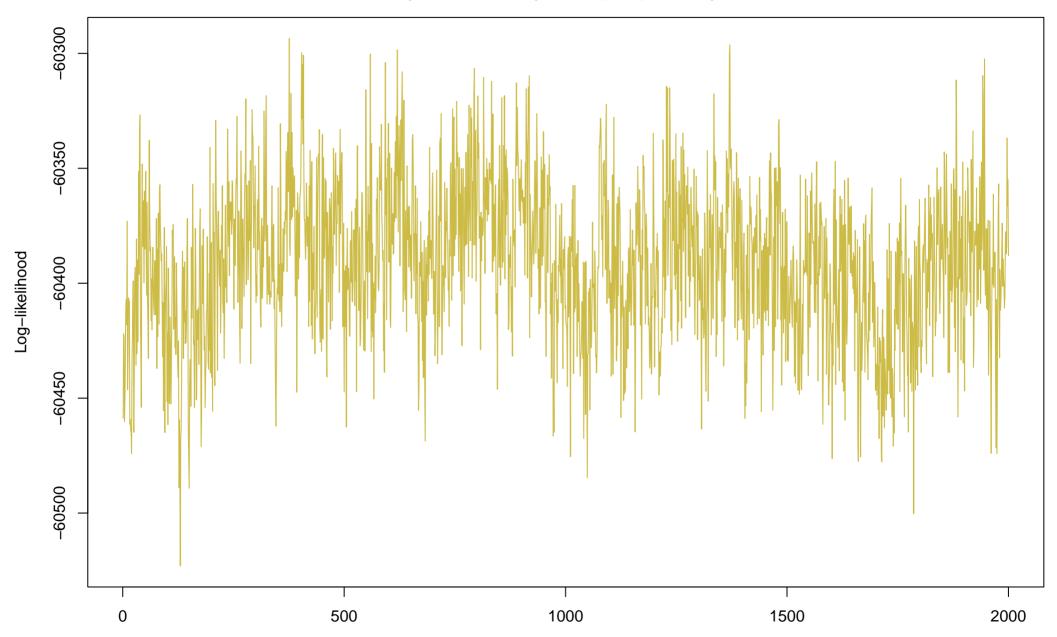
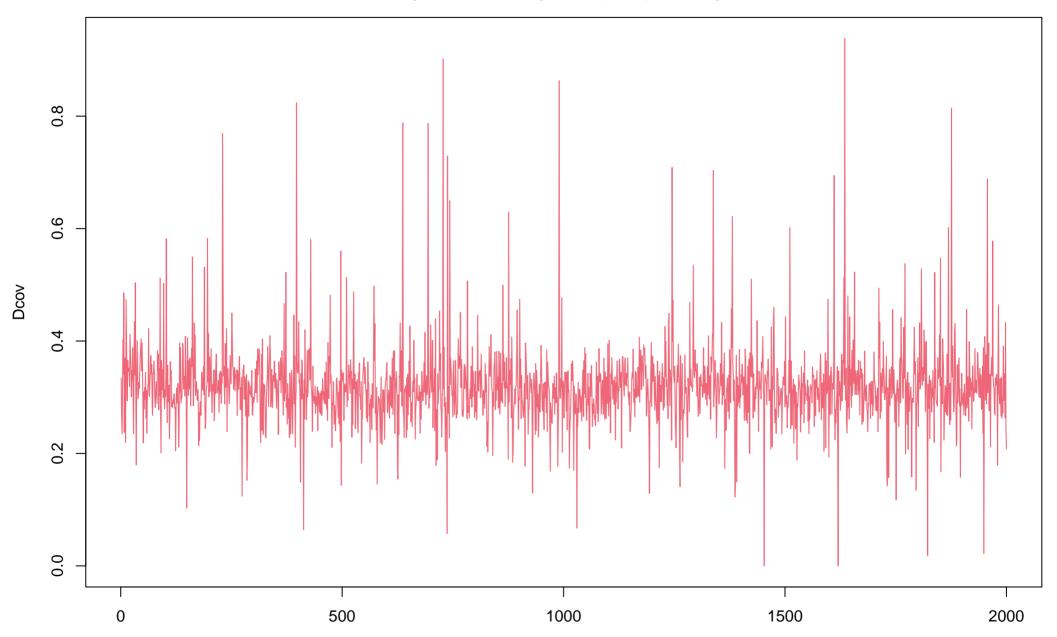


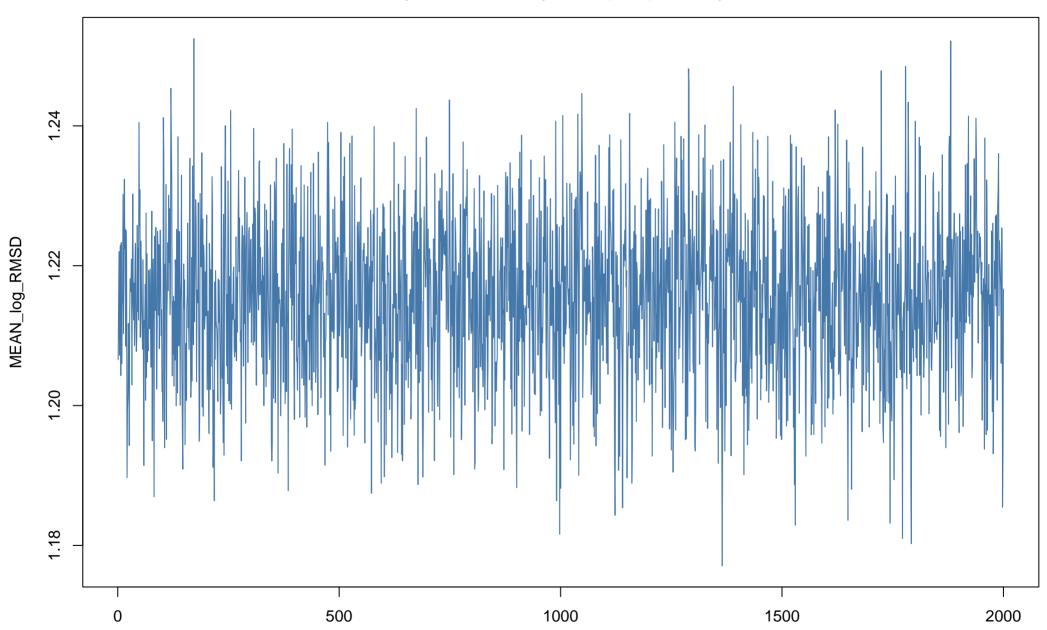
Log-likelihood ESS = 95.2 | BMK = 0.133 | MCSE(6.27) = 6.84 | stat: FALSE



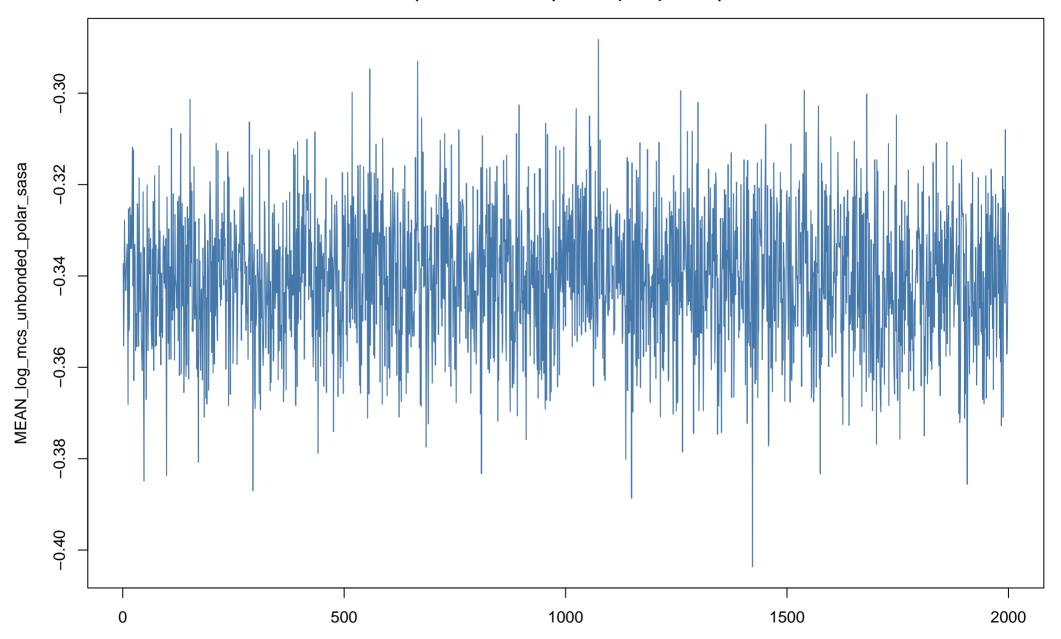
Dcov ESS = 1580 | BMK = 0.095 | MCSE(6.27) = 2.74 | stat: TRUE



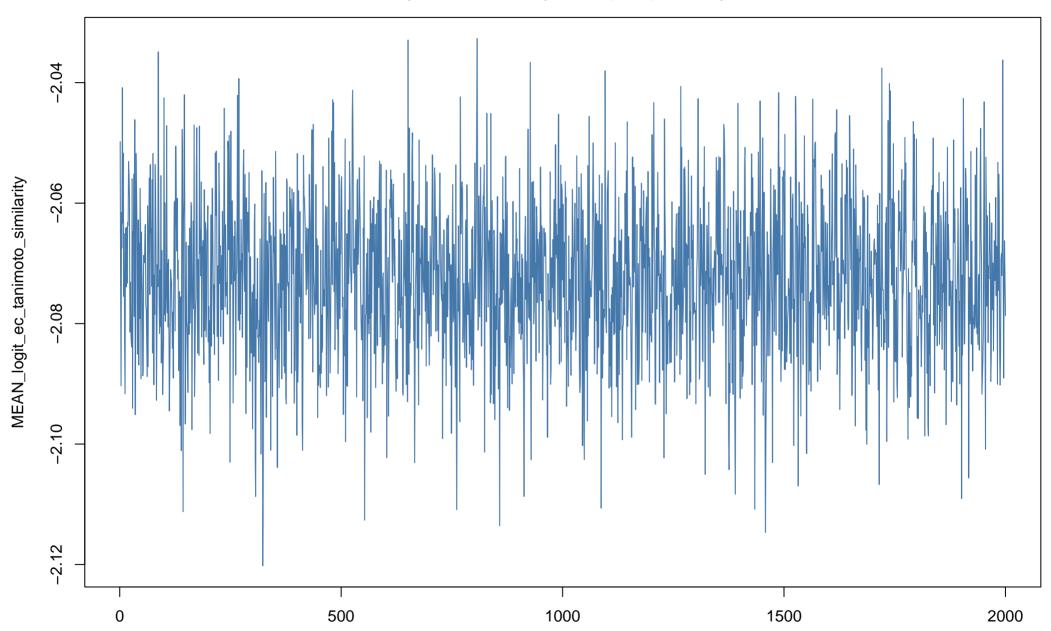
MEAN\_log\_RMSD ESS = 1750 | BMK = 0.0461 | MCSE(6.27) = 2.48 | stat: TRUE



