

-- STATS maxD --

min ESS = 34.6741684315747

max BMK = 0.248060967145648

max MCSE = 9.60384498868575

all stationary: FALSE

burn: 0

max rel.err.: 2.00543309742939

-- STATS 2D --

min ESS = 1743.88787429342

max BMK = 0.0603247304129974

max MCSE = 2.59175713787968

all stationary: TRUE

burn: 0

max rel.err.: 1.77001028802712

-- STATS 1D --

min ESS = 1494.42321337791

max BMK = 0.0835000099520056

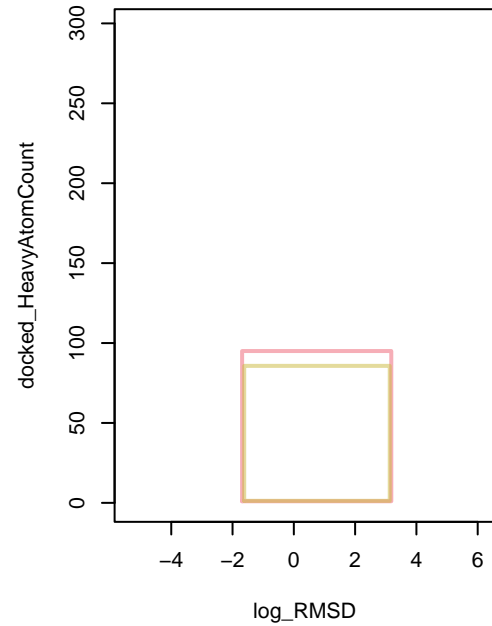
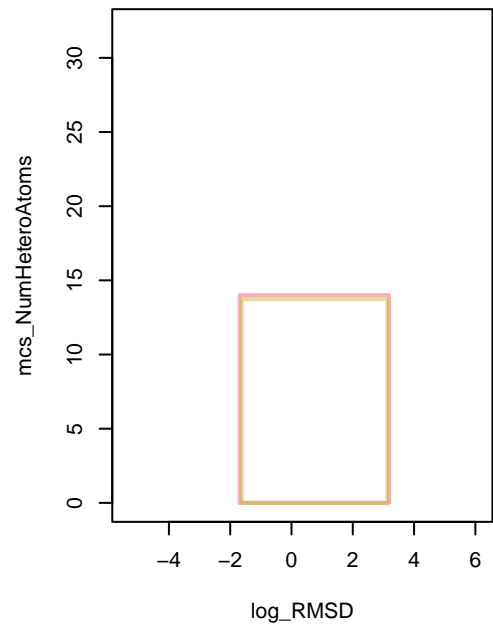
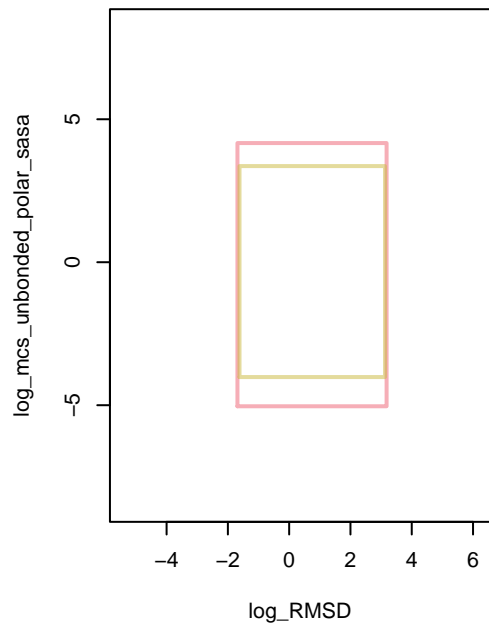
max MCSE = 3.06704602288849

