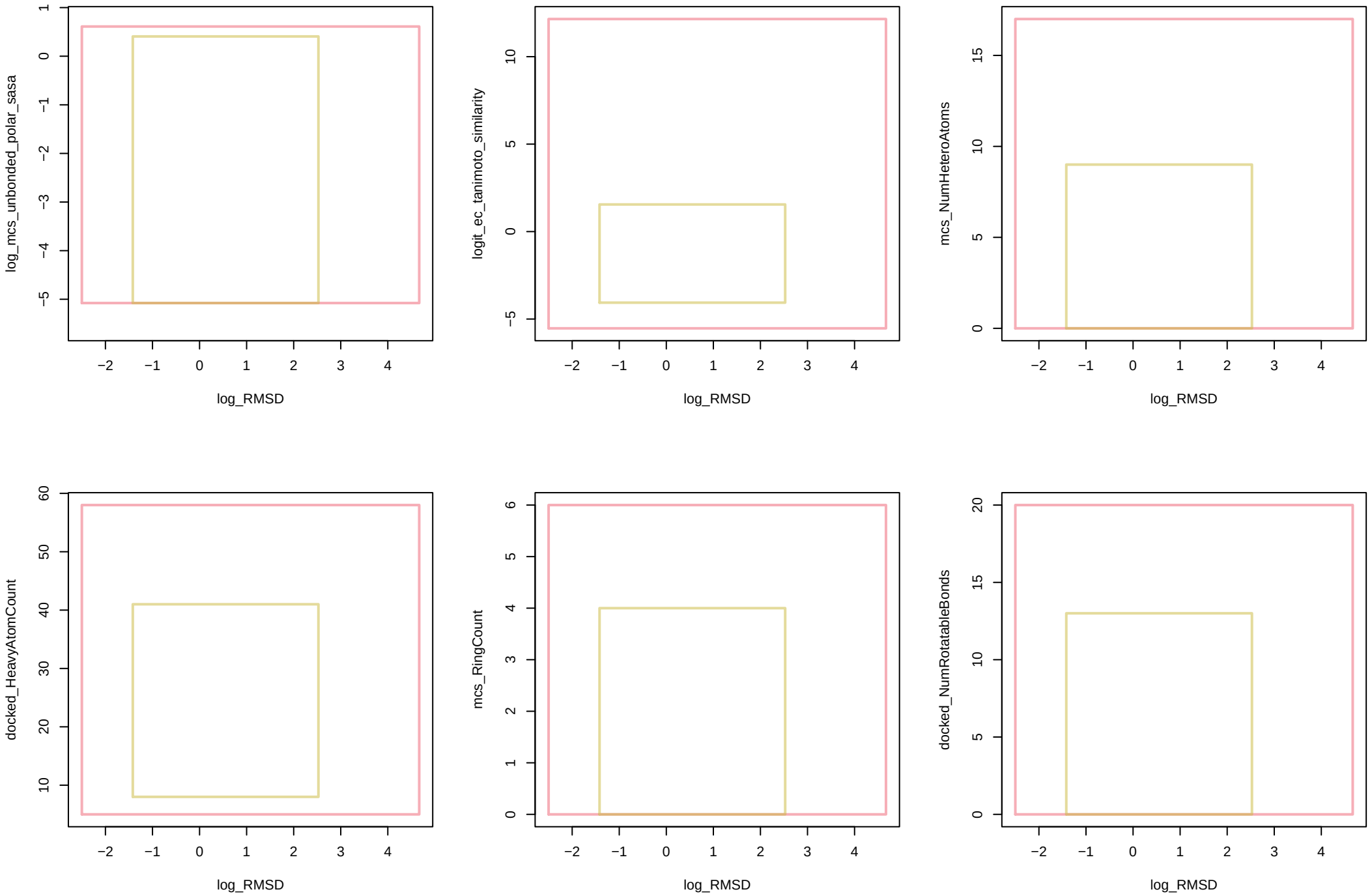
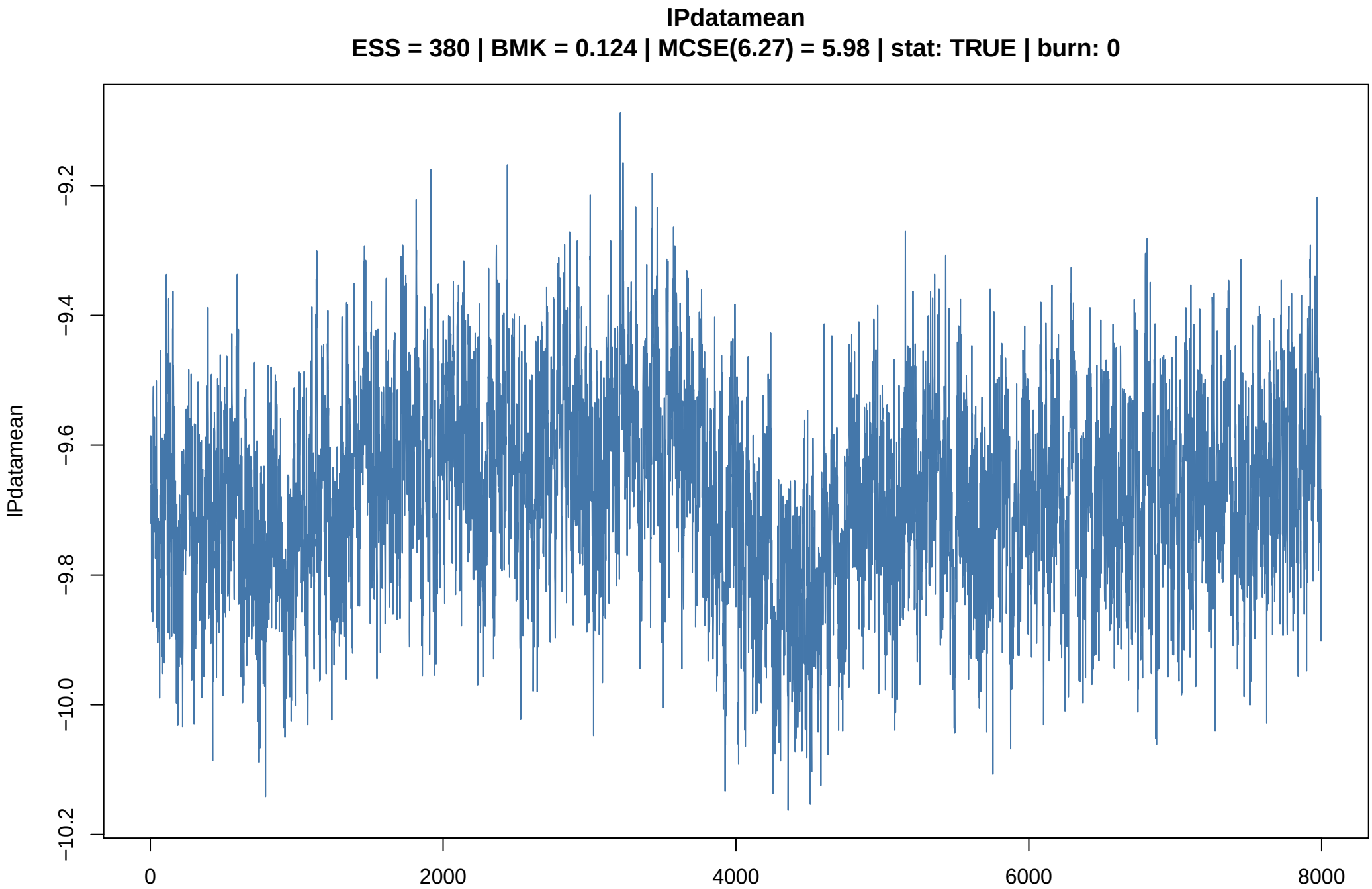
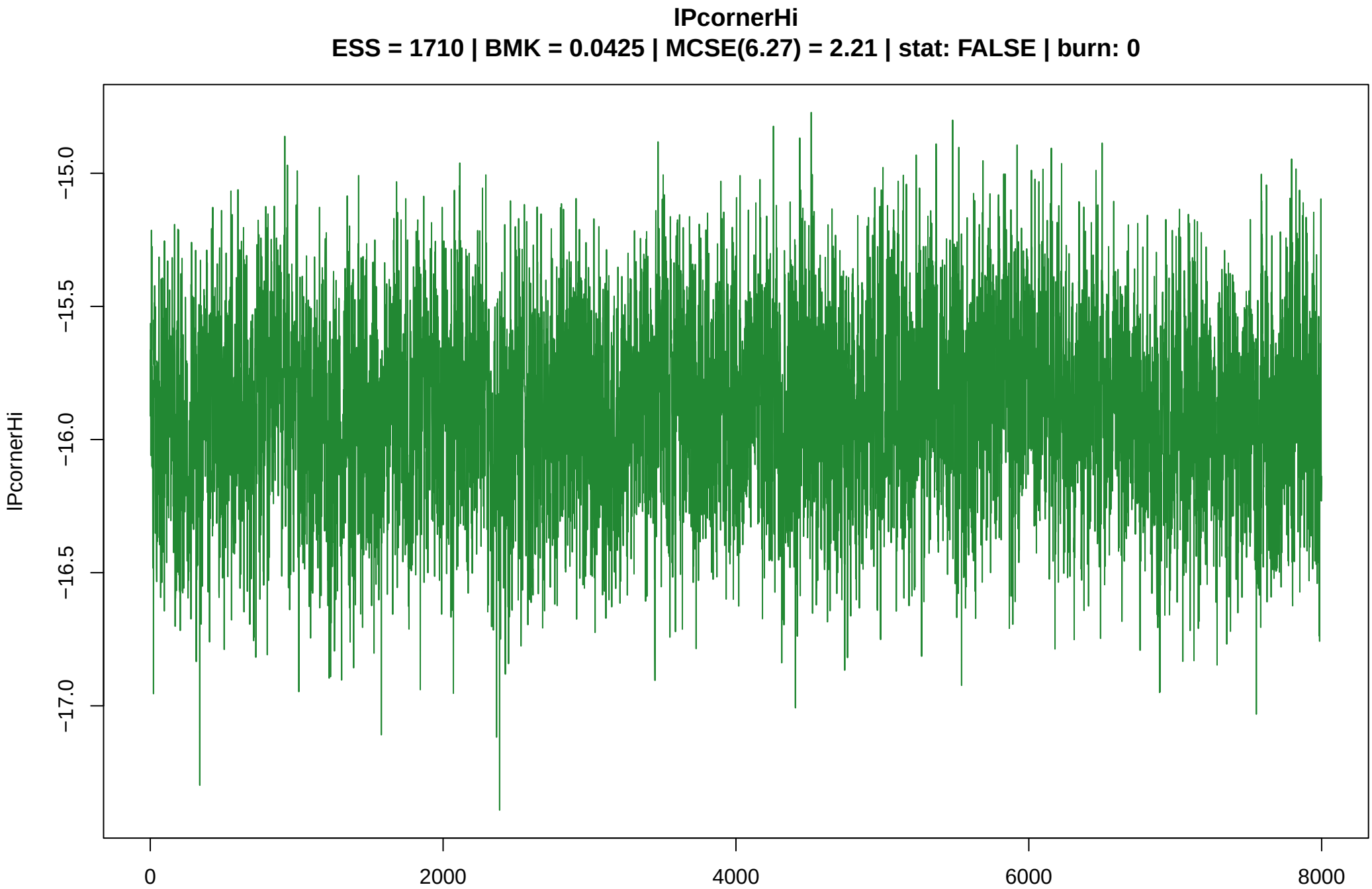
−− STATS maxD −−
min ESS = 68.1277238236928
max BMK = 0.308058036363699
max MCSE = 5.9808727615353
all stationary: FALSE
burn: 800

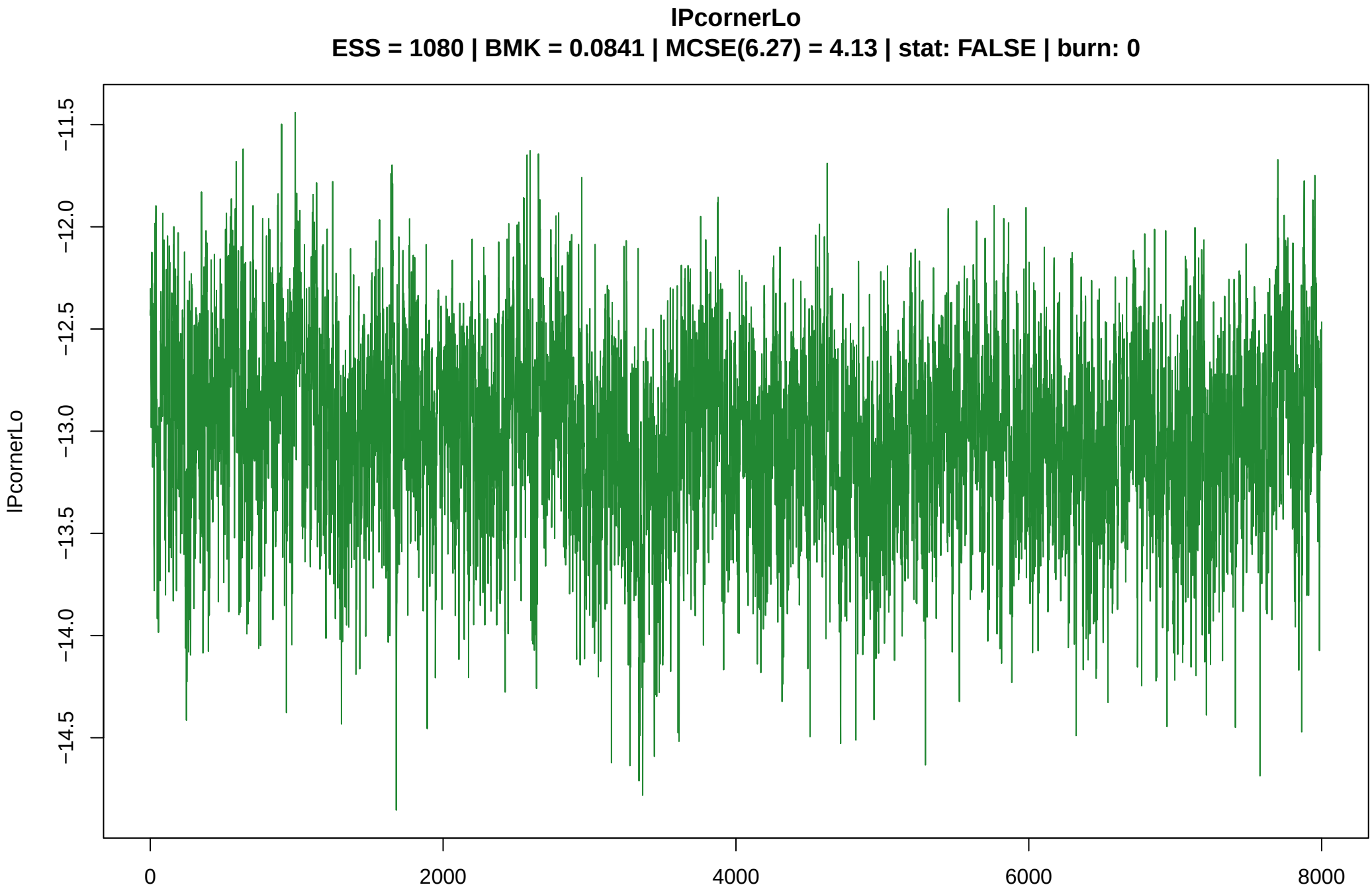
−− STATS 2D −−
min ESS = 1344.18684458699
max BMK = 0.0679760848274486
max MCSE = 1.5629288567136
all stationary: FALSE
burn: 0

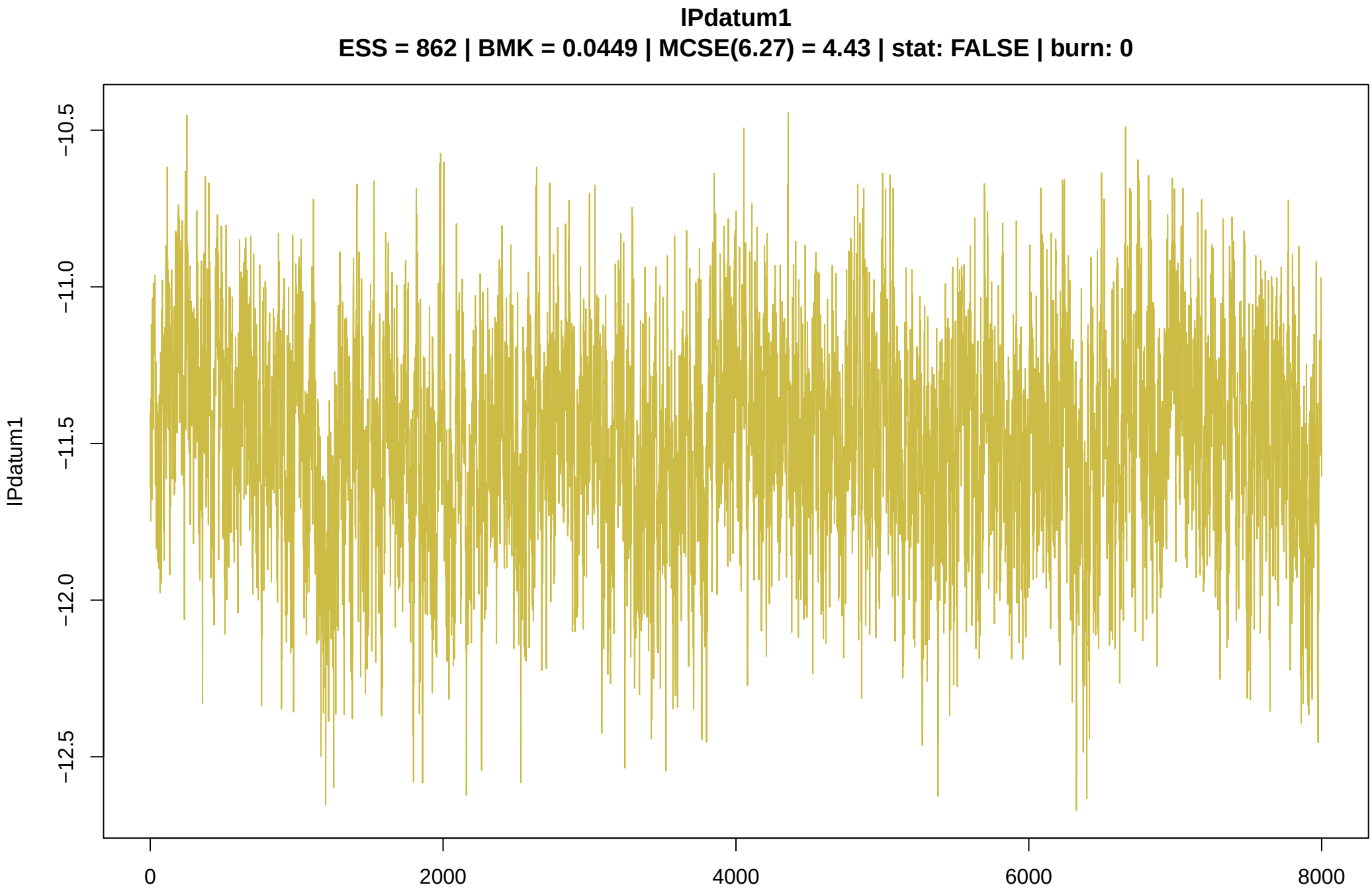
−− STATS 1D −−
min ESS = 860.548810035603
max BMK = 0.076684012180363 6
max MCSE = 1.77043245578415
all stationary: FALSE
burn: 0

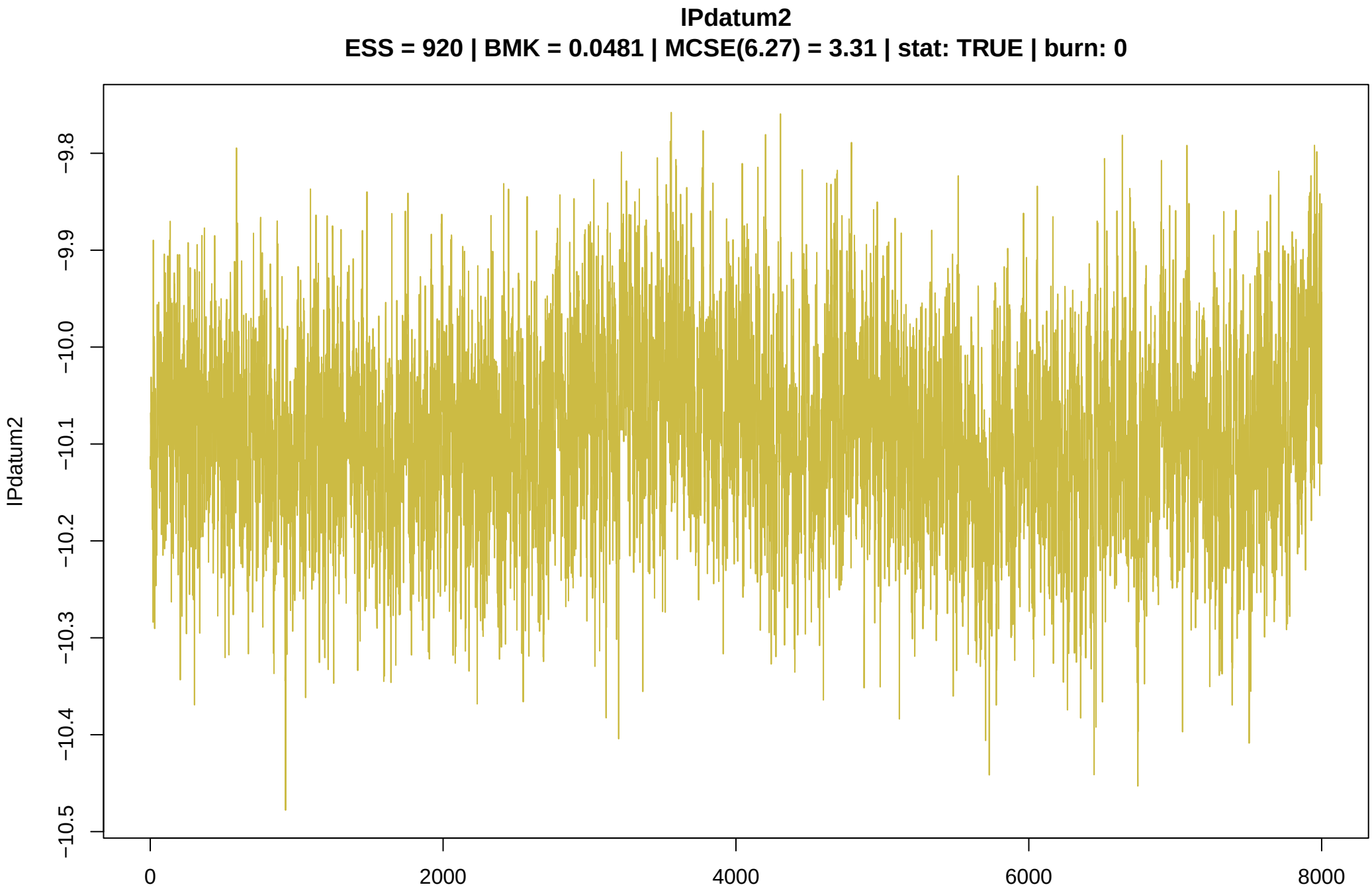

log_mcs_unbonded_polar_sasa
log_RMSD
logit_ec_tanimoto_similarity
log_RMSD
mcs_NumHeteroAtoms
log_RMSD
docked_HeavyAtomCount
log_RMSD
mcs_RingCount
log_RMSD
docked_NumRotatableBonds
log_RMSD

