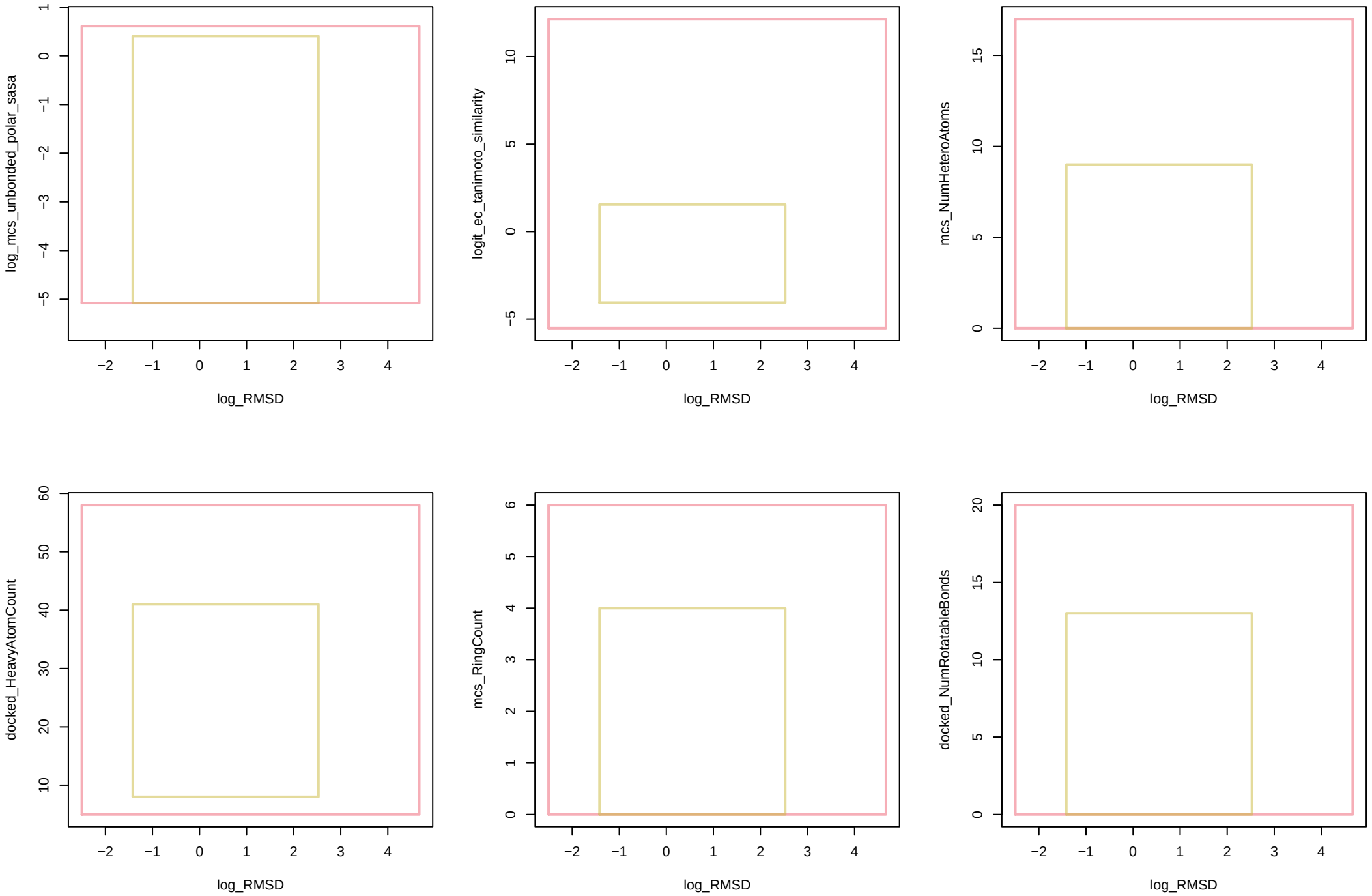
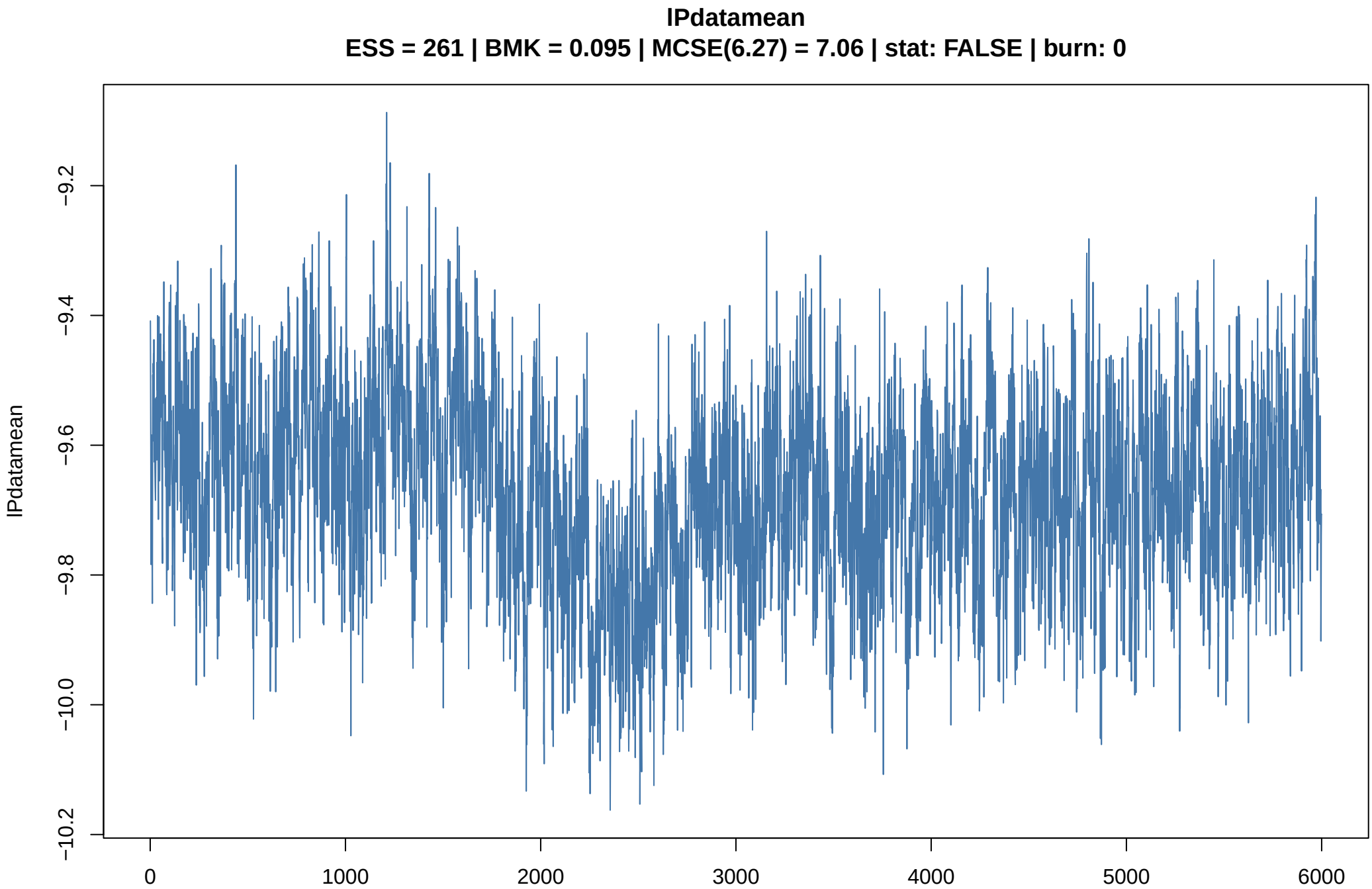
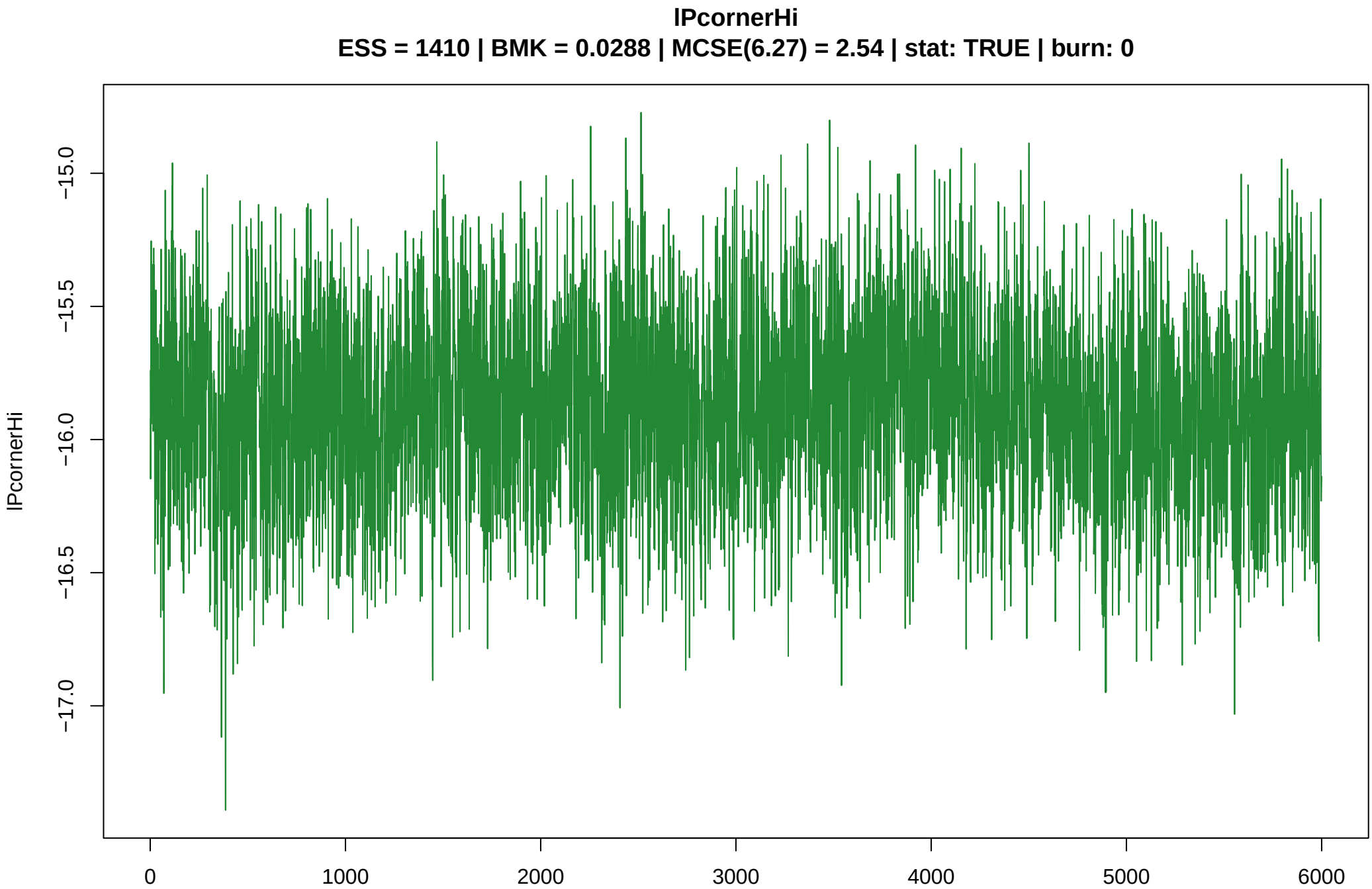
−− STATS maxD −−
min ESS = 71.1494805040645
max BMK = 0.275242459165424
max MCSE = 7.05508572314033
all stationary: FALSE
burn: 0

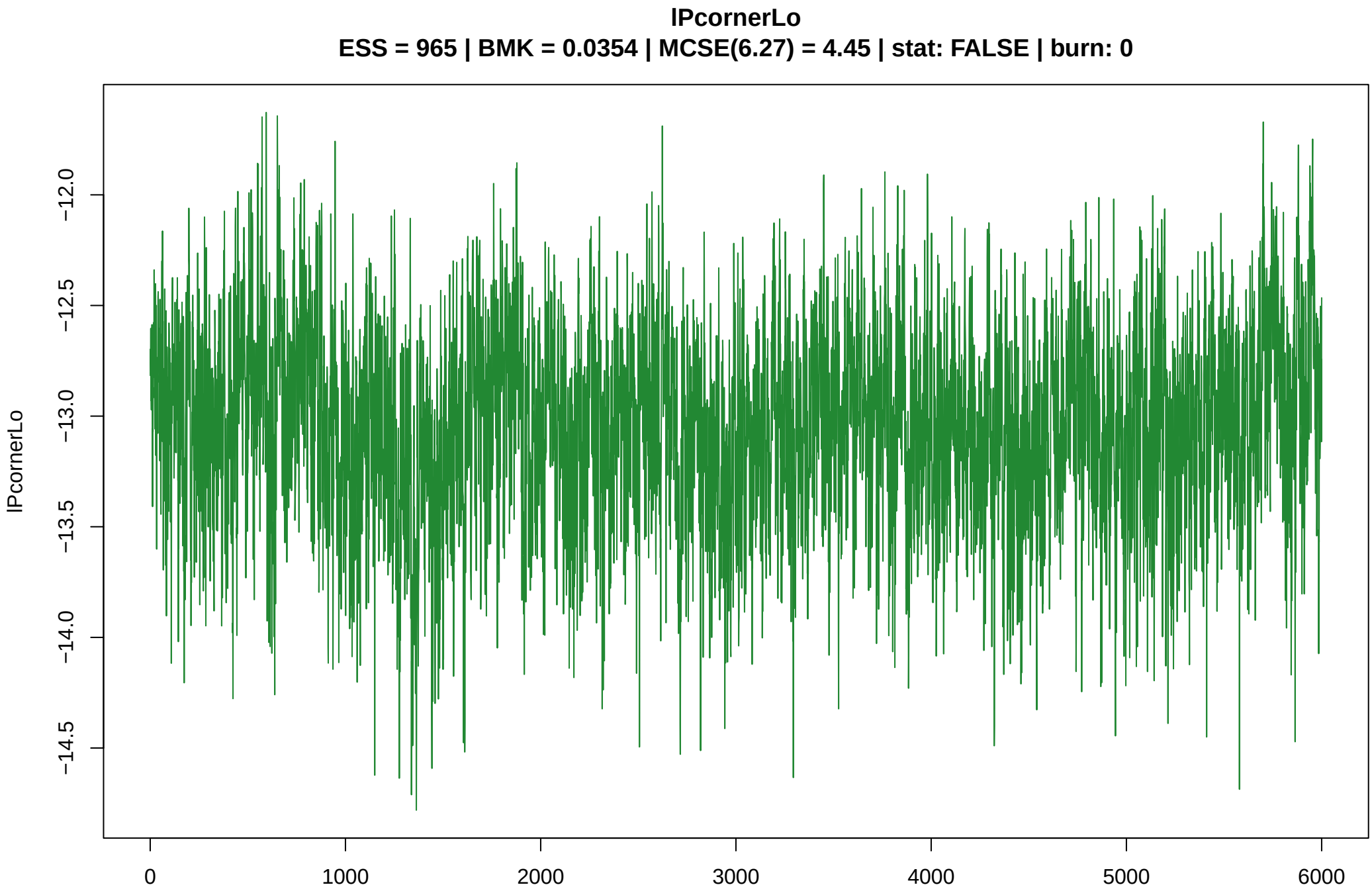
−− STATS 2D −−
min ESS = 813.677857478713
max BMK = 0.060874490179981
max MCSE = 1.79179682486954
all stationary: FALSE
burn: 0

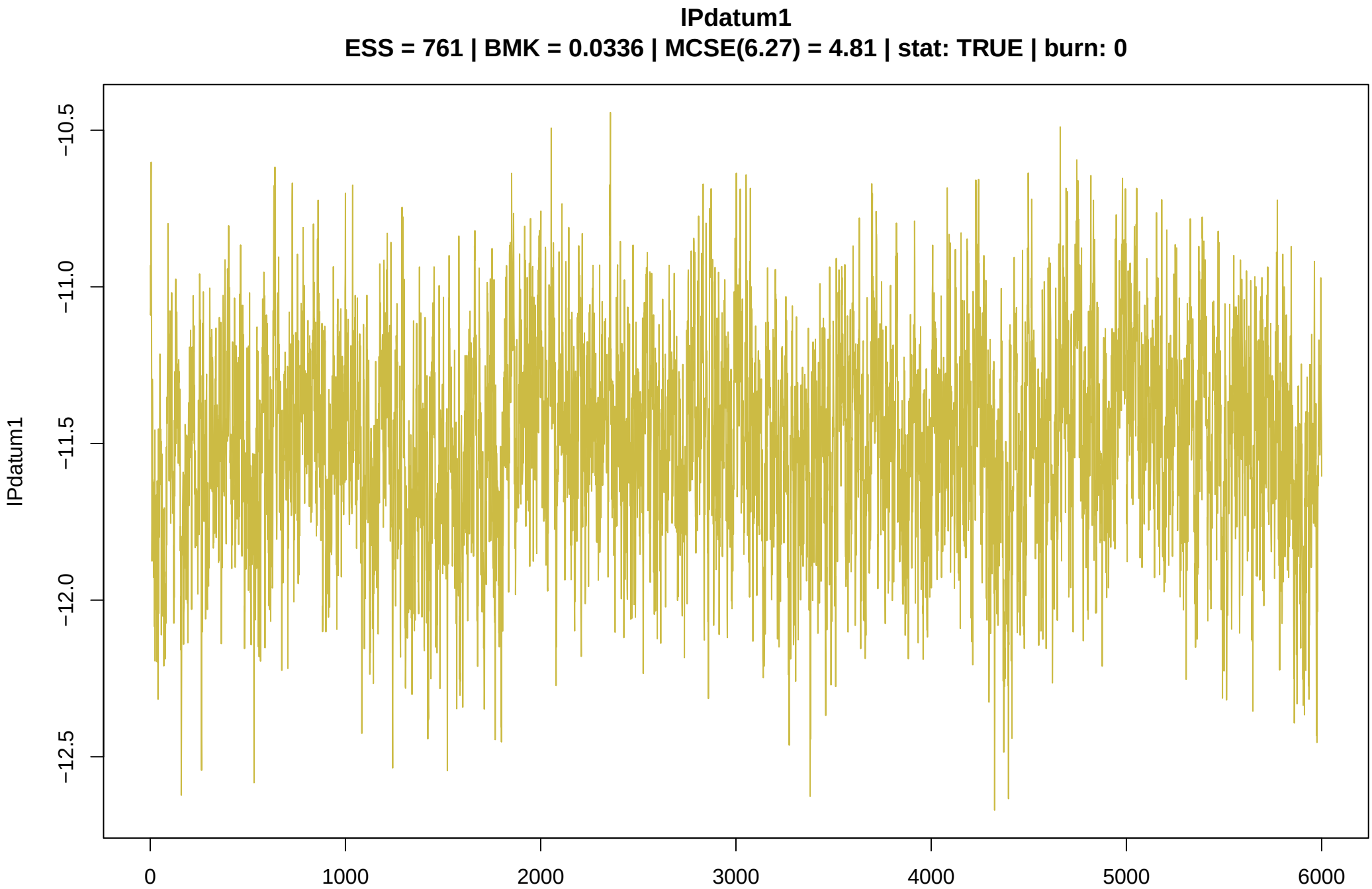
−− STATS 1D −−
min ESS = 961.904918402964
max BMK = 0.113330981777197
max MCSE = 1.92009072558012
all stationary: FALSE
burn: 0

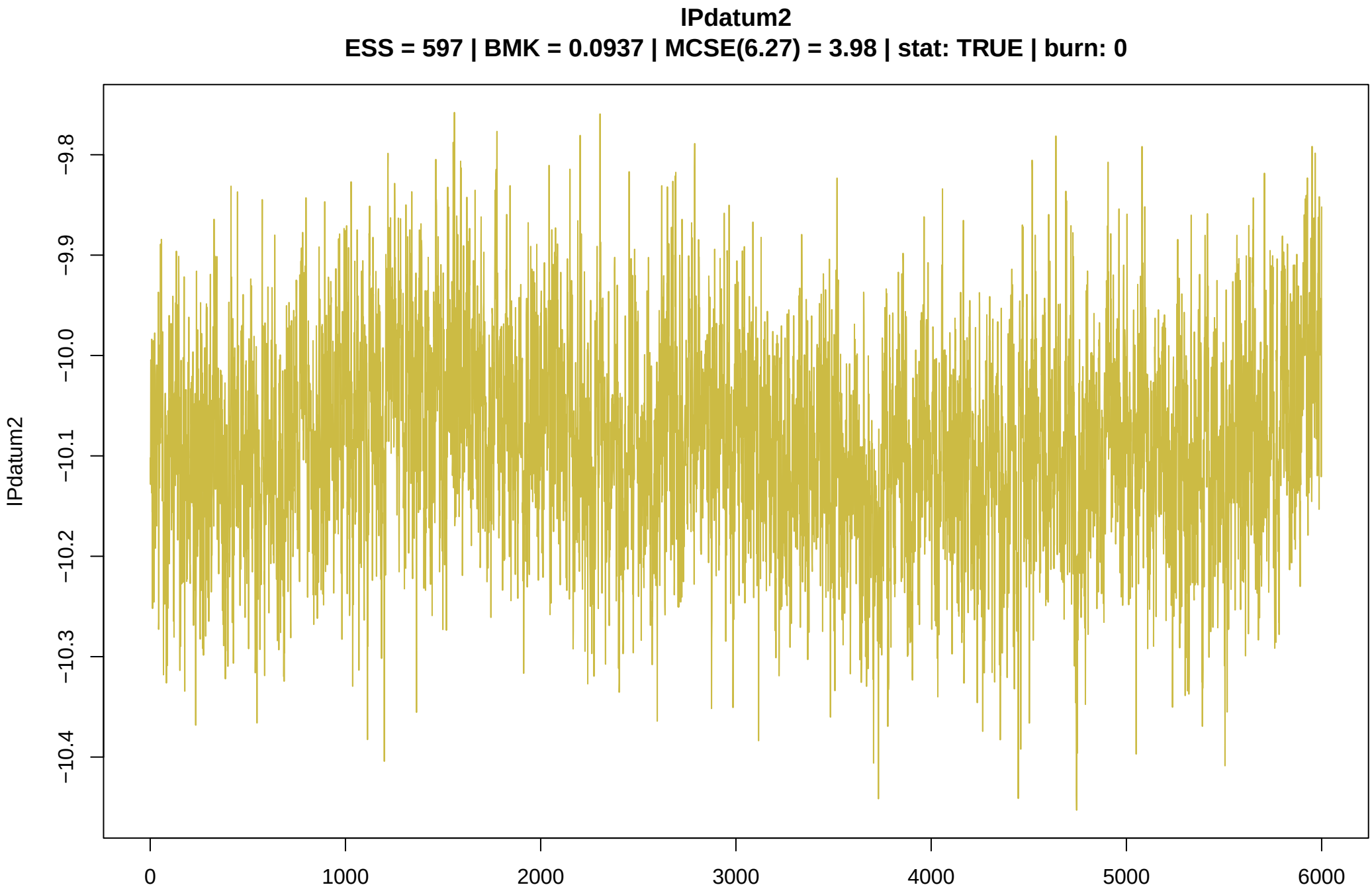

log_mcs_unbonded_polar_sasa
logit_ec_tanimoto_similarity
mcs_NumHeteroAtoms
docked_HeavyAtomCount
mcs_RingCount
docked_NumRotatableBonds
log_RMSD