all stationary: FALSE

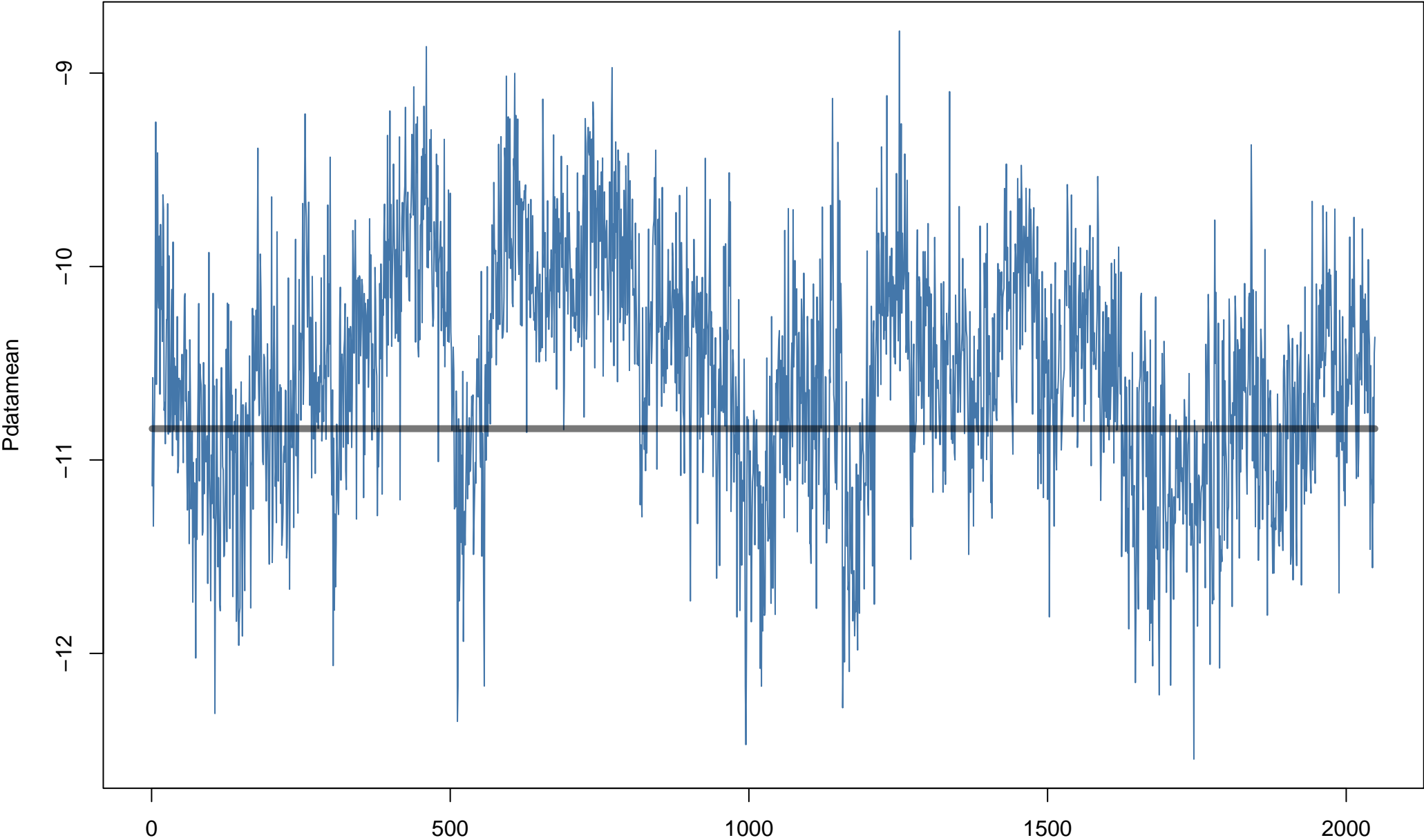
burn: 0

max rel.err.: 2.29372129484307

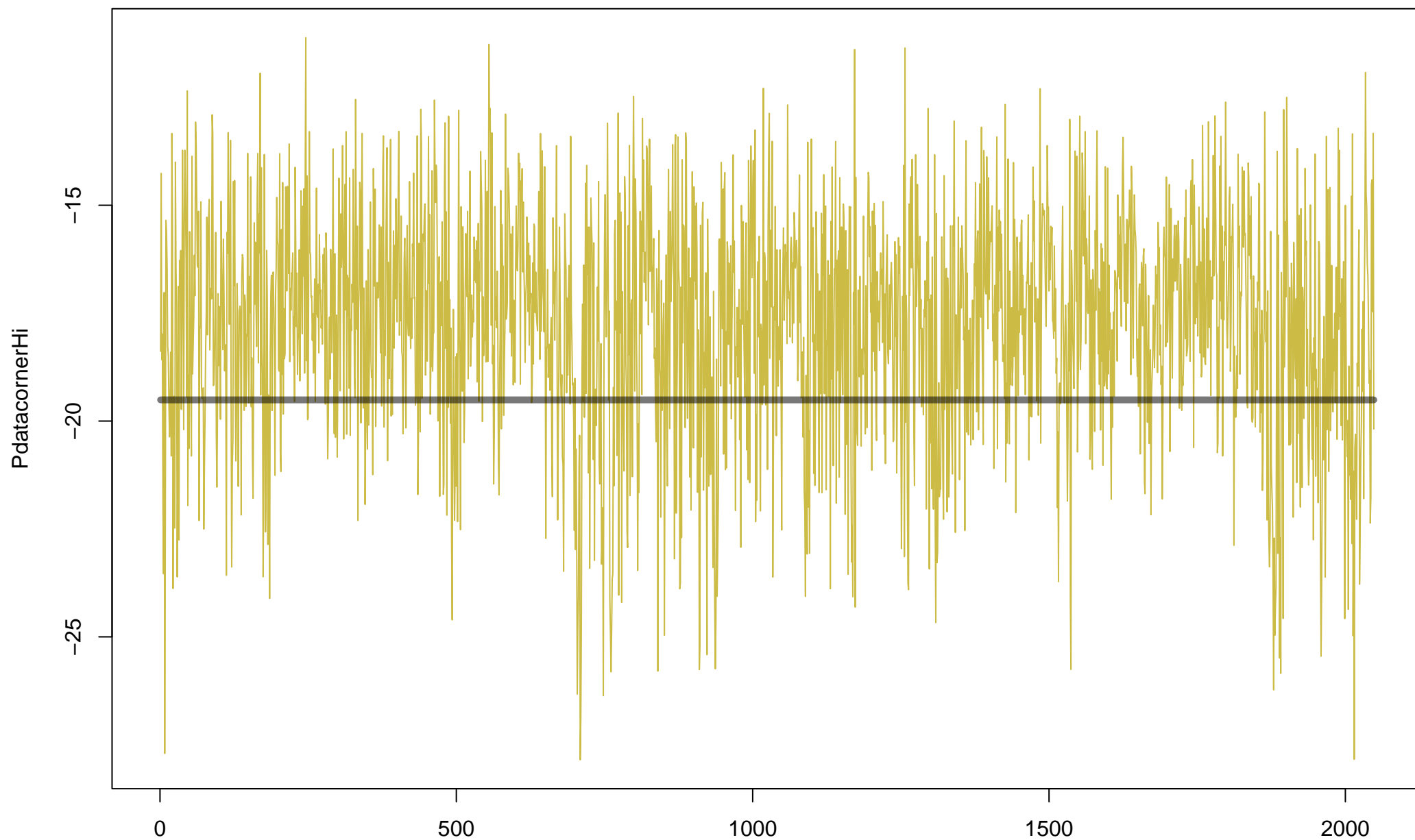
Occupied clusters: 10 of 16



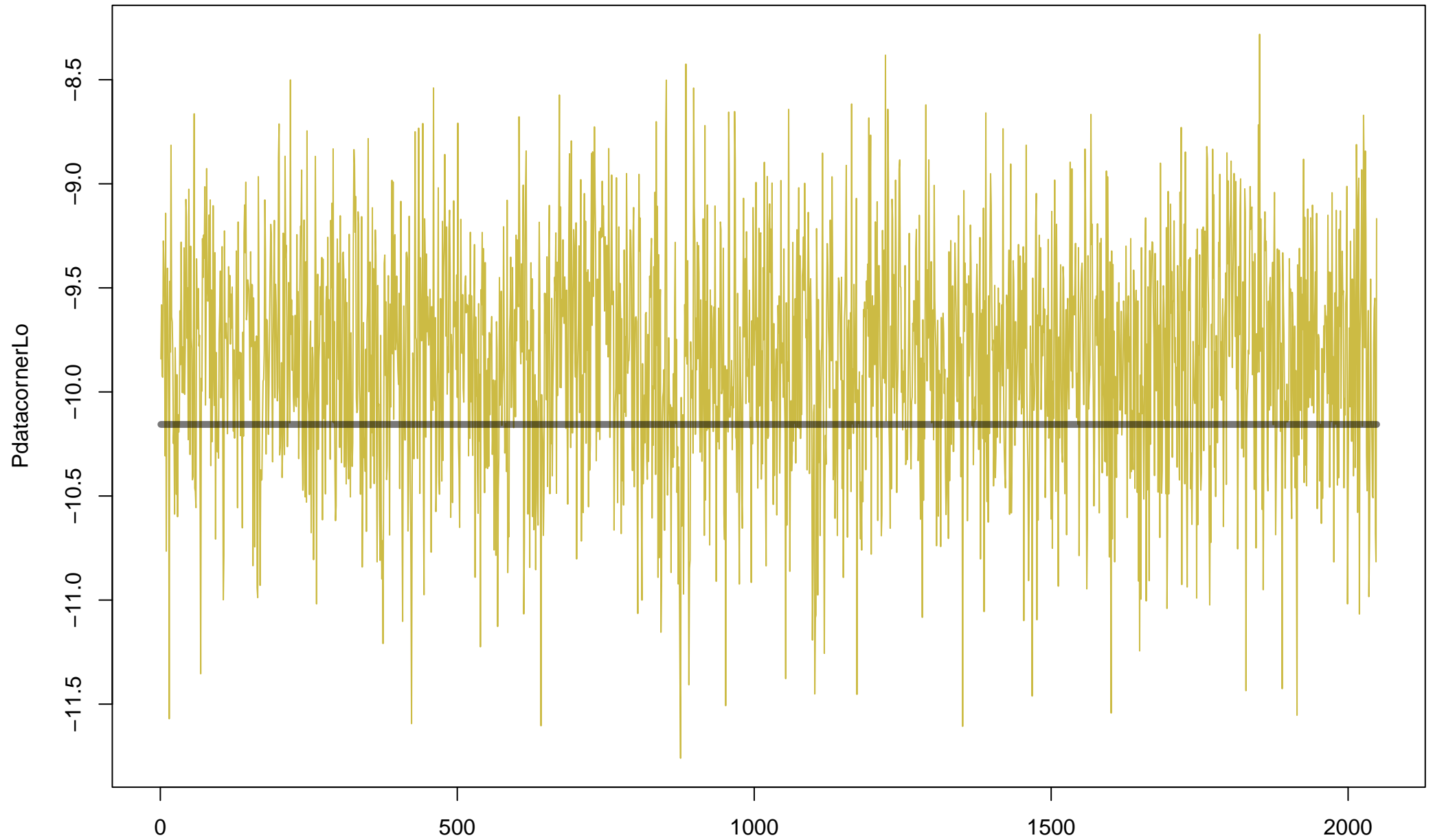
**Pdatamean**  
**ESS = 34.7 | BMK = 0.179 | MCSE(6.27) = 9.6 | stat: TRUE | burn: 0 | rel.err: 0.612**



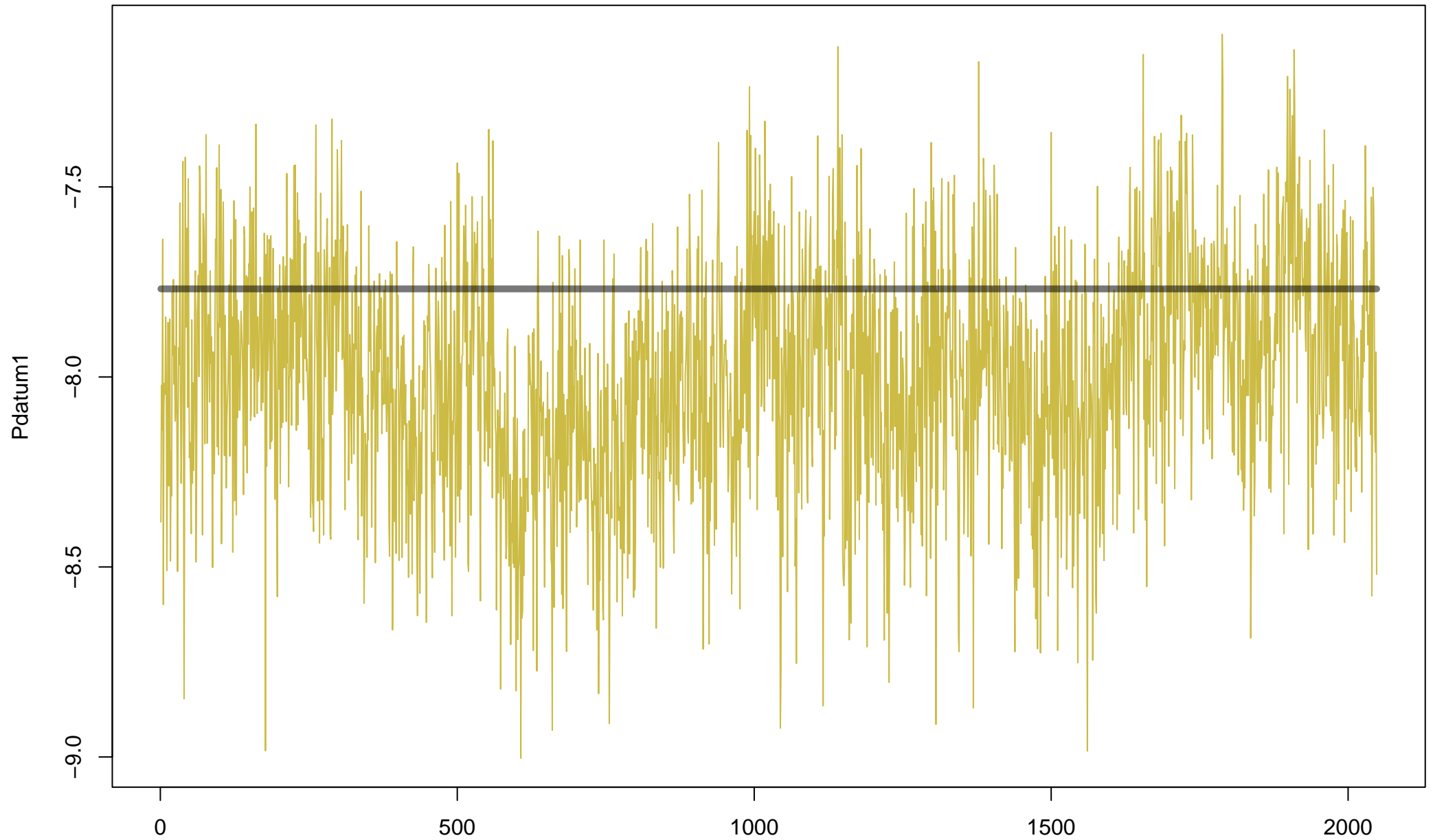
**PdatacornerHi**  
**ESS = 2050 | BMK = 0.138 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0 | rel.err: 0.272**



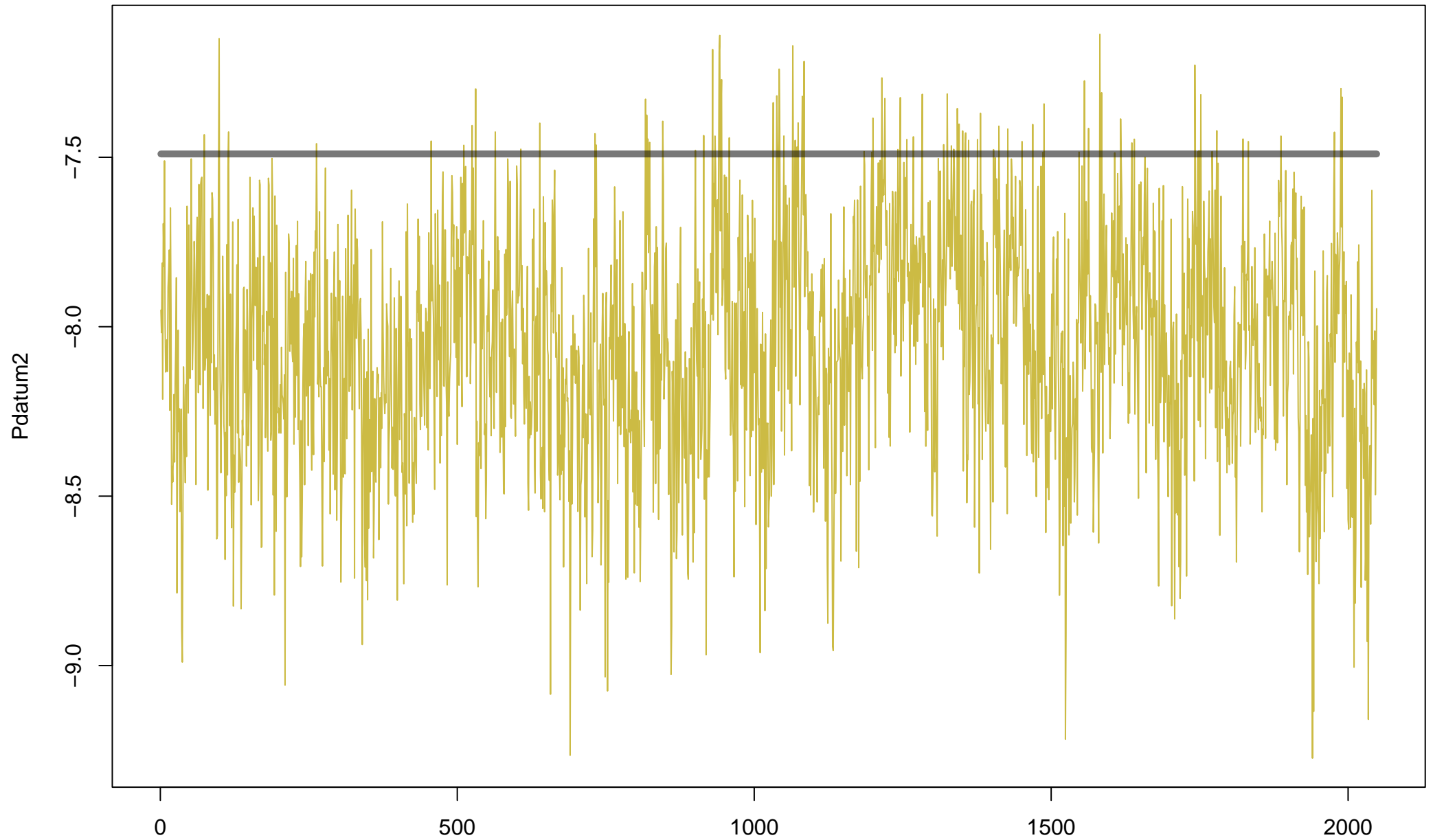
**PdatacornerLo**  
**ESS = 1610 | BMK = 0.057 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0 | rel.err: 0.676**



