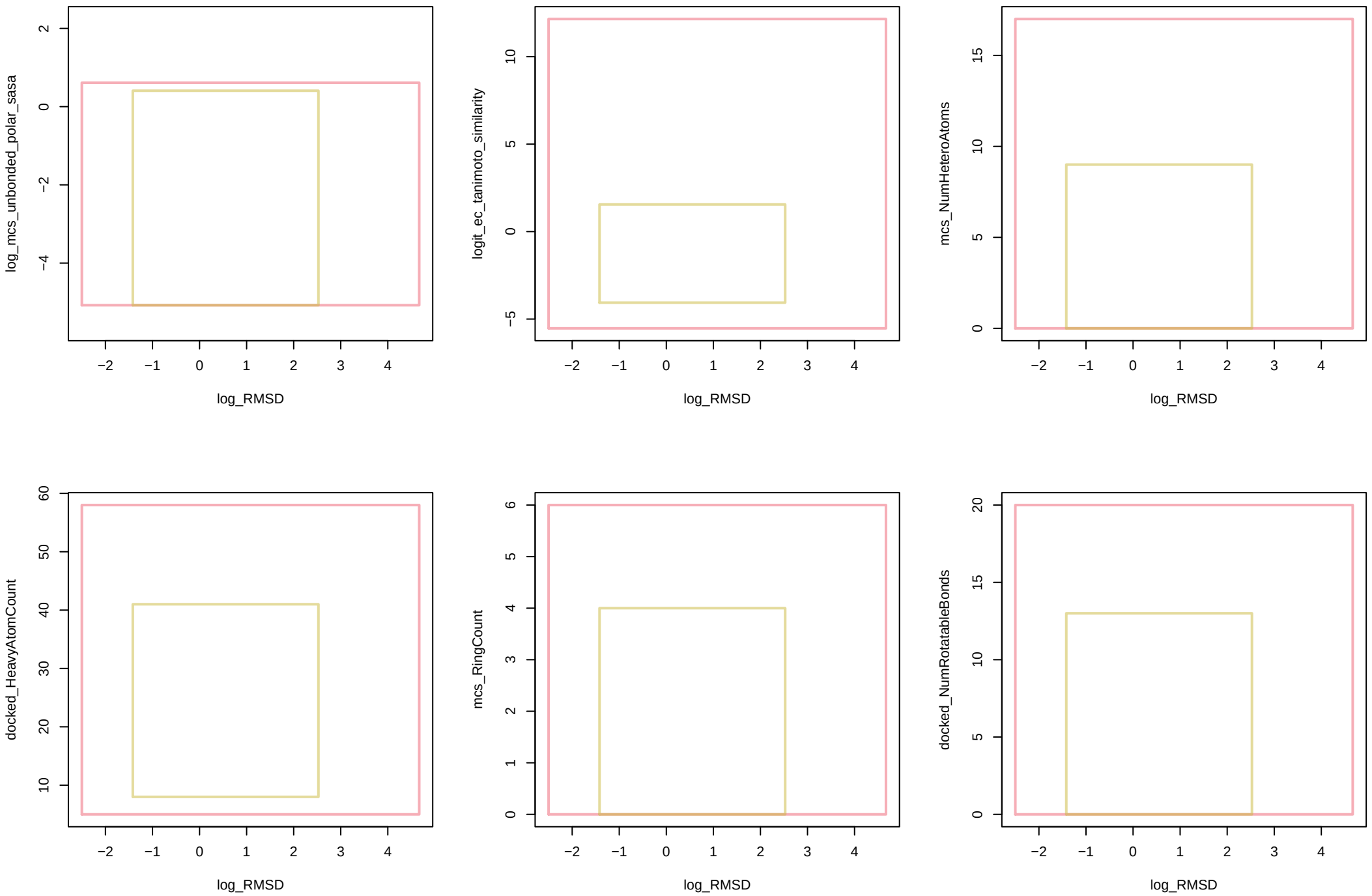
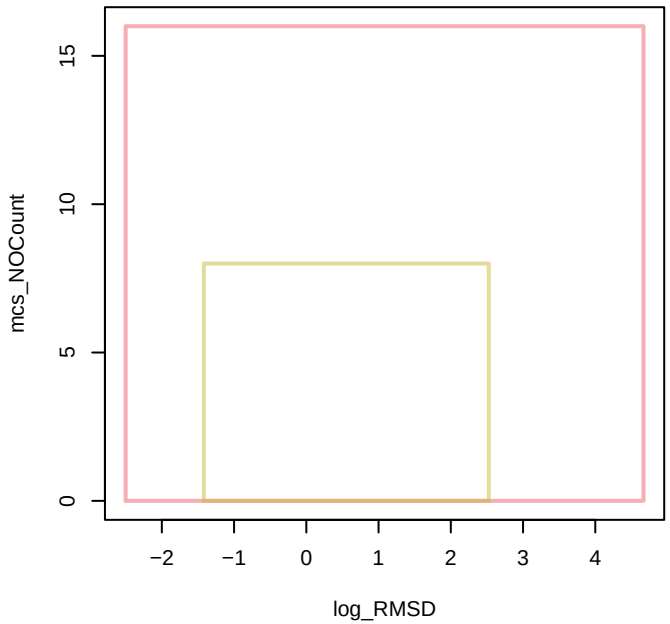
−− STATS maxD −−
min ESS = 4.06612840137564
max BMK = 0.836873733655051
max MCSE = 24.3631587703453
all stationary: FALSE
burn: 1224

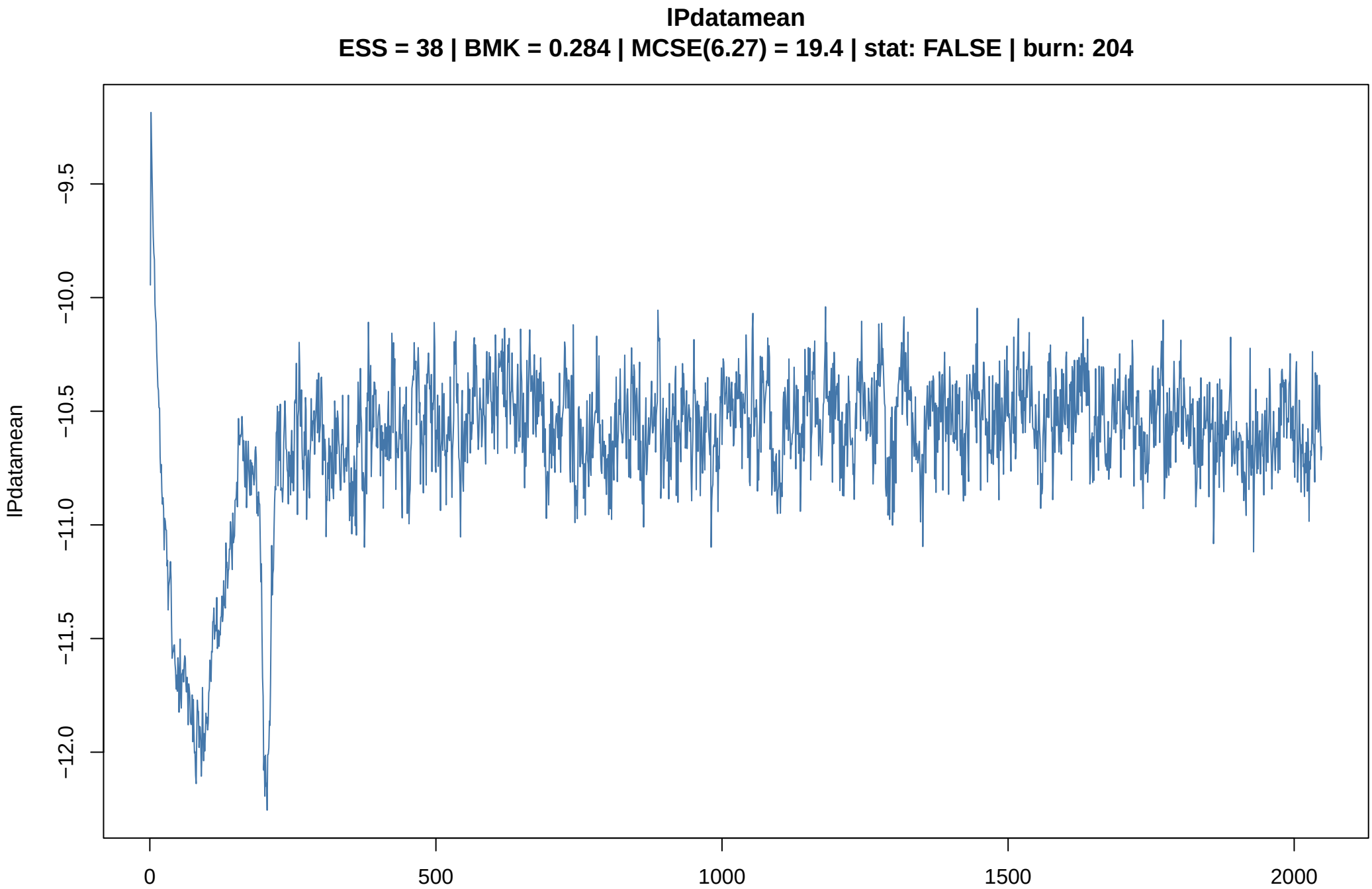
−− STATS 2D −−
min ESS = 8.12551786780056
max BMK = 0.348476374648908
max MCSE = 22.2464885914186
all stationary: FALSE
burn: 204

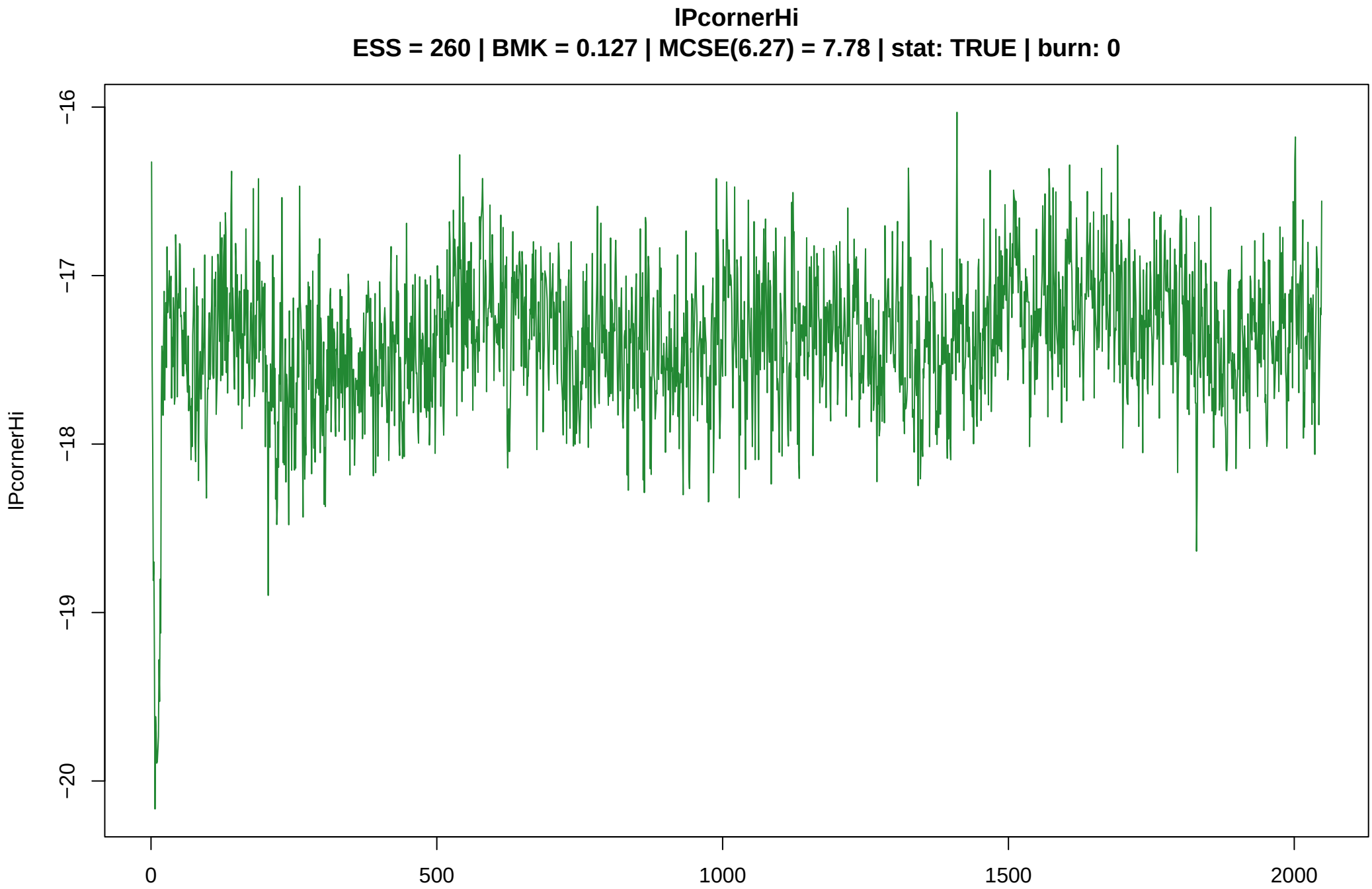
−− STATS 1D −−
min ESS = 9.88395324235386
max BMK = 0.278238770343452
max MCSE = 6.26706740732643
all stationary: FALSE
burn: 204

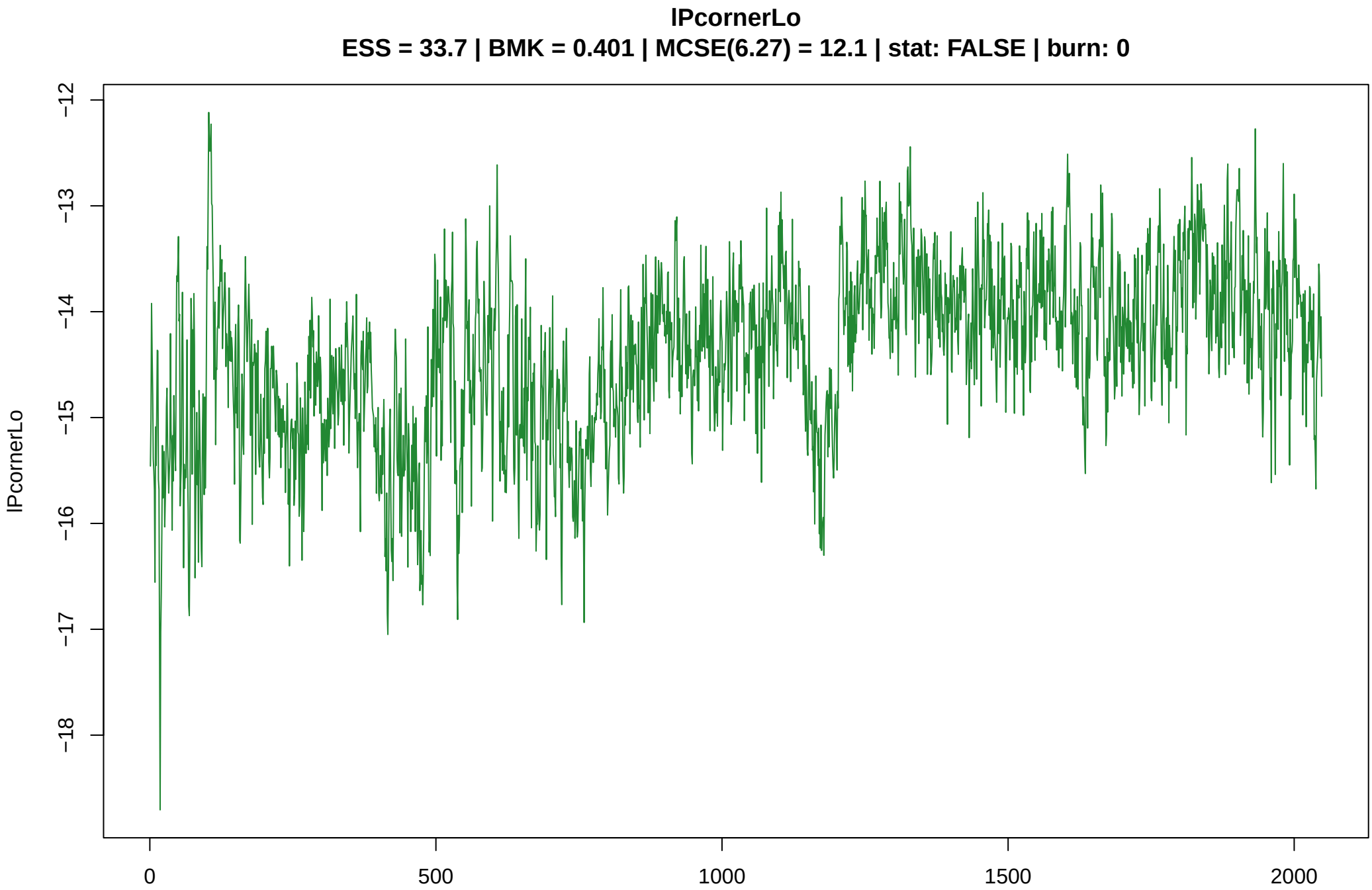
Occupied clusters: 20 of 64

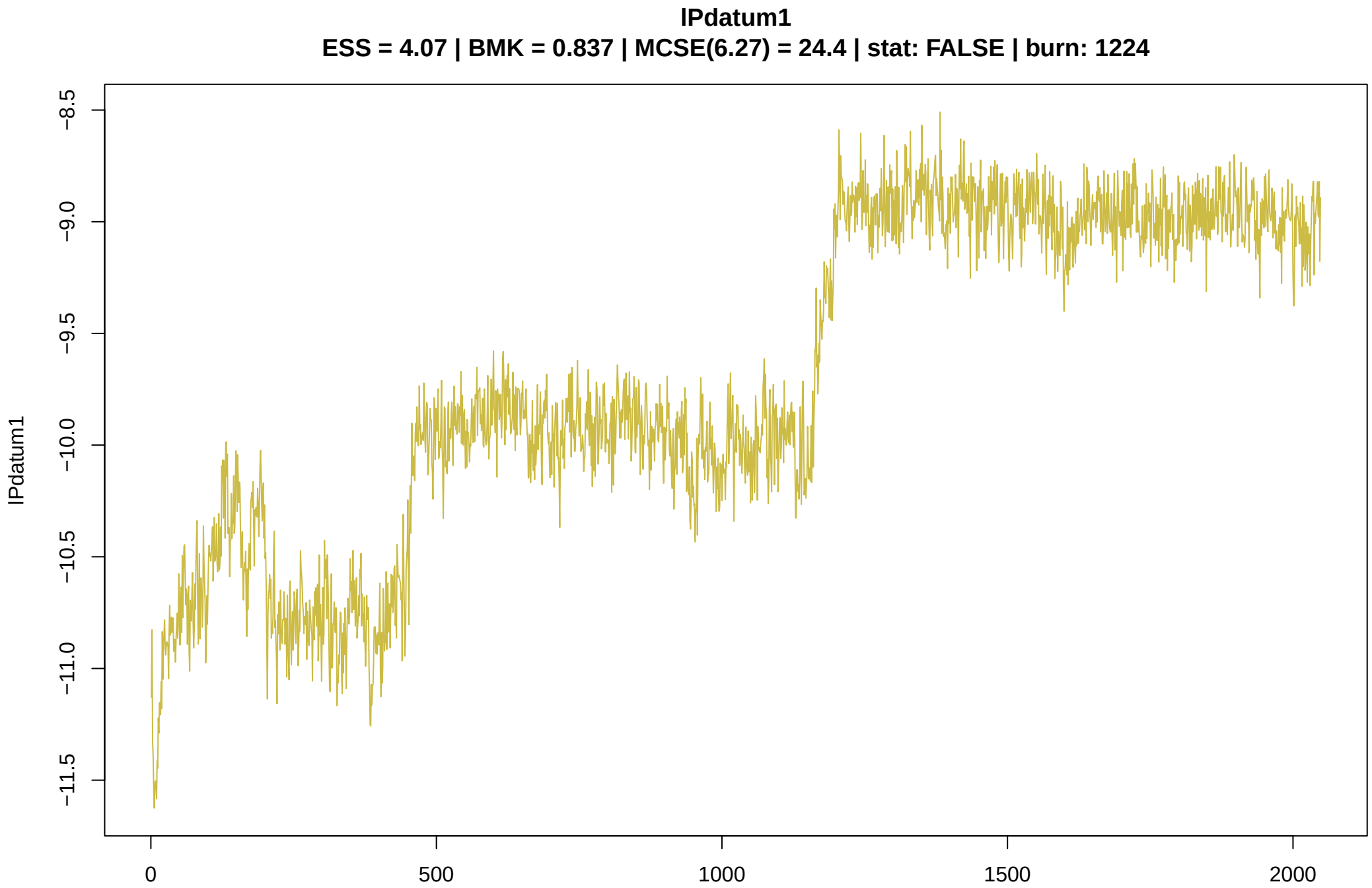

log_mcs_unbonded_polar_sasa
log_RMSD
logit_ec_tanimoto_similarity
log_RMSD
mcs_NumHeteroAtoms
log_RMSD
docked_HeavyAtomCount
log_RMSD
mcs_RingCount
log_RMSD
docked_NumRotatableBonds
log_RMSD

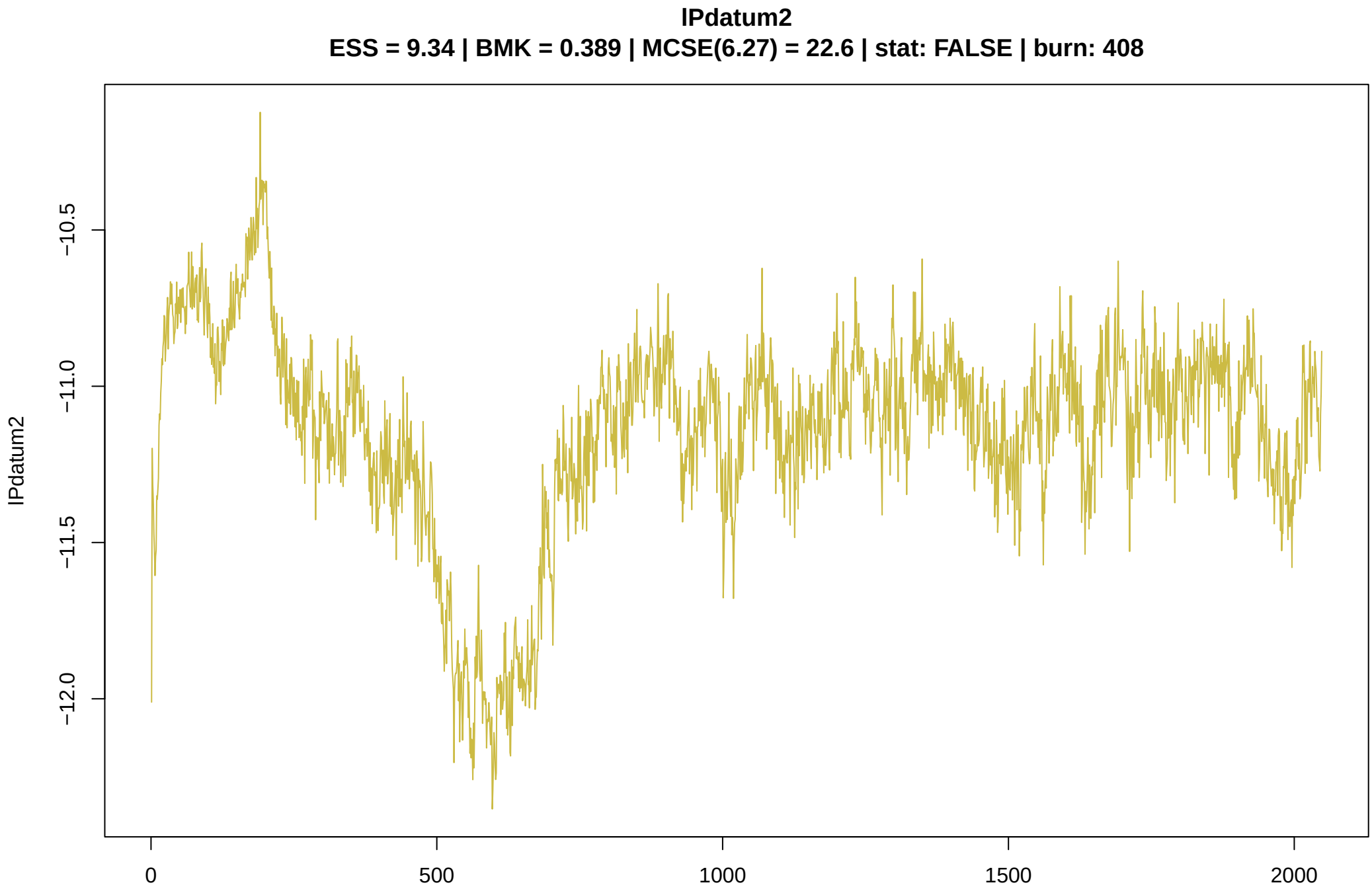

mcs_NOCount
0
5
10
15
−2
−1
0
1
2
3
4
log_RMSD

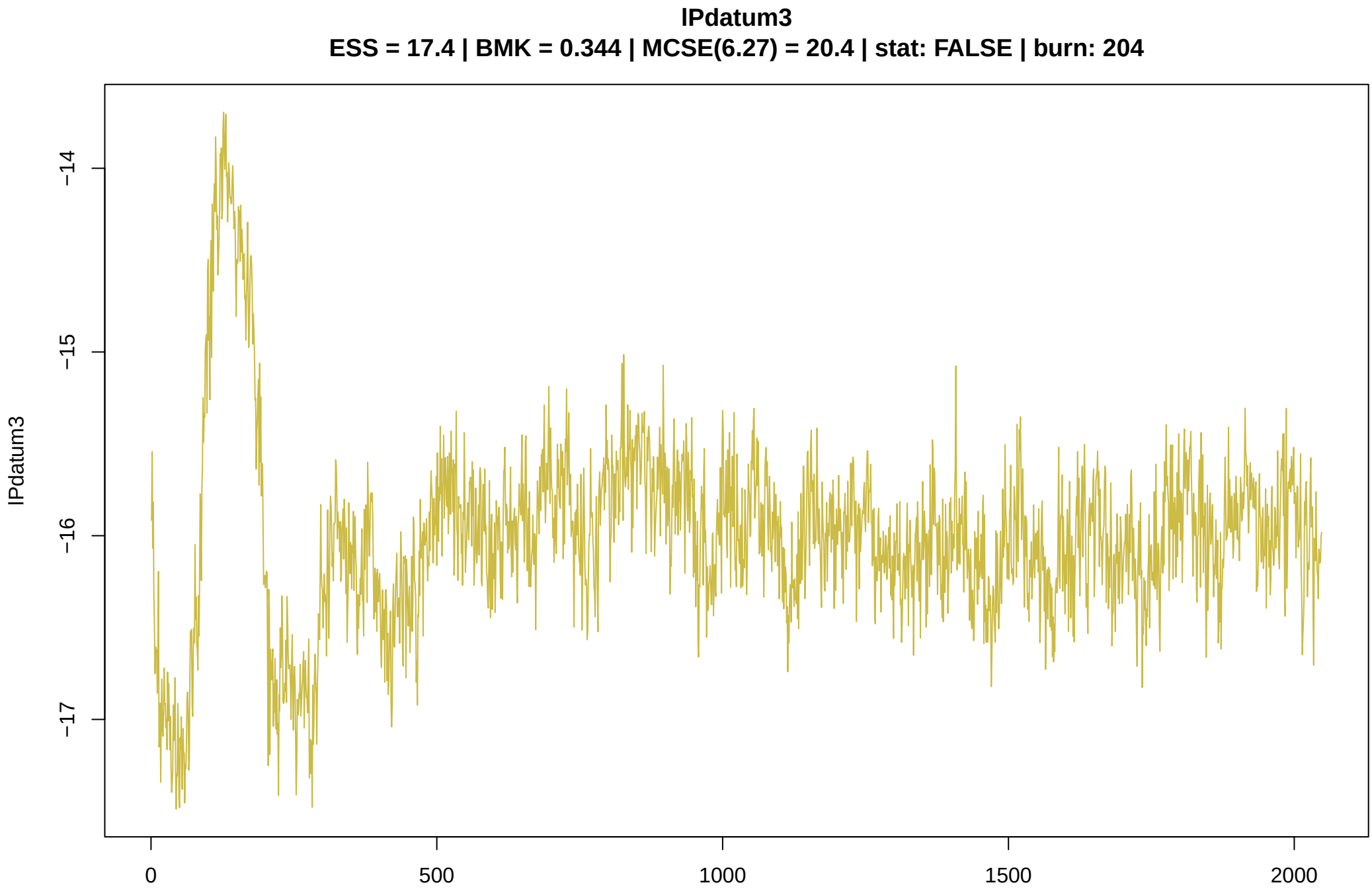

lPdatamean
ESS = 38 | BMK = 0.284 | MCSE(6.27) = 19.4 | stat: FALSE | burn: 204
lPdatamean
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

