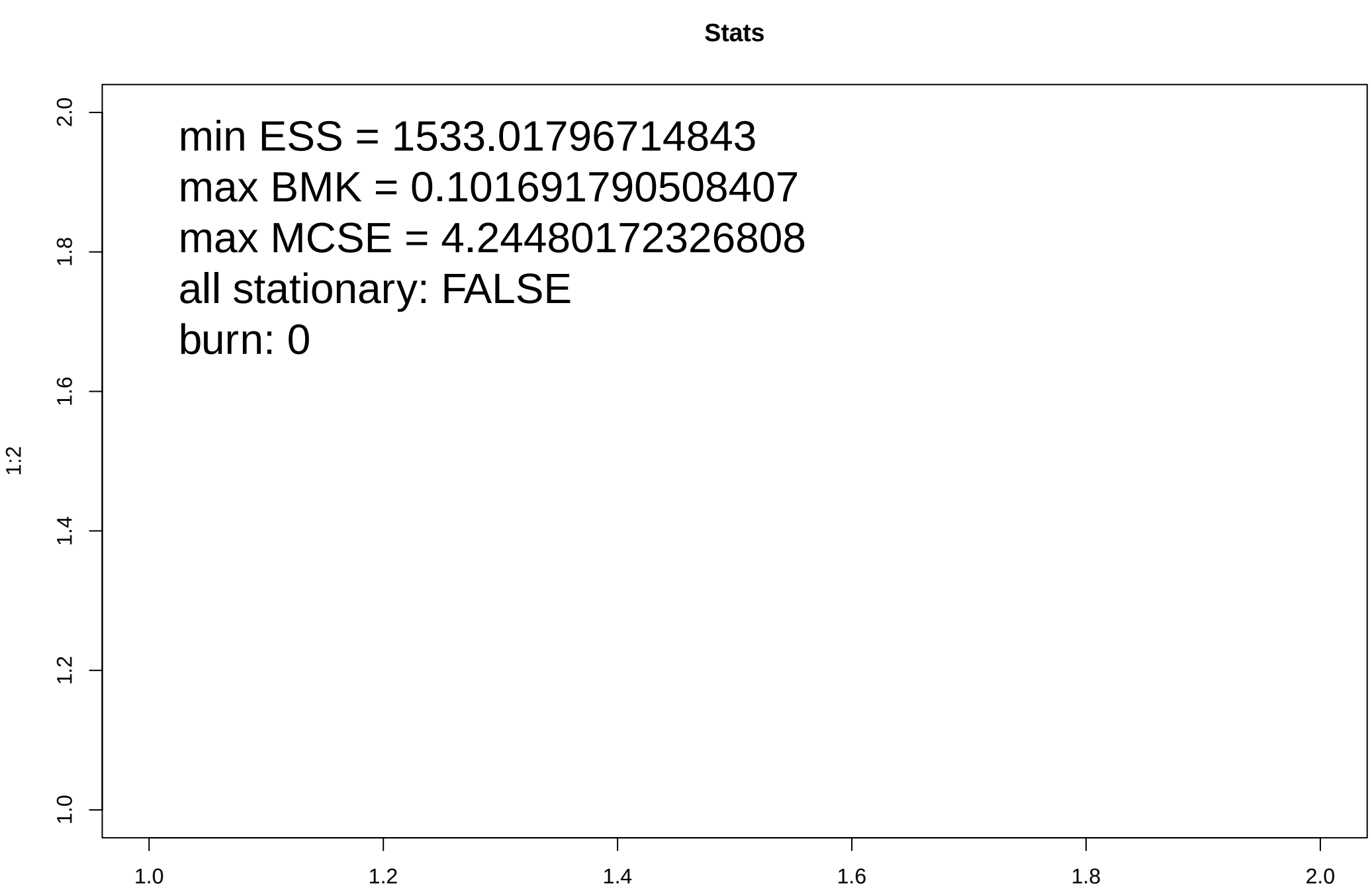
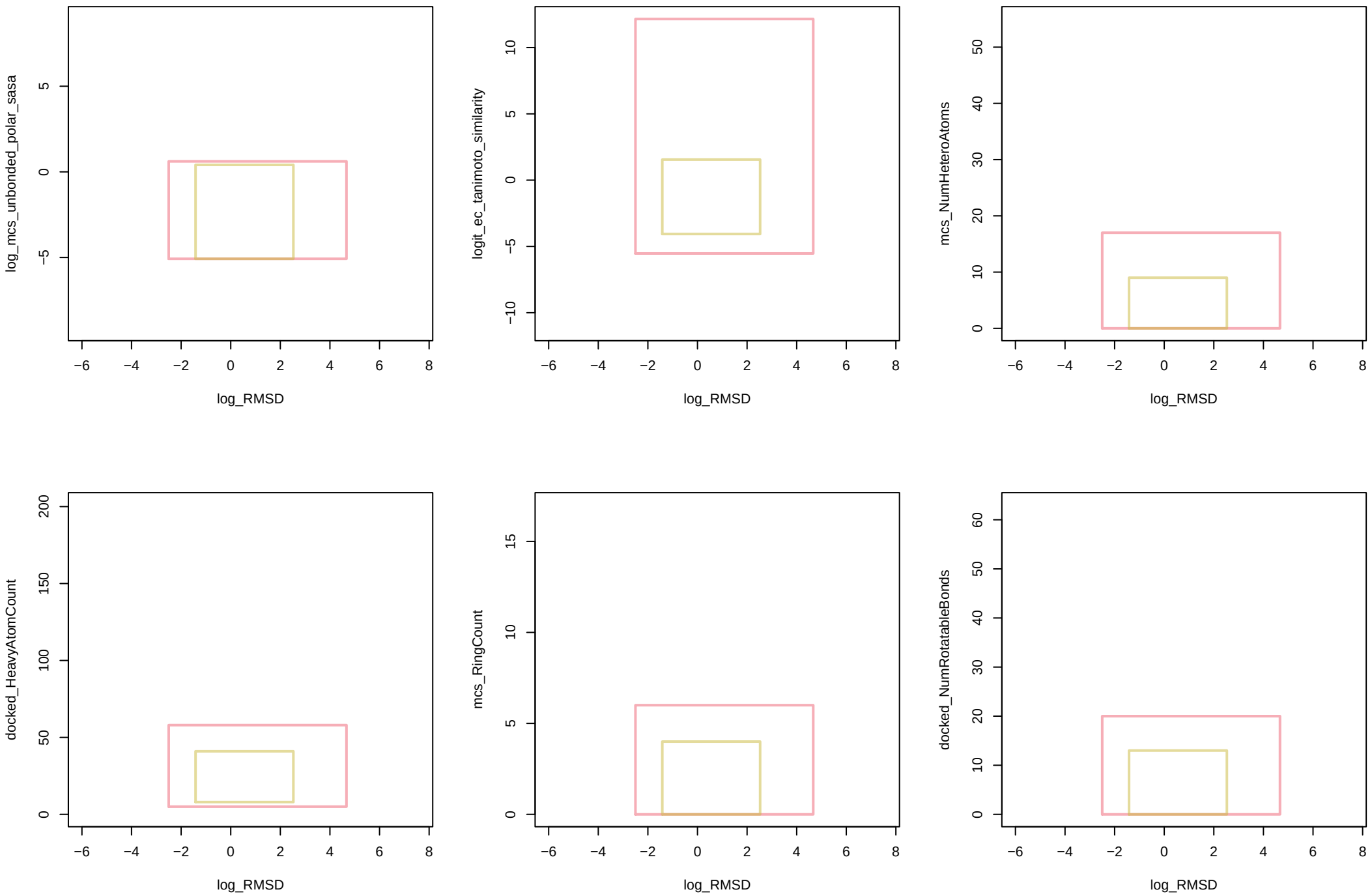
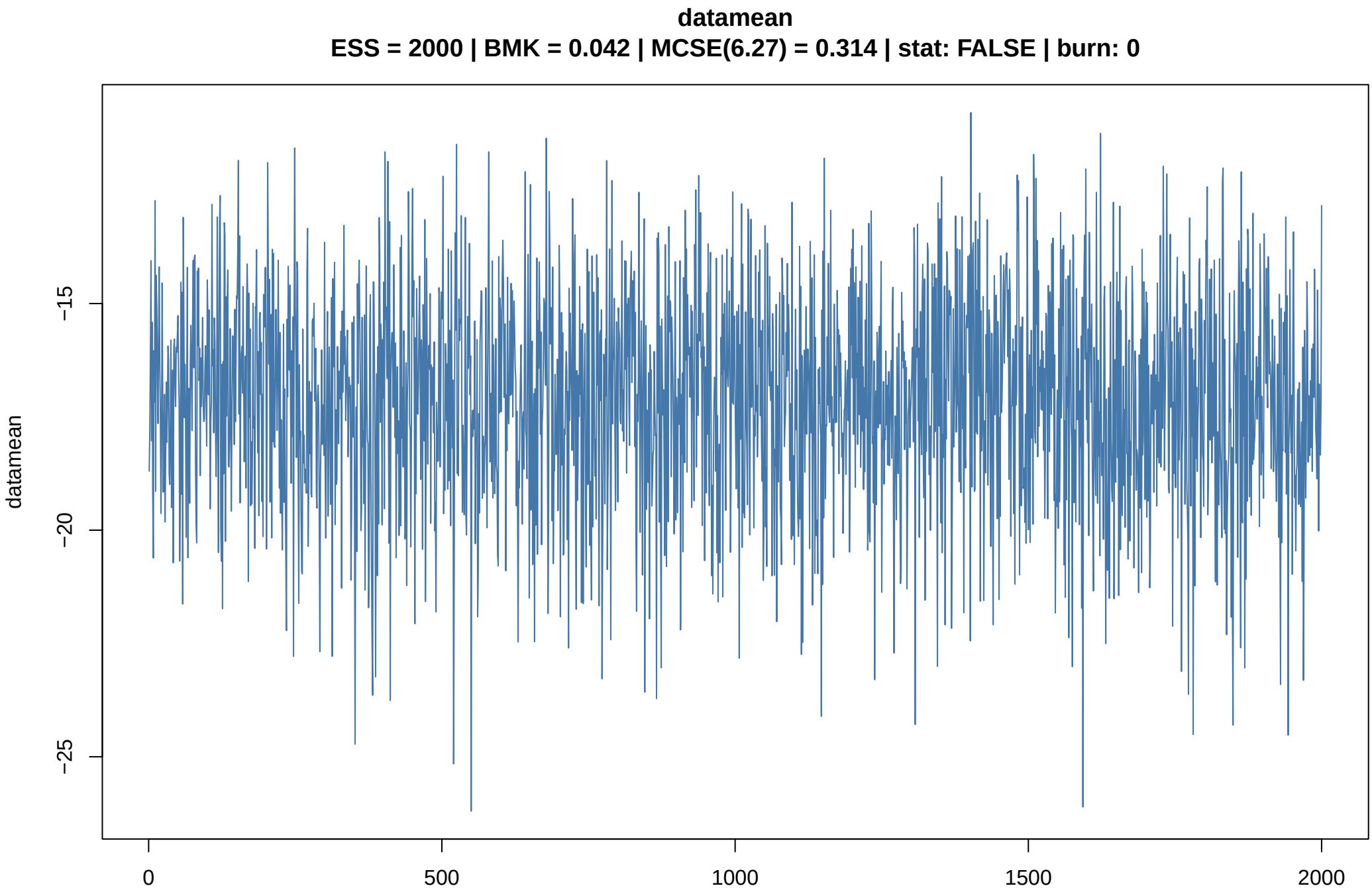
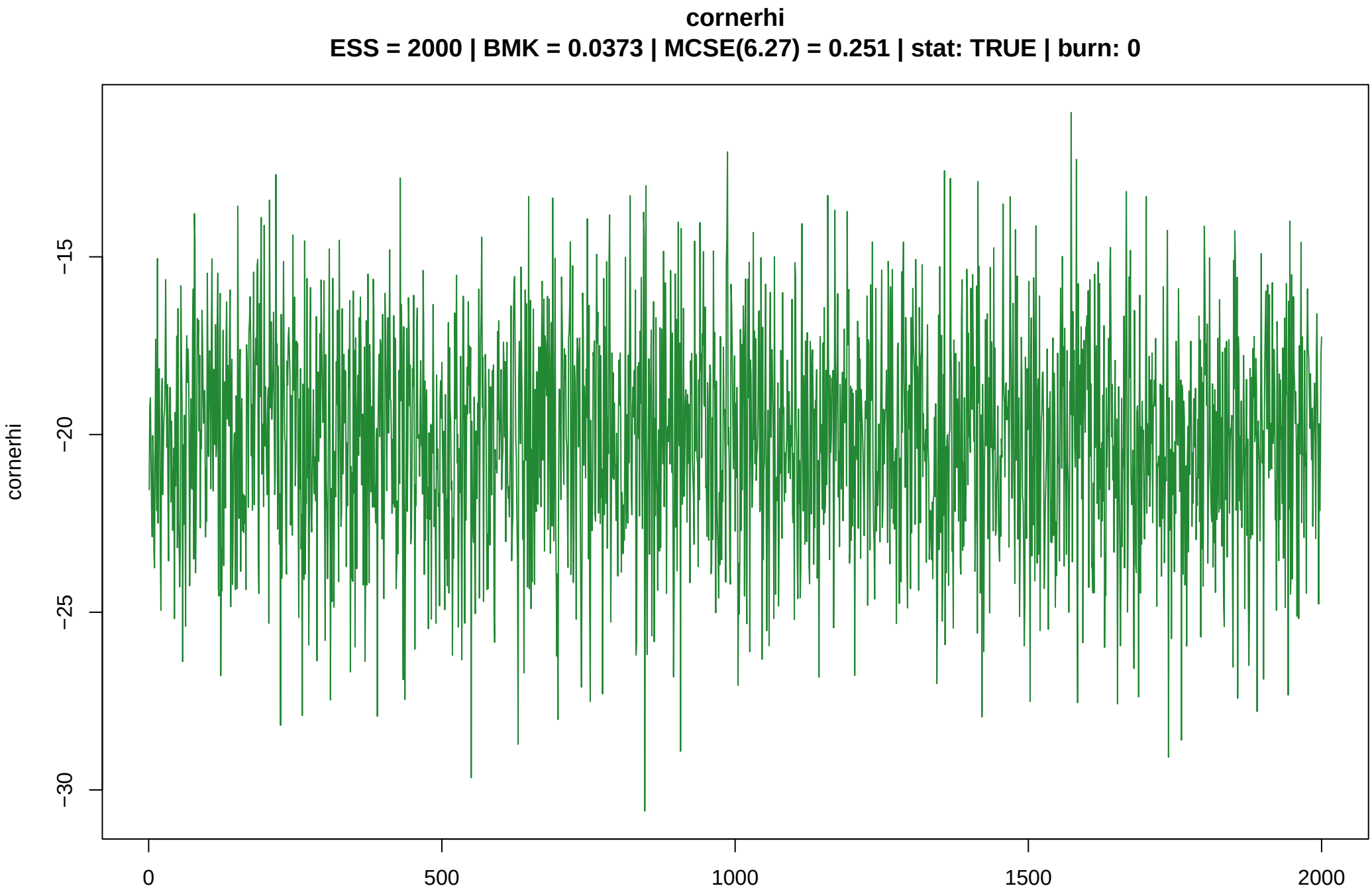
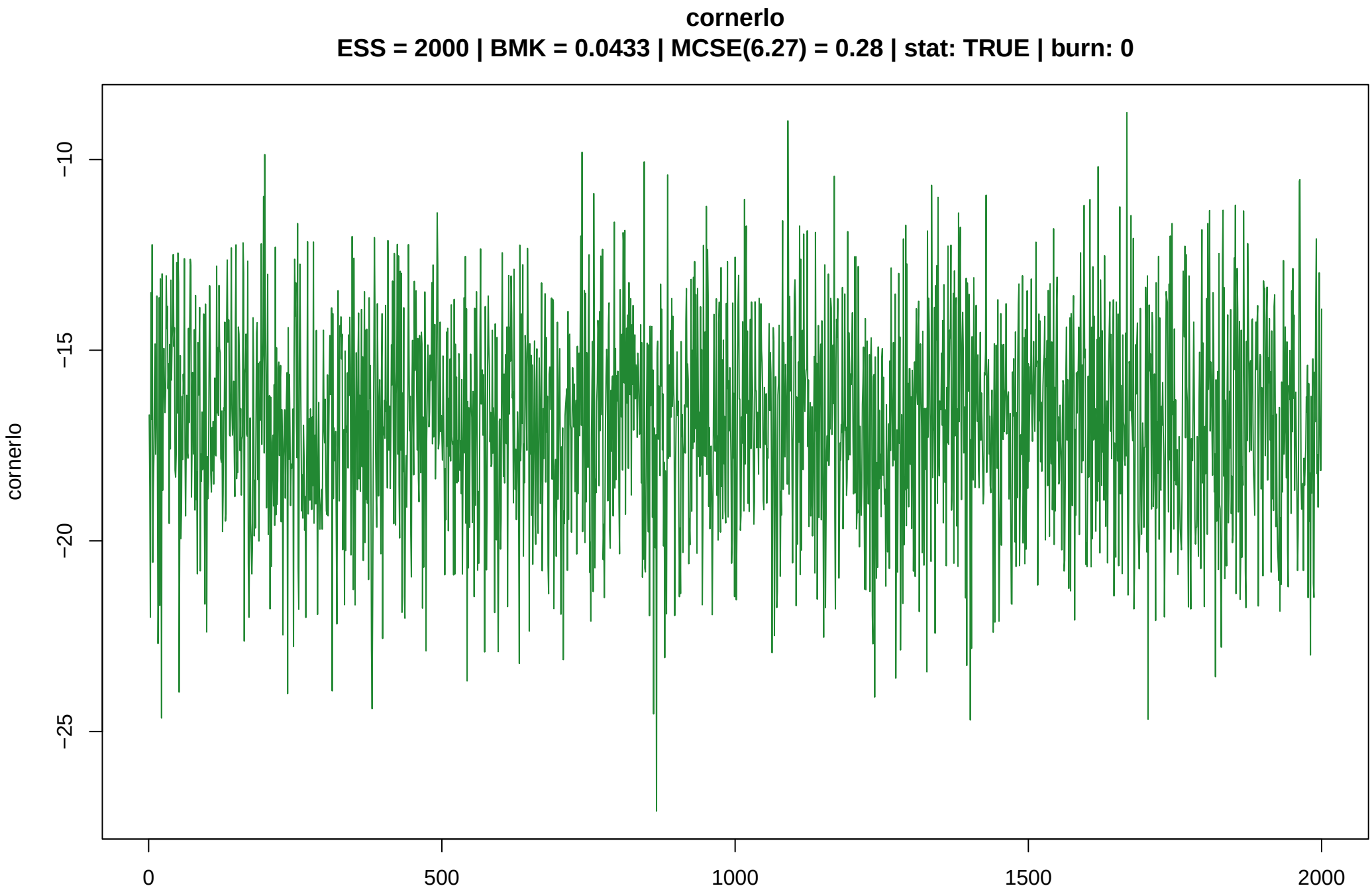
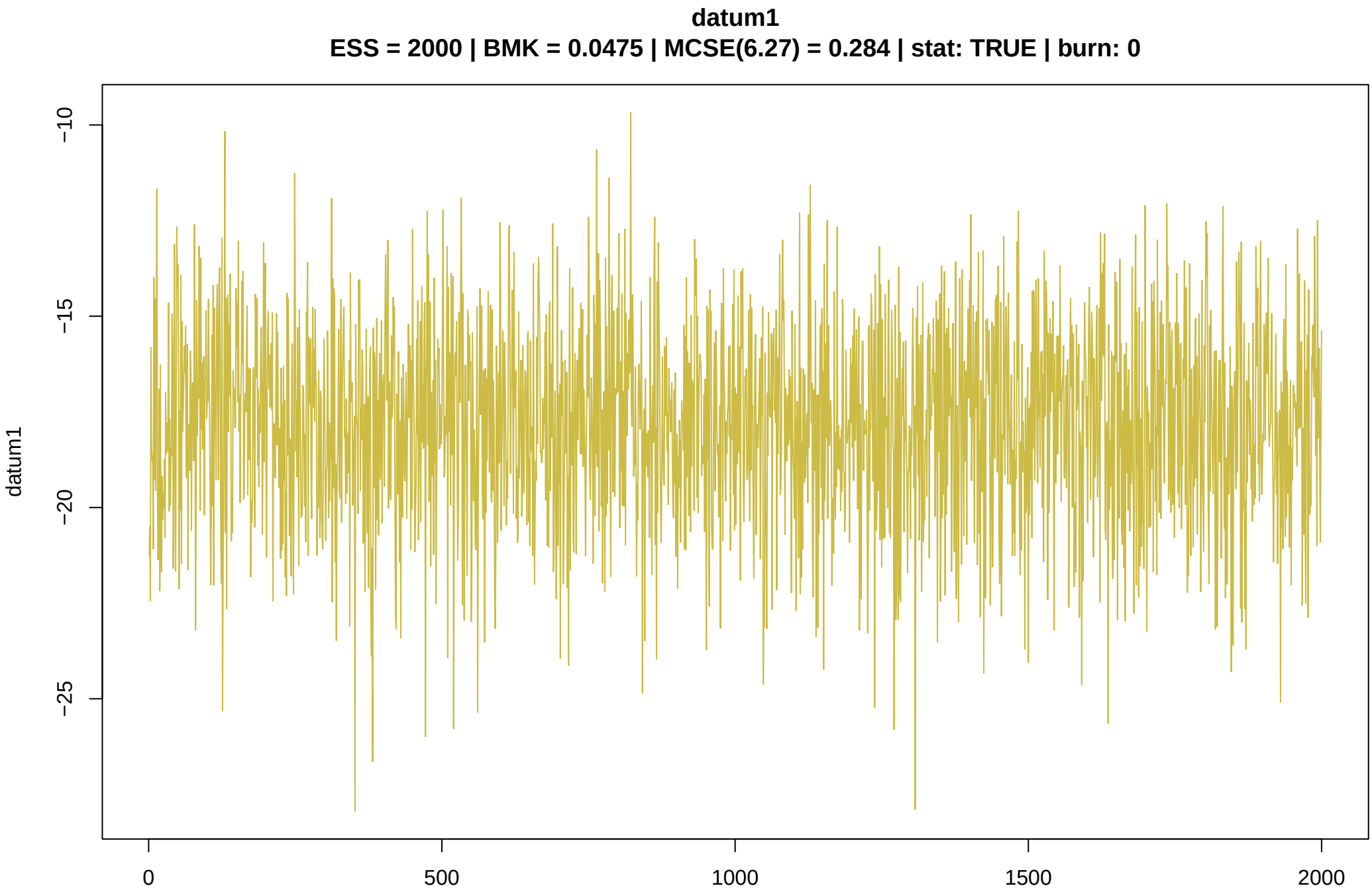

Stats
min ESS = 1533.01796714843
max BMK = 0.101691790508407
max MCSE = 4.24480172326808
all stationary: FALSE
burn: 0
1:2
1.0
1.2
1.4
1.6
1.8
2.0

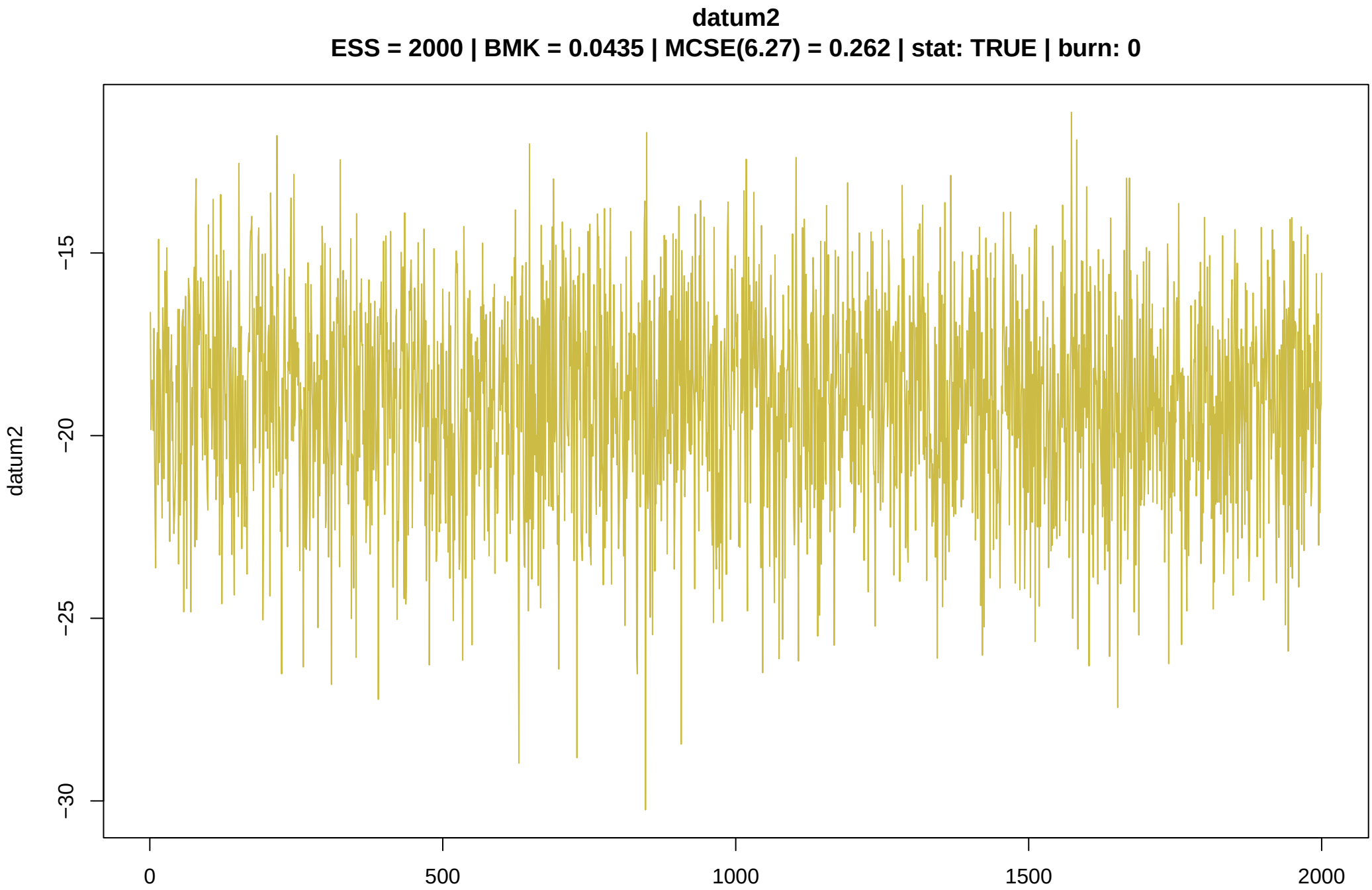

log_mcs_unbonded_polar_sasa
log_RMSD
logit_ec_tanimoto_similarity
log_RMSD
mcs_NumHeteroAtoms
log_RMSD
docked_HeavyAtomCount
log_RMSD
mcs_RingCount
log_RMSD
docked_NumRotatableBonds
log_RMSD

