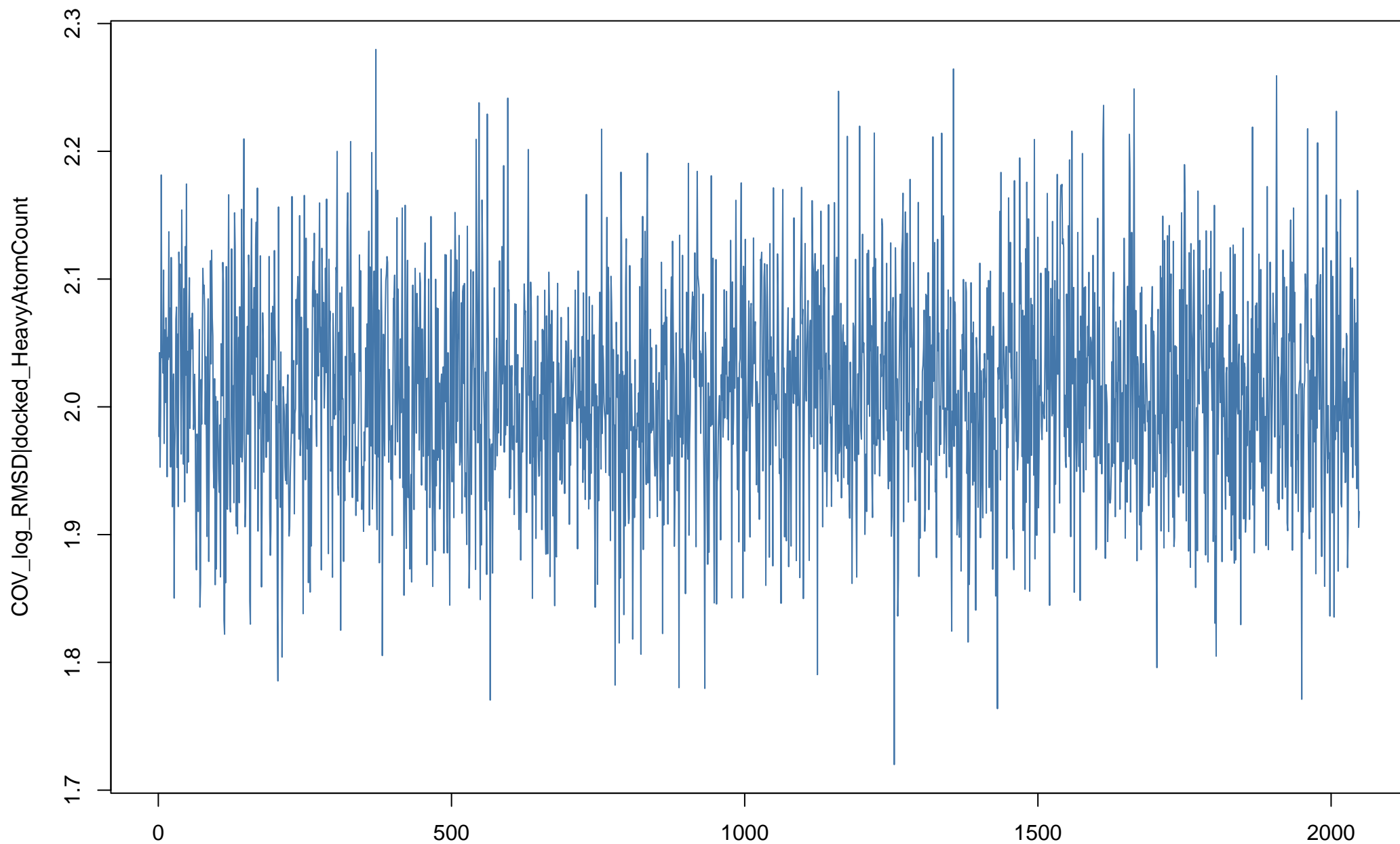


**COV\_log\_RMSD|Xtransf\_ec\_tanimoto\_similarity**  
**ESS = 1870 | BMK = 0.0396 | MCSE(6.27) = 2.86 | stat: FALSE | burn: 0**

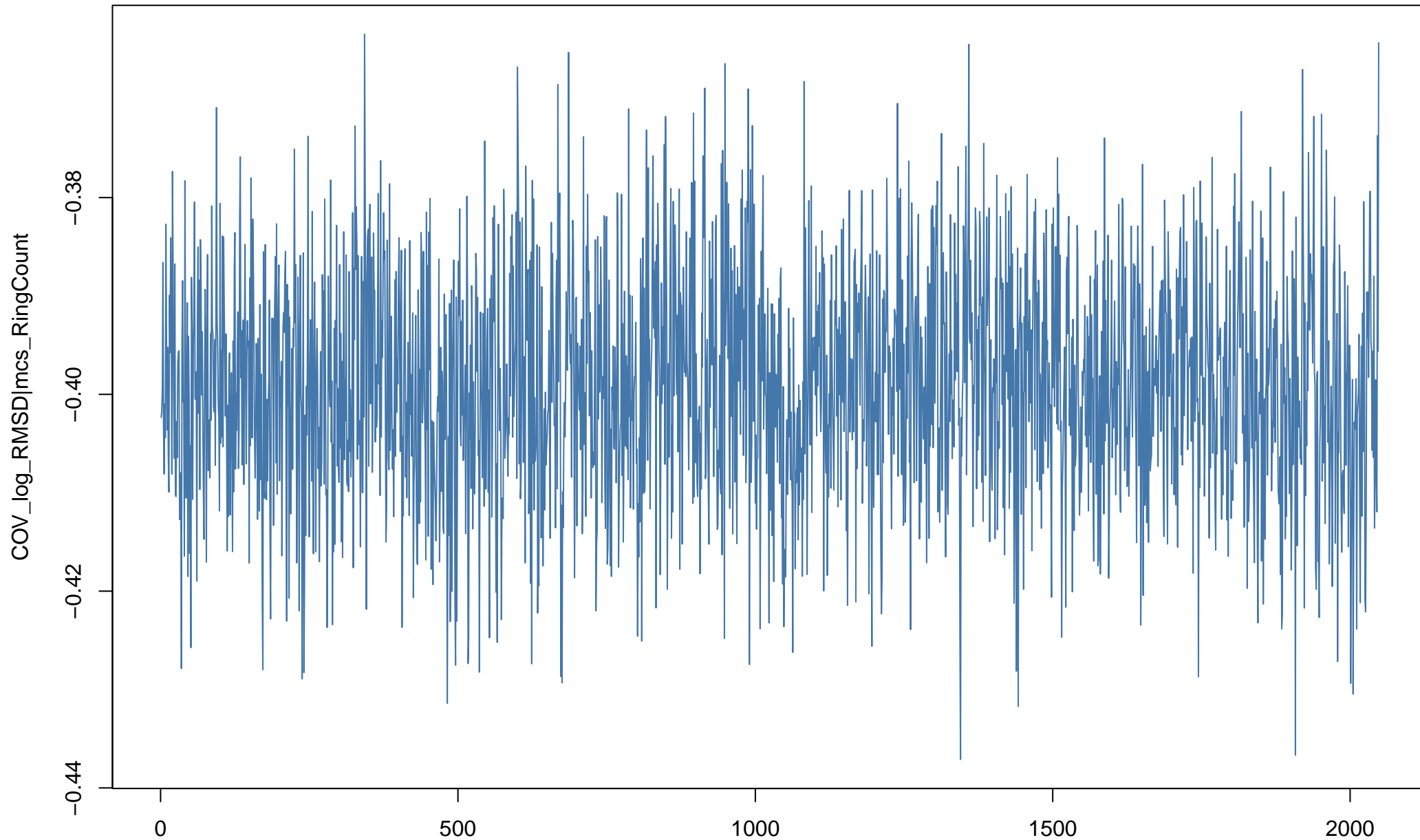




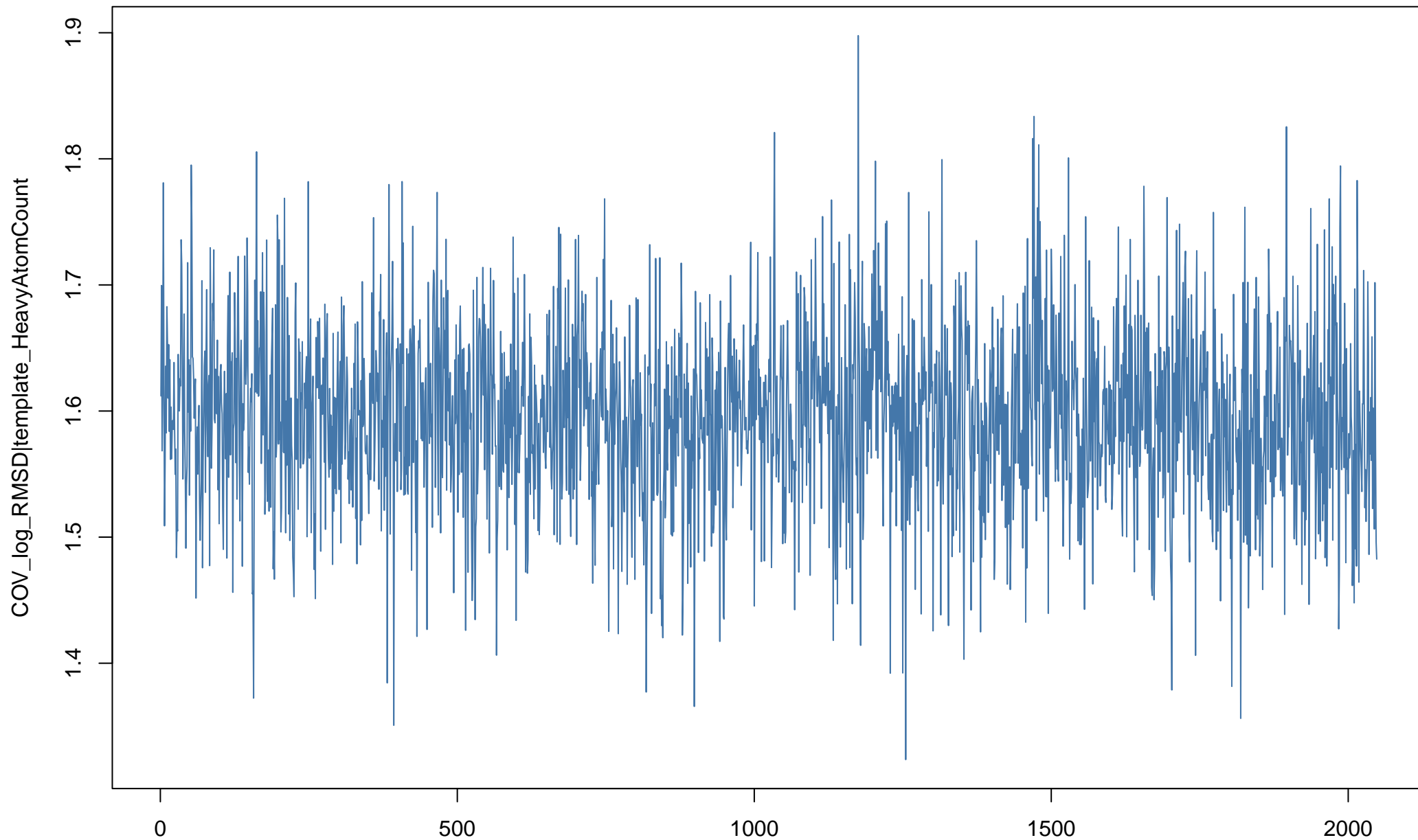
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0467 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0**



