

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 1

max MCSE = 34.3300137294225

all stationary: FALSE

burn: 20

min percent.: 0

-- STATS 2D --

min ESS = 5.85842798529857

max BMK = 0.763287358002483

max MCSE = 45.6955983673816

all stationary: FALSE

burn: 20

min percent.: 0

-- STATS 1D --

min ESS = 9.7150136796015

max BMK = 1

max MCSE = 32.1379088781033

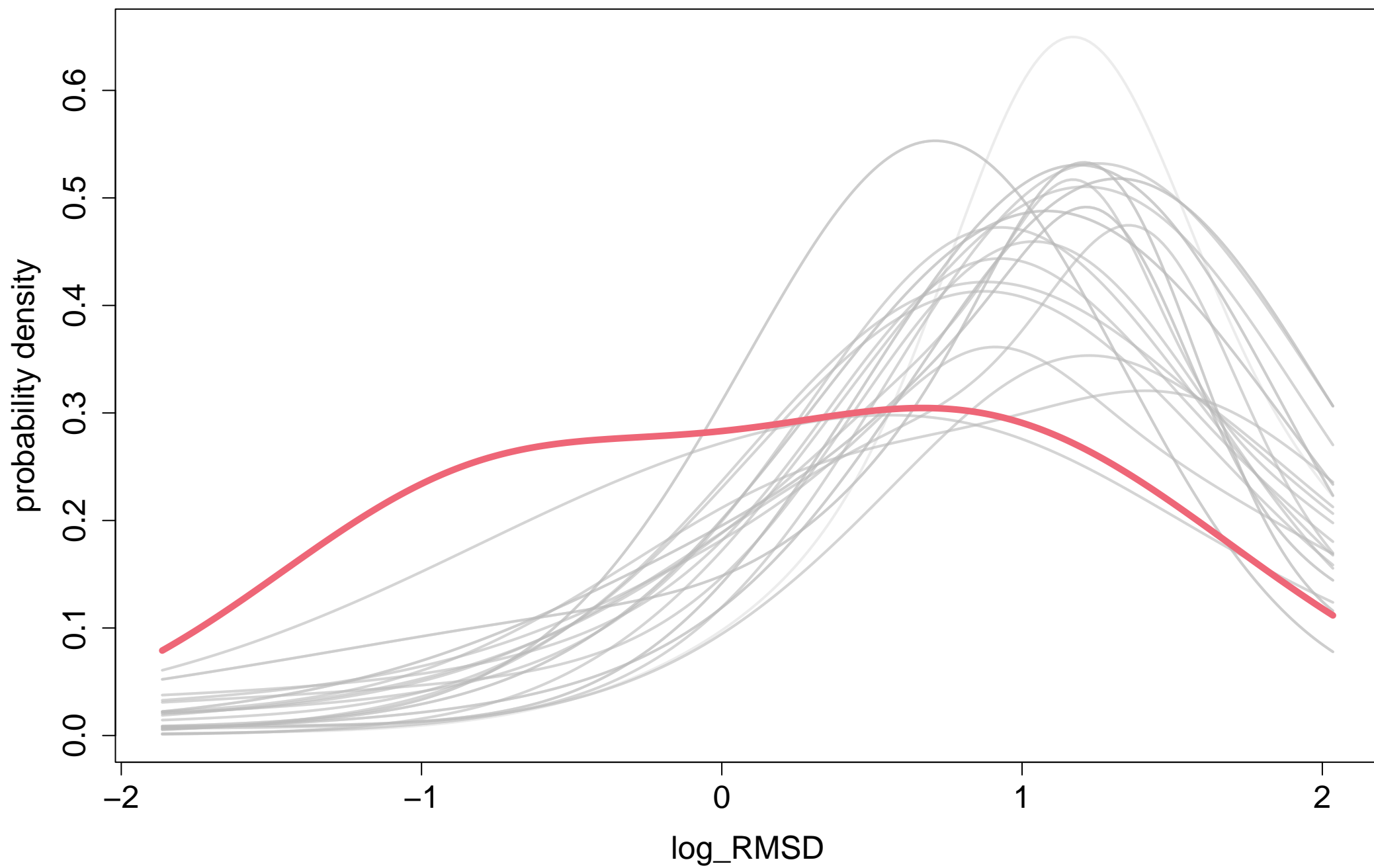
all stationary: FALSE

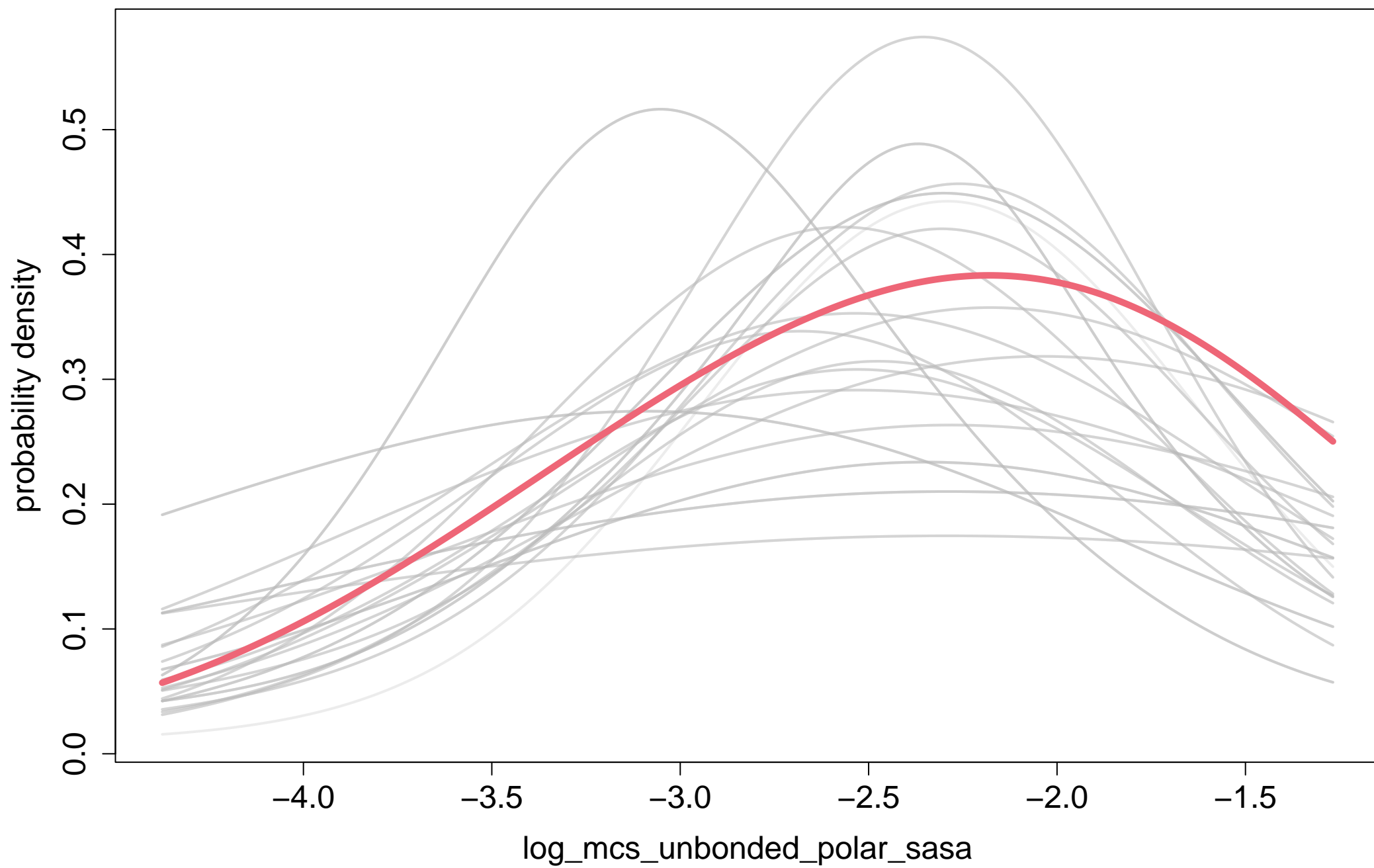
burn: 20

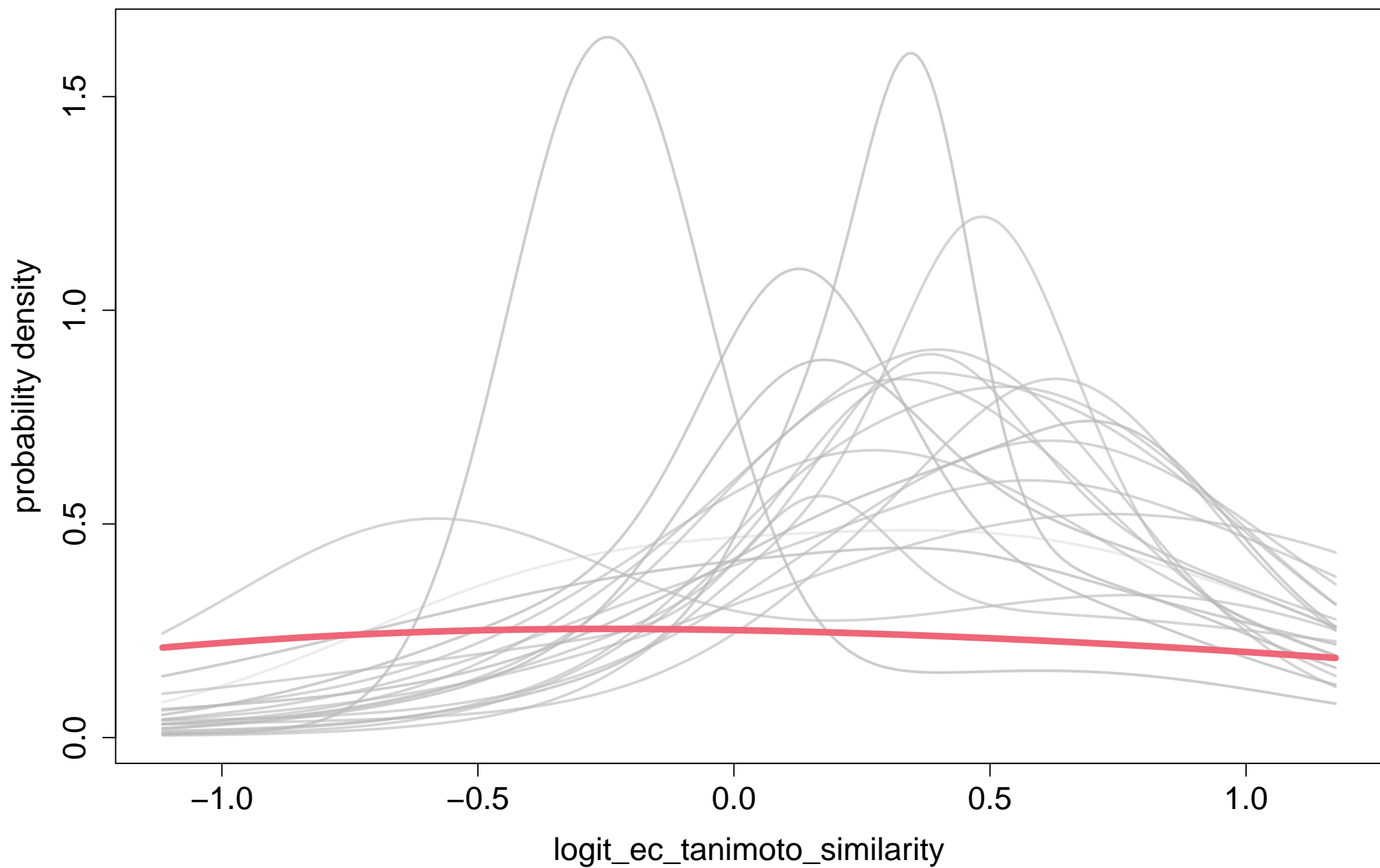
min percent.: 0

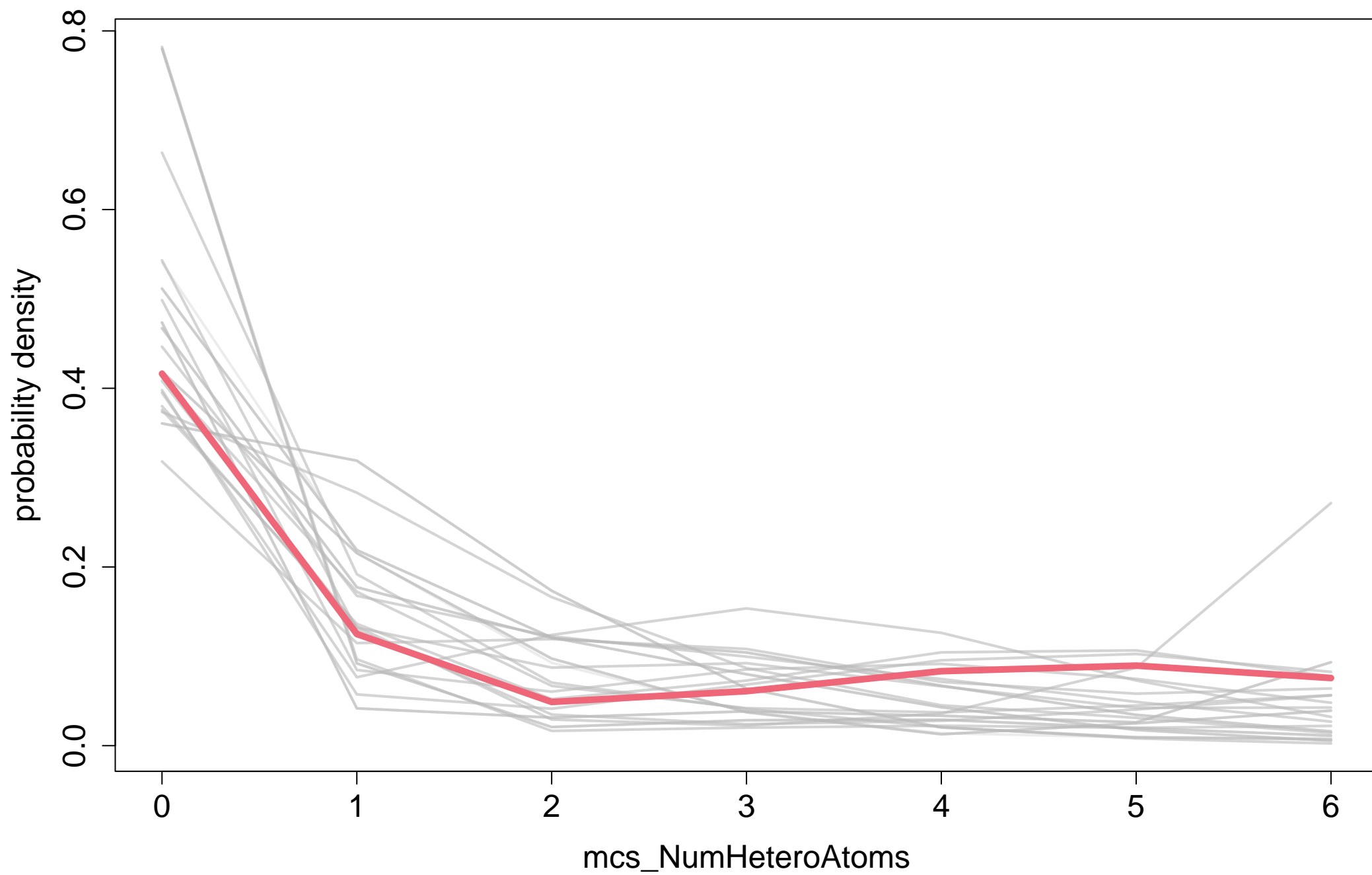
Occupied clusters: 3 of 4

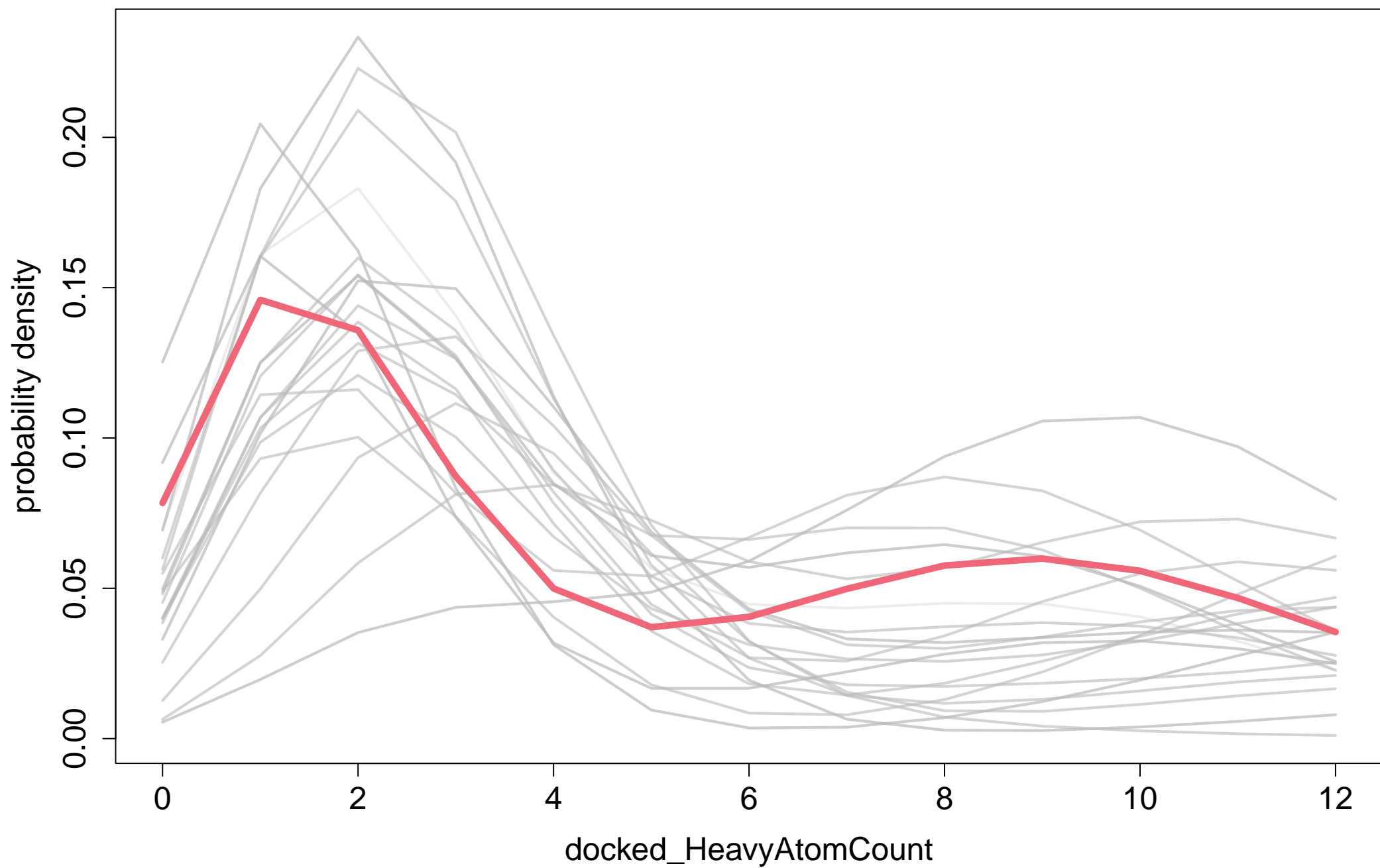
LL: -107 +- 3.03

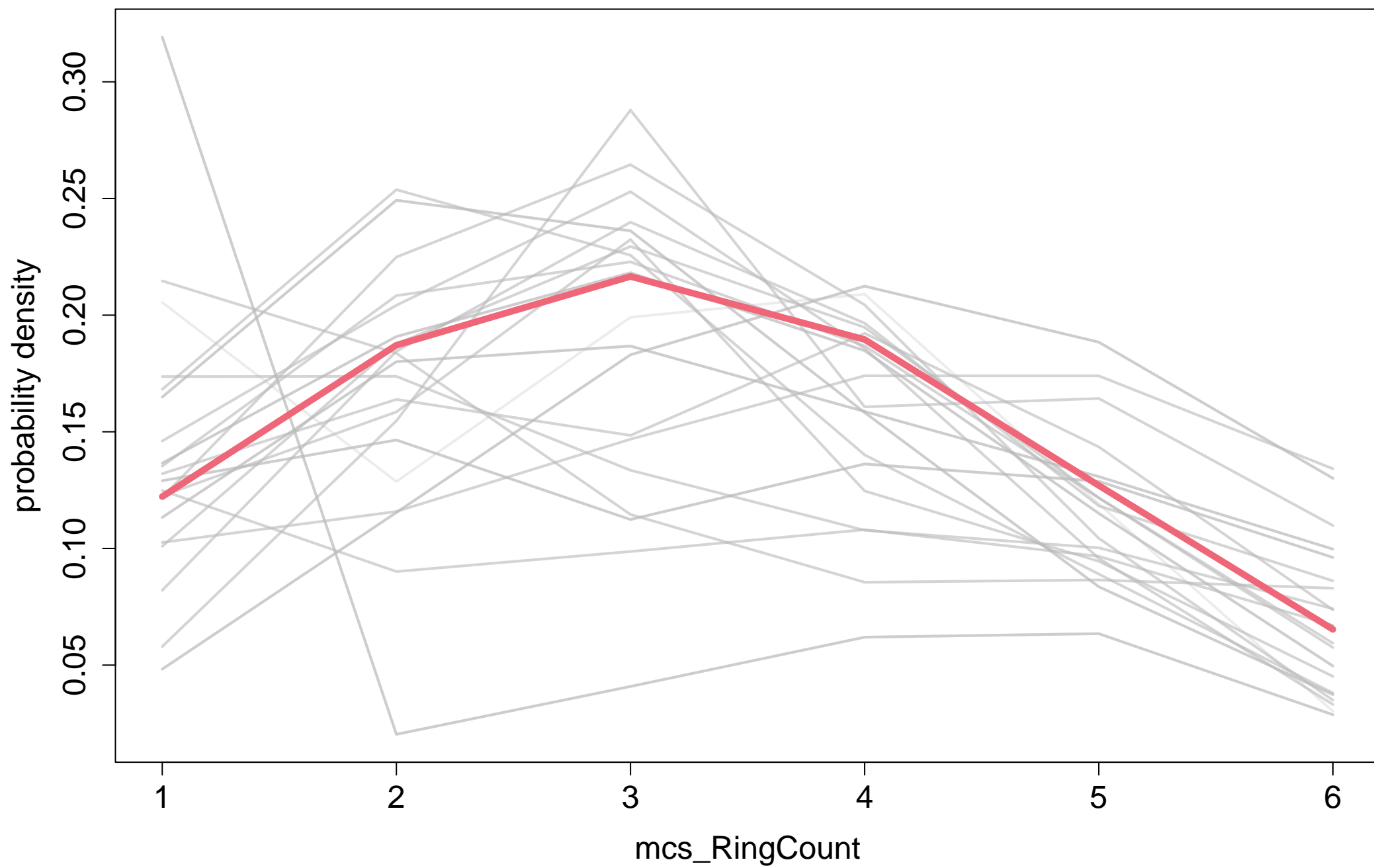


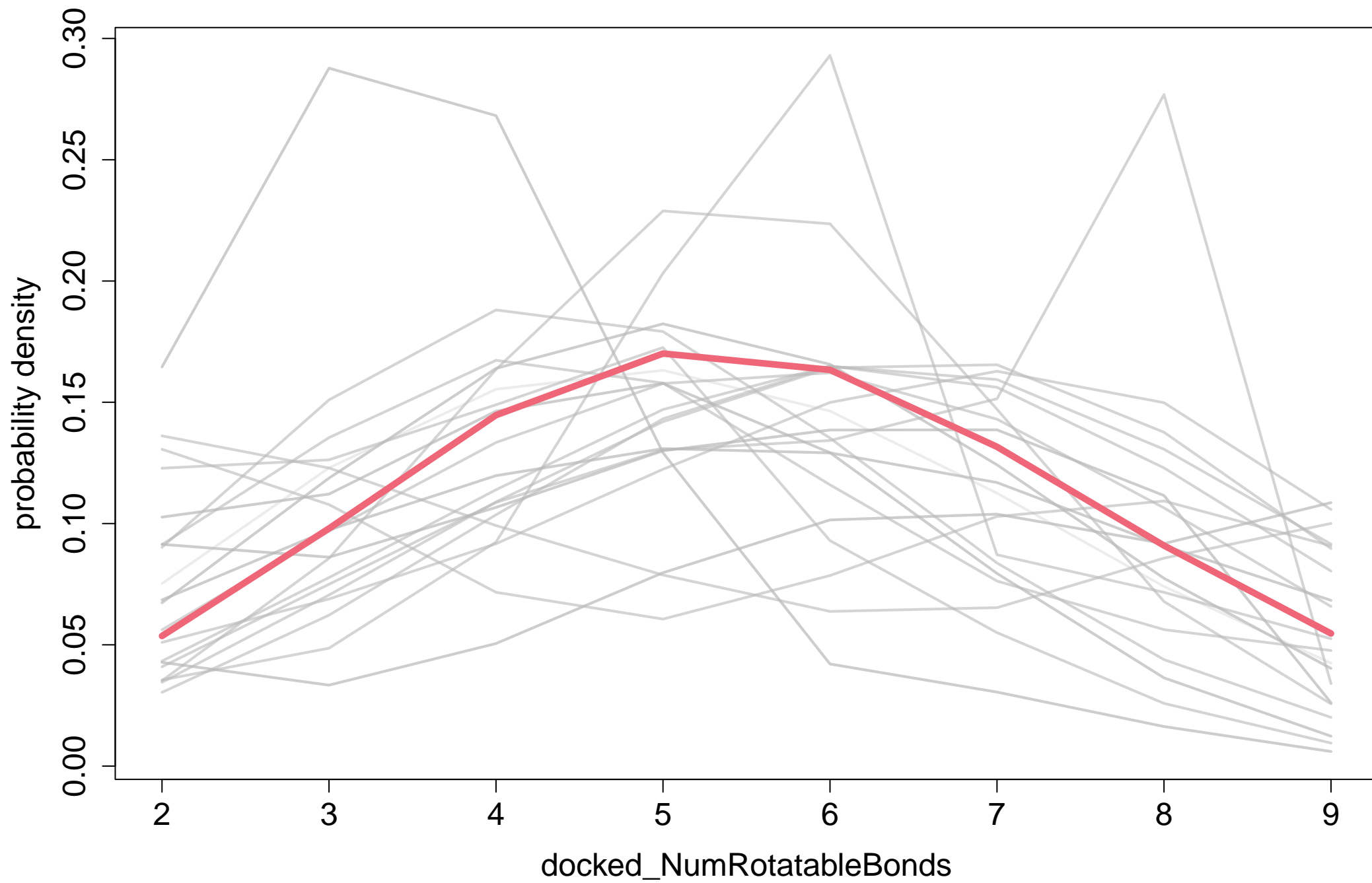




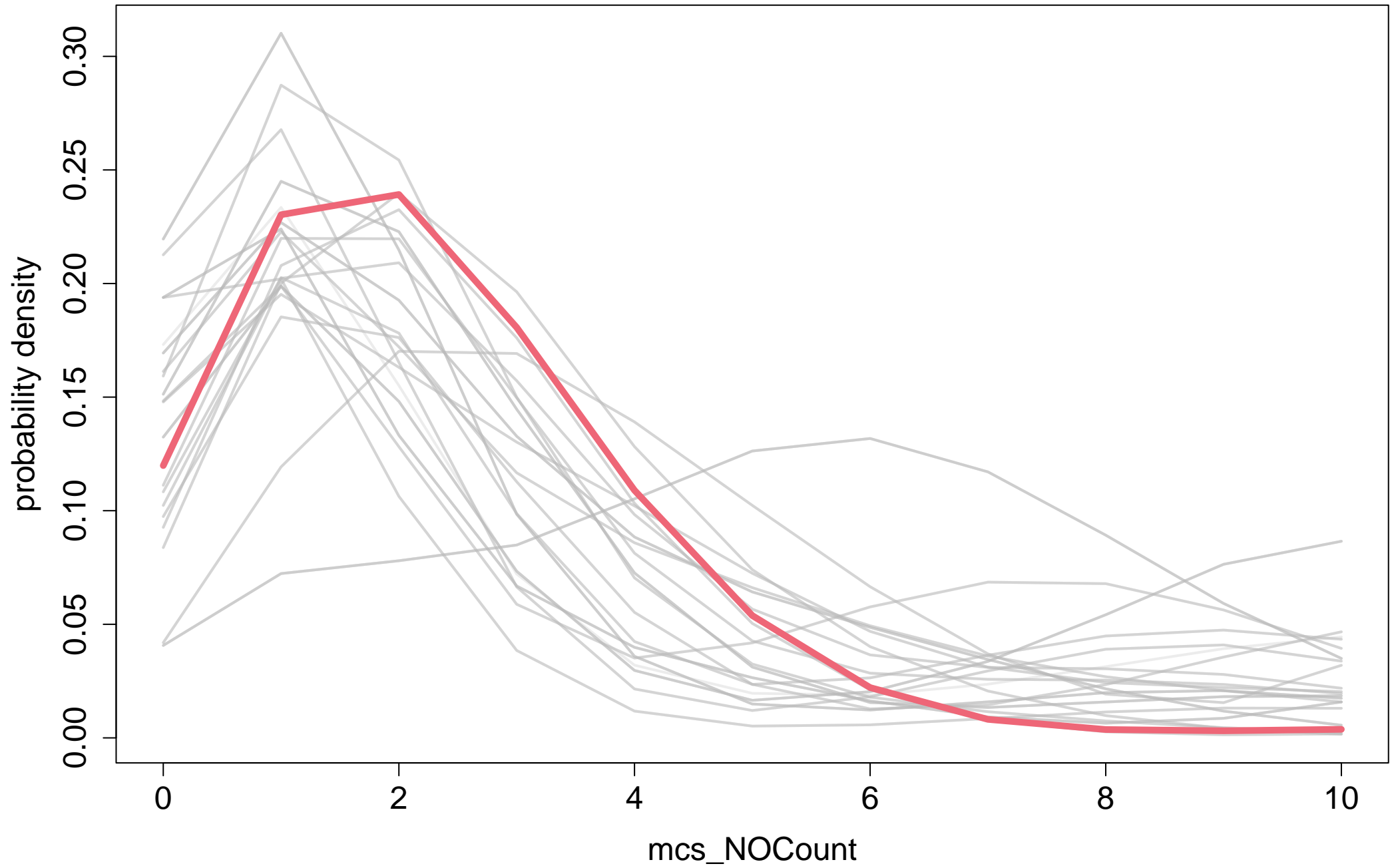


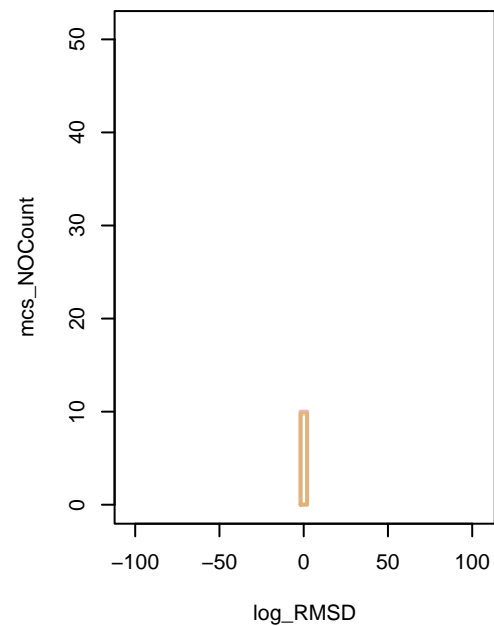
