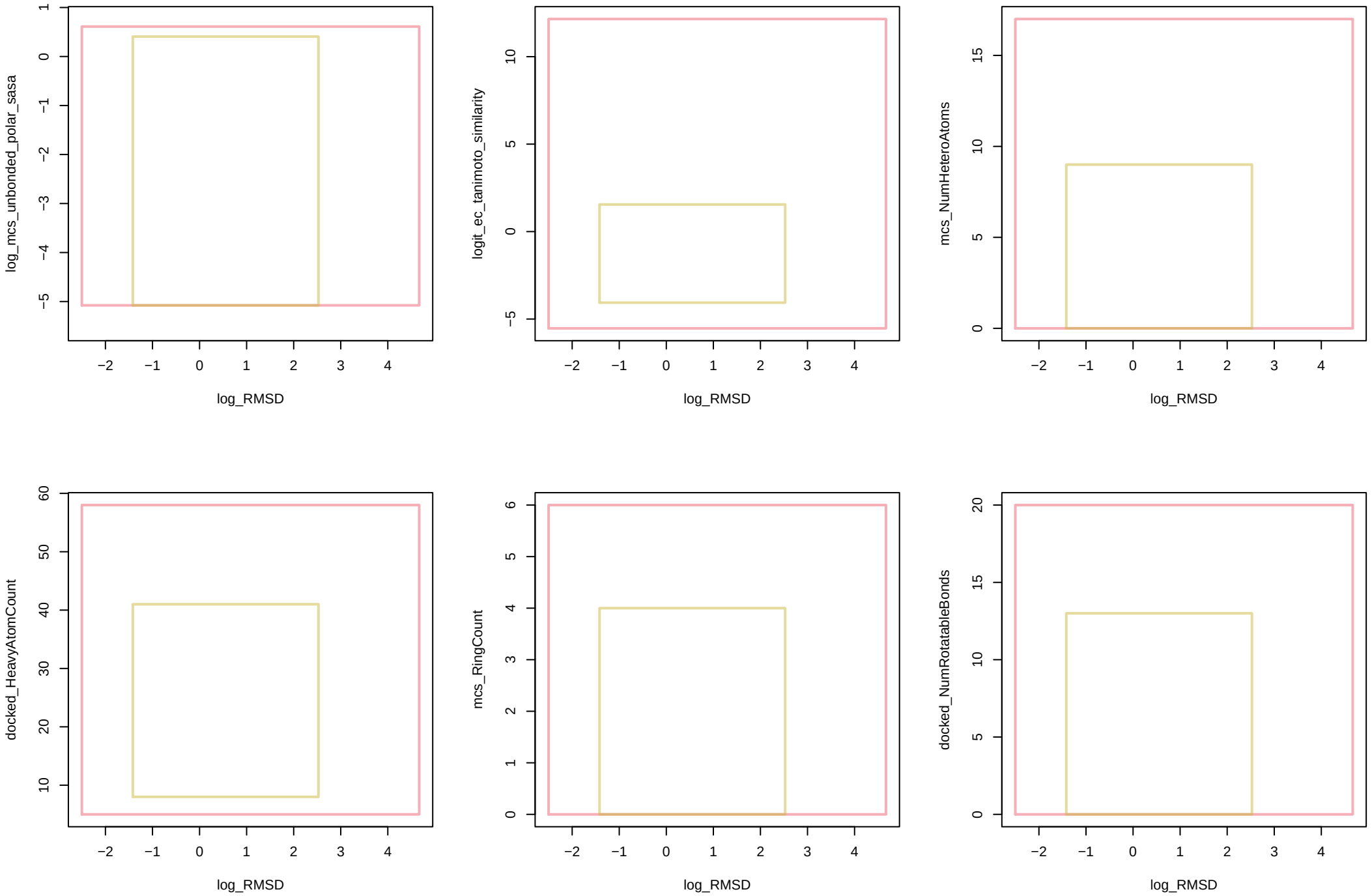
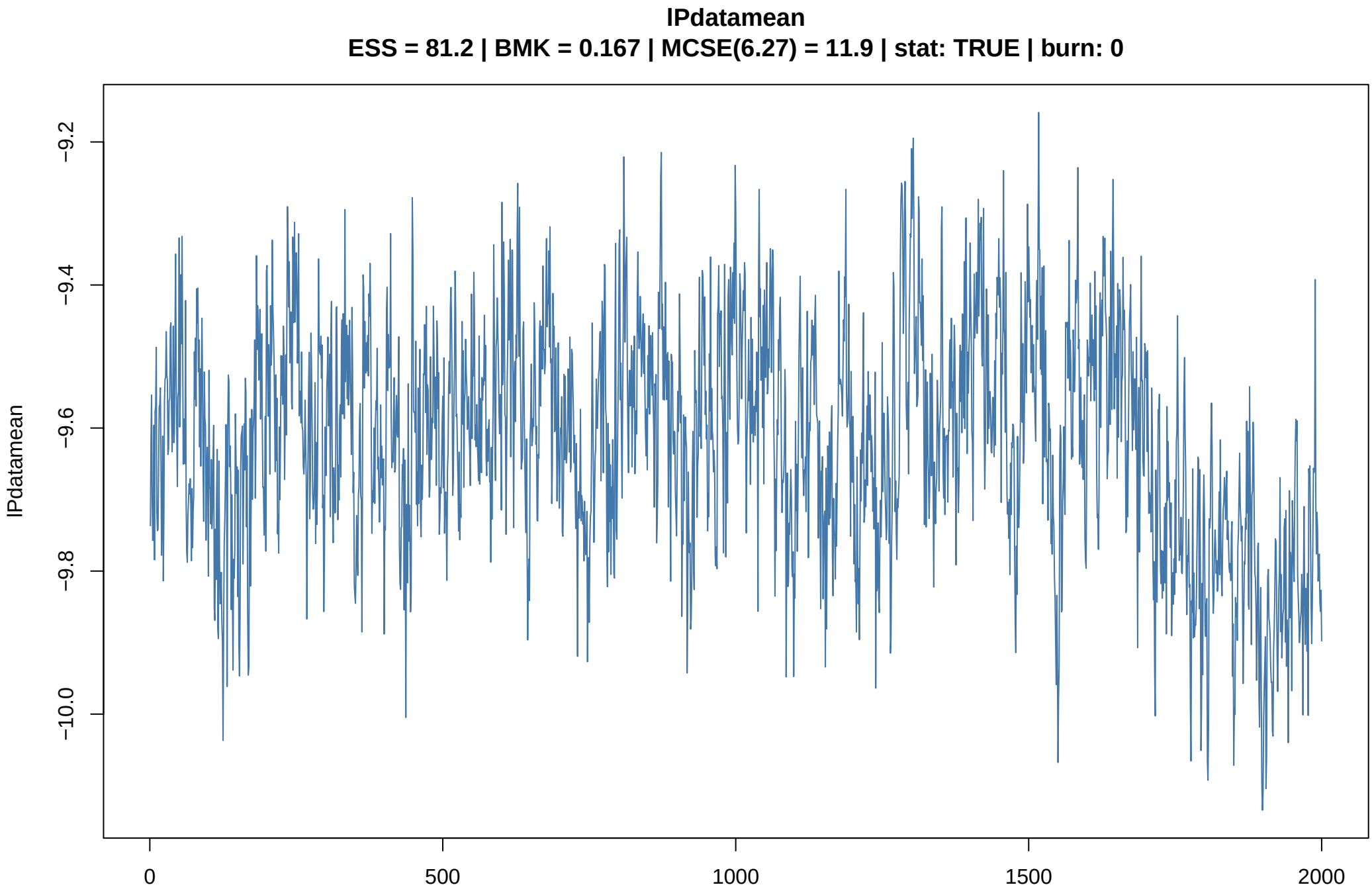
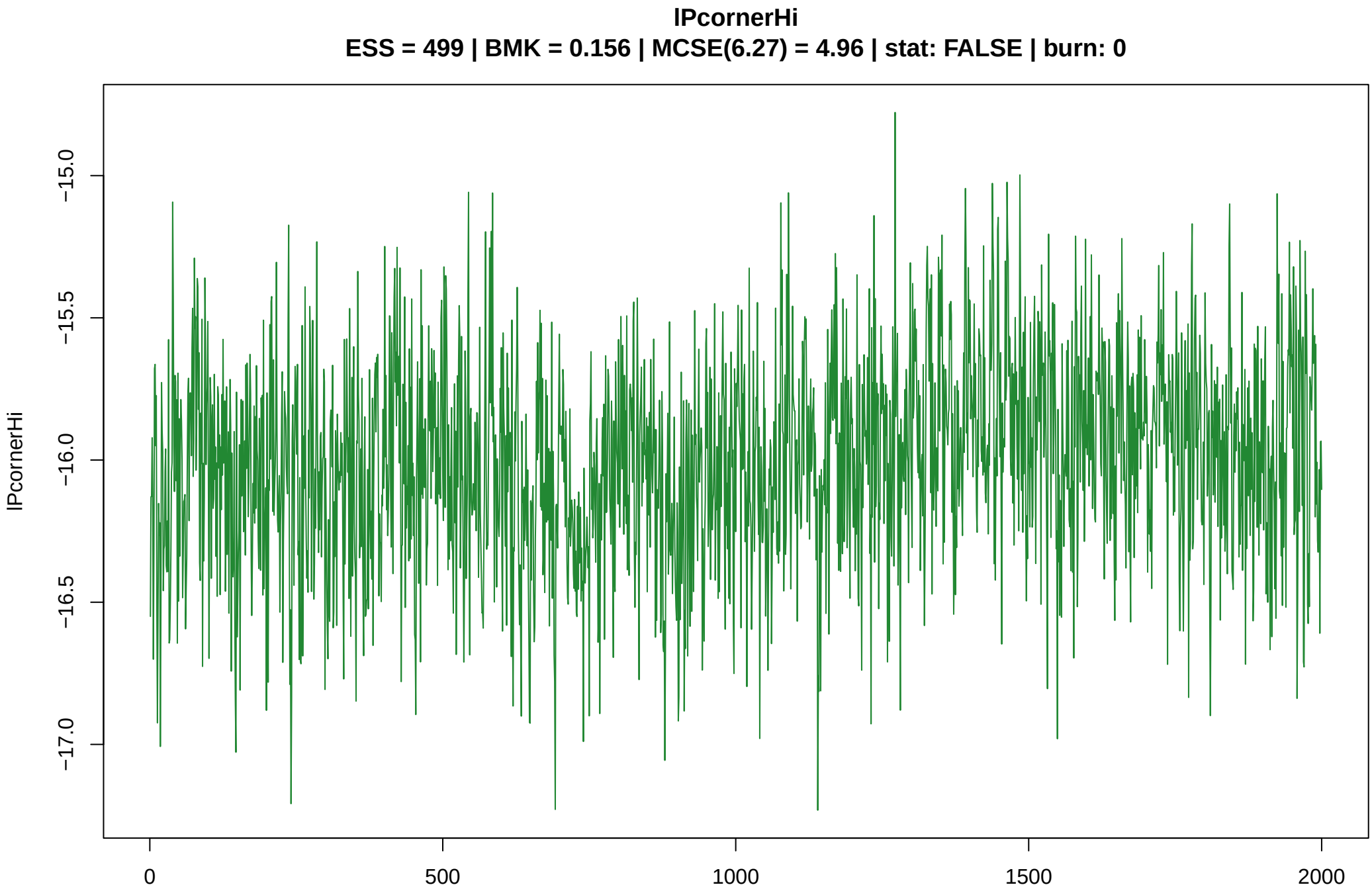
−− STATS maxD −−
min ESS = 81.1613267904487
max BMK = 0.174969685007296
max MCSE = 11.9232991242859
all stationary: FALSE
burn: 0

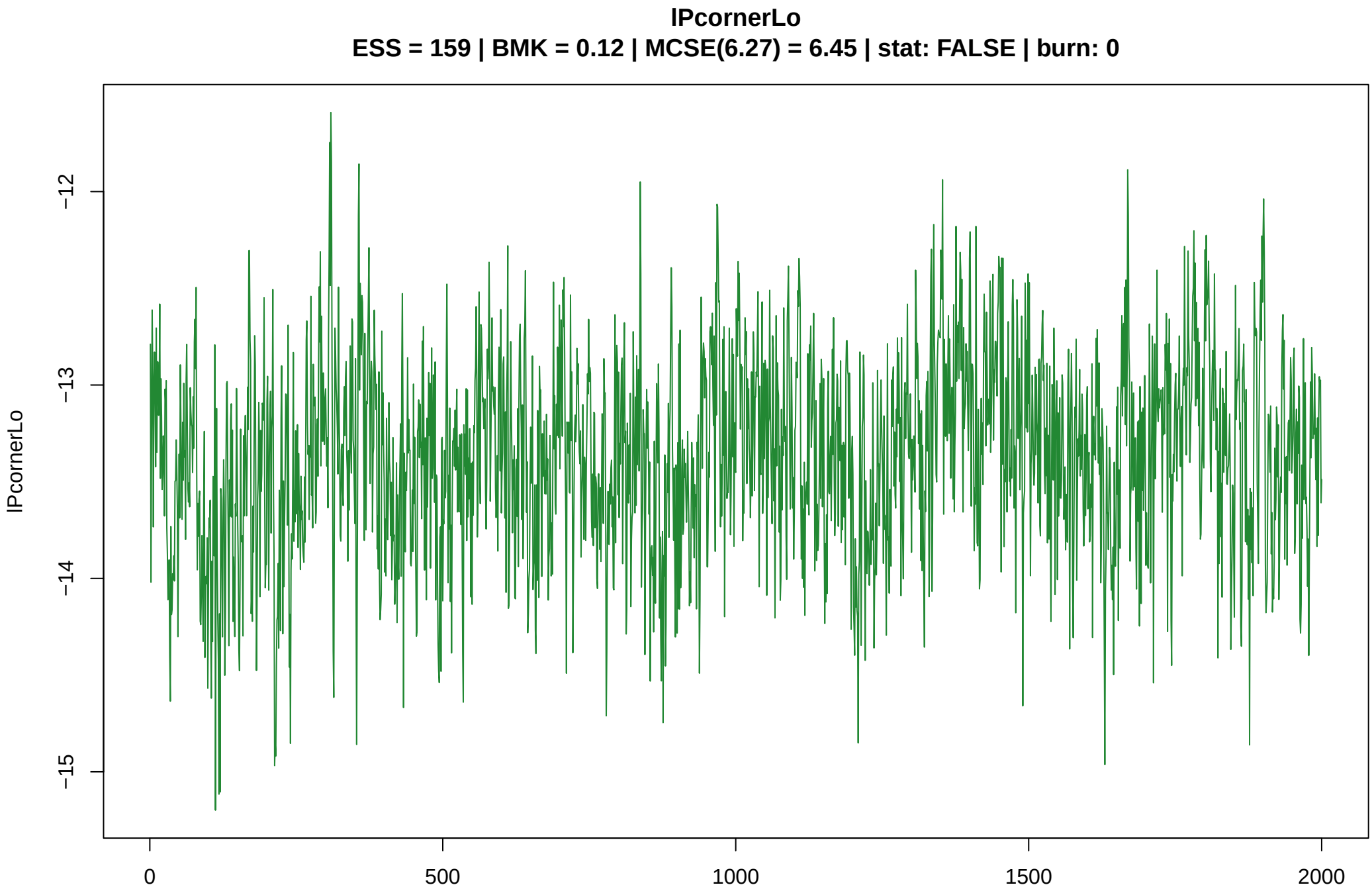
−− STATS 2D −−
min ESS = 1324.92419265124
max BMK = 0.085091206217596
max MCSE = 3.15739867470025
all stationary: FALSE
burn: 0

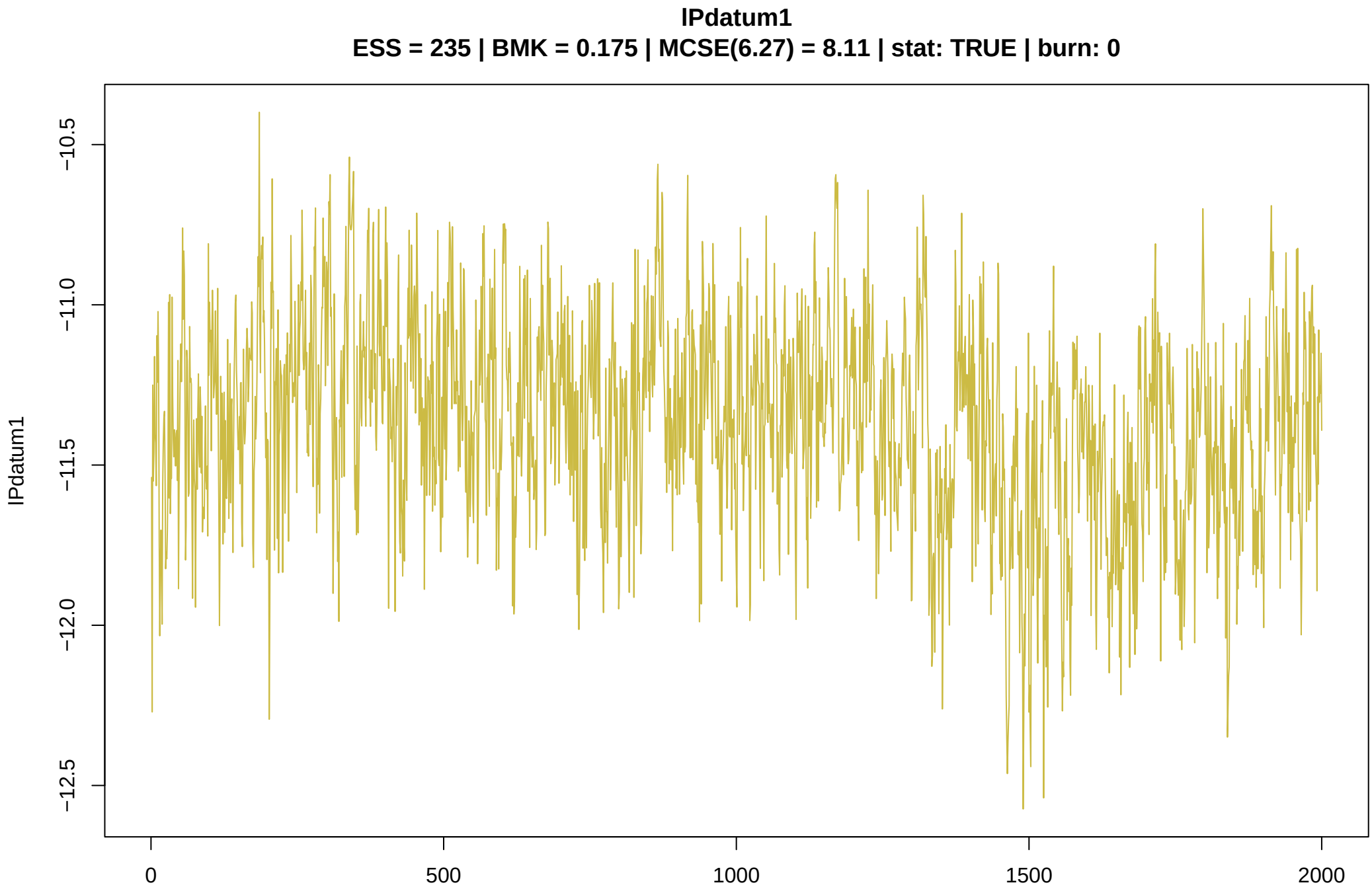
−− STATS 1D −−
min ESS = 562.549239297758
max BMK = 0.108479888629404
max MCSE = 2.98567298800275
all stationary: FALSE
burn: 0

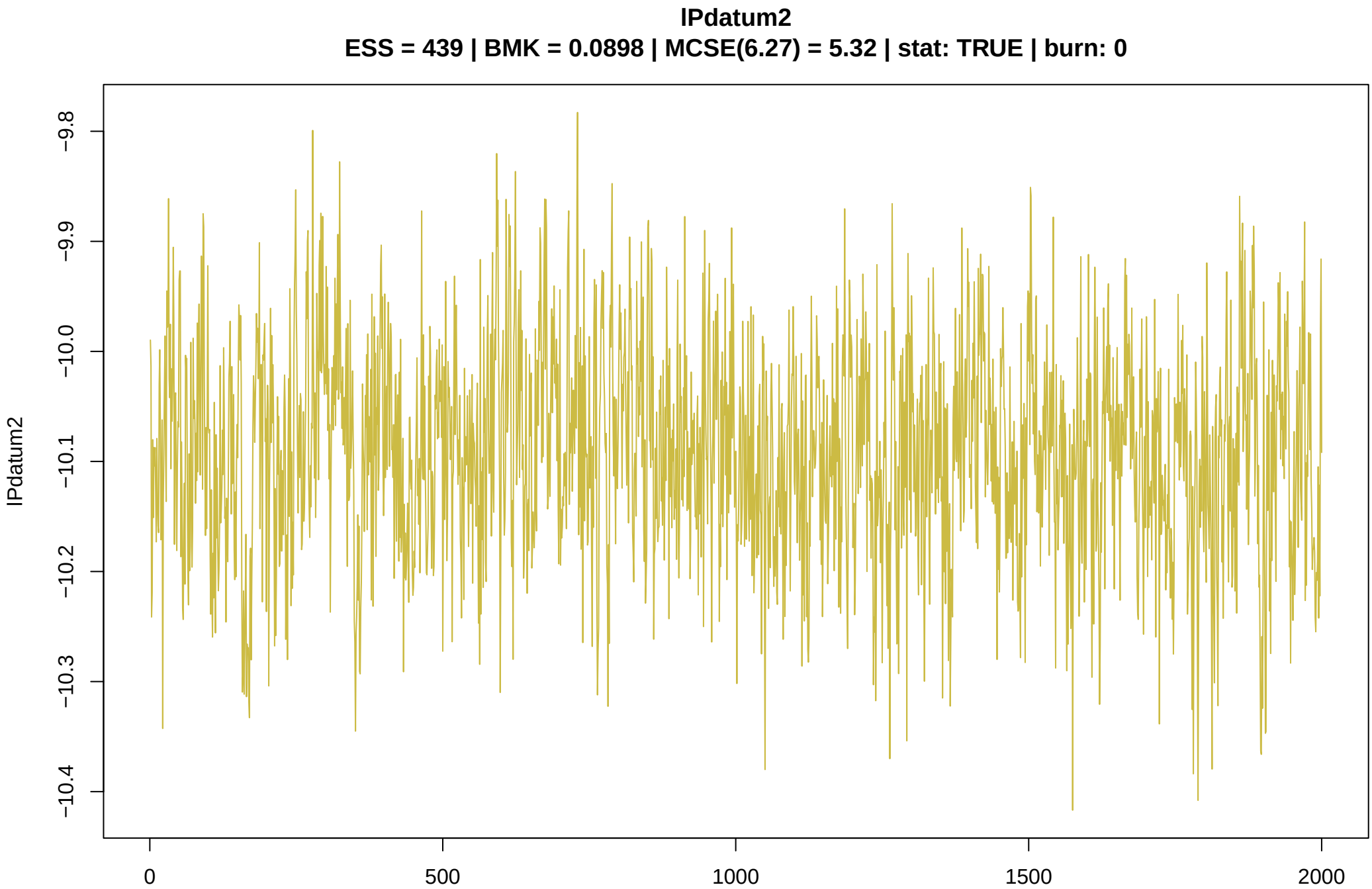

log_mcs_unbonded_polar_sasa
logit_ec_tanimoto_similarity
mcs_NumHeteroAtoms
docked_HeavyAtomCount
mcs_RingCount
docked_NumRotatableBonds
log_RMSD