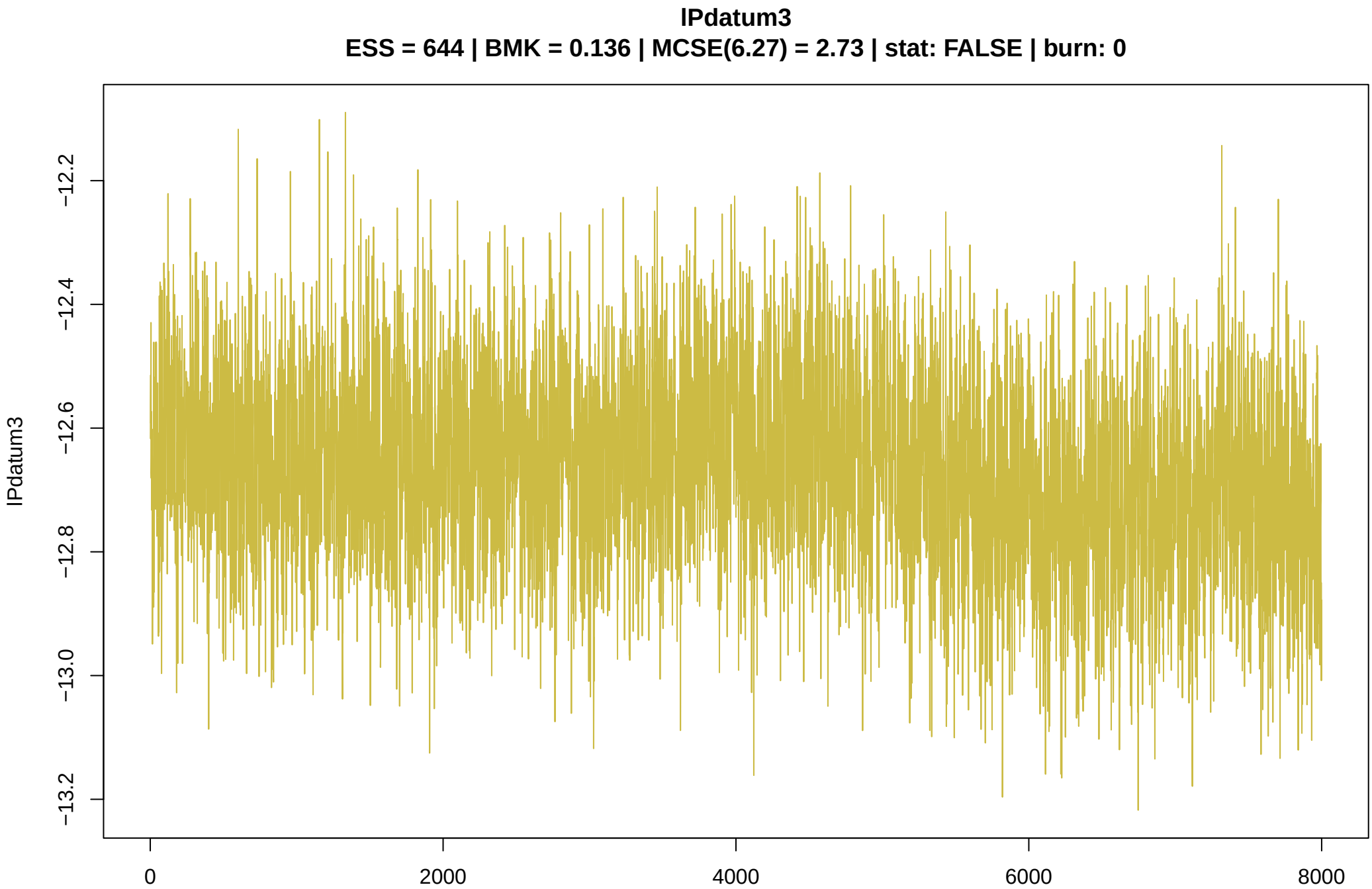

lPdatamean
ESS = 380 | BMK = 0.124 | MCSE(6.27) = 5.98 | stat: TRUE | burn: 0
lPdatamean
−9.2
−9.4
−9.6
−9.8
−10.0
−10.2
0
2000
4000
6000
8000

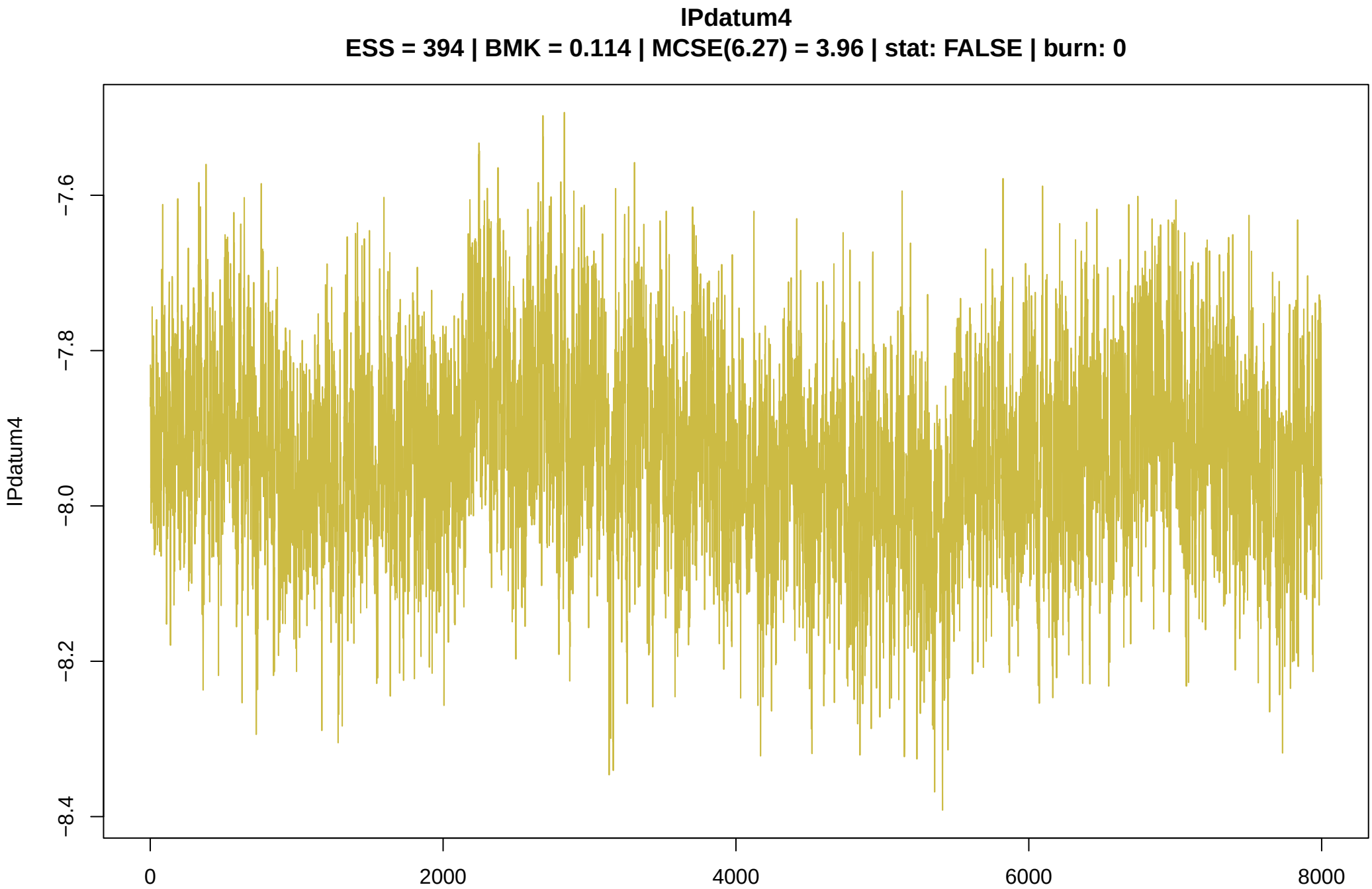

lPcornerHi
ESS = 1710 | BMK = 0.0425 | MCSE(6.27) = 2.21 | stat: FALSE | burn: 0
lPcornerHi
−15.0
−15.5
−16.0
−16.5
−17.0
0
2000
4000
6000
8000

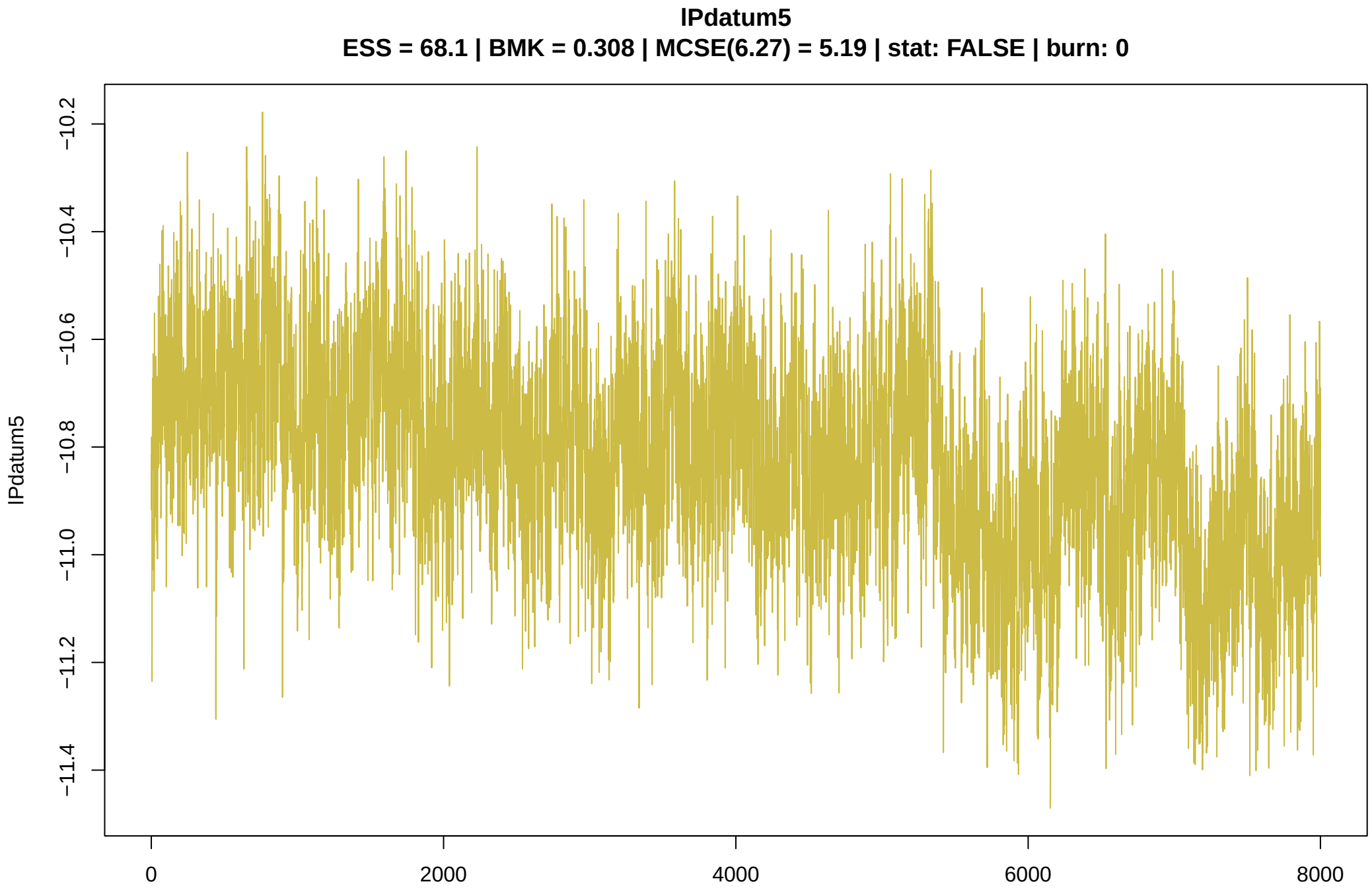

lPcornerLo
ESS = 1080 | BMK = 0.0841 | MCSE(6.27) = 4.13 | stat: FALSE | burn: 0
lPcornerLo
−11.5
−12.0
−12.5
−13.0
−13.5
−14.0
−14.5
0
2000
4000
6000
8000

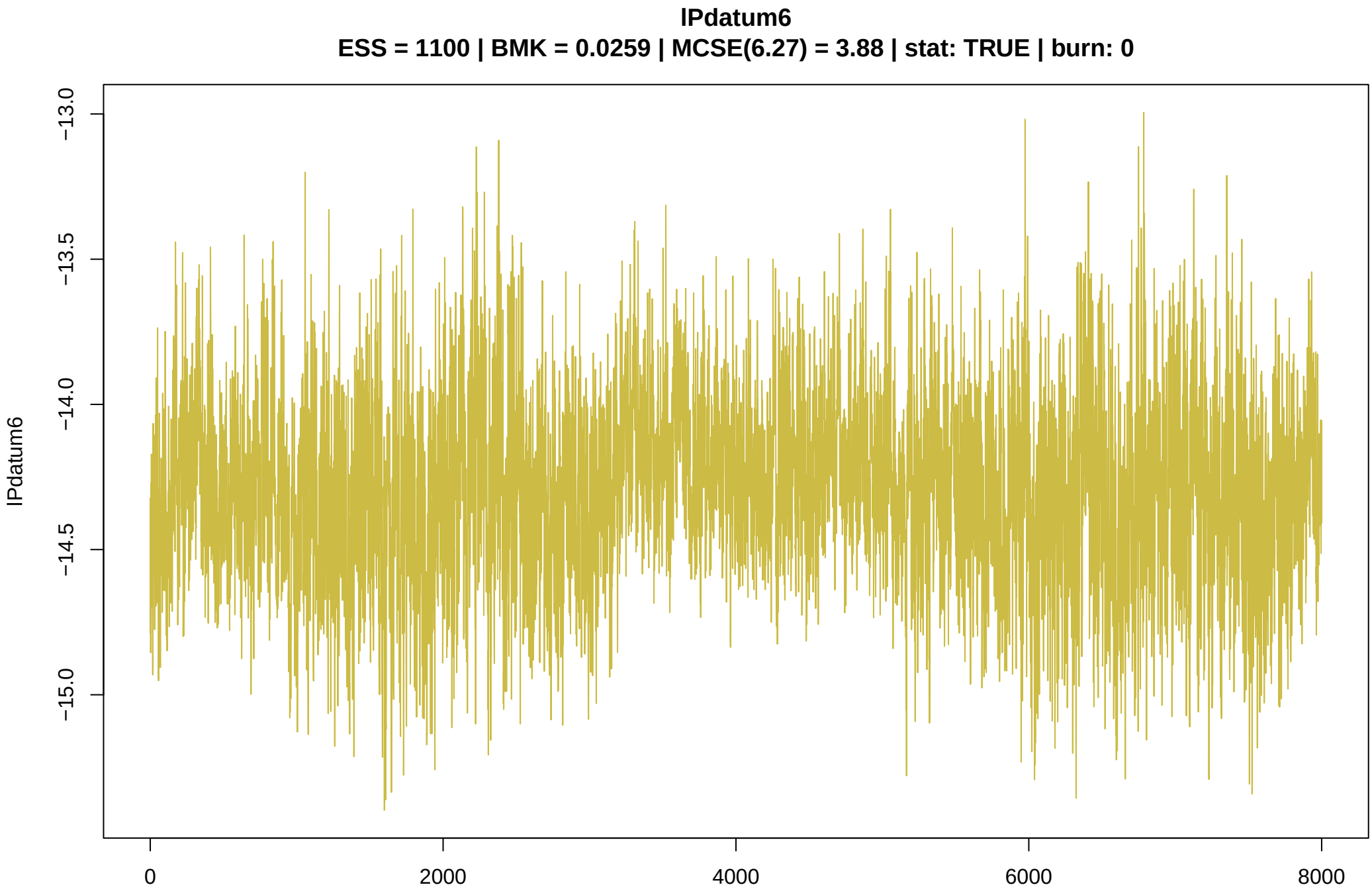

lPdatum1
ESS = 862 | BMK = 0.0449 | MCSE(6.27) = 4.43 | stat: FALSE | burn: 0
lPdatum1
−10.5
−11.0
−11.5
−12.0
−12.5
0
2000
4000
6000
8000

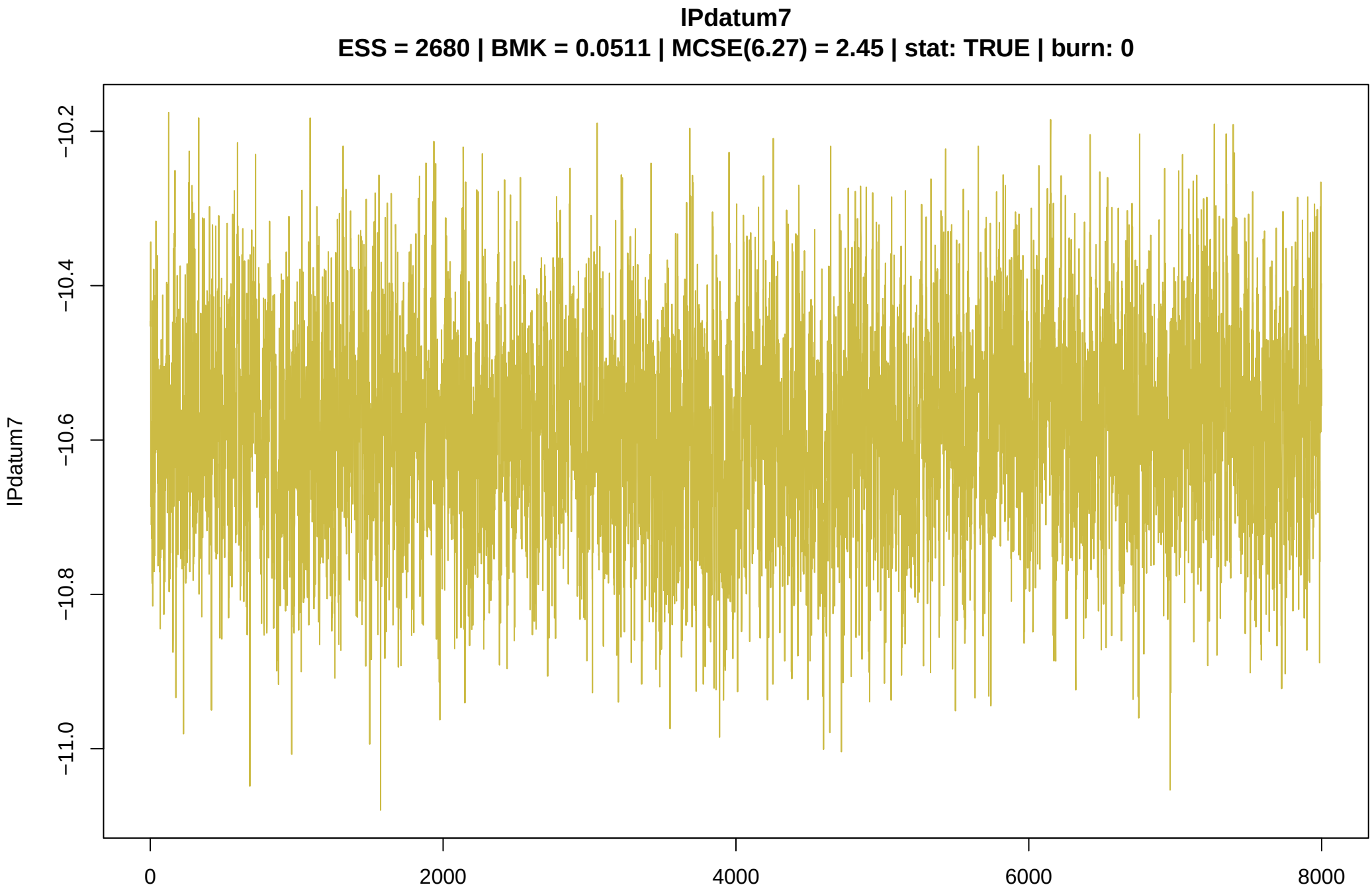

lPdatum2
ESS = 920 | BMK = 0.0481 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0
lPdatum2
−9.8
−9.9
−10.0
−10.1
−10.2
−10.3
−10.4
−10.5
0
2000
4000
6000
8000

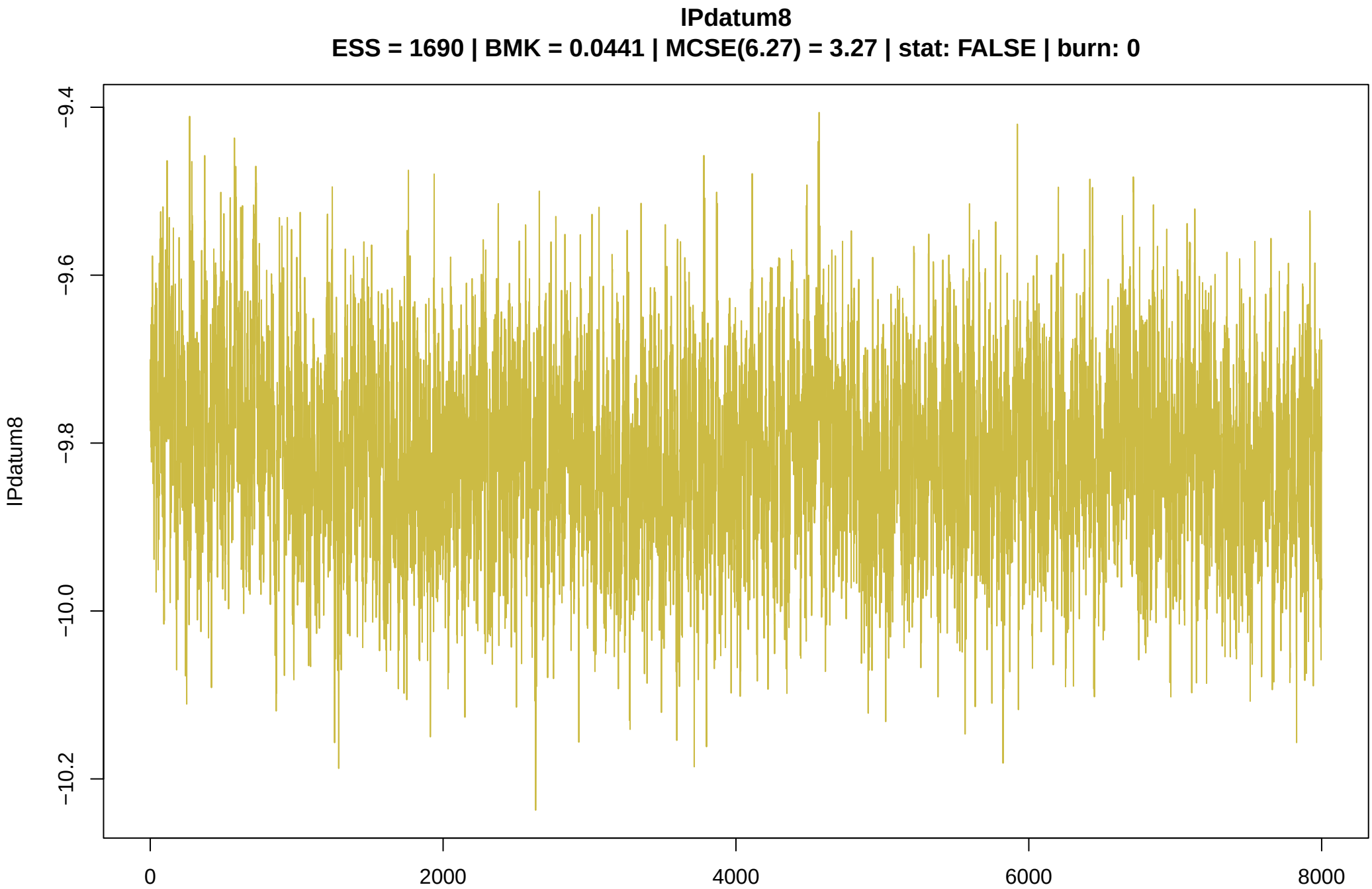

lPdatum3
ESS = 644 | BMK = 0.136 | MCSE(6.27) = 2.73 | stat: FALSE | burn: 0
lPdatum3
−12.2
−12.4
−12.6
−12.8
−13.0
−13.2
0
2000
4000
6000
8000

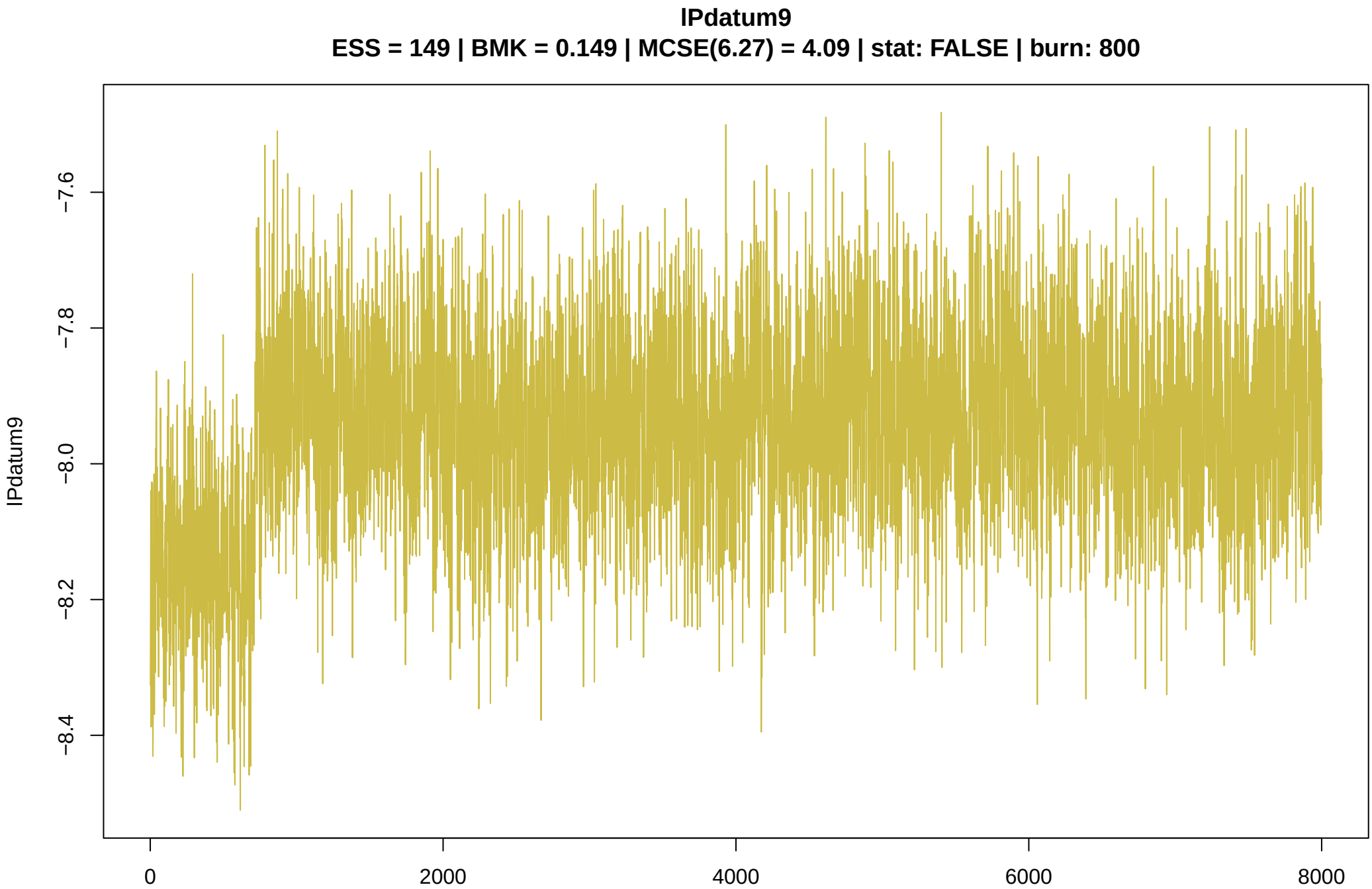

lPdatum4
ESS = 394 | BMK = 0.114 | MCSE(6.27) = 3.96 | stat: FALSE | burn: 0
lPdatum4
−7.6
−7.8
−8.0
−8.2
−8.4
0
2000
4000
6000
8000

