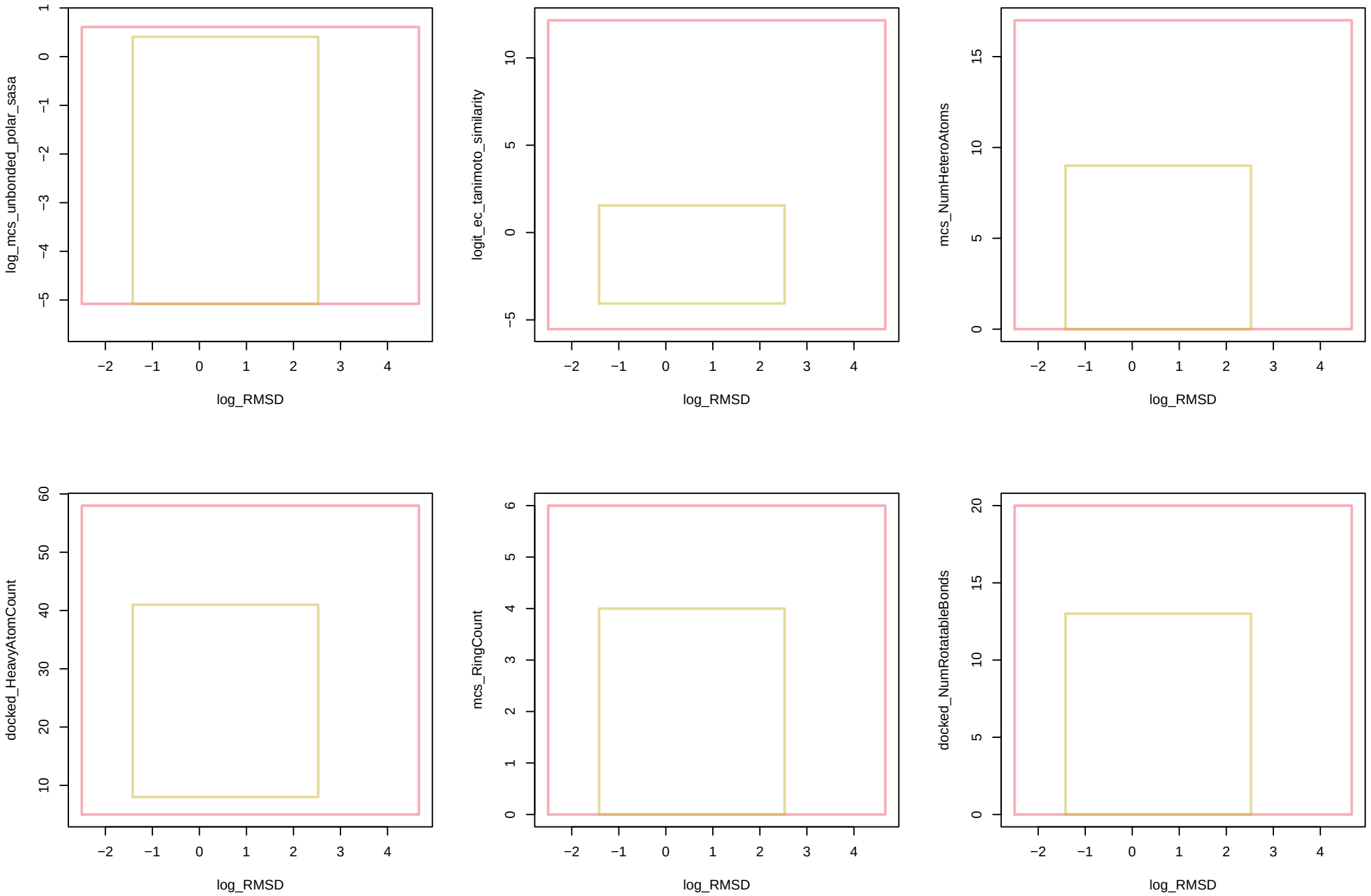
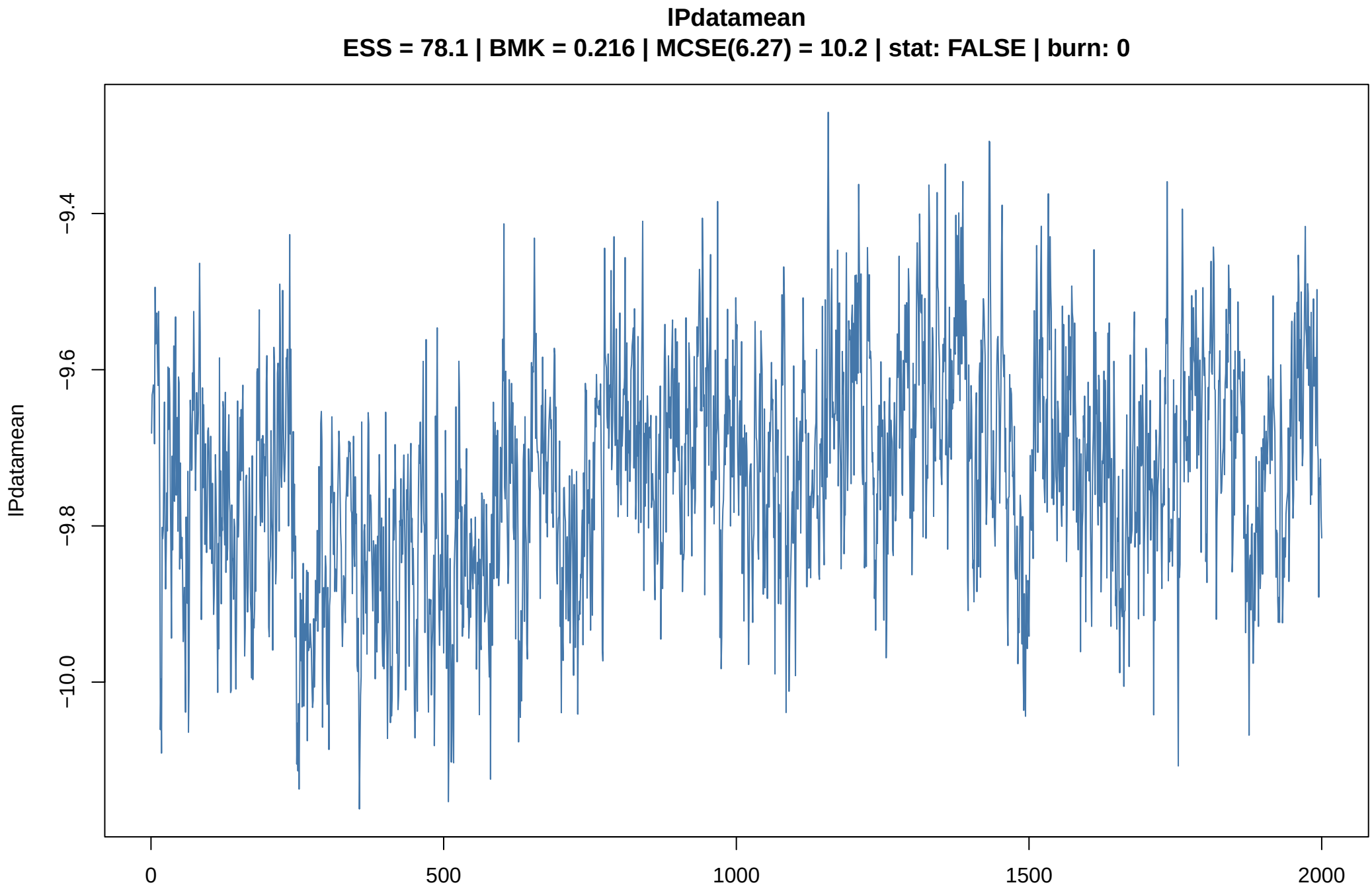
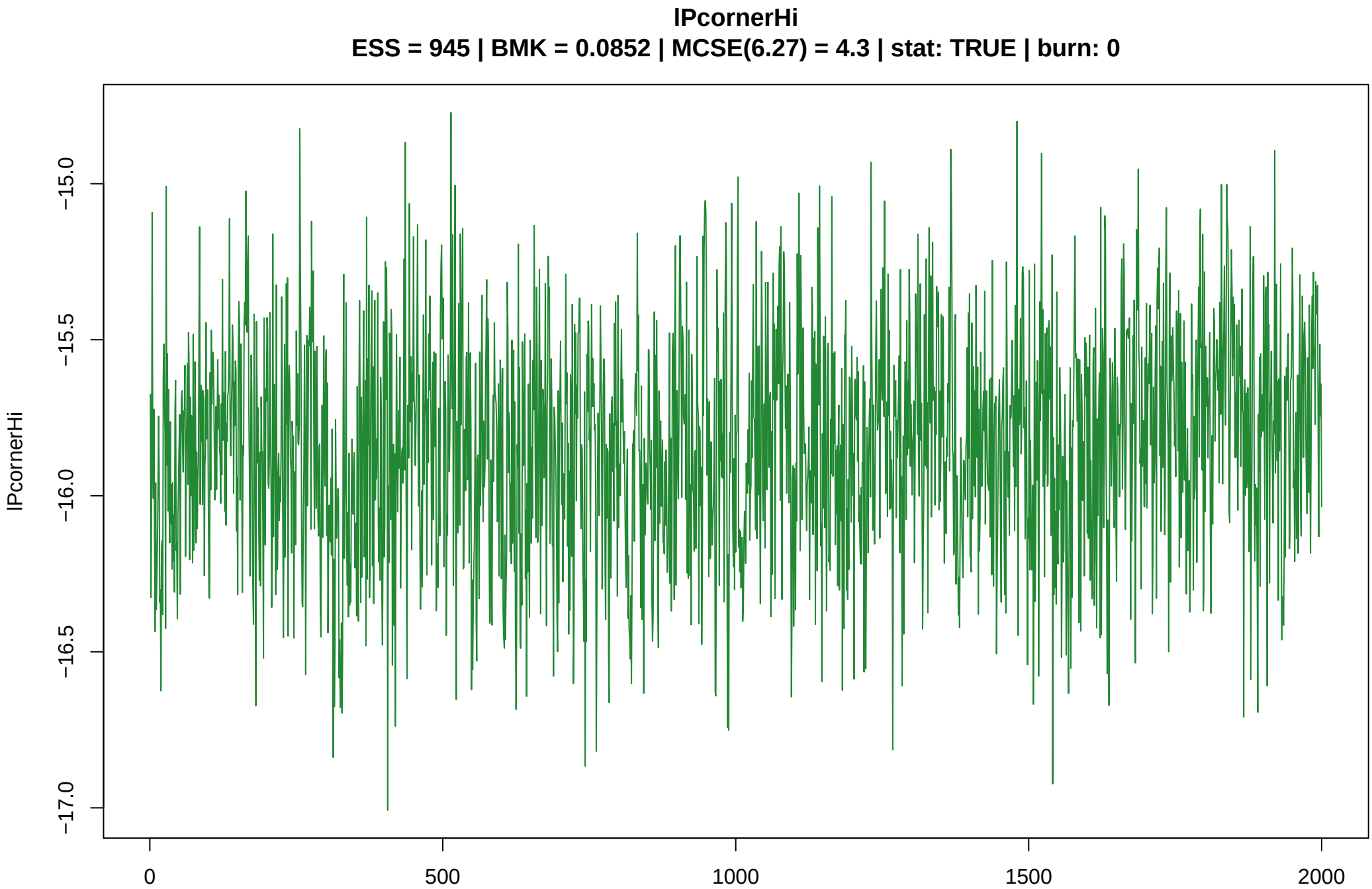
−− STATS maxD −−
min ESS = 78.1426263272921
max BMK = 0.215993717404799
max MCSE = 10.2317442870101
all stationary: FALSE
burn: 1400

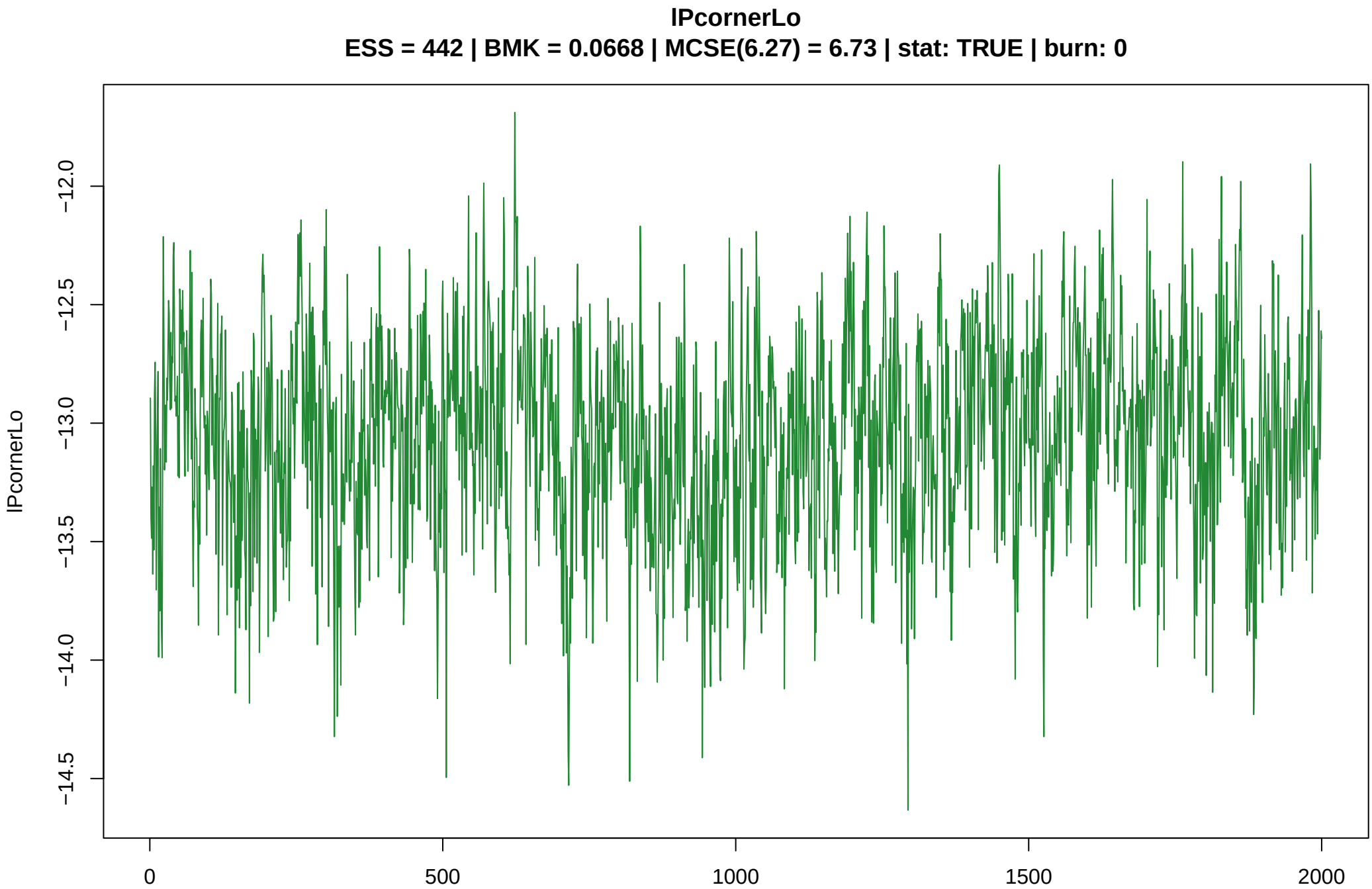
−− STATS 2D −−
min ESS = 520.328849474848
max BMK = 0.058107352917355 1
max MCSE = 3.23474230550864
all stationary: FALSE
burn: 0

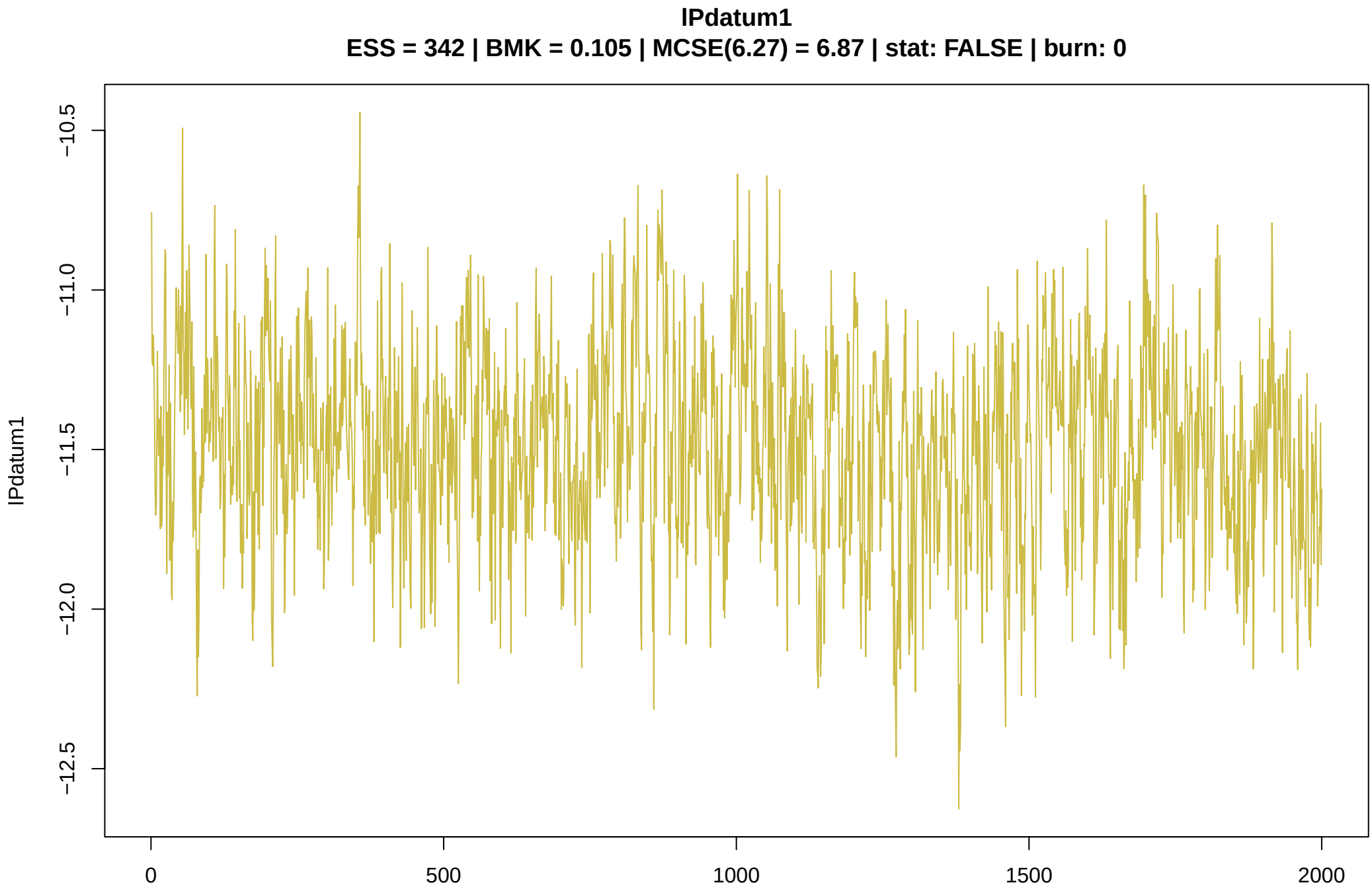
−− STATS 1D −−
min ESS = 234.132032797974
max BMK = 0.136568223603466
max MCSE = 2.68299263128896
all stationary: FALSE
burn: 0

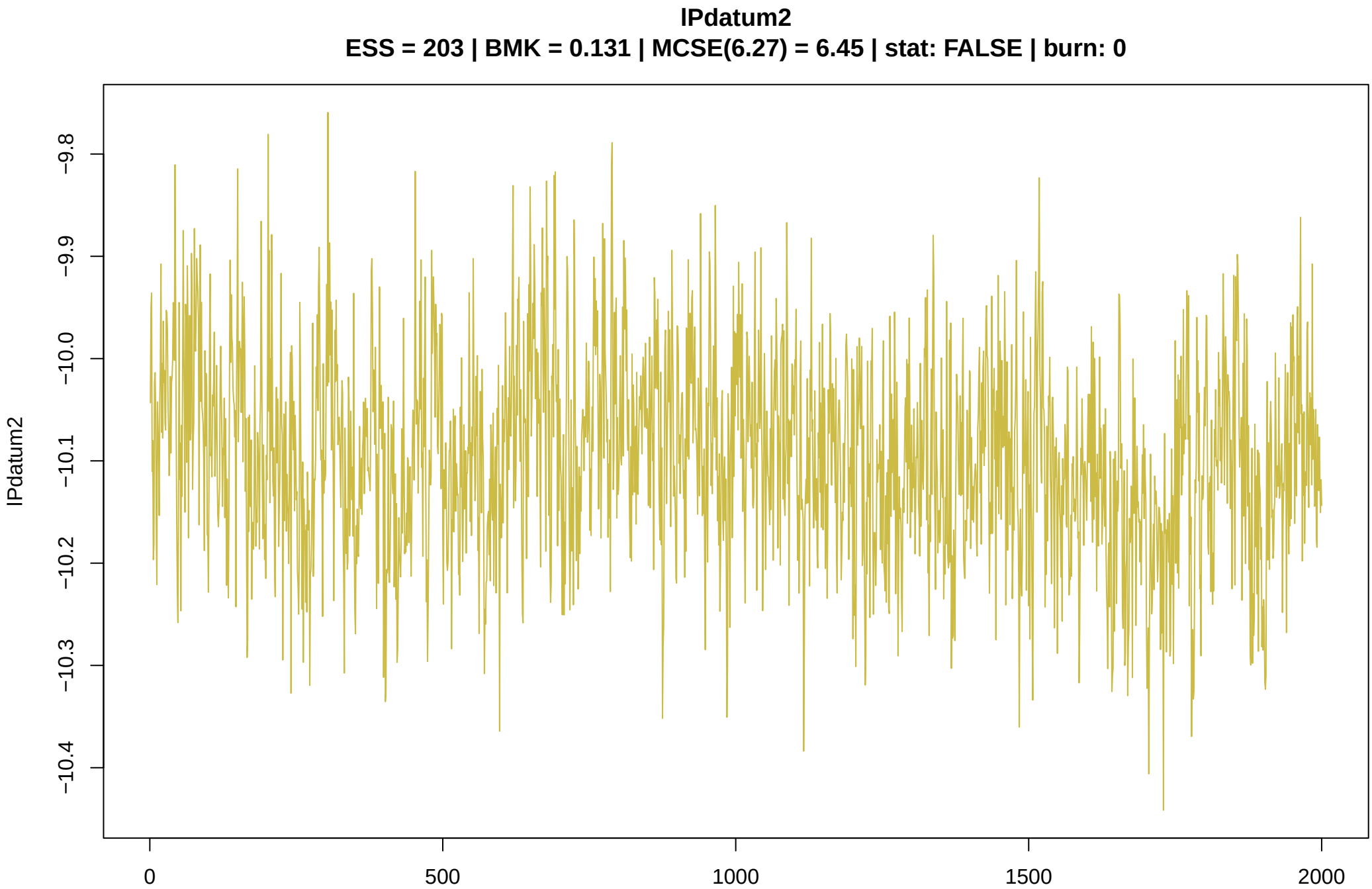

log_mcs_unbonded_polar_sasa
logit_ec_tanimoto_similarity
mcs_NumHeteroAtoms
docked_HeavyAtomCount
mcs_RingCount
docked_NumRotatableBonds
log_RMSD

