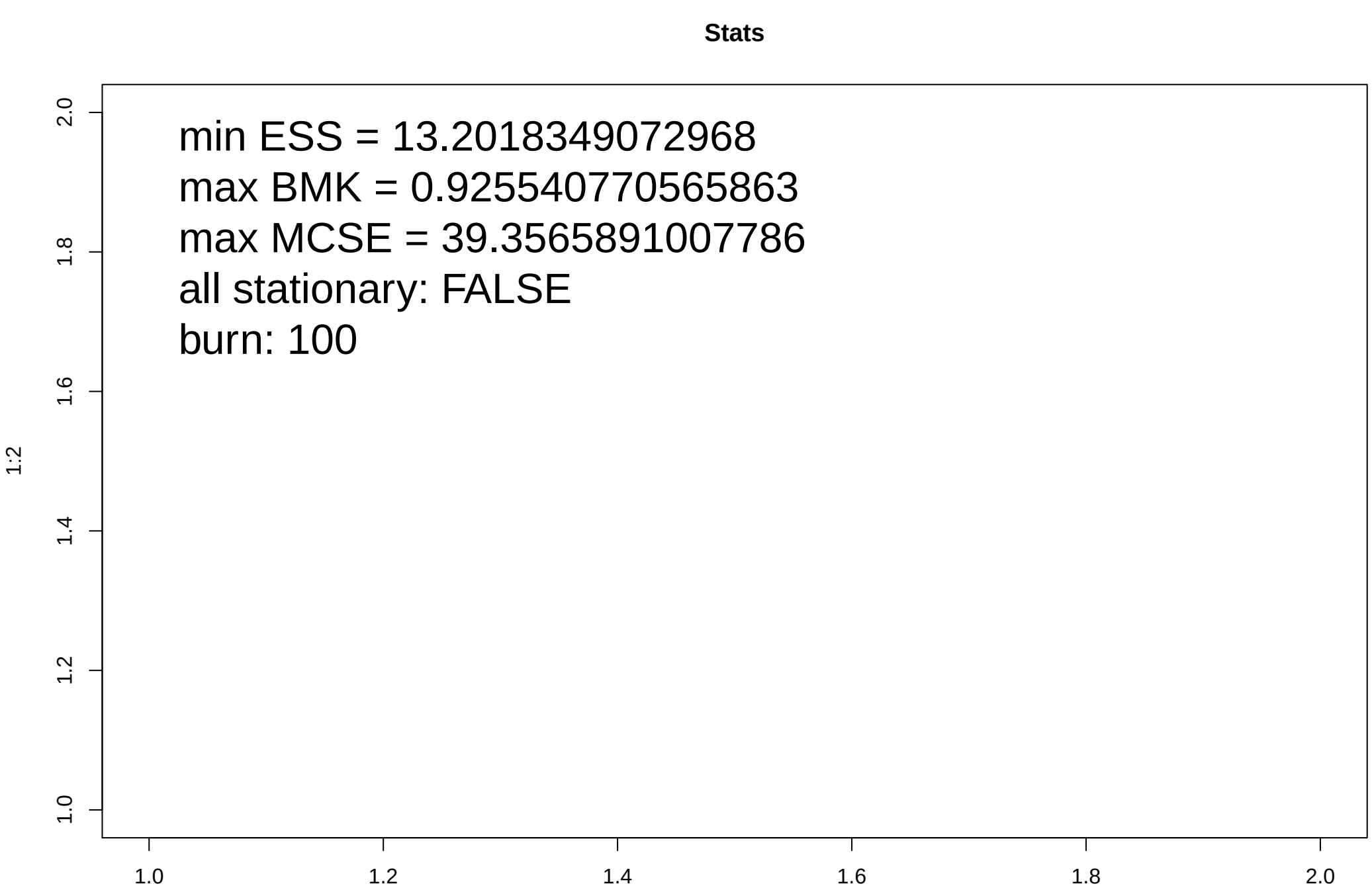
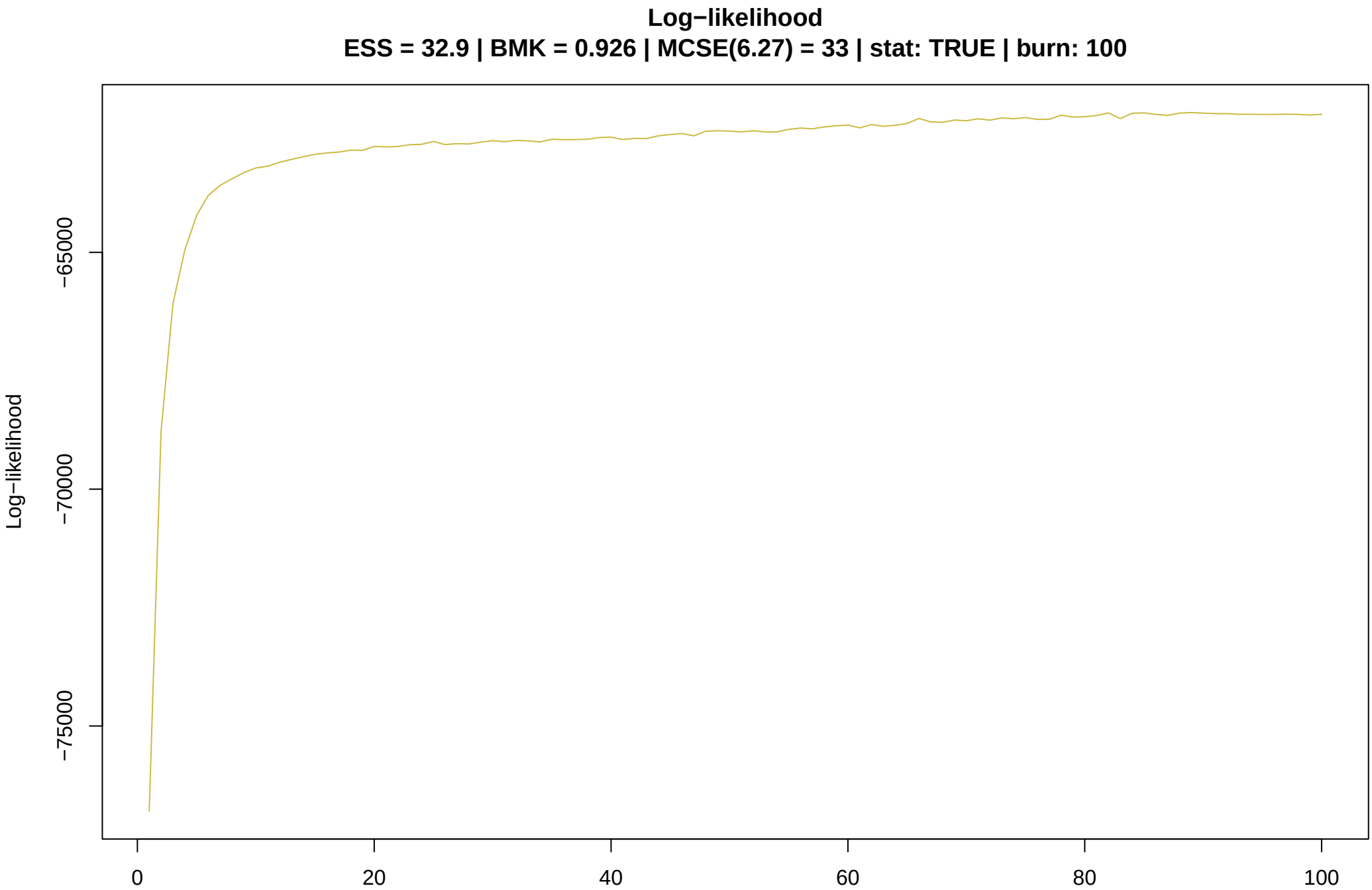
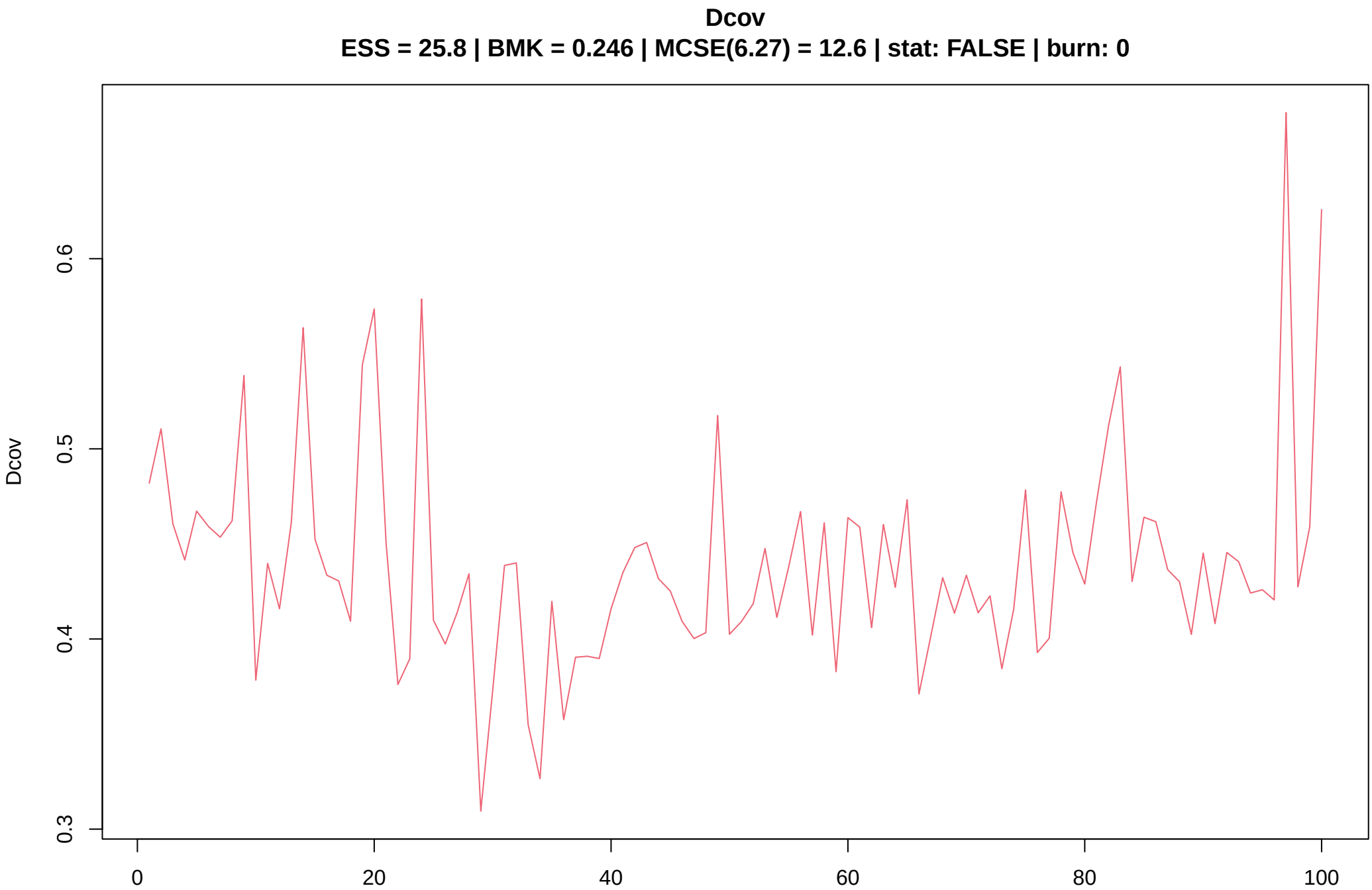
