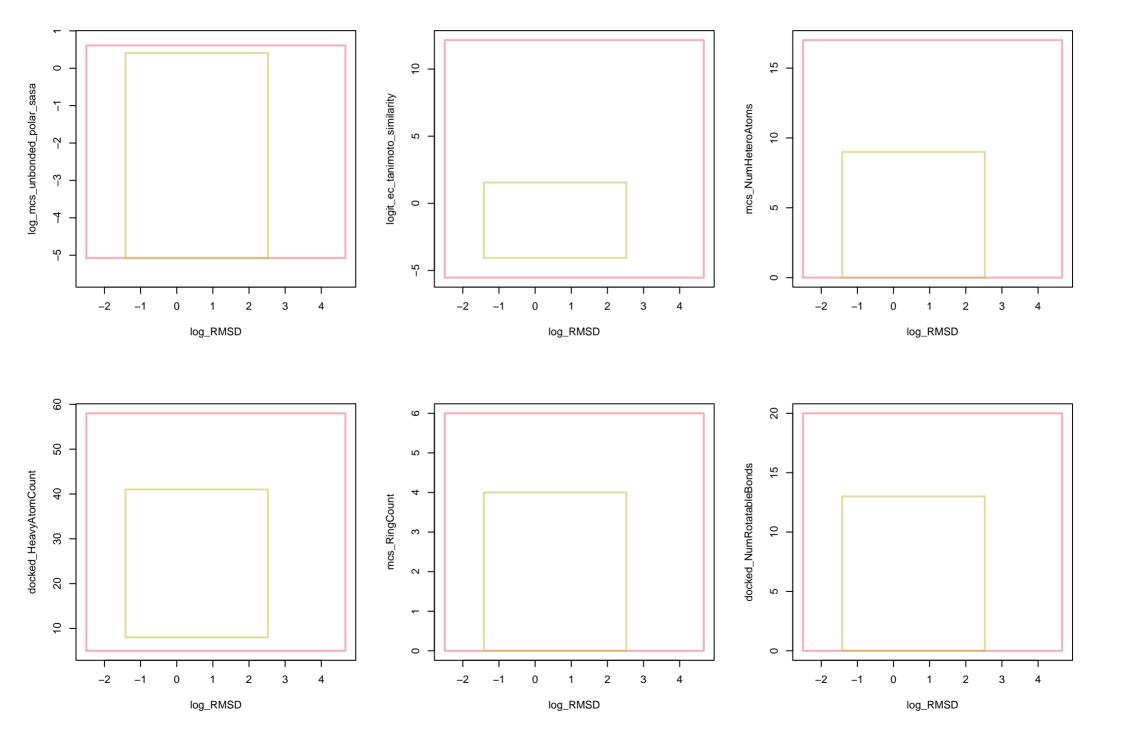
-- STATS maxD -min ESS = 179.183825321979 max BMK = 0.213258381007843 max MCSE = 10.0005977407497 all stationary: FALSE

burn: 0

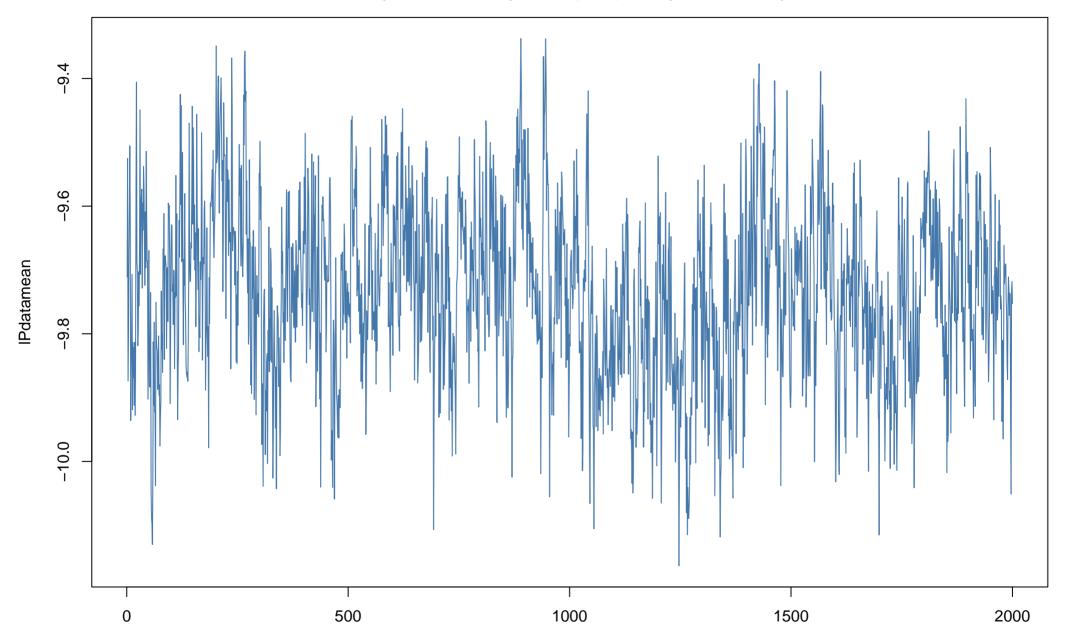
-- STATS 1D -min ESS = 1104.75389267184 max BMK = 0.0993112452914862 max MCSE = 3.16425884607483 all stationary: FALSE

burn: 0

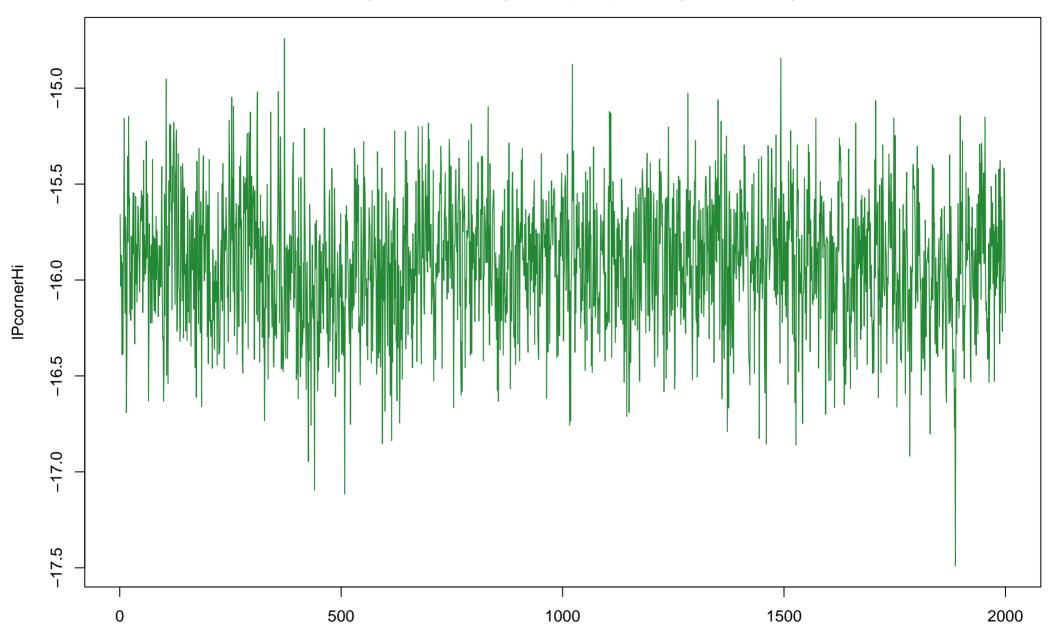
--- STATS 2D --min ESS = 789.906223907395
max BMK = 0.0966105648306887
max MCSE = 3.09034561334103
all stationary: FALSE
burn: 0



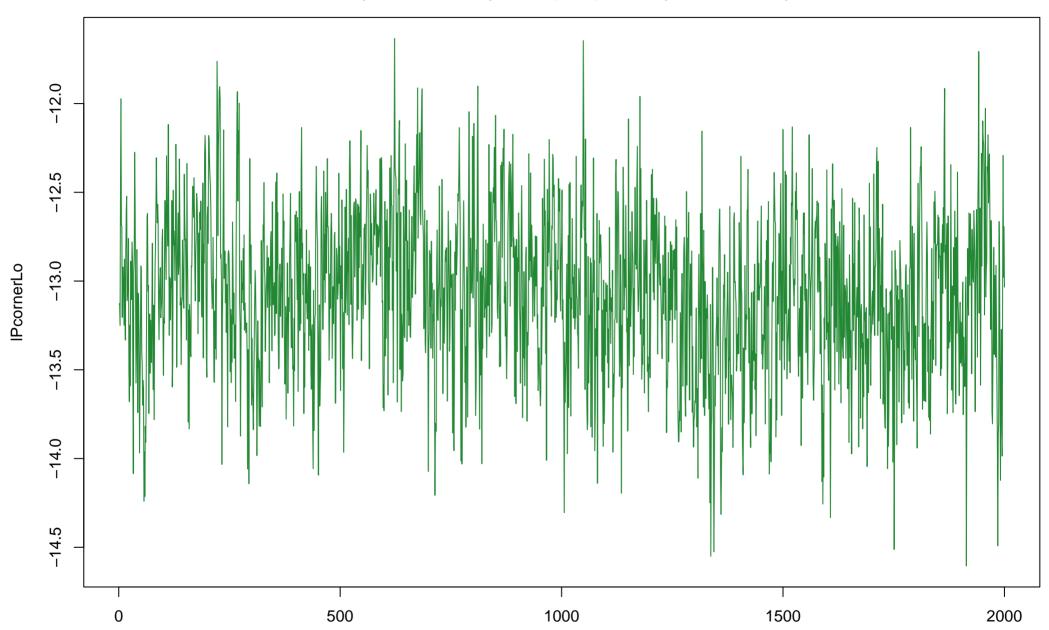
IPdatamean
ESS = 186 | BMK = 0.141 | MCSE(6.27) = 10 | stat: TRUE | burn: 0



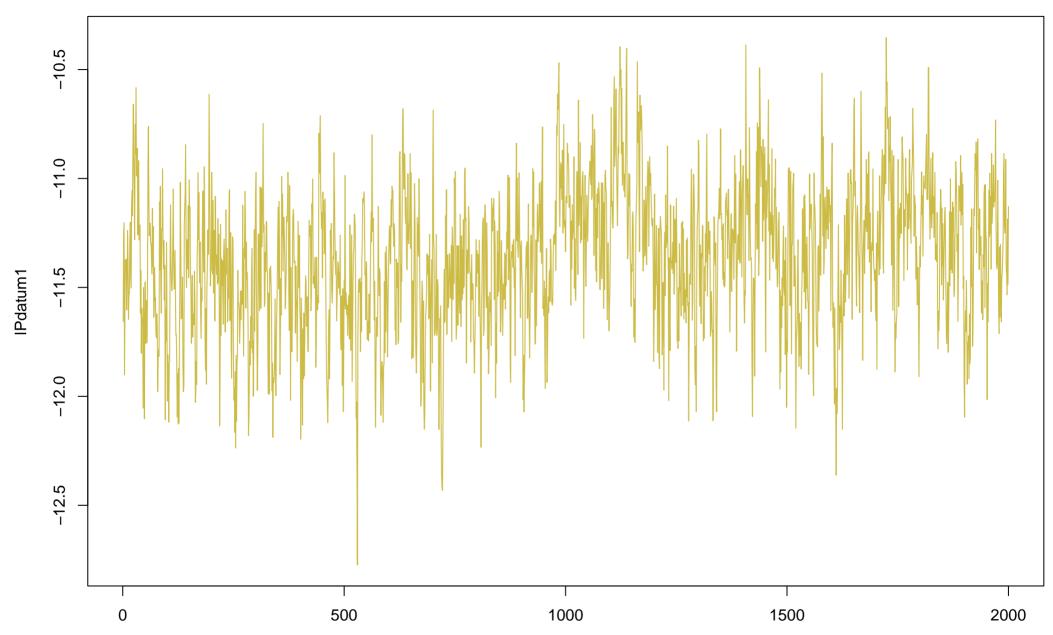
IPcornerHi
ESS = 1060 | BMK = 0.0501 | MCSE(6.27) = 3.77 | stat: TRUE | burn: 0



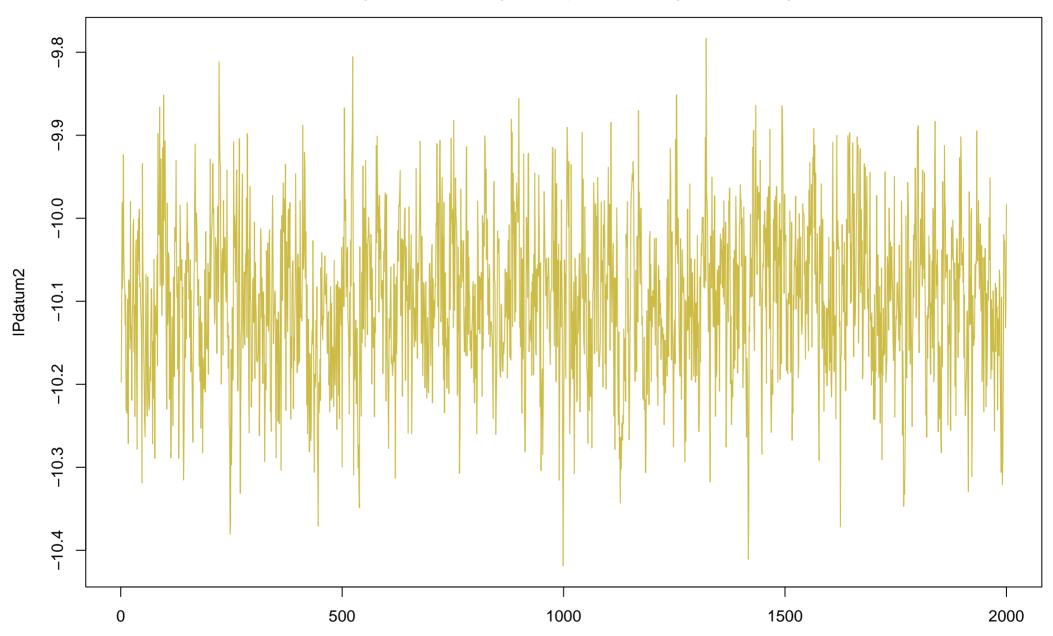
IPcornerLo
ESS = 313 | BMK = 0.135 | MCSE(6.27) = 5.86 | stat: FALSE | burn: 0