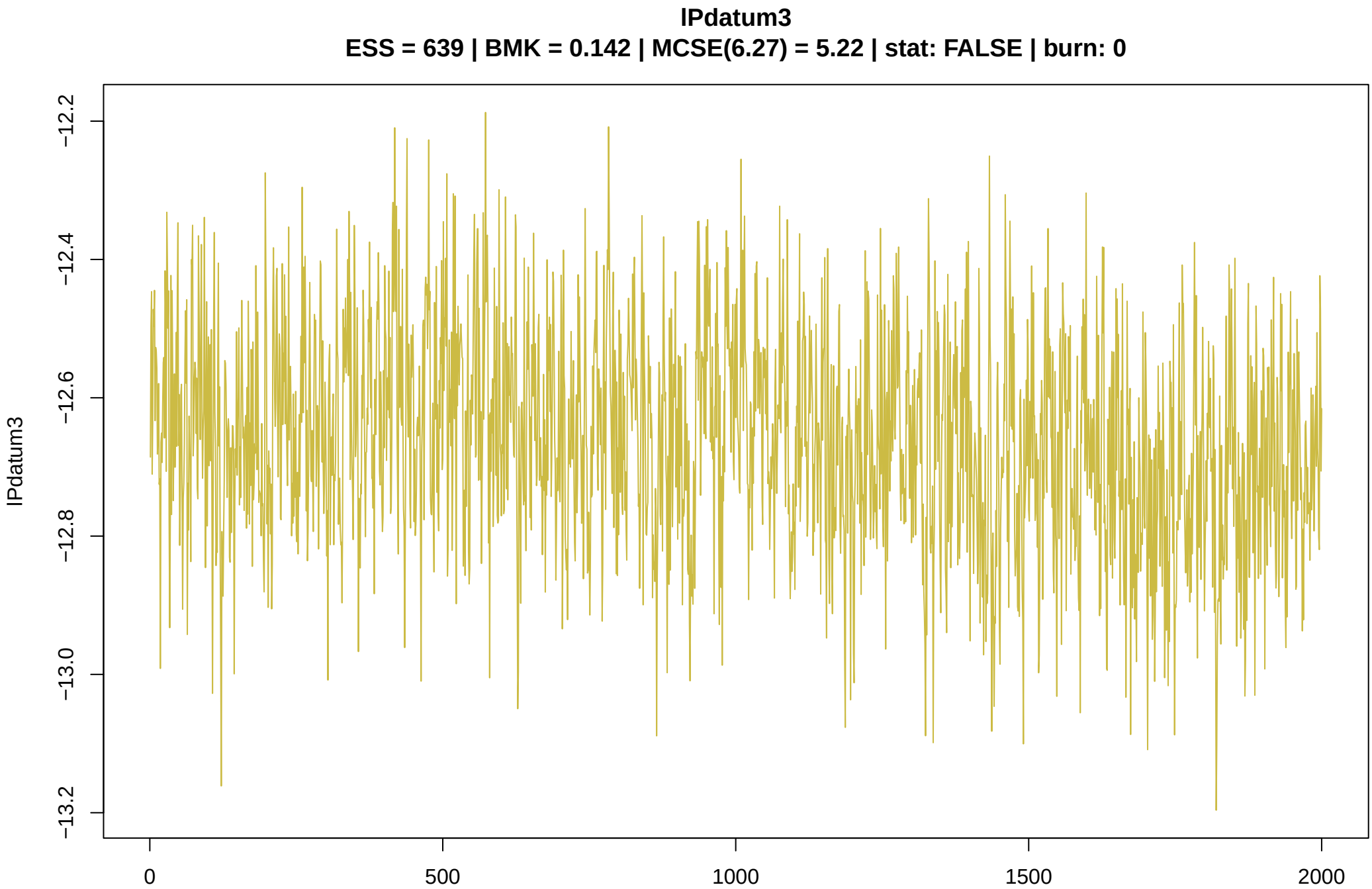

lPdatamean
ESS = 78.1 | BMK = 0.216 | MCSE(6.27) = 10.2 | stat: FALSE | burn: 0
lPdatamean
−9.4
−9.6
−9.8
−10.0
0
500
1000
1500
2000

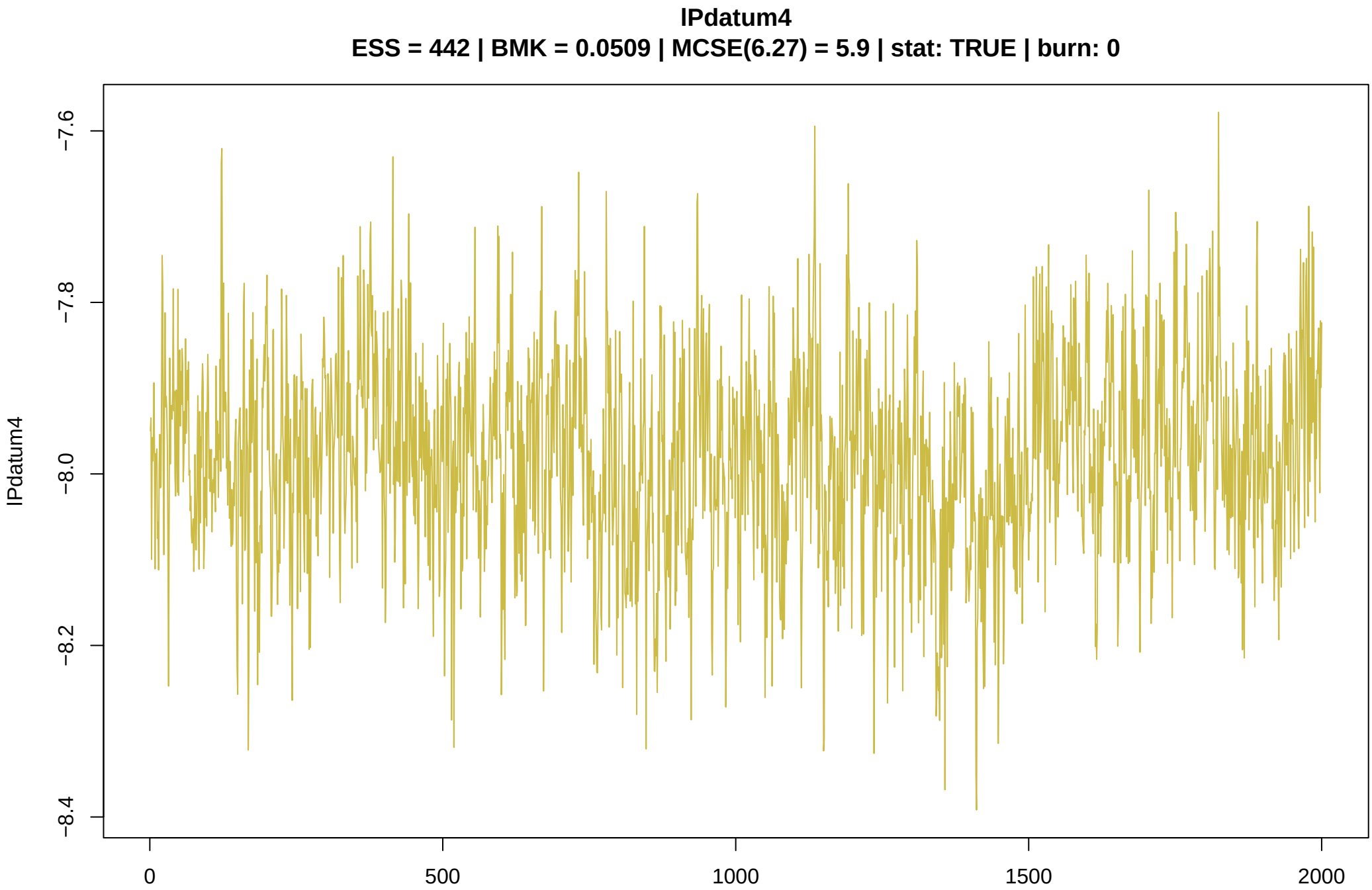

lPcornerHi
ESS = 945 | BMK = 0.0852 | MCSE(6.27) = 4.3 | stat: TRUE | burn: 0
lPcornerHi
−15.0
−15.5
−16.0
−16.5
−17.0
0
500
1000
1500
2000

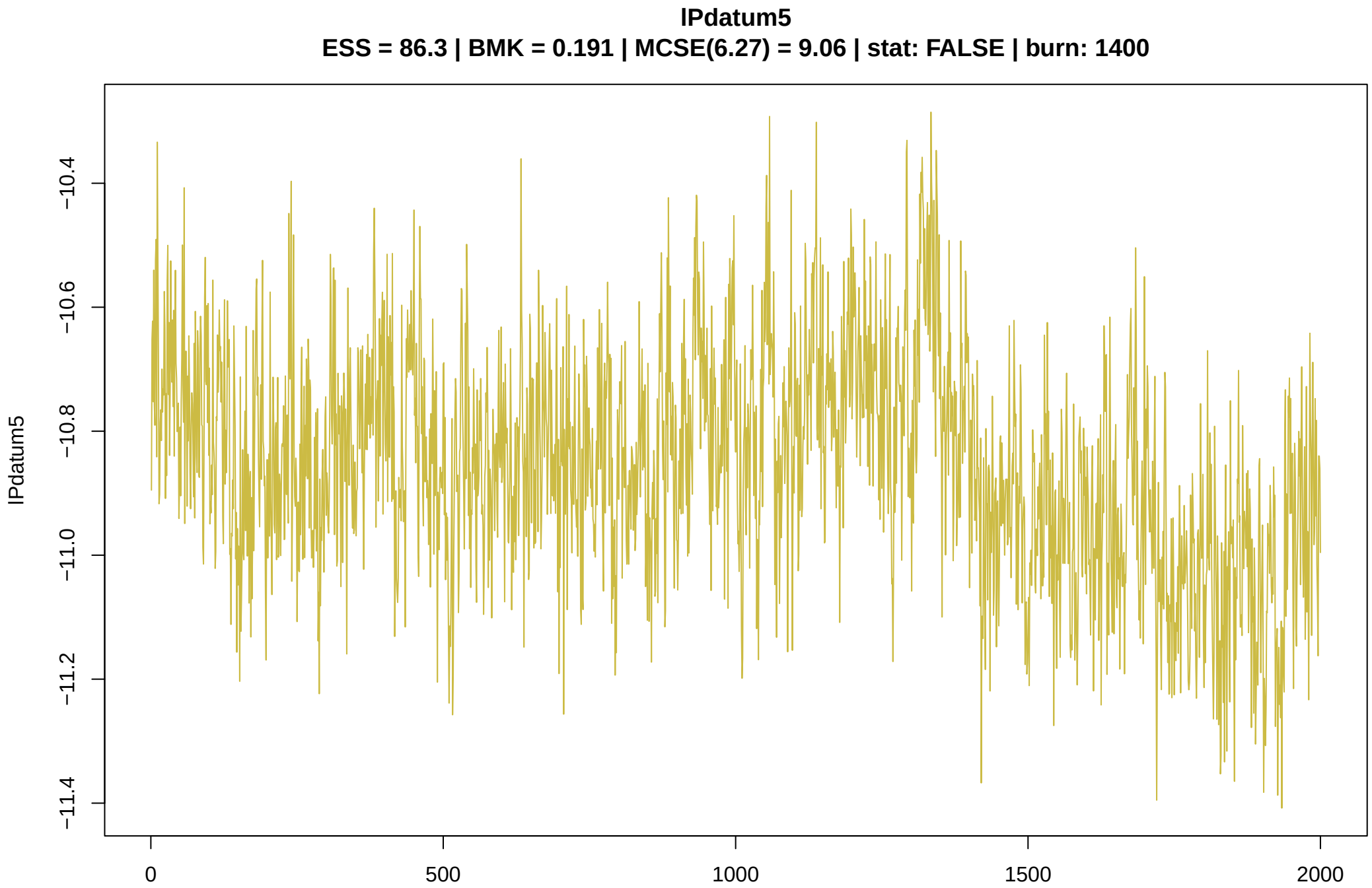

lPcornerLo
ESS = 442 | BMK = 0.0668 | MCSE(6.27) = 6.73 | stat: TRUE | burn: 0
lPcornerLo
−12.0
−12.5
−13.0
−13.5
−14.0
−14.5
0
500
1000
1500
2000

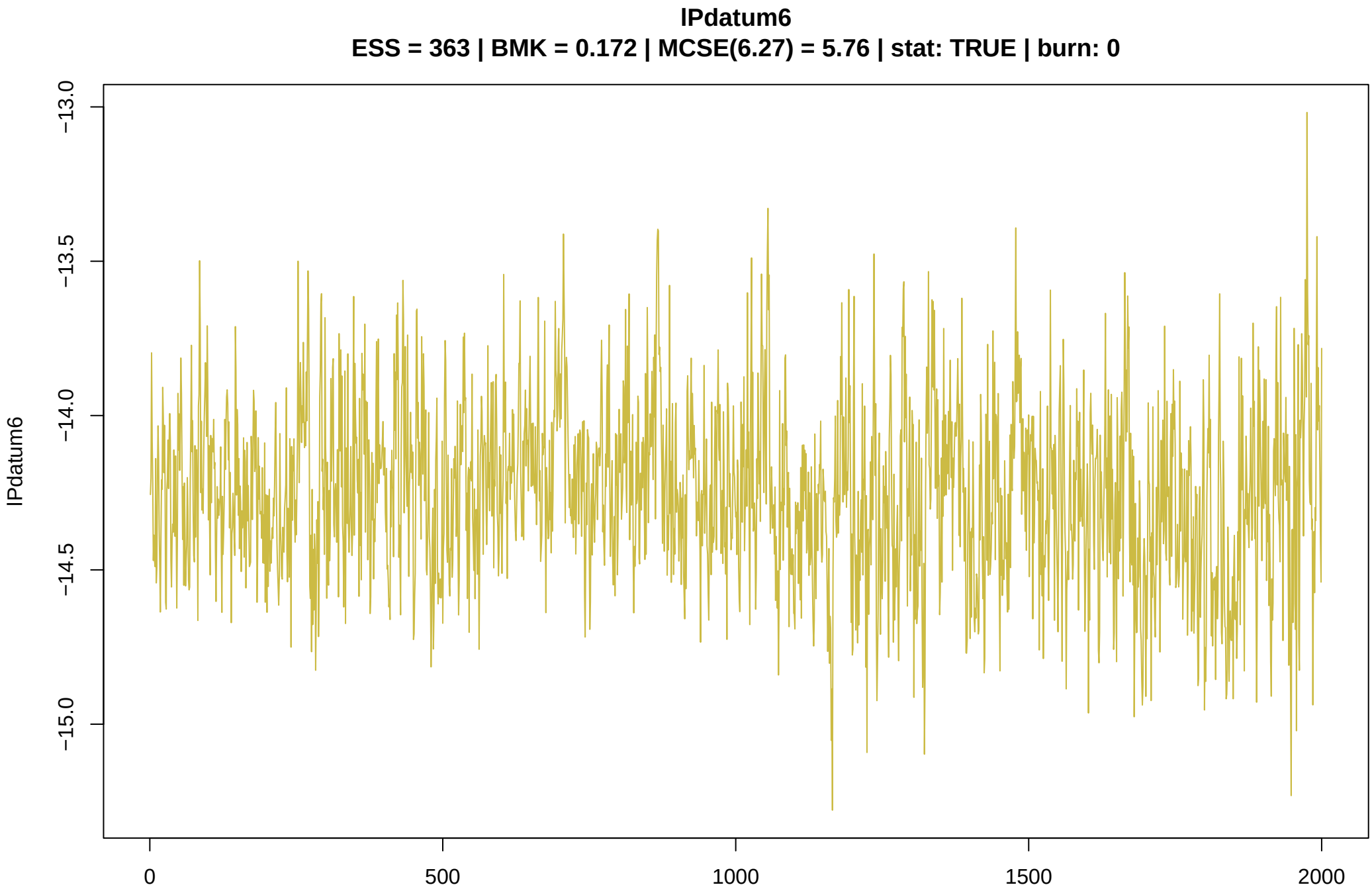

lPdatum1
ESS = 342 | BMK = 0.105 | MCSE(6.27) = 6.87 | stat: FALSE | burn: 0
lPdatum1
−10.5
−11.0
−11.5
−12.0
−12.5
0
500
1000
1500
2000

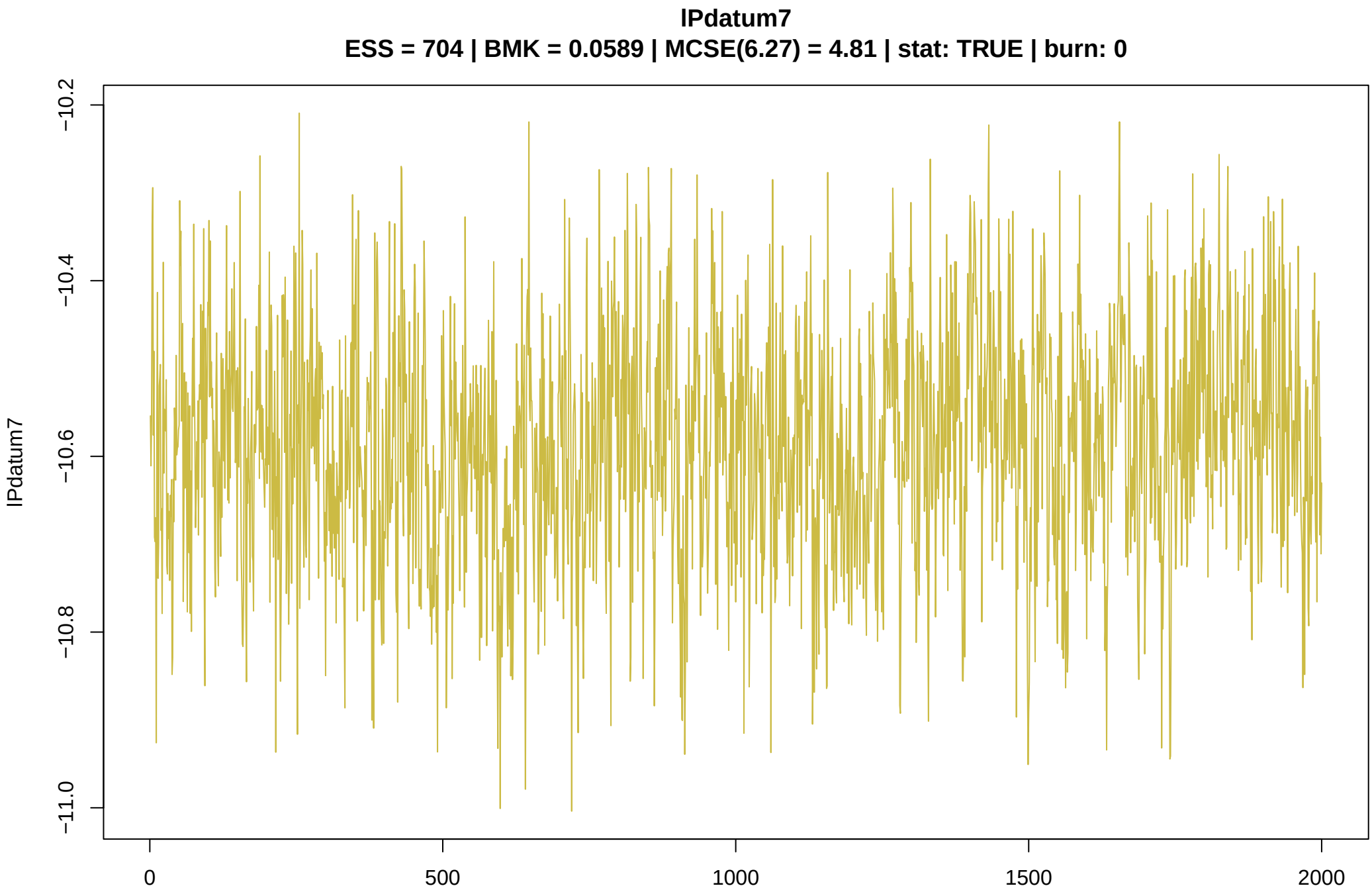

lPdatum2
ESS = 203 | BMK = 0.131 | MCSE(6.27) = 6.45 | stat: FALSE | burn: 0
lPdatum2
−9.8
−9.9
−10.0
−10.1
−10.2
−10.3
−10.4
0
500
1000
1500
2000

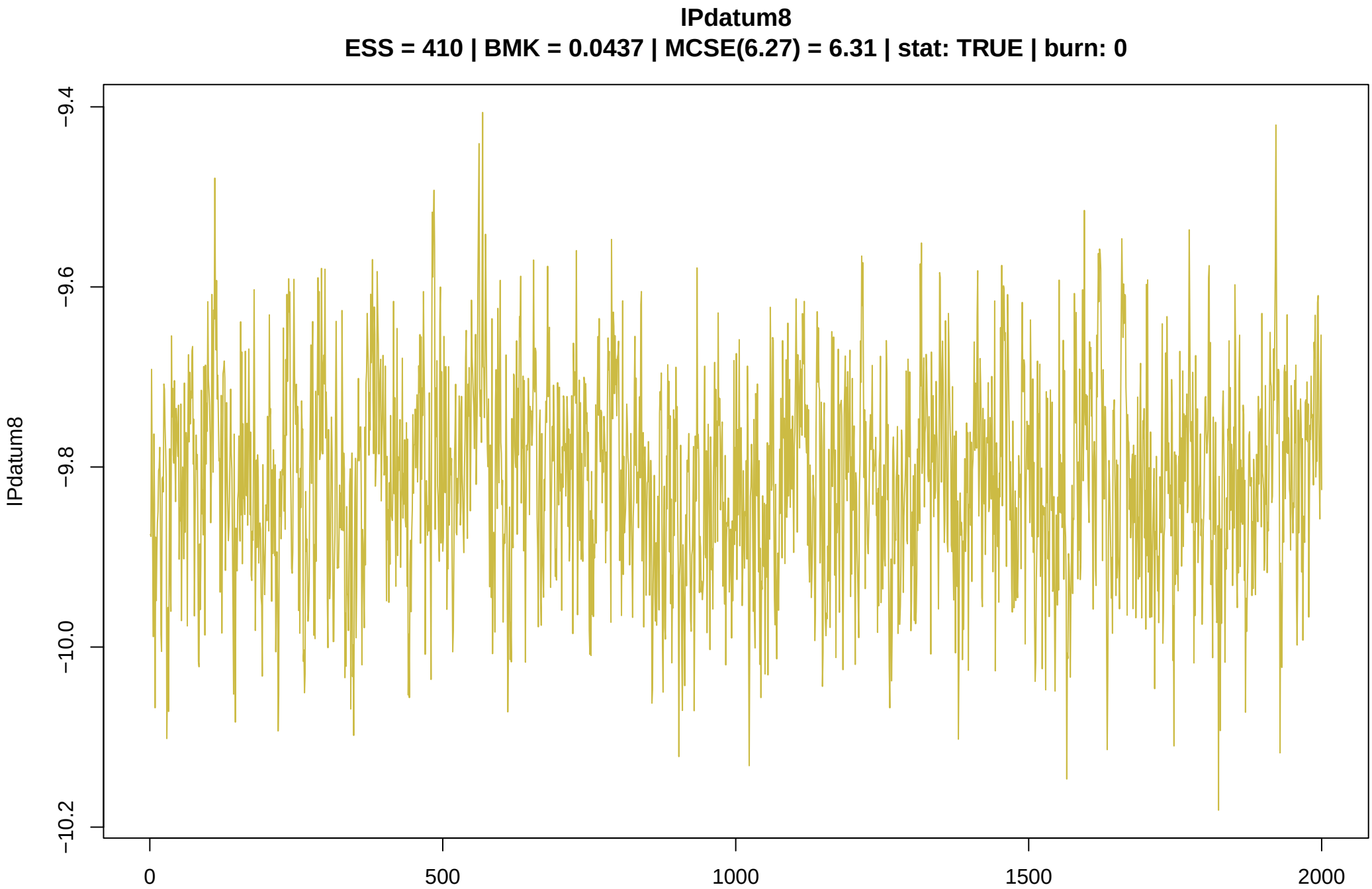

lPdatum3
ESS = 639 | BMK = 0.142 | MCSE(6.27) = 5.22 | stat: FALSE | burn: 0
lPdatum3
−12.2
−12.4
−12.6
−12.8
−13.0
−13.2
0
500
1000
1500
2000

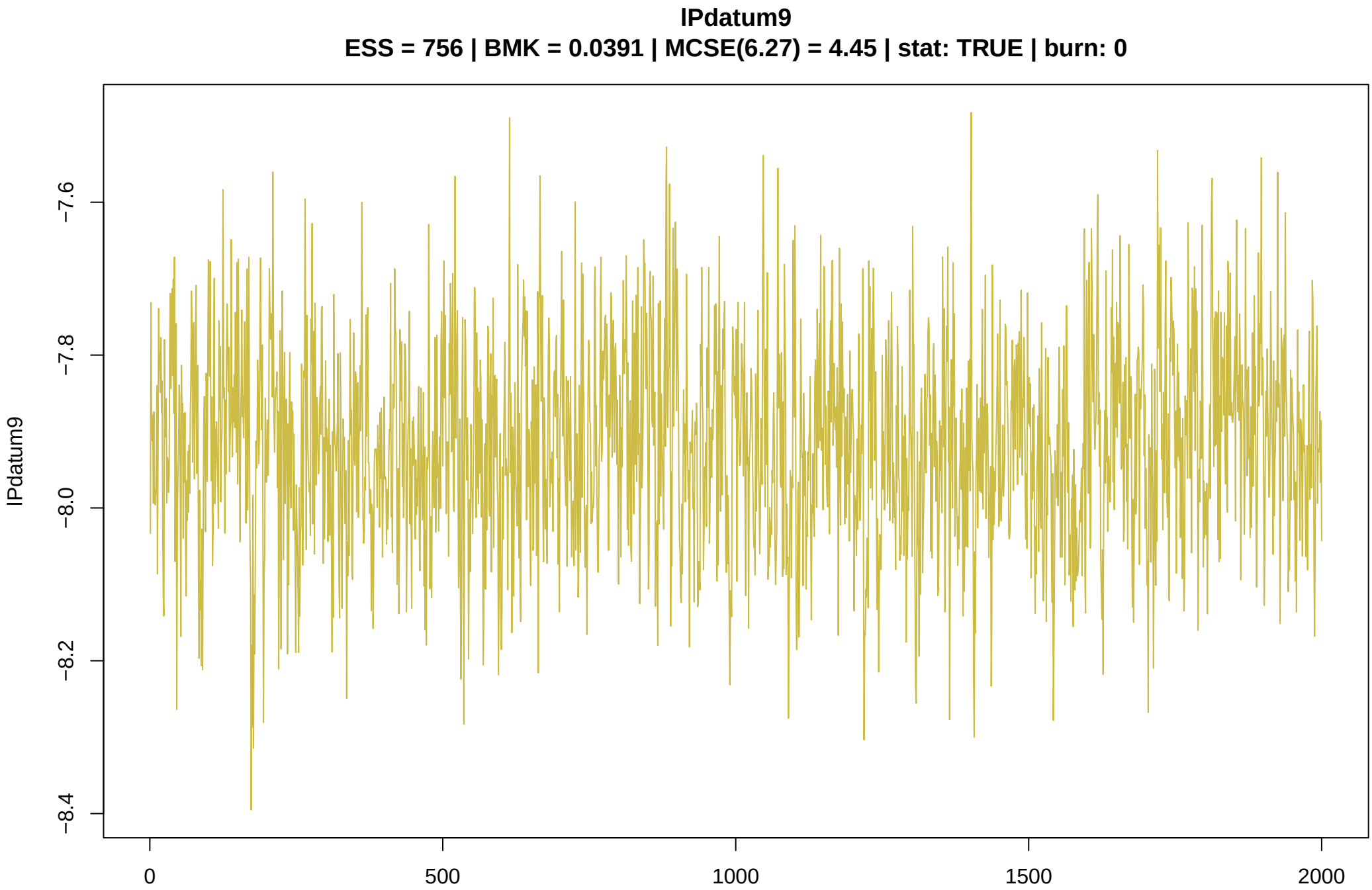

lPdatum4
ESS = 442 | BMK = 0.0509 | MCSE(6.27) = 5.9 | stat: TRUE | burn: 0
lPdatum4
−7.6
−7.8
−8.0
−8.2
−8.4
0
500
1000
1500
2000