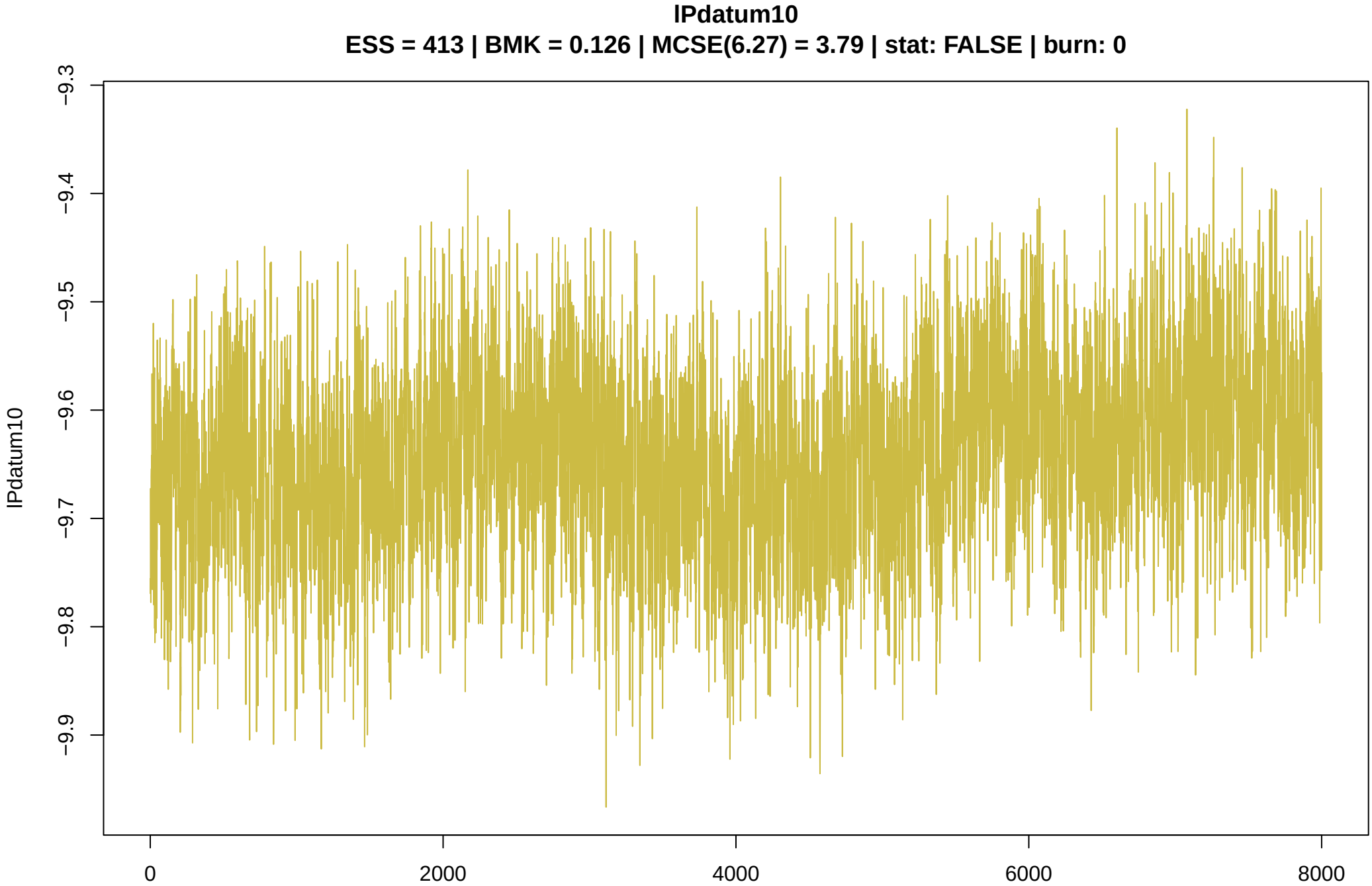

lPdatum5
ESS = 68.1 | BMK = 0.308 | MCSE(6.27) = 5.19 | stat: FALSE | burn: 0
lPdatum5
−10.2
−10.4
−10.6
−10.8
−11.0
−11.2
−11.4
0
2000
4000
6000
8000

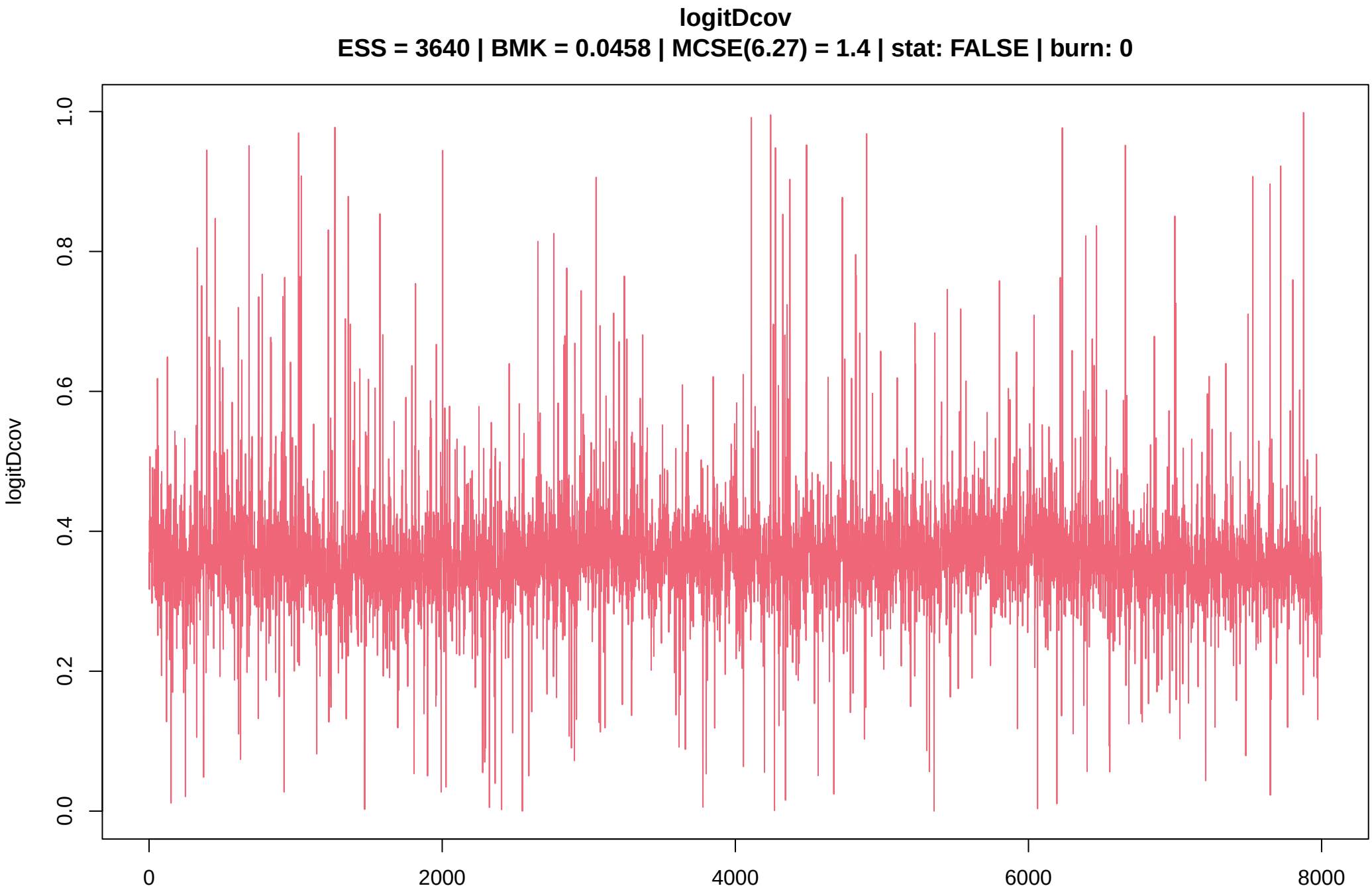

lPdatum6
ESS = 1100 | BMK = 0.0259 | MCSE(6.27) = 3.88 | stat: TRUE | burn: 0
lPdatum6
−13.0
−13.5
−14.0
−14.5
−15.0
0
2000
4000
6000
8000

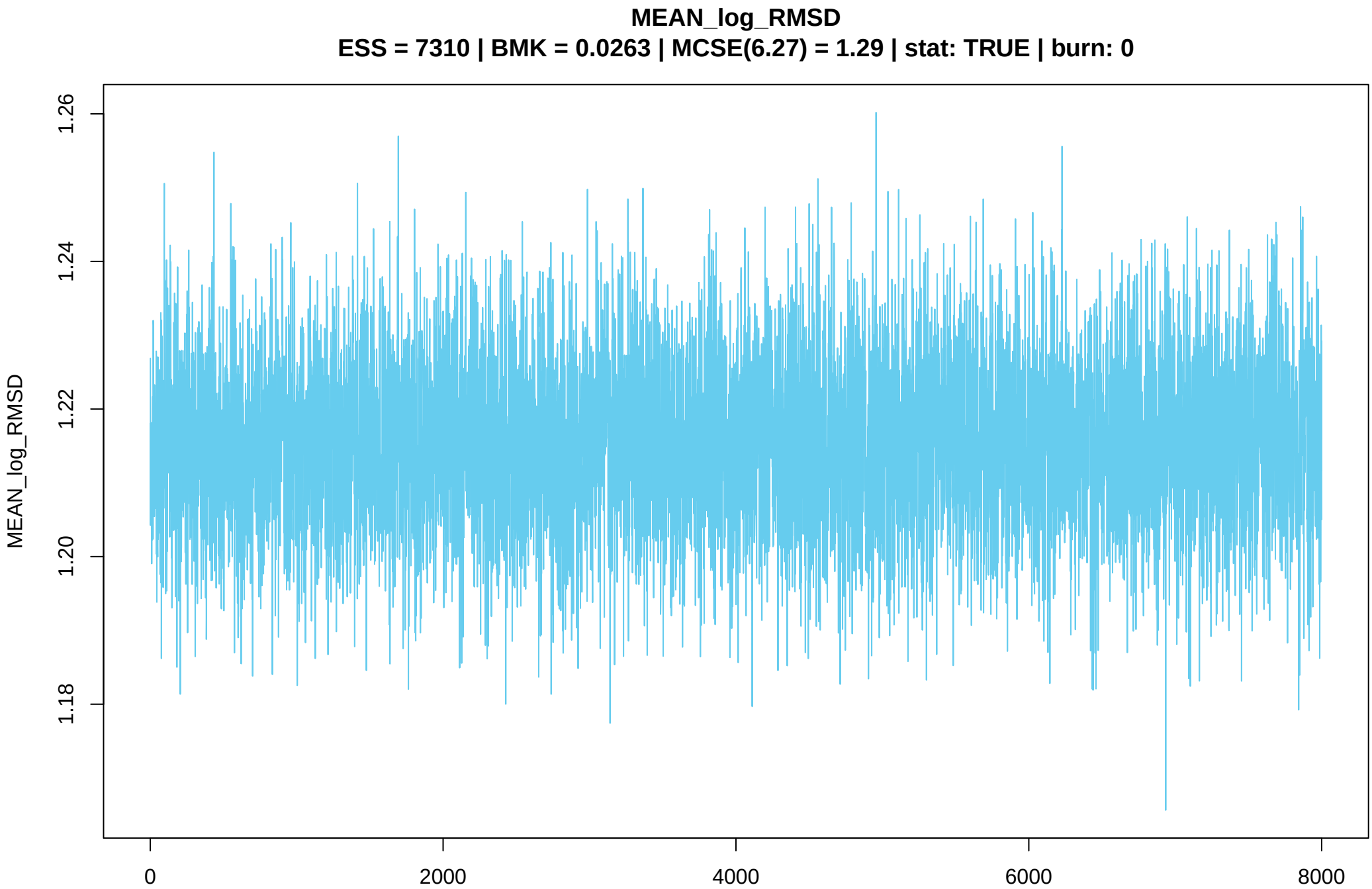

lPdatum7
ESS = 2680 | BMK = 0.0511 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0
lPdatum7
−10.2
−10.4
−10.6
−10.8
−11.0
0
2000
4000
6000
8000

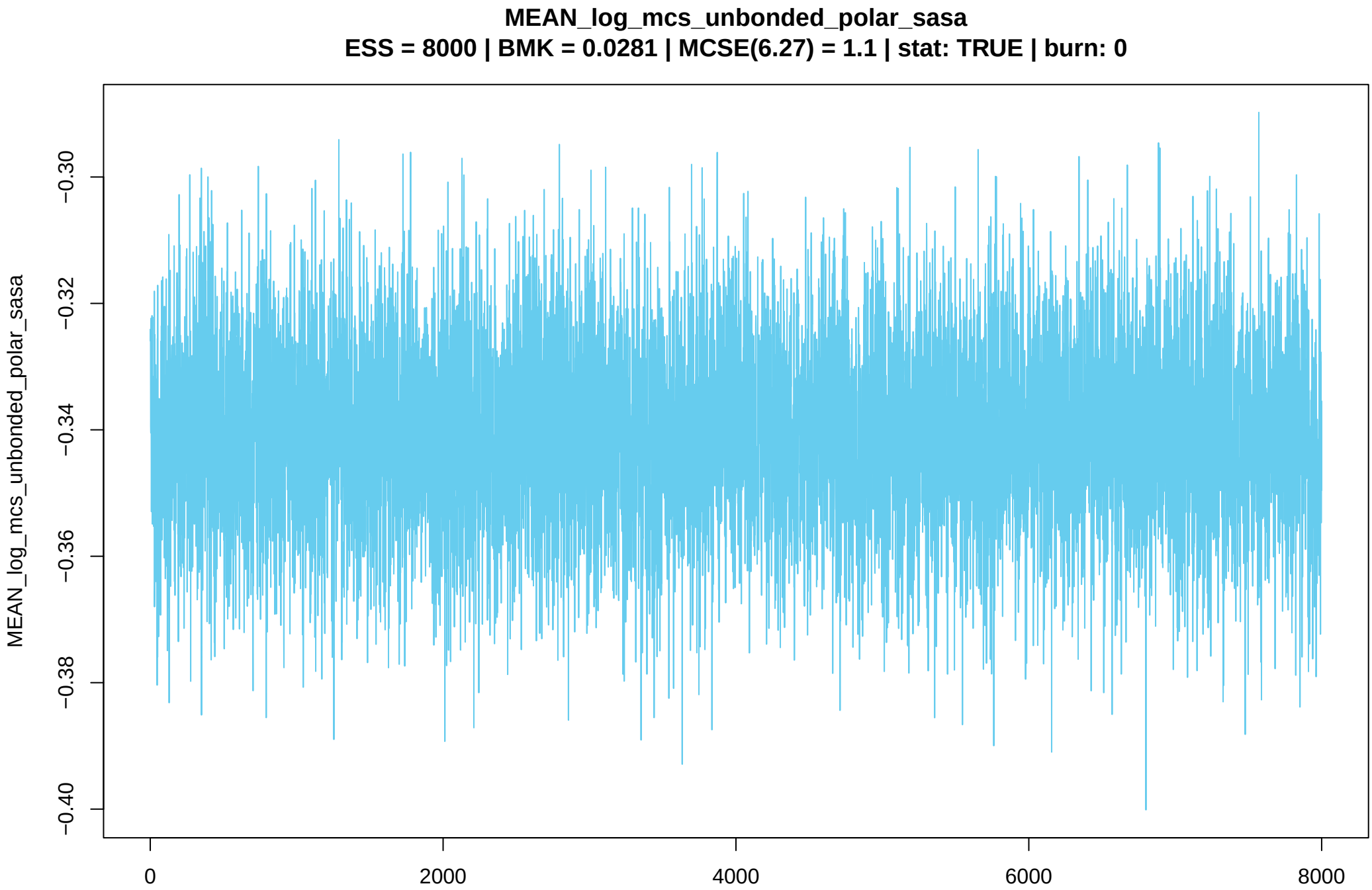

lPdatum8
ESS = 1690 | BMK = 0.0441 | MCSE(6.27) = 3.27 | stat: FALSE | burn: 0
lPdatum8
−9.4
−9.6
−9.8
−10.0
−10.2
0
2000
4000
6000
8000

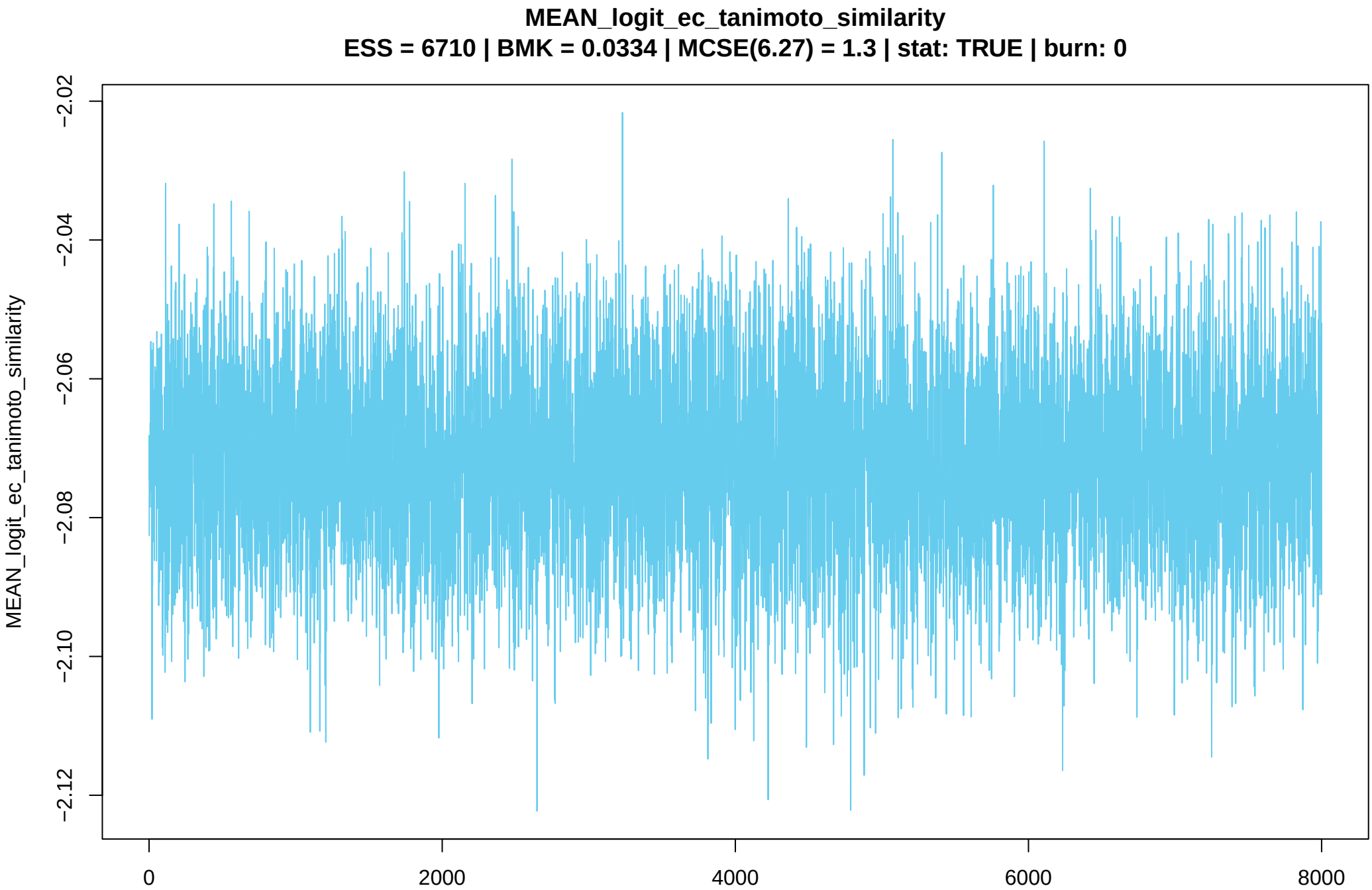

lPdatum9
ESS = 149 | BMK = 0.149 | MCSE(6.27) = 4.09 | stat: FALSE | burn: 800
lPdatum9
−7.6
−7.8
−8.0
−8.2
−8.4
0
2000
4000
6000
8000

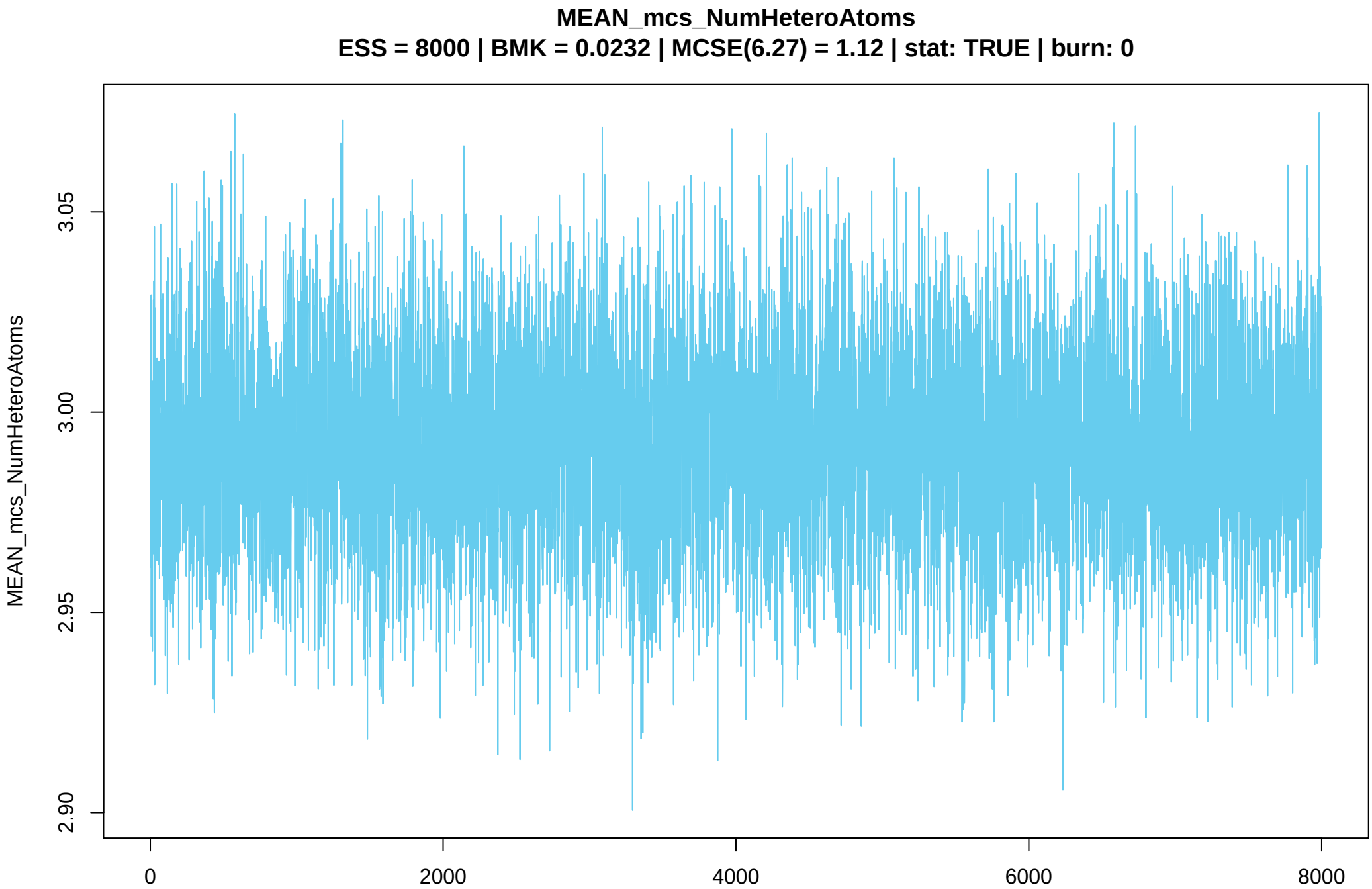

lPdatum10
ESS = 413 | BMK = 0.126 | MCSE(6.27) = 3.79 | stat: FALSE | burn: 0
lPdatum10
−9.3
−9.4
−9.5
−9.6
−9.7
−9.8
−9.9
0
2000
4000
6000
8000