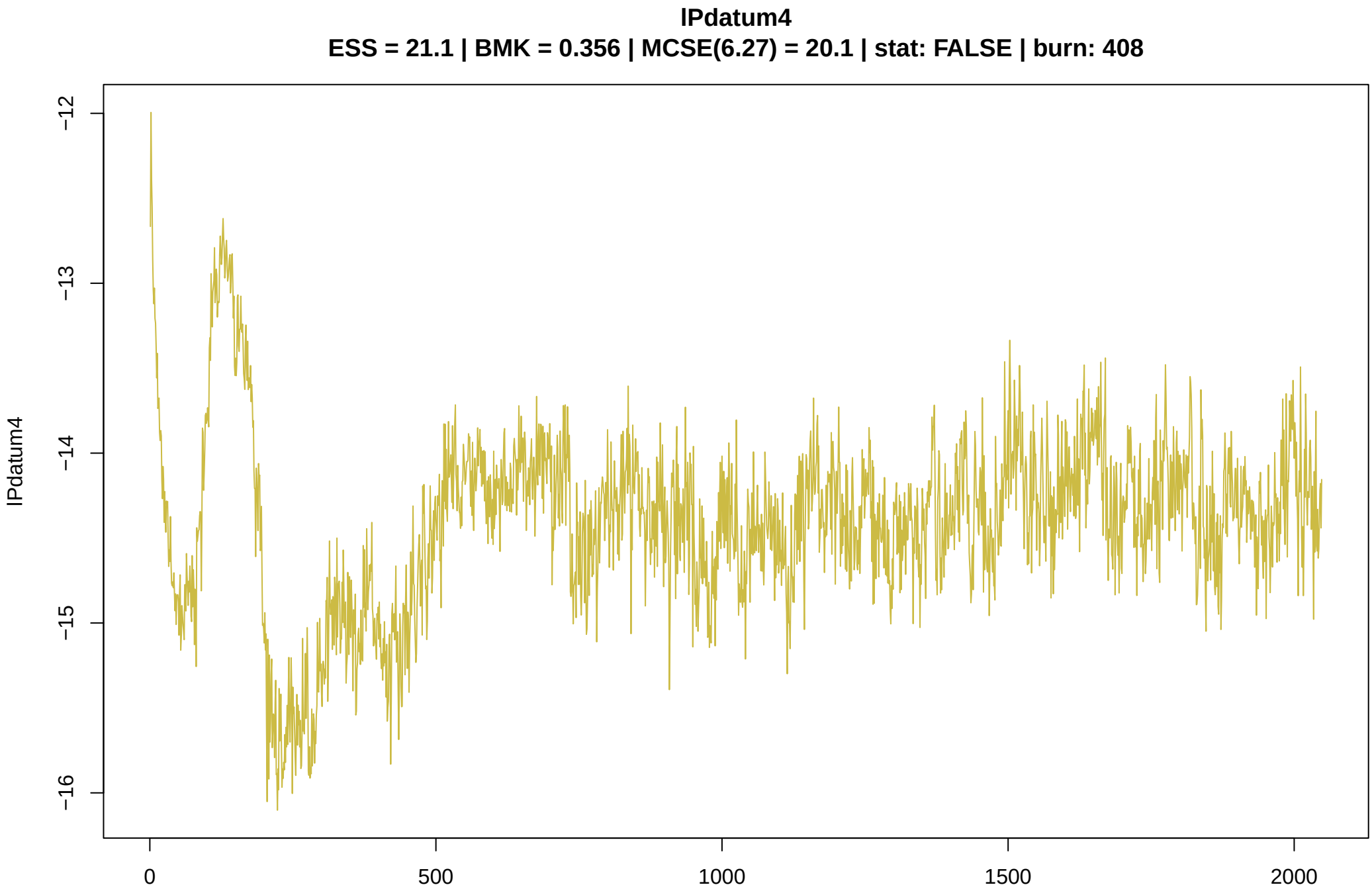

lPcornerHi
ESS = 260 | BMK = 0.127 | MCSE(6.27) = 7.78 | stat: TRUE | burn: 0
lPcornerHi
−16
−17
−18
−19
−20
0
500
1000
1500
2000

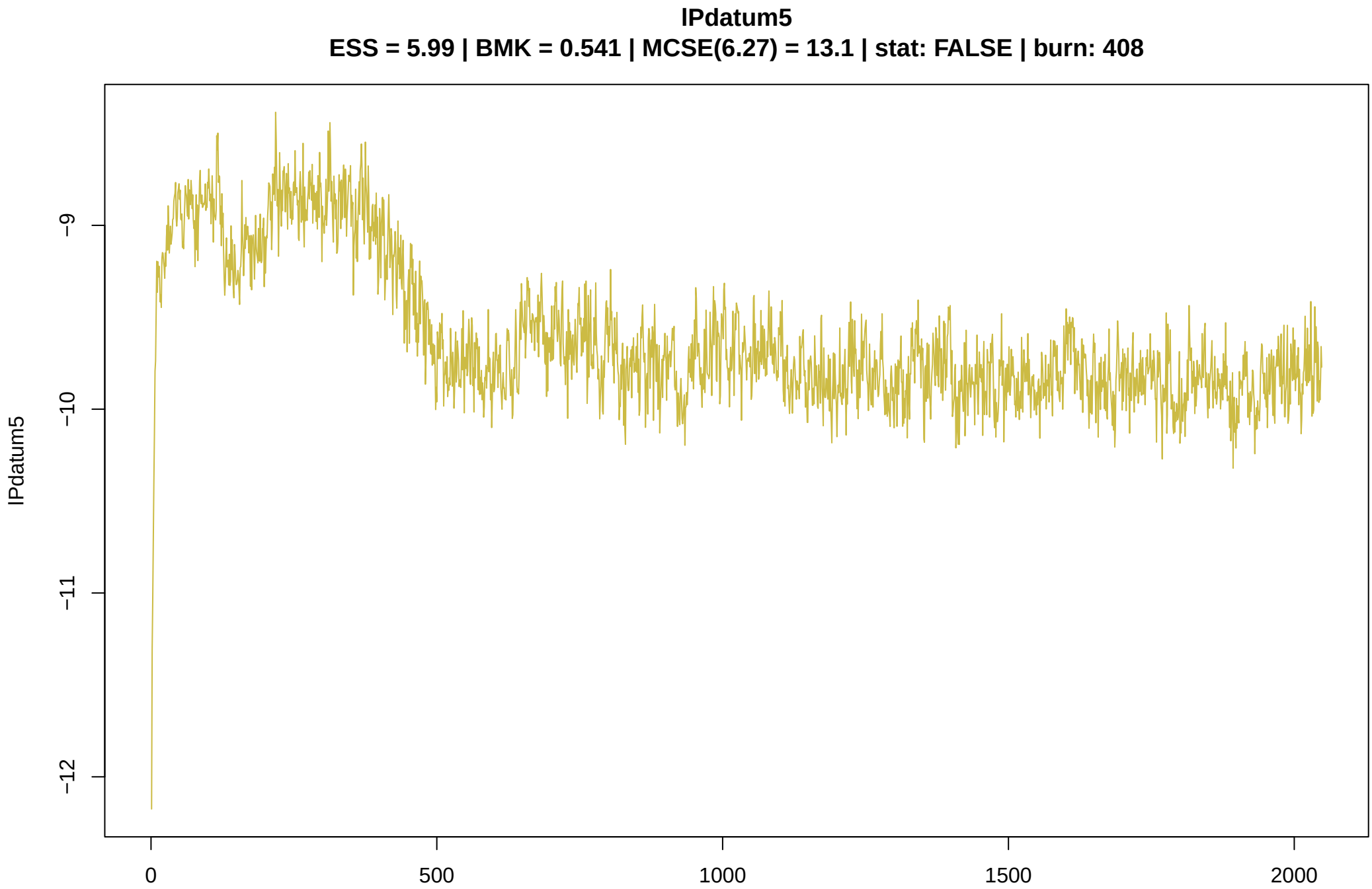

lPcornerLo
ESS = 33.7 | BMK = 0.401 | MCSE(6.27) = 12.1 | stat: FALSE | burn: 0
lPcornerLo
−12
−13
−14
−15
−16
−17
−18
0
500
1000
1500
2000

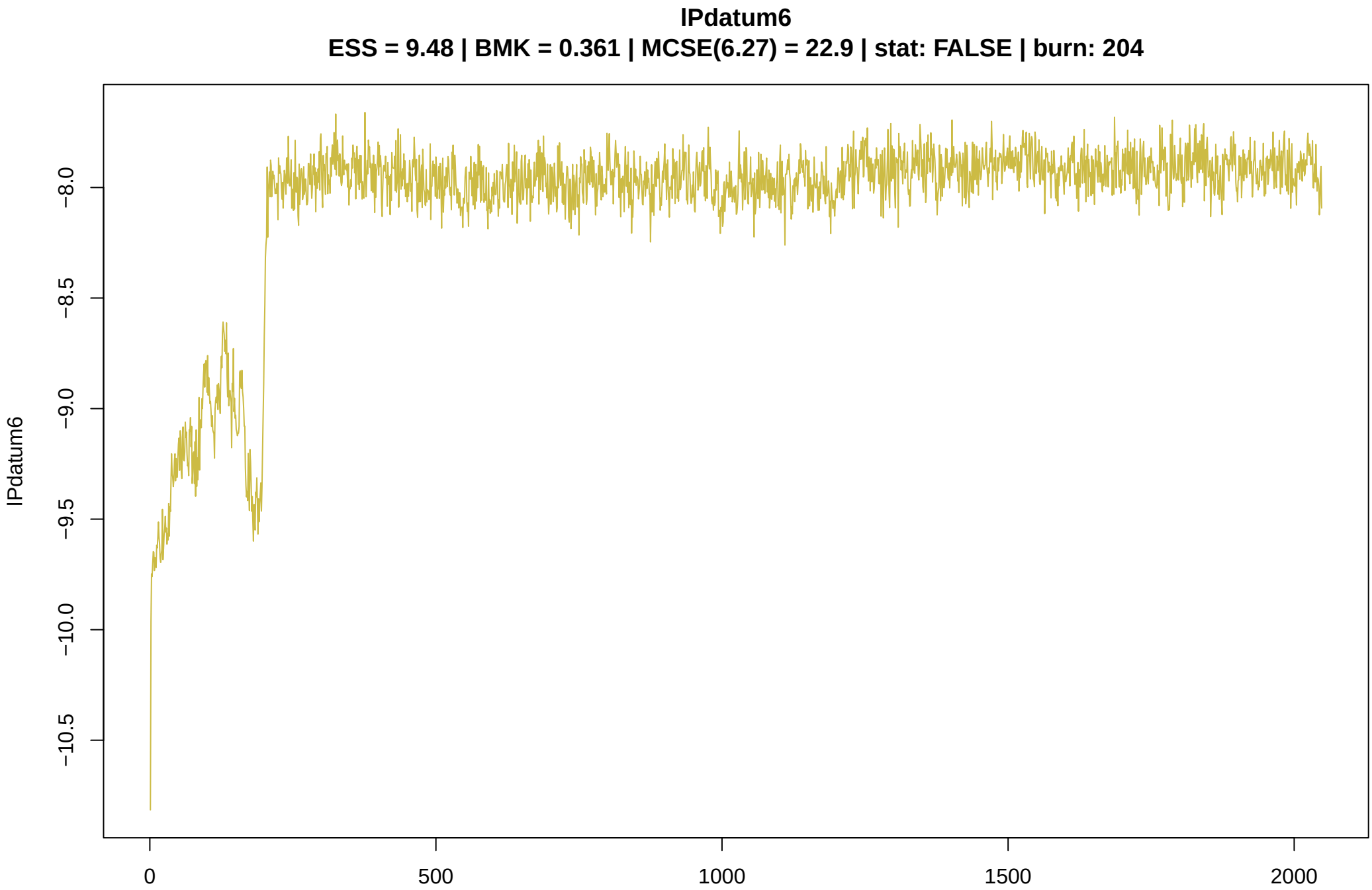

lPdatum1
ESS = 4.07 | BMK = 0.837 | MCSE(6.27) = 24.4 | stat: FALSE | burn: 1224
lPdatum1
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
0
500
1000
1500
2000

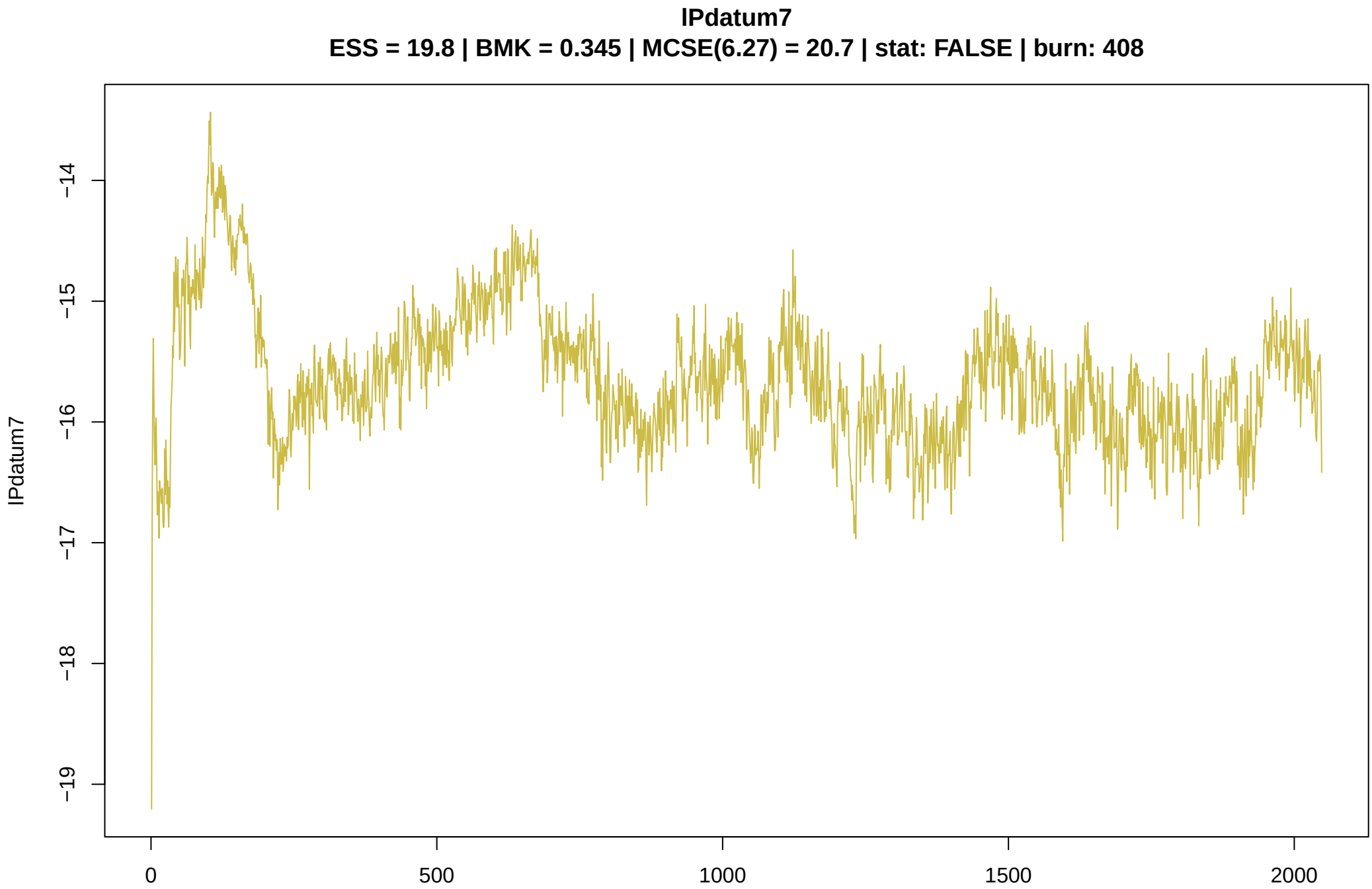

lPdatum2
ESS = 9.34 | BMK = 0.389 | MCSE(6.27) = 22.6 | stat: FALSE | burn: 408
lPdatum2
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

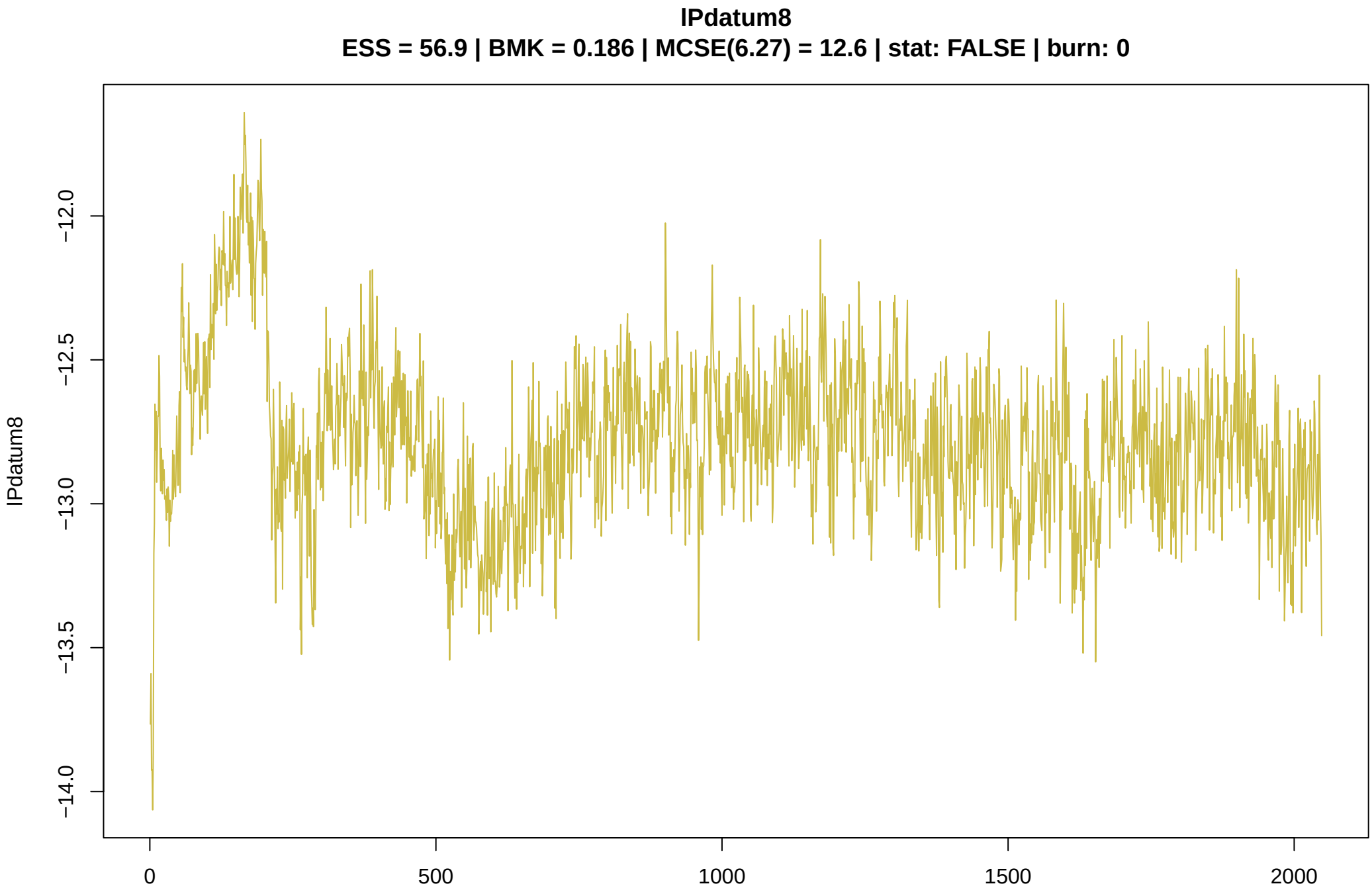

lPdatum3
ESS = 17.4 | BMK = 0.344 | MCSE(6.27) = 20.4 | stat: FALSE | burn: 204
lPdatum3
−14
−15
−16
−17
0
500
1000
1500
2000

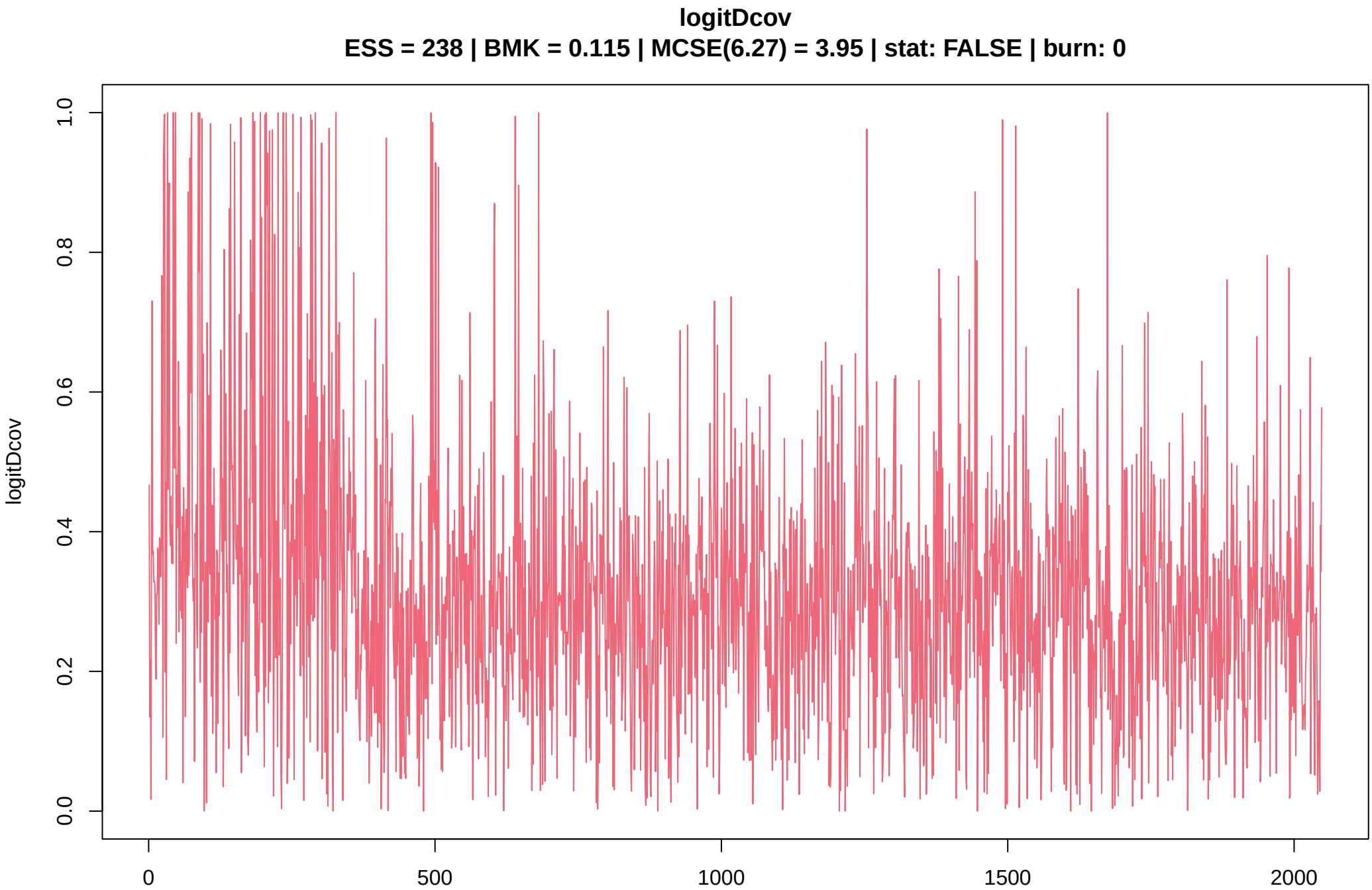

lPdatum4
ESS = 21.1 | BMK = 0.356 | MCSE(6.27) = 20.1 | stat: FALSE | burn: 408
lPdatum4
−12
−13
−14
−15
−16
0
500
1000
1500
2000

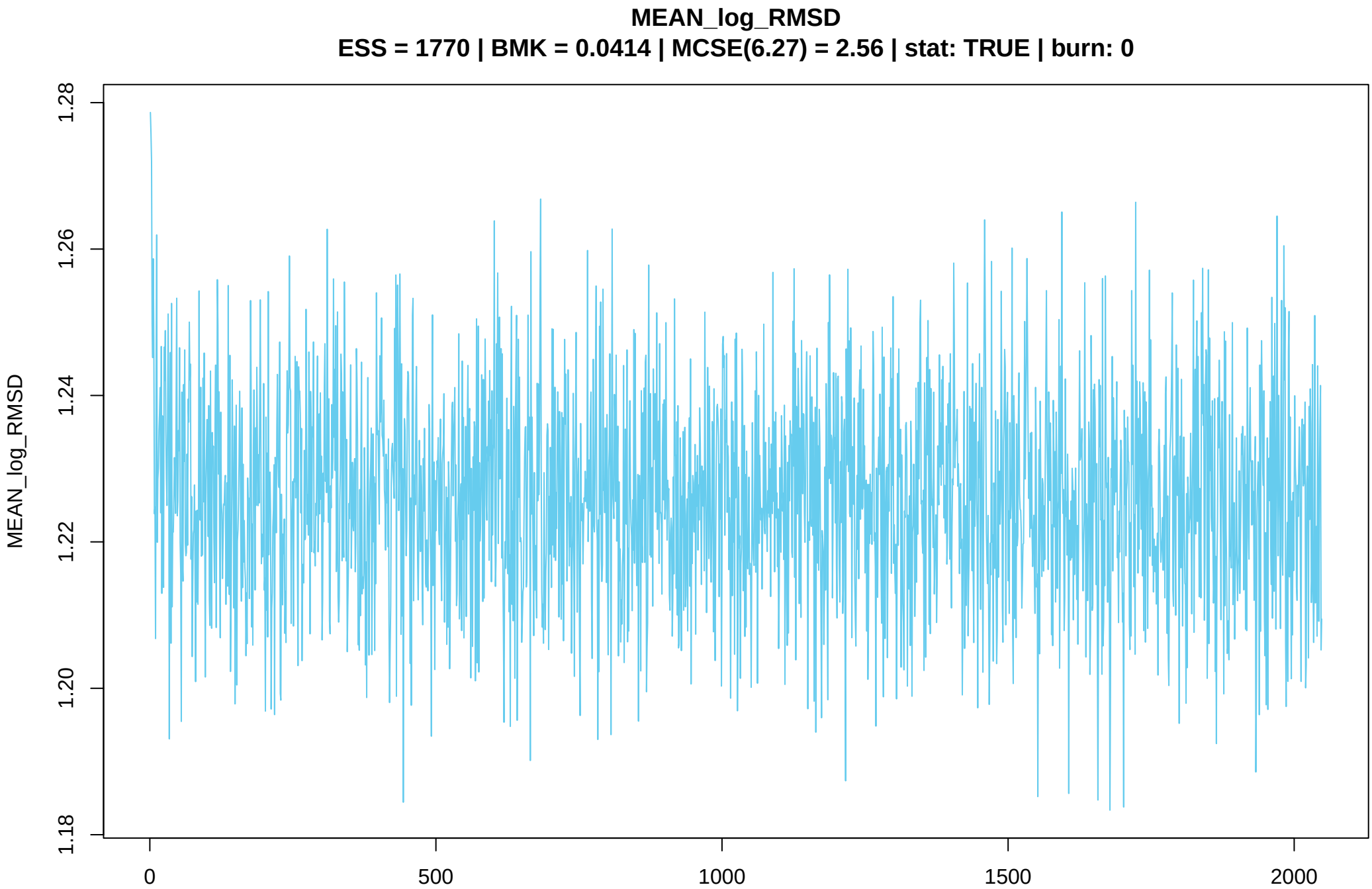

lPdatum5
ESS = 5.99 | BMK = 0.541 | MCSE(6.27) = 13.1 | stat: FALSE | burn: 408
lPdatum5
−9
−10
−11
−12
0
500
1000
1500
2000

