

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 1

max MCSE = 54.6660394059867

all stationary: FALSE

burn: 0

min percent.: 0

-- STATS 2D --

min ESS = 2.70826862105808

max BMK = 0.865259016067798

max MCSE = NaN

all stationary: FALSE

burn: 0

min percent.: 0

-- STATS 1D --

min ESS = 2.87910360620067

max BMK = 1

max MCSE = NaN

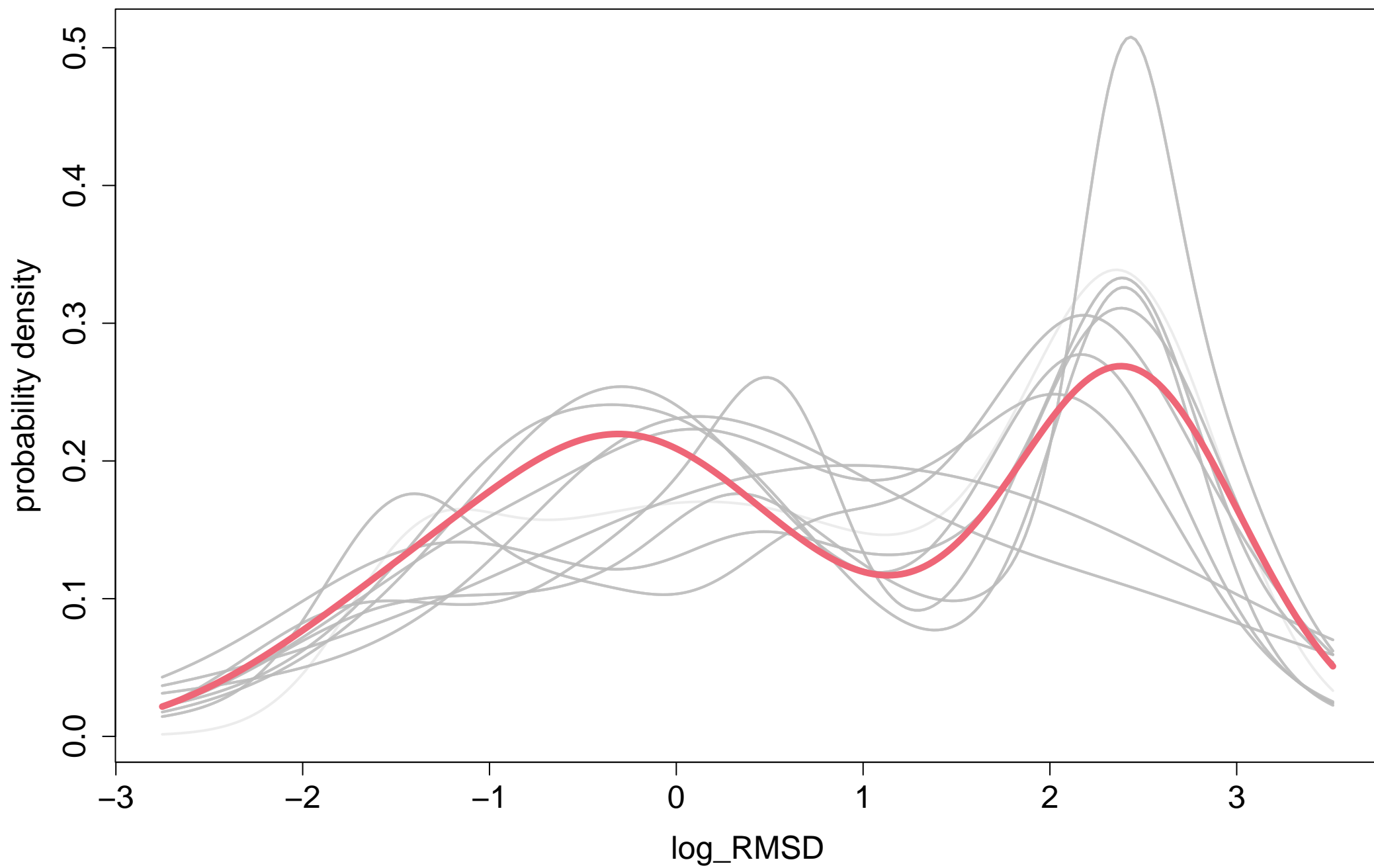
all stationary: FALSE

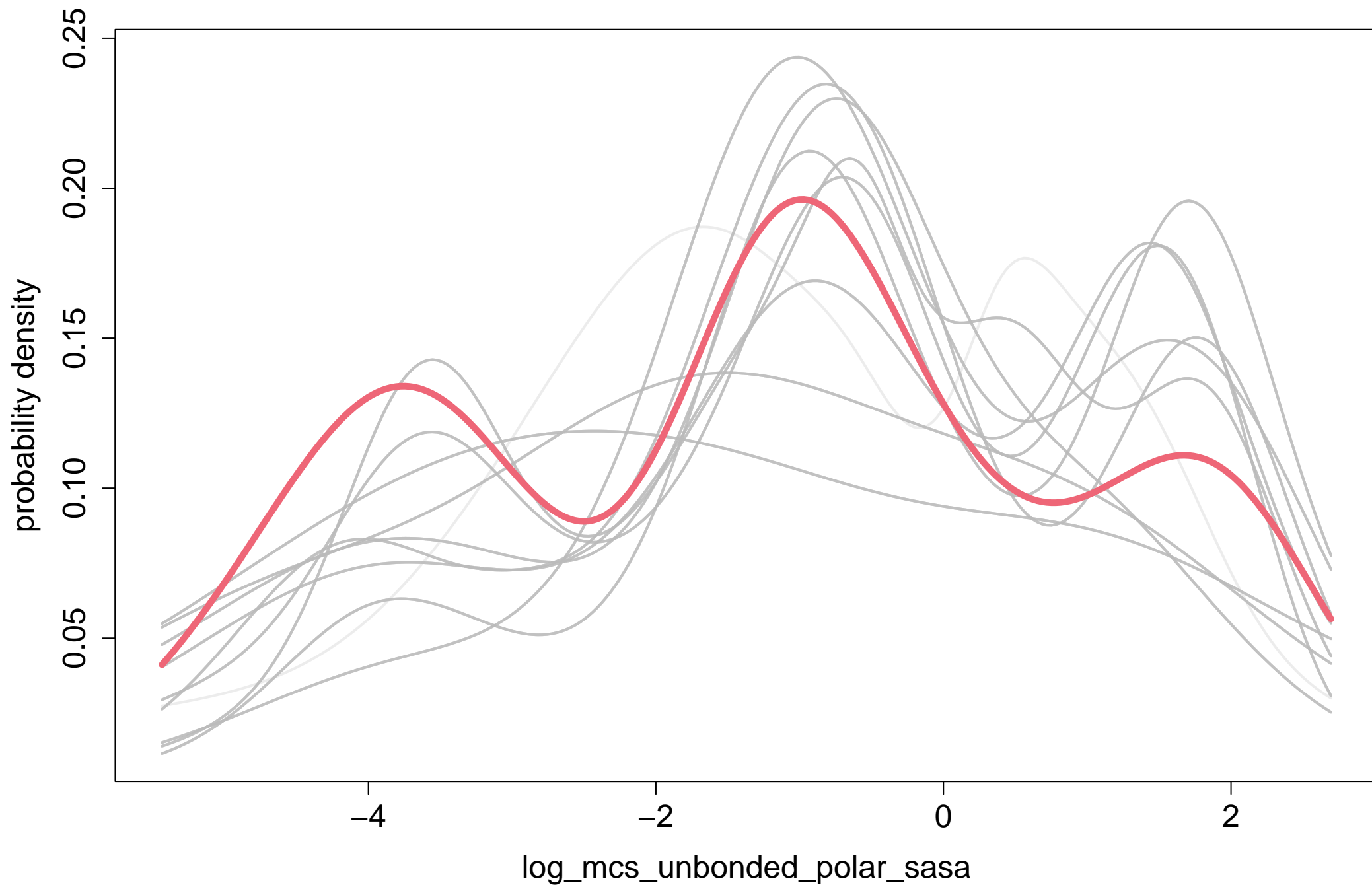
burn: 0

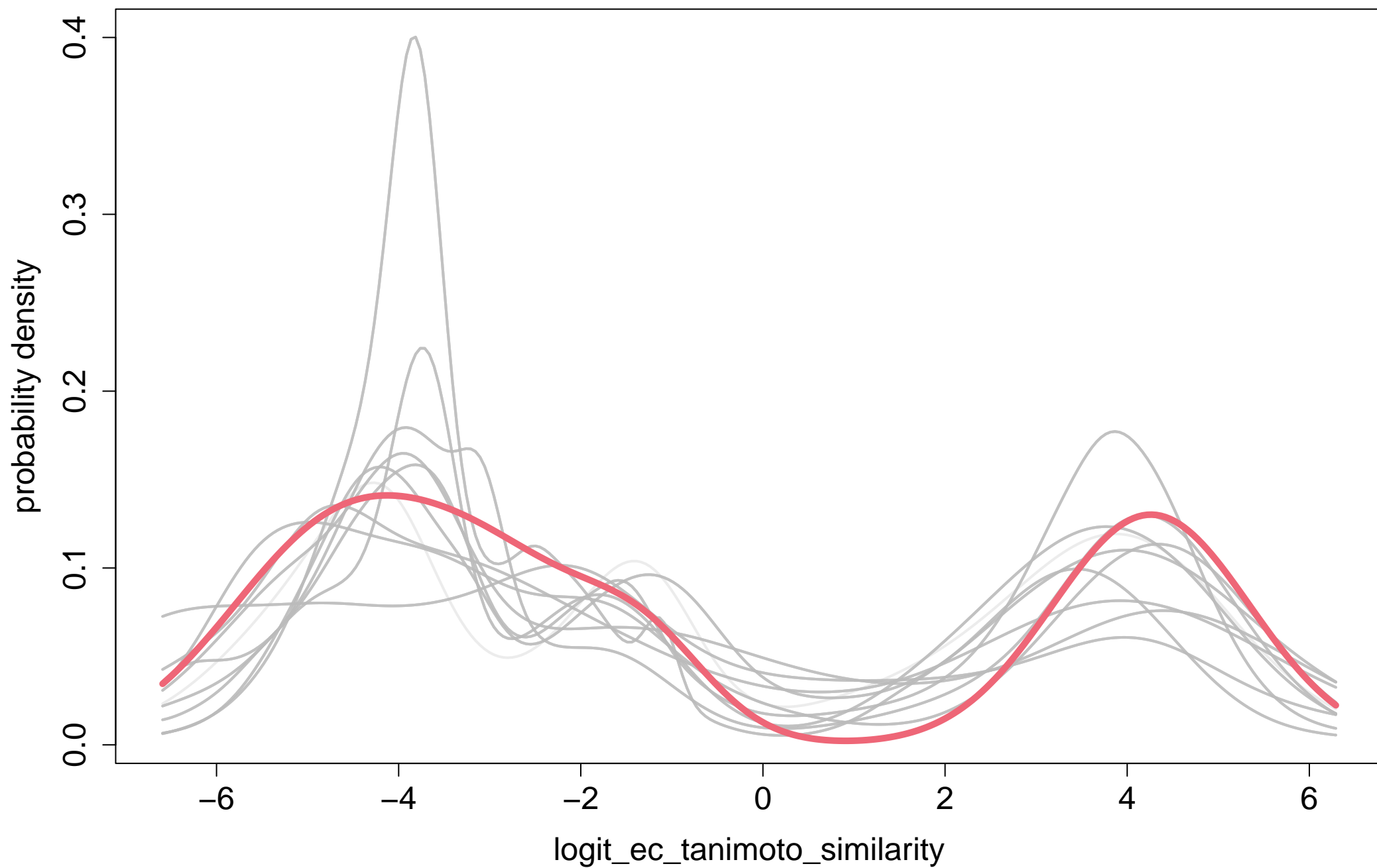
min percent.: 0

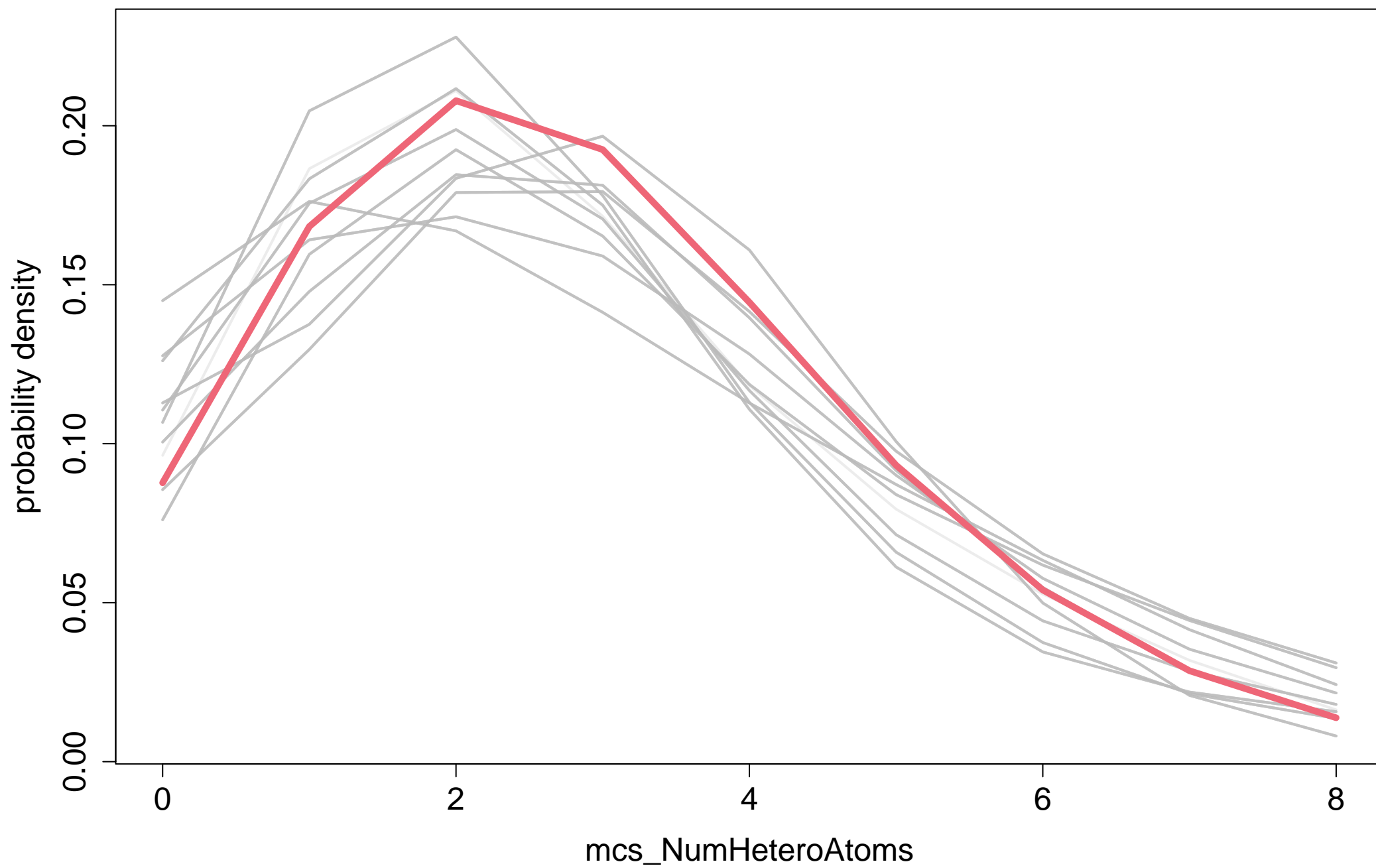
Occupied clusters: 25 of 64

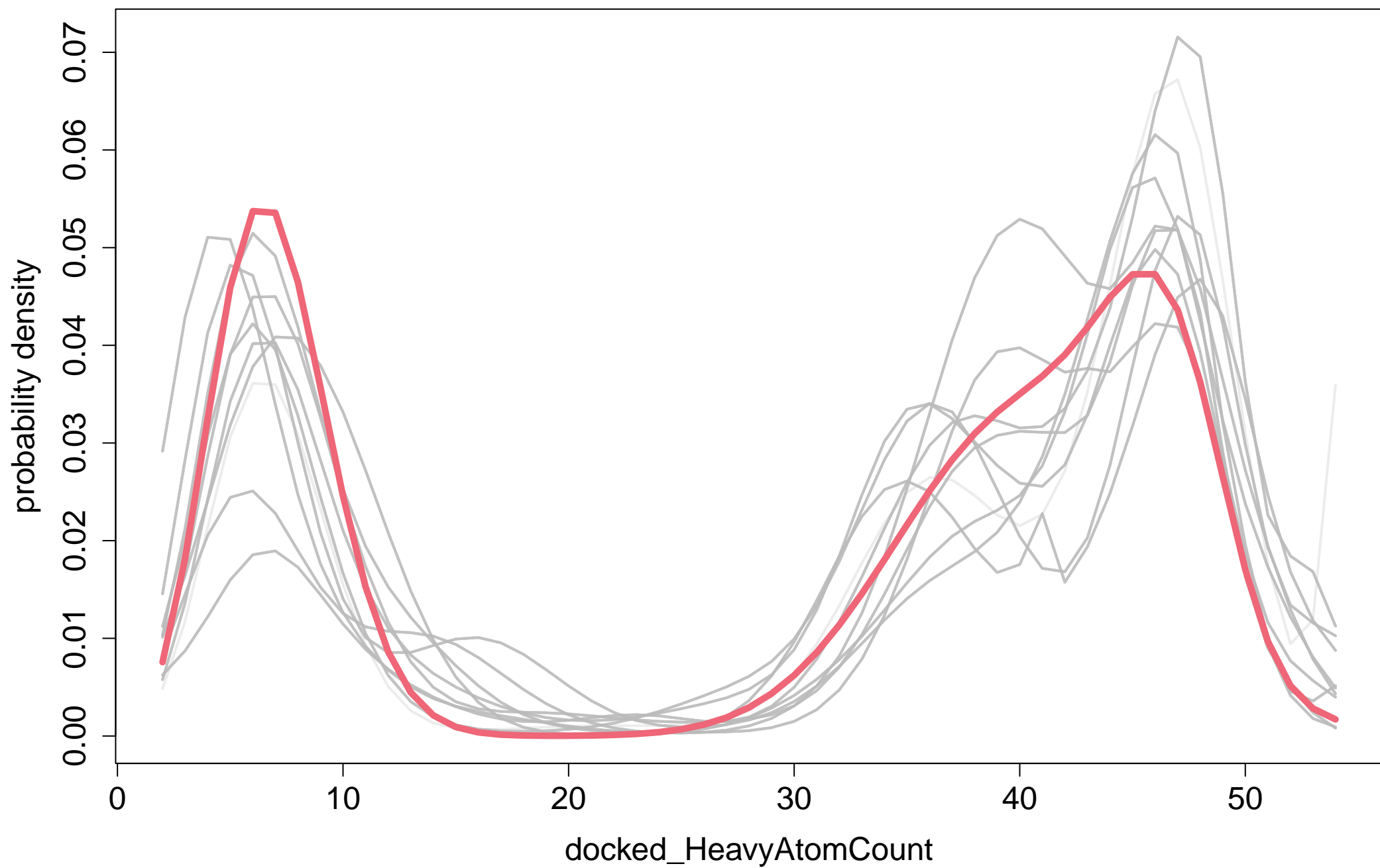
LL: -989 +- 49.9

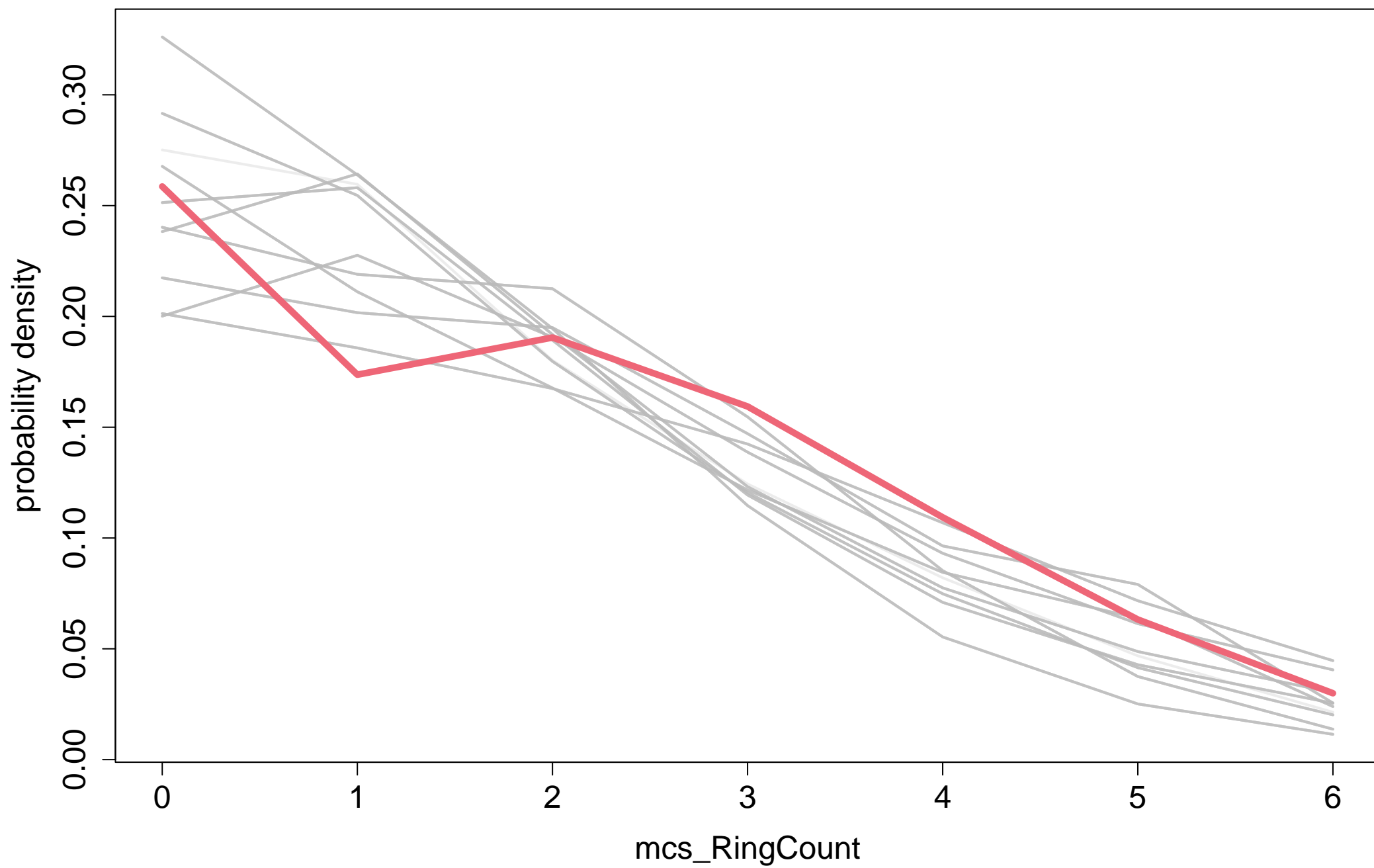


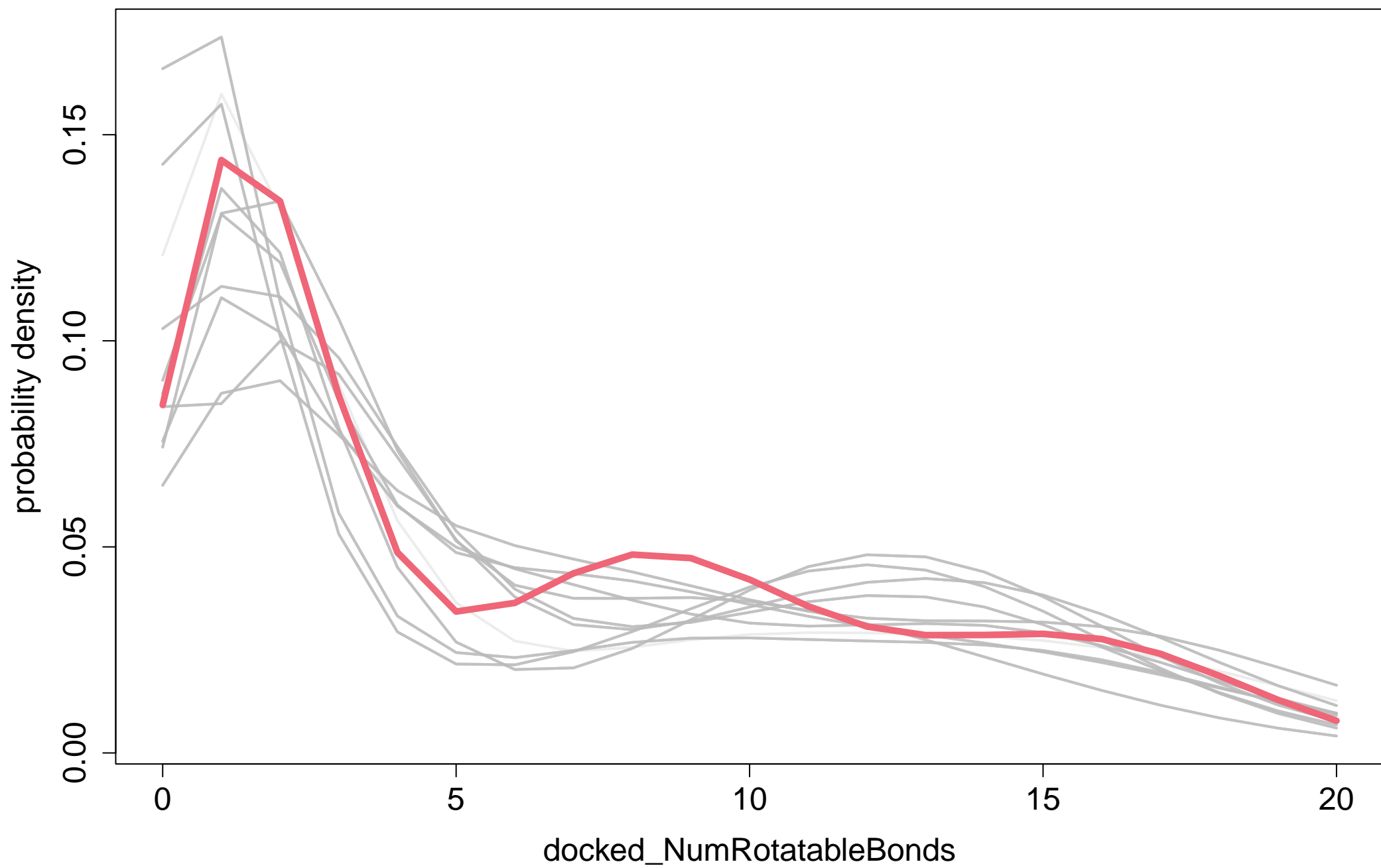




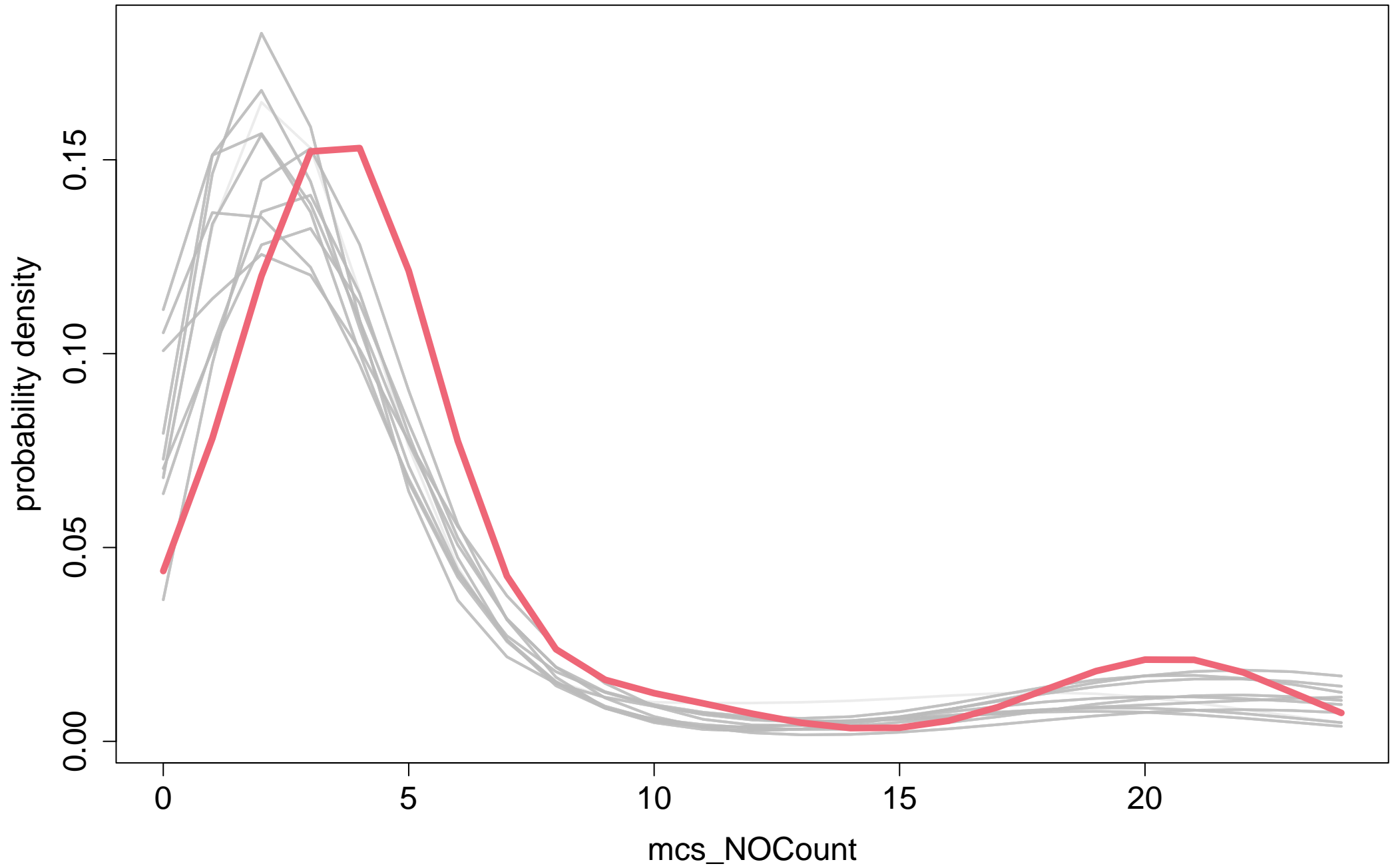


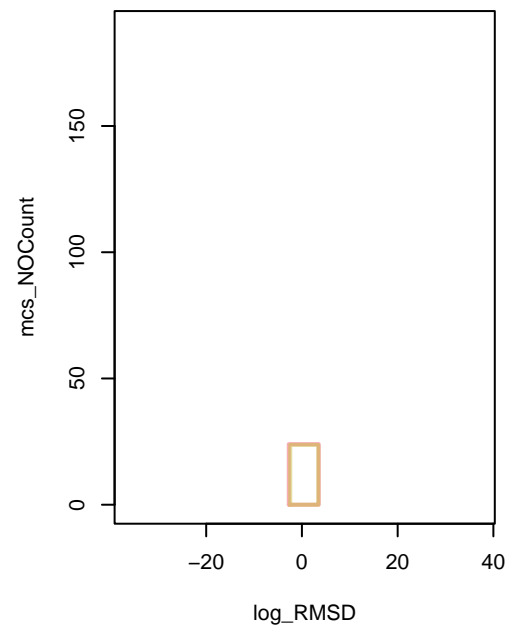
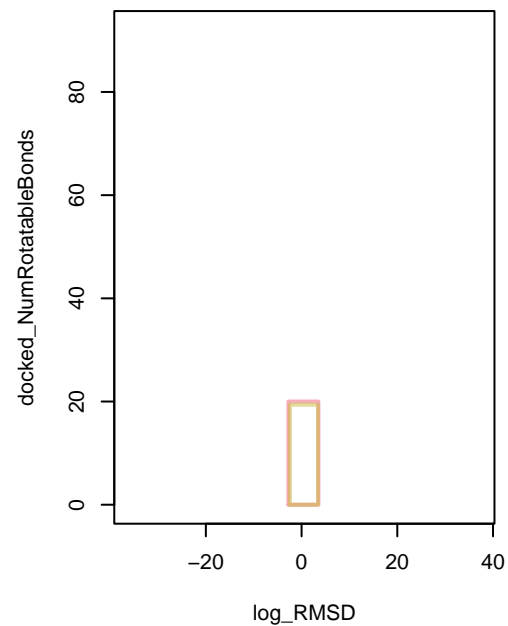
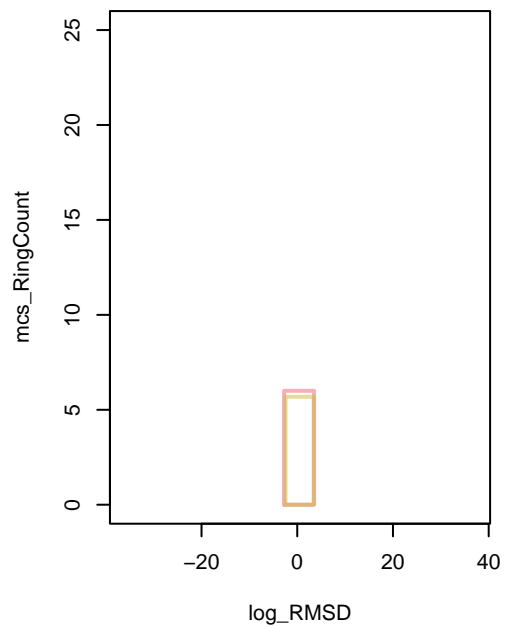
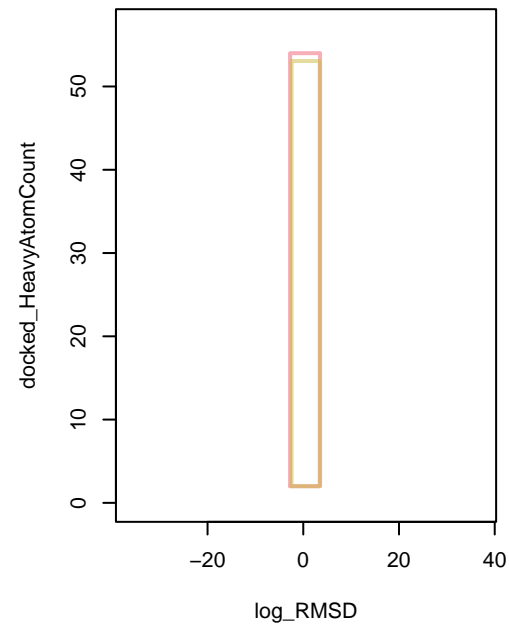
