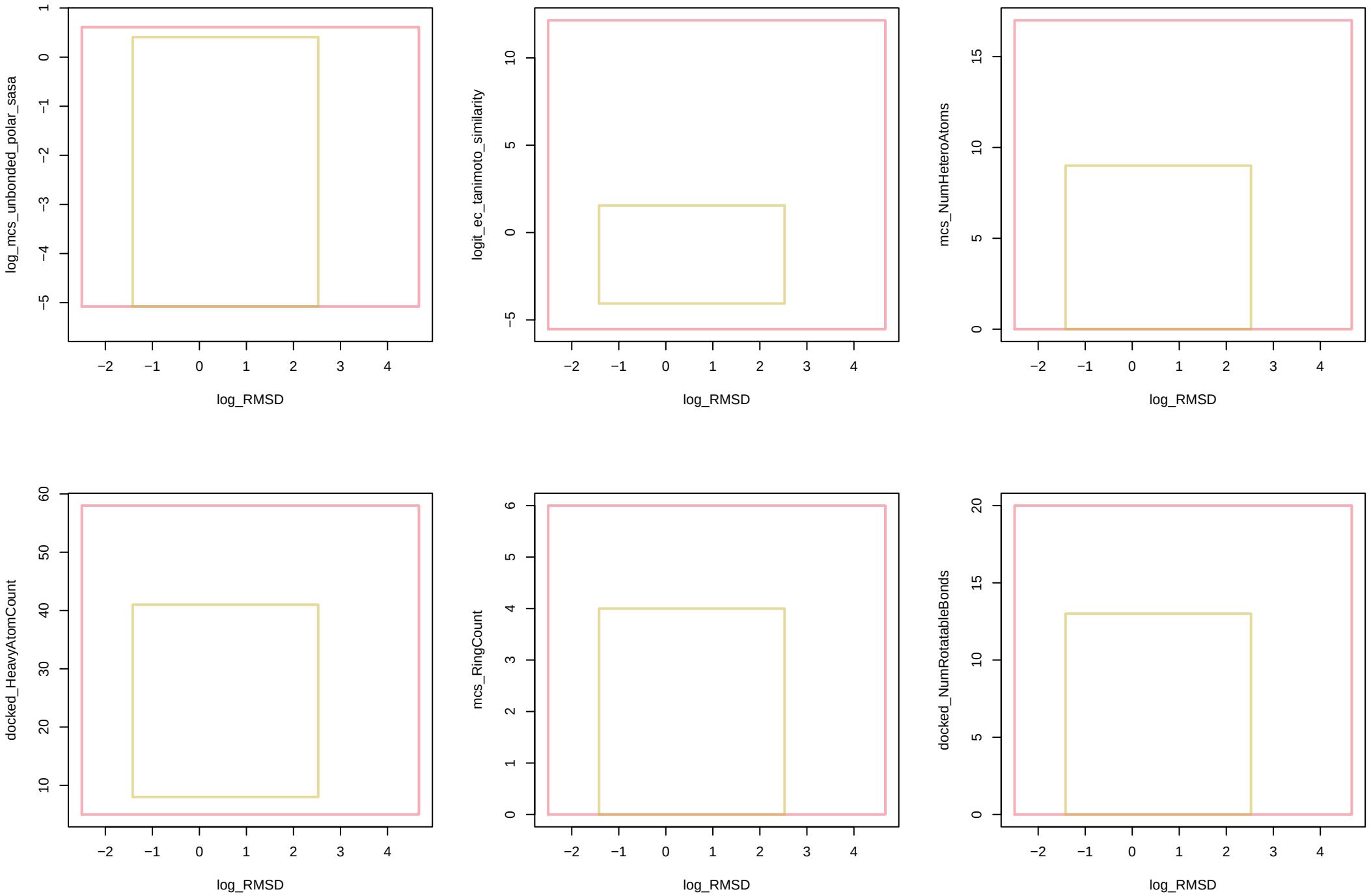
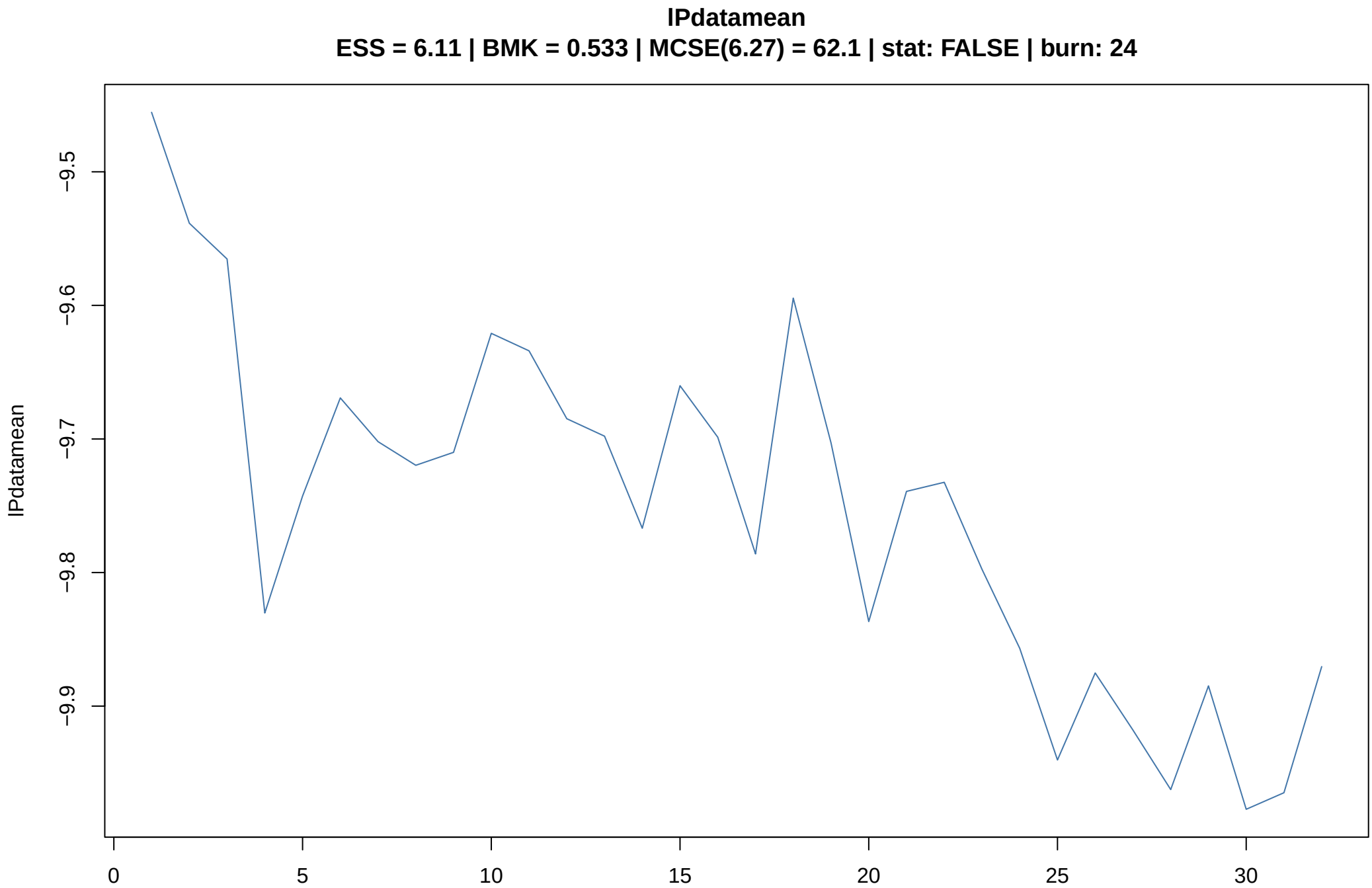
−− STATS maxD −−
min ESS = 4.8733946904484
max BMK = 0.533309096687053
max MCSE = 62.1201205535898
all stationary: FALSE
burn: 30

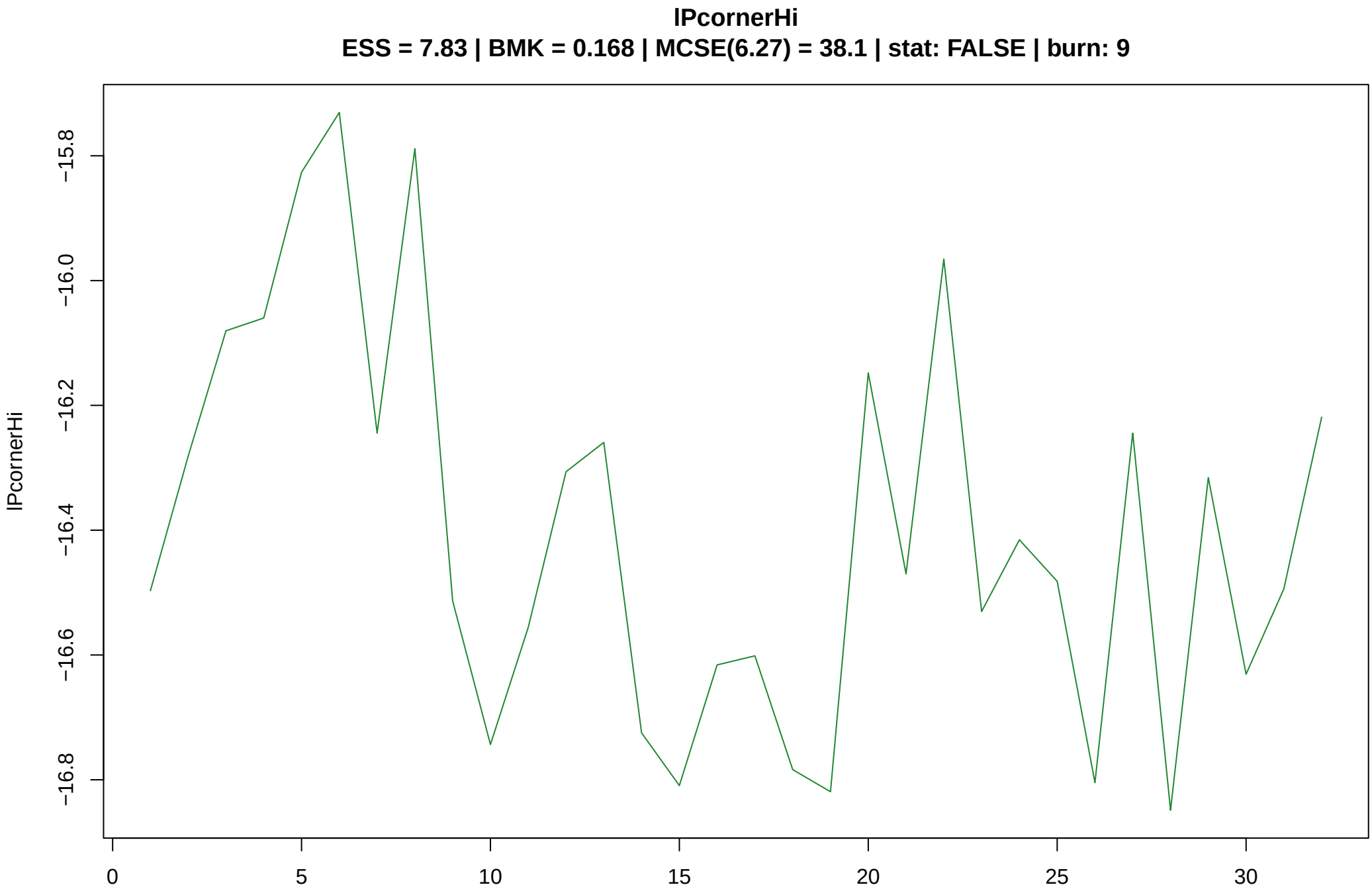
−− STATS 2D −−
min ESS = 16.913597499247
max BMK = 0.47852179393525
max MCSE = 34.803275524987
all stationary: FALSE
burn: 30

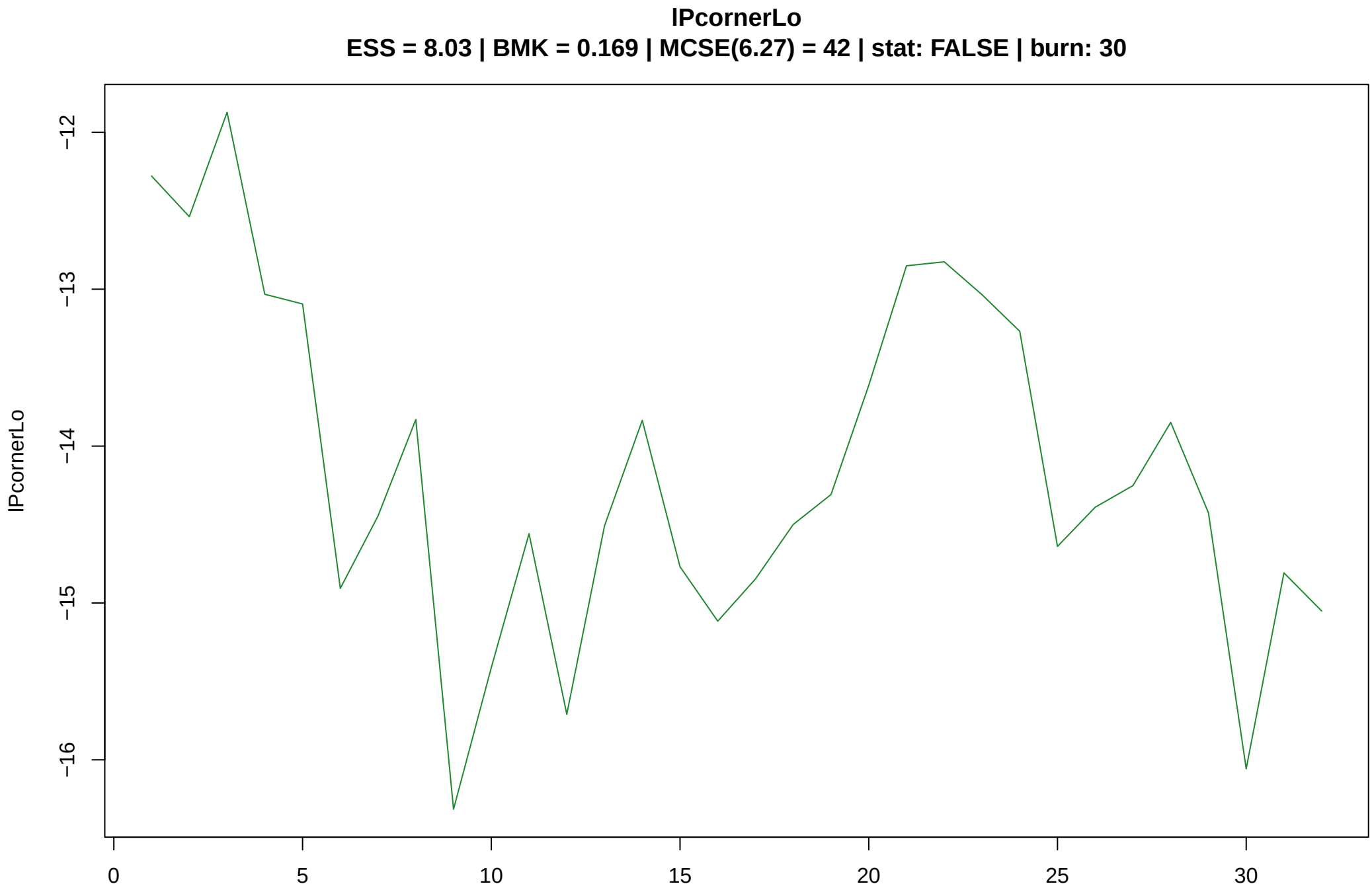
−− STATS 1D −−
min ESS = 14.9846254760828
max BMK = 0.33398071115542
max MCSE = 19.4025893795959
all stationary: FALSE
burn: 30

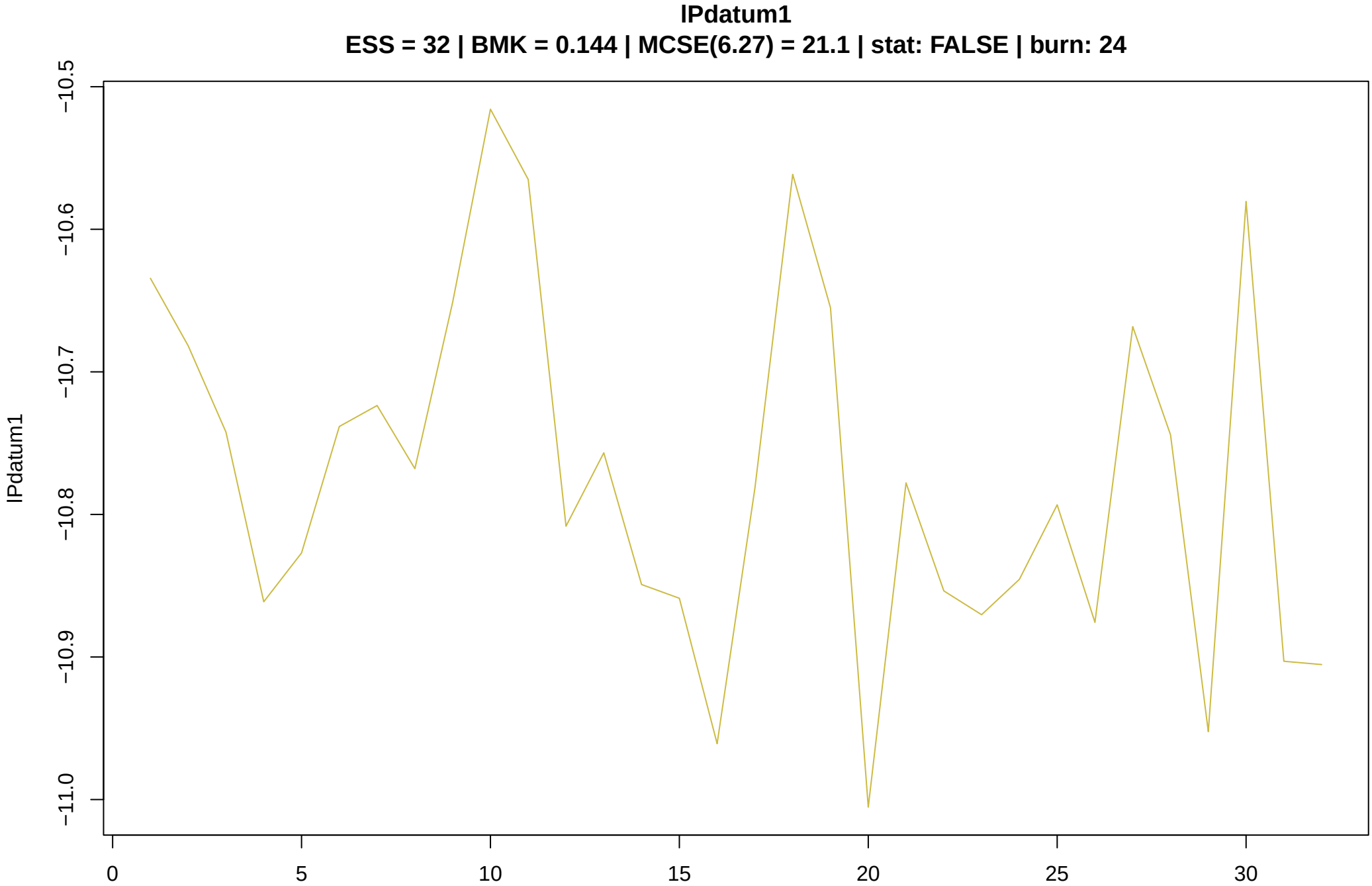
Occupied clusters: 17 of 64

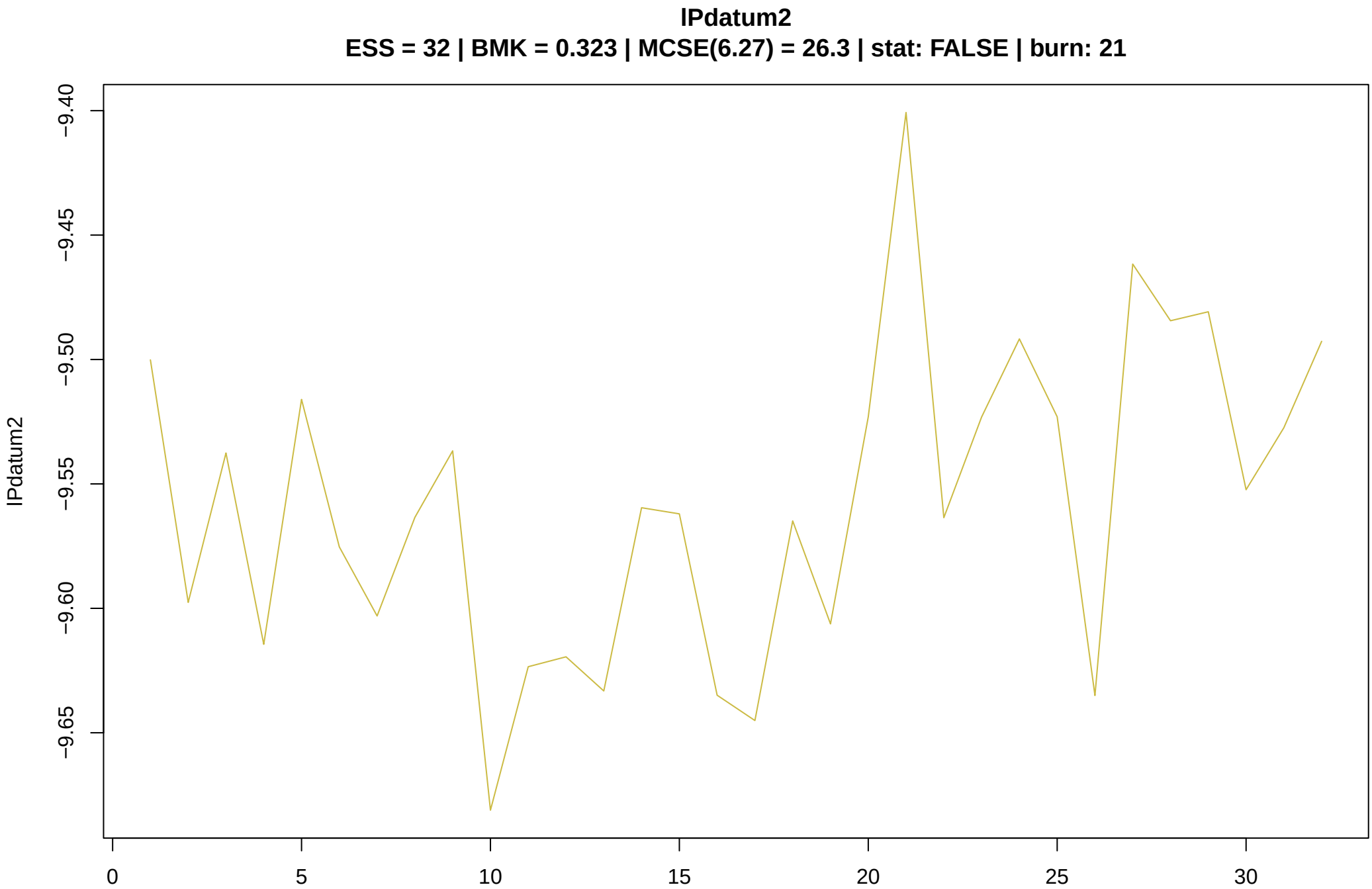

log_mcs_unbonded_polar_sasa
log_RMSD
logit_ec_tanimoto_similarity
log_RMSD
mcs_NumHeteroAtoms
log_RMSD
docked_HeavyAtomCount
log_RMSD
mcs_RingCount
log_RMSD
docked_NumRotatableBonds
log_RMSD

