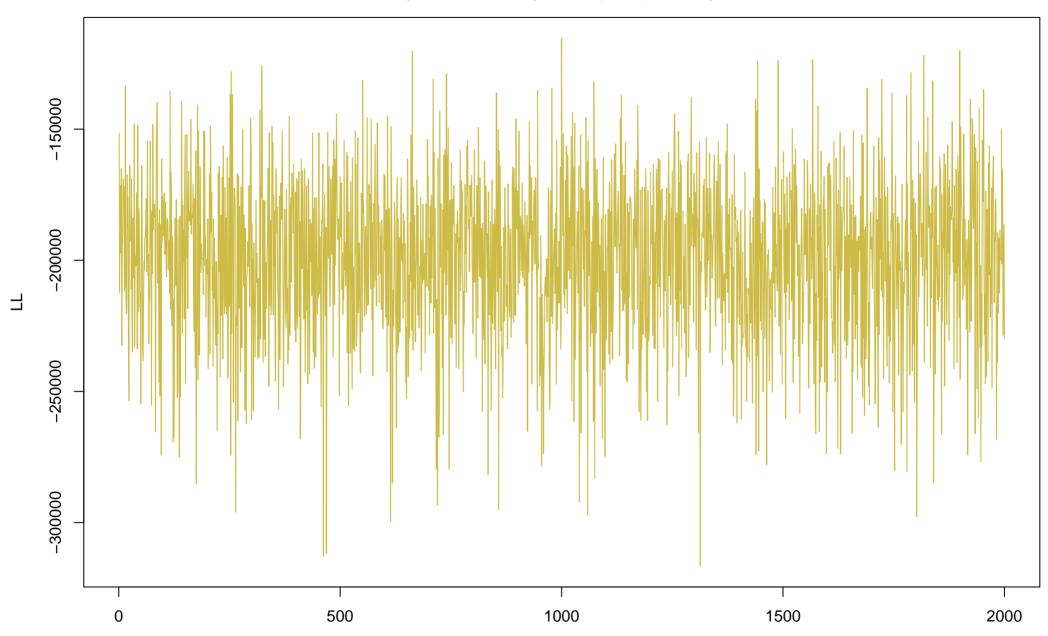
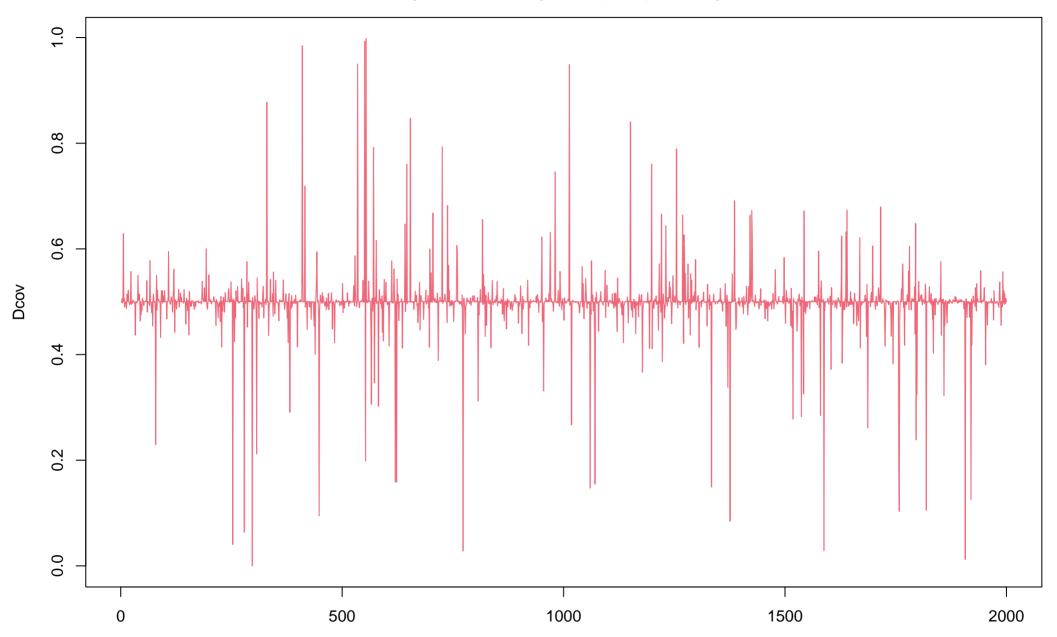
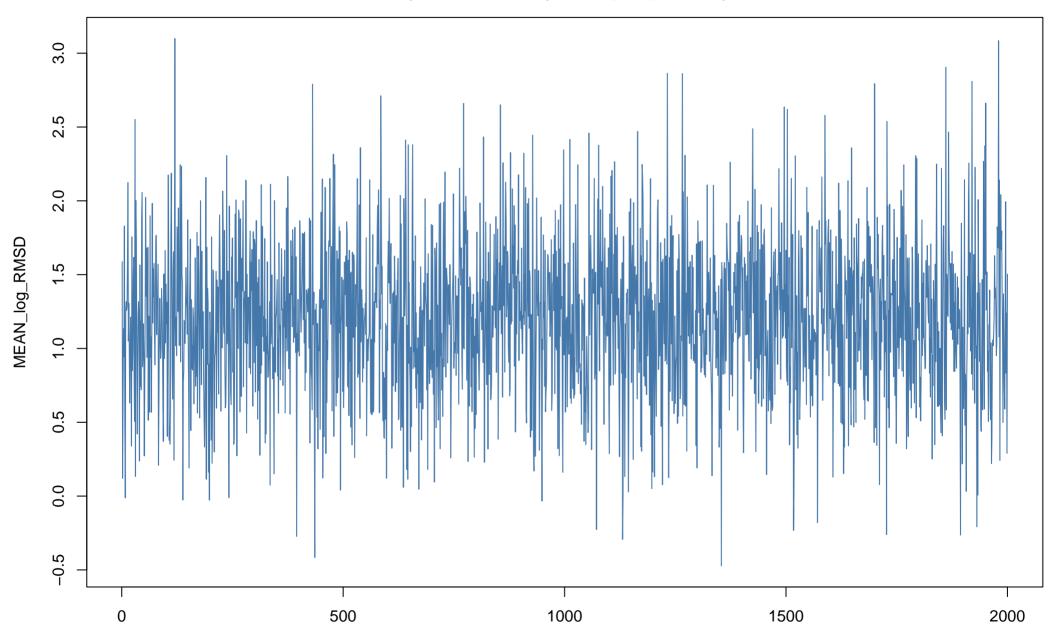
LL ESS = 1990 | BMK = 0.142 | MCSE(6.27) = 2.14 | stat: FALSE



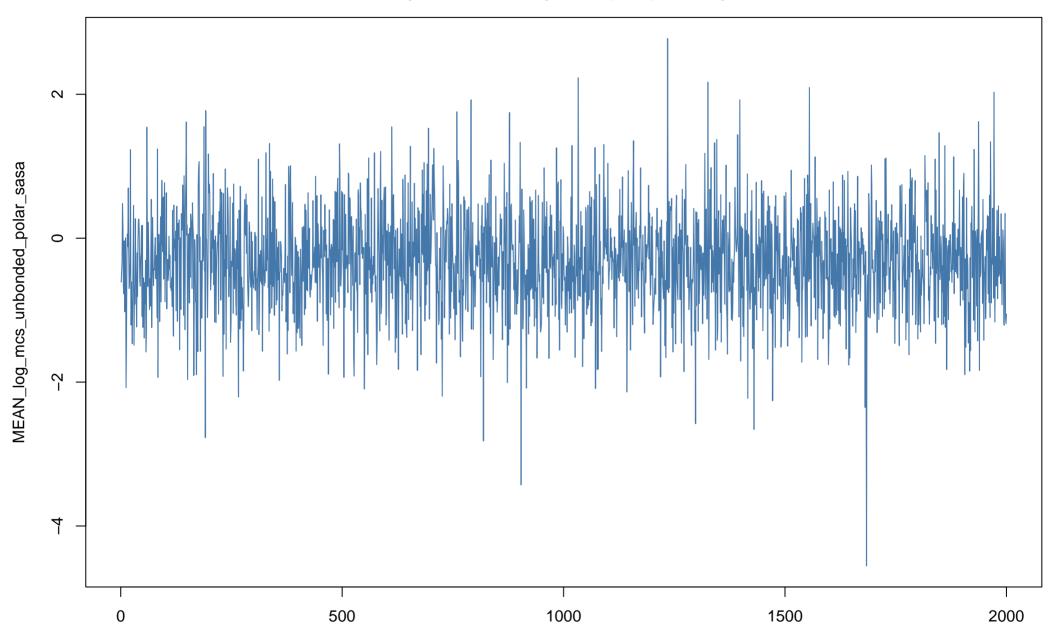
Dcov ESS = 2000 | BMK = 0.231 | MCSE(6.27) = 2.23 | stat: TRUE



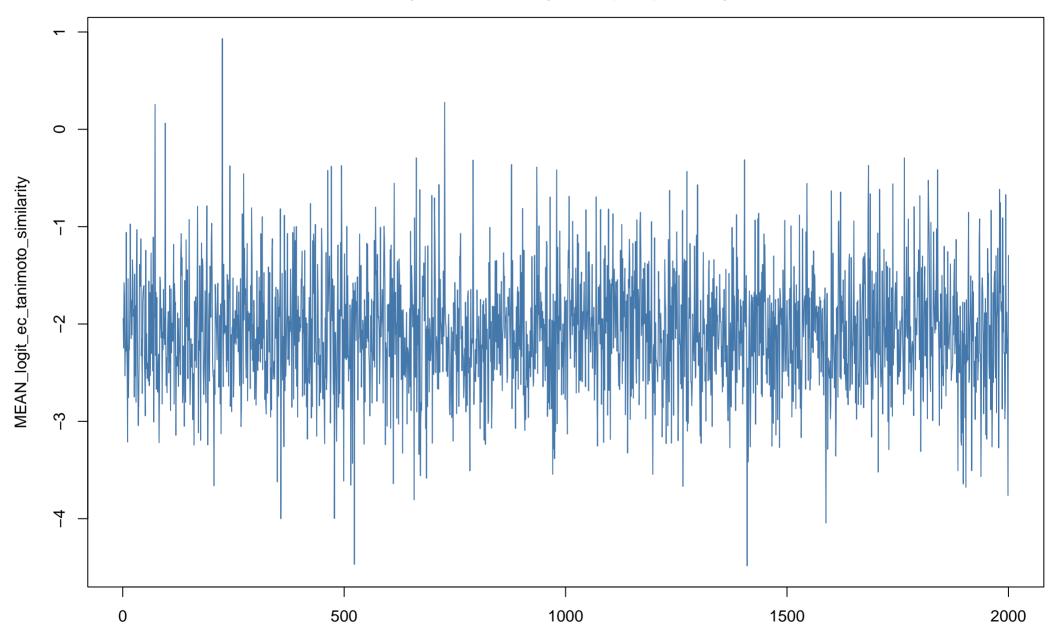
MEAN\_log\_RMSD ESS = 2000 | BMK = 0.0509 | MCSE(6.27) = 2.22 | stat: TRUE