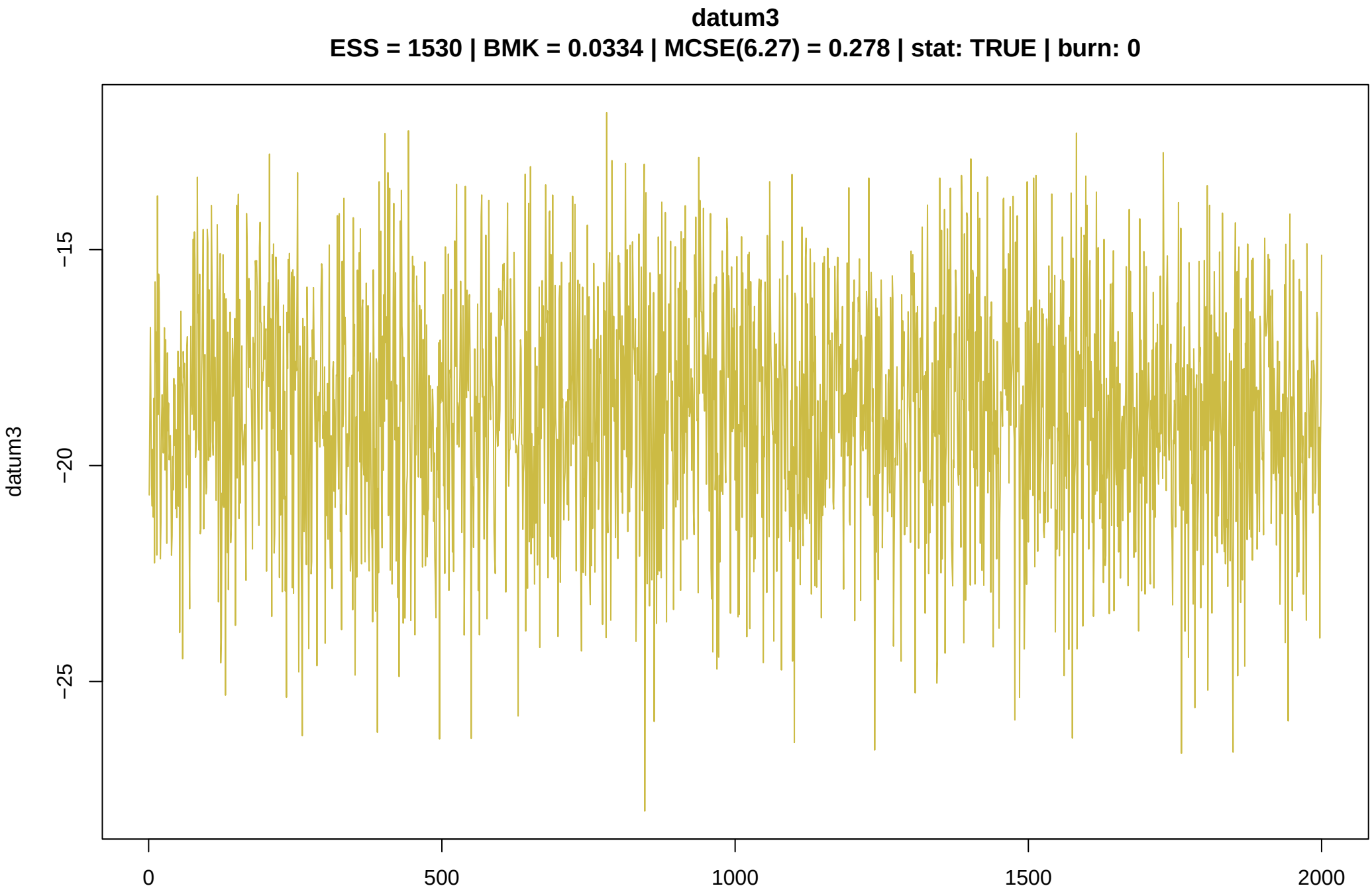

datamean
ESS = 2000 | BMK = 0.042 | MCSE(6.27) = 0.314 | stat: FALSE | burn: 0
datamean
−15
−20
−25
0
500
1000
1500
2000

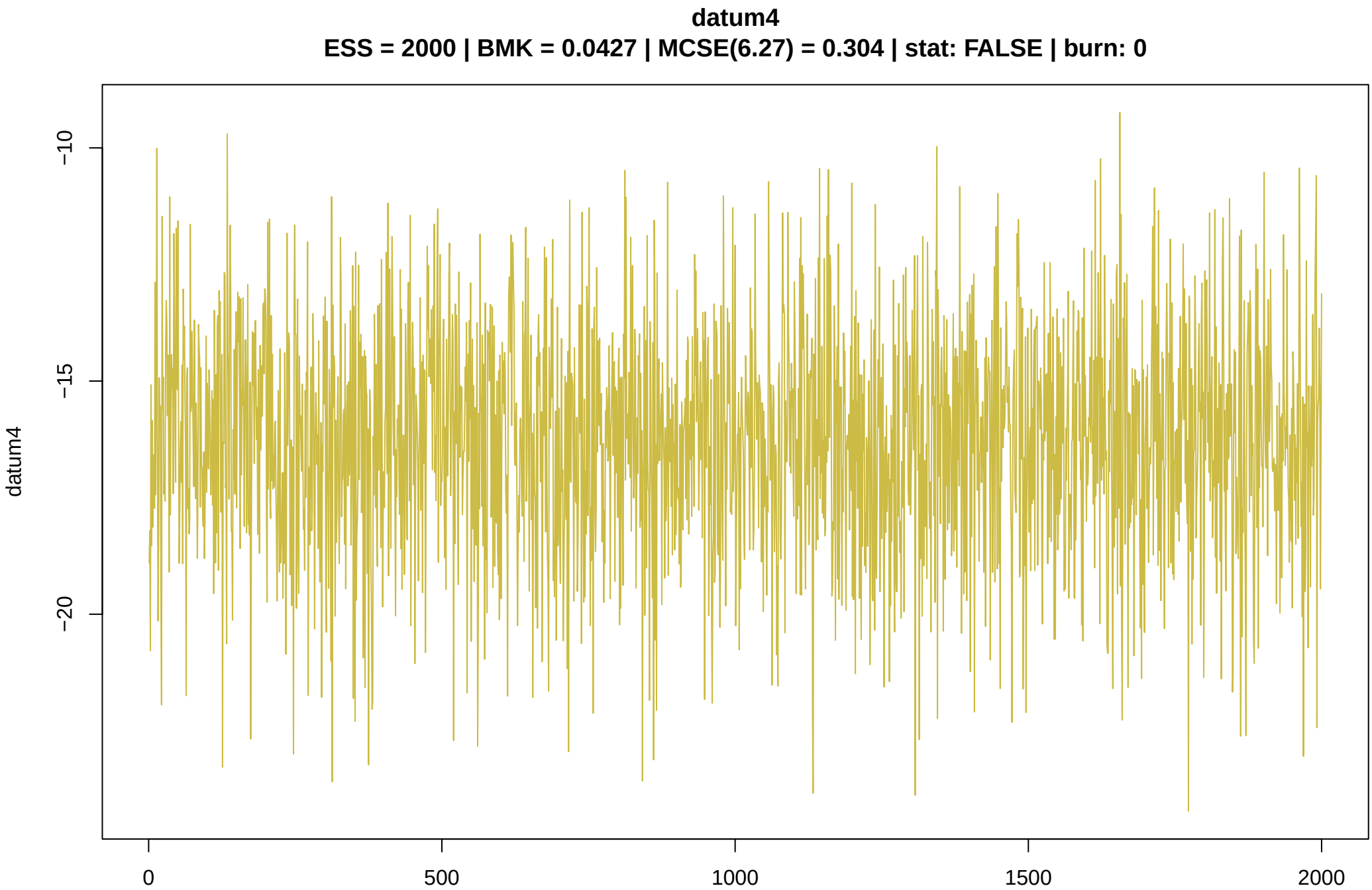

cornerhi
ESS = 2000 | BMK = 0.0373 | MCSE(6.27) = 0.251 | stat: TRUE | burn: 0
cornerhi
−15
−20
−25
−30
0
500
1000
1500
2000

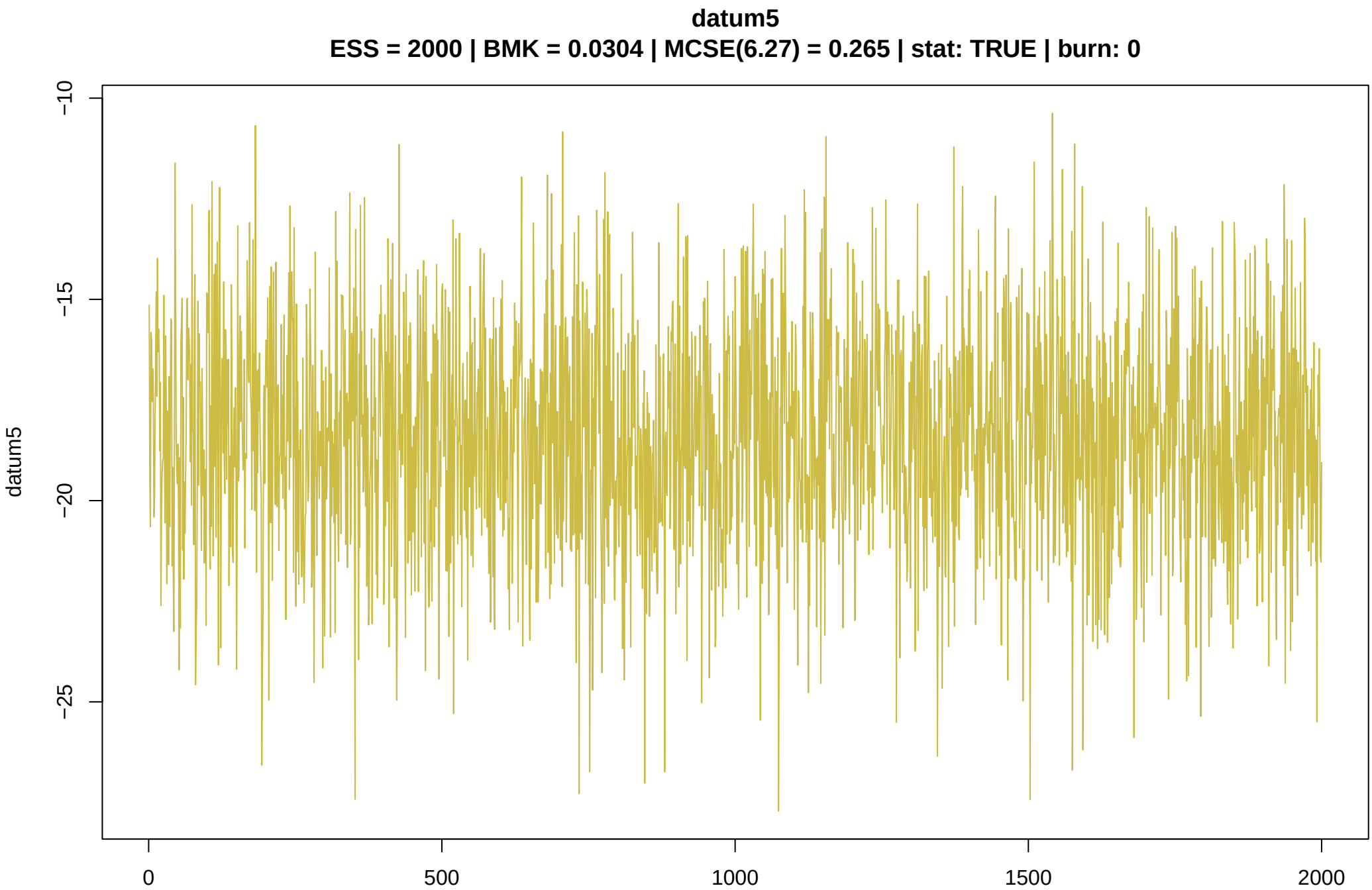

cornerlo
ESS = 2000 | BMK = 0.0433 | MCSE(6.27) = 0.28 | stat: TRUE | burn: 0
cornerlo
−10
−15
−20
−25
0
500
1000
1500
2000

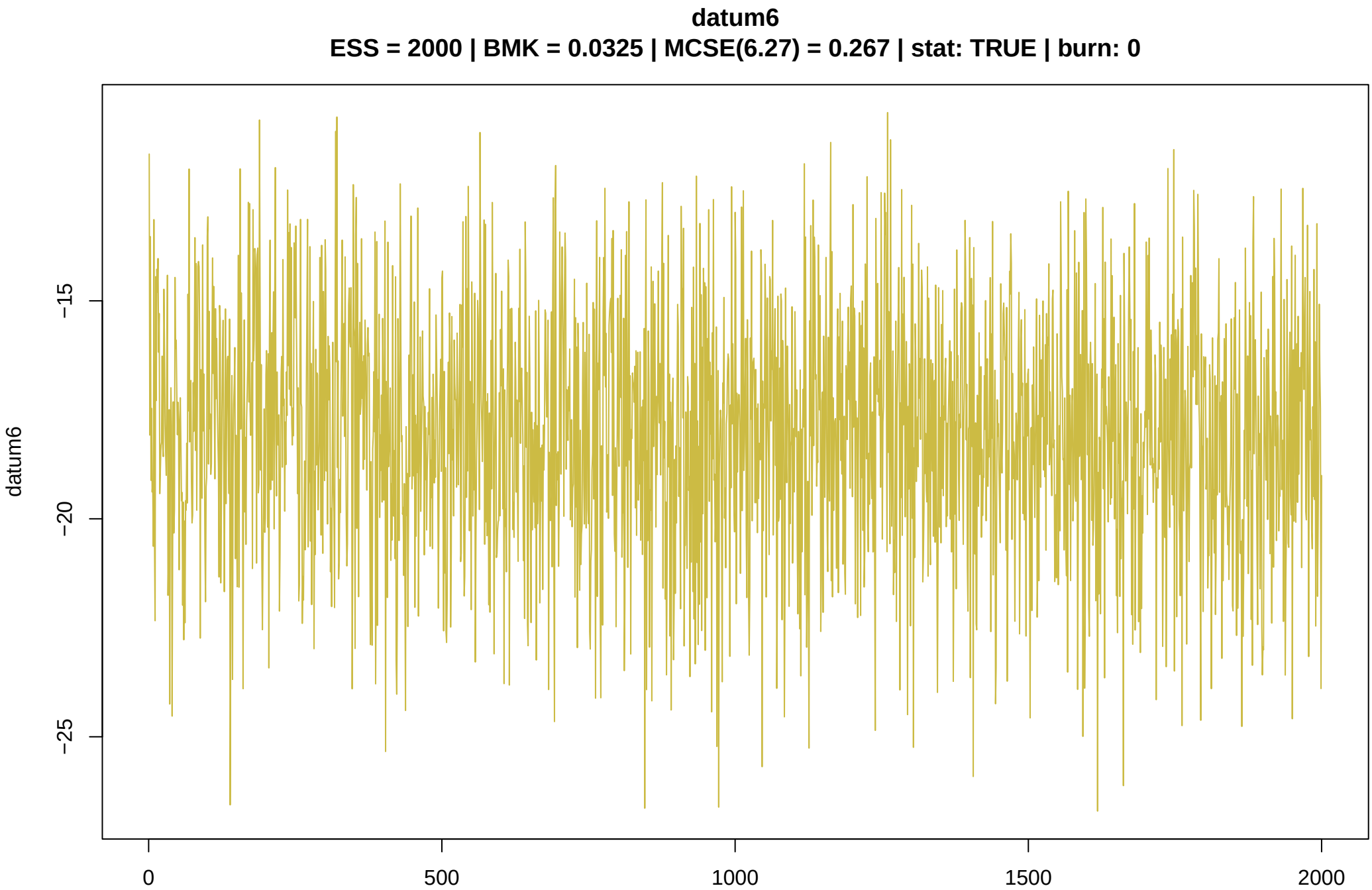

datum1
ESS = 2000 | BMK = 0.0475 | MCSE(6.27) = 0.284 | stat: TRUE | burn: 0
datum1
−10
−15
−20
−25
0
500
1000
1500
2000

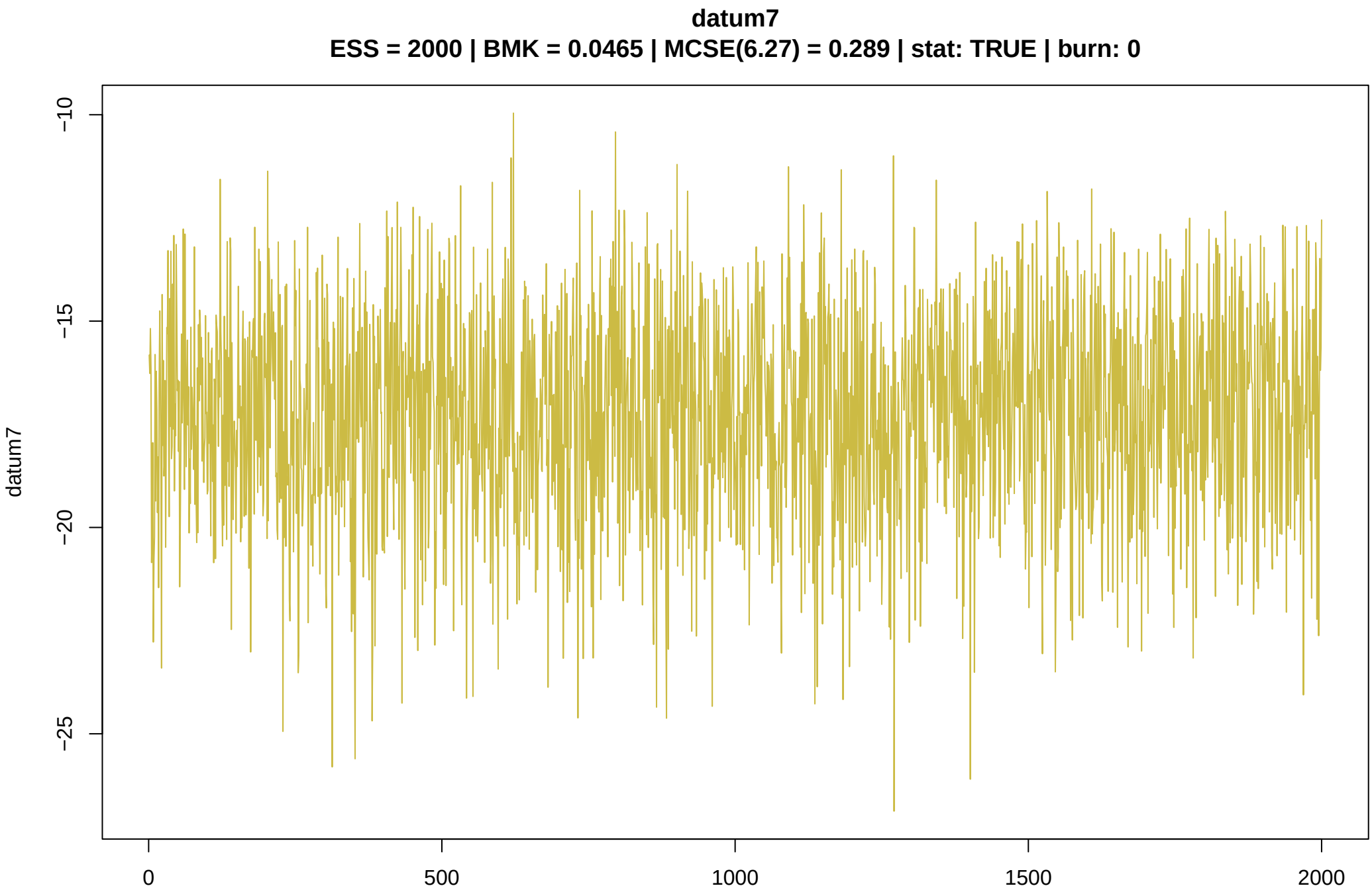

datum2
ESS = 2000 | BMK = 0.0435 | MCSE(6.27) = 0.262 | stat: TRUE | burn: 0
datum2
−15
−20
−25
−30
0
500
1000
1500
2000

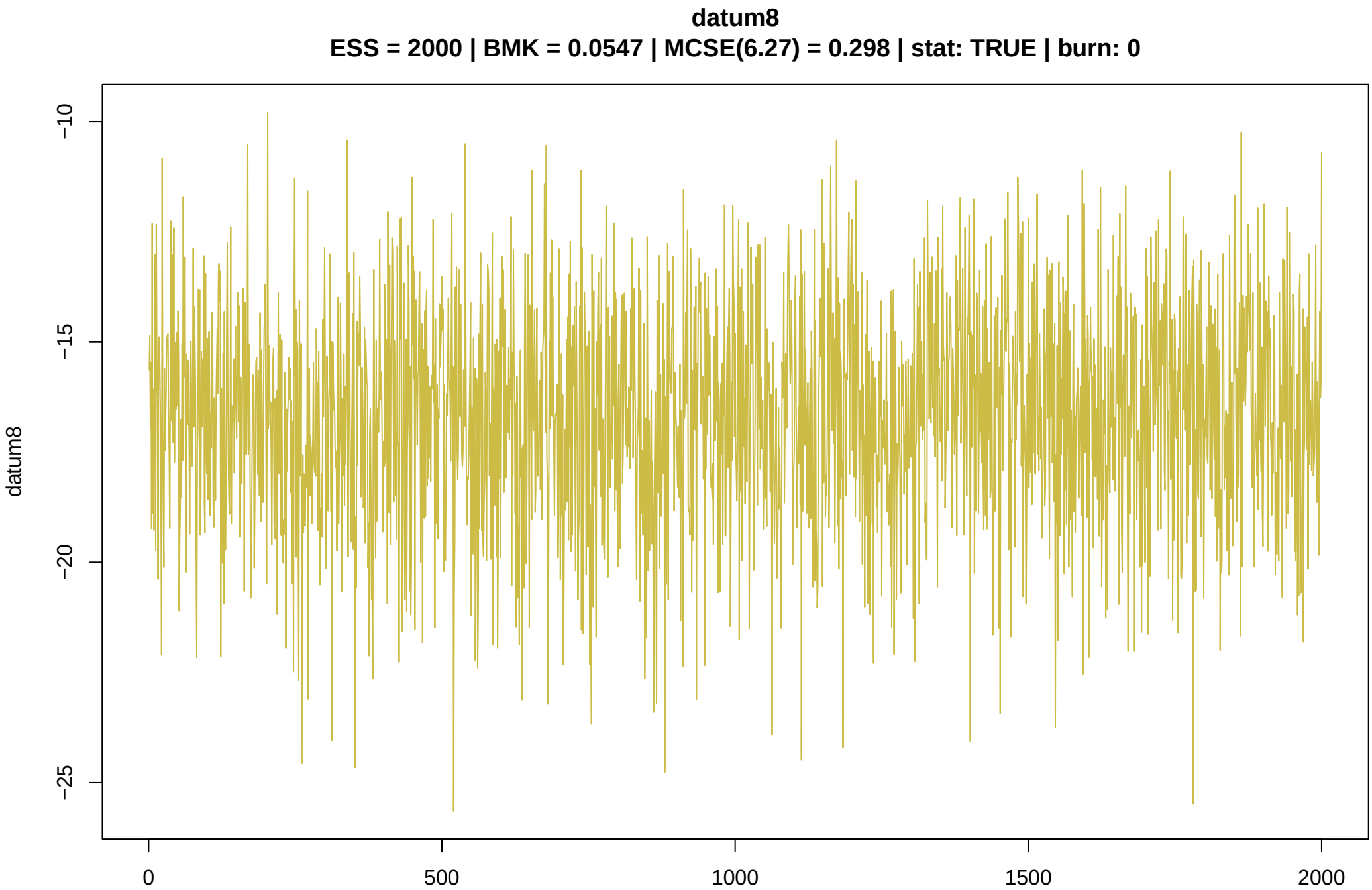

datum3
ESS = 1530 | BMK = 0.0334 | MCSE(6.27) = 0.278 | stat: TRUE | burn: 0
datum3
−15
−20
−25
0
500
1000
1500
2000