**Pdatum1**  
**ESS = 130 | BMK = 0.119 | MCSE(6.27) = 6.63 | stat: TRUE | burn: 0 | rel.err: -0.678**

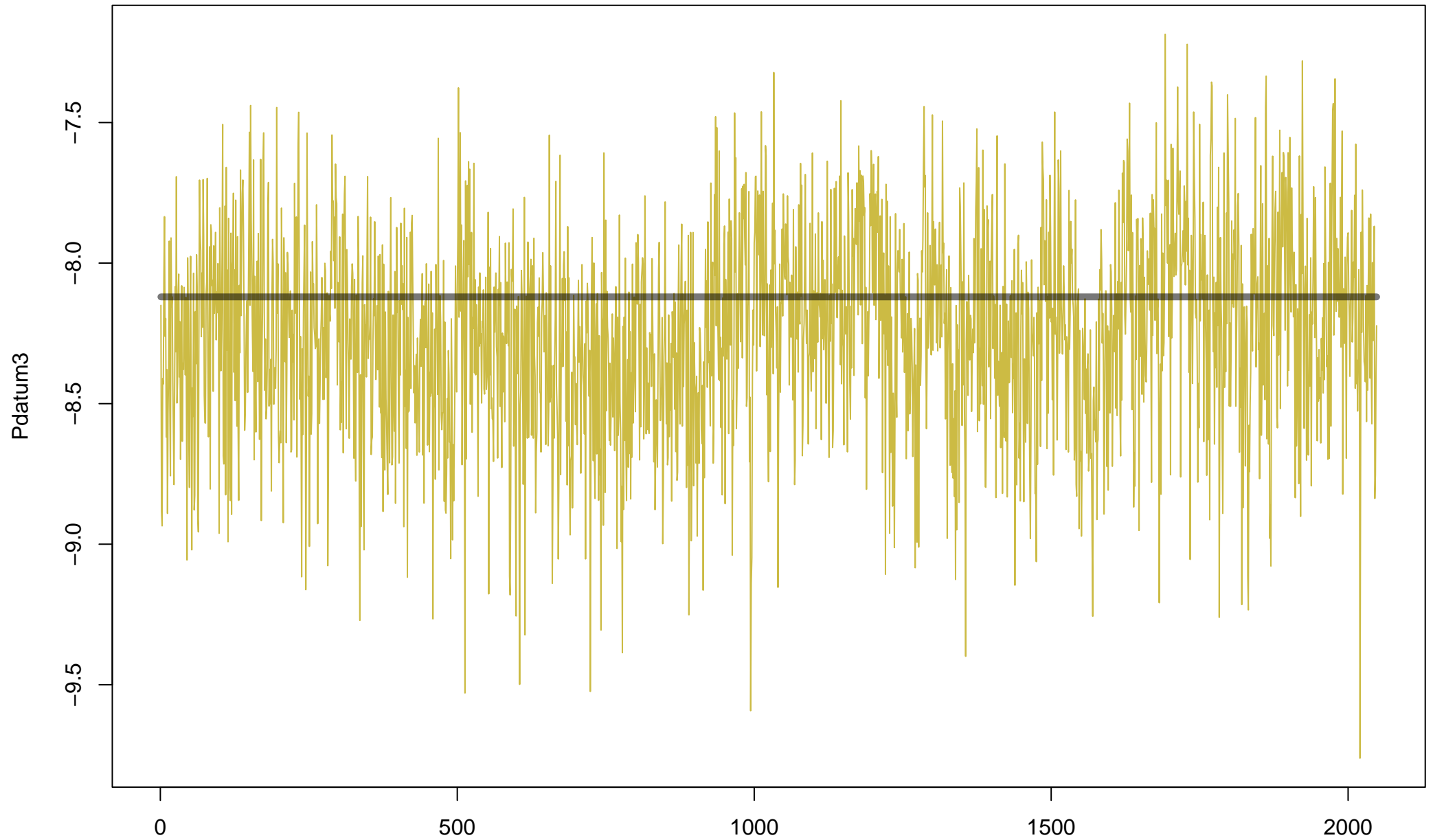


**Pdatum2**  
**ESS = 211 | BMK = 0.125 | MCSE(6.27) = 5.94 | stat: FALSE | burn: 0 | rel.err: -2.01**



**Pdatum3**

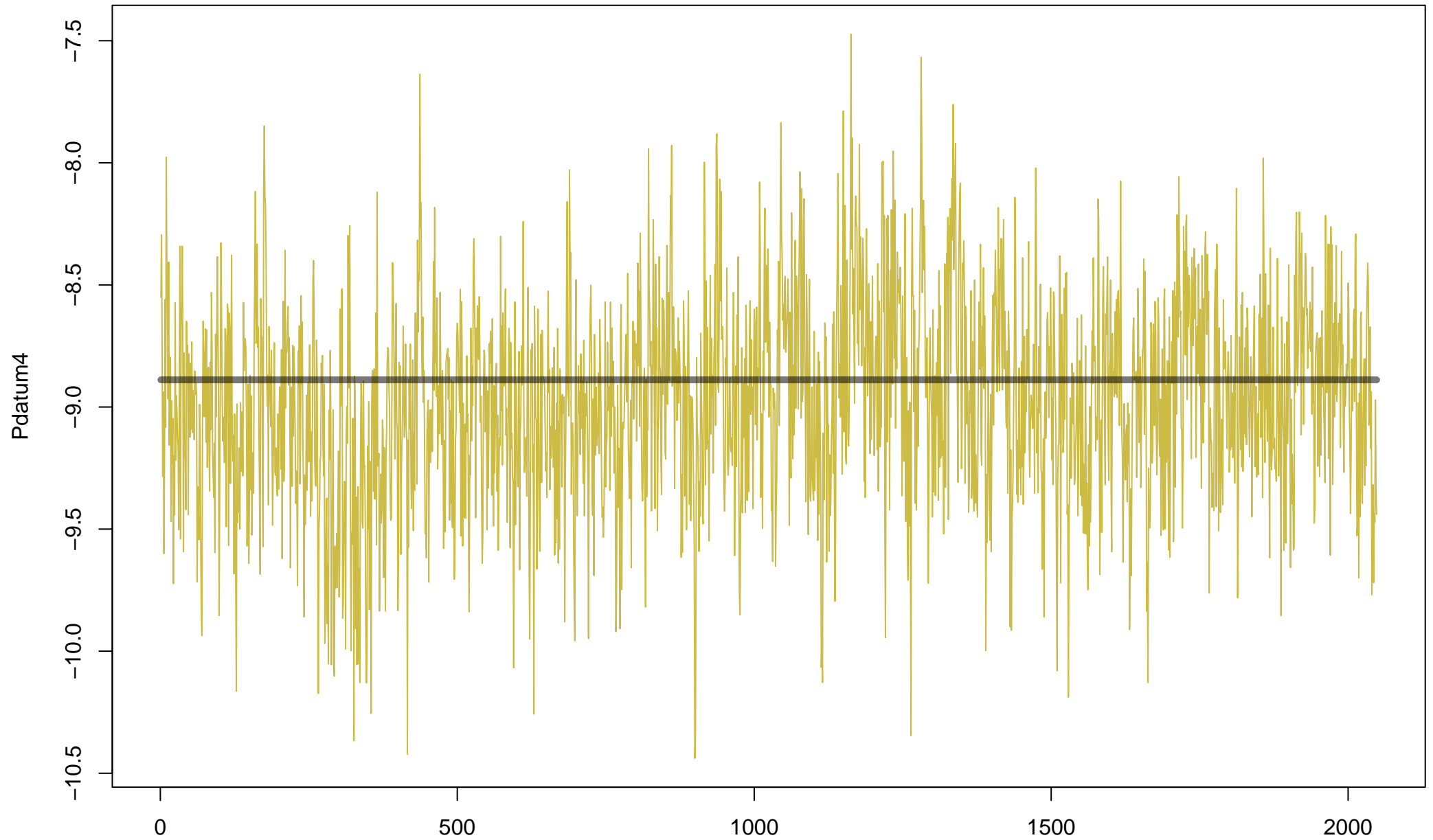
**ESS = 275 | BMK = 0.123 | MCSE(6.27) = 5.13 | stat: TRUE | burn: 0 | rel.err: -0.202**



