-- STATS maxD -min ESS = 3.4480532324482 max BMK = 0.542720101856772 max MCSE = 17.1435942153973 all stationary: FALSE

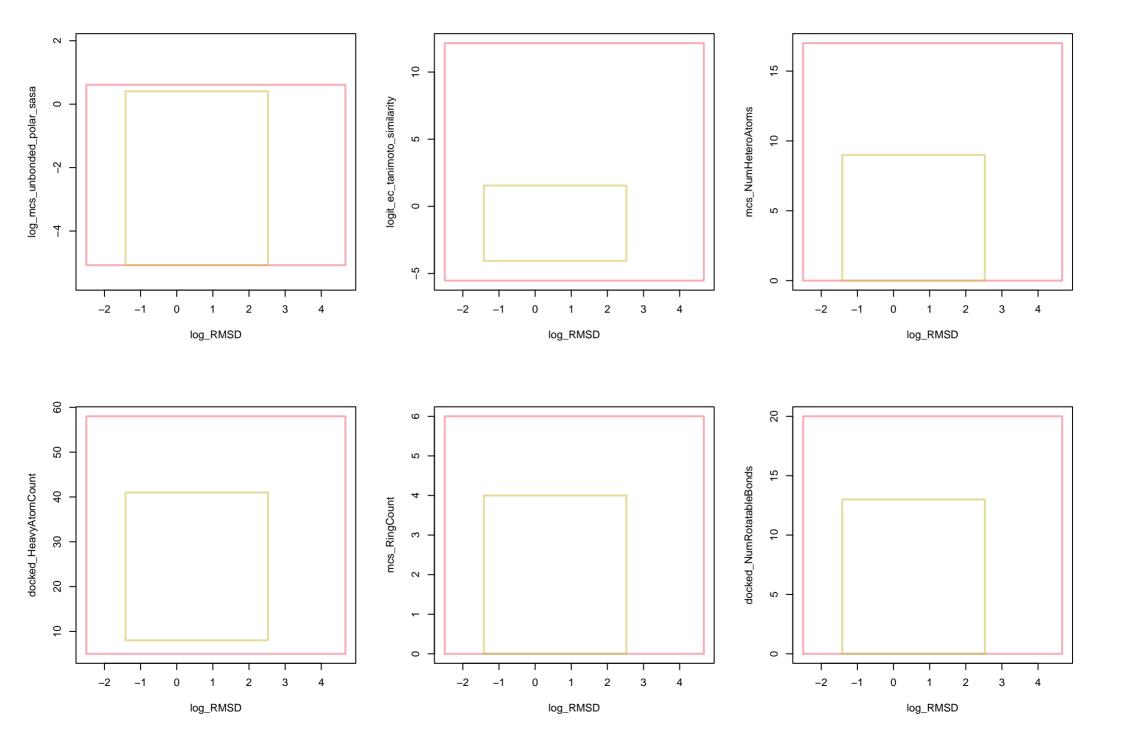
burn: 2000

--- STATS 1D --min ESS = 10.3427646548009 max BMK = 0.506963097474754 max MCSE = 9.7342285685163 all stationary: FALSE

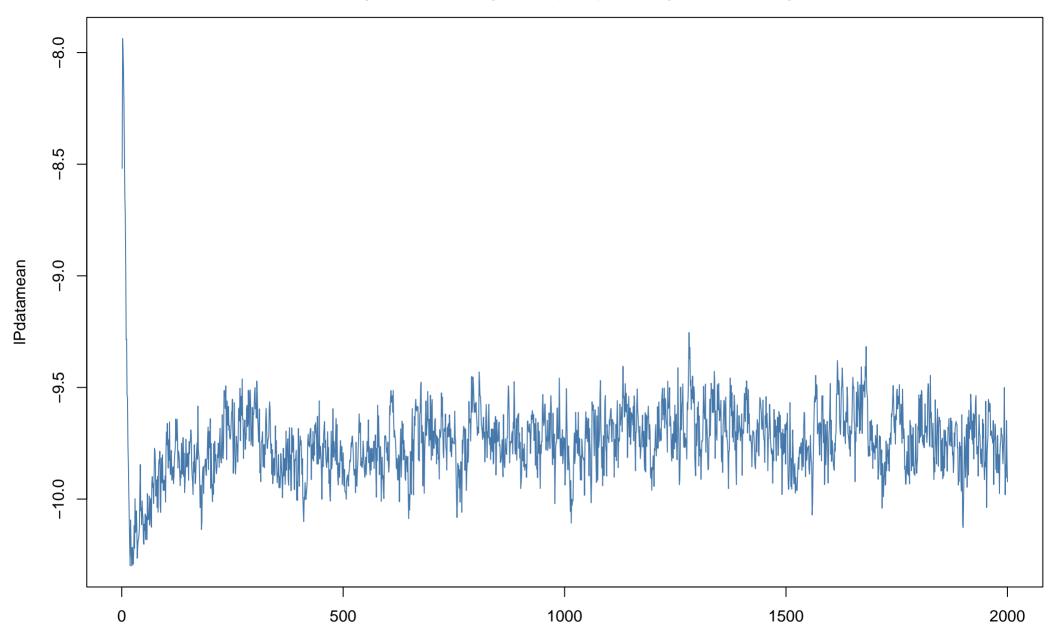
burn: 200

-- STATS 2D -min ESS = 38.1542130615616 max BMK = 0.376665432595328 max MCSE = 7.03085982363998 all stationary: FALSE

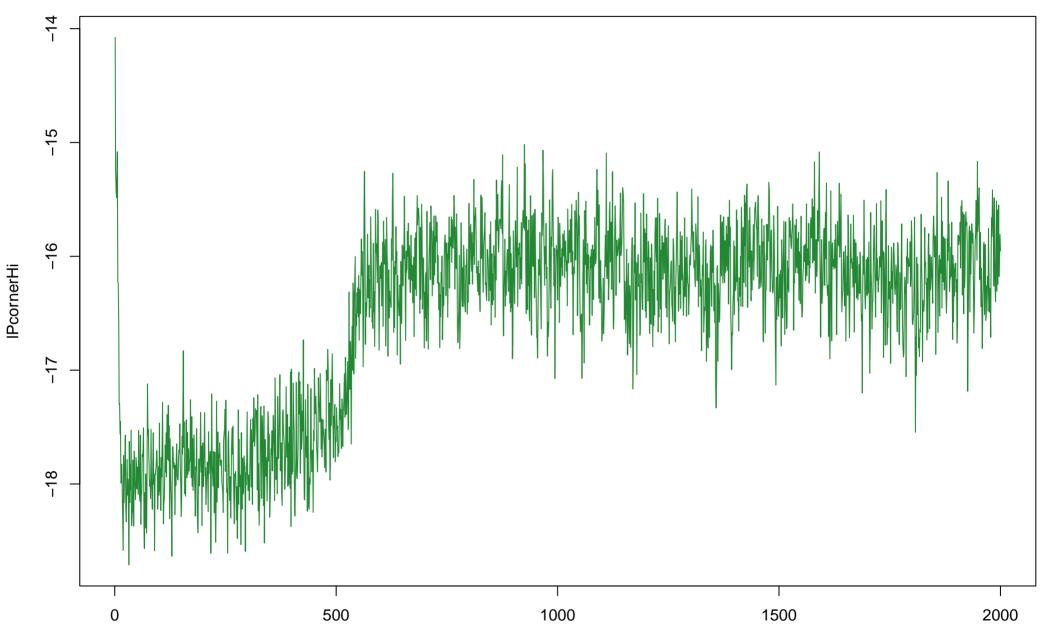
burn: 0



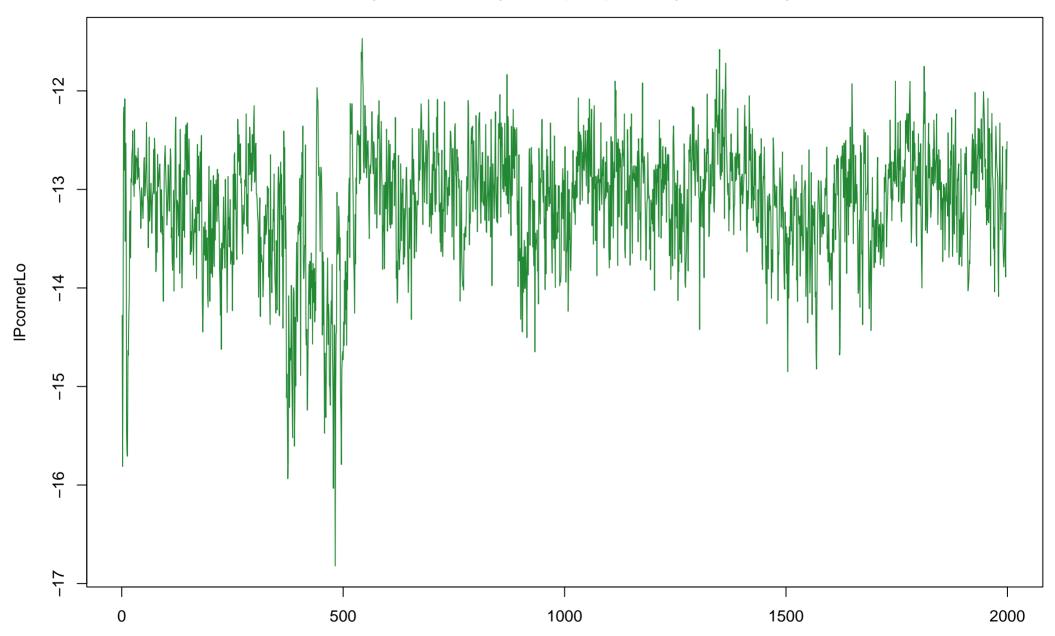
IPdatamean
ESS = 158 | BMK = 0.208 | MCSE(6.27) = 11.1 | stat: FALSE | burn: 0



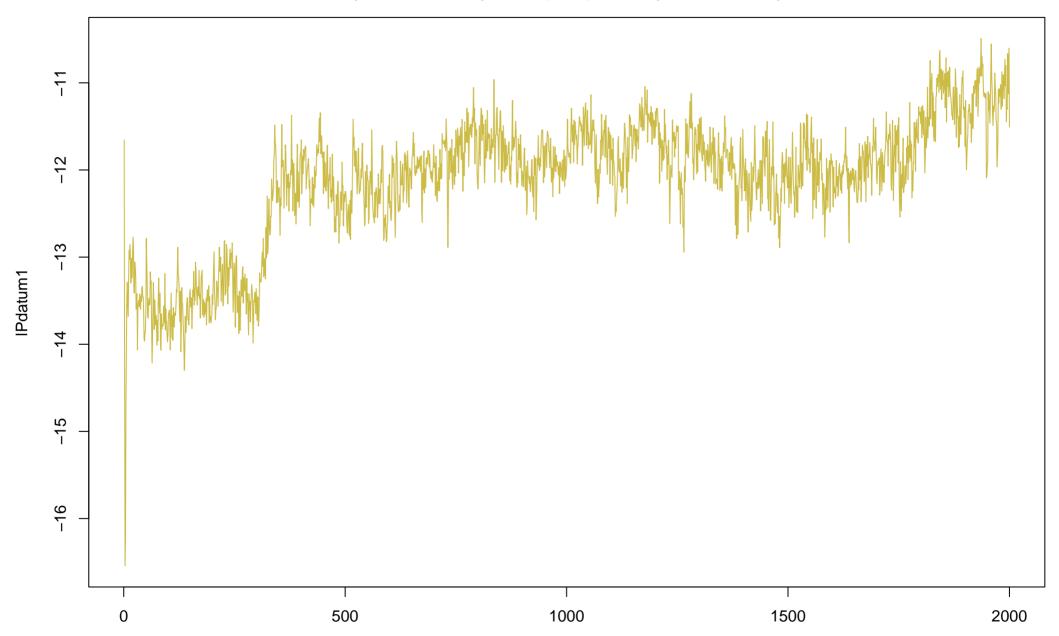
IPcornerHi
ESS = 3.45 | BMK = 0.52 | MCSE(6.27) = 9.8 | stat: FALSE | burn: 600



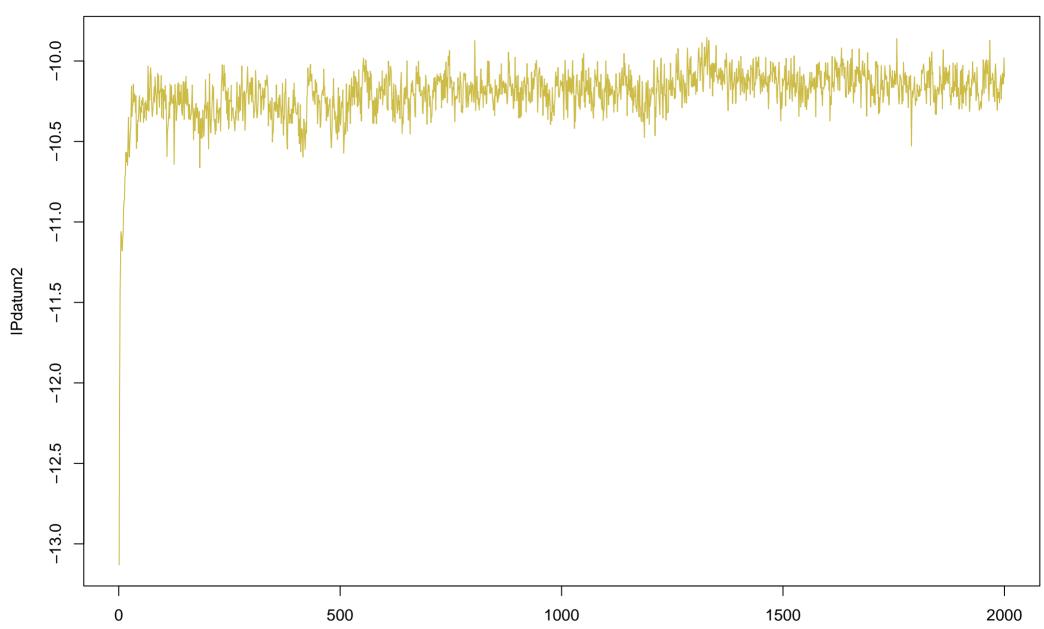
IPcornerLo ESS = 96.6 | BMK = 0.169 | MCSE(6.27) = 8.64 | stat: TRUE | burn: 0