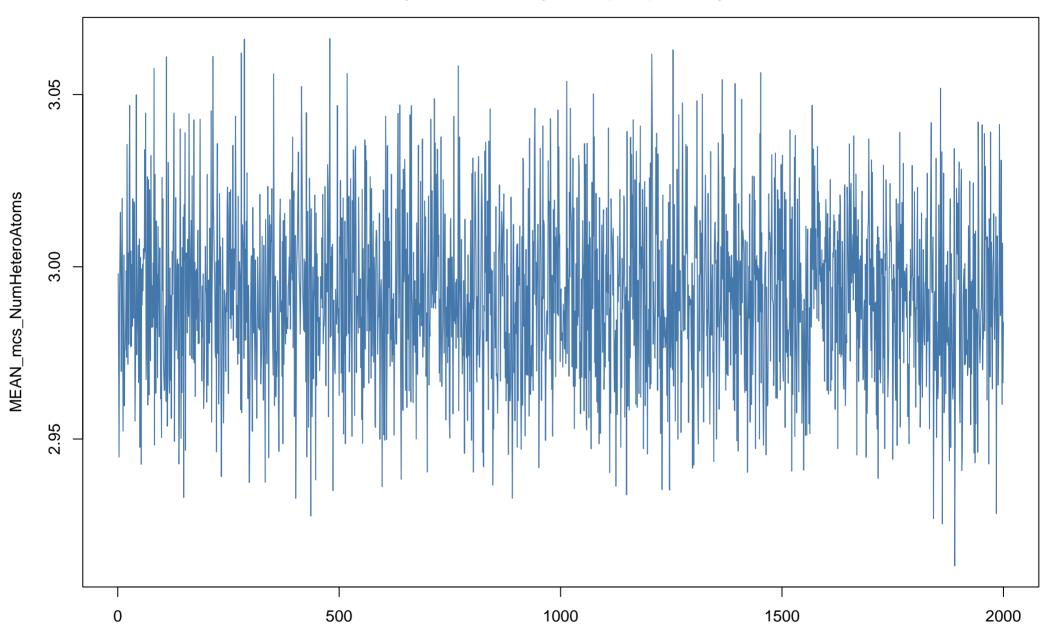
MEAN\_log\_mcs\_unbonded\_polar\_sasa ESS = 2000 | BMK = 0.0424 | MCSE(6.27) = 2.2 | stat: TRUE



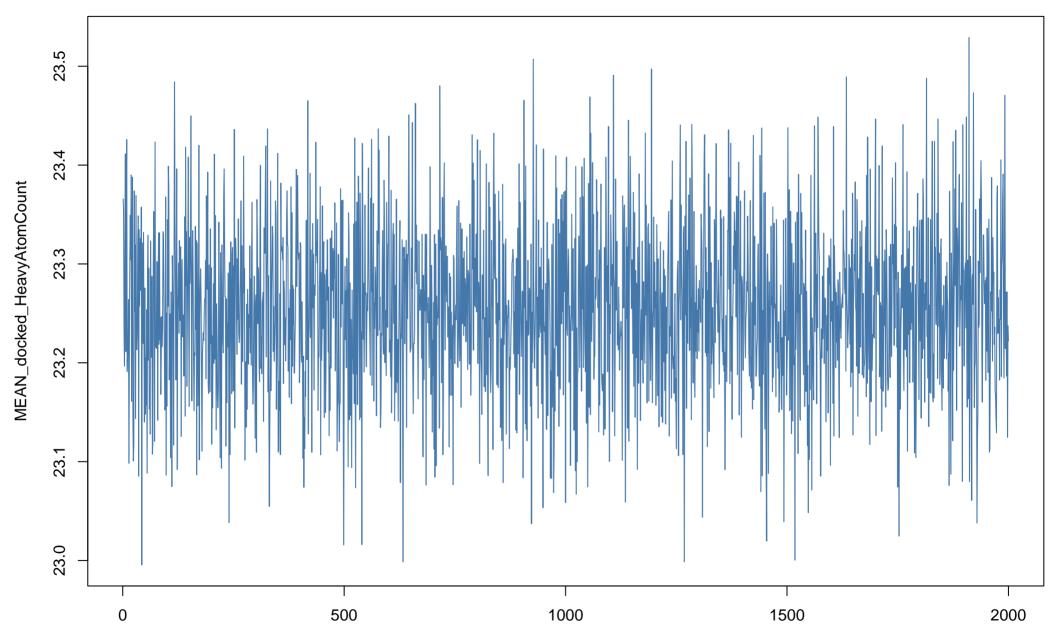
MEAN\_logit\_ec\_tanimoto\_similarity ESS = 1610 | BMK = 0.0287 | MCSE(6.27) = 2.68 | stat: TRUE



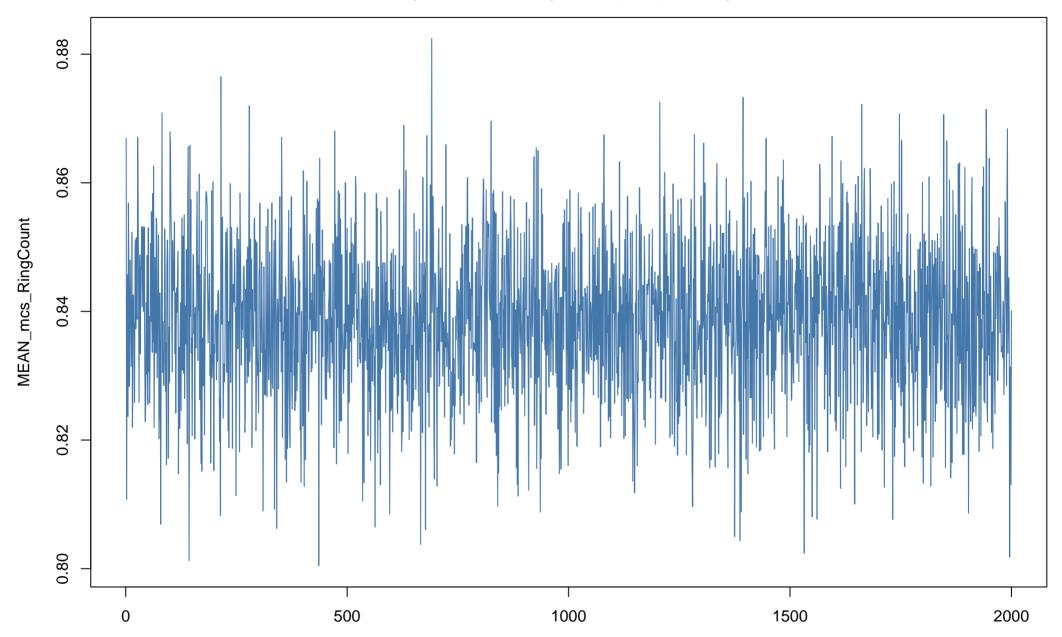
MEAN\_mcs\_NumHeteroAtoms ESS = 2000 | BMK = 0.0372 | MCSE(6.27) = 2.18 | stat: TRUE



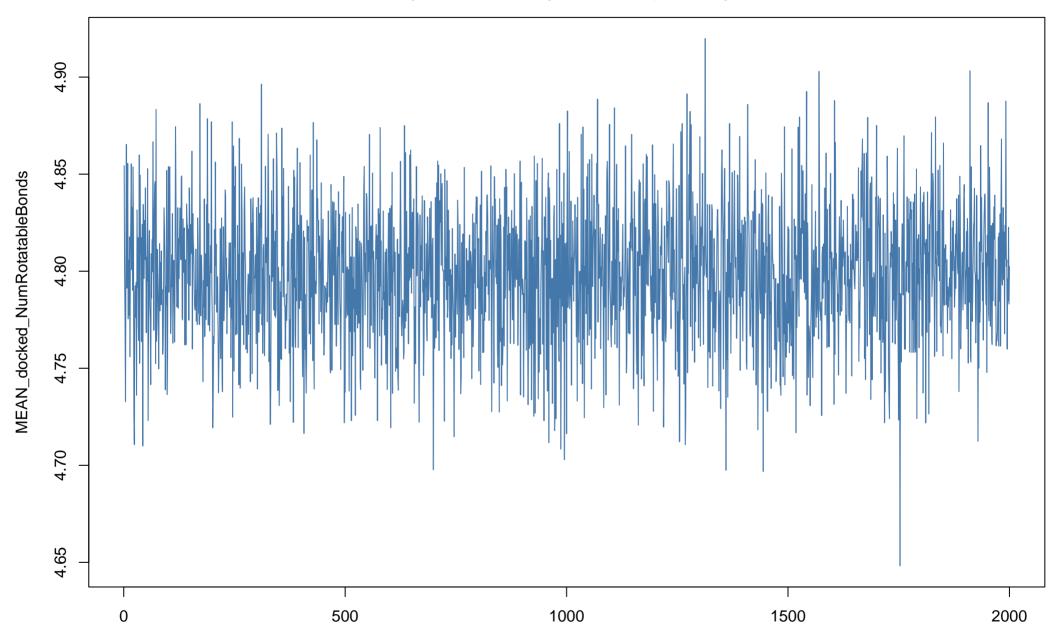
MEAN\_docked\_HeavyAtomCount ESS = 2000 | BMK = 0.0439 | MCSE(6.27) = 2.14 | stat: TRUE



