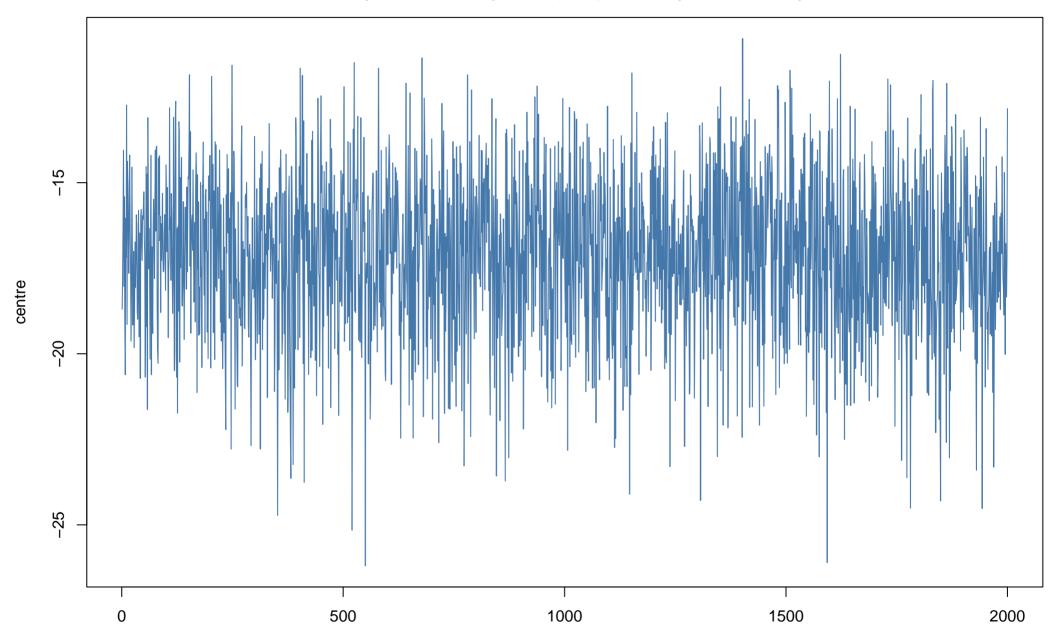
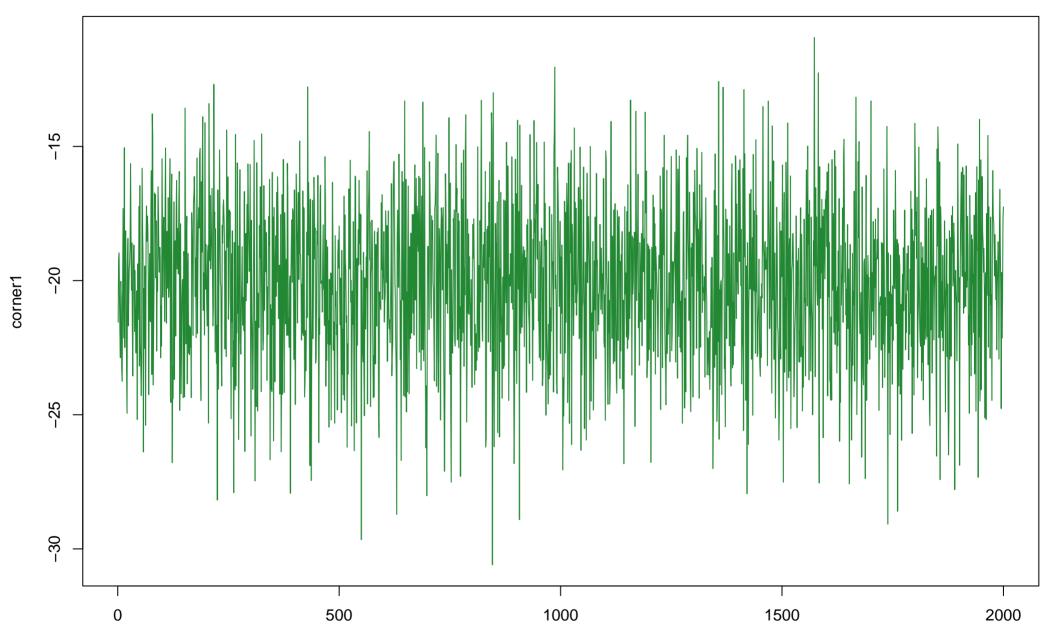


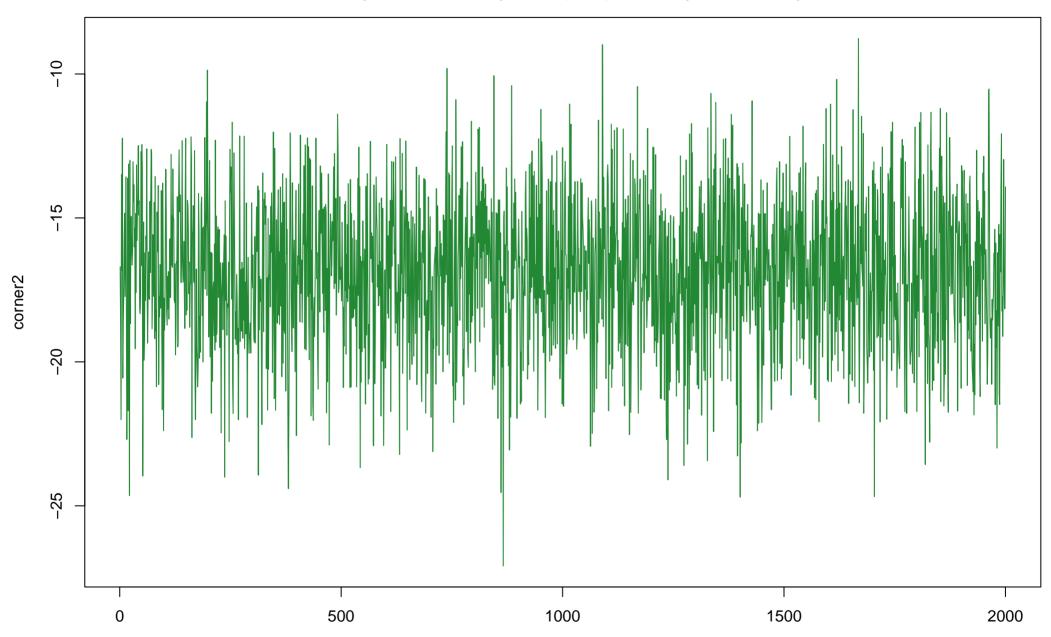
centre ESS = 2000 | BMK = 0.042 | MCSE(6.27) = 0.186 | stat: FALSE | burn: 0



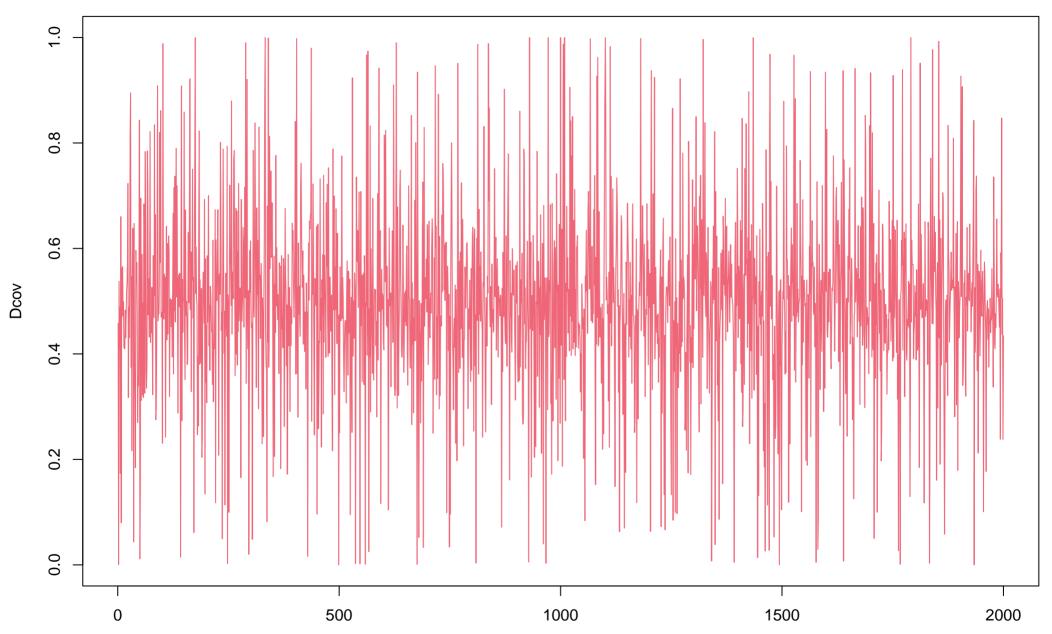
corner1 ESS = 2000 | BMK = 0.0373 | MCSE(6.27) = 0.149 | stat: TRUE | burn: 0



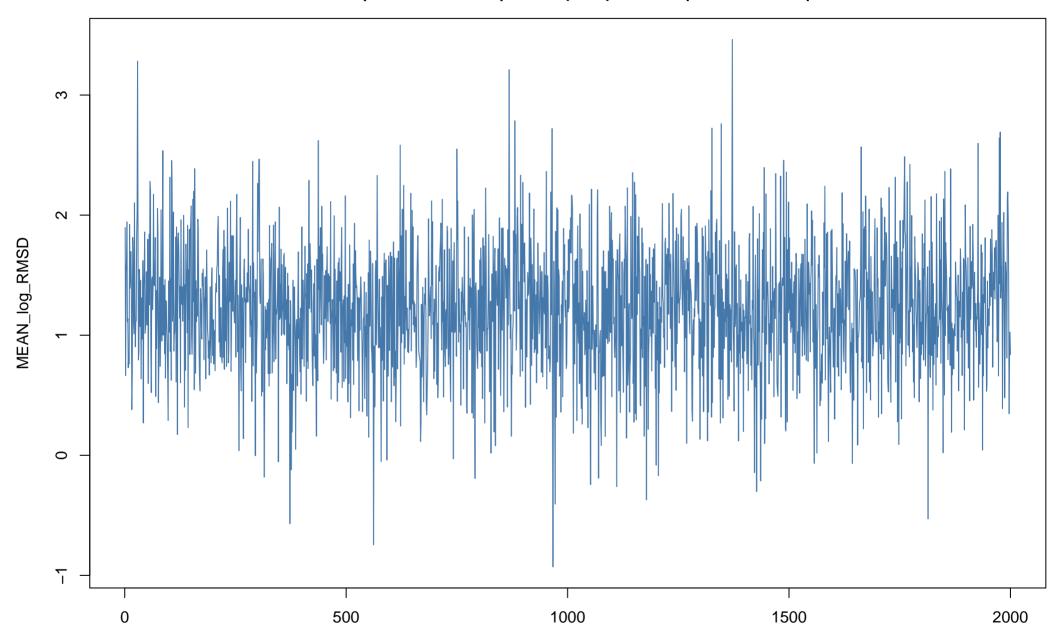
corner2 ESS = 2000 | BMK = 0.0433 | MCSE(6.27) = 0.166 | stat: TRUE | burn: 0



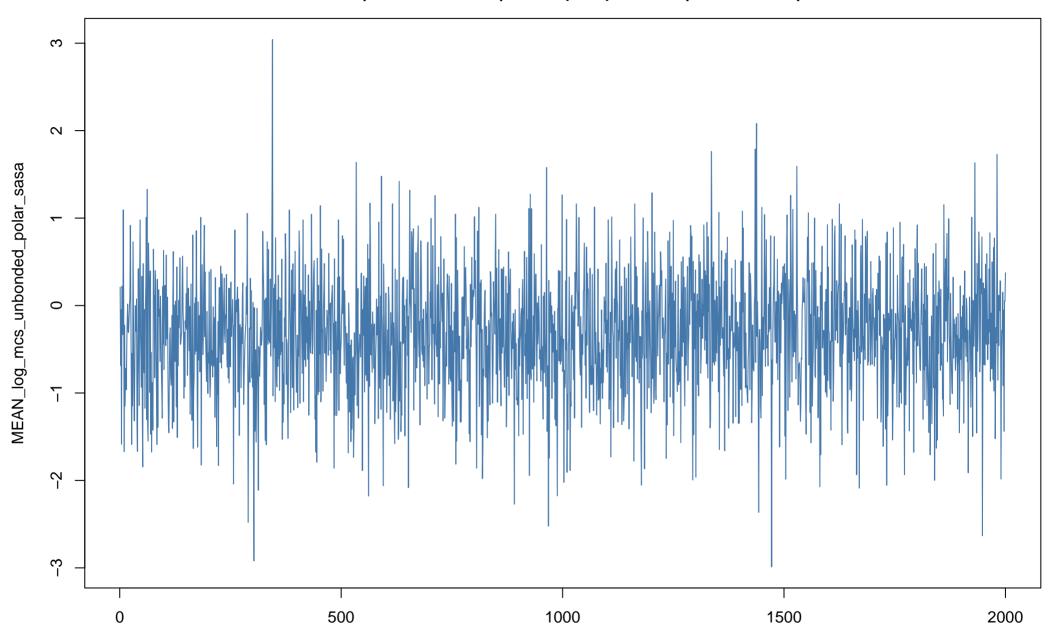
Dcov ESS = 2000 | BMK = 0.0448 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0



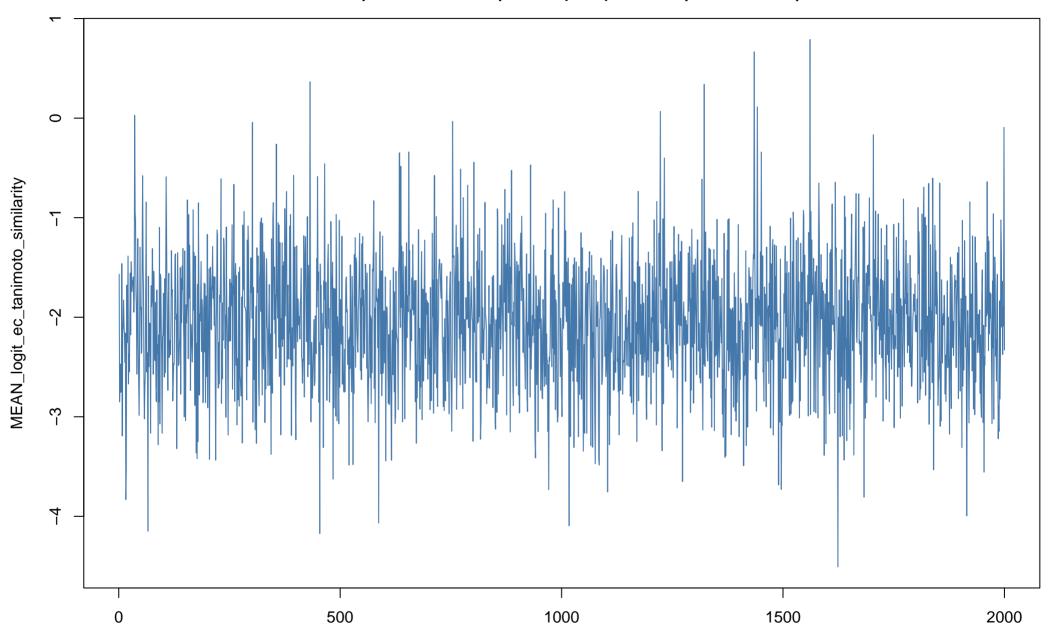
MEAN_log_RMSD ESS = 2000 | BMK = 0.0552 | MCSE(6.27) = 0.845 | stat: FALSE | burn: 0



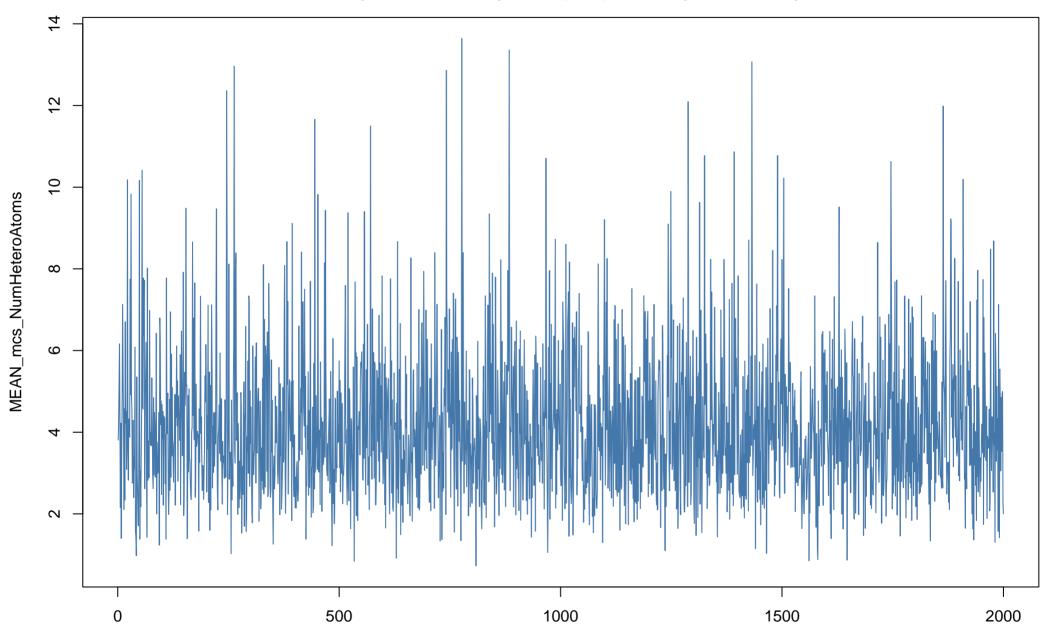
MEAN_log_mcs_unbonded_polar_sasa ESS = 2000 | BMK = 0.0564 | MCSE(6.27) = 0.642 | stat: TRUE | burn: 0



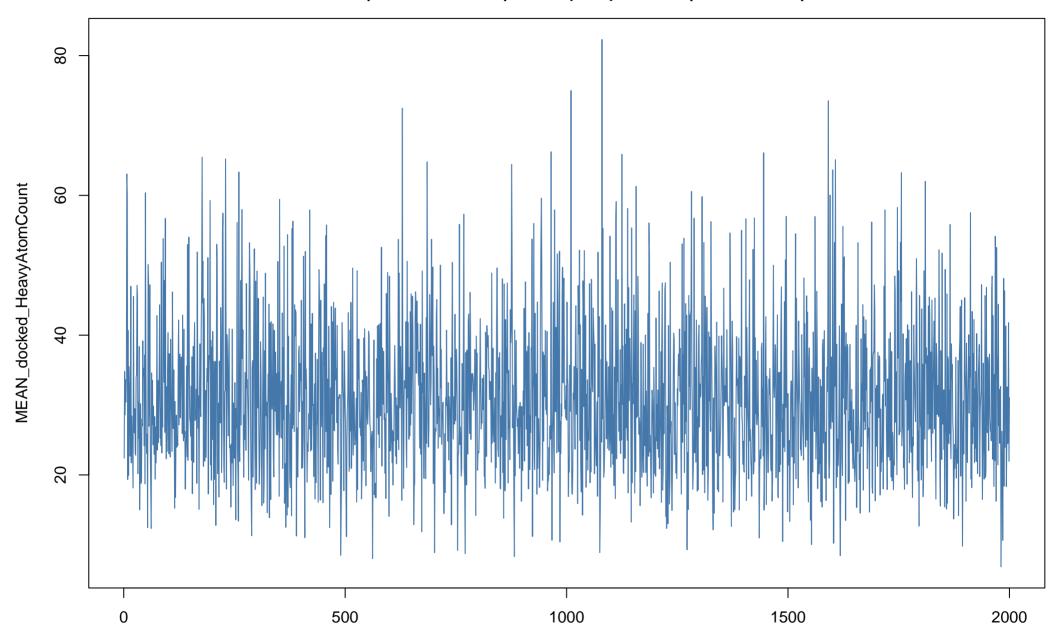
MEAN_logit_ec_tanimoto_similarity ESS = 1640 | BMK = 0.0476 | MCSE(6.27) = 0.687 | stat: TRUE | burn: 0



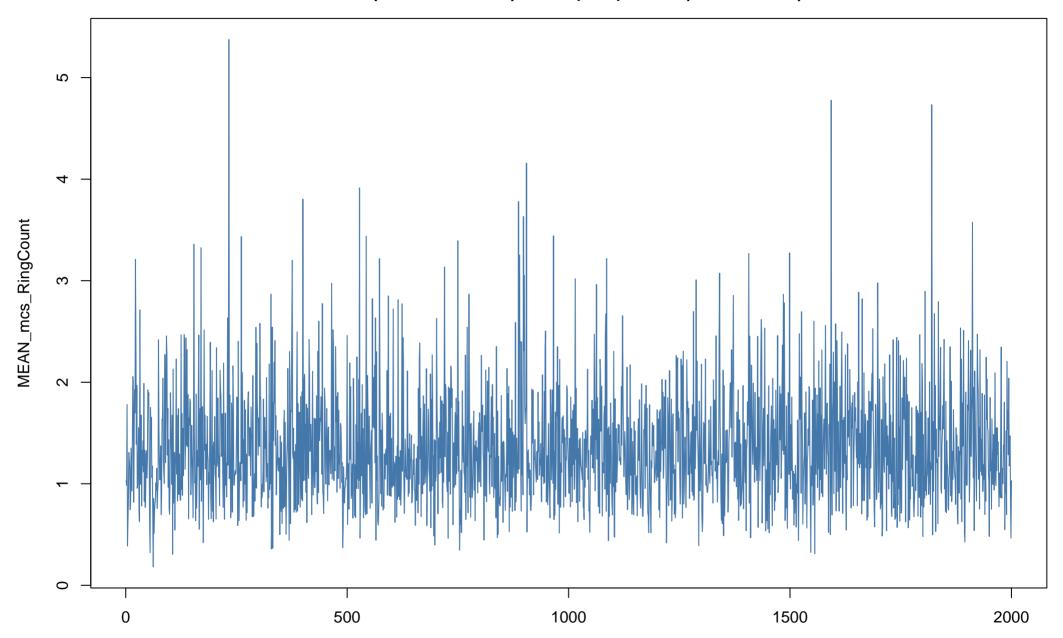
MEAN_mcs_NumHeteroAtoms ESS = 2000 | BMK = 0.0413 | MCSE(6.27) = 0.243 | stat: TRUE | burn: 0



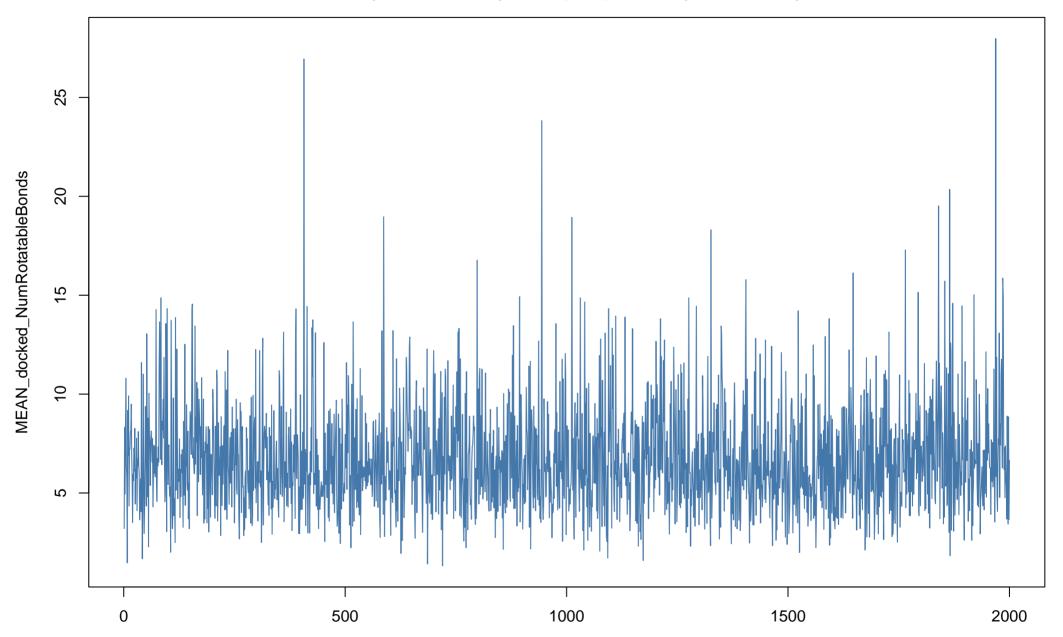
MEAN_docked_HeavyAtomCount ESS = 2000 | BMK = 0.0511 | MCSE(6.27) = 0.041 | stat: TRUE | burn: 0



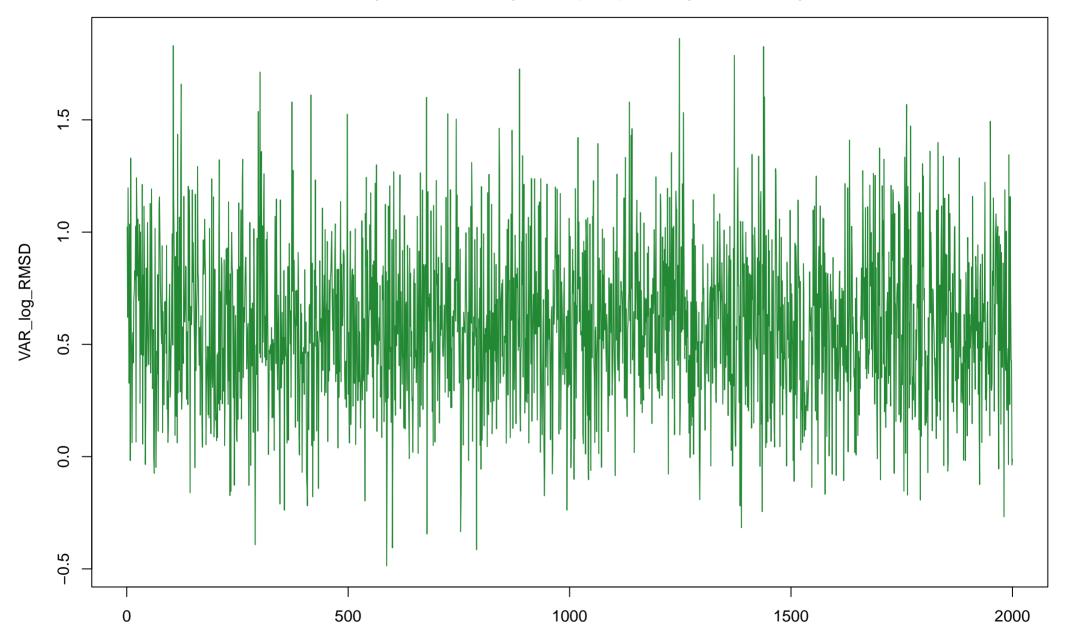
MEAN_mcs_RingCount ESS = 1800 | BMK = 0.0668 | MCSE(6.27) = 0.76 | stat: TRUE | burn: 0



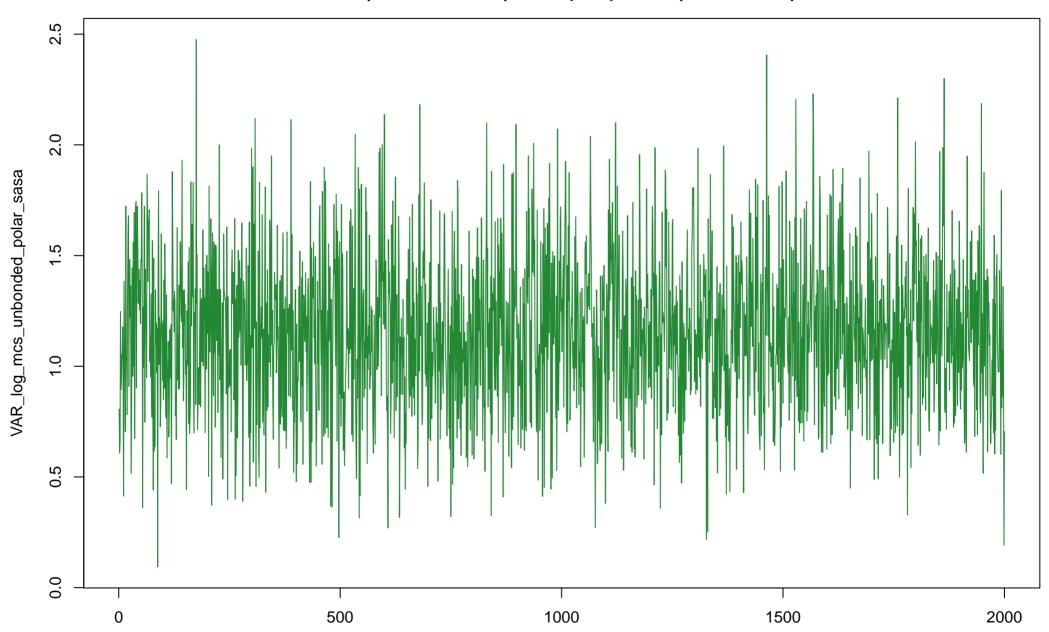
MEAN_docked_NumRotatableBonds ESS = 2000 | BMK = 0.055 | MCSE(6.27) = 0.158 | stat: TRUE | burn: 0



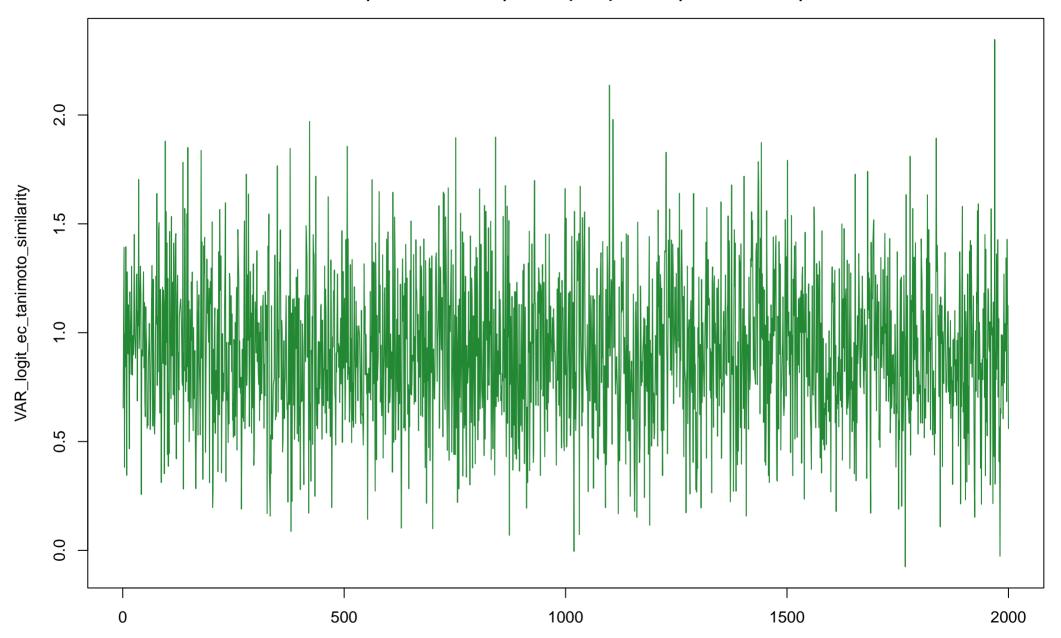
VAR_log_RMSD ESS = 2000 | BMK = 0.0403 | MCSE(6.27) = 1.23 | stat: TRUE | burn: 0



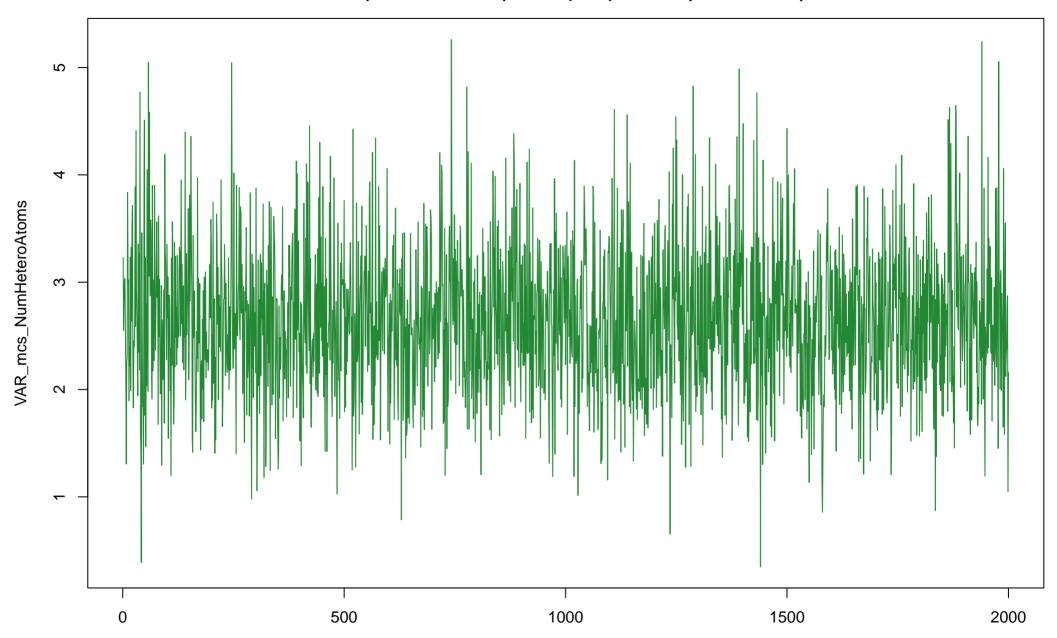
VAR_log_mcs_unbonded_polar_sasa ESS = 2000 | BMK = 0.0569 | MCSE(6.27) = 1.23 | stat: TRUE | burn: 0



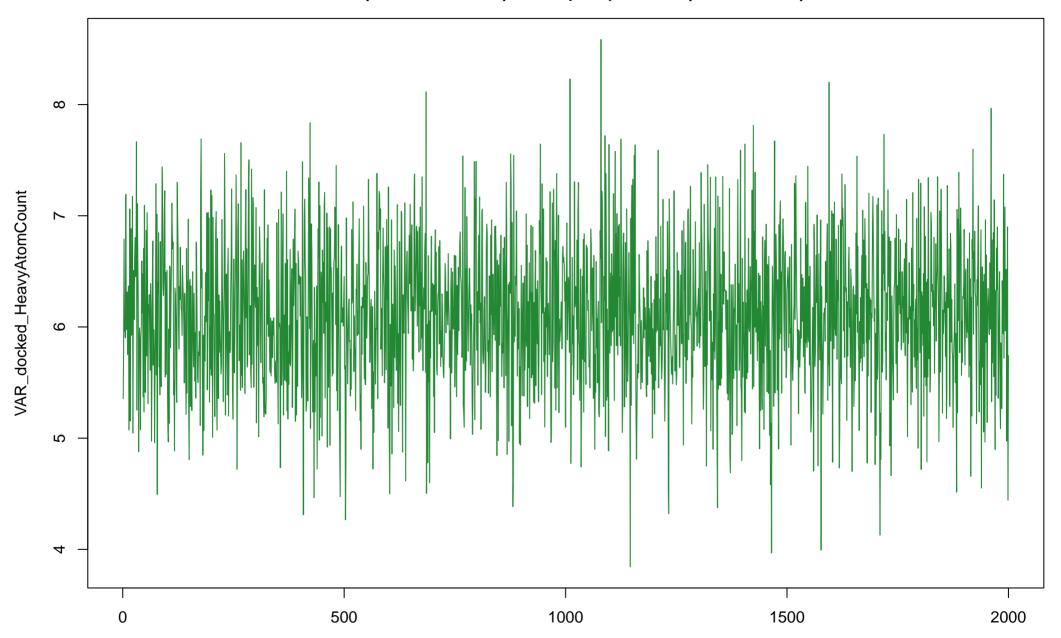
VAR_logit_ec_tanimoto_similarity ESS = 2000 | BMK = 0.0372 | MCSE(6.27) = 1.28 | stat: FALSE | burn: 0



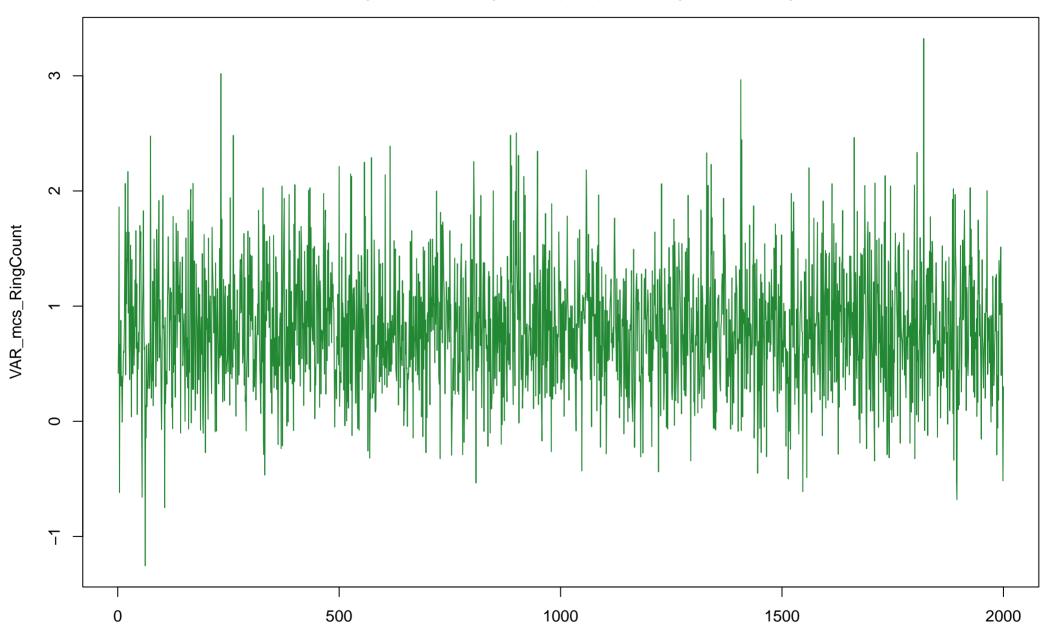
VAR_mcs_NumHeteroAtoms ESS = 1770 | BMK = 0.0324 | MCSE(6.27) = 0.627 | stat: TRUE | burn: 0