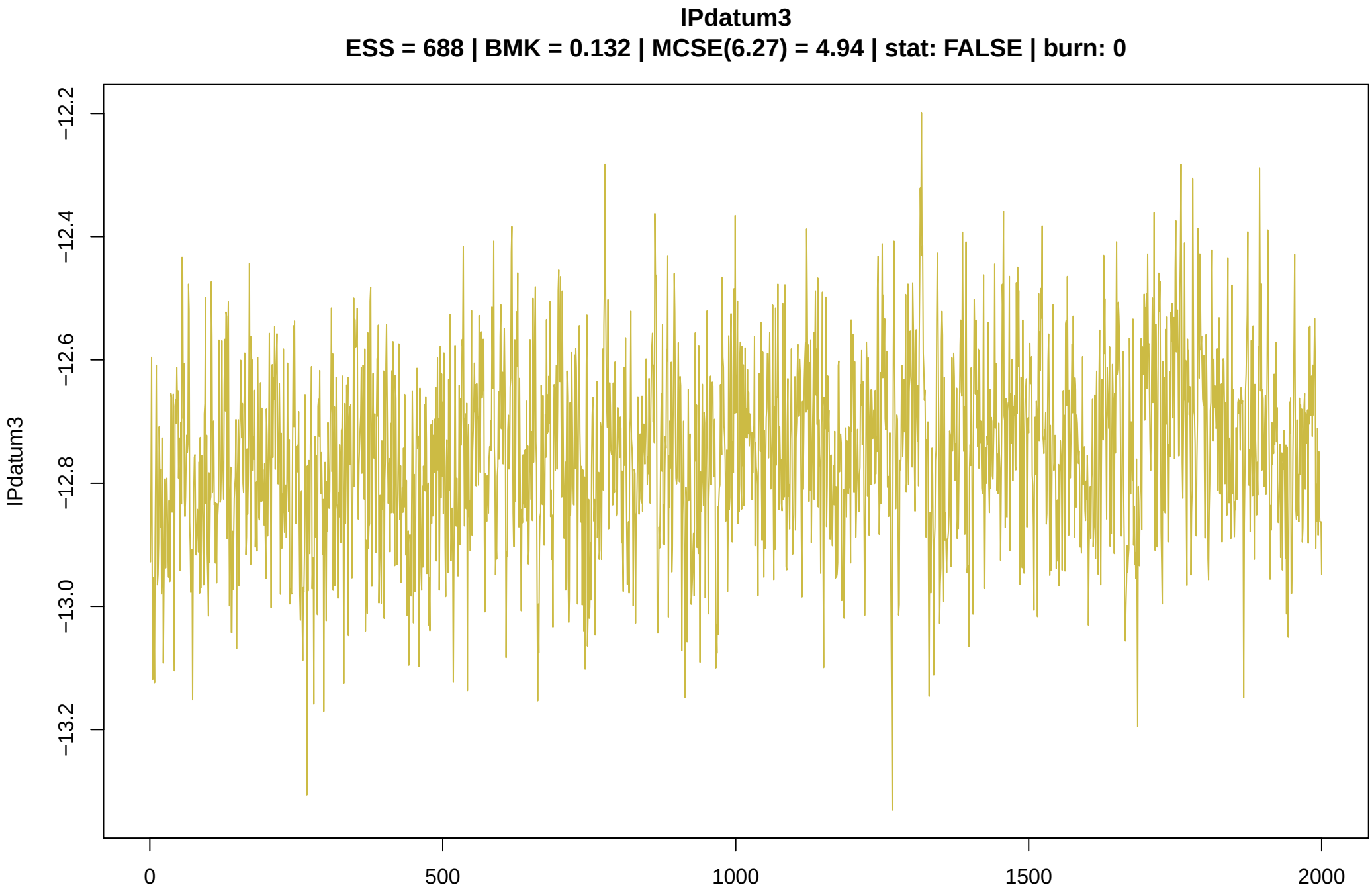

lPdatamean
ESS = 81.2 | BMK = 0.167 | MCSE(6.27) = 11.9 | stat: TRUE | burn: 0
lPdatamean
−9.2
−9.4
−9.6
−9.8
−10.0
0
500
1000
1500
2000

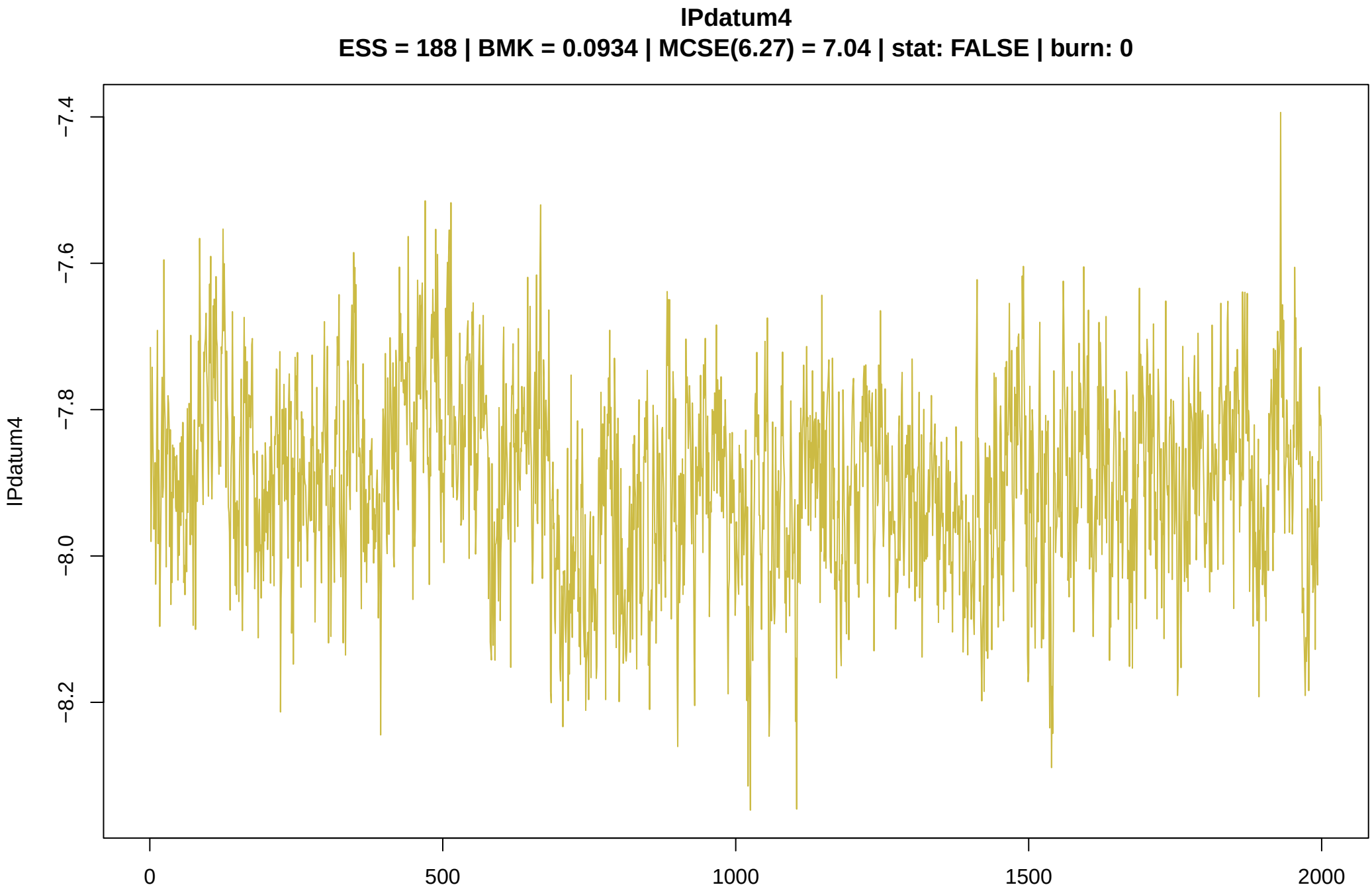

lPcornerHi
ESS = 499 | BMK = 0.156 | MCSE(6.27) = 4.96 | stat: FALSE | burn: 0
lPcornerHi
−15.0
−15.5
−16.0
−16.5
−17.0
0
500
1000
1500
2000

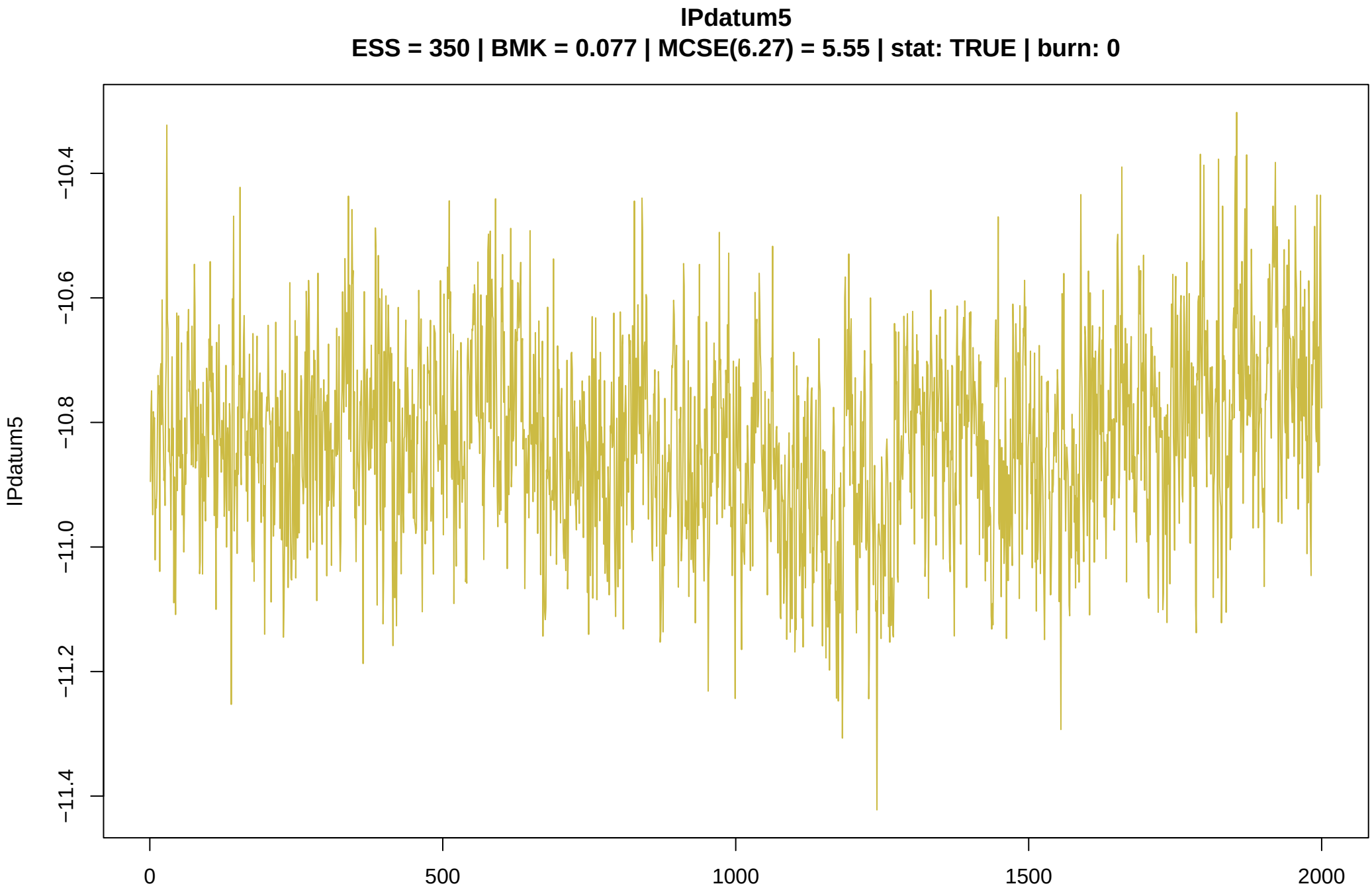

lPcornerLo
ESS = 159 | BMK = 0.12 | MCSE(6.27) = 6.45 | stat: FALSE | burn: 0
lPcornerLo
−12
−13
−14
−15
0
500
1000
1500
2000

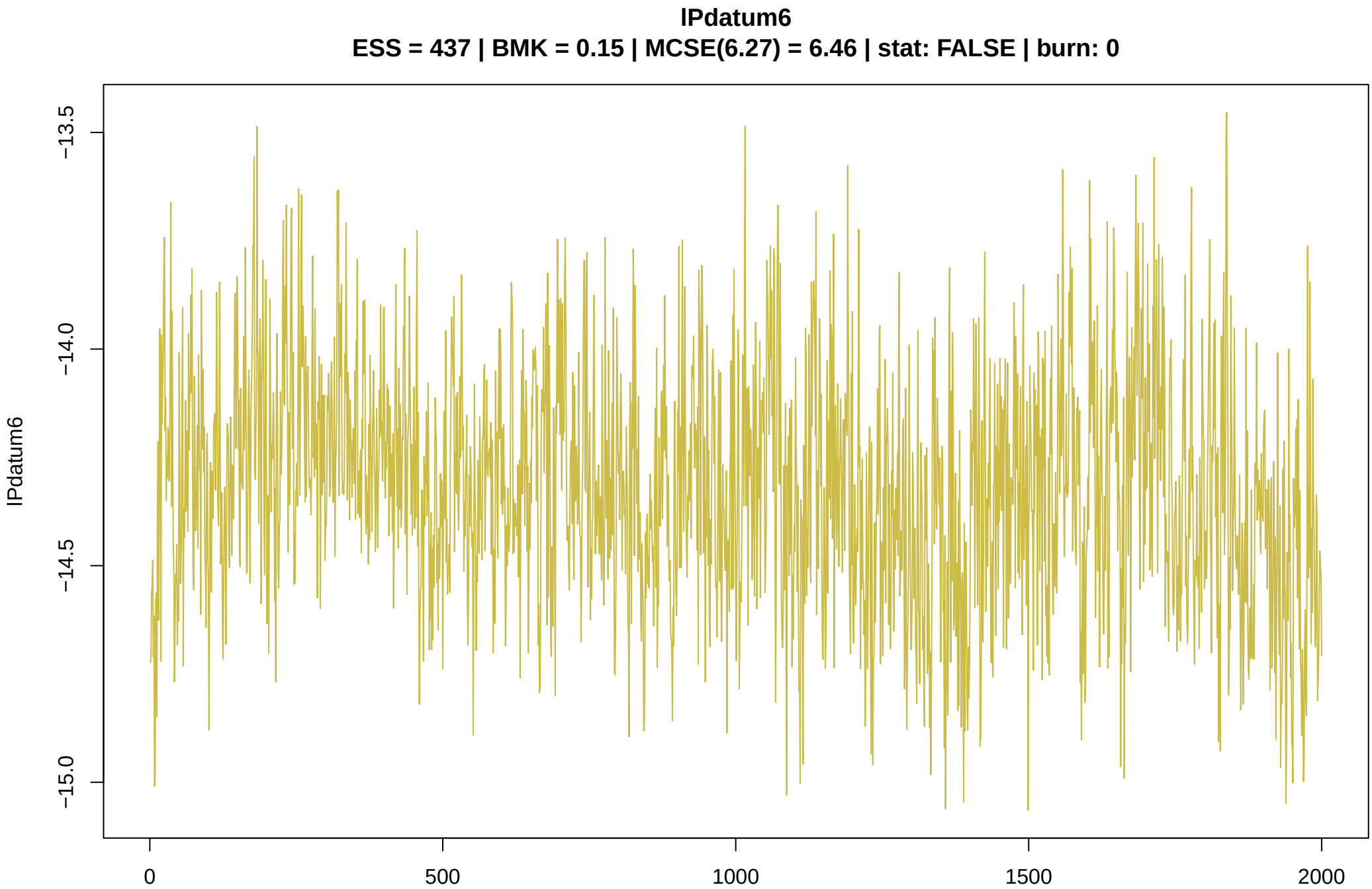

lPdatum1
ESS = 235 | BMK = 0.175 | MCSE(6.27) = 8.11 | stat: TRUE | burn: 0
lPdatum1
−10.5
−11.0
−11.5
−12.0
−12.5
0
500
1000
1500
2000

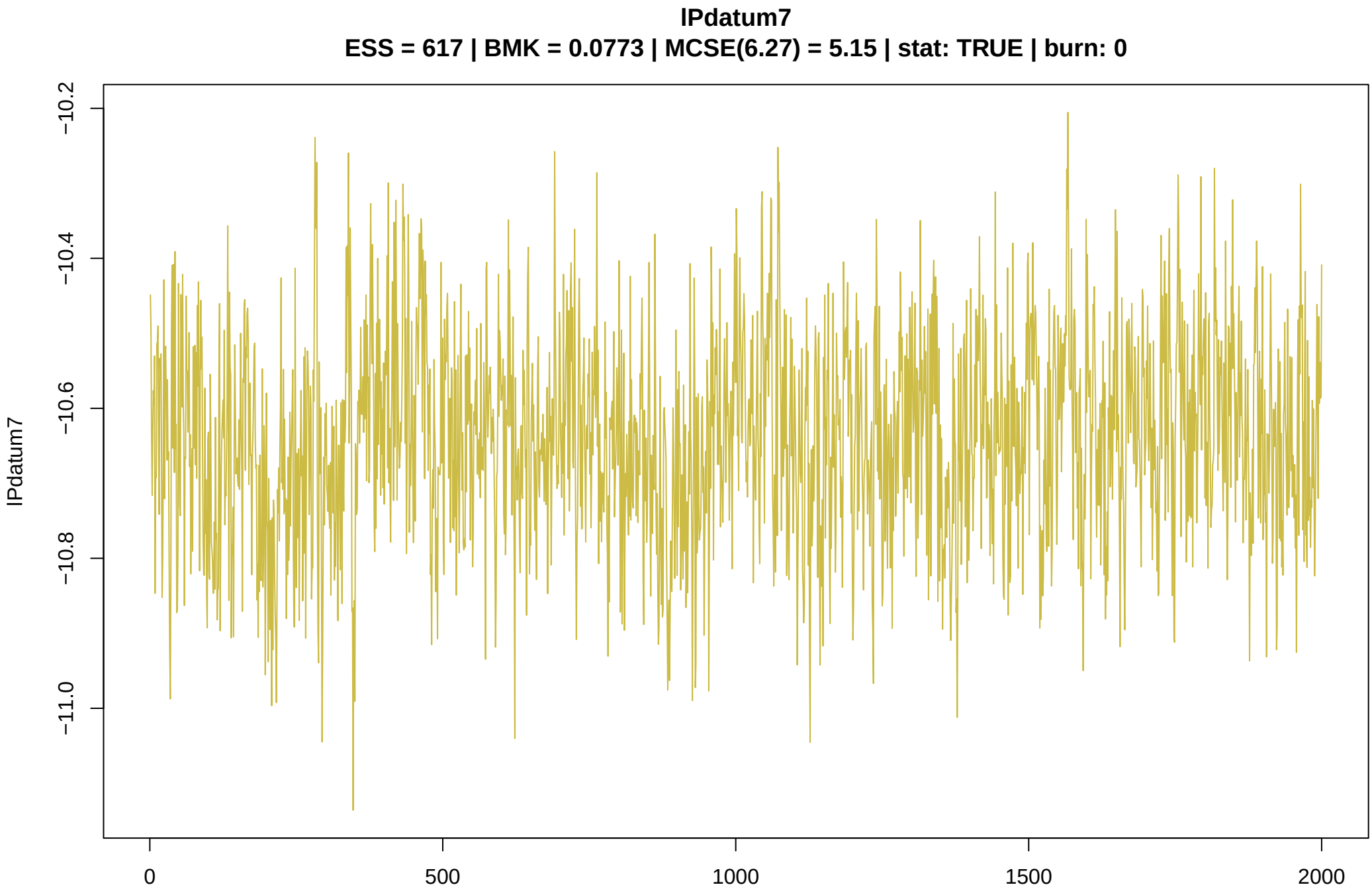

lPdatum2
ESS = 439 | BMK = 0.0898 | MCSE(6.27) = 5.32 | stat: TRUE | burn: 0
lPdatum2
−9.8
−9.9
−10.0
−10.1
−10.2
−10.3
−10.4
0
500
1000
1500
2000

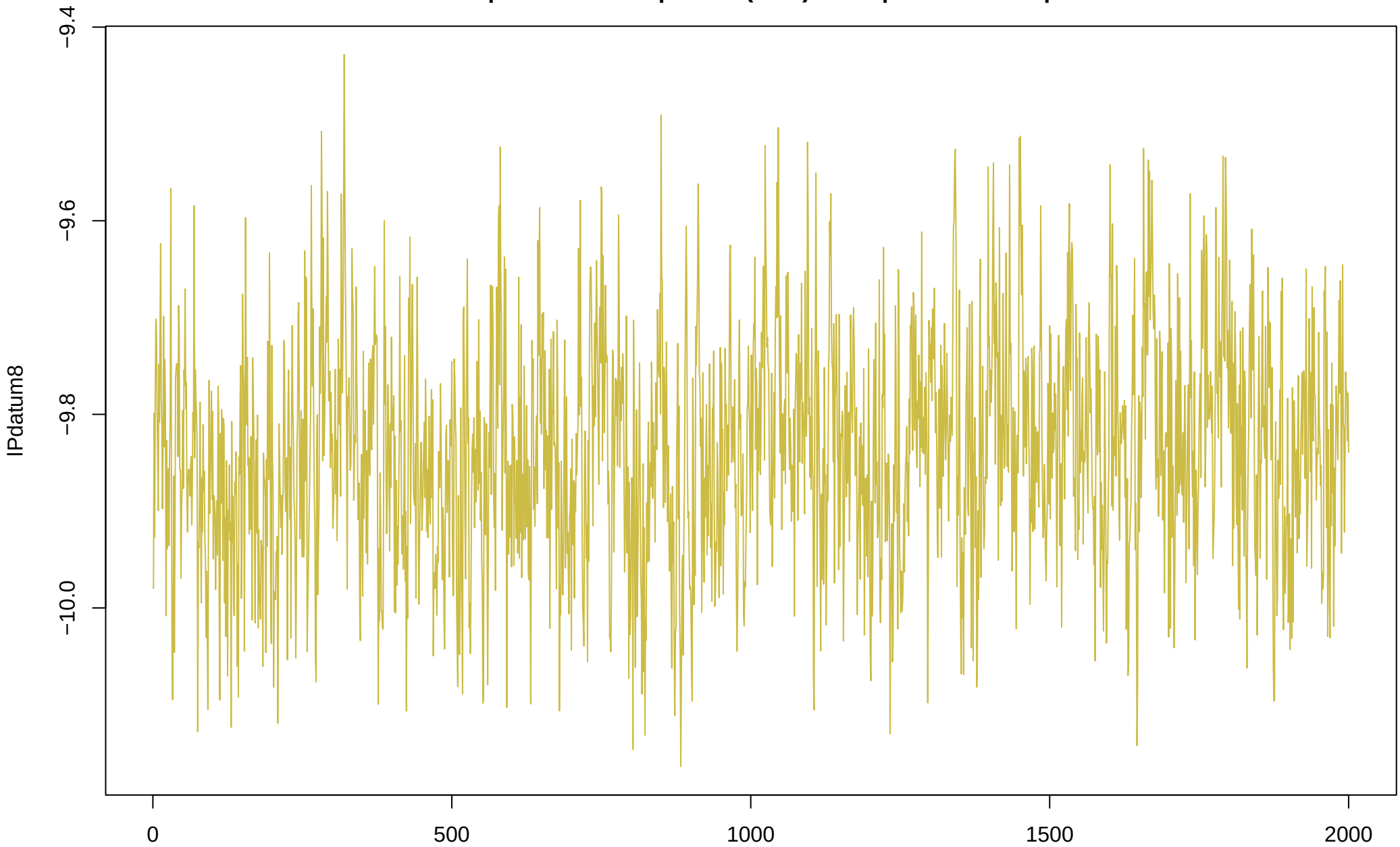

lPdatum3
ESS = 688 | BMK = 0.132 | MCSE(6.27) = 4.94 | stat: FALSE | burn: 0
lPdatum3
−12.2
−12.4
−12.6
−12.8
−13.0
−13.2
0
500
1000
1500
2000

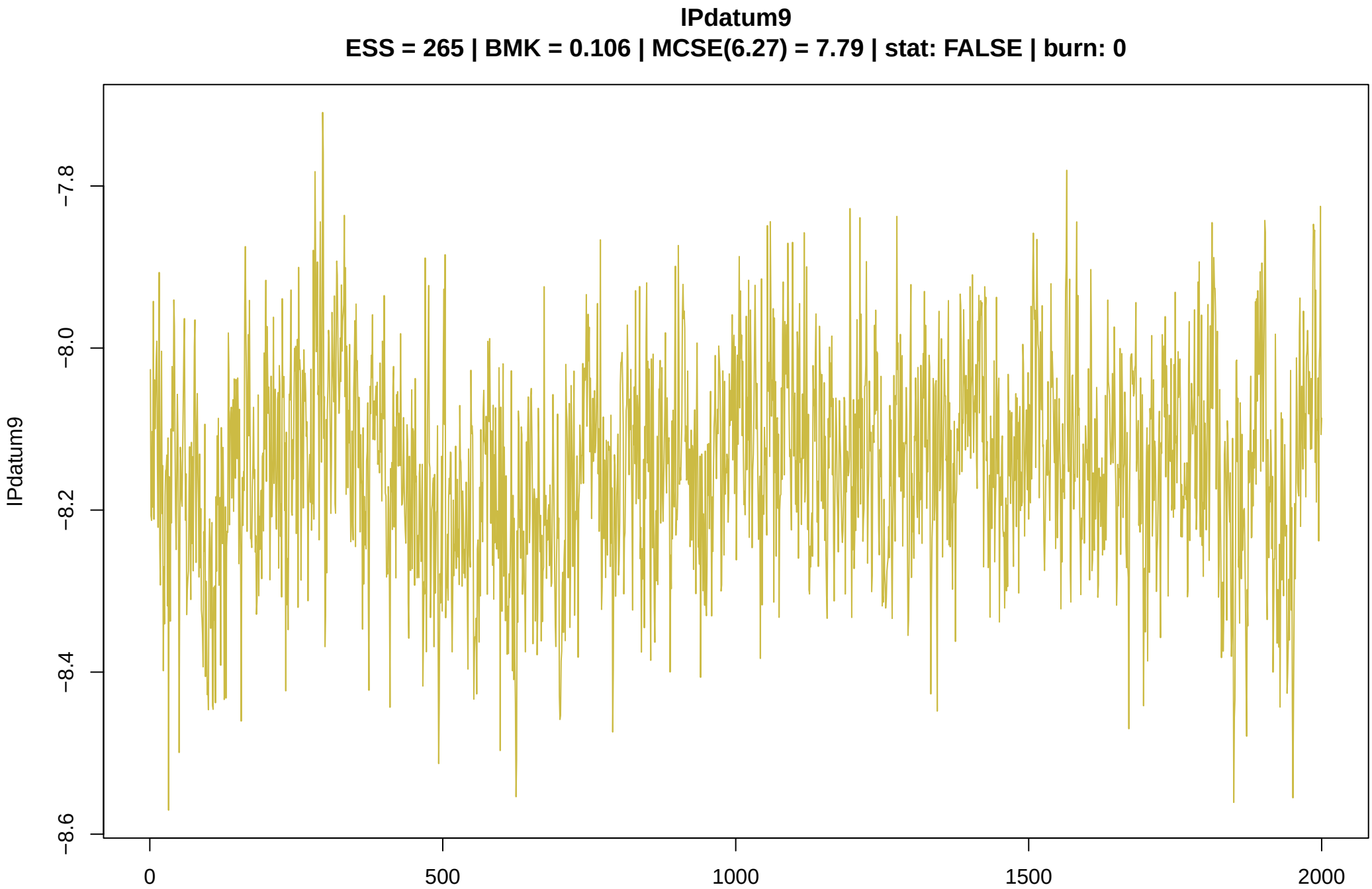

lPdatum4
ESS = 188 | BMK = 0.0934 | MCSE(6.27) = 7.04 | stat: FALSE | burn: 0
lPdatum4
−7.4
−7.6
−7.8
−8.0
−8.2
0
500
1000
1500
2000

