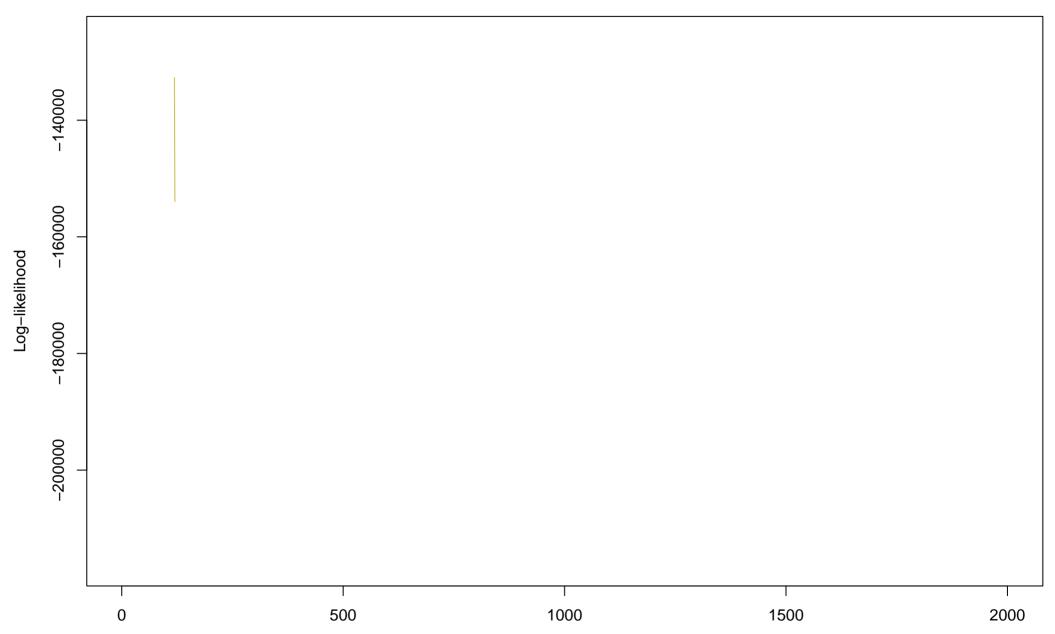
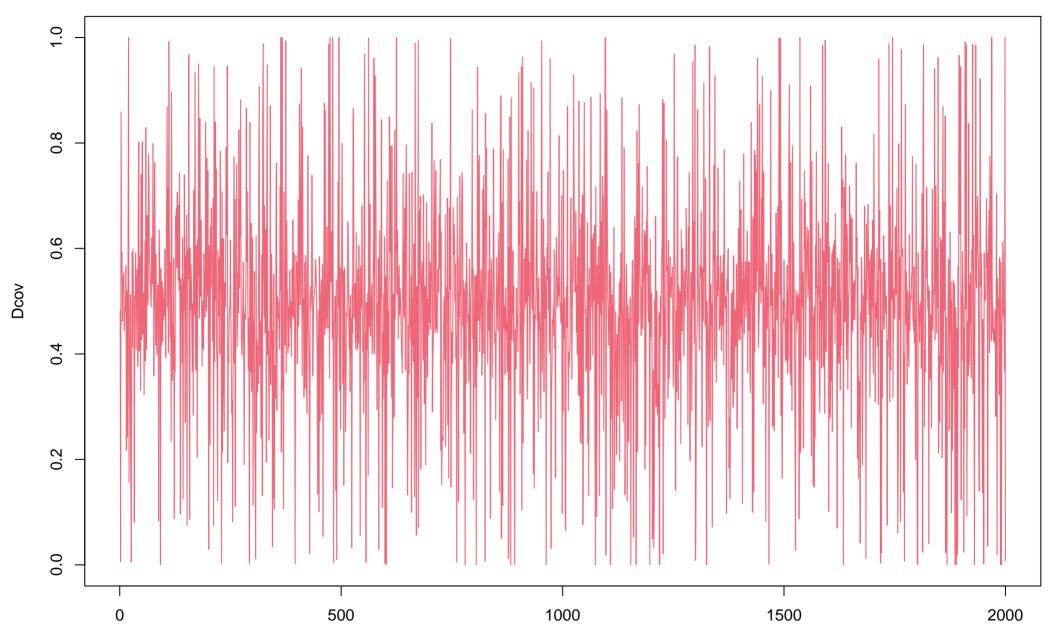


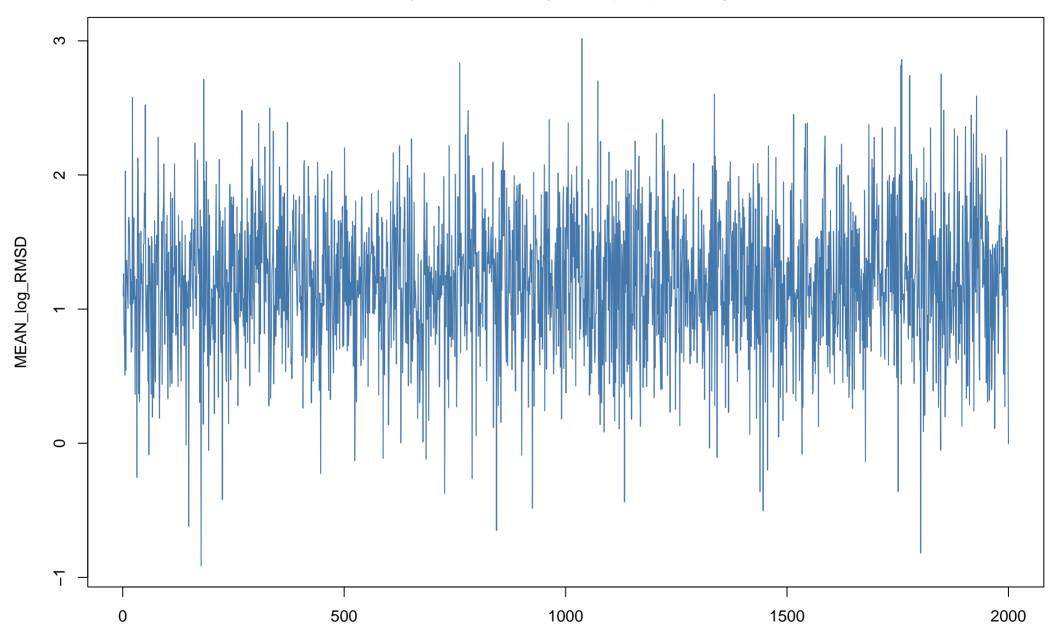
Log-likelihood ESS = NA | BMK = 0.0618 | MCSE(6.27) = 9.79 | stat: FALSE



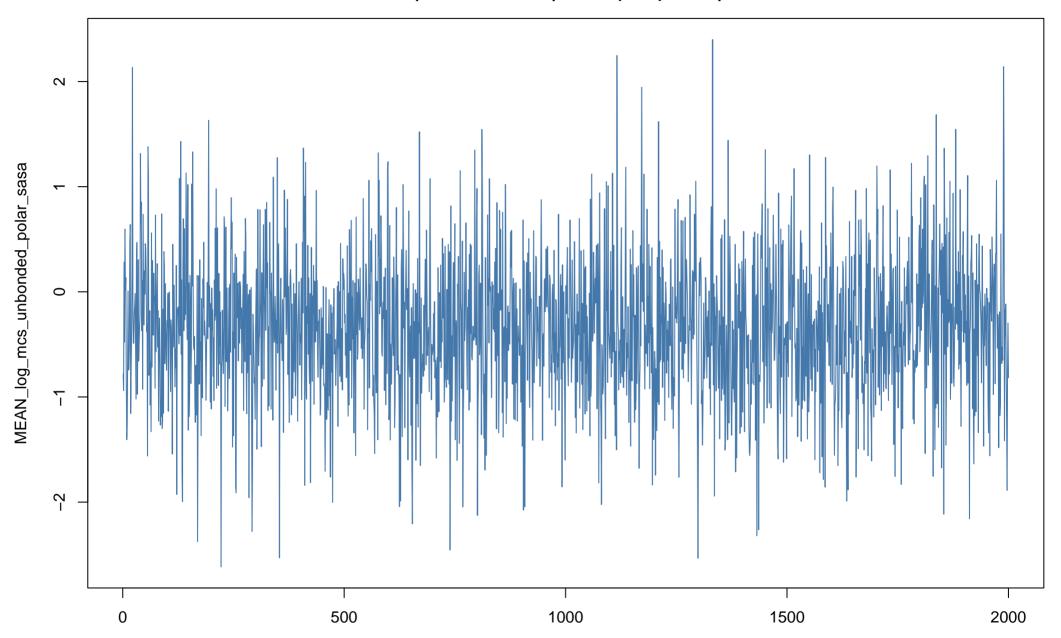
Dcov ESS = 2000 | BMK = 0.0516 | MCSE(6.27) = 2.19 | stat: TRUE



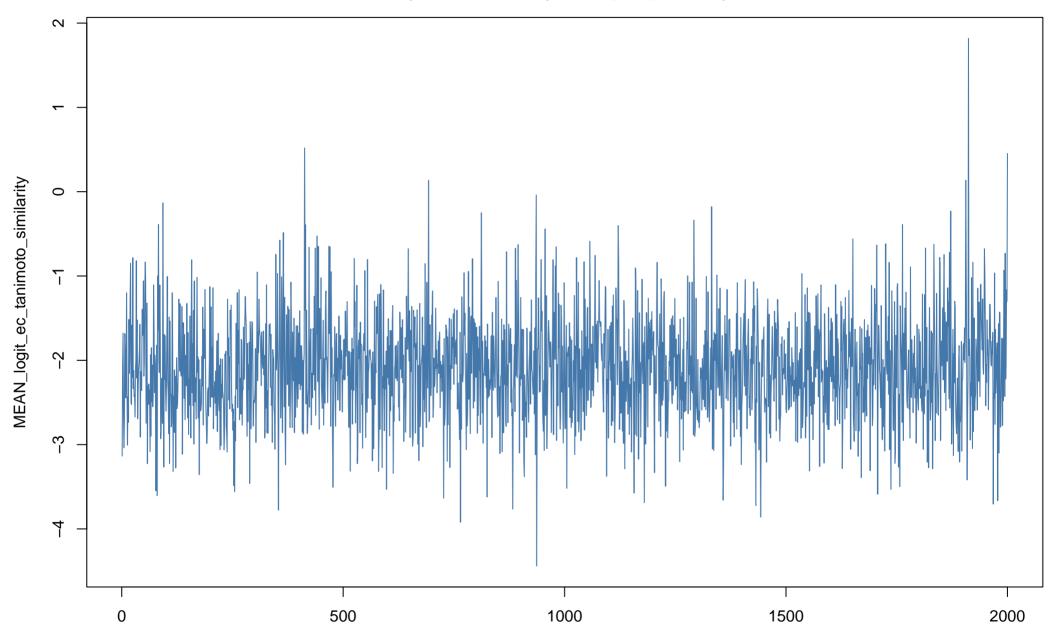
MEAN\_log\_RMSD ESS = 2000 | BMK = 0.0546 | MCSE(6.27) = 2.21 | stat: TRUE