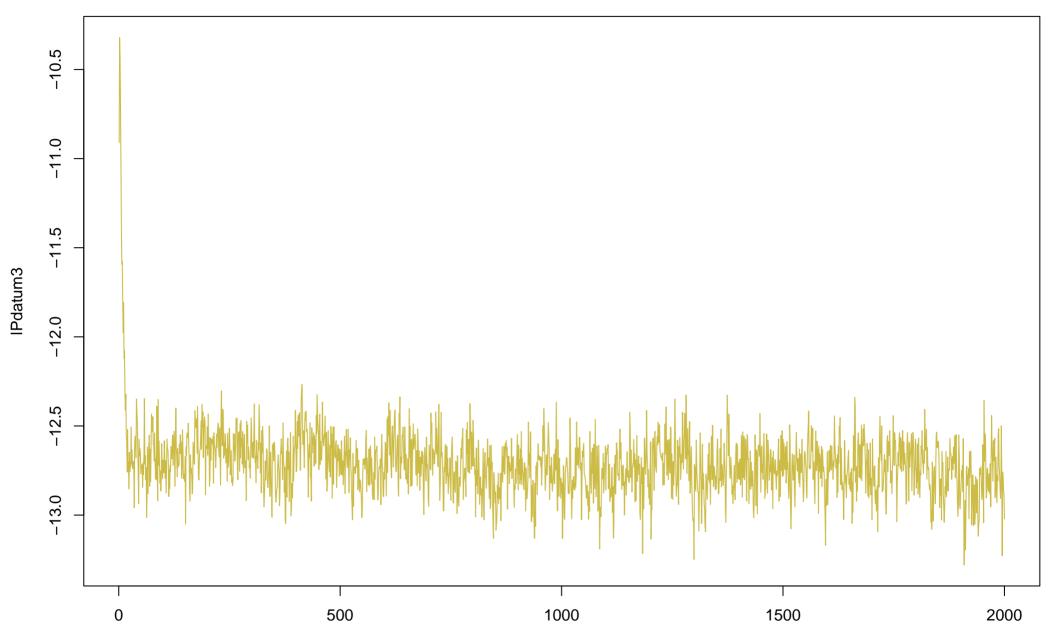
IPdatum1 ESS = 5.99 | BMK = 0.461 | MCSE(6.27) = 17.1 | stat: FALSE | burn: 2000



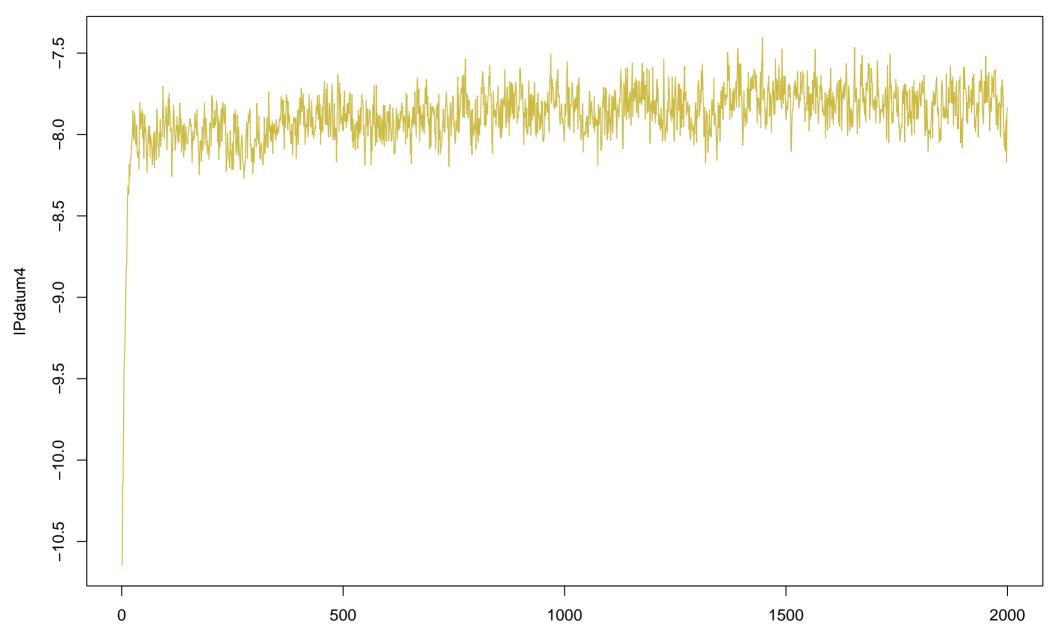
IPdatum2 ESS = 107 | BMK = 0.315 | MCSE(6.27) = 13.4 | stat: FALSE | burn: 0



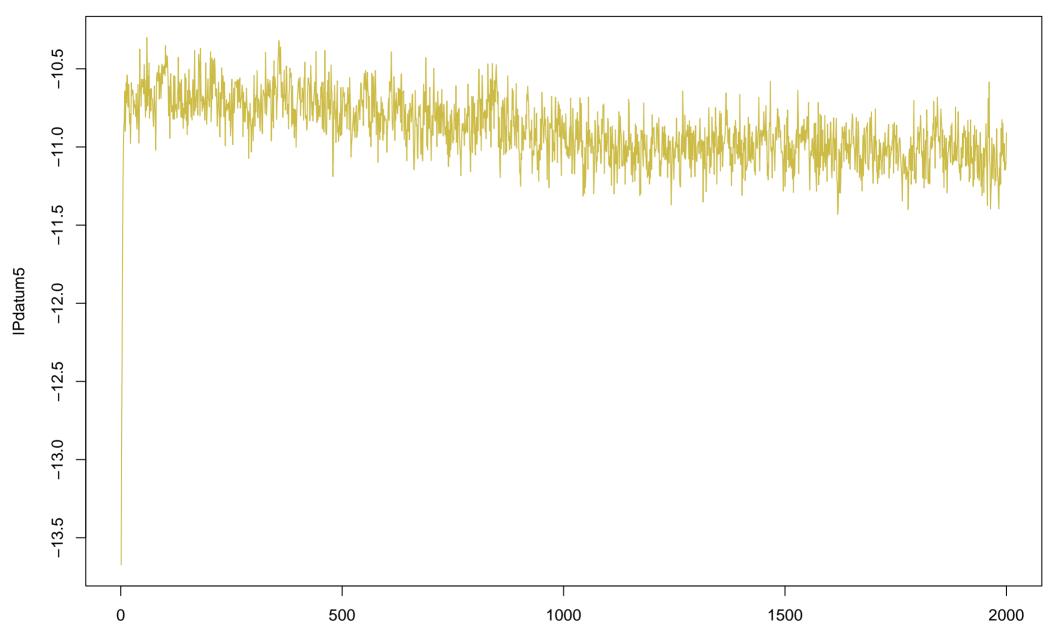
IPdatum3 ESS = 211 | BMK = 0.156 | MCSE(6.27) = 9.27 | stat: FALSE | burn: 0



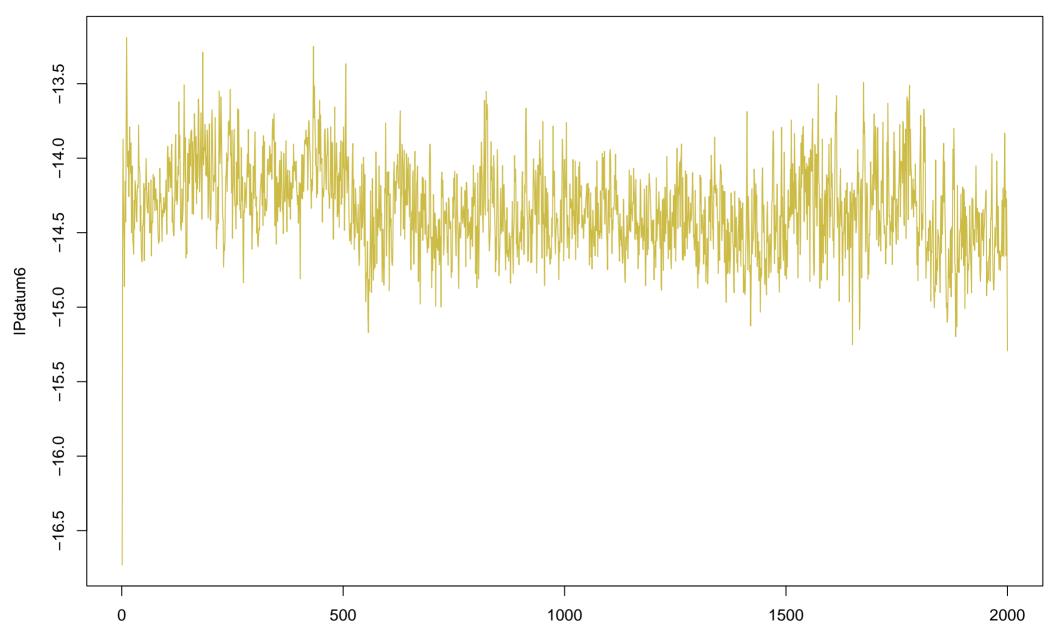
IPdatum4 ESS = 135 | BMK = 0.321 | MCSE(6.27) = 12.3 | stat: FALSE | burn: 0



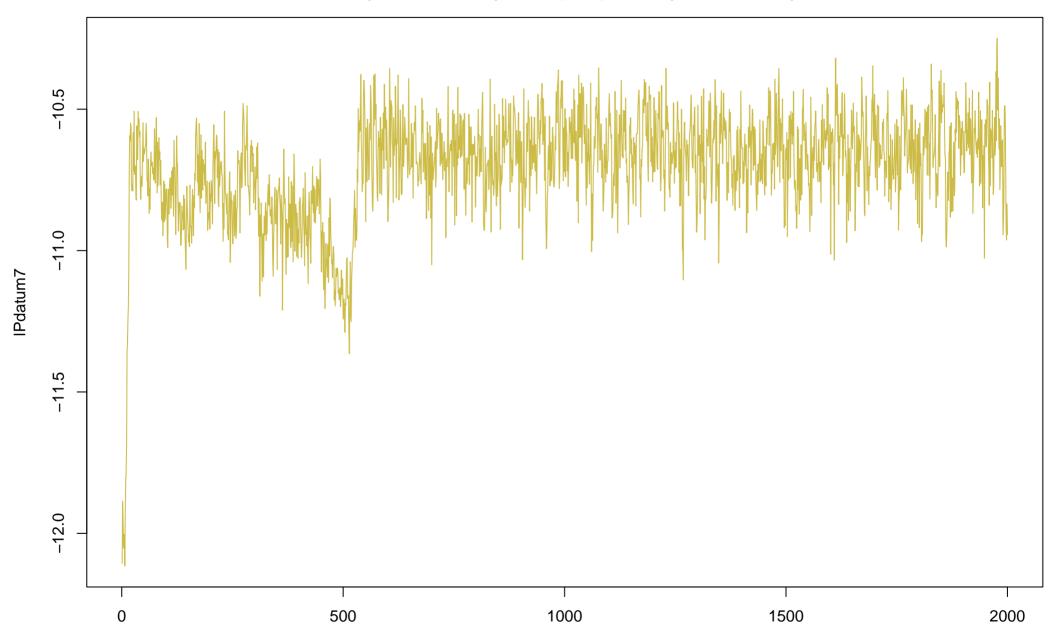
IPdatum5 ESS = 28.3 | BMK = 0.543 | MCSE(6.27) = 11 | stat: FALSE | burn: 0



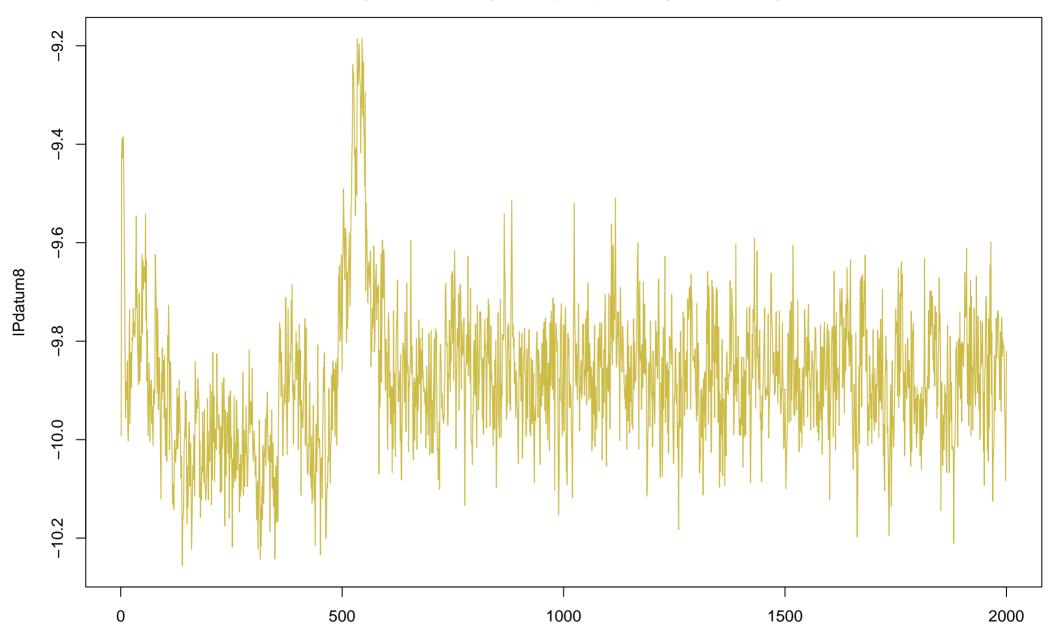
IPdatum6 ESS = 67.3 | BMK = 0.173 | MCSE(6.27) = 6.7 | stat: FALSE | burn: 0