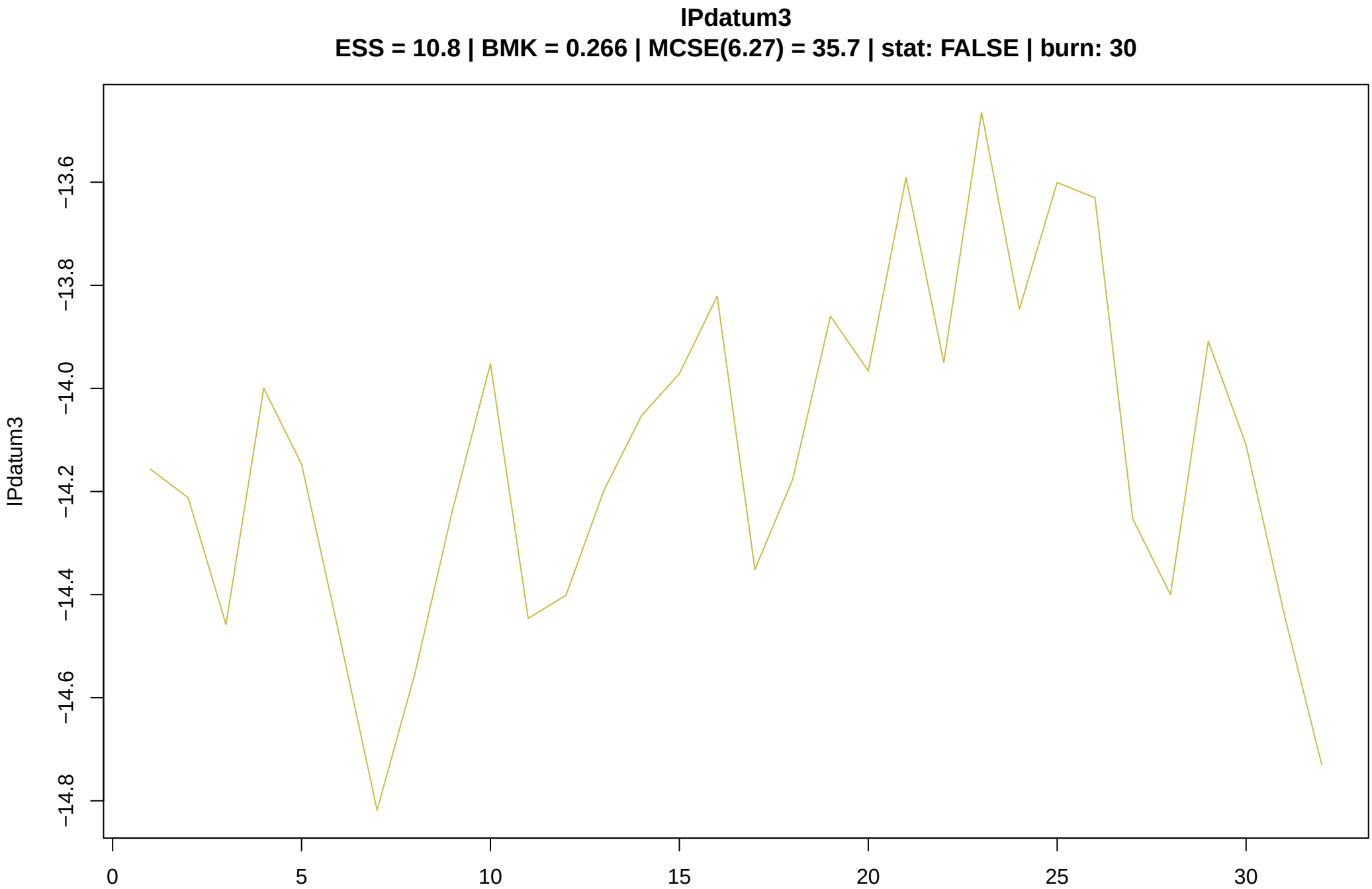

lPdatamean
ESS = 6.11 | BMK = 0.533 | MCSE(6.27) = 62.1 | stat: FALSE | burn: 24
lPdatamean
−9.5
−9.6
−9.7
−9.8
−9.9
0
5
10
15
20
25
30

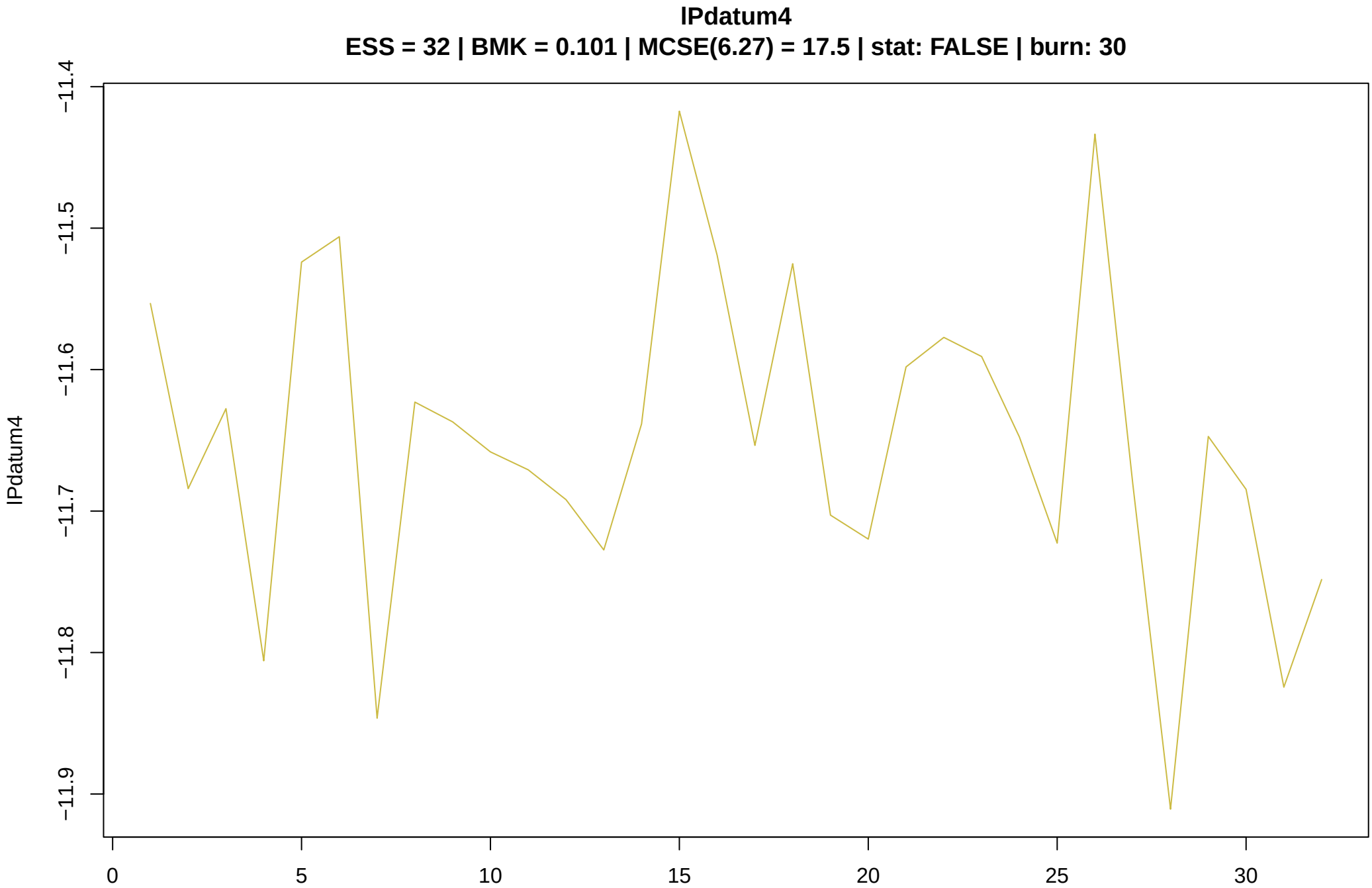

lPcornerHi
ESS = 7.83 | BMK = 0.168 | MCSE(6.27) = 38.1 | stat: FALSE | burn: 9
lPcornerHi
−15.8
−16.0
−16.2
−16.4
−16.6
−16.8
0
5
10
15
20
25
30

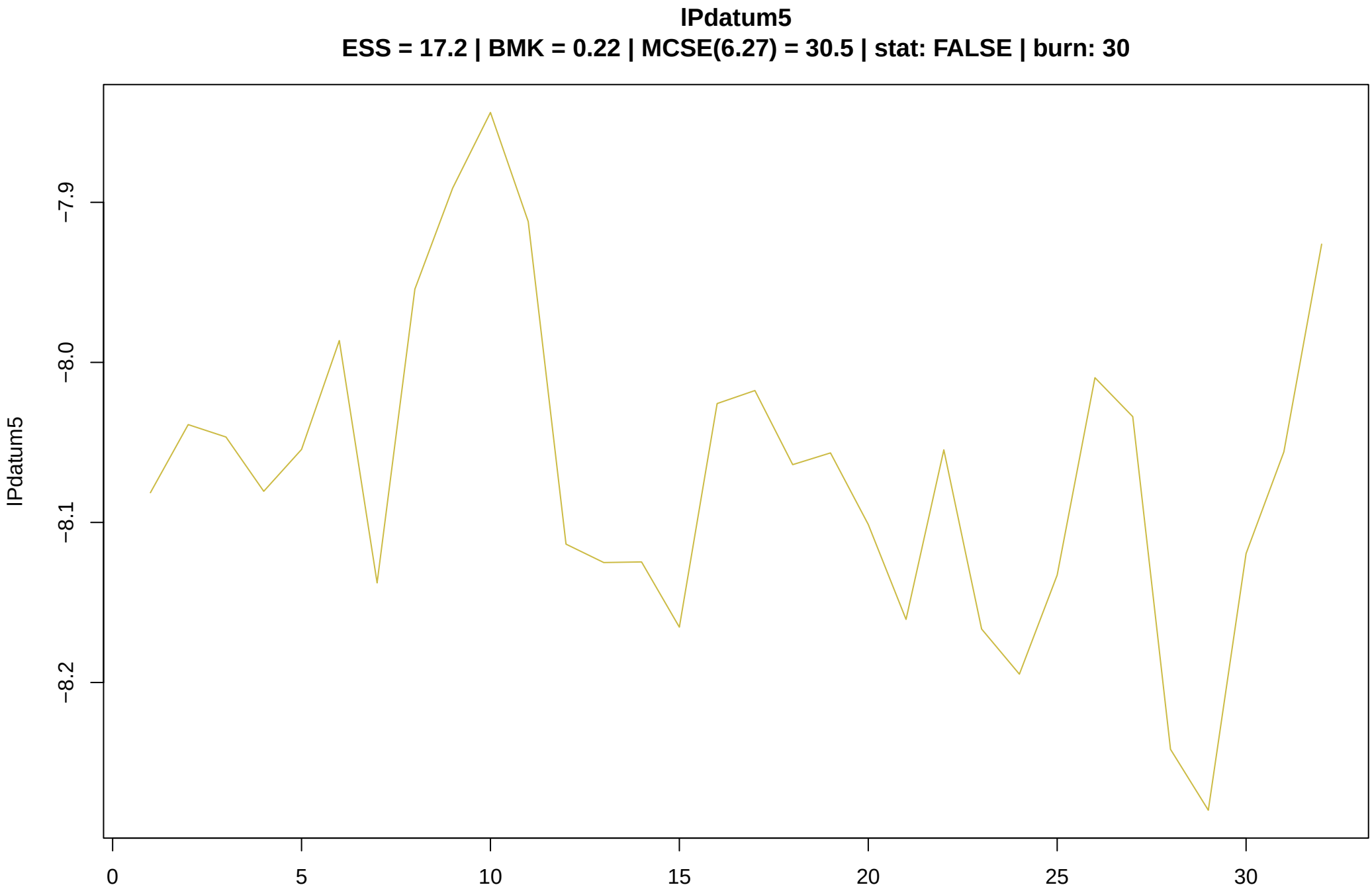

lPcornerLo
ESS = 8.03 | BMK = 0.169 | MCSE(6.27) = 42 | stat: FALSE | burn: 30
lPcornerLo
−12
−13
−14
−15
−16
0
5
10
15
20
25
30

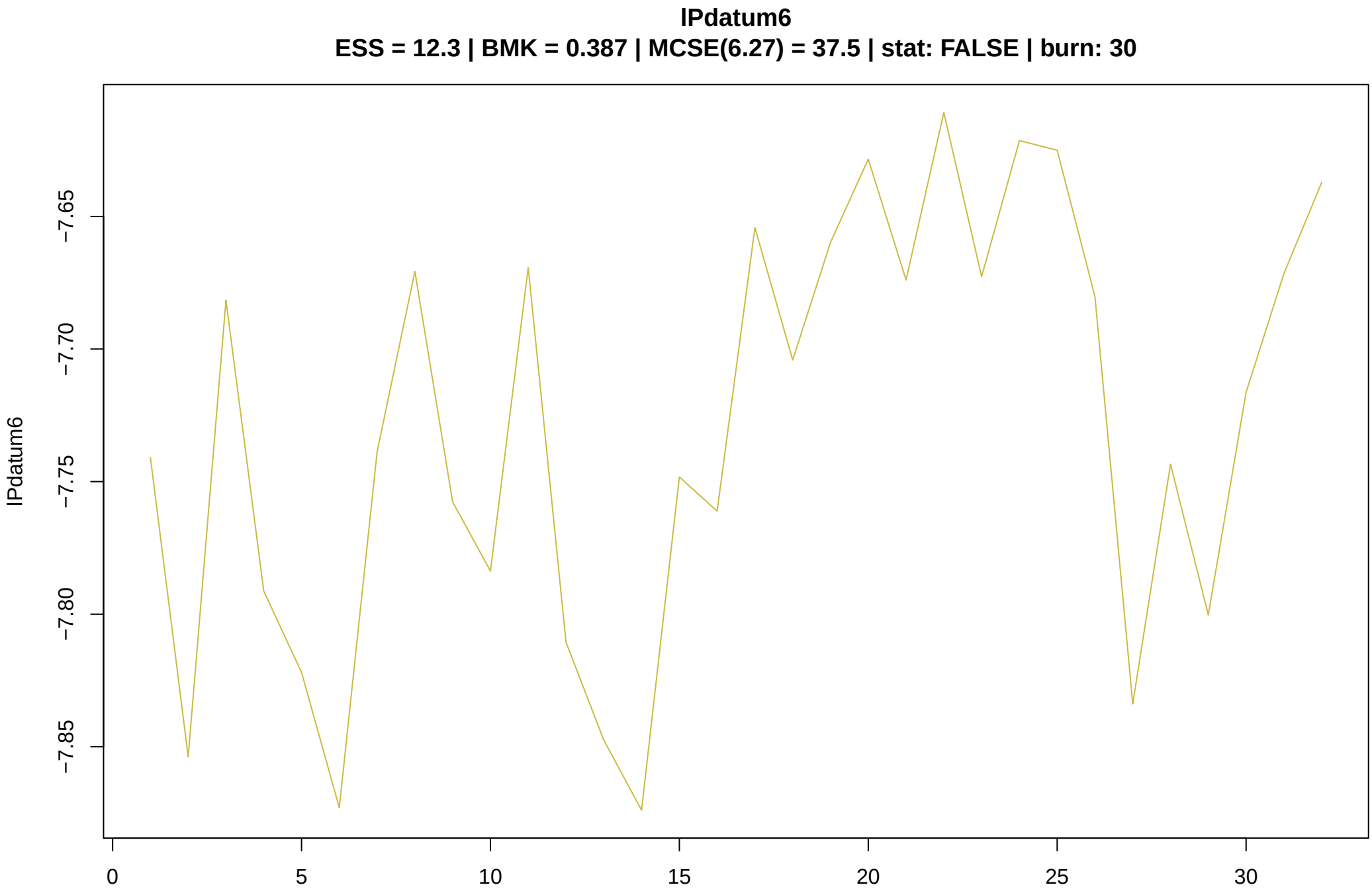

lPdatum1
ESS = 32 | BMK = 0.144 | MCSE(6.27) = 21.1 | stat: FALSE | burn: 24
lPdatum1
−10.5
−10.6
−10.7
−10.8
−10.9
−11.0
0
5
10
15
20
25
30

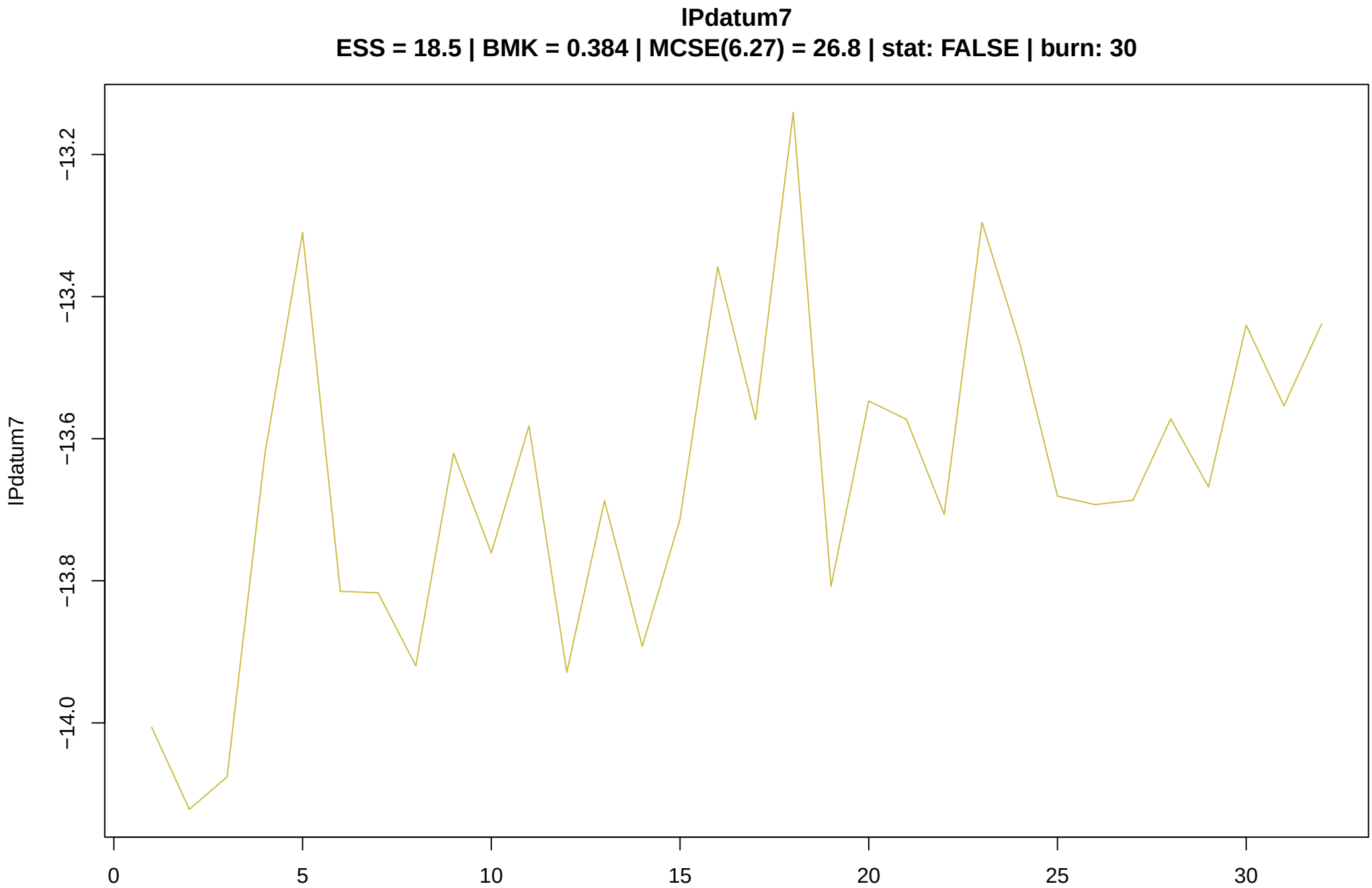

lPdatum2
ESS = 32 | BMK = 0.323 | MCSE(6.27) = 26.3 | stat: FALSE | burn: 21
lPdatum2
−9.40
−9.45
−9.50
−9.55
−9.60
−9.65
0
5
10
15
20
25
30

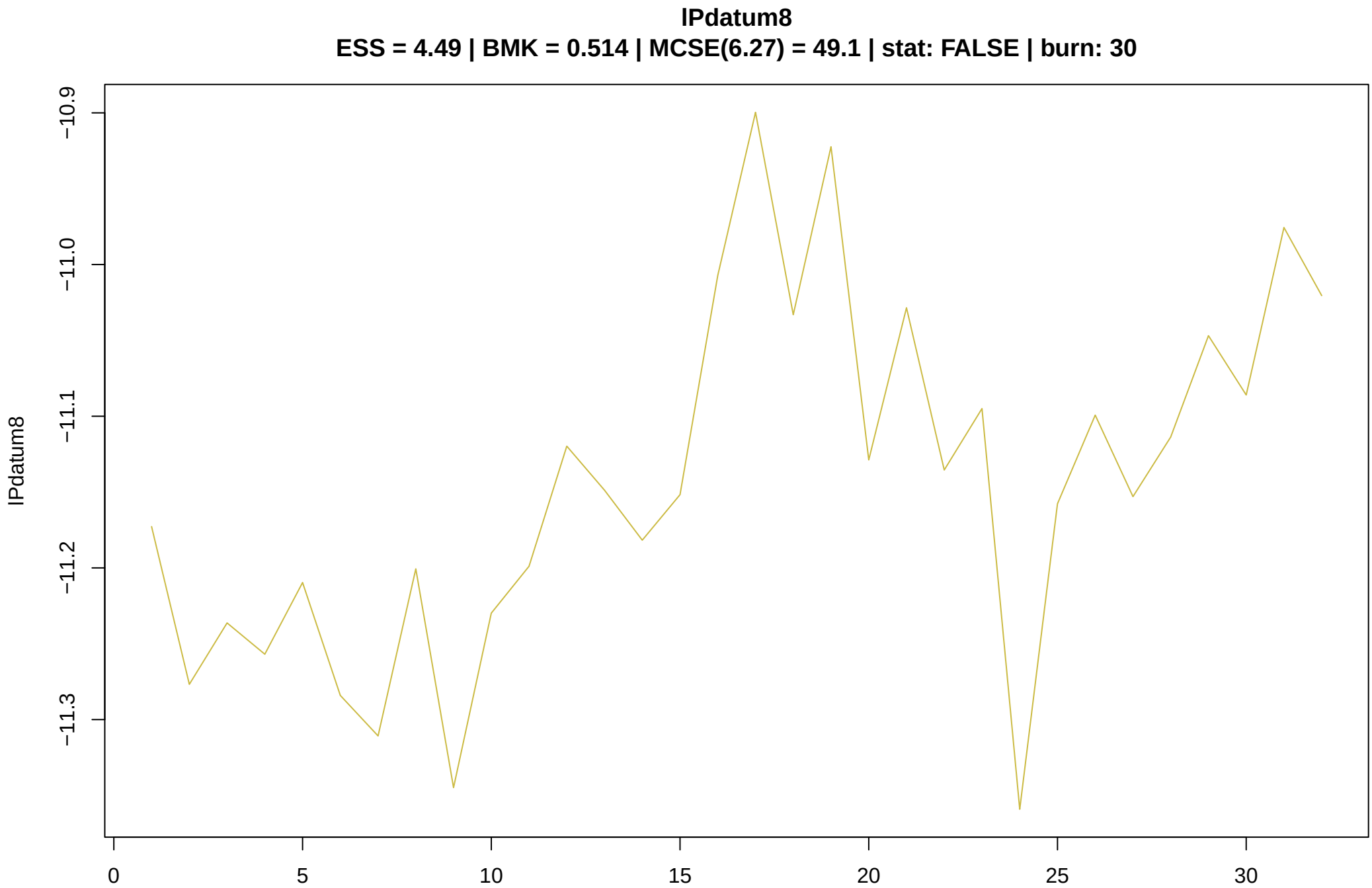

lPdatum3
ESS = 10.8 | BMK = 0.266 | MCSE(6.27) = 35.7 | stat: FALSE | burn: 30
lPdatum3
−13.6
−13.8
−14.0
−14.2
−14.4
−14.6
−14.8
0
5
10
15
20
25
30