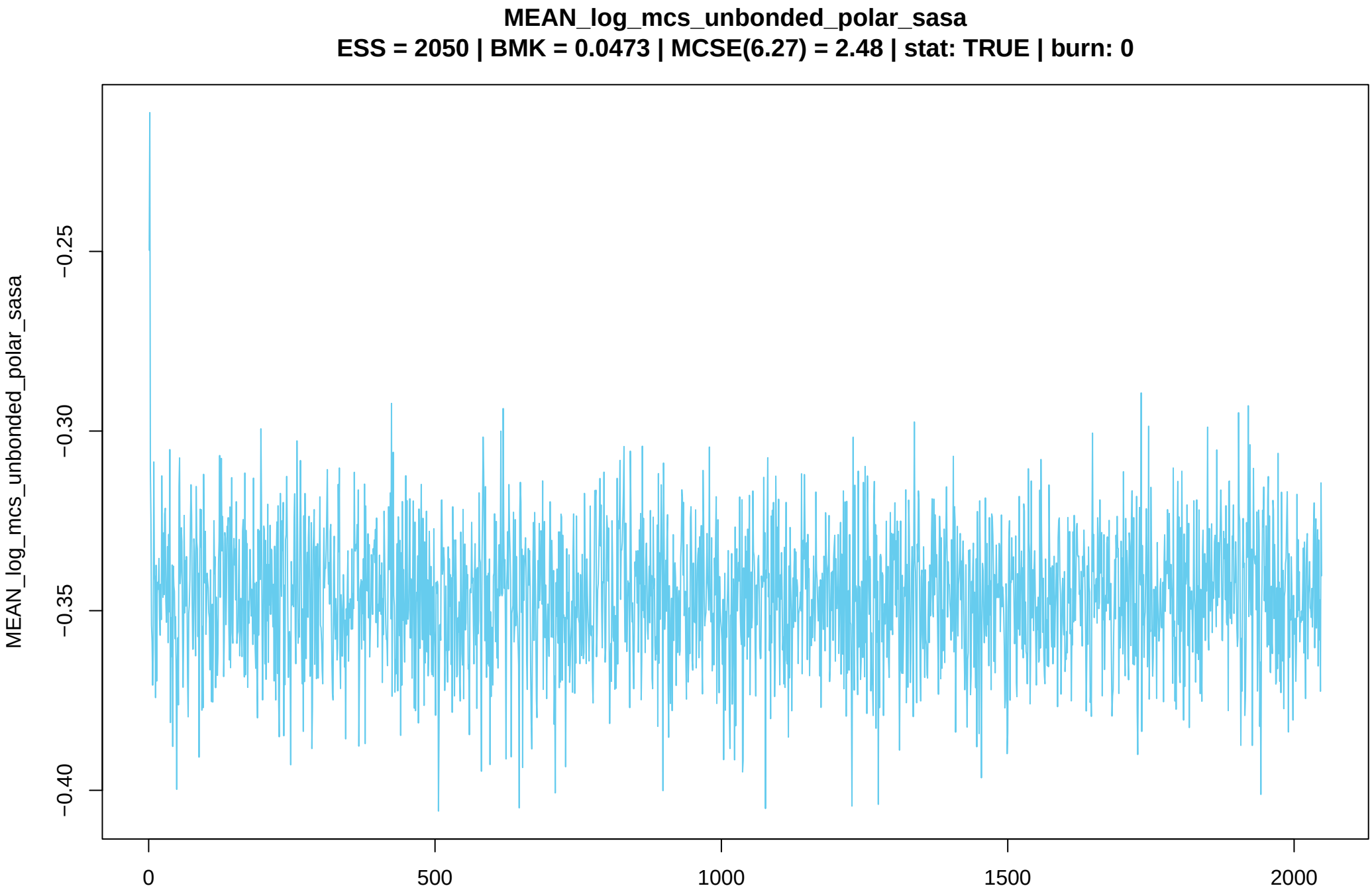

lPdatum6
ESS = 9.48 | BMK = 0.361 | MCSE(6.27) = 22.9 | stat: FALSE | burn: 204
lPdatum6
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
500
1000
1500
2000

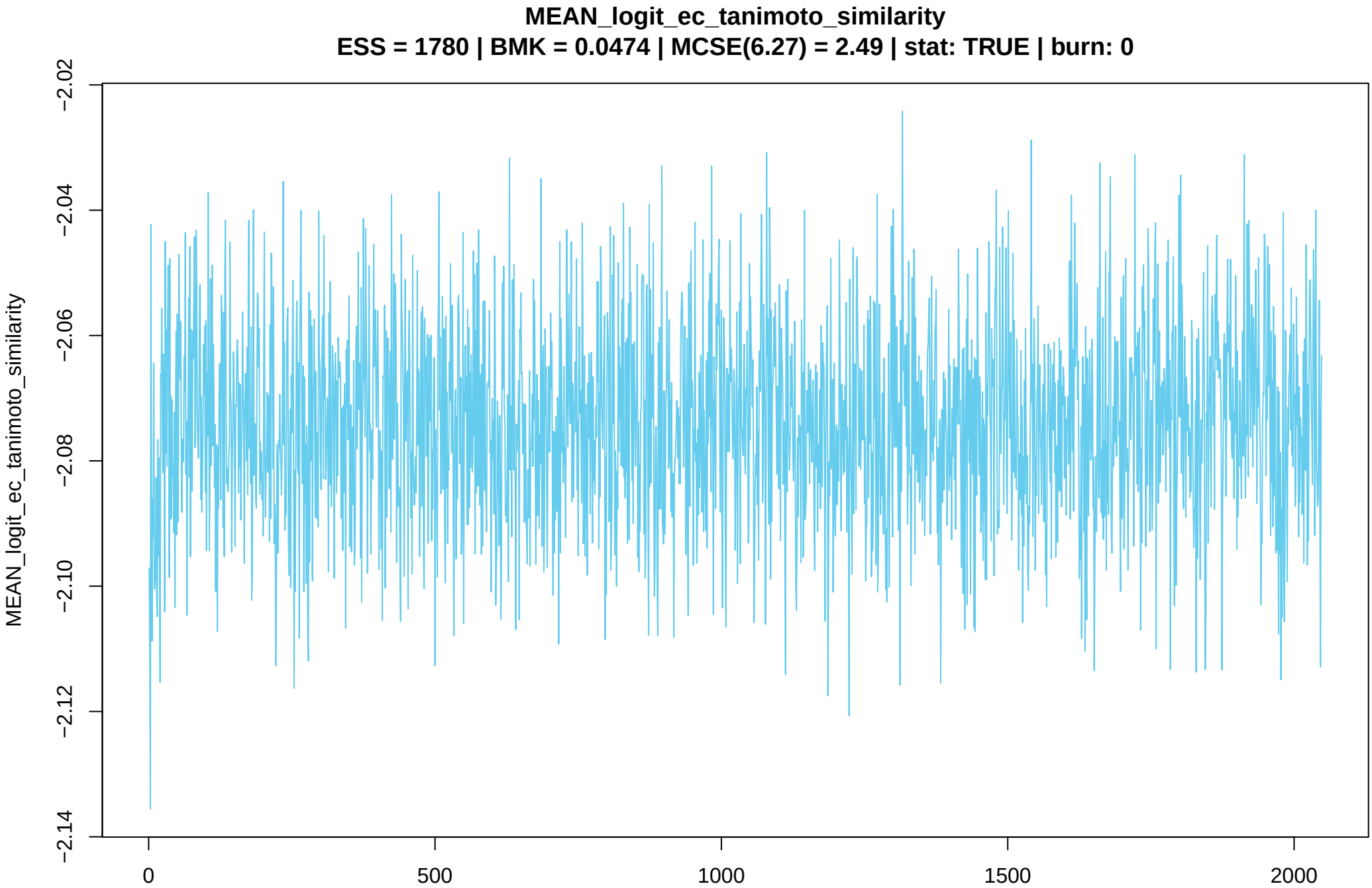

lPdatum7
ESS = 19.8 | BMK = 0.345 | MCSE(6.27) = 20.7 | stat: FALSE | burn: 408
lPdatum7
−14
−15
−16
−17
−18
−19
0
500
1000
1500
2000

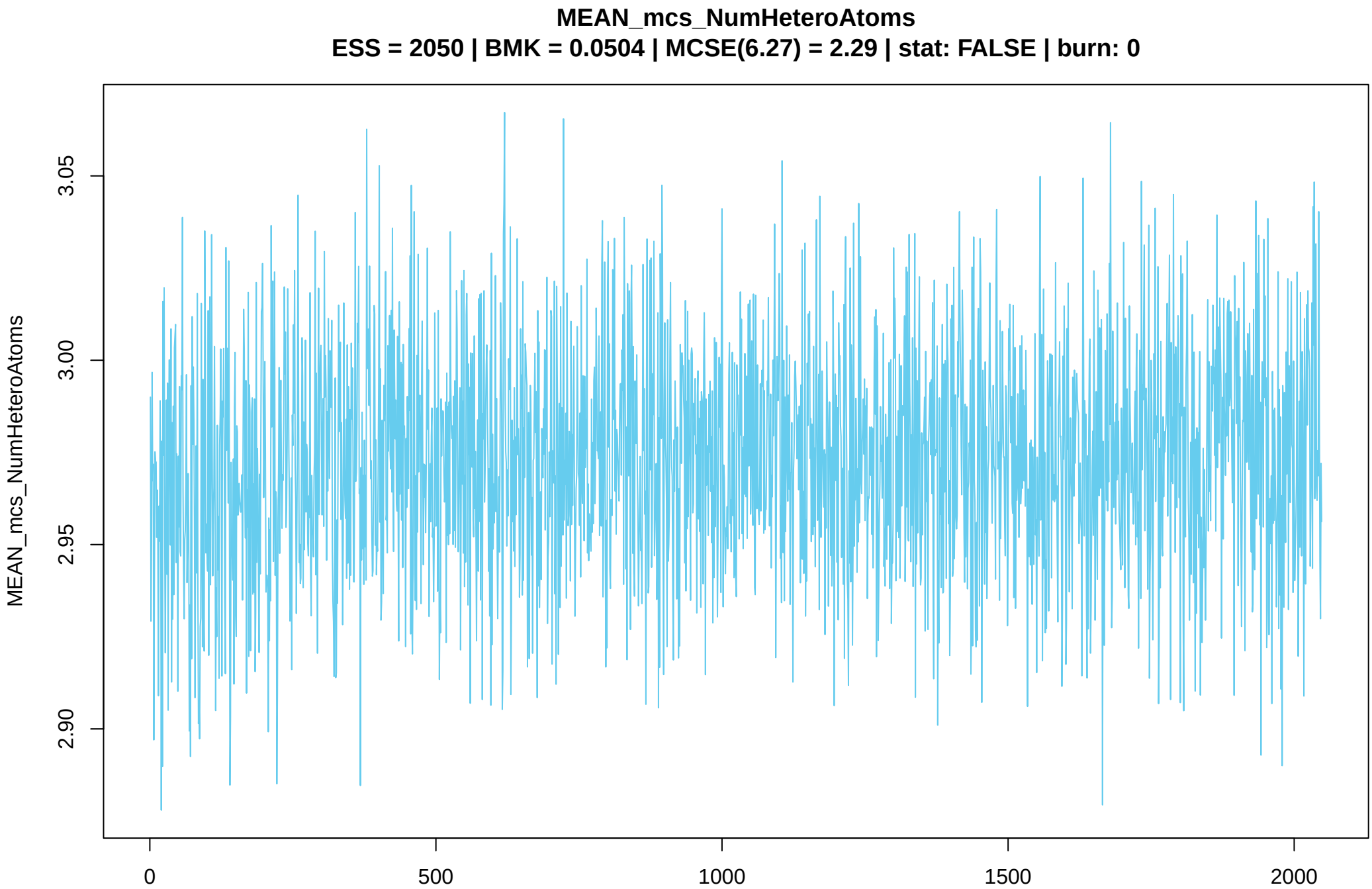

lPdatum8
ESS = 56.9 | BMK = 0.186 | MCSE(6.27) = 12.6 | stat: FALSE | burn: 0
lPdatum8
−12.0
−12.5
−13.0
−13.5
−14.0
0
500
1000
1500
2000

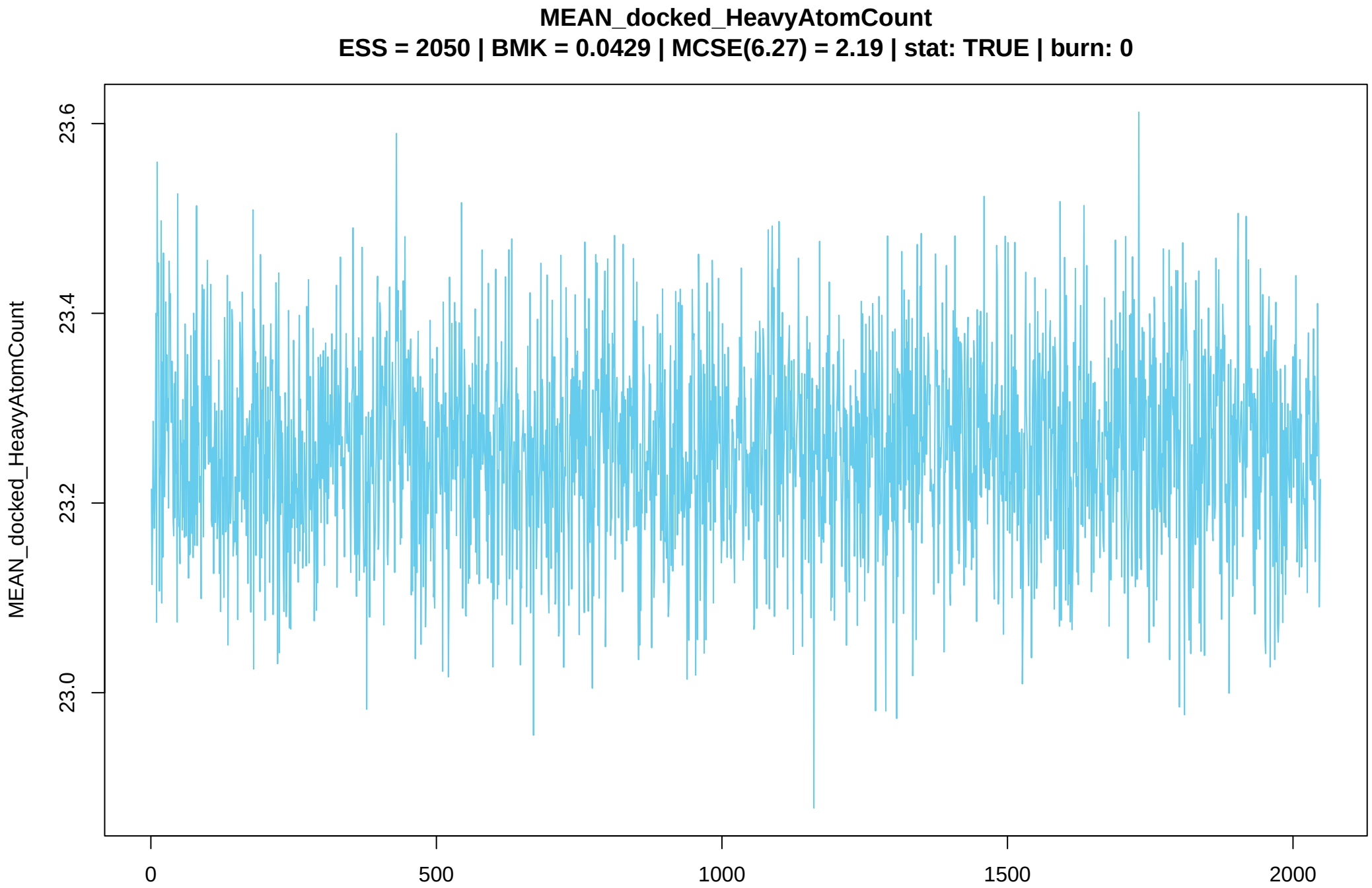

logitDcov
ESS = 238 | BMK = 0.115 | MCSE(6.27) = 3.95 | stat: FALSE | burn: 0
logitDcov
0.0
0.2
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

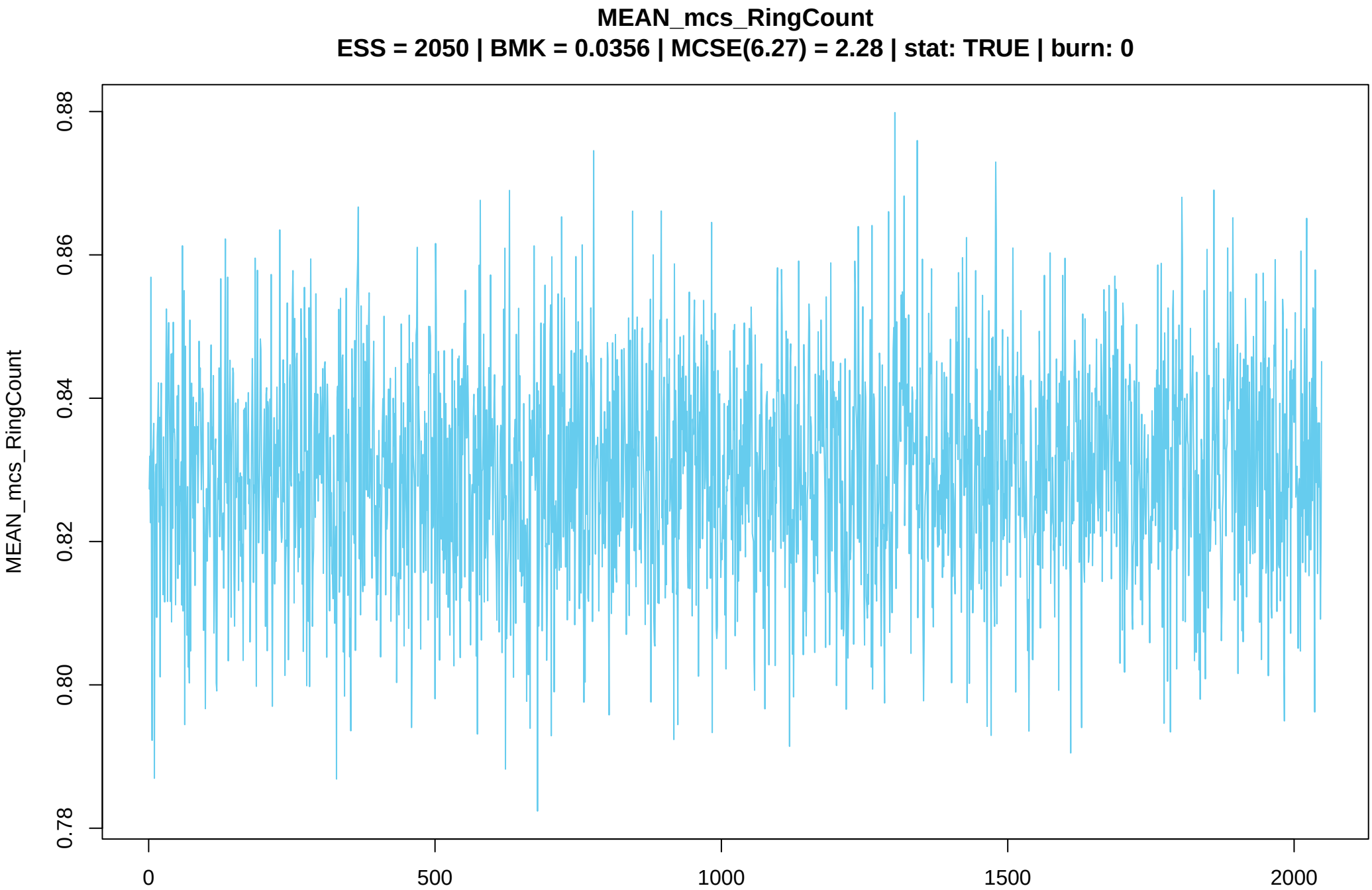

MEAN_log_RMSD
ESS = 1770 | BMK = 0.0414 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.18
1.20
1.22
1.24
1.26
1.28
0
500
1000
1500
2000

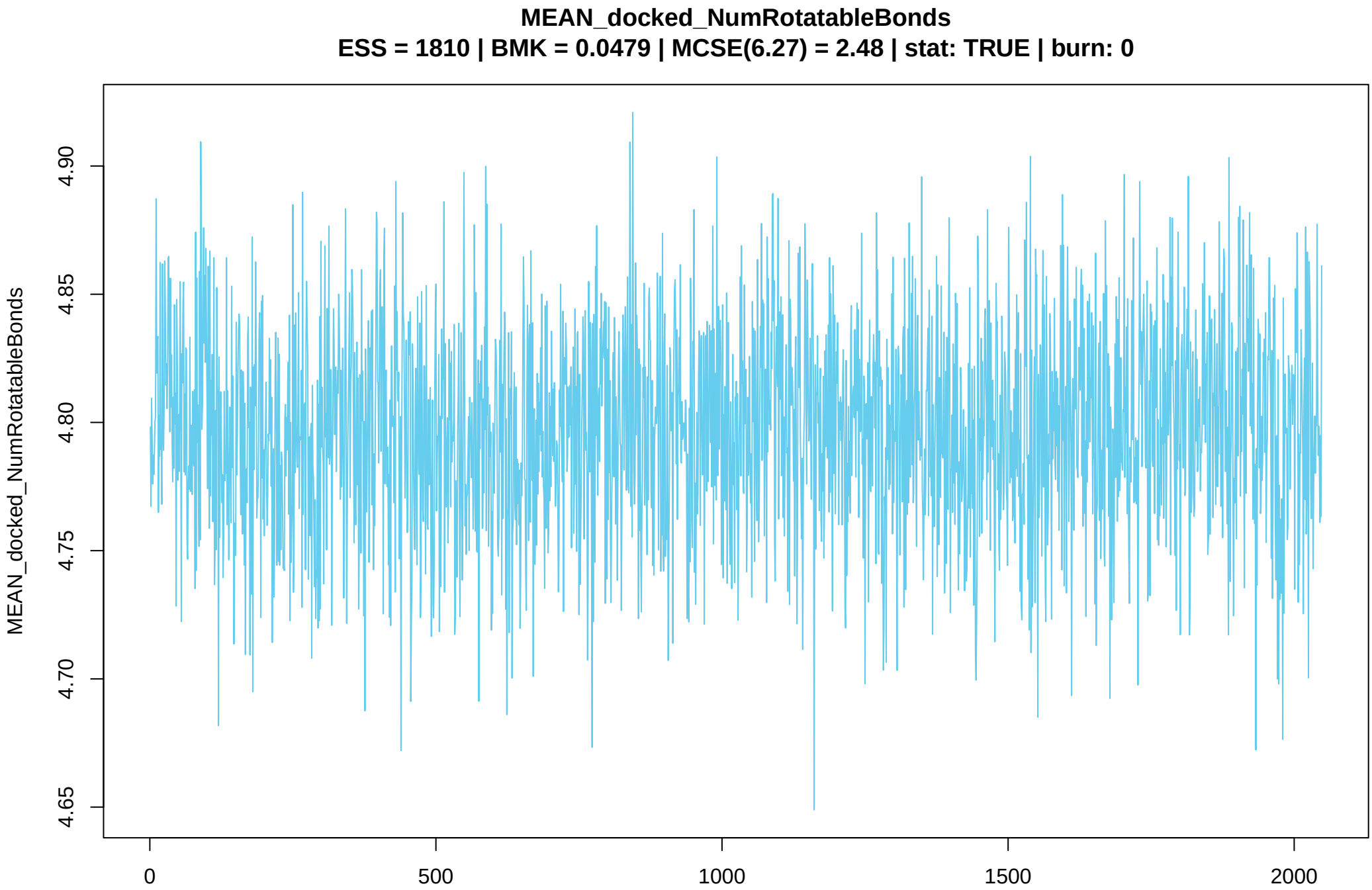

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0473 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0
MEAN_log_mcs_unbonded_polar_sasa
−0.25
−0.30
−0.35
−0.40
0
500
1000
1500
2000

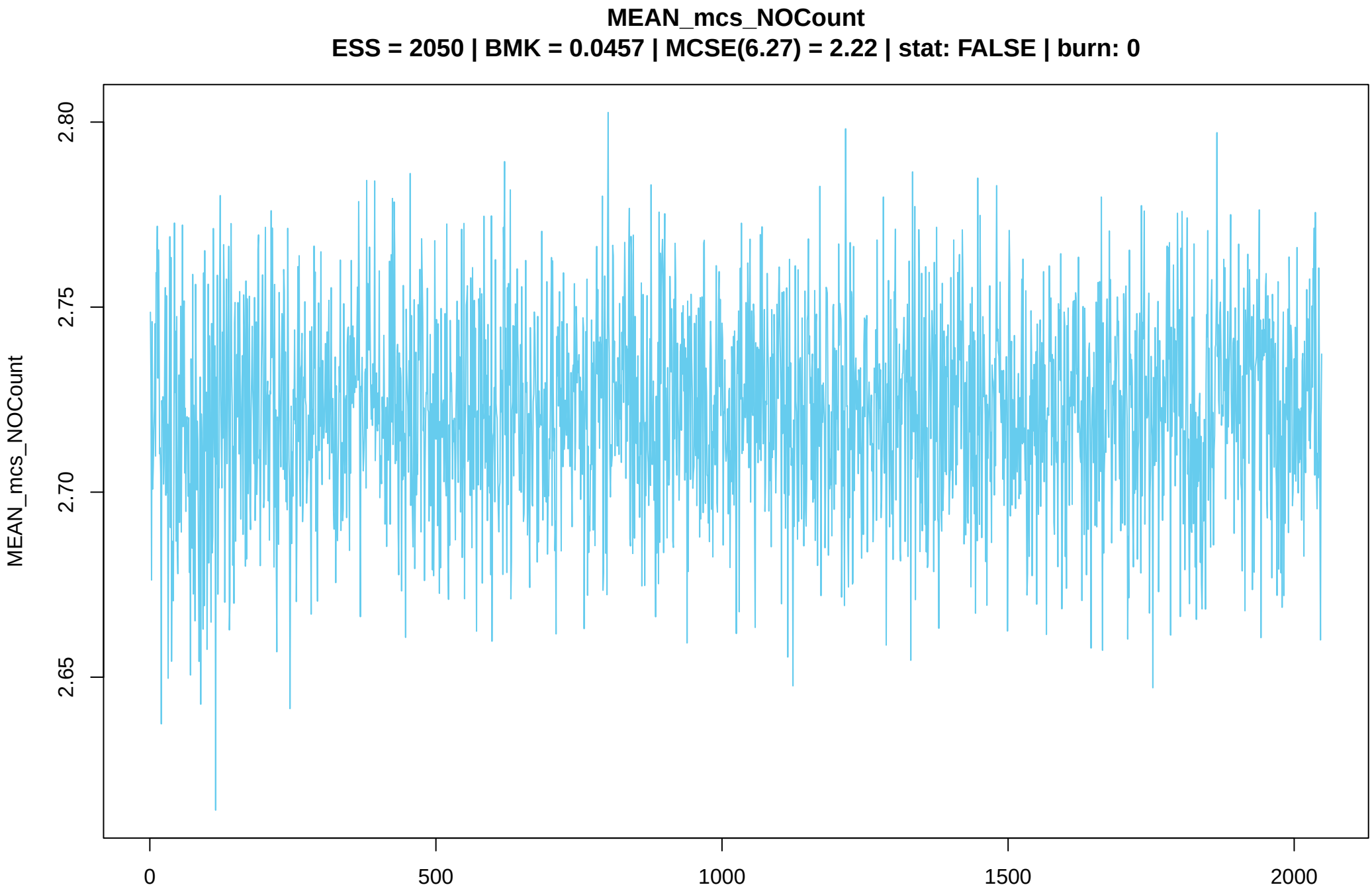

MEAN_logit_ec_tanimoto_similarity
ESS = 1780 | BMK = 0.0474 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0
MEAN_logit_ec_tanimoto_similarity
−2.02
−2.04
−2.06
−2.08
−2.10
−2.12
−2.14
0
500
1000
1500
2000