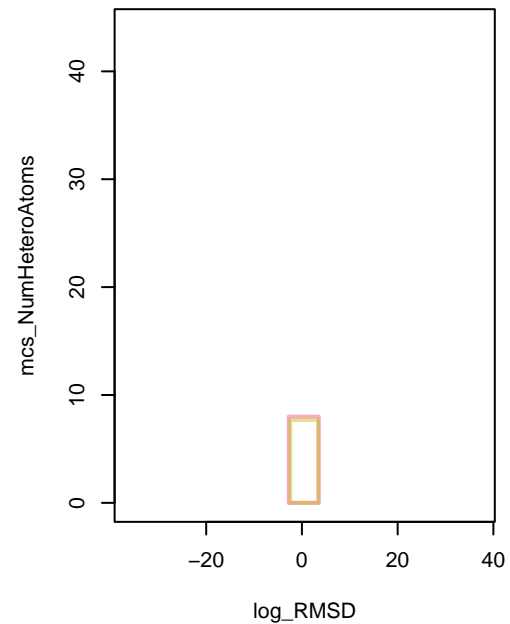
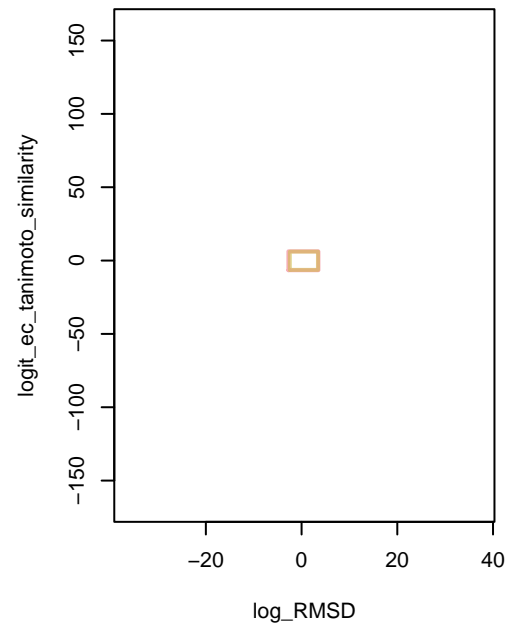
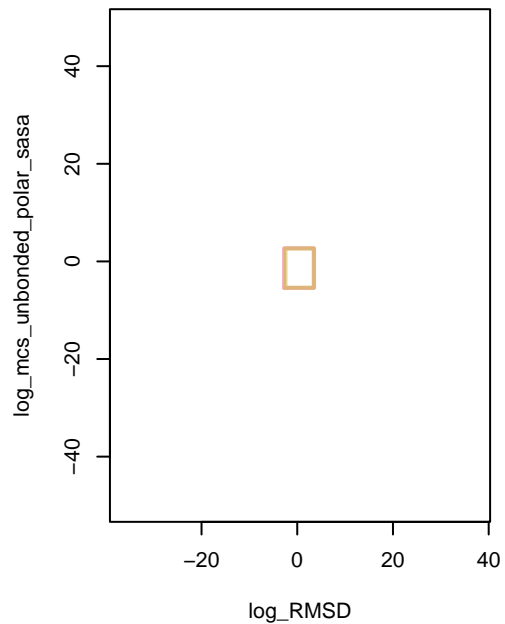




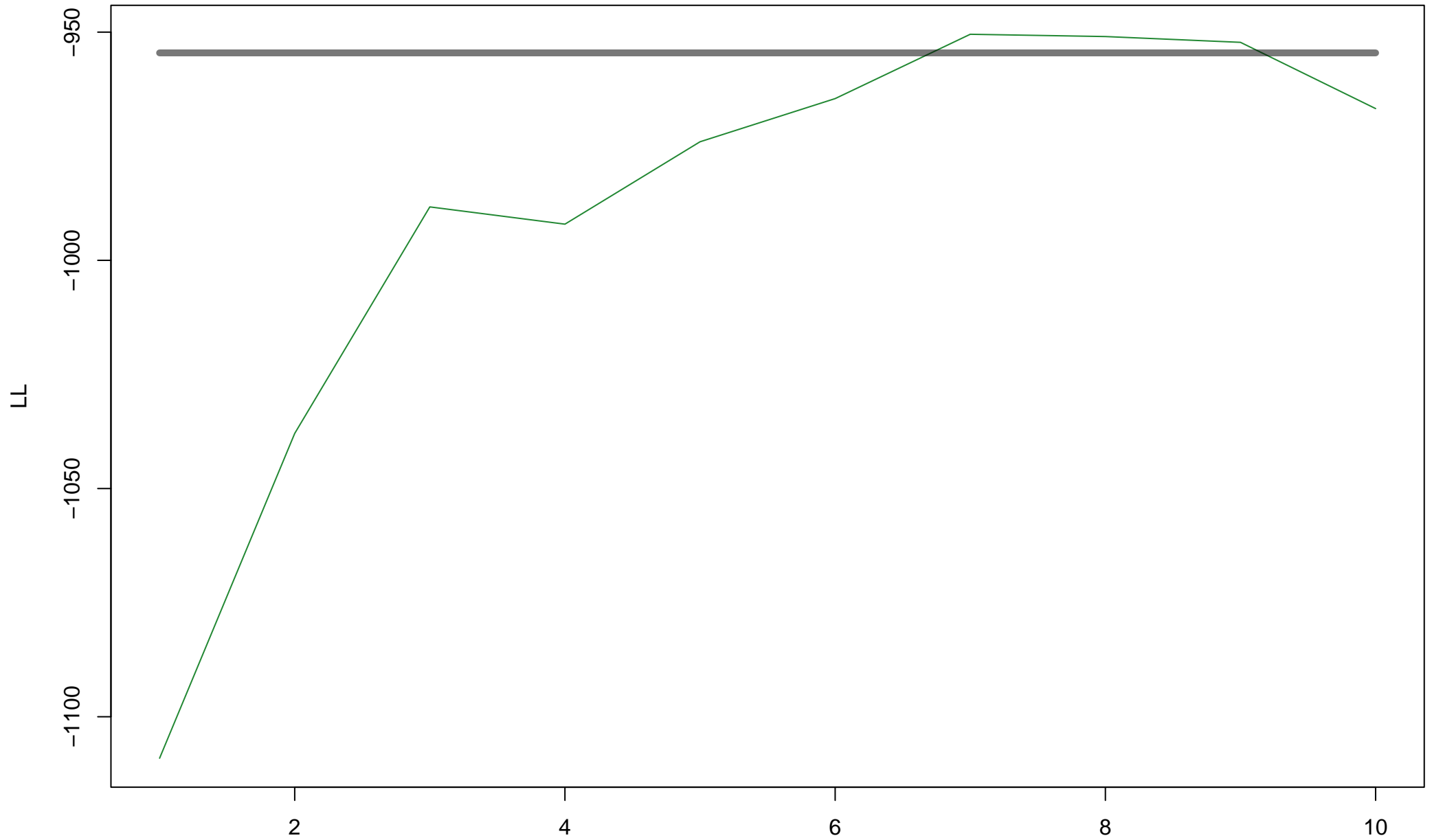






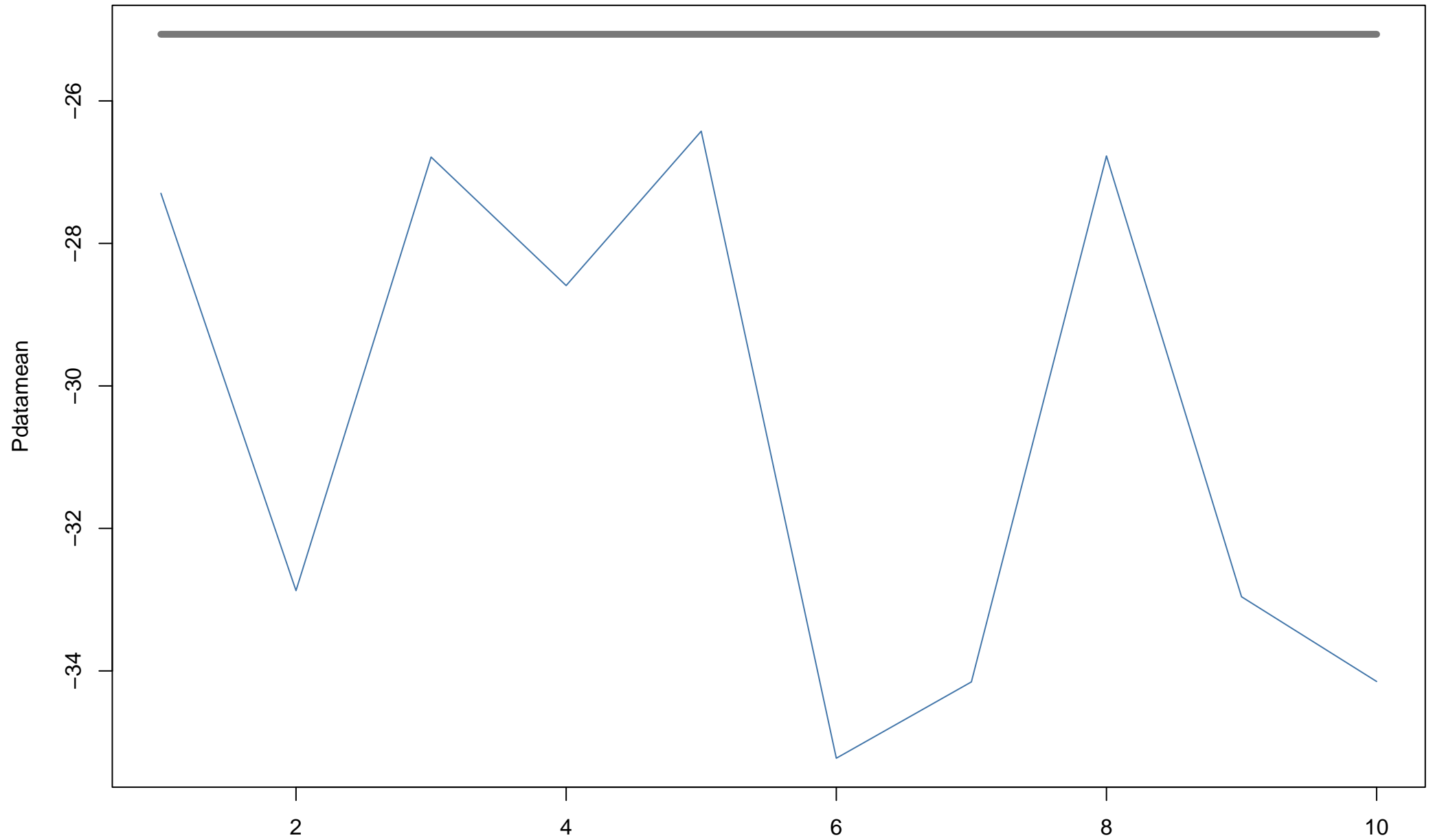


LL



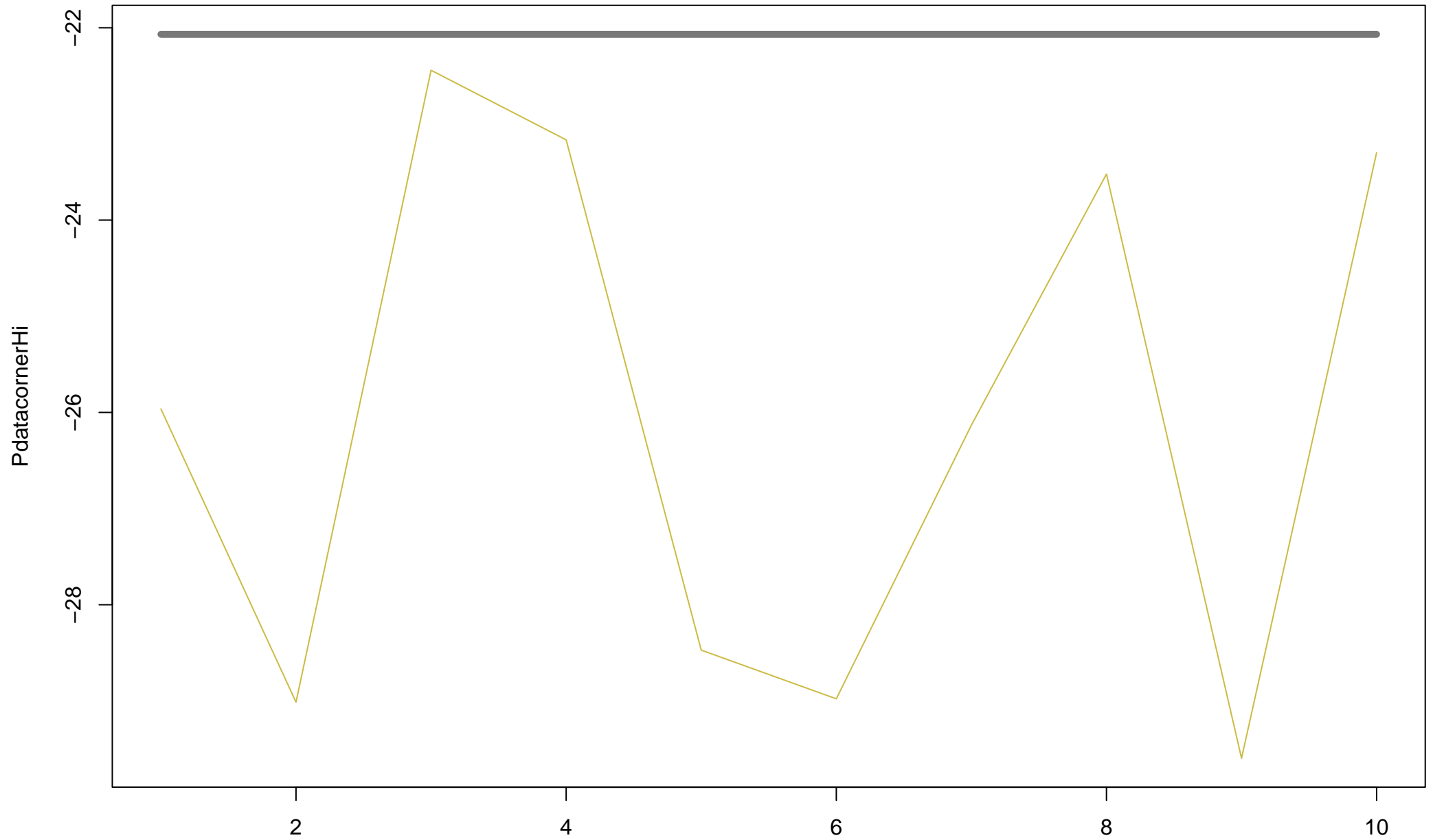
Pdatamean

ESS = 2.22e-16 | BMK = 1 | MCSE(6.27) = 5.77 | stat: FALSE | burn: 0 | percentile: 100



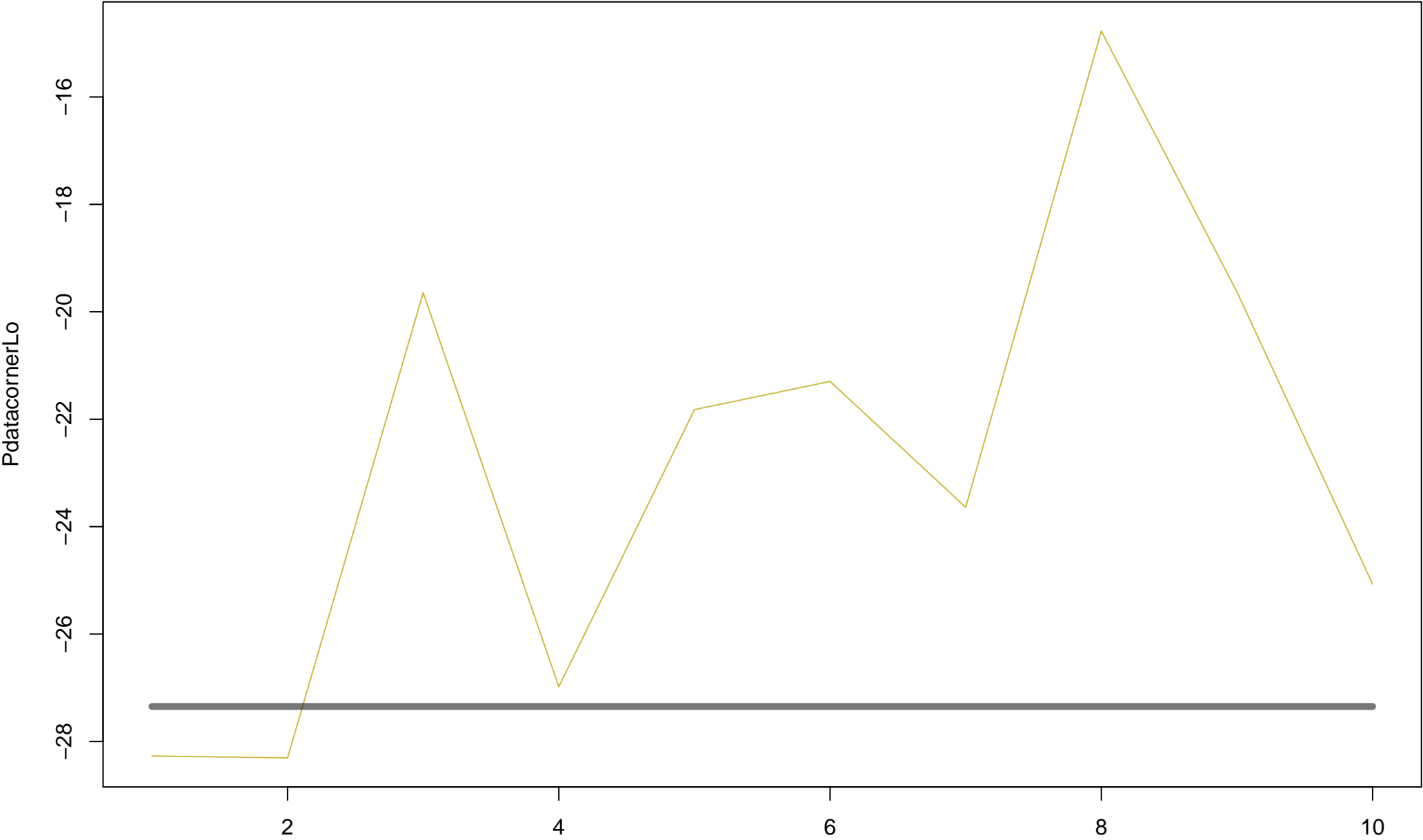
# PdatacornerHi

ESS = 2.22e-16 | BMK = 0.294 | MCSE(6.27) = 30.4 | stat: FALSE | burn: 0 | percentile: 100

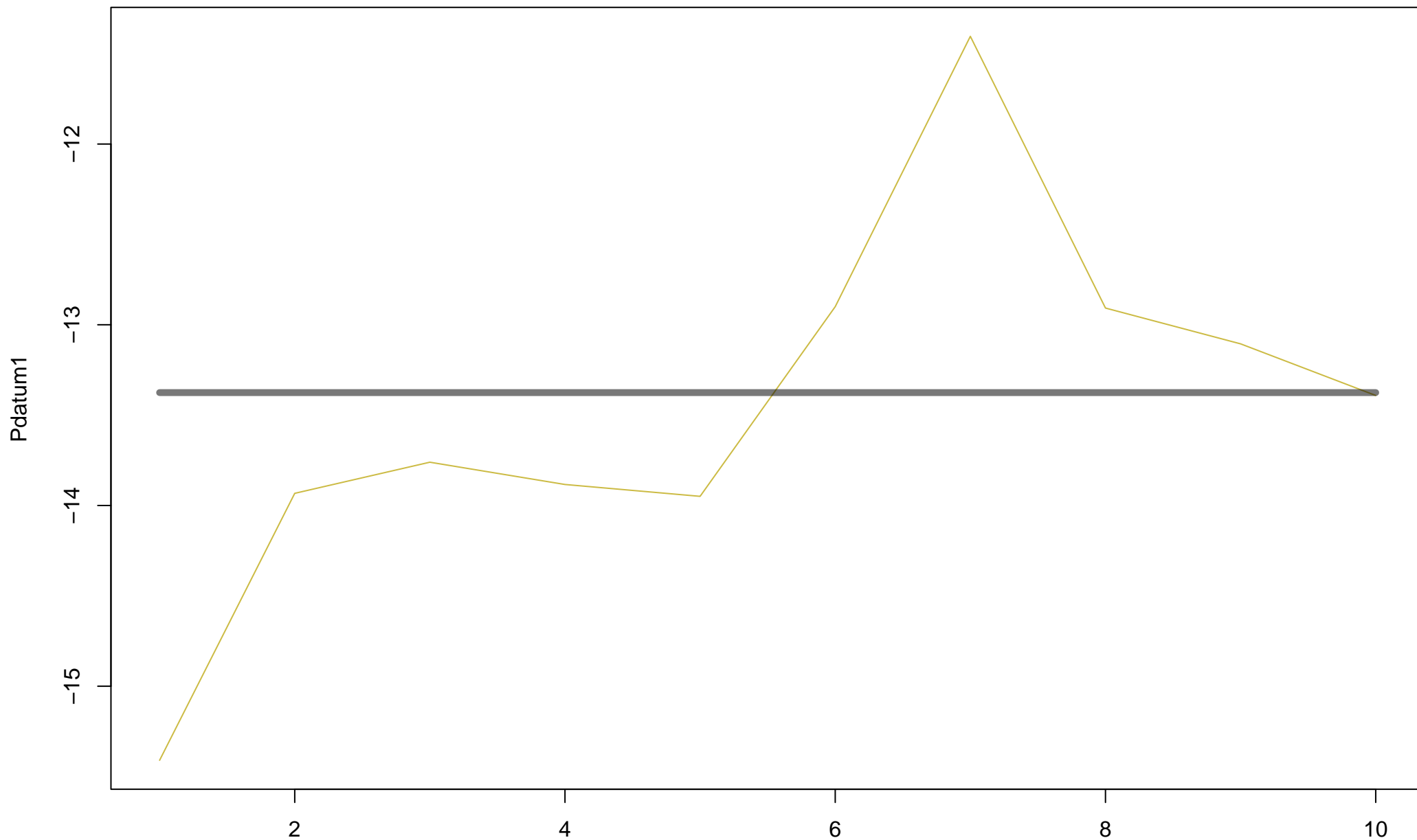


PdatacornerLo

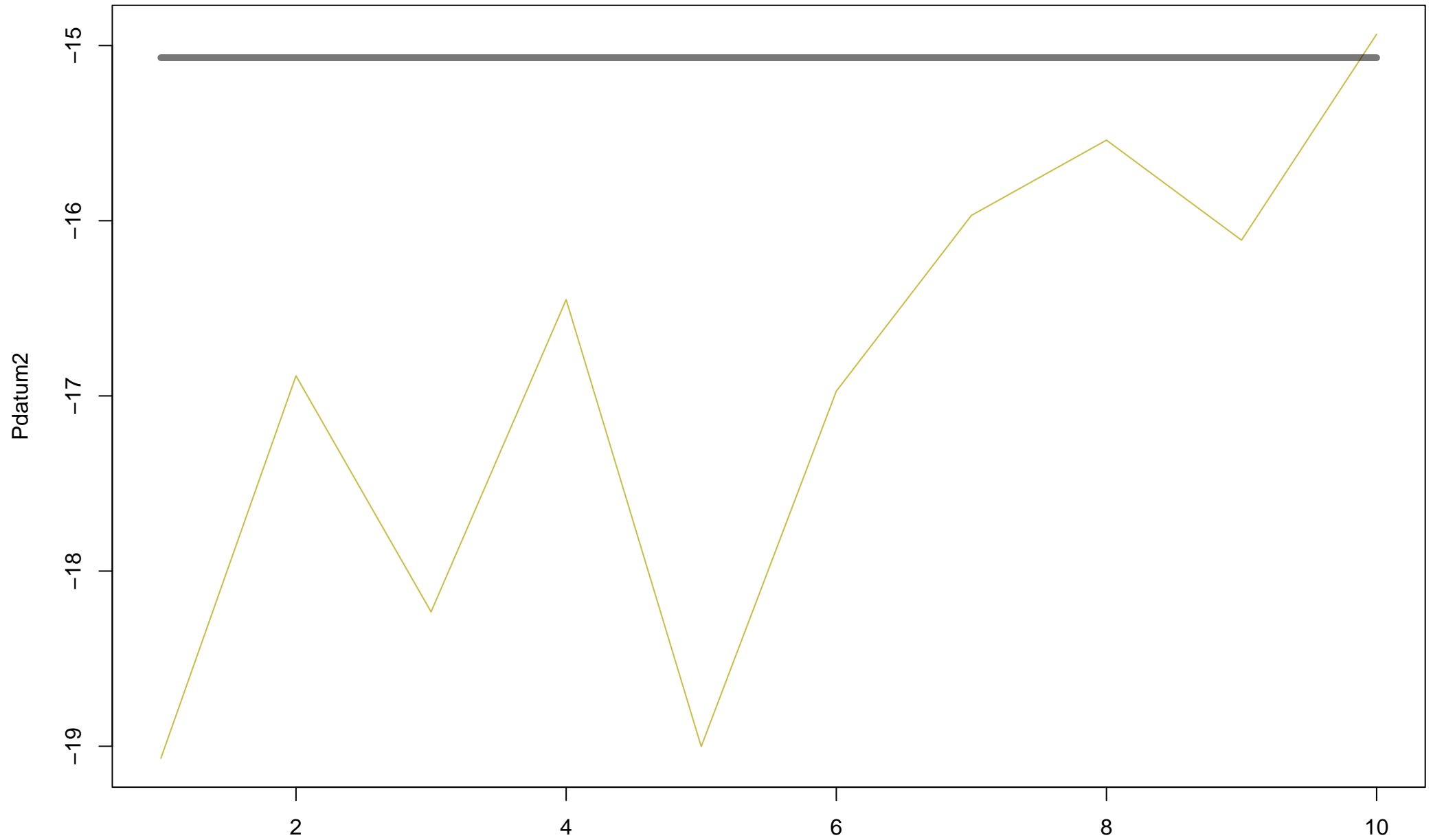
ESS = 10 | BMK = 1 | MCSE(6.27) = 26.2 | stat: FALSE | burn: 0 | percentile: 20



**Pdatum1**  
**ESS = 10 | BMK = 1 | MCSE(6.27) = 34.1 | stat: FALSE | burn: 0 | percentile: 60**



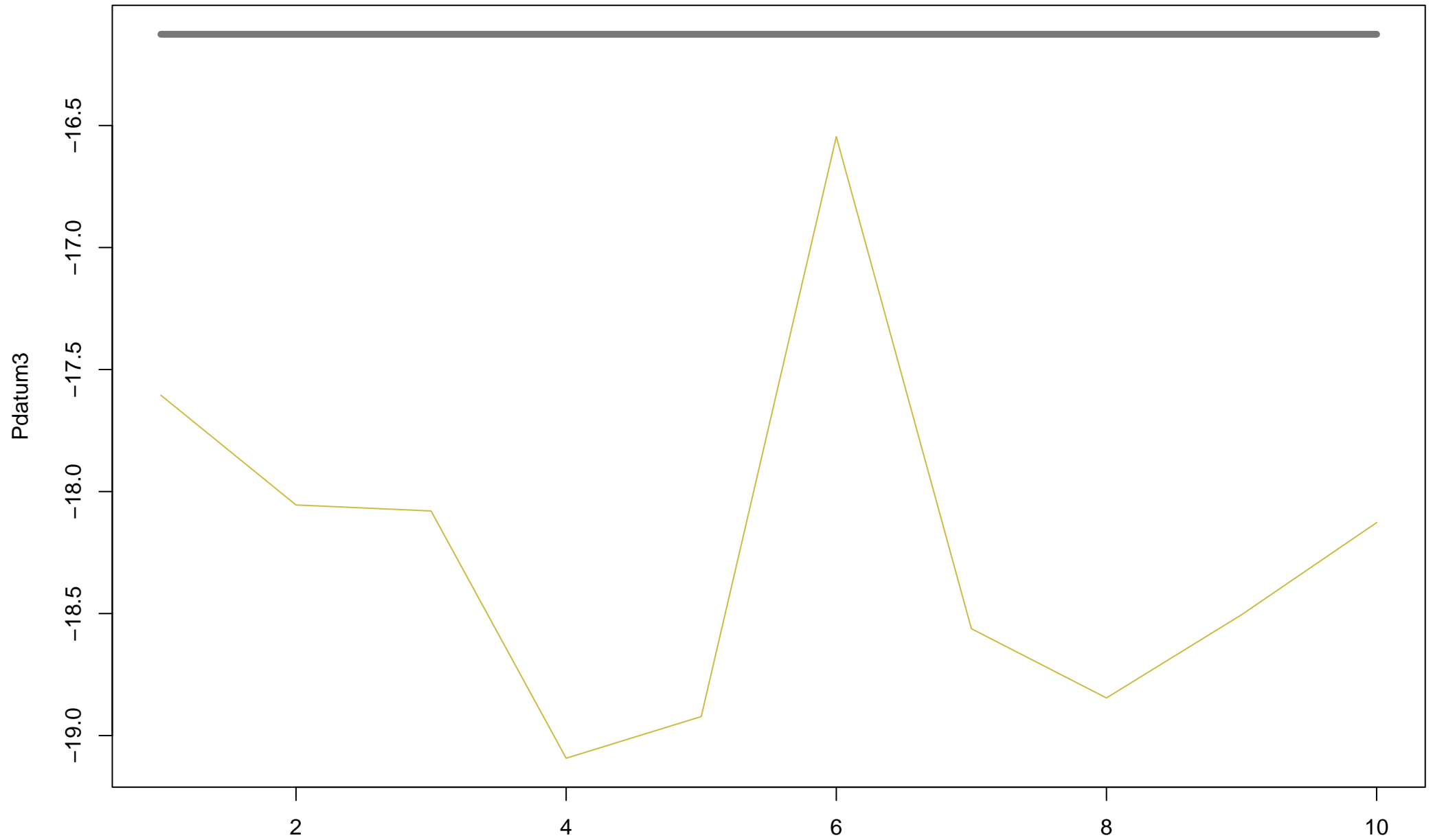
**Pdatum2**  
**ESS = 10 | BMK = 0.686 | MCSE(6.27) = 54.7 | stat: FALSE | burn: 0 | percentile: 90**