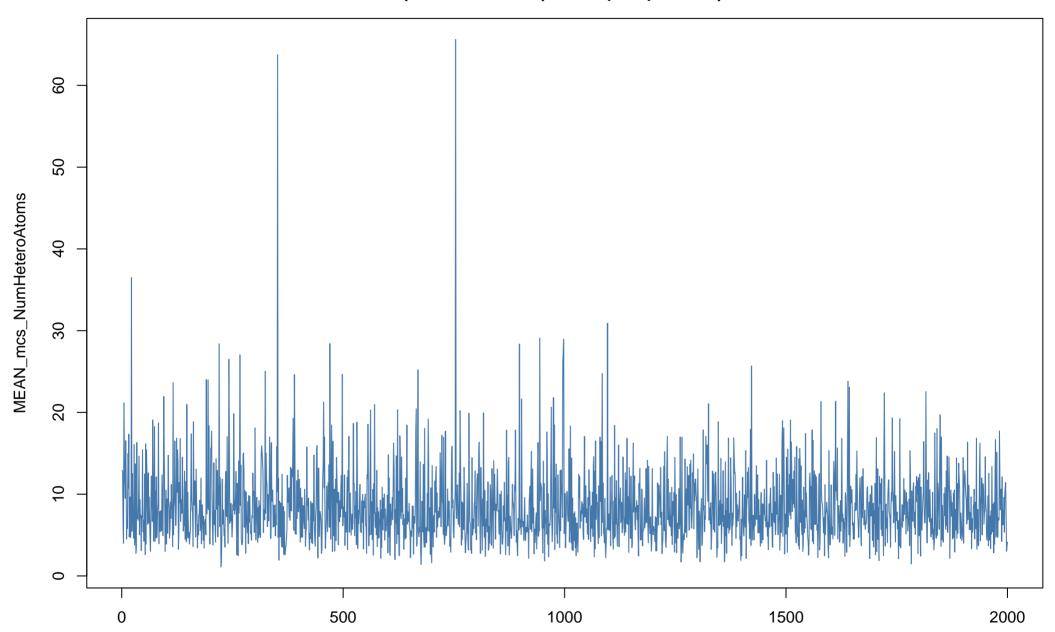
MEAN\_log\_mcs\_unbonded\_polar\_sasa ESS = 2000 | BMK = 0.0708 | MCSE(6.27) = 2.19 | stat: TRUE



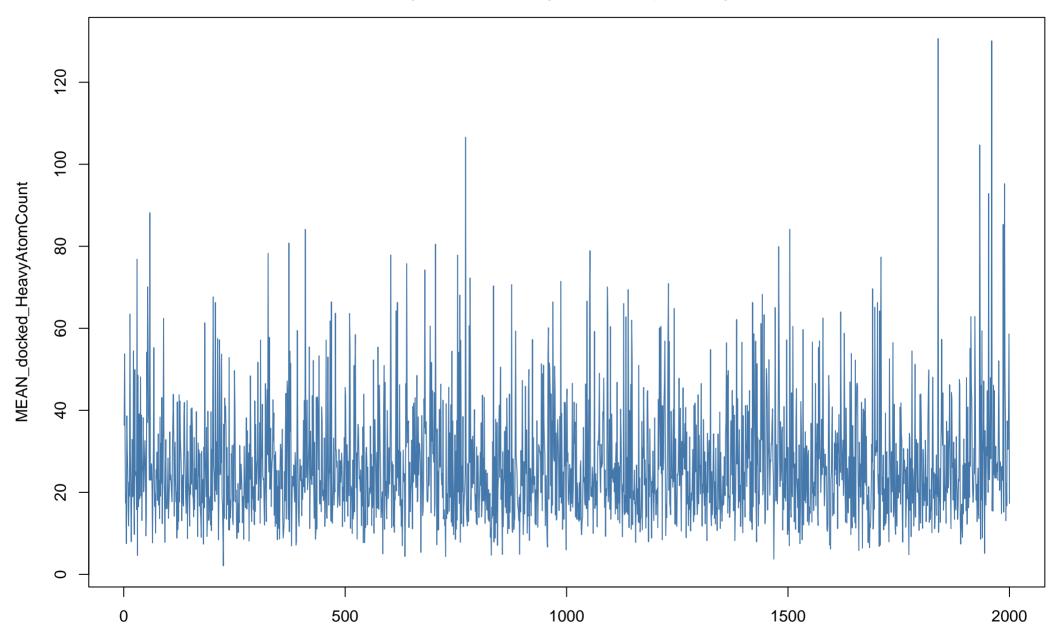
MEAN\_logit\_ec\_tanimoto\_similarity ESS = 2000 | BMK = 0.0574 | MCSE(6.27) = 2.21 | stat: TRUE



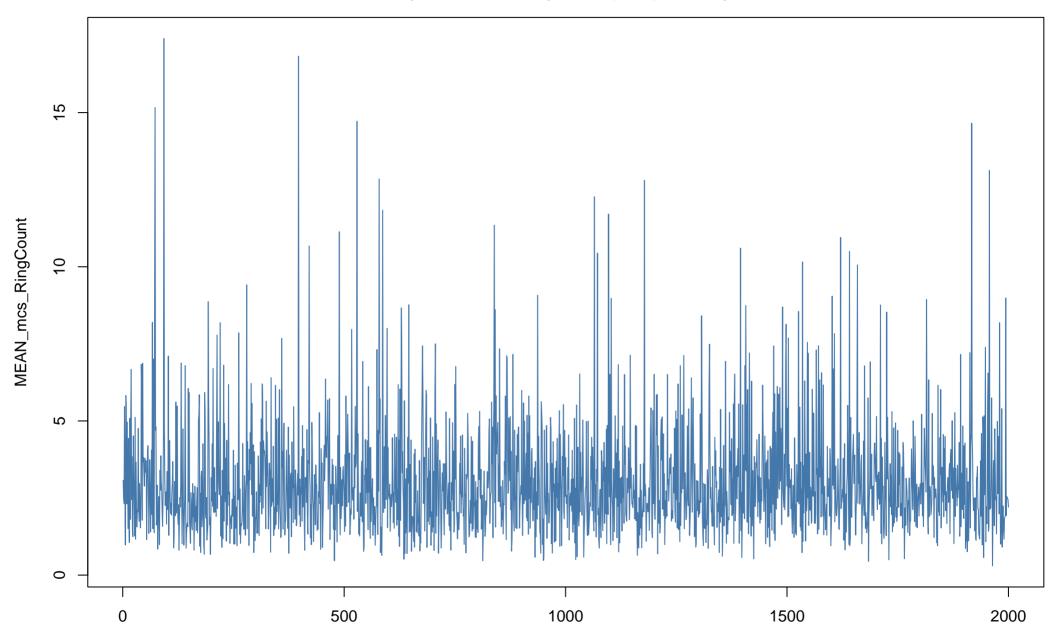
MEAN\_mcs\_NumHeteroAtoms ESS = 2000 | BMK = 0.0797 | MCSE(6.27) = 2.34 | stat: FALSE



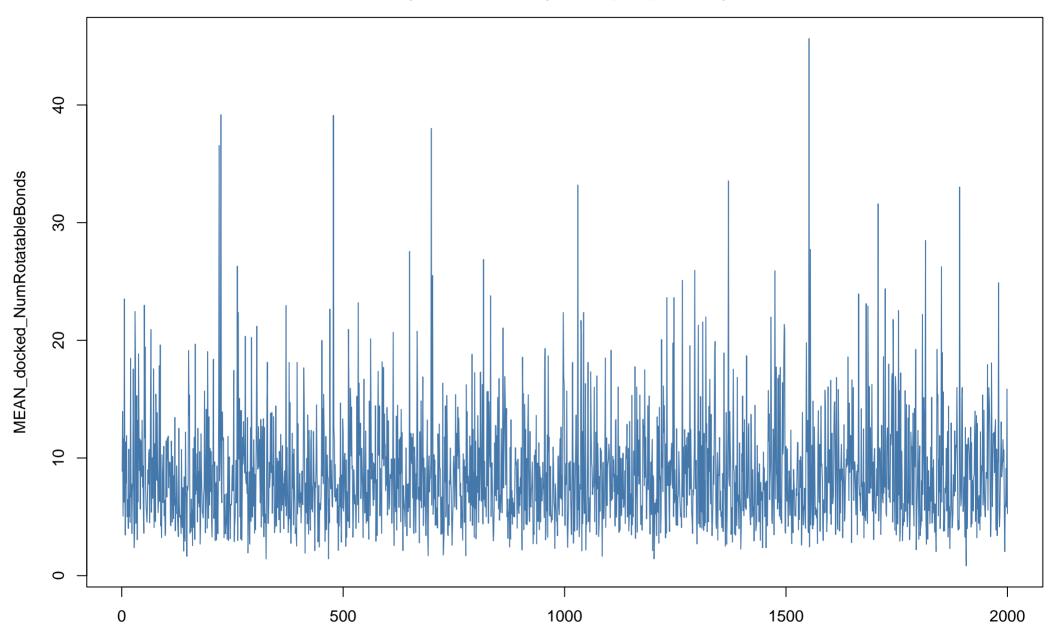
MEAN\_docked\_HeavyAtomCount ESS = 1740 | BMK = 0.0534 | MCSE(6.27) = 2.53 | stat: TRUE



