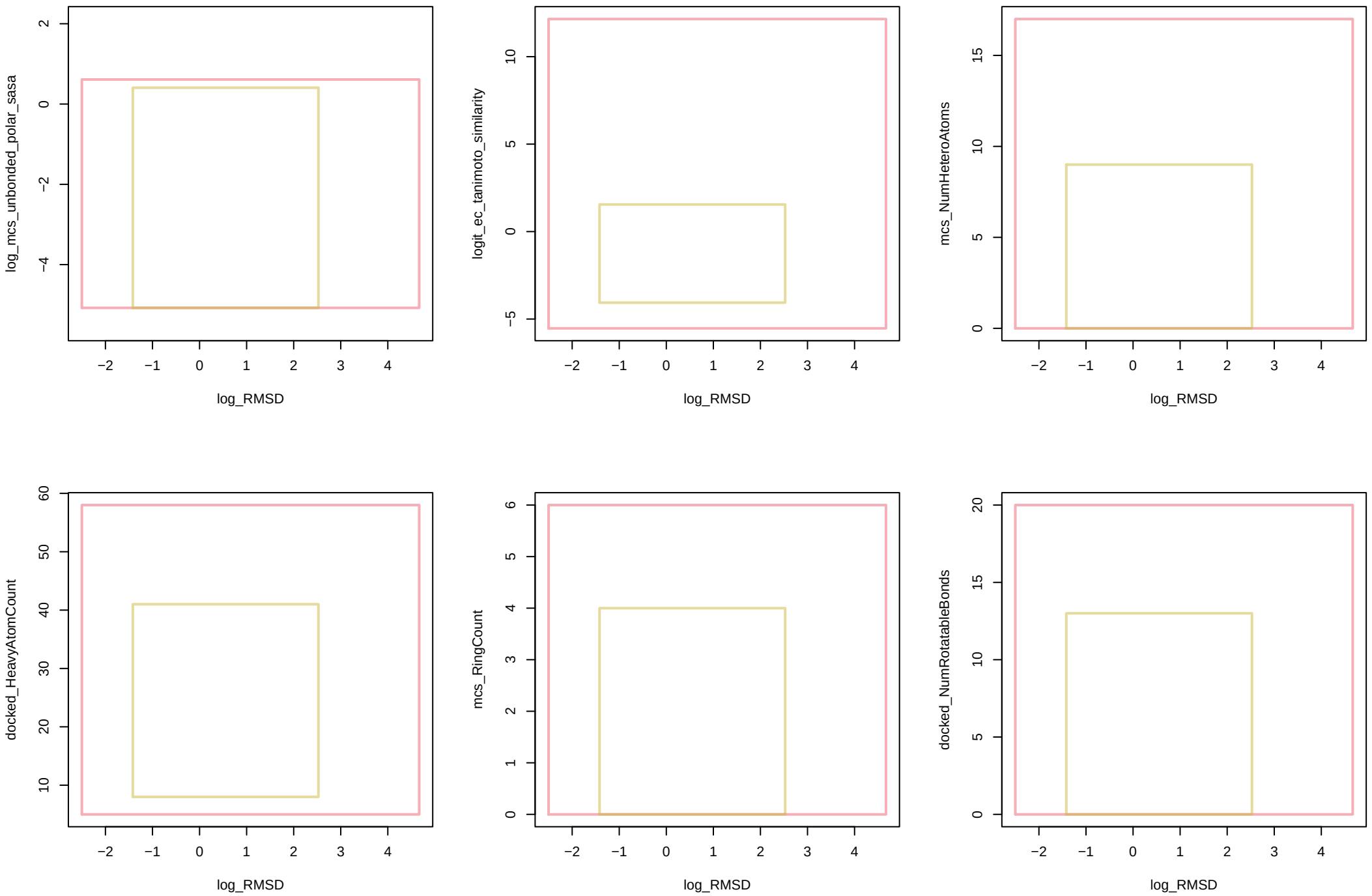
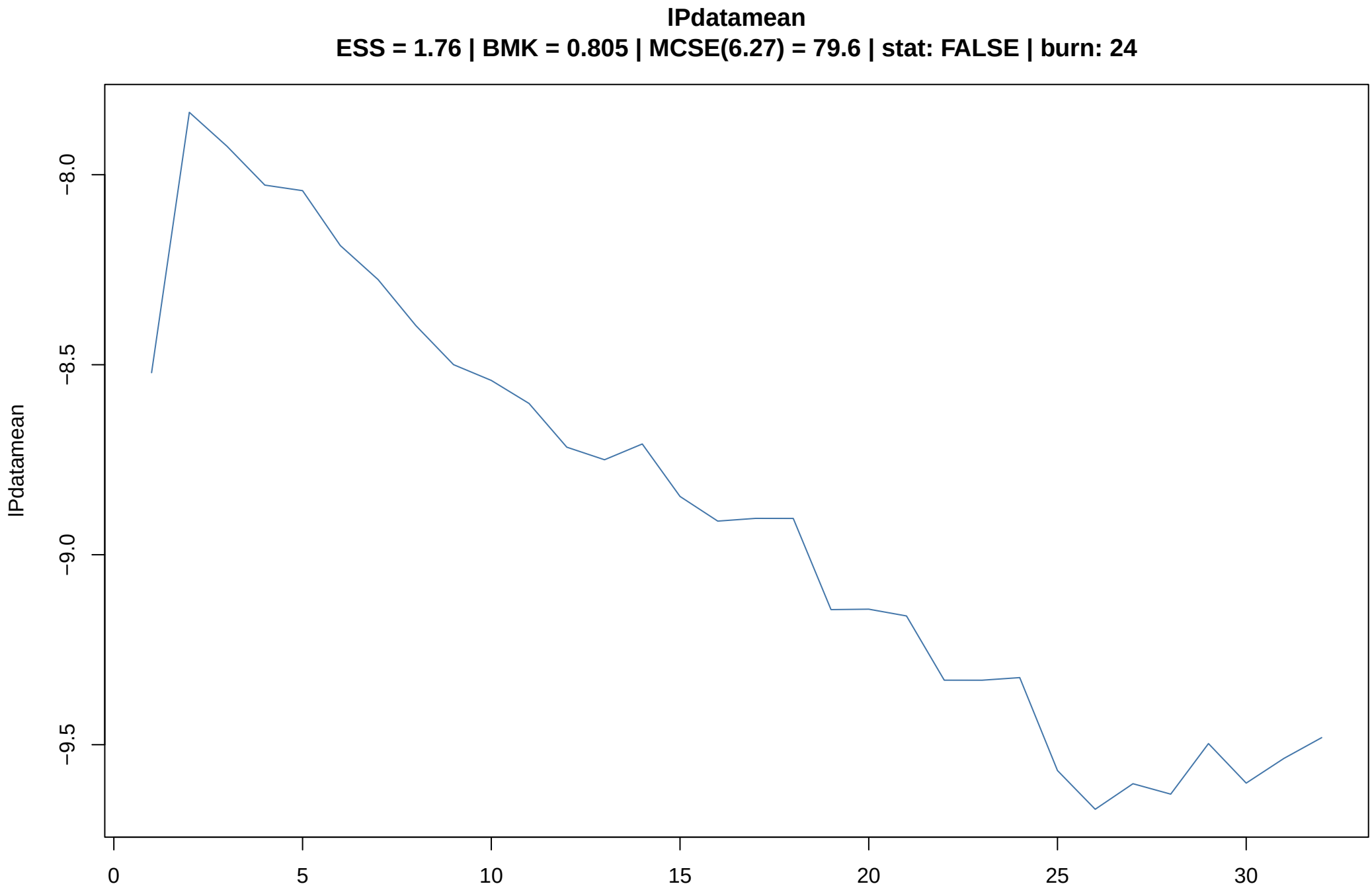
−− STATS maxD −−
min ESS = 1.75584040314641
max BMK = 0.870171859032433
max MCSE = 79.5869172949247
all stationary: FALSE
burn: 30

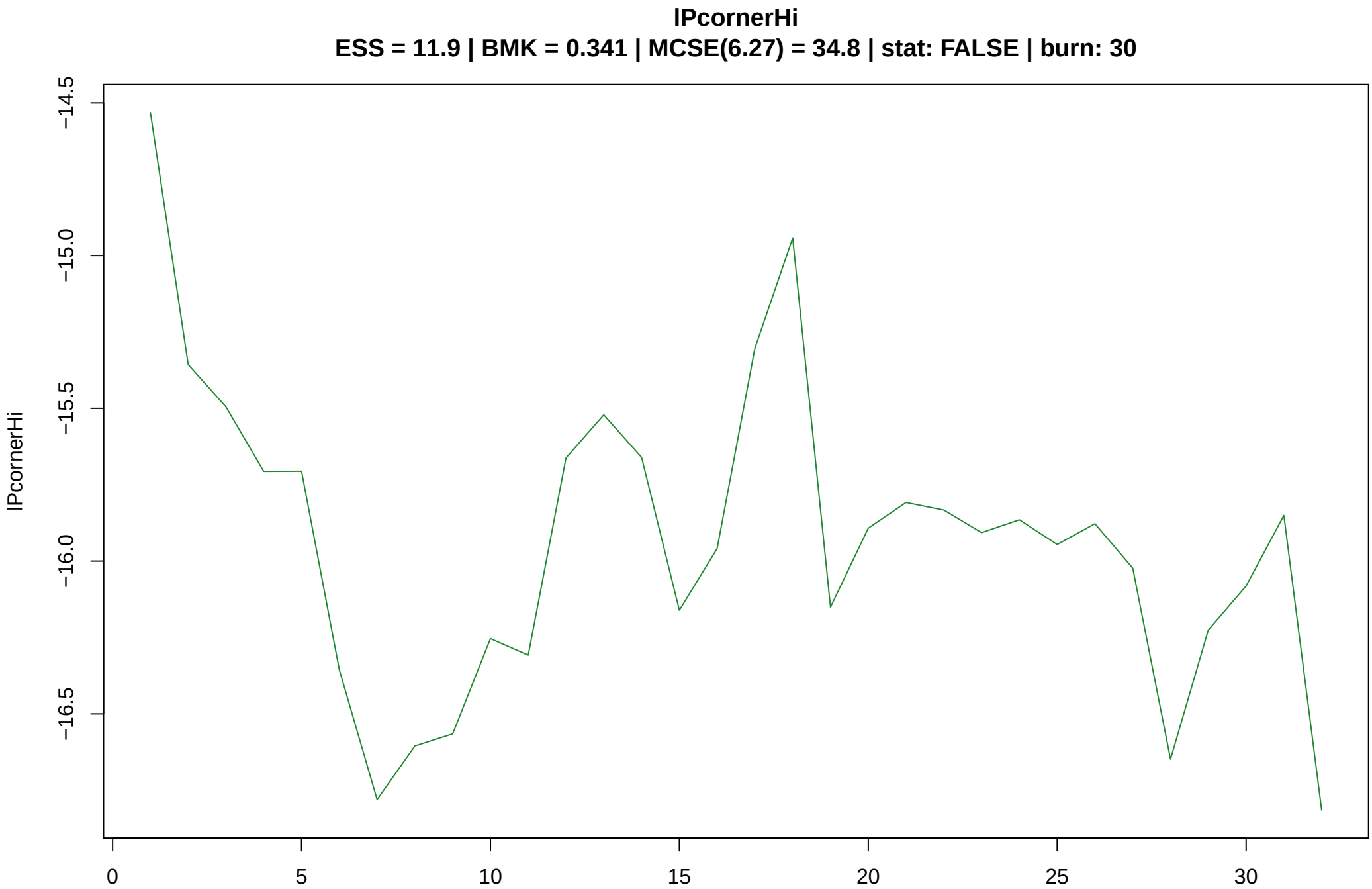
−− STATS 2D −−
min ESS = 3.58023161786877
max BMK = 0.764231904570669
max MCSE = 61.0000373883634
all stationary: FALSE
burn: 30

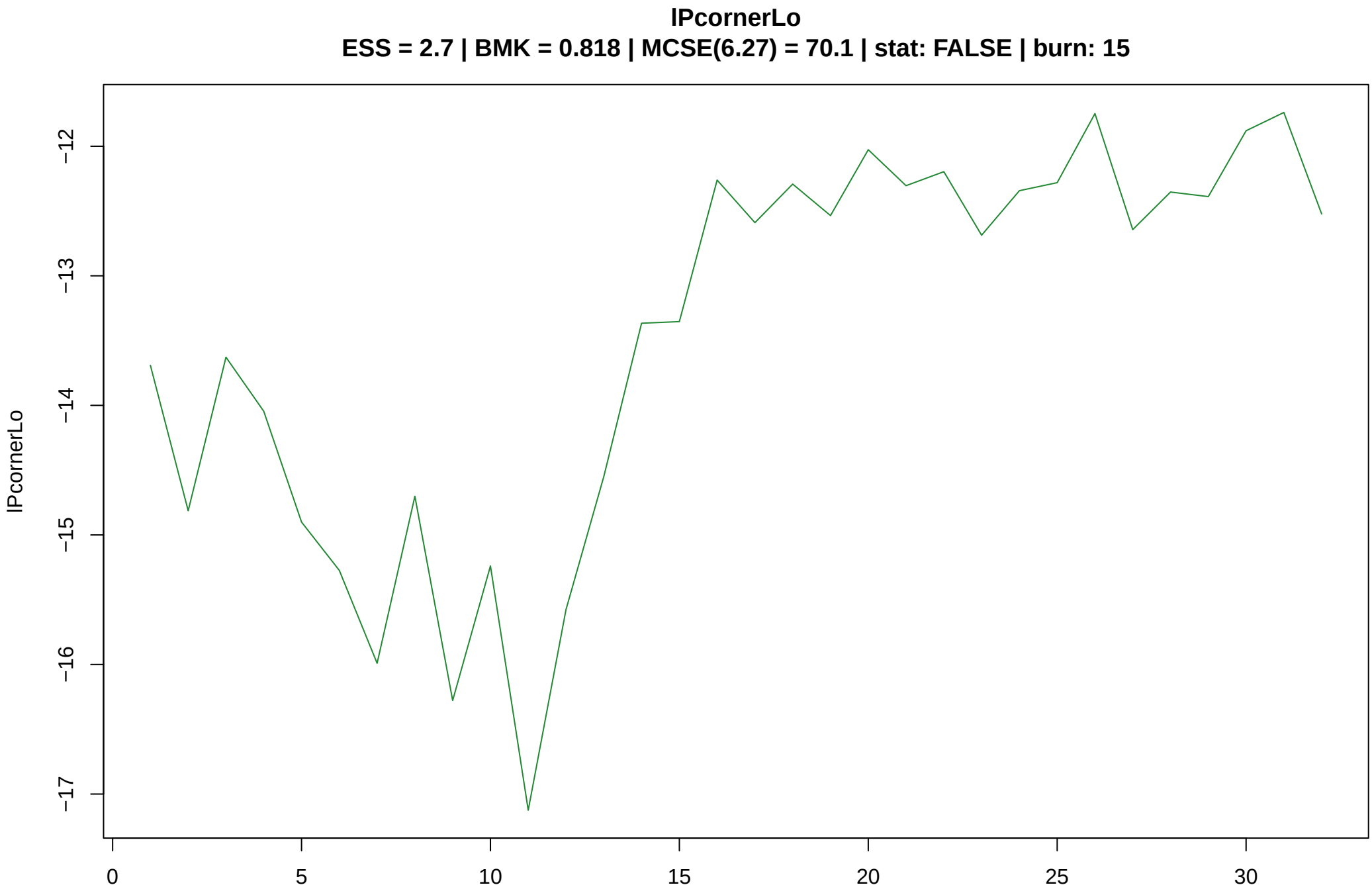
−− STATS 1D −−
min ESS = 8.2996019108569
max BMK = 0.468516743733029
max MCSE = 44.2419465831639
all stationary: FALSE
burn: 30

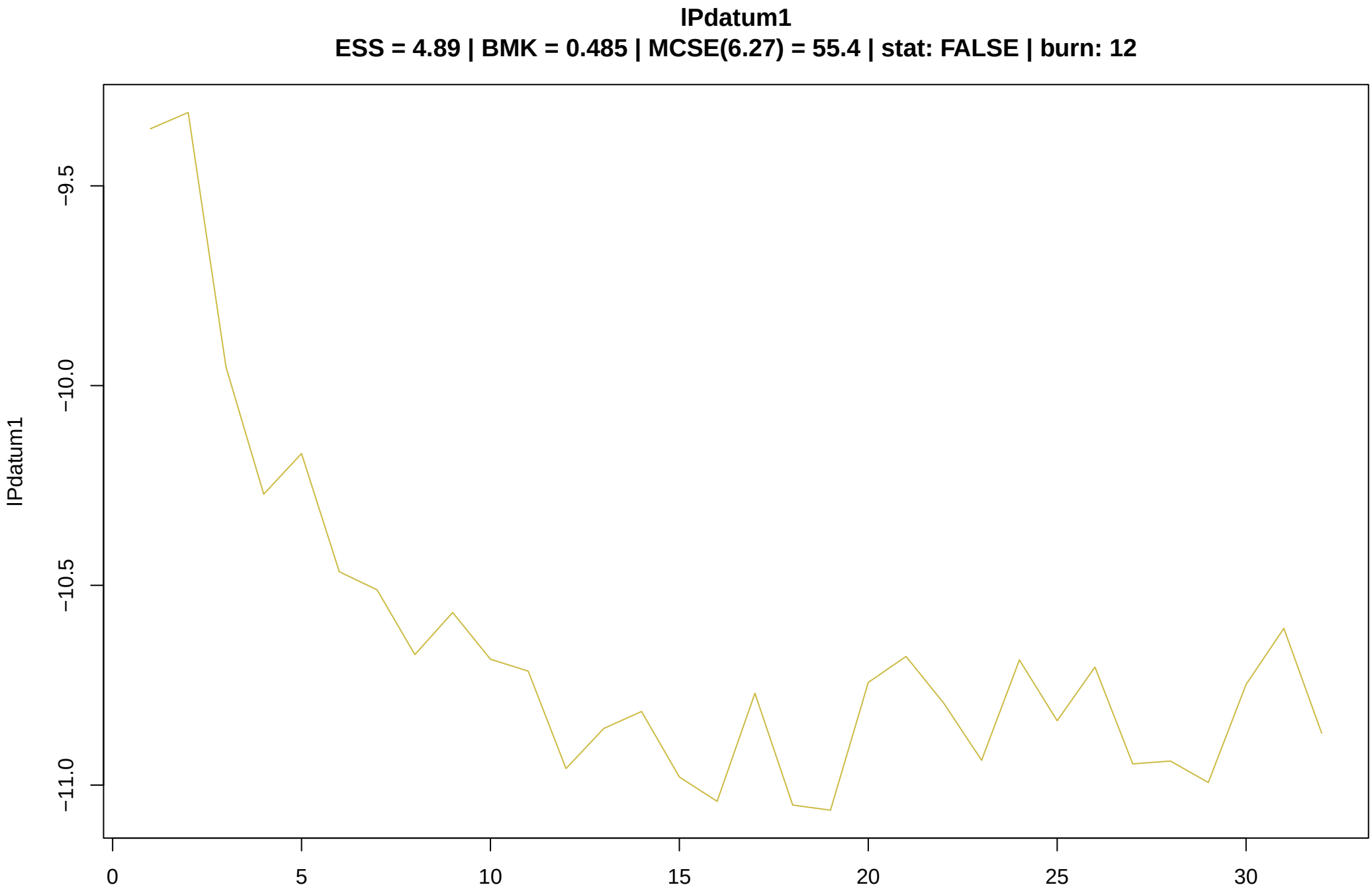
Occupied clusters: 15 of 64

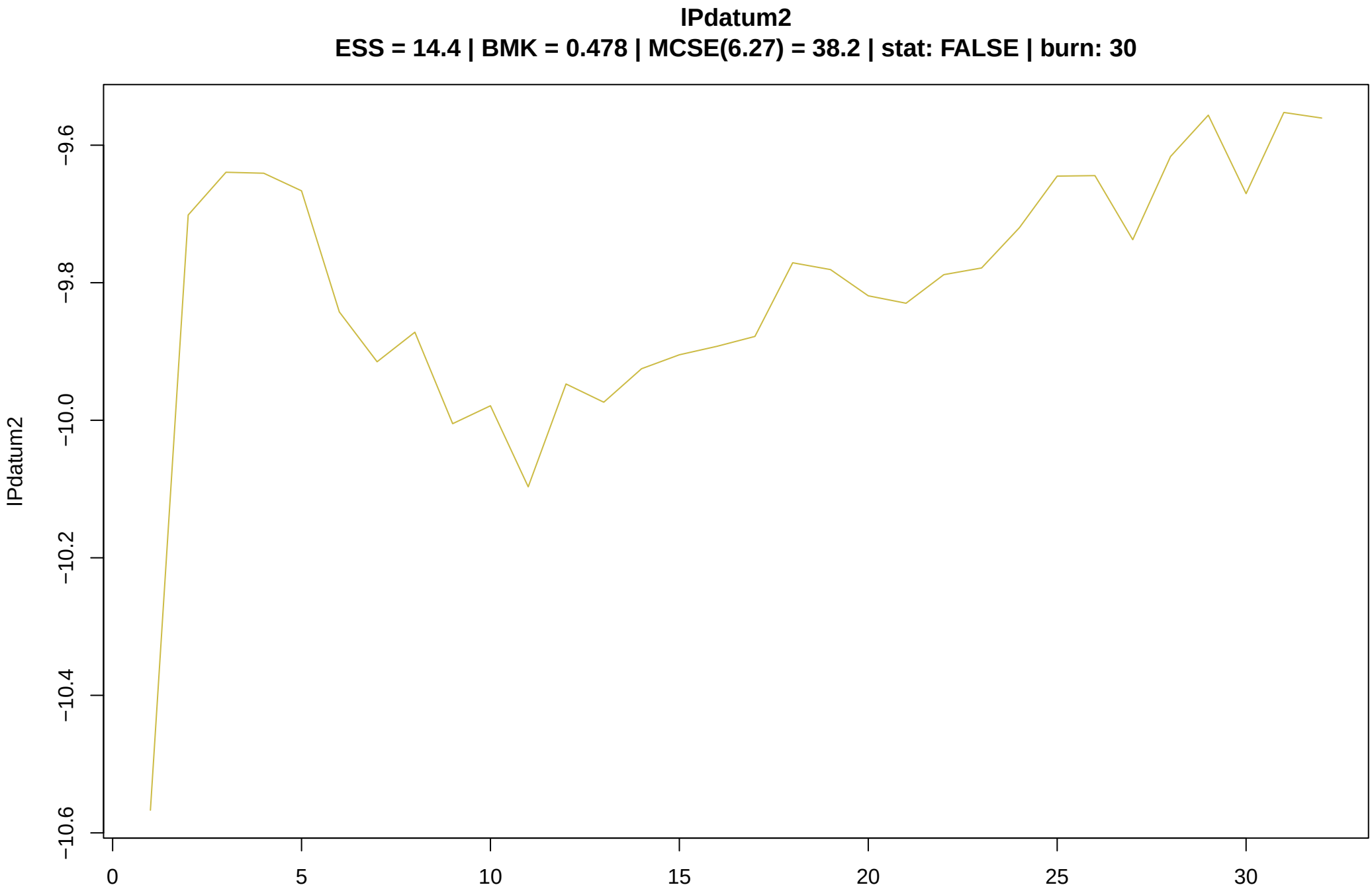

log_mcs_unbonded_polar_sasa
logit_ec_tanimoto_similarity
mcs_NumHeteroAtoms
docked_HeavyAtomCount
mcs_RingCount
docked_NumRotatableBonds
log_RMSD