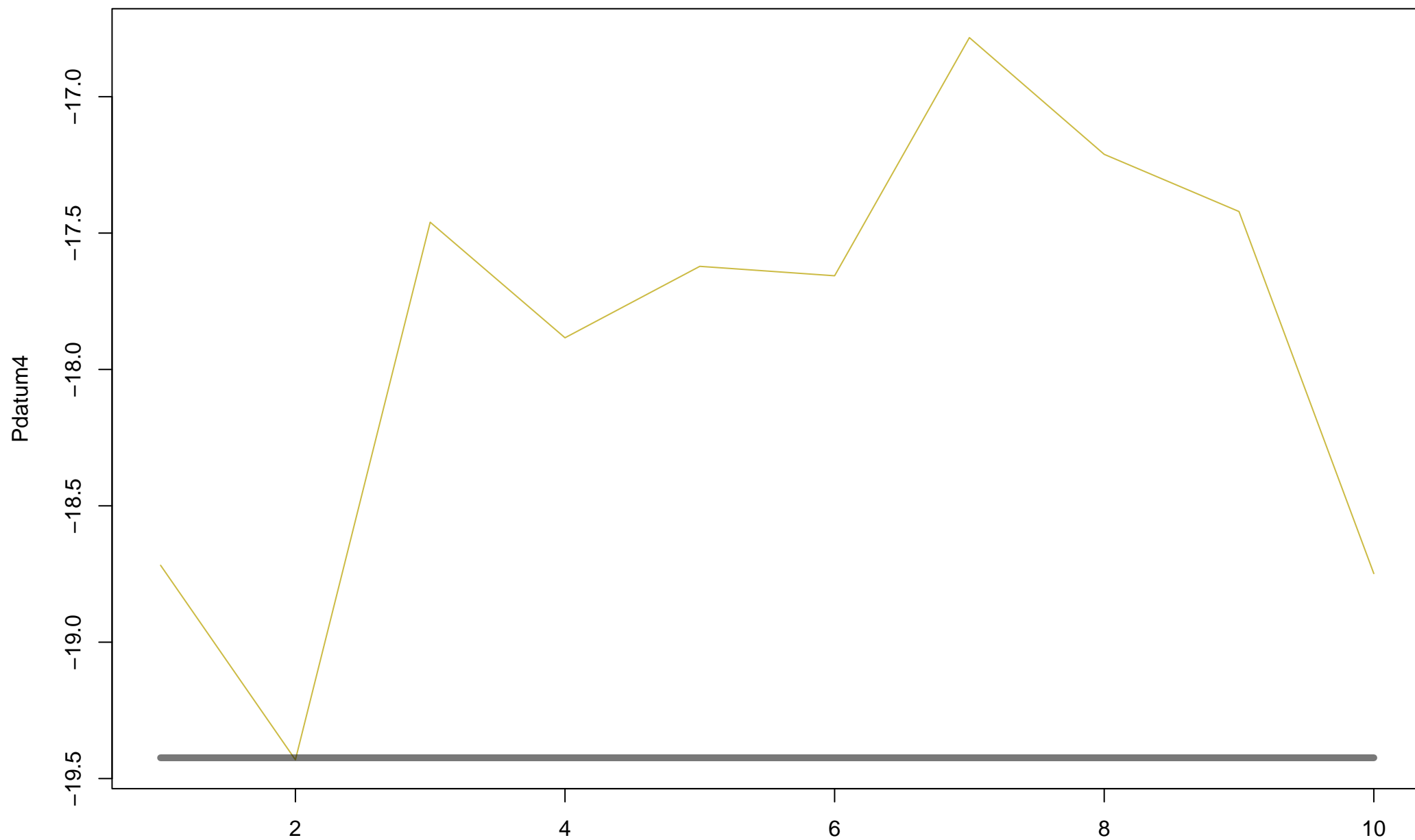


**Pdatum3**

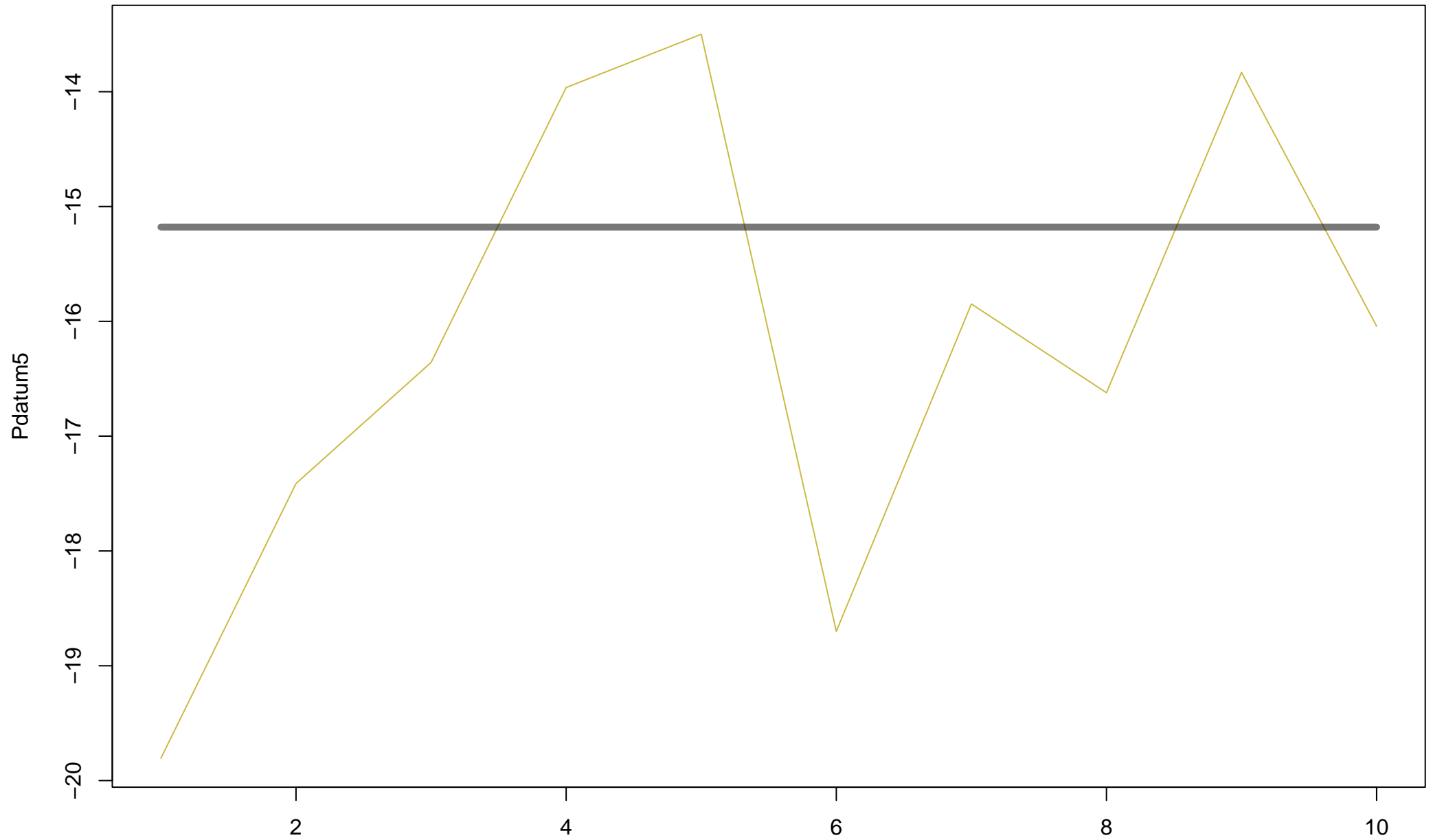
**ESS = 10 | BMK = 0.659 | MCSE(6.27) = 23.2 | stat: FALSE | burn: 0 | percentile: 100**



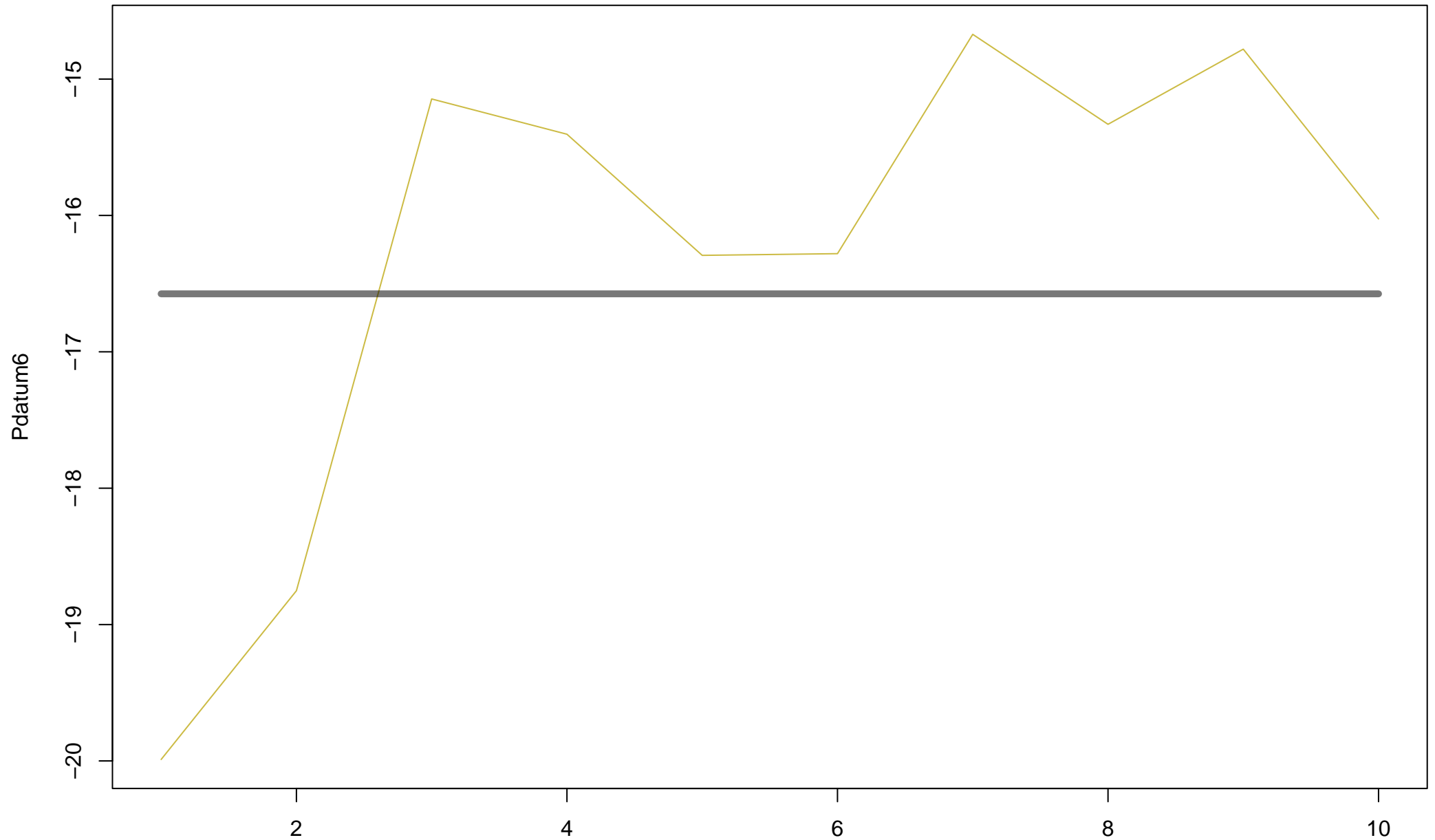
**Pdatum4**  
**ESS = 2.22e-16 | BMK = 0.372 | MCSE(6.27) = 43.3 | stat: FALSE | burn: 0 | percentile: 10**



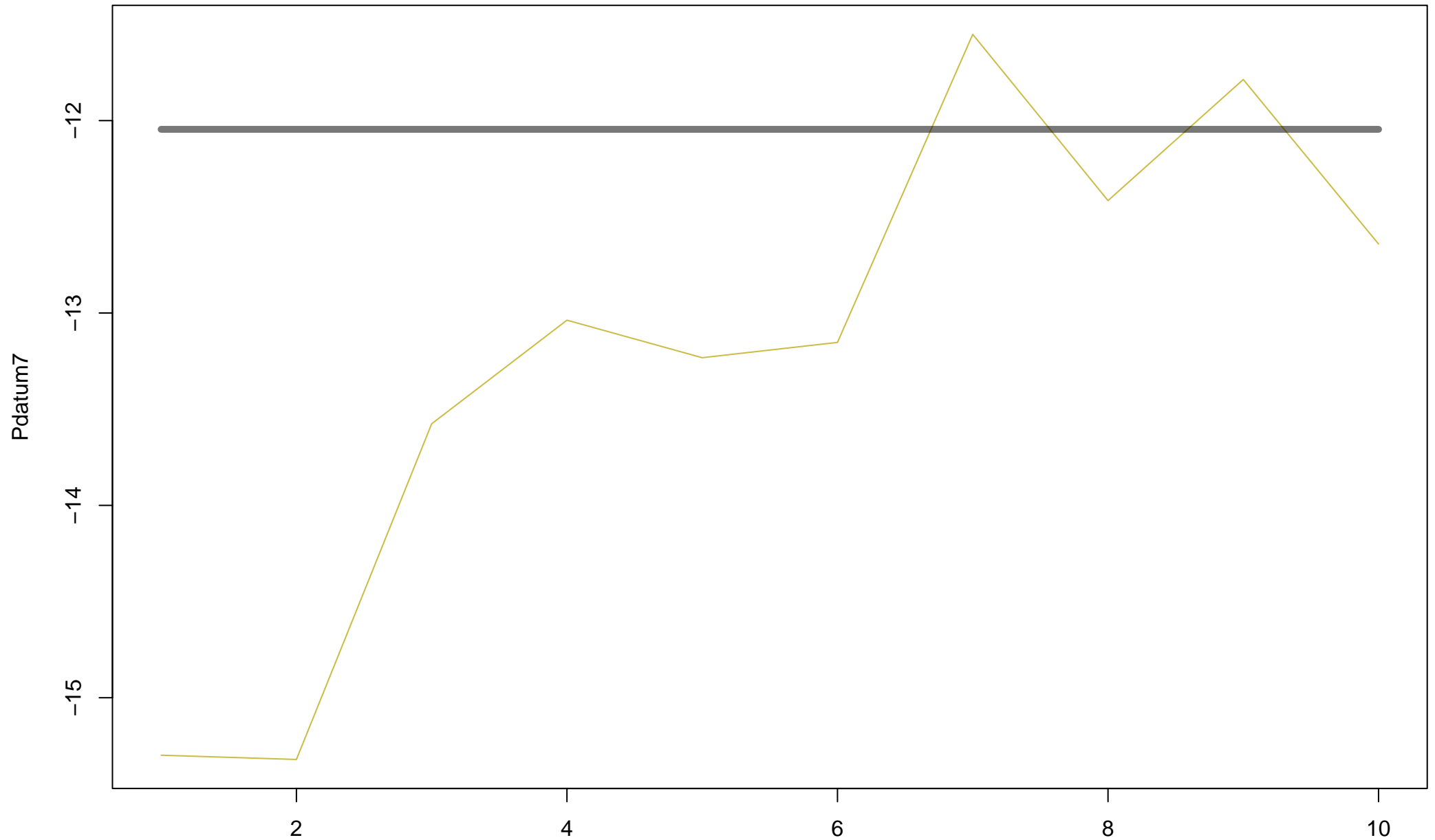
**Pdatum5**  
**ESS = 10 | BMK = 0.616 | MCSE(6.27) = 30.3 | stat: FALSE | burn: 0 | percentile: 70**



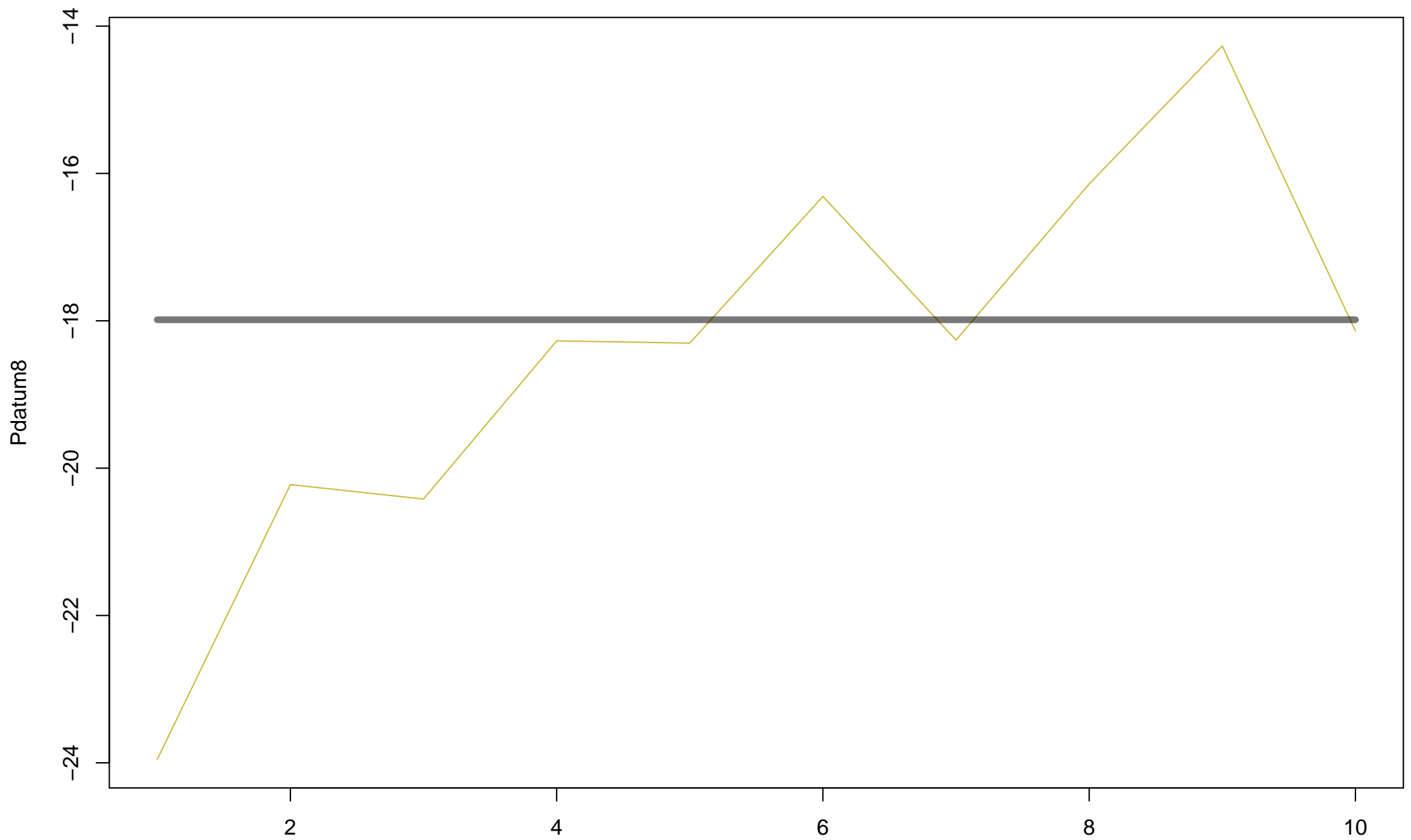
**Pdatum6**  
**ESS = 10 | BMK = 0.259 | MCSE(6.27) = 30.9 | stat: FALSE | burn: 0 | percentile: 20**



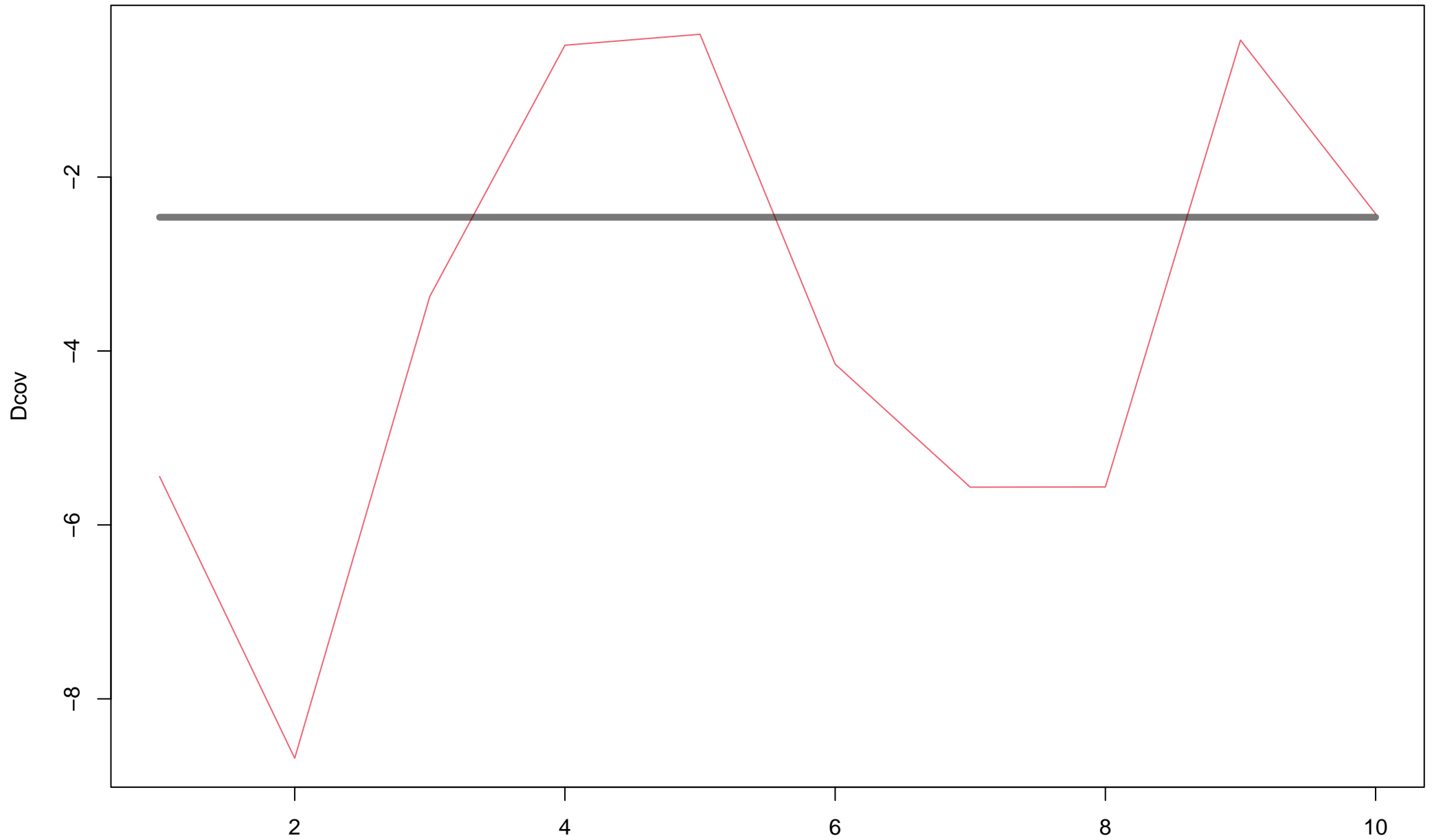
**Pdatum7**  
**ESS = 10 | BMK = 0.647 | MCSE(6.27) = 54.5 | stat: FALSE | burn: 0 | percentile: 80**



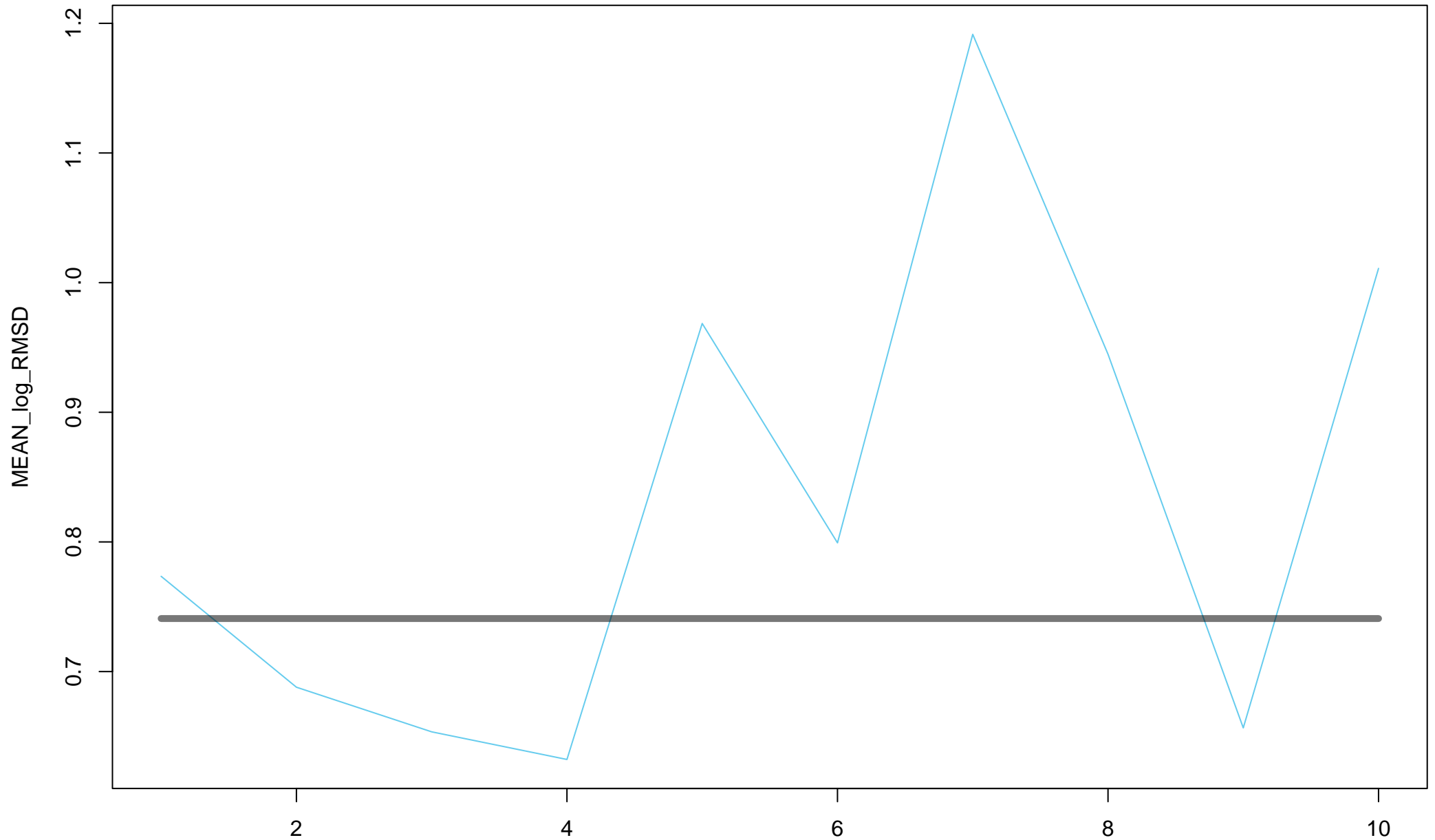
**Pdatum8**  
**ESS = 10 | BMK = 1 | MCSE(6.27) = 29.3 | stat: FALSE | burn: 0 | percentile: 70**