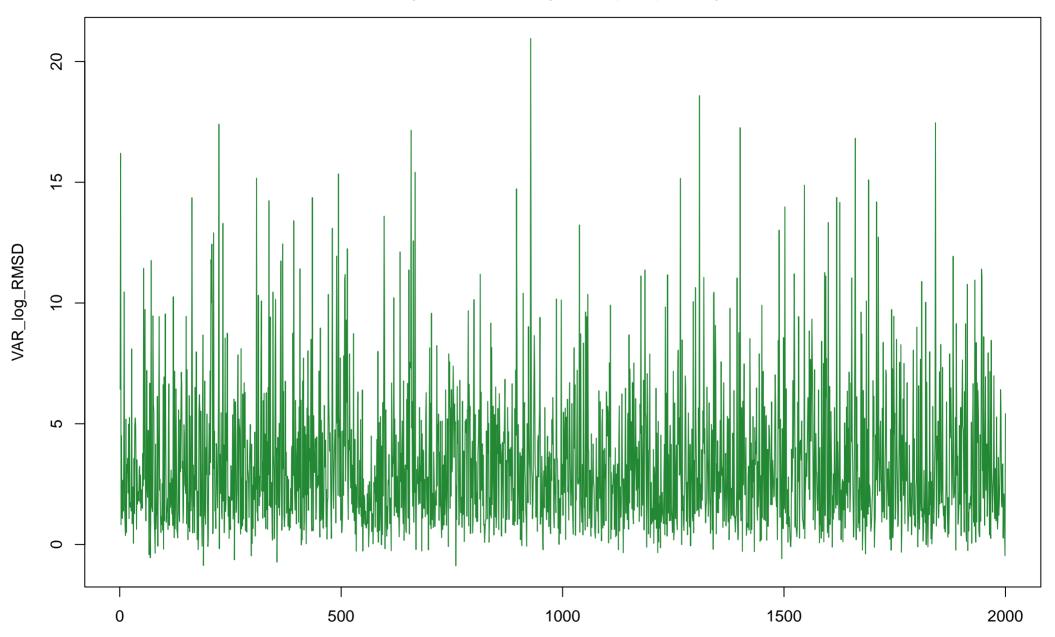
MEAN\_mcs\_RingCount ESS = 2000 | BMK = 0.0615 | MCSE(6.27) = 2.33 | stat: TRUE



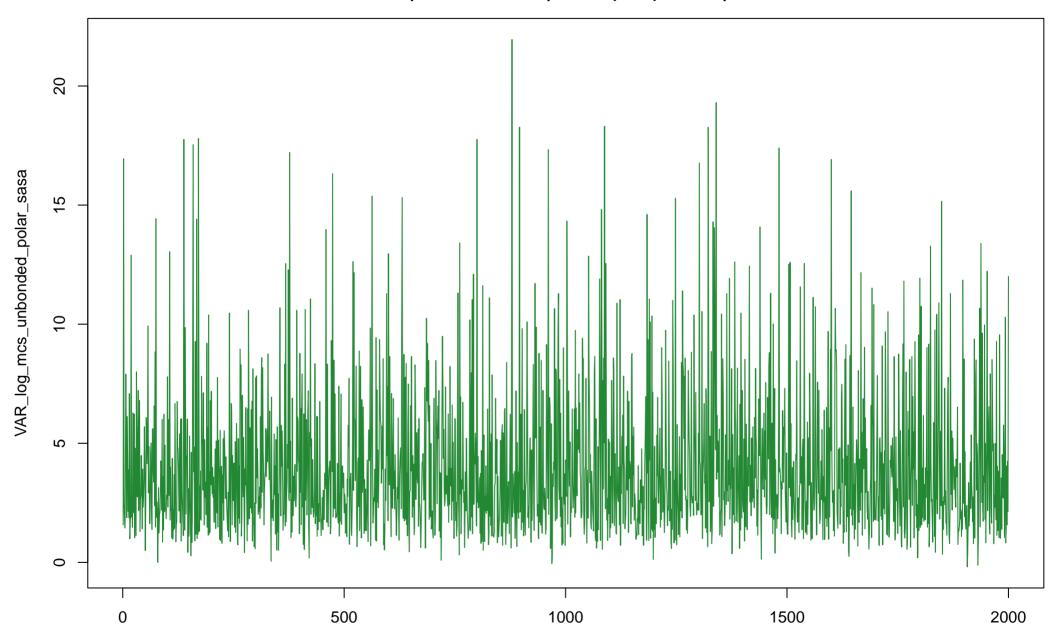
MEAN\_docked\_NumRotatableBonds ESS = 2000 | BMK = 0.0704 | MCSE(6.27) = 2.23 | stat: TRUE



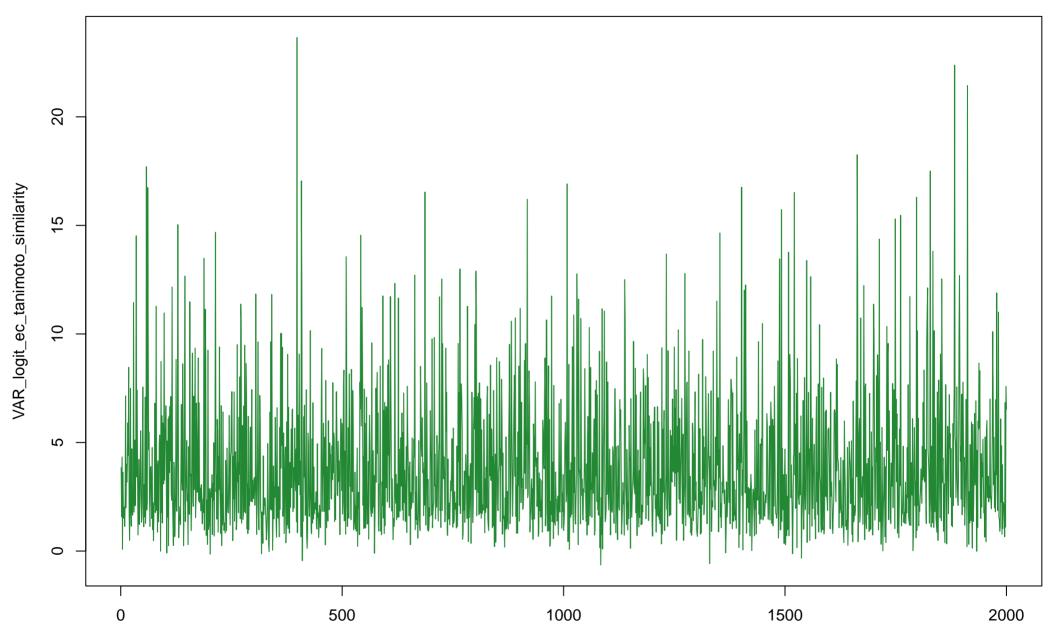
VAR\_log\_RMSD ESS = 2000 | BMK = 0.0435 | MCSE(6.27) = 2.2 | stat: TRUE



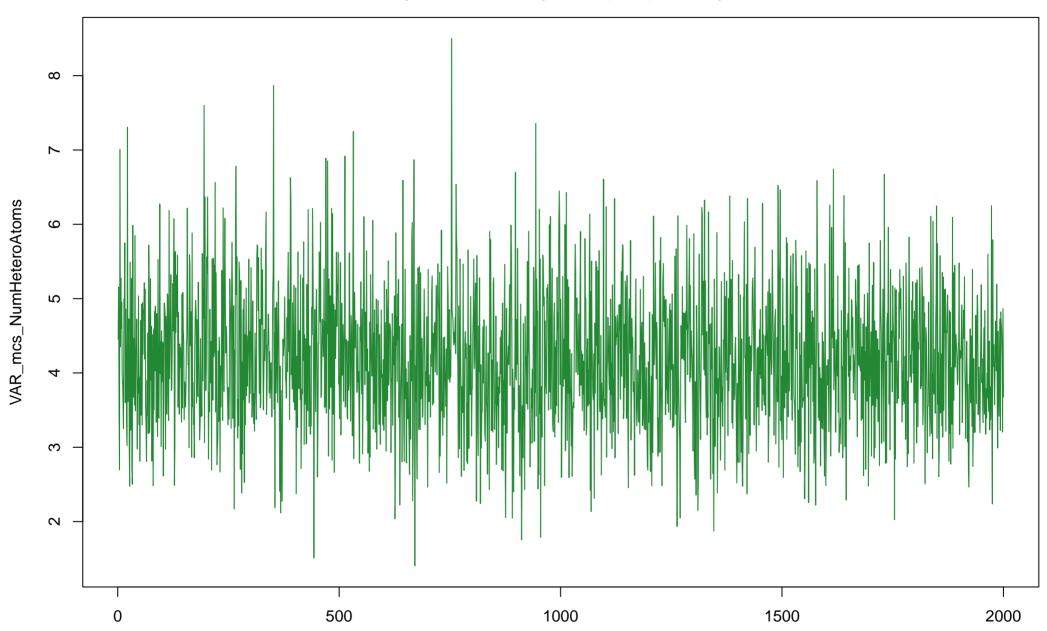
VAR\_log\_mcs\_unbonded\_polar\_sasa ESS = 2000 | BMK = 0.0601 | MCSE(6.27) = 2.19 | stat: TRUE