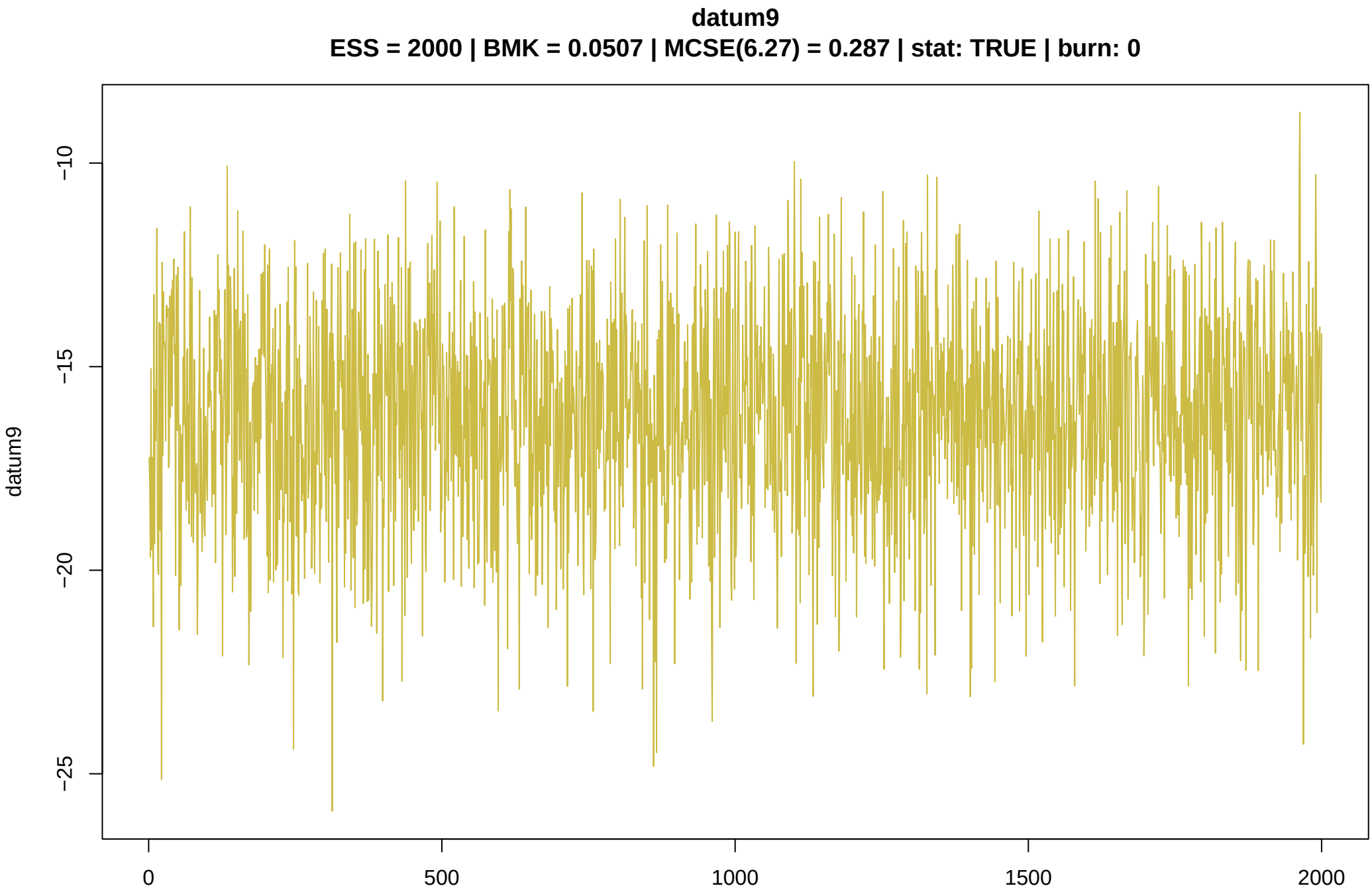

datum4
ESS = 2000 | BMK = 0.0427 | MCSE(6.27) = 0.304 | stat: FALSE | burn: 0
datum4
−10
−15
−20
0
500
1000
1500
2000

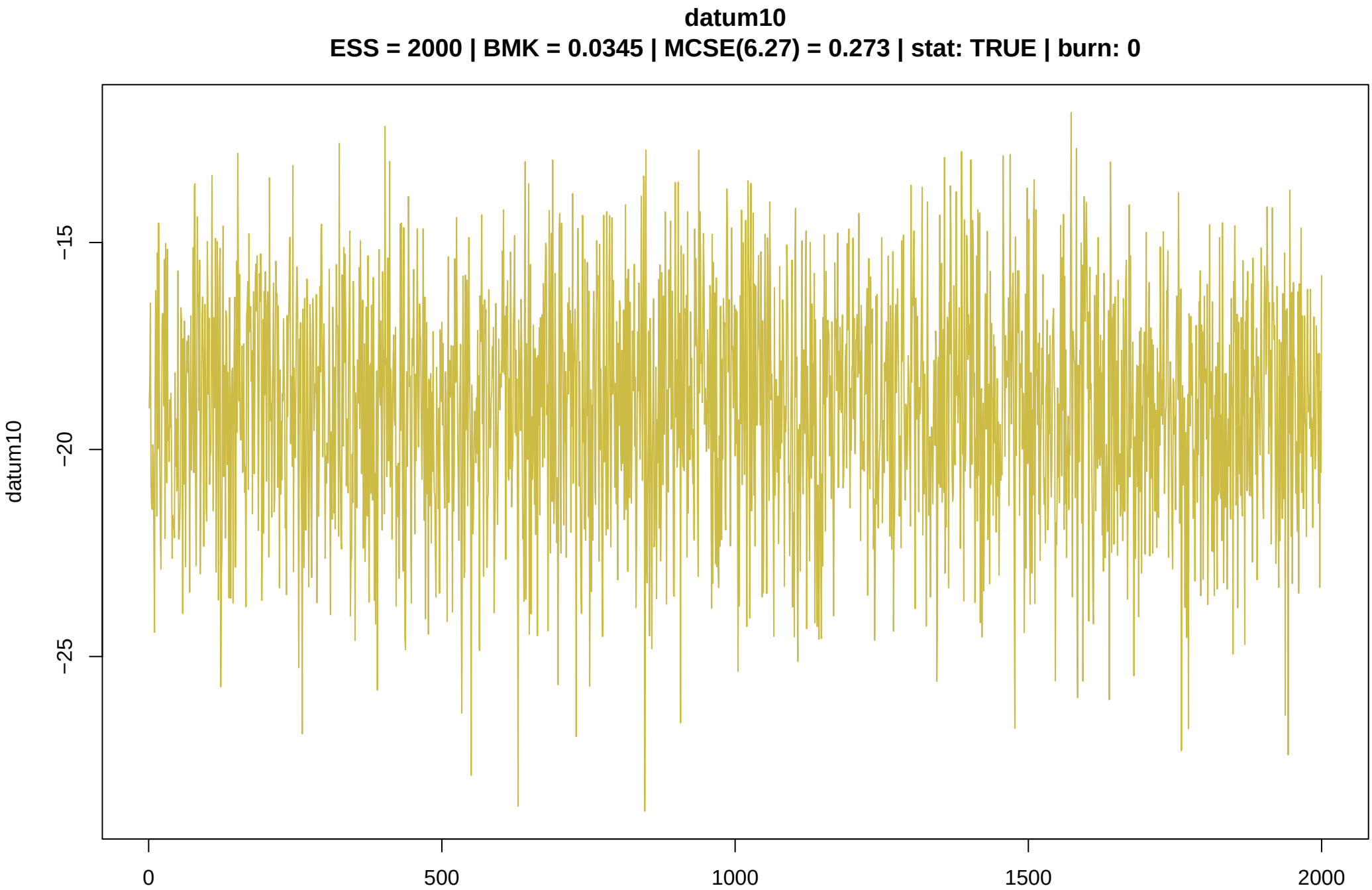

datum5
ESS = 2000 | BMK = 0.0304 | MCSE(6.27) = 0.265 | stat: TRUE | burn: 0
datum5
−10
−15
−20
−25
0
500
1000
1500
2000

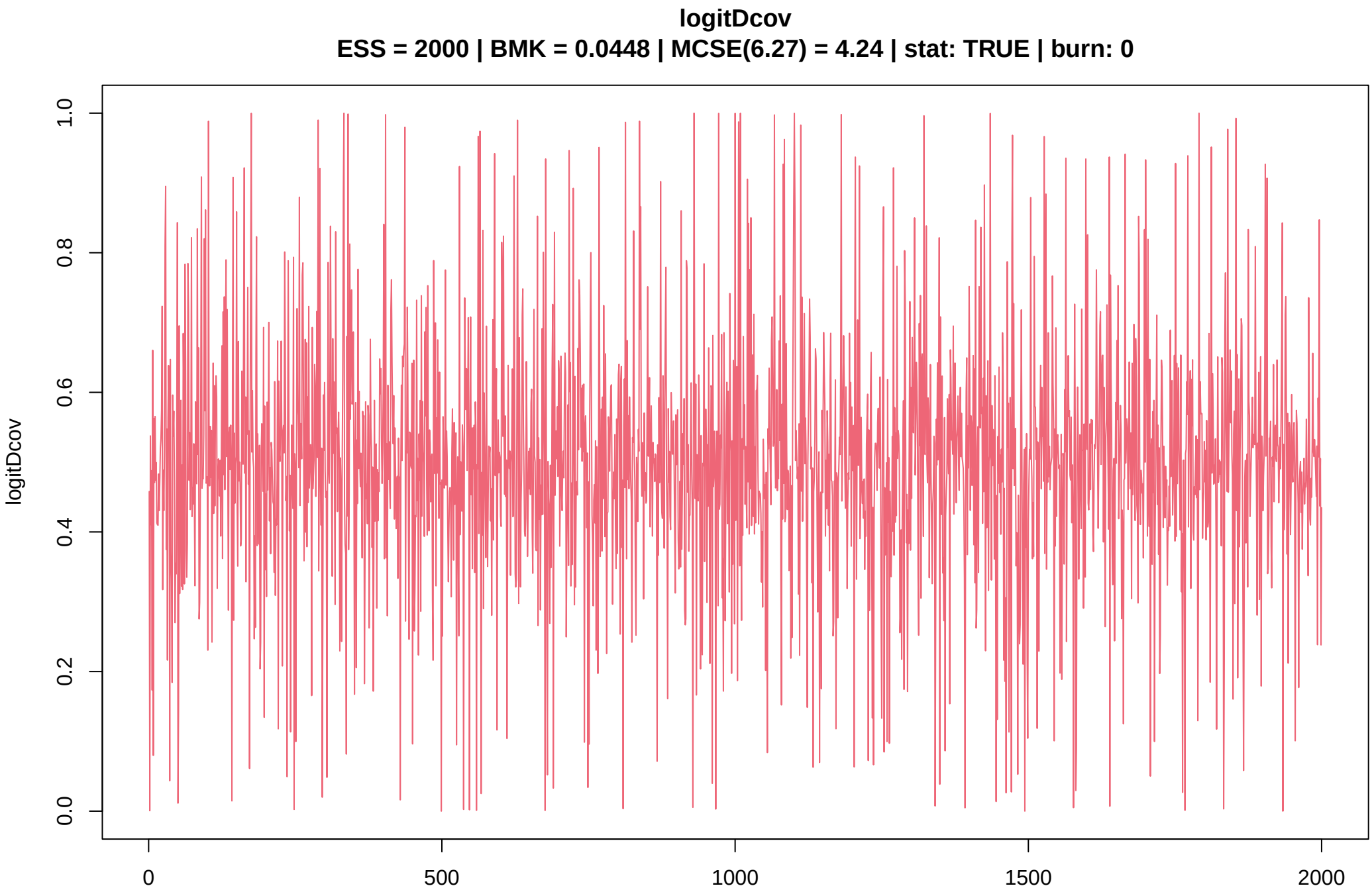

datum6
ESS = 2000 | BMK = 0.0325 | MCSE(6.27) = 0.267 | stat: TRUE | burn: 0
datum6
−15
−20
−25
0
500
1000
1500
2000

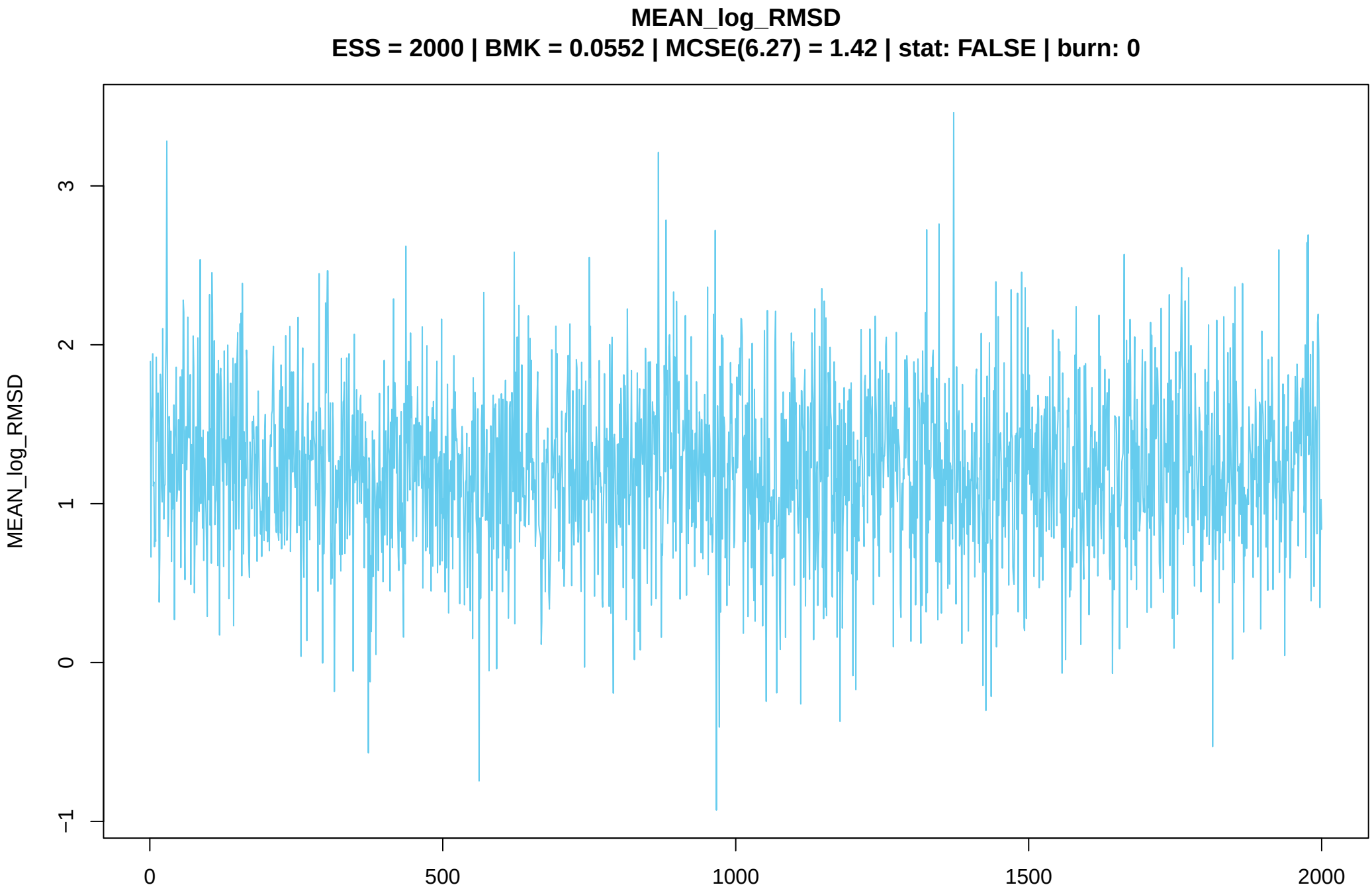

datum7
ESS = 2000 | BMK = 0.0465 | MCSE(6.27) = 0.289 | stat: TRUE | burn: 0
datum7
−10
−15
−20
−25
0
500
1000
1500
2000

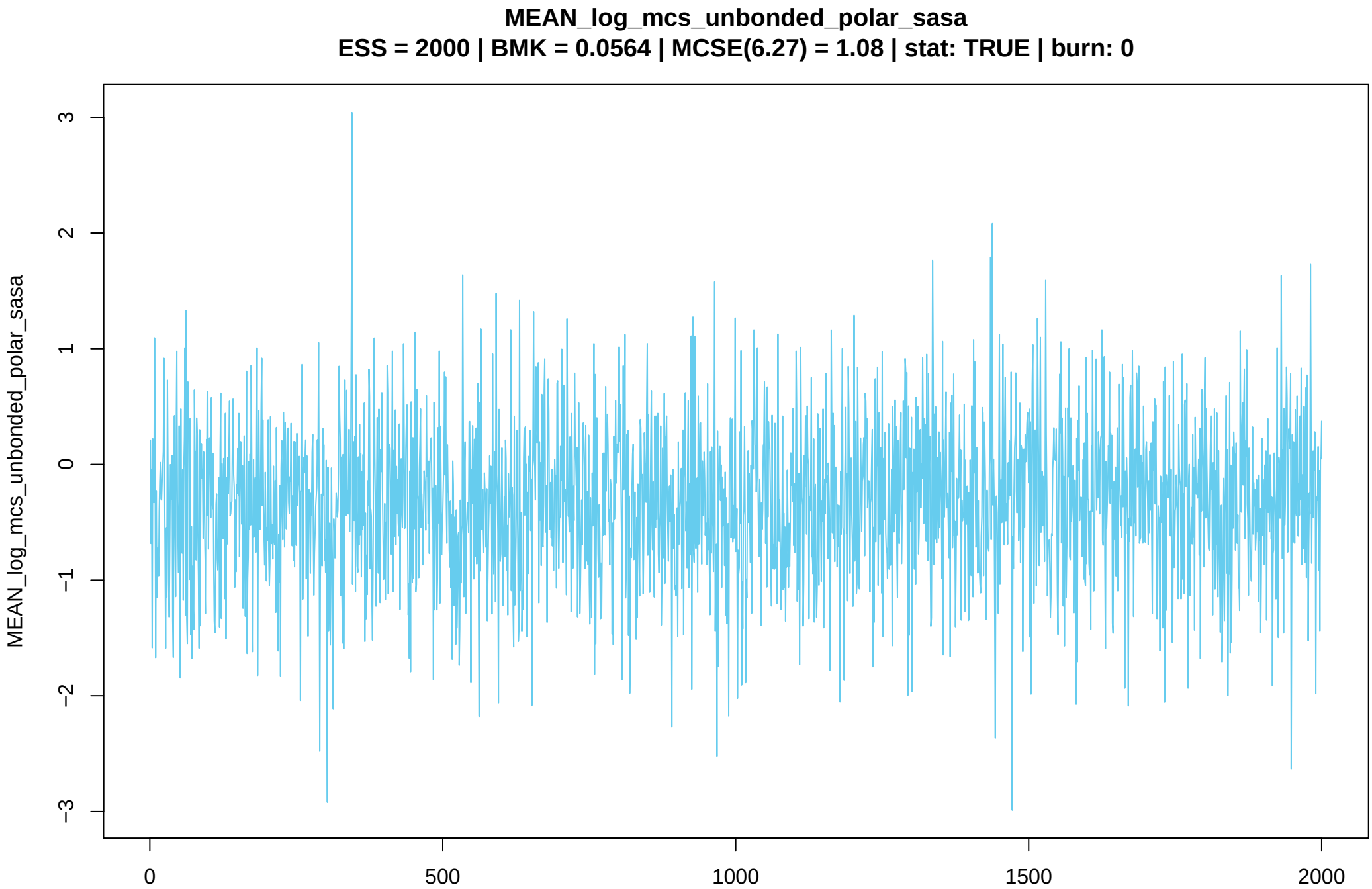

datum8
ESS = 2000 | BMK = 0.0547 | MCSE(6.27) = 0.298 | stat: TRUE | burn: 0
datum8
−10
−15
−20
−25
0
500
1000
1500
2000

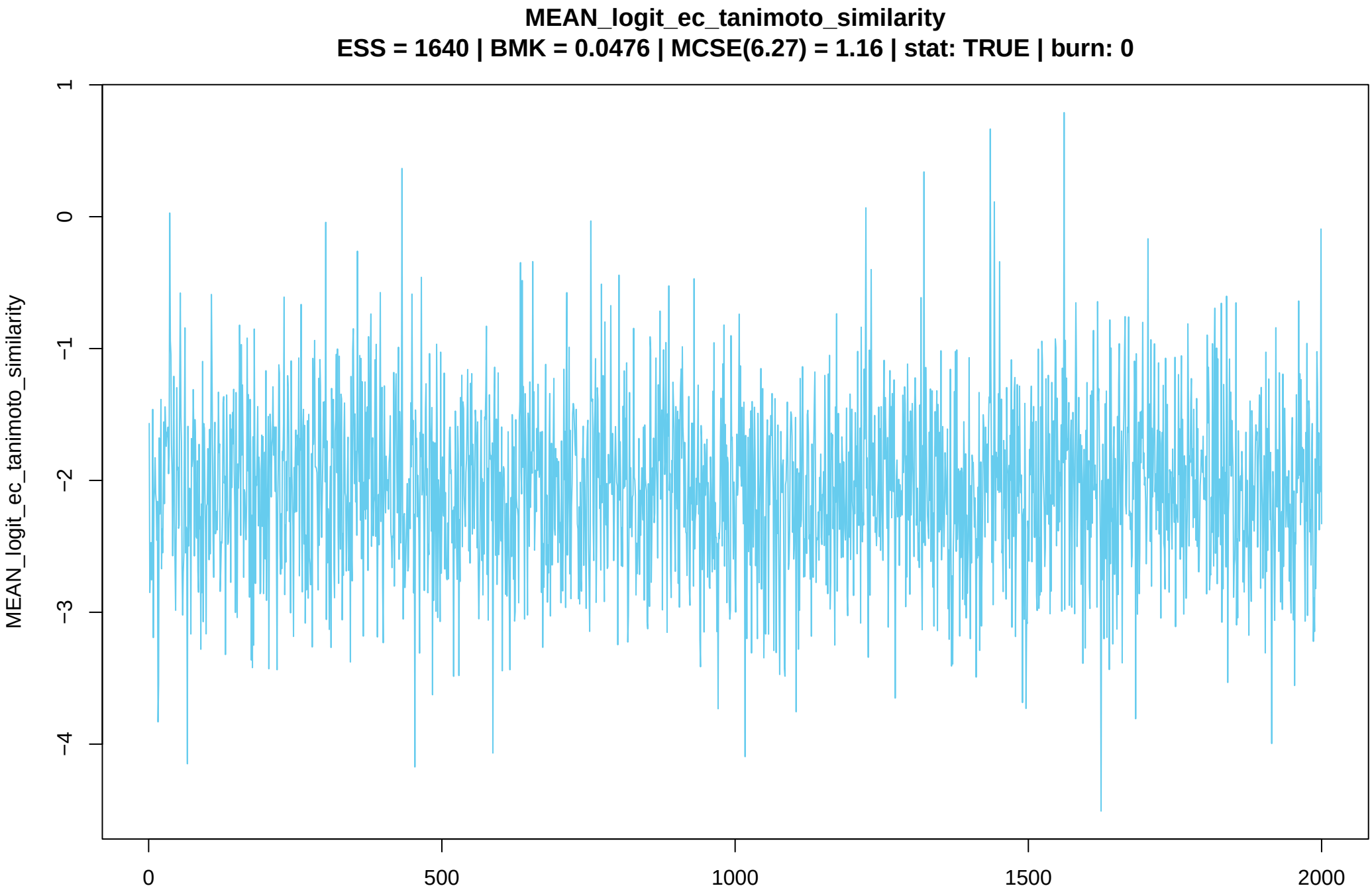

datum9
ESS = 2000 | BMK = 0.0507 | MCSE(6.27) = 0.287 | stat: TRUE | burn: 0
datum9
−10
−15
−20
−25
0
500
1000
1500
2000