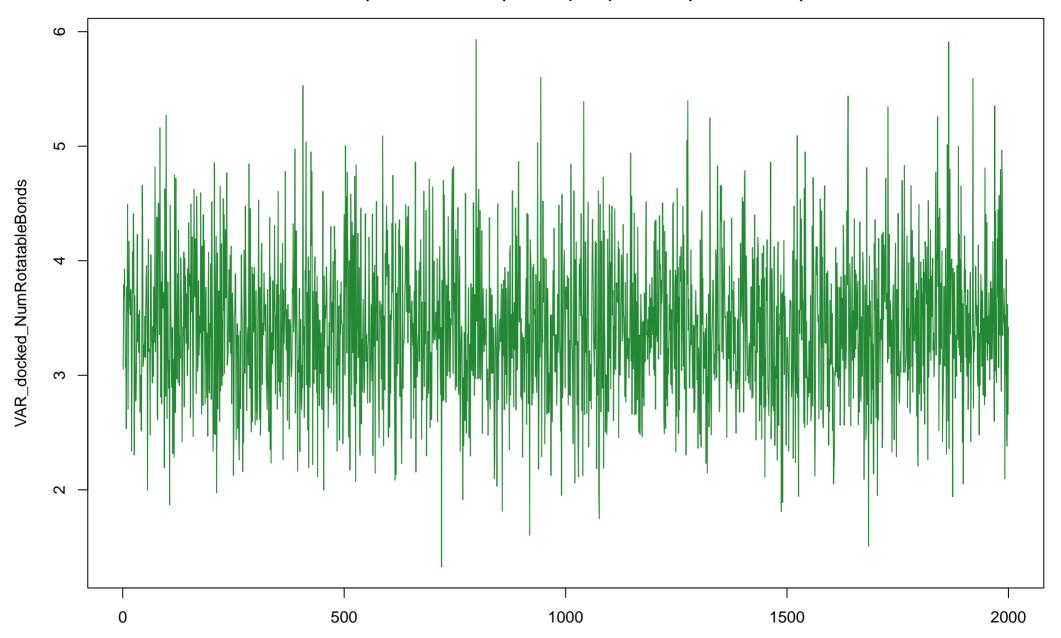
VAR_docked_HeavyAtomCount ESS = 2000 | BMK = 0.0456 | MCSE(6.27) = 0.675 | stat: TRUE | burn: 0



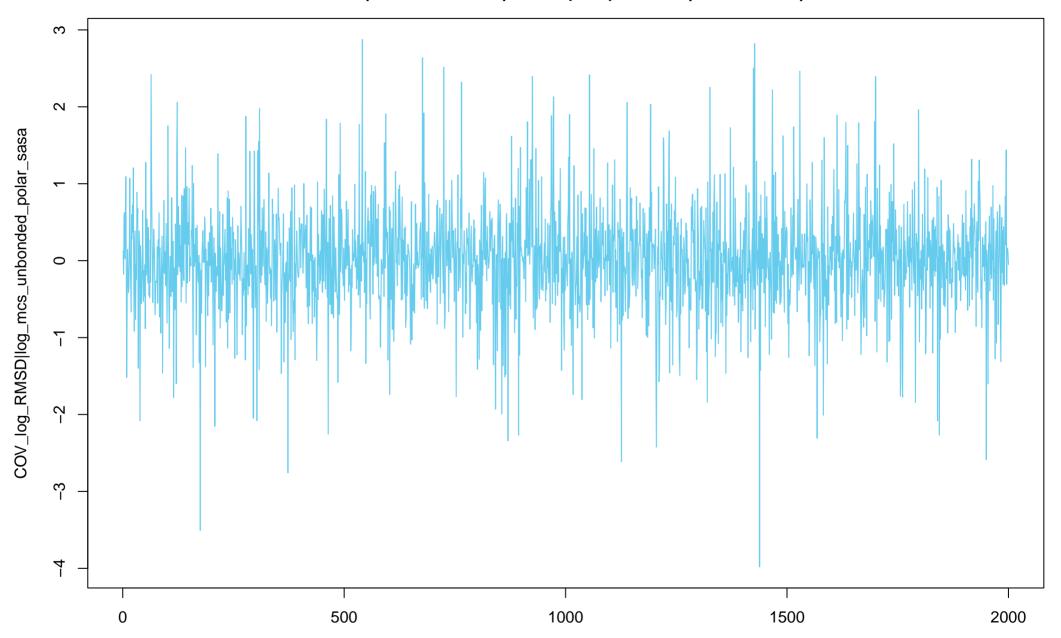
VAR_mcs_RingCount ESS = 2000 | BMK = 0.055 | MCSE(6.27) = 0.804 | stat: TRUE | burn: 0



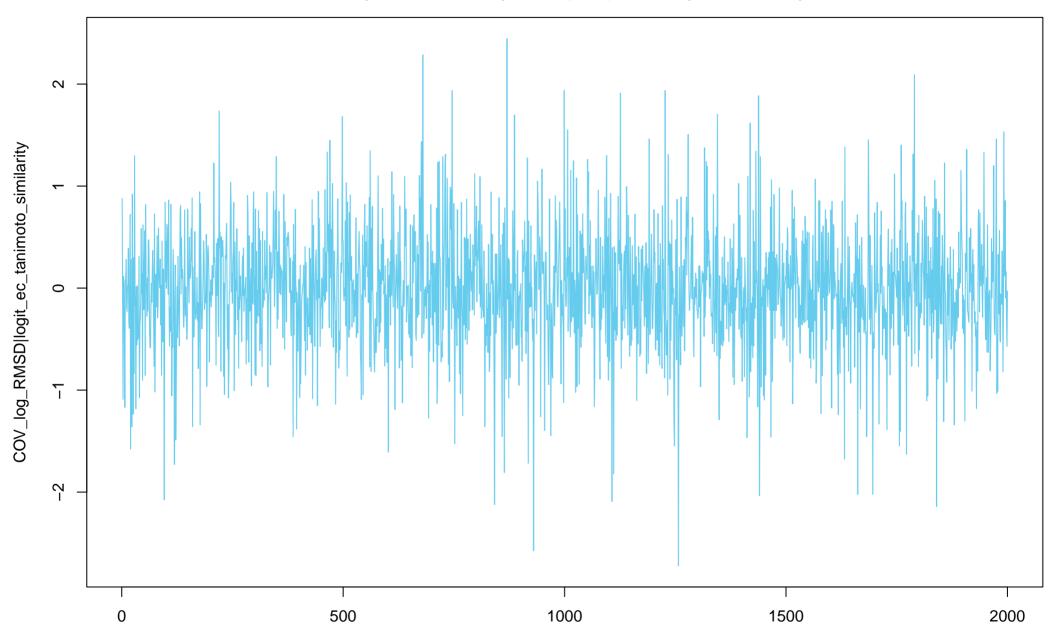
VAR_docked_NumRotatableBonds ESS = 2000 | BMK = 0.0352 | MCSE(6.27) = 0.672 | stat: TRUE | burn: 0



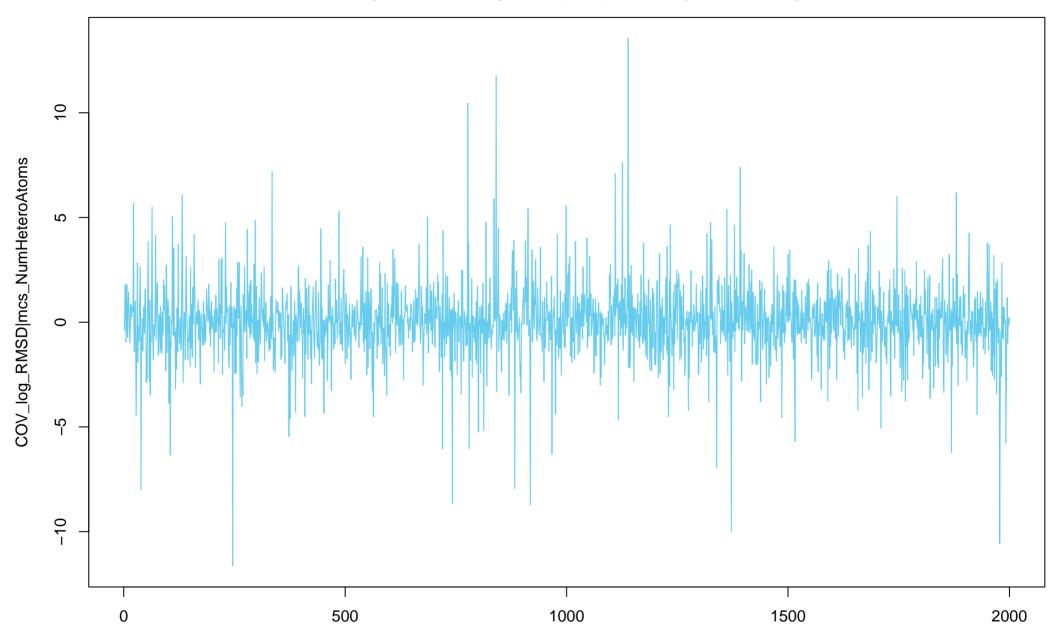
COV_log_RMSD|log_mcs_unbonded_polar_sasa ESS = 2000 | BMK = 0.0483 | MCSE(6.27) = 0.651 | stat: TRUE | burn: 0



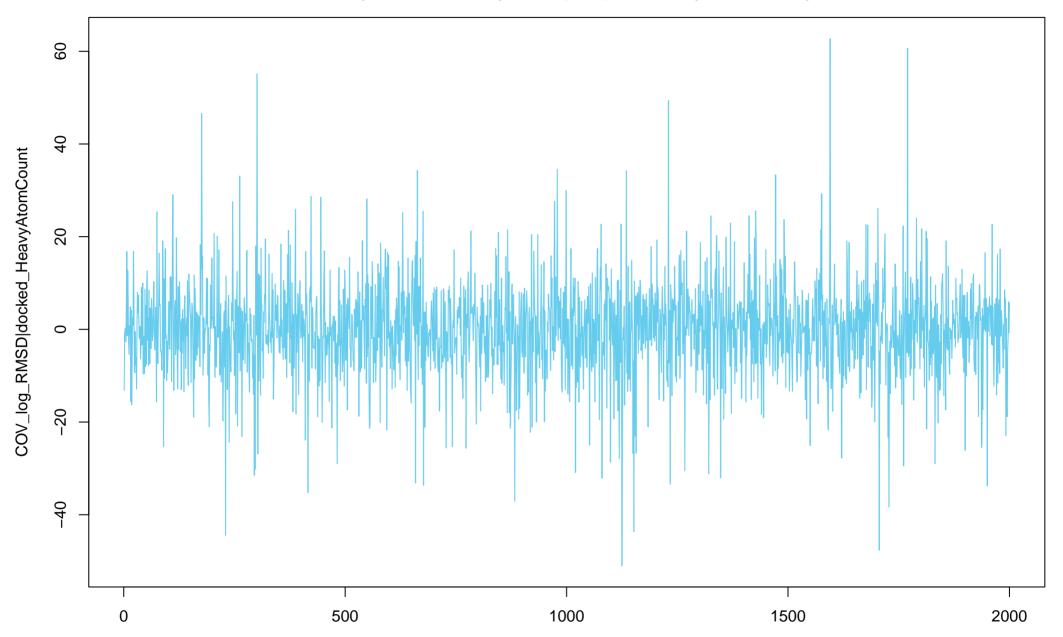
COV_log_RMSD|logit_ec_tanimoto_similarity ESS = 2000 | BMK = 0.0535 | MCSE(6.27) = 0.769 | stat: TRUE | burn: 0



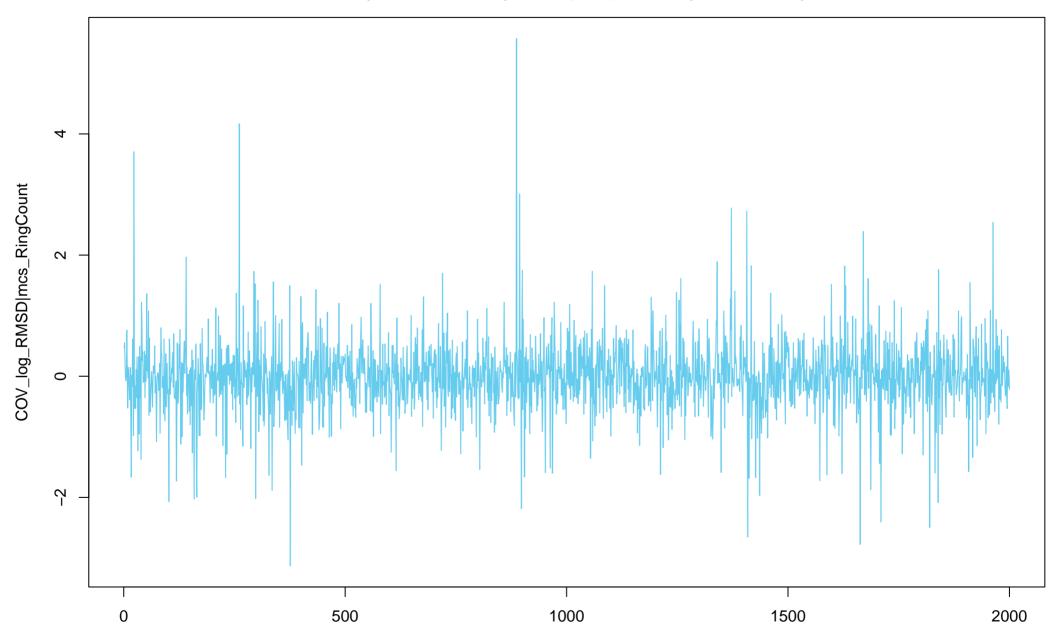
COV_log_RMSD|mcs_NumHeteroAtoms ESS = 2000 | BMK = 0.086 | MCSE(6.27) = 0.251 | stat: TRUE | burn: 0



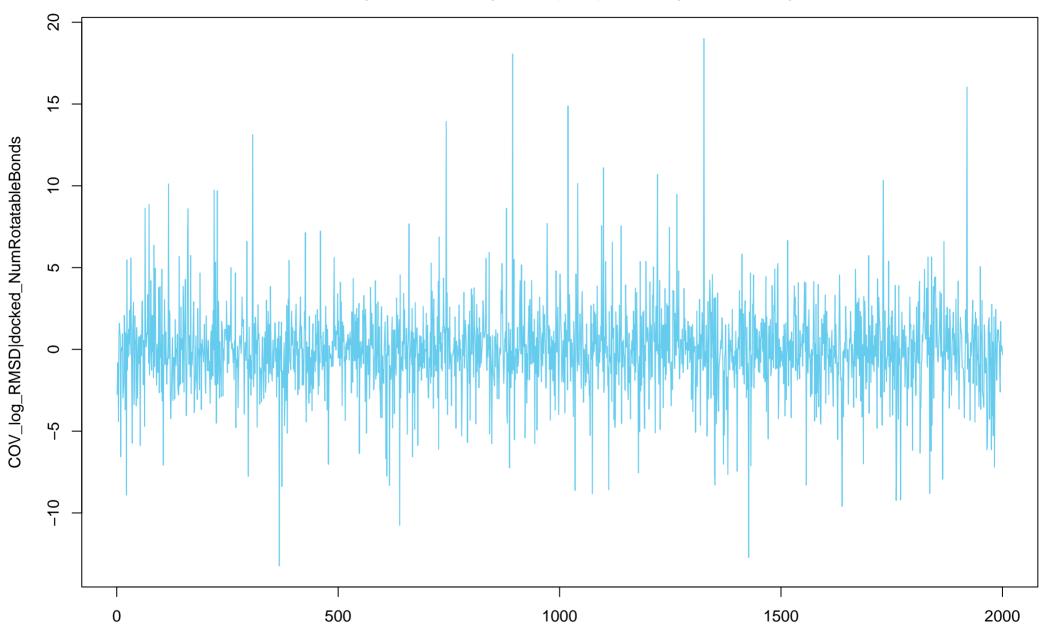
COV_log_RMSD|docked_HeavyAtomCount ESS = 2000 | BMK = 0.0751 | MCSE(6.27) = 0.0428 | stat: TRUE | burn: 0

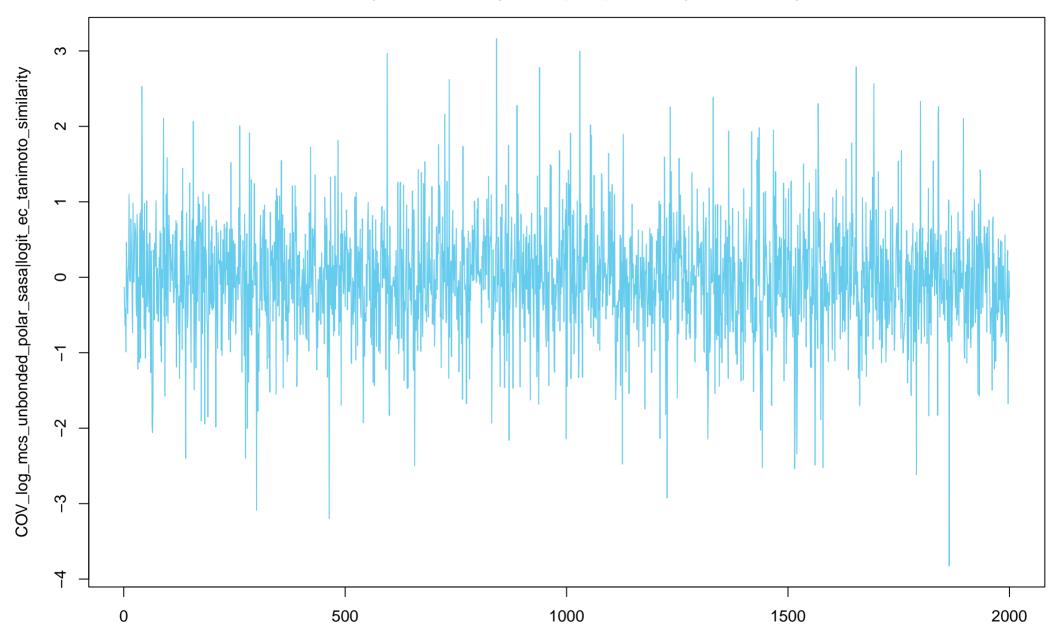


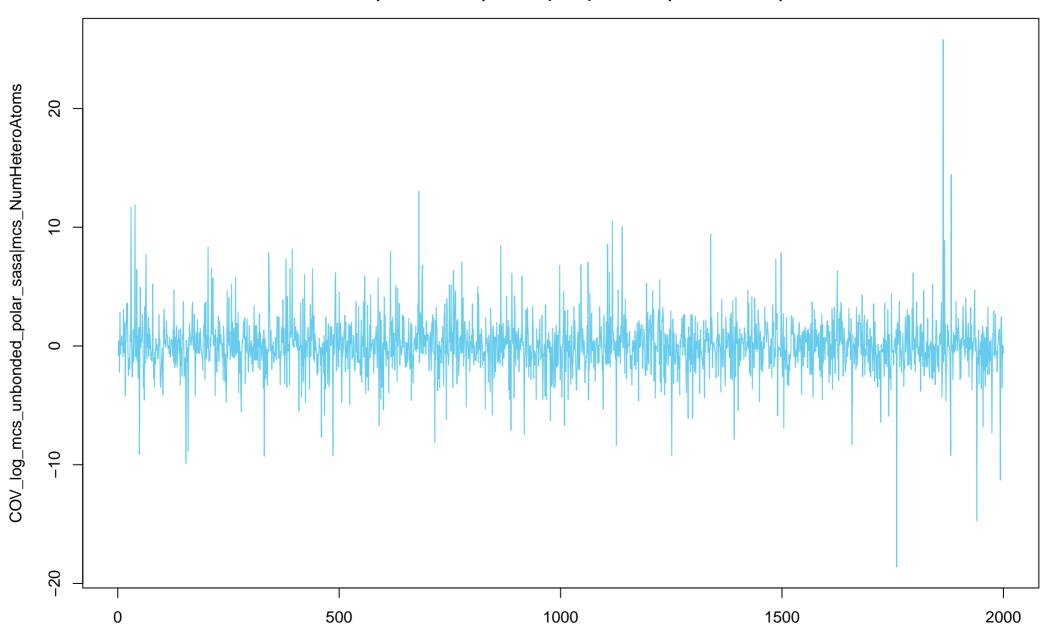
COV_log_RMSD|mcs_RingCount ESS = 2000 | BMK = 0.0902 | MCSE(6.27) = 0.752 | stat: TRUE | burn: 0

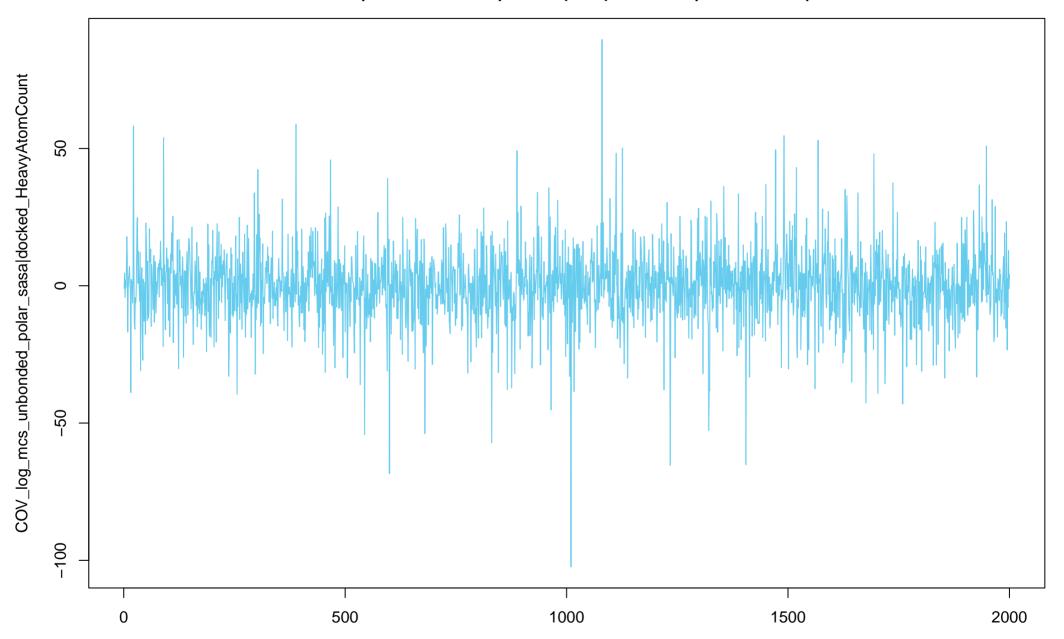


COV_log_RMSD|docked_NumRotatableBonds ESS = 2000 | BMK = 0.089 | MCSE(6.27) = 0.163 | stat: TRUE | burn: 0

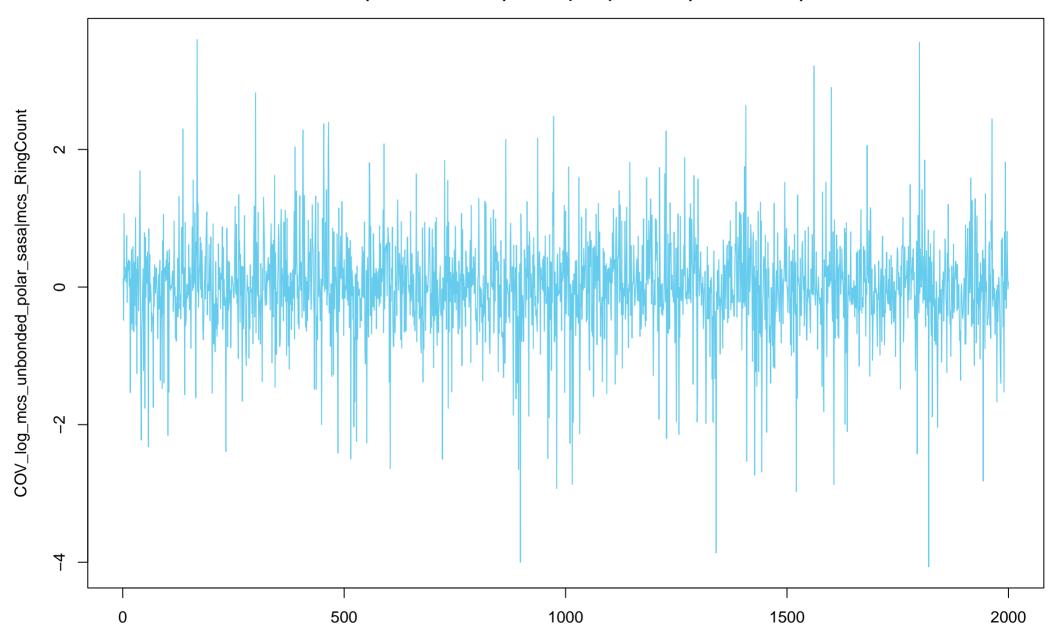


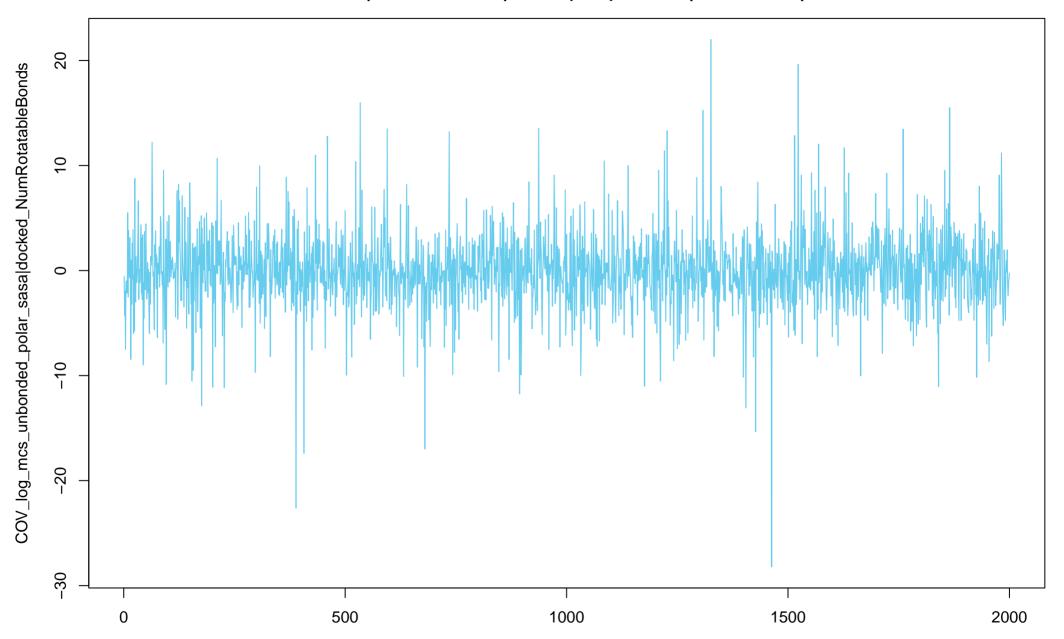




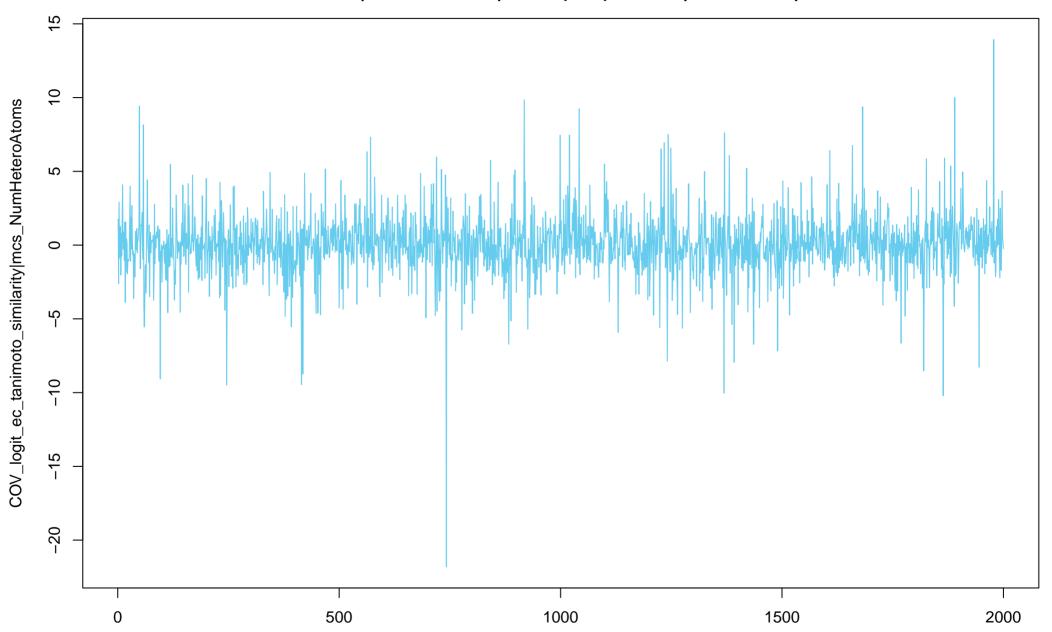


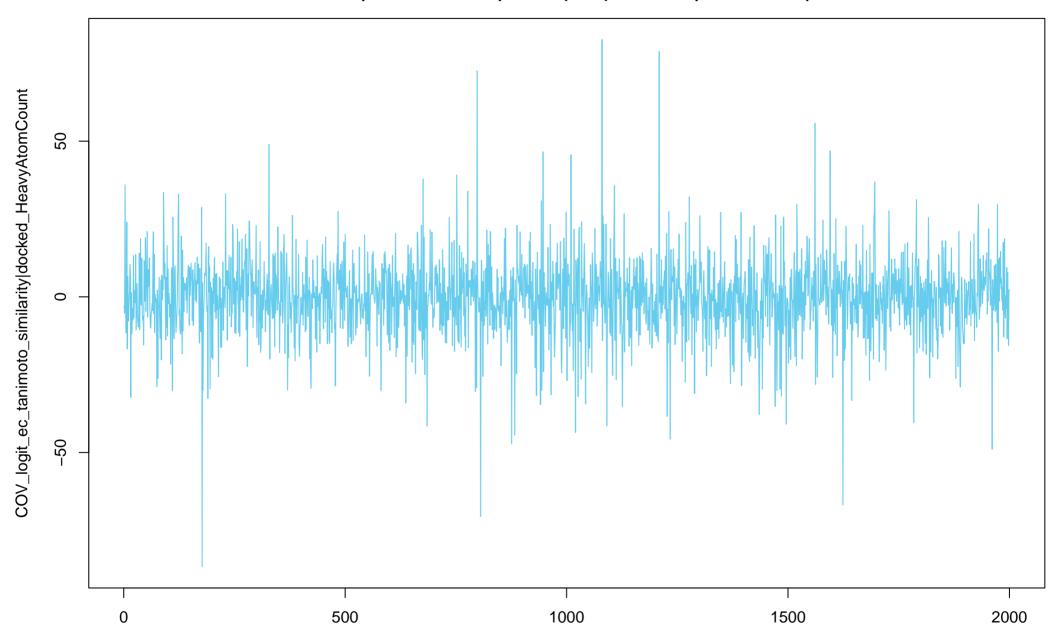
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount ESS = 1560 | BMK = 0.0652 | MCSE(6.27) = 0.595 | stat: TRUE | burn: 0



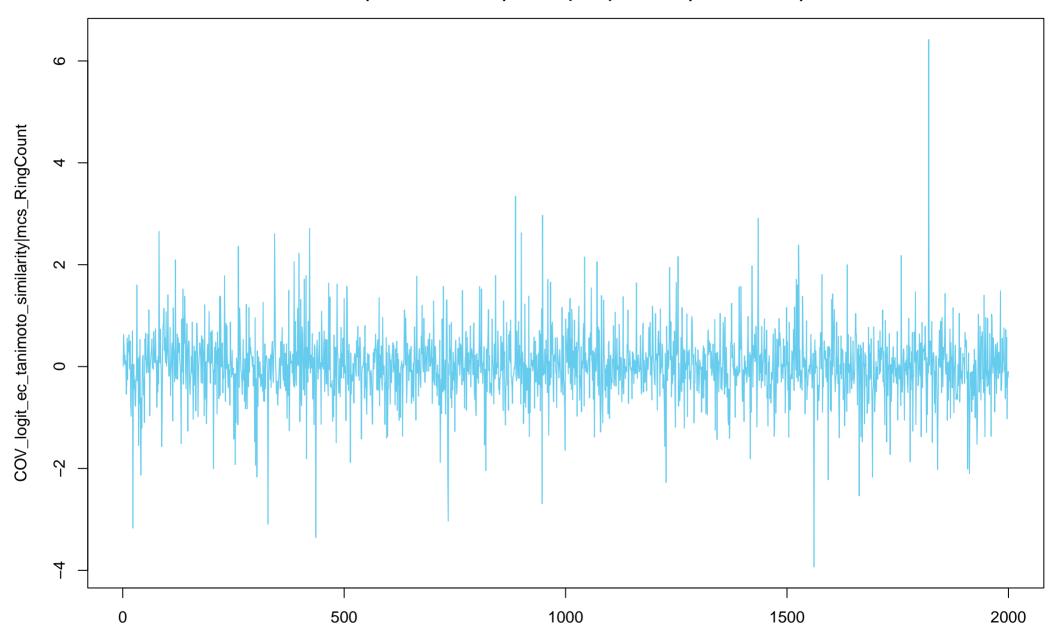


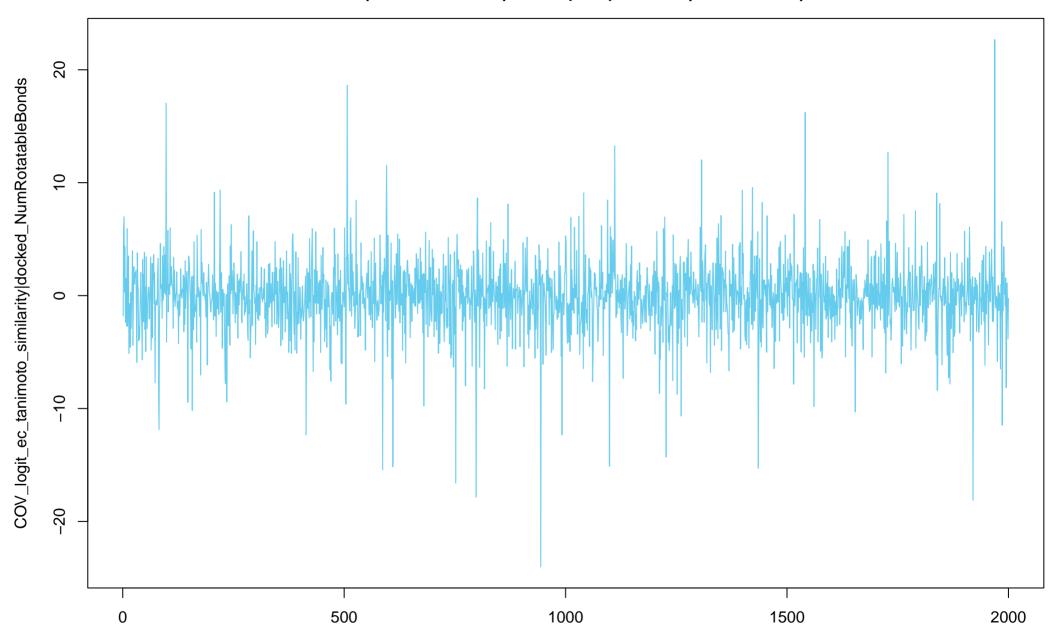
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms ESS = 2000 | BMK = 0.0804 | MCSE(6.27) = 0.211 | stat: TRUE | burn: 0



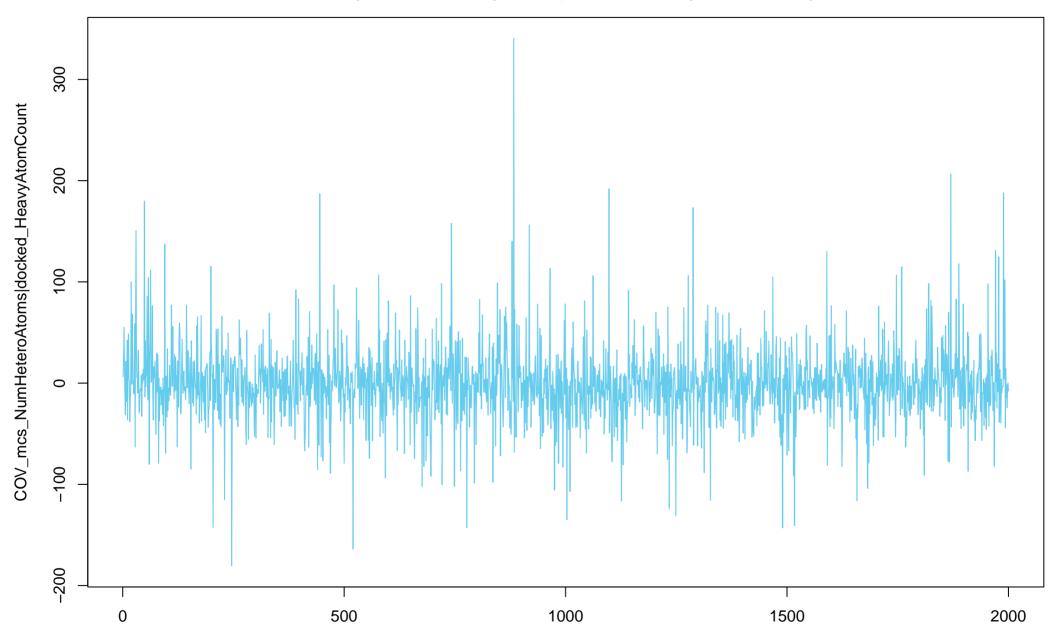


COV_logit_ec_tanimoto_similarity|mcs_RingCount ESS = 2000 | BMK = 0.0767 | MCSE(6.27) = 0.645 | stat: TRUE | burn: 0