**Dcov**  
**ESS = 10 | BMK = 0.808 | MCSE(6.27) = 29 | stat: FALSE | burn: 0 | percentile: 10**

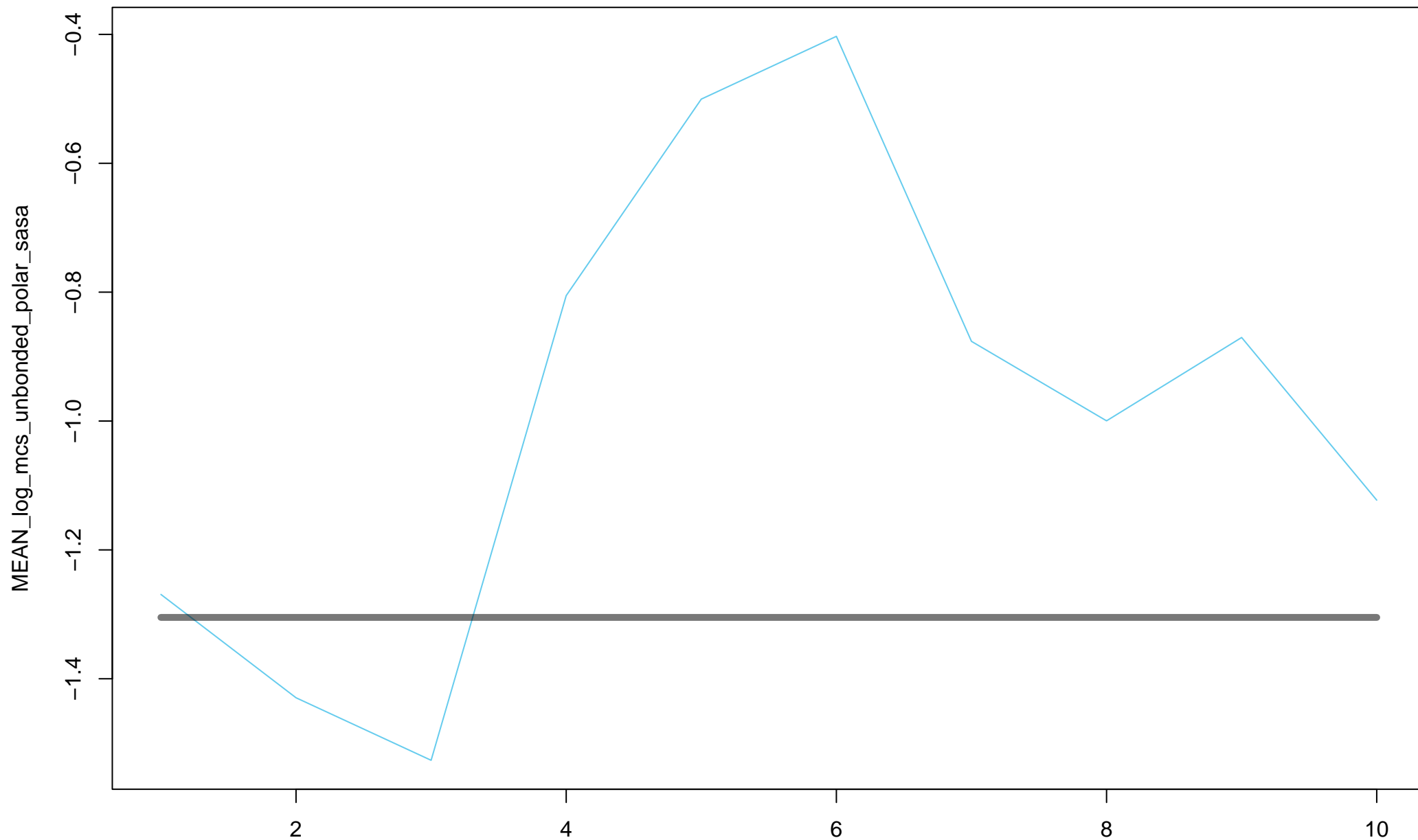


**MEAN\_log\_RMSD**  
**ESS = 10 | BMK = 0.393 | MCSE(6.27) = 37.5 | stat: FALSE | burn: 0 | percentile: 40**

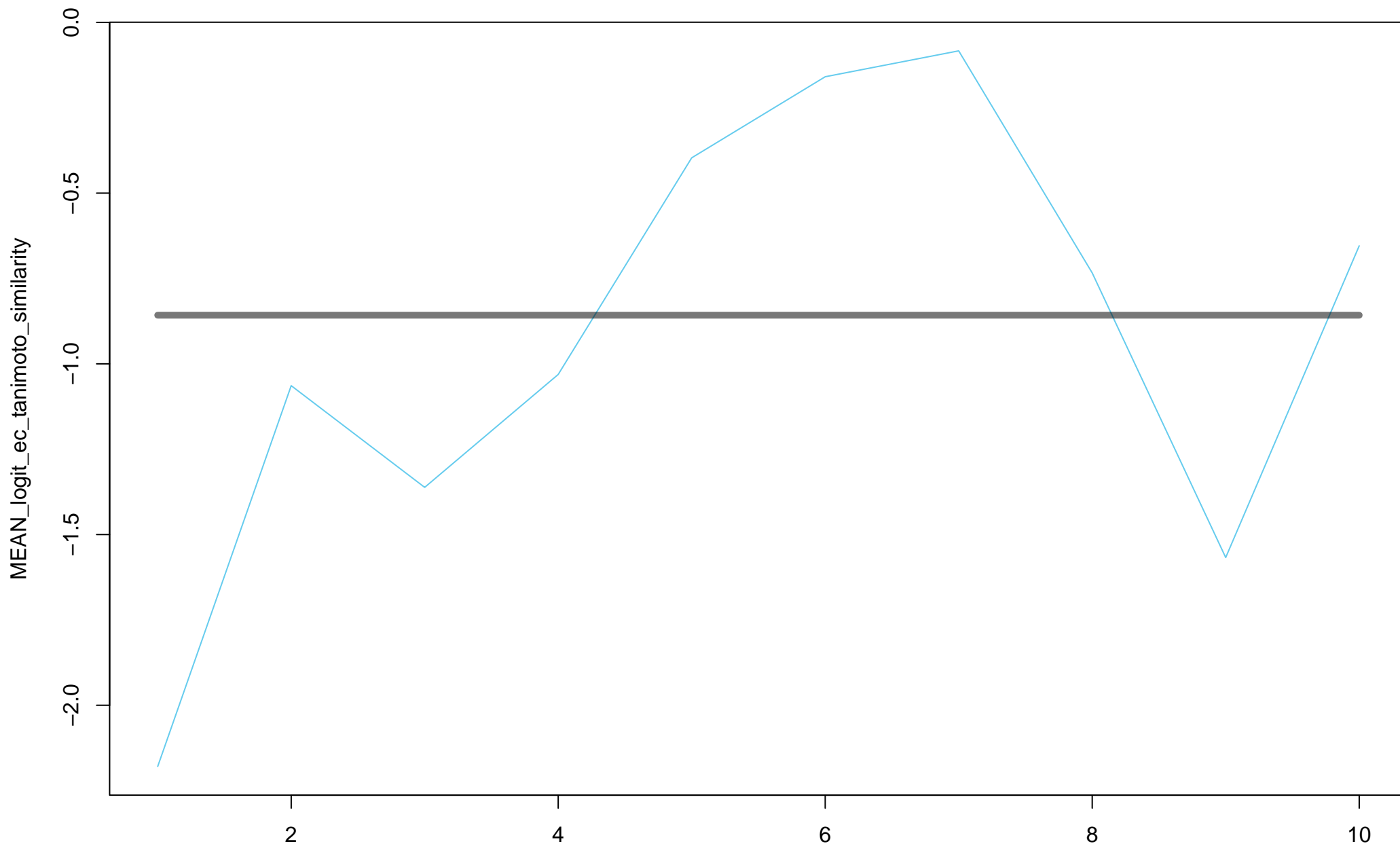




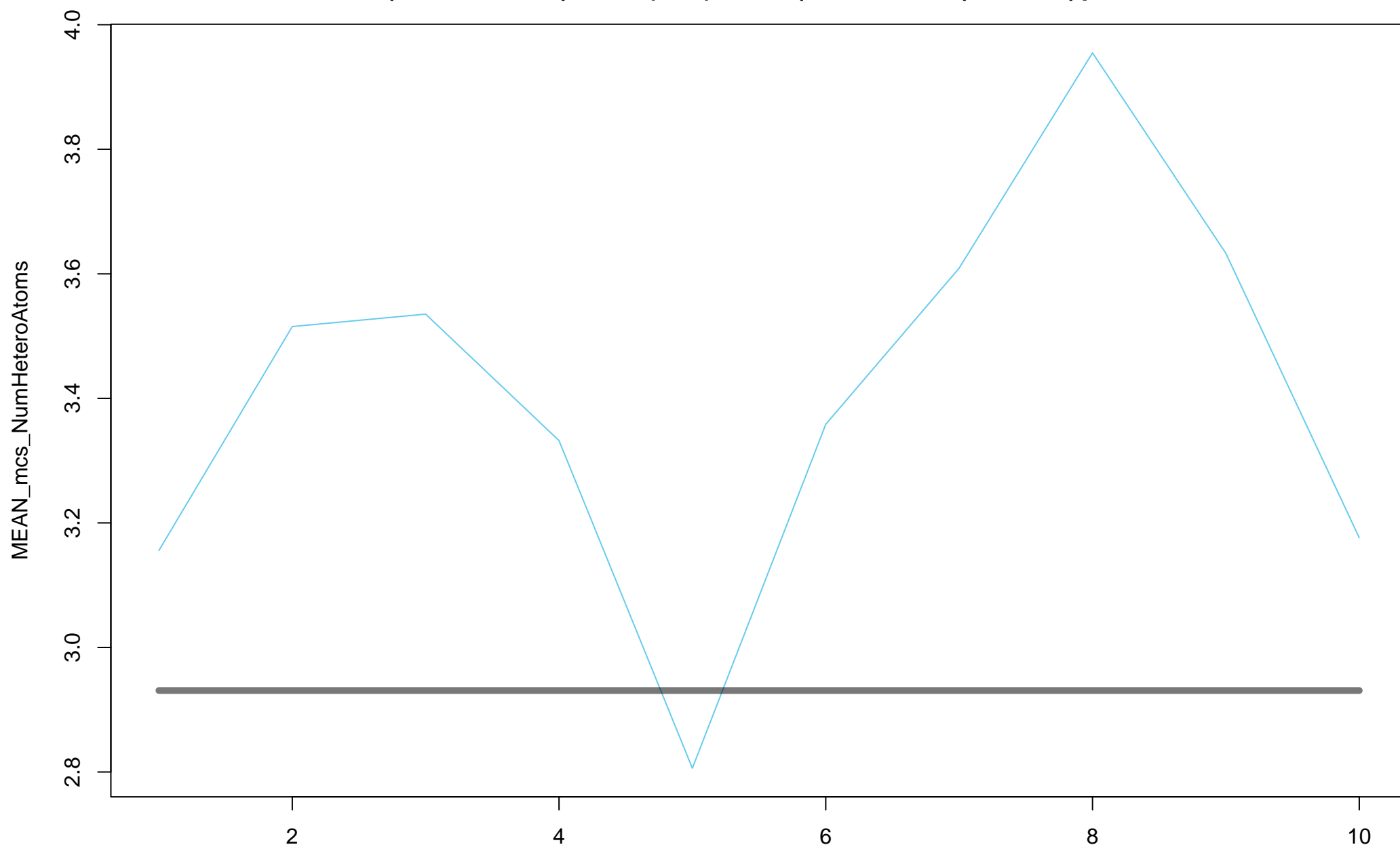
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 6.38 | BMK = 0.524 | MCSE(6.27) = 53.5 | stat: FALSE | burn: 0 | percentile: 20**



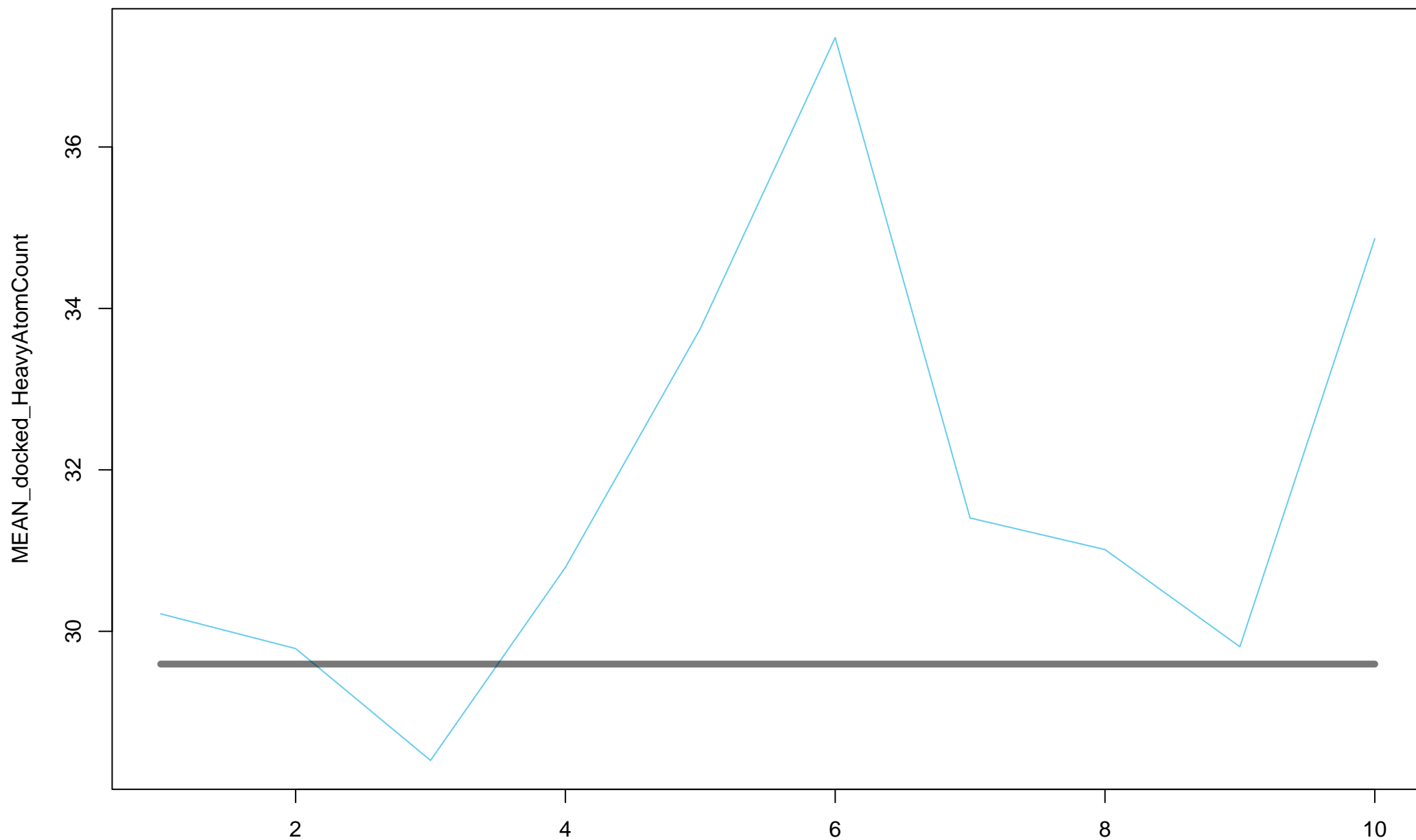
**MEAN\_logit\_ec\_tanimoto\_similarity**  
**ESS = 10 | BMK = 0.505 | MCSE(6.27) = 46 | stat: FALSE | burn: 0 | percentile: 50**



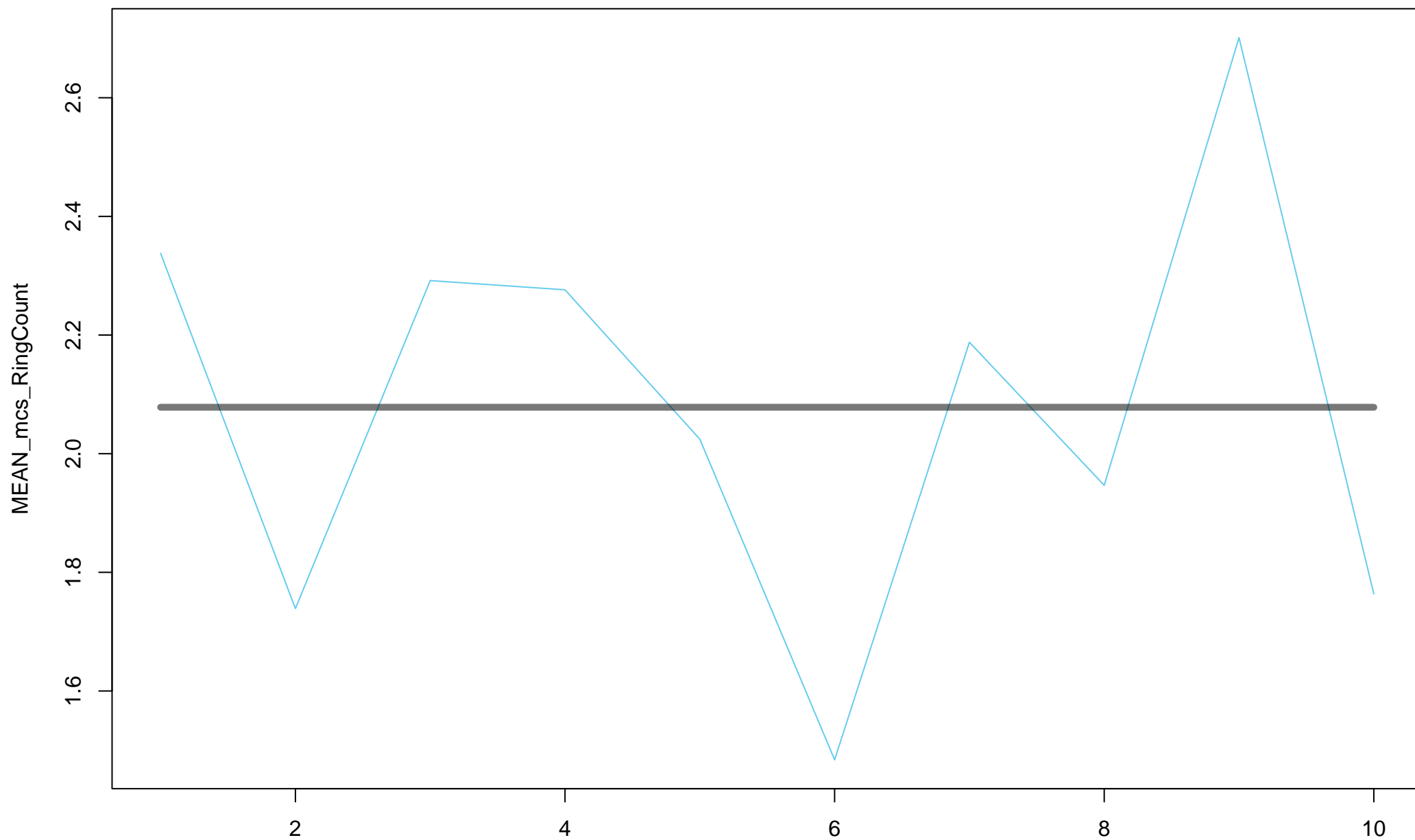
**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 10 | BMK = 0.342 | MCSE(6.27) = 36.7 | stat: FALSE | burn: 0 | percentile: 10**



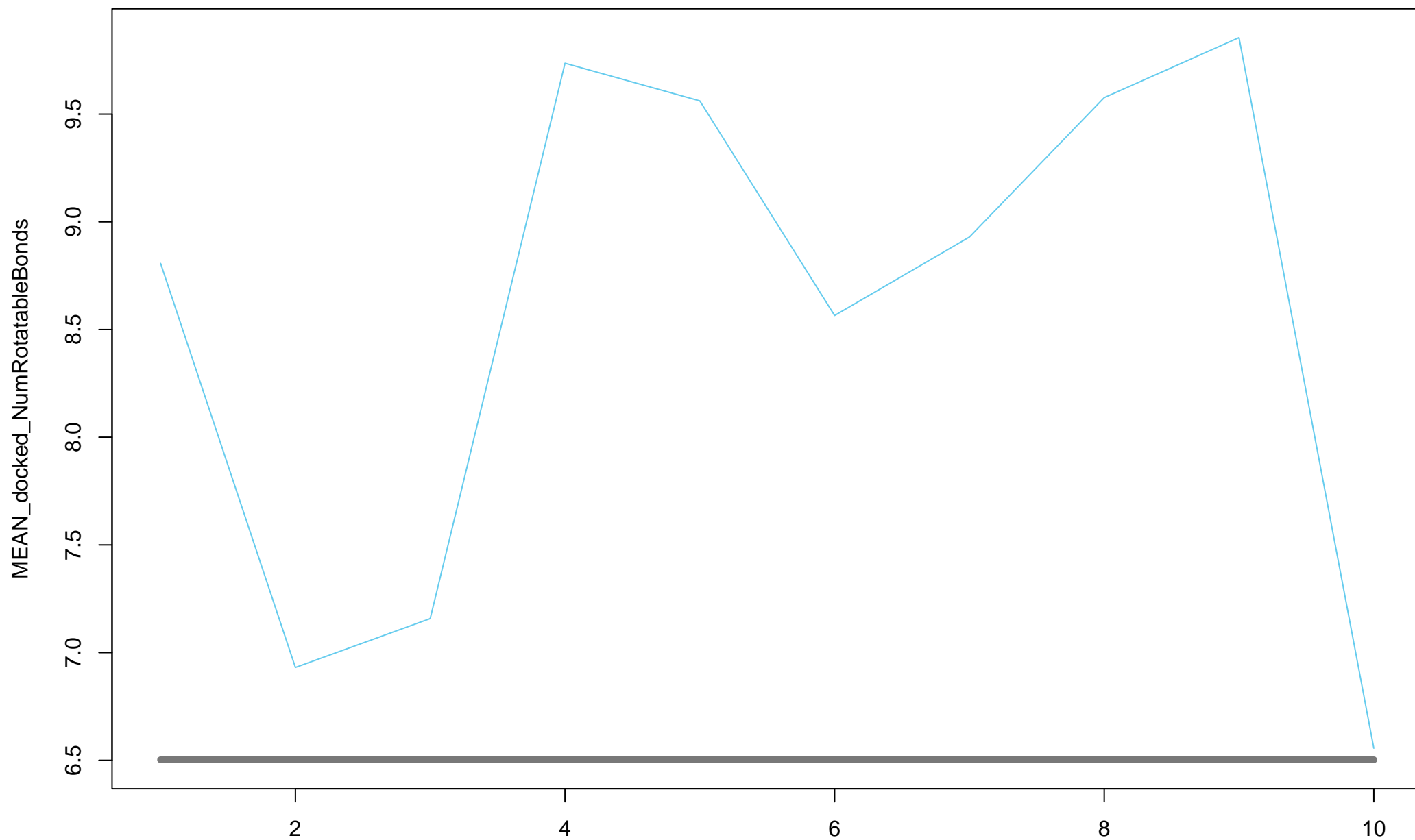
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 10 | BMK = 0.459 | MCSE(6.27) = 37.8 | stat: FALSE | burn: 0 | percentile: 10**



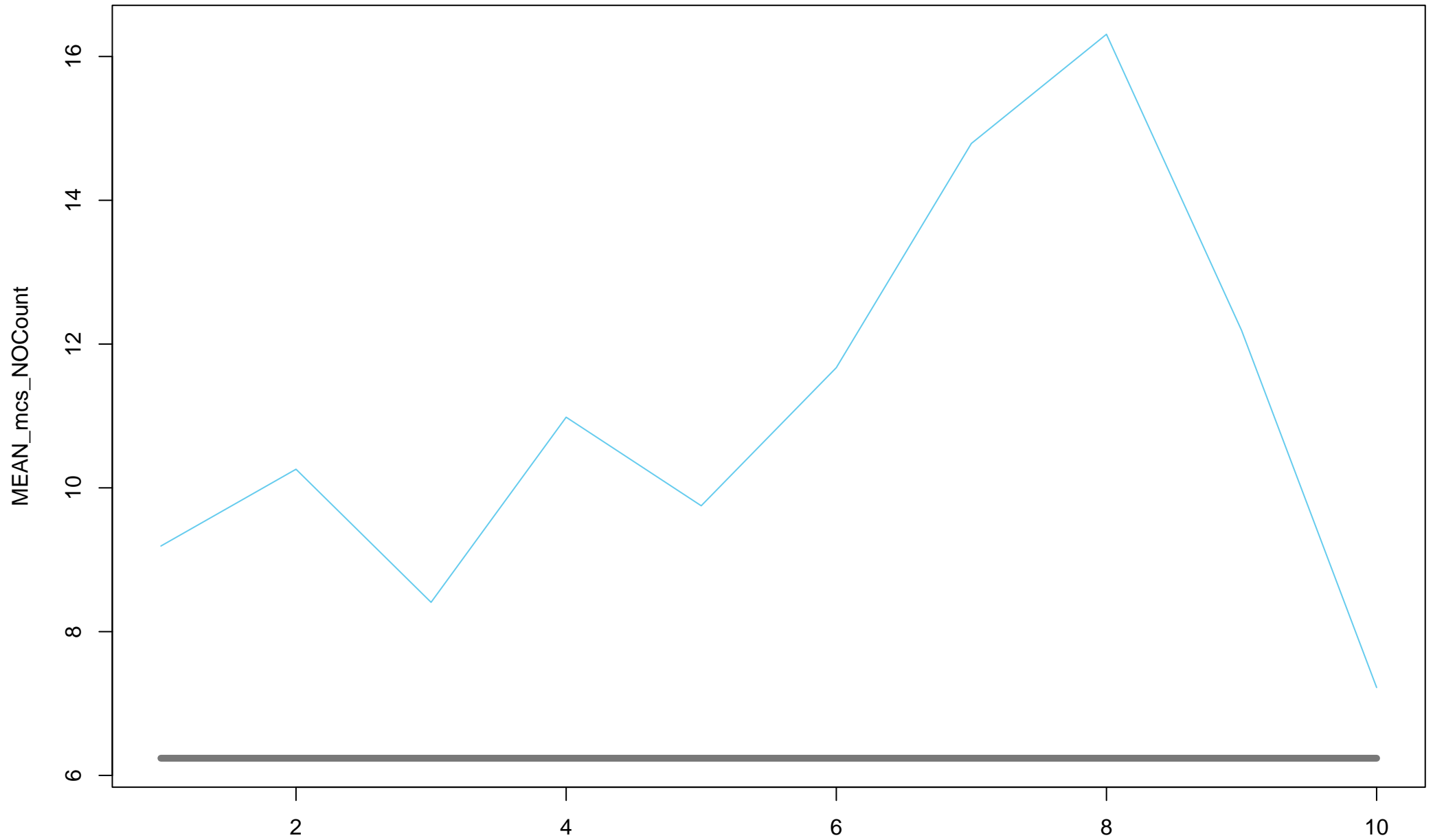
**MEAN\_mcs\_RingCount**  
**ESS = 10 | BMK = 0.347 | MCSE(6.27) = 13.5 | stat: FALSE | burn: 0 | percentile: 50**



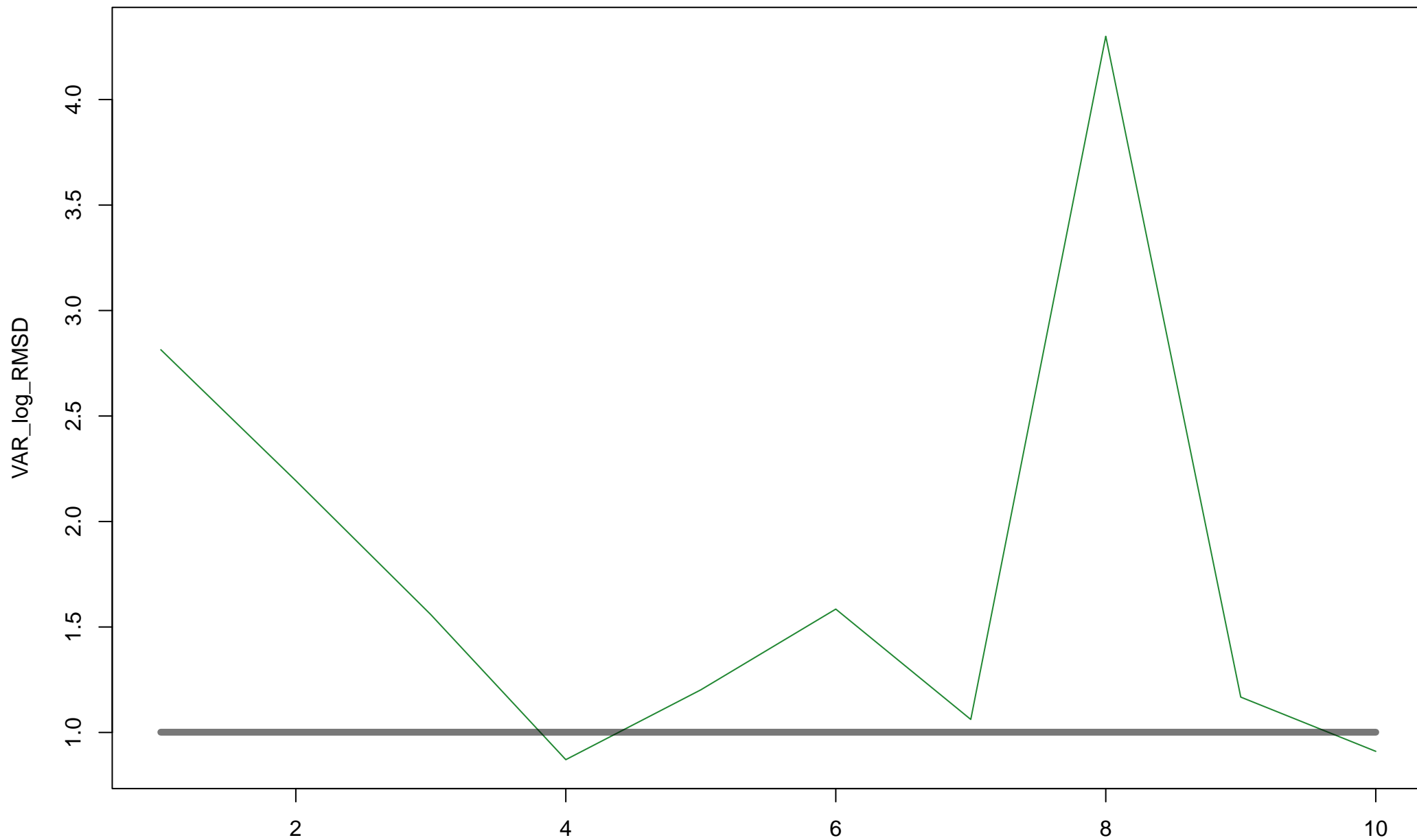
**MEAN\_docked\_NumRotatableBonds**  
**ESS = 10 | BMK = 0.178 | MCSE(6.27) = 31.1 | stat: FALSE | burn: 0 | percentile: 0**