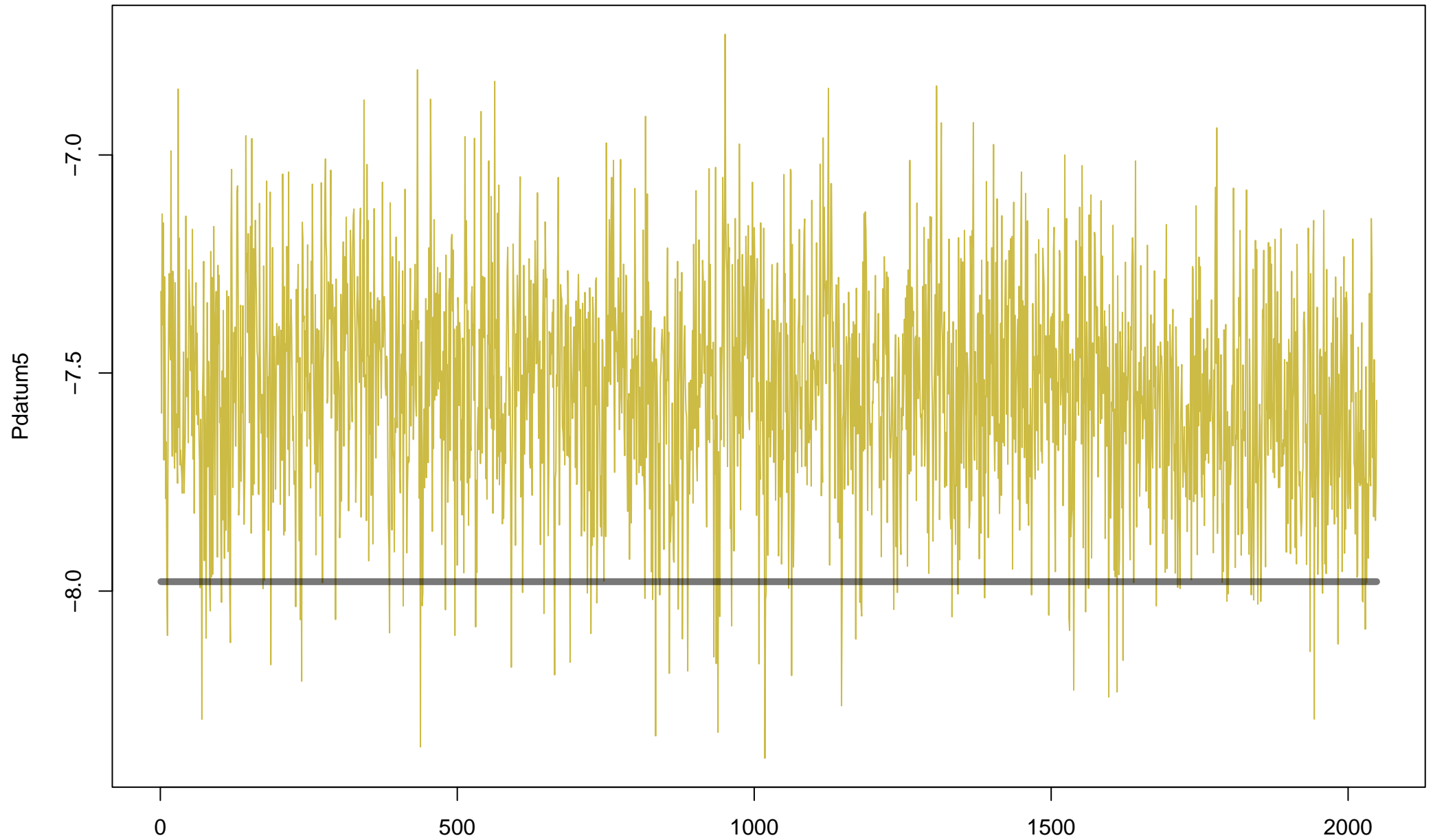


**Pdatum4**

**ESS = 319 | BMK = 0.139 | MCSE(6.27) = 5.4 | stat: FALSE | burn: 0 | rel.err: -0.00167**

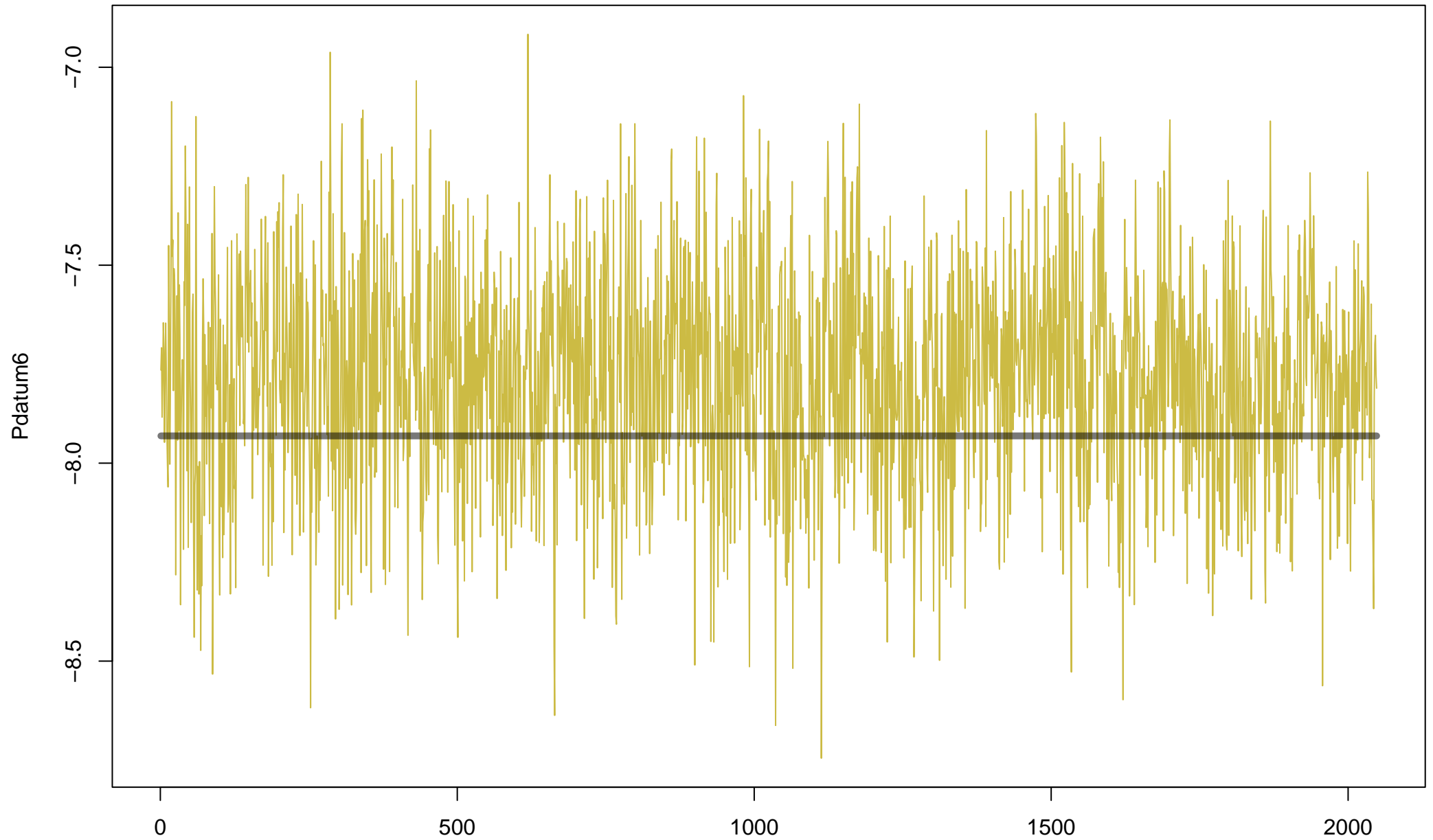


**Pdatum5**  
**ESS = 1040 | BMK = 0.0756 | MCSE(6.27) = 3.45 | stat: TRUE | burn: 0 | rel.err: 1.51**

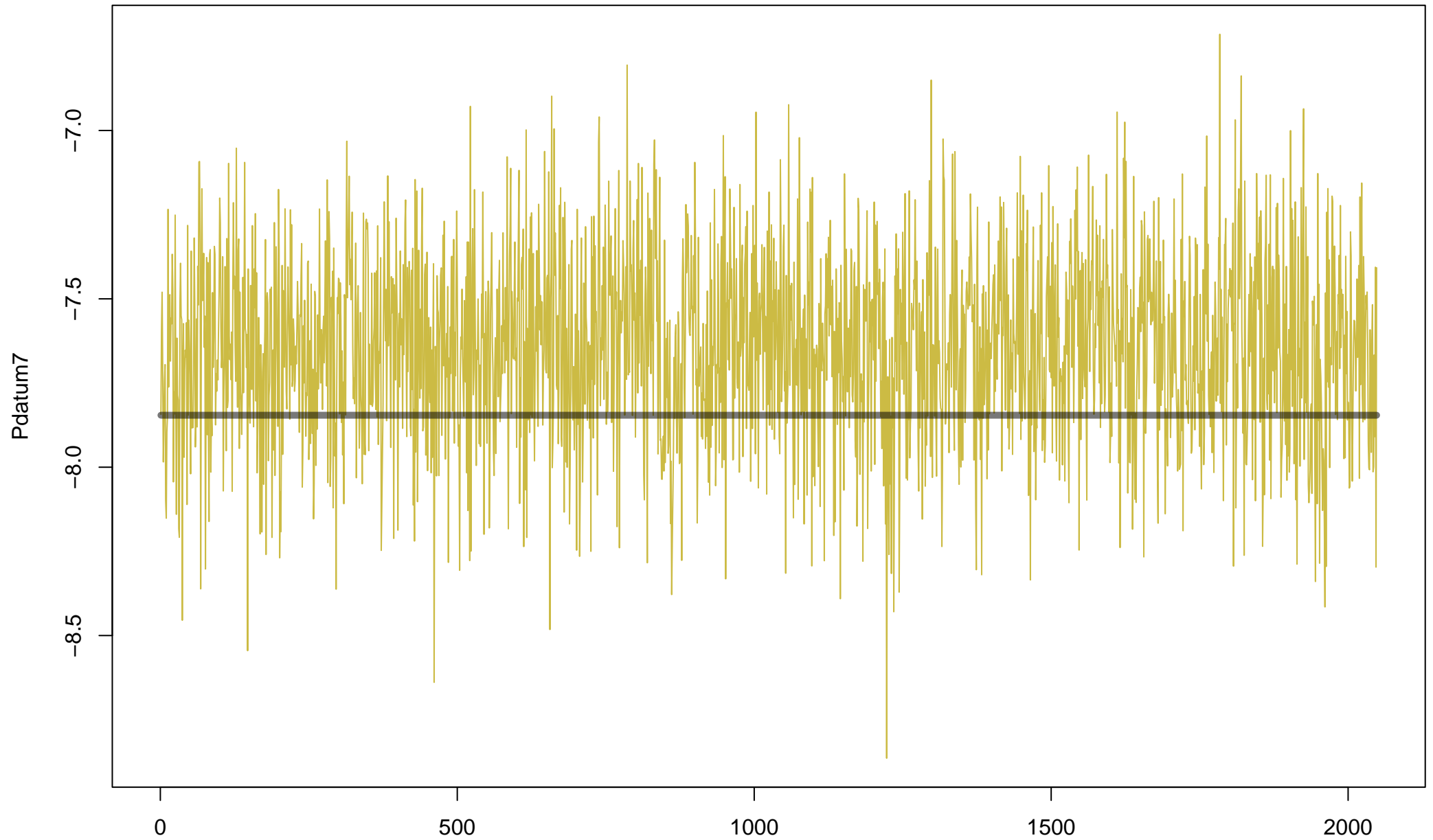


Pdatum6

ESS = 1050 | BMK = 0.0538 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | rel.err: 0.612