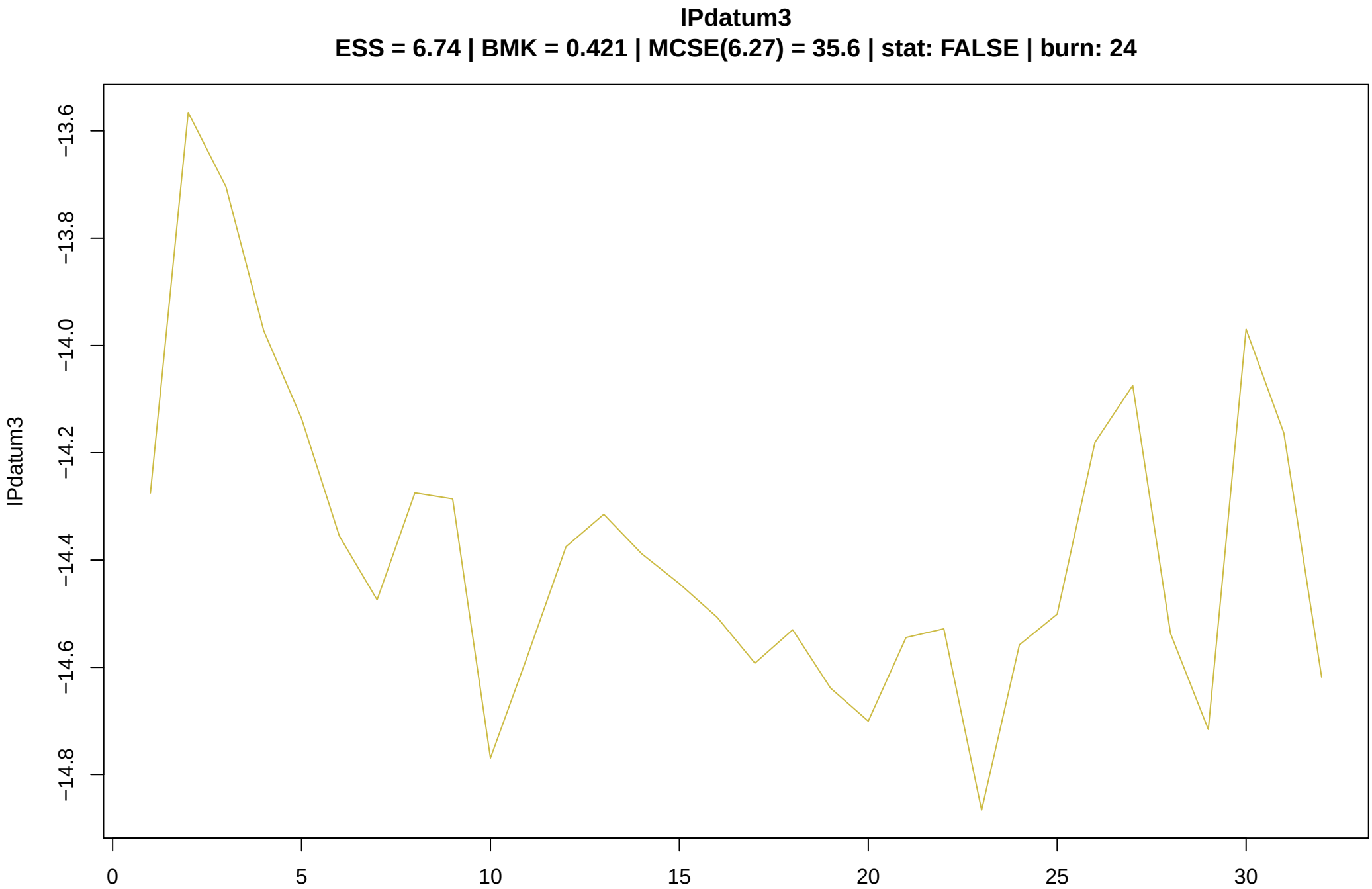

lPdatamean
ESS = 1.76 | BMK = 0.805 | MCSE(6.27) = 79.6 | stat: FALSE | burn: 24
lPdatamean
−8.0
−8.5
−9.0
−9.5
0
5
10
15
20
25
30

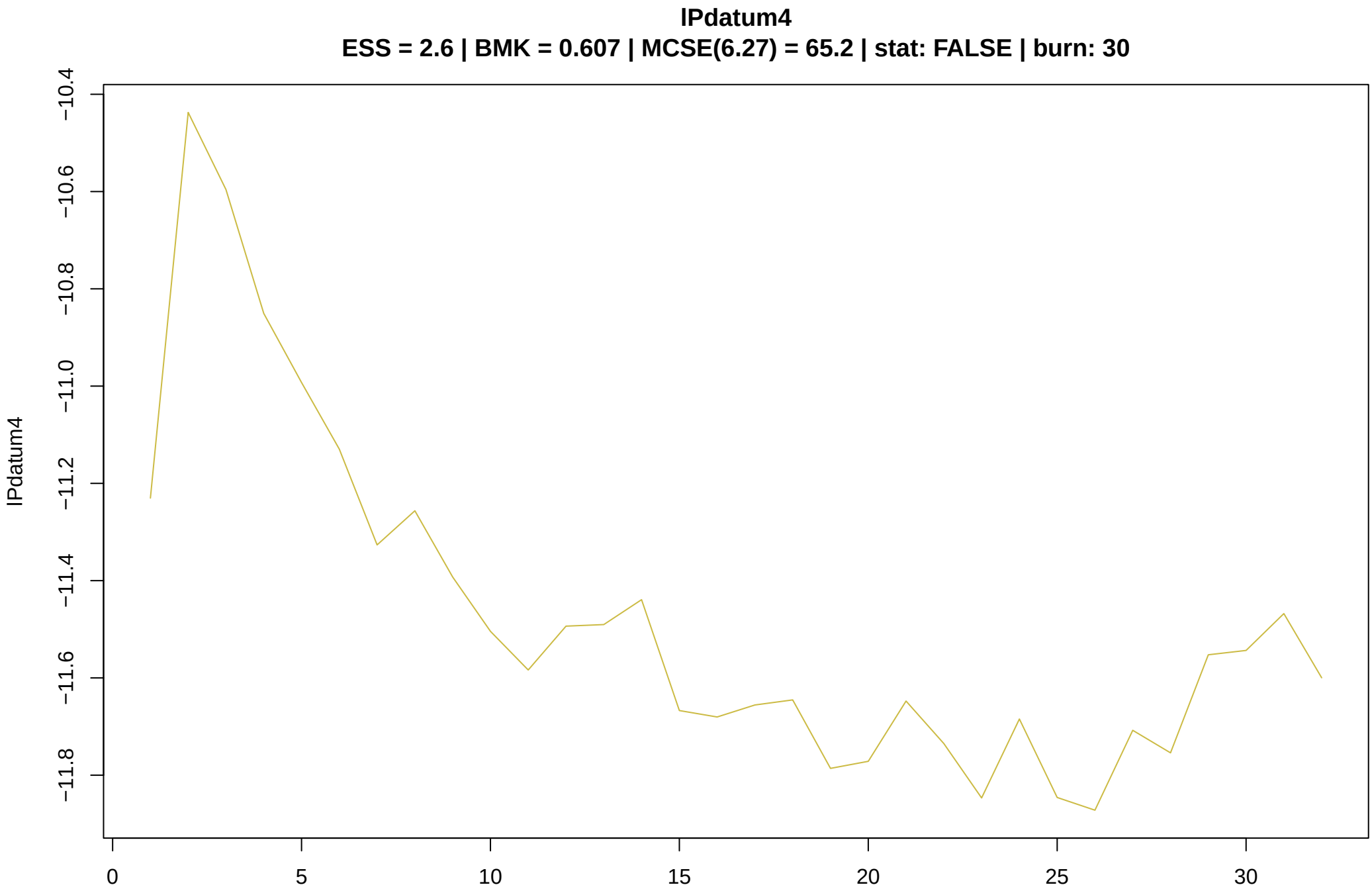

lPcornerHi
ESS = 11.9 | BMK = 0.341 | MCSE(6.27) = 34.8 | stat: FALSE | burn: 30
lPcornerHi
−14.5
−15.0
−15.5
−16.0
−16.5
0
5
10
15
20
25
30

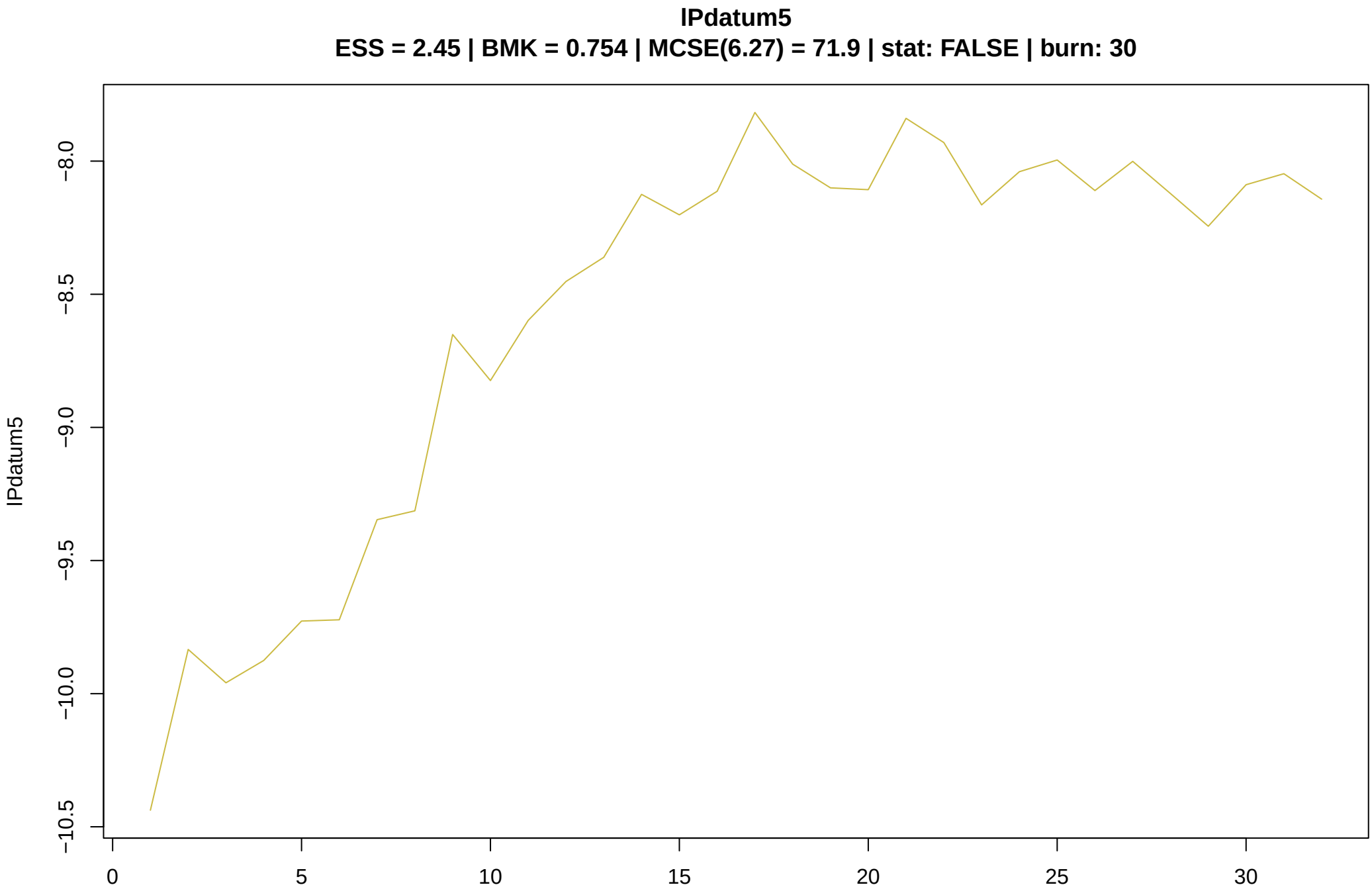

lPcornerLo
ESS = 2.7 | BMK = 0.818 | MCSE(6.27) = 70.1 | stat: FALSE | burn: 15
lPcornerLo
−12
−13
−14
−15
−16
−17
0
5
10
15
20
25
30

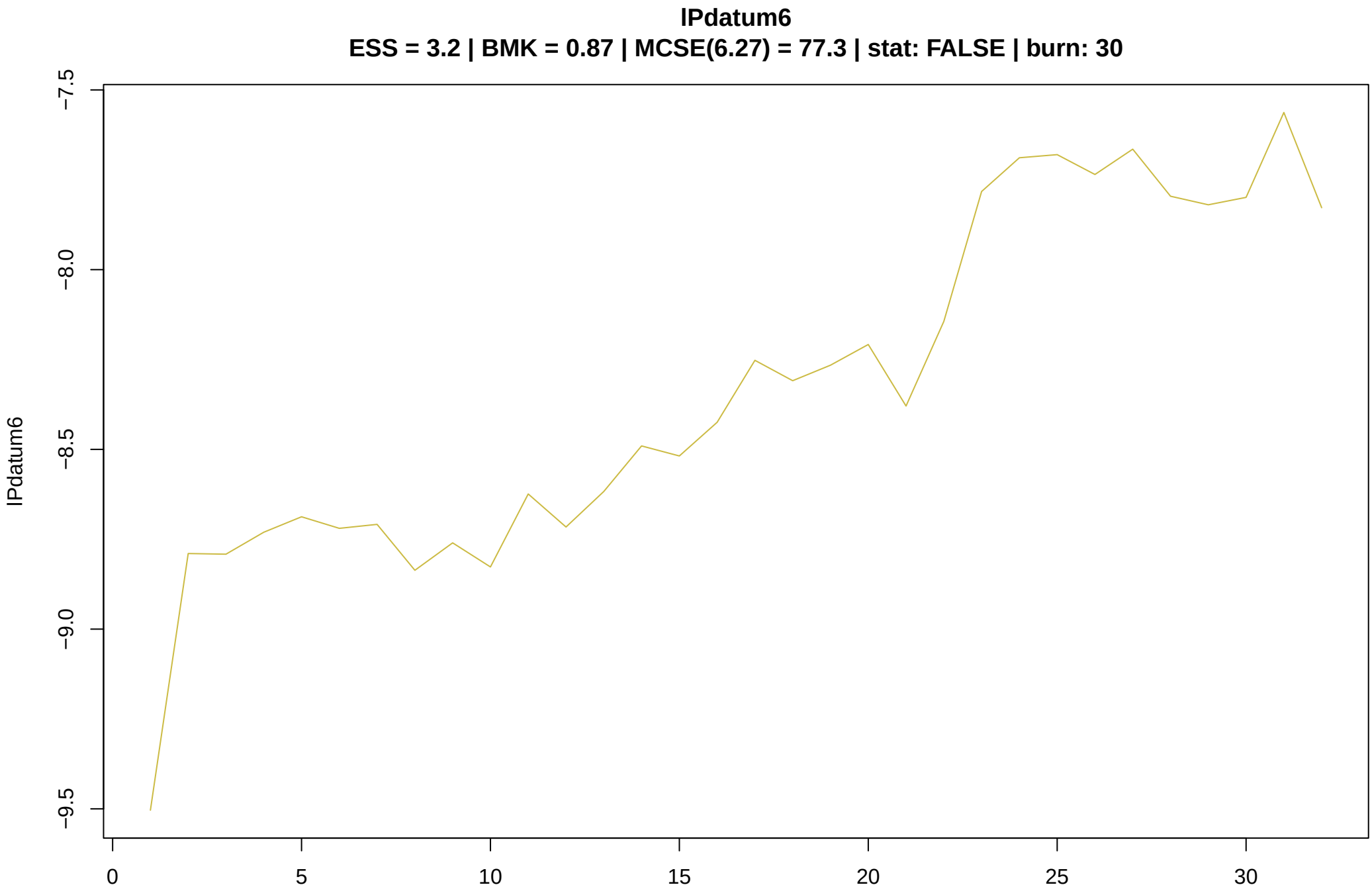

lPdatum1
ESS = 4.89 | BMK = 0.485 | MCSE(6.27) = 55.4 | stat: FALSE | burn: 12
lPdatum1
−9.5
−10.0
−10.5
−11.0
0
5
10
15
20
25
30

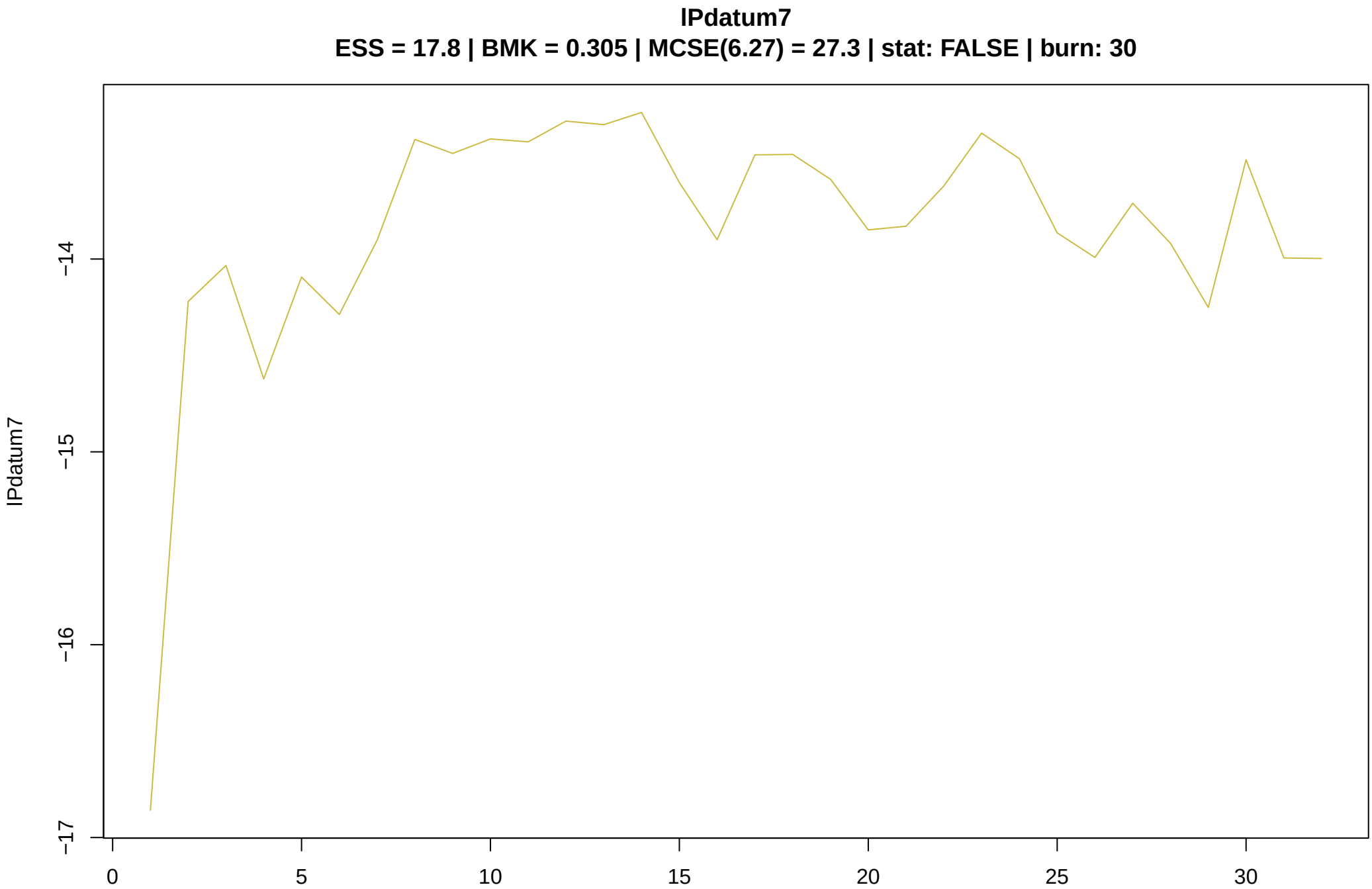

lPdatum2
ESS = 14.4 | BMK = 0.478 | MCSE(6.27) = 38.2 | stat: FALSE | burn: 30
lPdatum2
−9.6
−9.8
−10.0
−10.2
−10.4
−10.6
0
5
10
15
20
25
30

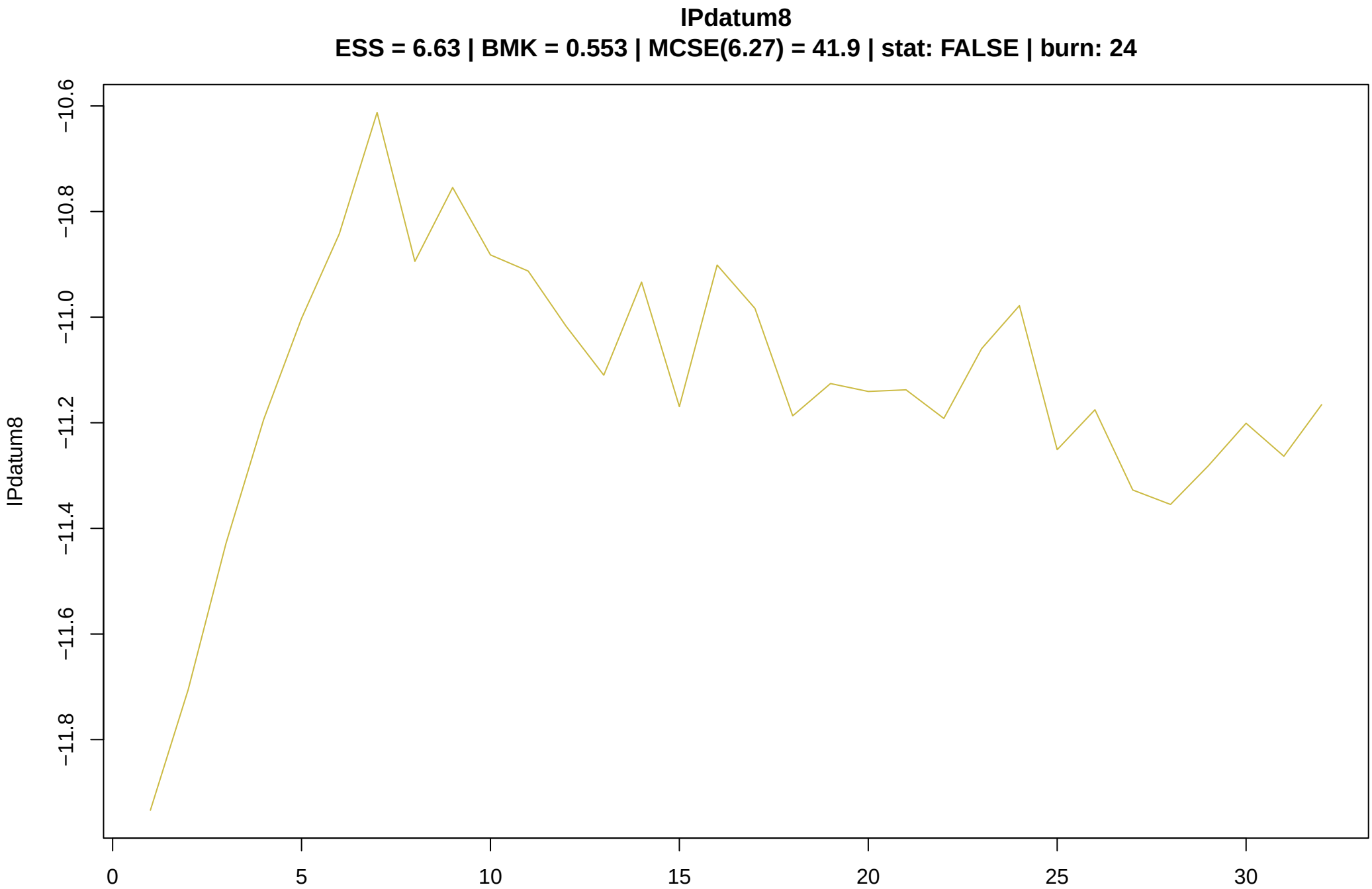

lPdatum3
ESS = 6.74 | BMK = 0.421 | MCSE(6.27) = 35.6 | stat: FALSE | burn: 24
lPdatum3
−13.6
−13.8
−14.0
−14.2
−14.4
−14.6
−14.8
0
5
10
15
20
25
30