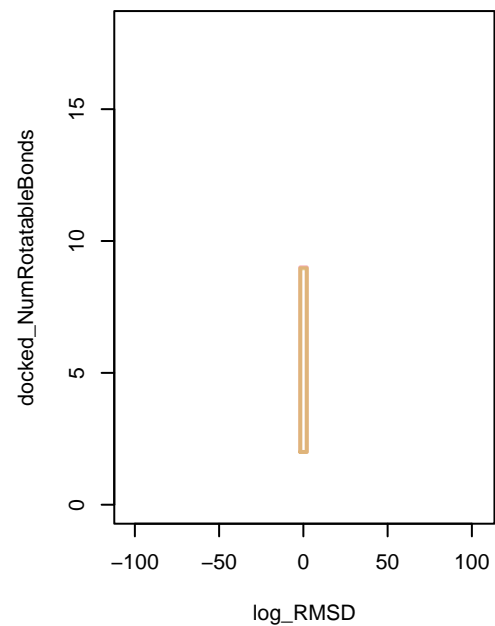
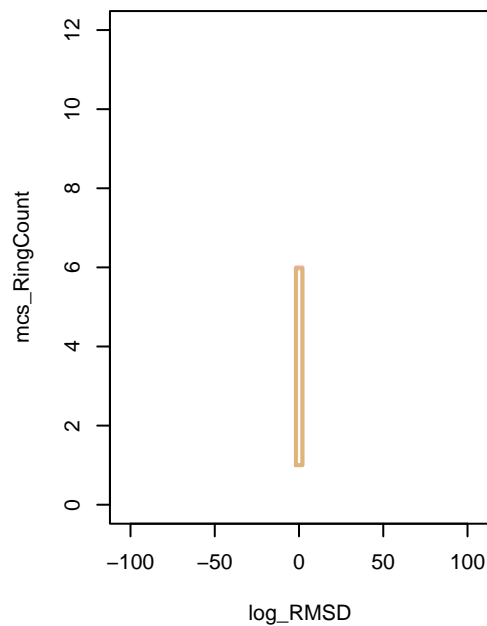
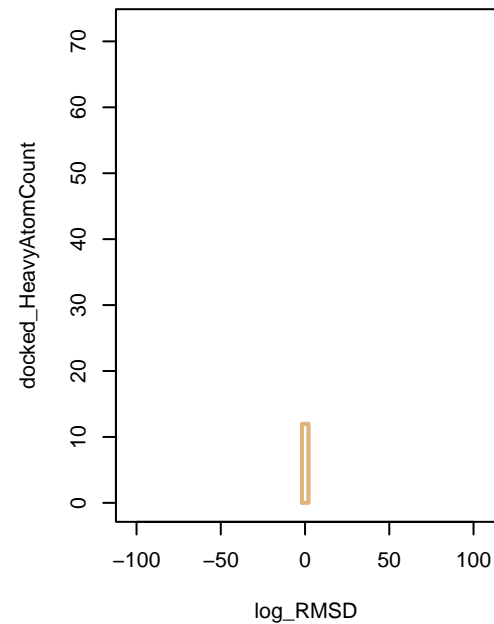
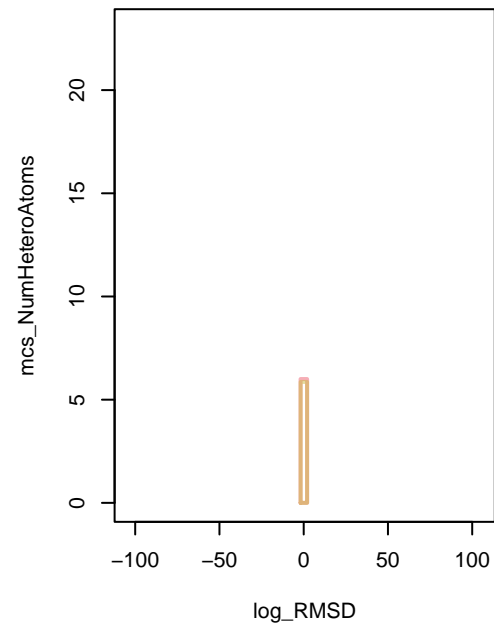
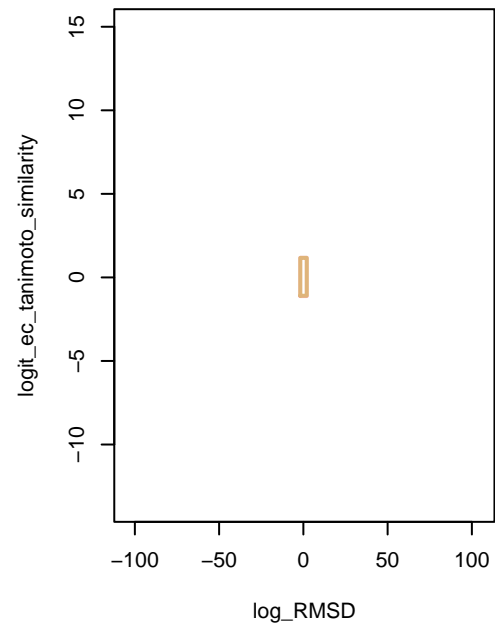
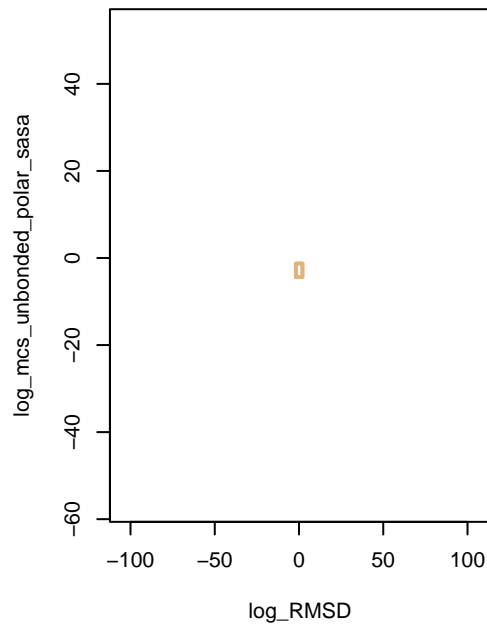




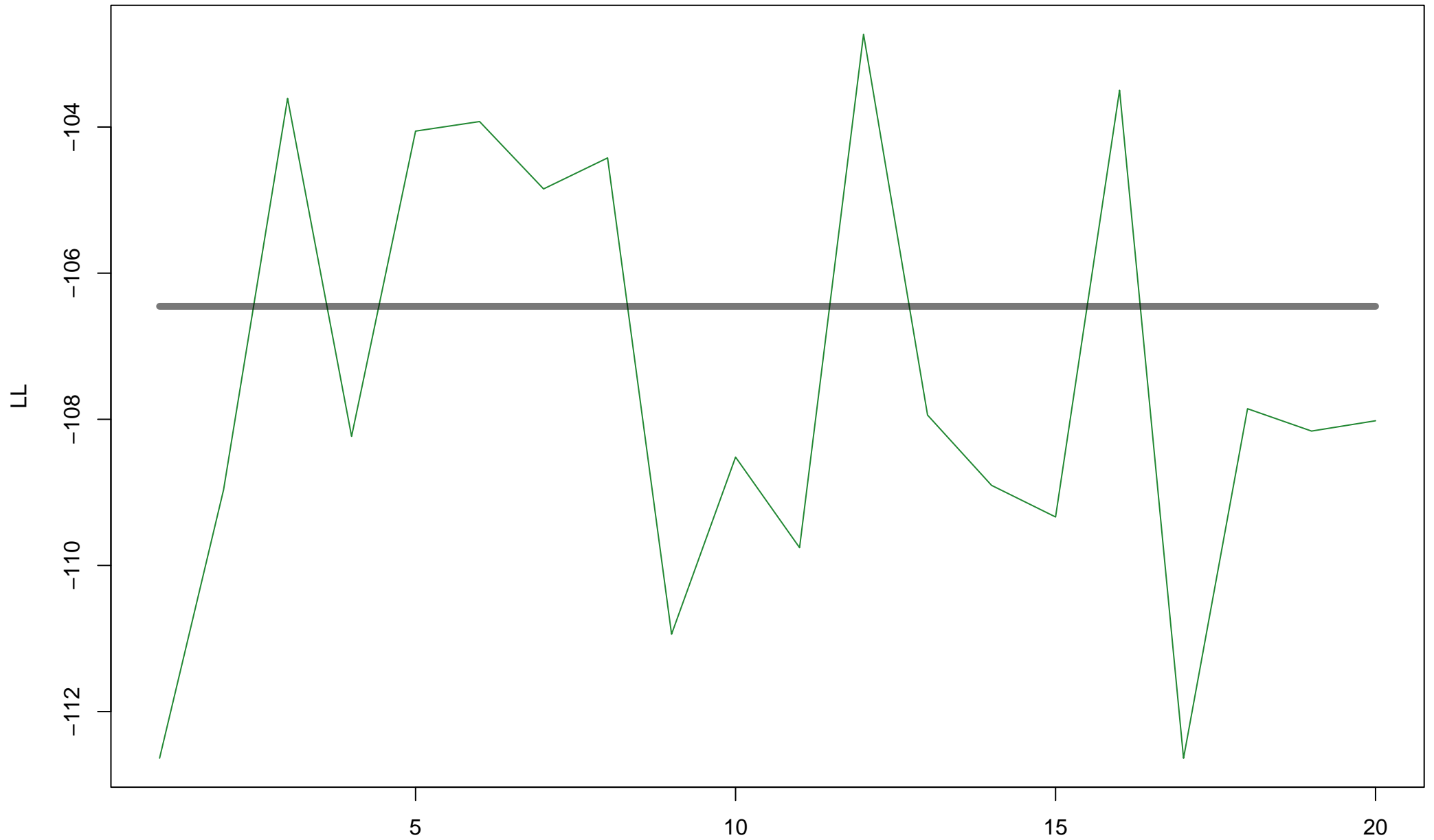




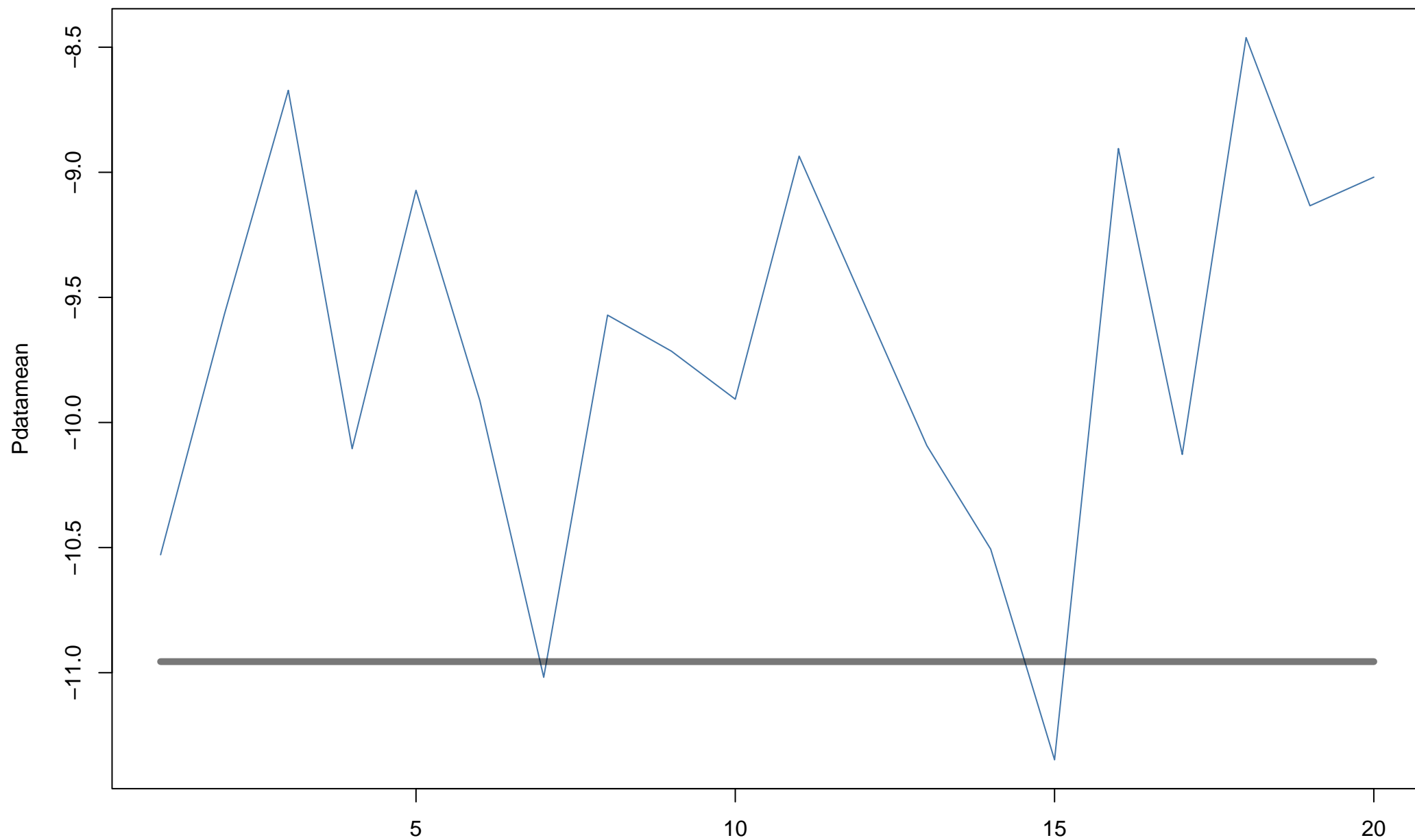




LL

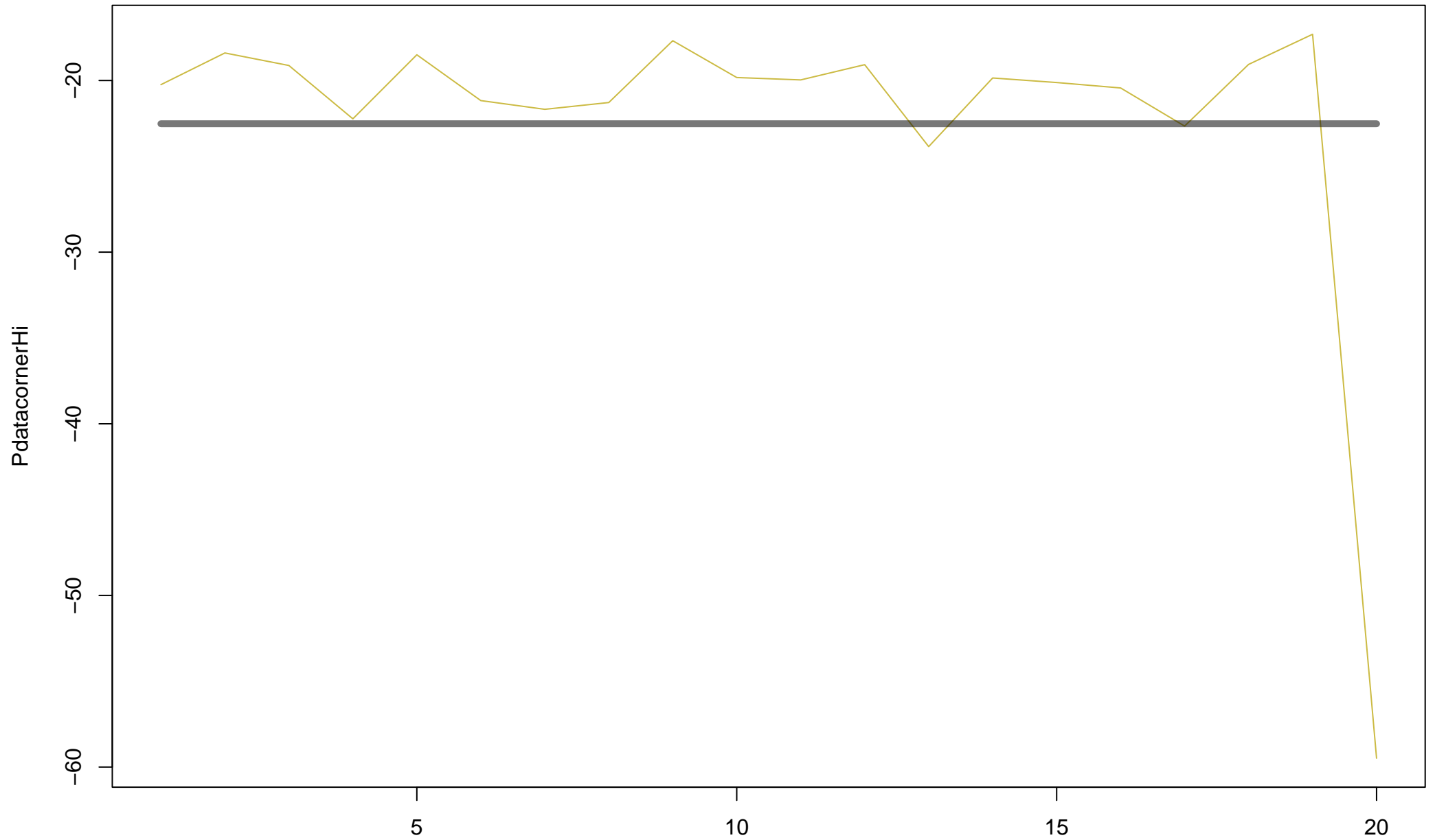


**Pdatamean**  
**ESS = 20 | BMK = 0.293 | MCSE(6.27) = 23.2 | stat: FALSE | burn: 20 | percentile: 10**

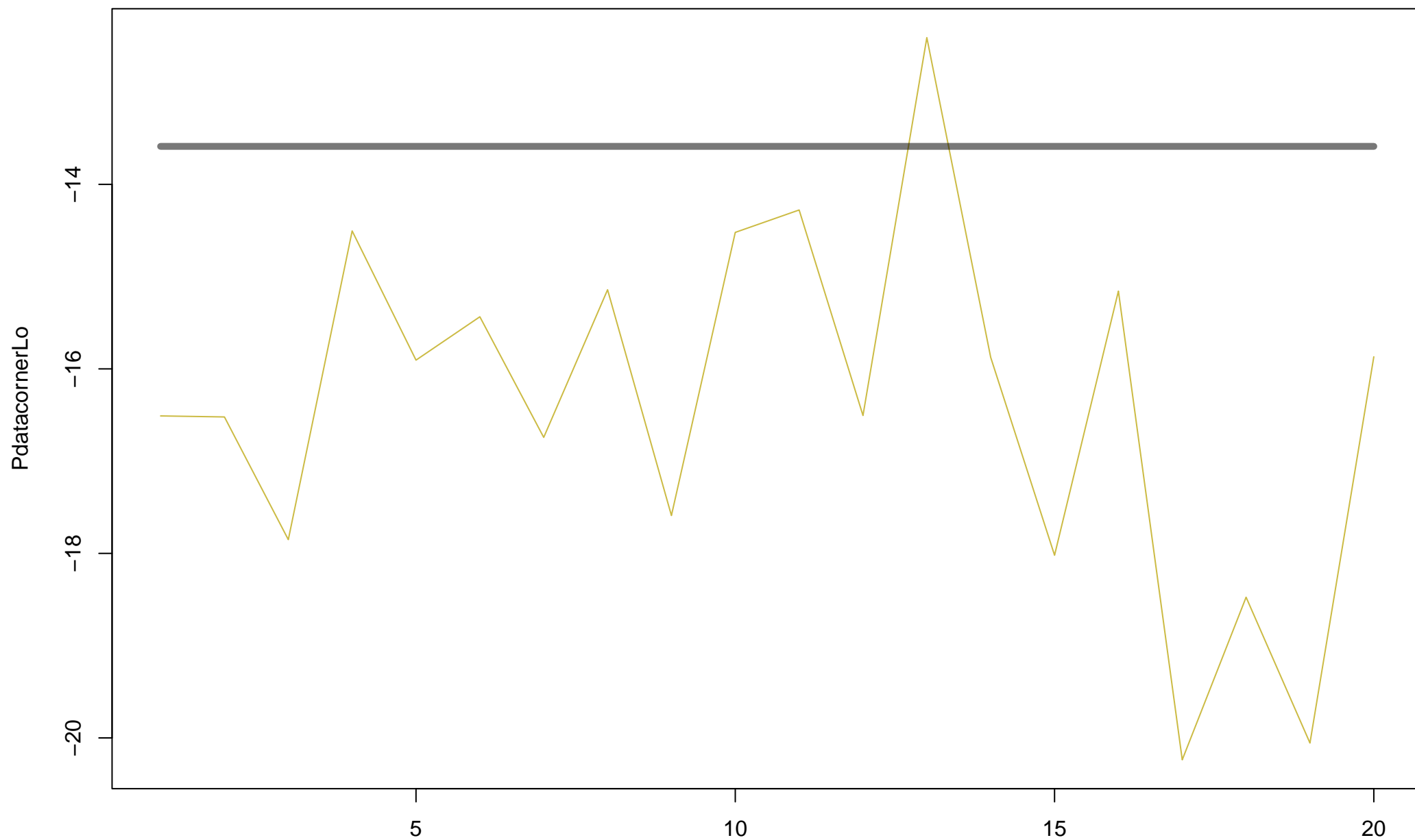


# PdatacornerHi

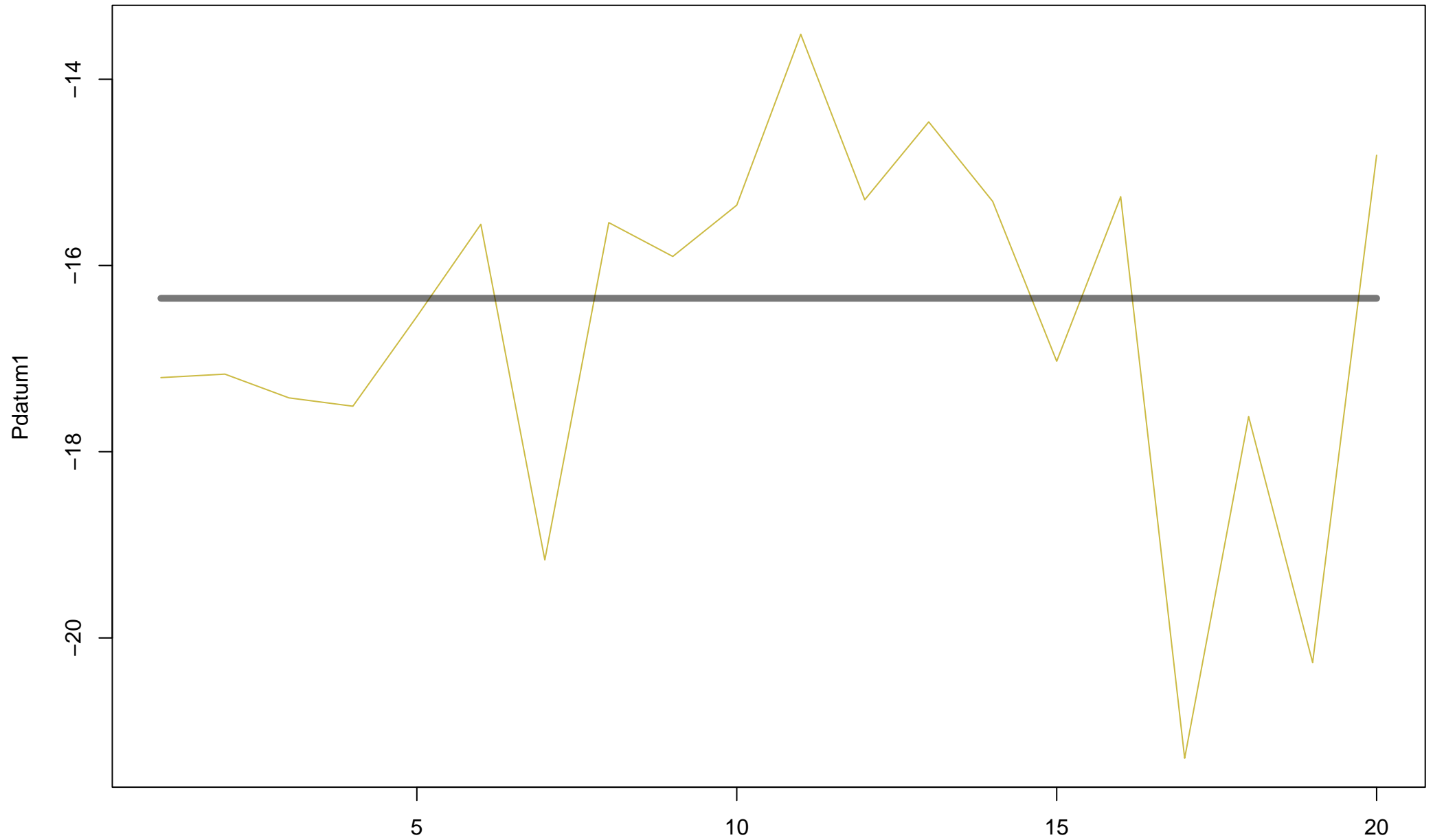
ESS = 2.22e-16 | BMK = 0.393 | MCSE(6.27) = 17.8 | stat: FALSE | burn: 20 | percentile: 15



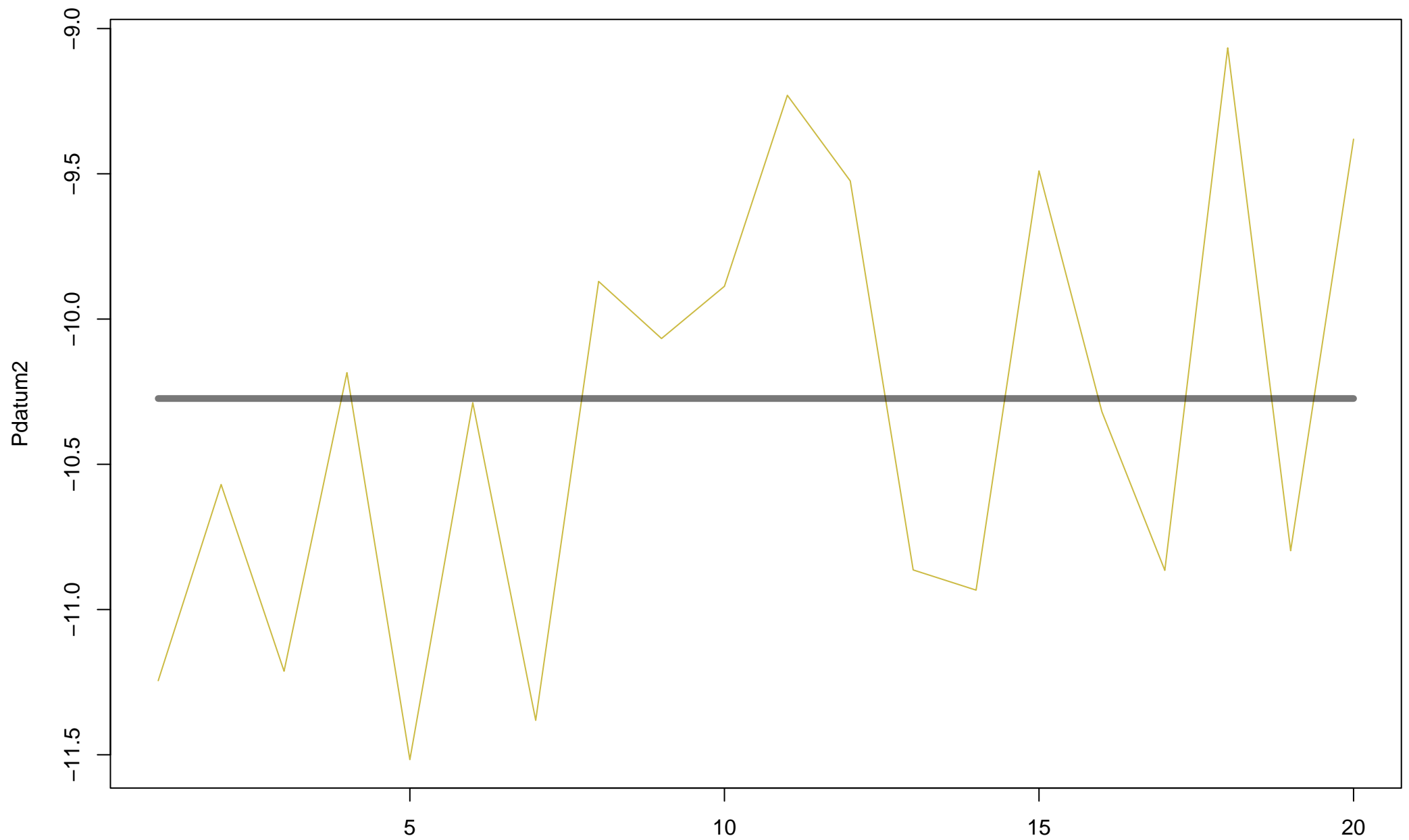
**PdatacornerLo**  
**ESS = 20 | BMK = 0.424 | MCSE(6.27) = 19.8 | stat: FALSE | burn: 20 | percentile: 95**