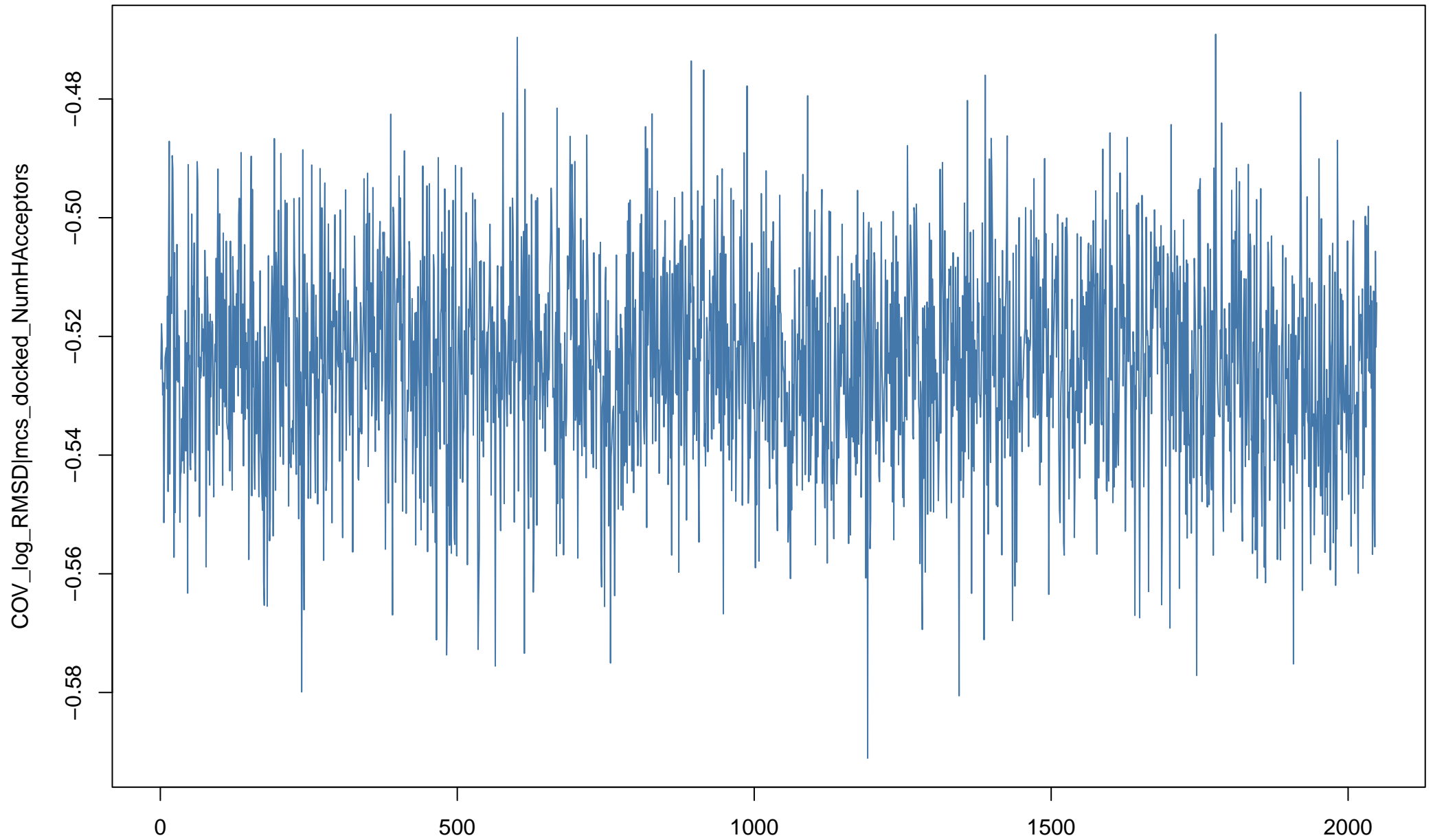
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 1520 | BMK = 0.0463 | MCSE(6.27) = 3.45 | stat: TRUE | burn: 0**



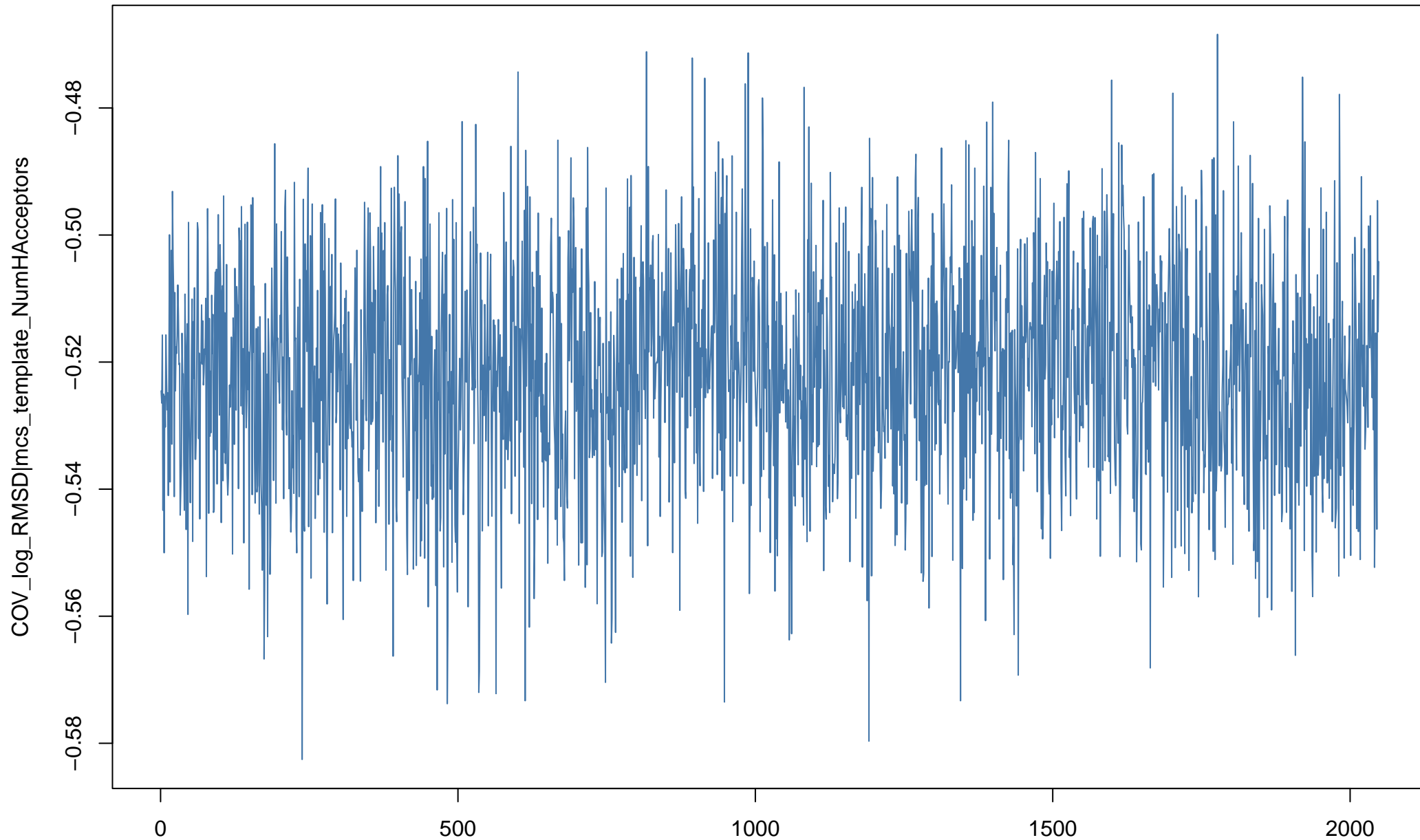
**COV\_log\_RMSD|template\_HeavyAtomCount**  
**ESS = 1520 | BMK = 0.054 | MCSE(6.27) = 3 | stat: TRUE | burn: 0**



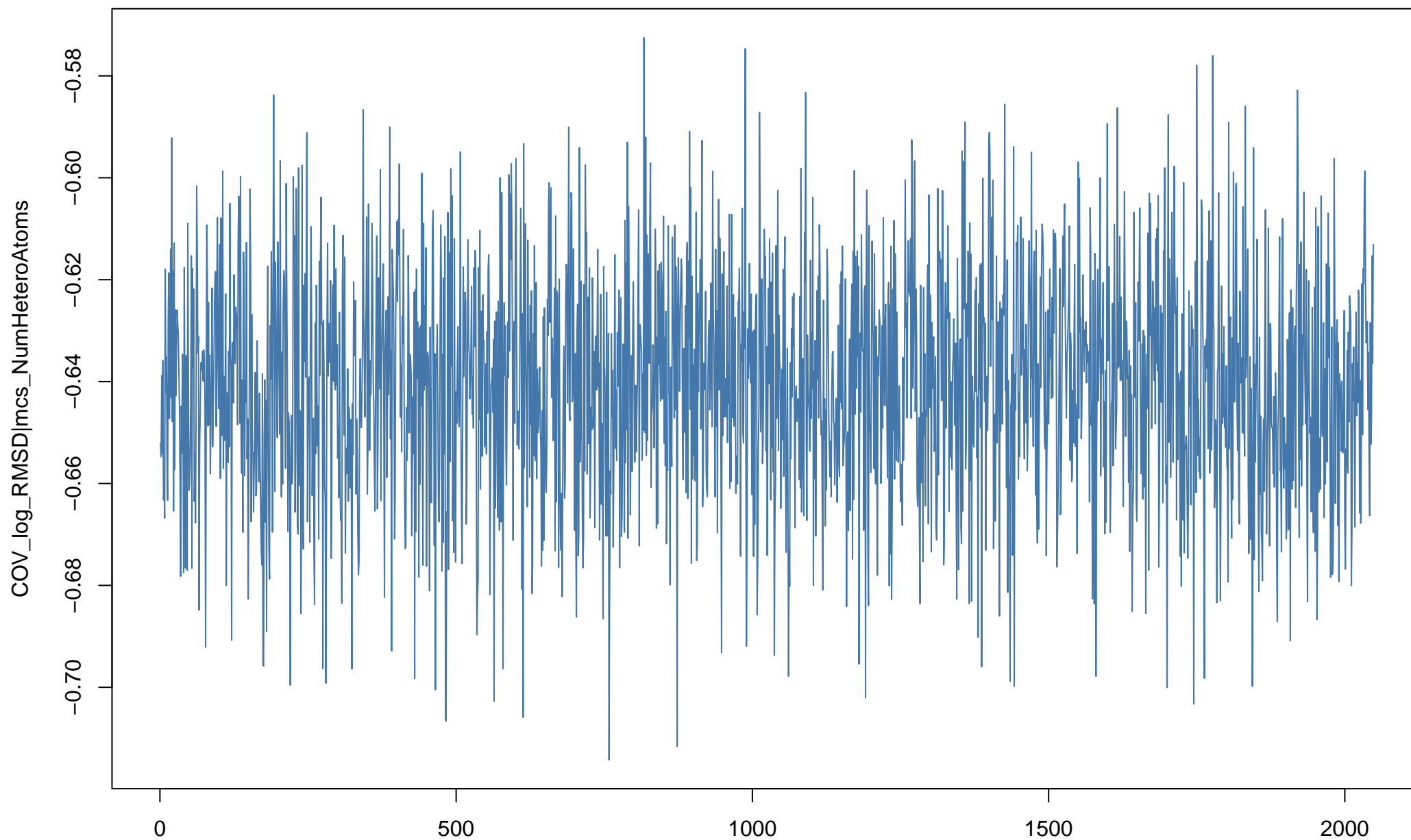
**COV\_log\_RMSD|mcs\_docked\_NumHAcceptors**  
**ESS = 1870 | BMK = 0.054 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0**