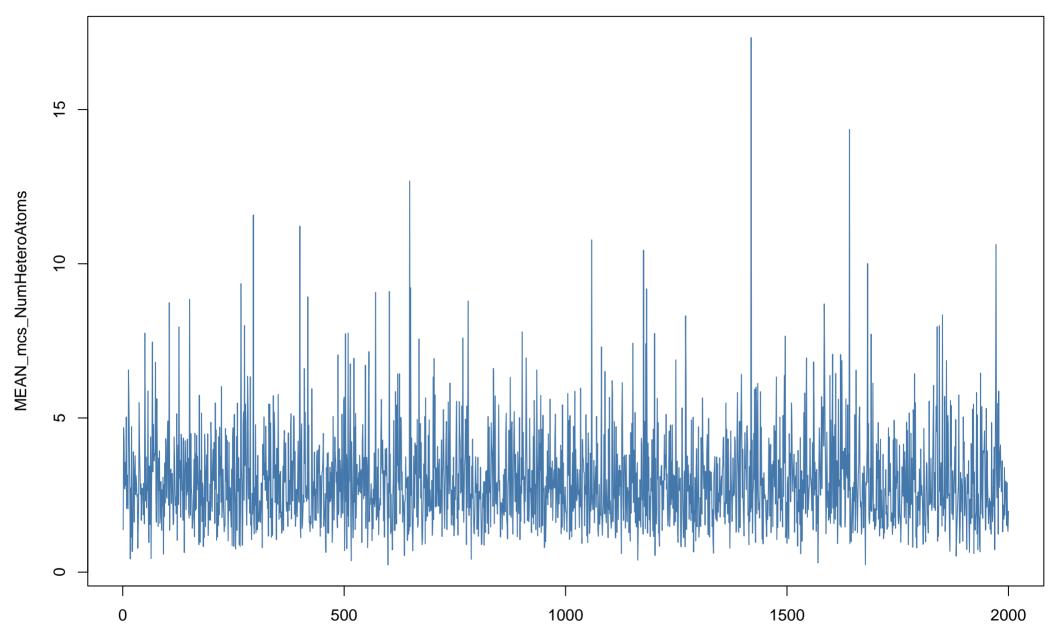
MEAN\_log\_mcs\_unbonded\_polar\_sasa ESS = 1780 | BMK = 0.0521 | MCSE(6.27) = 2.4 | stat: TRUE



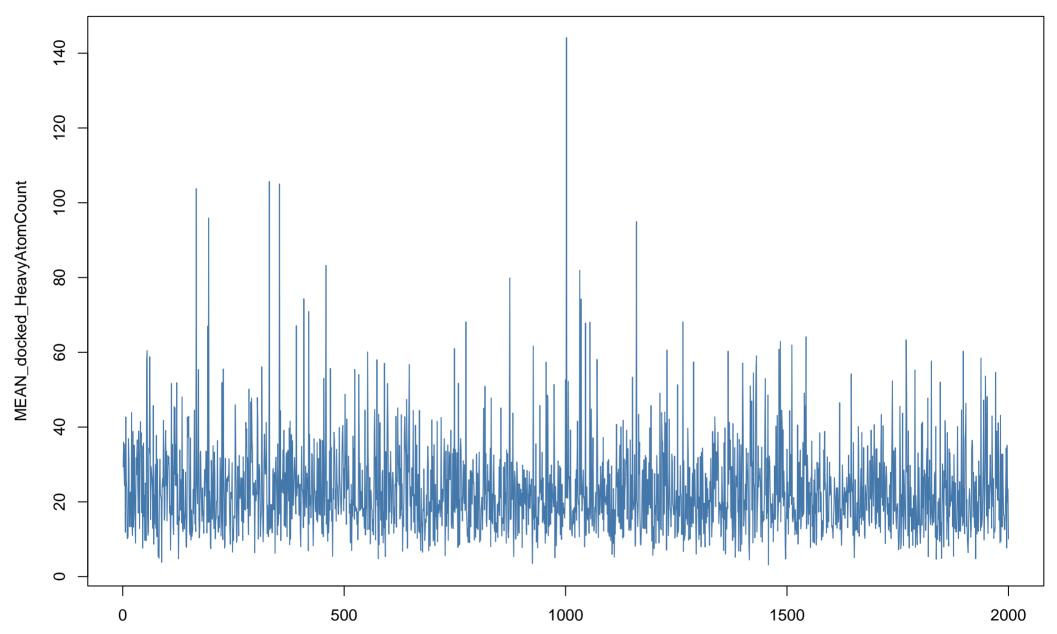
MEAN\_logit\_ec\_tanimoto\_similarity ESS = 2000 | BMK = 0.0343 | MCSE(6.27) = 2.28 | stat: TRUE



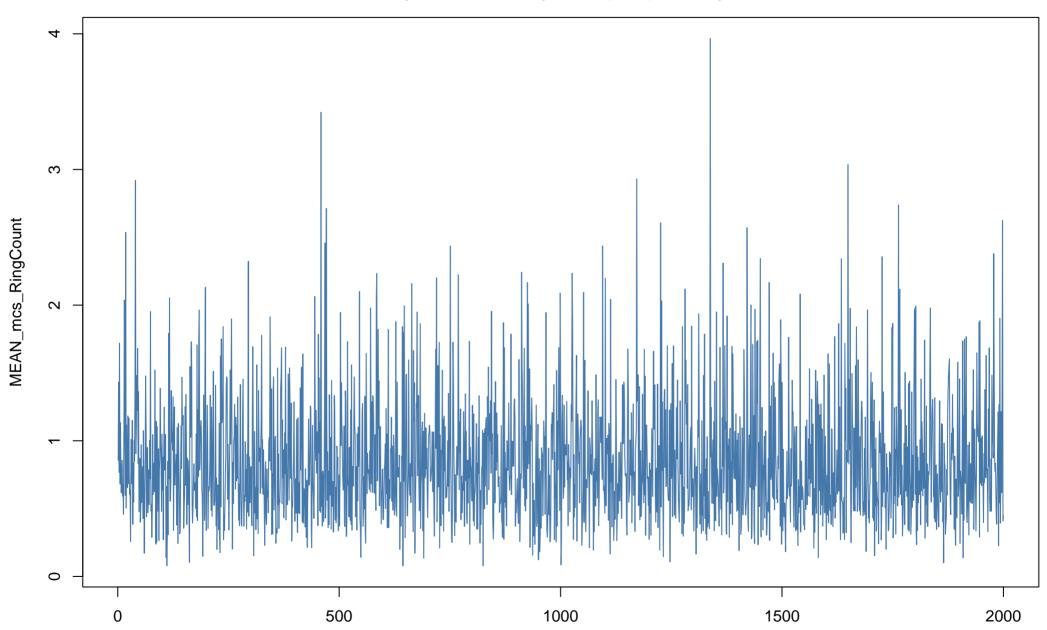
MEAN\_mcs\_NumHeteroAtoms ESS = 2000 | BMK = 0.0653 | MCSE(6.27) = 2.13 | stat: TRUE



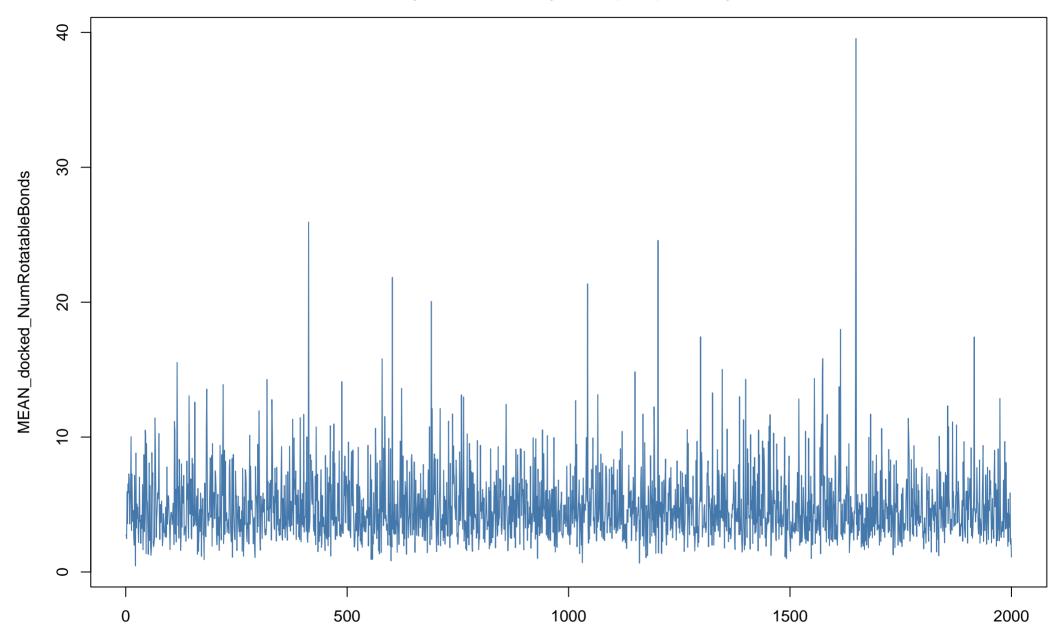
MEAN\_docked\_HeavyAtomCount ESS = 2000 | BMK = 0.0569 | MCSE(6.27) = 2.2 | stat: TRUE



