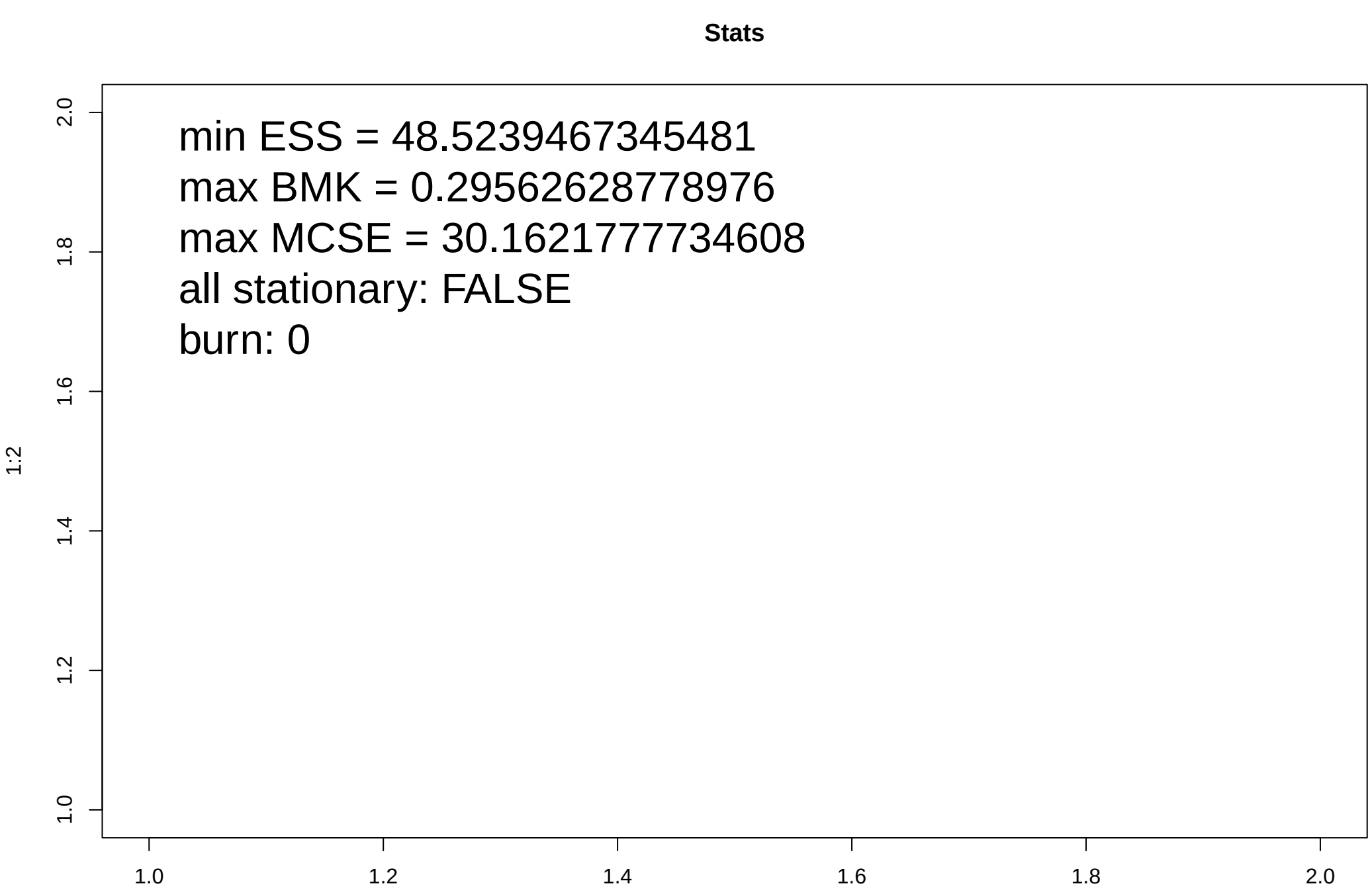
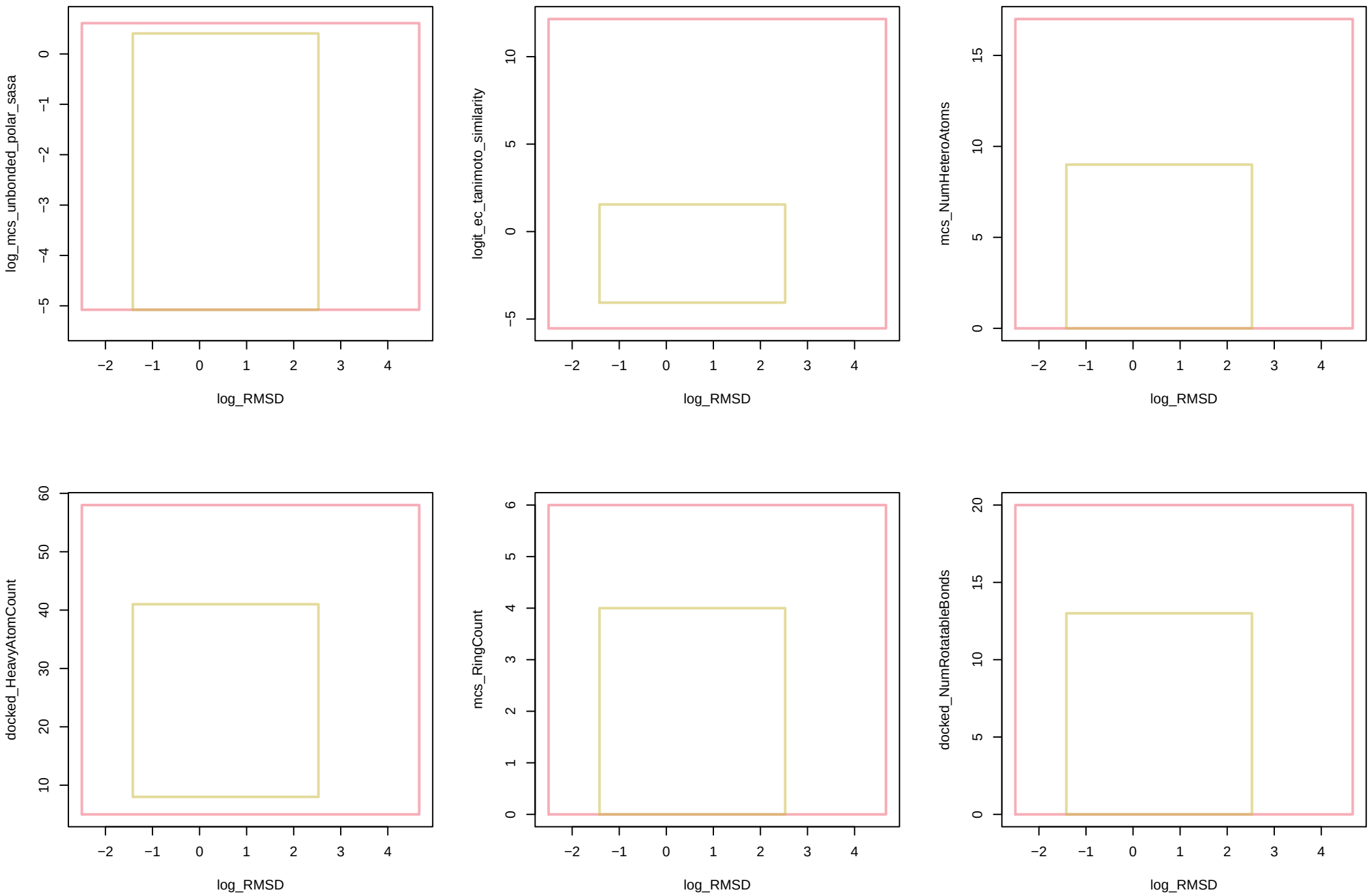
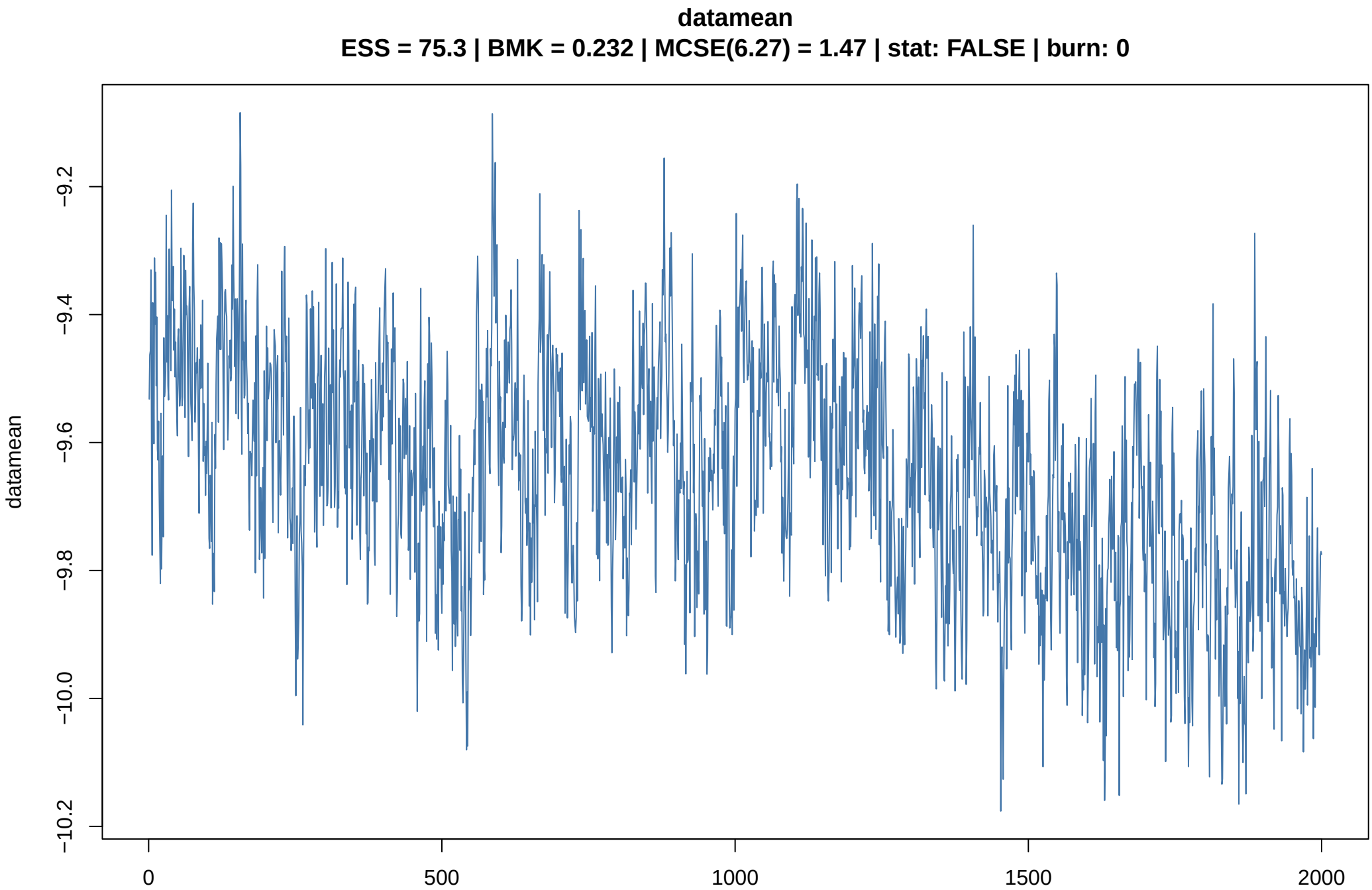
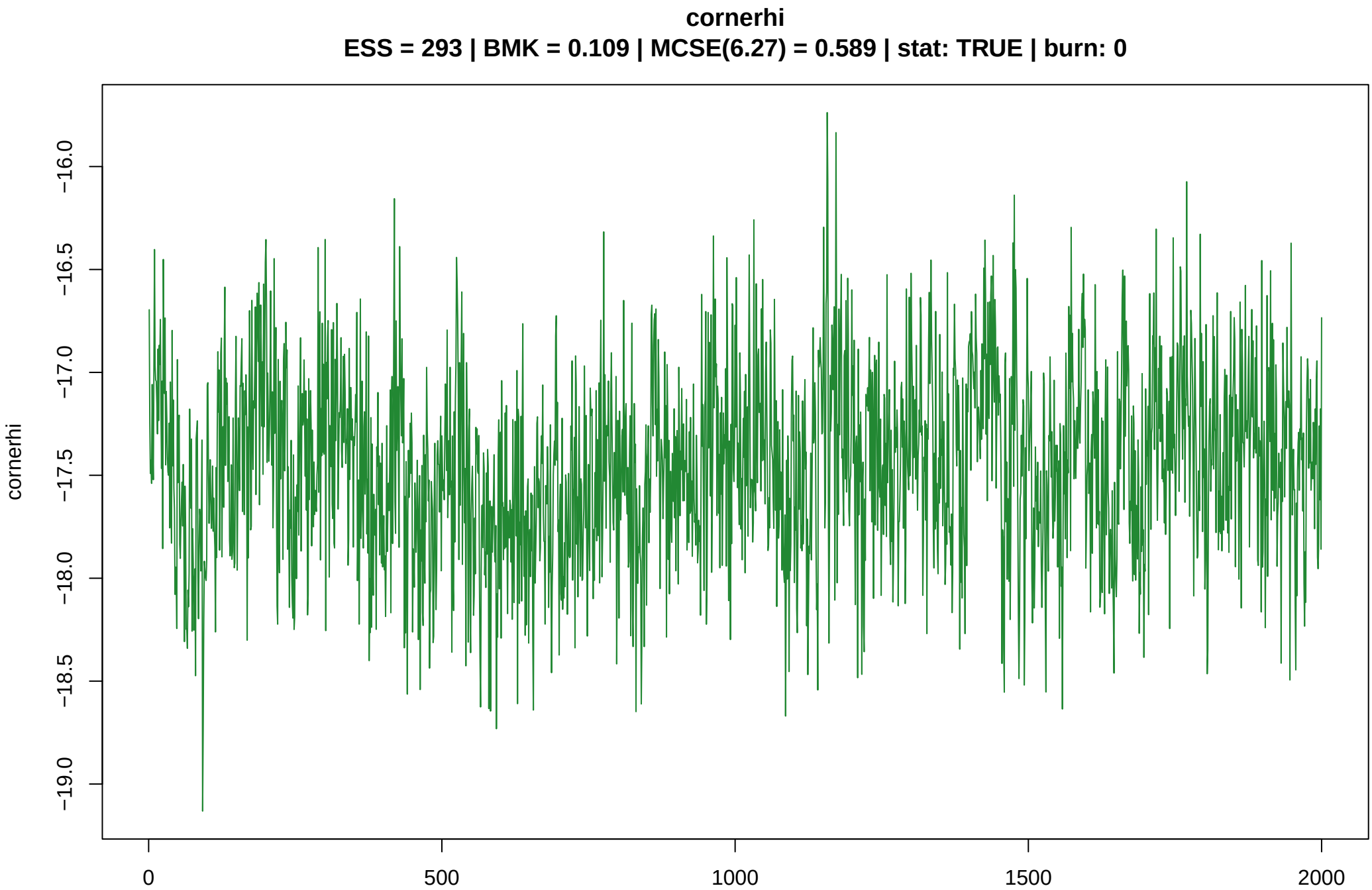
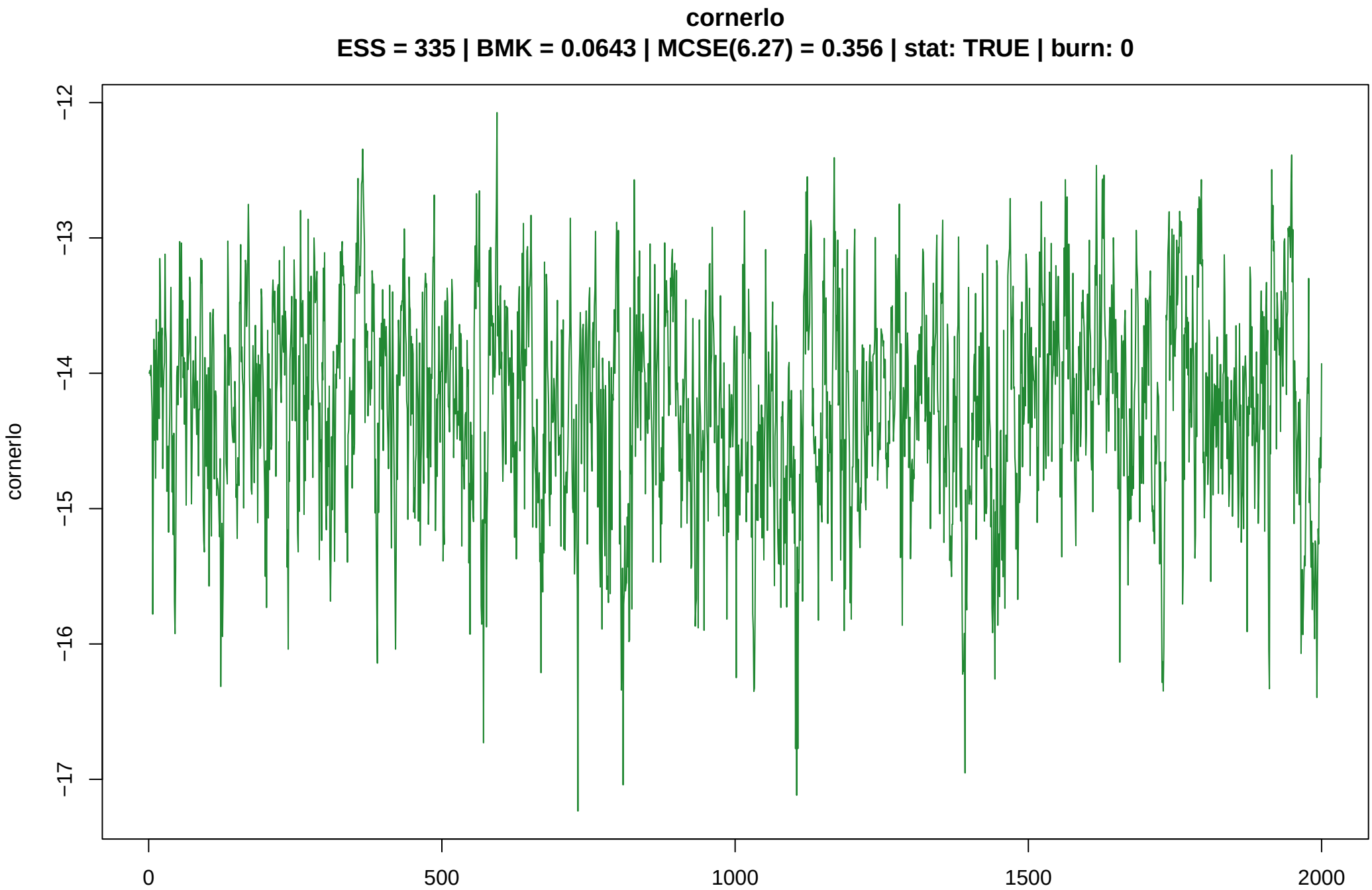
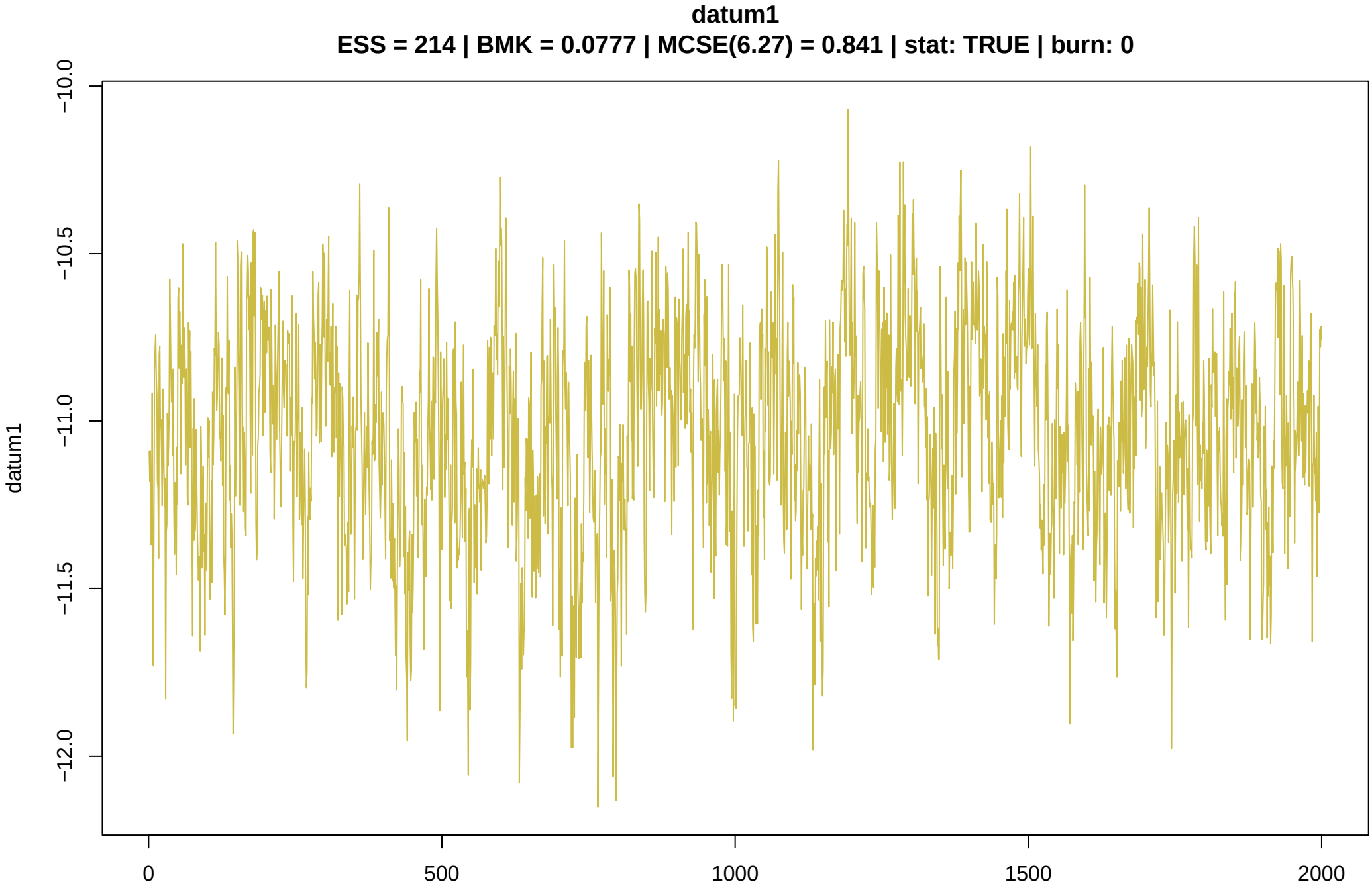

Stats
min ESS = 48.5239467345481
max BMK = 0.29562628778976
max MCSE = 30.1621777734608
all stationary: FALSE
burn: 0
1:2
1.0
1.2
1.4
1.6
1.8
2.0

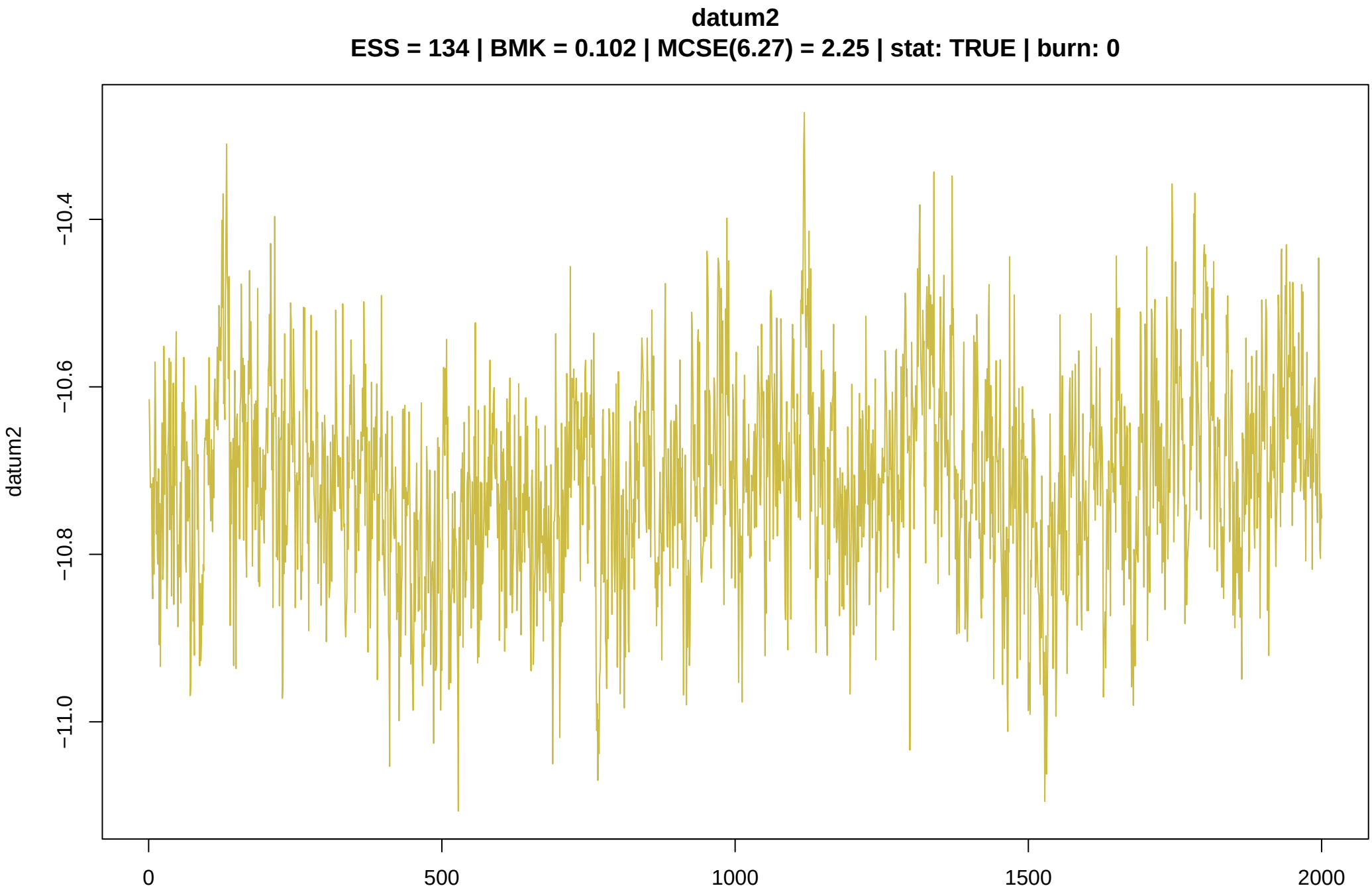

log_mcs_unbonded_polar_sasa
logit_ec_tanimoto_similarity
mcs_NumHeteroAtoms
docked_HeavyAtomCount
mcs_RingCount
docked_NumRotatableBonds
log_RMSD