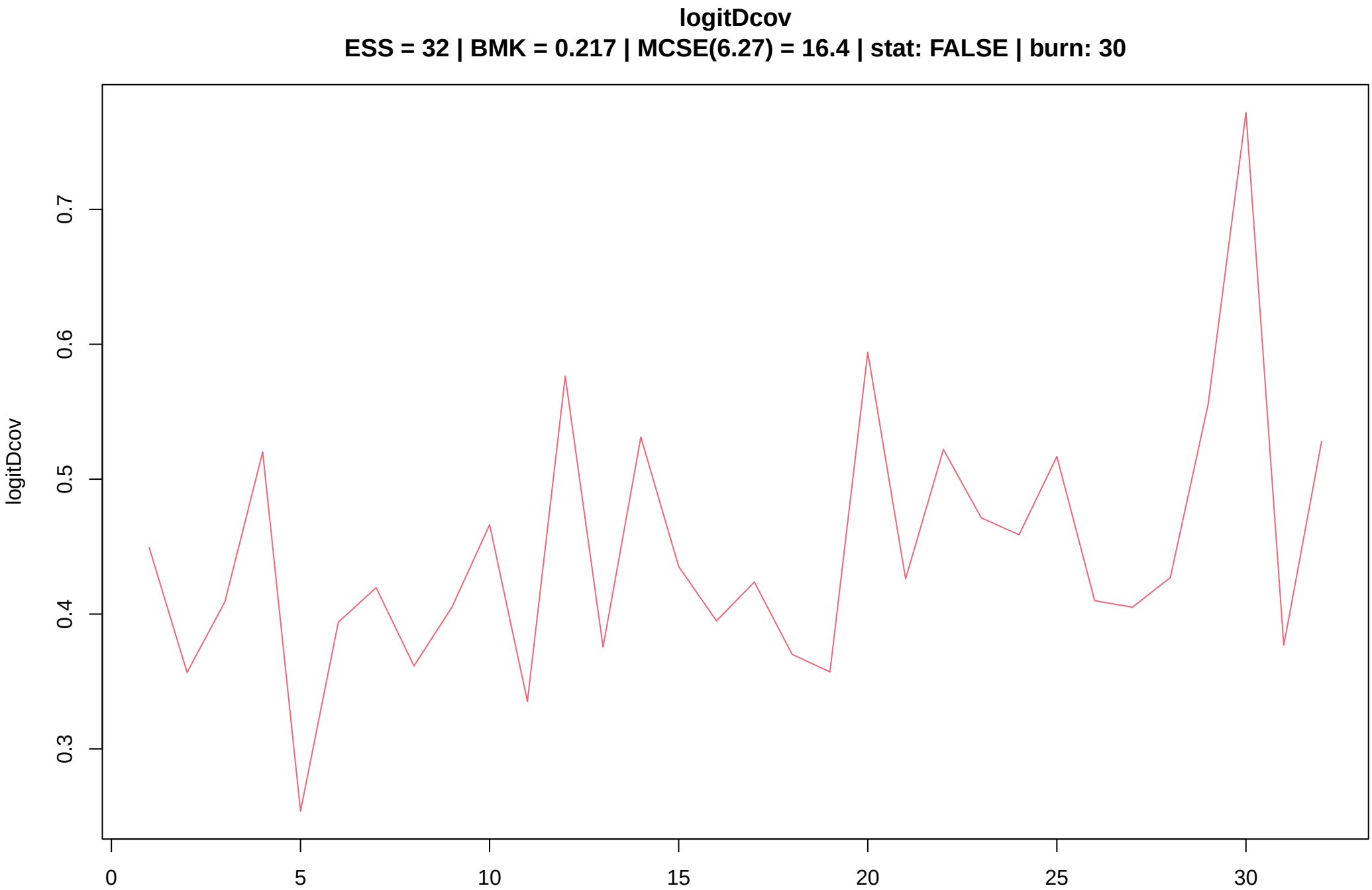

lPdatum4
ESS = 32 | BMK = 0.101 | MCSE(6.27) = 17.5 | stat: FALSE | burn: 30
lPdatum4
−11.4
−11.5
−11.6
−11.7
−11.8
−11.9
0
5
10
15
20
25
30

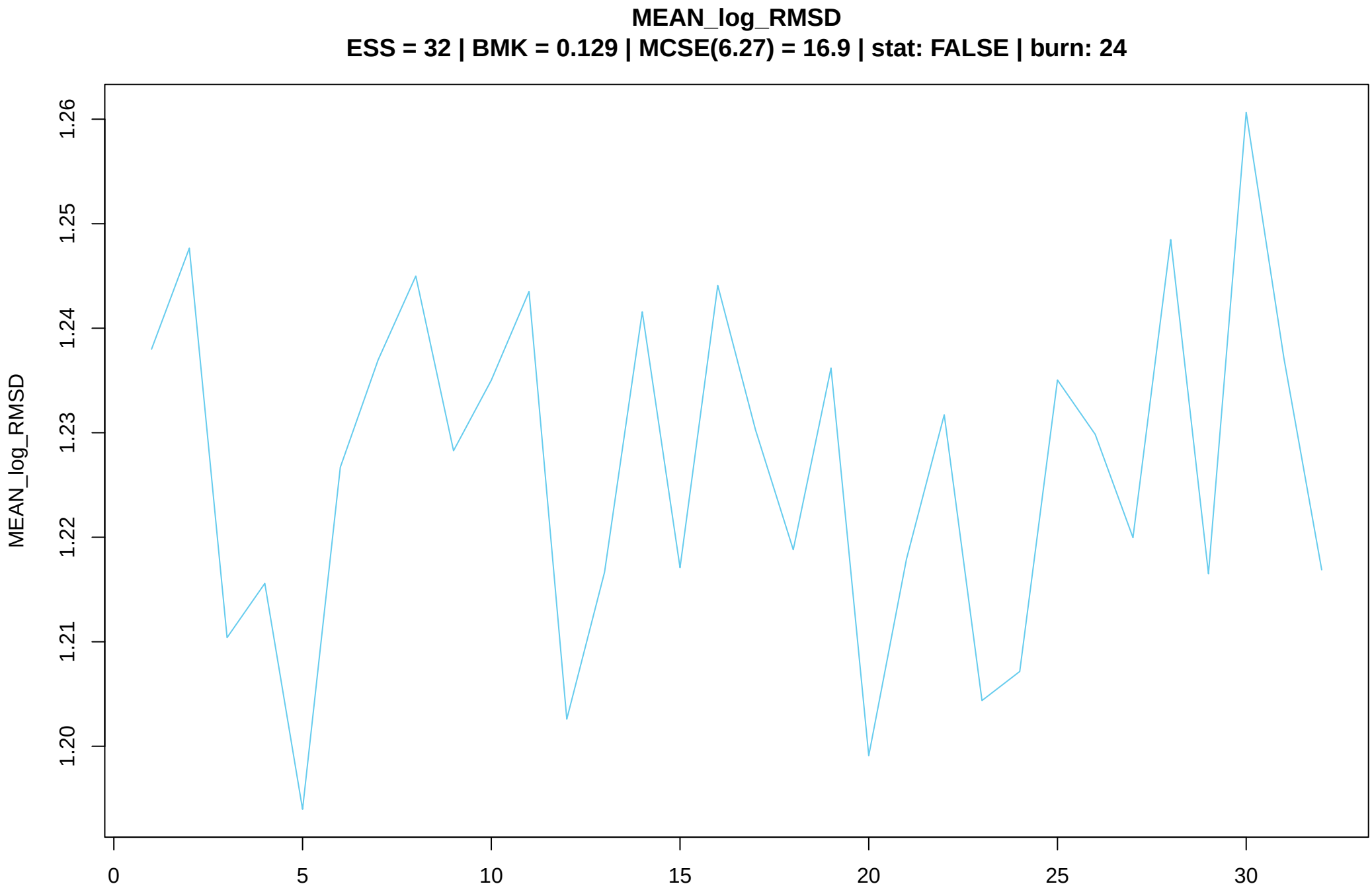

lPdatum5
ESS = 17.2 | BMK = 0.22 | MCSE(6.27) = 30.5 | stat: FALSE | burn: 30
lPdatum5
−7.9
−8.0
−8.1
−8.2
0
5
10
15
20
25
30

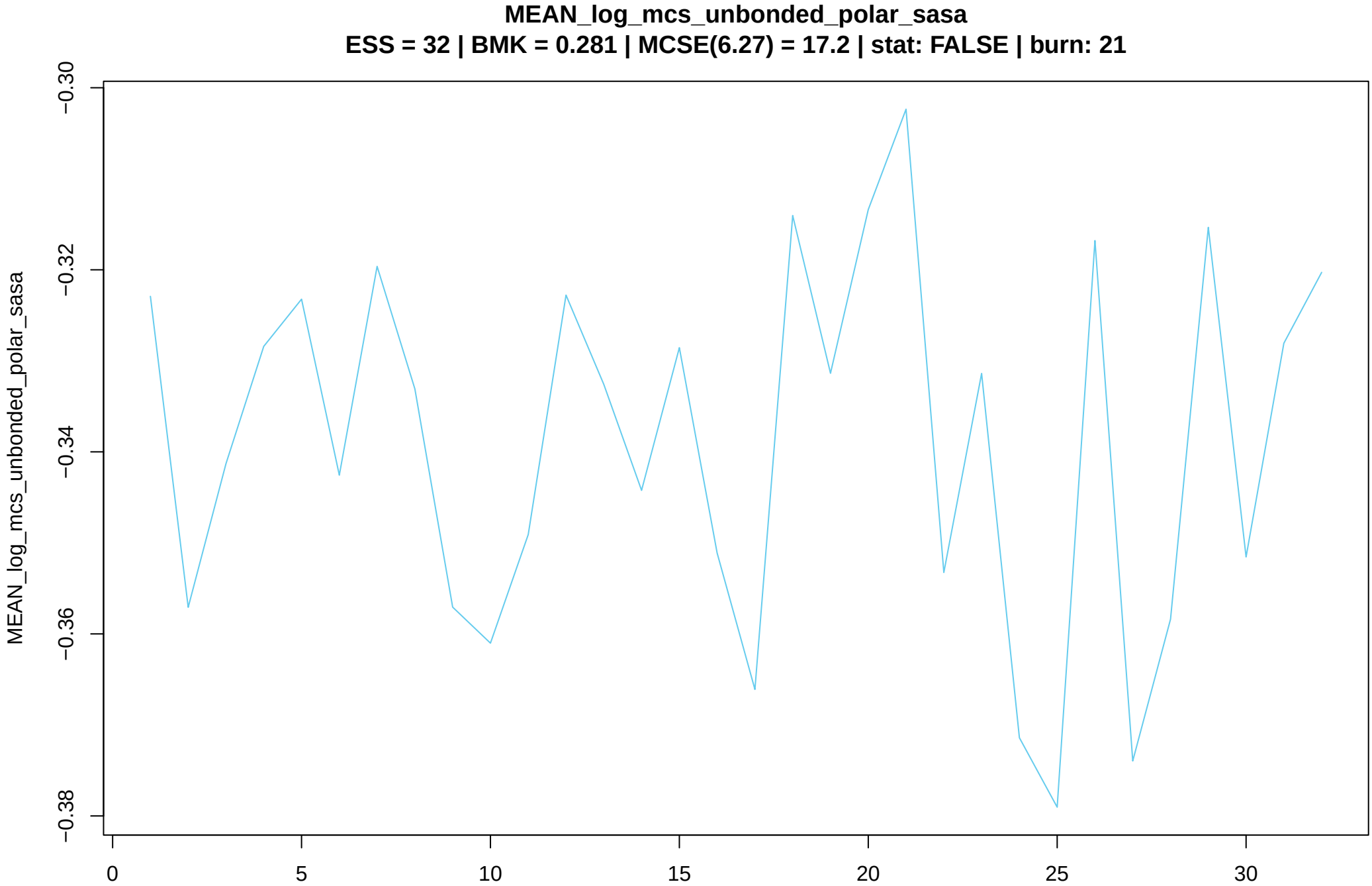

lPdatum6
ESS = 12.3 | BMK = 0.387 | MCSE(6.27) = 37.5 | stat: FALSE | burn: 30
lPdatum6
−7.65
−7.70
−7.75
−7.80
−7.85
0
5
10
15
20
25
30

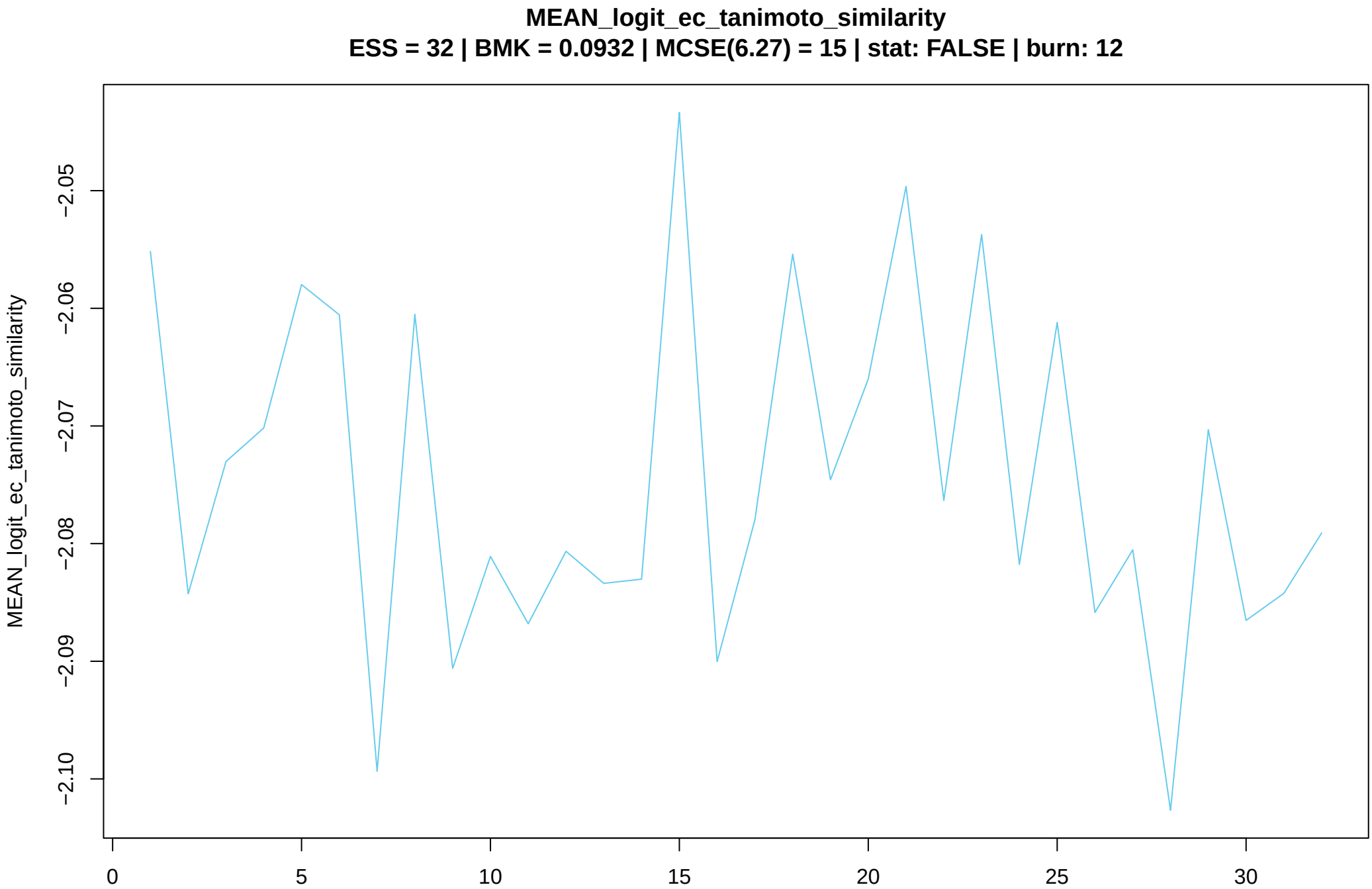

lPdatum7
ESS = 18.5 | BMK = 0.384 | MCSE(6.27) = 26.8 | stat: FALSE | burn: 30
lPdatum7
−13.2
−13.4
−13.6
−13.8
−14.0
0
5
10
15
20
25
30

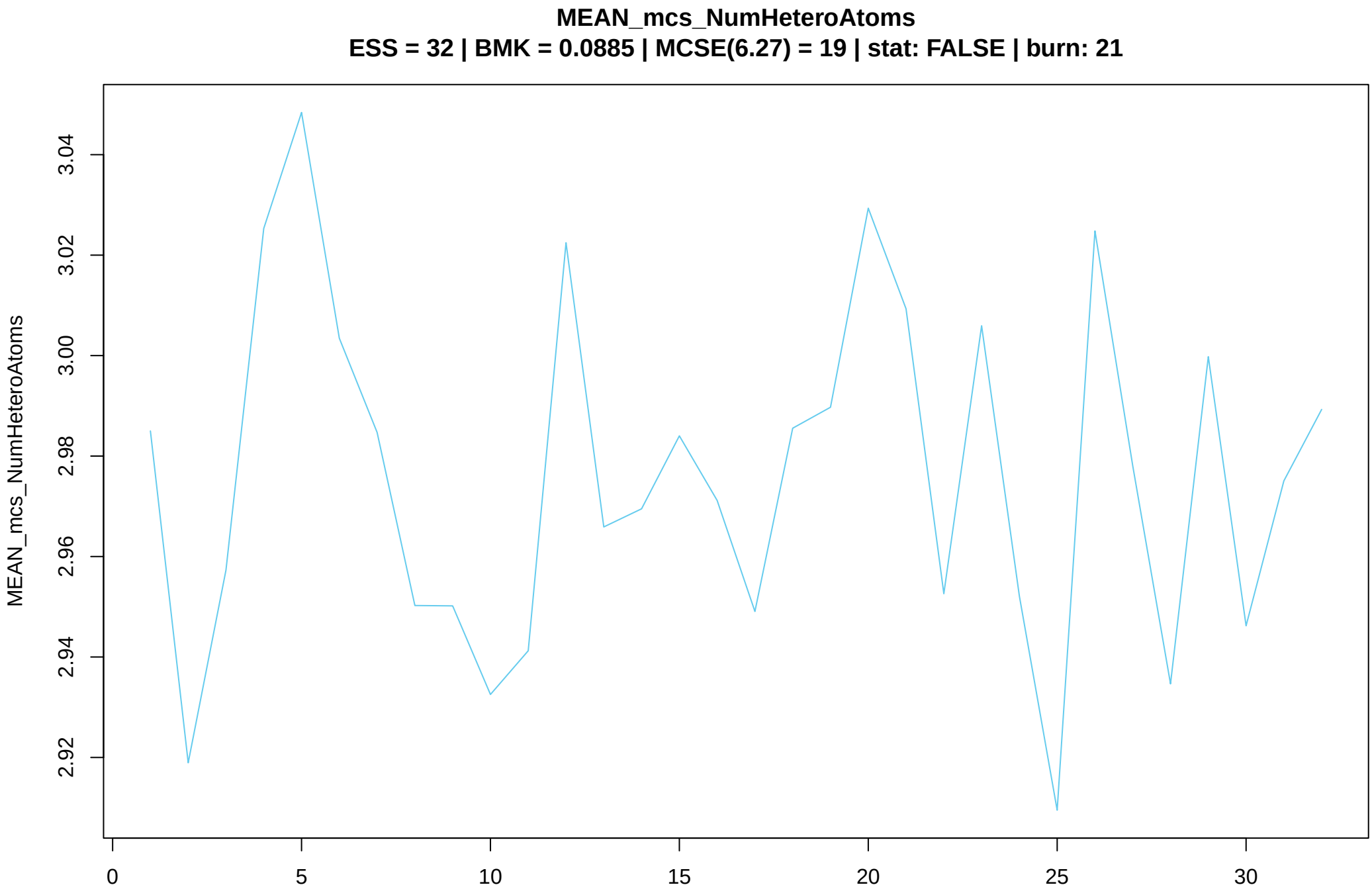

lPdatum8
ESS = 4.49 | BMK = 0.514 | MCSE(6.27) = 49.1 | stat: FALSE | burn: 30
lPdatum8
−10.9
−11.0
−11.1
−11.2
−11.3
0
5
10
15
20
25
30

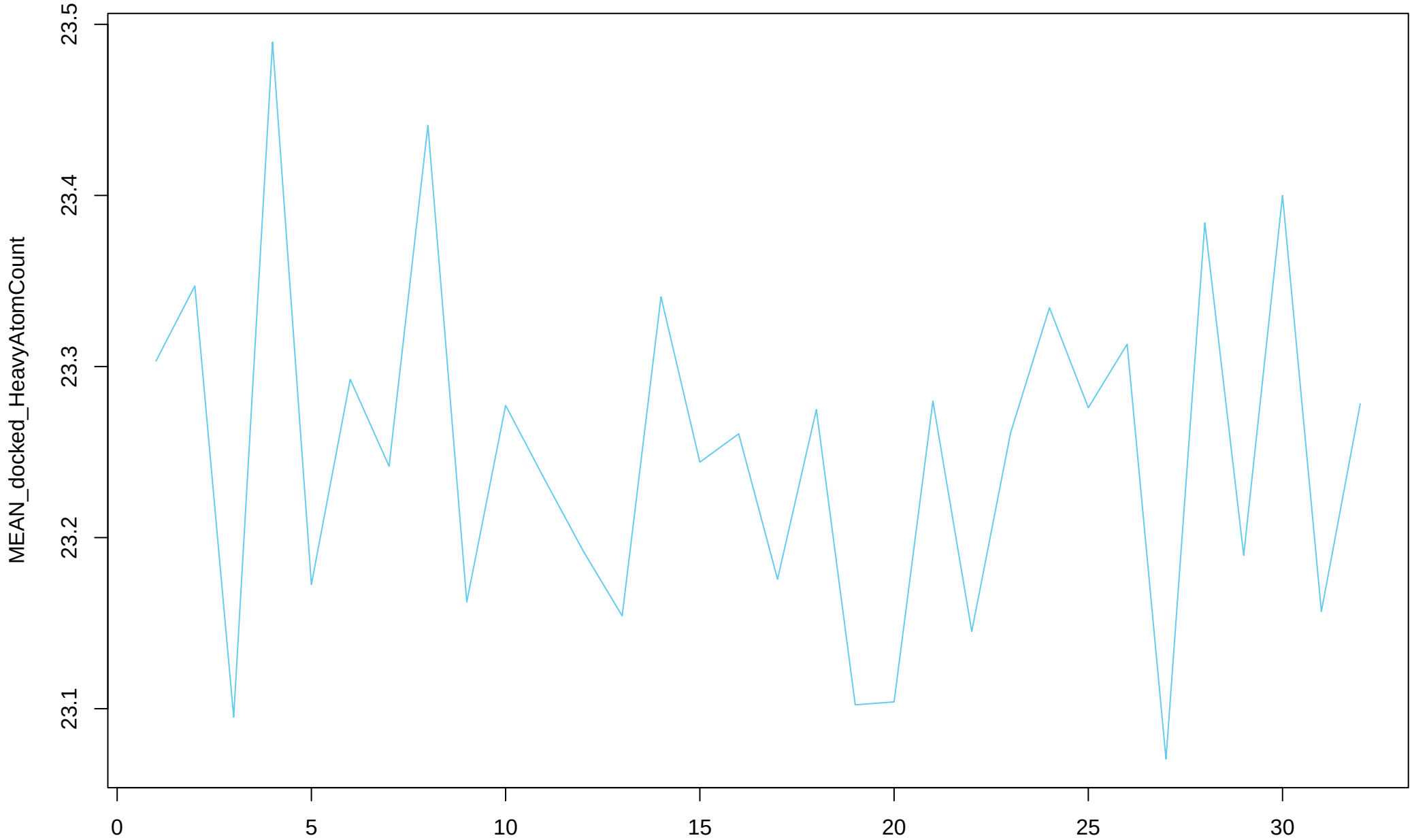

logitDcov
ESS = 32 | BMK = 0.217 | MCSE(6.27) = 16.4 | stat: FALSE | burn: 30
logitDcov
0.3
0.4
0.5
0.6
0.7
0
5
10
15
20
25
30