**MEAN\_mcs\_NOCount**  
**ESS = 10 | BMK = 0.63 | MCSE(6.27) = 44.9 | stat: FALSE | burn: 0 | percentile: 0**

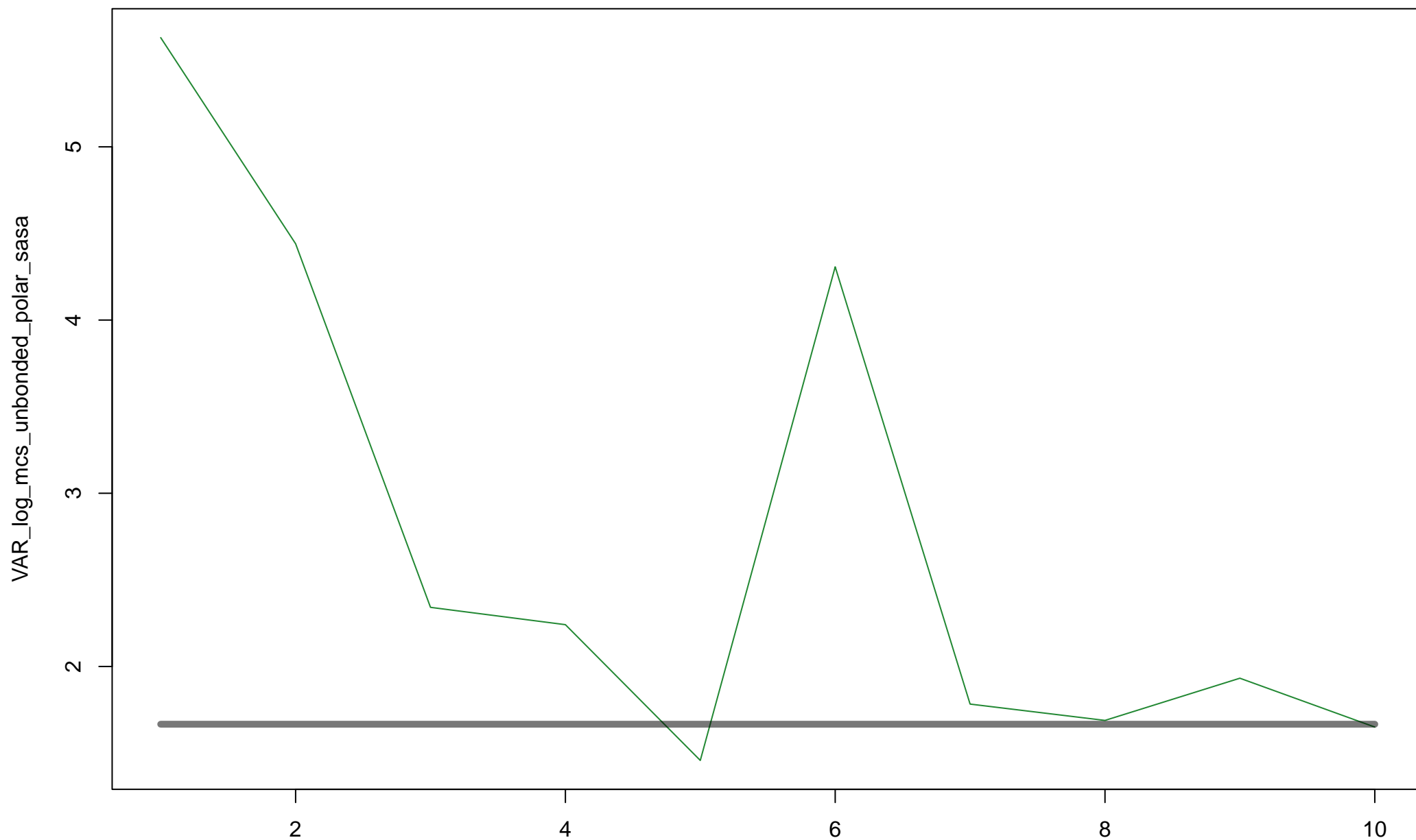


**VAR\_log\_RMSD**  
**ESS = 10 | BMK = 1 | MCSE(6.27) = 24.4 | stat: FALSE | burn: 0 | percentile: 20**

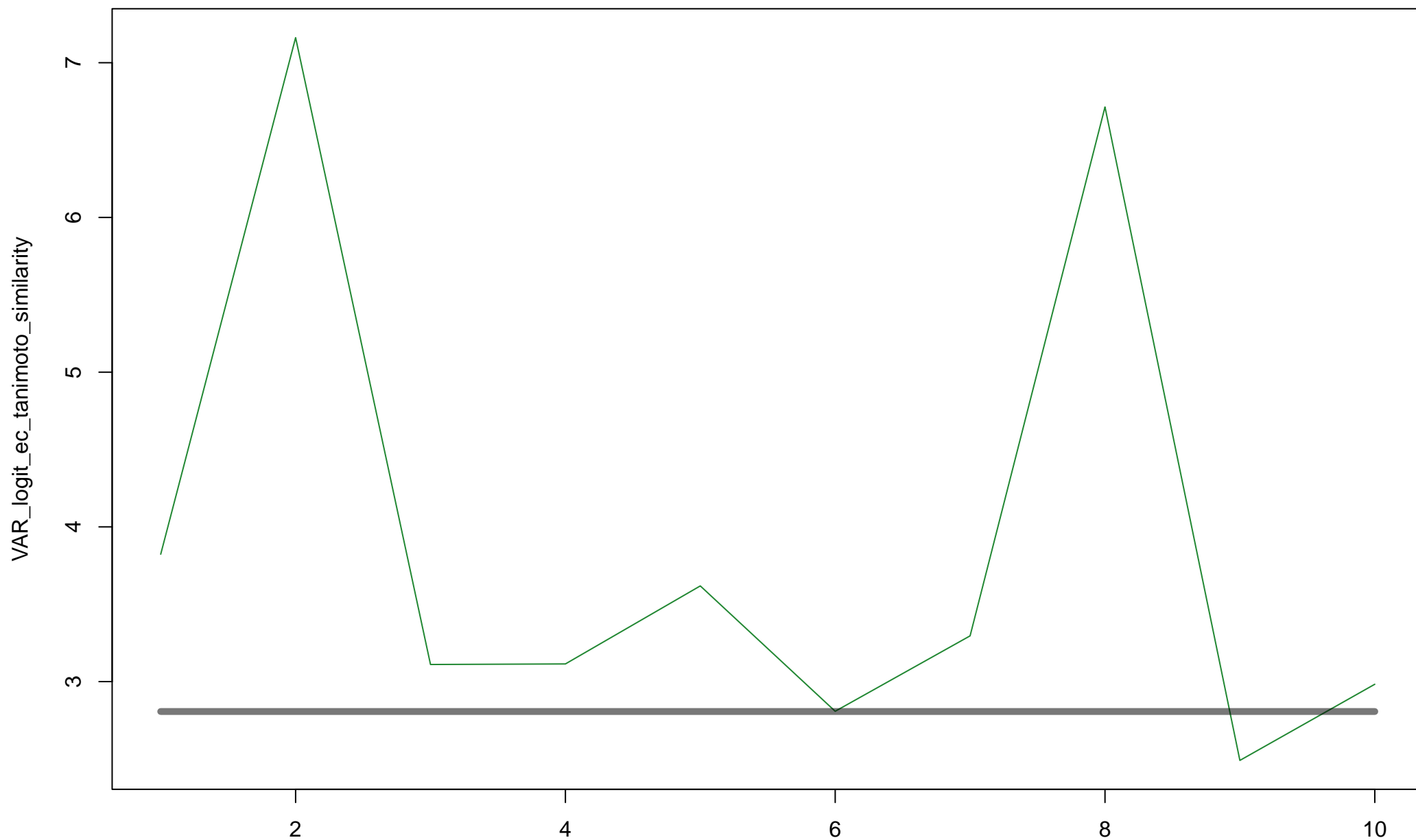




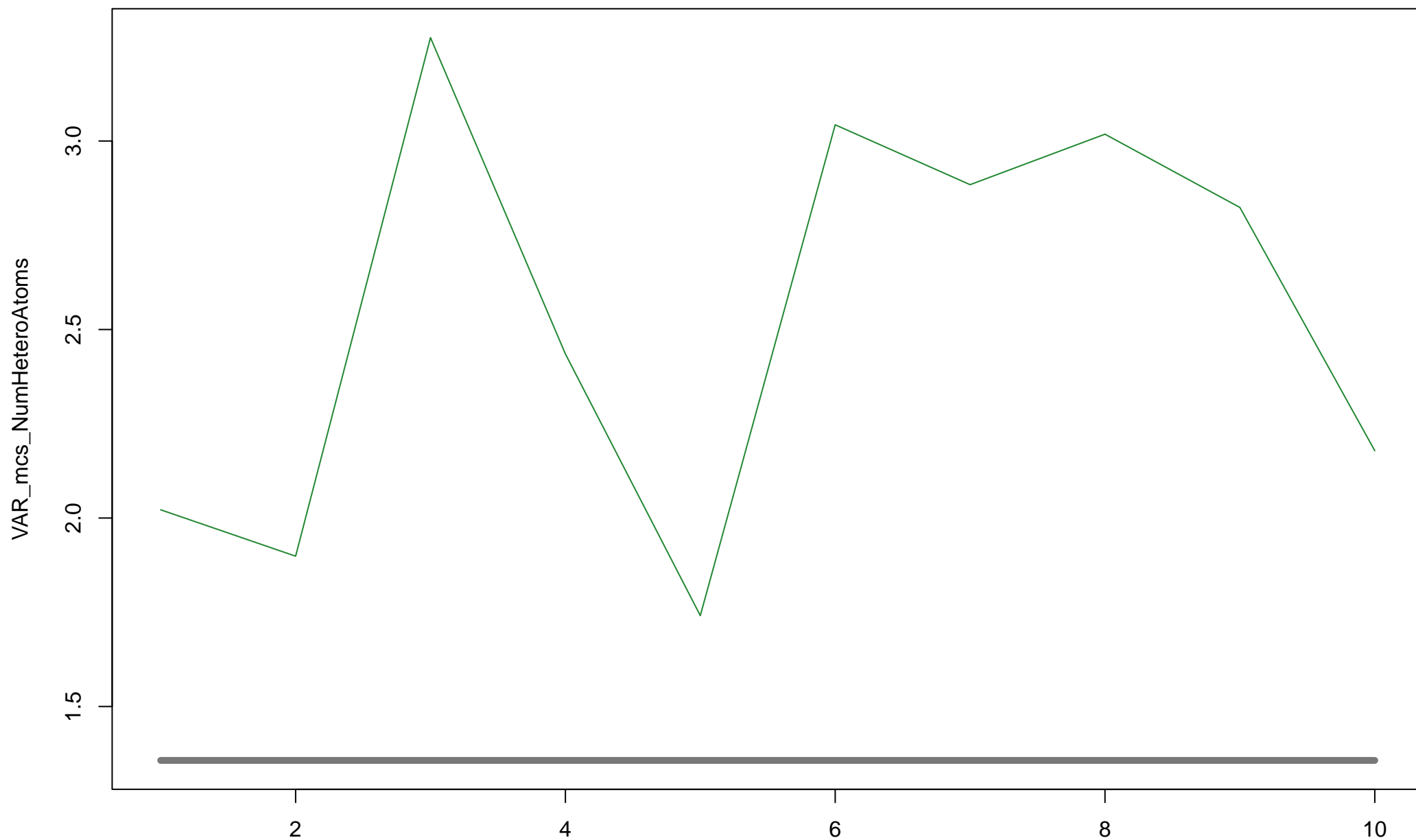
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 10 | BMK = 1 | MCSE(6.27) = 38.5 | stat: FALSE | burn: 0 | percentile: 20**



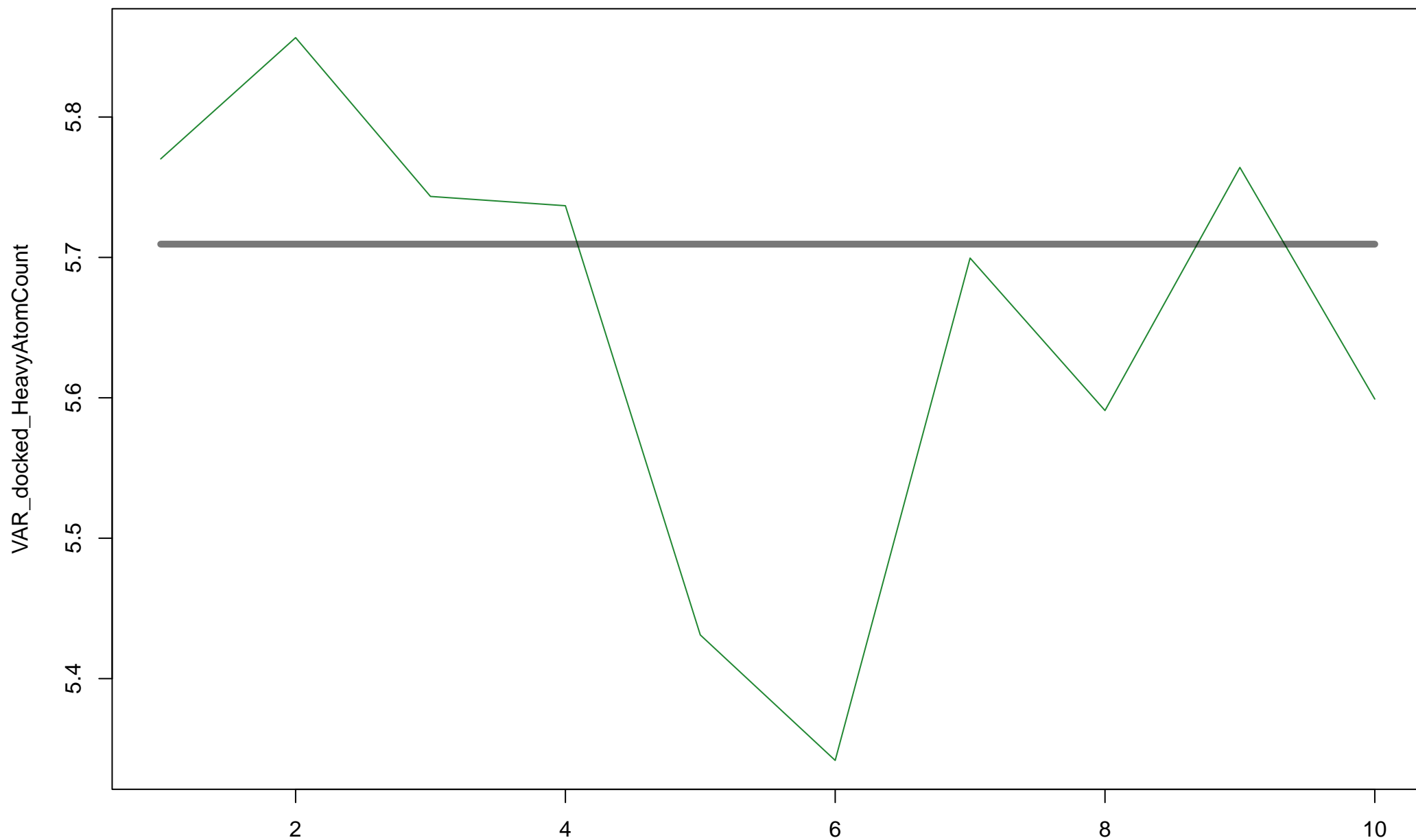
**VAR\_logit\_ec\_tanimoto\_similarity**  
**ESS = 10 | BMK = 1 | MCSE(6.27) = 21.2 | stat: FALSE | burn: 0 | percentile: 10**



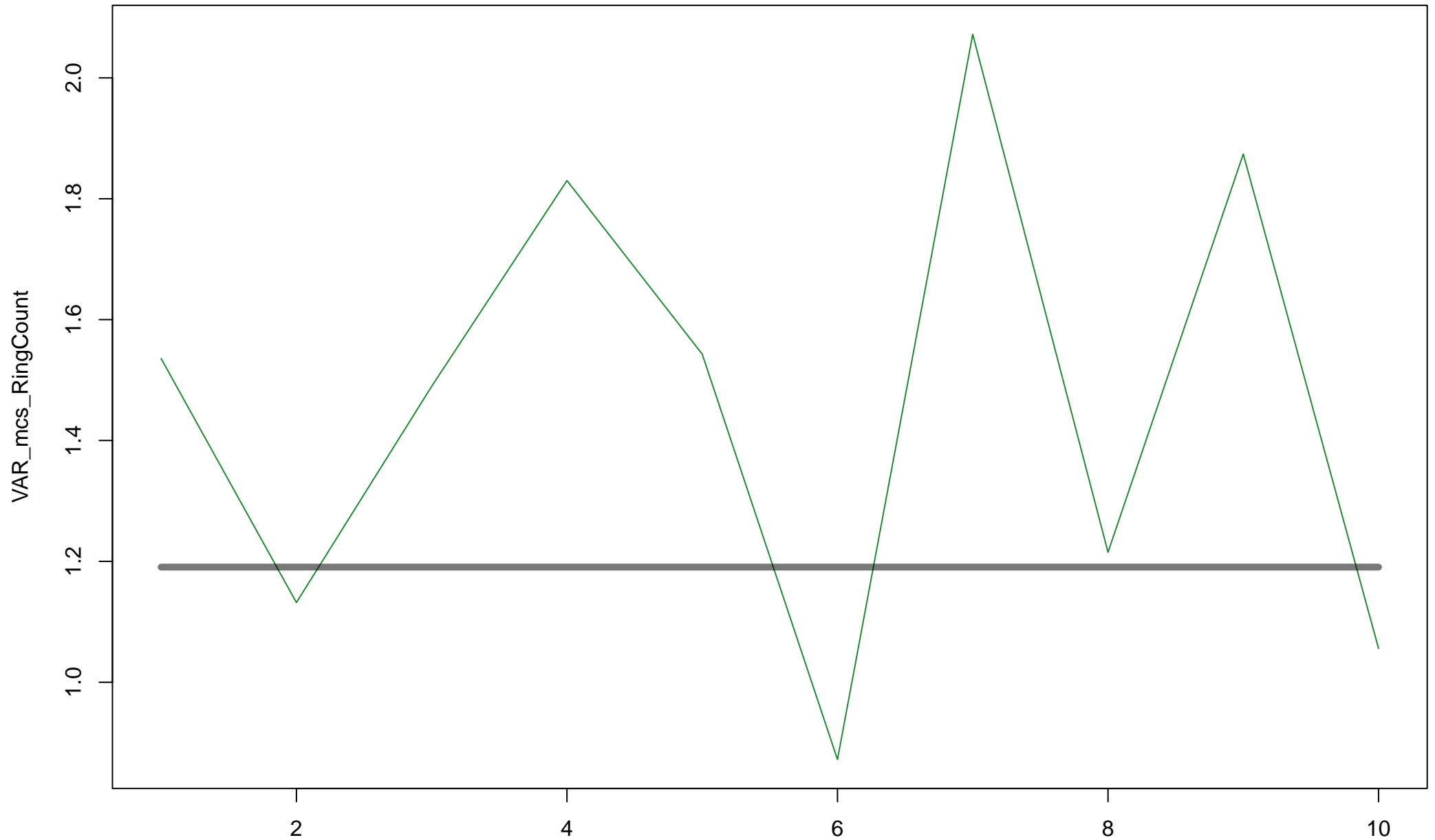
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 10 | BMK = 0.685 | MCSE(6.27) = 25.8 | stat: FALSE | burn: 0 | percentile: 0**



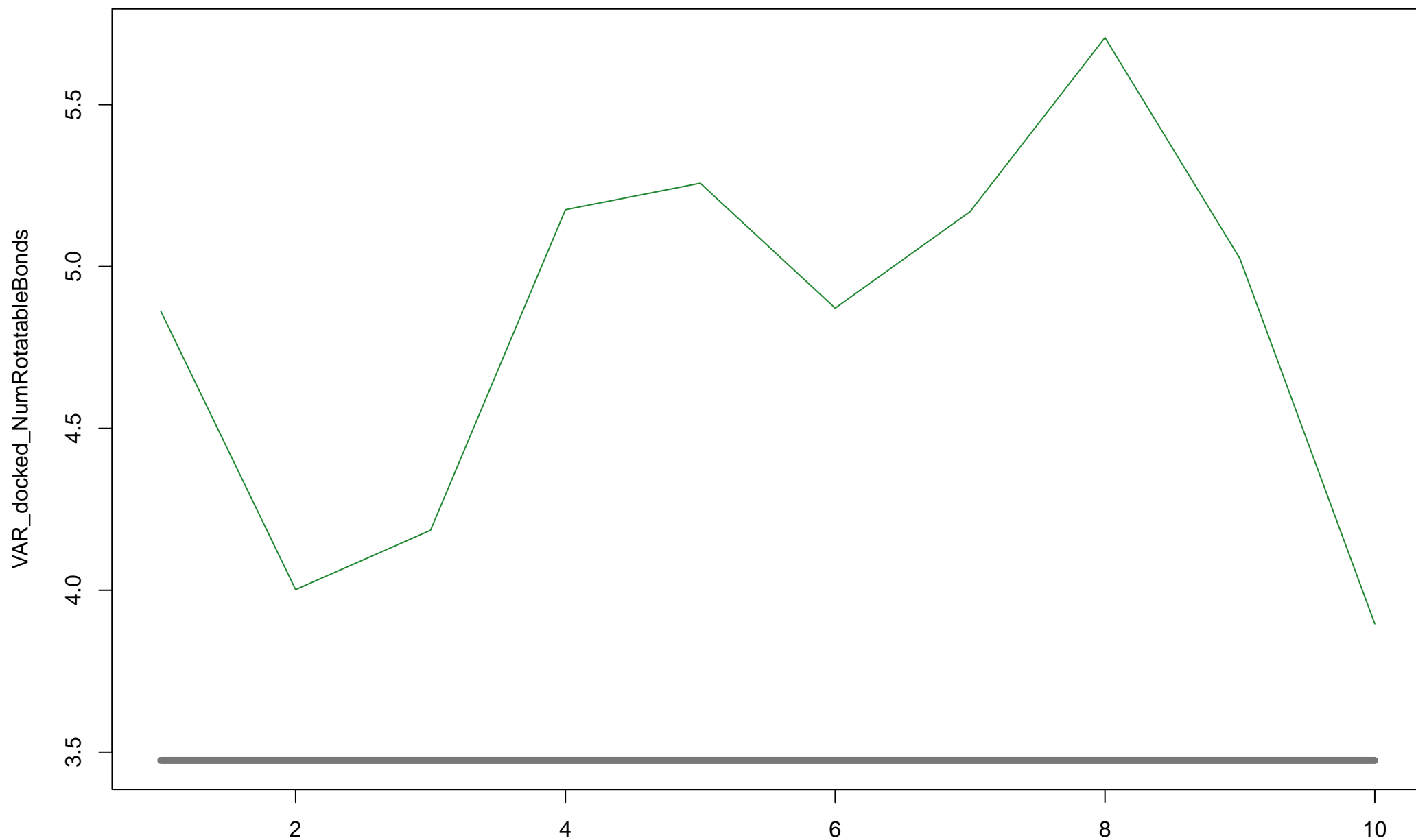
**VAR\_docked\_HeavyAtomCount**  
**ESS = 10 | BMK = 0.789 | MCSE(6.27) = 45.1 | stat: FALSE | burn: 0 | percentile: 50**



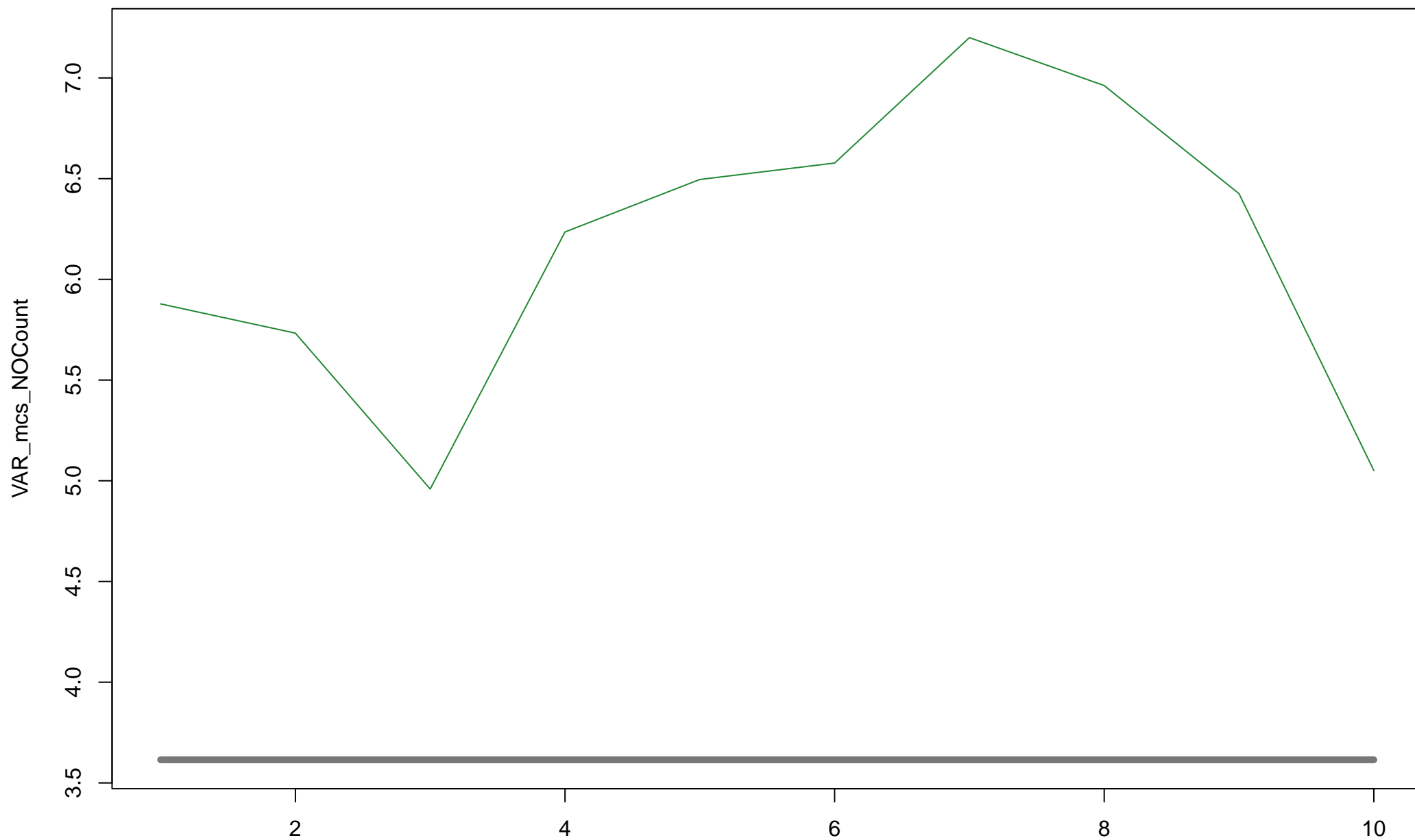
**VAR\_mcs\_RingCount**  
**ESS = 10 | BMK = 0.582 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 30**



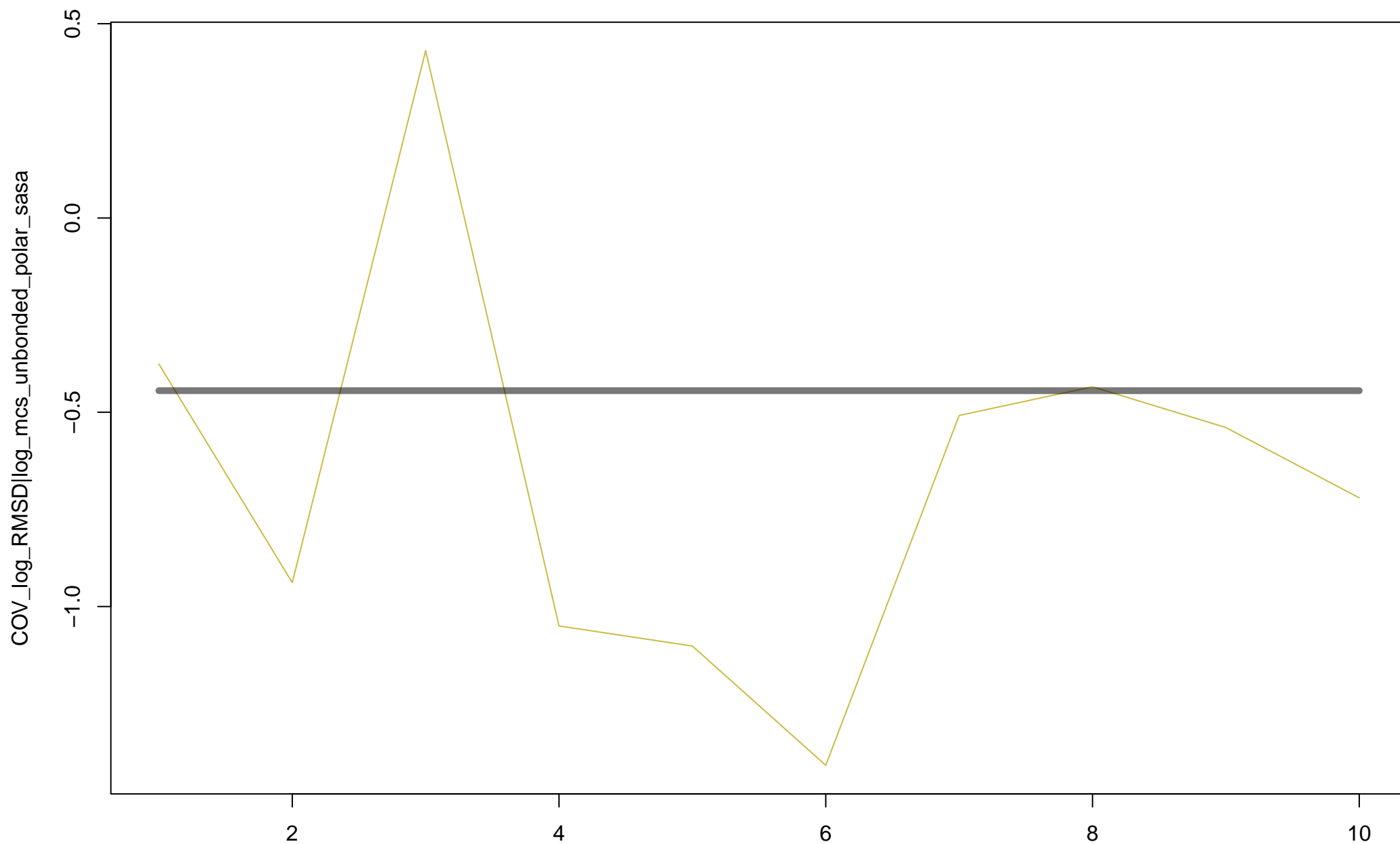
**VAR\_docked\_NumRotatableBonds**  
**ESS = 10 | BMK = 0.342 | MCSE(6.27) = 36.1 | stat: FALSE | burn: 0 | percentile: 0**



**VAR\_mcs\_NOCount**  
**ESS = 2.88 | BMK = 0.49 | MCSE(6.27) = 52.6 | stat: FALSE | burn: 0 | percentile: 0**

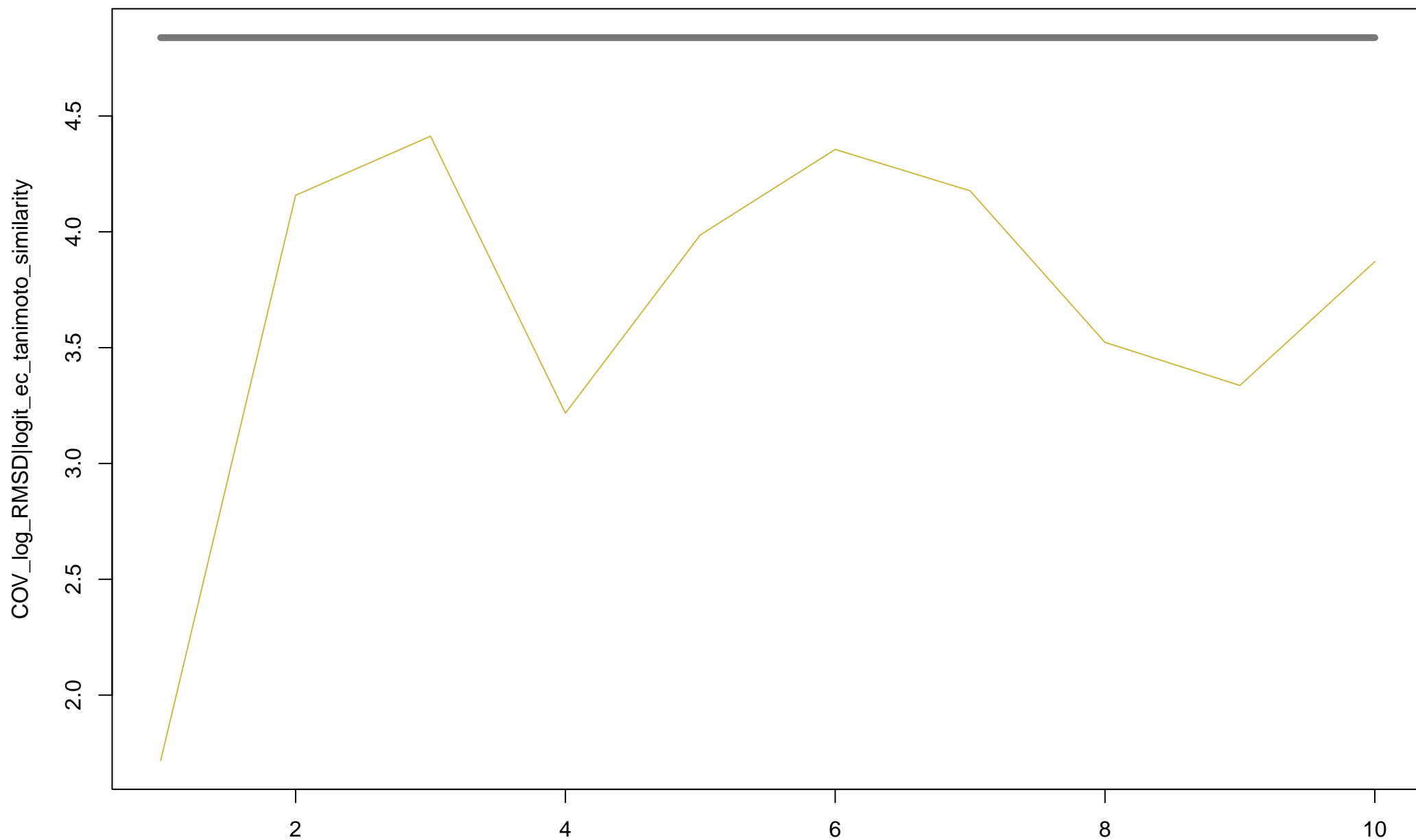


**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 10 | BMK = 0.604 | MCSE(6.27) = 24.9 | stat: FALSE | burn: 0 | percentile: 70**