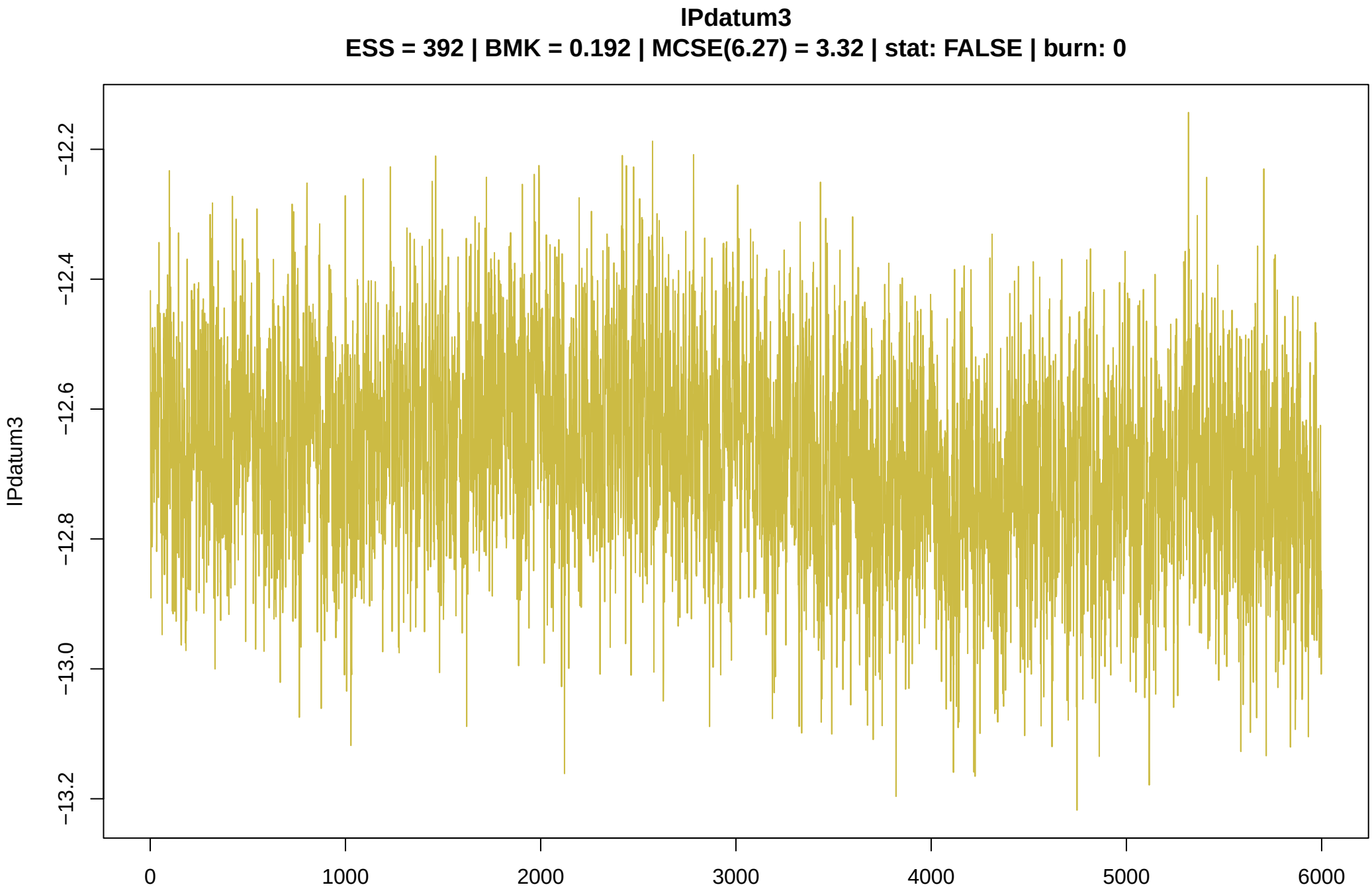

lPdatamean
ESS = 261 | BMK = 0.095 | MCSE(6.27) = 7.06 | stat: FALSE | burn: 0
lPdatamean
−9.2
−9.4
−9.6
−9.8
−10.0
−10.2
0
1000
2000
3000
4000
5000
6000

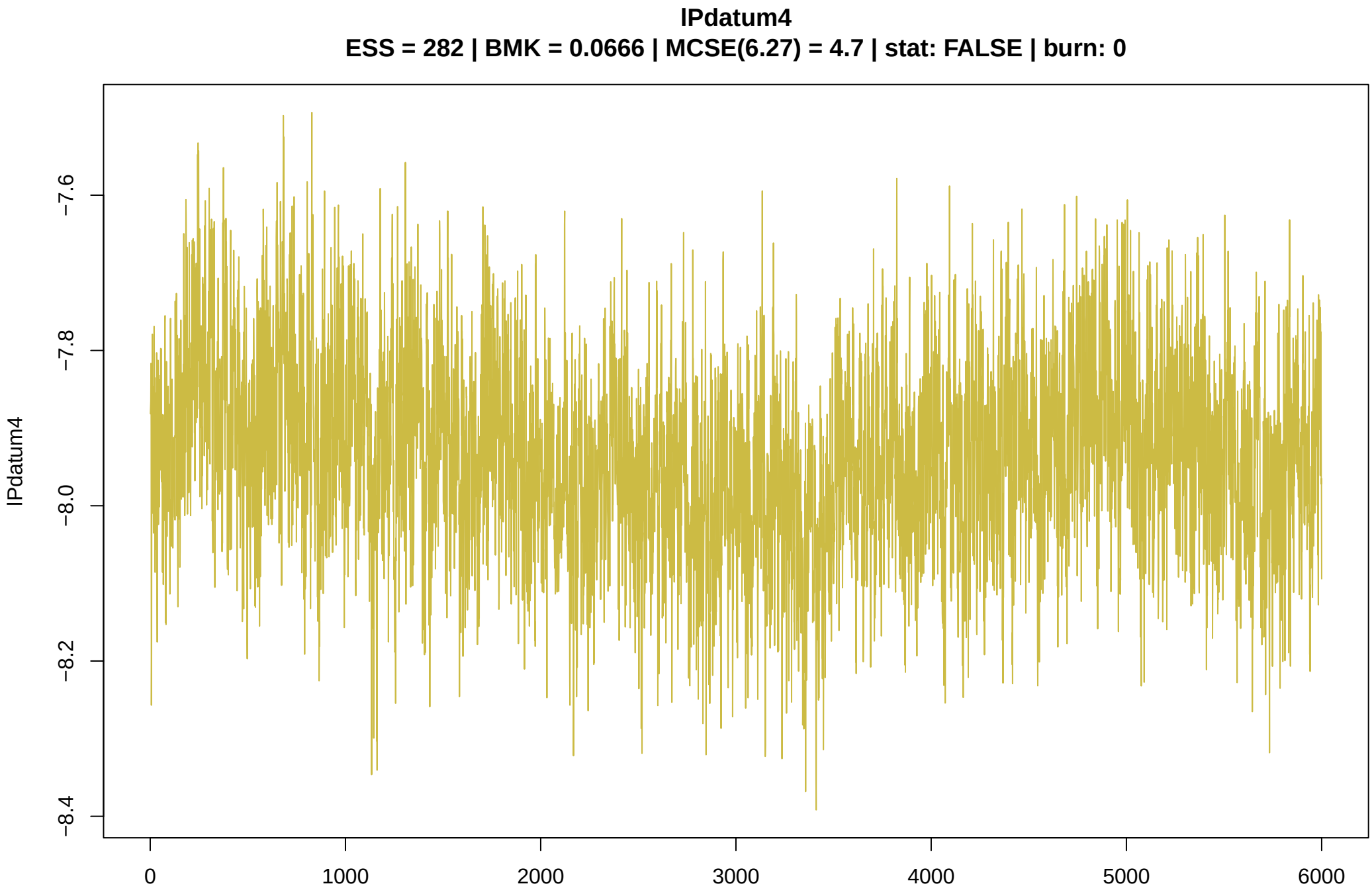

lPcornerHi
ESS = 1410 | BMK = 0.0288 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0
lPcornerHi
−15.0
−15.5
−16.0
−16.5
−17.0
0
1000
2000
3000
4000
5000
6000

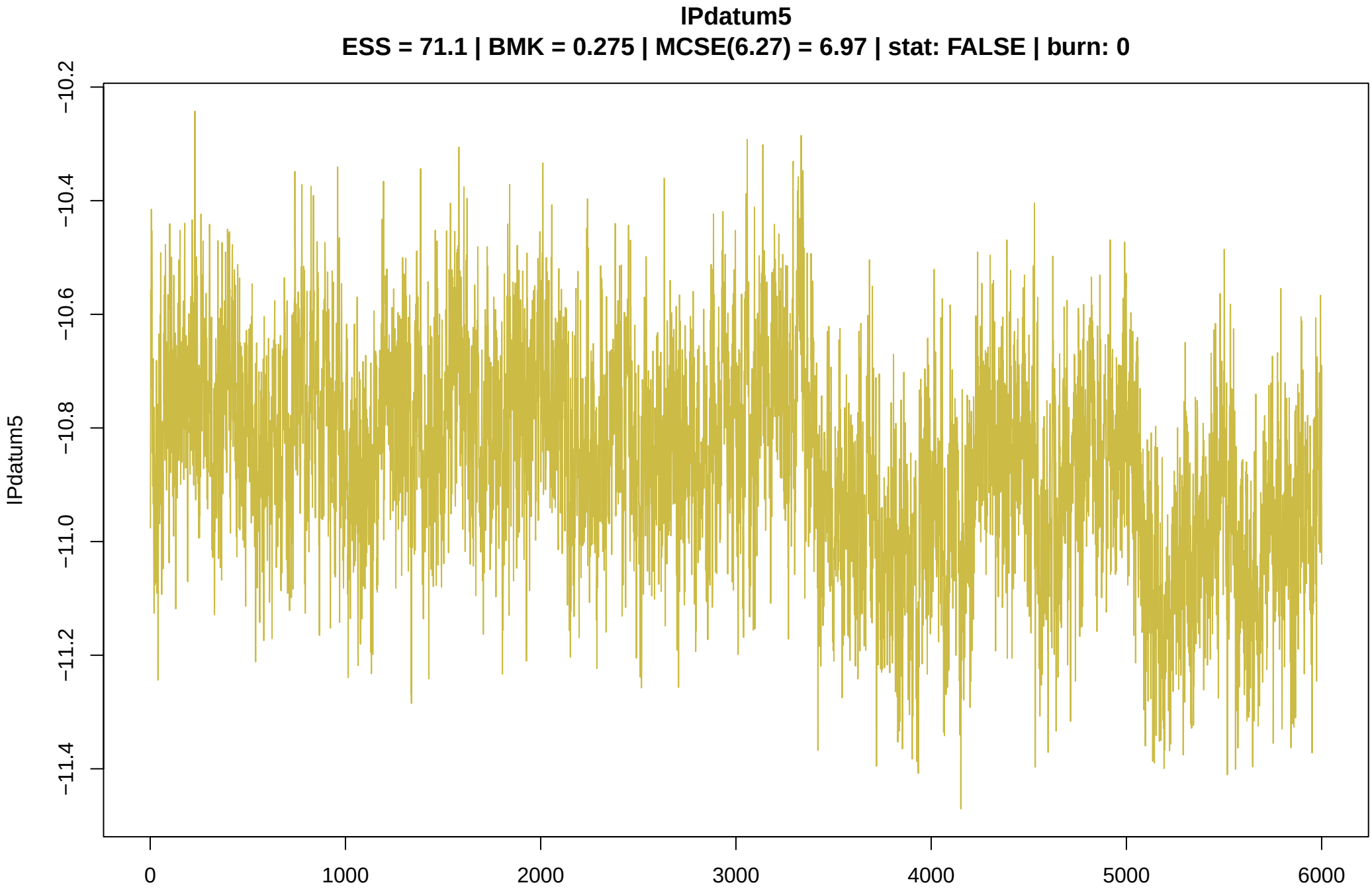

lPcornerLo
ESS = 965 | BMK = 0.0354 | MCSE(6.27) = 4.45 | stat: FALSE | burn: 0
lPcornerLo
−12.0
−12.5
−13.0
−13.5
−14.0
−14.5
0
1000
2000
3000
4000
5000
6000

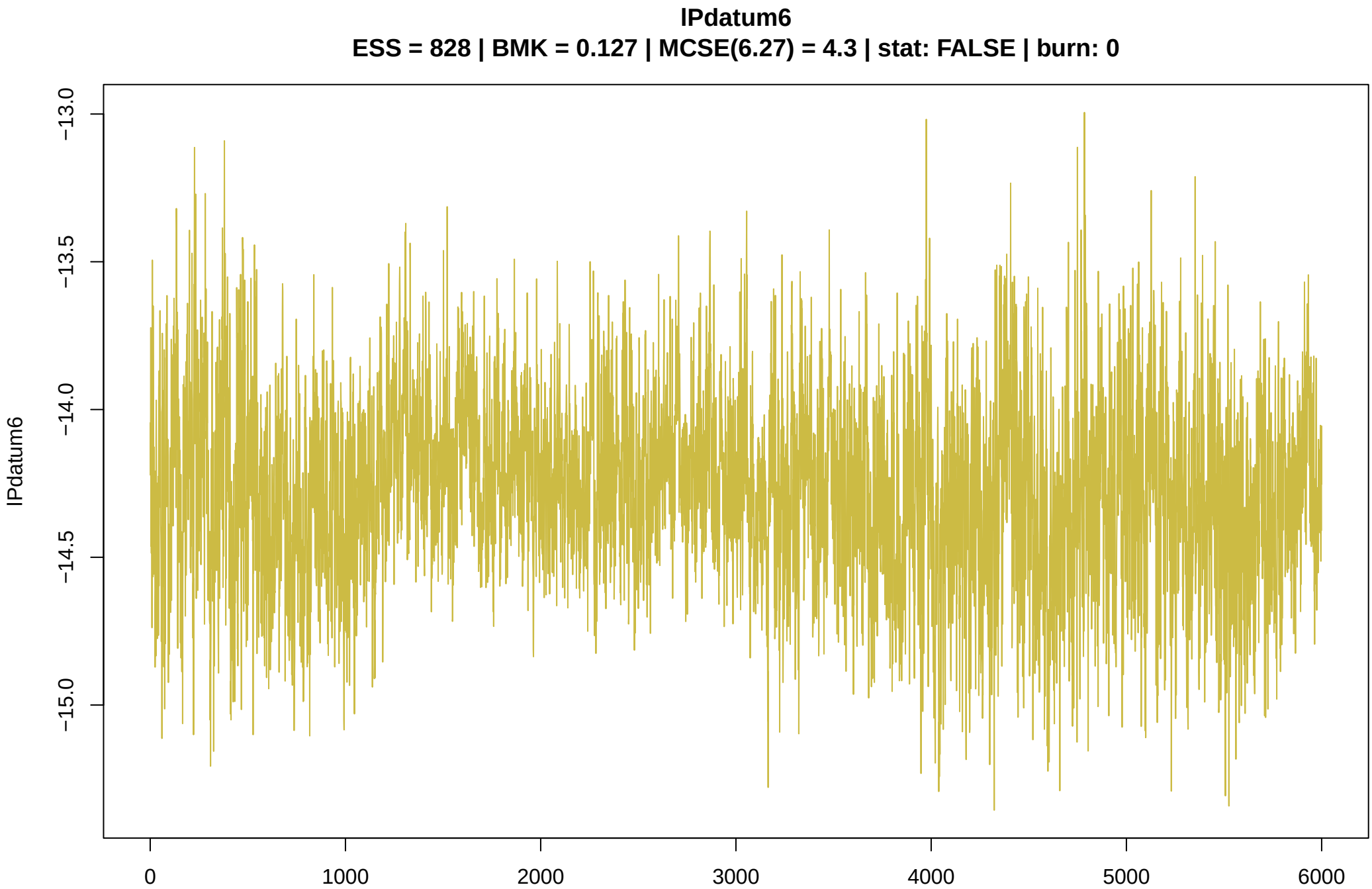

lPdatum1
ESS = 761 | BMK = 0.0336 | MCSE(6.27) = 4.81 | stat: TRUE | burn: 0
lPdatum1
−10.5
−11.0
−11.5
−12.0
−12.5
0
1000
2000
3000
4000
5000
6000

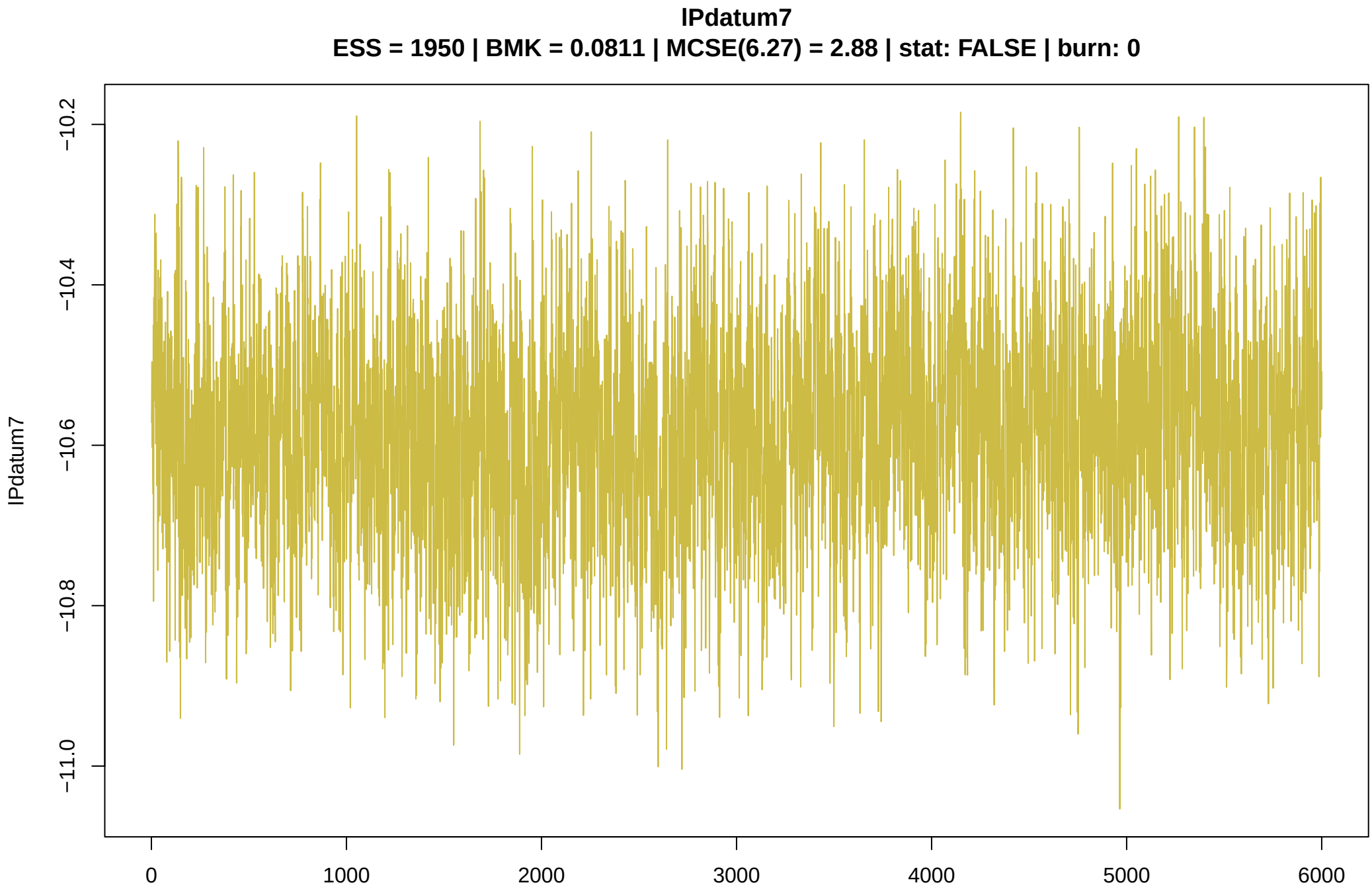

lPdatum2
ESS = 597 | BMK = 0.0937 | MCSE(6.27) = 3.98 | stat: TRUE | burn: 0
lPdatum2
−9.8
−9.9
−10.0
−10.1
−10.2
−10.3
−10.4
0
1000
2000
3000
4000
5000
6000

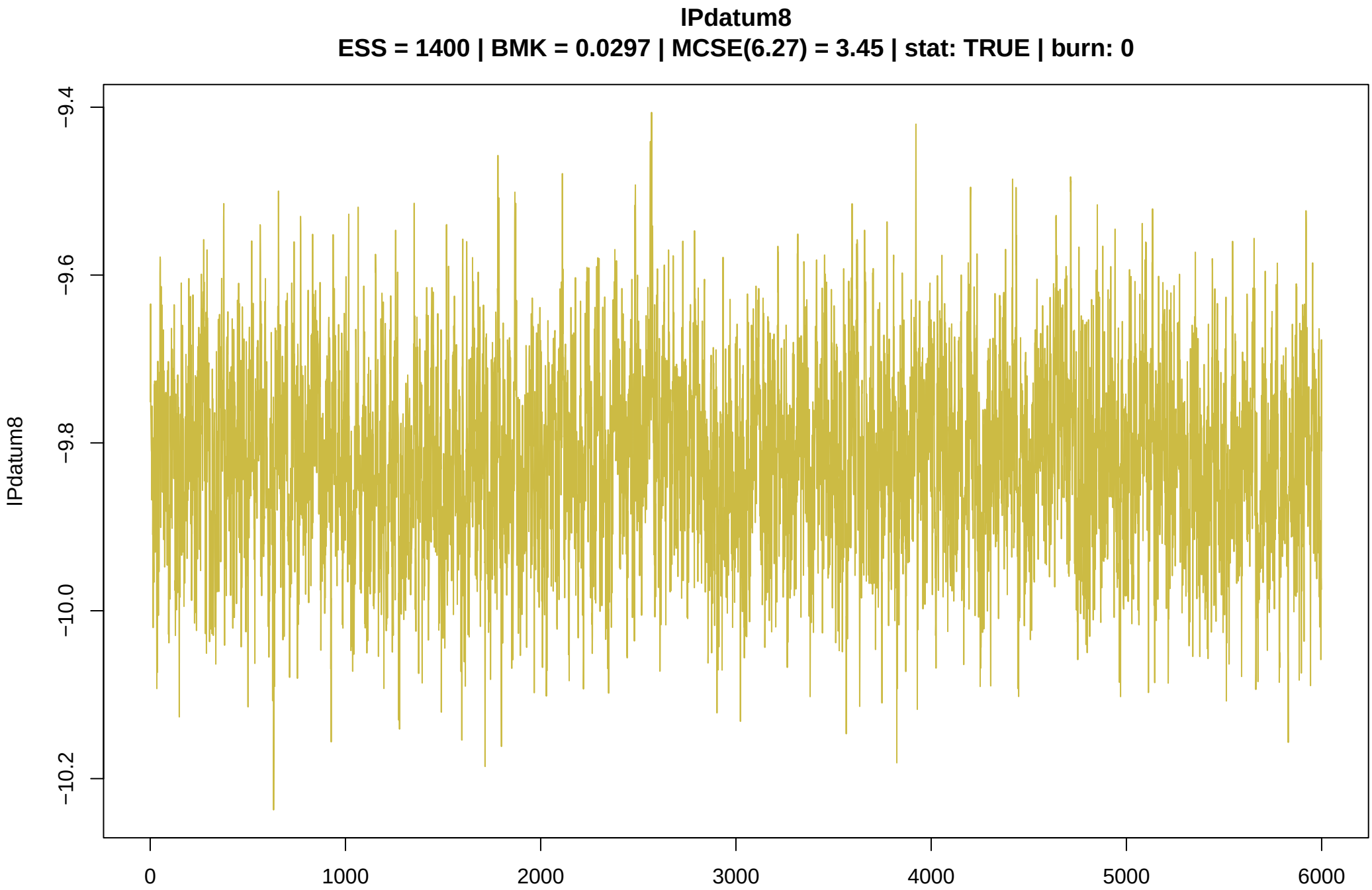

lPdatum3
ESS = 392 | BMK = 0.192 | MCSE(6.27) = 3.32 | stat: FALSE | burn: 0
lPdatum3
−12.2
−12.4
−12.6
−12.8
−13.0
−13.2
0
1000
2000
3000
4000
5000
6000

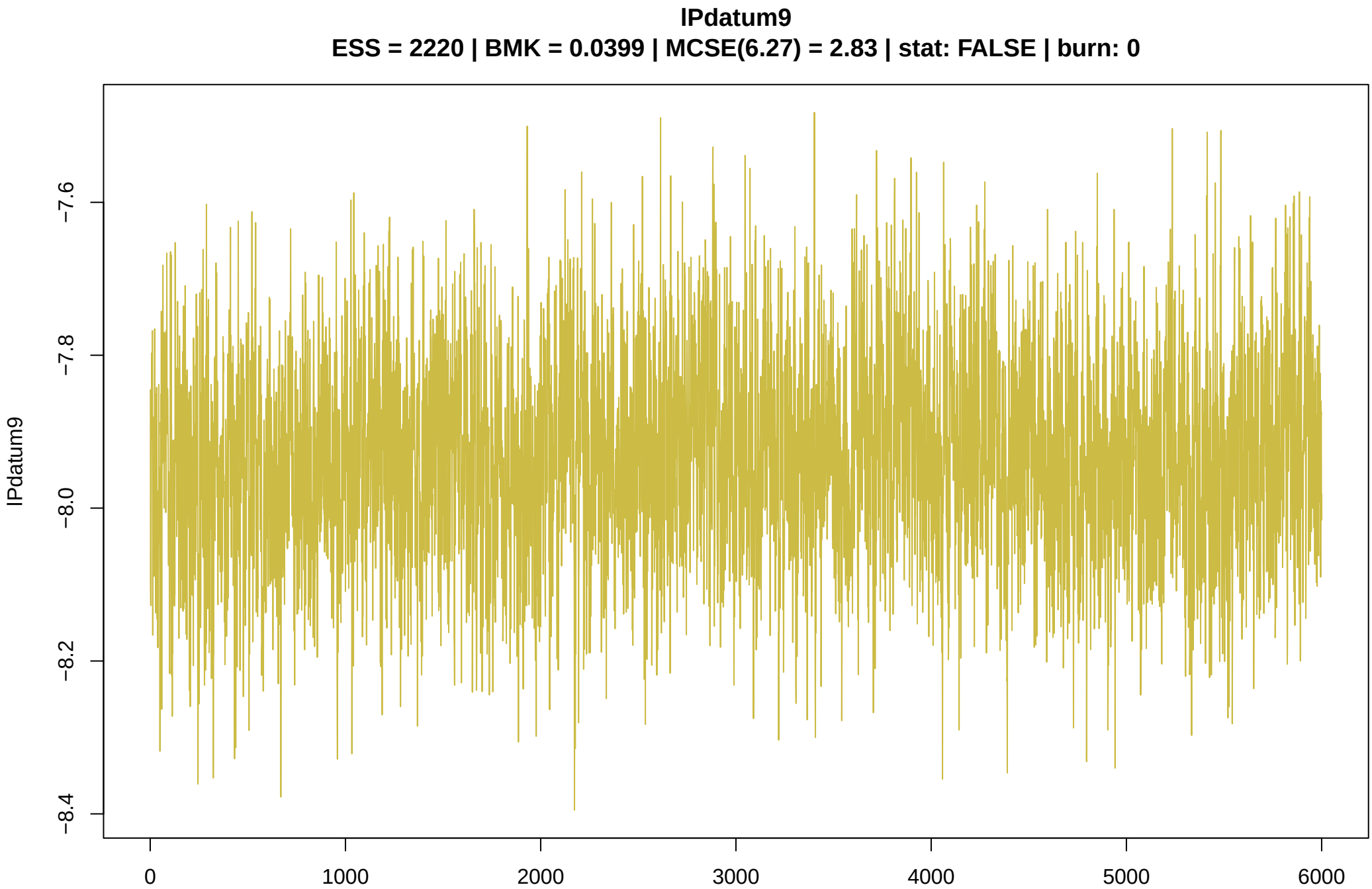

lPdatum4
ESS = 282 | BMK = 0.0666 | MCSE(6.27) = 4.7 | stat: FALSE | burn: 0
lPdatum4
−7.6
−7.8
−8.0
−8.2
−8.4
0
1000
2000
3000
4000
5000
6000