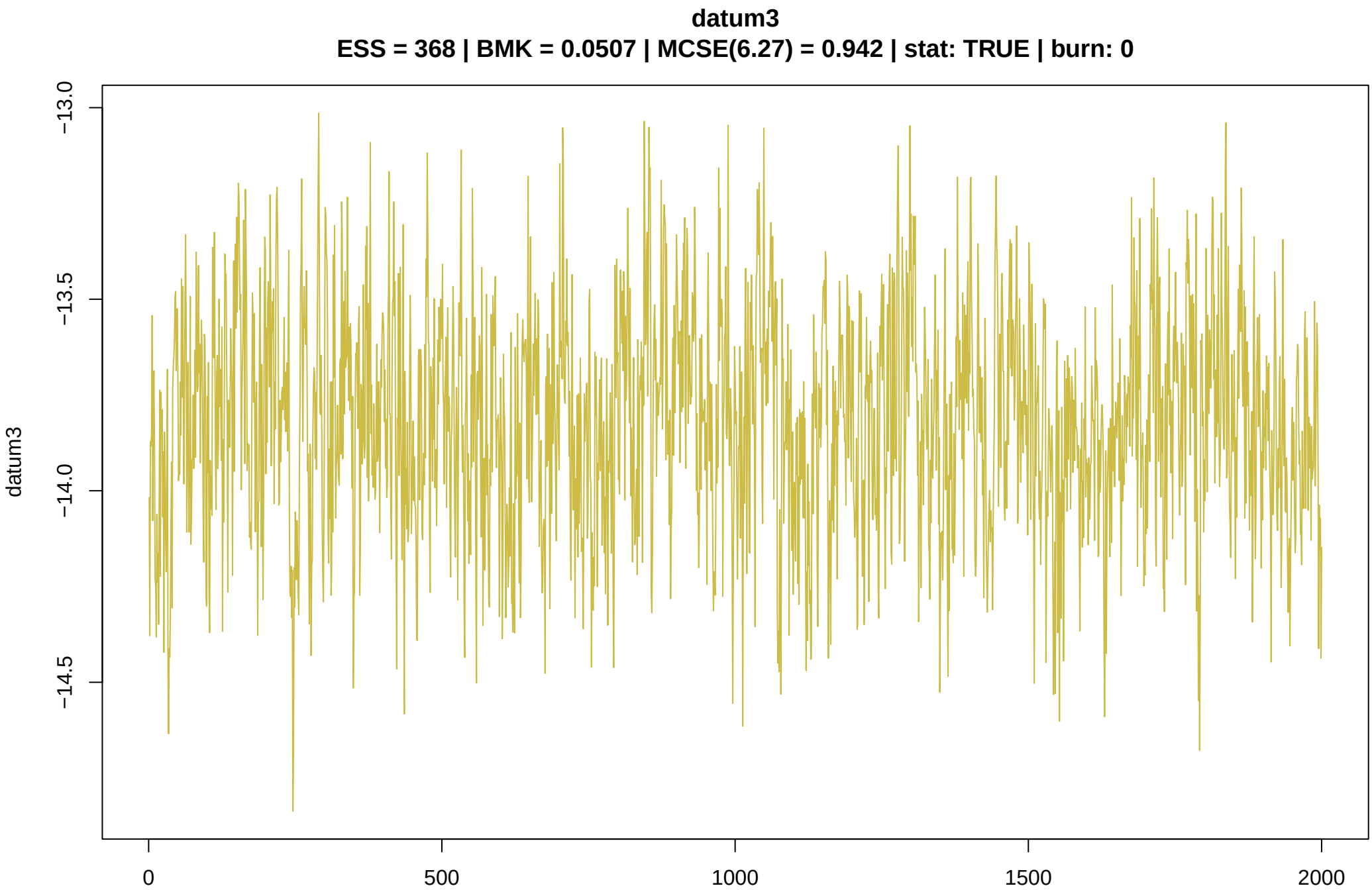

datamean
ESS = 75.3 | BMK = 0.232 | MCSE(6.27) = 1.47 | stat: FALSE | burn: 0
datamean
−9.2
−9.4
−9.6
−9.8
−10.0
−10.2
0
500
1000
1500
2000

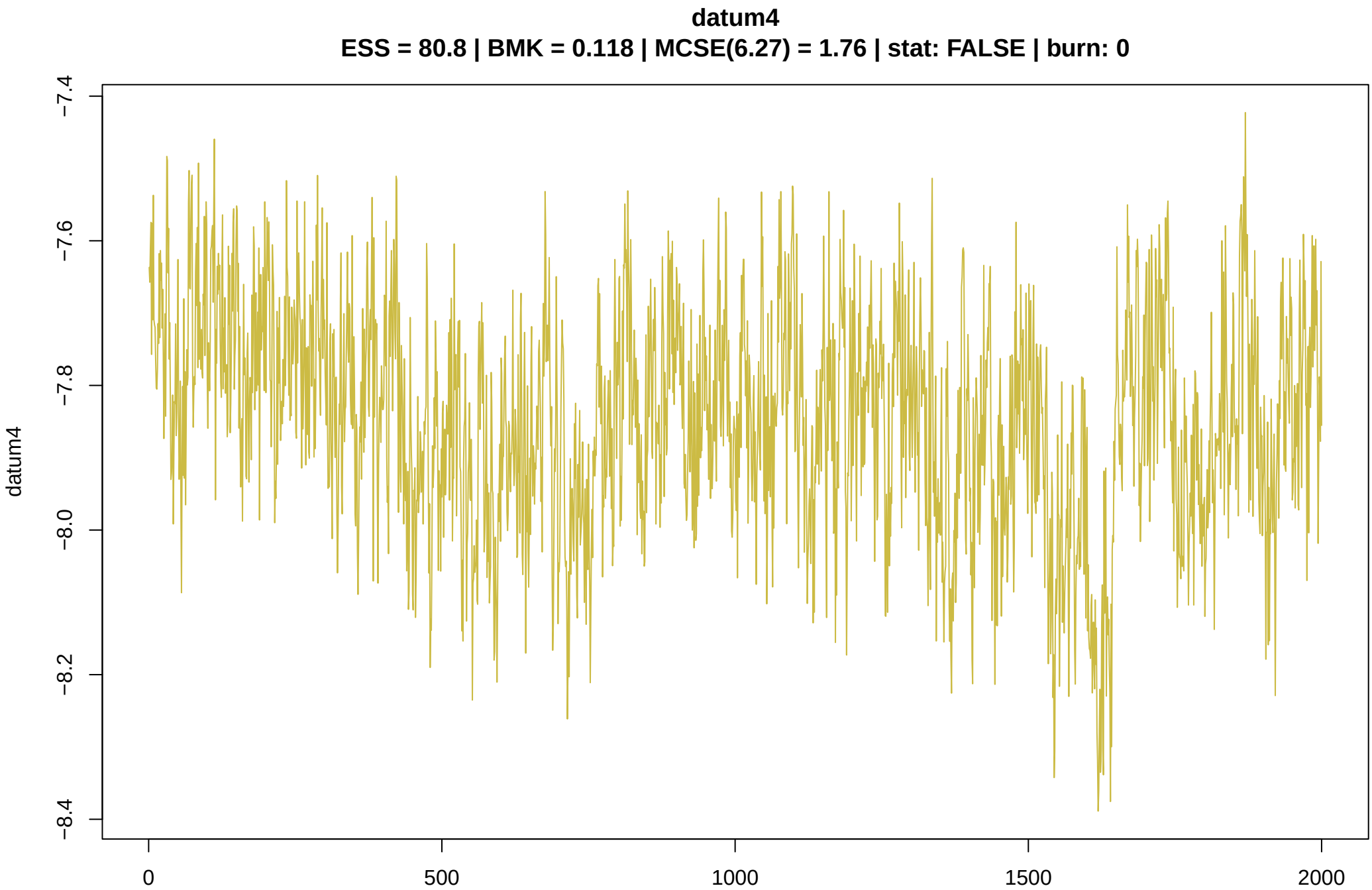

cornerhi
ESS = 293 | BMK = 0.109 | MCSE(6.27) = 0.589 | stat: TRUE | burn: 0
cornerhi
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
−19.0
0
500
1000
1500
2000

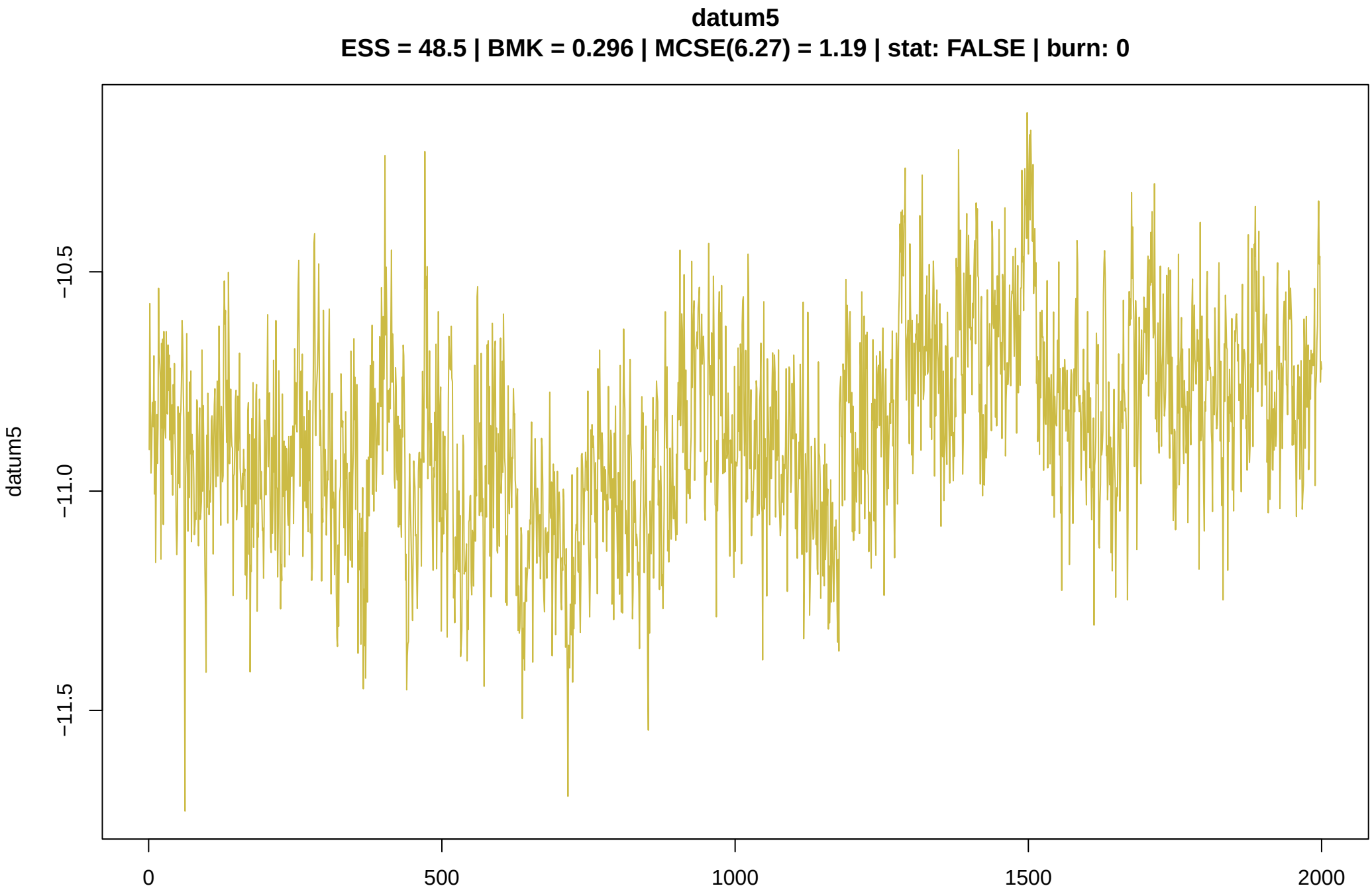

cornerlo
ESS = 335 | BMK = 0.0643 | MCSE(6.27) = 0.356 | stat: TRUE | burn: 0
cornerlo
−12
−13
−14
−15
−16
−17
0
500
1000
1500
2000

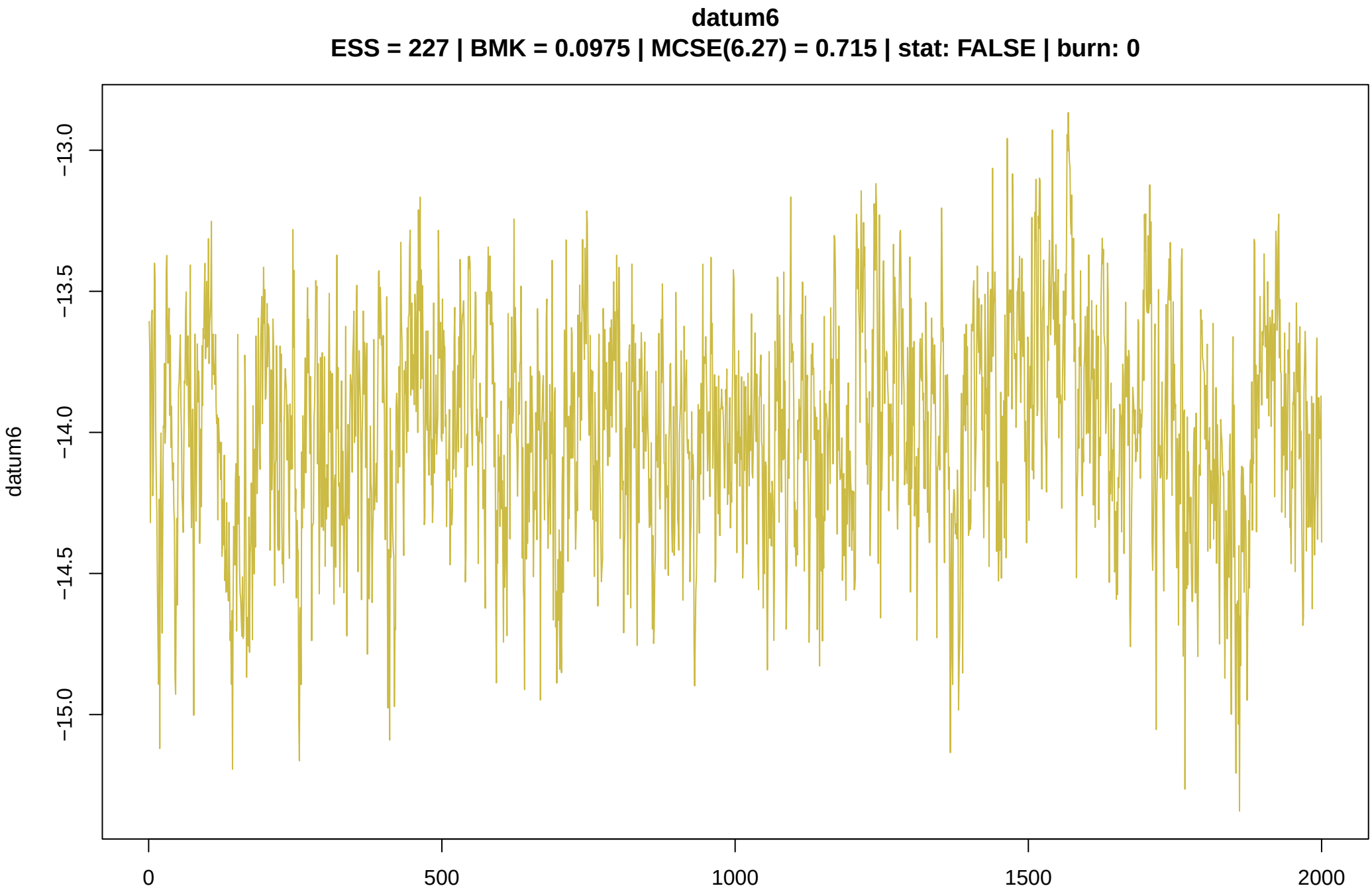

datum1
ESS = 214 | BMK = 0.0777 | MCSE(6.27) = 0.841 | stat: TRUE | burn: 0
datum1
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

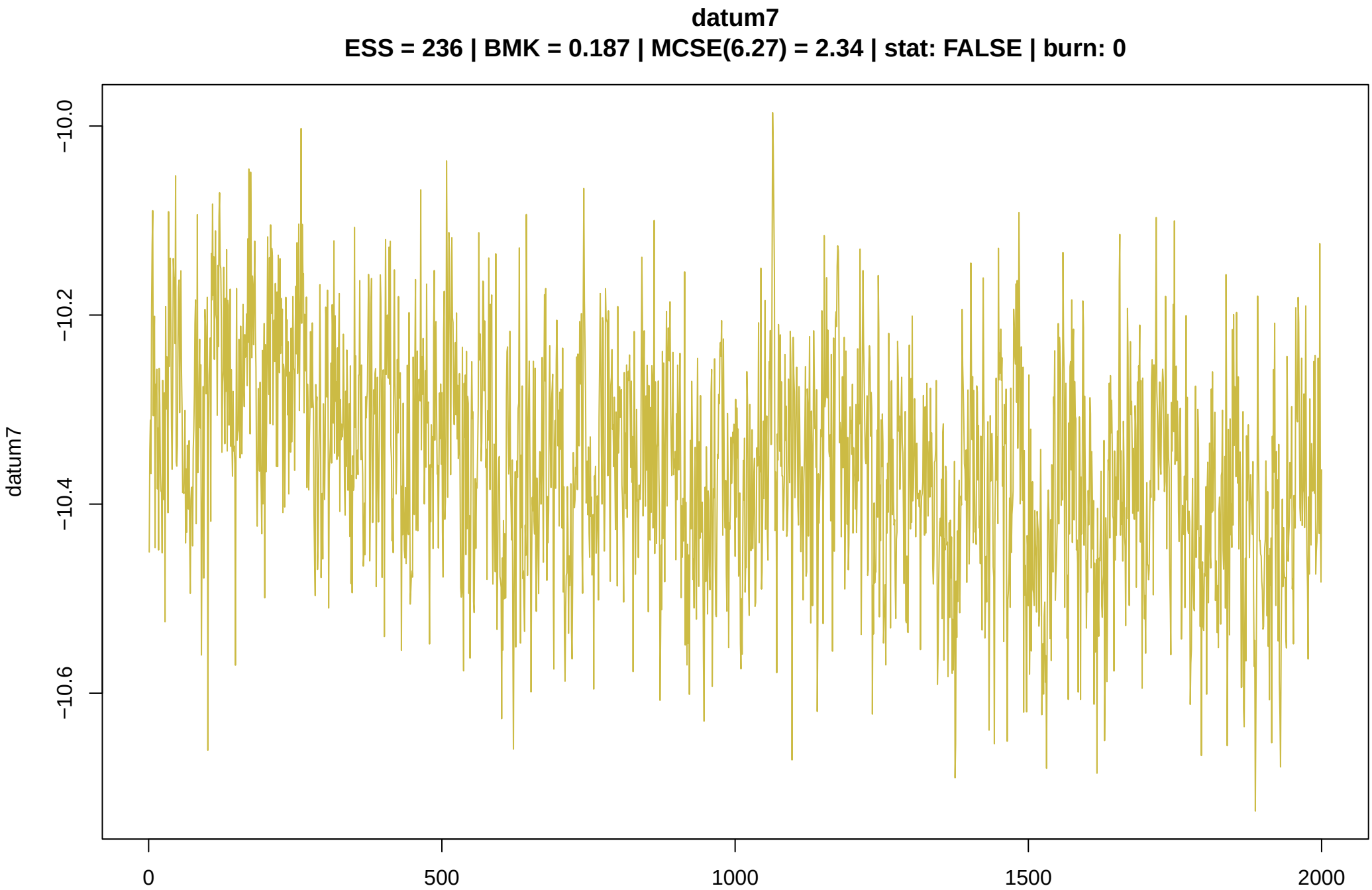

datum2
ESS = 134 | BMK = 0.102 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0
datum2
−10.4
−10.6
−10.8
−11.0
0
500
1000
1500
2000

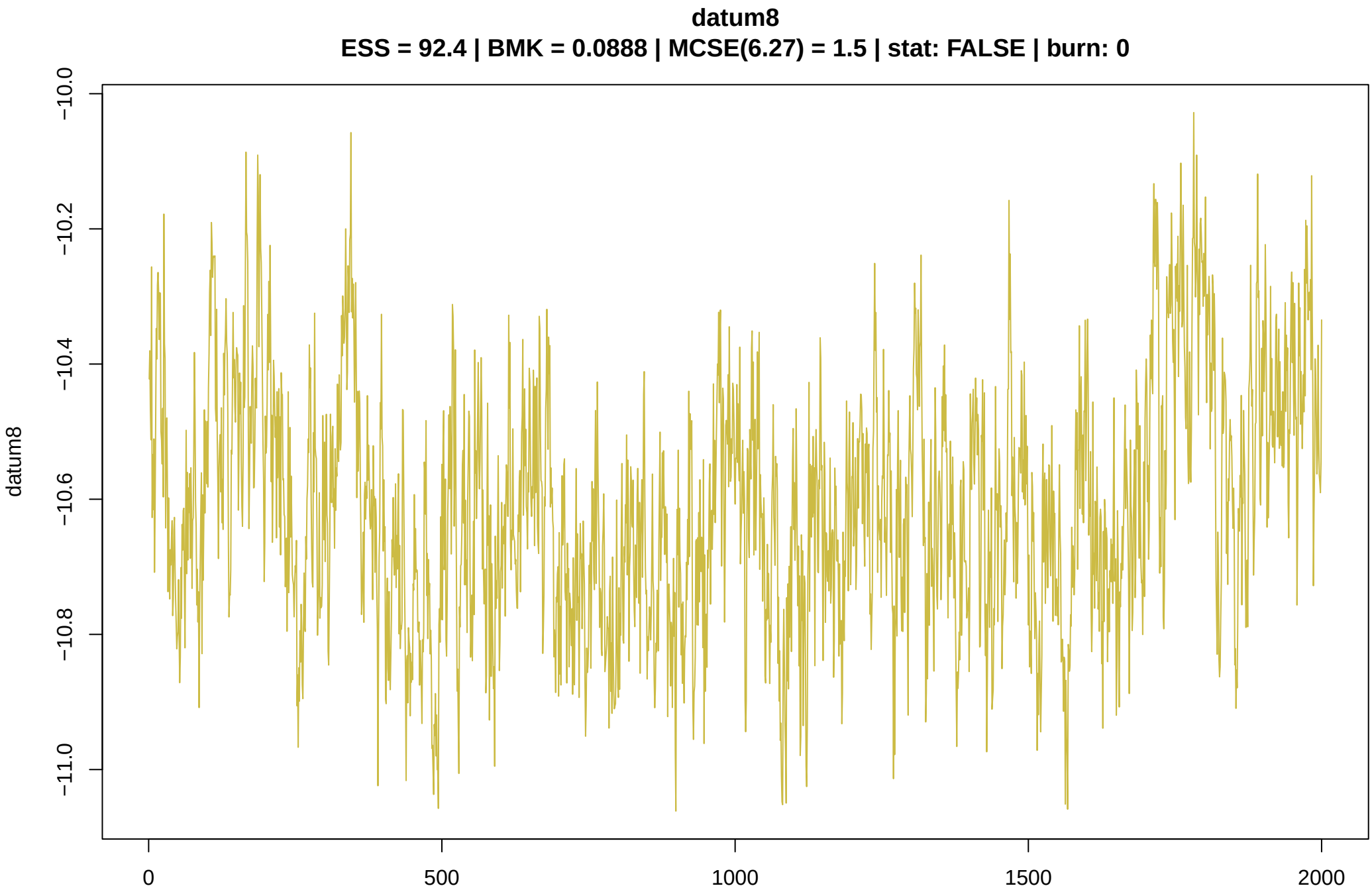

datum3
ESS = 368 | BMK = 0.0507 | MCSE(6.27) = 0.942 | stat: TRUE | burn: 0
datum3
−13.0
−13.5
−14.0
−14.5
0
500
1000
1500
2000