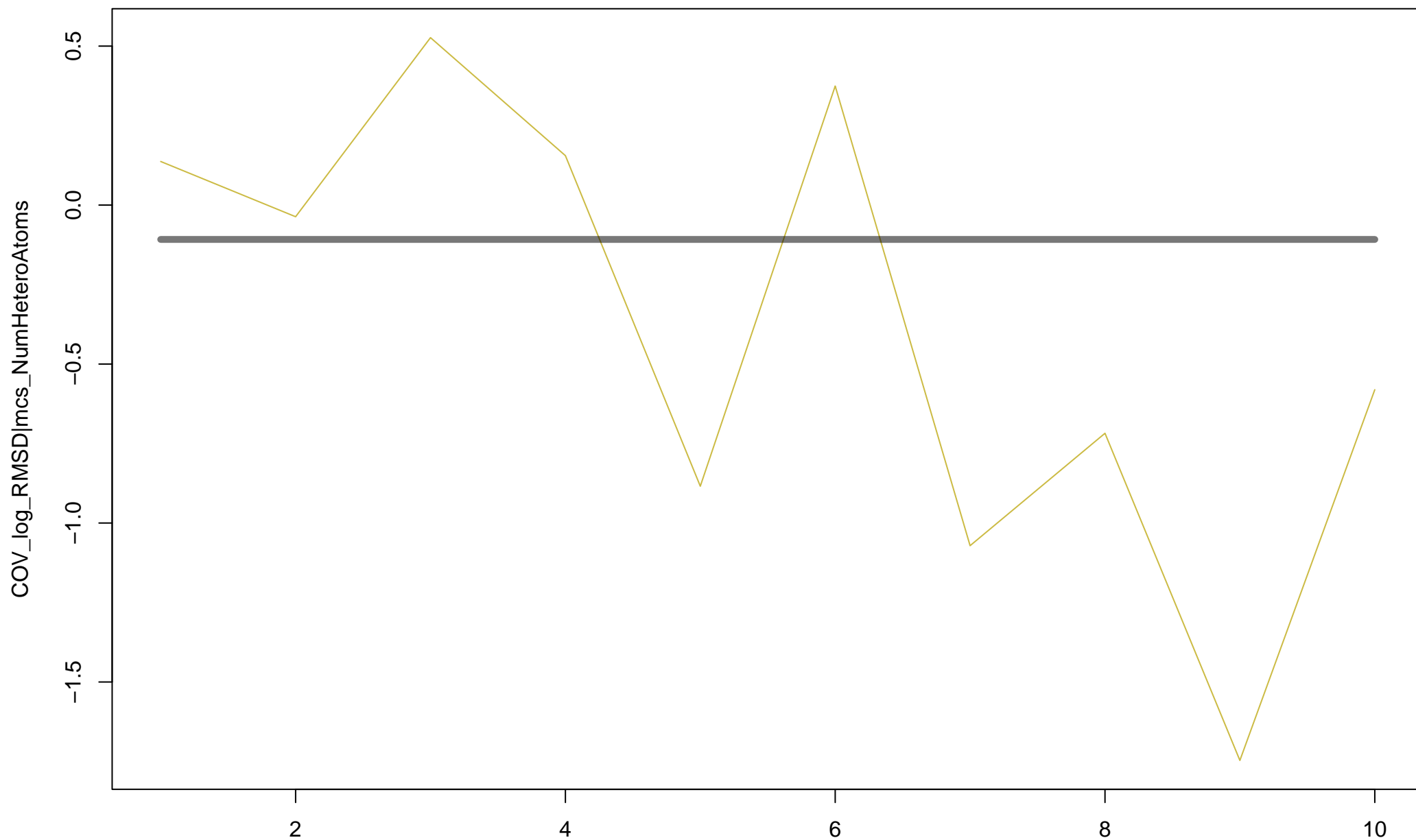




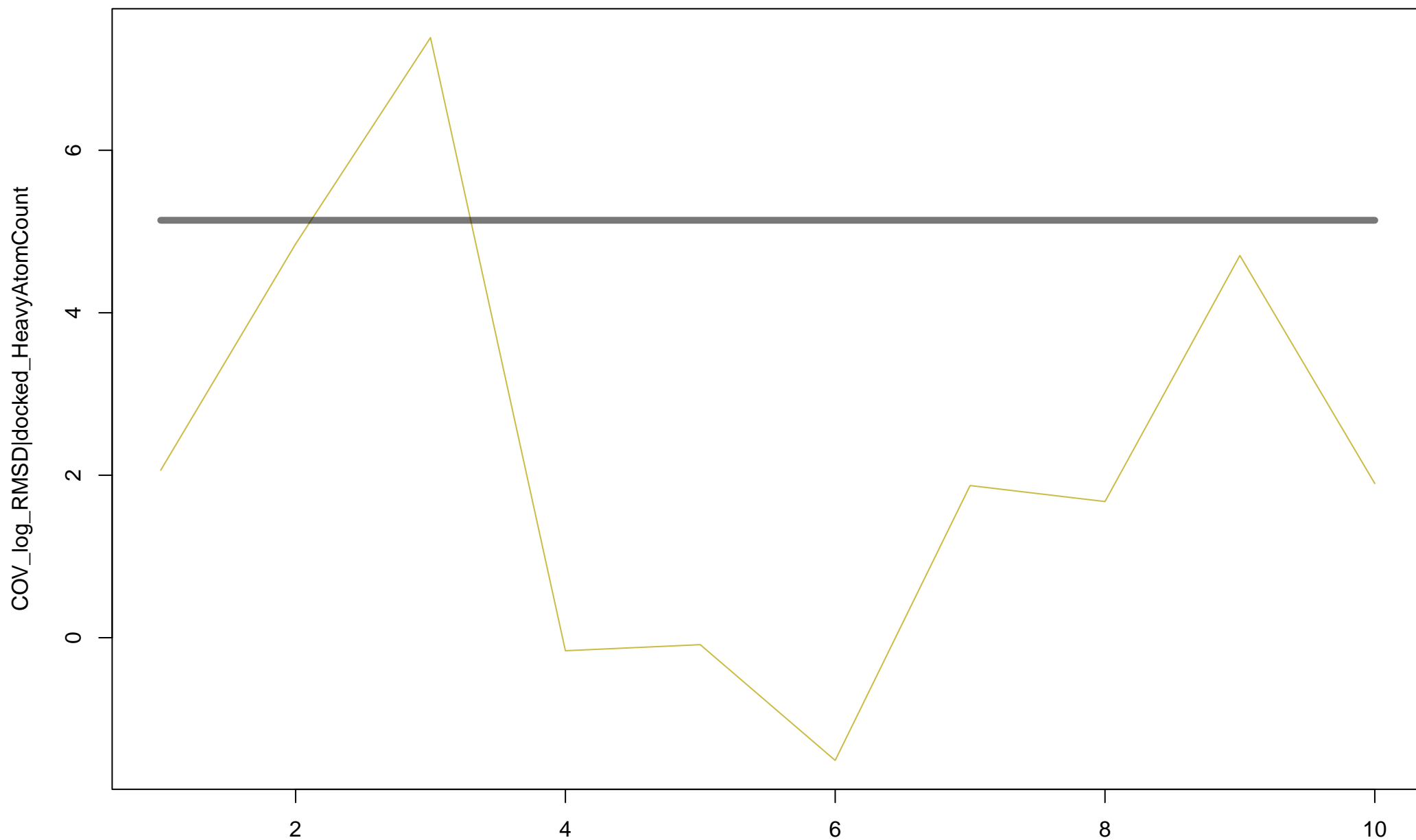
**COV\_log\_RMSD|logit\_ec\_tanimoto\_similarity**  
**ESS = 10 | BMK = 0.312 | MCSE(6.27) = 26.7 | stat: FALSE | burn: 0 | percentile: 100**



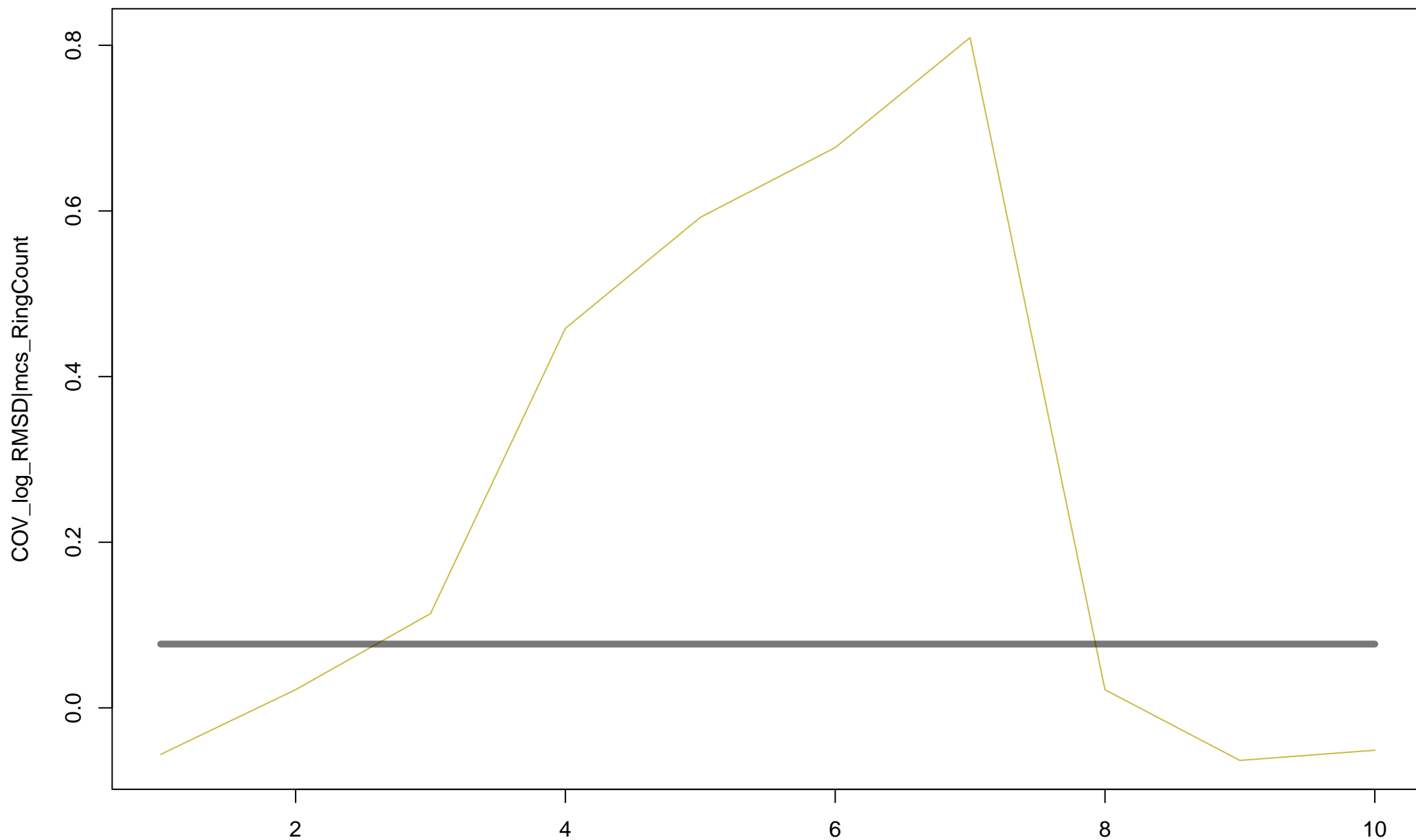
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 10 | BMK = 0.721 | MCSE(6.27) = 51.4 | stat: FALSE | burn: 0 | percentile: 50**



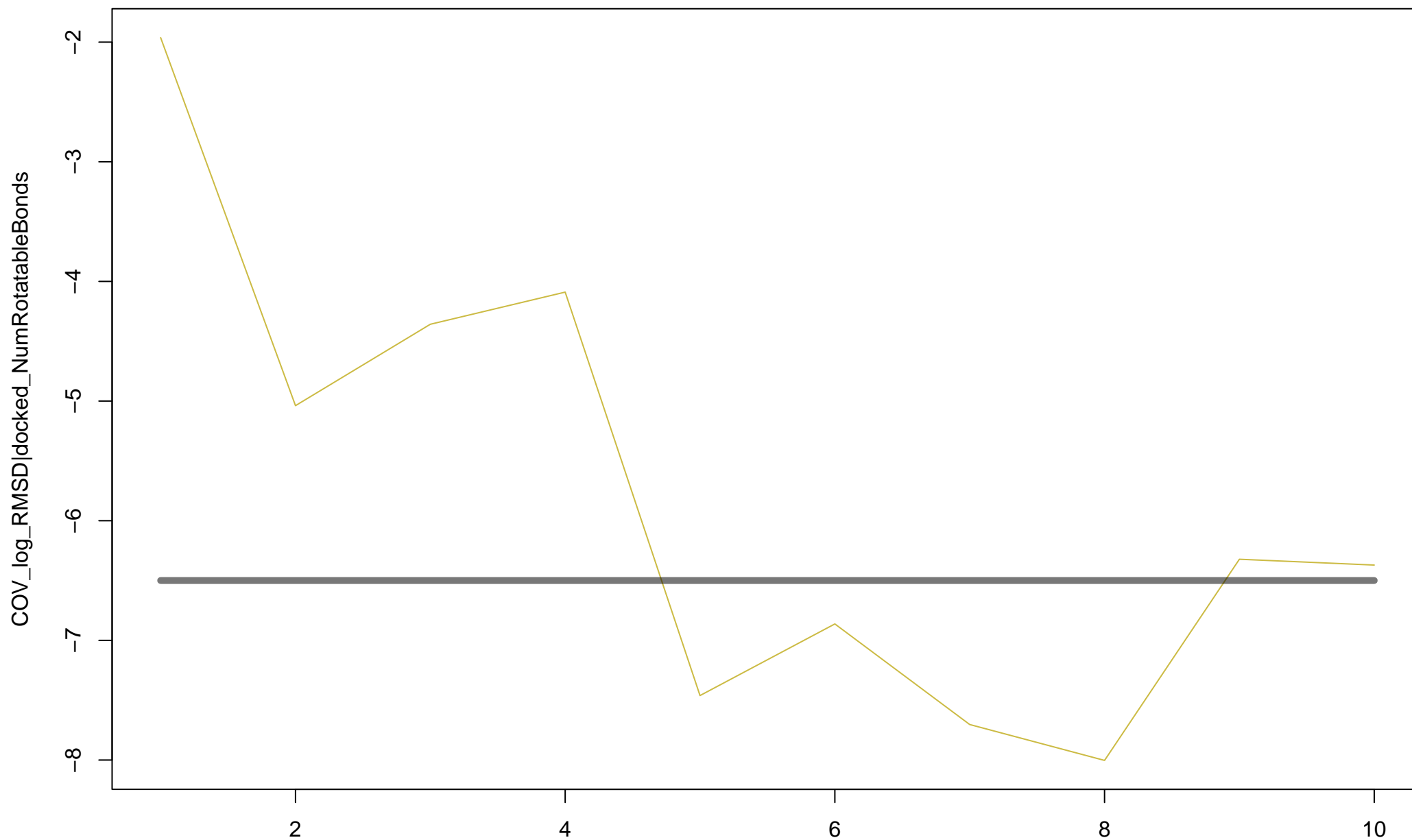
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 10 | BMK = 0.865 | MCSE(6.27) = 38.4 | stat: FALSE | burn: 0 | percentile: 90**



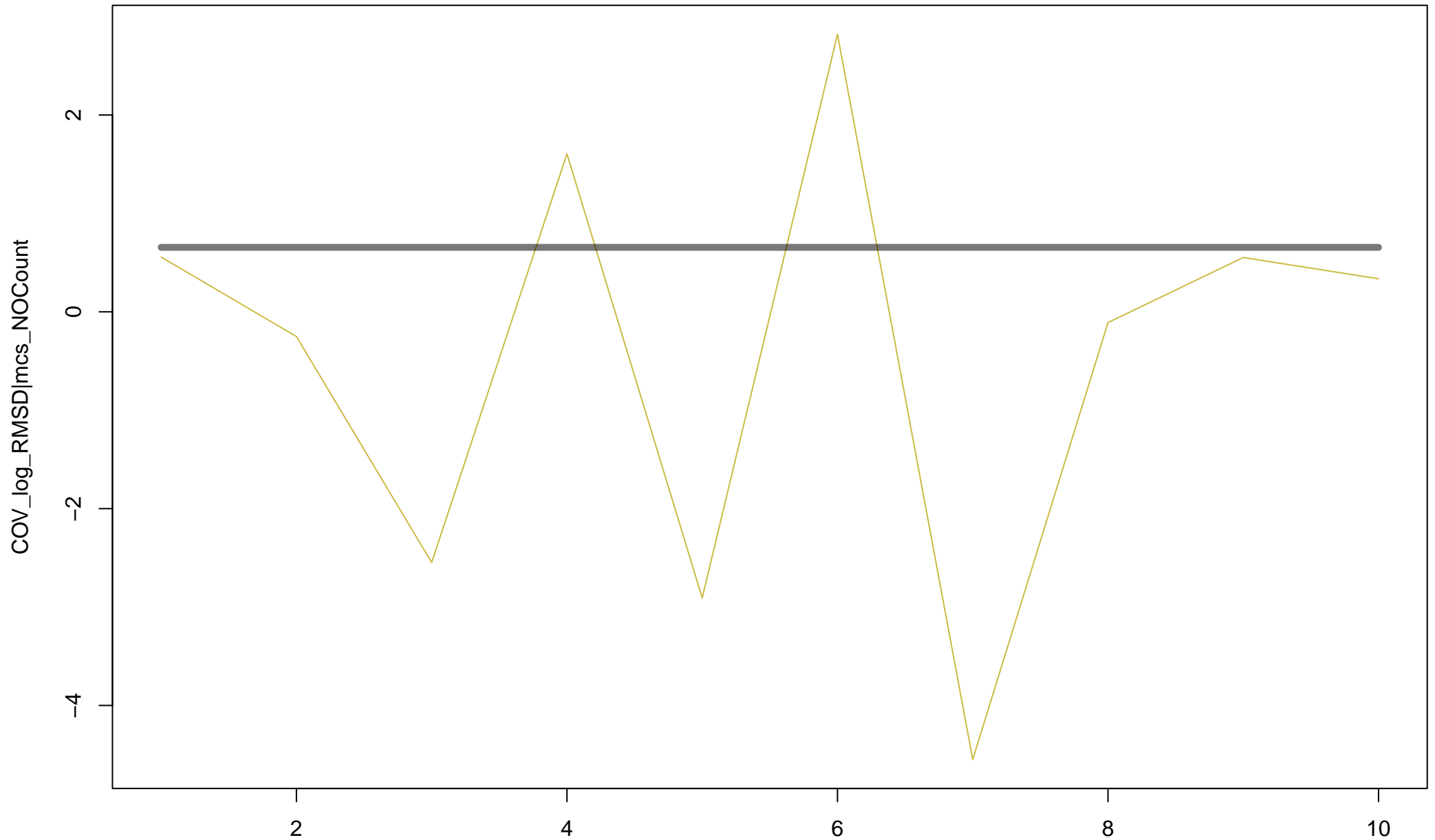
**COV\_log\_RMSD|mcs\_RingCount**  
**ESS = 2.71 | BMK = 0.128 | MCSE(6.27) = 53.4 | stat: FALSE | burn: 0 | percentile: 50**



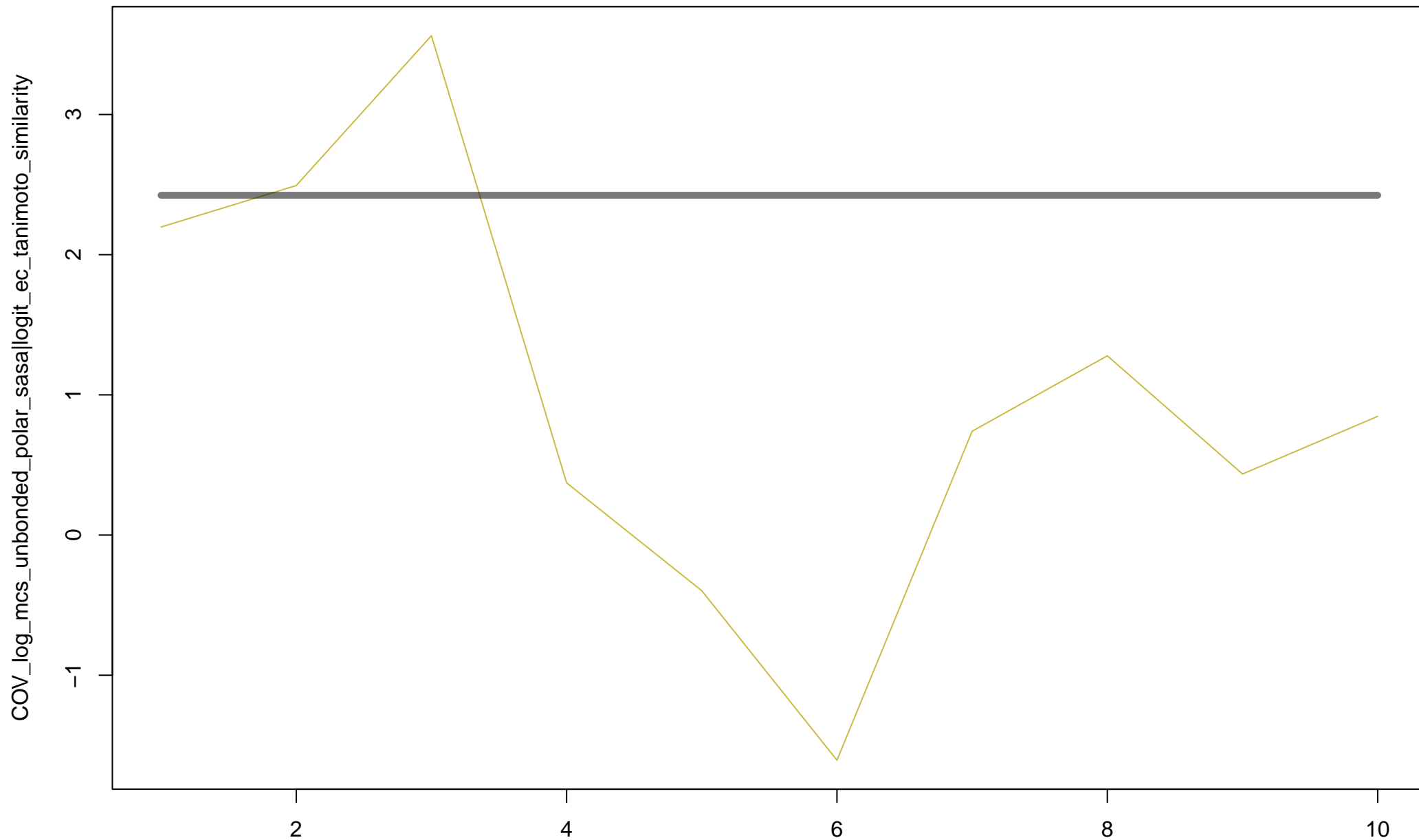
COV\_log\_RMSD|docked\_NumRotatableBonds  
ESS = 10 | BMK = 0.772 | MCSE(6.27) = 61.1 | stat: FALSE | burn: 0 | percentile: 40



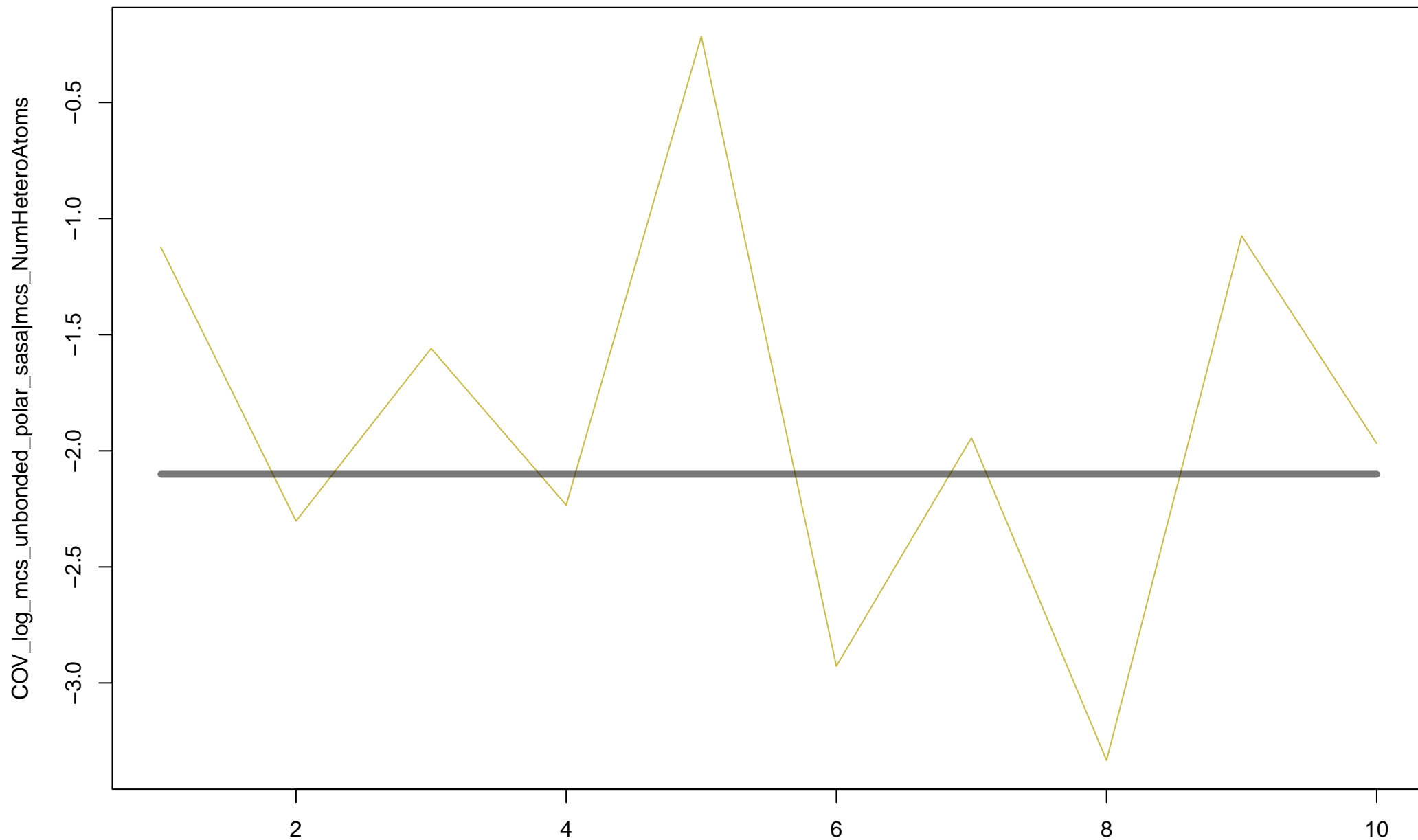
**COV\_log\_RMSD|mcs\_NOCount**  
**ESS = 10 | BMK = 0.566 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 80**



**COV\_log\_mcs\_unbonded\_polar\_sasa|logit\_ec\_tanimoto\_similarity**  
**ESS = 3.32 | BMK = 0.727 | MCSE(6.27) = 50.3 | stat: FALSE | burn: 0 | percentile: 80**

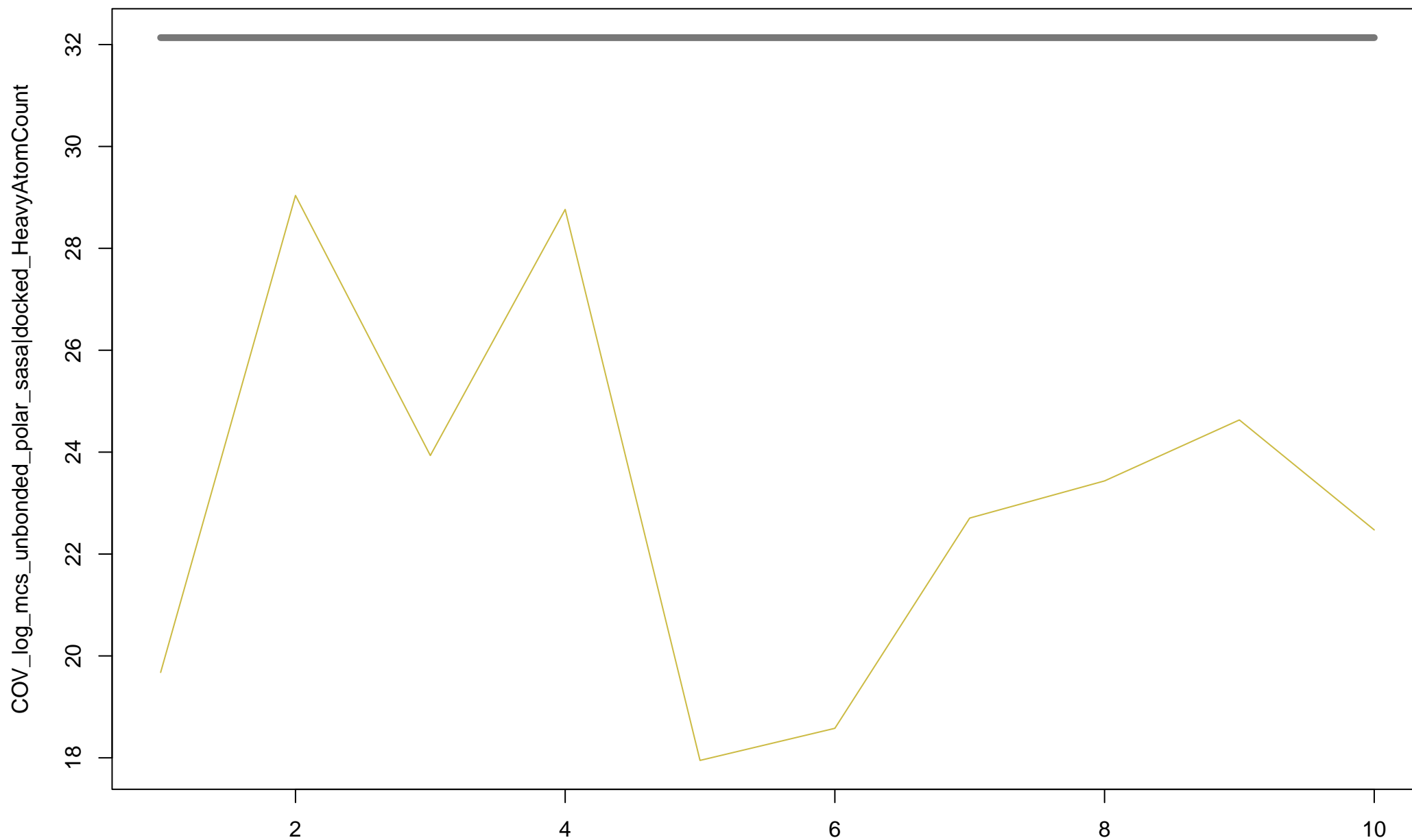


COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms  
ESS = 10 | BMK = 0.266 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 40