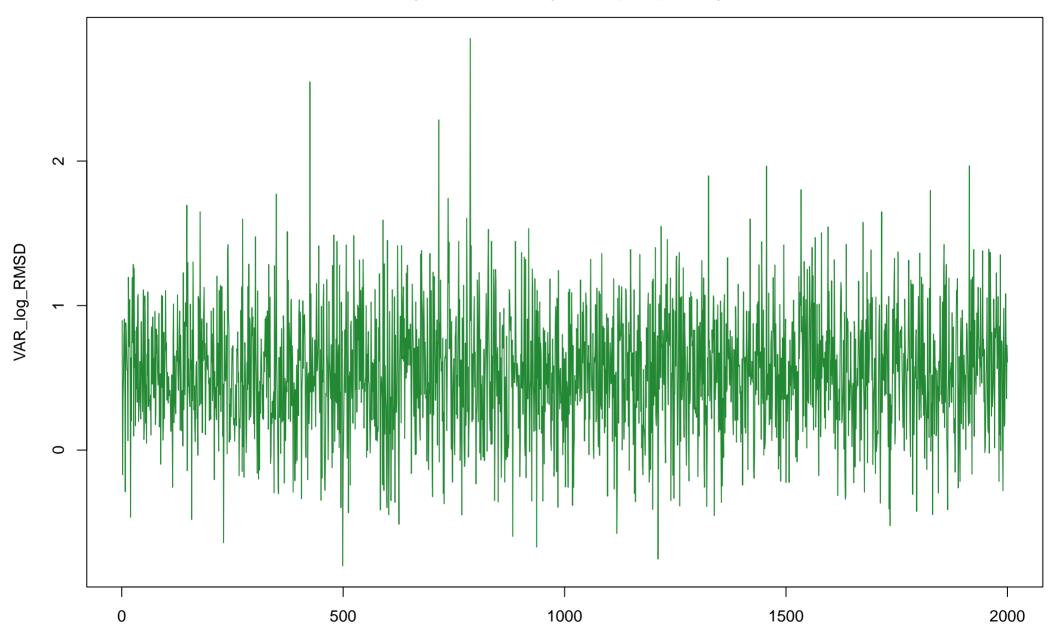
MEAN\_mcs\_RingCount ESS = 2000 | BMK = 0.0425 | MCSE(6.27) = 2.29 | stat: TRUE



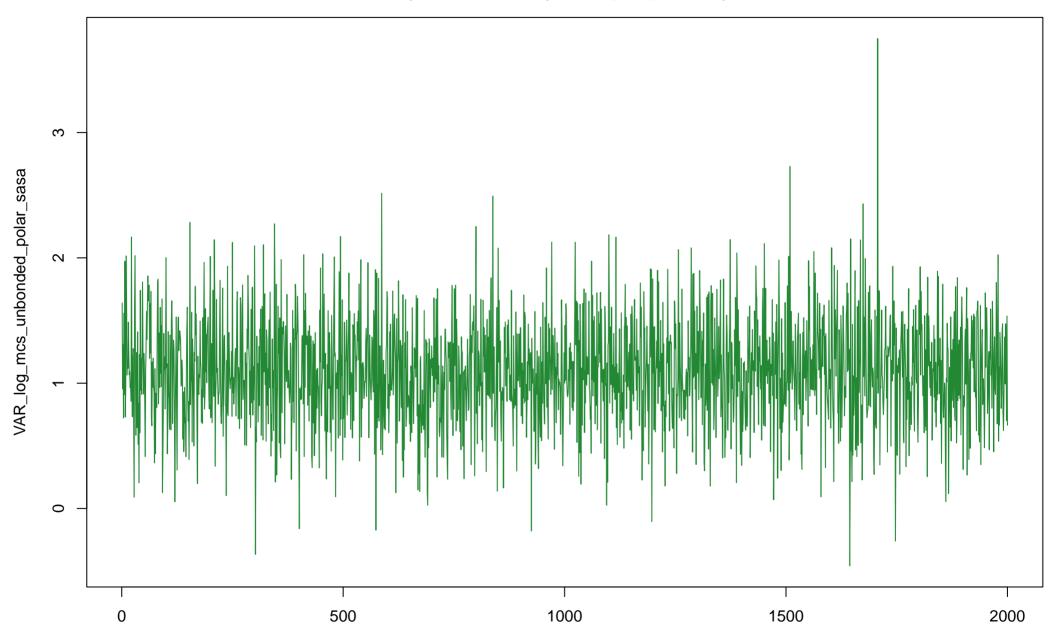
MEAN\_docked\_NumRotatableBonds ESS = 2000 | BMK = 0.0725 | MCSE(6.27) = 2.16 | stat: TRUE



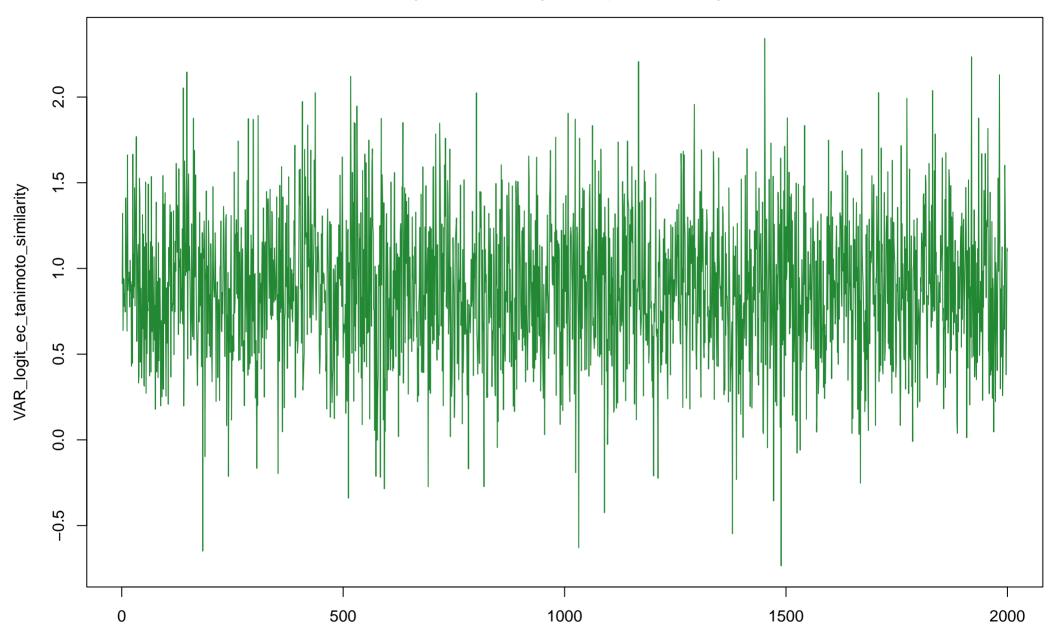
VAR\_log\_RMSD ESS = 2000 | BMK = 0.0521 | MCSE(6.27) = 2.3 | stat: TRUE



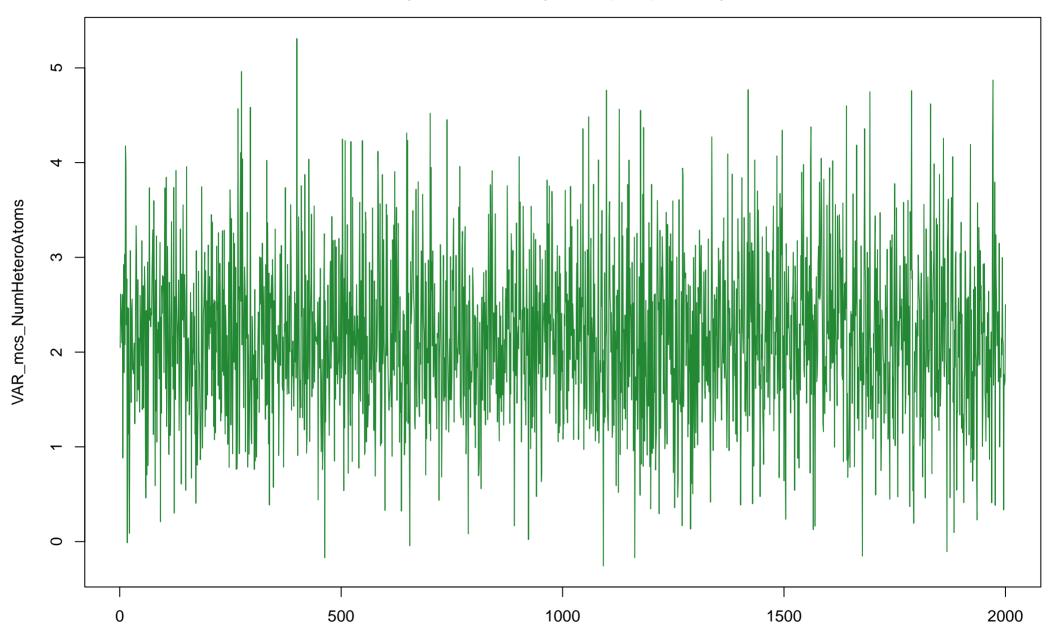
VAR\_log\_mcs\_unbonded\_polar\_sasa ESS = 2000 | BMK = 0.0424 | MCSE(6.27) = 2.26 | stat: TRUE