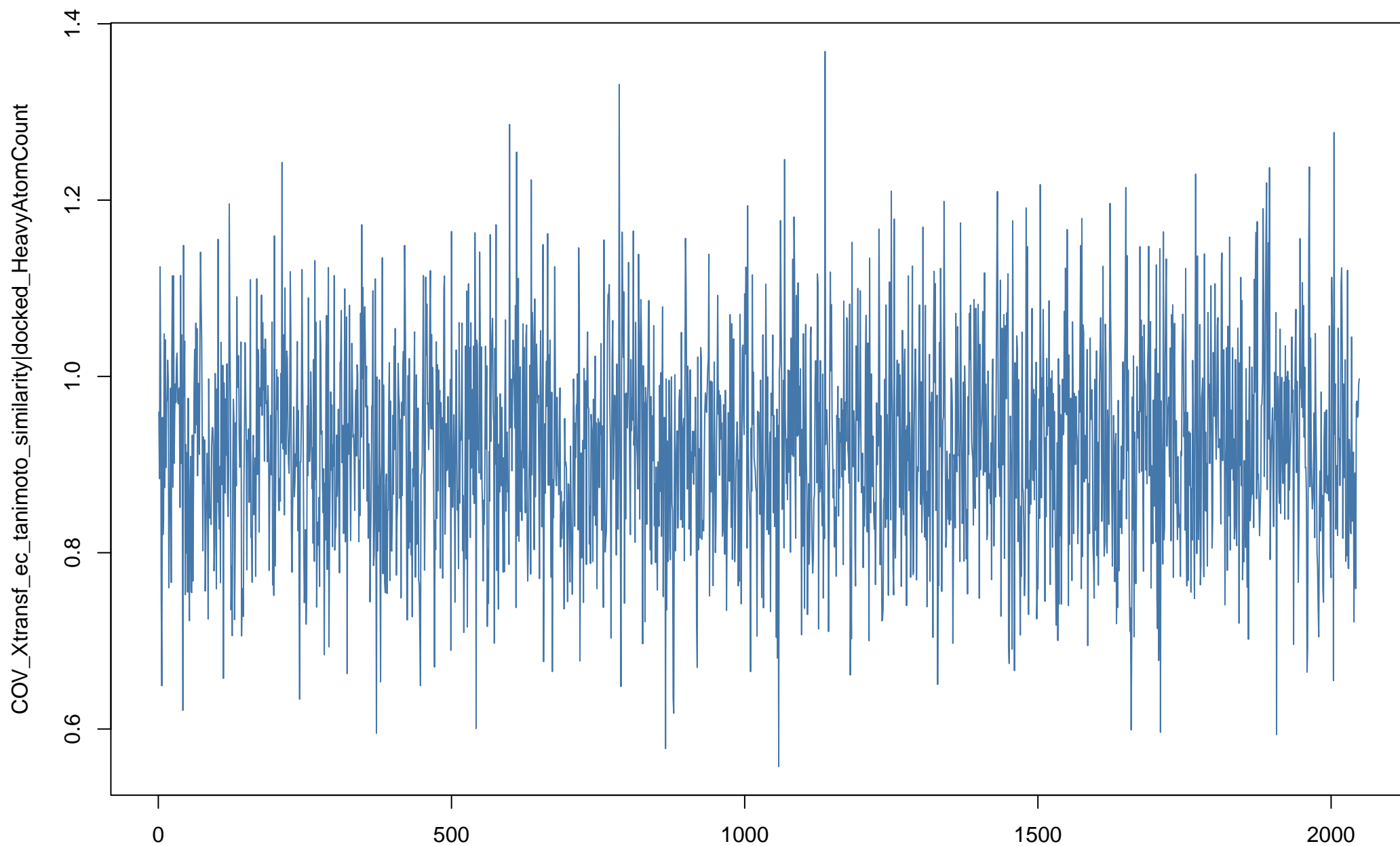
**COV\_log\_RMSD|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0459 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0**



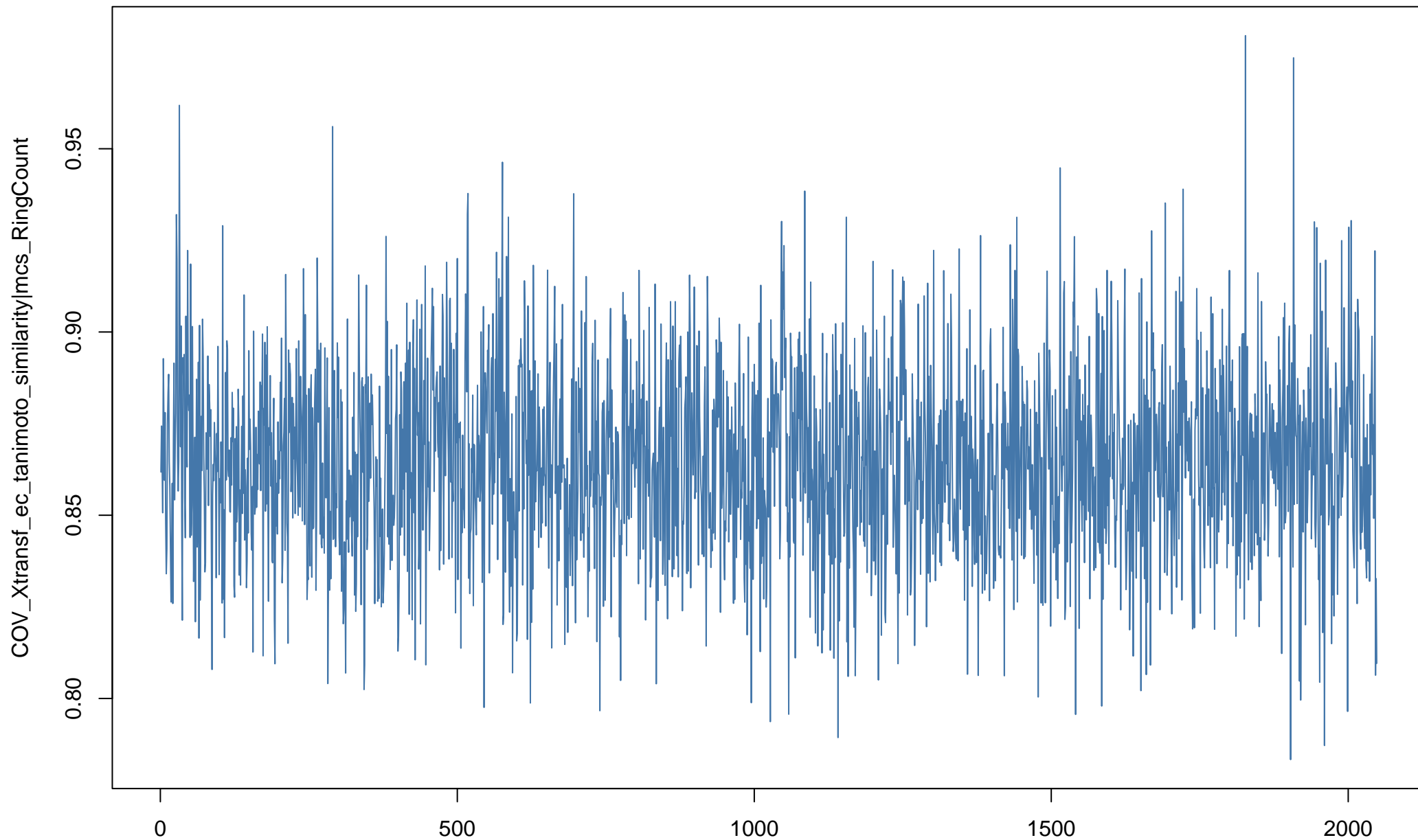
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 1750 | BMK = 0.0285 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0**



**COV\_Xtransf\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount**  
**ESS = 1650 | BMK = 0.0482 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0**

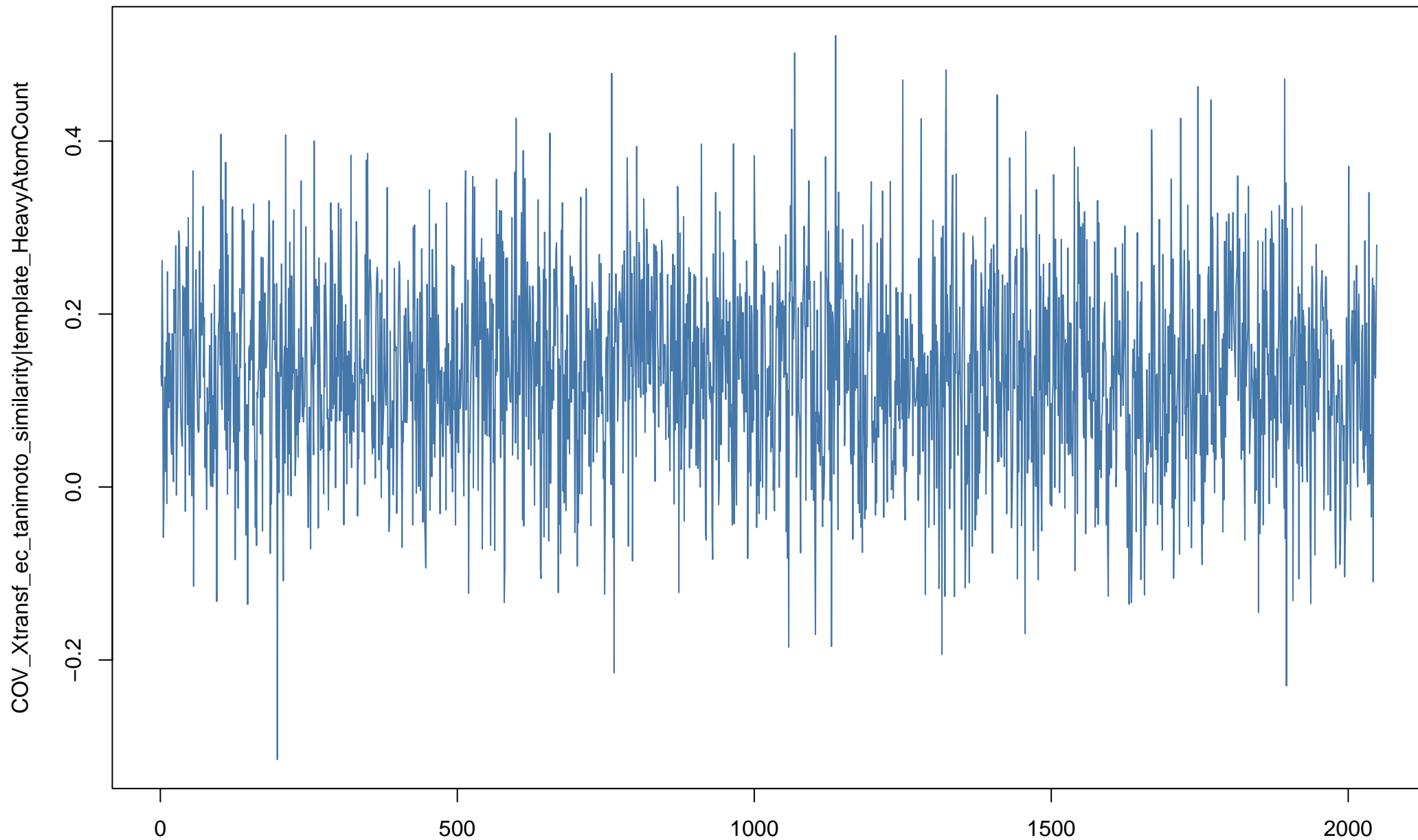


**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 2050 | BMK = 0.0529 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0**

