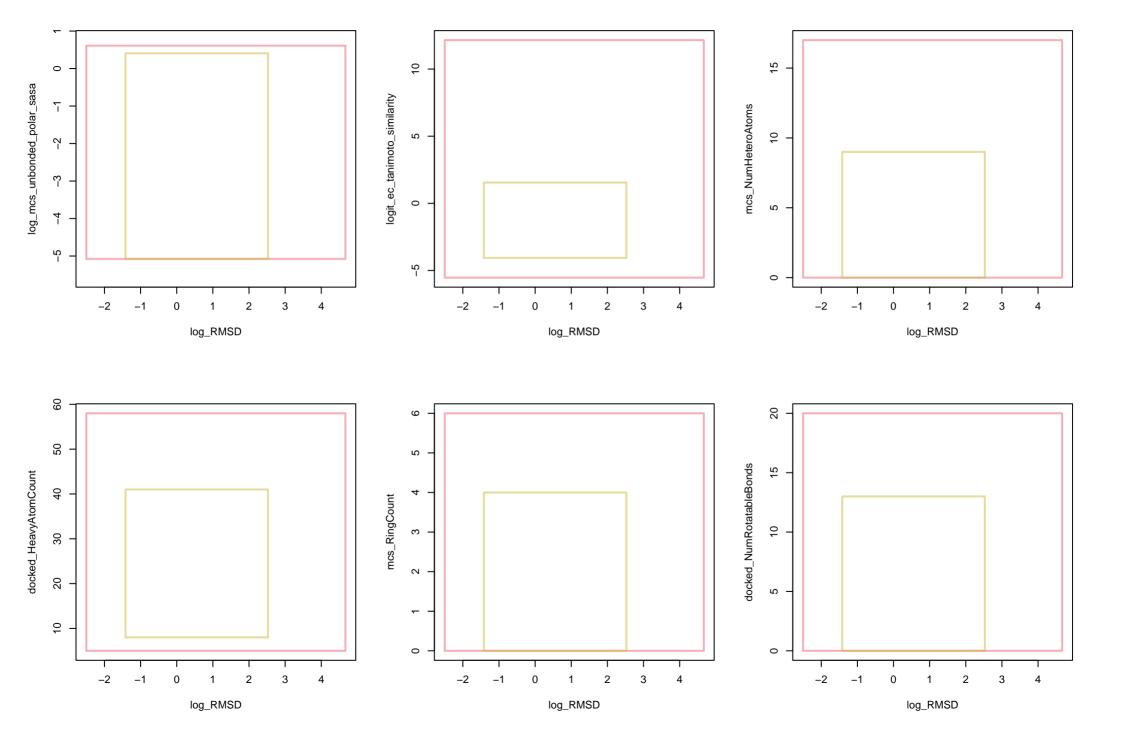
-- STATS maxD -min ESS = 45.9695092367089 max BMK = 0.35047765878268 max MCSE = 10.9148415280253 all stationary: FALSE

burn: 0

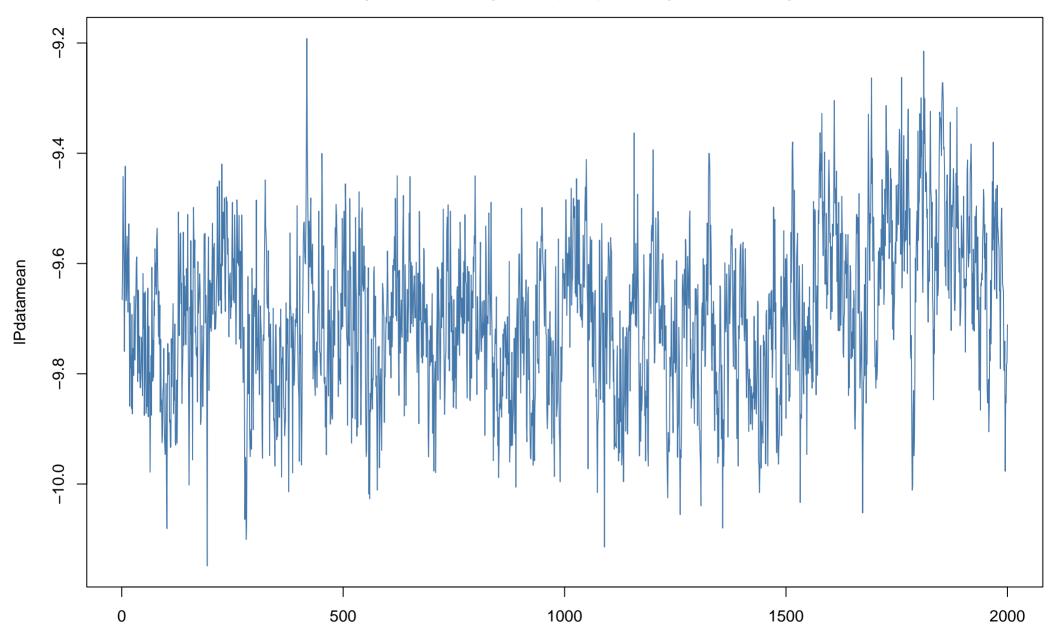
burn: 0

-- STATS 1D -min ESS = 504.283562003686 max BMK = 0.11808137970968 max MCSE = 2.89792648800152 all stationary: FALSE -- STATS 2D -min ESS = 569.178288003345 max BMK = 0.153569823562787 max MCSE = 3.42713310278508 all stationary: FALSE

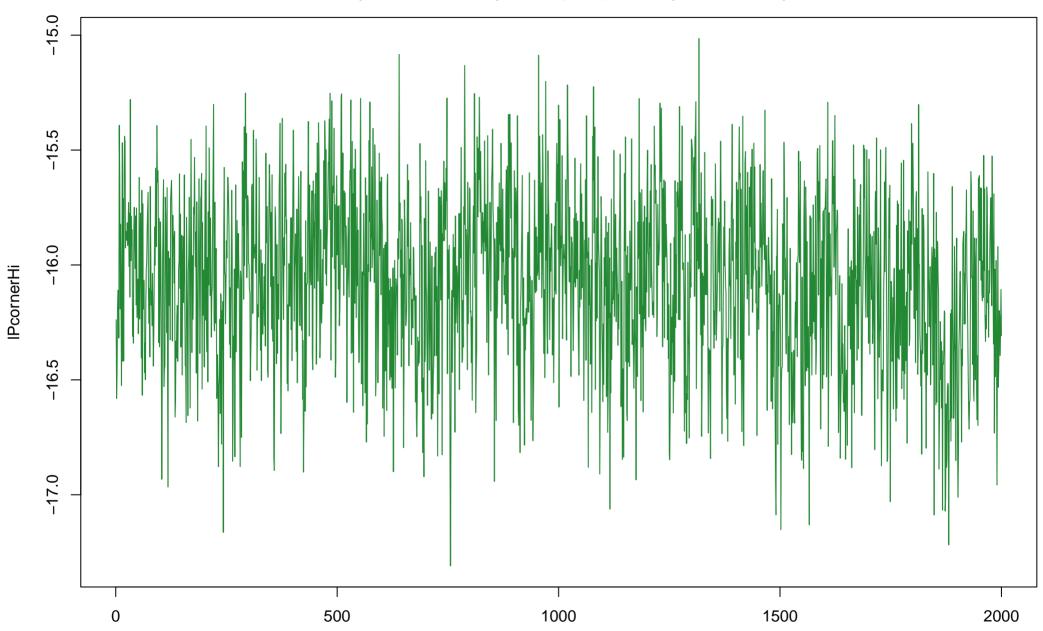
burn: 0



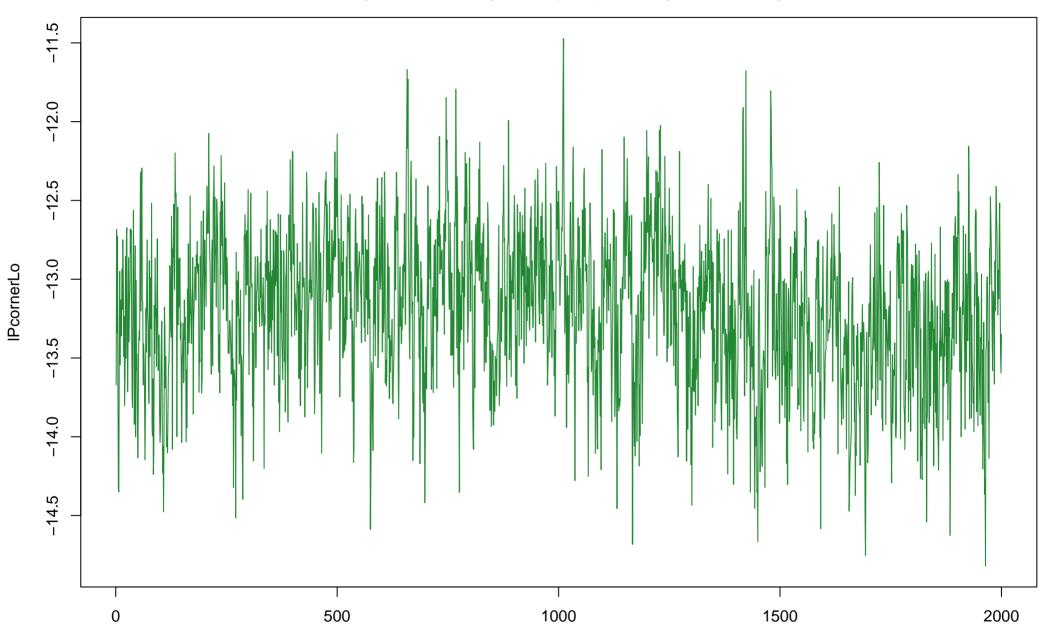
IPdatamean ESS = 160 | BMK = 0.183 | MCSE(6.27) = 10.9 | stat: FALSE | burn: 0



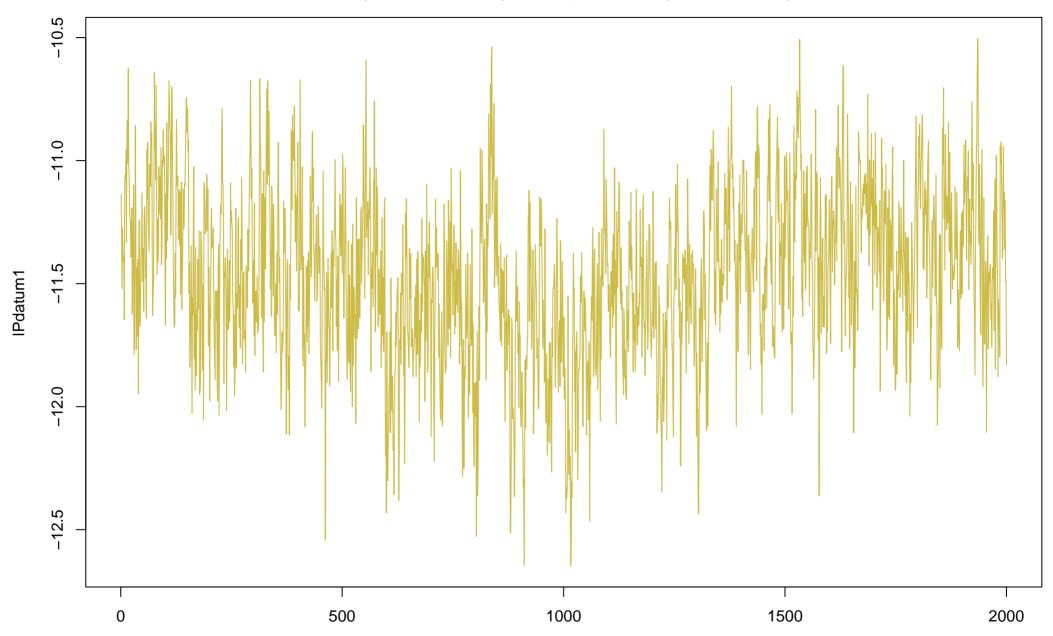
IPcornerHi
ESS = 596 | BMK = 0.0876 | MCSE(6.27) = 5.36 | stat: TRUE | burn: 0



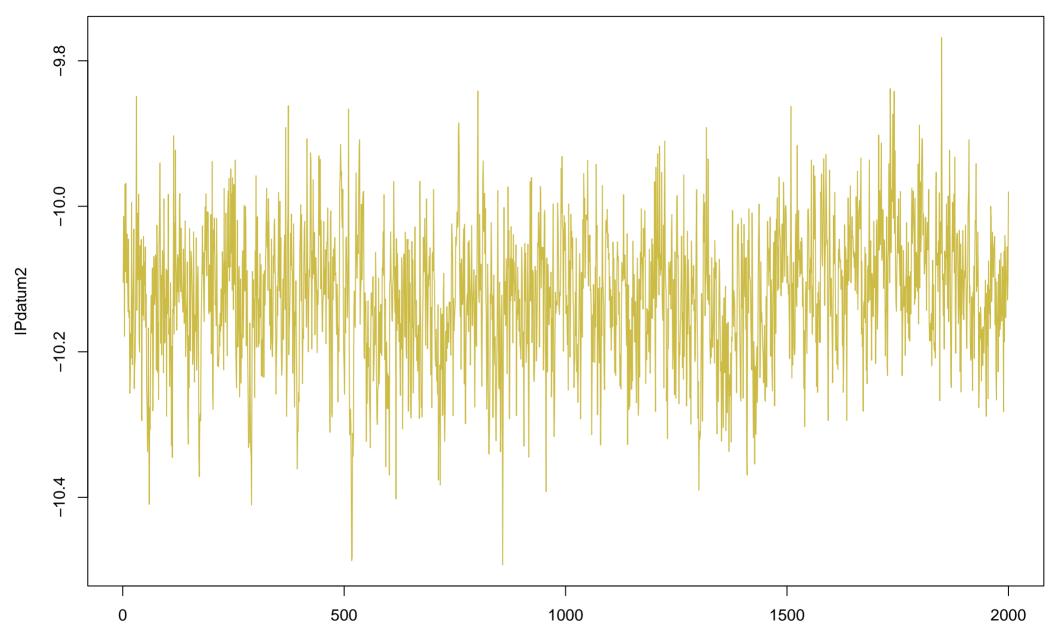
IPcornerLo
ESS = 241 | BMK = 0.124 | MCSE(6.27) = 5.73 | stat: TRUE | burn: 0