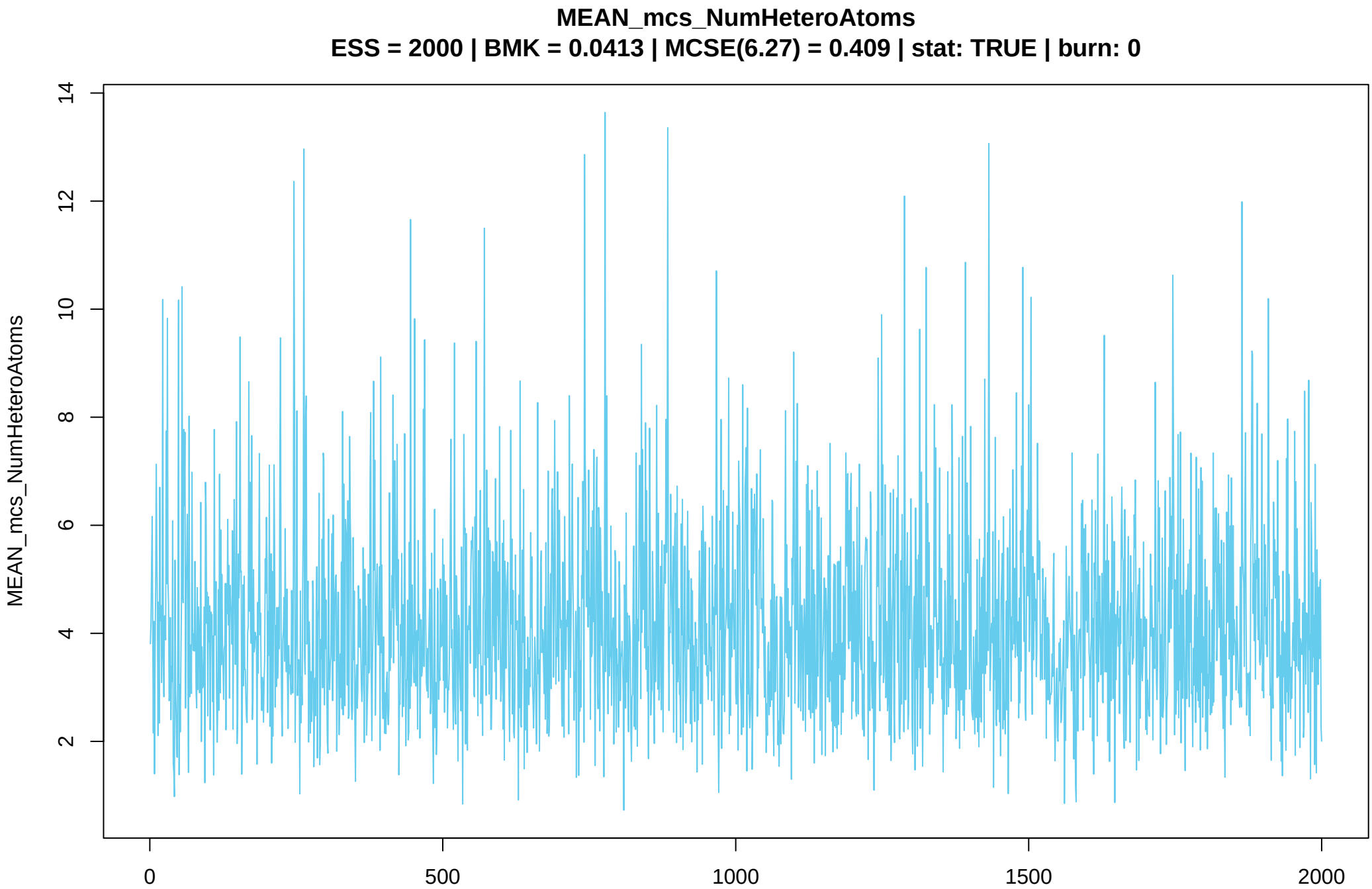

datum10
ESS = 2000 | BMK = 0.0345 | MCSE(6.27) = 0.273 | stat: TRUE | burn: 0
datum10
−15
−20
−25
0
500
1000
1500
2000

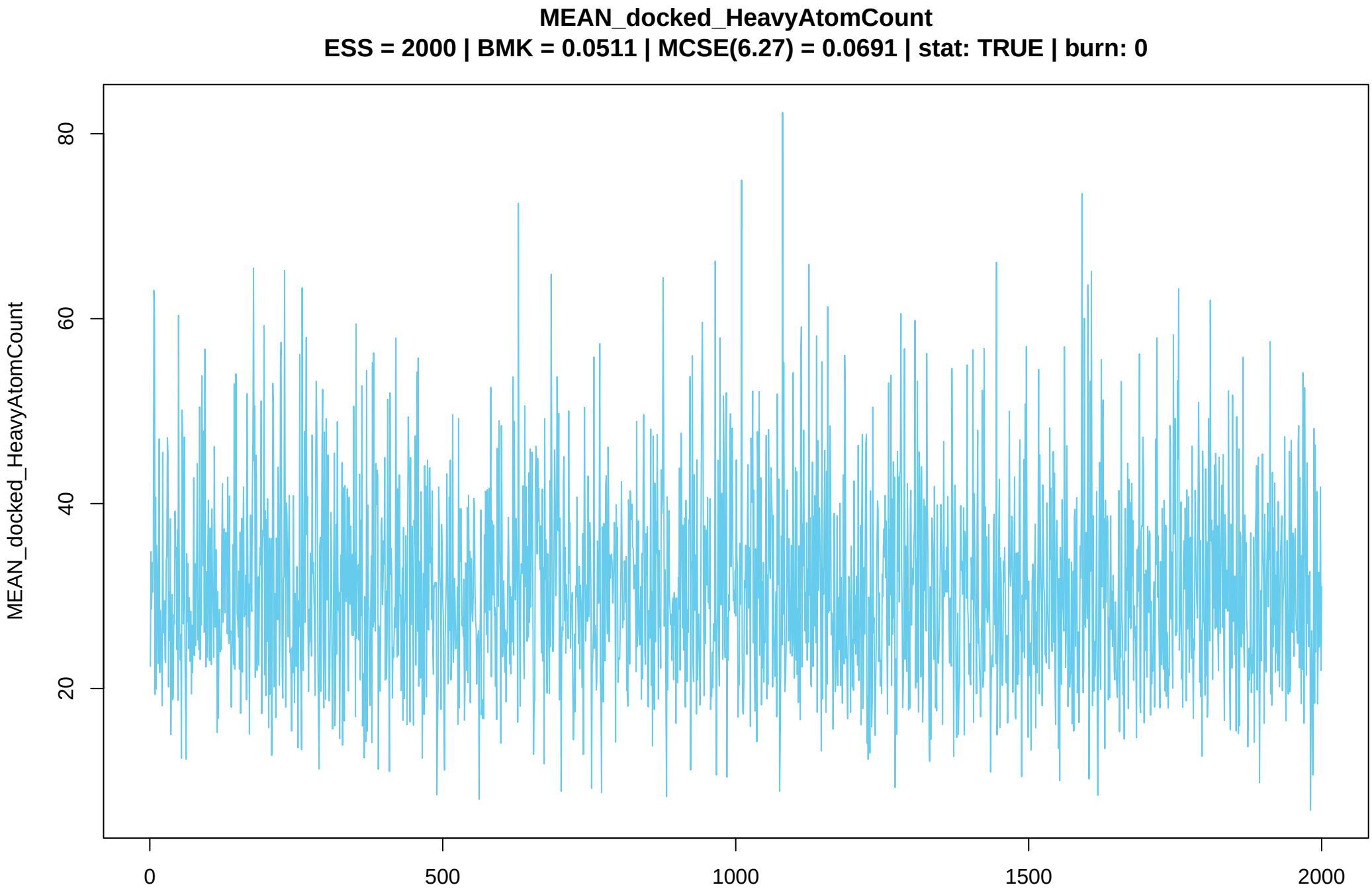

logitDcov
ESS = 2000 | BMK = 0.0448 | MCSE(6.27) = 4.24 | stat: TRUE | burn: 0
logitDcov
0.0
0.2
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

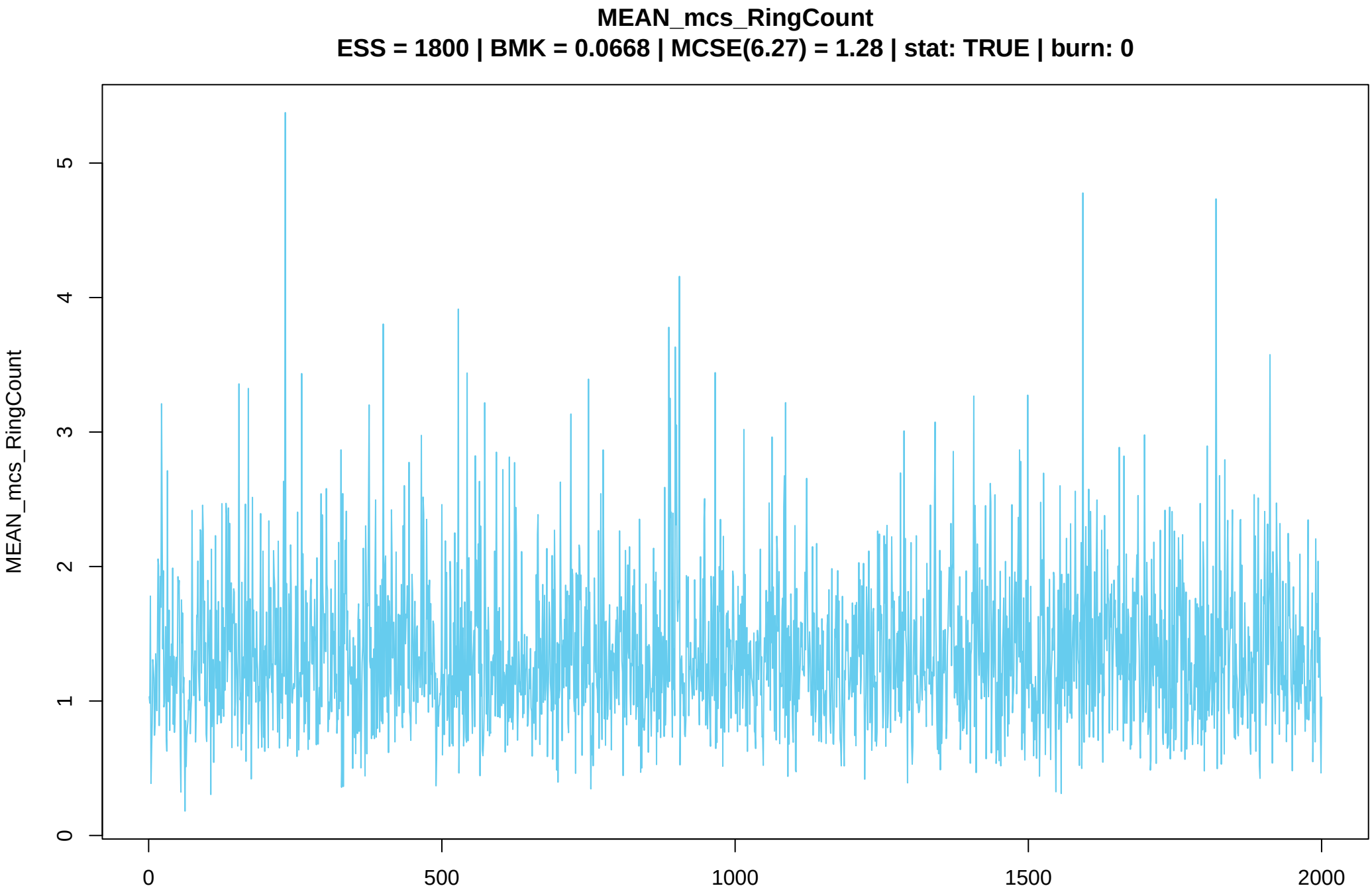

MEAN_log_RMSD
ESS = 2000 | BMK = 0.0552 | MCSE(6.27) = 1.42 | stat: FALSE | burn: 0
MEAN_log_RMSD
−1
0
1
2
3
0
500
1000
1500
2000

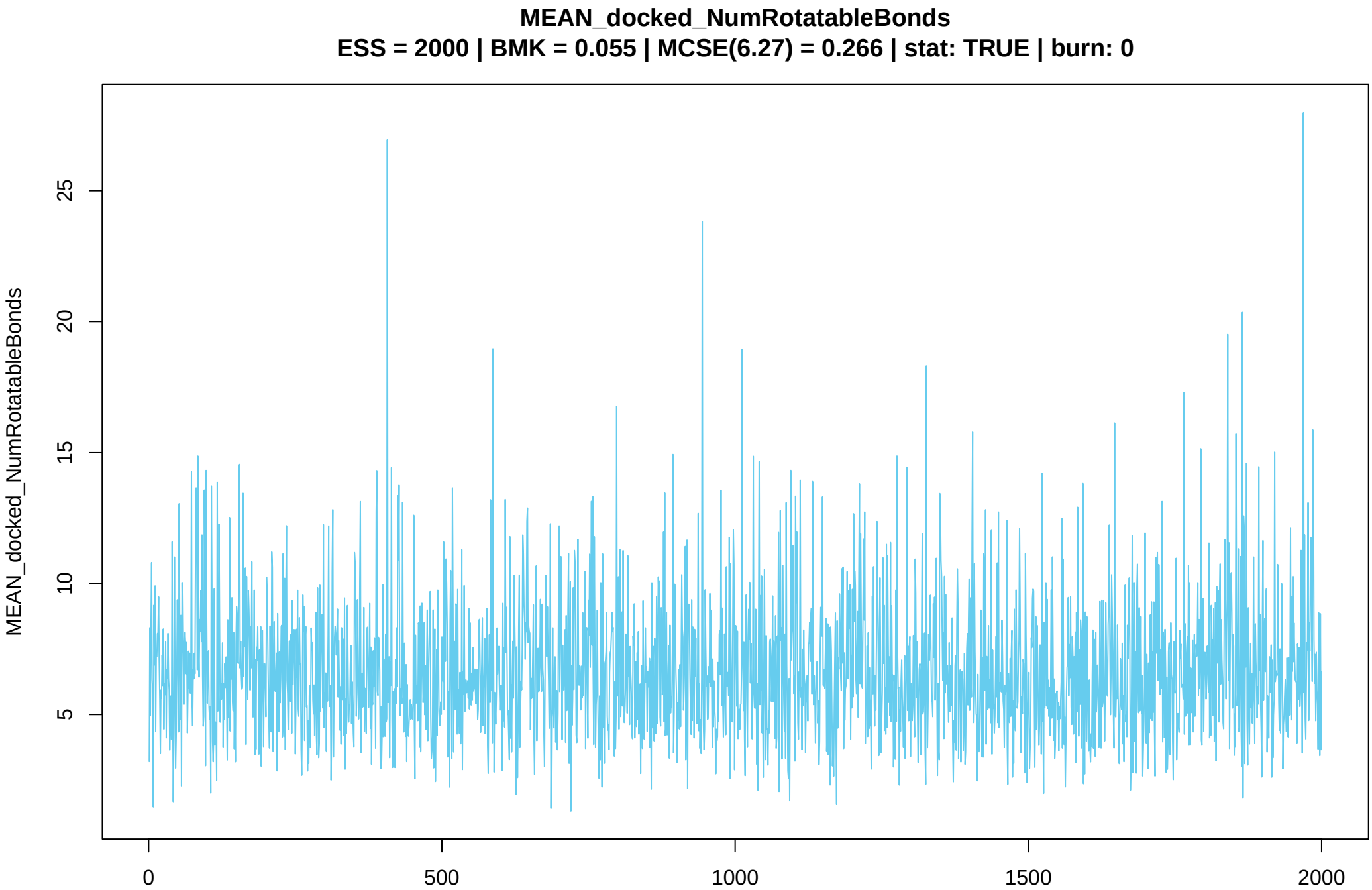

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0564 | MCSE(6.27) = 1.08 | stat: TRUE | burn: 0
MEAN_log_mcs_unbonded_polar_sasa
3
2
1
0
−1
−2
−3
0
500
1000
1500
2000

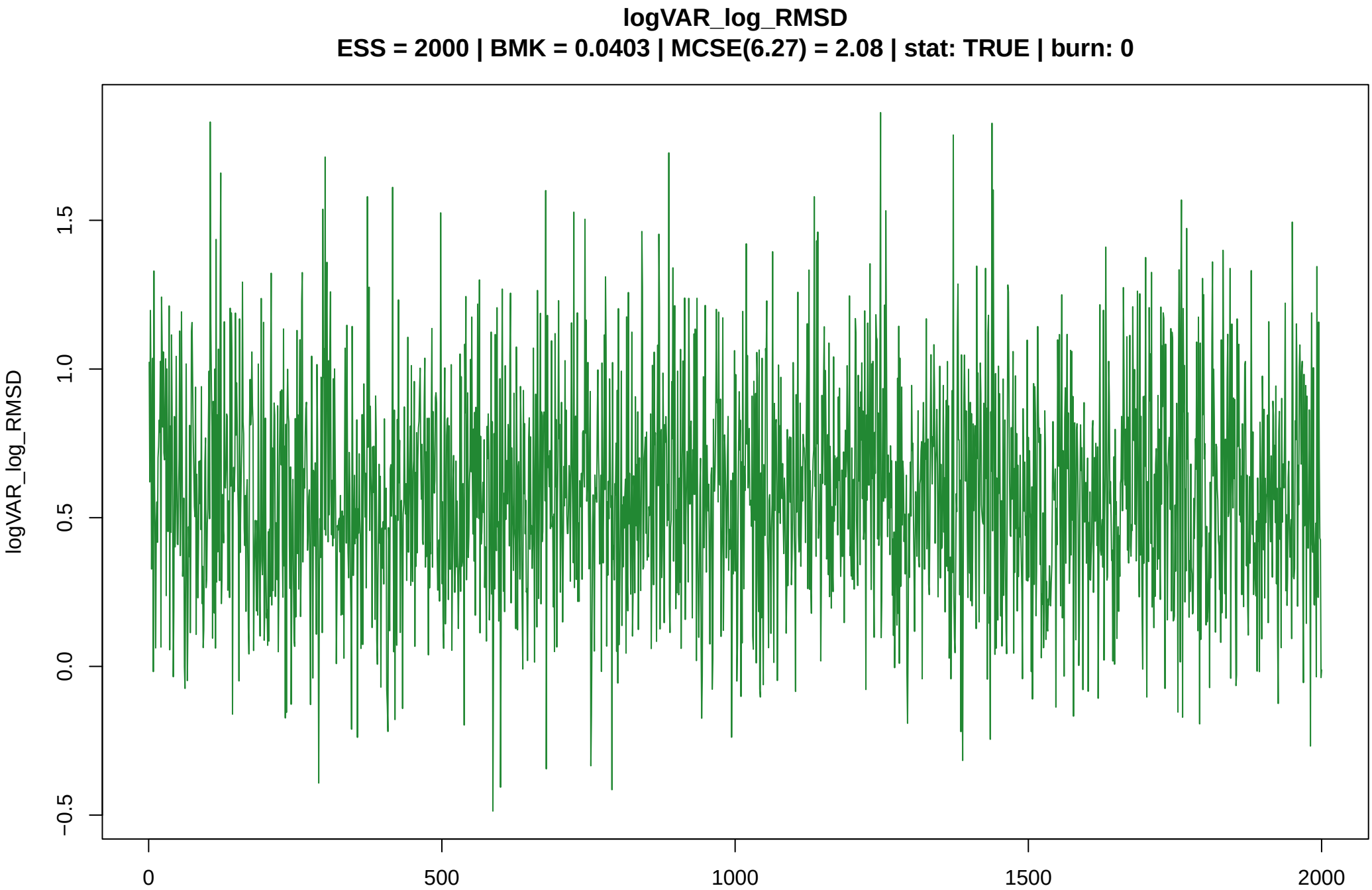

MEAN_logit_ec_tanimoto_similarity
ESS = 1640 | BMK = 0.0476 | MCSE(6.27) = 1.16 | stat: TRUE | burn: 0
MEAN_logit_ec_tanimoto_similarity
1
0
−1
−2
−3
−4
0
500
1000
1500
2000

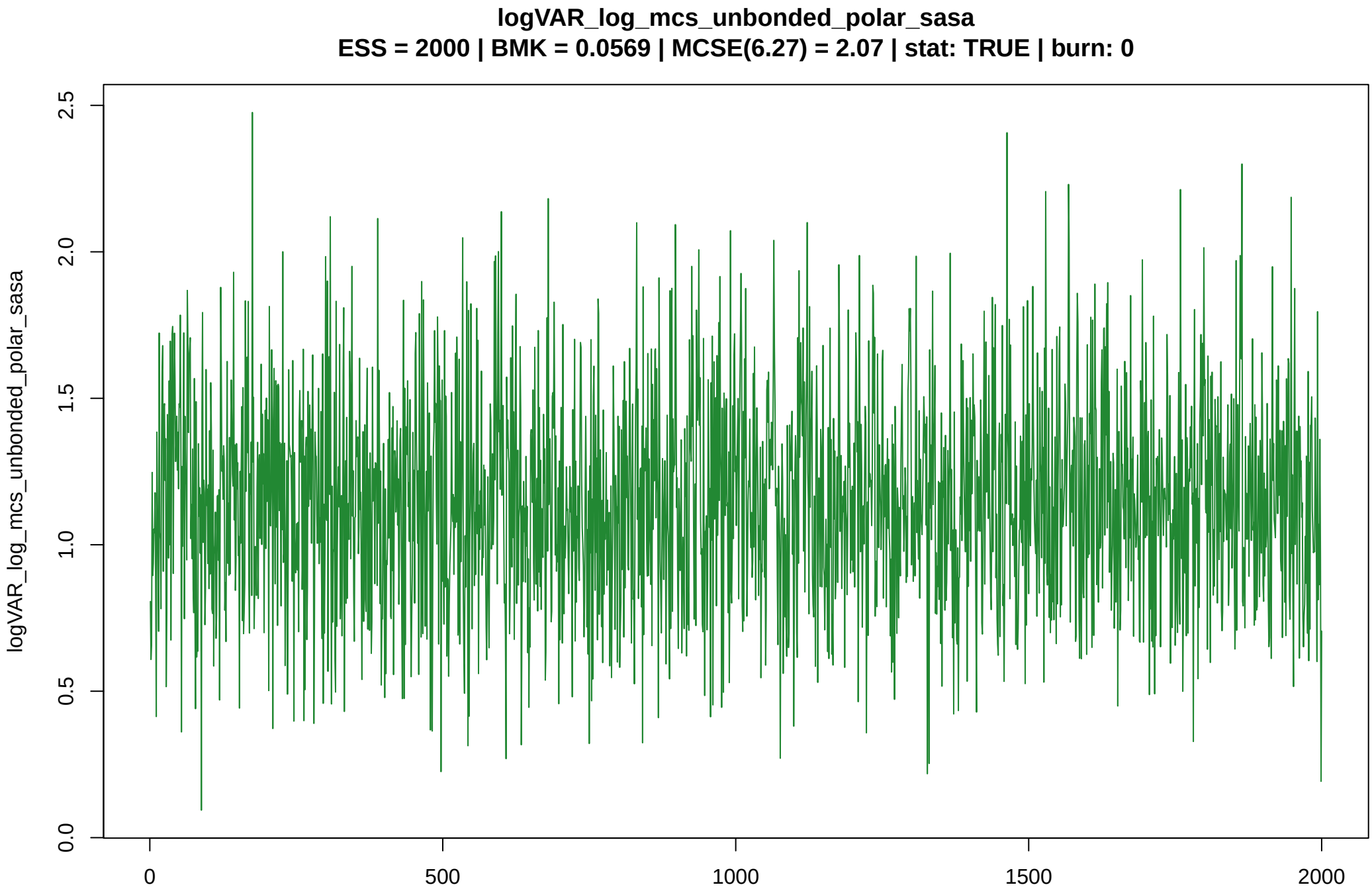

MEAN_mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0413 | MCSE(6.27) = 0.409 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
2
4
6
8
10
12
14
0
500
1000
1500
2000

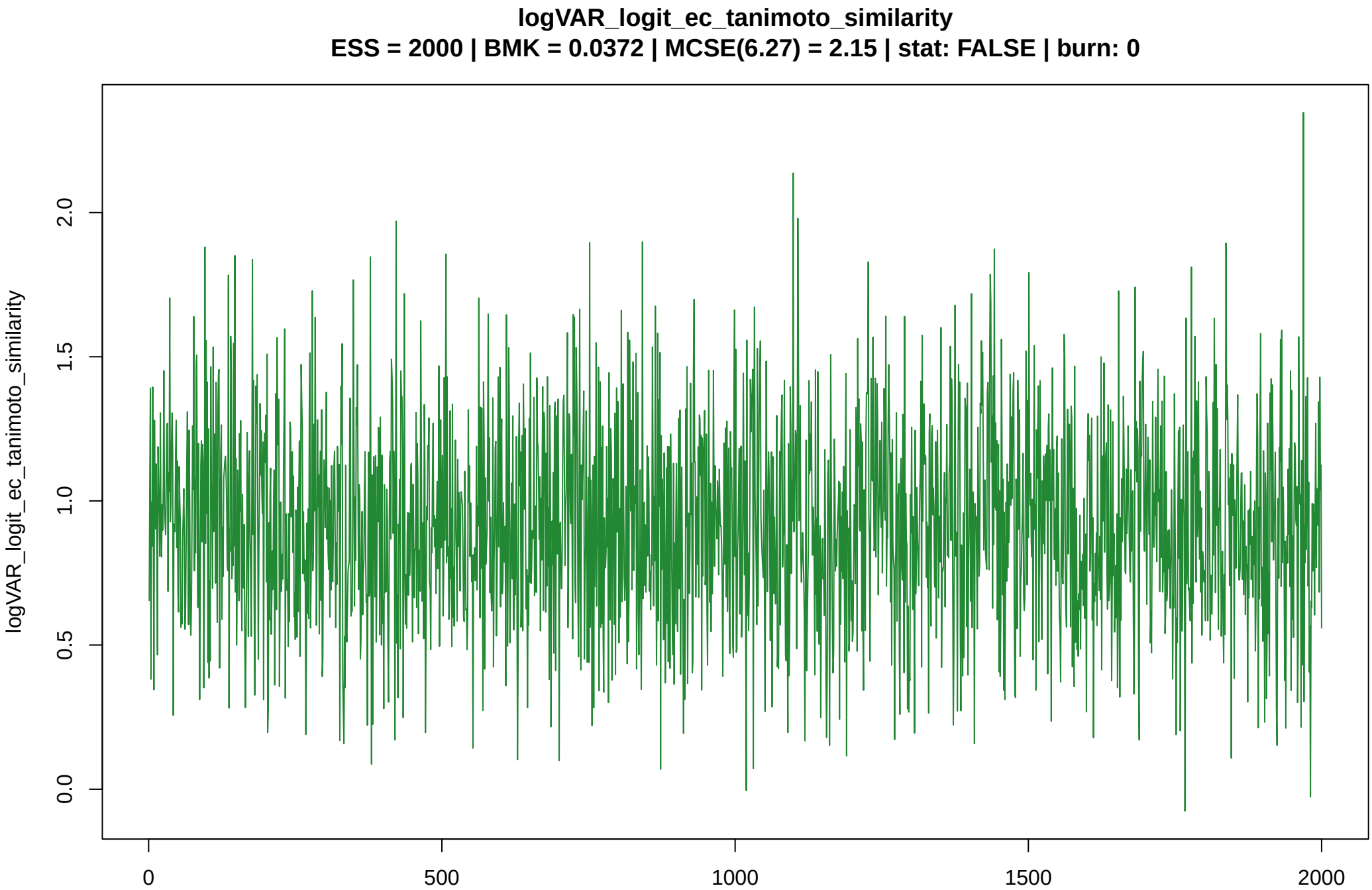

MEAN_docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0511 | MCSE(6.27) = 0.0691 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
20
40
60
80
0
500
1000
1500
2000