**Pdatum1**  
**ESS = 20 | BMK = 0.475 | MCSE(6.27) = 34.3 | stat: FALSE | burn: 20 | percentile: 50**

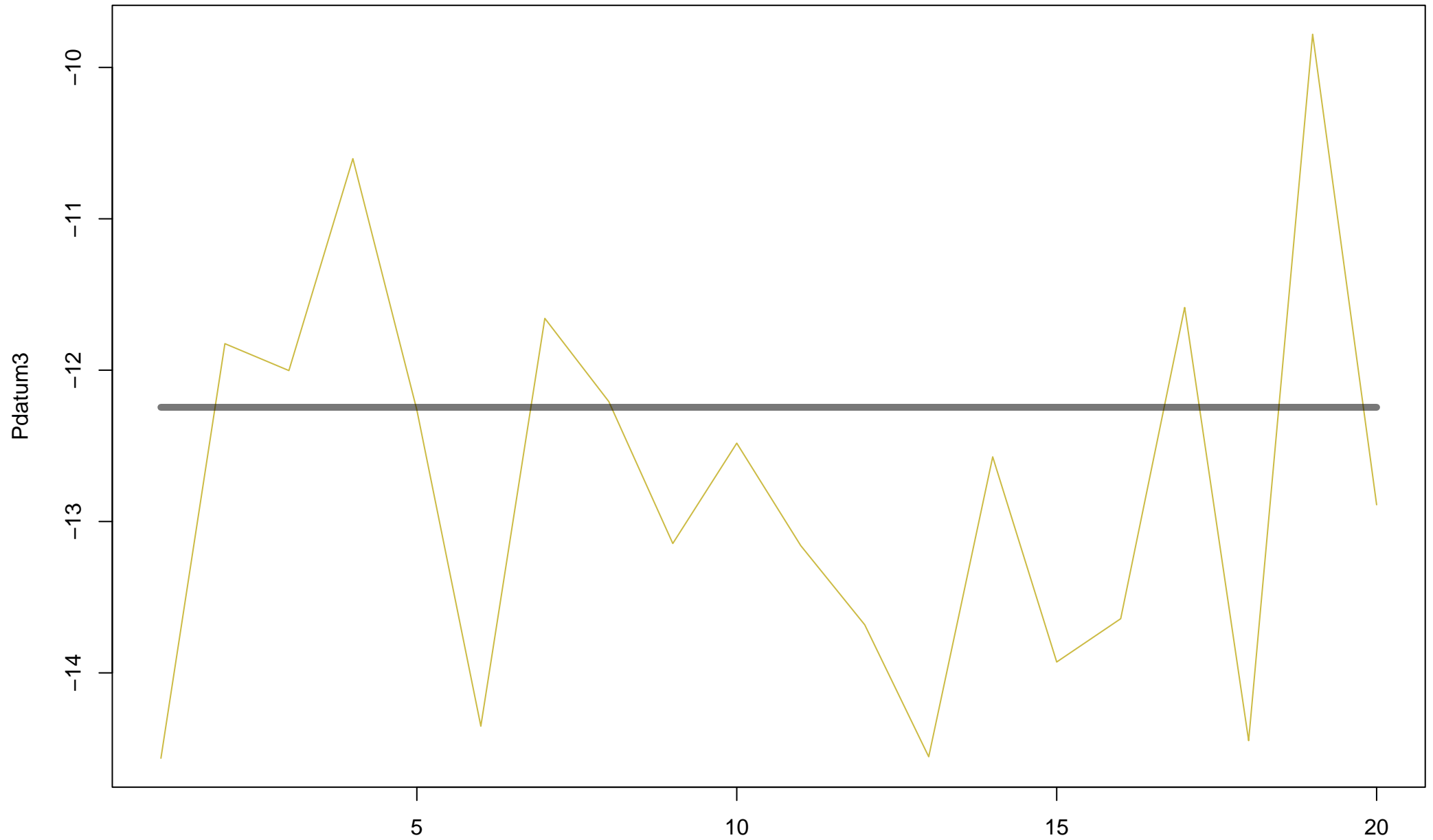


**Pdatum2**  
**ESS = 20 | BMK = 0.435 | MCSE(6.27) = 21.2 | stat: FALSE | burn: 16 | percentile: 55**

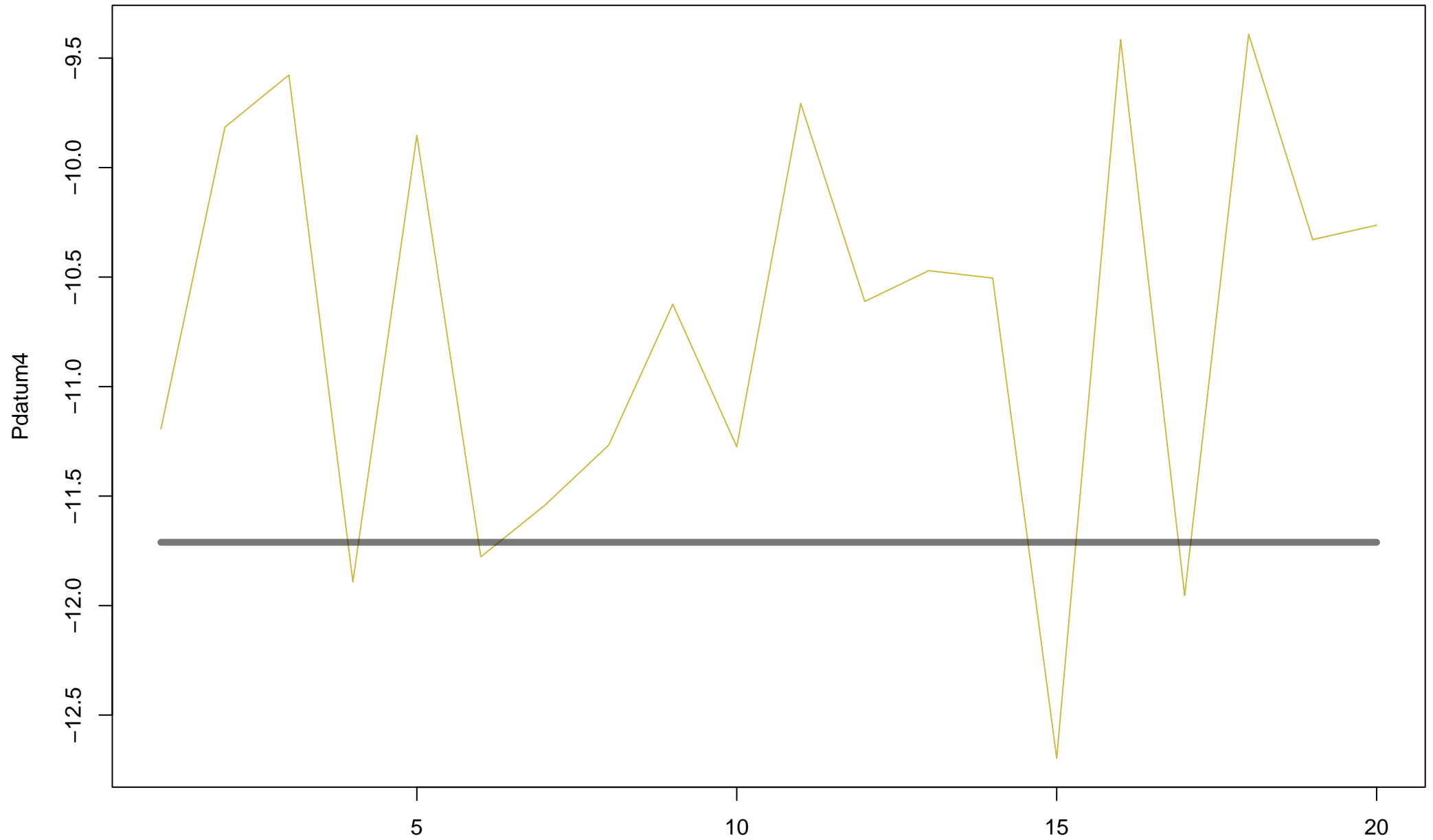




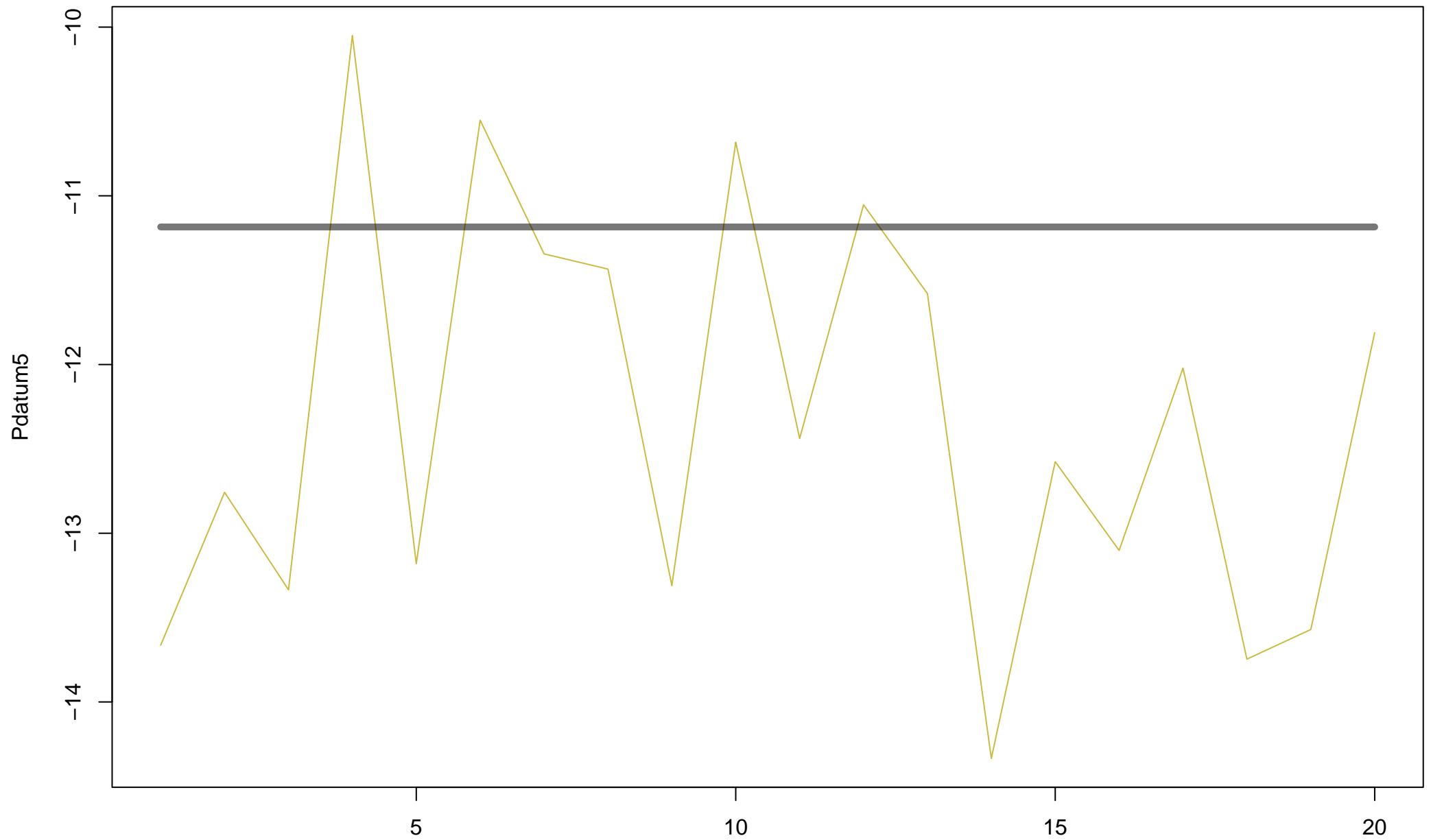
**Pdatum3**  
**ESS = 20 | BMK = 0.721 | MCSE(6.27) = 18.5 | stat: FALSE | burn: 20 | percentile: 65**



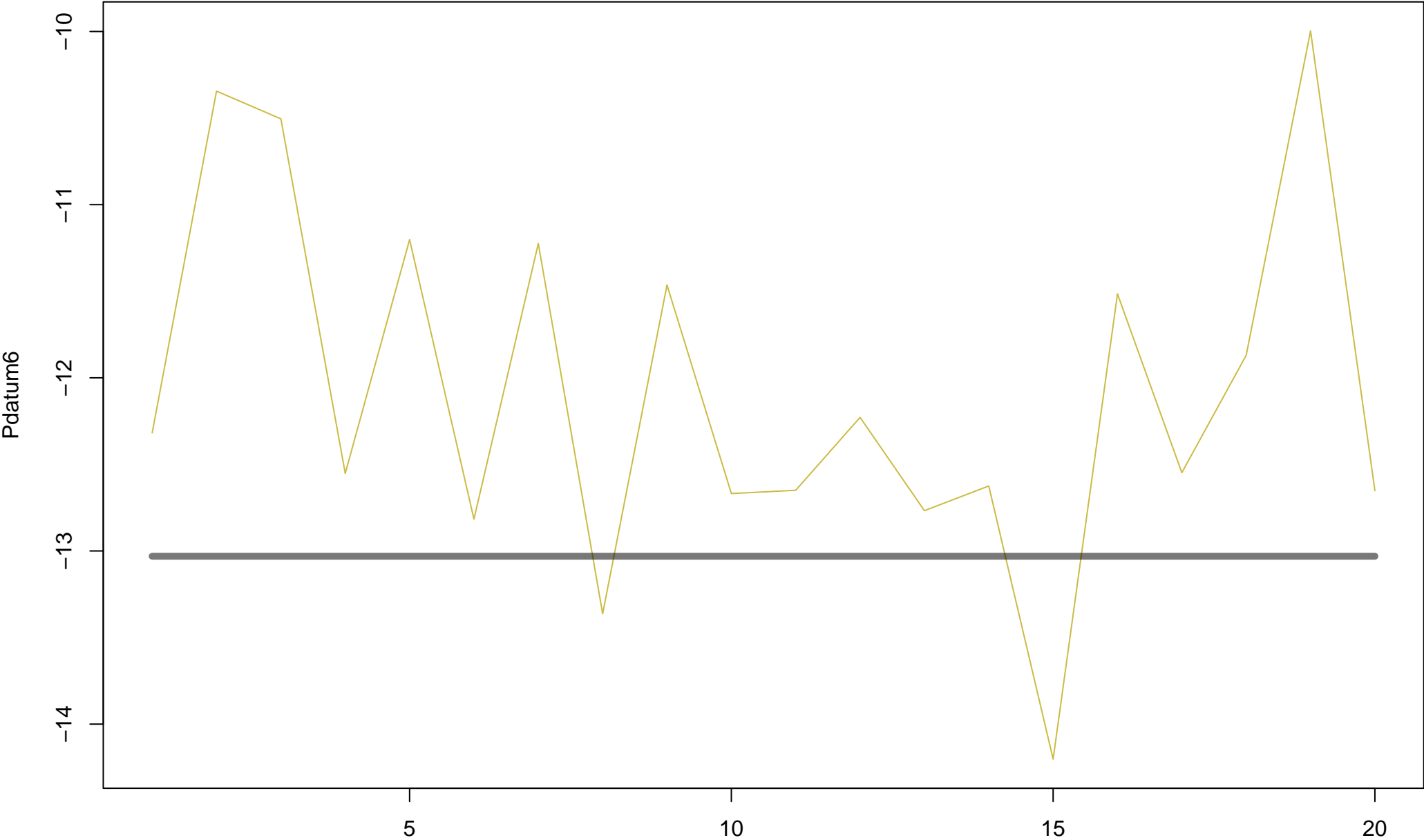
**Pdatum4**  
**ESS = 20 | BMK = 0.162 | MCSE(6.27) = 10.6 | stat: FALSE | burn: 20 | percentile: 20**



**Pdatum5**  
**ESS = 20 | BMK = 0.399 | MCSE(6.27) = 19.5 | stat: FALSE | burn: 16 | percentile: 80**

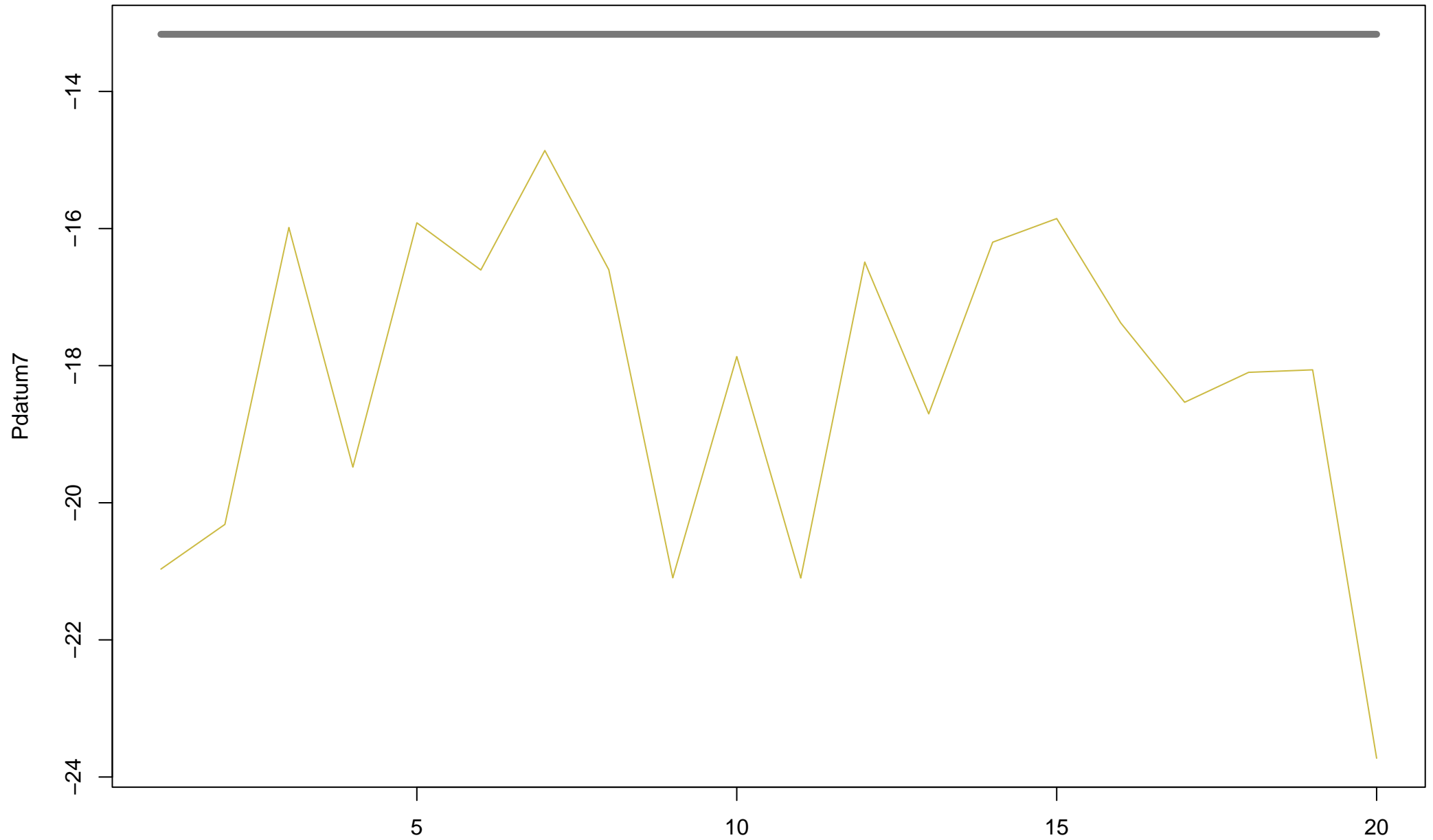


**Pdatum6**  
**ESS = 20 | BMK = 0.493 | MCSE(6.27) = 21.3 | stat: FALSE | burn: 20 | percentile: 10**

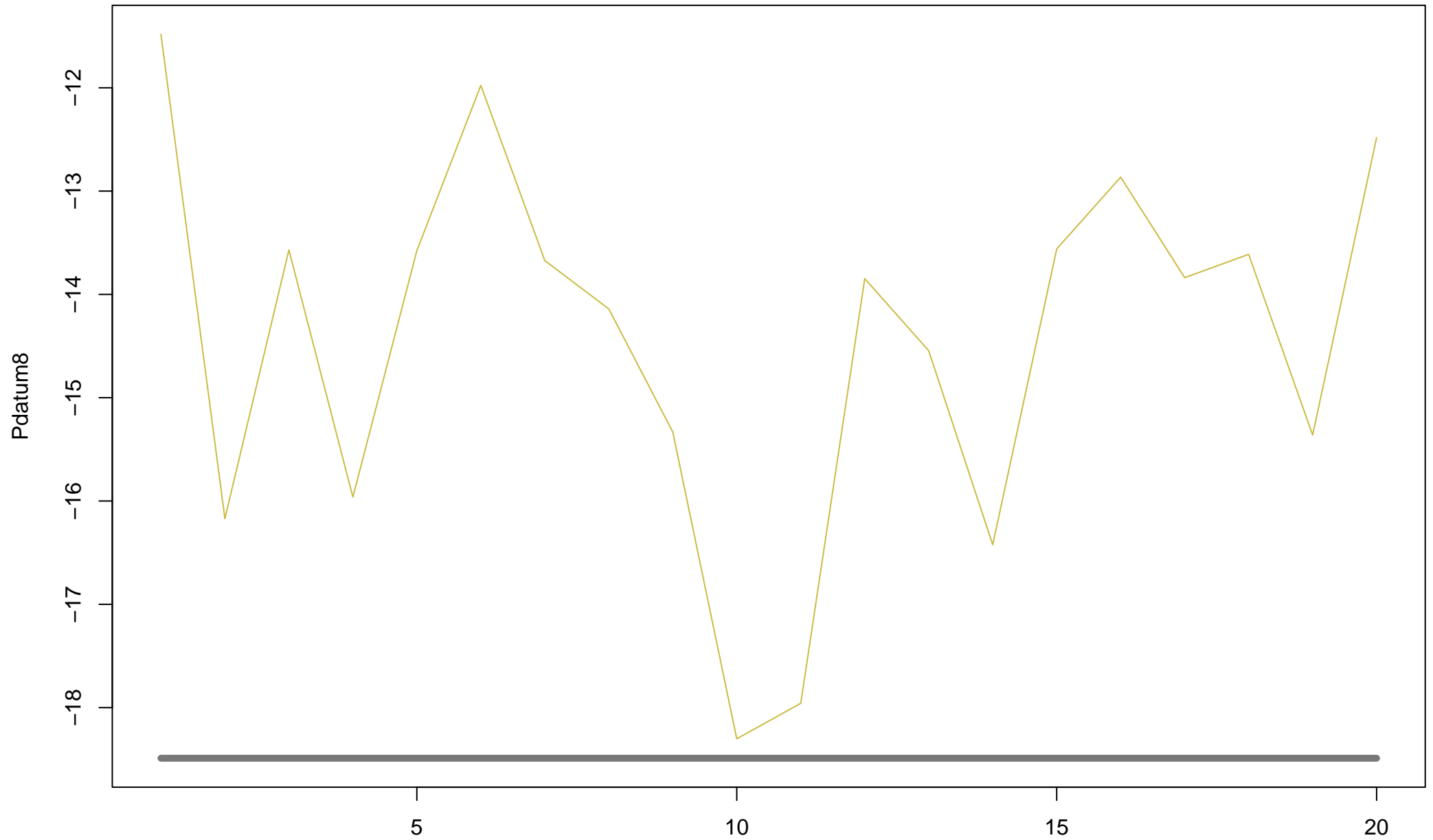


Pdatum7

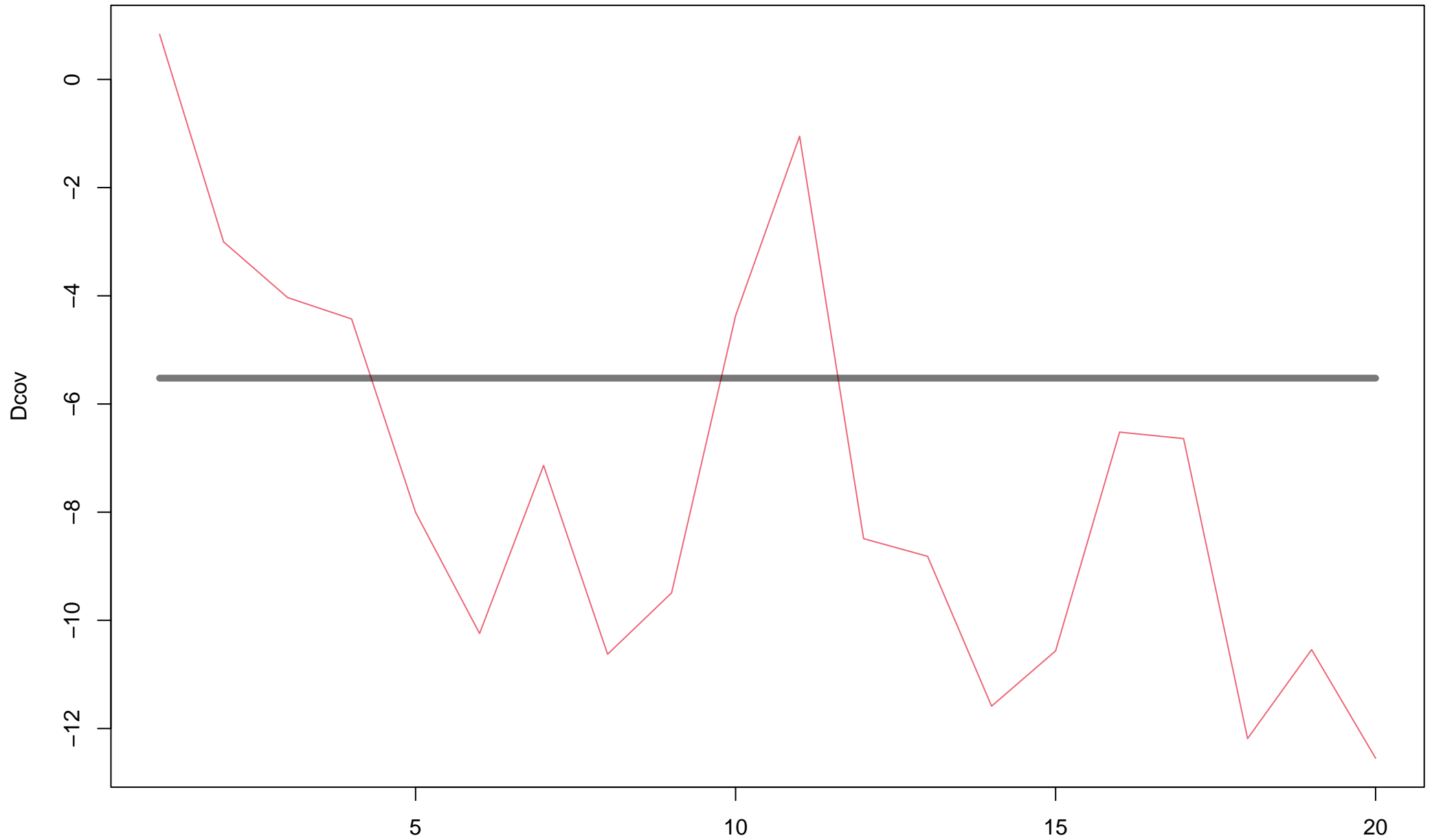
ESS = 20 | BMK = 0.247 | MCSE(6.27) = 25.1 | stat: FALSE | burn: 20 | percentile: 100



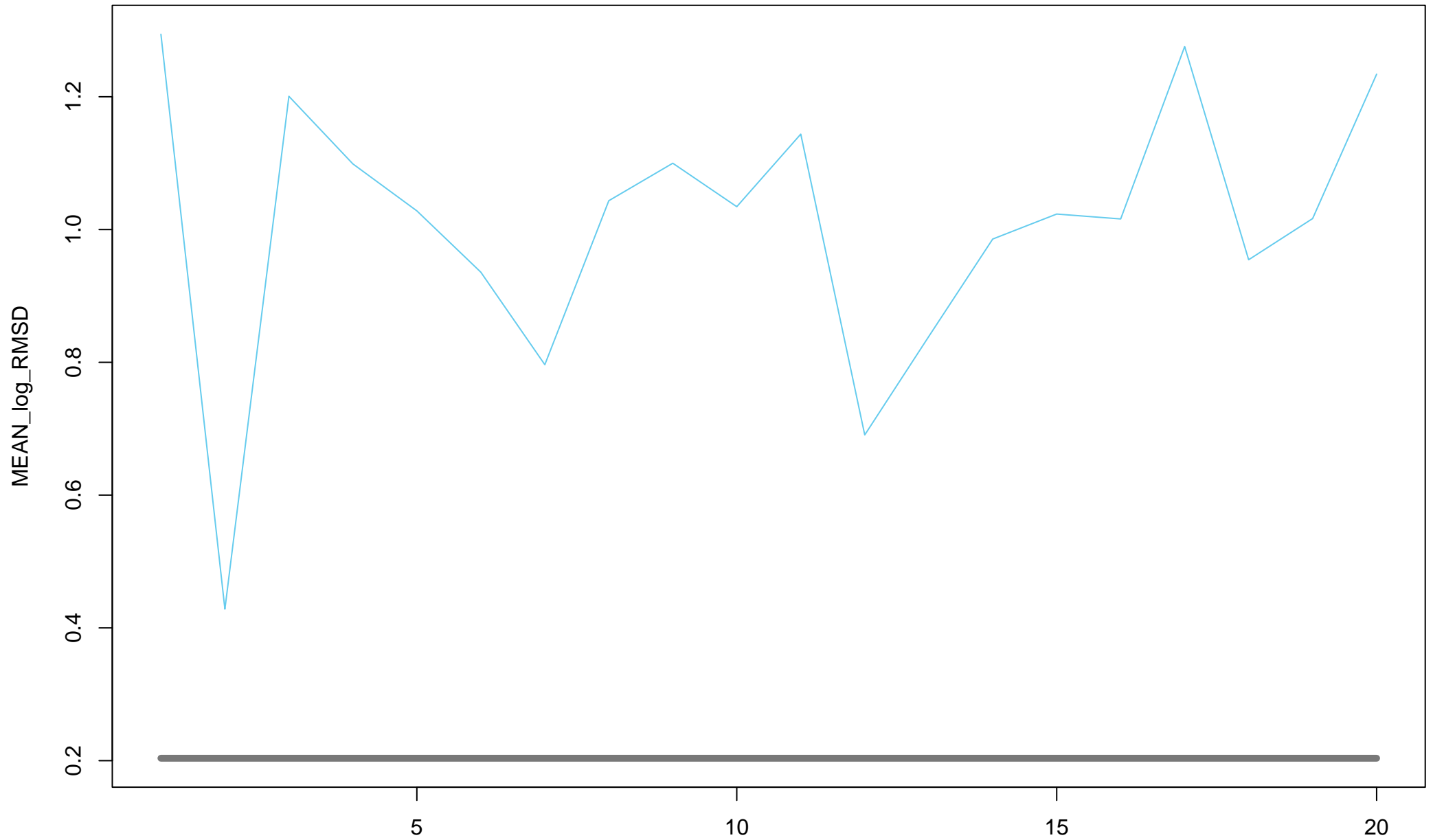
**Pdatum8**  
**ESS = 20 | BMK = 0.403 | MCSE(6.27) = 20.4 | stat: FALSE | burn: 20 | percentile: 0**