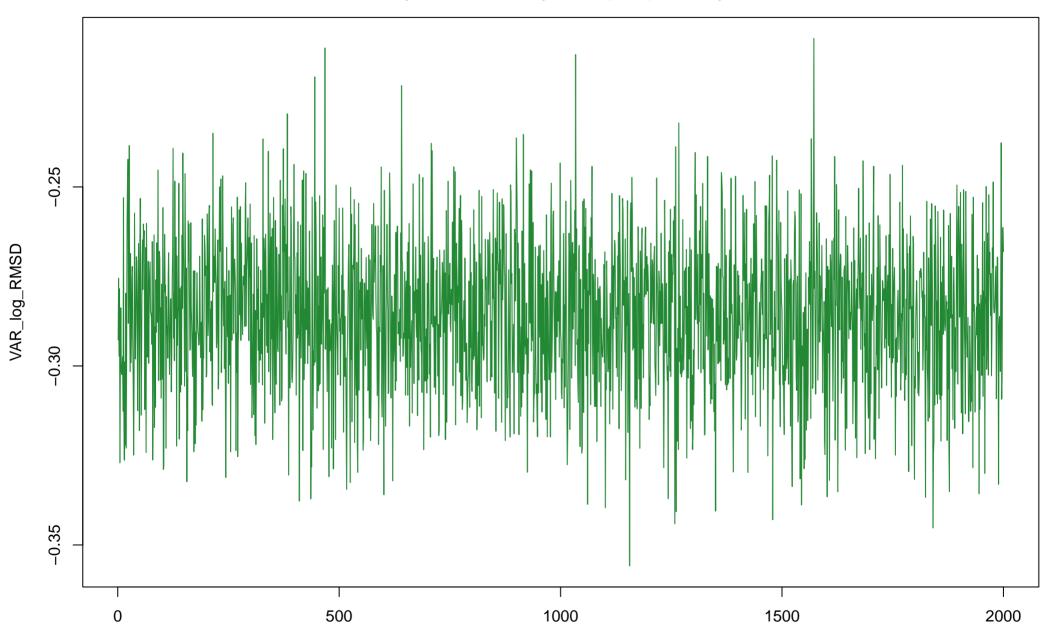
MEAN\_mcs\_RingCount ESS = 2000 | BMK = 0.0358 | MCSE(6.27) = 2.15 | stat: TRUE



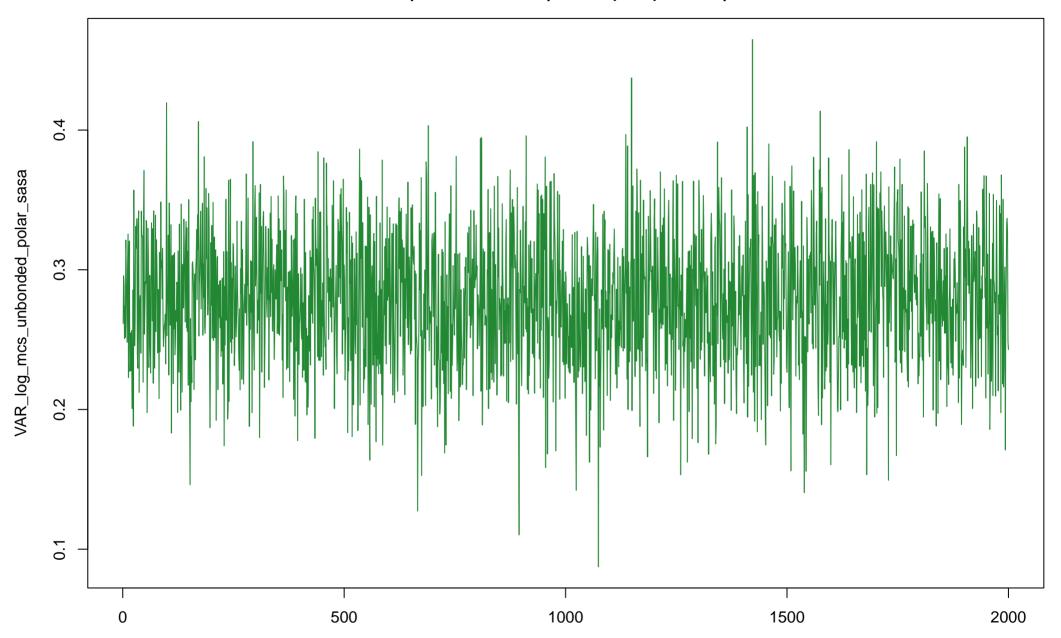
MEAN\_docked\_NumRotatableBonds ESS = 2000 | BMK = 0.0541 | MCSE(6.27) = 2.18 | stat: TRUE



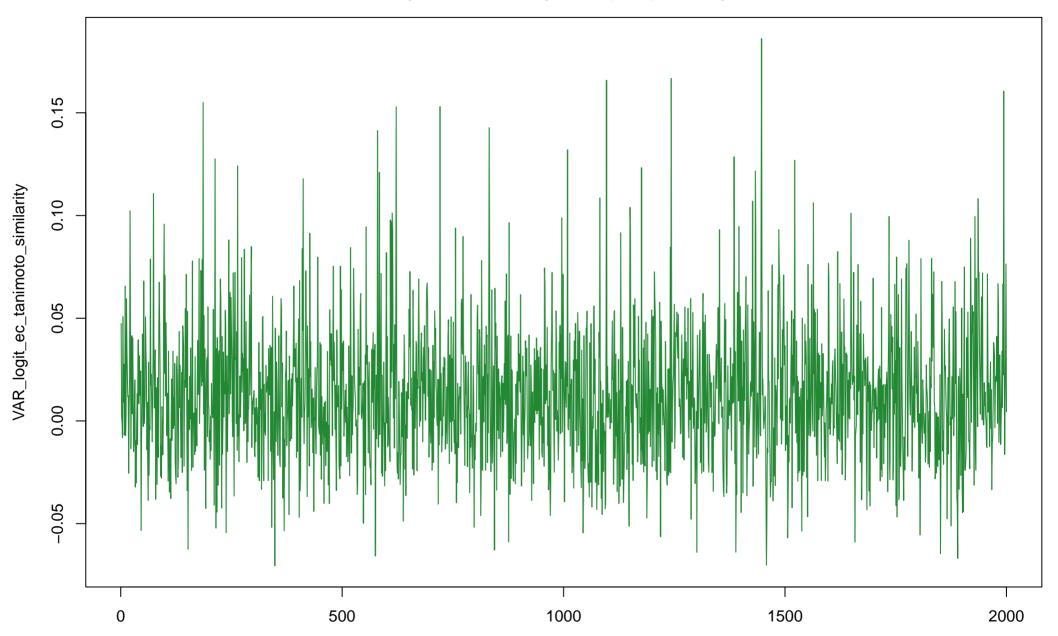
VAR\_log\_RMSD ESS = 1870 | BMK = 0.0543 | MCSE(6.27) = 2.31 | stat: TRUE



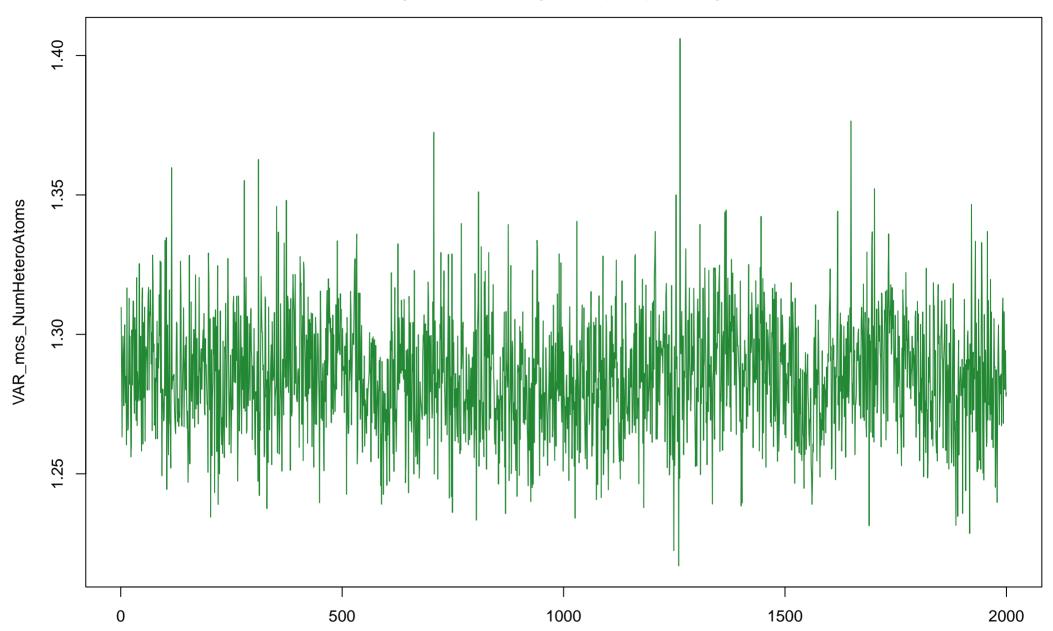
VAR\_log\_mcs\_unbonded\_polar\_sasa ESS = 1860 | BMK = 0.0389 | MCSE(6.27) = 2.17 | stat: TRUE



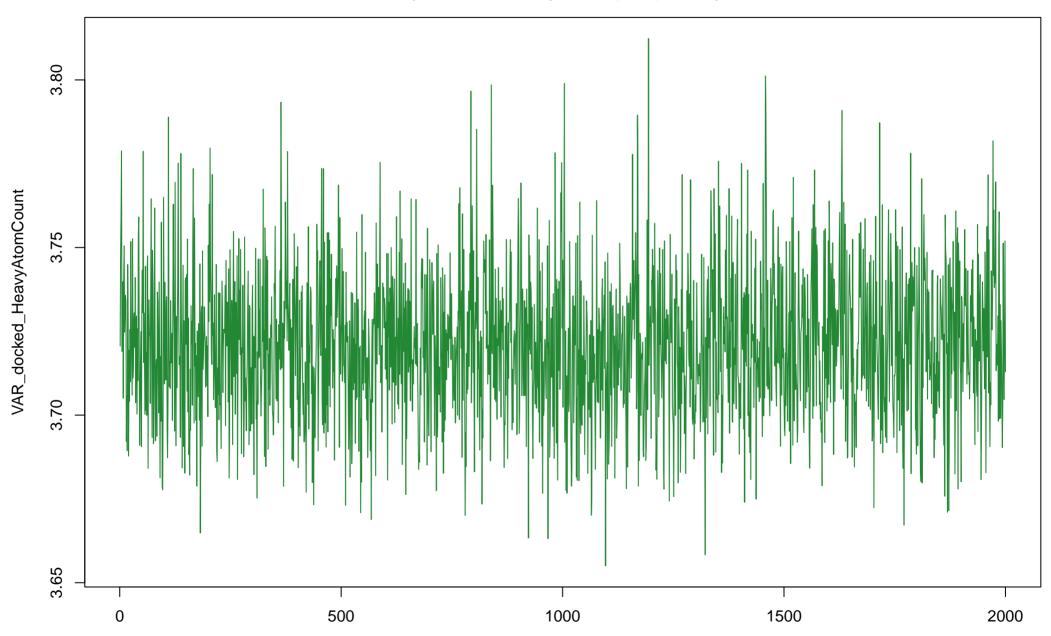
VAR\_logit\_ec\_tanimoto\_similarity ESS = 1600 | BMK = 0.0566 | MCSE(6.27) = 2.74 | stat: TRUE