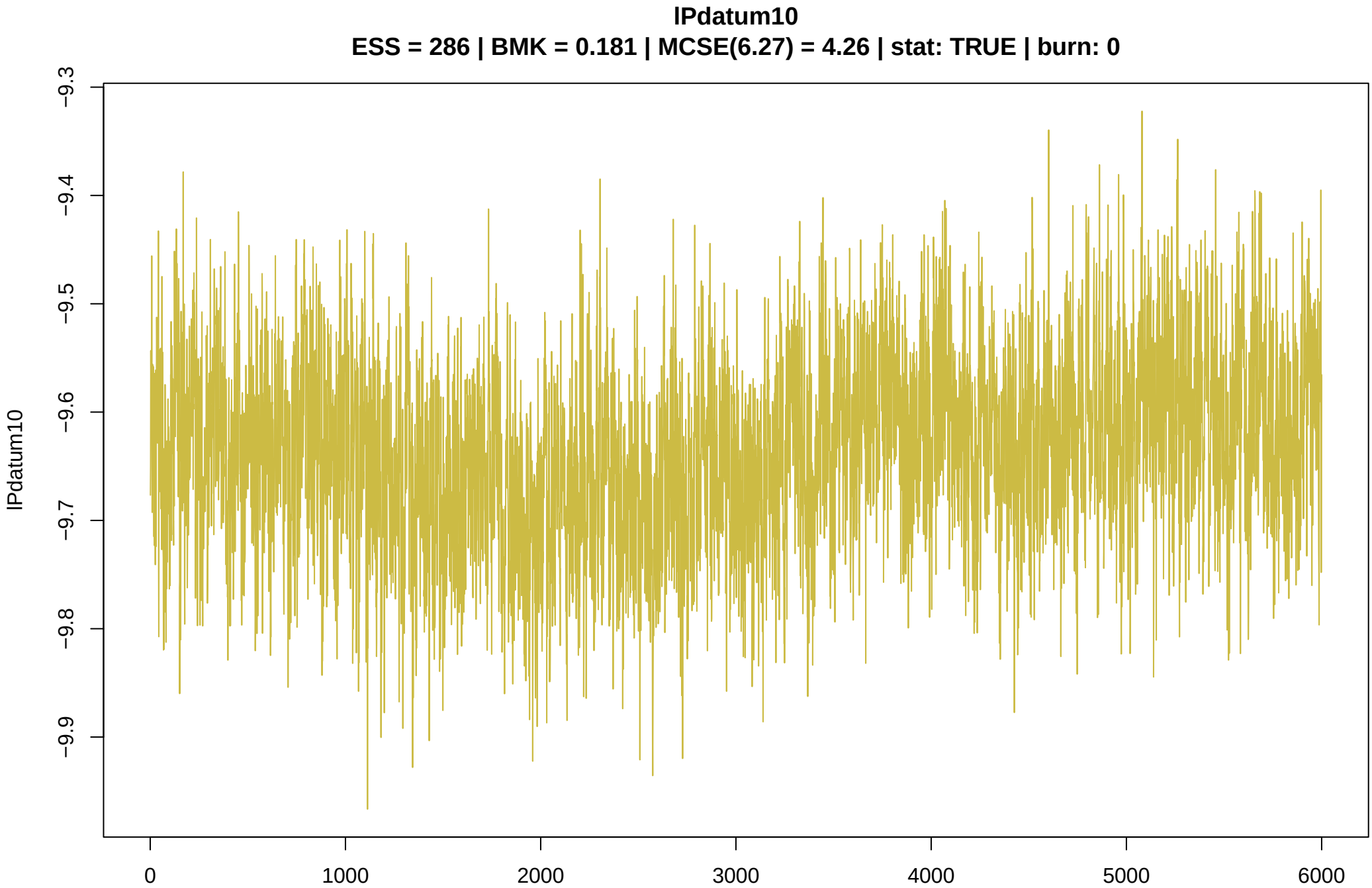

lPdatum5
ESS = 71.1 | BMK = 0.275 | MCSE(6.27) = 6.97 | stat: FALSE | burn: 0
lPdatum5
−10.2
−10.4
−10.6
−10.8
−11.0
−11.2
−11.4
0
1000
2000
3000
4000
5000
6000

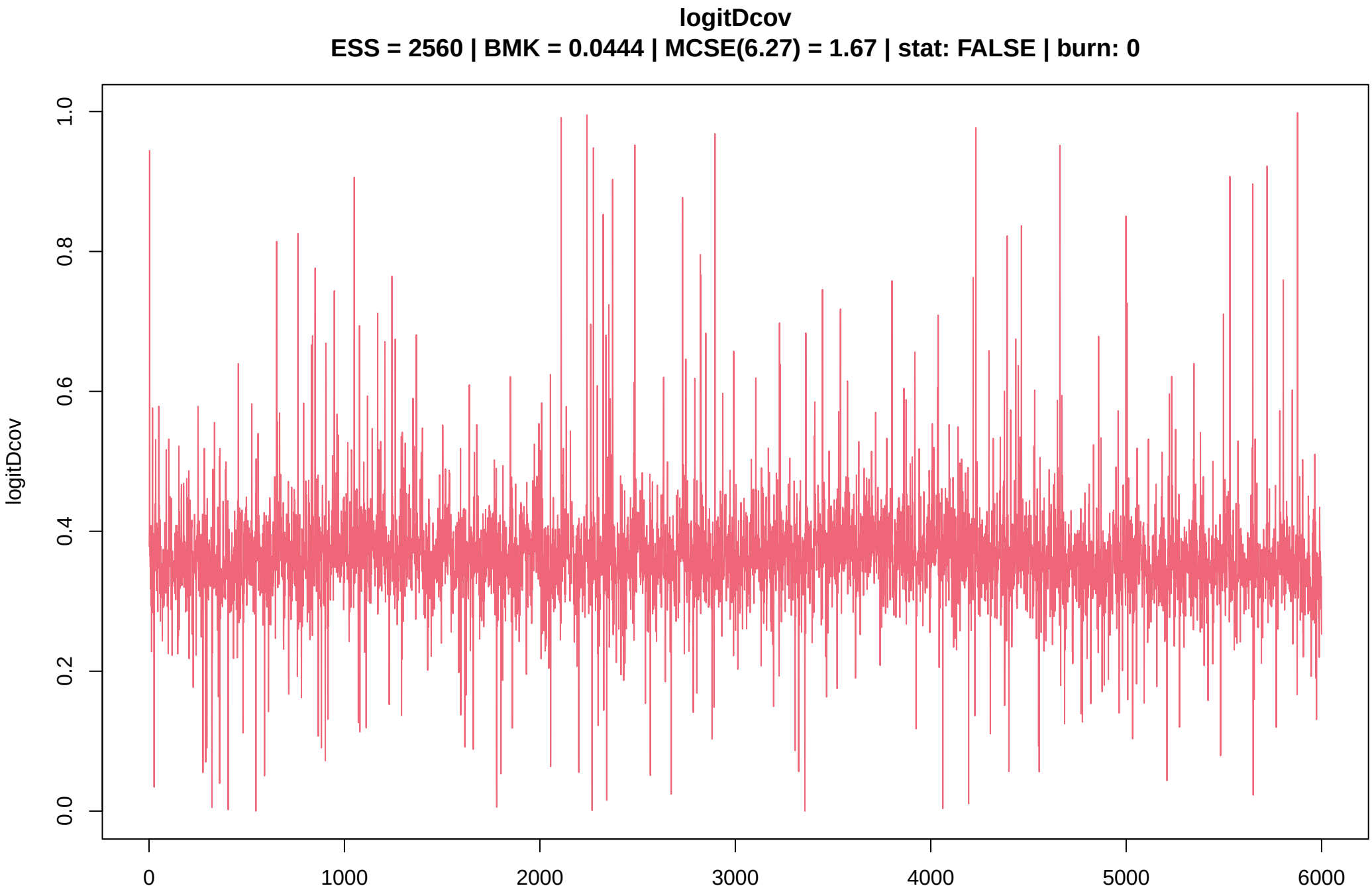

lPdatum6
ESS = 828 | BMK = 0.127 | MCSE(6.27) = 4.3 | stat: FALSE | burn: 0
lPdatum6
−13.0
−13.5
−14.0
−14.5
−15.0
0
1000
2000
3000
4000
5000
6000

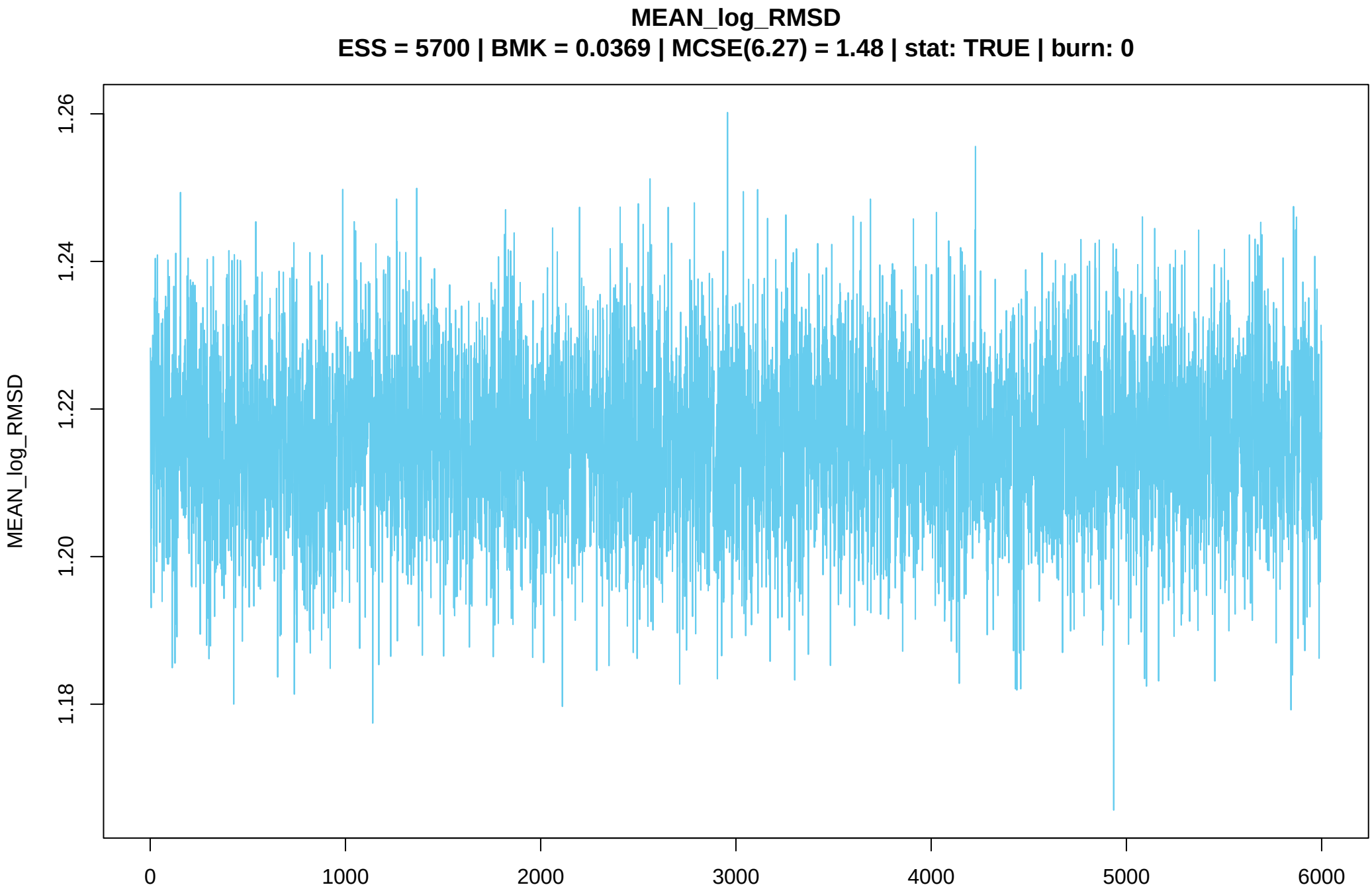

lPdatum7
ESS = 1950 | BMK = 0.0811 | MCSE(6.27) = 2.88 | stat: FALSE | burn: 0
lPdatum7
−10.2
−10.4
−10.6
−10.8
−11.0
0
1000
2000
3000
4000
5000
6000

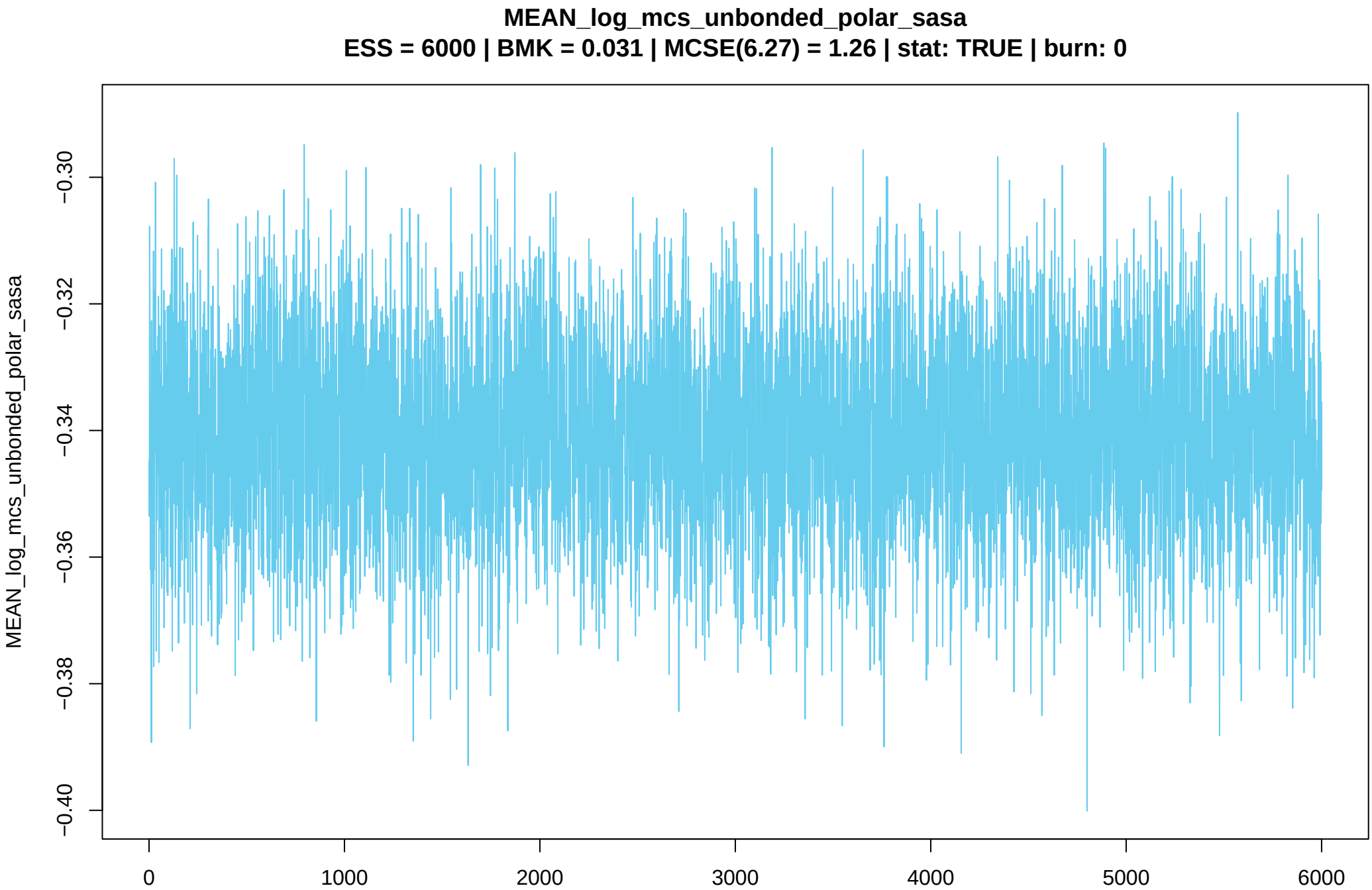

lPdatum8
ESS = 1400 | BMK = 0.0297 | MCSE(6.27) = 3.45 | stat: TRUE | burn: 0
lPdatum8
−9.4
−9.6
−9.8
−10.0
−10.2
0
1000
2000
3000
4000
5000
6000

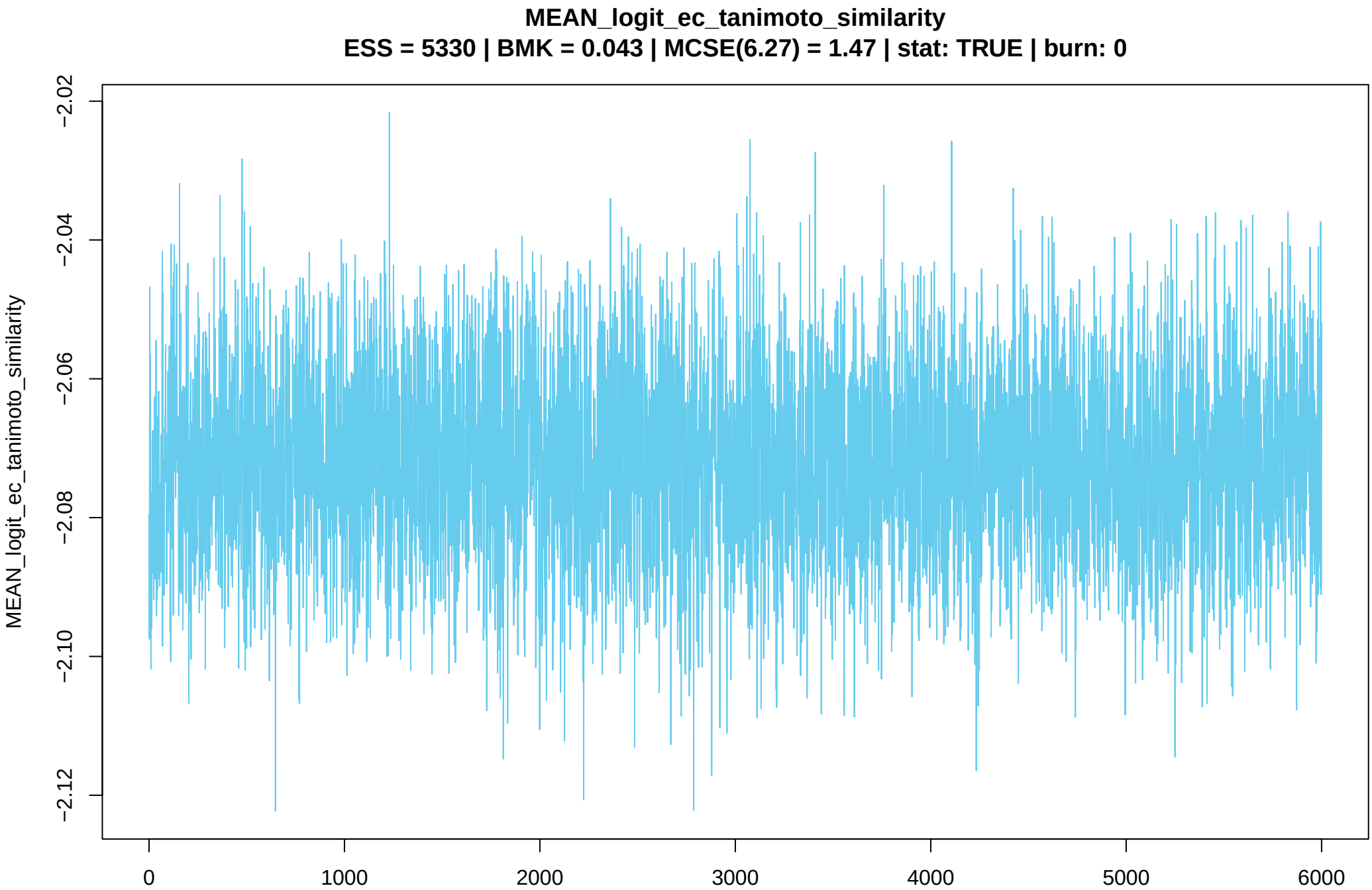

lPdatum9
ESS = 2220 | BMK = 0.0399 | MCSE(6.27) = 2.83 | stat: FALSE | burn: 0
lPdatum9
−7.6
−7.8
−8.0
−8.2
−8.4
0
1000
2000
3000
4000
5000
6000

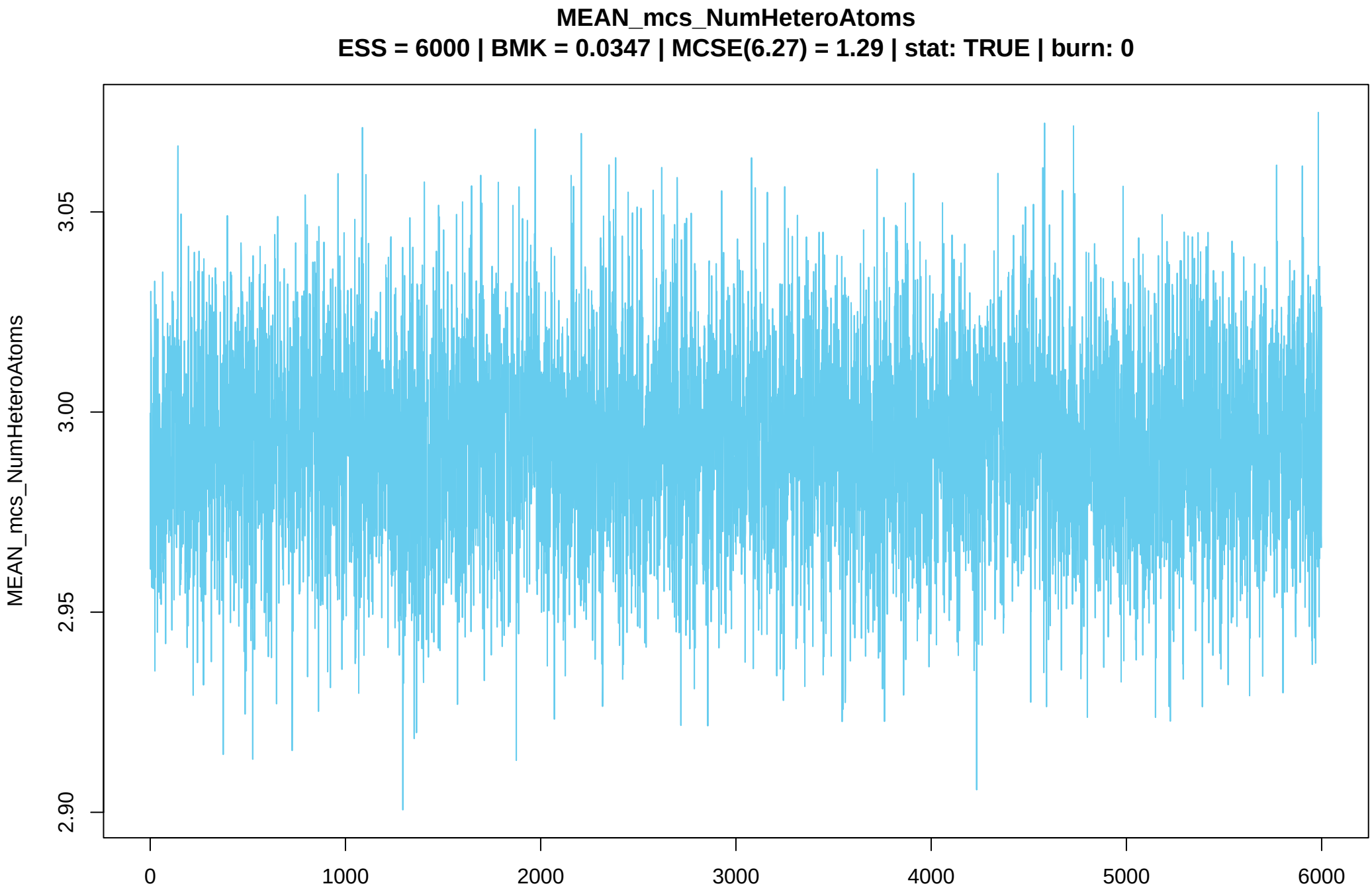

lPdatum10
ESS = 286 | BMK = 0.181 | MCSE(6.27) = 4.26 | stat: TRUE | burn: 0
lPdatum10
−9.3
−9.4
−9.5
−9.6
−9.7
−9.8
−9.9
0
1000
2000
3000
4000
5000
6000