**Dcov**  
**ESS = 20 | BMK = 1 | MCSE(6.27) = 21 | stat: FALSE | burn: 20 | percentile: 85**

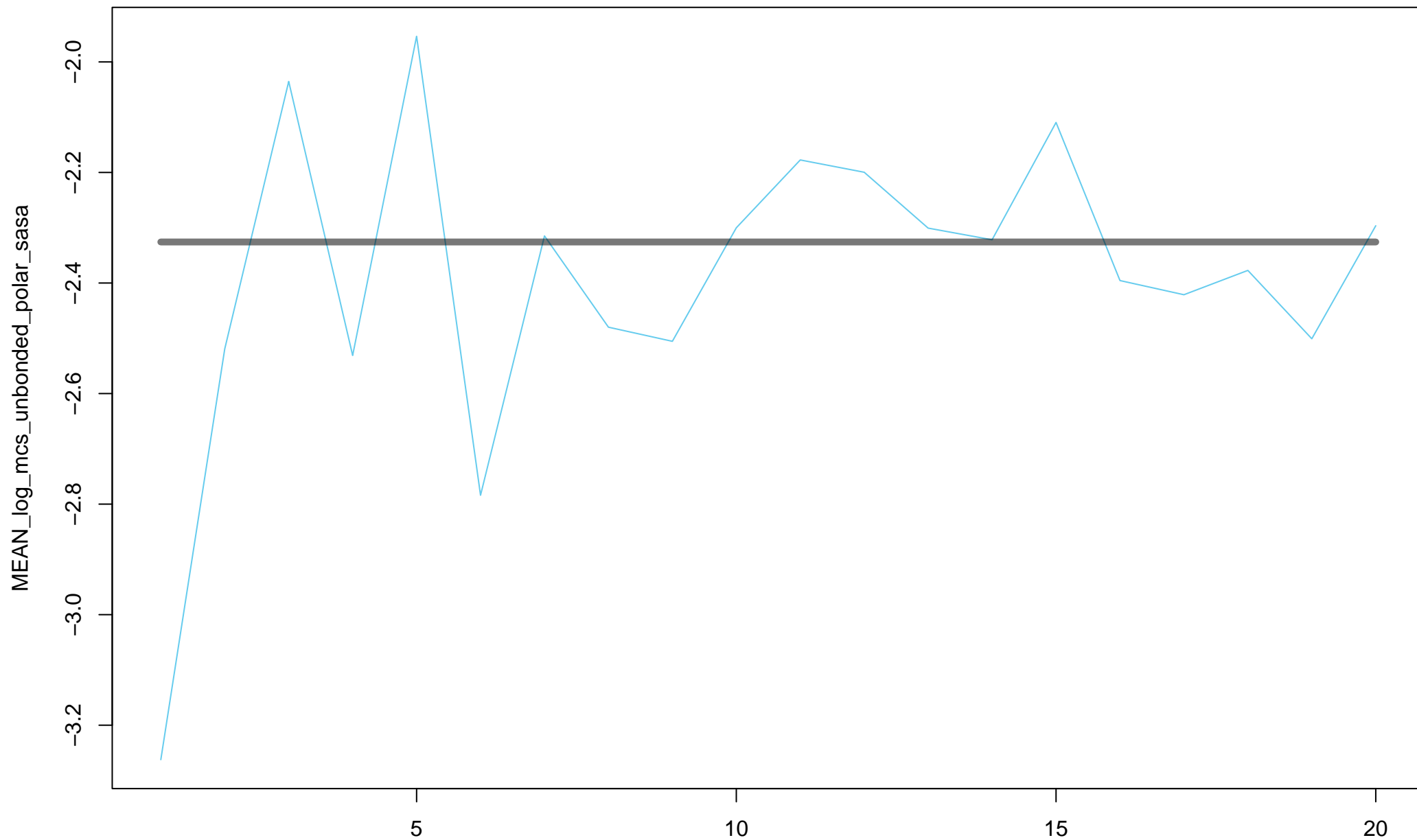


**MEAN\_log\_RMSD**  
**ESS = 20 | BMK = 0.248 | MCSE(6.27) = 13.8 | stat: FALSE | burn: 16 | percentile: 0**

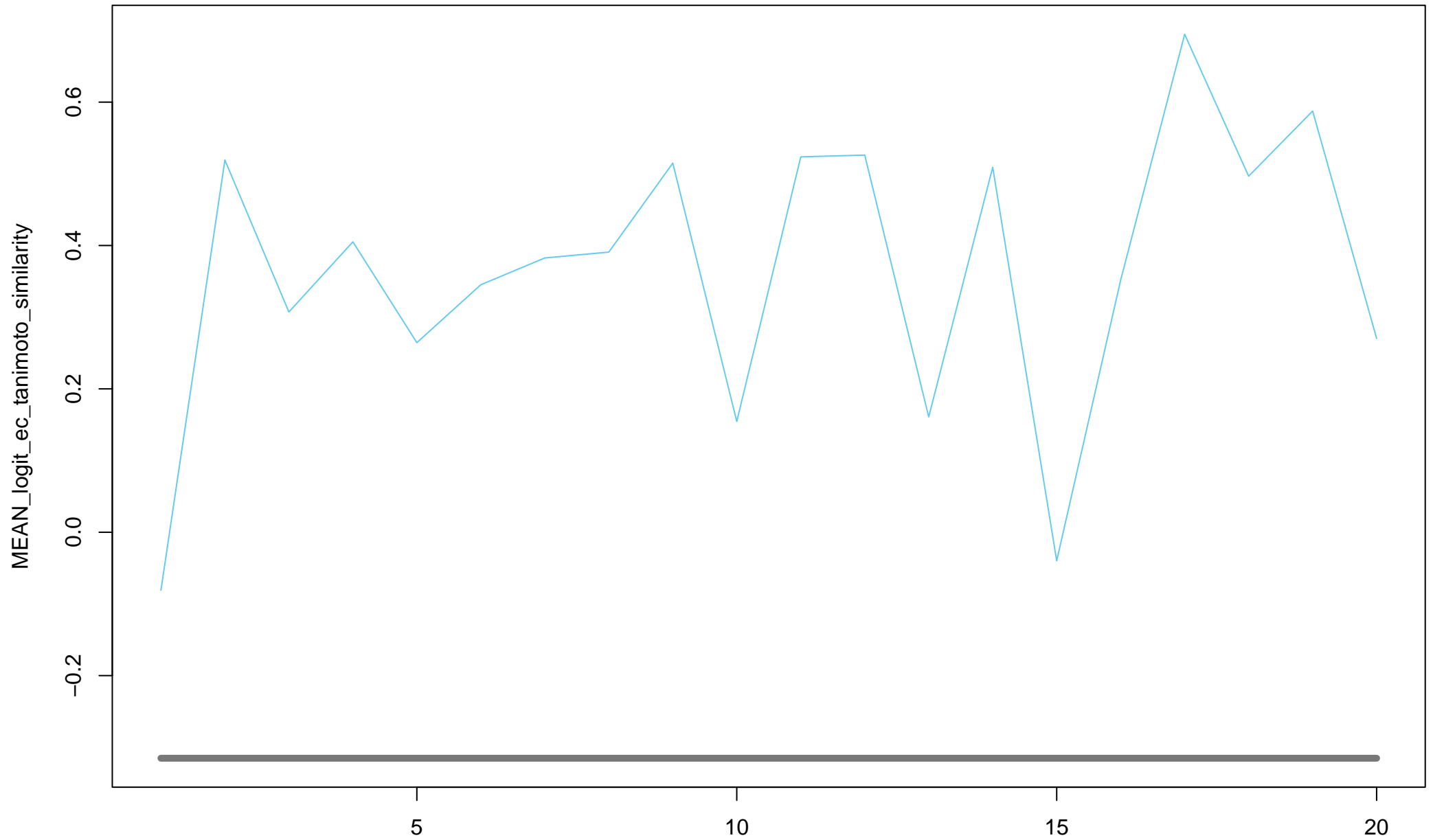




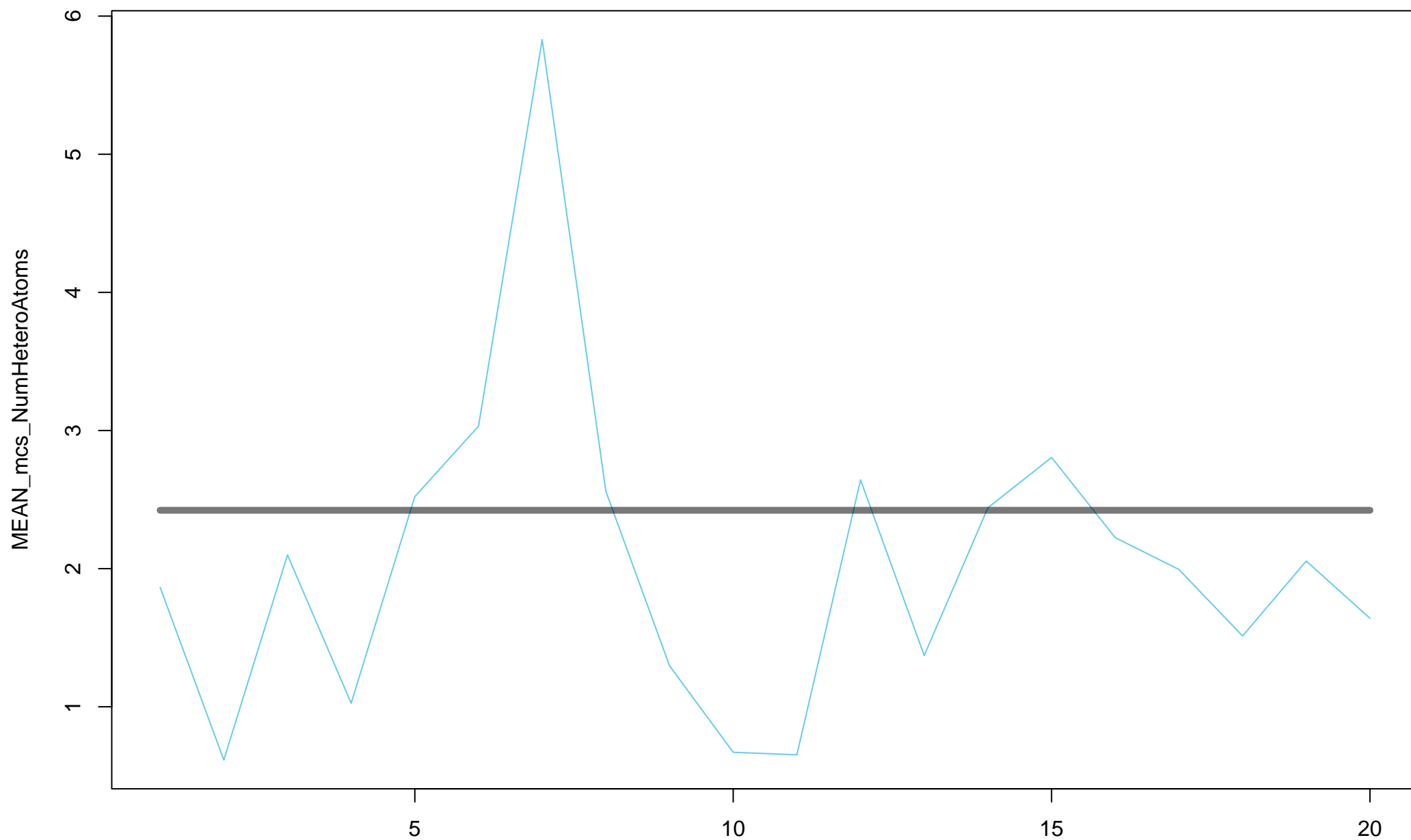
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 20 | BMK = 0.439 | MCSE(6.27) = 19.2 | stat: FALSE | burn: 20 | percentile: 50**



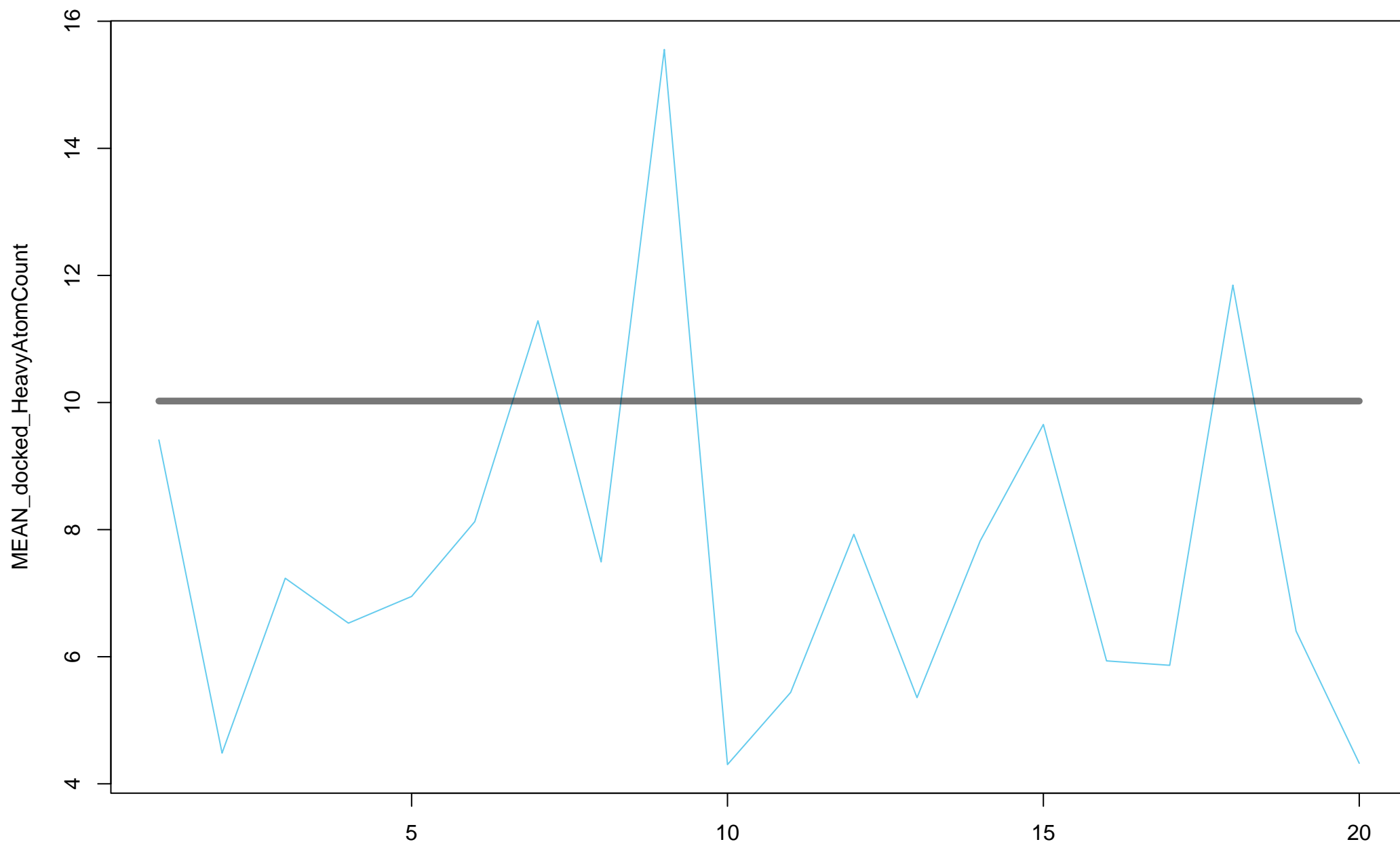
**MEAN\_logit\_ec\_tanimoto\_similarity**  
**ESS = 20 | BMK = 0.299 | MCSE(6.27) = 15.7 | stat: FALSE | burn: 20 | percentile: 0**



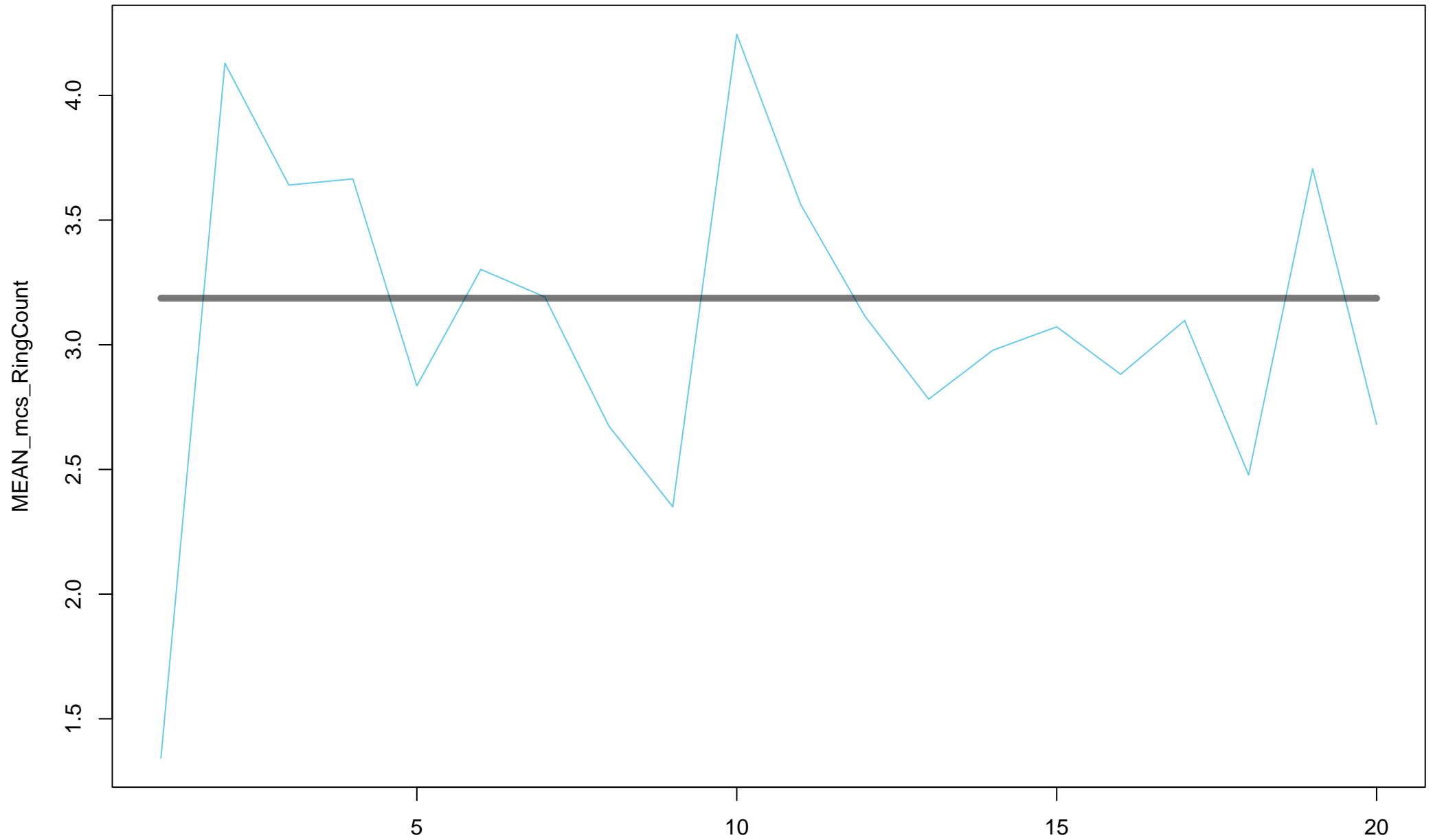
**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 20 | BMK = 0.262 | MCSE(6.27) = 32.1 | stat: FALSE | burn: 16 | percentile: 65**



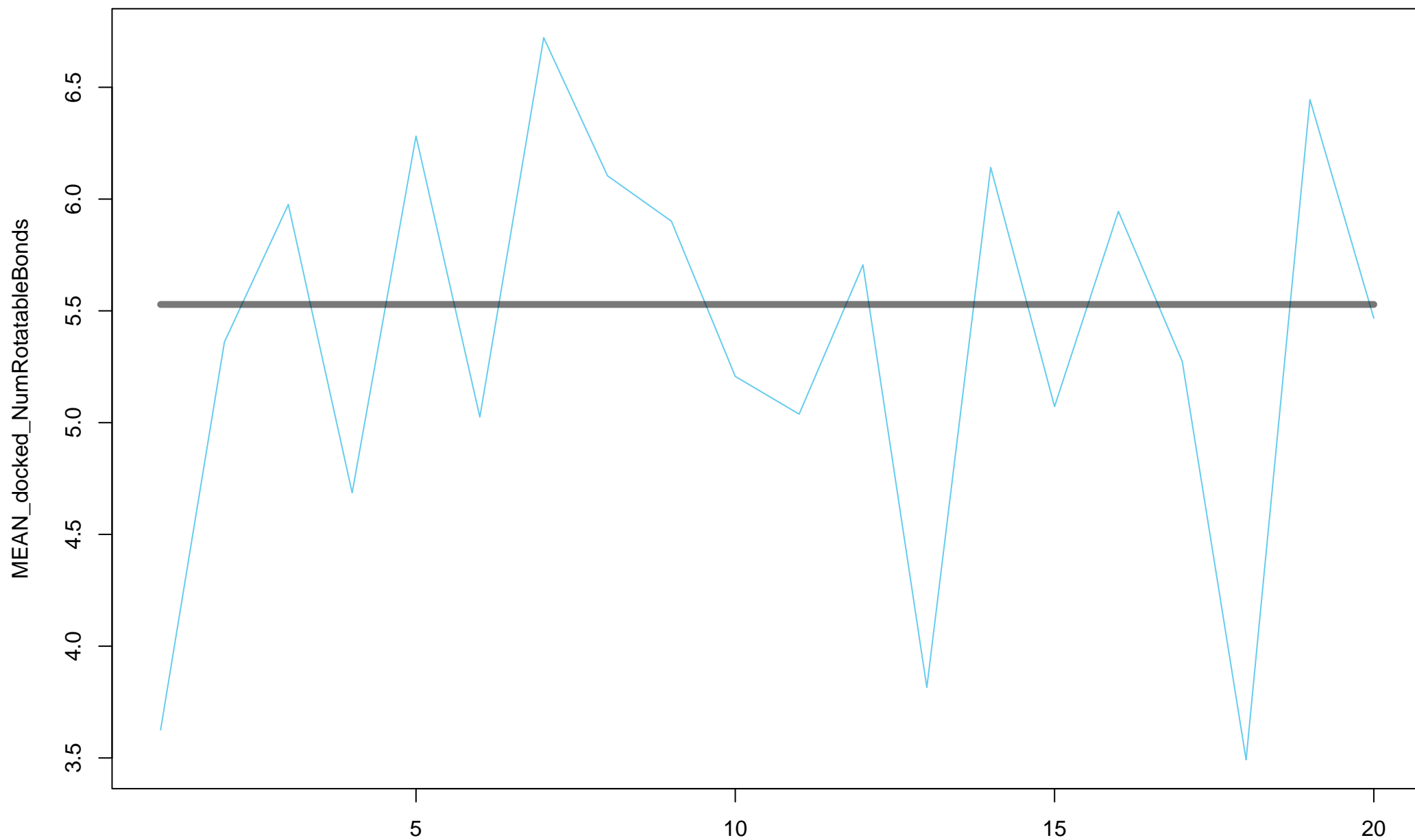
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 20 | BMK = 0.211 | MCSE(6.27) = 16.5 | stat: FALSE | burn: 20 | percentile: 85**



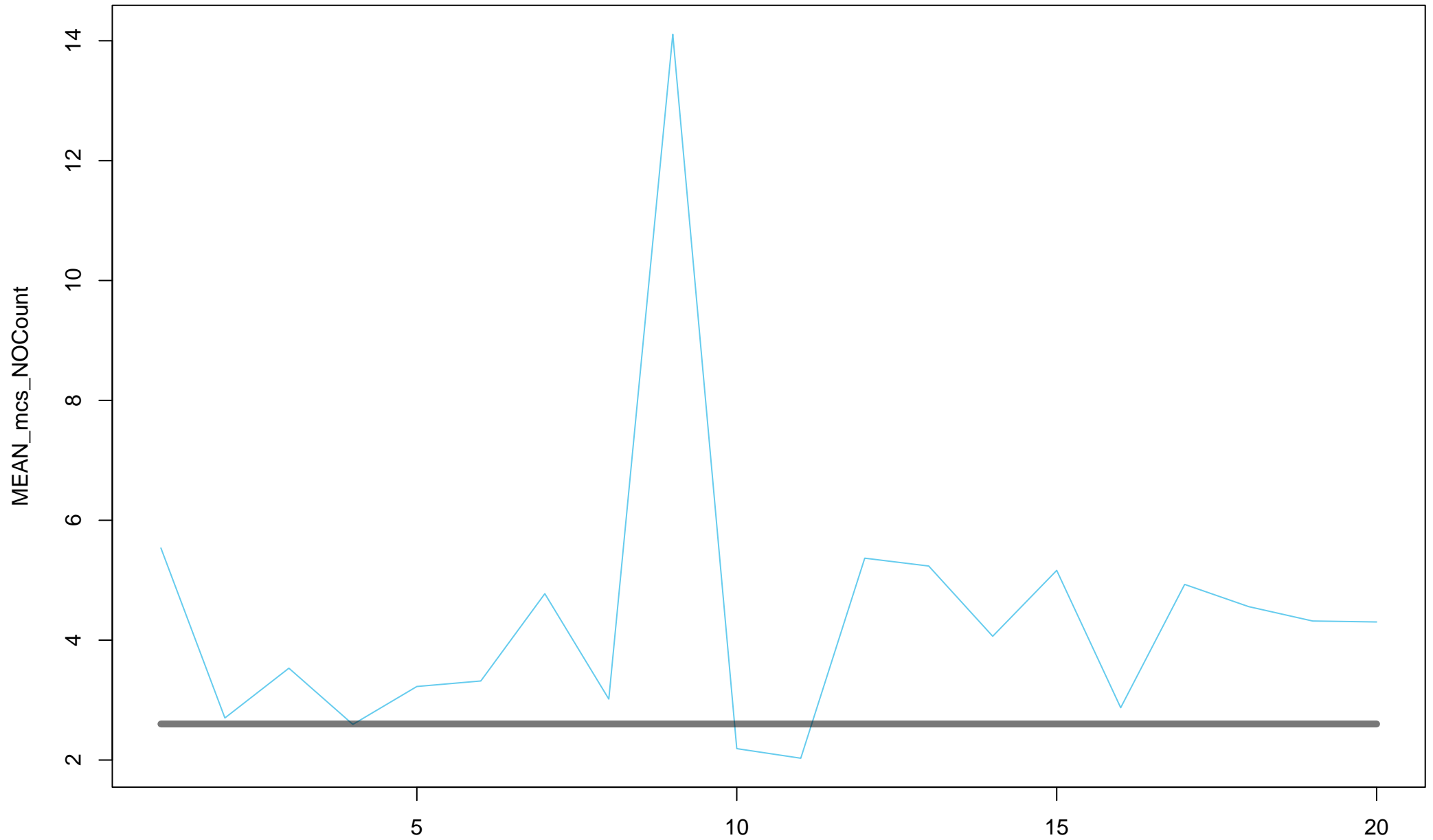
**MEAN\_mcs\_RingCount**  
**ESS = 20 | BMK = 0.4 | MCSE(6.27) = 16.6 | stat: FALSE | burn: 20 | percentile: 60**



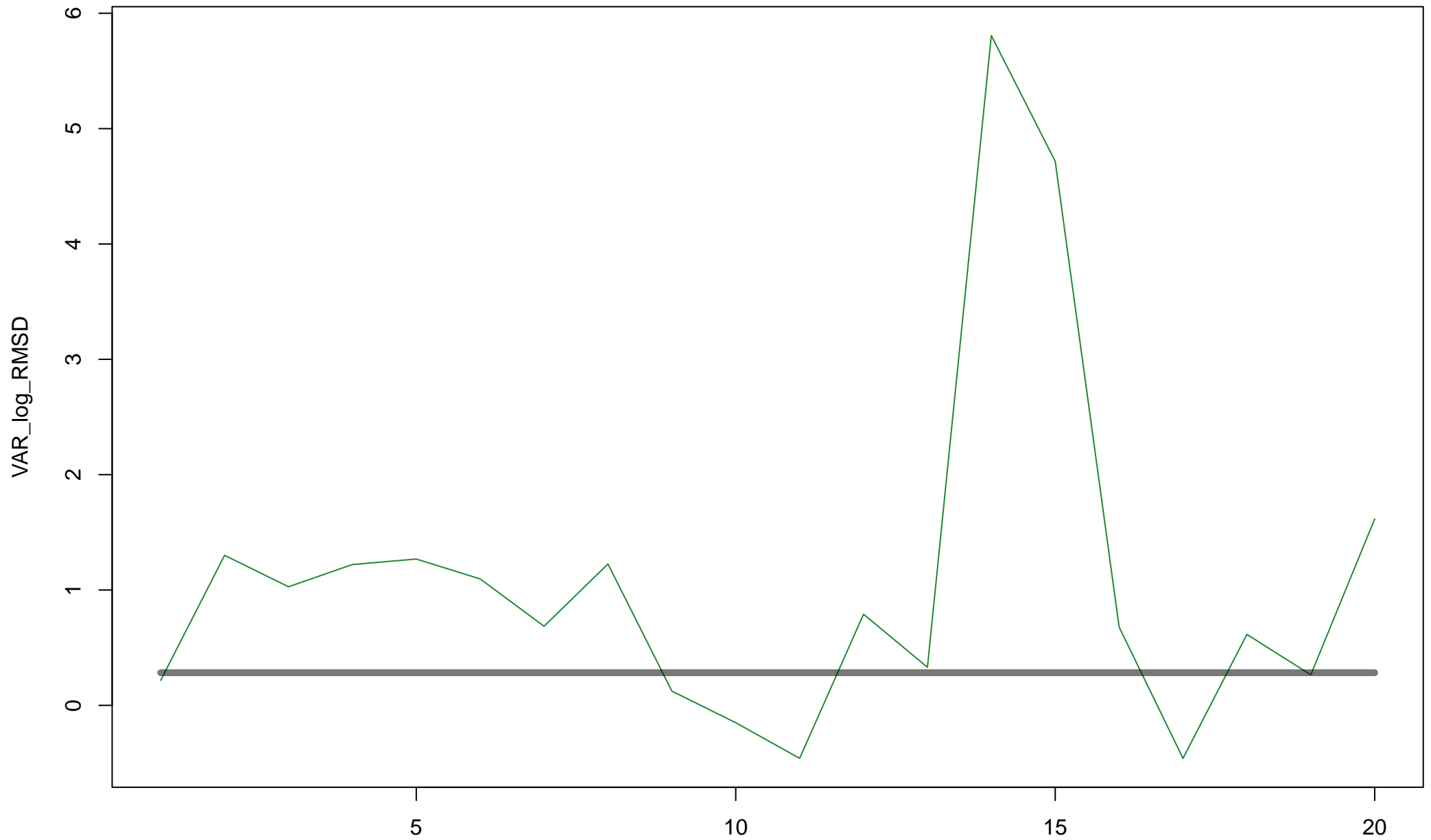
**MEAN\_docked\_NumRotatableBonds**  
**ESS = 20 | BMK = 0.108 | MCSE(6.27) = 14.4 | stat: FALSE | burn: 20 | percentile: 55**