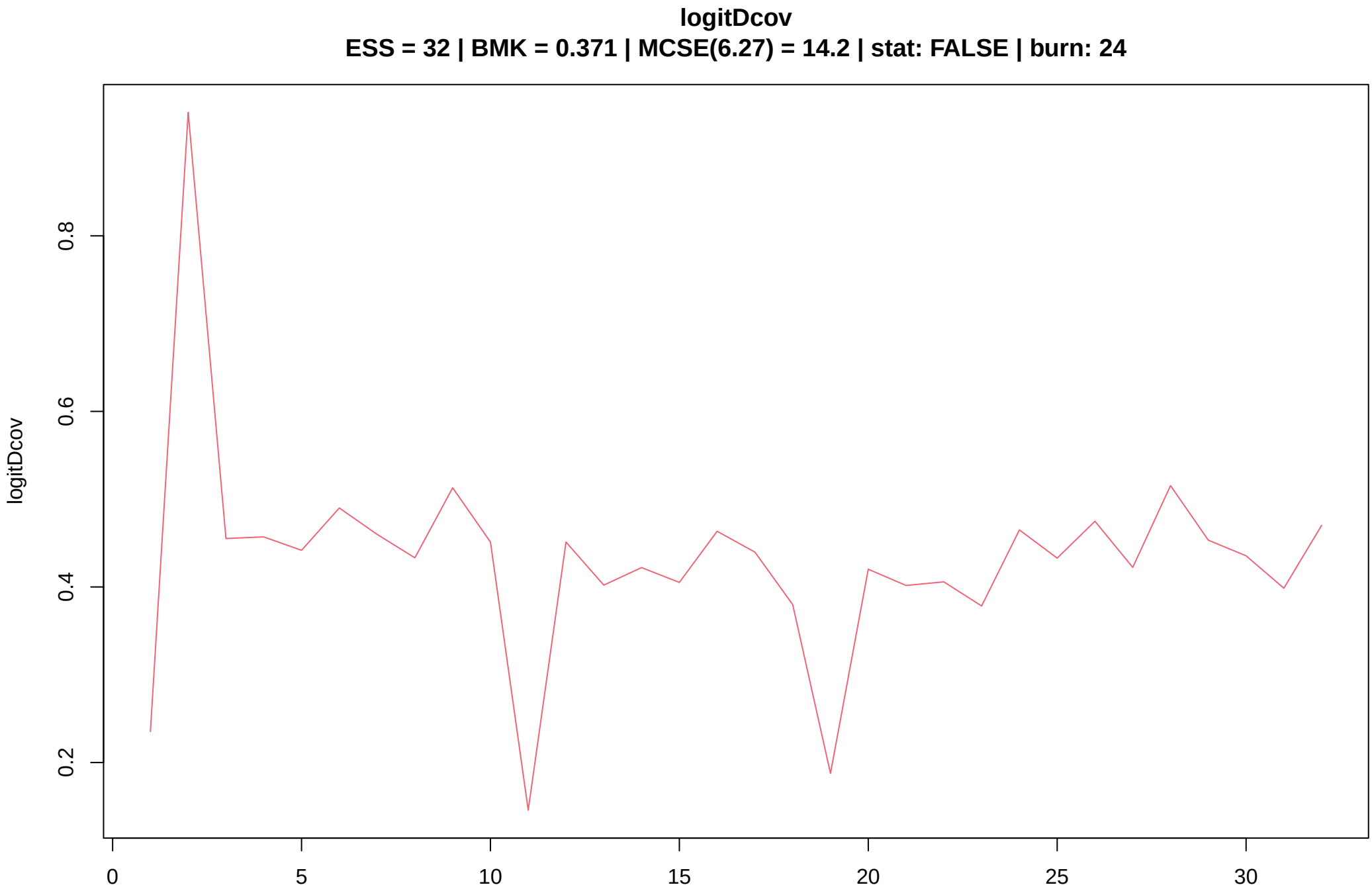

lPdatum4
ESS = 2.6 | BMK = 0.607 | MCSE(6.27) = 65.2 | stat: FALSE | burn: 30
lPdatum4
−10.4
−10.6
−10.8
−11.0
−11.2
−11.4
−11.6
−11.8
0
5
10
15
20
25
30

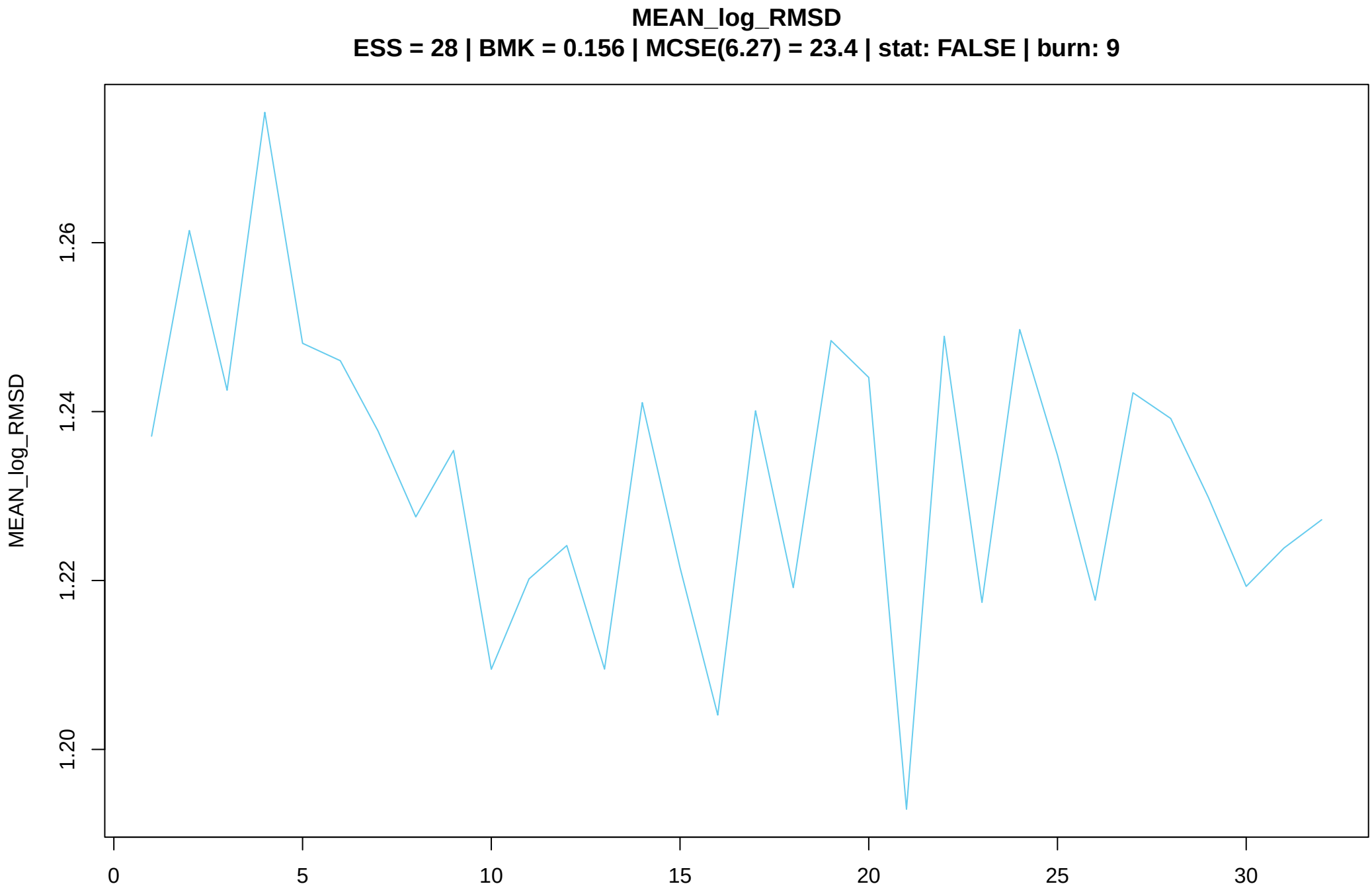

lPdatum5
ESS = 2.45 | BMK = 0.754 | MCSE(6.27) = 71.9 | stat: FALSE | burn: 30
lPdatum5
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
5
10
15
20
25
30

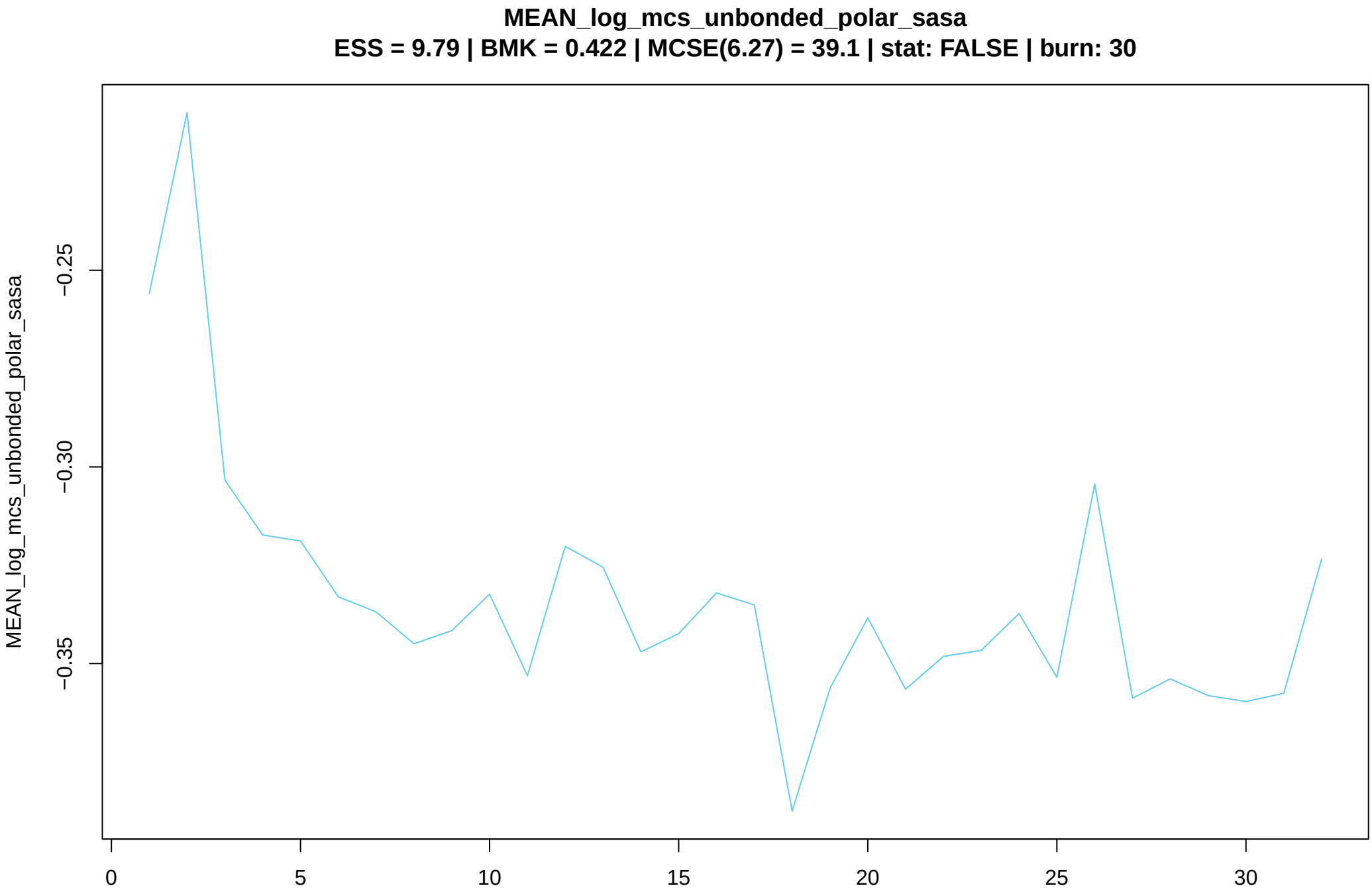

lPdatum6
ESS = 3.2 | BMK = 0.87 | MCSE(6.27) = 77.3 | stat: FALSE | burn: 30
lPdatum6
−7.5
−8.0
−8.5
−9.0
−9.5
0
5
10
15
20
25
30

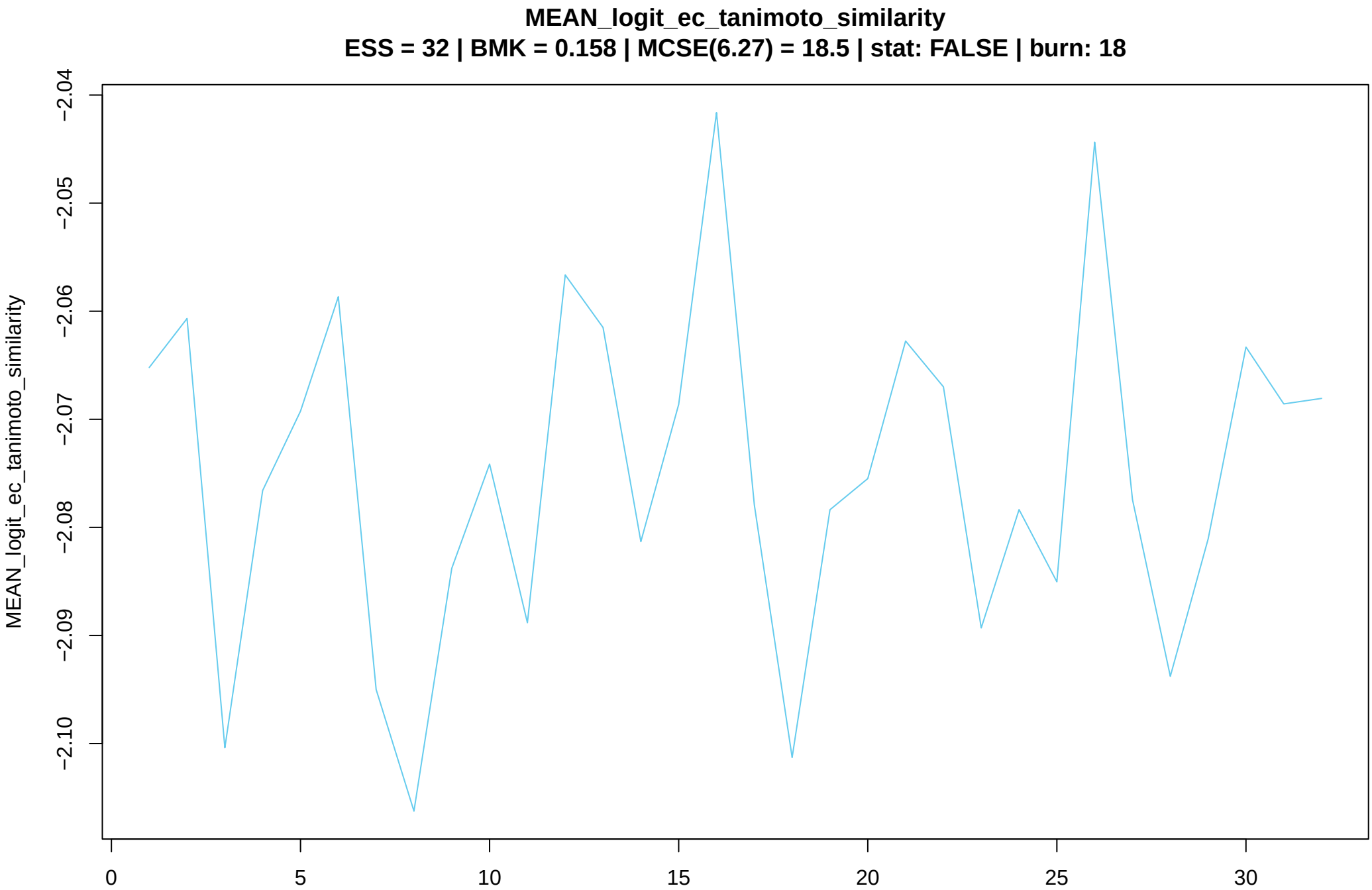

lPdatum7
ESS = 17.8 | BMK = 0.305 | MCSE(6.27) = 27.3 | stat: FALSE | burn: 30
lPdatum7
−14
−15
−16
−17
0
5
10
15
20
25
30

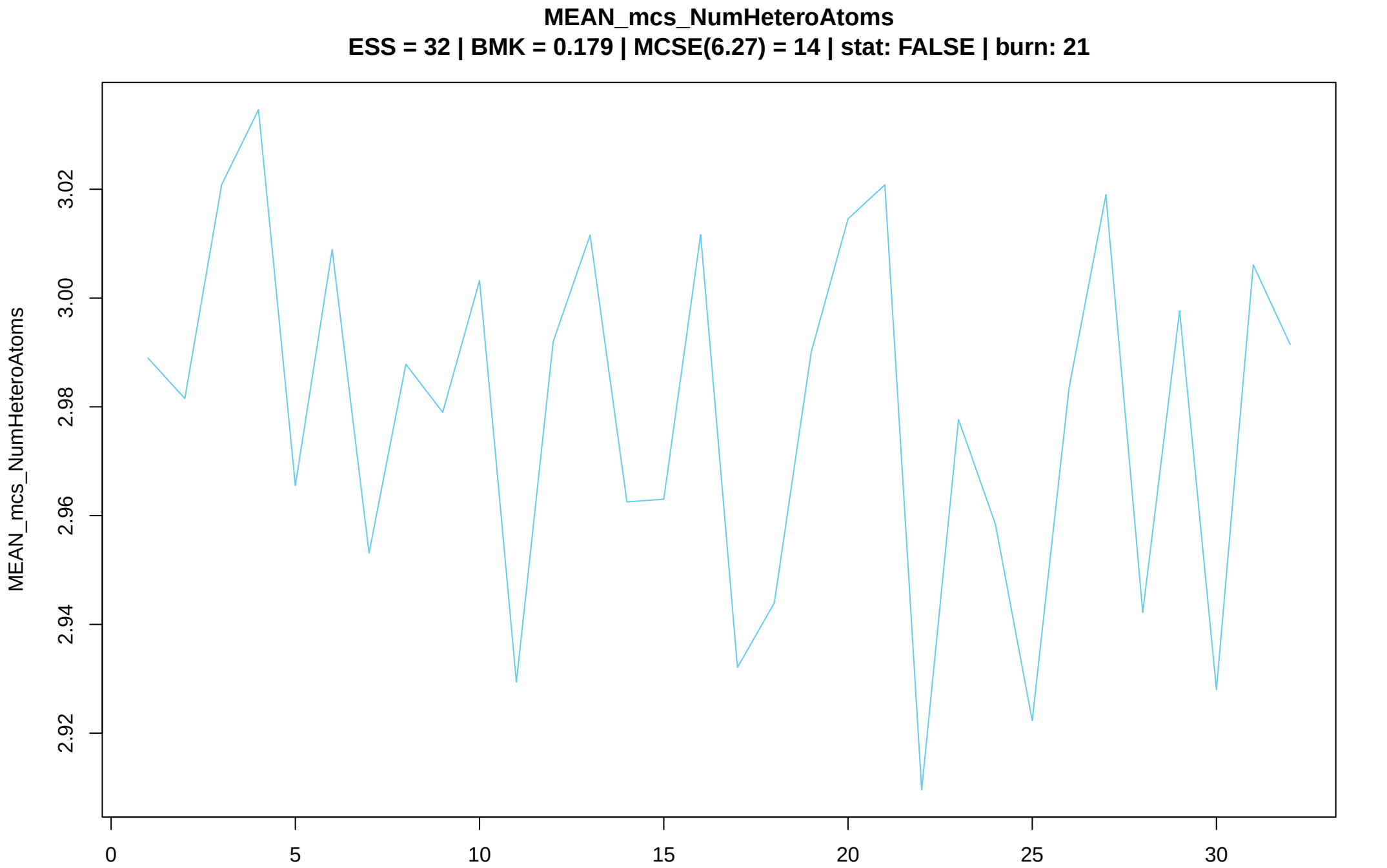

lPdatum8
ESS = 6.63 | BMK = 0.553 | MCSE(6.27) = 41.9 | stat: FALSE | burn: 24
lPdatum8
−10.6
−10.8
−11.0
−11.2
−11.4
−11.6
−11.8
0
5
10
15
20
25
30

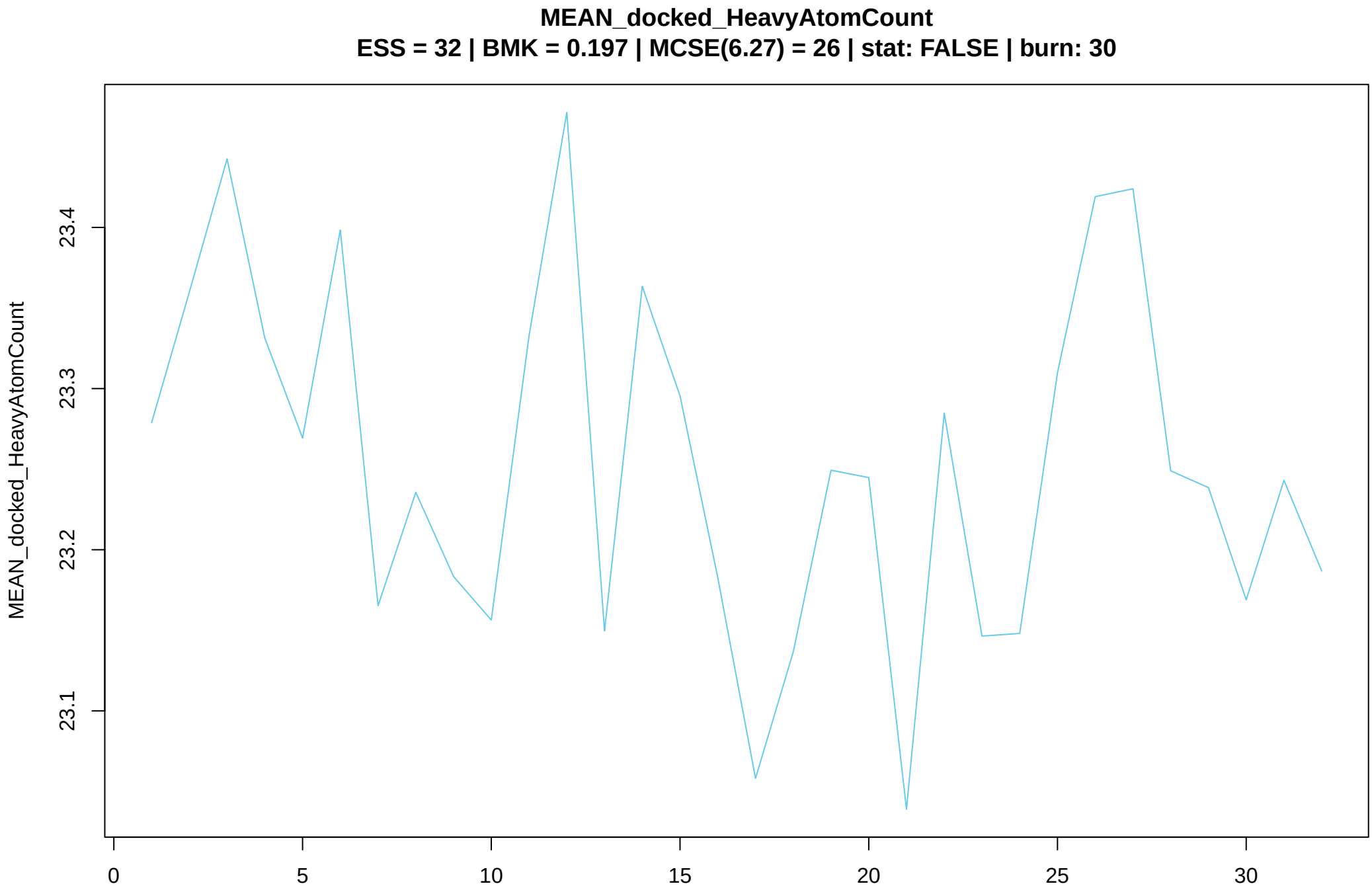

logitDcov
ESS = 32 | BMK = 0.371 | MCSE(6.27) = 14.2 | stat: FALSE | burn: 24
logitDcov
0.2
0.4
0.6
0.8
0
5
10
15
20
25
30