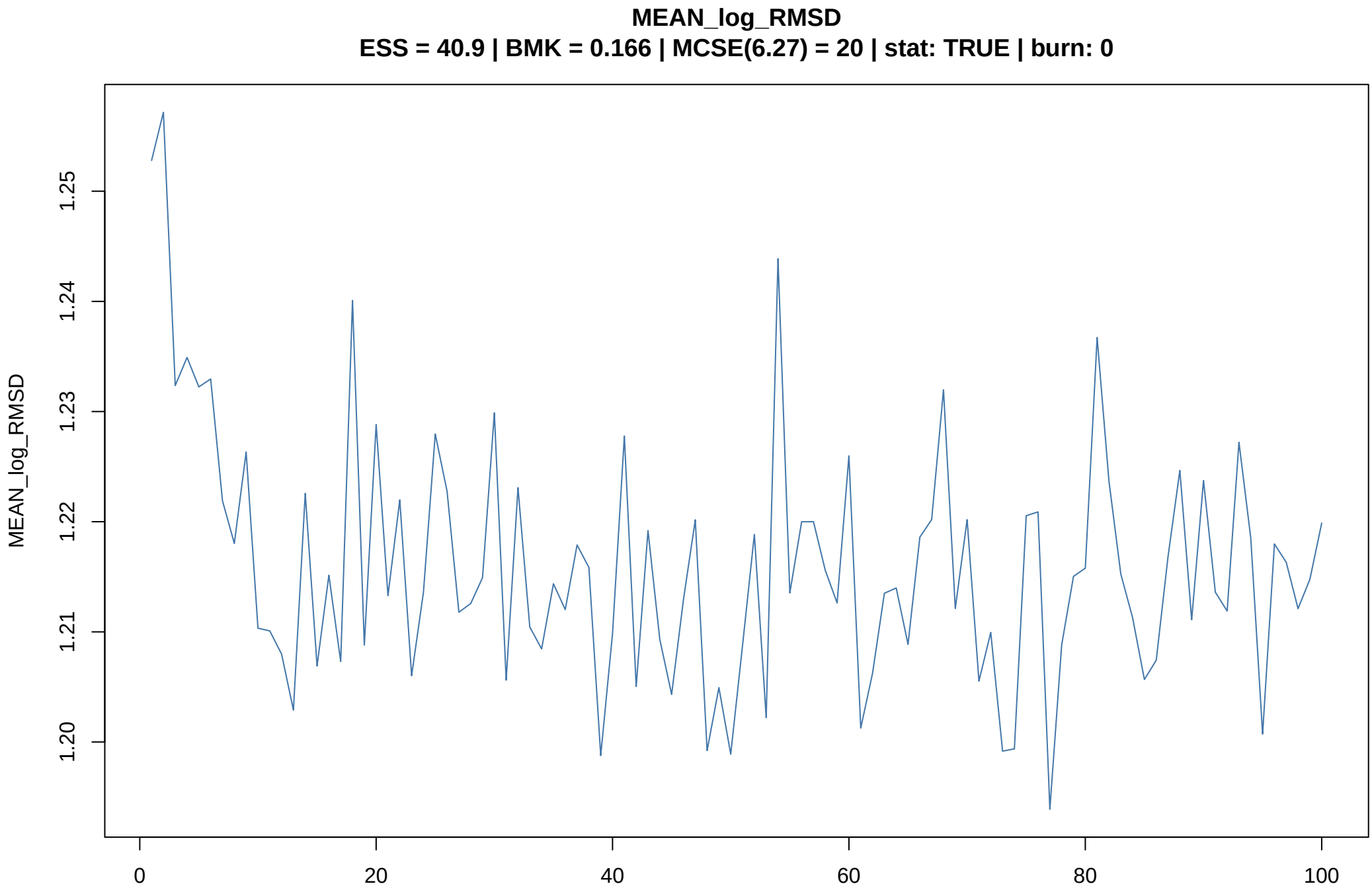
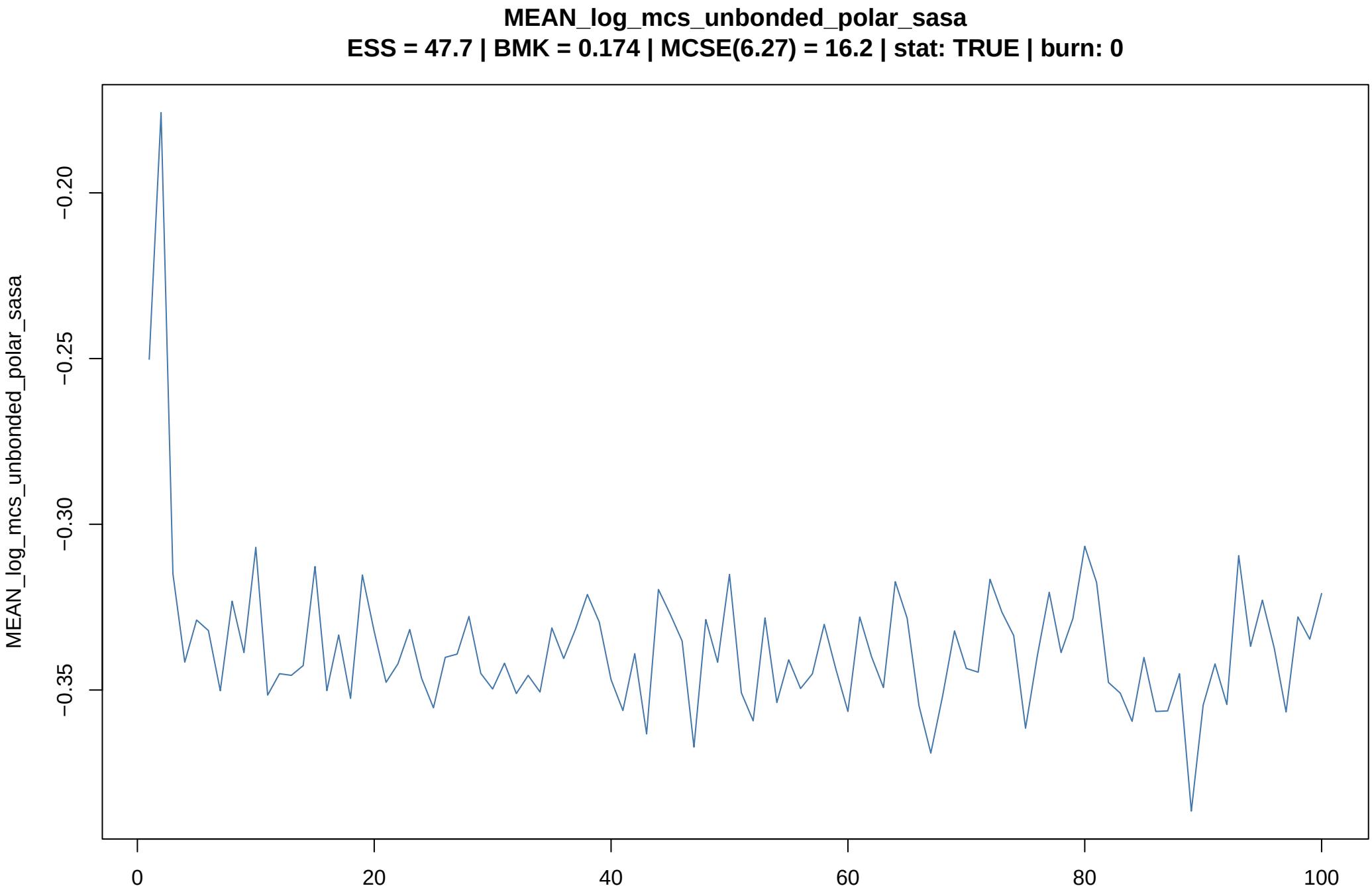
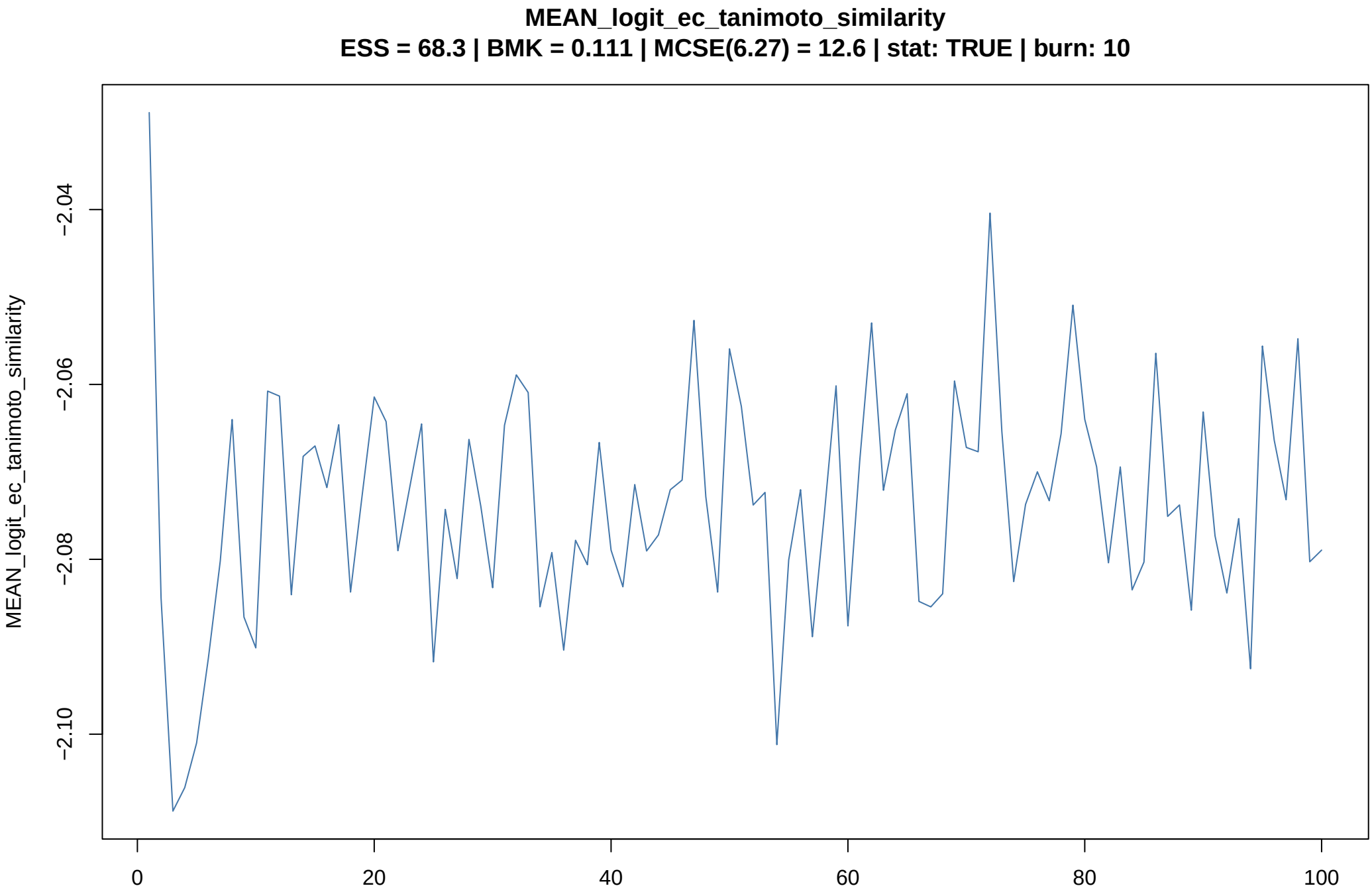