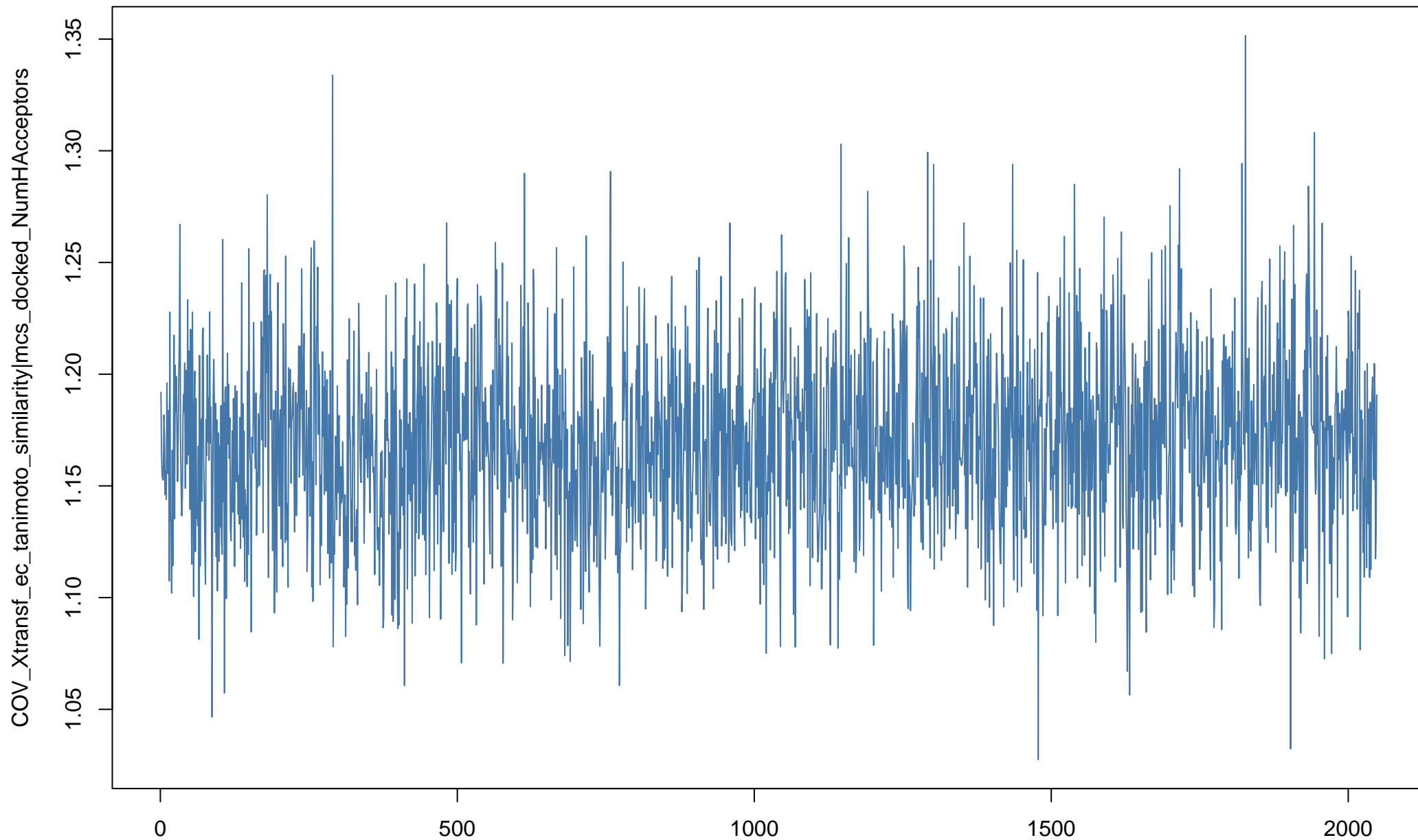




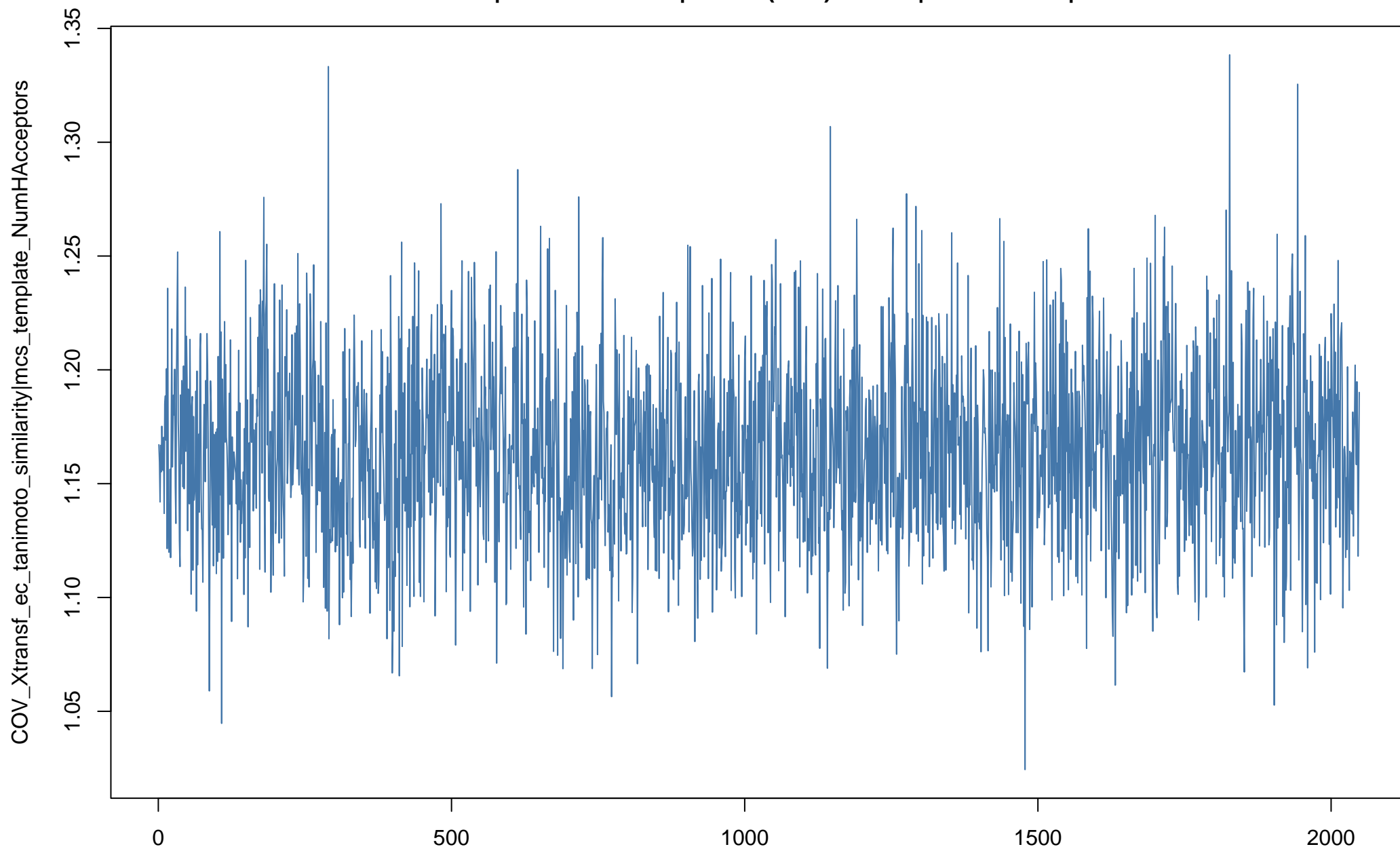
COV\_Xtransf\_ec\_tanimoto\_similarity|template\_HeavyAtomCount  
ESS = 1670 | BMK = 0.0659 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0



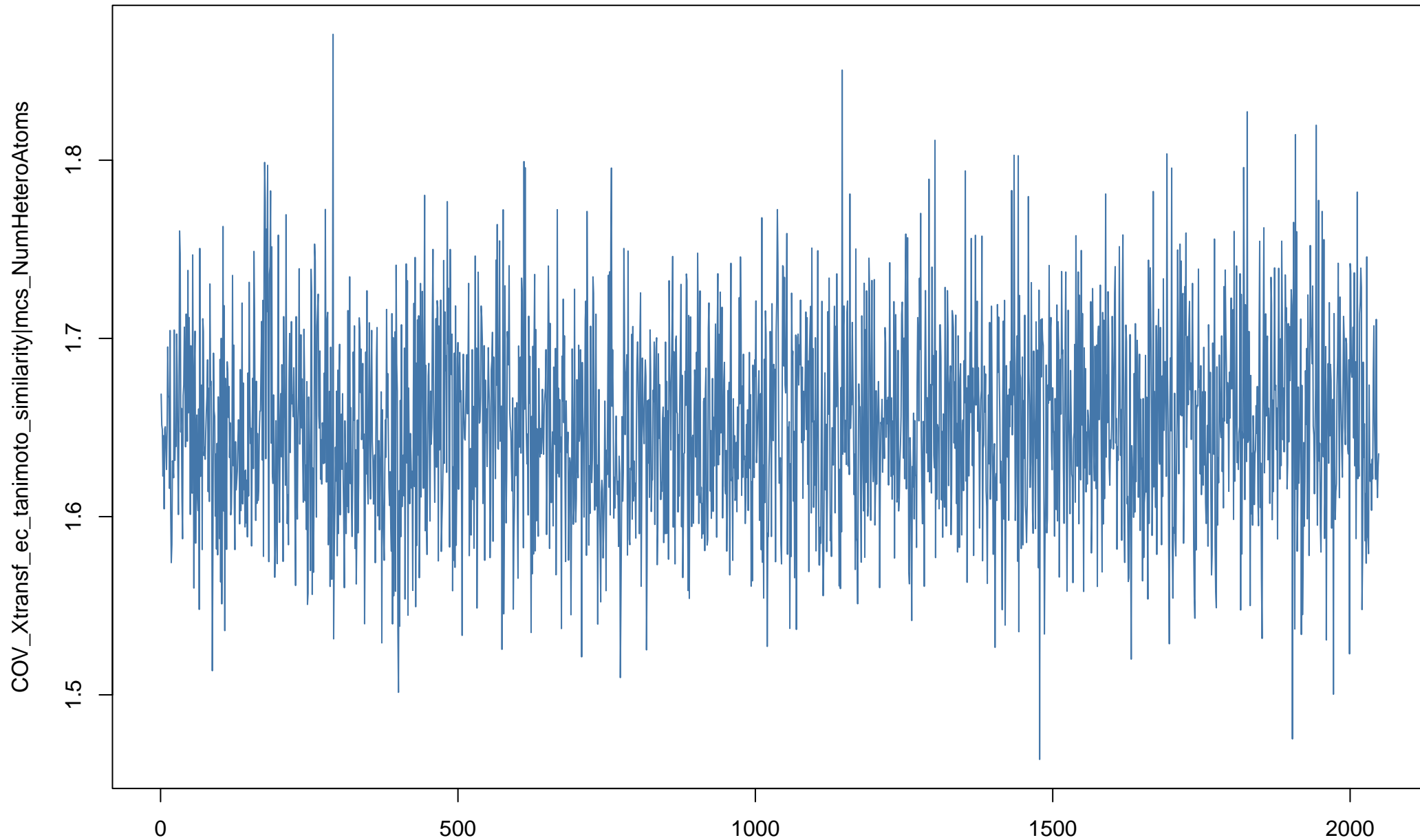
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.072 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0**



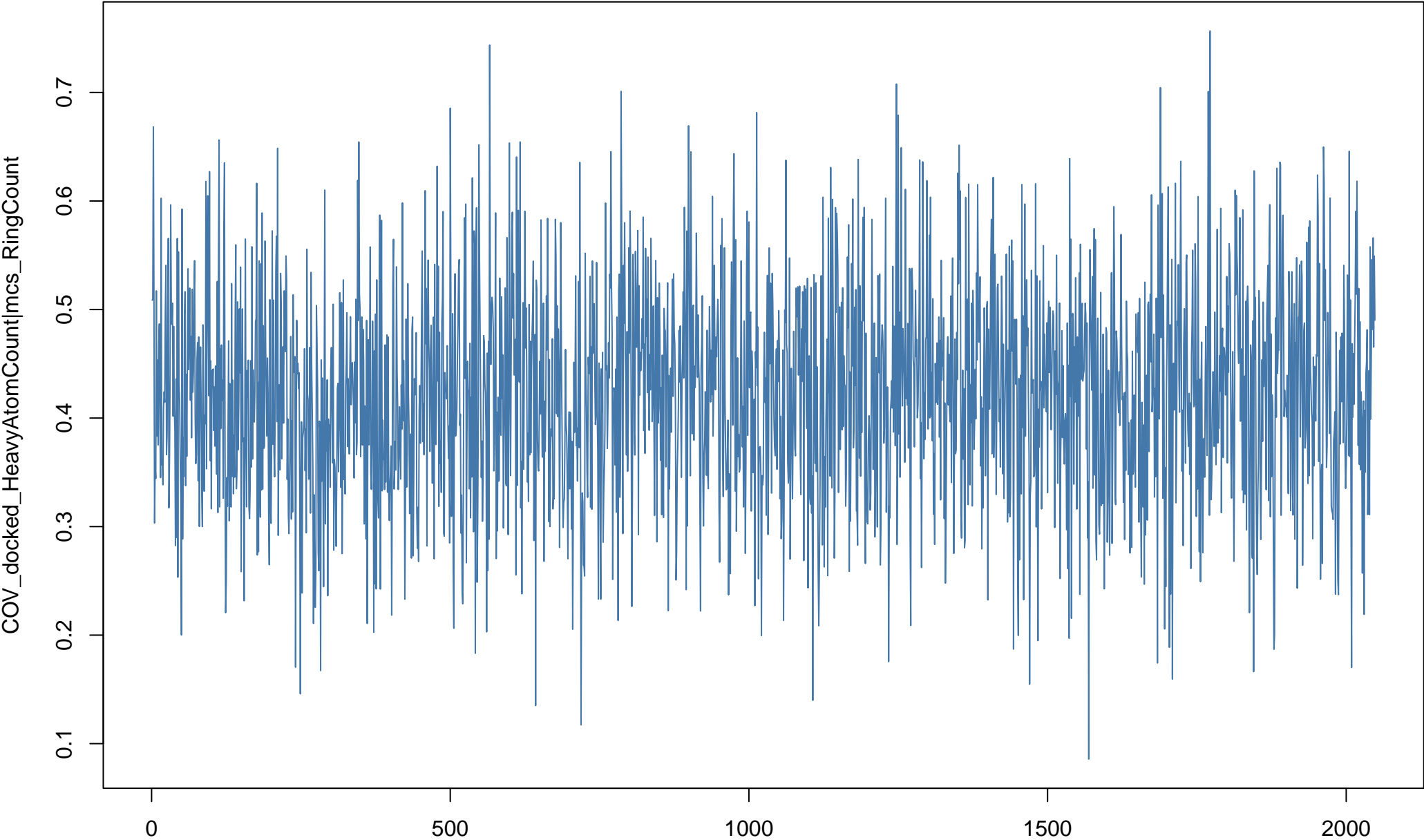
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0445 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0**