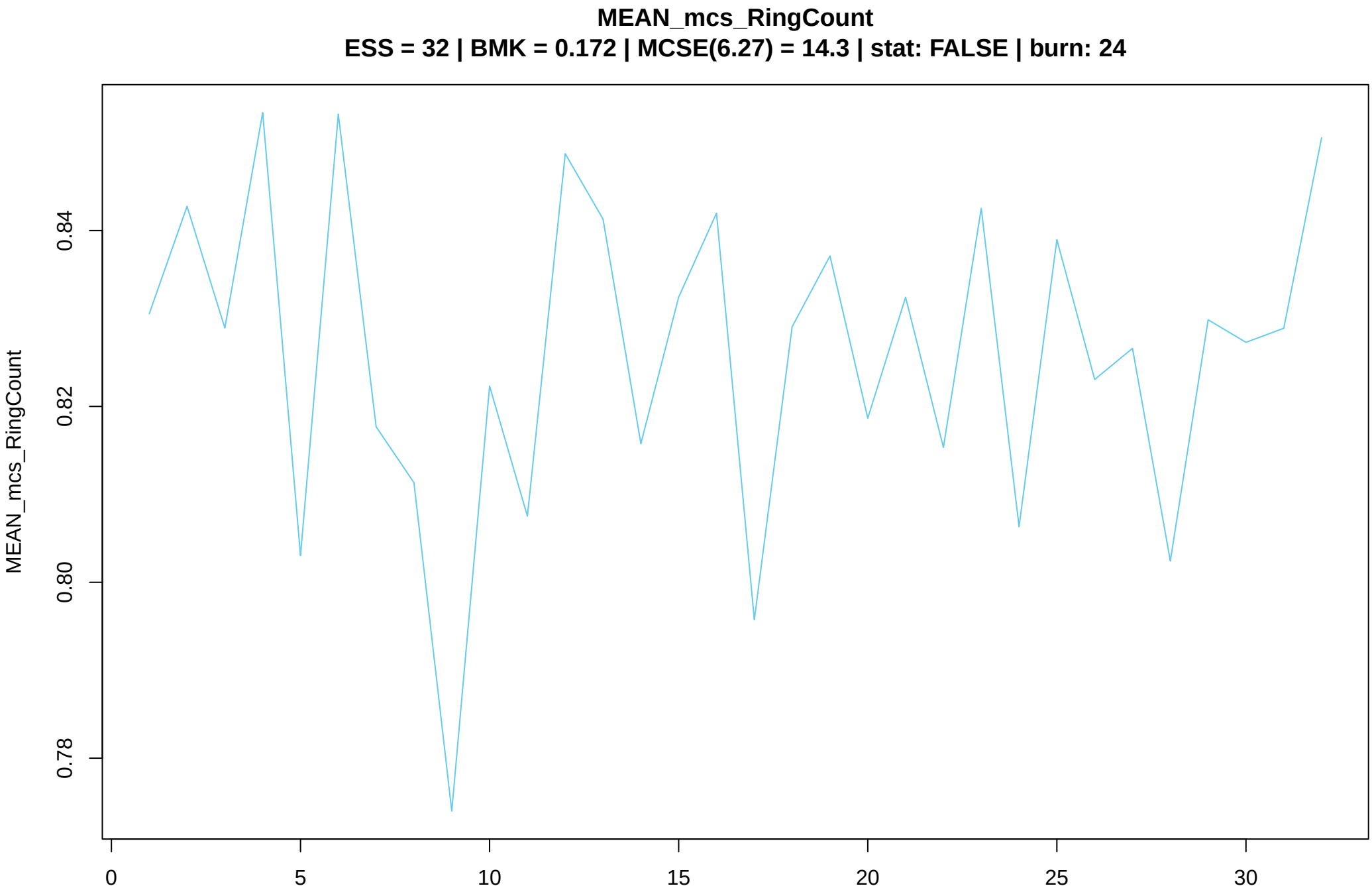

MEAN_log_RMSD
ESS = 28 | BMK = 0.156 | MCSE(6.27) = 23.4 | stat: FALSE | burn: 9
MEAN_log_RMSD
1.20
1.22
1.24
1.26
0
5
10
15
20
25
30

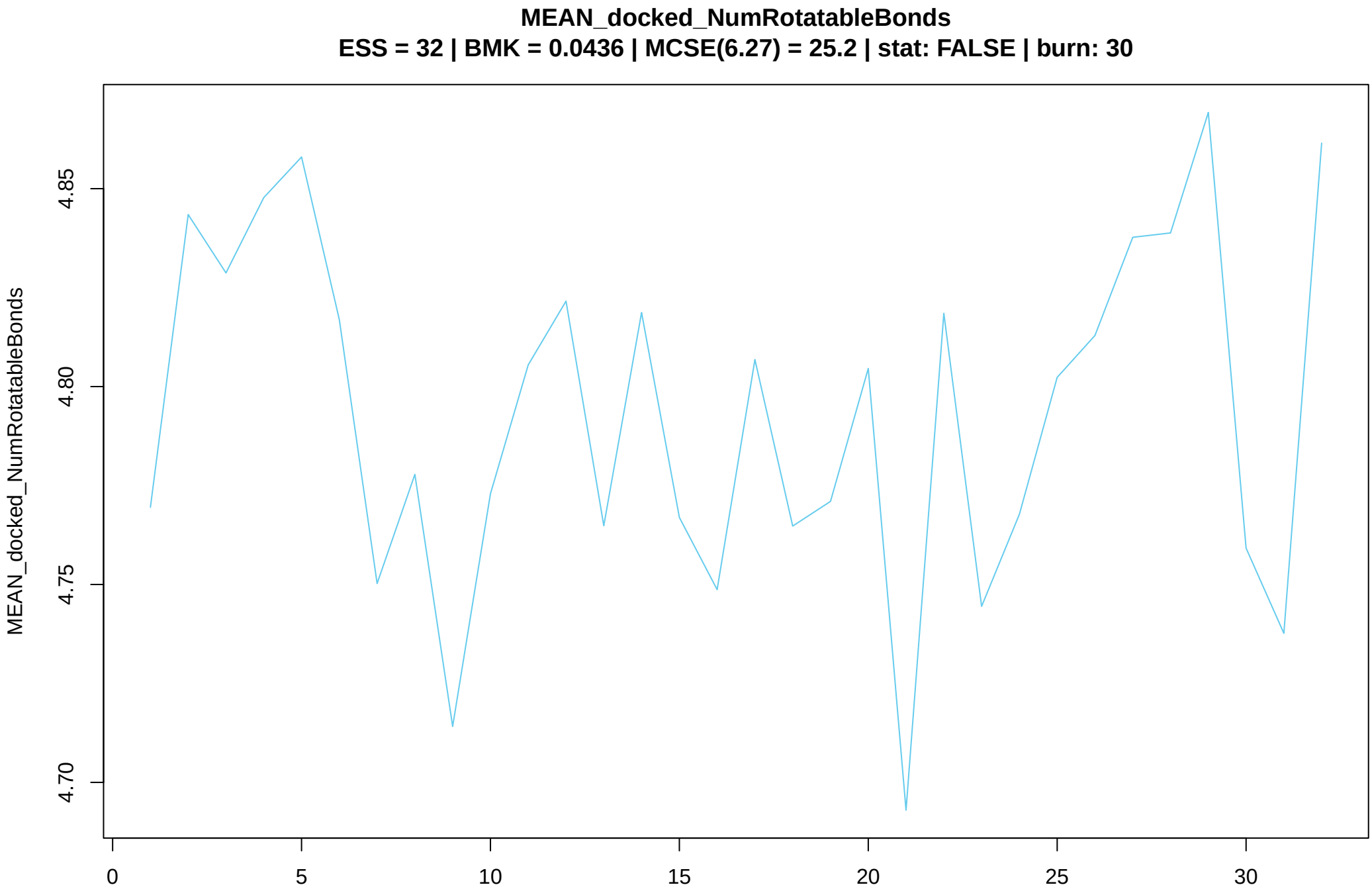

MEAN_log_mcs_unbonded_polar_sasa
ESS = 9.79 | BMK = 0.422 | MCSE(6.27) = 39.1 | stat: FALSE | burn: 30
MEAN_log_mcs_unbonded_polar_sasa
−0.25
−0.30
−0.35
0
5
10
15
20
25
30

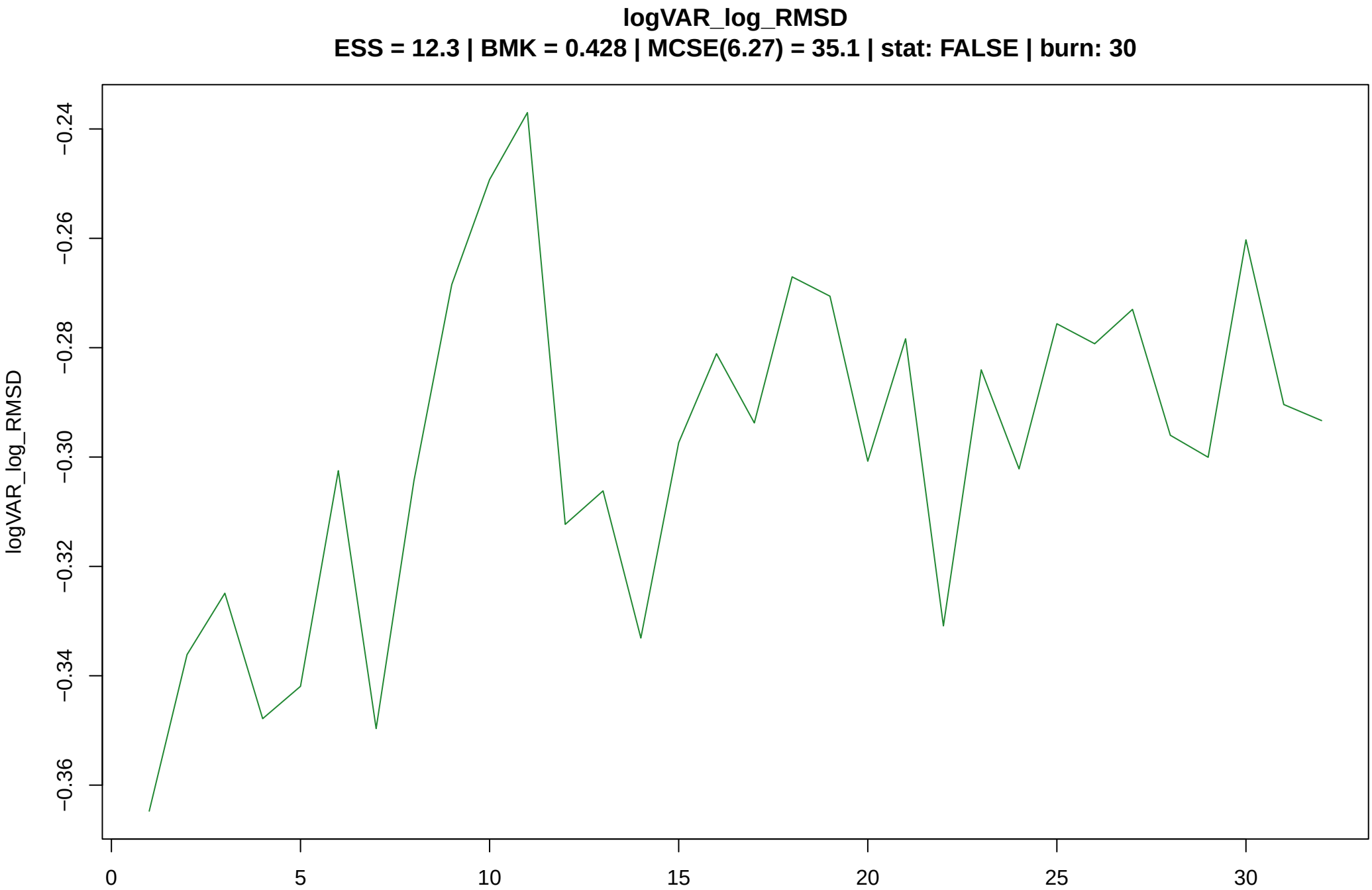

MEAN_logit_ec_tanimoto_similarity
ESS = 32 | BMK = 0.158 | MCSE(6.27) = 18.5 | stat: FALSE | burn: 18
MEAN_logit_ec_tanimoto_similarity
−2.04
−2.05
−2.06
−2.07
−2.08
−2.09
−2.10
0
5
10
15
20
25
30

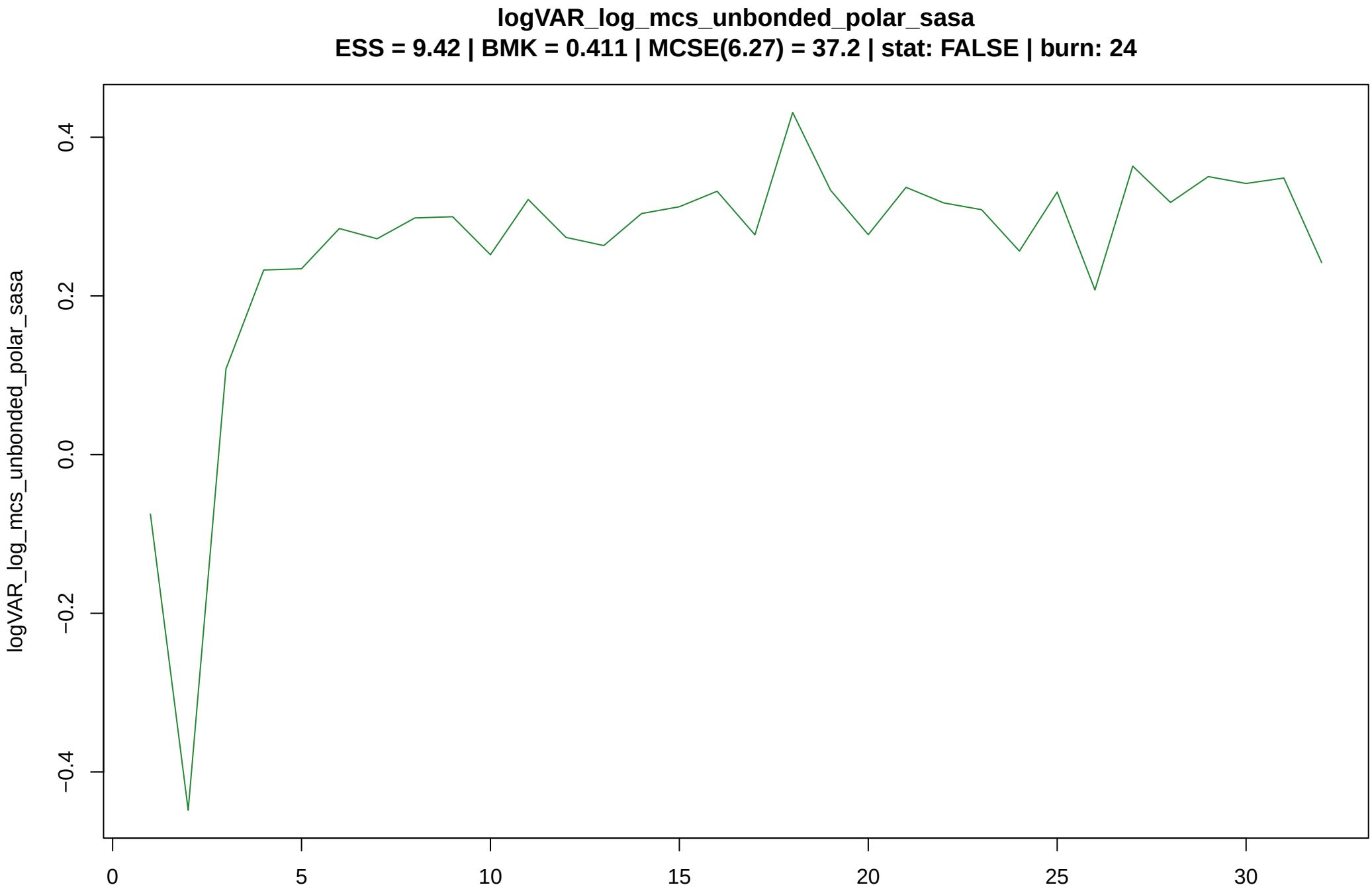

MEAN_mcs_NumHeteroAtoms
ESS = 32 | BMK = 0.179 | MCSE(6.27) = 14 | stat: FALSE | burn: 21
MEAN_mcs_NumHeteroAtoms
2.92
2.94
2.96
2.98
3.00
3.02
0
5
10
15
20
25
30

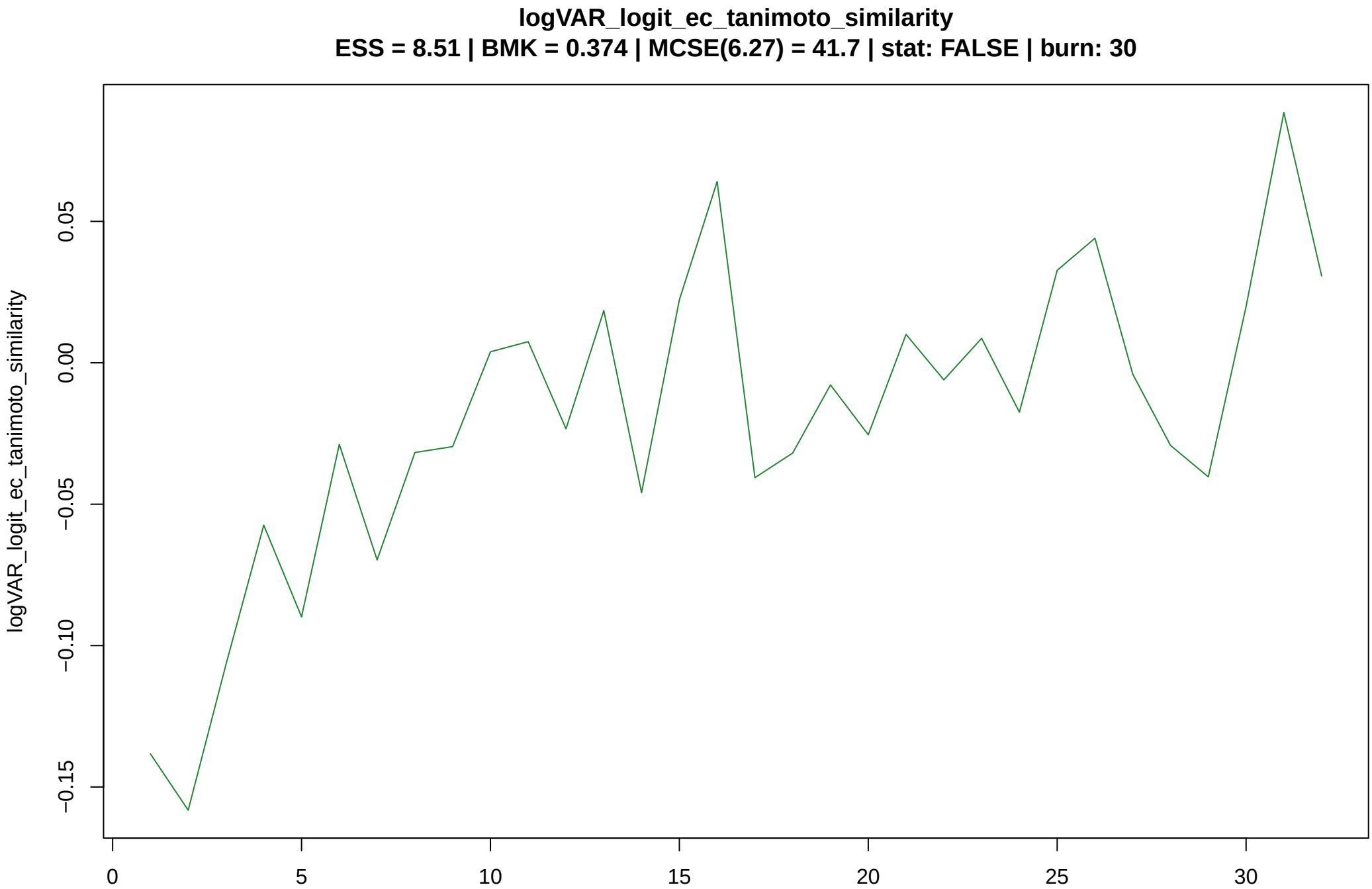

MEAN_docked_HeavyAtomCount
ESS = 32 | BMK = 0.197 | MCSE(6.27) = 26 | stat: FALSE | burn: 30
MEAN_docked_HeavyAtomCount
23.1
23.2
23.3
23.4
0
5
10
15
20
25
30

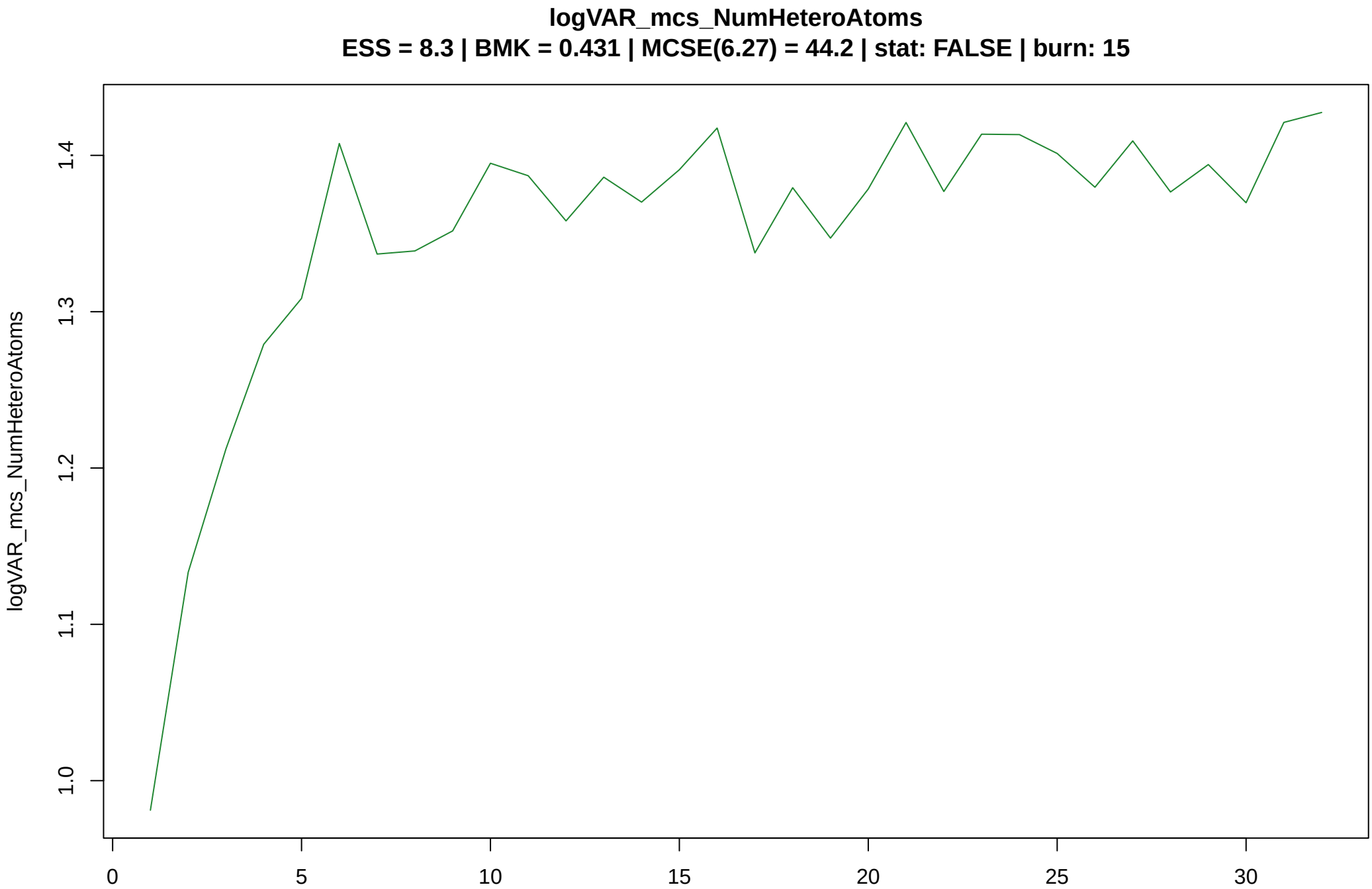

MEAN_mcs_RingCount
ESS = 32 | BMK = 0.172 | MCSE(6.27) = 14.3 | stat: FALSE | burn: 24
MEAN_mcs_RingCount
0.78
0.80
0.82
0.84
0
5
10
15
20
25
30