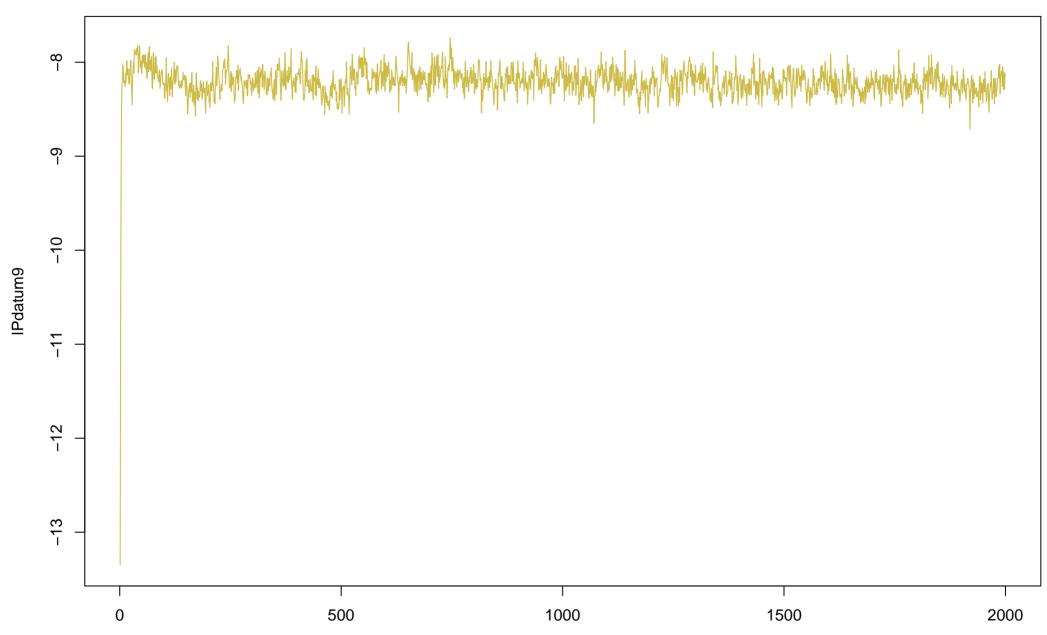
IPdatum7
ESS = 91.1 | BMK = 0.273 | MCSE(6.27) = 12.1 | stat: FALSE | burn: 0



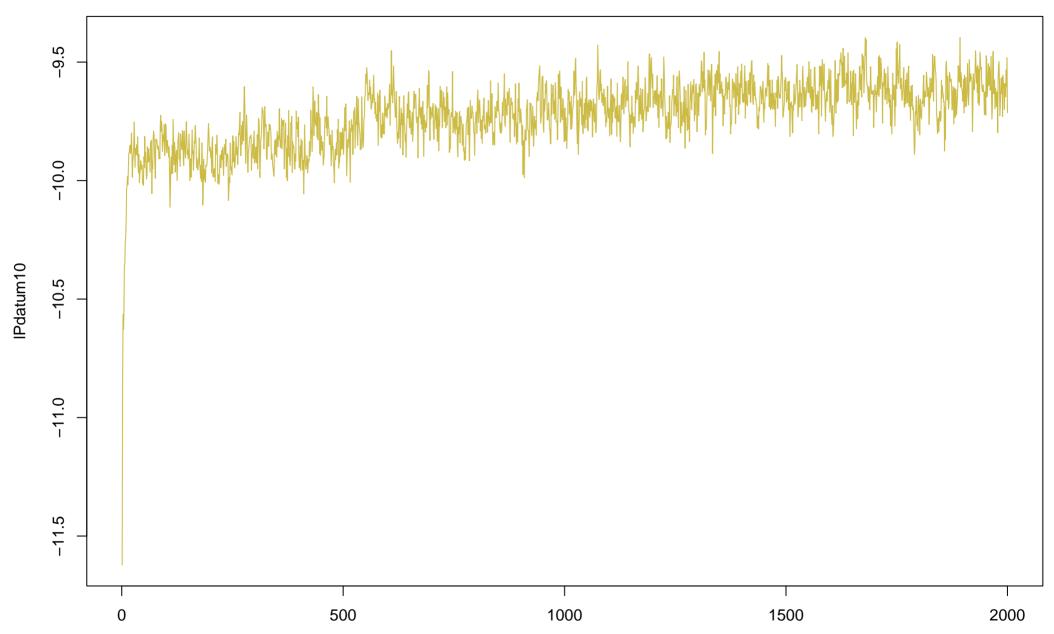
IPdatum8 ESS = 58 | BMK = 0.207 | MCSE(6.27) = 9.68 | stat: TRUE | burn: 0



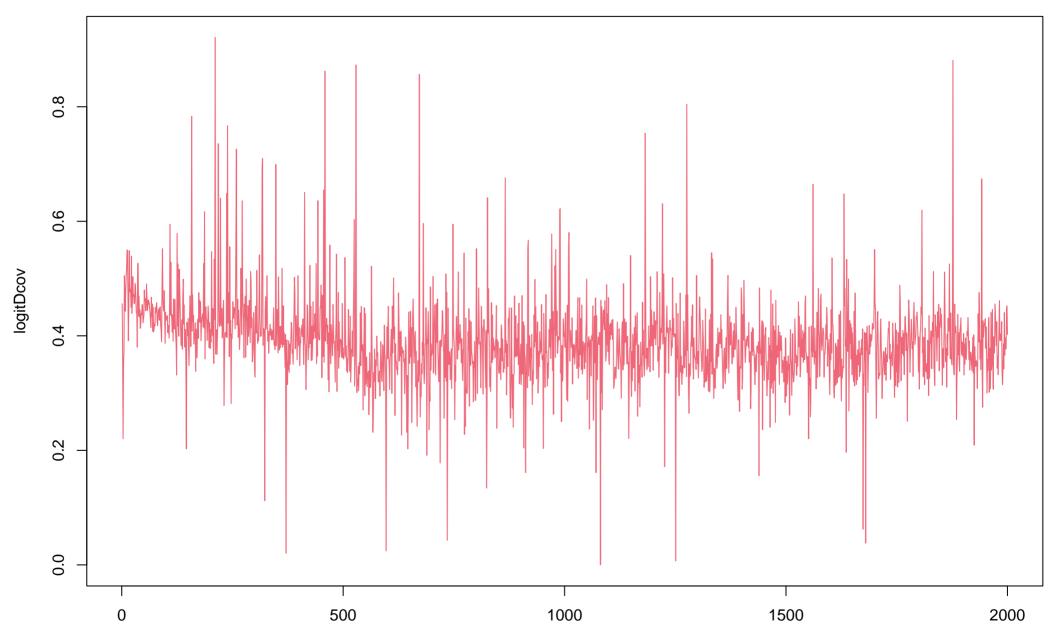
IPdatum9 ESS = 637 | BMK = 0.15 | MCSE(6.27) = 5.85 | stat: TRUE | burn: 0



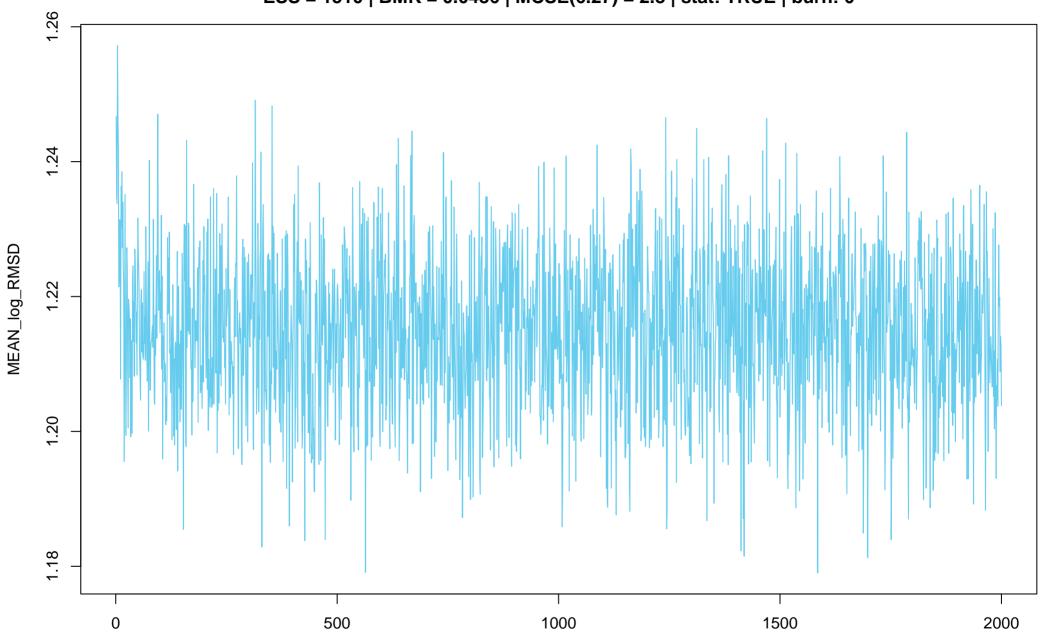
IPdatum10 ESS = 30 | BMK = 0.531 | MCSE(6.27) = 15.1 | stat: FALSE | burn: 0



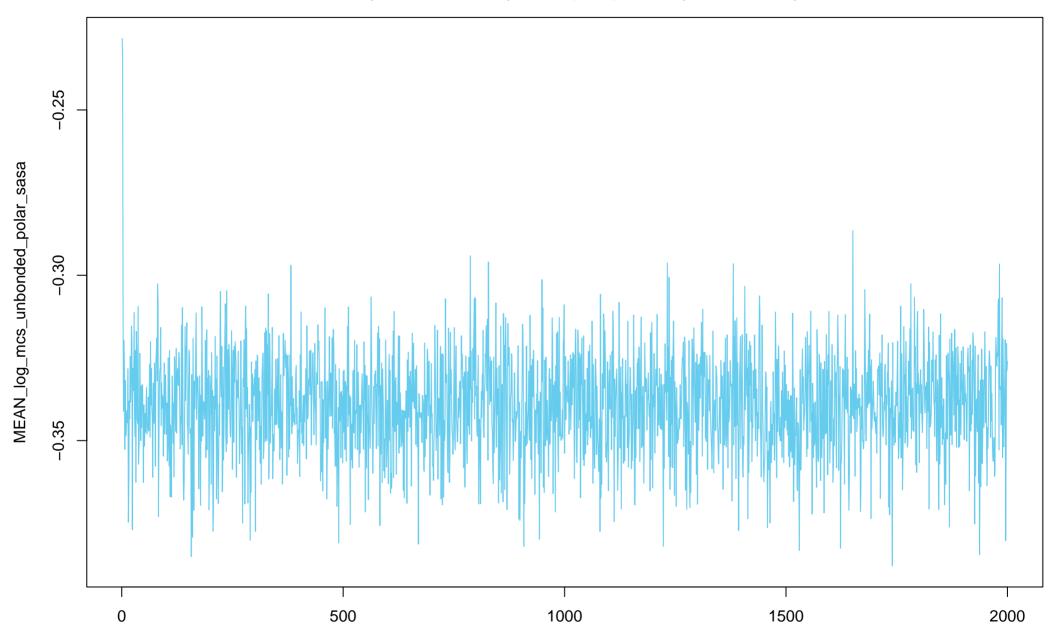
logitDcov ESS = 175 | BMK = 0.156 | MCSE(6.27) = 3.69 | stat: FALSE | burn: 0



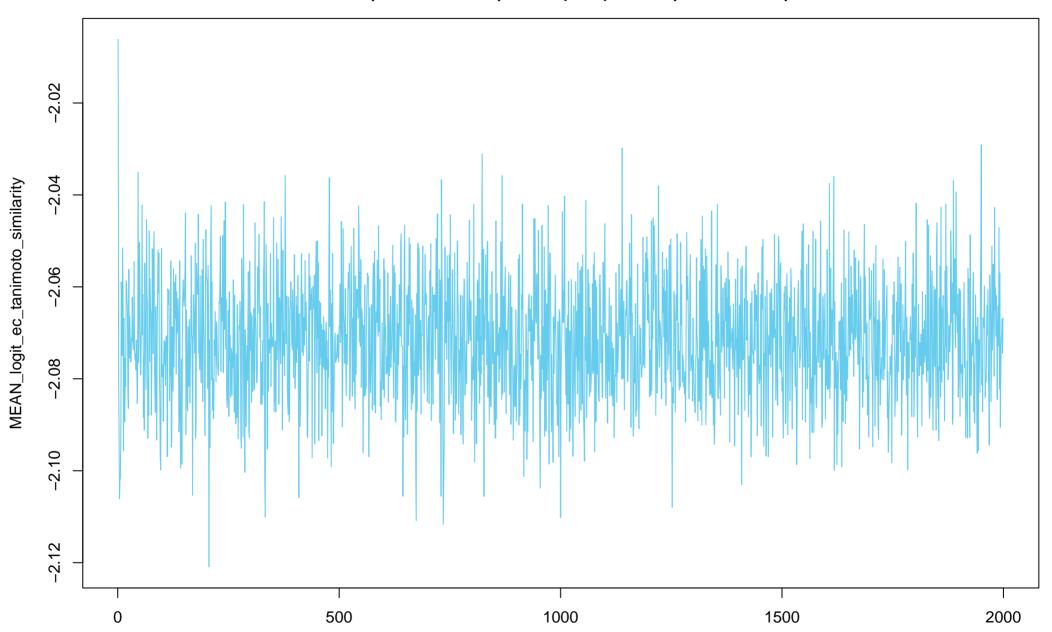
MEAN\_log\_RMSD ESS = 1510 | BMK = 0.0486 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0