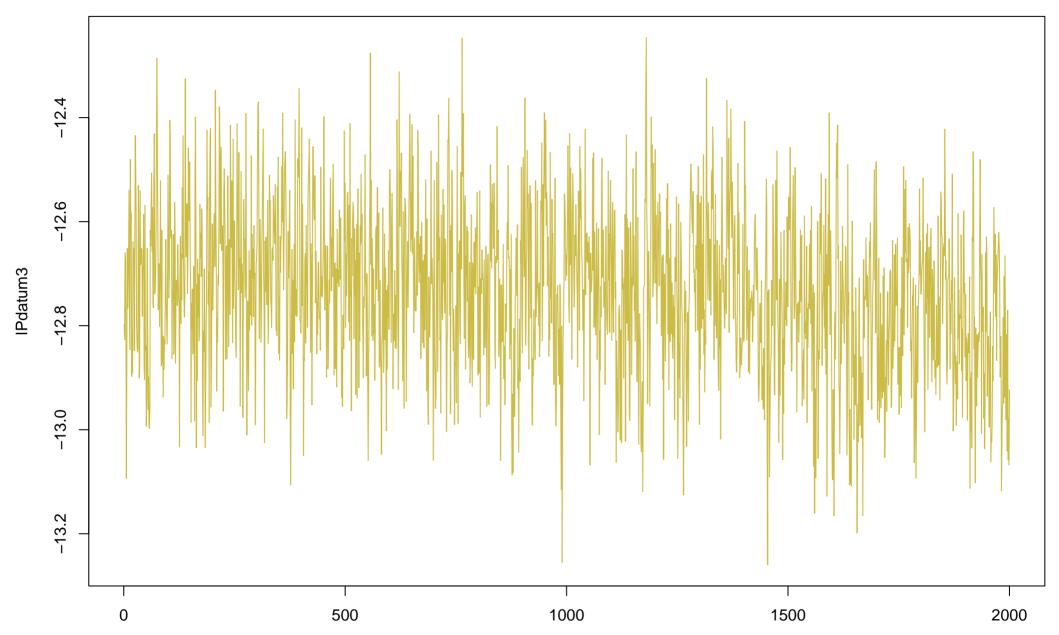
IPdatum1 ESS = 145 | BMK = 0.0796 | MCSE(6.27) = 9.6 | stat: FALSE | burn: 0



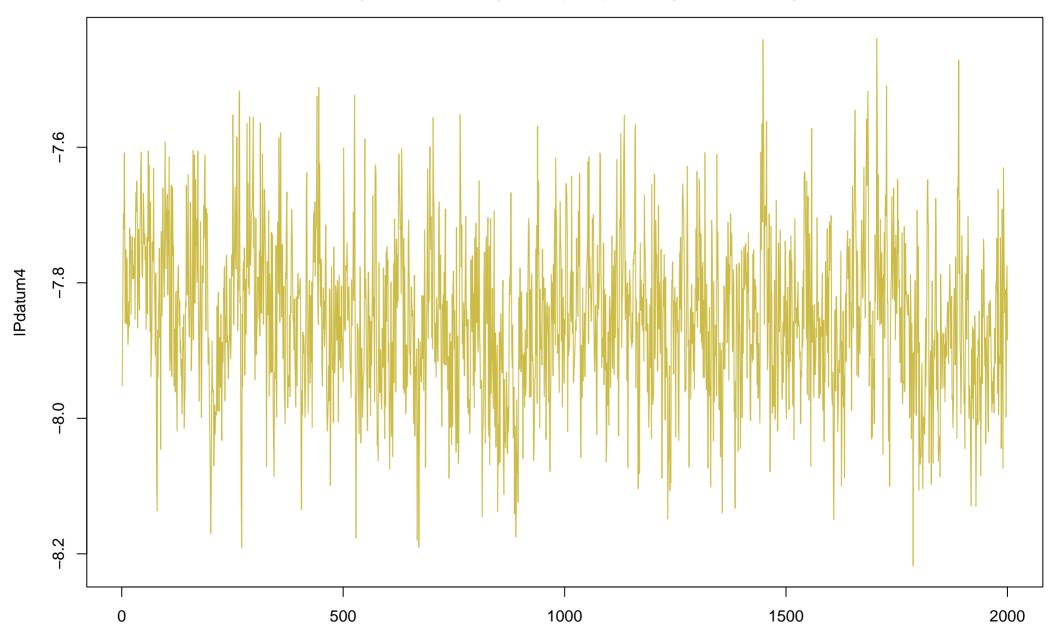
IPdatum2 ESS = 418 | BMK = 0.0802 | MCSE(6.27) = 6.49 | stat: TRUE | burn: 0



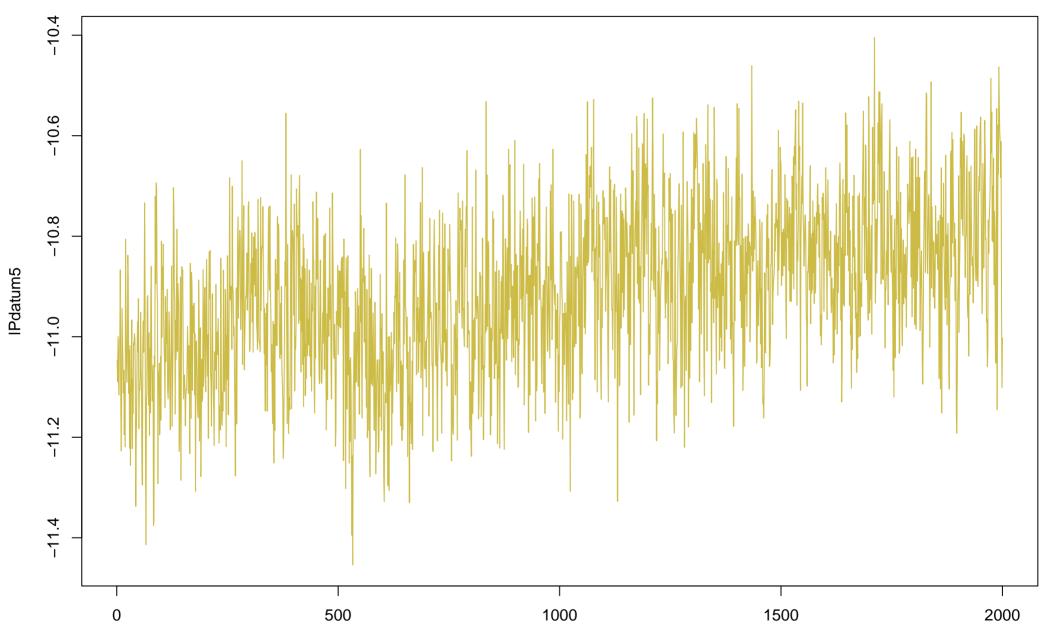
IPdatum3 ESS = 572 | BMK = 0.123 | MCSE(6.27) = 5.45 | stat: FALSE | burn: 0



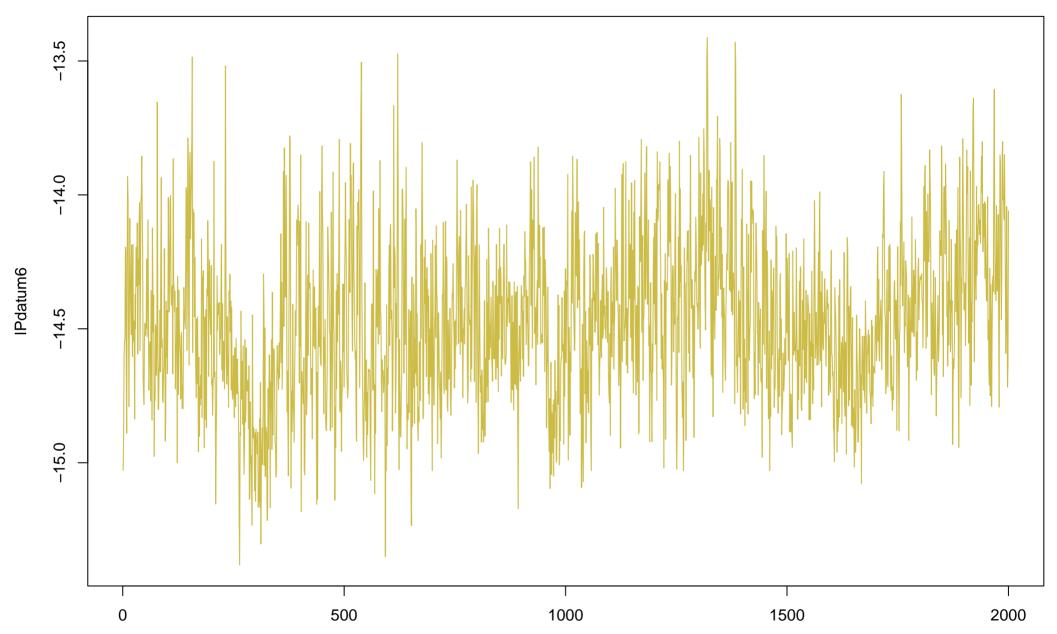
IPdatum4 ESS = 434 | BMK = 0.0508 | MCSE(6.27) = 6.47 | stat: FALSE | burn: 0



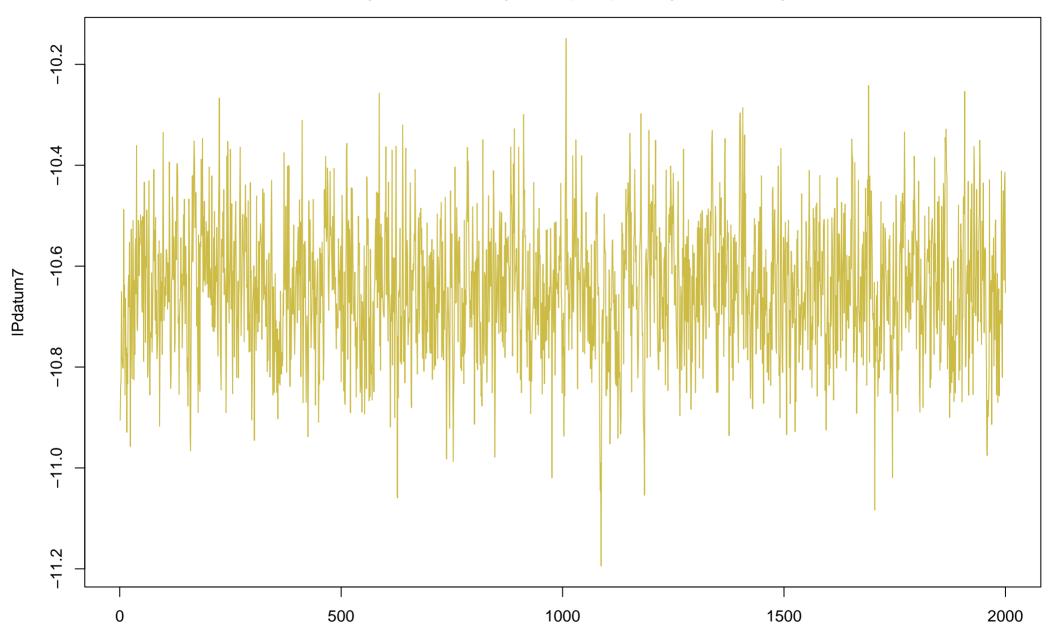
IPdatum5 ESS = 46 | BMK = 0.35 | MCSE(6.27) = 7.37 | stat: FALSE | burn: 0



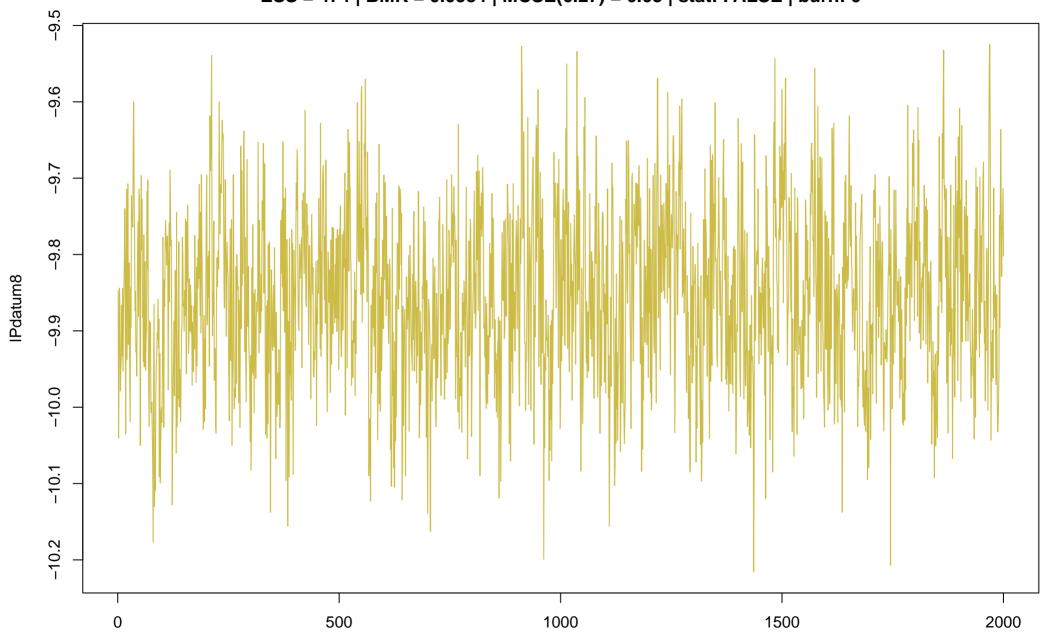
IPdatum6 ESS = 107 | BMK = 0.152 | MCSE(6.27) = 7.76 | stat: TRUE | burn: 0