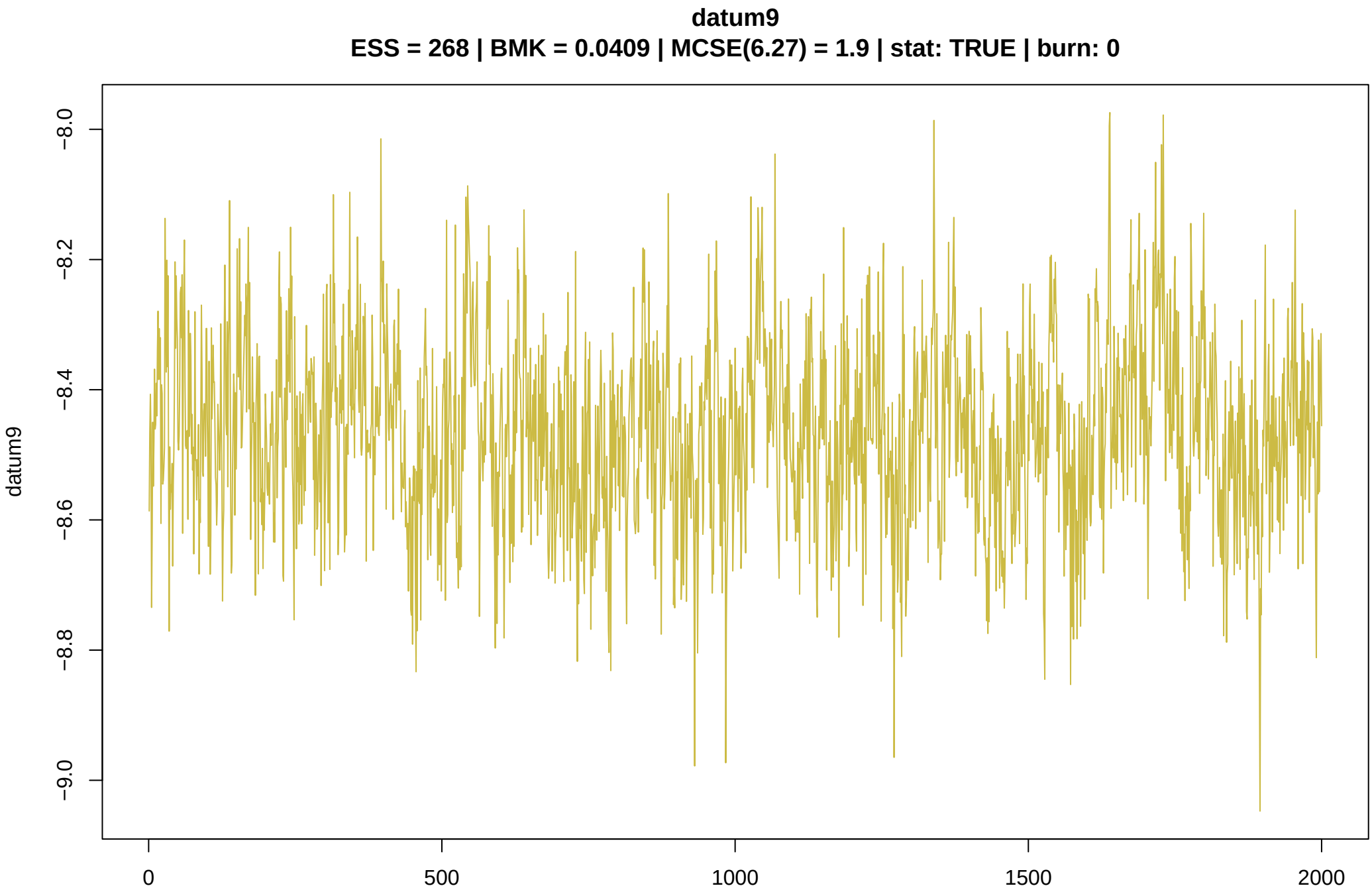

datum4
ESS = 80.8 | BMK = 0.118 | MCSE(6.27) = 1.76 | stat: FALSE | burn: 0
datum4
−7.4
−7.6
−7.8
−8.0
−8.2
−8.4
0
500
1000
1500
2000

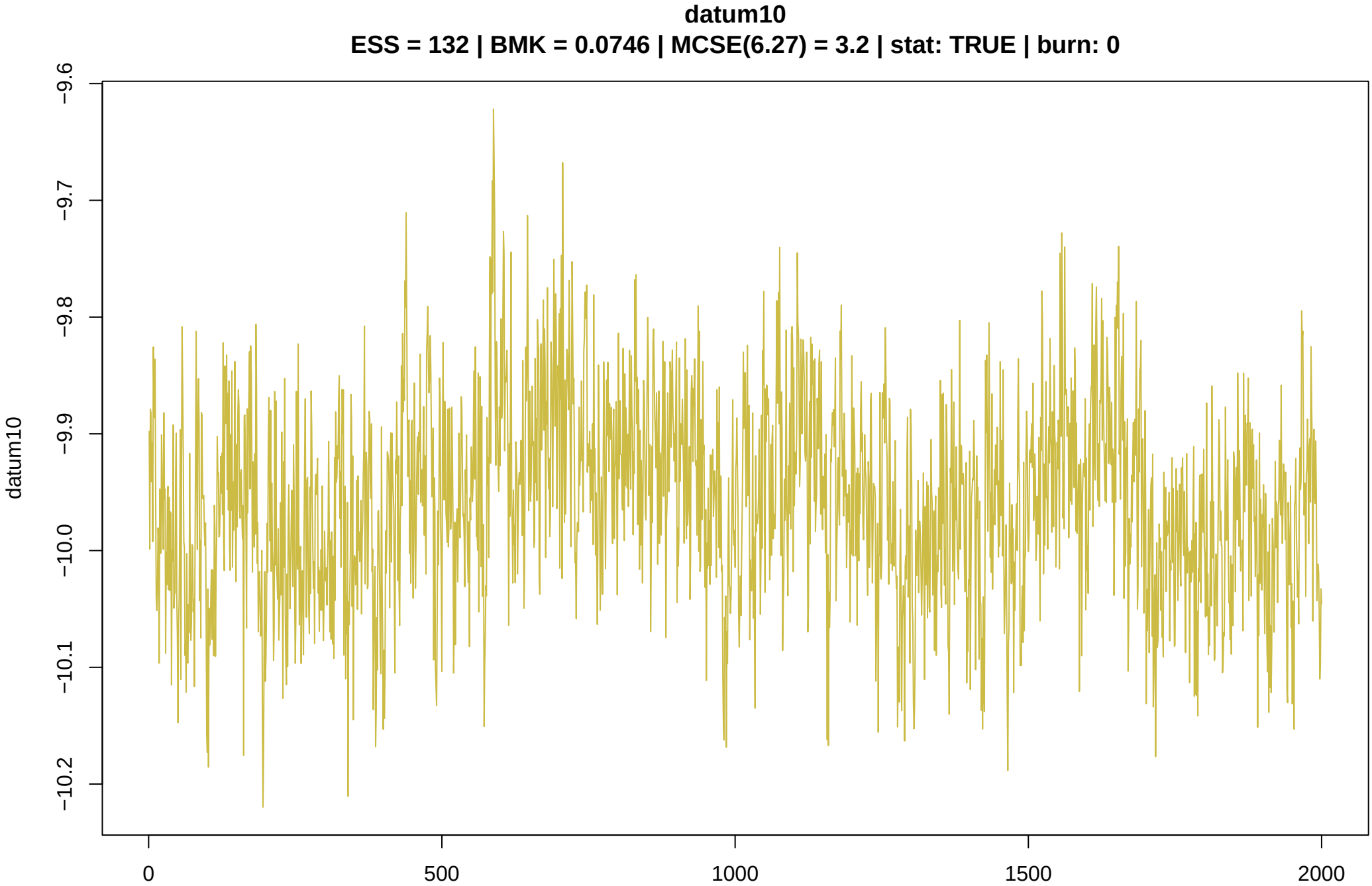

datum5
ESS = 48.5 | BMK = 0.296 | MCSE(6.27) = 1.19 | stat: FALSE | burn: 0
datum5
−10.5
−11.0
−11.5
0
500
1000
1500
2000

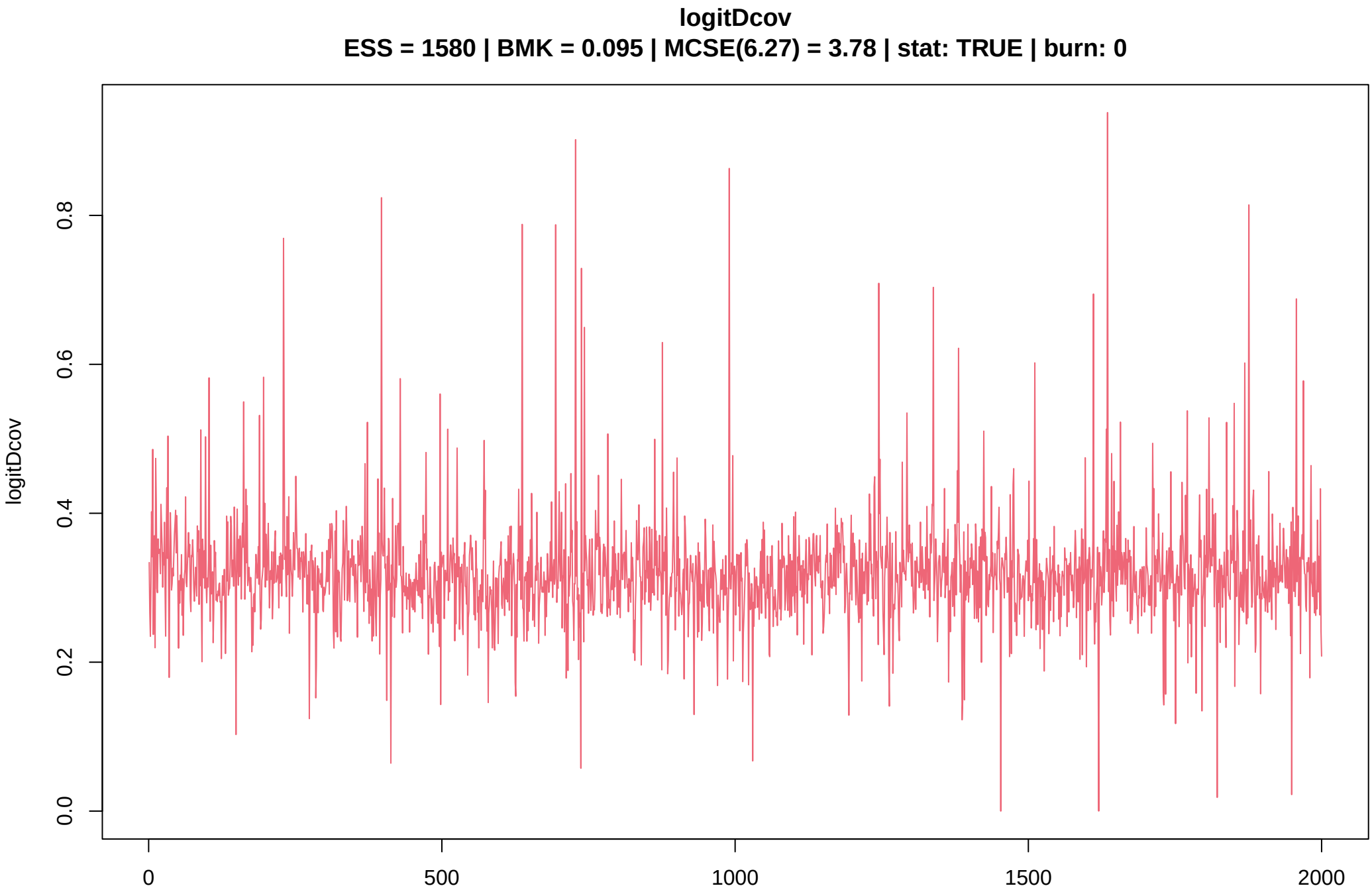

datum6
ESS = 227 | BMK = 0.0975 | MCSE(6.27) = 0.715 | stat: FALSE | burn: 0
datum6
−13.0
−13.5
−14.0
−14.5
−15.0
0
500
1000
1500
2000

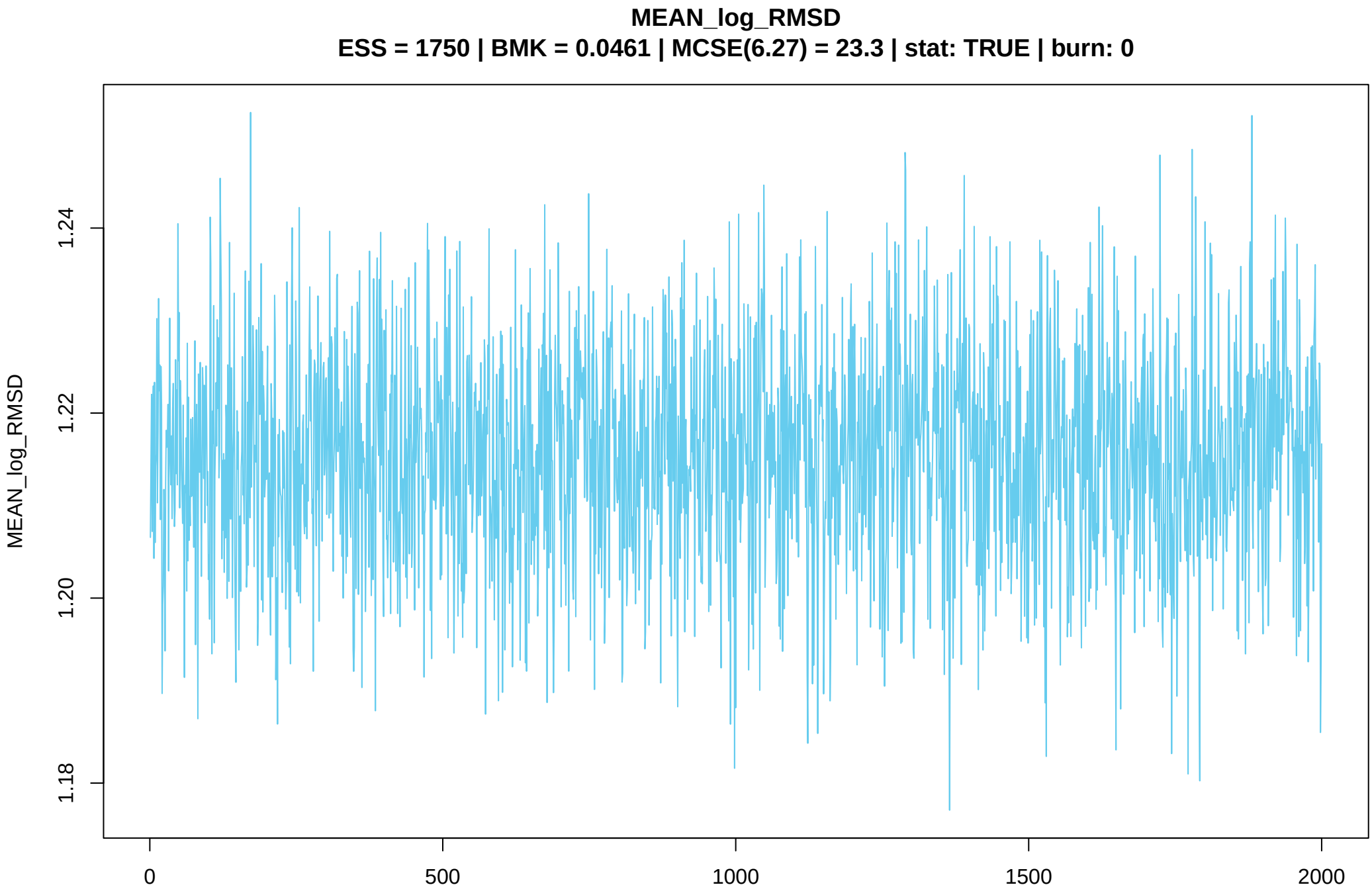

datum7
ESS = 236 | BMK = 0.187 | MCSE(6.27) = 2.34 | stat: FALSE | burn: 0
datum7
−10.0
−10.2
−10.4
−10.6
0
500
1000
1500
2000

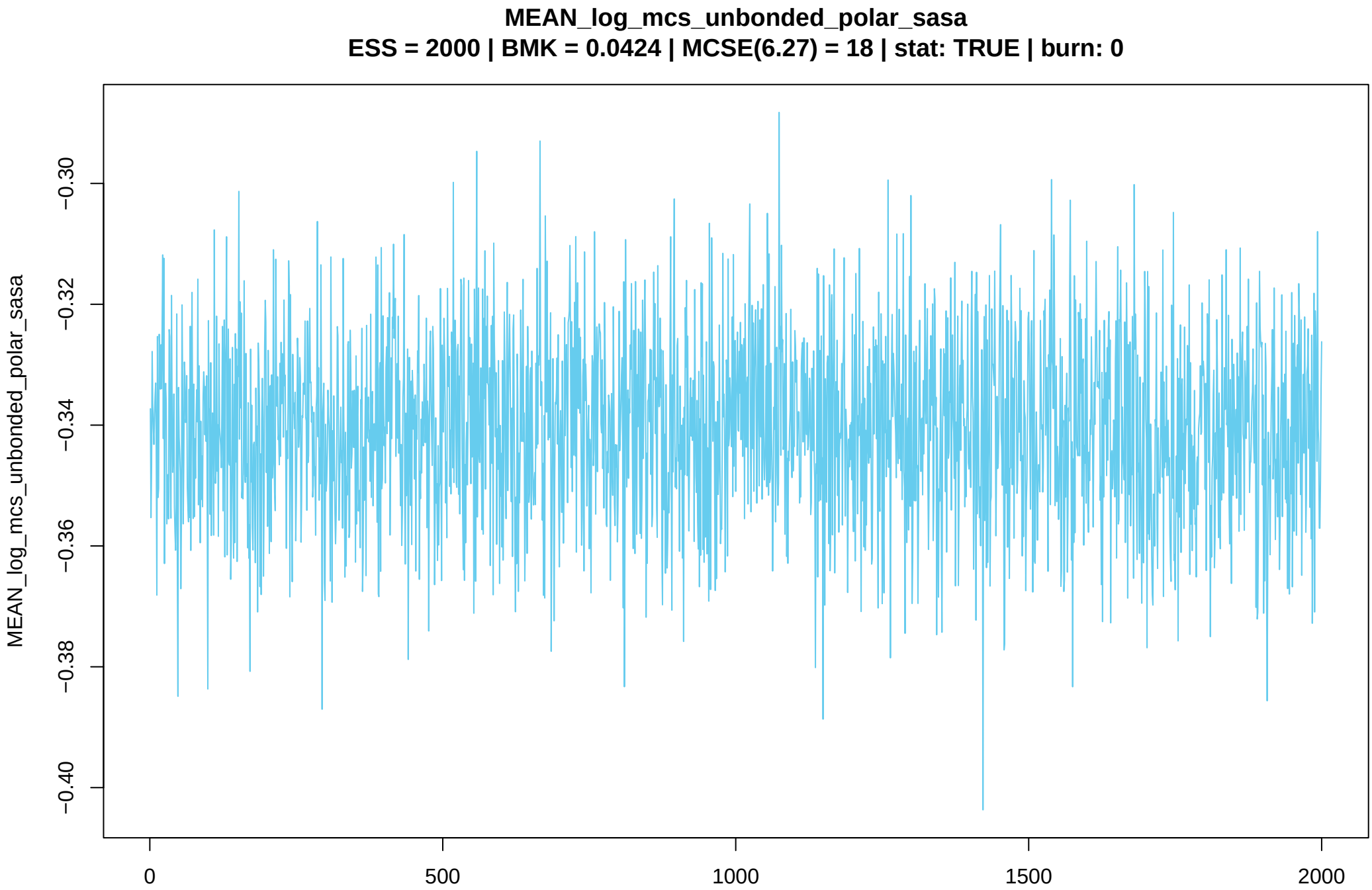

datum8
ESS = 92.4 | BMK = 0.0888 | MCSE(6.27) = 1.5 | stat: FALSE | burn: 0
datum8
−10.0
−10.2
−10.4
−10.6
−10.8
−11.0
0
500
1000
1500
2000

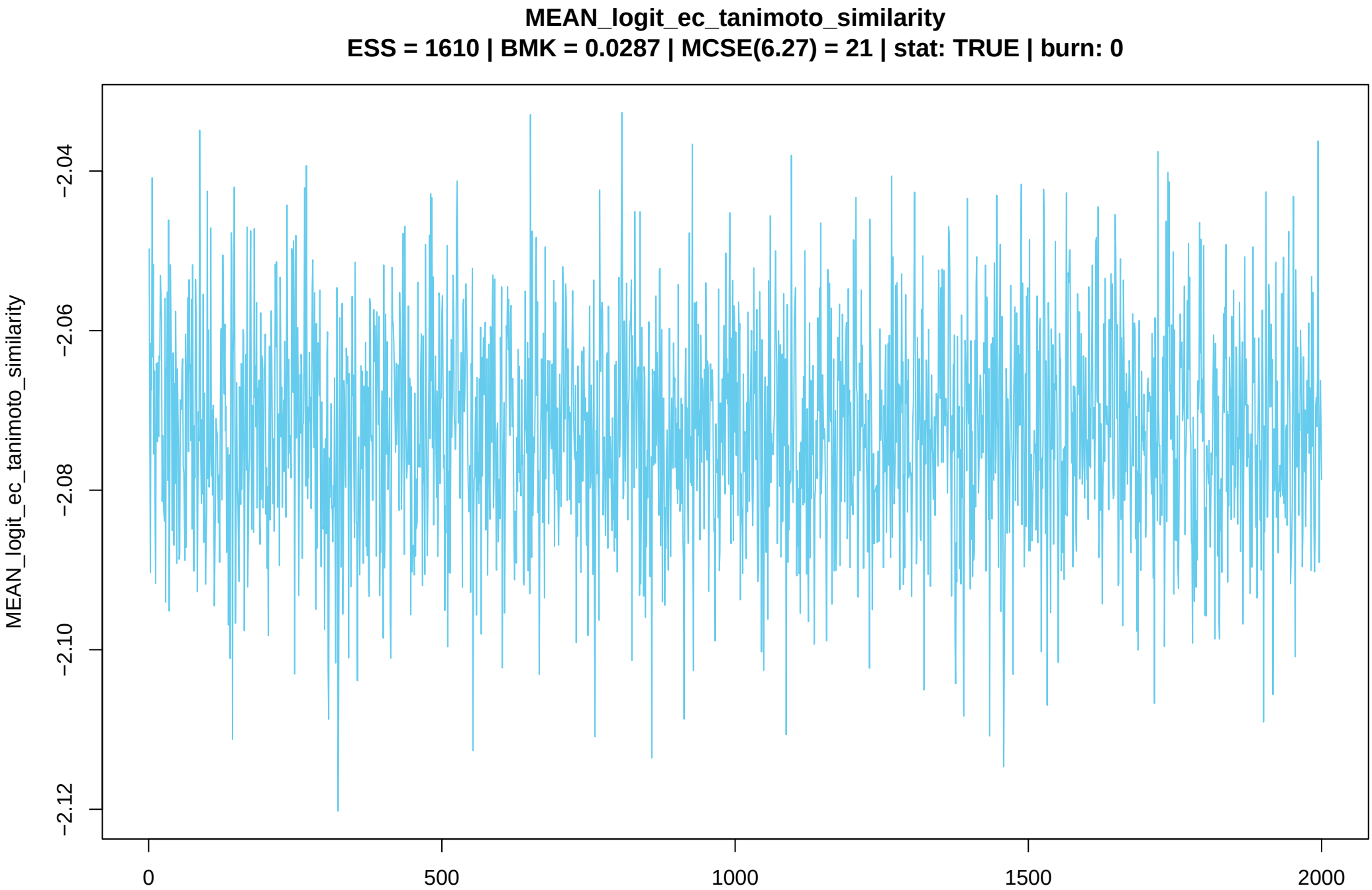

datum9
ESS = 268 | BMK = 0.0409 | MCSE(6.27) = 1.9 | stat: TRUE | burn: 0
datum9
−8.0
−8.2
−8.4
−8.6
−8.8
−9.0
0
500
1000
1500
2000