**MEAN\_mcs\_NOCount**  
**ESS = 20 | BMK = 0.407 | MCSE(6.27) = 15.6 | stat: FALSE | burn: 20 | percentile: 15**

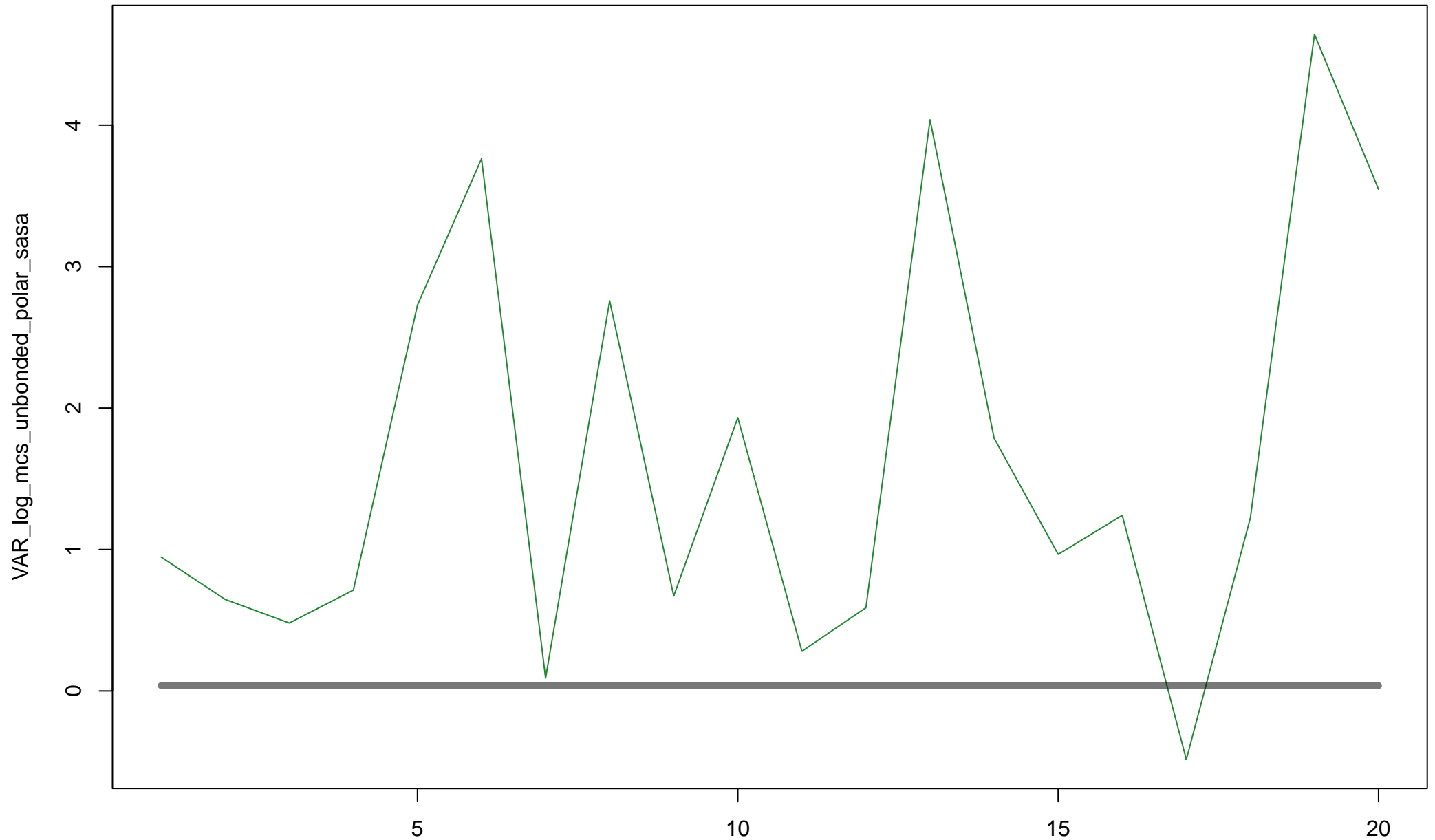


**VAR\_log\_RMSD**  
**ESS = 20 | BMK = 1 | MCSE(6.27) = 28.7 | stat: FALSE | burn: 20 | percentile: 30**

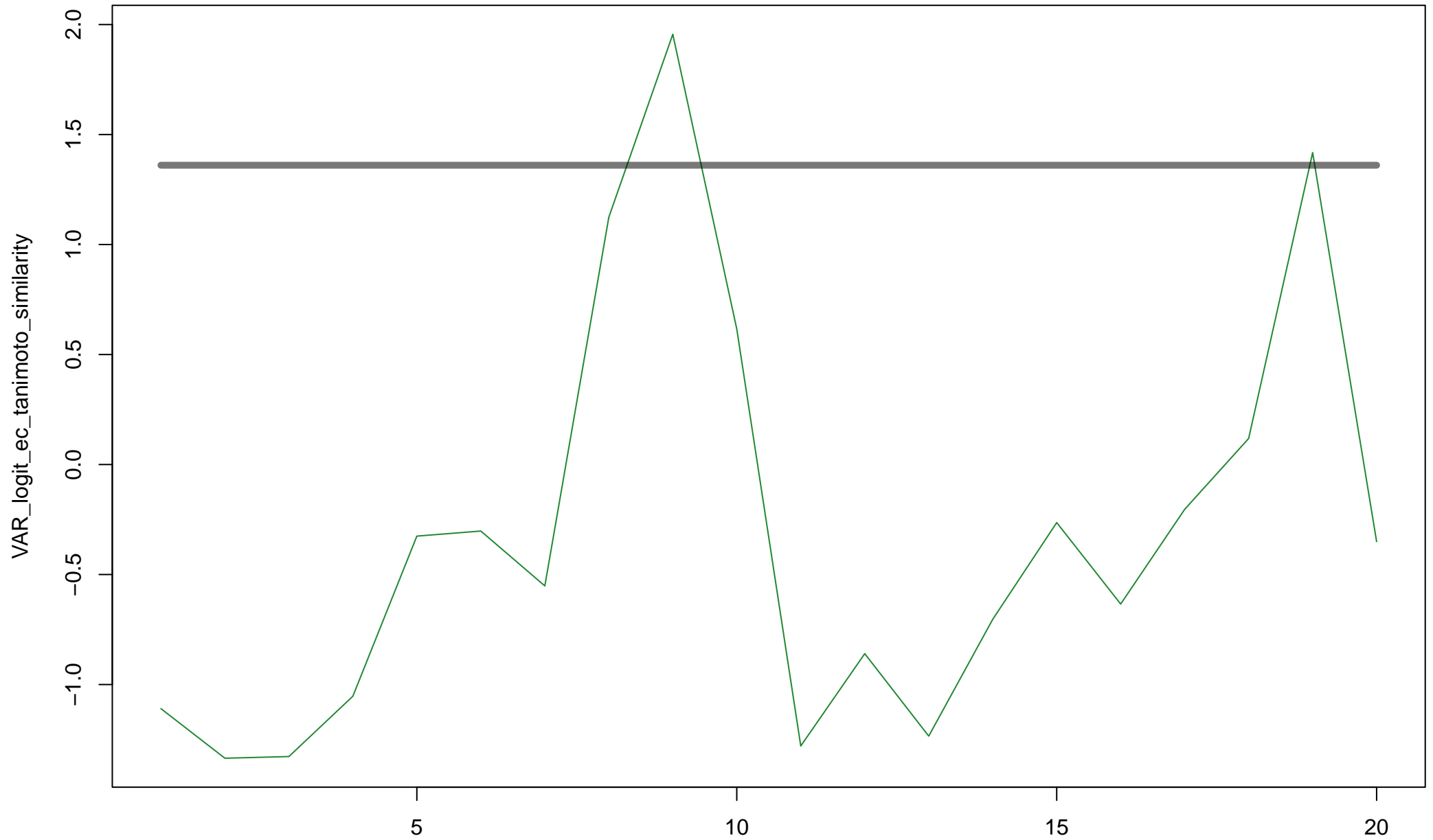




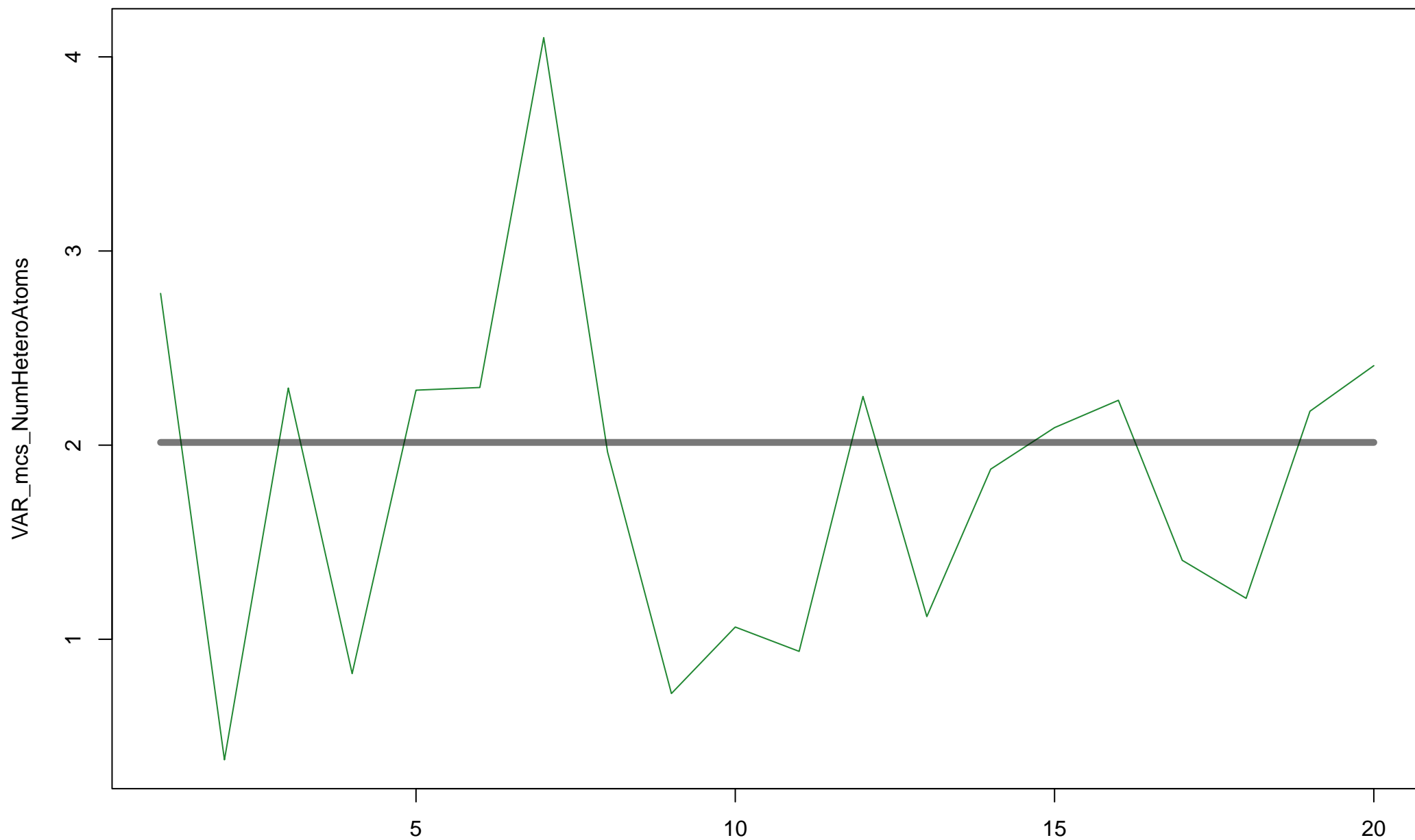
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 20 | BMK = 0.316 | MCSE(6.27) = 23.2 | stat: FALSE | burn: 20 | percentile: 5**



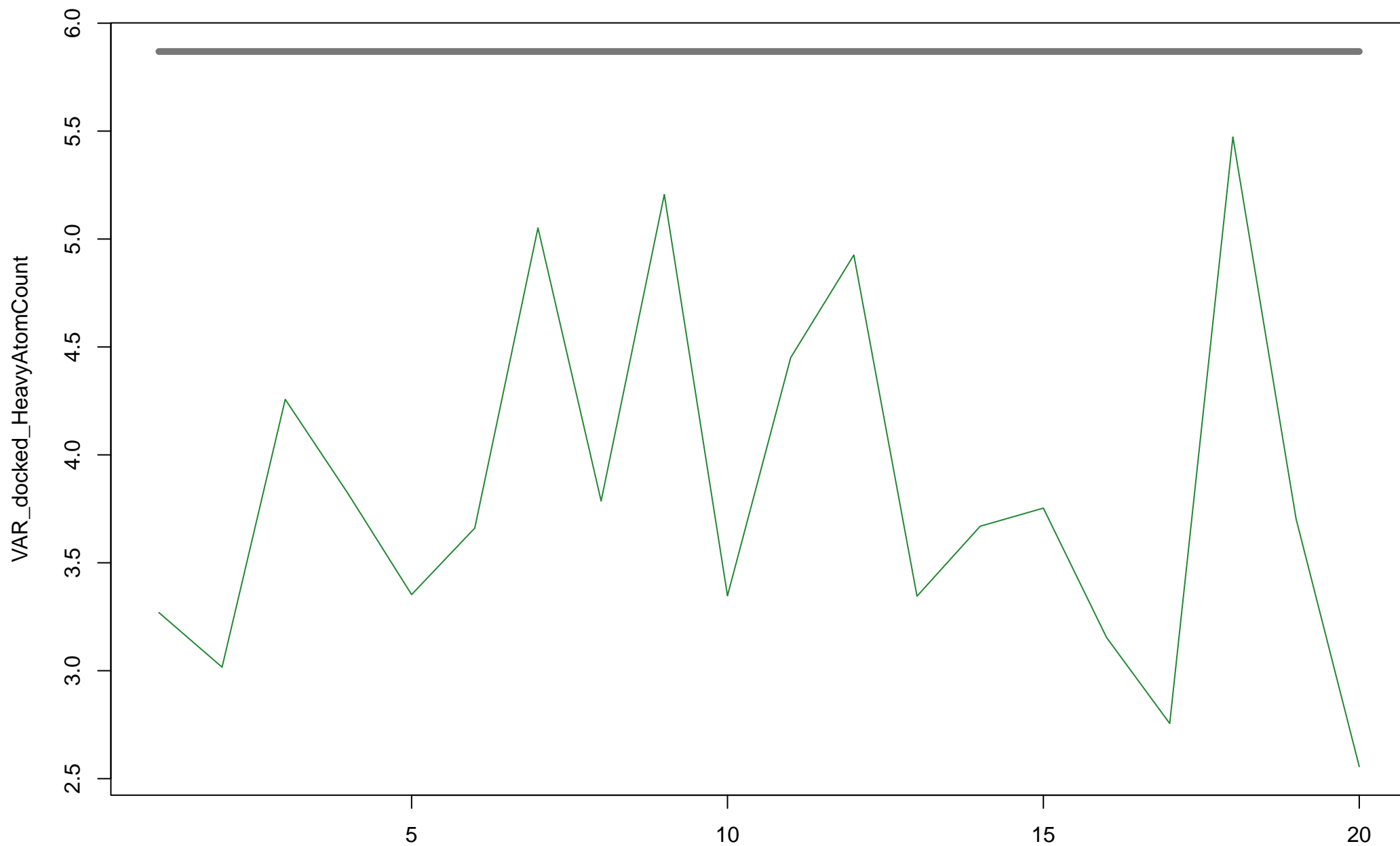
**VAR\_logit\_ec\_tanimoto\_similarity**  
**ESS = 9.72 | BMK = 0.452 | MCSE(6.27) = 31.6 | stat: FALSE | burn: 20 | percentile: 90**



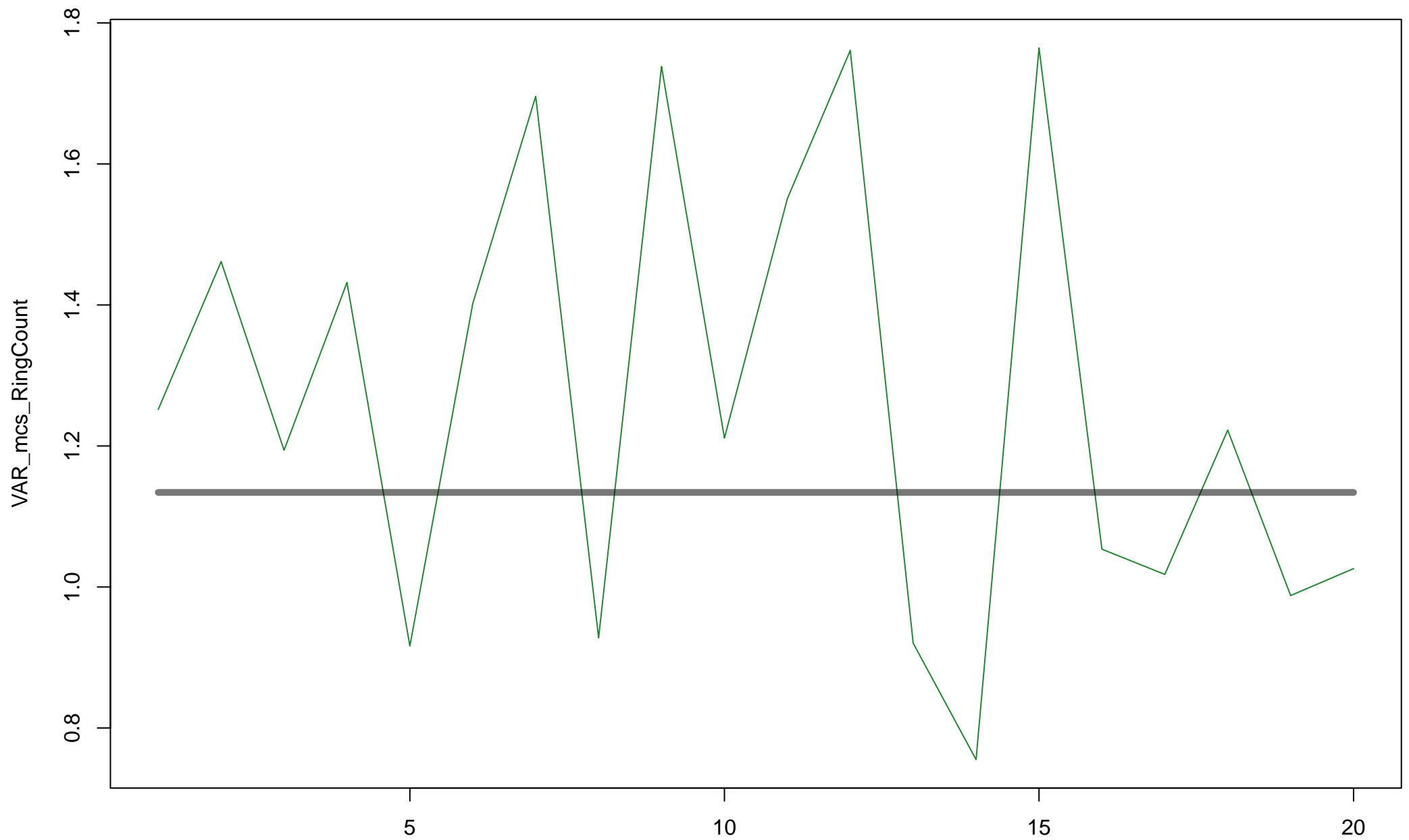
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 20 | BMK = 0.329 | MCSE(6.27) = 21.9 | stat: FALSE | burn: 20 | percentile: 50**



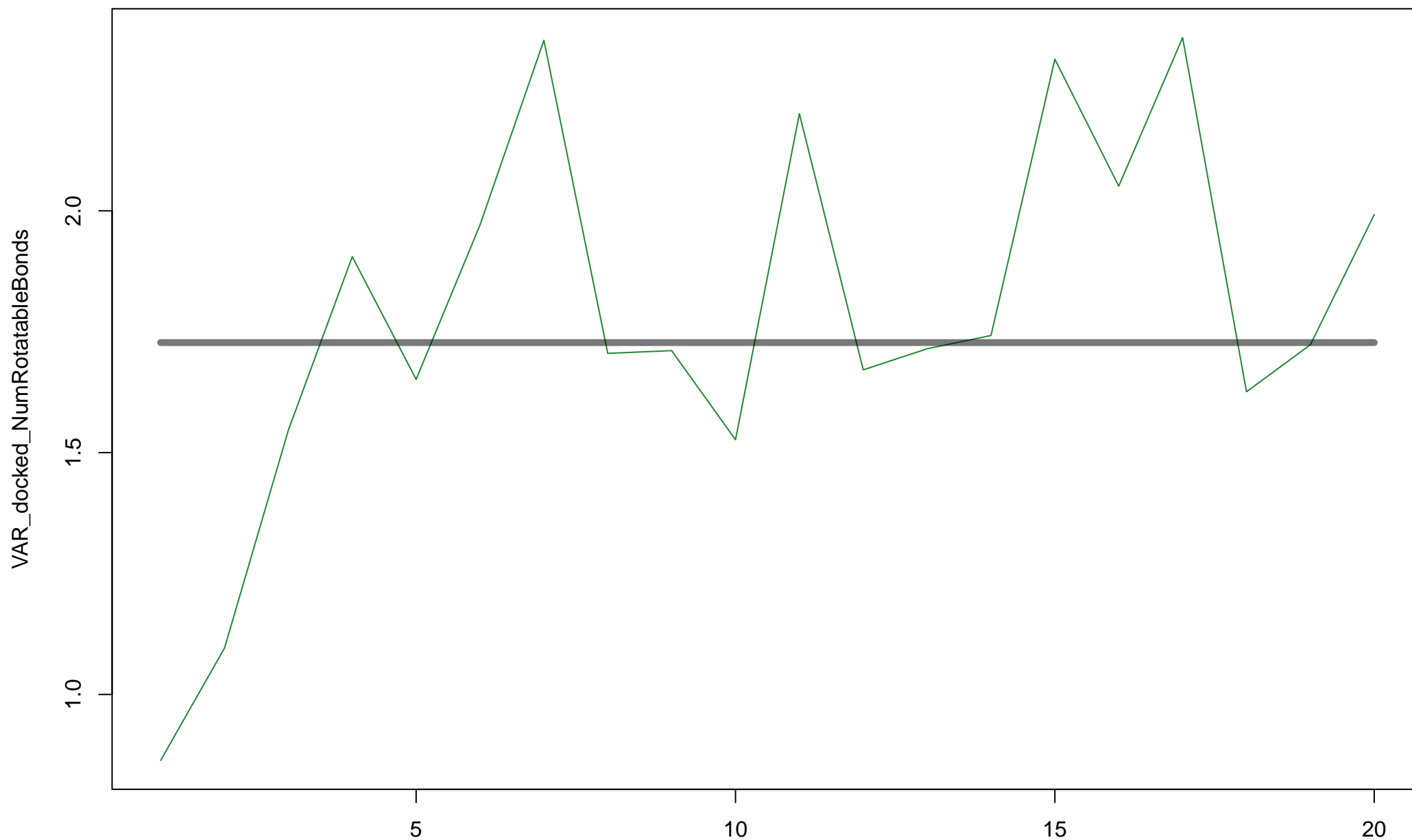
**VAR\_docked\_HeavyAtomCount**  
**ESS = 20 | BMK = 0.268 | MCSE(6.27) = 16.2 | stat: FALSE | burn: 20 | percentile: 100**



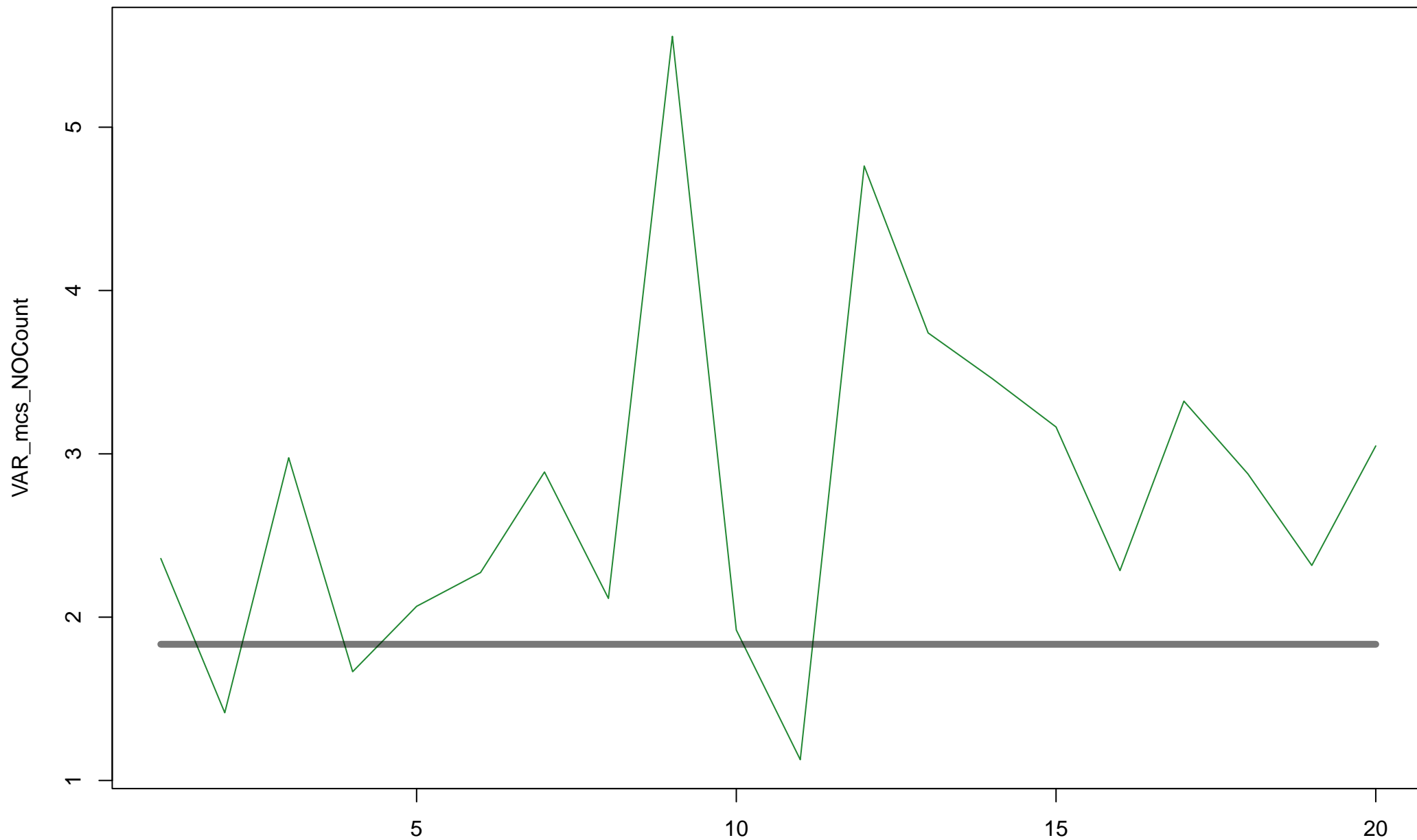
**VAR\_mcs\_RingCount**  
**ESS = 20 | BMK = 0.177 | MCSE(6.27) = 14.7 | stat: FALSE | burn: 20 | percentile: 40**



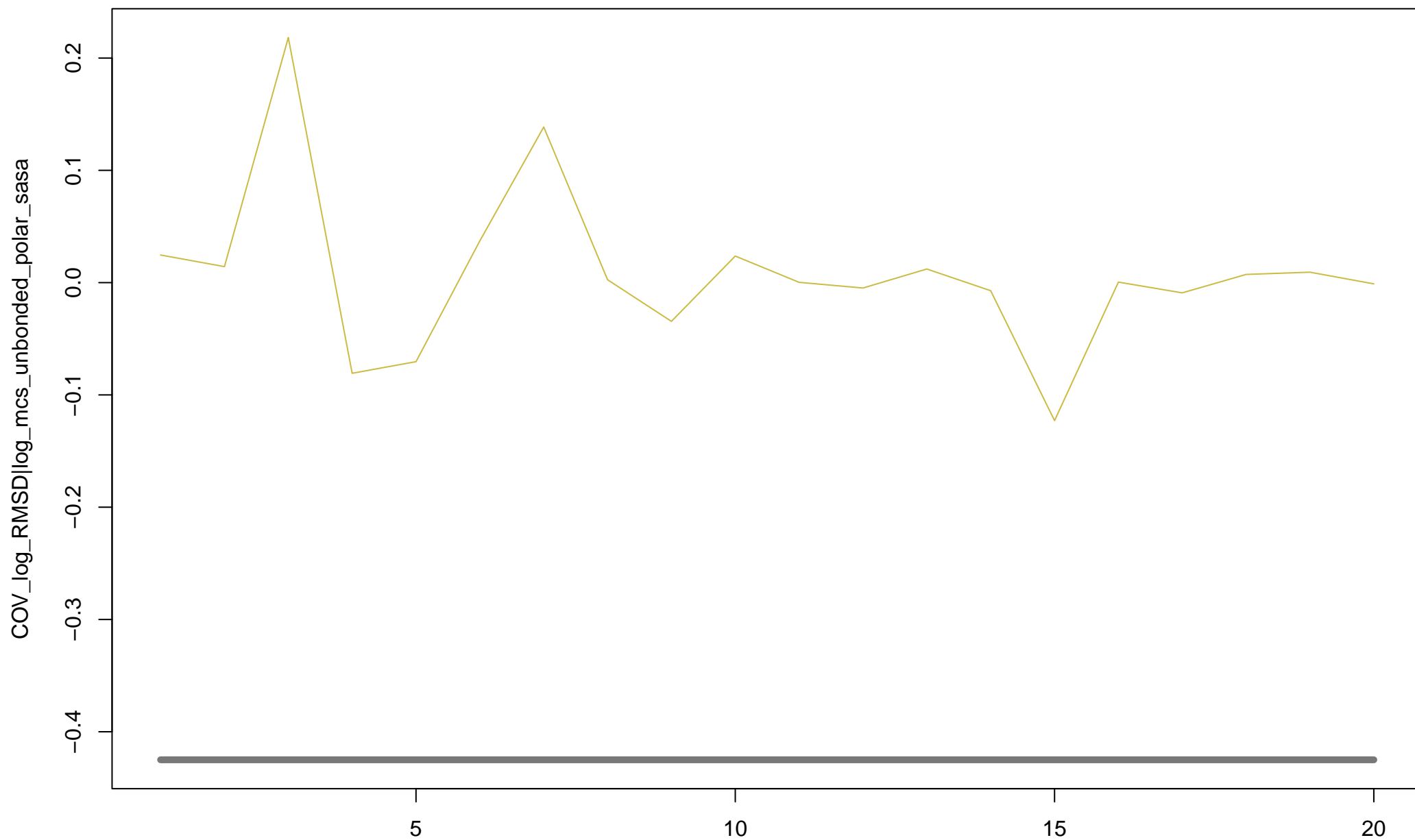
**VAR\_docked\_NumRotatableBonds**  
**ESS = 20 | BMK = 0.273 | MCSE(6.27) = 28.8 | stat: FALSE | burn: 20 | percentile: 55**



**VAR\_mcs\_NOCount**  
**ESS = 20 | BMK = 0.731 | MCSE(6.27) = 18.9 | stat: FALSE | burn: 20 | percentile: 15**

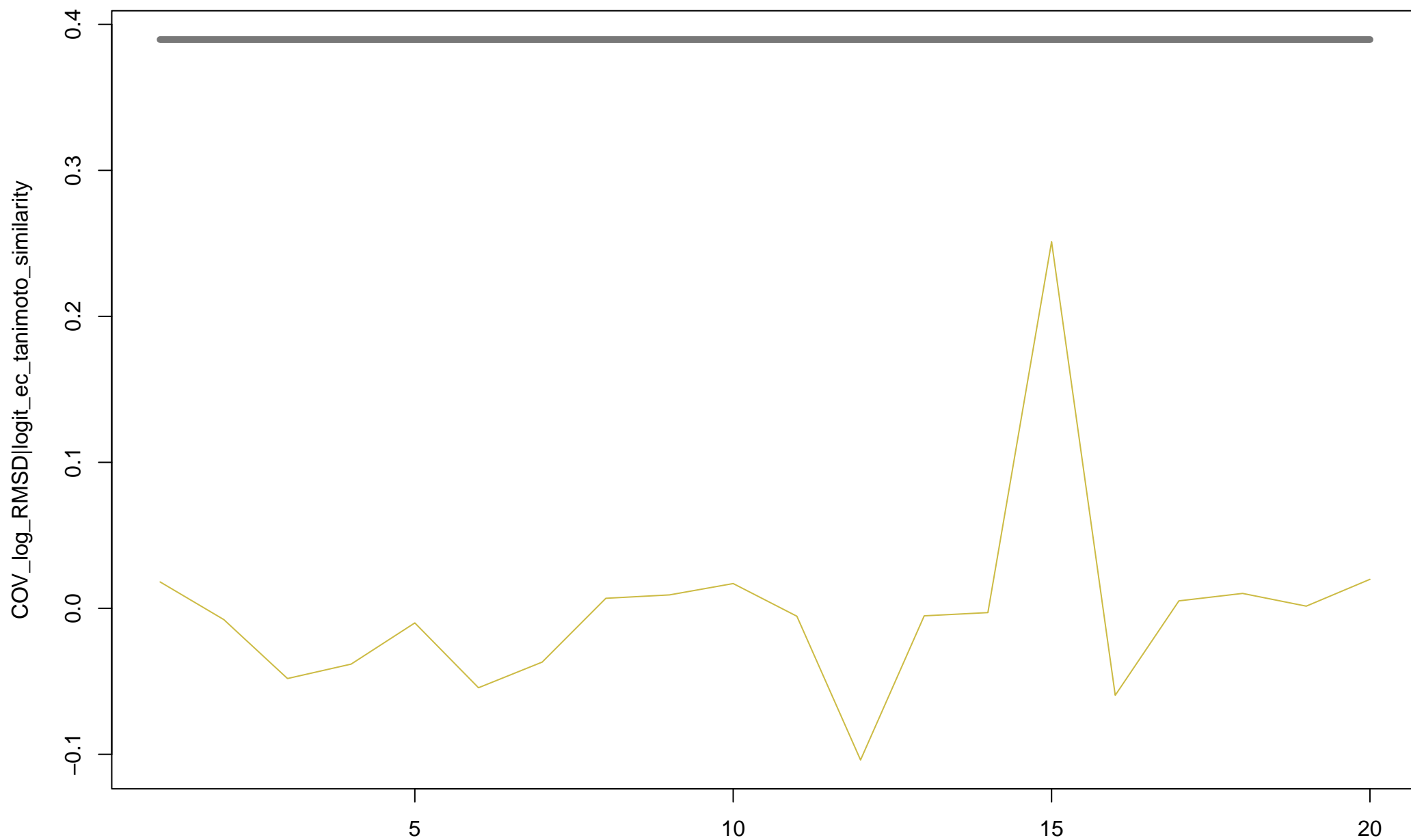


**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 20 | BMK = 0.763 | MCSE(6.27) = 20.2 | stat: FALSE | burn: 20 | percentile: 0**