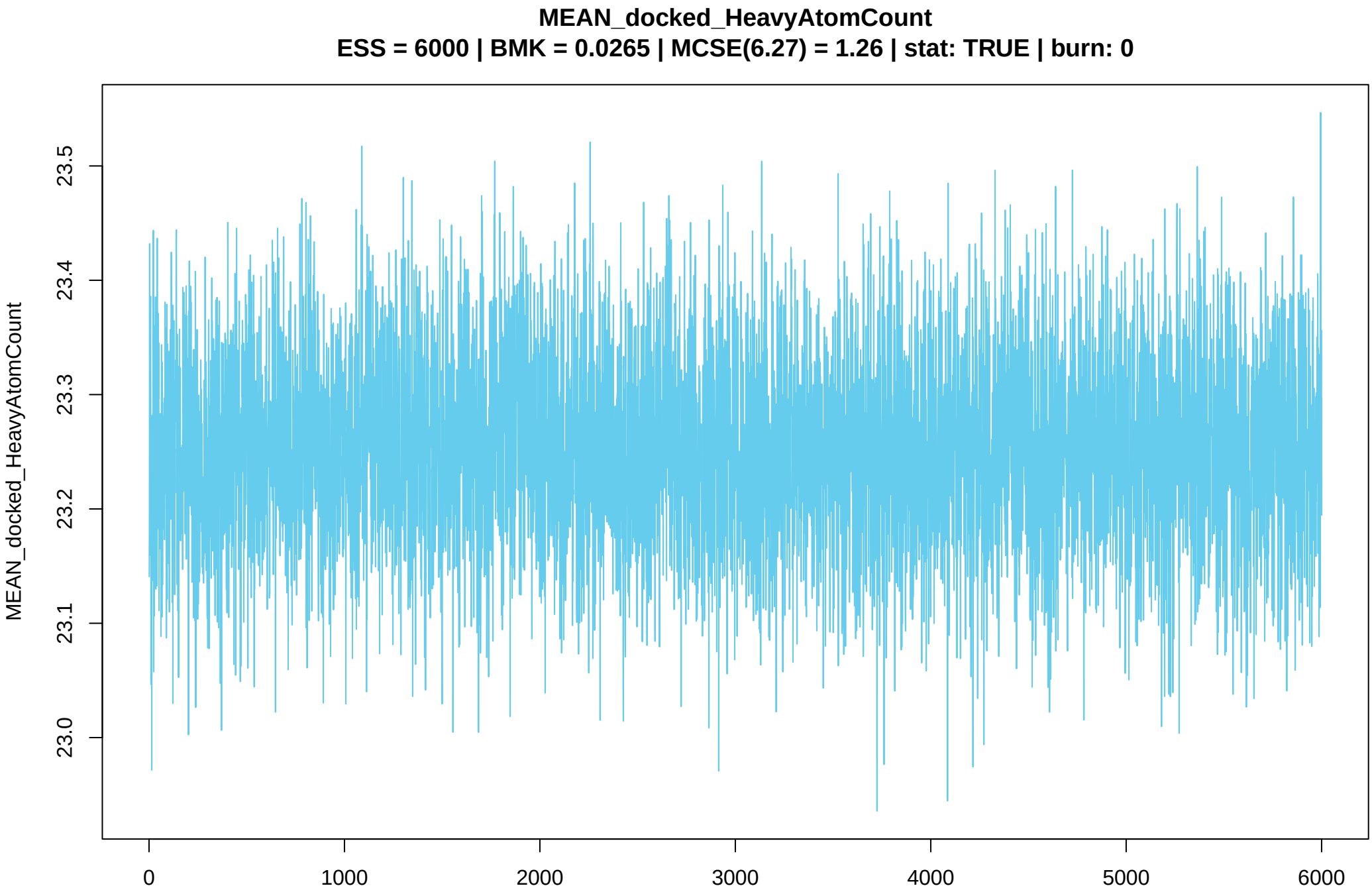

logitDcov
ESS = 2560 | BMK = 0.0444 | MCSE(6.27) = 1.67 | stat: FALSE | burn: 0
logitDcov
0.0
0.2
0.4
0.6
0.8
1.0
0
1000
2000
3000
4000
5000
6000

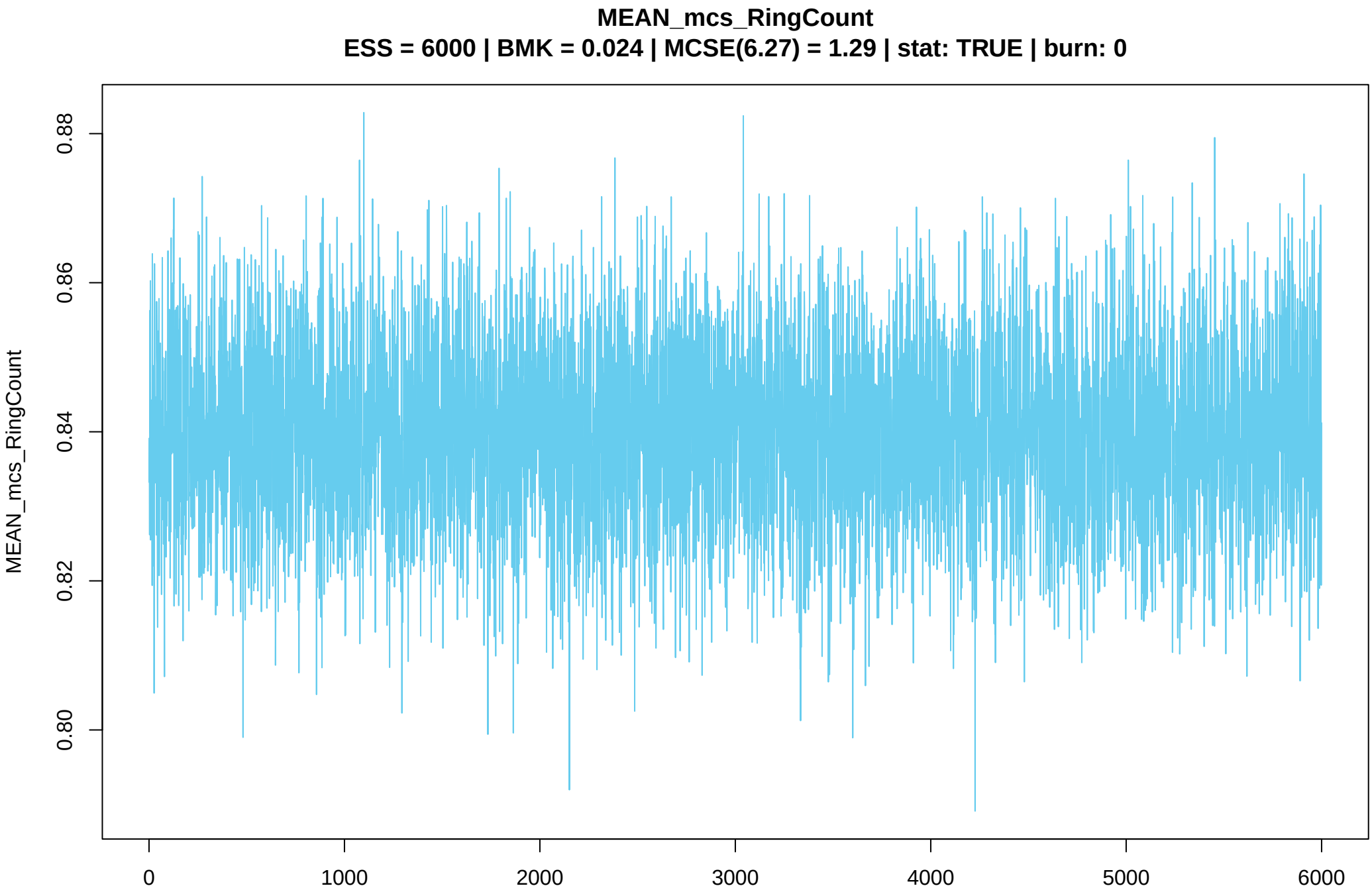

MEAN_log_RMSD
ESS = 5700 | BMK = 0.0369 | MCSE(6.27) = 1.48 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.26
1.24
1.22
1.20
1.18
0
1000
2000
3000
4000
5000
6000

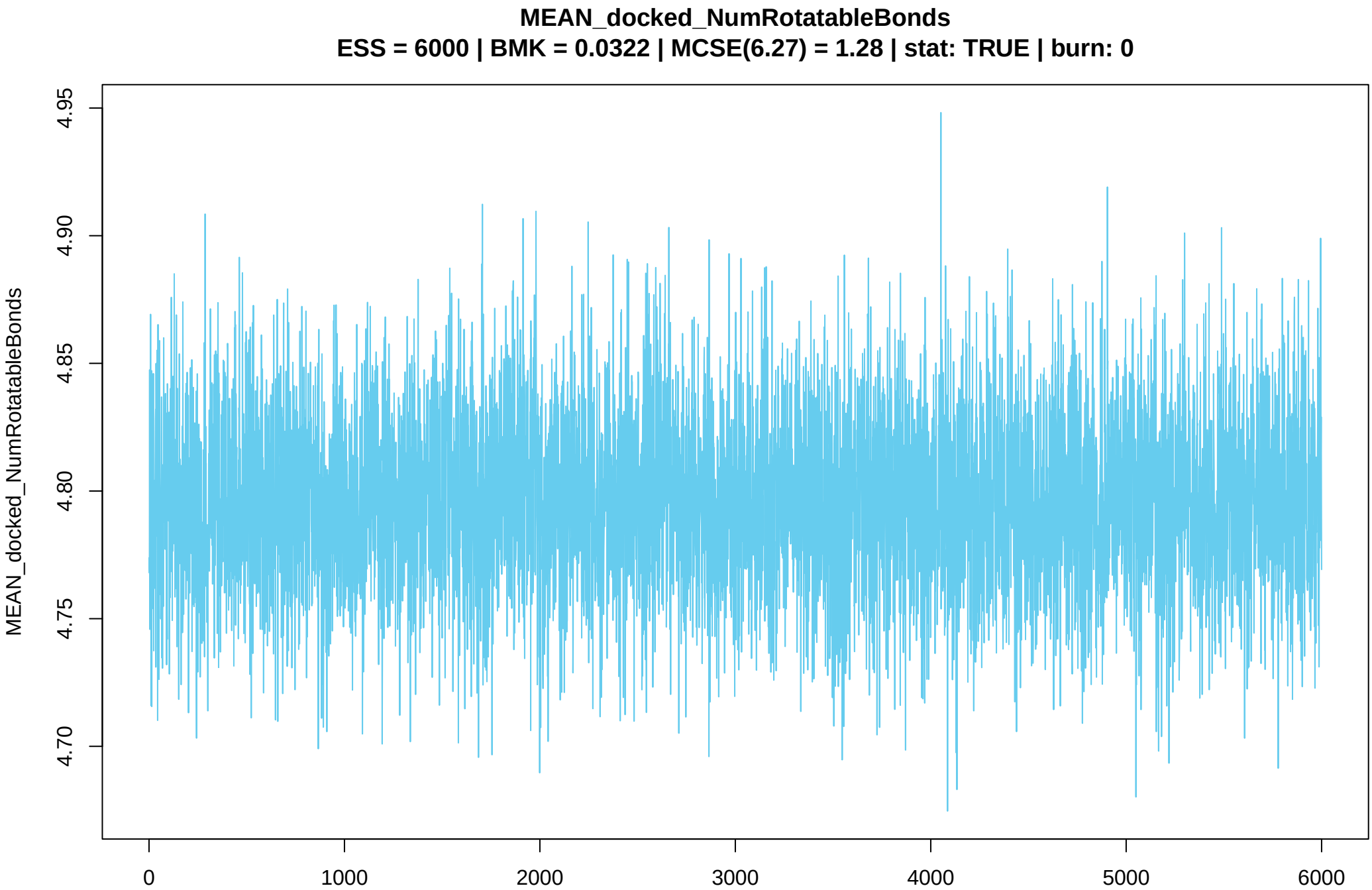

MEAN_log_mcs_unbonded_polar_sasa
ESS = 6000 | BMK = 0.031 | MCSE(6.27) = 1.26 | stat: TRUE | burn: 0
MEAN_log_mcs_unbonded_polar_sasa
−0.30
−0.32
−0.34
−0.36
−0.38
−0.40
0
1000
2000
3000
4000
5000
6000

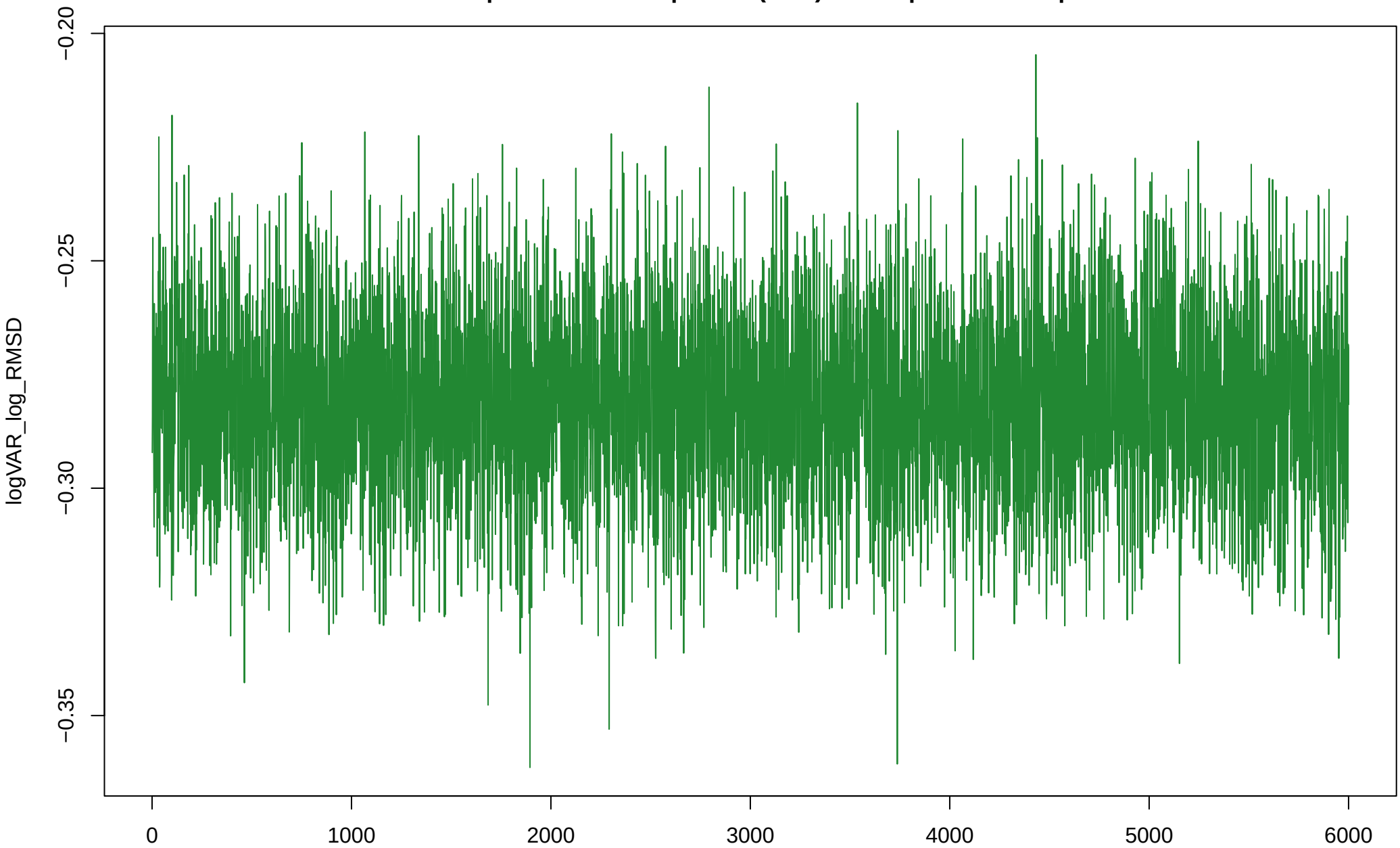

MEAN_logit_ec_tanimoto_similarity
ESS = 5330 | BMK = 0.043 | MCSE(6.27) = 1.47 | stat: TRUE | burn: 0
MEAN_logit_ec_tanimoto_similarity
−2.02
−2.04
−2.06
−2.08
−2.10
−2.12
0
1000
2000
3000
4000
5000
6000

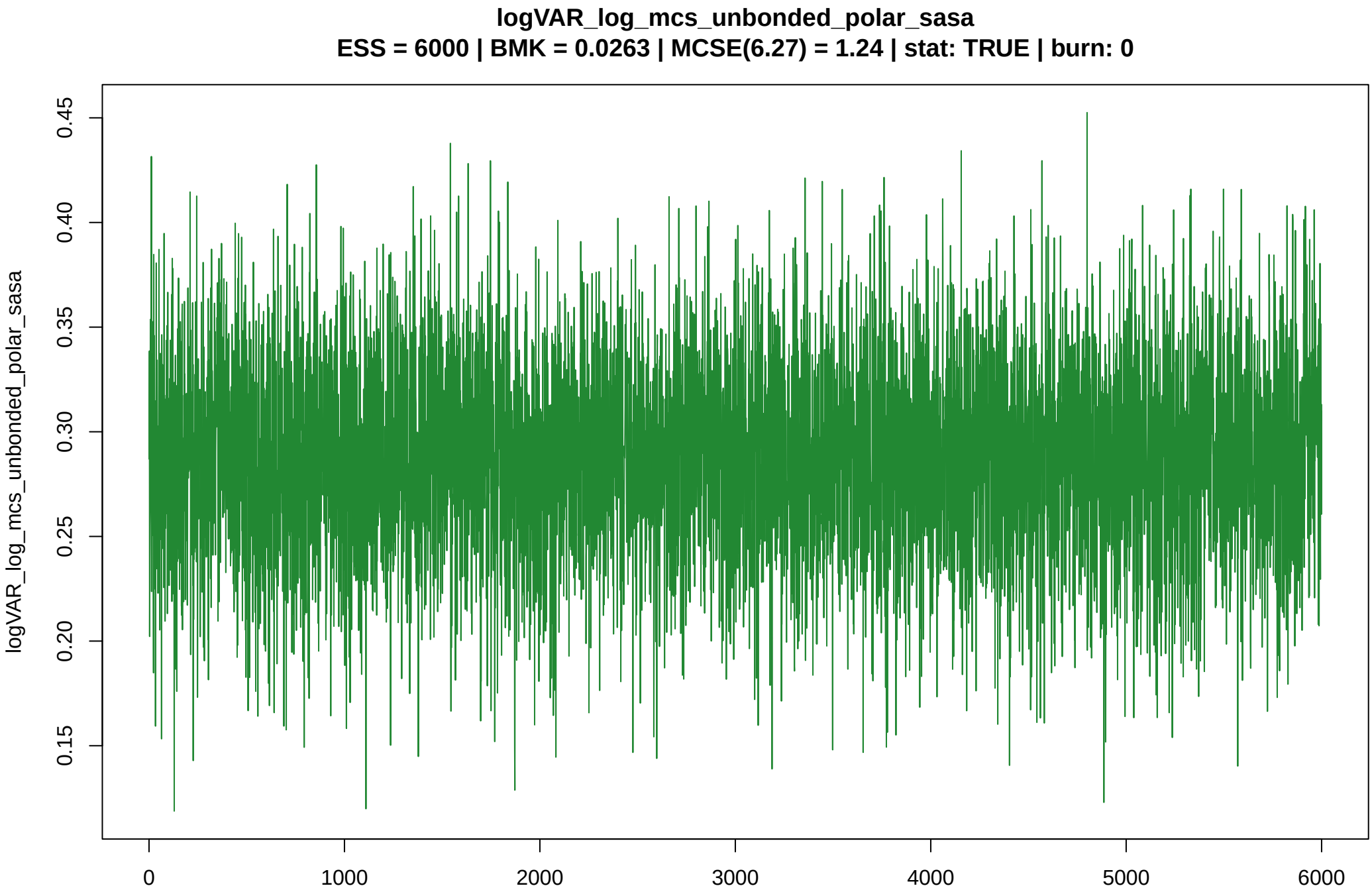

MEAN_mcs_NumHeteroAtoms
ESS = 6000 | BMK = 0.0347 | MCSE(6.27) = 1.29 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
2.90
2.95
3.00
3.05
0
1000
2000
3000
4000
5000
6000

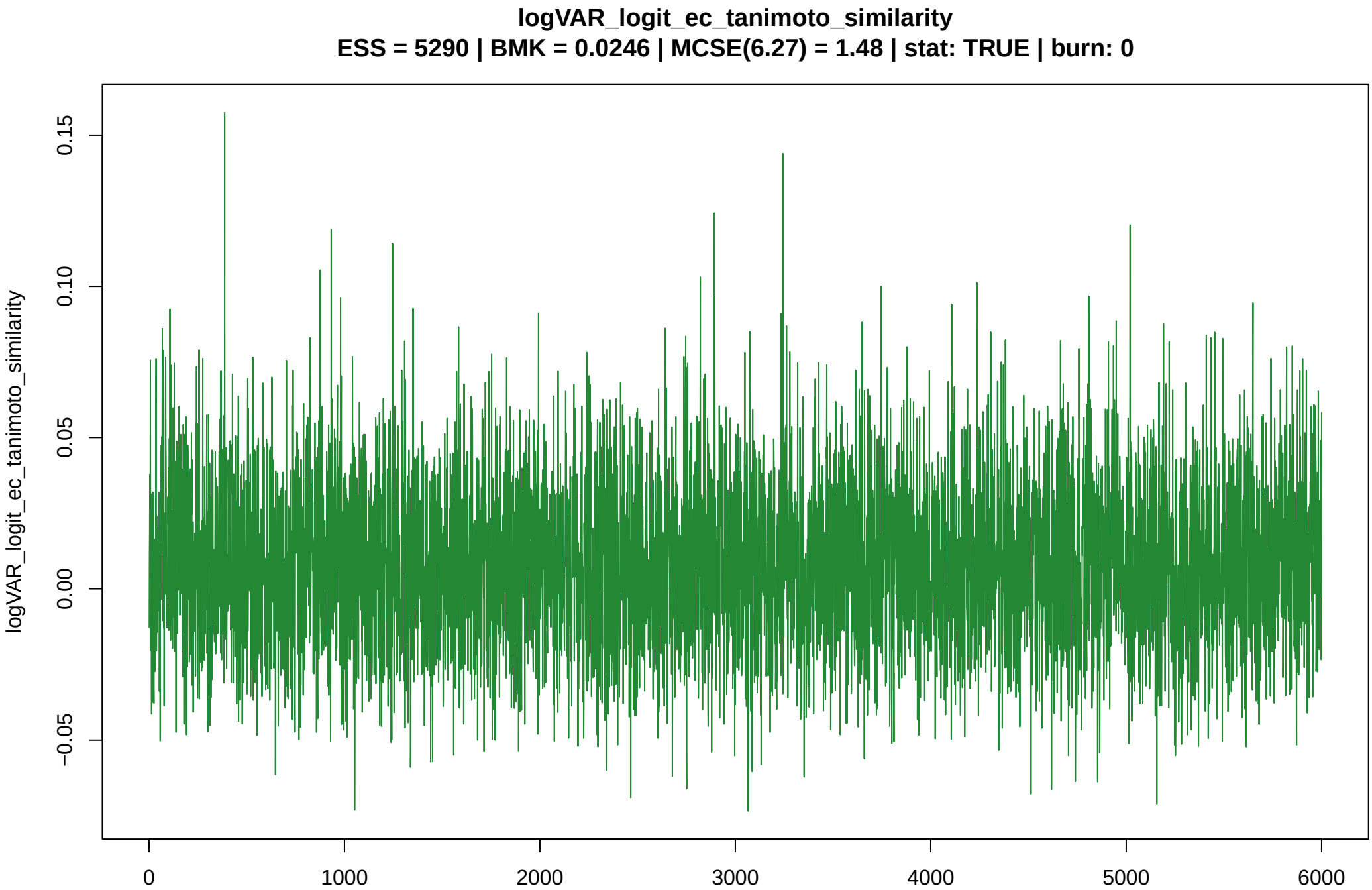

MEAN_docked_HeavyAtomCount
ESS = 6000 | BMK = 0.0265 | MCSE(6.27) = 1.26 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
23.0
23.1
23.2
23.3
23.4
23.5
0
1000
2000
3000
4000
5000
6000