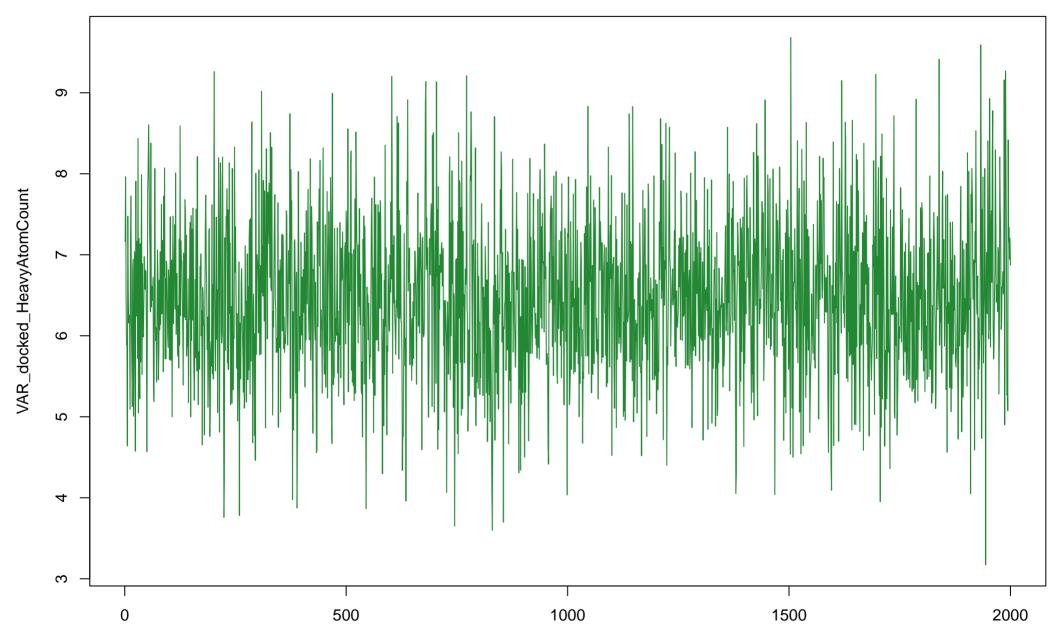
VAR\_logit\_ec\_tanimoto\_similarity ESS = 1880 | BMK = 0.0389 | MCSE(6.27) = 2.24 | stat: TRUE



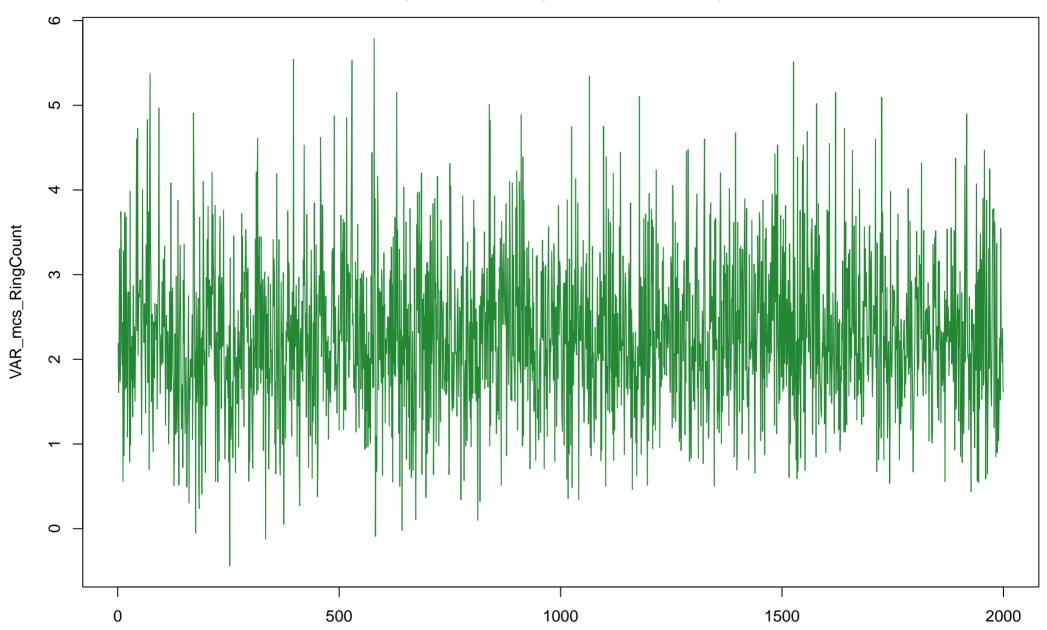
VAR\_mcs\_NumHeteroAtoms ESS = 2000 | BMK = 0.0661 | MCSE(6.27) = 2.25 | stat: TRUE



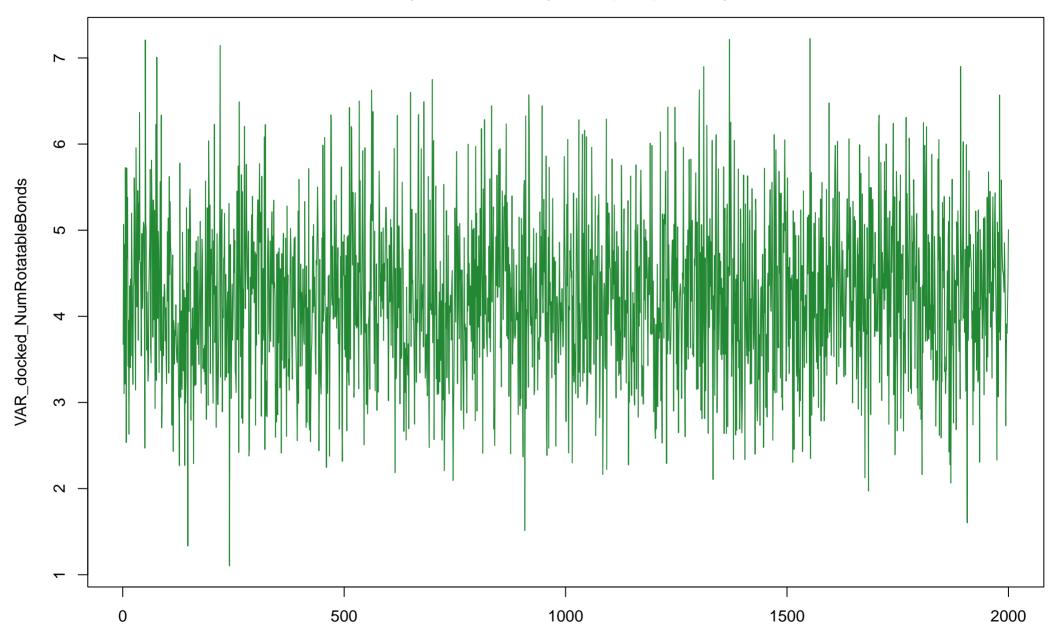
VAR\_docked\_HeavyAtomCount ESS = 1820 | BMK = 0.0383 | MCSE(6.27) = 2.51 | stat: TRUE

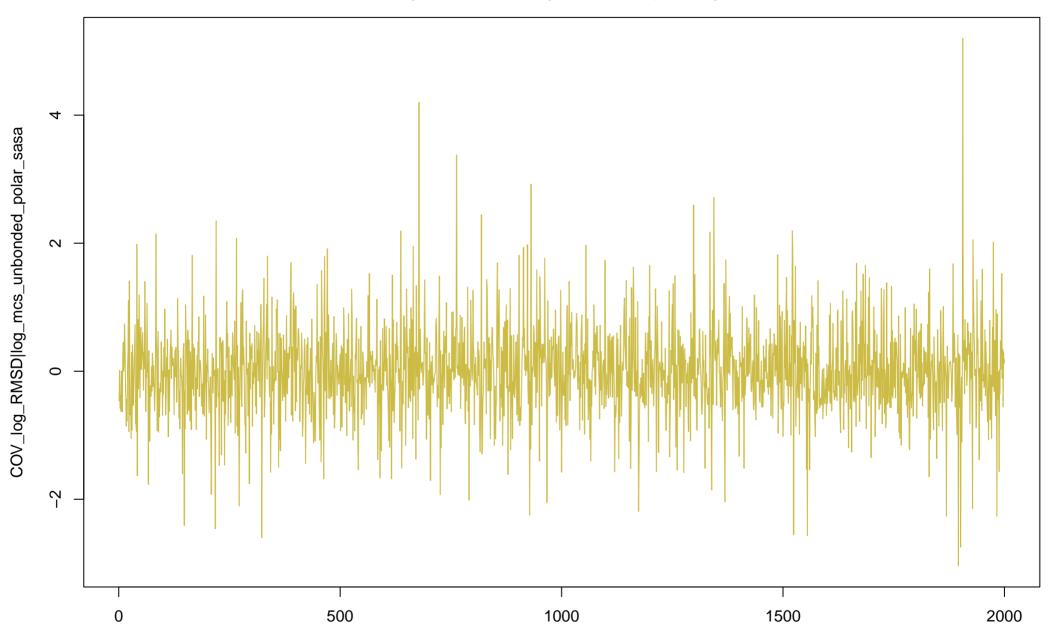


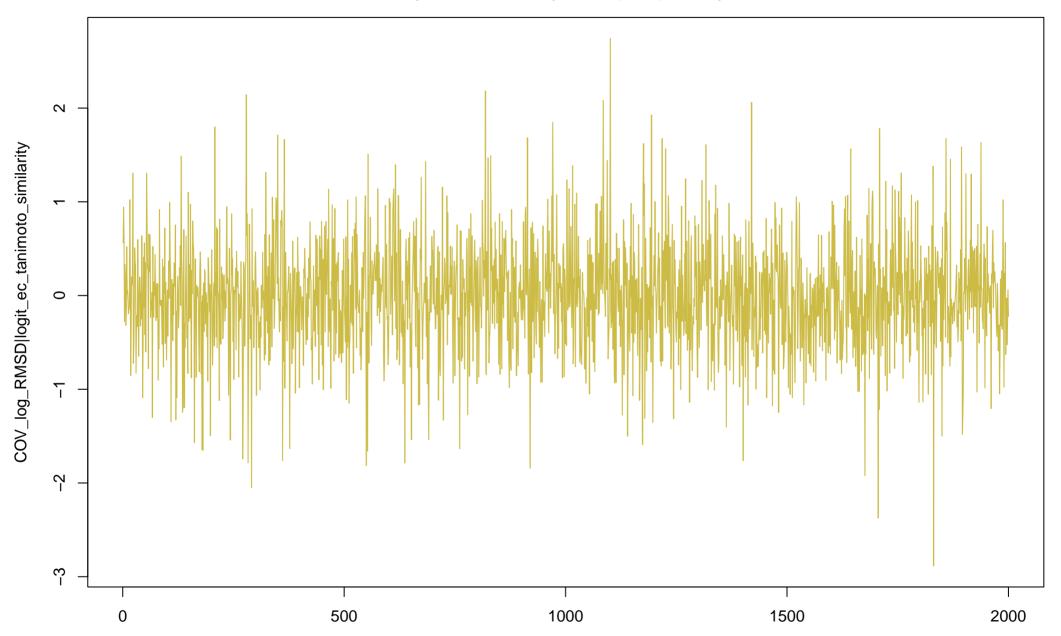
VAR\_mcs\_RingCount ESS = 2000 | BMK = 0.0672 | MCSE(6.27) = 2.46 | stat: TRUE