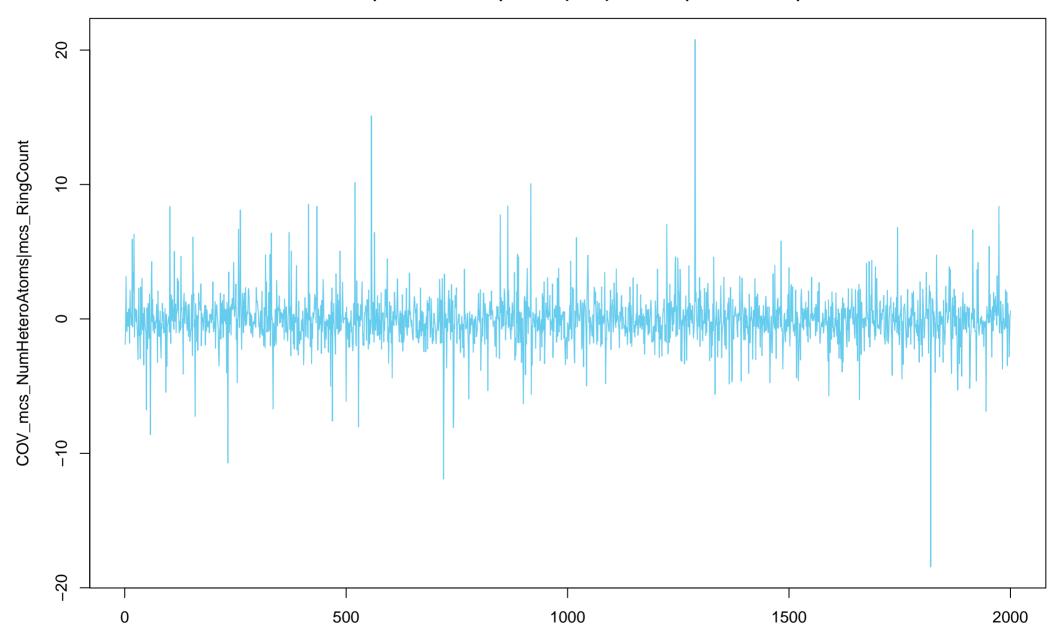




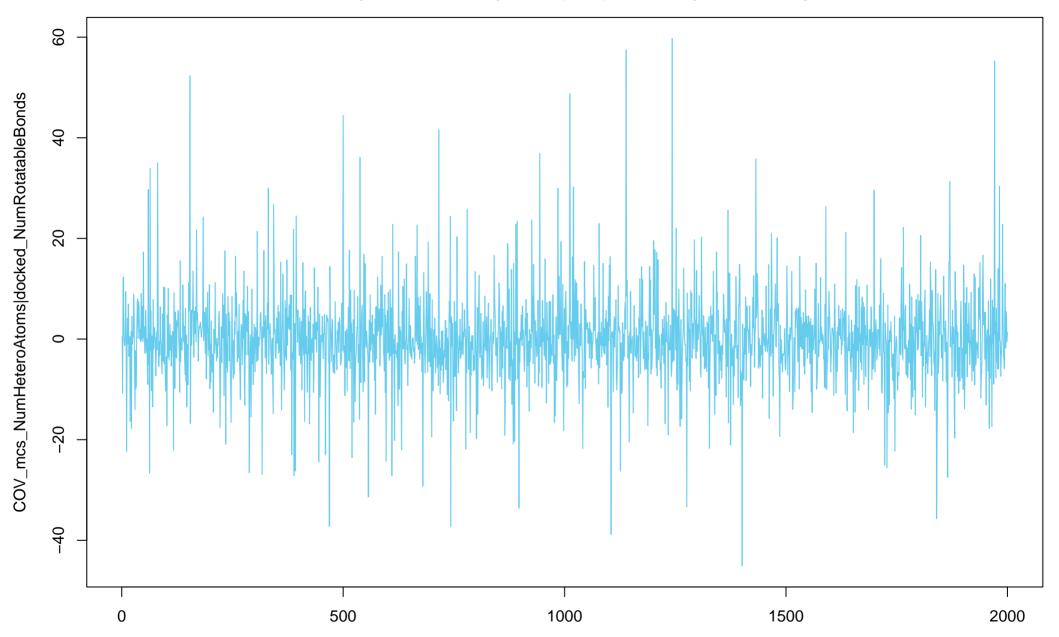
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount ESS = 2000 | BMK = 0.0794 | MCSE(6.27) = 0.0118 | stat: FALSE | burn: 0



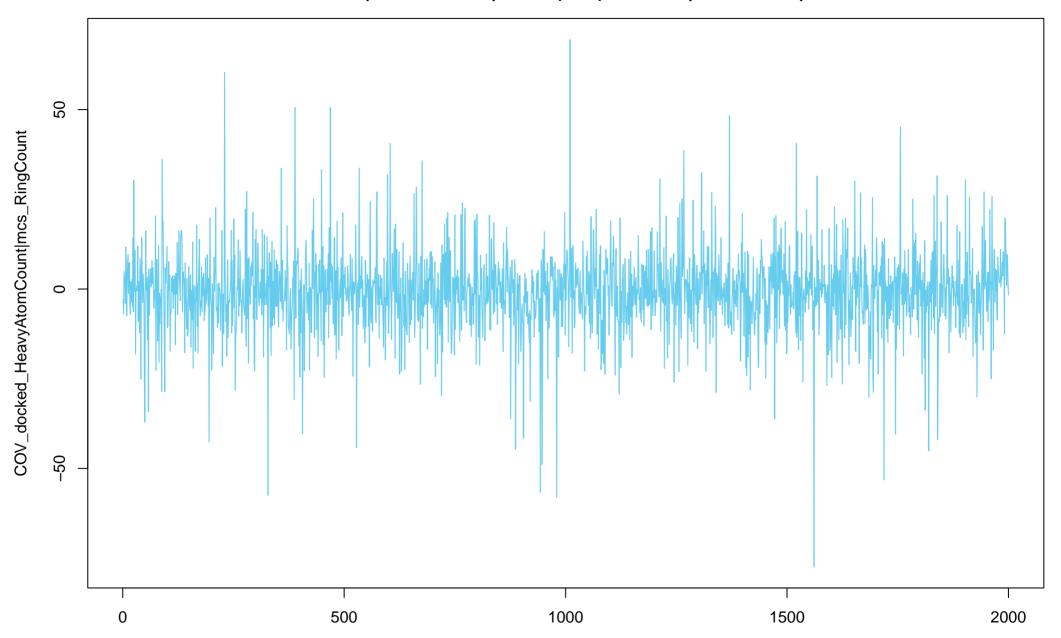
COV_mcs_NumHeteroAtoms|mcs_RingCount ESS = 1830 | BMK = 0.102 | MCSE(6.27) = 0.222 | stat: TRUE | burn: 0



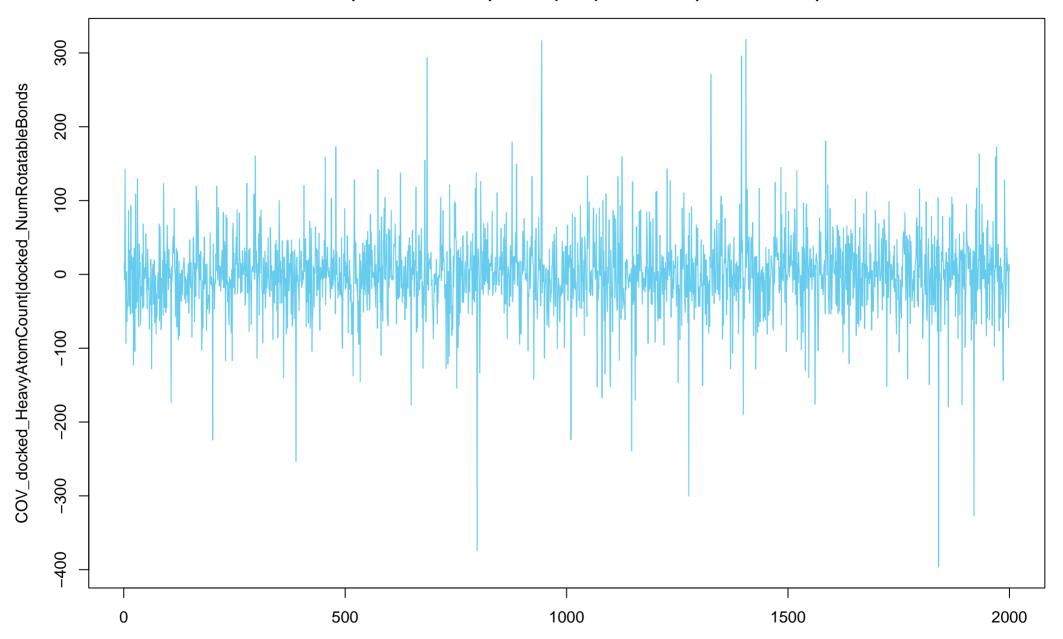
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds ESS = 2000 | BMK = 0.0819 | MCSE(6.27) = 0.0496 | stat: TRUE | burn: 0



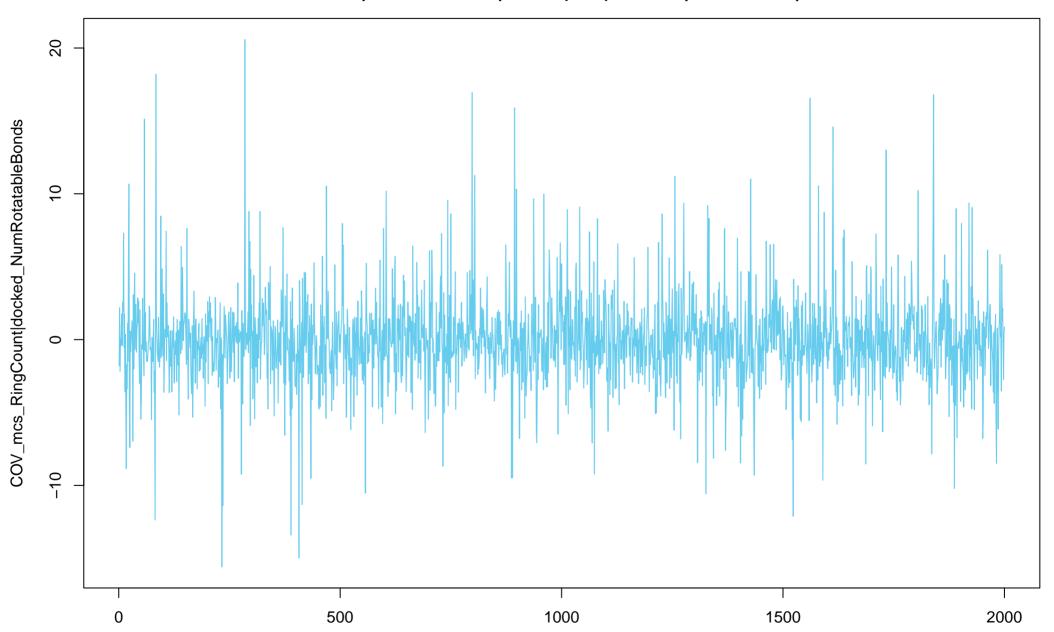
COV_docked_HeavyAtomCount|mcs_RingCount ESS = 2000 | BMK = 0.066 | MCSE(6.27) = 0.0386 | stat: TRUE | burn: 0



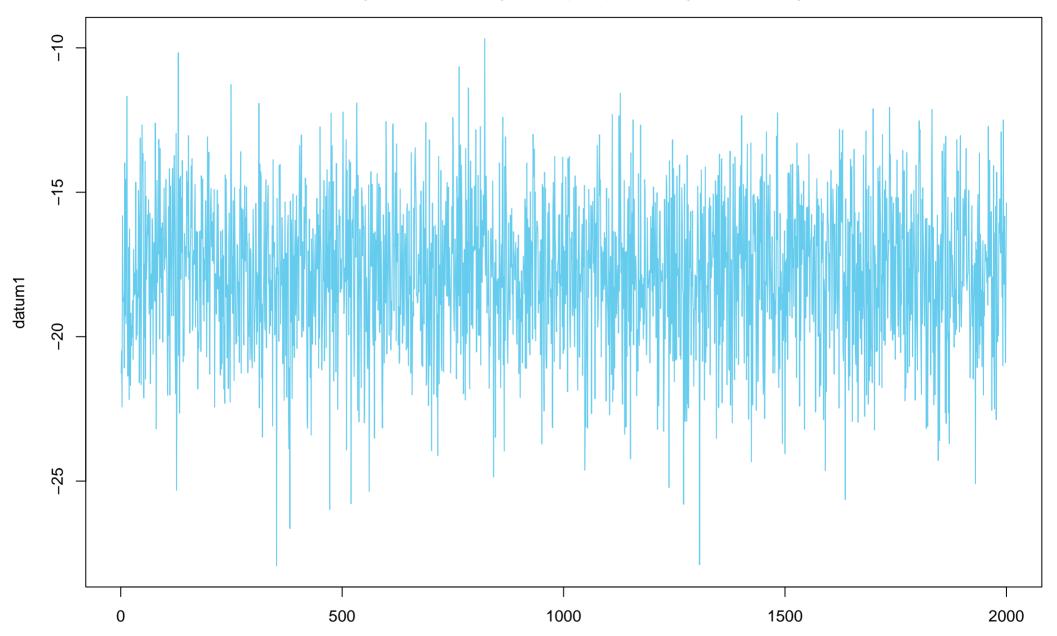
COV_docked_HeavyAtomCount|docked_NumRotatableBonds ESS = 2000 | BMK = 0.0811 | MCSE(6.27) = 0.00793 | stat: FALSE | burn: 0



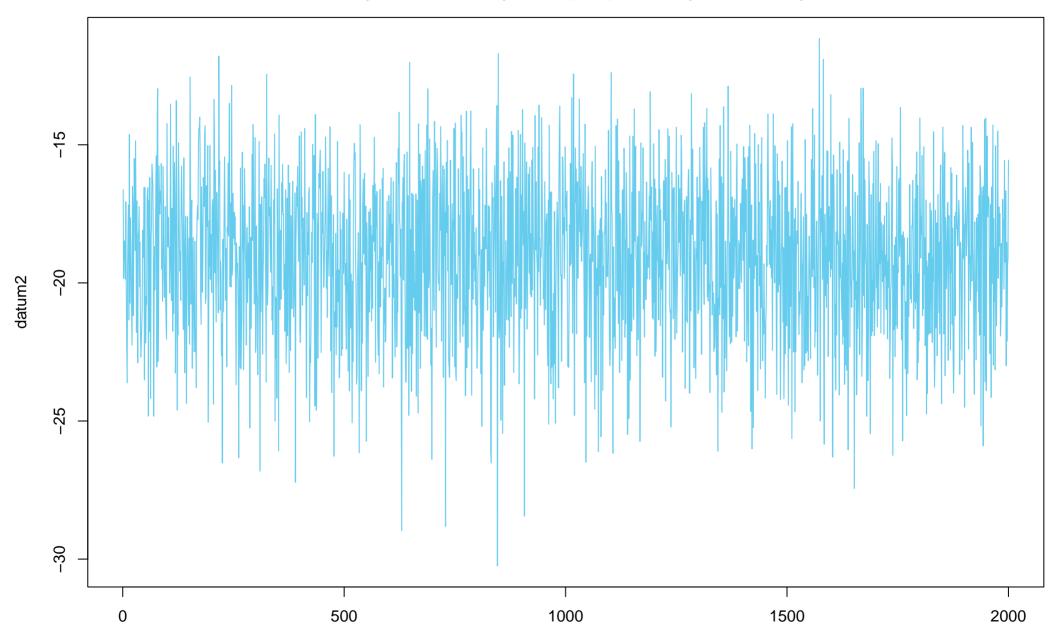
COV_mcs_RingCount|docked_NumRotatableBonds ESS = 1870 | BMK = 0.0691 | MCSE(6.27) = 0.142 | stat: TRUE | burn: 0



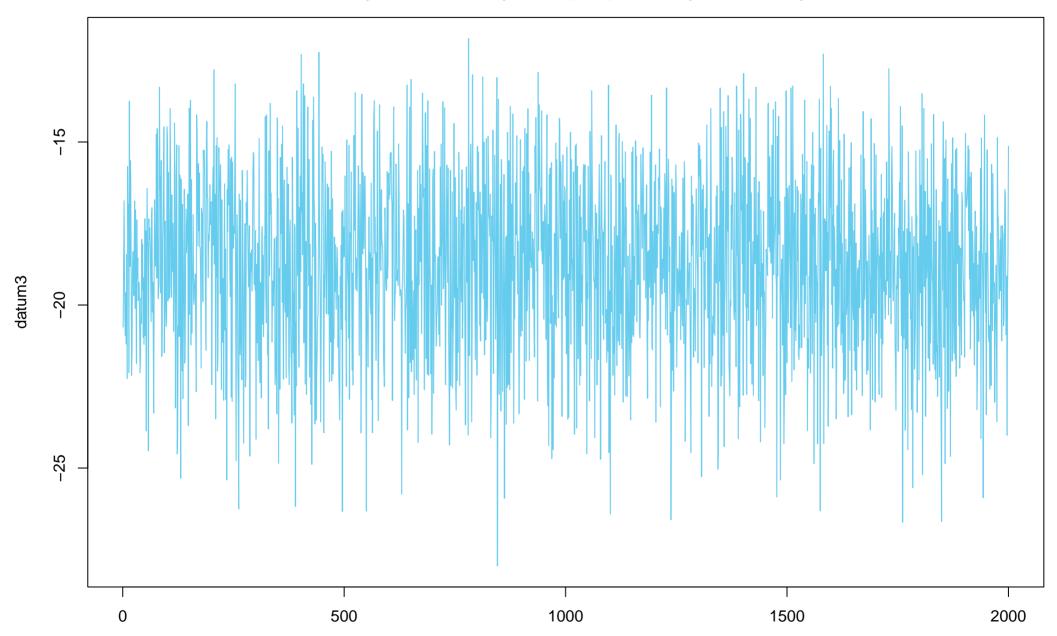
datum1 ESS = 2000 | BMK = 0.0475 | MCSE(6.27) = 0.169 | stat: TRUE | burn: 0



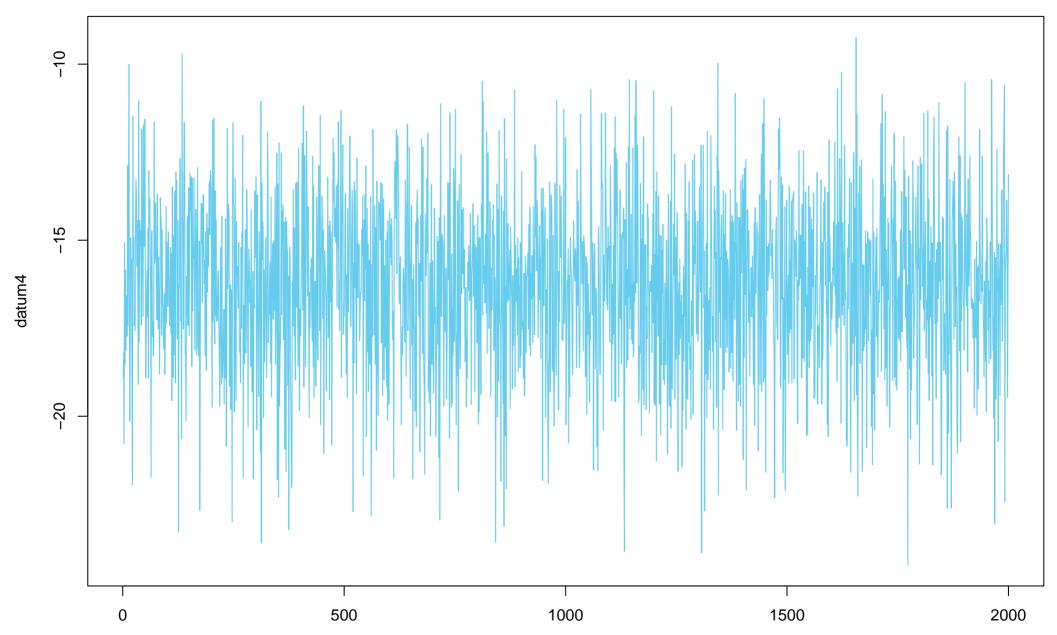
datum2 ESS = 2000 | BMK = 0.0435 | MCSE(6.27) = 0.156 | stat: TRUE | burn: 0



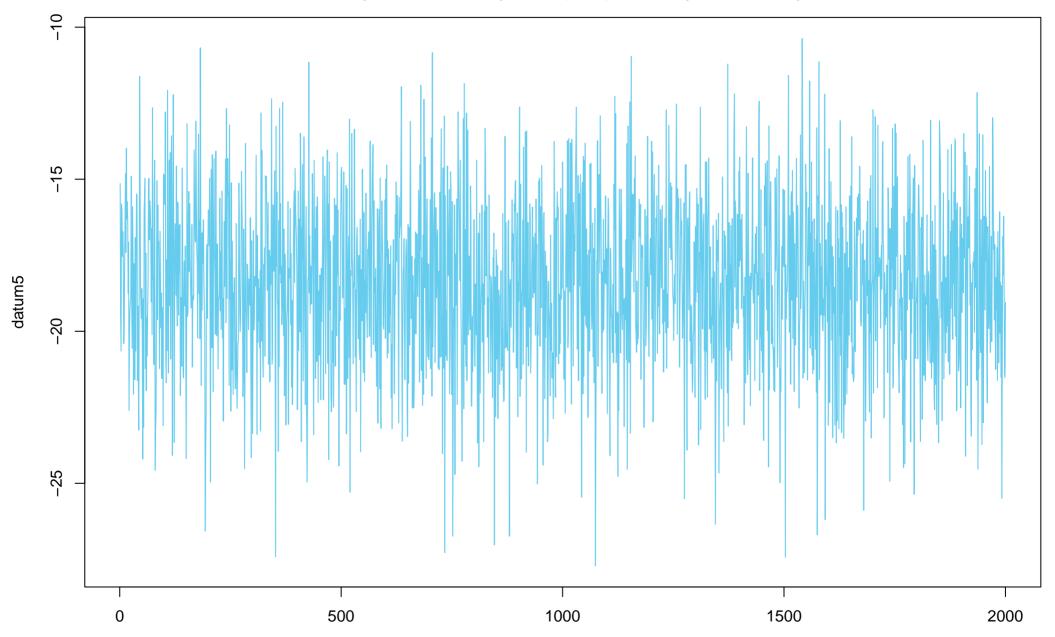
datum3 ESS = 1530 | BMK = 0.0334 | MCSE(6.27) = 0.165 | stat: TRUE | burn: 0



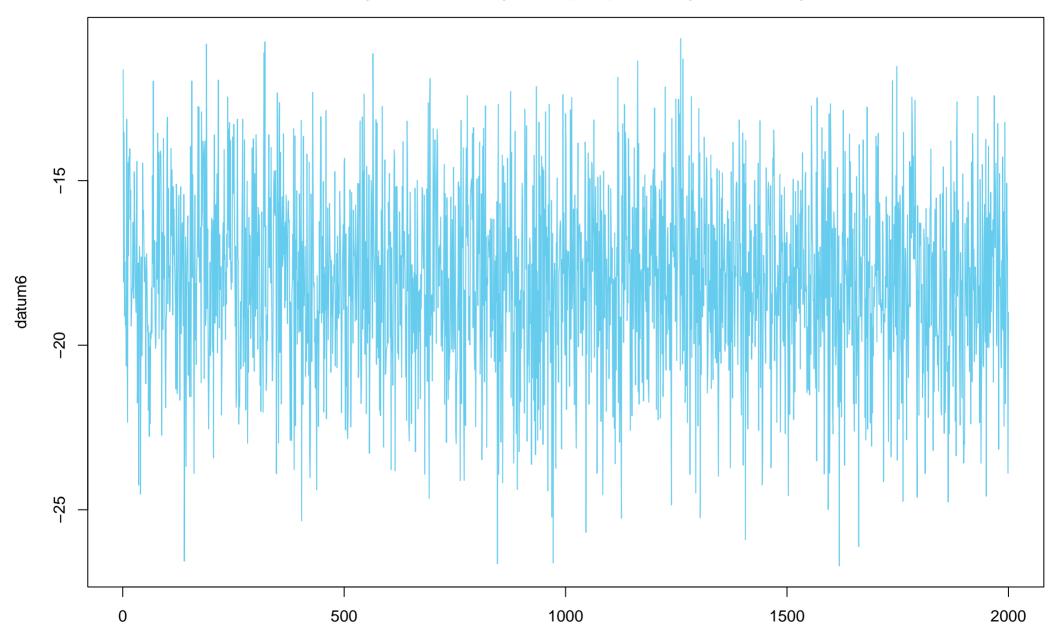
datum4 ESS = 2000 | BMK = 0.0427 | MCSE(6.27) = 0.181 | stat: FALSE | burn: 0



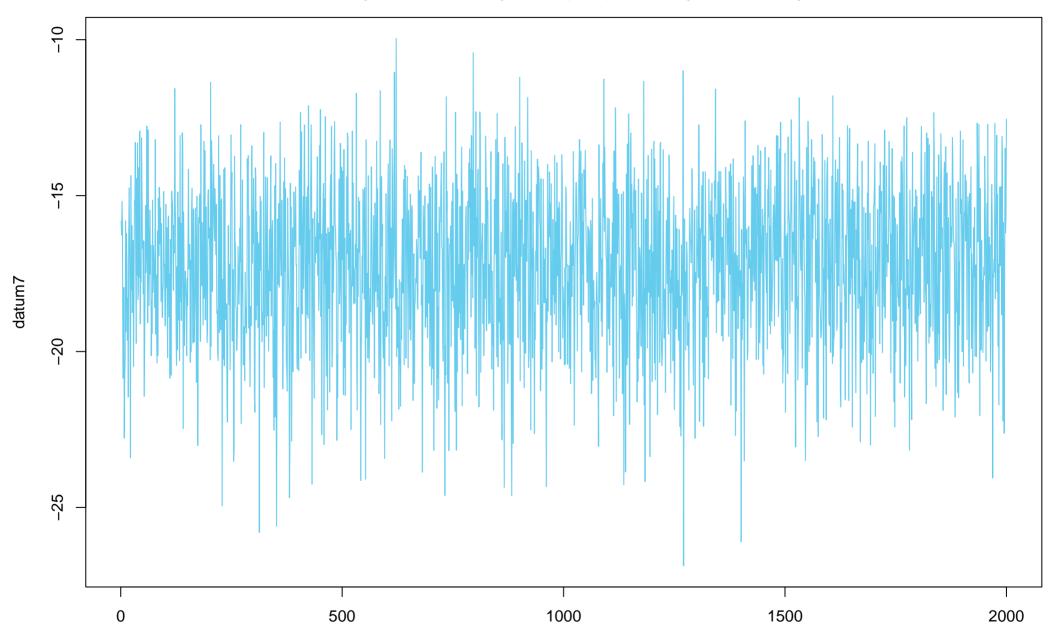
datum5 ESS = 2000 | BMK = 0.0304 | MCSE(6.27) = 0.158 | stat: TRUE | burn: 0



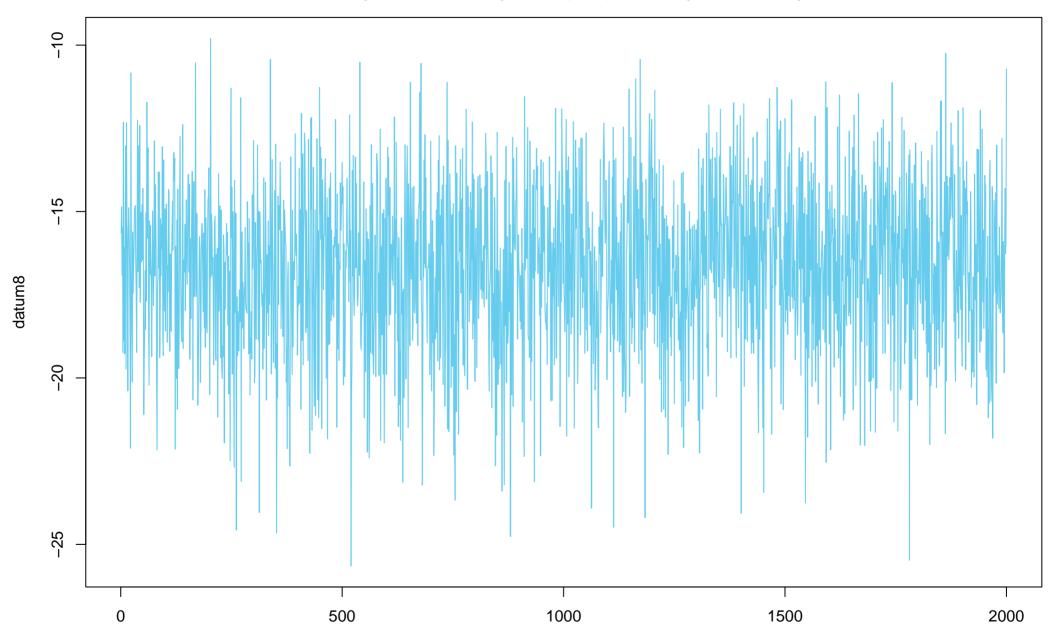
datum6 ESS = 2000 | BMK = 0.0325 | MCSE(6.27) = 0.159 | stat: TRUE | burn: 0



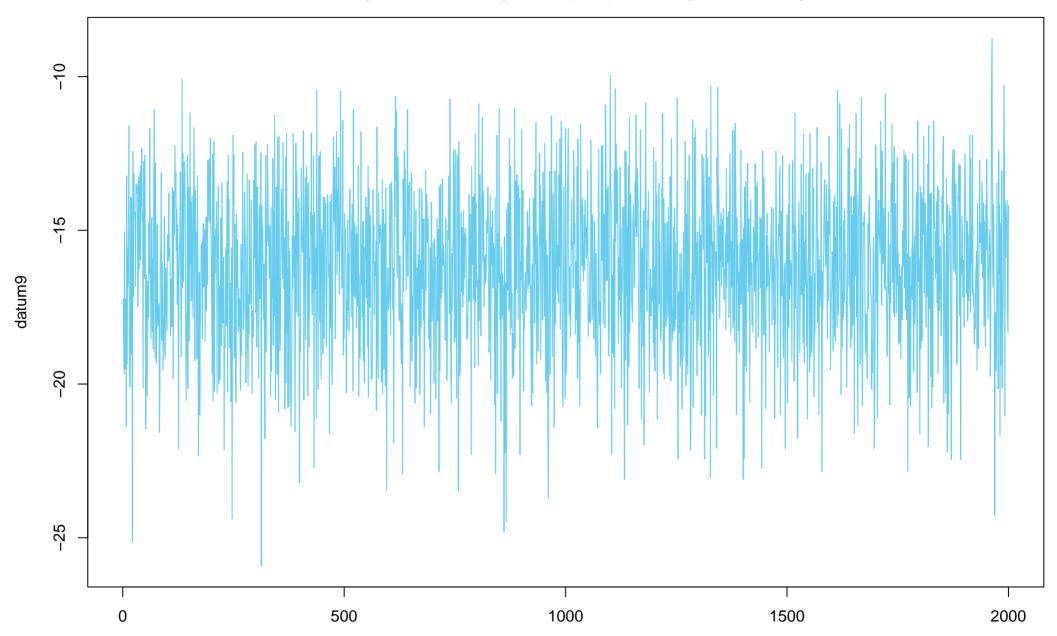
datum7 ESS = 2000 | BMK = 0.0465 | MCSE(6.27) = 0.172 | stat: TRUE | burn: 0



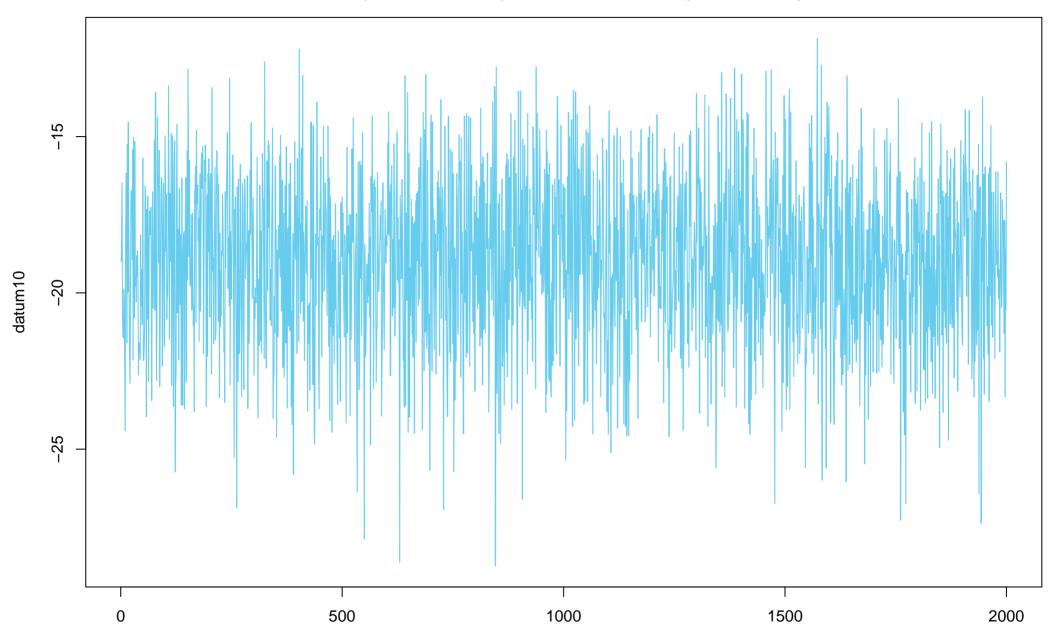
datum8 ESS = 2000 | BMK = 0.0547 | MCSE(6.27) = 0.177 | stat: TRUE | burn: 0



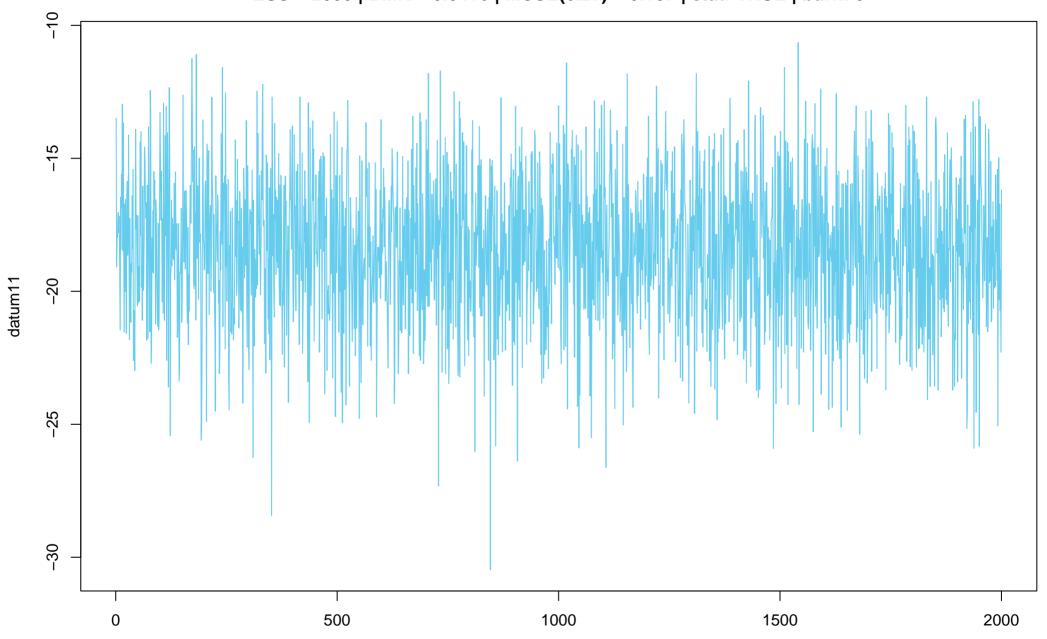
datum9 ESS = 2000 | BMK = 0.0507 | MCSE(6.27) = 0.171 | stat: TRUE | burn: 0



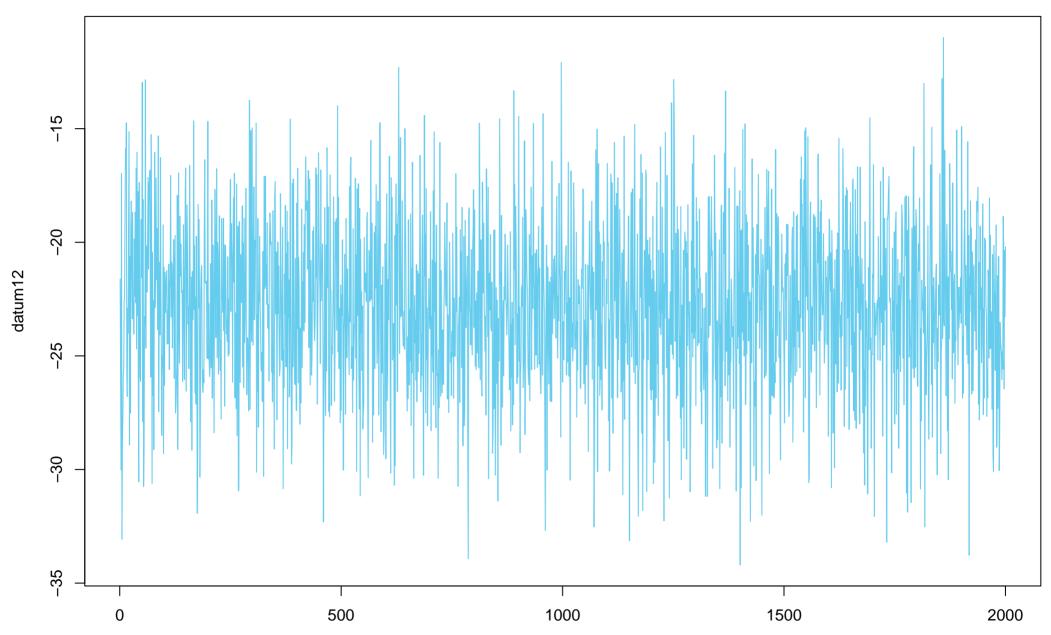
datum10 ESS = 2000 | BMK = 0.0345 | MCSE(6.27) = 0.162 | stat: TRUE | burn: 0



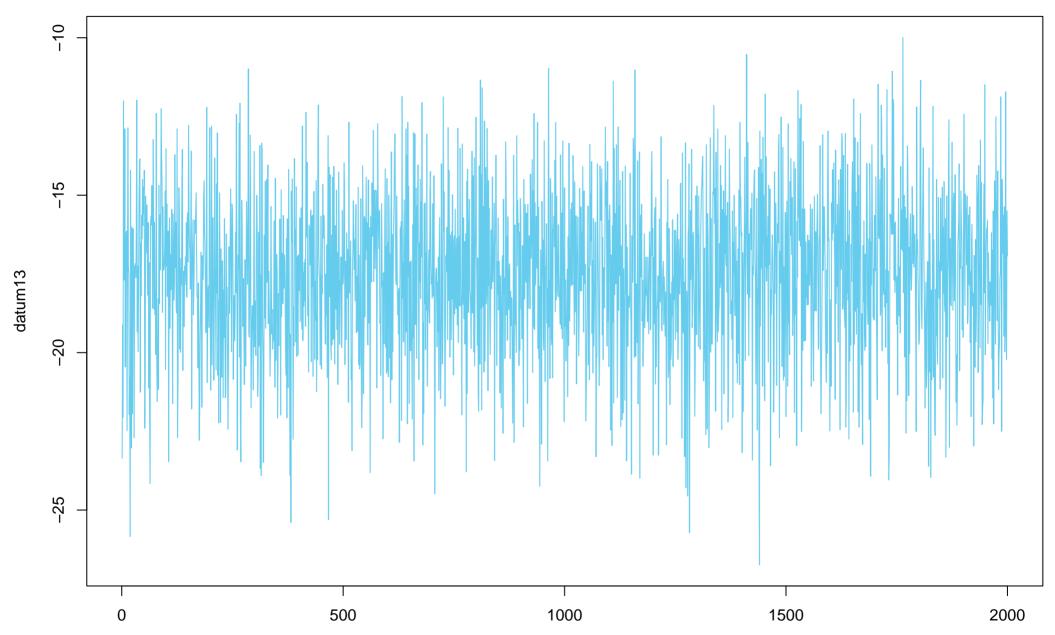
datum11 ESS = 2000 | BMK = 0.0416 | MCSE(6.27) = 0.157 | stat: TRUE | burn: 0