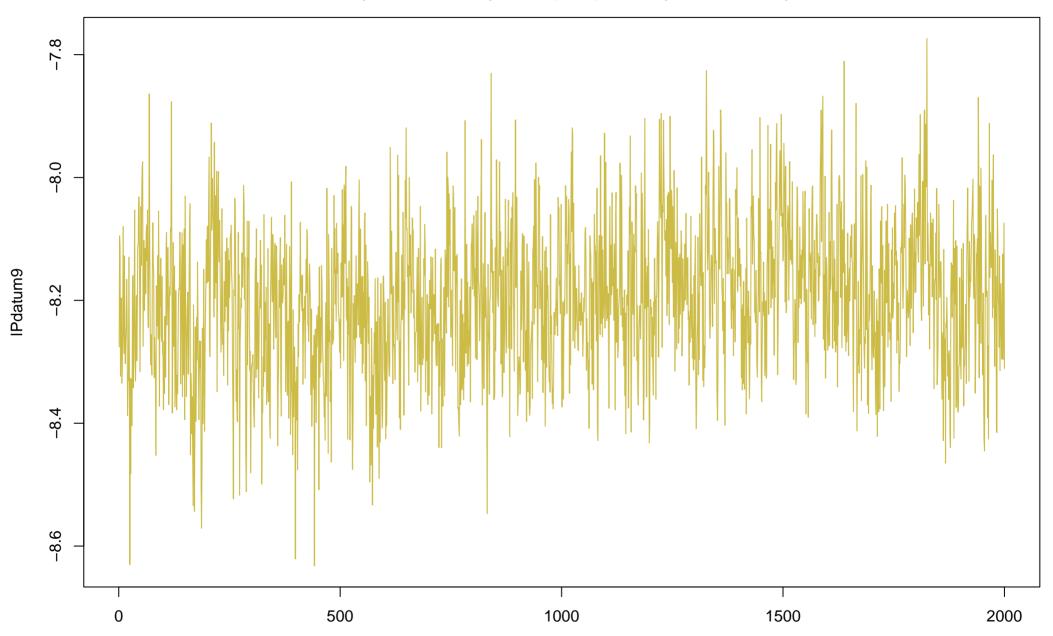
IPdatum7
ESS = 745 | BMK = 0.0382 | MCSE(6.27) = 4.1 | stat: TRUE | burn: 0



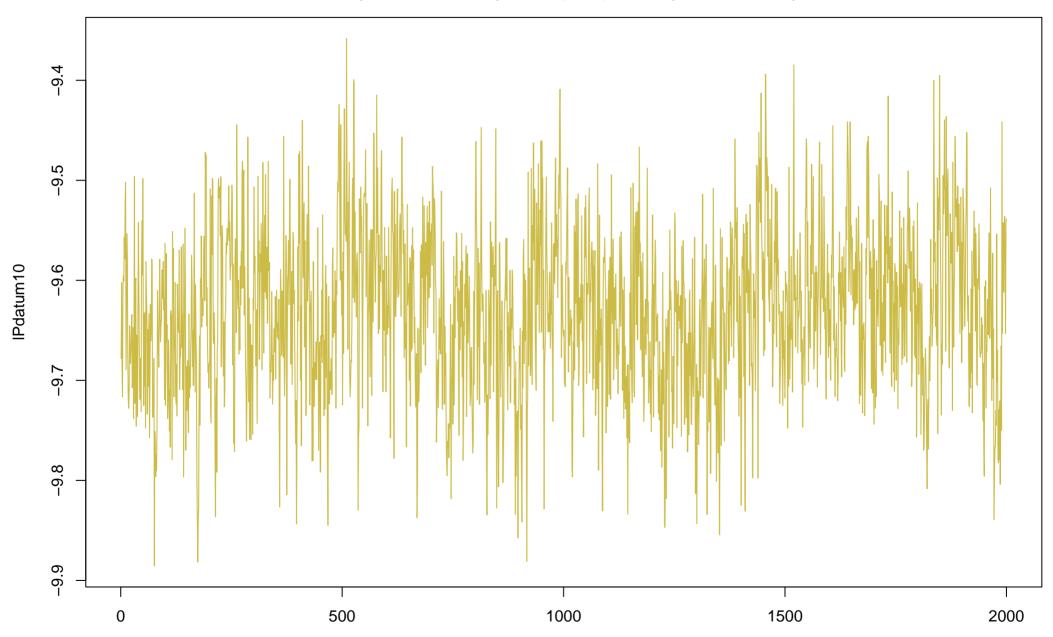
IPdatum8 ESS = 474 | BMK = 0.0584 | MCSE(6.27) = 6.05 | stat: FALSE | burn: 0



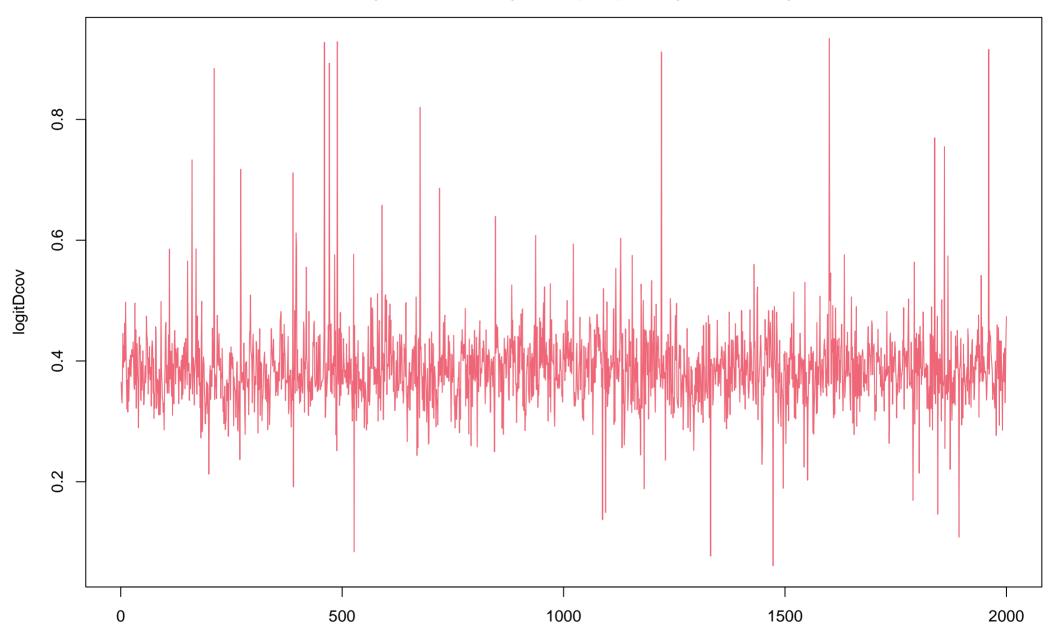
IPdatum9 ESS = 204 | BMK = 0.165 | MCSE(6.27) = 5.96 | stat: FALSE | burn: 0



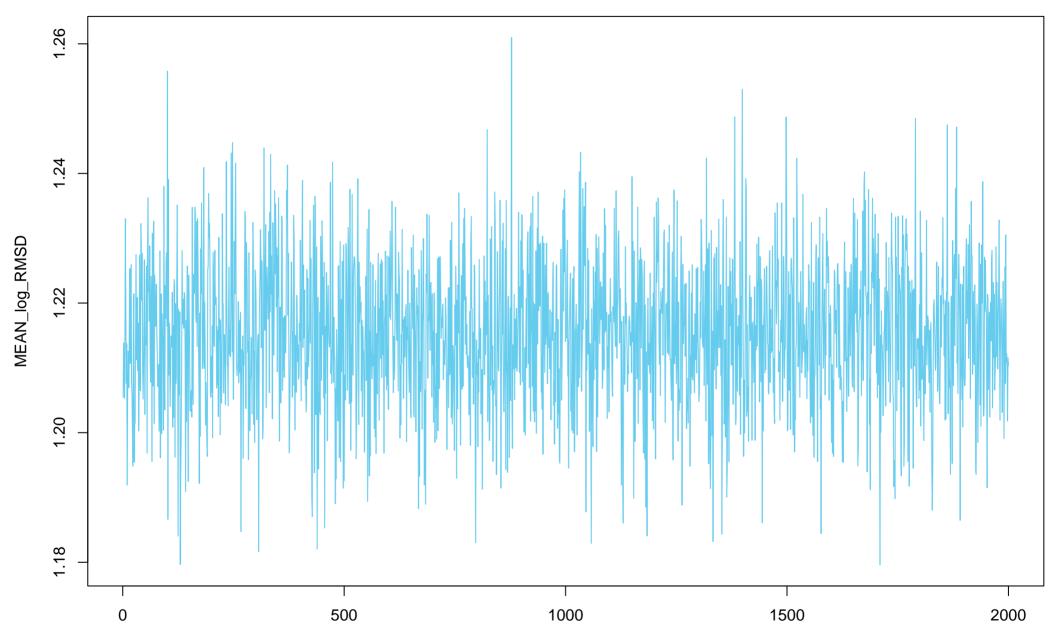
IPdatum10 ESS = 297 | BMK = 0.0389 | MCSE(6.27) = 6.27 | stat: FALSE | burn: 0



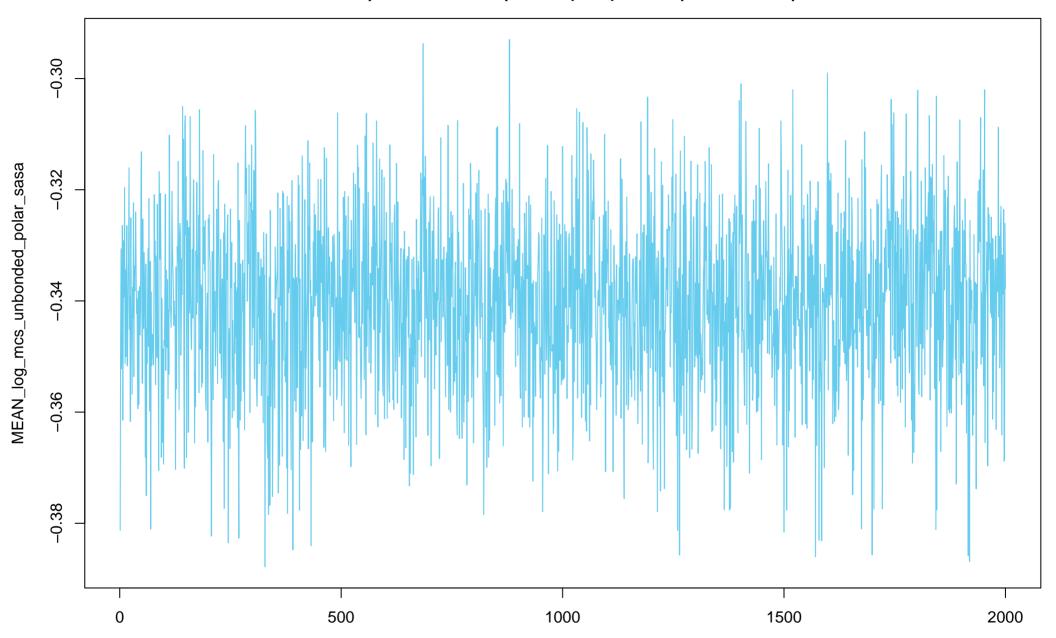
logitDcov ESS = 1660 | BMK = 0.0955 | MCSE(6.27) = 2.9 | stat: TRUE | burn: 0



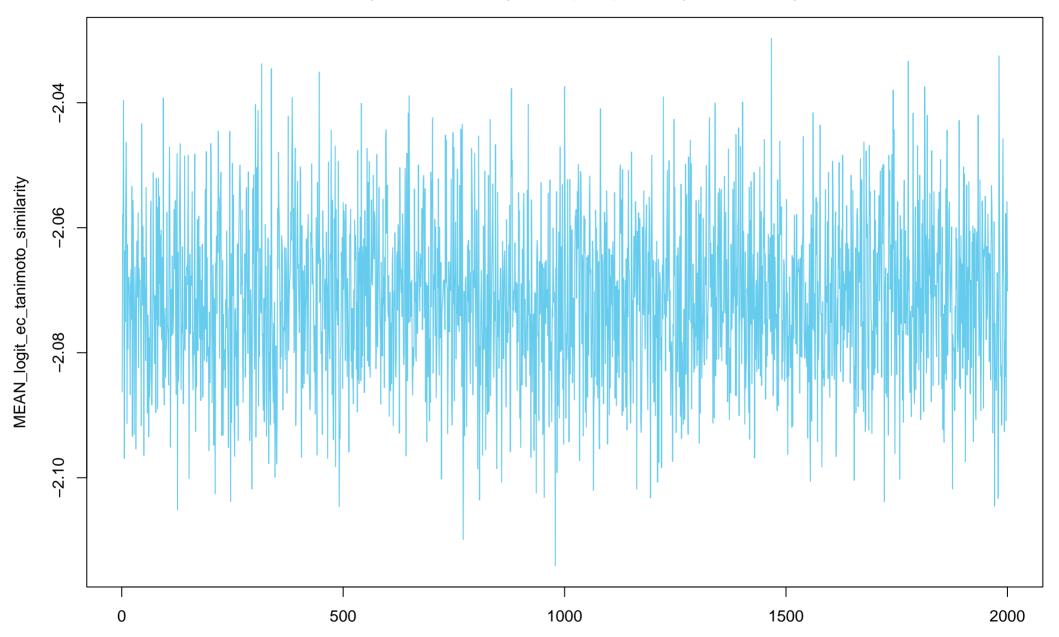
MEAN_log_RMSD ESS = 1630 | BMK = 0.0444 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0