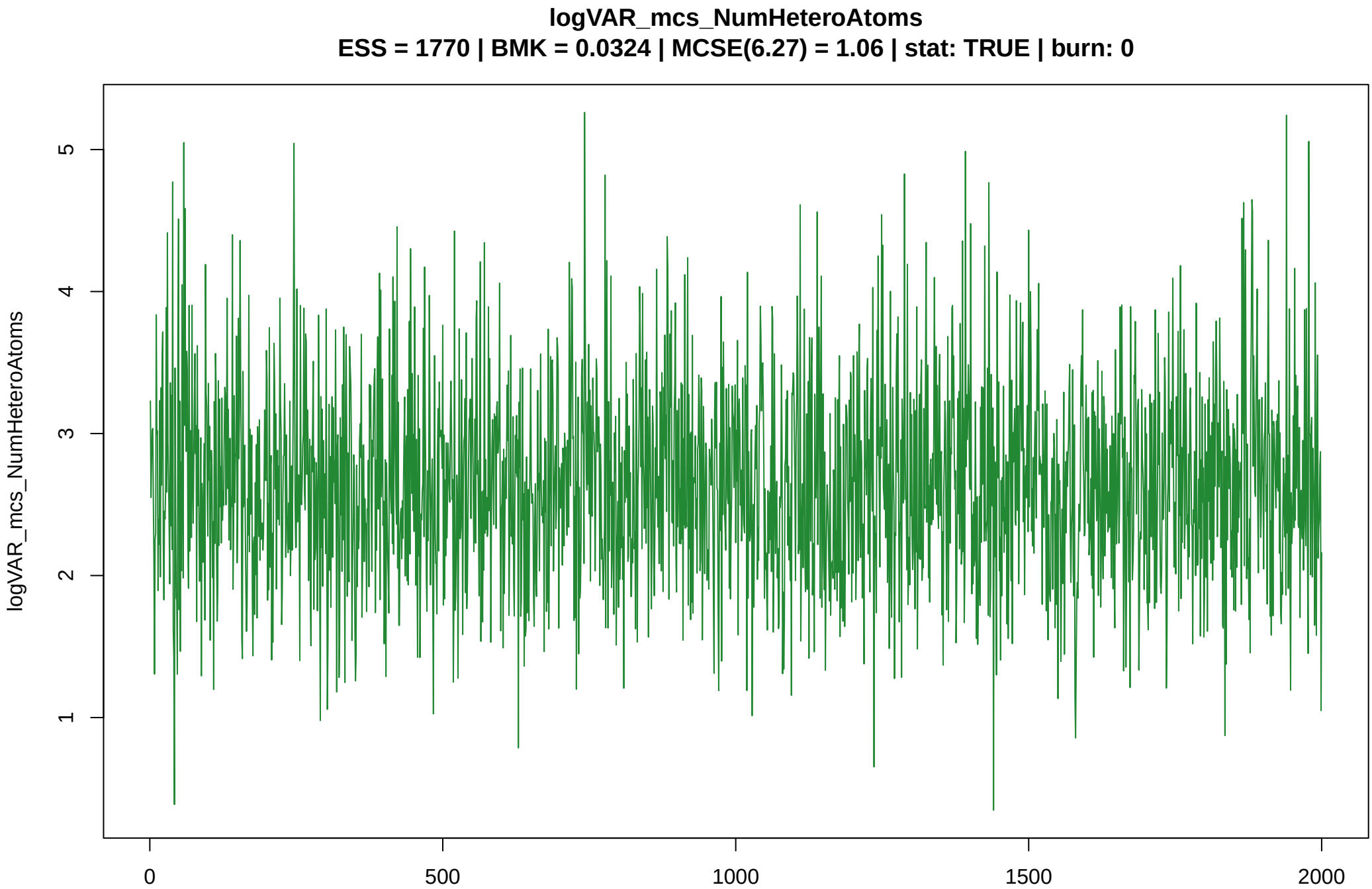

MEAN_mcs_RingCount
ESS = 1800 | BMK = 0.0668 | MCSE(6.27) = 1.28 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0
1
2
3
4
5
0
500
1000
1500
2000

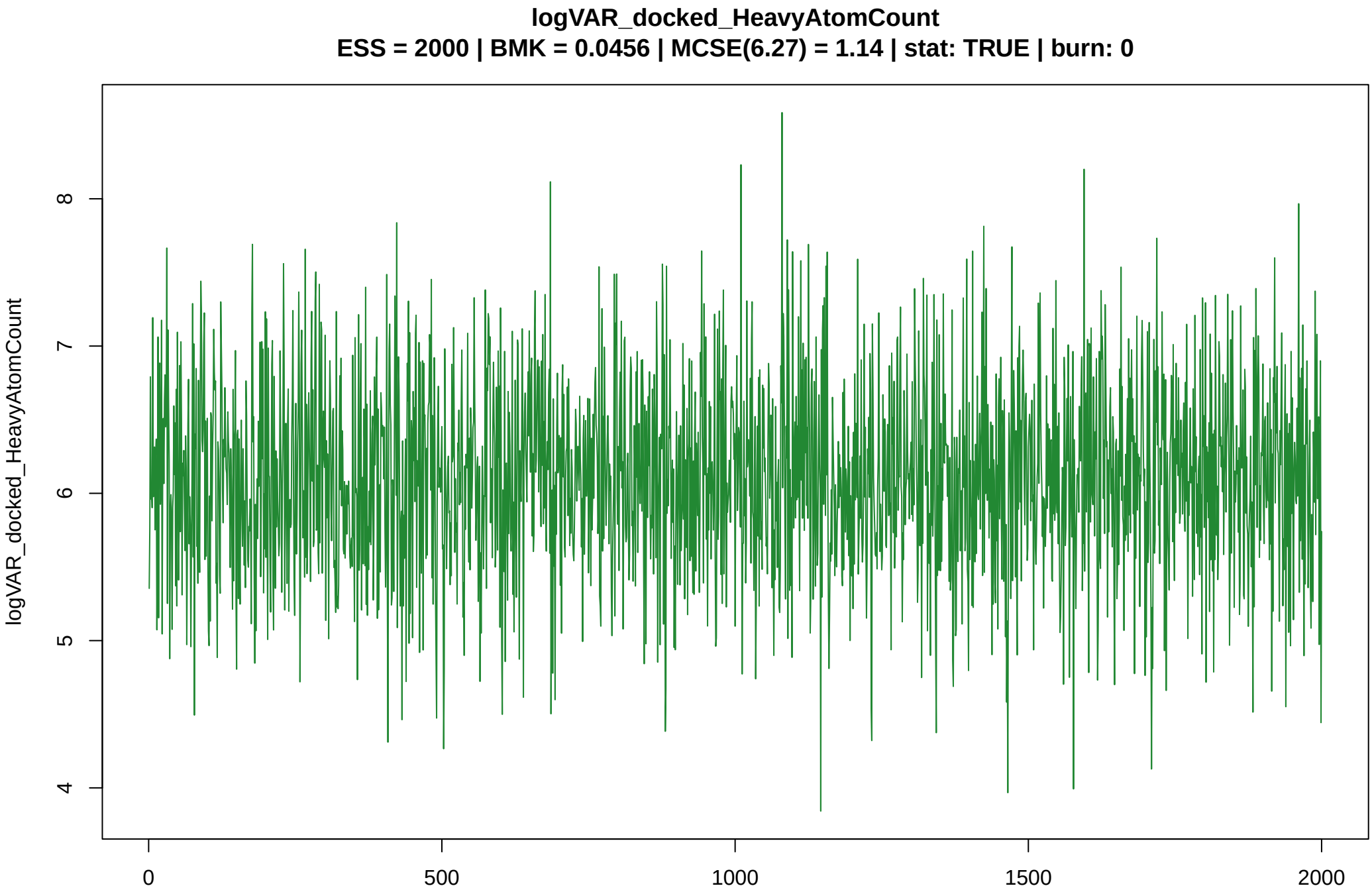

MEAN_docked_NumRotatableBonds
ESS = 2000 | BMK = 0.055 | MCSE(6.27) = 0.266 | stat: TRUE | burn: 0
MEAN_docked_NumRotatableBonds
5
10
15
20
25
0
500
1000
1500
2000

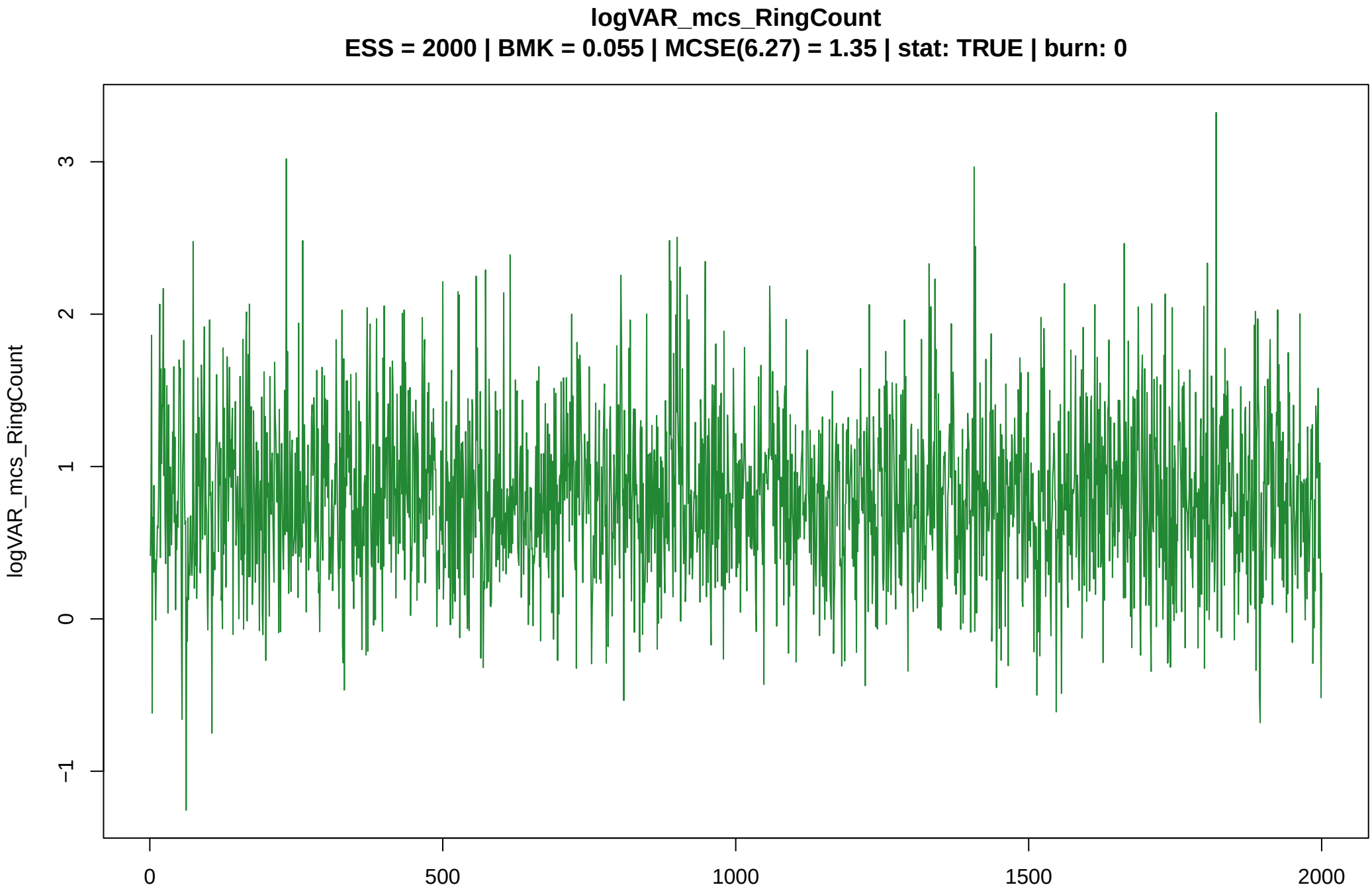

logVAR_log_RMSD
ESS = 2000 | BMK = 0.0403 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0
logVAR_log_RMSD
−0.5
0.0
0.5
1.0
1.5
0
500
1000
1500
2000

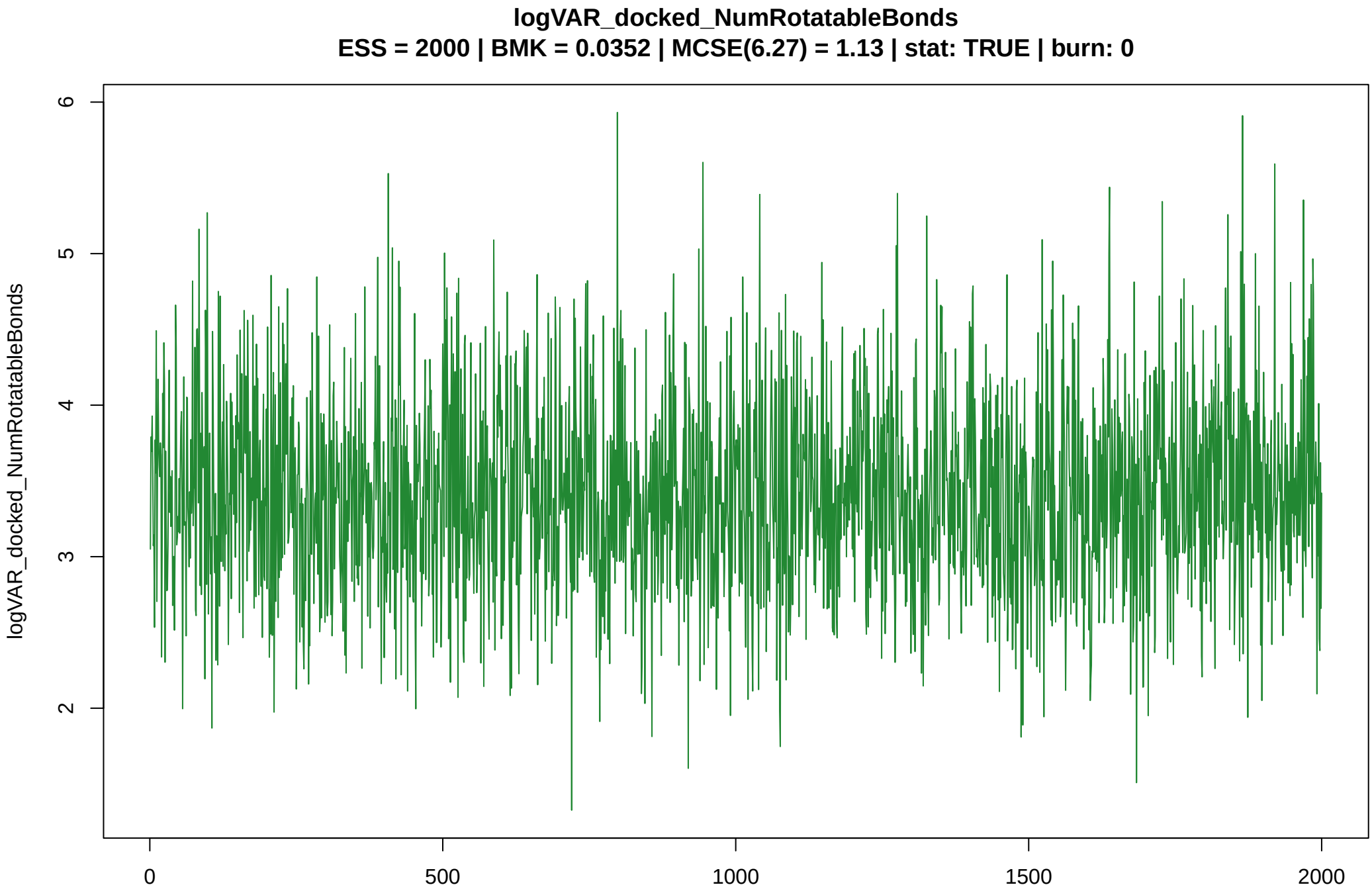

logVAR_log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0569 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0
logVAR_log_mcs_unbonded_polar_sasa
0.0
0.5
1.0
1.5
2.0
2.5
0
500
1000
1500
2000

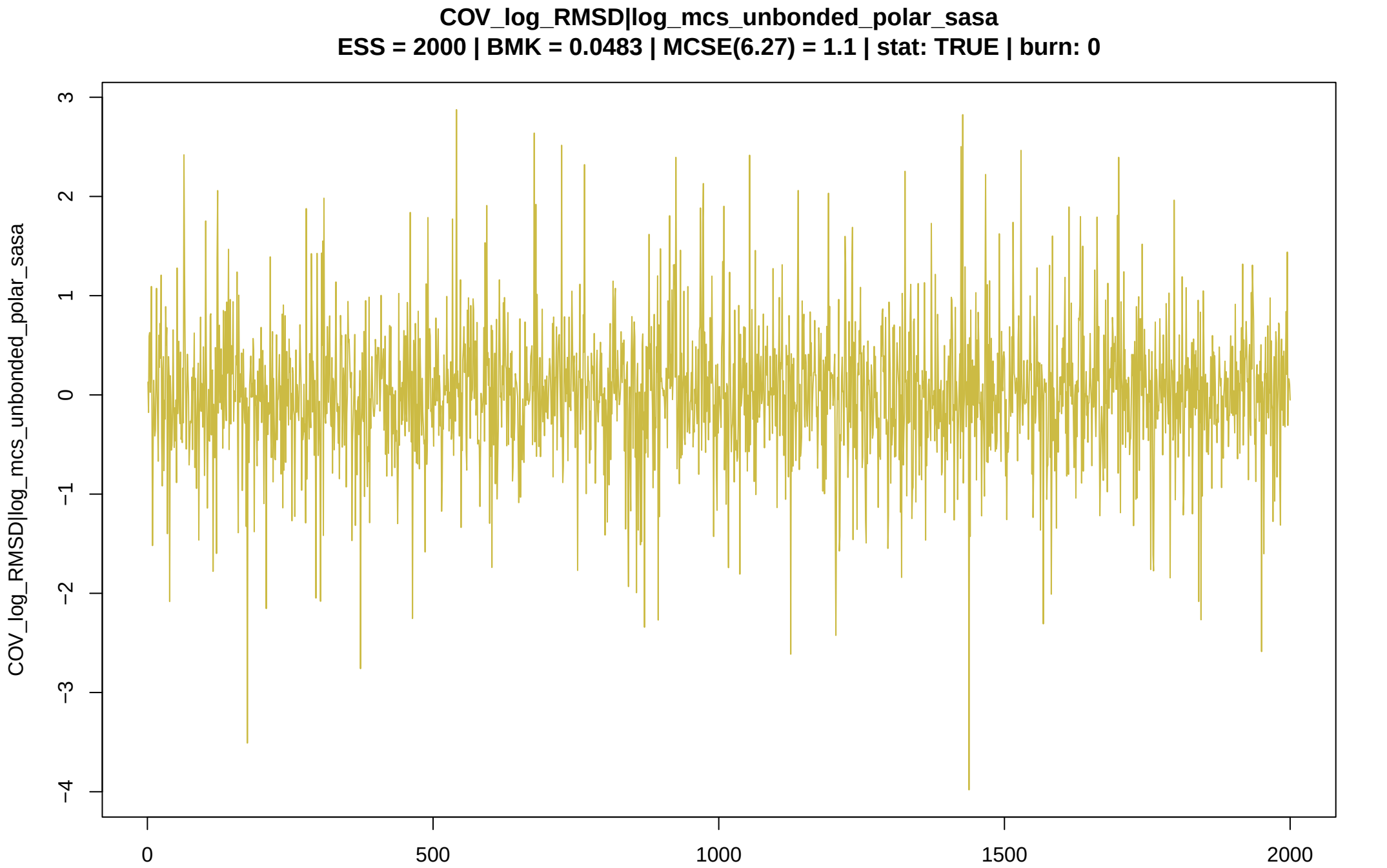

logVAR_logit_ec_tanimoto_similarity
ESS = 2000 | BMK = 0.0372 | MCSE(6.27) = 2.15 | stat: FALSE | burn: 0
logVAR_logit_ec_tanimoto_similarity
0.0
0.5
1.0
1.5
2.0
0
500
1000
1500
2000

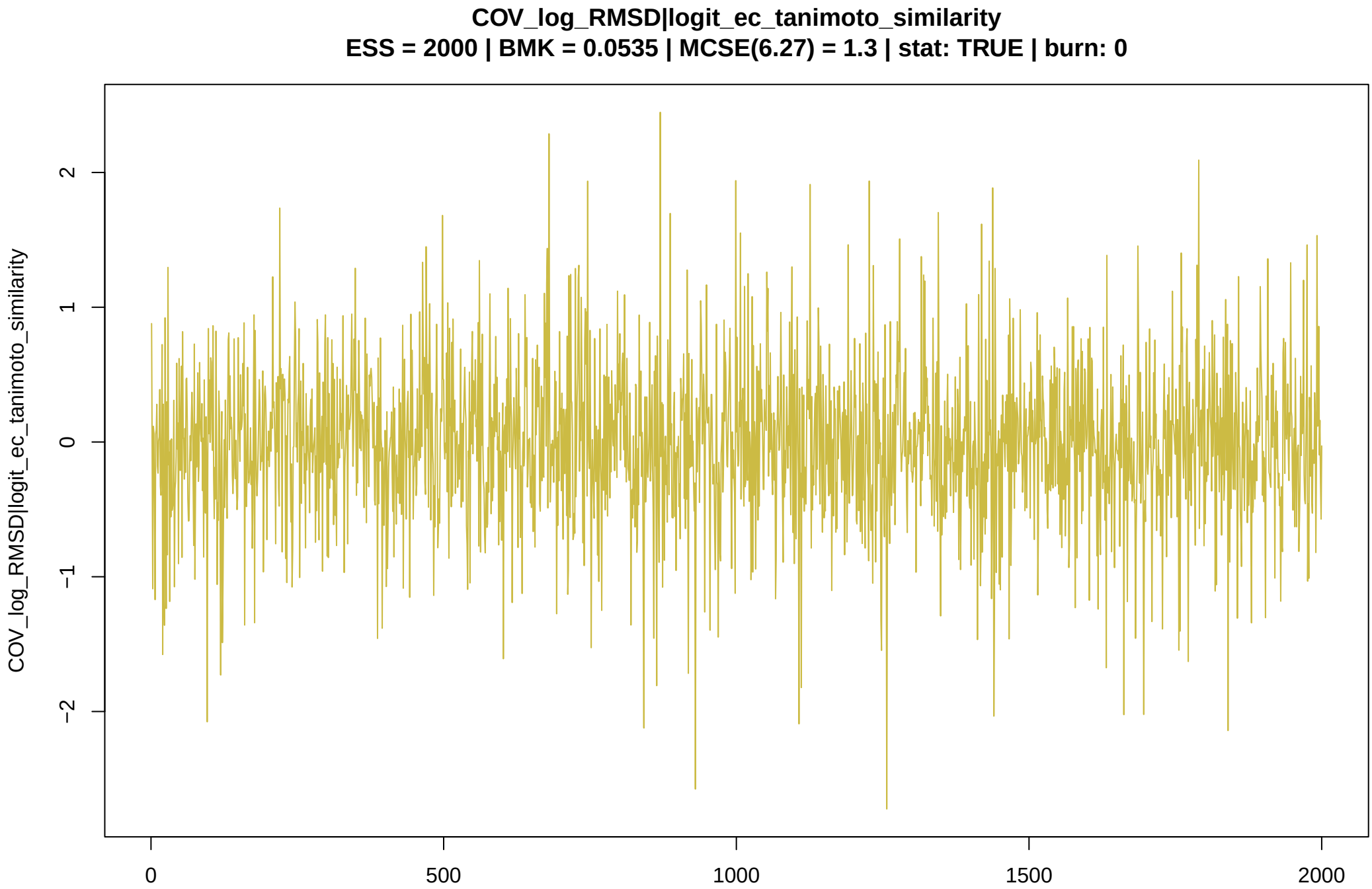

logVAR_mcs_NumHeteroAtoms
ESS = 1770 | BMK = 0.0324 | MCSE(6.27) = 1.06 | stat: TRUE | burn: 0
logVAR_mcs_NumHeteroAtoms
1
2
3
4
5
0
500
1000
1500
2000