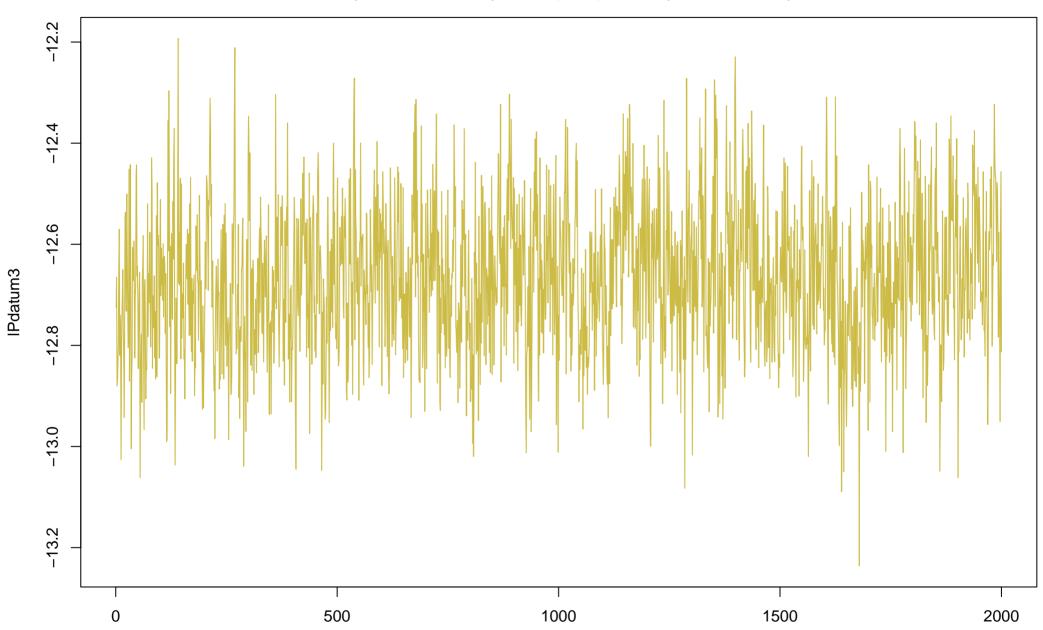
IPdatum1 ESS = 190 | BMK = 0.213 | MCSE(6.27) = 9.4 | stat: FALSE | burn: 0



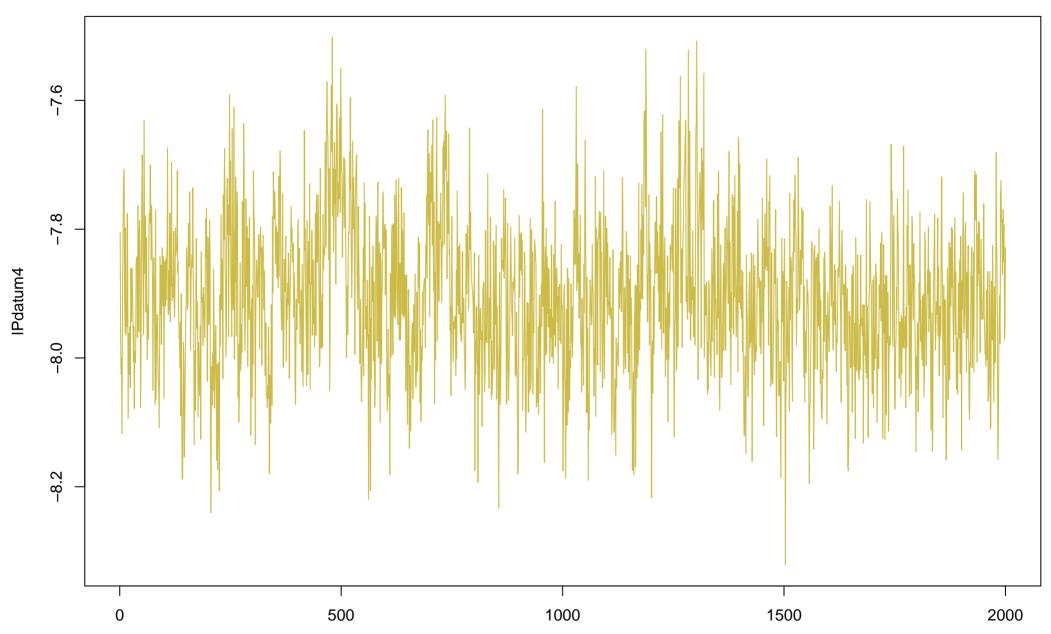
IPdatum2 ESS = 528 | BMK = 0.0363 | MCSE(6.27) = 5.62 | stat: TRUE | burn: 0



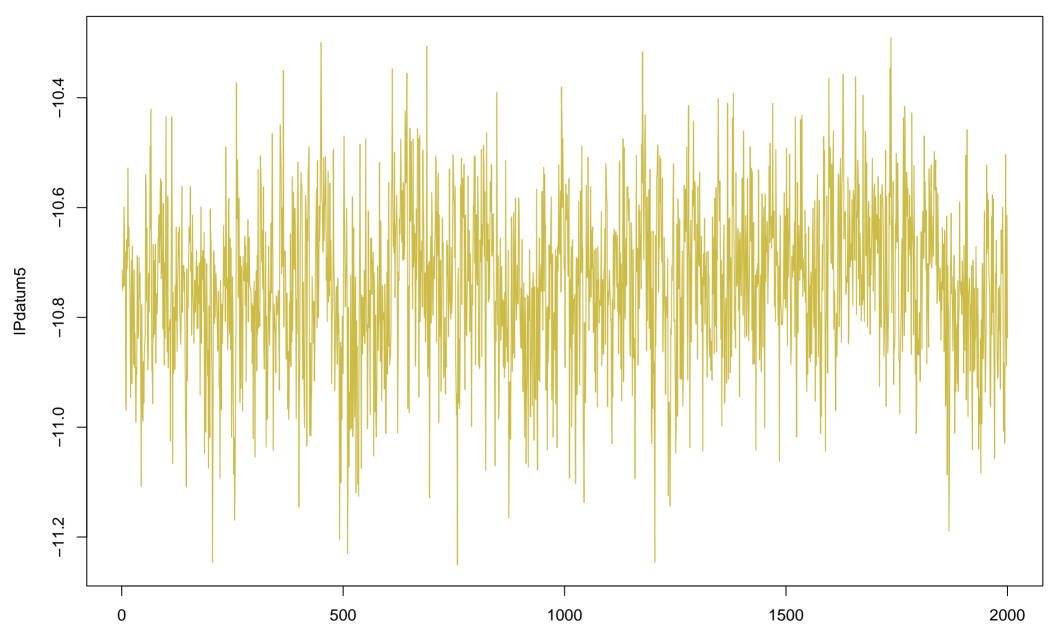
IPdatum3 ESS = 646 | BMK = 0.0592 | MCSE(6.27) = 4.81 | stat: FALSE | burn: 0



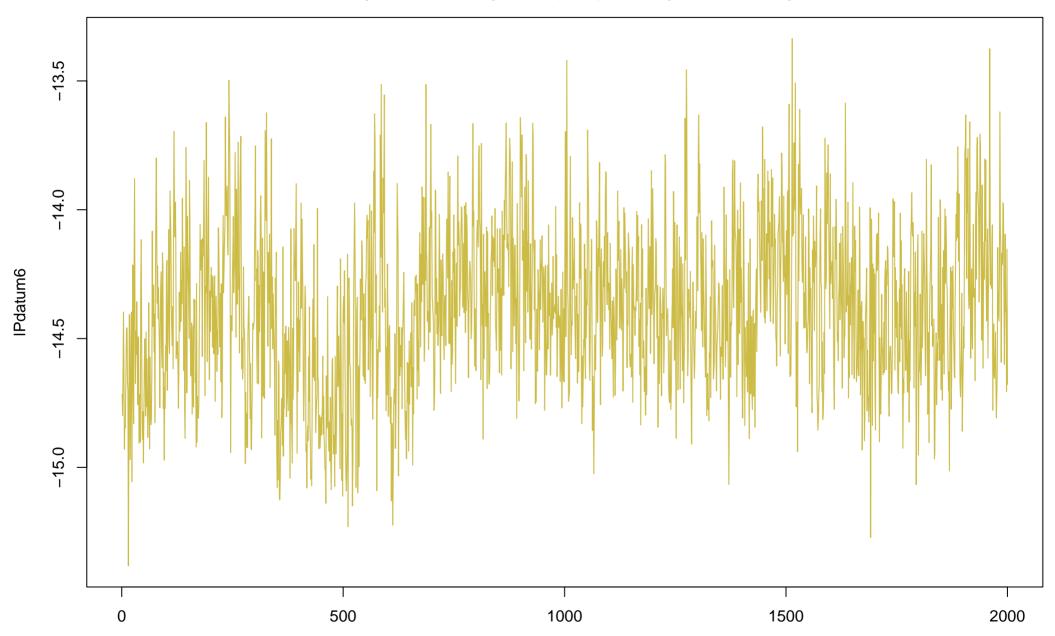
IPdatum4 ESS = 277 | BMK = 0.073 | MCSE(6.27) = 7.51 | stat: TRUE | burn: 0



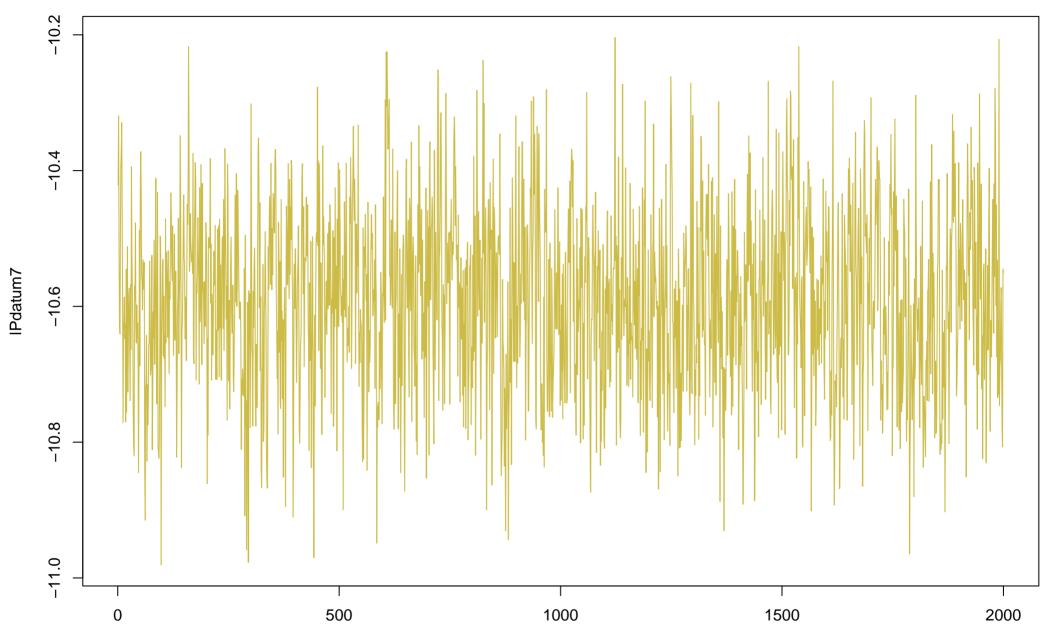
IPdatum5 ESS = 548 | BMK = 0.0772 | MCSE(6.27) = 5.66 | stat: FALSE | burn: 0



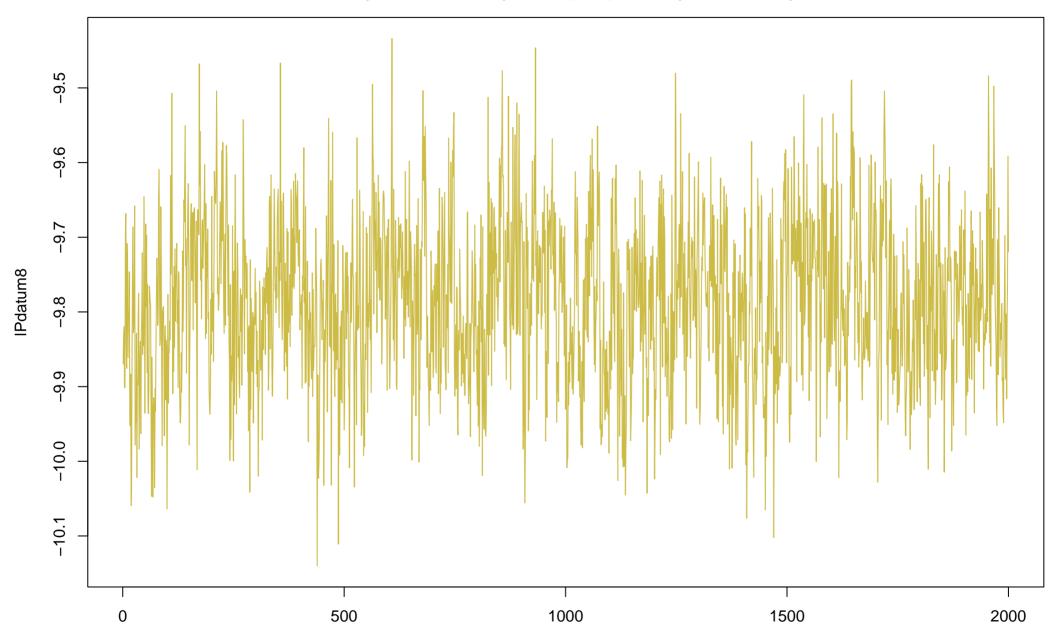
IPdatum6 ESS = 179 | BMK = 0.135 | MCSE(6.27) = 7.04 | stat: FALSE | burn: 0