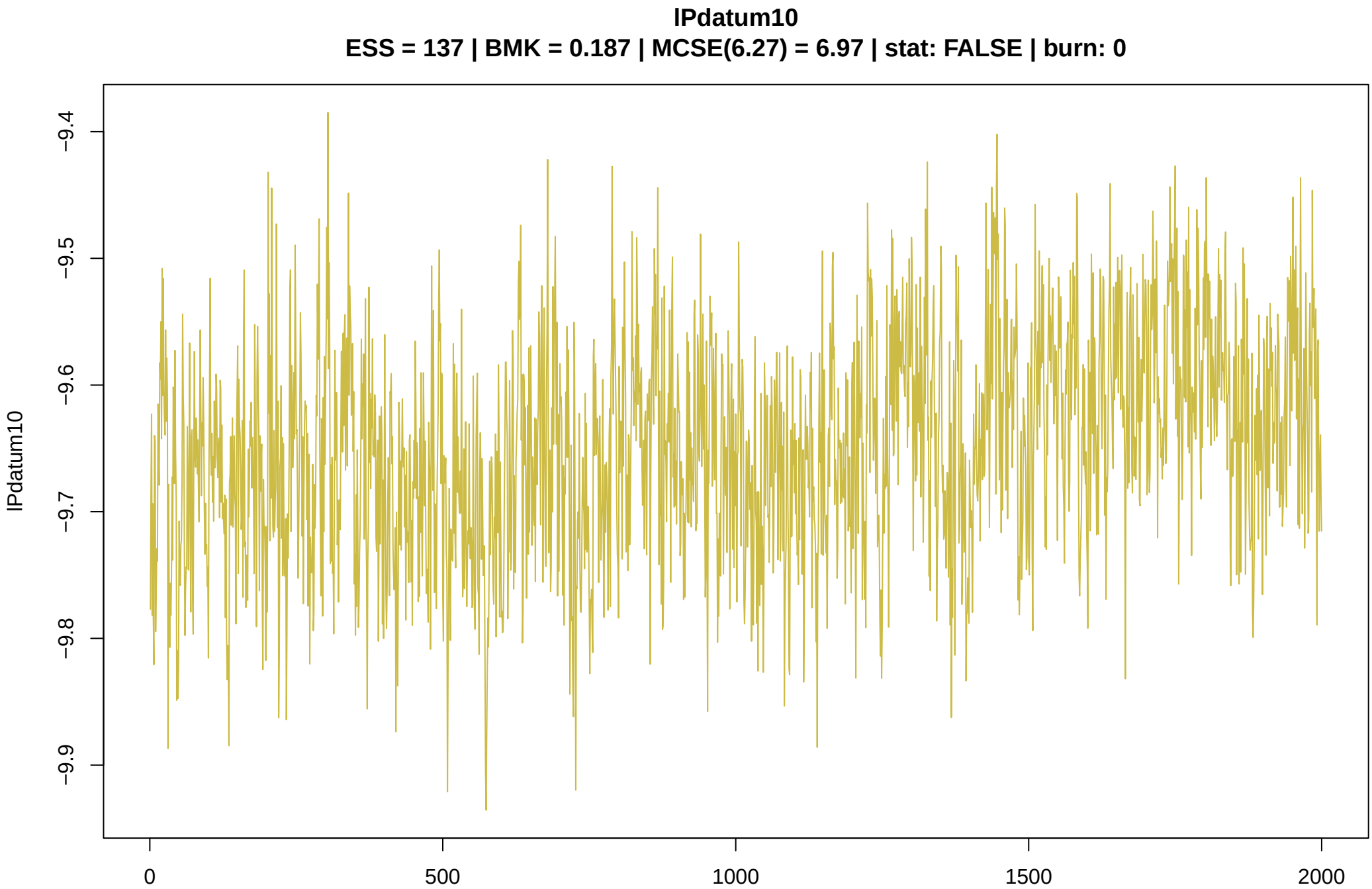

lPdatum5
ESS = 86.3 | BMK = 0.191 | MCSE(6.27) = 9.06 | stat: FALSE | burn: 1400
lPdatum5
−10.4
−10.6
−10.8
−11.0
−11.2
−11.4
0
500
1000
1500
2000

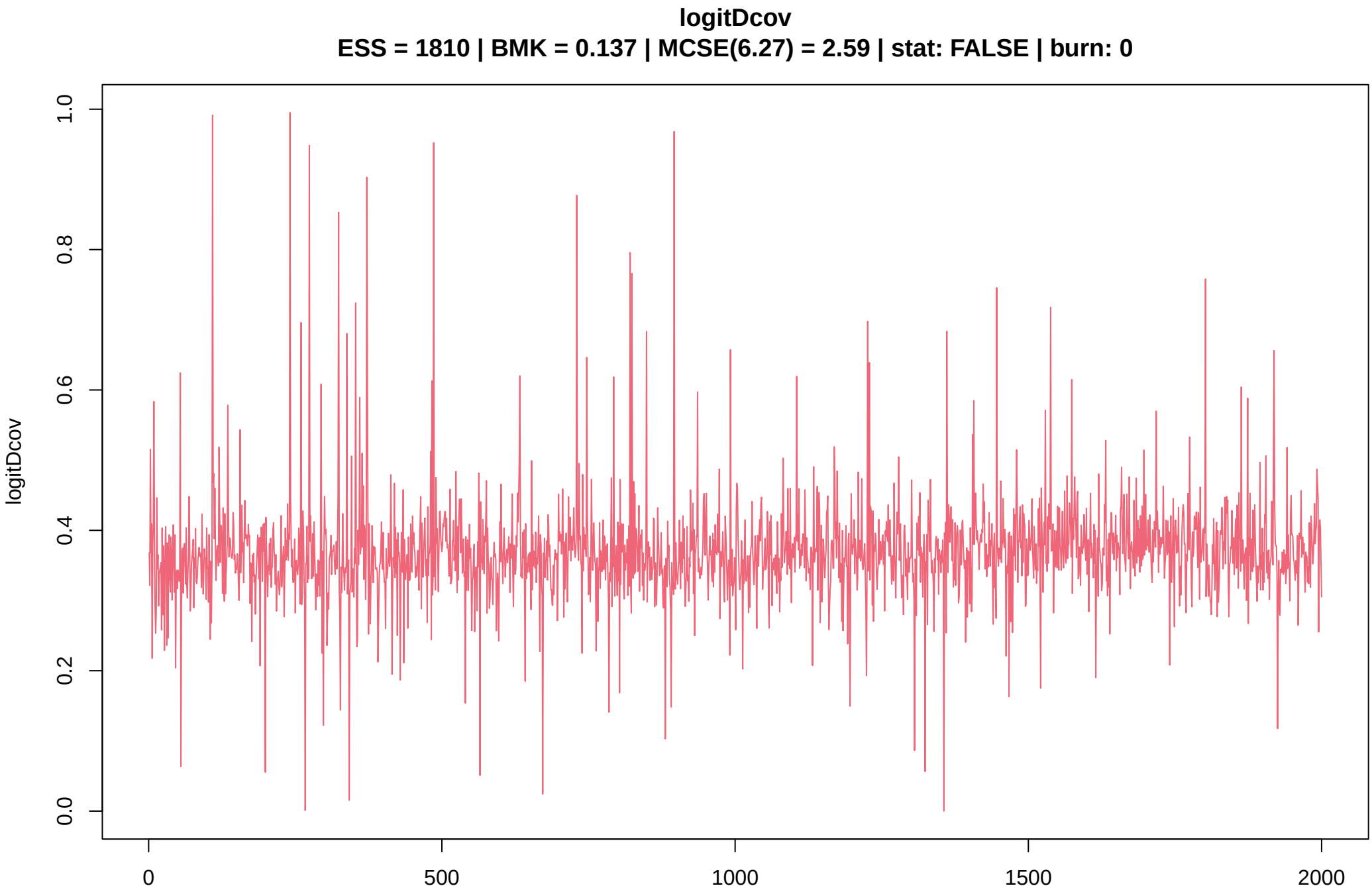

lPdatum6
ESS = 363 | BMK = 0.172 | MCSE(6.27) = 5.76 | stat: TRUE | burn: 0
lPdatum6
−13.0
−13.5
−14.0
−14.5
−15.0
0
500
1000
1500
2000

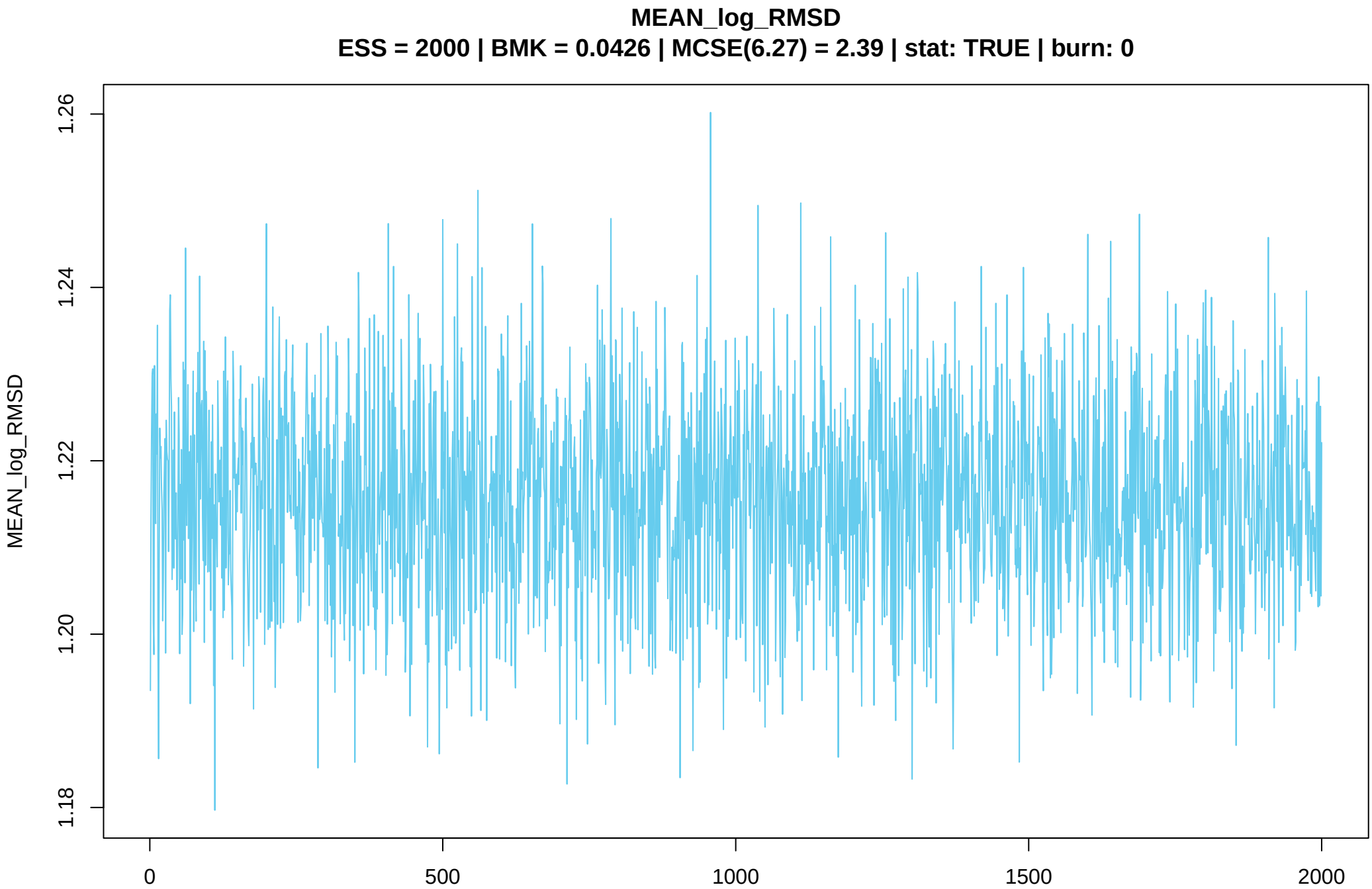

lPdatum7
ESS = 704 | BMK = 0.0589 | MCSE(6.27) = 4.81 | stat: TRUE | burn: 0
lPdatum7
−10.2
−10.4
−10.6
−10.8
−11.0
0
500
1000
1500
2000

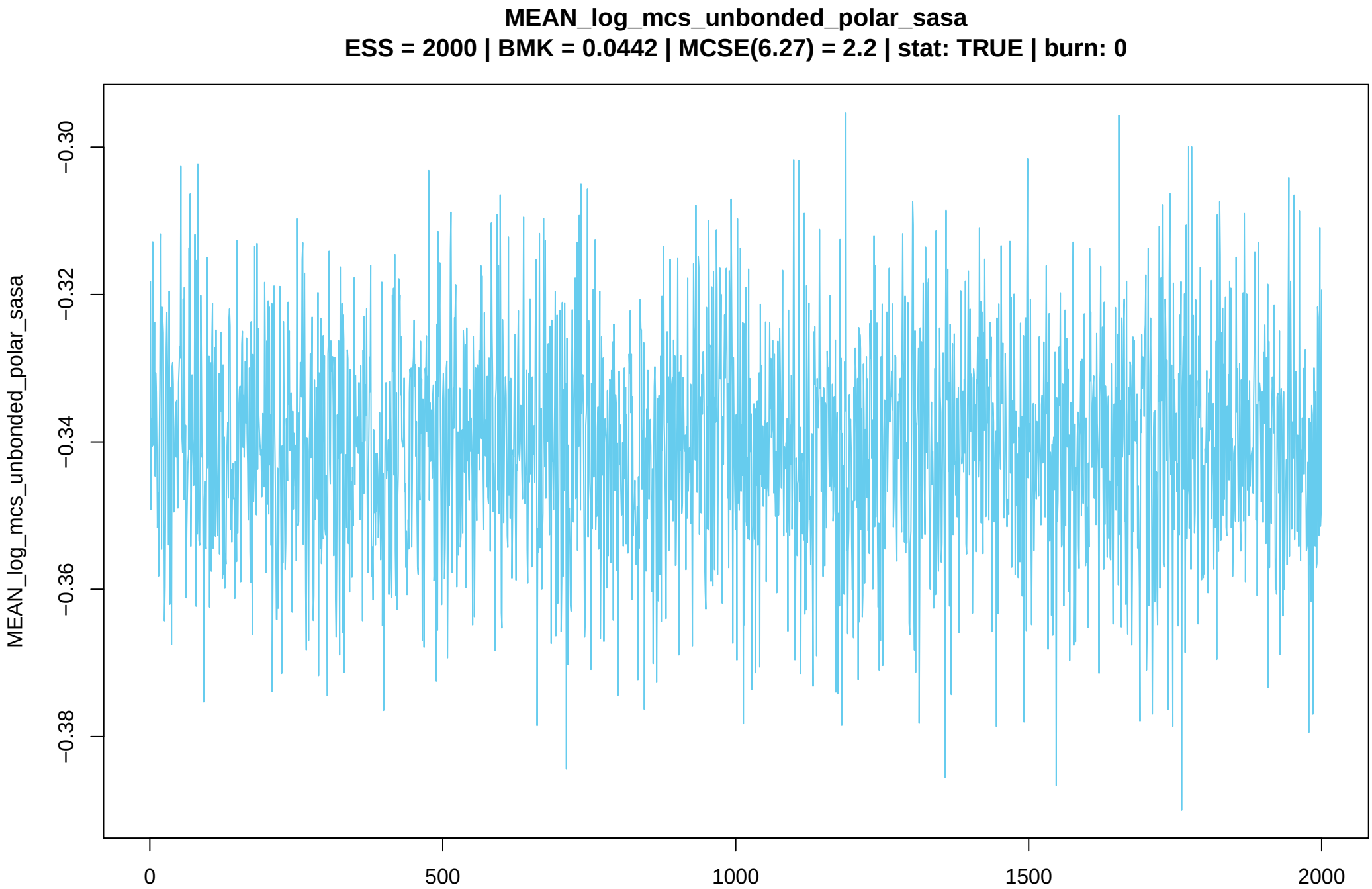

lPdatum8
ESS = 410 | BMK = 0.0437 | MCSE(6.27) = 6.31 | stat: TRUE | burn: 0
lPdatum8
−9.4
−9.6
−9.8
−10.0
−10.2
0
500
1000
1500
2000

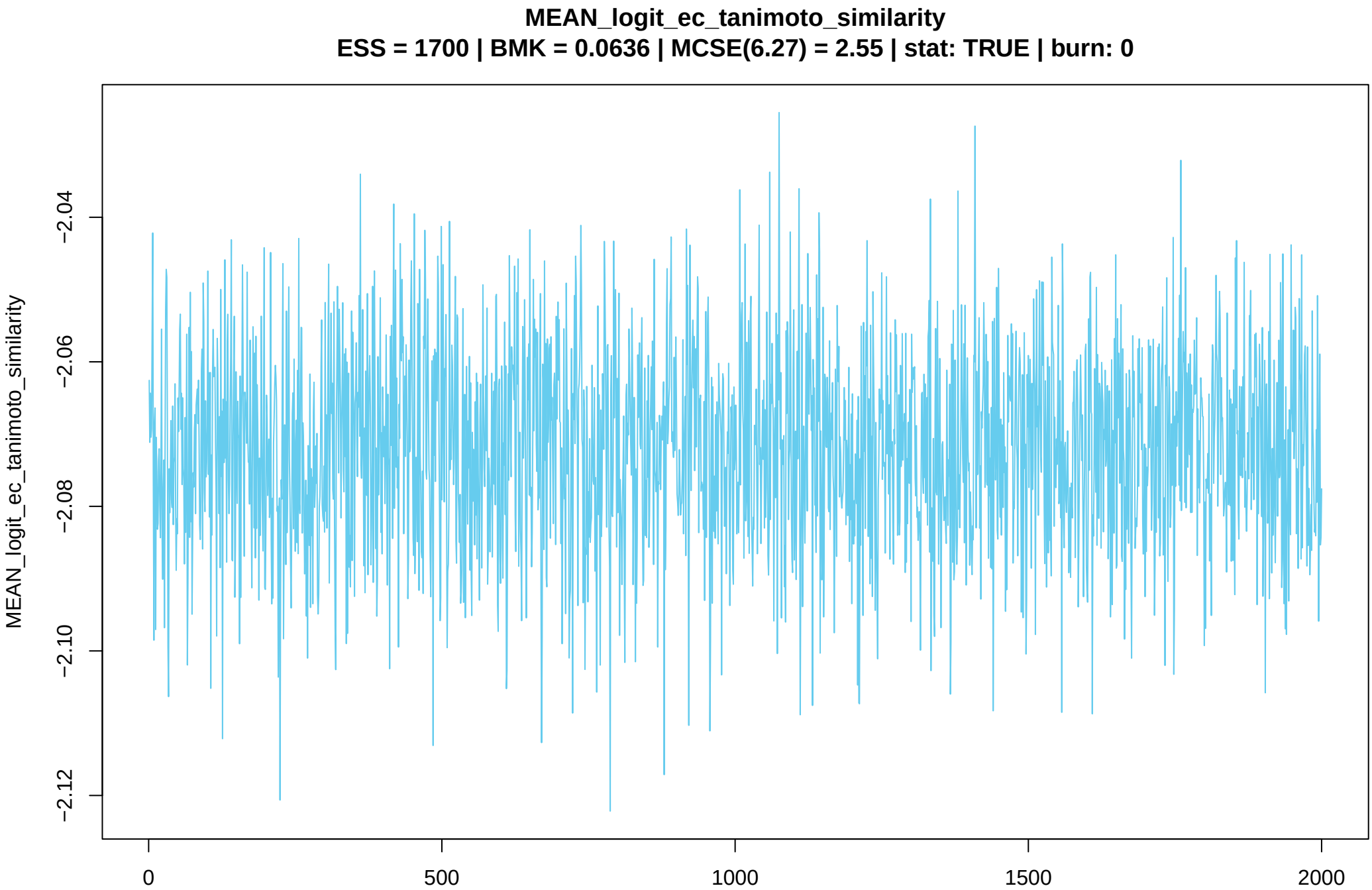

lPdatum9
ESS = 756 | BMK = 0.0391 | MCSE(6.27) = 4.45 | stat: TRUE | burn: 0
lPdatum9
−7.6
−7.8
−8.0
−8.2
−8.4
0
500
1000
1500
2000

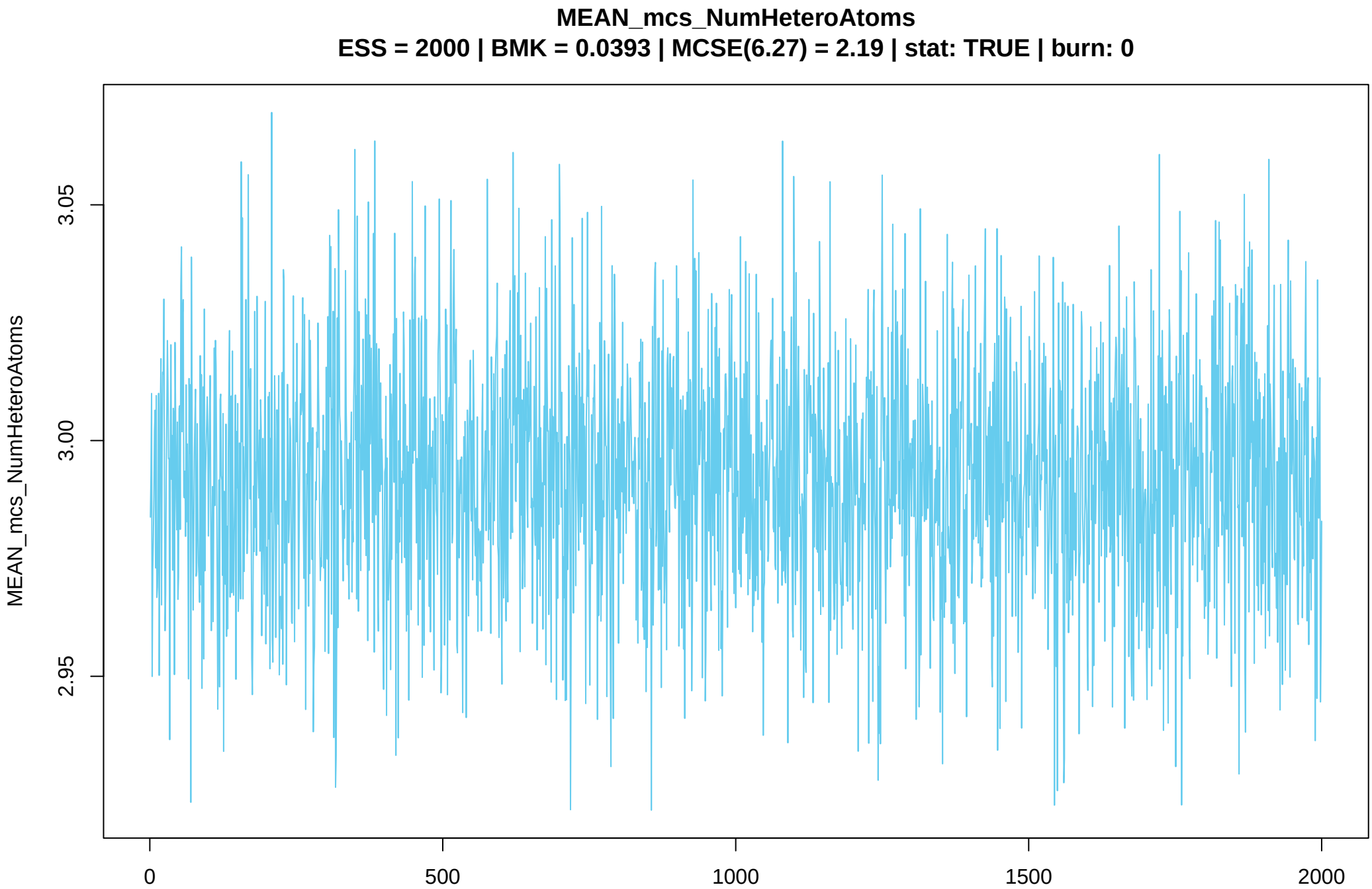

lPdatum10
ESS = 137 | BMK = 0.187 | MCSE(6.27) = 6.97 | stat: FALSE | burn: 0
lPdatum10
−9.4
−9.5
−9.6
−9.7
−9.8
−9.9
0
500
1000
1500
2000