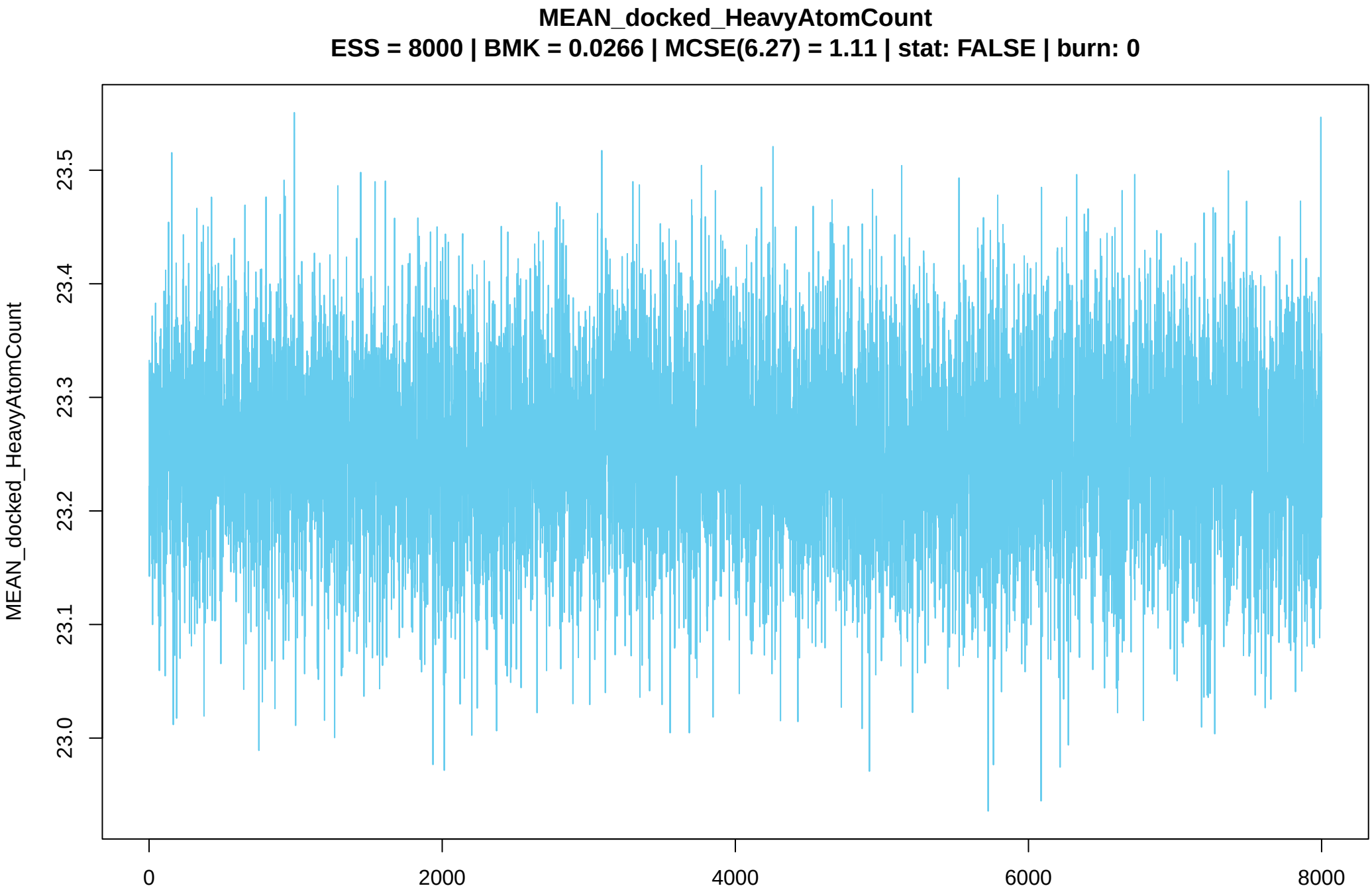

logitDcov
ESS = 3640 | BMK = 0.0458 | MCSE(6.27) = 1.4 | stat: FALSE | burn: 0
logitDcov
0.0
0.2
0.4
0.6
0.8
1.0
0
2000
4000
6000
8000

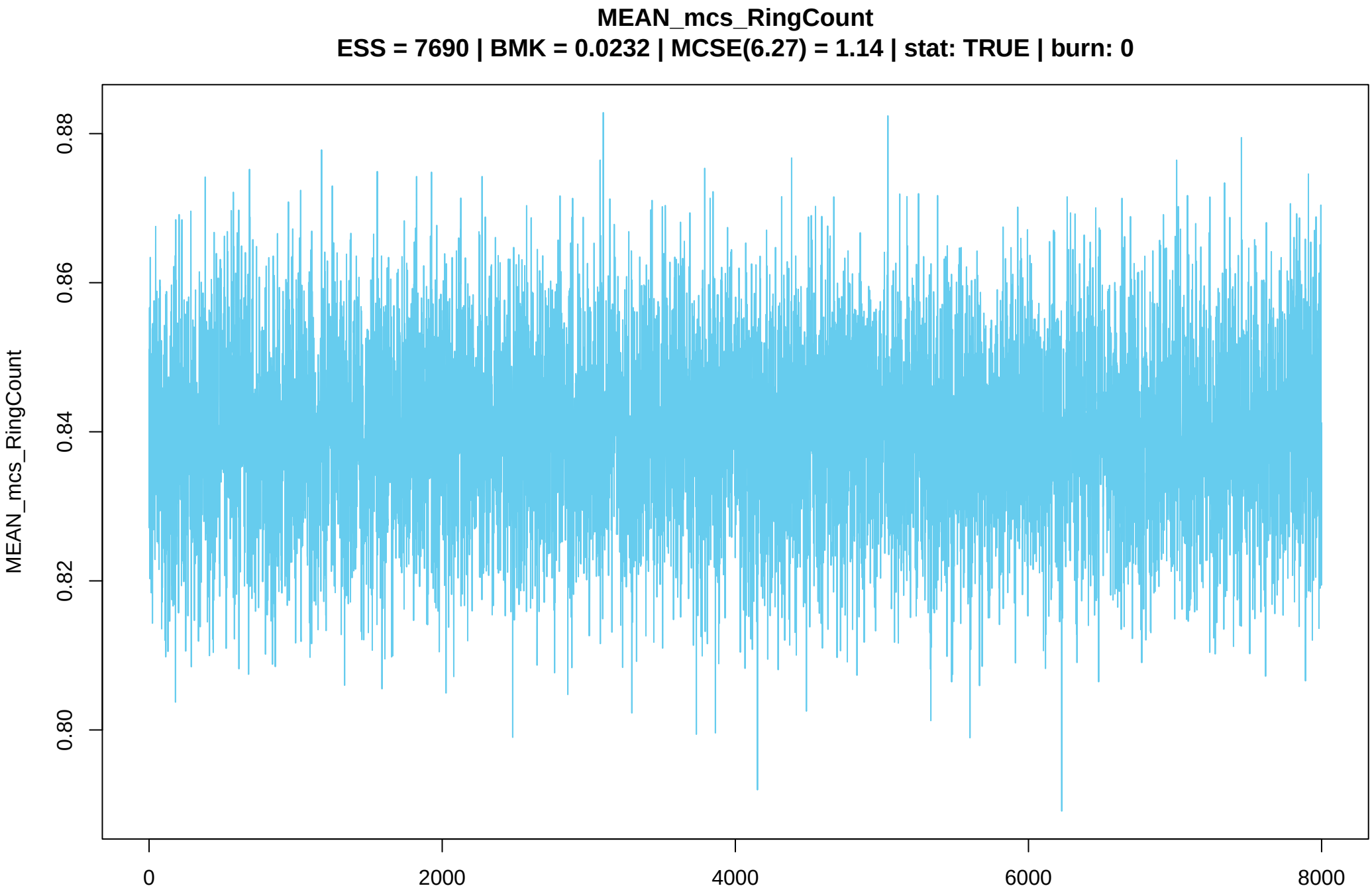

MEAN_log_RMSD
ESS = 7310 | BMK = 0.0263 | MCSE(6.27) = 1.29 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.26
1.24
1.22
1.20
1.18
0
2000
4000
6000
8000

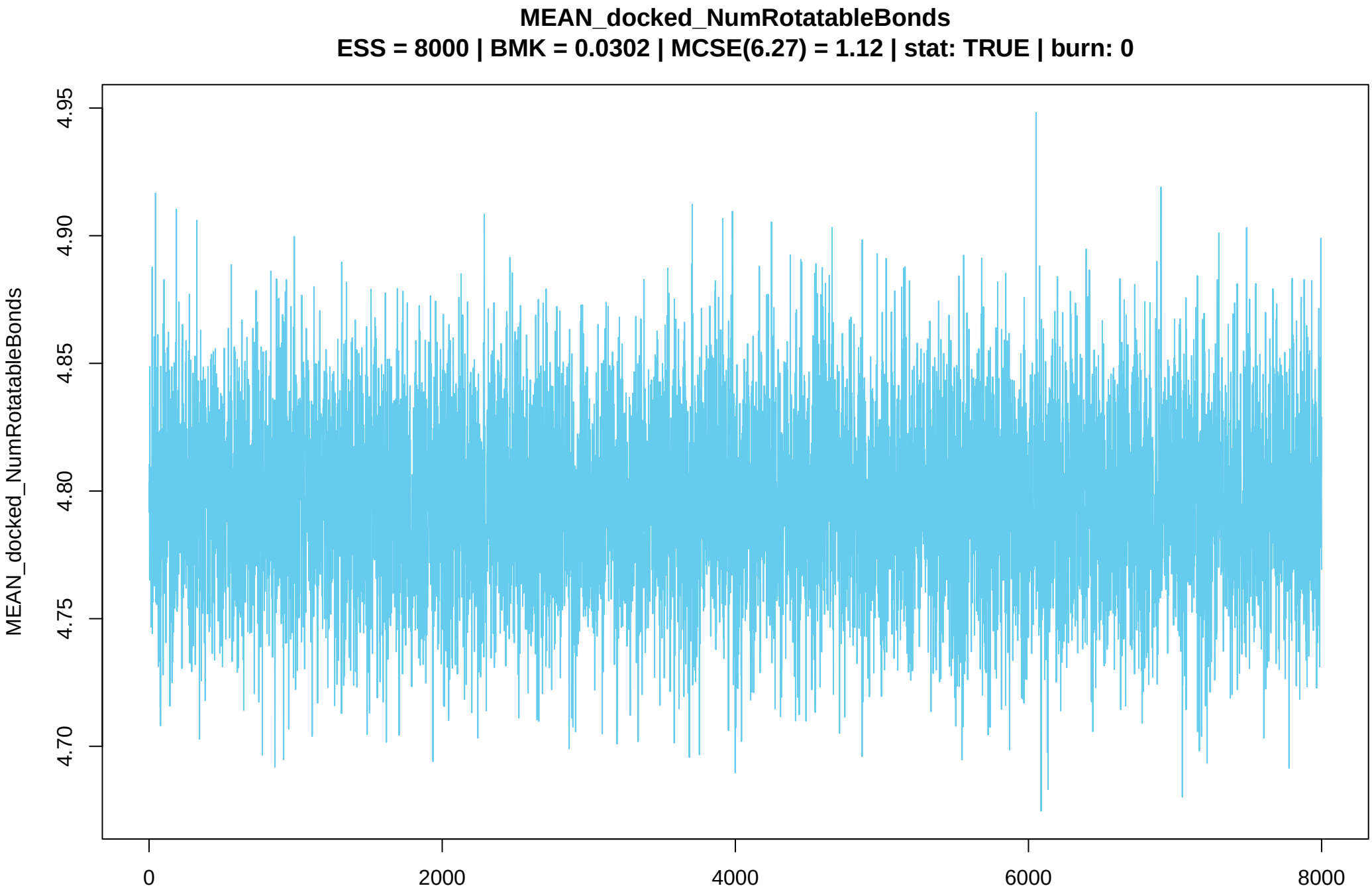

MEAN_log_mcs_unbonded_polar_sasa
ESS = 8000 | BMK = 0.0281 | MCSE(6.27) = 1.1 | stat: TRUE | burn: 0
MEAN_log_mcs_unbonded_polar_sasa
−0.30
−0.32
−0.34
−0.36
−0.38
−0.40
0
2000
4000
6000
8000

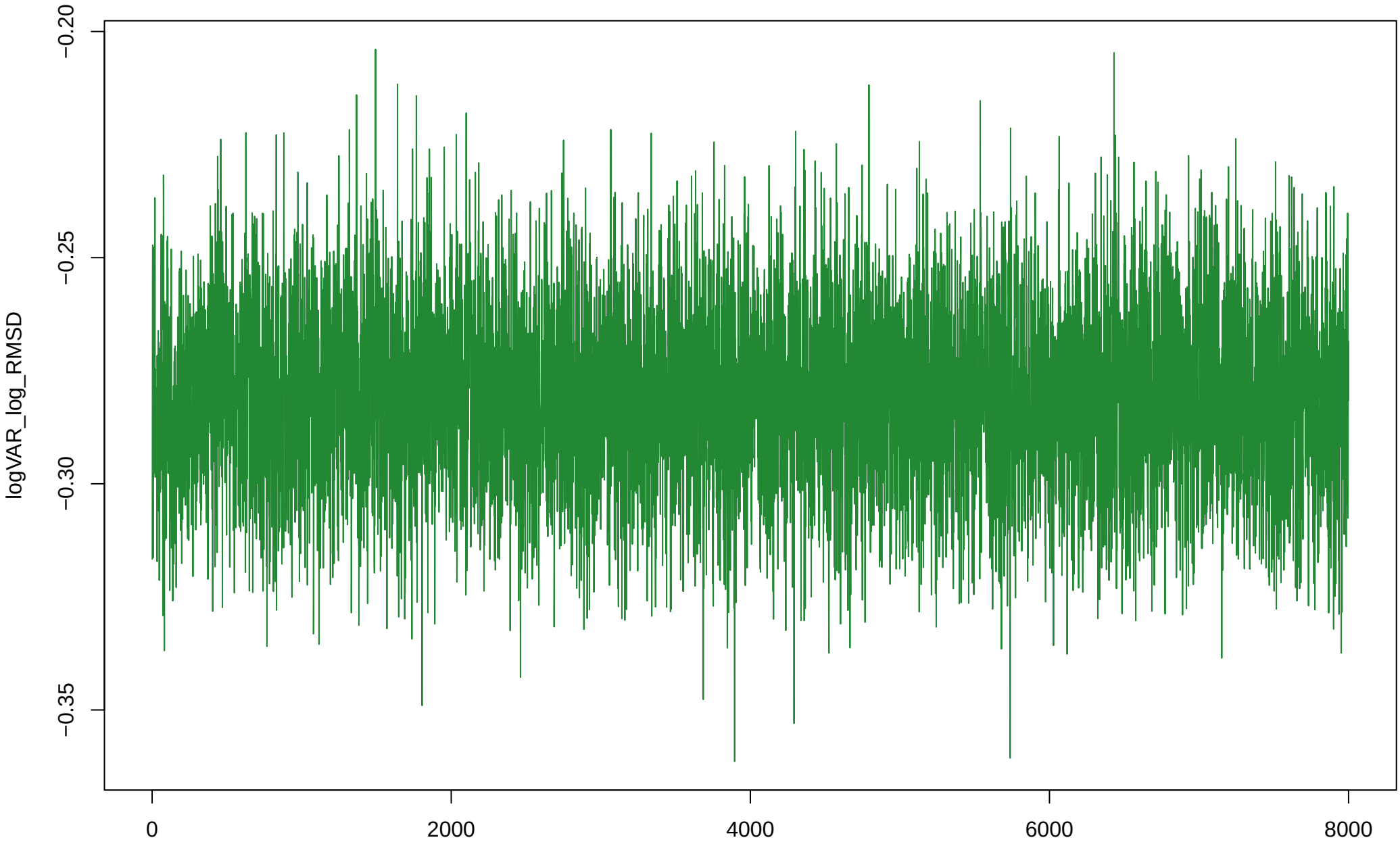

MEAN_logit_ec_tanimoto_similarity
ESS = 6710 | BMK = 0.0334 | MCSE(6.27) = 1.3 | stat: TRUE | burn: 0
MEAN_logit_ec_tanimoto_similarity
−2.02
−2.04
−2.06
−2.08
−2.10
−2.12
0
2000
4000
6000
8000

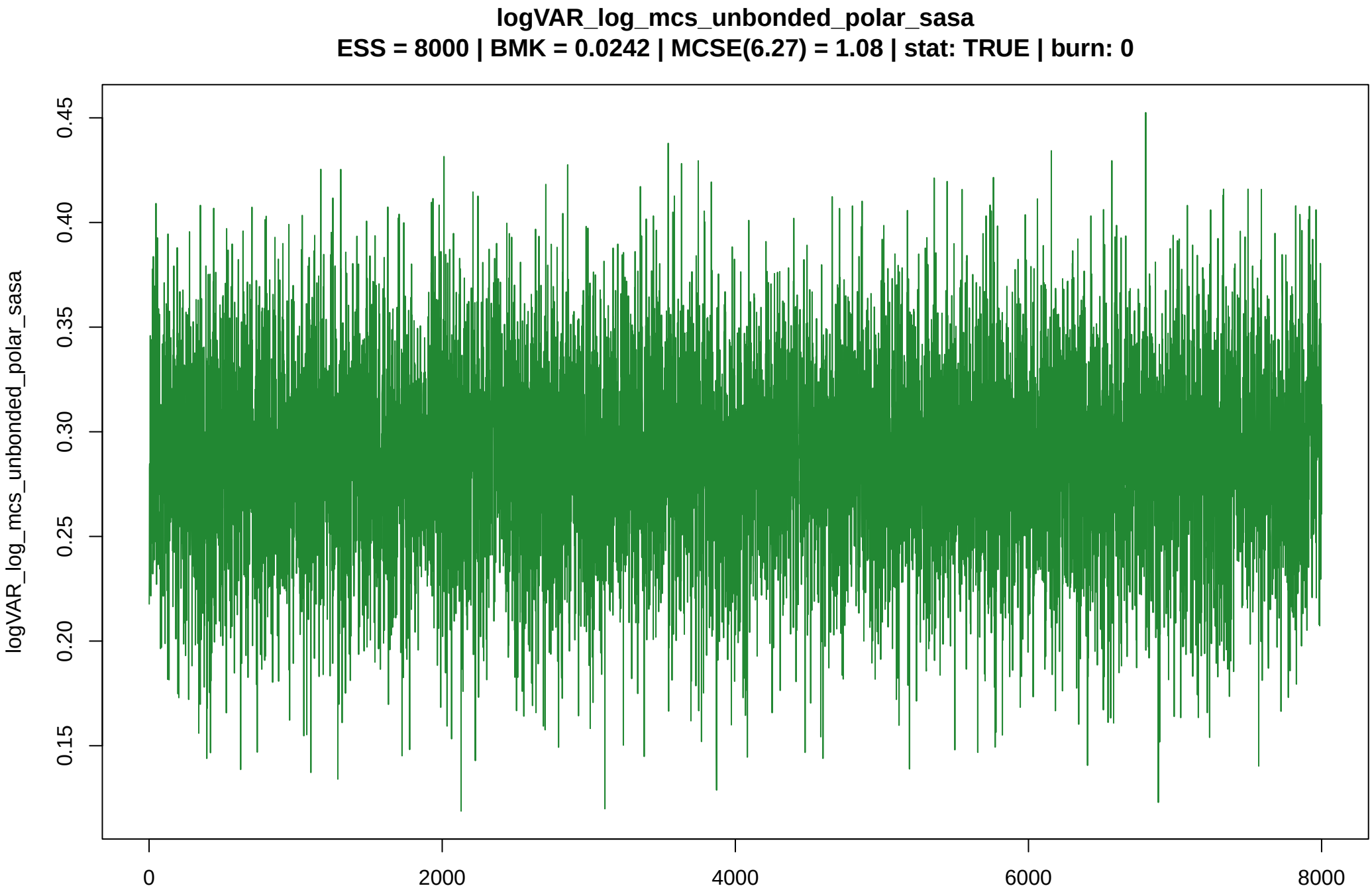

MEAN_mcs_NumHeteroAtoms
ESS = 8000 | BMK = 0.0232 | MCSE(6.27) = 1.12 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
2.90
2.95
3.00
3.05
0
2000
4000
6000
8000

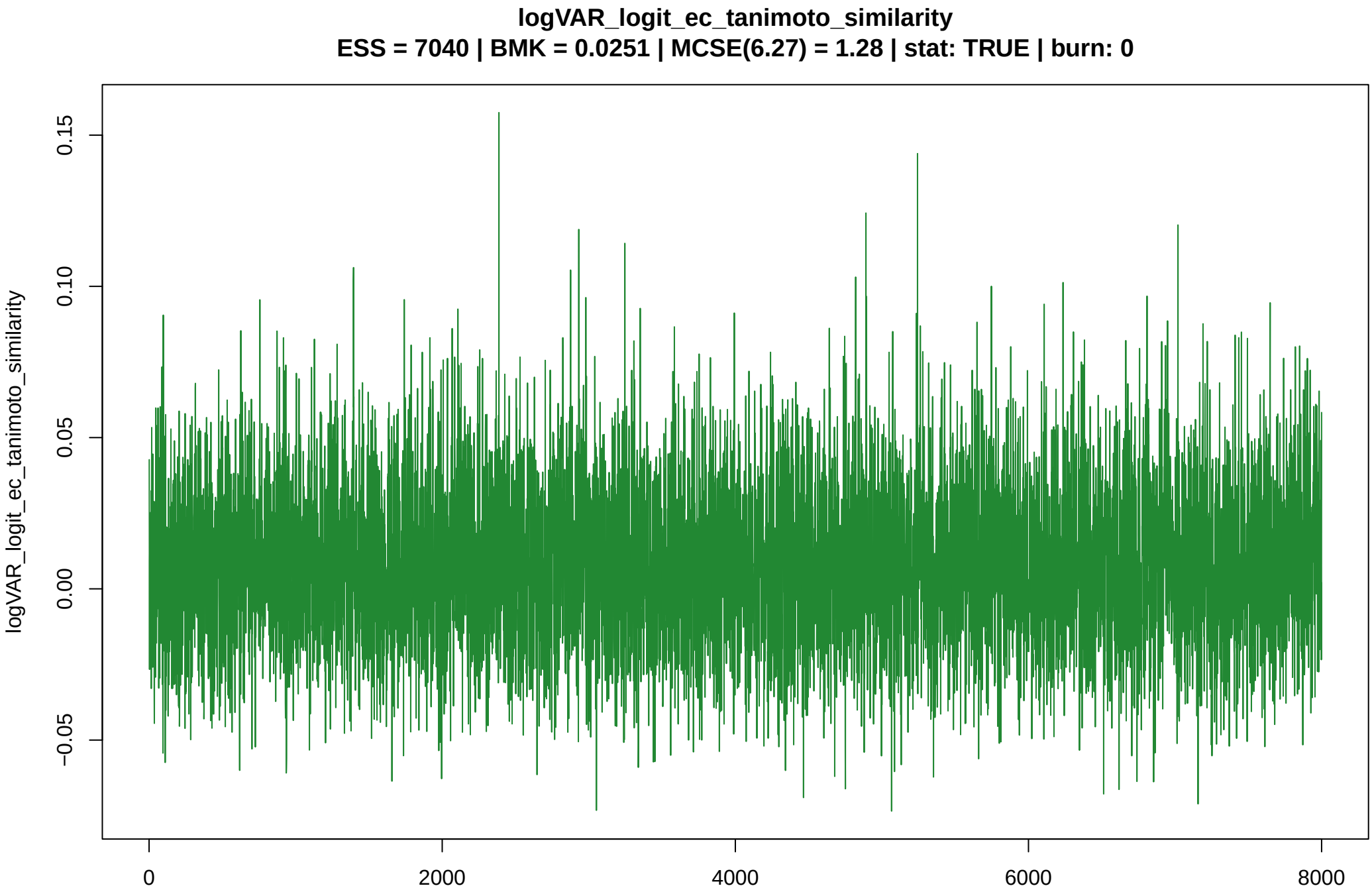

MEAN_docked_HeavyAtomCount
ESS = 8000 | BMK = 0.0266 | MCSE(6.27) = 1.11 | stat: FALSE | burn: 0
MEAN_docked_HeavyAtomCount
23.0
23.1
23.2
23.3
23.4
23.5
0
2000
4000
6000
8000