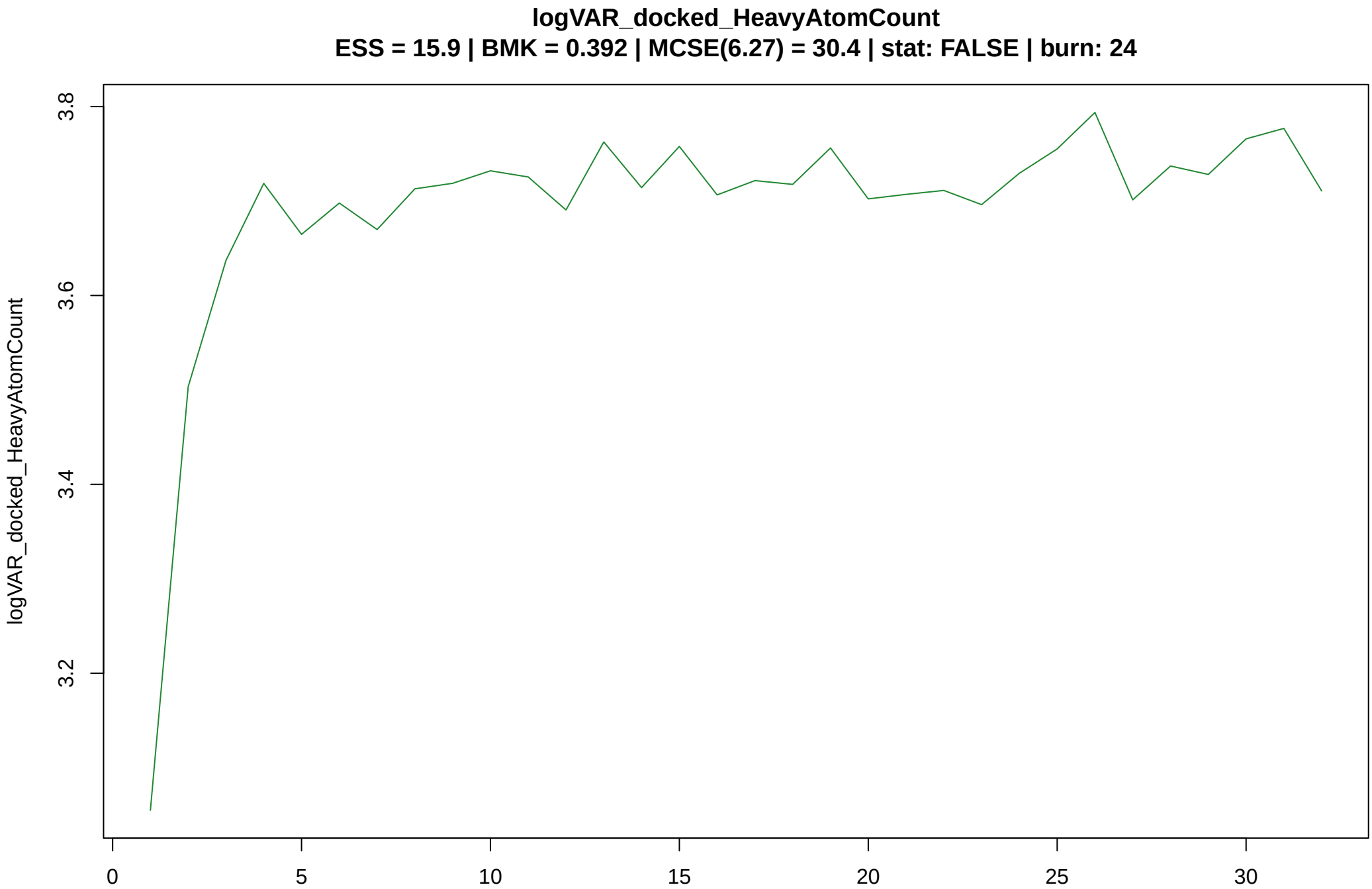

MEAN_docked_NumRotatableBonds
ESS = 32 | BMK = 0.0436 | MCSE(6.27) = 25.2 | stat: FALSE | burn: 30
MEAN_docked_NumRotatableBonds
4.70
4.75
4.80
4.85
0
5
10
15
20
25
30

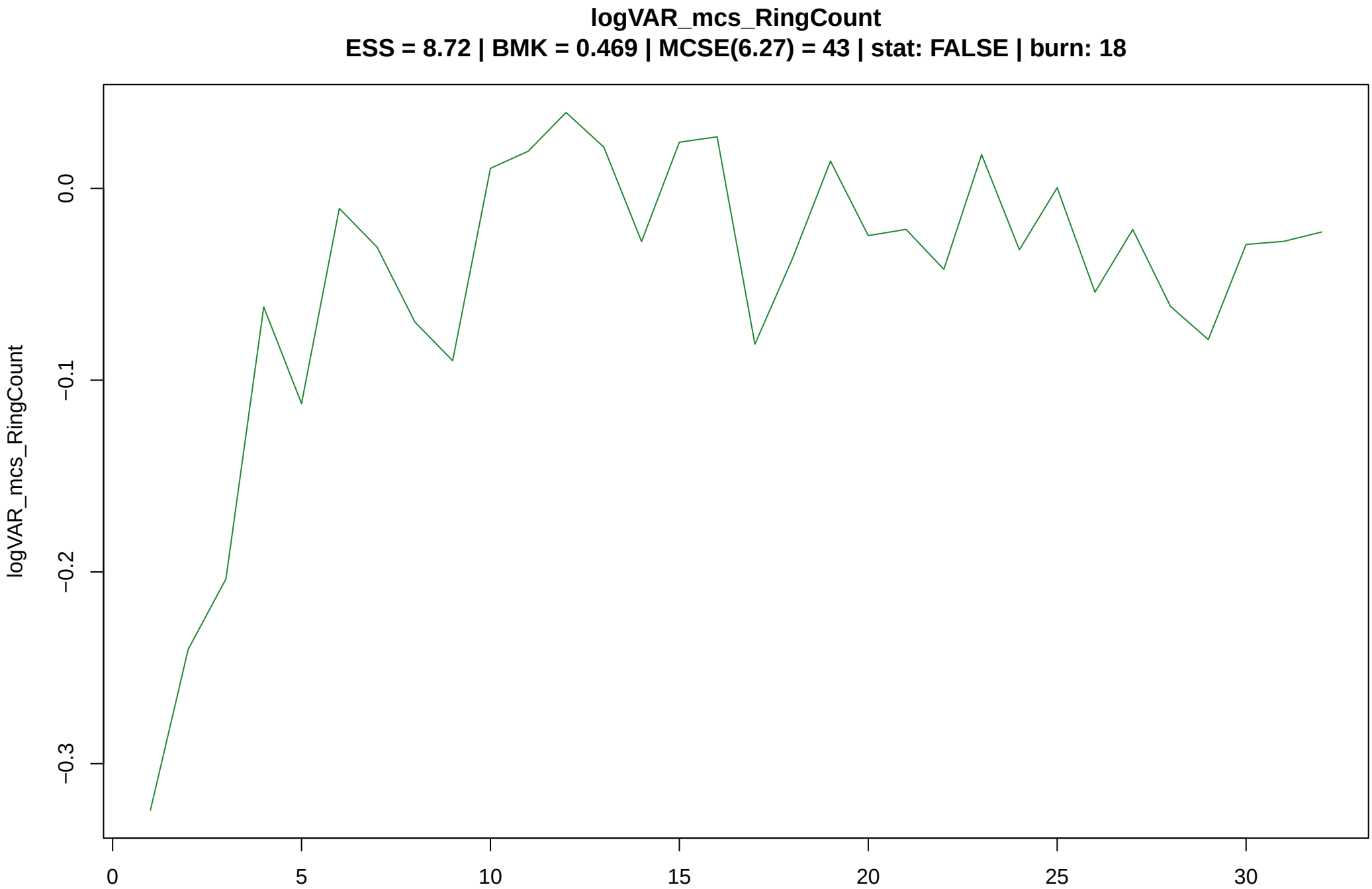

logVAR_log_RMSD
ESS = 12.3 | BMK = 0.428 | MCSE(6.27) = 35.1 | stat: FALSE | burn: 30
logVAR_log_RMSD
−0.24
−0.26
−0.28
−0.30
−0.32
−0.34
−0.36
0
5
10
15
20
25
30

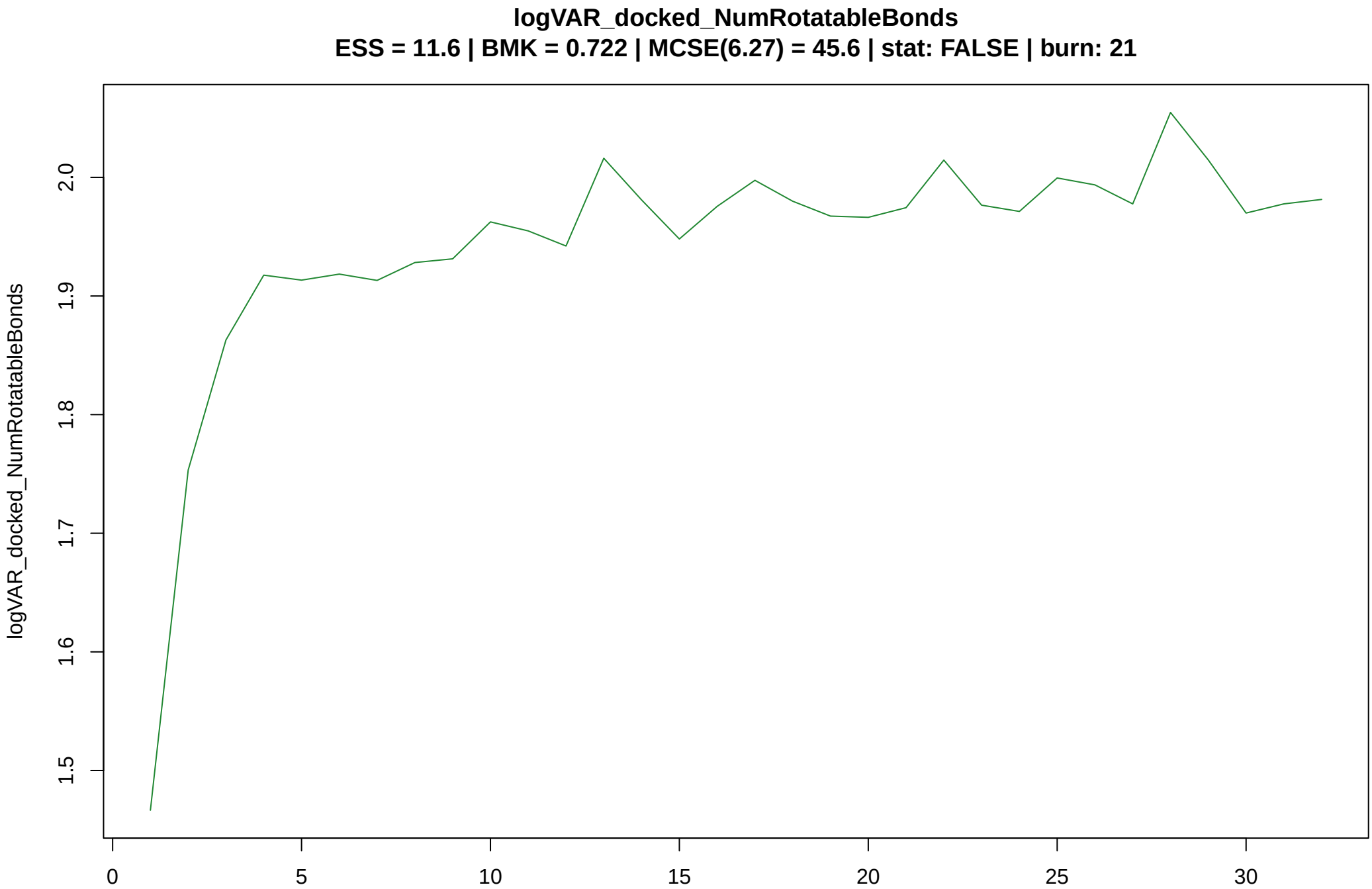

logVAR_log_mcs_unbonded_polar_sasa
ESS = 9.42 | BMK = 0.411 | MCSE(6.27) = 37.2 | stat: FALSE | burn: 24
logVAR_log_mcs_unbonded_polar_sasa
0.4
0.2
0.0
−0.2
−0.4
0
5
10
15
20
25
30

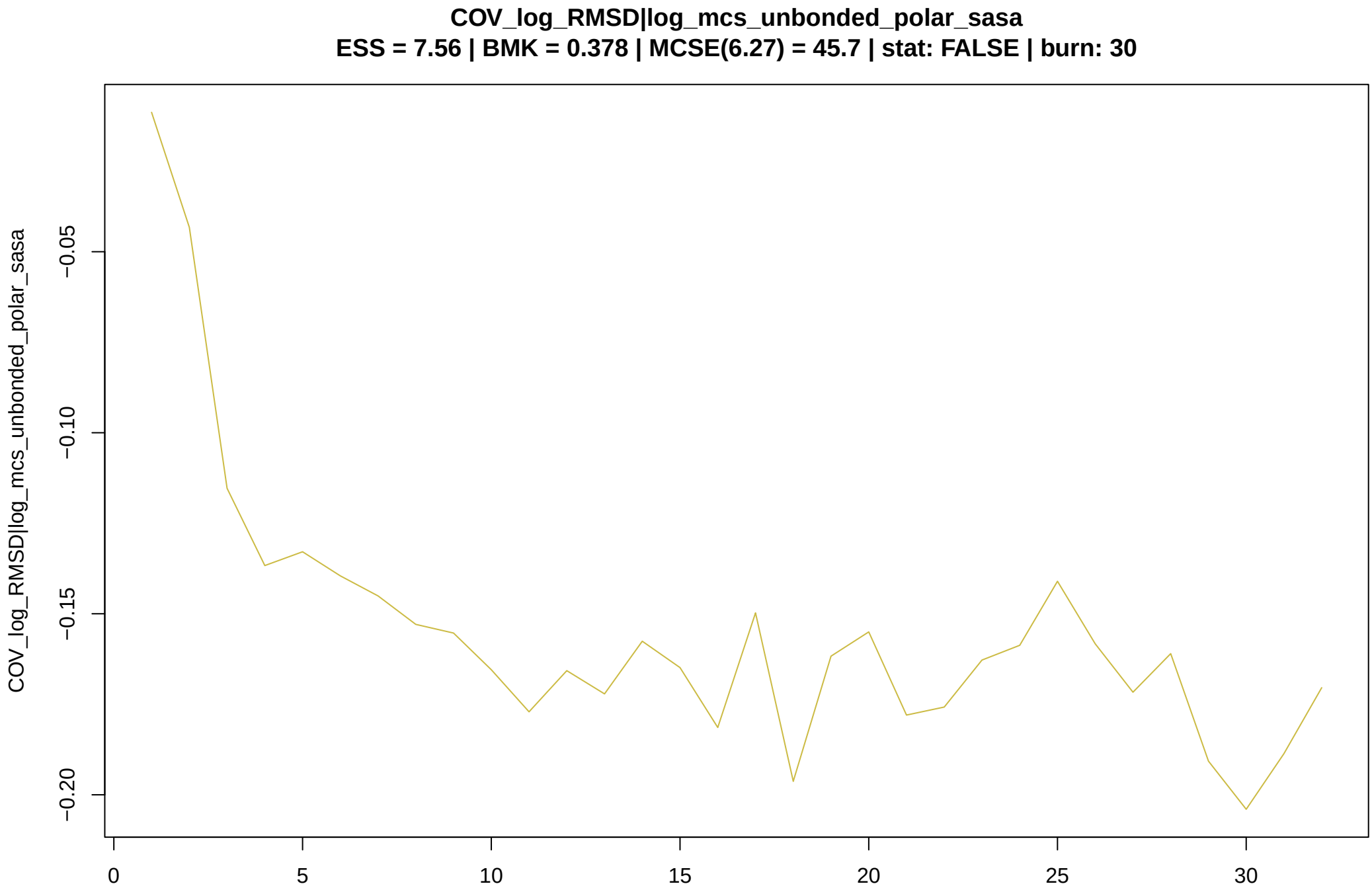

logVAR_logit_ec_tanimoto_similarity
ESS = 8.51 | BMK = 0.374 | MCSE(6.27) = 41.7 | stat: FALSE | burn: 30
logVAR_logit_ec_tanimoto_similarity
0.05
0.00
−0.05
−0.10
−0.15
0
5
10
15
20
25
30

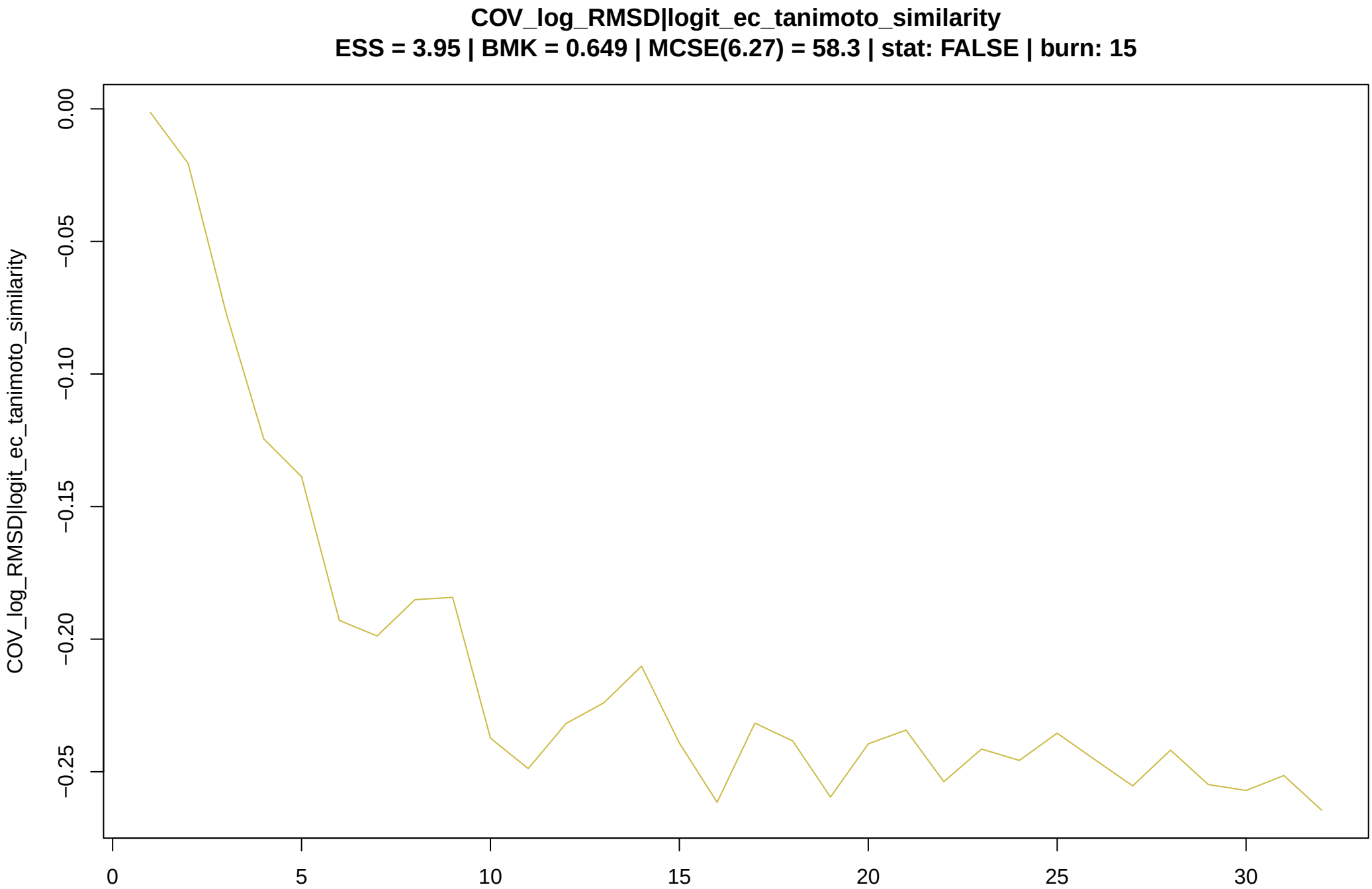

logVAR_mcs_NumHeteroAtoms
ESS = 8.3 | BMK = 0.431 | MCSE(6.27) = 44.2 | stat: FALSE | burn: 15
logVAR_mcs_NumHeteroAtoms
1.0
1.1
1.2
1.3
1.4
0
5
10
15
20
25
30

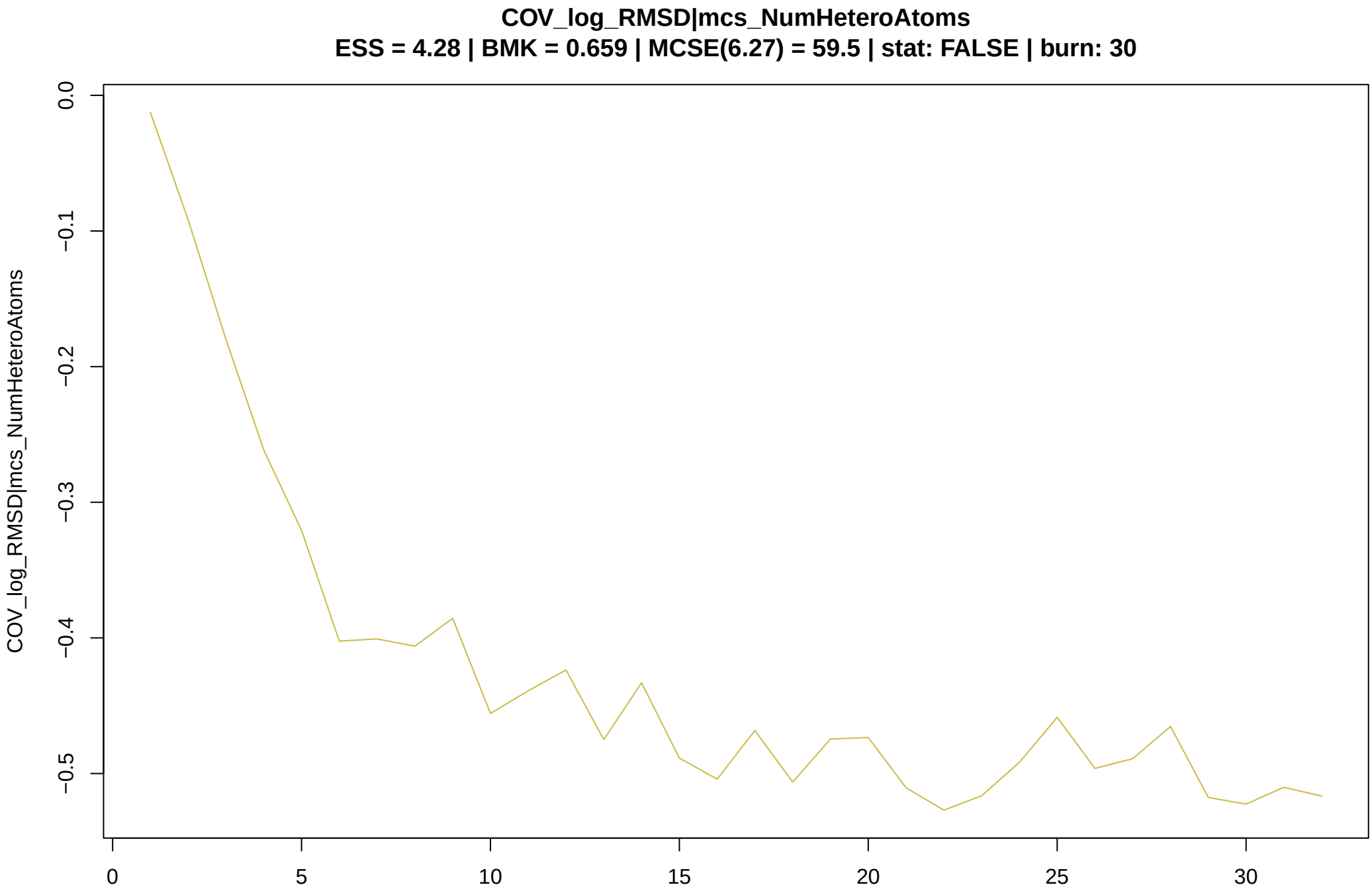

logVAR_docked_HeavyAtomCount
ESS = 15.9 | BMK = 0.392 | MCSE(6.27) = 30.4 | stat: FALSE | burn: 24
logVAR_docked_HeavyAtomCount
3.2
3.4
3.6
3.8
0
5
10
15
20
25
30