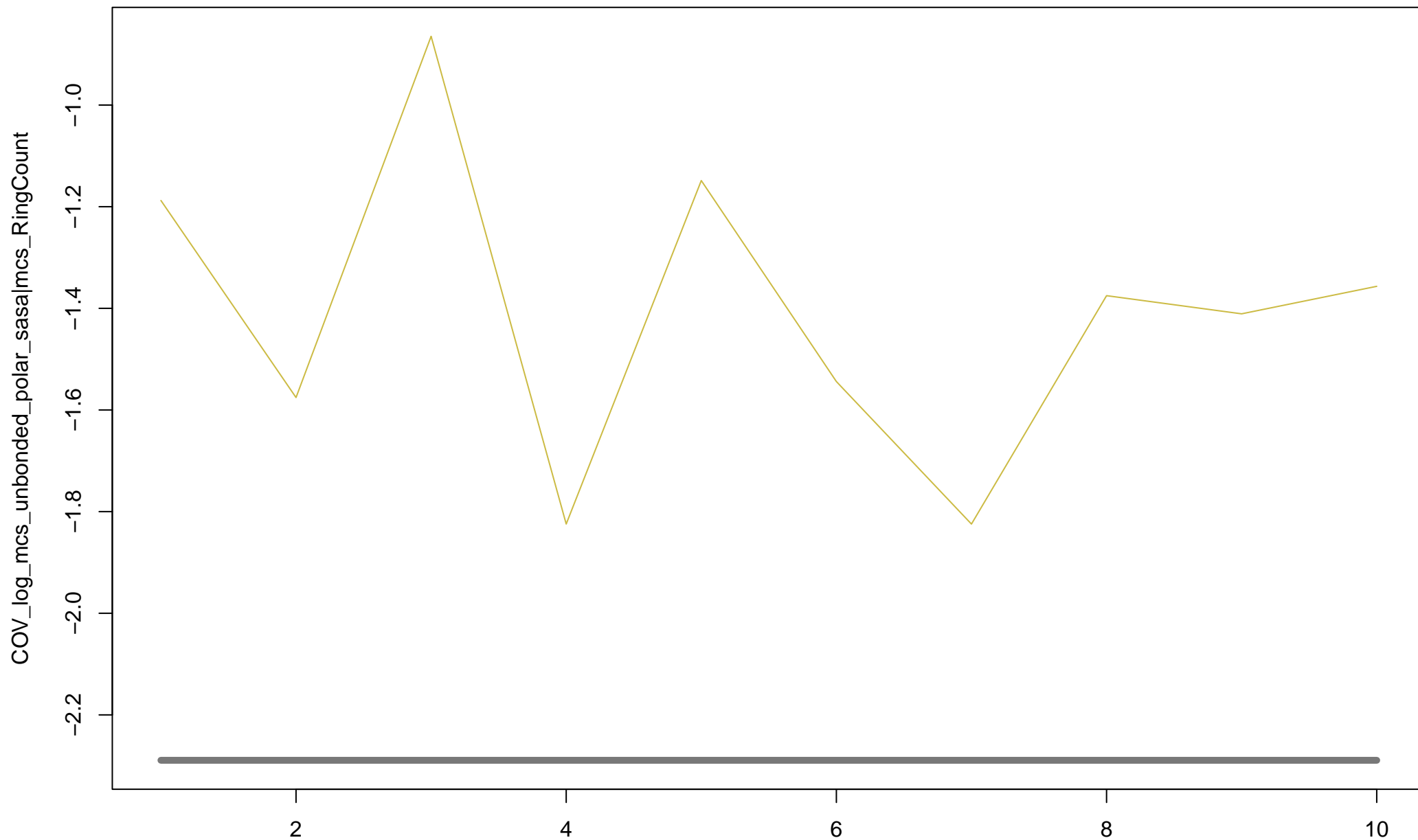




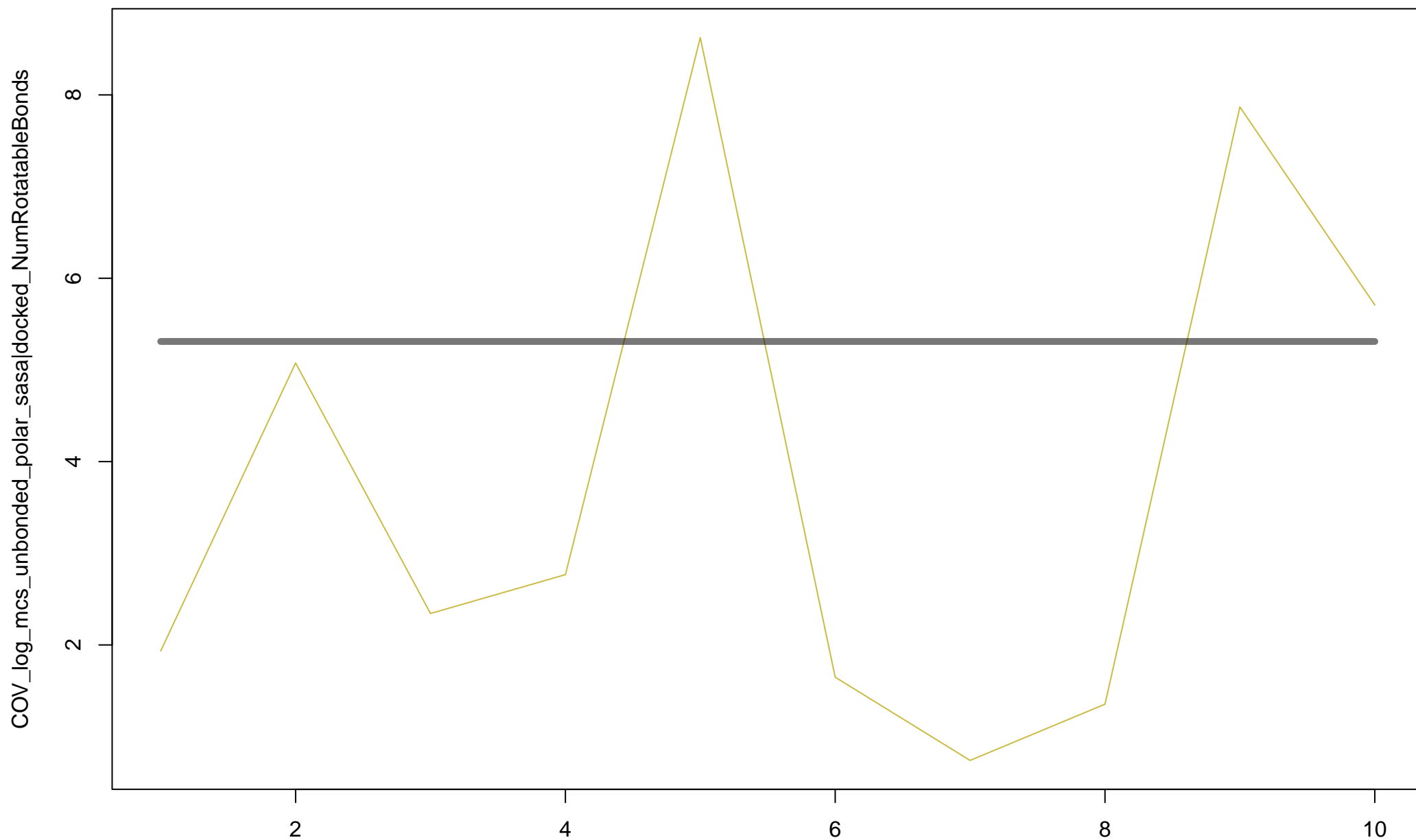
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 10 | BMK = 0.553 | MCSE(6.27) = 26.2 | stat: FALSE | burn: 0 | percentile: 100**



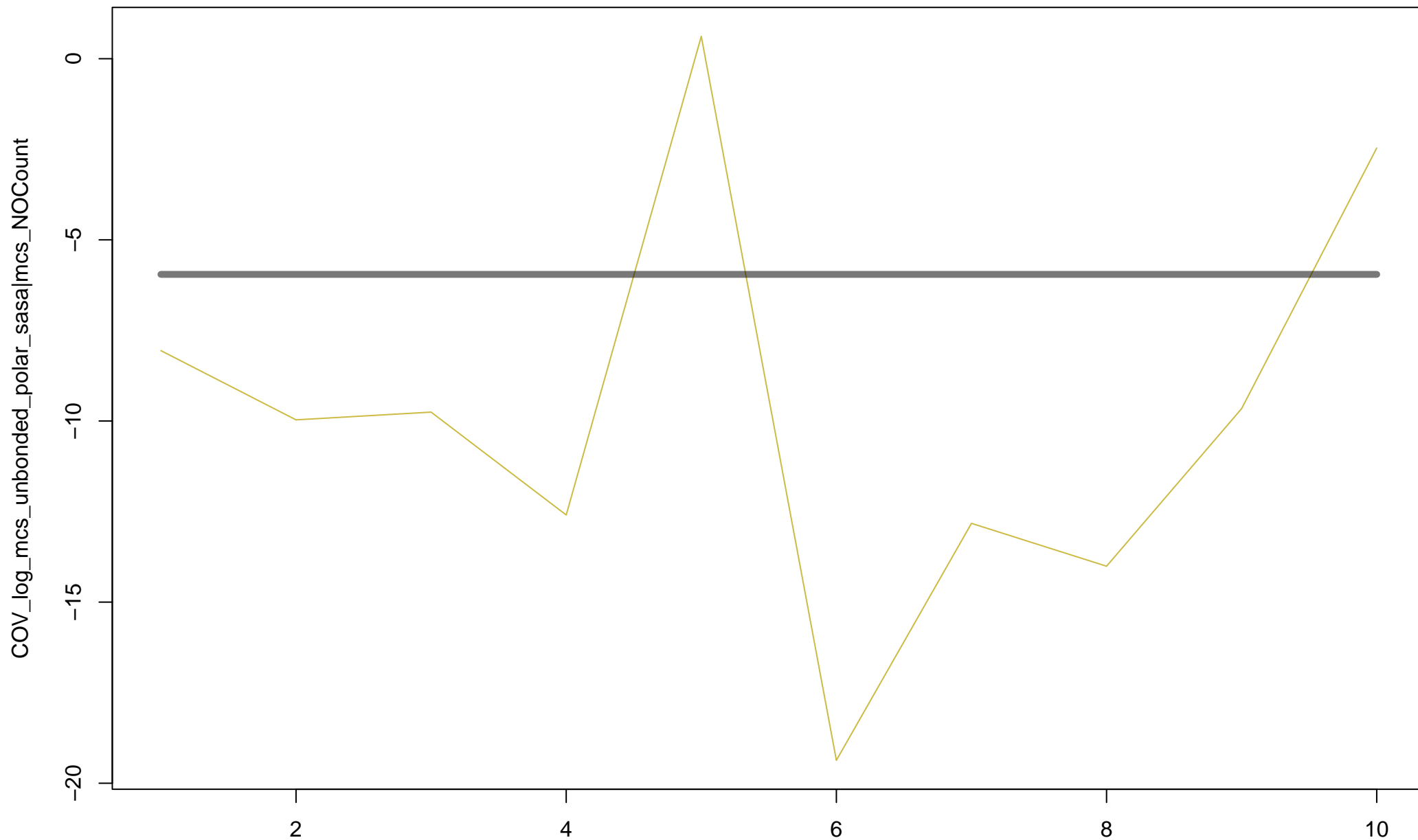
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_RingCount**  
**ESS = 10 | BMK = 0.49 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 0**



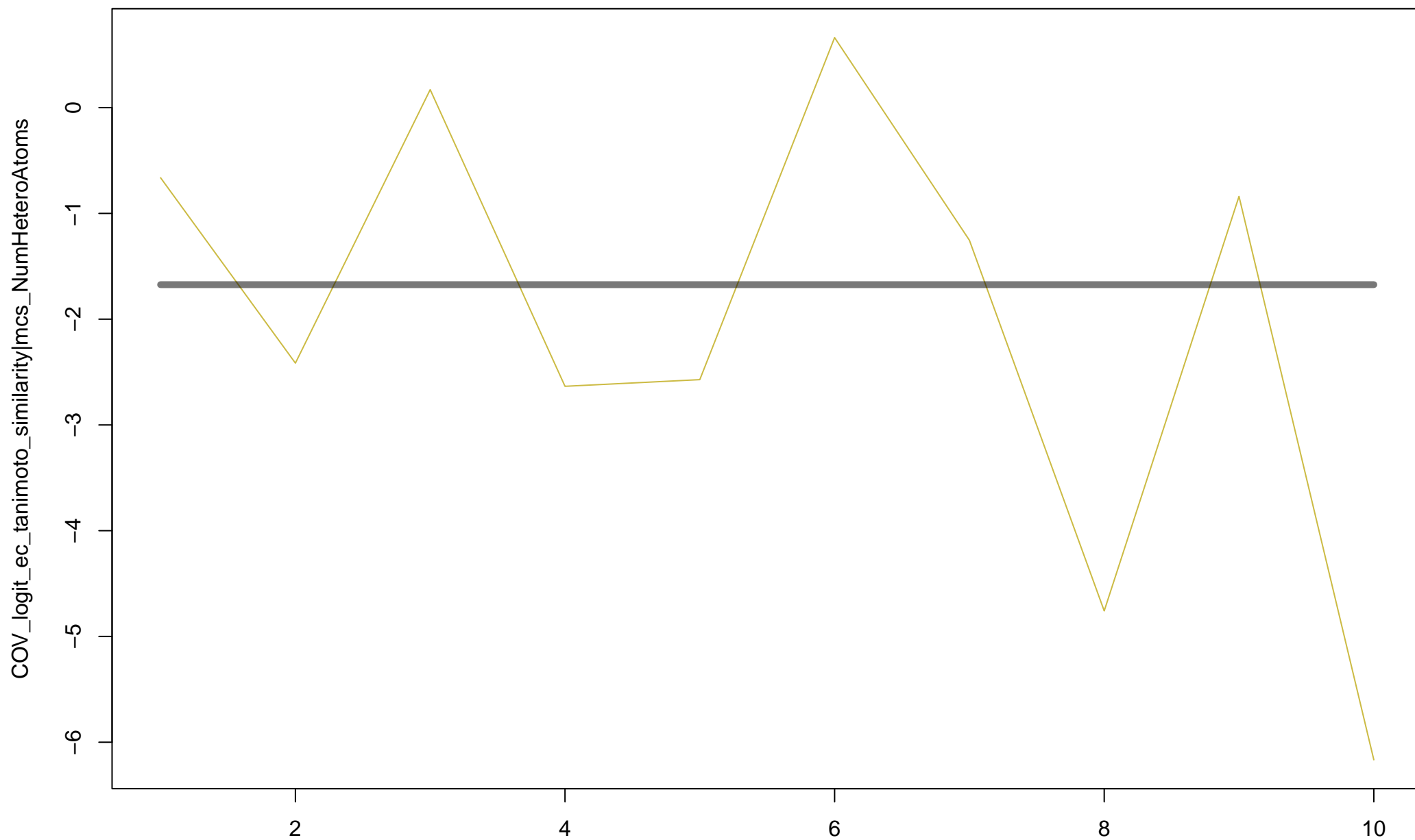
**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_NumRotatableBonds**  
**ESS = 10 | BMK = 0.124 | MCSE(6.27) = 27.3 | stat: FALSE | burn: 0 | percentile: 70**



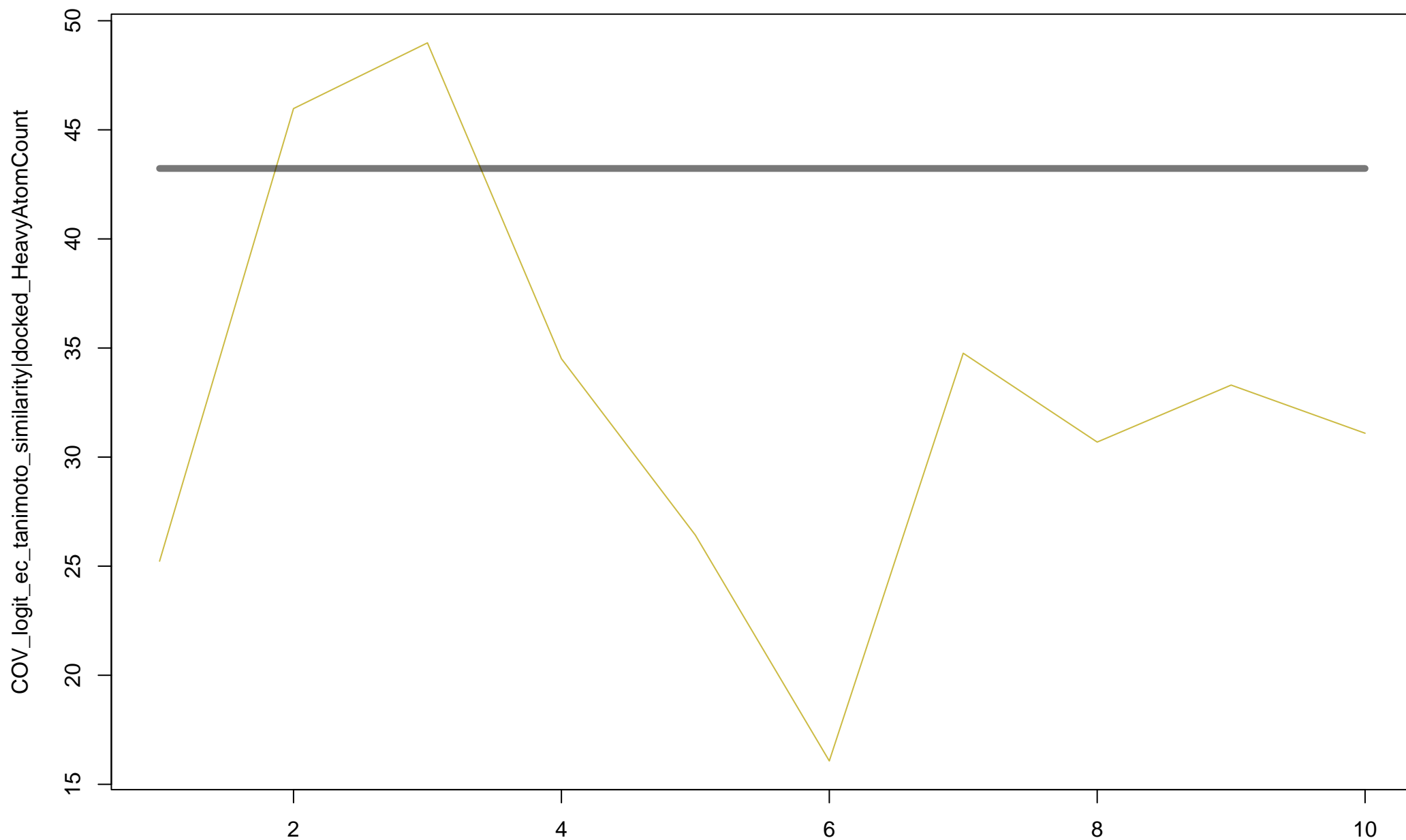
**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NOCount**  
**ESS = 10 | BMK = 0.629 | MCSE(6.27) = 19 | stat: FALSE | burn: 0 | percentile: 80**



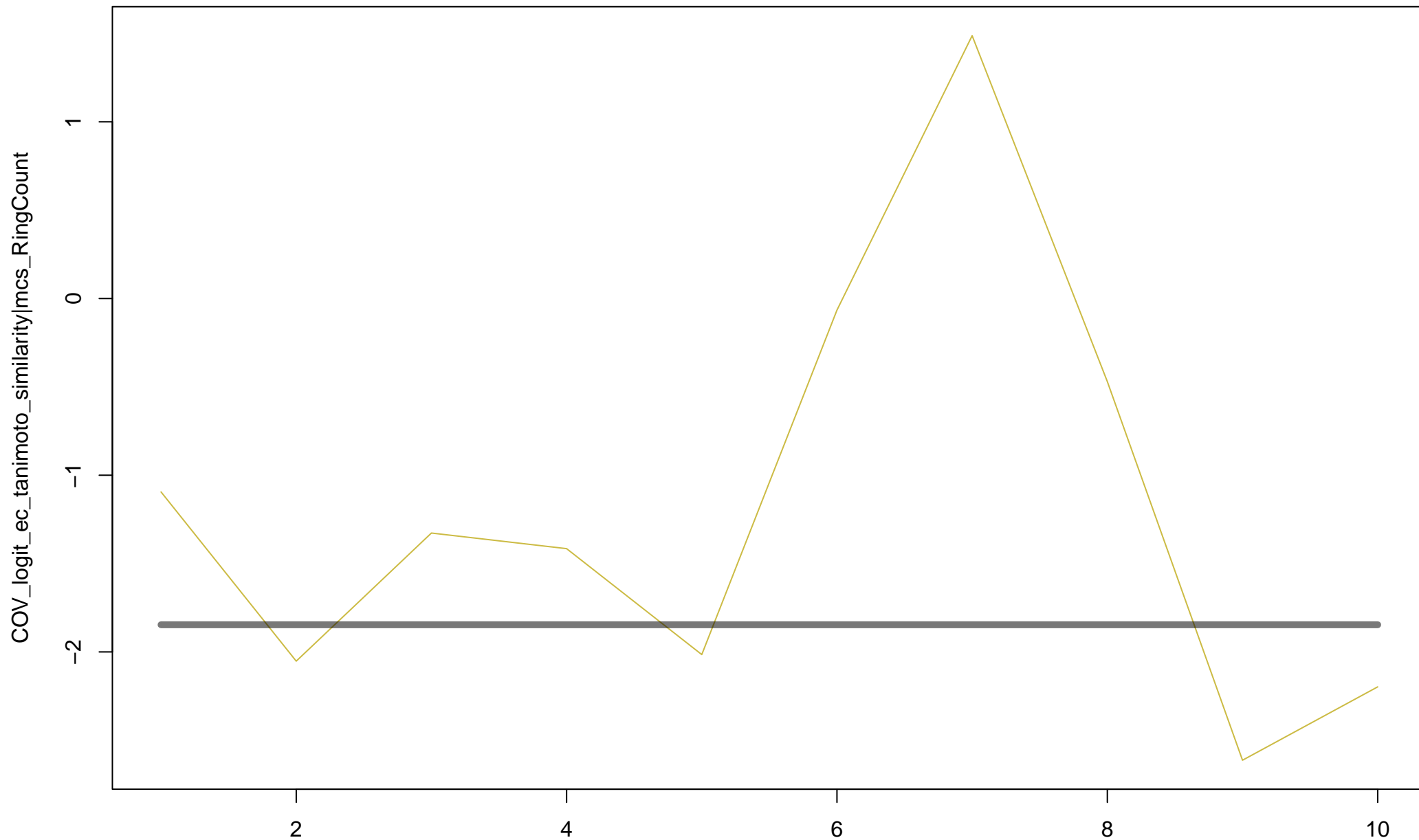
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms**  
**ESS = 10 | BMK = 0.356 | MCSE(6.27) = 19.4 | stat: FALSE | burn: 0 | percentile: 50**



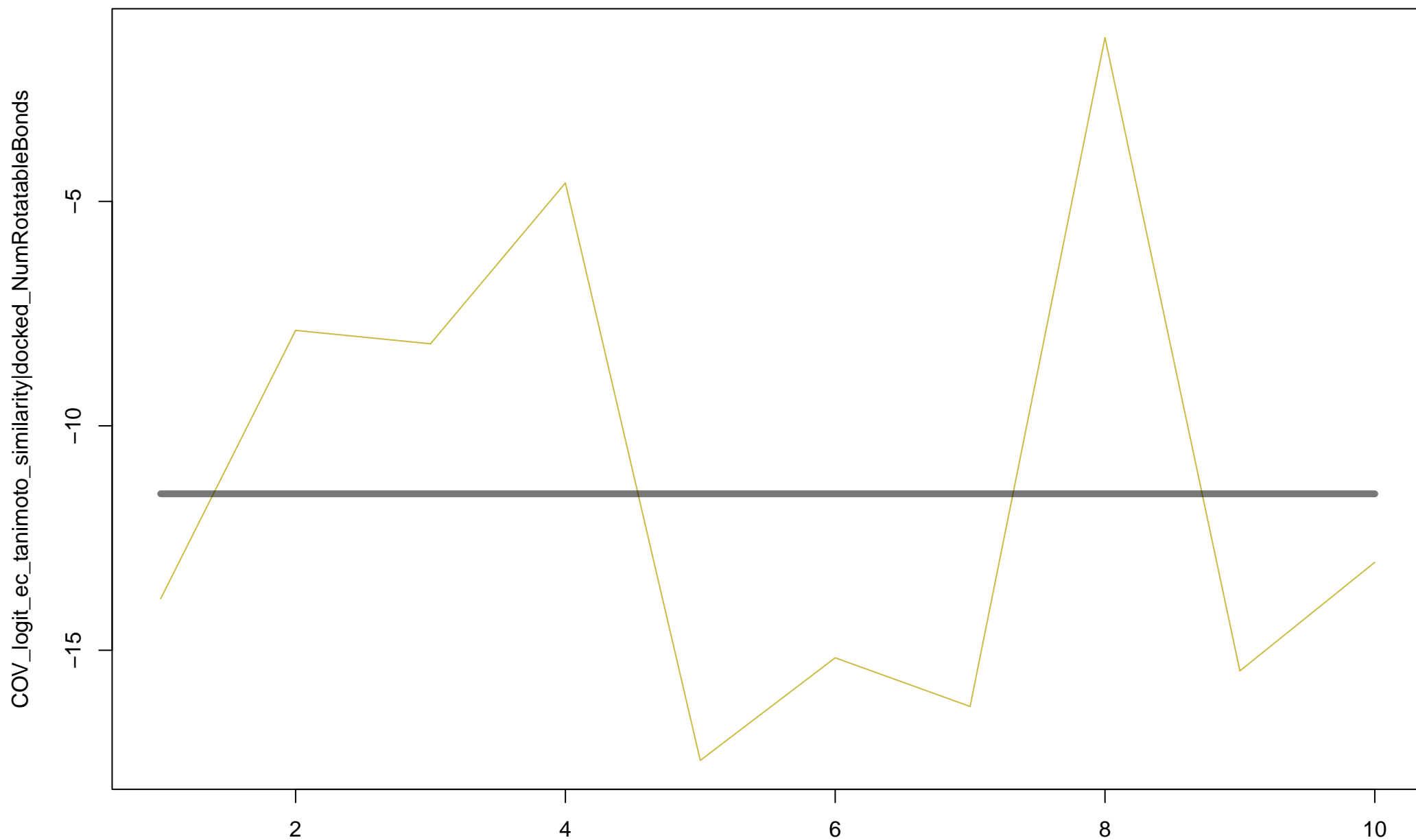
COV\_logit\_ec\_tanimoto\_similarity|docked\_HeavyAtomCount  
ESS = 10 | BMK = 0.73 | MCSE(6.27) = 36.5 | stat: FALSE | burn: 0 | percentile: 80



**COV\_logit\_ec\_tanimoto\_similarity|mcs\_RingCount**  
**ESS = 10 | BMK = 0.498 | MCSE(6.27) = 39 | stat: FALSE | burn: 0 | percentile: 40**

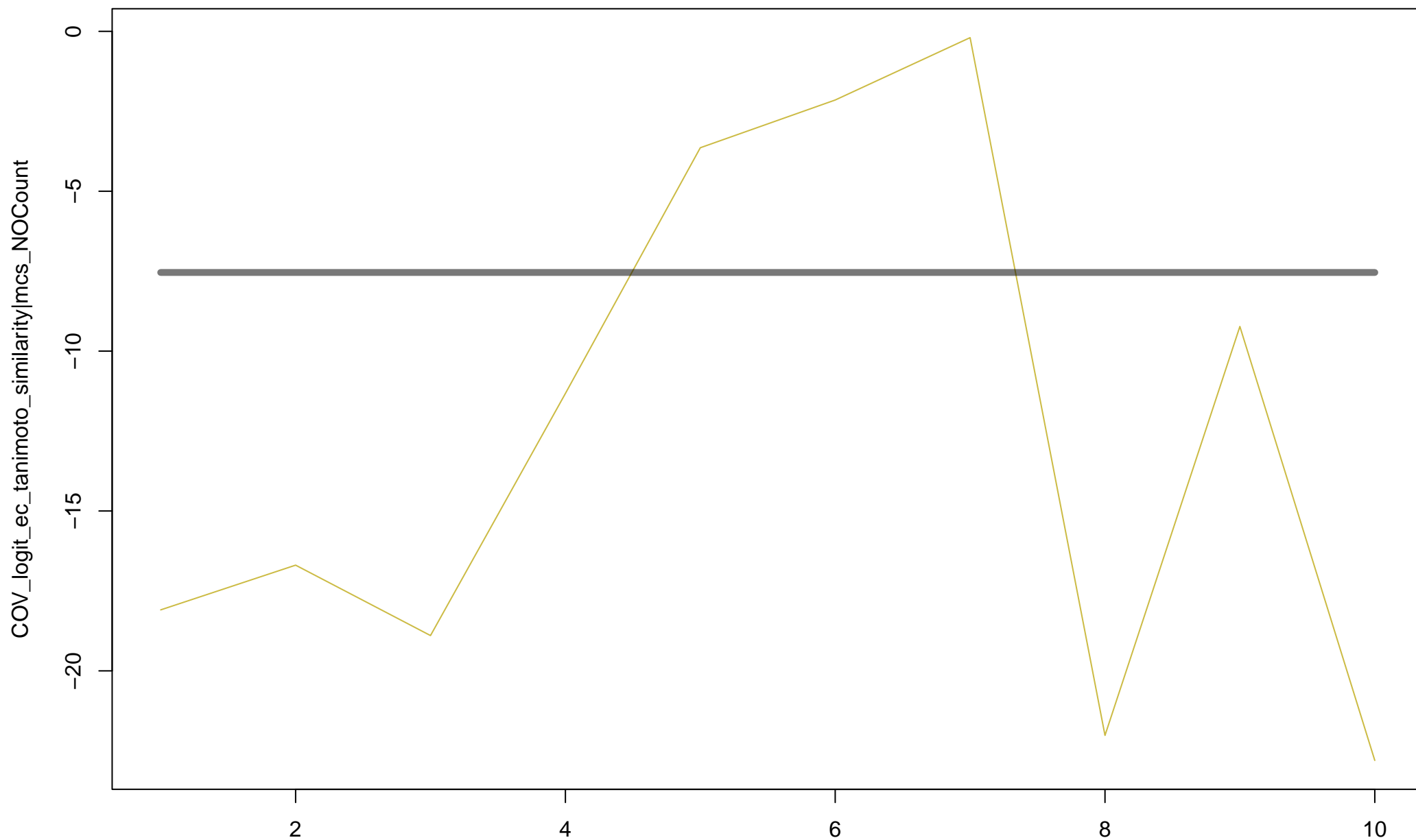


COV\_logit\_ec\_tanimoto\_similarity|docked\_NumRotatableBonds  
ESS = 10 | BMK = 0.53 | MCSE(6.27) = 22.5 | stat: FALSE | burn: 0 | percentile: 60