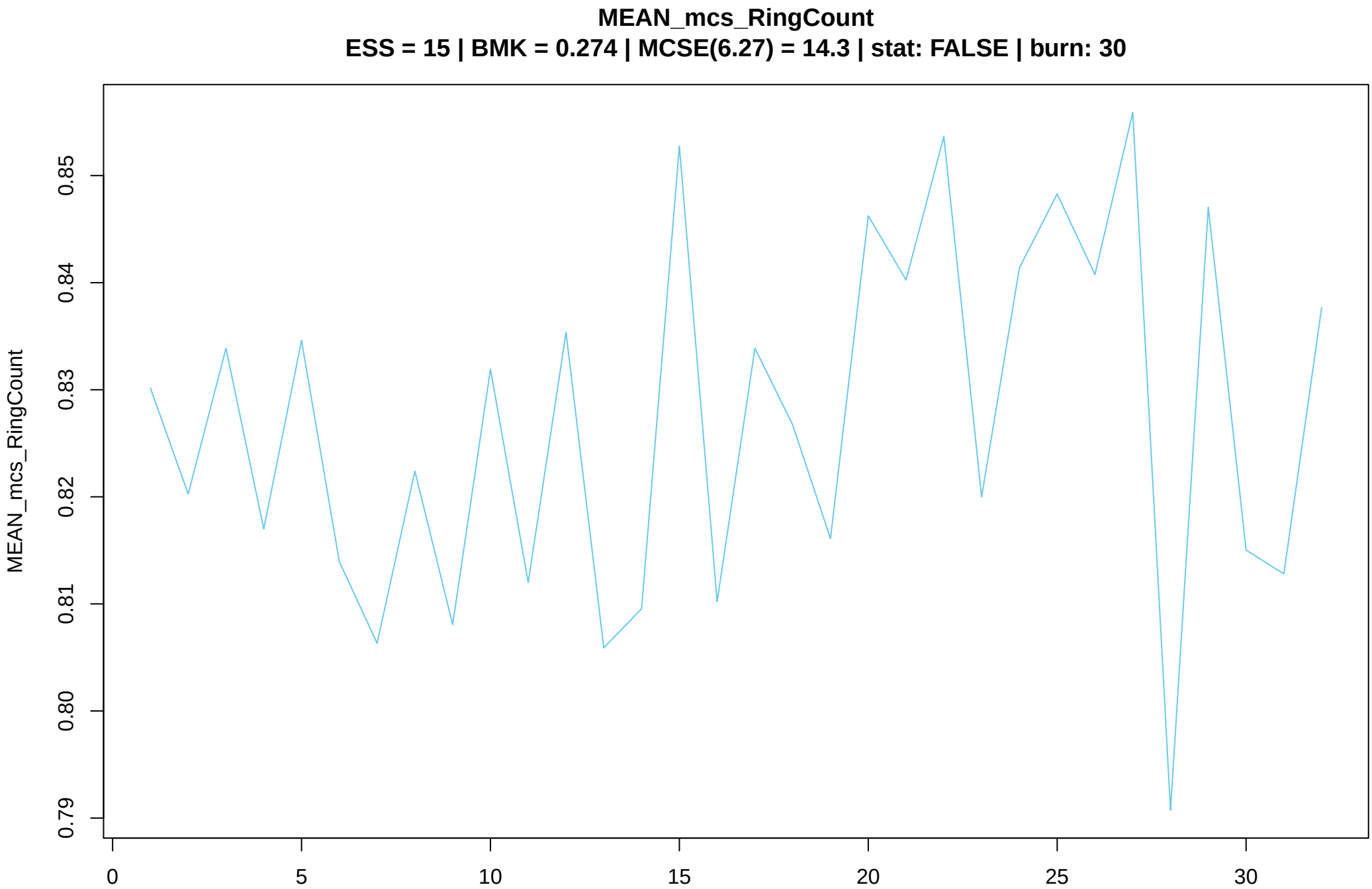

MEAN_log_RMSD
ESS = 32 | BMK = 0.129 | MCSE(6.27) = 16.9 | stat: FALSE | burn: 24
MEAN_log_RMSD
1.20
1.21
1.22
1.23
1.24
1.25
1.26
0
5
10
15
20
25
30

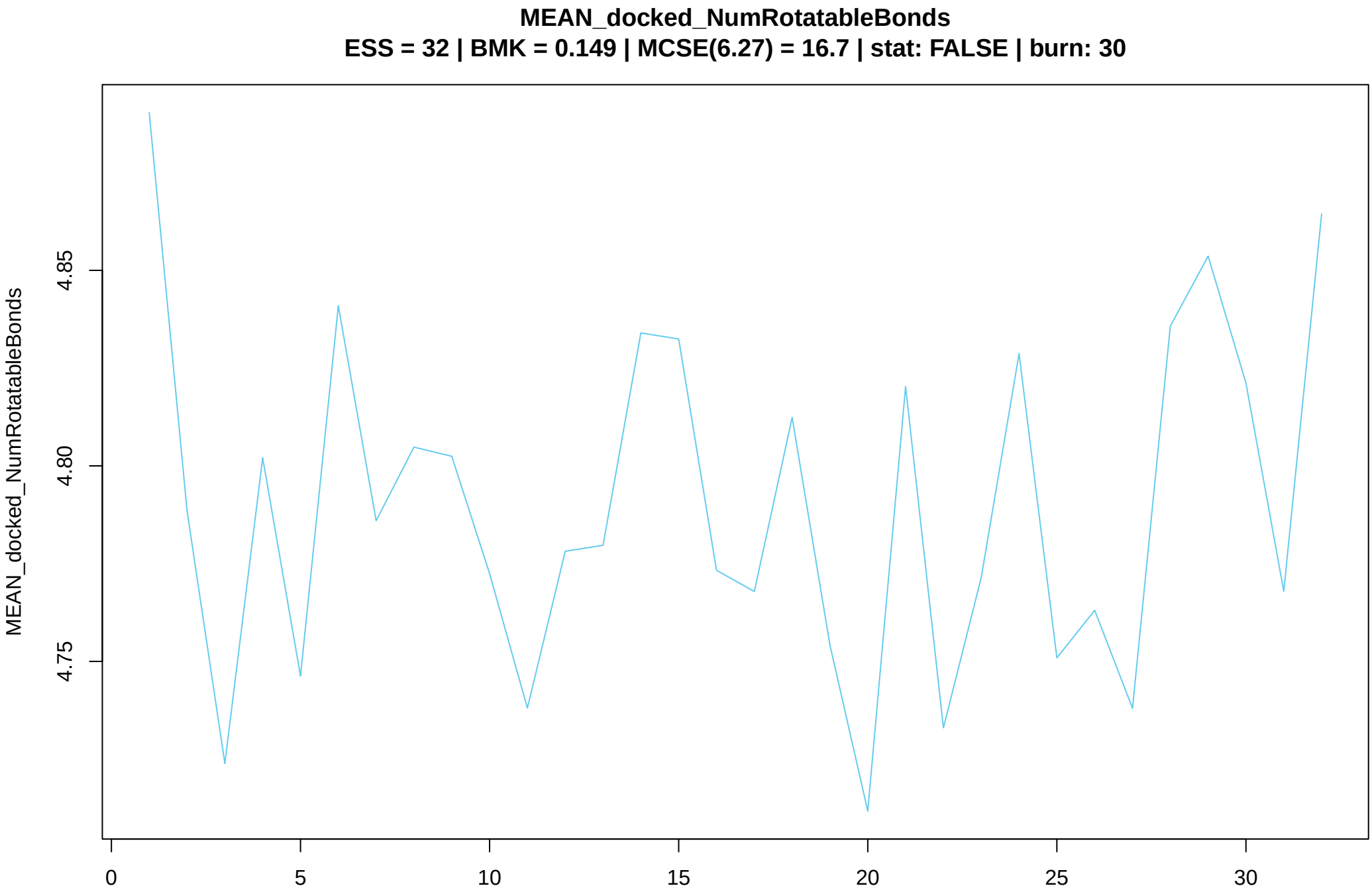

MEAN_log_mcs_unbonded_polar_sasa
ESS = 32 | BMK = 0.281 | MCSE(6.27) = 17.2 | stat: FALSE | burn: 21
MEAN_log_mcs_unbonded_polar_sasa
−0.30
−0.32
−0.34
−0.36
−0.38
0
5
10
15
20
25
30

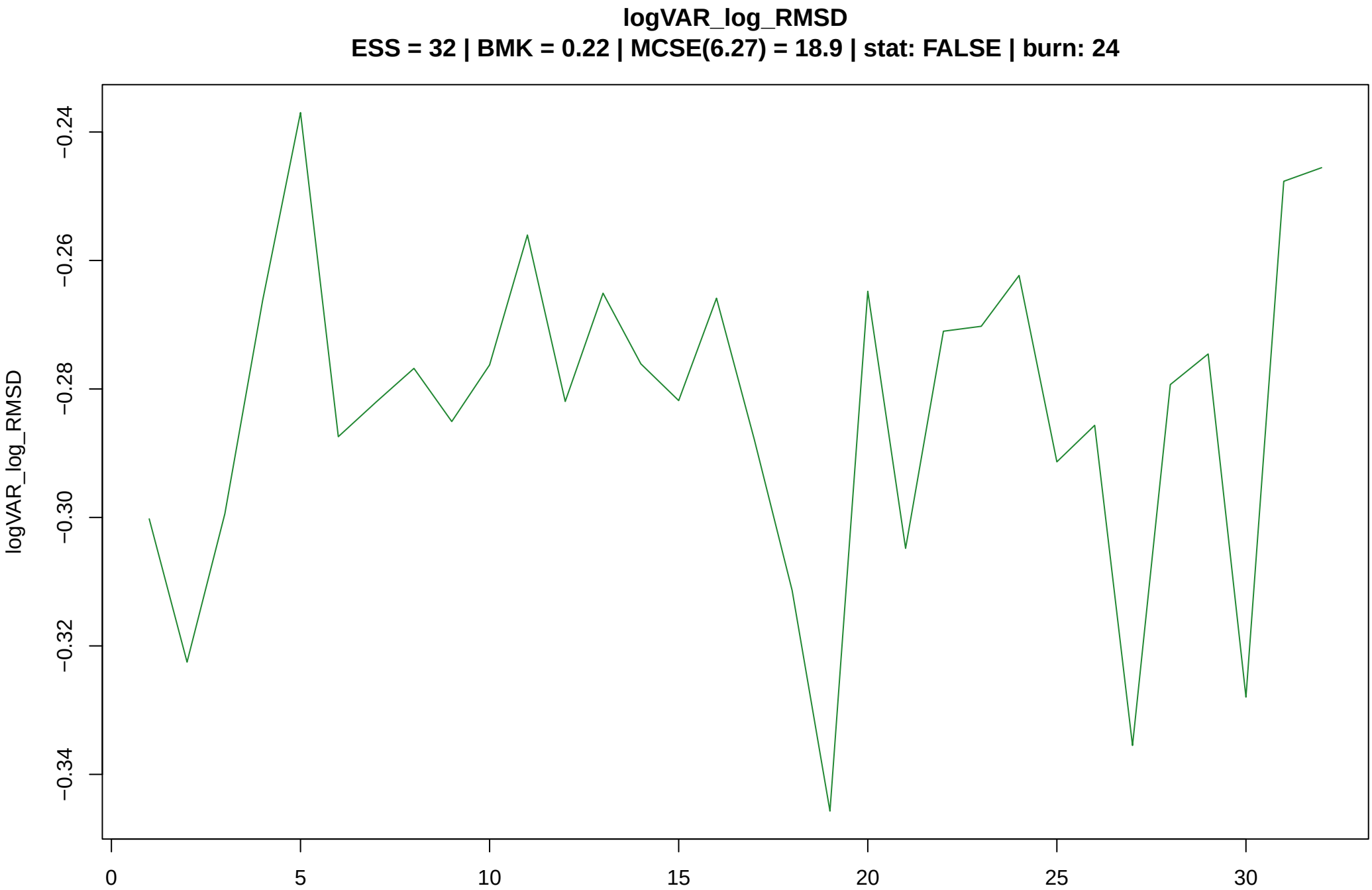

MEAN_logit_ec_tanimoto_similarity
ESS = 32 | BMK = 0.0932 | MCSE(6.27) = 15 | stat: FALSE | burn: 12
MEAN_logit_ec_tanimoto_similarity
−2.05
−2.06
−2.07
−2.08
−2.09
−2.10
0
5
10
15
20
25
30

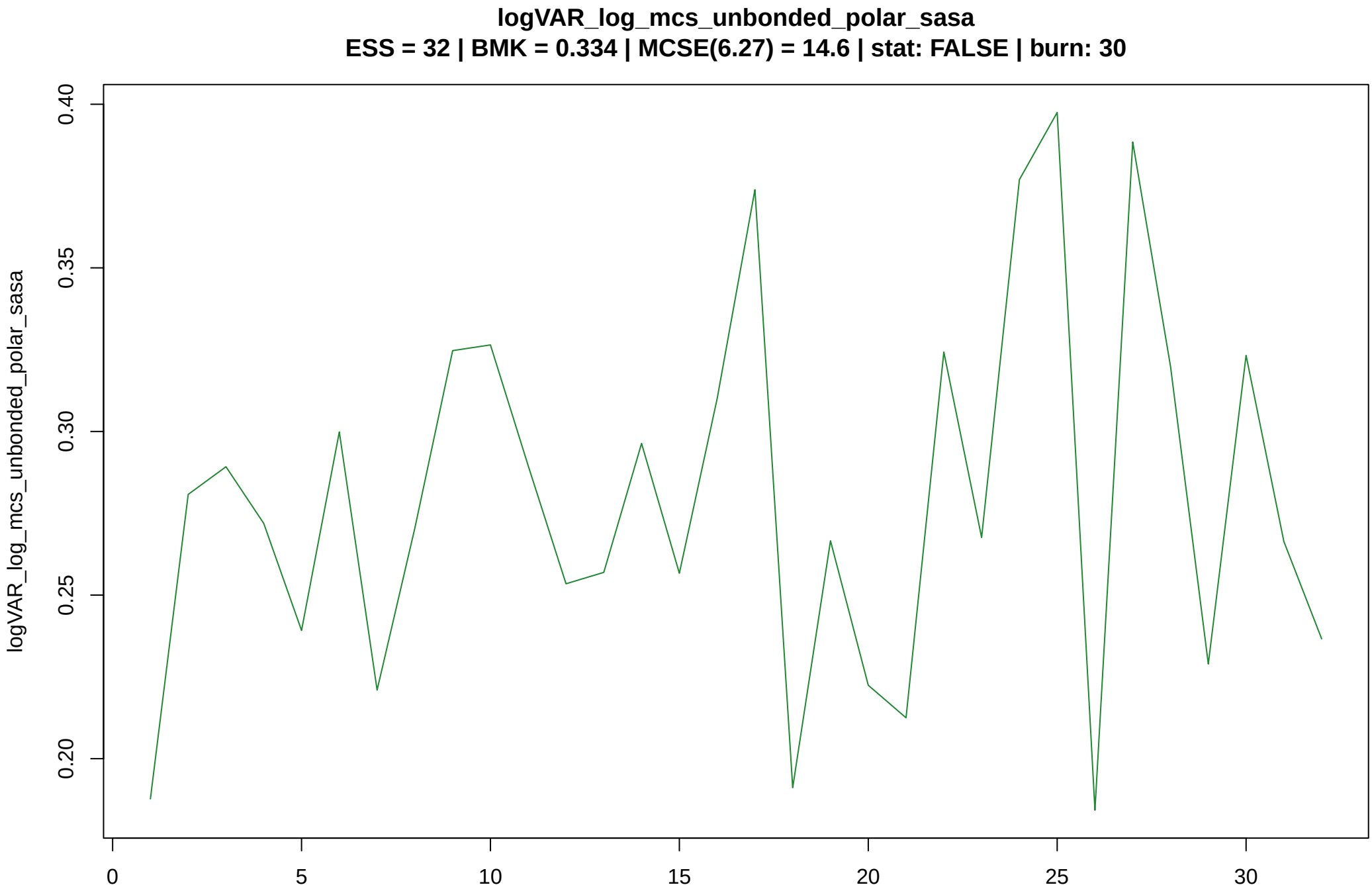

MEAN_mcs_NumHeteroAtoms
ESS = 32 | BMK = 0.0885 | MCSE(6.27) = 19 | stat: FALSE | burn: 21
MEAN_mcs_NumHeteroAtoms
2.92
2.94
2.96
2.98
3.00
3.02
3.04
0
5
10
15
20
25
30

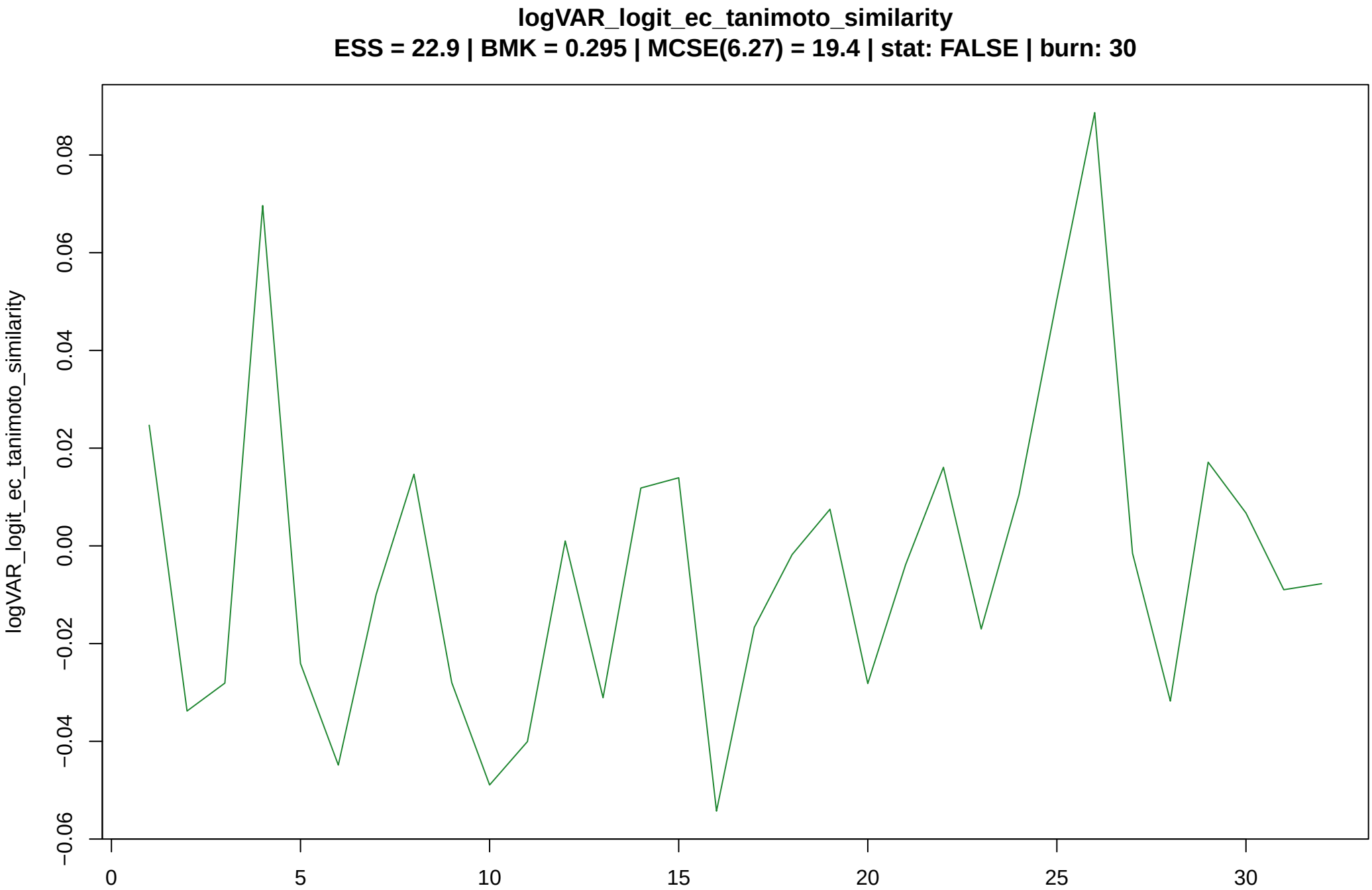

MEAN_docked_HeavyAtomCount
ESS = 32 | BMK = 0.113 | MCSE(6.27) = 4.78 | stat: FALSE | burn: 18
MEAN_docked_HeavyAtomCount
23.1
23.2
23.3
23.4
23.5
0
5
10
15
20
25
30

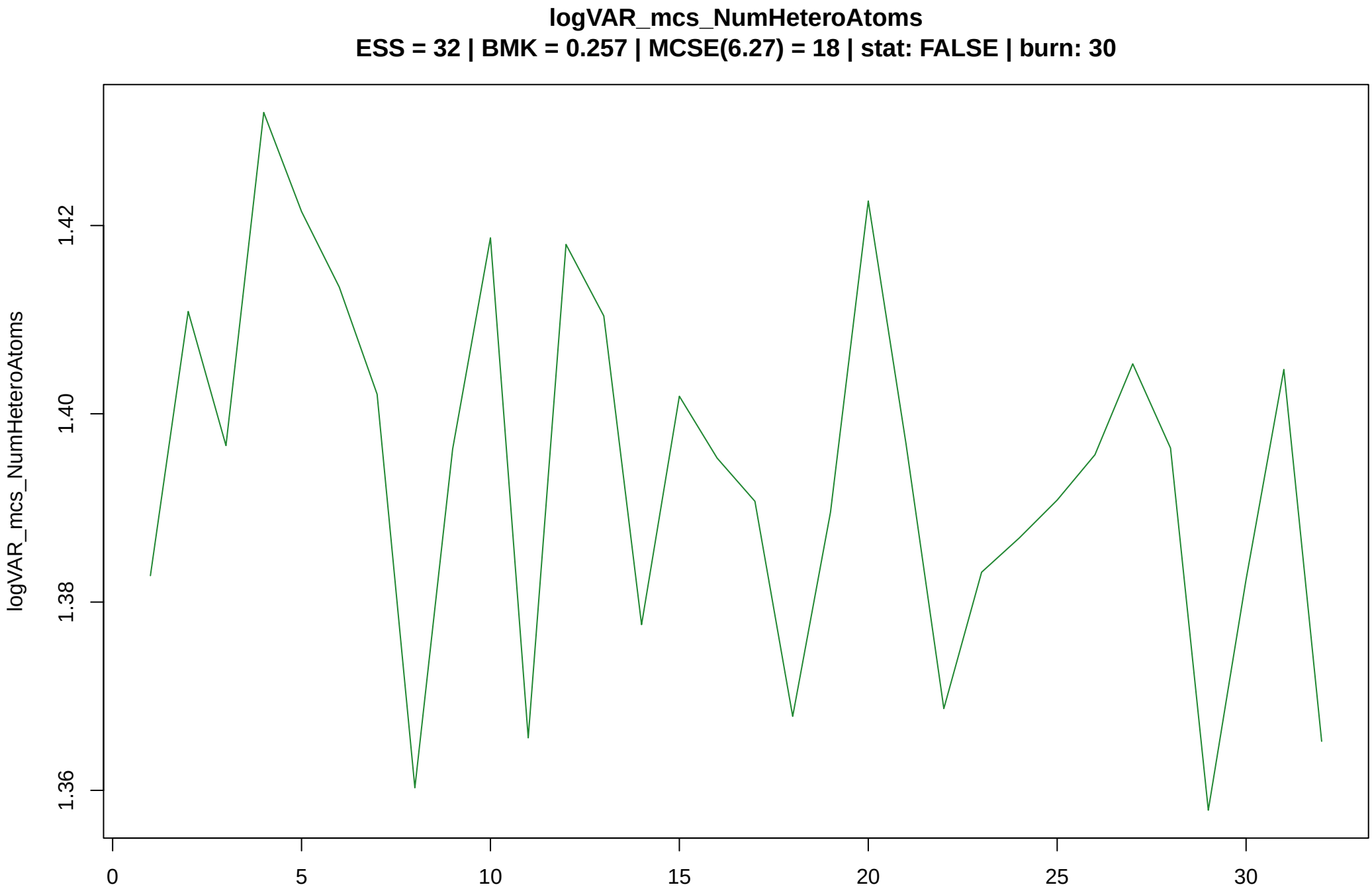

MEAN_mcs_RingCount
ESS = 15 | BMK = 0.274 | MCSE(6.27) = 14.3 | stat: FALSE | burn: 30
MEAN_mcs_RingCount
0.79
0.80
0.81
0.82
0.83
0.84
0.85
0
5
10
15
20
25
30