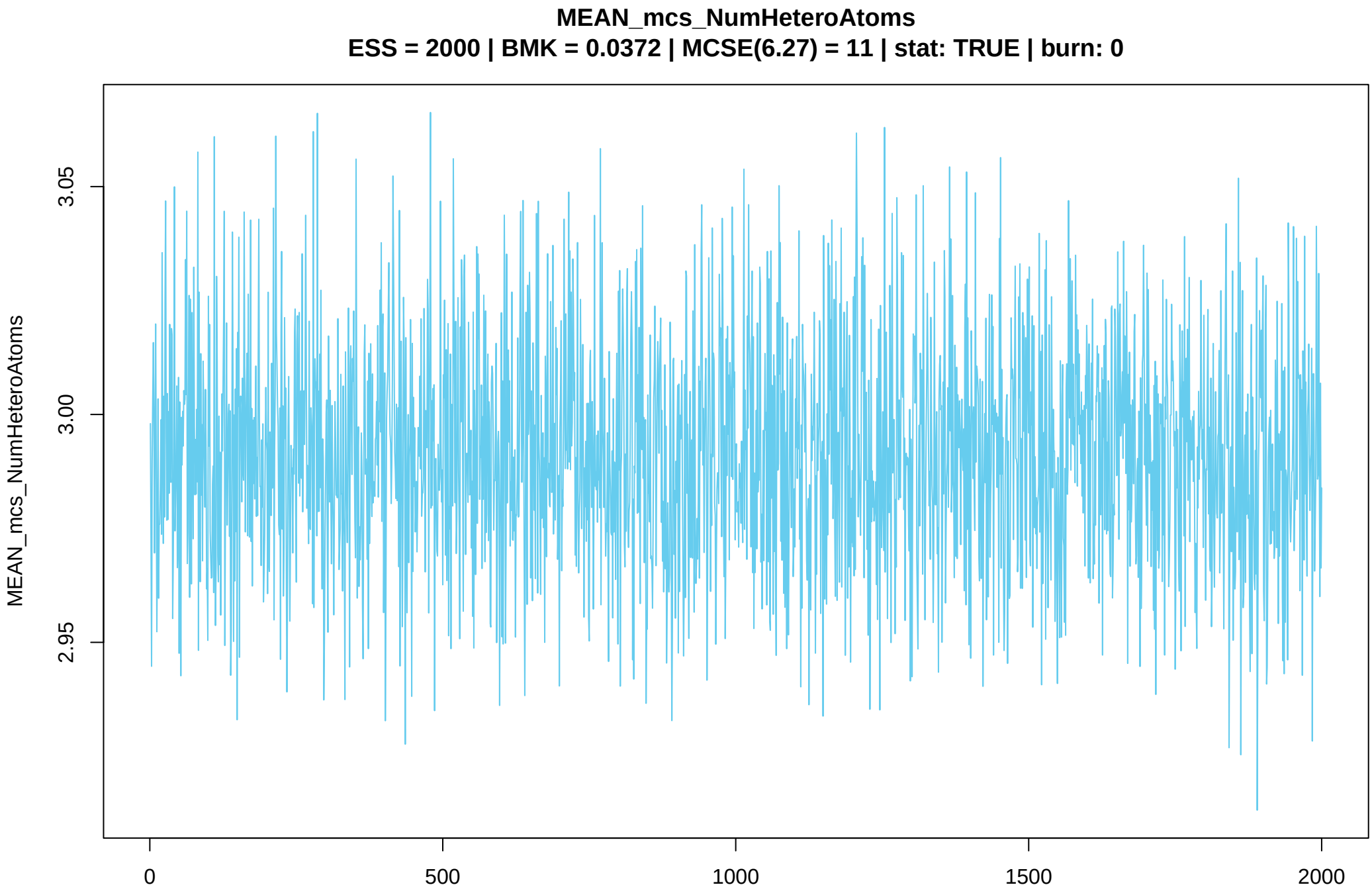

datum10
ESS = 132 | BMK = 0.0746 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0
datum10
−9.6
−9.7
−9.8
−9.9
−10.0
−10.1
−10.2
0
500
1000
1500
2000

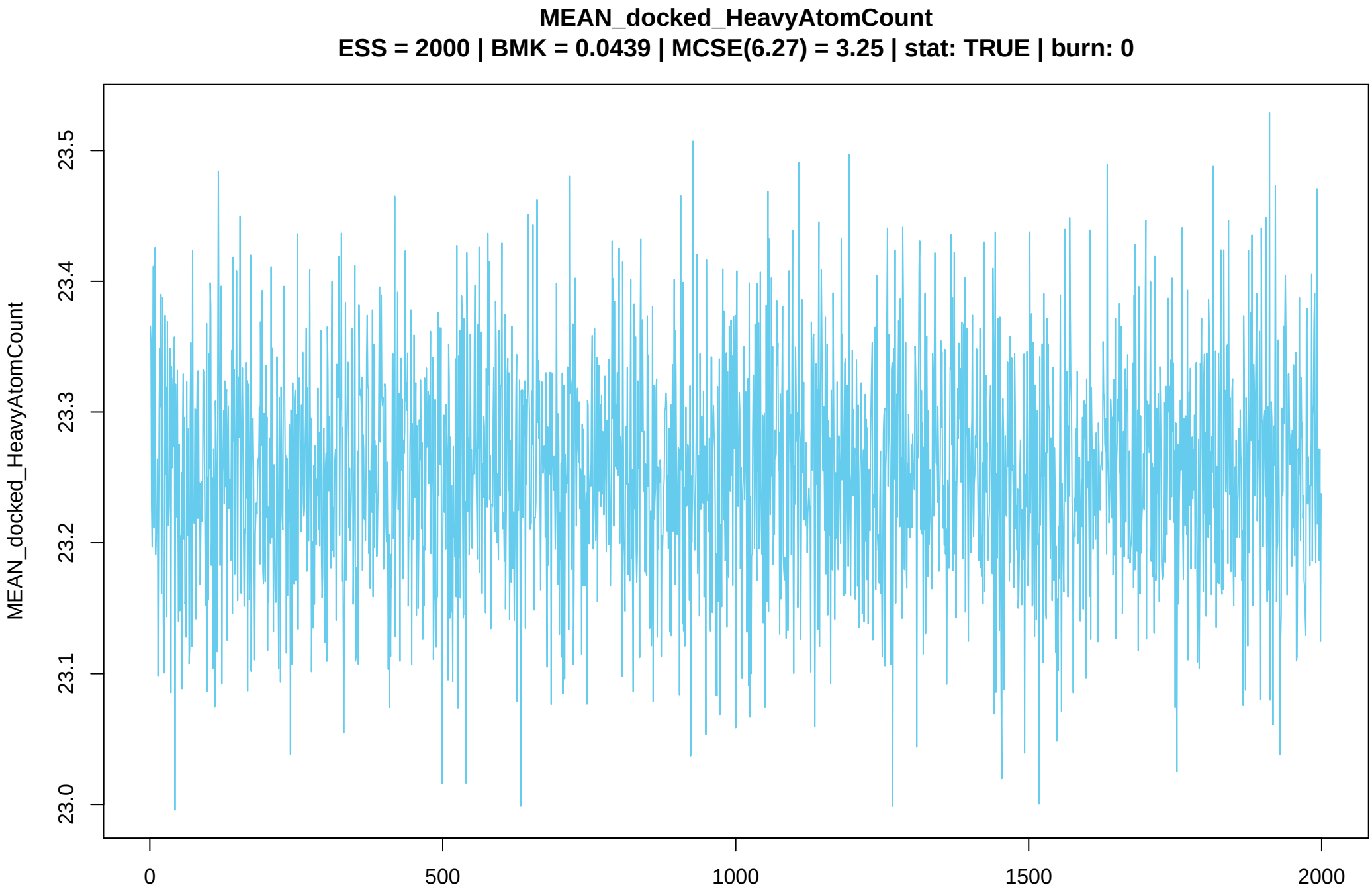

logitDcov
ESS = 1580 | BMK = 0.095 | MCSE(6.27) = 3.78 | stat: TRUE | burn: 0
logitDcov
0.0
0.2
0.4
0.6
0.8
0
500
1000
1500
2000

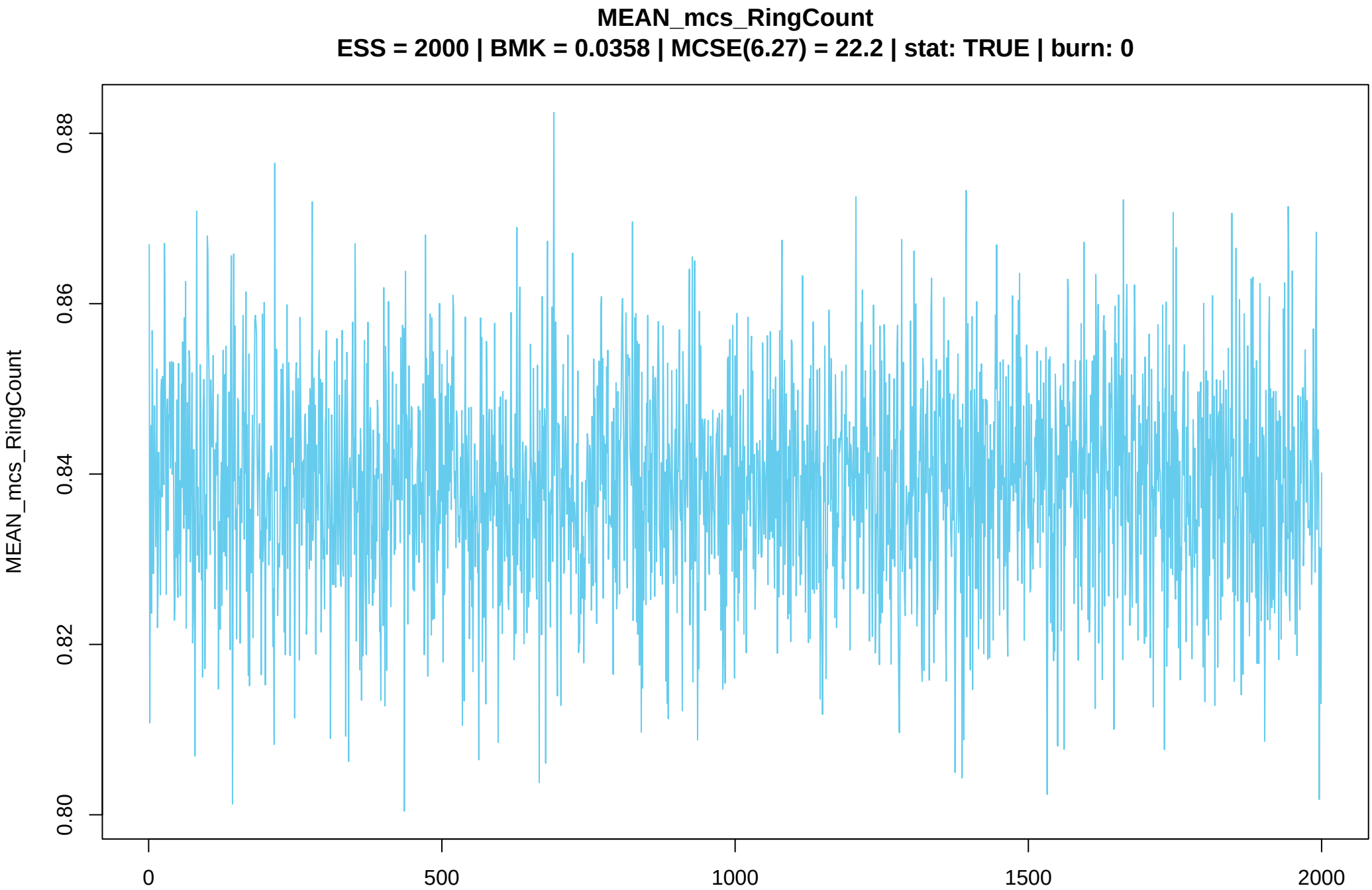

MEAN_log_RMSD
ESS = 1750 | BMK = 0.0461 | MCSE(6.27) = 23.3 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.18
1.20
1.22
1.24
0
500
1000
1500
2000

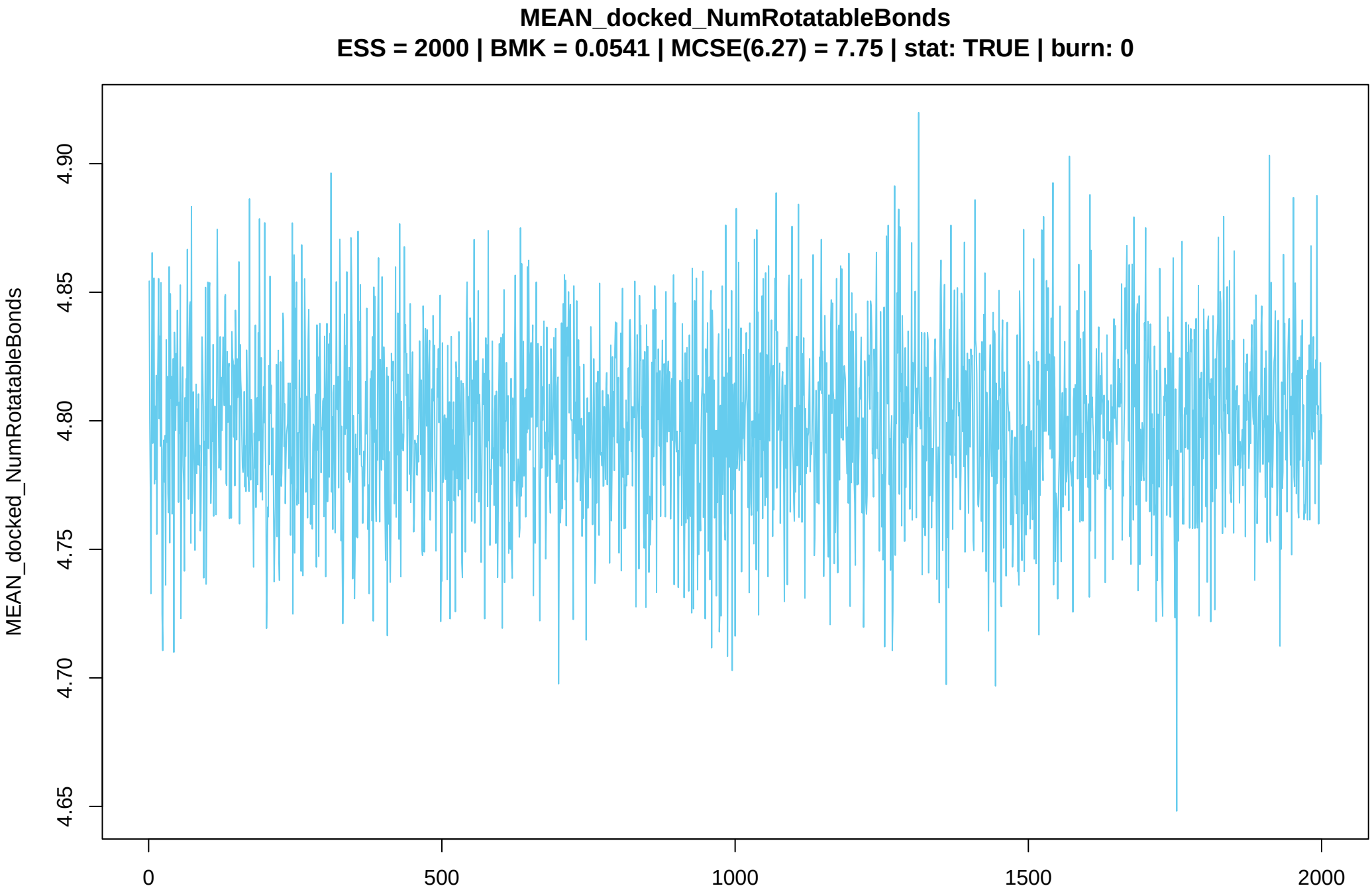

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0424 | MCSE(6.27) = 18 | stat: TRUE | burn: 0
MEAN_log_mcs_unbonded_polar_sasa
−0.30
−0.32
−0.34
−0.36
−0.38
−0.40
0
500
1000
1500
2000

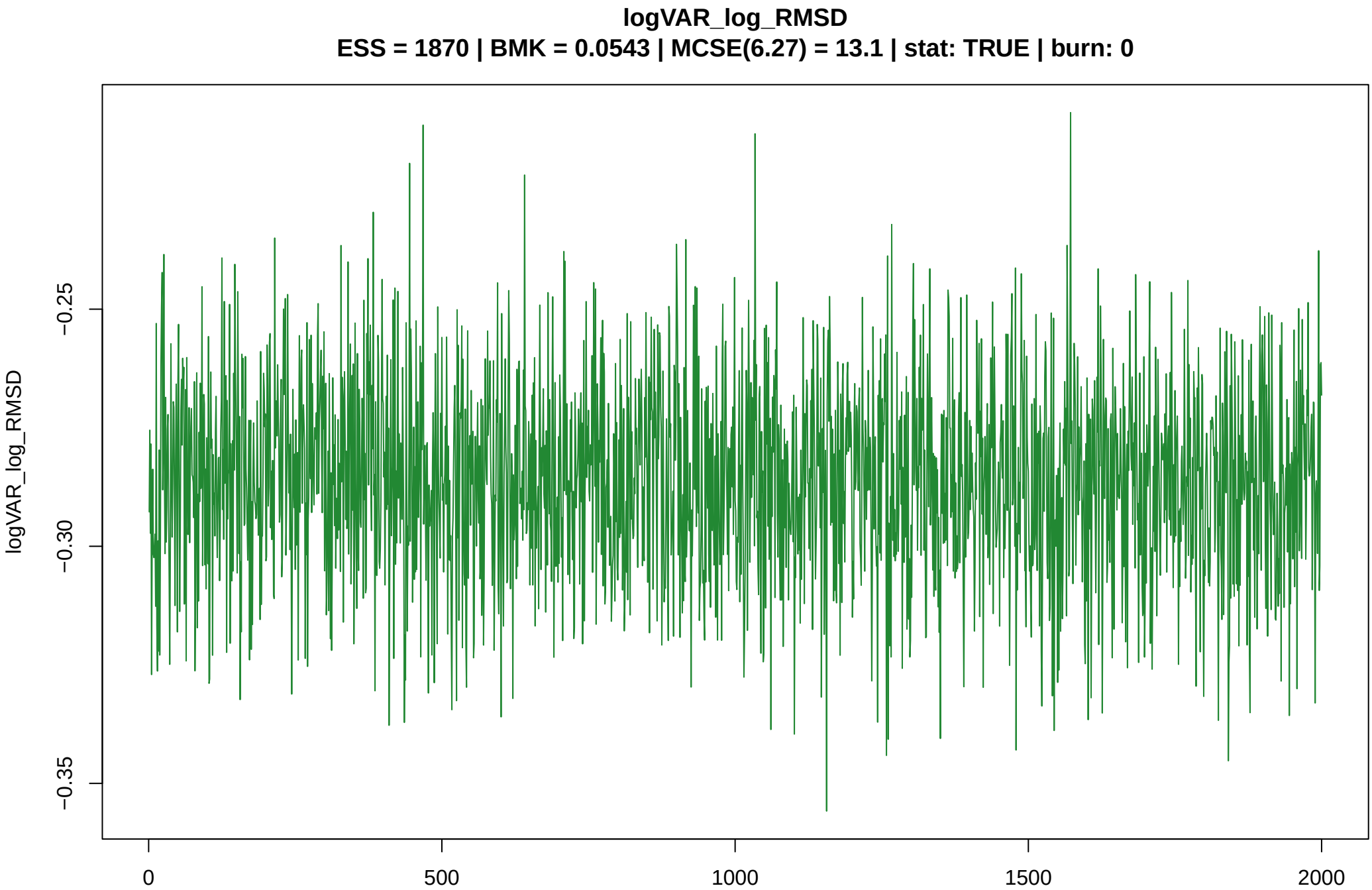

MEAN_logit_ec_tanimoto_similarity
ESS = 1610 | BMK = 0.0287 | MCSE(6.27) = 21 | stat: TRUE | burn: 0
MEAN_logit_ec_tanimoto_similarity
−2.04
−2.06
−2.08
−2.10
−2.12
0
500
1000
1500
2000

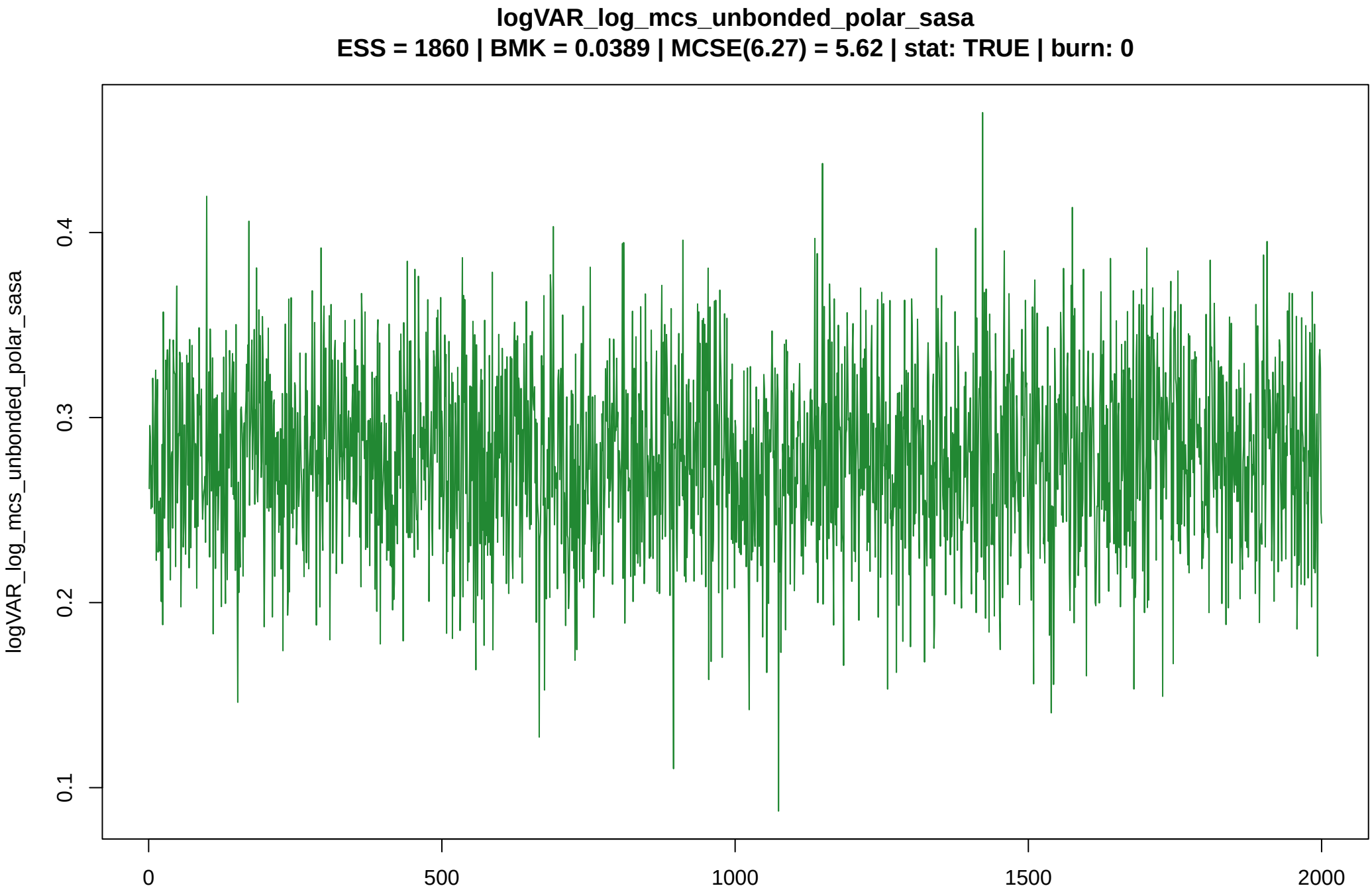

MEAN_mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0372 | MCSE(6.27) = 11 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
2.95
3.00
3.05
0
500
1000
1500
2000

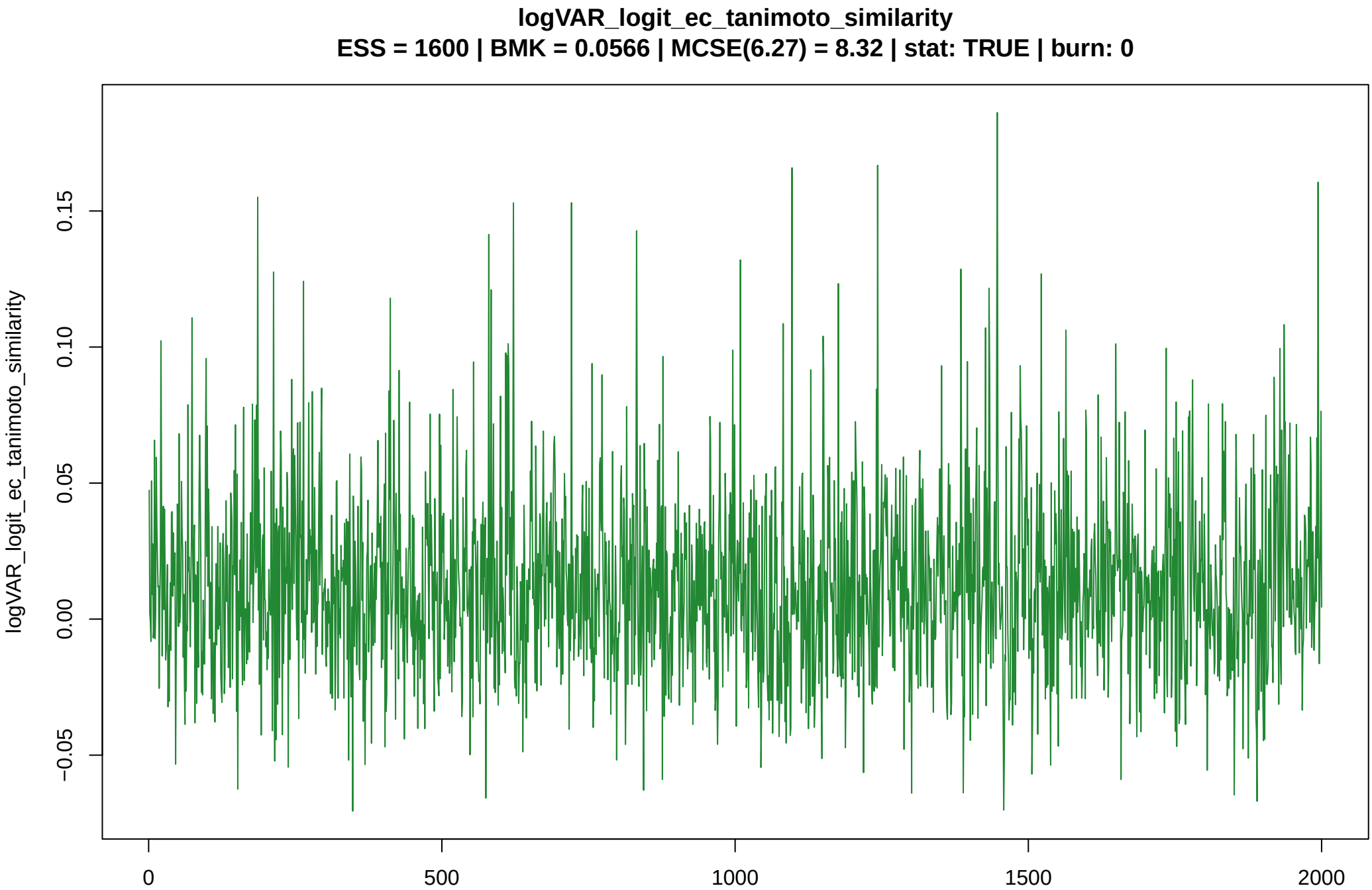

MEAN_docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0439 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
23.0
23.1
23.2
23.3
23.4
23.5
0
500
1000
1500
2000