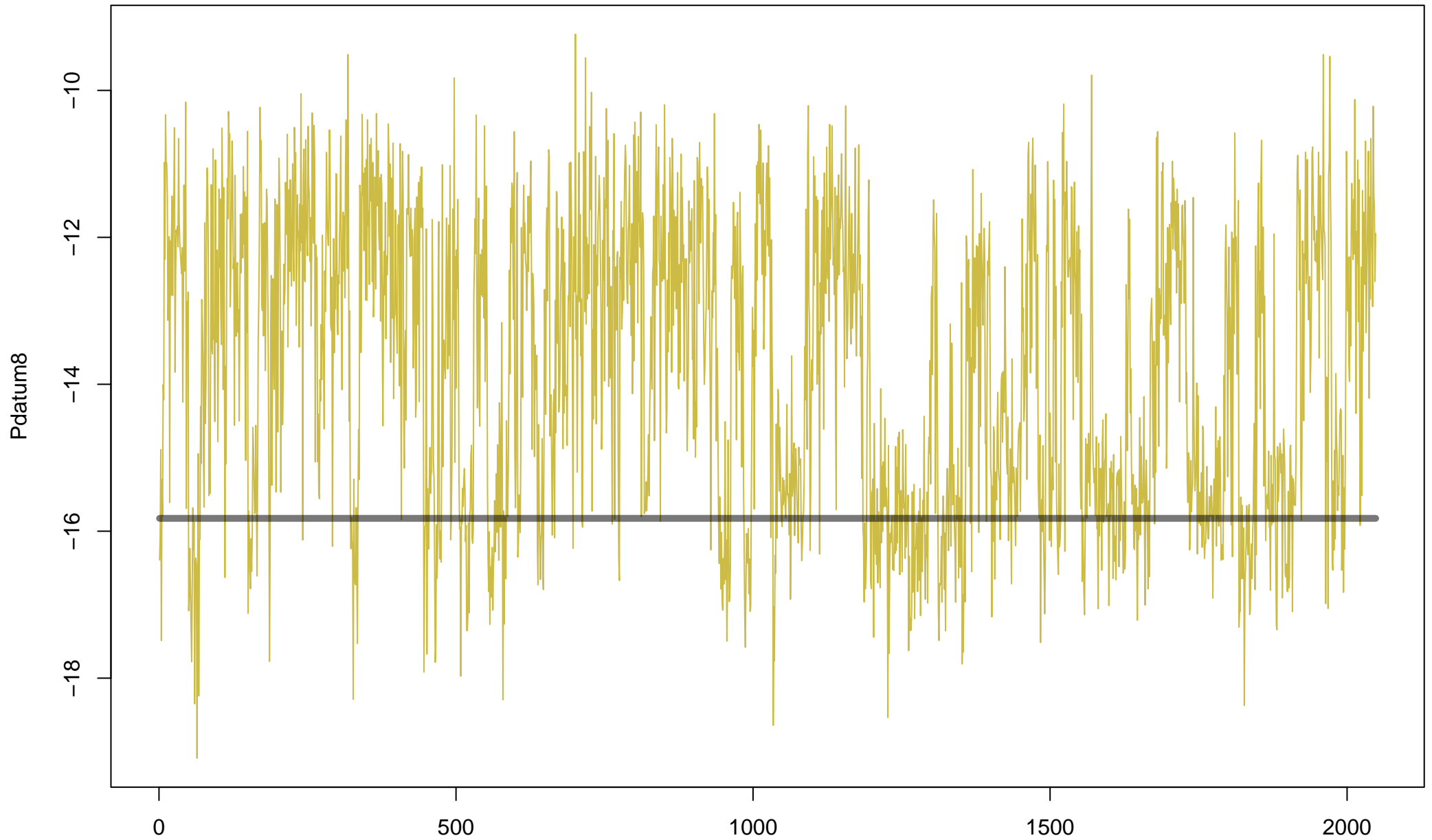


**Pdatum7**  
**ESS = 1520 | BMK = 0.032 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | rel.err: 0.771**

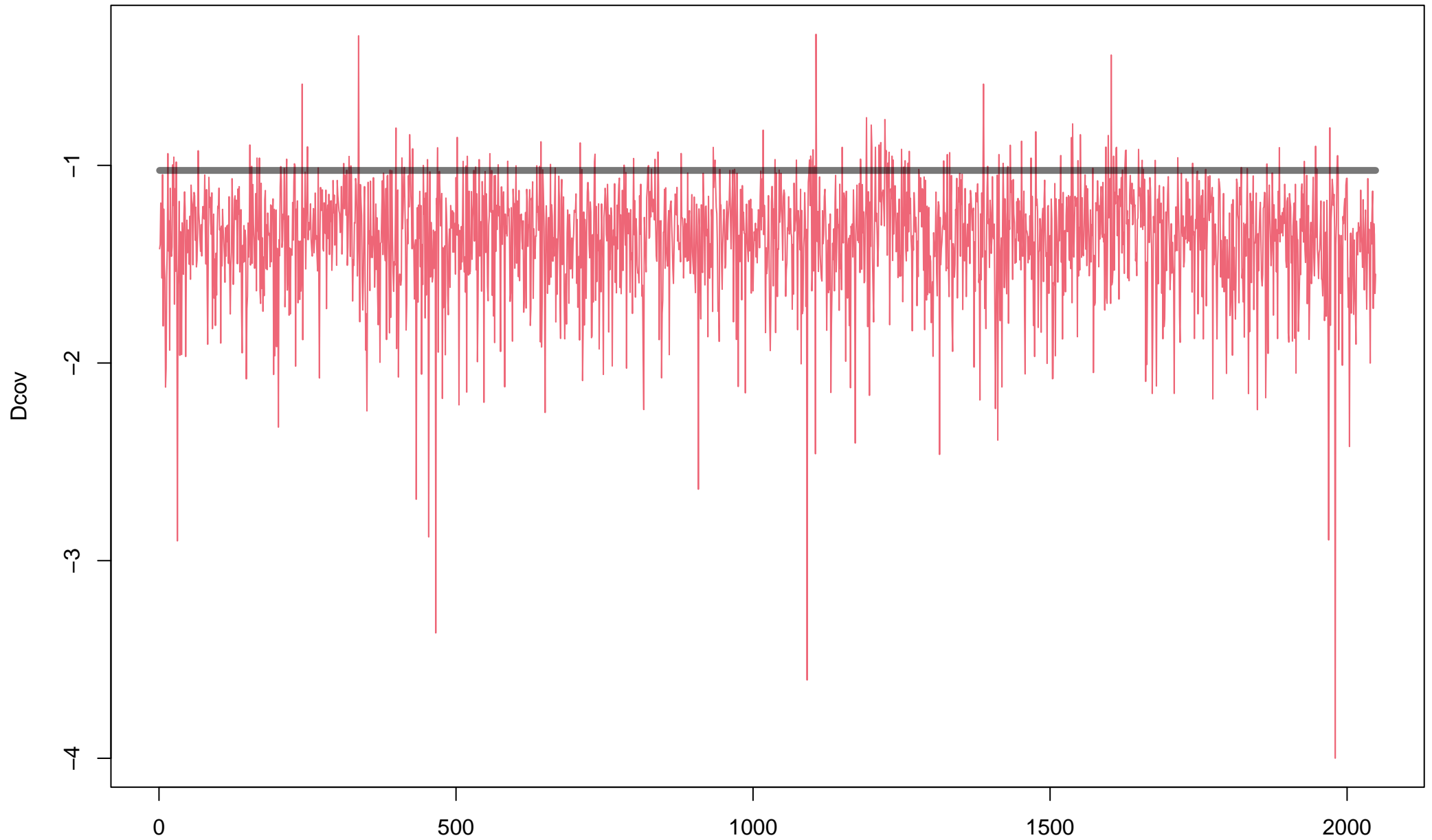


**Pdatum8**

**ESS = 258 | BMK = 0.248 | MCSE(6.27) = 5.39 | stat: FALSE | burn: 0 | rel.err: 0.56**

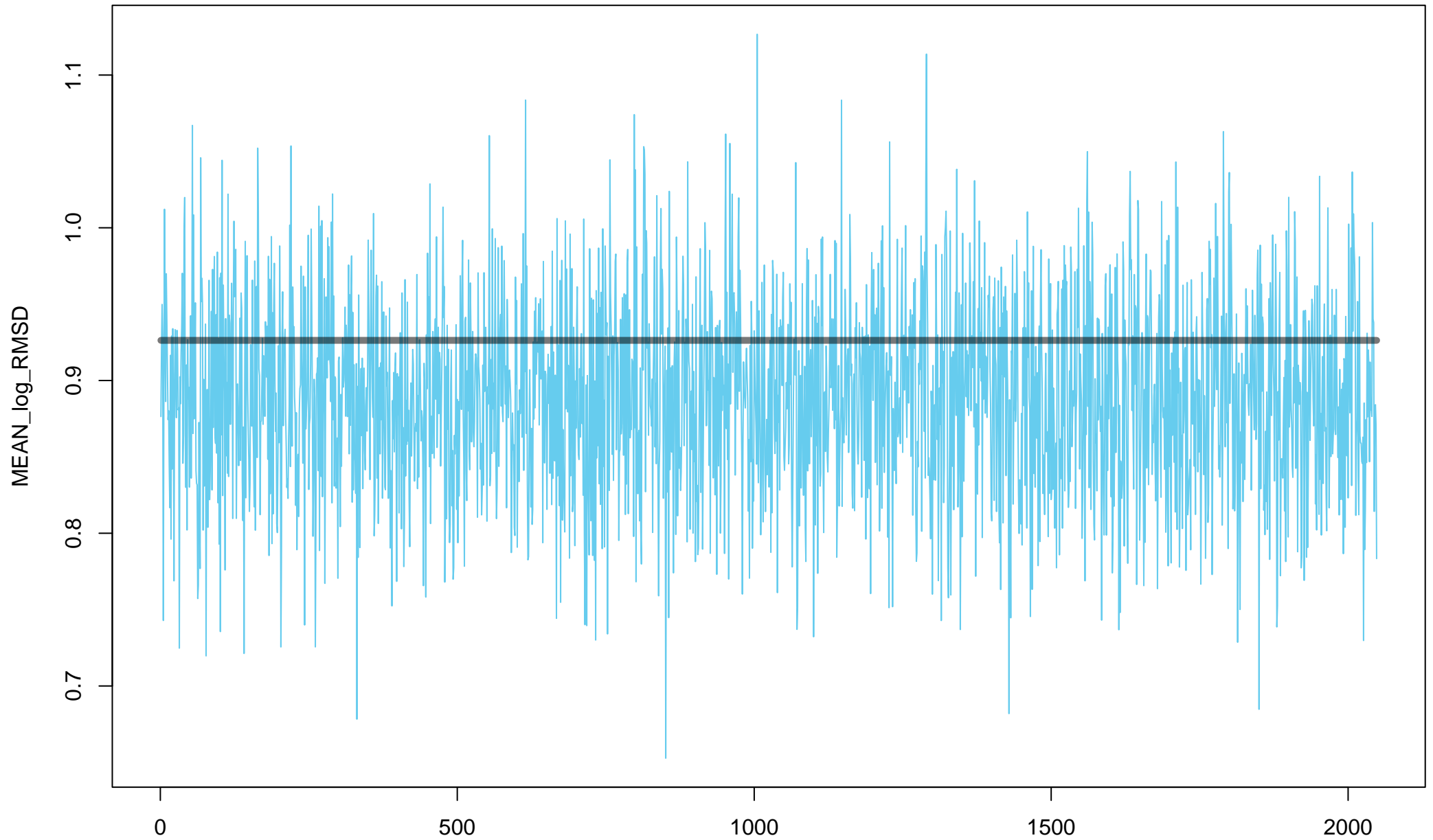


**Dcov**  
**ESS = 1910 | BMK = 0.0679 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0 | rel.err: 1.41**

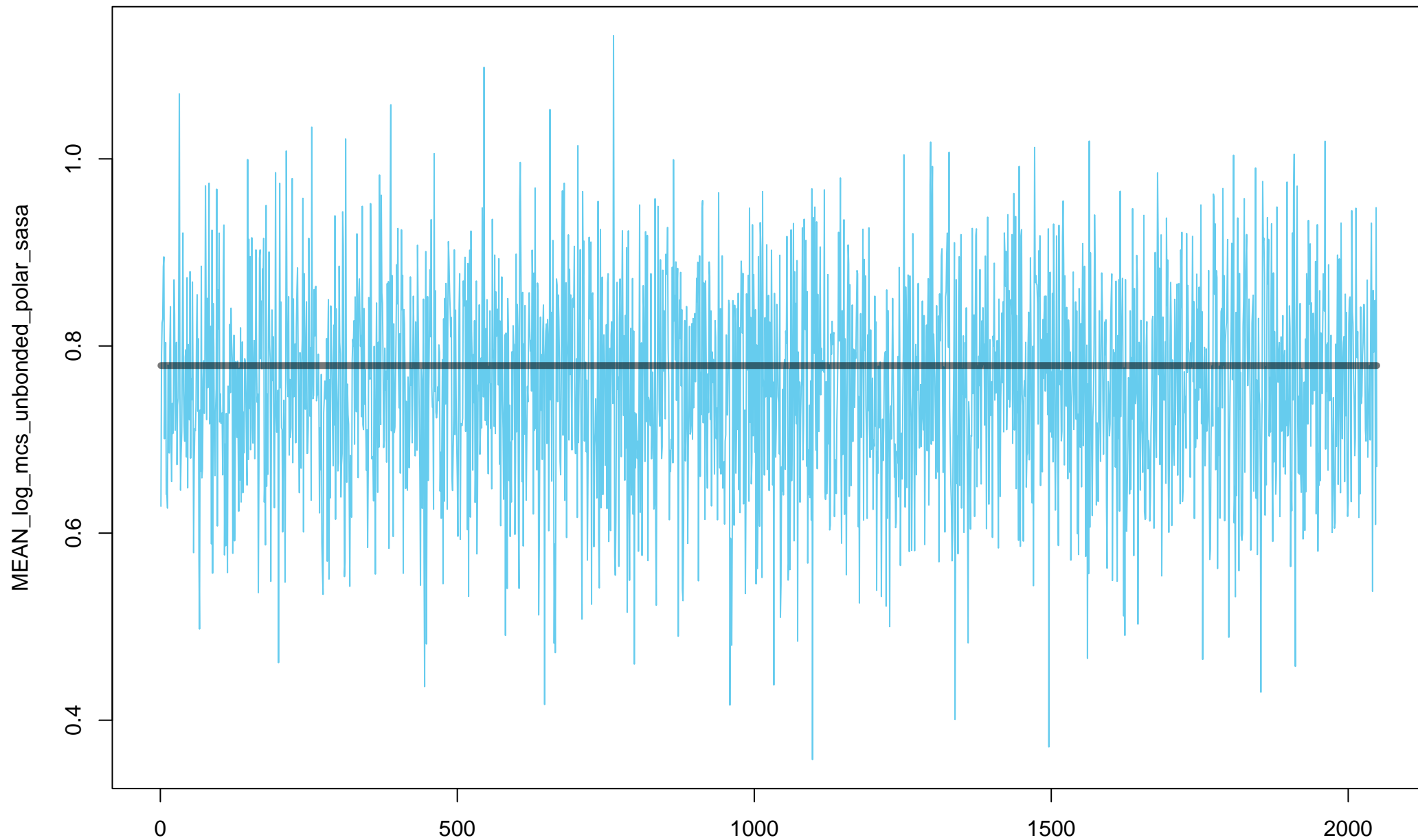


# MEAN\_log\_RMSD

ESS = 2050 | BMK = 0.0316 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0 | rel.err: -0.577



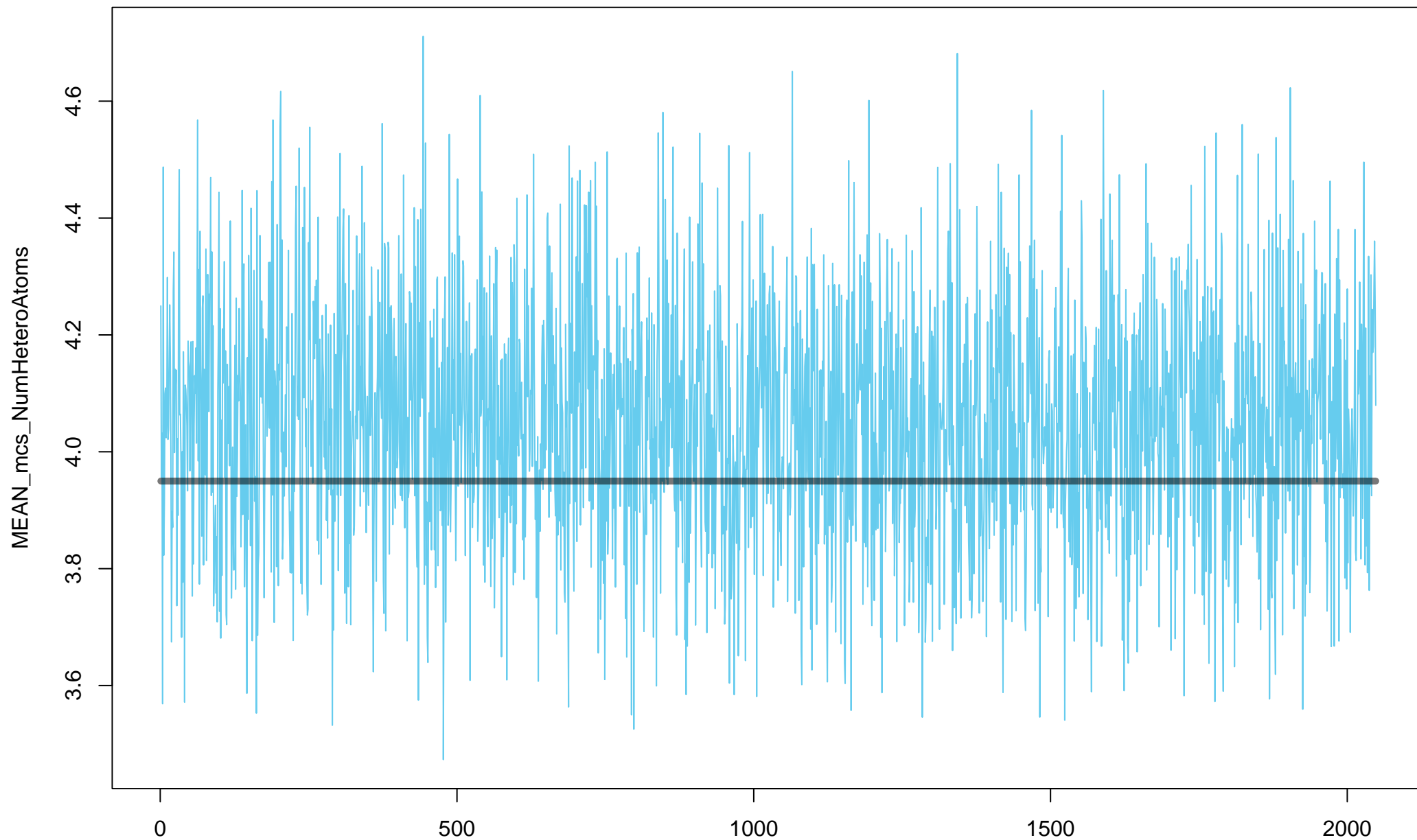
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0486 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0 | rel.err: -0.203**