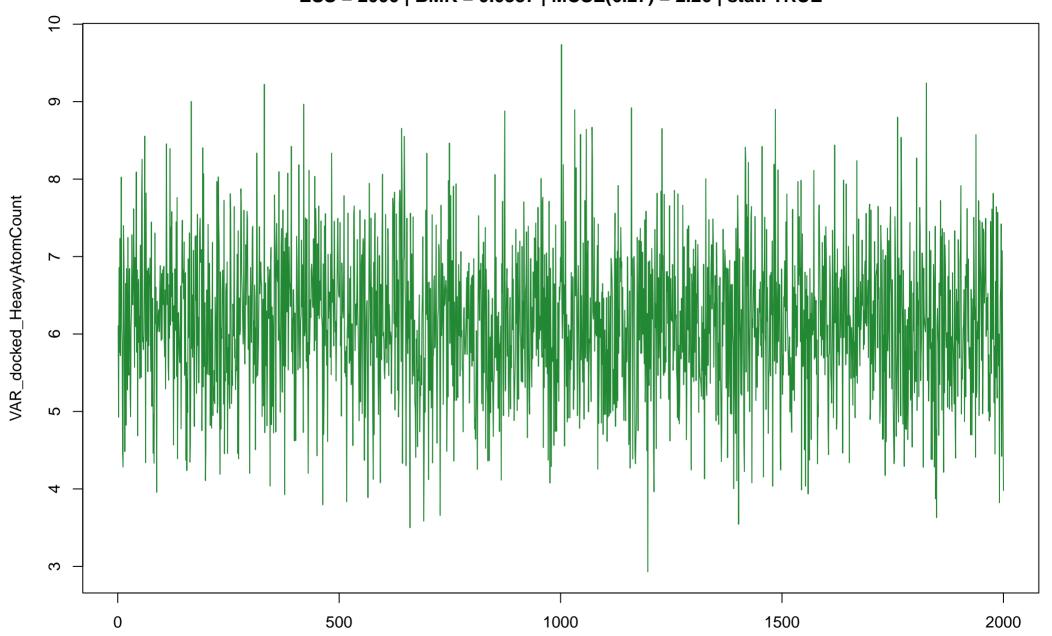
VAR\_logit\_ec\_tanimoto\_similarity ESS = 2000 | BMK = 0.029 | MCSE(6.27) = 2.27 | stat: TRUE



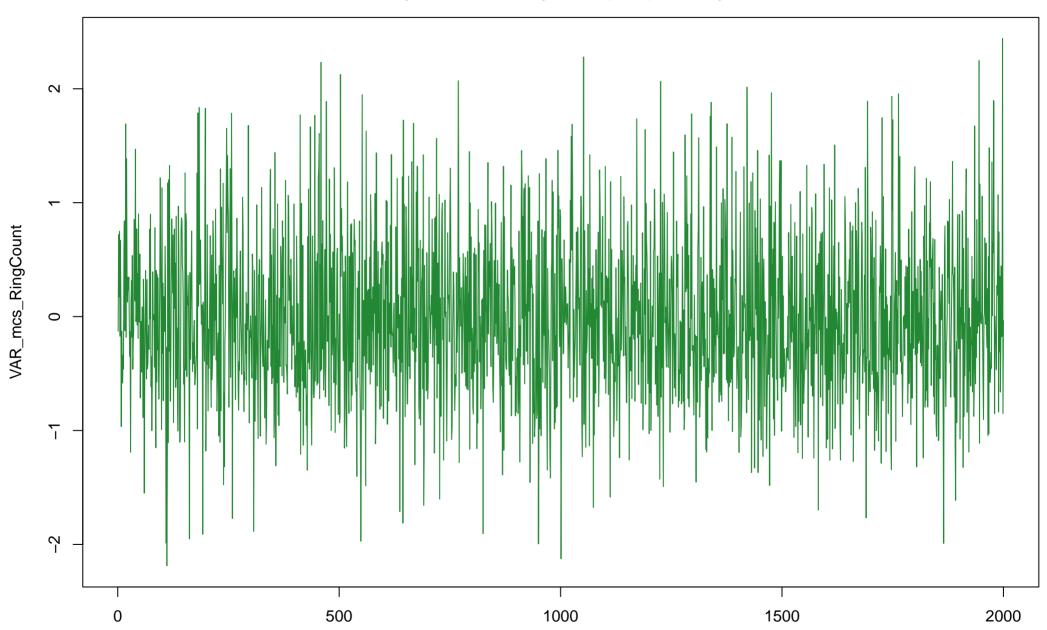
VAR\_mcs\_NumHeteroAtoms ESS = 2000 | BMK = 0.0461 | MCSE(6.27) = 2.23 | stat: TRUE



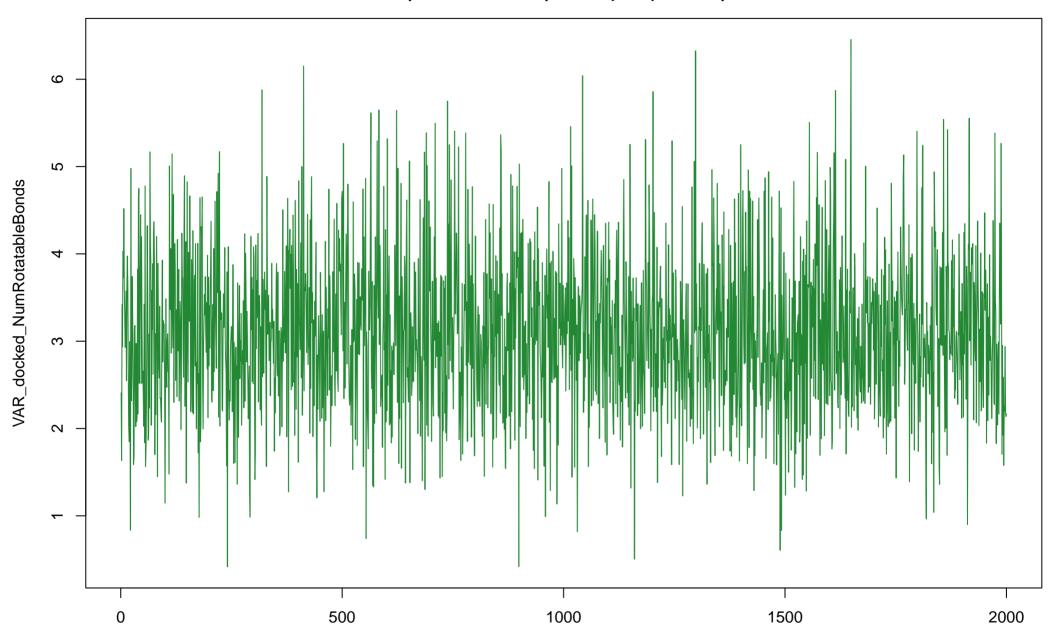
VAR\_docked\_HeavyAtomCount ESS = 2000 | BMK = 0.0387 | MCSE(6.27) = 2.26 | stat: TRUE

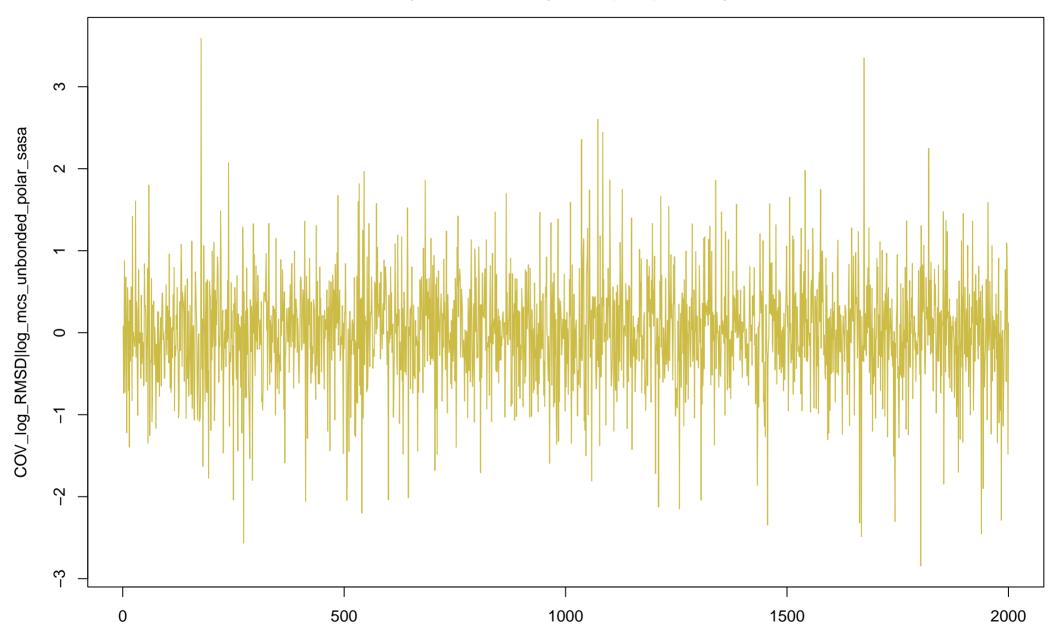


VAR\_mcs\_RingCount ESS = 2000 | BMK = 0.0411 | MCSE(6.27) = 2.19 | stat: TRUE

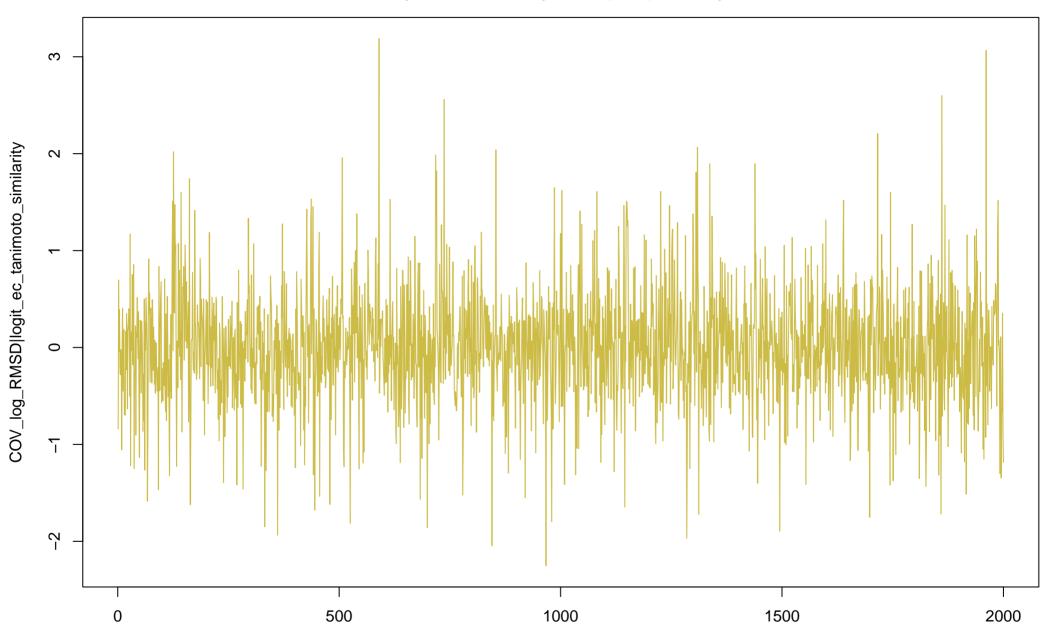


VAR\_docked\_NumRotatableBonds ESS = 2000 | BMK = 0.0321 | MCSE(6.27) = 2.22 | stat: TRUE