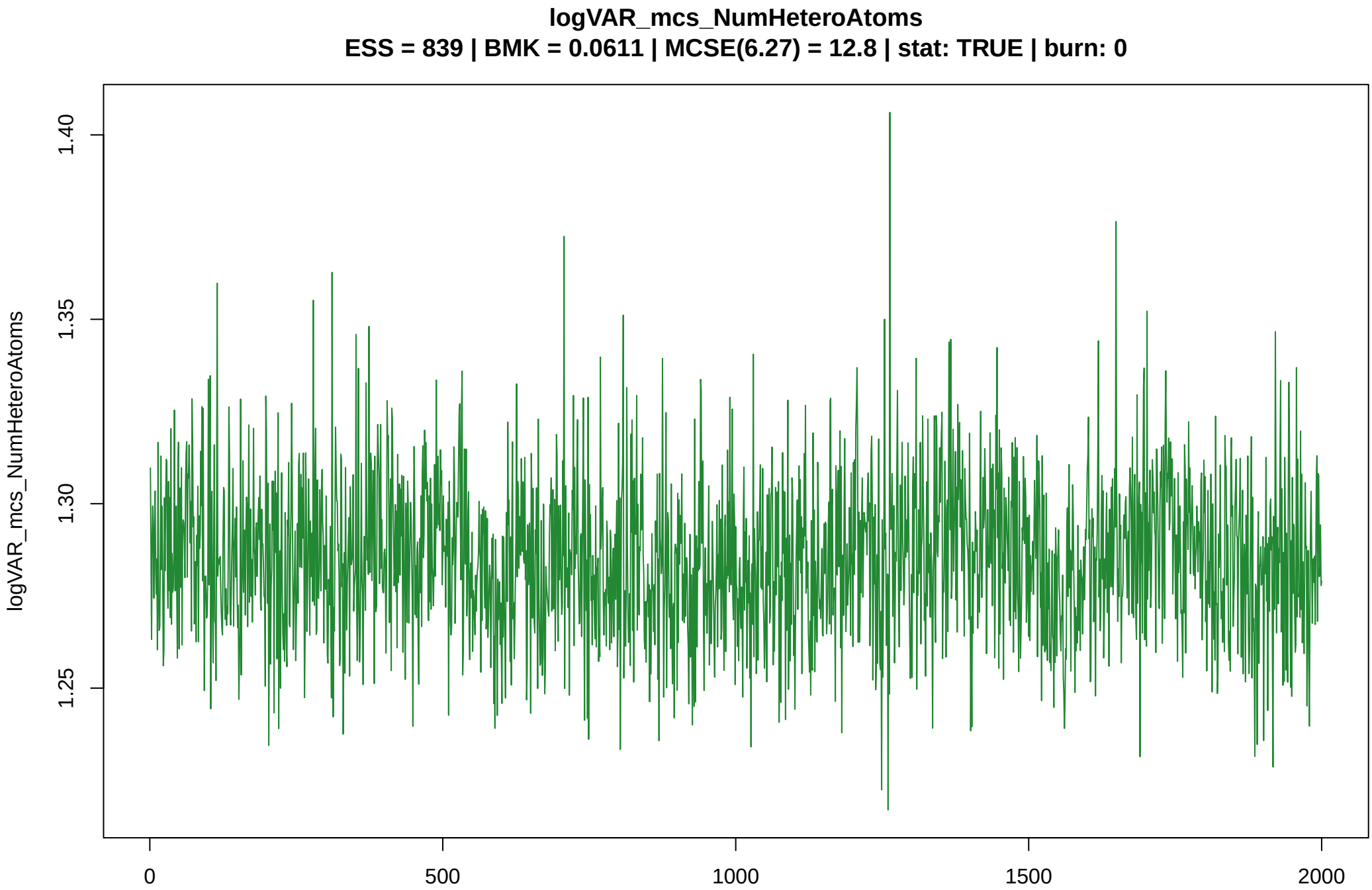

MEAN_mcs_RingCount
ESS = 2000 | BMK = 0.0358 | MCSE(6.27) = 22.2 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.80
0.82
0.84
0.86
0.88
0
500
1000
1500
2000

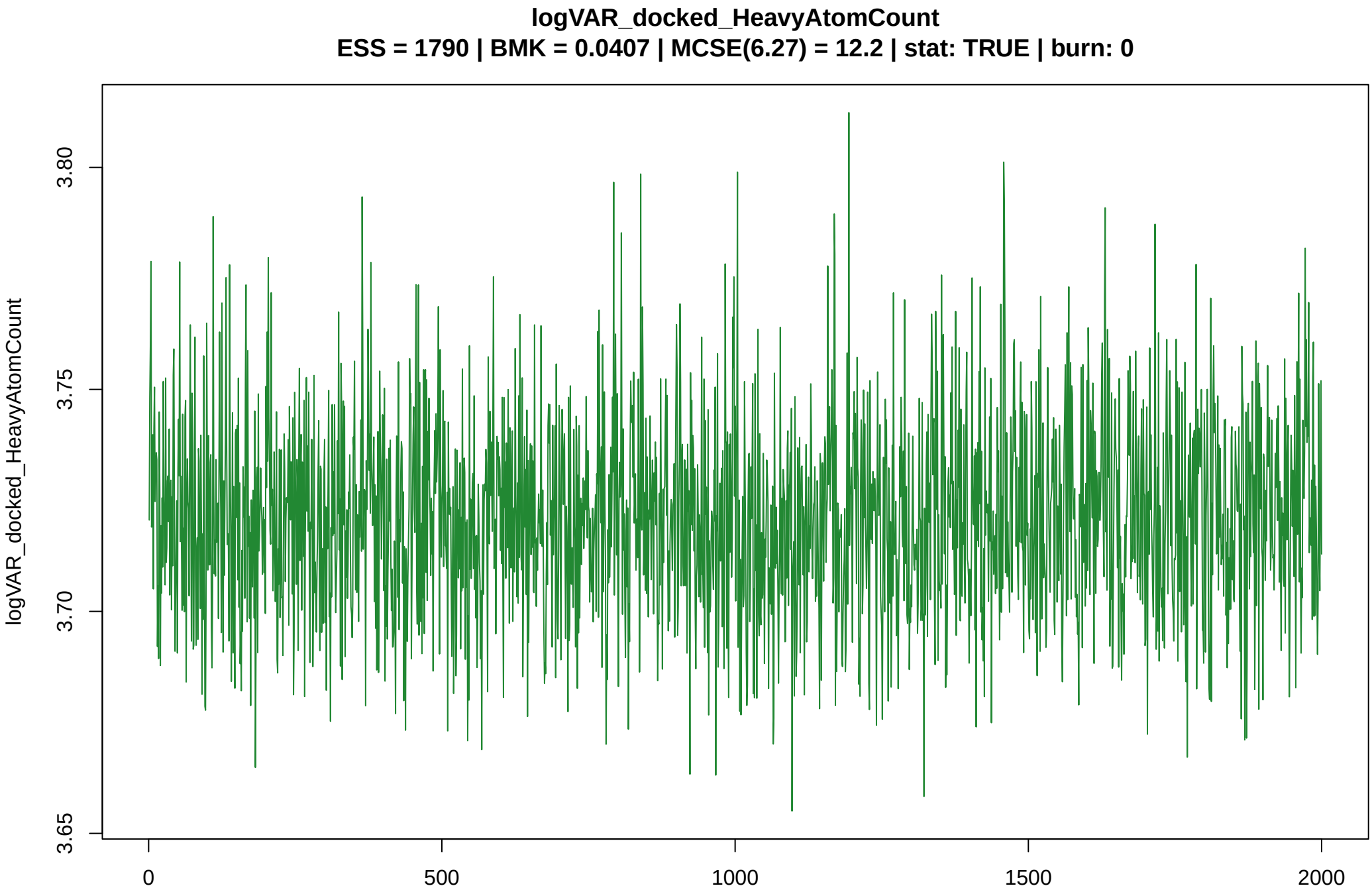

MEAN_docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0541 | MCSE(6.27) = 7.75 | stat: TRUE | burn: 0
MEAN_docked_NumRotatableBonds
4.65
4.70
4.75
4.80
4.85
4.90
0
500
1000
1500
2000

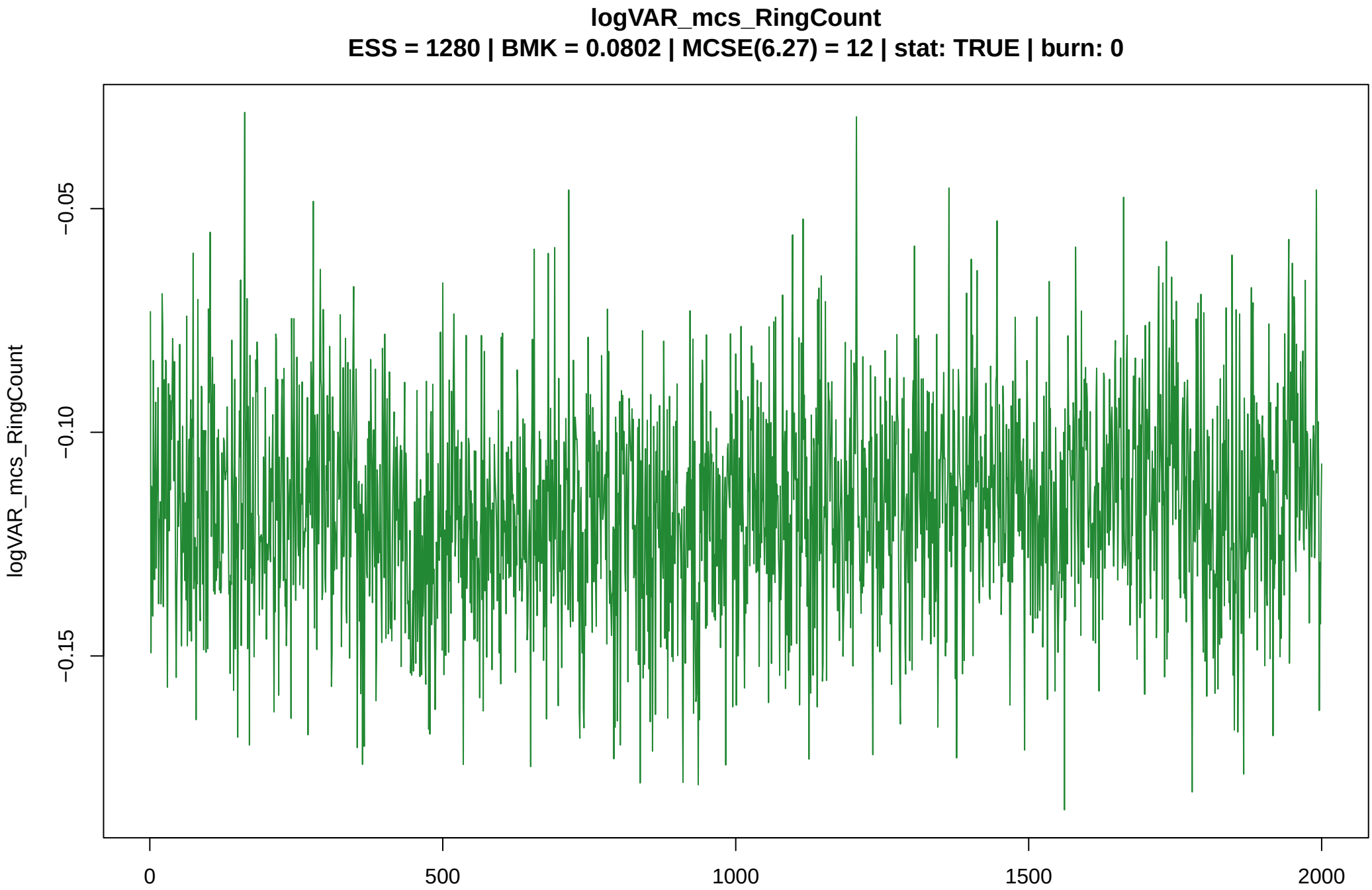

logVAR_log_RMSD
ESS = 1870 | BMK = 0.0543 | MCSE(6.27) = 13.1 | stat: TRUE | burn: 0
logVAR_log_RMSD
−0.25
−0.30
−0.35
0
500
1000
1500
2000

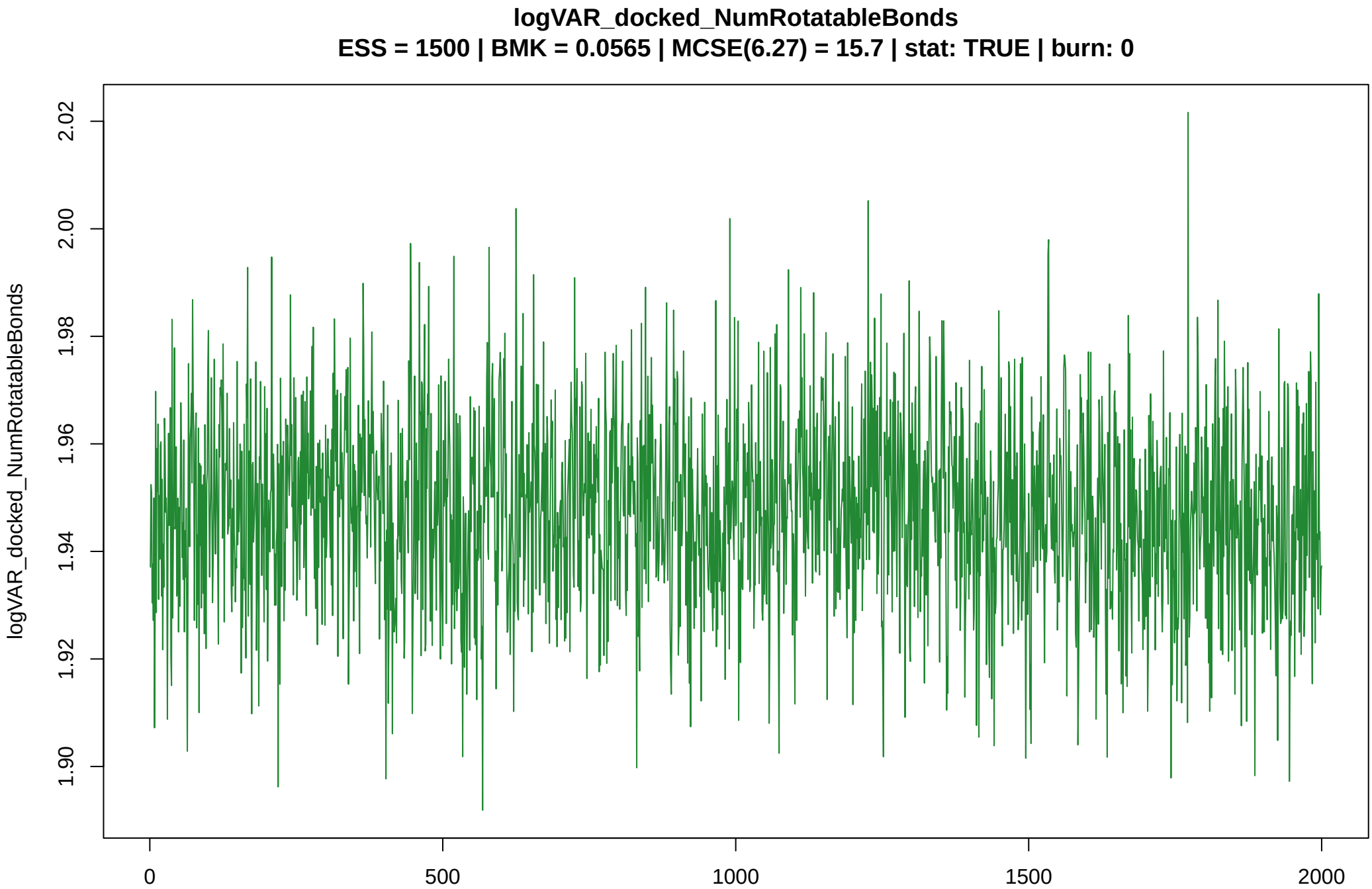

logVAR_log_mcs_unbonded_polar_sasa
ESS = 1860 | BMK = 0.0389 | MCSE(6.27) = 5.62 | stat: TRUE | burn: 0
logVAR_log_mcs_unbonded_polar_sasa
0.1
0.2
0.3
0.4
0
500
1000
1500
2000

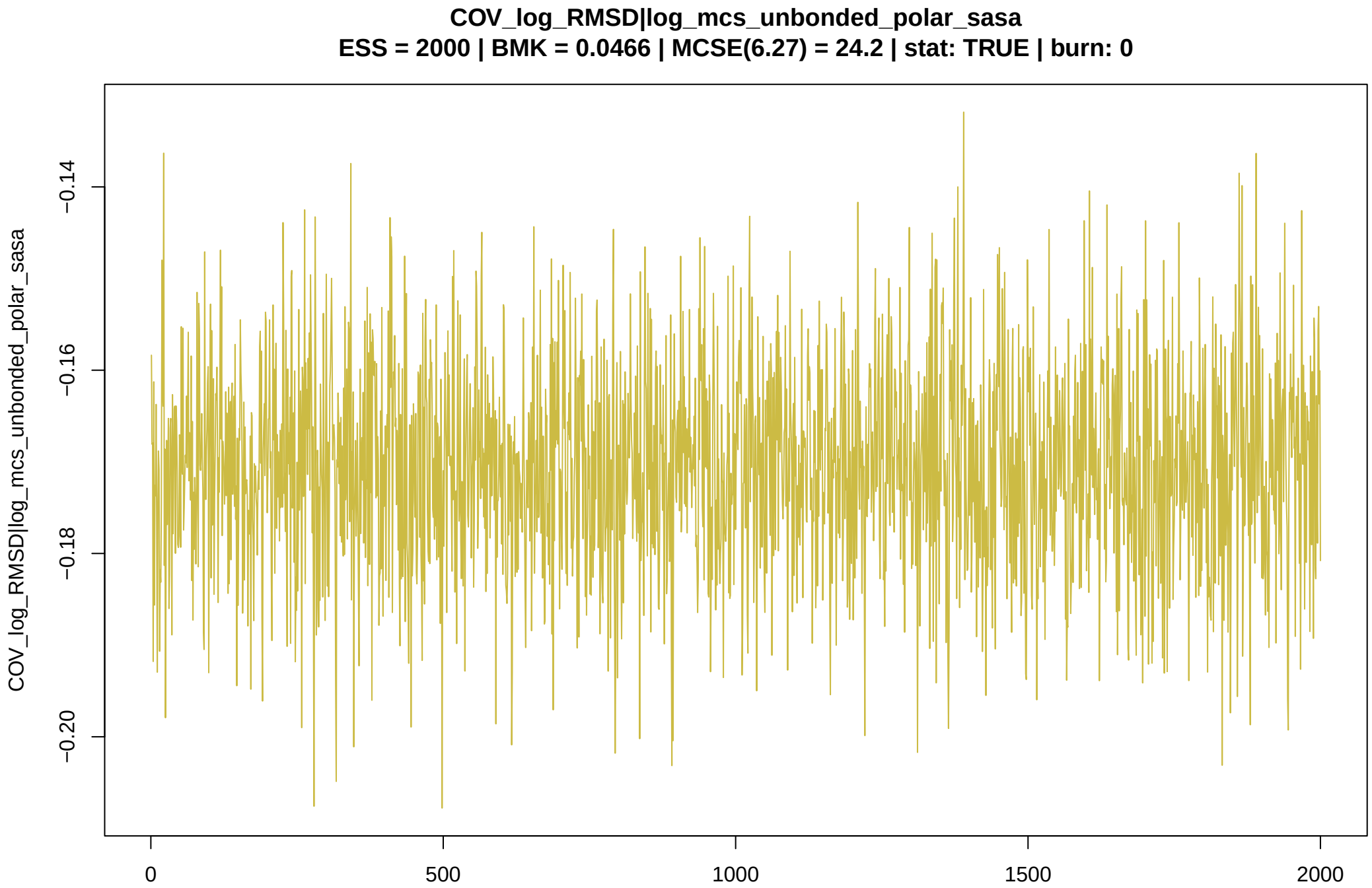

logVAR_logit_ec_tanimoto_similarity
ESS = 1600 | BMK = 0.0566 | MCSE(6.27) = 8.32 | stat: TRUE | burn: 0
logVAR_logit_ec_tanimoto_similarity
−0.05
0.00
0.05
0.10
0.15
0
500
1000
1500
2000

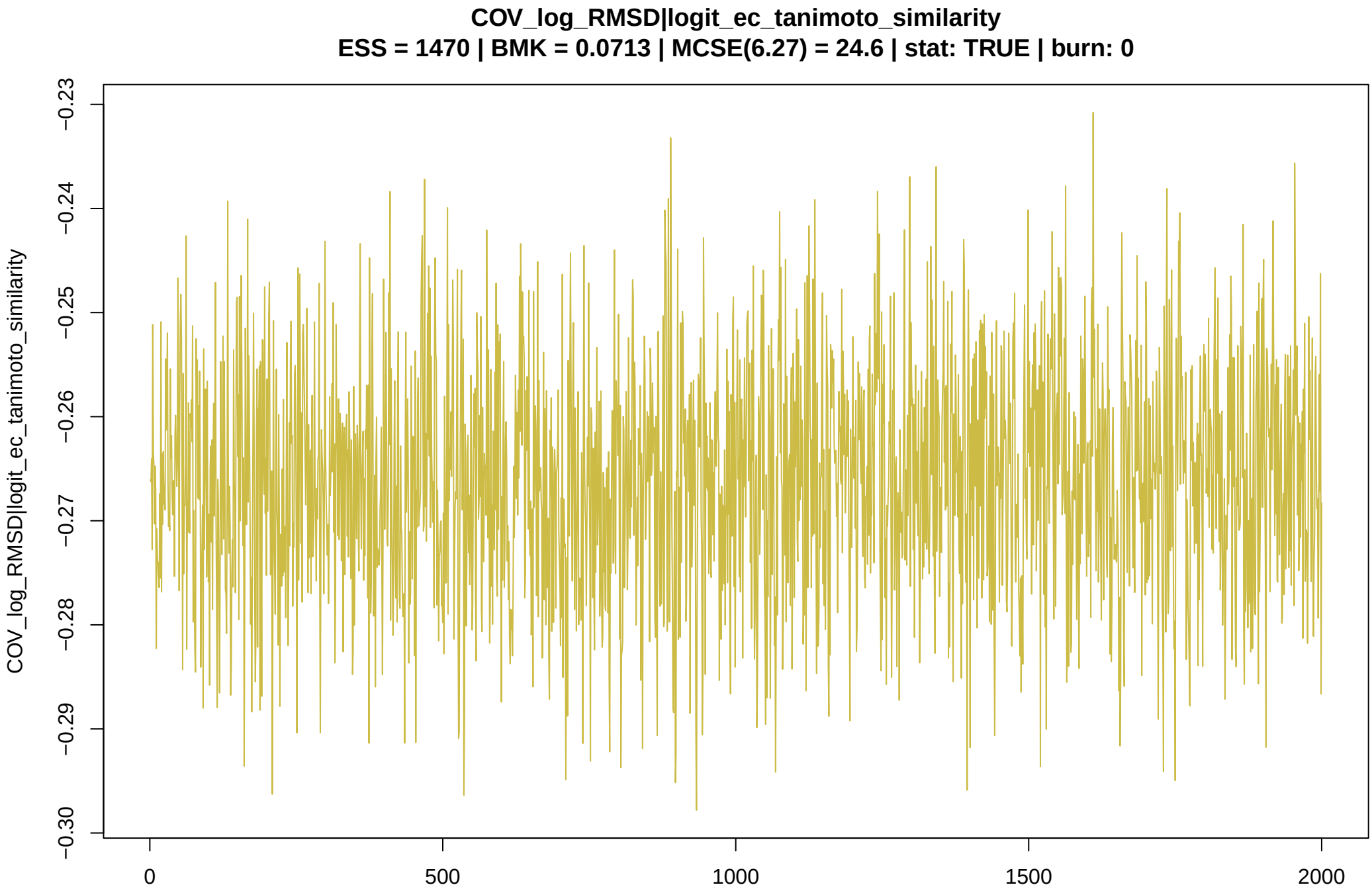

logVAR_mcs_NumHeteroAtoms
ESS = 839 | BMK = 0.0611 | MCSE(6.27) = 12.8 | stat: TRUE | burn: 0
logVAR_mcs_NumHeteroAtoms
1.40
1.35
1.30
1.25
0
500
1000
1500
2000