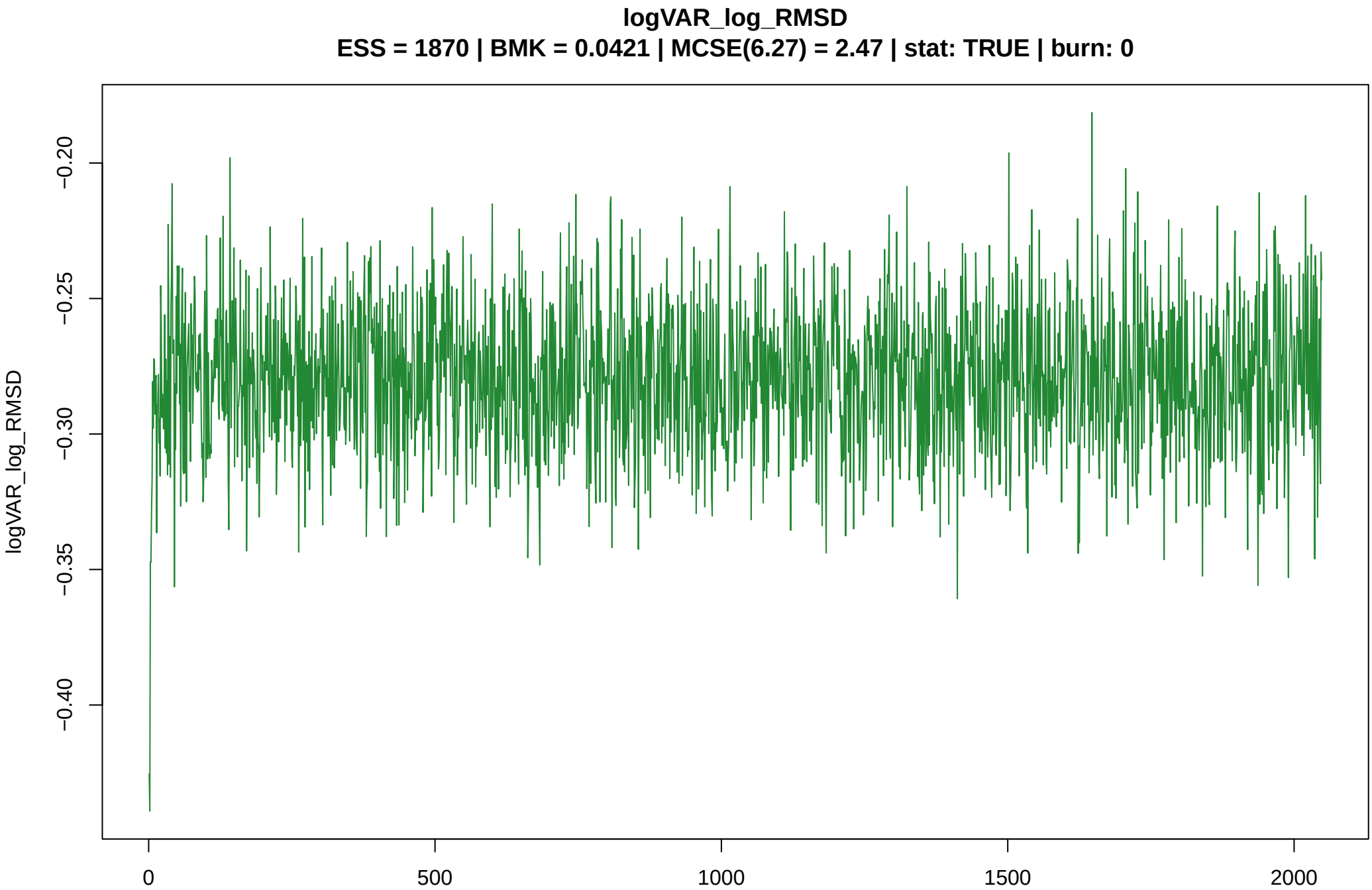

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0504 | MCSE(6.27) = 2.29 | stat: FALSE | burn: 0
MEAN_mcs_NumHeteroAtoms
2.90
2.95
3.00
3.05
0
500
1000
1500
2000

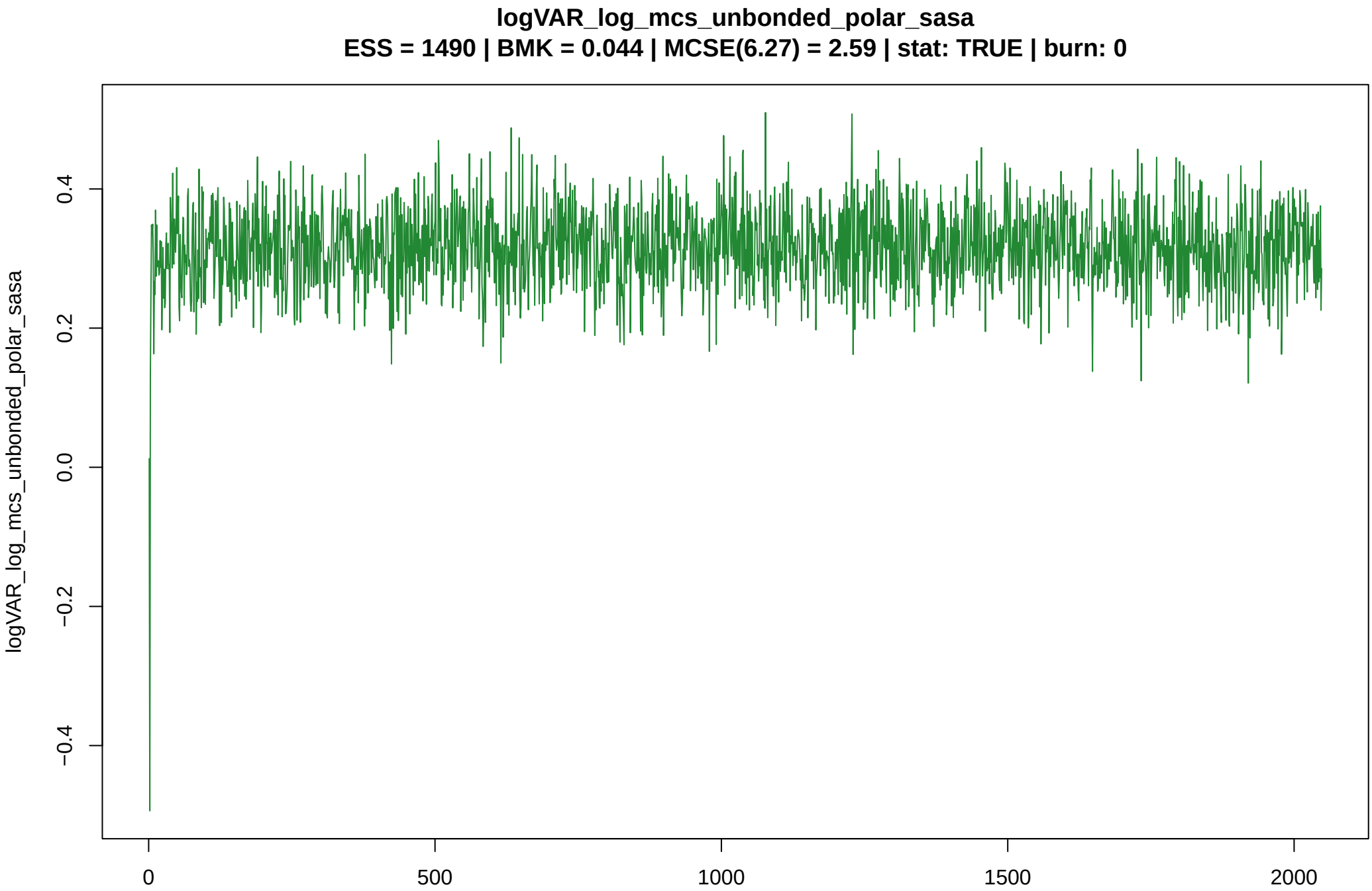

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0429 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
23.6
23.4
23.2
23.0
0
500
1000
1500
2000

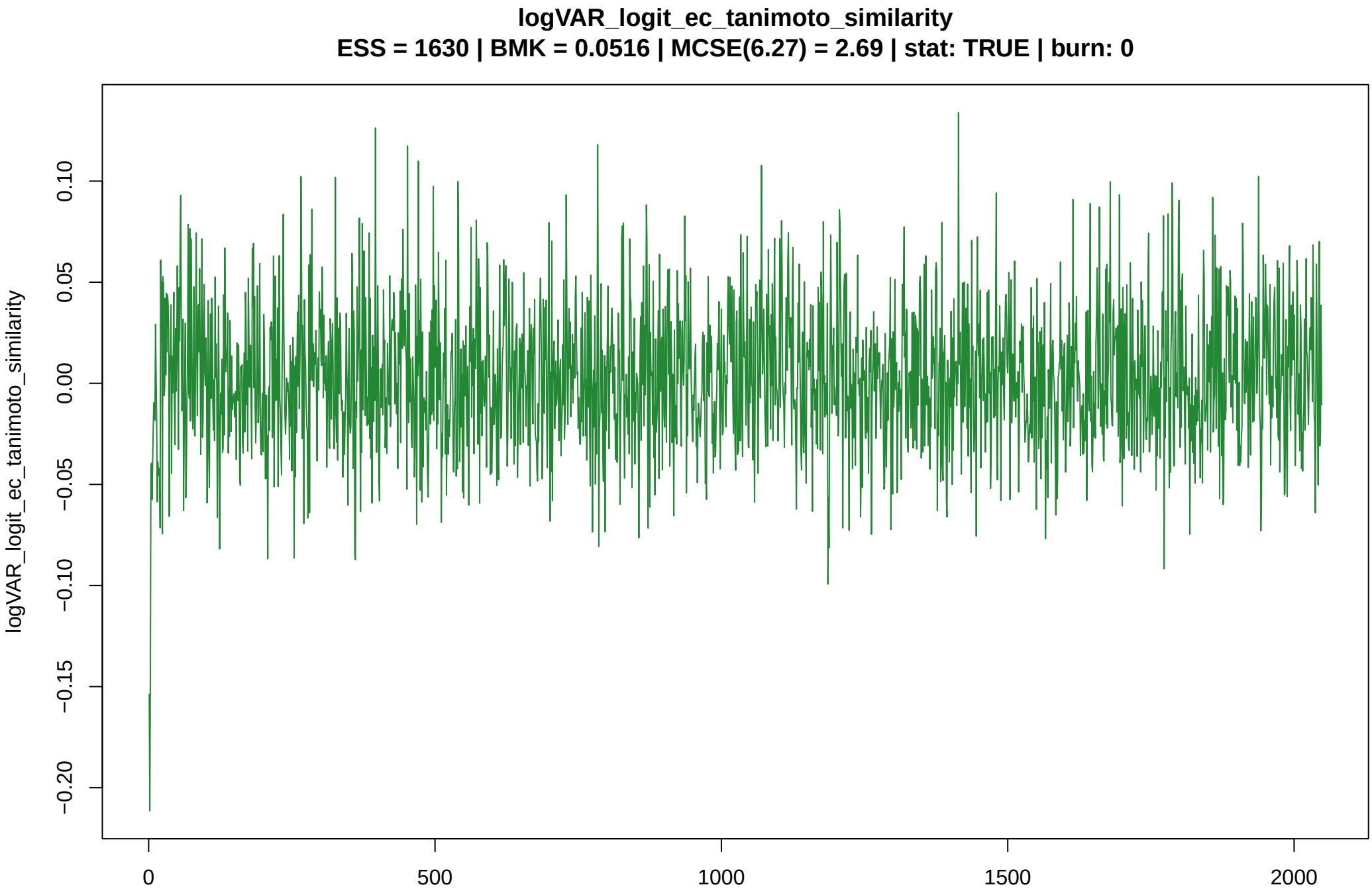

MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0356 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.78
0.80
0.82
0.84
0.86
0.88
0
500
1000
1500
2000

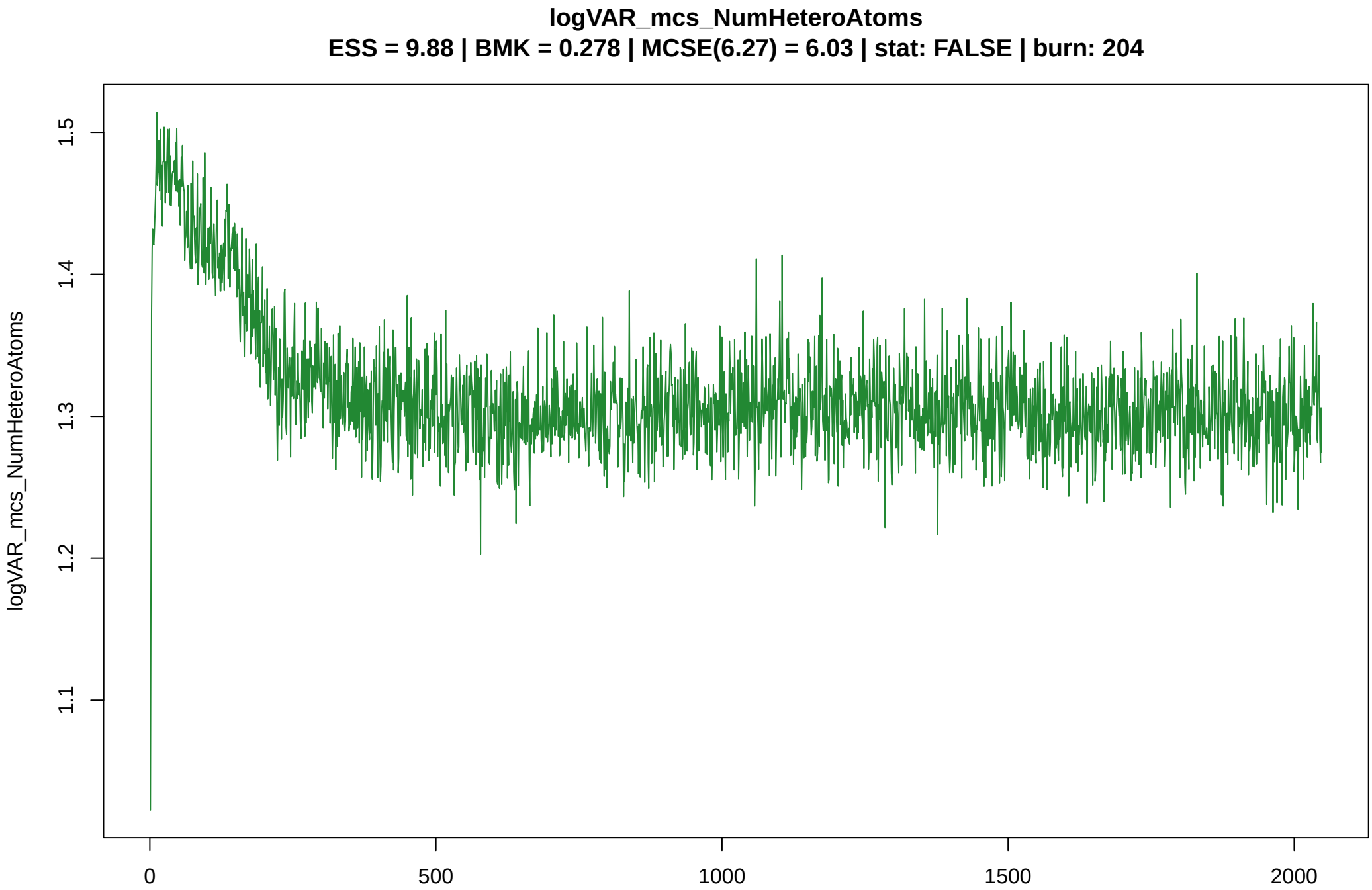

MEAN_docked_NumRotatableBonds
ESS = 1810 | BMK = 0.0479 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0
MEAN_docked_NumRotatableBonds
4.65
4.70
4.75
4.80
4.85
4.90
0
500
1000
1500
2000

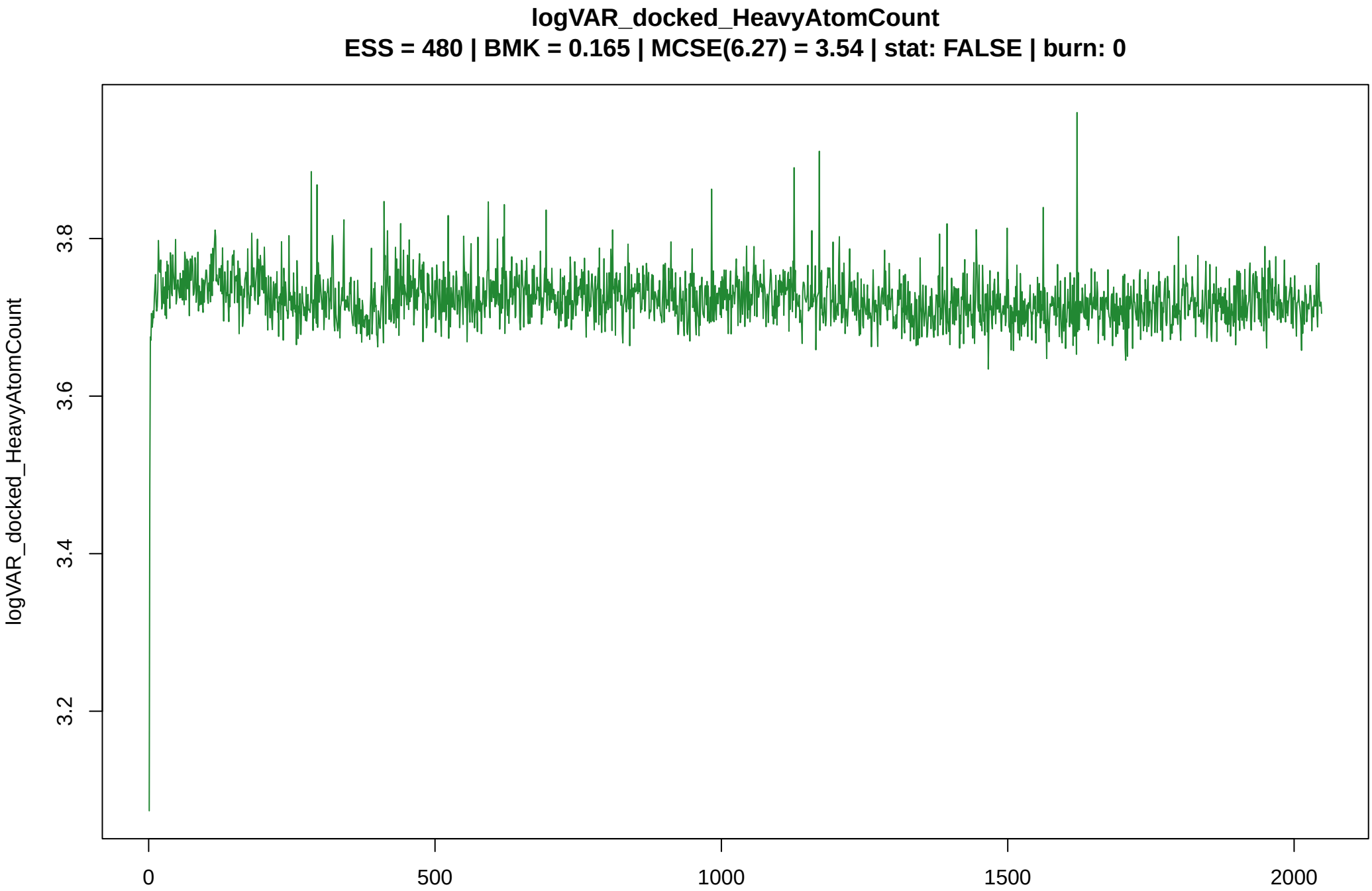

MEAN_mcs_NOCount
ESS = 2050 | BMK = 0.0457 | MCSE(6.27) = 2.22 | stat: FALSE | burn: 0
MEAN_mcs_NOCount
2.80
2.75
2.70
2.65
0
500
1000
1500
2000

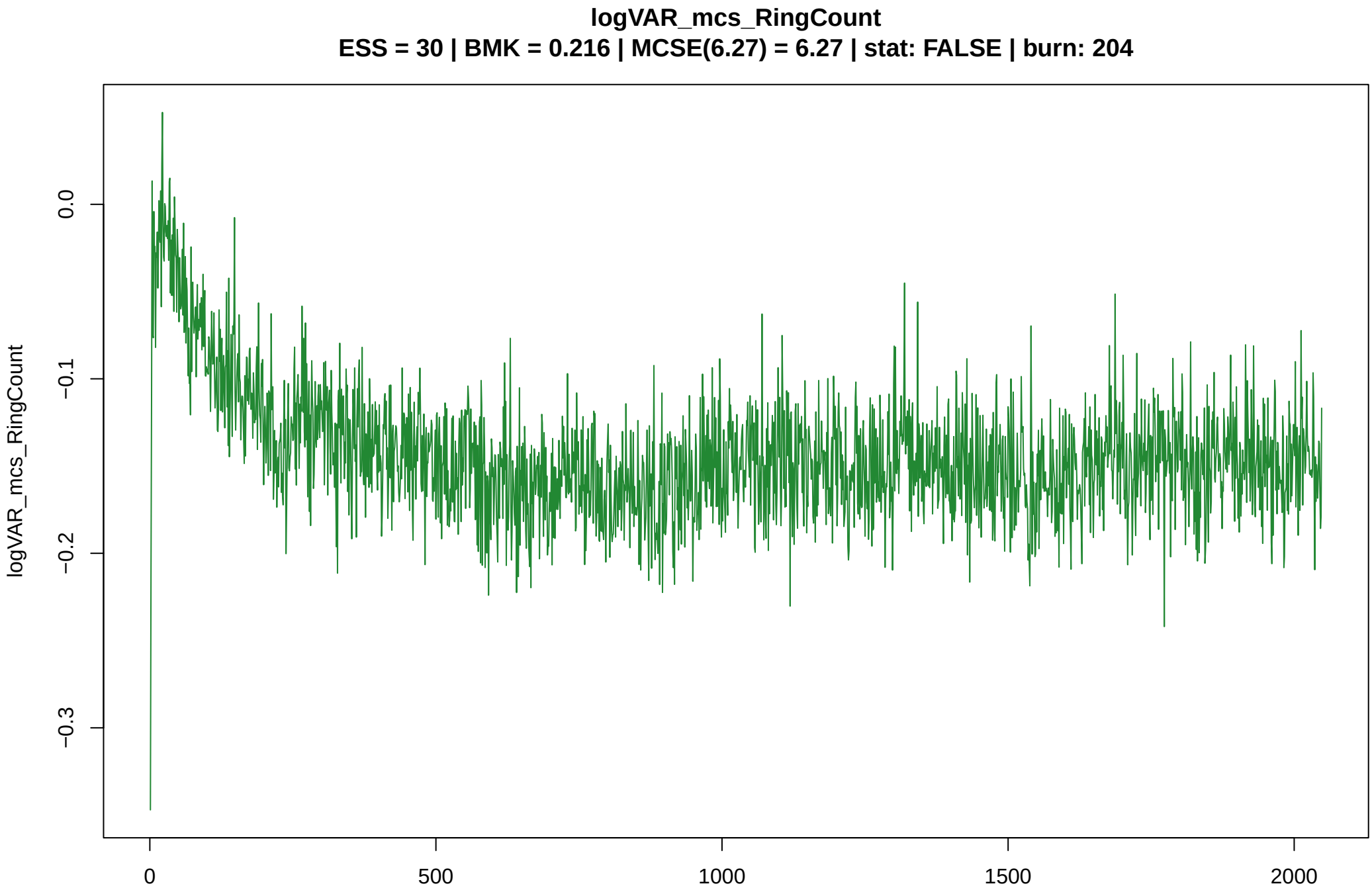

logVAR_log_RMSD
ESS = 1870 | BMK = 0.0421 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0
logVAR_log_RMSD
−0.20
−0.25
−0.30
−0.35
−0.40
0
500
1000
1500
2000

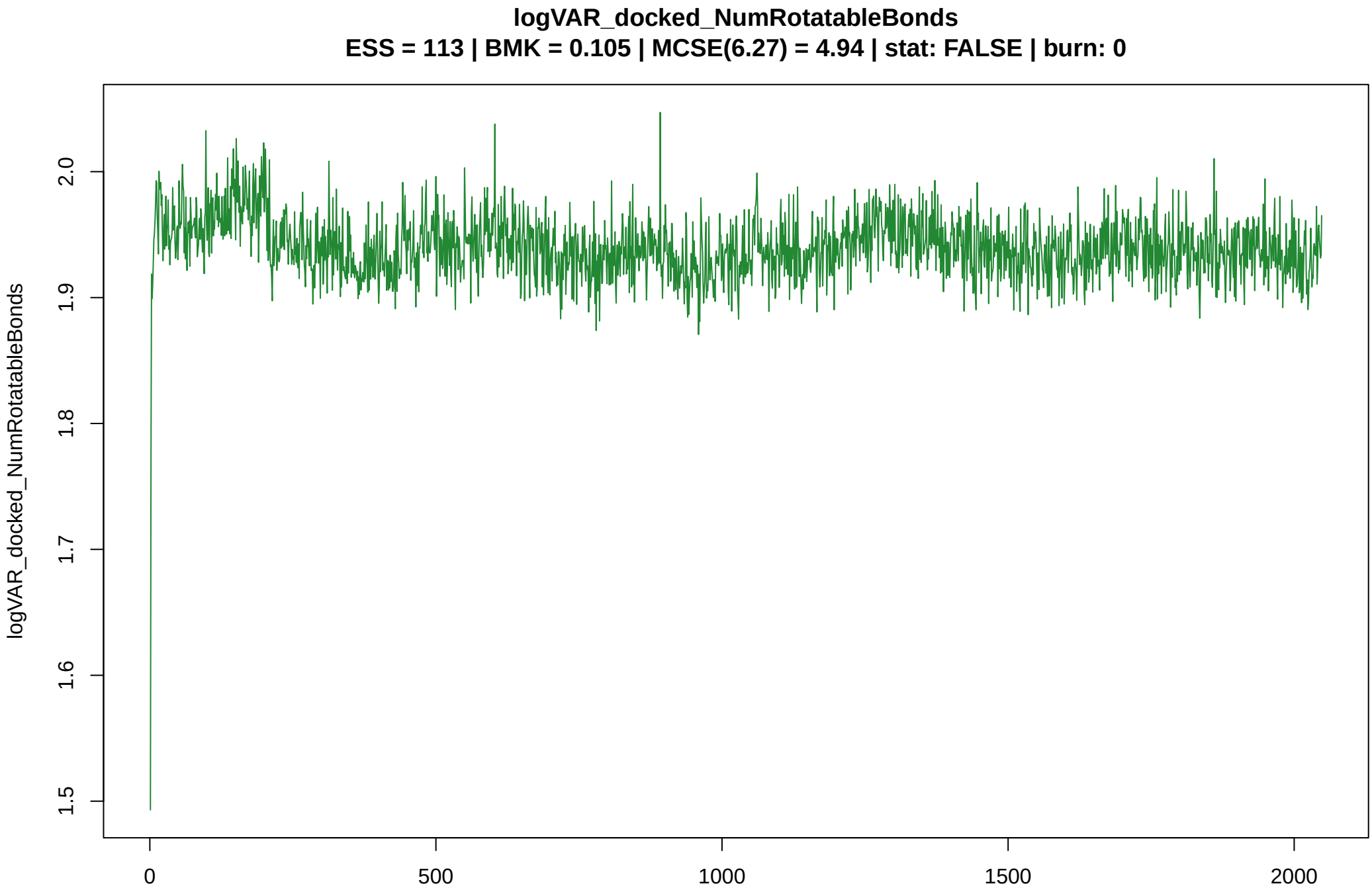

logVAR_log_mcs_unbonded_polar_sasa
ESS = 1490 | BMK = 0.044 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0
logVAR_log_mcs_unbonded_polar_sasa
0.4
0.2
0.0
−0.2
−0.4
0
500
1000
1500
2000