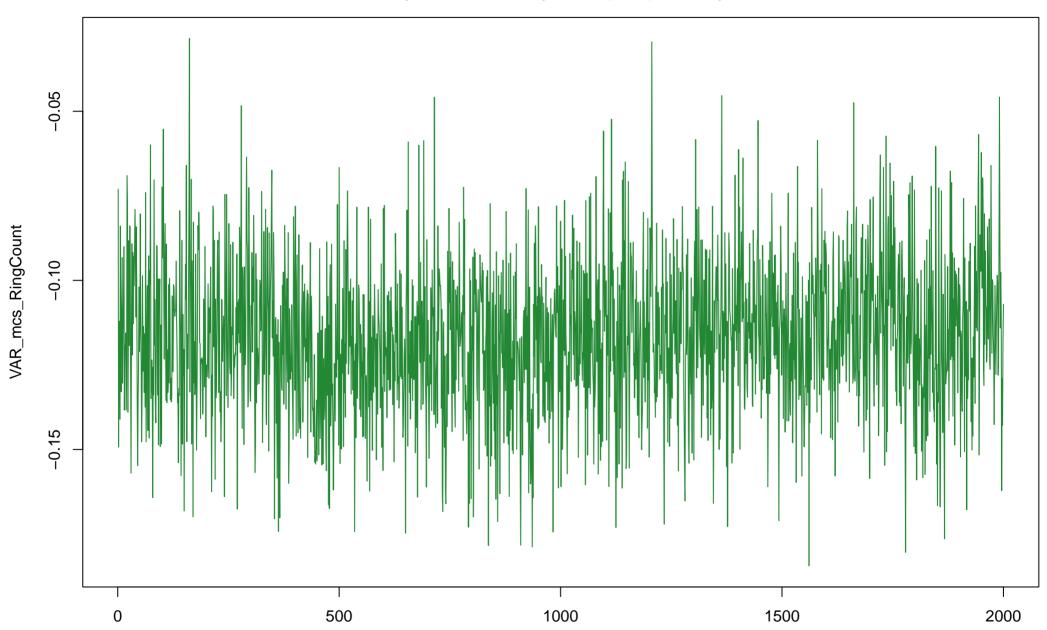
VAR\_mcs\_NumHeteroAtoms ESS = 839 | BMK = 0.0611 | MCSE(6.27) = 2.95 | stat: TRUE



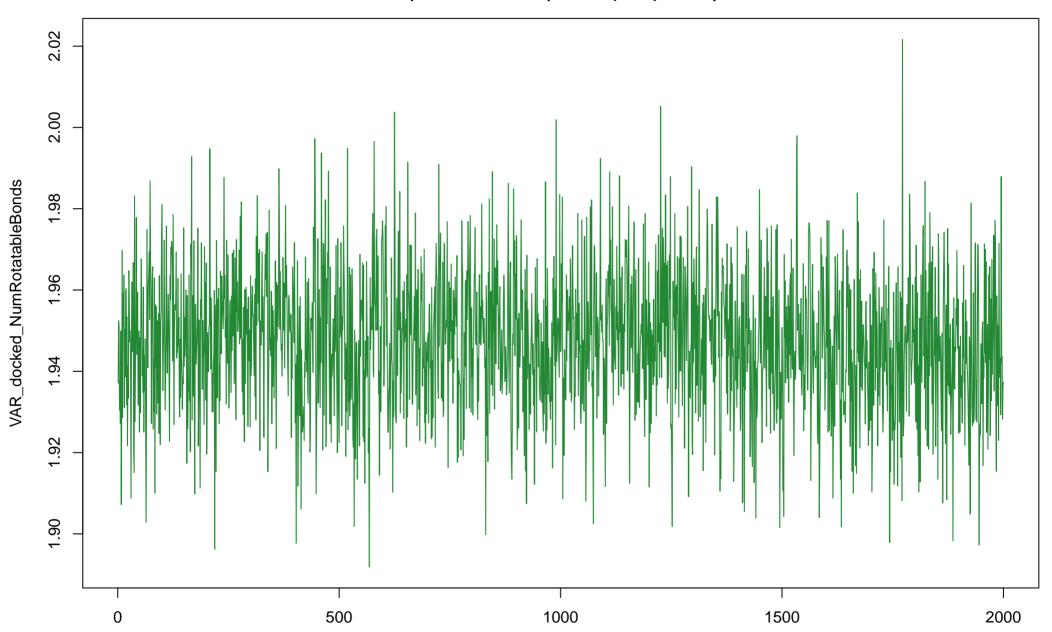
VAR\_docked\_HeavyAtomCount ESS = 1790 | BMK = 0.0407 | MCSE(6.27) = 2.6 | stat: TRUE



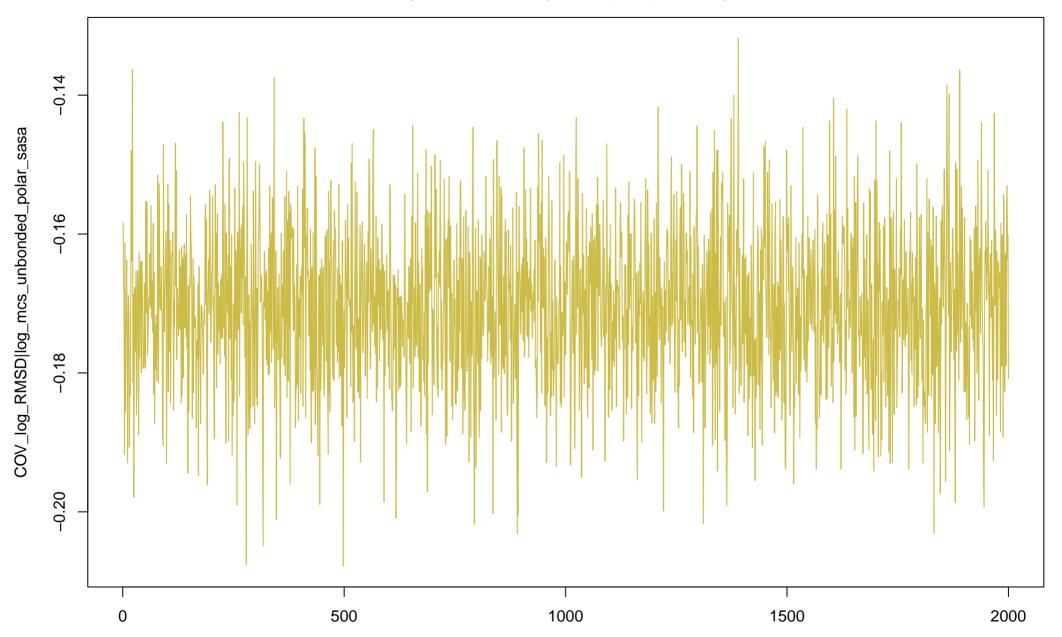
VAR\_mcs\_RingCount ESS = 1280 | BMK = 0.0802 | MCSE(6.27) = 2.82 | stat: TRUE



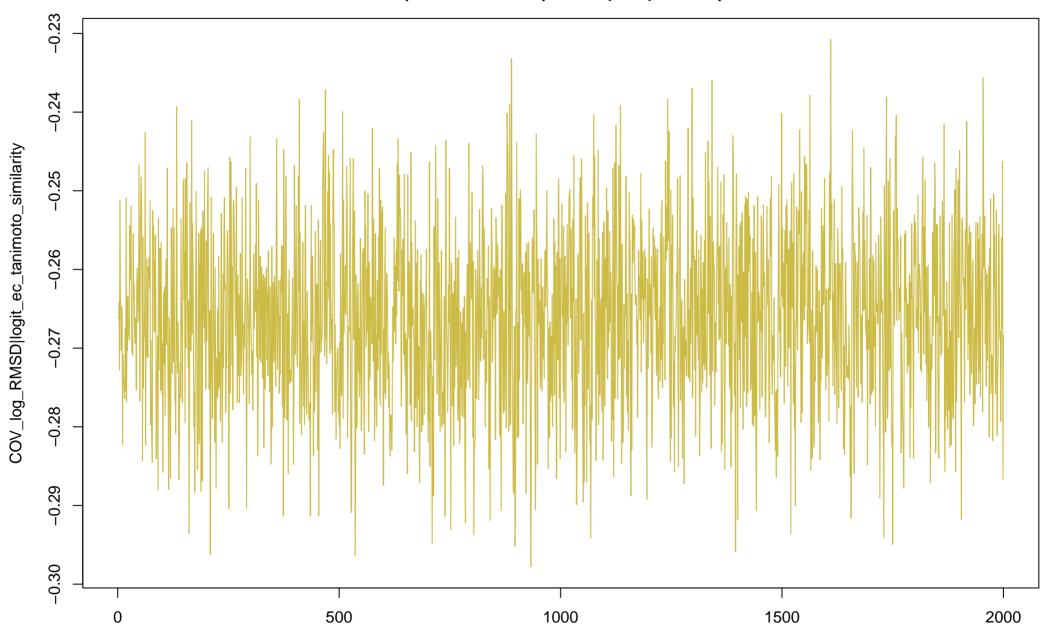
VAR\_docked\_NumRotatableBonds ESS = 1500 | BMK = 0.0565 | MCSE(6.27) = 2.9 | stat: TRUE