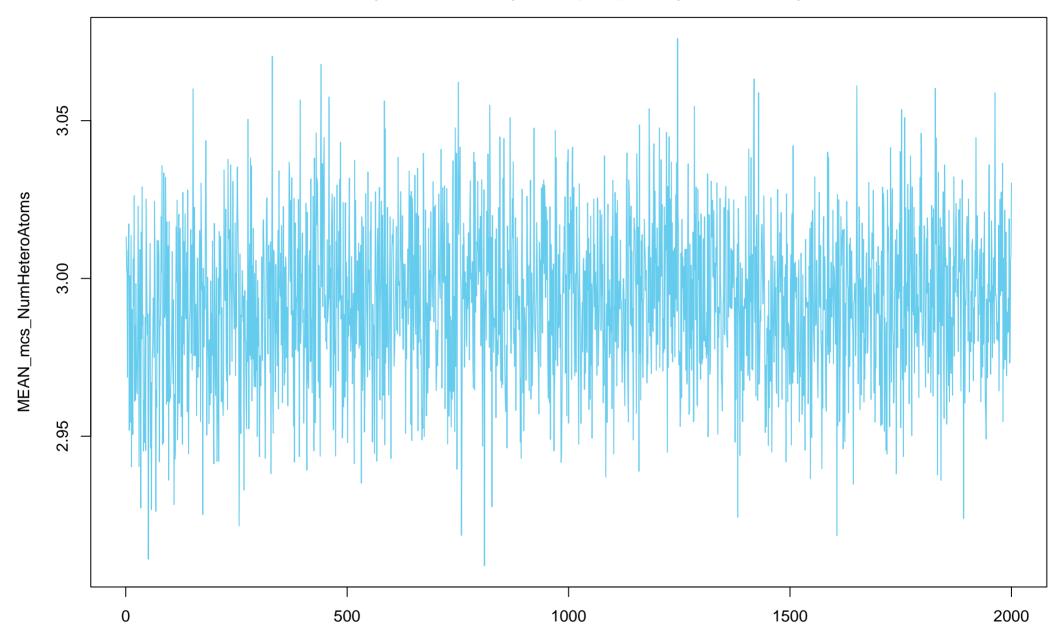
MEAN\_log\_mcs\_unbonded\_polar\_sasa ESS = 1780 | BMK = 0.0451 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0



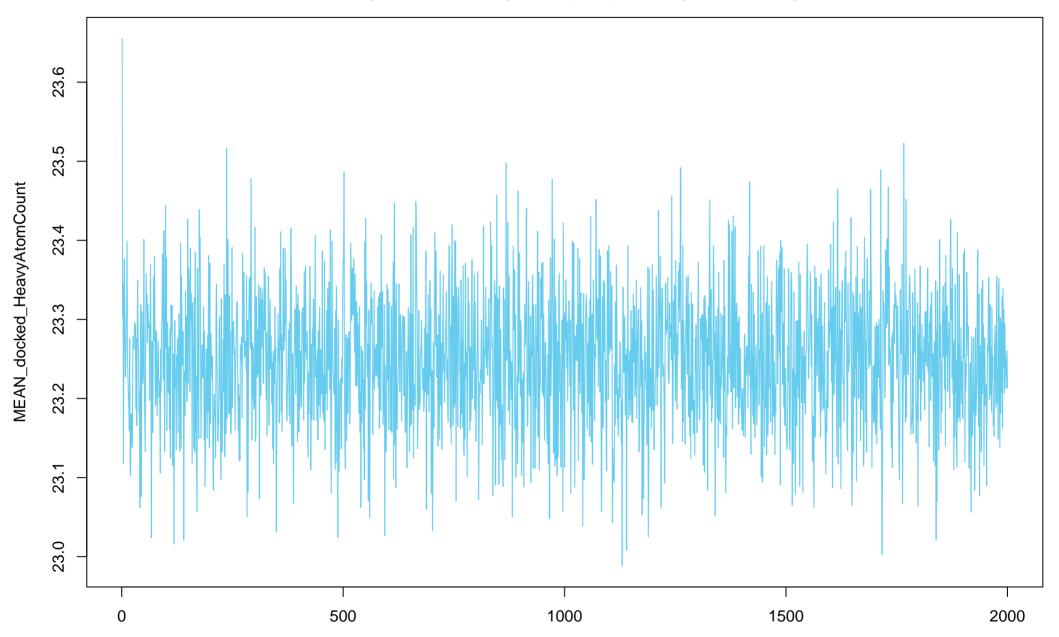
MEAN\_logit\_ec\_tanimoto\_similarity ESS = 1850 | BMK = 0.068 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0



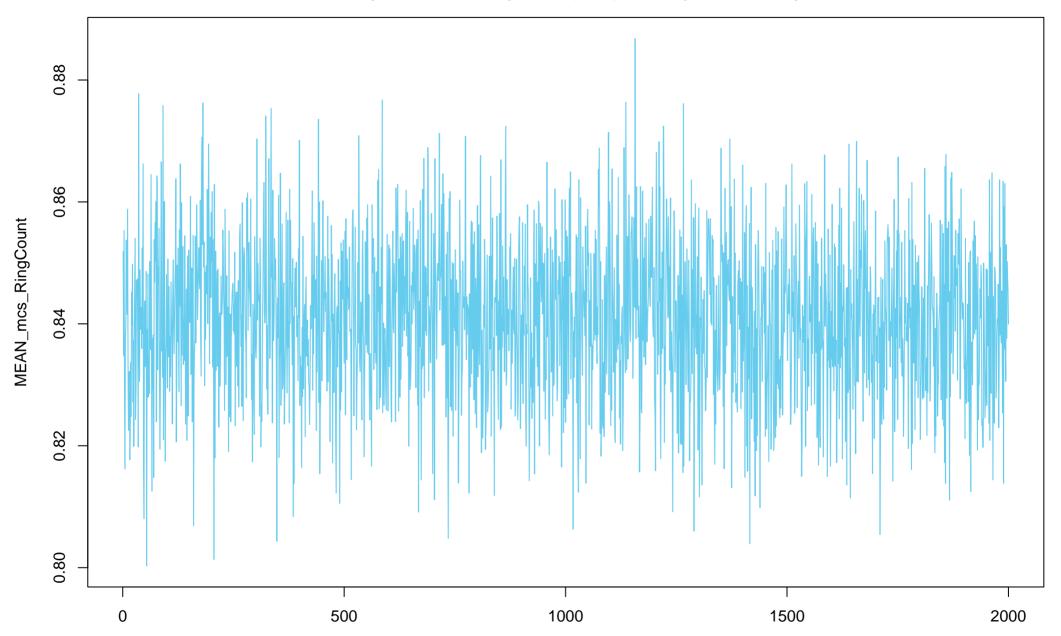
MEAN\_mcs\_NumHeteroAtoms ESS = 1270 | BMK = 0.0633 | MCSE(6.27) = 2.4 | stat: FALSE | burn: 0



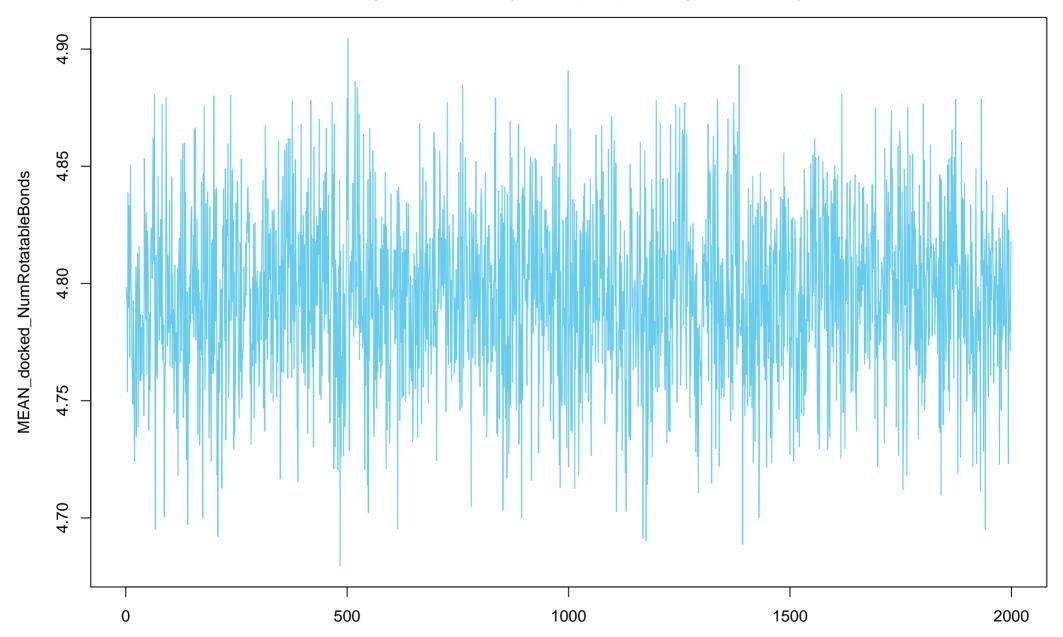
MEAN\_docked\_HeavyAtomCount ESS = 2000 | BMK = 0.0331 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0



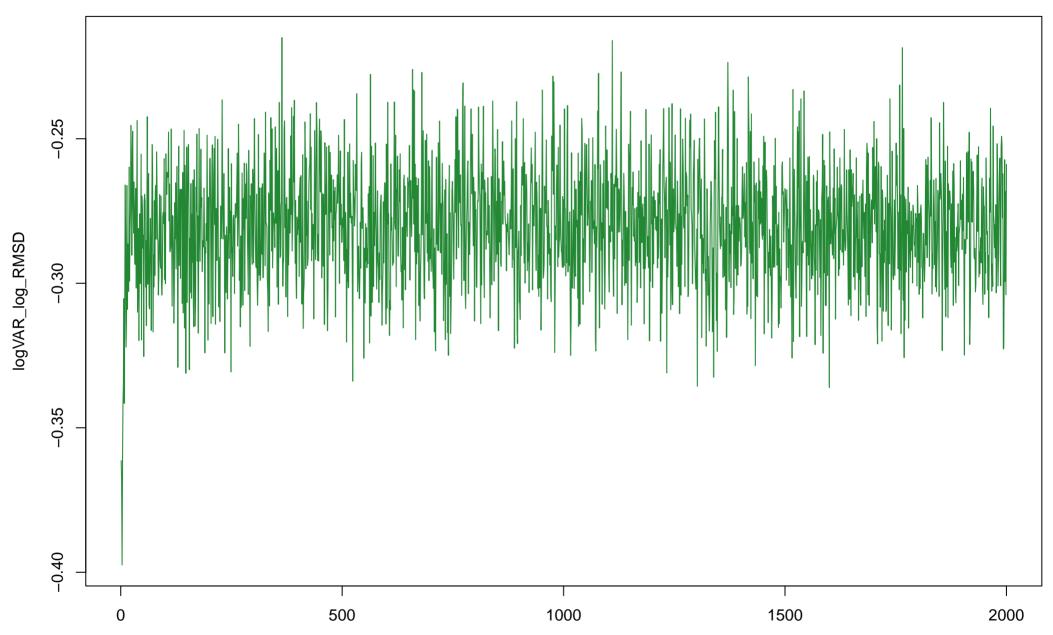
MEAN\_mcs\_RingCount ESS = 2000 | BMK = 0.0436 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0



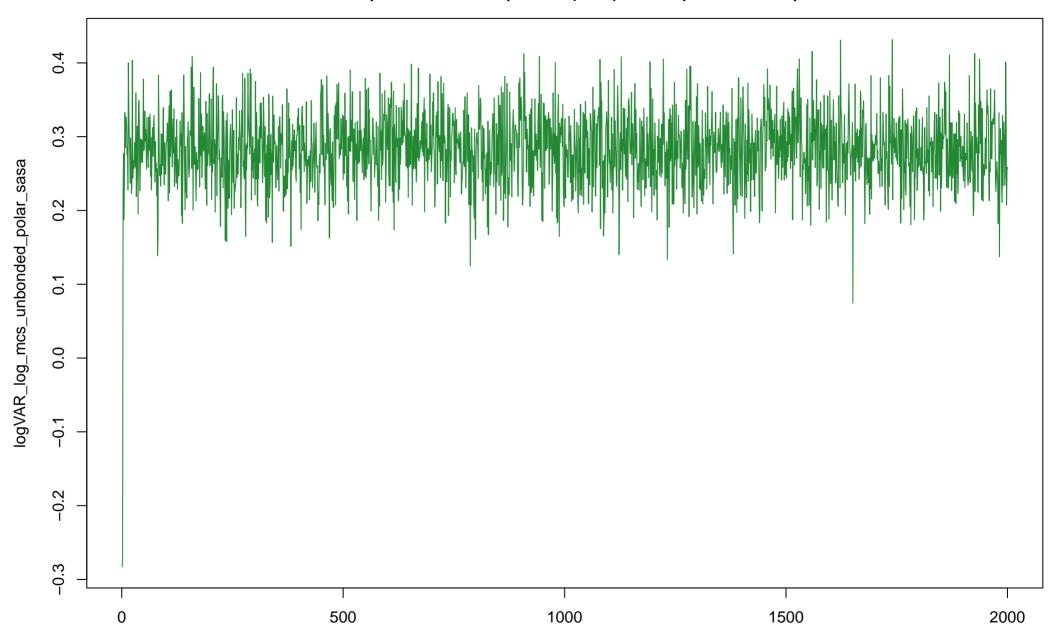
MEAN\_docked\_NumRotatableBonds ESS = 1690 | BMK = 0.0314 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0