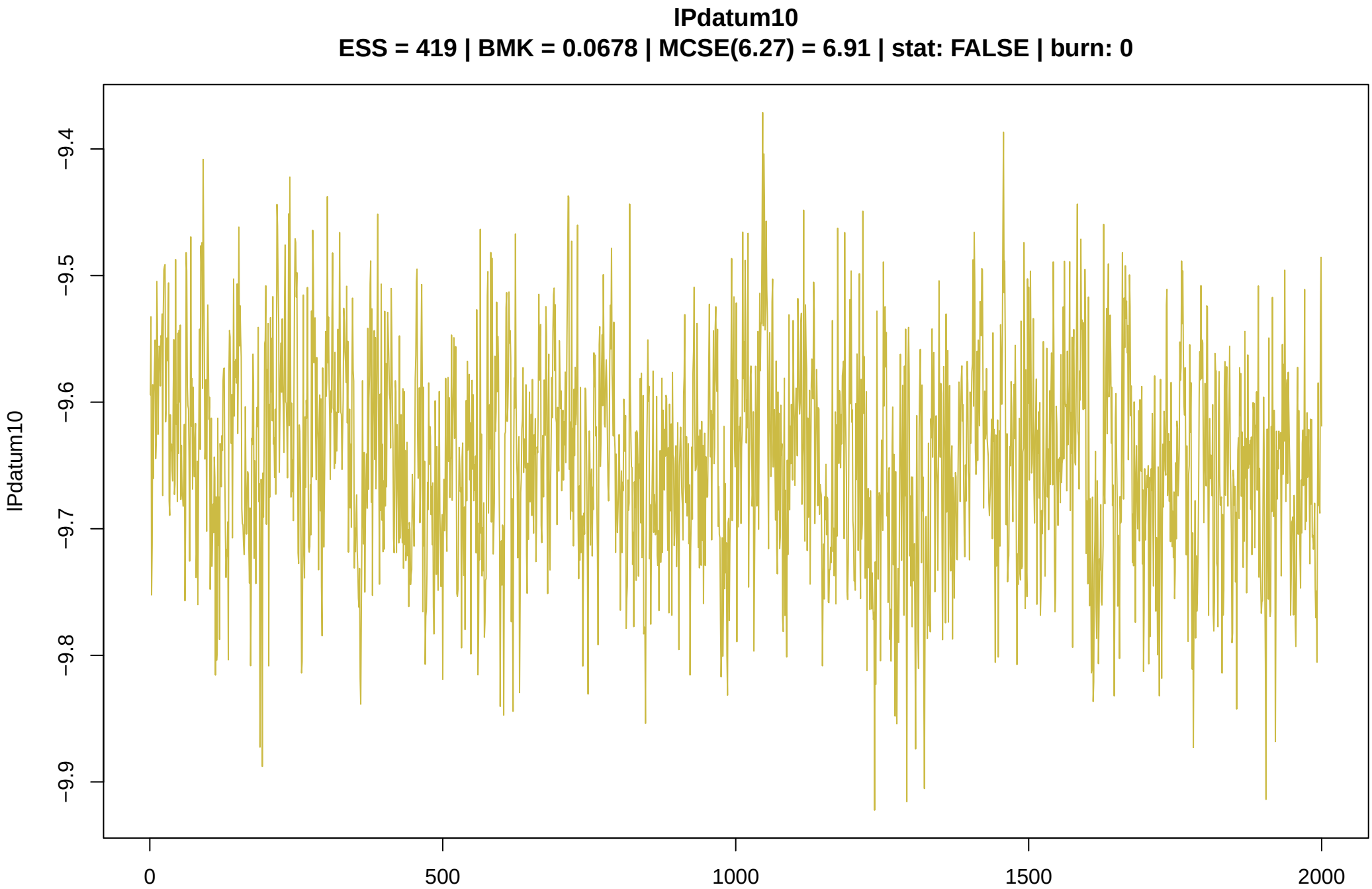

lPdatum5
ESS = 350 | BMK = 0.077 | MCSE(6.27) = 5.55 | stat: TRUE | burn: 0
lPdatum5
−10.4
−10.6
−10.8
−11.0
−11.2
−11.4
0
500
1000
1500
2000

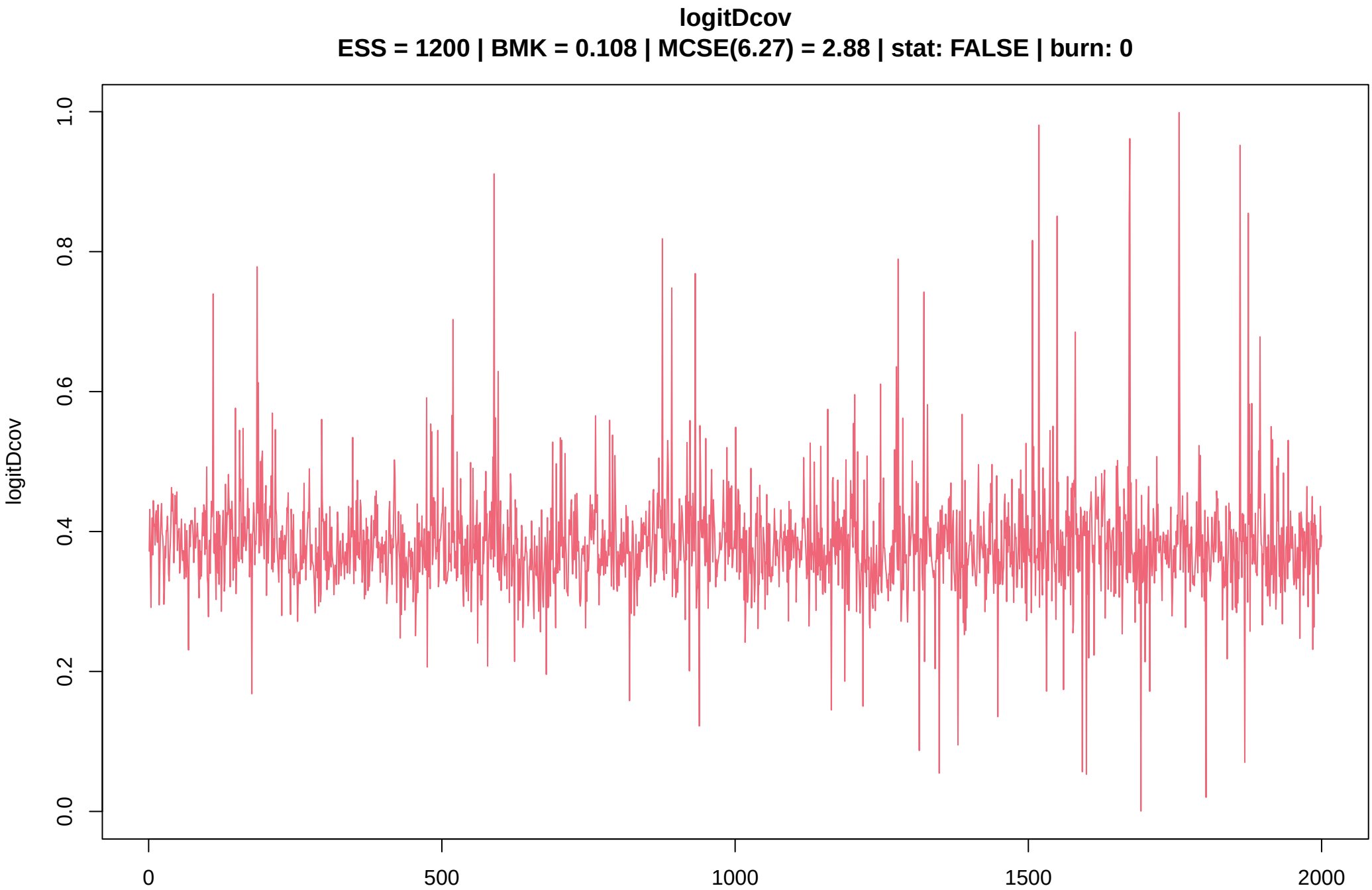

lPdatum6
ESS = 437 | BMK = 0.15 | MCSE(6.27) = 6.46 | stat: FALSE | burn: 0
lPdatum6
−13.5
−14.0
−14.5
−15.0
0
500
1000
1500
2000

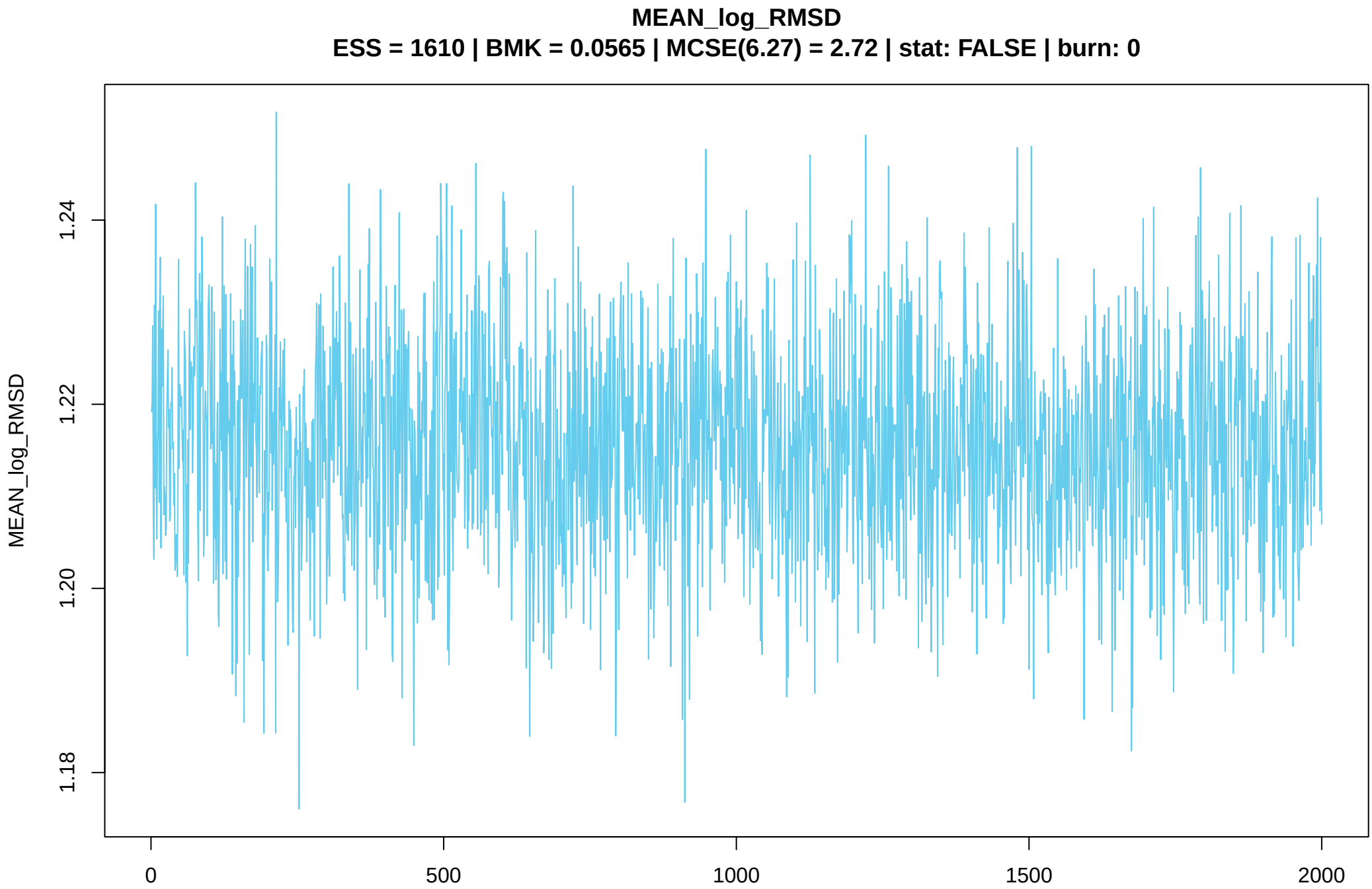

lPdatum7
ESS = 617 | BMK = 0.0773 | MCSE(6.27) = 5.15 | stat: TRUE | burn: 0
lPdatum7
−10.2
−10.4
−10.6
−10.8
−11.0
0
500
1000
1500
2000

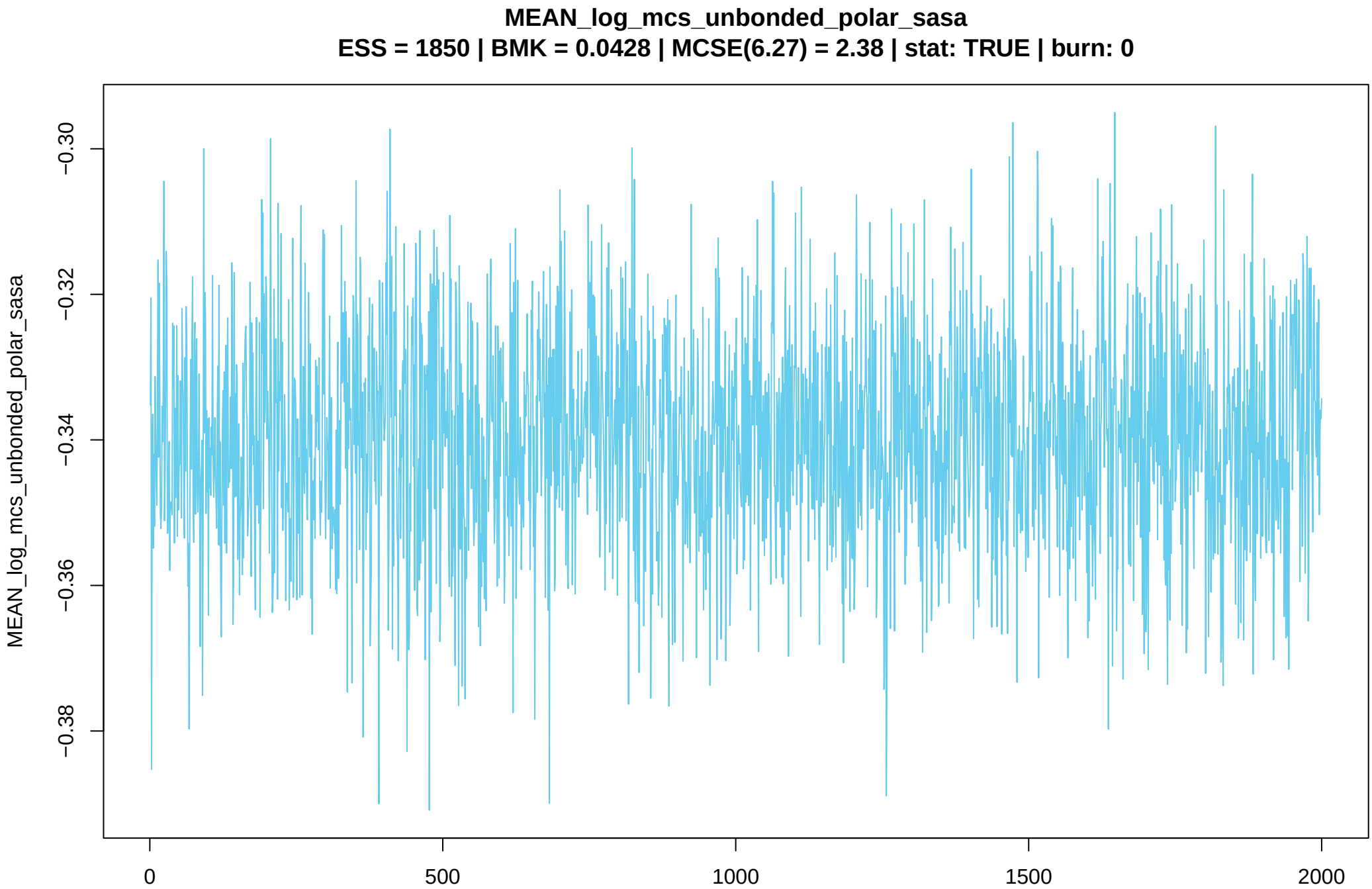

lPdatum8
ESS = 428 | BMK = 0.117 | MCSE(6.27) = 6.3 | stat: FALSE | burn: 0
lPdatum8
−9.4
−9.6
−9.8
−10.0
0
500
1000
1500
2000

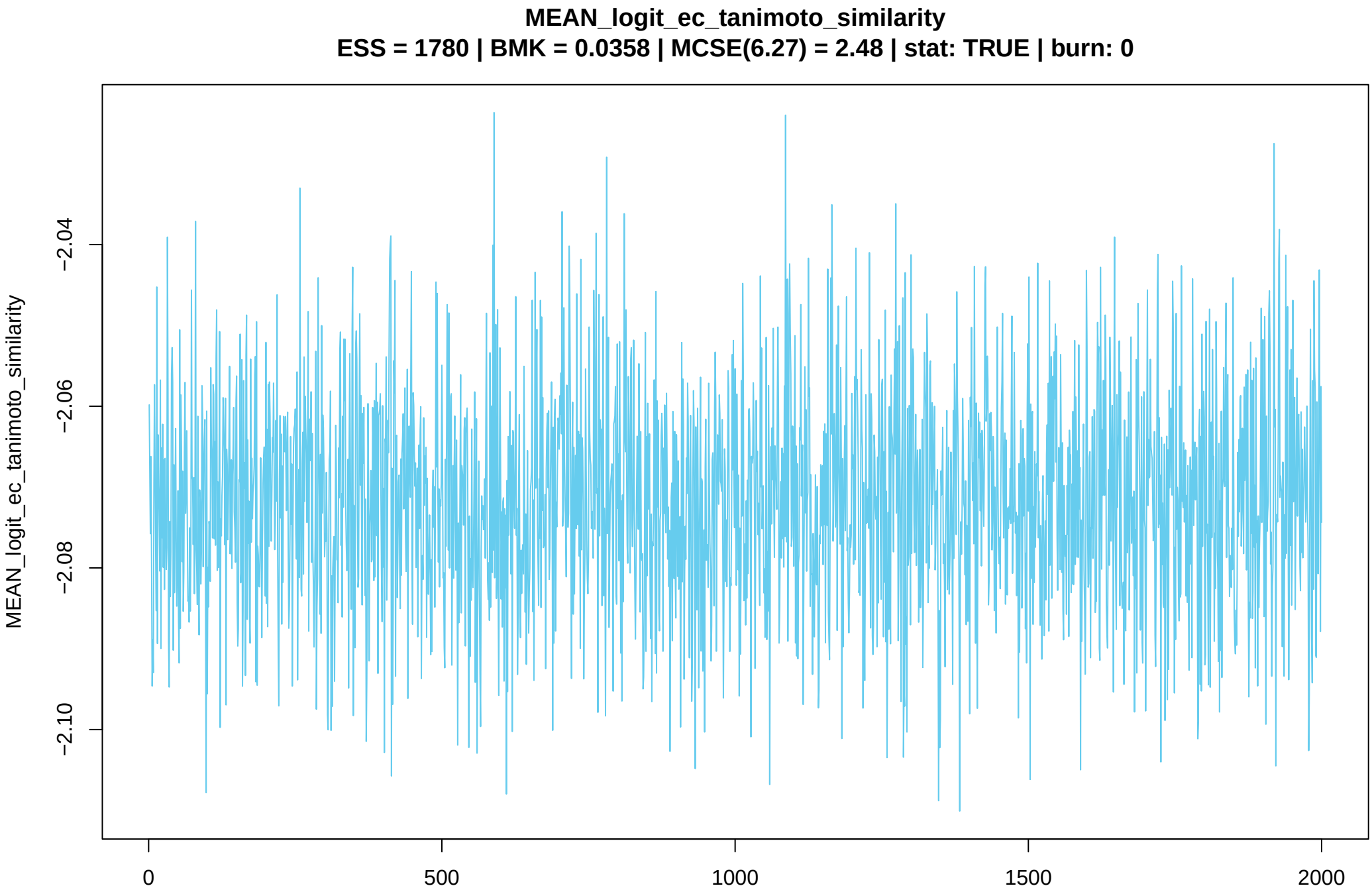

lPdatum9
ESS = 265 | BMK = 0.106 | MCSE(6.27) = 7.79 | stat: FALSE | burn: 0
lPdatum9
−7.8
−8.0
−8.2
−8.4
−8.6
0
500
1000
1500
2000

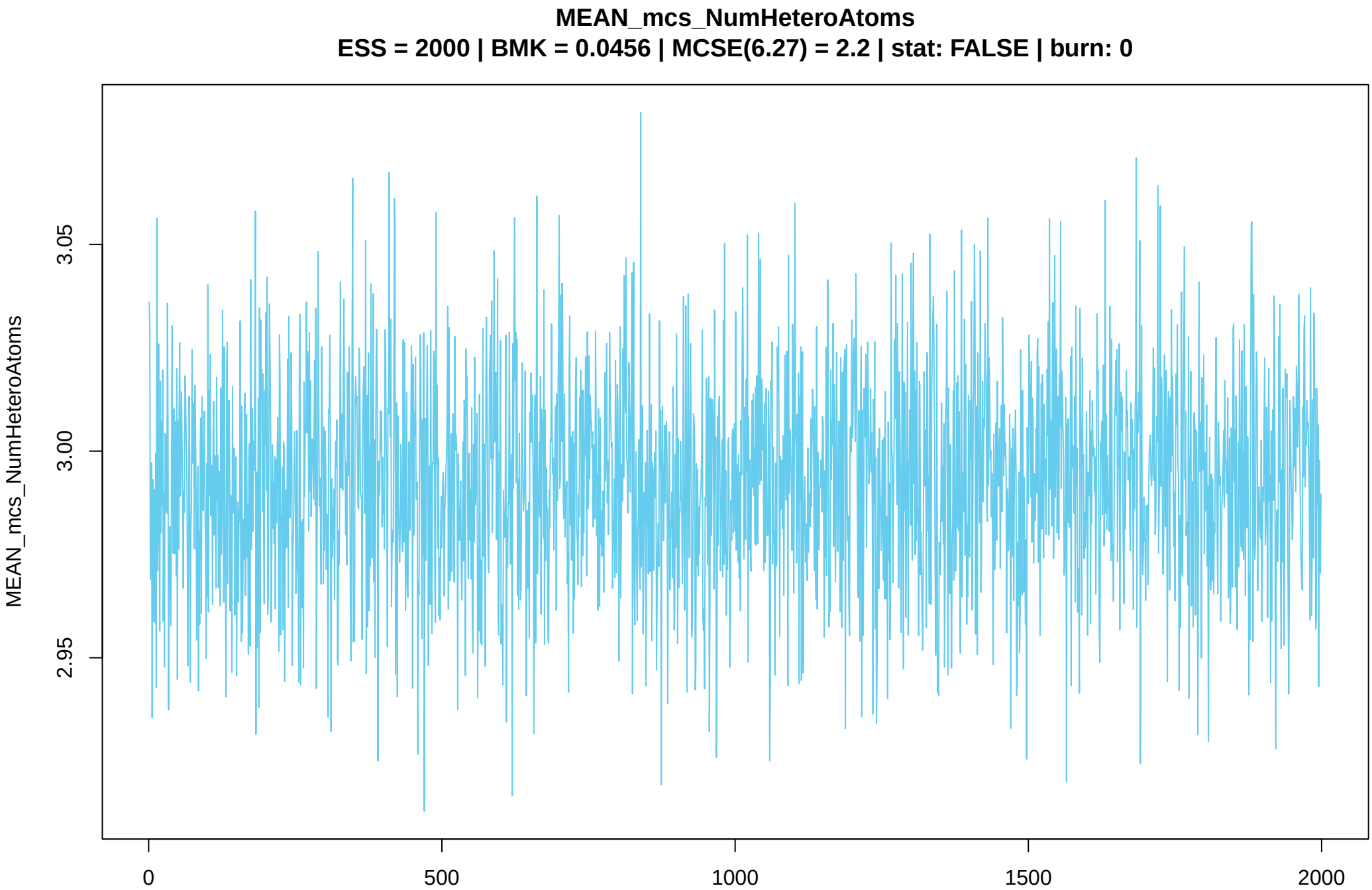

lPdatum10
ESS = 419 | BMK = 0.0678 | MCSE(6.27) = 6.91 | stat: FALSE | burn: 0
lPdatum10
−9.4
−9.5
−9.6
−9.7
−9.8
−9.9
0
500
1000
1500
2000