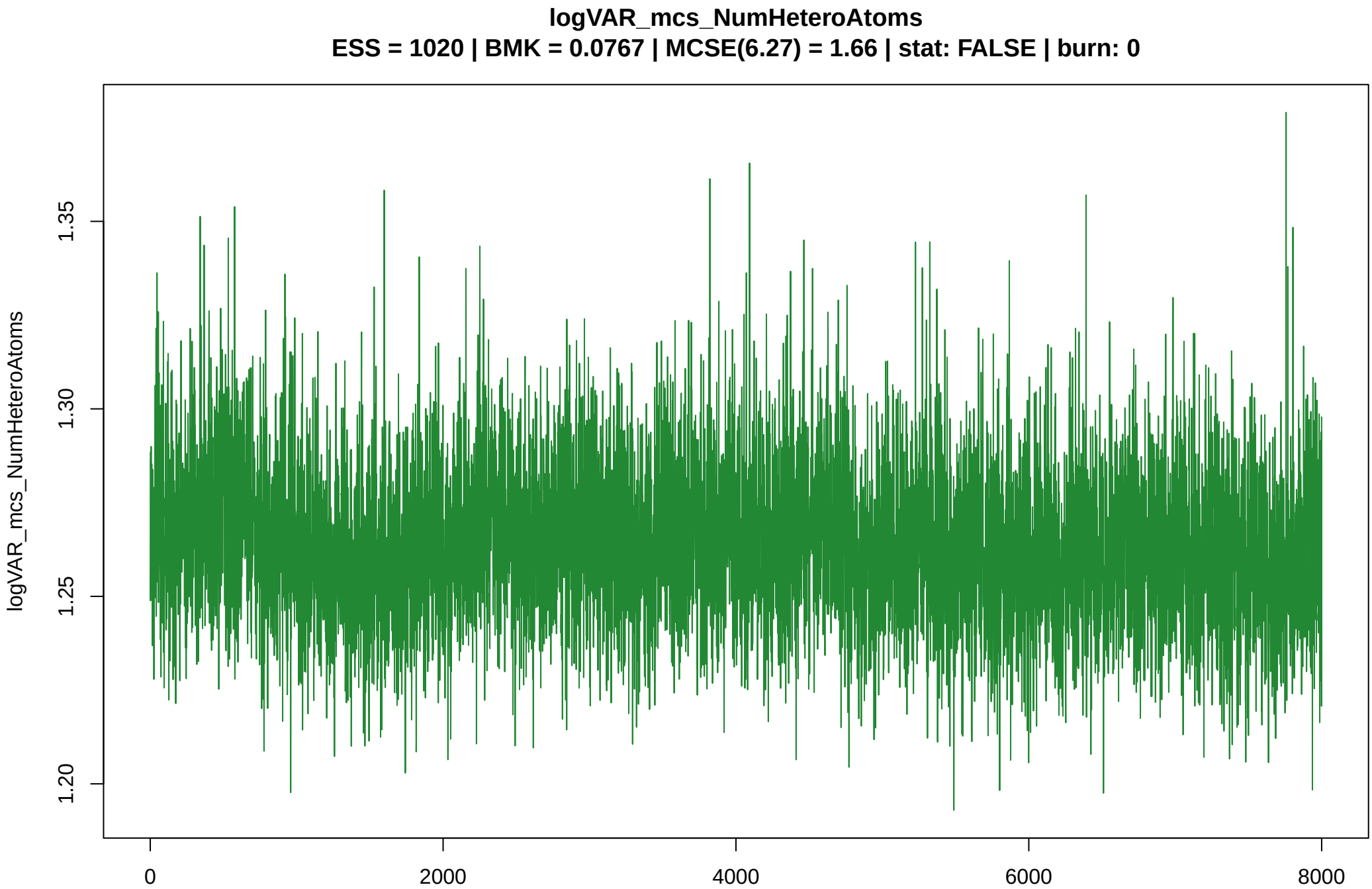

MEAN_mcs_RingCount
ESS = 7690 | BMK = 0.0232 | MCSE(6.27) = 1.14 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.80
0.82
0.84
0.86
0.88
0
2000
4000
6000
8000

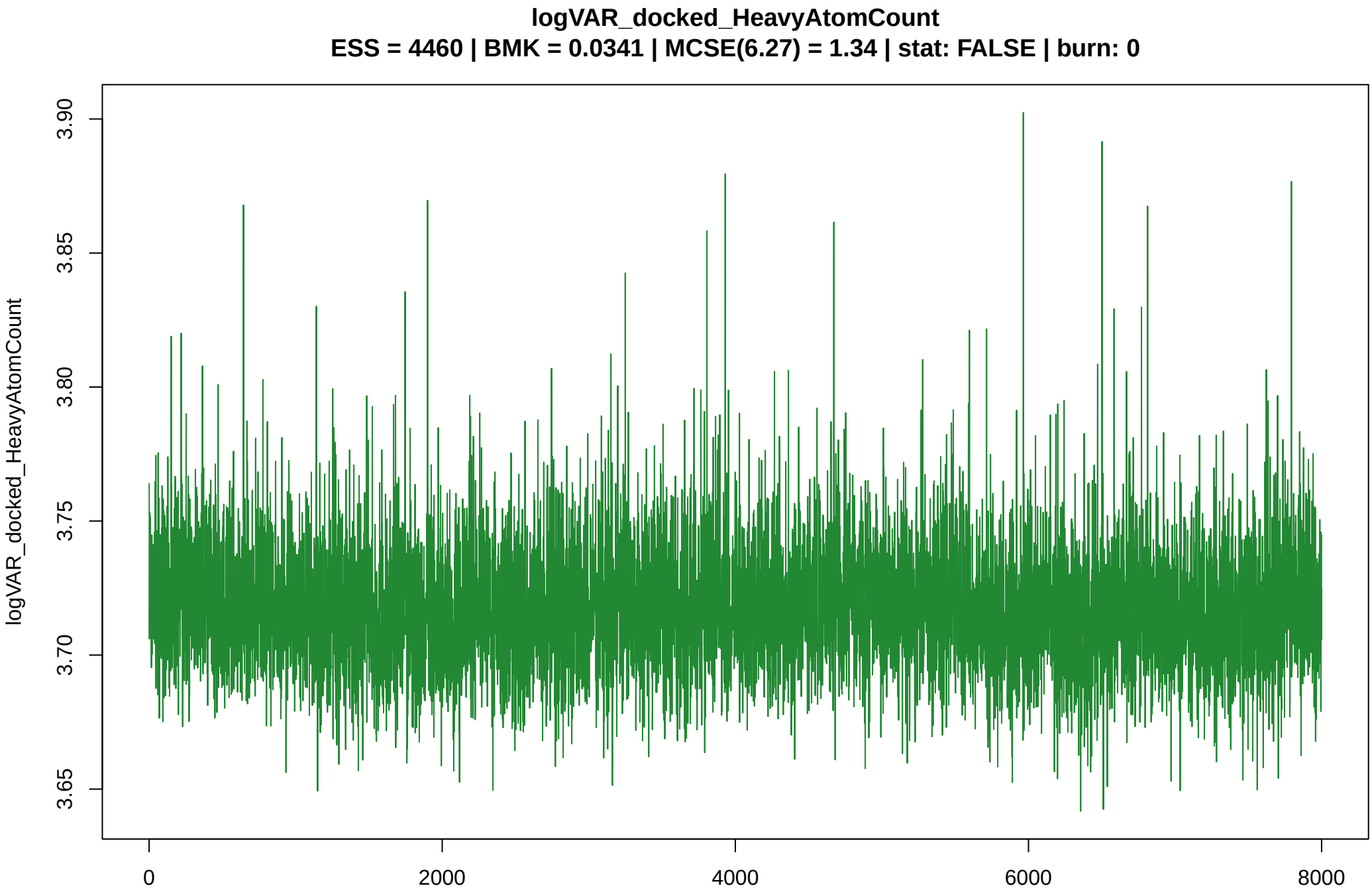

MEAN_docked_NumRotatableBonds
ESS = 8000 | BMK = 0.0302 | MCSE(6.27) = 1.12 | stat: TRUE | burn: 0
MEAN_docked_NumRotatableBonds
4.95
4.90
4.85
4.80
4.75
4.70
0
2000
4000
6000
8000

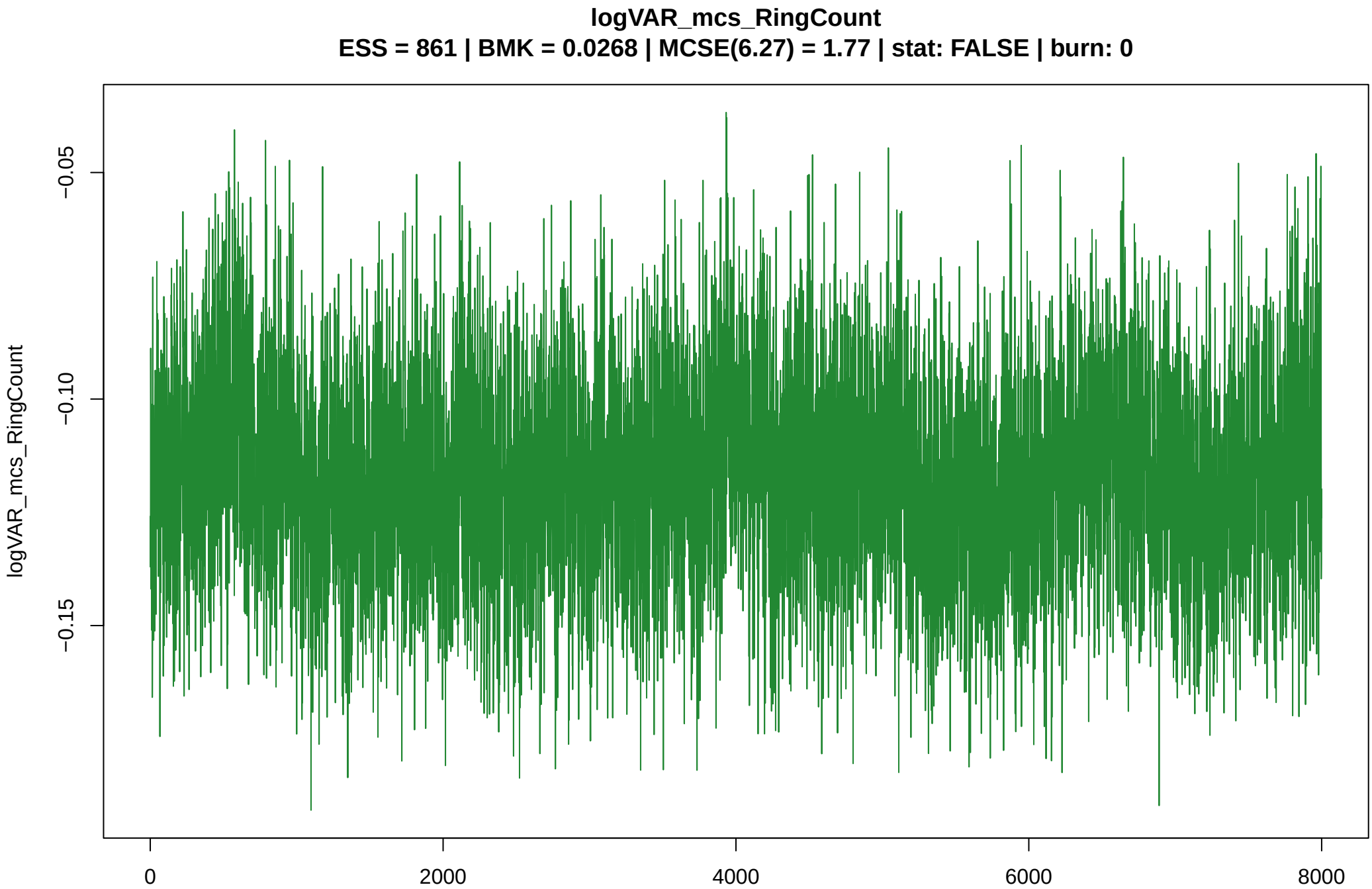

logVAR_log_RMSD
ESS = 6960 | BMK = 0.0211 | MCSE(6.27) = 1.26 | stat: TRUE | burn: 0
logVAR_log_RMSD
−0.20
−0.25
−0.30
−0.35
0
2000
4000
6000
8000

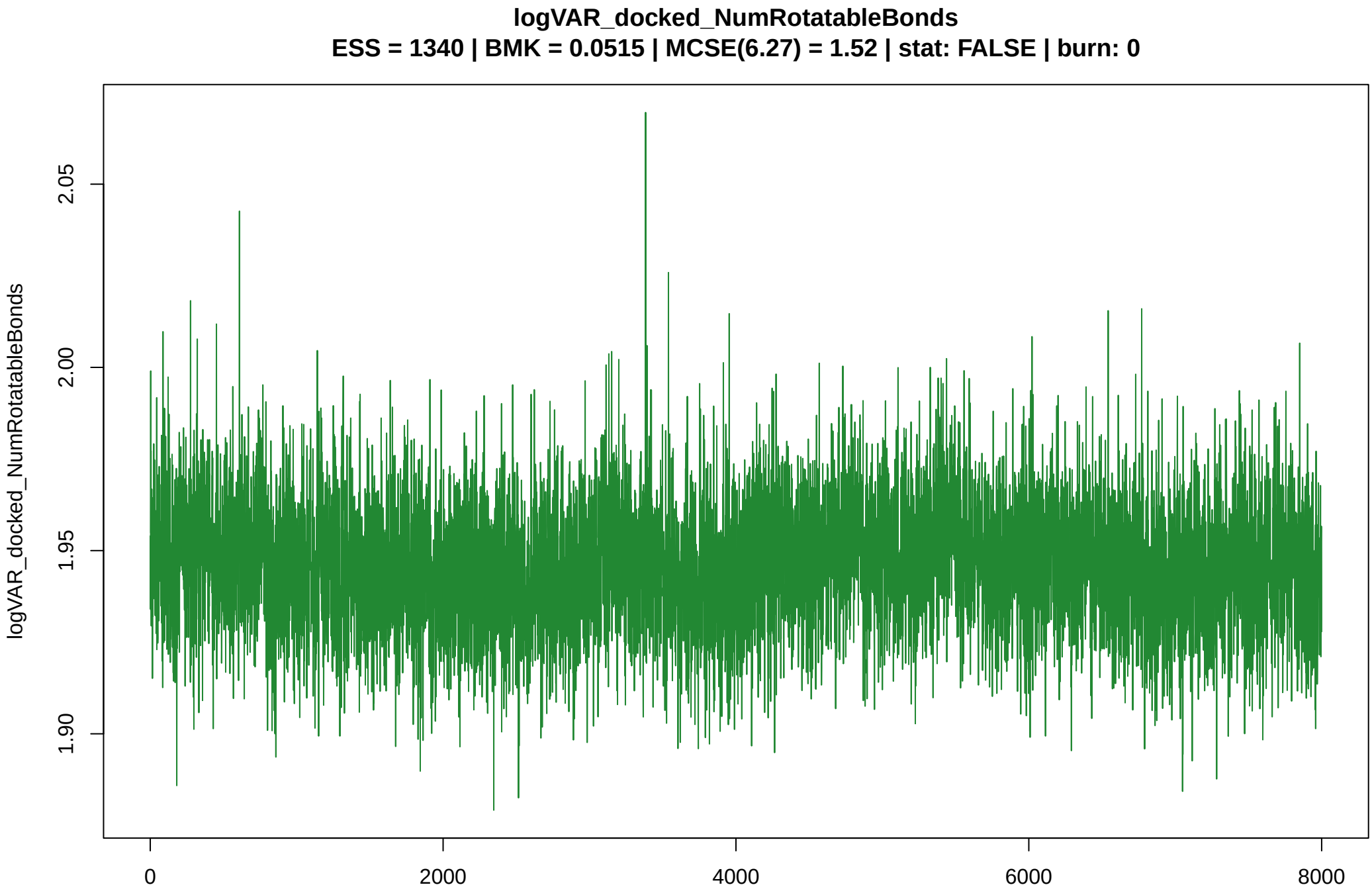

logVAR_log_mcs_unbonded_polar_sasa
ESS = 8000 | BMK = 0.0242 | MCSE(6.27) = 1.08 | stat: TRUE | burn: 0
logVAR_log_mcs_unbonded_polar_sasa
0.15
0.20
0.25
0.30
0.35
0.40
0.45
0
2000
4000
6000
8000

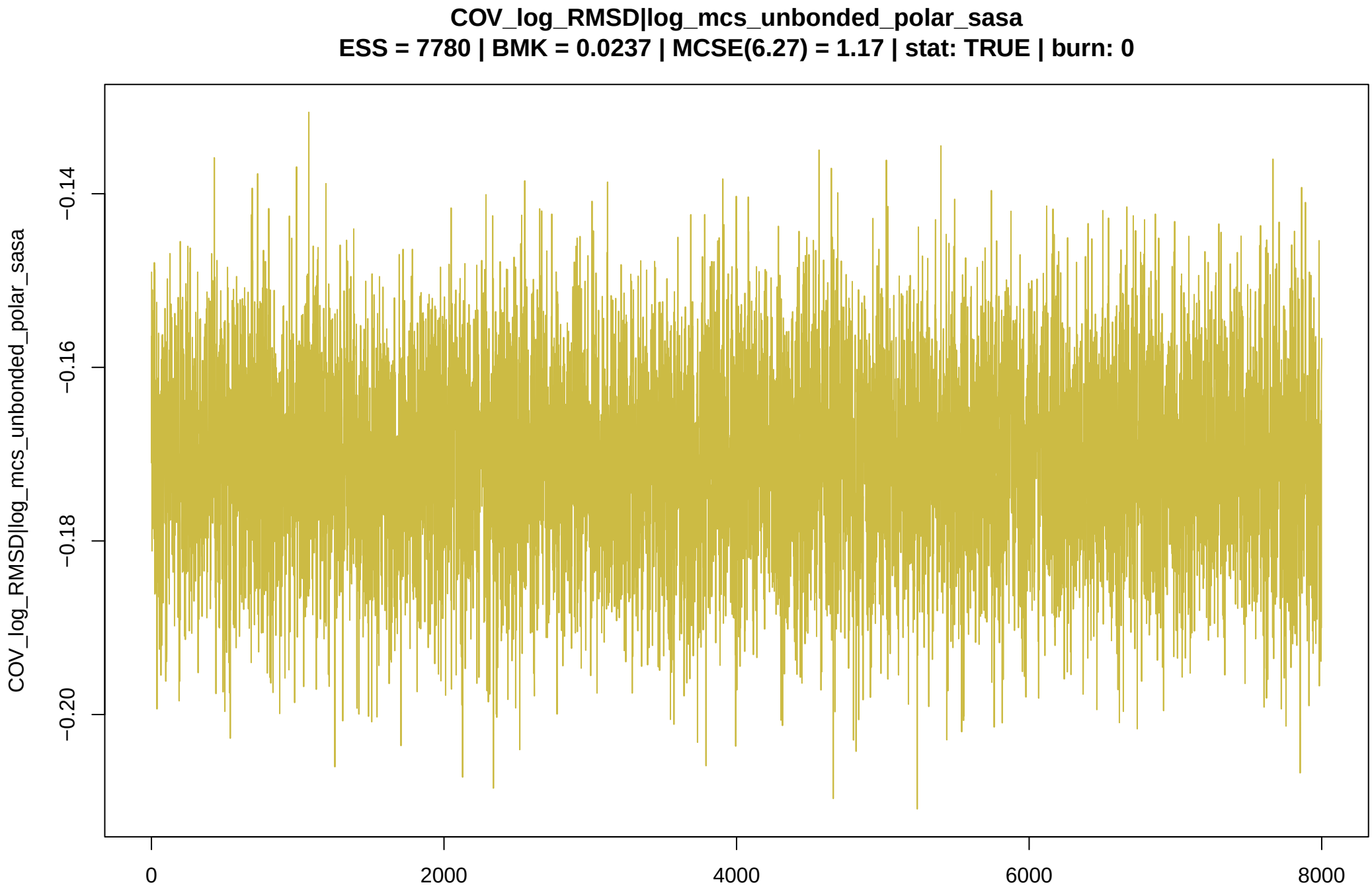

logVAR_logit_ec_tanimoto_similarity
ESS = 7040 | BMK = 0.0251 | MCSE(6.27) = 1.28 | stat: TRUE | burn: 0
logVAR_logit_ec_tanimoto_similarity
0.15
0.10
0.05
0.00
−0.05
0
2000
4000
6000
8000

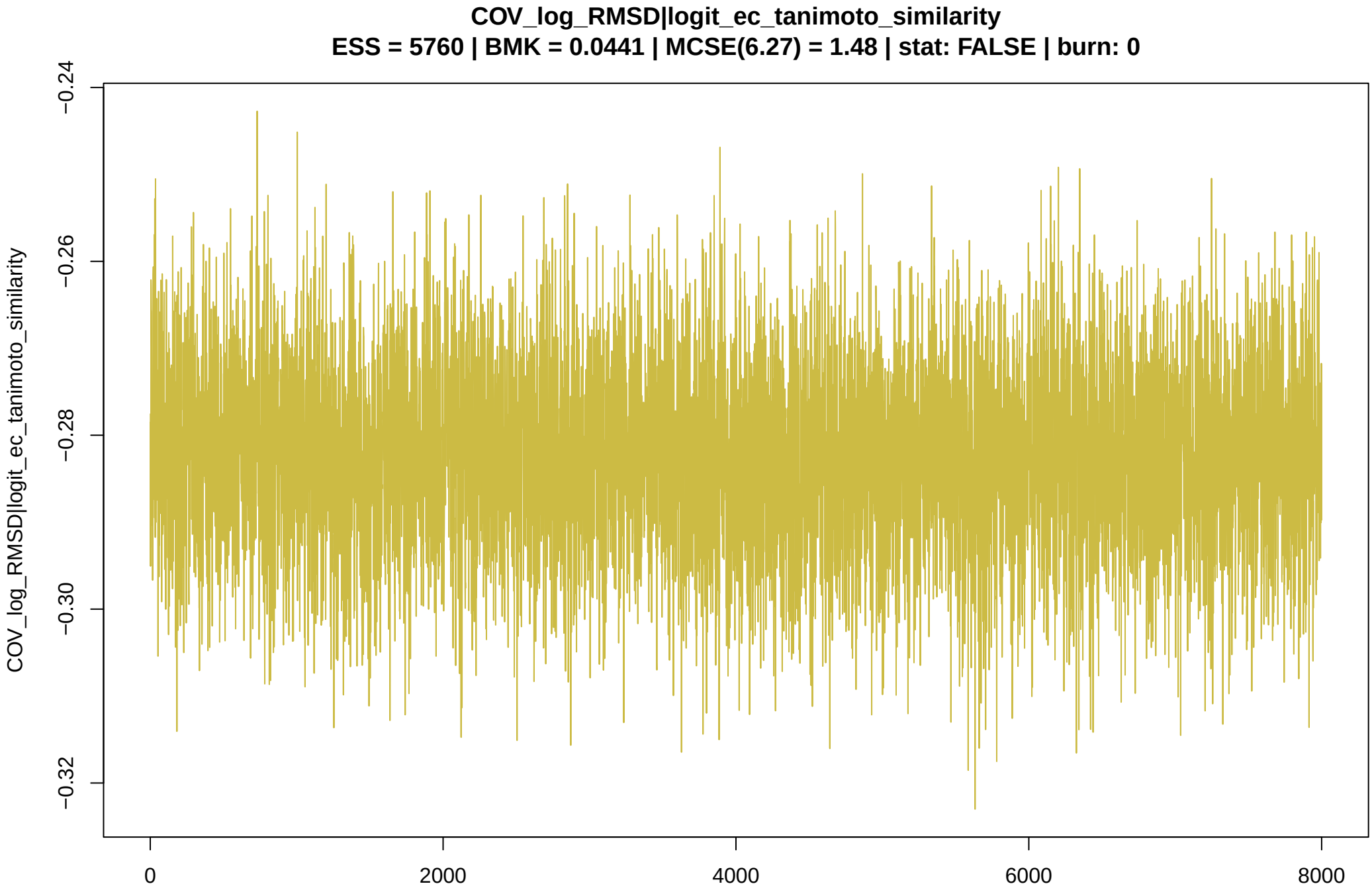

logVAR_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0767 | MCSE(6.27) = 1.66 | stat: FALSE | burn: 0
logVAR_mcs_NumHeteroAtoms
1.20
1.25
1.30
1.35
0
2000
4000
6000
8000