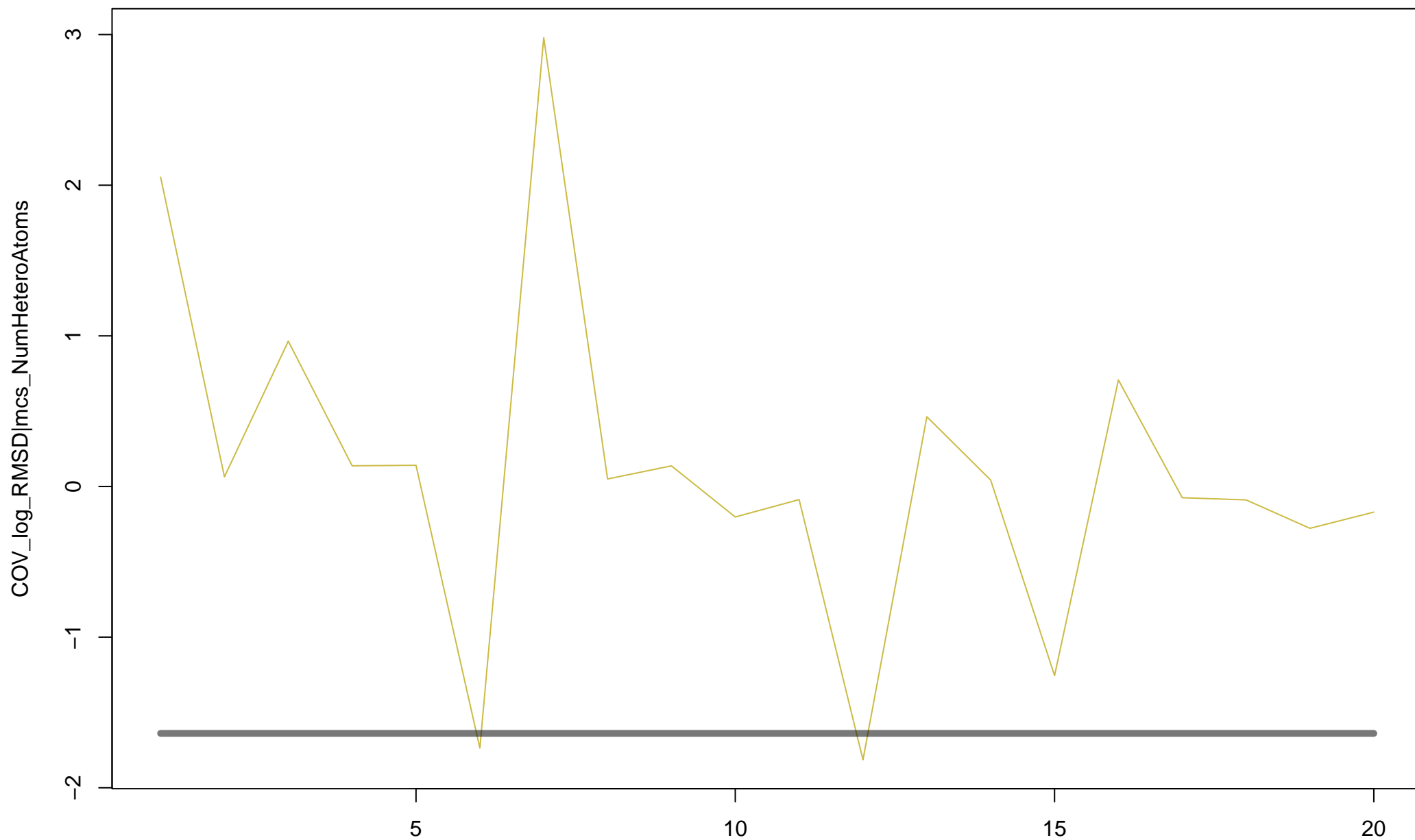




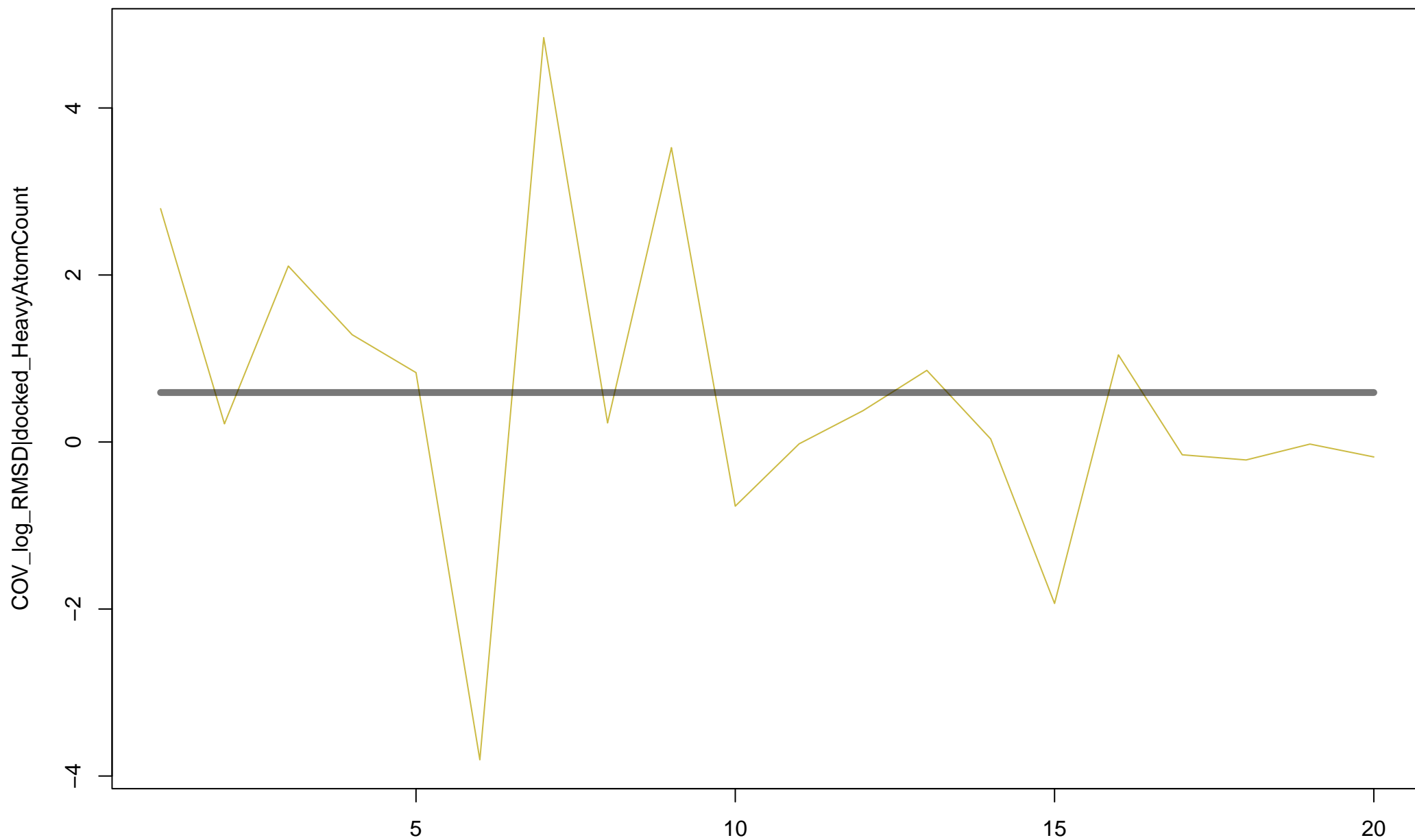
**COV\_log\_RMSD|logit\_ec\_tanimoto\_similarity**  
**ESS = 20 | BMK = 0.627 | MCSE(6.27) = 19.1 | stat: FALSE | burn: 20 | percentile: 100**



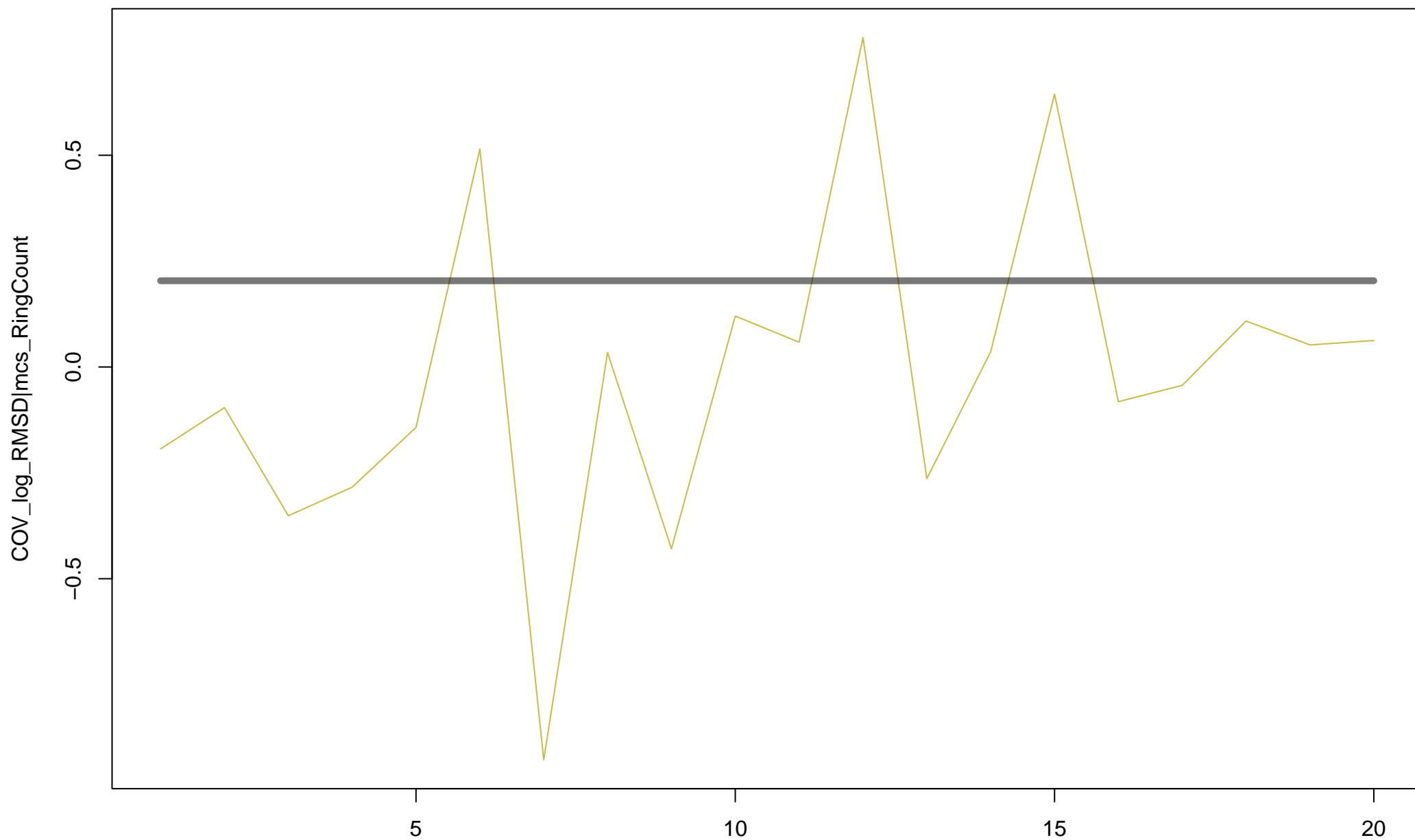
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 20 | BMK = 0.488 | MCSE(6.27) = 14.2 | stat: FALSE | burn: 20 | percentile: 10**



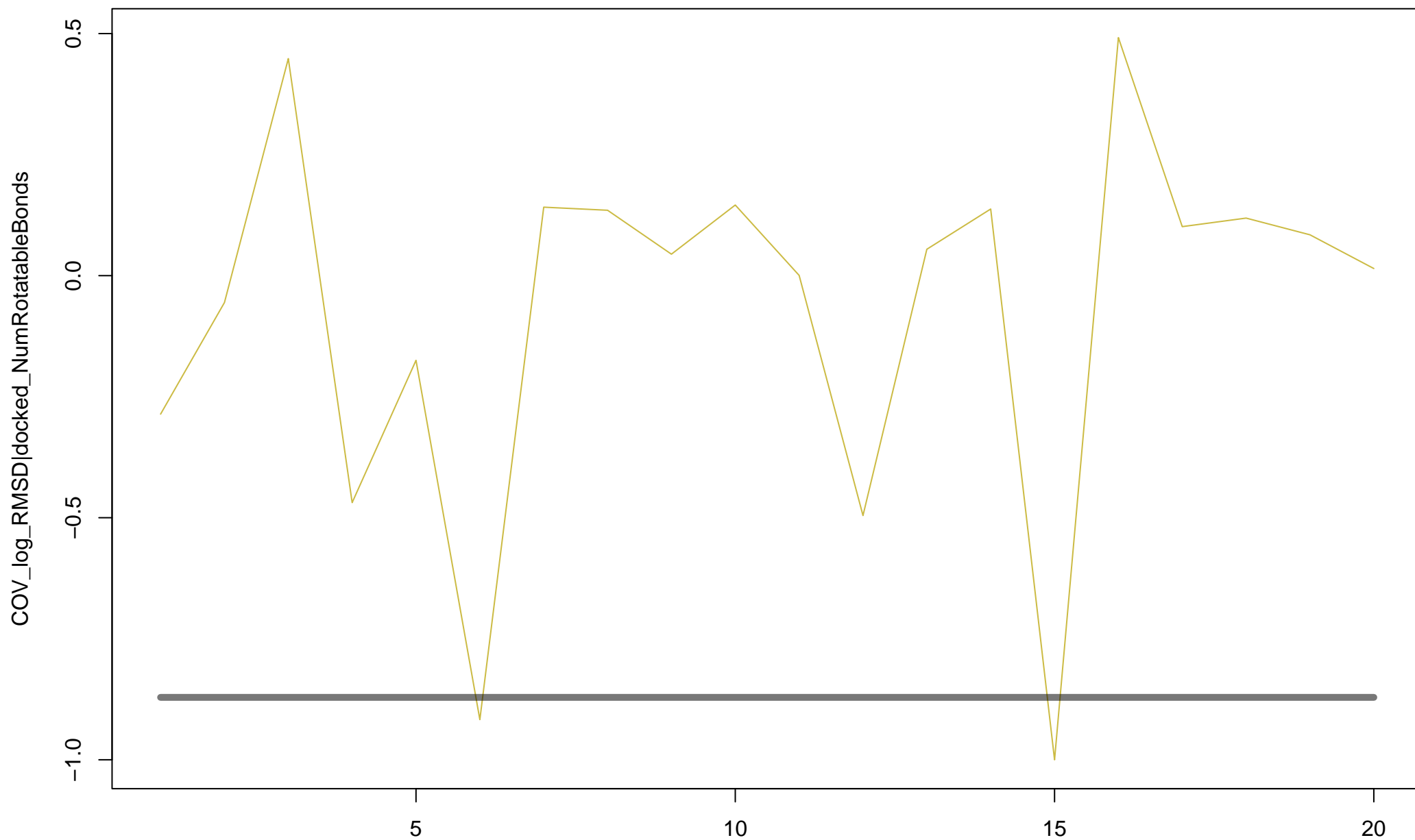
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 20 | BMK = 0.698 | MCSE(6.27) = 11 | stat: FALSE | burn: 20 | percentile: 60**



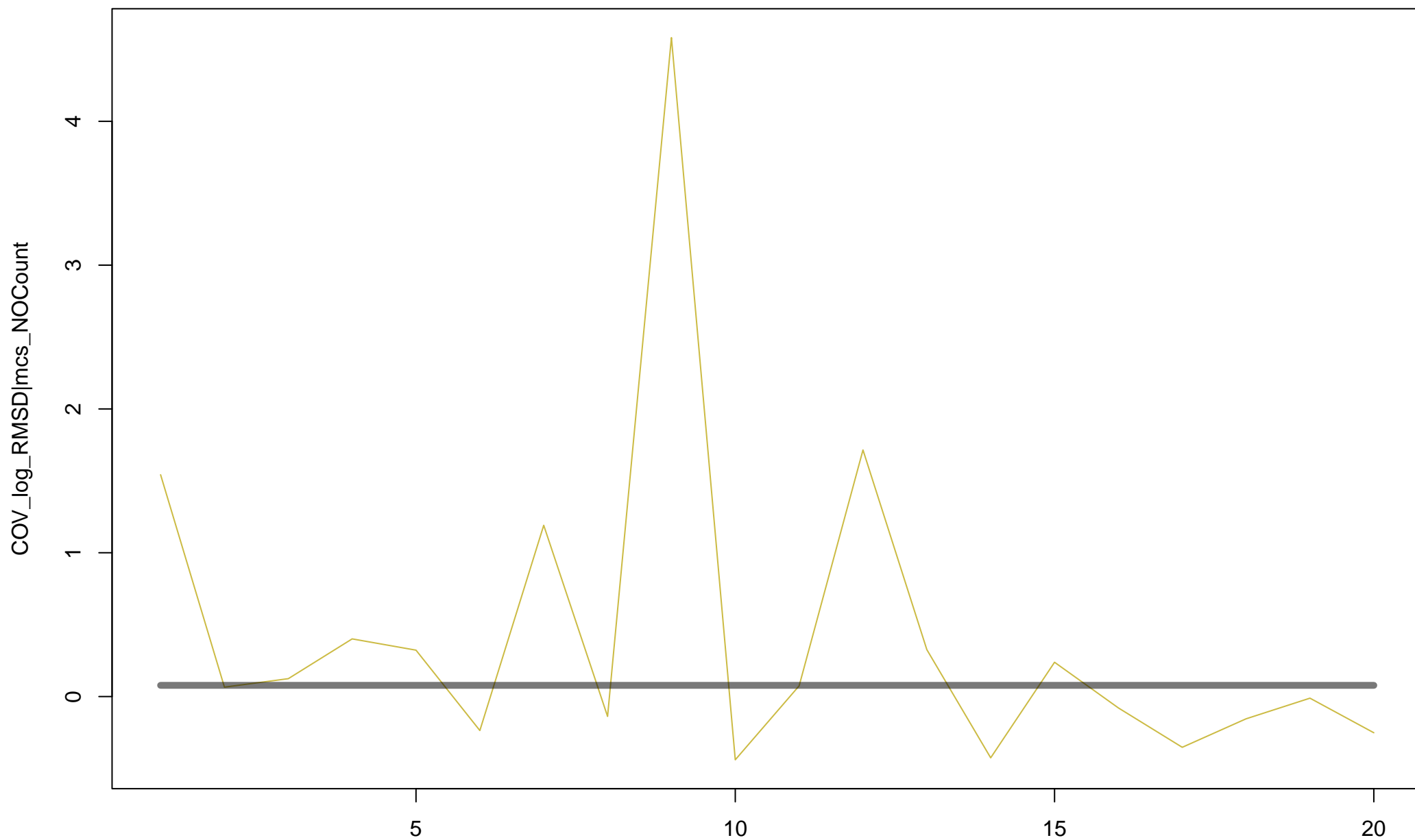
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 20 | BMK = 0.531 | MCSE(6.27) = 15.8 | stat: FALSE | burn: 20 | percentile: 85**



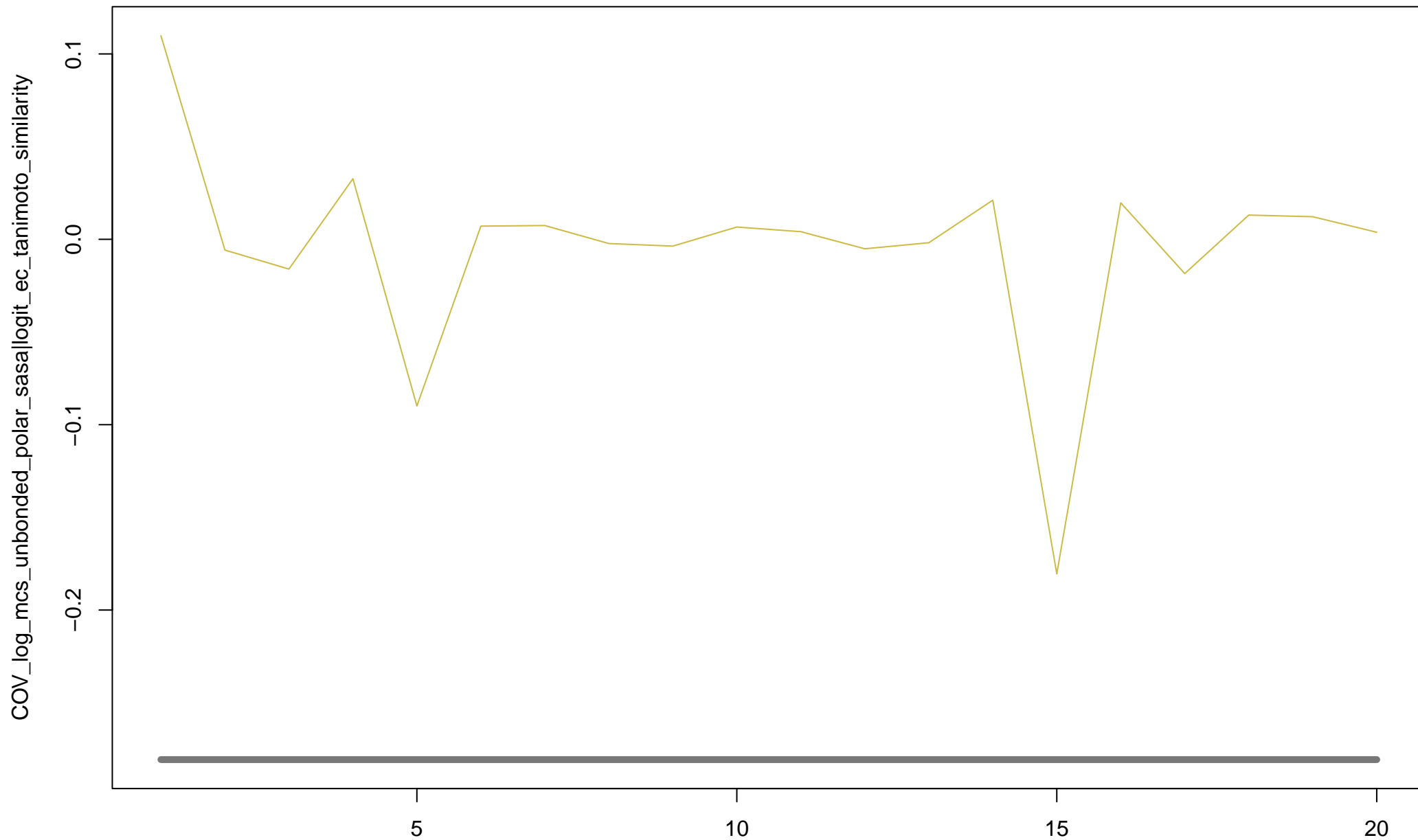
**COV\_log\_RMSD|docked\_NumRotatableBonds**  
**ESS = 20 | BMK = 0.507 | MCSE(6.27) = 15.1 | stat: FALSE | burn: 20 | percentile: 10**



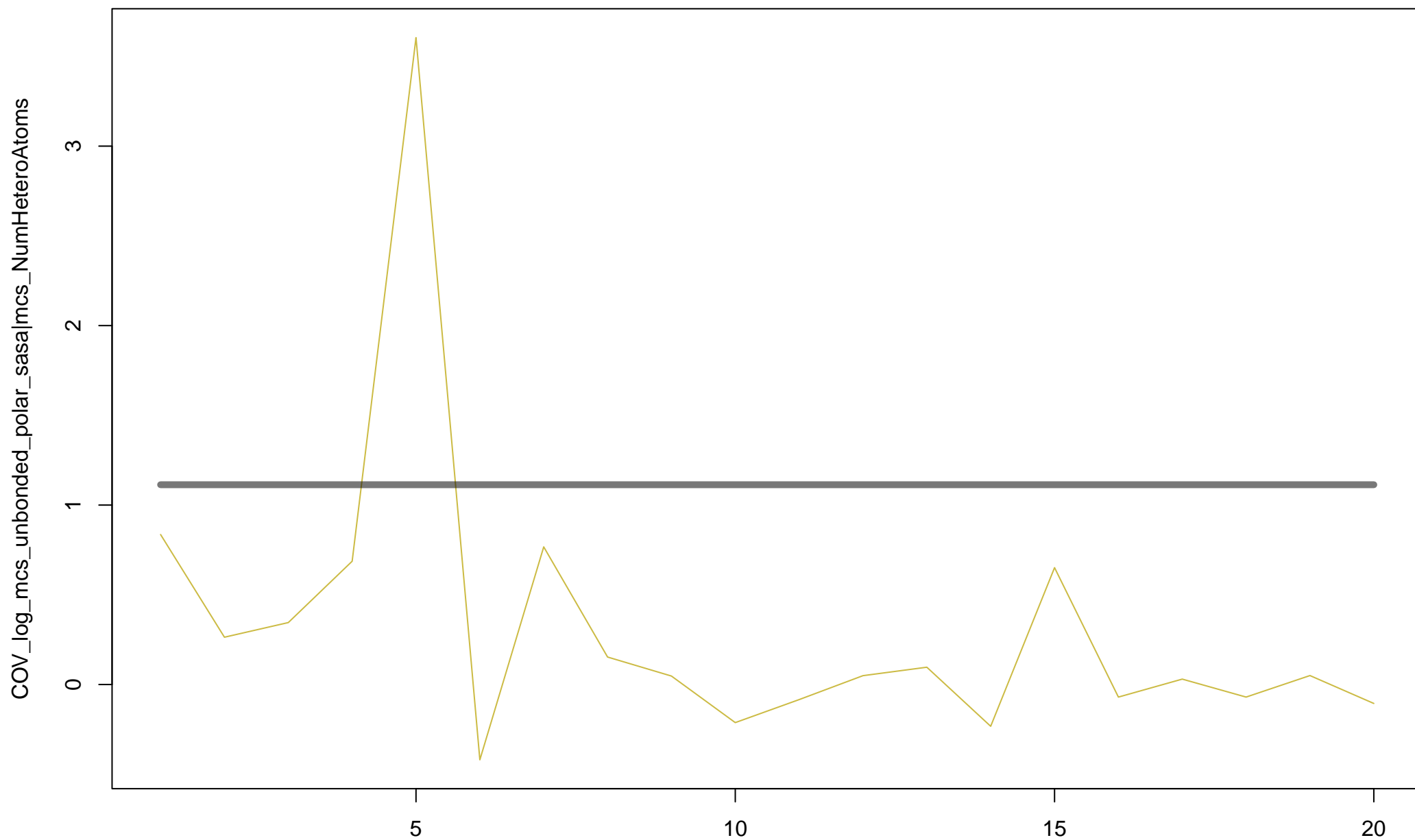
**COV\_log\_RMSD|mcs\_NOCount**  
**ESS = 20 | BMK = 0.377 | MCSE(6.27) = 16.2 | stat: FALSE | burn: 20 | percentile: 55**



**COV\_log\_mcs\_unbonded\_polar\_sasa|logit\_ec\_tanimoto\_similarity**  
**ESS = 20 | BMK = 0.551 | MCSE(6.27) = 15.7 | stat: FALSE | burn: 20 | percentile: 0**

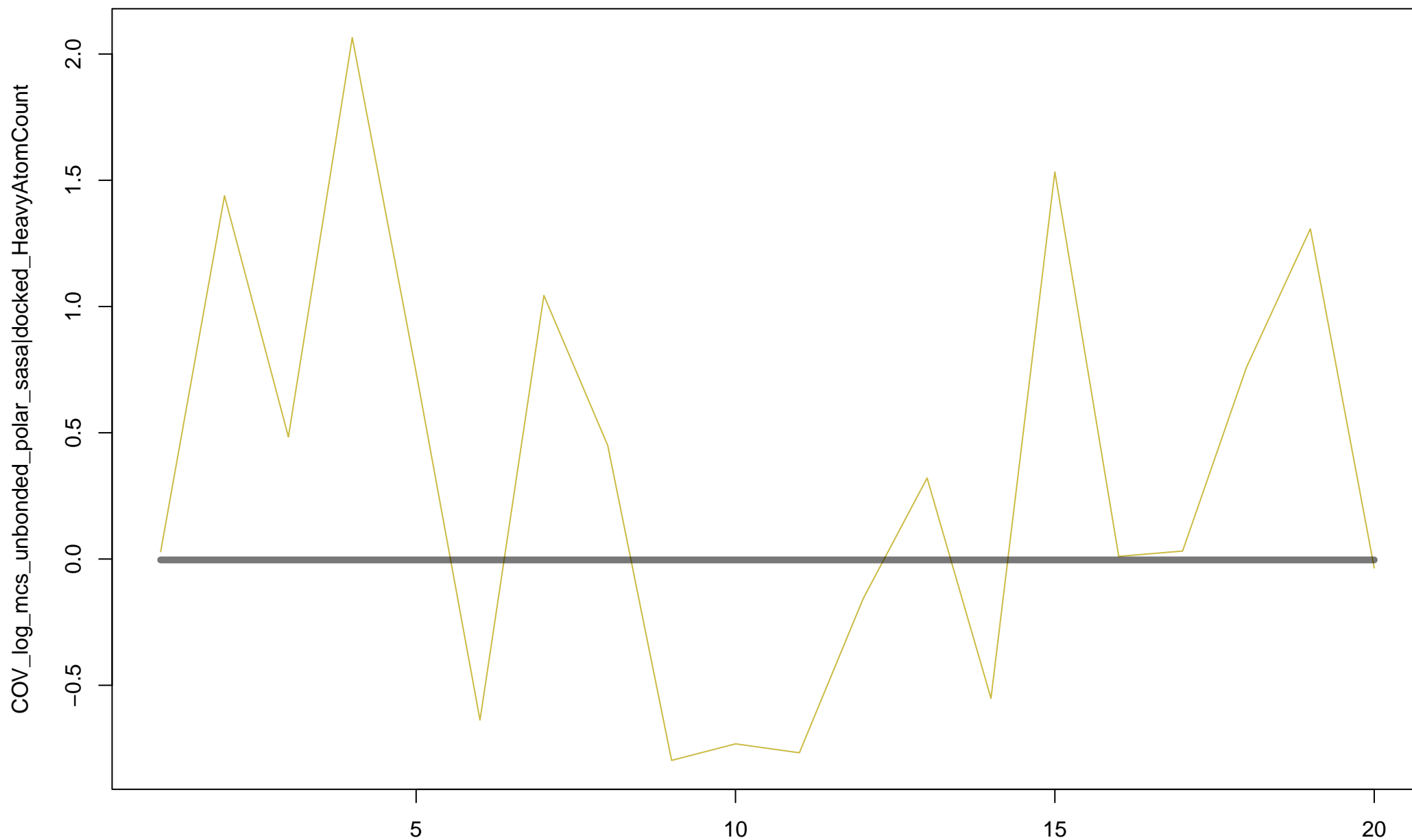


**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 20 | BMK = 0.703 | MCSE(6.27) = 22.8 | stat: FALSE | burn: 16 | percentile: 95**