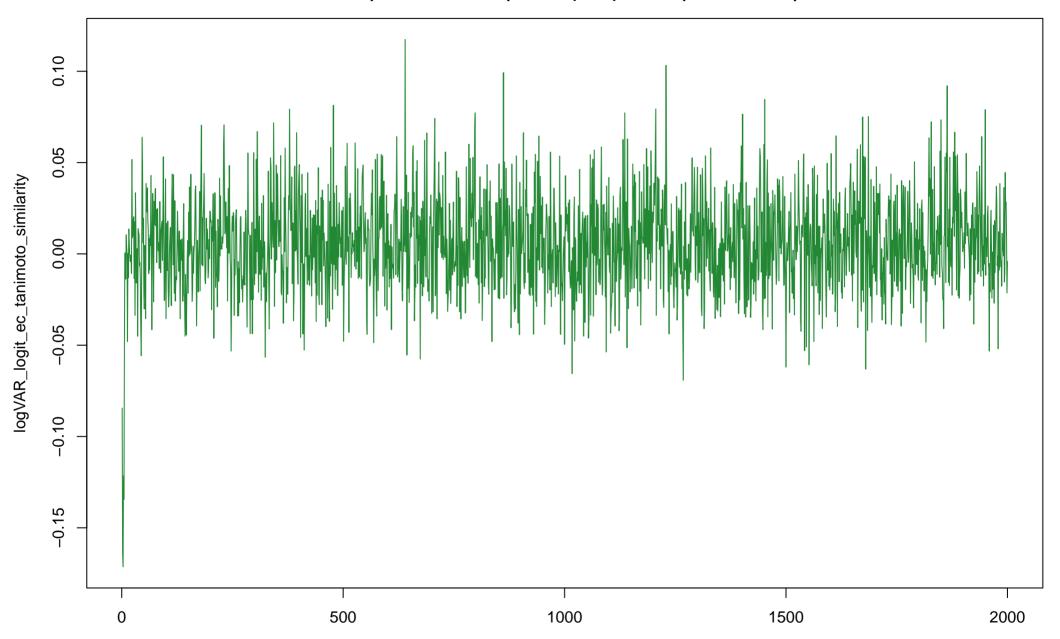
logVAR\_log\_RMSD ESS = 1550 | BMK = 0.051 | MCSE(6.27) = 2.82 | stat: FALSE | burn: 0



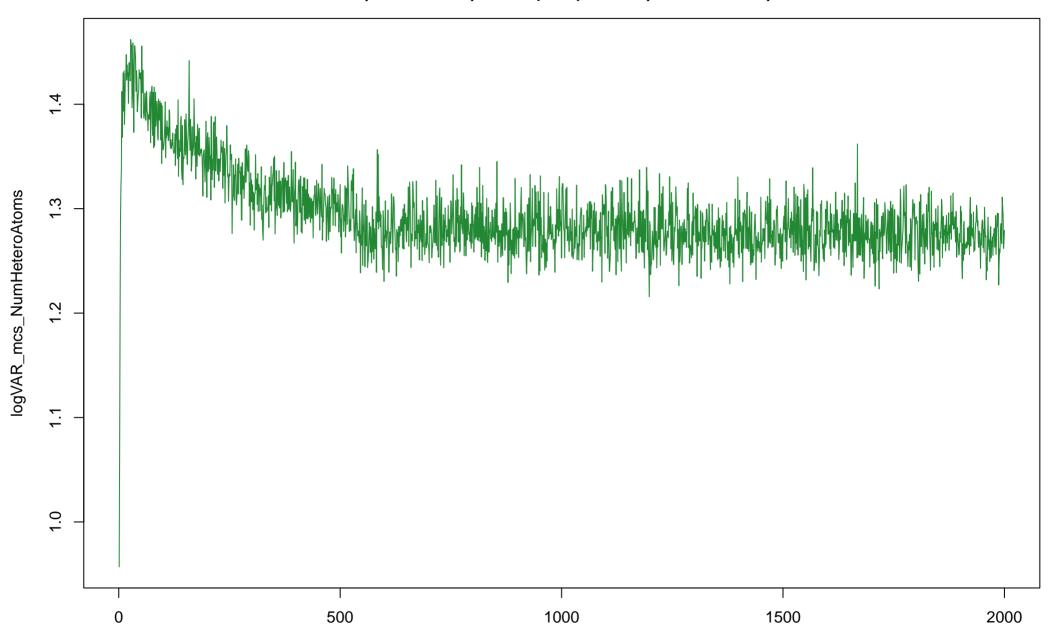
logVAR\_log\_mcs\_unbonded\_polar\_sasa ESS = 1710 | BMK = 0.0618 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0



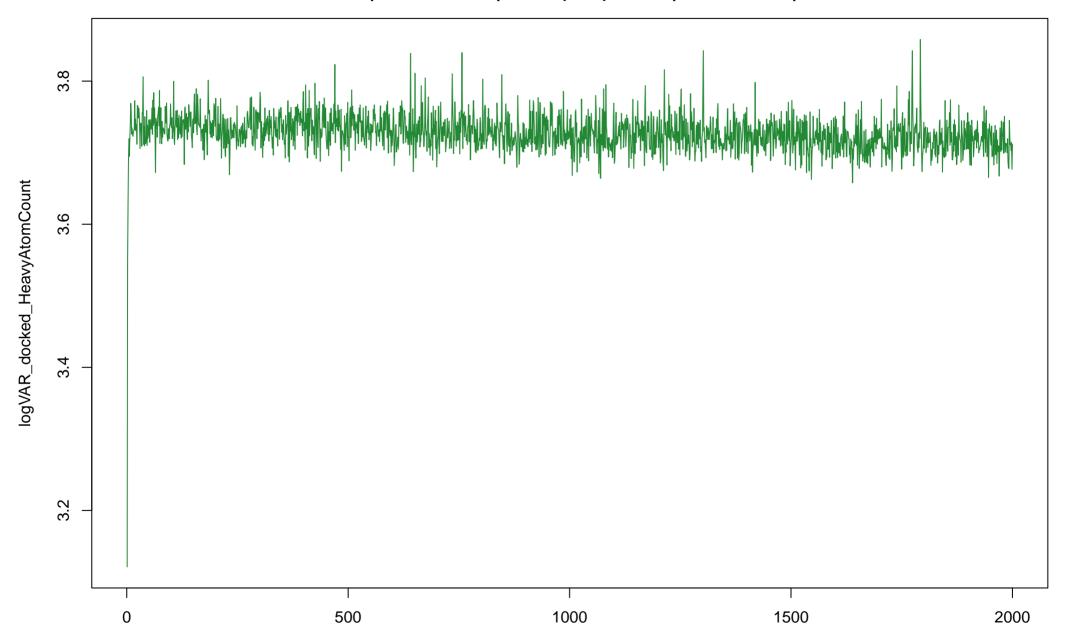
logVAR\_logit\_ec\_tanimoto\_similarity ESS = 1260 | BMK = 0.0585 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0



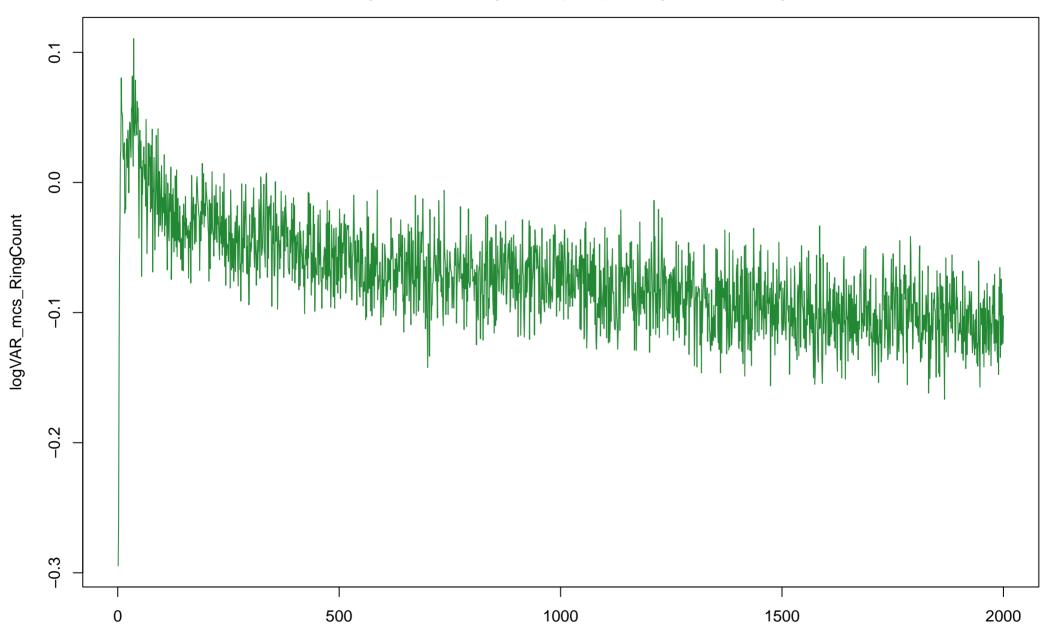
logVAR\_mcs\_NumHeteroAtoms ESS = 10.4 | BMK = 0.4 | MCSE(6.27) = 9.73 | stat: FALSE | burn: 200



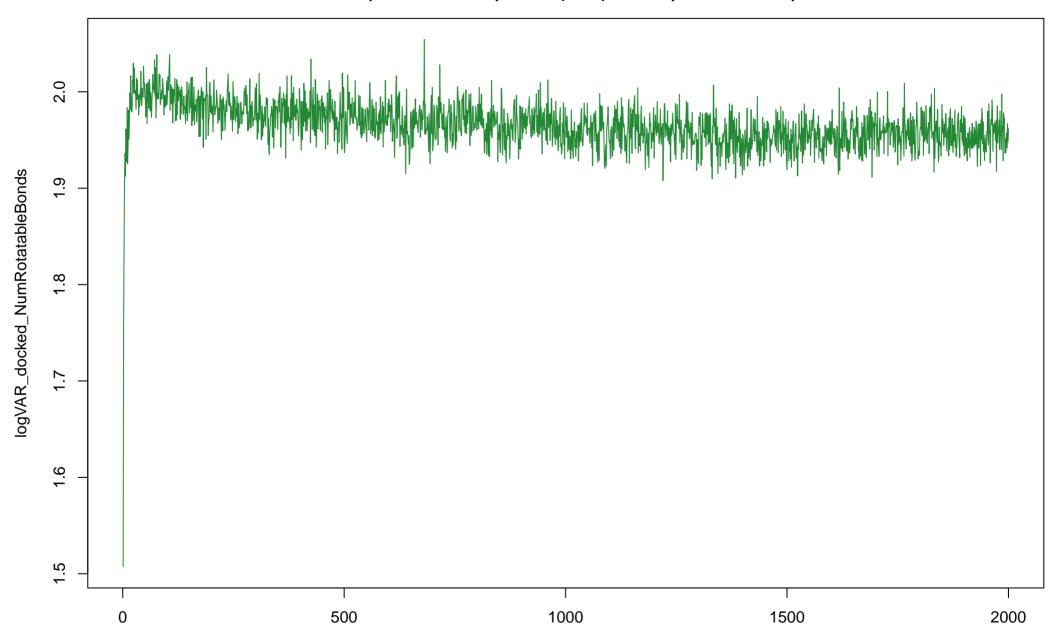
logVAR\_docked\_HeavyAtomCount ESS = 481 | BMK = 0.209 | MCSE(6.27) = 3.56 | stat: FALSE | burn: 0



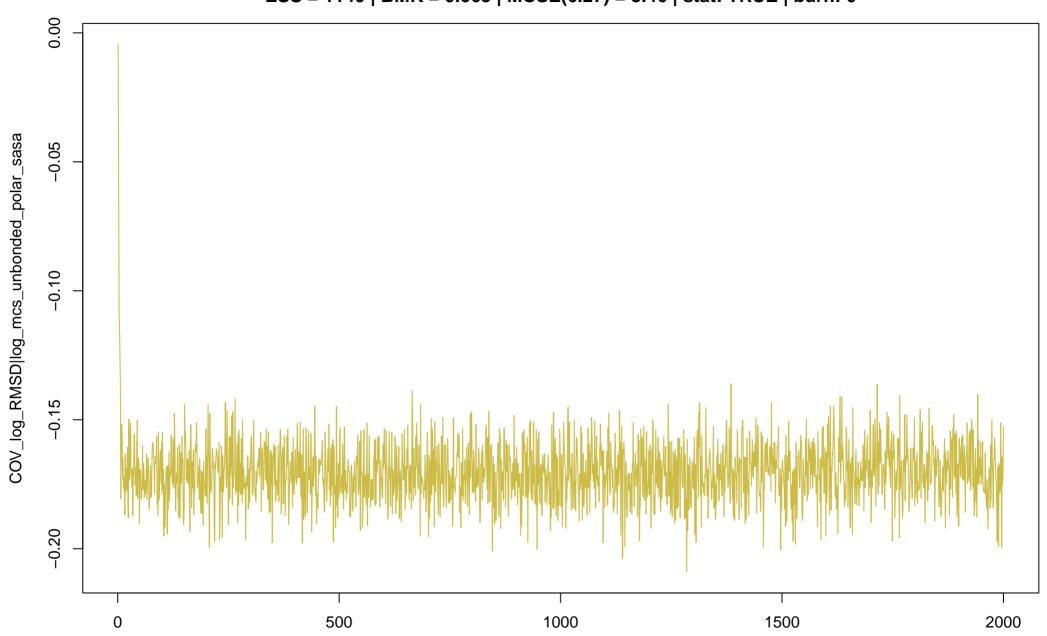
logVAR\_mcs\_RingCount ESS = 10.3 | BMK = 0.507 | MCSE(6.27) = 9.7 | stat: FALSE | burn: 0



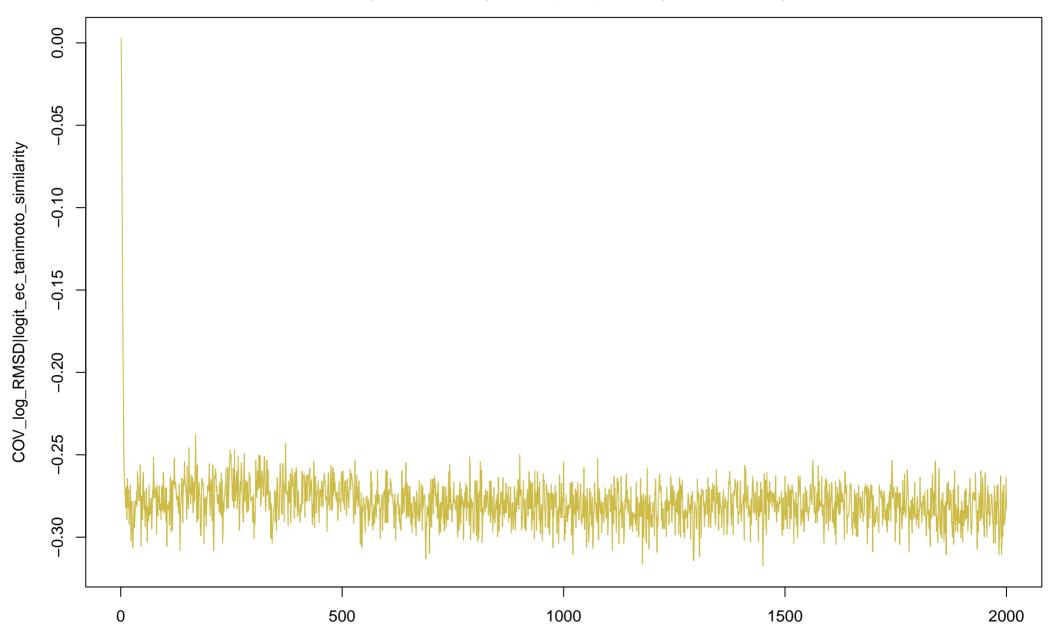
logVAR\_docked\_NumRotatableBonds ESS = 70.6 | BMK = 0.377 | MCSE(6.27) = 5.95 | stat: FALSE | burn: 0