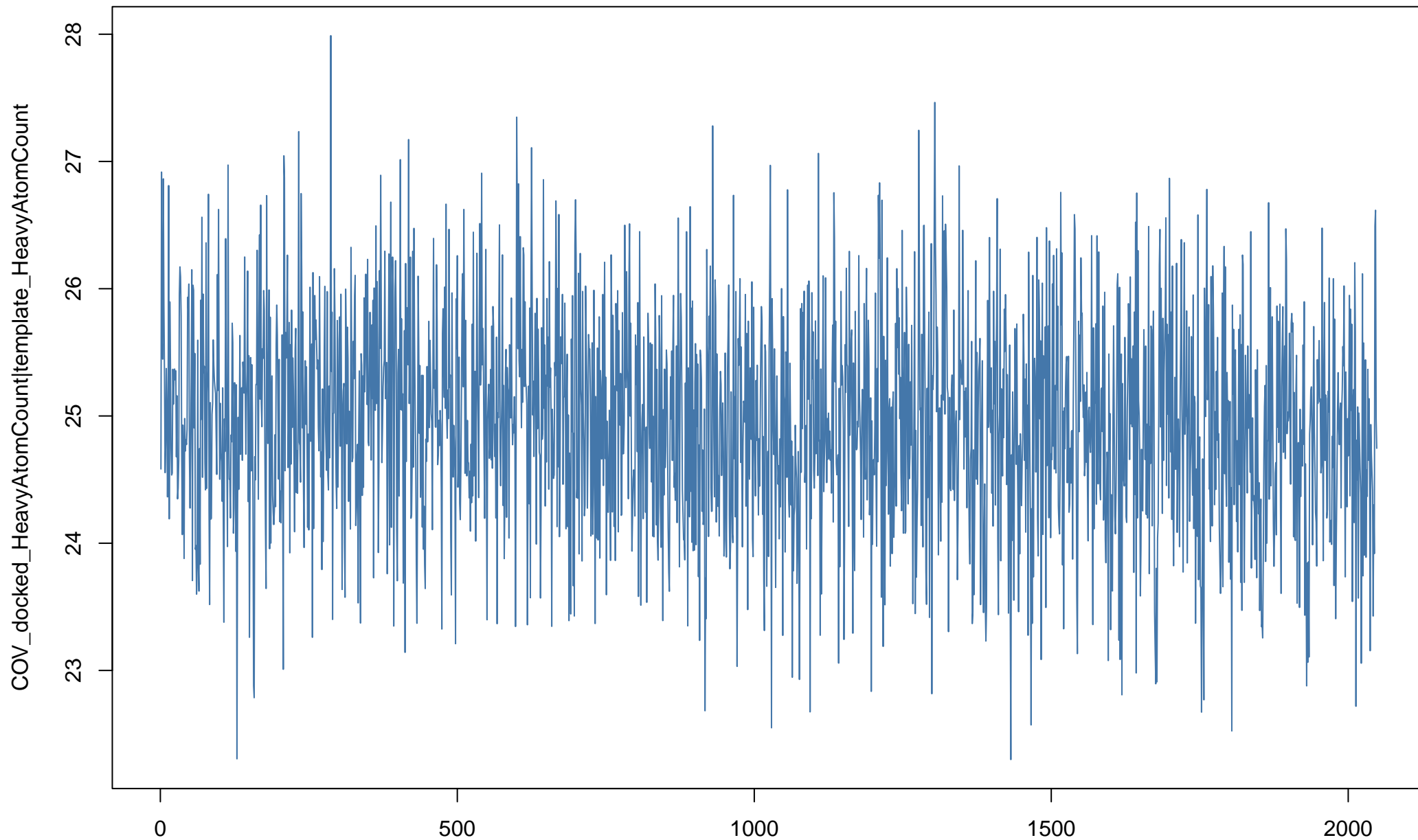
**COV\_Xtransf\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0641 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0**



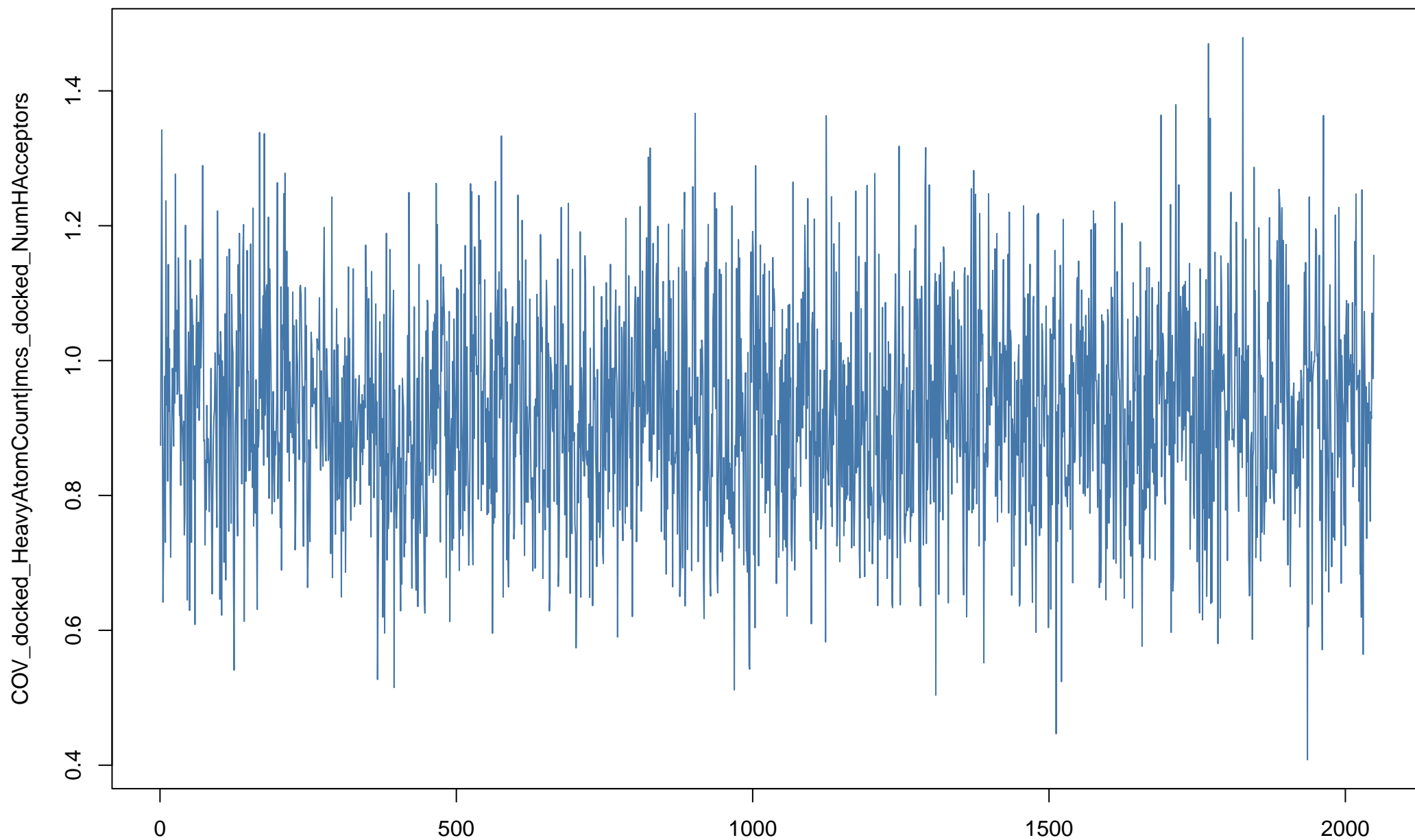
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 1790 | BMK = 0.0499 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0**



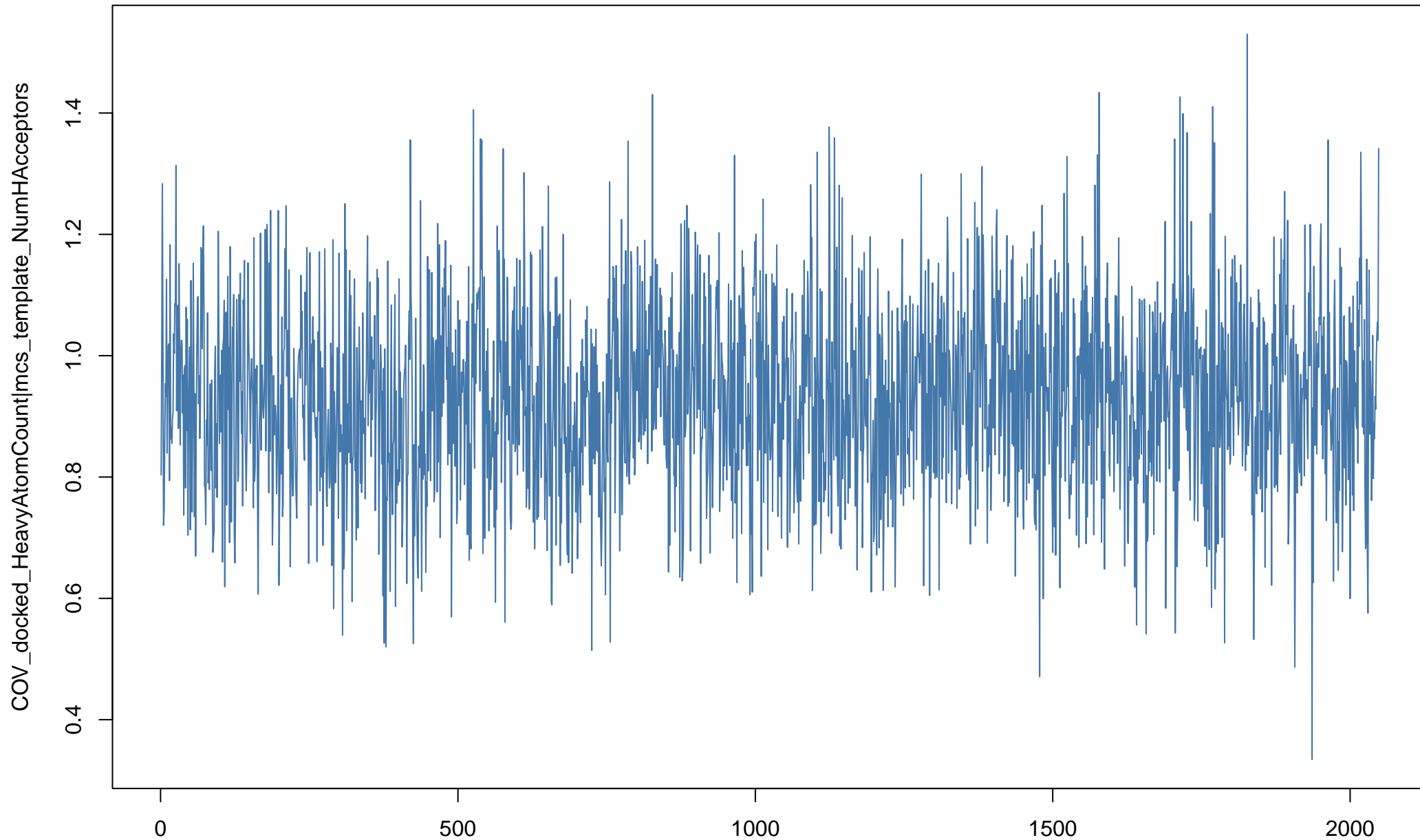
**COV\_docked\_HeavyAtomCount|template\_HeavyAtomCount**  
**ESS = 1470 | BMK = 0.0796 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0**



**COV\_docked\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 1740 | BMK = 0.038 | MCSE(6.27) = 2.67 | stat: TRUE | burn: 0**