Stats
min ESS = 13.2018349072968
max BMK = 0.925540770565863
max MCSE = 39.3565891007786
all stationary: FALSE
burn: 100
1:2
1.0
1.2
1.4
1.6
1.8
2.0

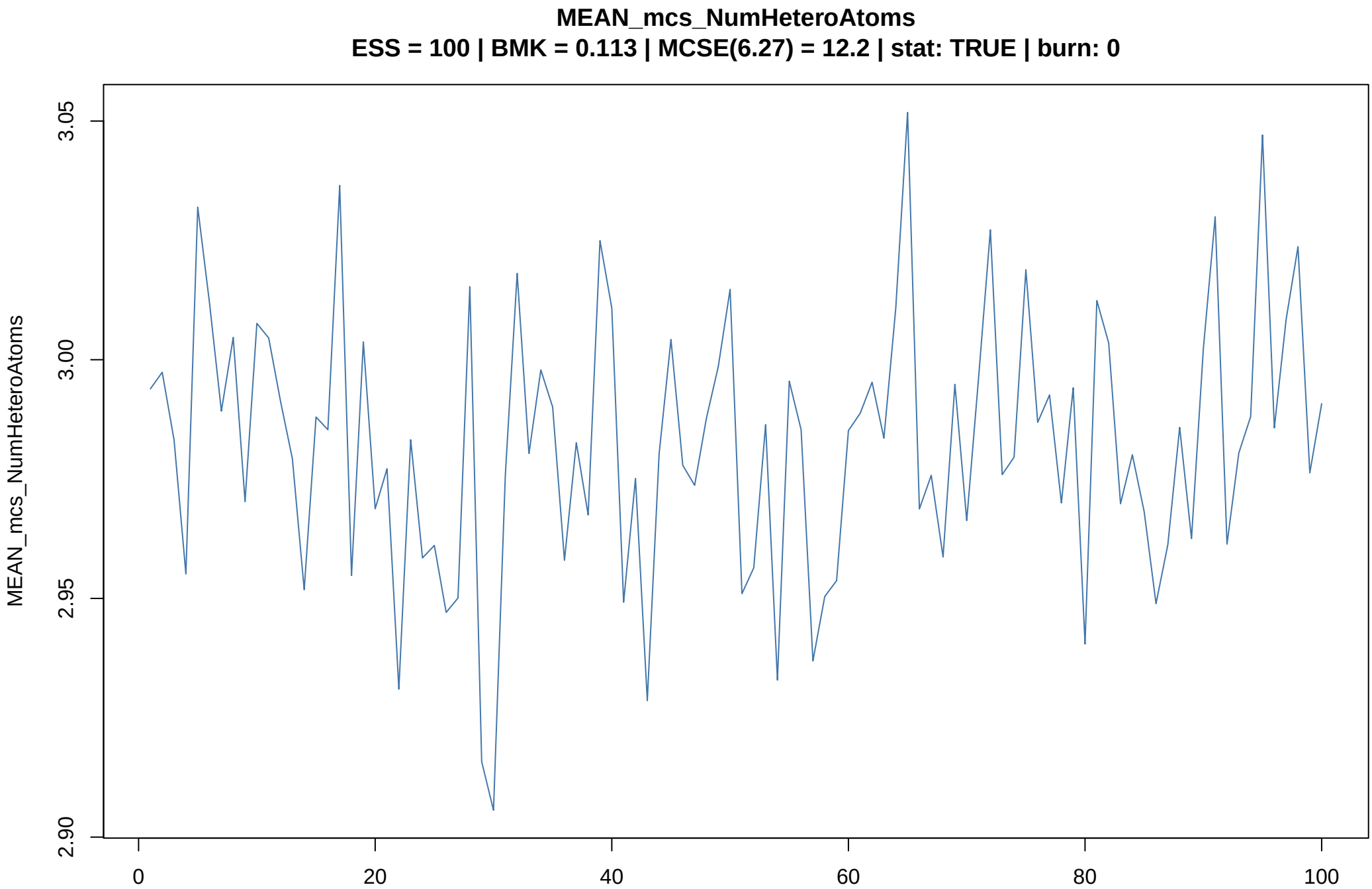

Log−likelihood
ESS = 32.9 | BMK = 0.926 | MCSE(6.27) = 33 | stat: TRUE | burn: 100
Log−likelihood
−65000
−70000
−75000
0
20
40
60
80
100

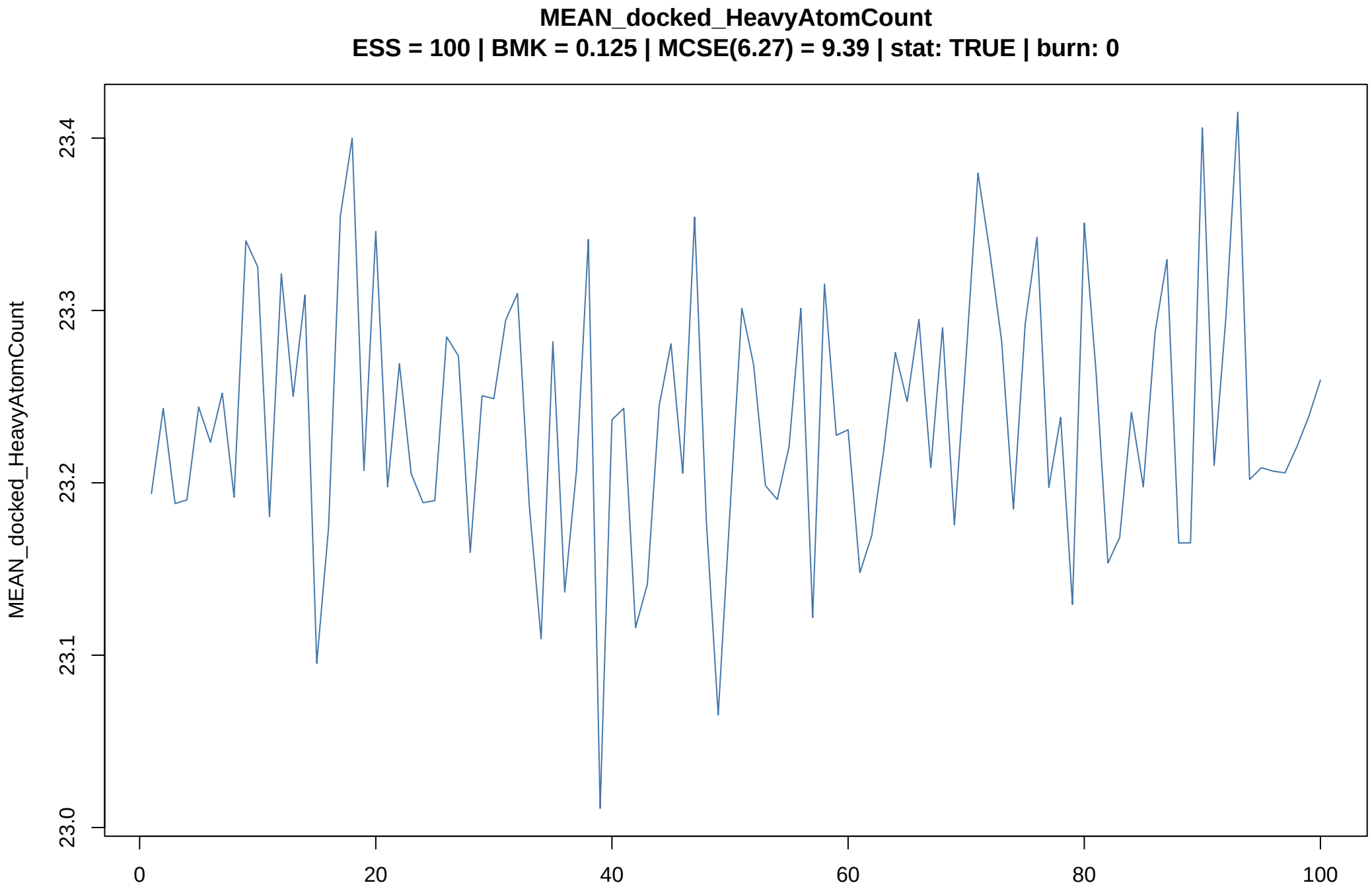

Dcov
ESS = 25.8 | BMK = 0.246 | MCSE(6.27) = 12.6 | stat: FALSE | burn: 0
Dcov
0.3
0.4
0.5
0.6
0
20
40
60
80
100