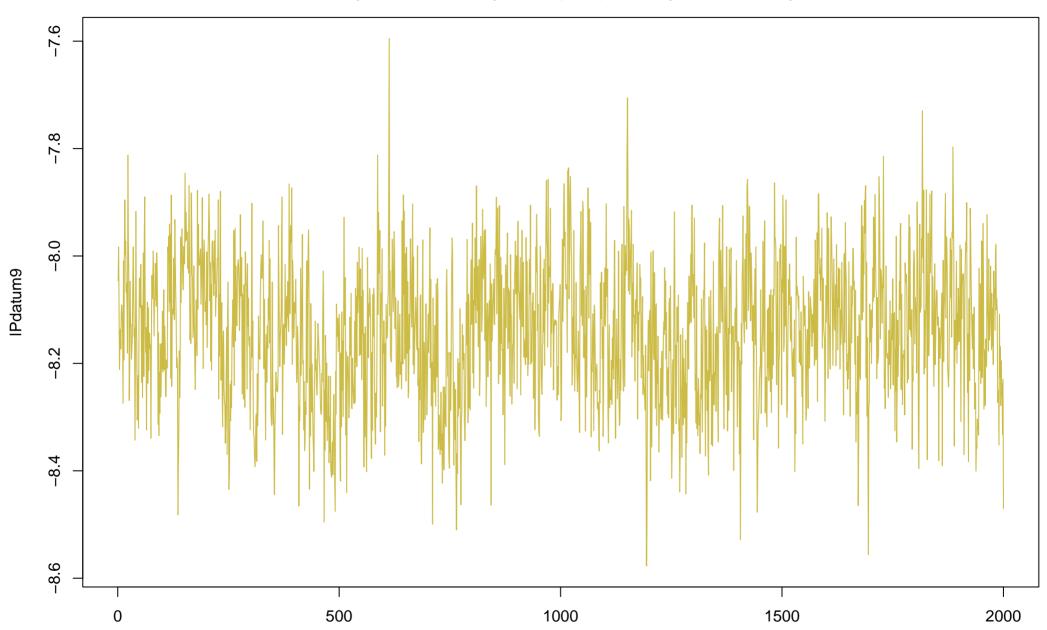
IPdatum7 ESS = 826 | BMK = 0.0557 | MCSE(6.27) = 4.47 | stat: TRUE | burn: 0



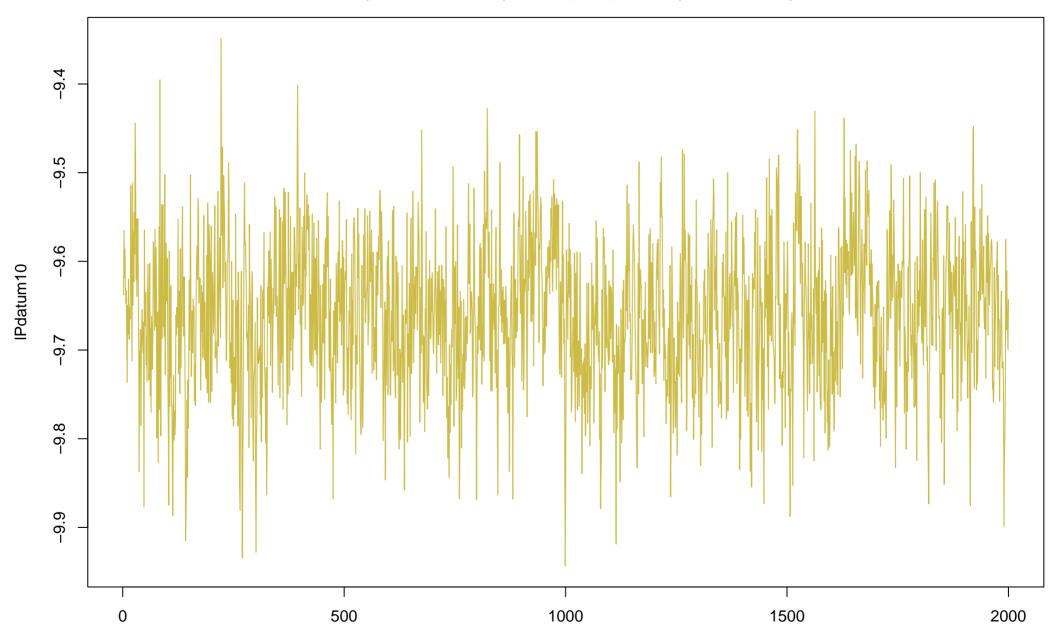
IPdatum8 ESS = 490 | BMK = 0.0477 | MCSE(6.27) = 6.12 | stat: TRUE | burn: 0



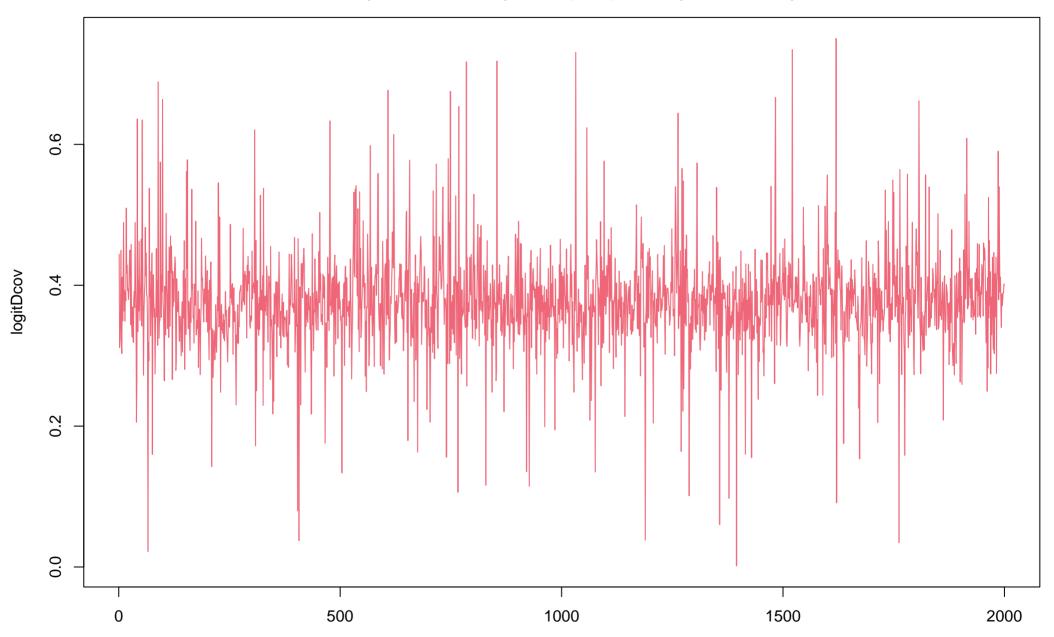
IPdatum9 ESS = 307 | BMK = 0.0599 | MCSE(6.27) = 6.25 | stat: FALSE | burn: 0



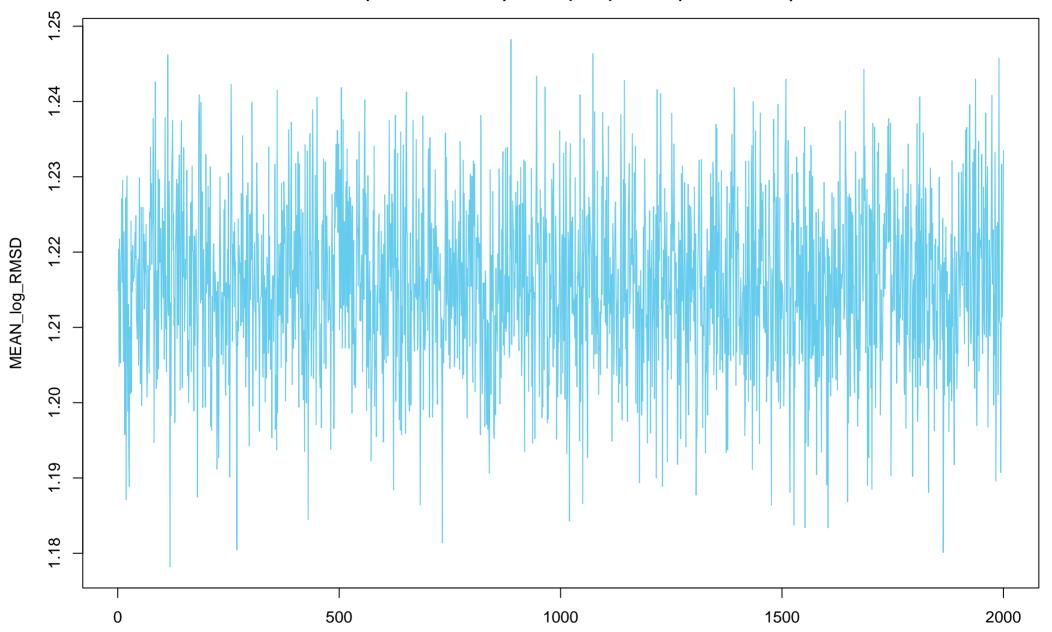
IPdatum10 ESS = 519 | BMK = 0.0641 | MCSE(6.27) = 5.97 | stat: TRUE | burn: 0



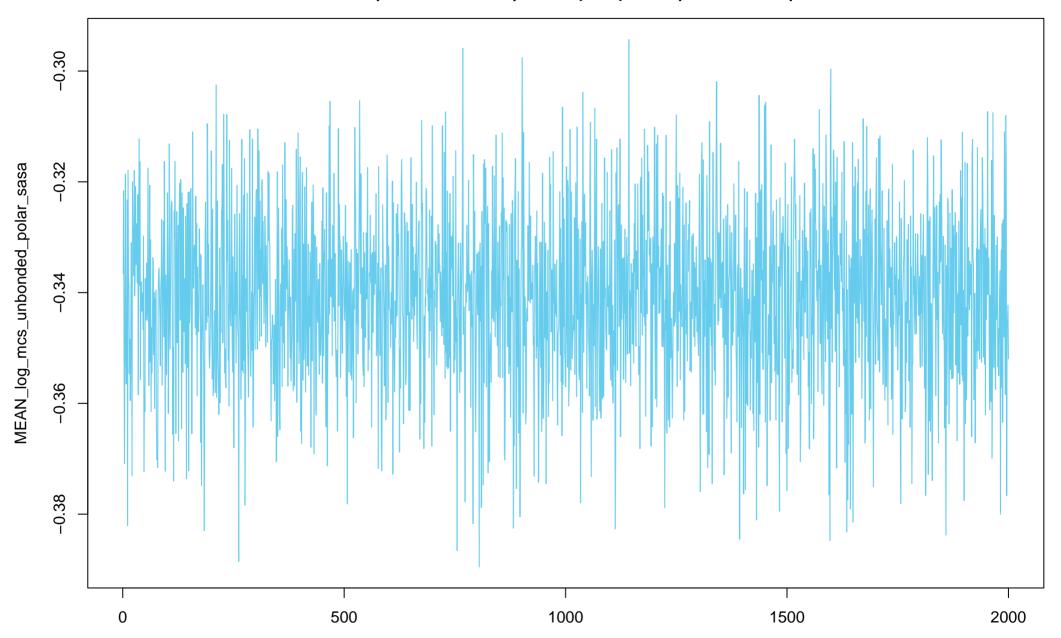
logitDcov ESS = 1540 | BMK = 0.0696 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0



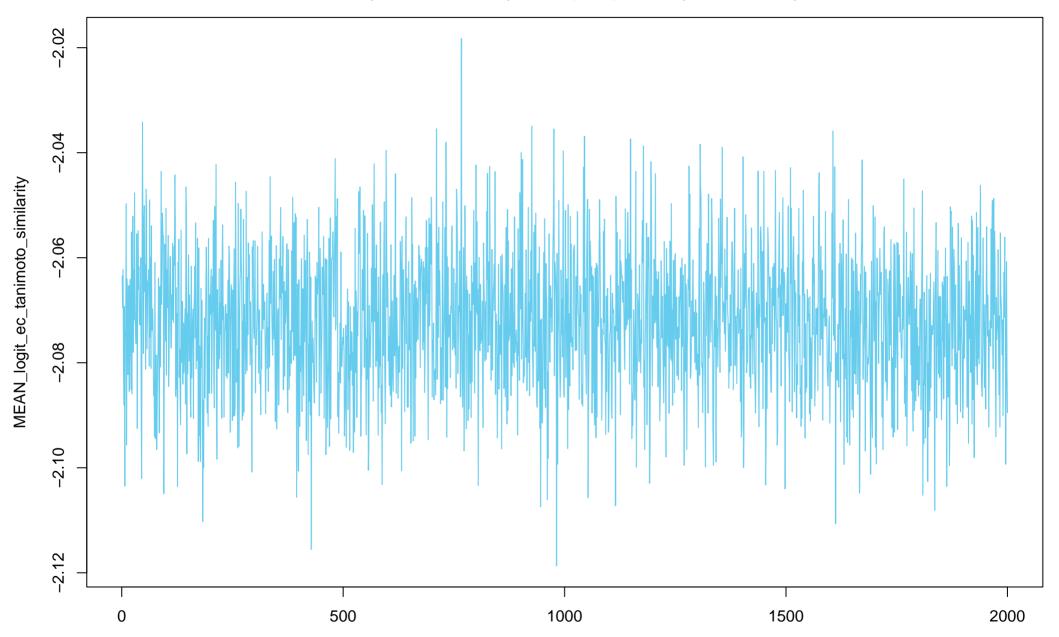
MEAN_log_RMSD ESS = 1660 | BMK = 0.0446 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0