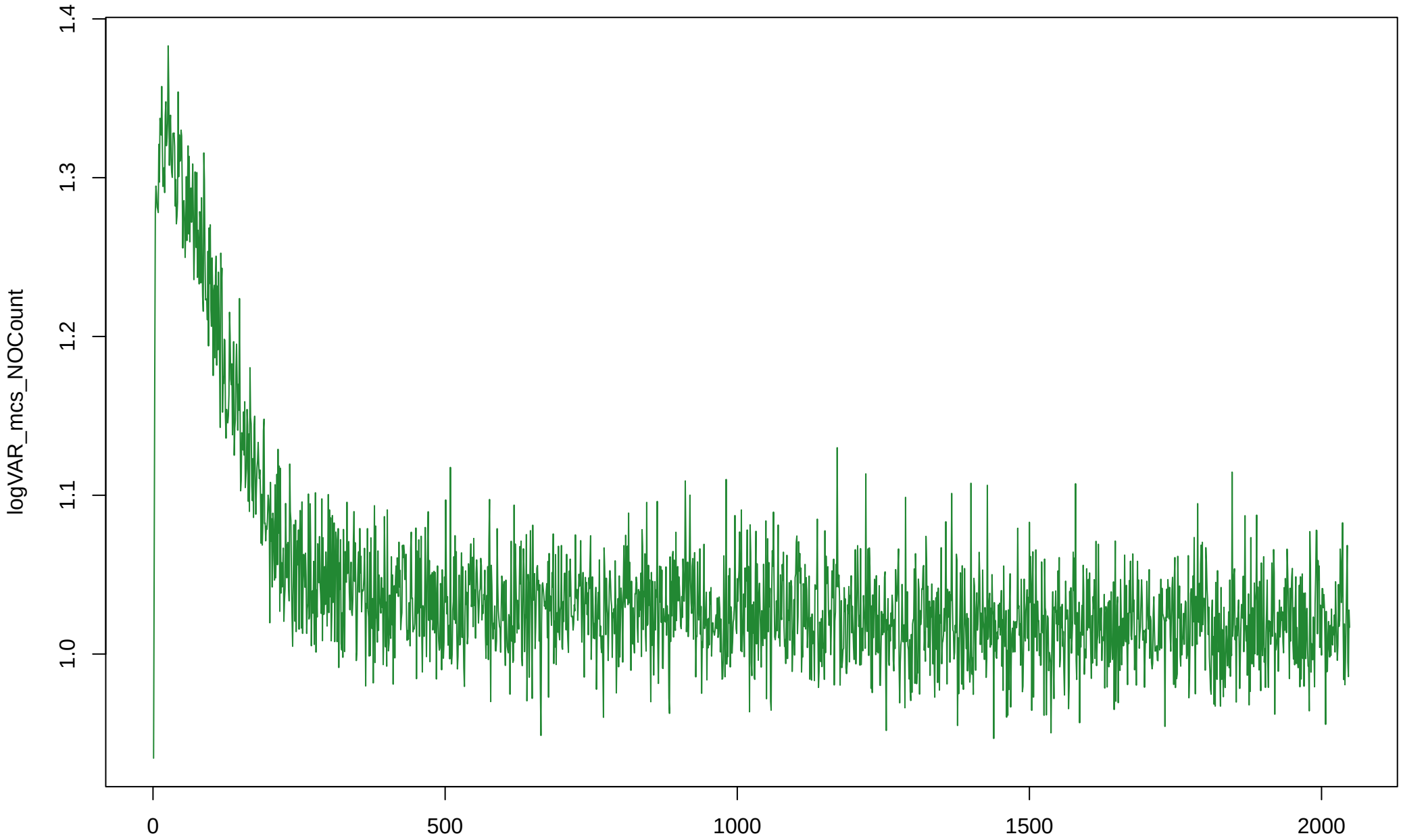

logVAR_logit_ec_tanimoto_similarity
ESS = 1630 | BMK = 0.0516 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0
logVAR_logit_ec_tanimoto_similarity
0.10
0.05
0.00
−0.05
−0.10
−0.15
−0.20
0
500
1000
1500
2000

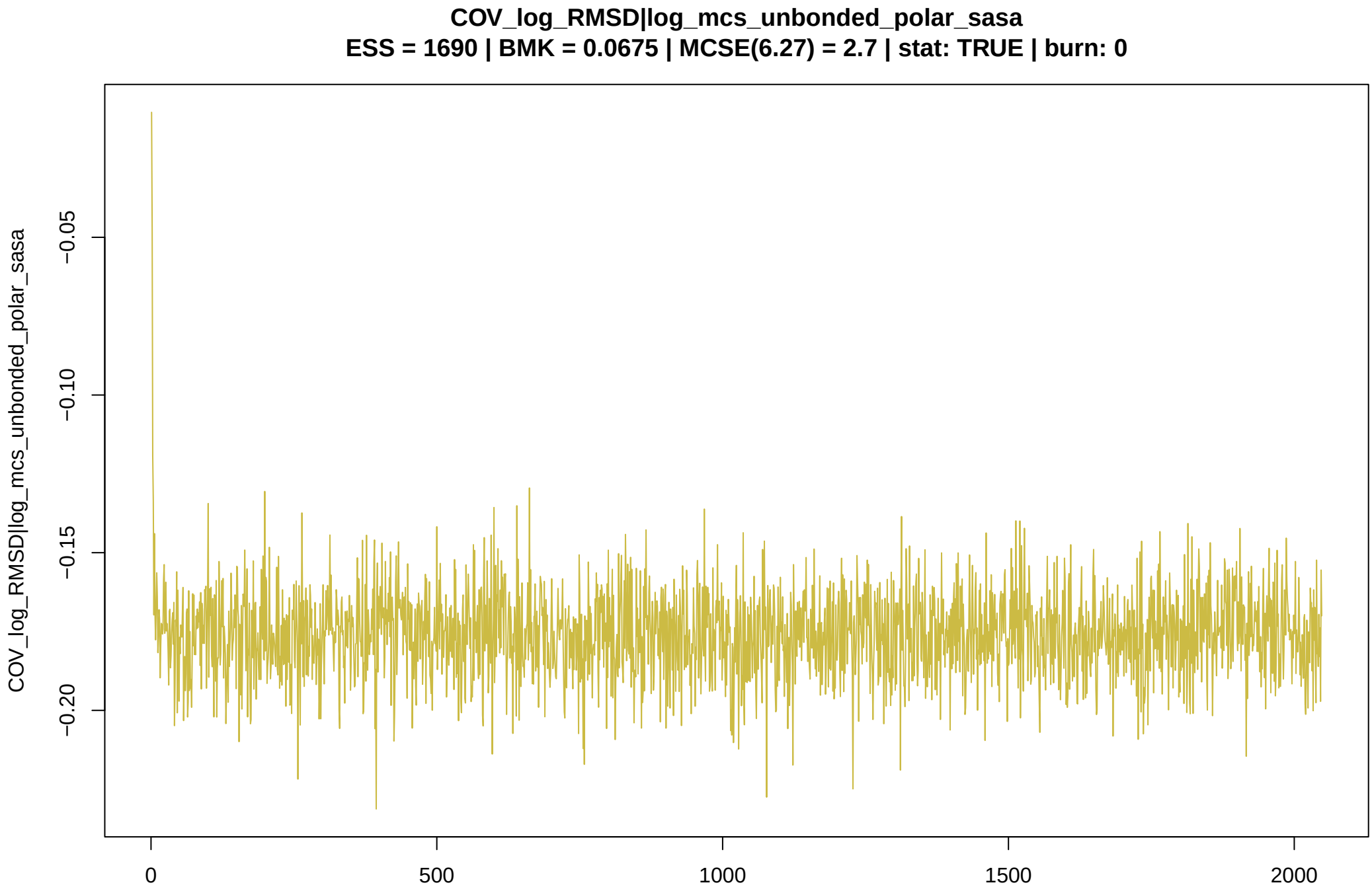

logVAR_mcs_NumHeteroAtoms
ESS = 9.88 | BMK = 0.278 | MCSE(6.27) = 6.03 | stat: FALSE | burn: 204
logVAR_mcs_NumHeteroAtoms
1.1
1.2
1.3
1.4
1.5
0
500
1000
1500
2000

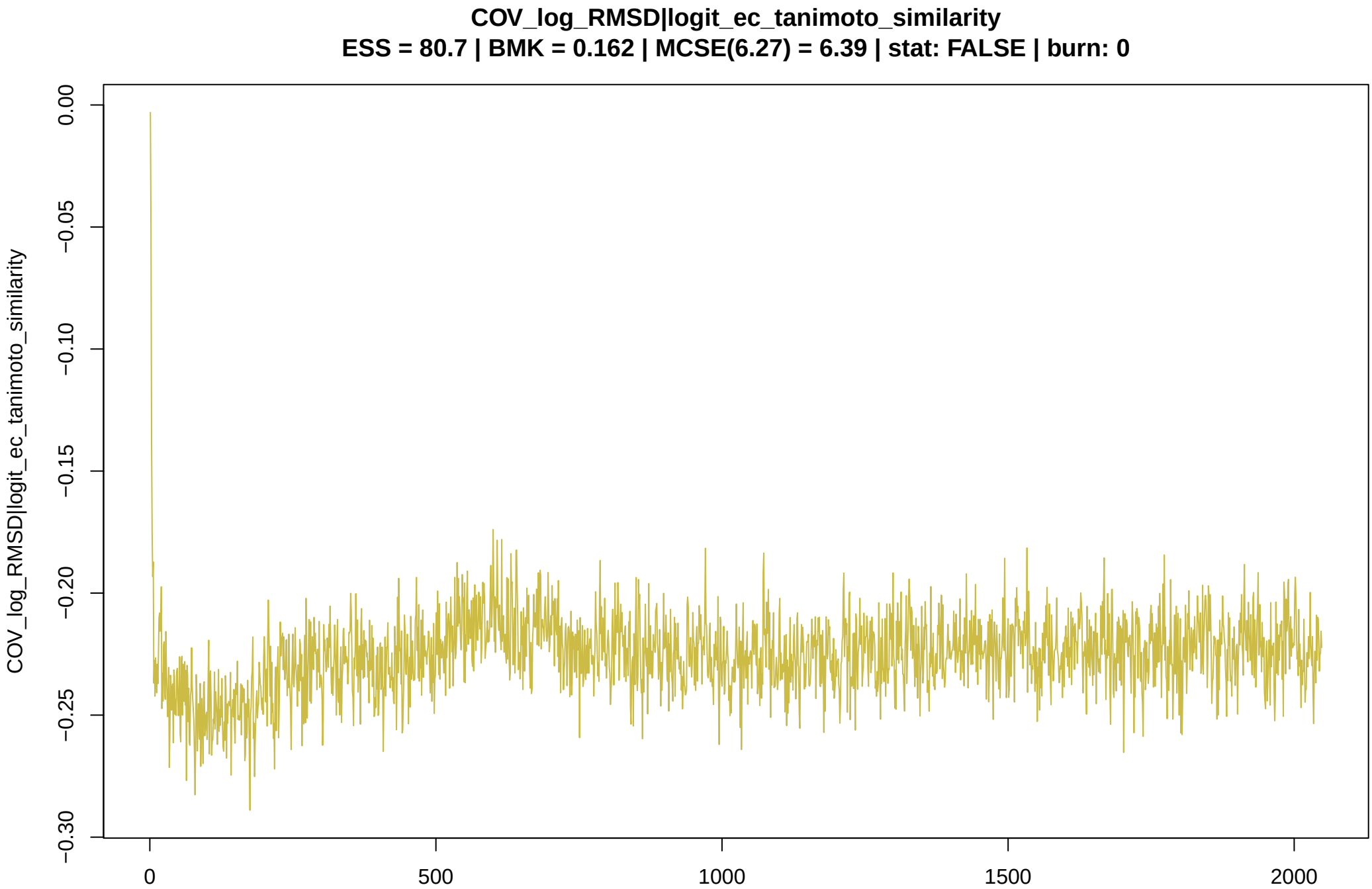

logVAR_docked_HeavyAtomCount
ESS = 480 | BMK = 0.165 | MCSE(6.27) = 3.54 | stat: FALSE | burn: 0
logVAR_docked_HeavyAtomCount
3.2
3.4
3.6
3.8
0
500
1000
1500
2000

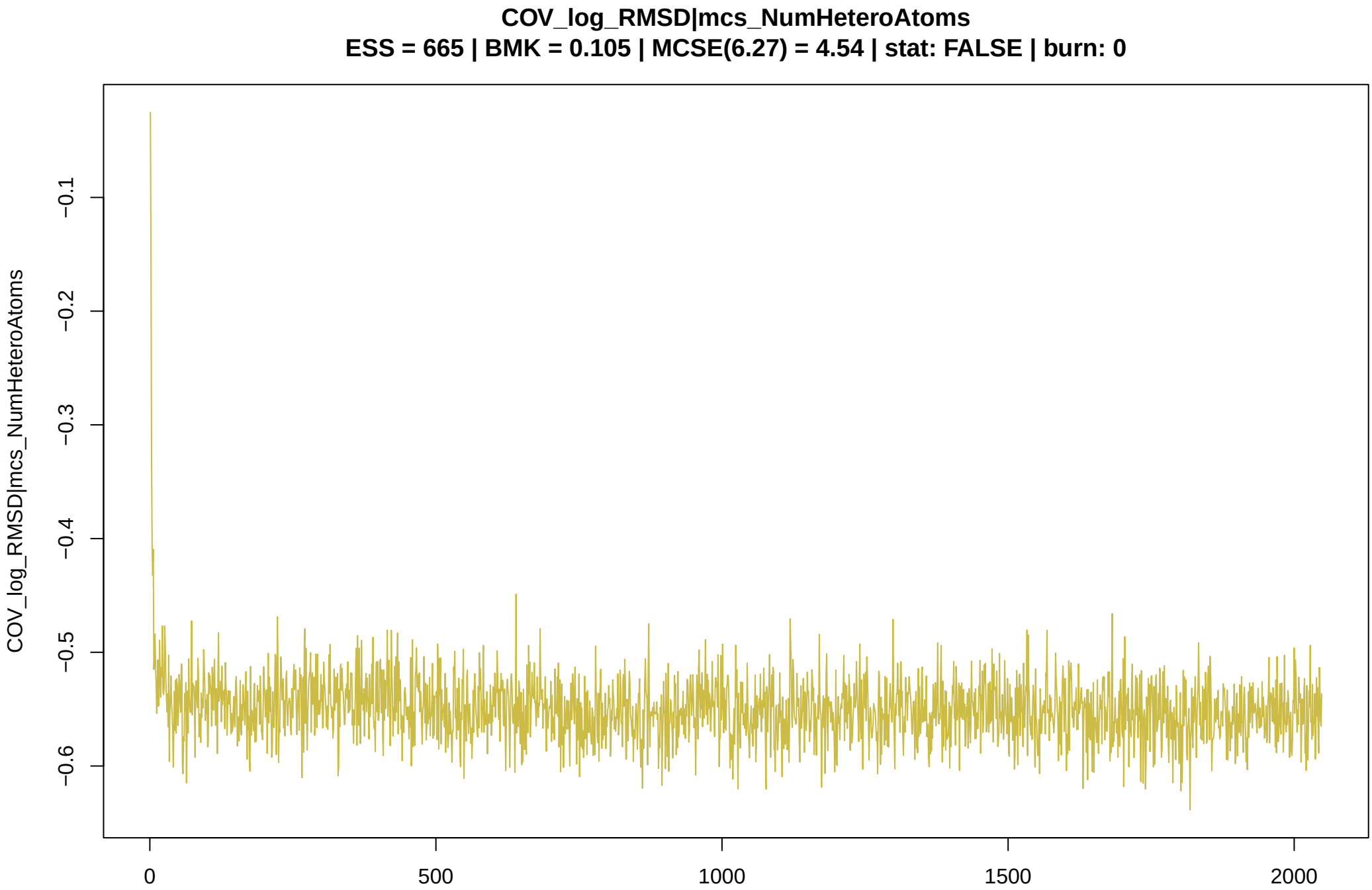

logVAR_mcs_RingCount
ESS = 30 | BMK = 0.216 | MCSE(6.27) = 6.27 | stat: FALSE | burn: 204
logVAR_mcs_RingCount
0.0
−0.1
−0.2
−0.3
0
500
1000
1500
2000

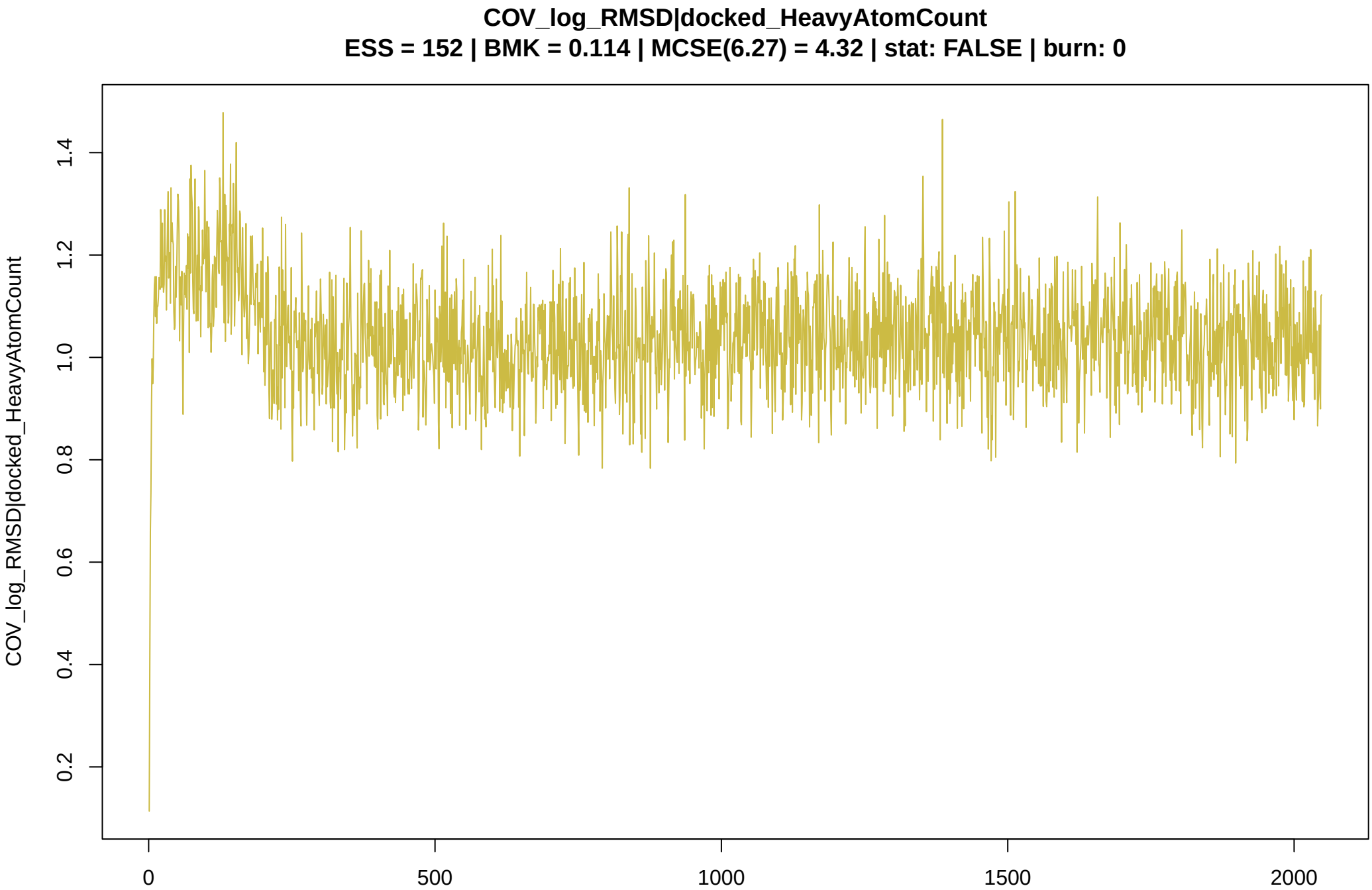

logVAR_docked_NumRotatableBonds
ESS = 113 | BMK = 0.105 | MCSE(6.27) = 4.94 | stat: FALSE | burn: 0
logVAR_docked_NumRotatableBonds
1.5
1.6
1.7
1.8
1.9
2.0
0
500
1000
1500
2000

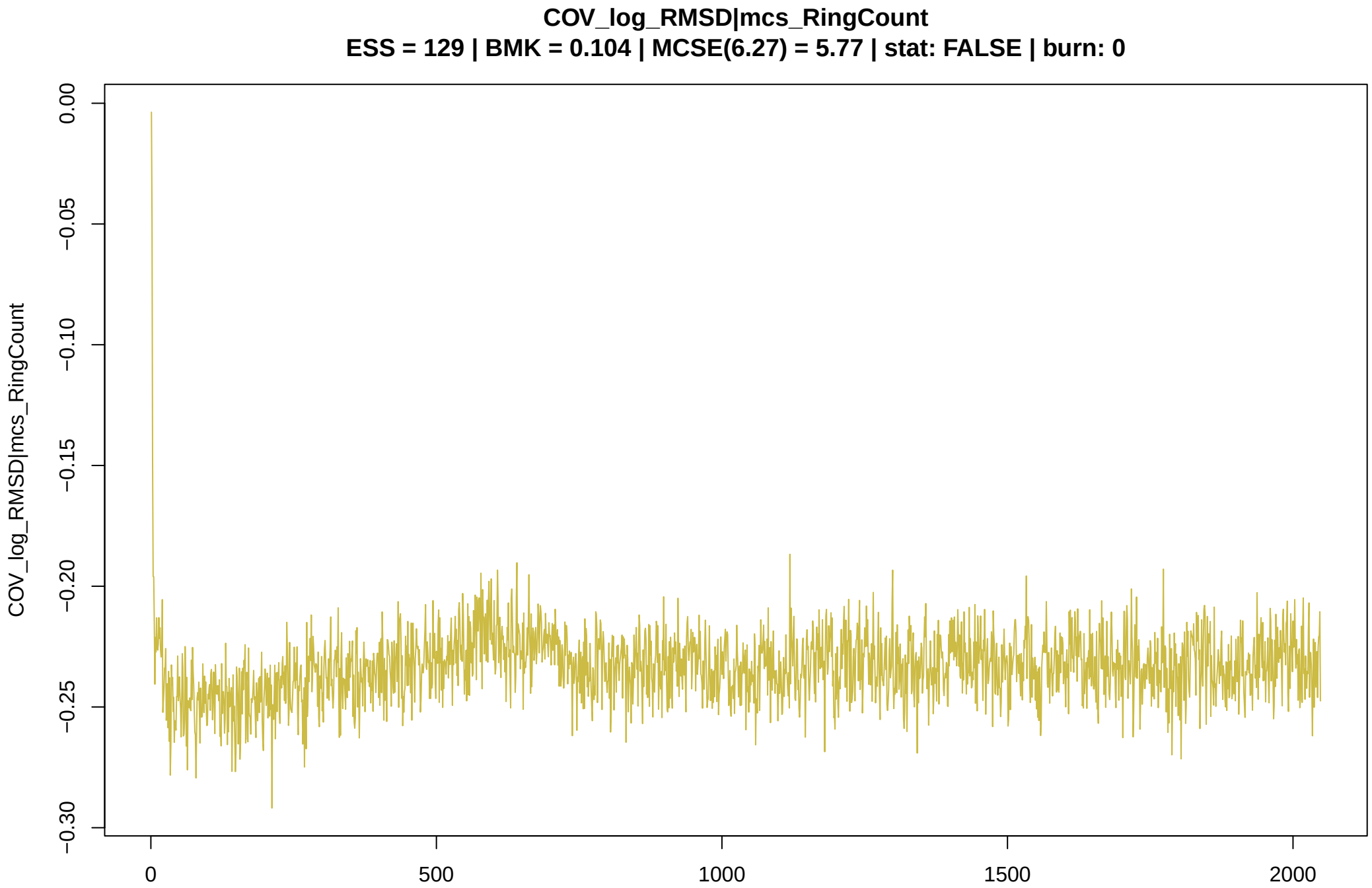

logVAR_mcs_NOCount
ESS = 8.13 | BMK = 0.348 | MCSE(6.27) = 22.2 | stat: FALSE | burn: 204
logVAR_mcs_NOCount
1.0
1.1
1.2
1.3
1.4
0
500
1000
1500
2000

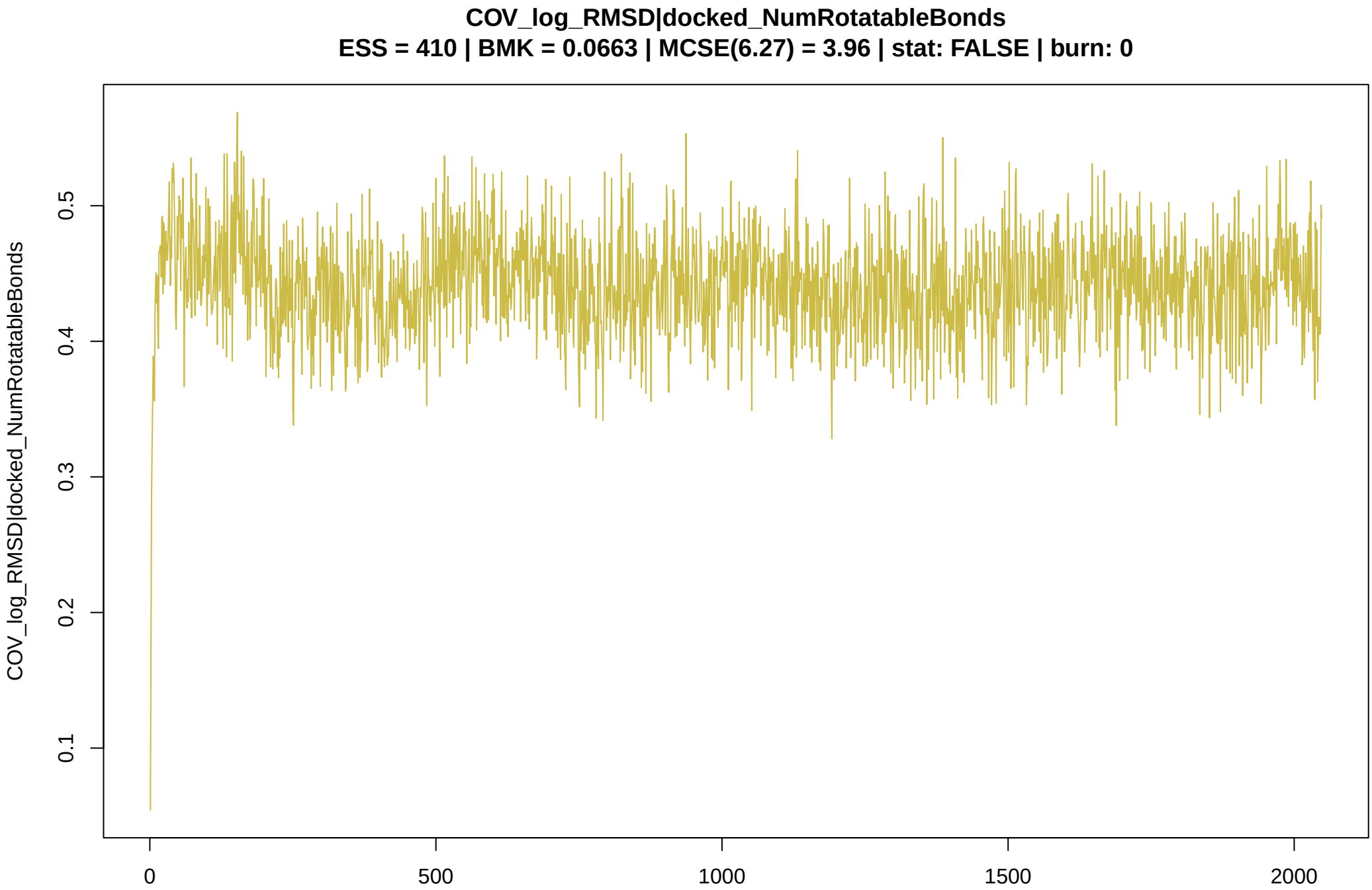

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1690 | BMK = 0.0675 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.05
−0.10
−0.15
−0.20
0
500
1000
1500
2000

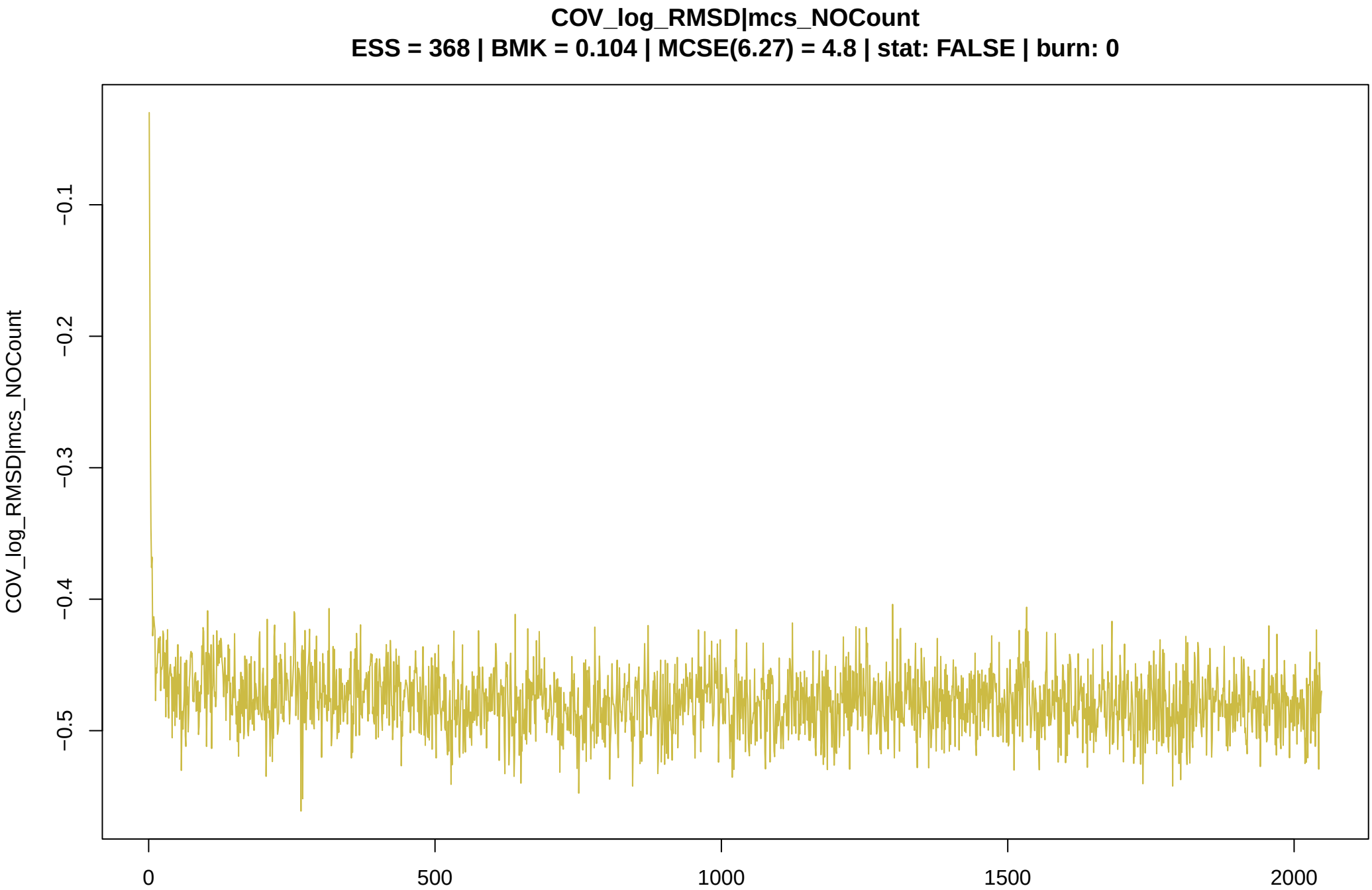

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 80.7 | BMK = 0.162 | MCSE(6.27) = 6.39 | stat: FALSE | burn: 0
COV_log_RMSD|logit_ec_tanimoto_similarity
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
0
500
1000
1500
2000