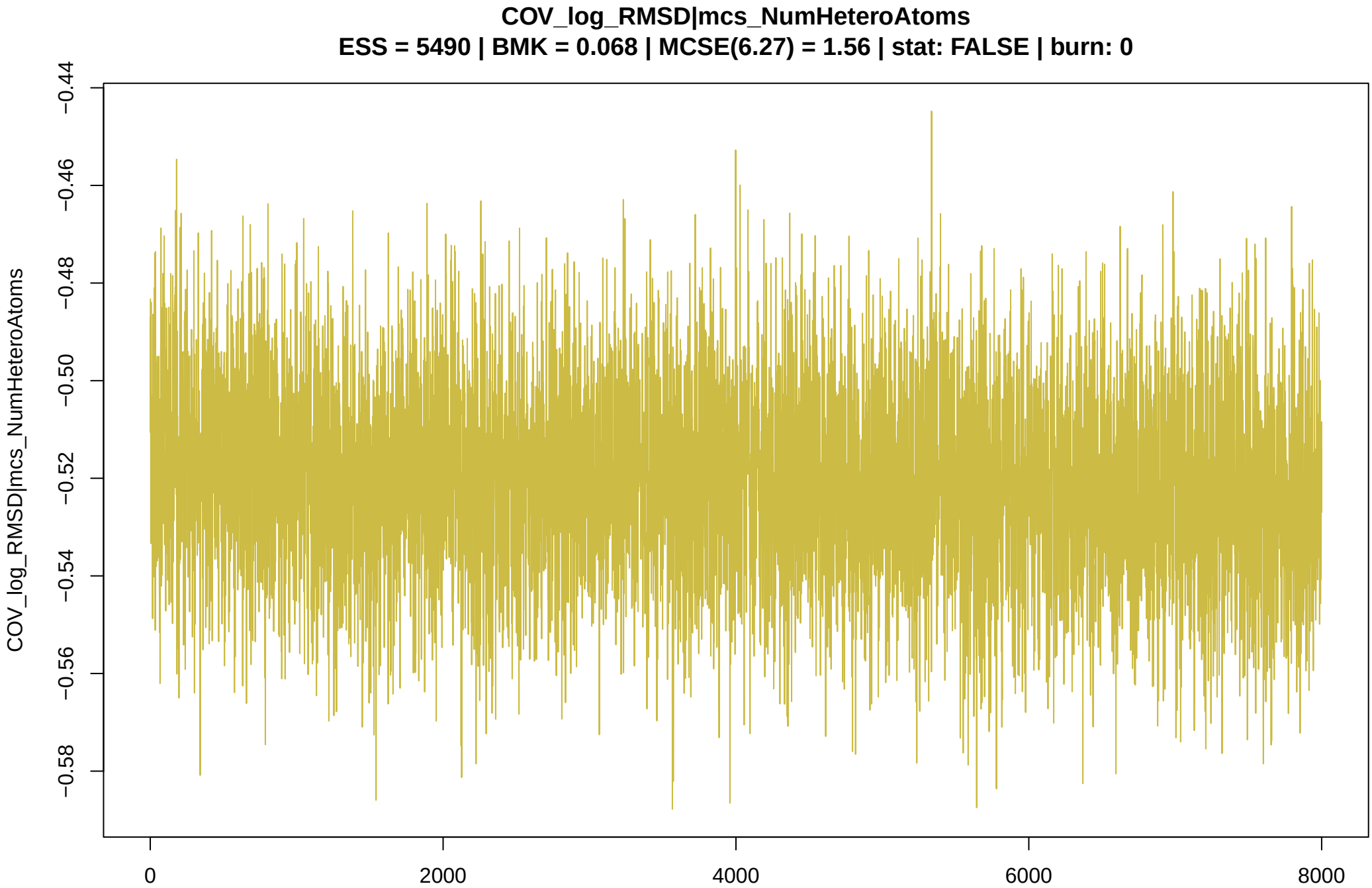

logVAR_docked_HeavyAtomCount
ESS = 4460 | BMK = 0.0341 | MCSE(6.27) = 1.34 | stat: FALSE | burn: 0
logVAR_docked_HeavyAtomCount
3.65
3.70
3.75
3.80
3.85
3.90
0
2000
4000
6000
8000

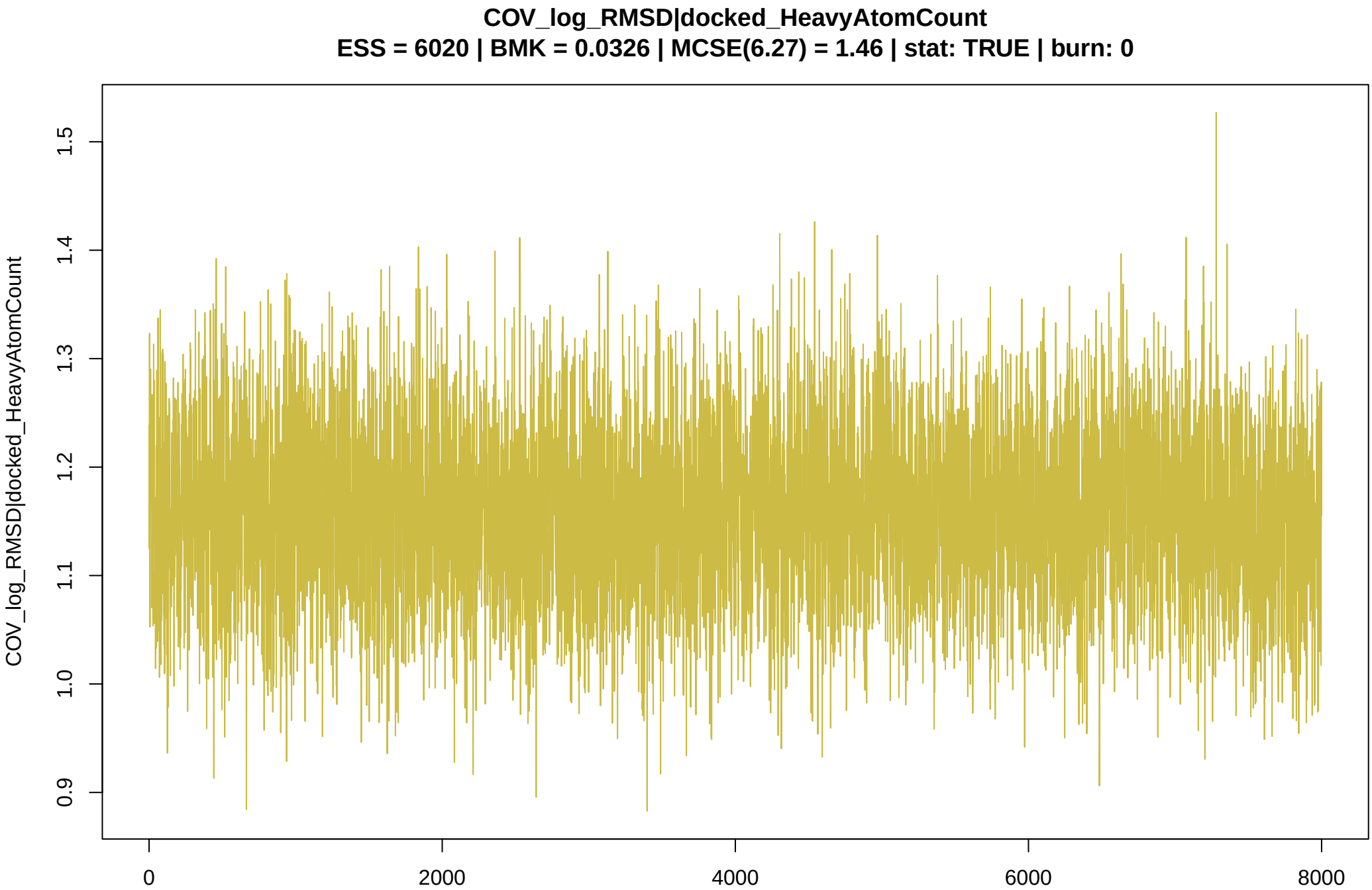

logVAR_mcs_RingCount
ESS = 861 | BMK = 0.0268 | MCSE(6.27) = 1.77 | stat: FALSE | burn: 0
logVAR_mcs_RingCount
−0.05
−0.10
−0.15
0
2000
4000
6000
8000

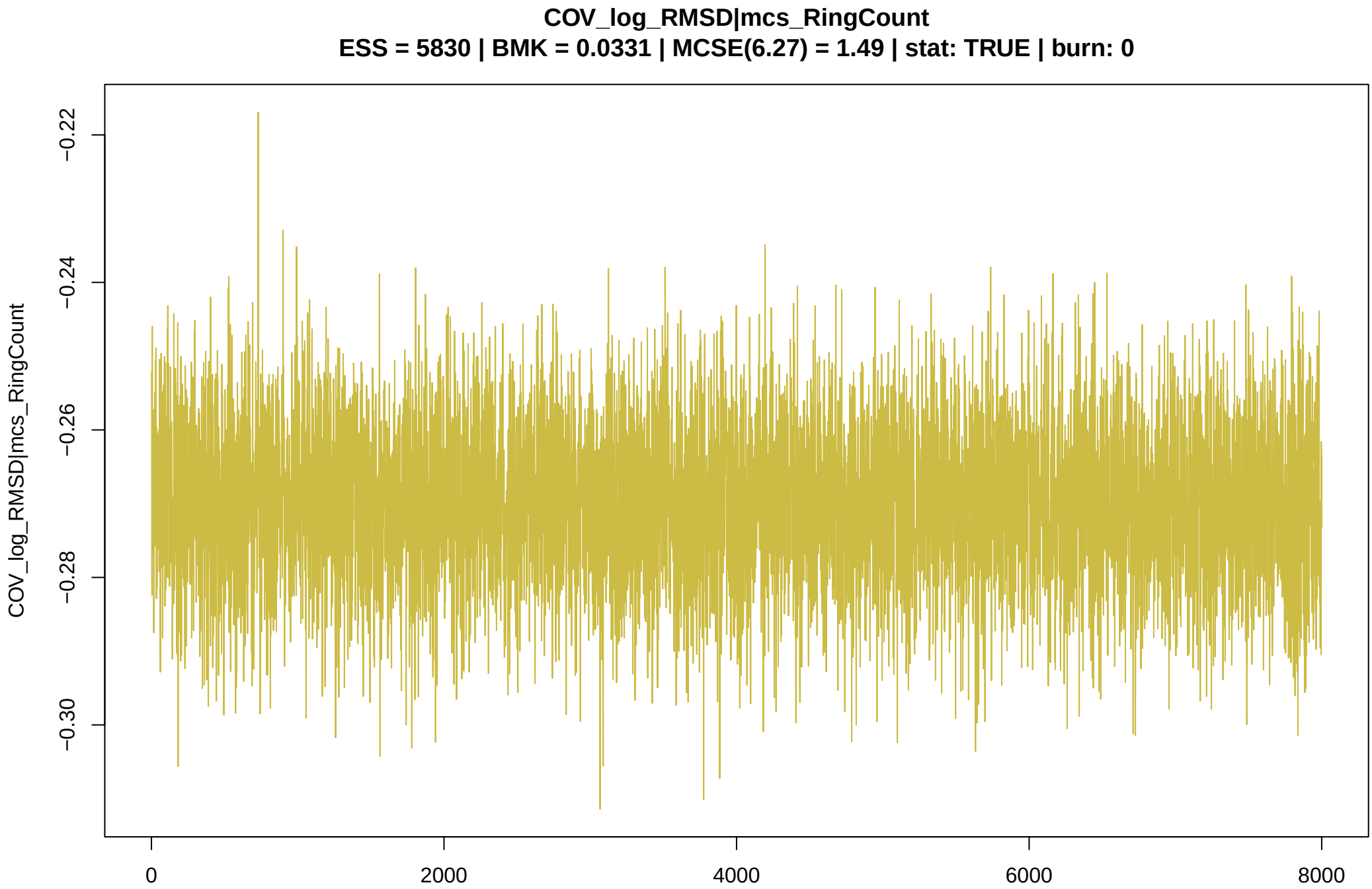

logVAR_docked_NumRotatableBonds
ESS = 1340 | BMK = 0.0515 | MCSE(6.27) = 1.52 | stat: FALSE | burn: 0
logVAR_docked_NumRotatableBonds
1.90
1.95
2.00
2.05
0
2000
4000
6000
8000

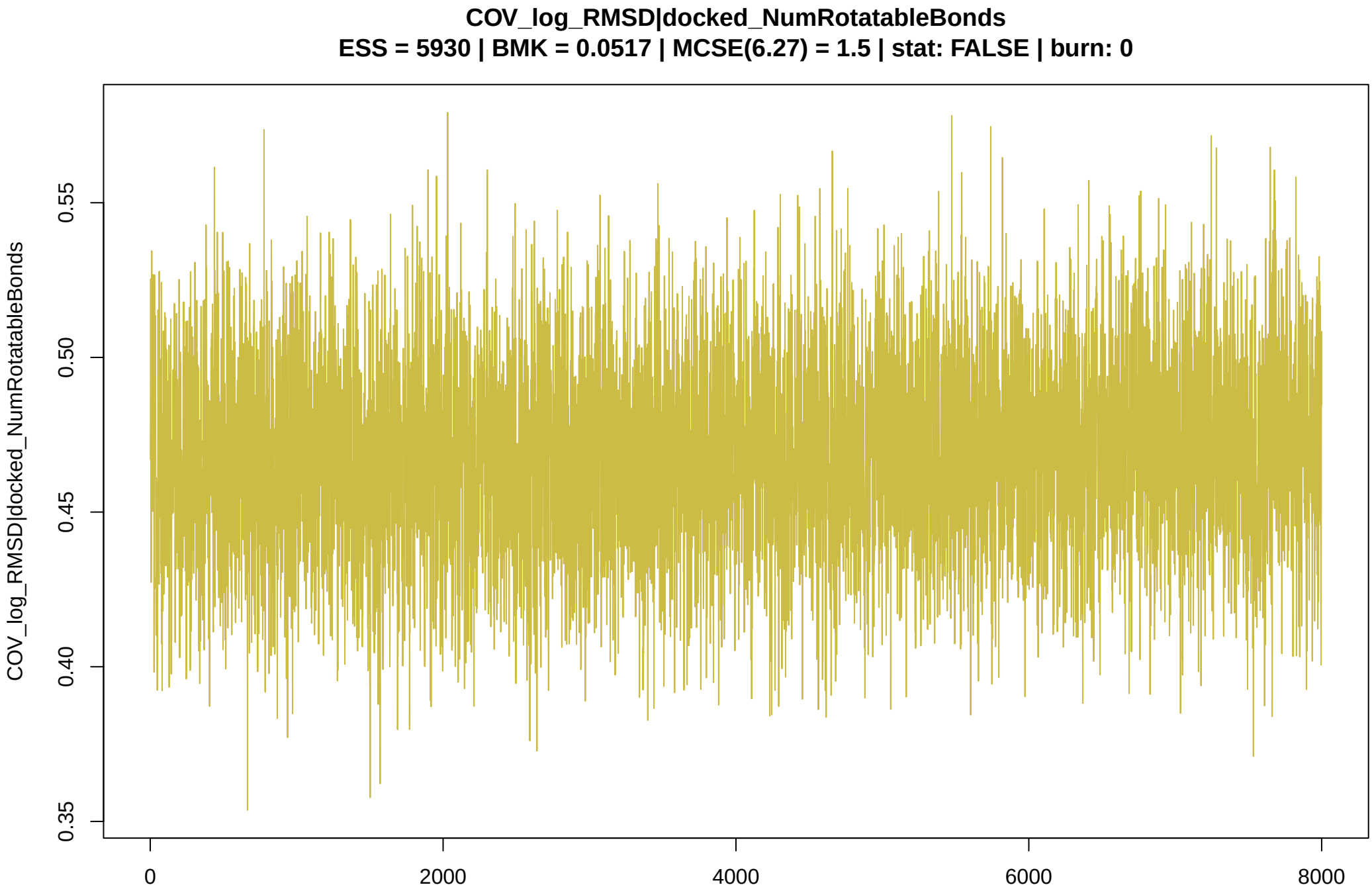

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 7780 | BMK = 0.0237 | MCSE(6.27) = 1.17 | stat: TRUE | burn: 0
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.14
−0.16
−0.18
−0.20
0
2000
4000
6000
8000

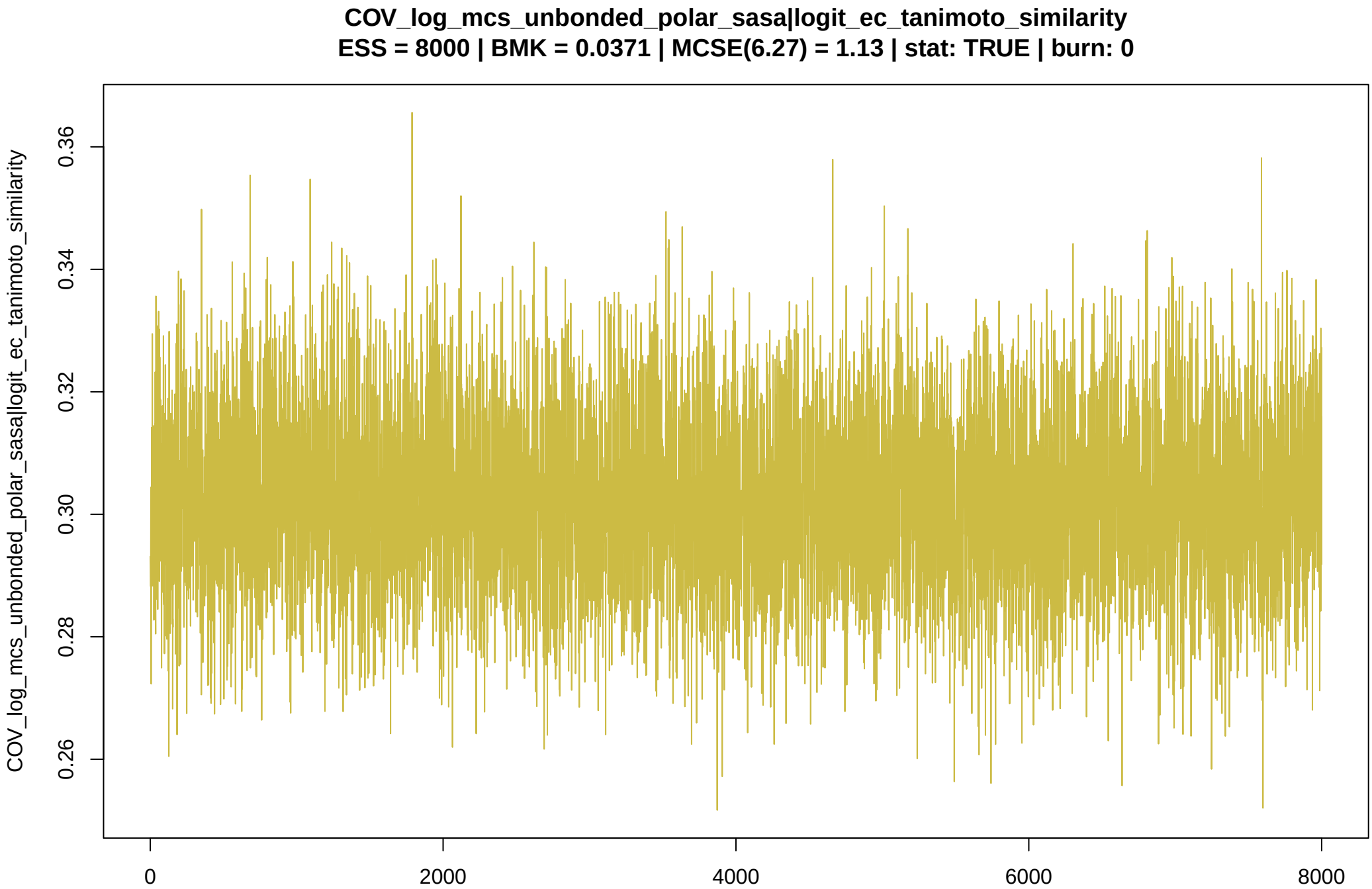

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 5760 | BMK = 0.0441 | MCSE(6.27) = 1.48 | stat: FALSE | burn: 0
COV_log_RMSD|logit_ec_tanimoto_similarity
−0.24
−0.26
−0.28
−0.30
−0.32
0
2000
4000
6000
8000

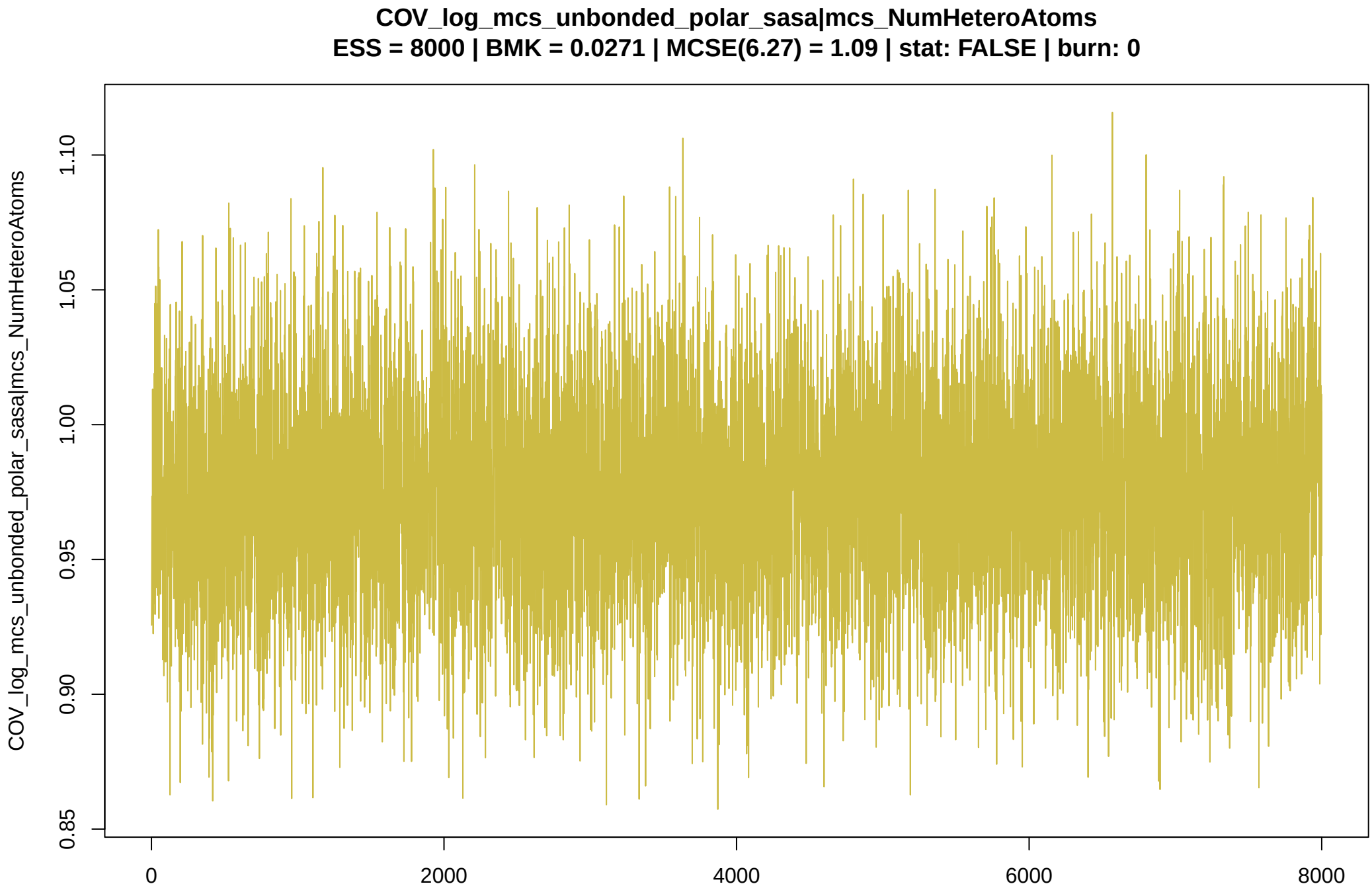

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 5490 | BMK = 0.068 | MCSE(6.27) = 1.56 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.44
−0.46
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
2000
4000
6000
8000

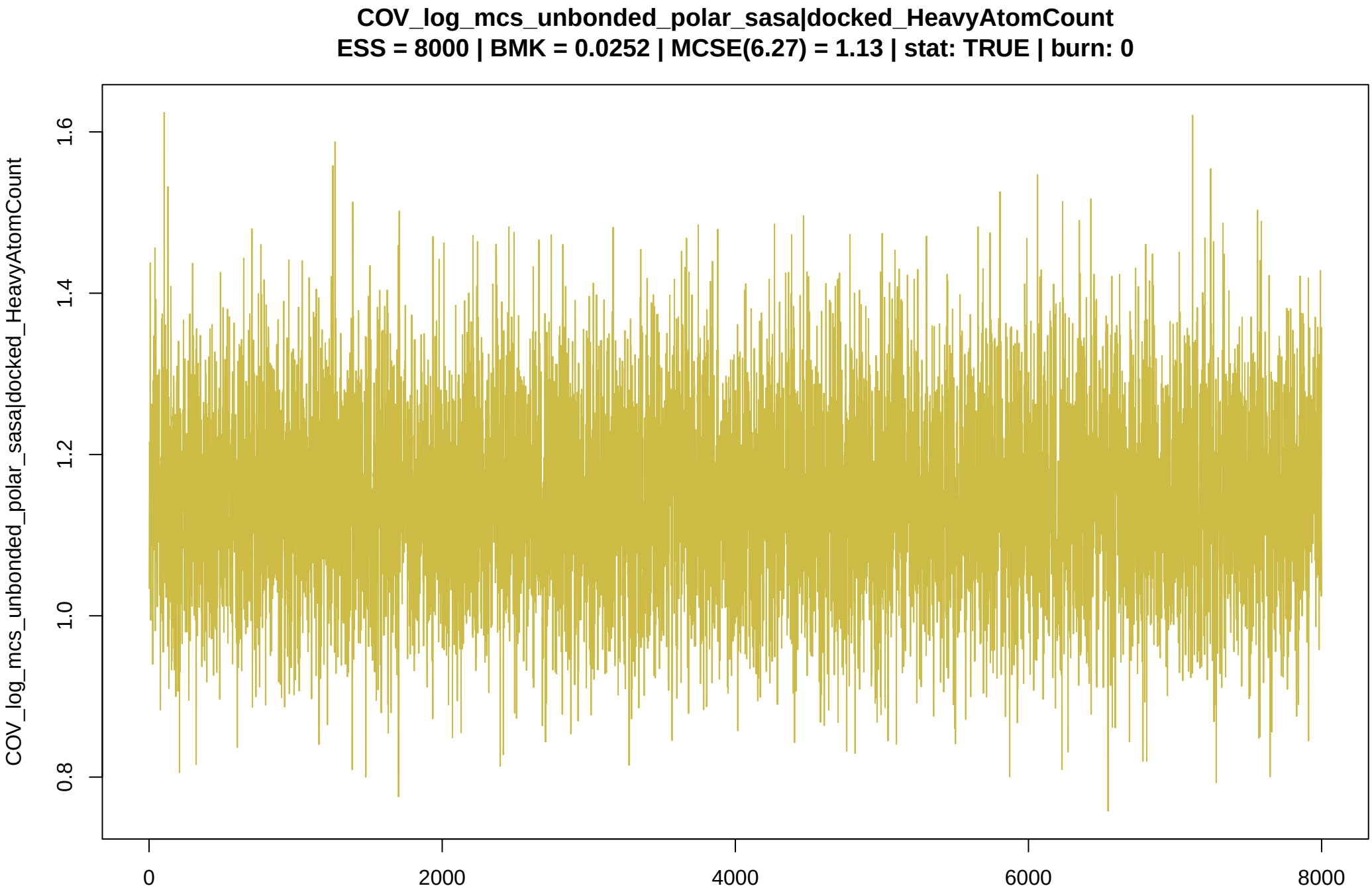

COV_log_RMSD|docked_HeavyAtomCount
ESS = 6020 | BMK = 0.0326 | MCSE(6.27) = 1.46 | stat: TRUE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
0.9
1.0
1.1
1.2
1.3
1.4
1.5
0
2000
4000
6000
8000