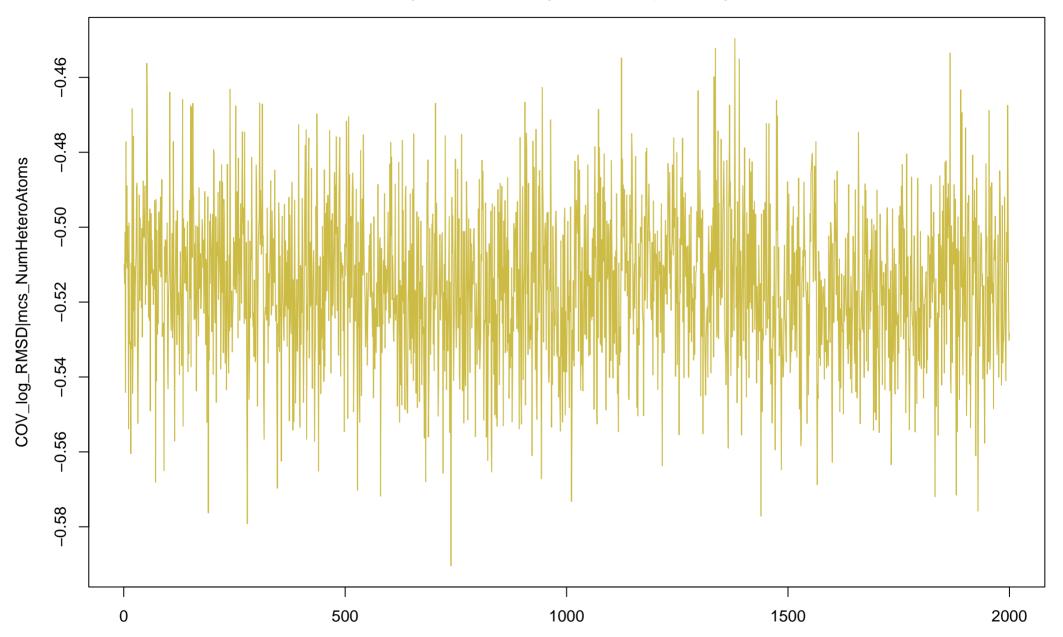
COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa ESS = 2000 | BMK = 0.0466 | MCSE(6.27) = 2.44 | stat: TRUE



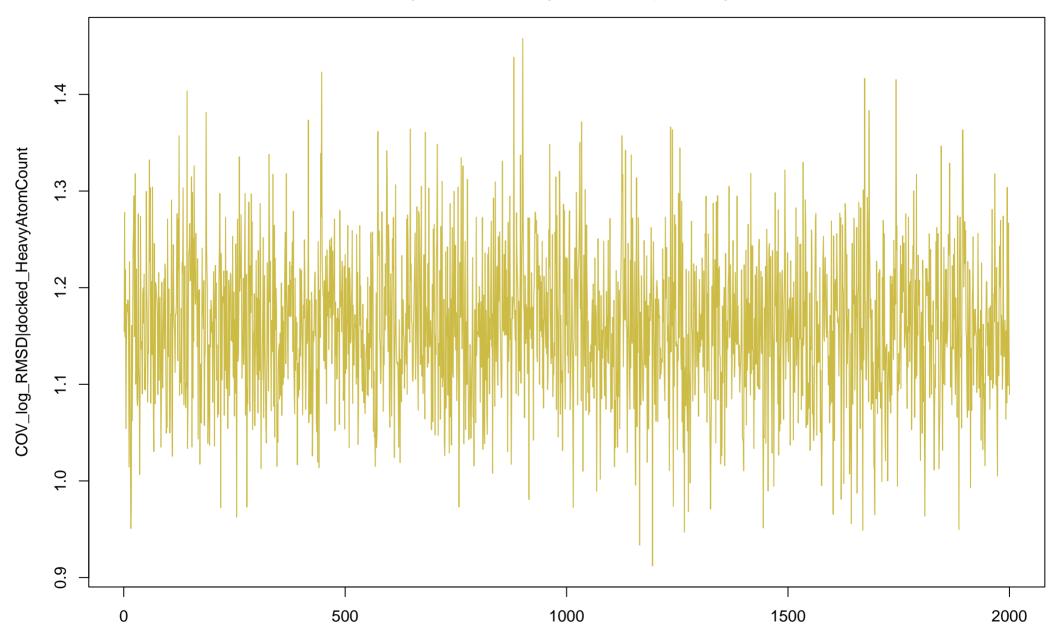
COV\_log\_RMSD|logit\_ec\_tanimoto\_similarity ESS = 1470 | BMK = 0.0713 | MCSE(6.27) = 2.93 | stat: TRUE



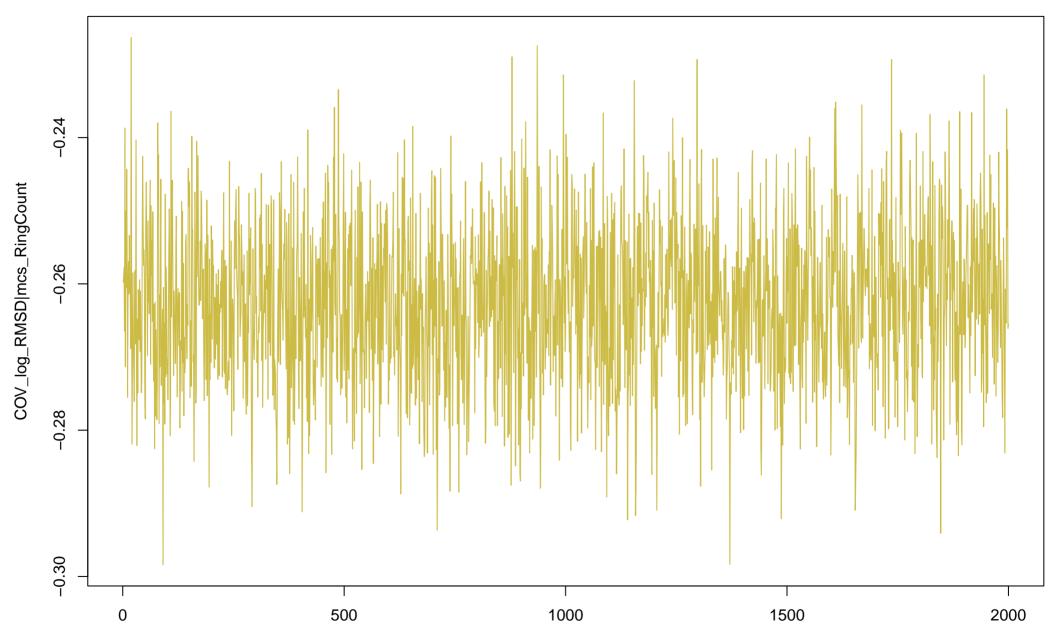
COV\_log\_RMSD|mcs\_NumHeteroAtoms ESS = 1520 | BMK = 0.0481 | MCSE(6.27) = 3.01 | stat: TRUE



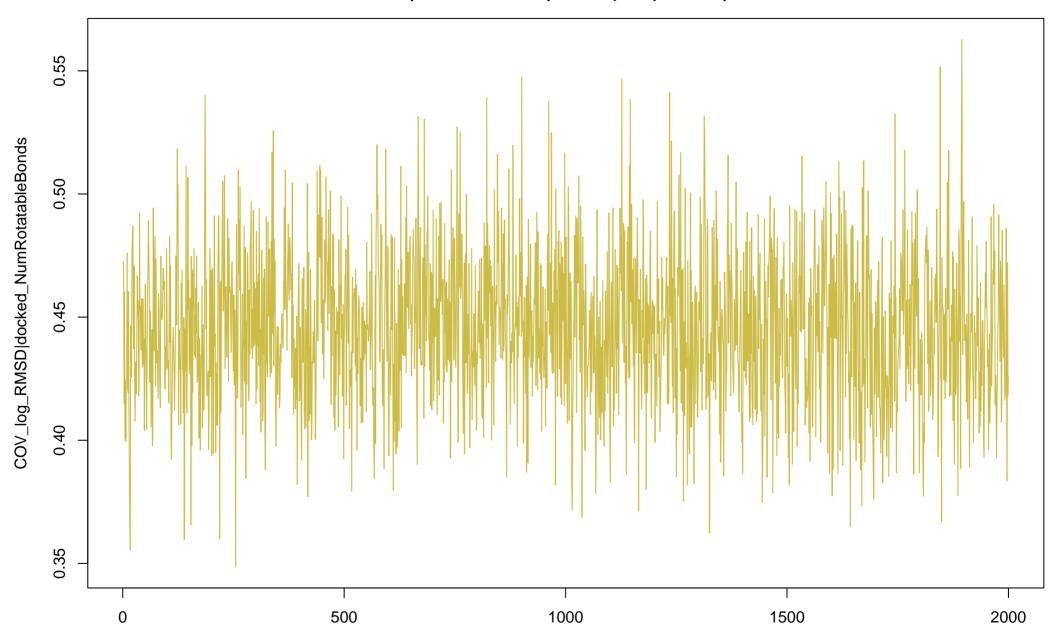
COV\_log\_RMSD|docked\_HeavyAtomCount ESS = 1550 | BMK = 0.0615 | MCSE(6.27) = 2.82 | stat: TRUE