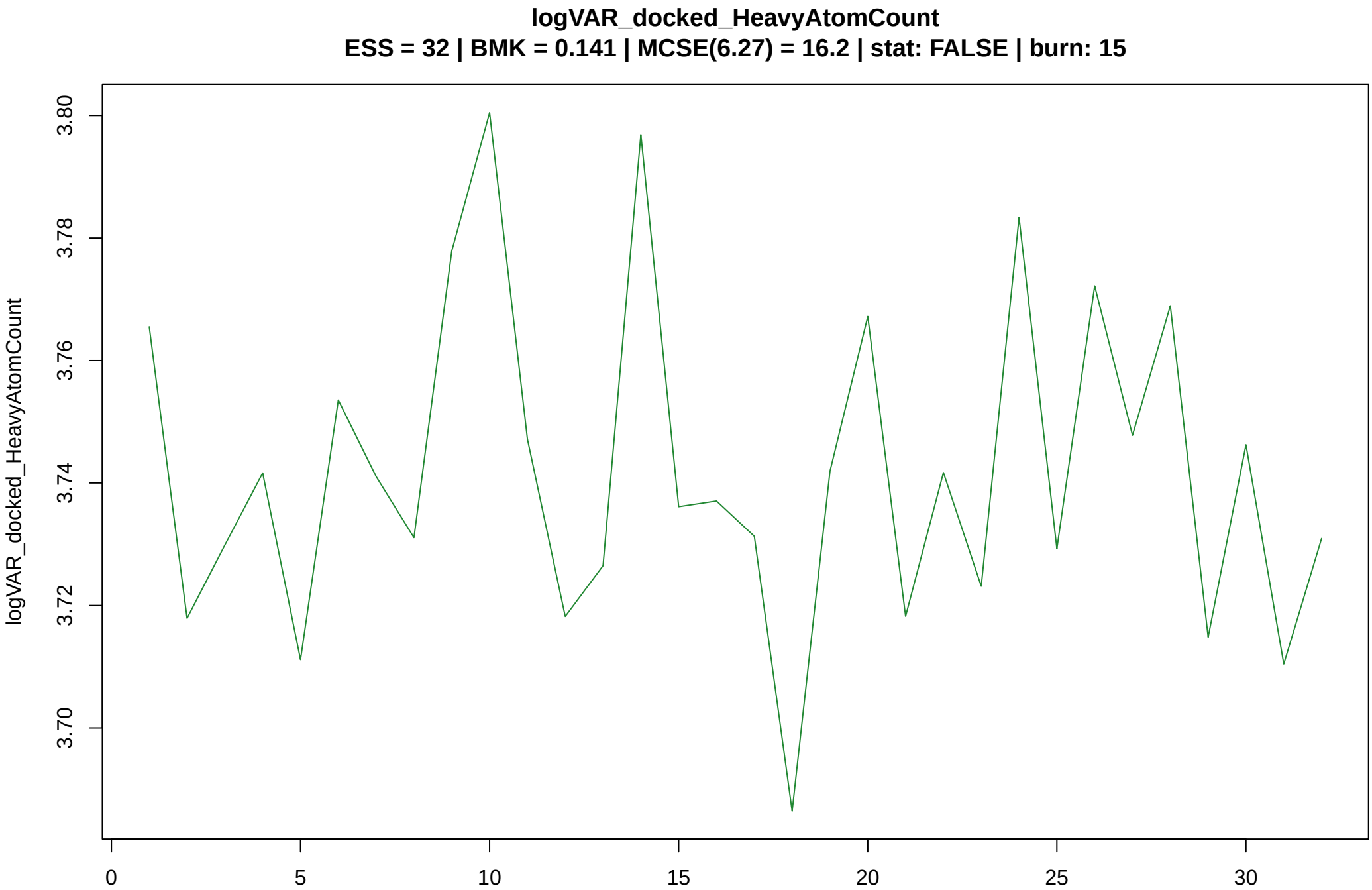

MEAN_docked_NumRotatableBonds
ESS = 32 | BMK = 0.149 | MCSE(6.27) = 16.7 | stat: FALSE | burn: 30
MEAN_docked_NumRotatableBonds
4.75
4.80
4.85
0
5
10
15
20
25
30

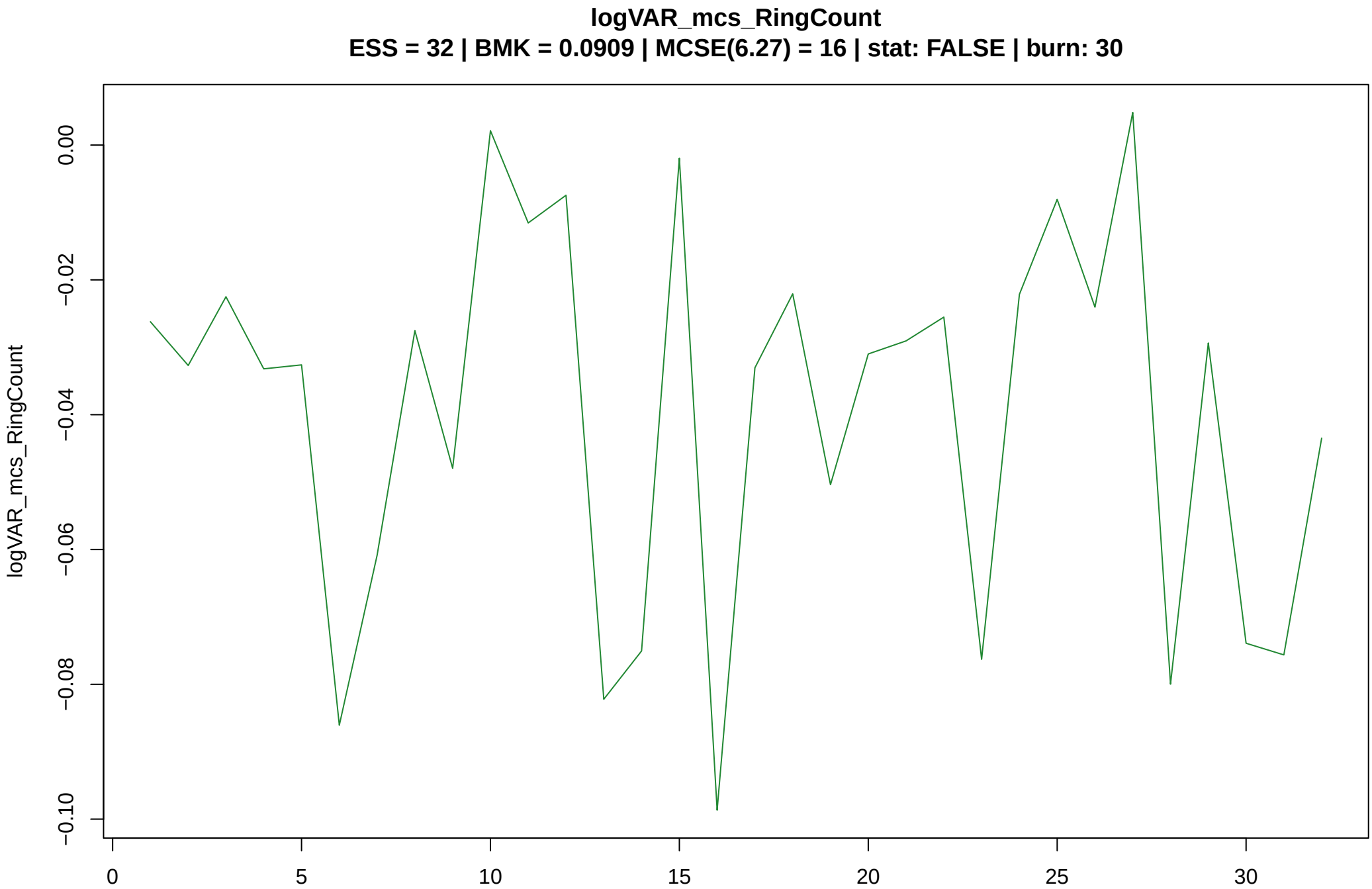

logVAR_log_RMSD
ESS = 32 | BMK = 0.22 | MCSE(6.27) = 18.9 | stat: FALSE | burn: 24
logVAR_log_RMSD
−0.24
−0.26
−0.28
−0.30
−0.32
−0.34
0
5
10
15
20
25
30

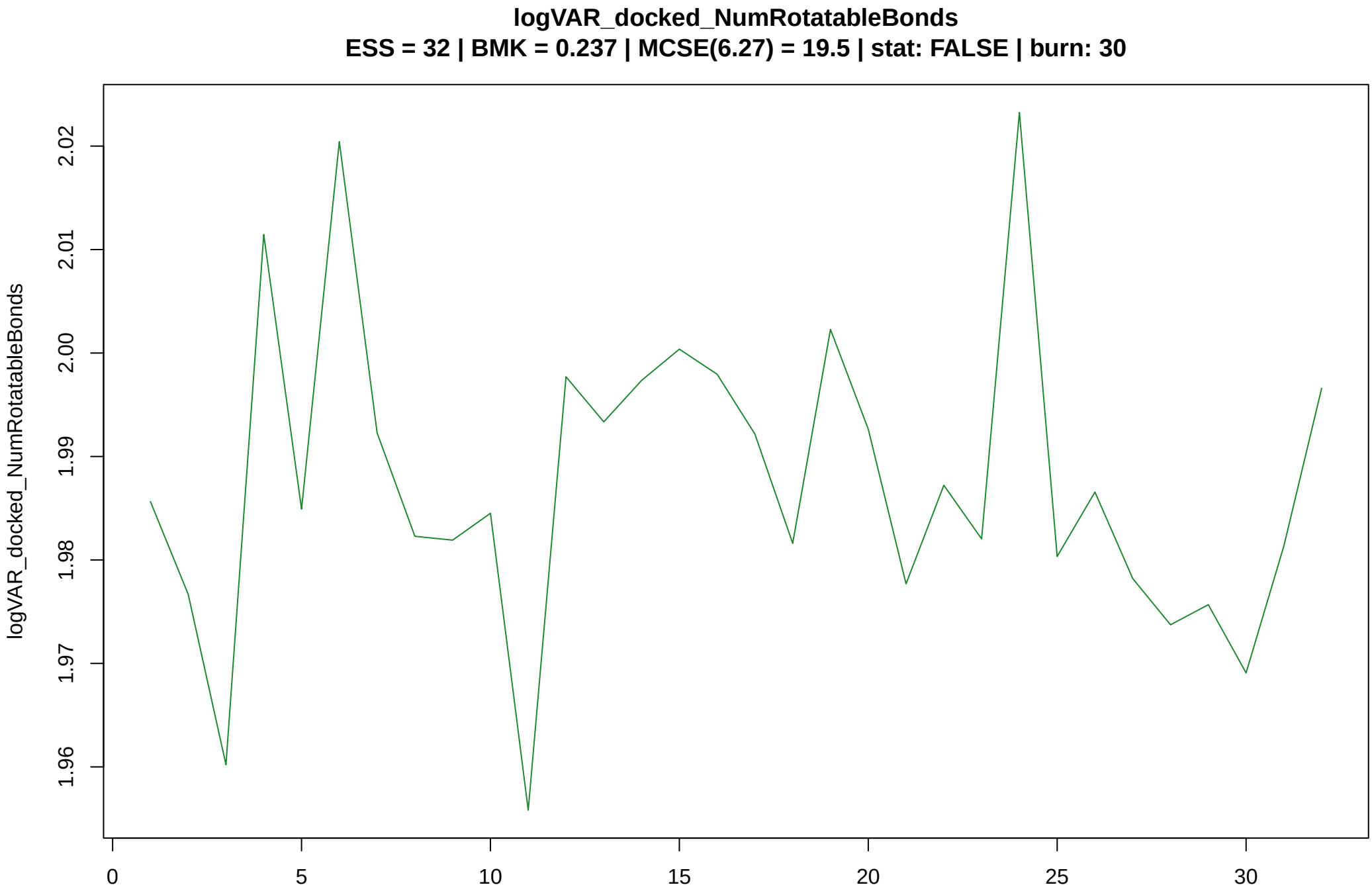

logVAR_log_mcs_unbonded_polar_sasa
ESS = 32 | BMK = 0.334 | MCSE(6.27) = 14.6 | stat: FALSE | burn: 30
logVAR_log_mcs_unbonded_polar_sasa
0.20
0.25
0.30
0.35
0.40
0
5
10
15
20
25
30

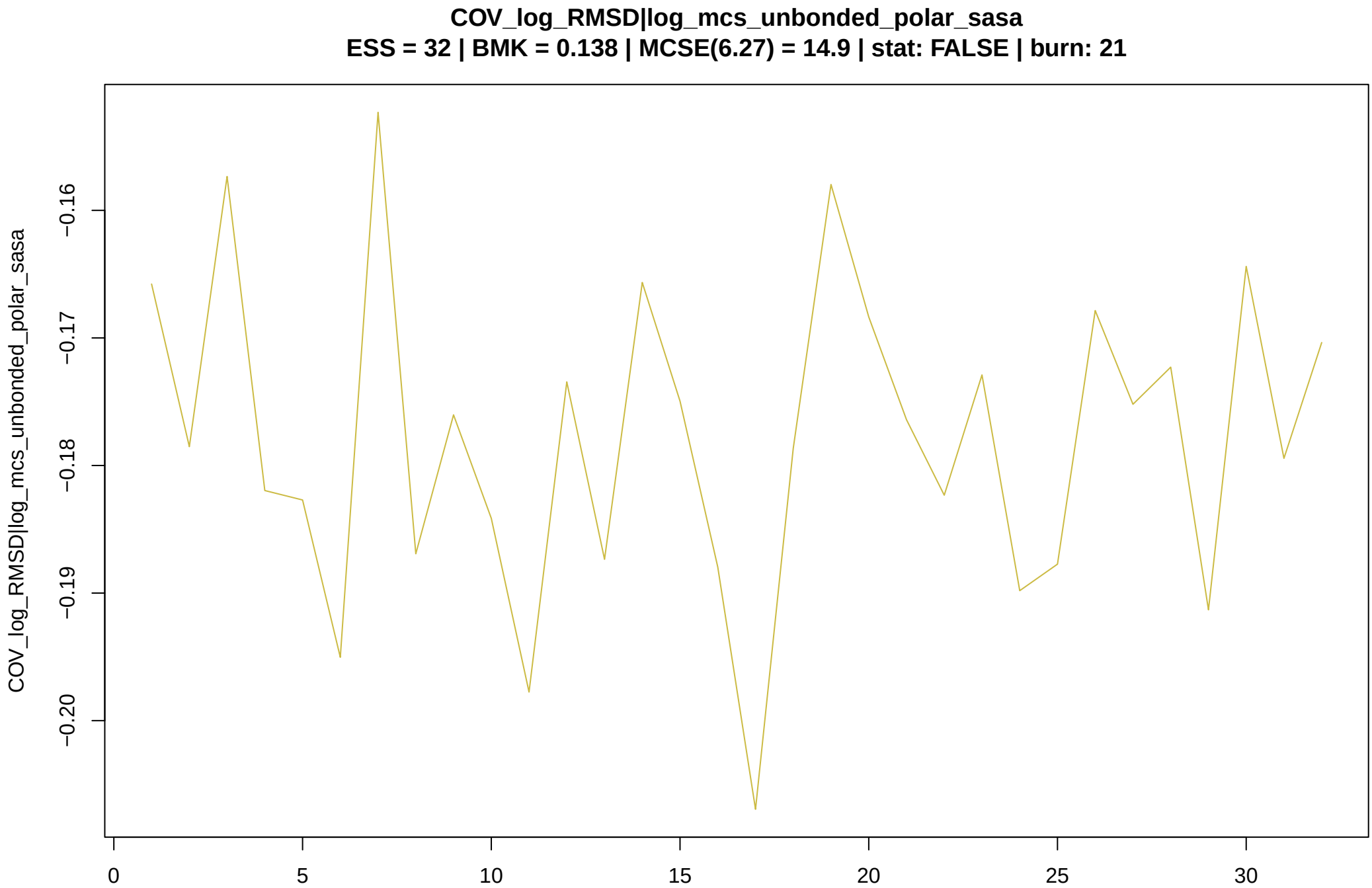

logVAR_logit_ec_tanimoto_similarity
ESS = 22.9 | BMK = 0.295 | MCSE(6.27) = 19.4 | stat: FALSE | burn: 30
logVAR_logit_ec_tanimoto_similarity
−0.06
−0.04
−0.02
0.00
0.02
0.04
0.06
0.08
0
5
10
15
20
25
30

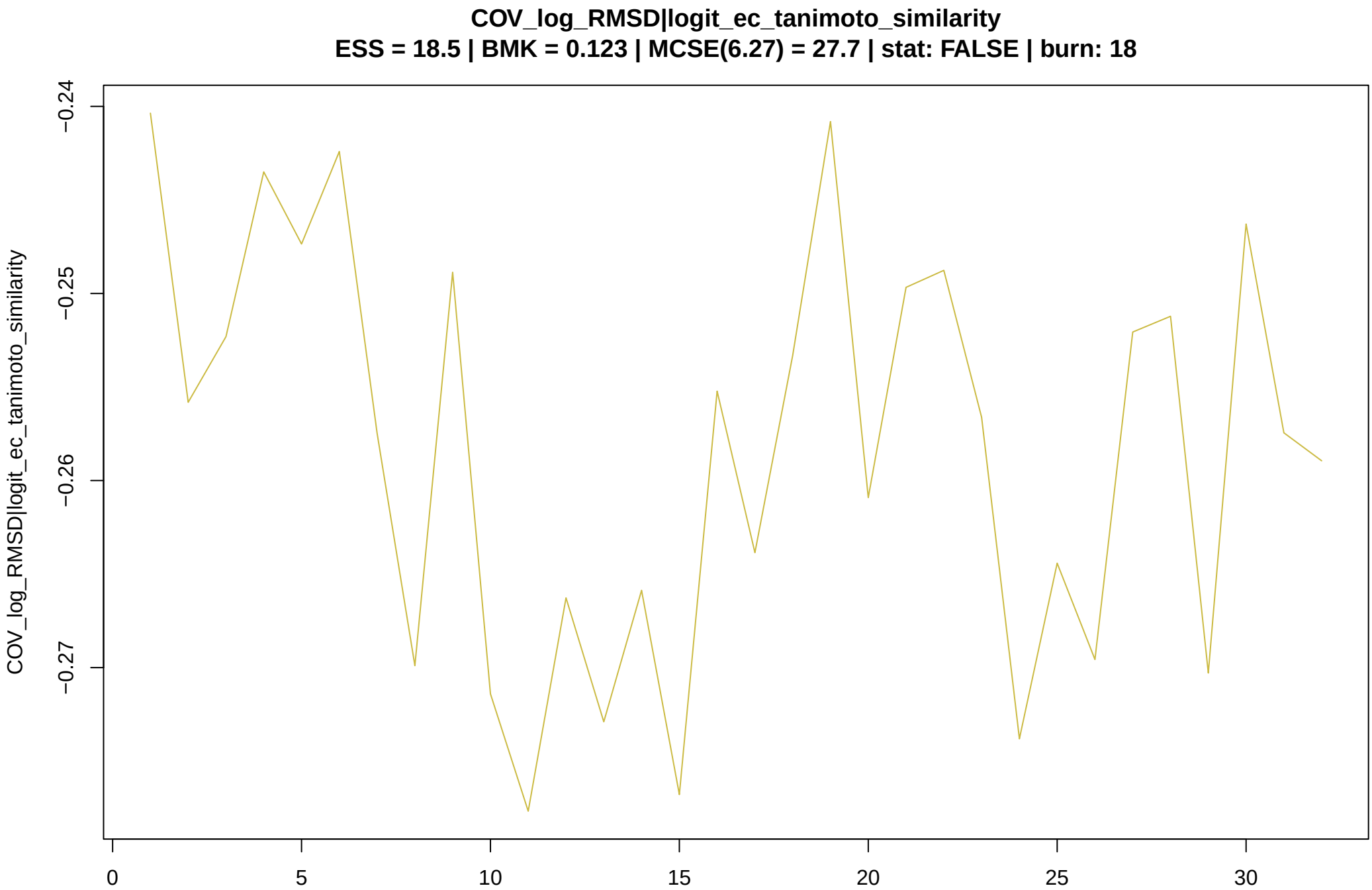

logVAR_mcs_NumHeteroAtoms
ESS = 32 | BMK = 0.257 | MCSE(6.27) = 18 | stat: FALSE | burn: 30
logVAR_mcs_NumHeteroAtoms
1.36
1.38
1.40
1.42
0
5
10
15
20
25
30

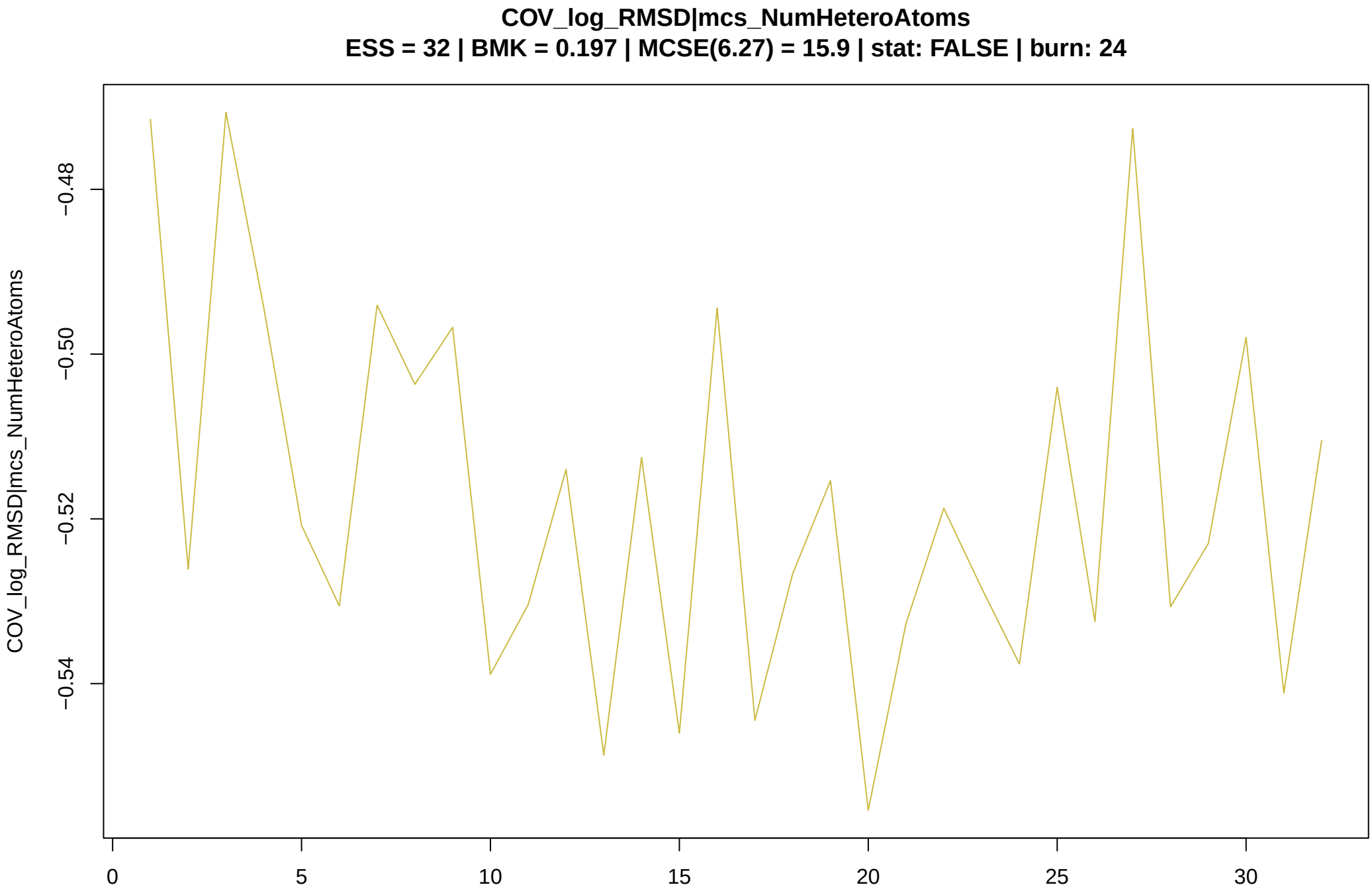

logVAR_docked_HeavyAtomCount
ESS = 32 | BMK = 0.141 | MCSE(6.27) = 16.2 | stat: FALSE | burn: 15
logVAR_docked_HeavyAtomCount
3.70
3.72
3.74
3.76
3.78
3.80
0
5
10
15
20
25
30