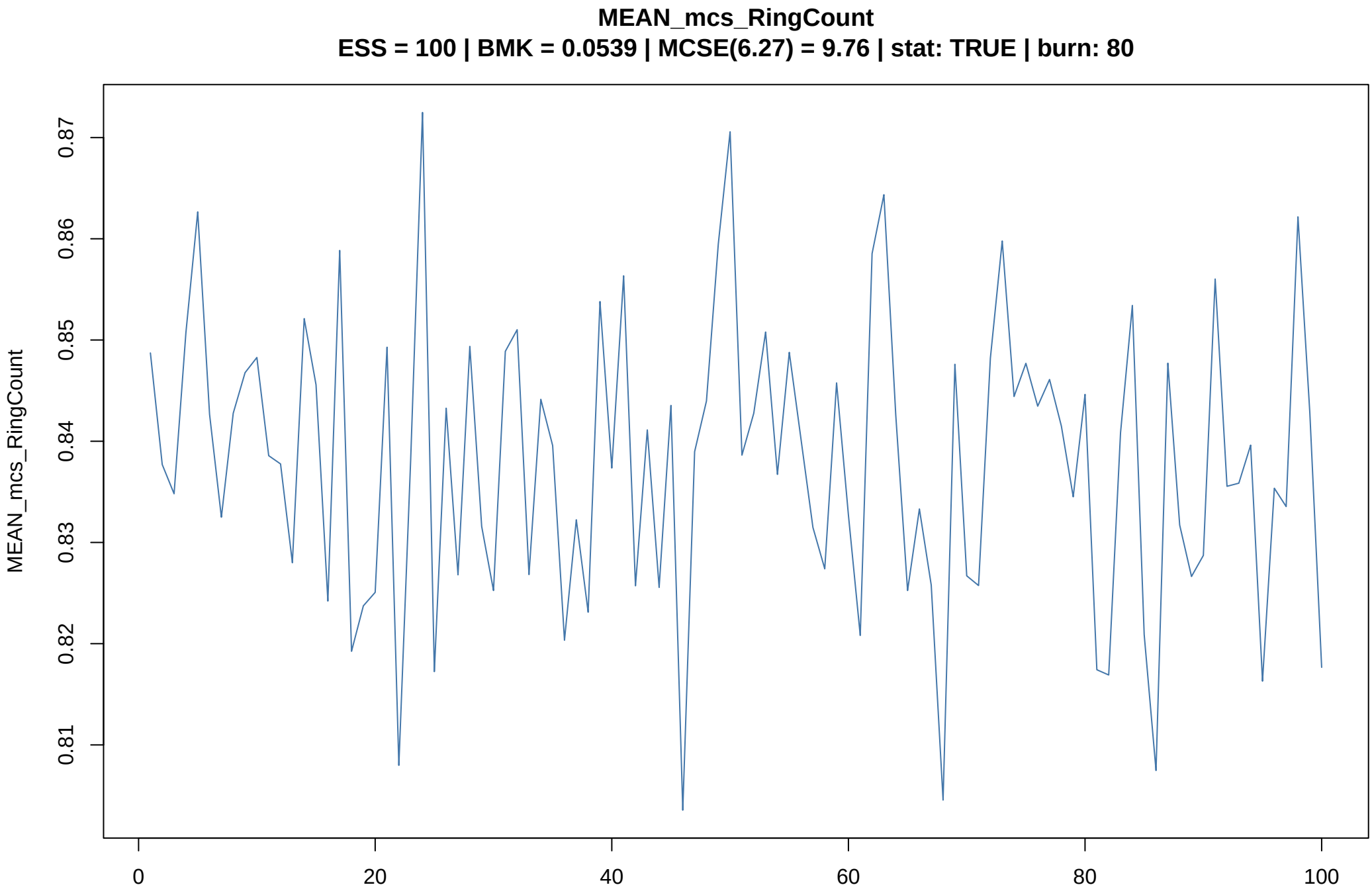

MEAN_log_RMSD
ESS = 40.9 | BMK = 0.166 | MCSE(6.27) = 20 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.20
1.21
1.22
1.23
1.24
1.25
0
20
40
60
80
100

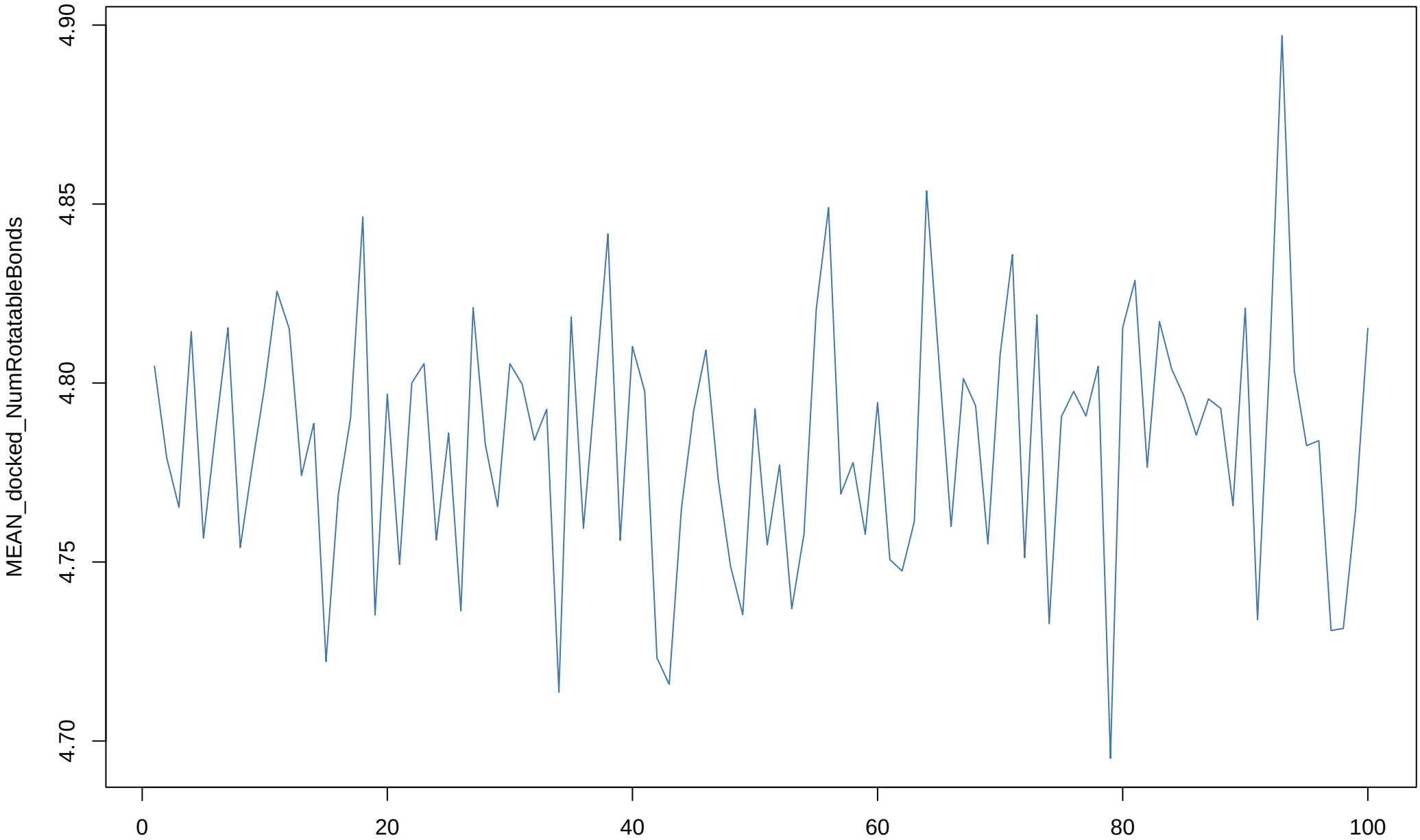

MEAN_log_mcs_unbonded_polar_sasa
ESS = 47.7 | BMK = 0.174 | MCSE(6.27) = 16.2 | stat: TRUE | burn: 0
MEAN_log_mcs_unbonded_polar_sasa
−0.20
−0.25
−0.30
−0.35
0
20
40
60
80
100