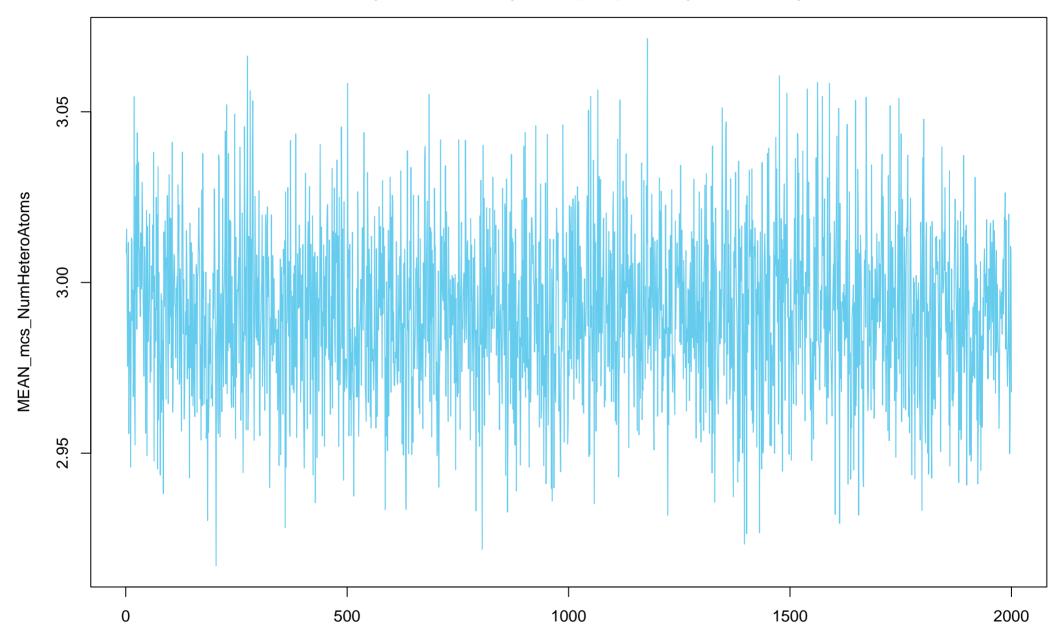
MEAN_log_mcs_unbonded_polar_sasa ESS = 2000 | BMK = 0.0369 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0



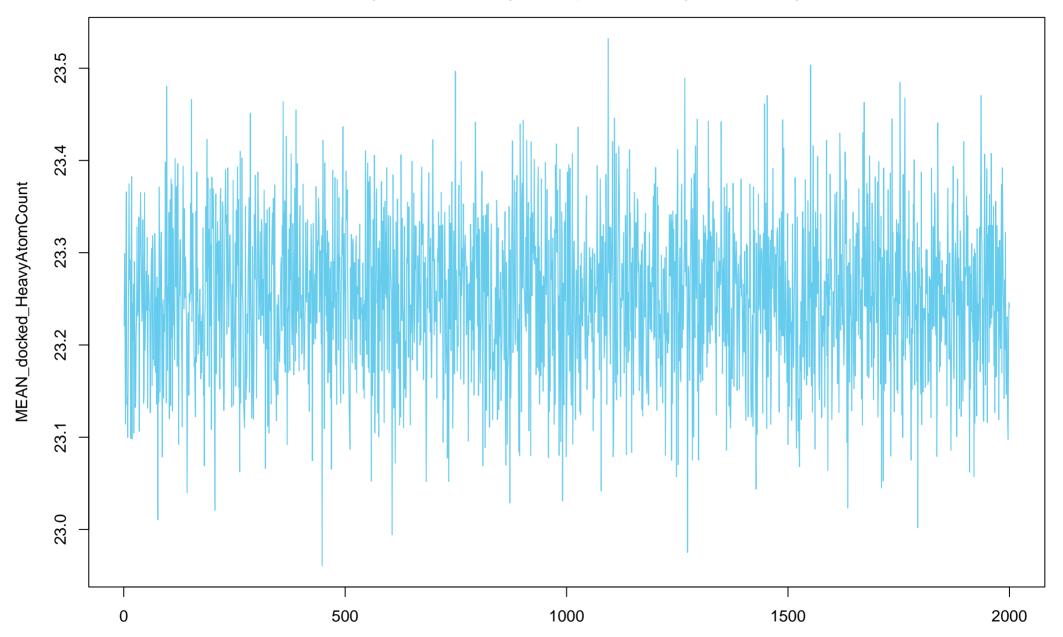
MEAN_logit_ec_tanimoto_similarity ESS = 1850 | BMK = 0.0408 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0



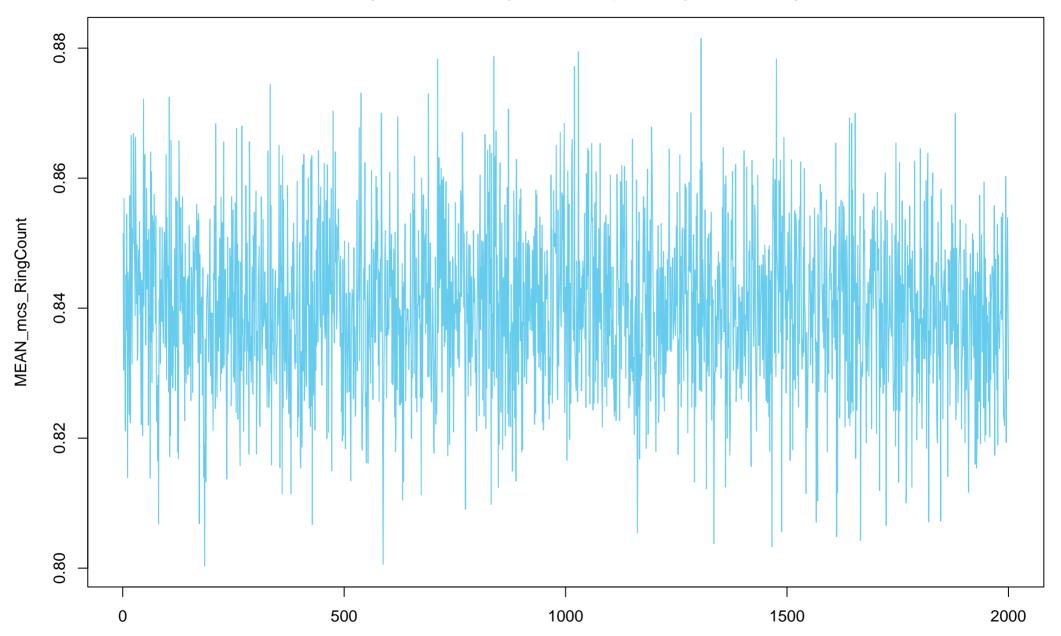
MEAN_mcs_NumHeteroAtoms ESS = 2000 | BMK = 0.0317 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0



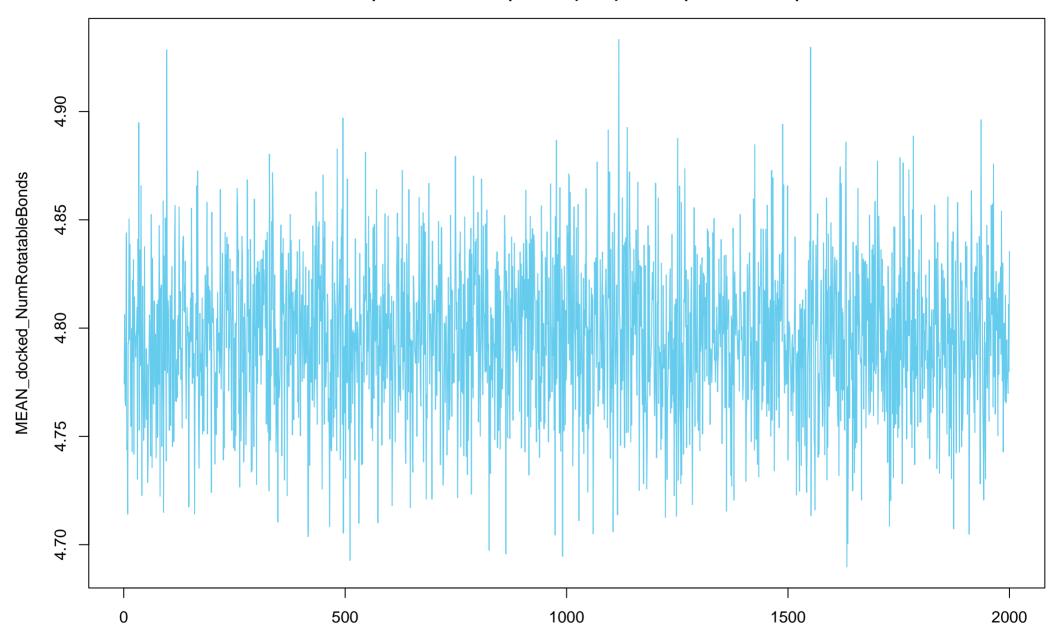
MEAN_docked_HeavyAtomCount ESS = 2000 | BMK = 0.0433 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0



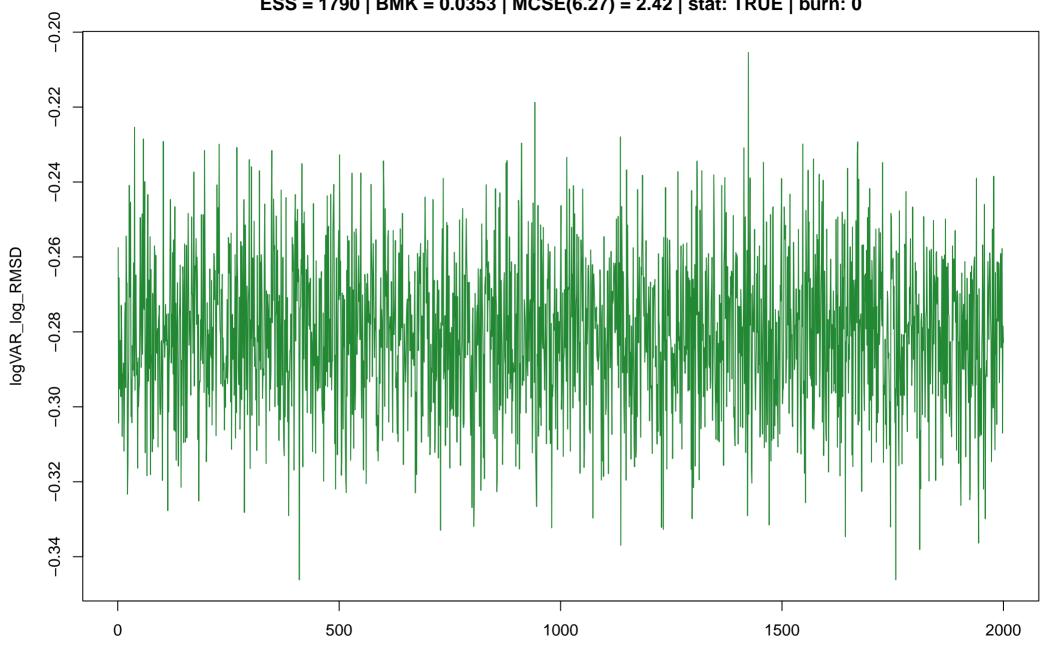
MEAN_mcs_RingCount ESS = 2000 | BMK = 0.0433 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0



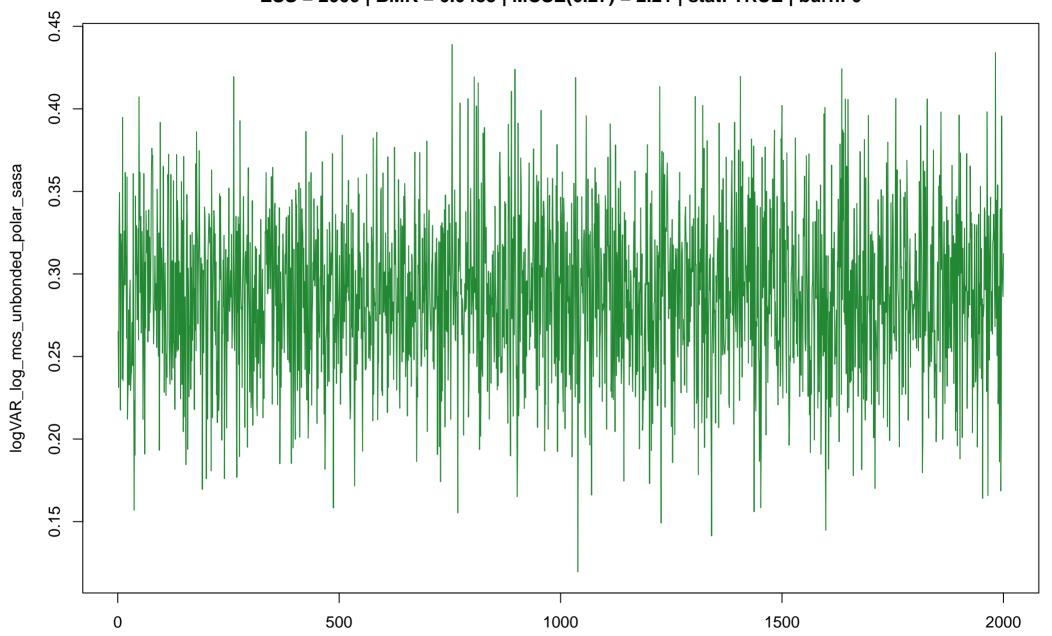
MEAN_docked_NumRotatableBonds ESS = 2000 | BMK = 0.0348 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