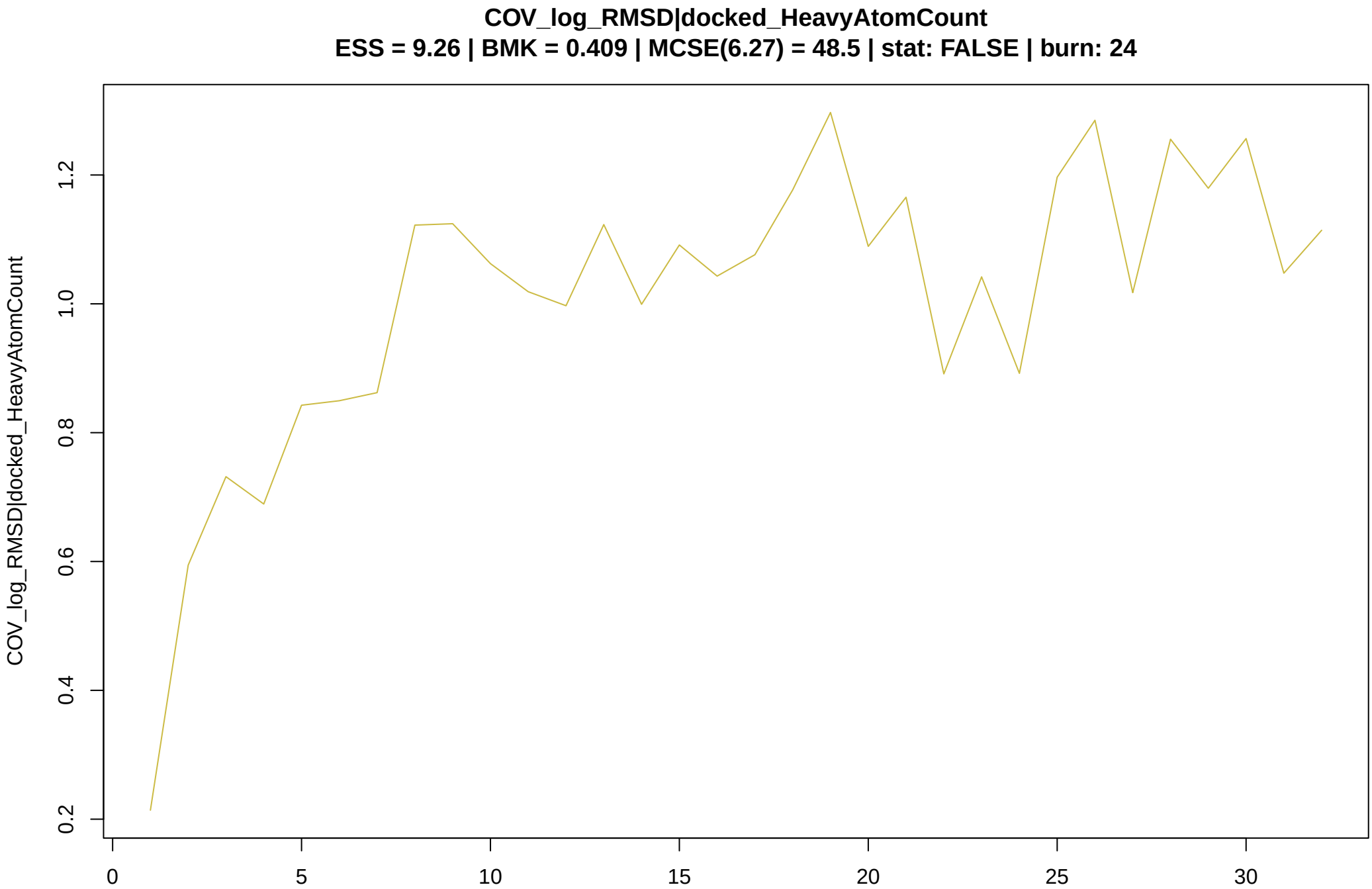

logVAR_mcs_RingCount
ESS = 8.72 | BMK = 0.469 | MCSE(6.27) = 43 | stat: FALSE | burn: 18
logVAR_mcs_RingCount
0.0
−0.1
−0.2
−0.3
0
5
10
15
20
25
30

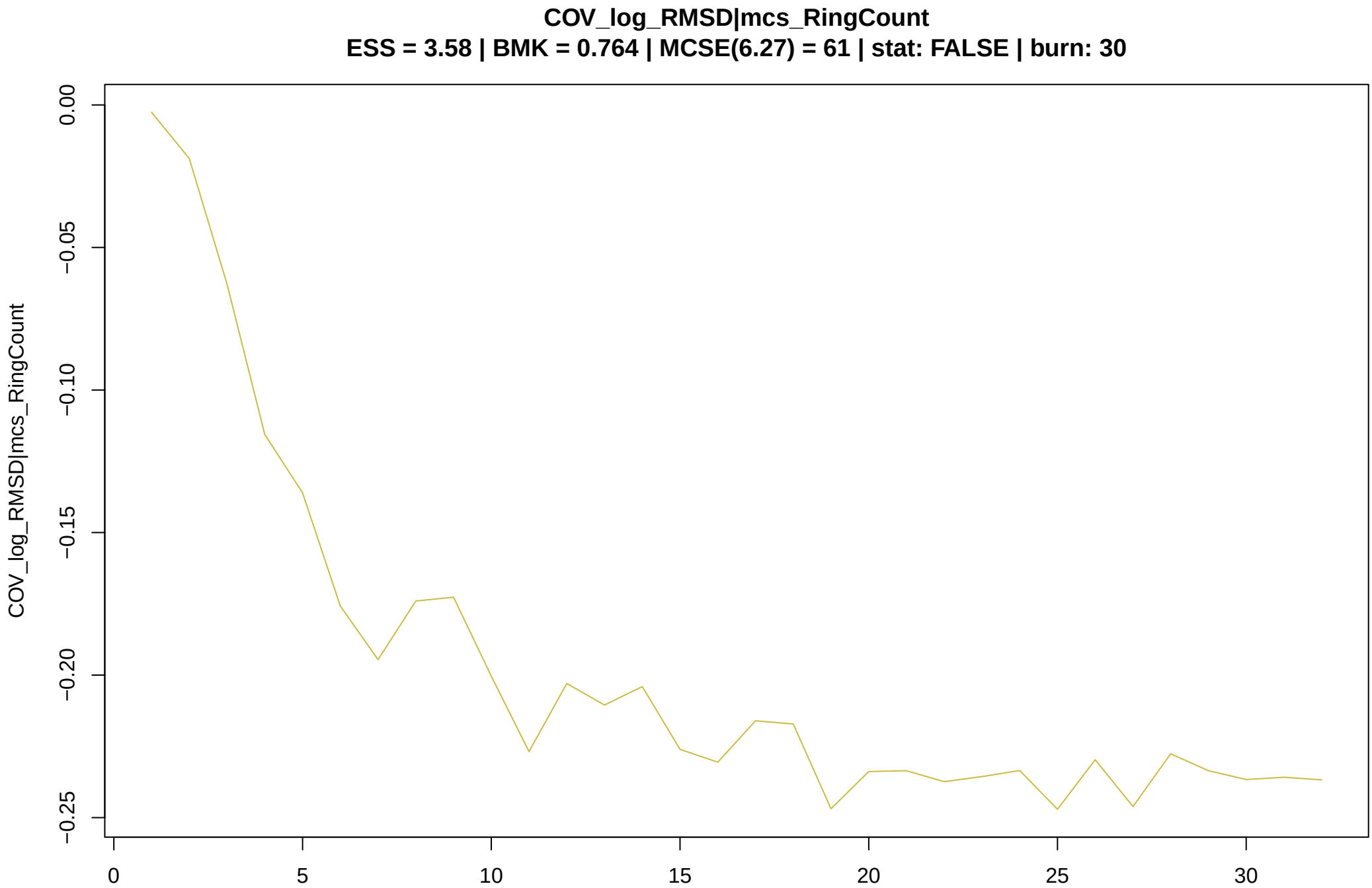

logVAR_docked_NumRotatableBonds
ESS = 11.6 | BMK = 0.722 | MCSE(6.27) = 45.6 | stat: FALSE | burn: 21
logVAR_docked_NumRotatableBonds
1.5
1.6
1.7
1.8
1.9
2.0
0
5
10
15
20
25
30

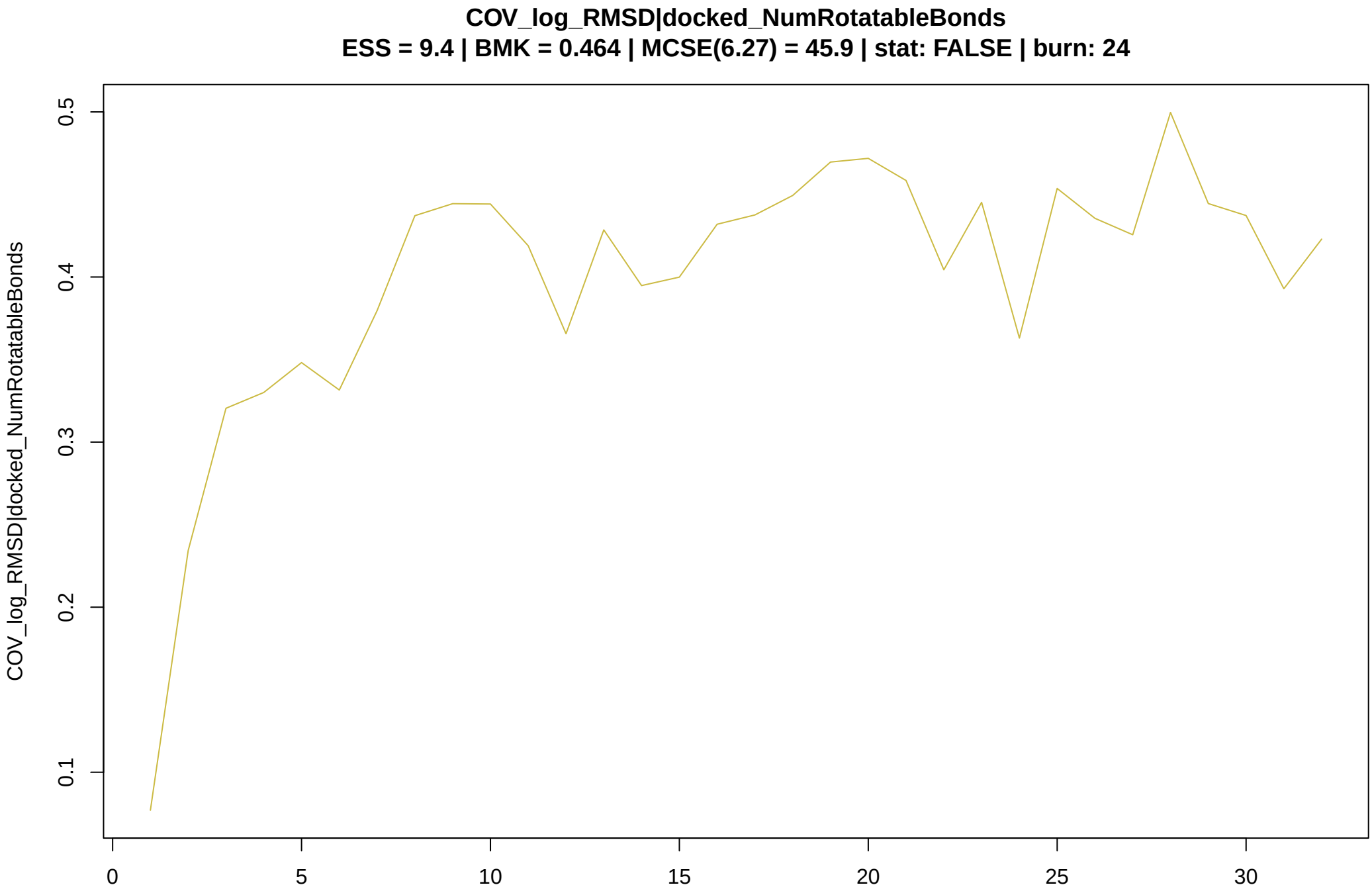

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 7.56 | BMK = 0.378 | MCSE(6.27) = 45.7 | stat: FALSE | burn: 30
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.05
−0.10
−0.15
−0.20
0
5
10
15
20
25
30

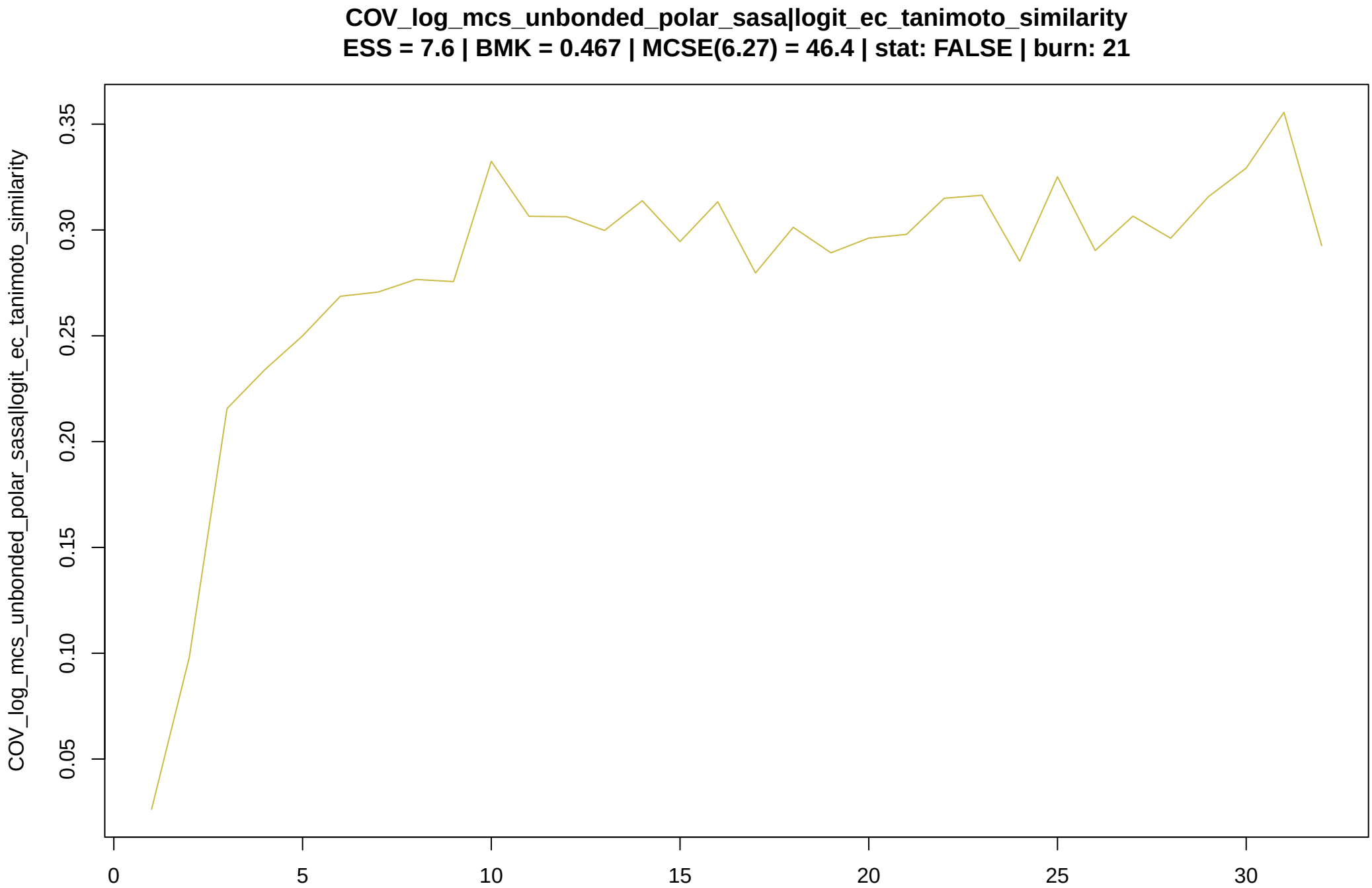

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 3.95 | BMK = 0.649 | MCSE(6.27) = 58.3 | stat: FALSE | burn: 15
COV_log_RMSD|logit_ec_tanimoto_similarity
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
0
5
10
15
20
25
30

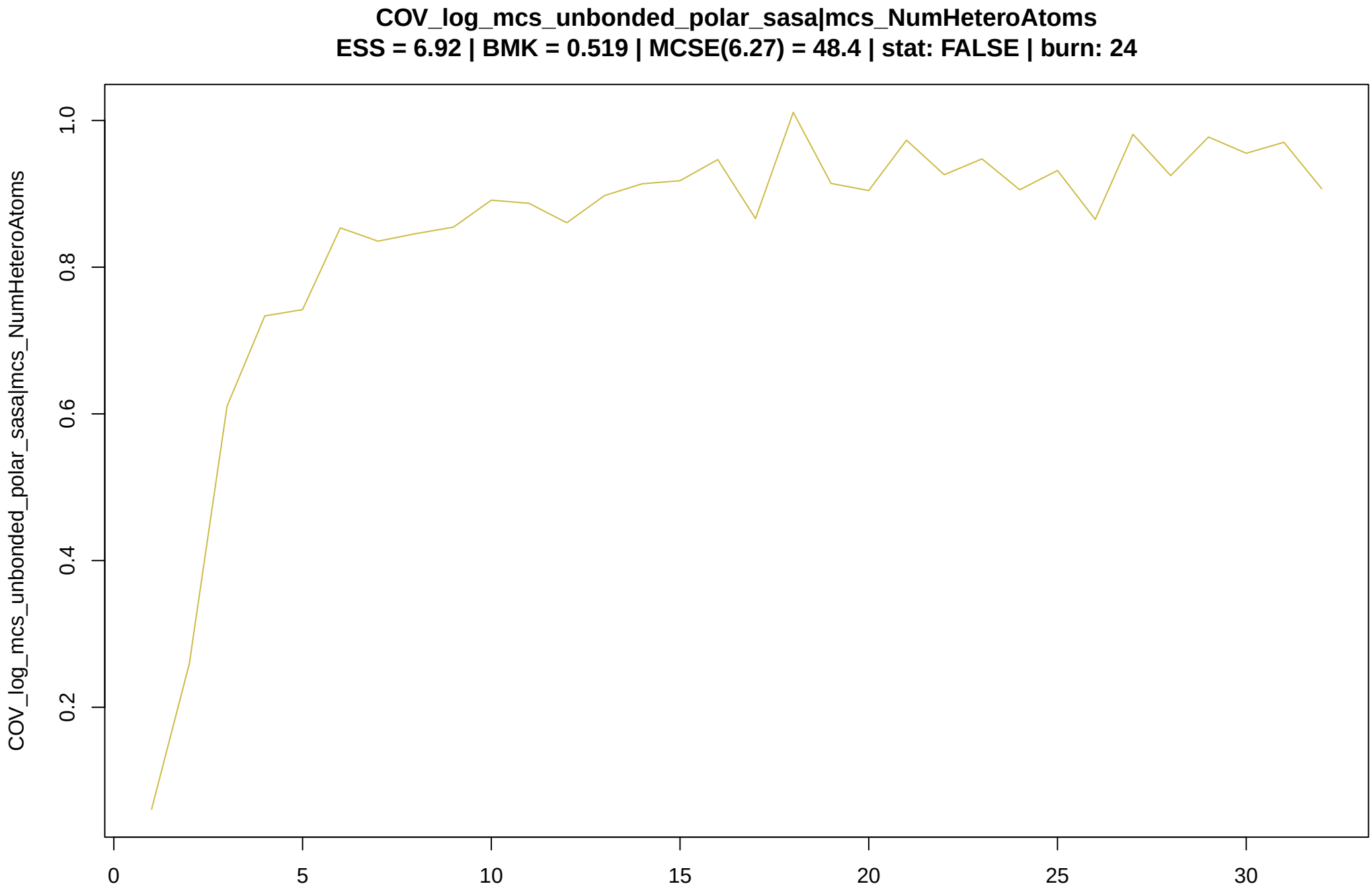

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 4.28 | BMK = 0.659 | MCSE(6.27) = 59.5 | stat: FALSE | burn: 30
COV_log_RMSD|mcs_NumHeteroAtoms
0.0
−0.1
−0.2
−0.3
−0.4
−0.5
0
5
10
15
20
25
30

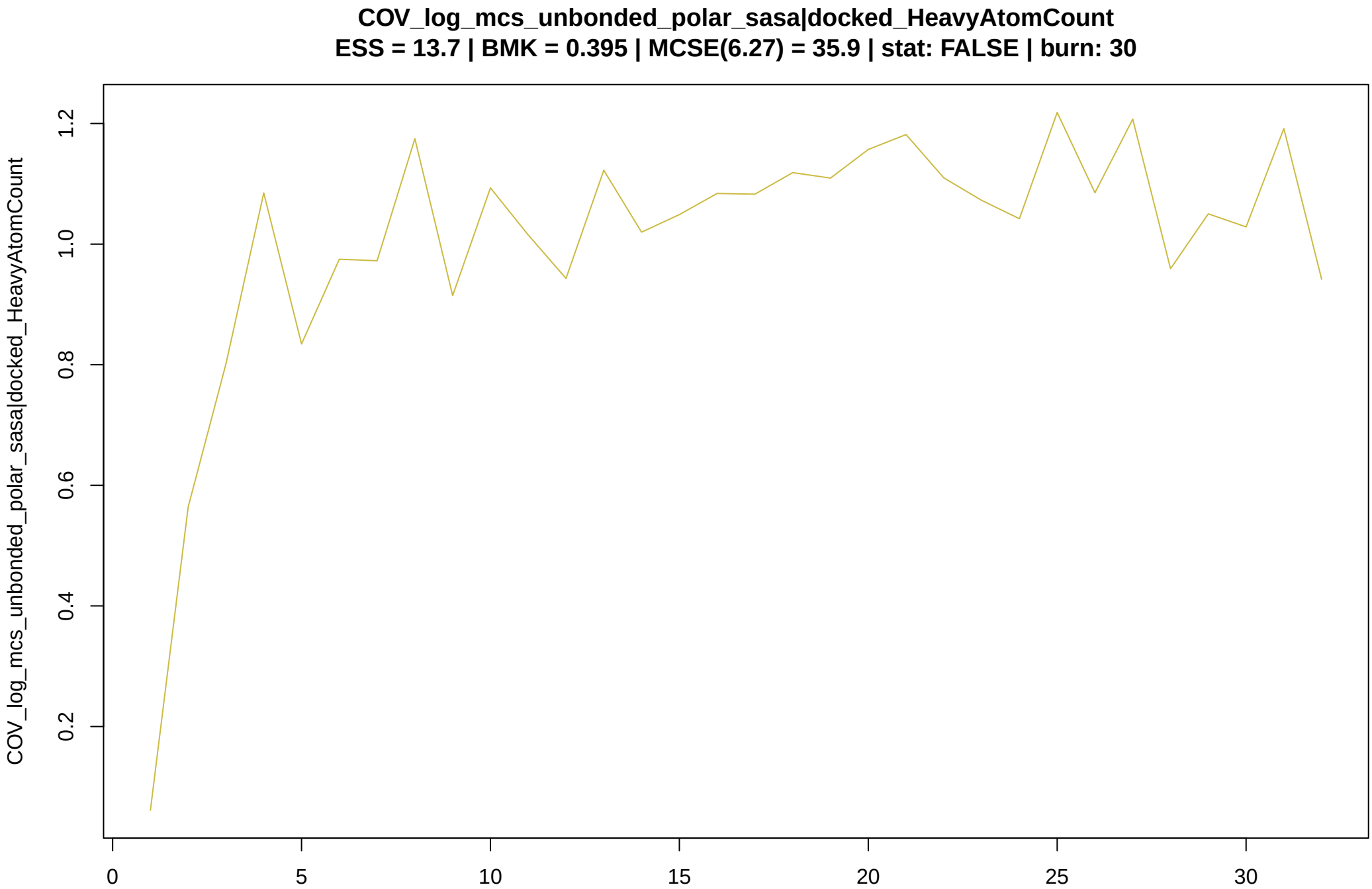

COV_log_RMSD|docked_HeavyAtomCount
ESS = 9.26 | BMK = 0.409 | MCSE(6.27) = 48.5 | stat: FALSE | burn: 24
COV_log_RMSD|docked_HeavyAtomCount
0.2
0.4
0.6
0.8
1.0
1.2
0
5
10
15
20
25
30