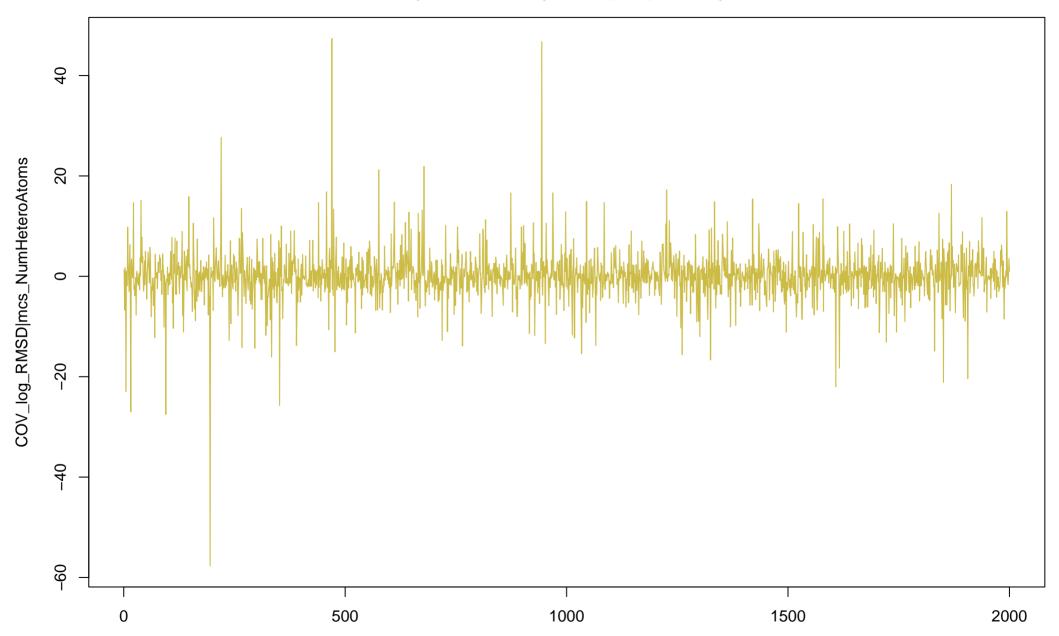
VAR\_docked\_NumRotatableBonds ESS = 2000 | BMK = 0.0444 | MCSE(6.27) = 2.33 | stat: TRUE



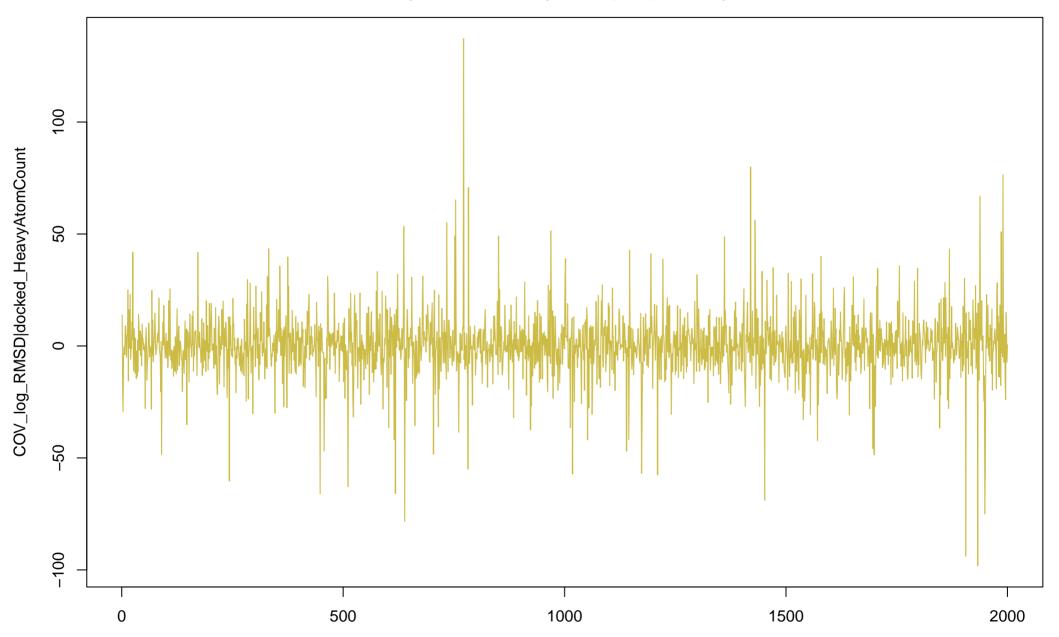




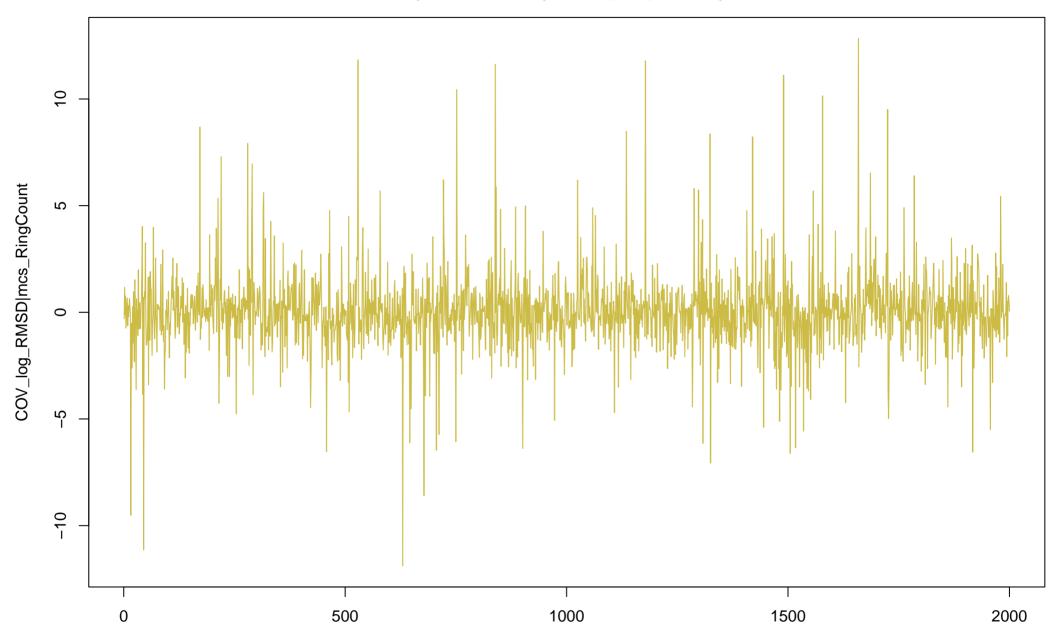
COV\_log\_RMSD|mcs\_NumHeteroAtoms ESS = 2000 | BMK = 0.091 | MCSE(6.27) = 2.28 | stat: TRUE



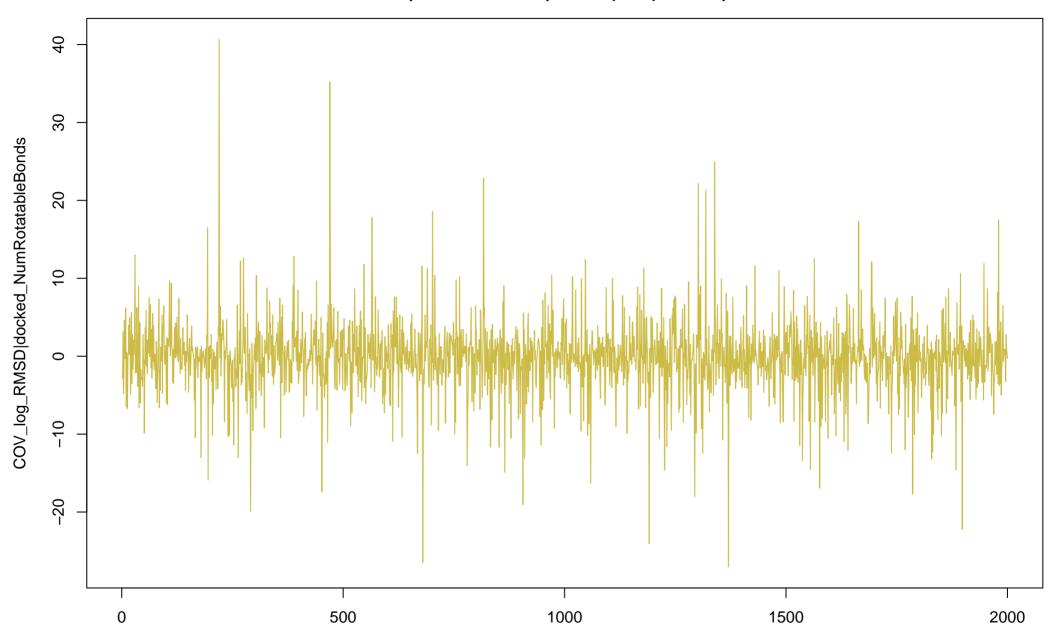
COV\_log\_RMSD|docked\_HeavyAtomCount ESS = 2000 | BMK = 0.0717 | MCSE(6.27) = 2.27 | stat: TRUE