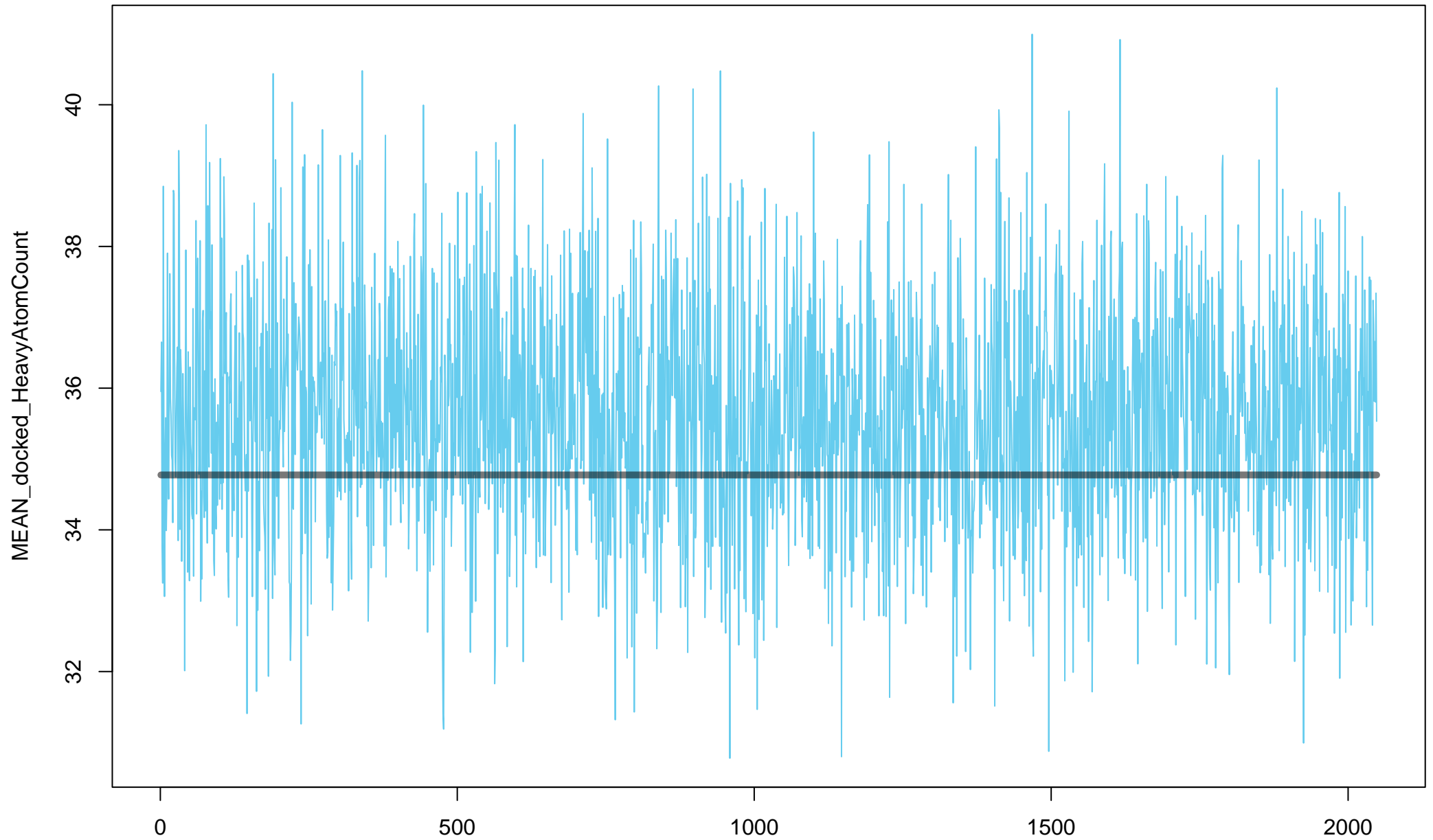


# MEAN\_mcs\_NumHeteroAtoms

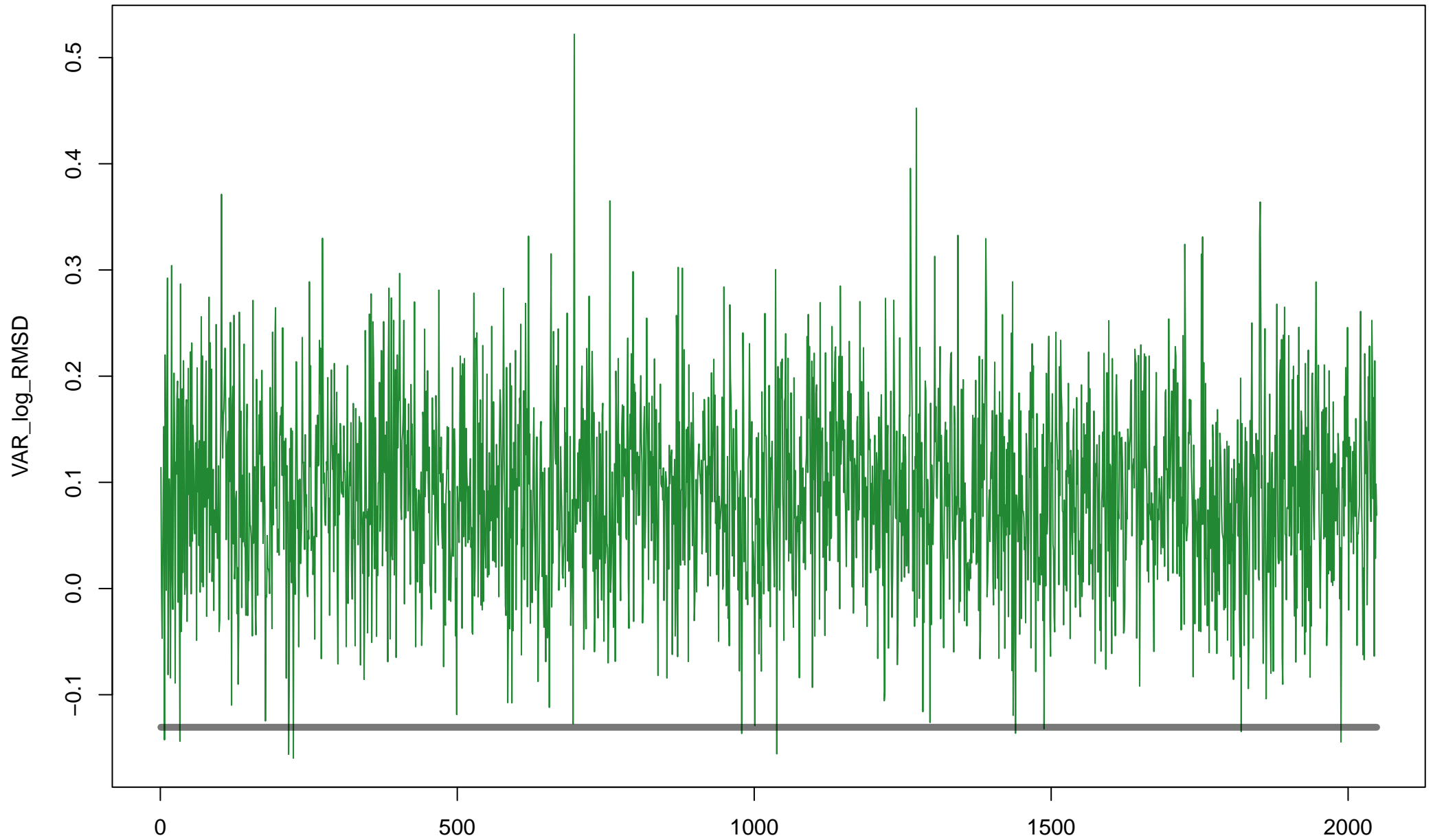
ESS = 2050 | BMK = 0.0468 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0 | rel.err: 0.474



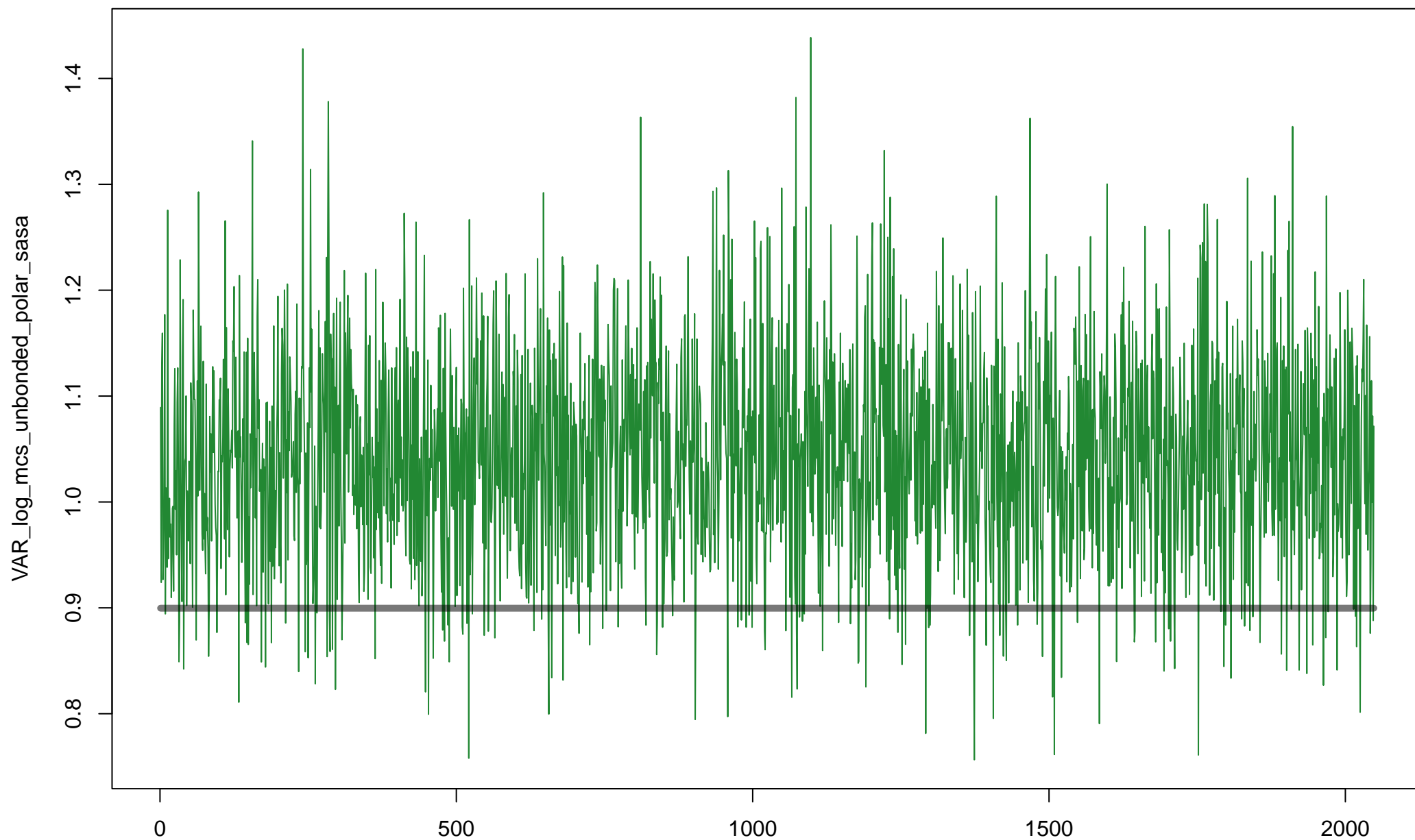
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 2010 | BMK = 0.0512 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0 | rel.err: 0.51**