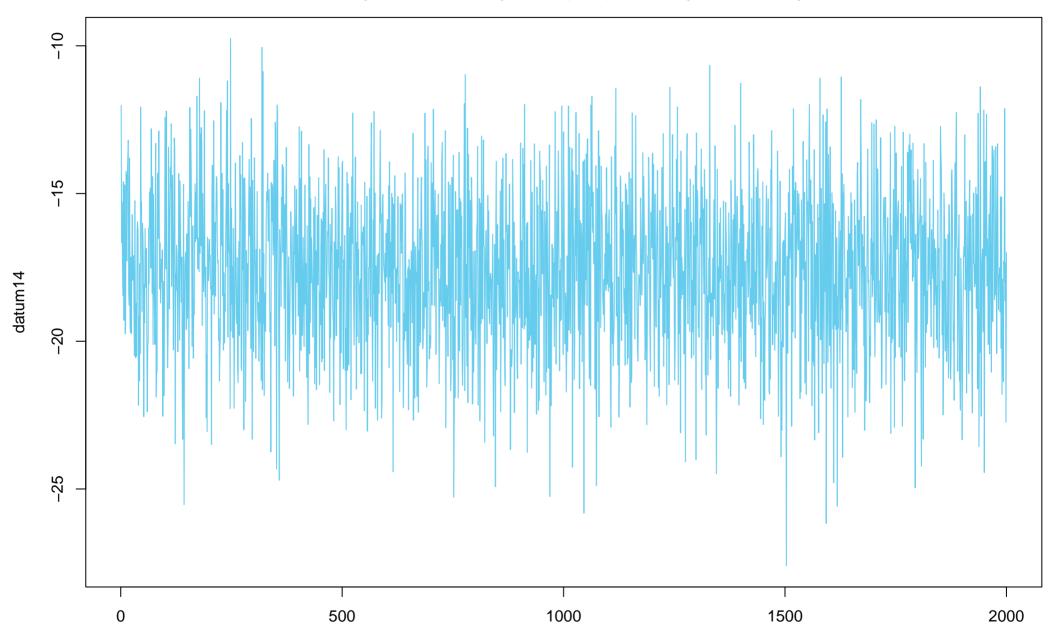
datum12 ESS = 2000 | BMK = 0.0423 | MCSE(6.27) = 0.118 | stat: TRUE | burn: 0



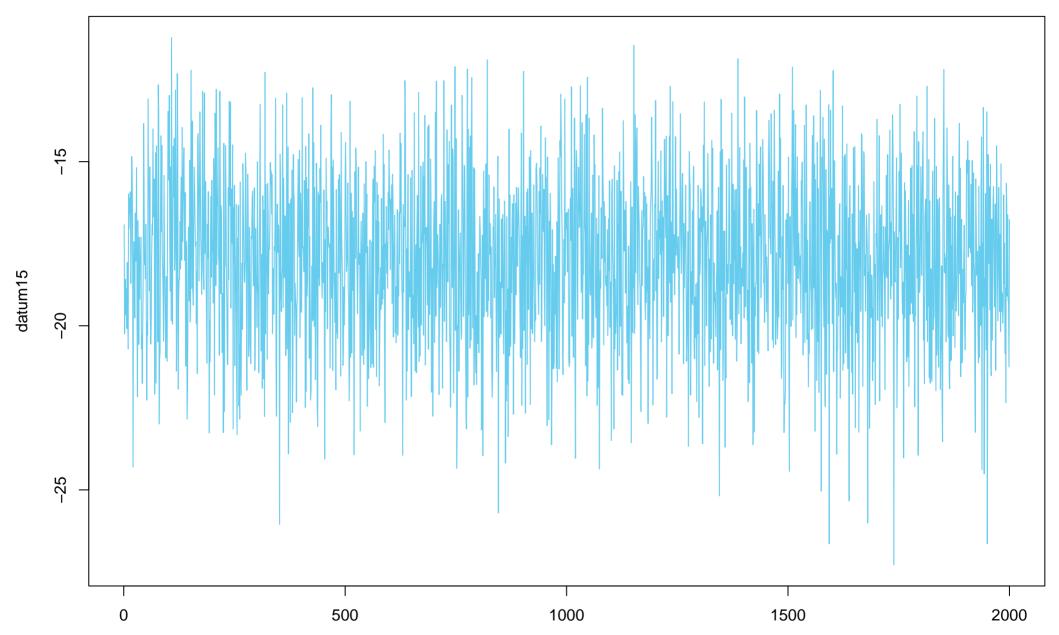
datum13 ESS = 2000 | BMK = 0.037 | MCSE(6.27) = 0.168 | stat: TRUE | burn: 0



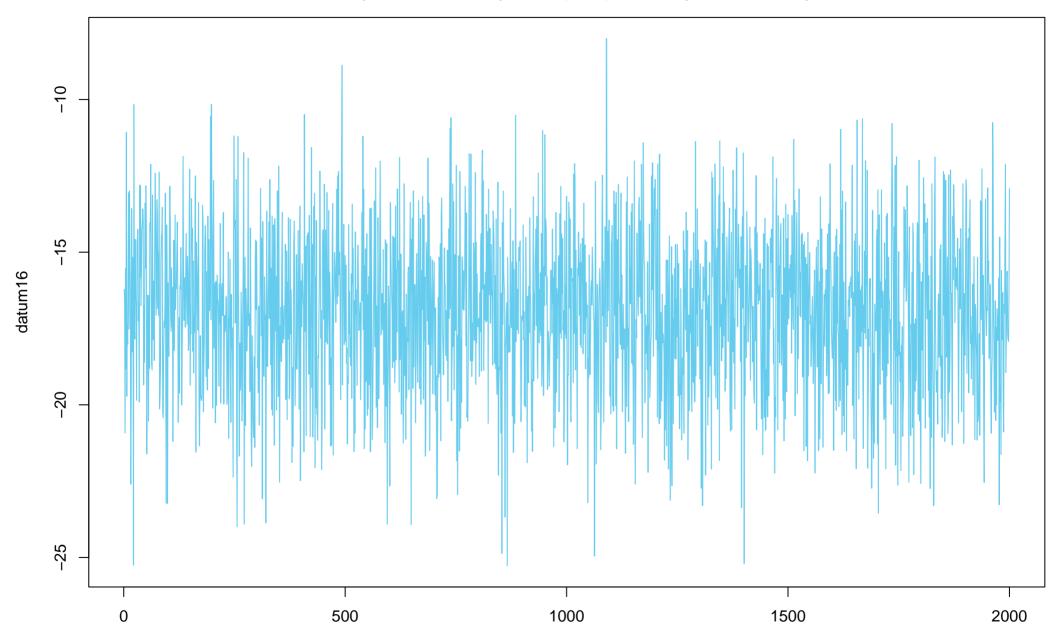
datum14 ESS = 2000 | BMK = 0.0301 | MCSE(6.27) = 0.163 | stat: TRUE | burn: 0



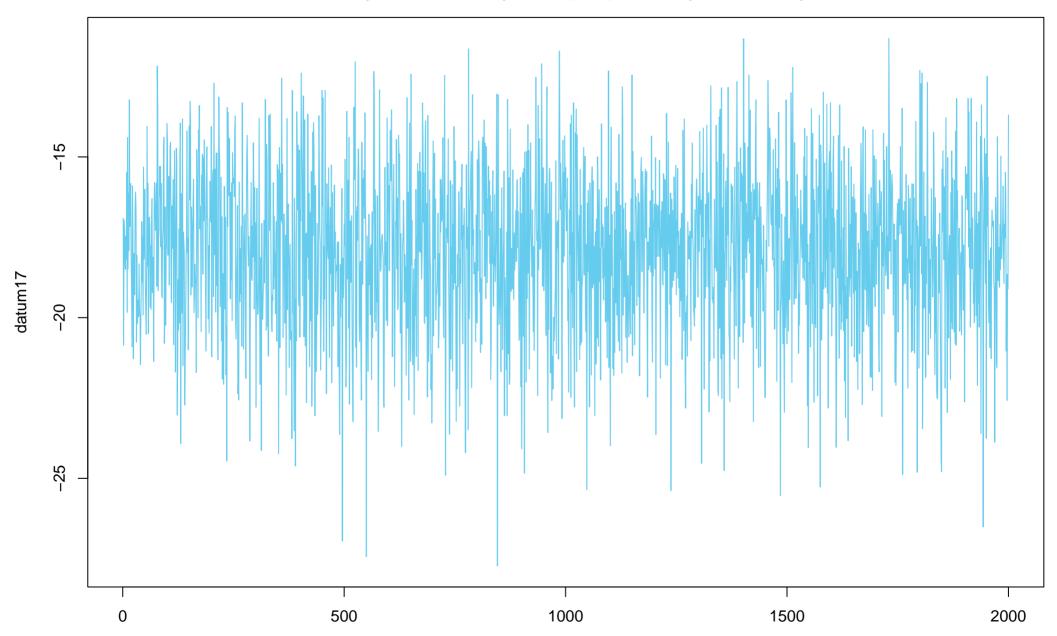
datum15 ESS = 2000 | BMK = 0.0392 | MCSE(6.27) = 0.173 | stat: TRUE | burn: 0



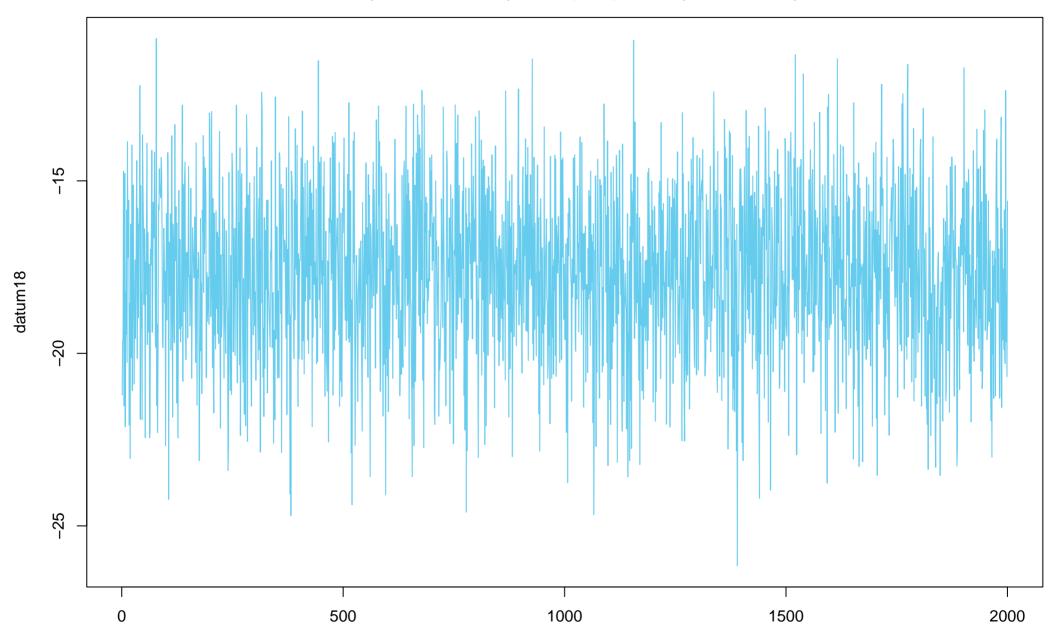
datum16 ESS = 2000 | BMK = 0.0408 | MCSE(6.27) = 0.167 | stat: FALSE | burn: 0



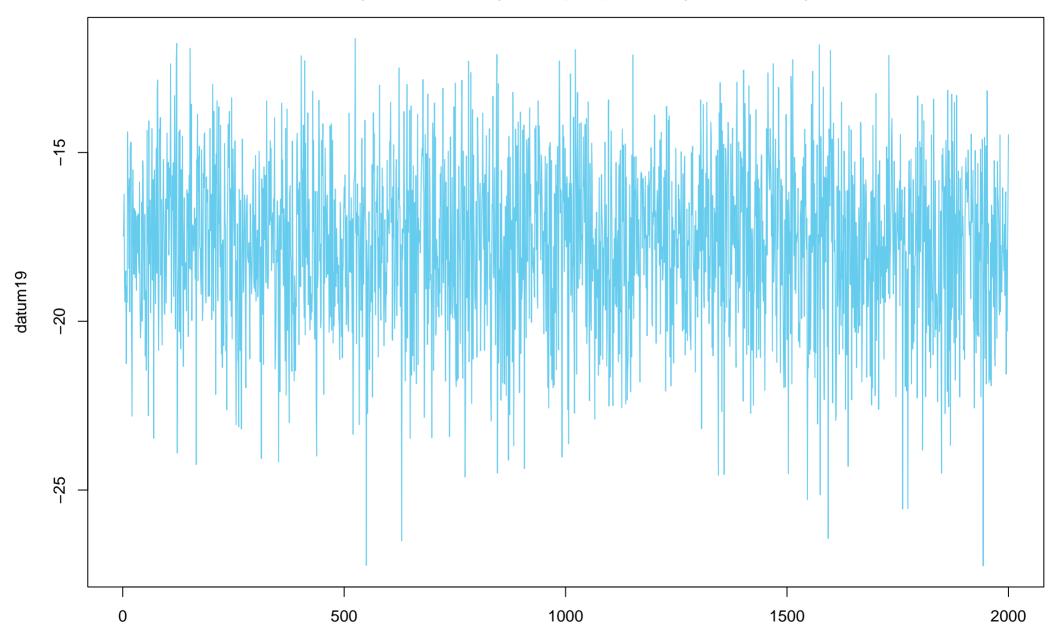
datum17 ESS = 1720 | BMK = 0.0499 | MCSE(6.27) = 0.173 | stat: TRUE | burn: 0



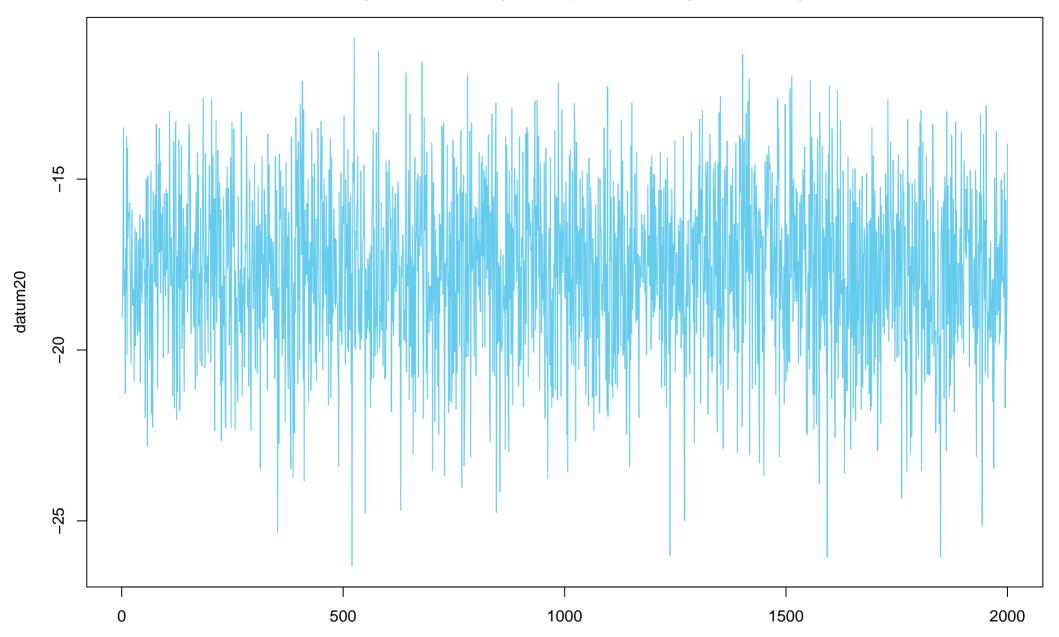
datum18 ESS = 2000 | BMK = 0.0344 | MCSE(6.27) = 0.18 | stat: TRUE | burn: 0



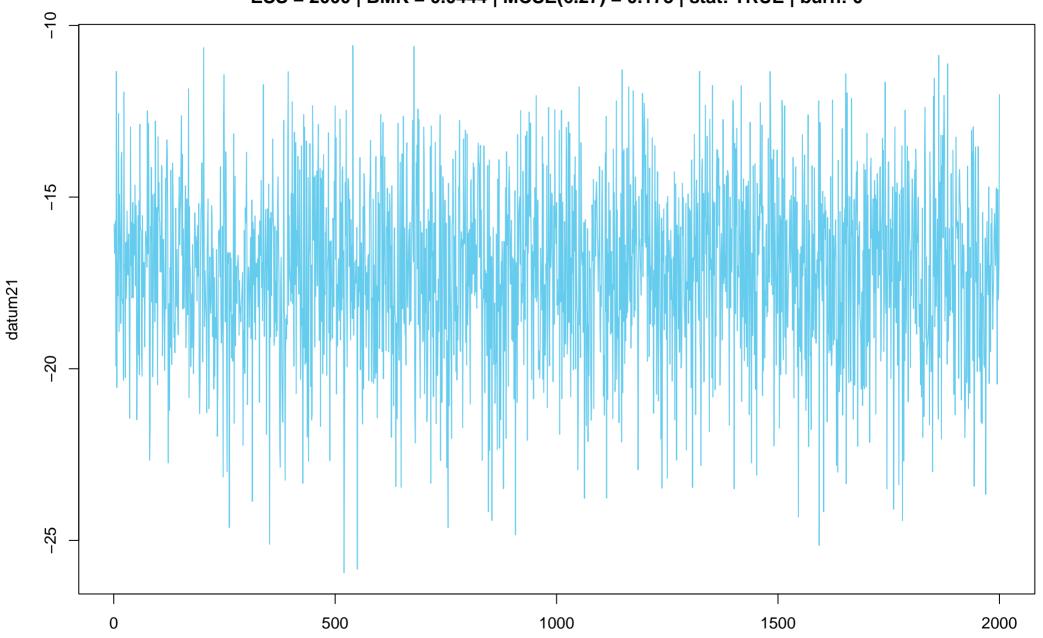
datum19 ESS = 2000 | BMK = 0.0496 | MCSE(6.27) = 0.177 | stat: FALSE | burn: 0



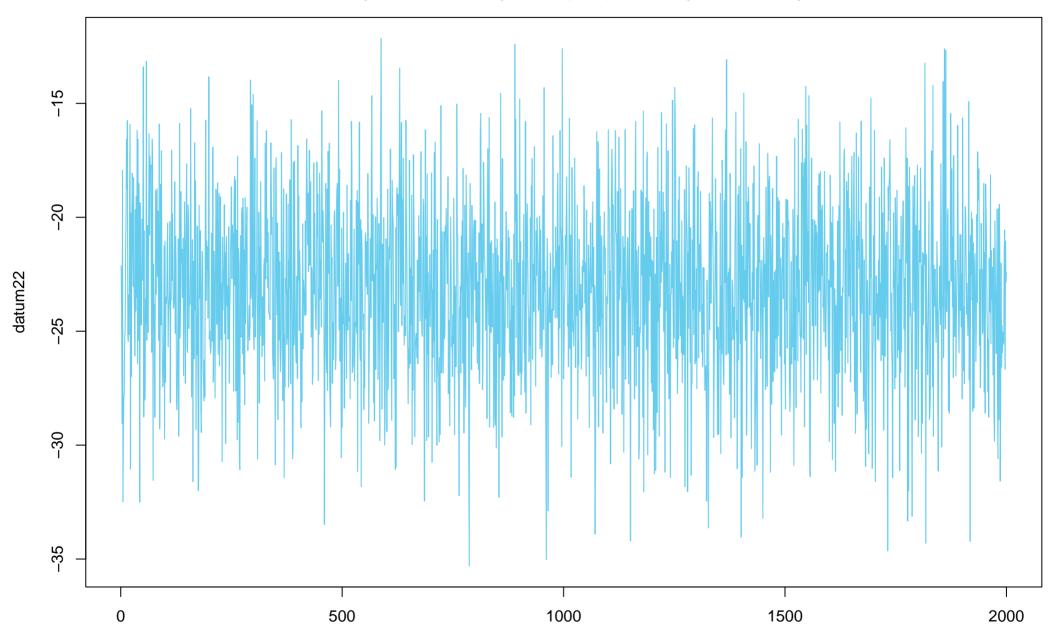
datum20 ESS = 2000 | BMK = 0.0289 | MCSE(6.27) = 0.179 | stat: TRUE | burn: 0



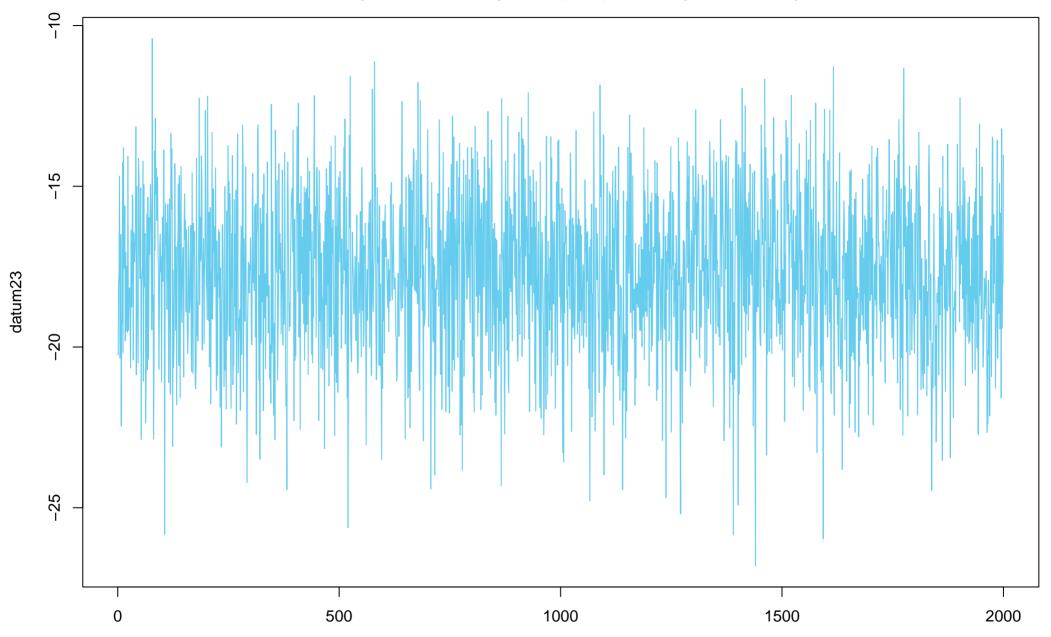
datum21 ESS = 2000 | BMK = 0.0444 | MCSE(6.27) = 0.173 | stat: TRUE | burn: 0



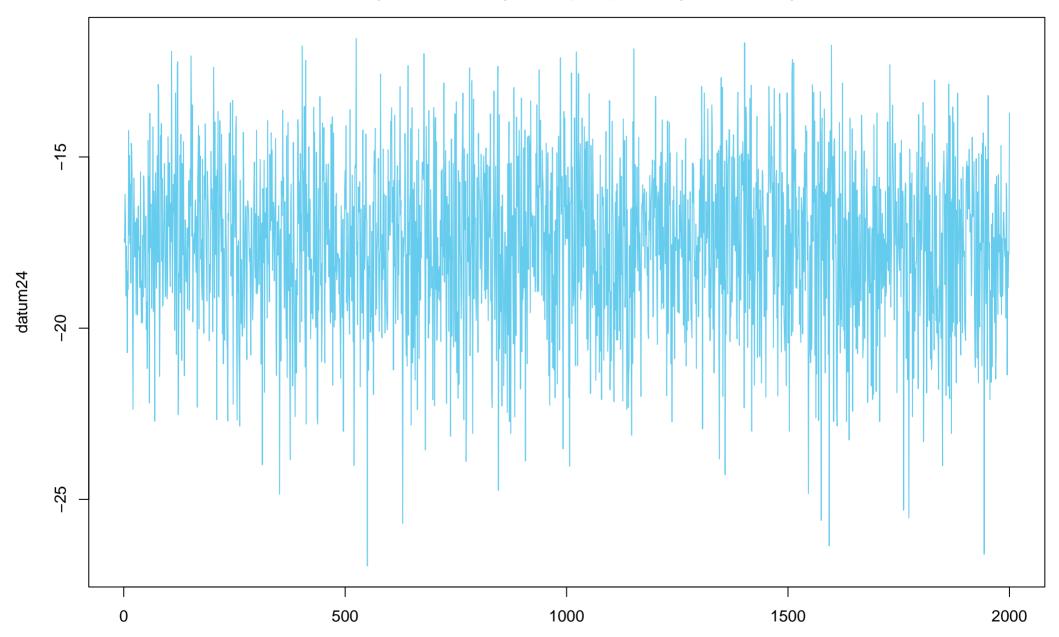
datum22 ESS = 2000 | BMK = 0.0357 | MCSE(6.27) = 0.114 | stat: TRUE | burn: 0



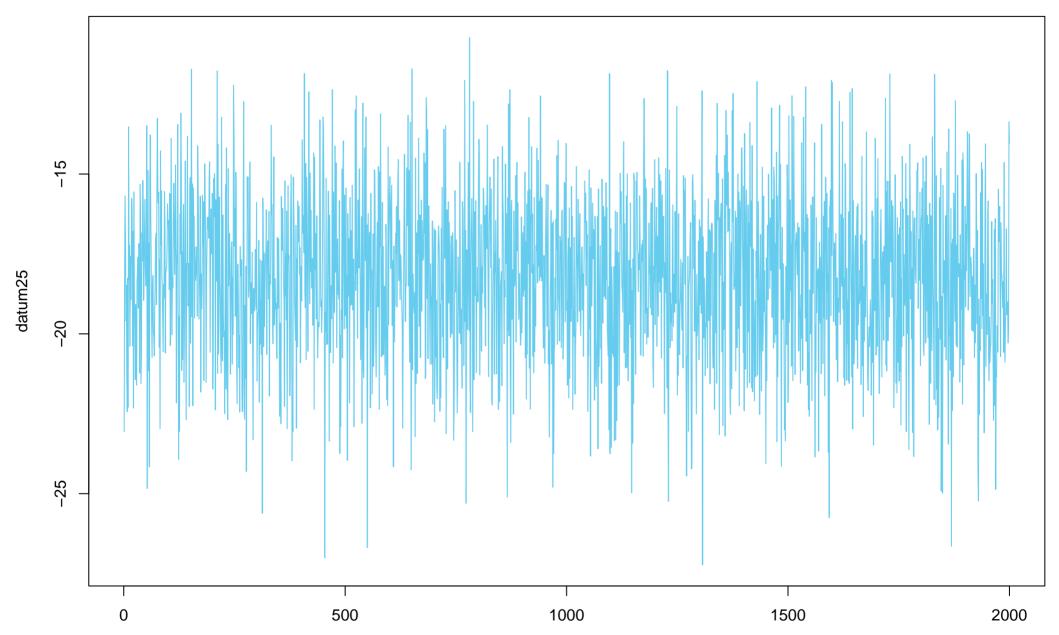
datum23 ESS = 2000 | BMK = 0.0304 | MCSE(6.27) = 0.177 | stat: TRUE | burn: 0



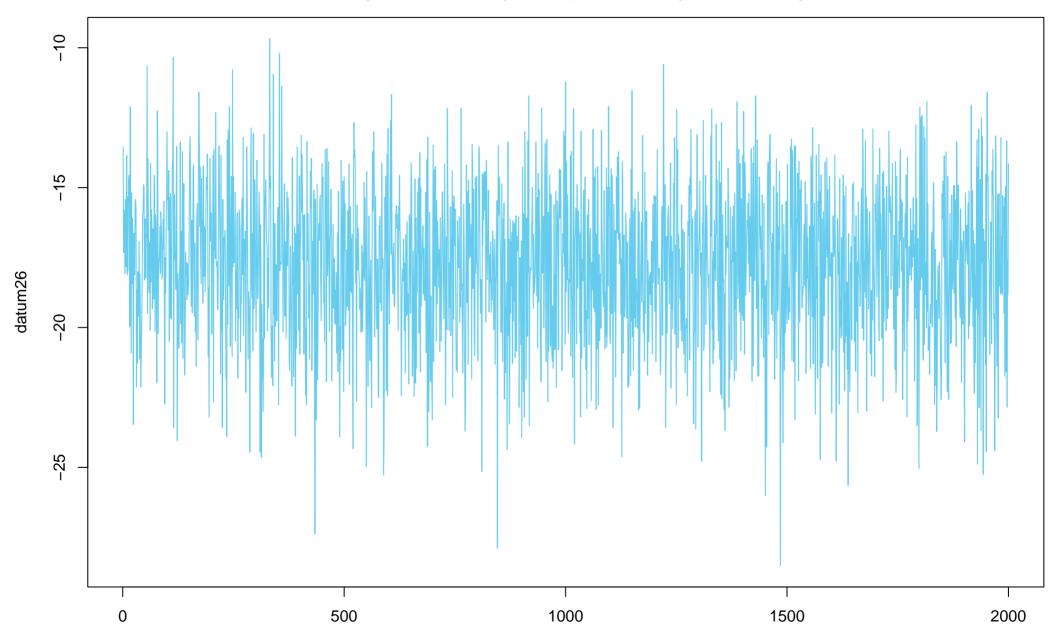
datum24 ESS = 2000 | BMK = 0.042 | MCSE(6.27) = 0.18 | stat: TRUE | burn: 0



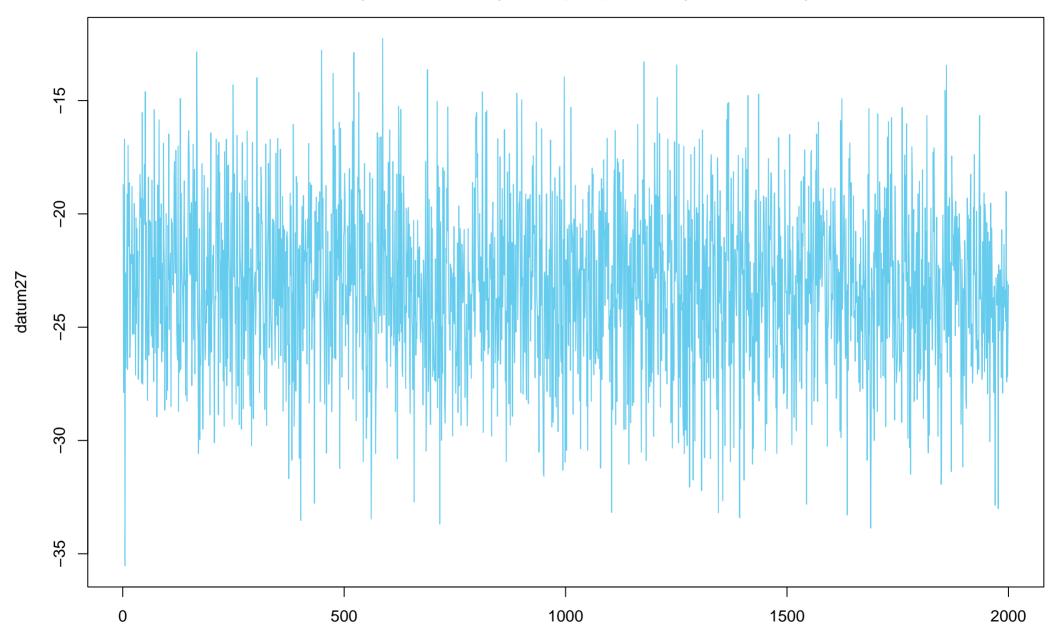
datum25 ESS = 2000 | BMK = 0.0385 | MCSE(6.27) = 0.17 | stat: FALSE | burn: 0



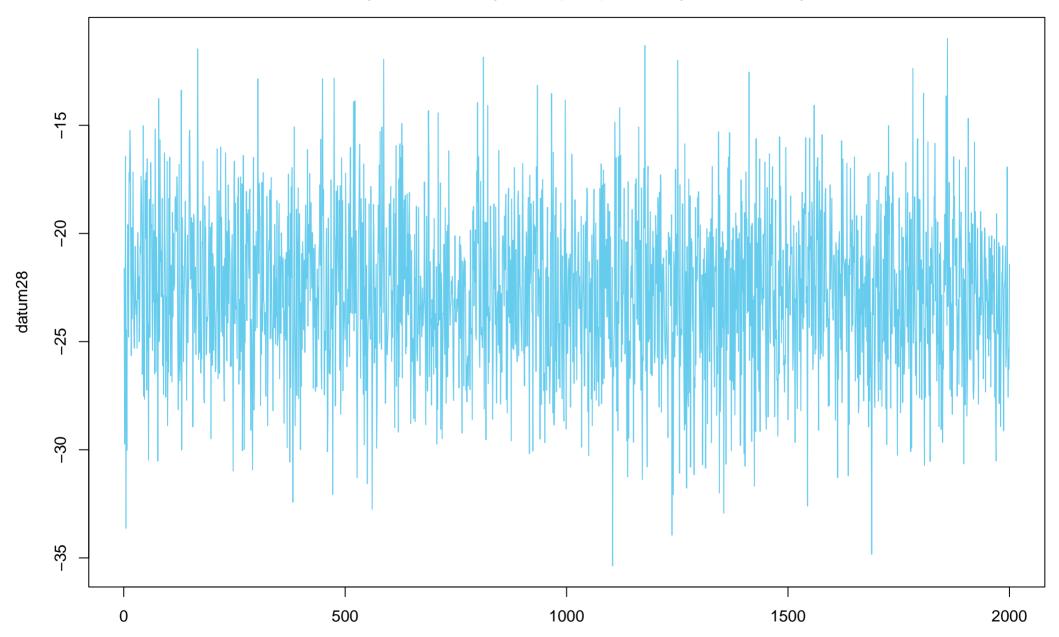
datum26 ESS = 2000 | BMK = 0.0377 | MCSE(6.27) = 0.16 | stat: FALSE | burn: 0



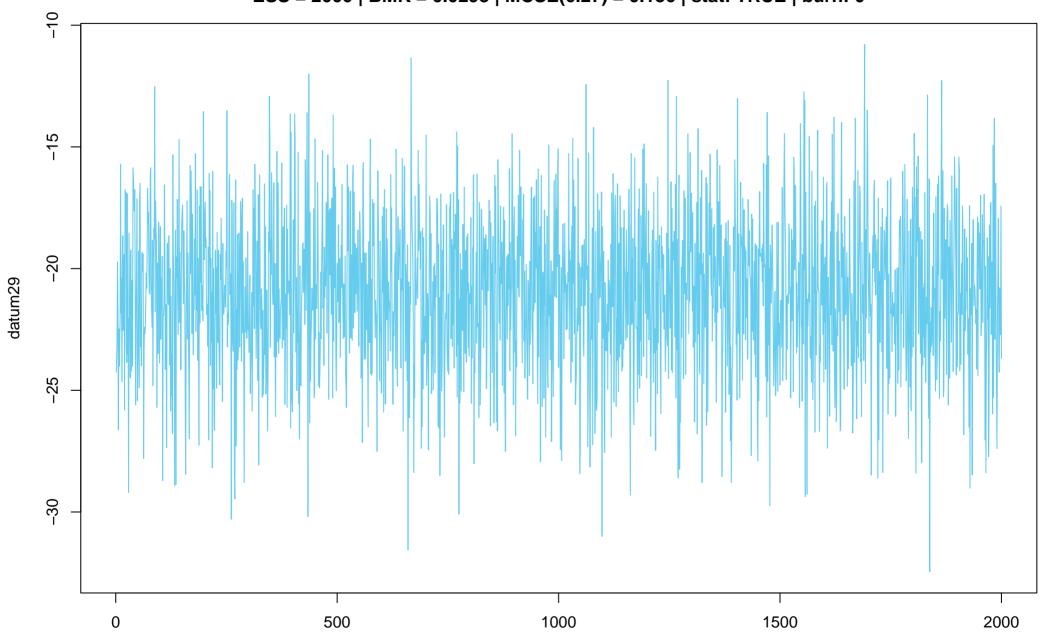
datum27 ESS = 2000 | BMK = 0.0519 | MCSE(6.27) = 0.118 | stat: FALSE | burn: 0



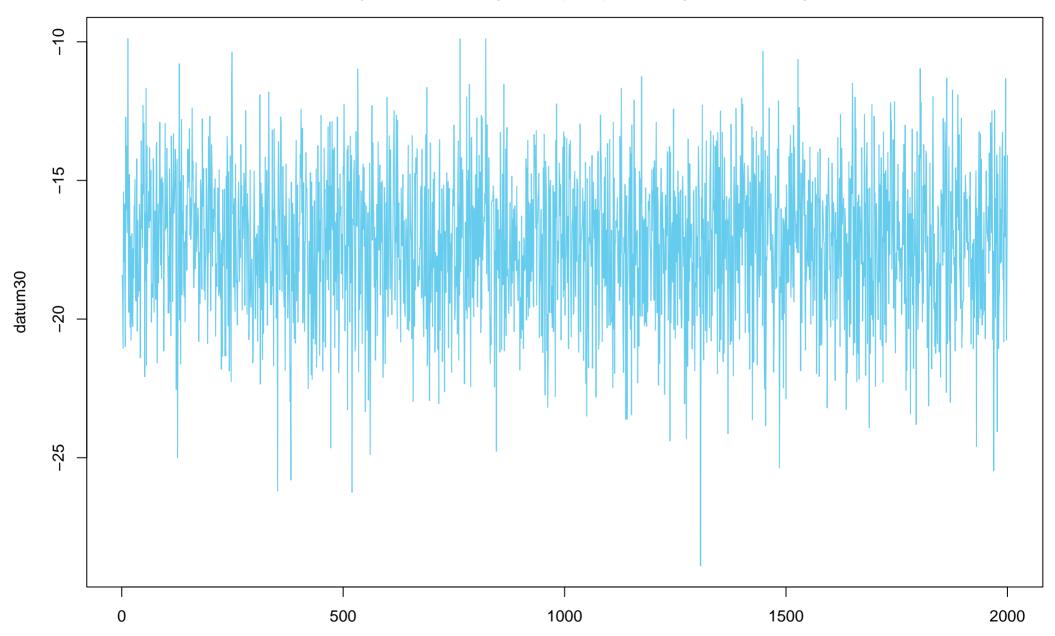
datum28 ESS = 2000 | BMK = 0.052 | MCSE(6.27) = 0.118 | stat: FALSE | burn: 0