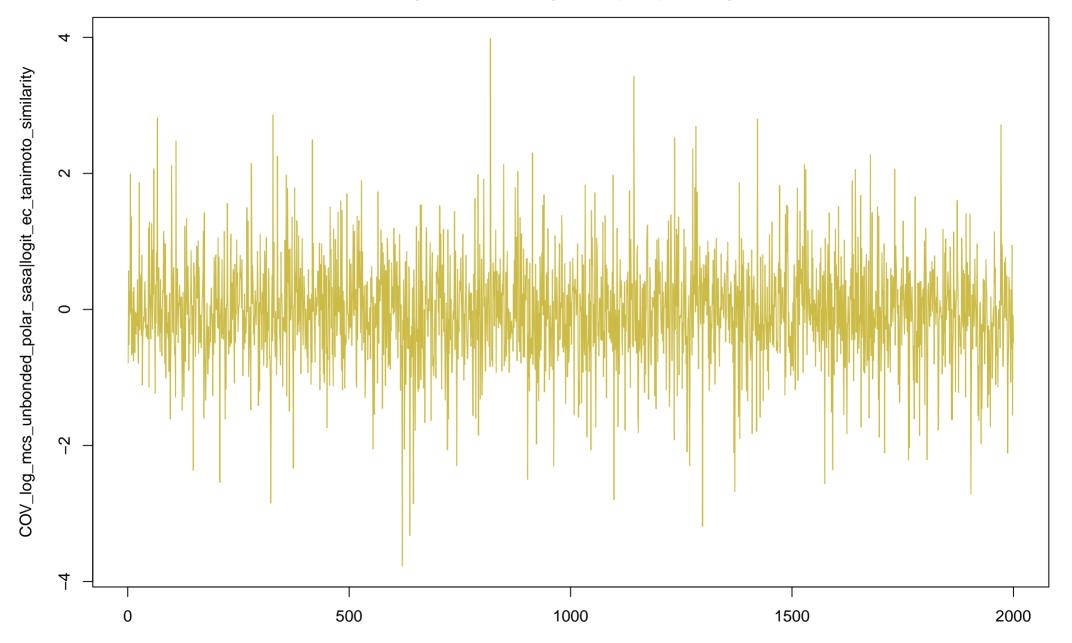


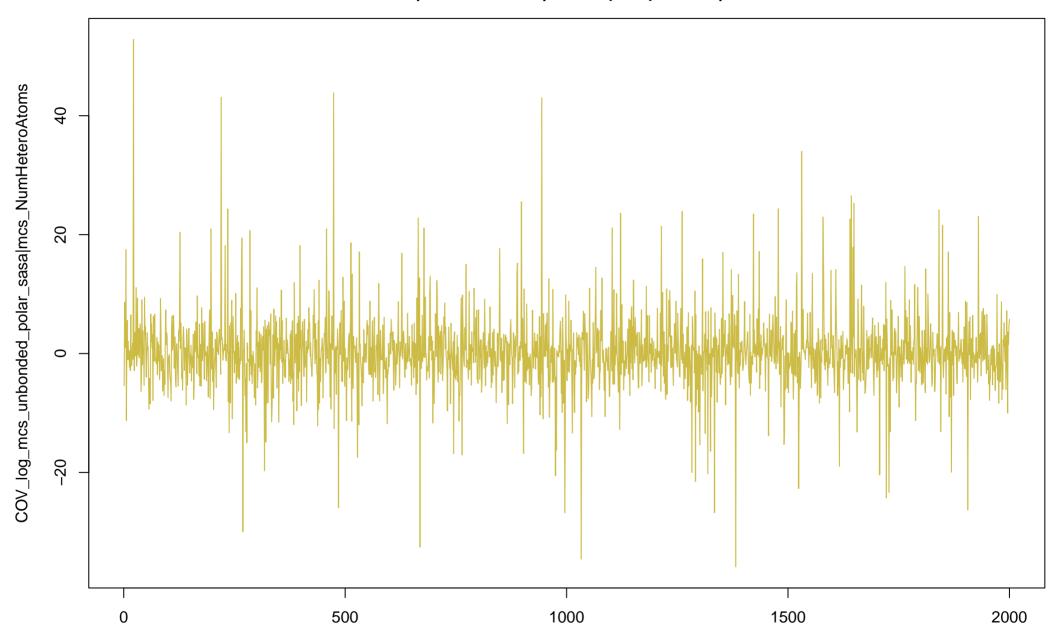
COV\_log\_RMSD|mcs\_RingCount ESS = 2000 | BMK = 0.076 | MCSE(6.27) = 2.36 | stat: TRUE

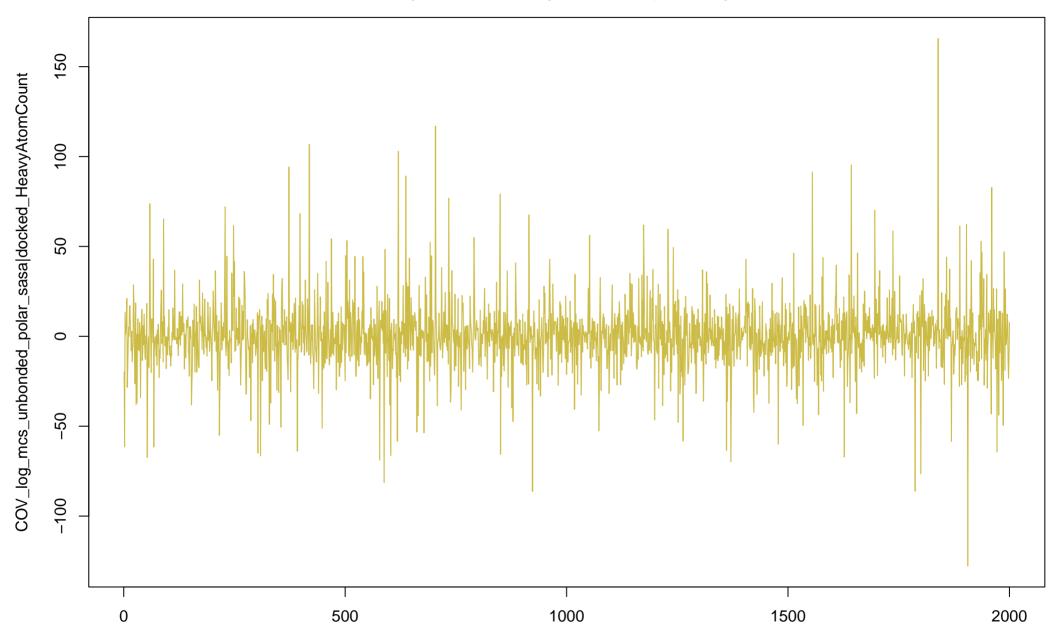


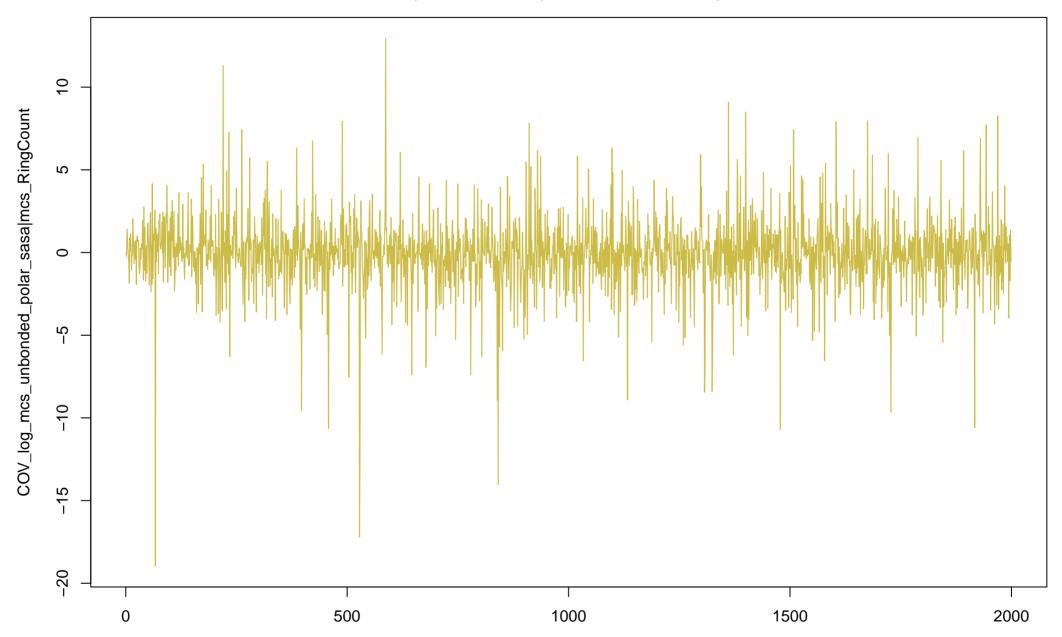
COV\_log\_RMSD|docked\_NumRotatableBonds ESS = 1870 | BMK = 0.0824 | MCSE(6.27) = 2.36 | stat: TRUE