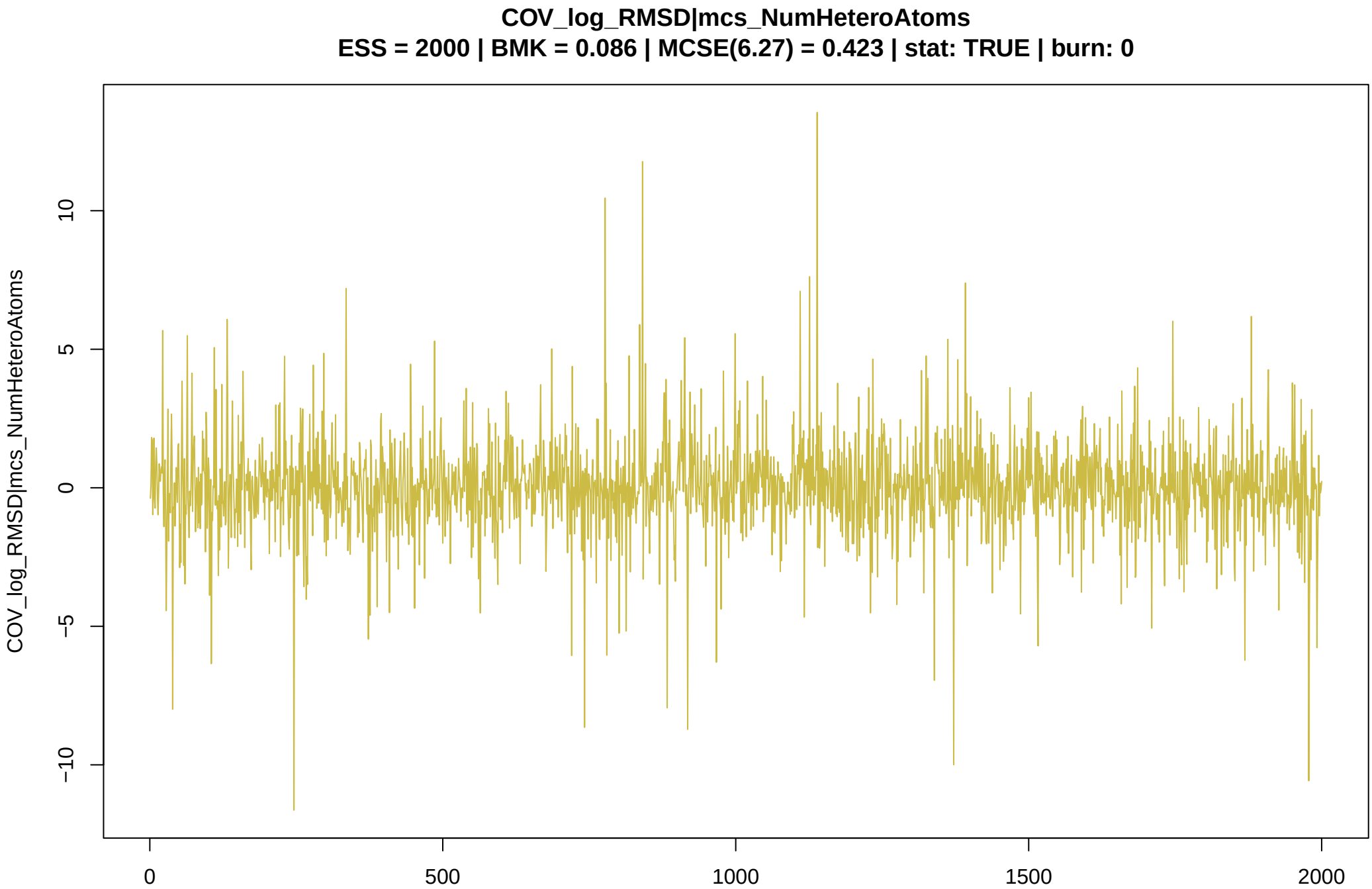

logVAR_docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0456 | MCSE(6.27) = 1.14 | stat: TRUE | burn: 0
logVAR_docked_HeavyAtomCount
4
5
6
7
8
0
500
1000
1500
2000

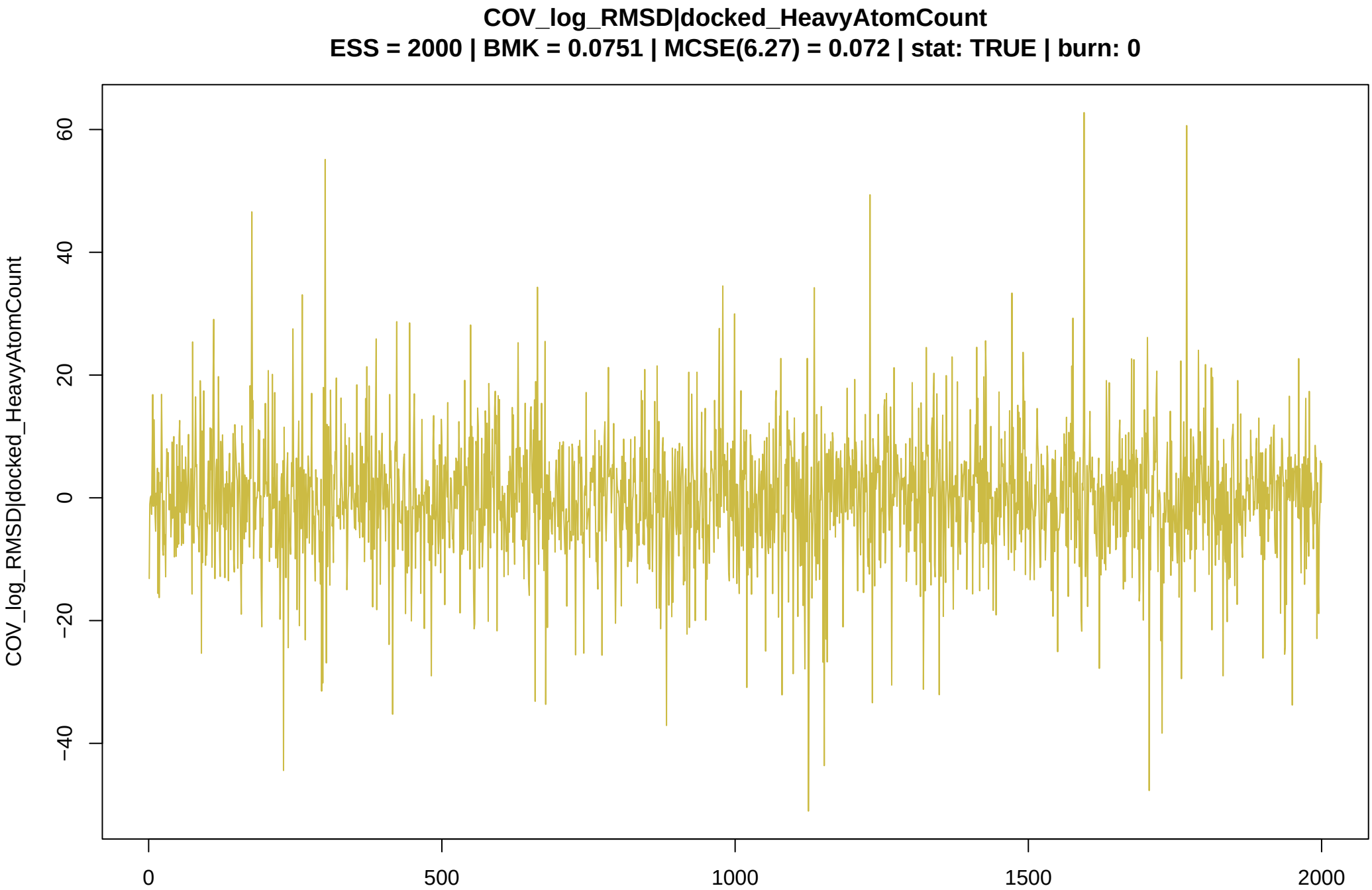

logVAR_mcs_RingCount
ESS = 2000 | BMK = 0.055 | MCSE(6.27) = 1.35 | stat: TRUE | burn: 0
logVAR_mcs_RingCount
3
2
1
0
−1
0
500
1000
1500
2000

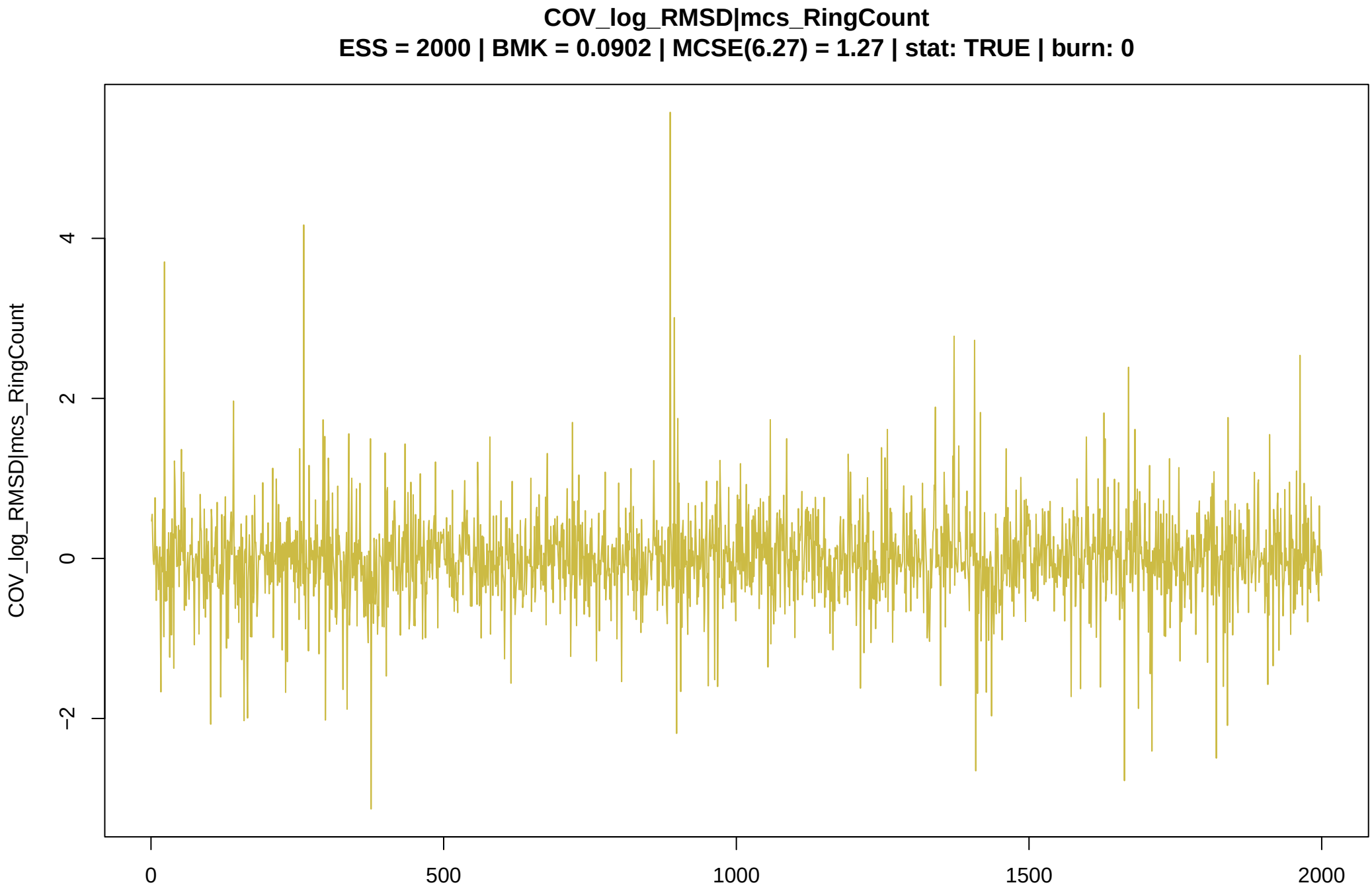

logVAR_docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0352 | MCSE(6.27) = 1.13 | stat: TRUE | burn: 0
logVAR_docked_NumRotatableBonds
2
3
4
5
6
0
500
1000
1500
2000

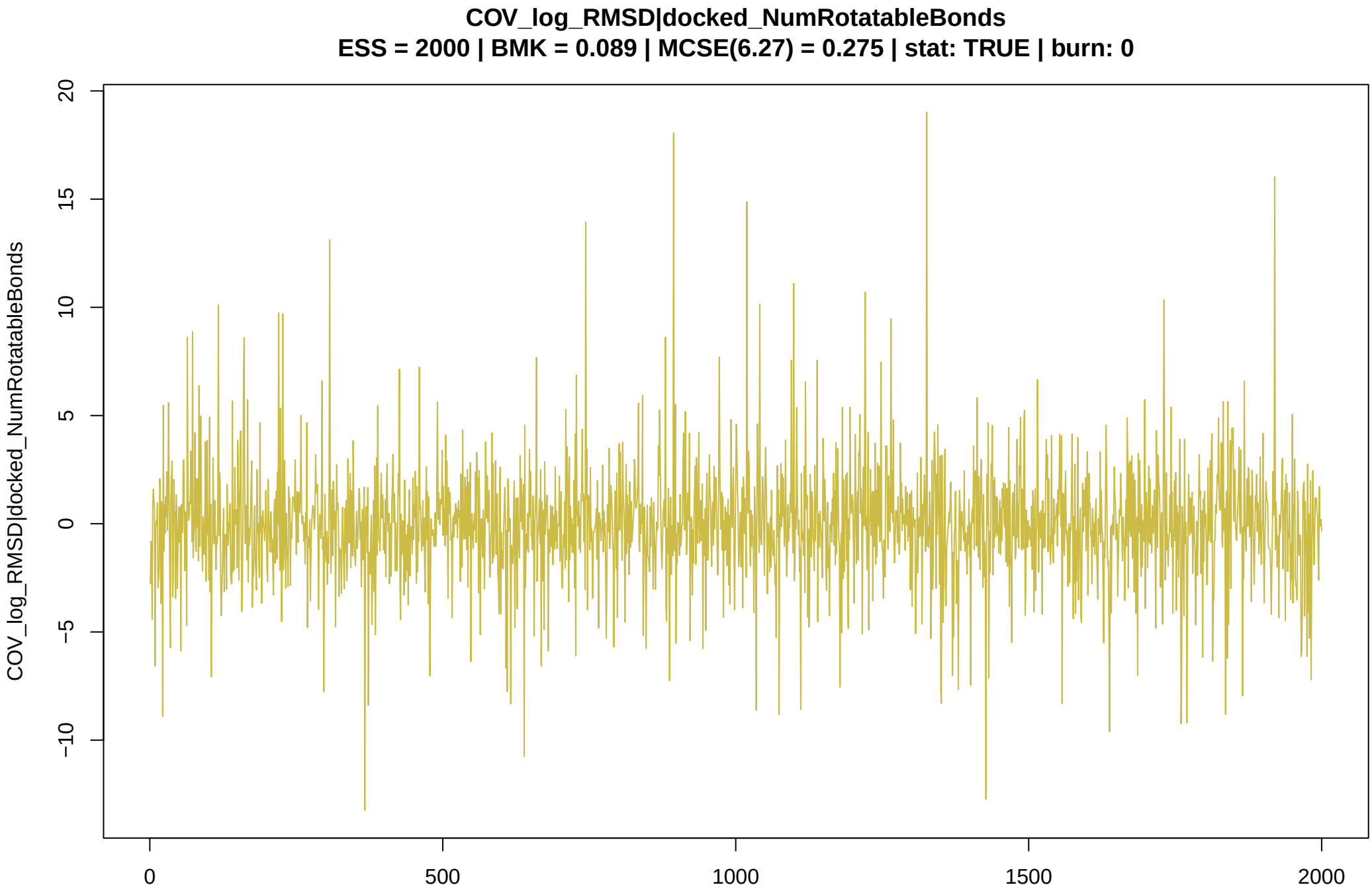

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0483 | MCSE(6.27) = 1.1 | stat: TRUE | burn: 0
COV_log_RMSD|log_mcs_unbonded_polar_sasa
3
2
1
0
−1
−2
−3
−4
0
500
1000
1500
2000

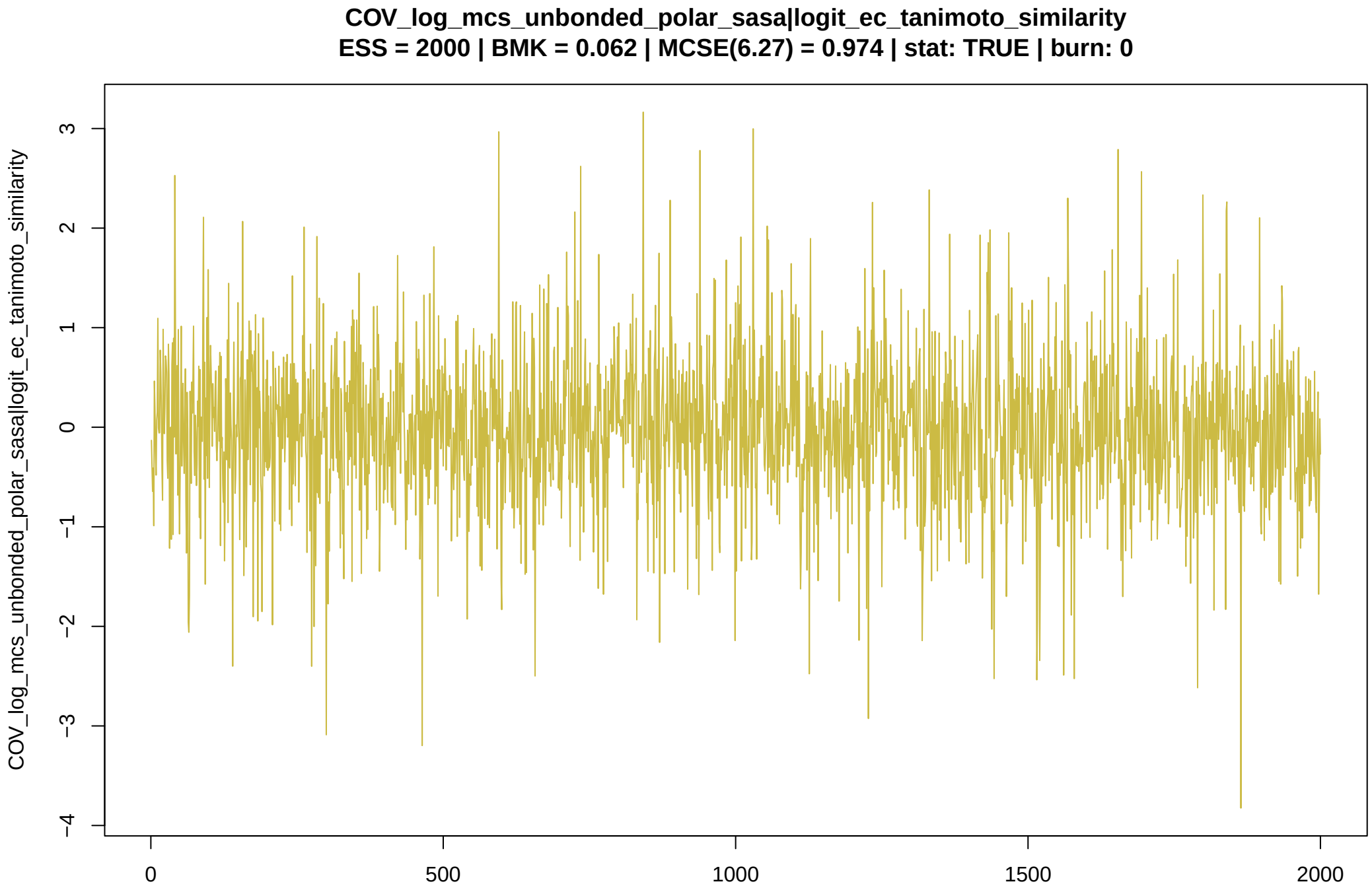

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 2000 | BMK = 0.0535 | MCSE(6.27) = 1.3 | stat: TRUE | burn: 0
COV_log_RMSD|logit_ec_tanimoto_similarity
2
1
0
−1
−2
0
500
1000
1500
2000

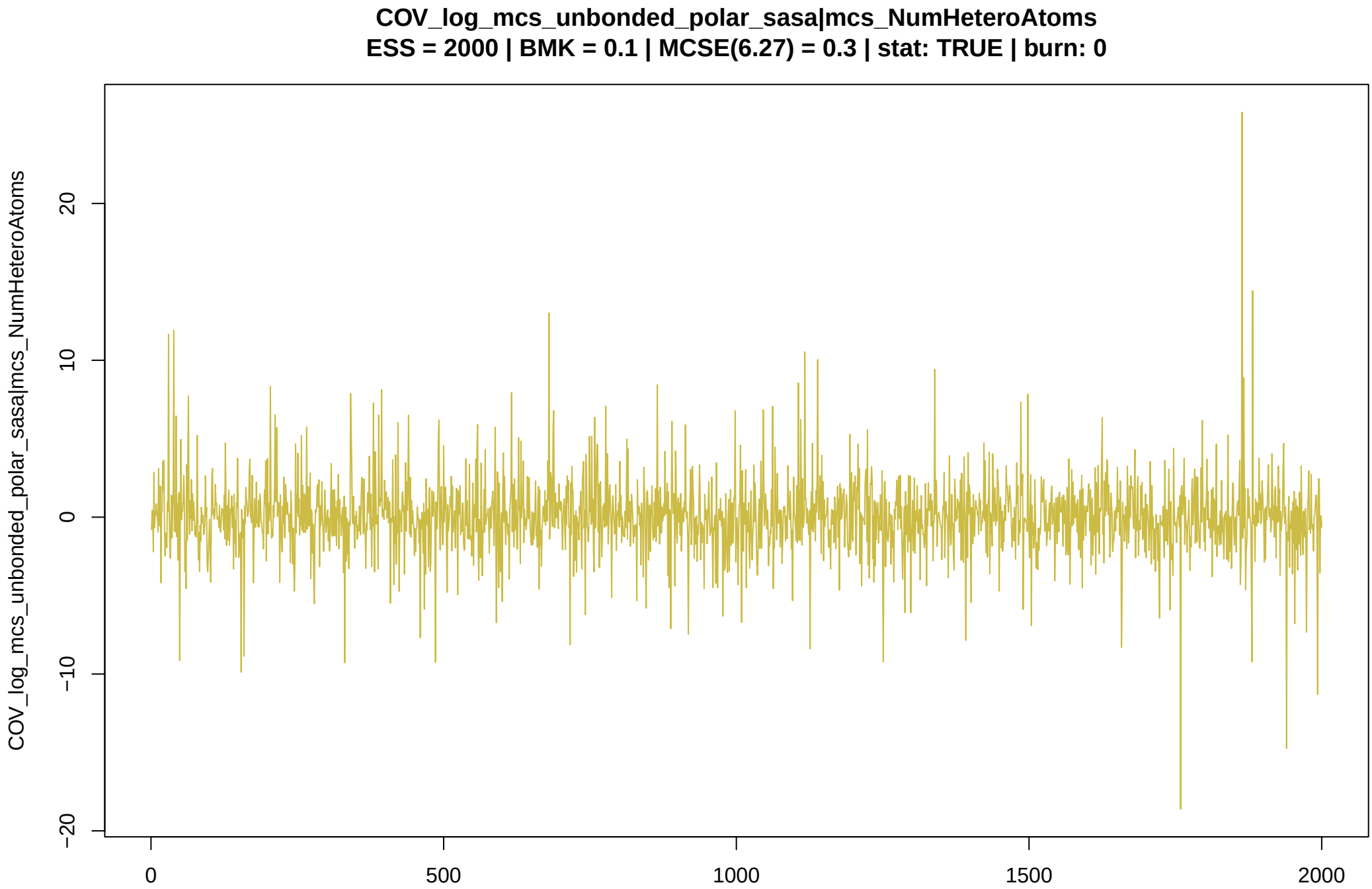

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.086 | MCSE(6.27) = 0.423 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
10
5
0
−5
−10
0
500
1000
1500
2000