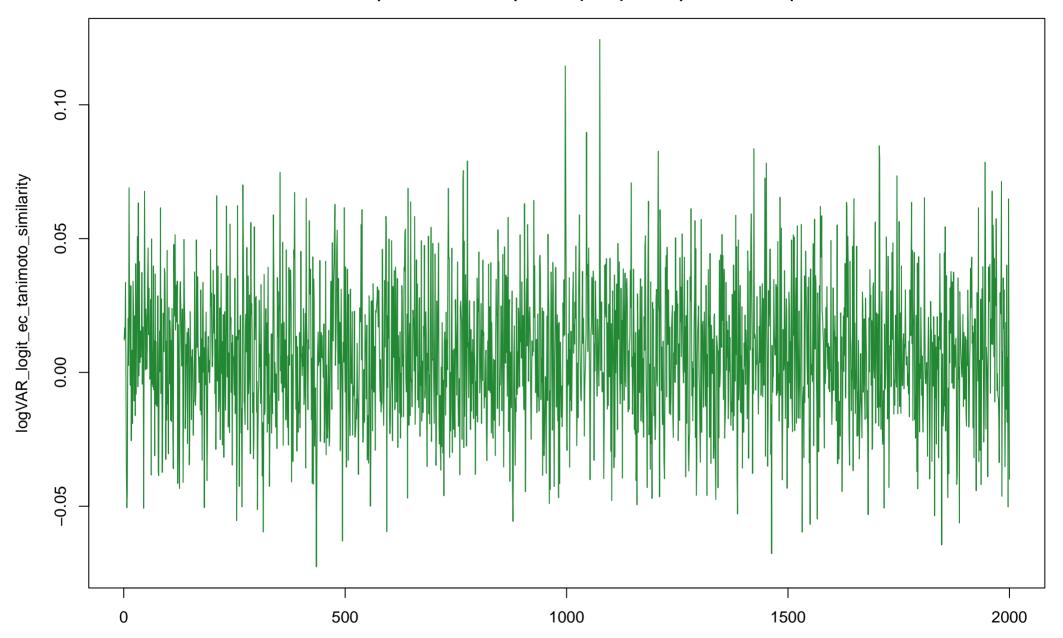
logVAR_log_RMSD ESS = 1790 | BMK = 0.0353 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0



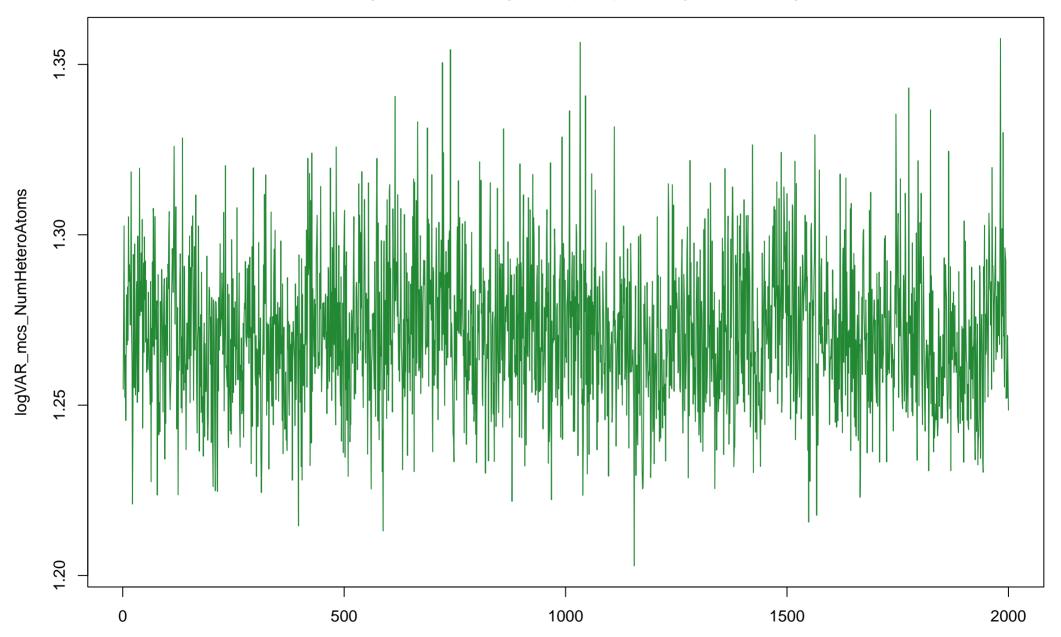
logVAR_log_mcs_unbonded_polar_sasa ESS = 2000 | BMK = 0.0435 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



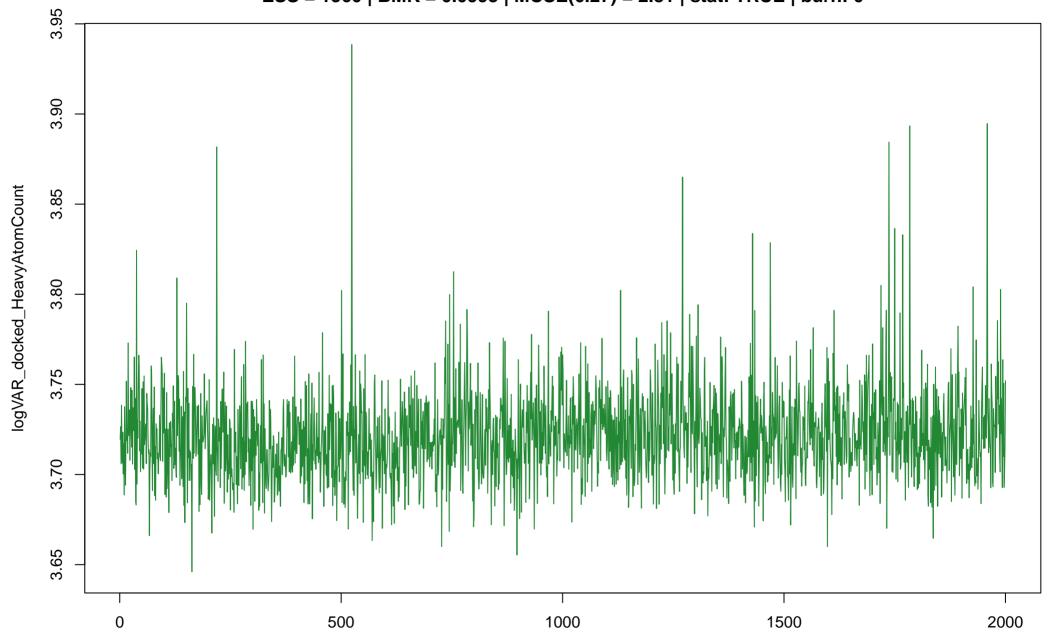
logVAR_logit_ec_tanimoto_similarity ESS = 1660 | BMK = 0.0426 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0



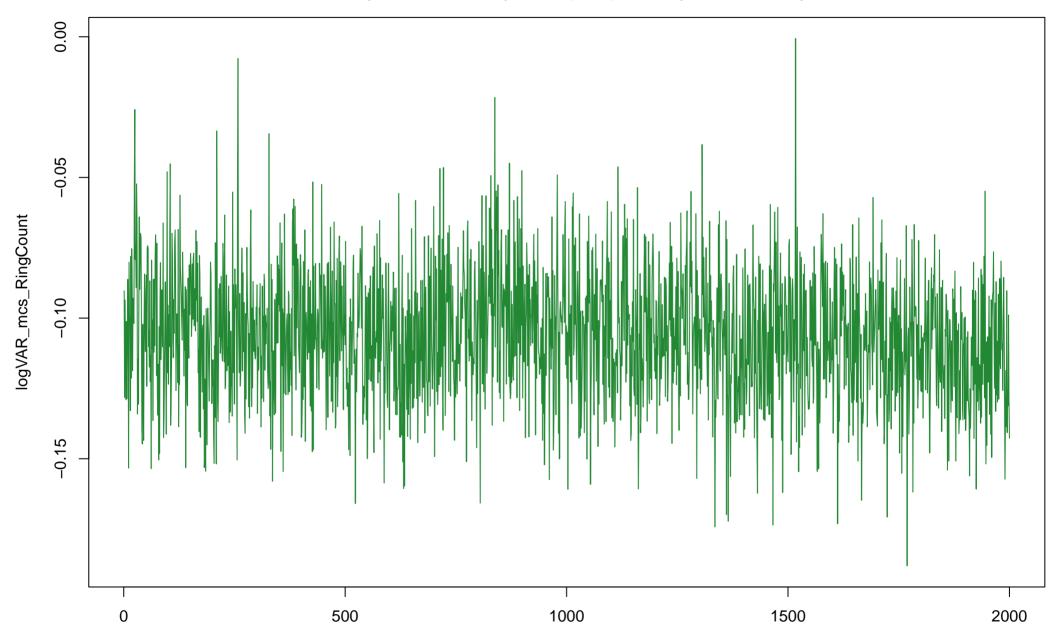
logVAR_mcs_NumHeteroAtoms ESS = 1100 | BMK = 0.0496 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0



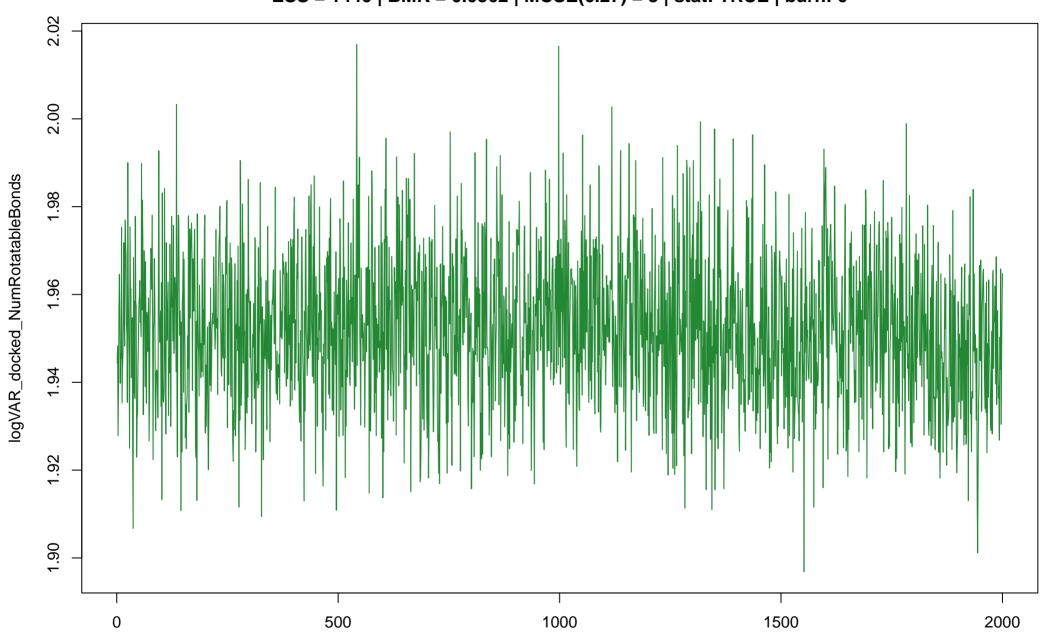
logVAR_docked_HeavyAtomCount ESS = 1560 | BMK = 0.0993 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0



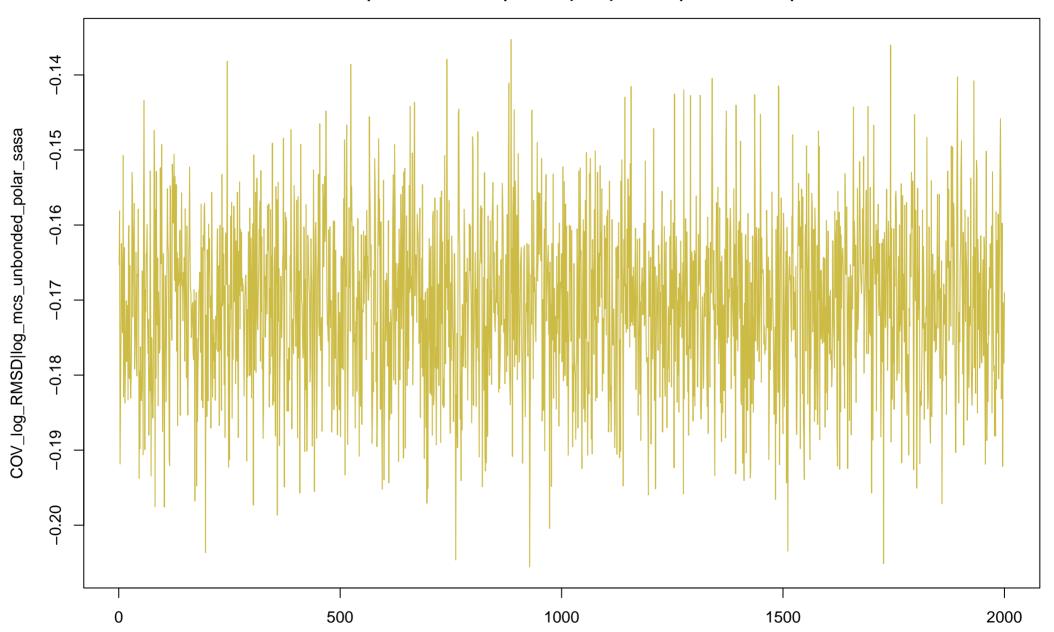
logVAR_mcs_RingCount ESS = 1450 | BMK = 0.0875 | MCSE(6.27) = 3.06 | stat: FALSE | burn: 0