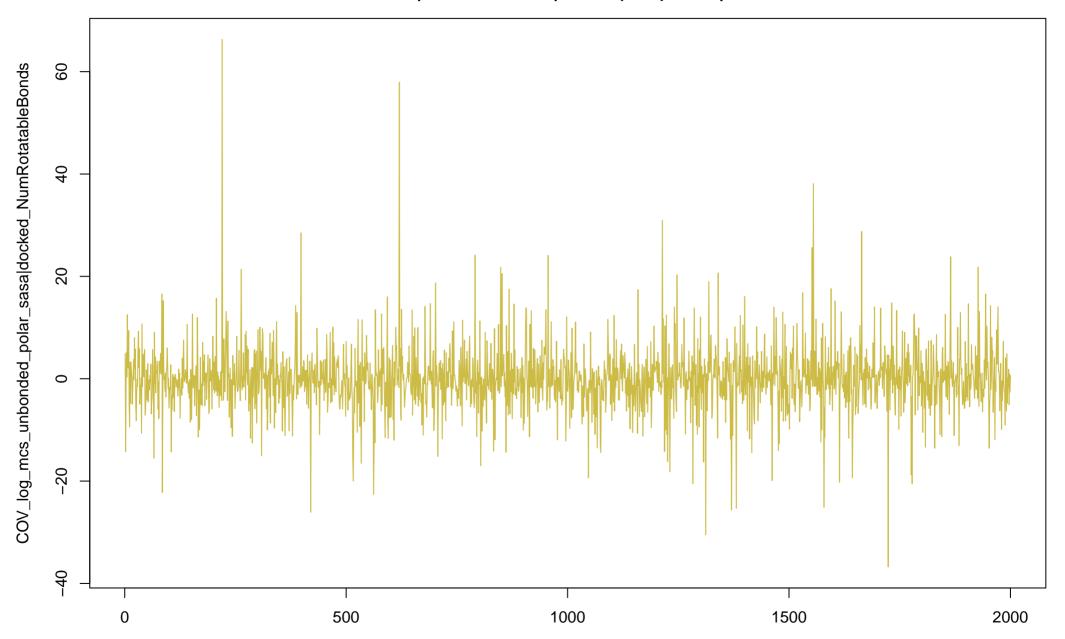


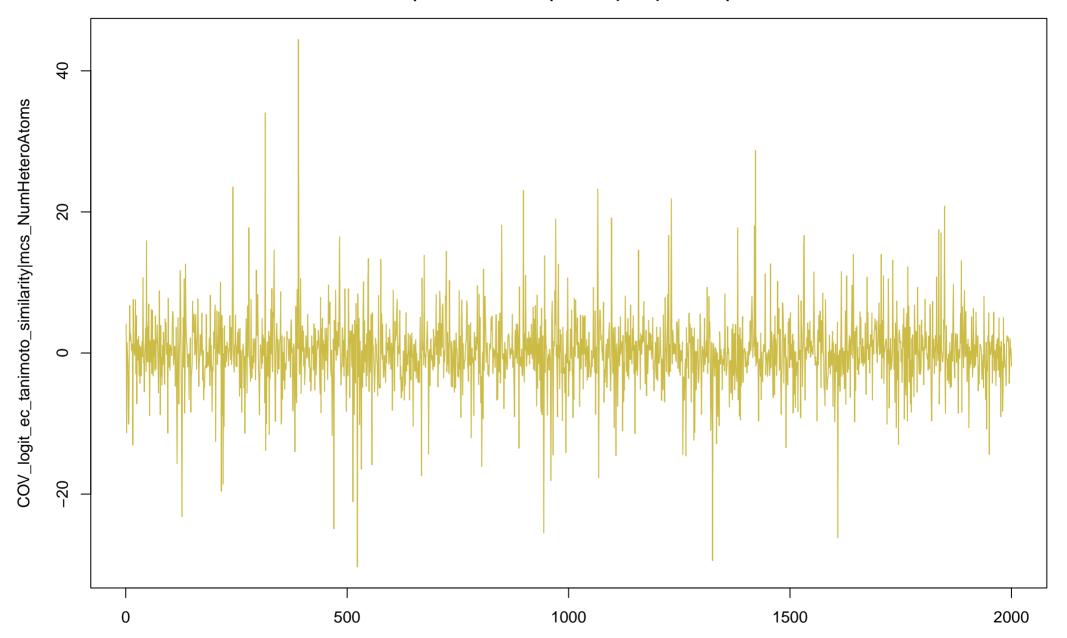


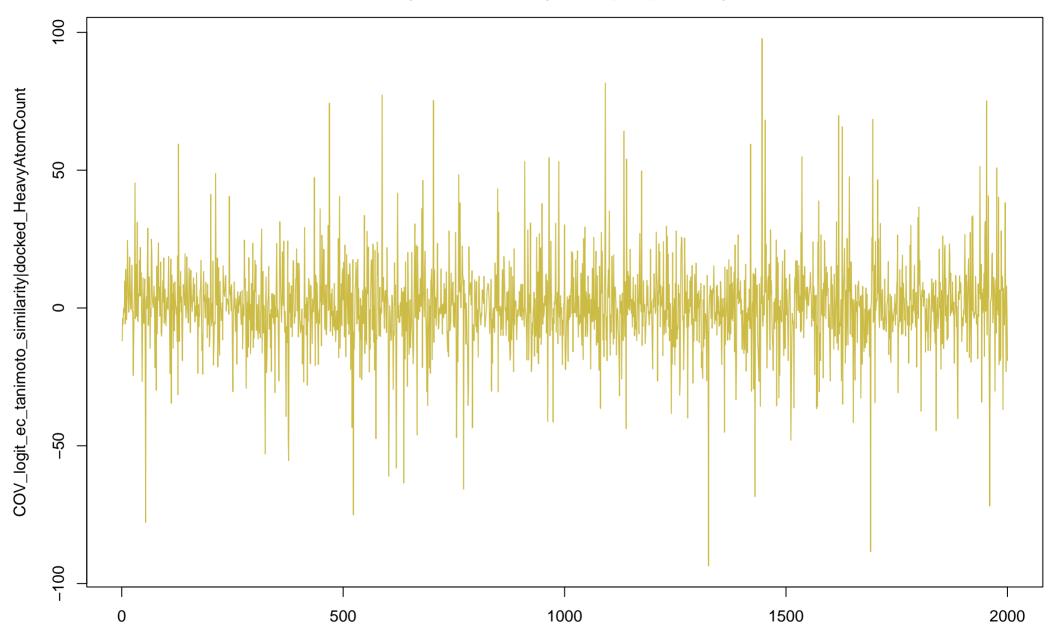


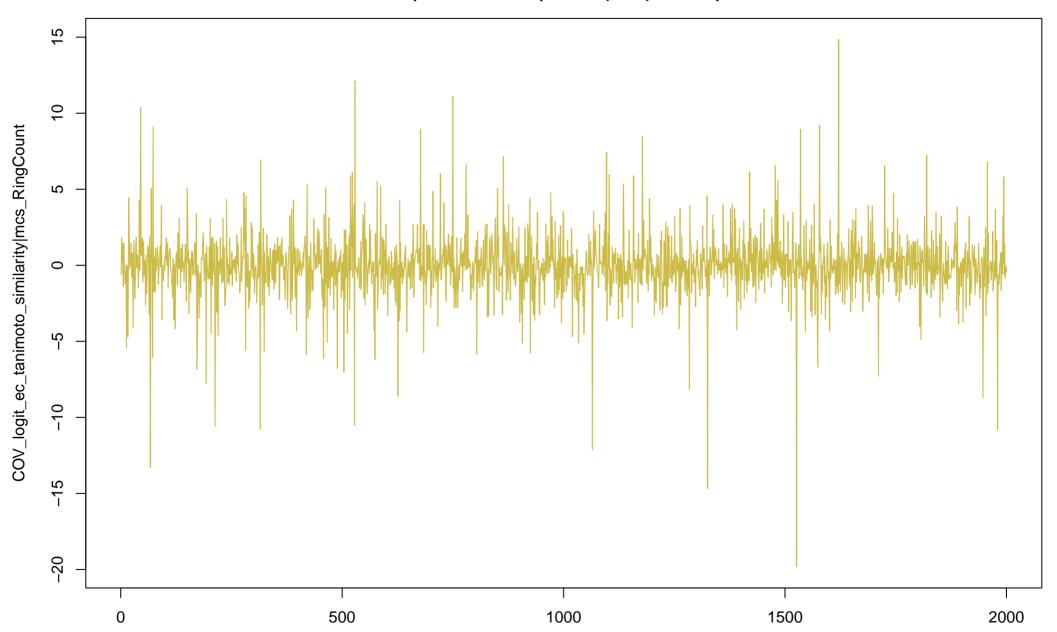


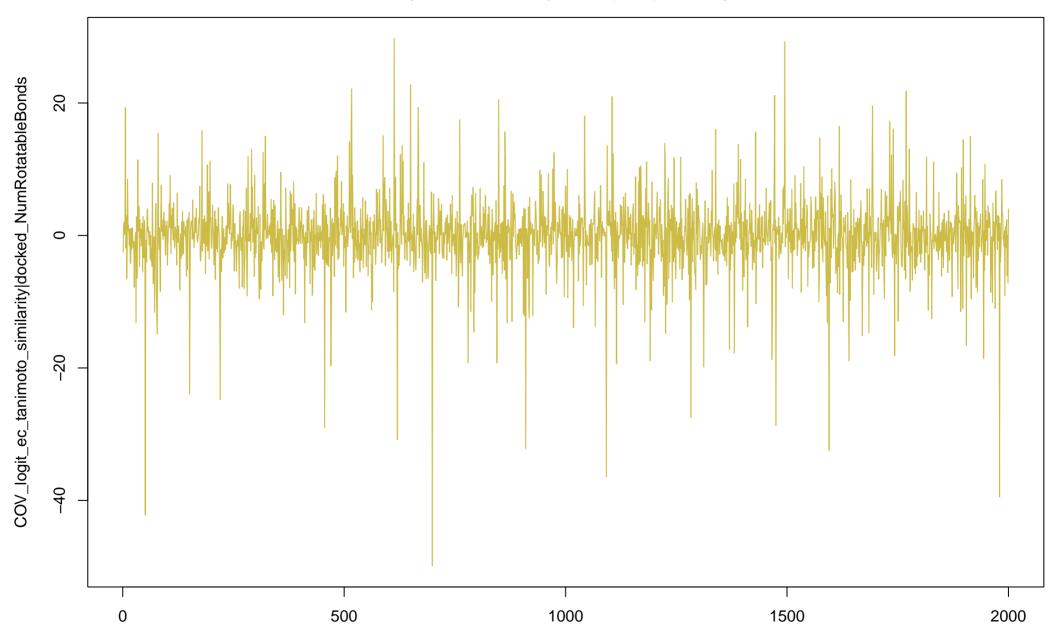


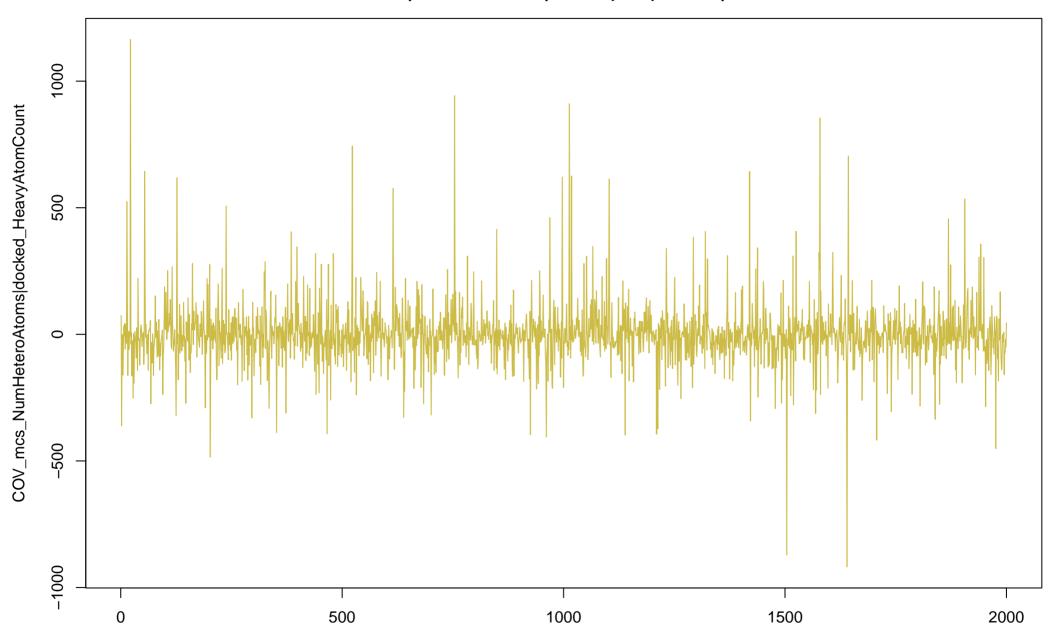




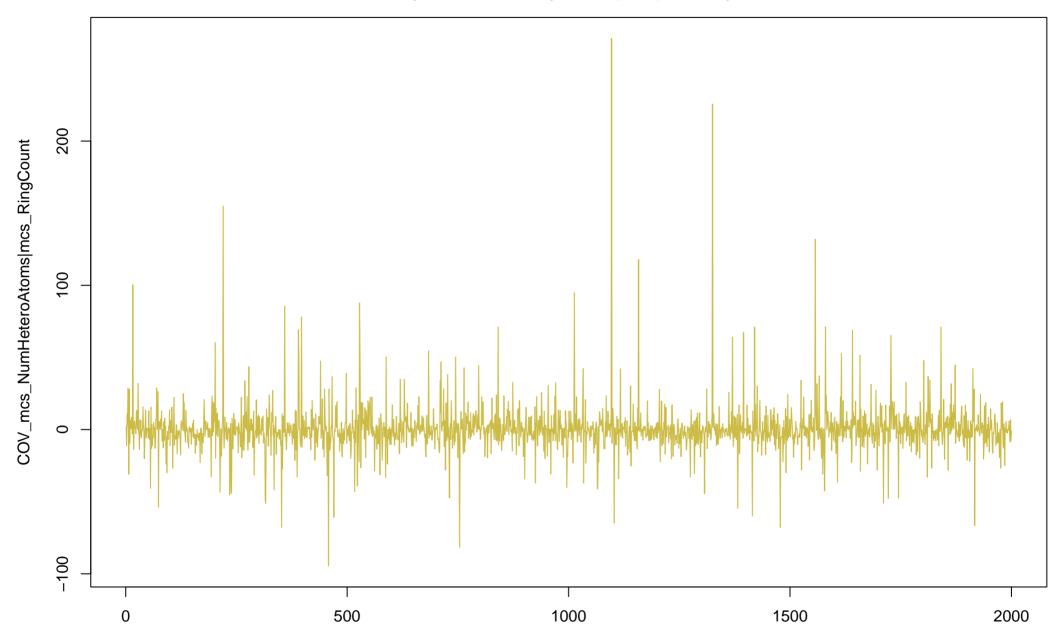


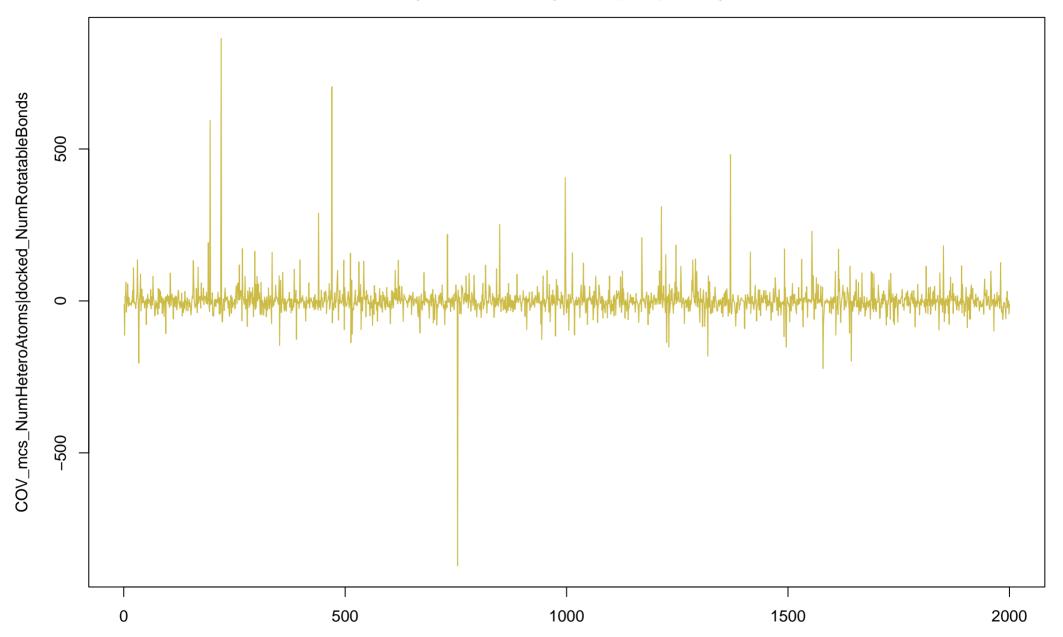




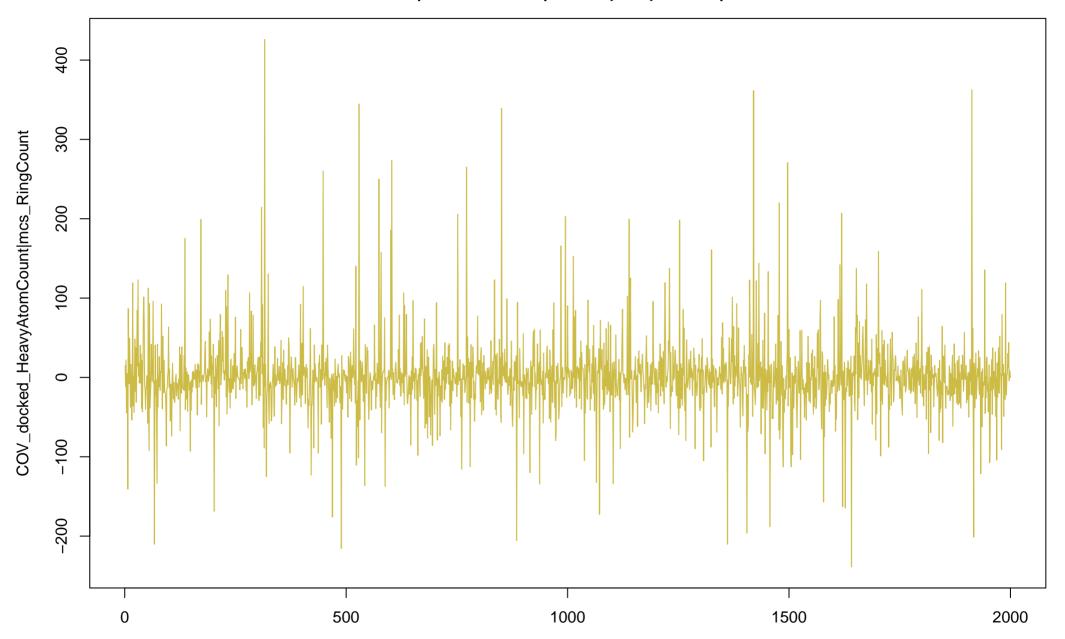