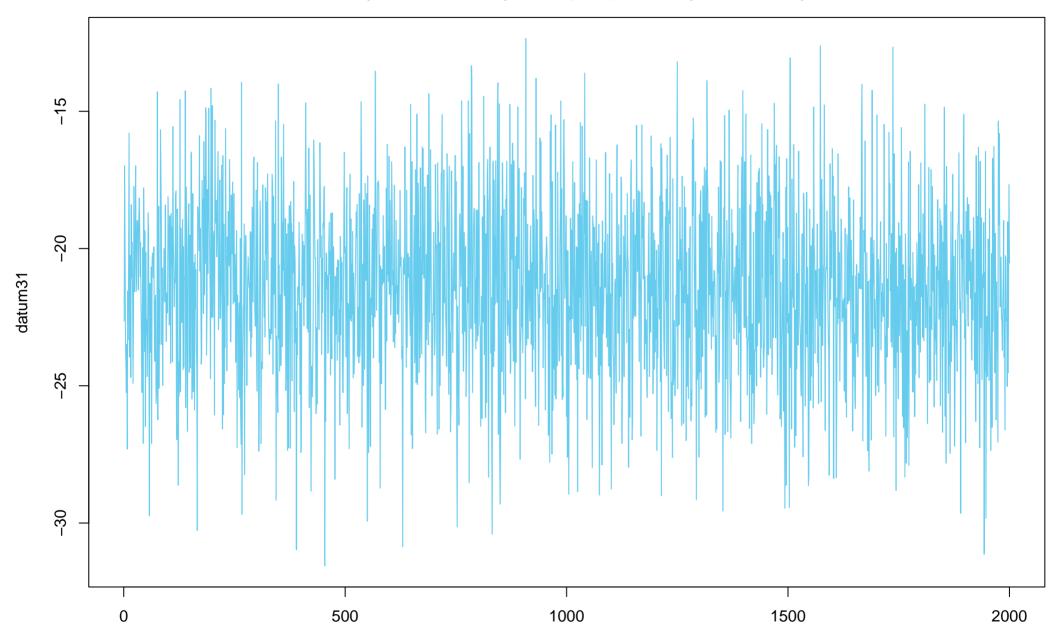
datum29 ESS = 2000 | BMK = 0.0298 | MCSE(6.27) = 0.136 | stat: TRUE | burn: 0



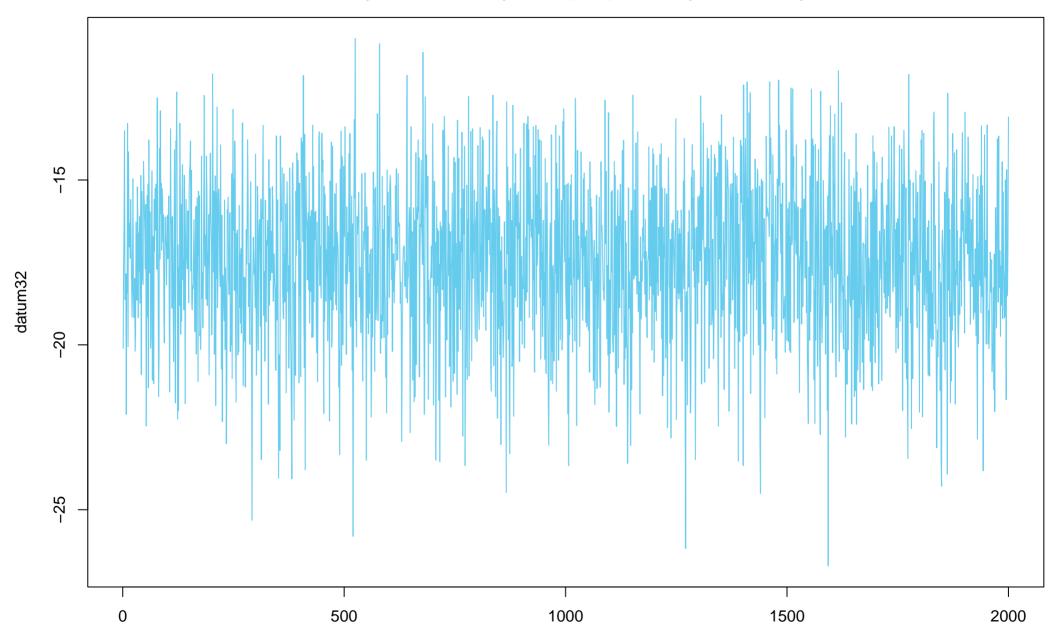
datum30 ESS = 2000 | BMK = 0.0566 | MCSE(6.27) = 0.166 | stat: FALSE | burn: 0



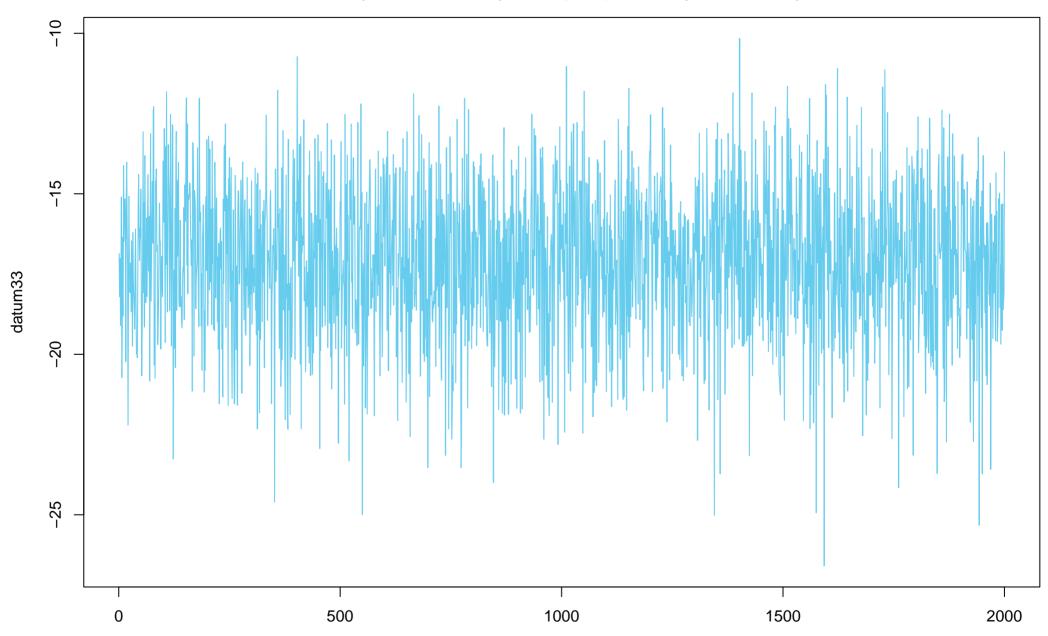
datum31 ESS = 2000 | BMK = 0.0539 | MCSE(6.27) = 0.138 | stat: TRUE | burn: 0



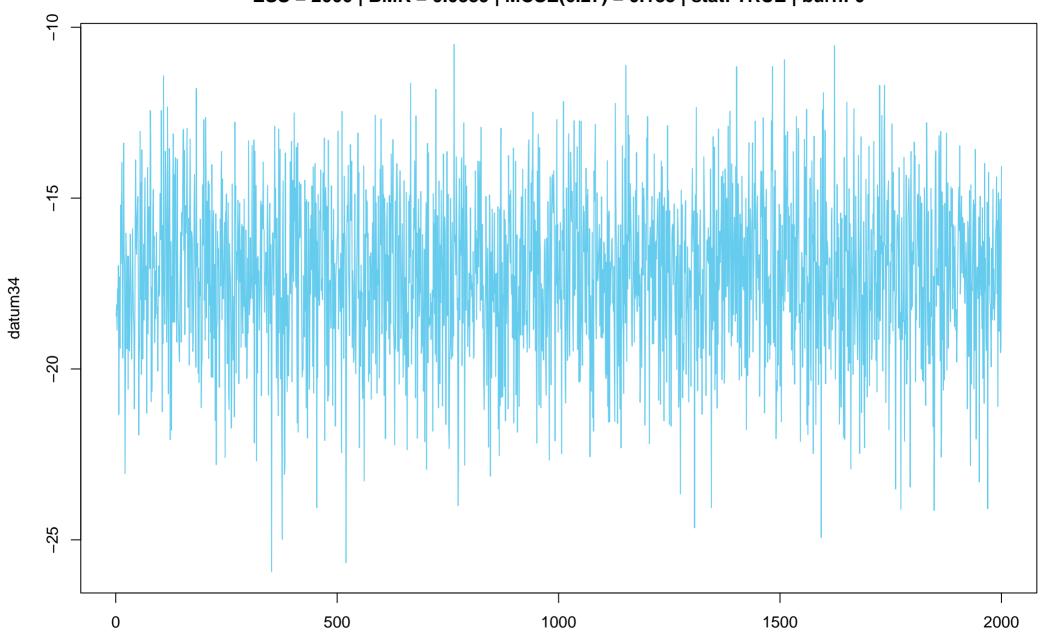
datum32 ESS = 2000 | BMK = 0.0364 | MCSE(6.27) = 0.181 | stat: TRUE | burn: 0



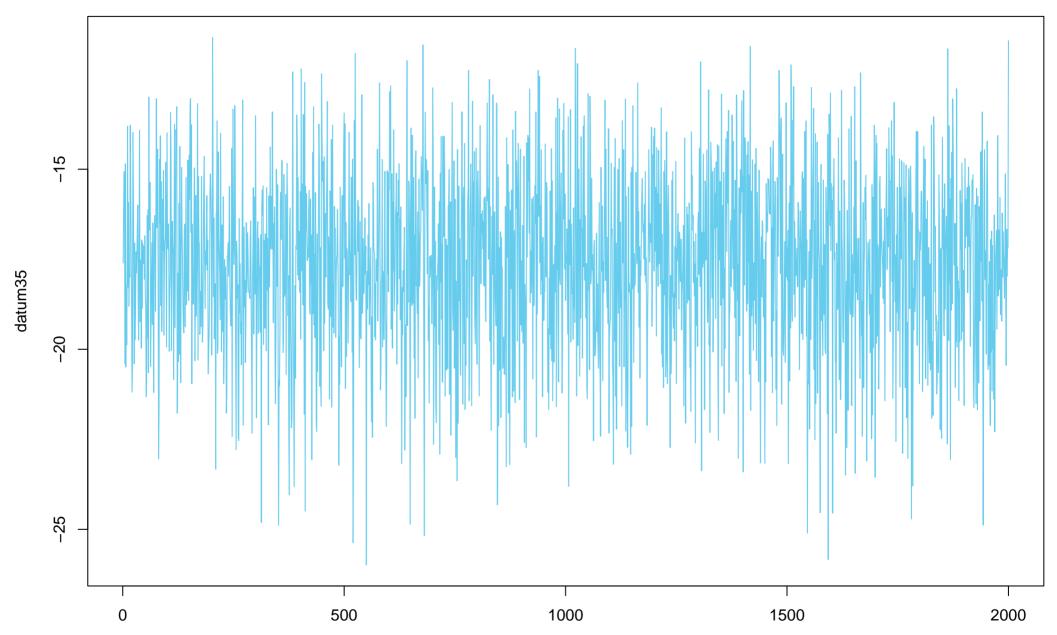
datum33 ESS = 2000 | BMK = 0.0414 | MCSE(6.27) = 0.184 | stat: TRUE | burn: 0



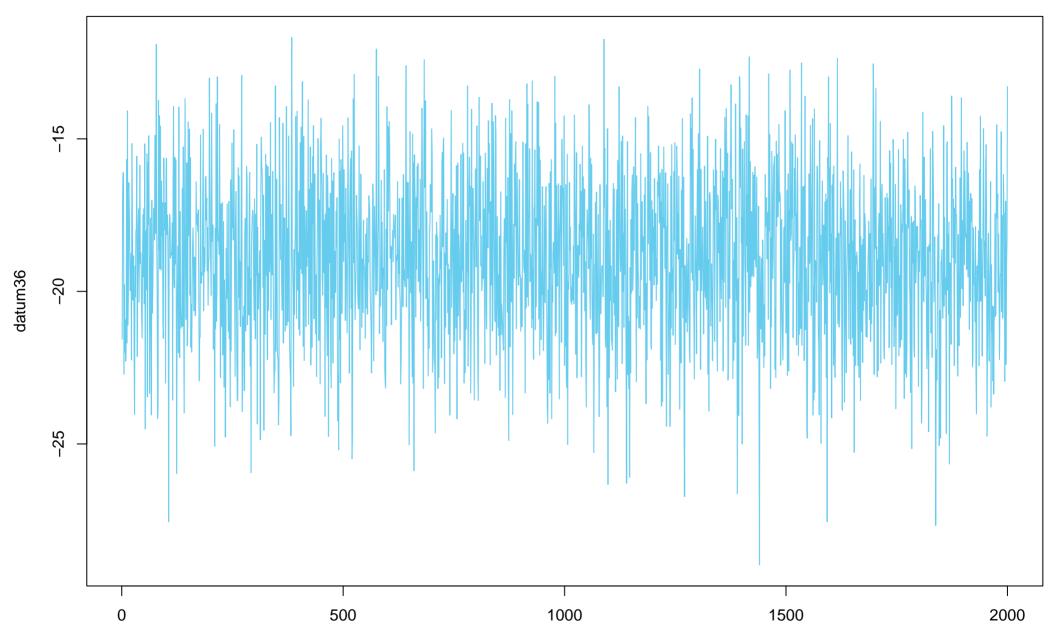
datum34 ESS = 2000 | BMK = 0.0339 | MCSE(6.27) = 0.183 | stat: TRUE | burn: 0



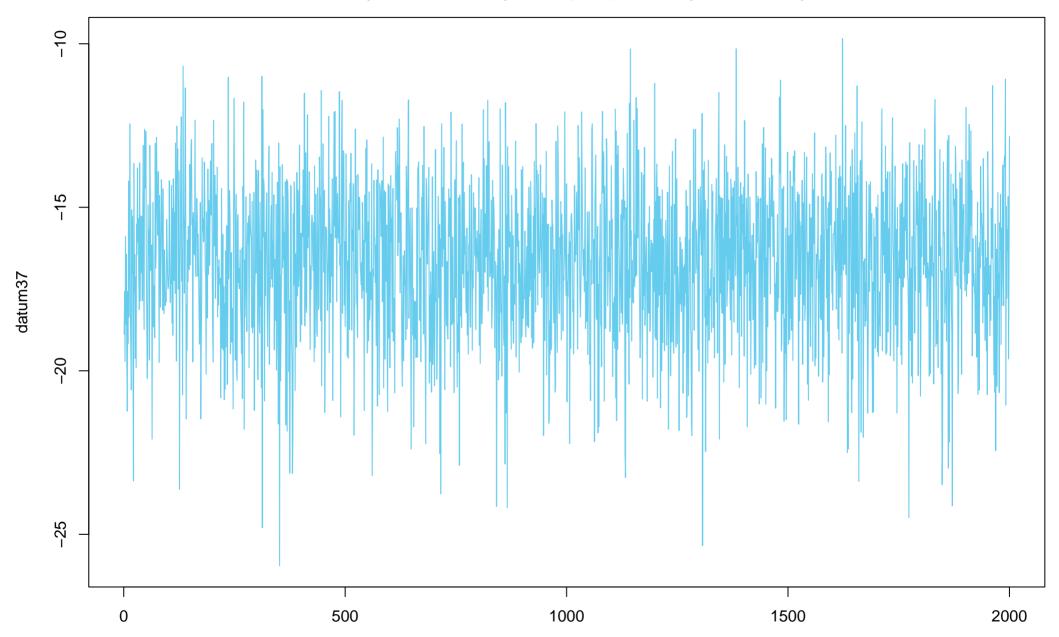
datum35 ESS = 2000 | BMK = 0.0241 | MCSE(6.27) = 0.177 | stat: TRUE | burn: 0



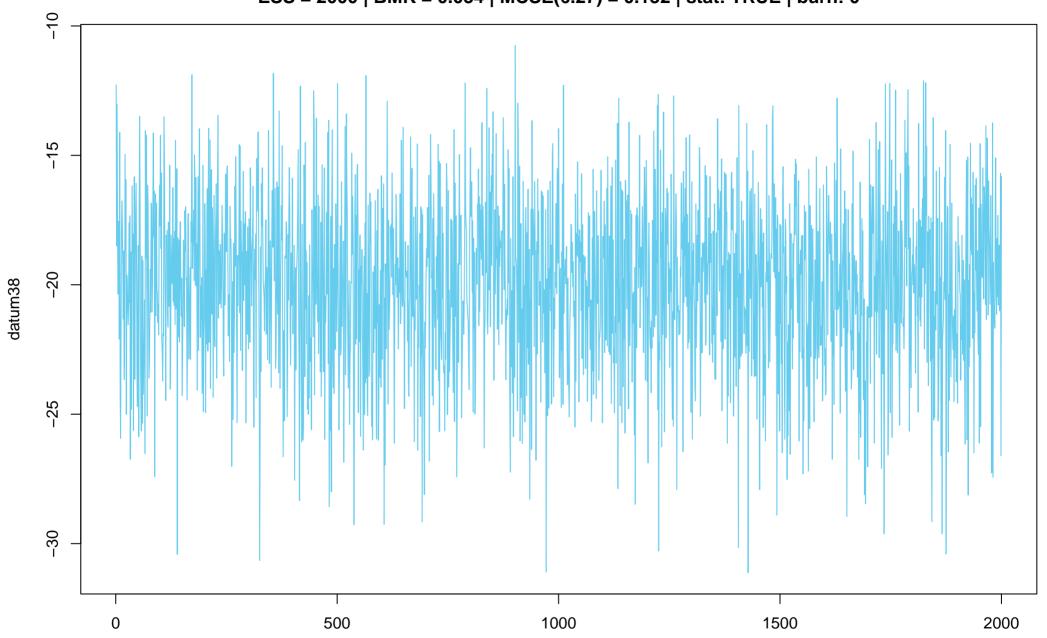
datum36 ESS = 2000 | BMK = 0.0411 | MCSE(6.27) = 0.164 | stat: TRUE | burn: 0



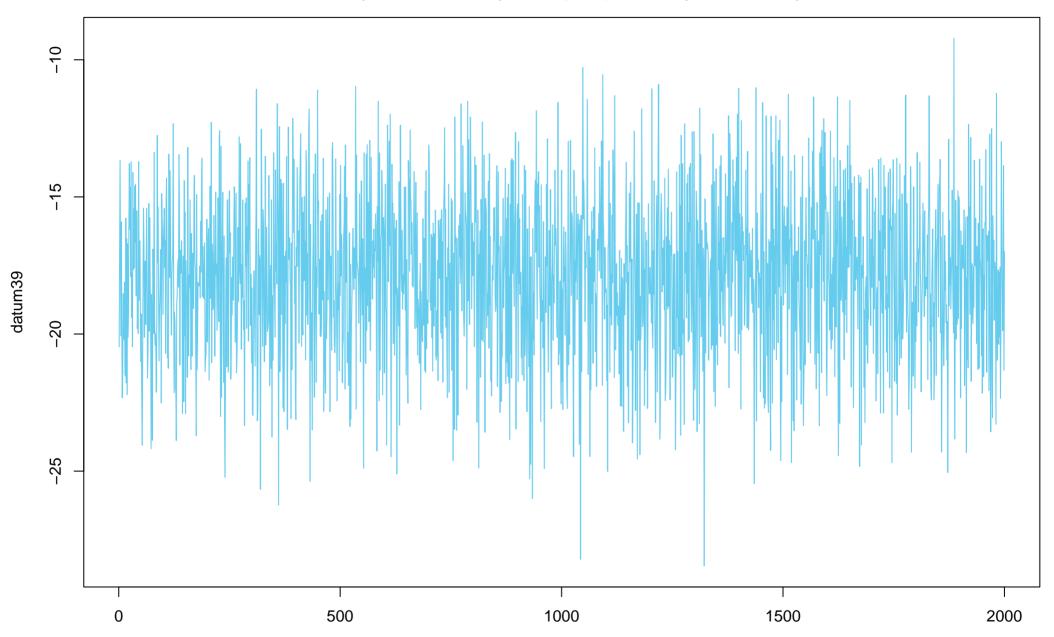
datum37 ESS = 2000 | BMK = 0.0296 | MCSE(6.27) = 0.184 | stat: TRUE | burn: 0



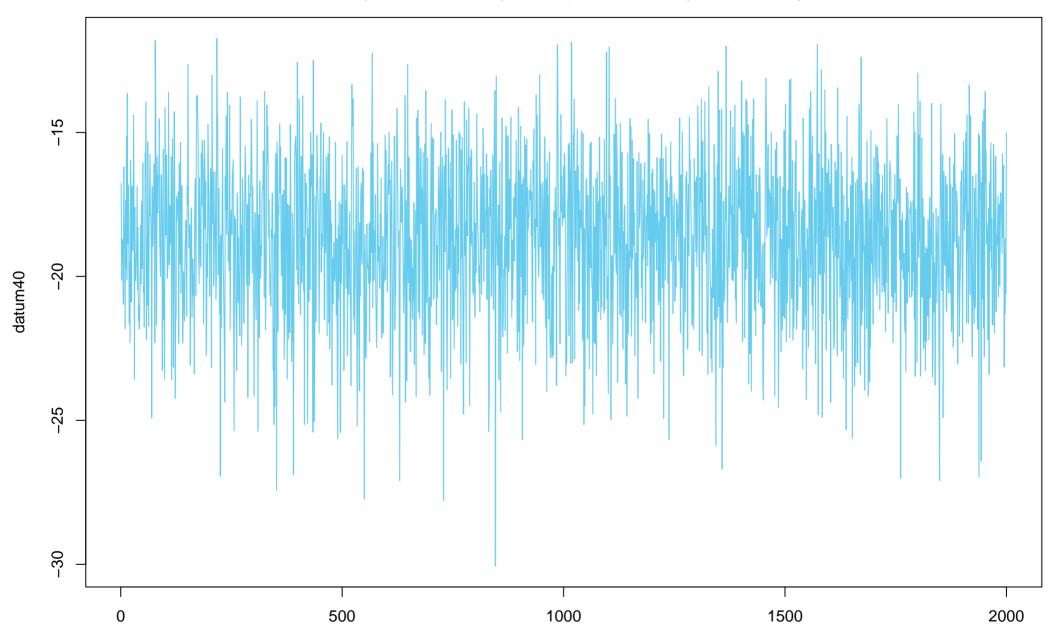
datum38 ESS = 2000 | BMK = 0.034 | MCSE(6.27) = 0.132 | stat: TRUE | burn: 0



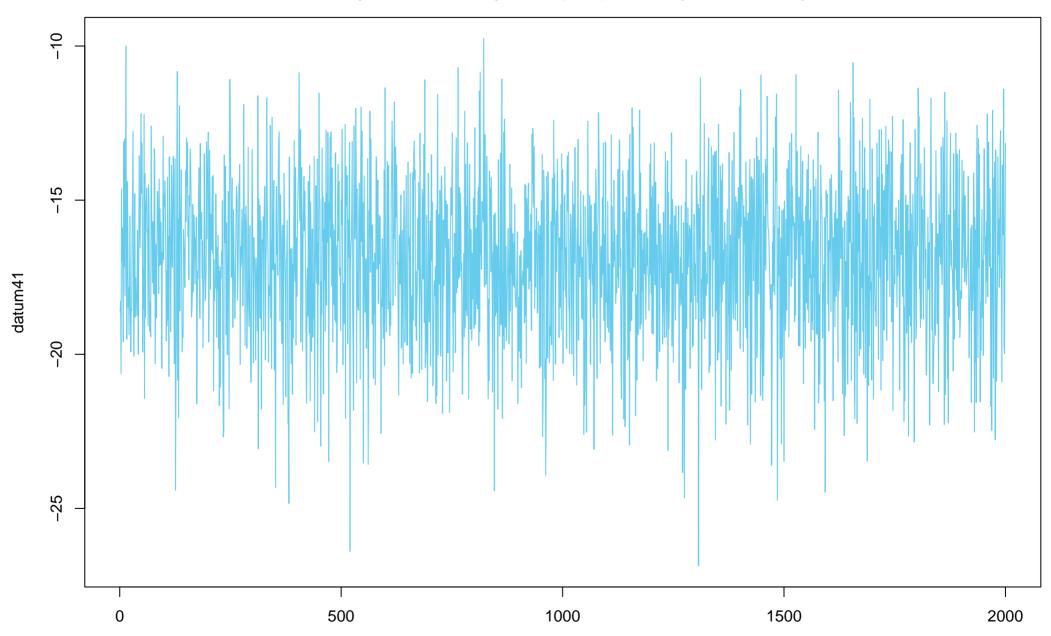
datum39 ESS = 2000 | BMK = 0.0492 | MCSE(6.27) = 0.151 | stat: TRUE | burn: 0



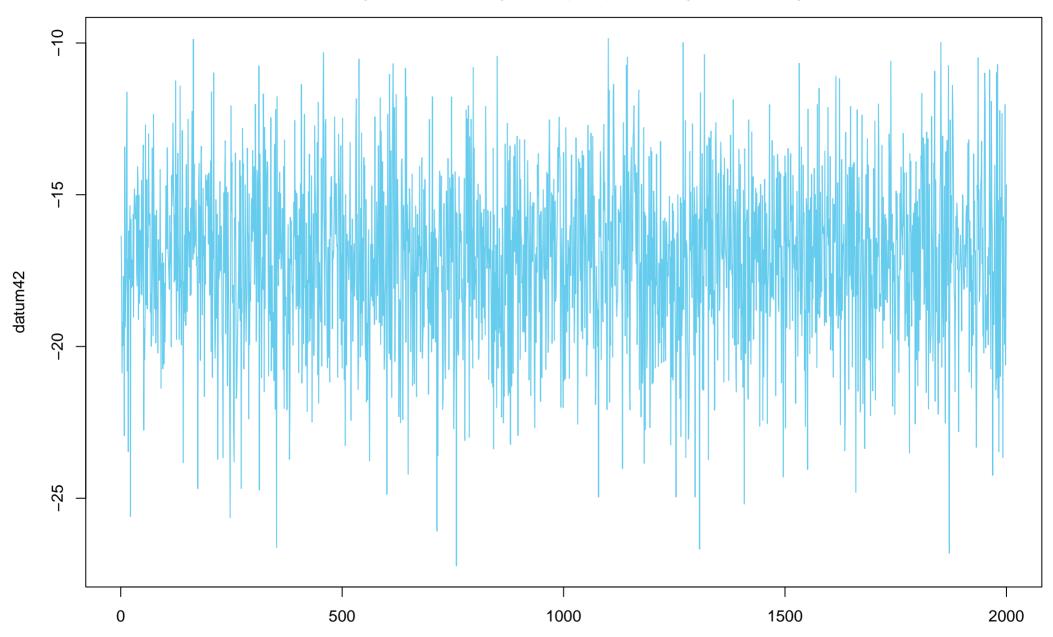
datum40 ESS = 2000 | BMK = 0.0301 | MCSE(6.27) = 0.162 | stat: TRUE | burn: 0



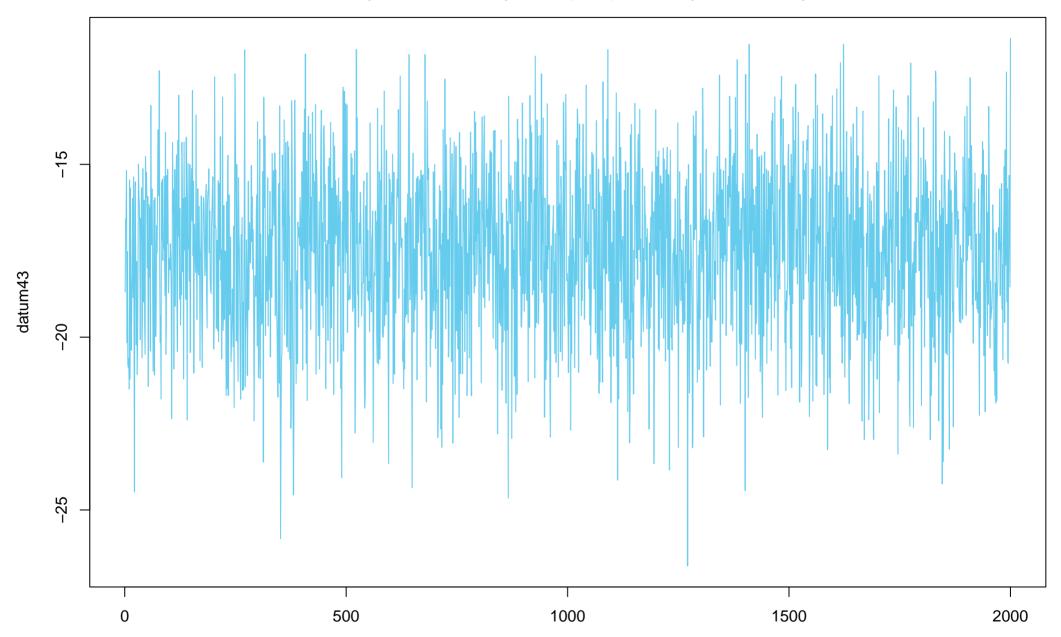
datum41 ESS = 2000 | BMK = 0.0334 | MCSE(6.27) = 0.171 | stat: FALSE | burn: 0



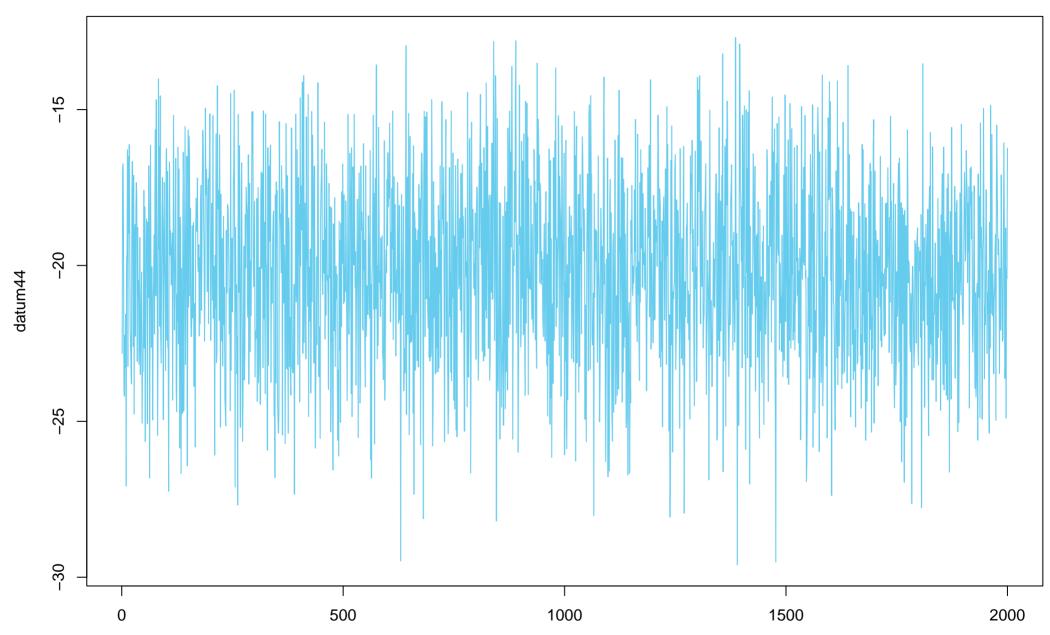
datum42 ESS = 2000 | BMK = 0.0248 | MCSE(6.27) = 0.157 | stat: TRUE | burn: 0



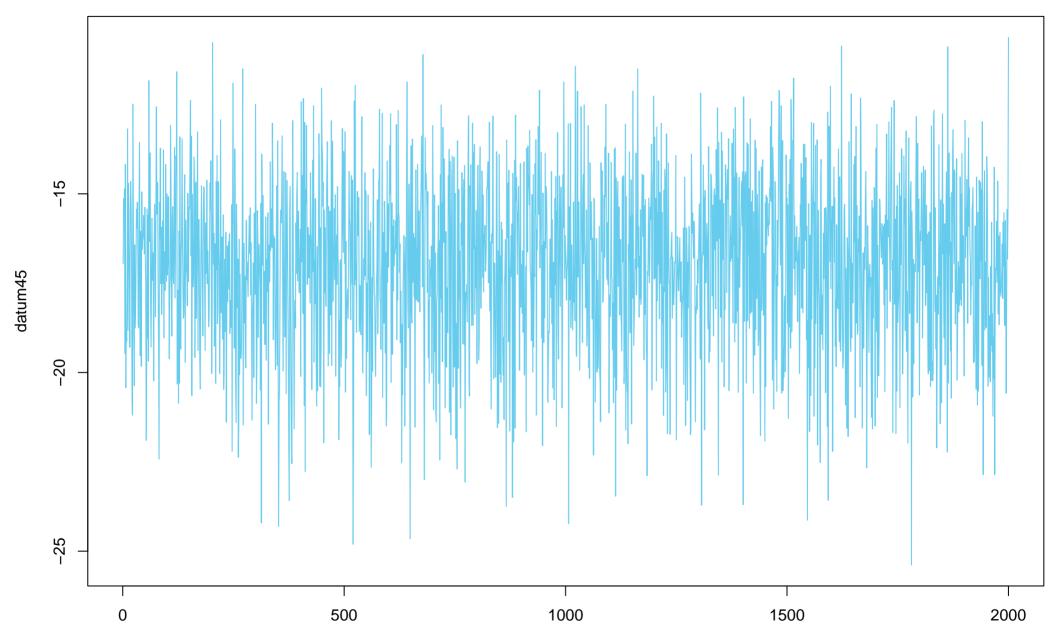
datum43 ESS = 2000 | BMK = 0.0402 | MCSE(6.27) = 0.183 | stat: TRUE | burn: 0



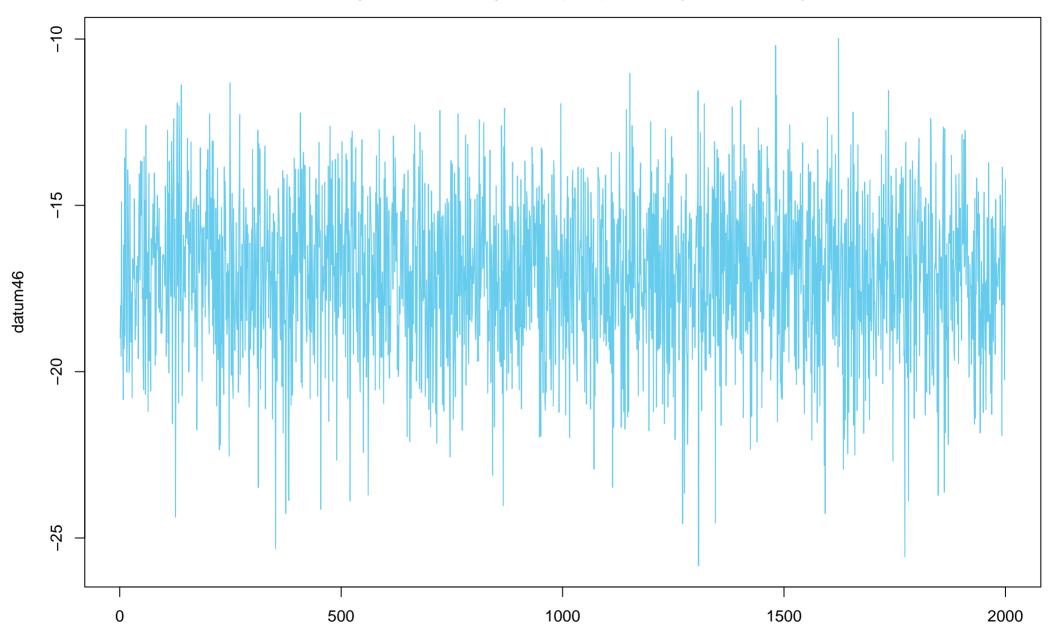
datum44 ESS = 2000 | BMK = 0.0413 | MCSE(6.27) = 0.148 | stat: TRUE | burn: 0



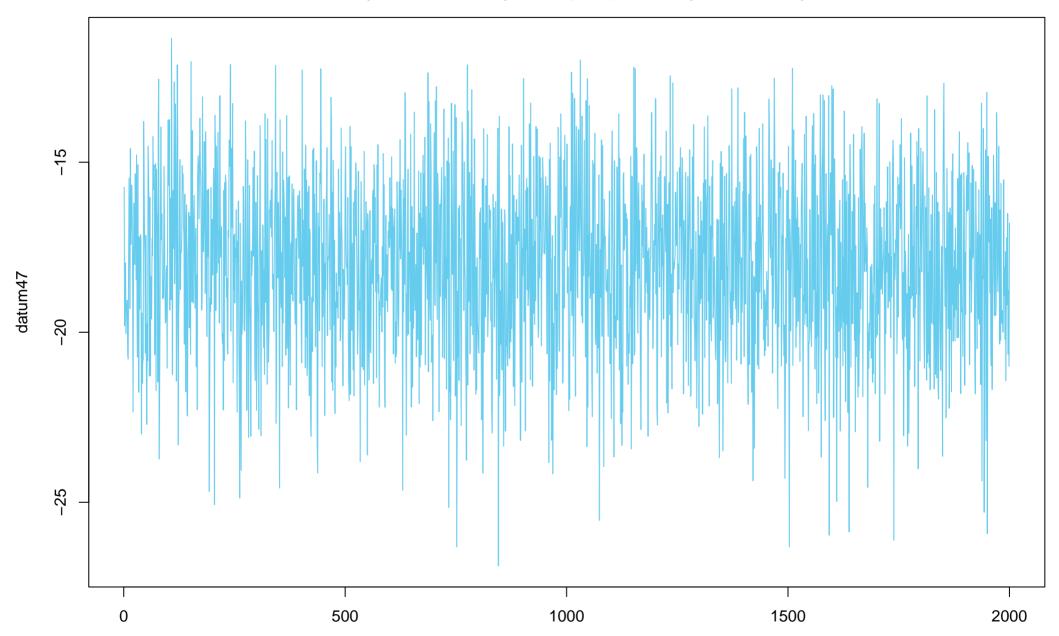
datum45 ESS = 2000 | BMK = 0.022 | MCSE(6.27) = 0.185 | stat: TRUE | burn: 0