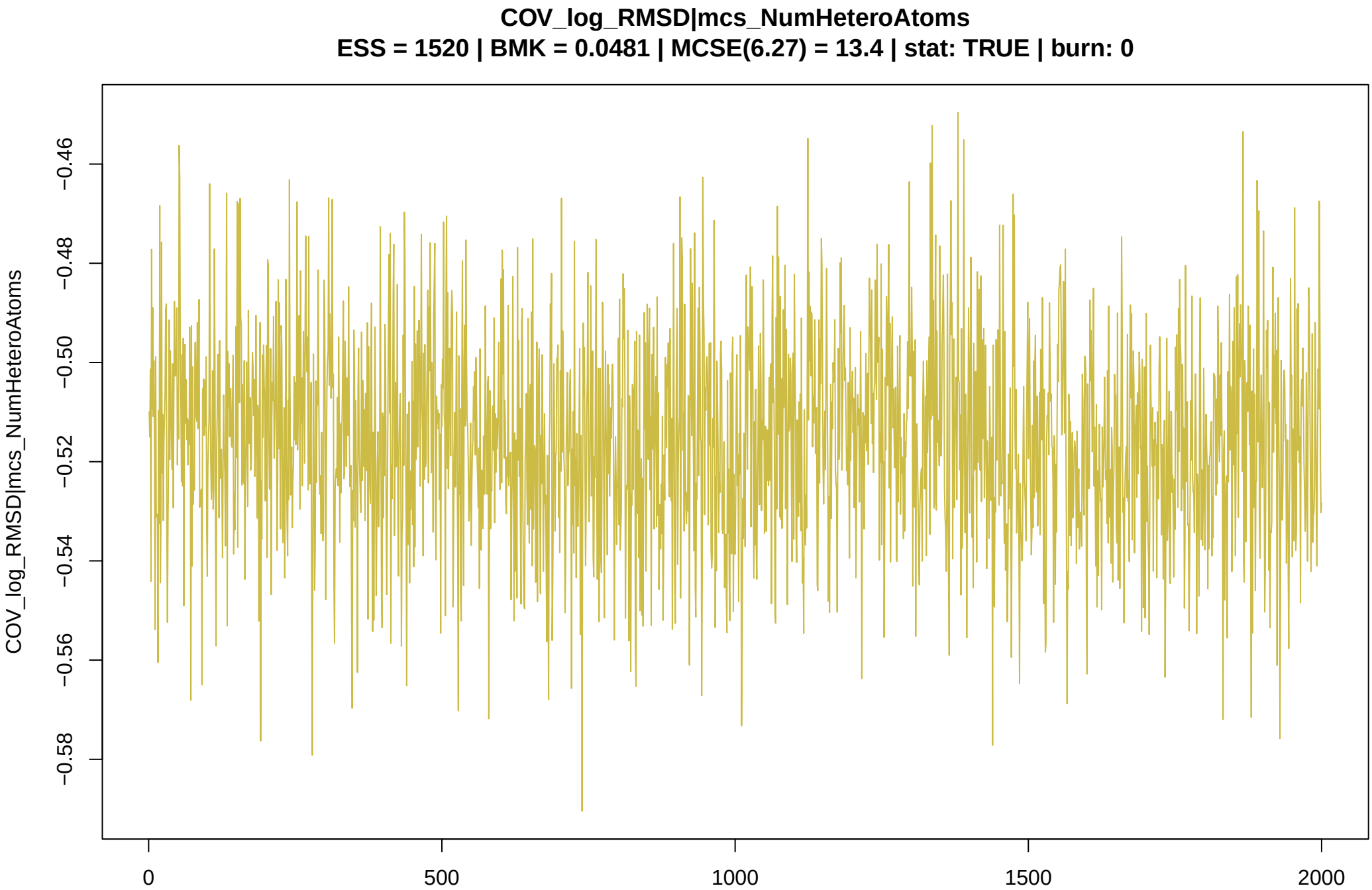

logVAR_docked_HeavyAtomCount
ESS = 1790 | BMK = 0.0407 | MCSE(6.27) = 12.2 | stat: TRUE | burn: 0
logVAR_docked_HeavyAtomCount
3.65
3.70
3.75
3.80
0
500
1000
1500
2000

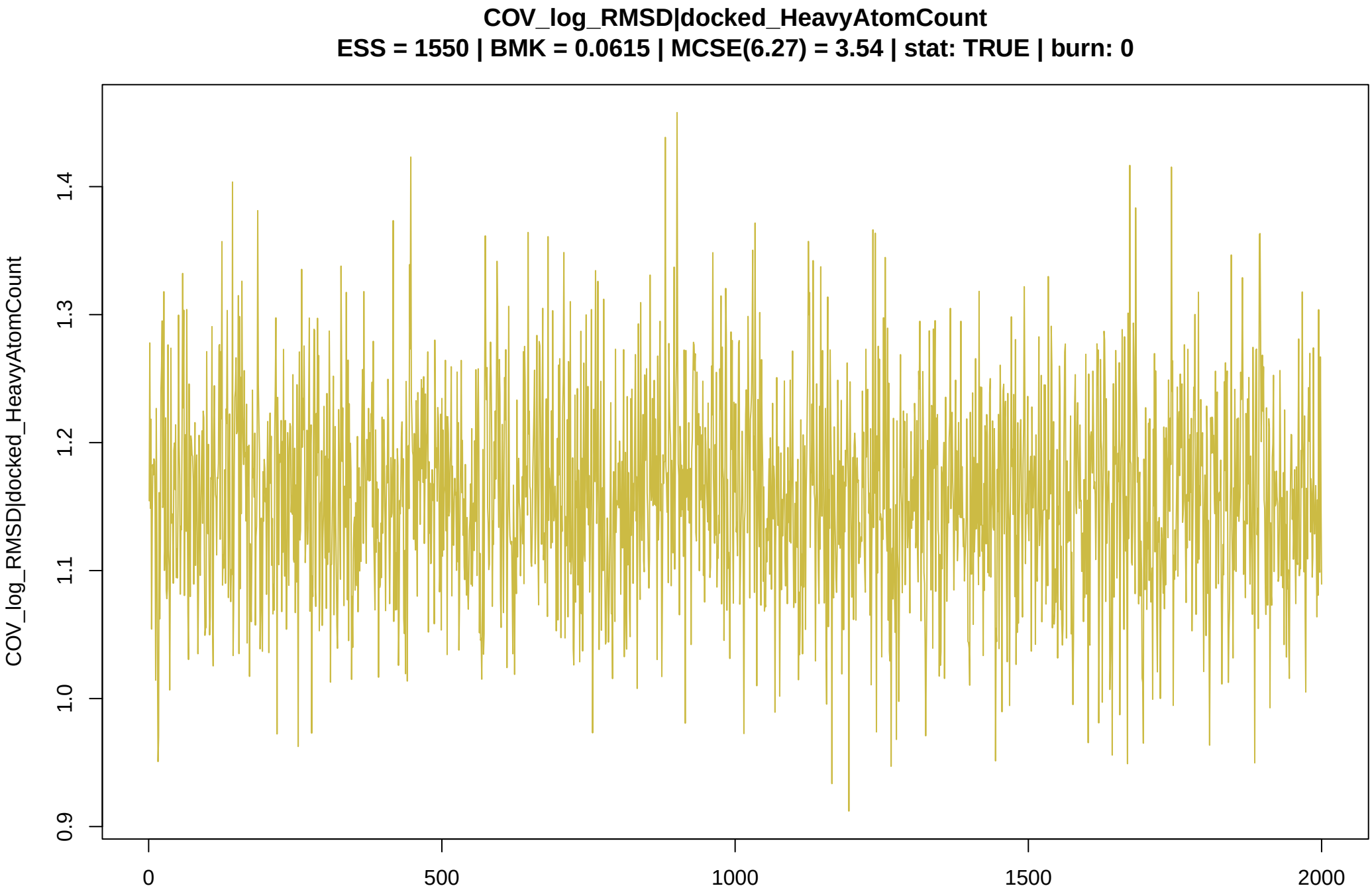

logVAR_mcs_RingCount
ESS = 1280 | BMK = 0.0802 | MCSE(6.27) = 12 | stat: TRUE | burn: 0
logVAR_mcs_RingCount
−0.05
−0.10
−0.15
0
500
1000
1500
2000

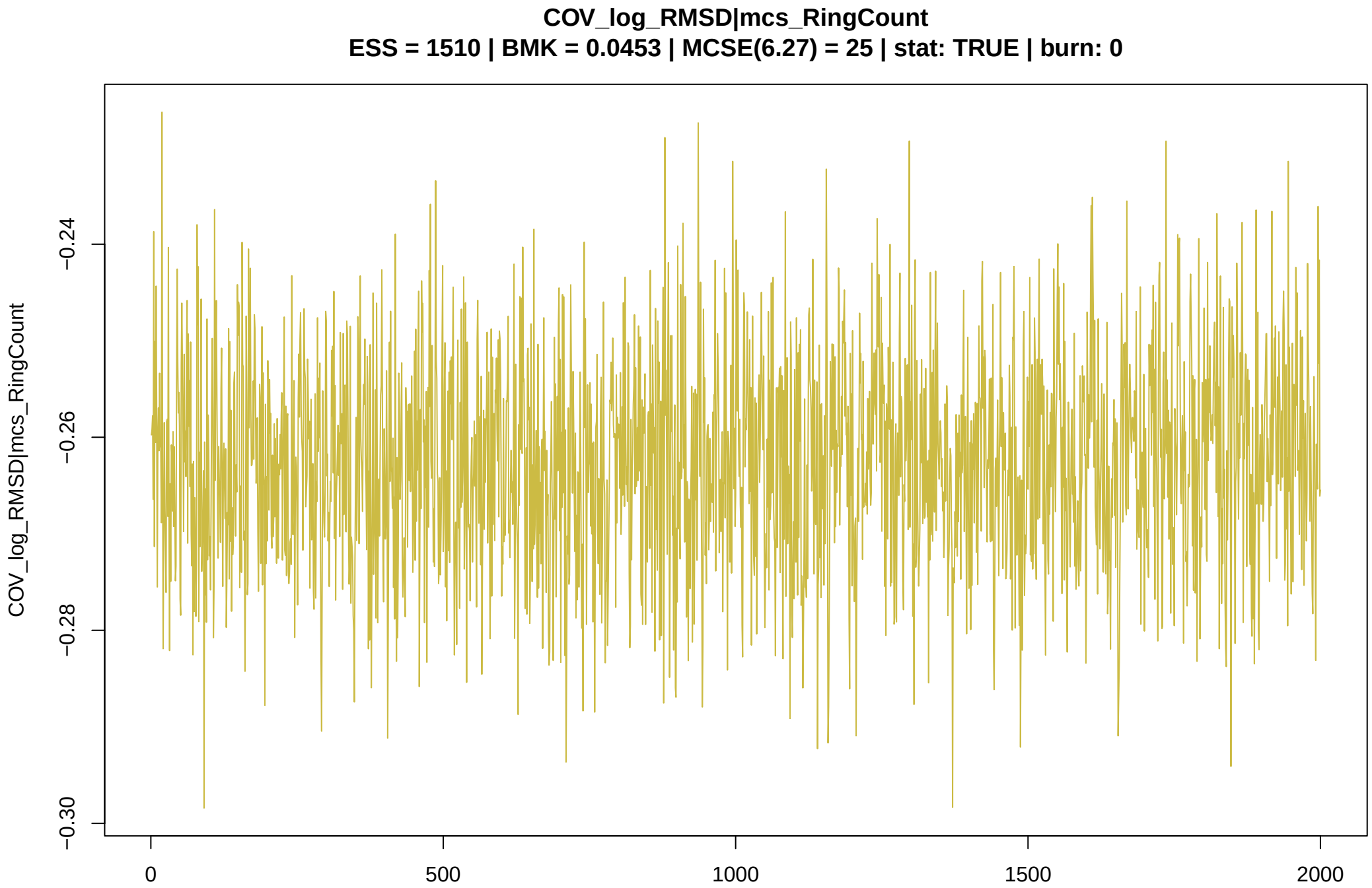

logVAR_docked_NumRotatableBonds
ESS = 1500 | BMK = 0.0565 | MCSE(6.27) = 15.7 | stat: TRUE | burn: 0
logVAR_docked_NumRotatableBonds
1.90
1.92
1.94
1.96
1.98
2.00
2.02
0
500
1000
1500
2000

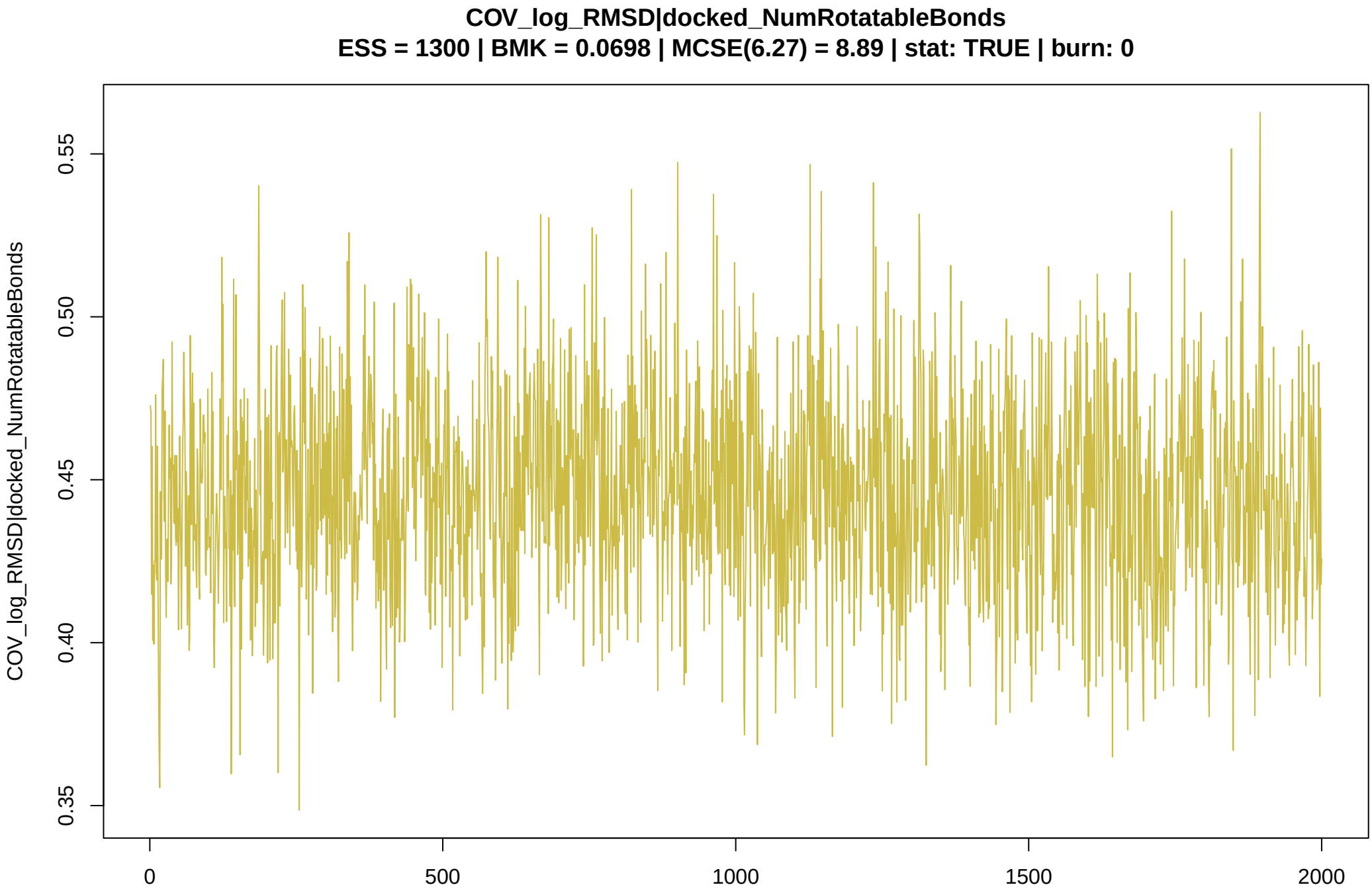

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0466 | MCSE(6.27) = 24.2 | stat: TRUE | burn: 0
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.14
−0.16
−0.18
−0.20
0
500
1000
1500
2000

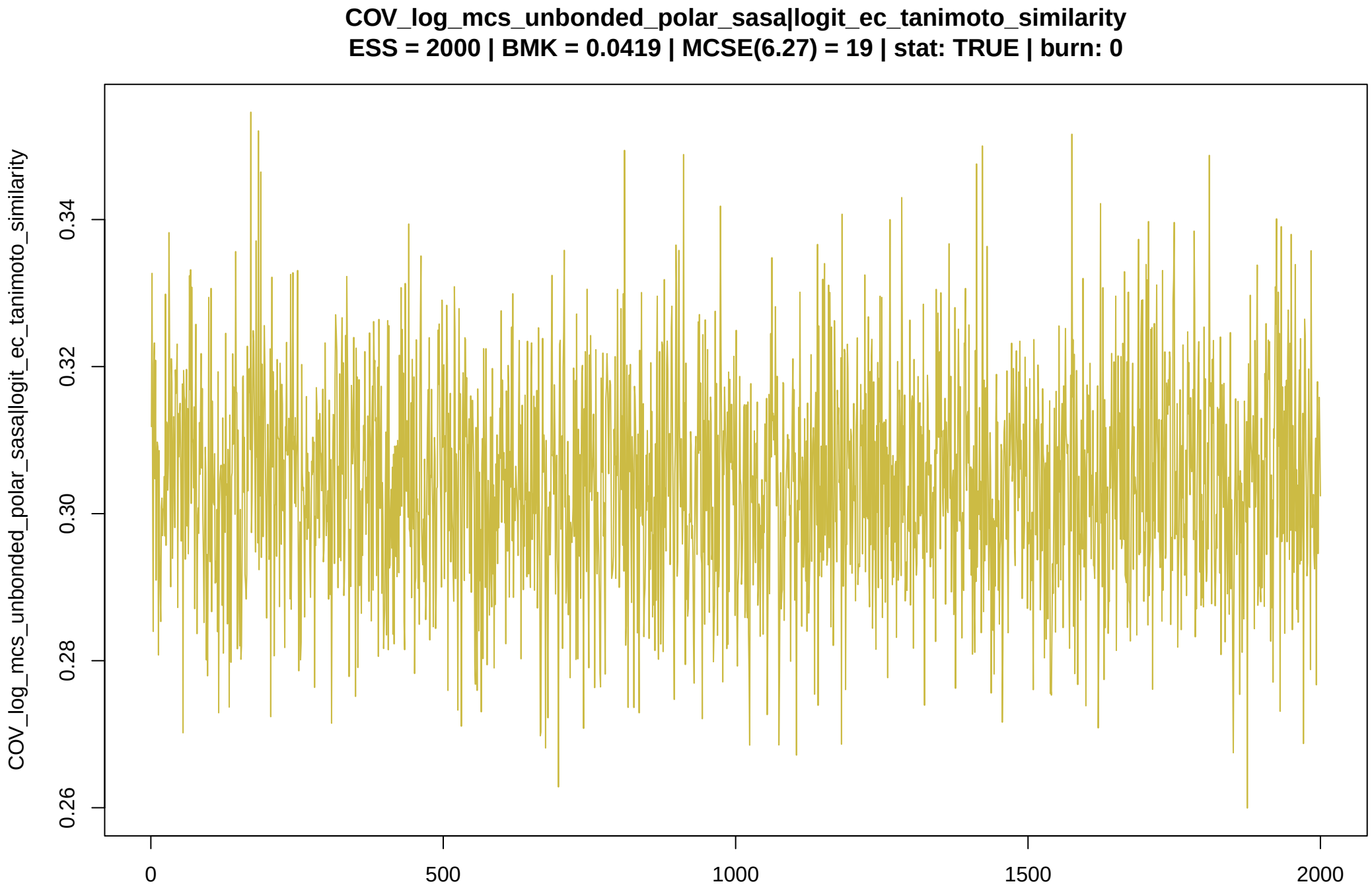

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1470 | BMK = 0.0713 | MCSE(6.27) = 24.6 | stat: TRUE | burn: 0
COV_log_RMSD|logit_ec_tanimoto_similarity
−0.23
−0.24
−0.25
−0.26
−0.27
−0.28
−0.29
−0.30
0
500
1000
1500
2000

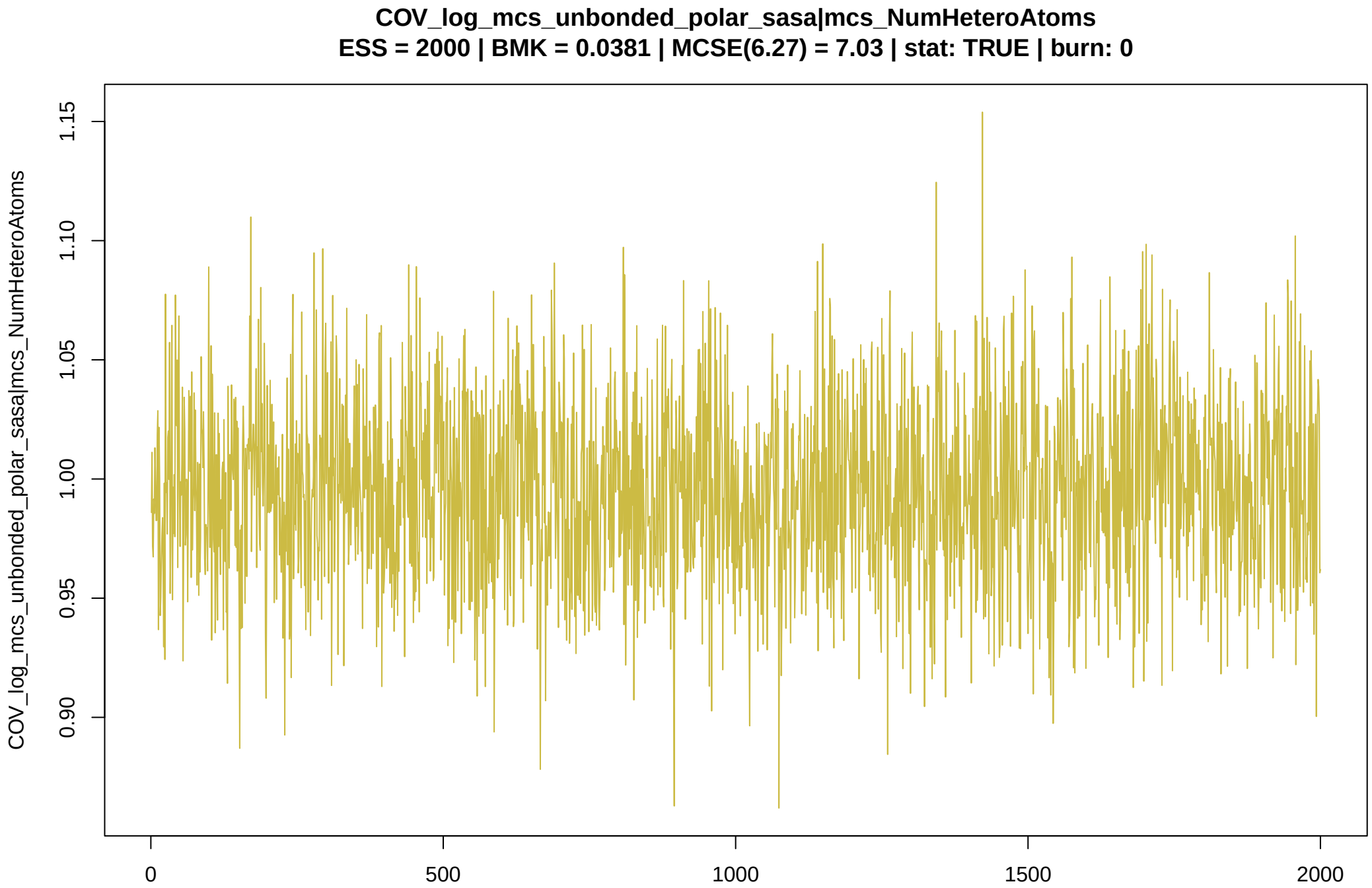

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1520 | BMK = 0.0481 | MCSE(6.27) = 13.4 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.46
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