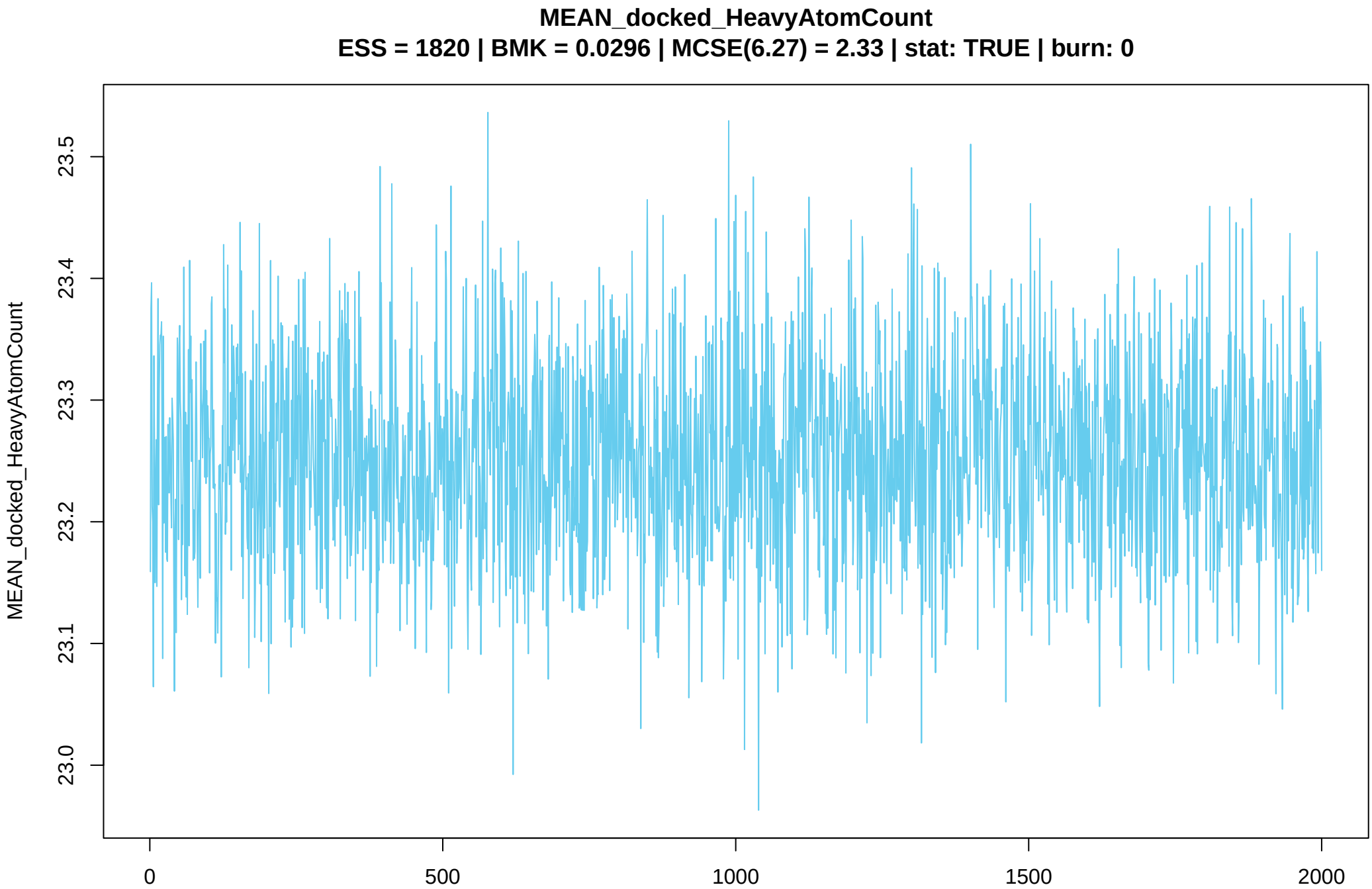

logitDcov
ESS = 1200 | BMK = 0.108 | MCSE(6.27) = 2.88 | stat: FALSE | burn: 0
logitDcov
0.0
0.2
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

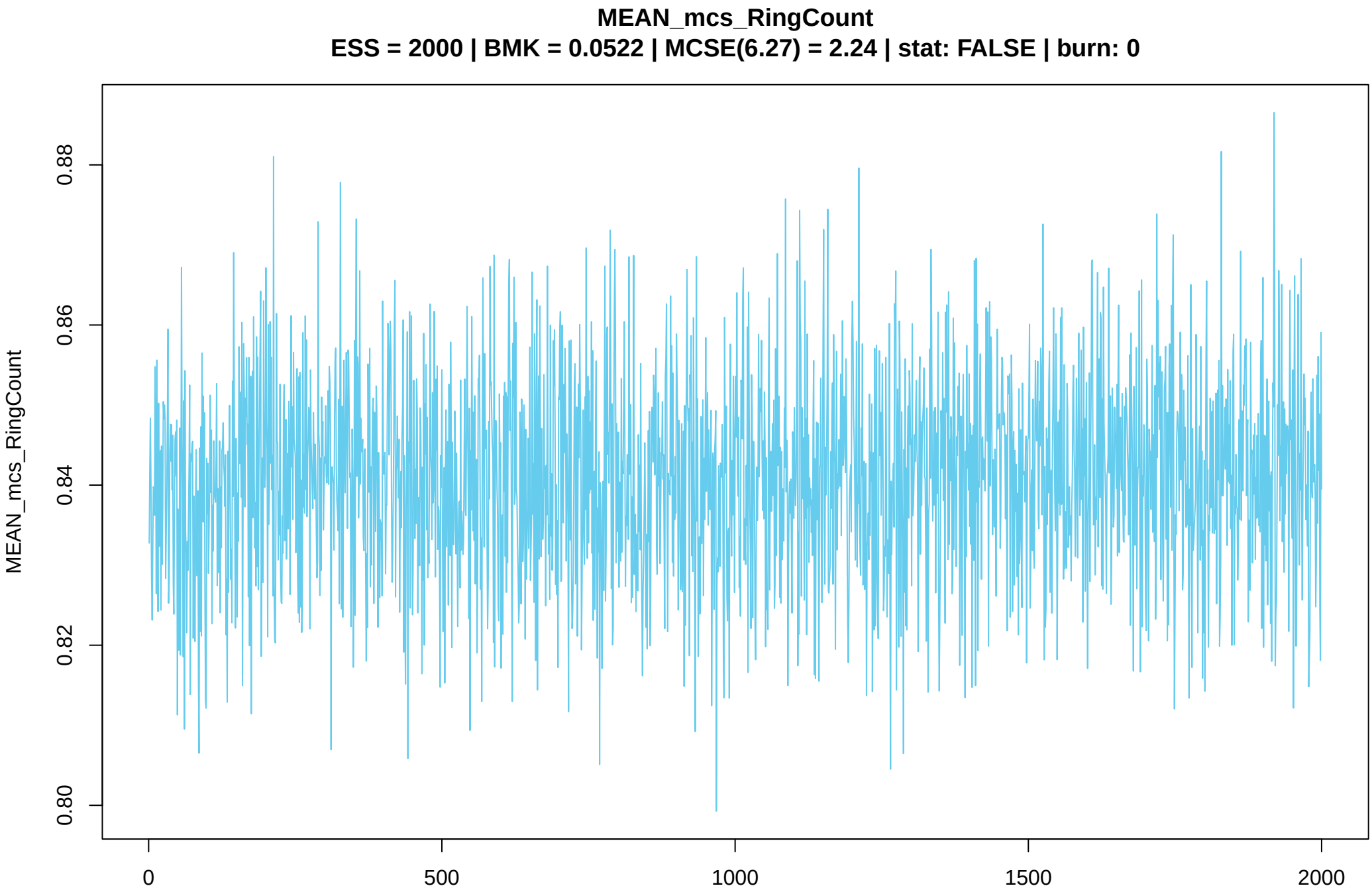

MEAN_log_RMSD
ESS = 1610 | BMK = 0.0565 | MCSE(6.27) = 2.72 | stat: FALSE | burn: 0
MEAN_log_RMSD
1.18
1.20
1.22
1.24
0
500
1000
1500
2000

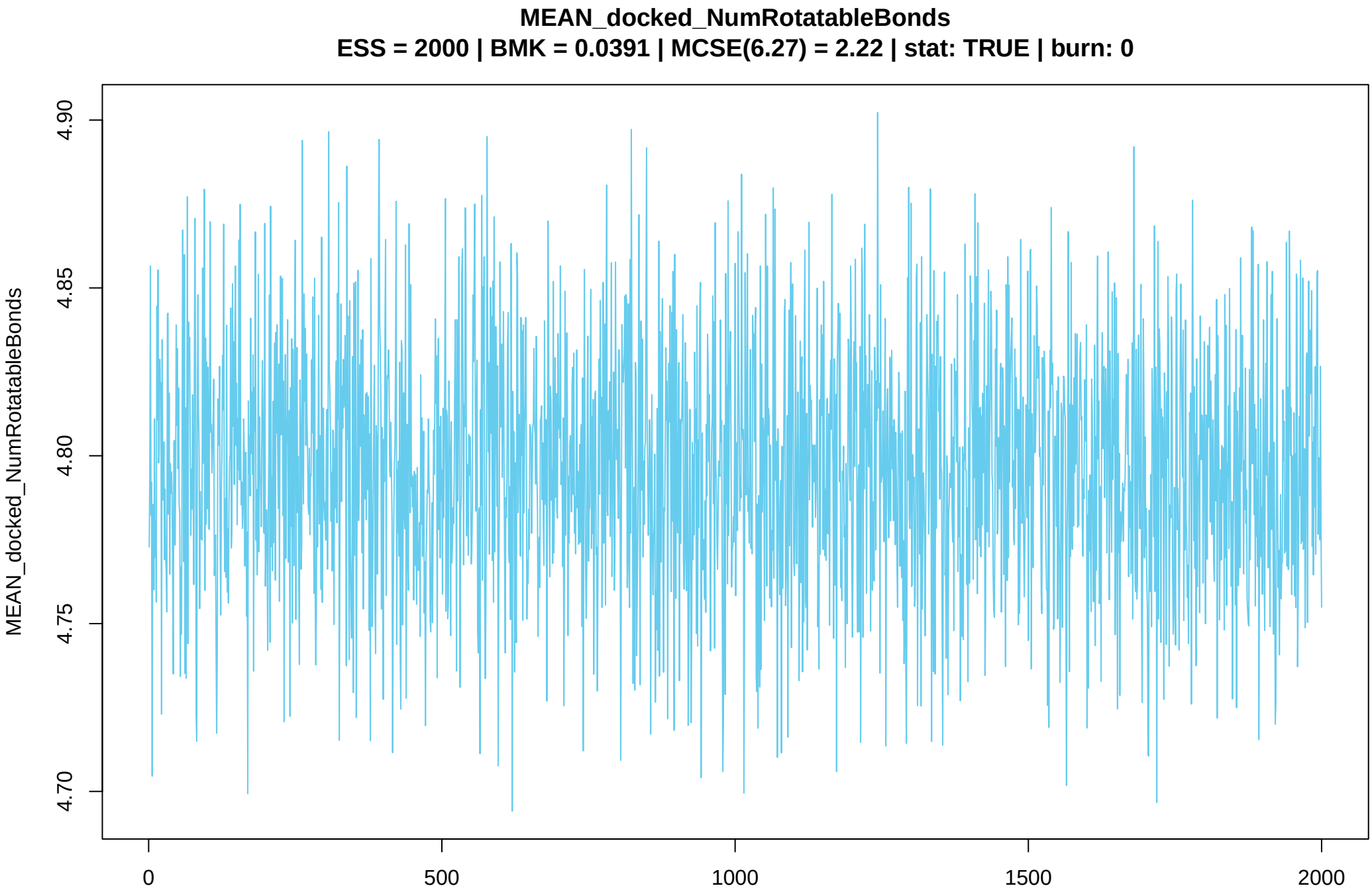

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1850 | BMK = 0.0428 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0
MEAN_log_mcs_unbonded_polar_sasa
−0.30
−0.32
−0.34
−0.36
−0.38
0
500
1000
1500
2000

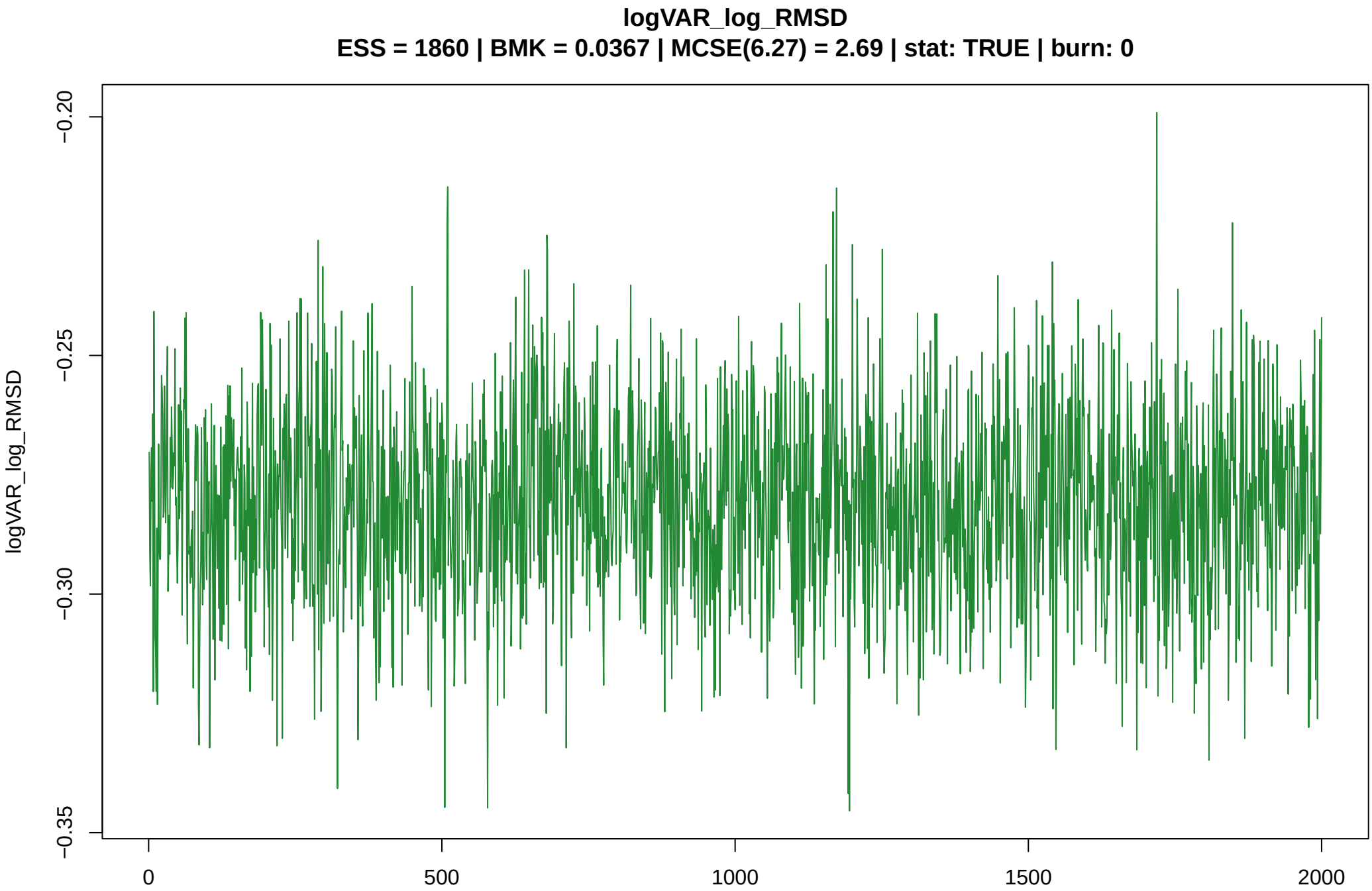

MEAN_logit_ec_tanimoto_similarity
ESS = 1780 | BMK = 0.0358 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0
MEAN_logit_ec_tanimoto_similarity
−2.04
−2.06
−2.08
−2.10
0
500
1000
1500
2000

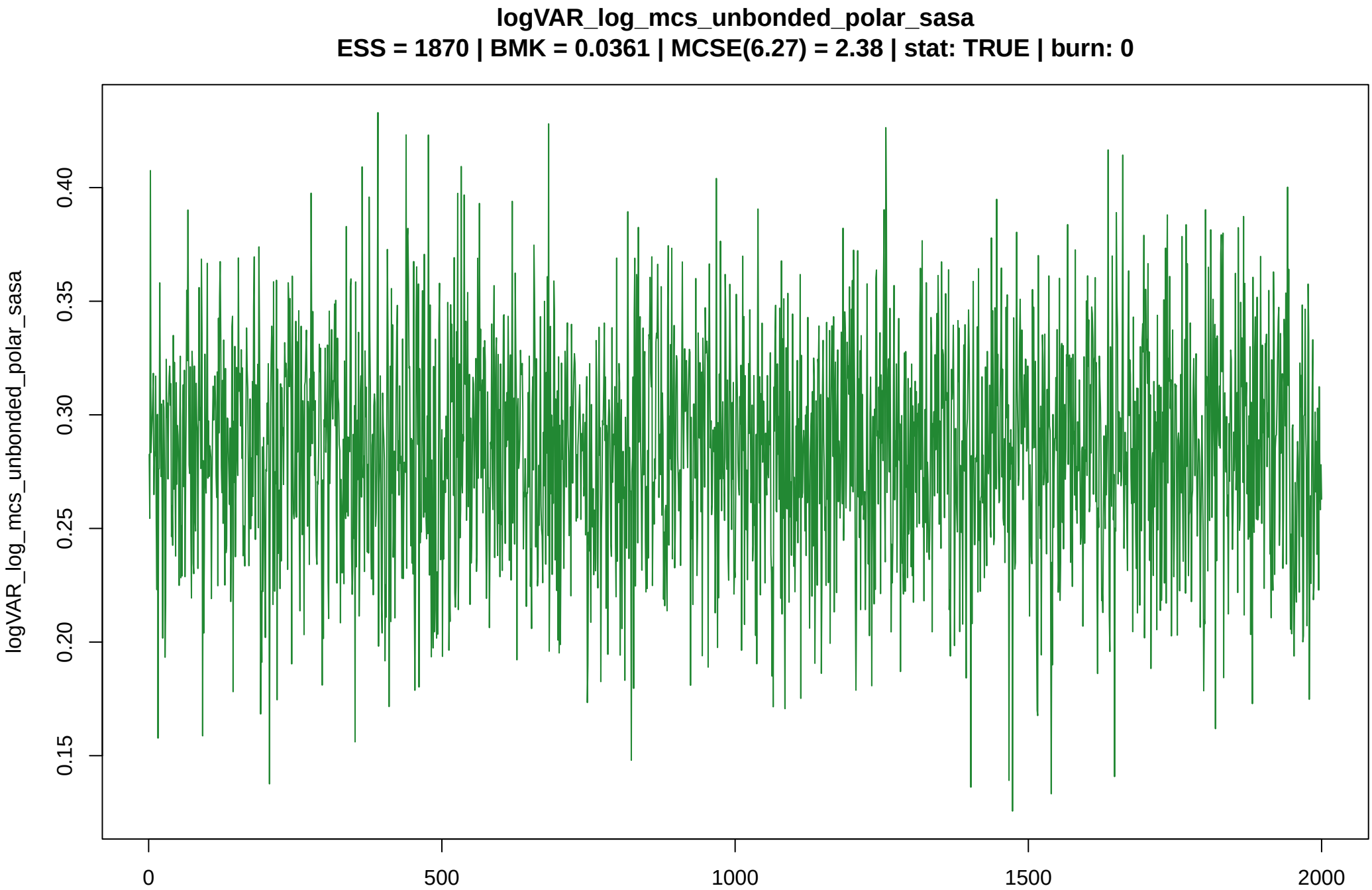

MEAN_mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0456 | MCSE(6.27) = 2.2 | stat: FALSE | burn: 0
MEAN_mcs_NumHeteroAtoms
2.95
3.00
3.05
0
500
1000
1500
2000

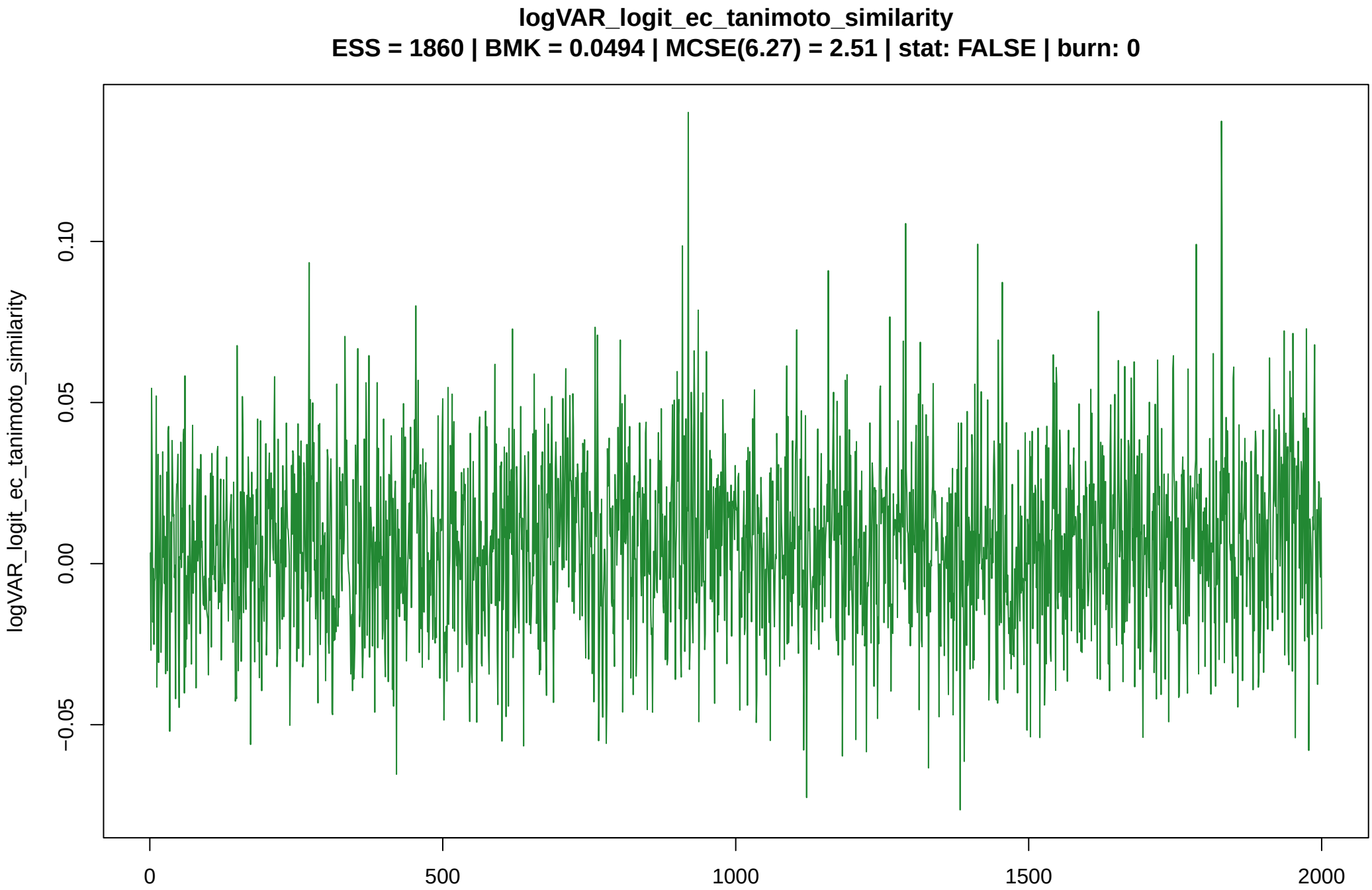

MEAN_docked_HeavyAtomCount
ESS = 1820 | BMK = 0.0296 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
23.0
23.1
23.2
23.3
23.4
23.5
0
500
1000
1500
2000