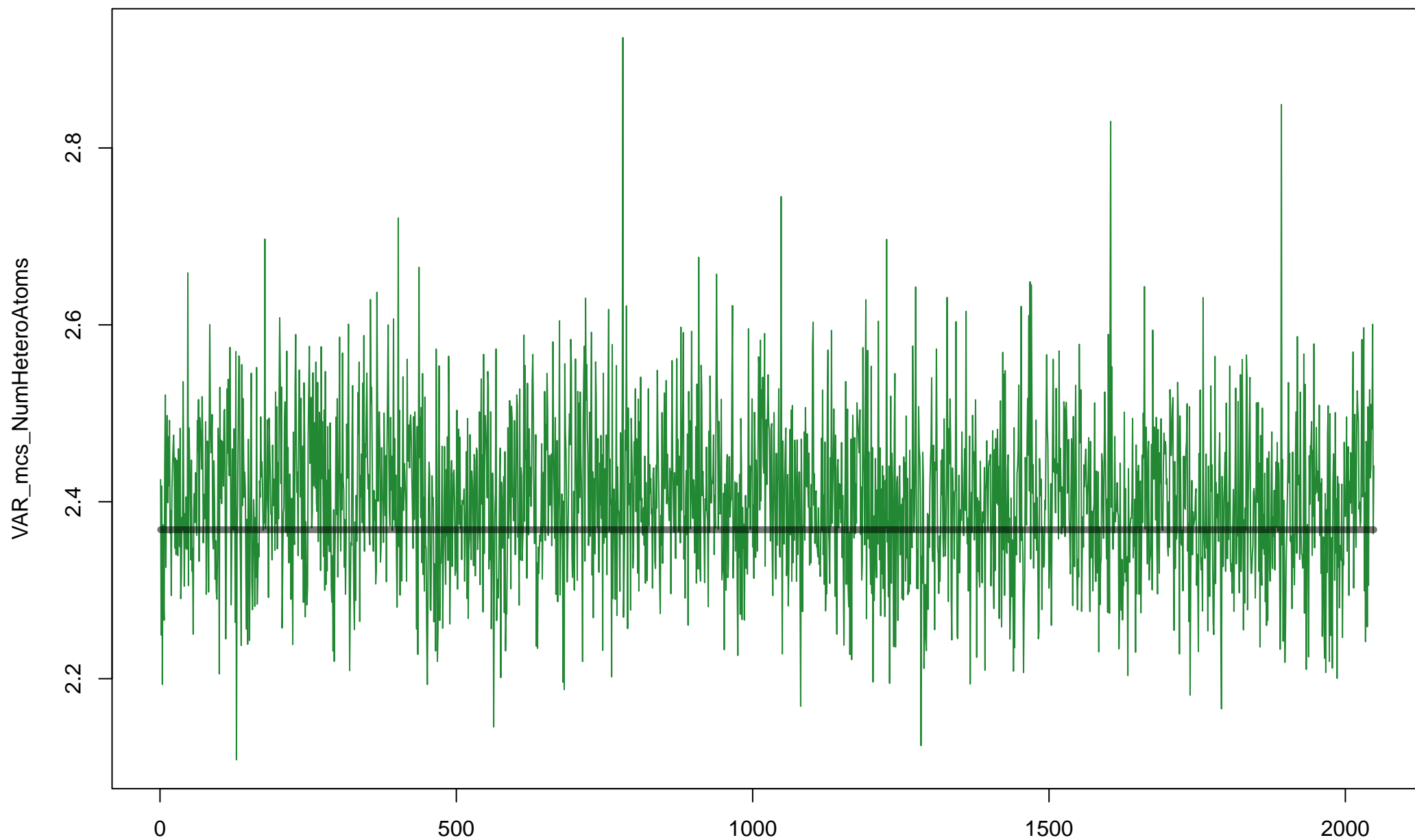
**VAR\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0495 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | rel.err: 2.29**



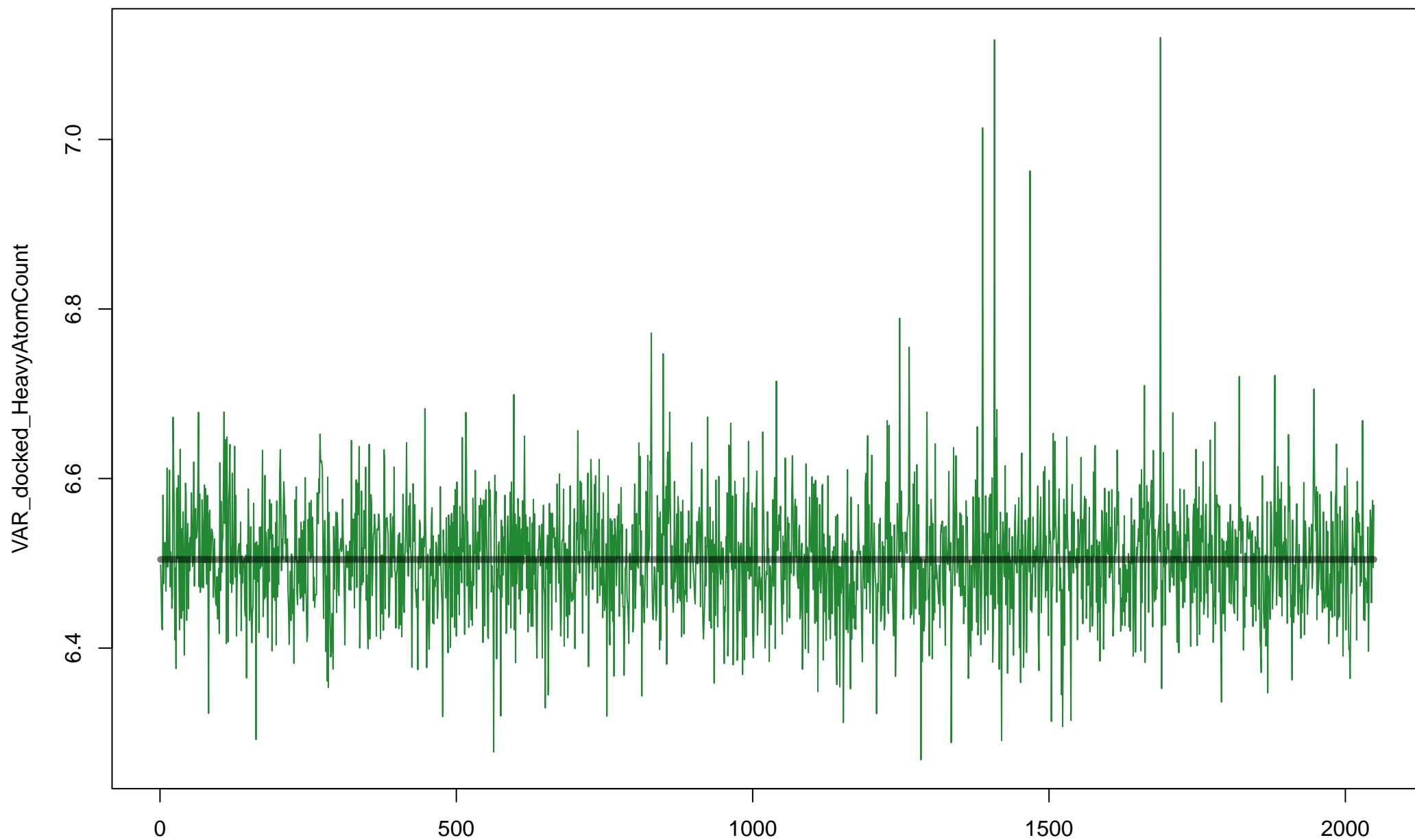
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0352 | MCSE(6.27) = 2.06 | stat: FALSE | burn: 0 | rel.err: 1.4**



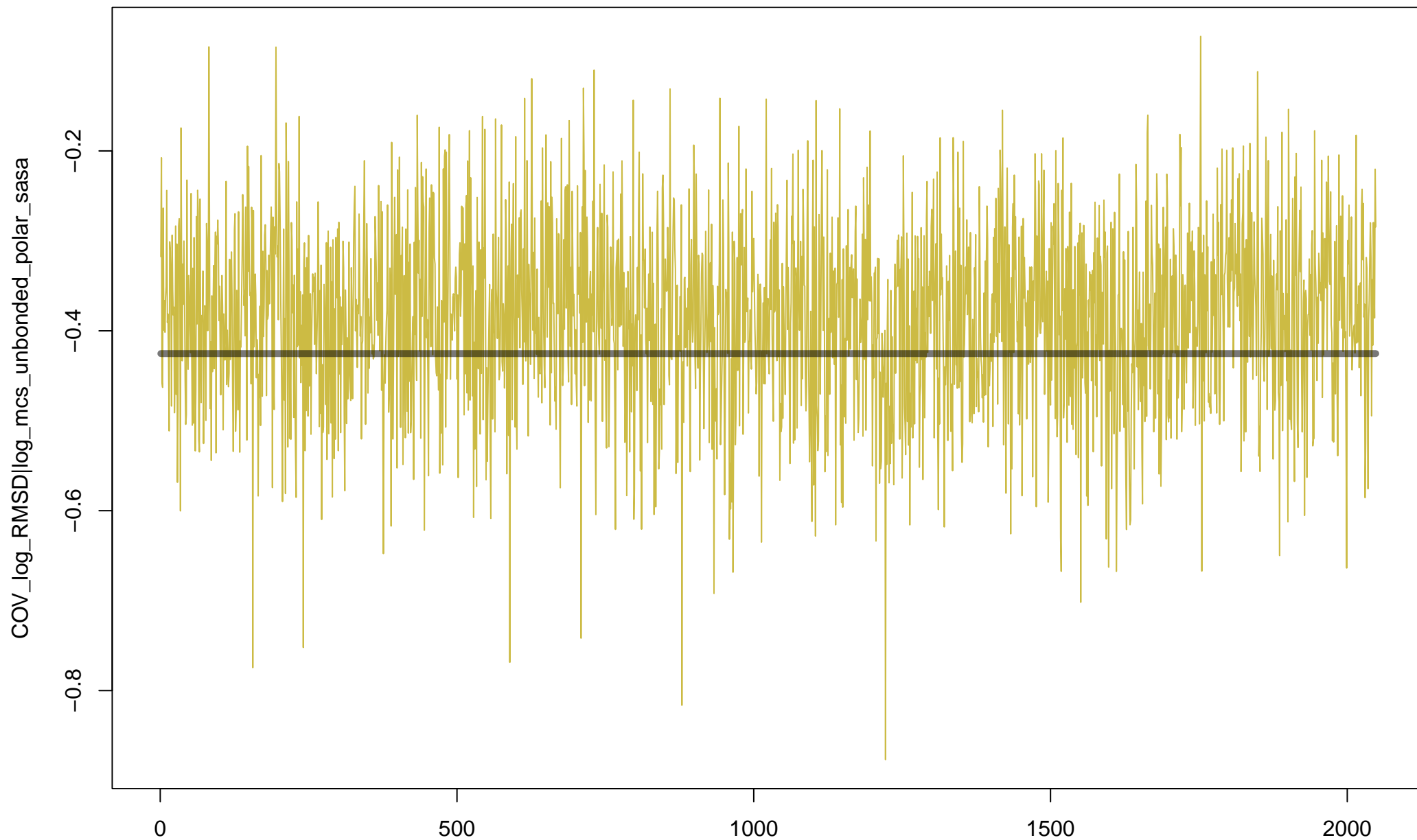
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 1490 | BMK = 0.0835 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | rel.err: 0.417**



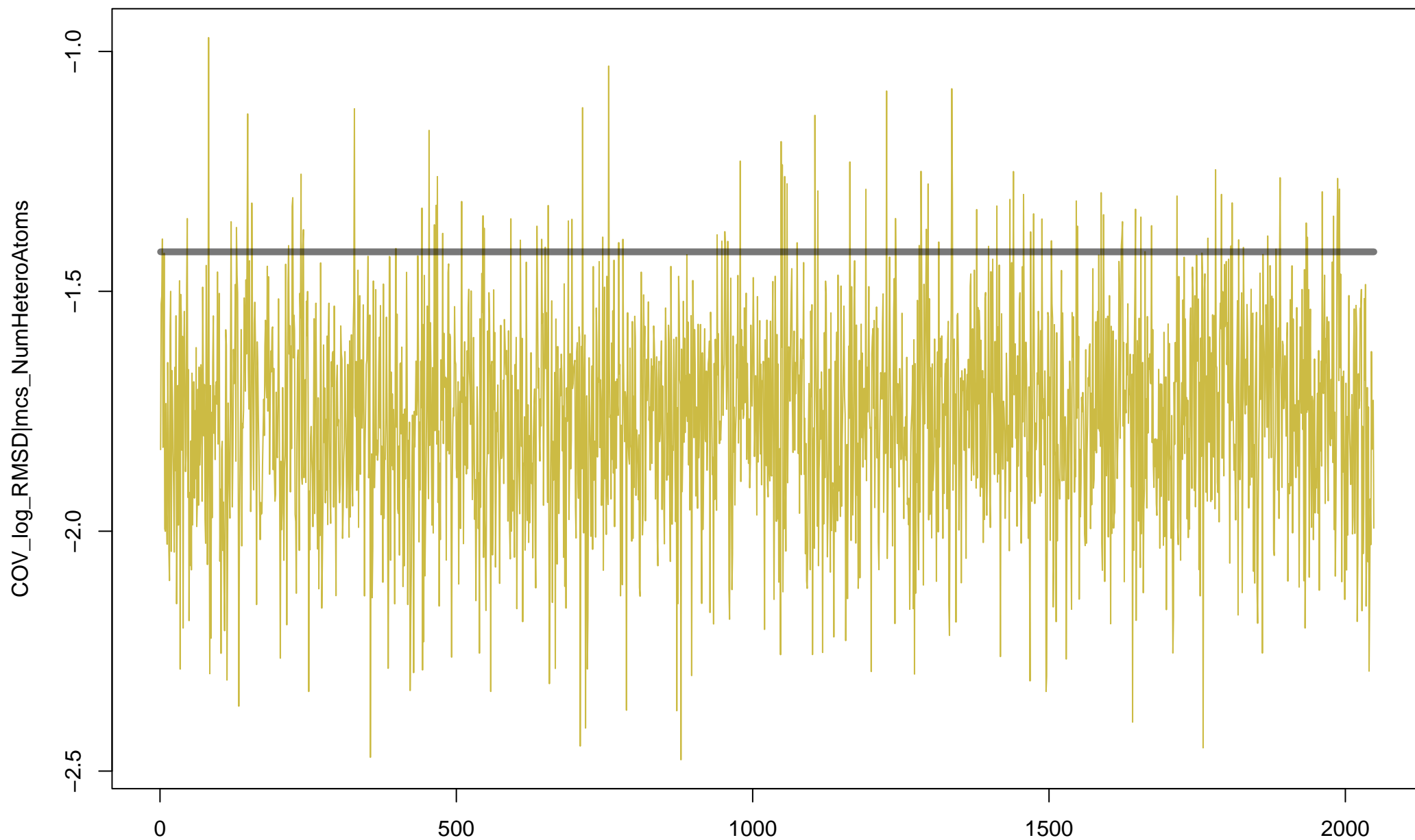
**VAR\_docked\_HeavyAtomCount**  
**ESS = 1900 | BMK = 0.0606 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 0 | rel.err: 0.0449**