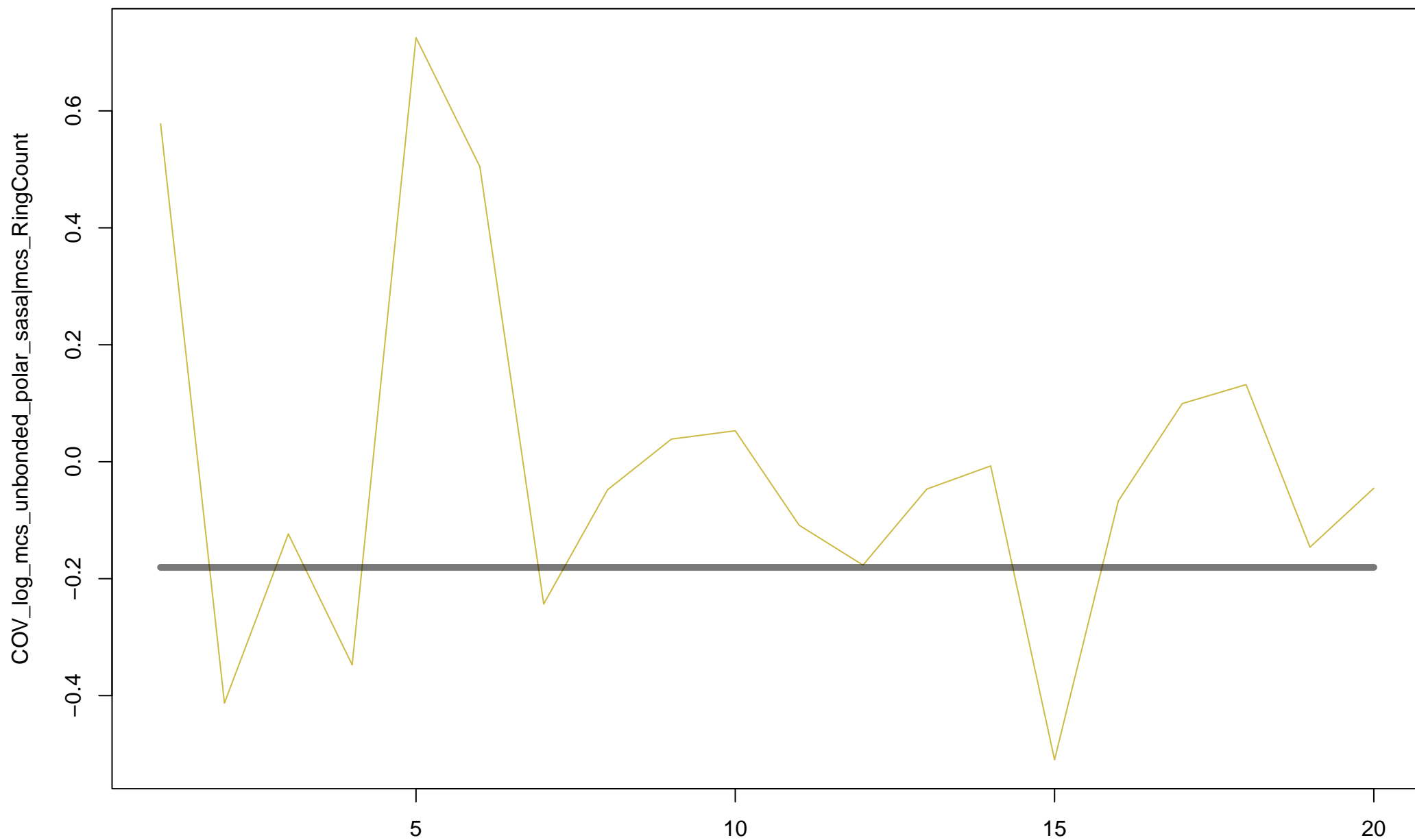




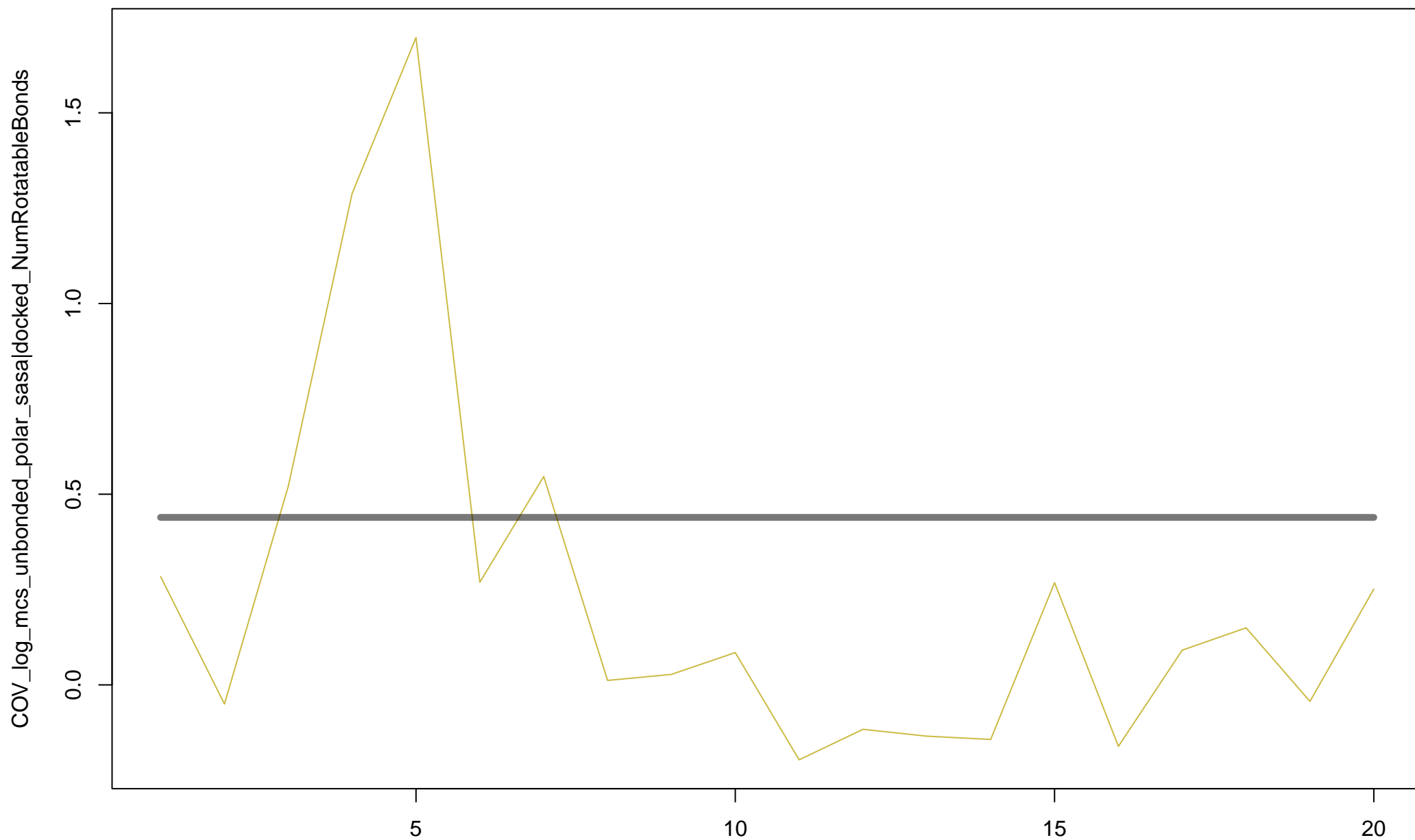
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 20 | BMK = 0.139 | MCSE(6.27) = 26.7 | stat: FALSE | burn: 16 | percentile: 35**



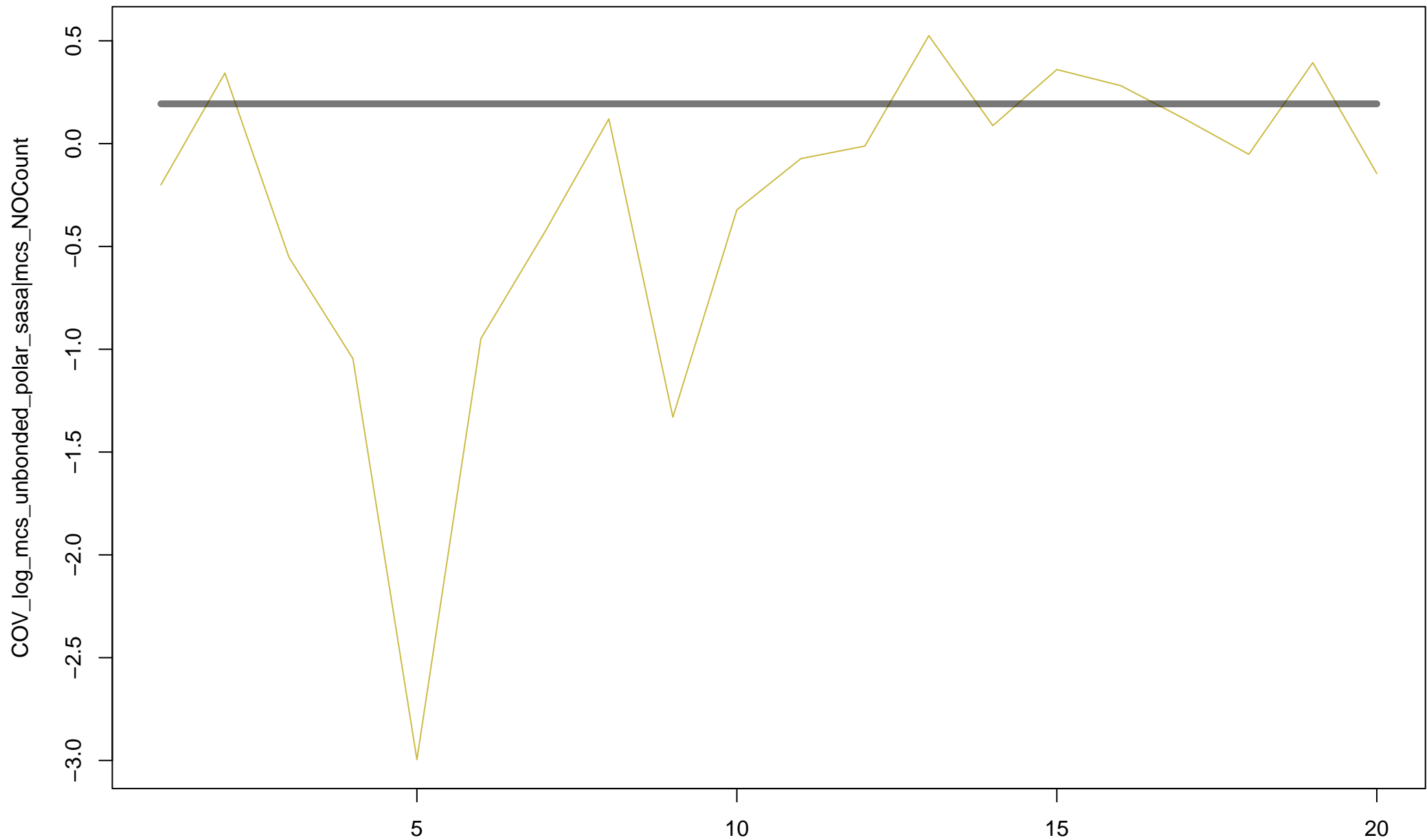
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_RingCount**  
**ESS = 20 | BMK = 0.474 | MCSE(6.27) = 20.7 | stat: FALSE | burn: 20 | percentile: 20**



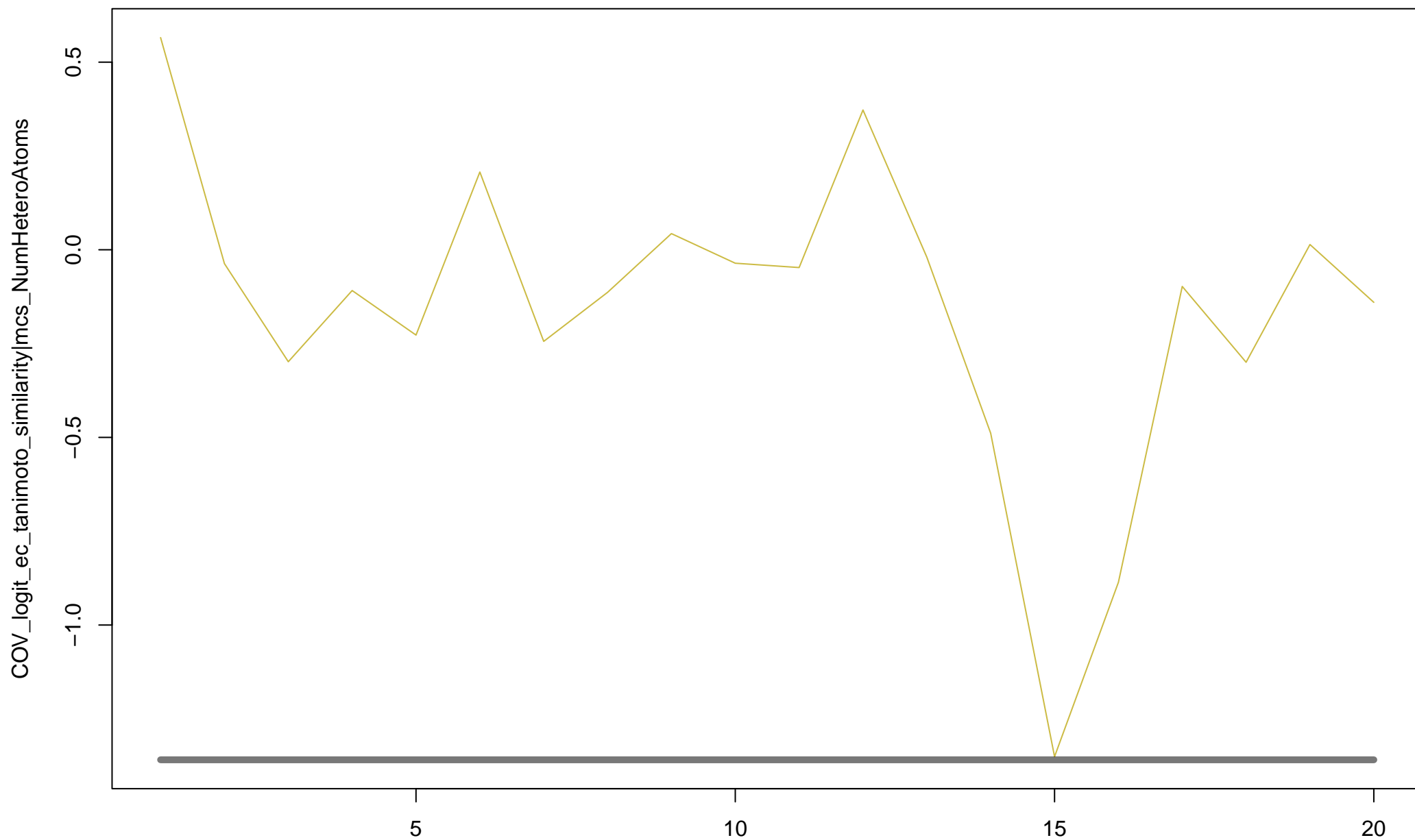
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_NumRotatableBonds**  
**ESS = 5.86 | BMK = 0.463 | MCSE(6.27) = 45.7 | stat: FALSE | burn: 20 | percentile: 80**



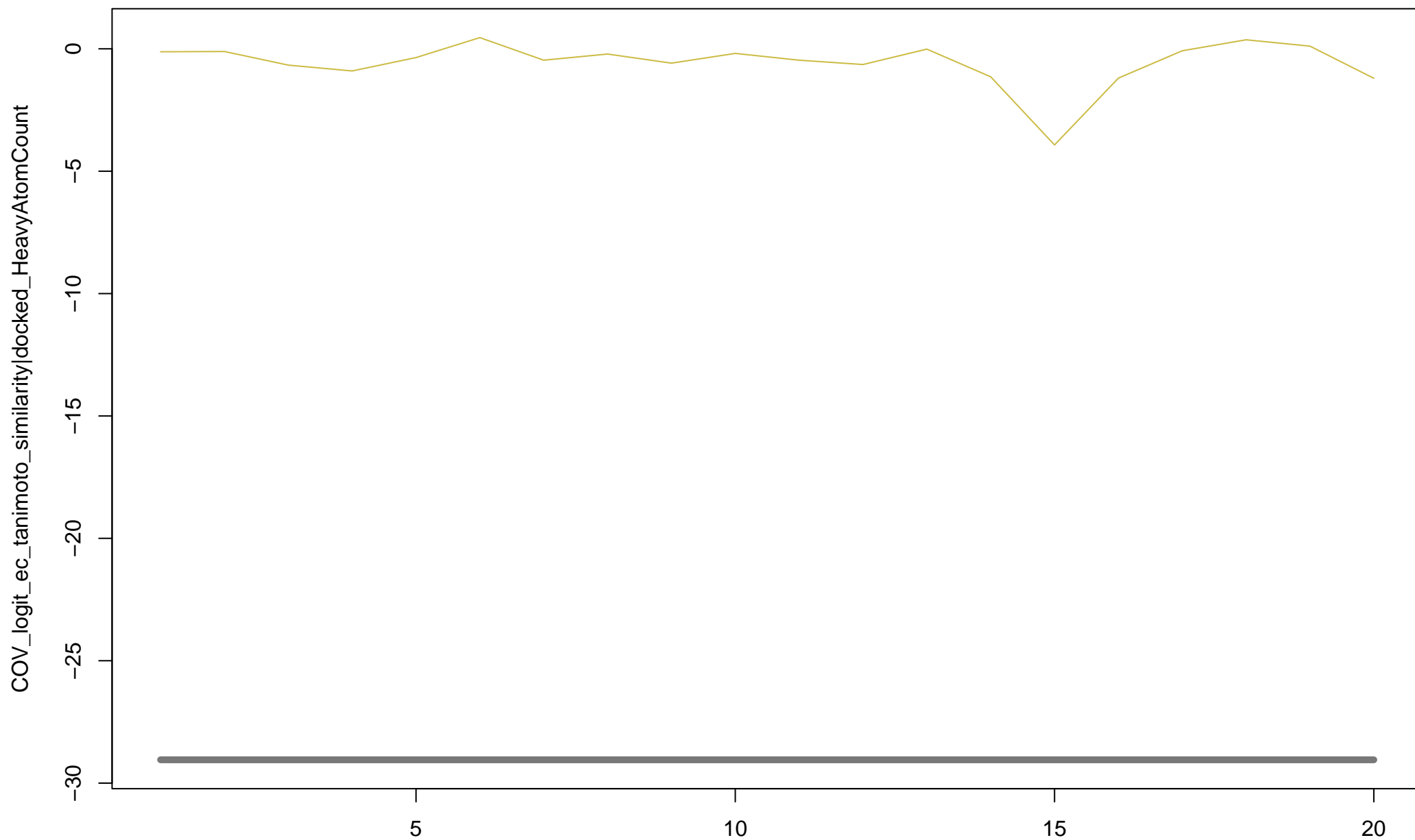
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NOCount**  
**ESS = 7.56 | BMK = 0.587 | MCSE(6.27) = 41.7 | stat: FALSE | burn: 20 | percentile: 75**



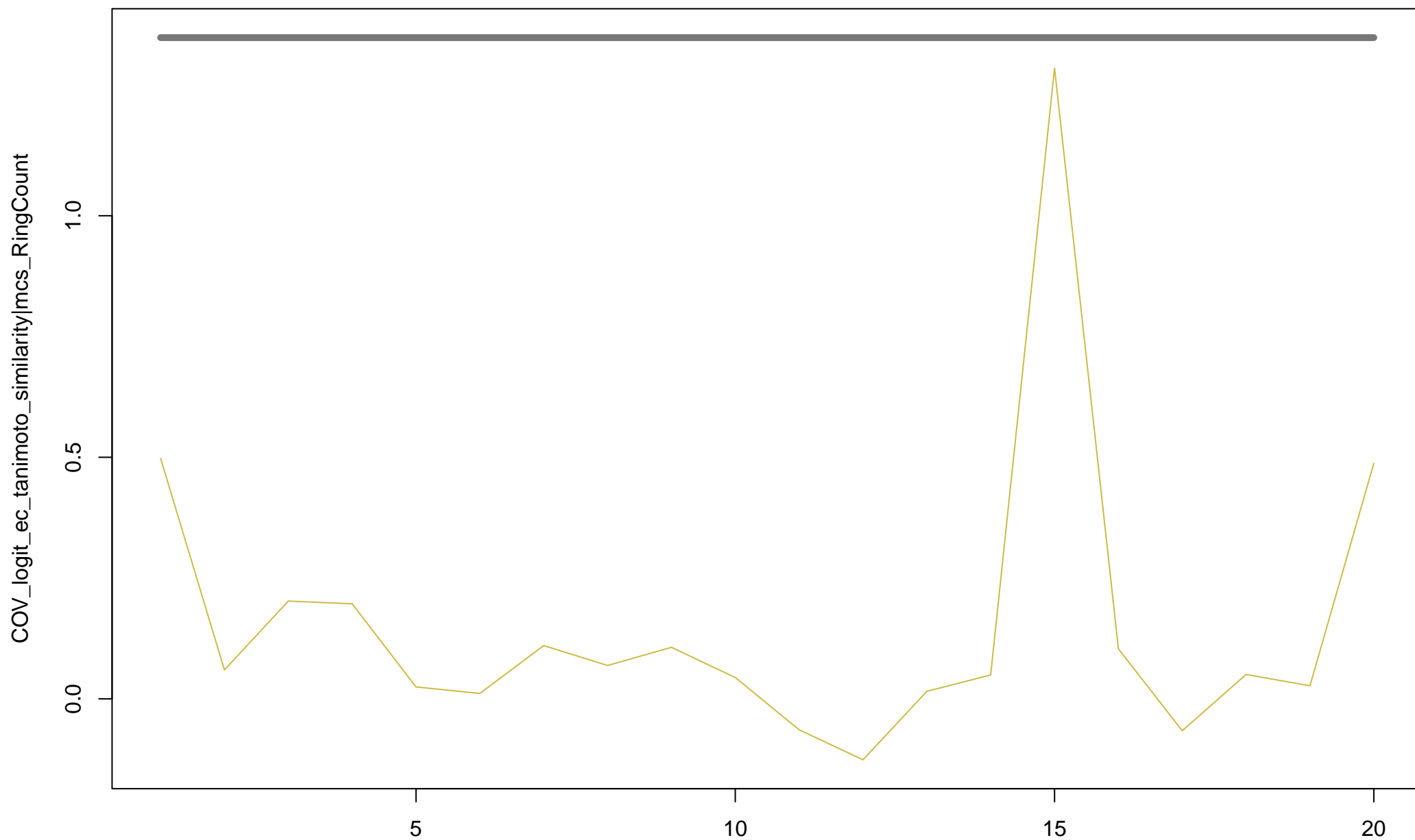
COV\_logit\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms  
ESS = 7.85 | BMK = 0.379 | MCSE(6.27) = 35.4 | stat: FALSE | burn: 20 | percentile: 0



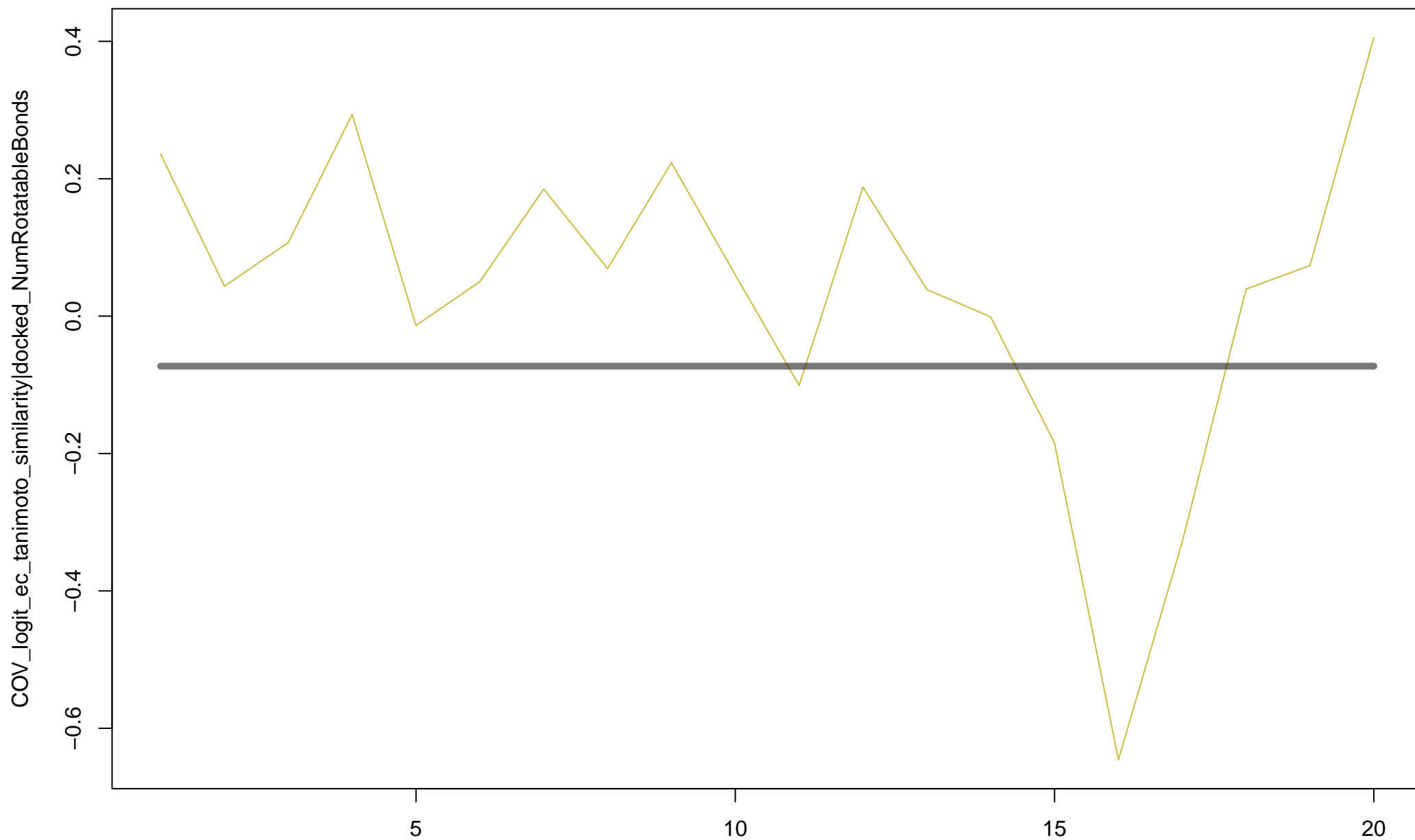
**COV\_logit\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount**  
**ESS = 20 | BMK = 0.373 | MCSE(6.27) = 27.8 | stat: FALSE | burn: 20 | percentile: 0**



COV\_logit\_ec\_tanimoto\_similarity|mcs\_RingCount  
ESS = 20 | BMK = 0.451 | MCSE(6.27) = 21.4 | stat: FALSE | burn: 20 | percentile: 100

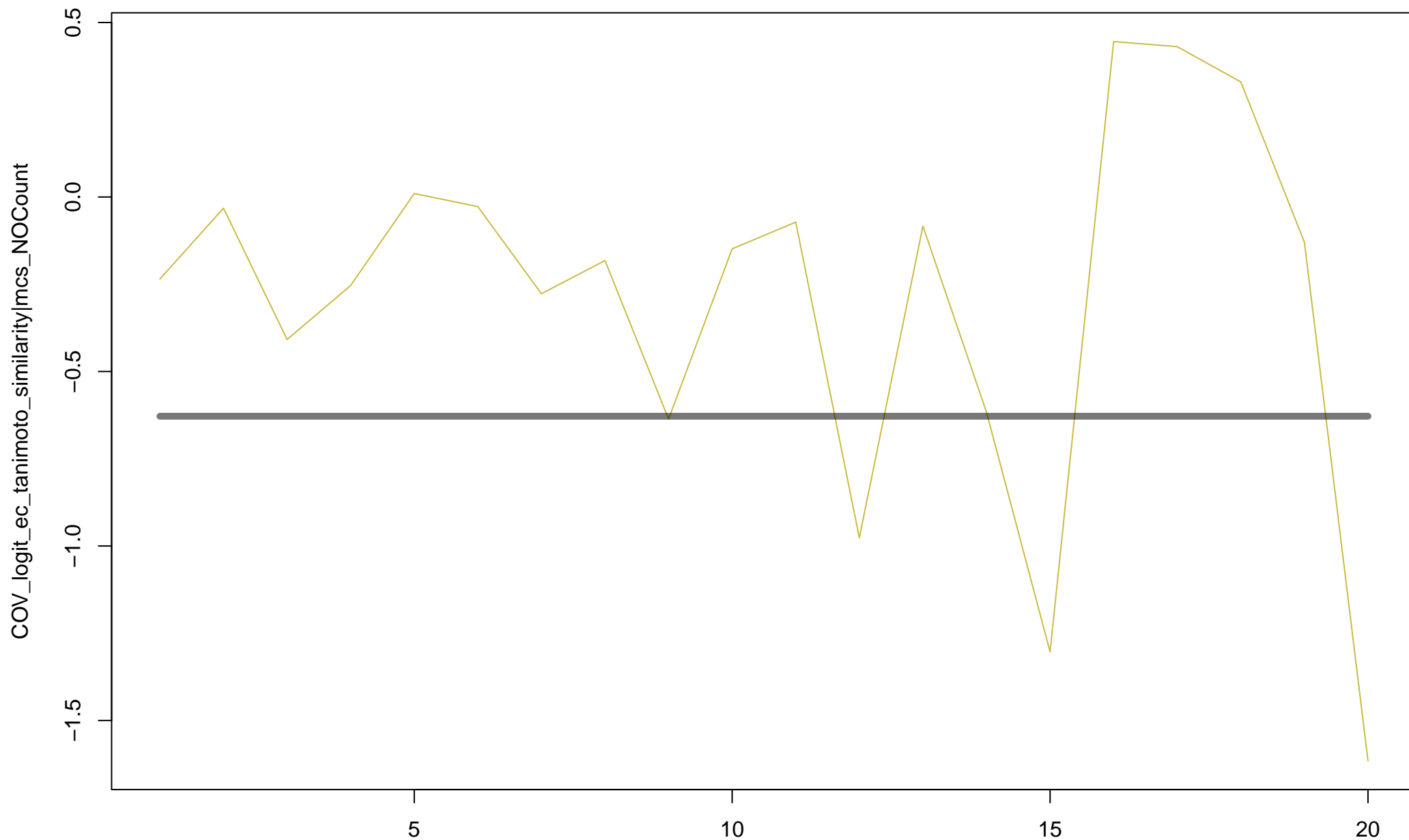


**COV\_logit\_ec\_tanimoto\_similarity|docked\_NumRotatableBonds**  
**ESS = 7.71 | BMK = 0.452 | MCSE(6.27) = 37.6 | stat: FALSE | burn: 20 | percentile: 20**