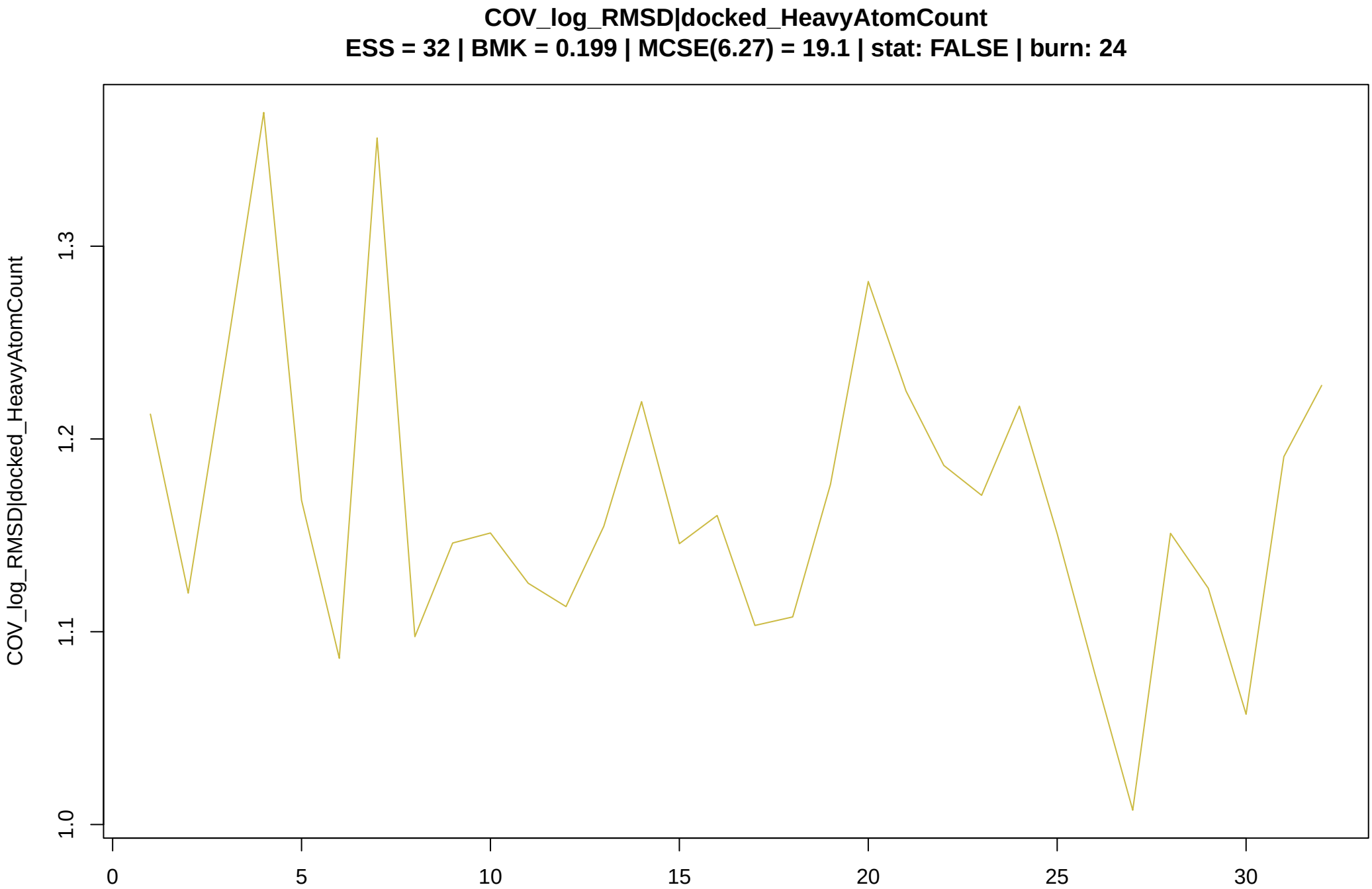

logVAR_mcs_RingCount
ESS = 32 | BMK = 0.0909 | MCSE(6.27) = 16 | stat: FALSE | burn: 30
logVAR_mcs_RingCount
0.00
−0.02
−0.04
−0.06
−0.08
−0.10
0
5
10
15
20
25
30

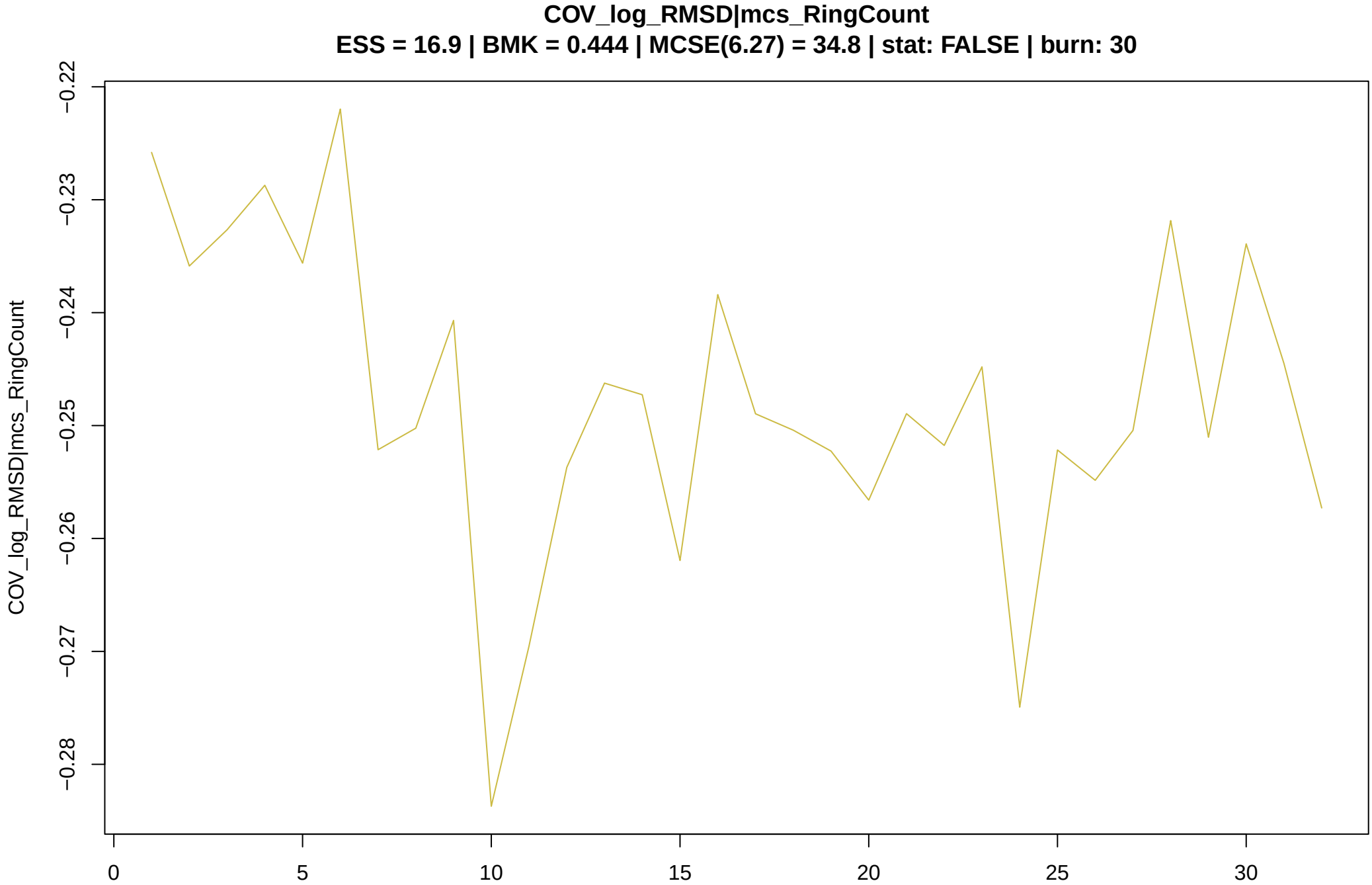

logVAR_docked_NumRotatableBonds
ESS = 32 | BMK = 0.237 | MCSE(6.27) = 19.5 | stat: FALSE | burn: 30
logVAR_docked_NumRotatableBonds
1.96
1.97
1.98
1.99
2.00
2.01
2.02
0
5
10
15
20
25
30

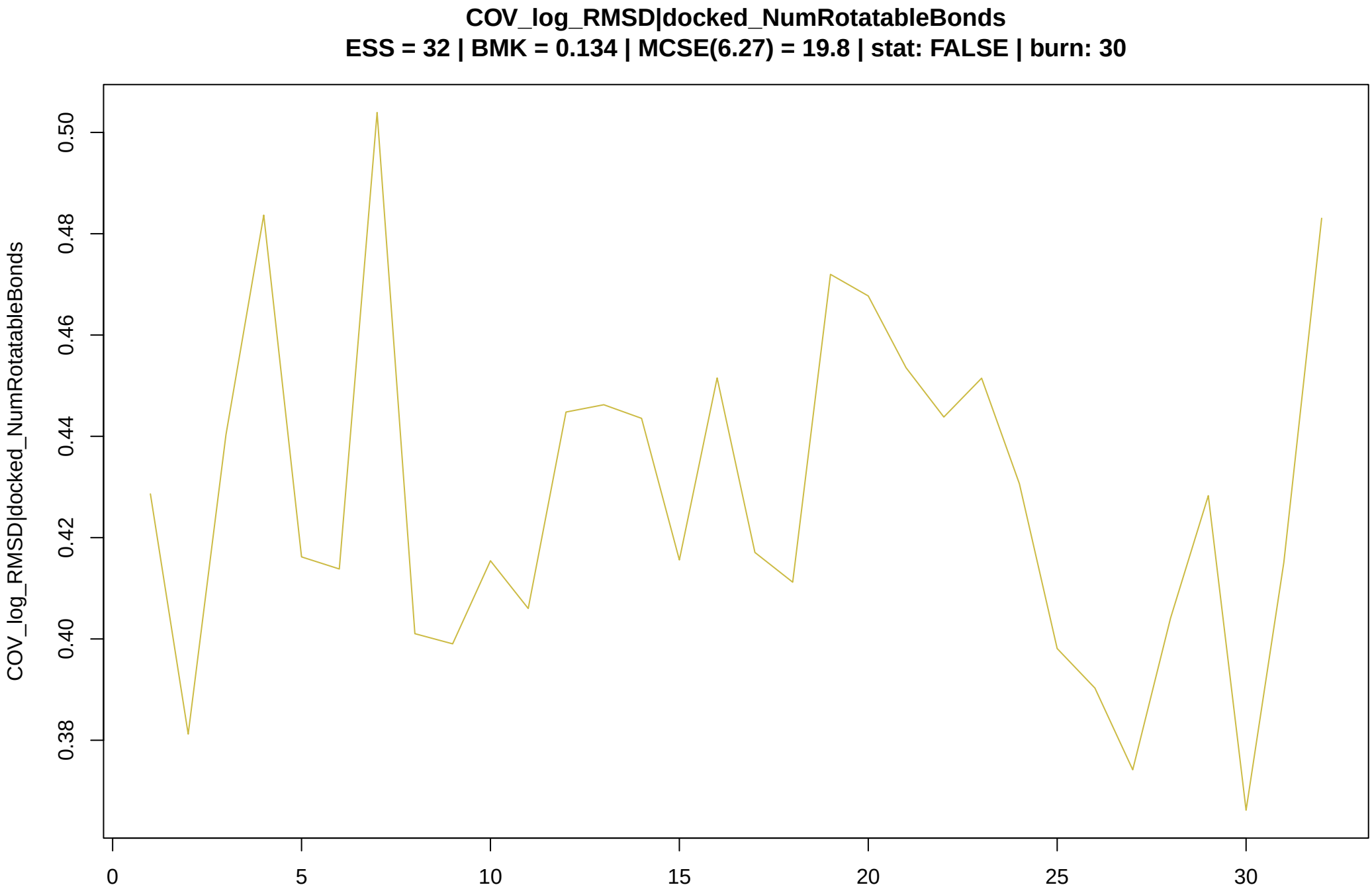

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 32 | BMK = 0.138 | MCSE(6.27) = 14.9 | stat: FALSE | burn: 21
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.16
−0.17
−0.18
−0.19
−0.20
0
5
10
15
20
25
30

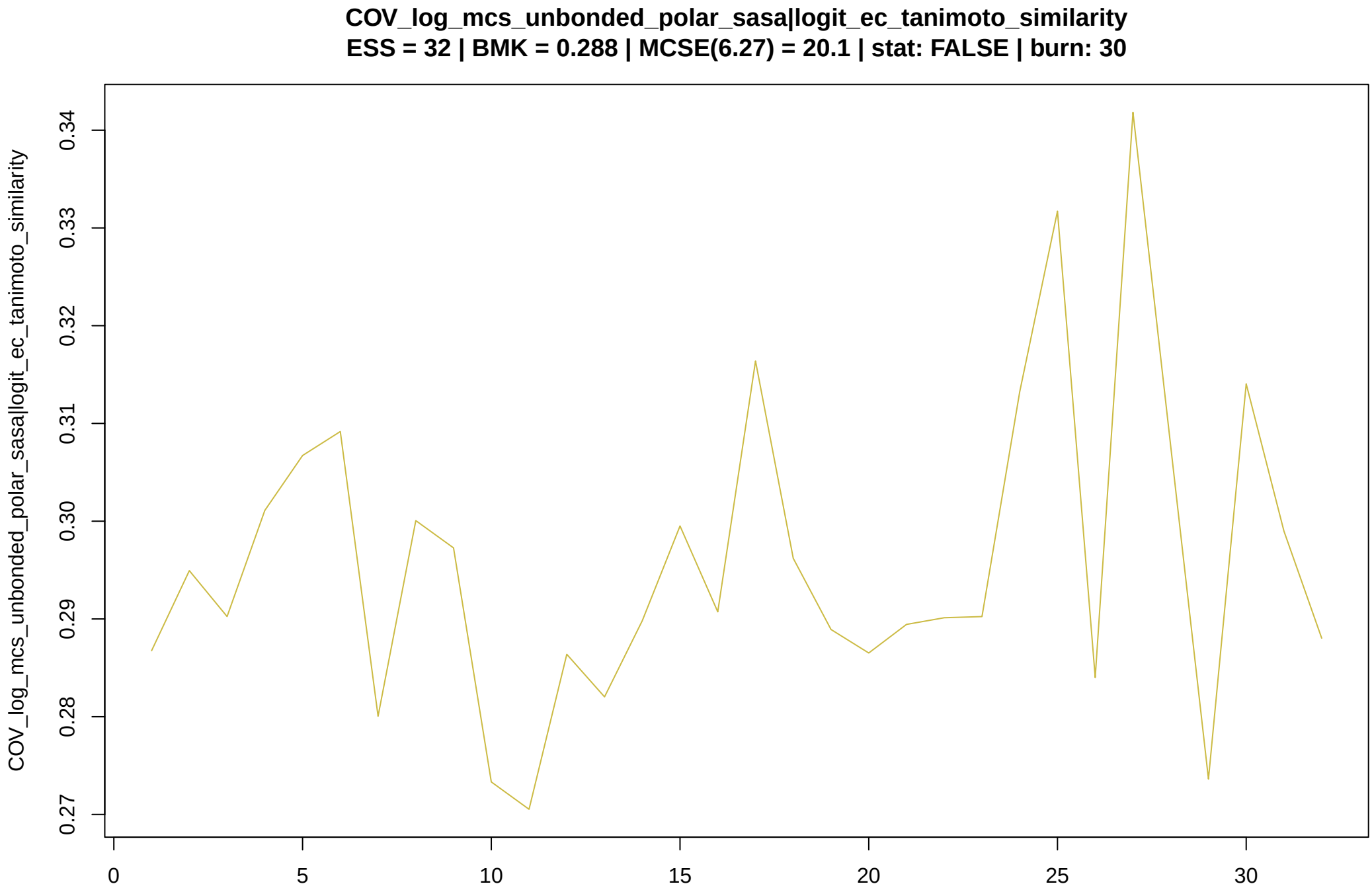

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 18.5 | BMK = 0.123 | MCSE(6.27) = 27.7 | stat: FALSE | burn: 18
COV_log_RMSD|logit_ec_tanimoto_similarity
−0.24
−0.25
−0.26
−0.27
0
5
10
15
20
25
30

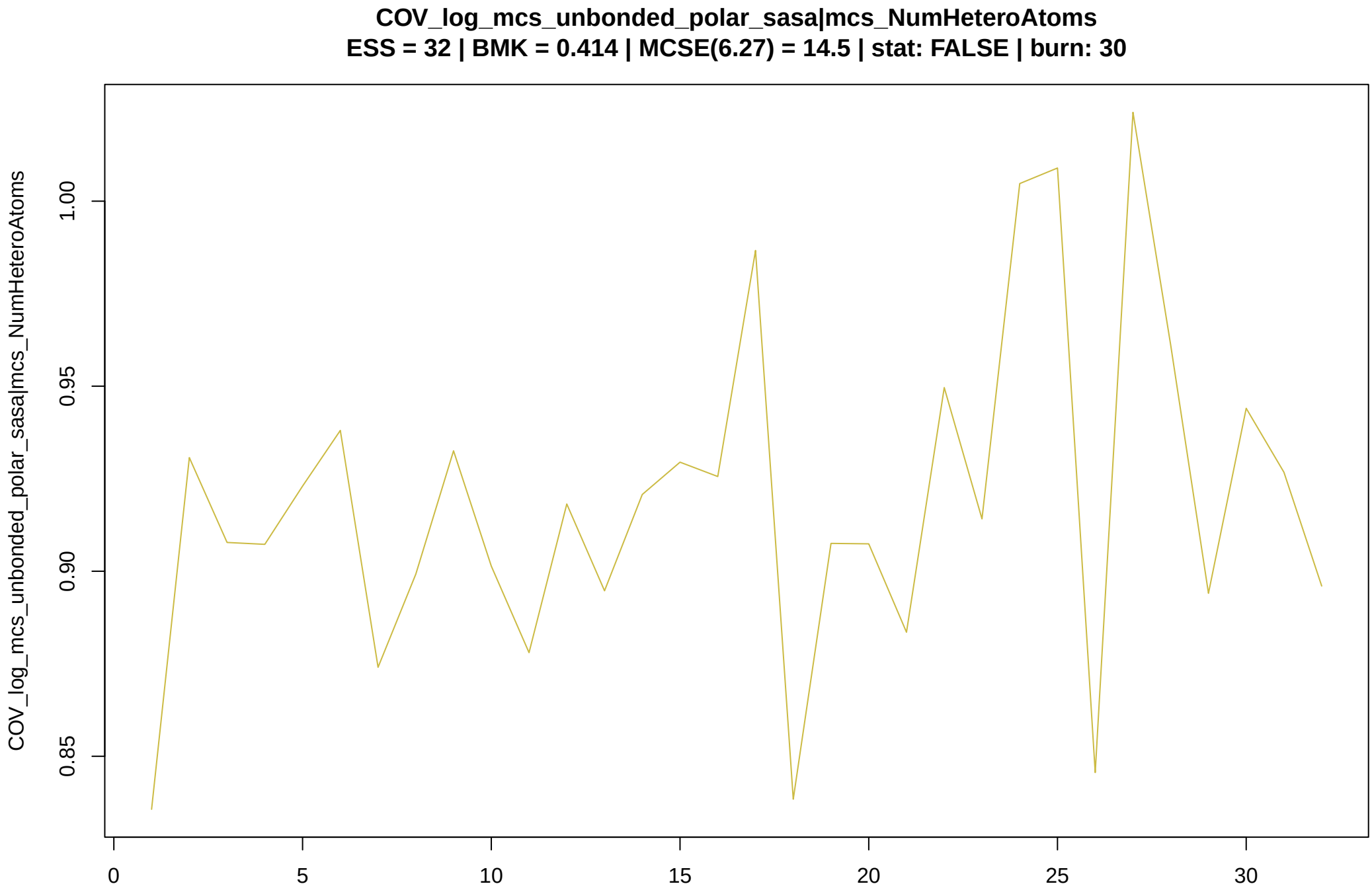

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 32 | BMK = 0.197 | MCSE(6.27) = 15.9 | stat: FALSE | burn: 24
COV_log_RMSD|mcs_NumHeteroAtoms
−0.48
−0.50
−0.52
−0.54
0
5
10
15
20
25
30

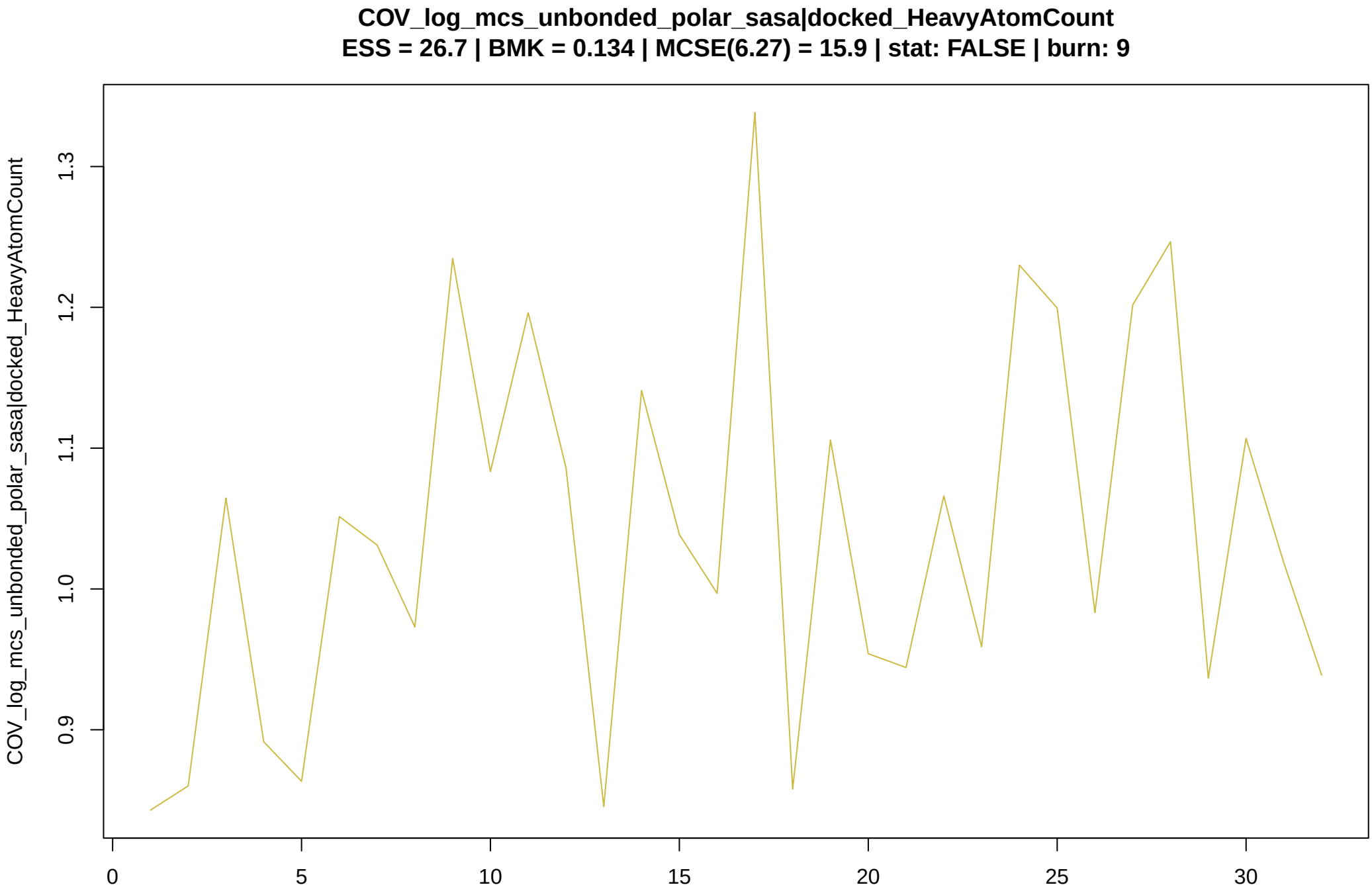

COV_log_RMSD|docked_HeavyAtomCount
ESS = 32 | BMK = 0.199 | MCSE(6.27) = 19.1 | stat: FALSE | burn: 24
COV_log_RMSD|docked_HeavyAtomCount
1.0
1.1
1.2
1.3
0
5
10
15
20
25
30