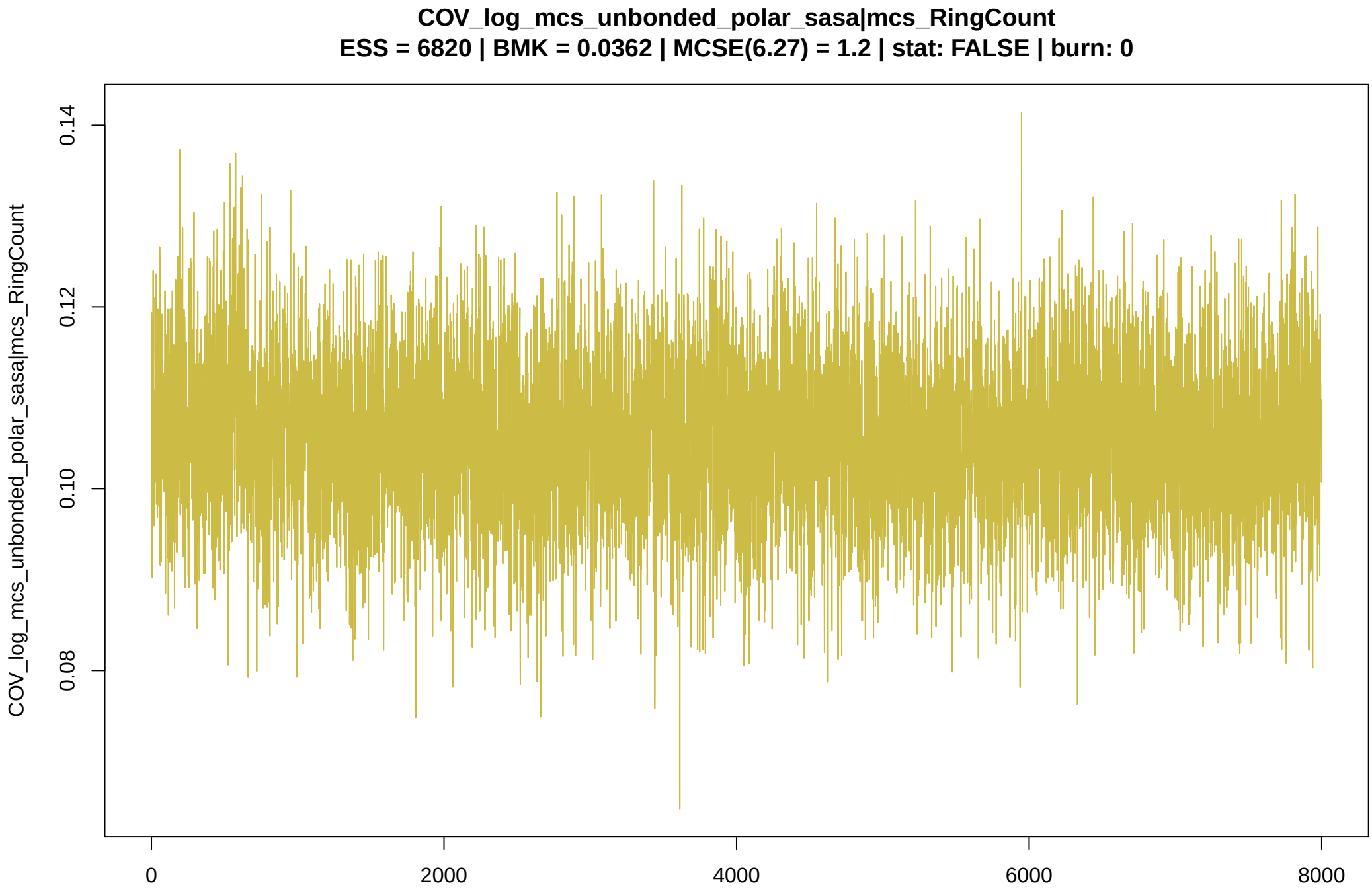

COV_log_RMSD|mcs_RingCount
ESS = 5830 | BMK = 0.0331 | MCSE(6.27) = 1.49 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.22
−0.24
−0.26
−0.28
−0.30
0
2000
4000
6000
8000

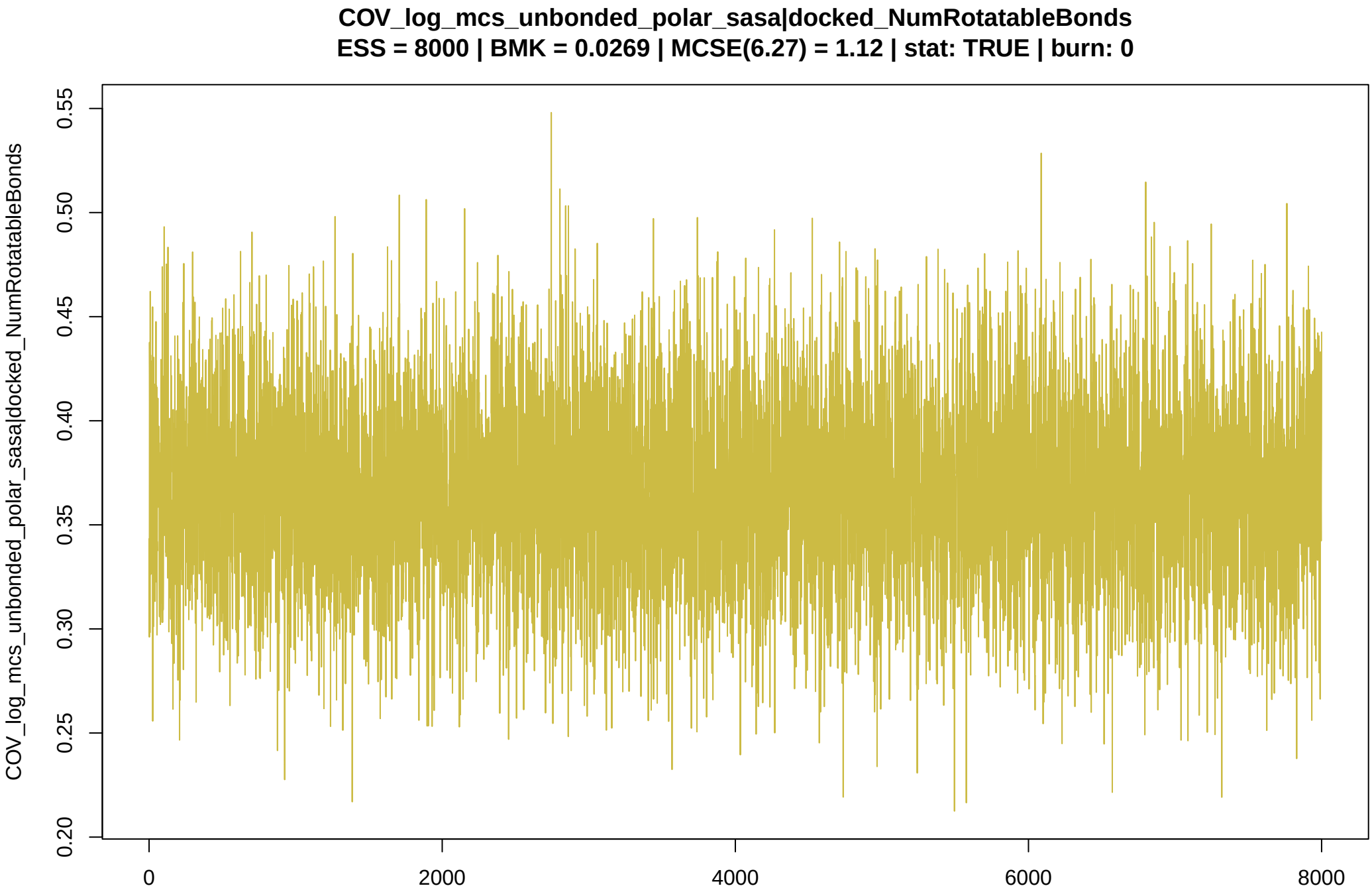

COV_log_RMSD|docked_NumRotatableBonds
ESS = 5930 | BMK = 0.0517 | MCSE(6.27) = 1.5 | stat: FALSE | burn: 0
COV_log_RMSD|docked_NumRotatableBonds
0.35
0.40
0.45
0.50
0.55
0
2000
4000
6000
8000

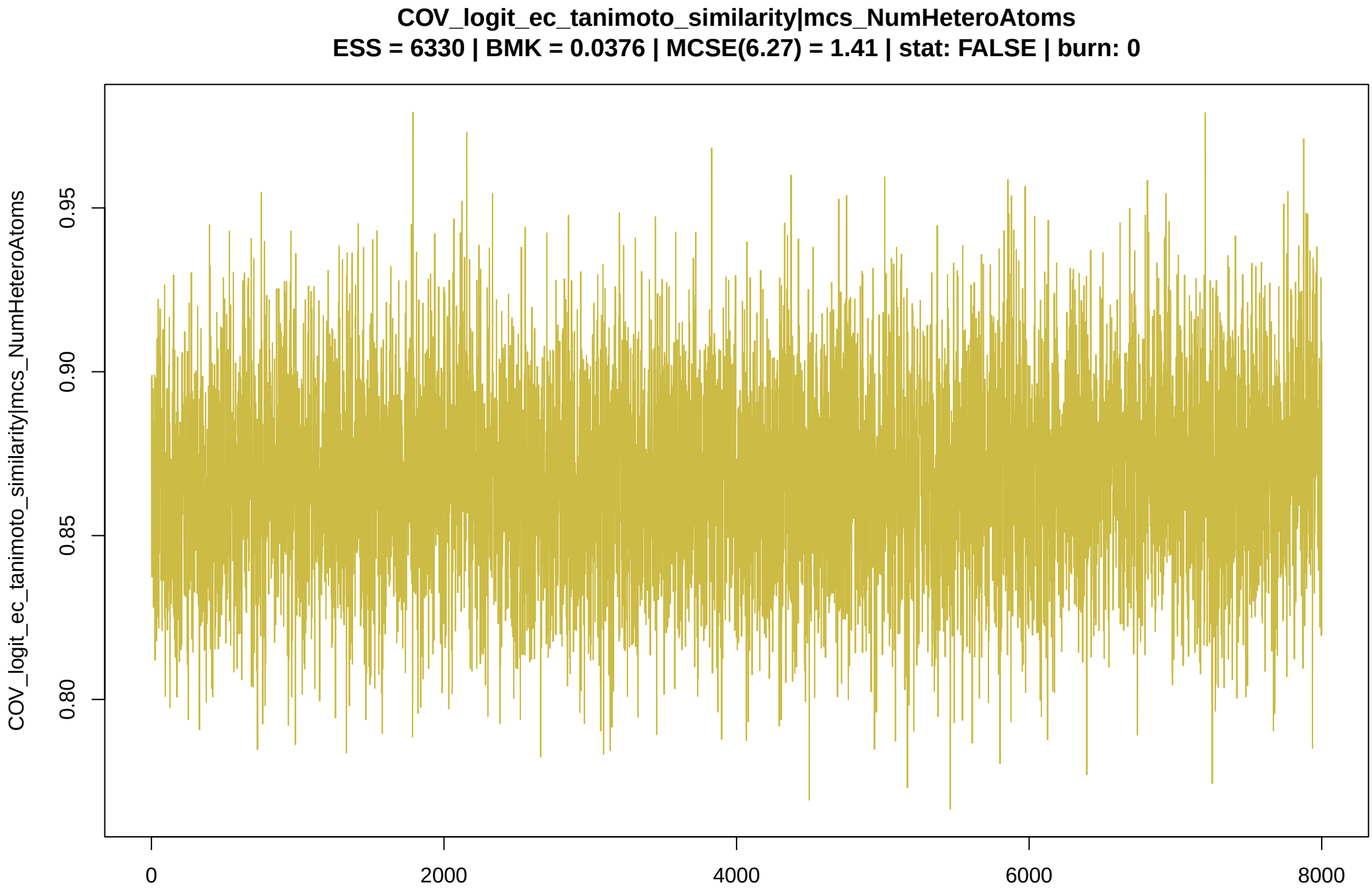

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 8000 | BMK = 0.0371 | MCSE(6.27) = 1.13 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0.26
0.28
0.30
0.32
0.34
0.36
0
2000
4000
6000
8000

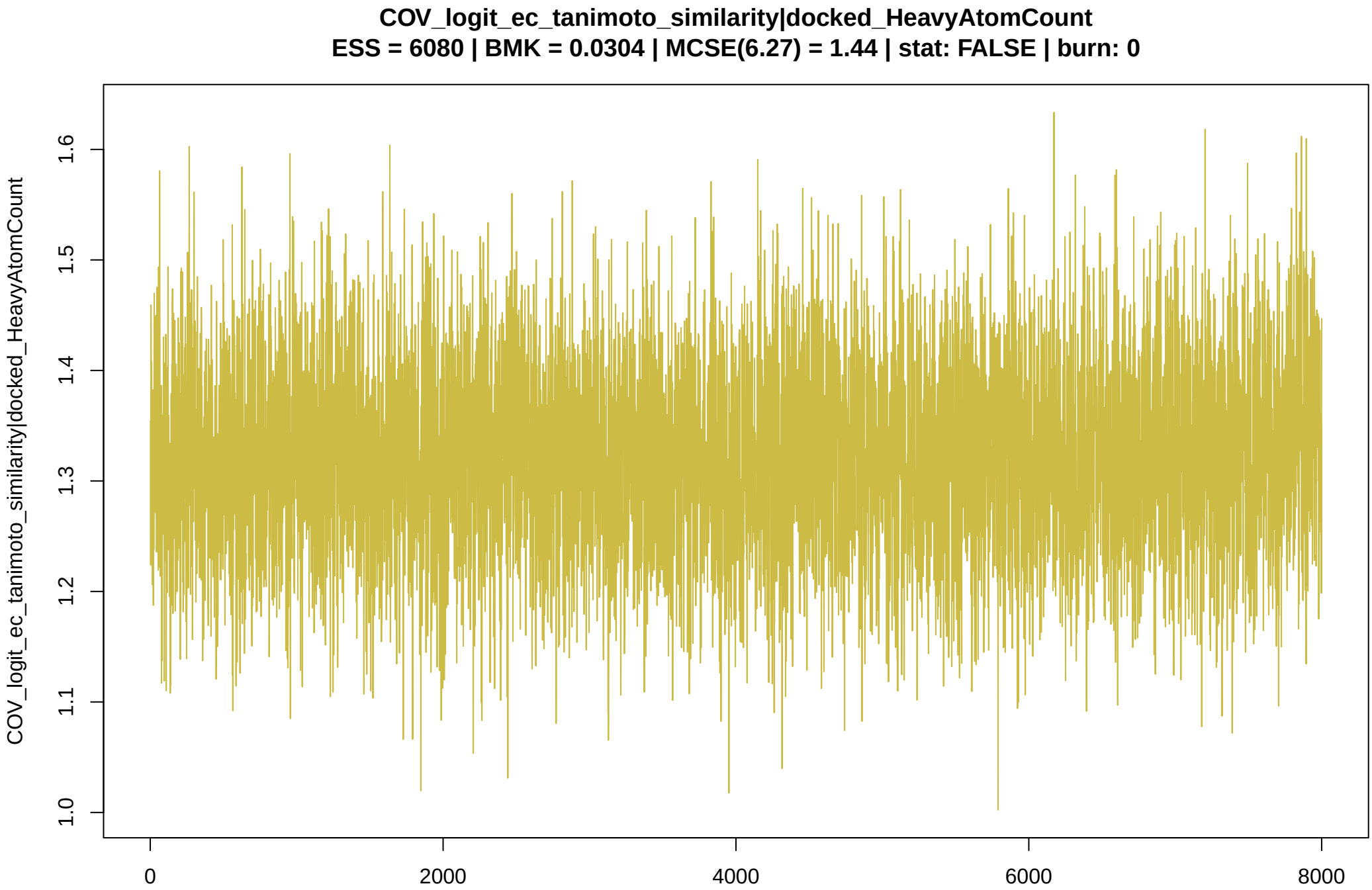

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 8000 | BMK = 0.0271 | MCSE(6.27) = 1.09 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.85
0.90
0.95
1.00
1.05
1.10
0
2000
4000
6000
8000

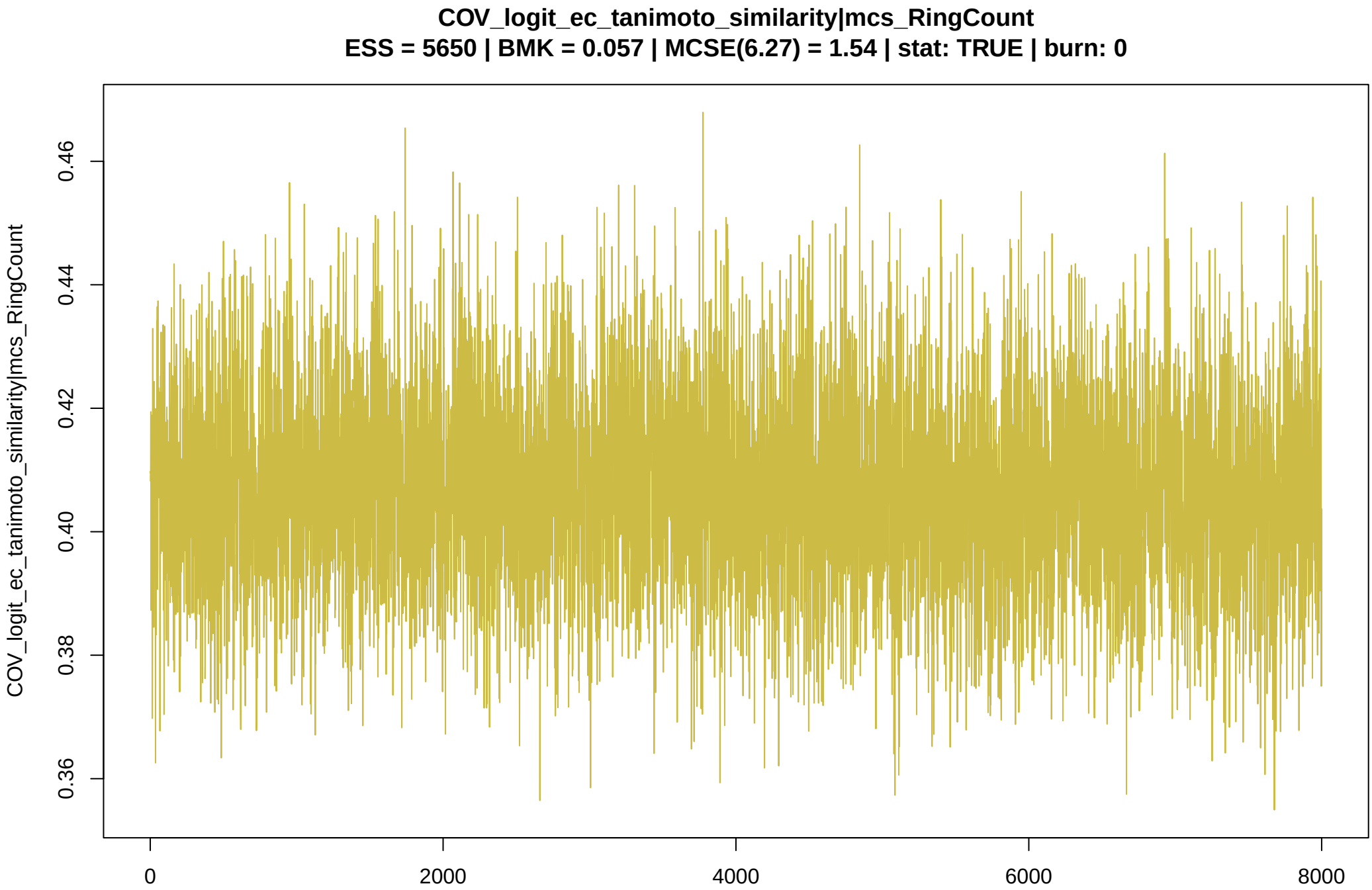

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 8000 | BMK = 0.0252 | MCSE(6.27) = 1.13 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0.8
1.0
1.2
1.4
1.6
0
2000
4000
6000
8000

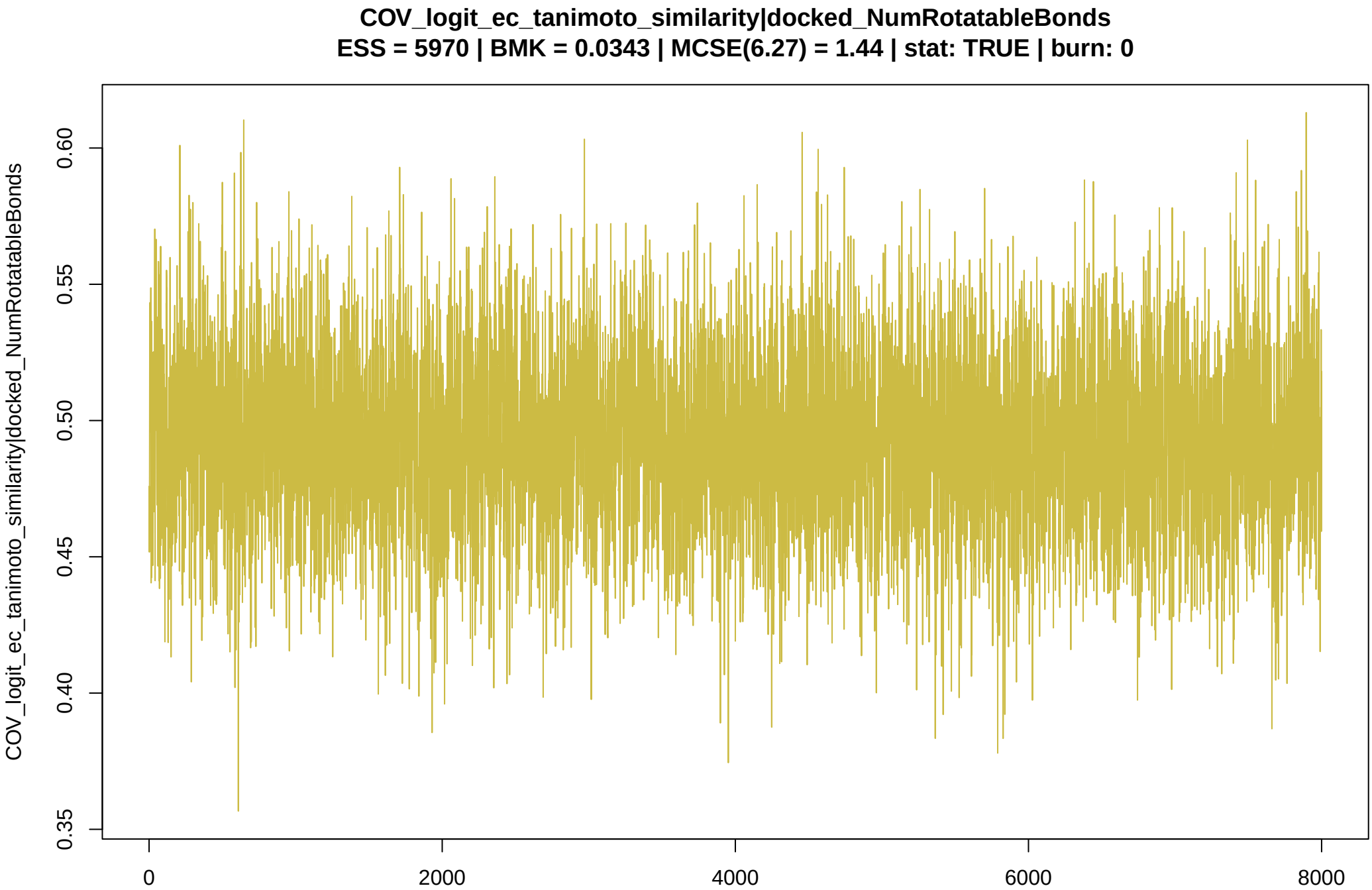

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 6820 | BMK = 0.0362 | MCSE(6.27) = 1.2 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
0.08
0.10
0.12
0.14
0
2000
4000
6000
8000