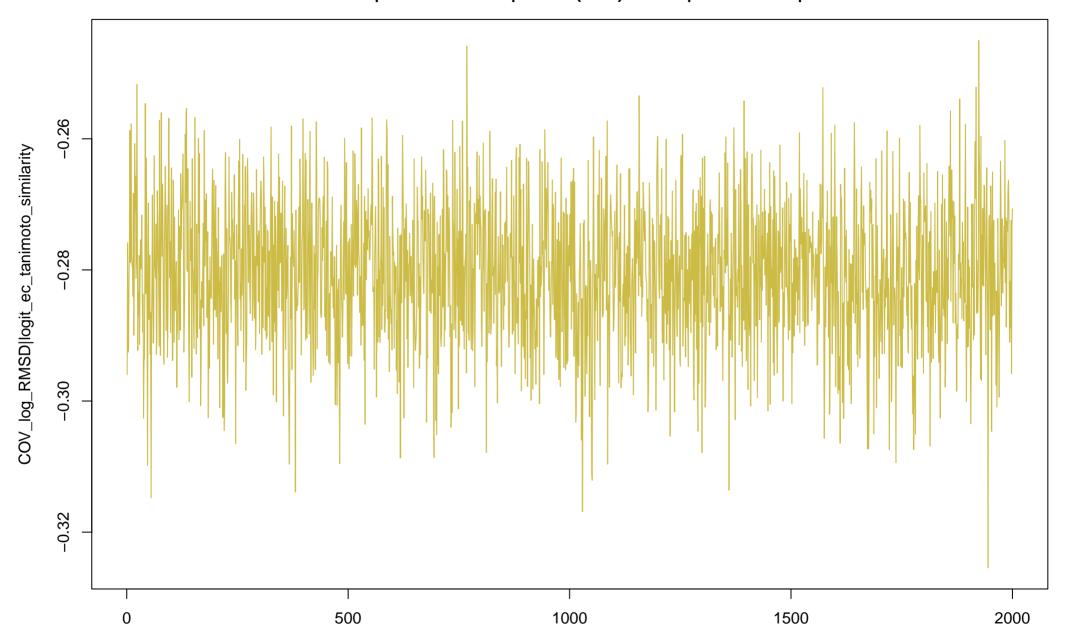
logVAR_docked_NumRotatableBonds ESS = 1440 | BMK = 0.0562 | MCSE(6.27) = 3 | stat: TRUE | burn: 0



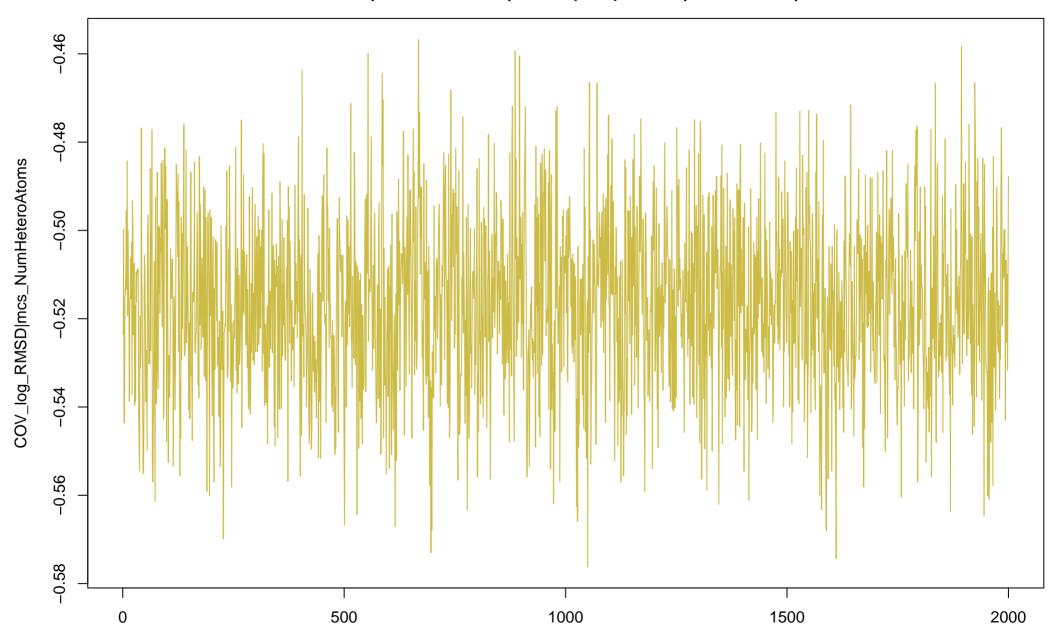
COV_log_RMSD|log_mcs_unbonded_polar_sasa ESS = 1770 | BMK = 0.0341 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0



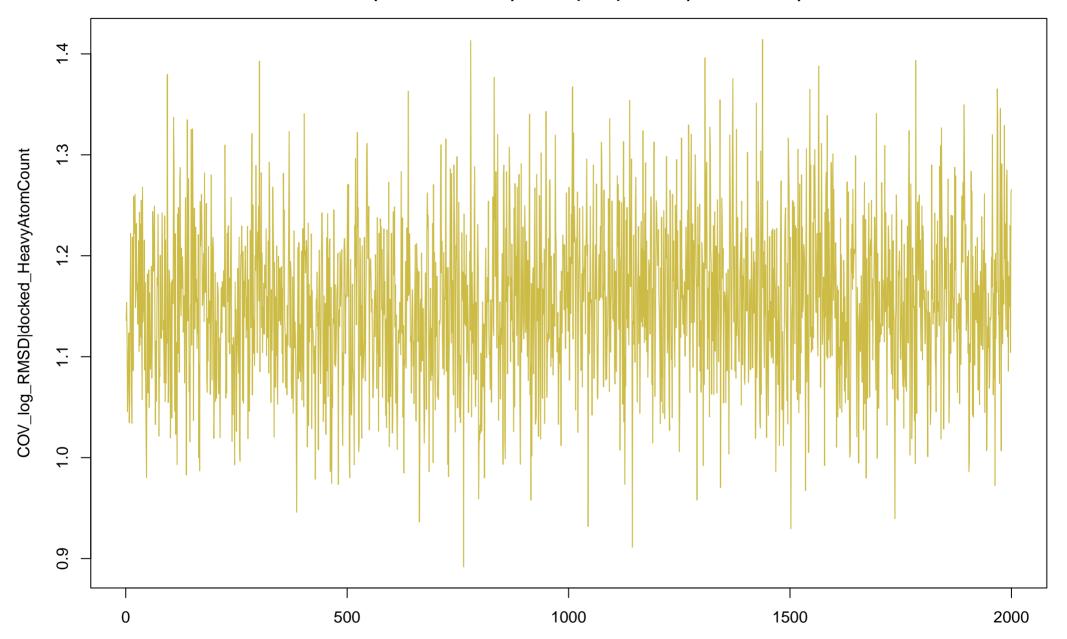
COV_log_RMSD|logit_ec_tanimoto_similarity ESS = 1610 | BMK = 0.0568 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0



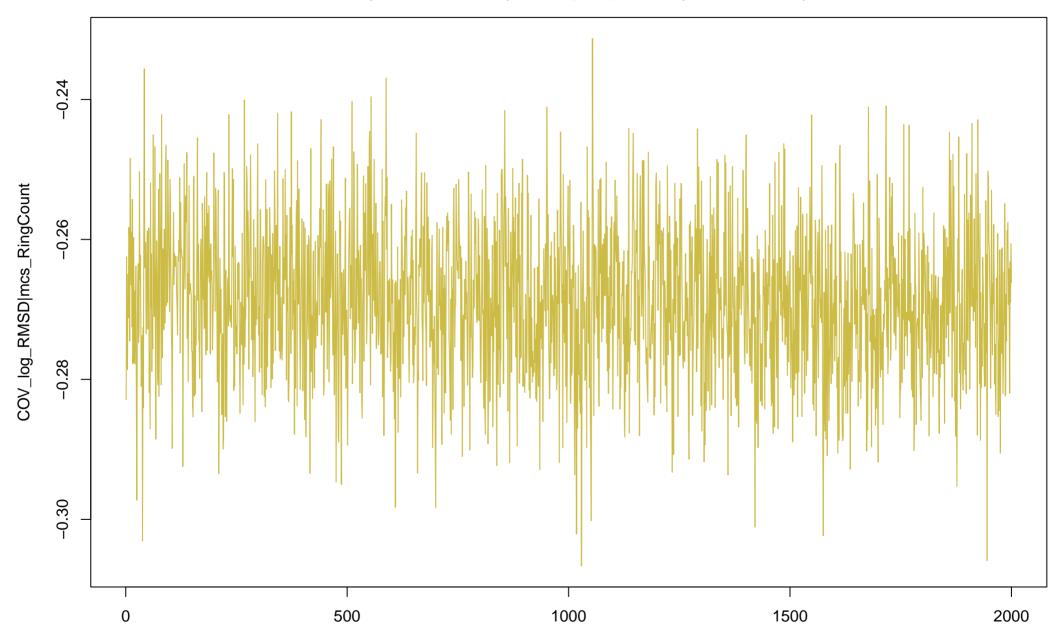
COV_log_RMSD|mcs_NumHeteroAtoms ESS = 1470 | BMK = 0.0289 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0



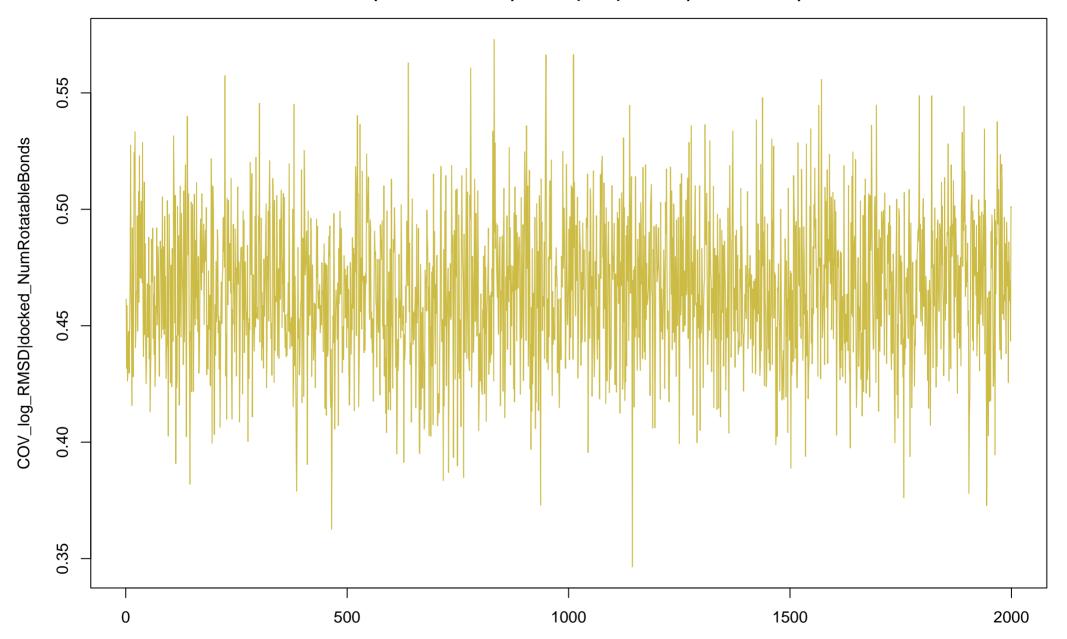
COV_log_RMSD|docked_HeavyAtomCount ESS = 1540 | BMK = 0.0796 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0

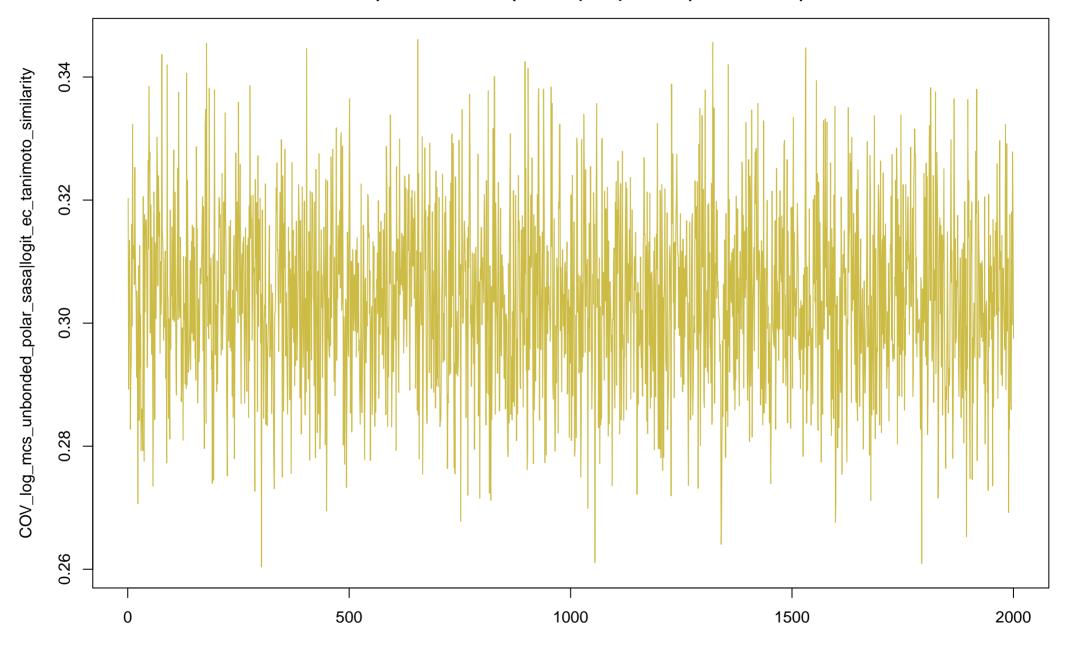


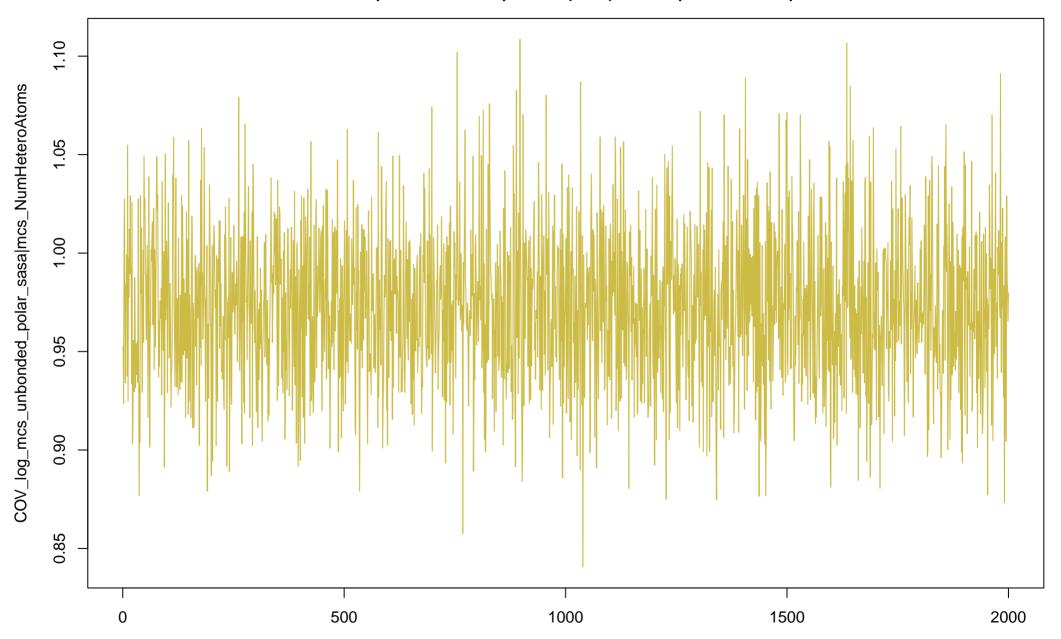
COV_log_RMSD|mcs_RingCount ESS = 1480 | BMK = 0.0672 | MCSE(6.27) = 3.01 | stat: FALSE | burn: 0