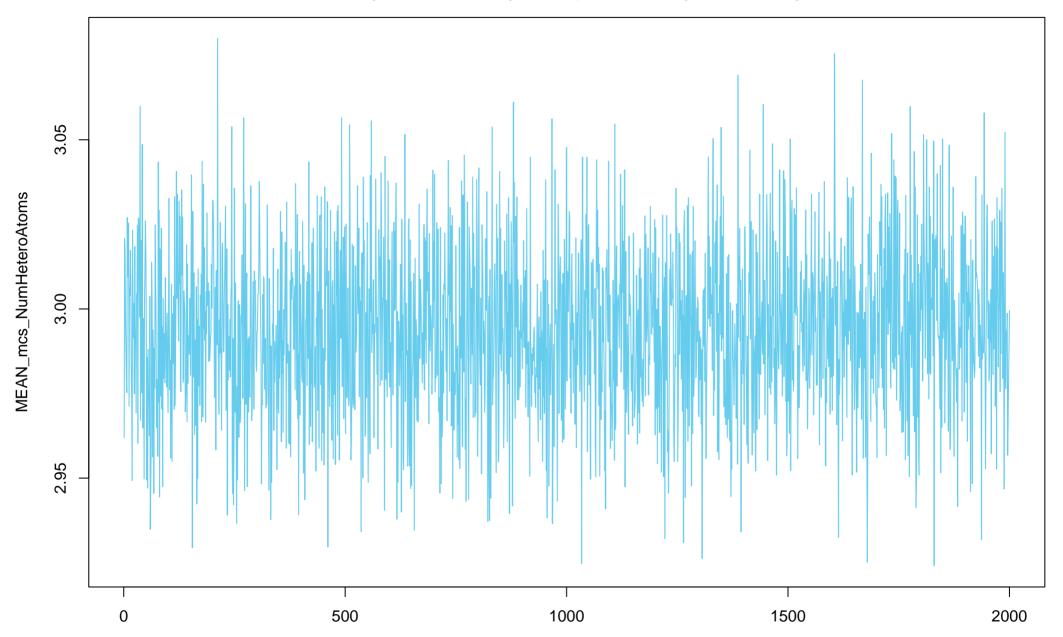
MEAN_log_mcs_unbonded_polar_sasa ESS = 1480 | BMK = 0.0346 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0



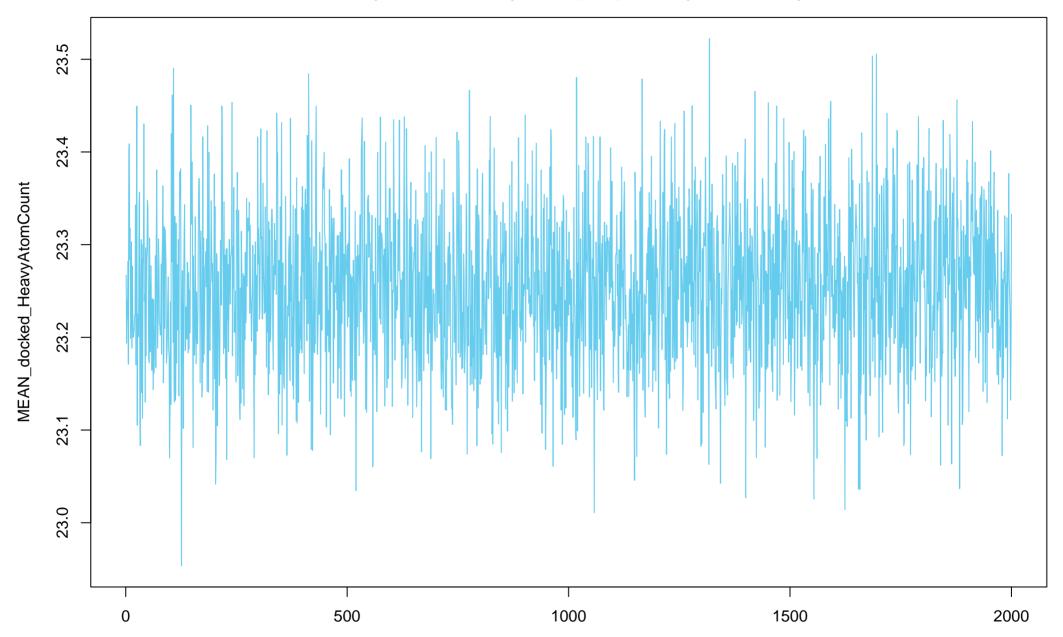
MEAN_logit_ec_tanimoto_similarity ESS = 2000 | BMK = 0.0493 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0



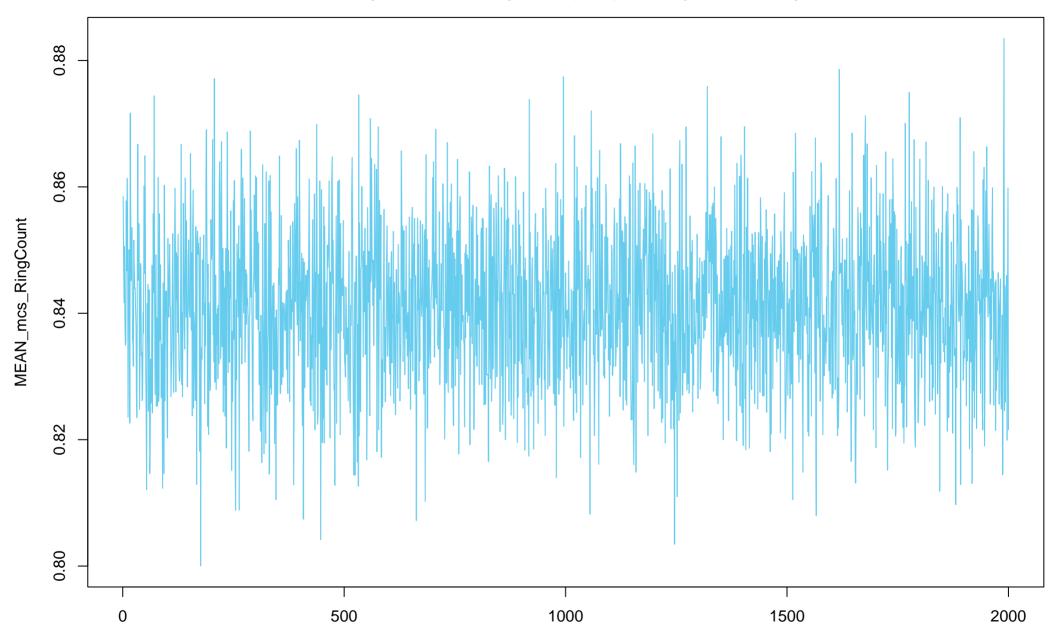
MEAN_mcs_NumHeteroAtoms ESS = 2000 | BMK = 0.0544 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



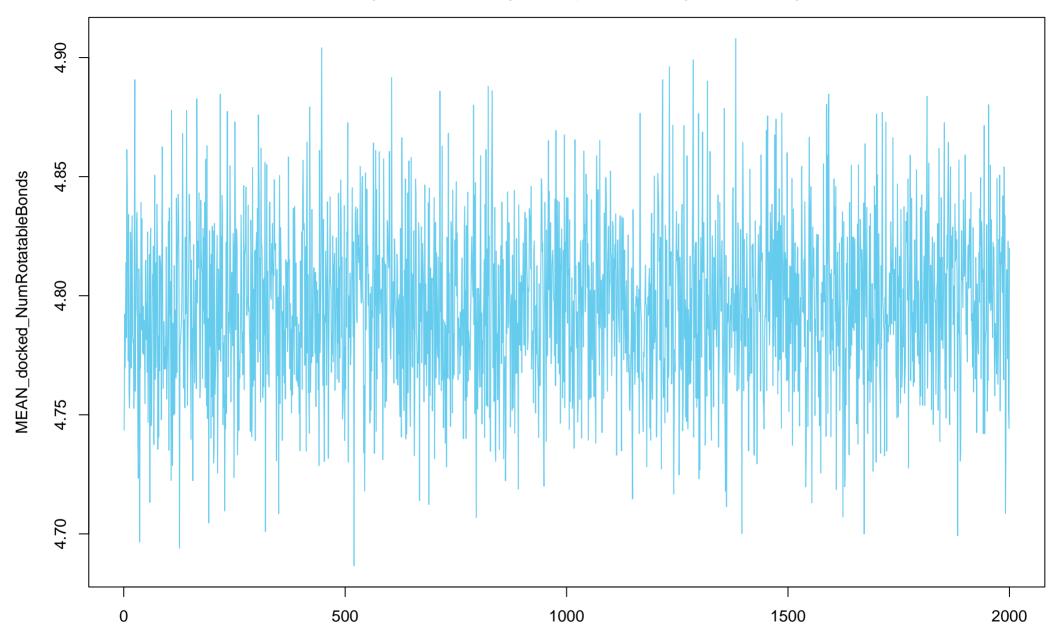
MEAN_docked_HeavyAtomCount ESS = 1870 | BMK = 0.0581 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0



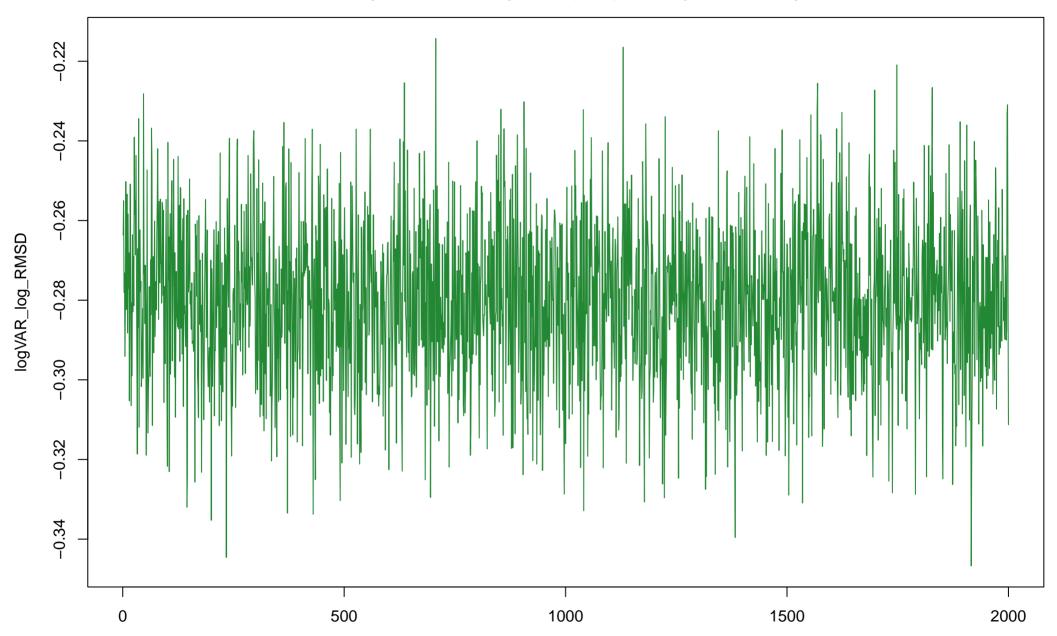
MEAN_mcs_RingCount ESS = 2000 | BMK = 0.0301 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0



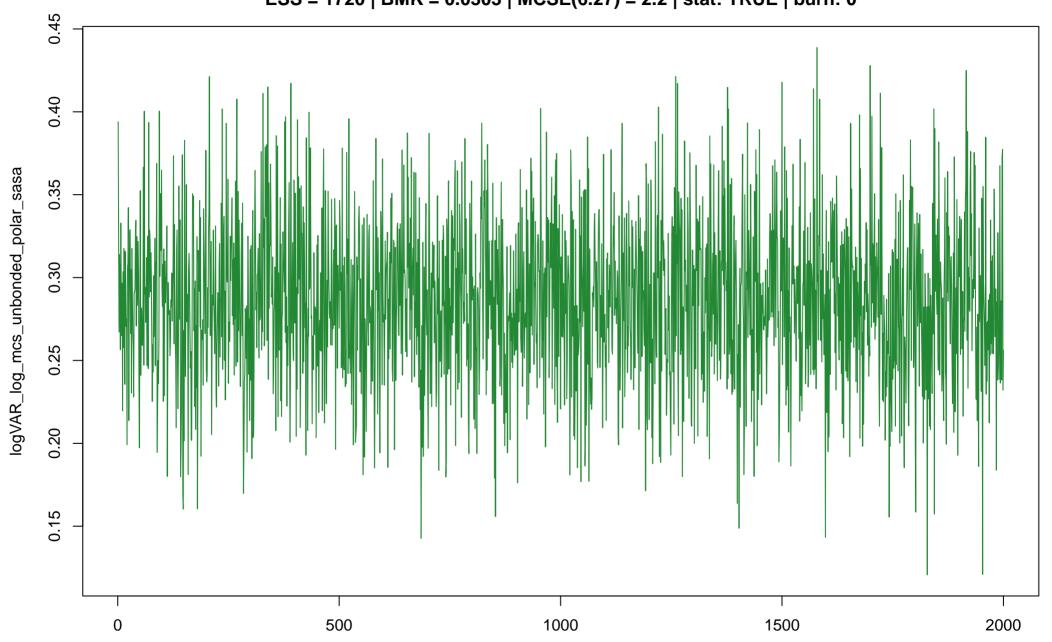
MEAN_docked_NumRotatableBonds ESS = 2000 | BMK = 0.0456 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0