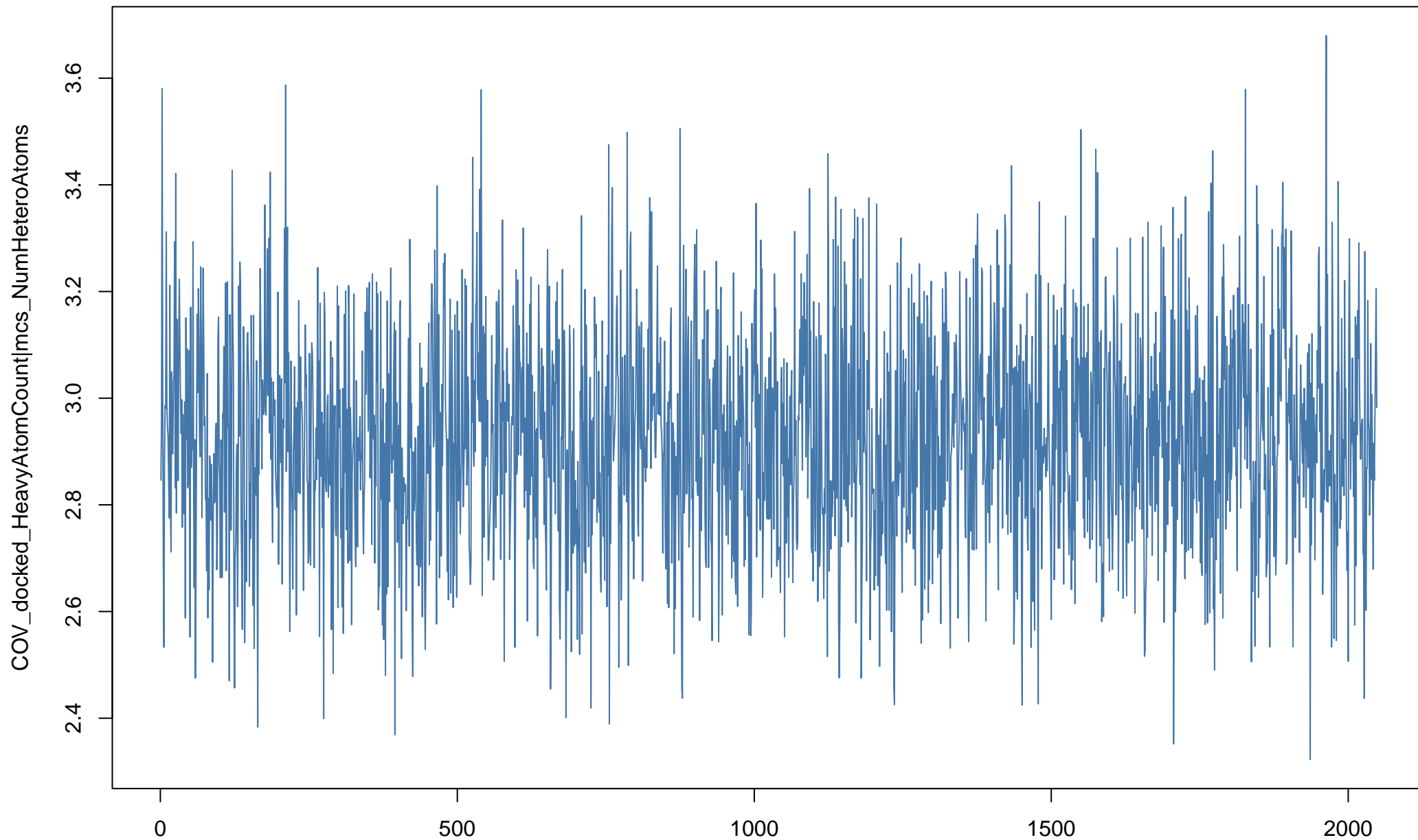


**COV\_docked\_HeavyAtomCount|mcs\_template\_NumHAcceptors**  
**ESS = 1870 | BMK = 0.0453 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0**

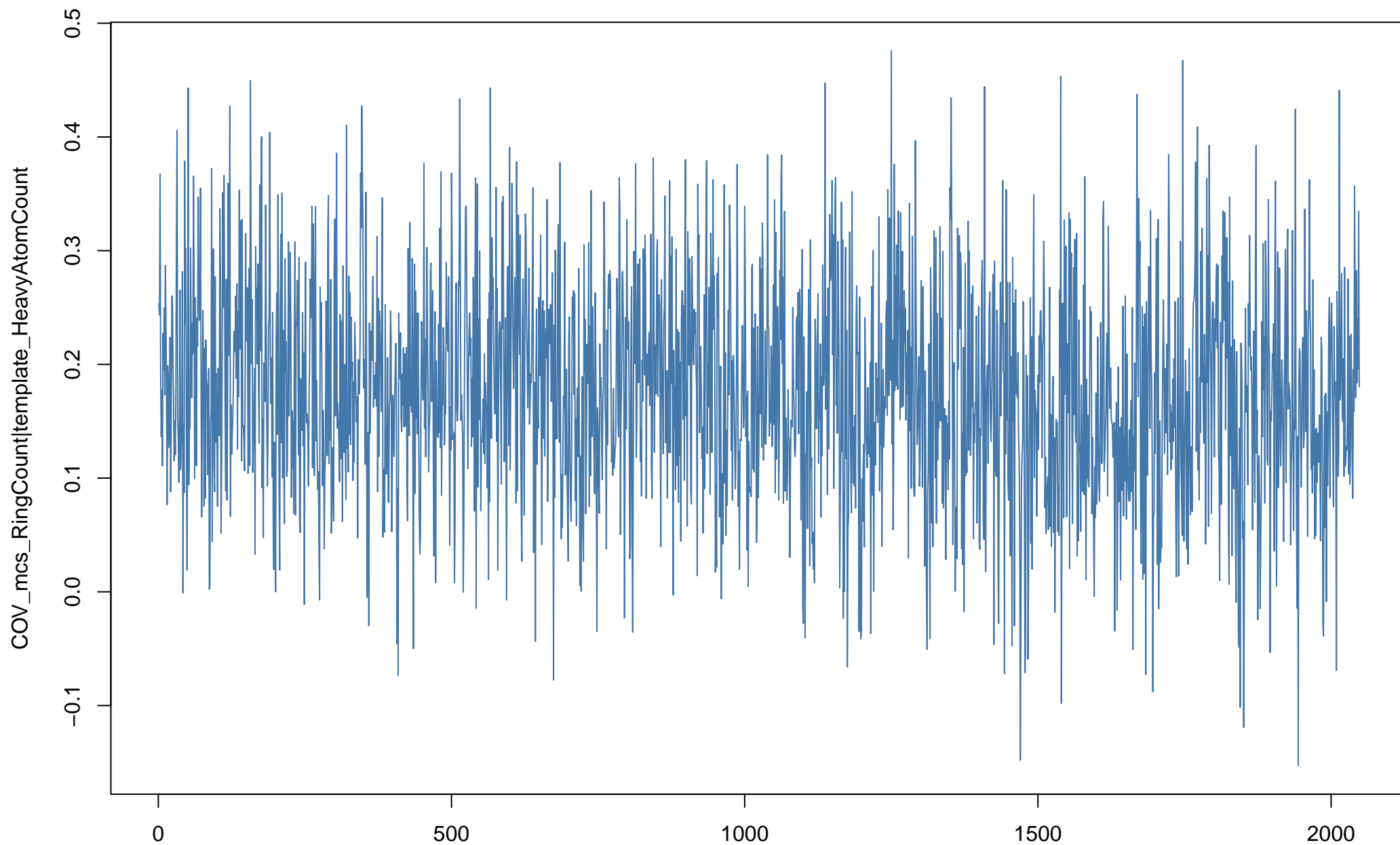




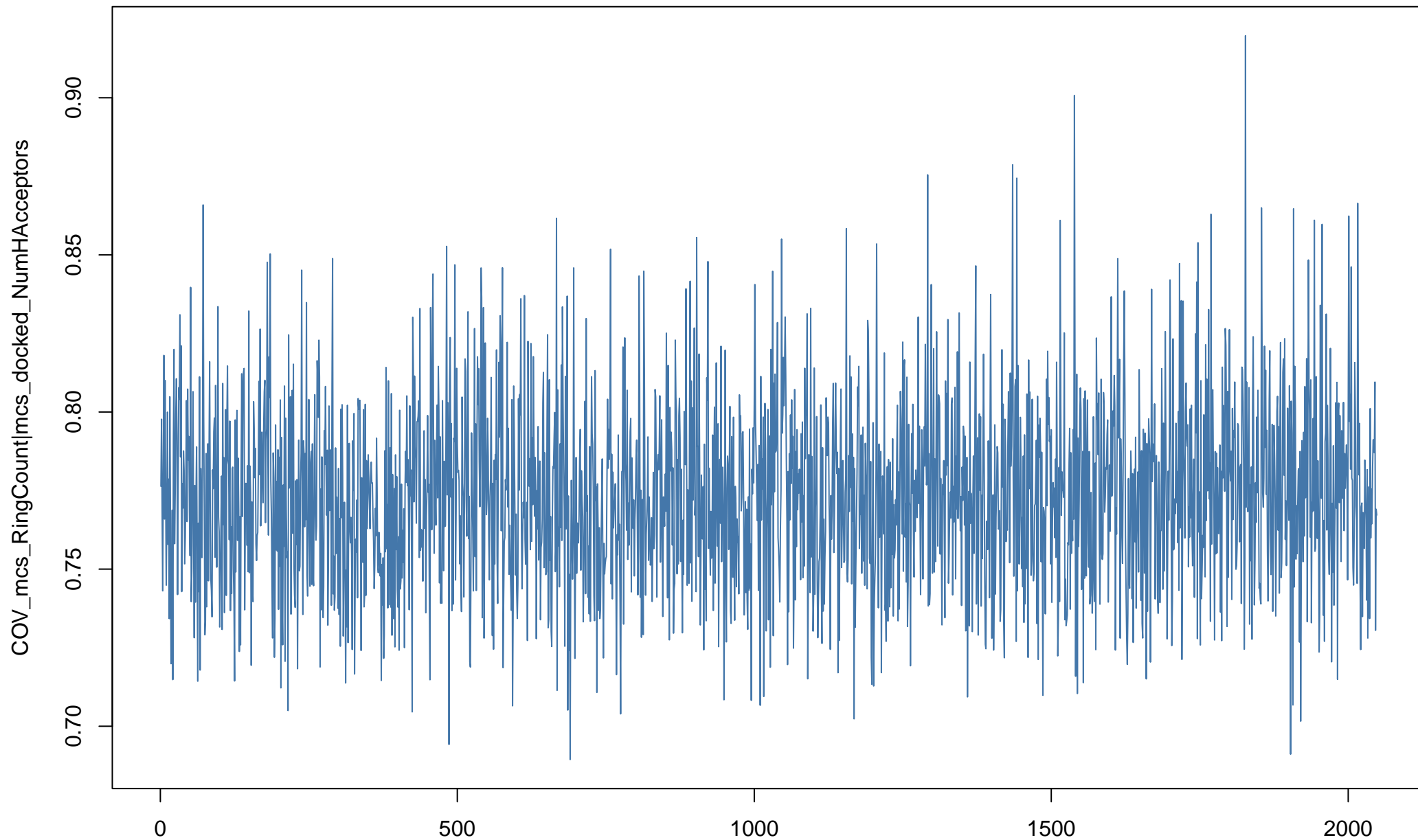
**COV\_docked\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 1730 | BMK = 0.0462 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0**



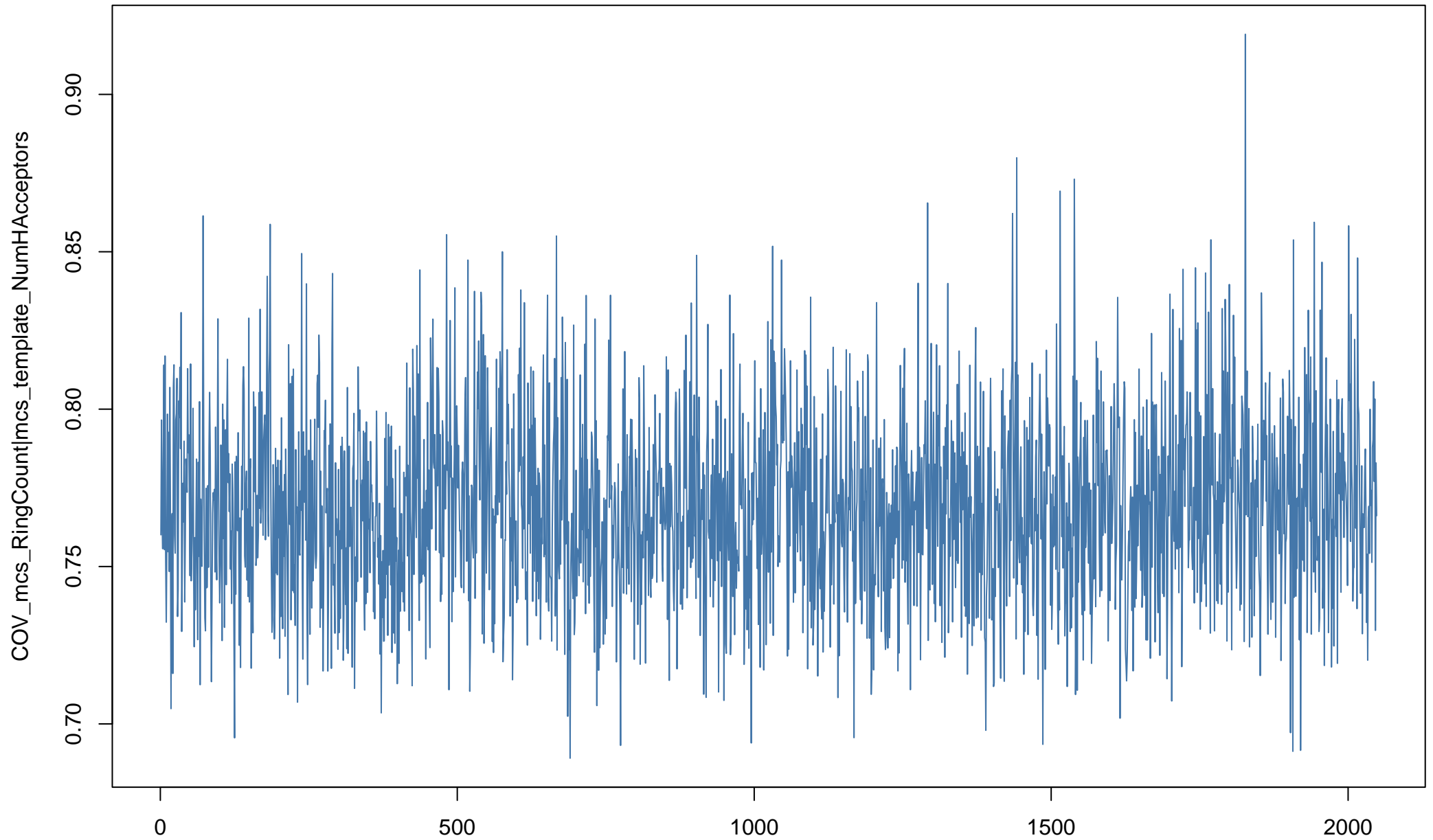
**COV\_mcs\_RingCount|template\_HeavyAtomCount**  
**ESS = 802 | BMK = 0.0915 | MCSE(6.27) = 3.45 | stat: FALSE | burn: 0**