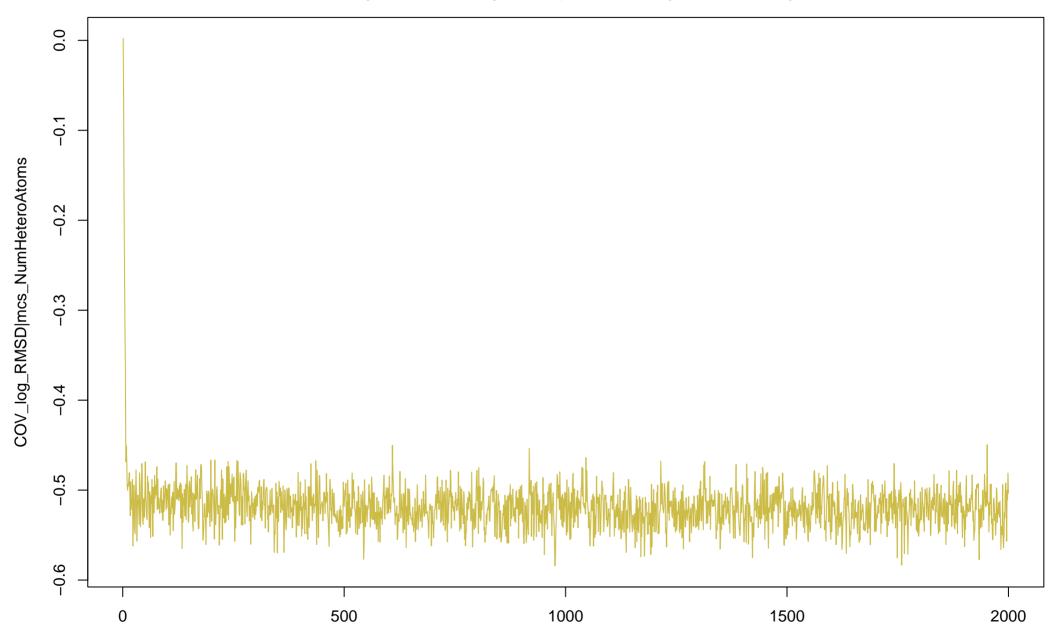
COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa ESS = 1140 | BMK = 0.065 | MCSE(6.27) = 3.46 | stat: TRUE | burn: 0



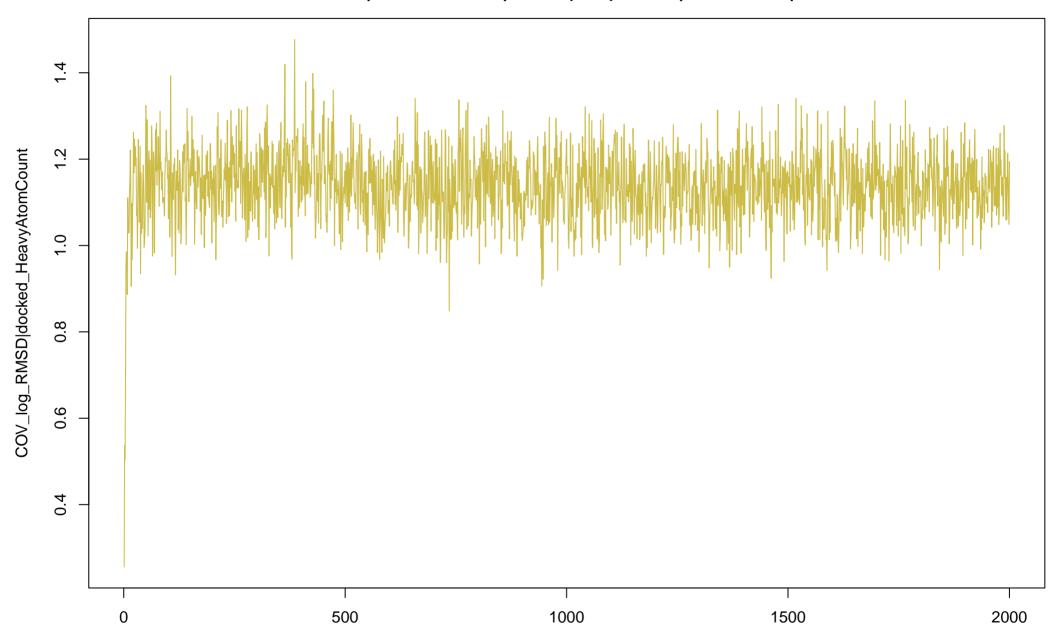
COV\_log\_RMSD|logit\_ec\_tanimoto\_similarity ESS = 500 | BMK = 0.16 | MCSE(6.27) = 6.07 | stat: FALSE | burn: 0



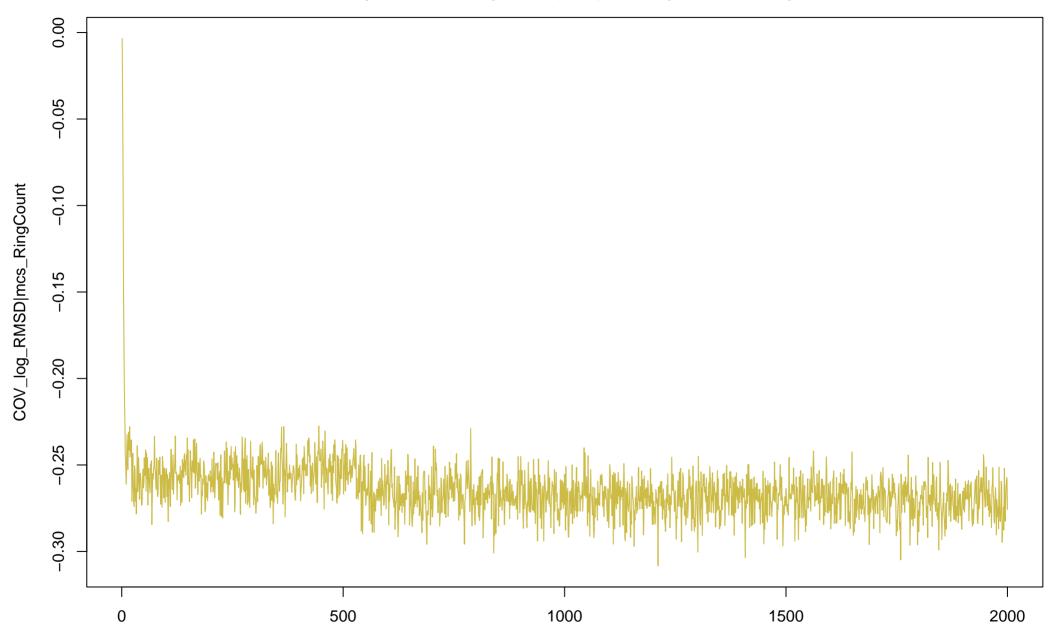
COV\_log\_RMSD|mcs\_NumHeteroAtoms ESS = 490 | BMK = 0.103 | MCSE(6.27) = 5.93 | stat: FALSE | burn: 0



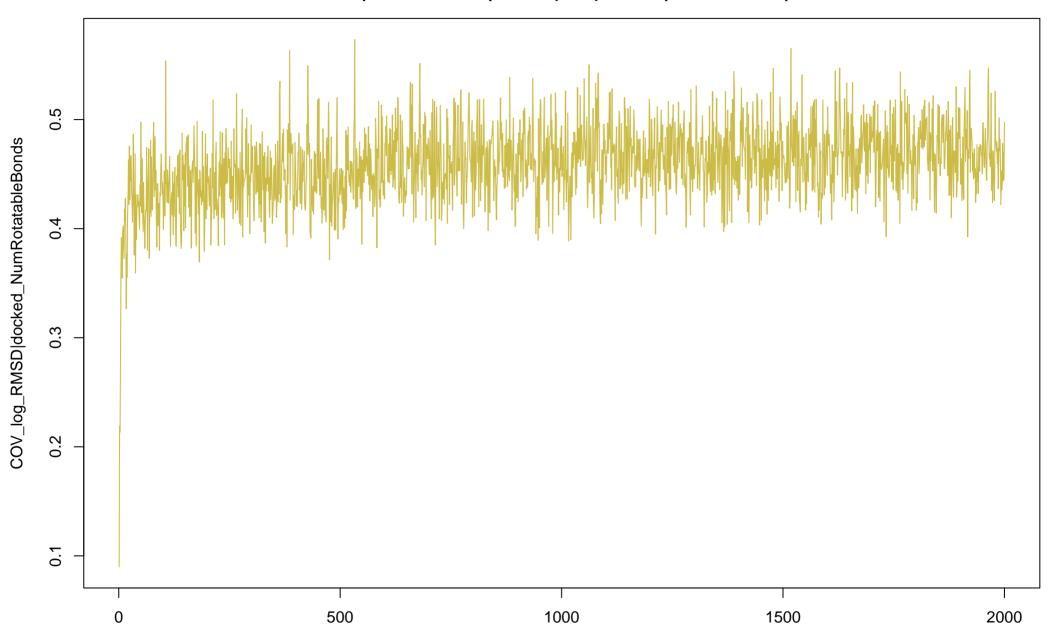
COV\_log\_RMSD|docked\_HeavyAtomCount ESS = 832 | BMK = 0.0945 | MCSE(6.27) = 3.87 | stat: TRUE | burn: 0

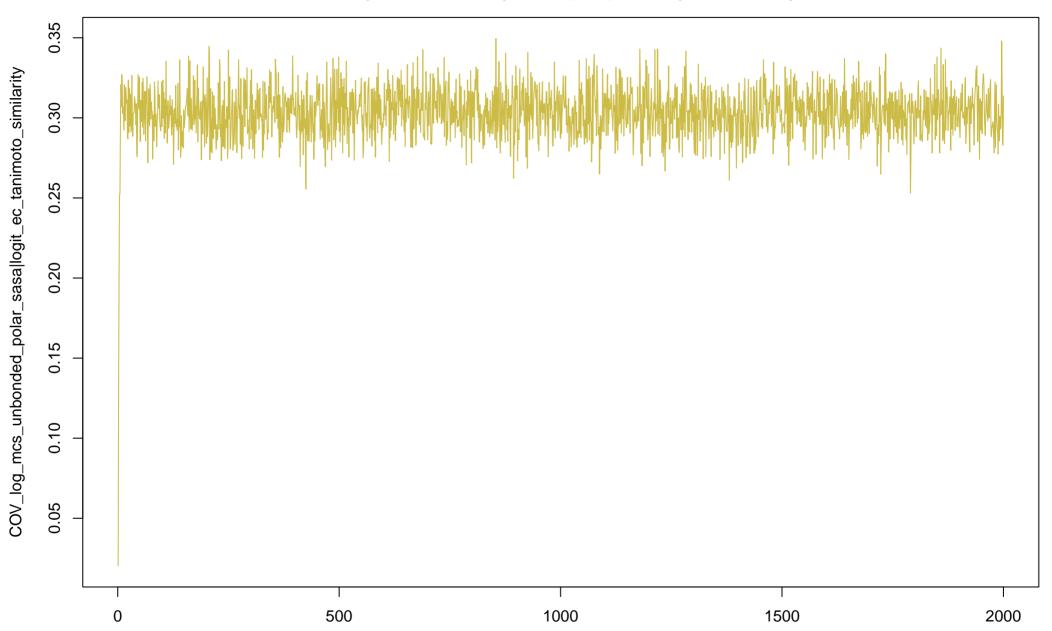


COV\_log\_RMSD|mcs\_RingCount ESS = 140 | BMK = 0.298 | MCSE(6.27) = 7.03 | stat: FALSE | burn: 0