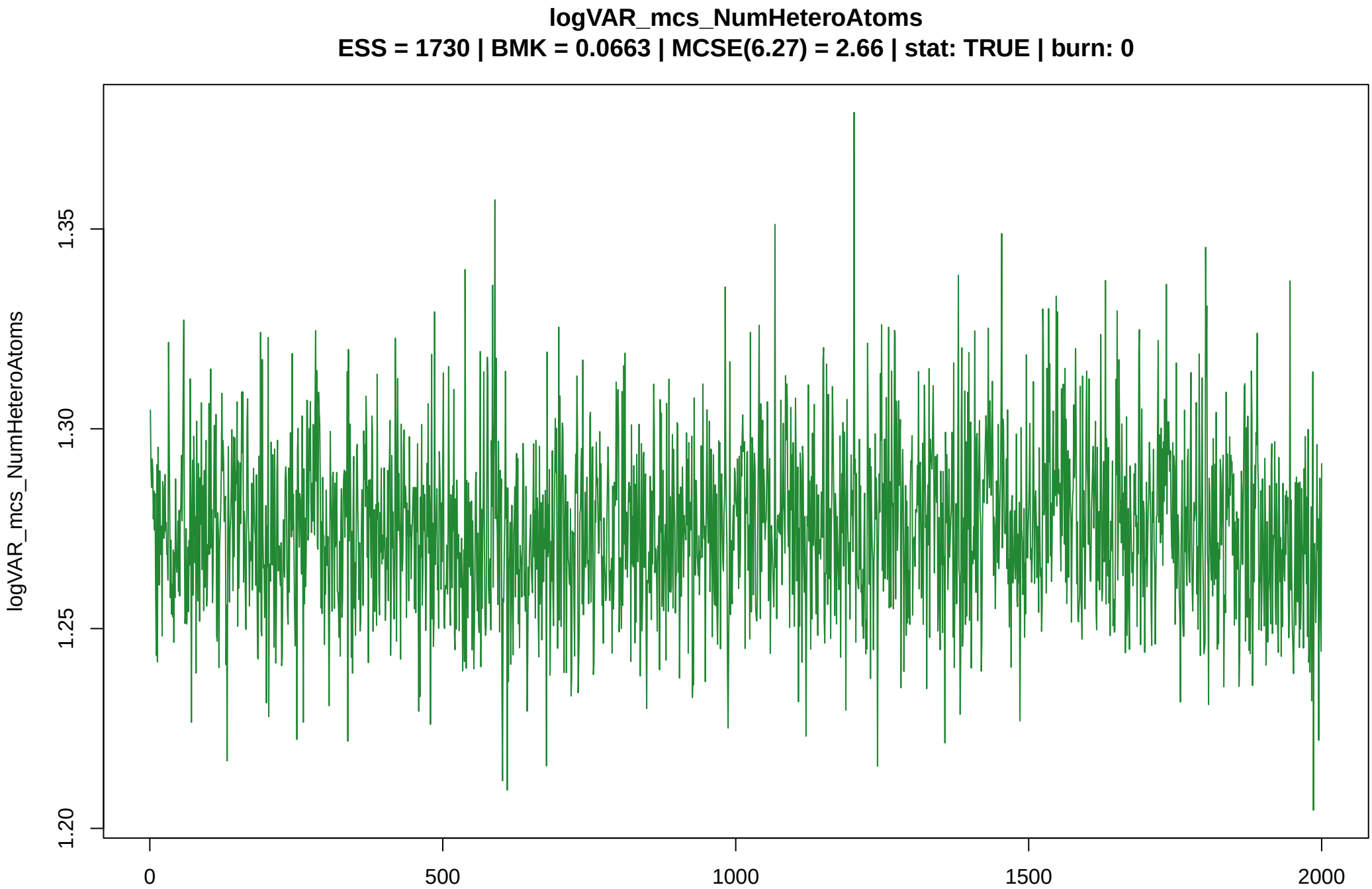

MEAN_mcs_RingCount
ESS = 2000 | BMK = 0.0522 | MCSE(6.27) = 2.24 | stat: FALSE | burn: 0
MEAN_mcs_RingCount
0.80
0.82
0.84
0.86
0.88
0
500
1000
1500
2000

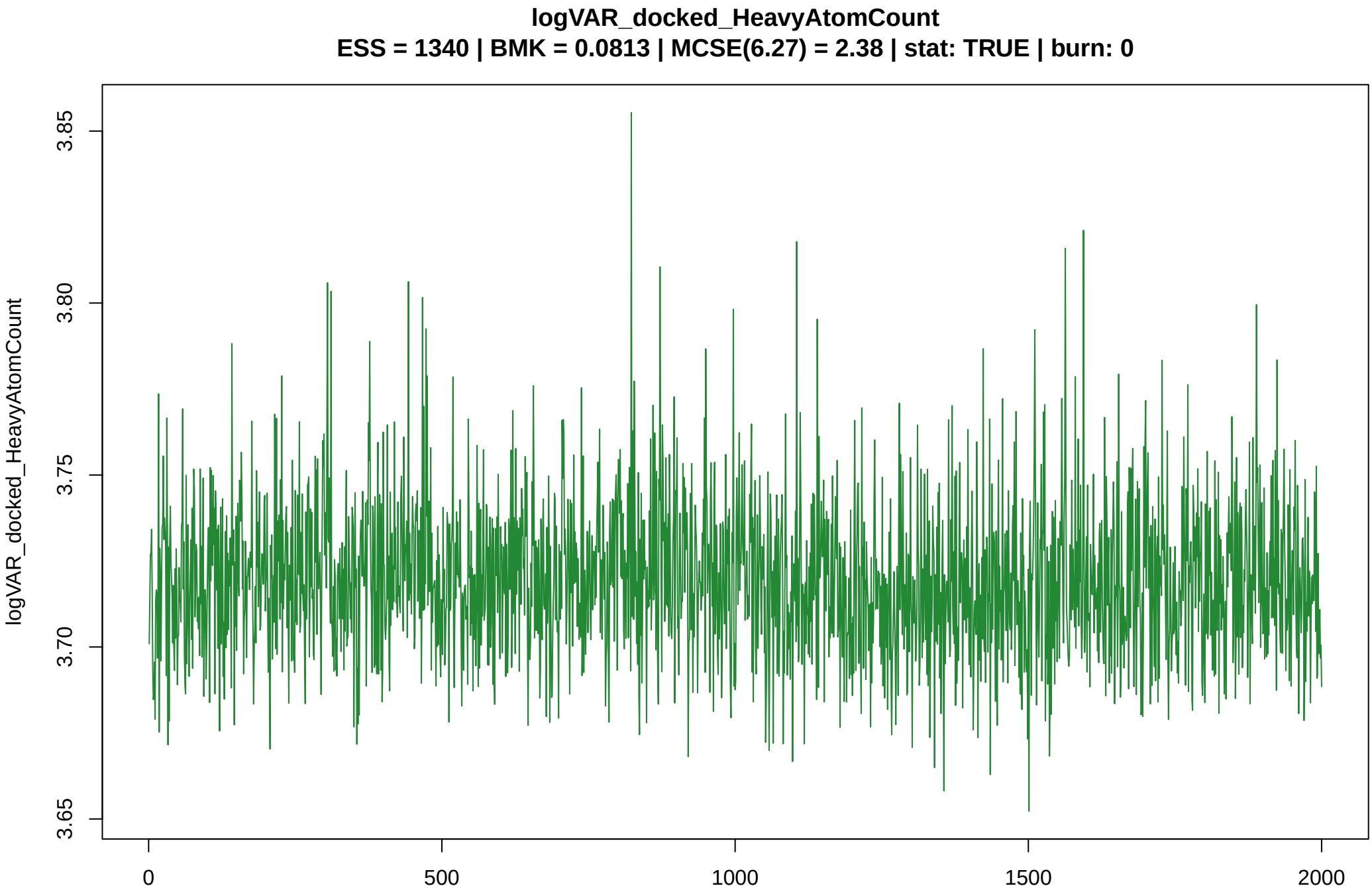

MEAN_docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0391 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0
MEAN_docked_NumRotatableBonds
4.70
4.75
4.80
4.85
4.90
0
500
1000
1500
2000

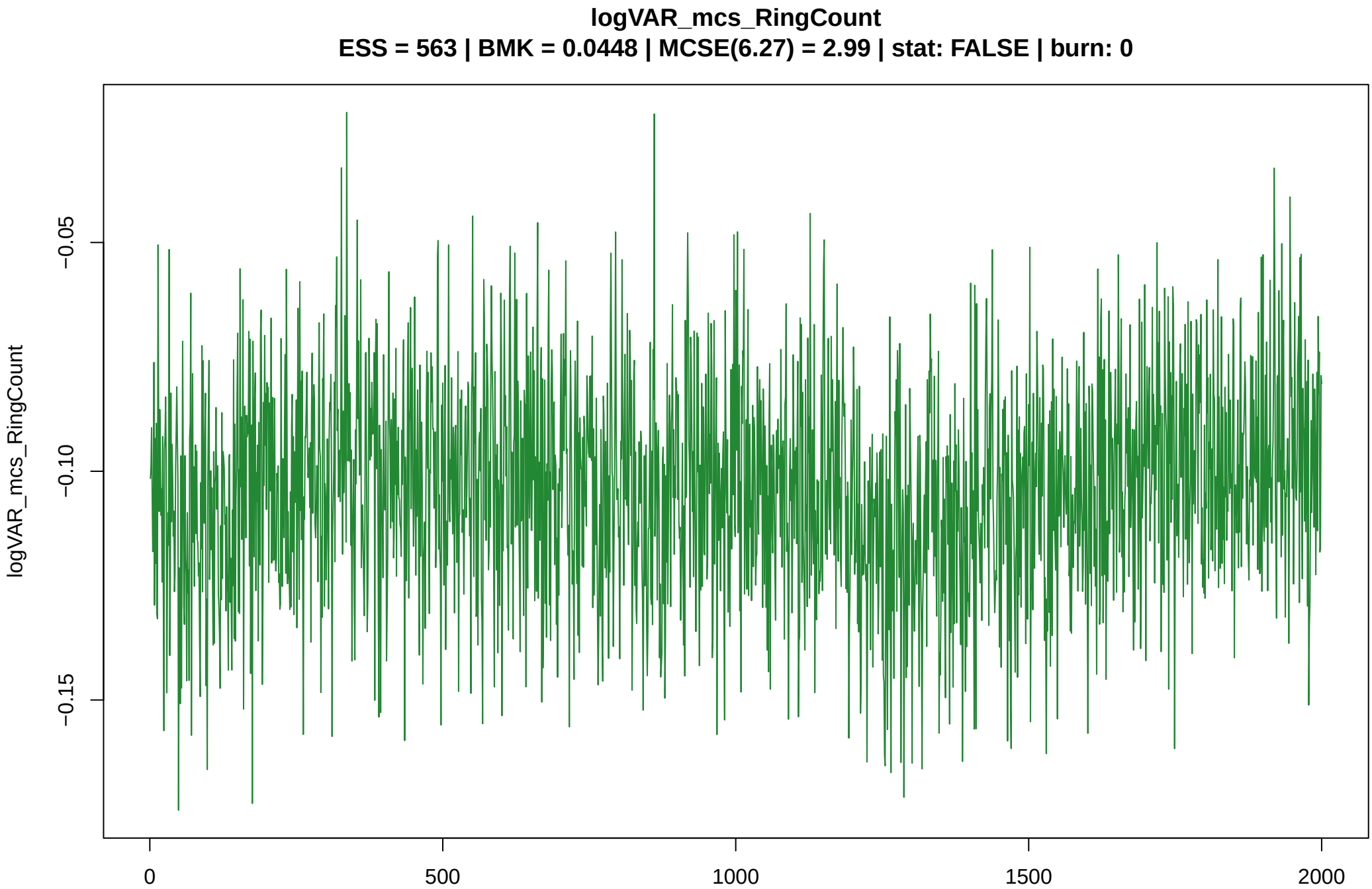

logVAR_log_RMSD
ESS = 1860 | BMK = 0.0367 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0
logVAR_log_RMSD
−0.20
−0.25
−0.30
−0.35
0
500
1000
1500
2000

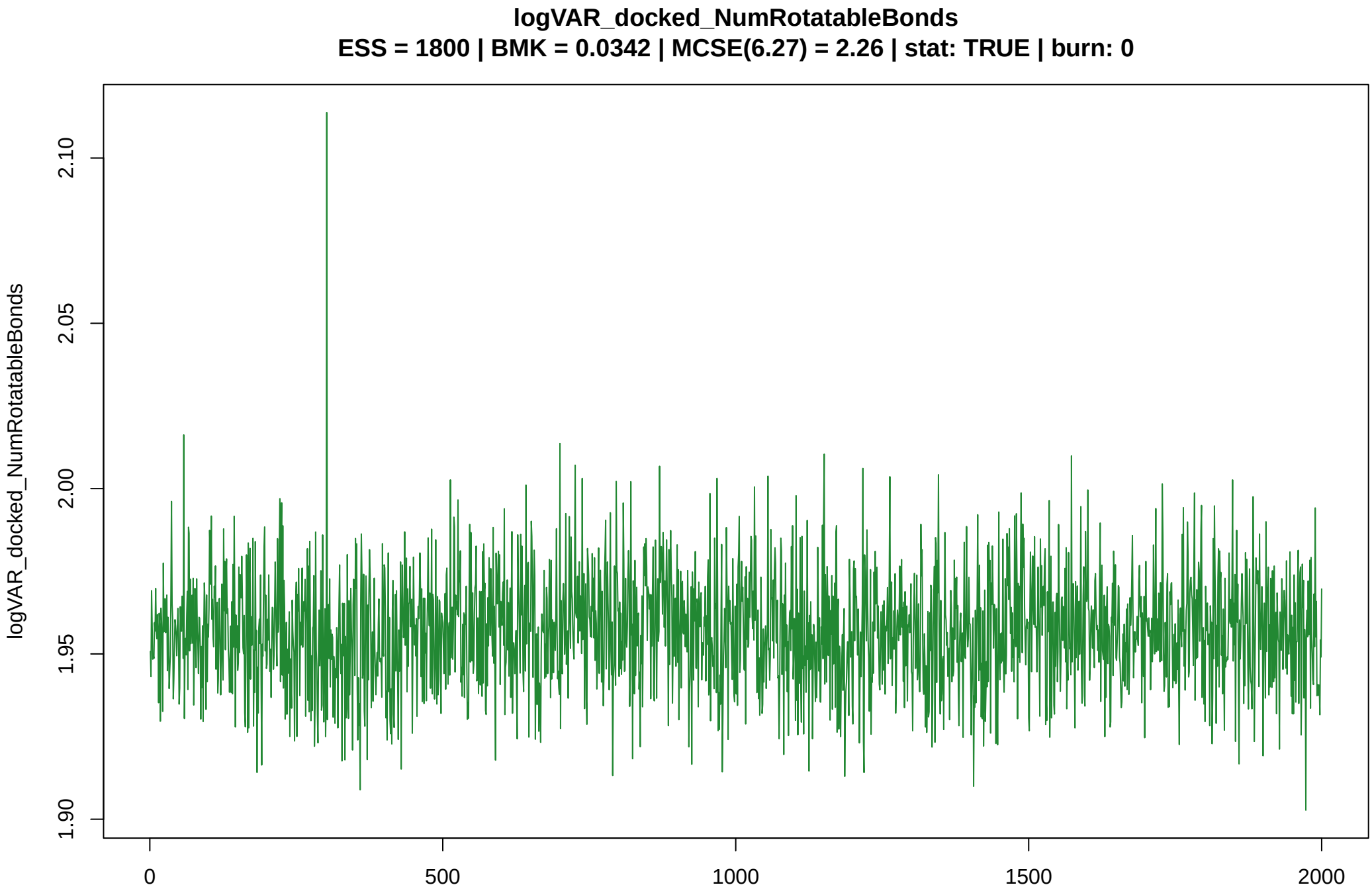

logVAR_log_mcs_unbonded_polar_sasa
ESS = 1870 | BMK = 0.0361 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0
logVAR_log_mcs_unbonded_polar_sasa
0.15
0.20
0.25
0.30
0.35
0.40
0
500
1000
1500
2000

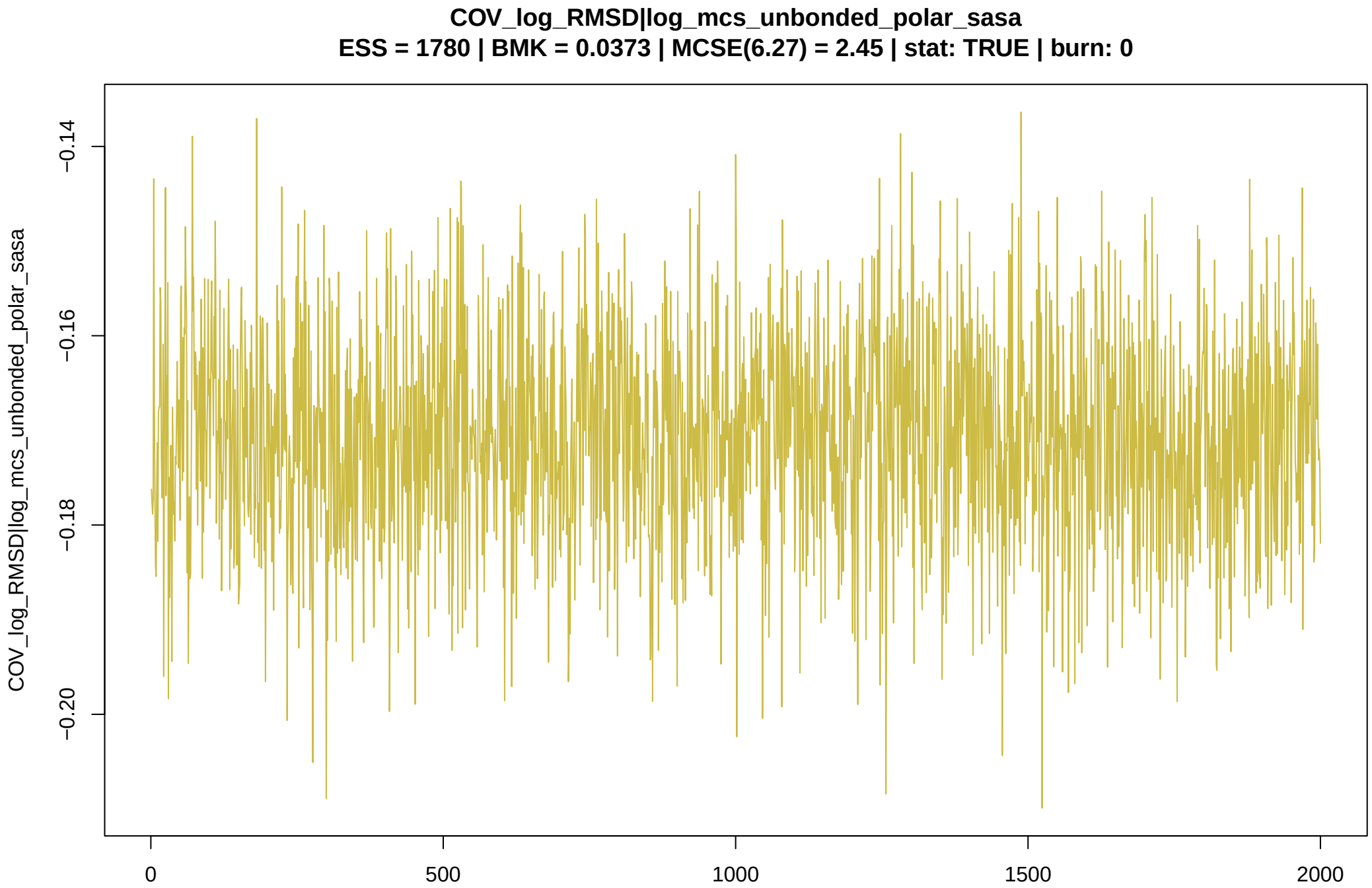

logVAR_logit_ec_tanimoto_similarity
ESS = 1860 | BMK = 0.0494 | MCSE(6.27) = 2.51 | stat: FALSE | burn: 0
logVAR_logit_ec_tanimoto_similarity
0.10
0.05
0.00
−0.05
0
500
1000
1500
2000

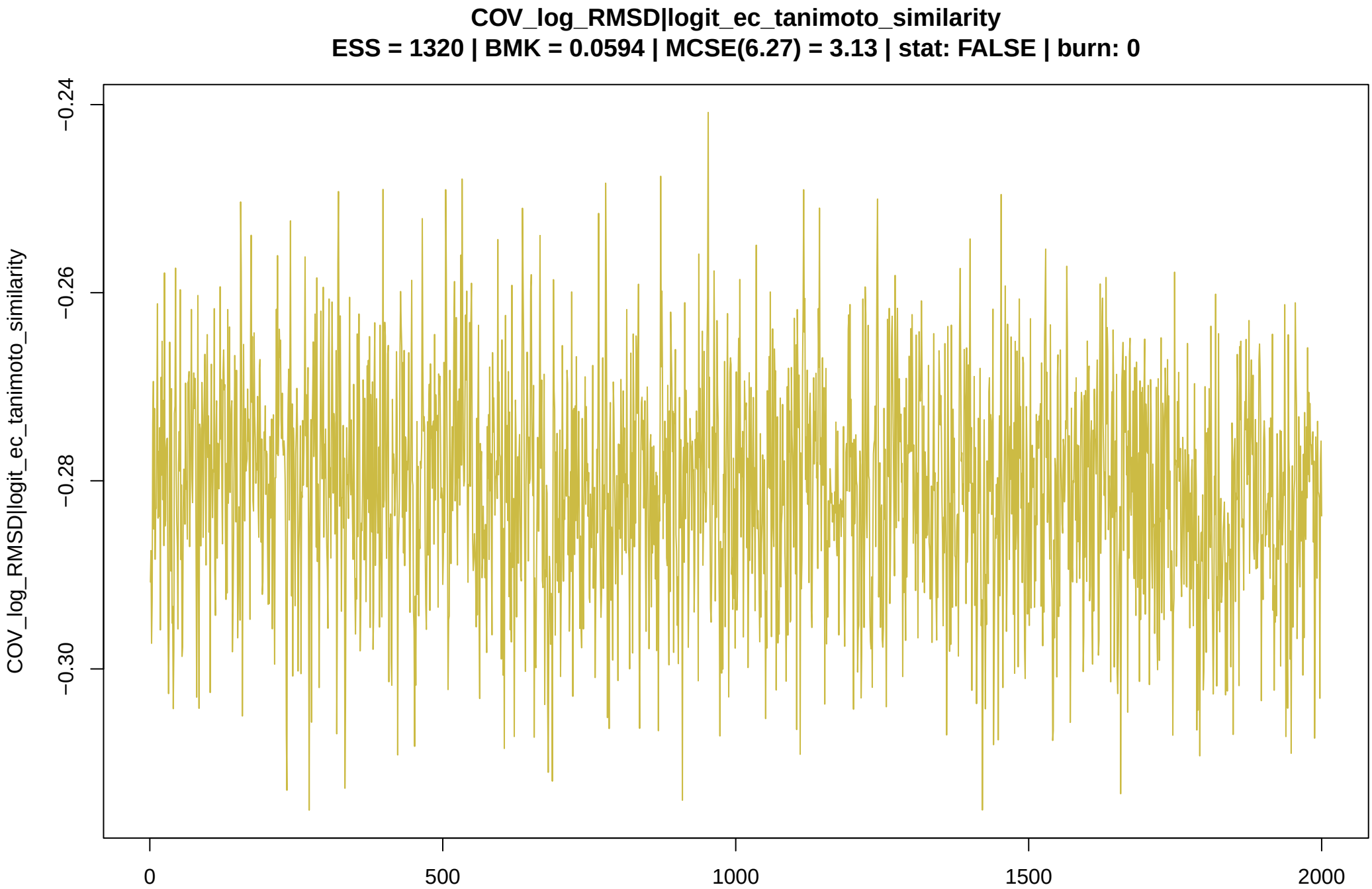

logVAR_mcs_NumHeteroAtoms
ESS = 1730 | BMK = 0.0663 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0
logVAR_mcs_NumHeteroAtoms
1.20
1.25
1.30
1.35
0
500
1000
1500
2000