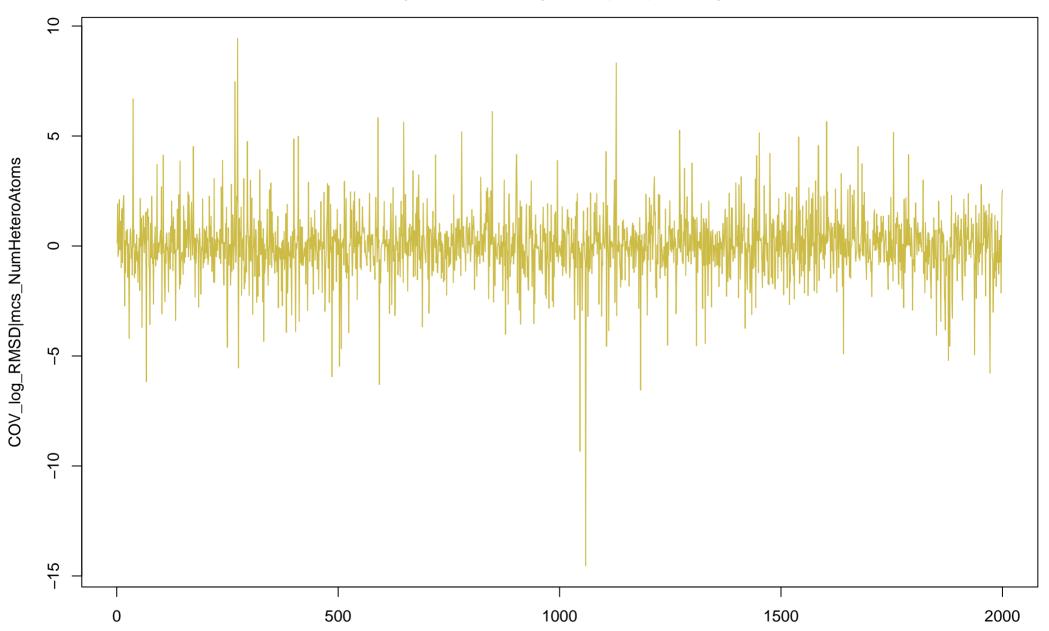




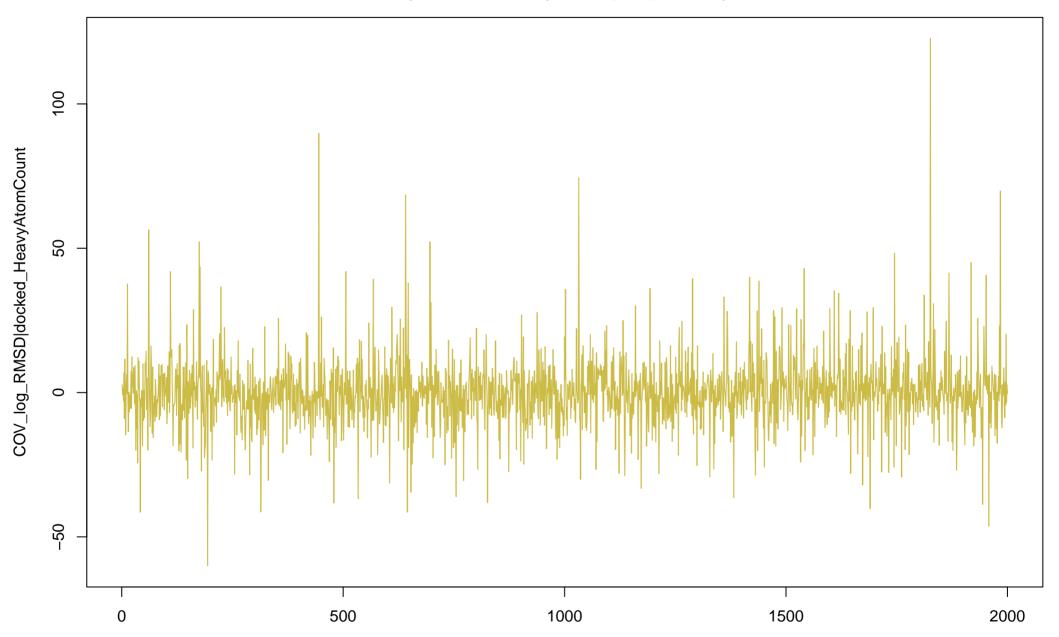
COV\_log\_RMSD|logit\_ec\_tanimoto\_similarity ESS = 1840 | BMK = 0.0503 | MCSE(6.27) = 2.58 | stat: TRUE



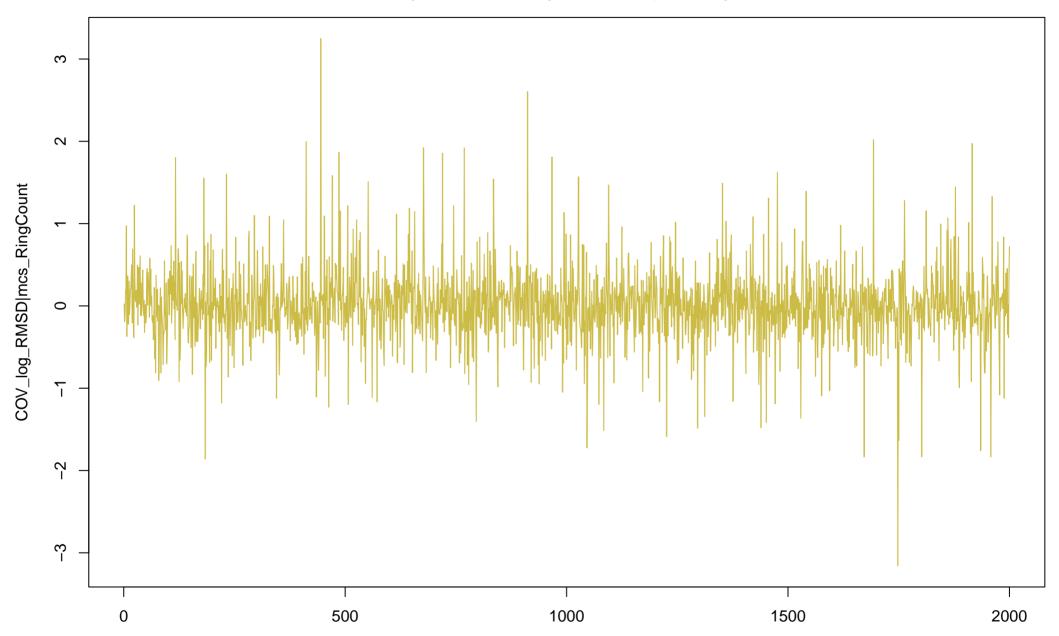
COV\_log\_RMSD|mcs\_NumHeteroAtoms ESS = 1870 | BMK = 0.0764 | MCSE(6.27) = 2.32 | stat: TRUE



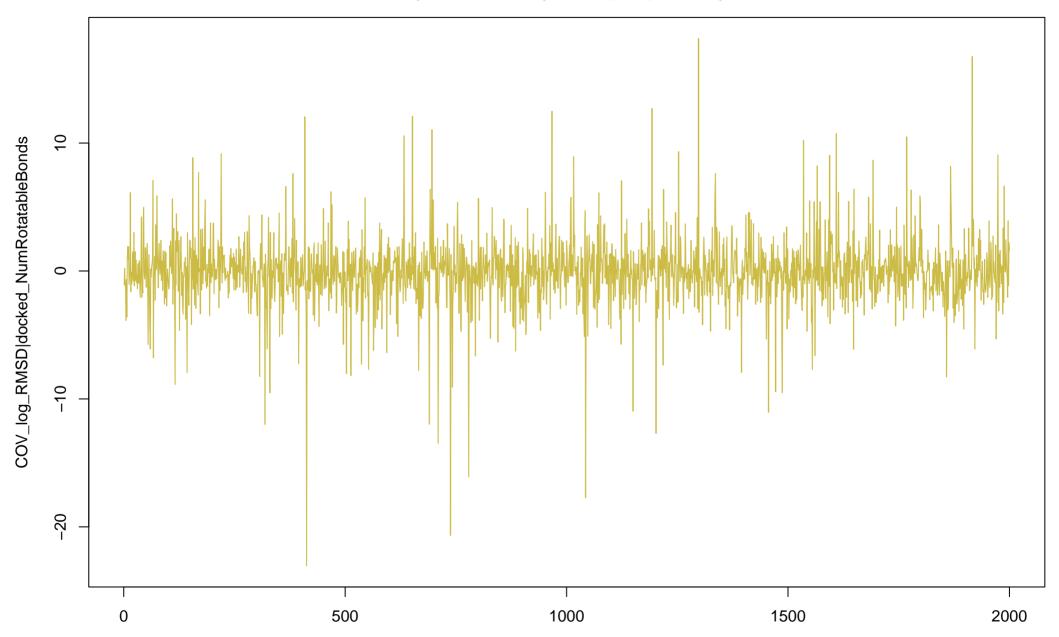
COV\_log\_RMSD|docked\_HeavyAtomCount ESS = 2000 | BMK = 0.0978 | MCSE(6.27) = 2.27 | stat: TRUE