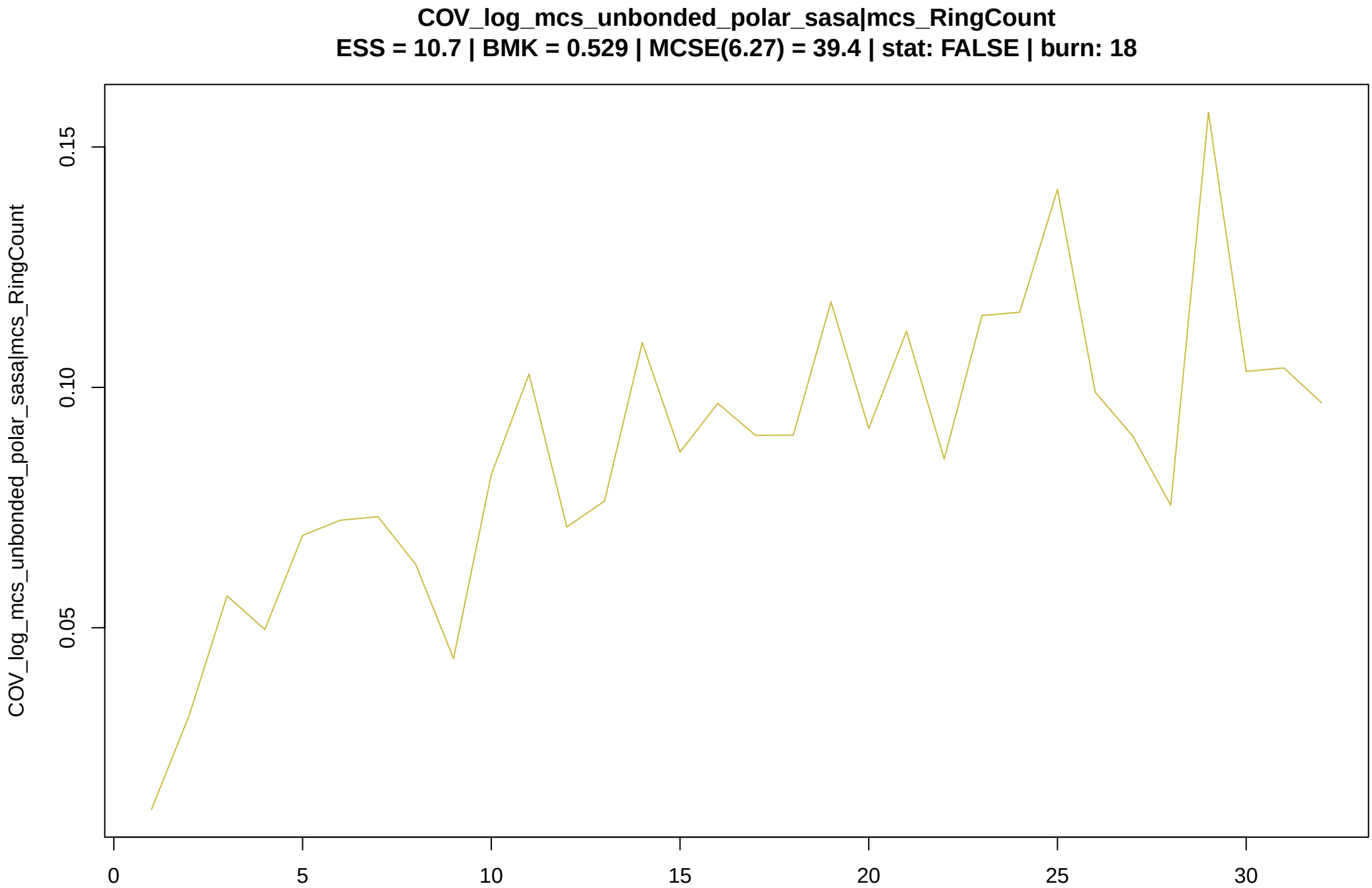

COV_log_RMSD|mcs_RingCount
ESS = 3.58 | BMK = 0.764 | MCSE(6.27) = 61 | stat: FALSE | burn: 30
COV_log_RMSD|mcs_RingCount
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
0
5
10
15
20
25
30

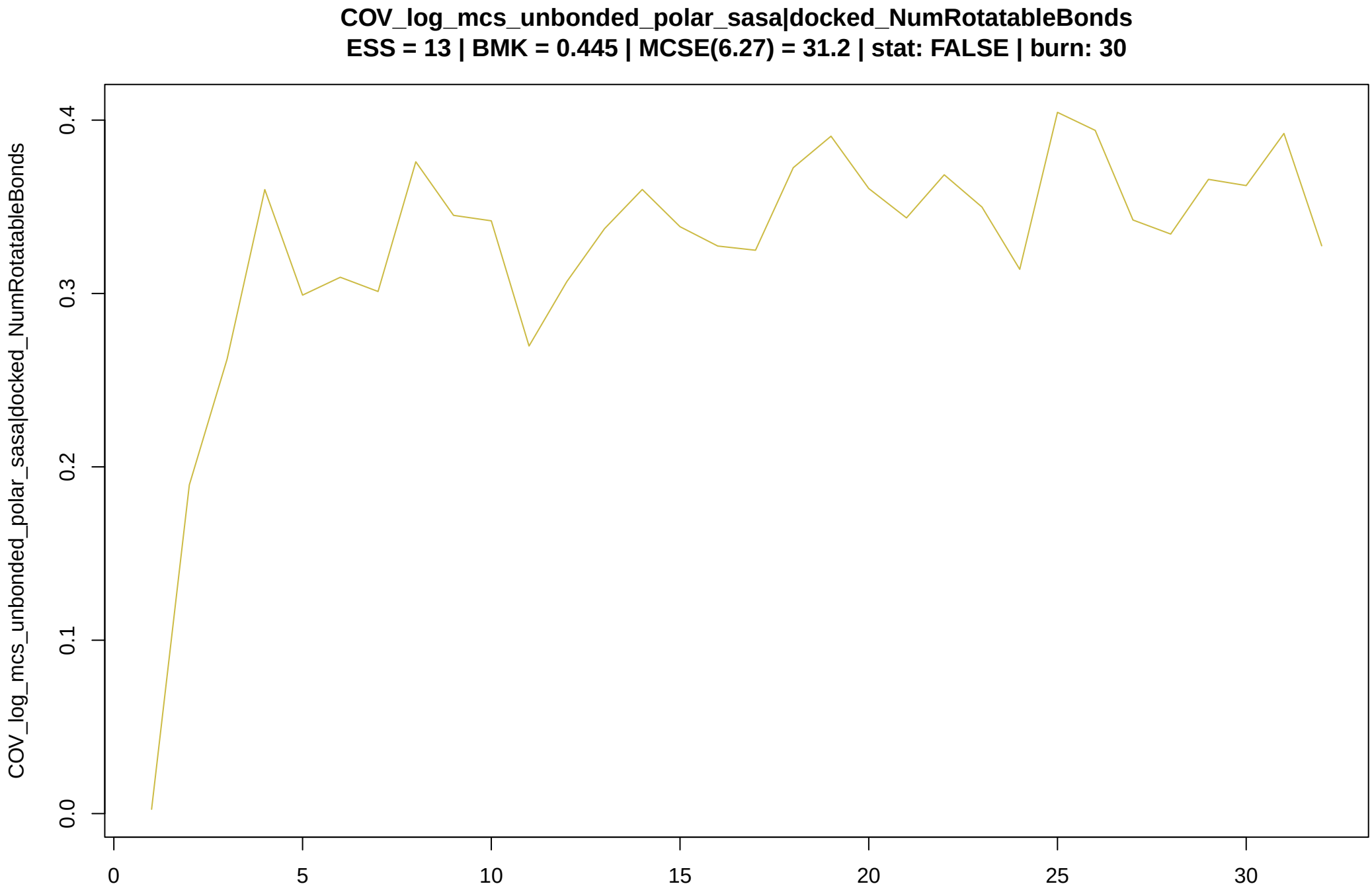

COV_log_RMSD|docked_NumRotatableBonds
ESS = 9.4 | BMK = 0.464 | MCSE(6.27) = 45.9 | stat: FALSE | burn: 24
COV_log_RMSD|docked_NumRotatableBonds
0.1
0.2
0.3
0.4
0.5
0
5
10
15
20
25
30

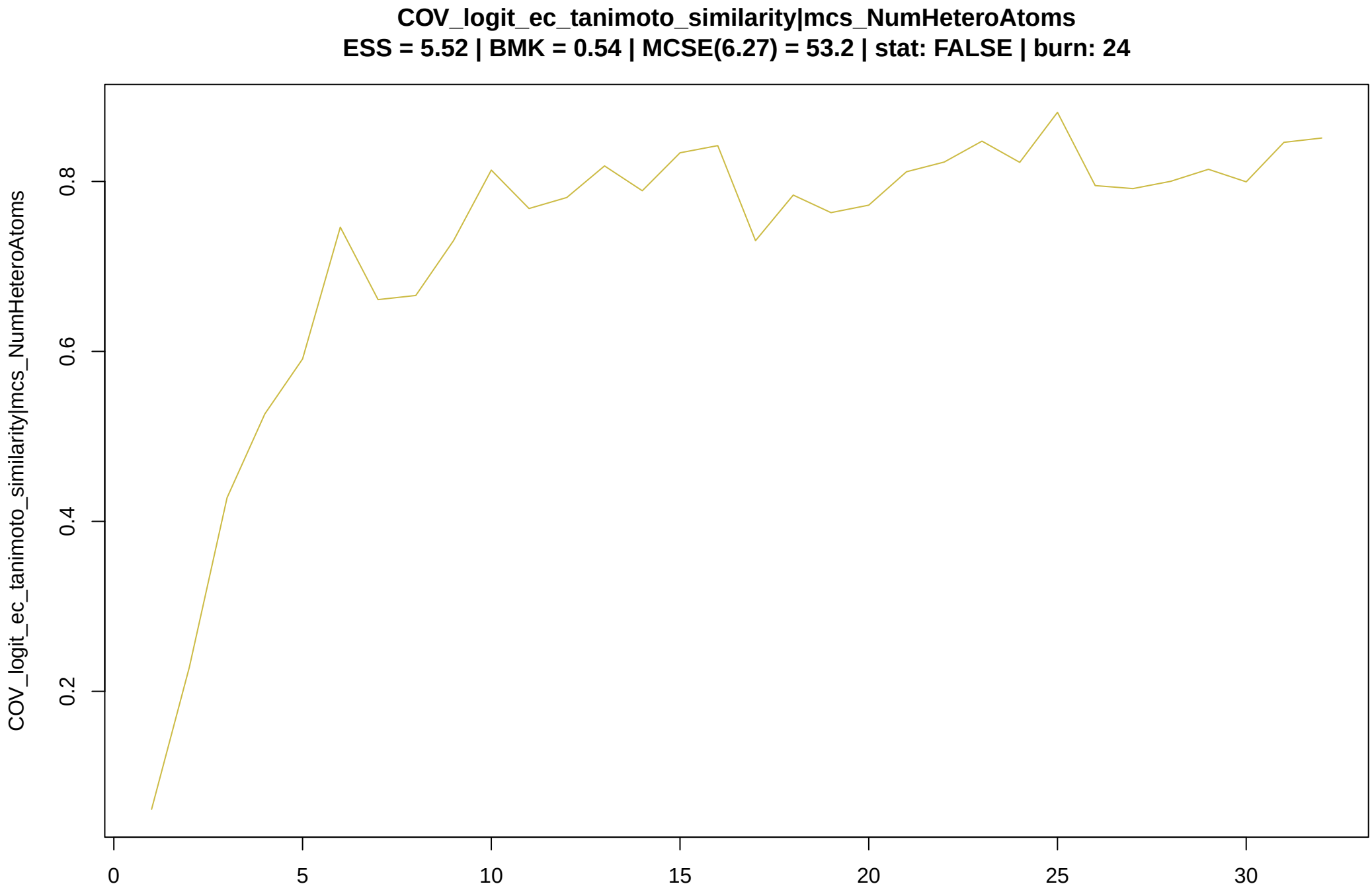

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 7.6 | BMK = 0.467 | MCSE(6.27) = 46.4 | stat: FALSE | burn: 21
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0
5
10
15
20
25
30

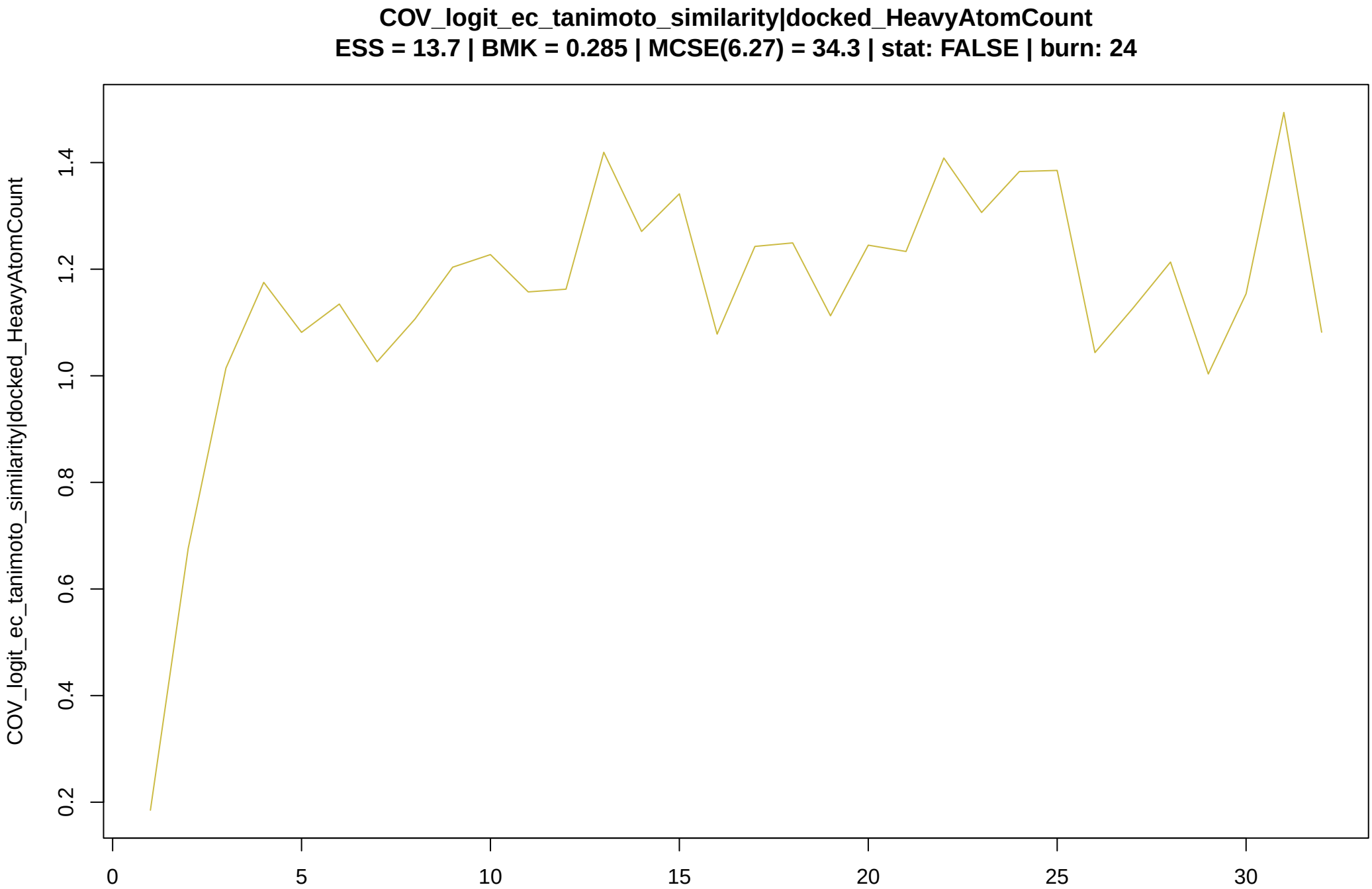

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 6.92 | BMK = 0.519 | MCSE(6.27) = 48.4 | stat: FALSE | burn: 24
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.2
0.4
0.6
0.8
1.0
0
5
10
15
20
25
30

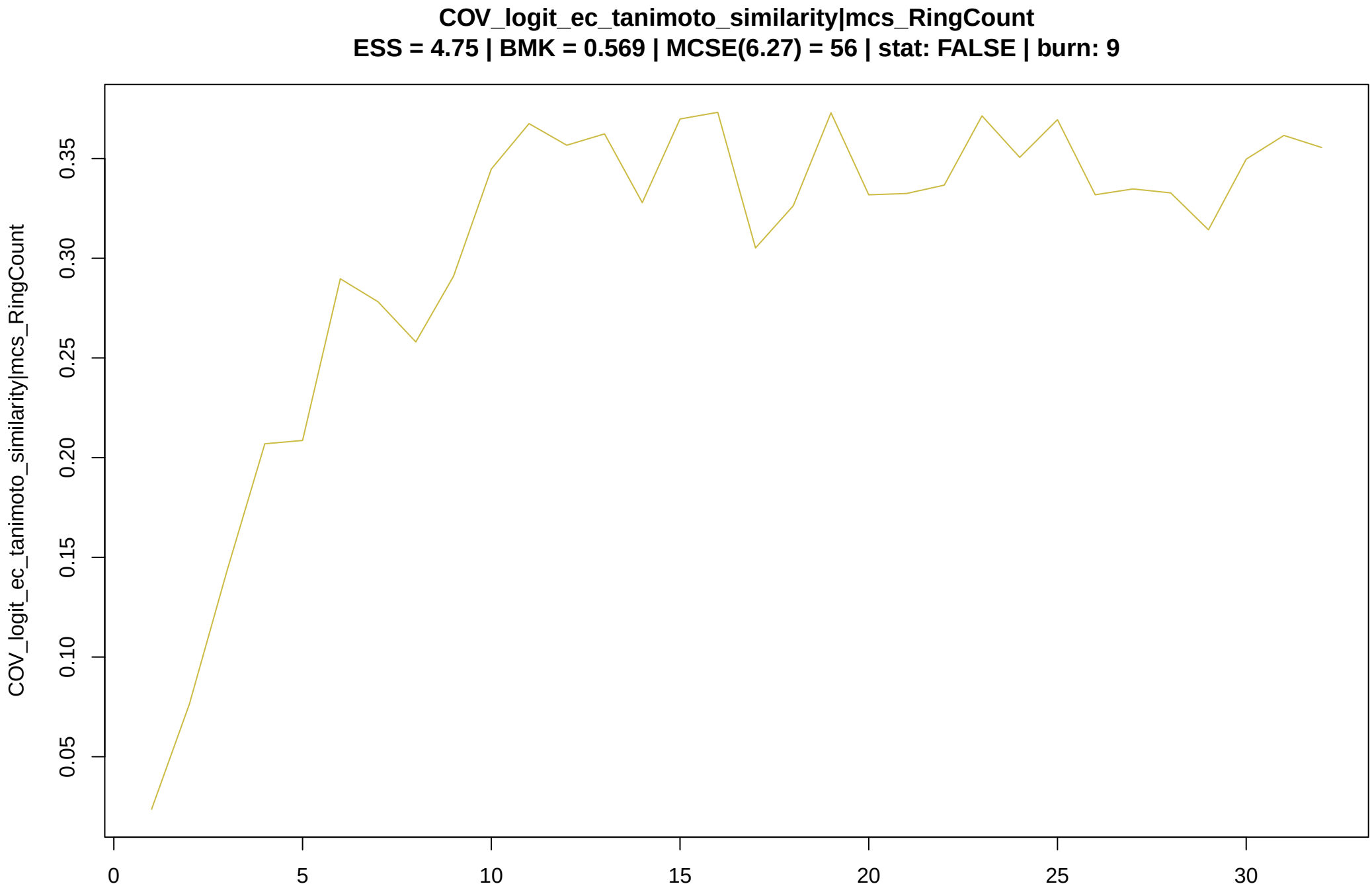

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 13.7 | BMK = 0.395 | MCSE(6.27) = 35.9 | stat: FALSE | burn: 30
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0.2
0.4
0.6
0.8
1.0
1.2
0
5
10
15
20
25
30

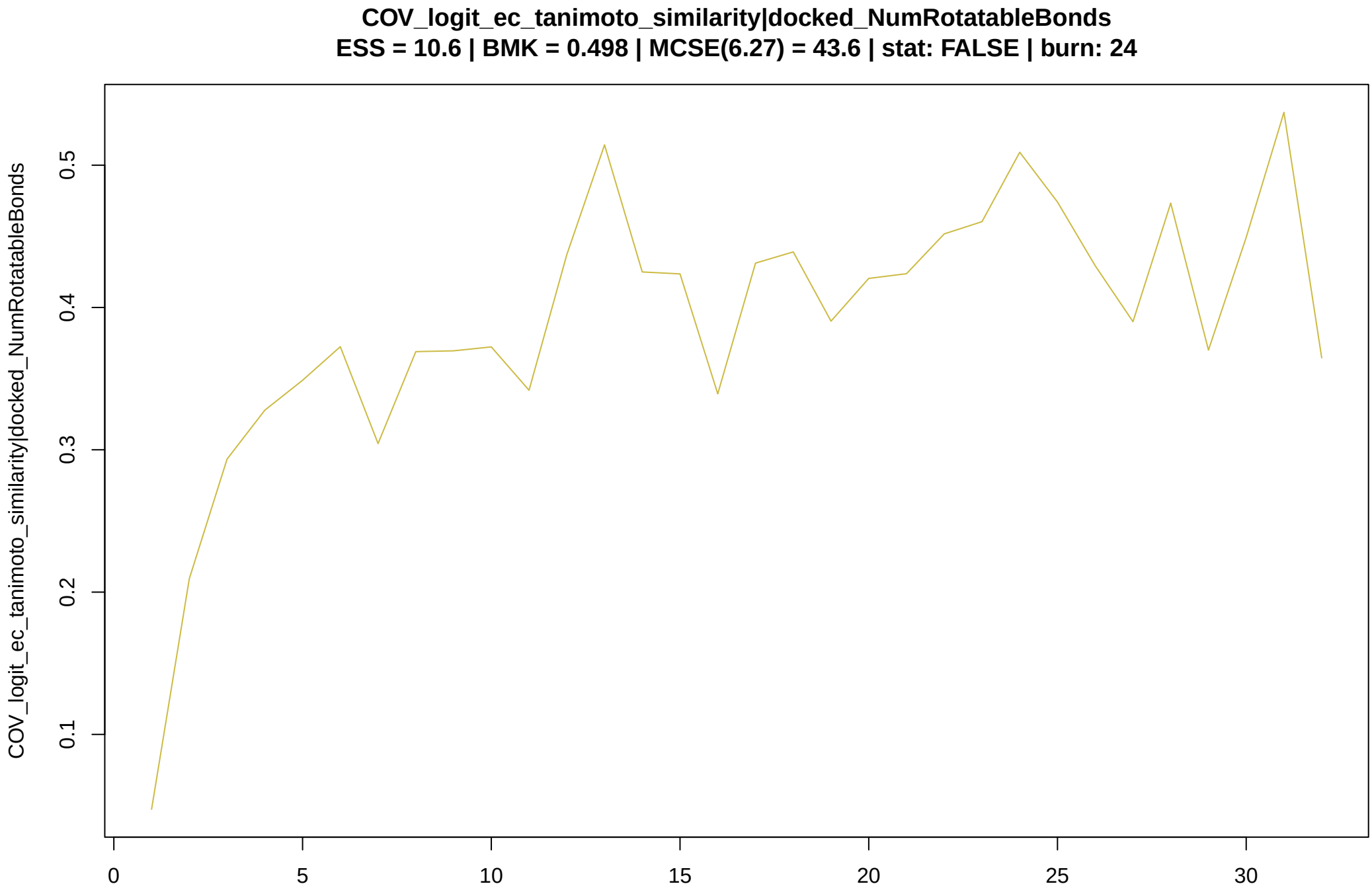

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 10.7 | BMK = 0.529 | MCSE(6.27) = 39.4 | stat: FALSE | burn: 18
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
0.05
0.10
0.15
0
5
10
15
20
25
30