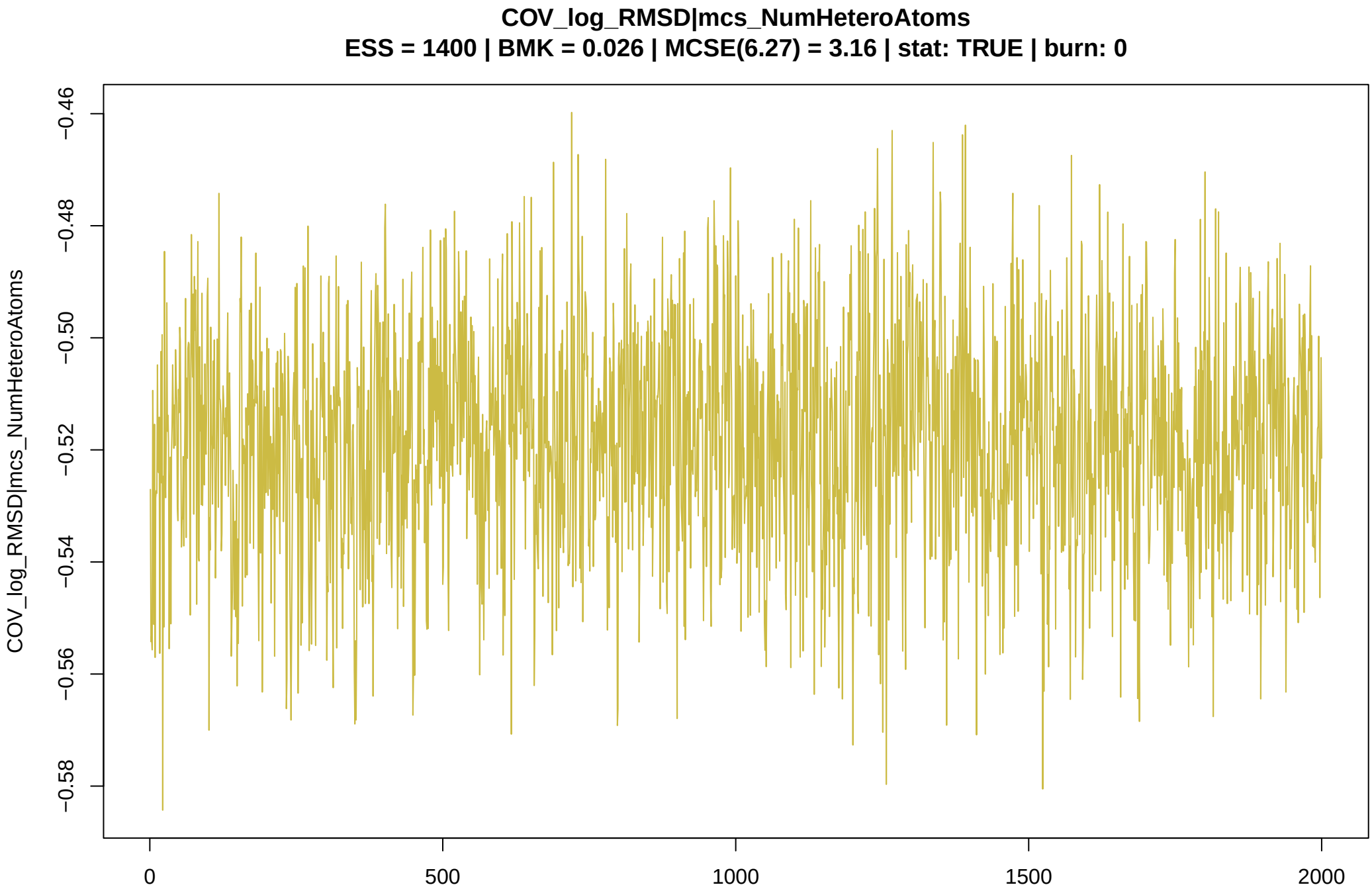

logVAR_docked_HeavyAtomCount
ESS = 1340 | BMK = 0.0813 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0
logVAR_docked_HeavyAtomCount
3.65
3.70
3.75
3.80
3.85
0
500
1000
1500
2000

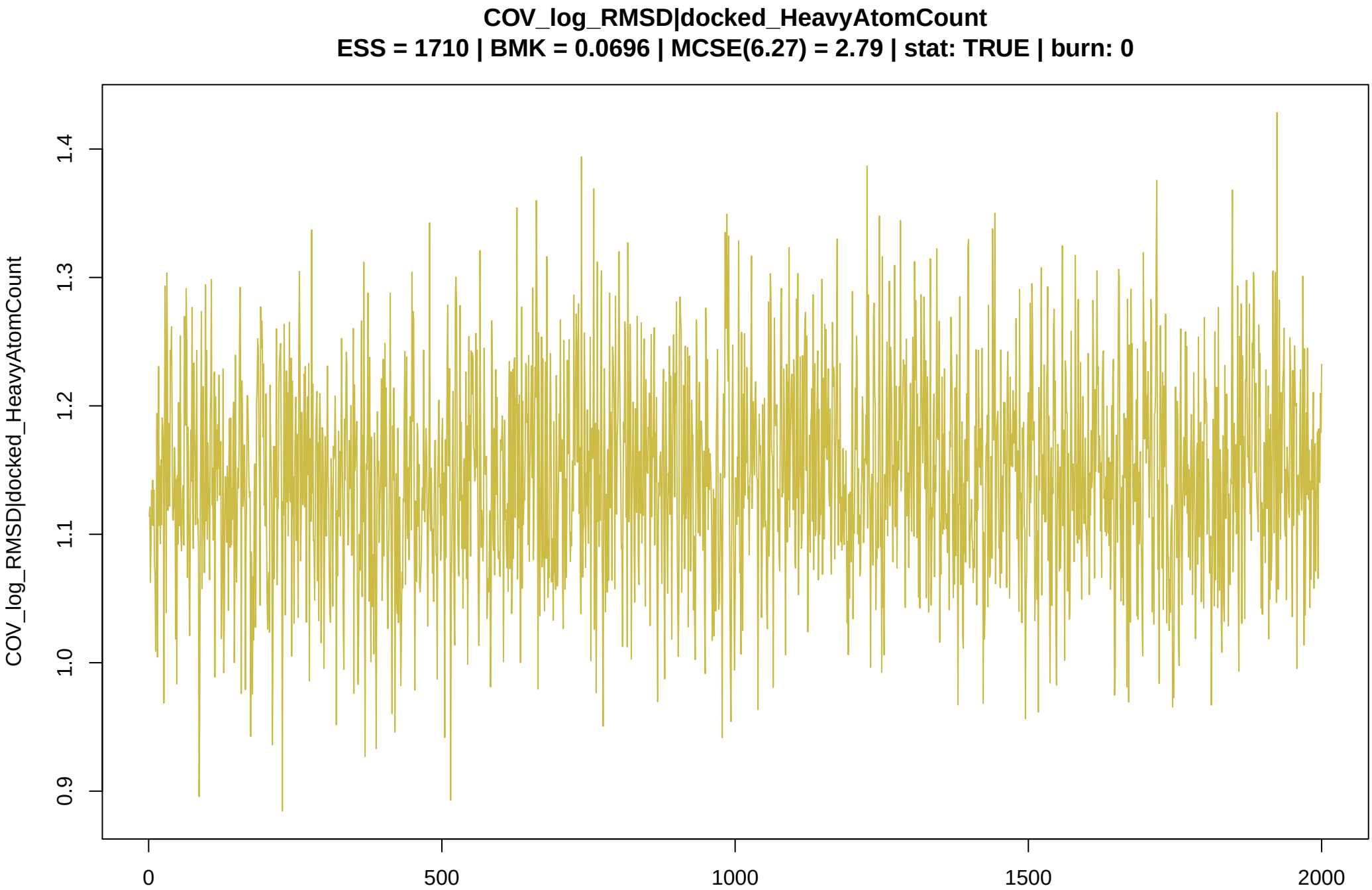

logVAR_mcs_RingCount
ESS = 563 | BMK = 0.0448 | MCSE(6.27) = 2.99 | stat: FALSE | burn: 0
logVAR_mcs_RingCount
−0.05
−0.10
−0.15
0
500
1000
1500
2000

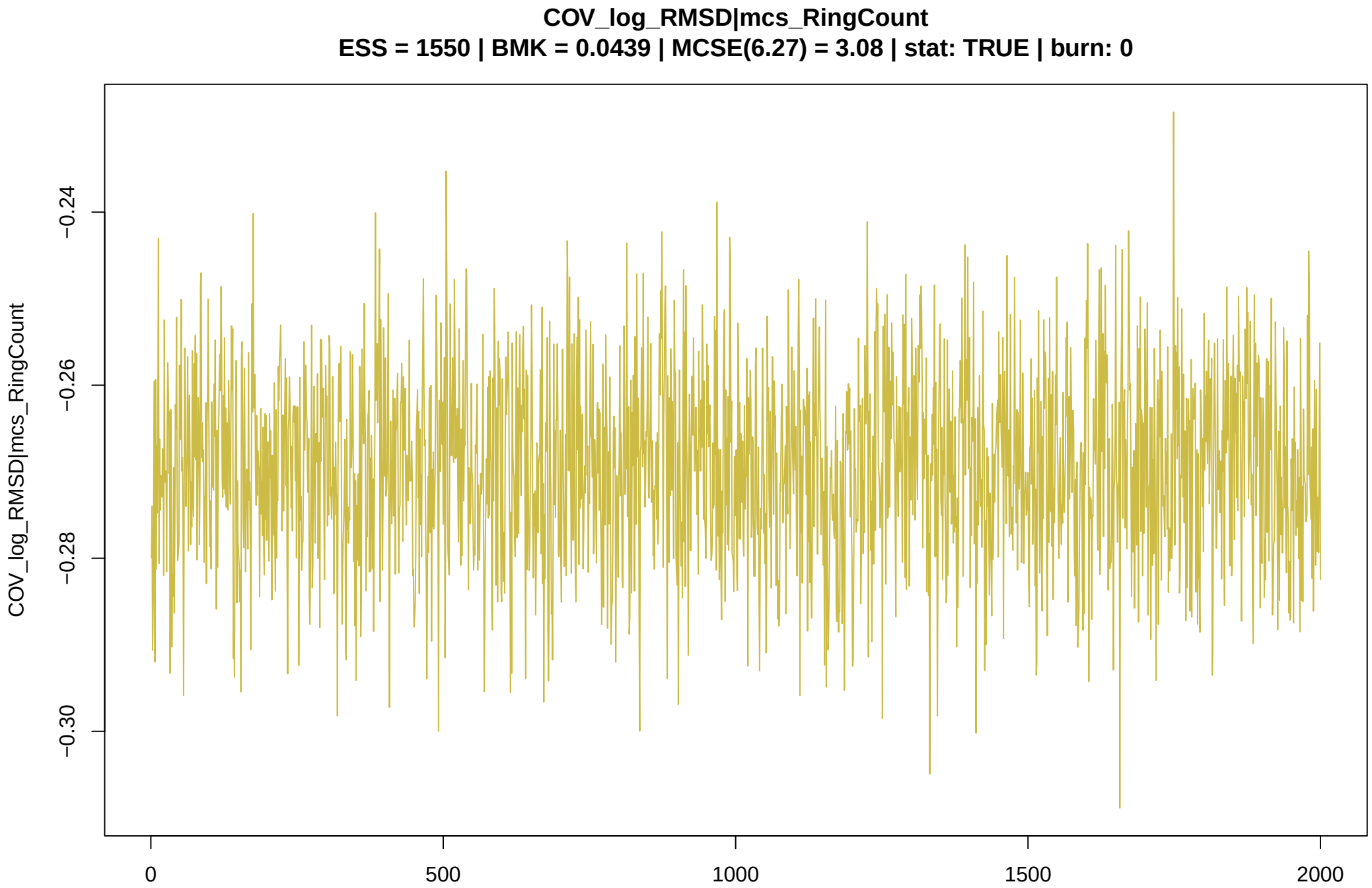

logVAR_docked_NumRotatableBonds
ESS = 1800 | BMK = 0.0342 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0
logVAR_docked_NumRotatableBonds
1.90
1.95
2.00
2.05
2.10
0
500
1000
1500
2000

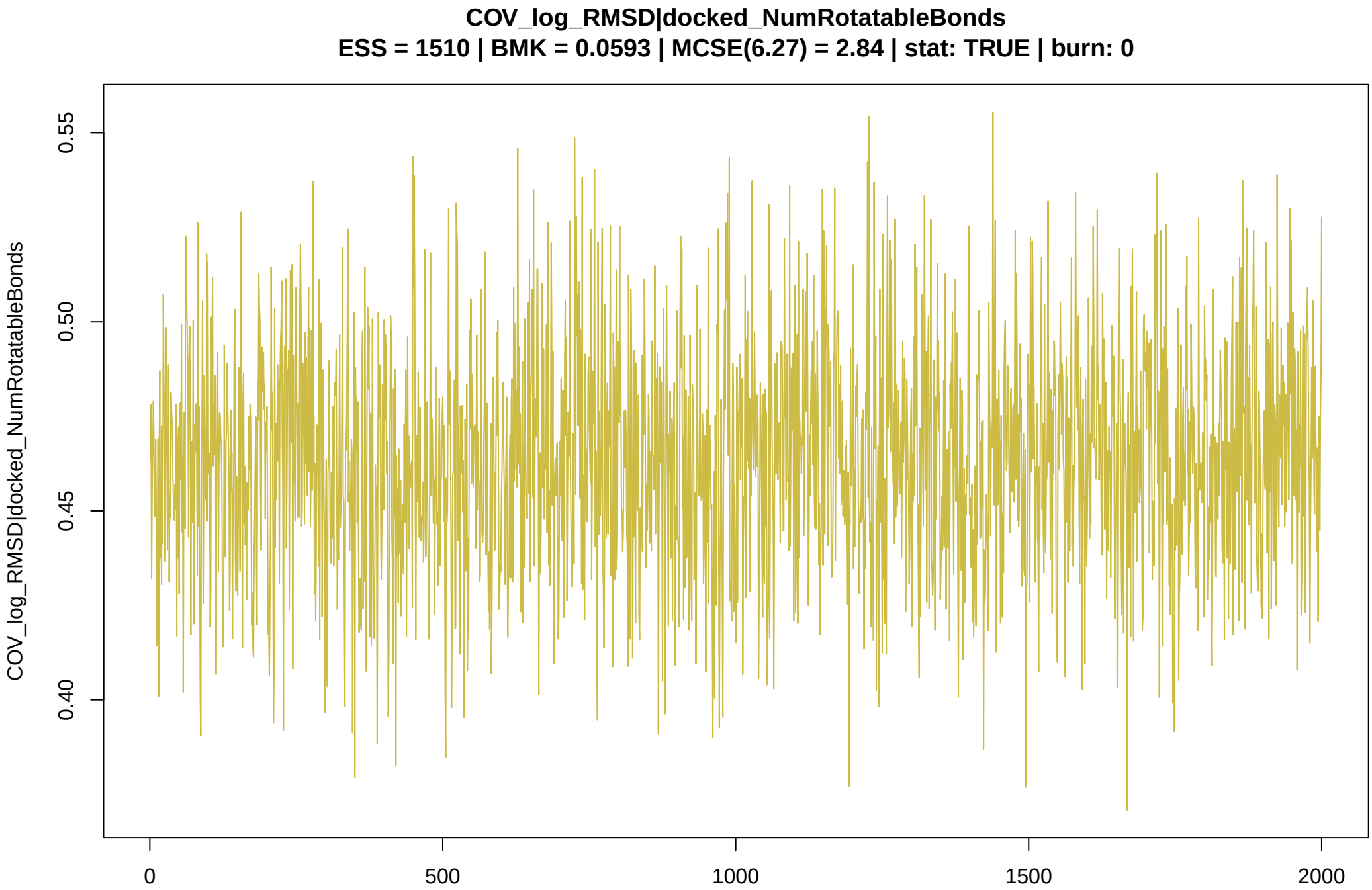

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1780 | BMK = 0.0373 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.14
−0.16
−0.18
−0.20
0
500
1000
1500
2000

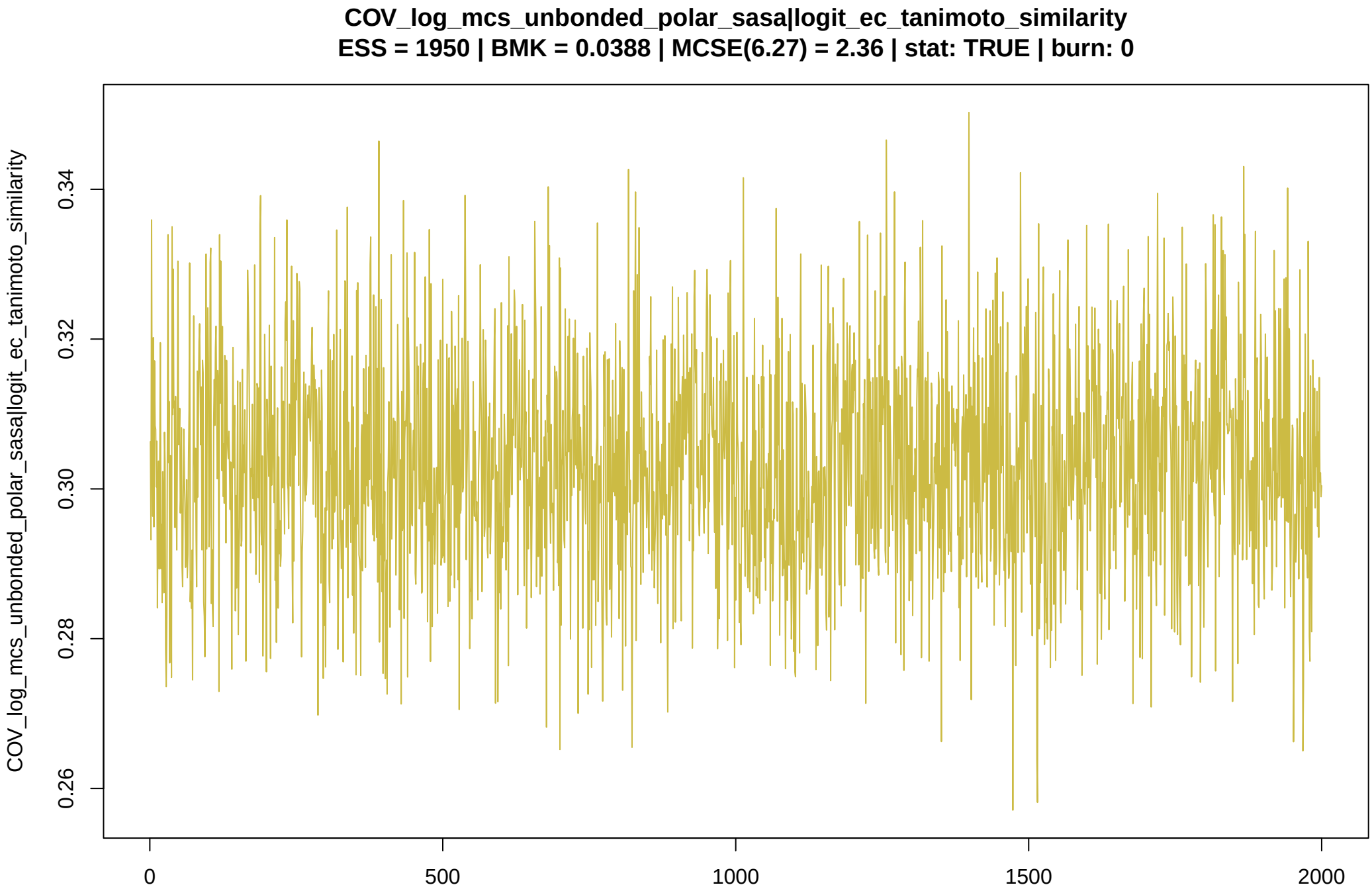

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1320 | BMK = 0.0594 | MCSE(6.27) = 3.13 | stat: FALSE | burn: 0
COV_log_RMSD|logit_ec_tanimoto_similarity
−0.24
−0.26
−0.28
−0.30
0
500
1000
1500
2000

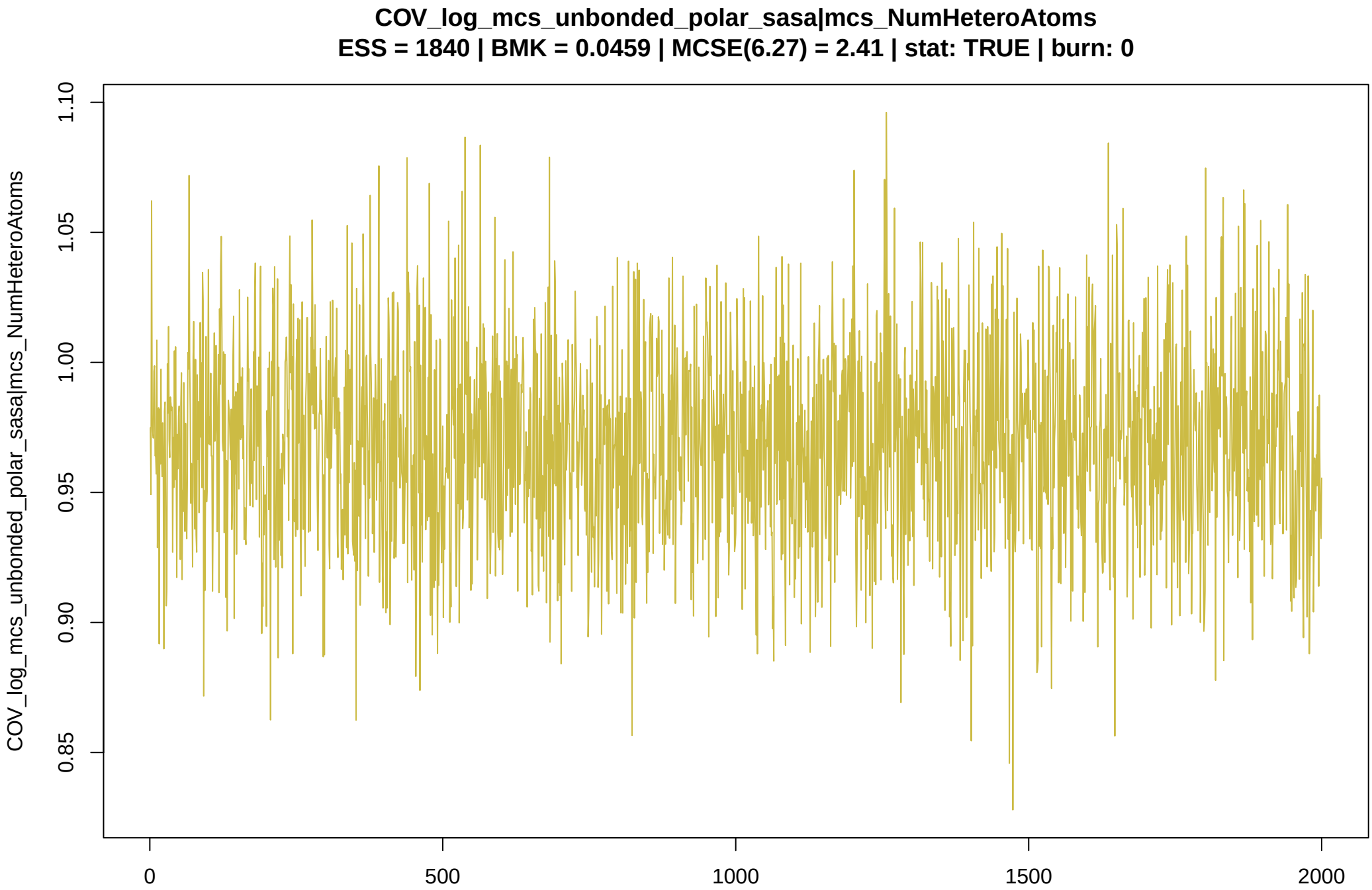

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1400 | BMK = 0.026 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.46
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