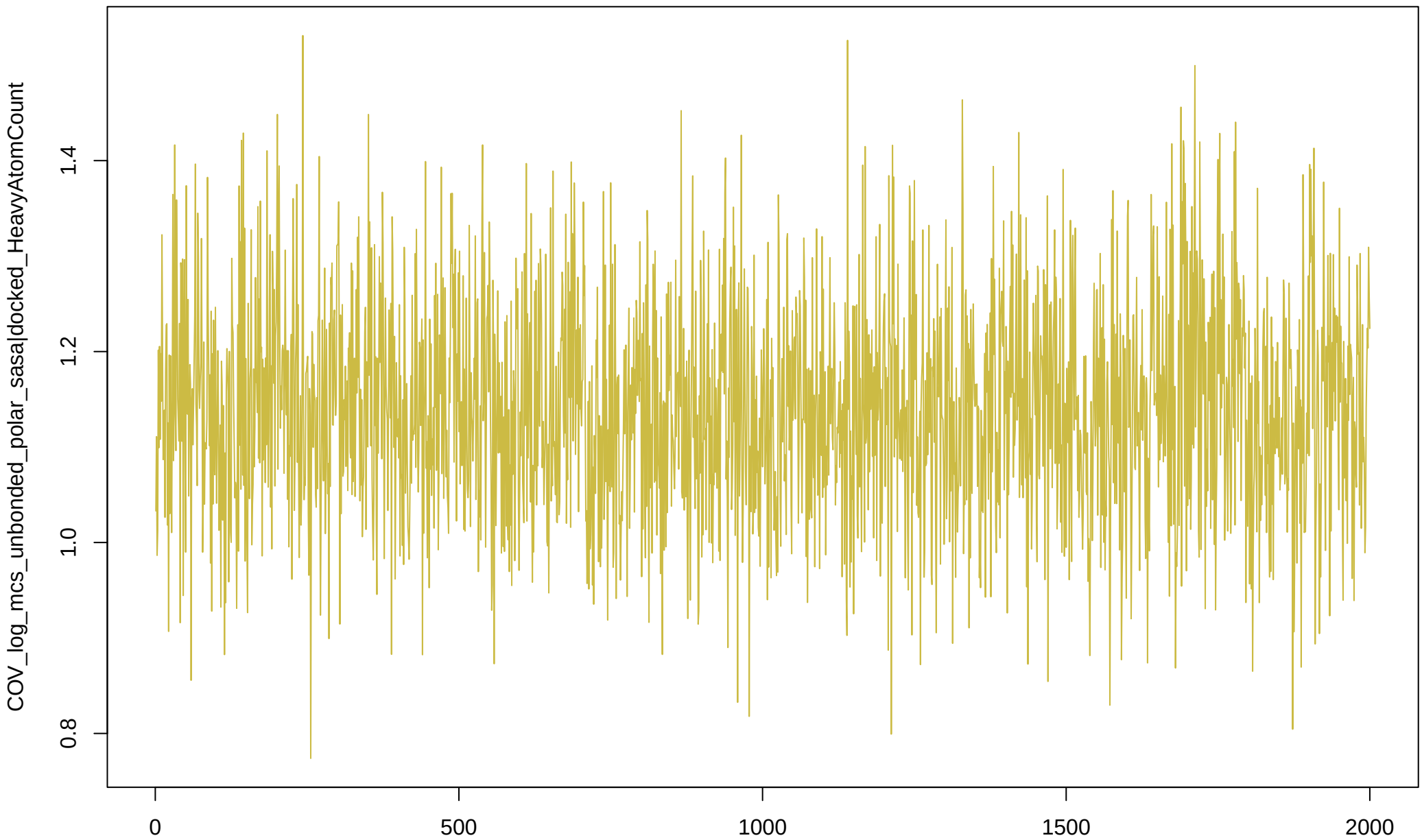

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1550 | BMK = 0.0615 | MCSE(6.27) = 3.54 | stat: TRUE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
0.9
1.0
1.1
1.2
1.3
1.4
0
500
1000
1500
2000

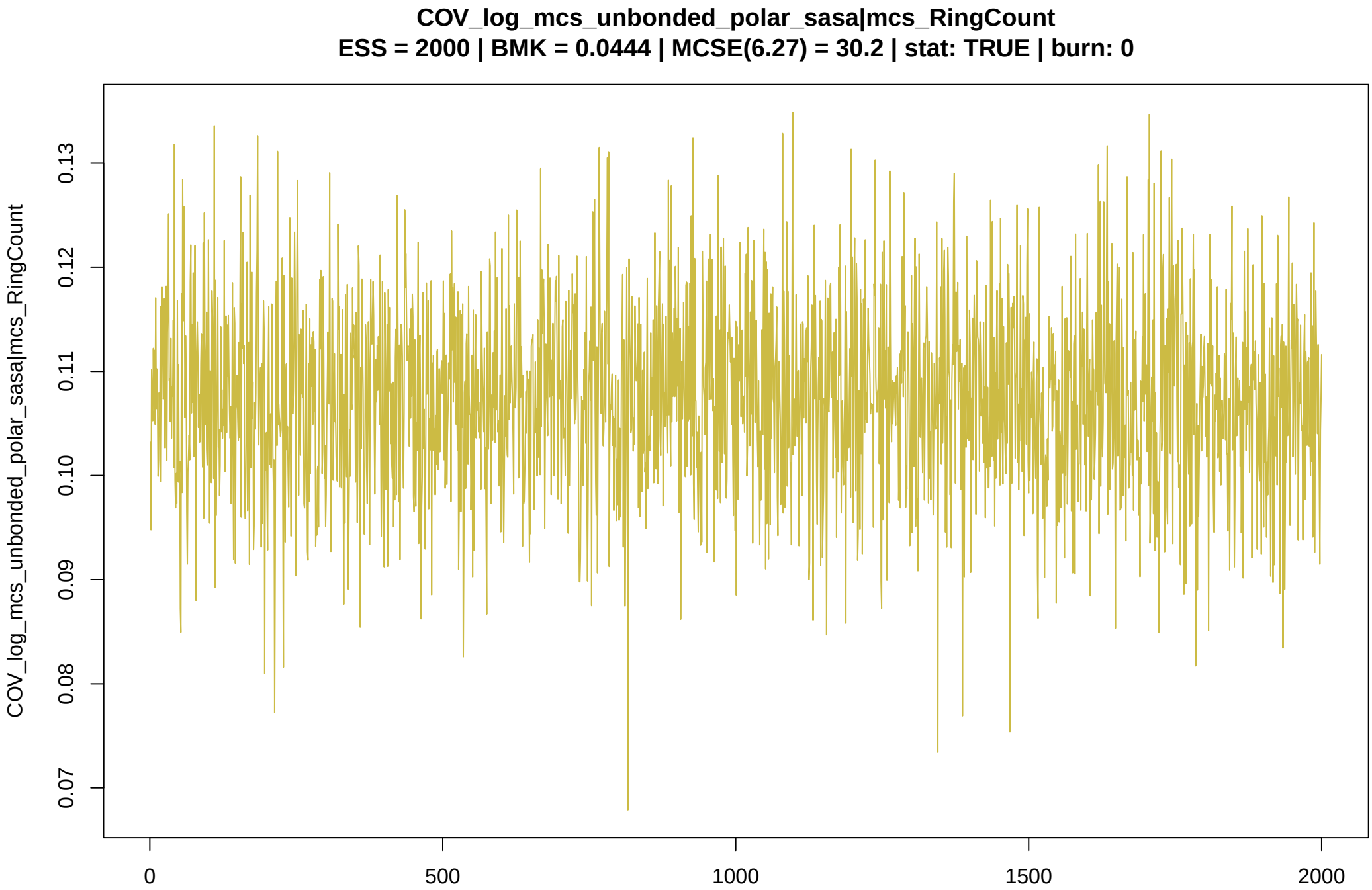

COV_log_RMSD|mcs_RingCount
ESS = 1510 | BMK = 0.0453 | MCSE(6.27) = 25 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.24
−0.26
−0.28
−0.30
0
500
1000
1500
2000

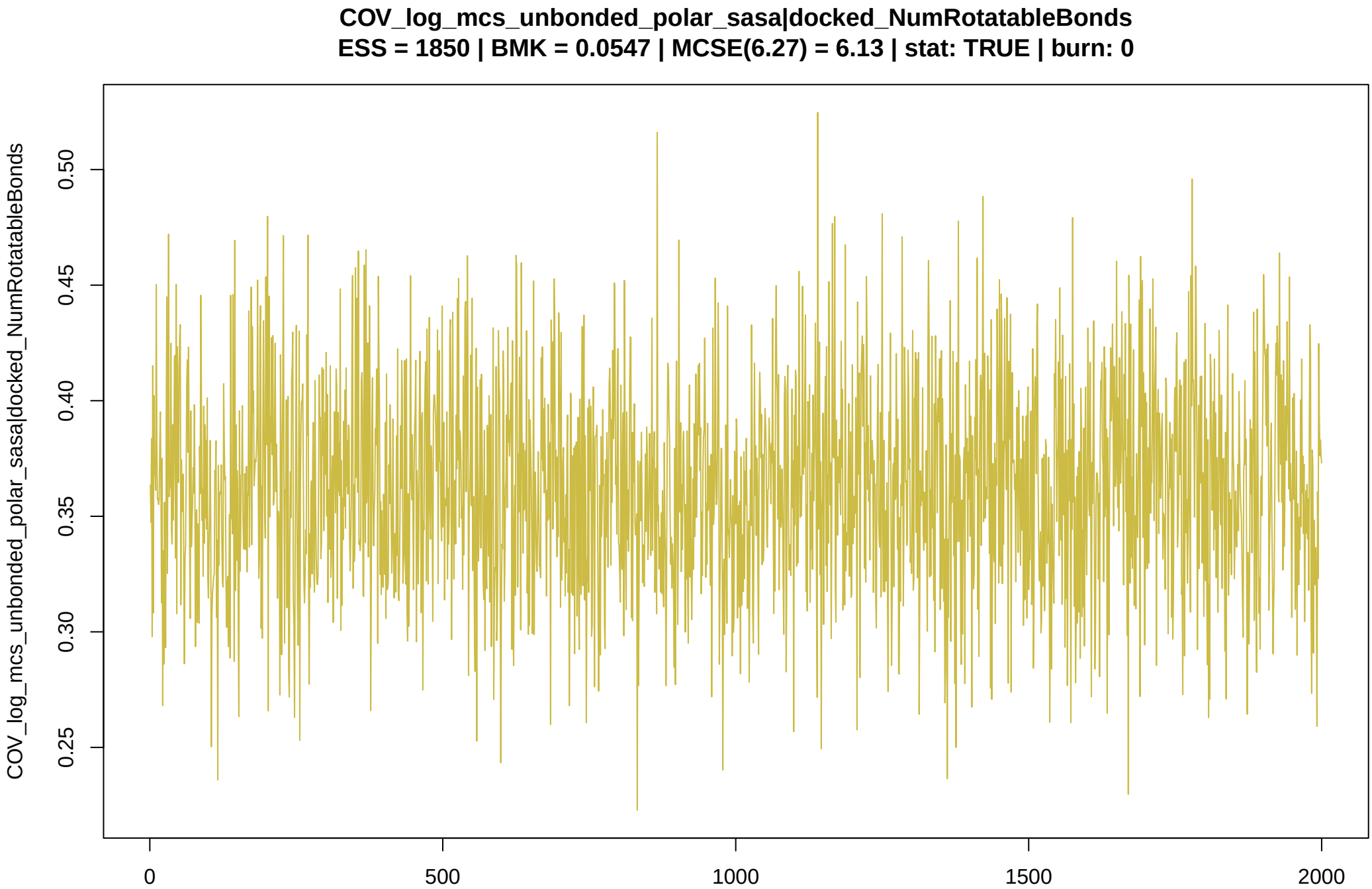

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1300 | BMK = 0.0698 | MCSE(6.27) = 8.89 | stat: TRUE | burn: 0
COV_log_RMSD|docked_NumRotatableBonds
0.35
0.40
0.45
0.50
0.55
0
500
1000
1500
2000

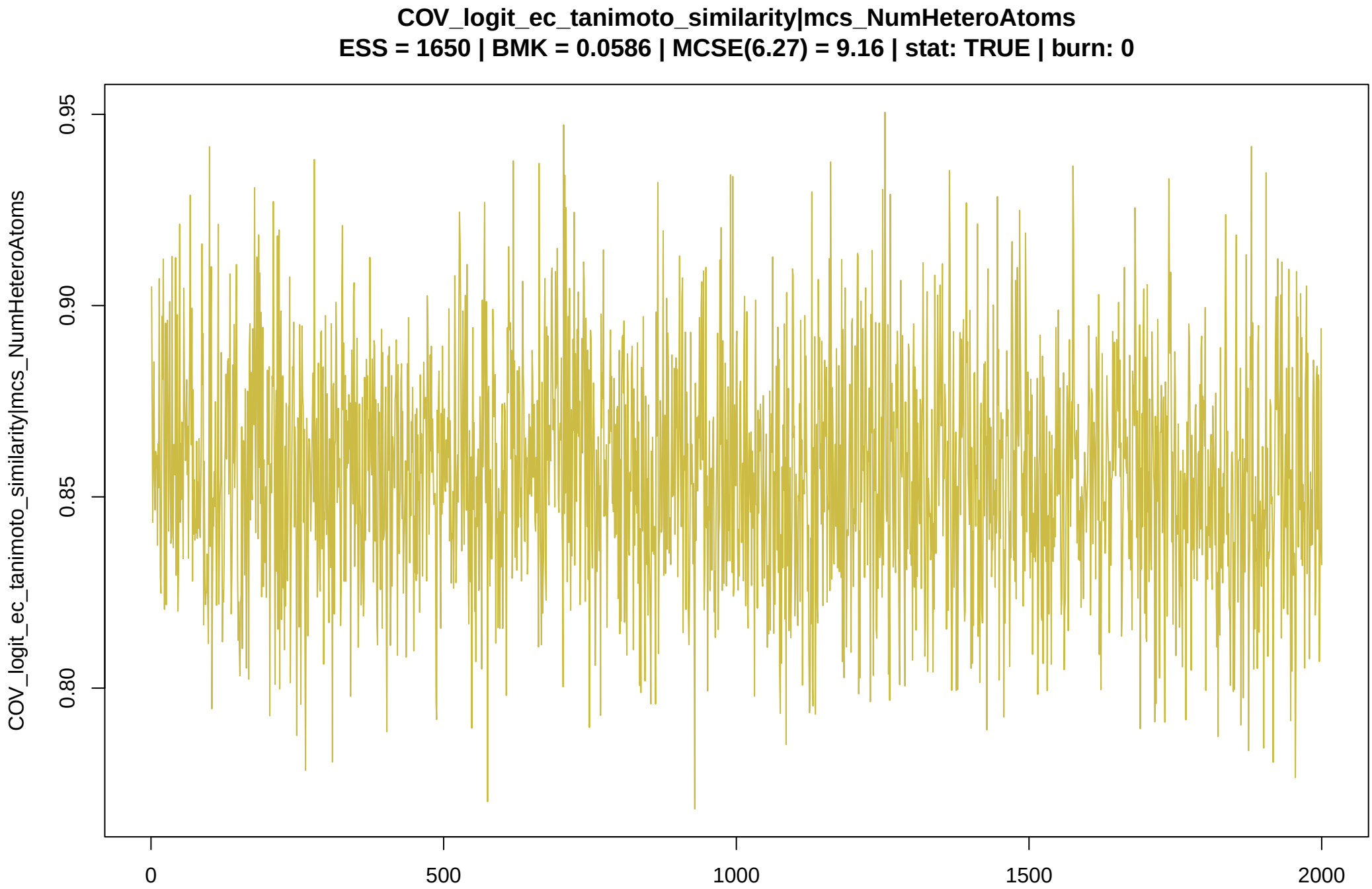

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 2000 | BMK = 0.0419 | MCSE(6.27) = 19 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0.26
0.28
0.30
0.32
0.34
0
500
1000
1500
2000

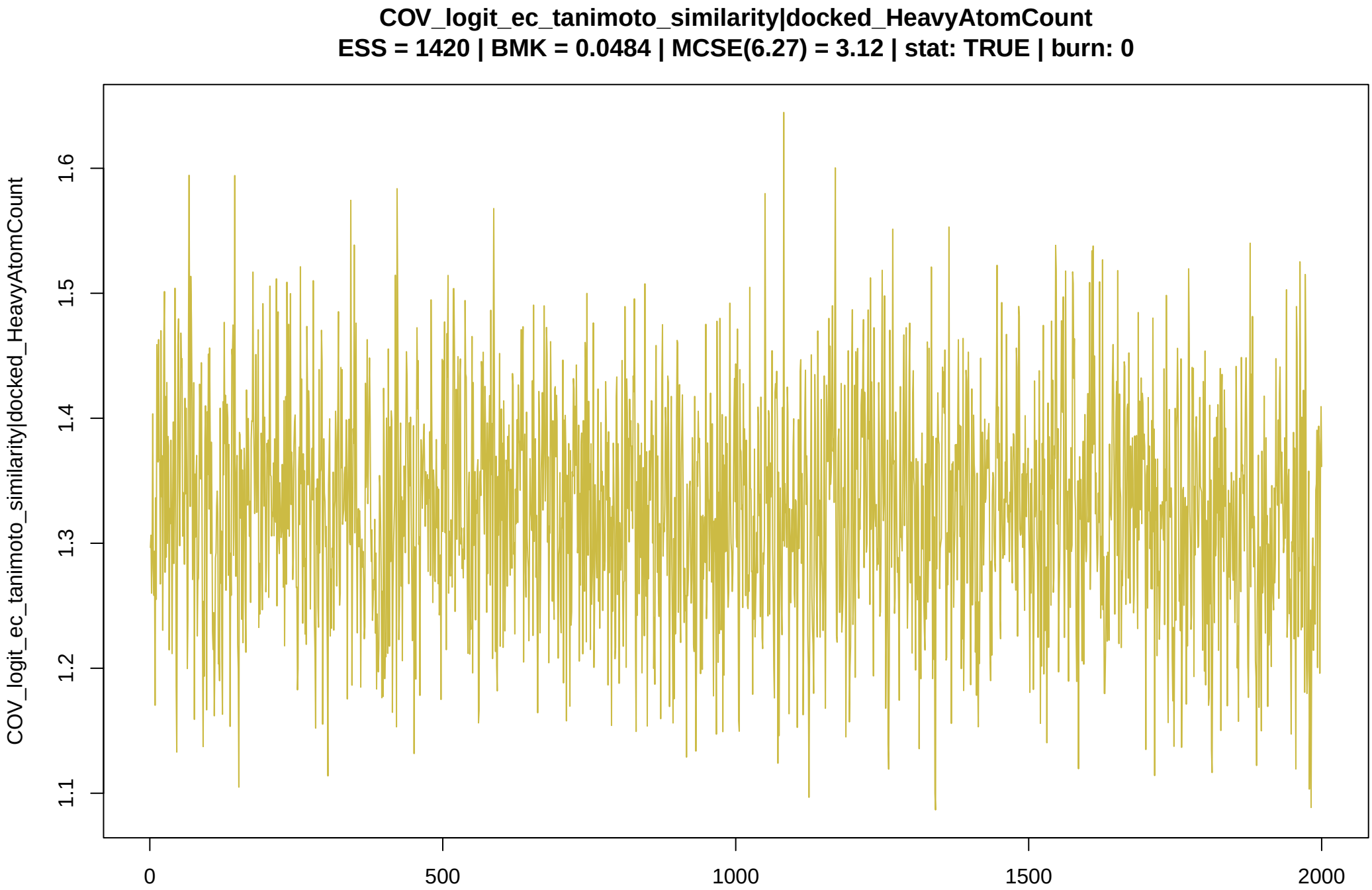

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0381 | MCSE(6.27) = 7.03 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.90
0.95
1.00
1.05
1.10
1.15
0
500
1000
1500
2000

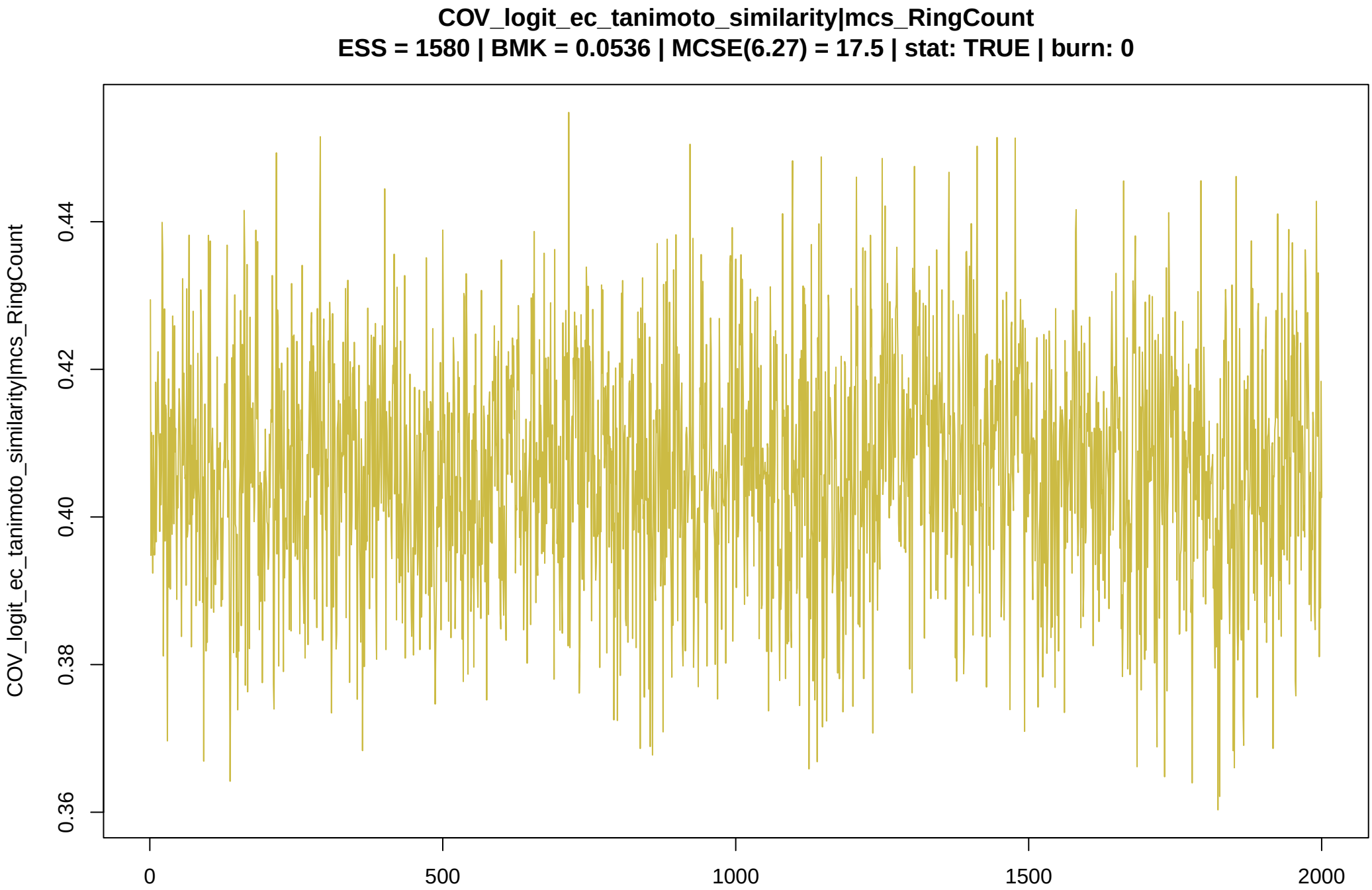

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1680 | BMK = 0.0378 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

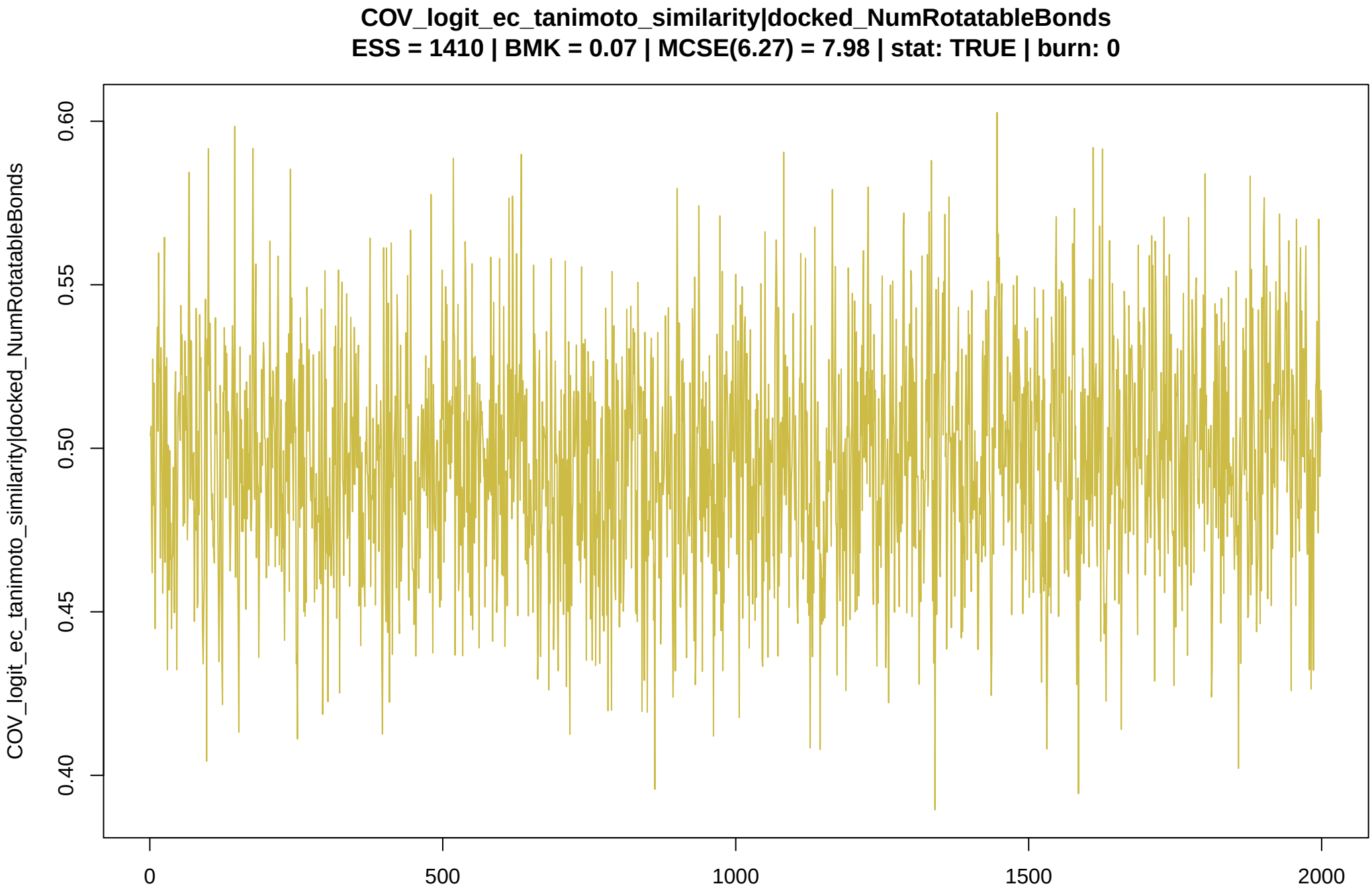

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 2000 | BMK = 0.0444 | MCSE(6.27) = 30.2 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
0.07
0.08
0.09
0.10
0.11
0.12
0.13
0
500
1000
1500
2000