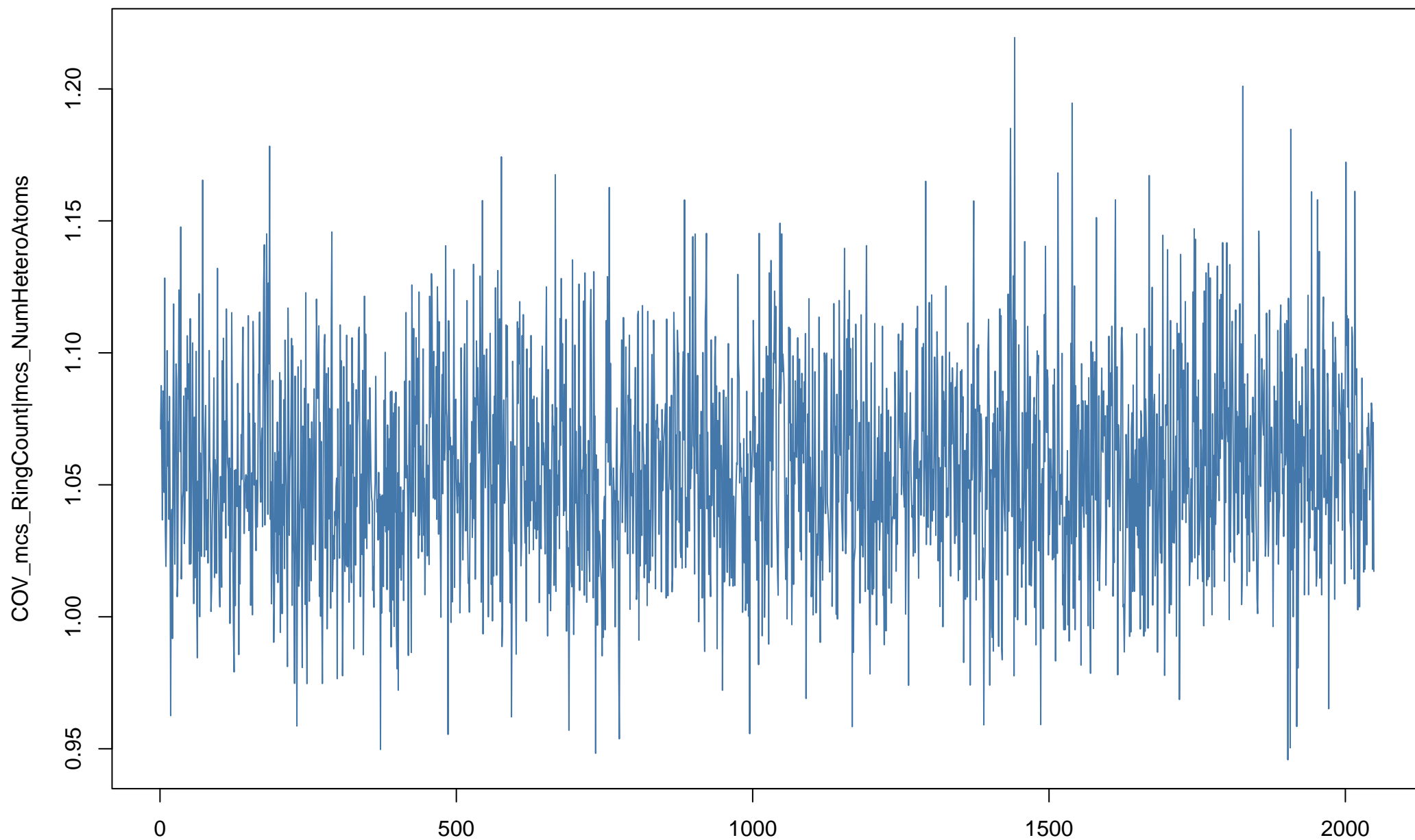
**COV\_mcs\_RingCount|mcs\_docked\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.0636 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0**



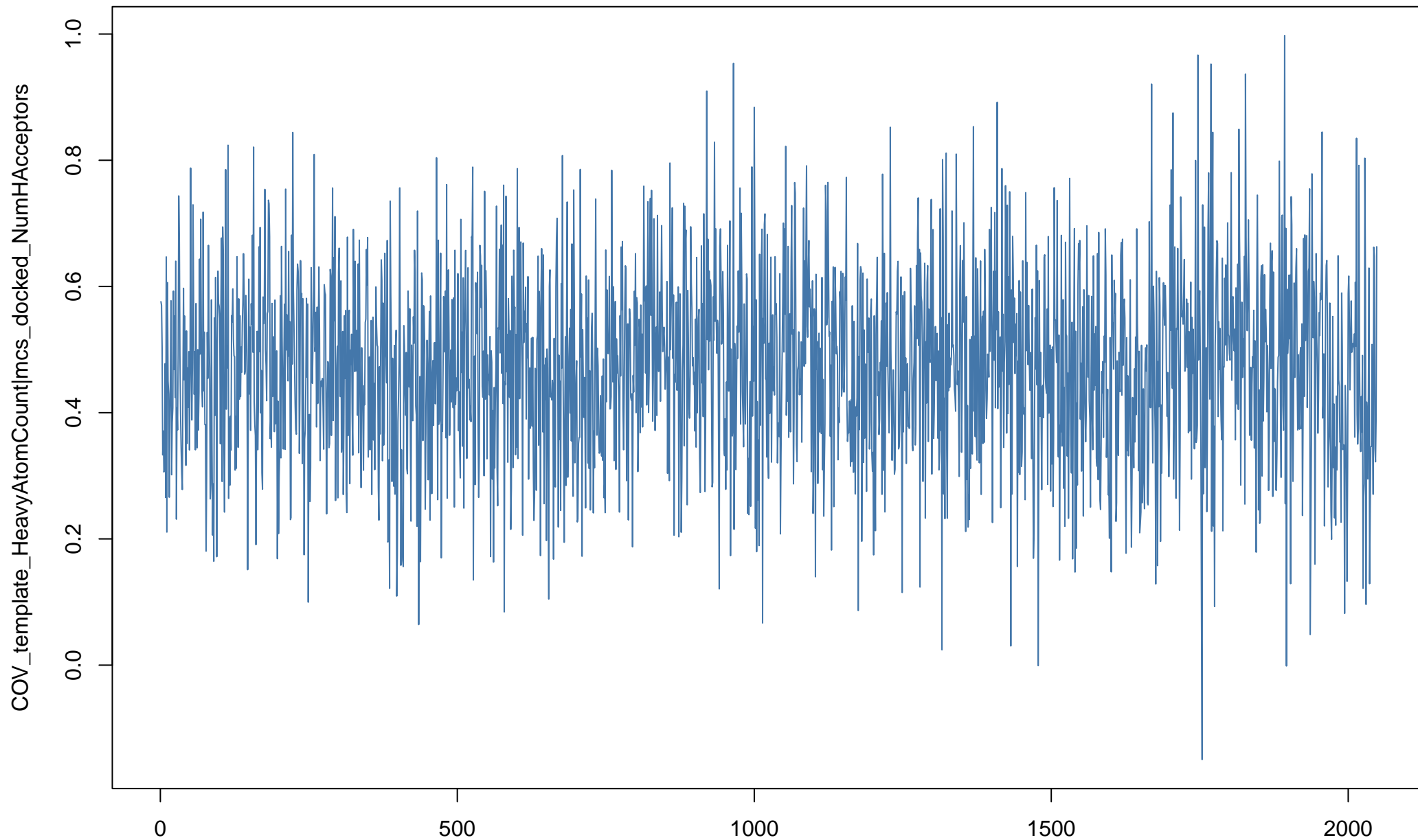
**COV\_mcs\_RingCount|mcs\_template\_NumHAcceptors**  
**ESS = 2050 | BMK = 0.052 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0**



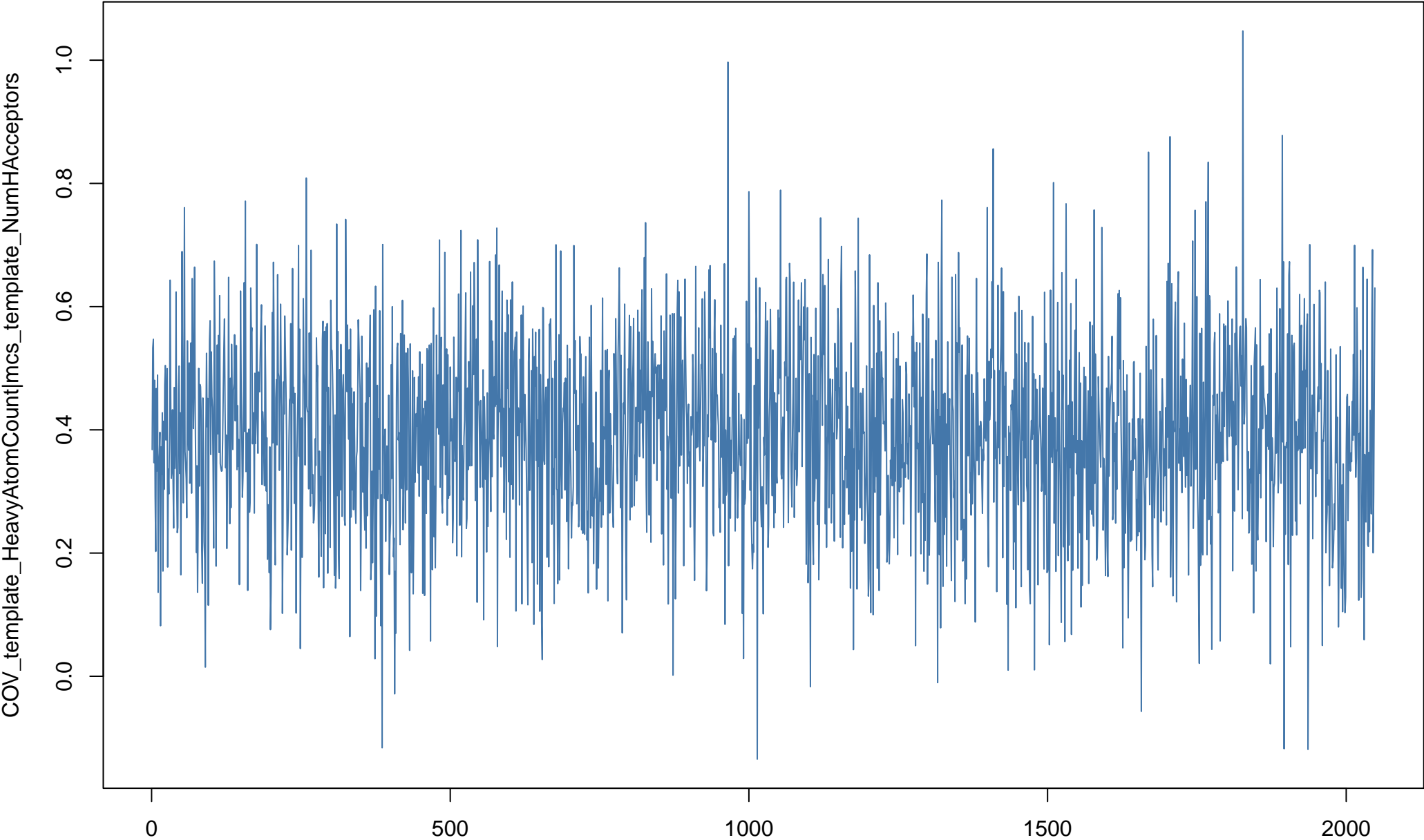
**COV\_mcs\_RingCount|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0541 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0**