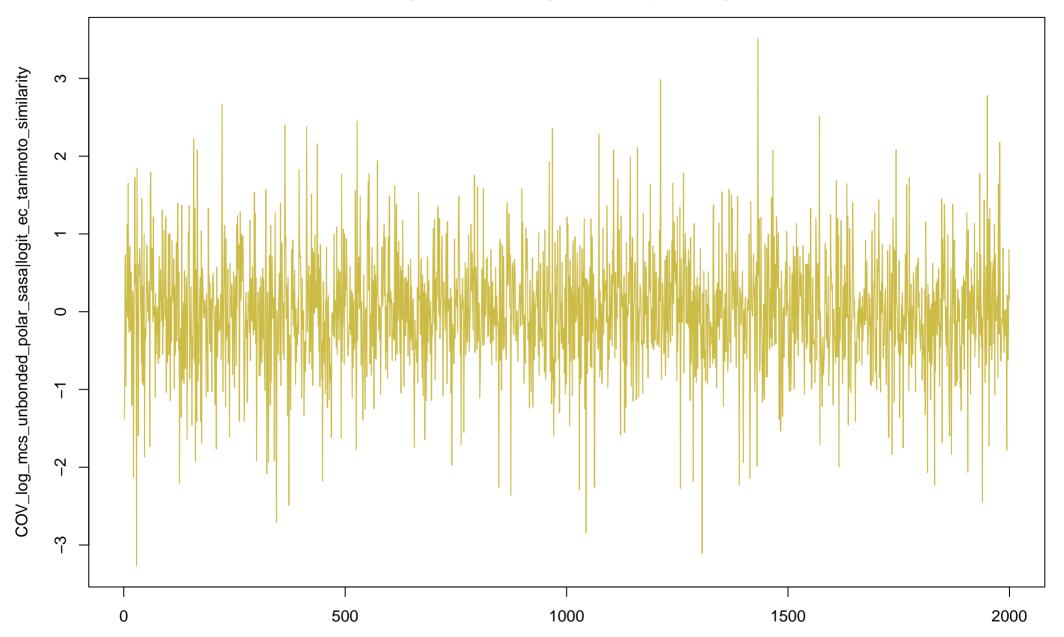


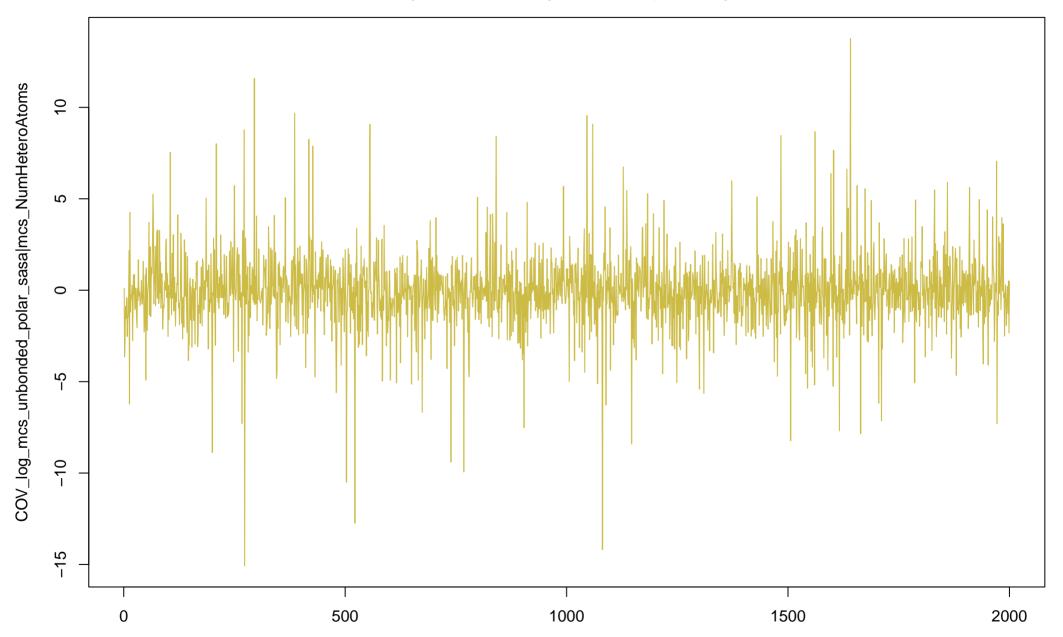
COV\_log\_RMSD|mcs\_RingCount ESS = 2000 | BMK = 0.0921 | MCSE(6.27) = 2.26 | stat: TRUE

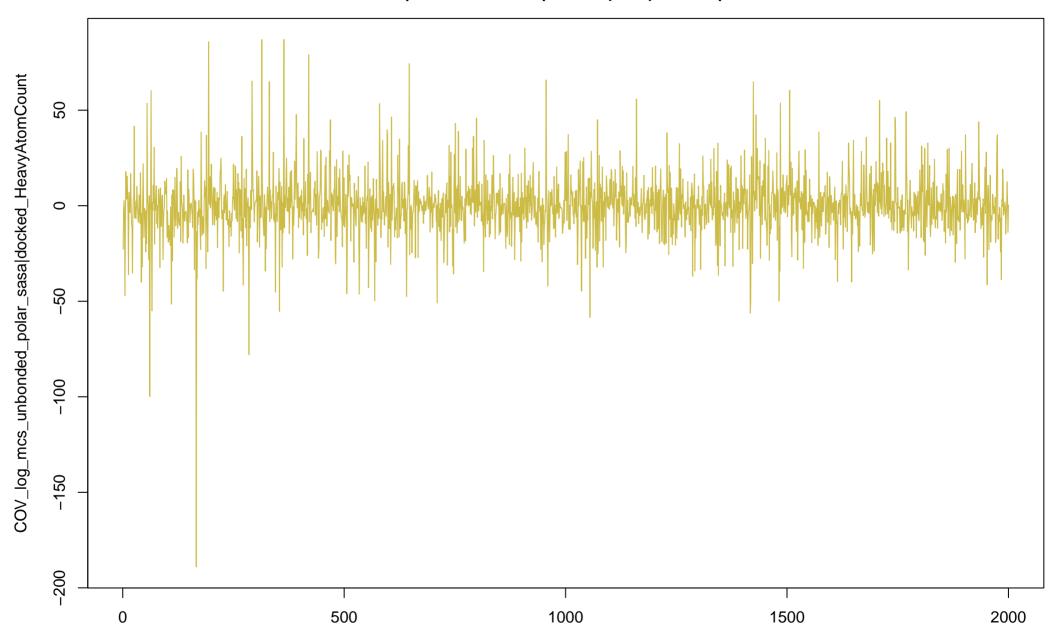


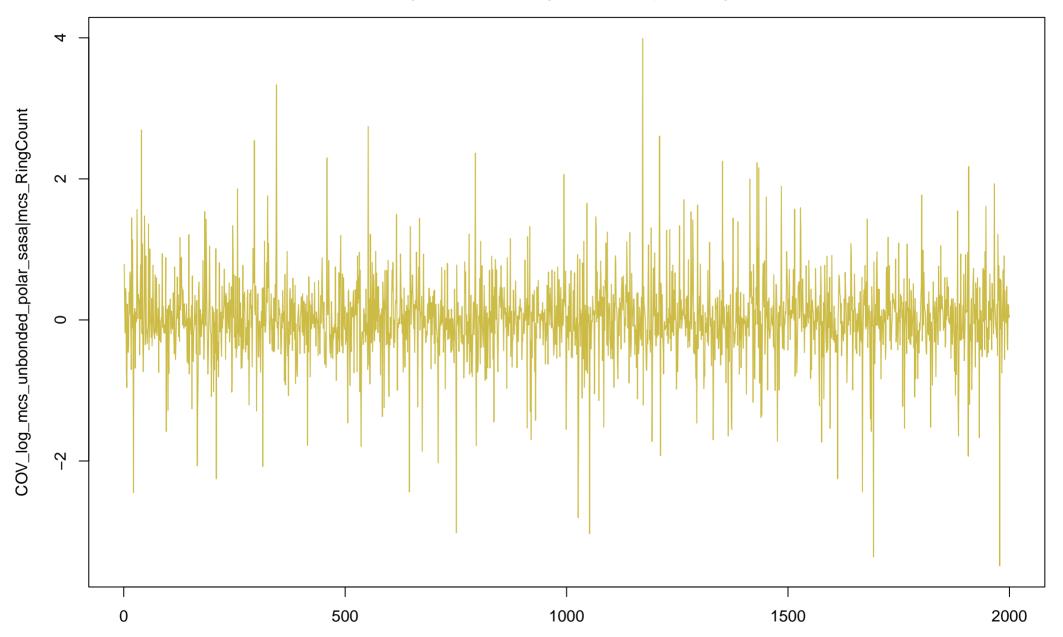
## COV\_log\_RMSD|docked\_NumRotatableBonds ESS = 2000 | BMK = 0.088 | MCSE(6.27) = 2.32 | stat: TRUE