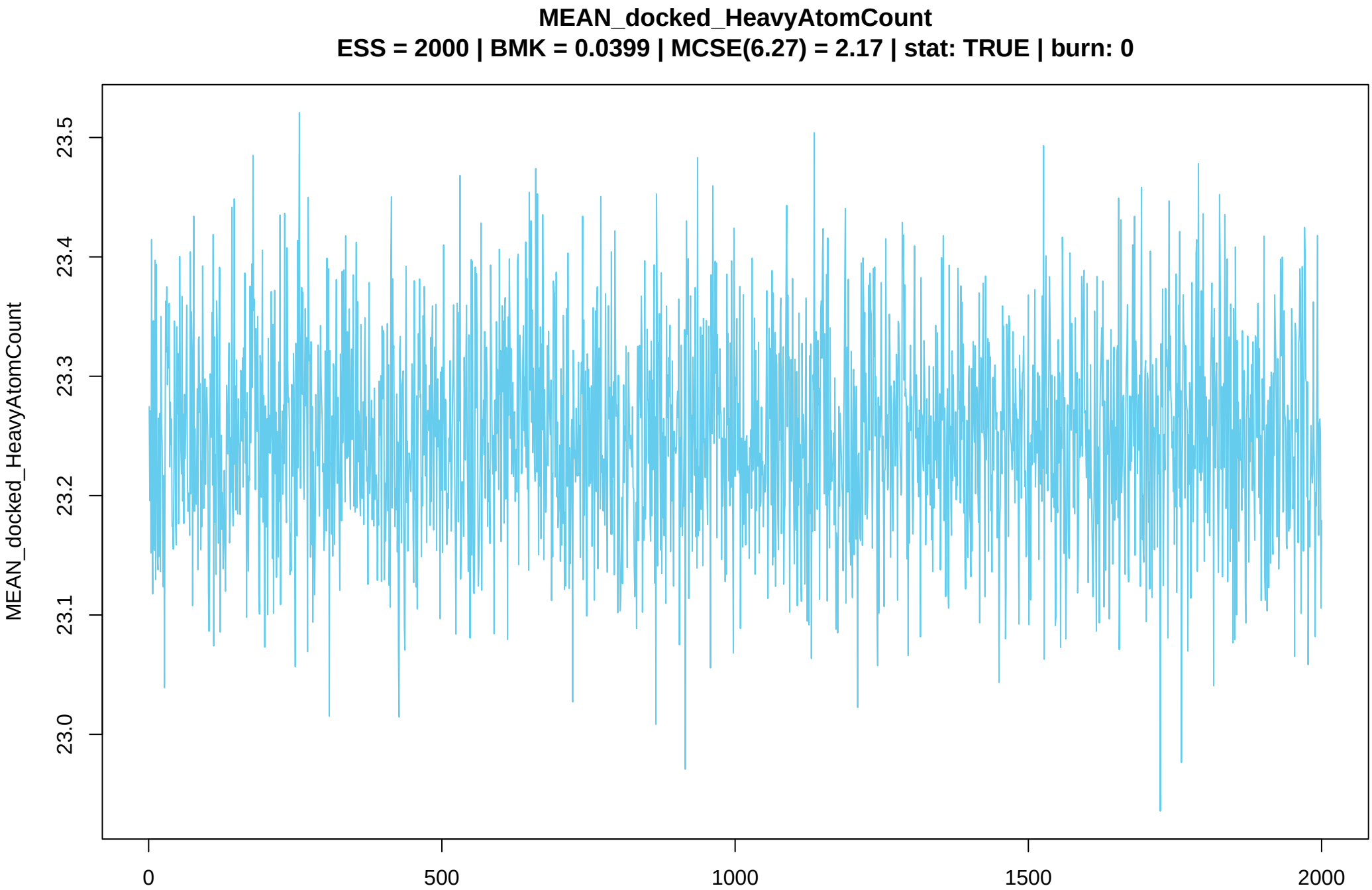

logitDcov
ESS = 1810 | BMK = 0.137 | MCSE(6.27) = 2.59 | stat: FALSE | burn: 0
logitDcov
0.0
0.2
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

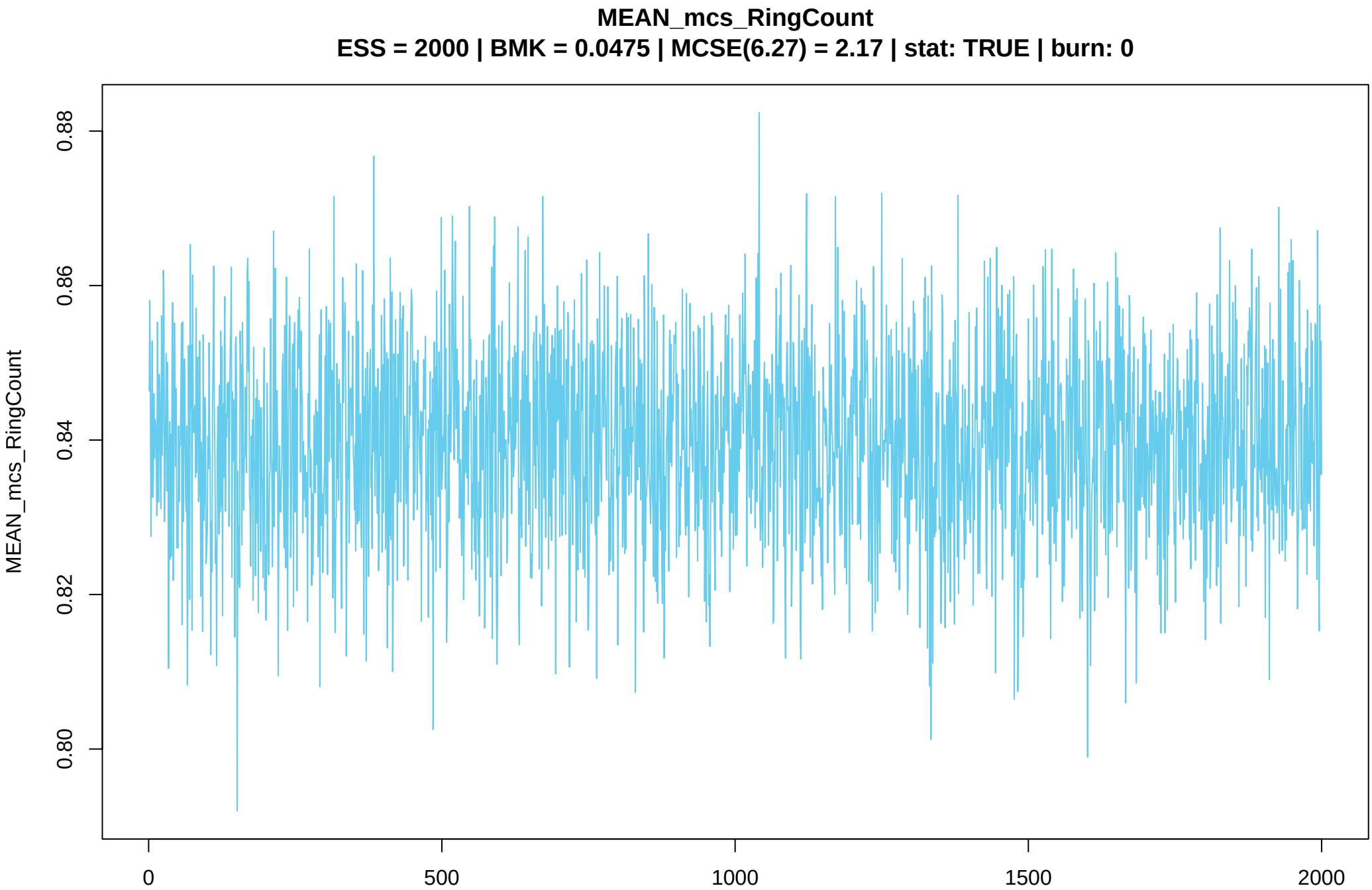

MEAN_log_RMSD
ESS = 2000 | BMK = 0.0426 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.18
1.20
1.22
1.24
1.26
0
500
1000
1500
2000

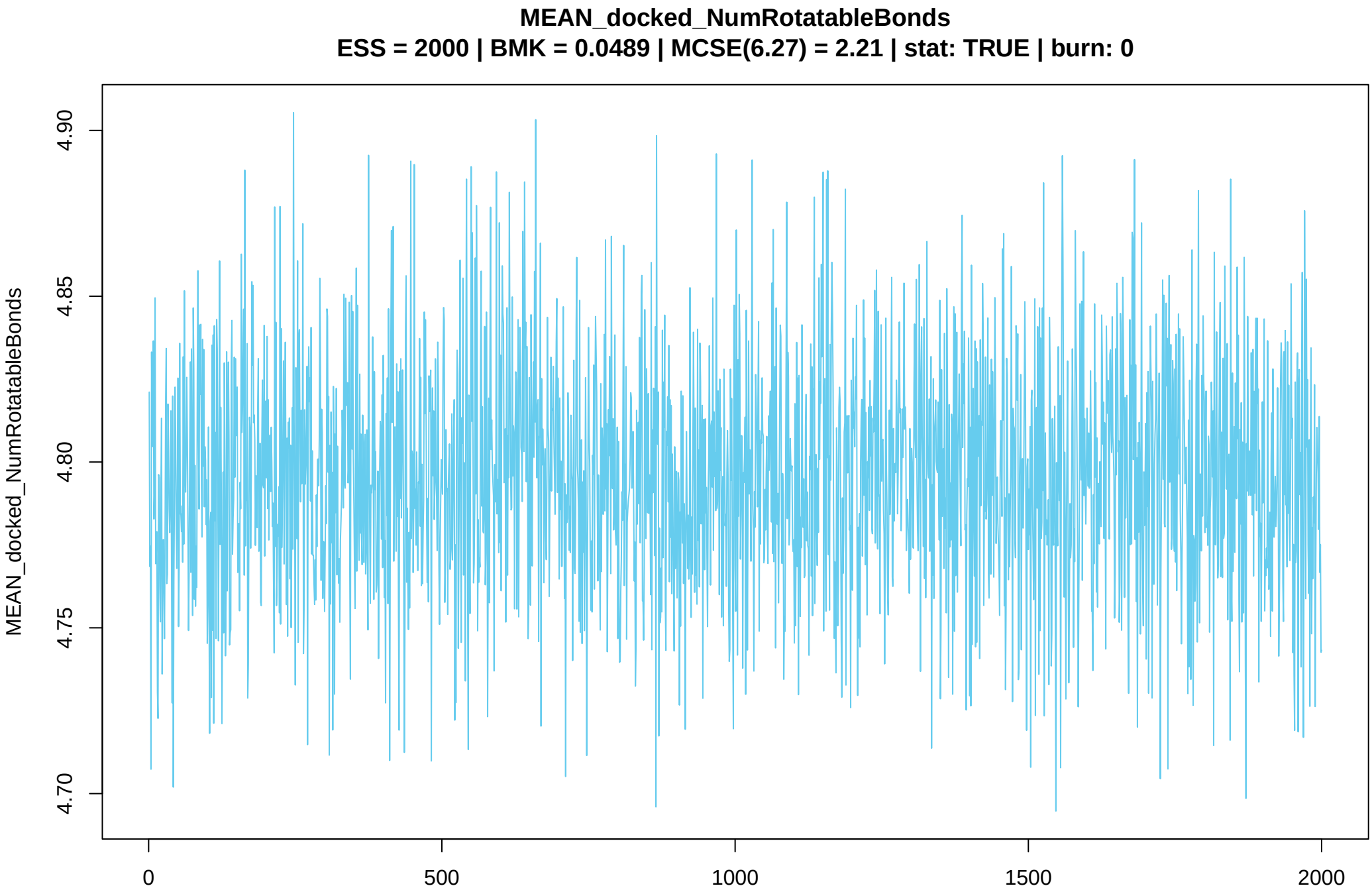

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0442 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0
MEAN_log_mcs_unbonded_polar_sasa
−0.30
−0.32
−0.34
−0.36
−0.38
0
500
1000
1500
2000

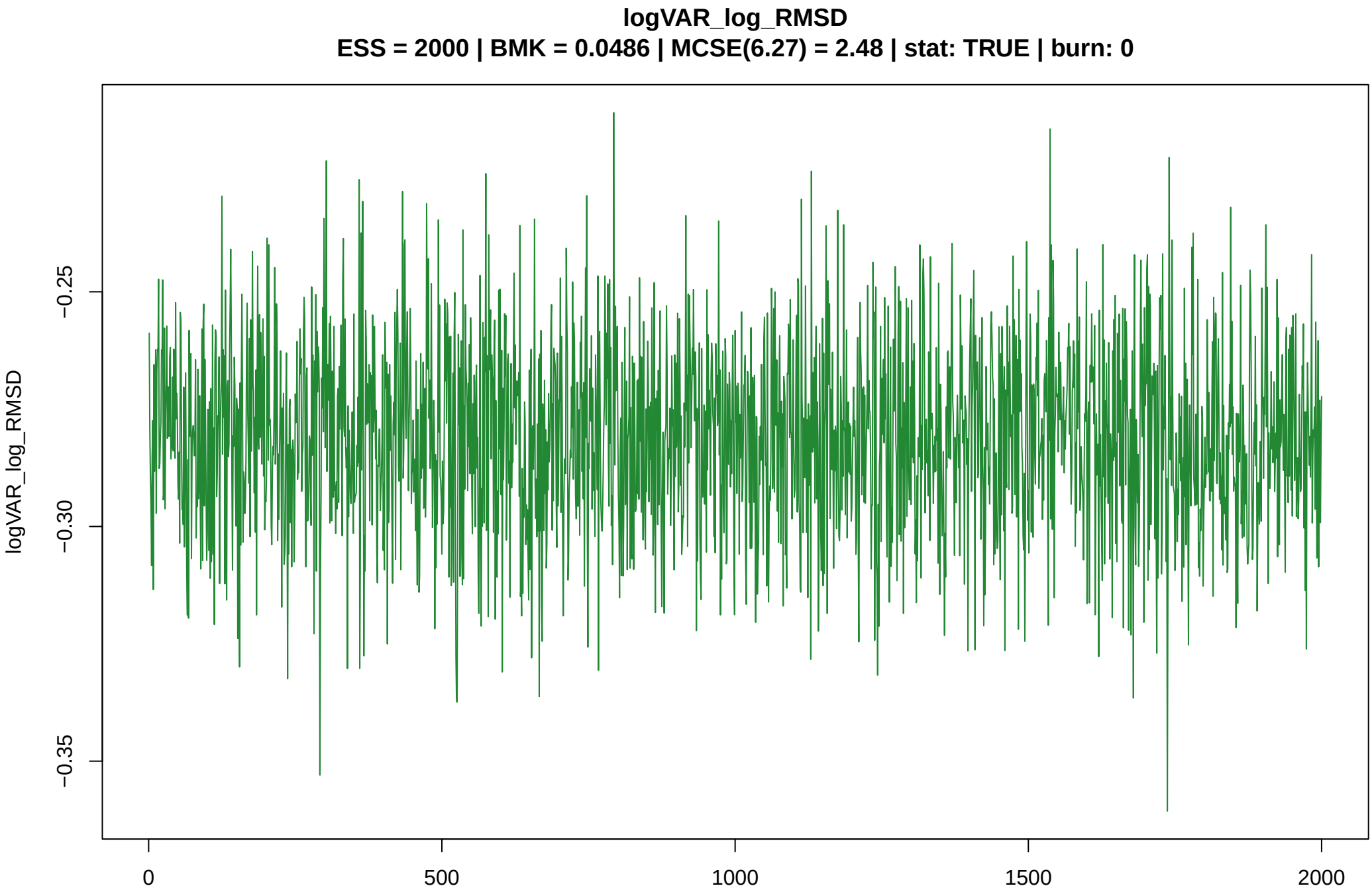

MEAN_logit_ec_tanimoto_similarity
ESS = 1700 | BMK = 0.0636 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0
MEAN_logit_ec_tanimoto_similarity
−2.04
−2.06
−2.08
−2.10
−2.12
0
500
1000
1500
2000

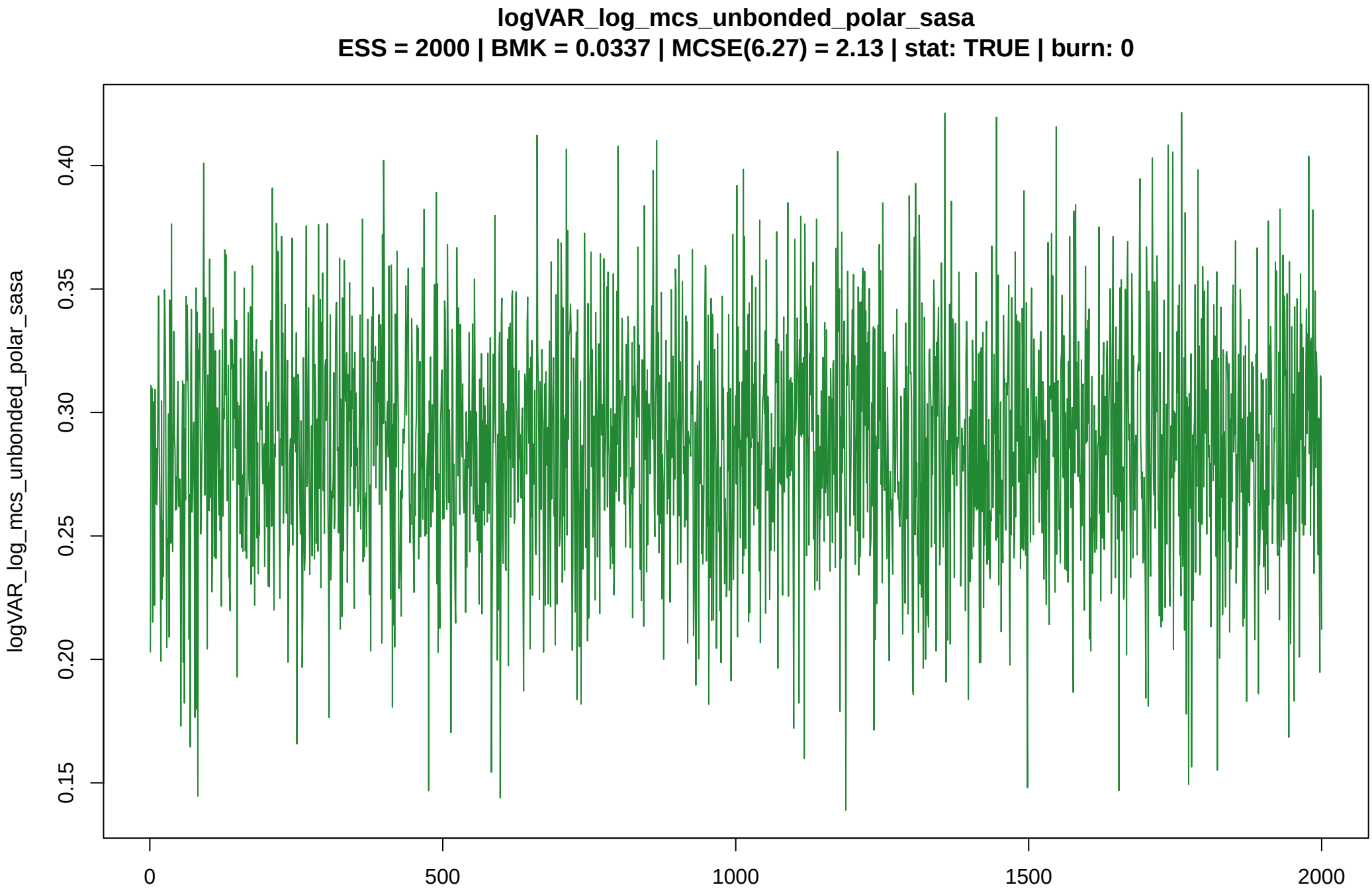

MEAN_mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0393 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
2.95
3.00
3.05
0
500
1000
1500
2000

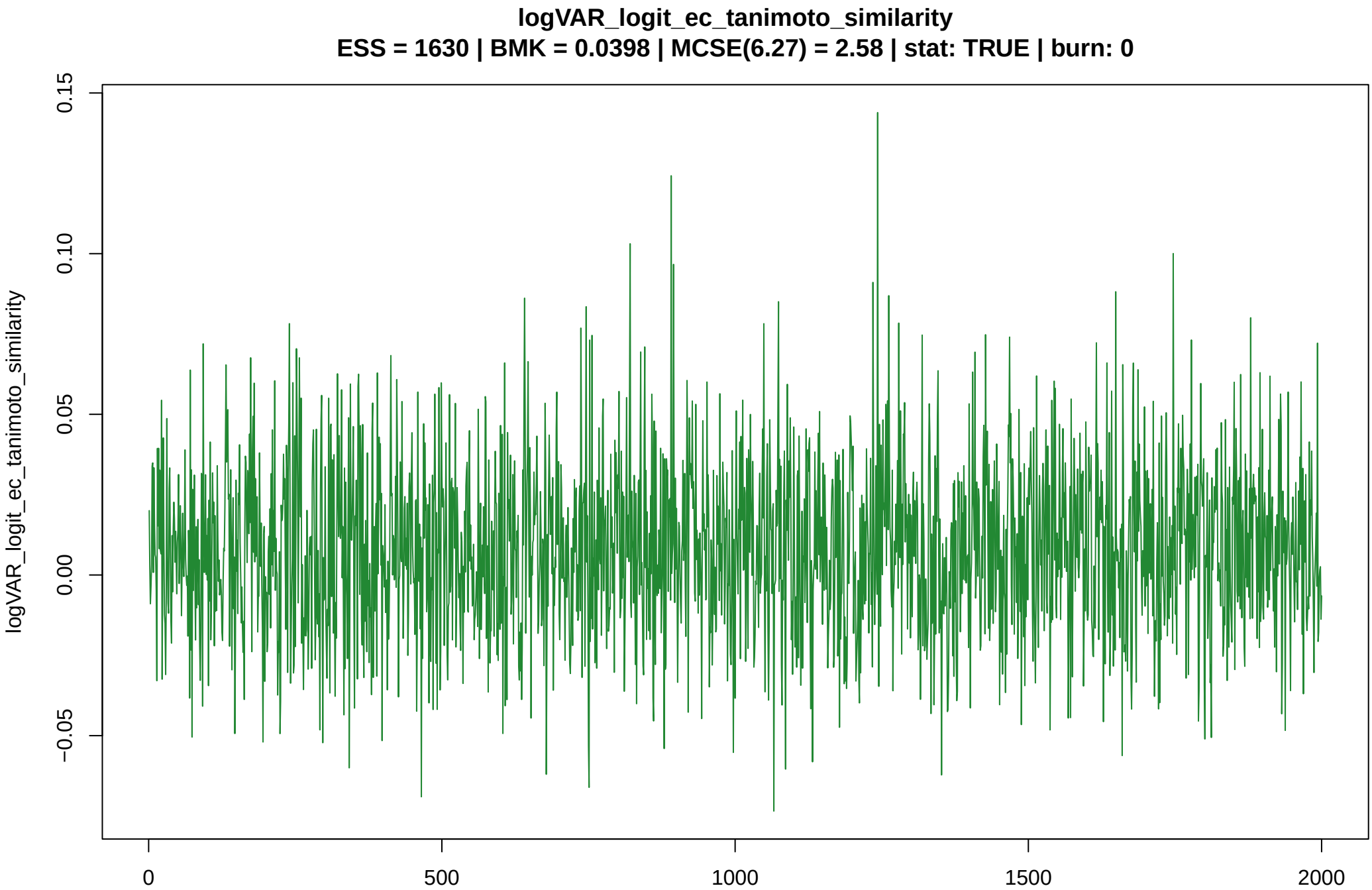

MEAN_docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0399 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
23.0
23.1
23.2
23.3
23.4
23.5
0
500
1000
1500
2000