**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0603 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0 | rel.err: 0.392**

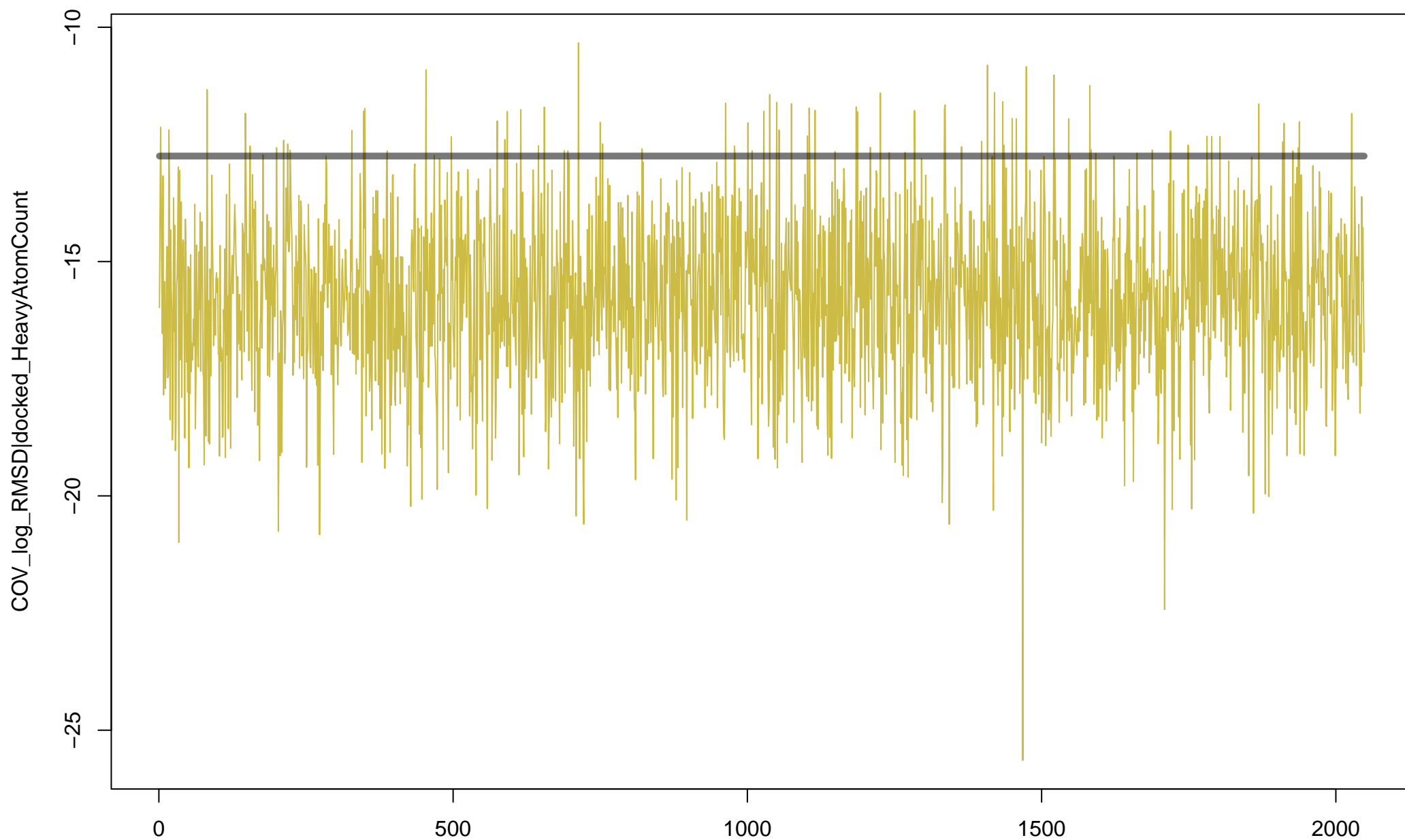


**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 1740 | BMK = 0.0515 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0 | rel.err: -1.61**

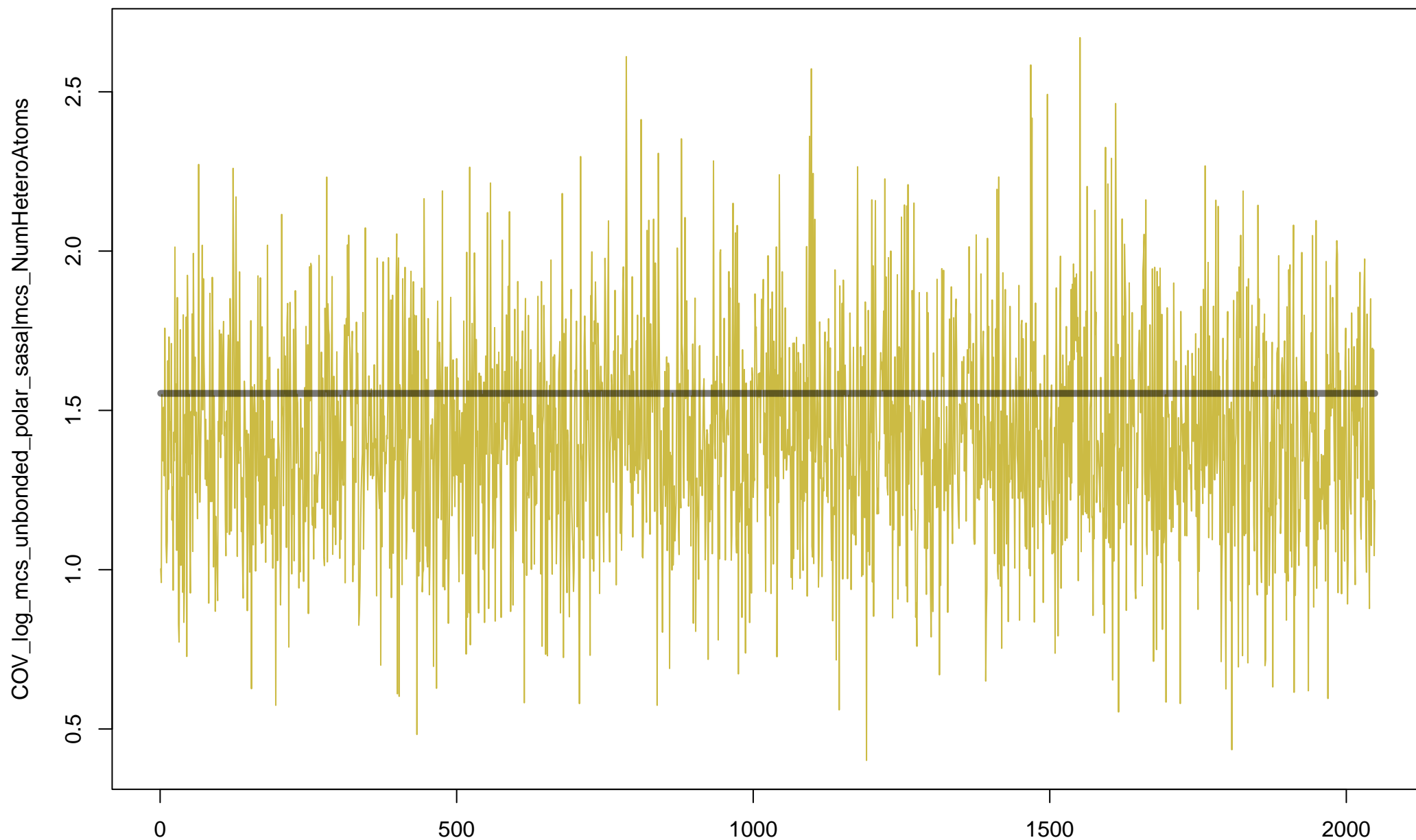




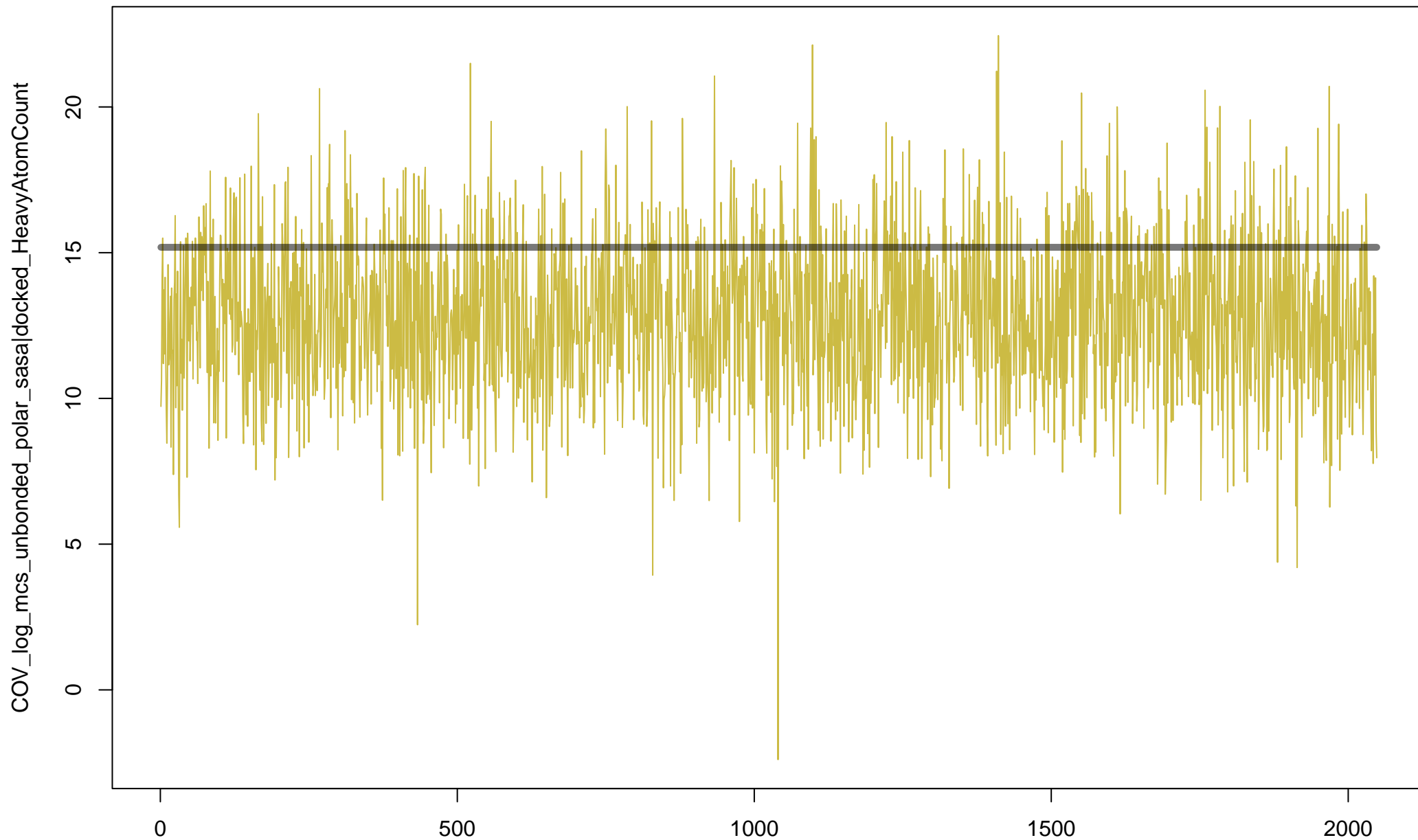
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 1900 | BMK = 0.0552 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0 | rel.err: -1.77**



**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0348 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0 | rel.err: -0.409**



**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0484 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0 | rel.err: -0.89**



**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0265 | MCSE(6.27) = 1.91 | stat: TRUE | burn: 0 | rel.err: 0.437**