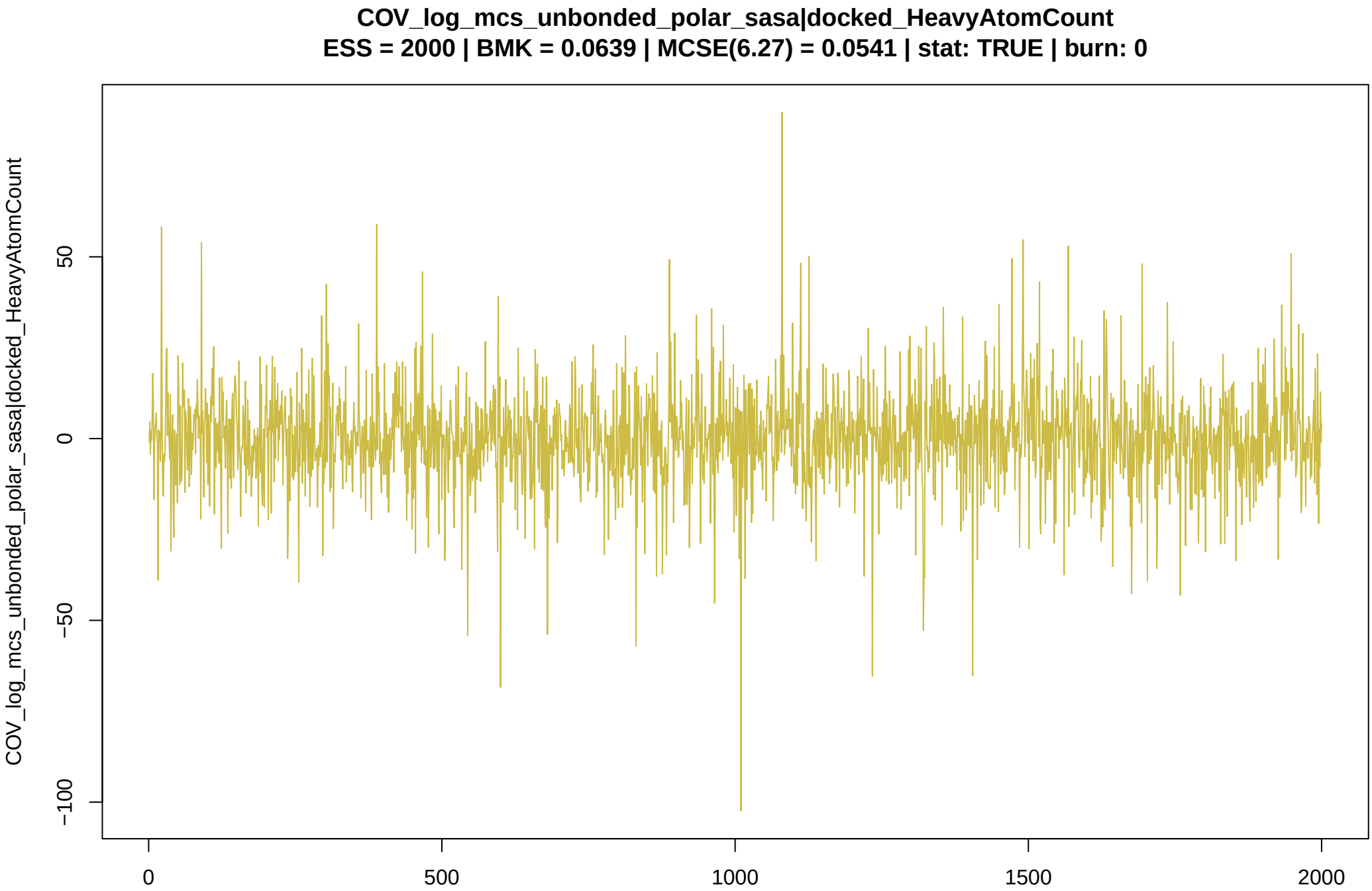

COV_log_RMSD|docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0751 | MCSE(6.27) = 0.072 | stat: TRUE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
60
40
20
0
−20
−40
0
500
1000
1500
2000

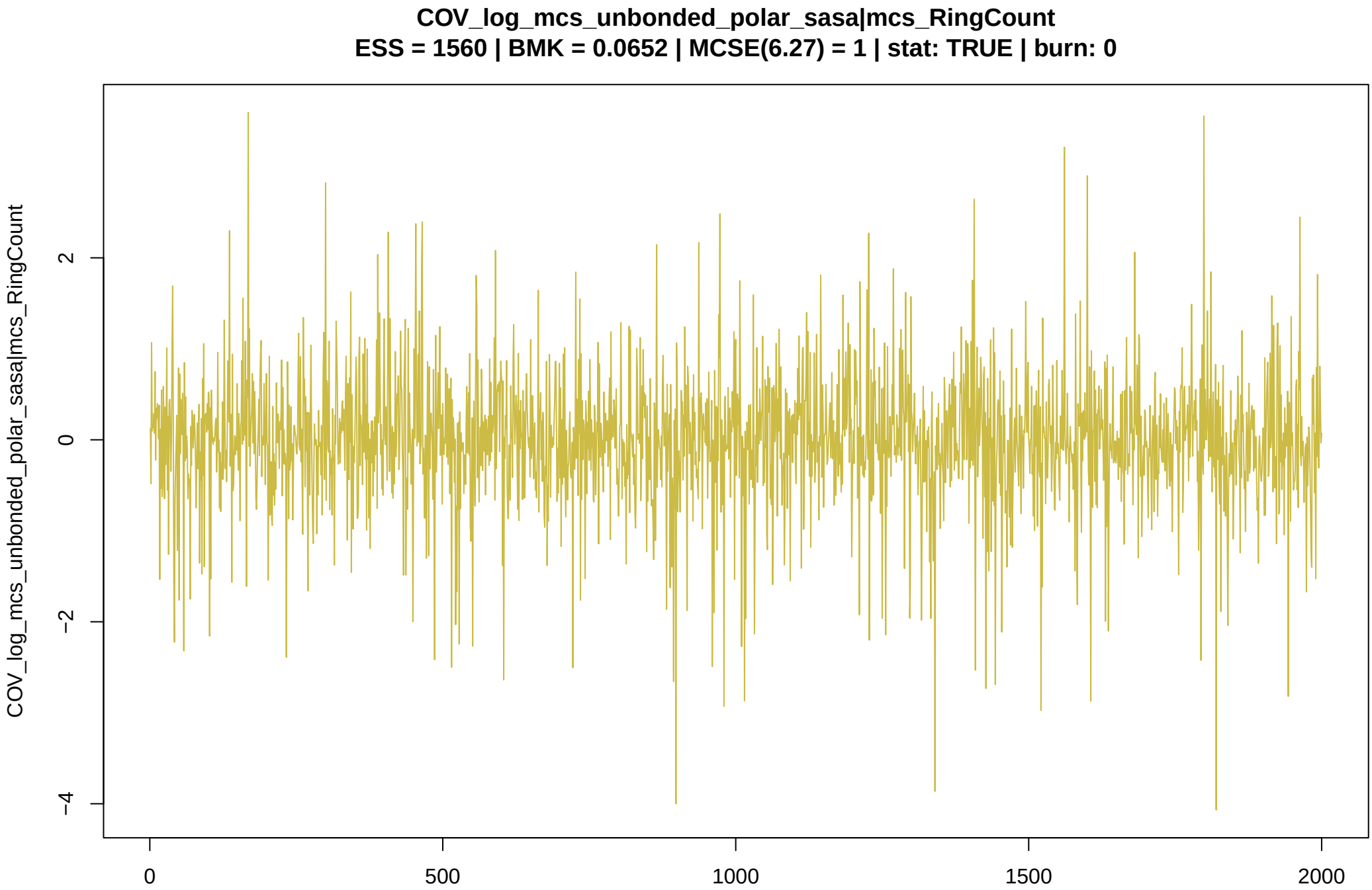

COV_log_RMSD|mcs_RingCount
ESS = 2000 | BMK = 0.0902 | MCSE(6.27) = 1.27 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_RingCount
4
2
0
−2
0
500
1000
1500
2000

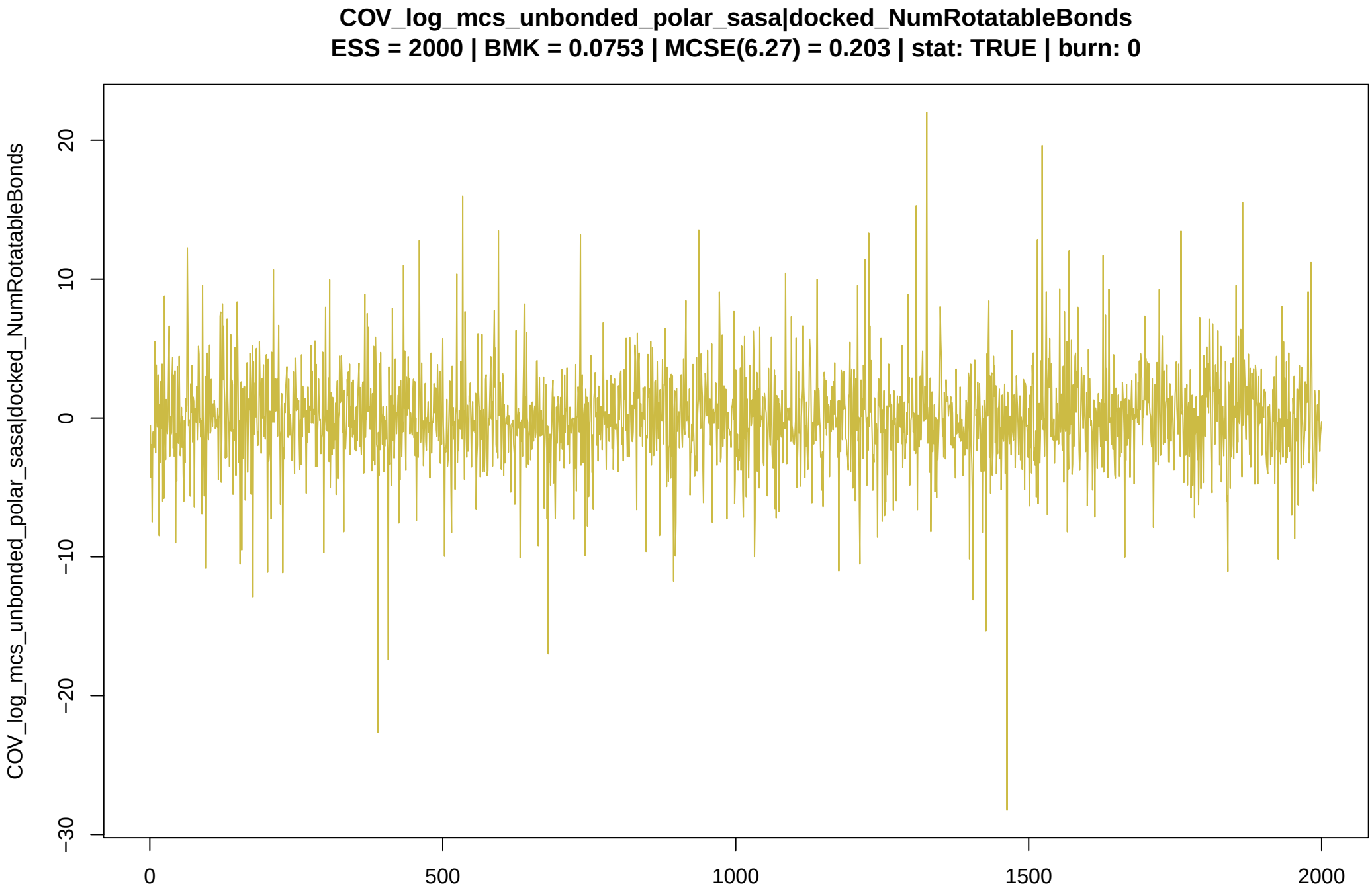

COV_log_RMSD|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.089 | MCSE(6.27) = 0.275 | stat: TRUE | burn: 0
COV_log_RMSD|docked_NumRotatableBonds
20
15
10
5
0
−5
−10
0
500
1000
1500
2000

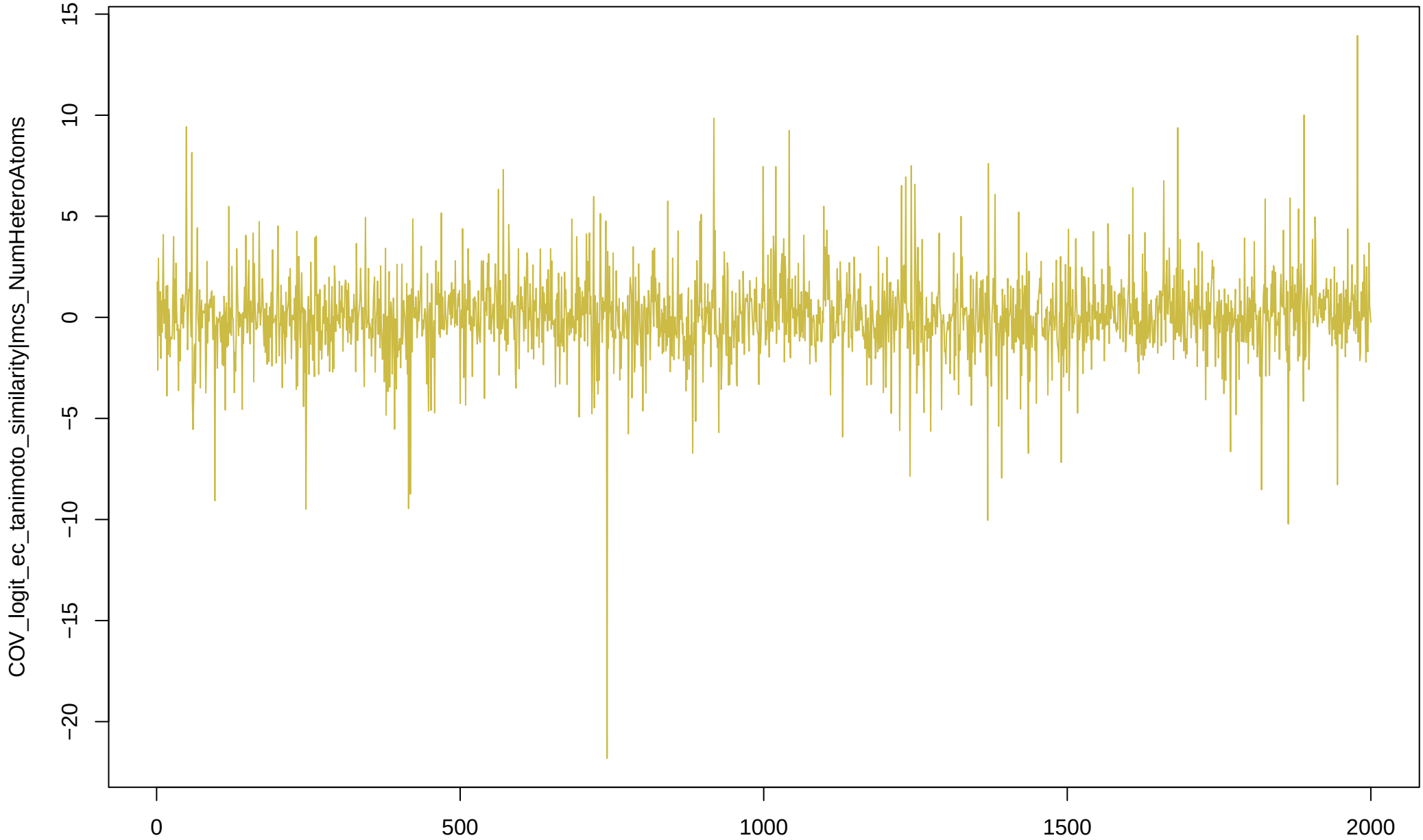

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 2000 | BMK = 0.062 | MCSE(6.27) = 0.974 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
3
2
1
0
−1
−2
−3
−4
0
500
1000
1500
2000

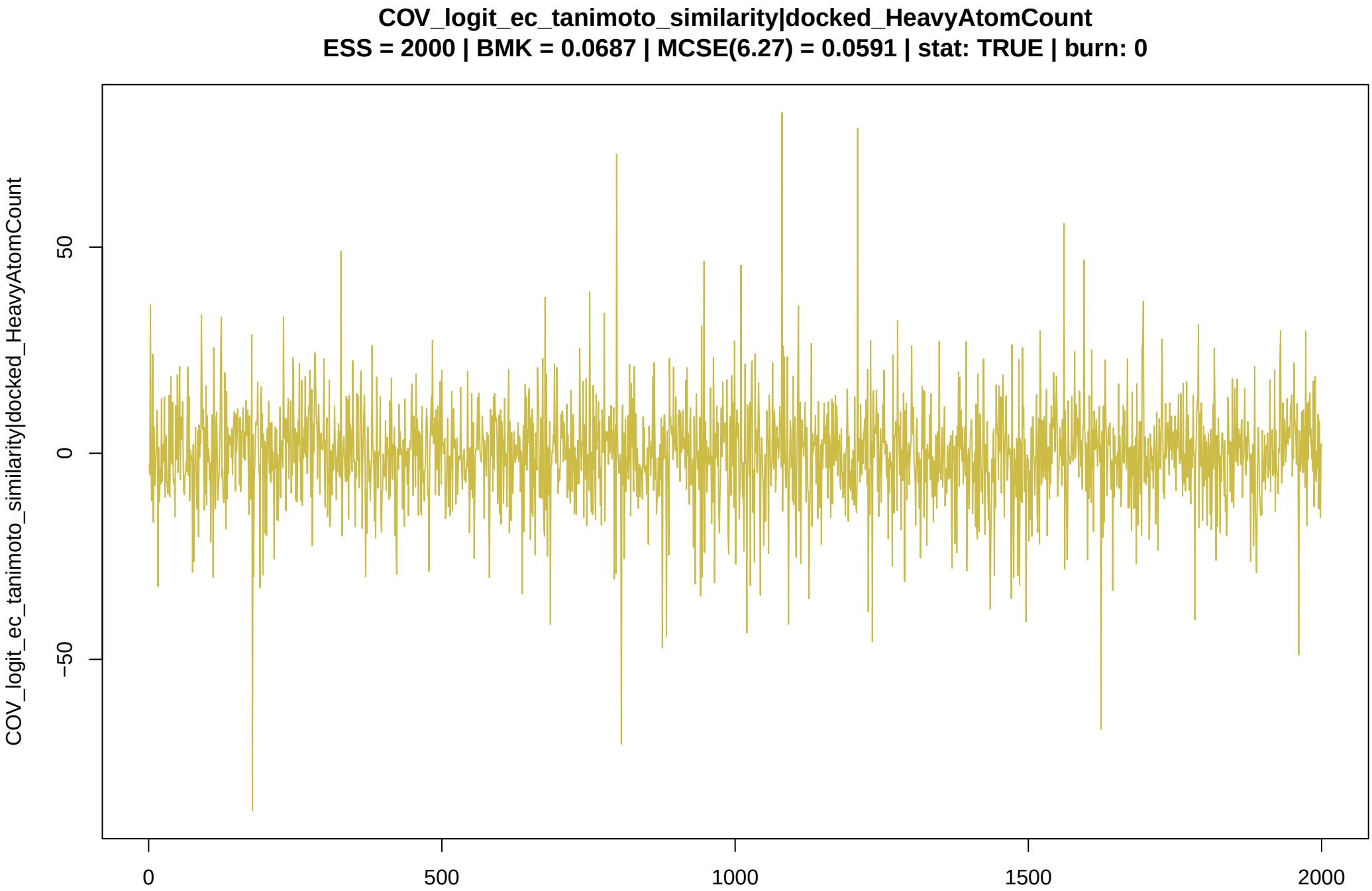

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.1 | MCSE(6.27) = 0.3 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
20
10
0
−10
−20
0
500
1000
1500
2000

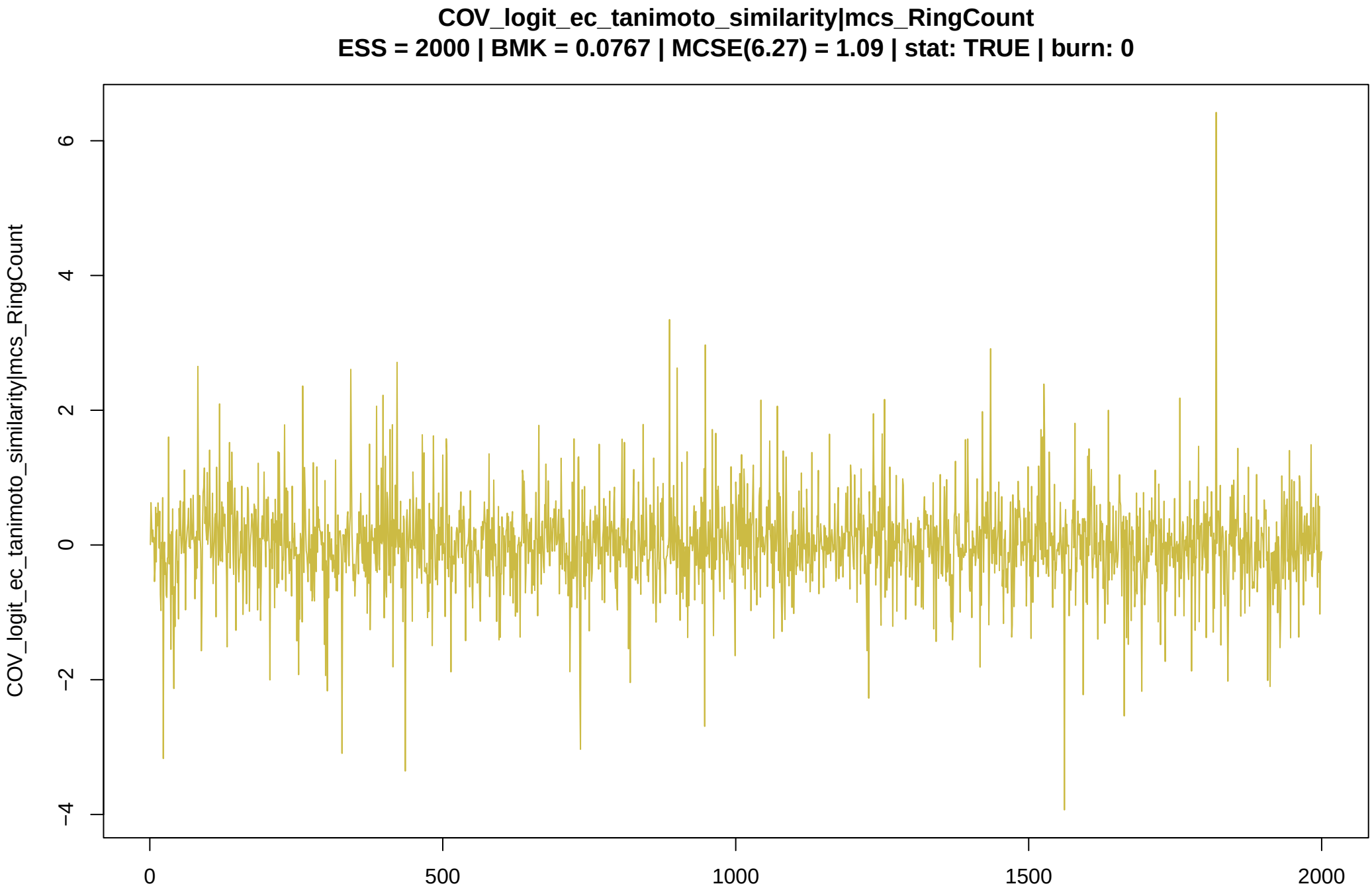

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0639 | MCSE(6.27) = 0.0541 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
50
0
−50
−100
0
500
1000
1500
2000

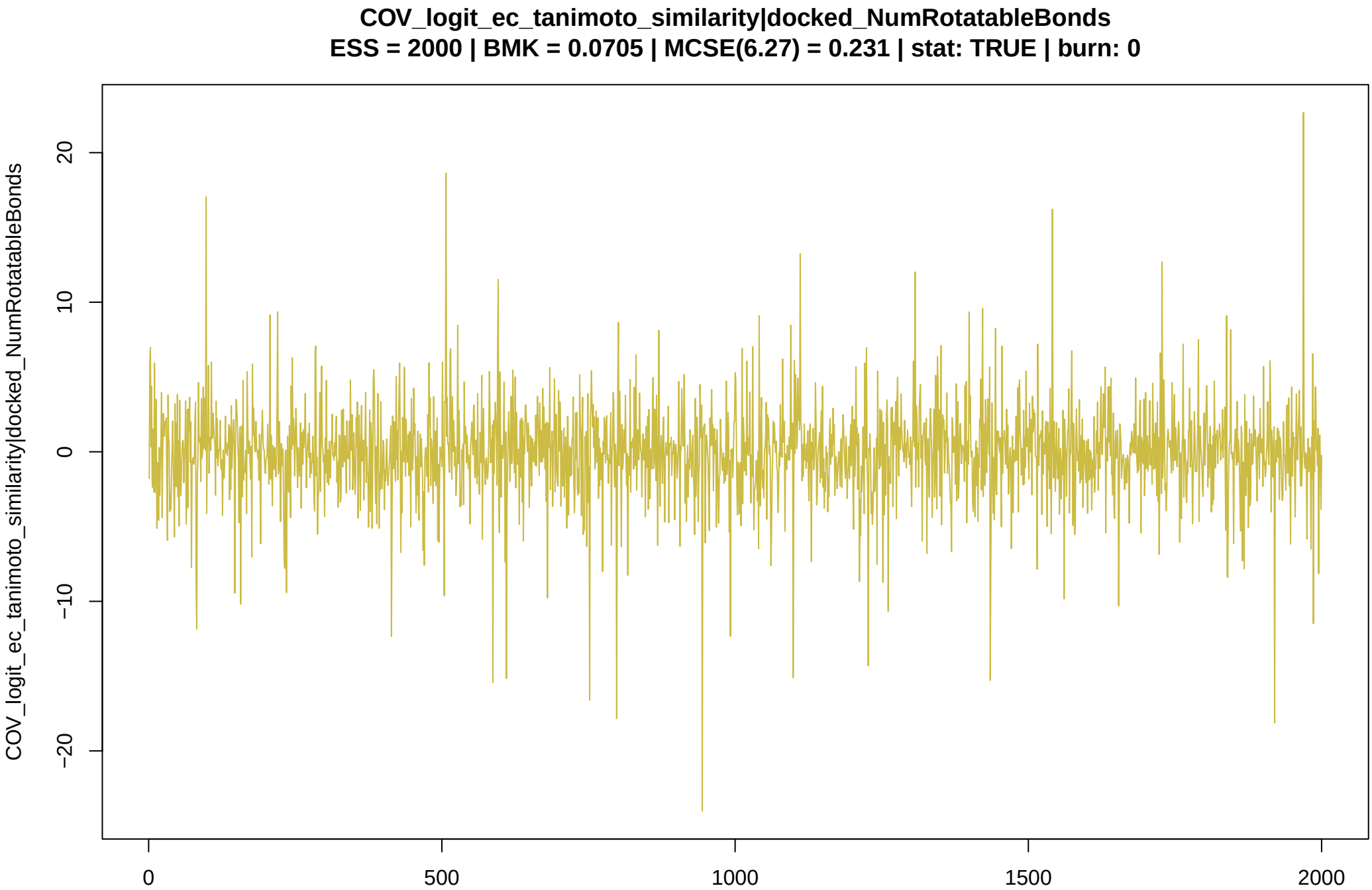

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1560 | BMK = 0.0652 | MCSE(6.27) = 1 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
2
0
−2
−4
0
500
1000
1500
2000