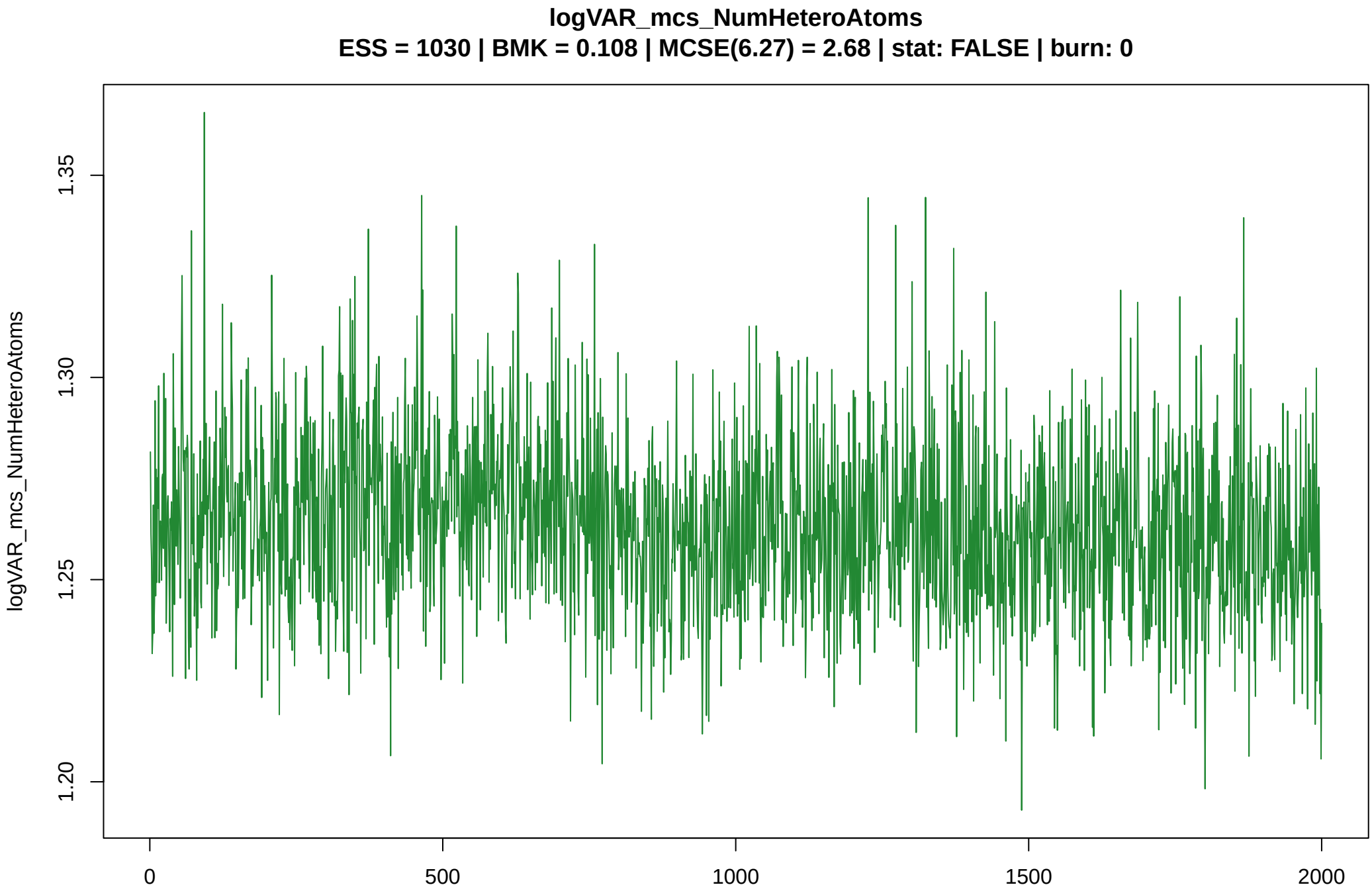

MEAN_mcs_RingCount
ESS = 2000 | BMK = 0.0475 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.80
0.82
0.84
0.86
0.88
0
500
1000
1500
2000

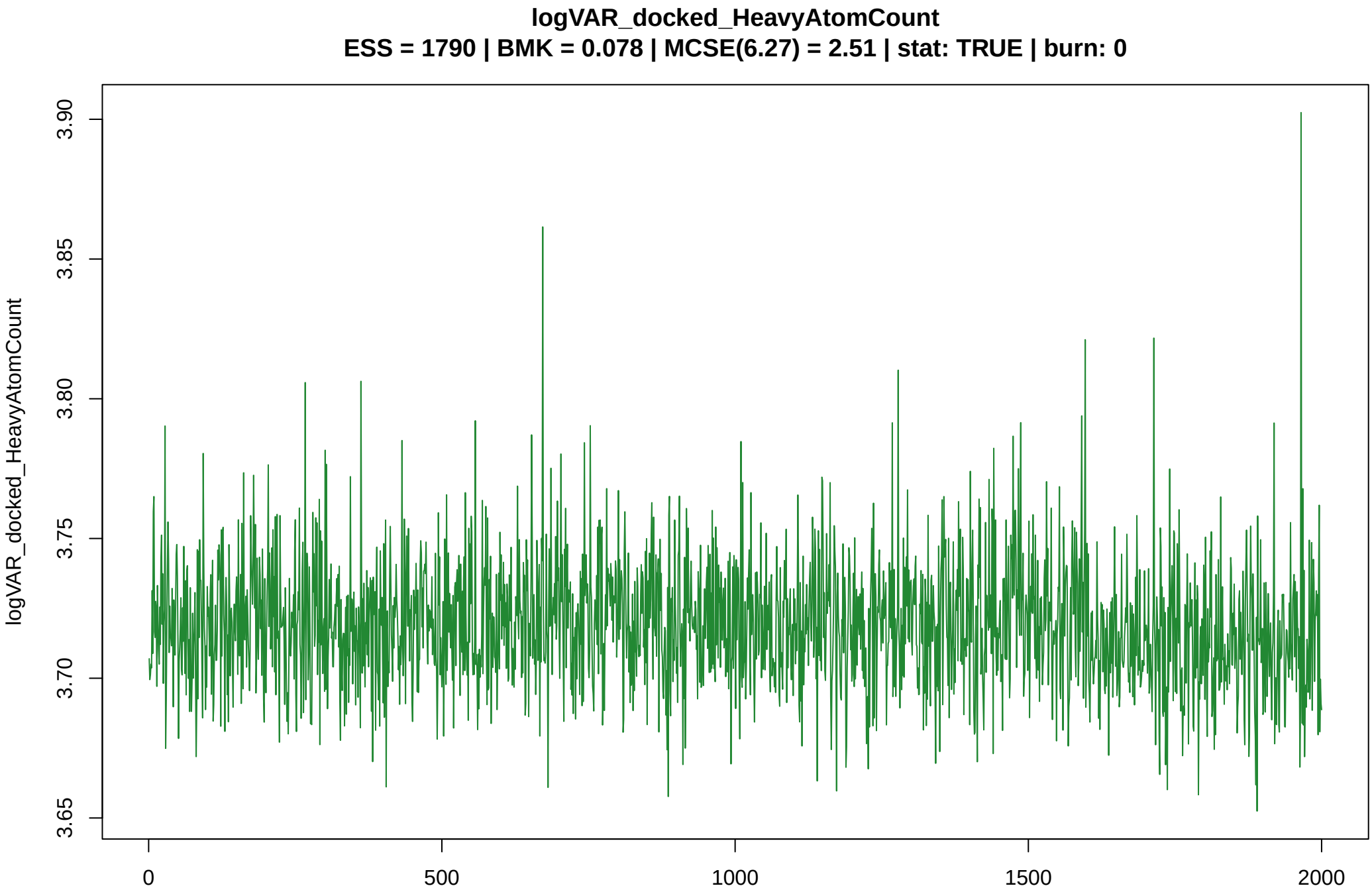

MEAN_docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0489 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0
MEAN_docked_NumRotatableBonds
4.70
4.75
4.80
4.85
4.90
0
500
1000
1500
2000

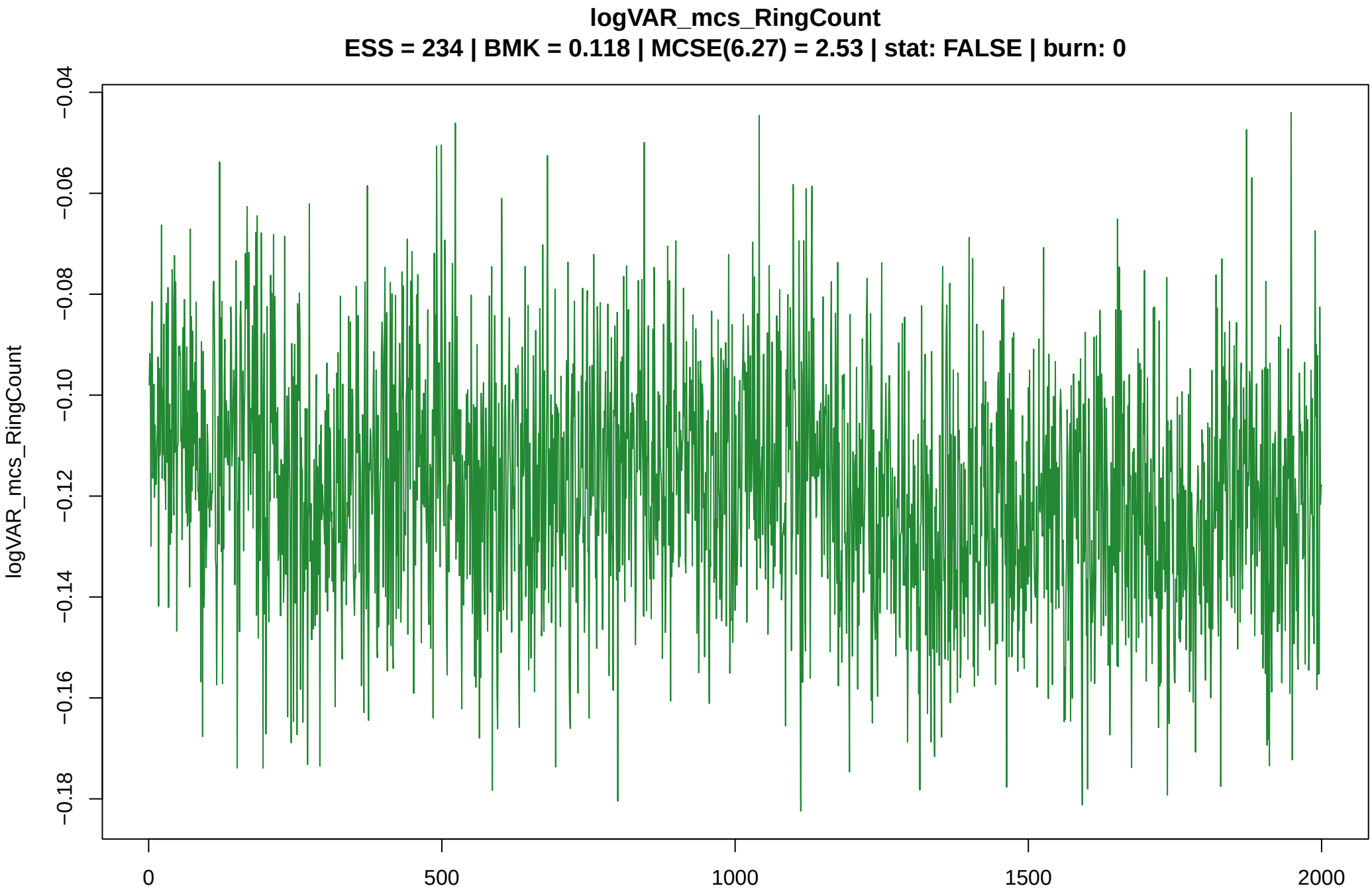

logVAR_log_RMSD
ESS = 2000 | BMK = 0.0486 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0
logVAR_log_RMSD
−0.25
−0.30
−0.35
0
500
1000
1500
2000

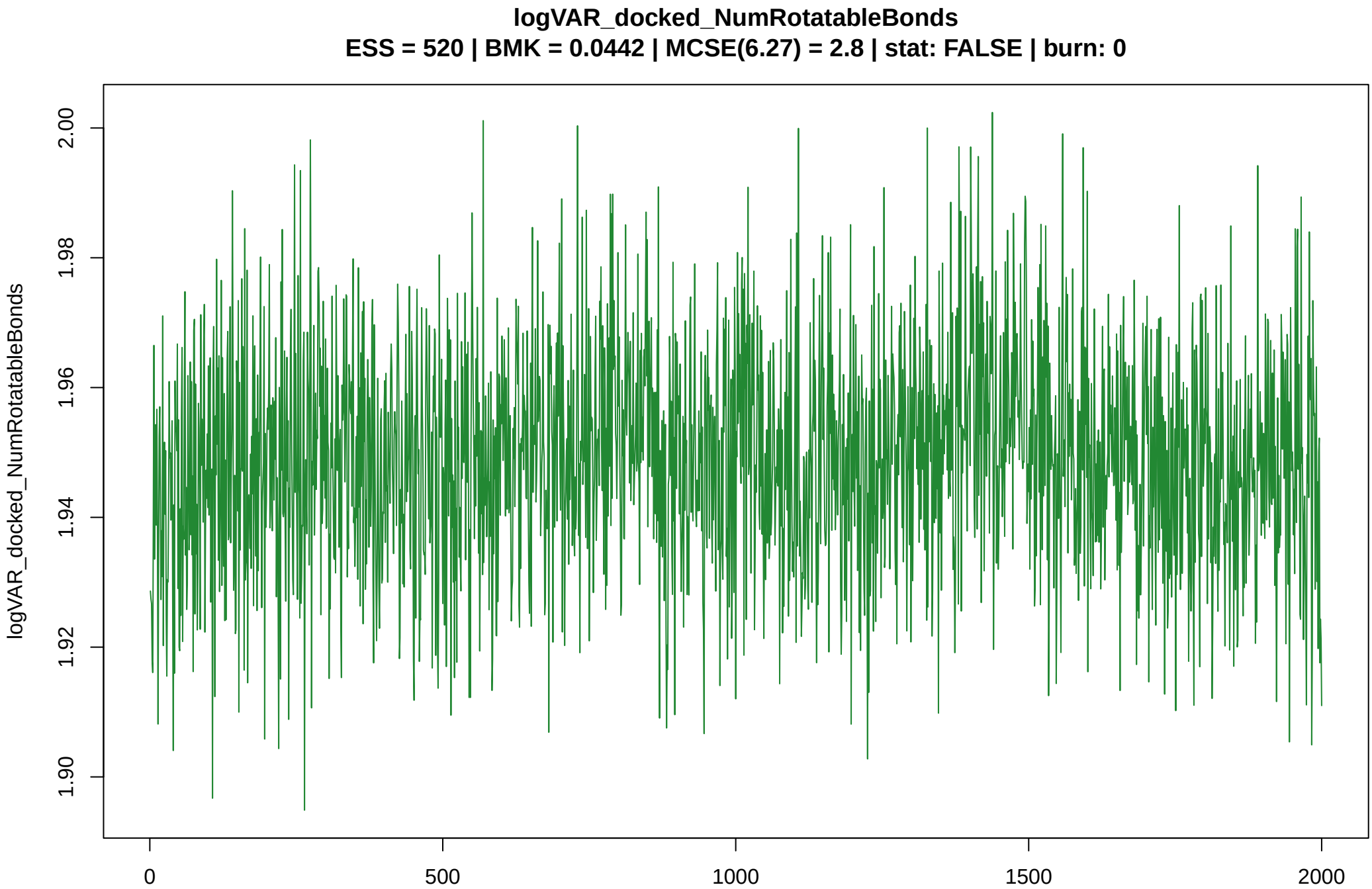

logVAR_log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0337 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0
logVAR_log_mcs_unbonded_polar_sasa
0.15
0.20
0.25
0.30
0.35
0.40
0
500
1000
1500
2000

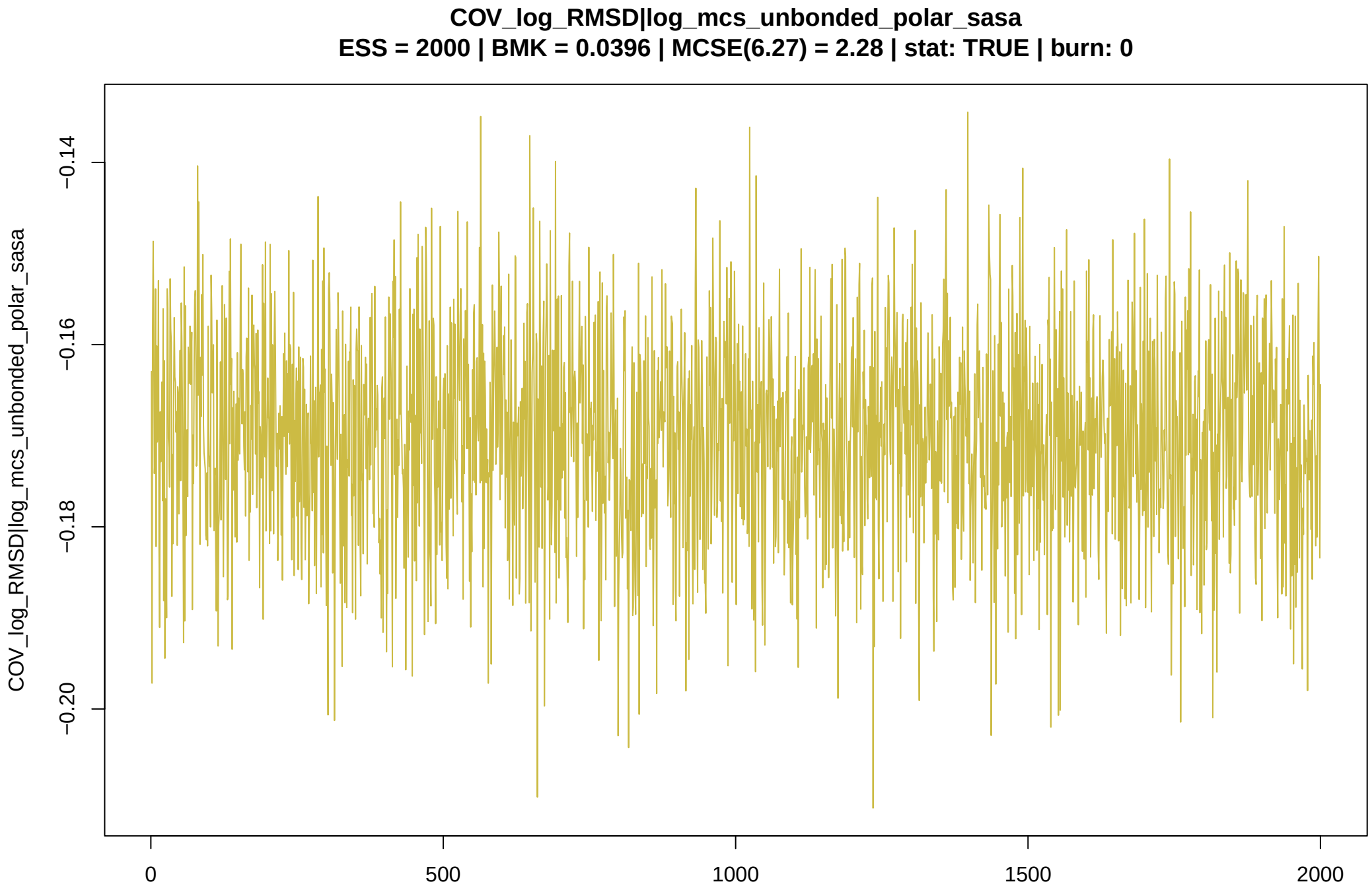

logVAR_logit_ec_tanimoto_similarity
ESS = 1630 | BMK = 0.0398 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0
logVAR_logit_ec_tanimoto_similarity
0.15
0.10
0.05
0.00
−0.05
0
500
1000
1500
2000

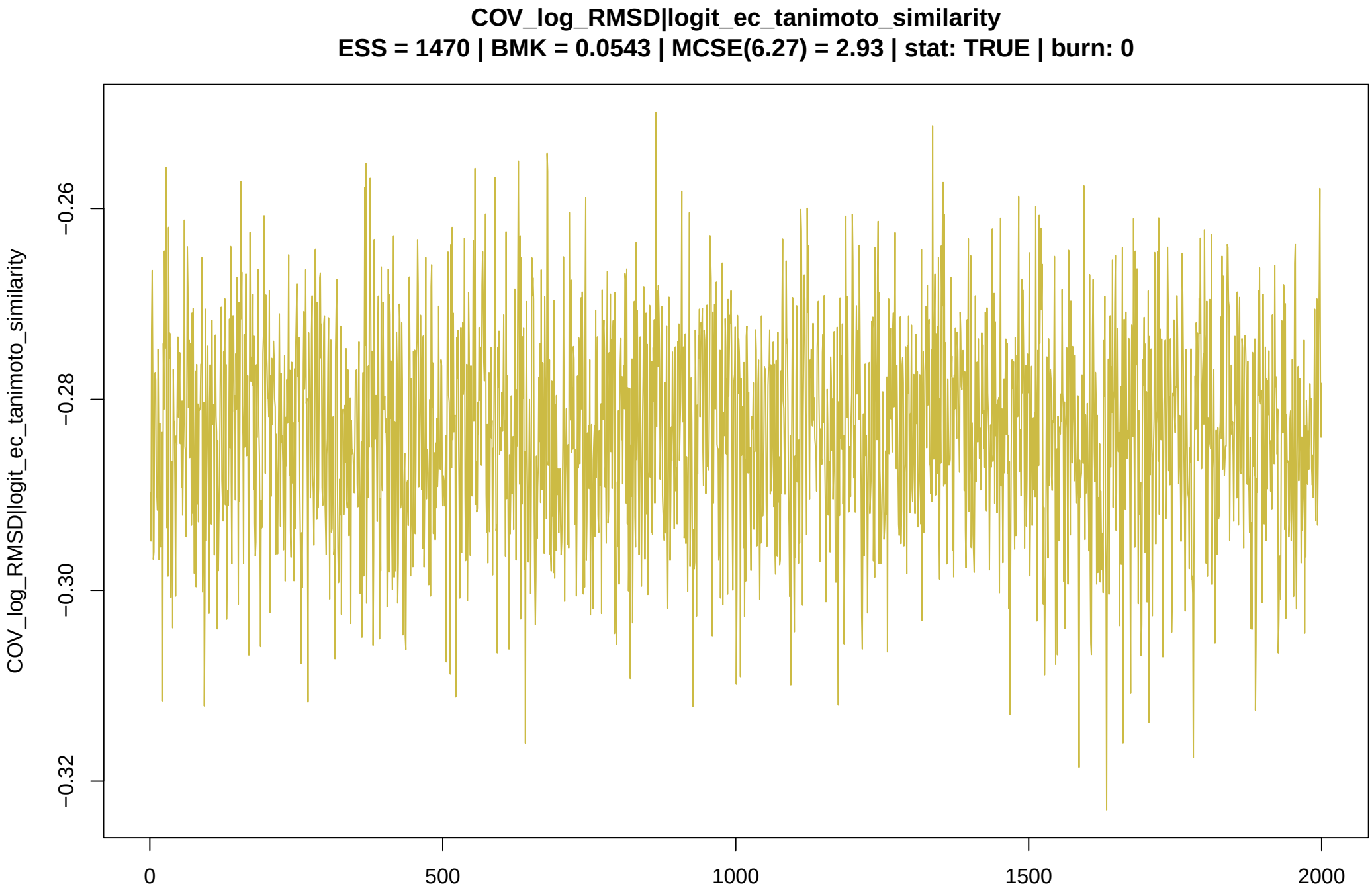

logVAR_mcs_NumHeteroAtoms
ESS = 1030 | BMK = 0.108 | MCSE(6.27) = 2.68 | stat: FALSE | burn: 0
logVAR_mcs_NumHeteroAtoms
1.20
1.25
1.30
1.35
0
500
1000
1500
2000