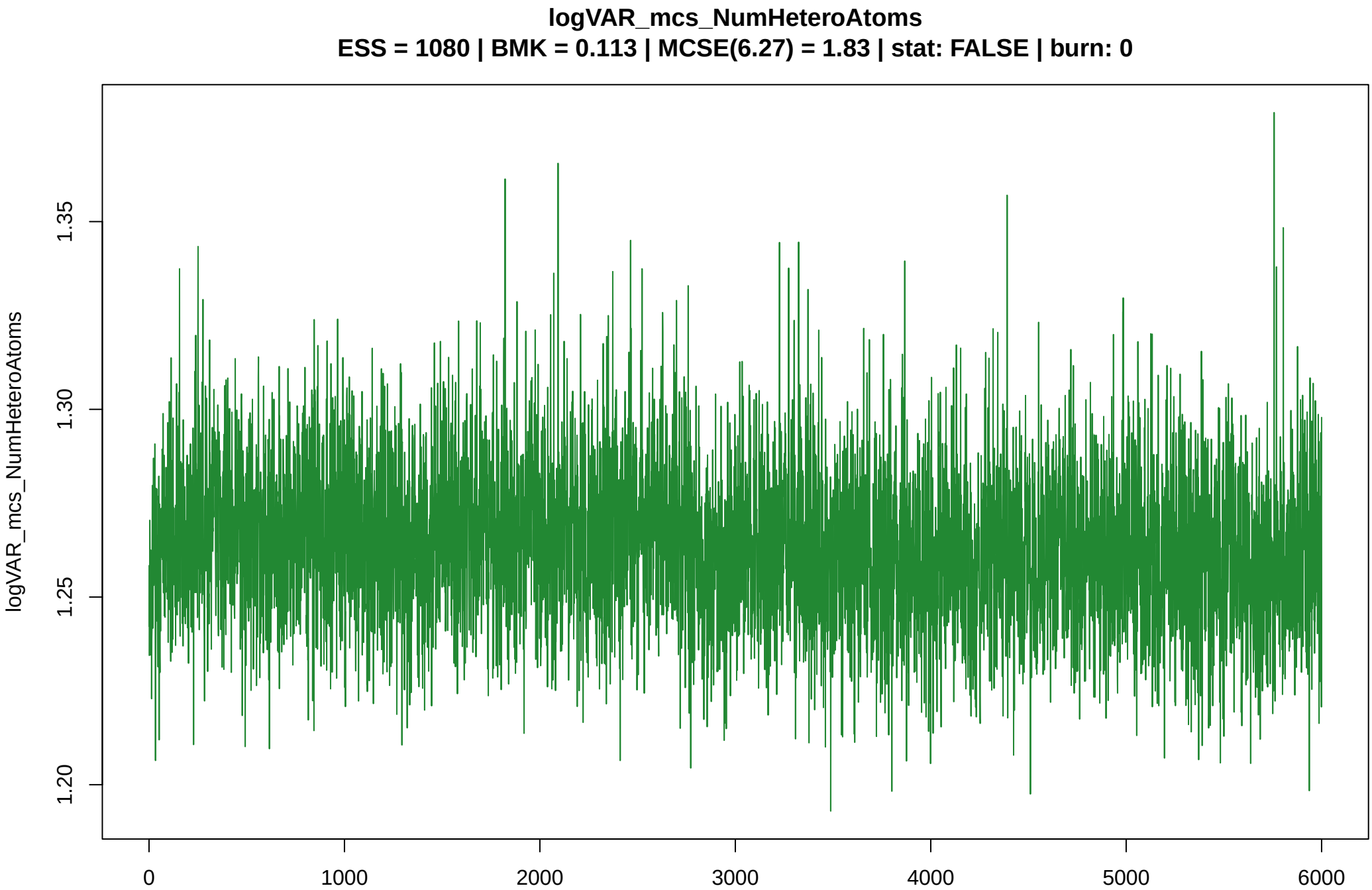

MEAN_mcs_RingCount
ESS = 6000 | BMK = 0.024 | MCSE(6.27) = 1.29 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.80
0.82
0.84
0.86
0.88
0
1000
2000
3000
4000
5000
6000

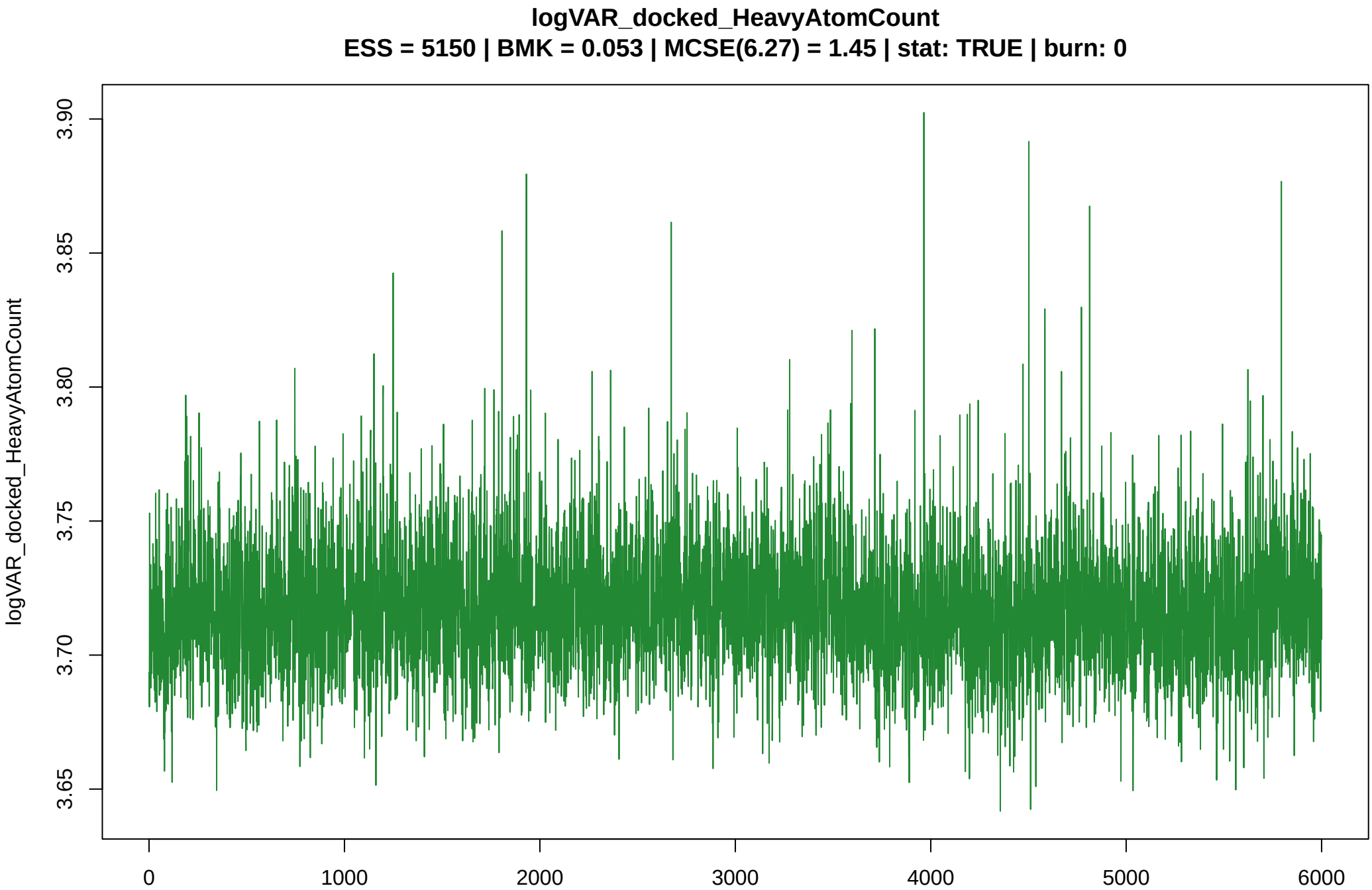

MEAN_docked_NumRotatableBonds
ESS = 6000 | BMK = 0.0322 | MCSE(6.27) = 1.28 | stat: TRUE | burn: 0
MEAN_docked_NumRotatableBonds
4.70
4.75
4.80
4.85
4.90
4.95
0
1000
2000
3000
4000
5000
6000

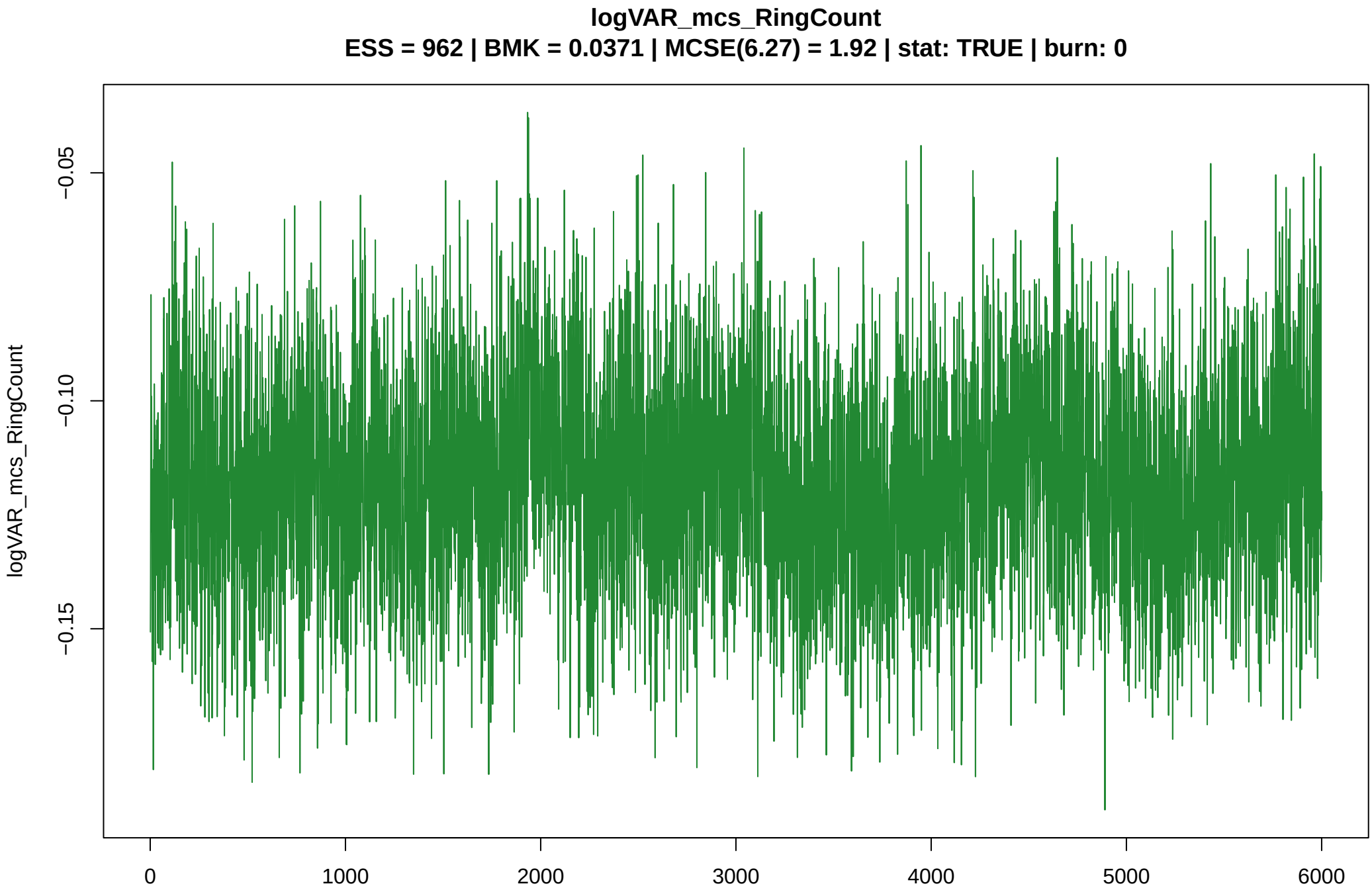

logVAR_log_RMSD
ESS = 5350 | BMK = 0.0201 | MCSE(6.27) = 1.42 | stat: TRUE | burn: 0
logVAR_log_RMSD
−0.20
−0.25
−0.30
−0.35
0
1000
2000
3000
4000
5000
6000

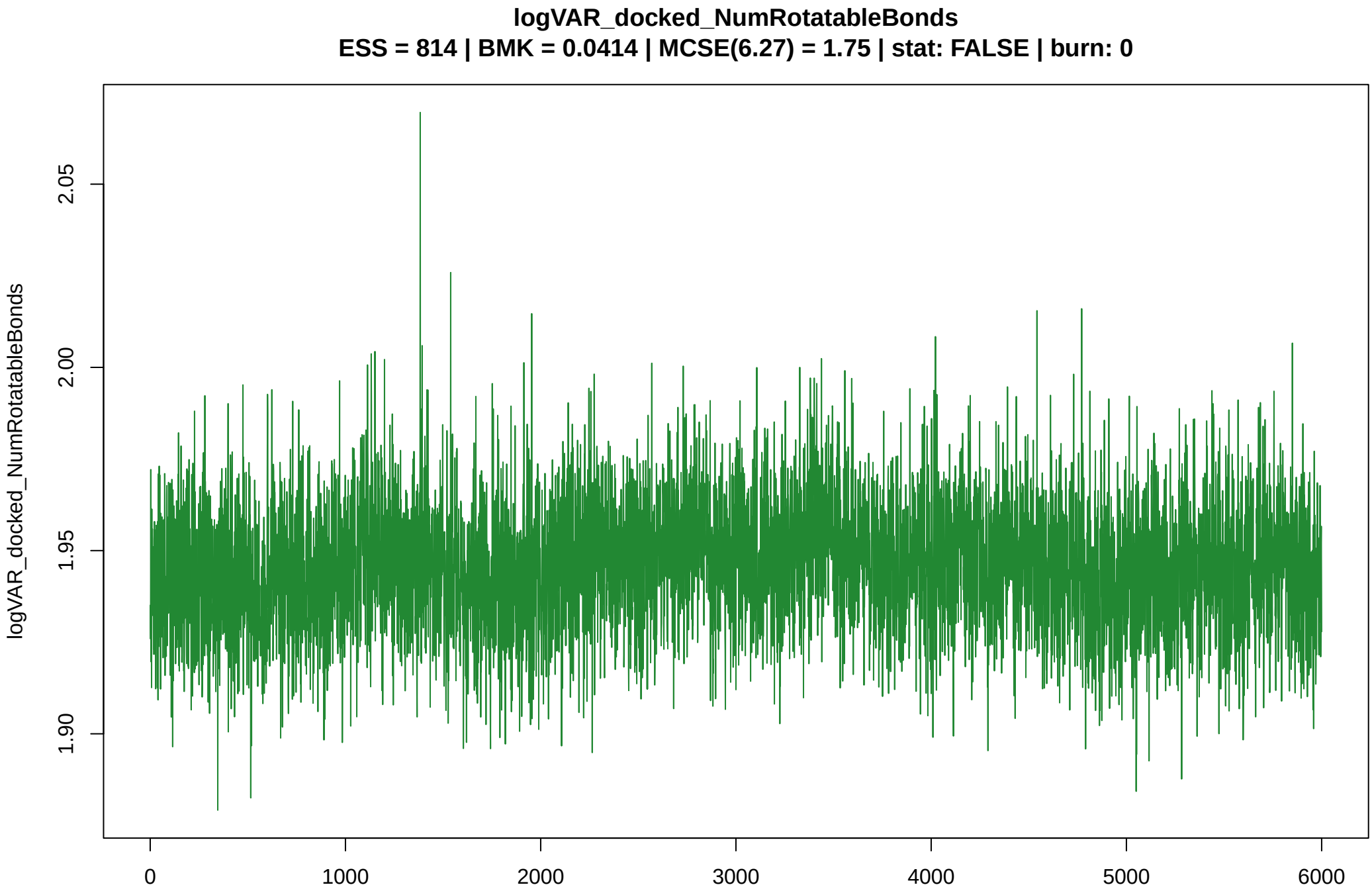

logVAR_log_mcs_unbonded_polar_sasa
ESS = 6000 | BMK = 0.0263 | MCSE(6.27) = 1.24 | stat: TRUE | burn: 0
logVAR_log_mcs_unbonded_polar_sasa
0.15
0.20
0.25
0.30
0.35
0.40
0.45
0
1000
2000
3000
4000
5000
6000

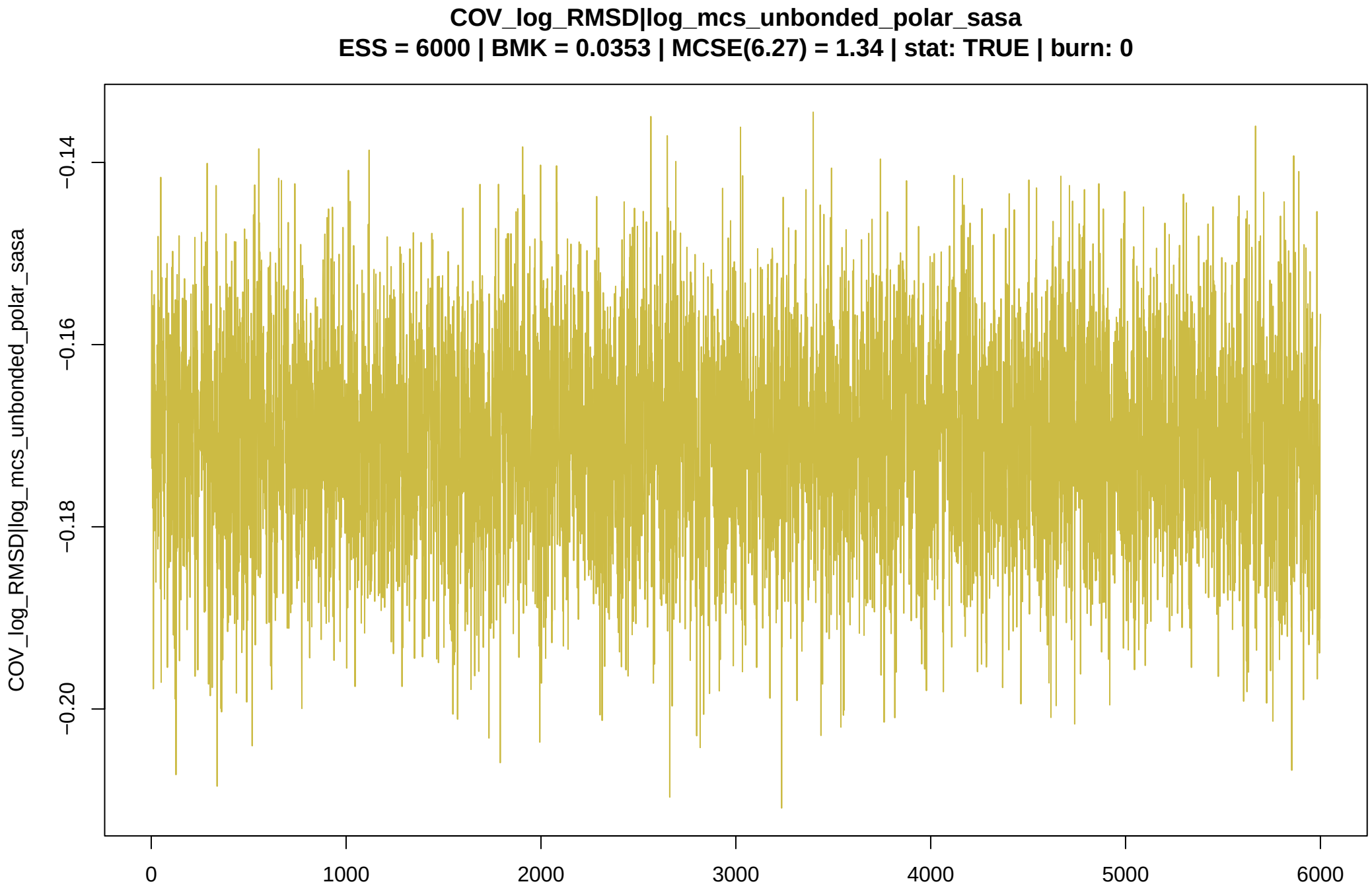

logVAR_logit_ec_tanimoto_similarity
ESS = 5290 | BMK = 0.0246 | MCSE(6.27) = 1.48 | stat: TRUE | burn: 0
logVAR_logit_ec_tanimoto_similarity
0.15
0.10
0.05
0.00
−0.05
0
1000
2000
3000
4000
5000
6000

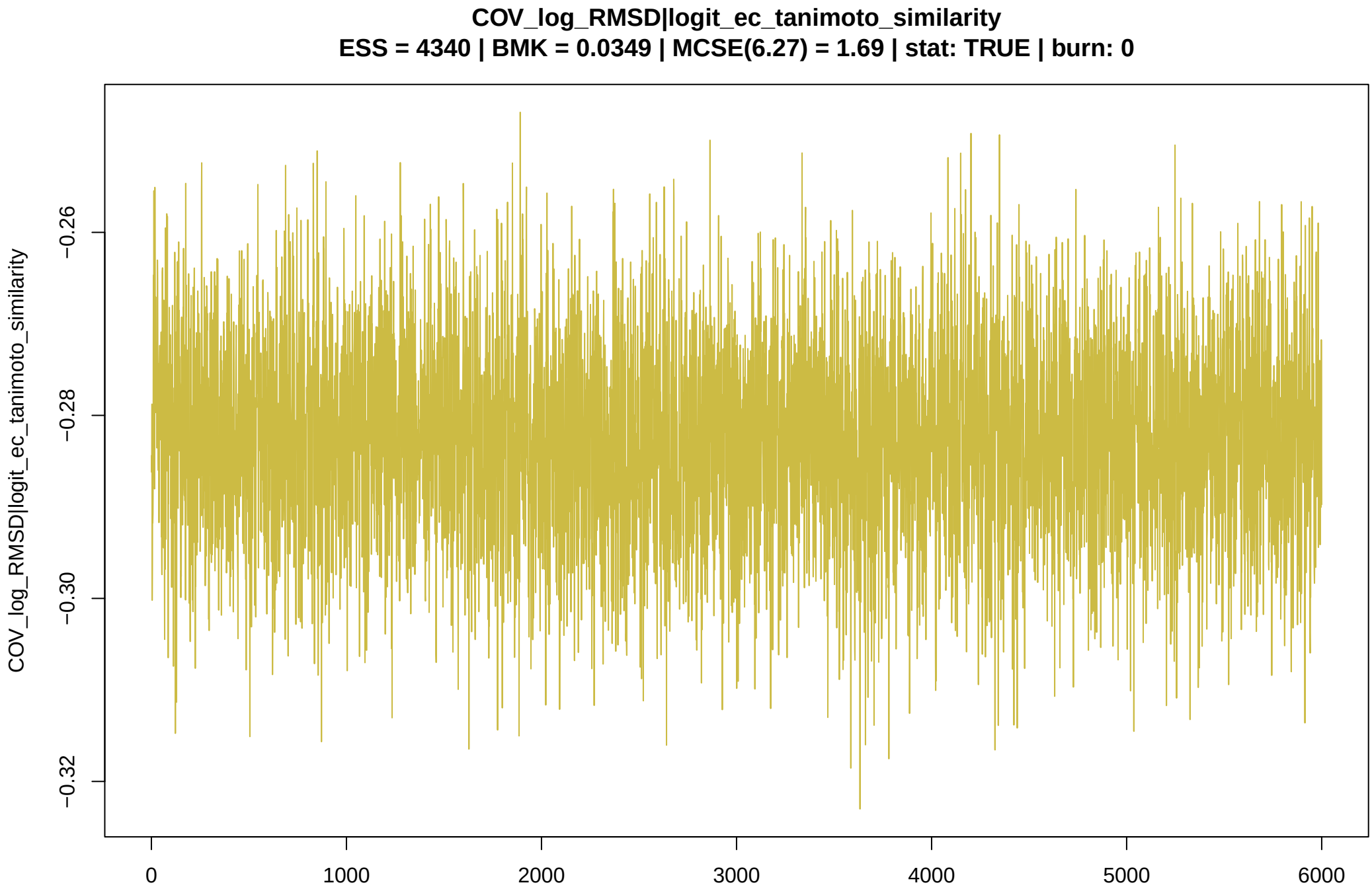

logVAR_mcs_NumHeteroAtoms
ESS = 1080 | BMK = 0.113 | MCSE(6.27) = 1.83 | stat: FALSE | burn: 0
logVAR_mcs_NumHeteroAtoms
1.20
1.25
1.30
1.35
0
1000
2000
3000
4000
5000
6000