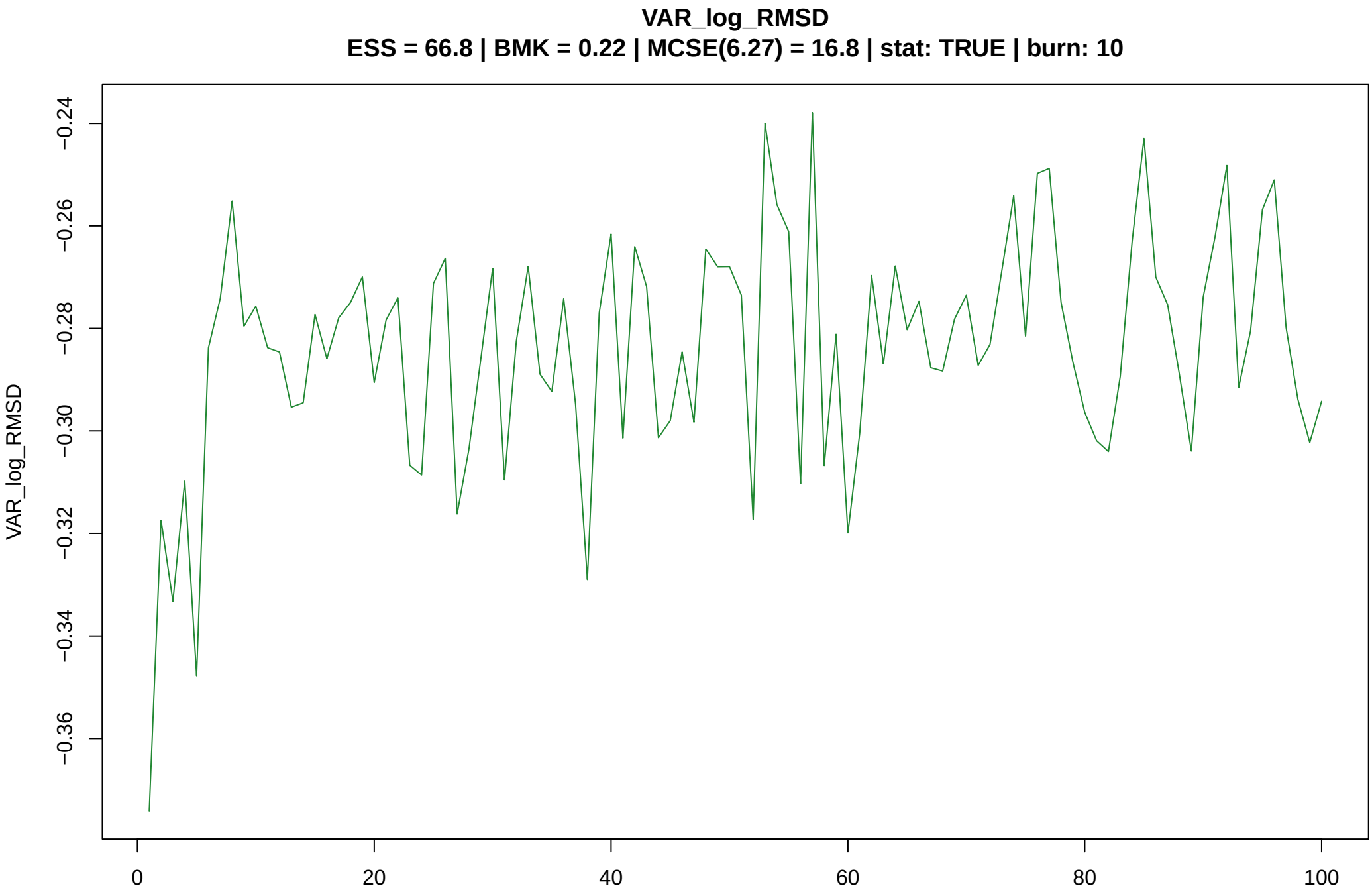

MEAN_logit_ec_tanimoto_similarity
ESS = 68.3 | BMK = 0.111 | MCSE(6.27) = 12.6 | stat: TRUE | burn: 10
MEAN_logit_ec_tanimoto_similarity
−2.04
−2.06
−2.08
−2.10
0
20
40
60
80
100

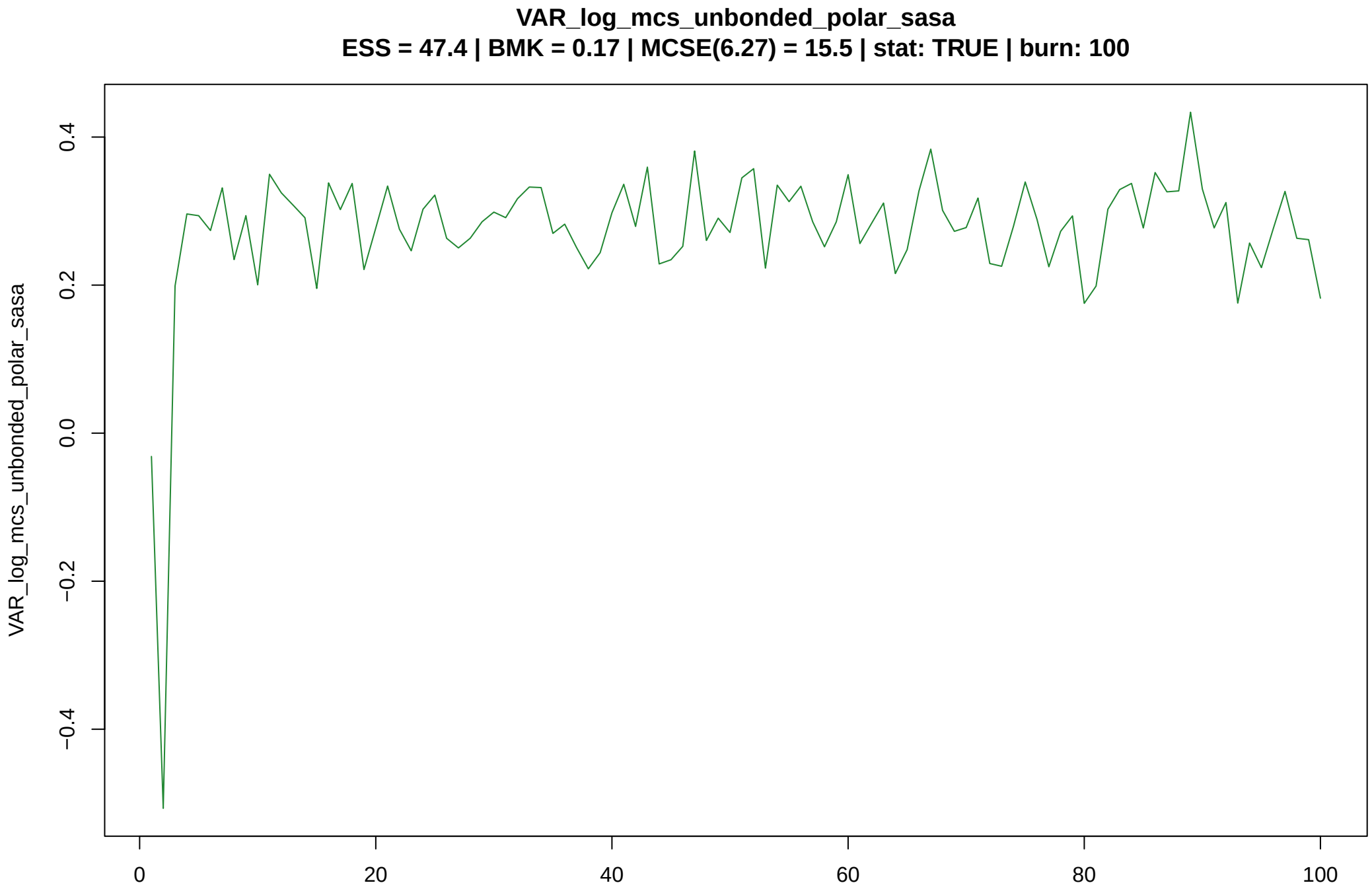

MEAN_mcs_NumHeteroAtoms
ESS = 100 | BMK = 0.113 | MCSE(6.27) = 12.2 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
2.90
2.95
3.00
3.05
0
20
40
60
80
100

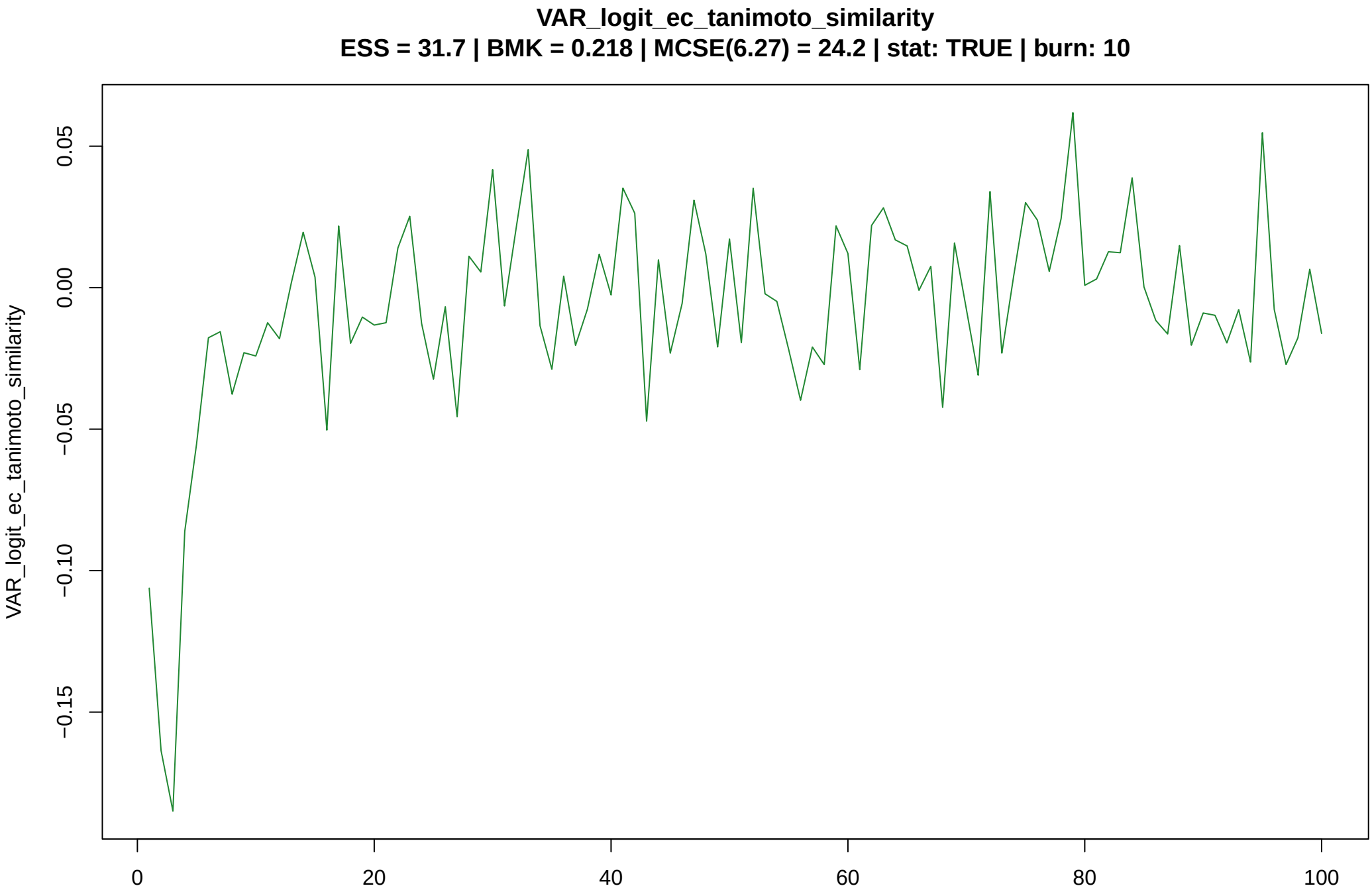

MEAN_docked_HeavyAtomCount
ESS = 100 | BMK = 0.125 | MCSE(6.27) = 9.39 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
23.0
23.1
23.2
23.3
23.4
0
20
40
60
80
100