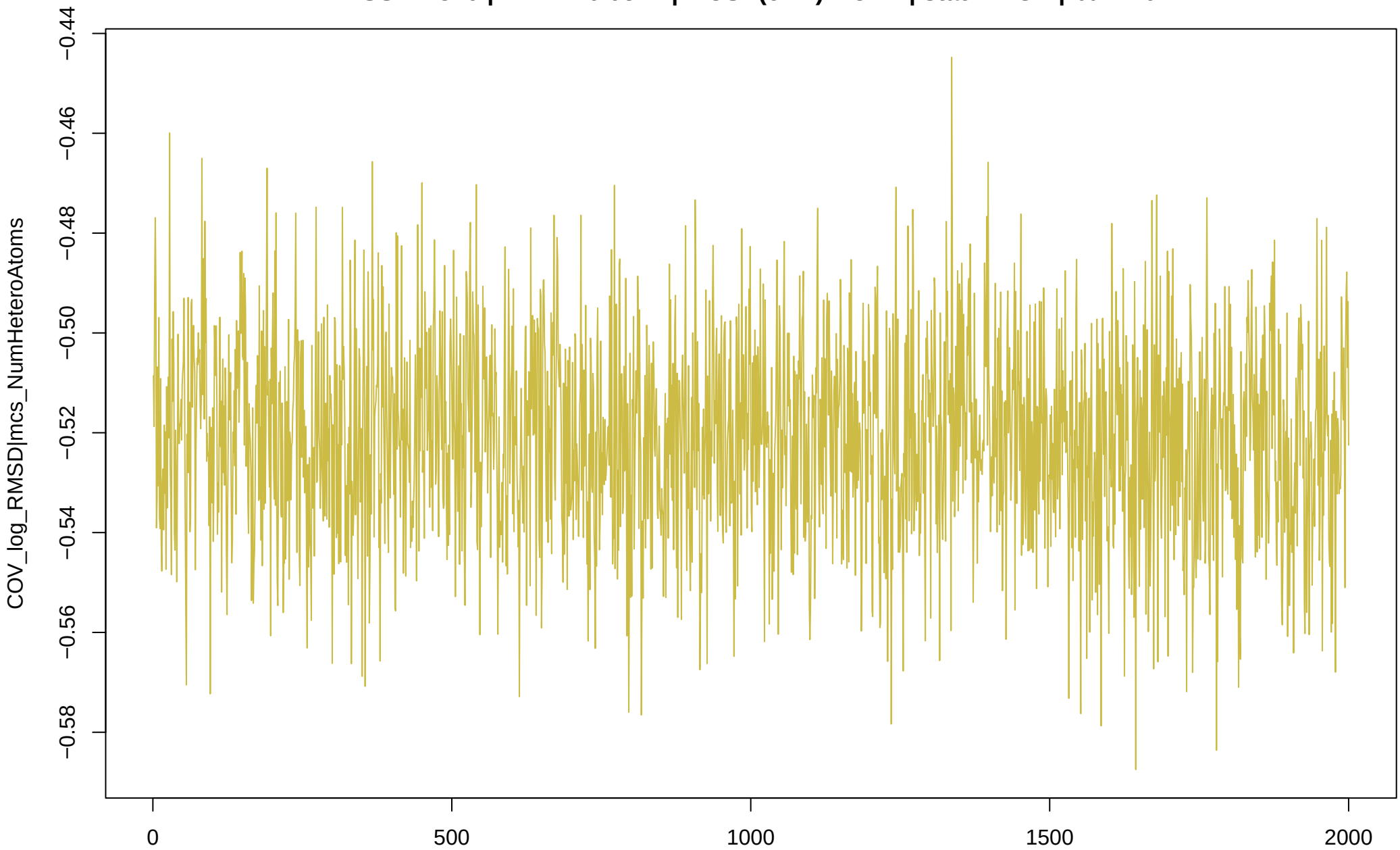

logVAR_docked_HeavyAtomCount
ESS = 1790 | BMK = 0.078 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0
logVAR_docked_HeavyAtomCount
3.65
3.70
3.75
3.80
3.85
3.90
0
500
1000
1500
2000

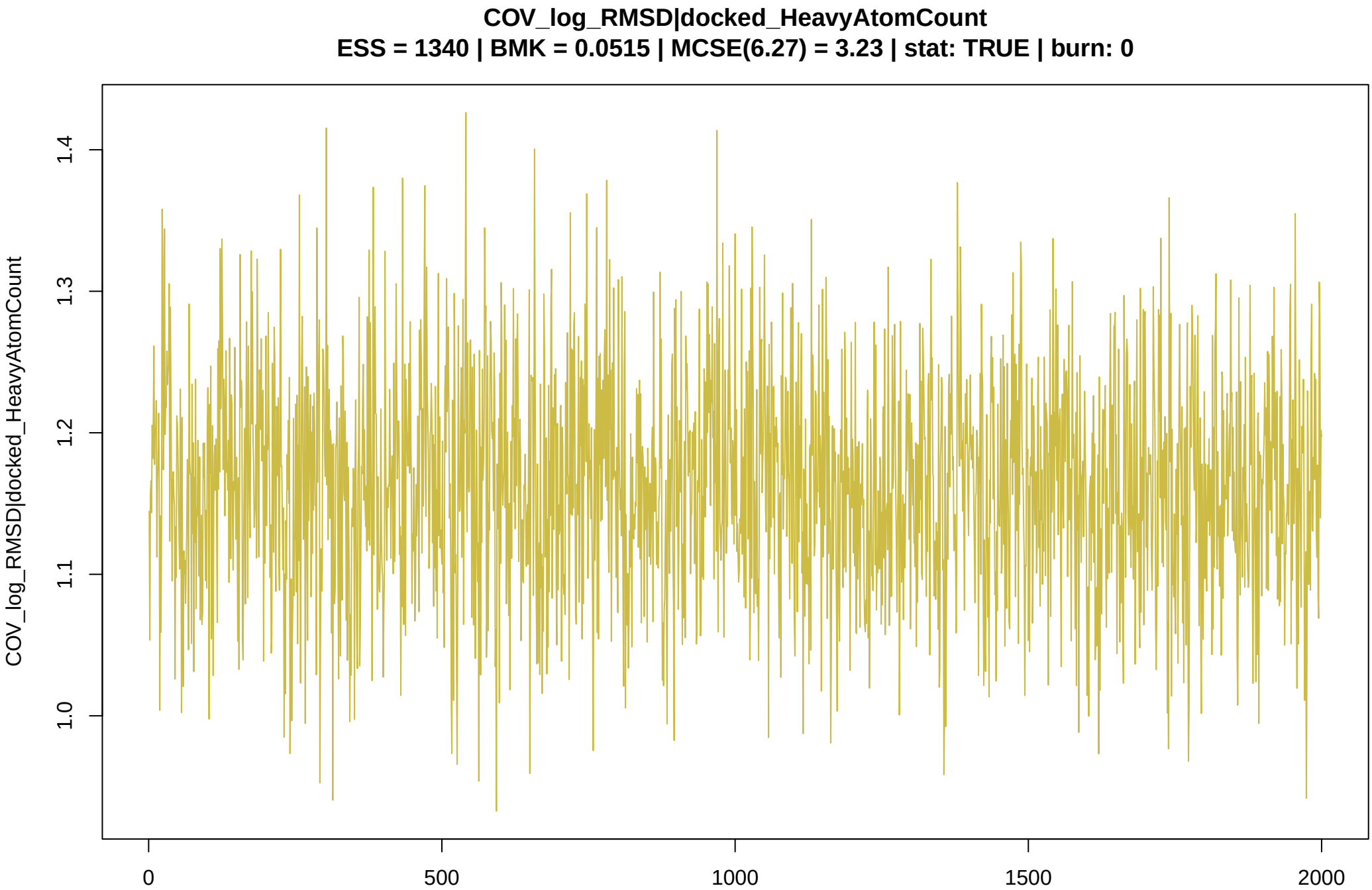

logVAR_mcs_RingCount
ESS = 234 | BMK = 0.118 | MCSE(6.27) = 2.53 | stat: FALSE | burn: 0
logVAR_mcs_RingCount
−0.04
−0.06
−0.08
−0.10
−0.12
−0.14
−0.16
−0.18
0
500
1000
1500
2000

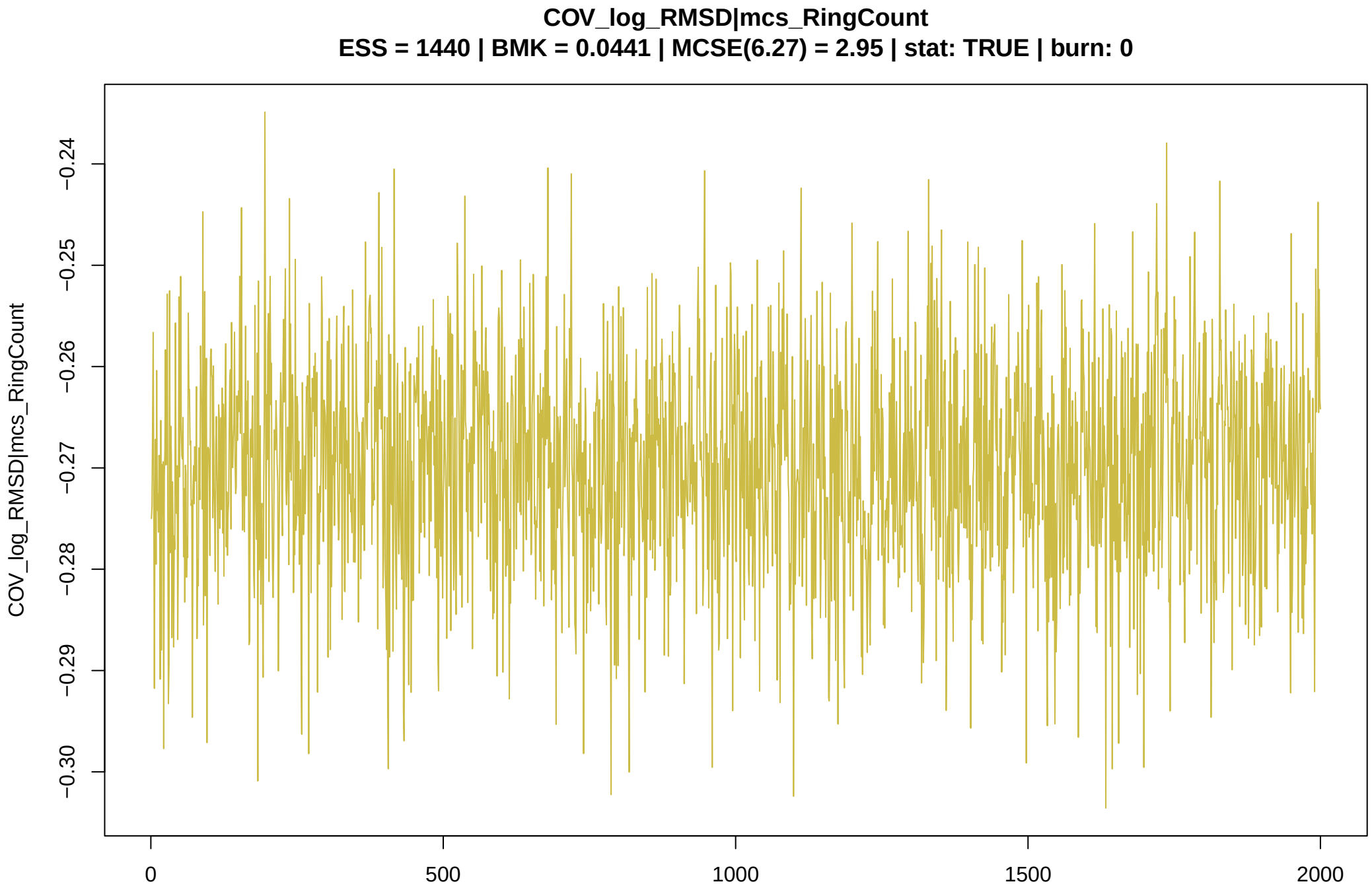

logVAR_docked_NumRotatableBonds
ESS = 520 | BMK = 0.0442 | MCSE(6.27) = 2.8 | stat: FALSE | burn: 0
logVAR_docked_NumRotatableBonds
1.90
1.92
1.94
1.96
1.98
2.00
0
500
1000
1500
2000

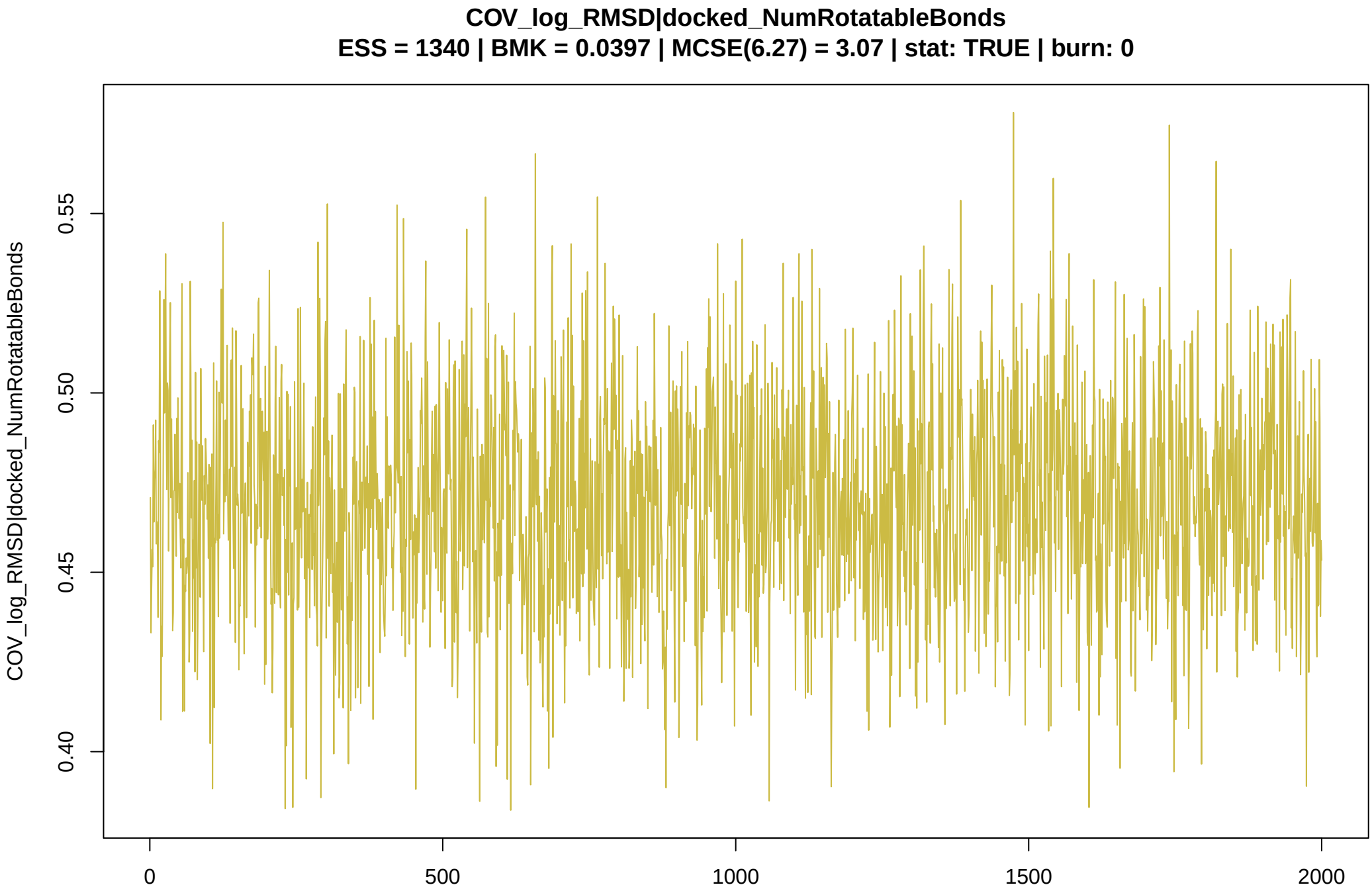

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0396 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.14
−0.16
−0.18
−0.20
0
500
1000
1500
2000

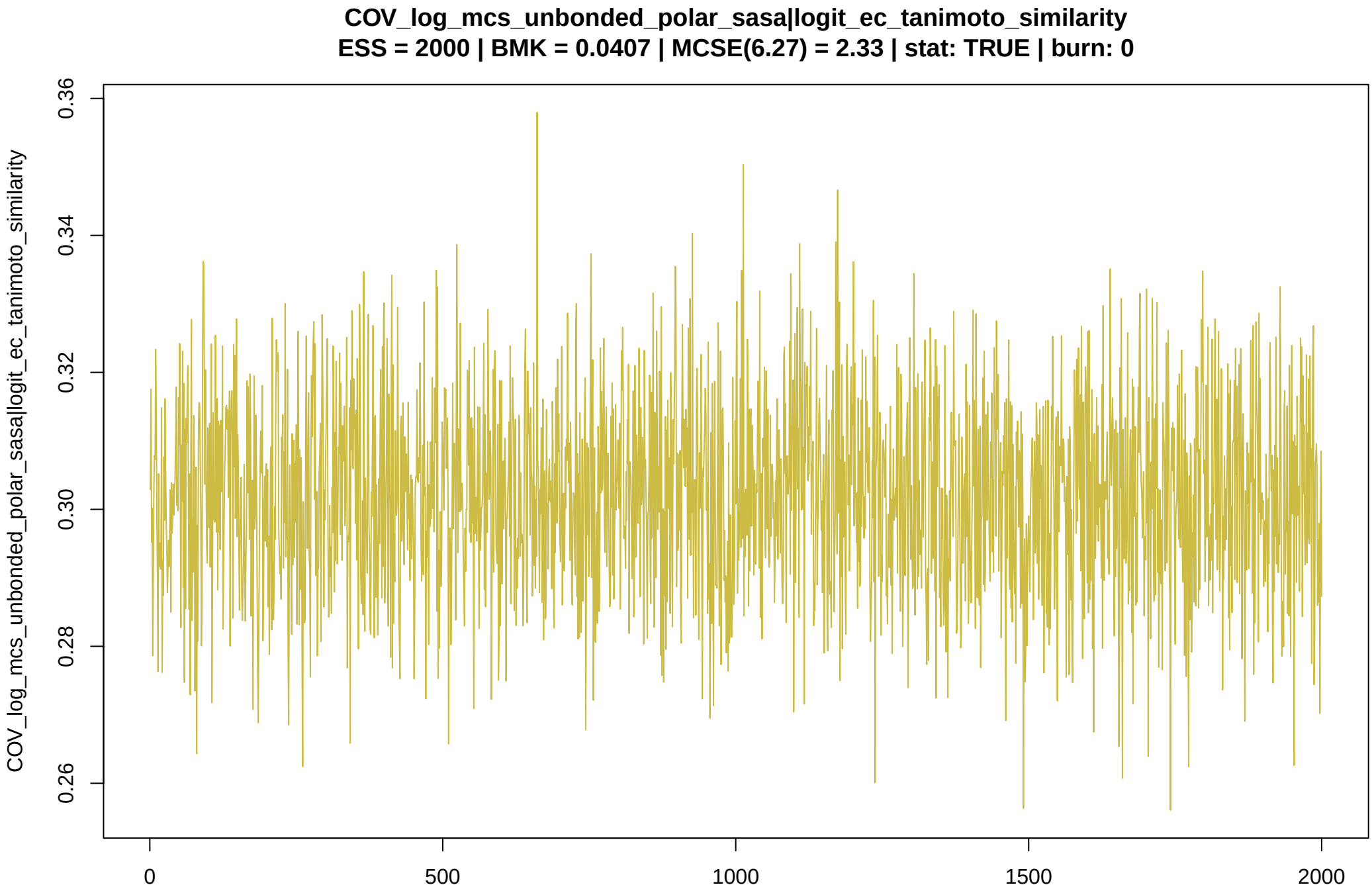

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1470 | BMK = 0.0543 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0
COV_log_RMSD|logit_ec_tanimoto_similarity
−0.26
−0.28
−0.30
−0.32
0
500
1000
1500
2000

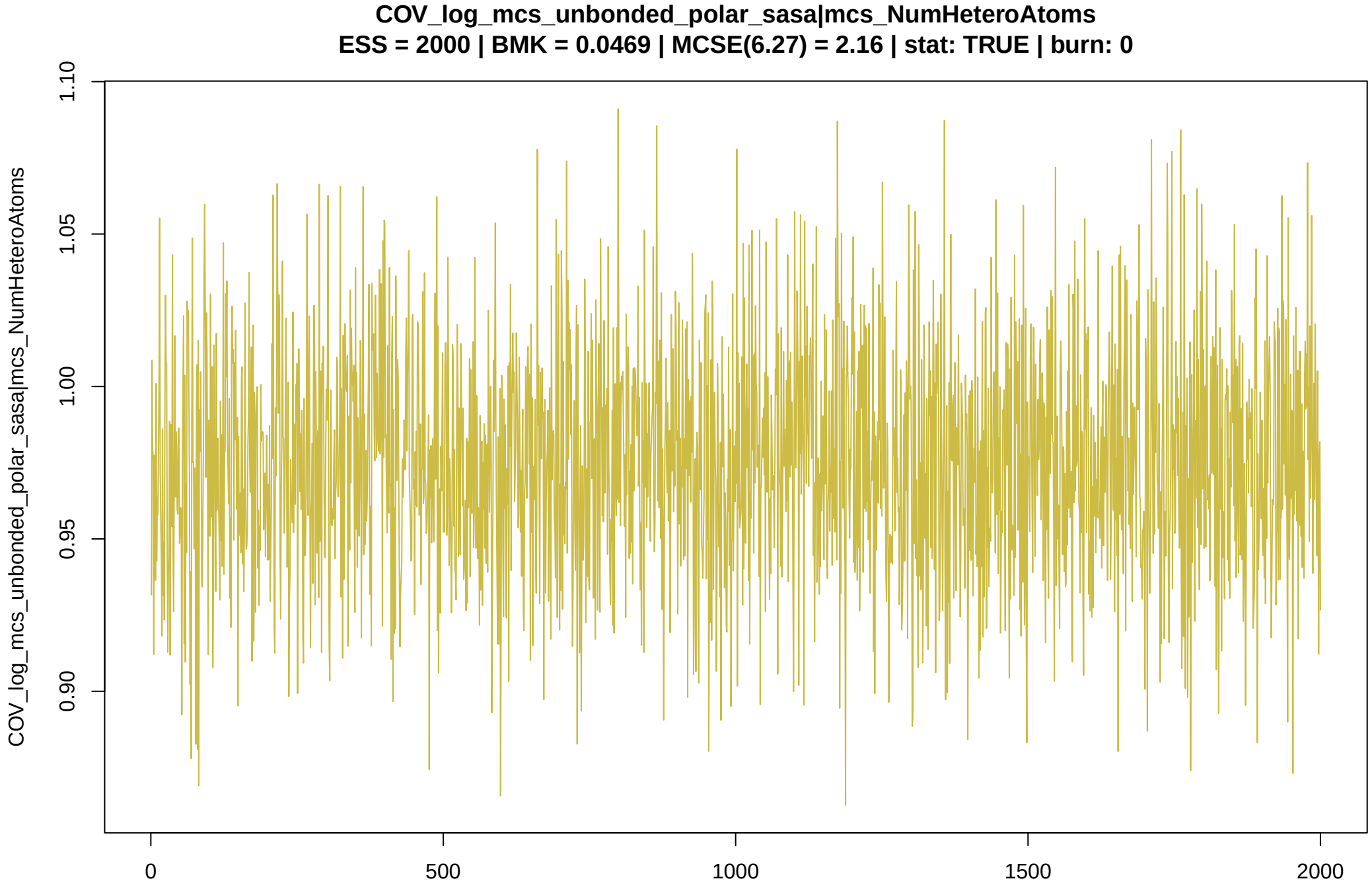

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1540 | BMK = 0.0524 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.44
−0.46
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