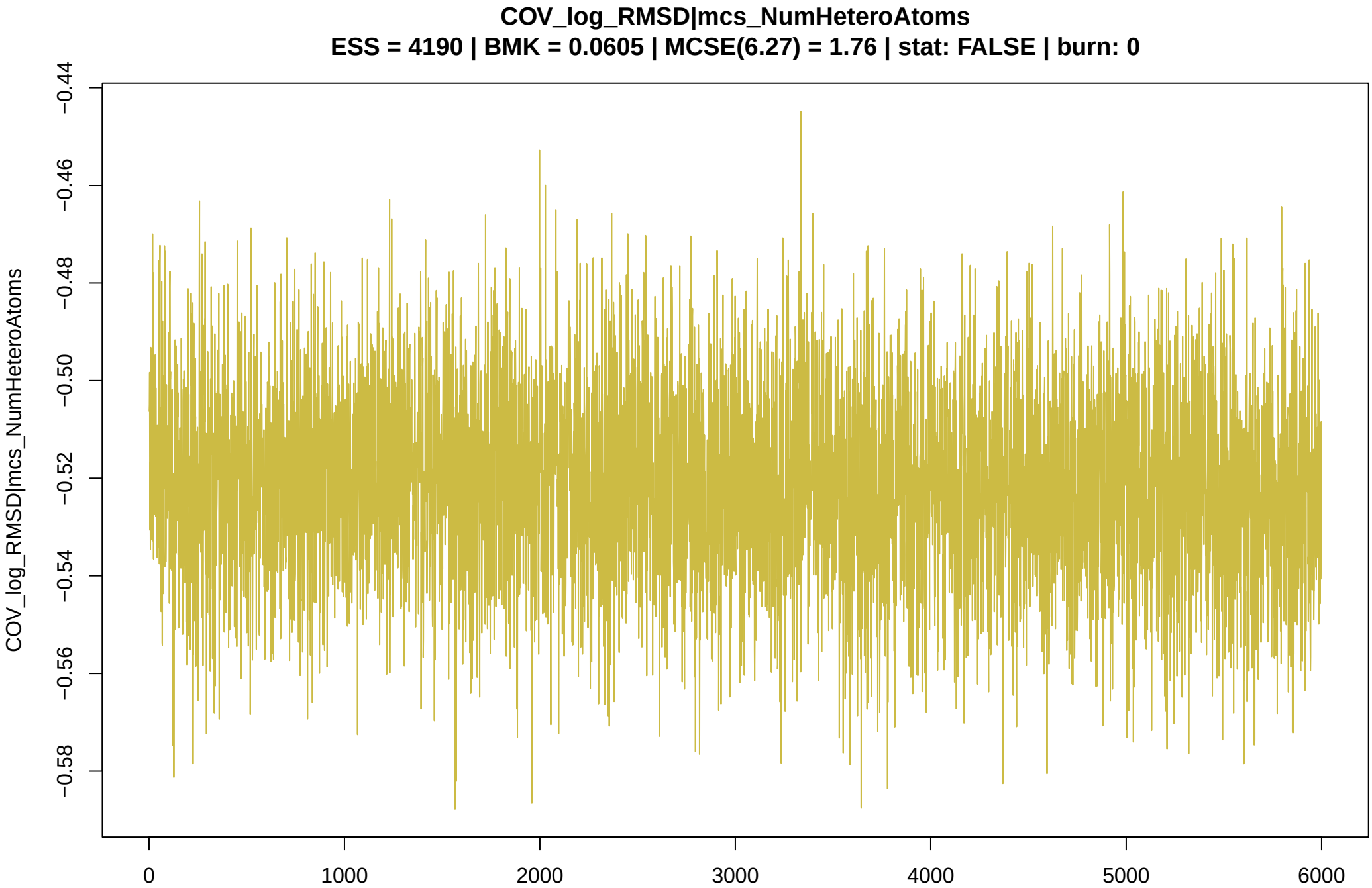

logVAR_docked_HeavyAtomCount
ESS = 5150 | BMK = 0.053 | MCSE(6.27) = 1.45 | stat: TRUE | burn: 0
logVAR_docked_HeavyAtomCount
3.65
3.70
3.75
3.80
3.85
3.90
0
1000
2000
3000
4000
5000
6000

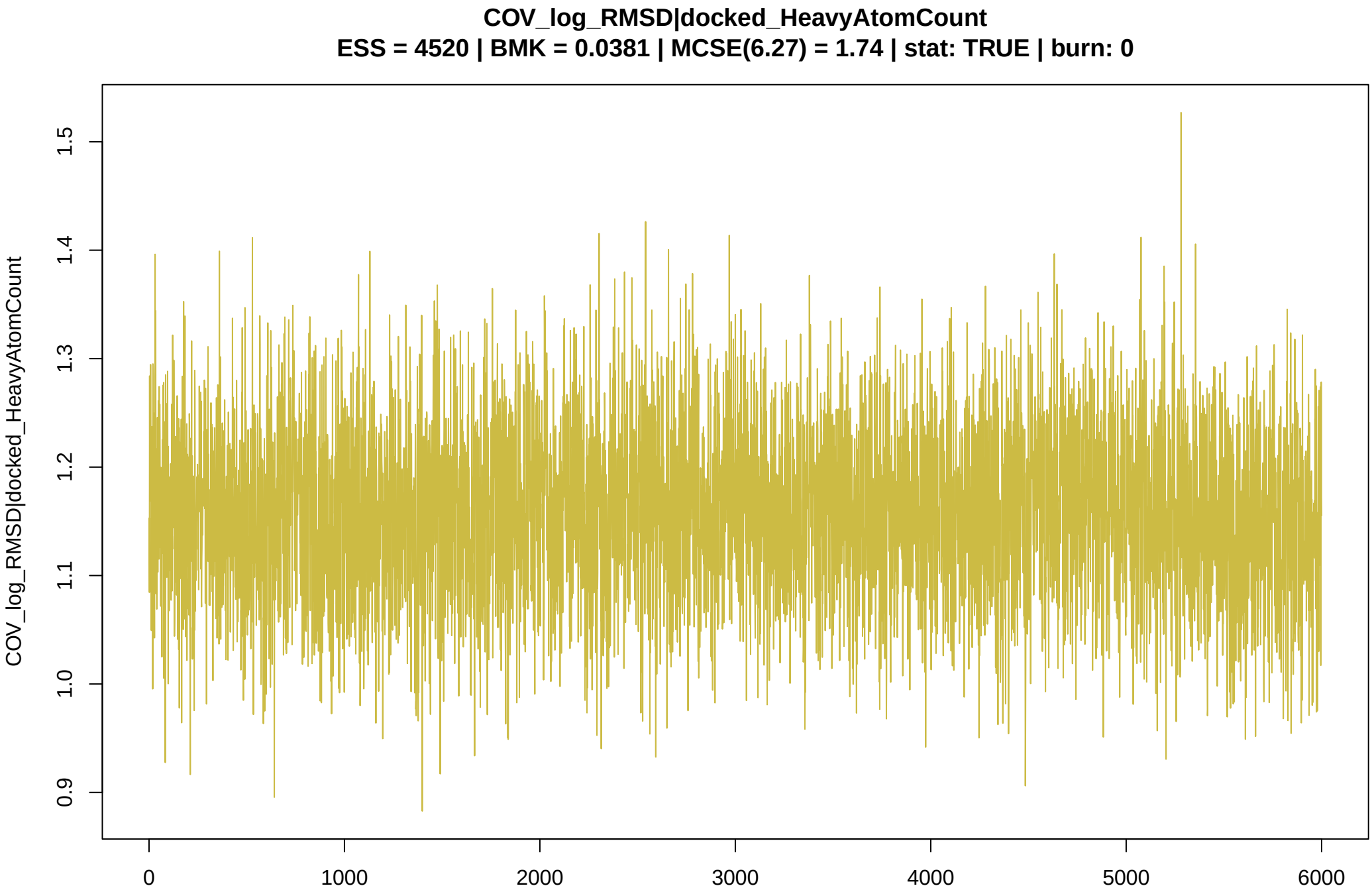

logVAR_mcs_RingCount
ESS = 962 | BMK = 0.0371 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0
logVAR_mcs_RingCount
−0.05
−0.10
−0.15
0
1000
2000
3000
4000
5000
6000

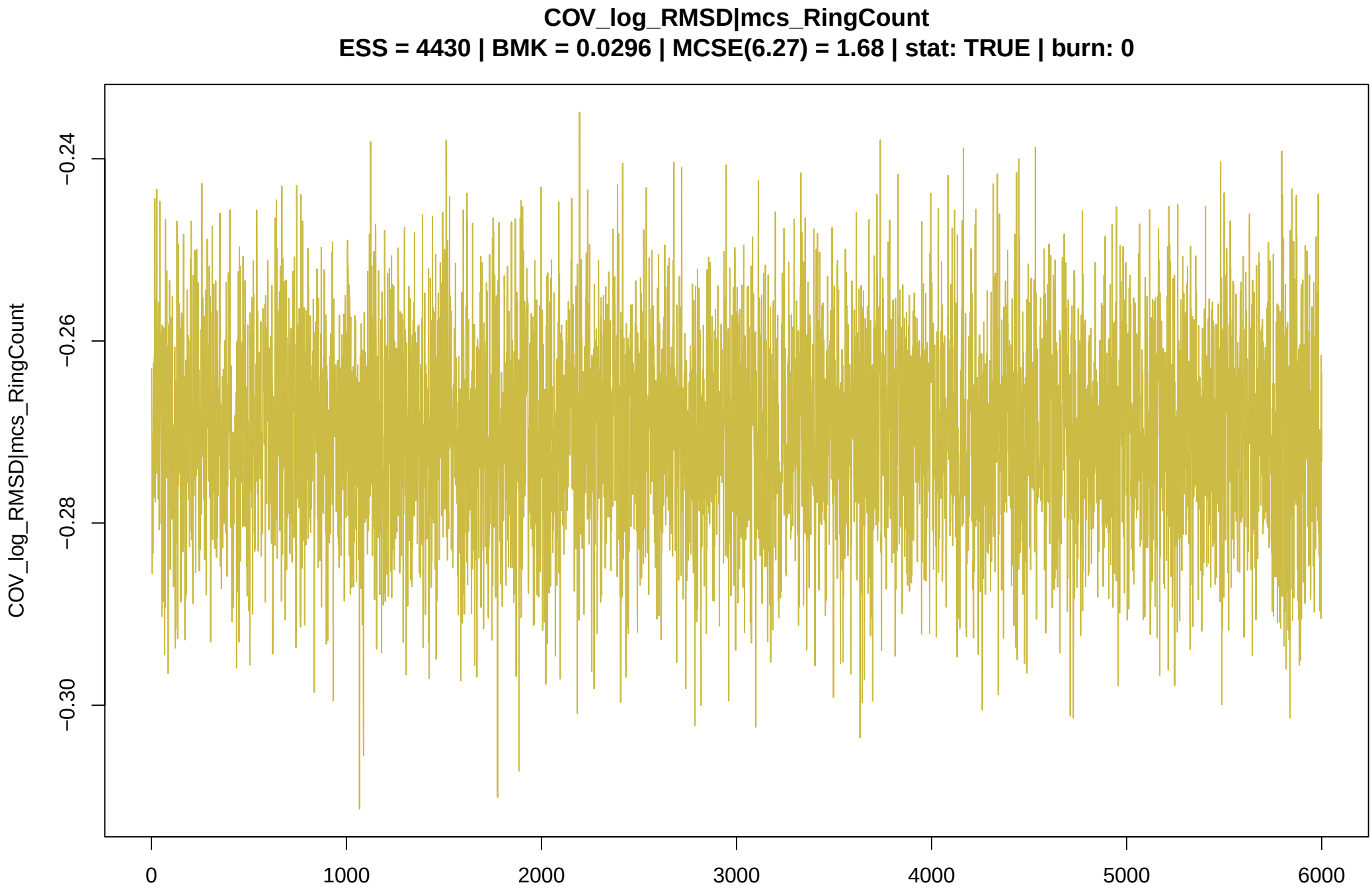

logVAR_docked_NumRotatableBonds
ESS = 814 | BMK = 0.0414 | MCSE(6.27) = 1.75 | stat: FALSE | burn: 0
logVAR_docked_NumRotatableBonds
1.90
1.95
2.00
2.05
0
1000
2000
3000
4000
5000
6000

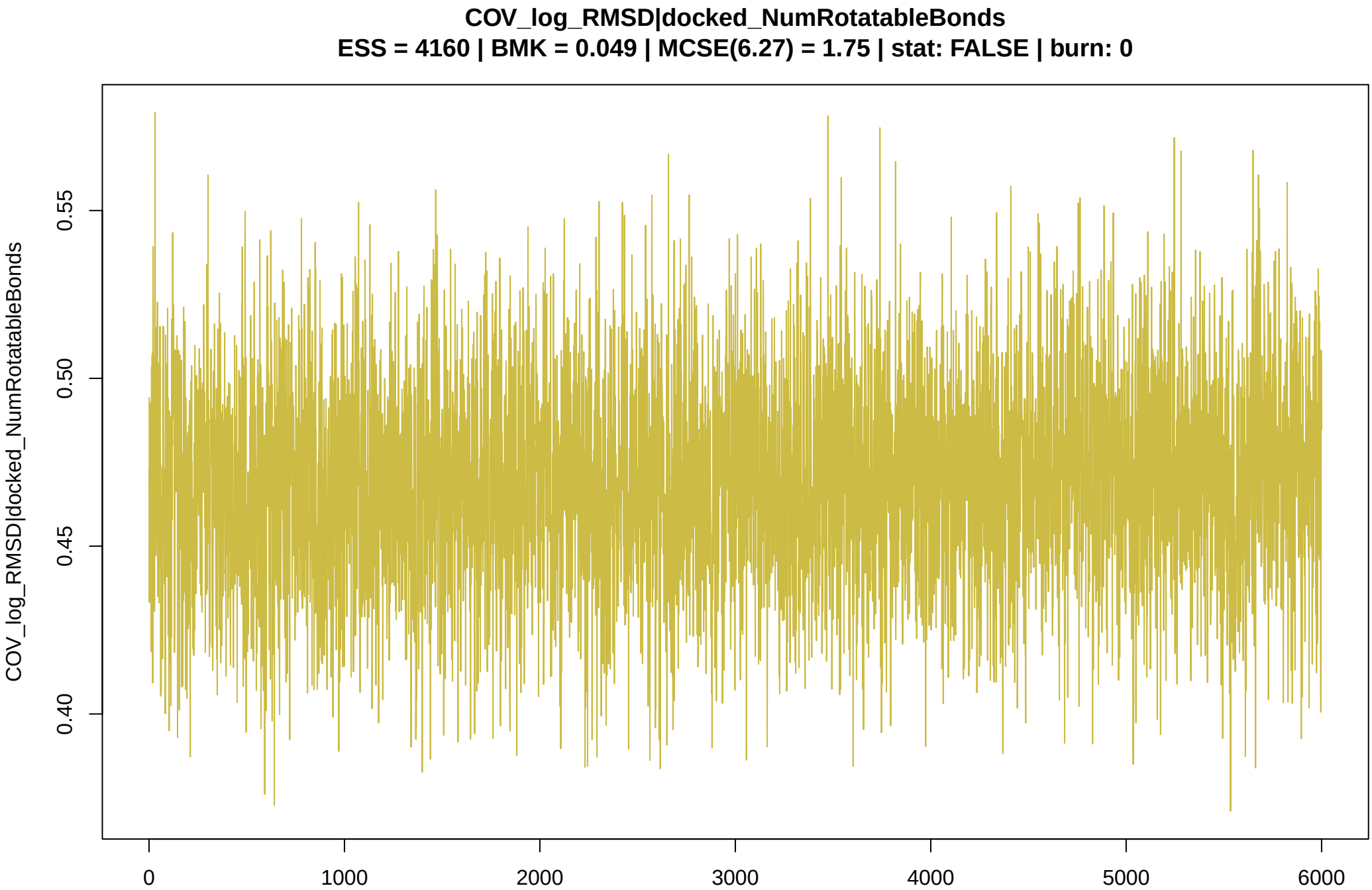

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 6000 | BMK = 0.0353 | MCSE(6.27) = 1.34 | stat: TRUE | burn: 0
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.14
−0.16
−0.18
−0.20
0
1000
2000
3000
4000
5000
6000

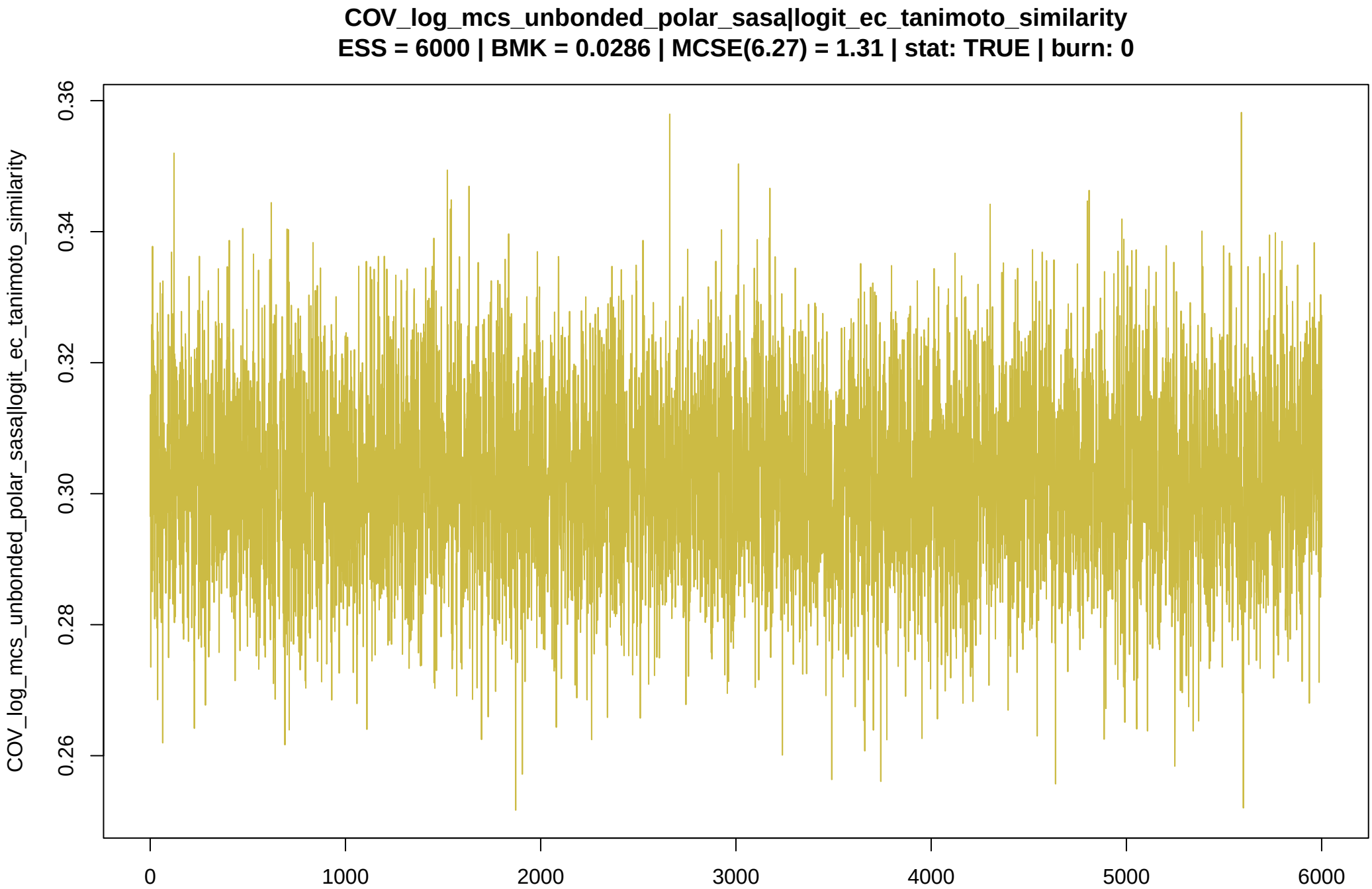

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 4340 | BMK = 0.0349 | MCSE(6.27) = 1.69 | stat: TRUE | burn: 0
COV_log_RMSD|logit_ec_tanimoto_similarity
−0.26
−0.28
−0.30
−0.32
0
1000
2000
3000
4000
5000
6000

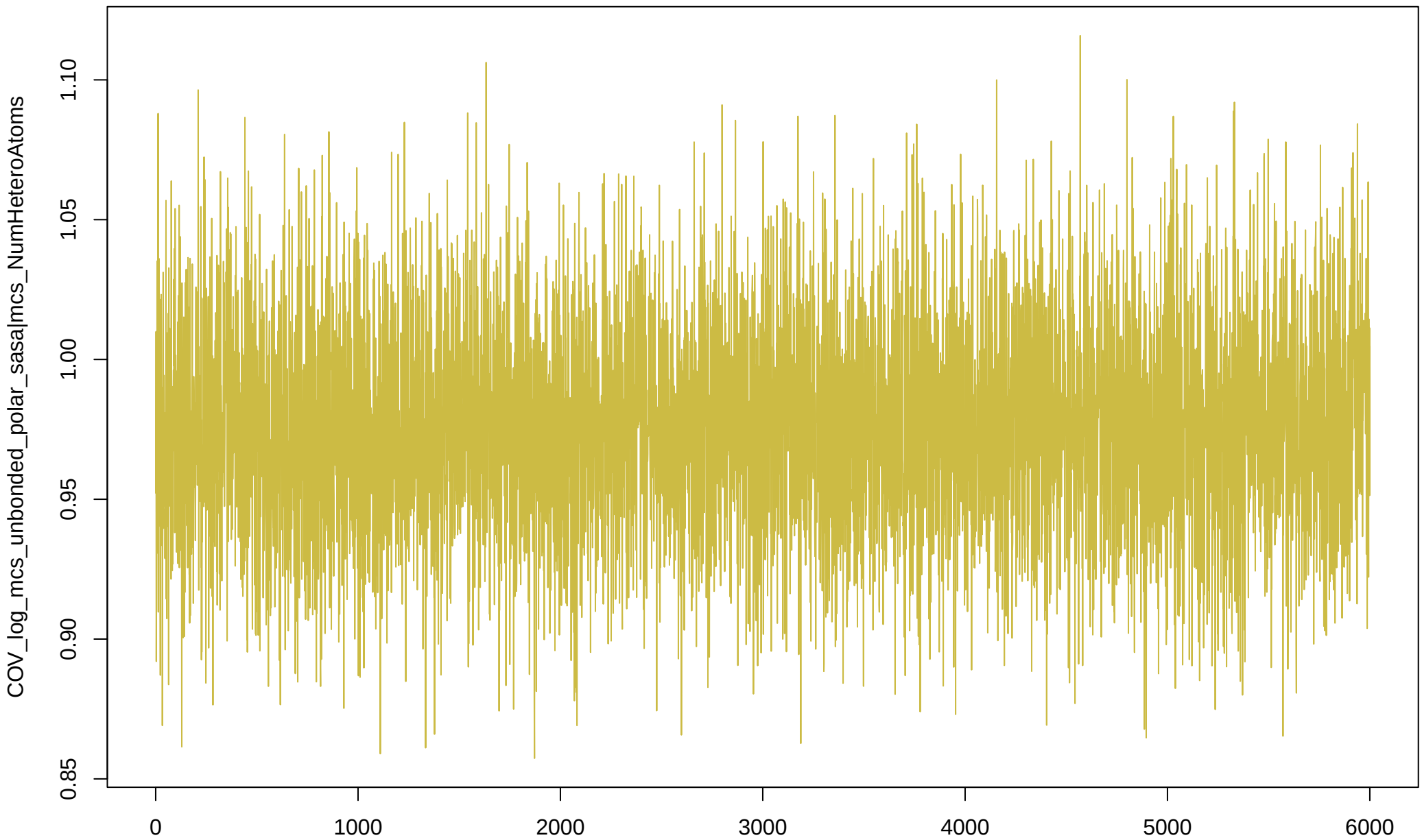

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 4190 | BMK = 0.0605 | MCSE(6.27) = 1.76 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.44
−0.46
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
1000
2000
3000
4000
5000
6000

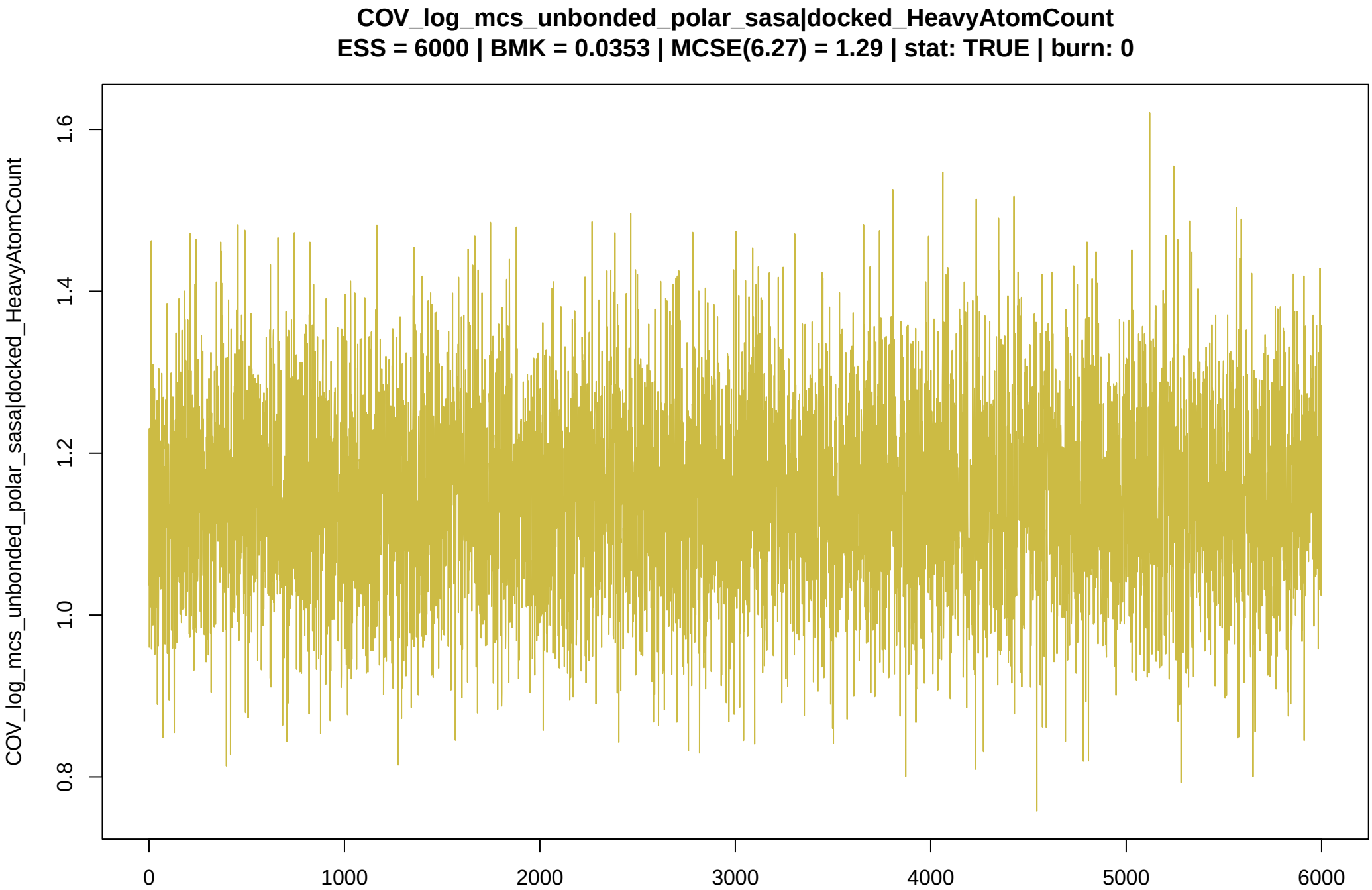

COV_log_RMSD|docked_HeavyAtomCount
ESS = 4520 | BMK = 0.0381 | MCSE(6.27) = 1.74 | stat: TRUE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
0.9
1.0
1.1
1.2
1.3
1.4
1.5
0
1000
2000
3000
4000
5000
6000