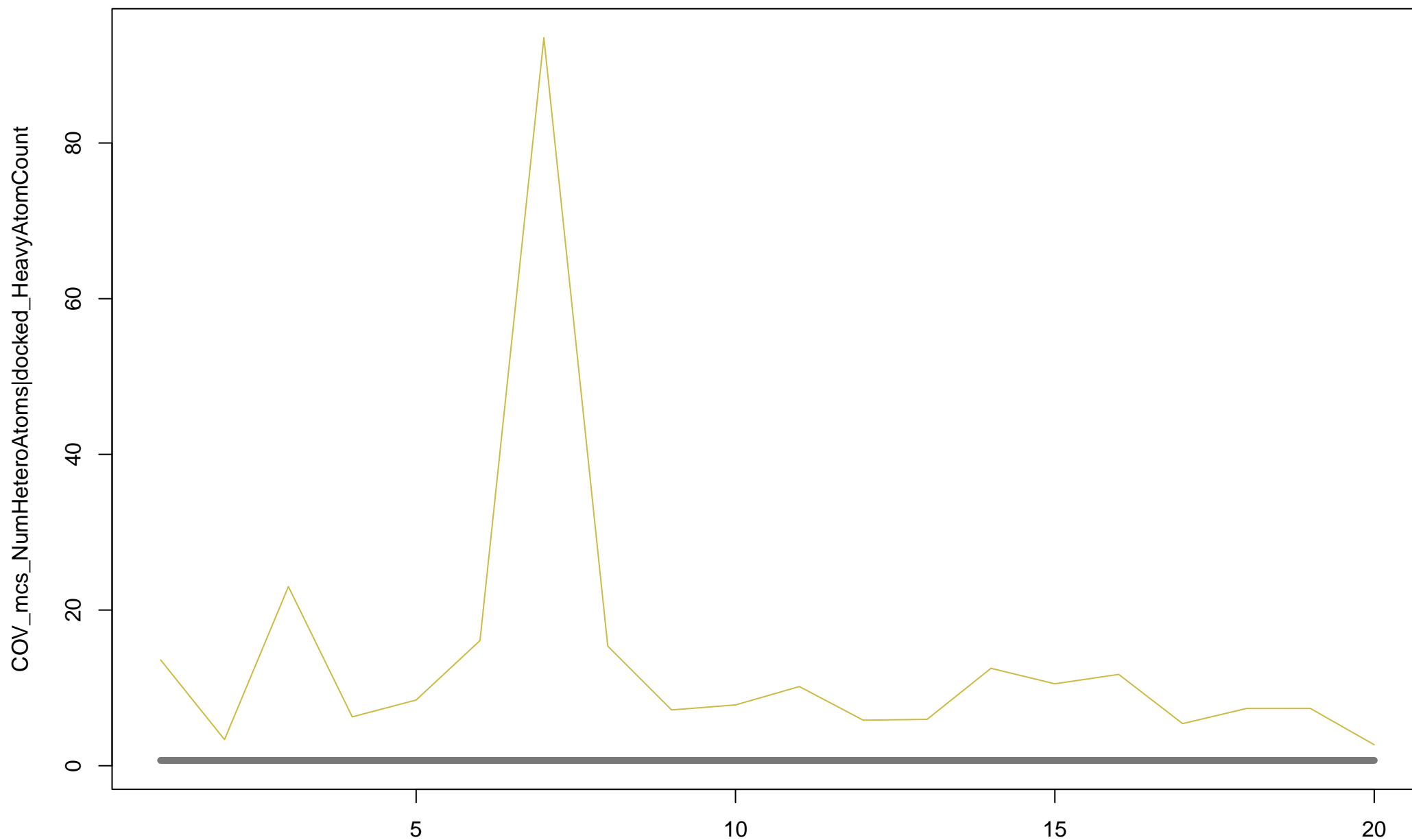




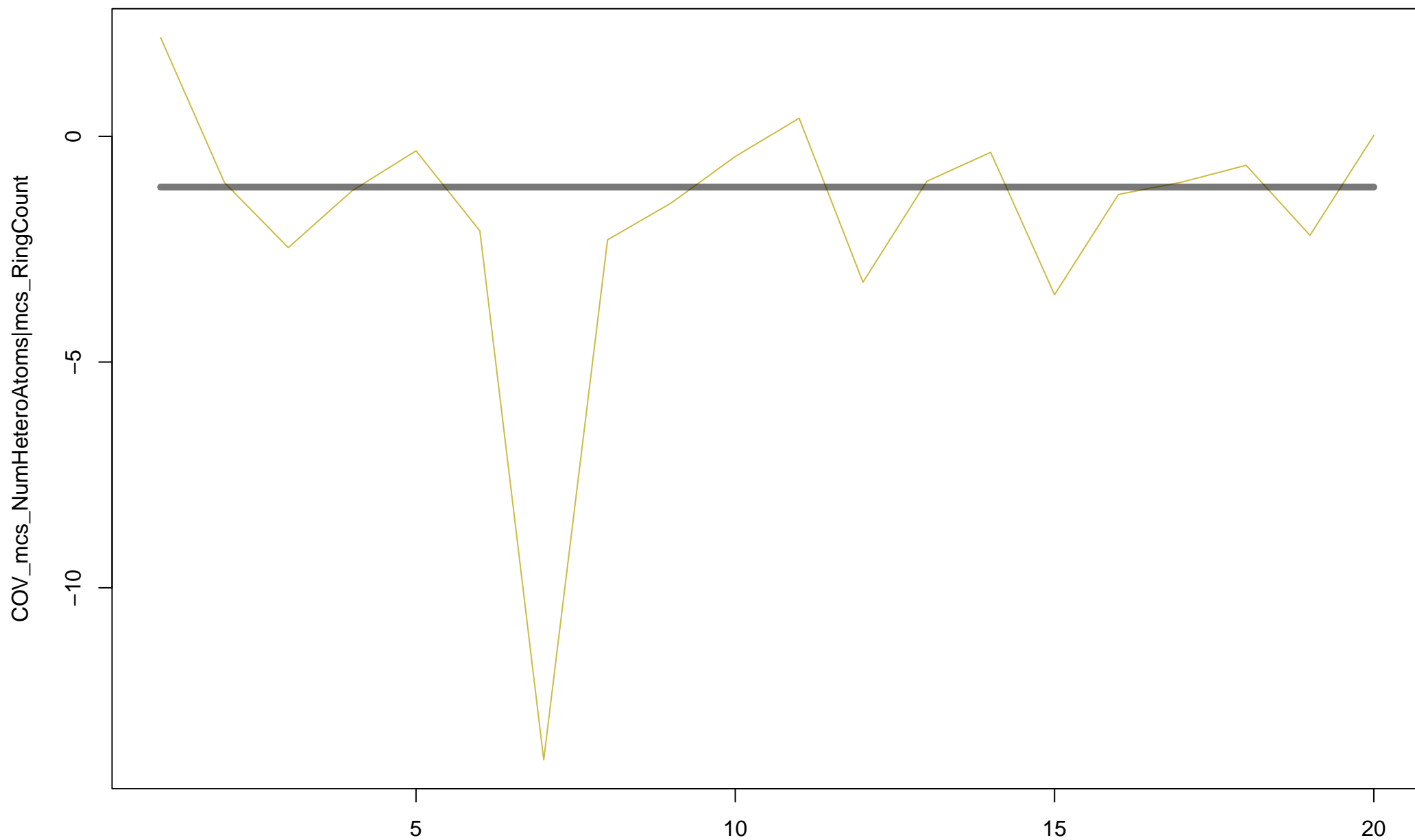
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NOCount**  
**ESS = 20 | BMK = 0.537 | MCSE(6.27) = 22.2 | stat: FALSE | burn: 20 | percentile: 20**



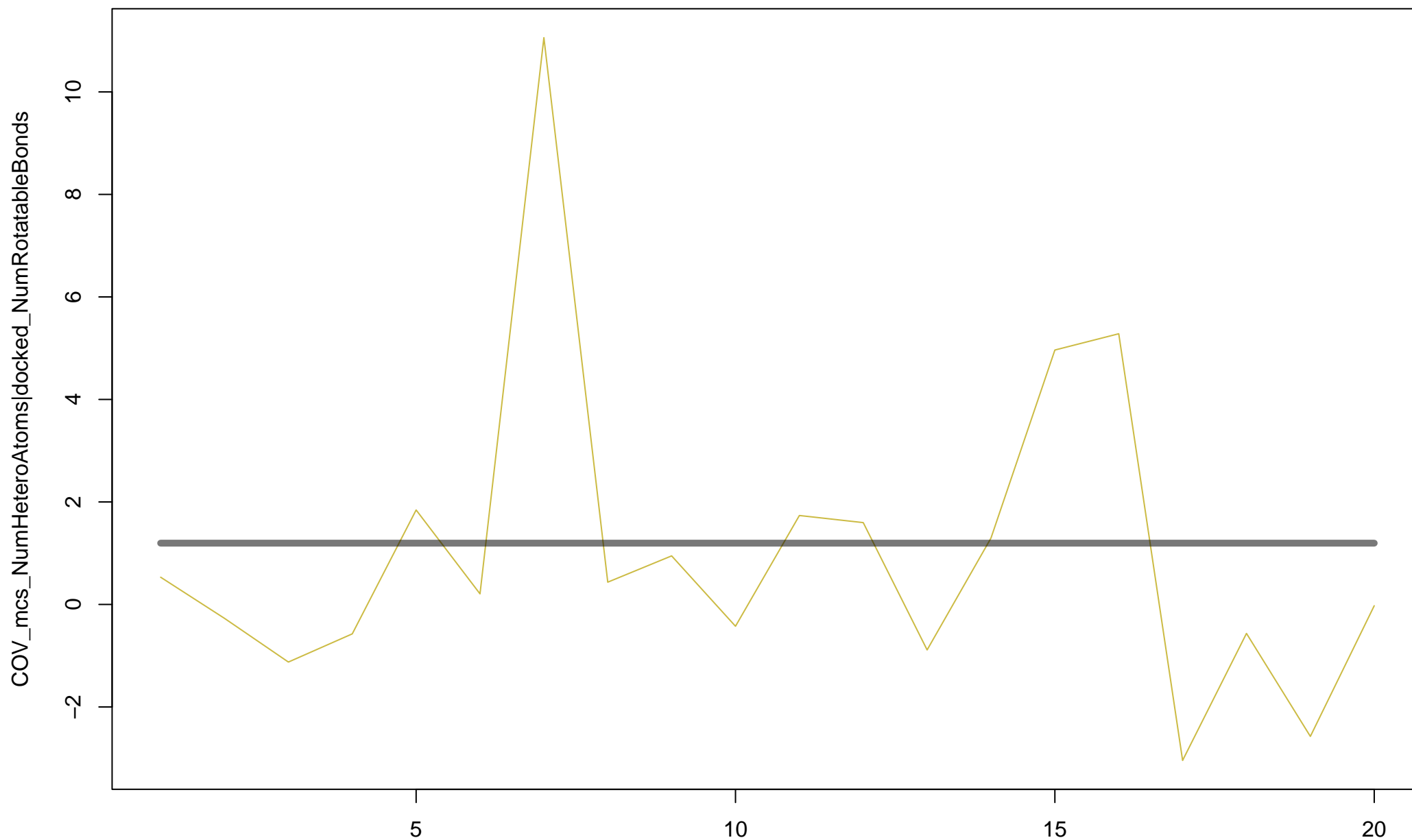
**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 20 | BMK = 0.377 | MCSE(6.27) = 23.3 | stat: FALSE | burn: 20 | percentile: 0**



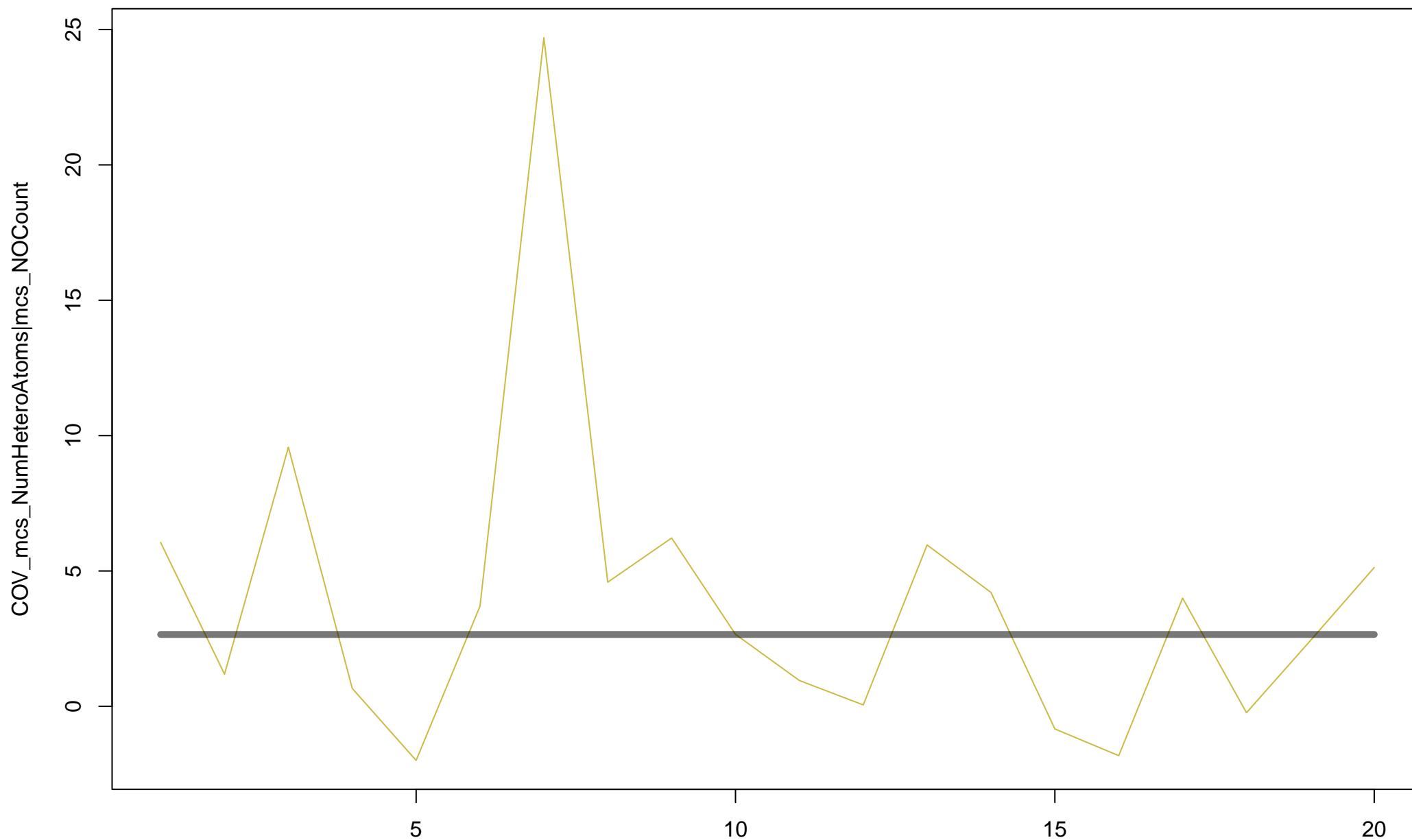
**COV\_mcs\_NumHeteroAtoms|mcs\_RingCount**  
**ESS = 20 | BMK = 0.34 | MCSE(6.27) = 22.8 | stat: FALSE | burn: 20 | percentile: 50**



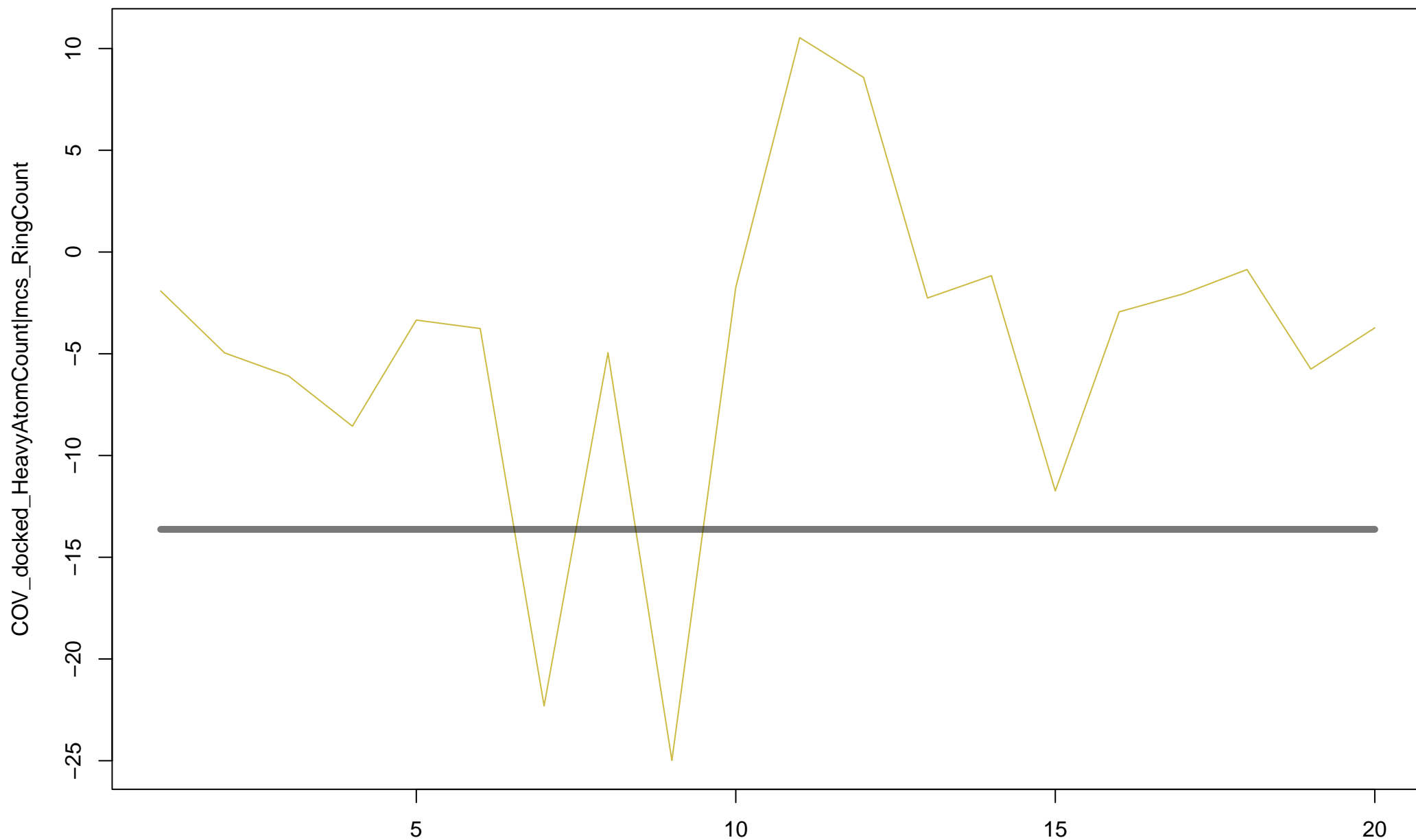
**COV\_mcs\_NumHeteroAtoms|docked\_NumRotatableBonds**  
**ESS = 20 | BMK = 0.52 | MCSE(6.27) = 22.6 | stat: FALSE | burn: 16 | percentile: 65**



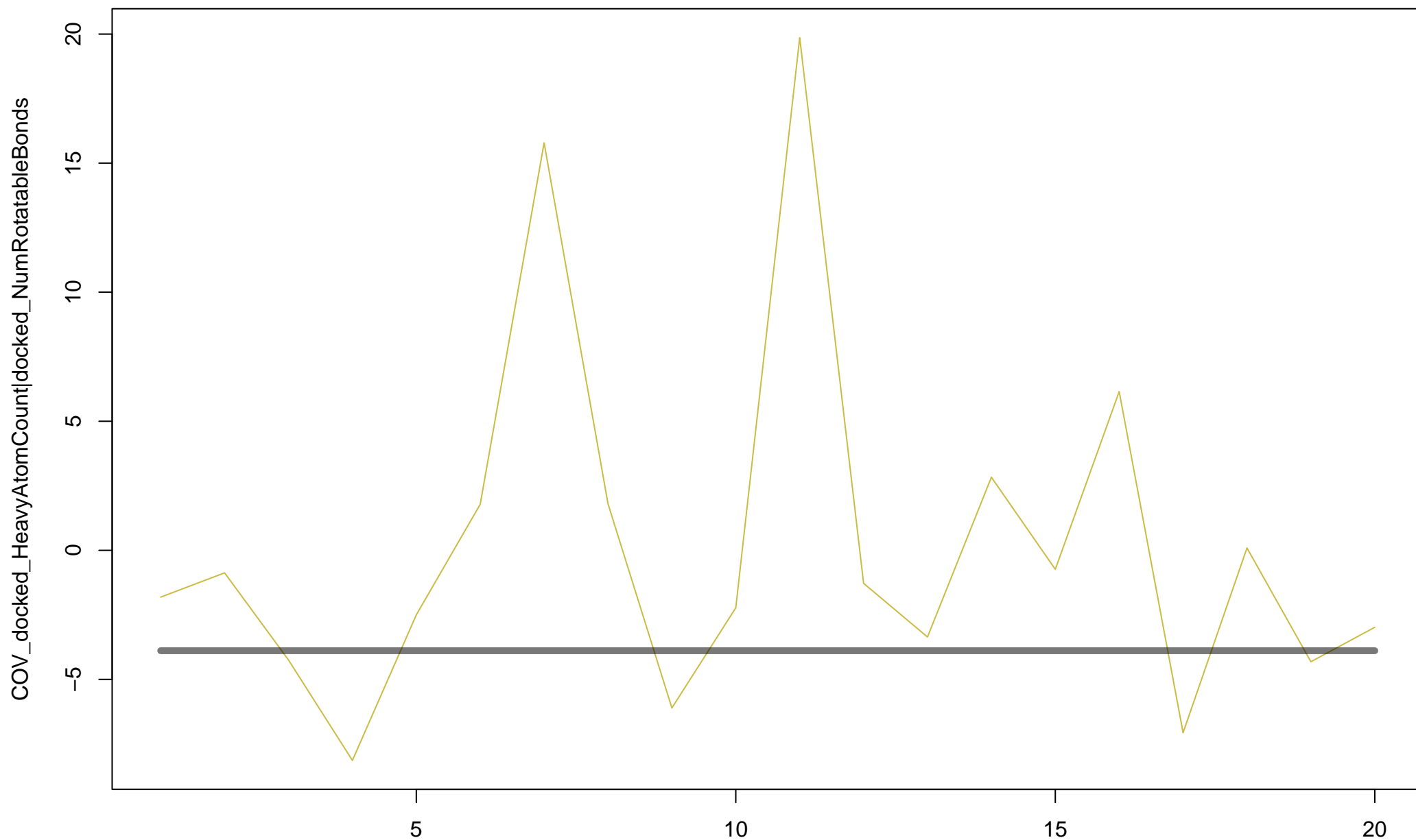
**COV\_mcs\_NumHeteroAtoms|mcs\_NOCount**  
**ESS = 20 | BMK = 0.301 | MCSE(6.27) = 22.7 | stat: FALSE | burn: 20 | percentile: 45**



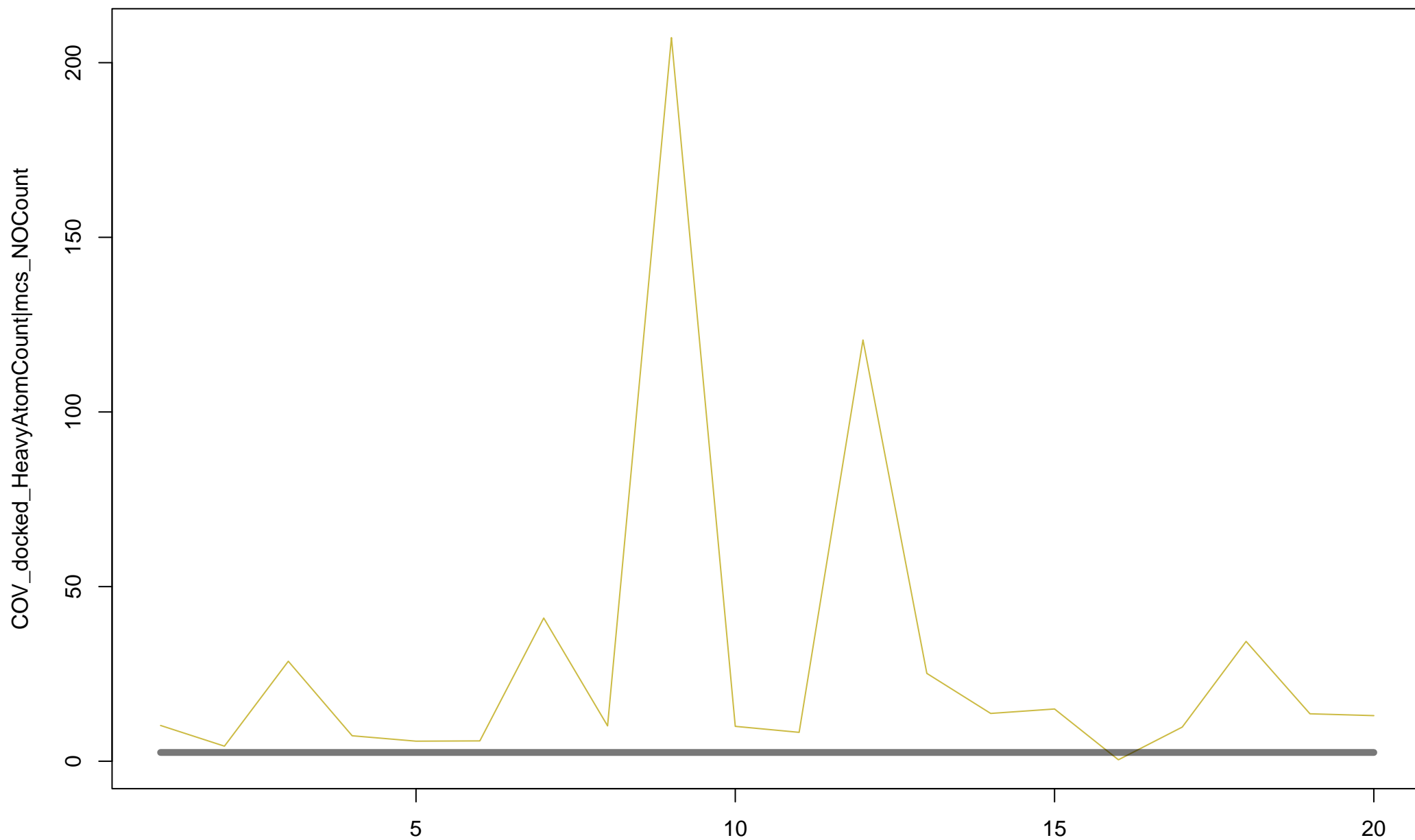
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 20 | BMK = 0.531 | MCSE(6.27) = 29.3 | stat: FALSE | burn: 20 | percentile: 10**



**COV\_docked\_HeavyAtomCount|docked\_NumRotatableBonds**  
**ESS = 20 | BMK = 0.212 | MCSE(6.27) = 21.8 | stat: FALSE | burn: 20 | percentile: 25**

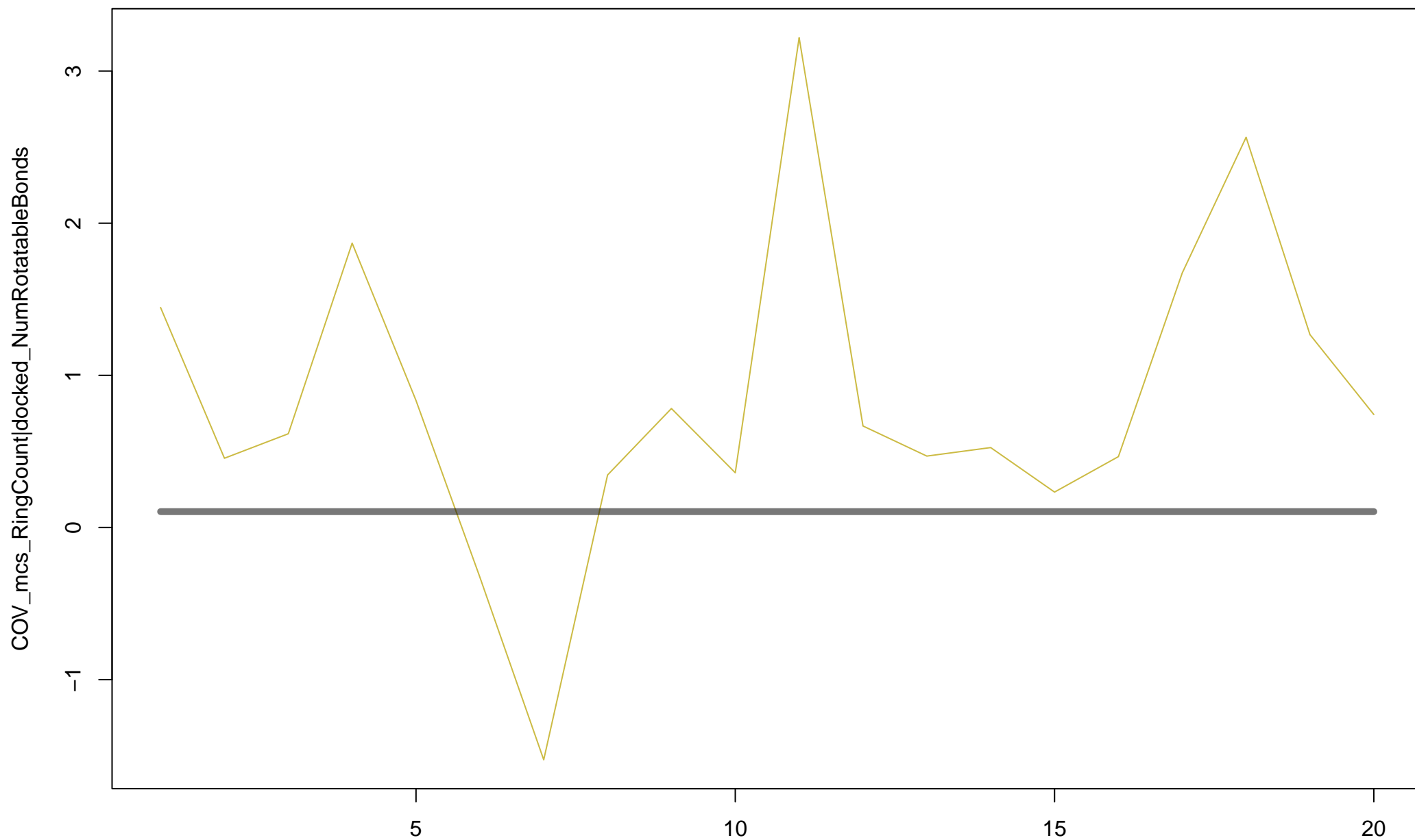


**COV\_docked\_HeavyAtomCount|mcs\_NOCount**  
**ESS = 20 | BMK = 0.4 | MCSE(6.27) = 18.6 | stat: FALSE | burn: 20 | percentile: 5**

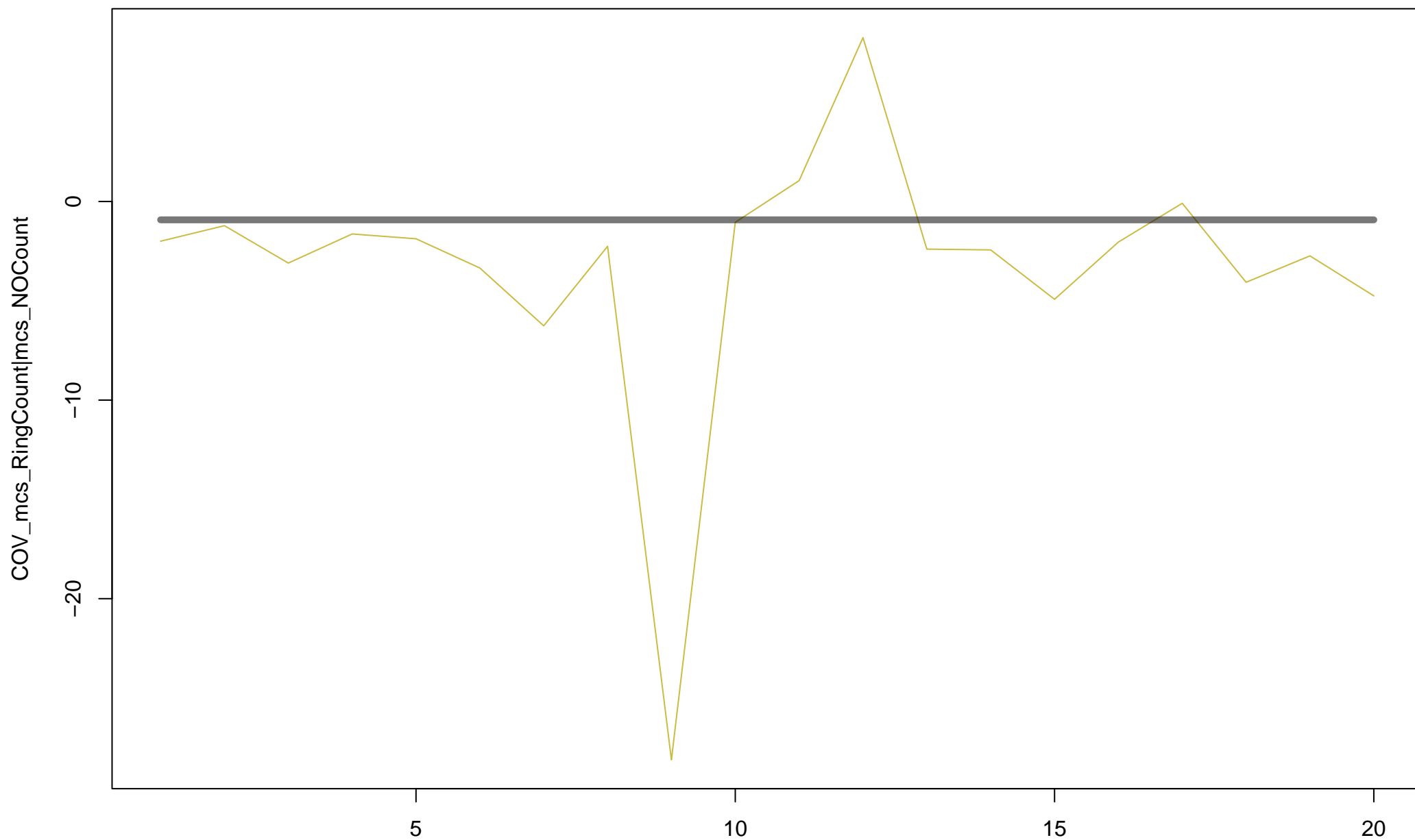




**COV\_mcs\_RingCount|docked\_NumRotatableBonds**  
**ESS = 20 | BMK = 0.377 | MCSE(6.27) = 28.3 | stat: FALSE | burn: 20 | percentile: 10**



**COV\_mcs\_RingCount|mcs\_NOCount**  
**ESS = 20 | BMK = 0.483 | MCSE(6.27) = 21.5 | stat: FALSE | burn: 20 | percentile: 85**



**COV\_docked\_NumRotatableBonds|mcs\_NOCount**  
**ESS = 20 | BMK = 0.451 | MCSE(6.27) = 29.1 | stat: FALSE | burn: 20 | percentile: 85**