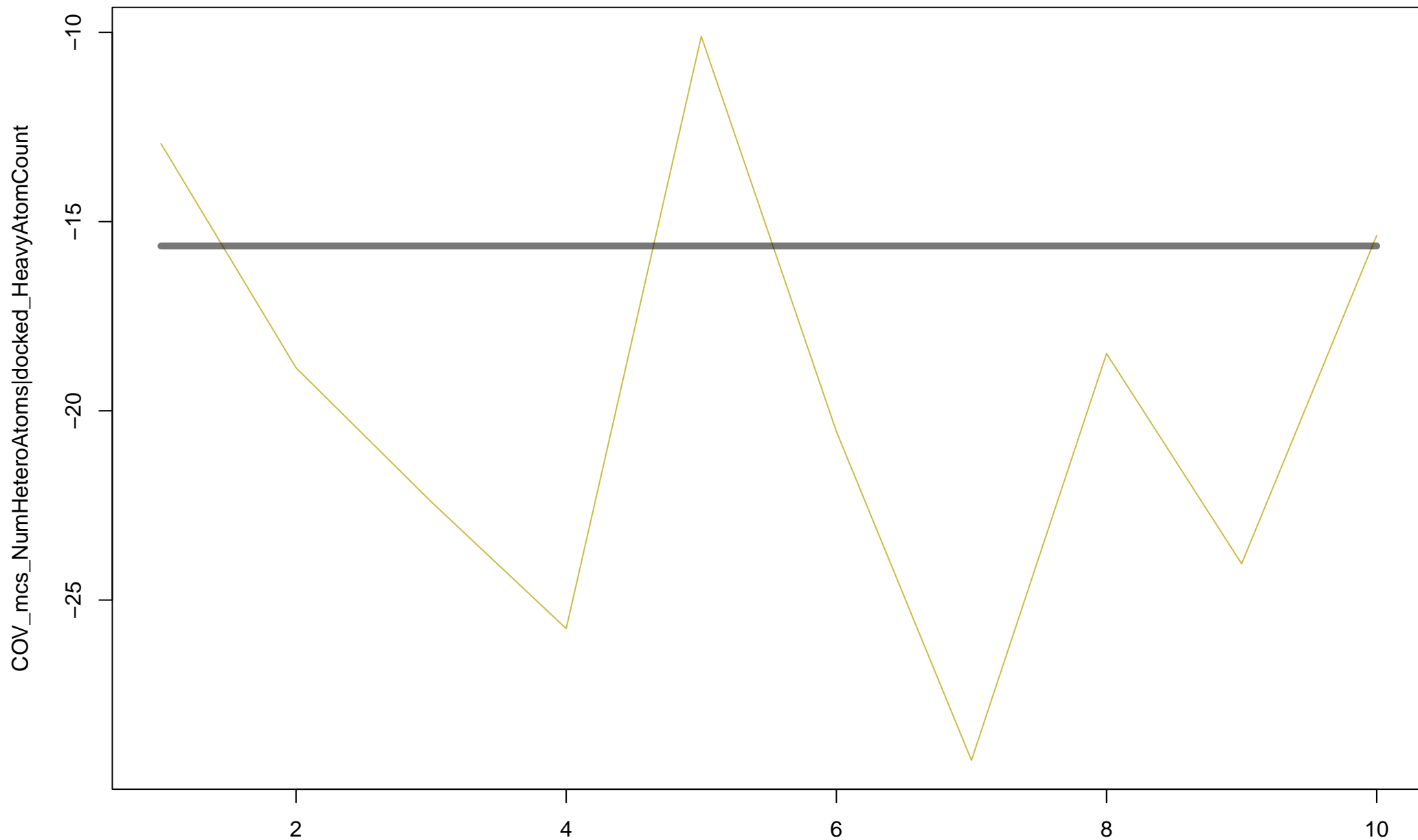




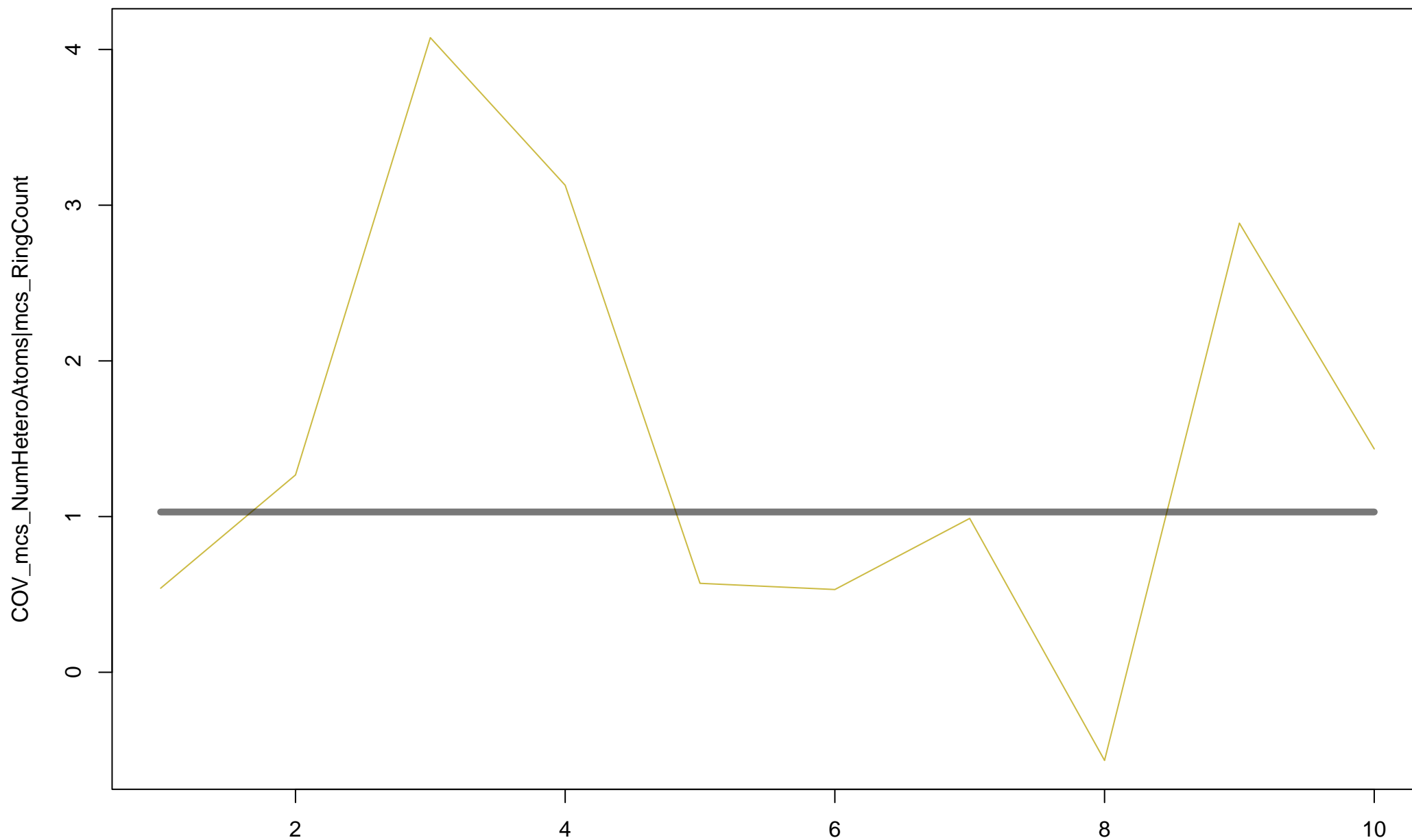
**COV\_logit\_ec\_tanimoto\_similarity|mcs\_NOCount**  
**ESS = 10 | BMK = 0.215 | MCSE(6.27) = 42.4 | stat: FALSE | burn: 0 | percentile: 70**



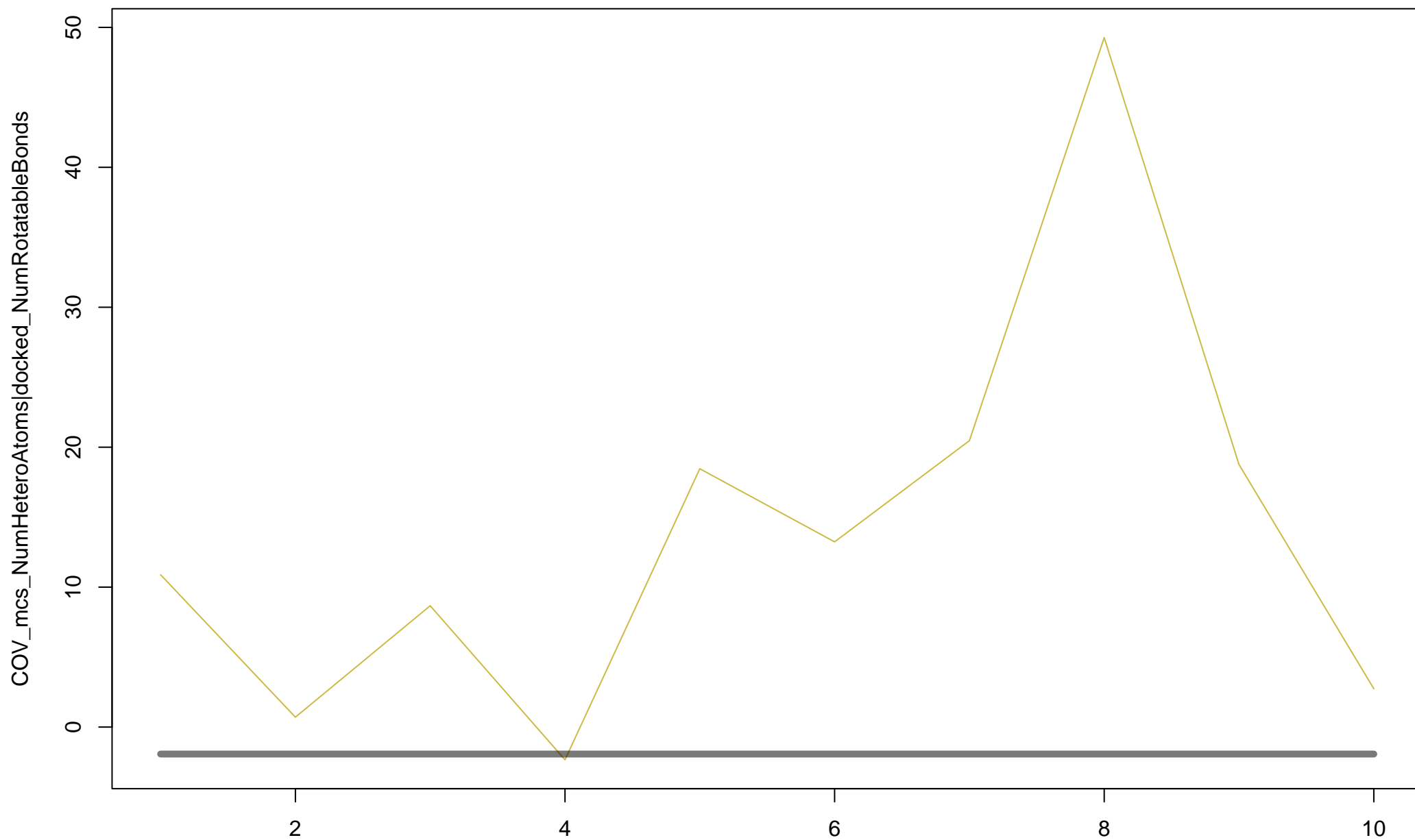
**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 10 | BMK = 0.217 | MCSE(6.27) = 21.7 | stat: FALSE | burn: 0 | percentile: 70**



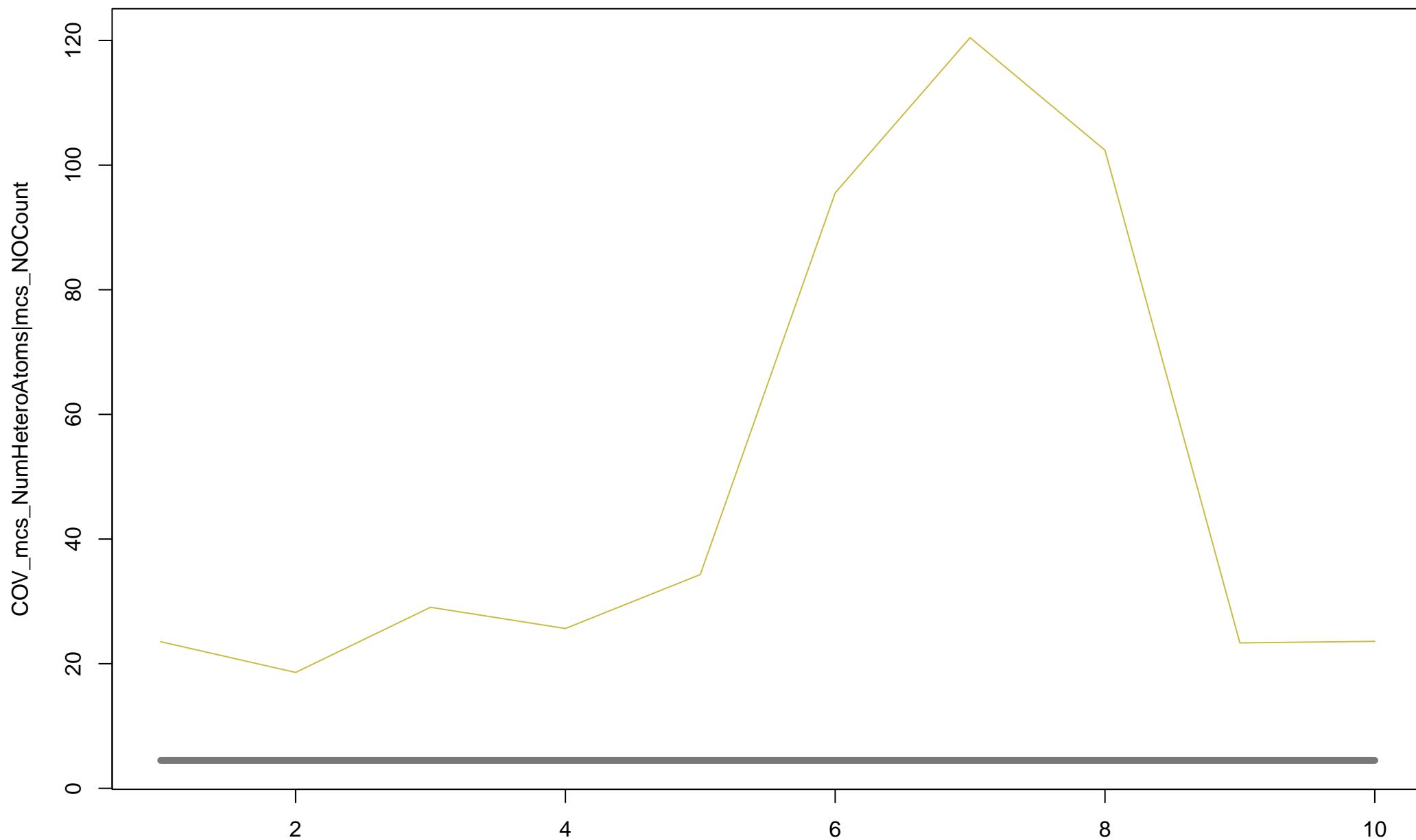
**COV\_mcs\_NumHeteroAtoms|mcs\_RingCount**  
**ESS = 10 | BMK = 0.256 | MCSE(6.27) = 32.8 | stat: FALSE | burn: 0 | percentile: 50**



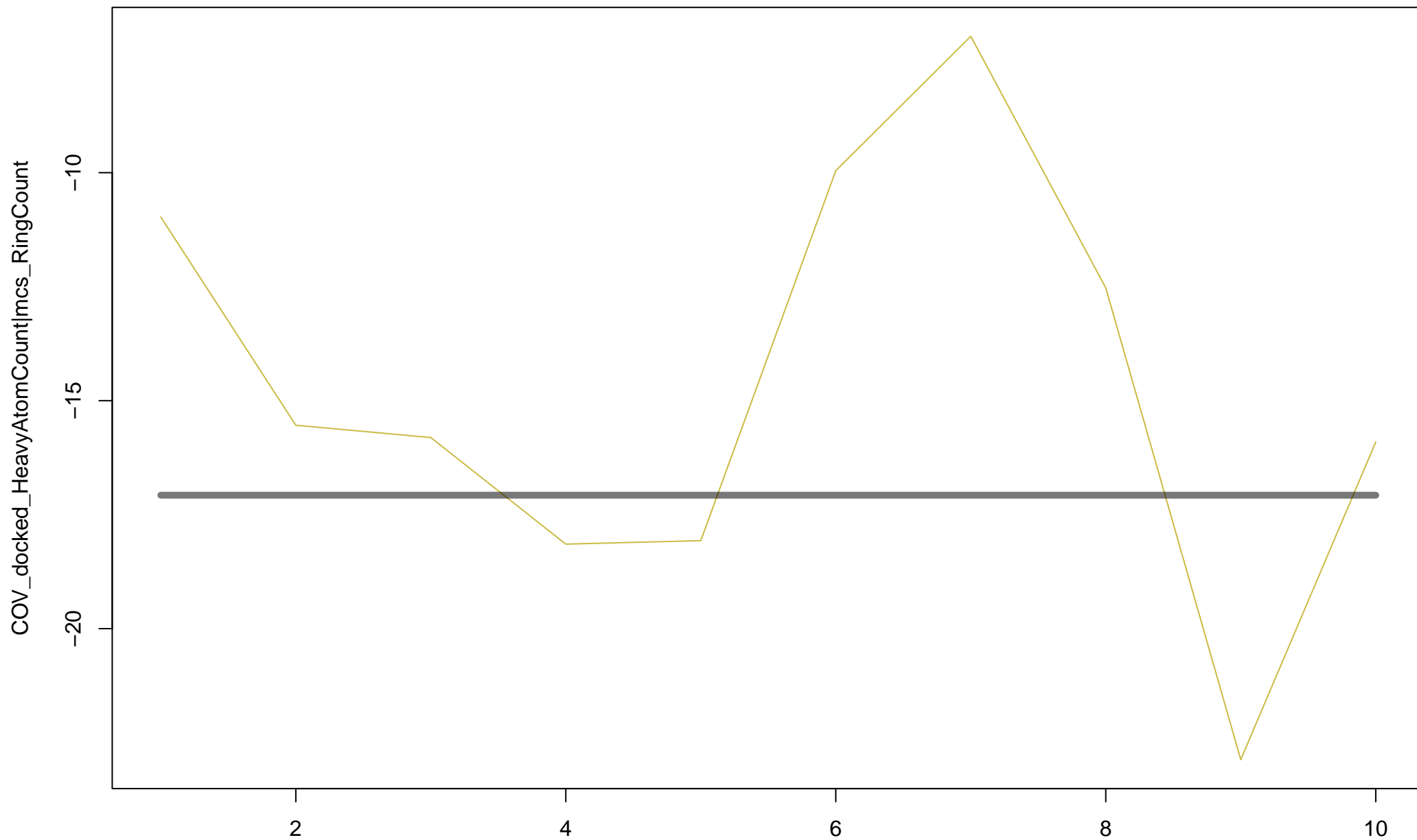
**COV\_mcs\_NumHeteroAtoms|docked\_NumRotatableBonds**  
**ESS = 10 | BMK = 0.483 | MCSE(6.27) = 40.2 | stat: FALSE | burn: 0 | percentile: 10**



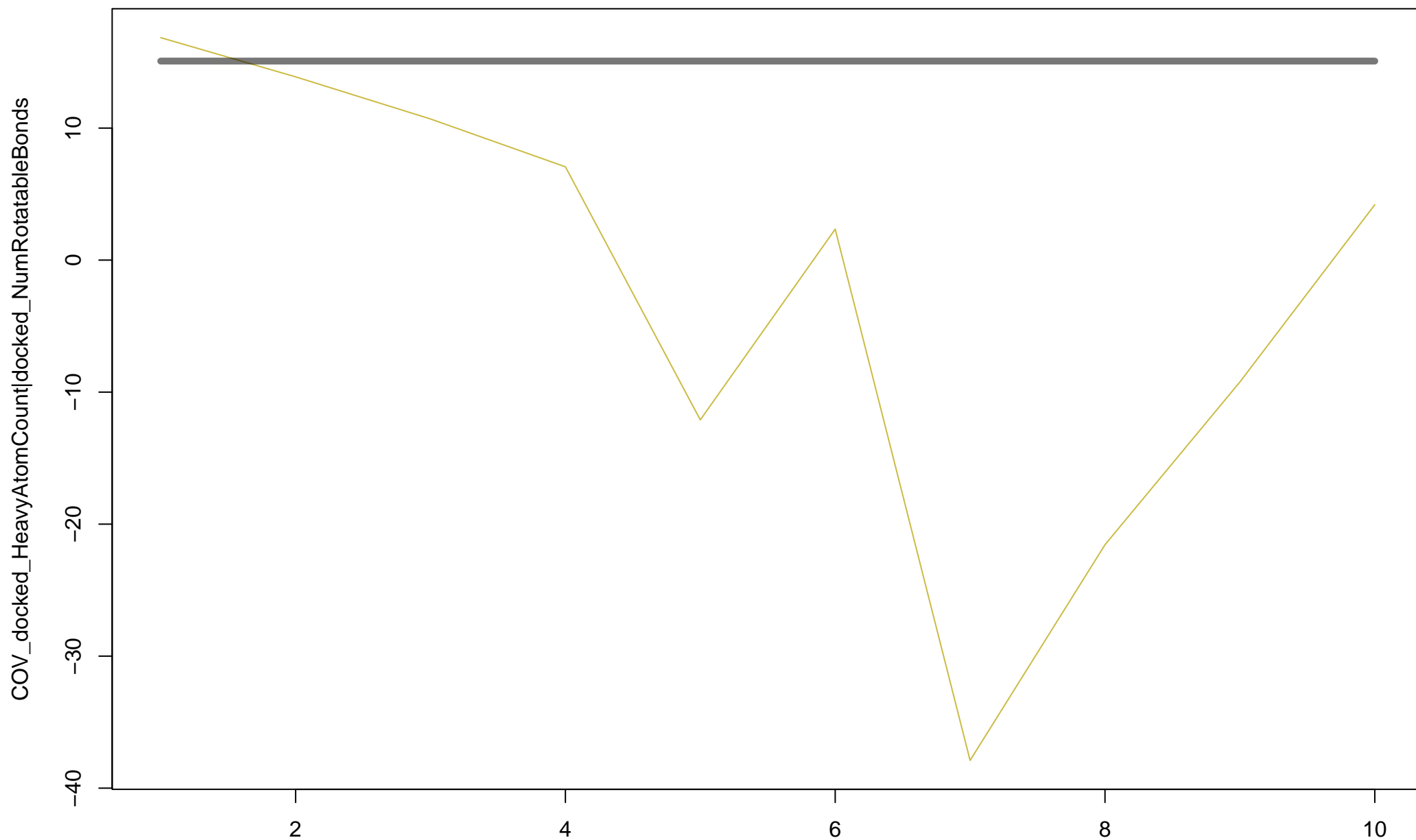
**COV\_mcs\_NumHeteroAtoms|mcs\_NOCount**  
**ESS = 8.7 | BMK = 0.694 | MCSE(6.27) = 52.2 | stat: FALSE | burn: 0 | percentile: 0**



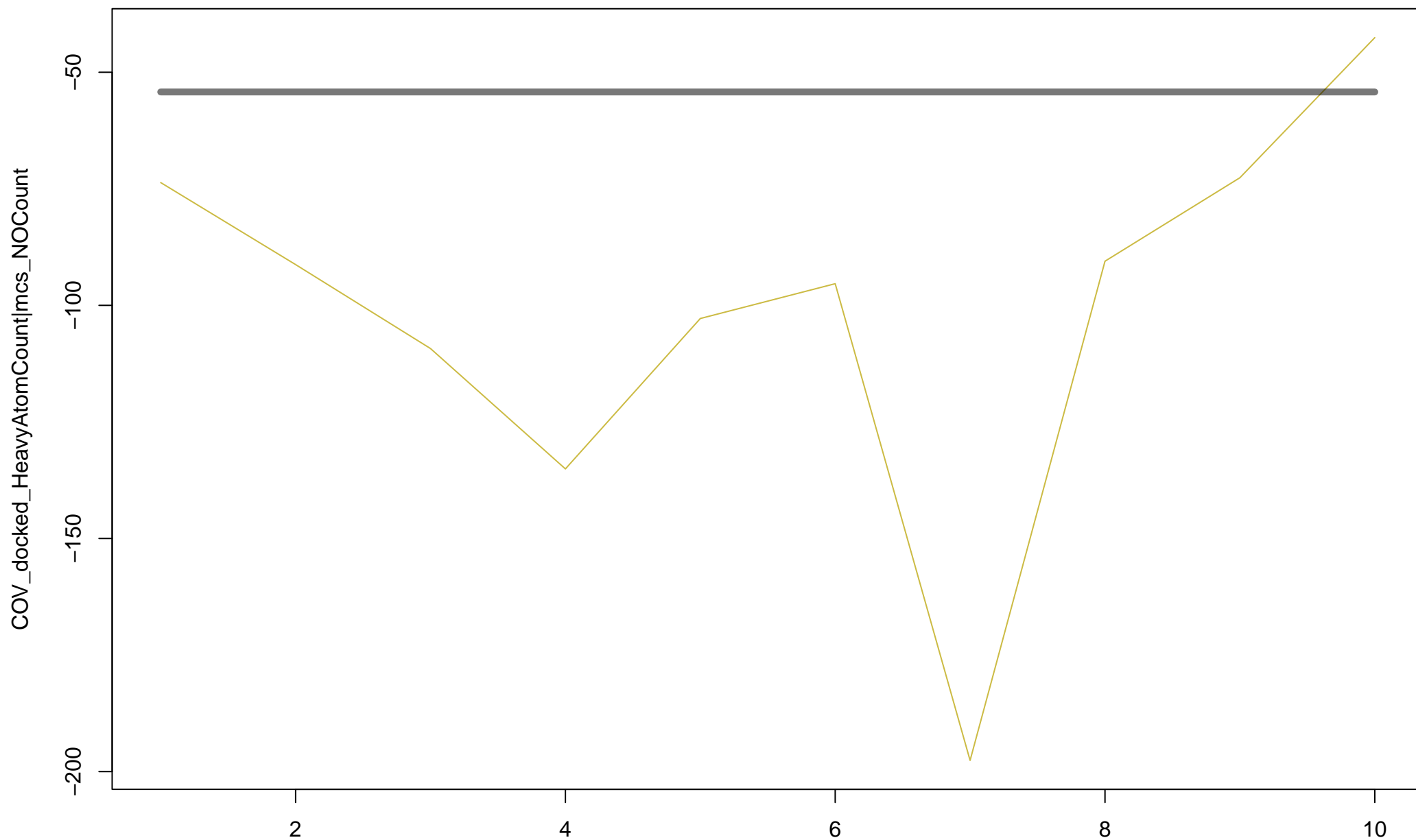
**COV\_docked\_HeavyAtomCount|mcs\_RingCount**  
**ESS = 10 | BMK = 0.452 | MCSE(6.27) = 36 | stat: FALSE | burn: 0 | percentile: 30**



**COV\_docked\_HeavyAtomCount|docked\_NumRotatableBonds**  
**ESS = 10 | BMK = 0.514 | MCSE(6.27) = 55.2 | stat: FALSE | burn: 0 | percentile: 90**

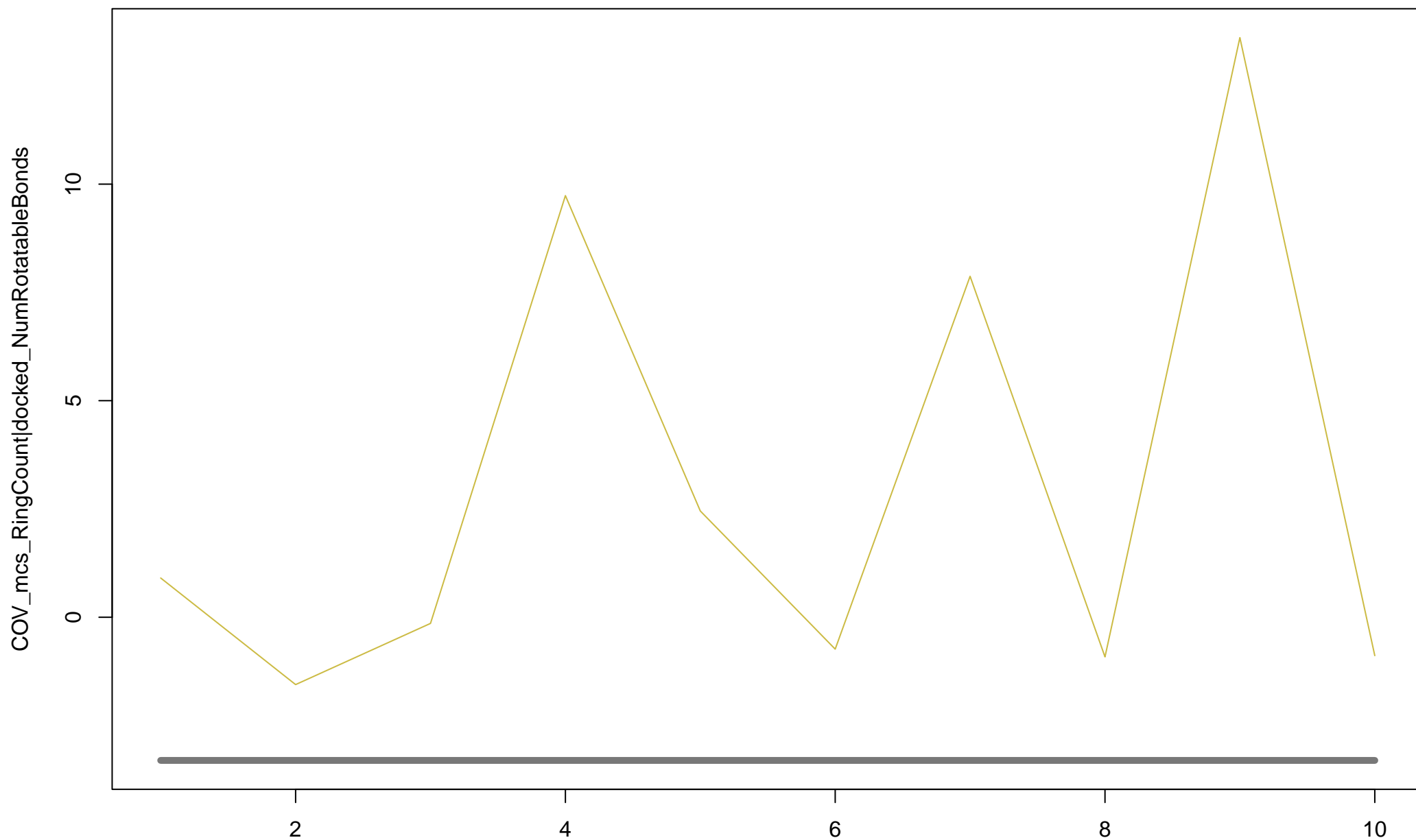


**COV\_docked\_HeavyAtomCount|mcs\_NOCount**  
**ESS = 10 | BMK = 0.585 | MCSE(6.27) = 31.7 | stat: FALSE | burn: 0 | percentile: 90**

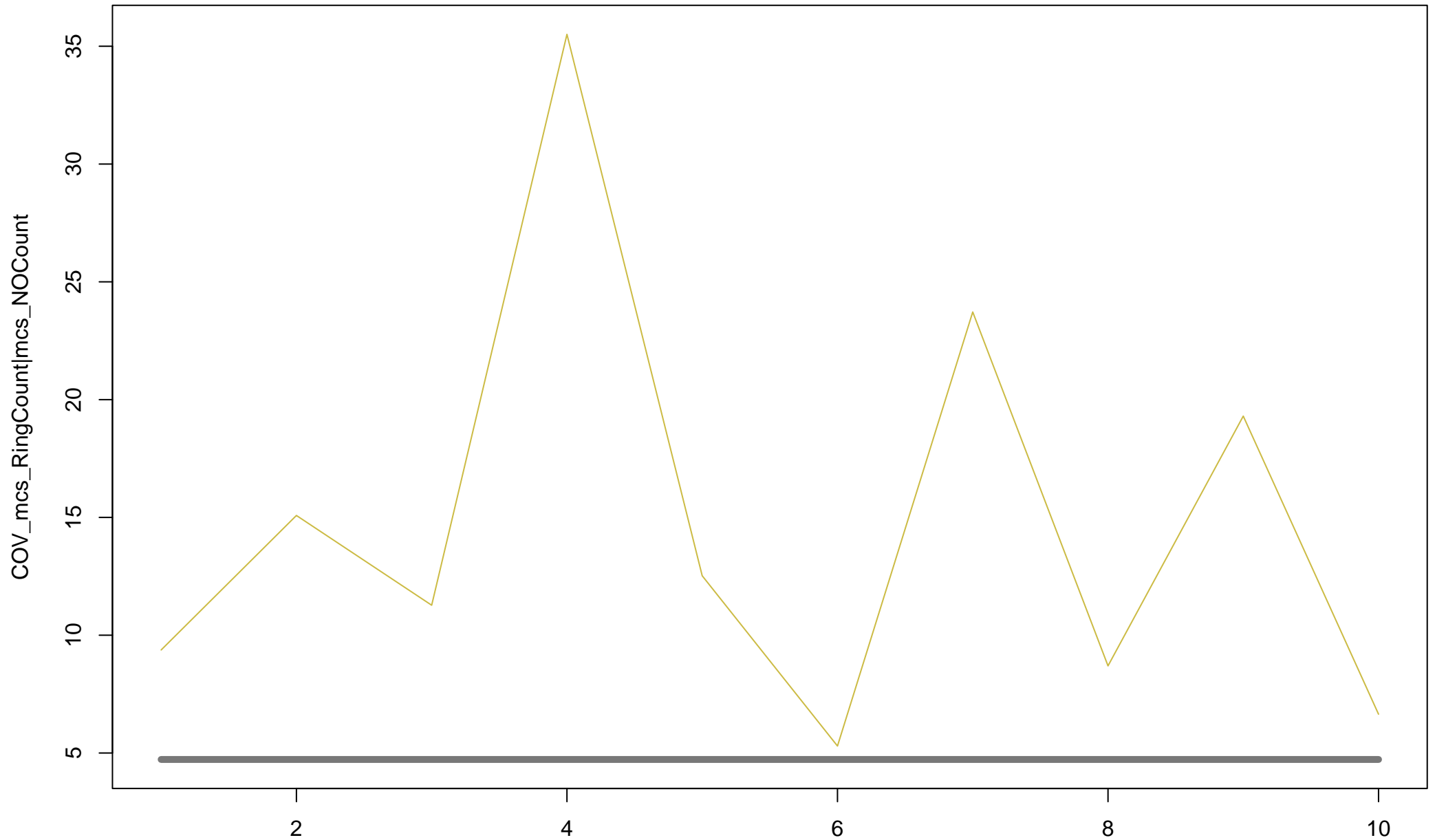




**COV\_mcs\_RingCount|docked\_NumRotatableBonds**  
**ESS = 10 | BMK = 0.343 | MCSE(6.27) = 8.79 | stat: FALSE | burn: 0 | percentile: 0**



**COV\_mcs\_RingCount|mcs\_NOCount**  
**ESS = 10 | BMK = 0.618 | MCSE(6.27) = 13.8 | stat: FALSE | burn: 0 | percentile: 0**



**COV\_docked\_NumRotatableBonds|mcs\_NOCount**  
**ESS = 10 | BMK = 0.223 | MCSE(6.27) = 42.1 | stat: FALSE | burn: 0 | percentile: 0**