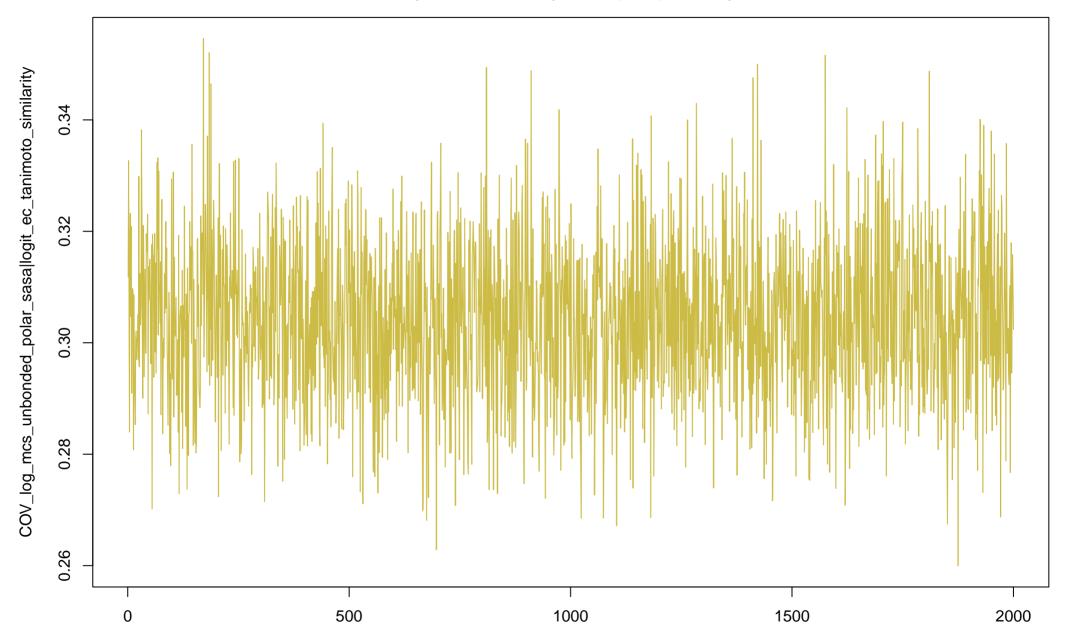


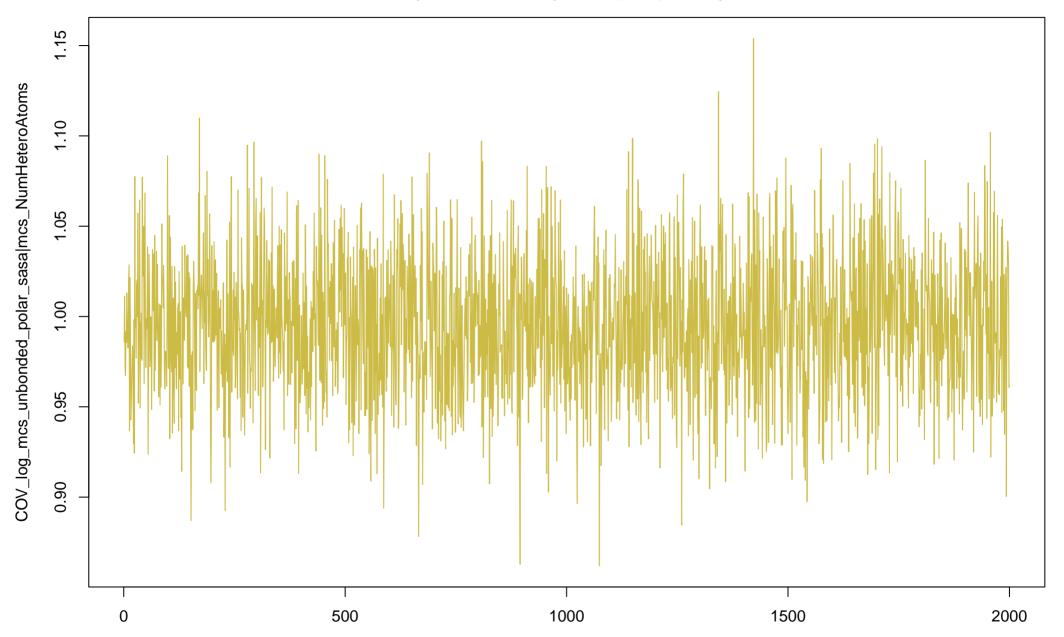
COV\_log\_RMSD|mcs\_RingCount ESS = 1510 | BMK = 0.0453 | MCSE(6.27) = 3.16 | stat: TRUE

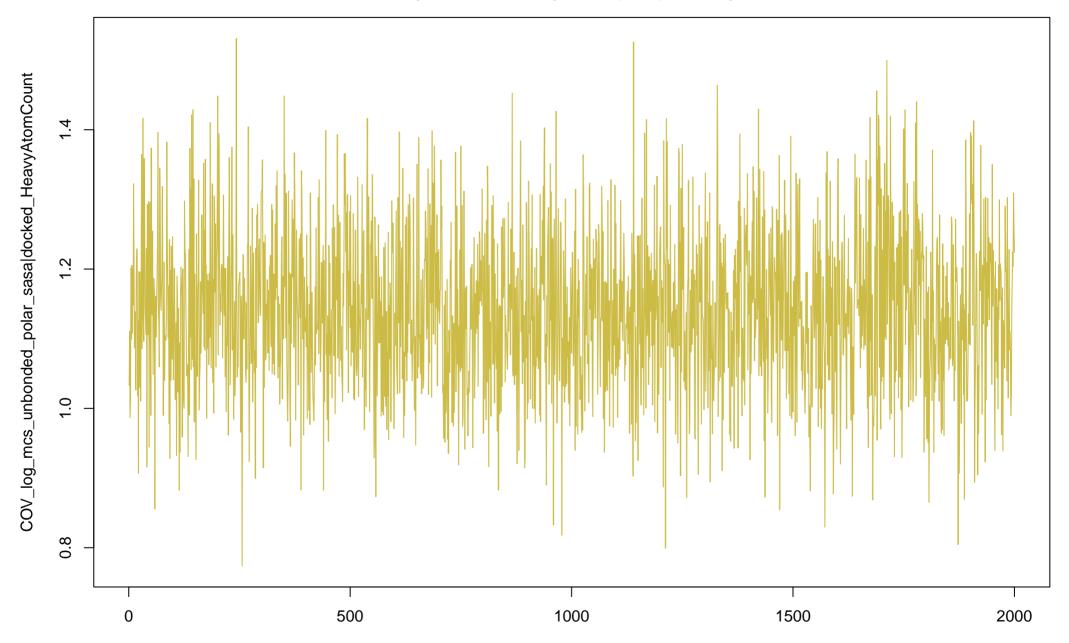


COV\_log\_RMSD|docked\_NumRotatableBonds ESS = 1300 | BMK = 0.0698 | MCSE(6.27) = 3.23 | stat: TRUE