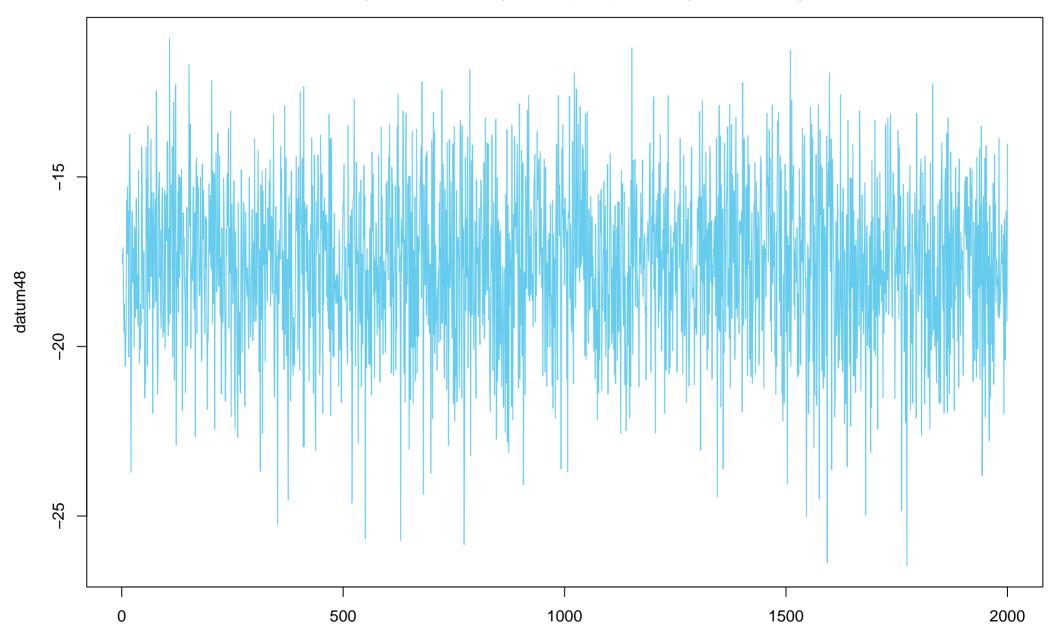
datum46 ESS = 2000 | BMK = 0.0359 | MCSE(6.27) = 0.185 | stat: FALSE | burn: 0



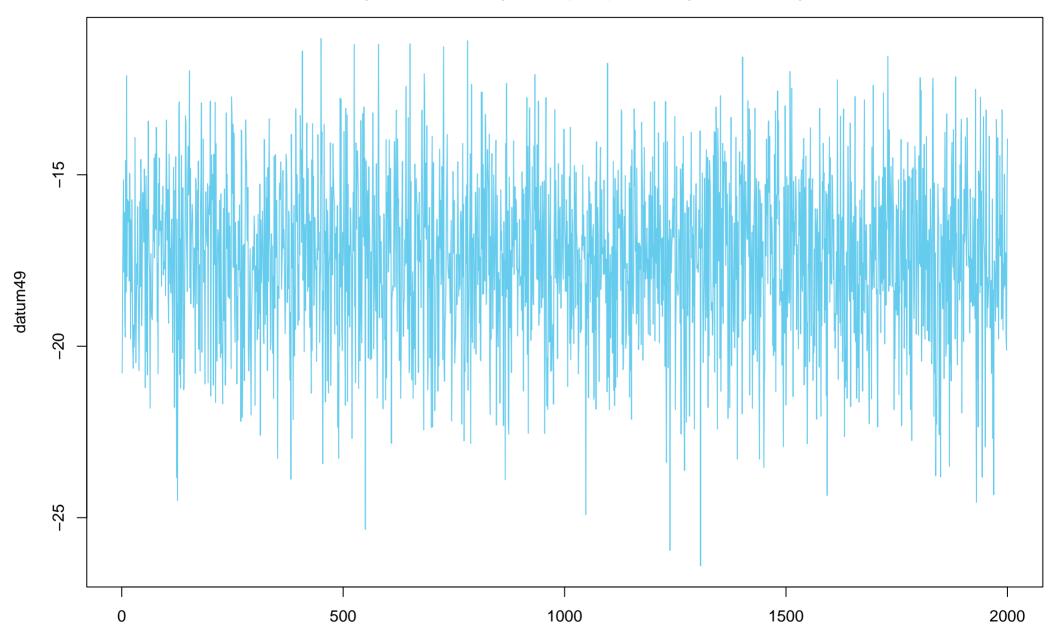
datum47 ESS = 2000 | BMK = 0.0345 | MCSE(6.27) = 0.171 | stat: TRUE | burn: 0



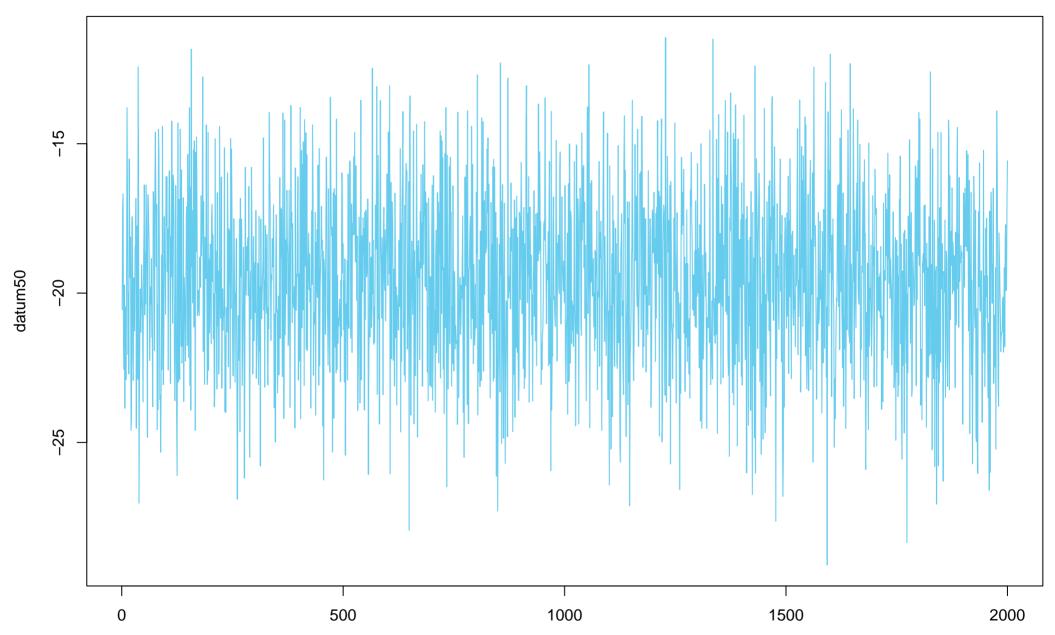
datum48 ESS = 2000 | BMK = 0.0305 | MCSE(6.27) = 0.181 | stat: TRUE | burn: 0



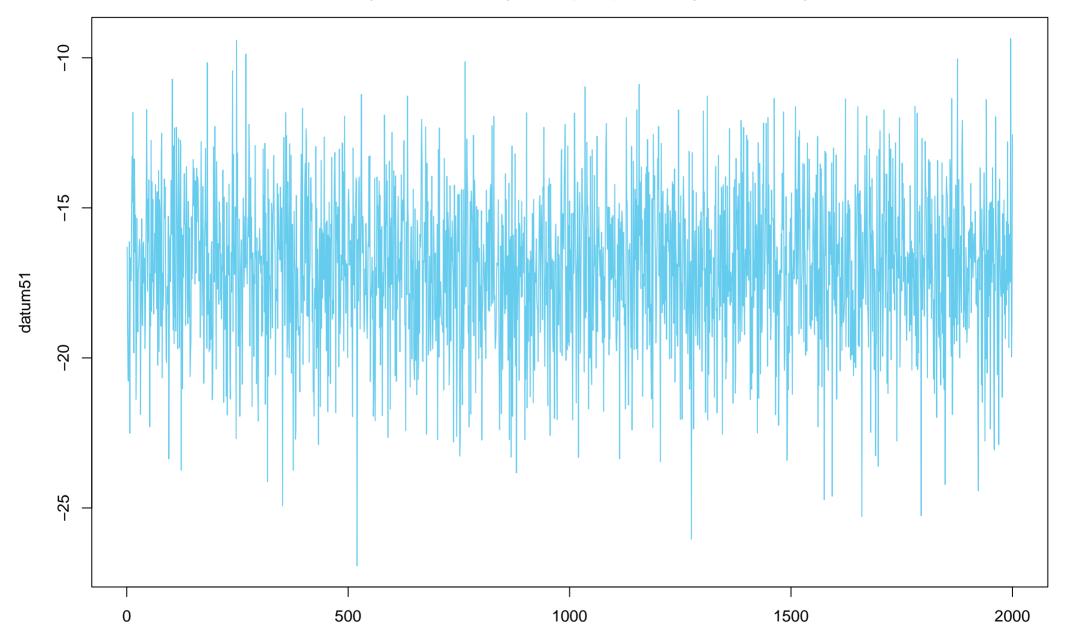
datum49 ESS = 2000 | BMK = 0.0324 | MCSE(6.27) = 0.181 | stat: TRUE | burn: 0



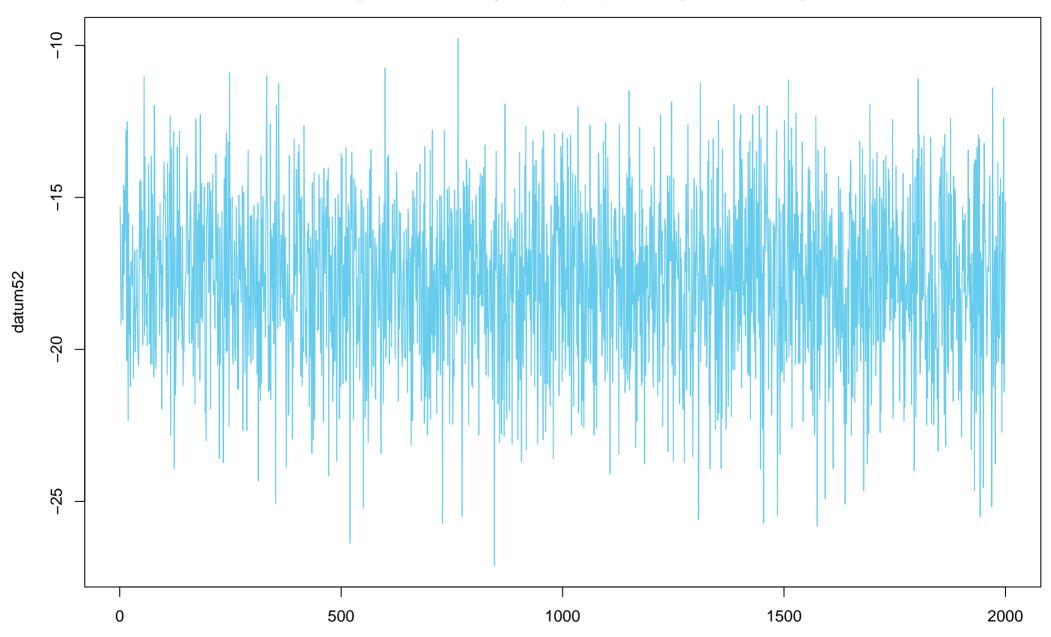
datum50 ESS = 2000 | BMK = 0.0318 | MCSE(6.27) = 0.152 | stat: TRUE | burn: 0



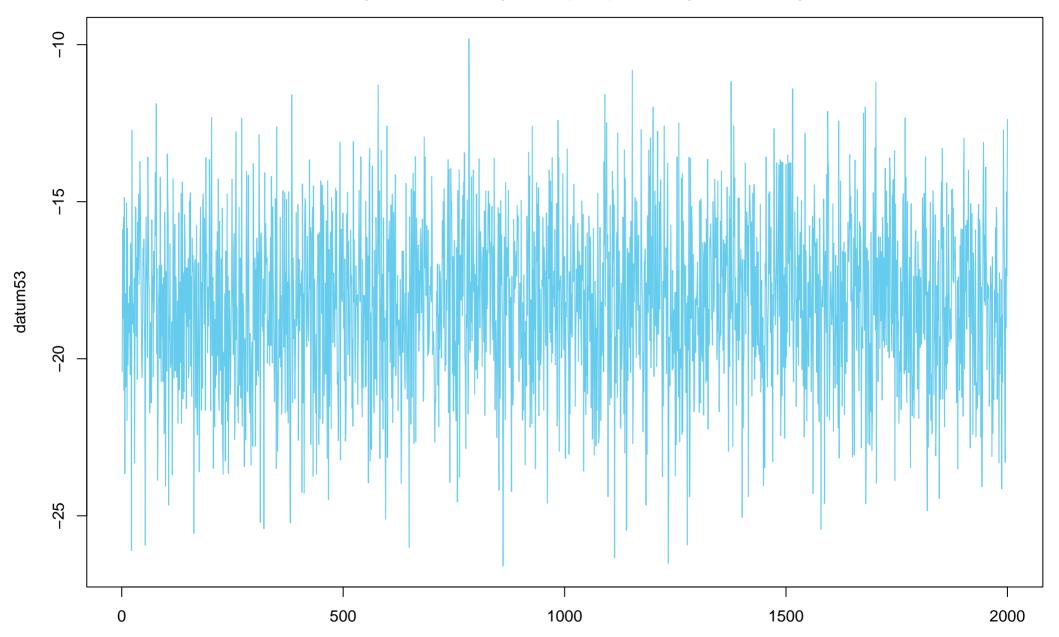
datum51 ESS = 2000 | BMK = 0.0374 | MCSE(6.27) = 0.172 | stat: TRUE | burn: 0



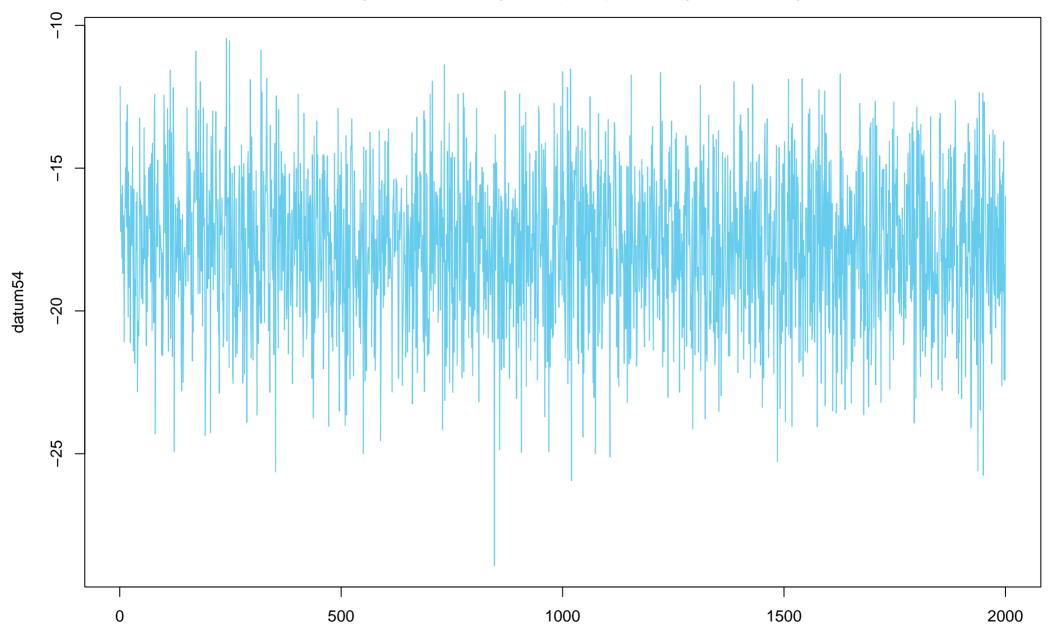
datum52 ESS = 2000 | BMK = 0.0395 | MCSE(6.27) = 0.163 | stat: FALSE | burn: 0



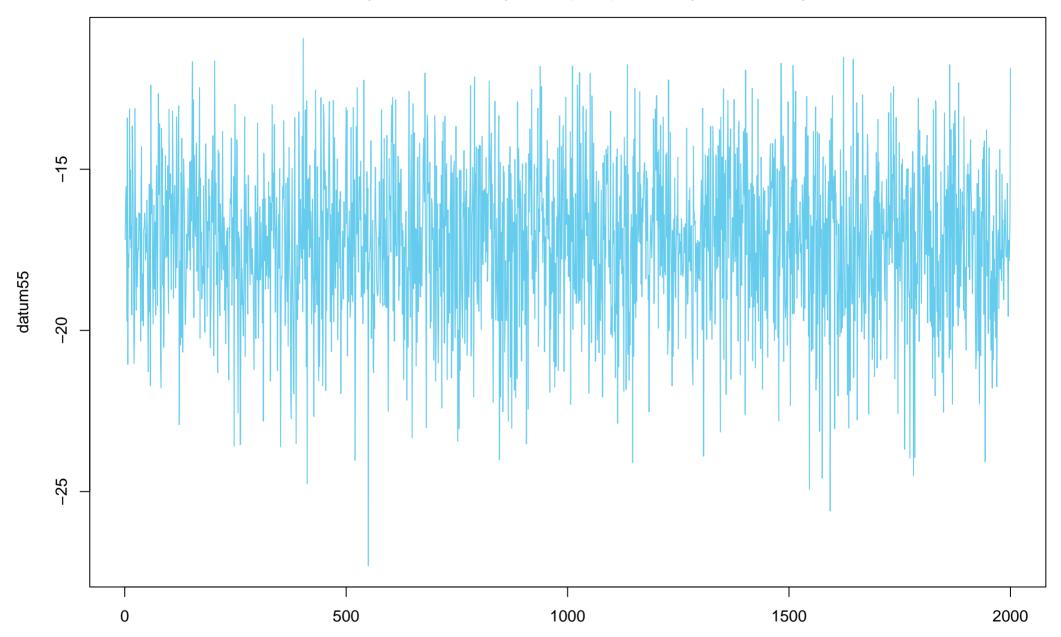
datum53 ESS = 2000 | BMK = 0.0339 | MCSE(6.27) = 0.162 | stat: TRUE | burn: 0



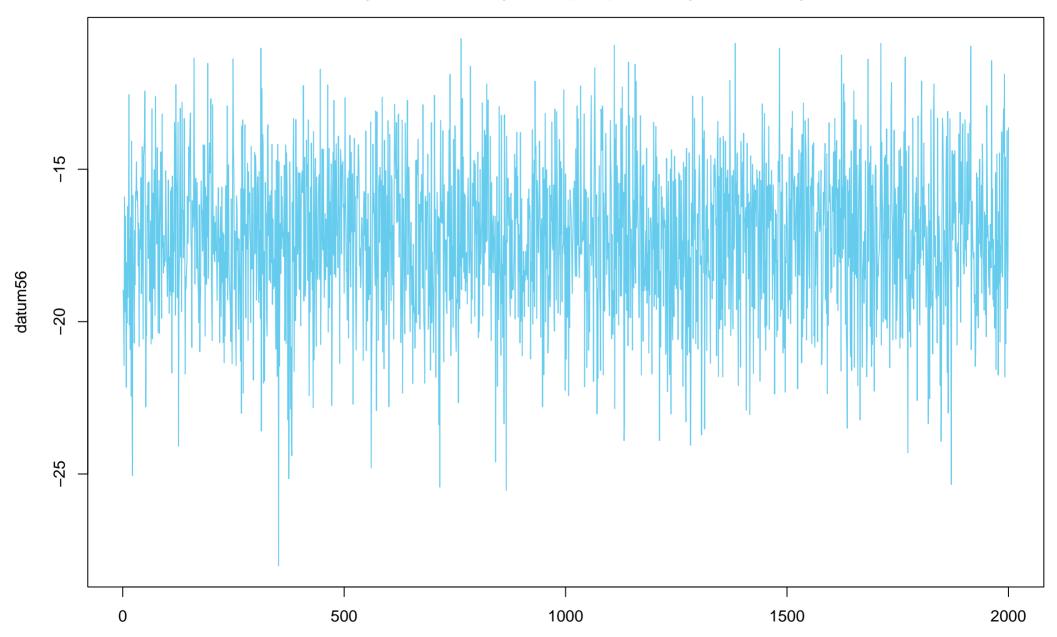
datum54 ESS = 2000 | BMK = 0.0494 | MCSE(6.27) = 0.163 | stat: TRUE | burn: 0



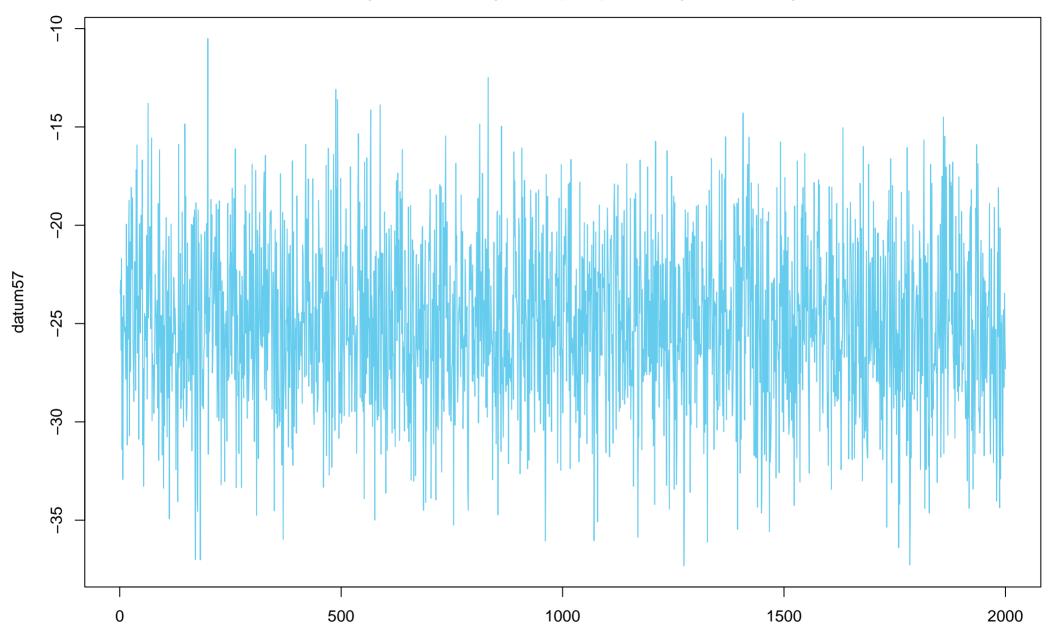
datum55 ESS = 1570 | BMK = 0.0338 | MCSE(6.27) = 0.183 | stat: TRUE | burn: 0



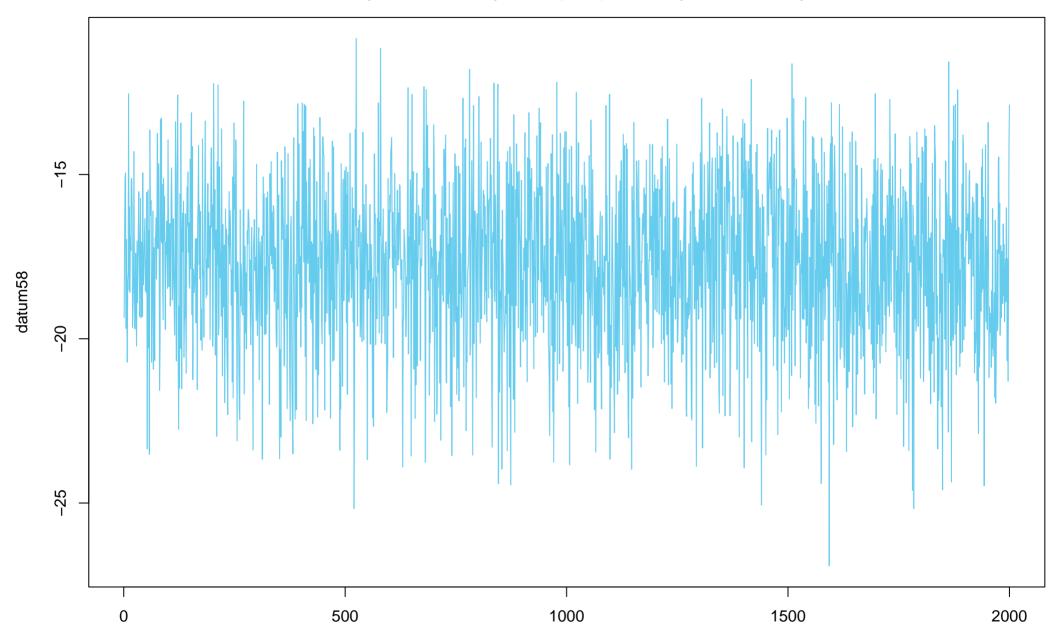
datum56 ESS = 2000 | BMK = 0.0462 | MCSE(6.27) = 0.173 | stat: TRUE | burn: 0



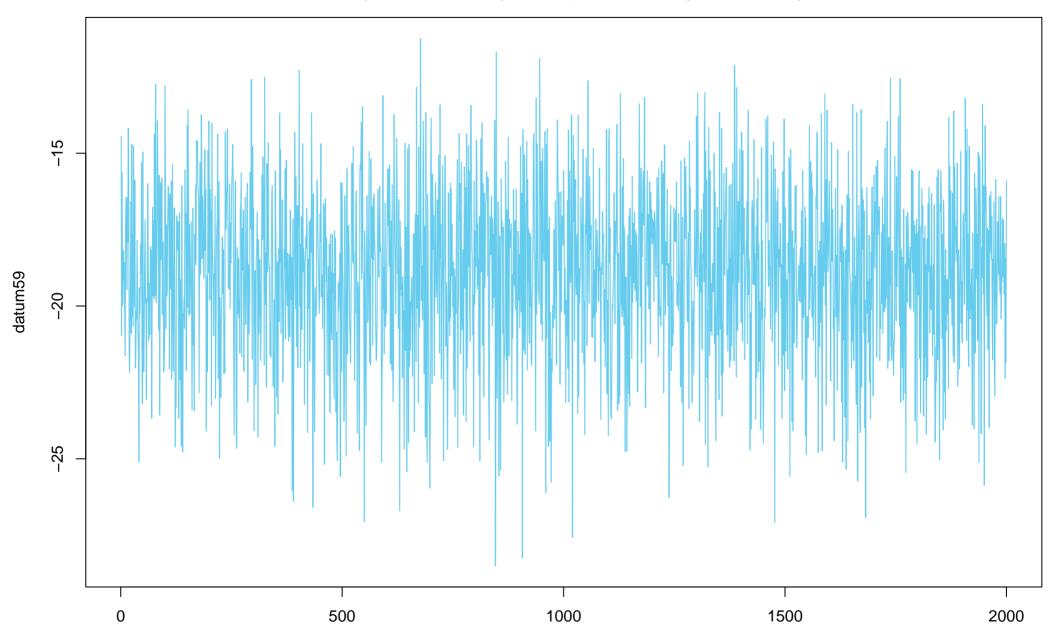
datum57 ESS = 2000 | BMK = 0.043 | MCSE(6.27) = 0.103 | stat: TRUE | burn: 0



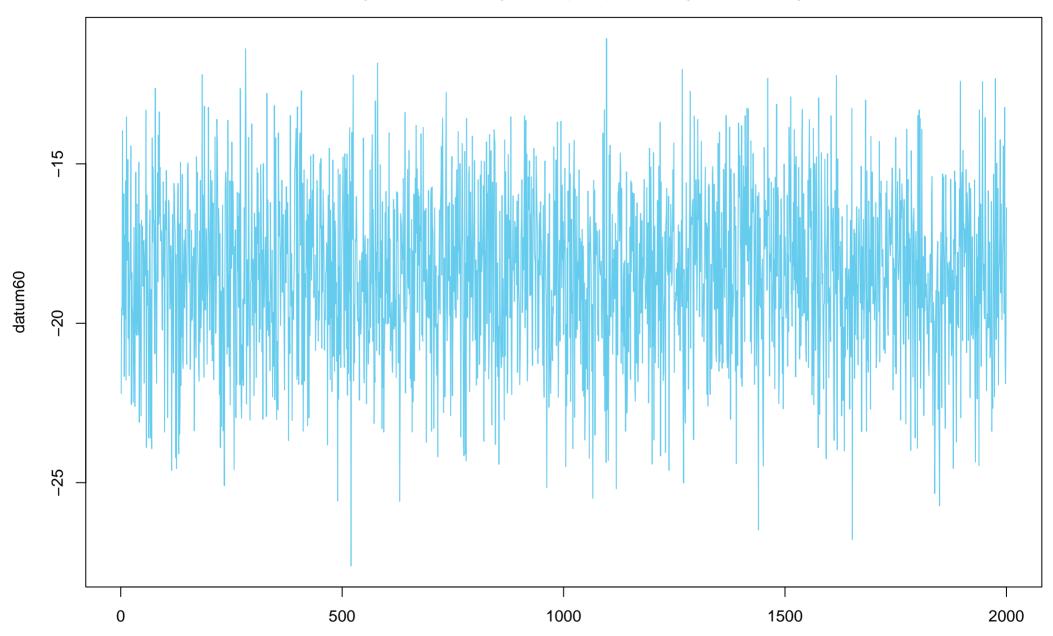
datum58 ESS = 2000 | BMK = 0.054 | MCSE(6.27) = 0.177 | stat: FALSE | burn: 0



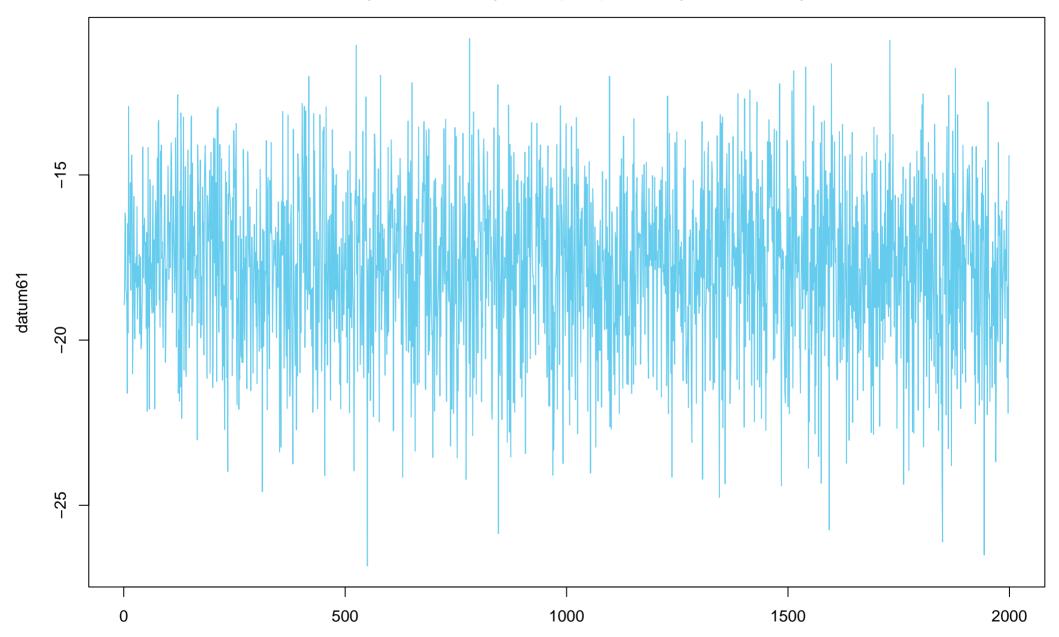
datum59 ESS = 2000 | BMK = 0.0337 | MCSE(6.27) = 0.159 | stat: TRUE | burn: 0



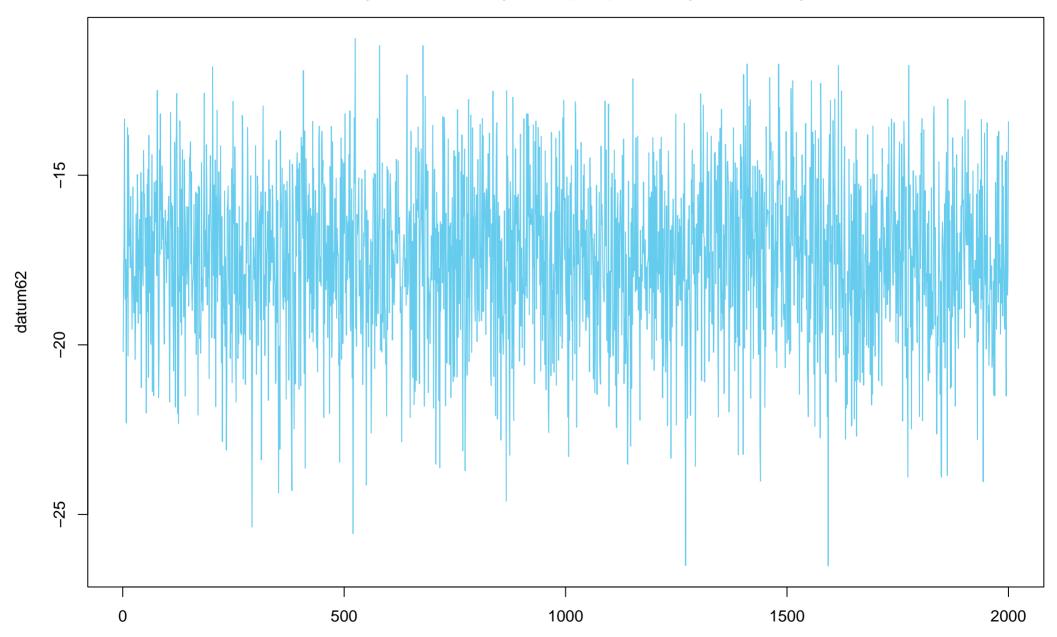
datum60 ESS = 2000 | BMK = 0.0364 | MCSE(6.27) = 0.167 | stat: TRUE | burn: 0



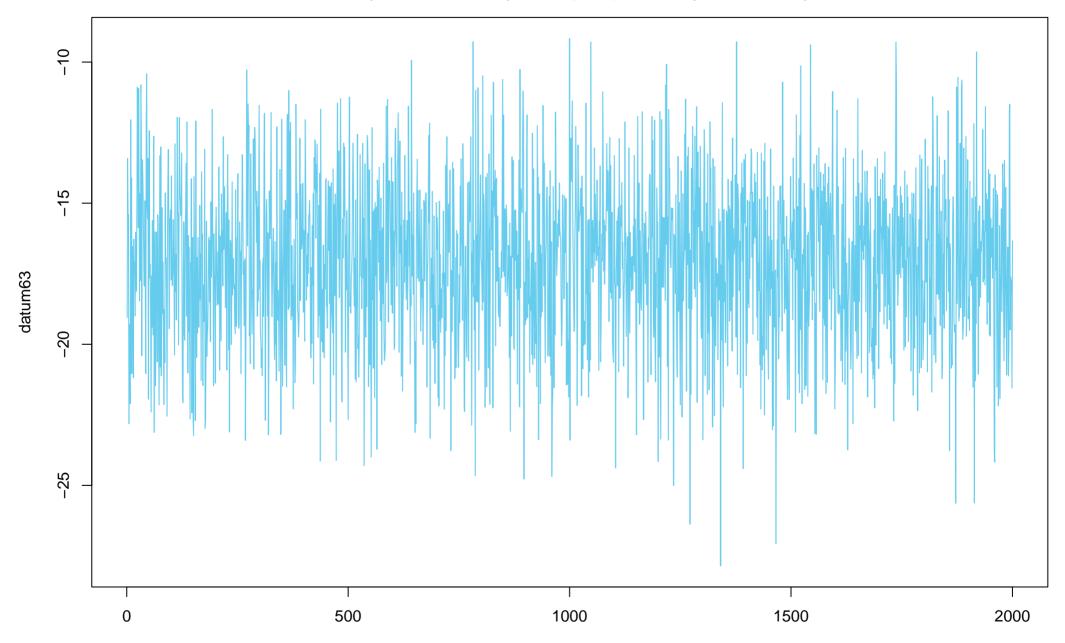
datum61 ESS = 1870 | BMK = 0.031 | MCSE(6.27) = 0.175 | stat: FALSE | burn: 0



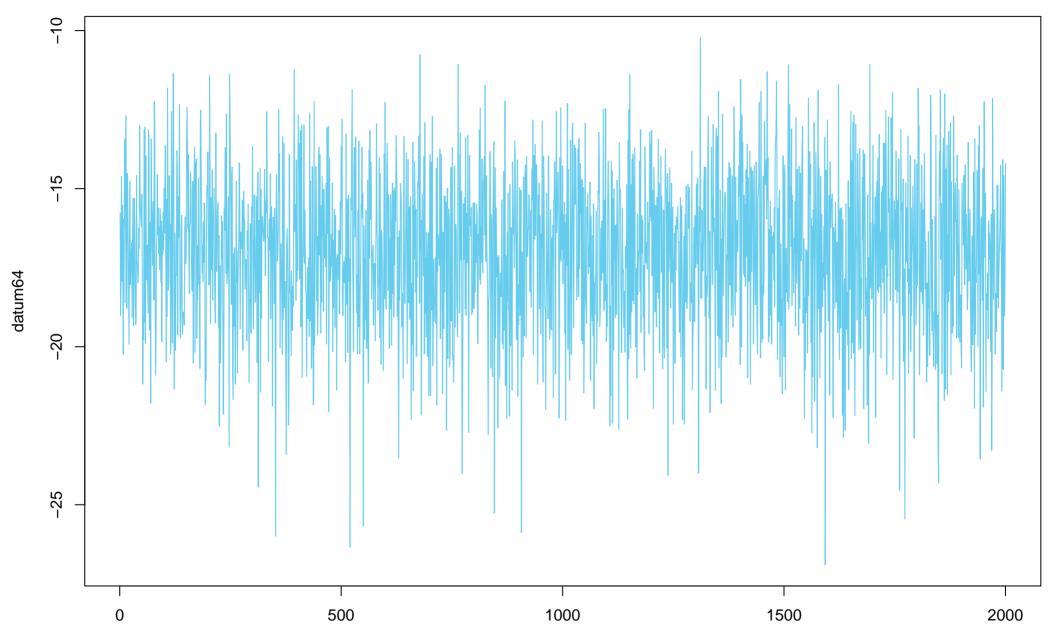
datum62 ESS = 2000 | BMK = 0.0367 | MCSE(6.27) = 0.182 | stat: TRUE | burn: 0



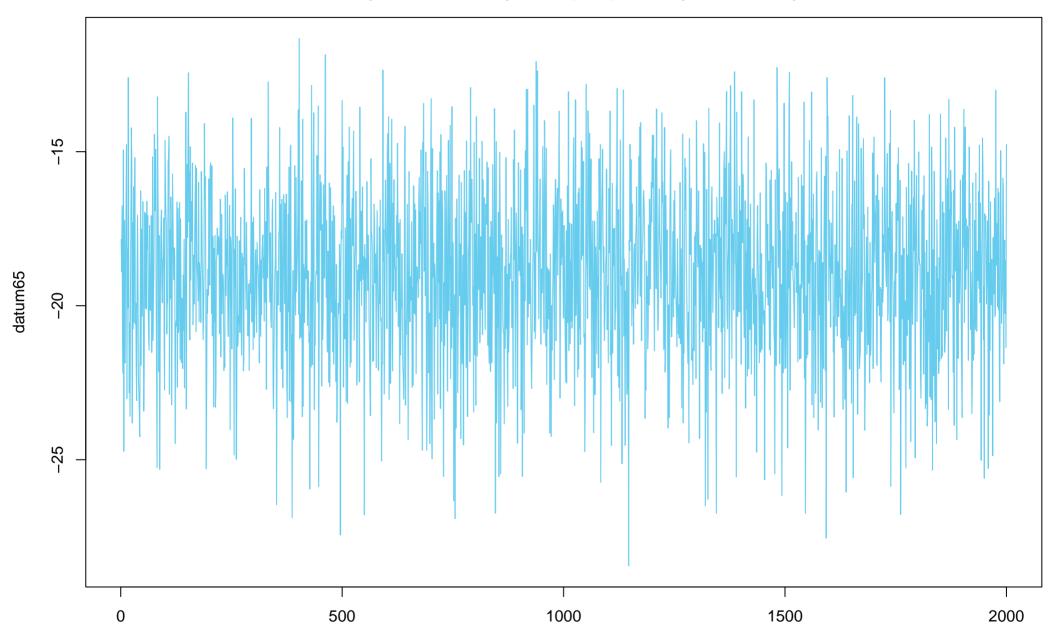
datum63 ESS = 2000 | BMK = 0.0515 | MCSE(6.27) = 0.153 | stat: TRUE | burn: 0