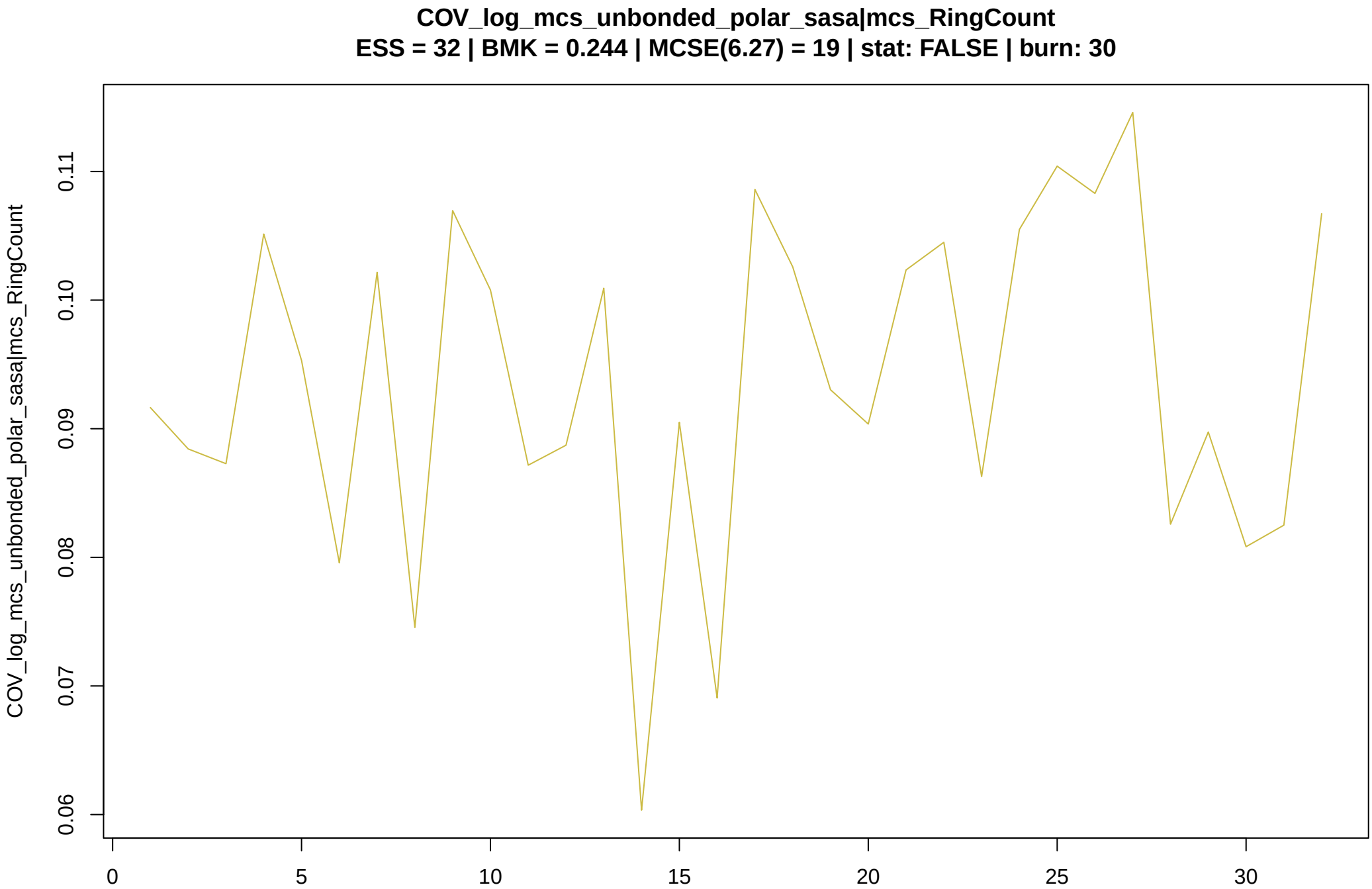

COV_log_RMSD|mcs_RingCount
ESS = 16.9 | BMK = 0.444 | MCSE(6.27) = 34.8 | stat: FALSE | burn: 30
COV_log_RMSD|mcs_RingCount
−0.22
−0.23
−0.24
−0.25
−0.26
−0.27
−0.28
0
5
10
15
20
25
30

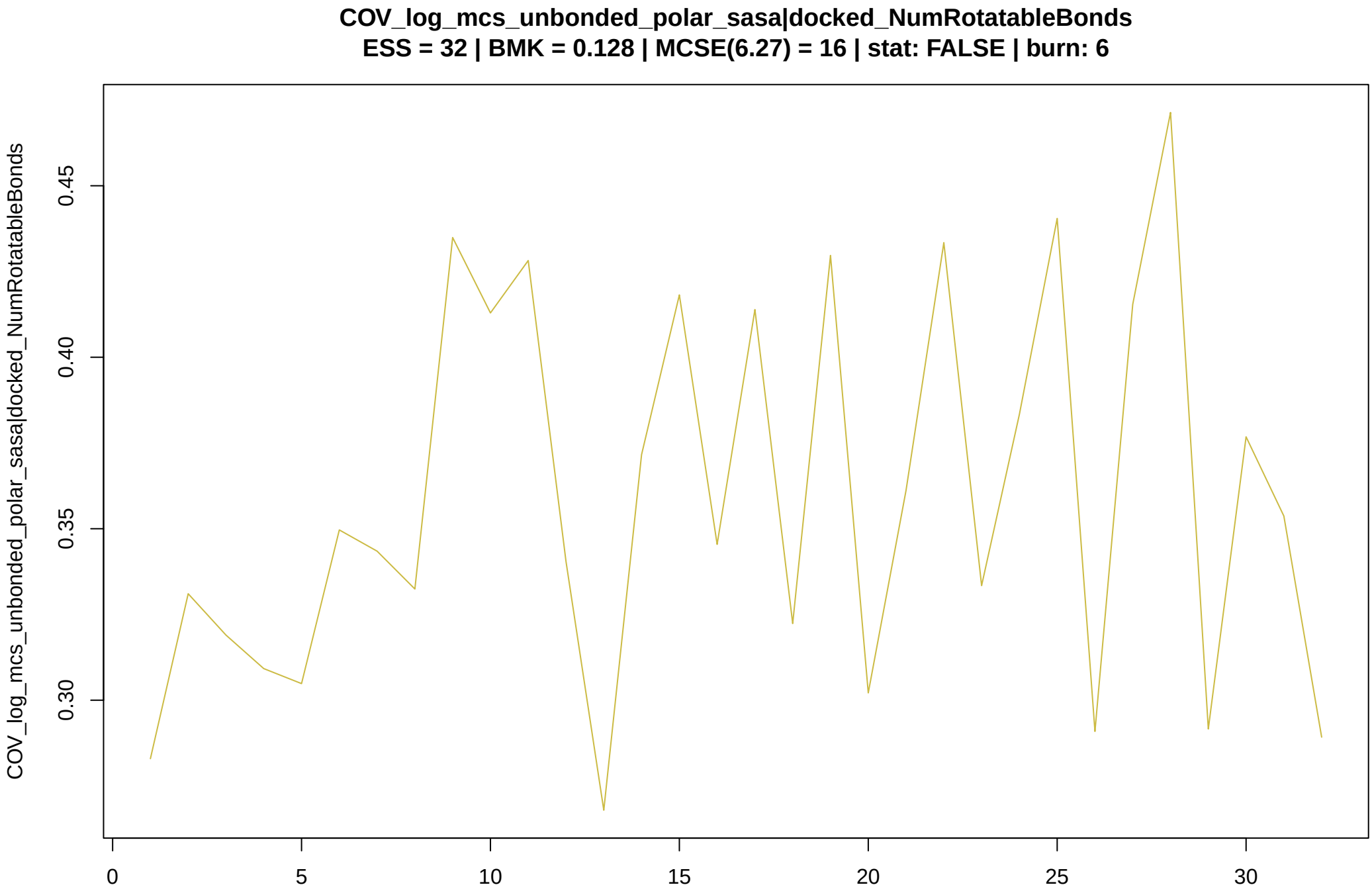

COV_log_RMSD|docked_NumRotatableBonds
ESS = 32 | BMK = 0.134 | MCSE(6.27) = 19.8 | stat: FALSE | burn: 30
COV_log_RMSD|docked_NumRotatableBonds
0.38
0.40
0.42
0.44
0.46
0.48
0.50
0
5
10
15
20
25
30

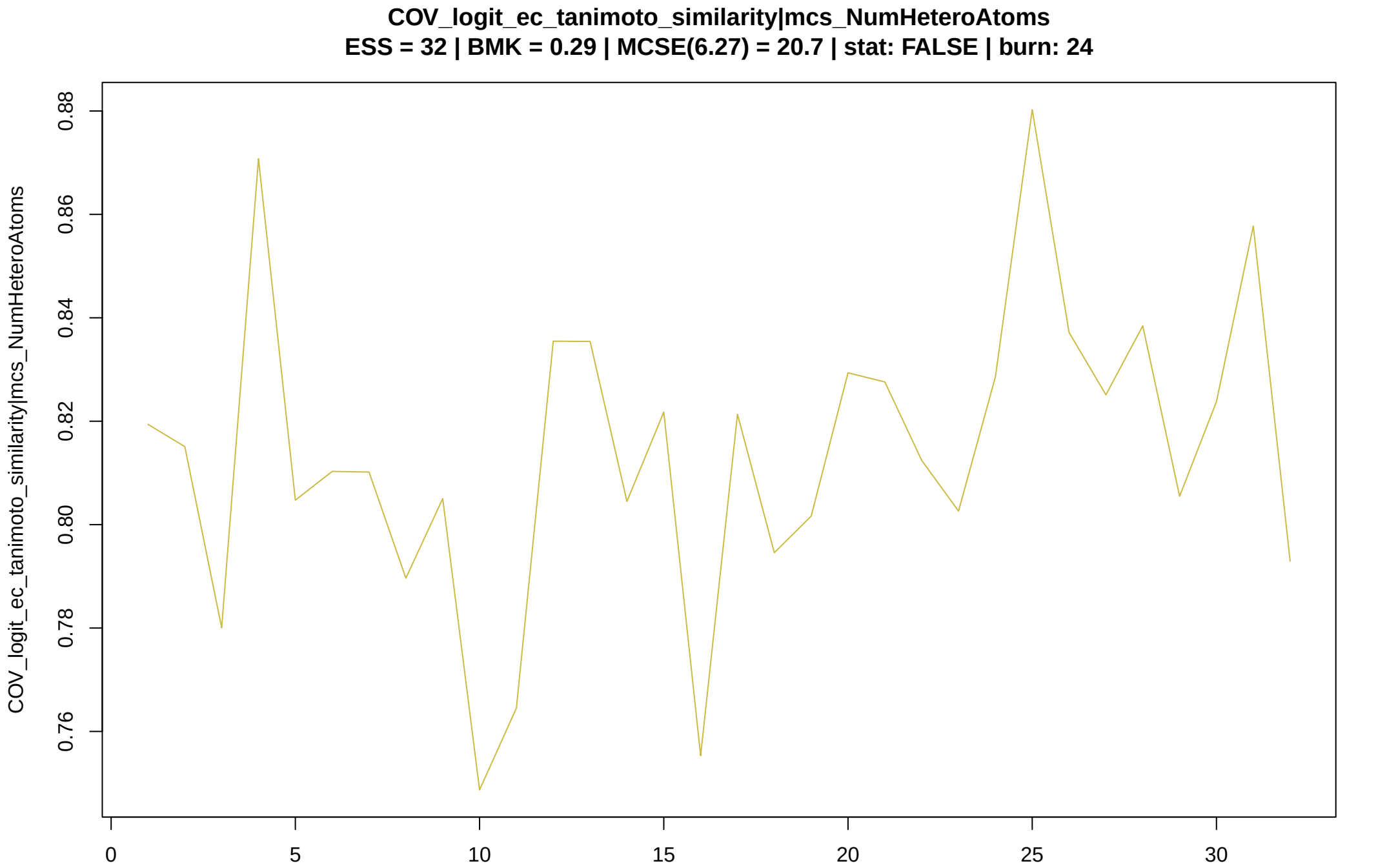

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 32 | BMK = 0.288 | MCSE(6.27) = 20.1 | stat: FALSE | burn: 30
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0.27
0.28
0.29
0.30
0.31
0.32
0.33
0.34
0
5
10
15
20
25
30

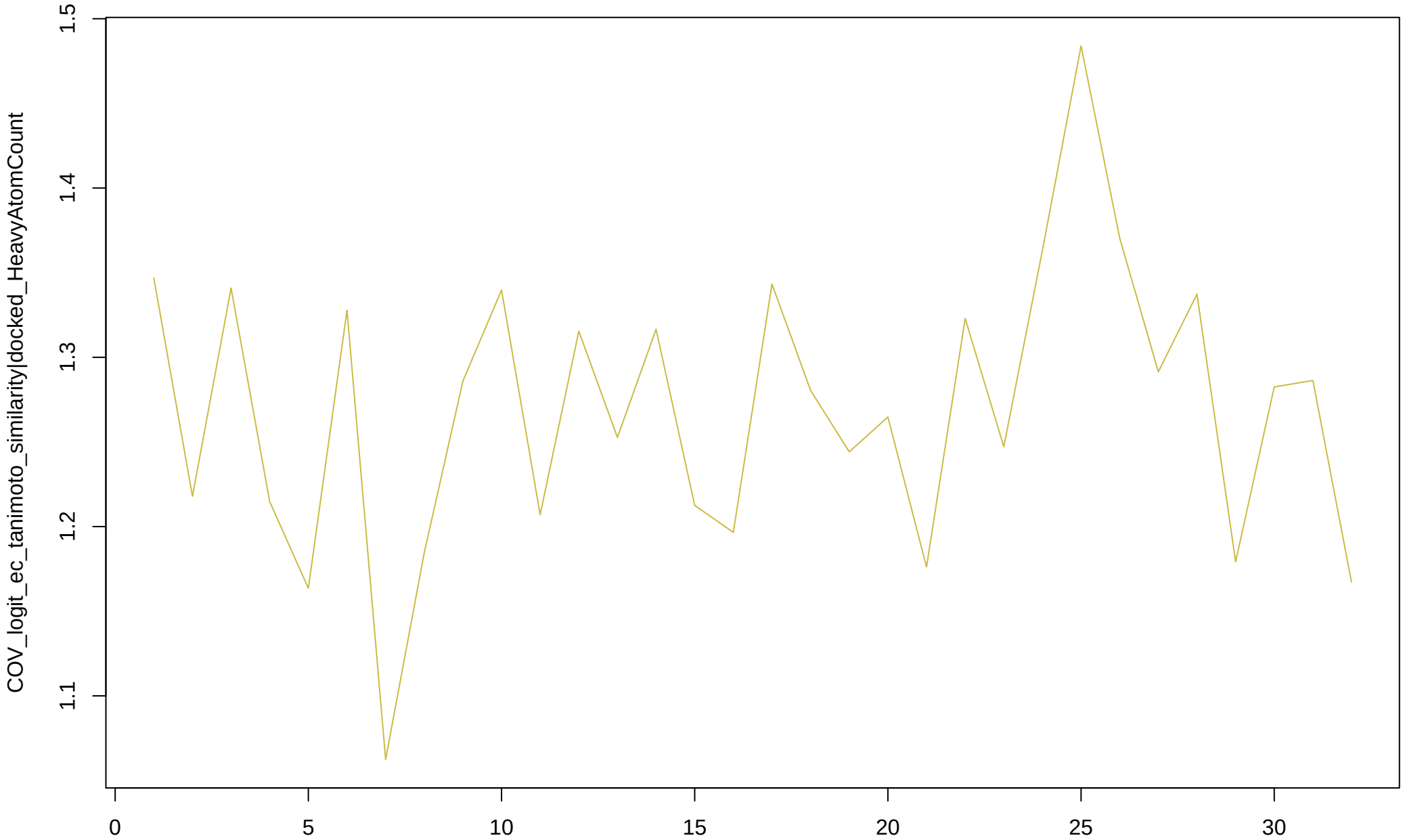

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 32 | BMK = 0.414 | MCSE(6.27) = 14.5 | stat: FALSE | burn: 30
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.85
0.90
0.95
1.00
0
5
10
15
20
25
30

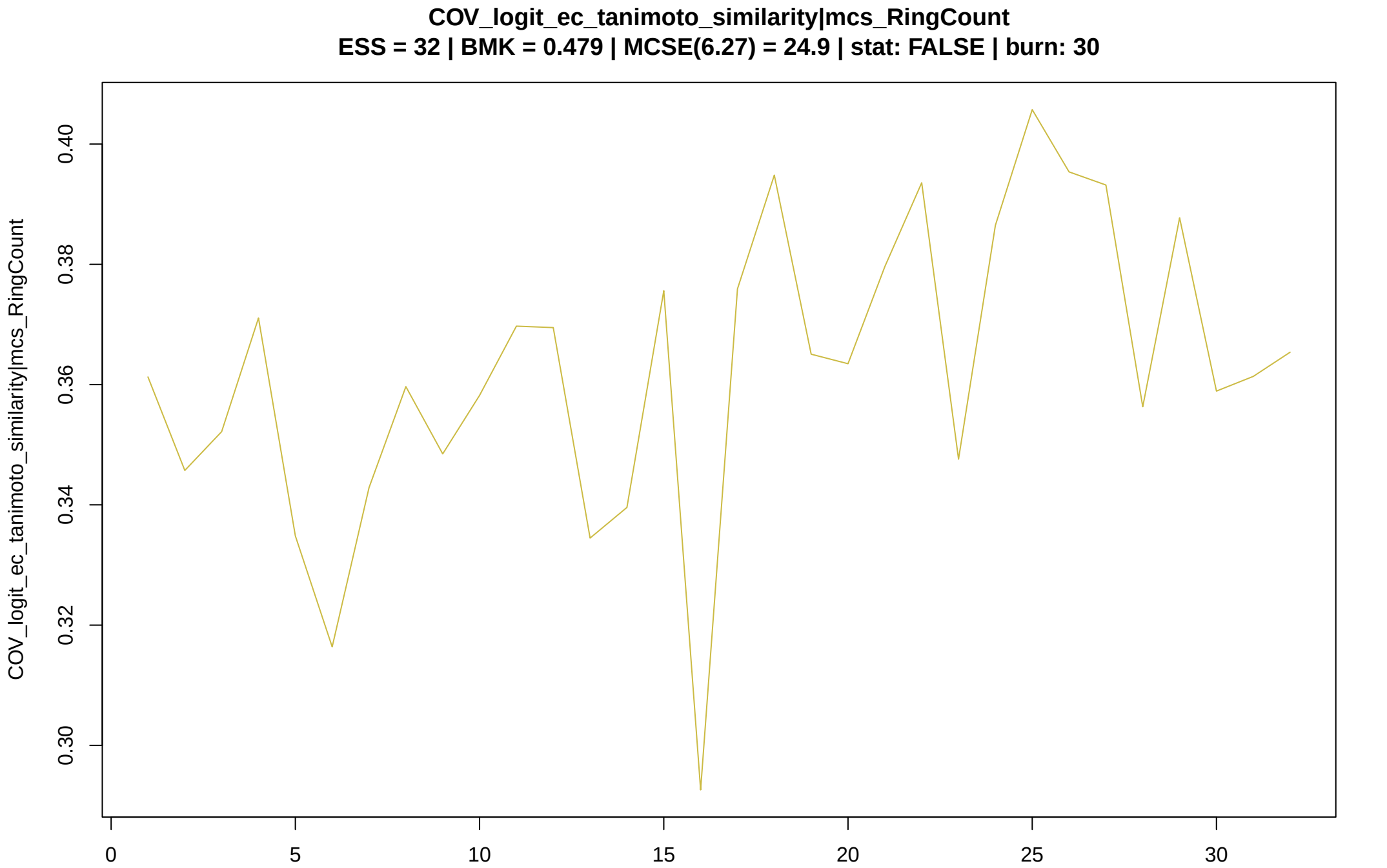

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 26.7 | BMK = 0.134 | MCSE(6.27) = 15.9 | stat: FALSE | burn: 9
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0.9
1.0
1.1
1.2
1.3
0
5
10
15
20
25
30

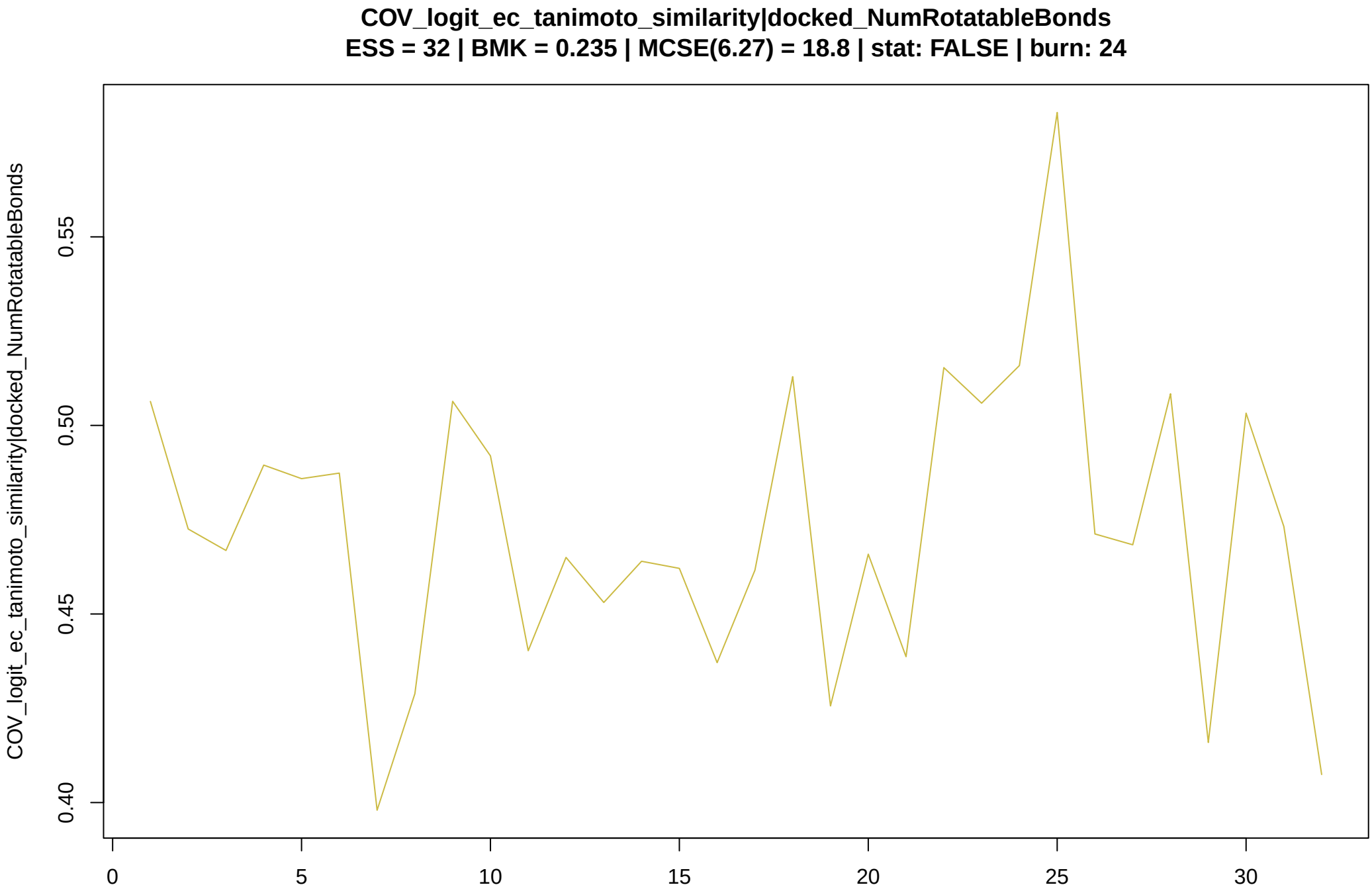

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 32 | BMK = 0.244 | MCSE(6.27) = 19 | stat: FALSE | burn: 30
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
0.06
0.07
0.08
0.09
0.10
0.11
0
5
10
15
20
25
30