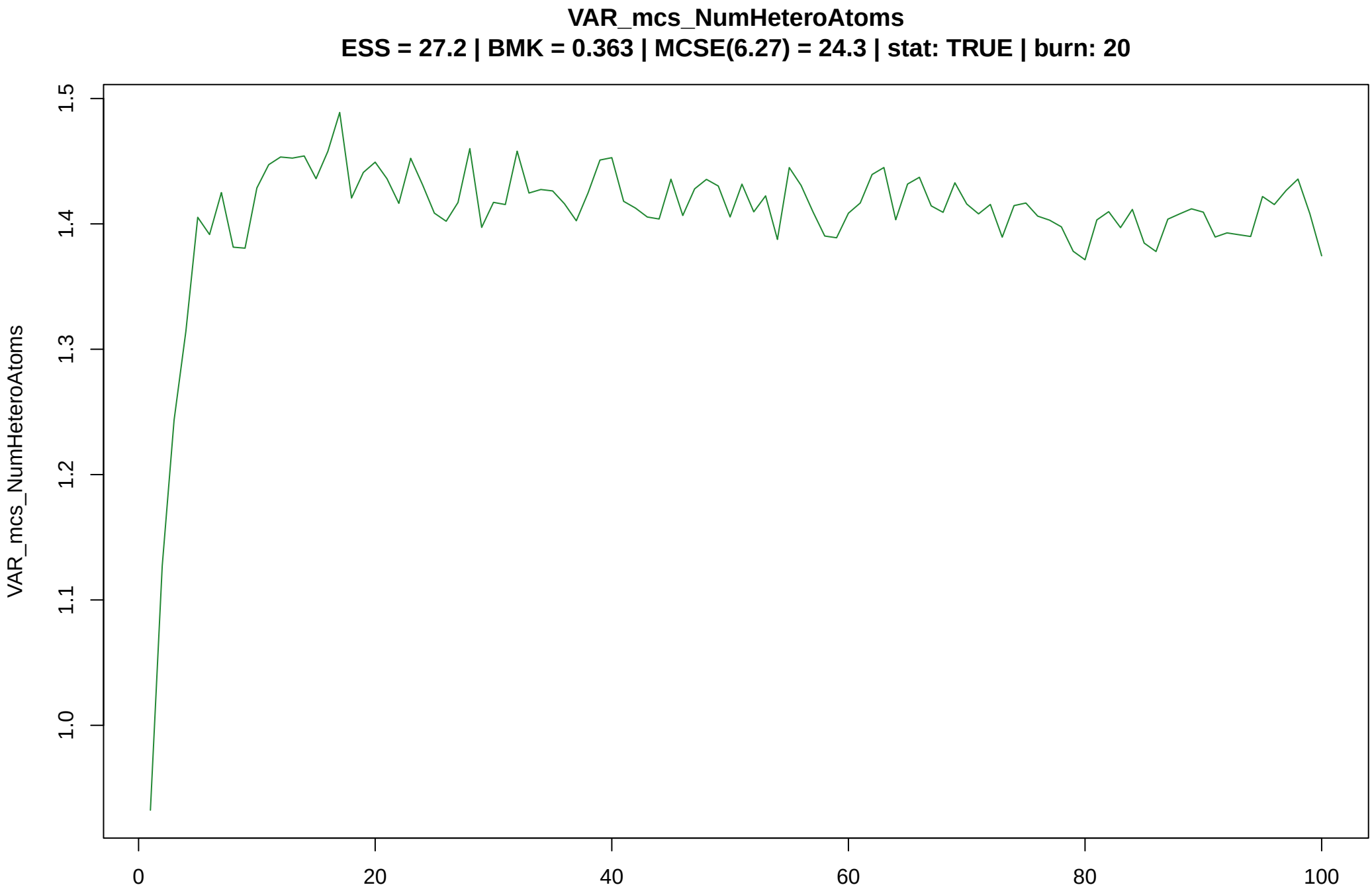

MEAN_mcs_RingCount
ESS = 100 | BMK = 0.0539 | MCSE(6.27) = 9.76 | stat: TRUE | burn: 80
MEAN_mcs_RingCount
0.81
0.82
0.83
0.84
0.85
0.86
0.87
0
20
40
60
80
100

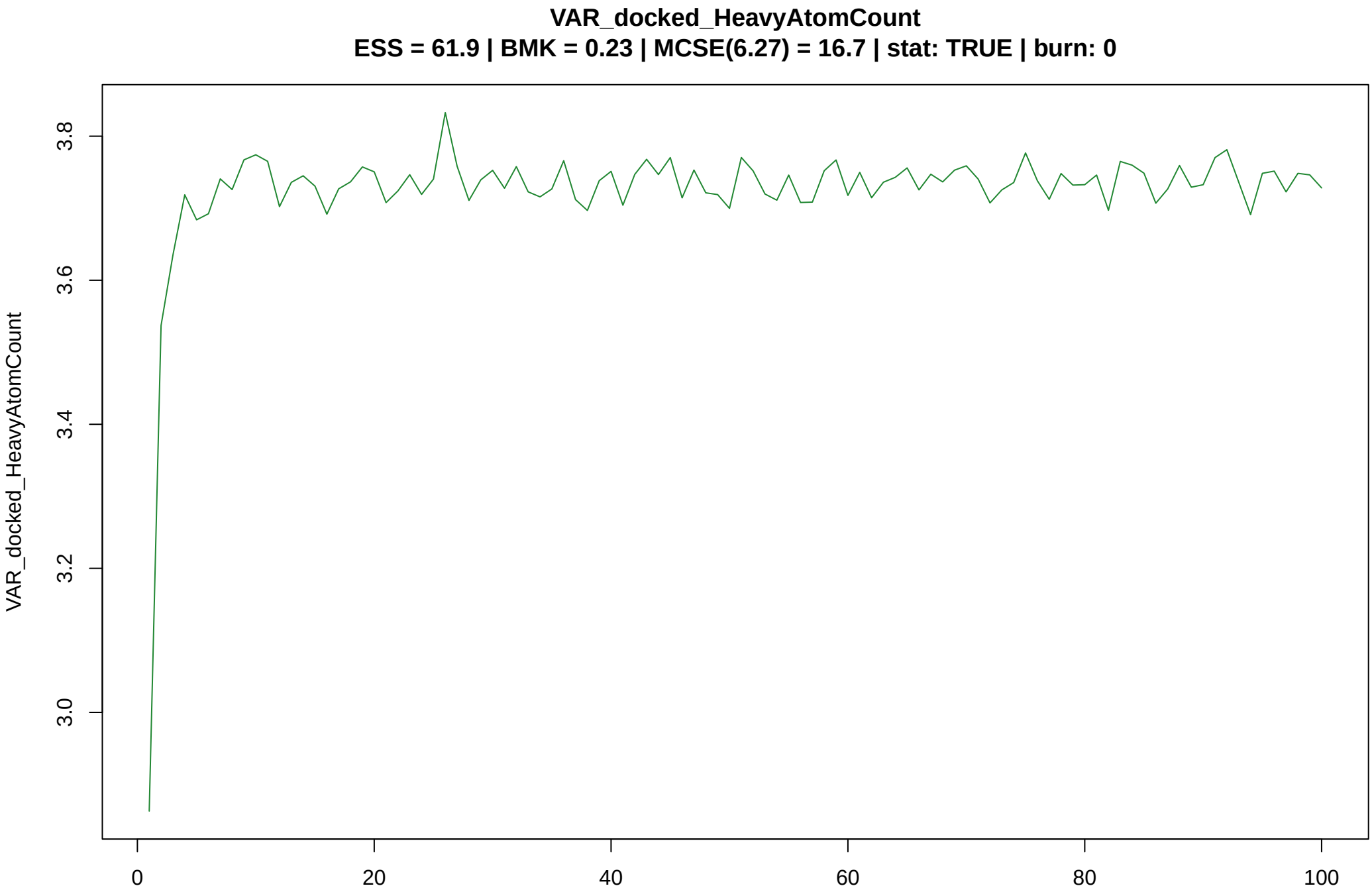

MEAN_docked_NumRotatableBonds
ESS = 100 | BMK = 0.0929 | MCSE(6.27) = 9.41 | stat: TRUE | burn: 0
MEAN_docked_NumRotatableBonds
4.70
4.75
4.80
4.85
4.90
0
20
40
60
80
100