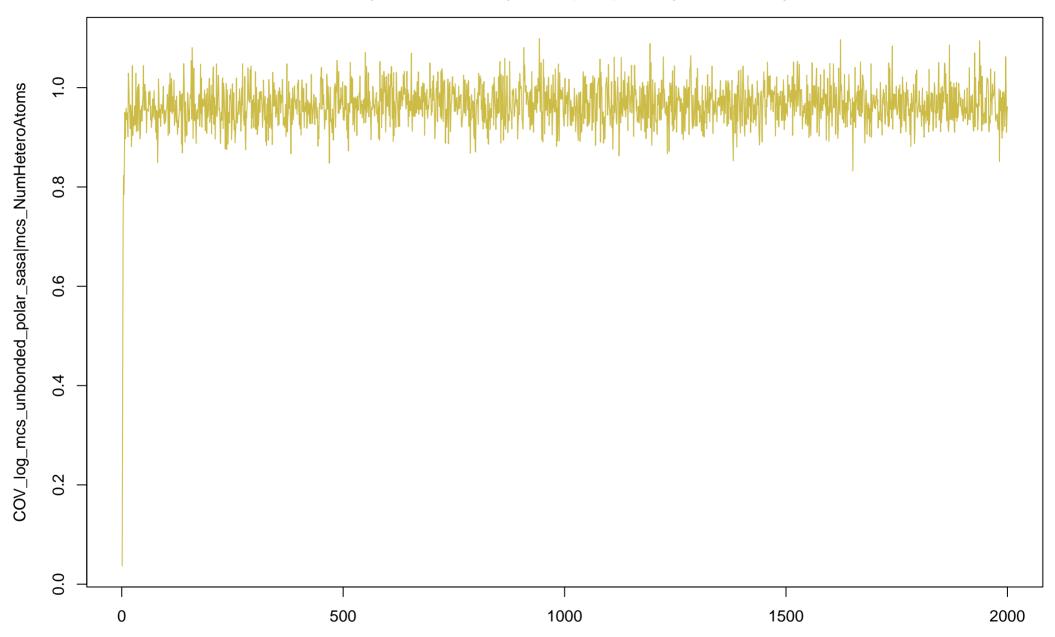


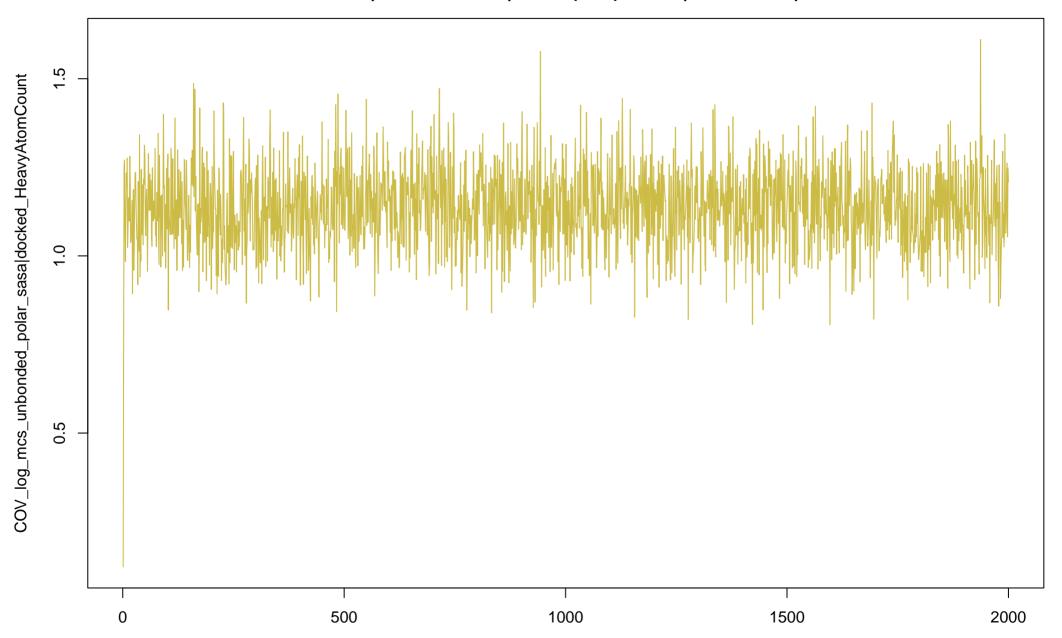
COV\_log\_RMSD|docked\_NumRotatableBonds ESS = 133 | BMK = 0.213 | MCSE(6.27) = 5.76 | stat: FALSE | burn: 0



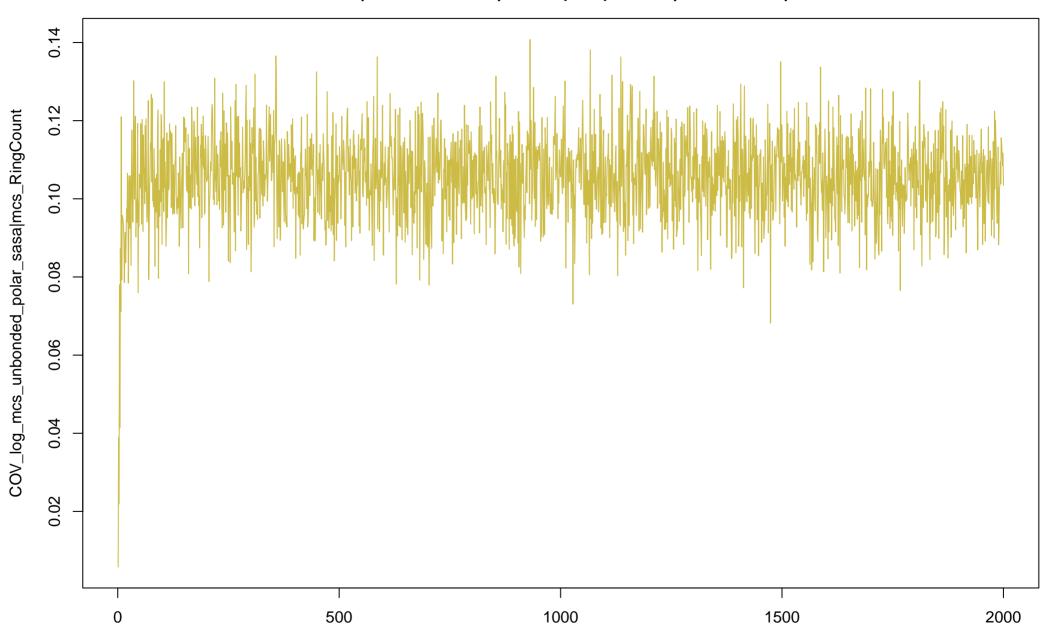


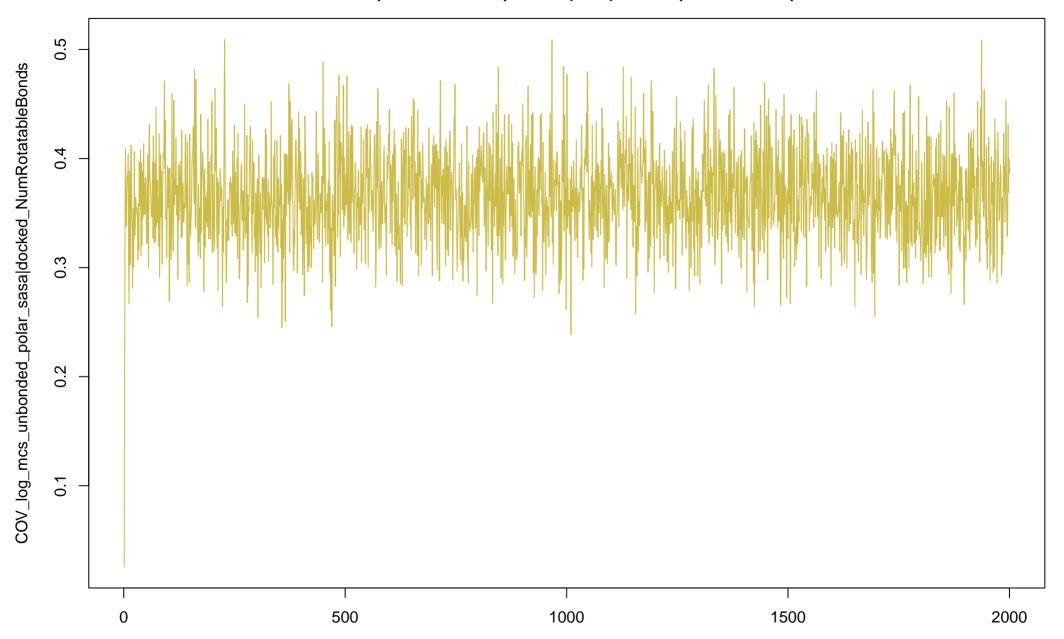
COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms ESS = 945 | BMK = 0.0621 | MCSE(6.27) = 3.9 | stat: TRUE | burn: 0



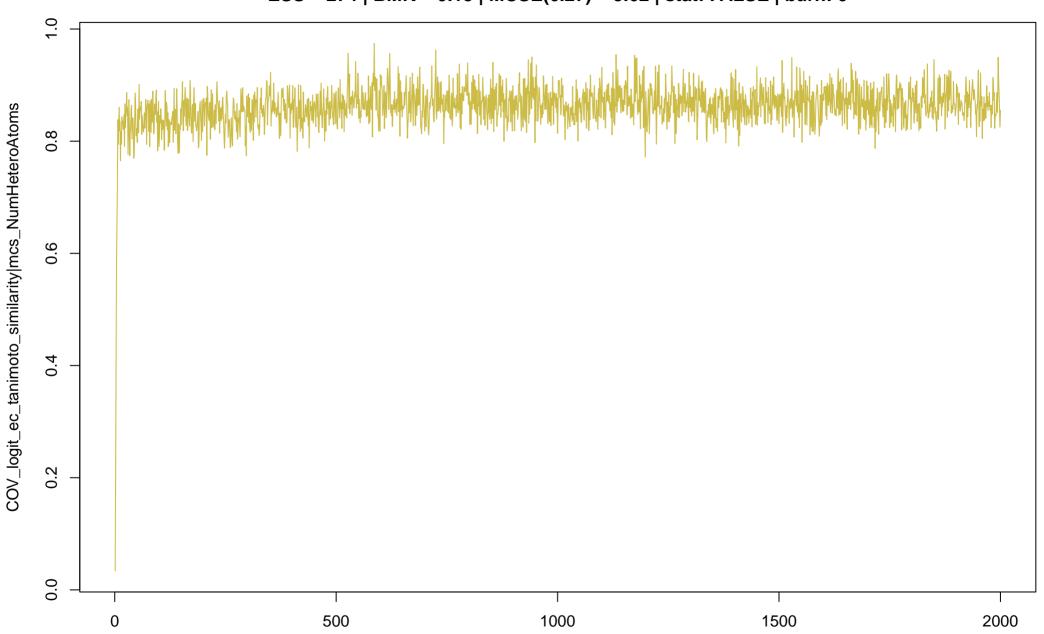


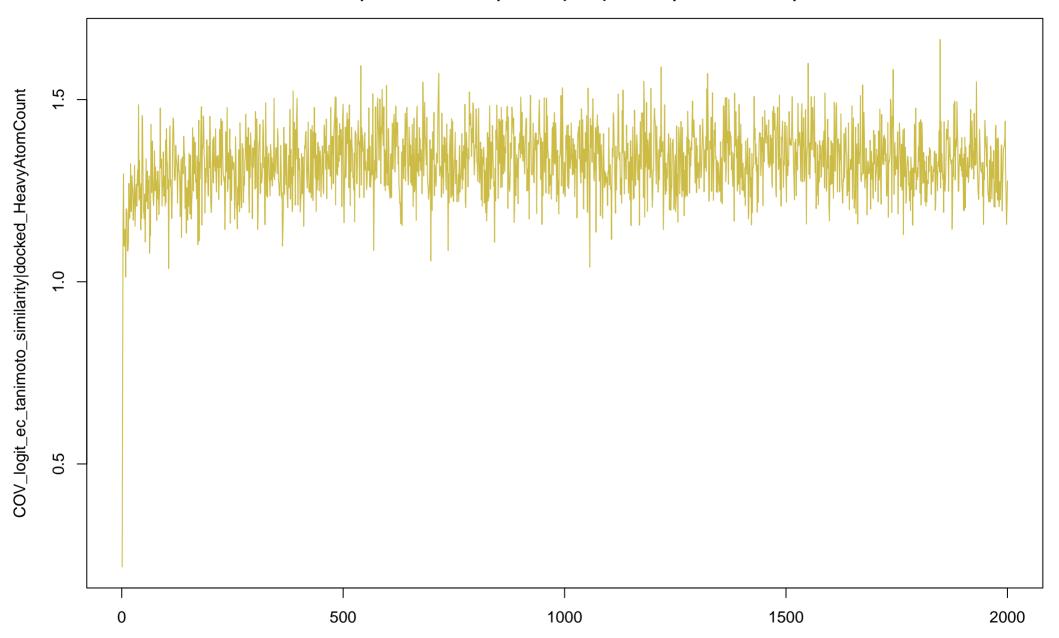
COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_RingCount ESS = 933 | BMK = 0.0562 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0



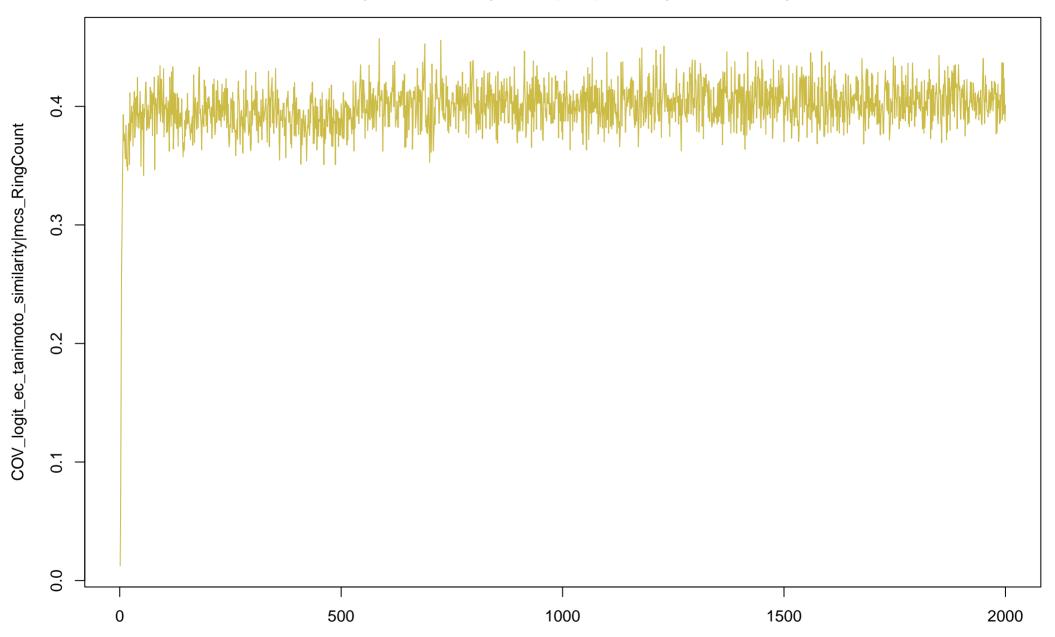


COV\_logit\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms ESS = 274 | BMK = 0.13 | MCSE(6.27) = 5.62 | stat: FALSE | burn: 0