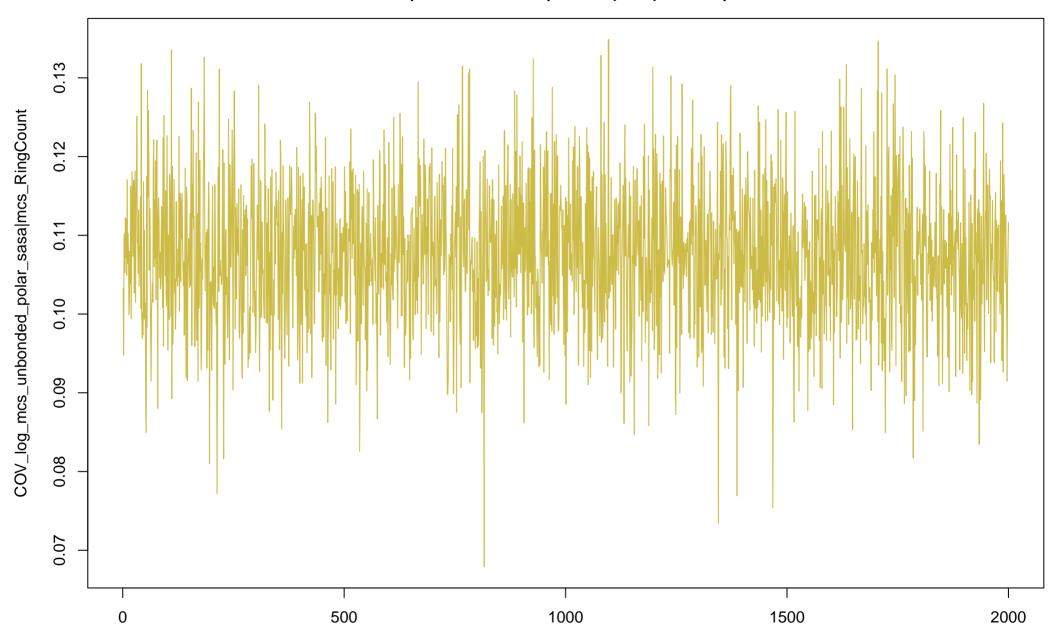




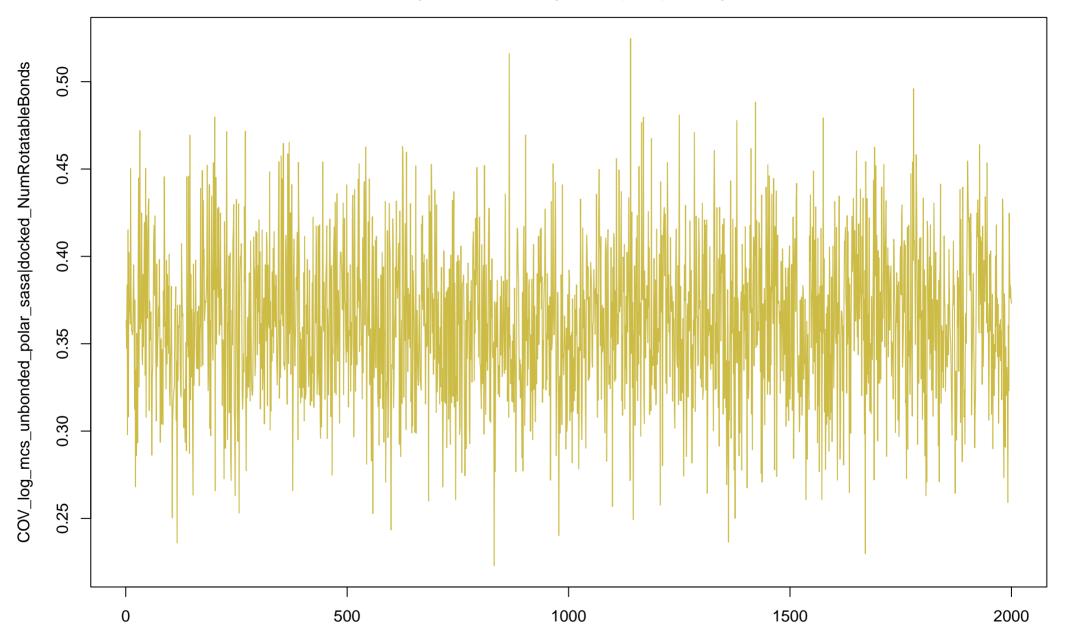




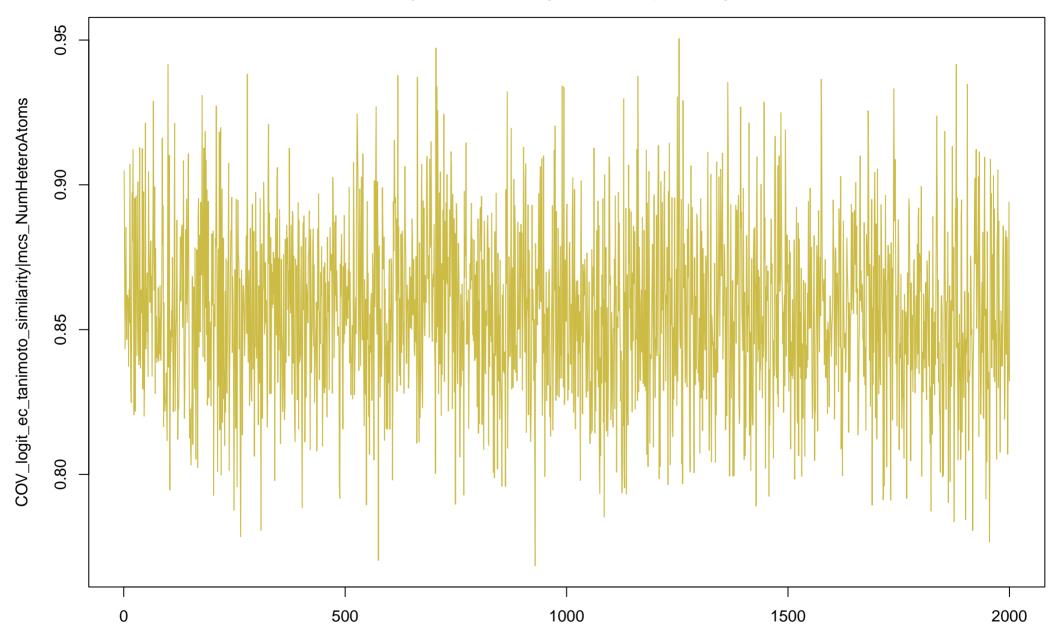
COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_RingCount ESS = 2000 | BMK = 0.0444 | MCSE(6.27) = 2.23 | stat: TRUE

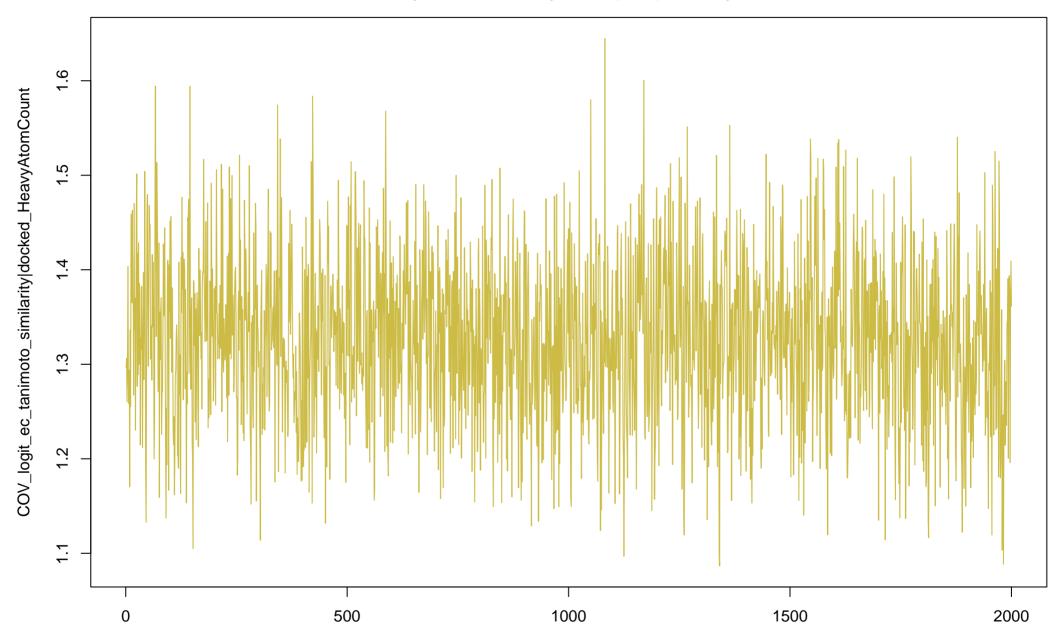


## COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_NumRotatableBonds ESS = 1850 | BMK = 0.0547 | MCSE(6.27) = 2.7 | stat: TRUE

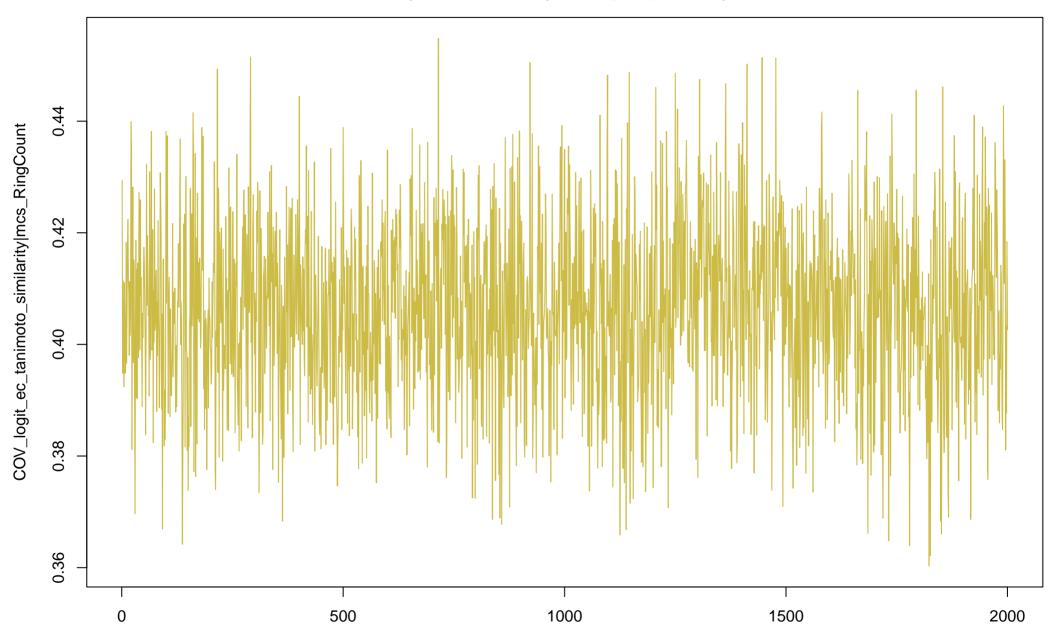


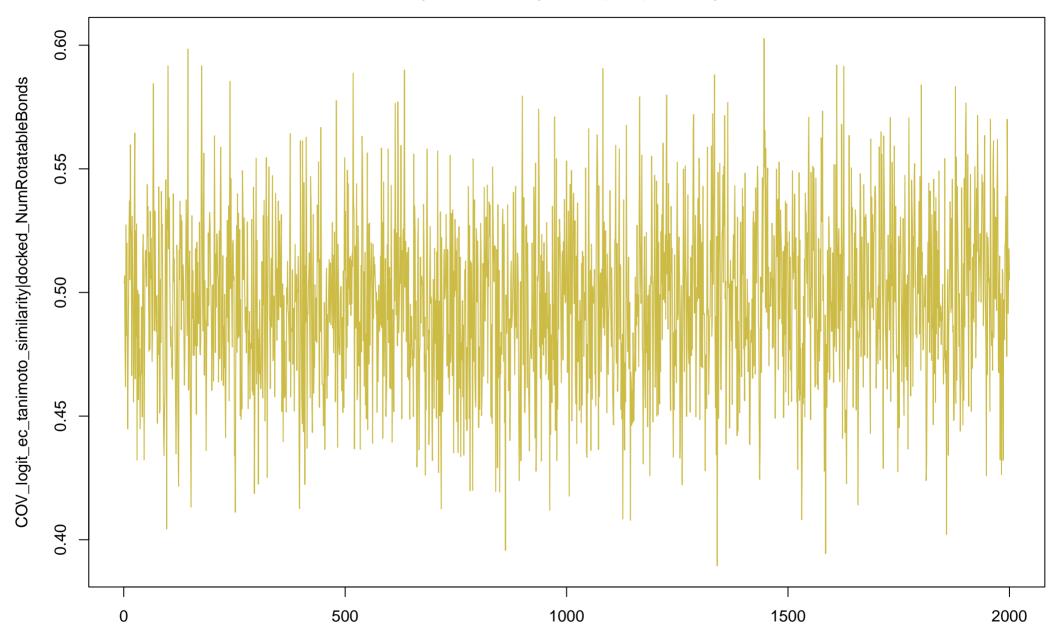
COV\_logit\_ec\_tanimoto\_similarity|mcs\_NumHeteroAtoms ESS = 1650 | BMK = 0.0586 | MCSE(6.27) = 2.61 | stat: TRUE