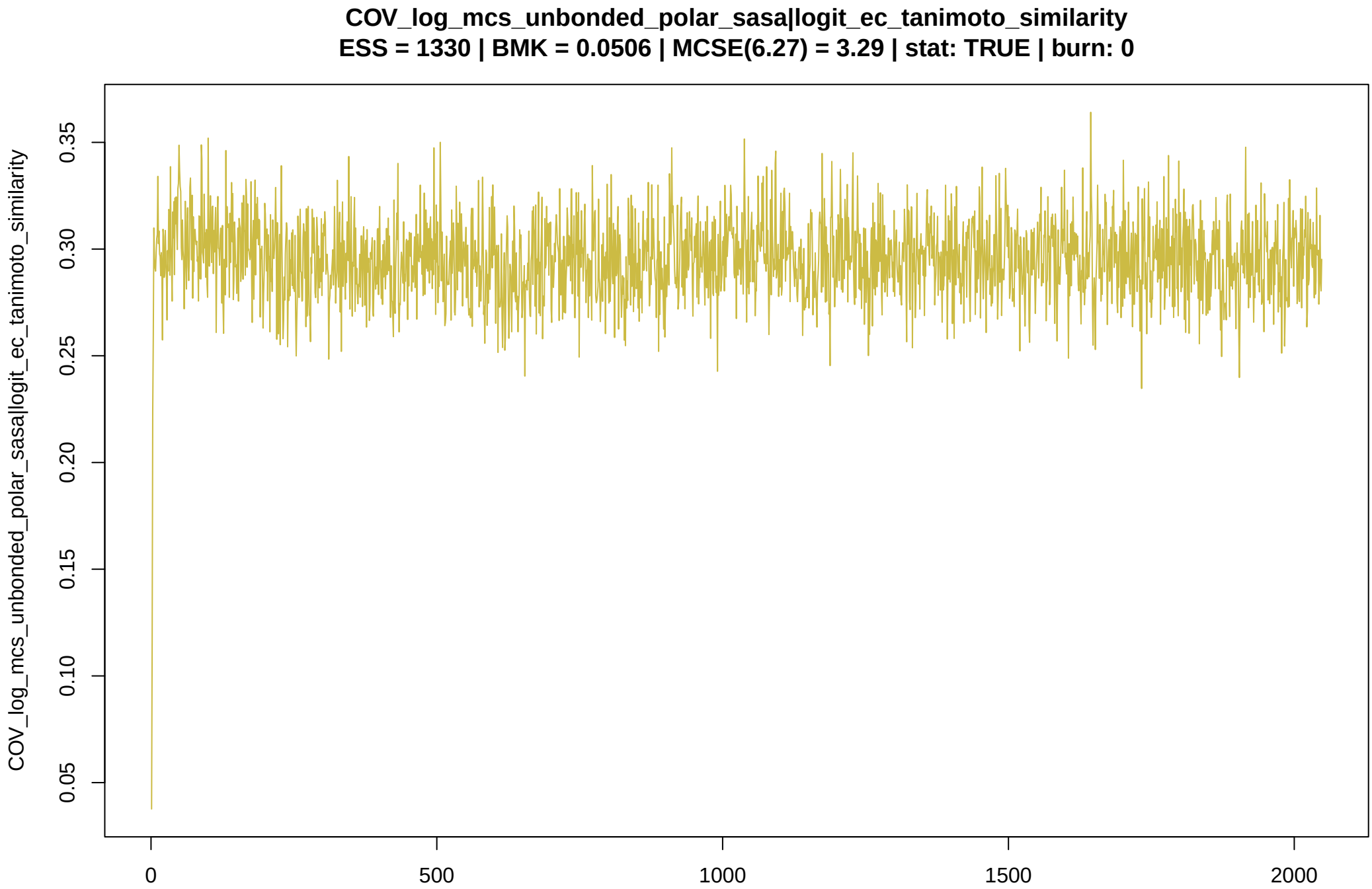

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 665 | BMK = 0.105 | MCSE(6.27) = 4.54 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
0
500
1000
1500
2000

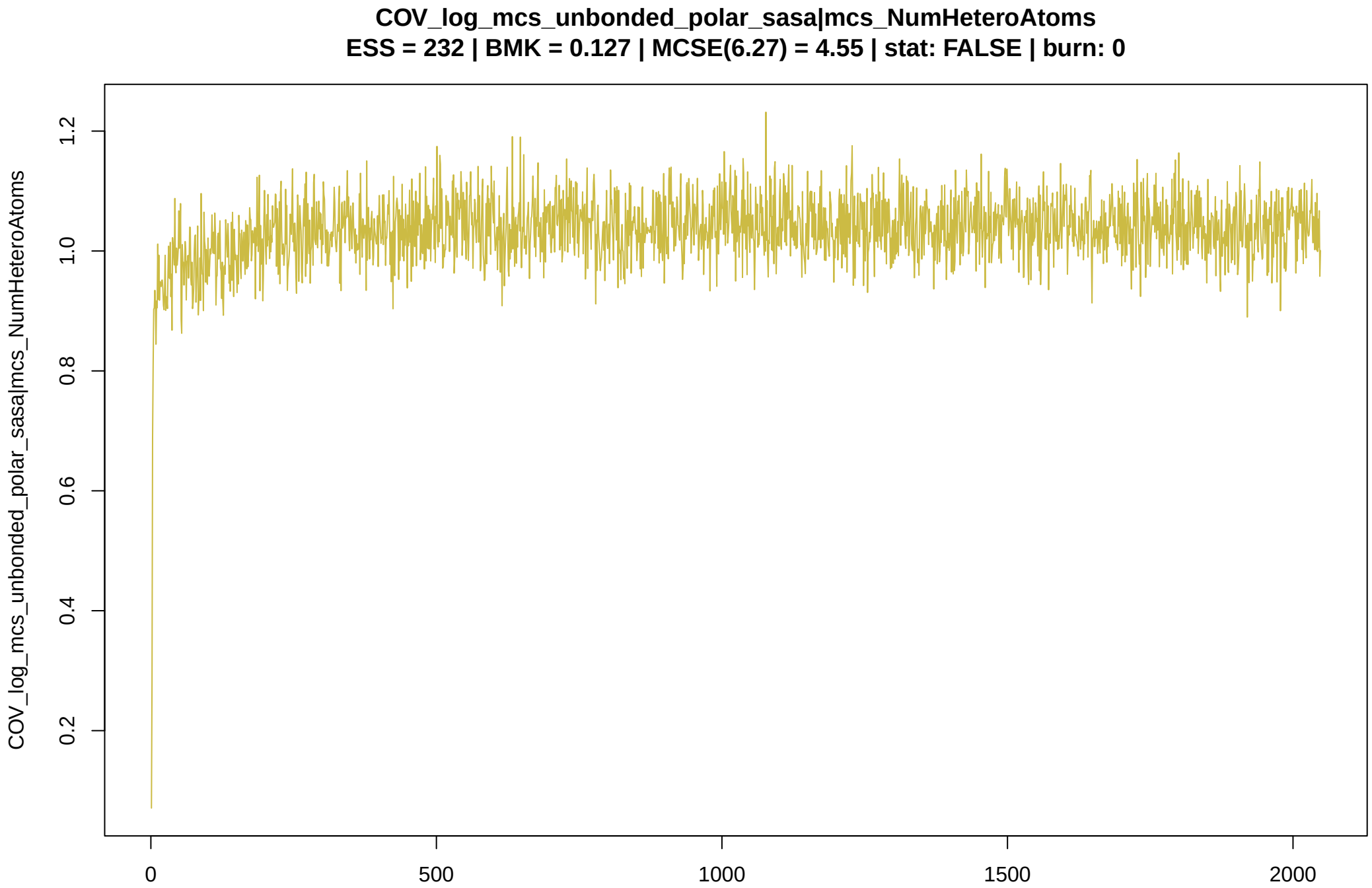

COV_log_RMSD|docked_HeavyAtomCount
ESS = 152 | BMK = 0.114 | MCSE(6.27) = 4.32 | stat: FALSE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

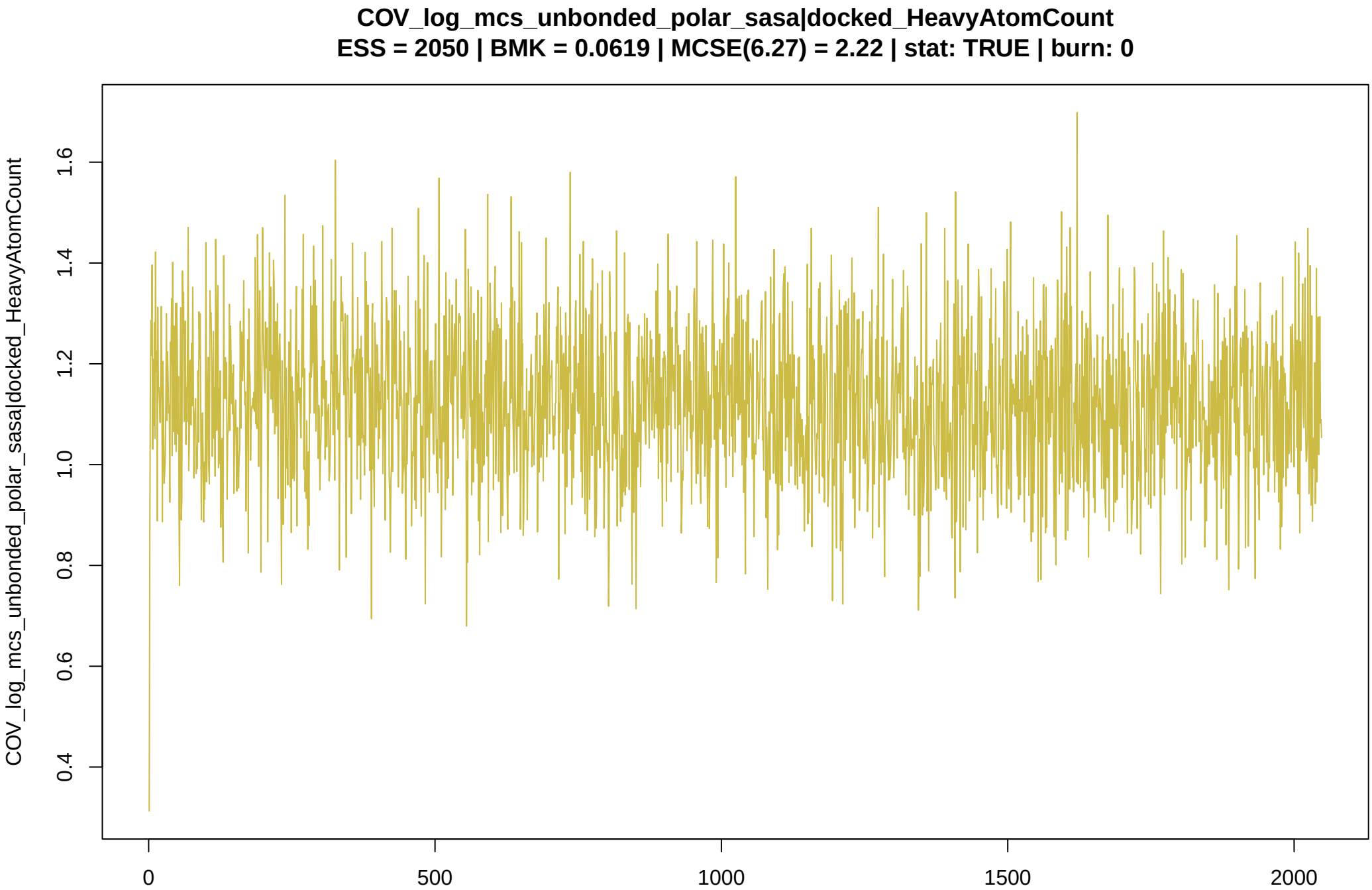

COV_log_RMSD|mcs_RingCount
ESS = 129 | BMK = 0.104 | MCSE(6.27) = 5.77 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_RingCount
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
0
500
1000
1500
2000

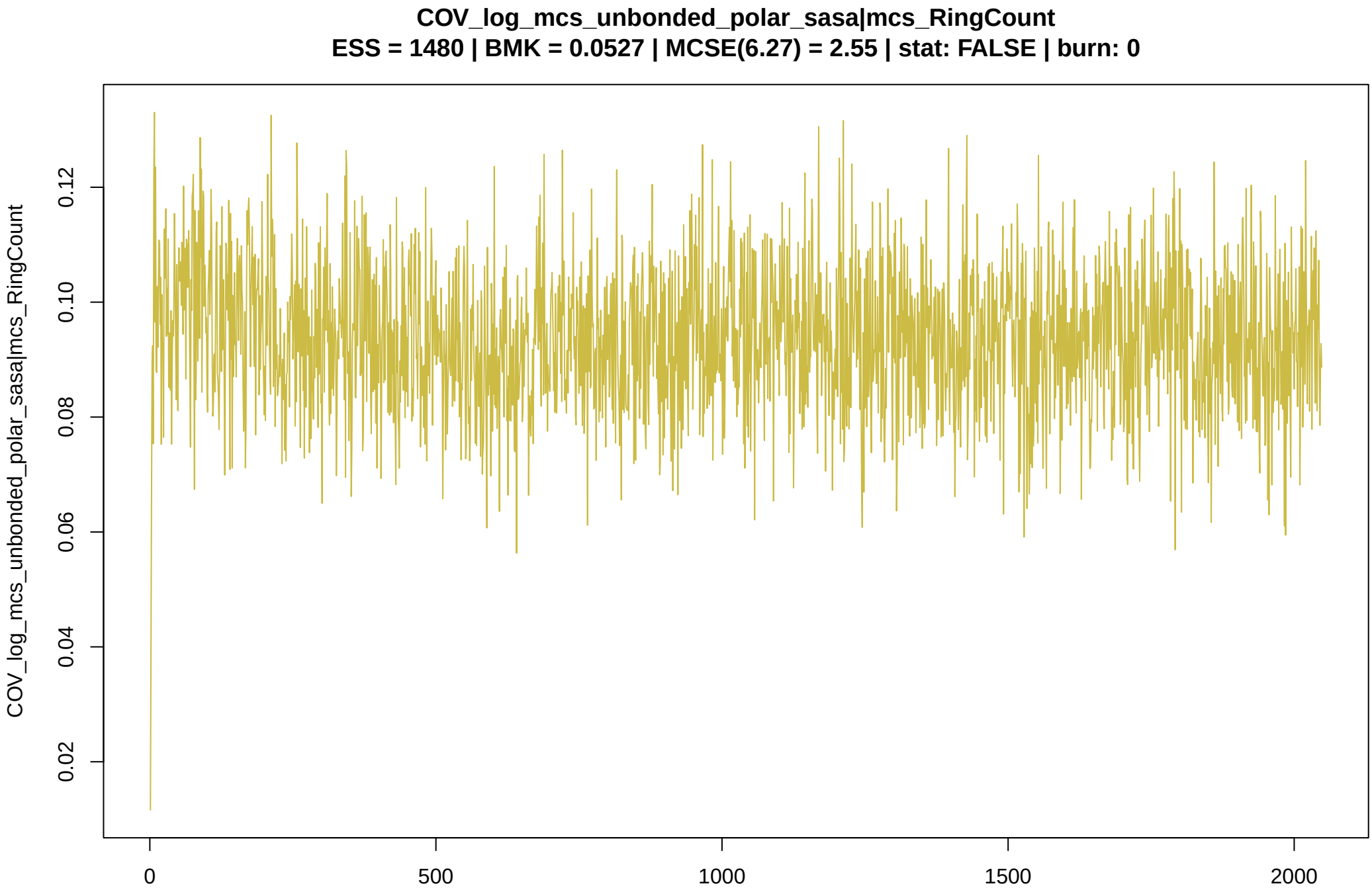

COV_log_RMSD|docked_NumRotatableBonds
ESS = 410 | BMK = 0.0663 | MCSE(6.27) = 3.96 | stat: FALSE | burn: 0
COV_log_RMSD|docked_NumRotatableBonds
0.1
0.2
0.3
0.4
0.5
0
500
1000
1500
2000

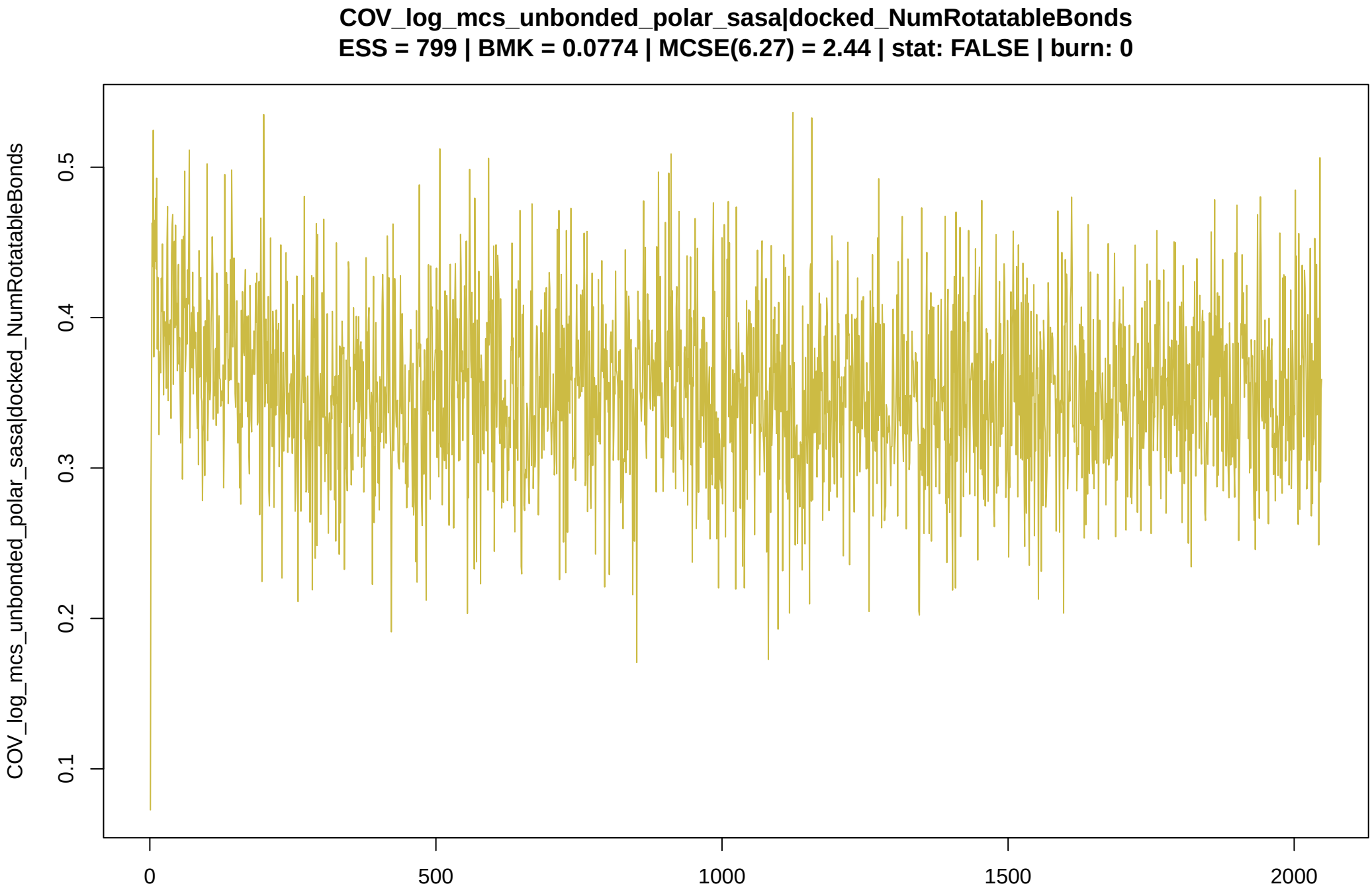

COV_log_RMSD|mcs_NOCount
ESS = 368 | BMK = 0.104 | MCSE(6.27) = 4.8 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_NOCount
−0.1
−0.2
−0.3
−0.4
−0.5
0
500
1000
1500
2000

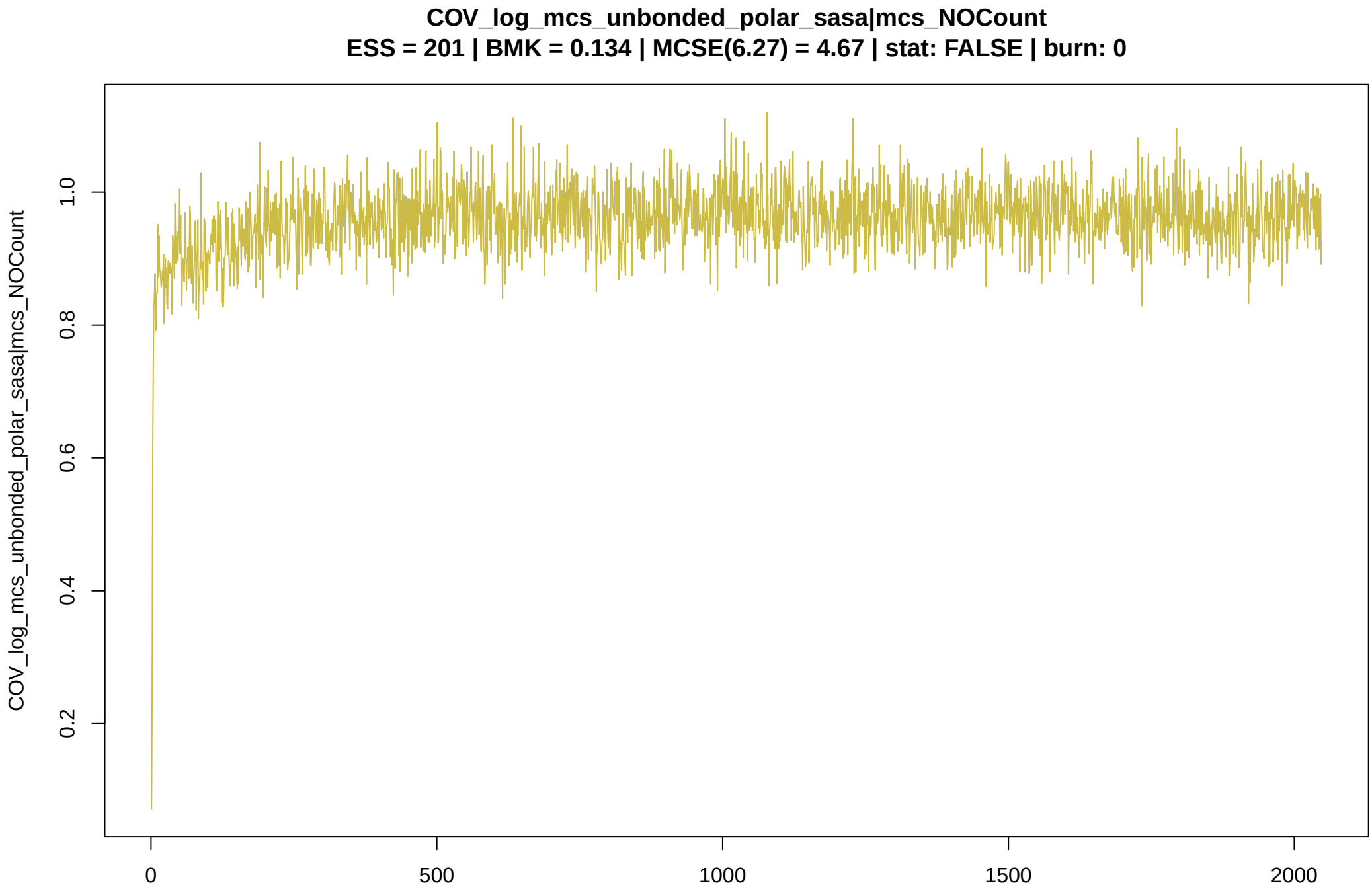

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1330 | BMK = 0.0506 | MCSE(6.27) = 3.29 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0
500
1000
1500
2000

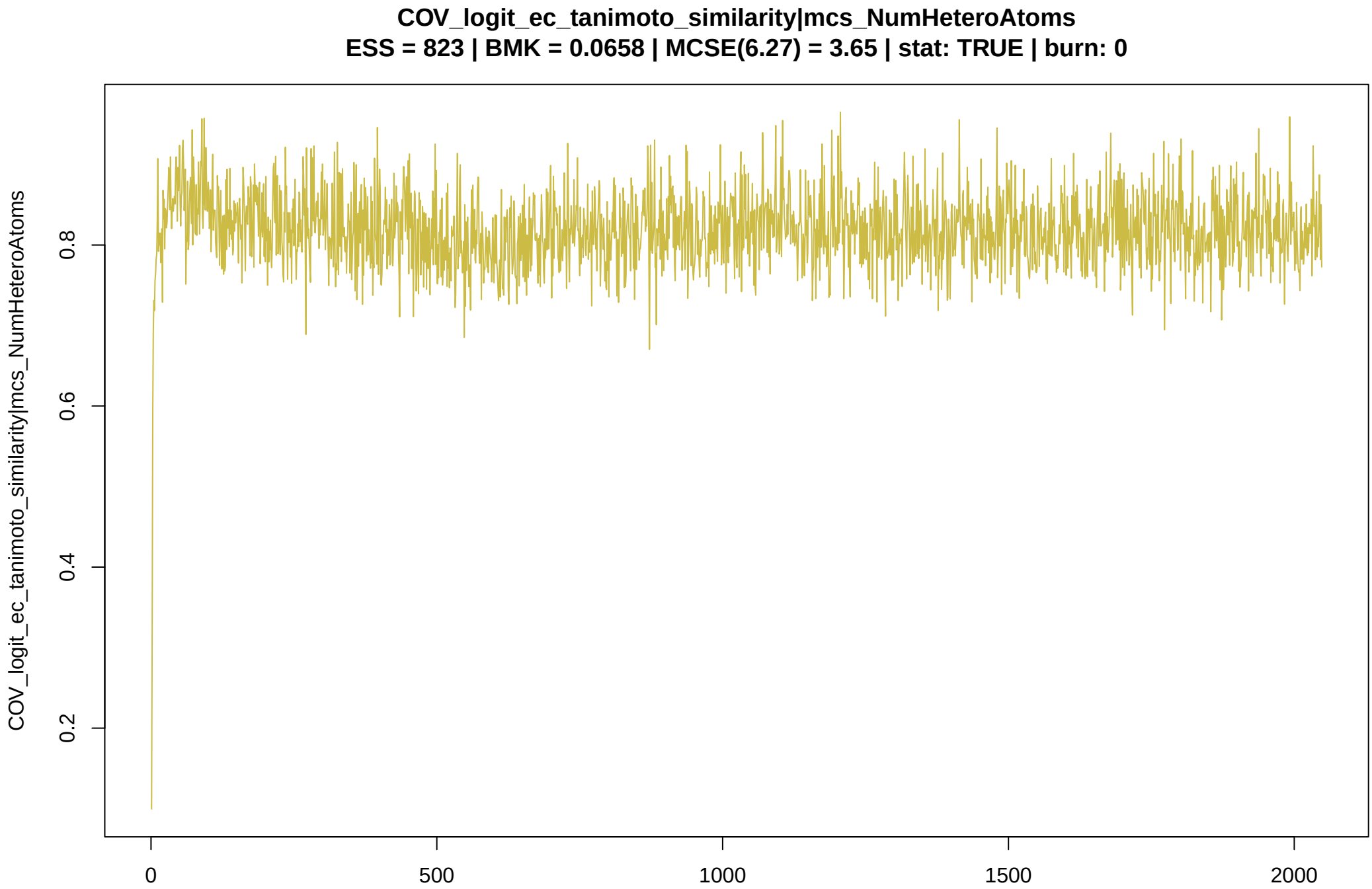

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 232 | BMK = 0.127 | MCSE(6.27) = 4.55 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.2
0.4
0.6
0.8
1.0
1.2
0
500
1000
1500
2000