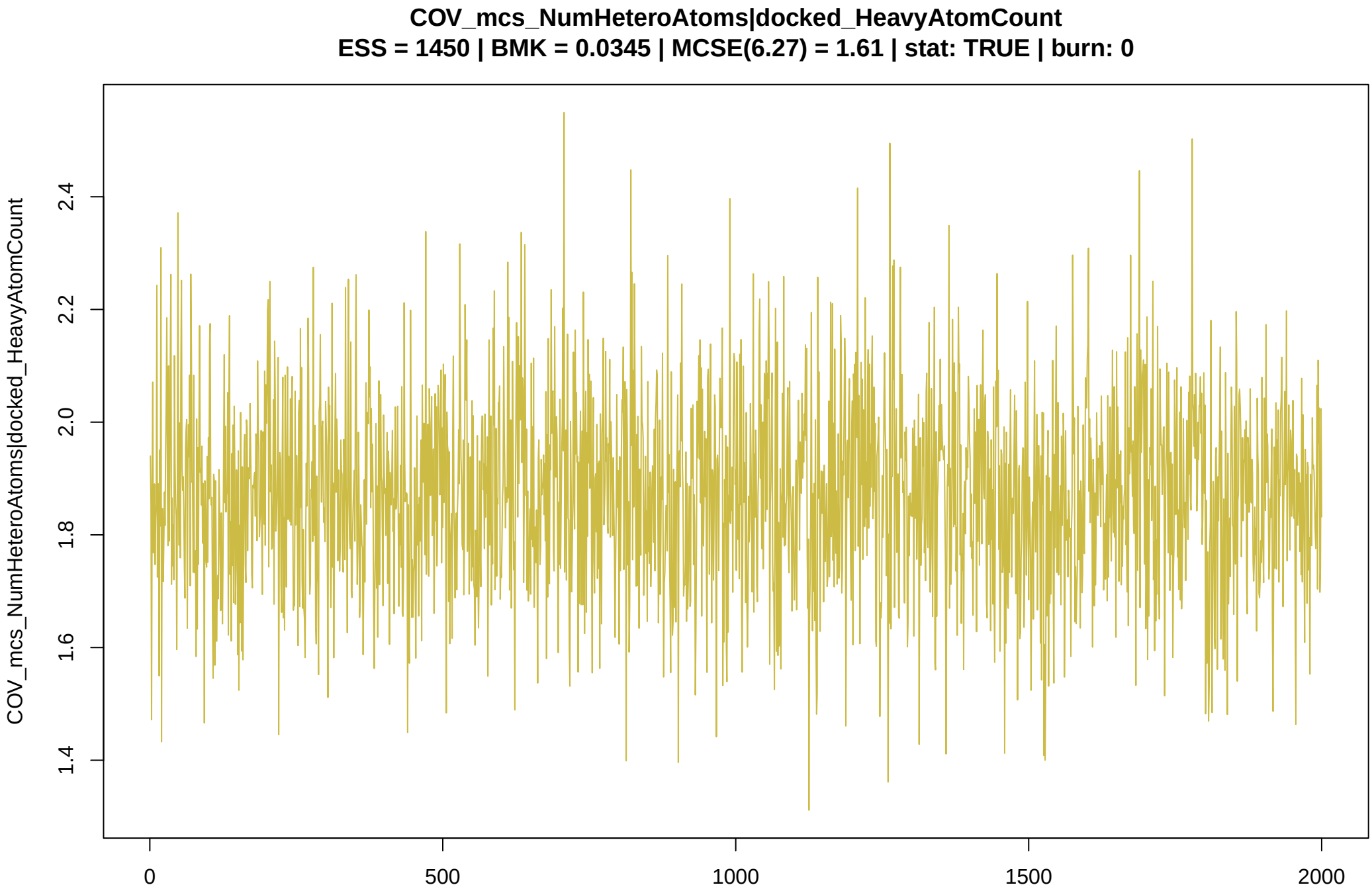

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1850 | BMK = 0.0547 | MCSE(6.27) = 6.13 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
0.25
0.30
0.35
0.40
0.45
0.50
0
500
1000
1500
2000

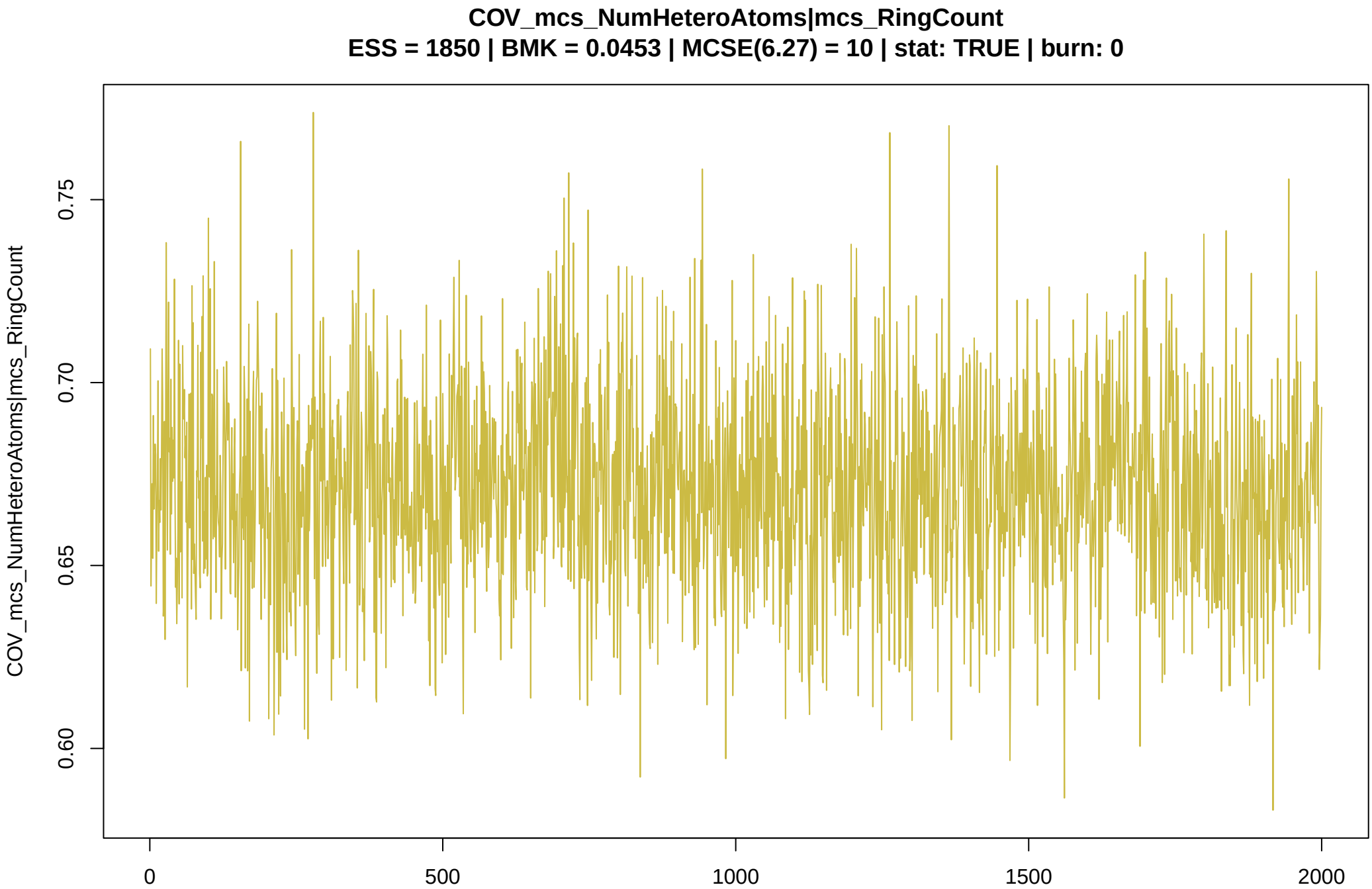

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1650 | BMK = 0.0586 | MCSE(6.27) = 9.16 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.80
0.85
0.90
0.95
0
500
1000
1500
2000

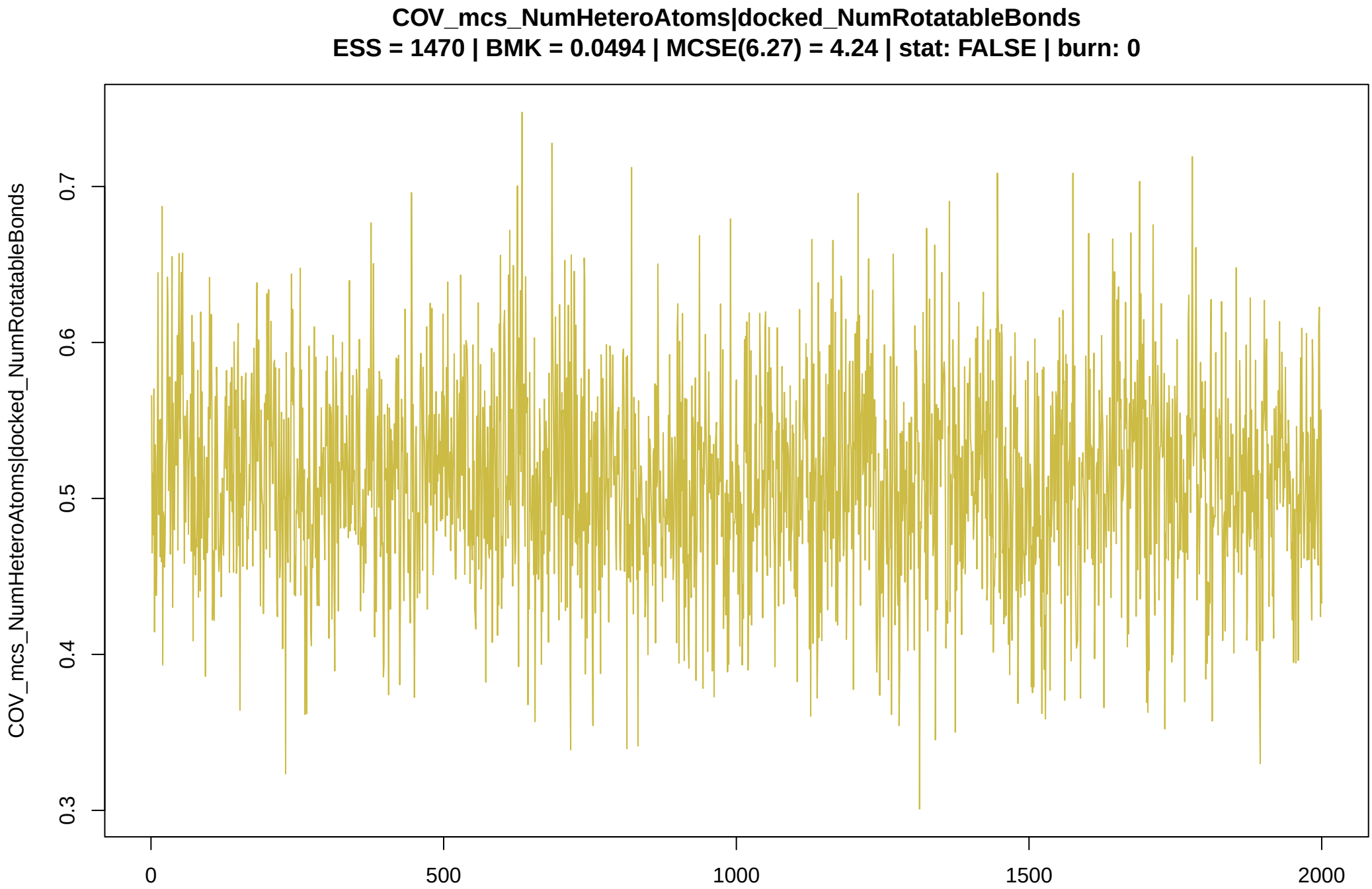

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1420 | BMK = 0.0484 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
1.1
1.2
1.3
1.4
1.5
1.6
0
500
1000
1500
2000

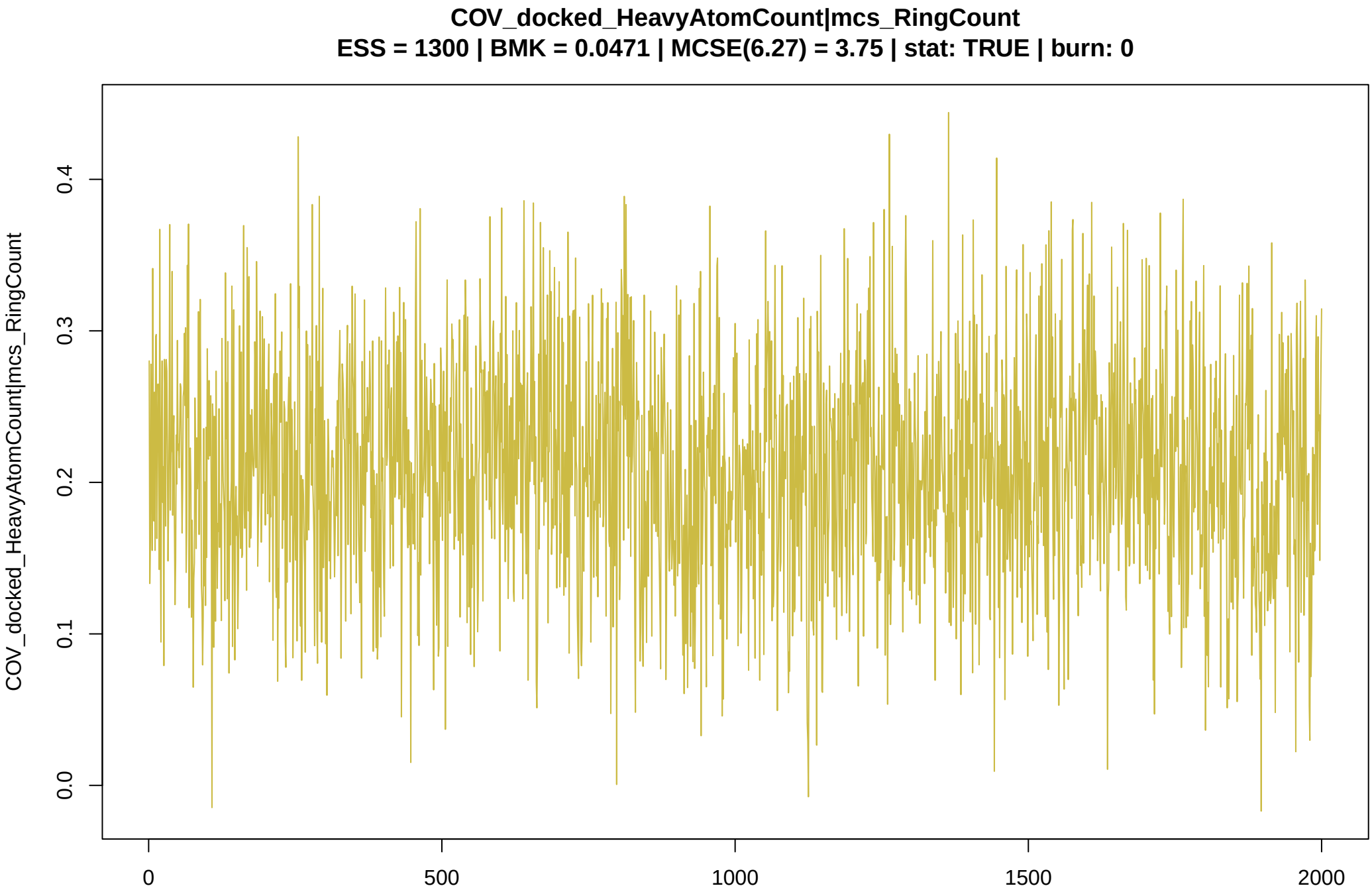

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1580 | BMK = 0.0536 | MCSE(6.27) = 17.5 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.36
0.38
0.40
0.42
0.44
0
500
1000
1500
2000

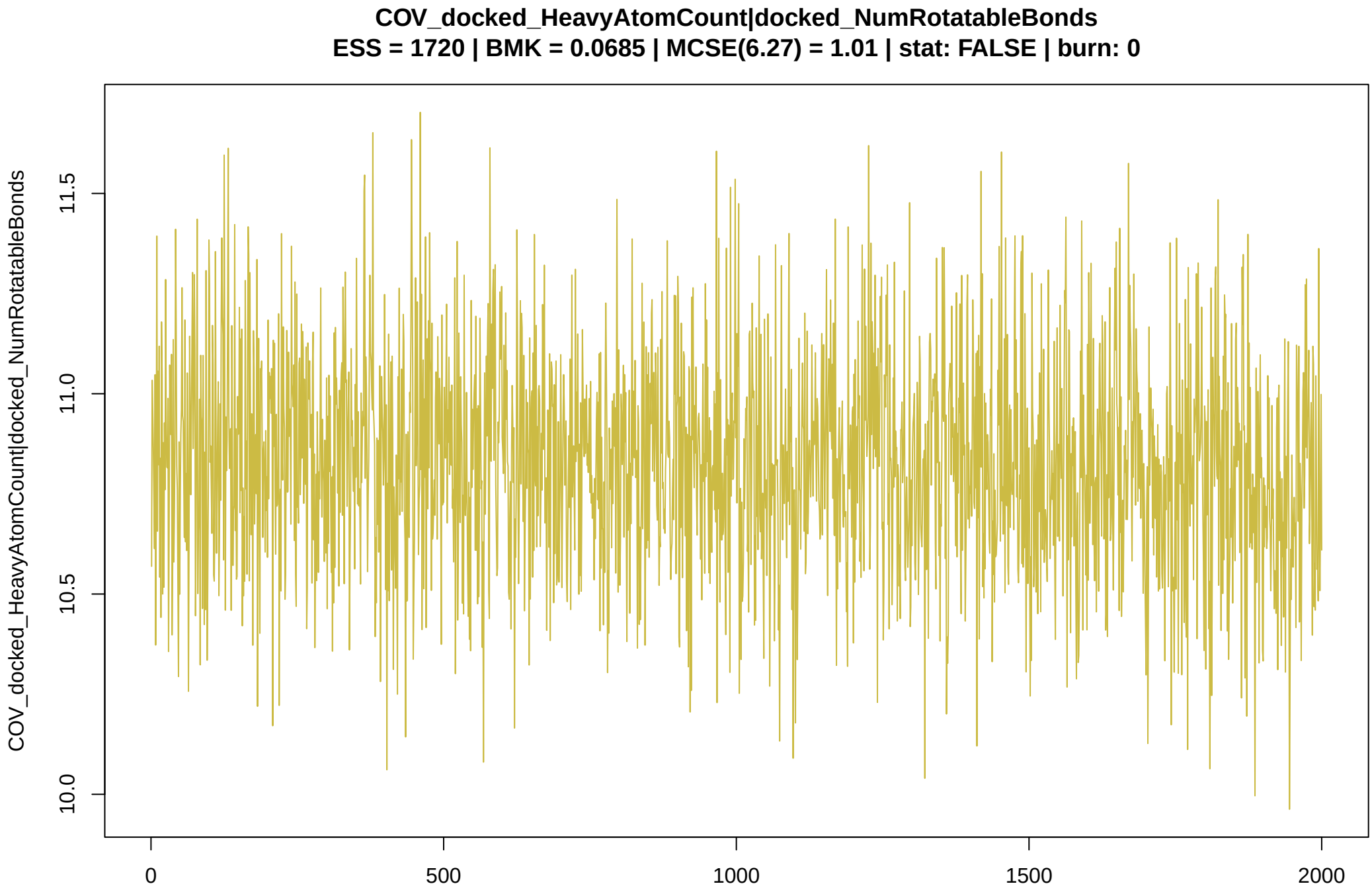

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1410 | BMK = 0.07 | MCSE(6.27) = 7.98 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
0.40
0.45
0.50
0.55
0.60
0
500
1000
1500
2000

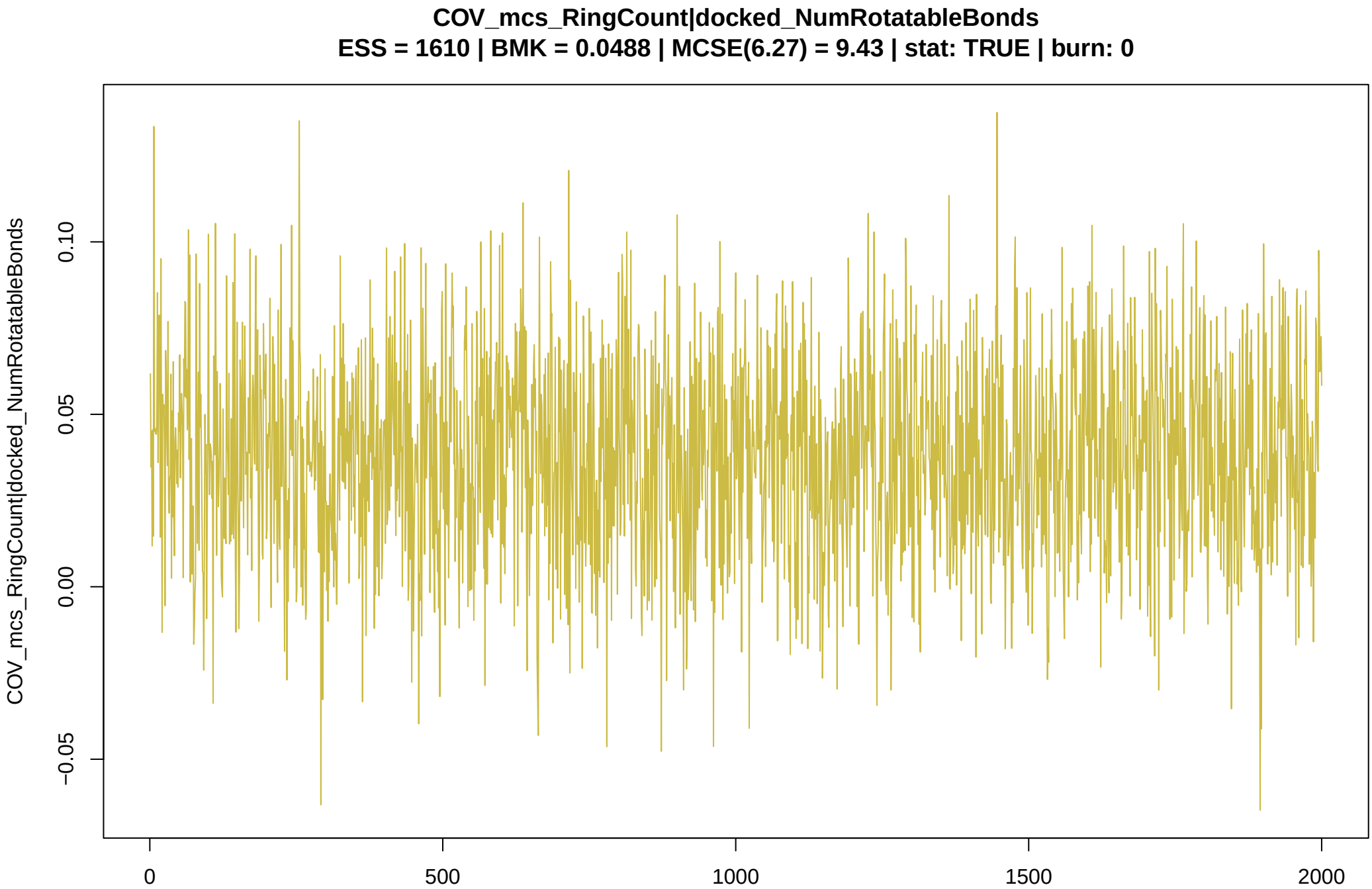

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1450 | BMK = 0.0345 | MCSE(6.27) = 1.61 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
1.4
1.6
1.8
2.0
2.2
2.4
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1850 | BMK = 0.0453 | MCSE(6.27) = 10 | 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 = 1470 | BMK = 0.0494 | MCSE(6.27) = 4.24 | stat: FALSE | burn: 0
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
0.3
0.4
0.5
0.6
0.7
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1300 | BMK = 0.0471 | MCSE(6.27) = 3.75 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.0
0.1
0.2
0.3
0.4
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1720 | BMK = 0.0685 | MCSE(6.27) = 1.01 | 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 = 1610 | BMK = 0.0488 | MCSE(6.27) = 9.43 | stat: TRUE | burn: 0
COV_mcs_RingCount|docked_NumRotatableBonds
0.10
0.05
0.00
−0.05
0
500
1000
1500
2000