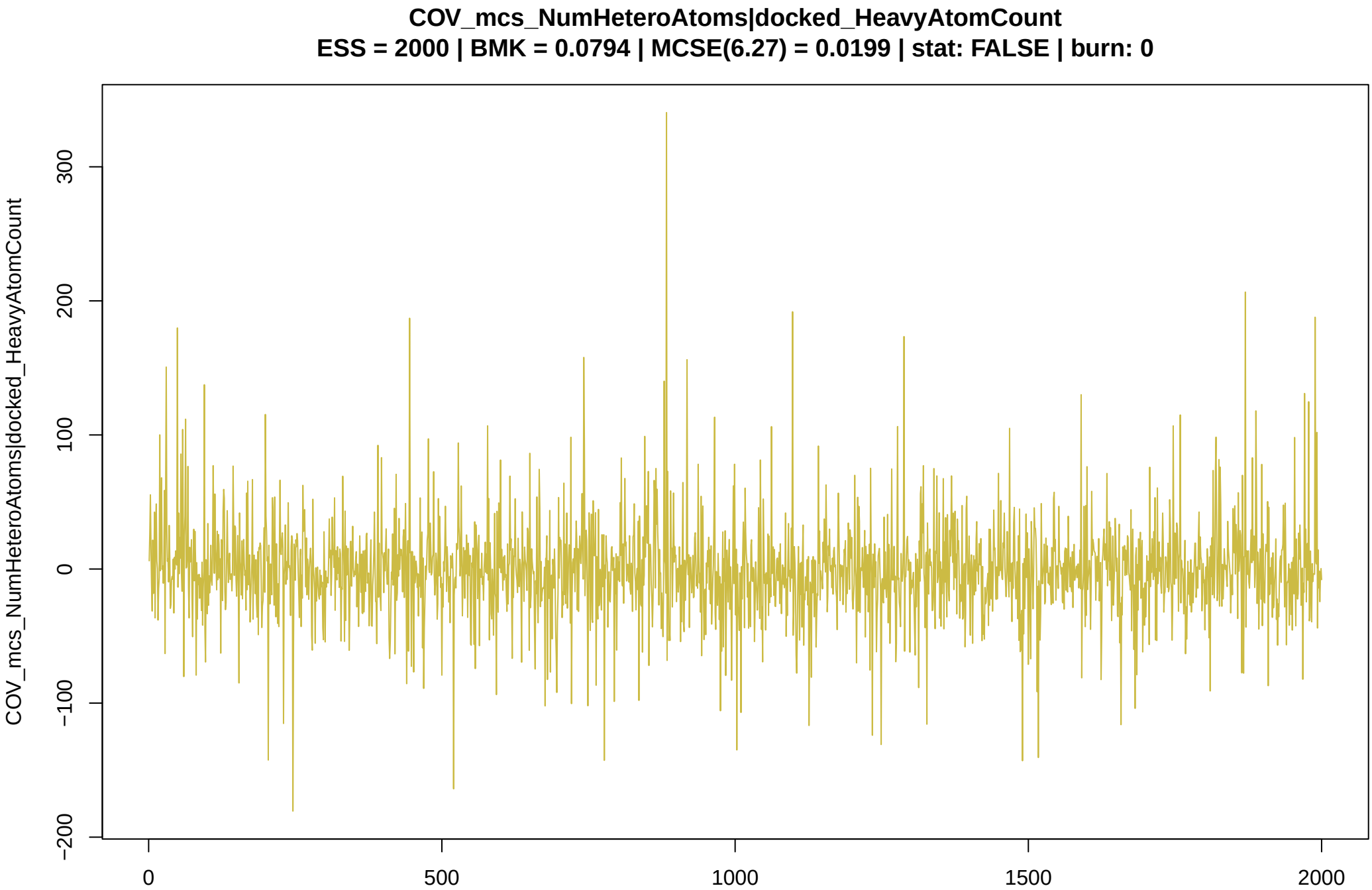

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0753 | MCSE(6.27) = 0.203 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
20
10
0
−10
−20
−30
0
500
1000
1500
2000

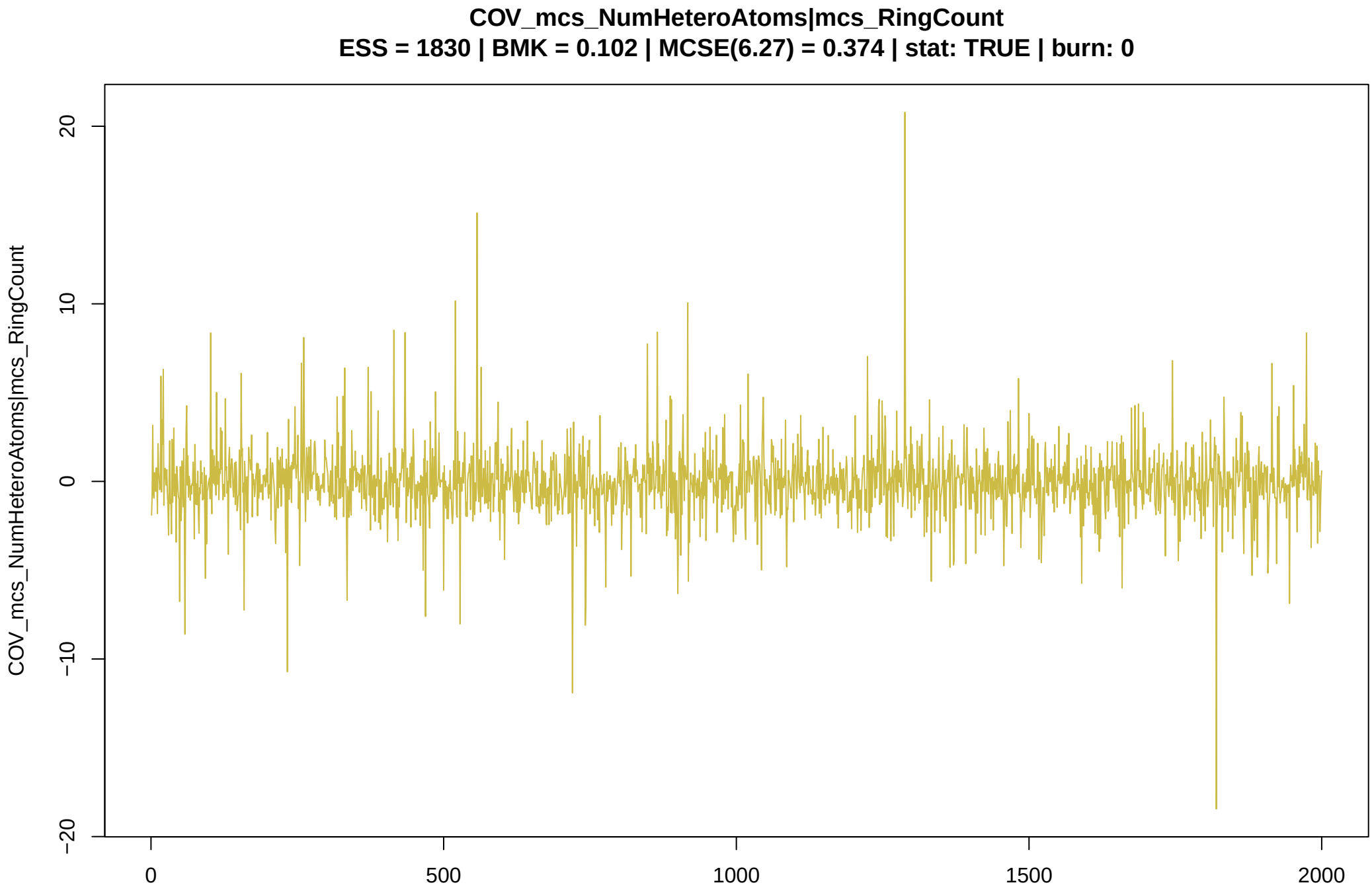

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0804 | MCSE(6.27) = 0.355 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
15
10
5
0
−5
−10
−15
−20
0
500
1000
1500
2000

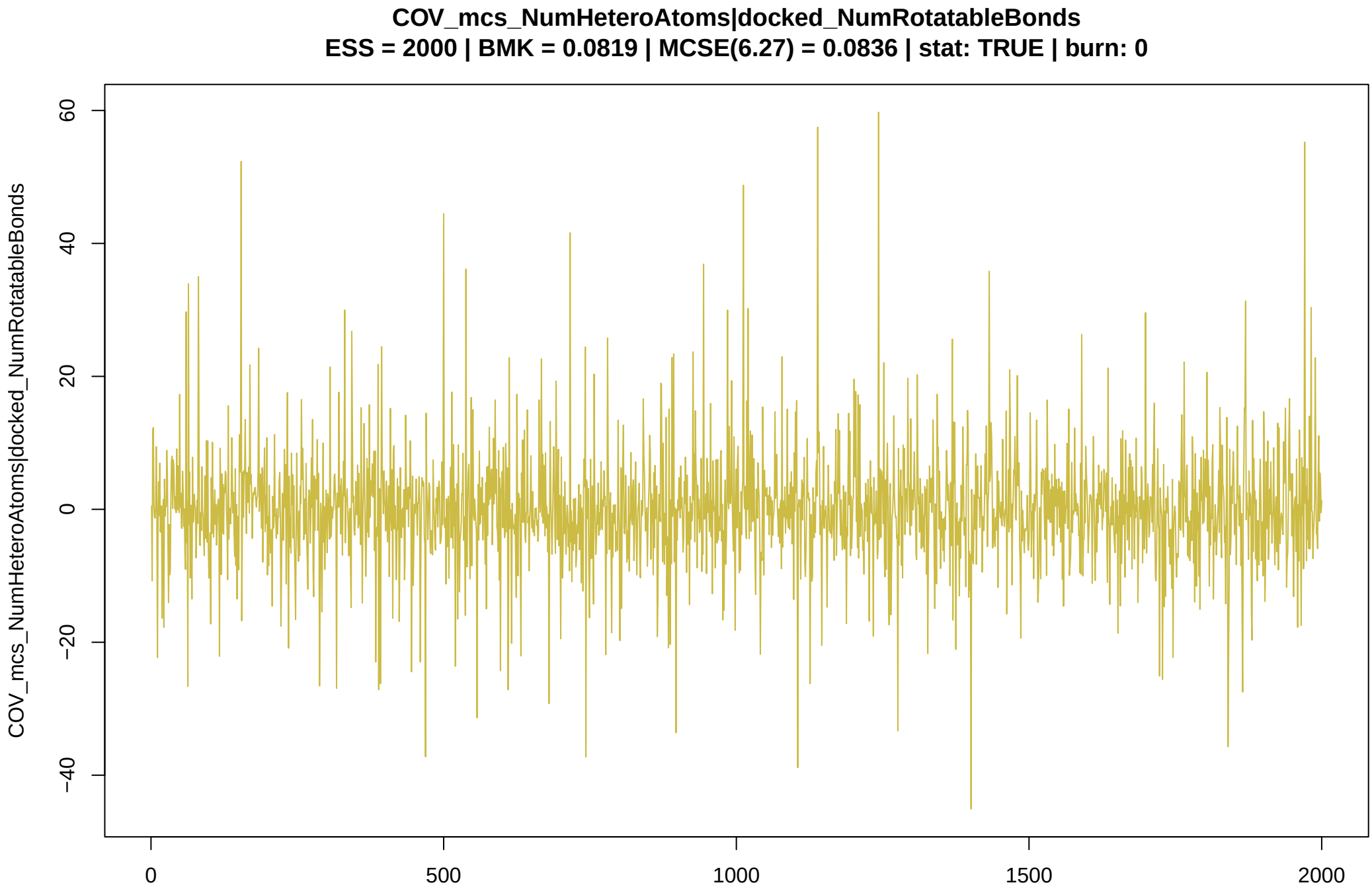

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0687 | MCSE(6.27) = 0.0591 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
50
0
−50
0
500
1000
1500
2000

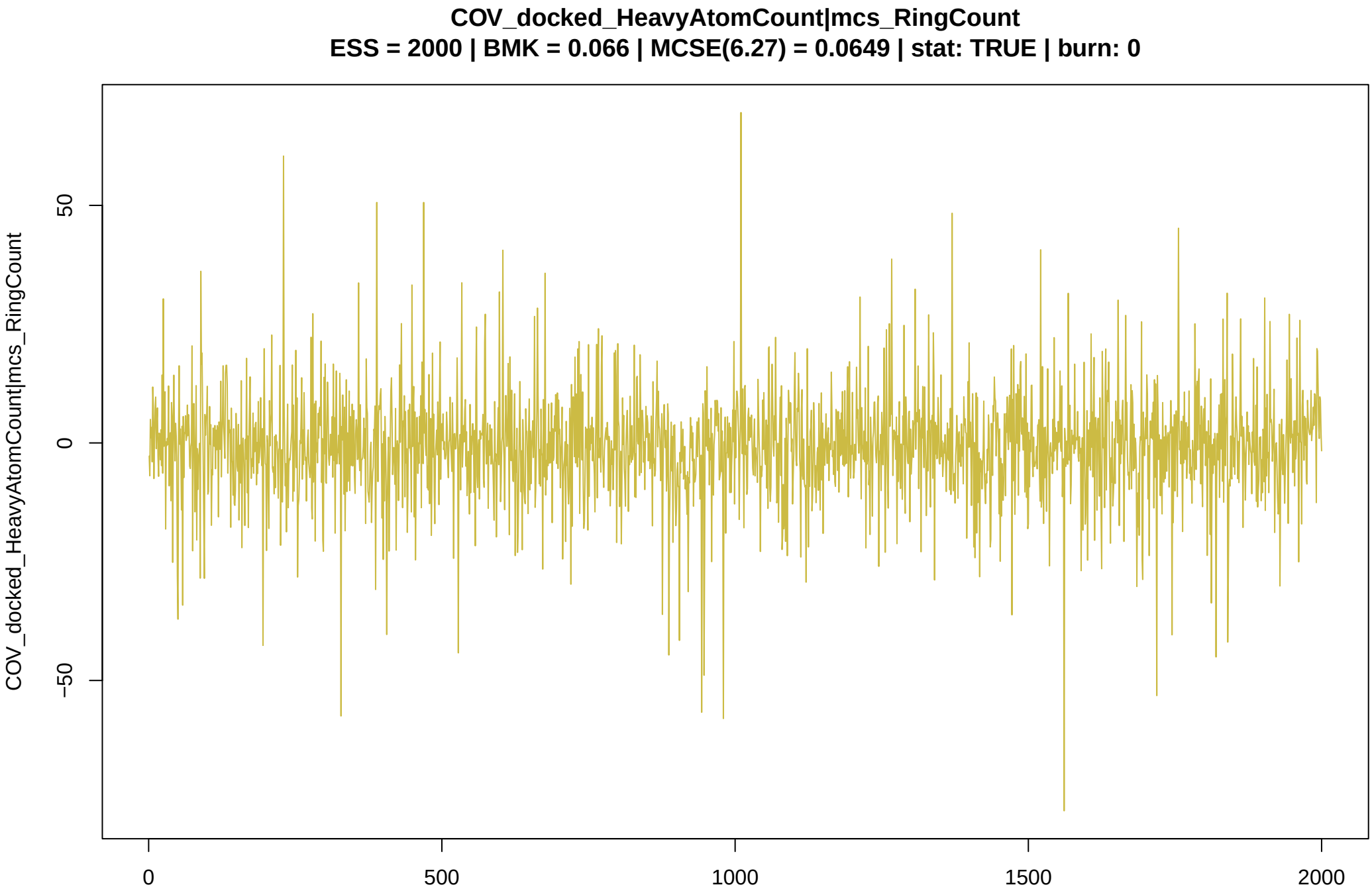

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 2000 | BMK = 0.0767 | MCSE(6.27) = 1.09 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_RingCount
6
4
2
0
−2
−4
0
500
1000
1500
2000

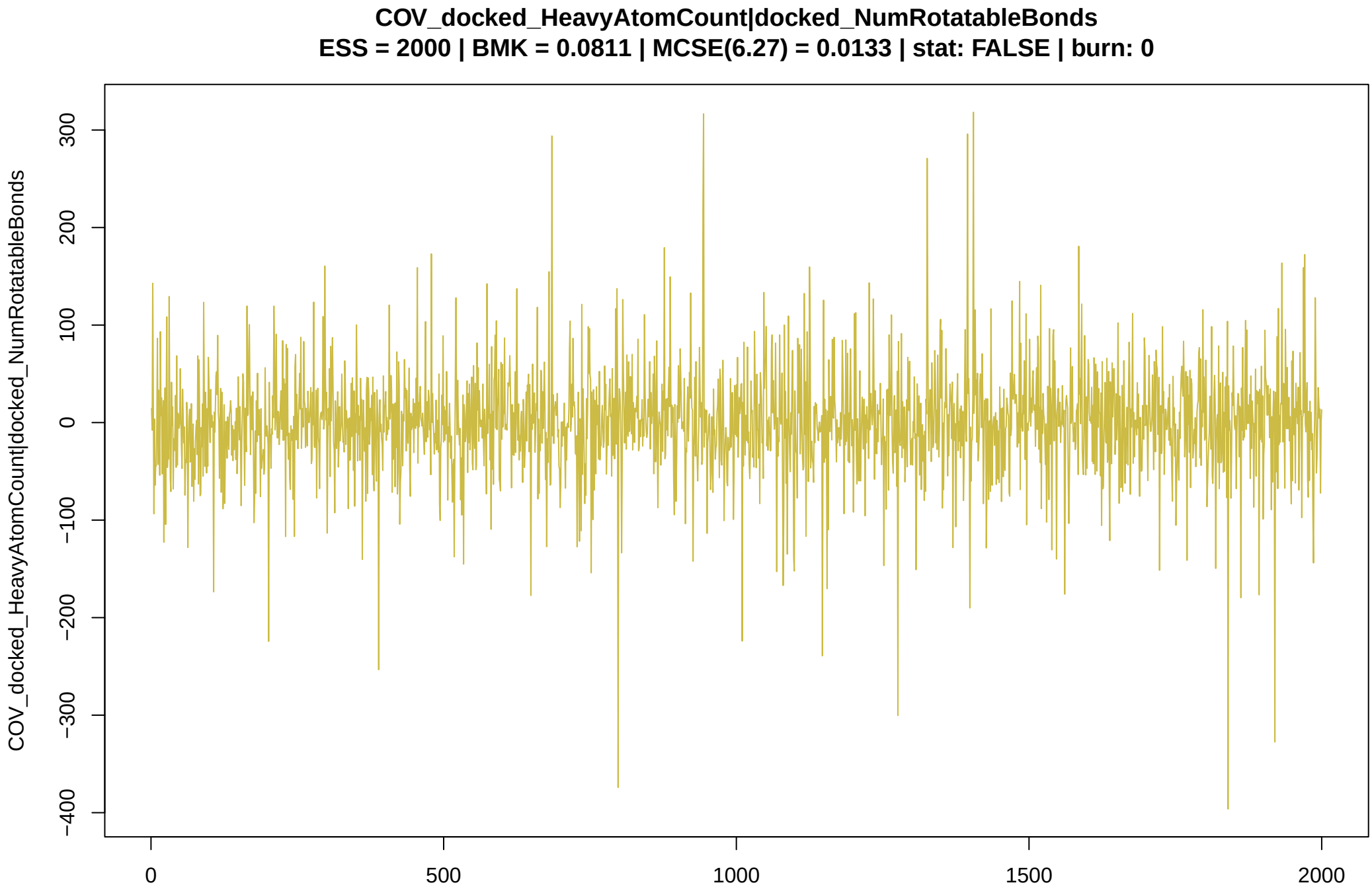

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0705 | MCSE(6.27) = 0.231 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
20
10
0
−10
−20
0
500
1000
1500
2000

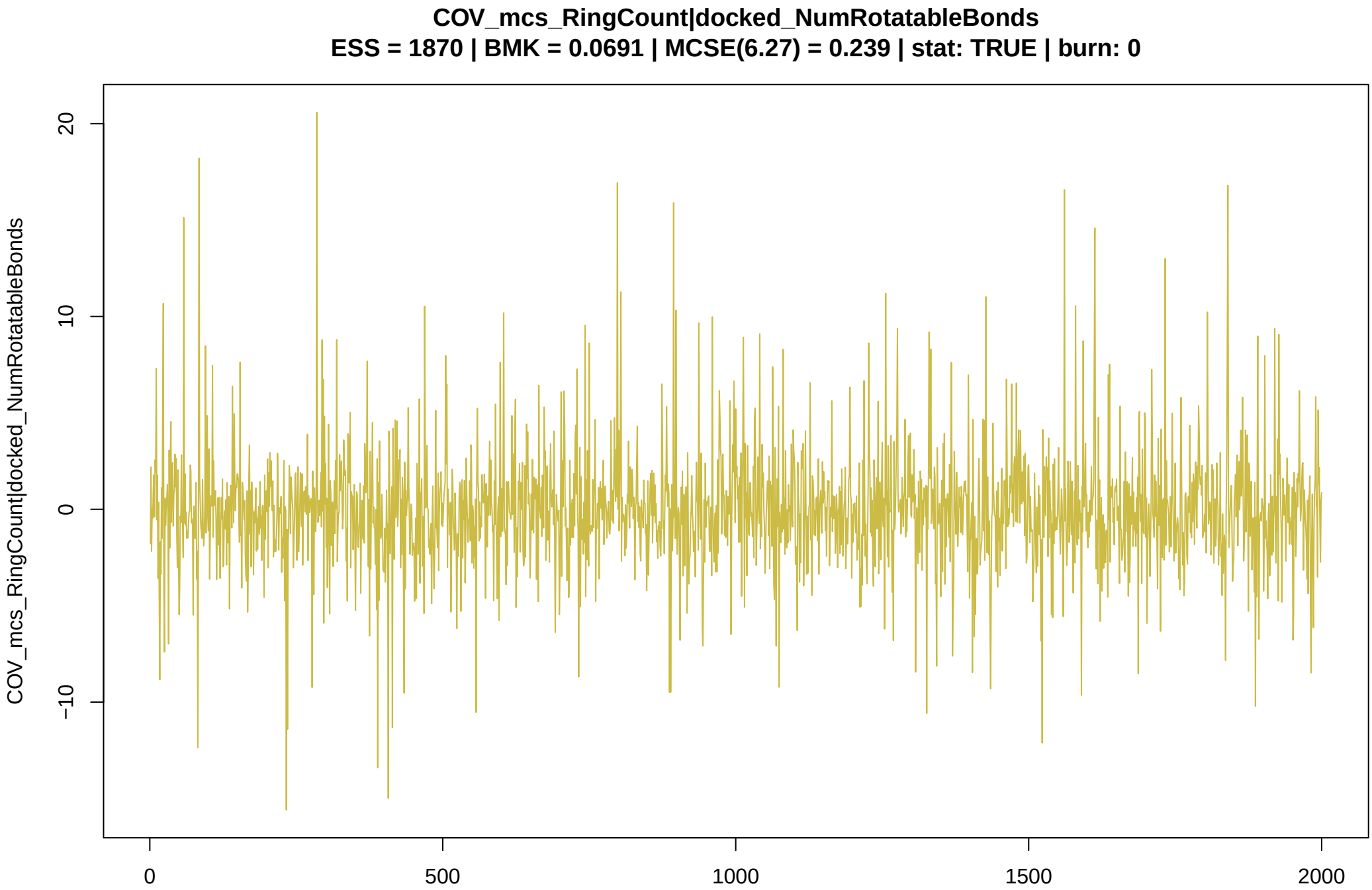

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0794 | MCSE(6.27) = 0.0199 | stat: FALSE | burn: 0
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
300
200
100
0
−100
−200
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1830 | BMK = 0.102 | MCSE(6.27) = 0.374 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|mcs_RingCount
20
10
0
−10
−20
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0819 | MCSE(6.27) = 0.0836 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
60
40
20
0
−20
−40
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 2000 | BMK = 0.066 | MCSE(6.27) = 0.0649 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
50
0
−50
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0811 | MCSE(6.27) = 0.0133 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
300
200
100
0
−100
−200
−300
−400
0
500
1000
1500
2000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1870 | BMK = 0.0691 | MCSE(6.27) = 0.239 | stat: TRUE | burn: 0
COV_mcs_RingCount|docked_NumRotatableBonds
20
10
0
−10
0
500
1000
1500
2000