COV\_mcs\_NumHeteroAtoms|mcs\_RingCount ESS = 2000 | BMK = 0.0982 | MCSE(6.27) = 2.23 | stat: TRUE

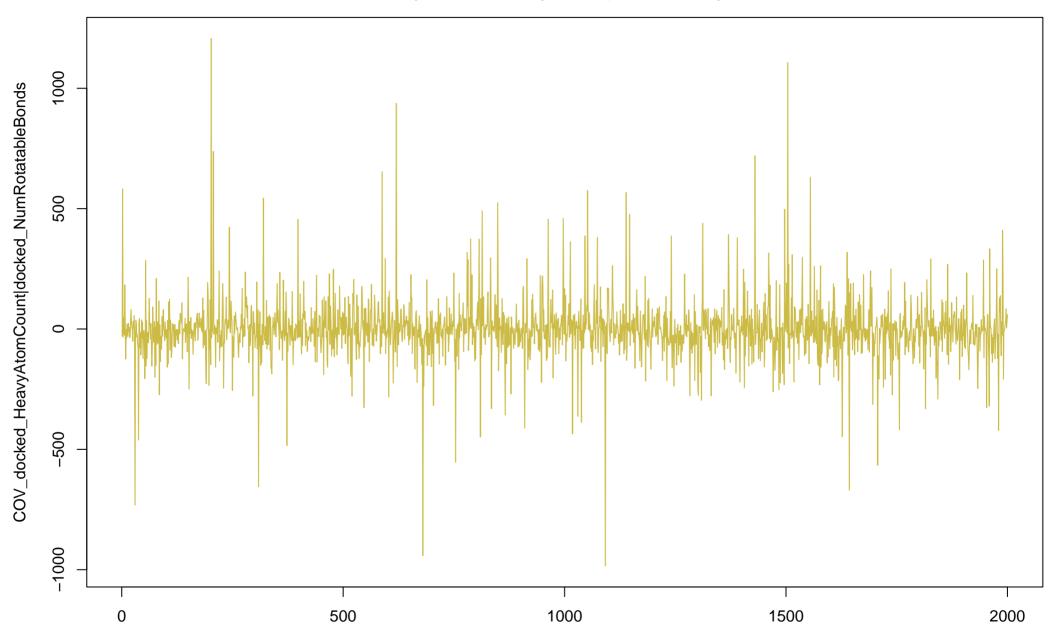




## COV\_docked\_HeavyAtomCount|mcs\_RingCount ESS = 2000 | BMK = 0.103 | MCSE(6.27) = 2.12 | stat: TRUE



## COV\_docked\_HeavyAtomCount|docked\_NumRotatableBonds ESS = 2000 | BMK = 0.092 | MCSE(6.27) = 2.28 | stat: TRUE



## COV\_mcs\_RingCount|docked\_NumRotatableBonds ESS = 2000 | BMK = 0.107 | MCSE(6.27) = 2.17 | stat: TRUE