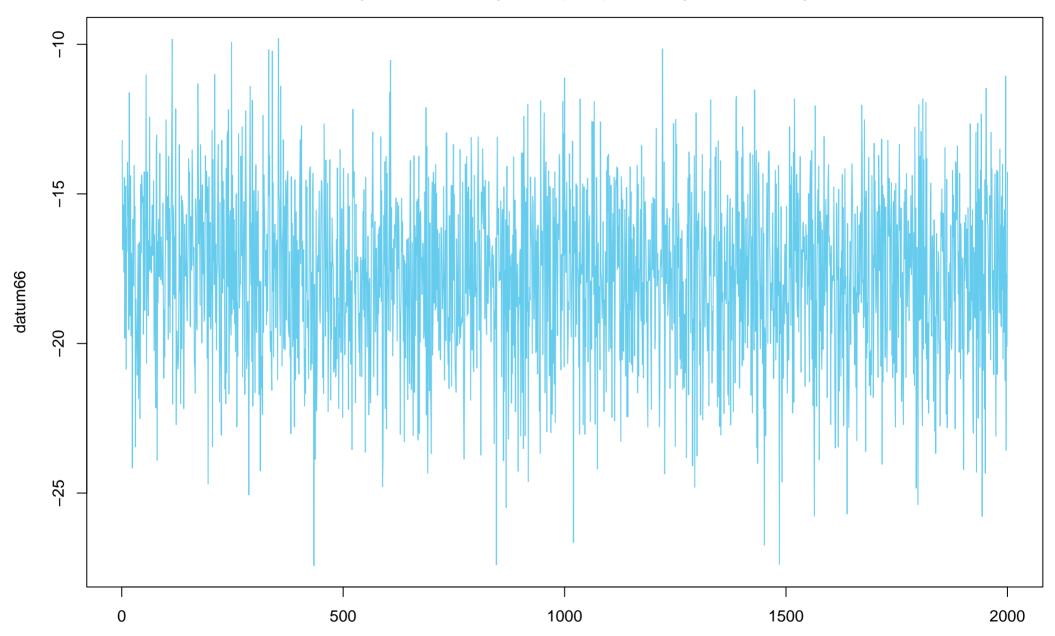
datum64 ESS = 2000 | BMK = 0.0371 | MCSE(6.27) = 0.176 | stat: TRUE | burn: 0



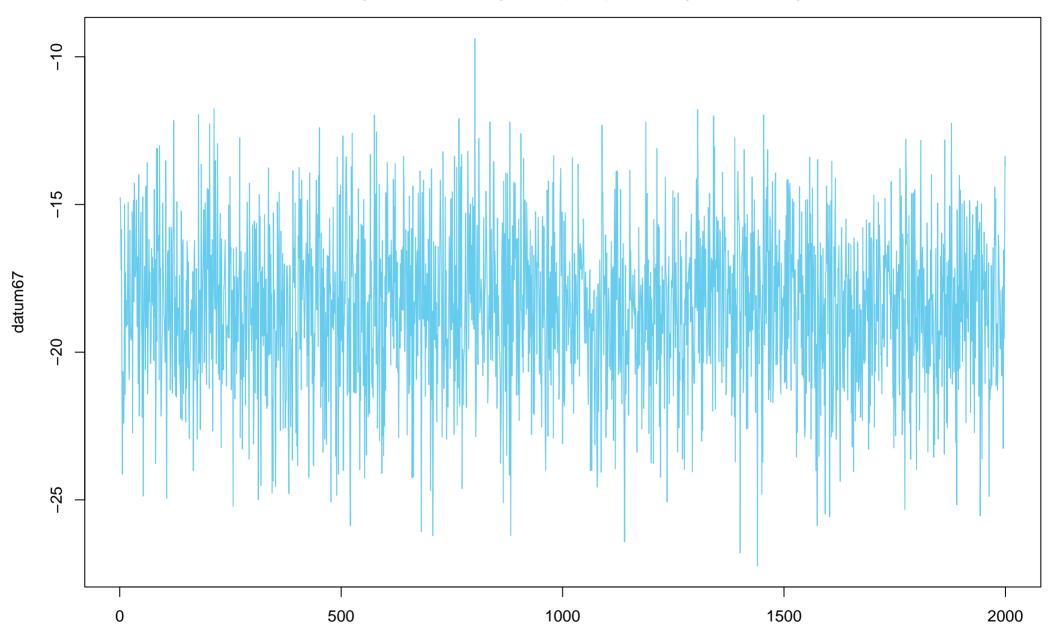
datum65 ESS = 1990 | BMK = 0.0261 | MCSE(6.27) = 0.16 | stat: TRUE | burn: 0



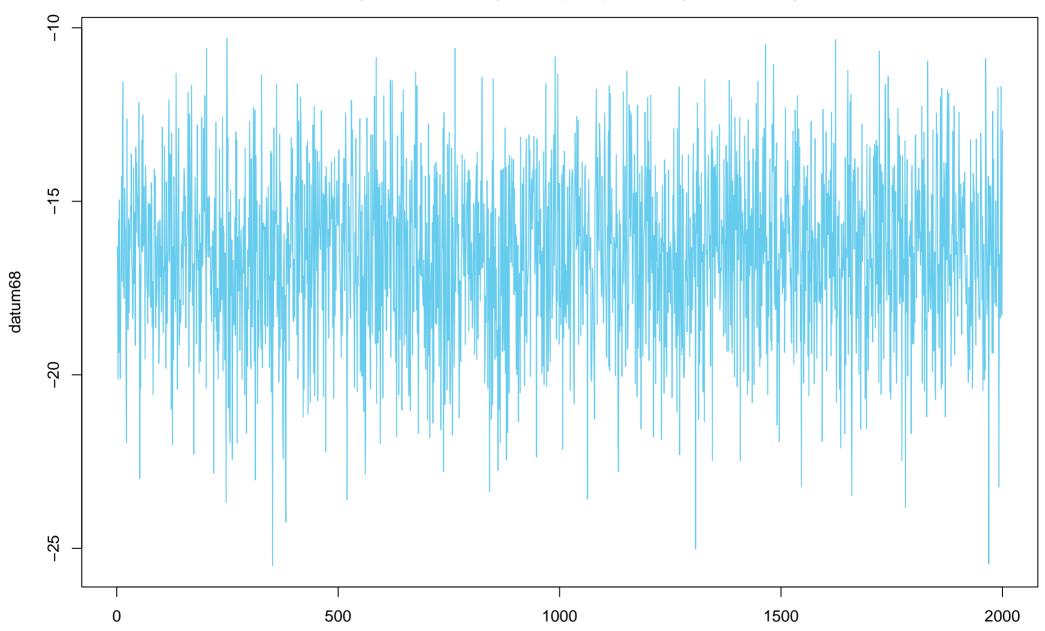
datum66 ESS = 2000 | BMK = 0.0367 | MCSE(6.27) = 0.155 | stat: FALSE | burn: 0



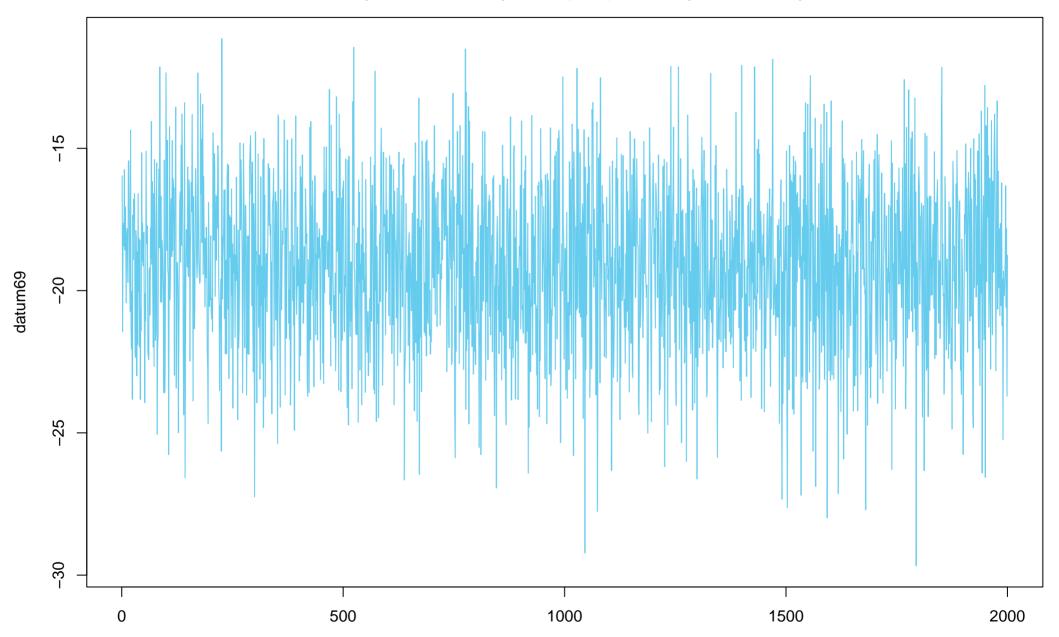
datum67 ESS = 2000 | BMK = 0.0488 | MCSE(6.27) = 0.164 | stat: TRUE | burn: 0



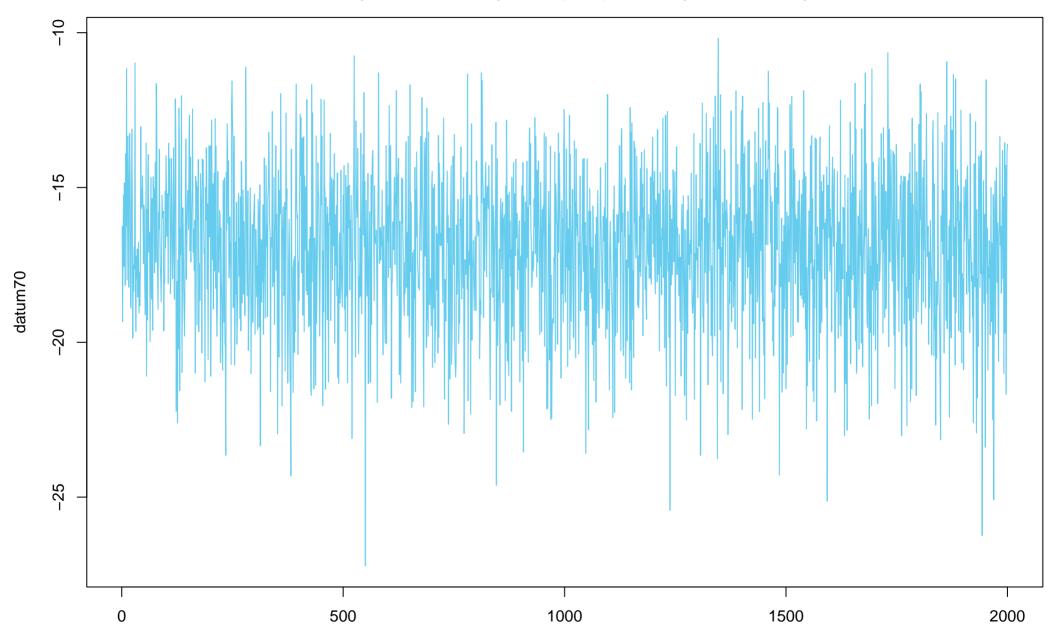
datum68 ESS = 2000 | BMK = 0.0477 | MCSE(6.27) = 0.179 | stat: TRUE | burn: 0



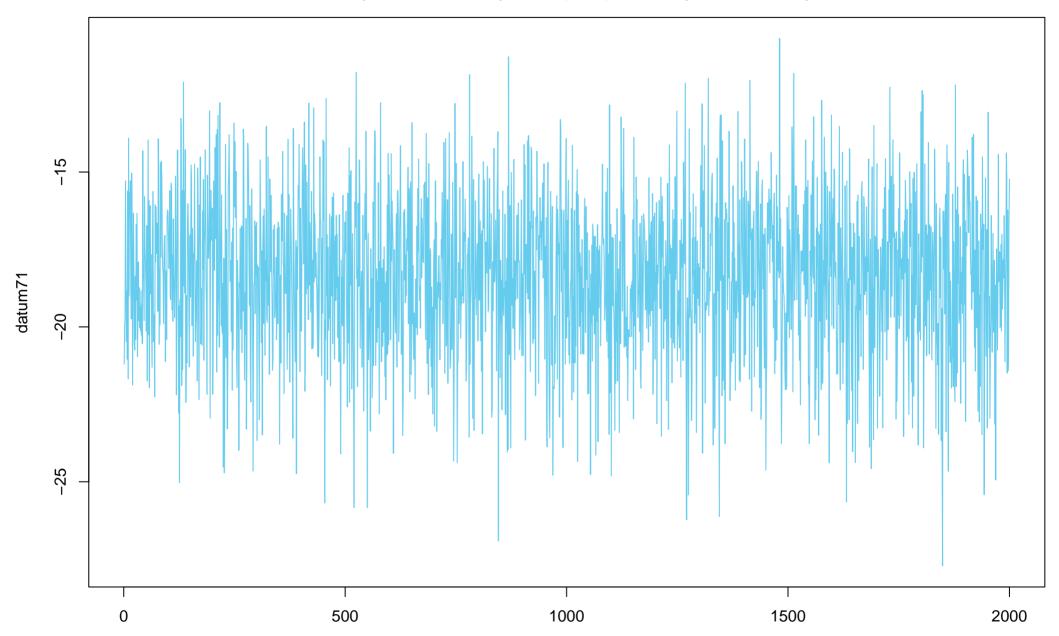
datum69 ESS = 2000 | BMK = 0.0507 | MCSE(6.27) = 0.151 | stat: TRUE | burn: 0



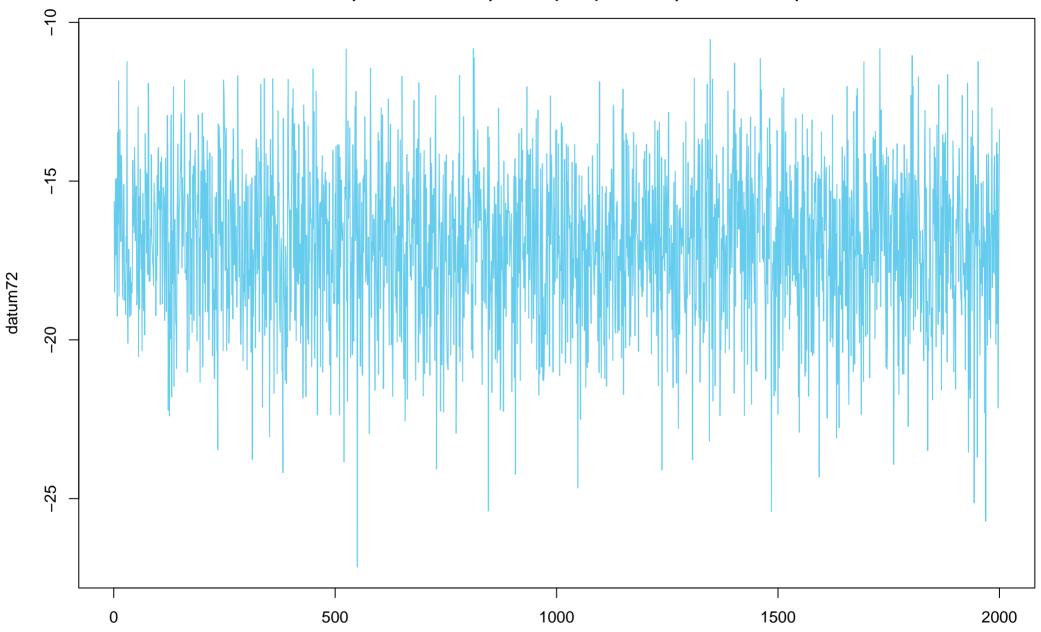
datum70 ESS = 2000 | BMK = 0.0434 | MCSE(6.27) = 0.177 | stat: FALSE | burn: 0



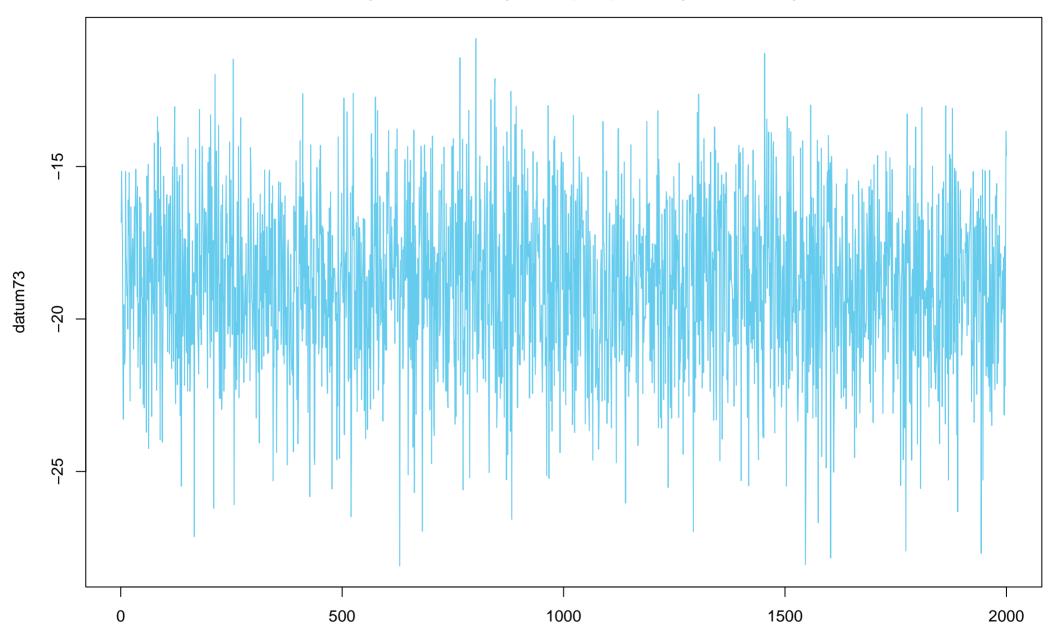
datum71 ESS = 2000 | BMK = 0.0441 | MCSE(6.27) = 0.171 | stat: FALSE | burn: 0



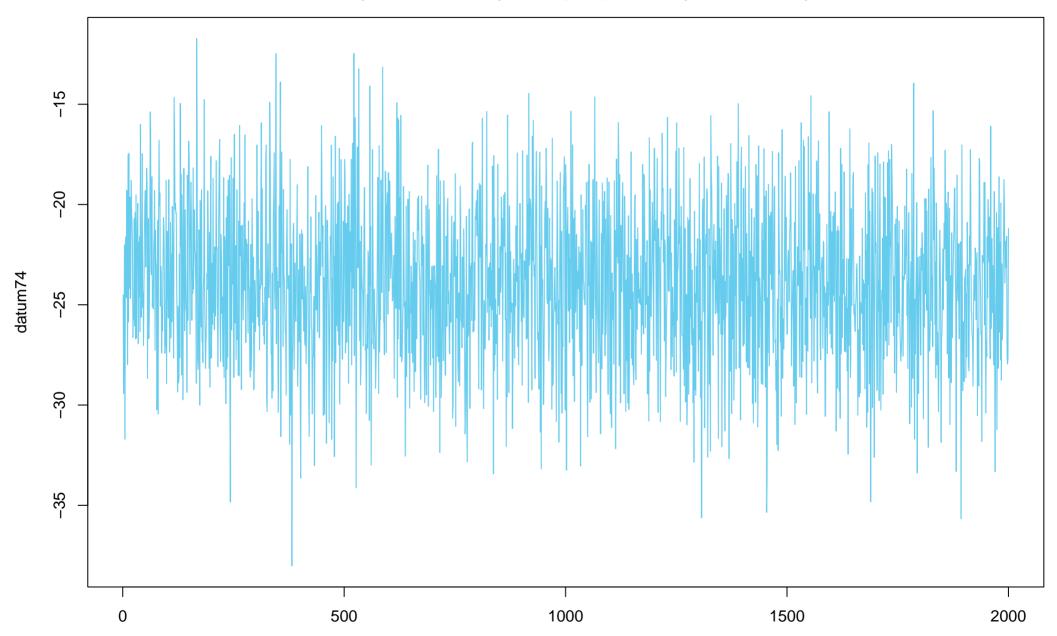
datum72 ESS = 2000 | BMK = 0.0308 | MCSE(6.27) = 0.176 | stat: FALSE | burn: 0



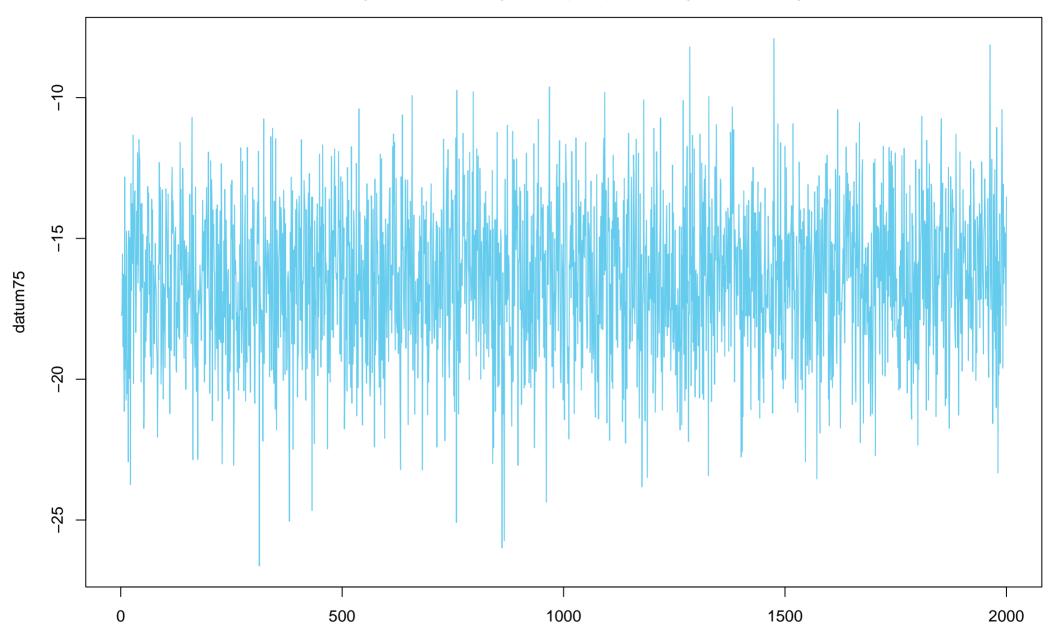
datum73 ESS = 2000 | BMK = 0.0463 | MCSE(6.27) = 0.16 | stat: TRUE | burn: 0



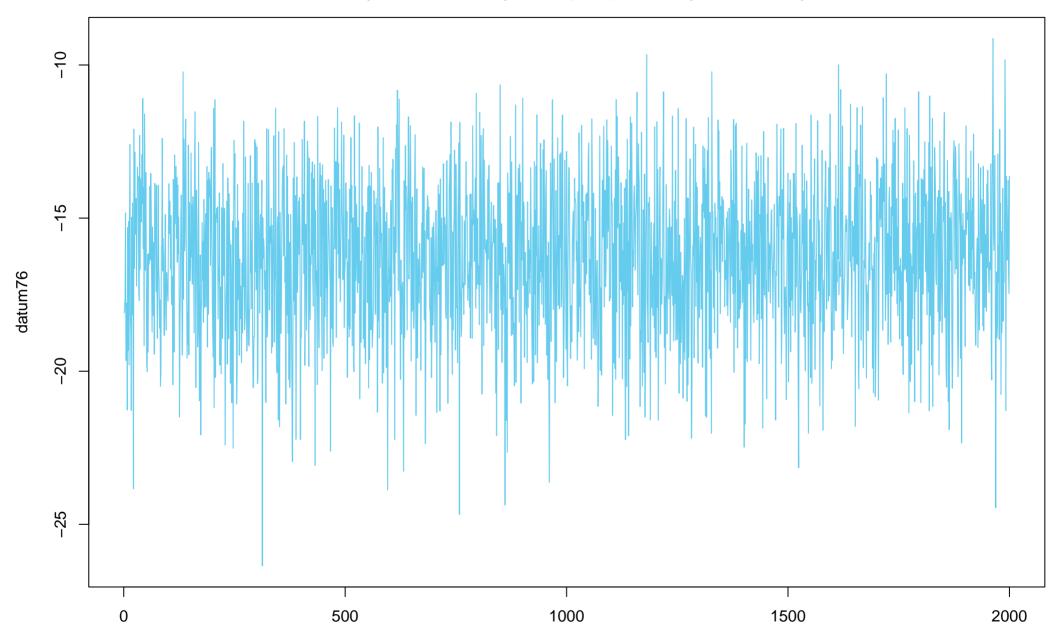
datum74 ESS = 2000 | BMK = 0.0494 | MCSE(6.27) = 0.112 | stat: FALSE | burn: 0



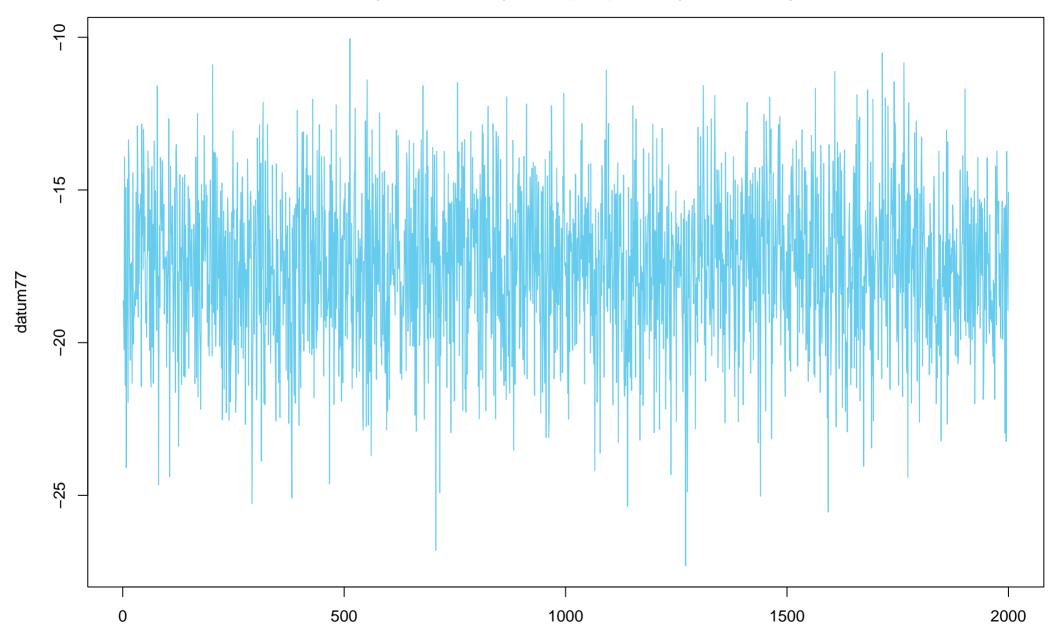
datum75 ESS = 2000 | BMK = 0.0574 | MCSE(6.27) = 0.161 | stat: TRUE | burn: 0



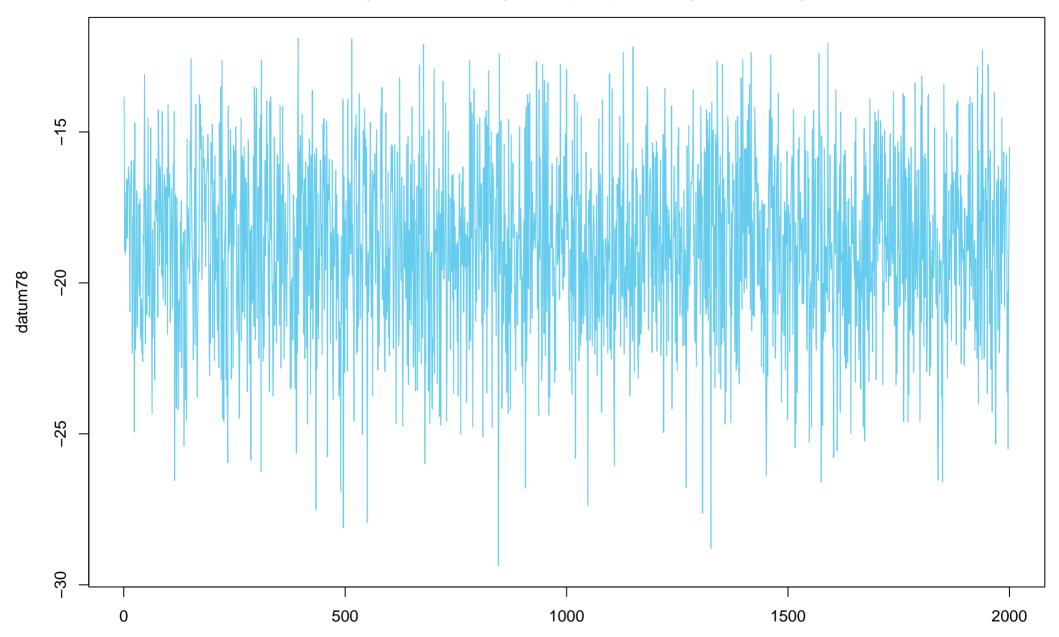
datum76 ESS = 2000 | BMK = 0.0506 | MCSE(6.27) = 0.175 | stat: TRUE | burn: 0



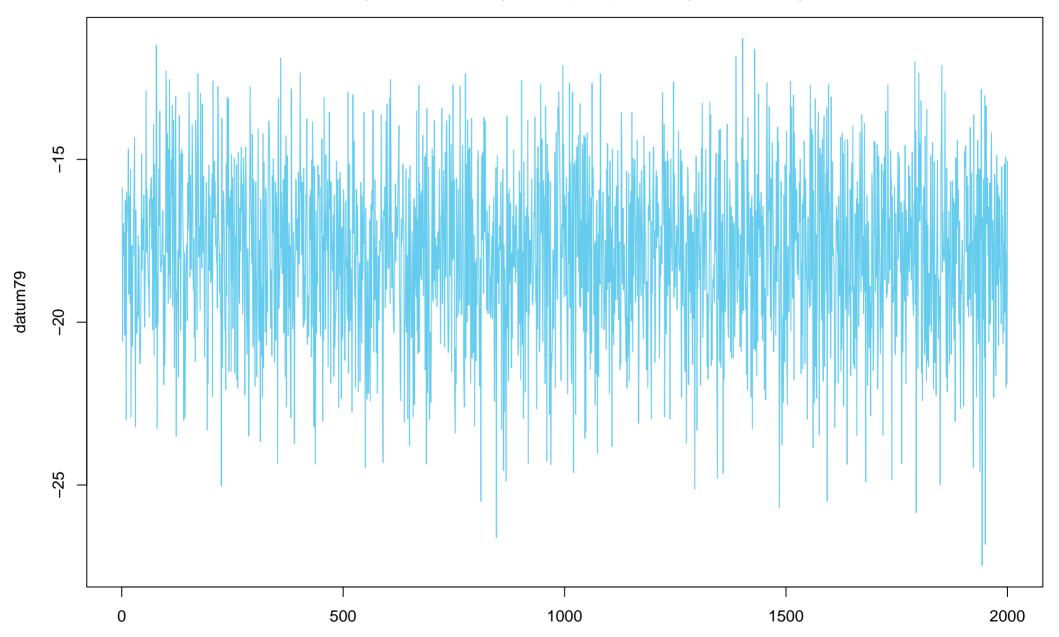
datum77 ESS = 2000 | BMK = 0.035 | MCSE(6.27) = 0.17 | stat: TRUE | burn: 0



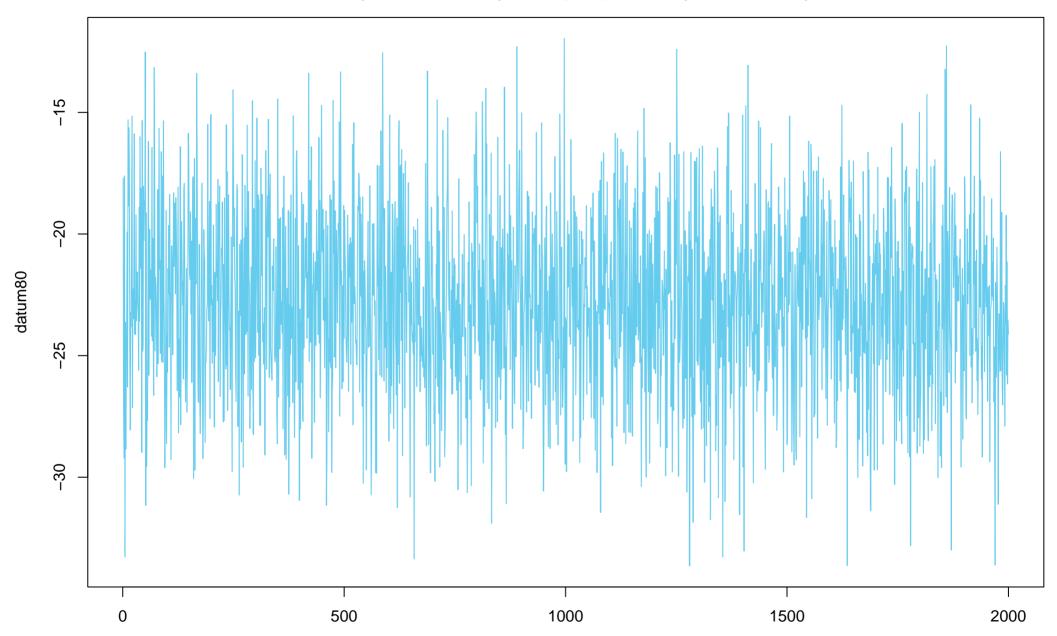
datum78 ESS = 1860 | BMK = 0.0359 | MCSE(6.27) = 0.152 | stat: TRUE | burn: 0



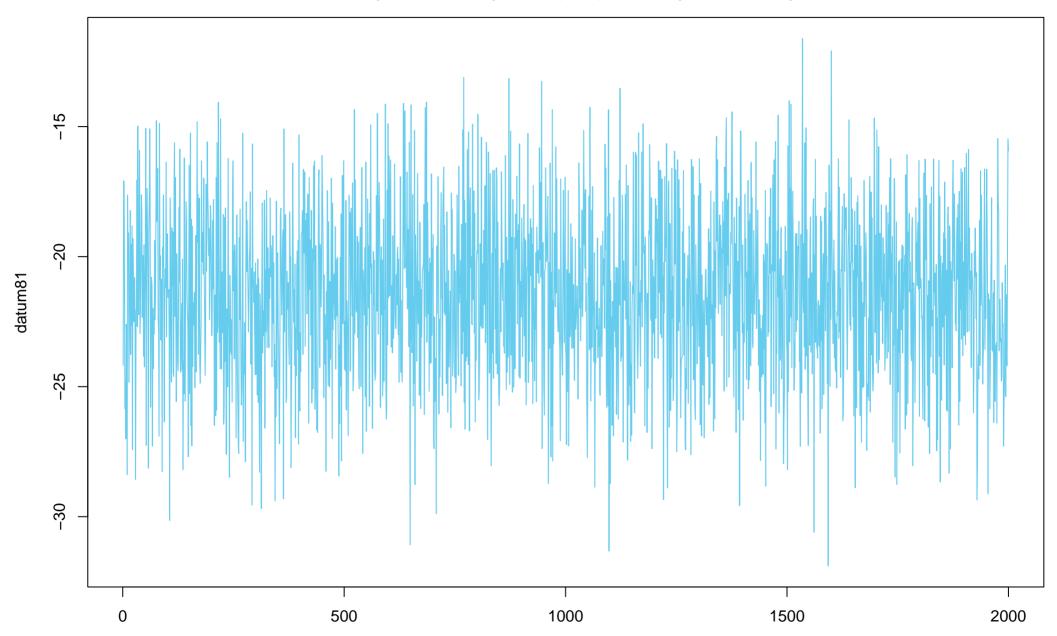
datum79 ESS = 2000 | BMK = 0.0457 | MCSE(6.27) = 0.167 | stat: TRUE | burn: 0



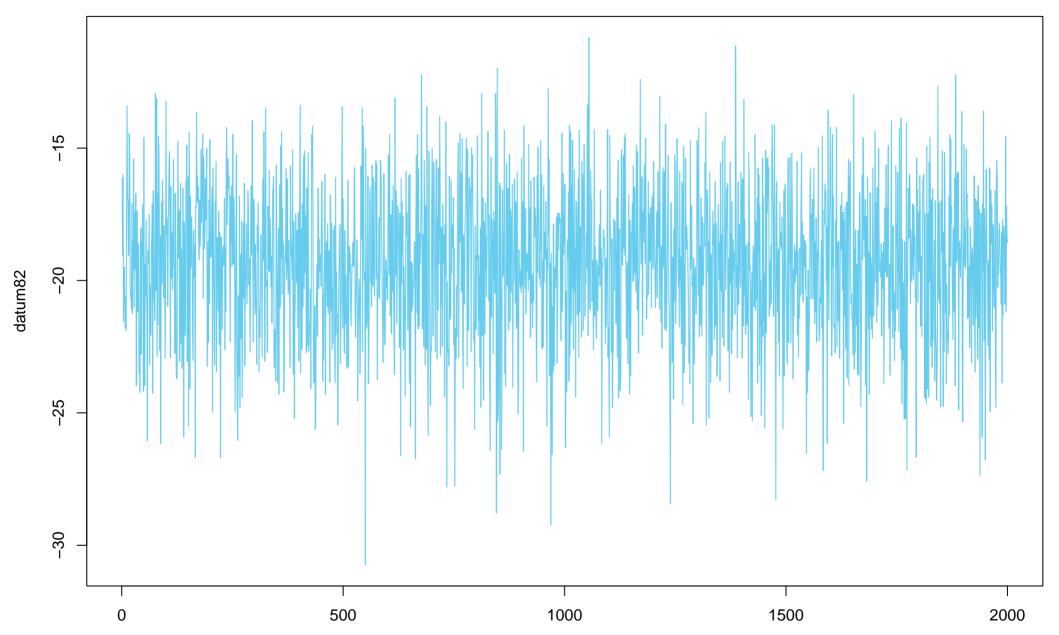
datum80 ESS = 2000 | BMK = 0.0553 | MCSE(6.27) = 0.118 | stat: FALSE | burn: 0