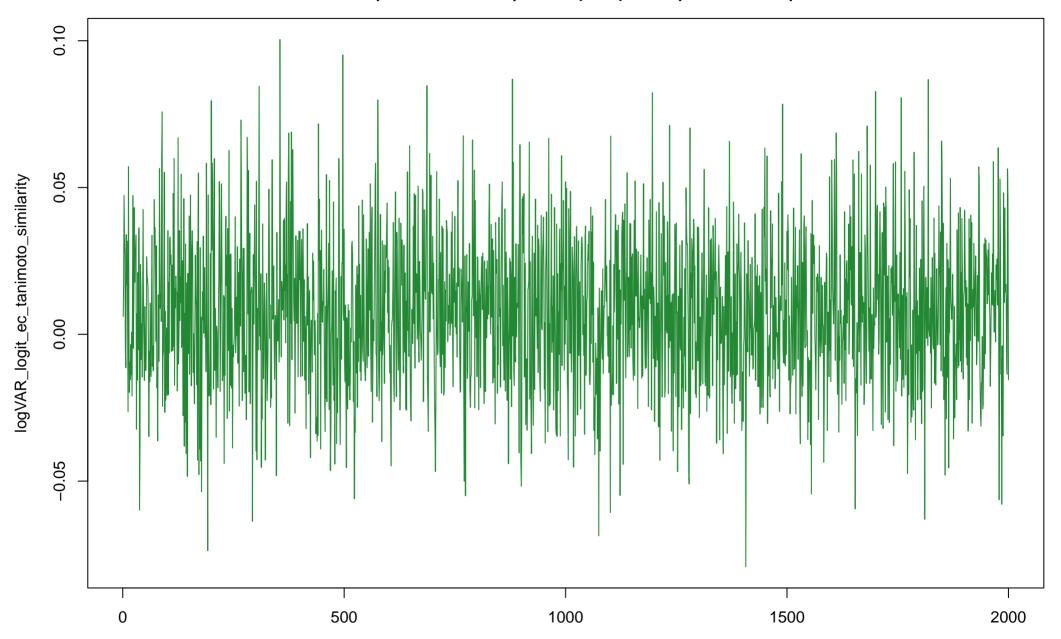
logVAR_log_RMSD ESS = 1950 | BMK = 0.0329 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0



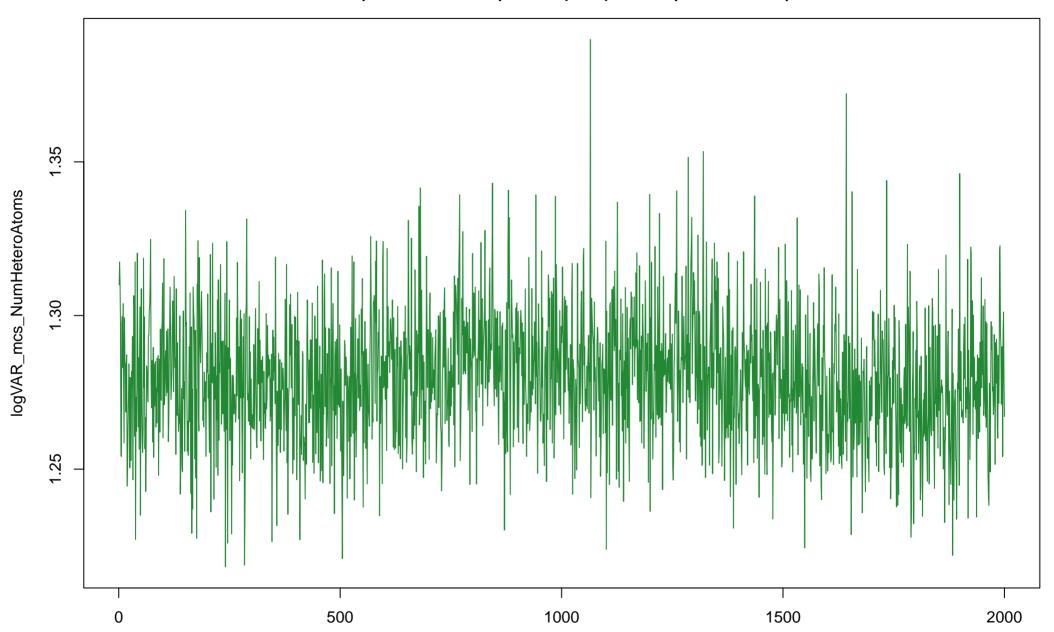
logVAR_log_mcs_unbonded_polar_sasa ESS = 1720 | BMK = 0.0303 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0



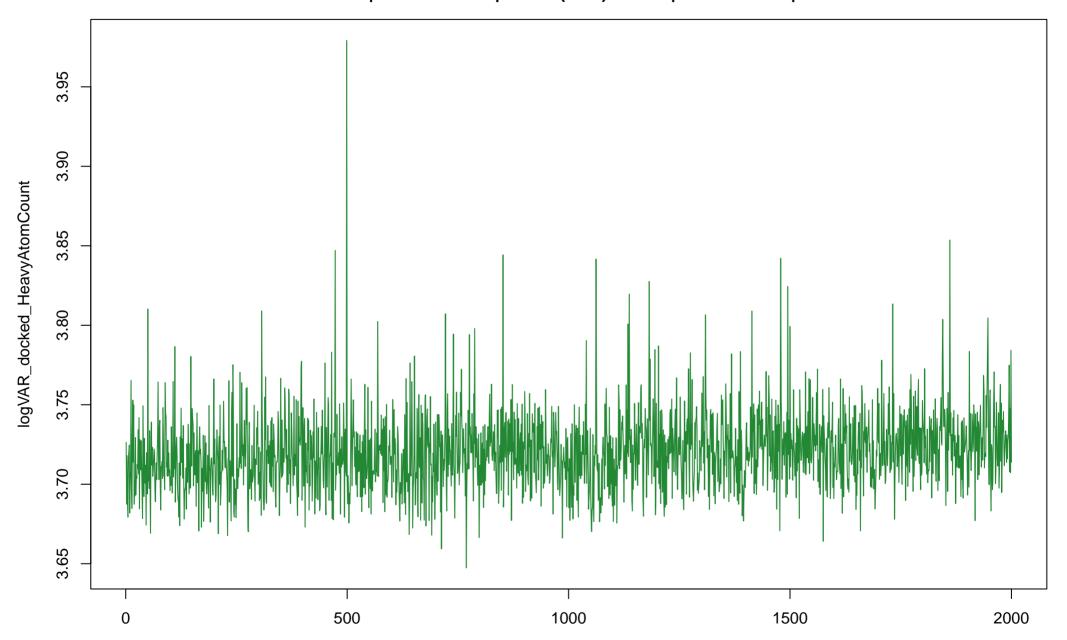
logVAR_logit_ec_tanimoto_similarity ESS = 1930 | BMK = 0.0433 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0



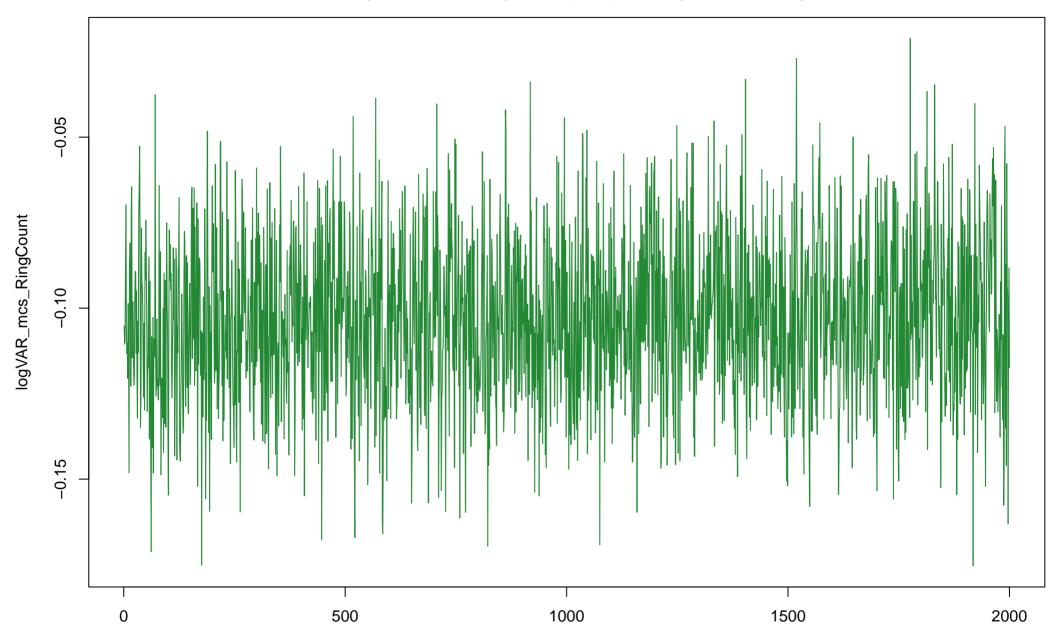
logVAR_mcs_NumHeteroAtoms ESS = 946 | BMK = 0.0594 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0



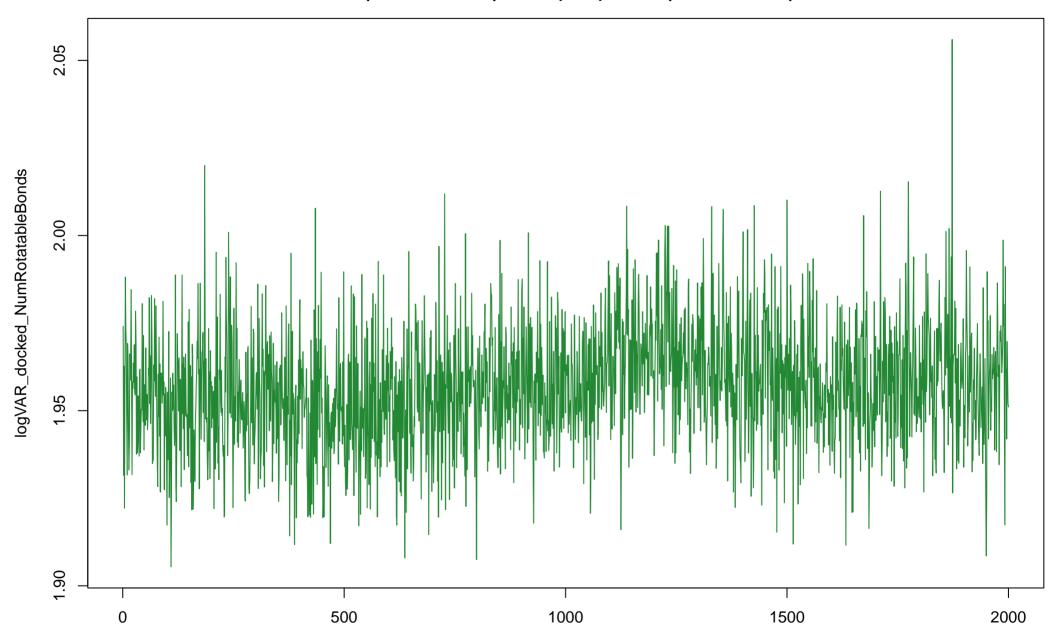
logVAR_docked_HeavyAtomCount ESS = 504 | BMK = 0.118 | MCSE(6.27) = 2.87 | stat: FALSE | burn: 0



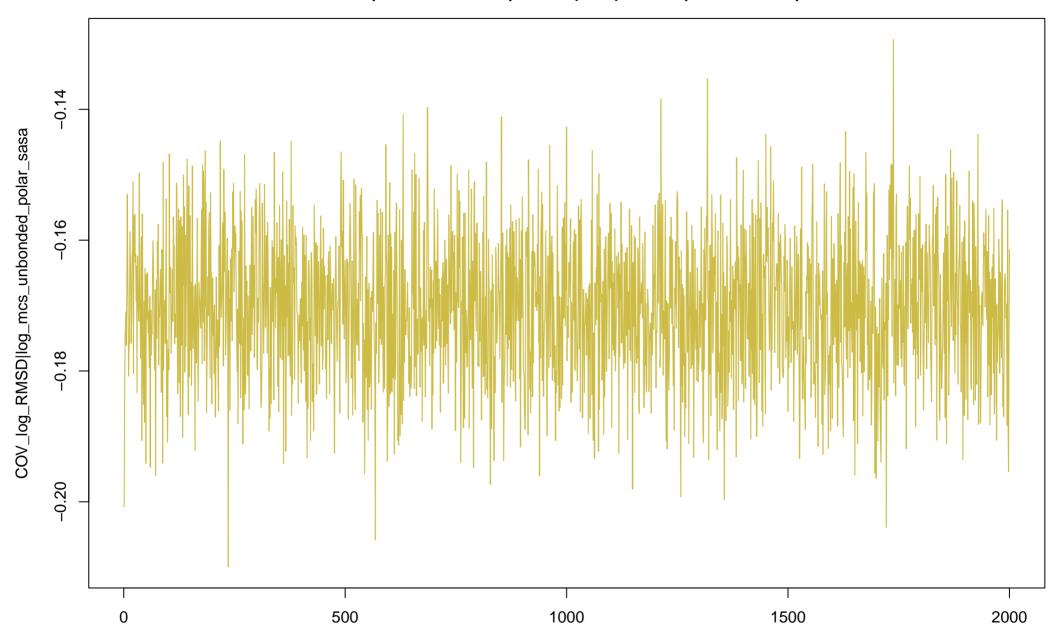
logVAR_mcs_RingCount ESS = 1780 | BMK = 0.0525 | MCSE(6.27) = 2.64 | stat: FALSE | burn: 0