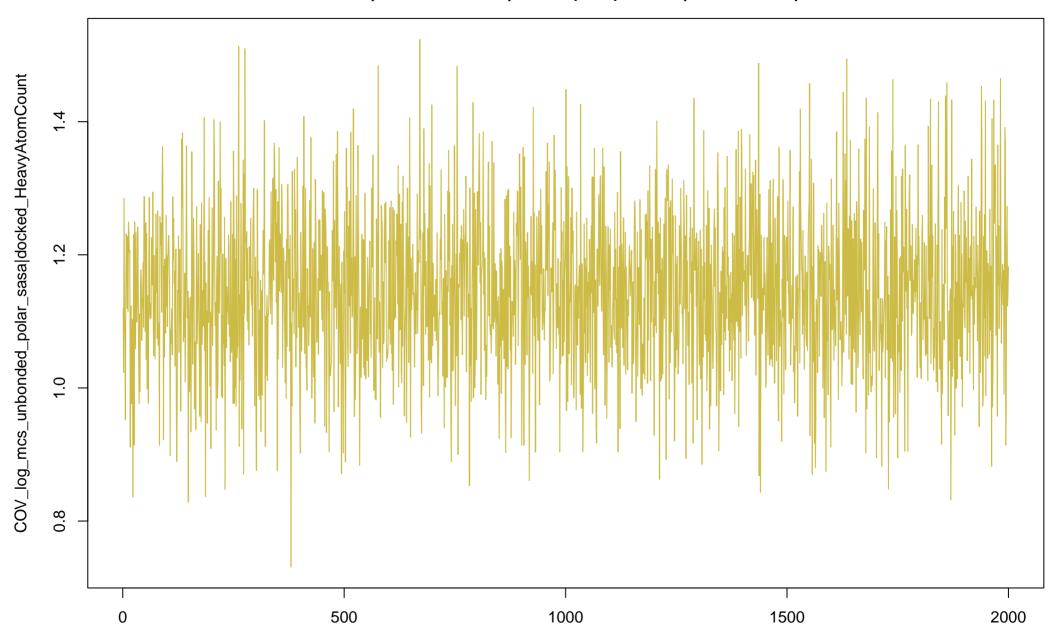


COV_log_RMSD|docked_NumRotatableBonds ESS = 1530 | BMK = 0.0601 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0

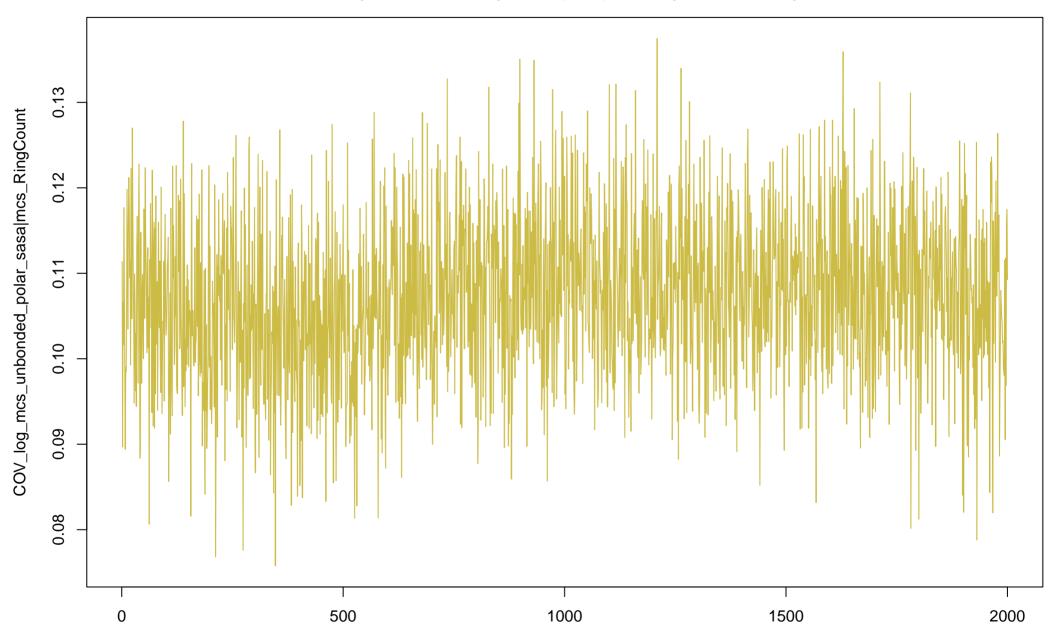


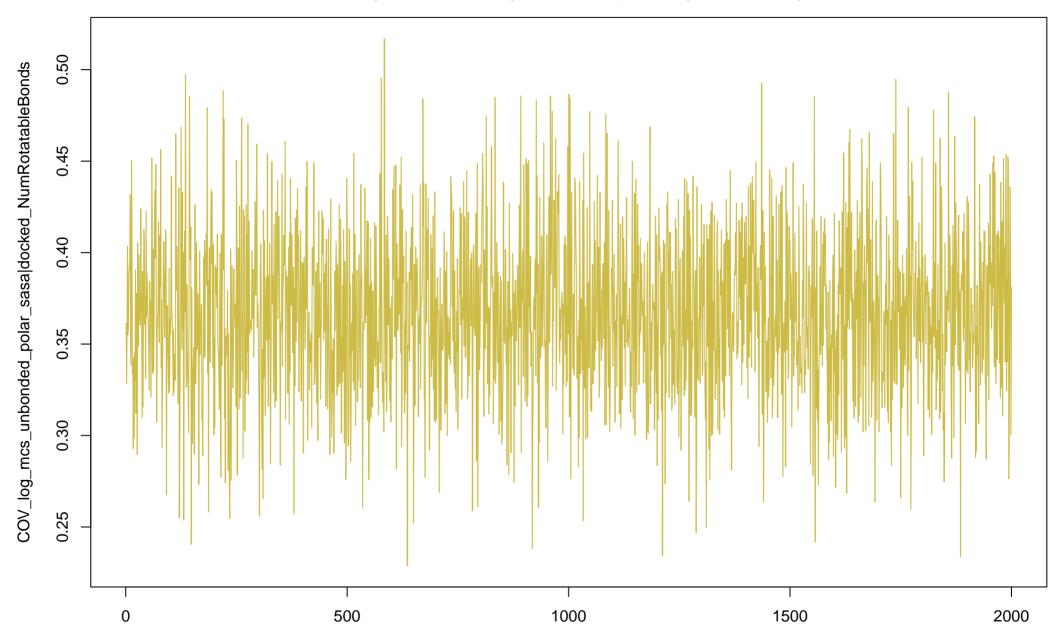




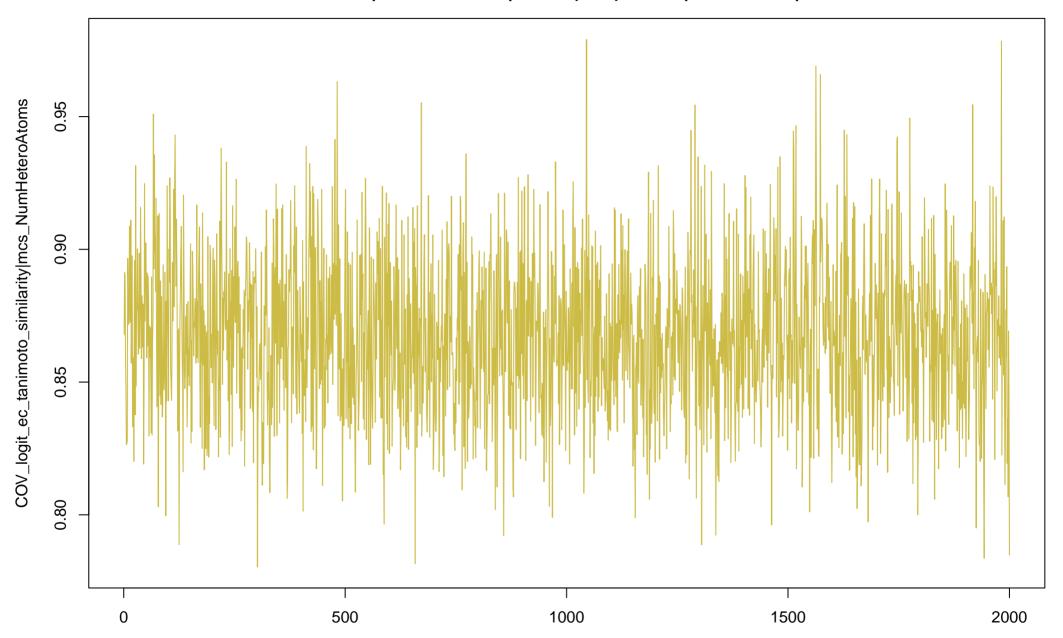


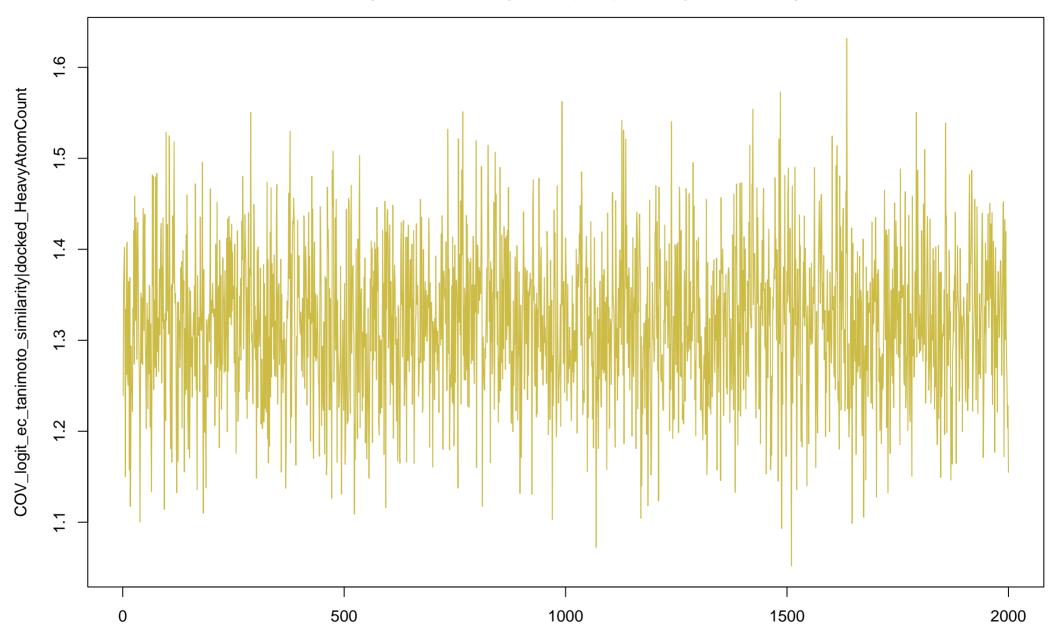
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount ESS = 790 | BMK = 0.0966 | MCSE(6.27) = 2.57 | stat: FALSE | burn: 0