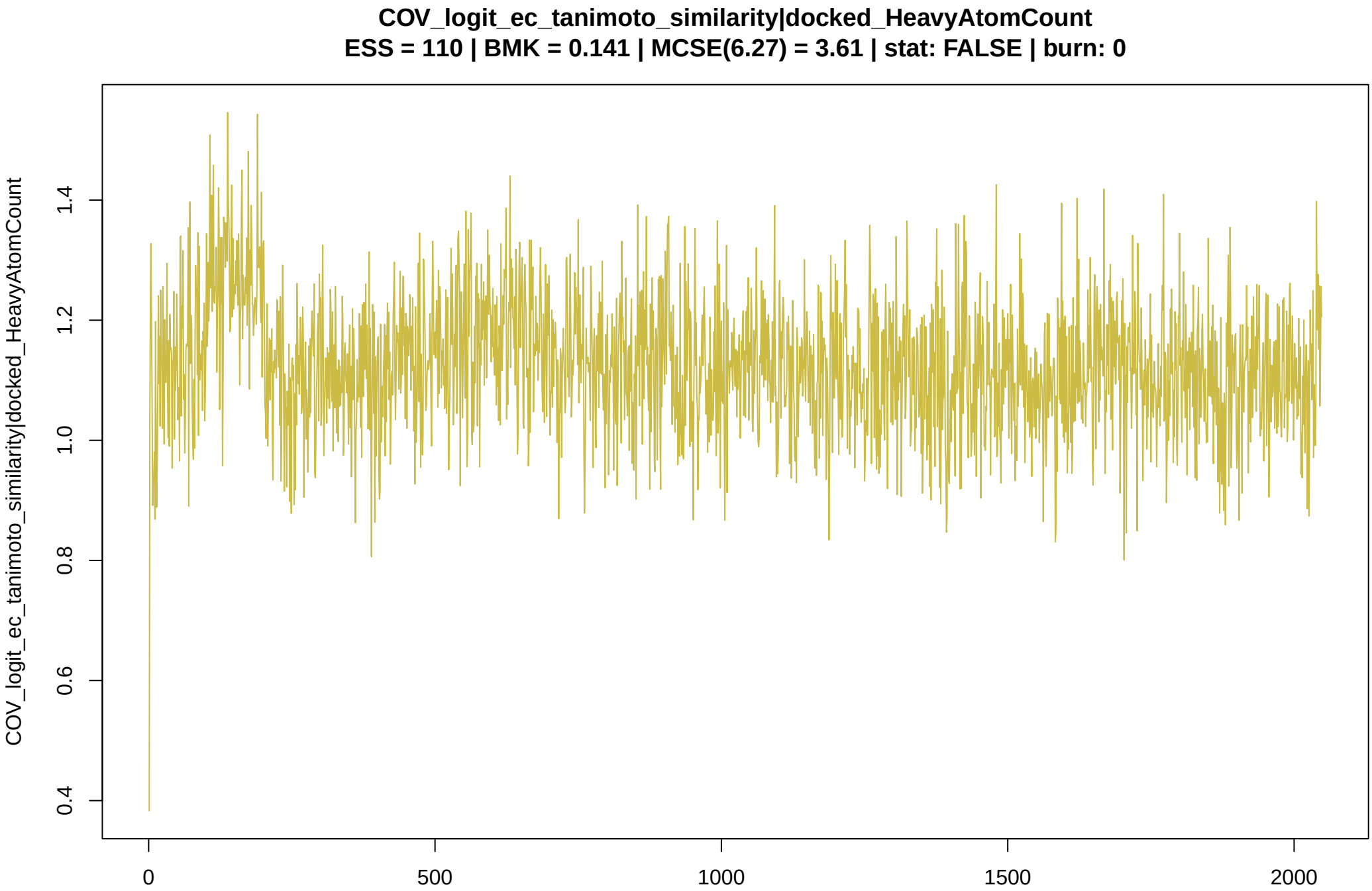

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0619 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
500
1000
1500
2000

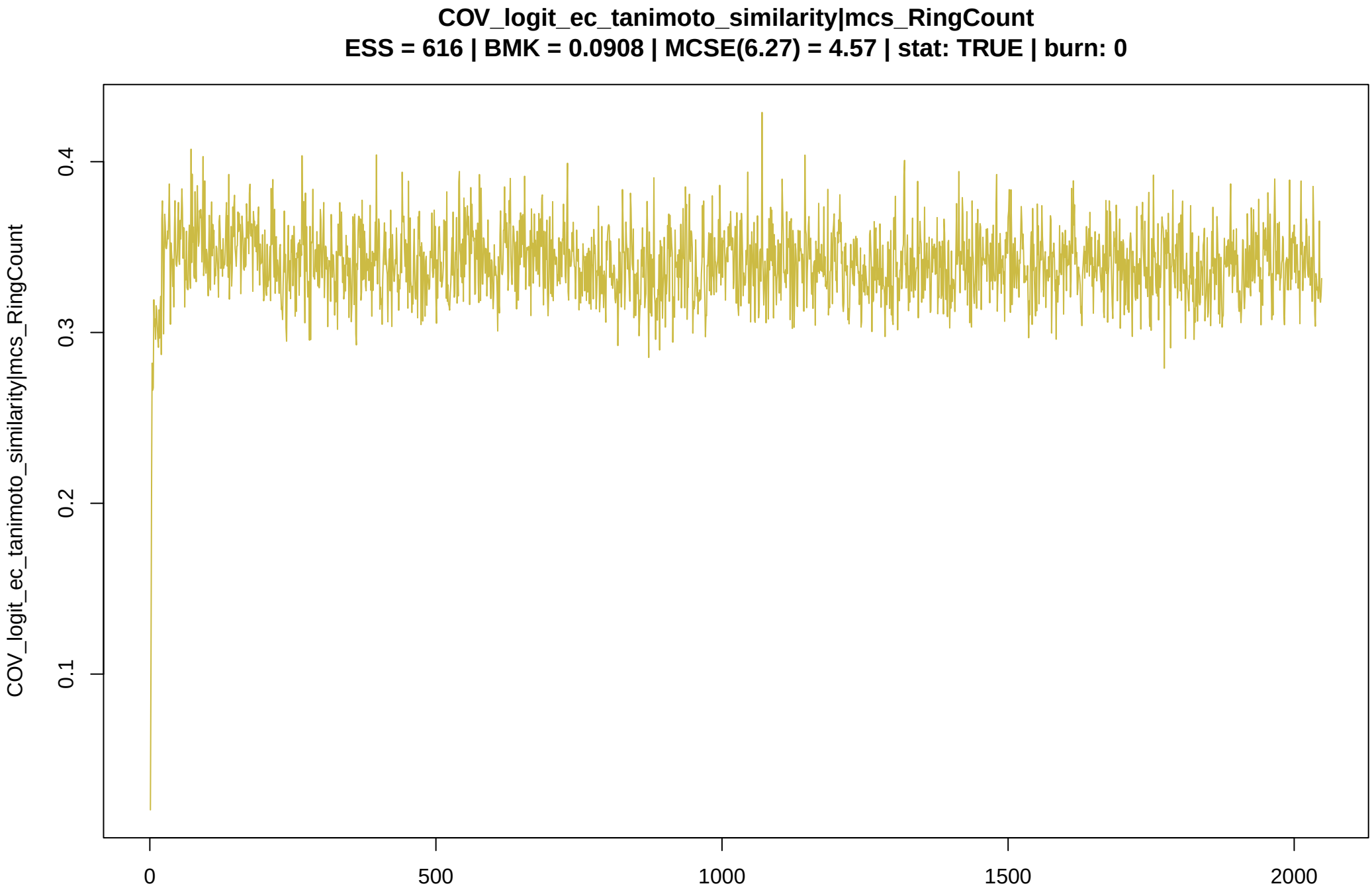

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1480 | BMK = 0.0527 | MCSE(6.27) = 2.55 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
0.02
0.04
0.06
0.08
0.10
0.12
0
500
1000
1500
2000

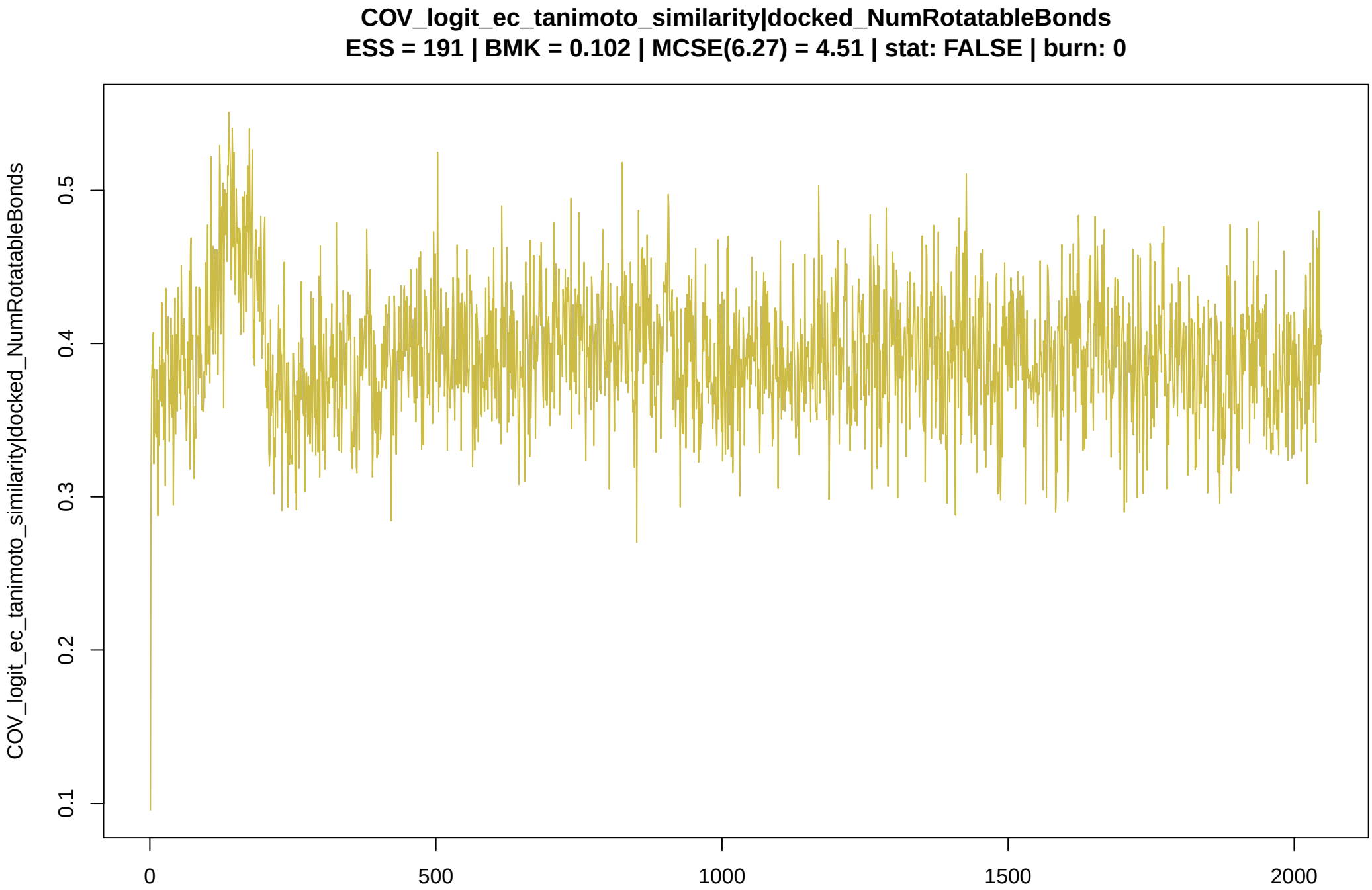

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 799 | BMK = 0.0774 | MCSE(6.27) = 2.44 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
0.1
0.2
0.3
0.4
0.5
0
500
1000
1500
2000

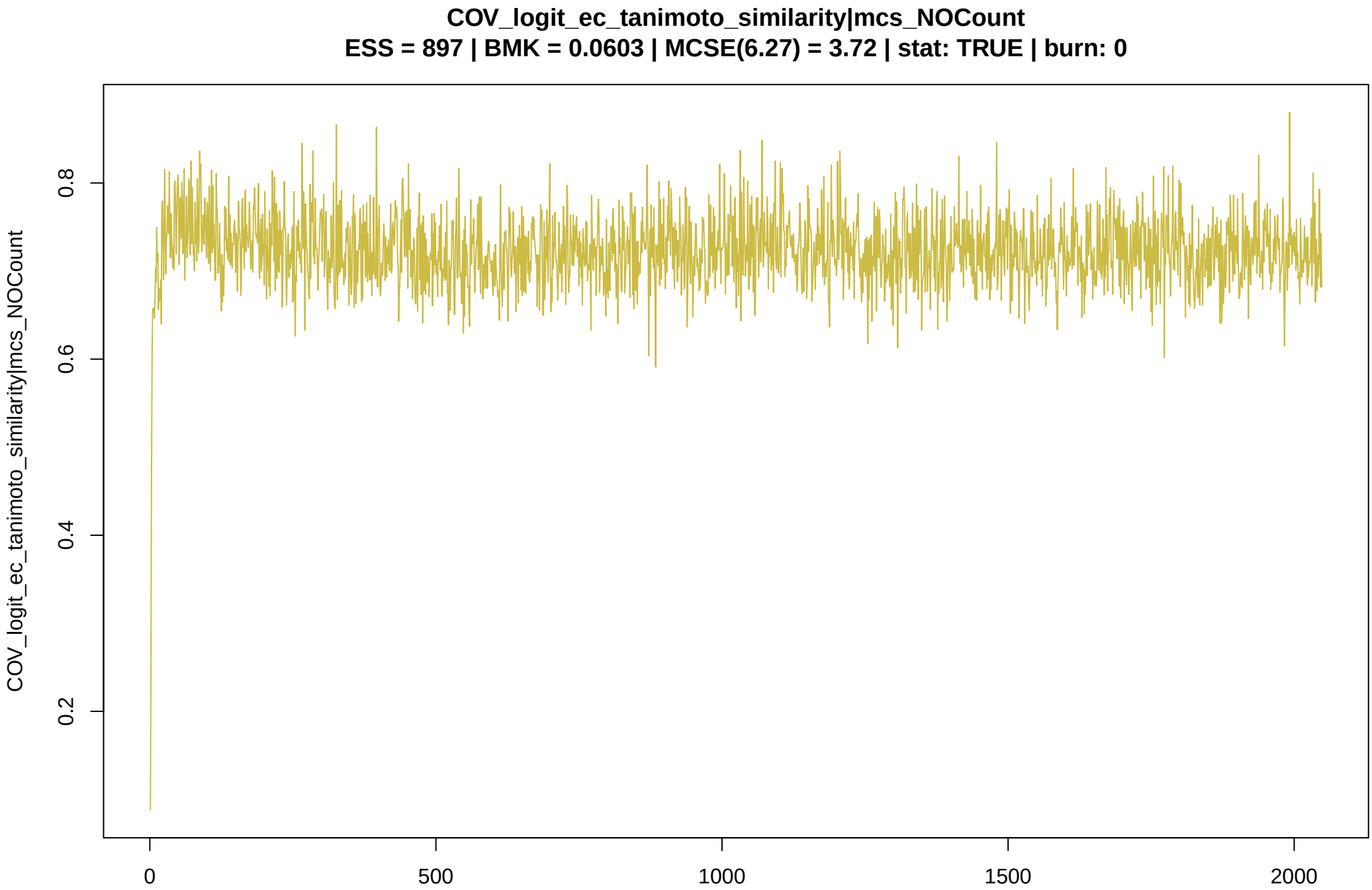

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 201 | BMK = 0.134 | MCSE(6.27) = 4.67 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
0.2
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

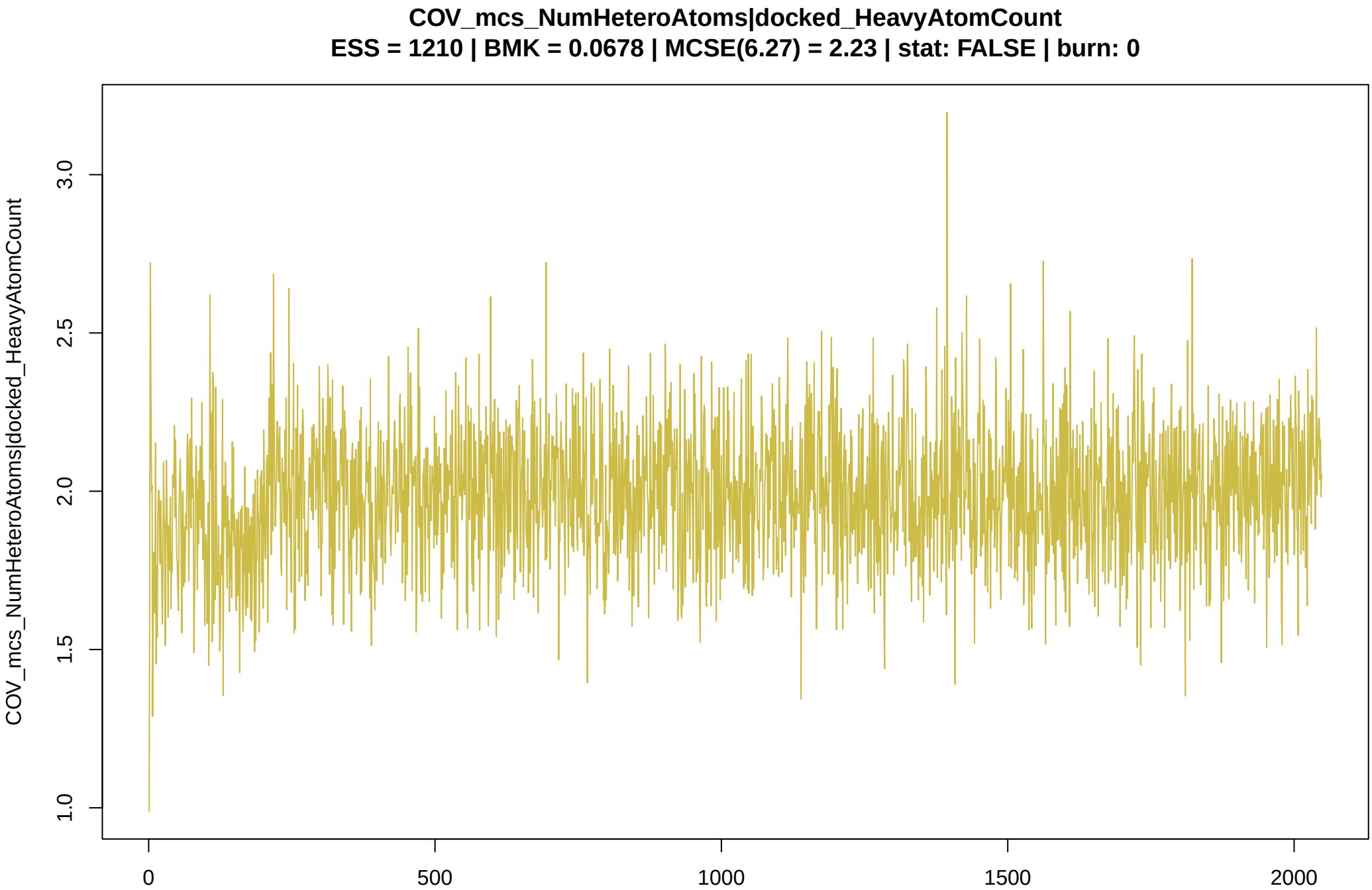

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 823 | BMK = 0.0658 | MCSE(6.27) = 3.65 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.2
0.4
0.6
0.8
0
500
1000
1500
2000

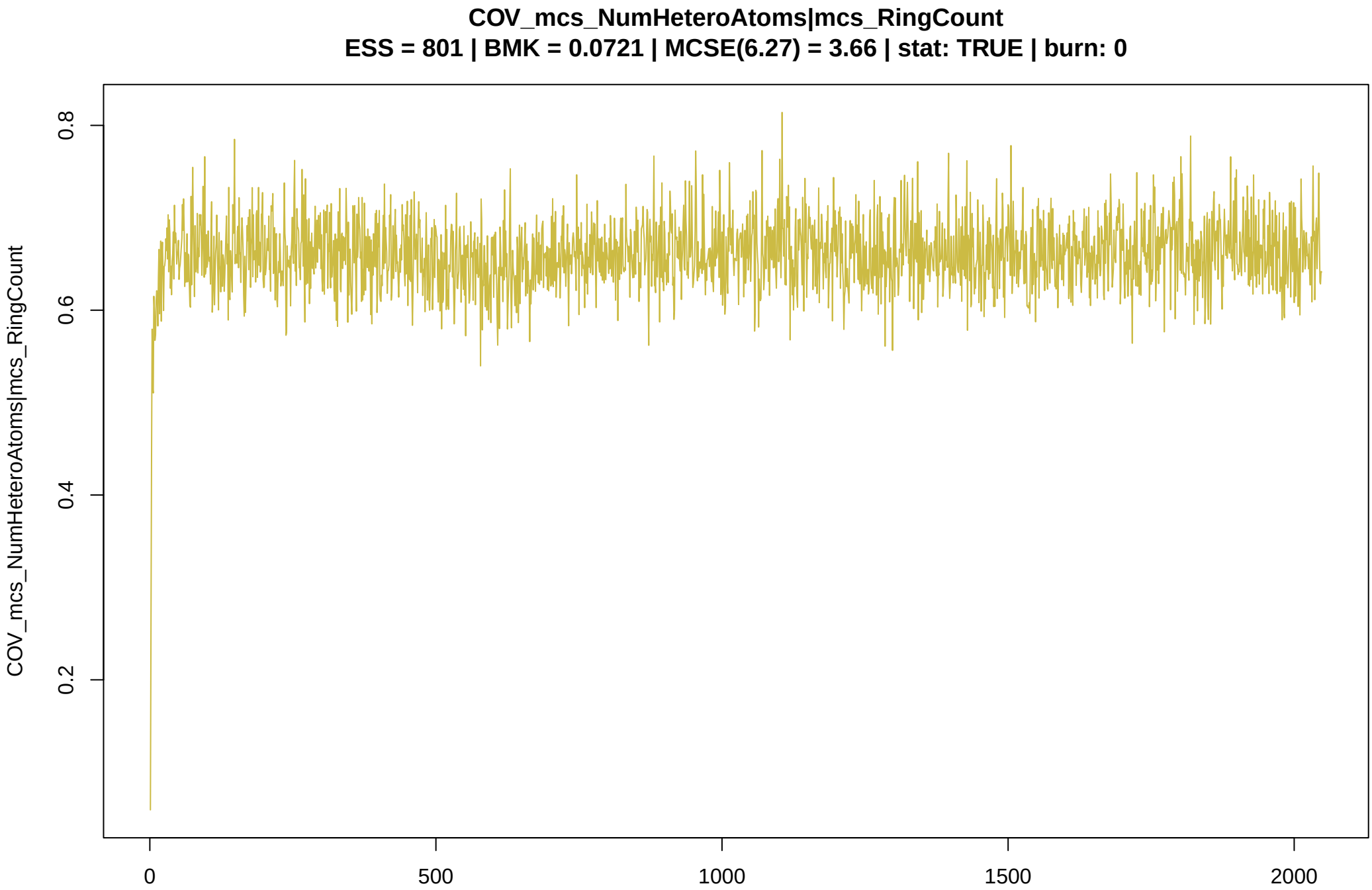

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 110 | BMK = 0.141 | MCSE(6.27) = 3.61 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
0.4
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

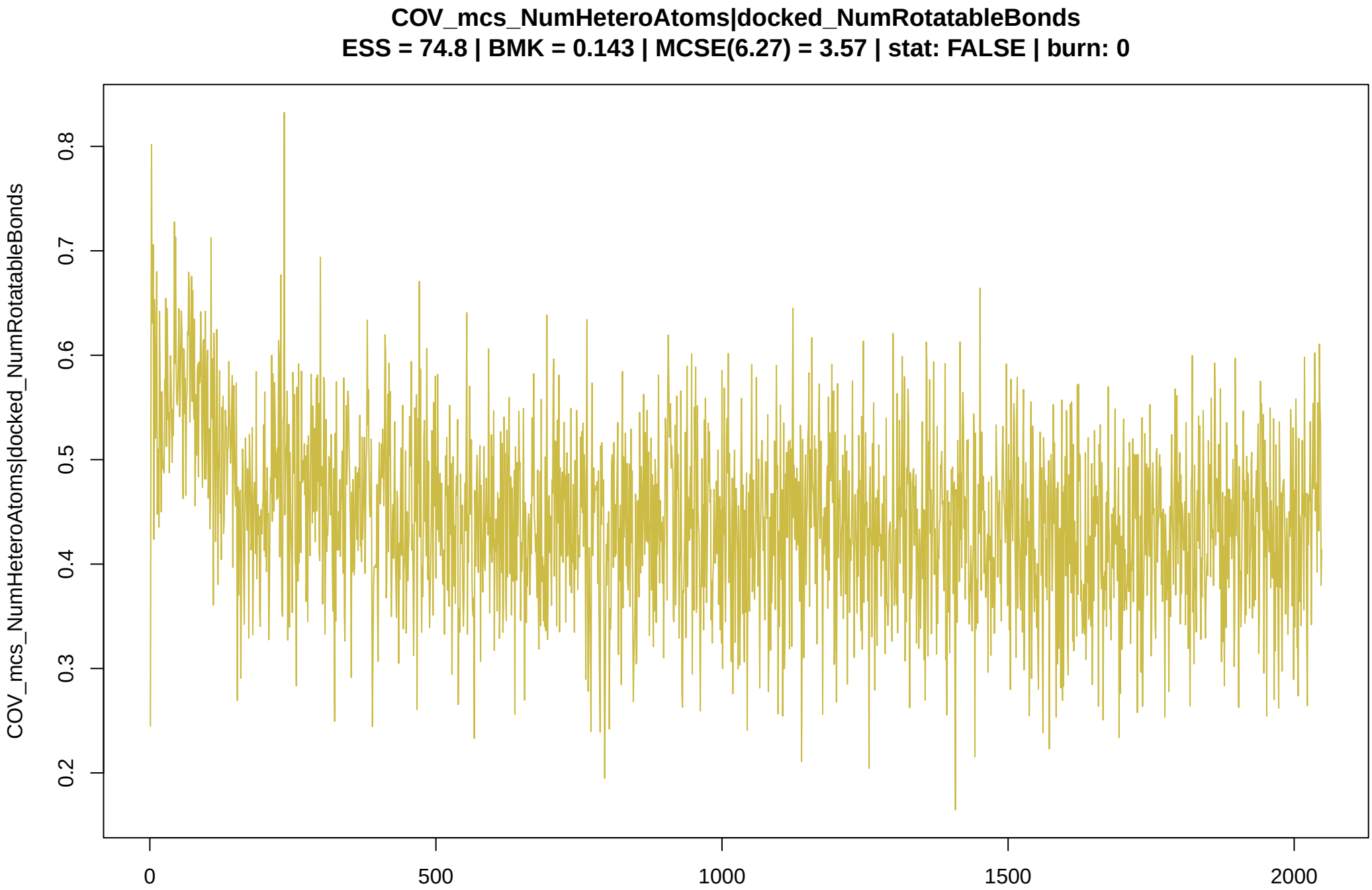

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 616 | BMK = 0.0908 | MCSE(6.27) = 4.57 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.1
0.2
0.3
0.4
0
500
1000
1500
2000