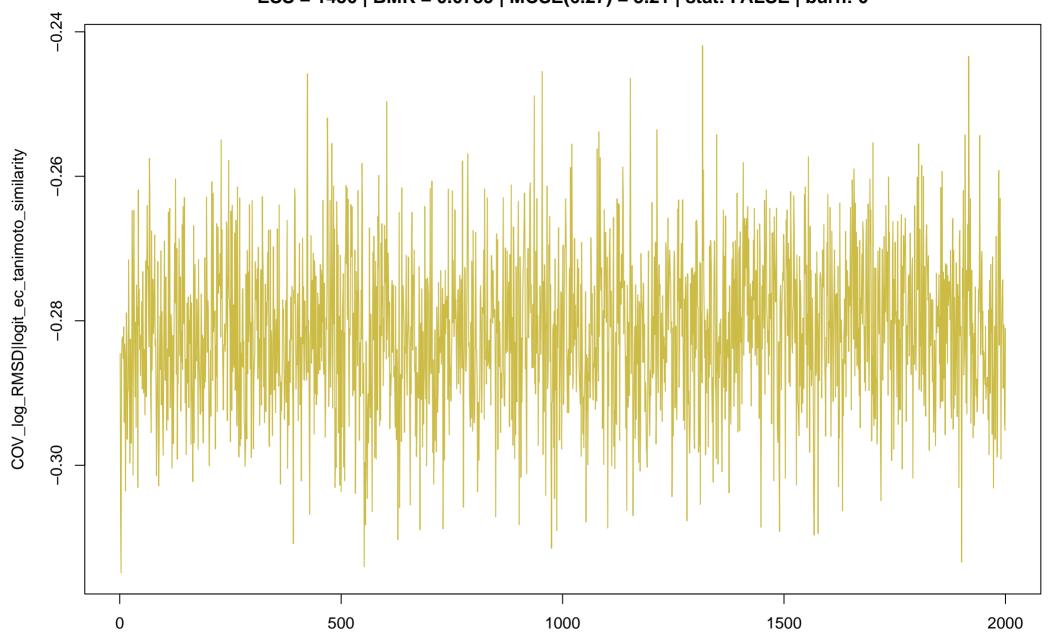
logVAR_docked_NumRotatableBonds ESS = 569 | BMK = 0.154 | MCSE(6.27) = 3.43 | stat: FALSE | burn: 0



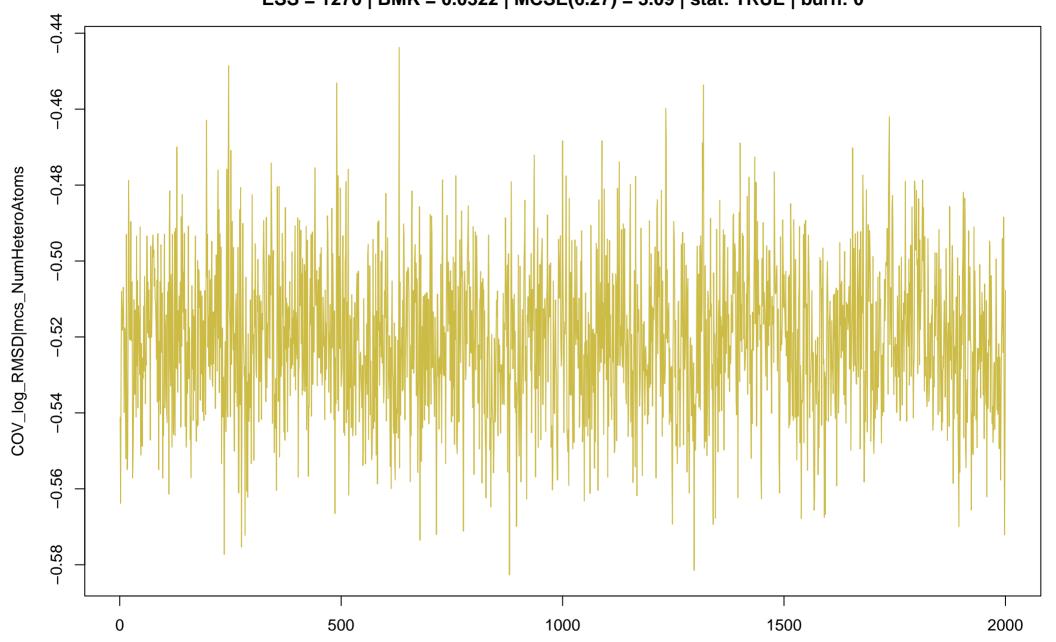
COV_log_RMSD|log_mcs_unbonded_polar_sasa ESS = 2000 | BMK = 0.0414 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0



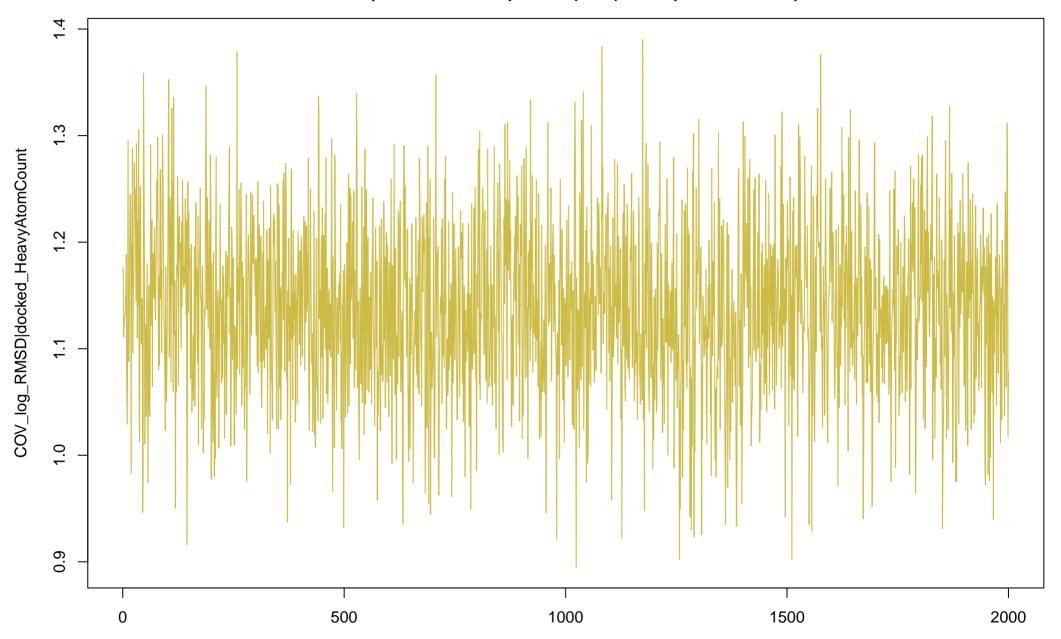
COV_log_RMSD|logit_ec_tanimoto_similarity ESS = 1450 | BMK = 0.0739 | MCSE(6.27) = 3.21 | stat: FALSE | burn: 0



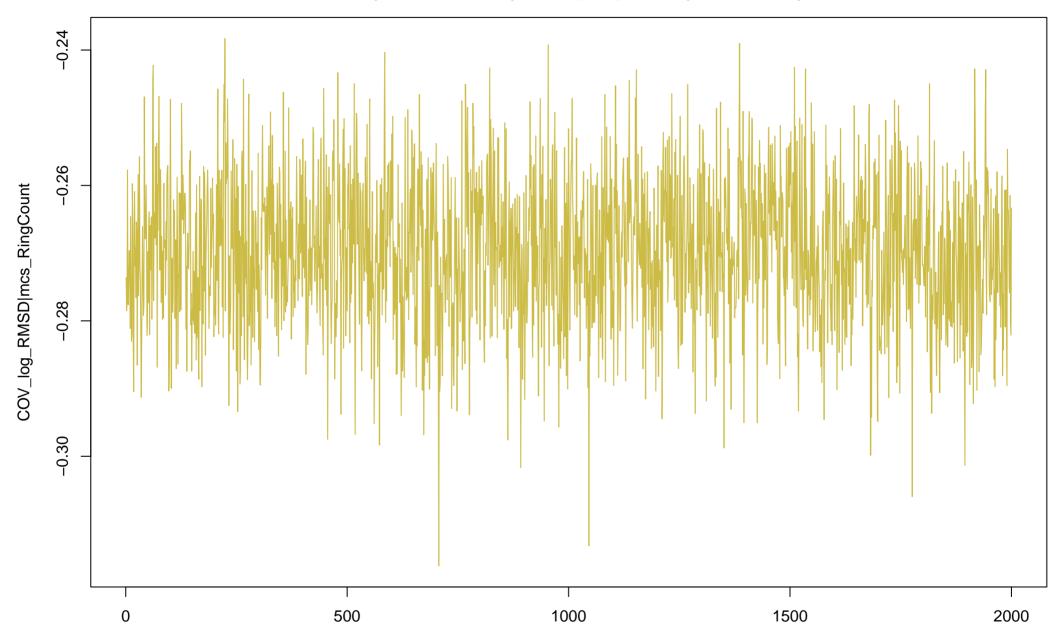
COV_log_RMSD|mcs_NumHeteroAtoms ESS = 1270 | BMK = 0.0322 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0



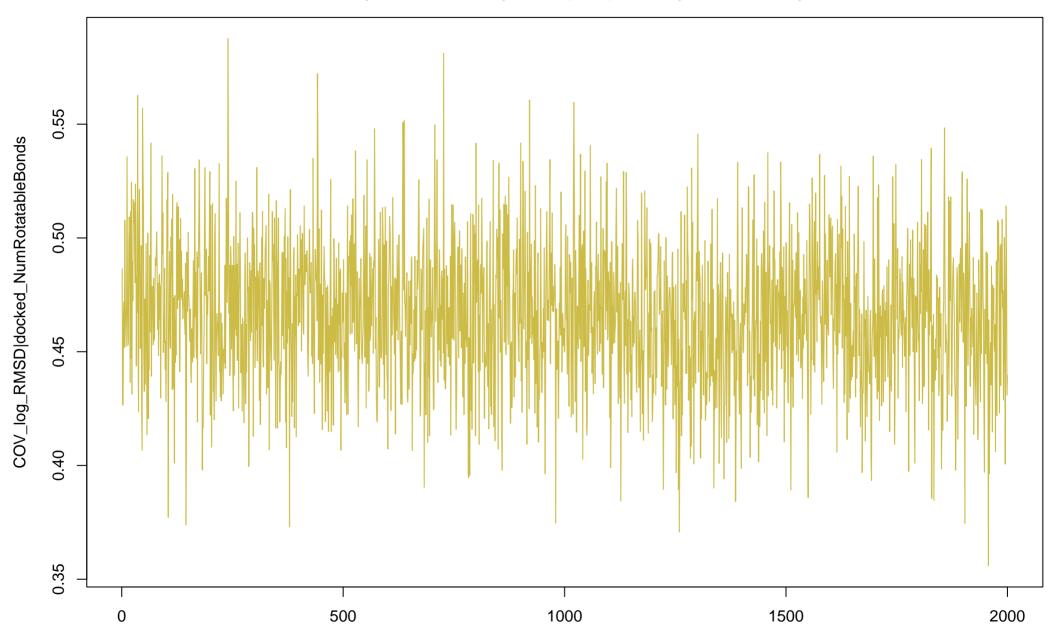
COV_log_RMSD|docked_HeavyAtomCount ESS = 1690 | BMK = 0.0435 | MCSE(6.27) = 2.7 | stat: FALSE | burn: 0

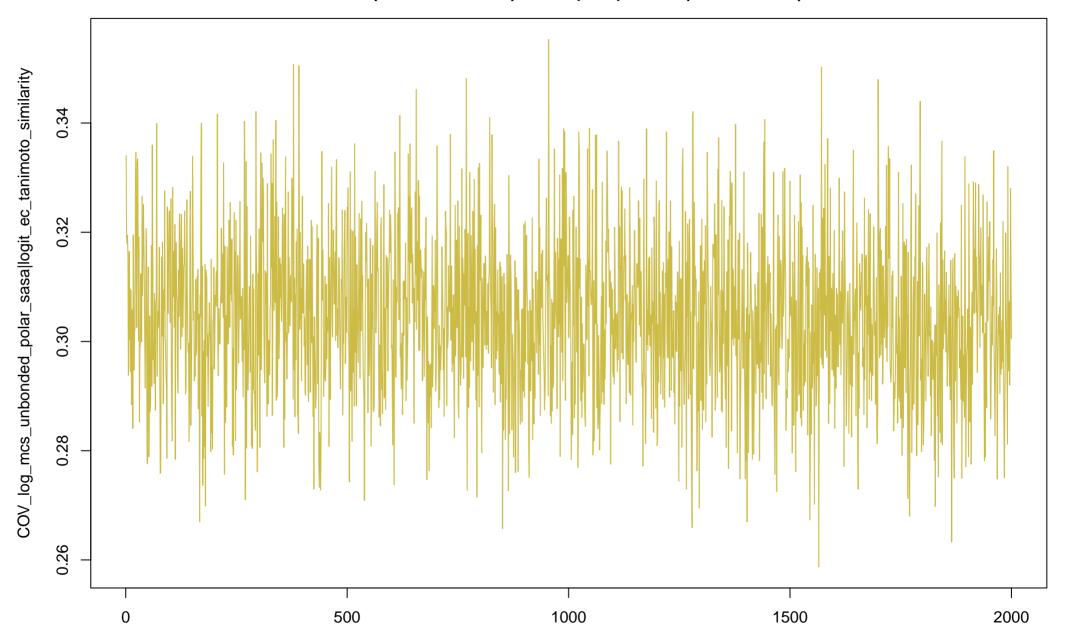


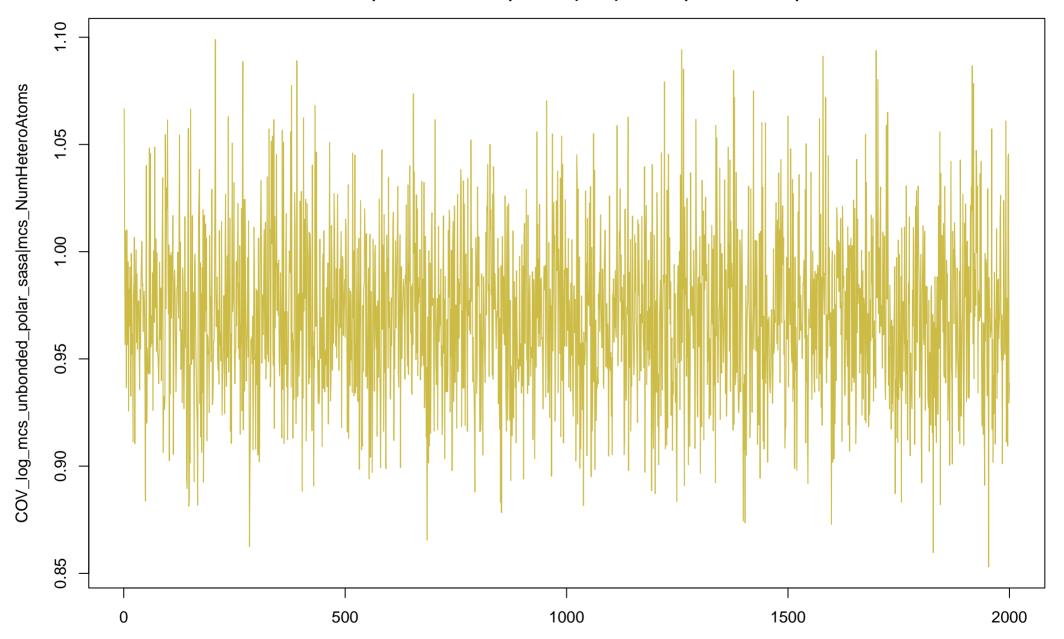
COV_log_RMSD|mcs_RingCount ESS = 1410 | BMK = 0.0327 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0