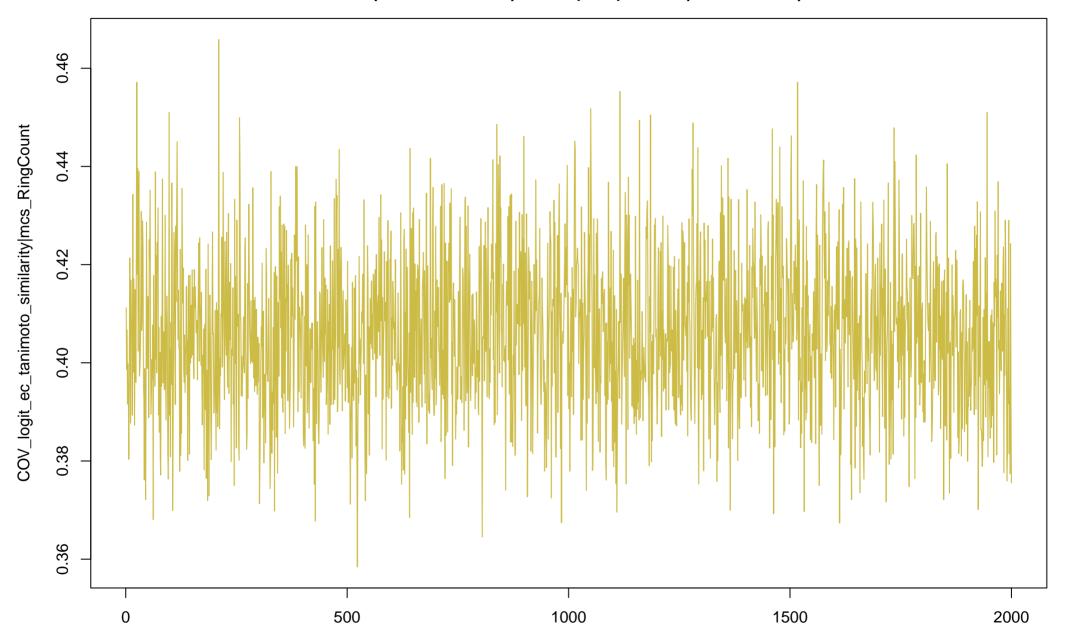


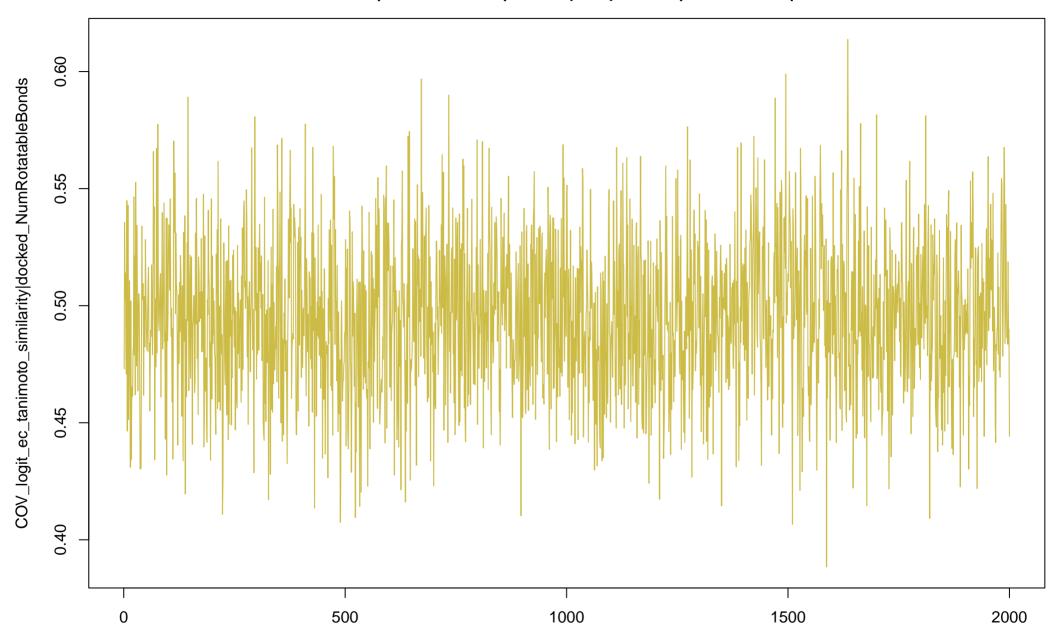
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms ESS = 1450 | BMK = 0.0492 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0

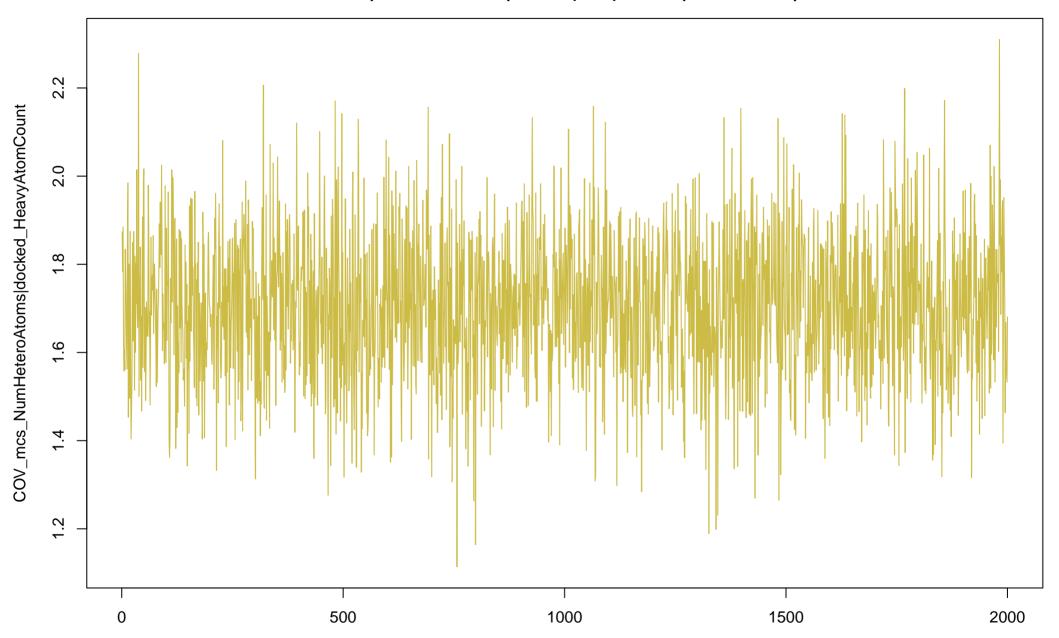




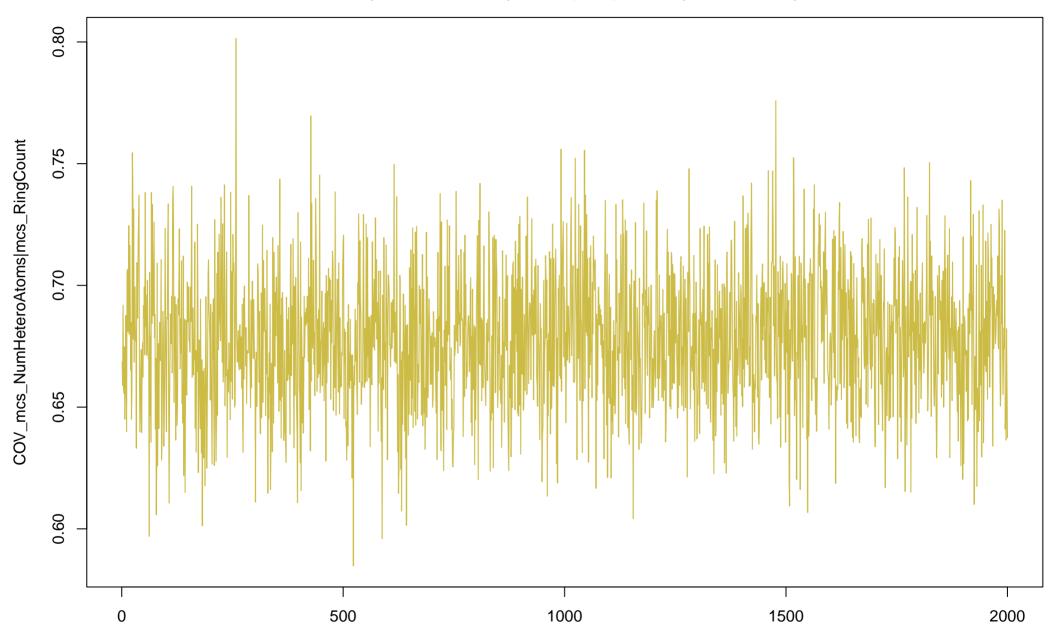
COV_logit_ec_tanimoto_similarity|mcs_RingCount ESS = 1500 | BMK = 0.0437 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0

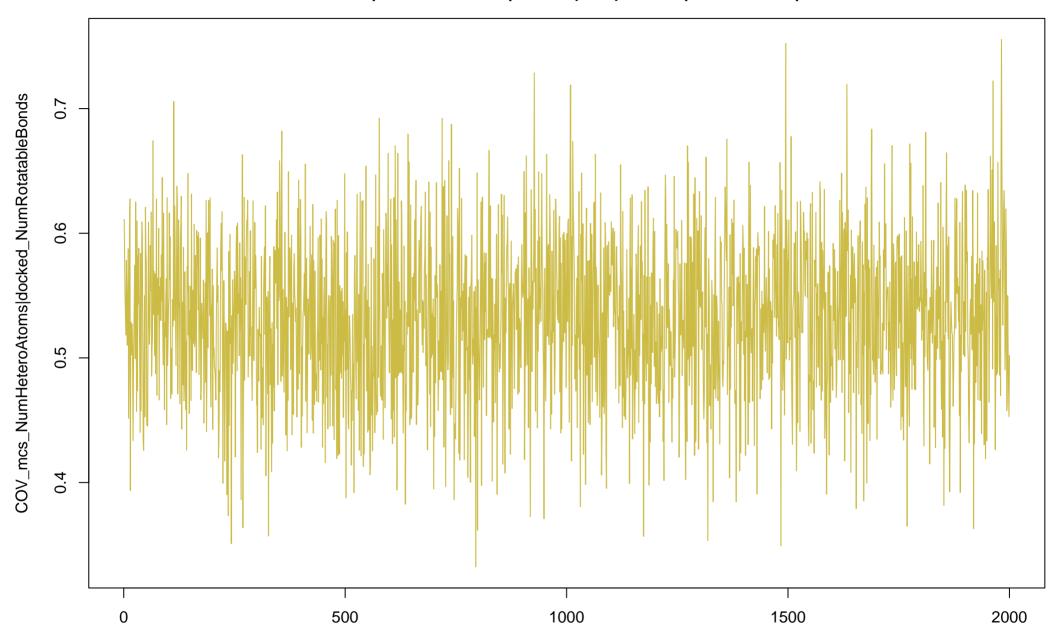


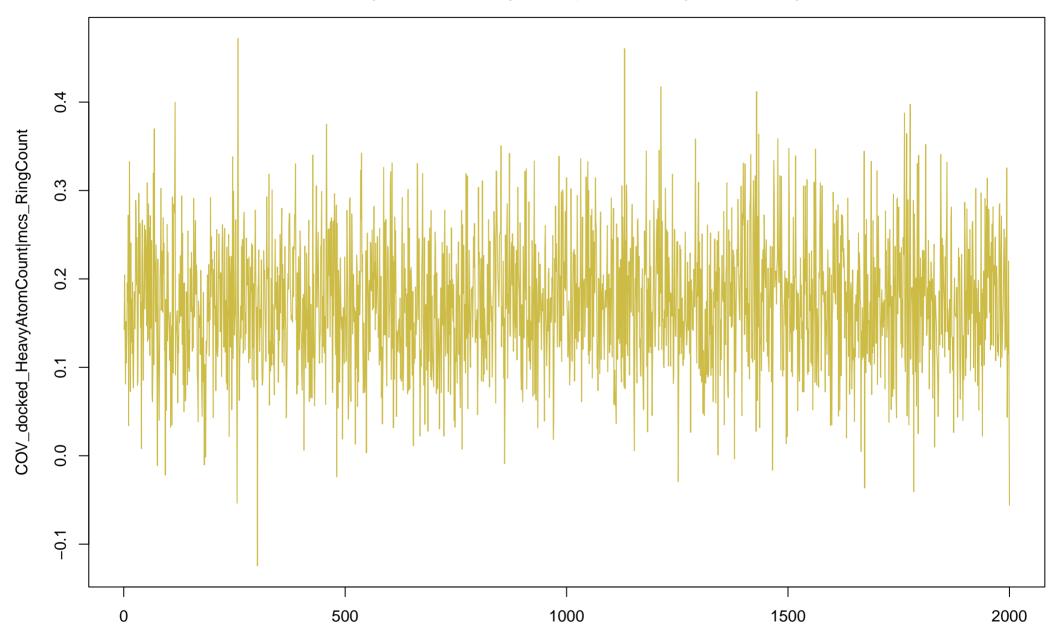


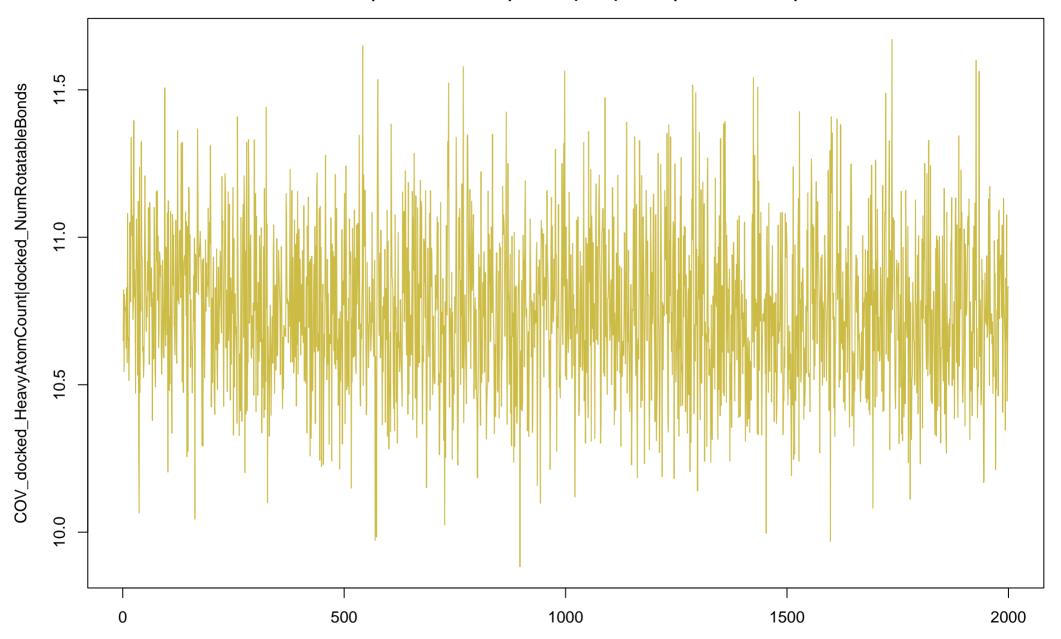


COV_mcs_NumHeteroAtoms|mcs_RingCount ESS = 1520 | BMK = 0.0562 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0









COV_mcs_RingCount|docked_NumRotatableBonds ESS = 1850 | BMK = 0.0701 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0