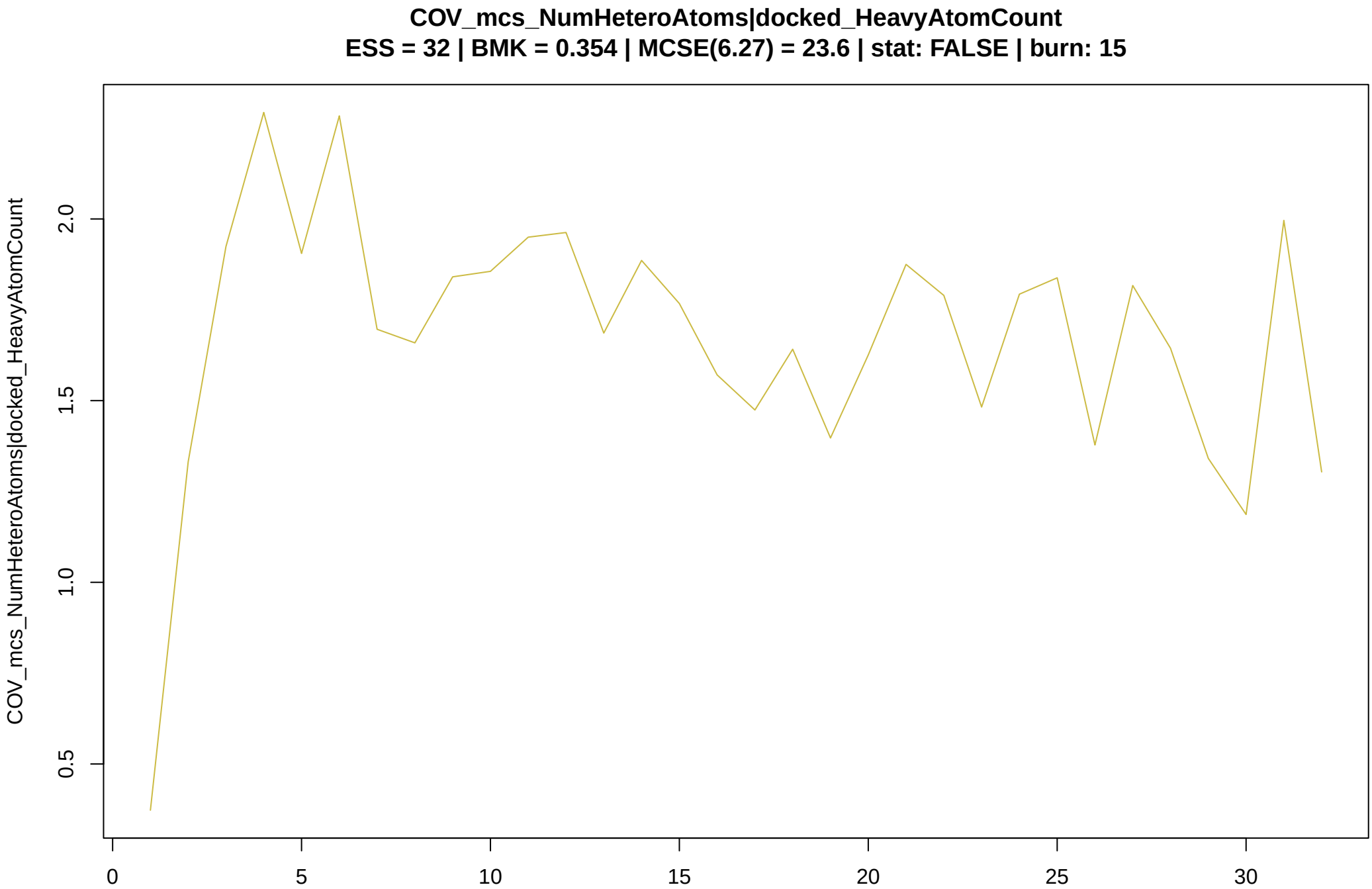

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 13 | BMK = 0.445 | MCSE(6.27) = 31.2 | stat: FALSE | burn: 30
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
0.0
0.1
0.2
0.3
0.4
0
5
10
15
20
25
30

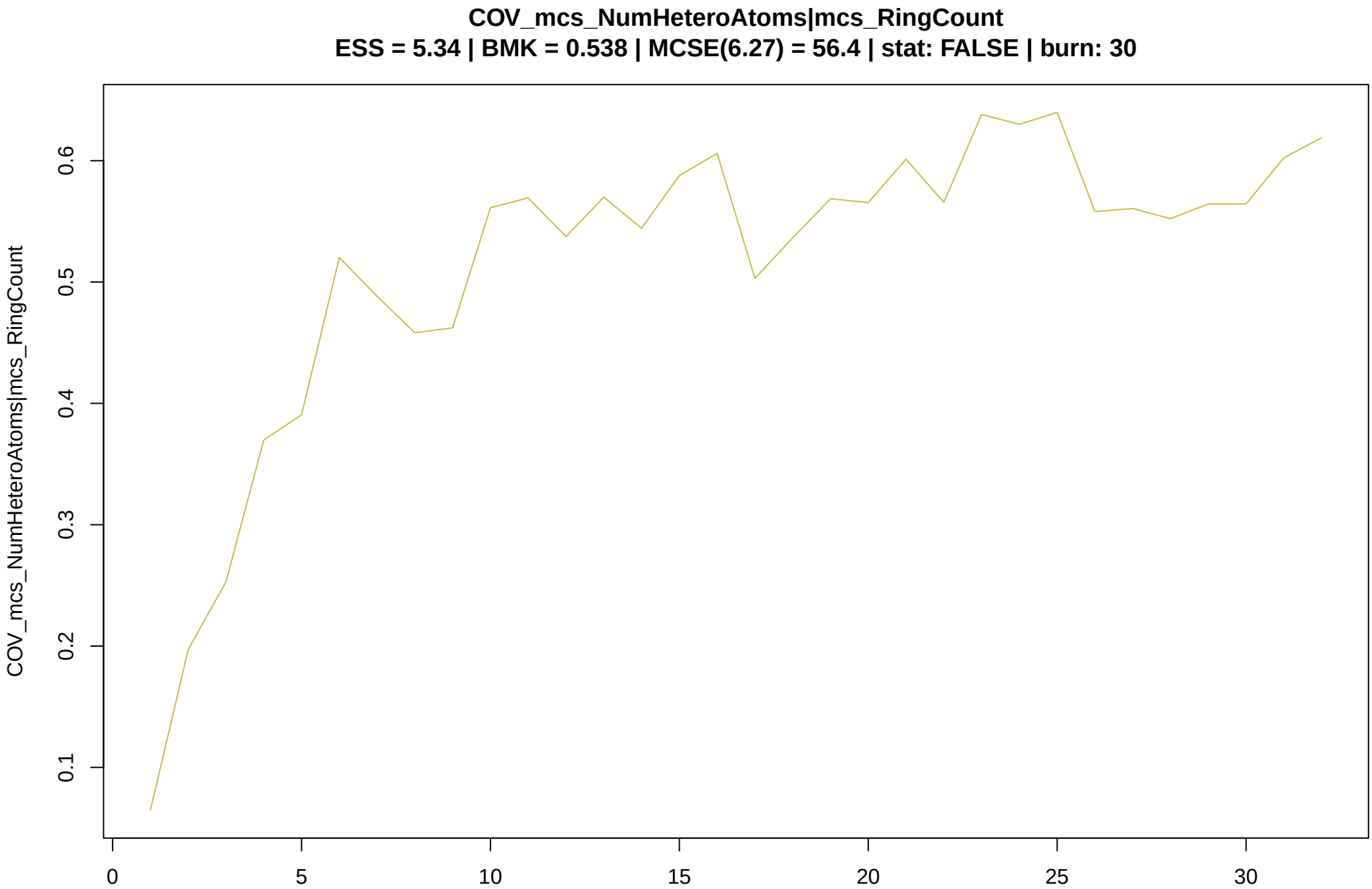

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 5.52 | BMK = 0.54 | MCSE(6.27) = 53.2 | stat: FALSE | burn: 24
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.2
0.4
0.6
0.8
0
5
10
15
20
25
30

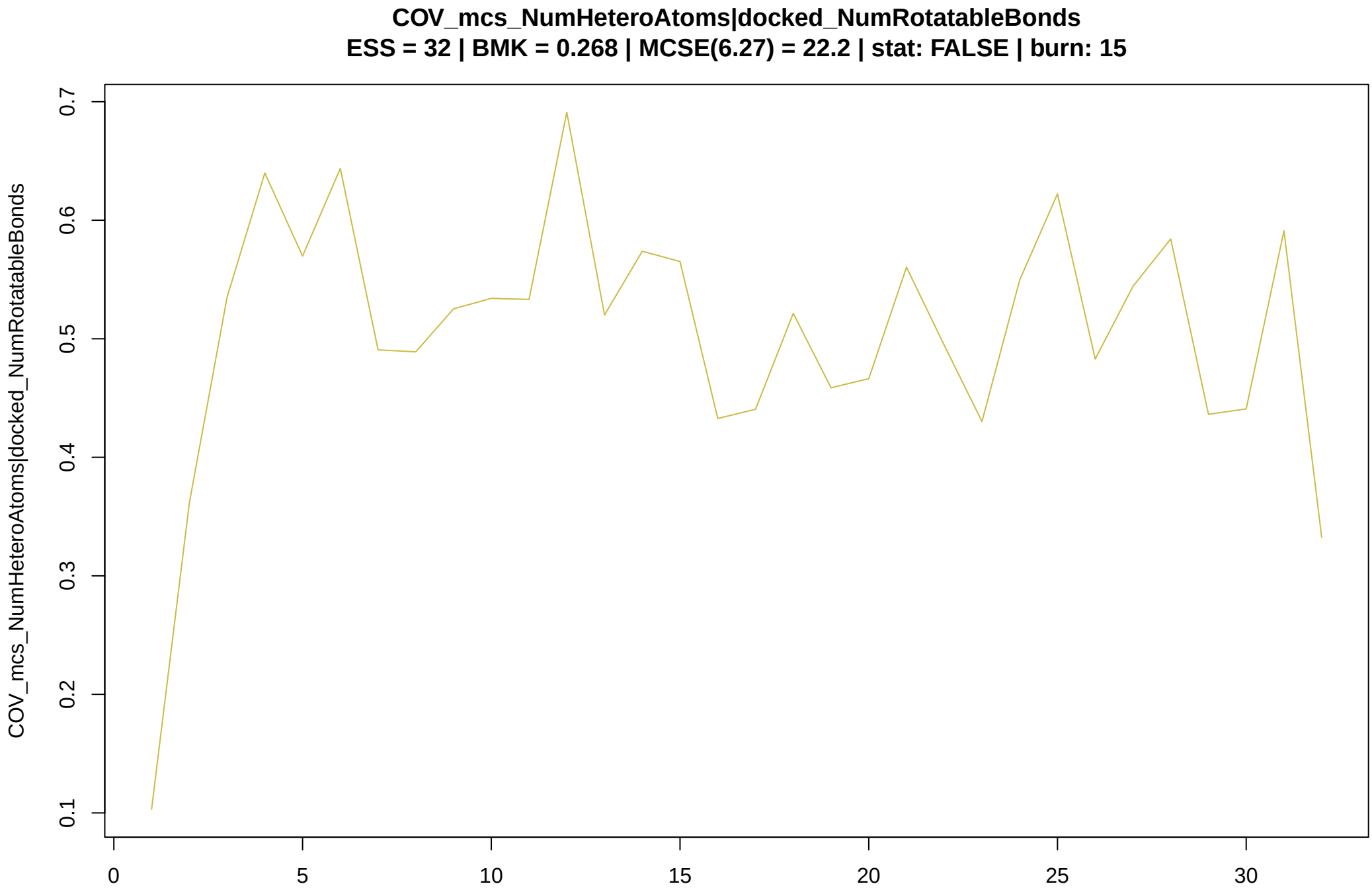

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 13.7 | BMK = 0.285 | MCSE(6.27) = 34.3 | stat: FALSE | burn: 24
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
5
10
15
20
25
30

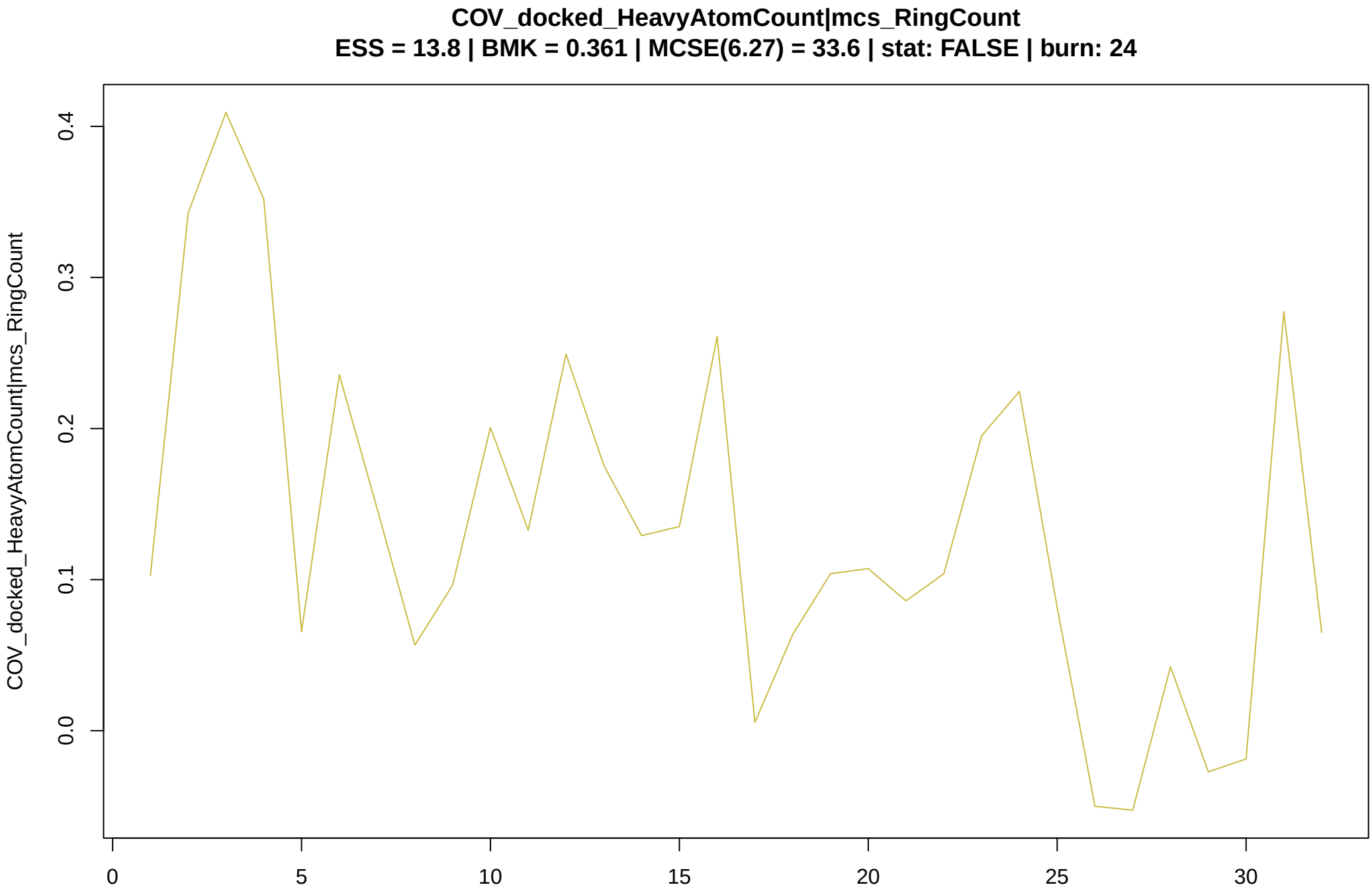

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 4.75 | BMK = 0.569 | MCSE(6.27) = 56 | stat: FALSE | burn: 9
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0
5
10
15
20
25
30

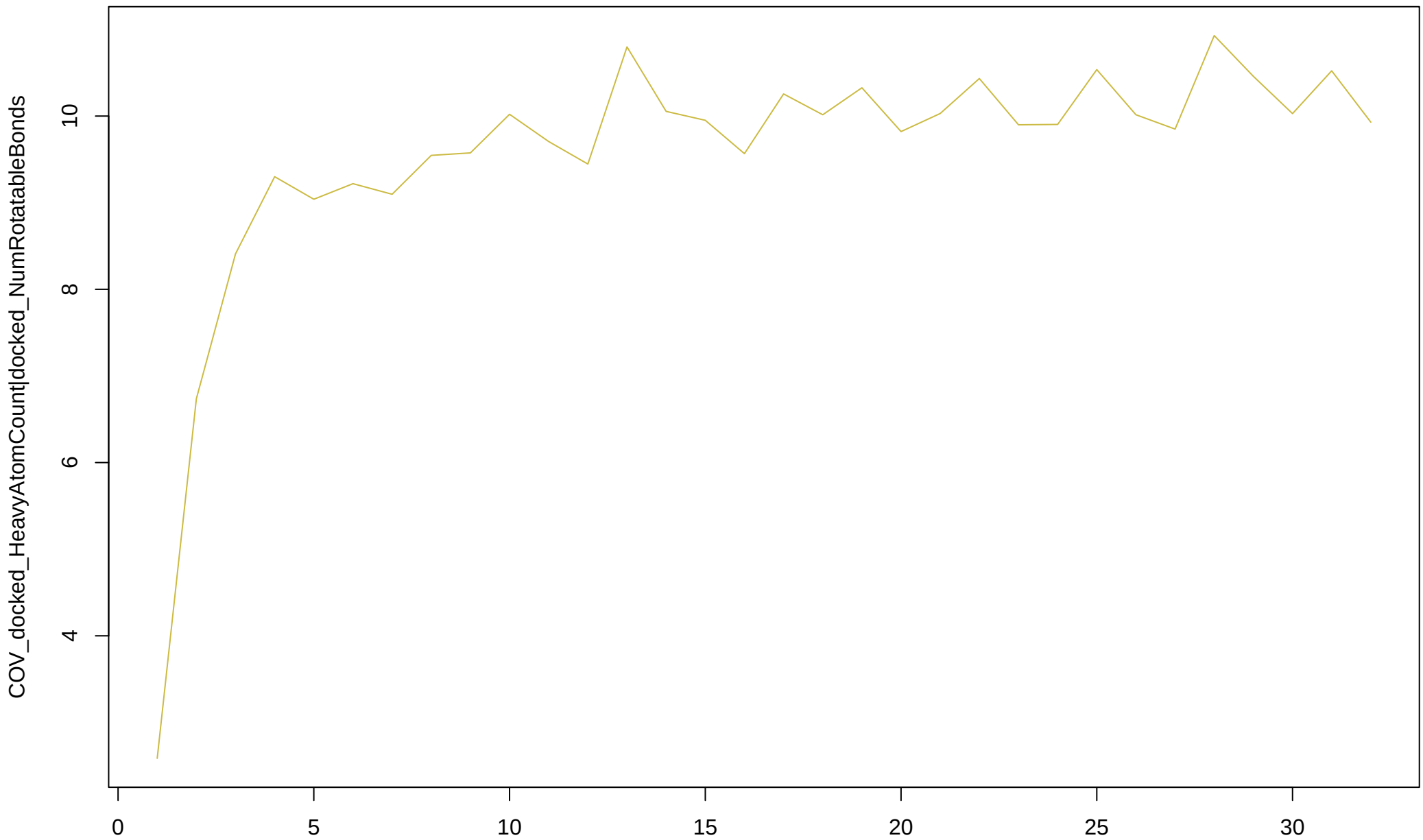

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 10.6 | BMK = 0.498 | MCSE(6.27) = 43.6 | stat: FALSE | burn: 24
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
0.1
0.2
0.3
0.4
0.5
0
5
10
15
20
25
30

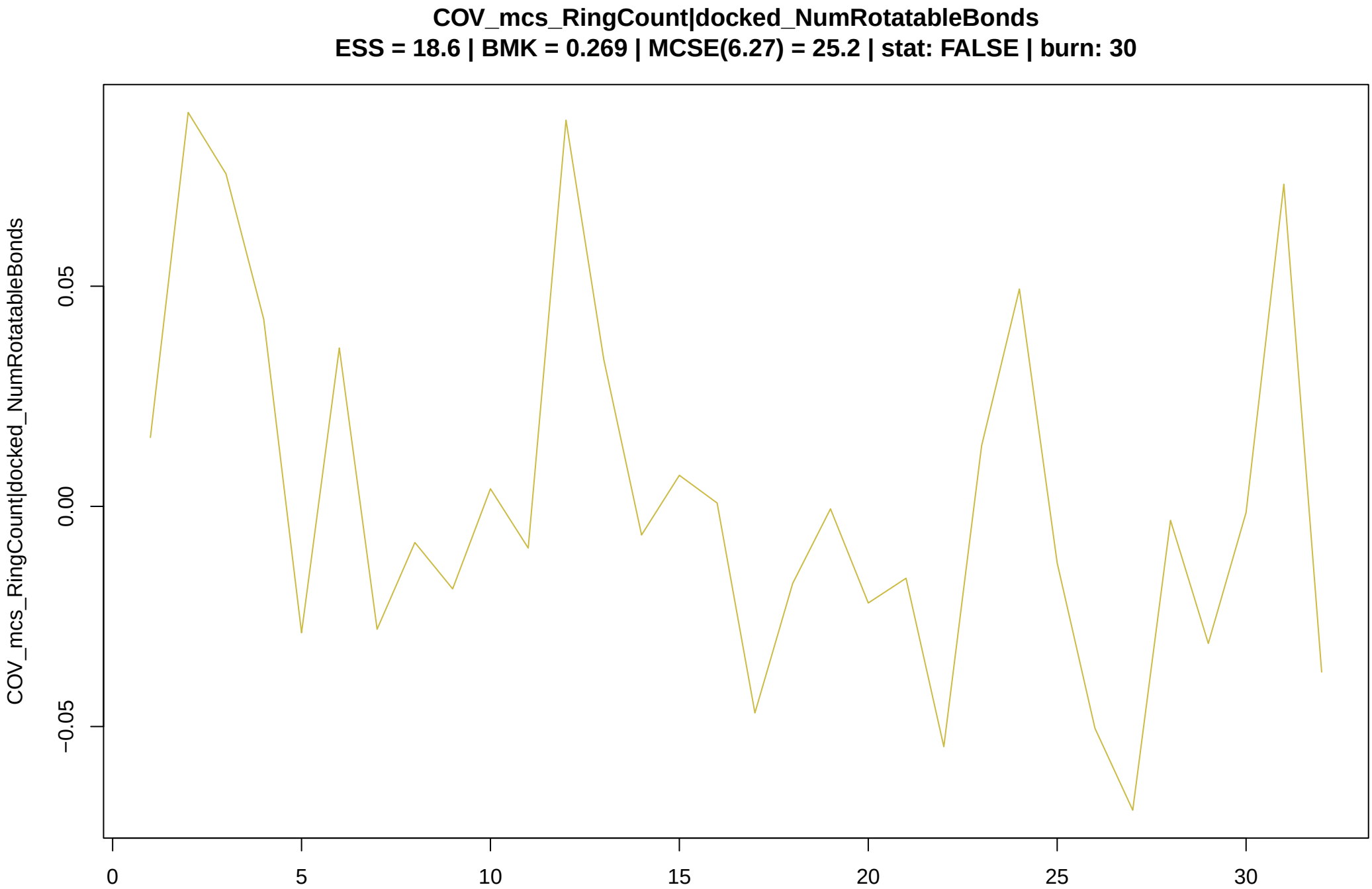

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 32 | BMK = 0.354 | MCSE(6.27) = 23.6 | stat: FALSE | burn: 15
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
0.5
1.0
1.5
2.0
0
5
10
15
20
25
30


COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 5.34 | BMK = 0.538 | MCSE(6.27) = 56.4 | stat: FALSE | burn: 30
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.1
0.2
0.3
0.4
0.5
0.6
0
5
10
15
20
25
30


COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 32 | BMK = 0.268 | MCSE(6.27) = 22.2 | stat: FALSE | burn: 15
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
5
10
15
20
25
30


COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 13.8 | BMK = 0.361 | MCSE(6.27) = 33.6 | stat: FALSE | burn: 24
COV_docked_HeavyAtomCount|mcs_RingCount
0.0
0.1
0.2
0.3
0.4
0
5
10
15
20
25
30


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 12.1 | BMK = 0.602 | MCSE(6.27) = 43.3 | stat: FALSE | burn: 12
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
4
6
8
10
0
5
10
15
20
25
30


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 18.6 | BMK = 0.269 | MCSE(6.27) = 25.2 | stat: FALSE | burn: 30
COV_mcs_RingCount|docked_NumRotatableBonds
0.05
0.00
−0.05
0
5
10
15
20
25
30