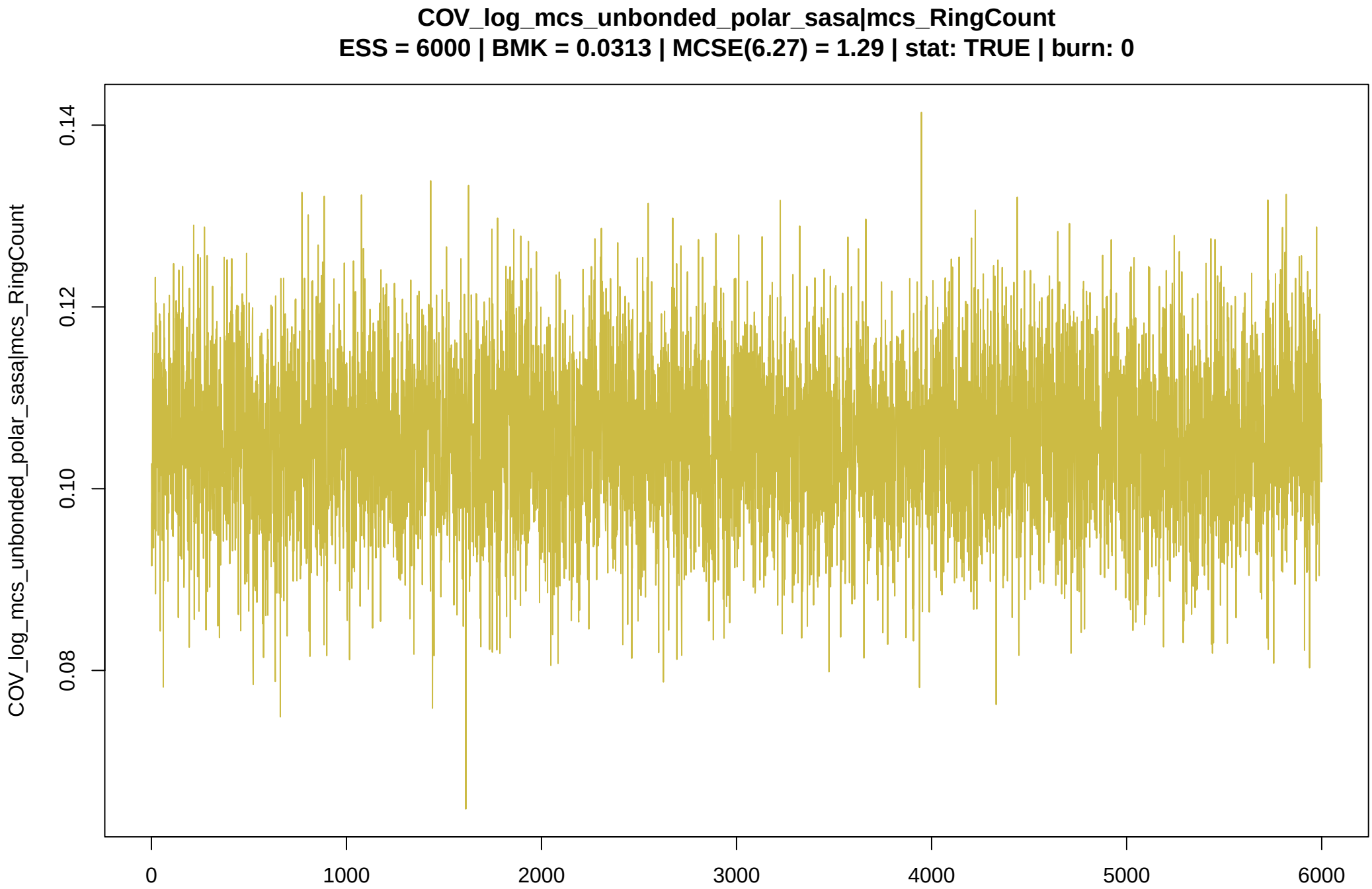

COV_log_RMSD|mcs_RingCount
ESS = 4430 | BMK = 0.0296 | MCSE(6.27) = 1.68 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.24
−0.26
−0.28
−0.30
0
1000
2000
3000
4000
5000
6000

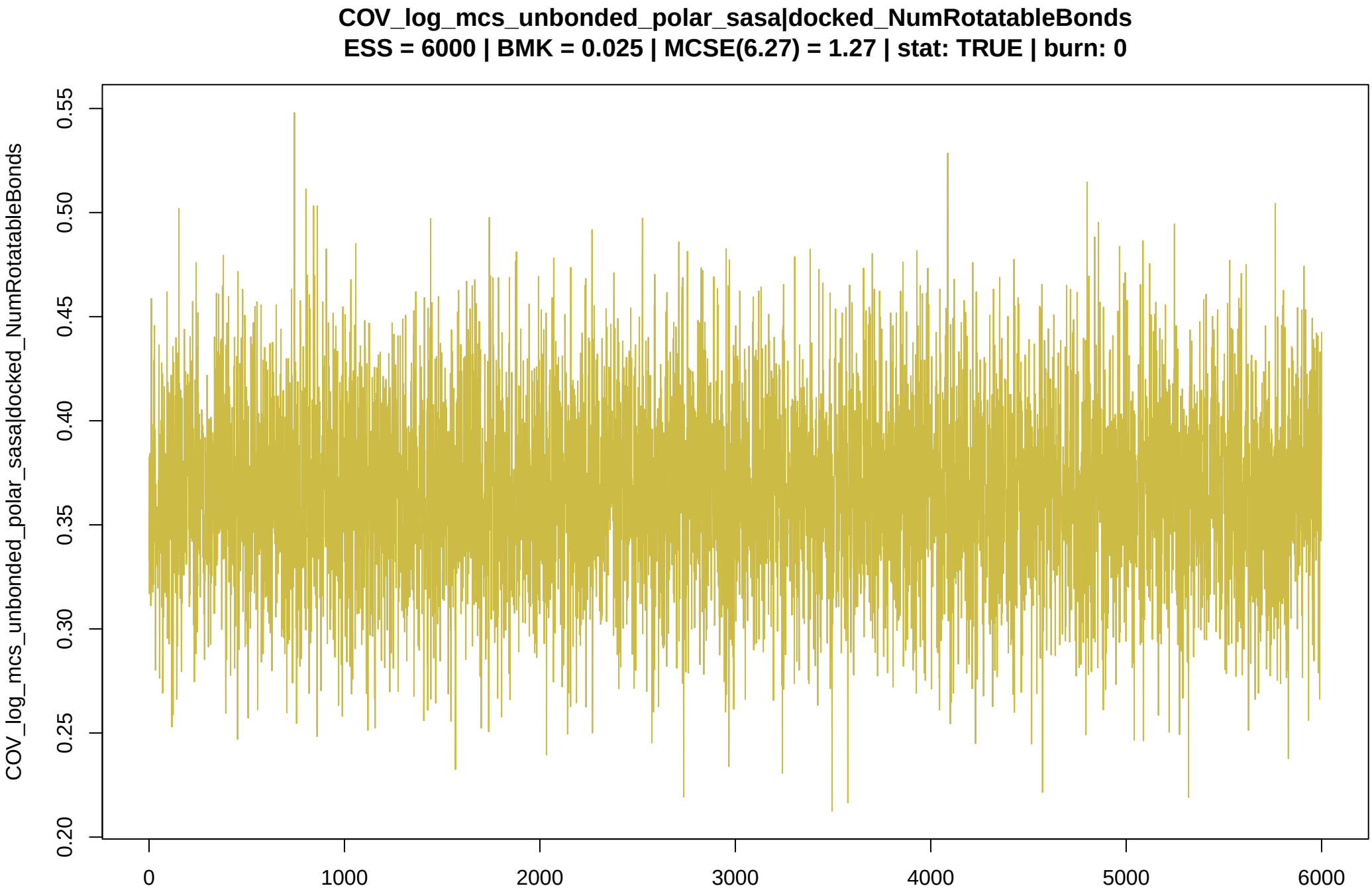

COV_log_RMSD|docked_NumRotatableBonds
ESS = 4160 | BMK = 0.049 | MCSE(6.27) = 1.75 | stat: FALSE | burn: 0
COV_log_RMSD|docked_NumRotatableBonds
0.40
0.45
0.50
0.55
0
1000
2000
3000
4000
5000
6000

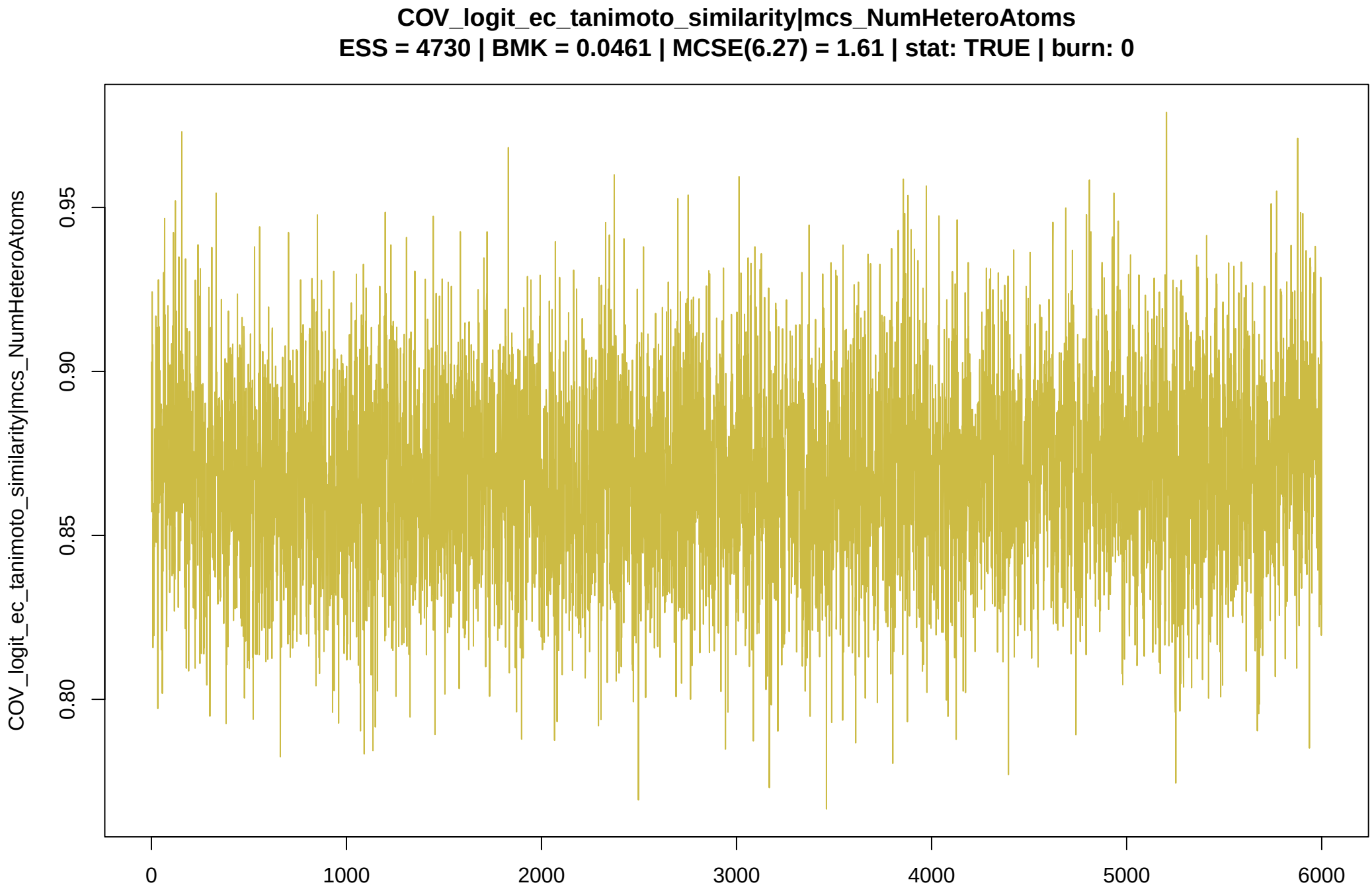

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 6000 | BMK = 0.0286 | MCSE(6.27) = 1.31 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0.26
0.28
0.30
0.32
0.34
0.36
0
1000
2000
3000
4000
5000
6000

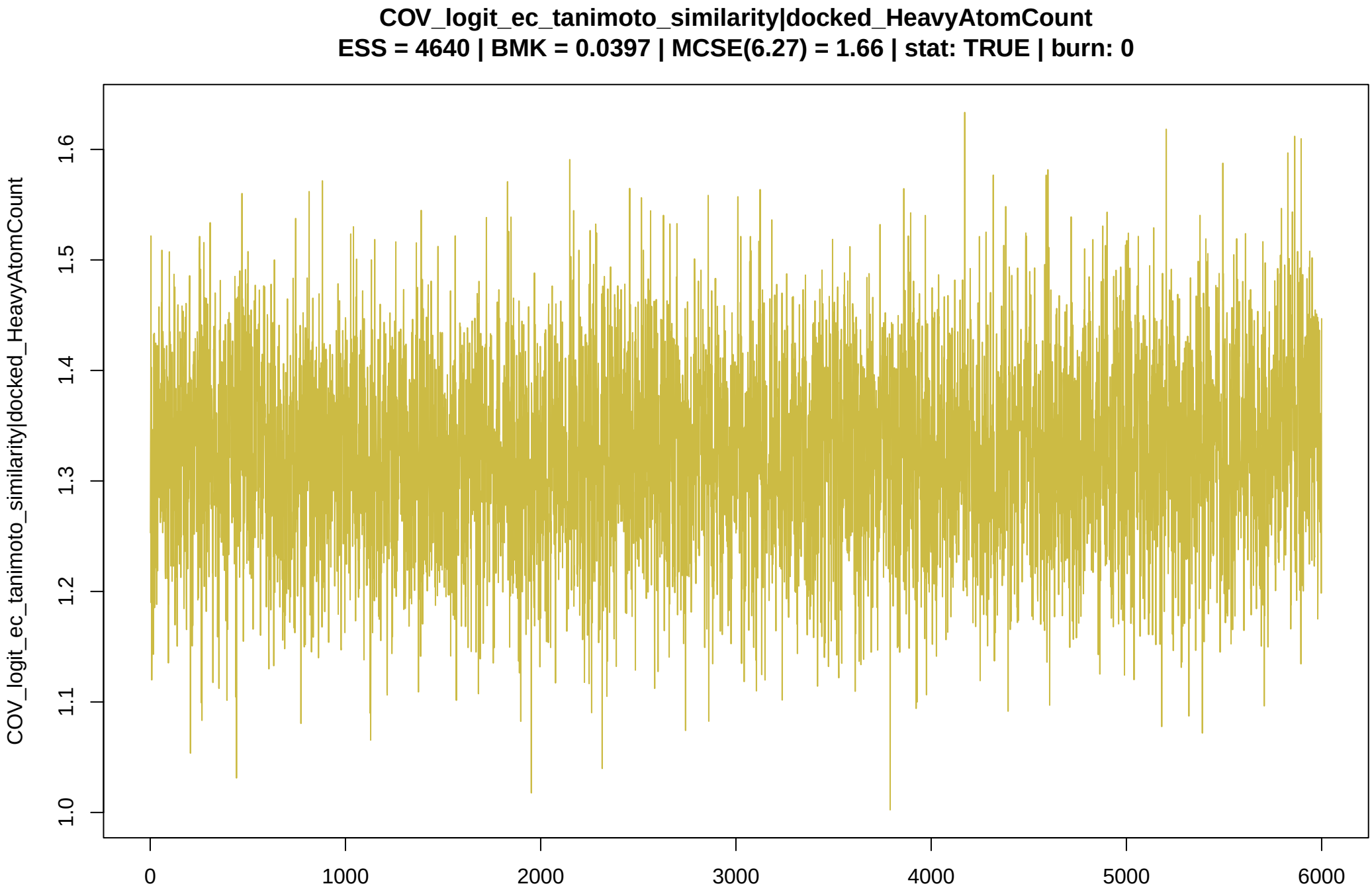

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 6000 | BMK = 0.0285 | MCSE(6.27) = 1.25 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.85
0.90
0.95
1.00
1.05
1.10
0
1000
2000
3000
4000
5000
6000

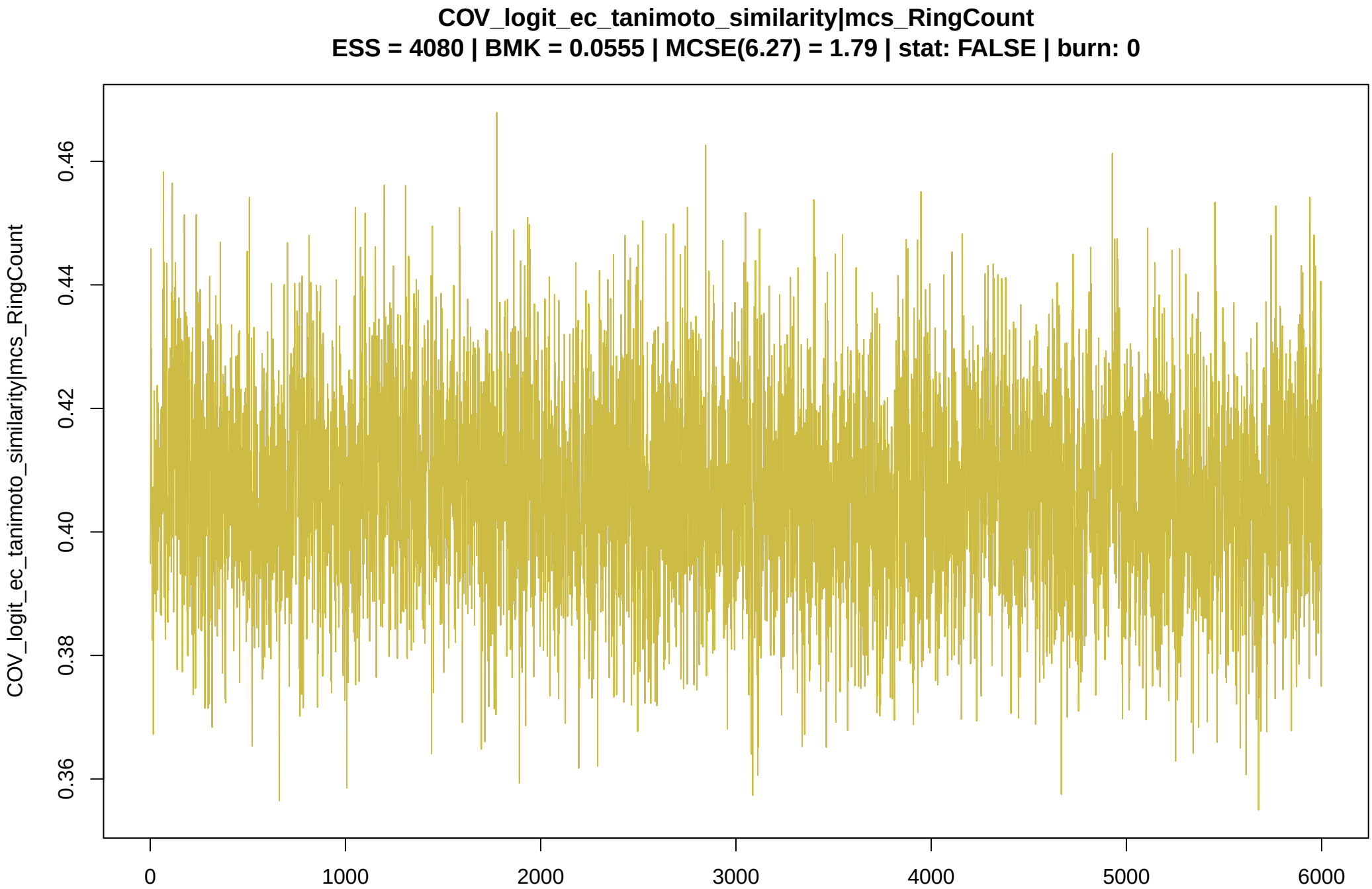

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 6000 | BMK = 0.0353 | MCSE(6.27) = 1.29 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0.8
1.0
1.2
1.4
1.6
0
1000
2000
3000
4000
5000
6000

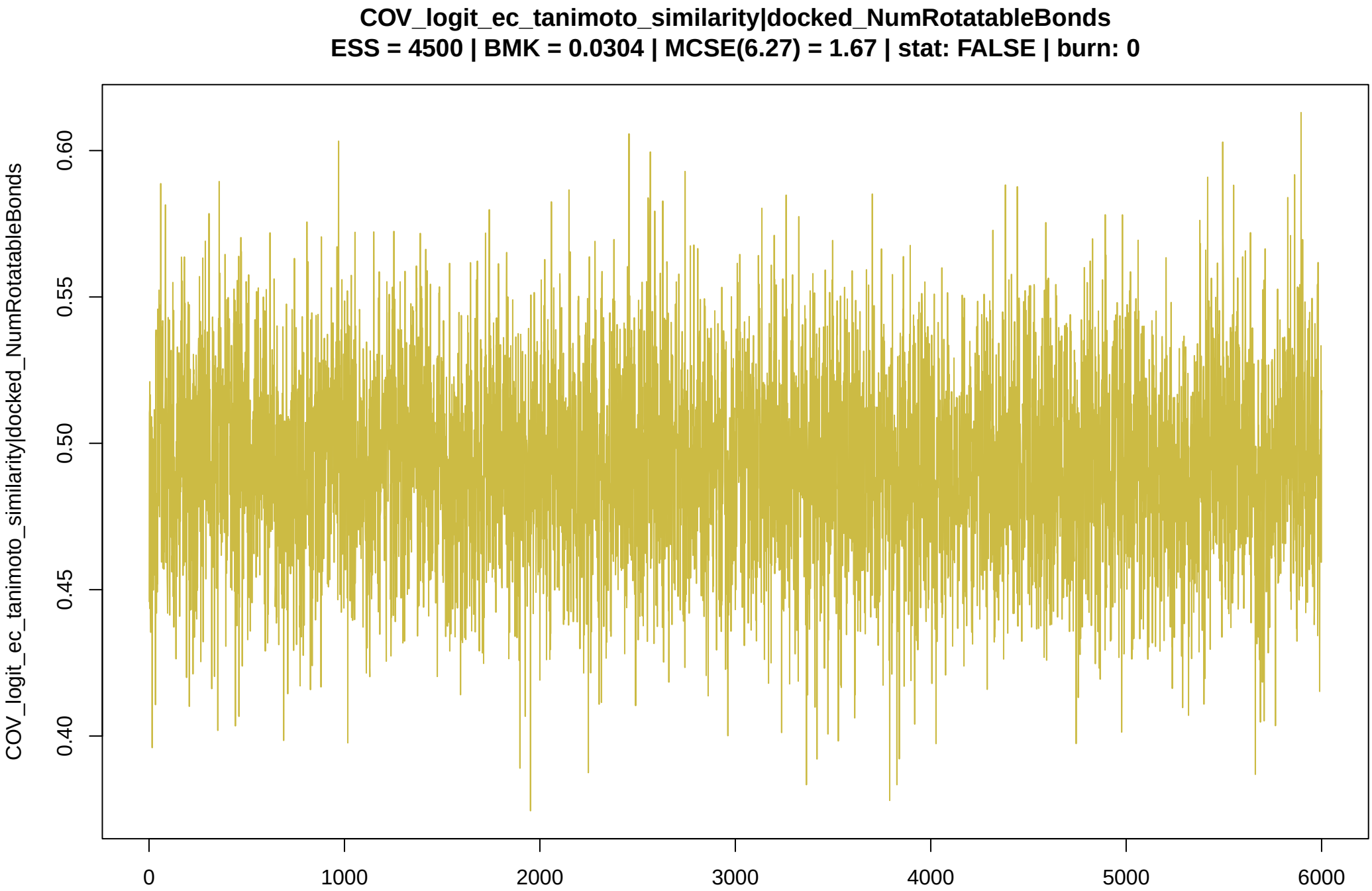

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 6000 | BMK = 0.0313 | MCSE(6.27) = 1.29 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
0.08
0.10
0.12
0.14
0
1000
2000
3000
4000
5000
6000