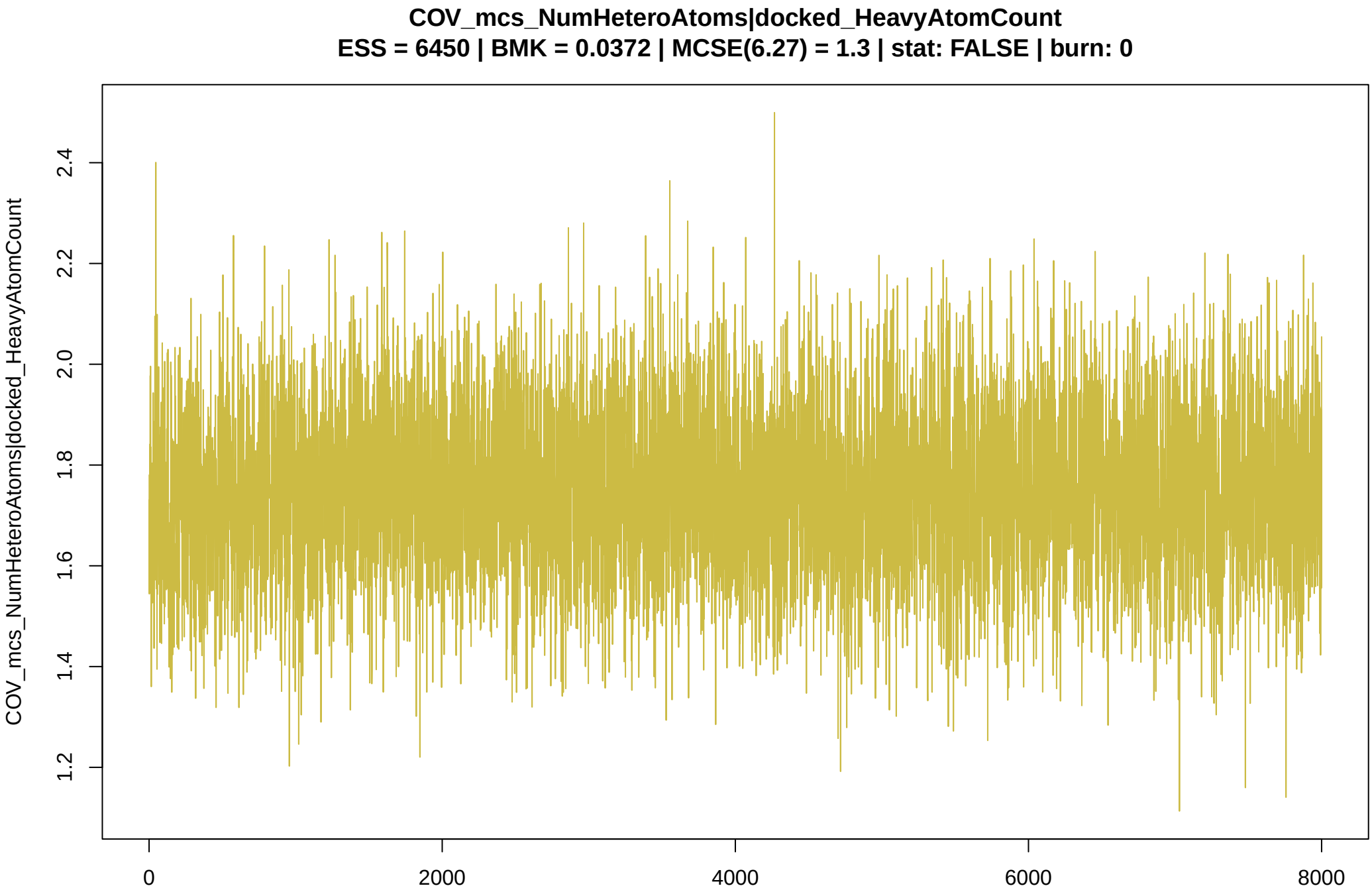

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 8000 | BMK = 0.0269 | MCSE(6.27) = 1.12 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
0.20
0.25
0.30
0.35
0.40
0.45
0.50
0.55
0
2000
4000
6000
8000

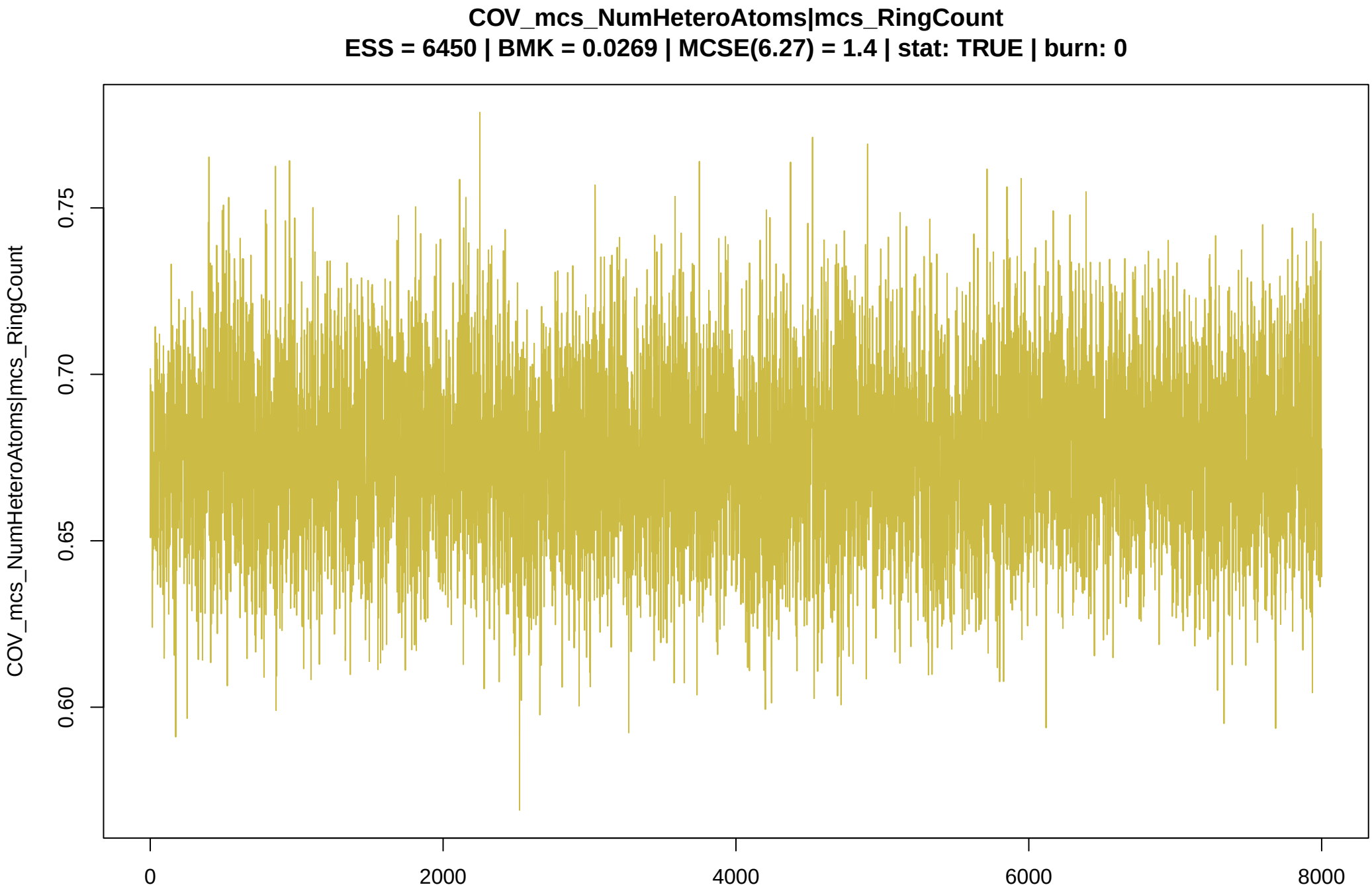

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 6330 | BMK = 0.0376 | MCSE(6.27) = 1.41 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.80
0.85
0.90
0.95
0
2000
4000
6000
8000

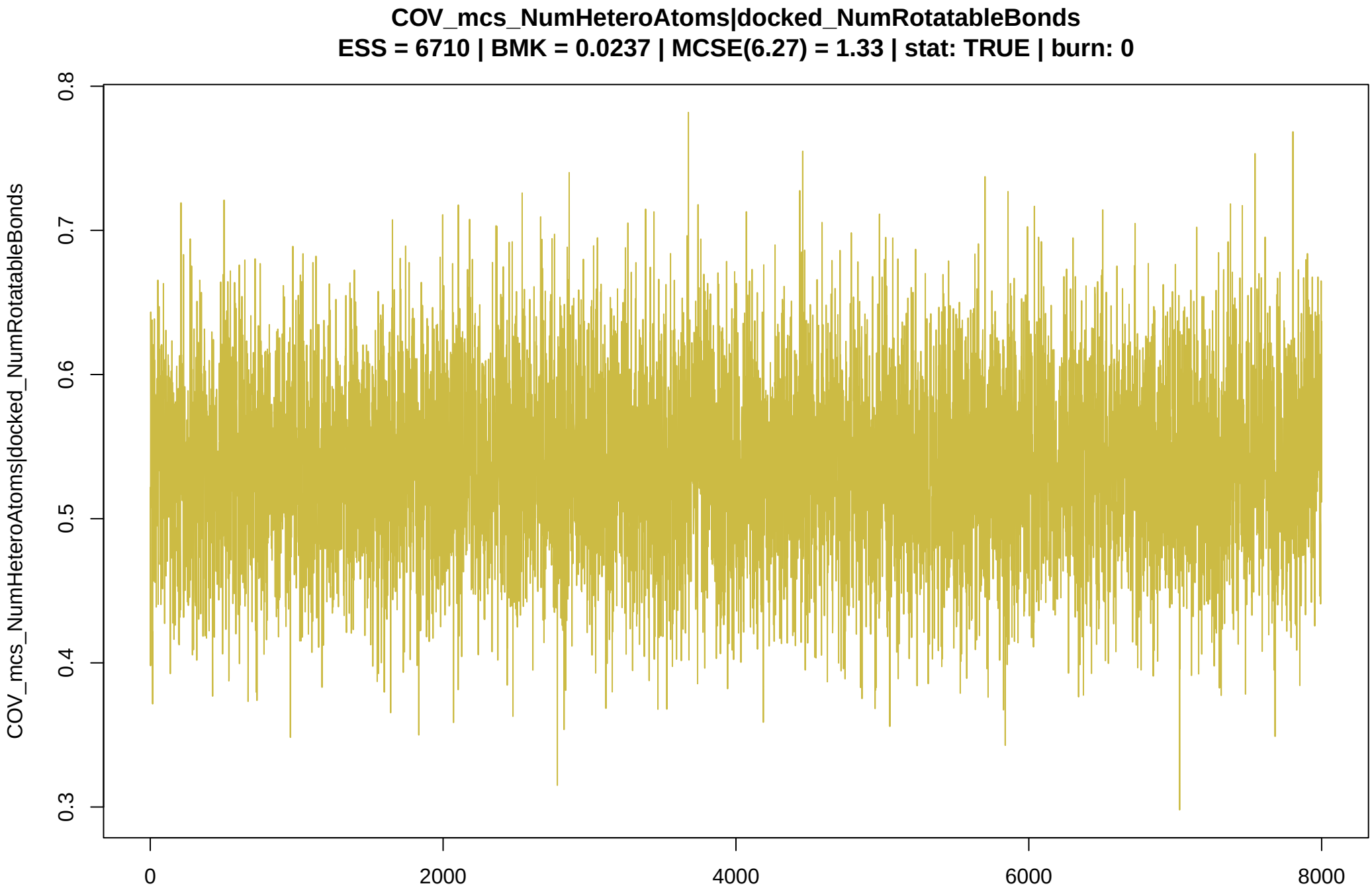

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 6080 | BMK = 0.0304 | MCSE(6.27) = 1.44 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
1.0
1.1
1.2
1.3
1.4
1.5
1.6
0
2000
4000
6000
8000

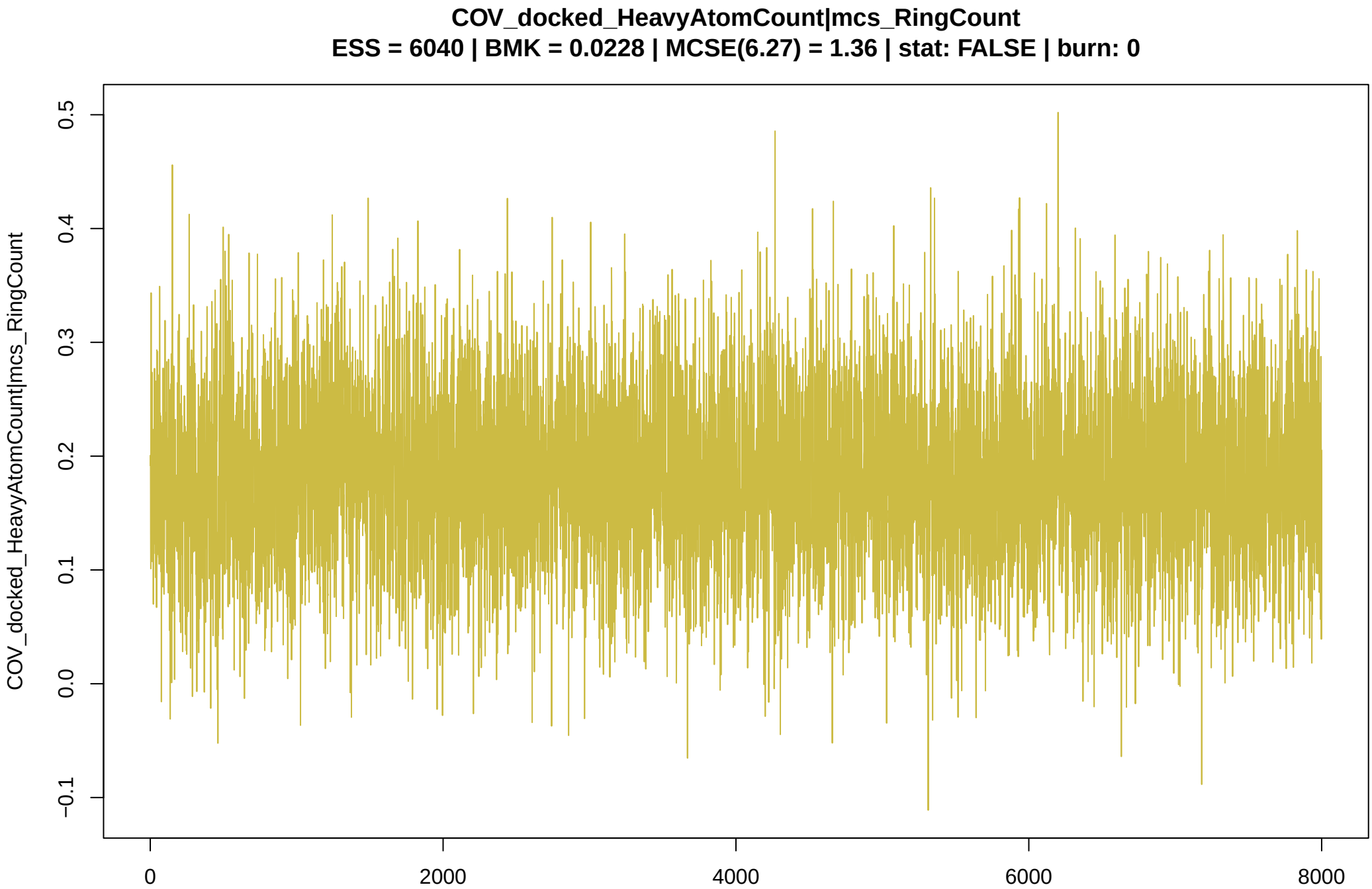

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 5650 | BMK = 0.057 | MCSE(6.27) = 1.54 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.36
0.38
0.40
0.42
0.44
0.46
0
2000
4000
6000
8000

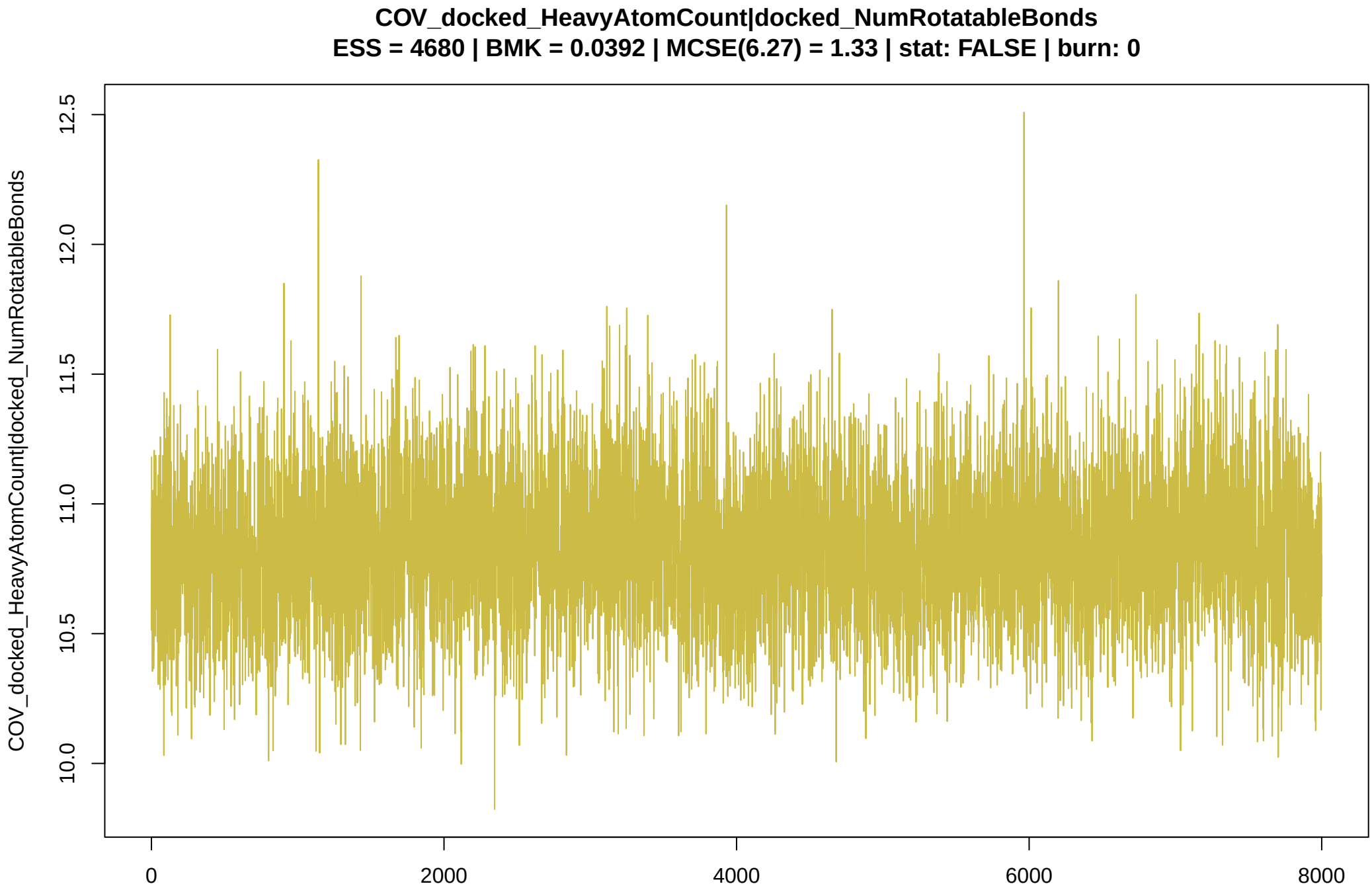

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 5970 | BMK = 0.0343 | MCSE(6.27) = 1.44 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
0.35
0.40
0.45
0.50
0.55
0.60
0
2000
4000
6000
8000

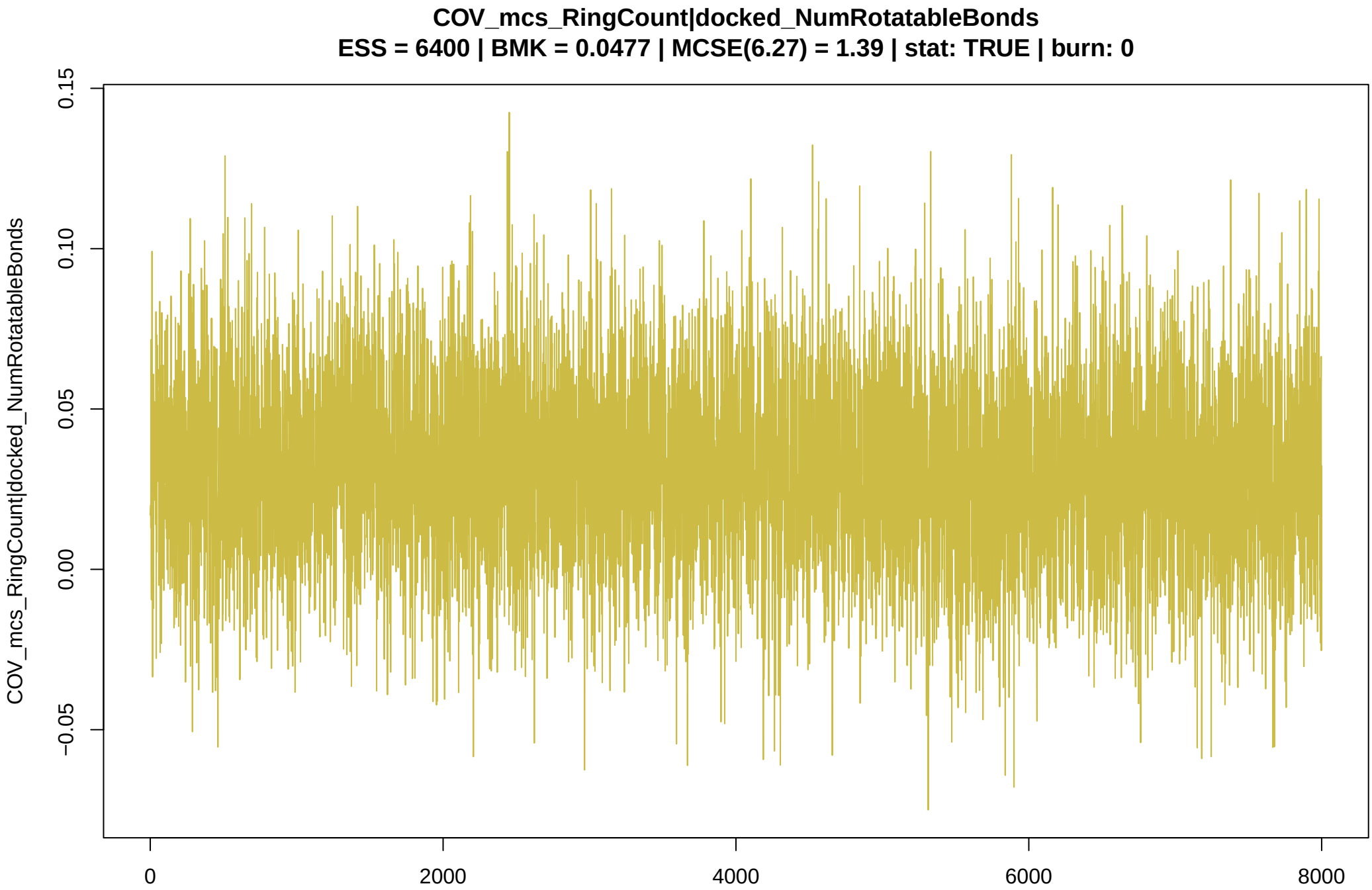

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 6450 | BMK = 0.0372 | MCSE(6.27) = 1.3 | stat: FALSE | burn: 0
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
1.2
1.4
1.6
1.8
2.0
2.2
2.4
0
2000
4000
6000
8000


COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 6450 | BMK = 0.0269 | MCSE(6.27) = 1.4 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.60
0.65
0.70
0.75
0
2000
4000
6000
8000


COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 6710 | BMK = 0.0237 | MCSE(6.27) = 1.33 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
0.3
0.4
0.5
0.6
0.7
0.8
0
2000
4000
6000
8000


COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 6040 | BMK = 0.0228 | MCSE(6.27) = 1.36 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.5
0.4
0.3
0.2
0.1
0.0
−0.1
0
2000
4000
6000
8000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 4680 | BMK = 0.0392 | MCSE(6.27) = 1.33 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10.0
10.5
11.0
11.5
12.0
12.5
0
2000
4000
6000
8000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 6400 | BMK = 0.0477 | MCSE(6.27) = 1.39 | stat: TRUE | burn: 0
COV_mcs_RingCount|docked_NumRotatableBonds
0.15
0.10
0.05
0.00
−0.05
0
2000
4000
6000
8000