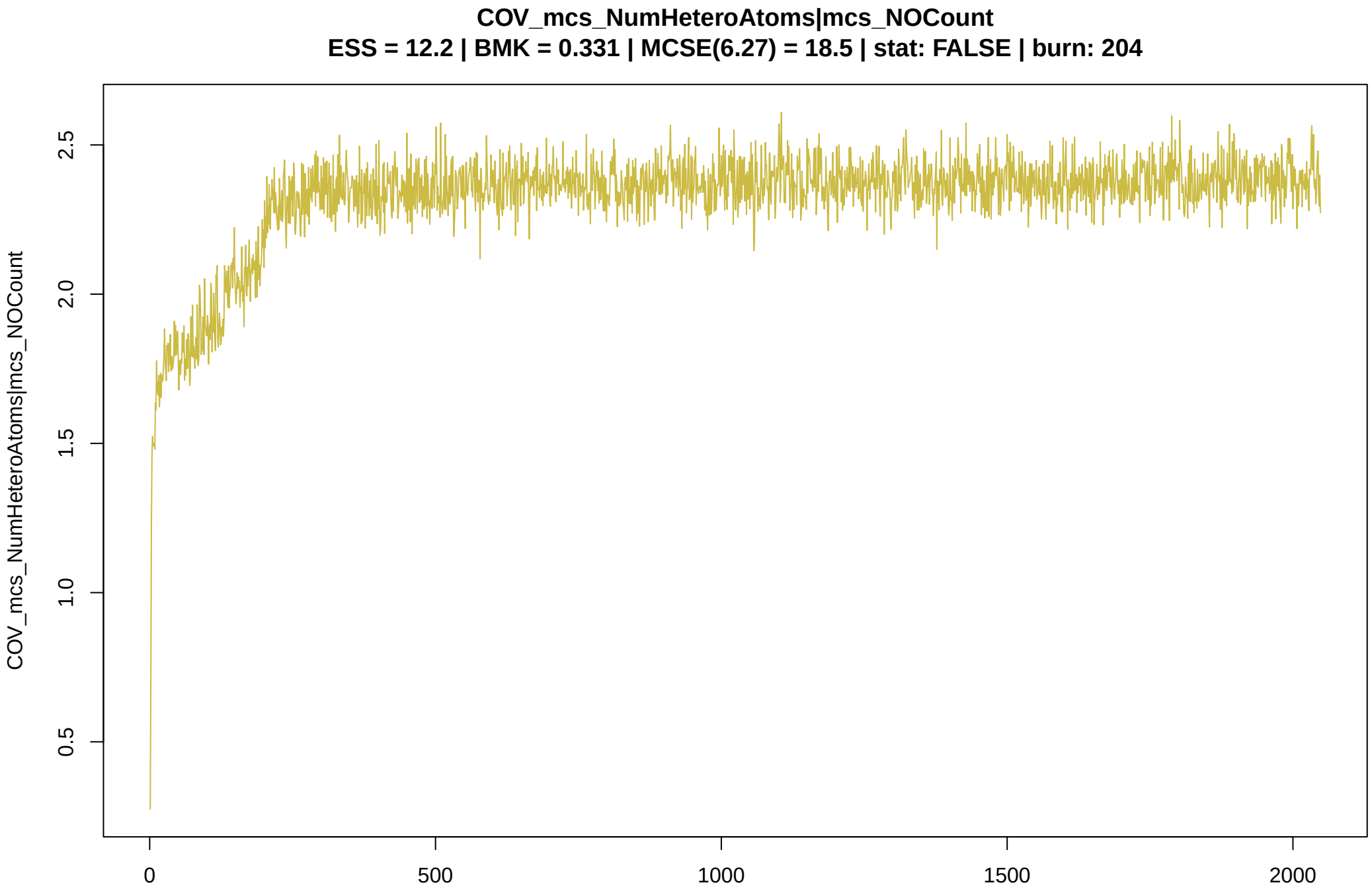

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 191 | BMK = 0.102 | MCSE(6.27) = 4.51 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
0.1
0.2
0.3
0.4
0.5
0
500
1000
1500
2000

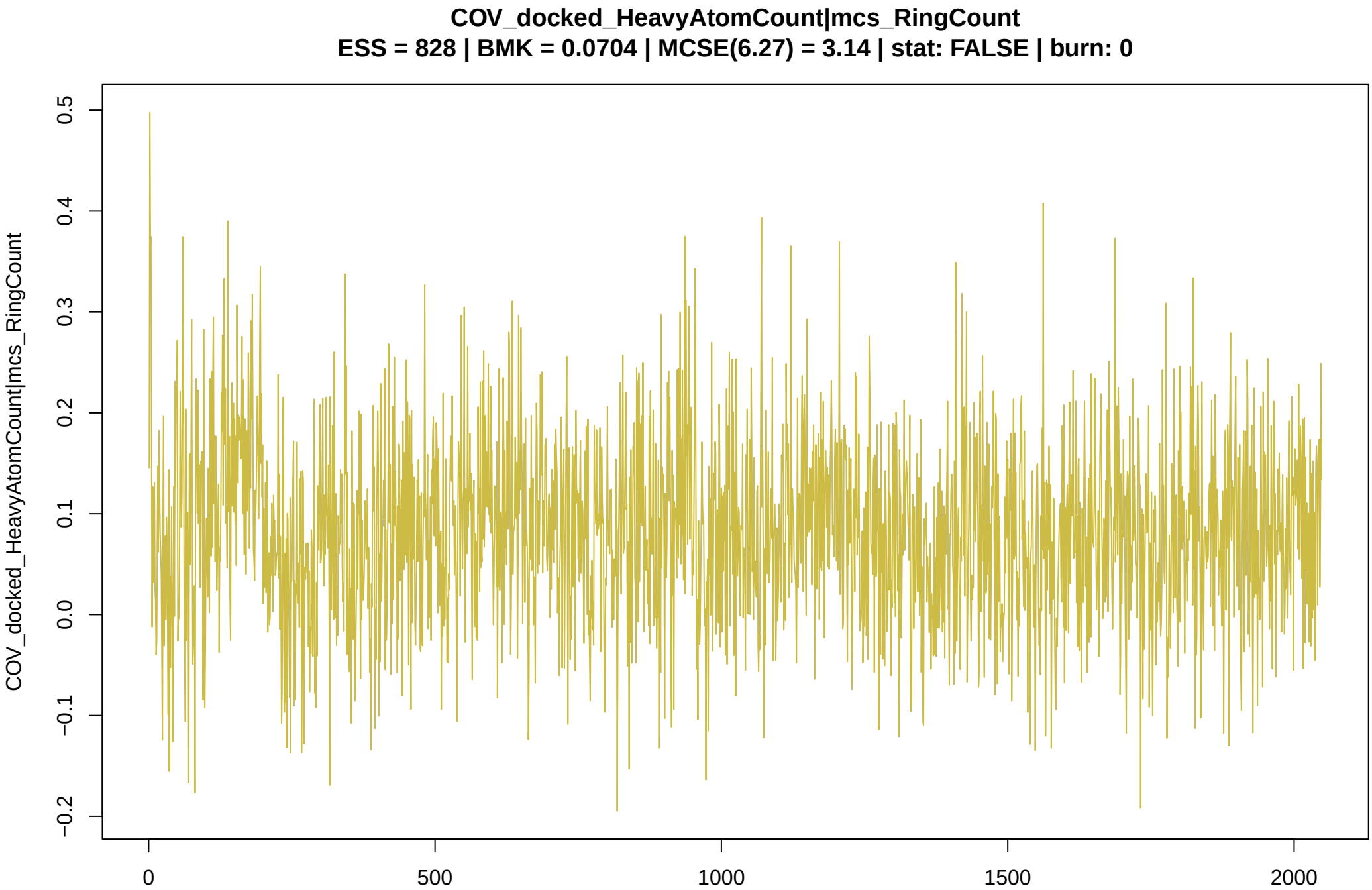

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 897 | BMK = 0.0603 | MCSE(6.27) = 3.72 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NOCount
0.2
0.4
0.6
0.8
0
500
1000
1500
2000

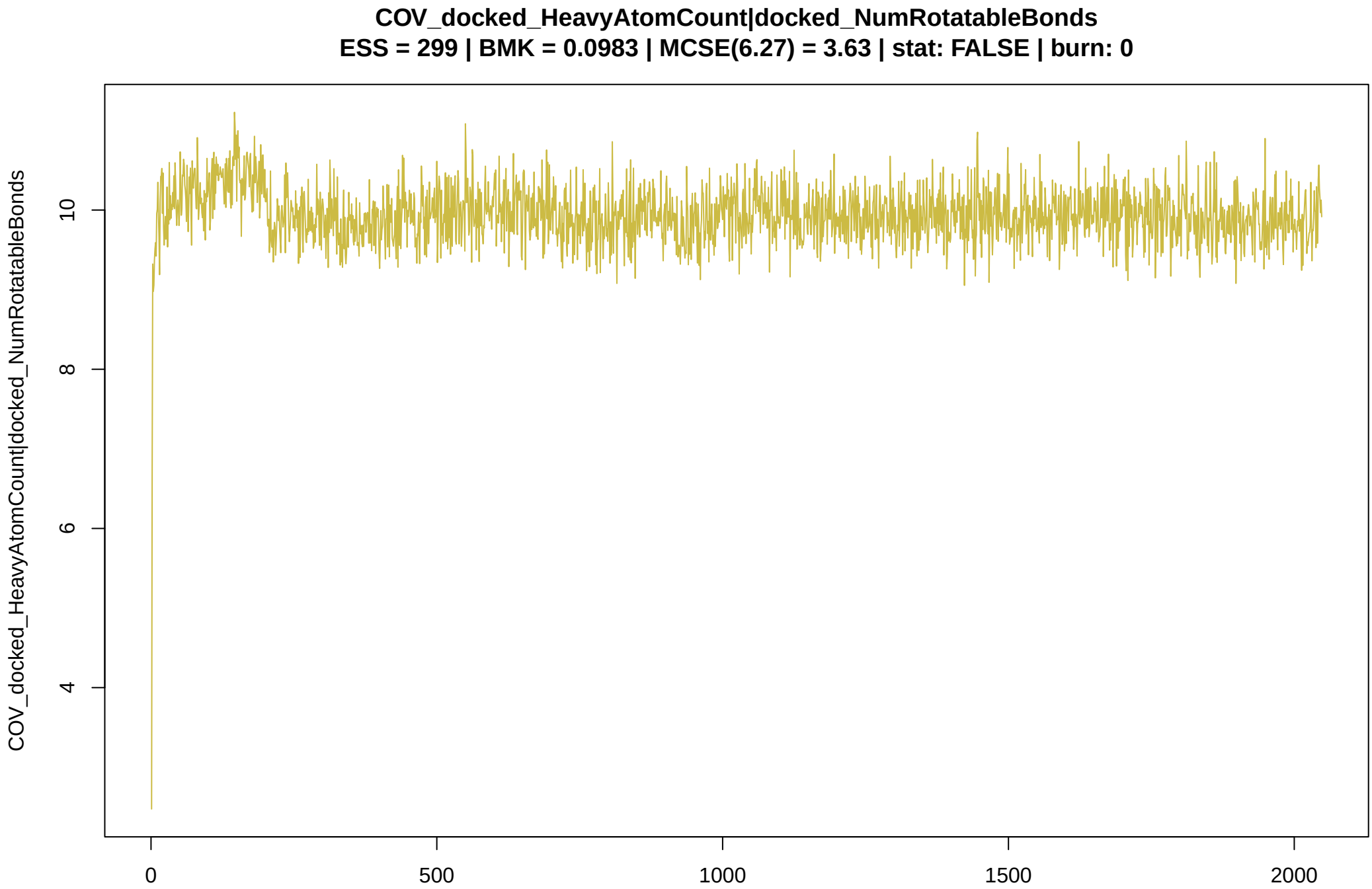

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1210 | BMK = 0.0678 | MCSE(6.27) = 2.23 | stat: FALSE | burn: 0
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
1.0
1.5
2.0
2.5
3.0
0
500
1000
1500
2000

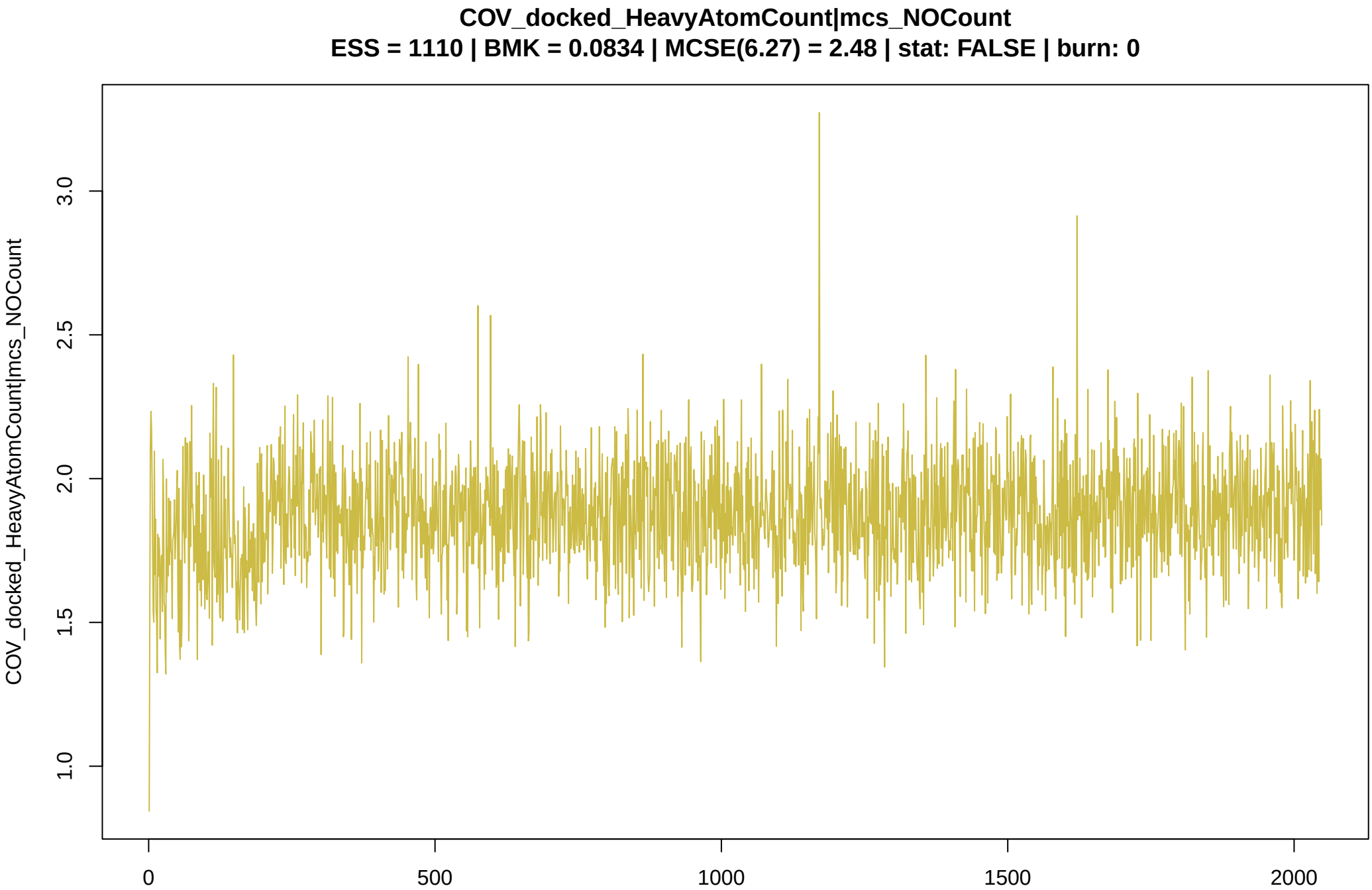

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 801 | BMK = 0.0721 | MCSE(6.27) = 3.66 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.2
0.4
0.6
0.8
0
500
1000
1500
2000

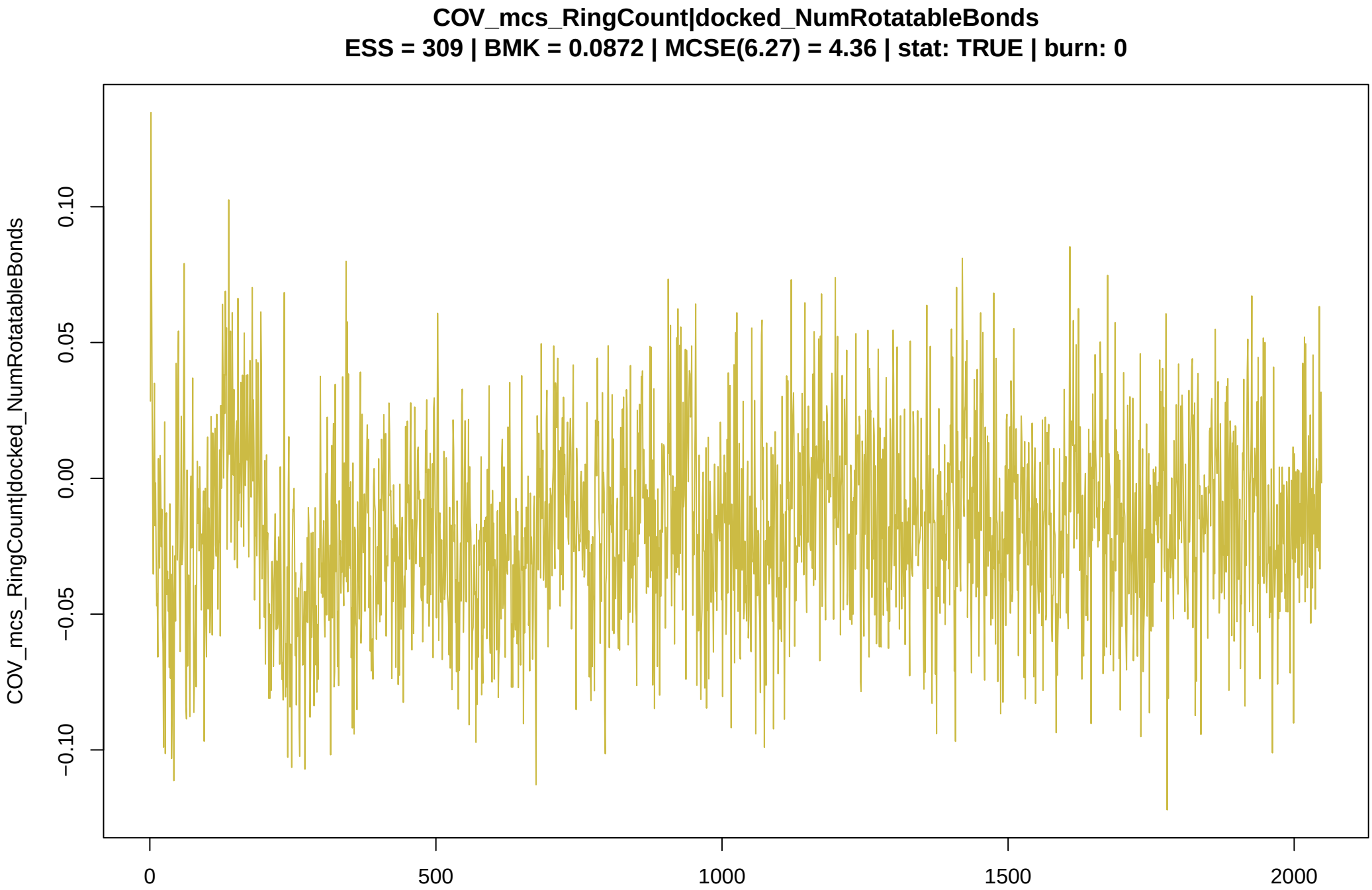

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 74.8 | BMK = 0.143 | MCSE(6.27) = 3.57 | stat: FALSE | burn: 0
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0
500
1000
1500
2000

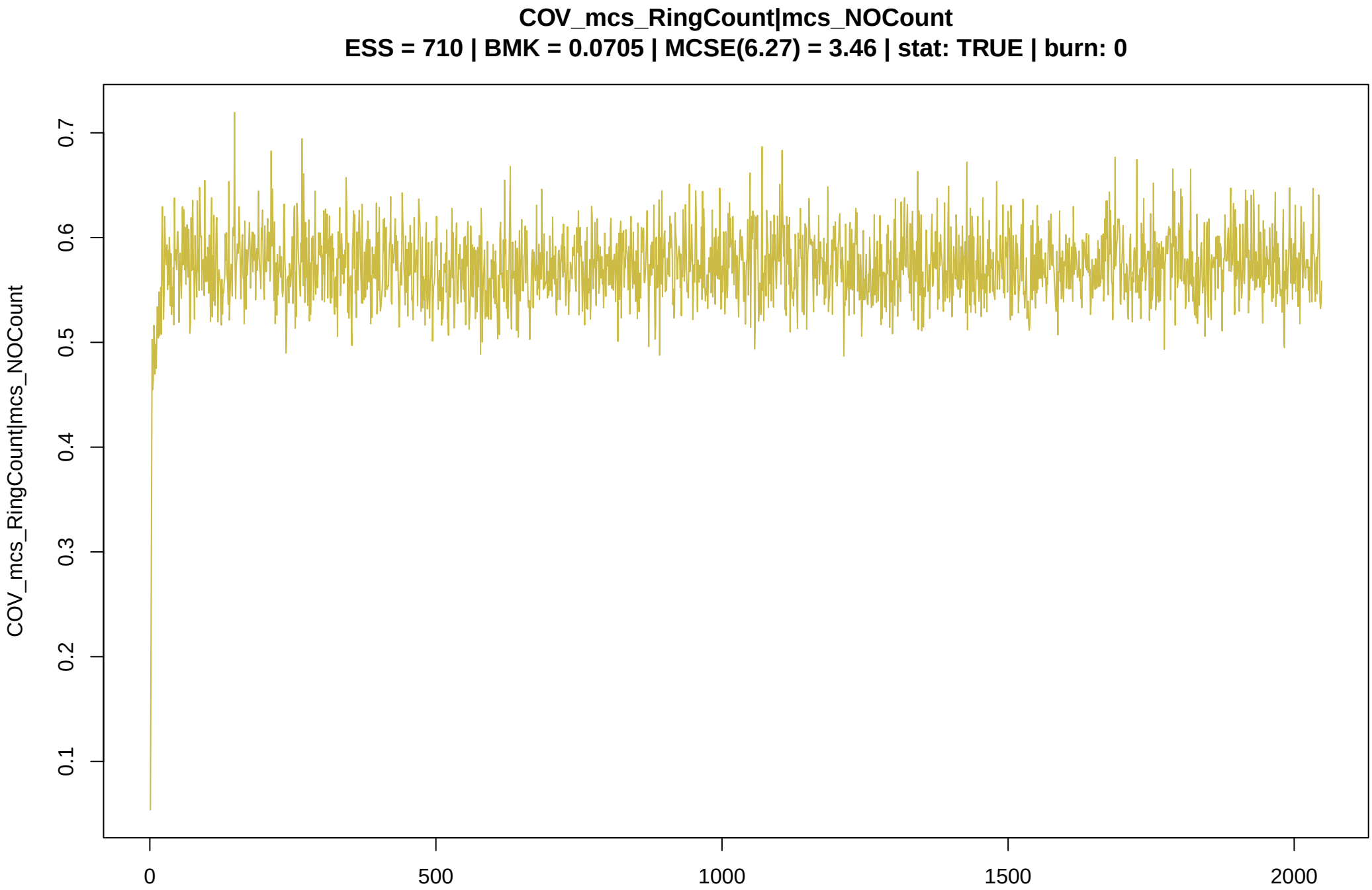

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 12.2 | BMK = 0.331 | MCSE(6.27) = 18.5 | stat: FALSE | burn: 204
COV_mcs_NumHeteroAtoms|mcs_NOCount
0.5
1.0
1.5
2.0
2.5
0
500
1000
1500
2000

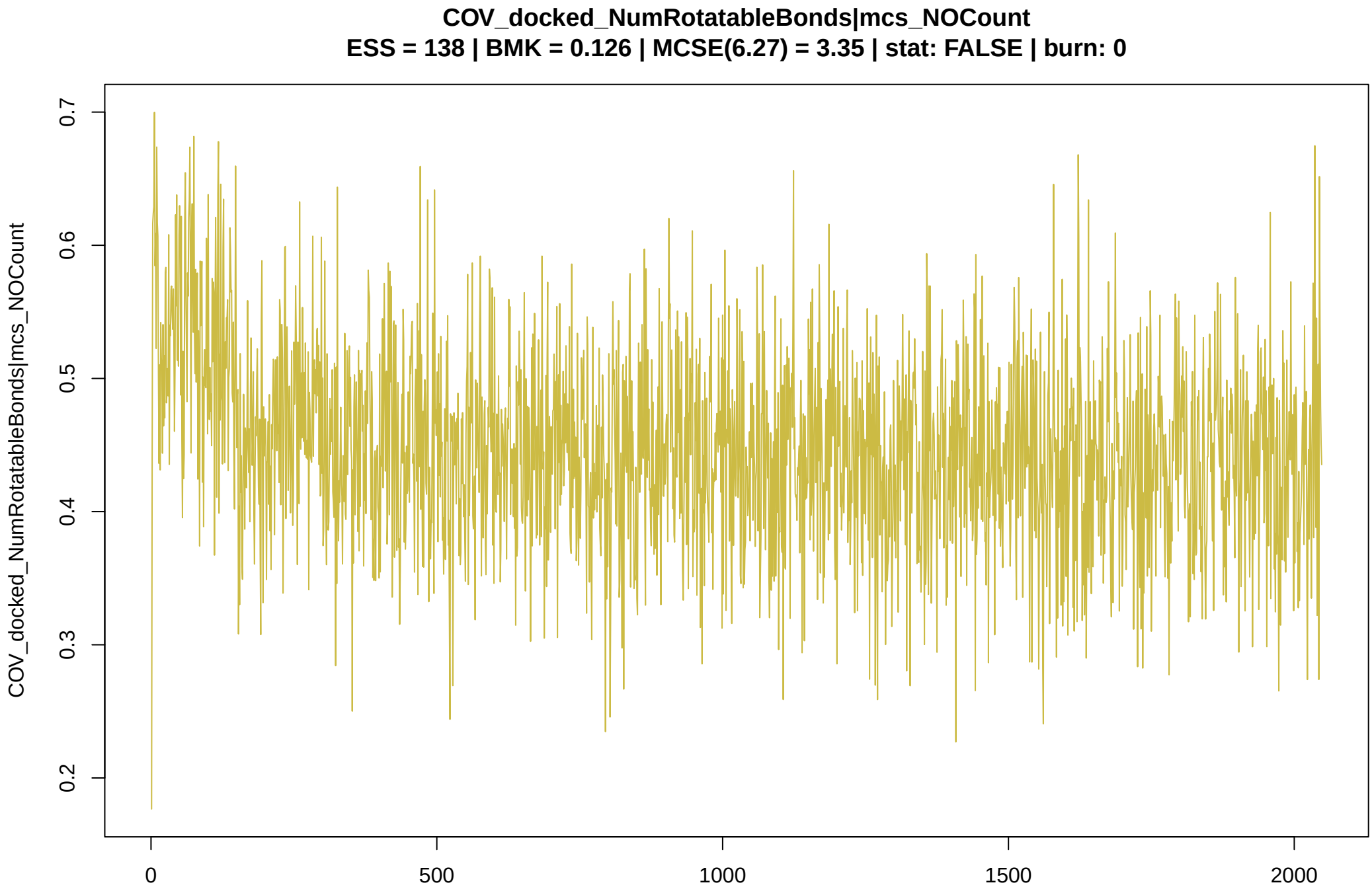

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 828 | BMK = 0.0704 | MCSE(6.27) = 3.14 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.5
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 299 | BMK = 0.0983 | MCSE(6.27) = 3.63 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
4
6
8
10
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1110 | BMK = 0.0834 | MCSE(6.27) = 2.48 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|mcs_NOCount
1.0
1.5
2.0
2.5
3.0
0
500
1000
1500
2000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 309 | BMK = 0.0872 | MCSE(6.27) = 4.36 | stat: TRUE | burn: 0
COV_mcs_RingCount|docked_NumRotatableBonds
0.10
0.05
0.00
−0.05
−0.10
0
500
1000
1500
2000


COV_mcs_RingCount|mcs_NOCount
ESS = 710 | BMK = 0.0705 | MCSE(6.27) = 3.46 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_NOCount
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
500
1000
1500
2000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 138 | BMK = 0.126 | MCSE(6.27) = 3.35 | stat: FALSE | burn: 0
COV_docked_NumRotatableBonds|mcs_NOCount
0.2
0.3
0.4
0.5
0.6
0.7
0
500
1000
1500
2000