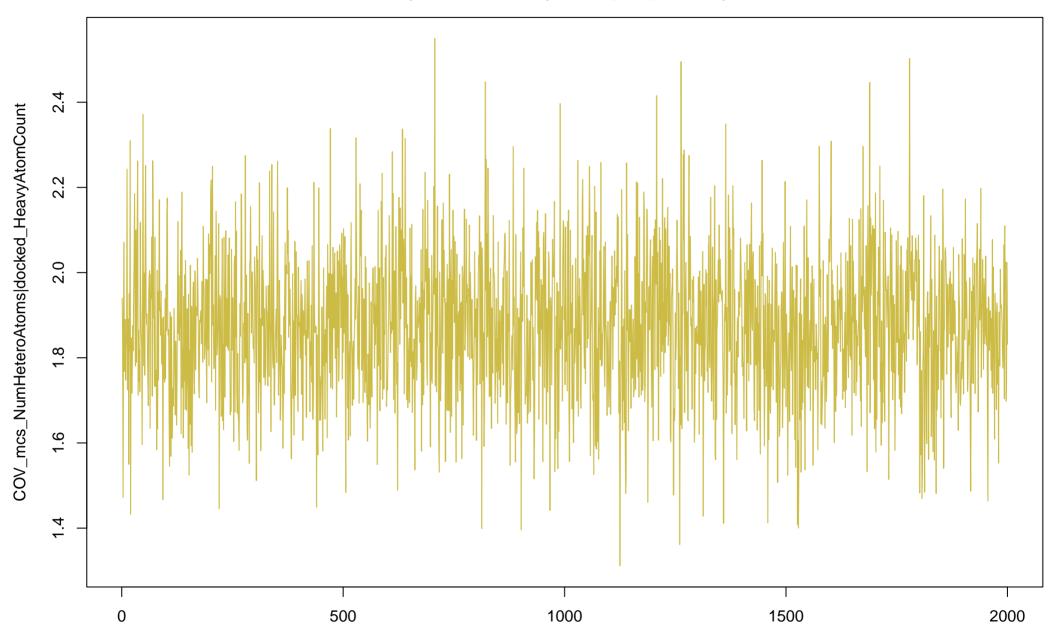




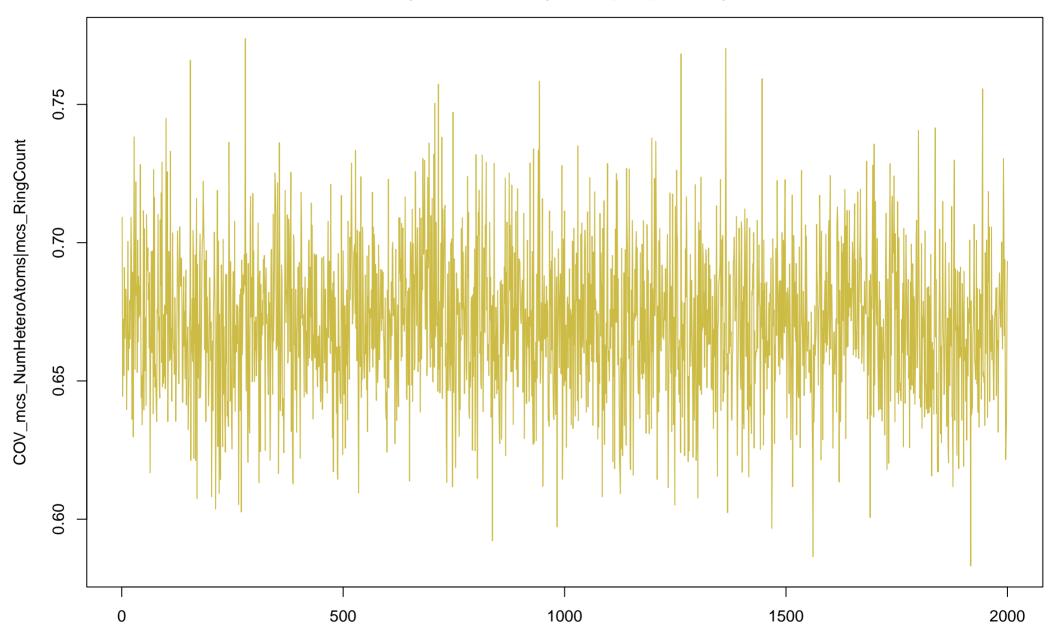
COV\_logit\_ec\_tanimoto\_similarity|mcs\_RingCount ESS = 1580 | BMK = 0.0536 | MCSE(6.27) = 2.88 | stat: TRUE

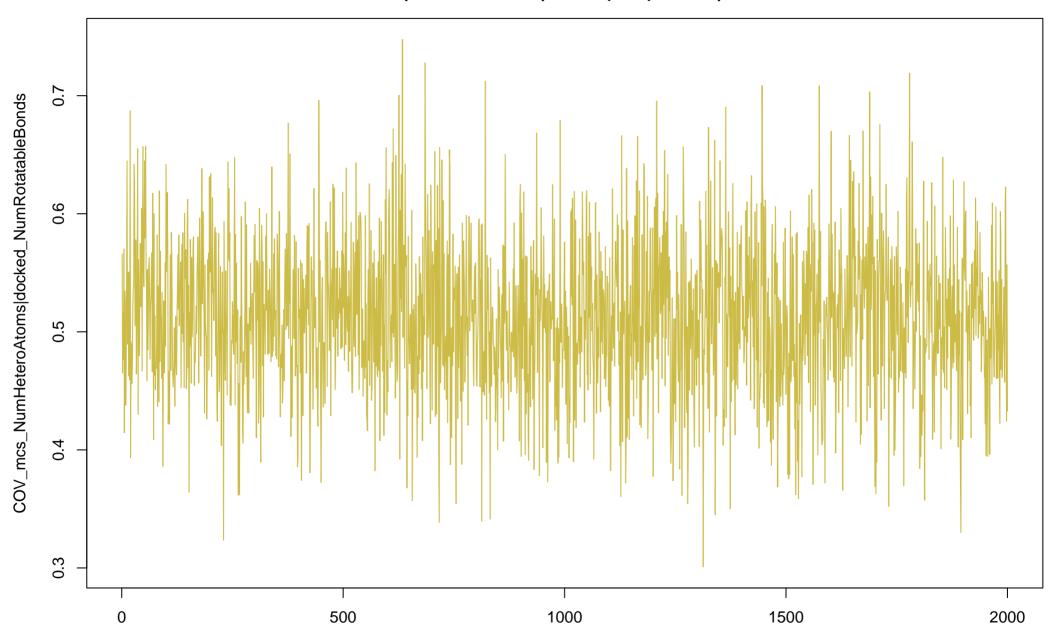




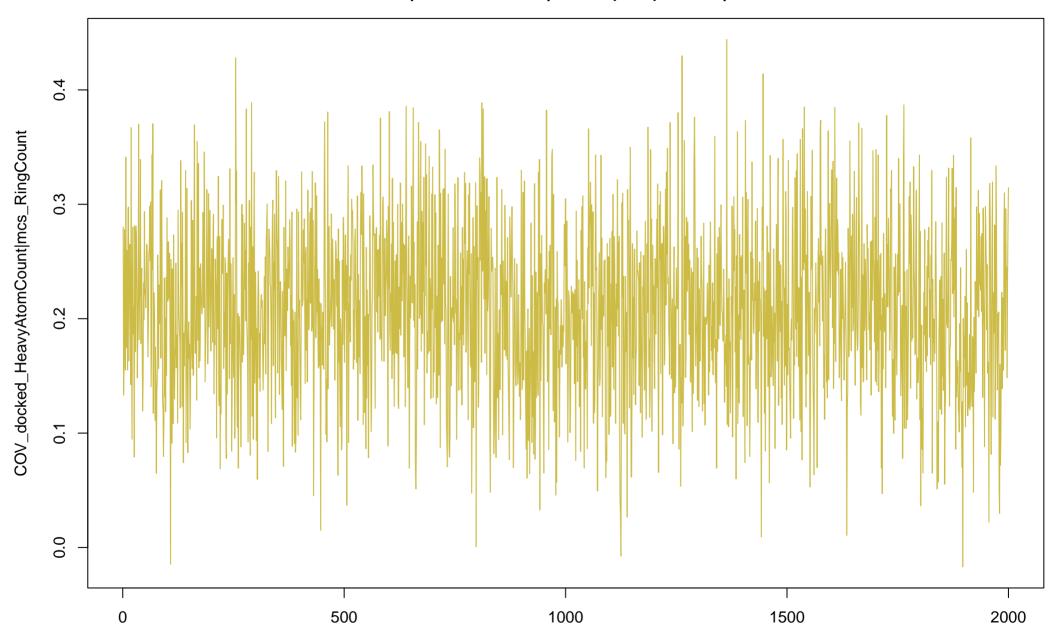


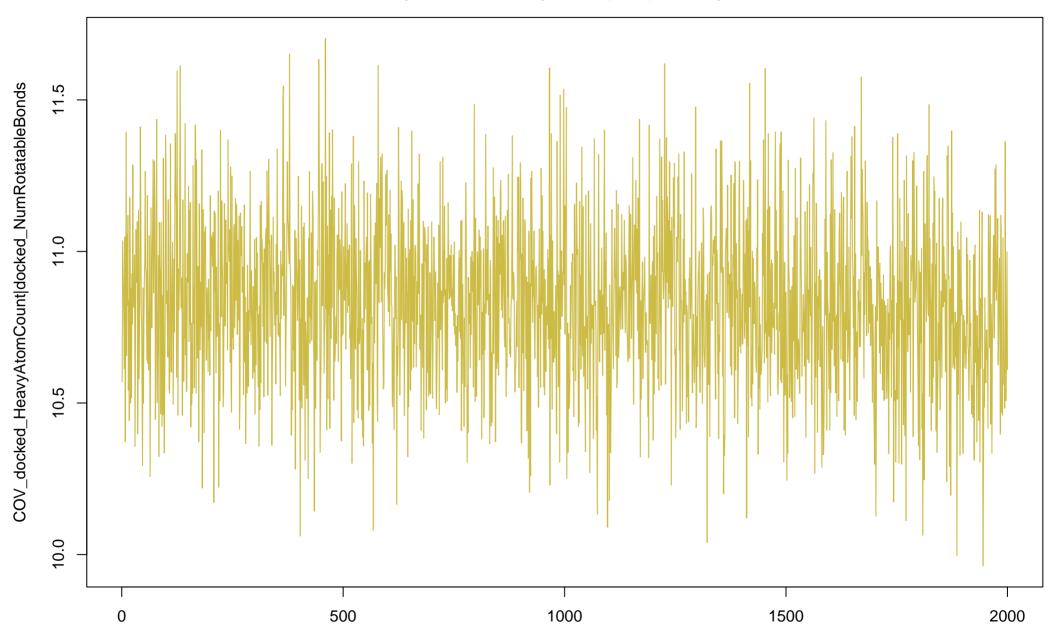
COV\_mcs\_NumHeteroAtoms|mcs\_RingCount ESS = 1850 | BMK = 0.0453 | MCSE(6.27) = 2.42 | stat: TRUE





## COV\_docked\_HeavyAtomCount|mcs\_RingCount ESS = 1300 | BMK = 0.0471 | MCSE(6.27) = 2.72 | stat: TRUE





## COV\_mcs\_RingCount|docked\_NumRotatableBonds ESS = 1610 | BMK = 0.0488 | MCSE(6.27) = 2.74 | stat: TRUE