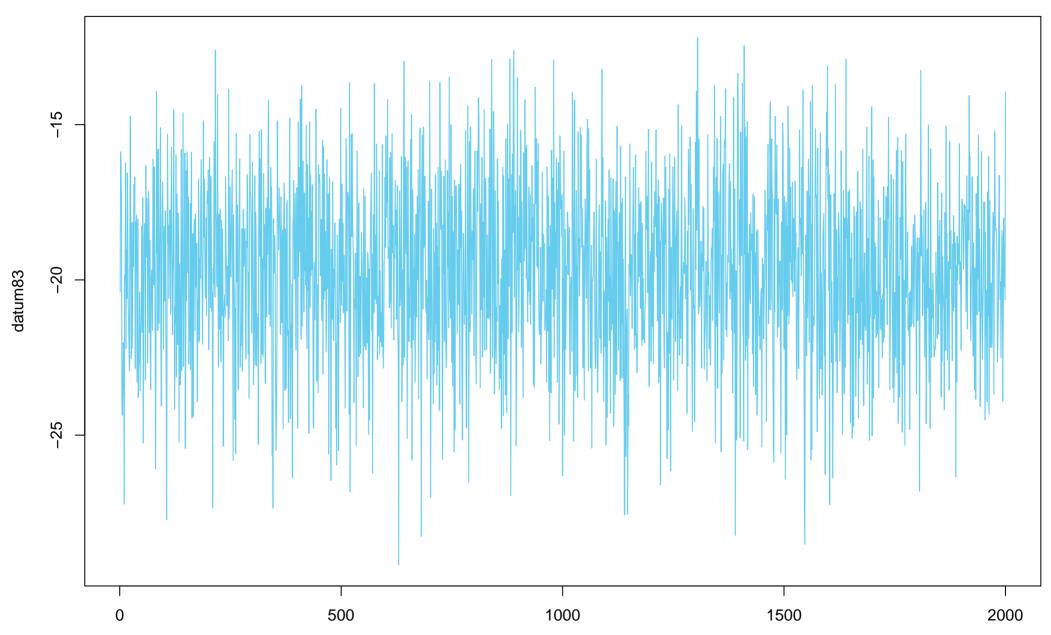
datum81 ESS = 2000 | BMK = 0.03 | MCSE(6.27) = 0.137 | stat: TRUE | burn: 0



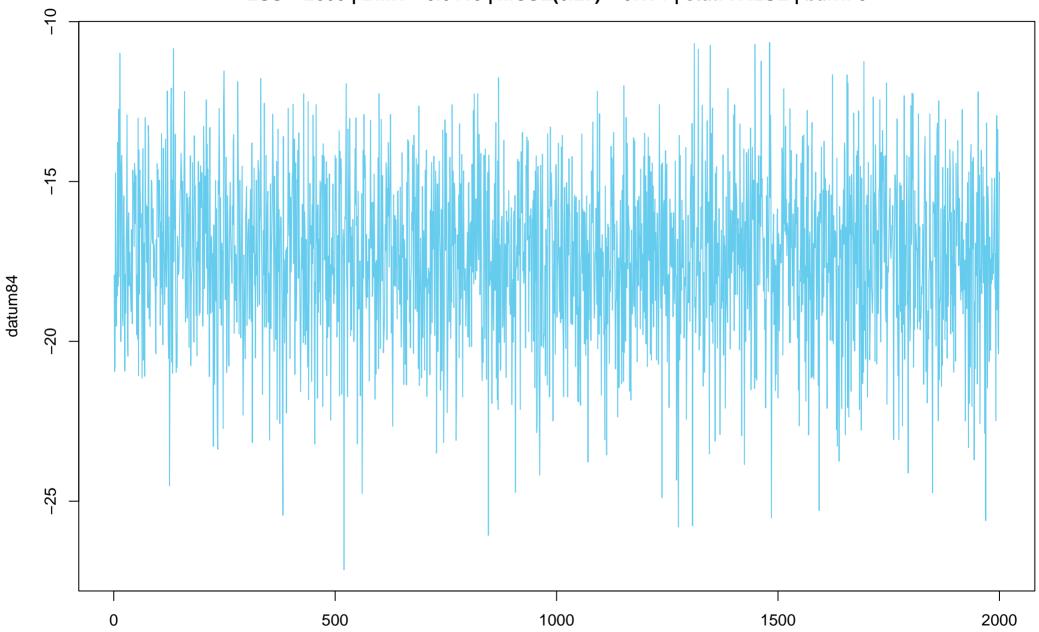
datum82 ESS = 2000 | BMK = 0.0378 | MCSE(6.27) = 0.153 | stat: TRUE | burn: 0



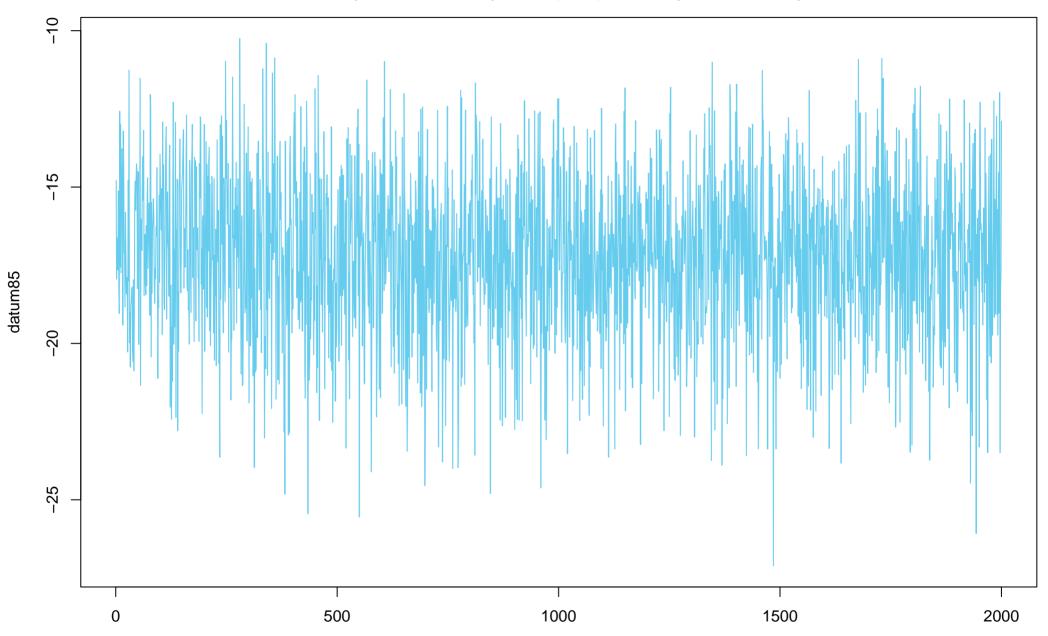
datum83 ESS = 2000 | BMK = 0.0395 | MCSE(6.27) = 0.156 | stat: TRUE | burn: 0



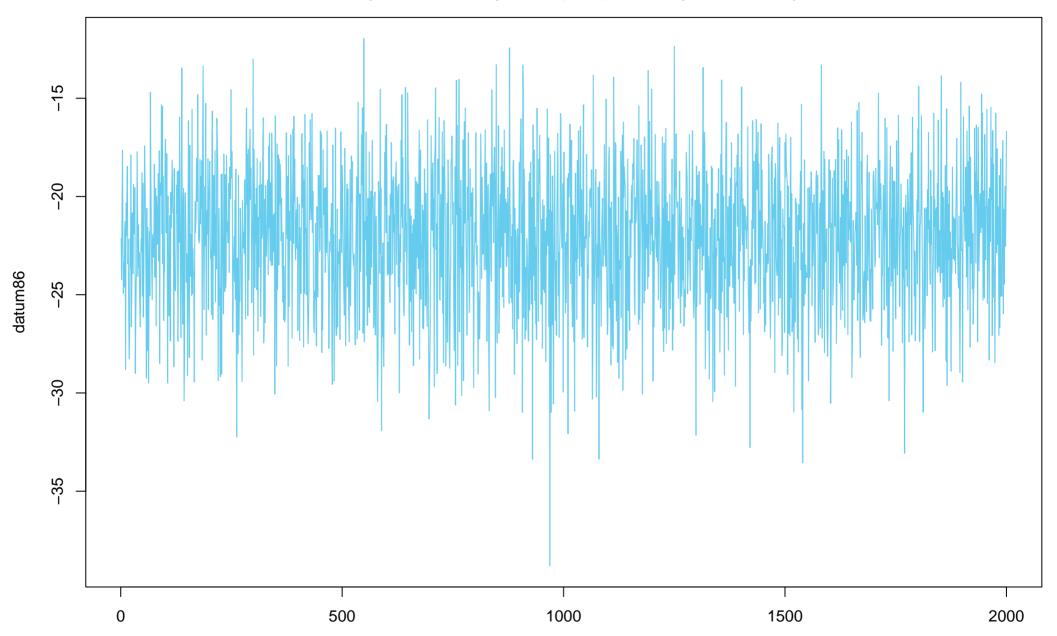
datum84 ESS = 2000 | BMK = 0.0418 | MCSE(6.27) = 0.171 | stat: FALSE | burn: 0



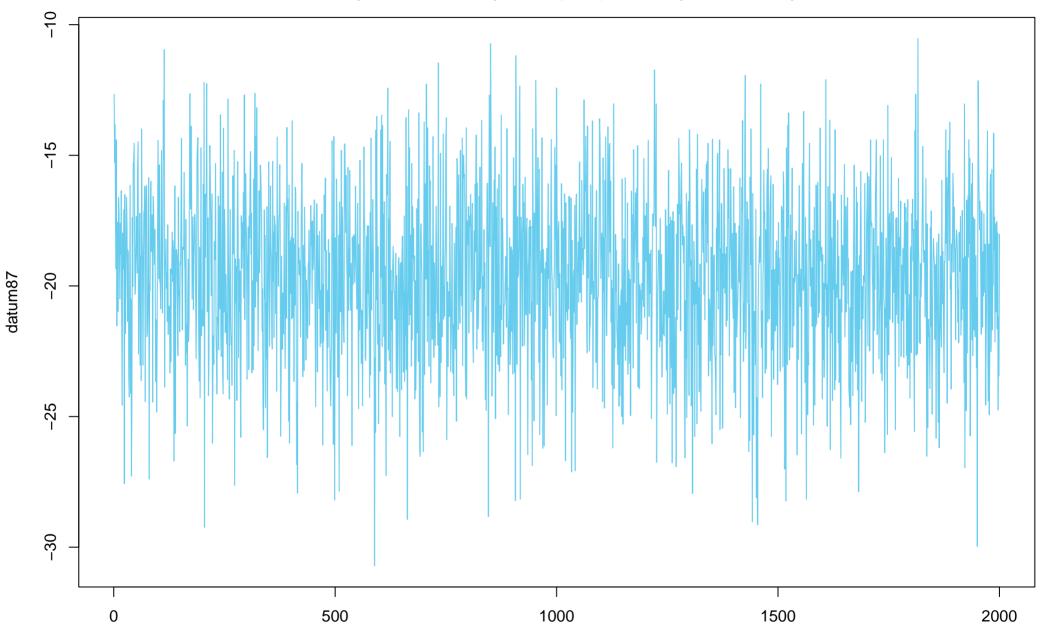
datum85 ESS = 2000 | BMK = 0.0487 | MCSE(6.27) = 0.166 | stat: FALSE | burn: 0



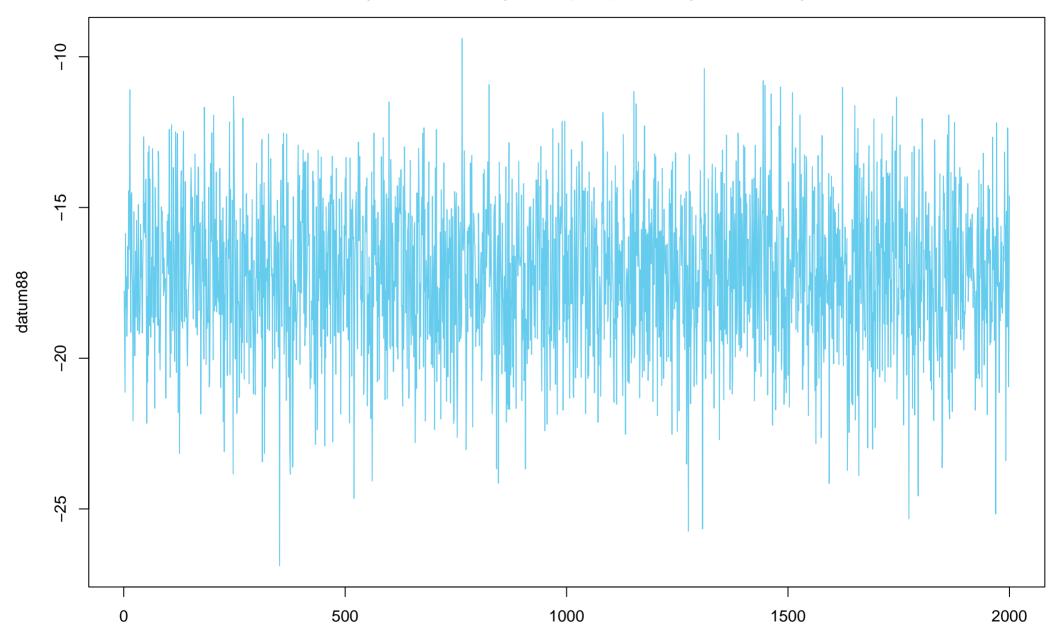
datum86 ESS = 2000 | BMK = 0.041 | MCSE(6.27) = 0.121 | stat: TRUE | burn: 0



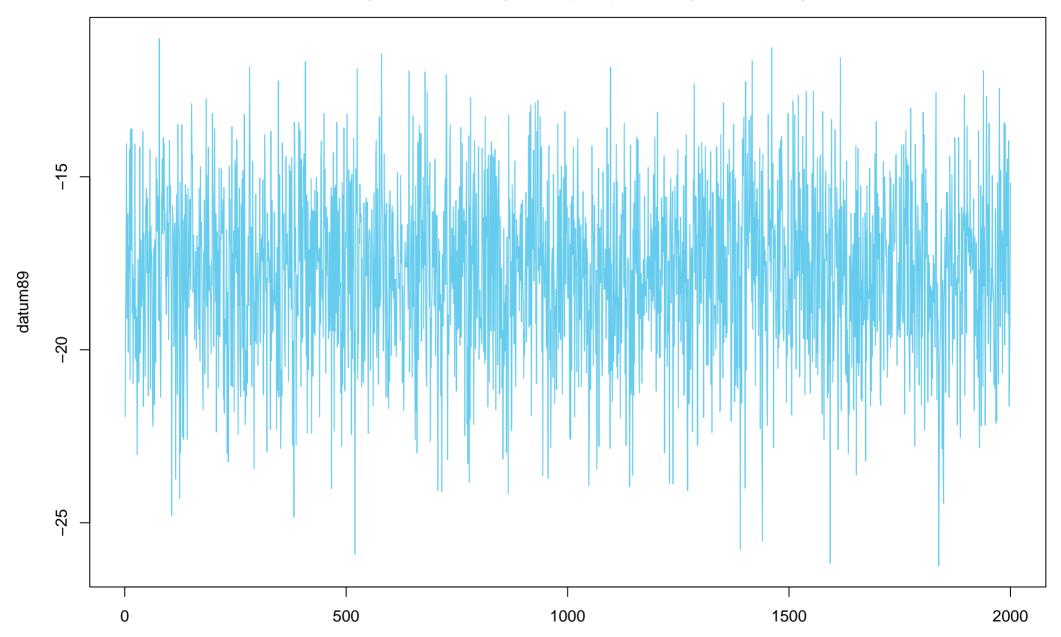
datum87 ESS = 1800 | BMK = 0.0414 | MCSE(6.27) = 0.138 | stat: TRUE | burn: 0



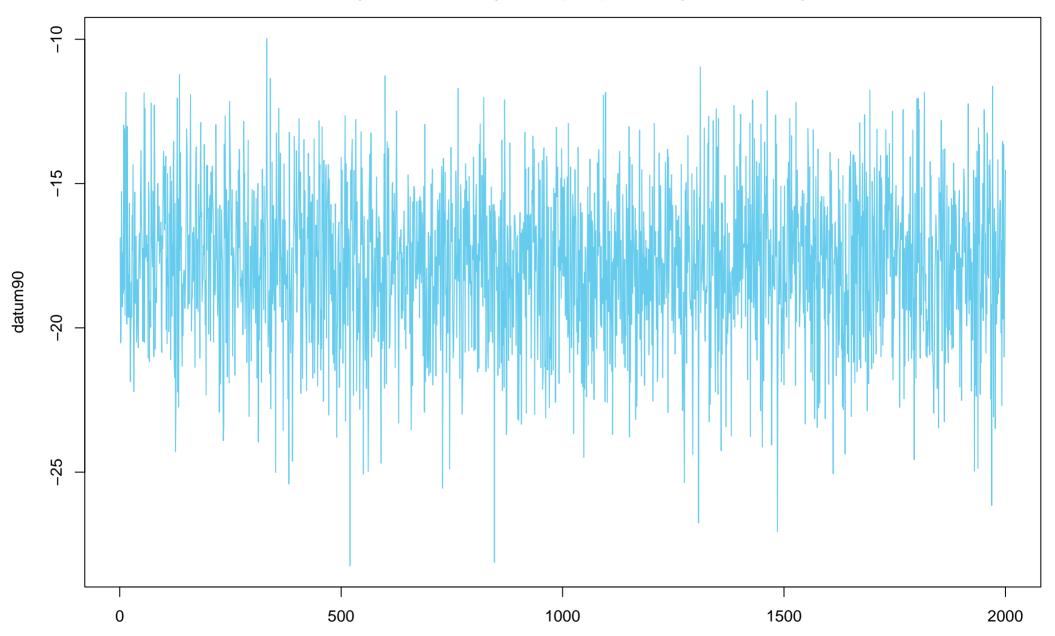
datum88 ESS = 2000 | BMK = 0.0396 | MCSE(6.27) = 0.173 | stat: TRUE | burn: 0



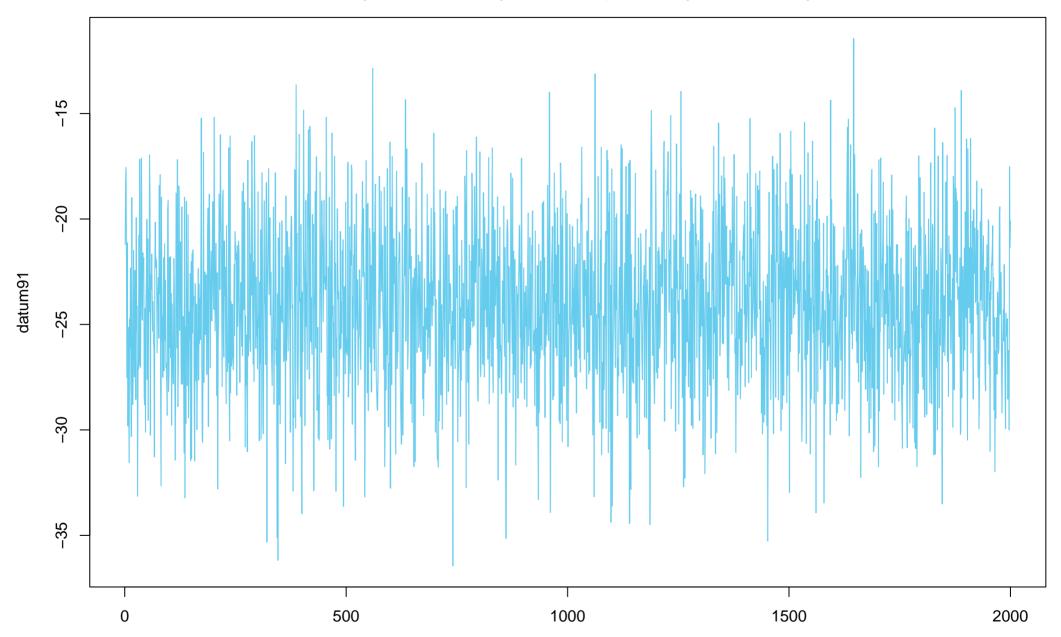
datum89 ESS = 2000 | BMK = 0.0217 | MCSE(6.27) = 0.176 | stat: TRUE | burn: 0



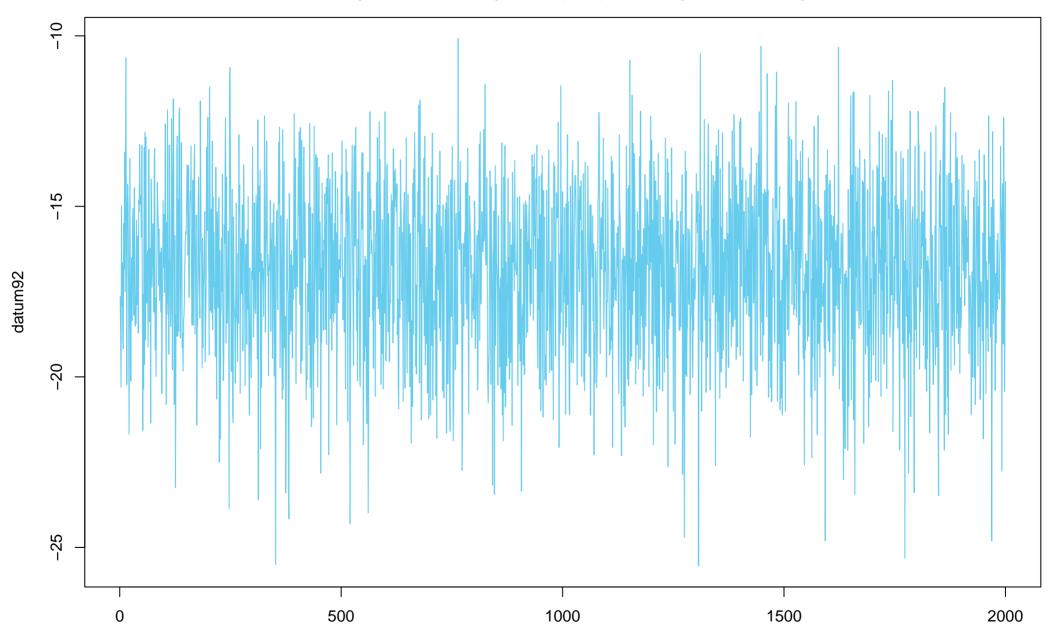
datum90 ESS = 2000 | BMK = 0.0401 | MCSE(6.27) = 0.164 | stat: FALSE | burn: 0



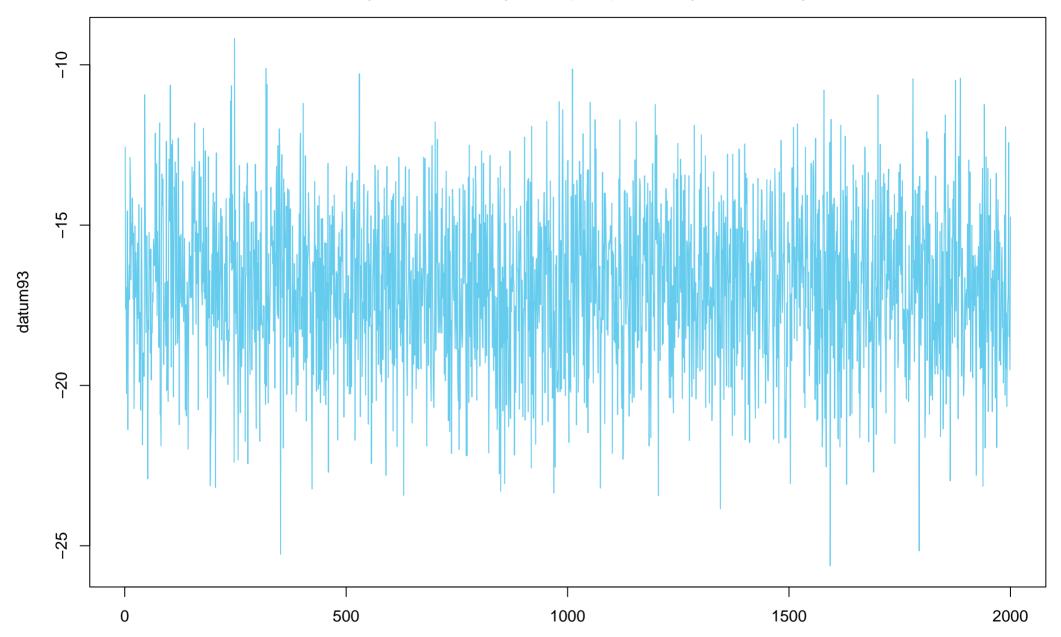
datum91 ESS = 2000 | BMK = 0.0355 | MCSE(6.27) = 0.113 | stat: FALSE | burn: 0



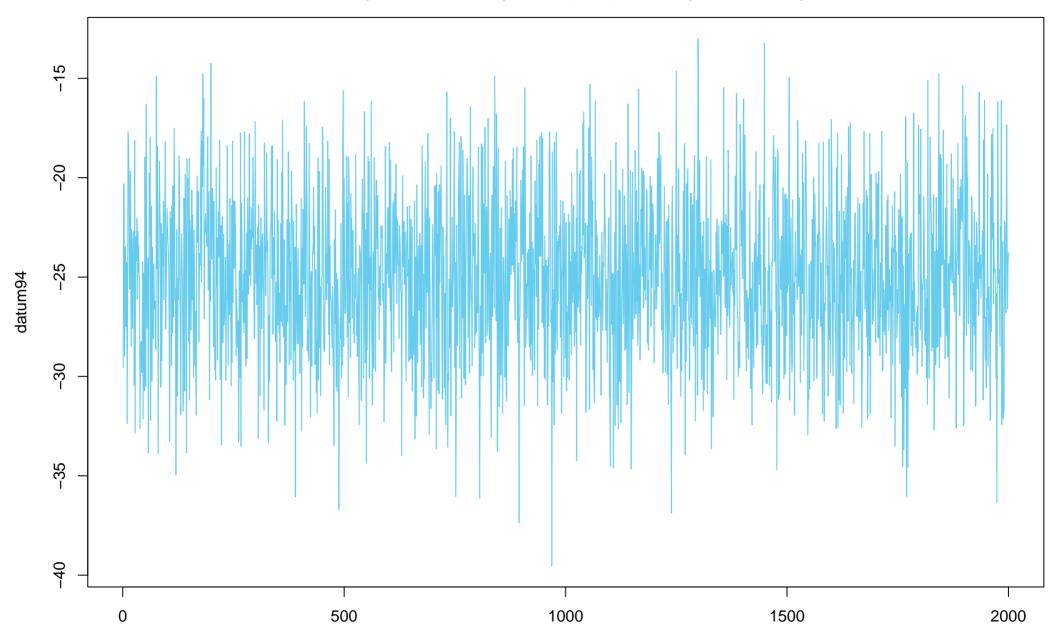
datum92 ESS = 2000 | BMK = 0.0359 | MCSE(6.27) = 0.177 | stat: FALSE | burn: 0



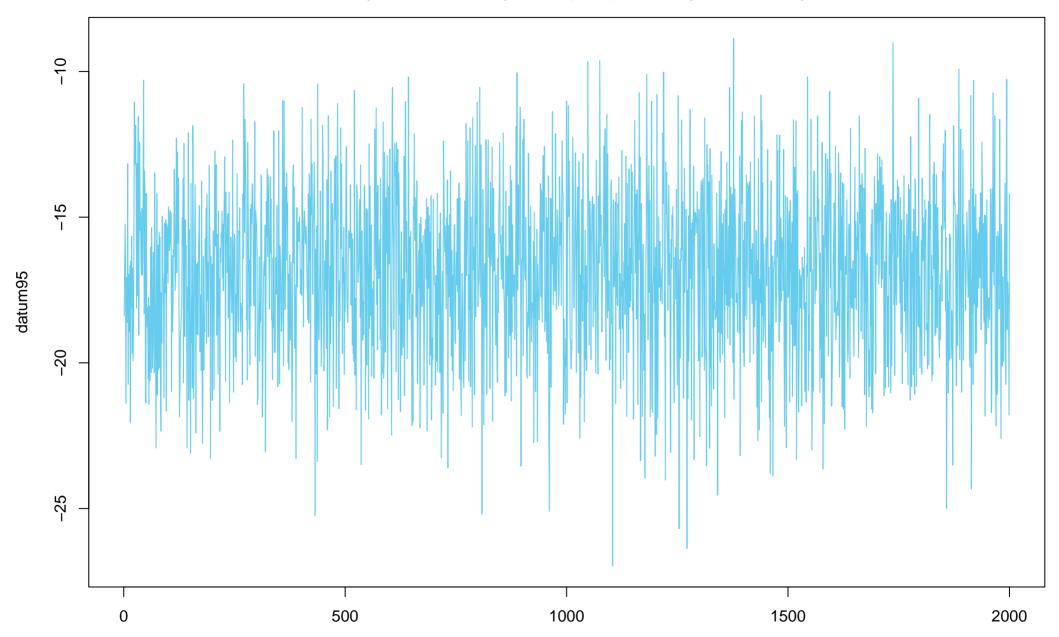
datum93 ESS = 2000 | BMK = 0.0248 | MCSE(6.27) = 0.176 | stat: TRUE | burn: 0



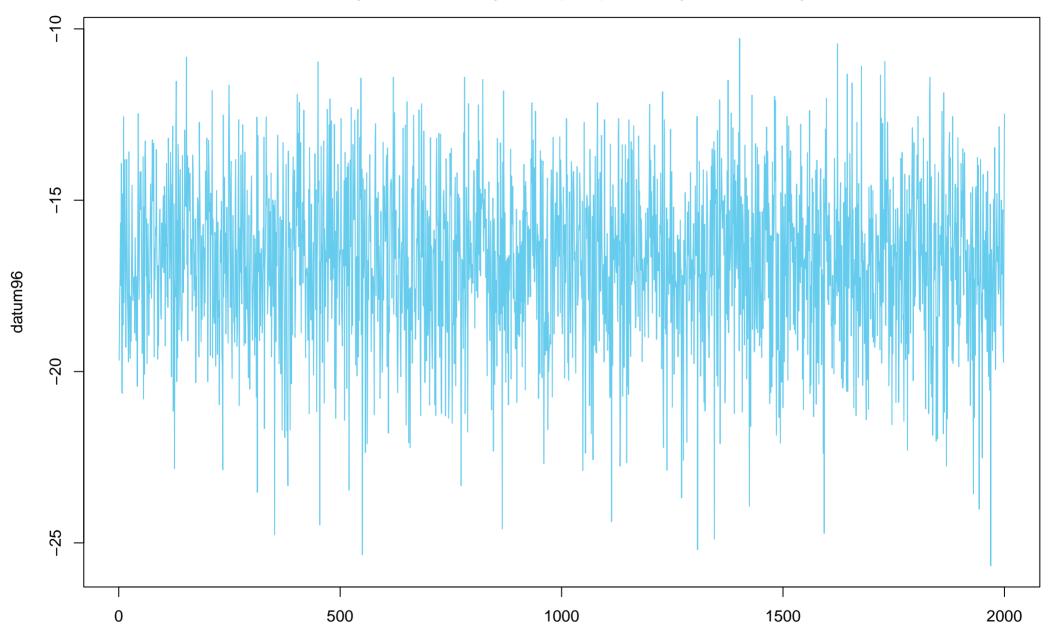
datum94 ESS = 2000 | BMK = 0.0564 | MCSE(6.27) = 0.109 | stat: TRUE | burn: 0



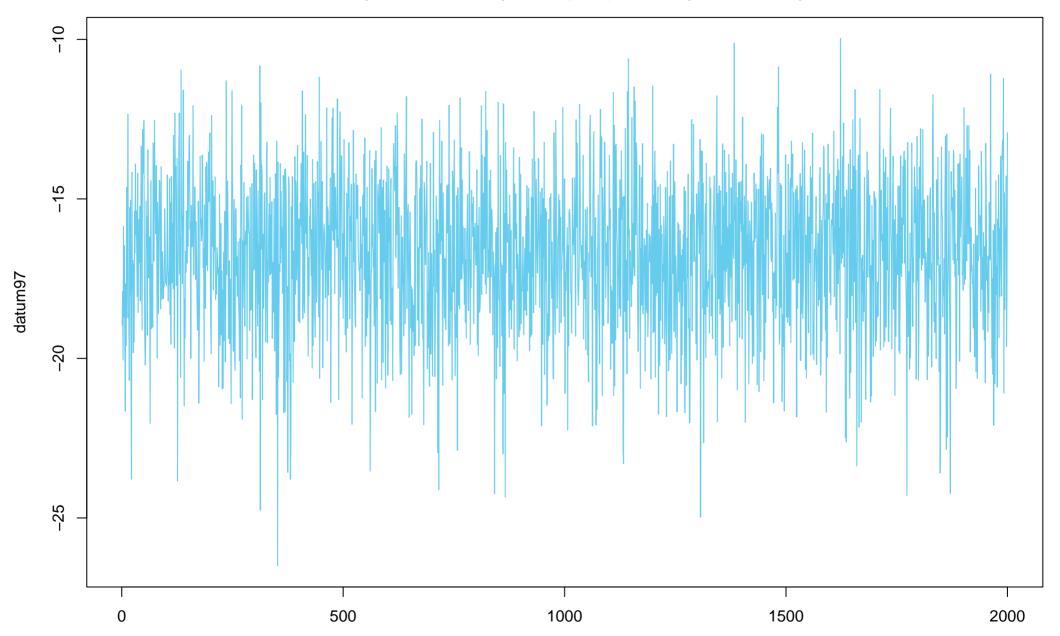
datum95 ESS = 2000 | BMK = 0.0395 | MCSE(6.27) = 0.155 | stat: TRUE | burn: 0



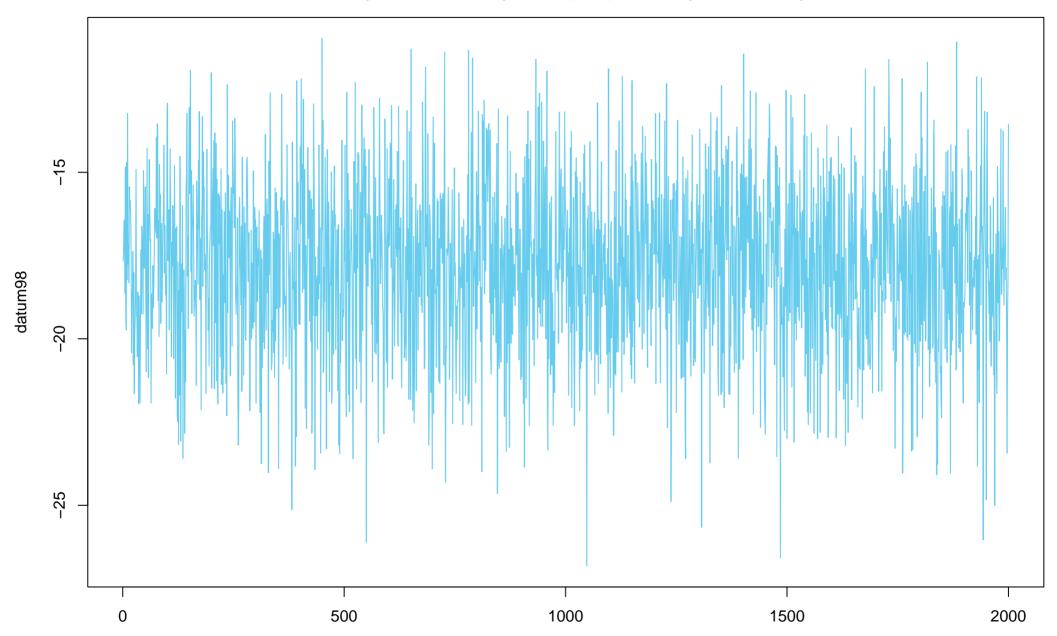
datum96 ESS = 2000 | BMK = 0.0343 | MCSE(6.27) = 0.182 | stat: FALSE | burn: 0



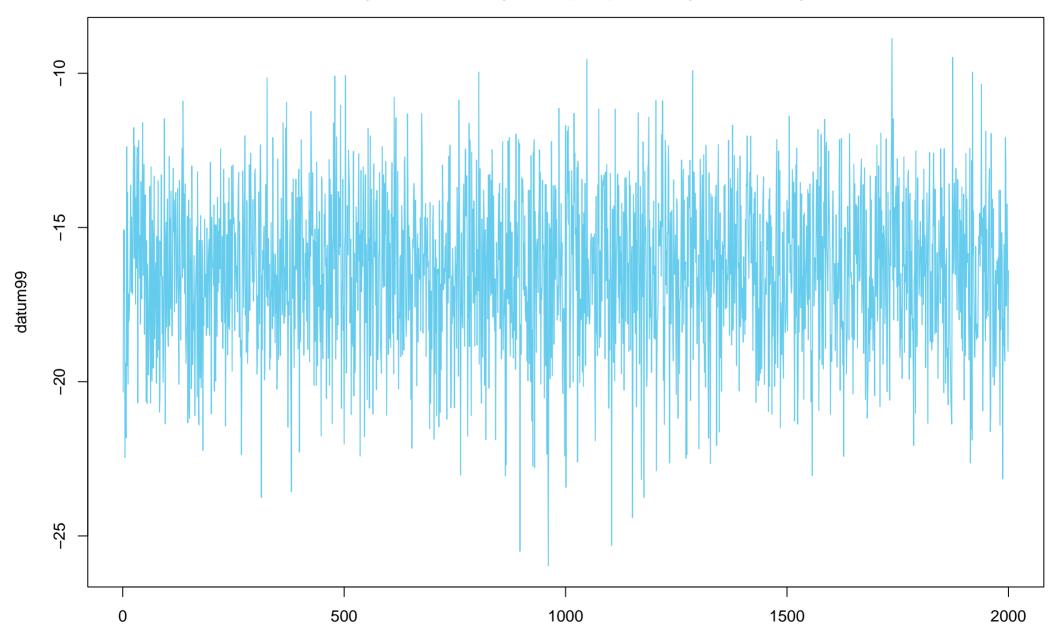
datum97 ESS = 2000 | BMK = 0.0375 | MCSE(6.27) = 0.183 | stat: TRUE | burn: 0



datum98 ESS = 2000 | BMK = 0.0435 | MCSE(6.27) = 0.171 | stat: TRUE | burn: 0



datum99 ESS = 2000 | BMK = 0.0308 | MCSE(6.27) = 0.173 | stat: TRUE | burn: 0



datum100 ESS = 2000 | BMK = 0.0275 | MCSE(6.27) = 0.115 | stat: TRUE | burn: 0