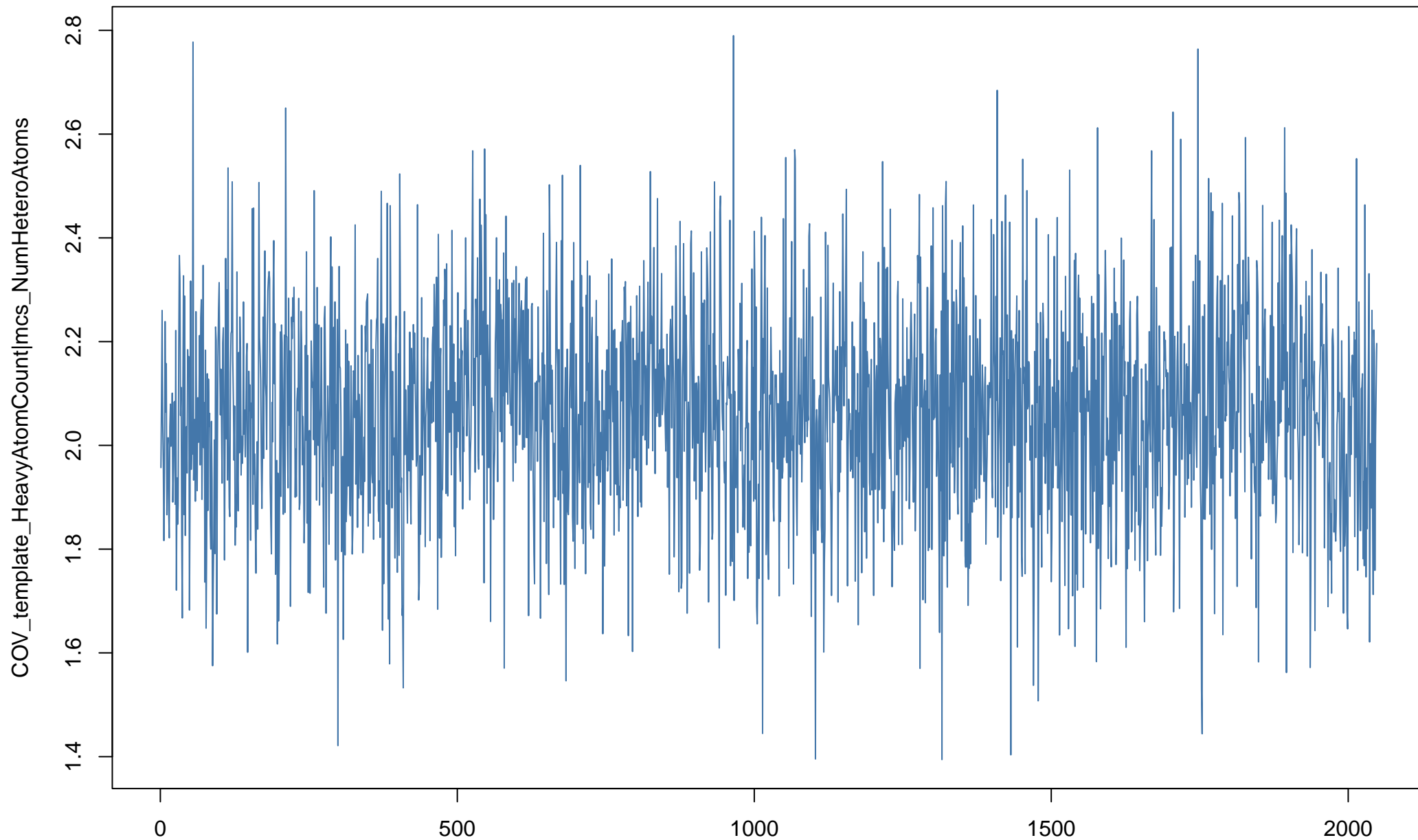
**COV\_template\_HeavyAtomCount|mcs\_docked\_NumHAcceptors**  
**ESS = 1880 | BMK = 0.0487 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0**



COV\_template\_HeavyAtomCount|mcs\_template\_NumHAcceptors  
ESS = 2050 | BMK = 0.0584 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0

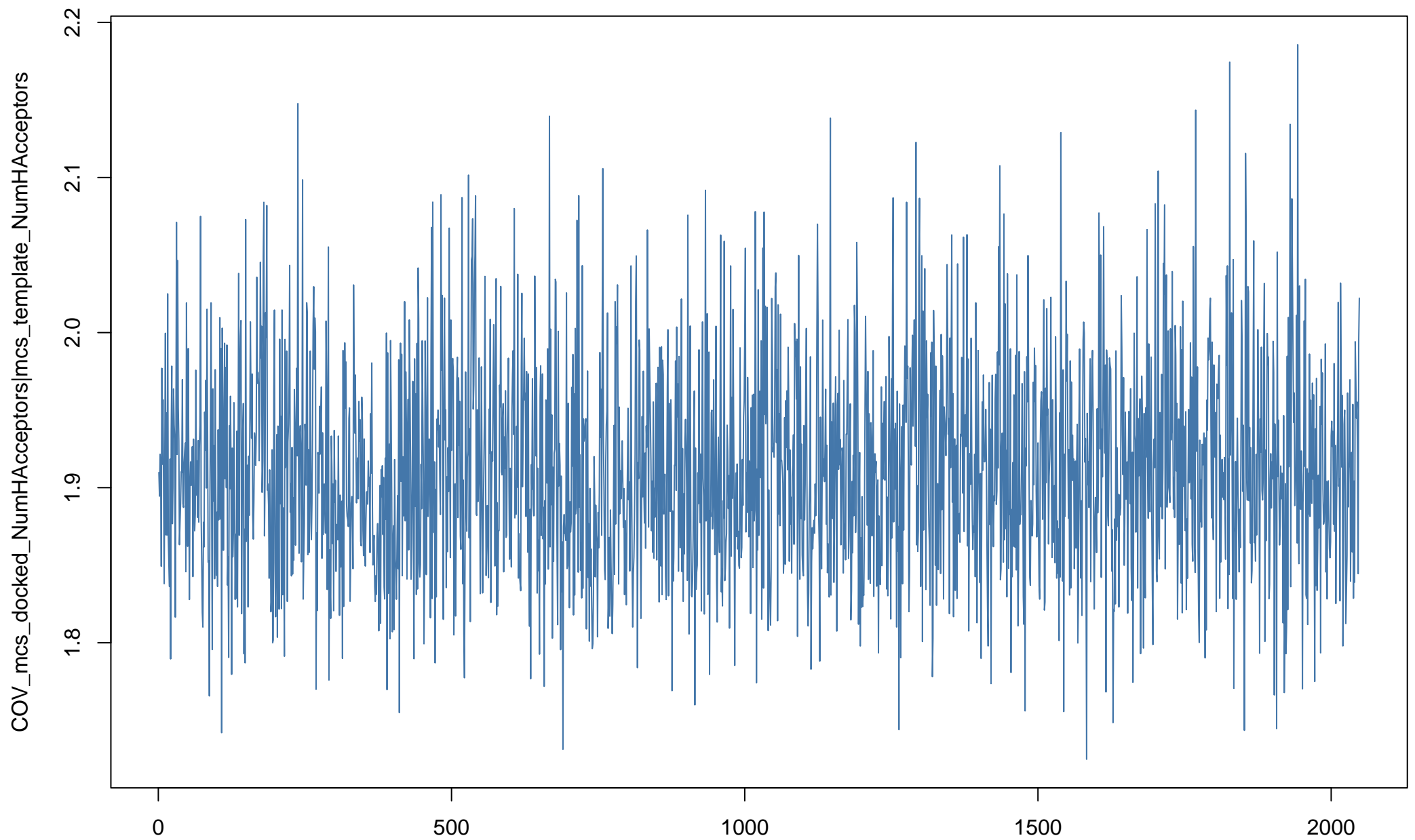


**COV\_template\_HeavyAtomCount|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0431 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0**

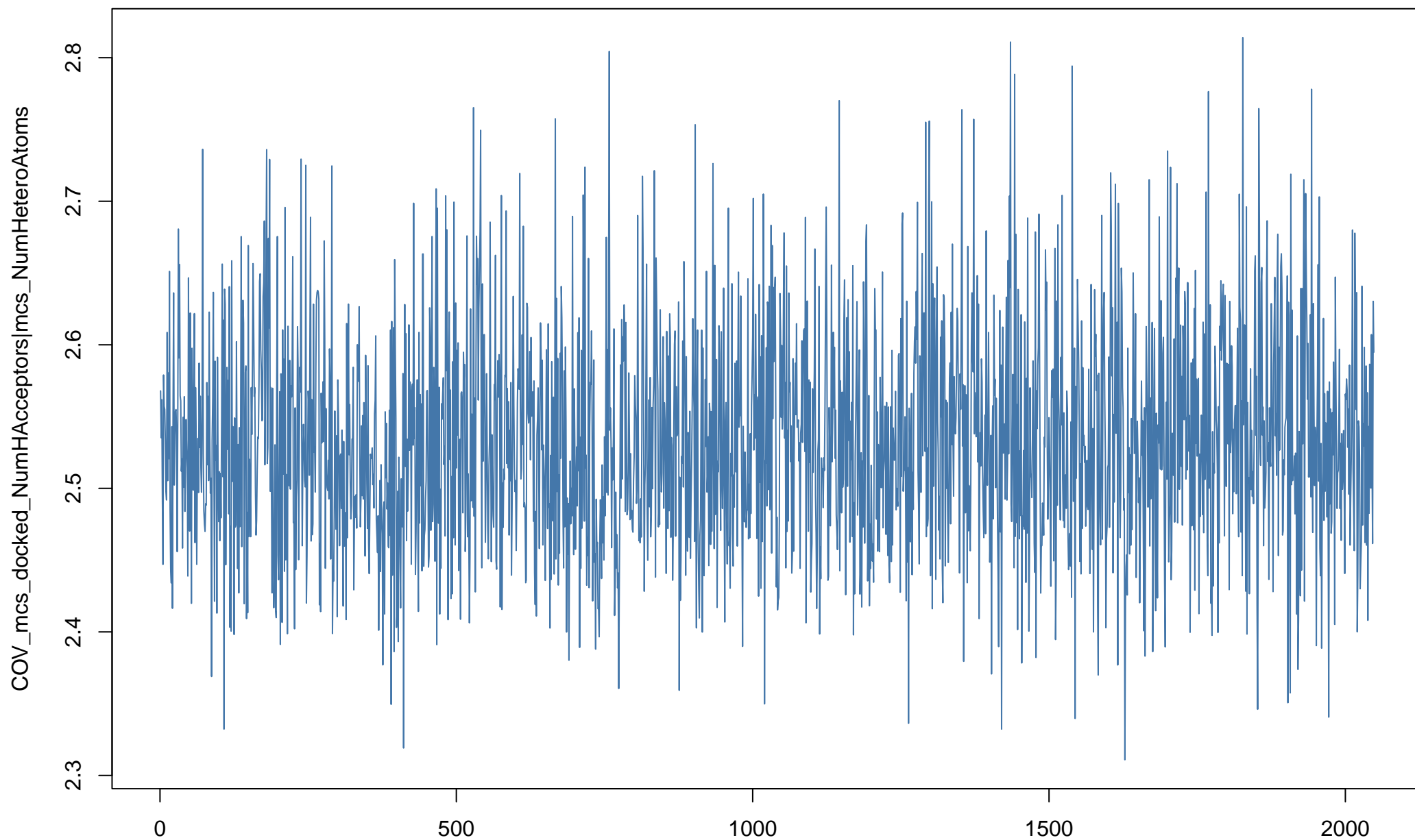




**COV\_mcs\_docked\_NumHAcceptors|mcs\_template\_NumHAcceptors**  
**ESS = 1710 | BMK = 0.0501 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0**



**COV\_mcs\_docked\_NumHAcceptors|mcs\_NumHeteroAtoms**  
**ESS = 1720 | BMK = 0.0626 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0**



**COV\_mcs\_template\_NumHAcceptors|mcs\_NumHeteroAtoms**  
**ESS = 1740 | BMK = 0.0526 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0**