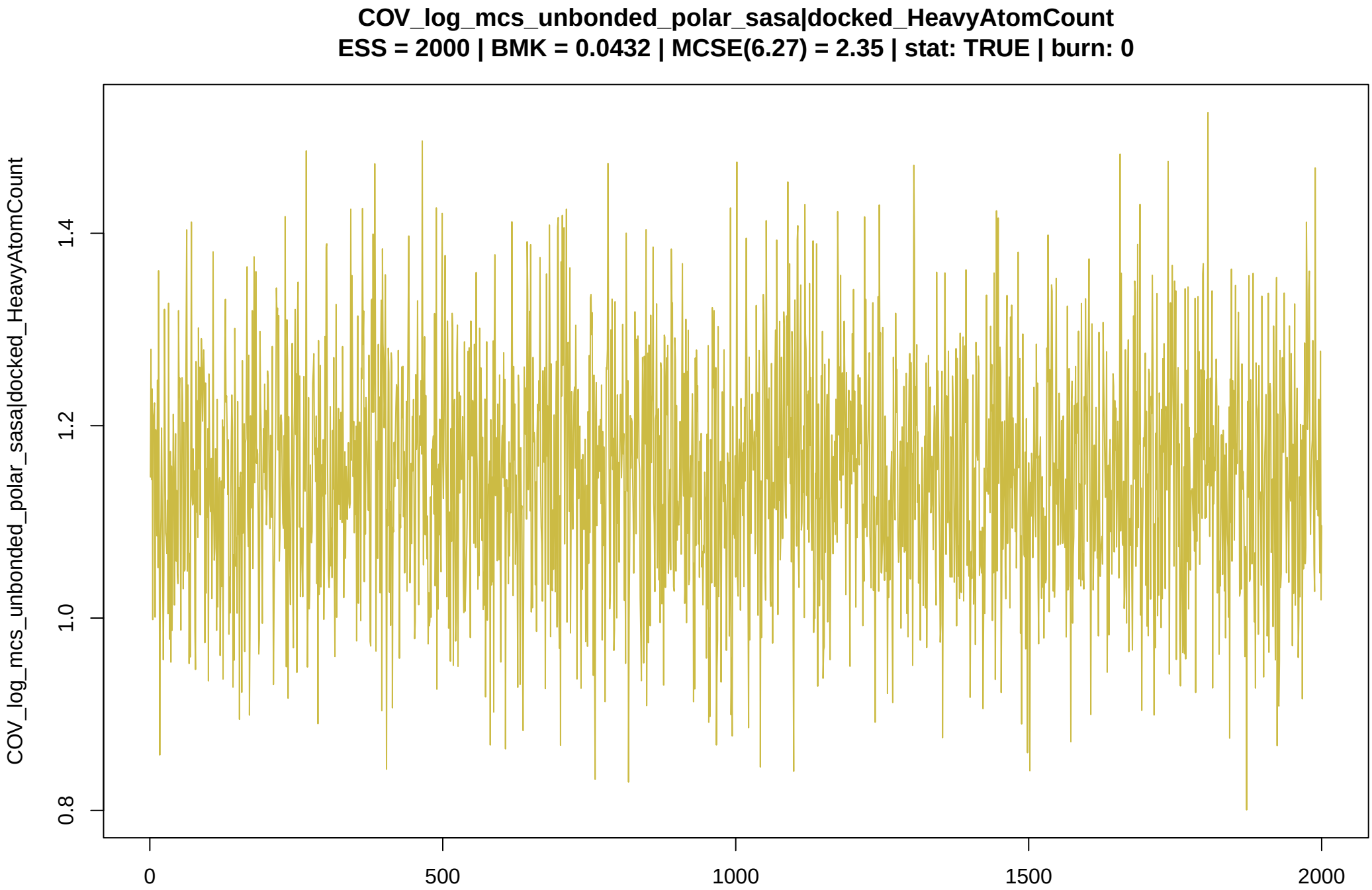

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1340 | BMK = 0.0515 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
1.0
1.1
1.2
1.3
1.4
0
500
1000
1500
2000

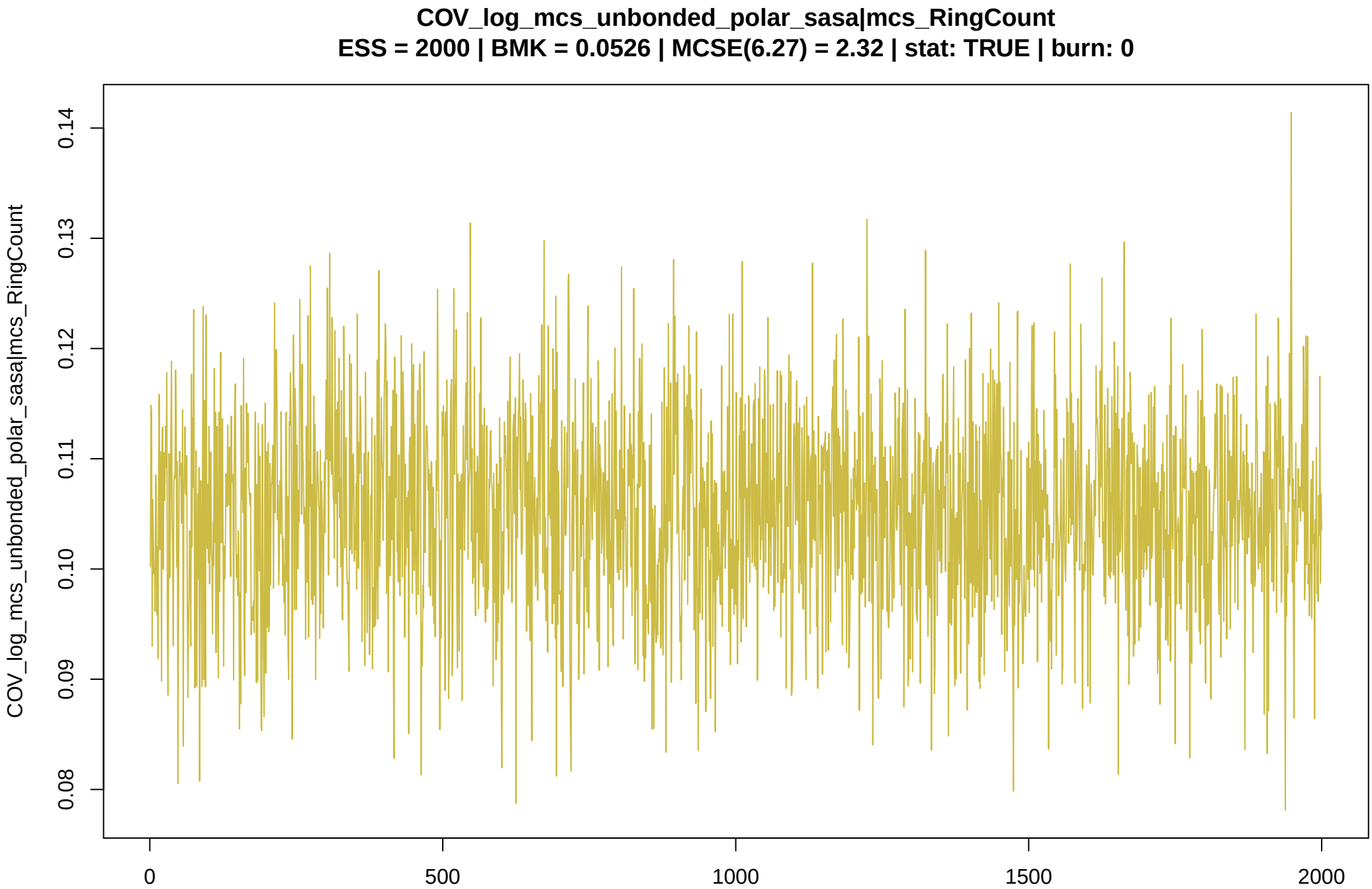

COV_log_RMSD|mcs_RingCount
ESS = 1440 | BMK = 0.0441 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.24
−0.25
−0.26
−0.27
−0.28
−0.29
−0.30
0
500
1000
1500
2000

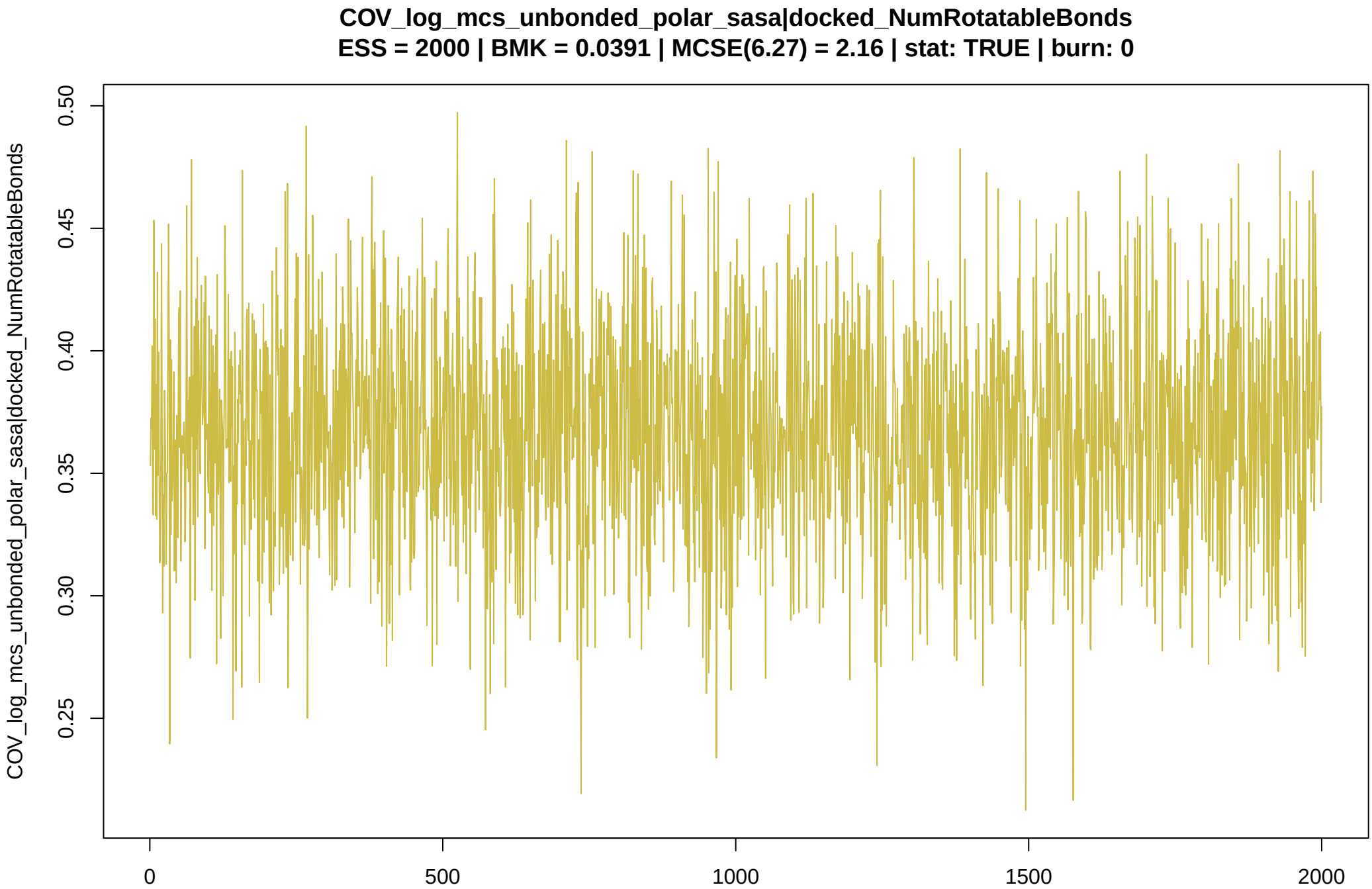

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1340 | BMK = 0.0397 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0
COV_log_RMSD|docked_NumRotatableBonds
0.40
0.45
0.50
0.55
0
500
1000
1500
2000

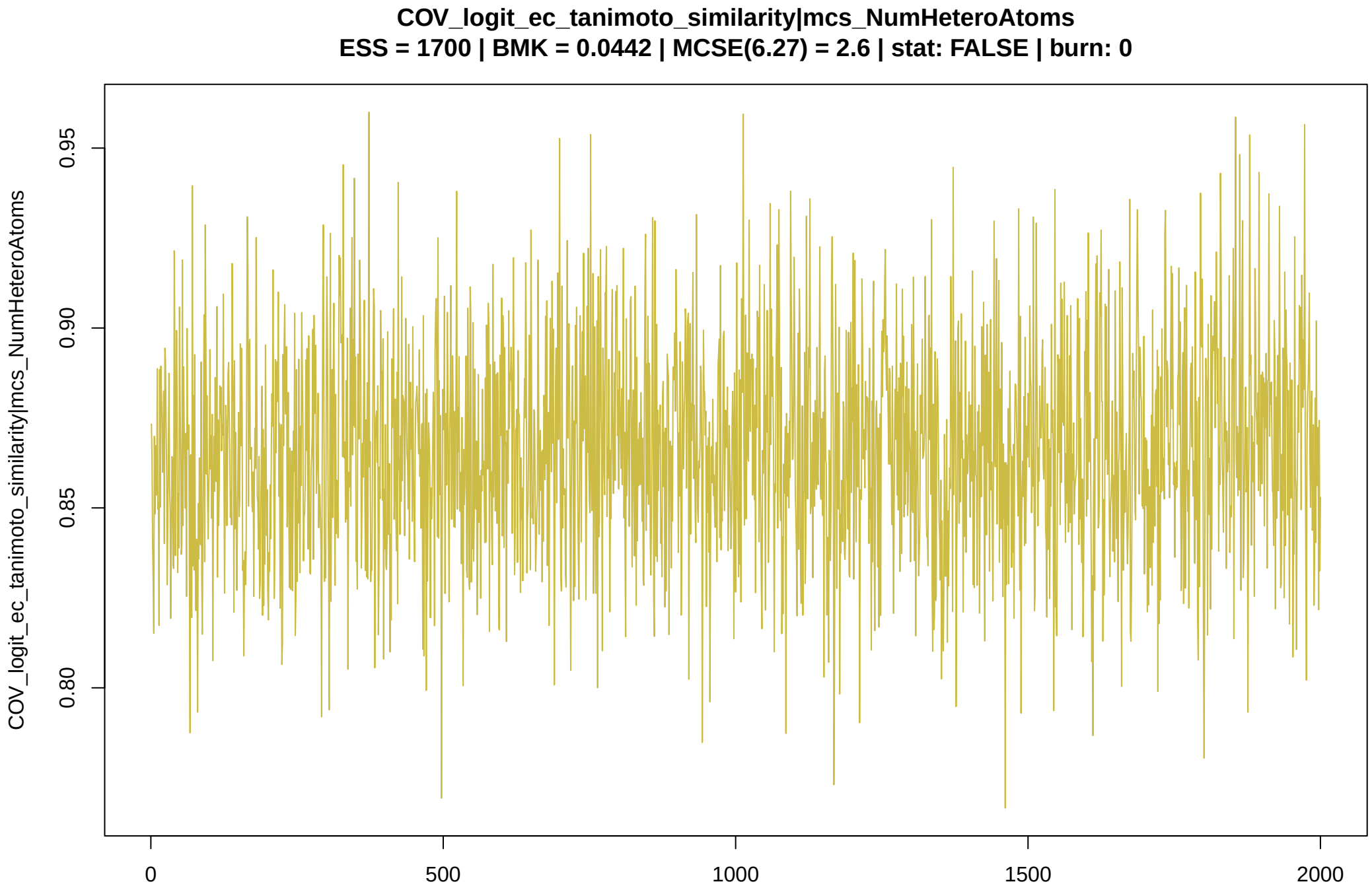

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 2000 | BMK = 0.0407 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0.26
0.28
0.30
0.32
0.34
0.36
0
500
1000
1500
2000

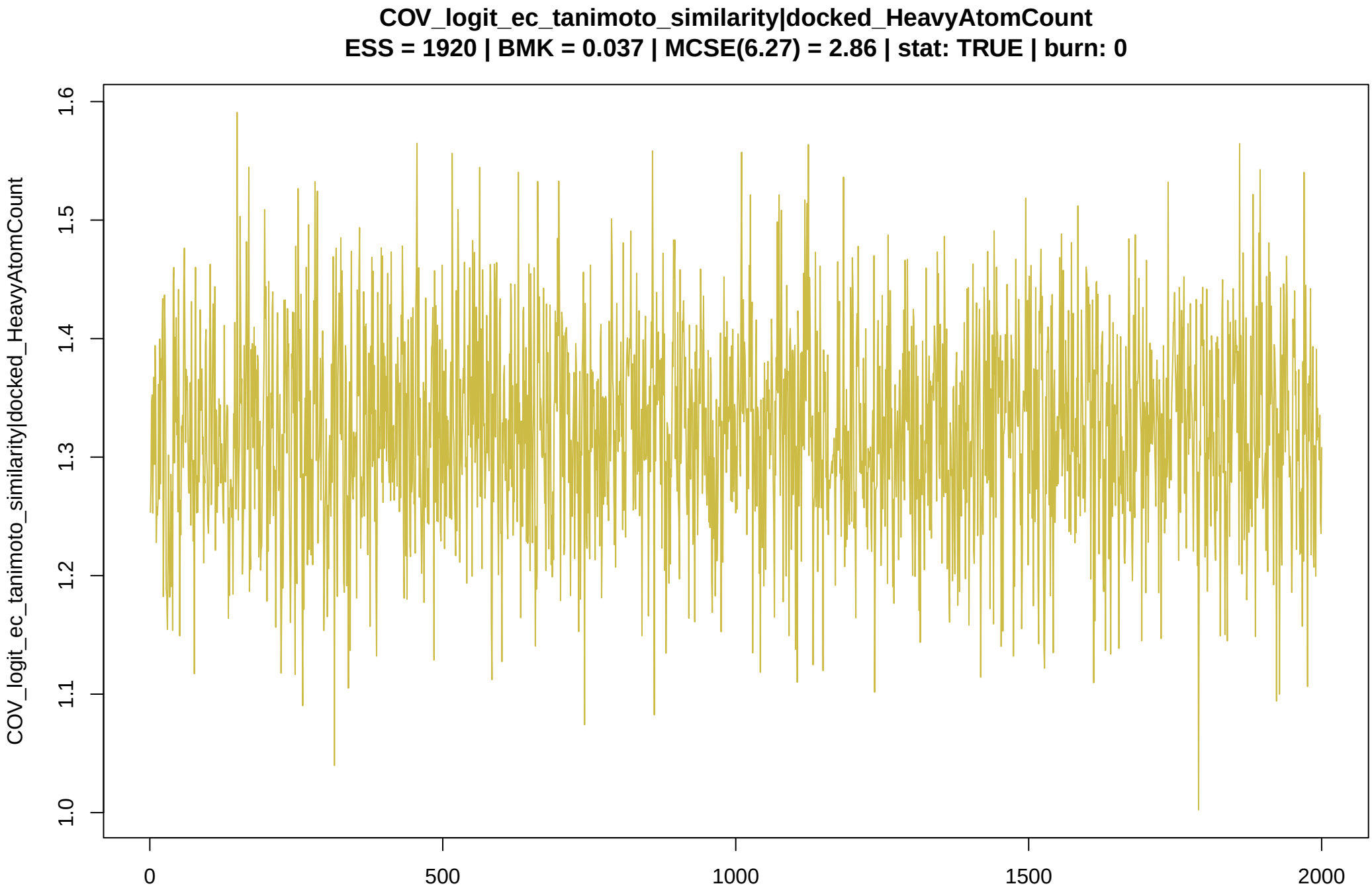

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0469 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
1.10
1.05
1.00
0.95
0.90
0
500
1000
1500
2000

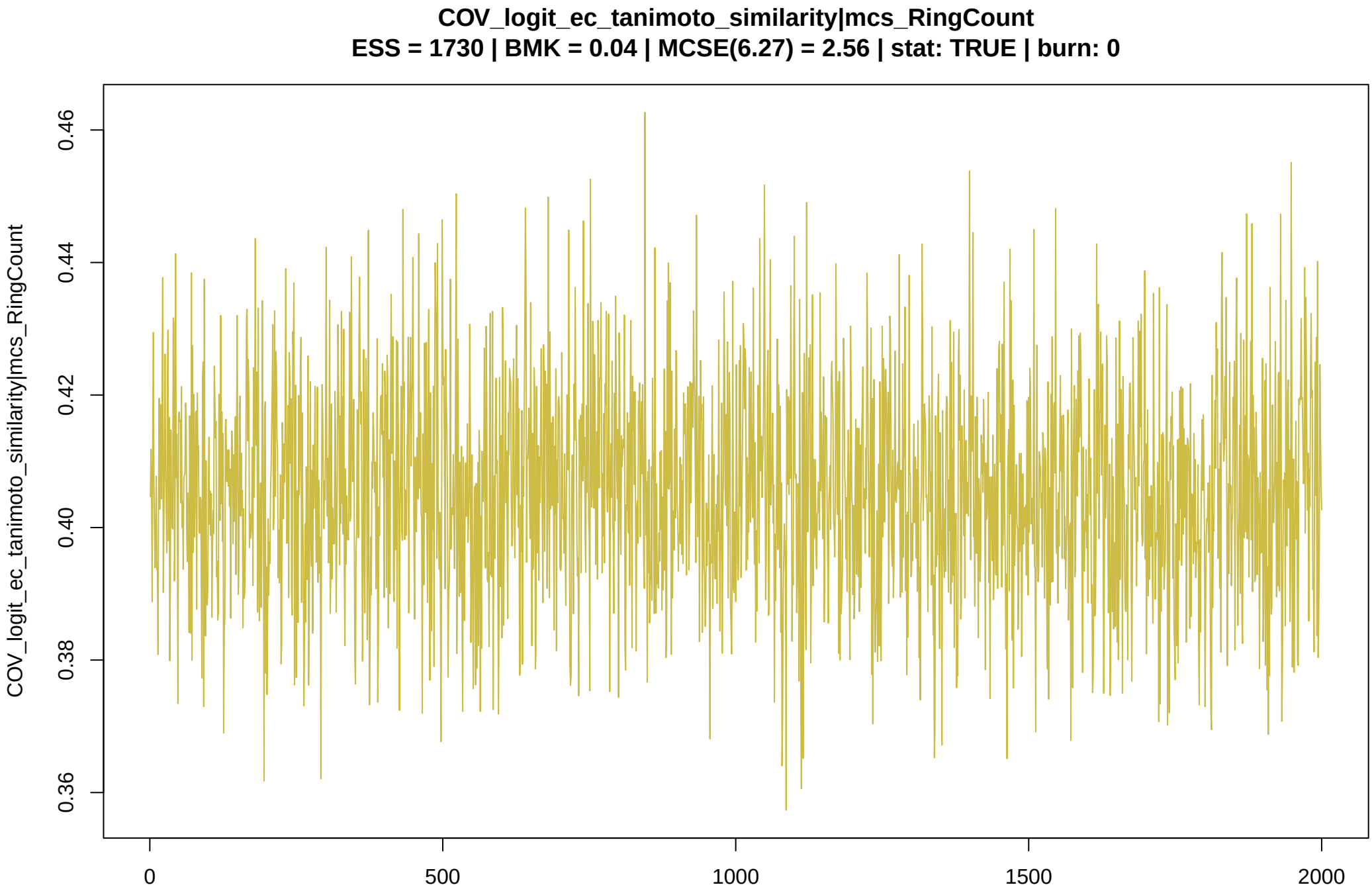

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0432 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

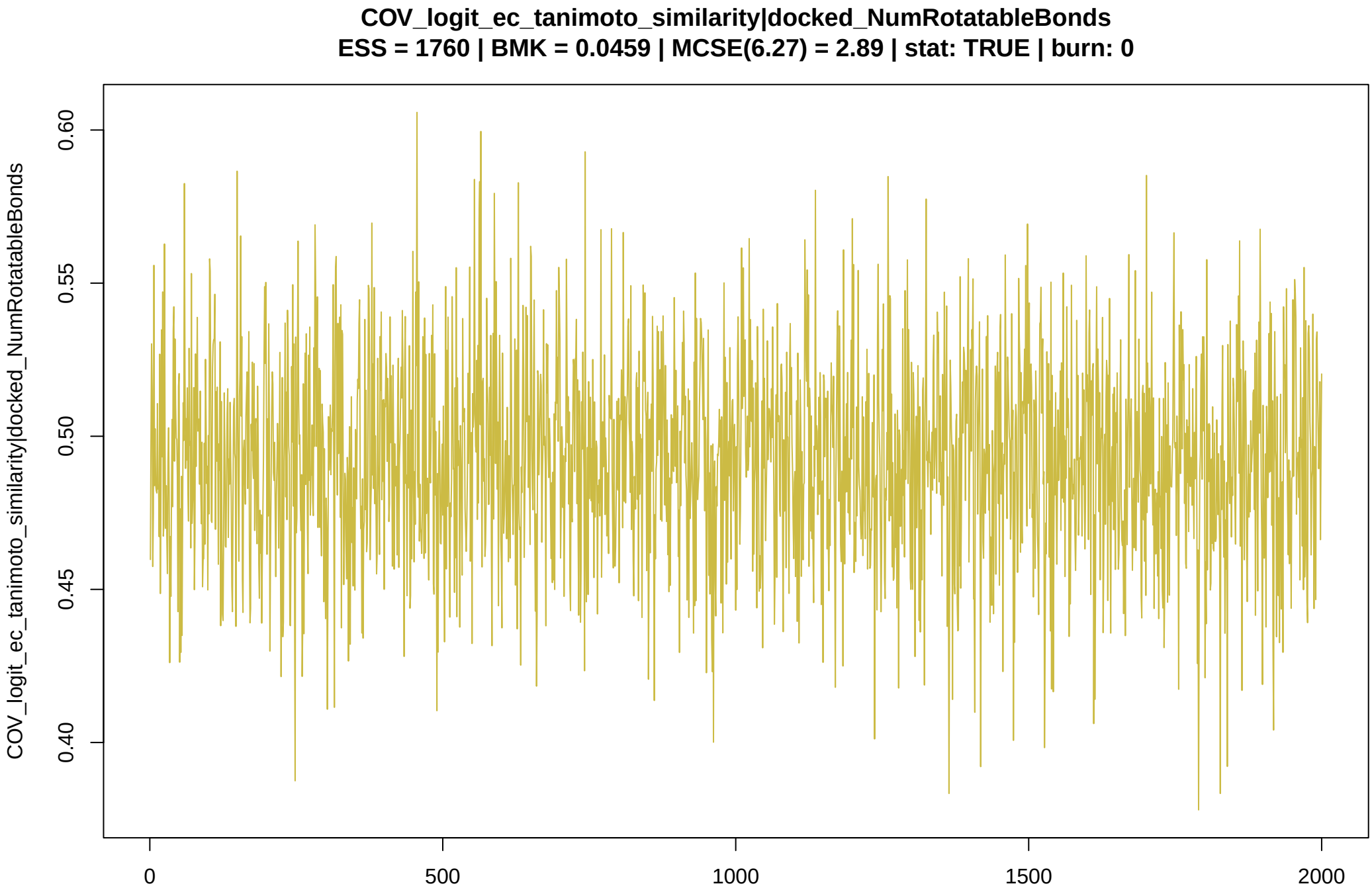

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 2000 | BMK = 0.0526 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
0.08
0.09
0.10
0.11
0.12
0.13
0.14
0
500
1000
1500
2000