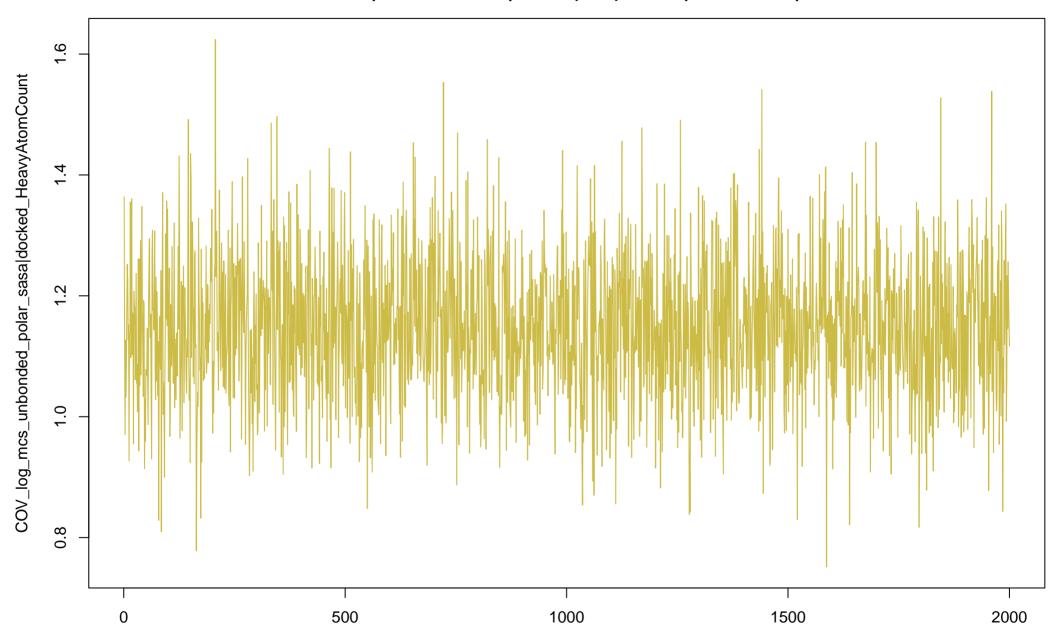


COV_log_RMSD|docked_NumRotatableBonds ESS = 1600 | BMK = 0.0827 | MCSE(6.27) = 2.72 | stat: FALSE | burn: 0

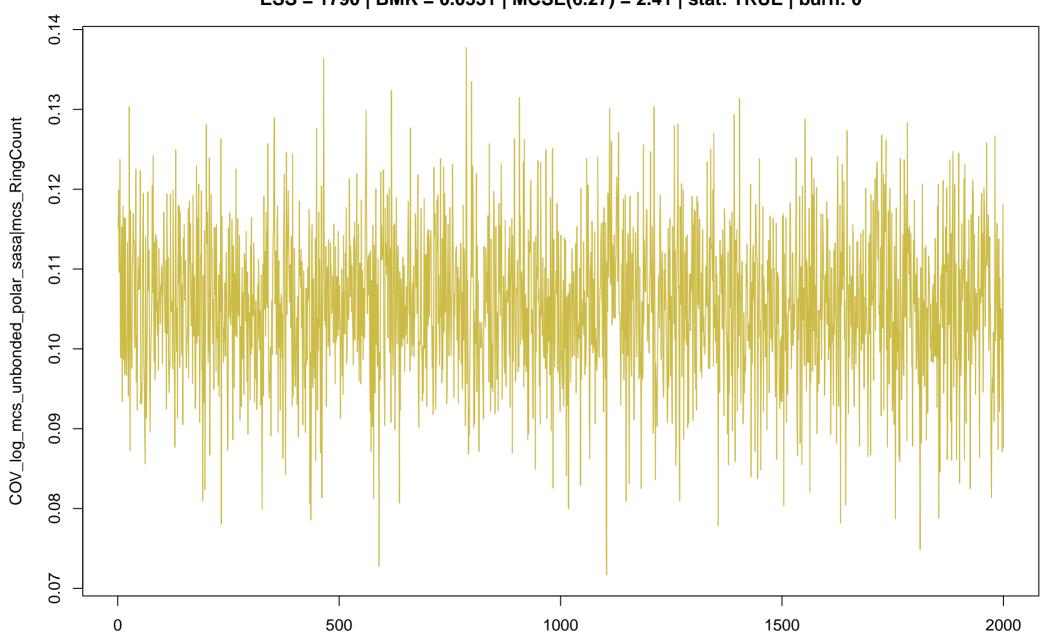


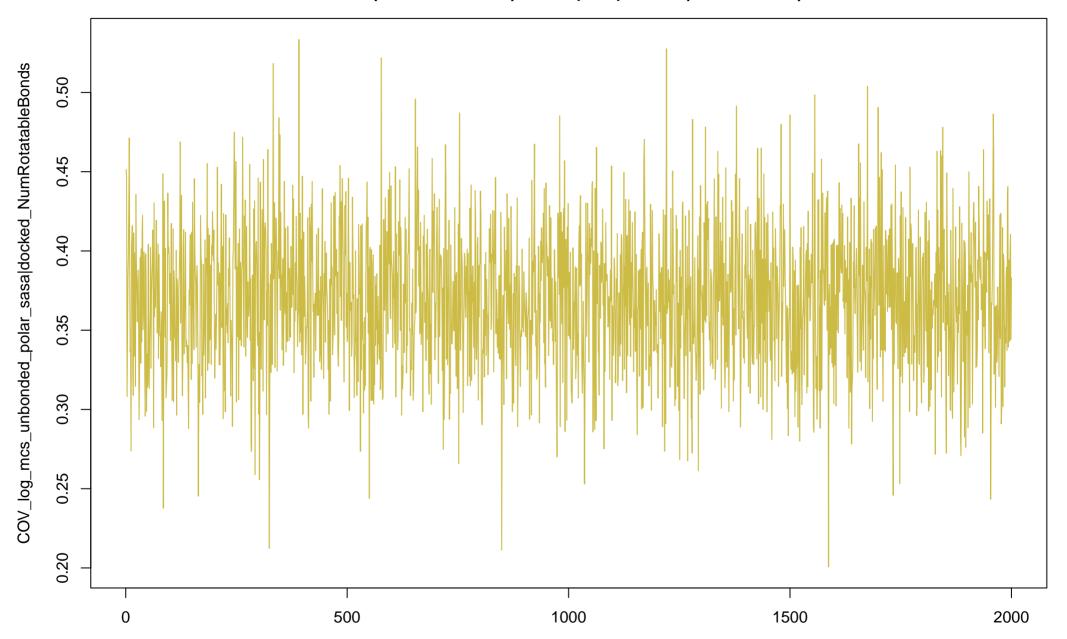




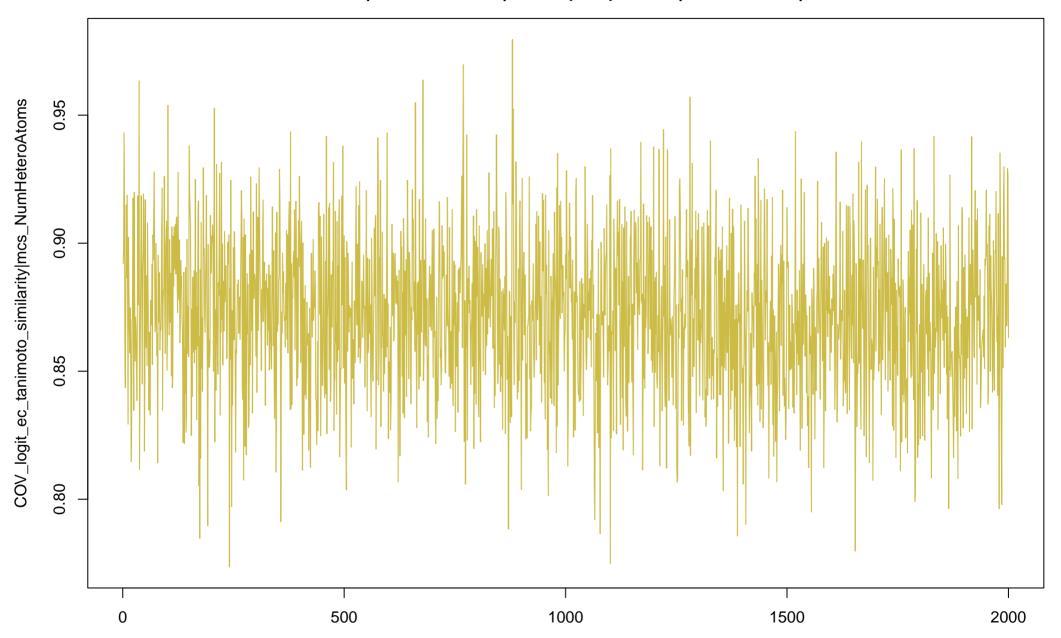


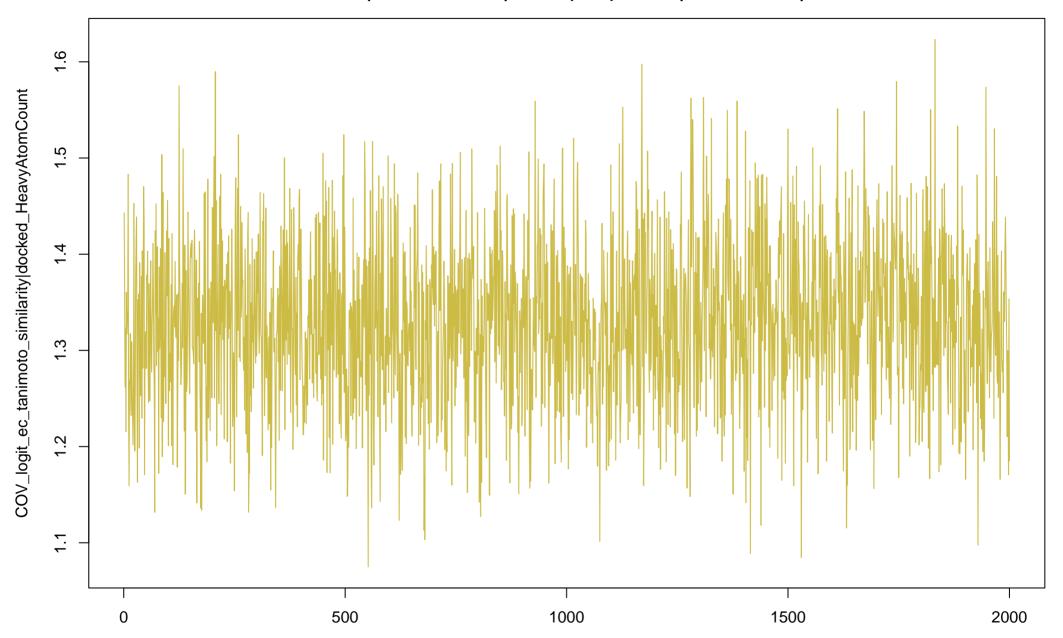
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount ESS = 1790 | BMK = 0.0531 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0