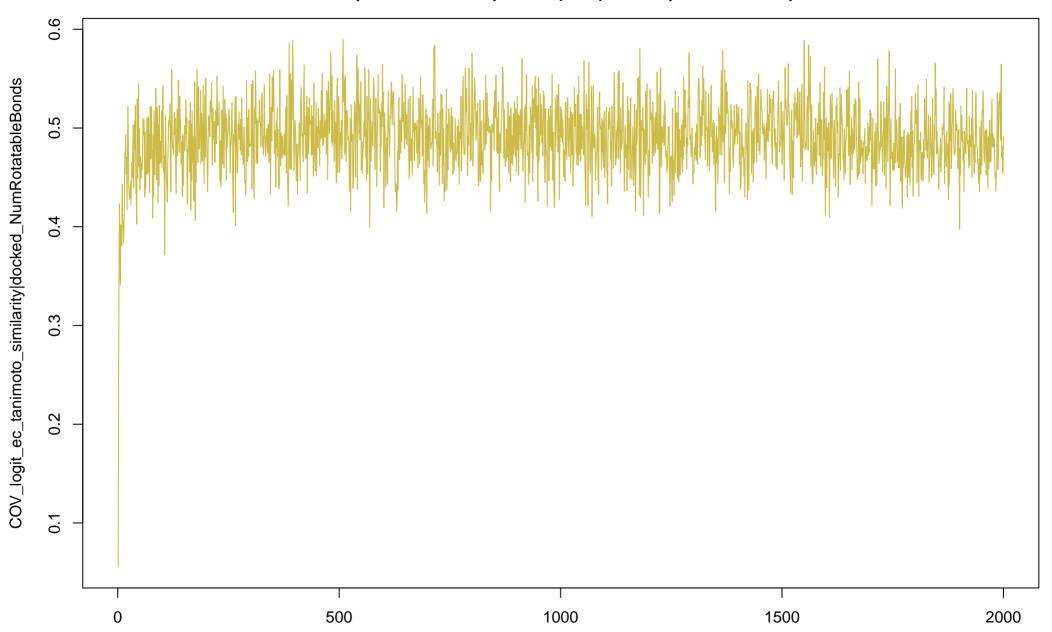


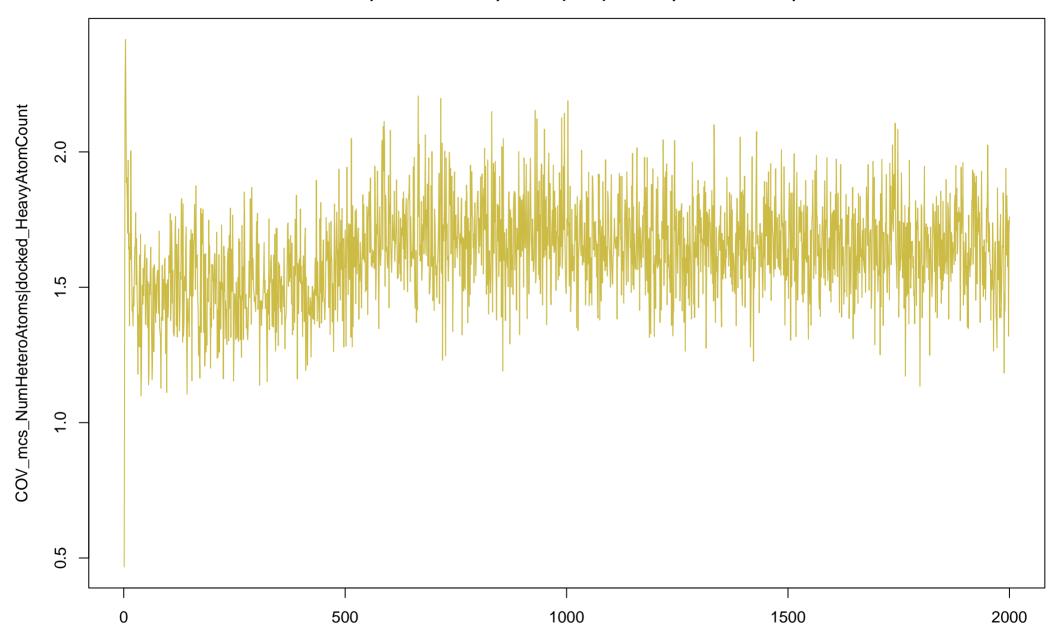


COV\_logit\_ec\_tanimoto\_similarity|mcs\_RingCount ESS = 246 | BMK = 0.181 | MCSE(6.27) = 5.61 | stat: FALSE | burn: 0

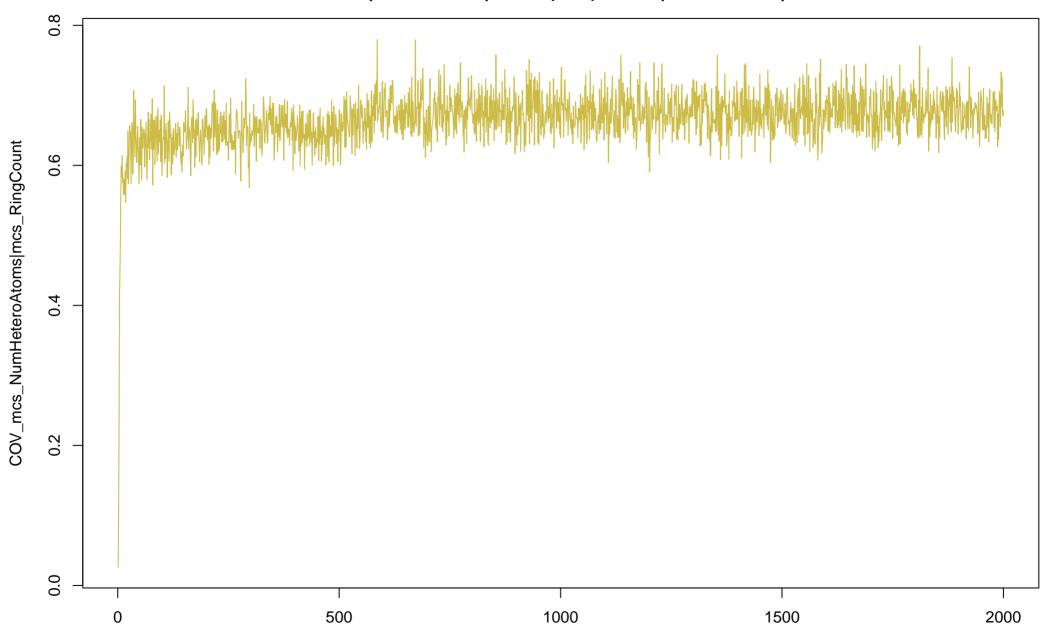


COV\_logit\_ec\_tanimoto\_similarity|docked\_NumRotatableBonds ESS = 683 | BMK = 0.0946 | MCSE(6.27) = 3.55 | stat: FALSE | burn: 0

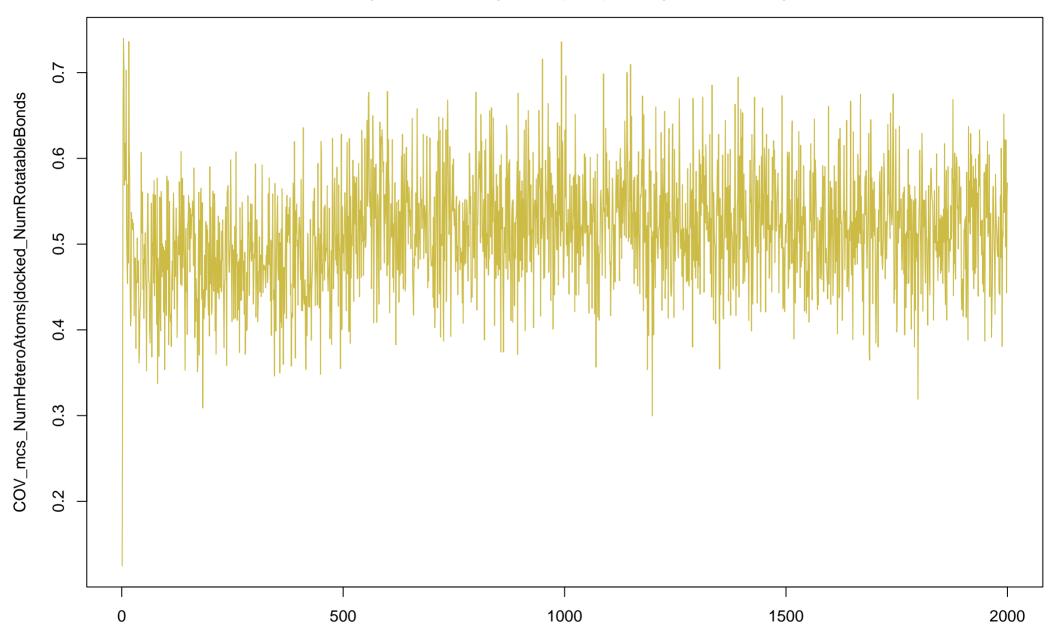




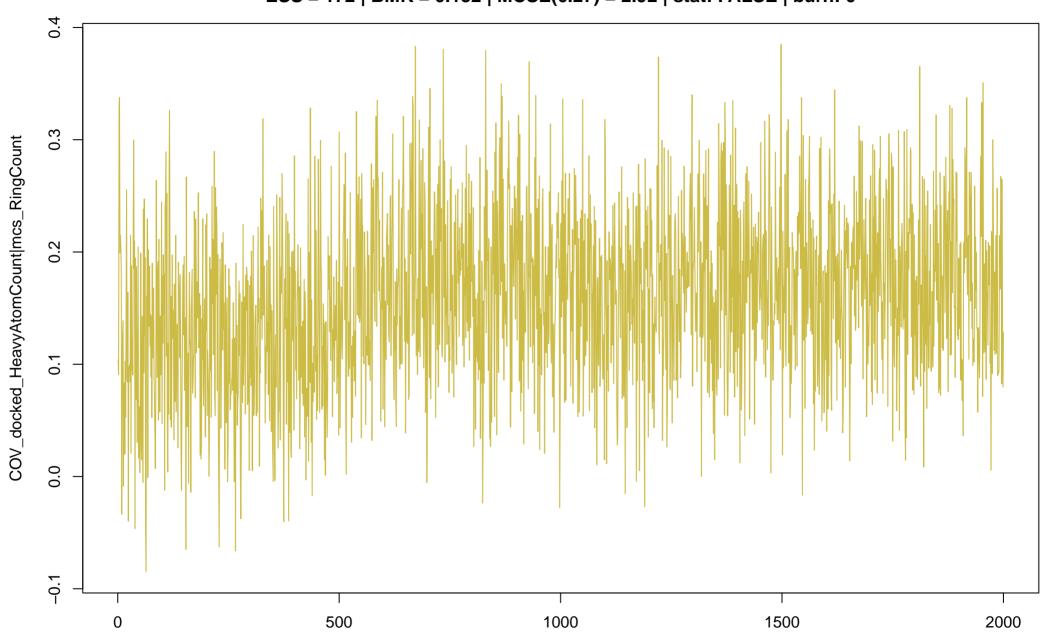
COV\_mcs\_NumHeteroAtoms|mcs\_RingCount ESS = 99.3 | BMK = 0.23 | MCSE(6.27) = 6.66 | stat: FALSE | burn: 0



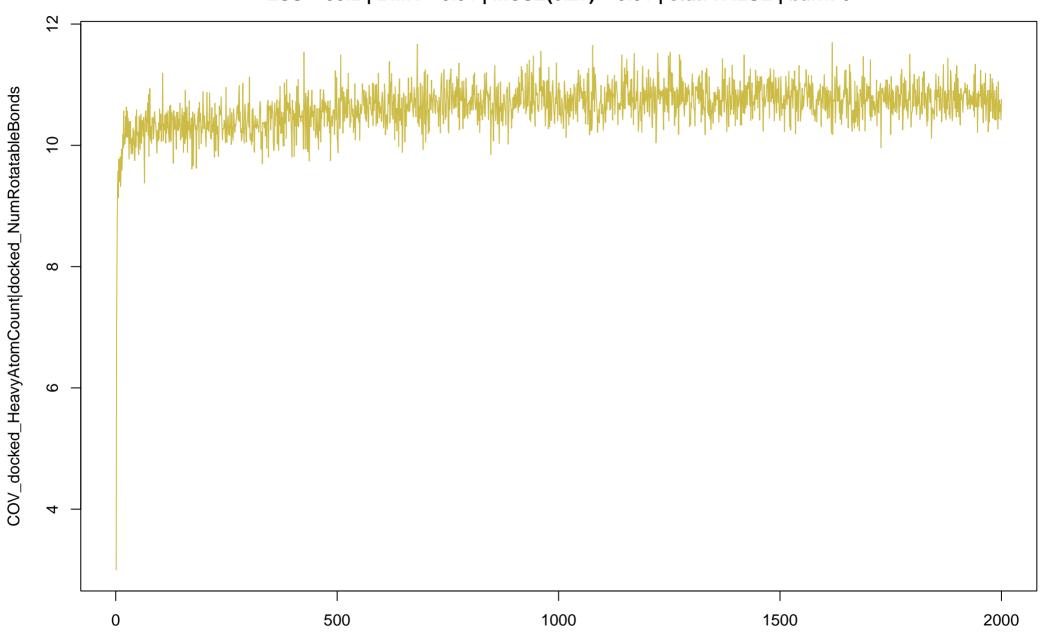
## COV\_mcs\_NumHeteroAtoms|docked\_NumRotatableBonds ESS = 409 | BMK = 0.111 | MCSE(6.27) = 3.2 | stat: FALSE | burn: 0



COV\_docked\_HeavyAtomCount|mcs\_RingCount ESS = 172 | BMK = 0.132 | MCSE(6.27) = 2.92 | stat: FALSE | burn: 0



## COV\_docked\_HeavyAtomCount|docked\_NumRotatableBonds ESS = 38.2 | BMK = 0.31 | MCSE(6.27) = 5.31 | stat: FALSE | burn: 0



COV\_mcs\_RingCount|docked\_NumRotatableBonds ESS = 1620 | BMK = 0.0439 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0