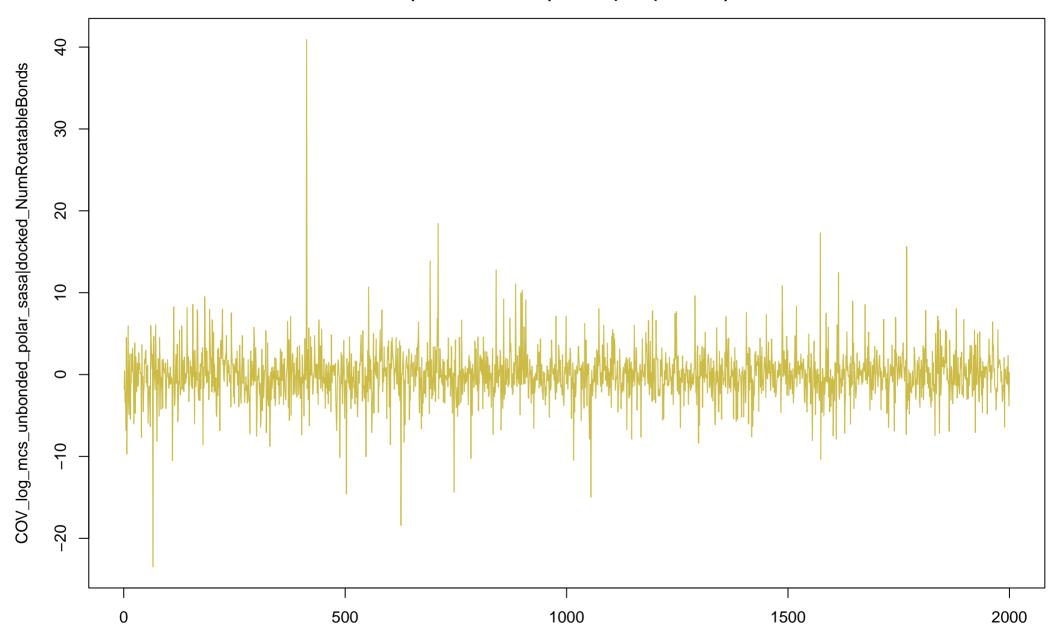


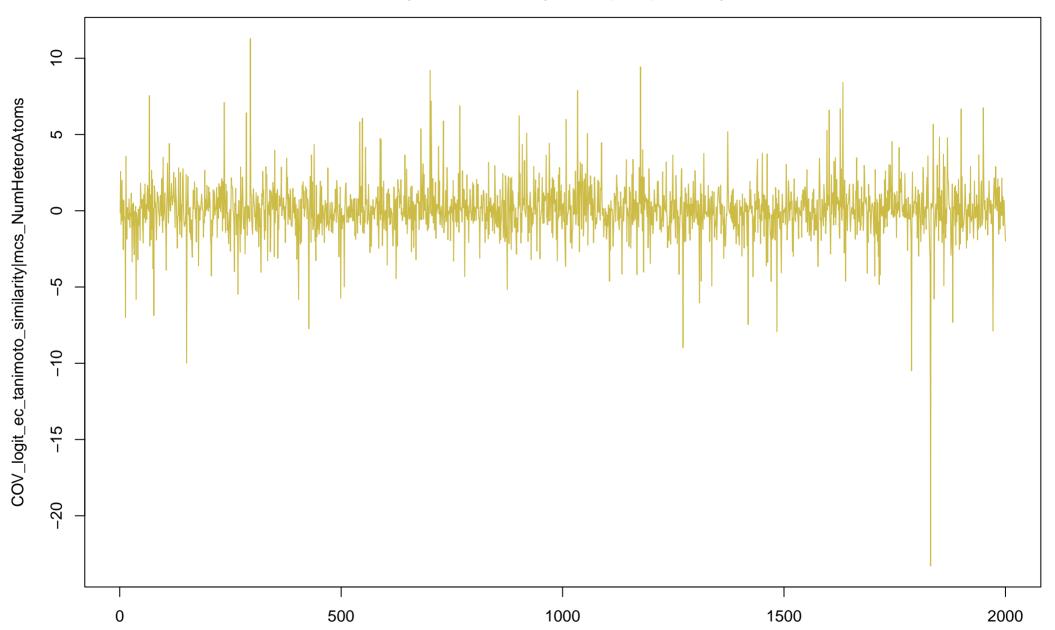


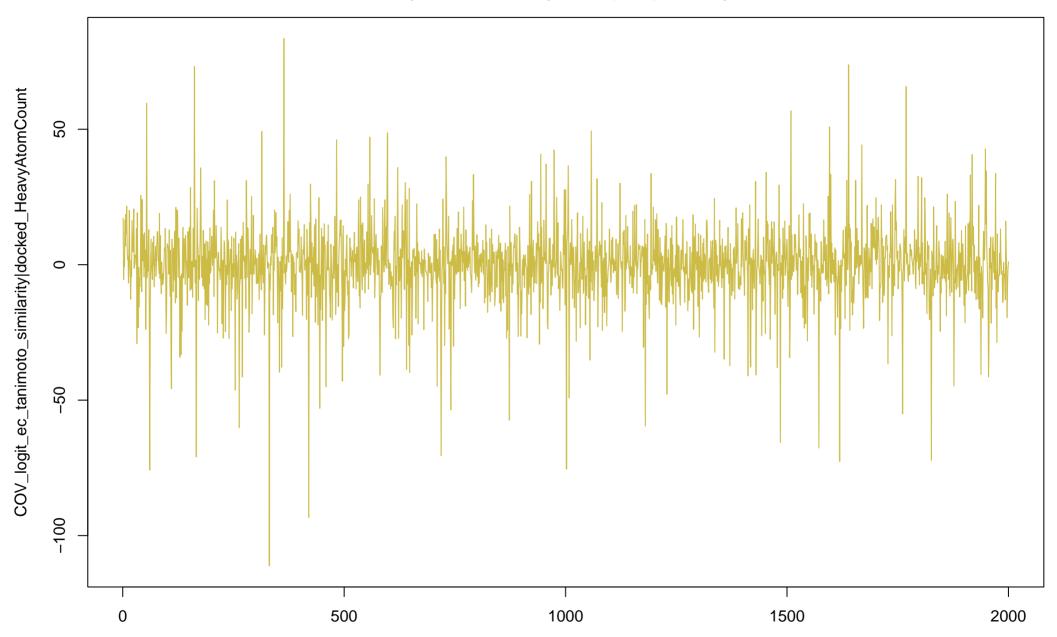


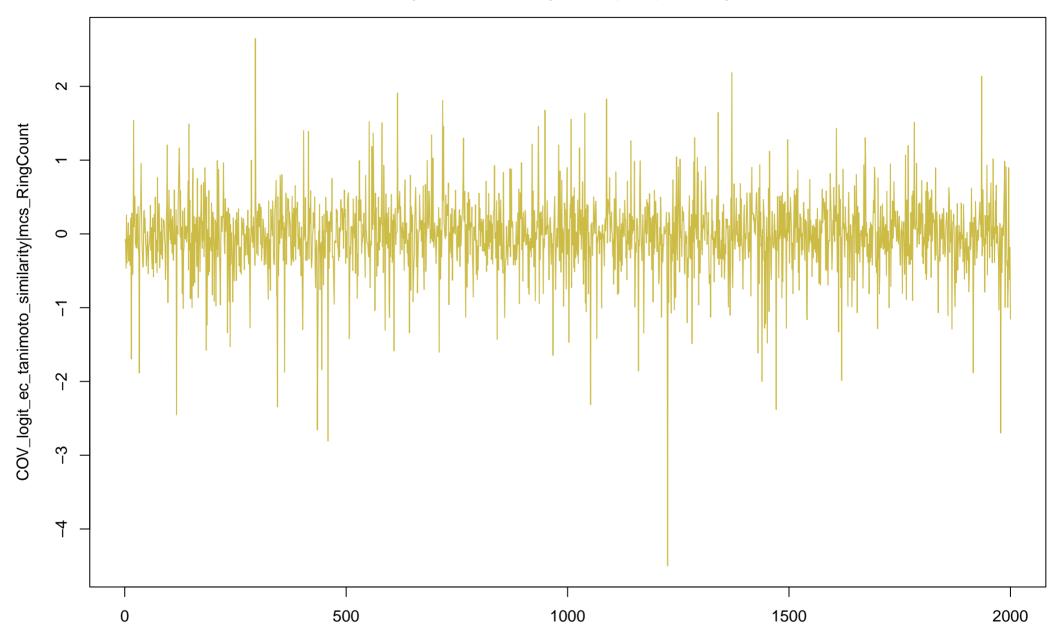


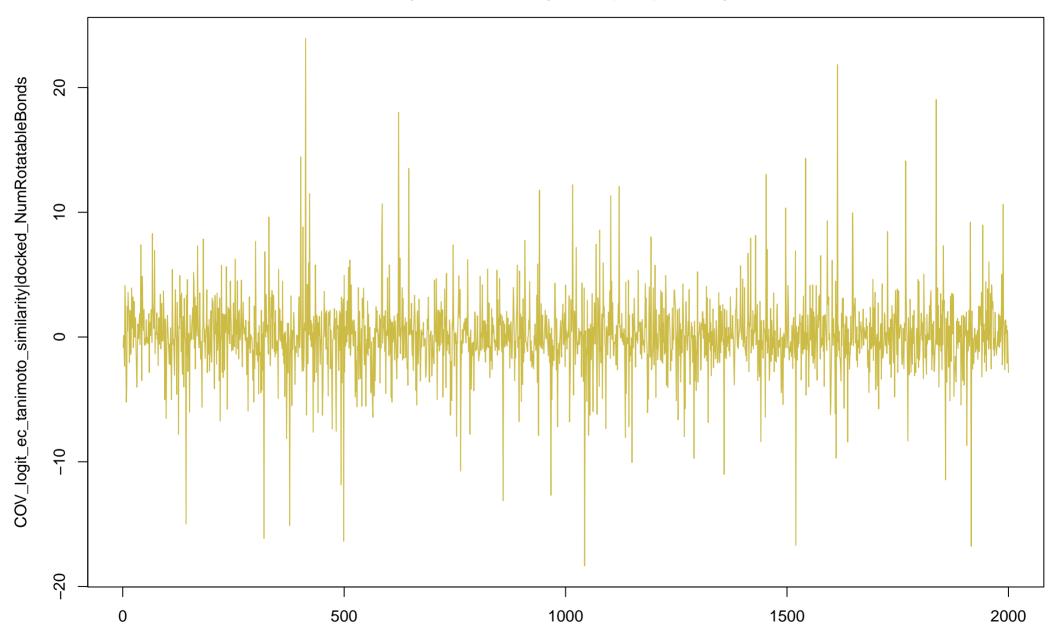


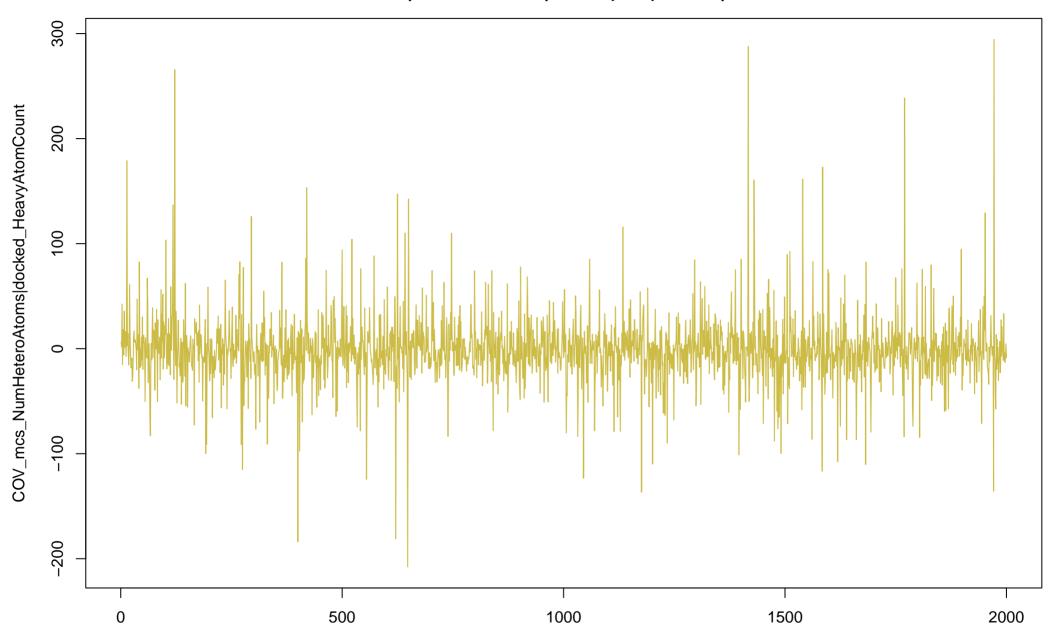




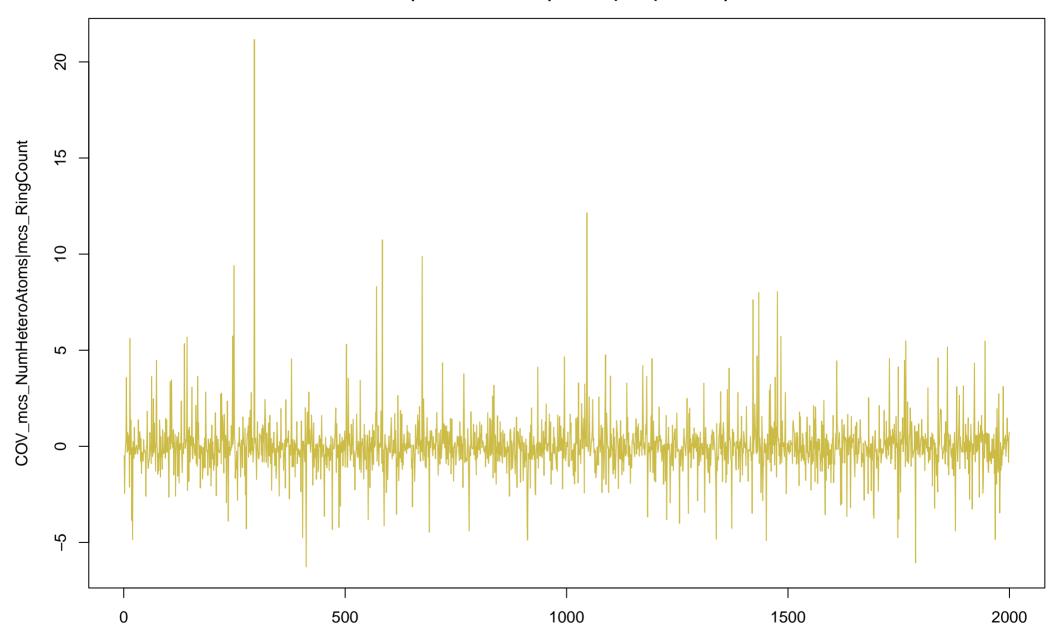


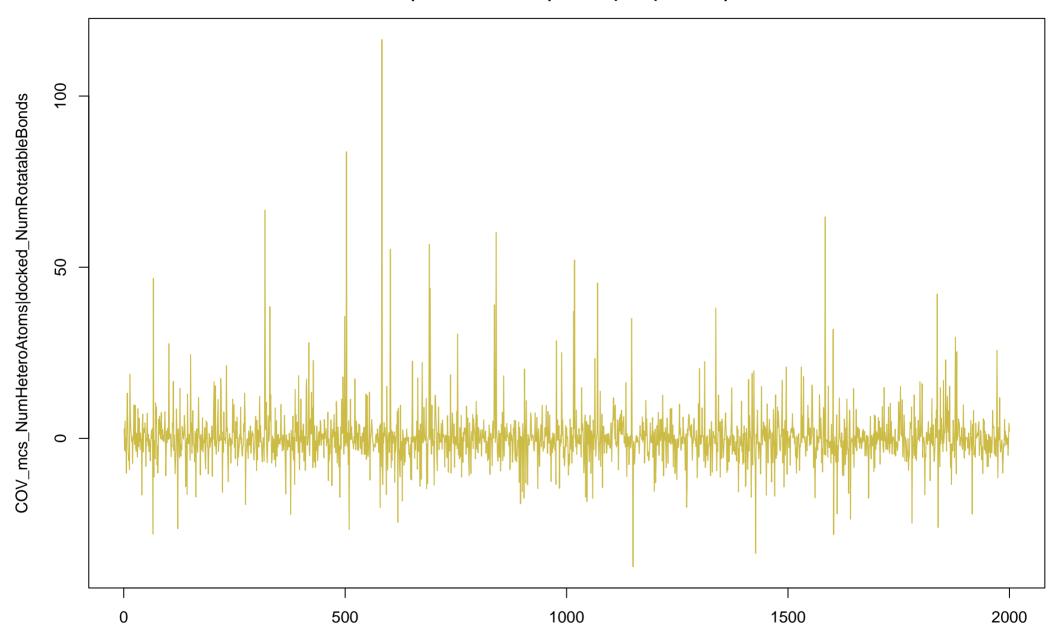




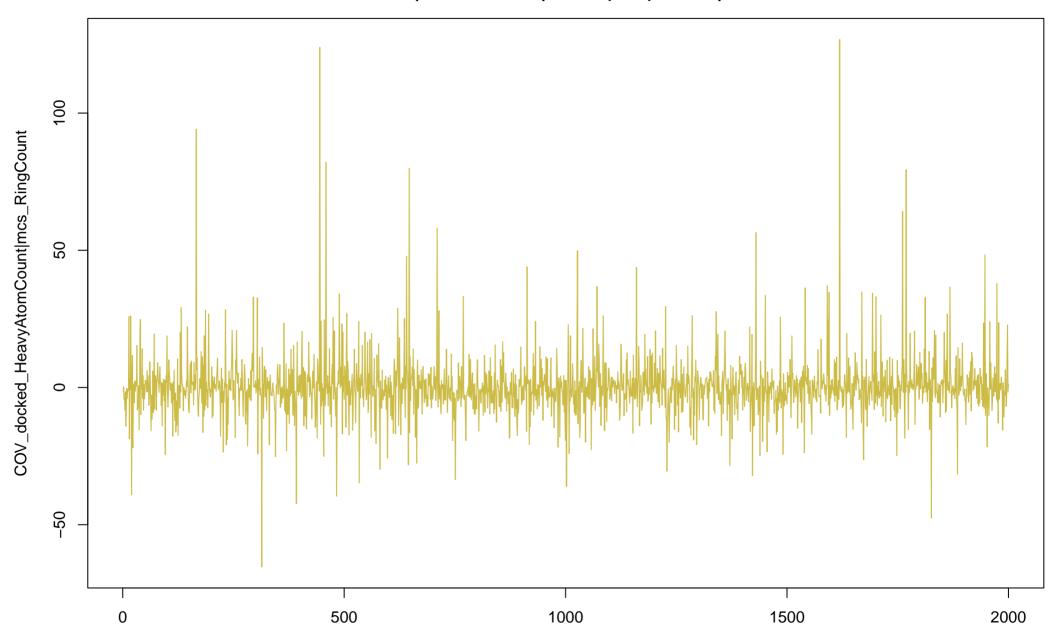