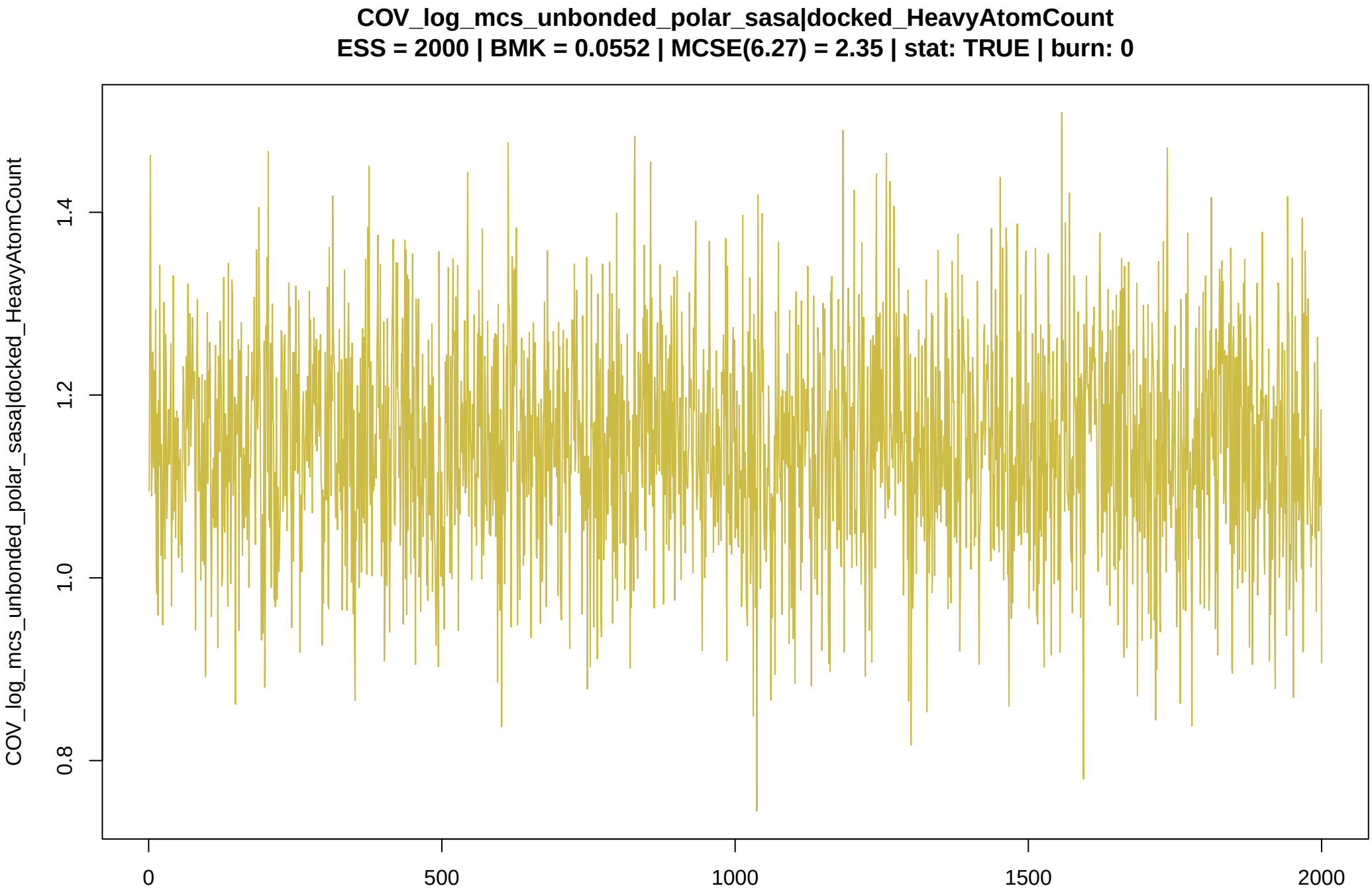

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1710 | BMK = 0.0696 | MCSE(6.27) = 2.79 | stat: TRUE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
0.9
1.0
1.1
1.2
1.3
1.4
0
500
1000
1500
2000

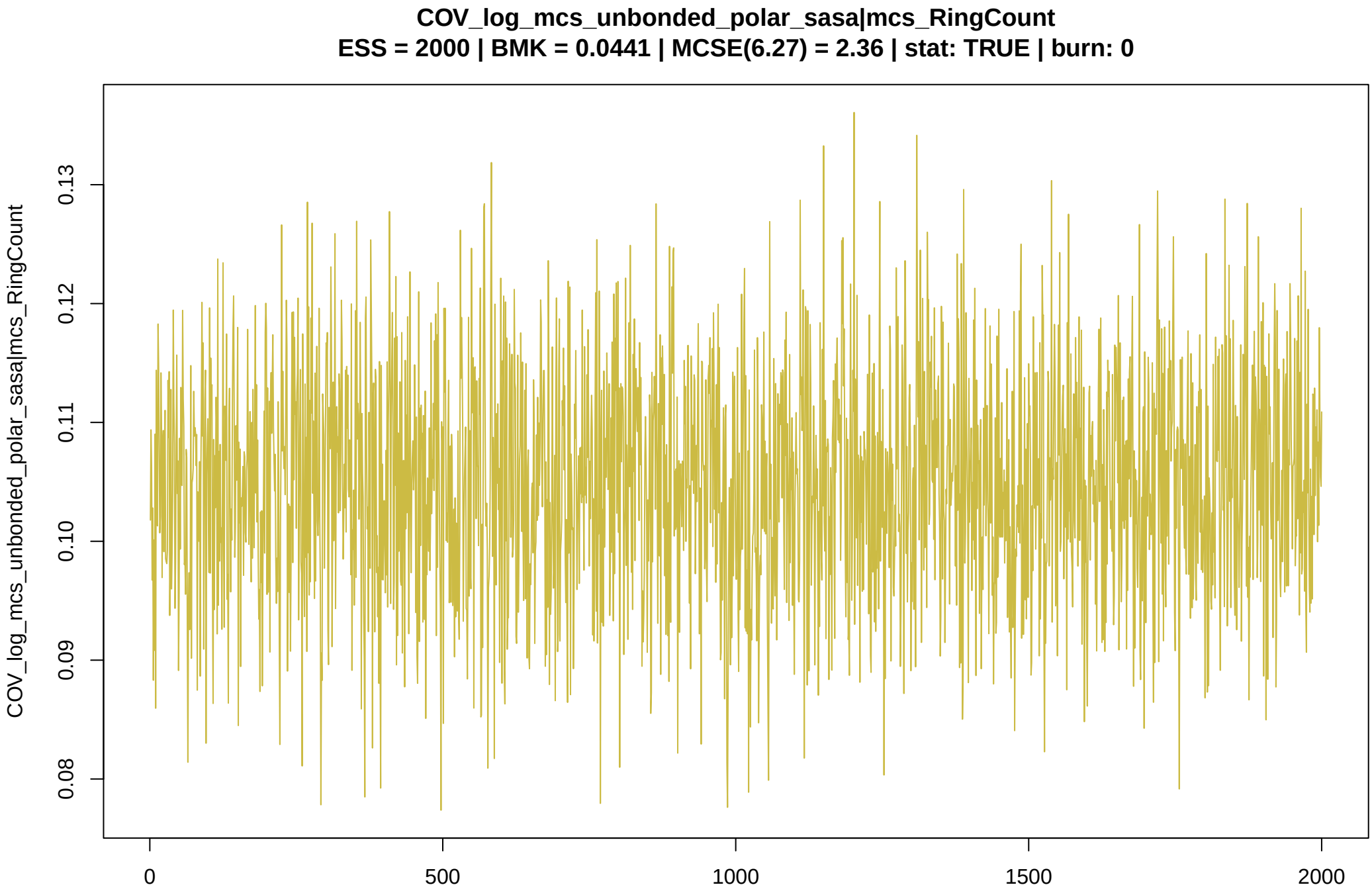

COV_log_RMSD|mcs_RingCount
ESS = 1550 | BMK = 0.0439 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.24
−0.26
−0.28
−0.30
0
500
1000
1500
2000

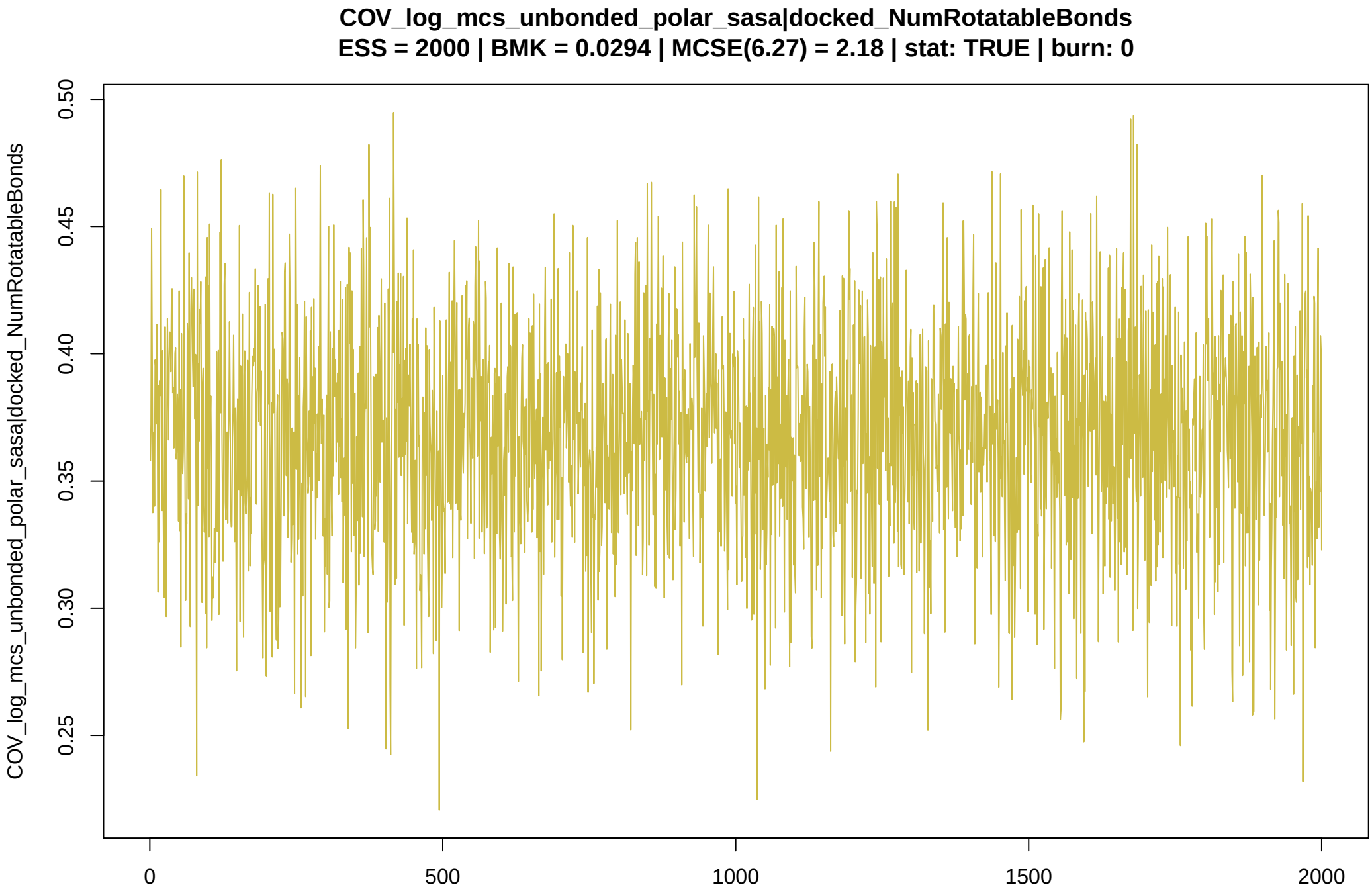

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1510 | BMK = 0.0593 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0
COV_log_RMSD|docked_NumRotatableBonds
0.40
0.45
0.50
0.55
0
500
1000
1500
2000

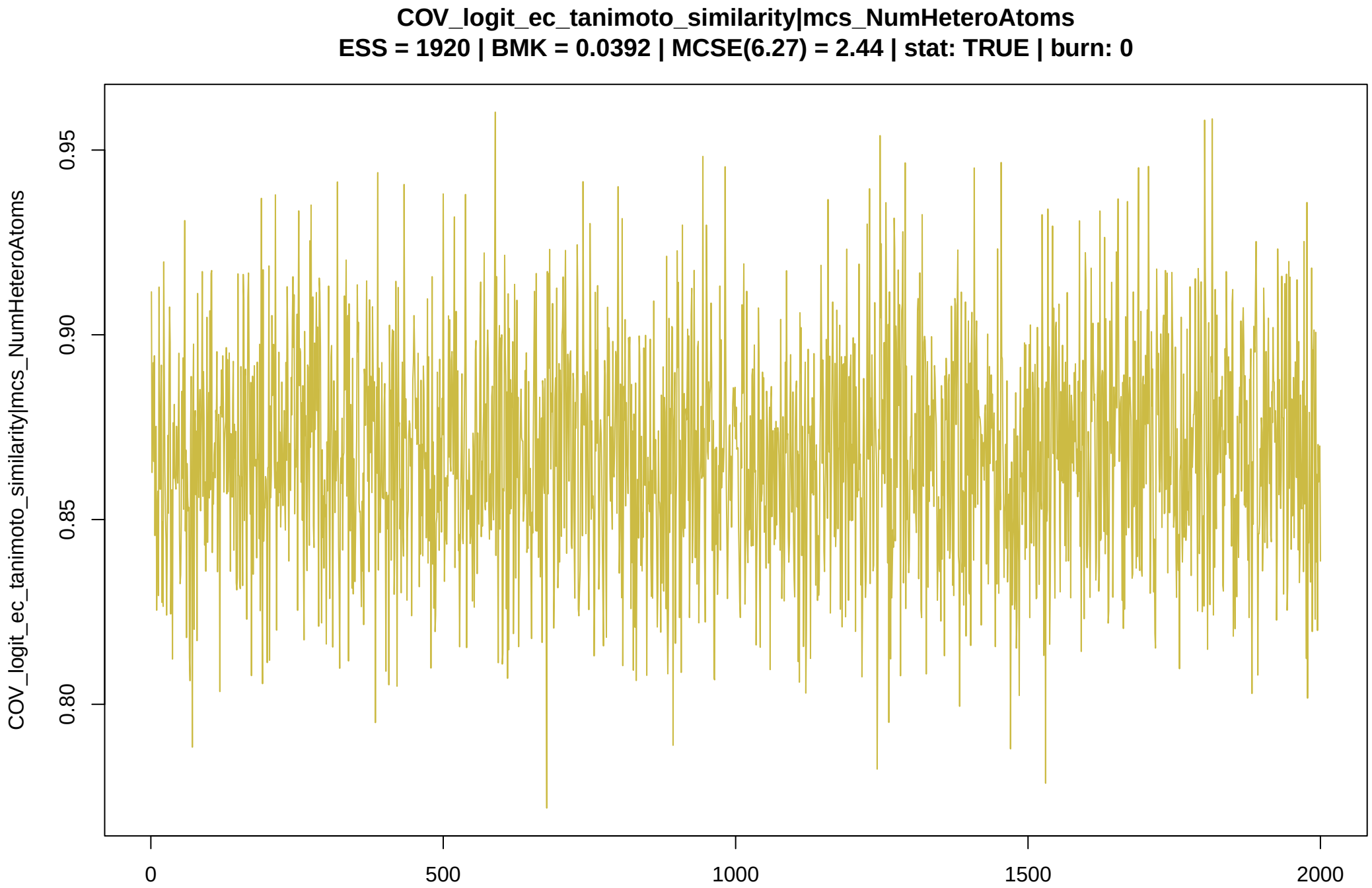

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1950 | BMK = 0.0388 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0.26
0.28
0.30
0.32
0.34
0
500
1000
1500
2000

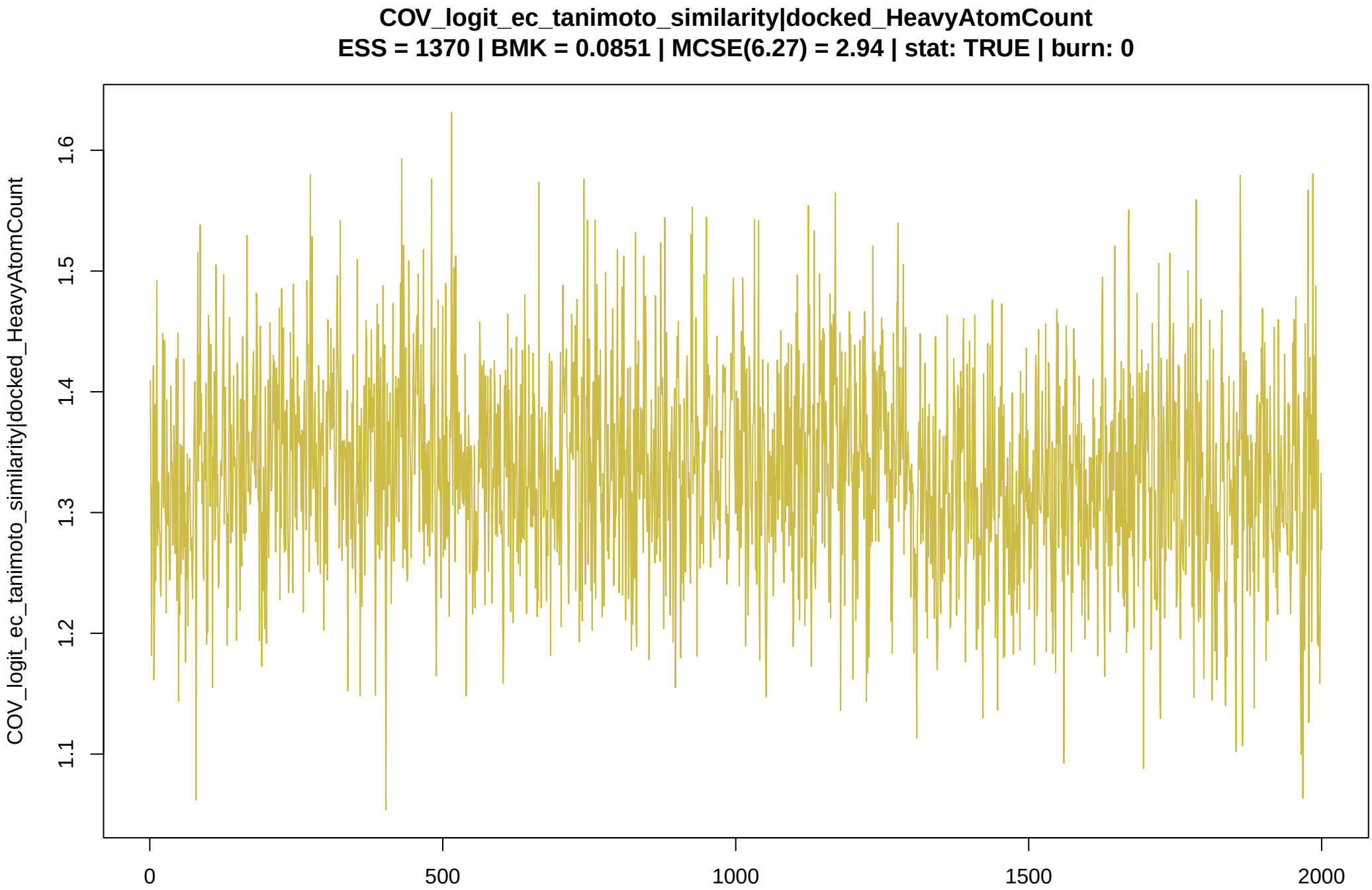

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1840 | BMK = 0.0459 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
1.10
1.05
1.00
0.95
0.90
0.85
0
500
1000
1500
2000

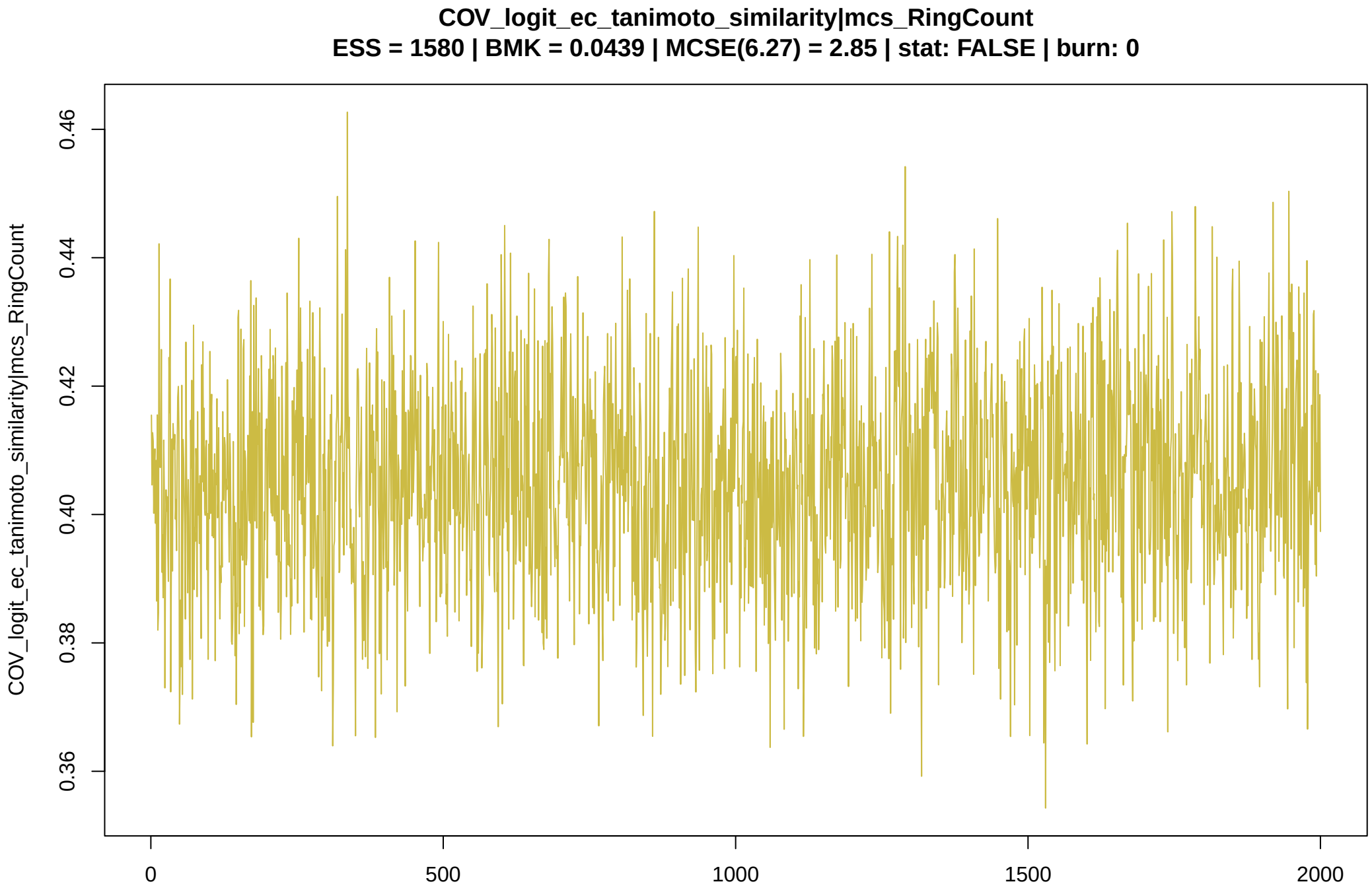

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0552 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

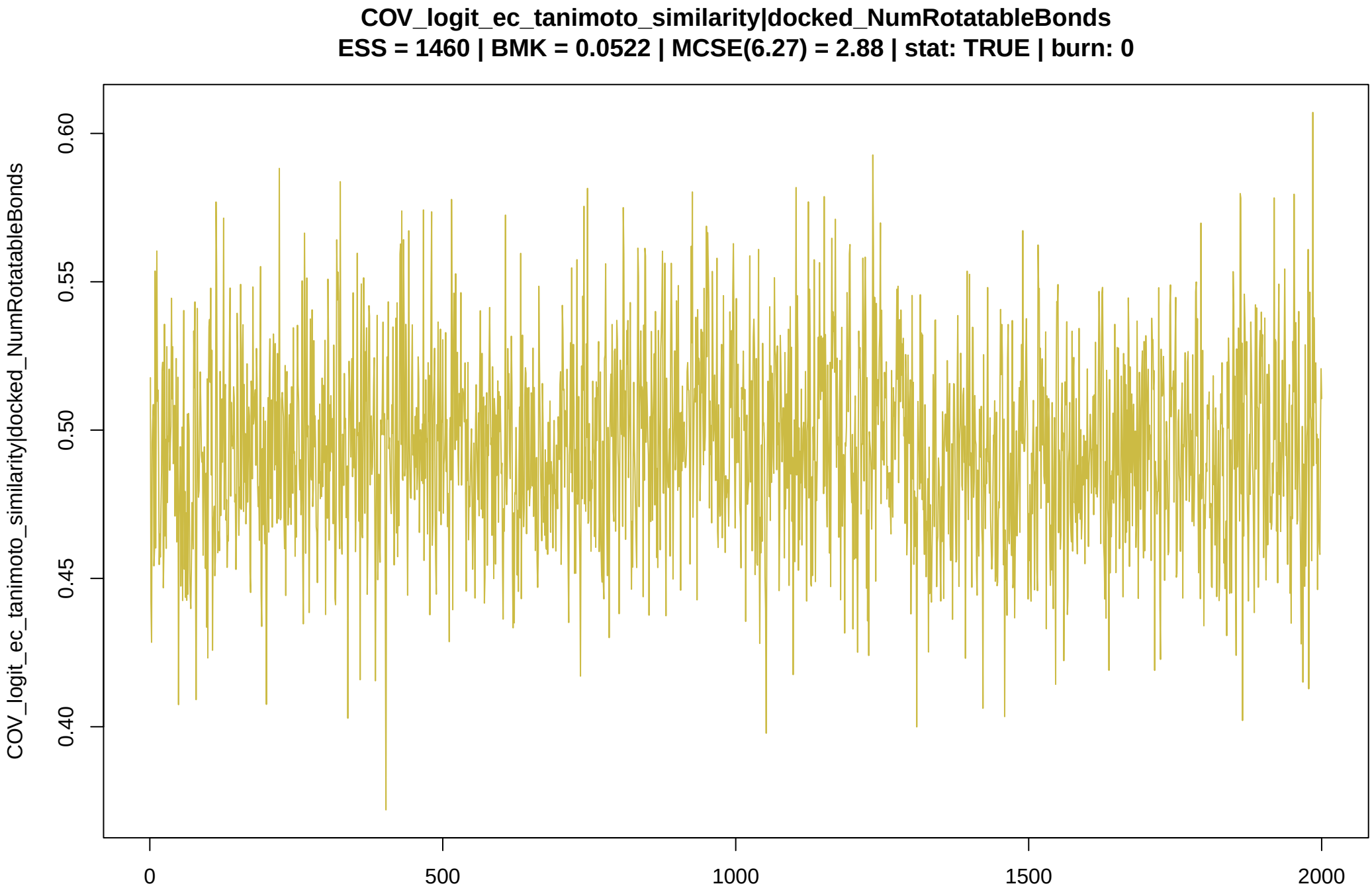

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 2000 | BMK = 0.0441 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
0.08
0.09
0.10
0.11
0.12
0.13
0
500
1000
1500
2000