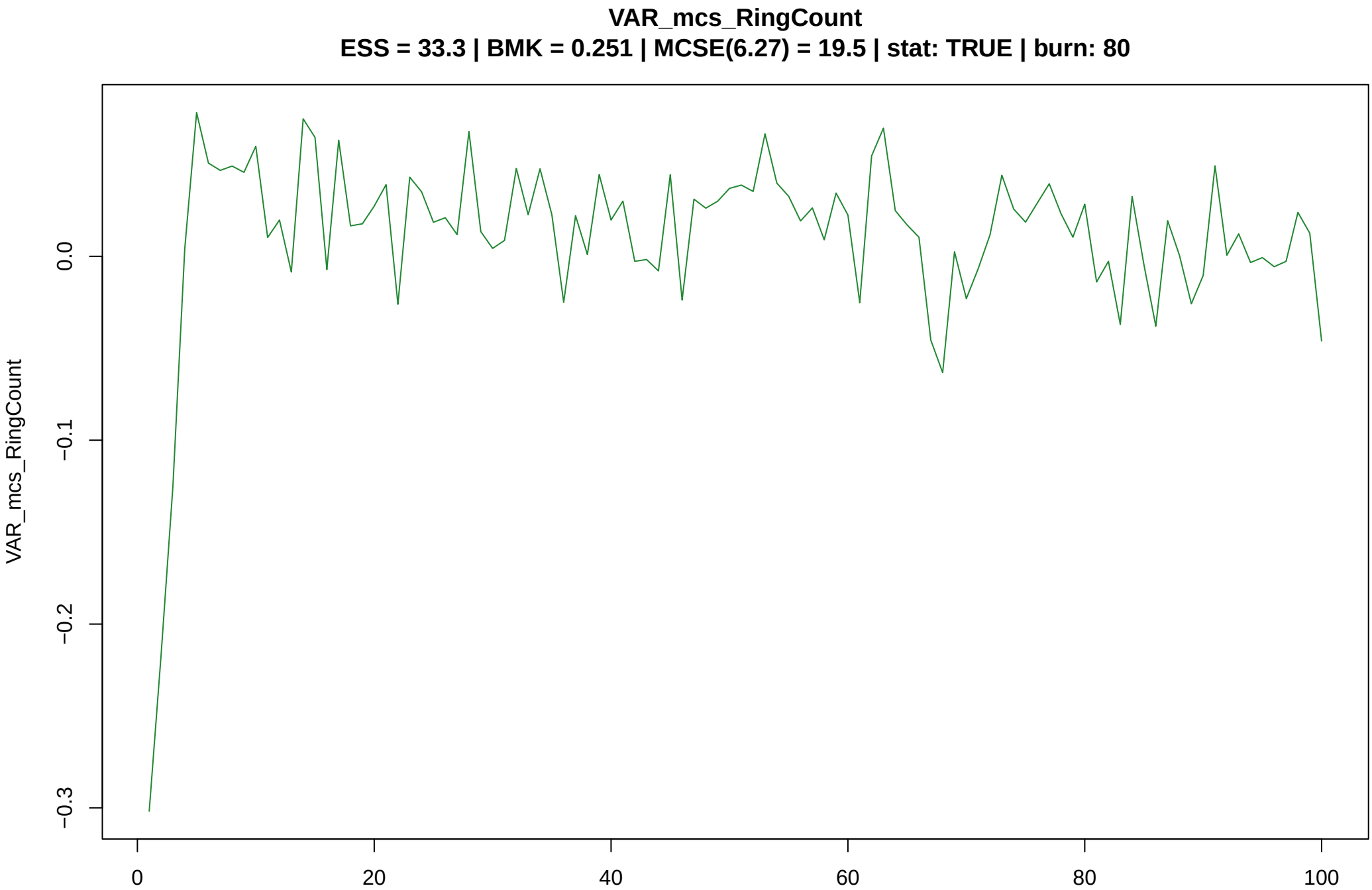

VAR_log_RMSD
ESS = 66.8 | BMK = 0.22 | MCSE(6.27) = 16.8 | stat: TRUE | burn: 10
VAR_log_RMSD
−0.24
−0.26
−0.28
−0.30
−0.32
−0.34
−0.36
0
20
40
60
80
100

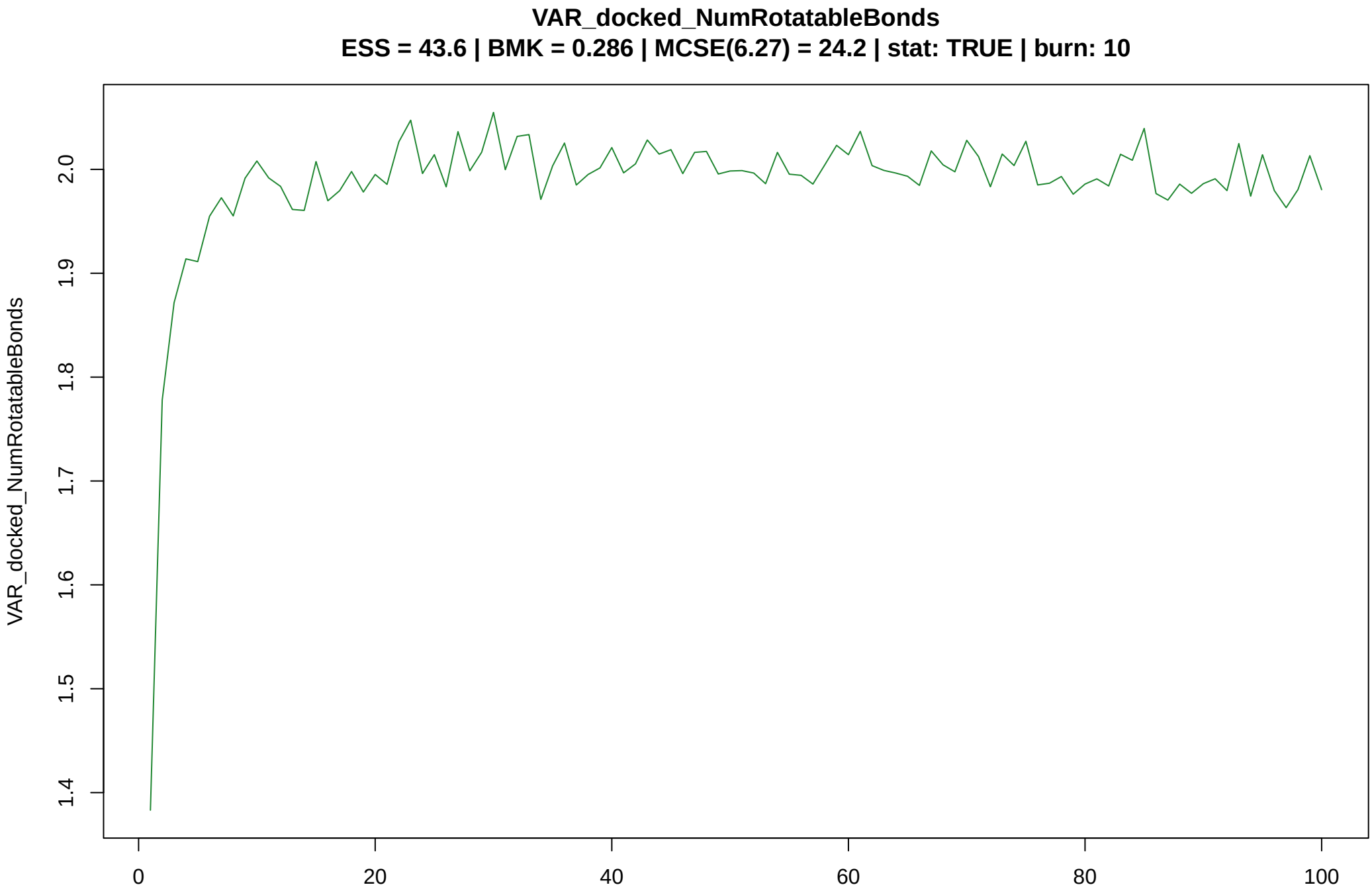

VAR_log_mcs_unbonded_polar_sasa
ESS = 47.4 | BMK = 0.17 | MCSE(6.27) = 15.5 | stat: TRUE | burn: 100
VAR_log_mcs_unbonded_polar_sasa
0.4
0.2
0.0
−0.2
−0.4
0
20
40
60
80
100