COV\_mcs\_NumHeteroAtoms|mcs\_RingCount ESS = 2000 | BMK = 0.0899 | MCSE(6.27) = 2.22 | stat: TRUE

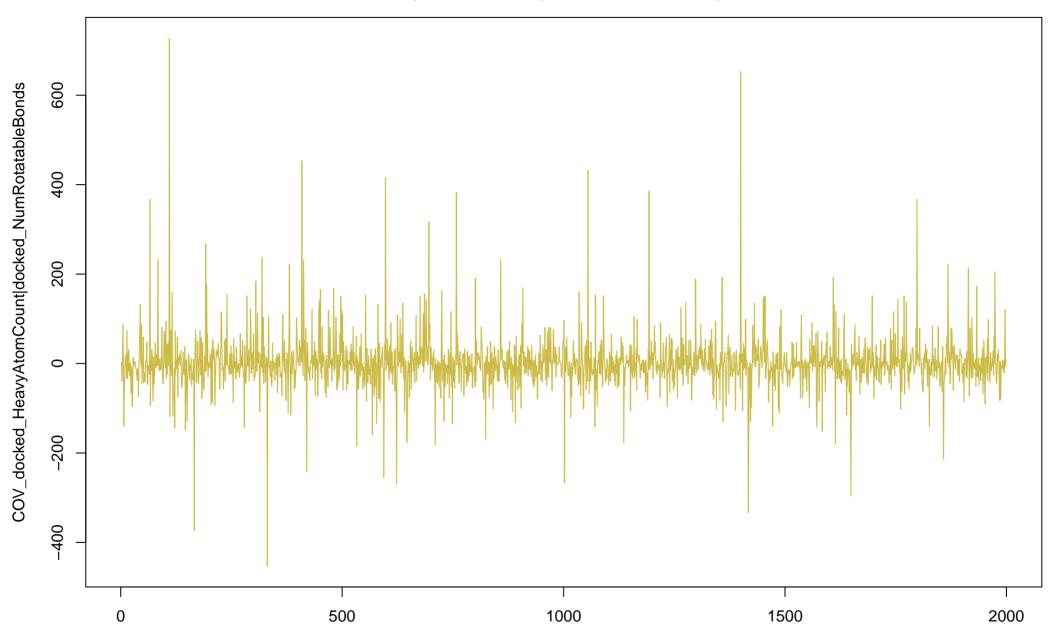




## COV\_docked\_HeavyAtomCount|mcs\_RingCount ESS = 2000 | BMK = 0.093 | MCSE(6.27) = 2.23 | stat: TRUE



## COV\_docked\_HeavyAtomCount|docked\_NumRotatableBonds ESS = 2000 | BMK = 0.105 | MCSE(6.27) = 2.38 | stat: TRUE



## COV\_mcs\_RingCount|docked\_NumRotatableBonds ESS = 2000 | BMK = 0.105 | MCSE(6.27) = 2.33 | stat: TRUE