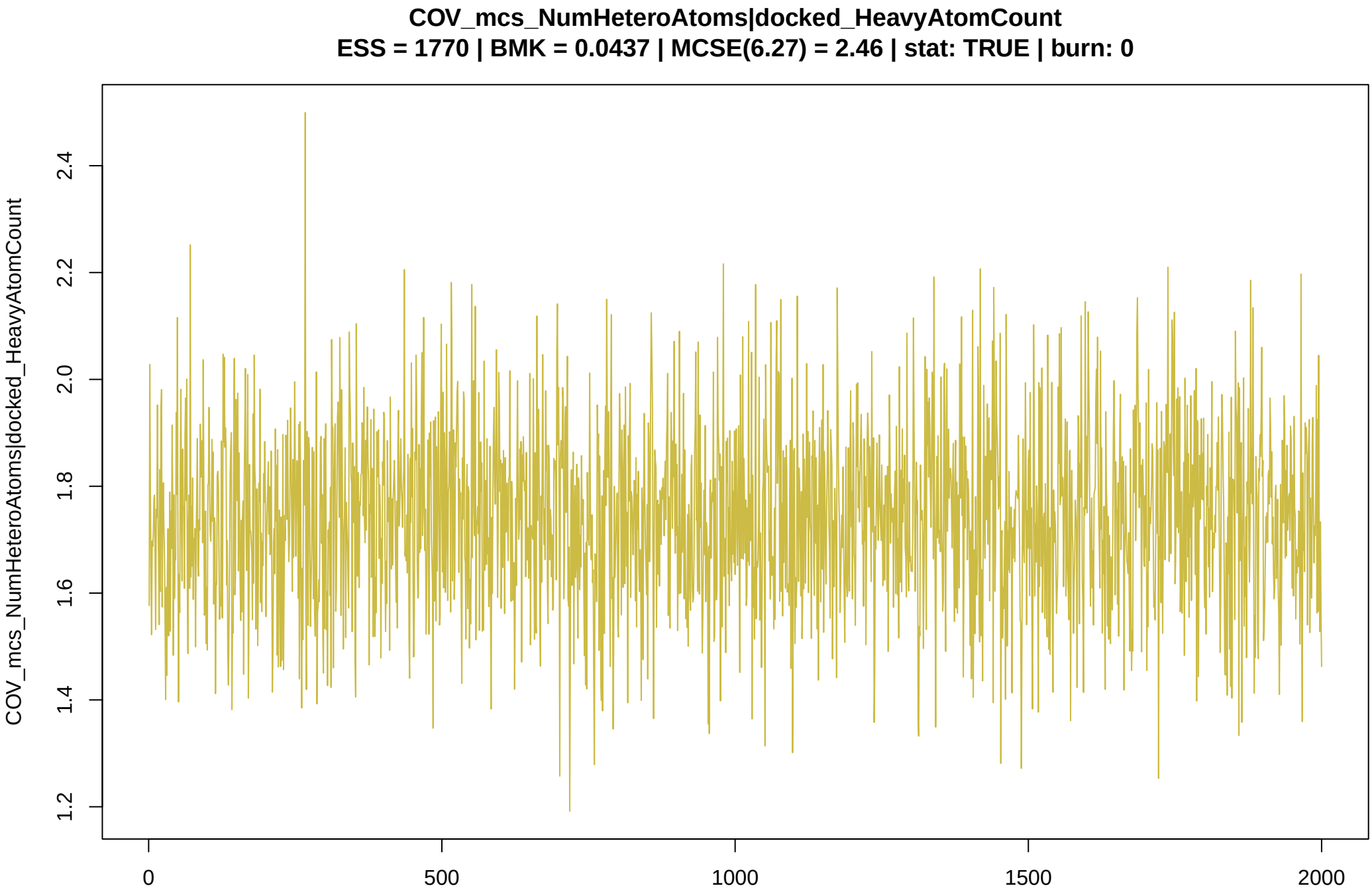

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0391 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
0.25
0.30
0.35
0.40
0.45
0.50
0
500
1000
1500
2000

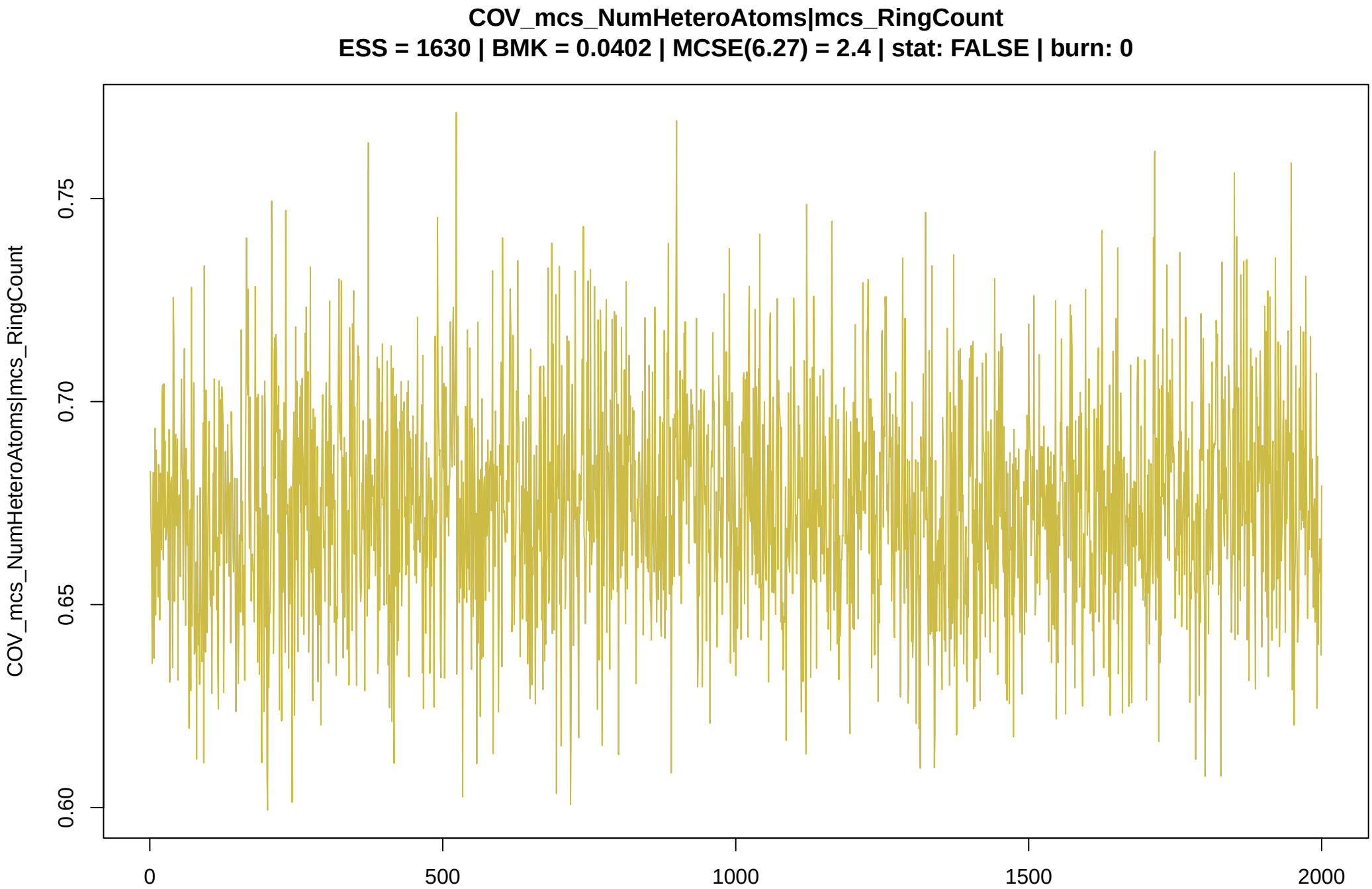

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1700 | BMK = 0.0442 | MCSE(6.27) = 2.6 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.80
0.85
0.90
0.95
0
500
1000
1500
2000

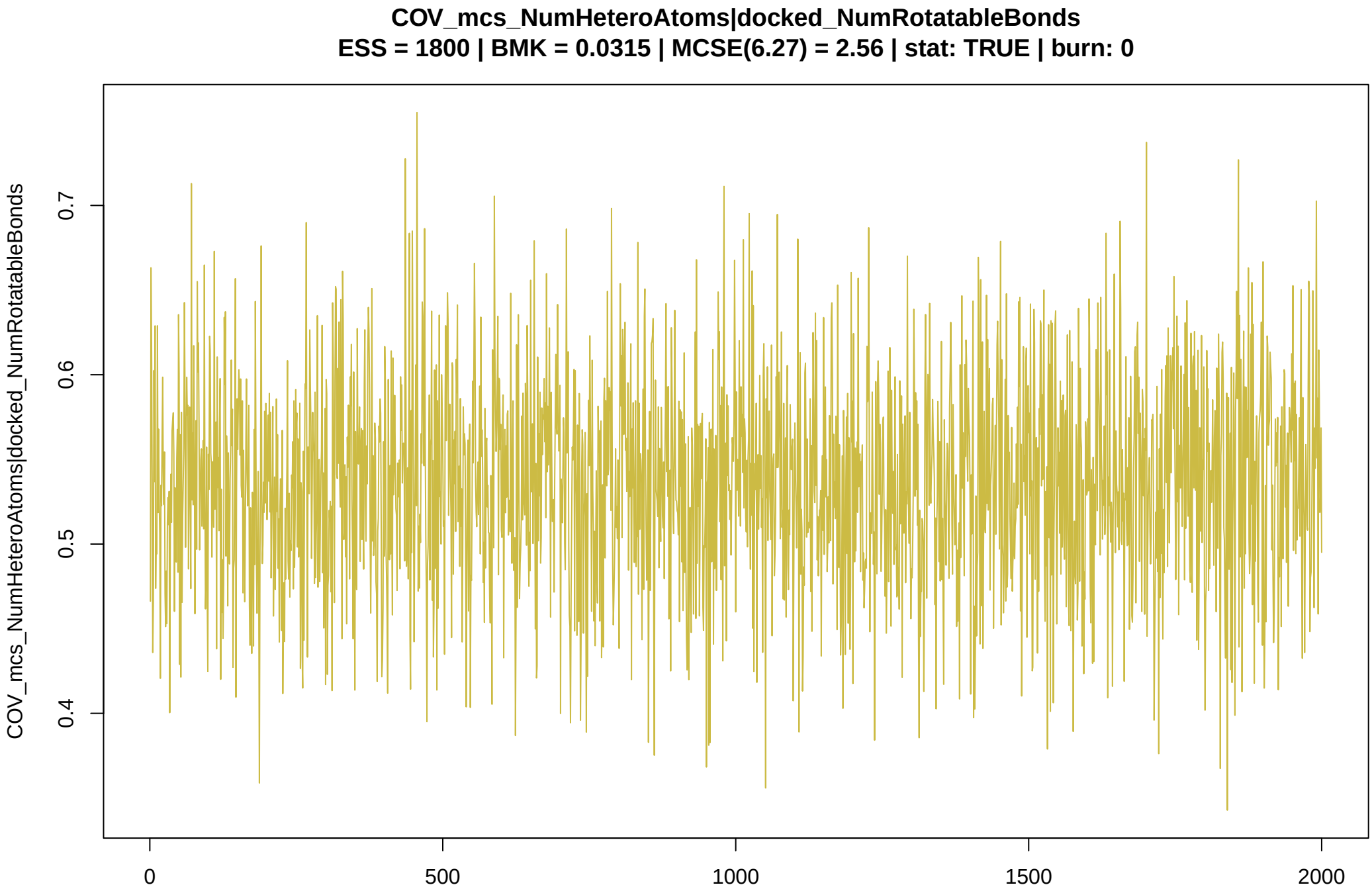

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1920 | BMK = 0.037 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
1.0
1.1
1.2
1.3
1.4
1.5
1.6
0
500
1000
1500
2000

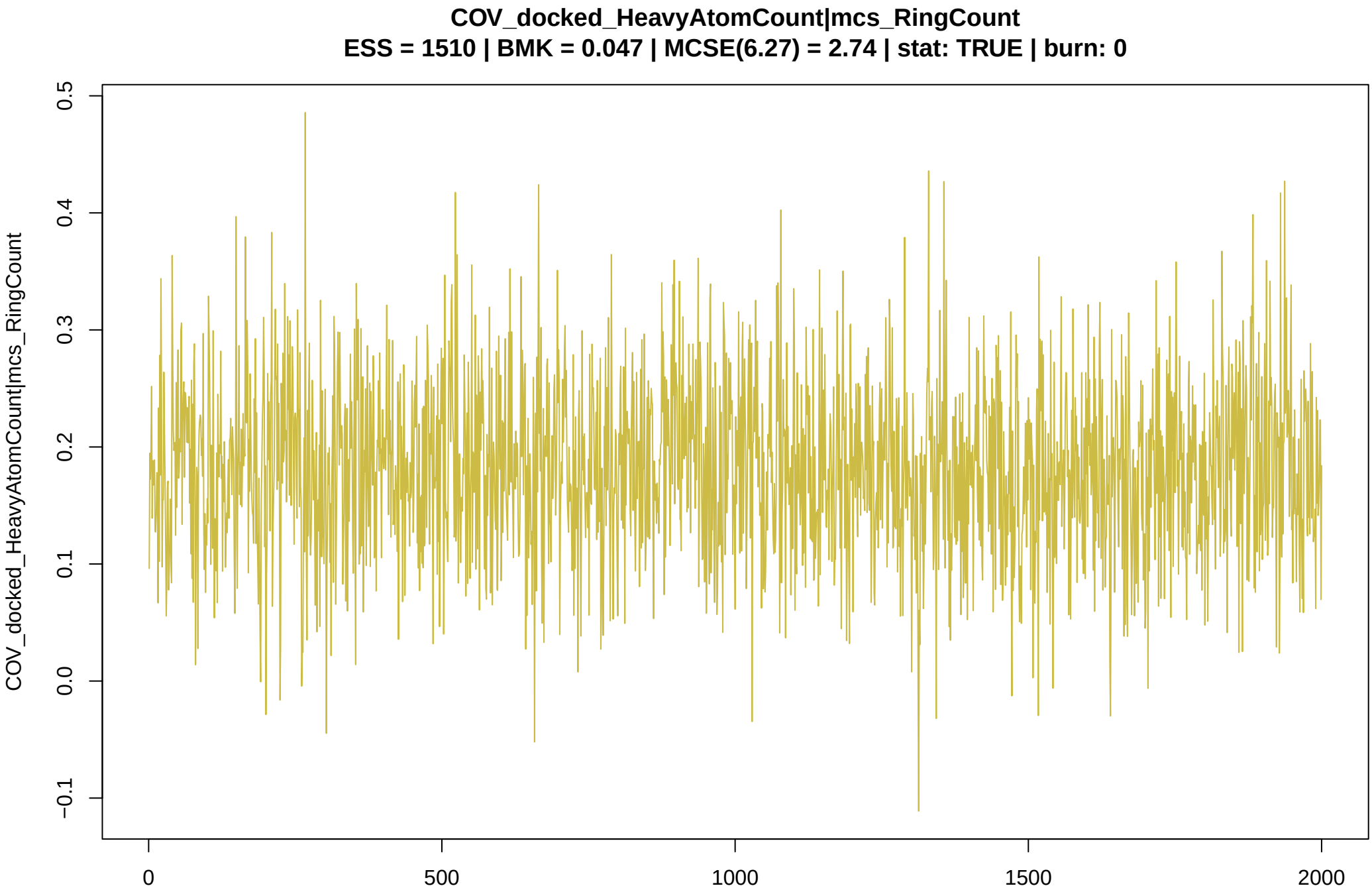

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1730 | BMK = 0.04 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.36
0.38
0.40
0.42
0.44
0.46
0
500
1000
1500
2000

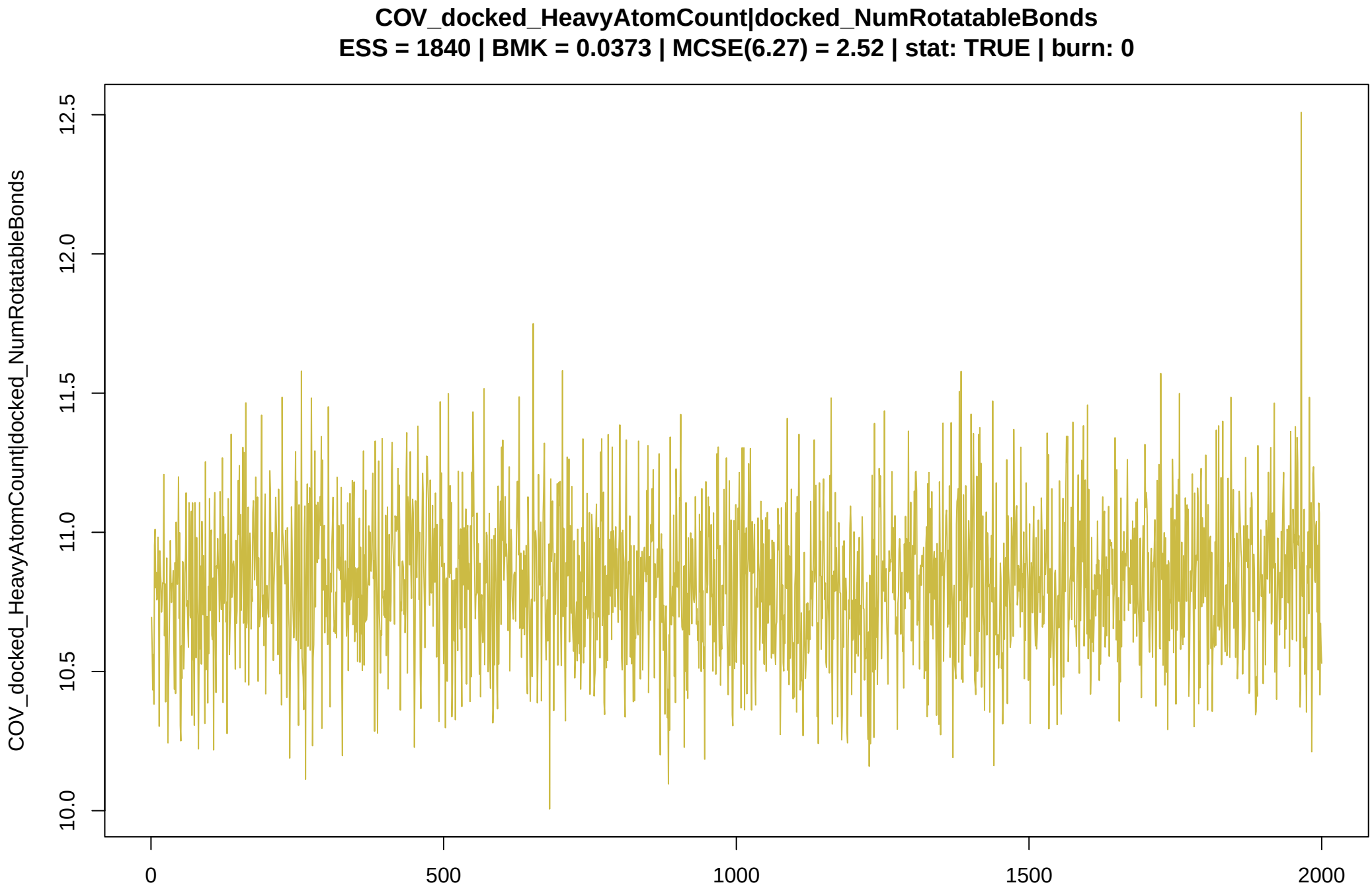

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1760 | BMK = 0.0459 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
0.40
0.45
0.50
0.55
0.60
0
500
1000
1500
2000

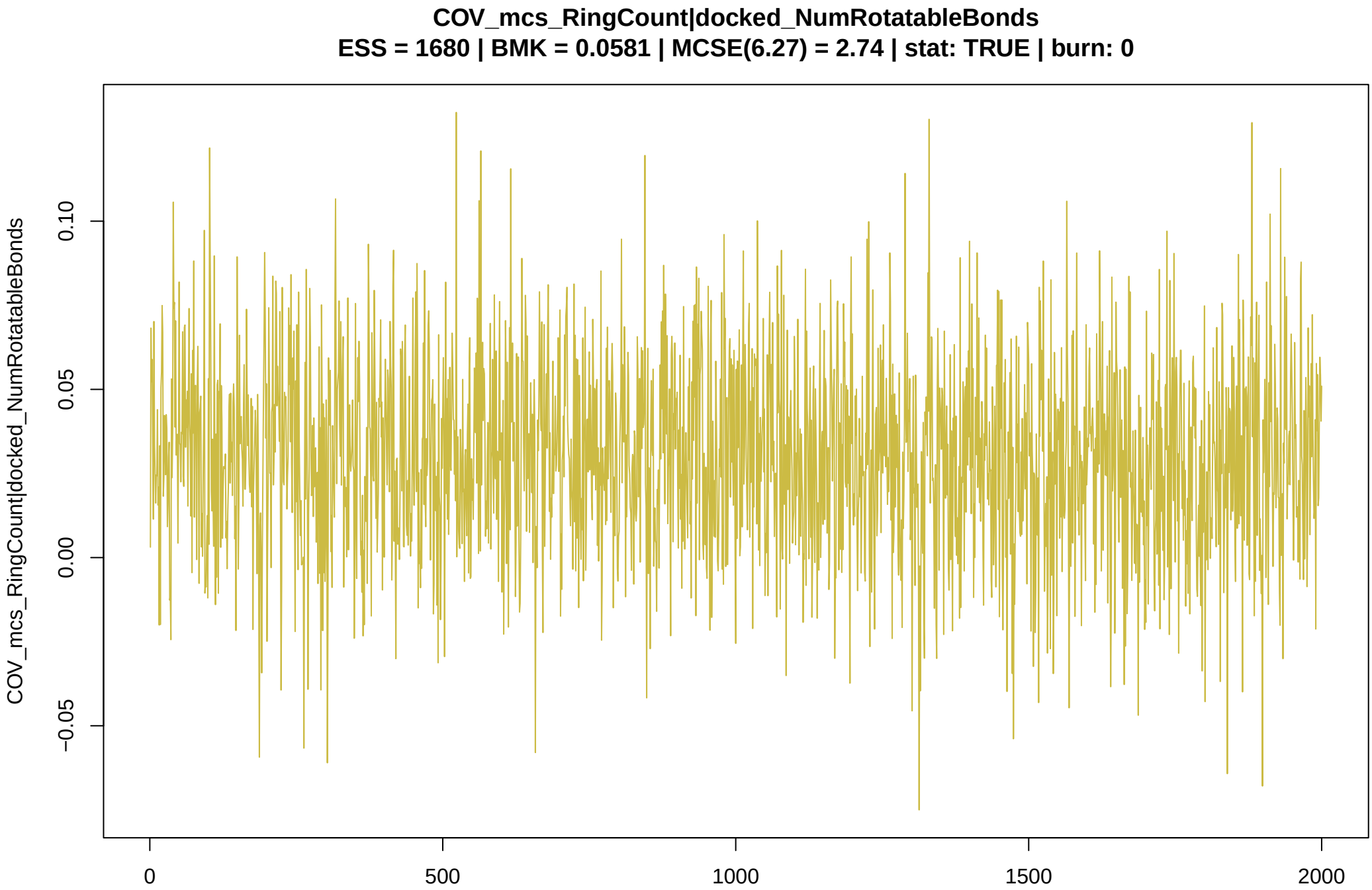

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1770 | BMK = 0.0437 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
1.2
1.4
1.6
1.8
2.0
2.2
2.4
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1630 | BMK = 0.0402 | MCSE(6.27) = 2.4 | stat: FALSE | burn: 0
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.60
0.65
0.70
0.75
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1800 | BMK = 0.0315 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
0.4
0.5
0.6
0.7
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1510 | BMK = 0.047 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.5
0.4
0.3
0.2
0.1
0.0
−0.1
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1840 | BMK = 0.0373 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10.0
10.5
11.0
11.5
12.0
12.5
0
500
1000
1500
2000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1680 | BMK = 0.0581 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0
COV_mcs_RingCount|docked_NumRotatableBonds
0.10
0.05
0.00
−0.05
0
500
1000
1500
2000