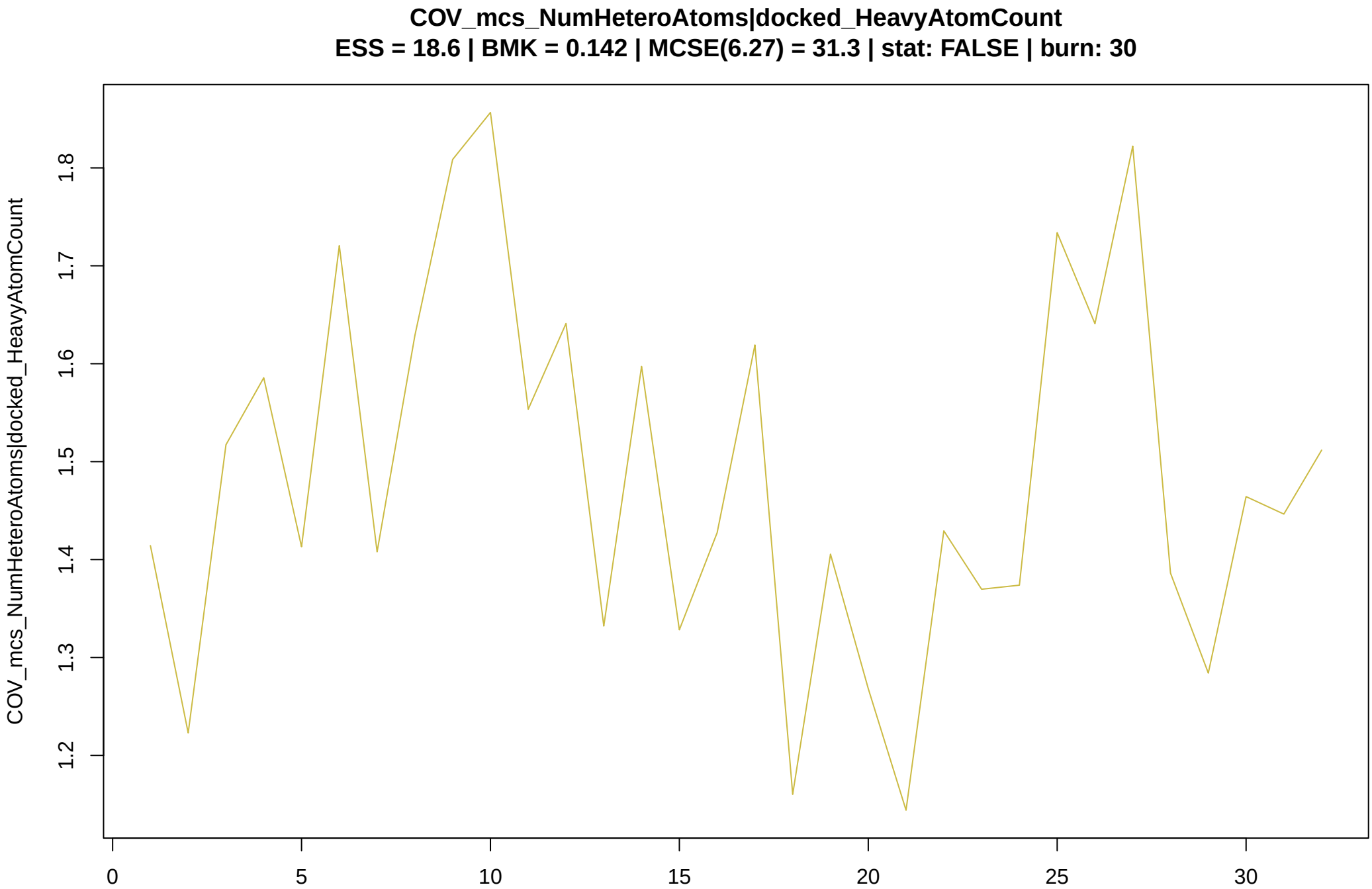

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 32 | BMK = 0.128 | MCSE(6.27) = 16 | stat: FALSE | burn: 6
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
0.30
0.35
0.40
0.45
0
5
10
15
20
25
30

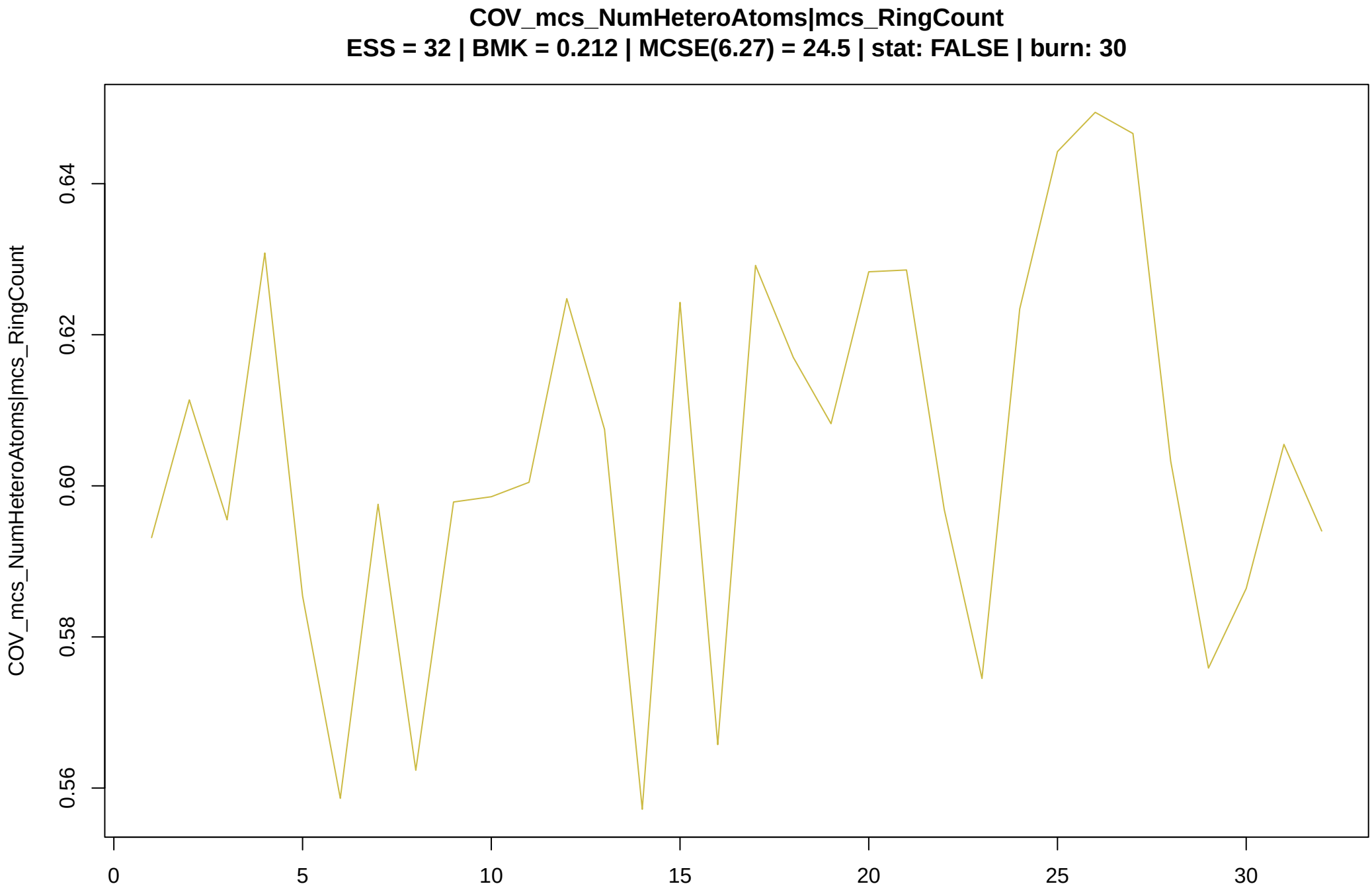

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 32 | BMK = 0.29 | MCSE(6.27) = 20.7 | stat: FALSE | burn: 24
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.76
0.78
0.80
0.82
0.84
0.86
0.88
0
5
10
15
20
25
30

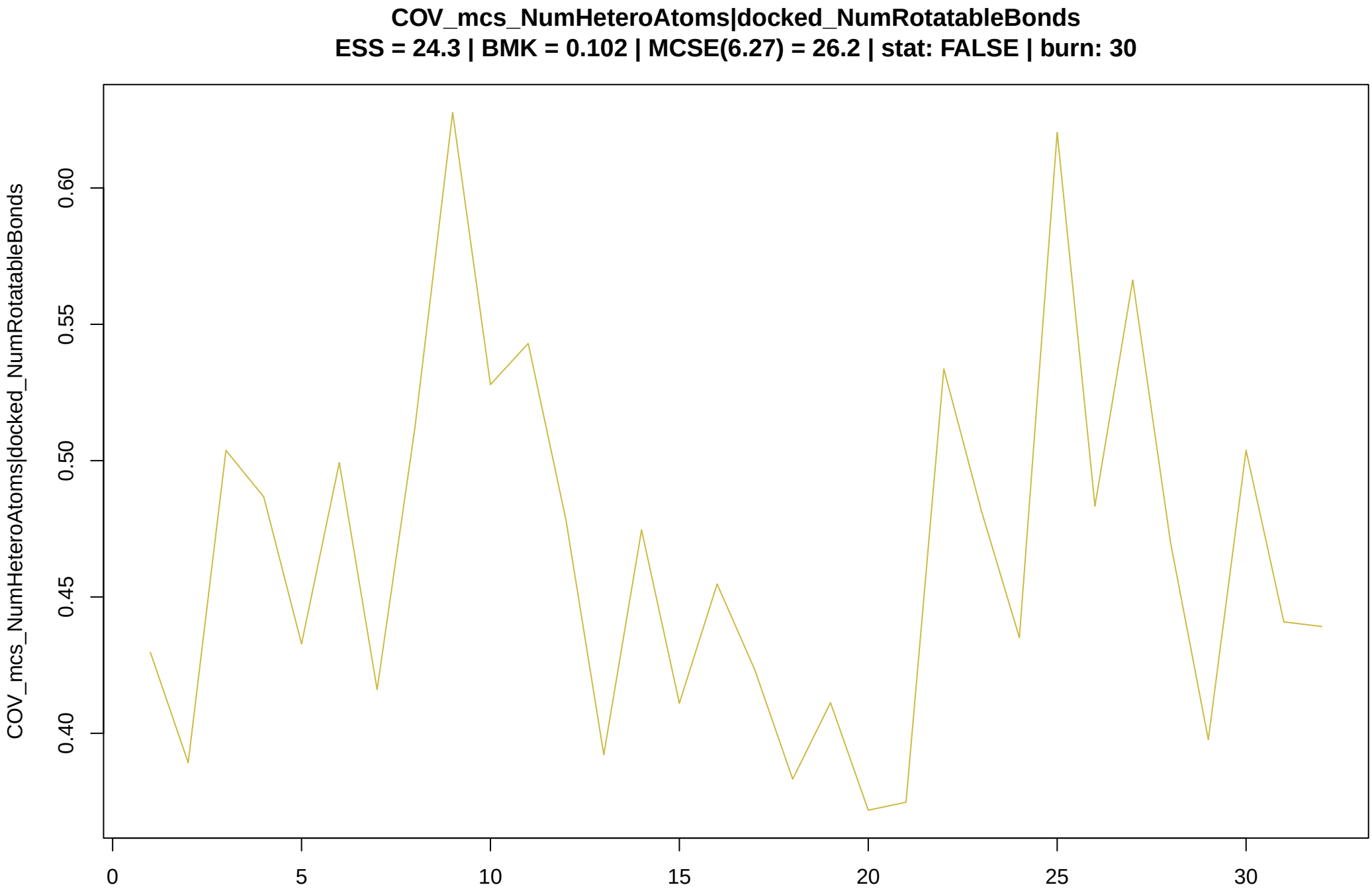

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 32 | BMK = 0.179 | MCSE(6.27) = 20.6 | stat: FALSE | burn: 30
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
1.1
1.2
1.3
1.4
1.5
0
5
10
15
20
25
30

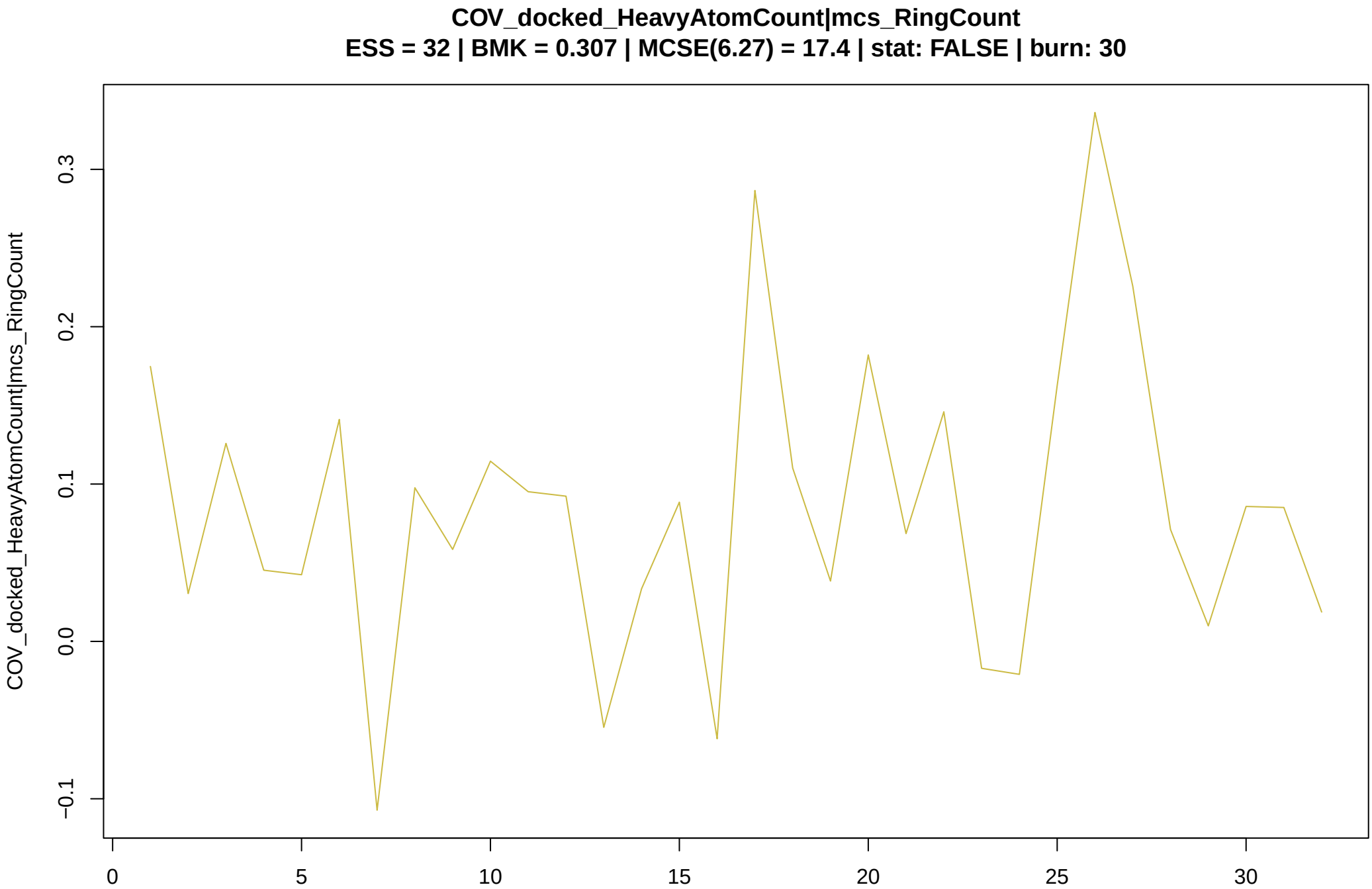

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 32 | BMK = 0.479 | MCSE(6.27) = 24.9 | stat: FALSE | burn: 30
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.30
0.32
0.34
0.36
0.38
0.40
0
5
10
15
20
25
30

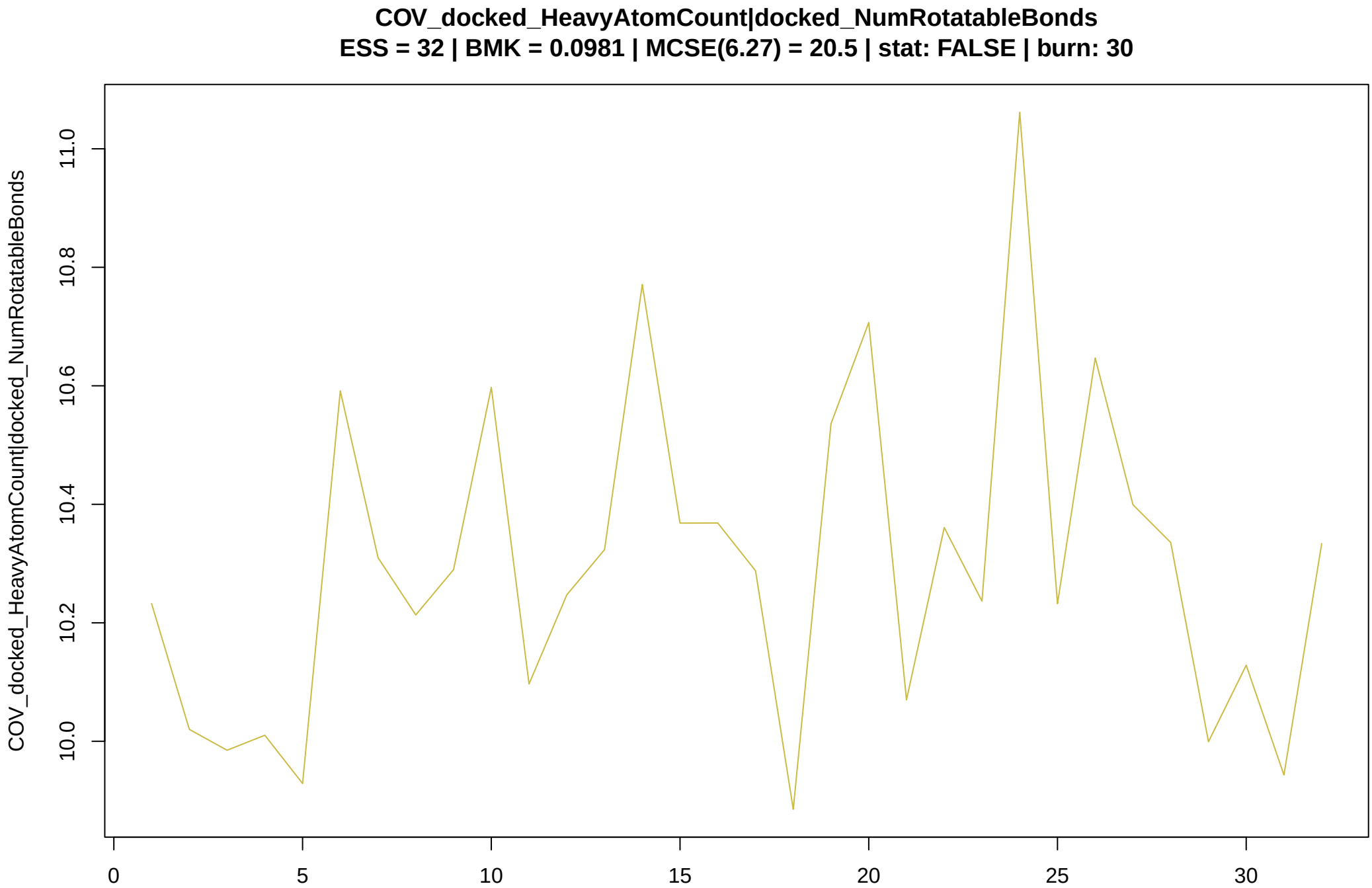

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 32 | BMK = 0.235 | MCSE(6.27) = 18.8 | stat: FALSE | burn: 24
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
0.40
0.45
0.50
0.55
0
5
10
15
20
25
30

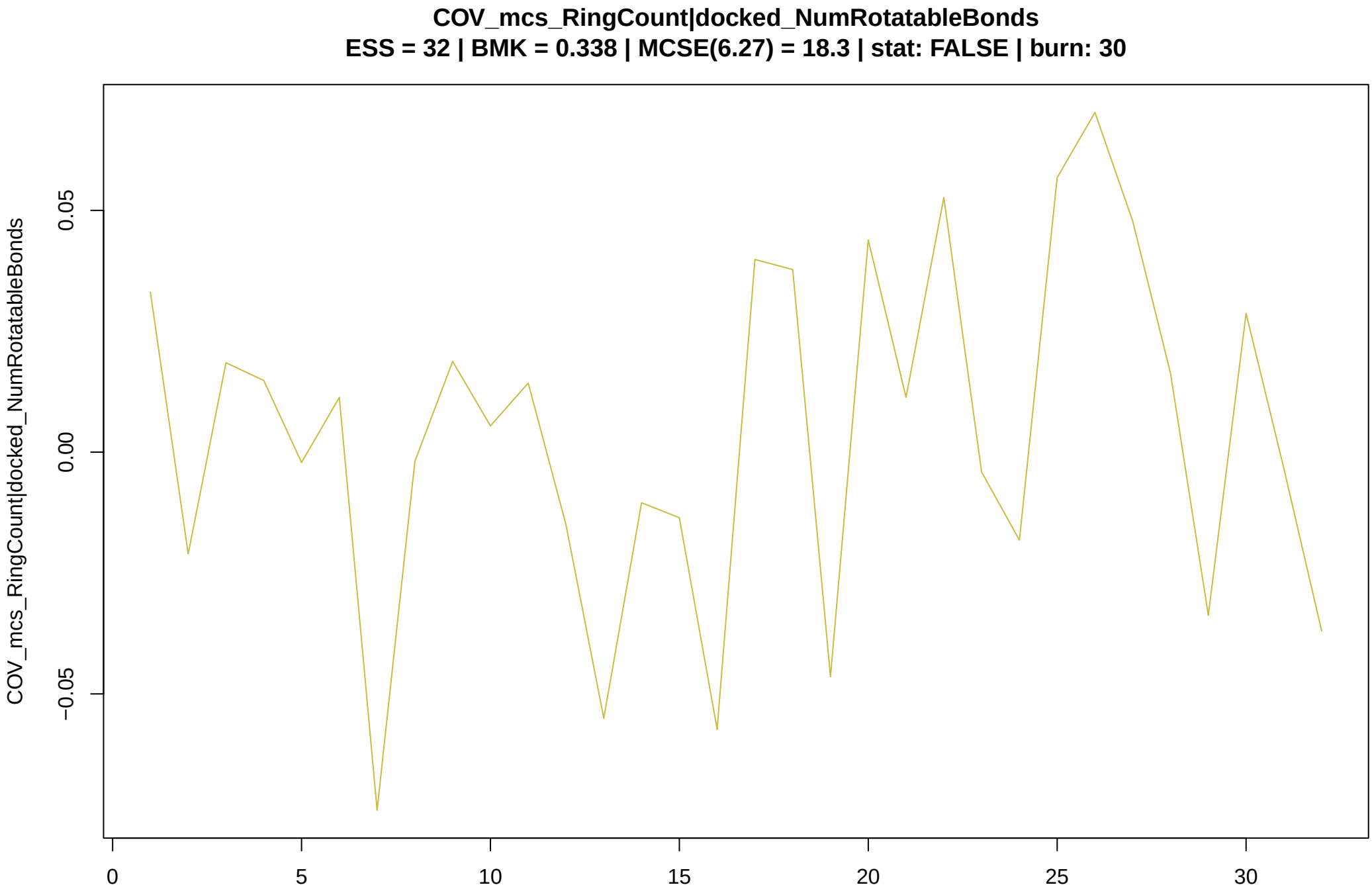

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 18.6 | BMK = 0.142 | MCSE(6.27) = 31.3 | stat: FALSE | burn: 30
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
1.2
1.3
1.4
1.5
1.6
1.7
1.8
0
5
10
15
20
25
30


COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 32 | BMK = 0.212 | MCSE(6.27) = 24.5 | stat: FALSE | burn: 30
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.56
0.58
0.60
0.62
0.64
0
5
10
15
20
25
30


COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 24.3 | BMK = 0.102 | MCSE(6.27) = 26.2 | stat: FALSE | burn: 30
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
0.40
0.45
0.50
0.55
0.60
0
5
10
15
20
25
30


COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 32 | BMK = 0.307 | MCSE(6.27) = 17.4 | stat: FALSE | burn: 30
COV_docked_HeavyAtomCount|mcs_RingCount
−0.1
0.0
0.1
0.2
0.3
0
5
10
15
20
25
30


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 32 | BMK = 0.0981 | MCSE(6.27) = 20.5 | stat: FALSE | burn: 30
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10.0
10.2
10.4
10.6
10.8
11.0
0
5
10
15
20
25
30


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 32 | BMK = 0.338 | MCSE(6.27) = 18.3 | stat: FALSE | burn: 30
COV_mcs_RingCount|docked_NumRotatableBonds
0.05
0.00
−0.05
0
5
10
15
20
25
30