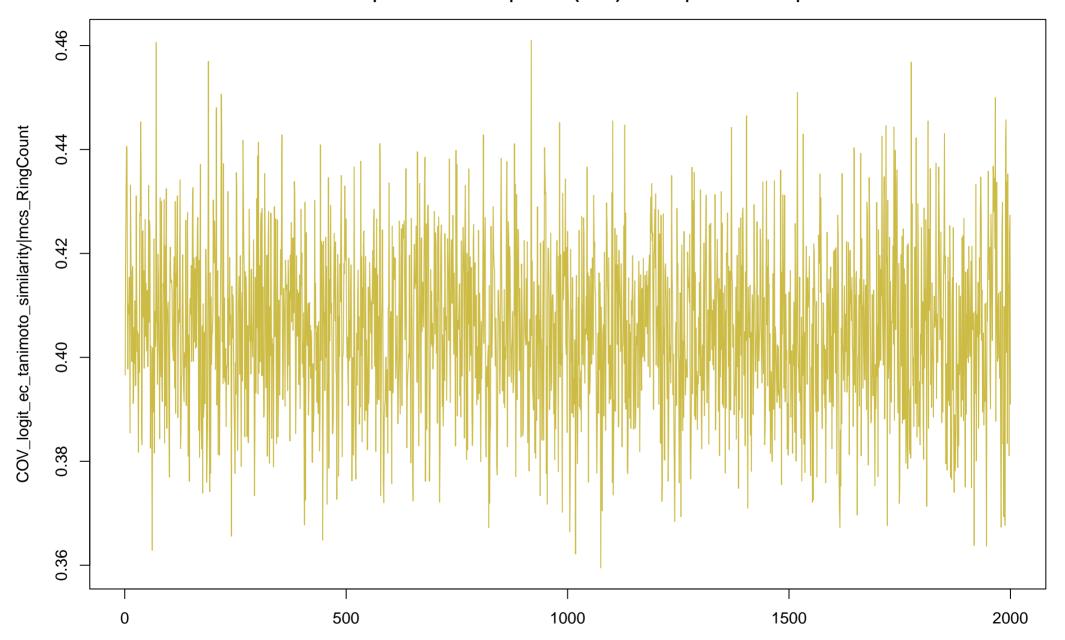


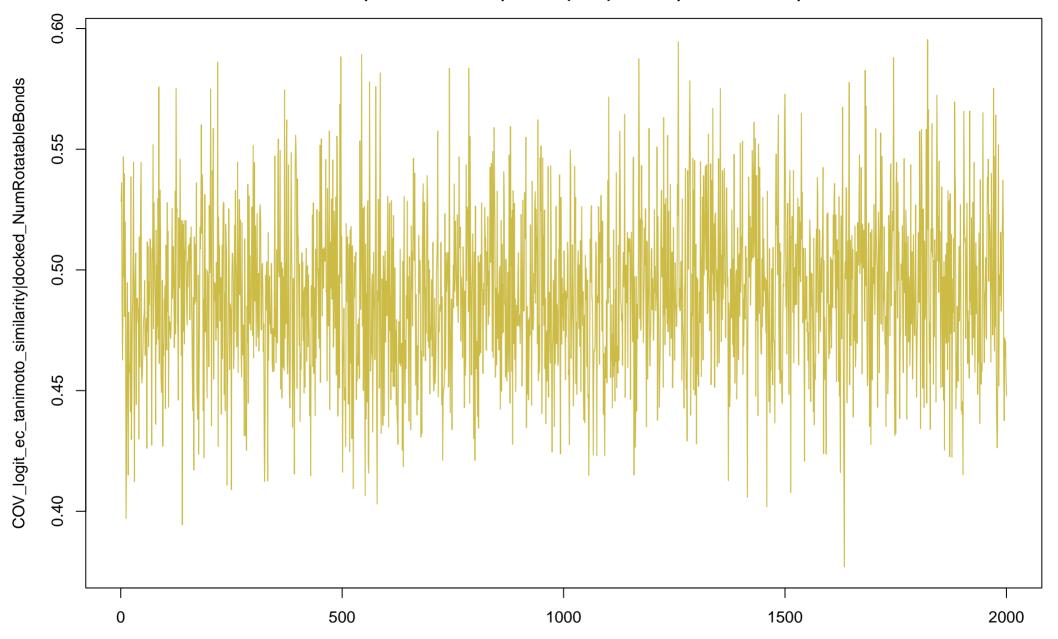
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms ESS = 1670 | BMK = 0.0667 | MCSE(6.27) = 2.57 | stat: FALSE | burn: 0



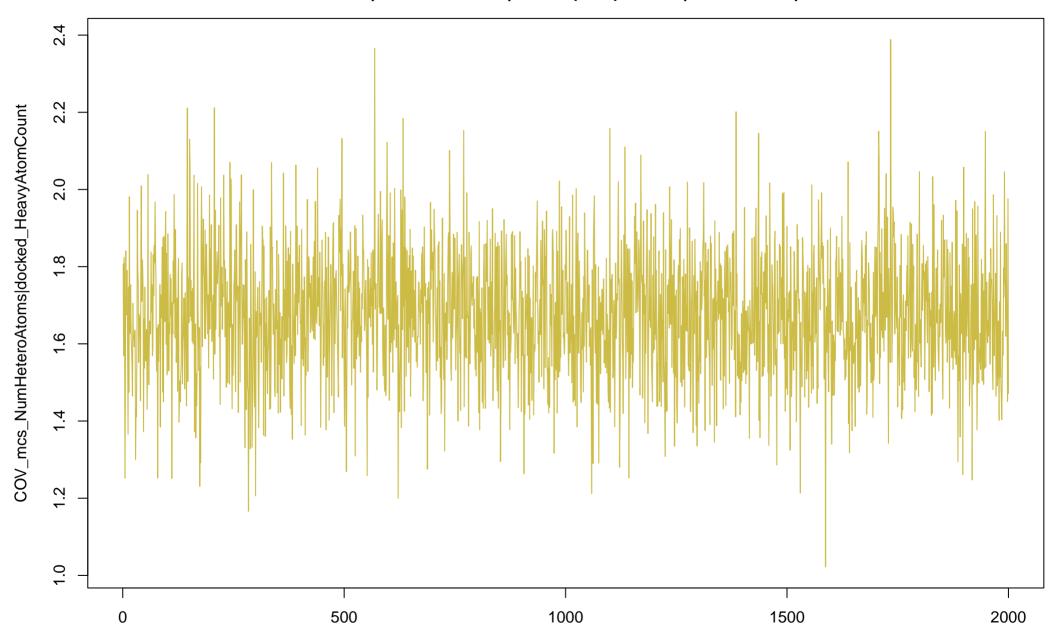


COV_logit_ec_tanimoto_similarity|mcs_RingCount ESS = 1750 | BMK = 0.0454 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0

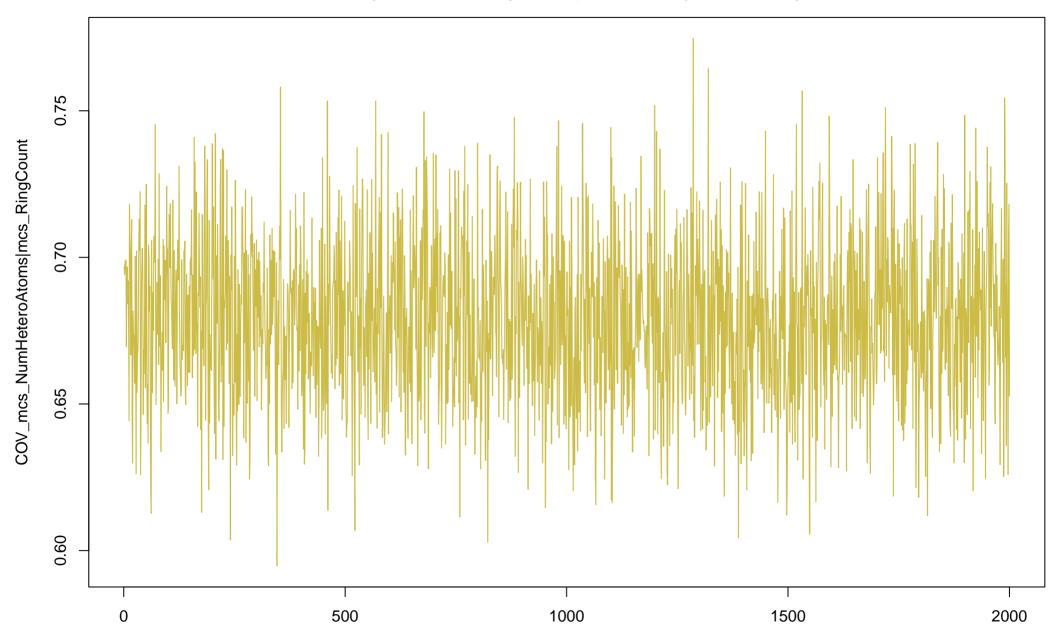


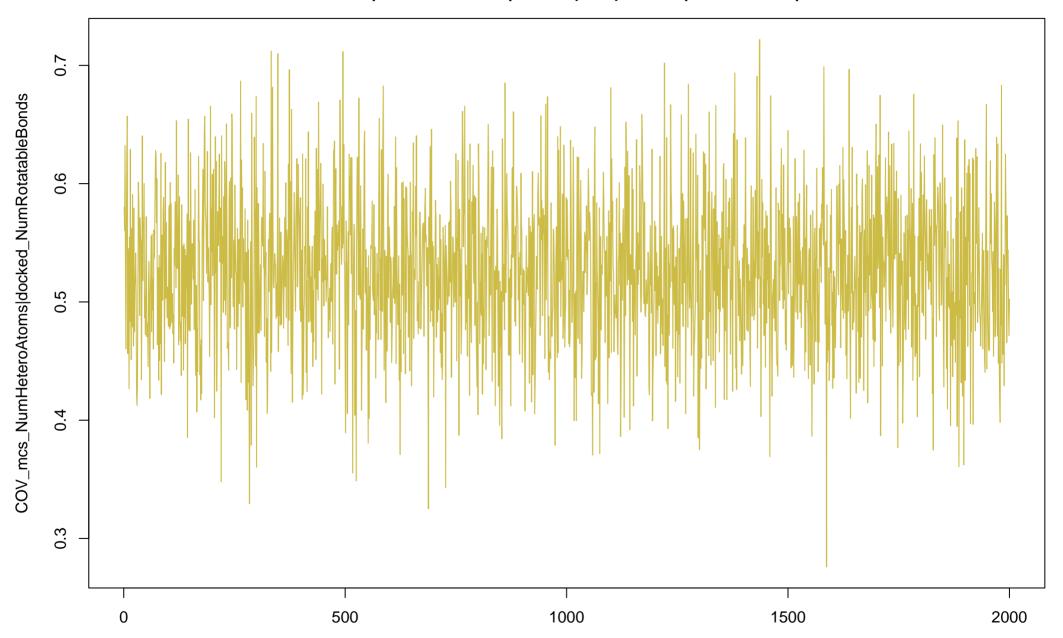


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount ESS = 1820 | BMK = 0.0354 | MCSE(6.27) = 2.67 | stat: TRUE | burn: 0

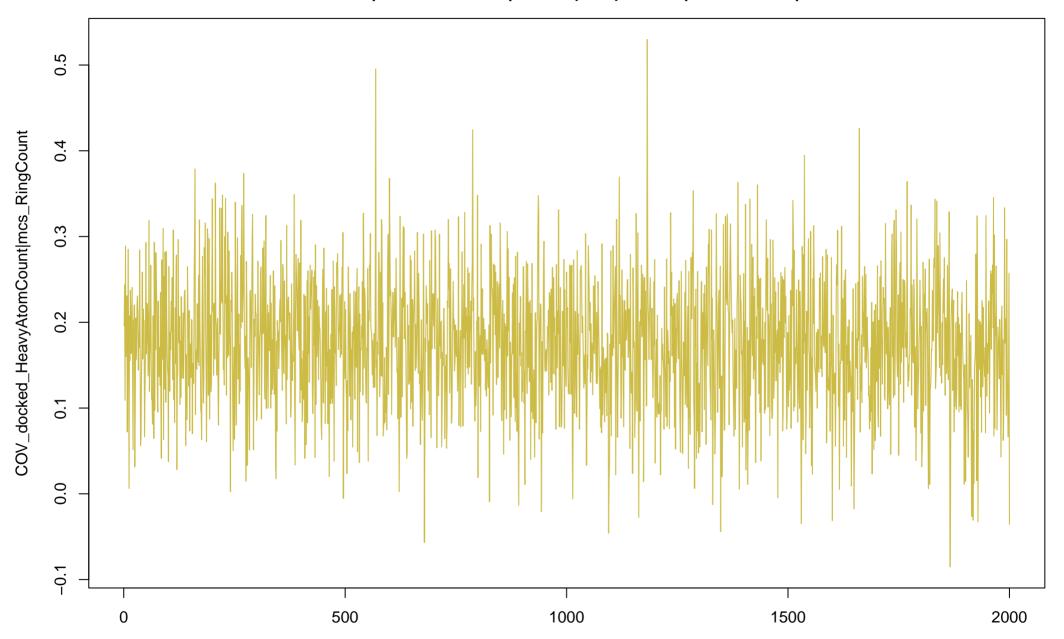


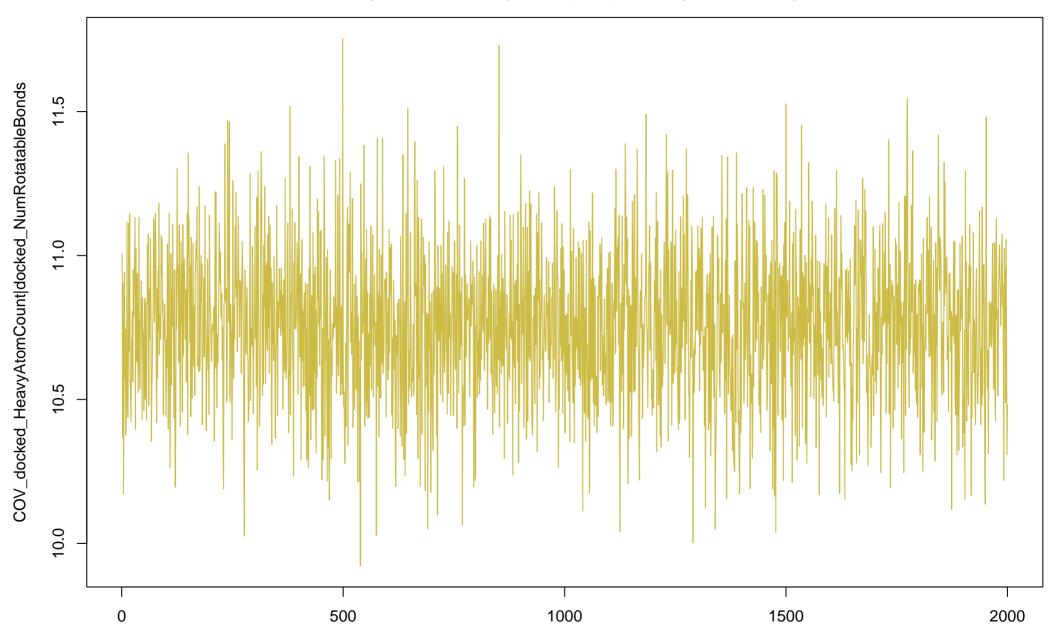
COV_mcs_NumHeteroAtoms|mcs_RingCount ESS = 1700 | BMK = 0.0468 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0





COV_docked_HeavyAtomCount|mcs_RingCount ESS = 1600 | BMK = 0.0634 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0





COV_mcs_RingCount|docked_NumRotatableBonds ESS = 1630 | BMK = 0.0669 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0