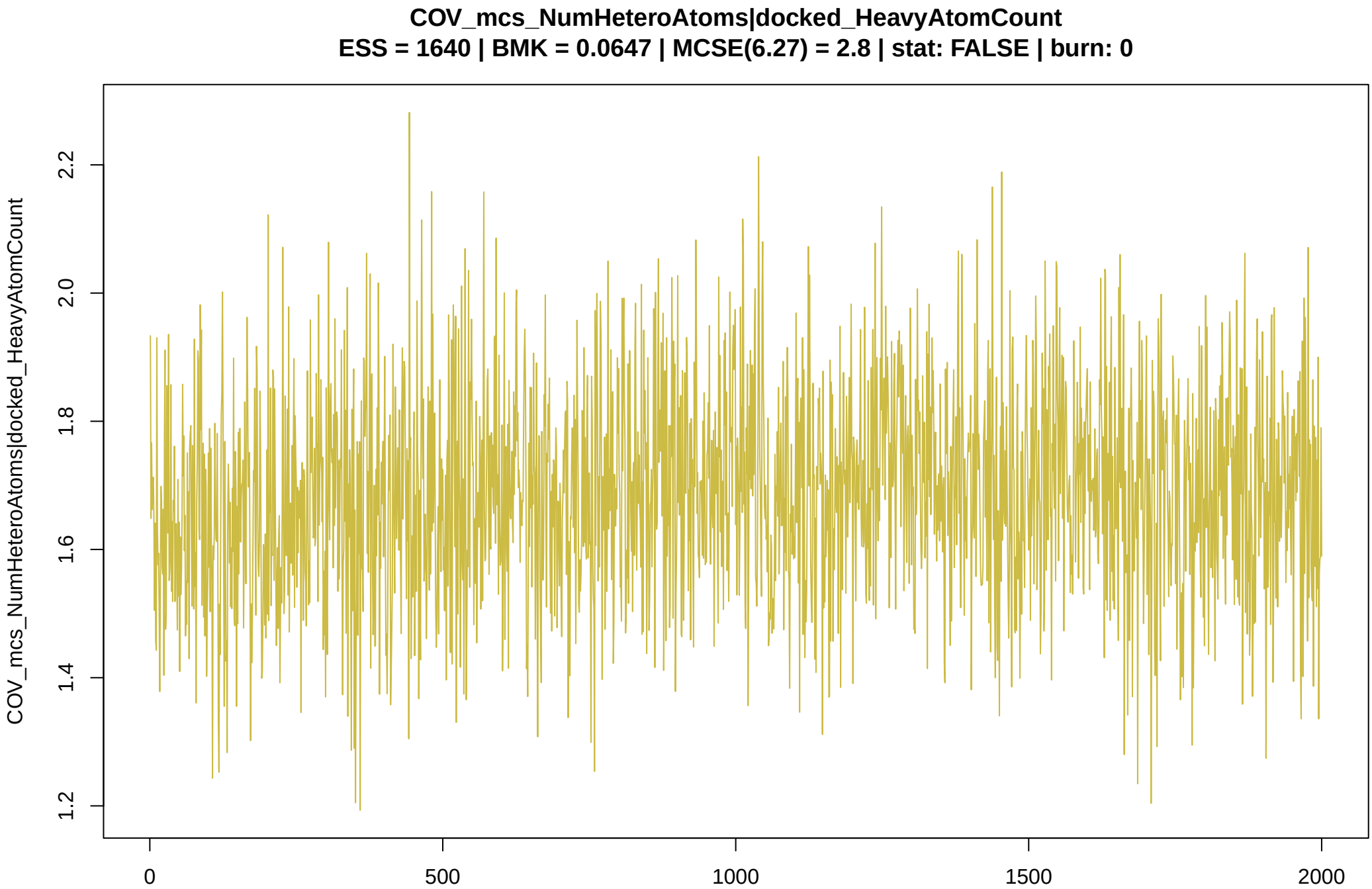

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0294 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
0.25
0.30
0.35
0.40
0.45
0.50
0
500
1000
1500
2000

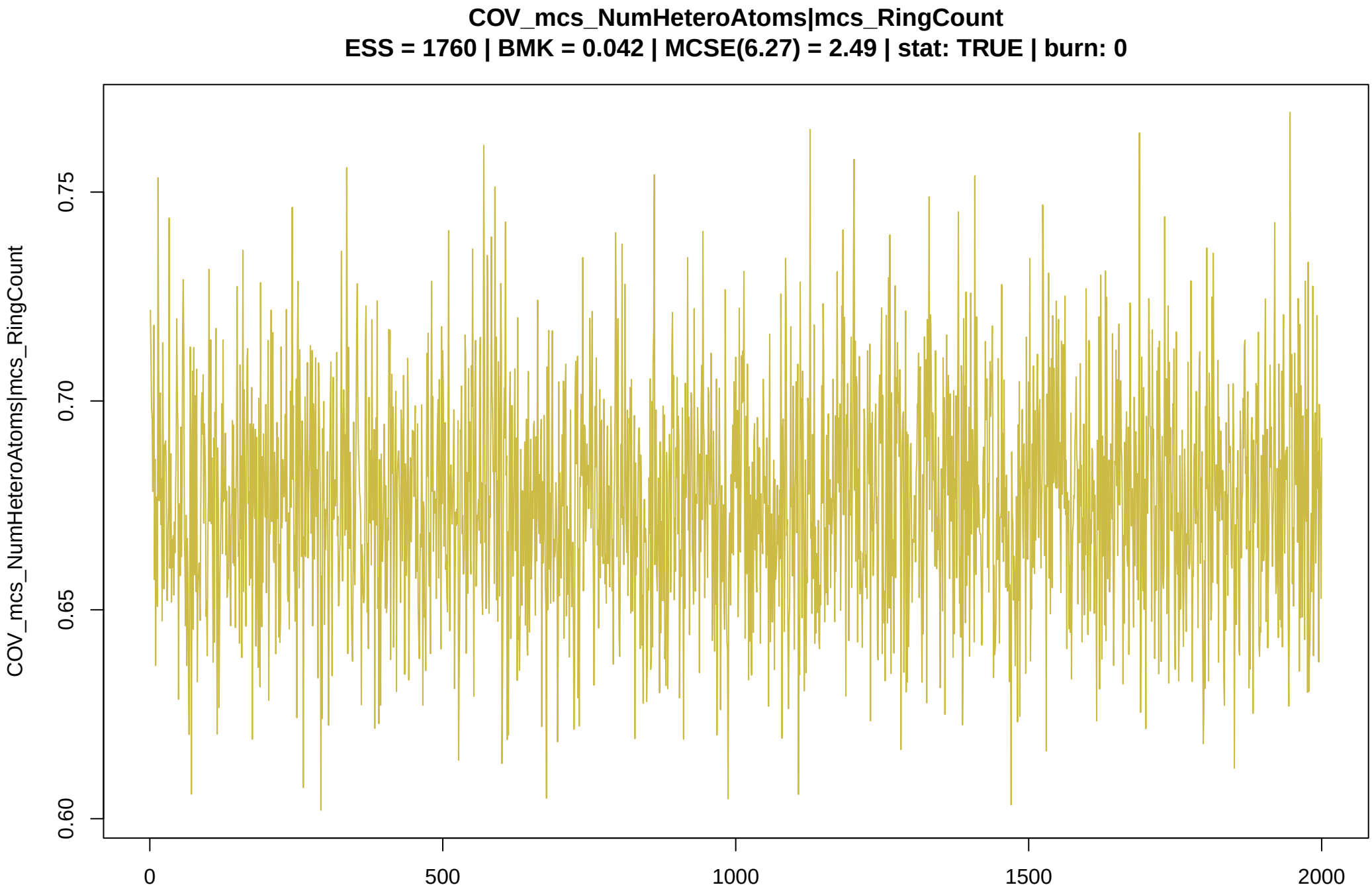

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1920 | BMK = 0.0392 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.80
0.85
0.90
0.95
0
500
1000
1500
2000

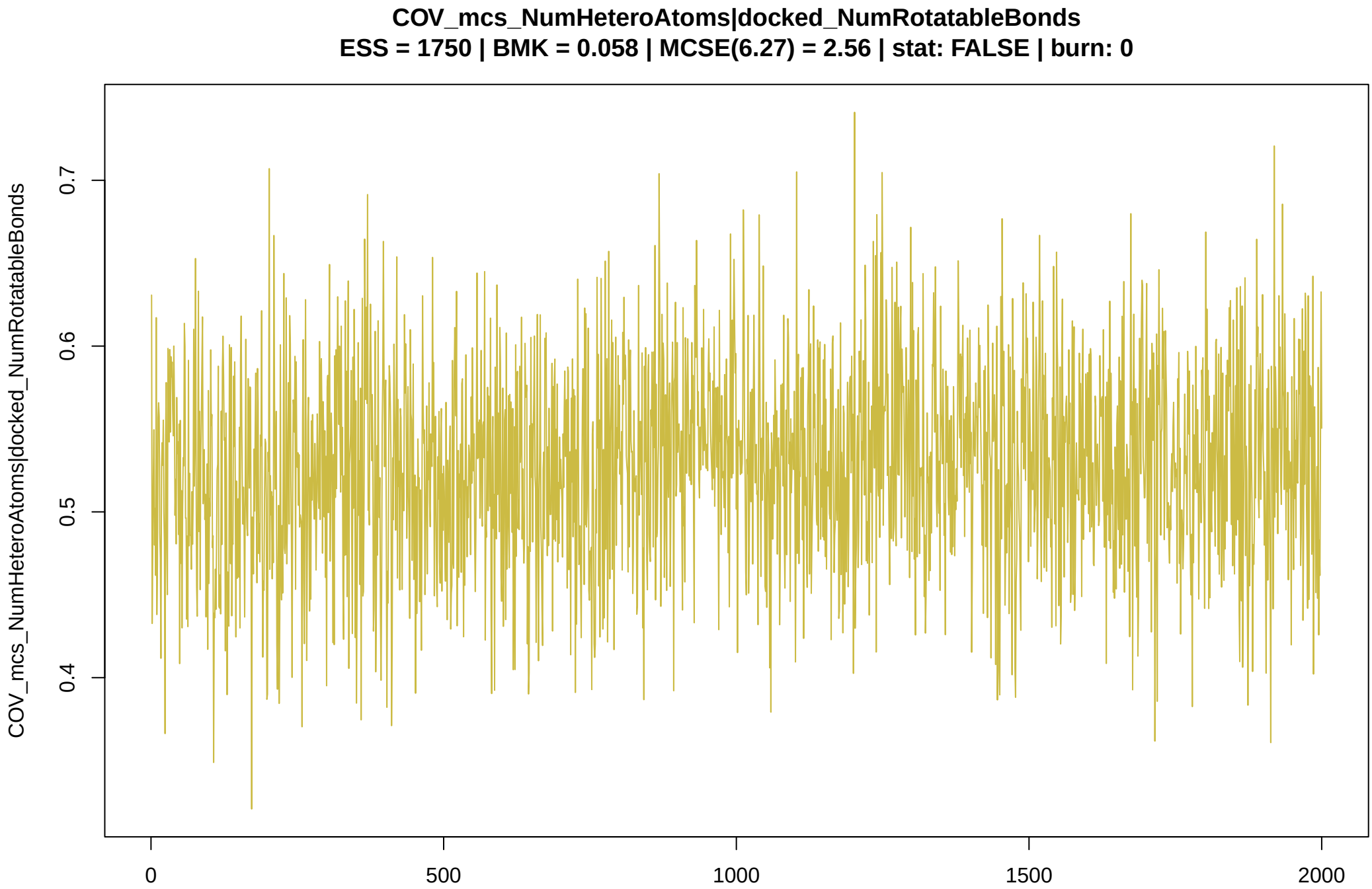

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1370 | BMK = 0.0851 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
1.1
1.2
1.3
1.4
1.5
1.6
0
500
1000
1500
2000

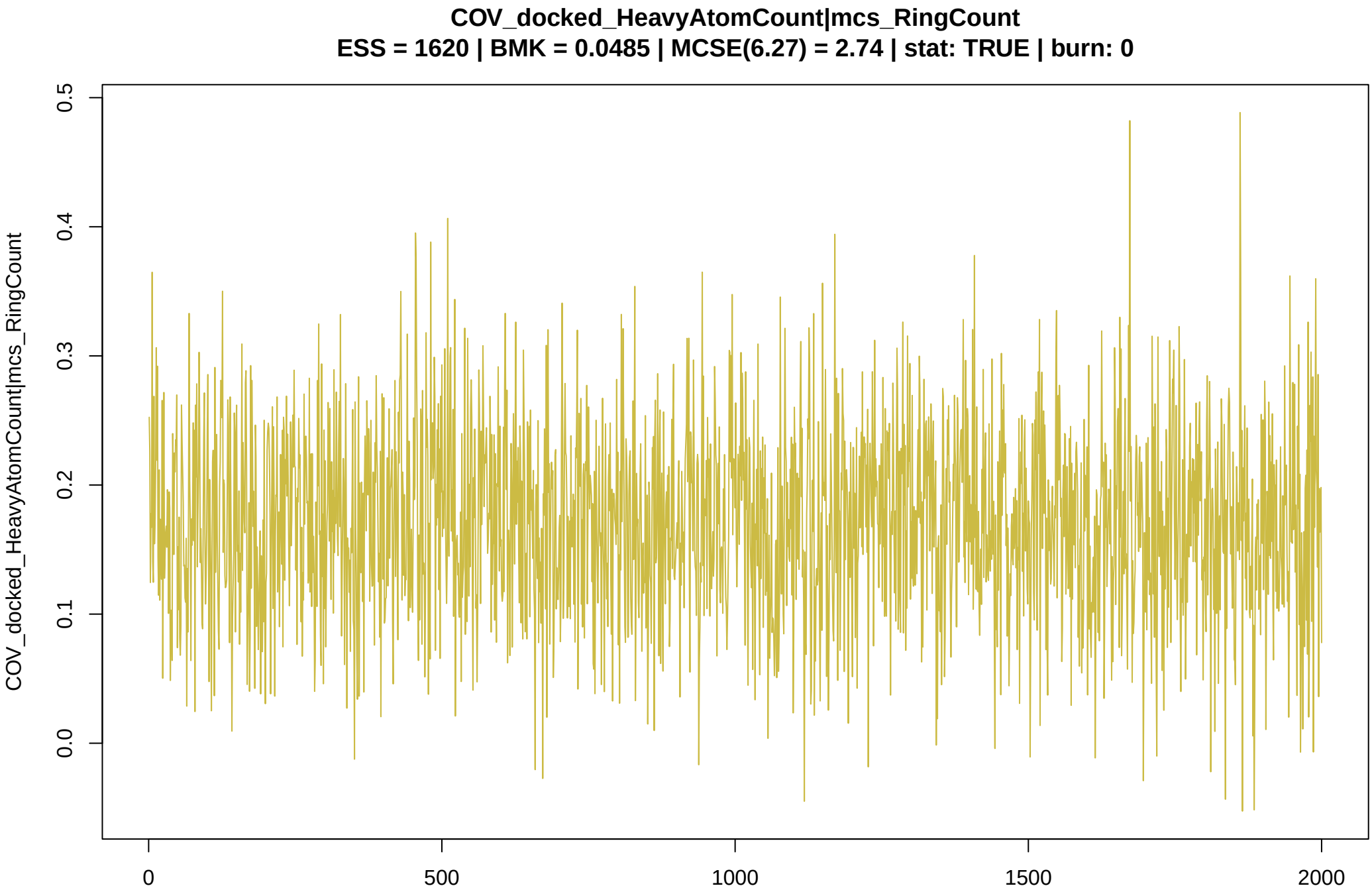

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1580 | BMK = 0.0439 | MCSE(6.27) = 2.85 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.36
0.38
0.40
0.42
0.44
0.46
0
500
1000
1500
2000

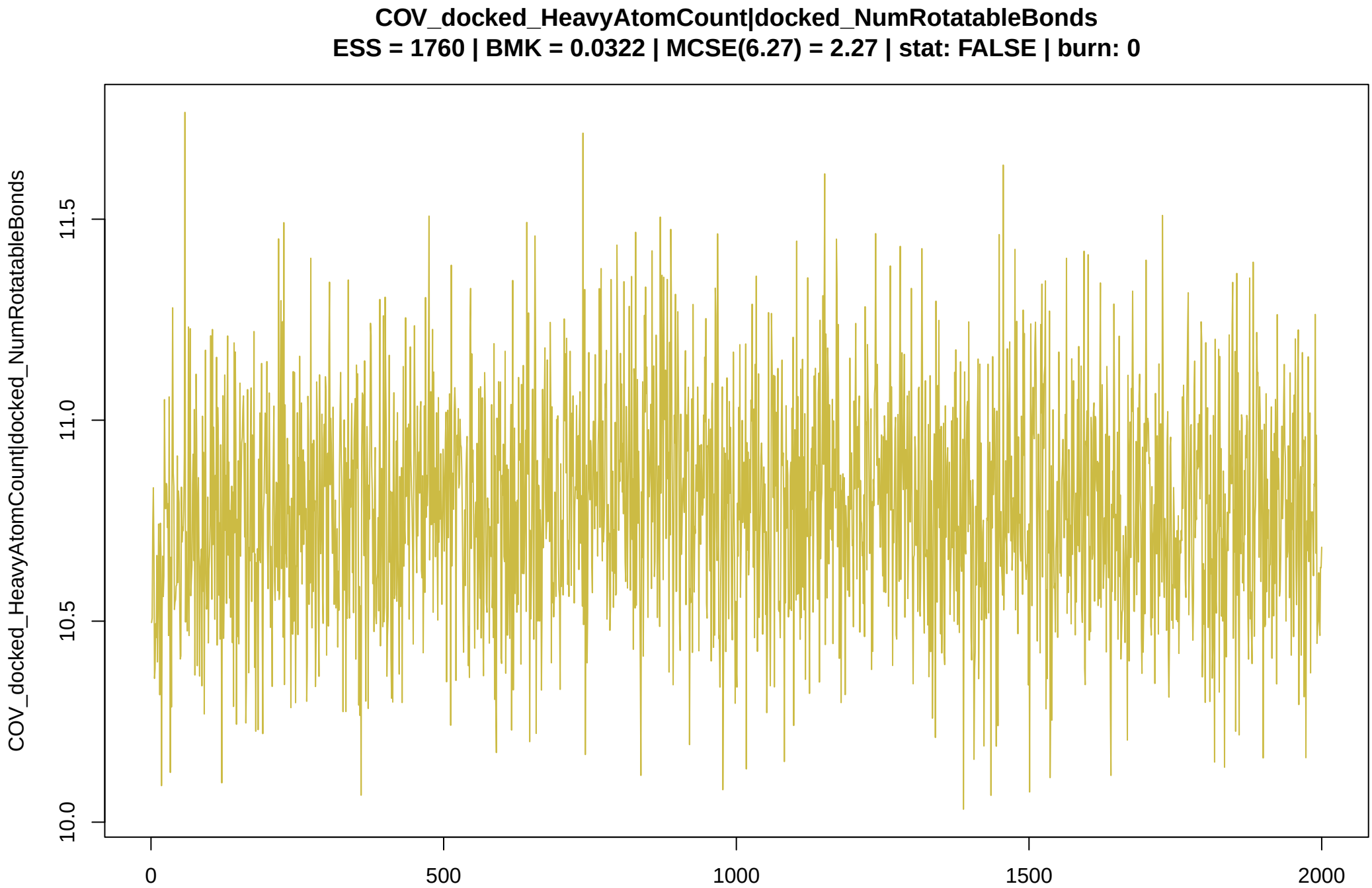

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1460 | BMK = 0.0522 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
0.40
0.45
0.50
0.55
0.60
0
500
1000
1500
2000

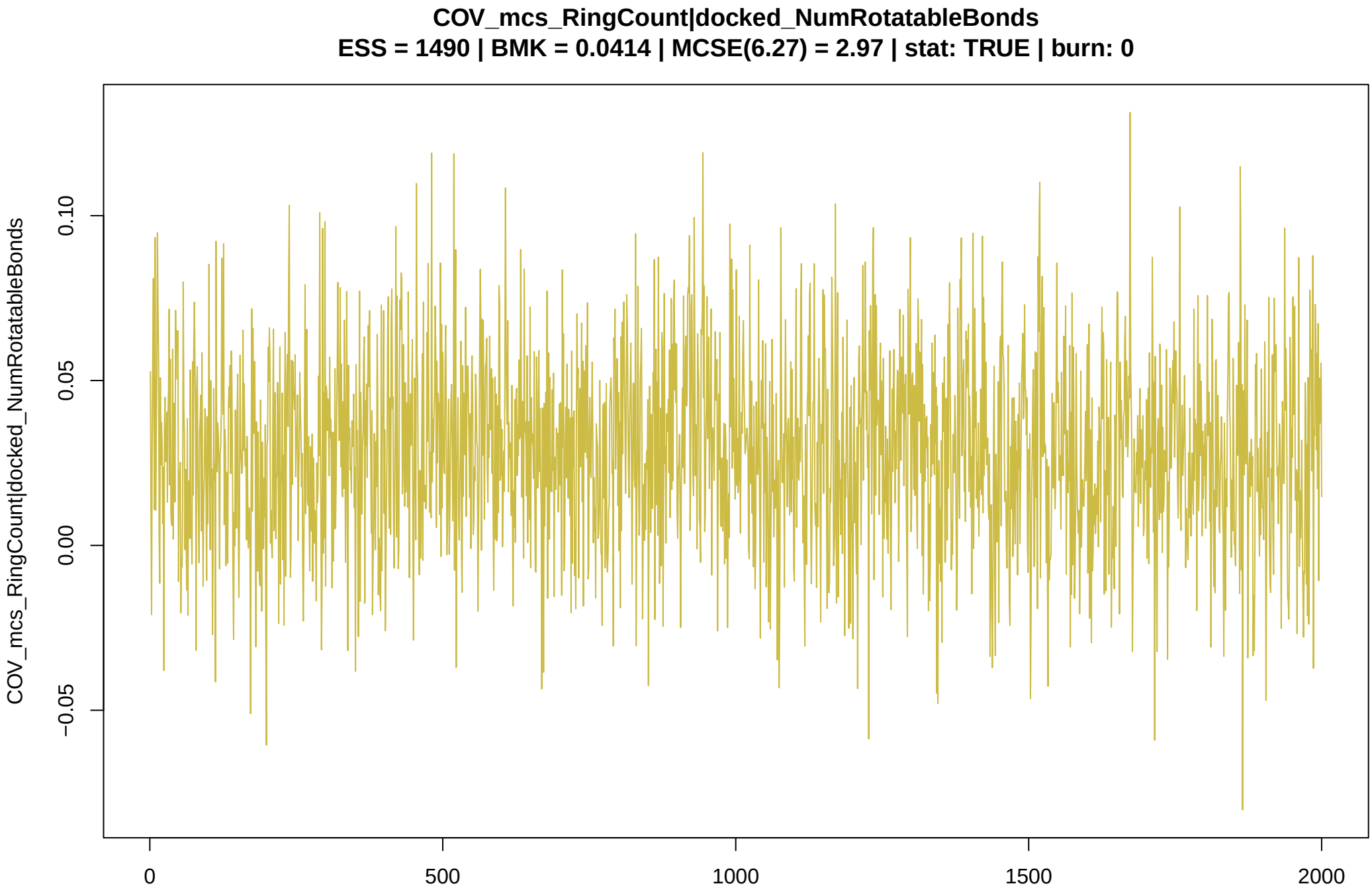

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1640 | BMK = 0.0647 | MCSE(6.27) = 2.8 | stat: FALSE | burn: 0
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
1.2
1.4
1.6
1.8
2.0
2.2
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1760 | BMK = 0.042 | MCSE(6.27) = 2.49 | stat: TRUE | 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 = 1750 | BMK = 0.058 | MCSE(6.27) = 2.56 | stat: FALSE | 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 = 1620 | BMK = 0.0485 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.0
0.1
0.2
0.3
0.4
0.5
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1760 | BMK = 0.0322 | MCSE(6.27) = 2.27 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10.0
10.5
11.0
11.5
0
500
1000
1500
2000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1490 | BMK = 0.0414 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 0
COV_mcs_RingCount|docked_NumRotatableBonds
0.10
0.05
0.00
−0.05
0
500
1000
1500
2000