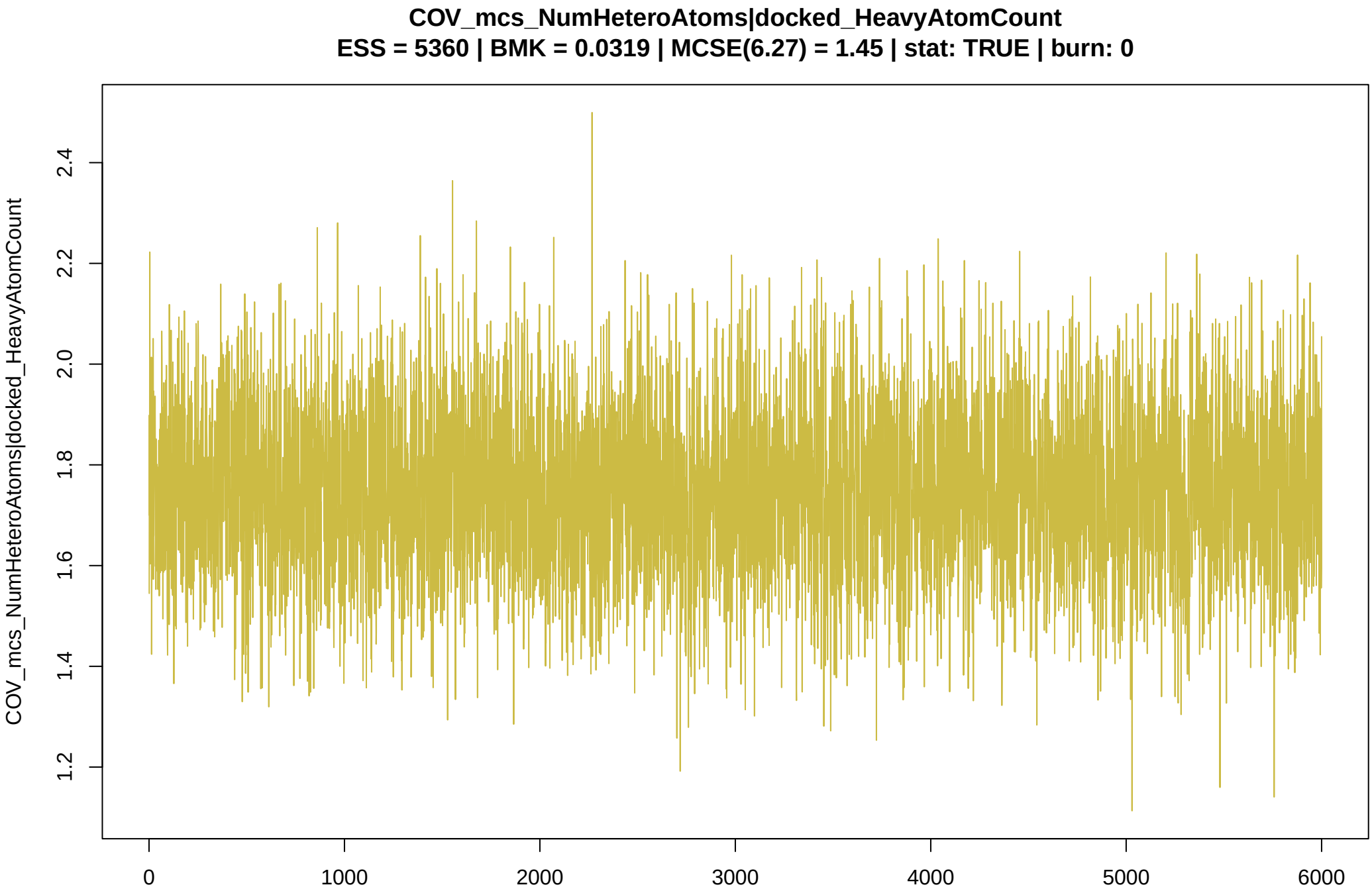

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 6000 | BMK = 0.025 | MCSE(6.27) = 1.27 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
0.20
0.25
0.30
0.35
0.40
0.45
0.50
0.55
0
1000
2000
3000
4000
5000
6000

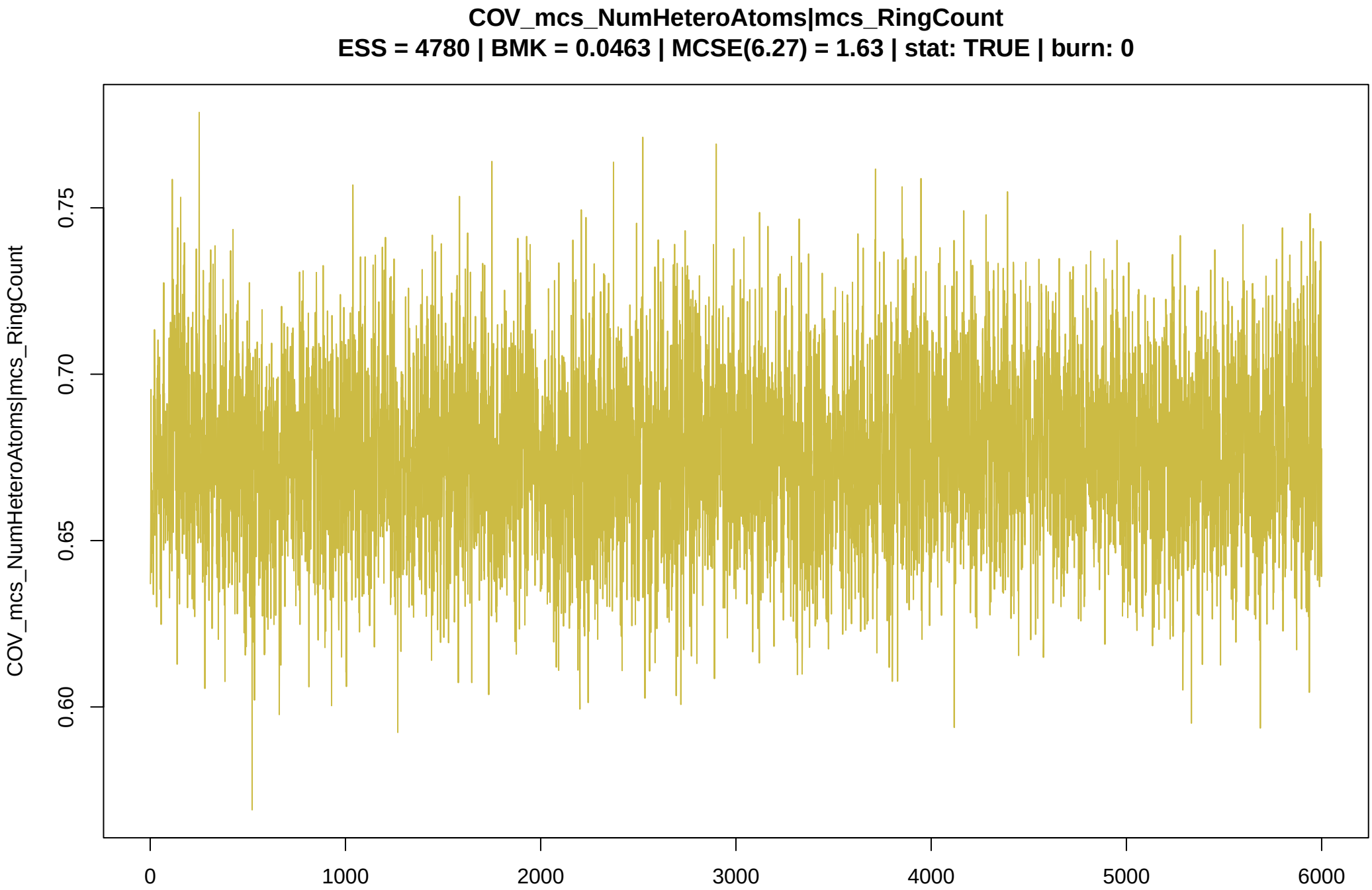

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 4730 | BMK = 0.0461 | MCSE(6.27) = 1.61 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.80
0.85
0.90
0.95
0
1000
2000
3000
4000
5000
6000

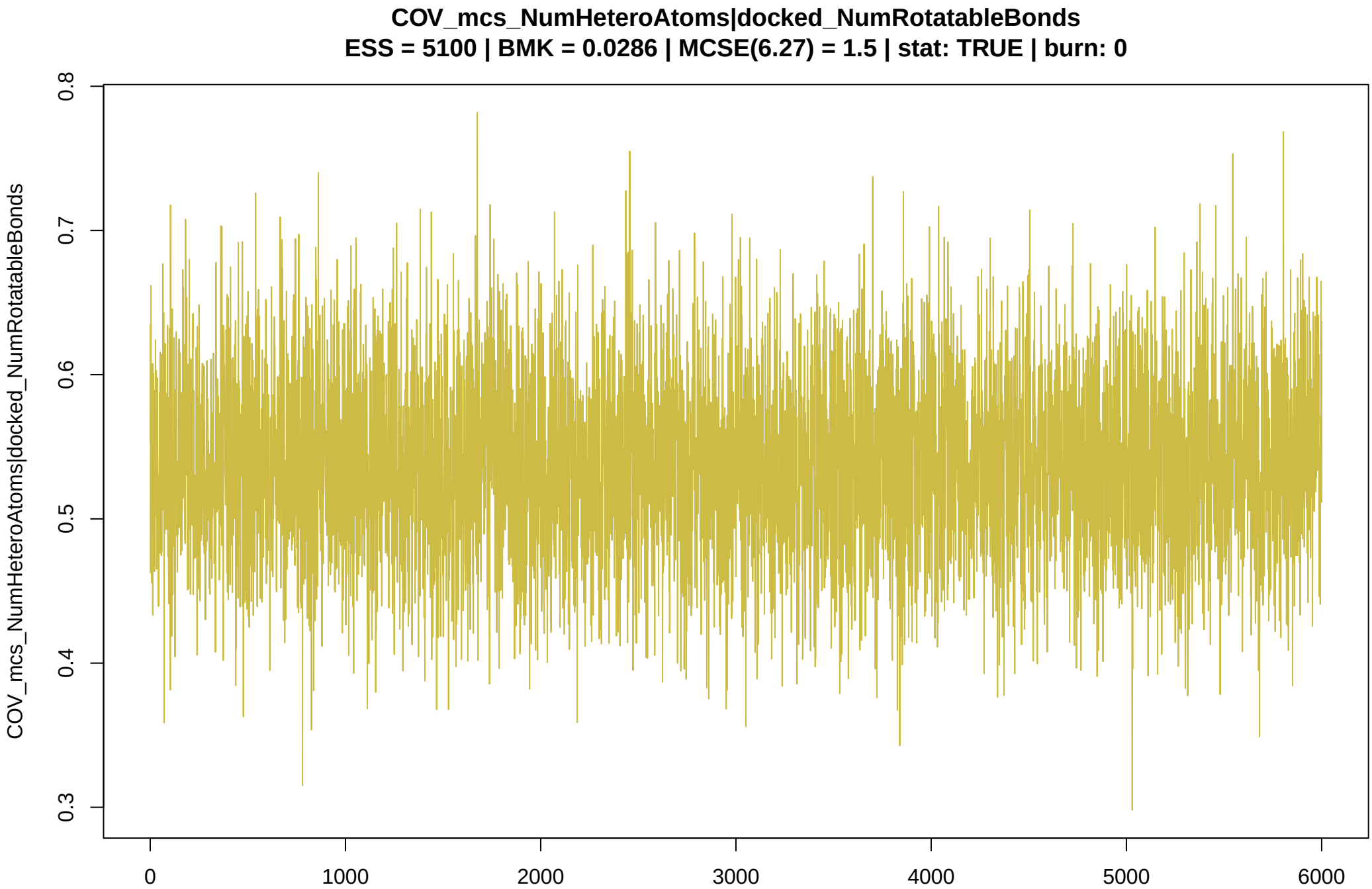

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 4640 | BMK = 0.0397 | MCSE(6.27) = 1.66 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
1.0
1.1
1.2
1.3
1.4
1.5
1.6
0
1000
2000
3000
4000
5000
6000

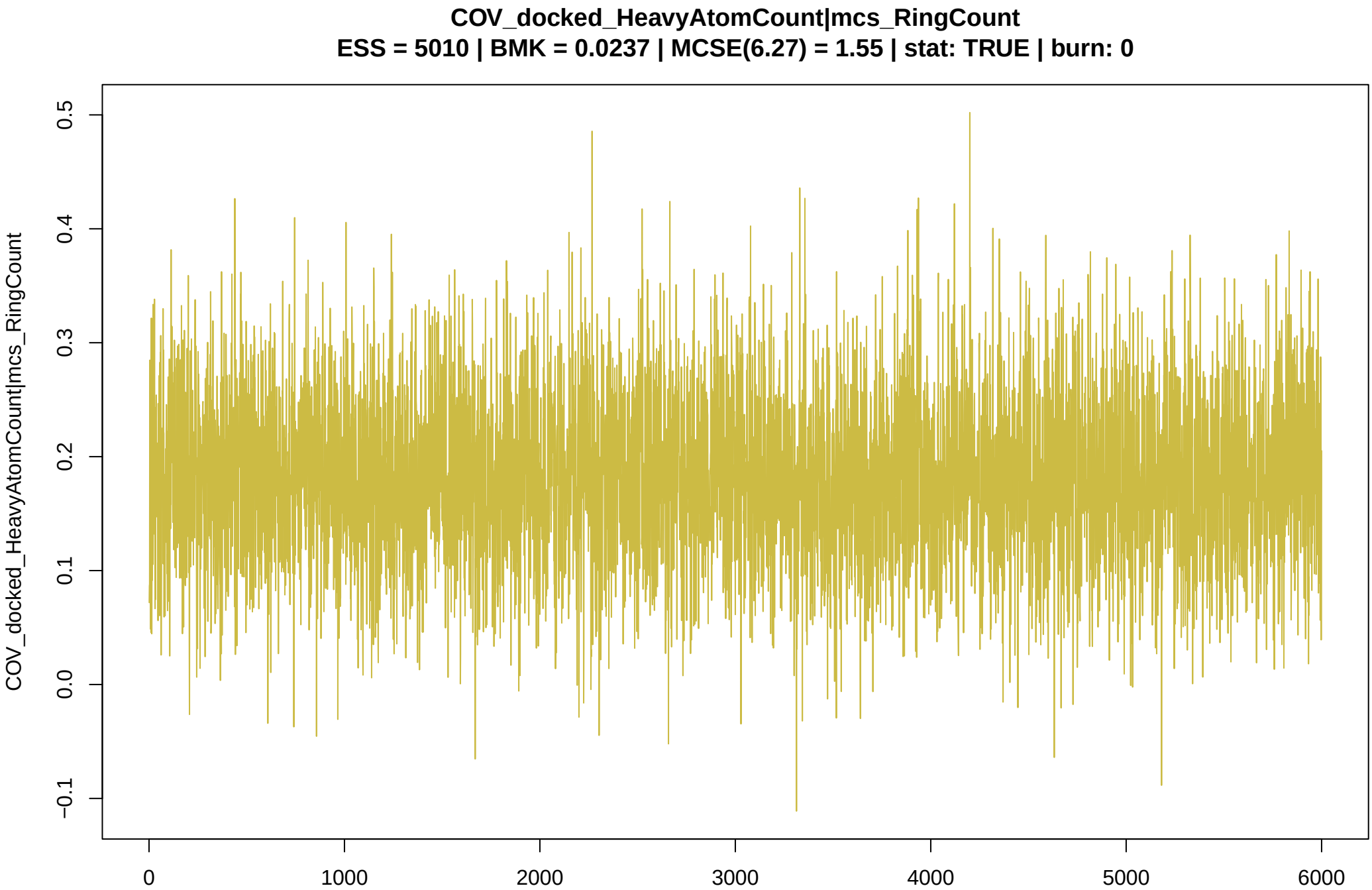

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 4080 | BMK = 0.0555 | MCSE(6.27) = 1.79 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.36
0.38
0.40
0.42
0.44
0.46
0
1000
2000
3000
4000
5000
6000

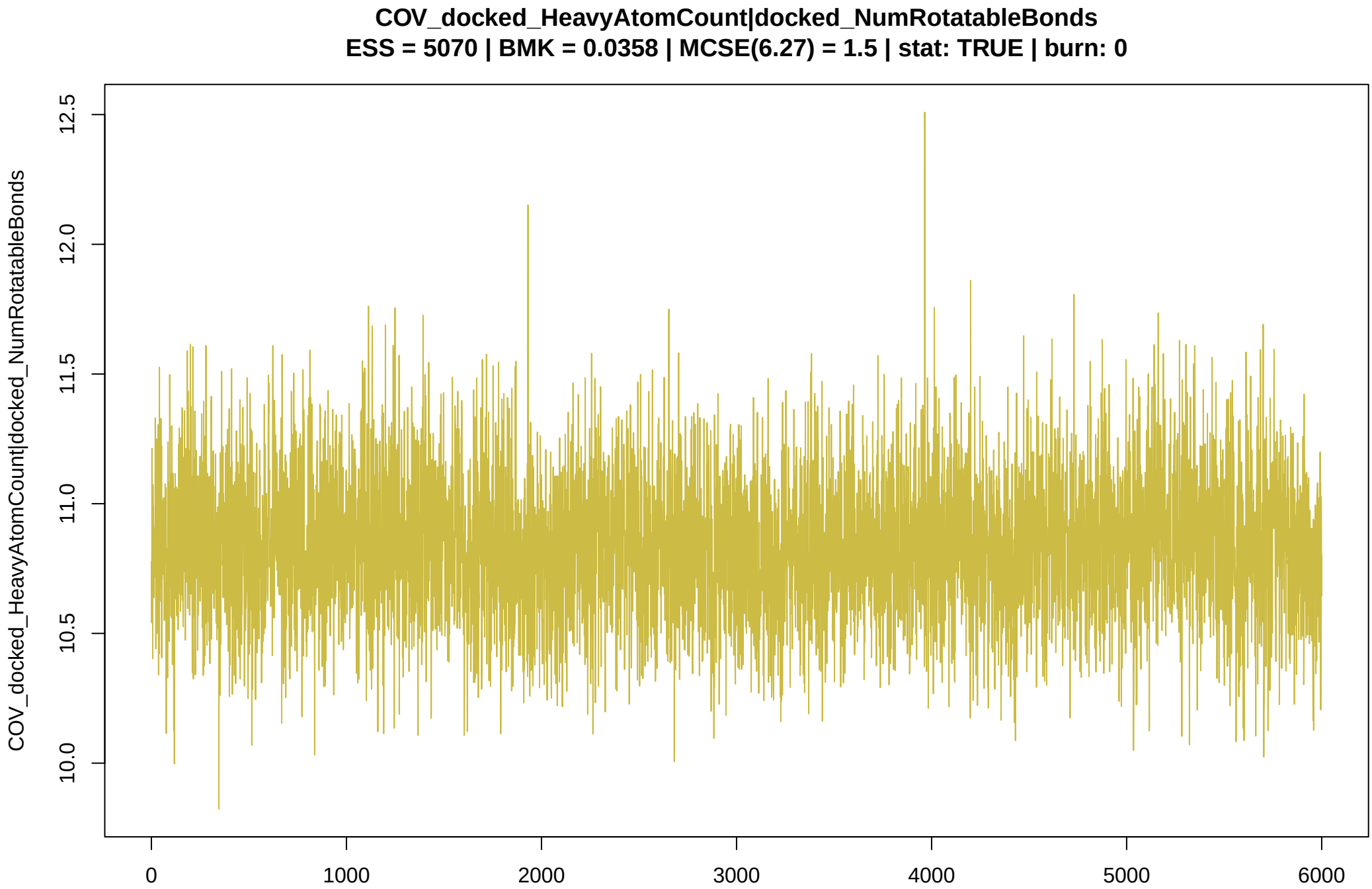

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 4500 | BMK = 0.0304 | MCSE(6.27) = 1.67 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
0.40
0.45
0.50
0.55
0.60
0
1000
2000
3000
4000
5000
6000

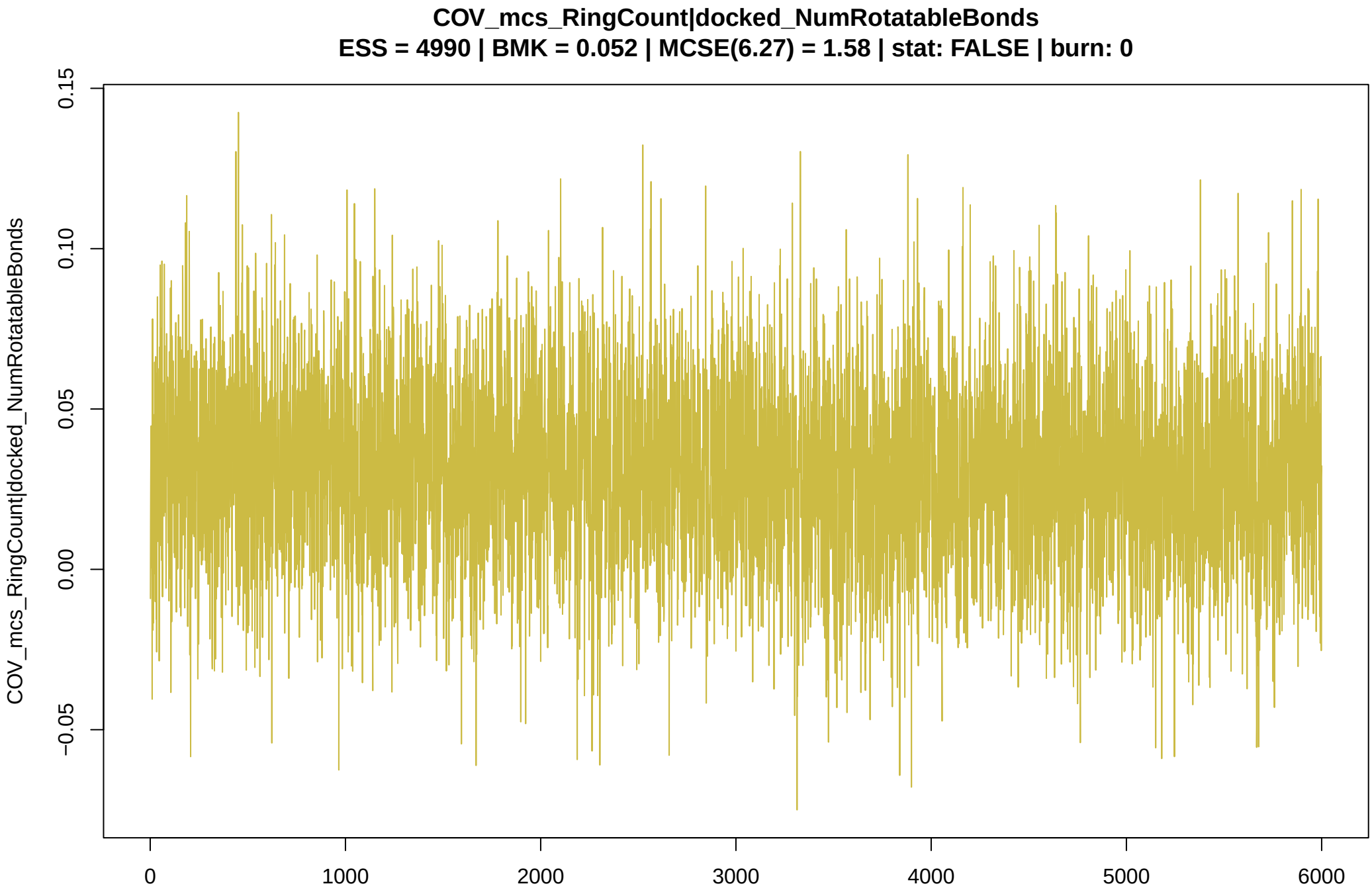

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 5360 | BMK = 0.0319 | MCSE(6.27) = 1.45 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
1.2
1.4
1.6
1.8
2.0
2.2
2.4
0
1000
2000
3000
4000
5000
6000


COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 4780 | BMK = 0.0463 | MCSE(6.27) = 1.63 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.60
0.65
0.70
0.75
0
1000
2000
3000
4000
5000
6000


COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 5100 | BMK = 0.0286 | MCSE(6.27) = 1.5 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
0.3
0.4
0.5
0.6
0.7
0.8
0
1000
2000
3000
4000
5000
6000


COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 5010 | BMK = 0.0237 | MCSE(6.27) = 1.55 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.5
0.4
0.3
0.2
0.1
0.0
−0.1
0
1000
2000
3000
4000
5000
6000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 5070 | BMK = 0.0358 | MCSE(6.27) = 1.5 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10.0
10.5
11.0
11.5
12.0
12.5
0
1000
2000
3000
4000
5000
6000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 4990 | BMK = 0.052 | MCSE(6.27) = 1.58 | stat: FALSE | burn: 0
COV_mcs_RingCount|docked_NumRotatableBonds
0.15
0.10
0.05
0.00
−0.05
0
1000
2000
3000
4000
5000
6000