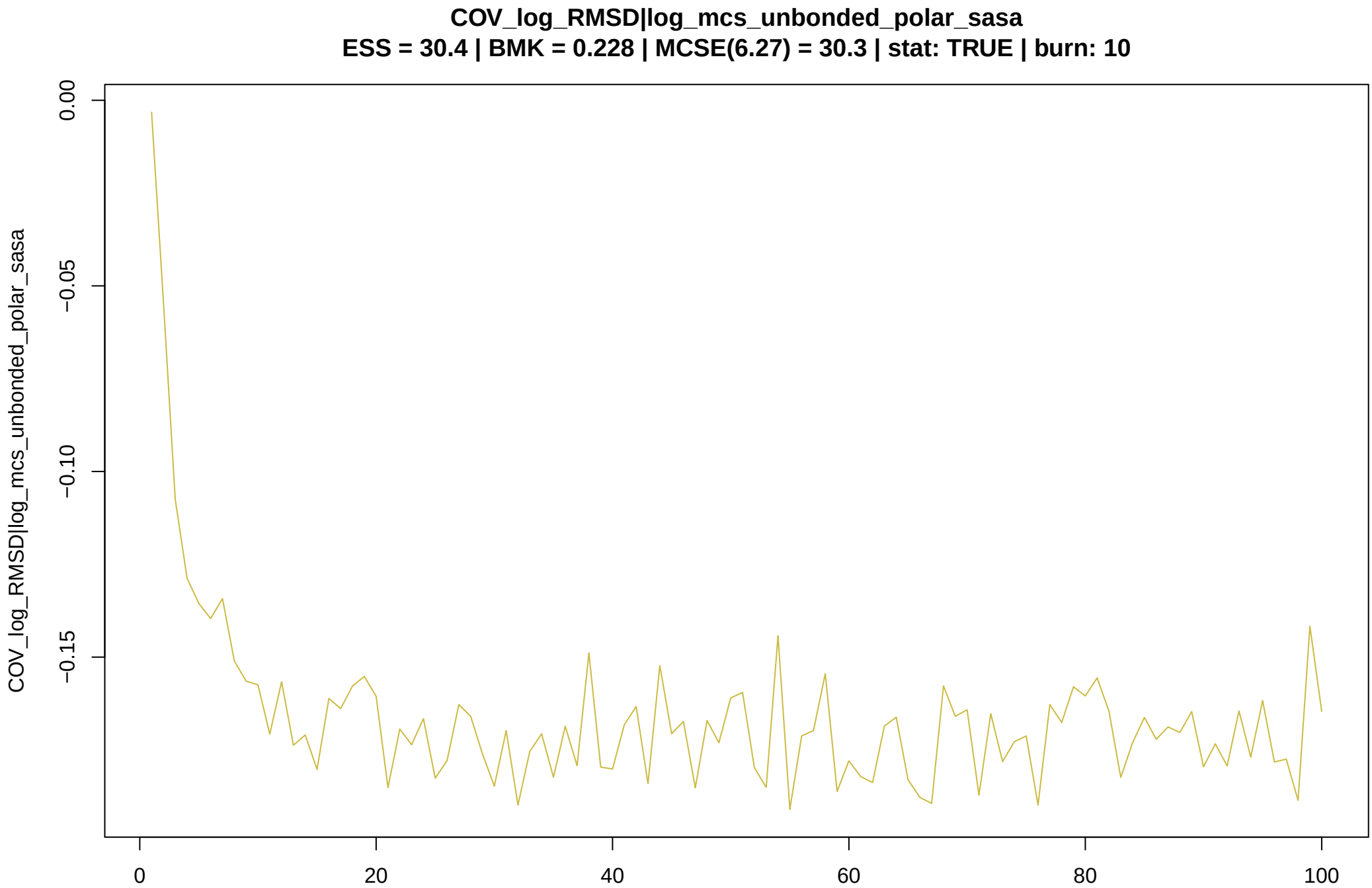

VAR_logit_ec_tanimoto_similarity
ESS = 31.7 | BMK = 0.218 | MCSE(6.27) = 24.2 | stat: TRUE | burn: 10
VAR_logit_ec_tanimoto_similarity
0.05
0.00
−0.05
−0.10
−0.15
0
20
40
60
80
100

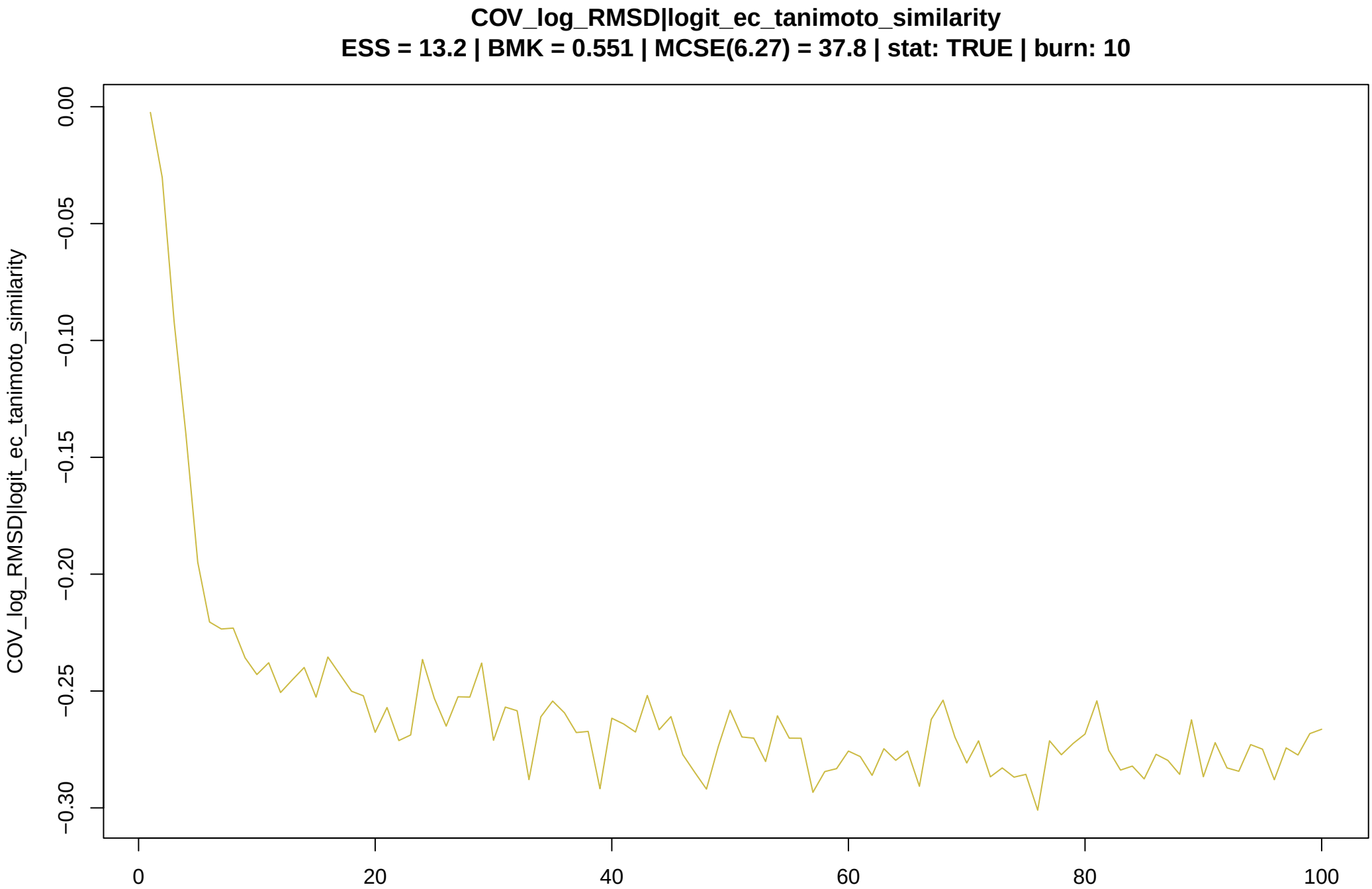

VAR_mcs_NumHeteroAtoms
ESS = 27.2 | BMK = 0.363 | MCSE(6.27) = 24.3 | stat: TRUE | burn: 20
VAR_mcs_NumHeteroAtoms
1.0
1.1
1.2
1.3
1.4
1.5
0
20
40
60
80
100

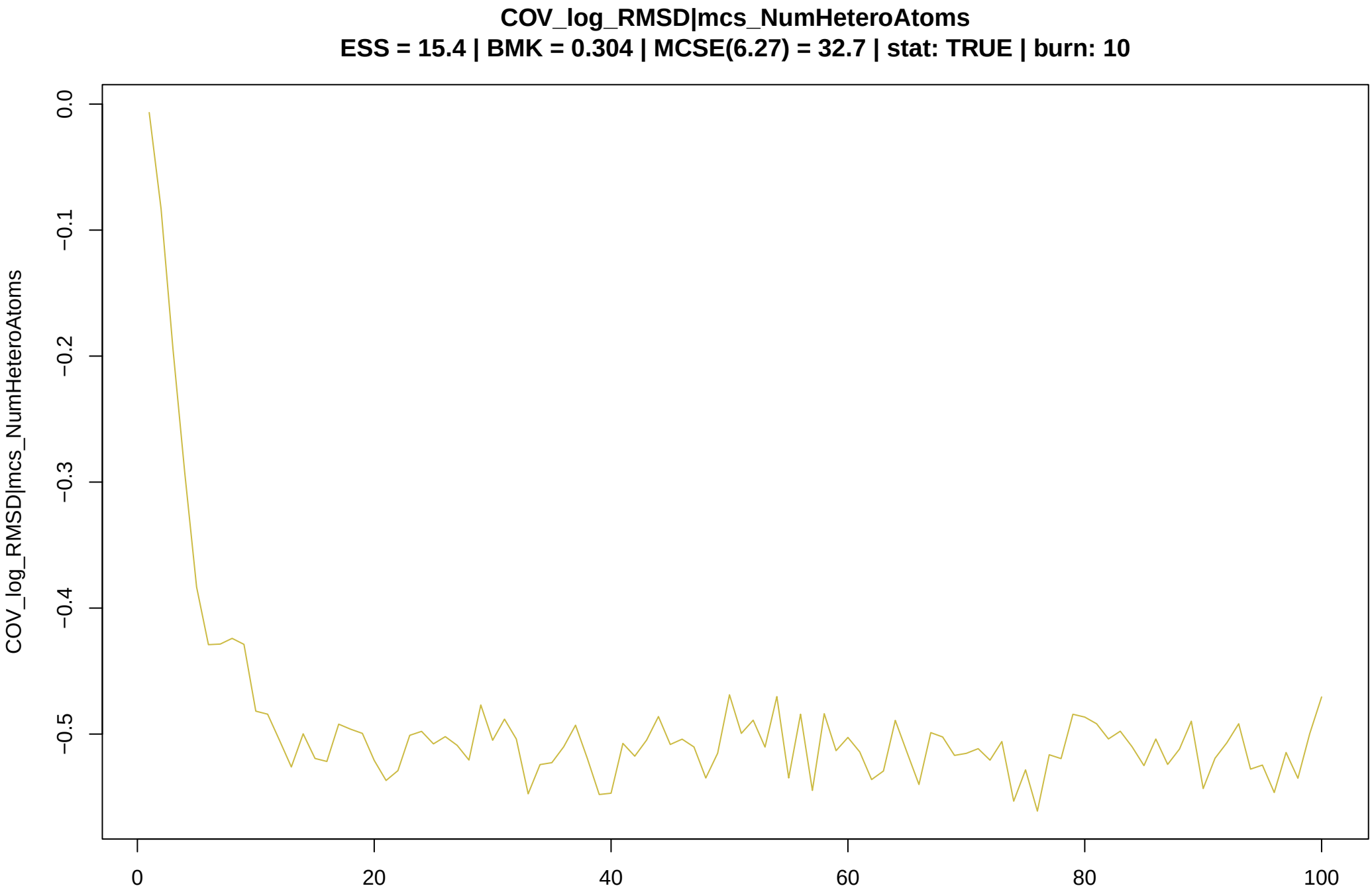

VAR_docked_HeavyAtomCount
ESS = 61.9 | BMK = 0.23 | MCSE(6.27) = 16.7 | stat: TRUE | burn: 0
VAR_docked_HeavyAtomCount
3.0
3.2
3.4
3.6
3.8
0
20
40
60
80
100

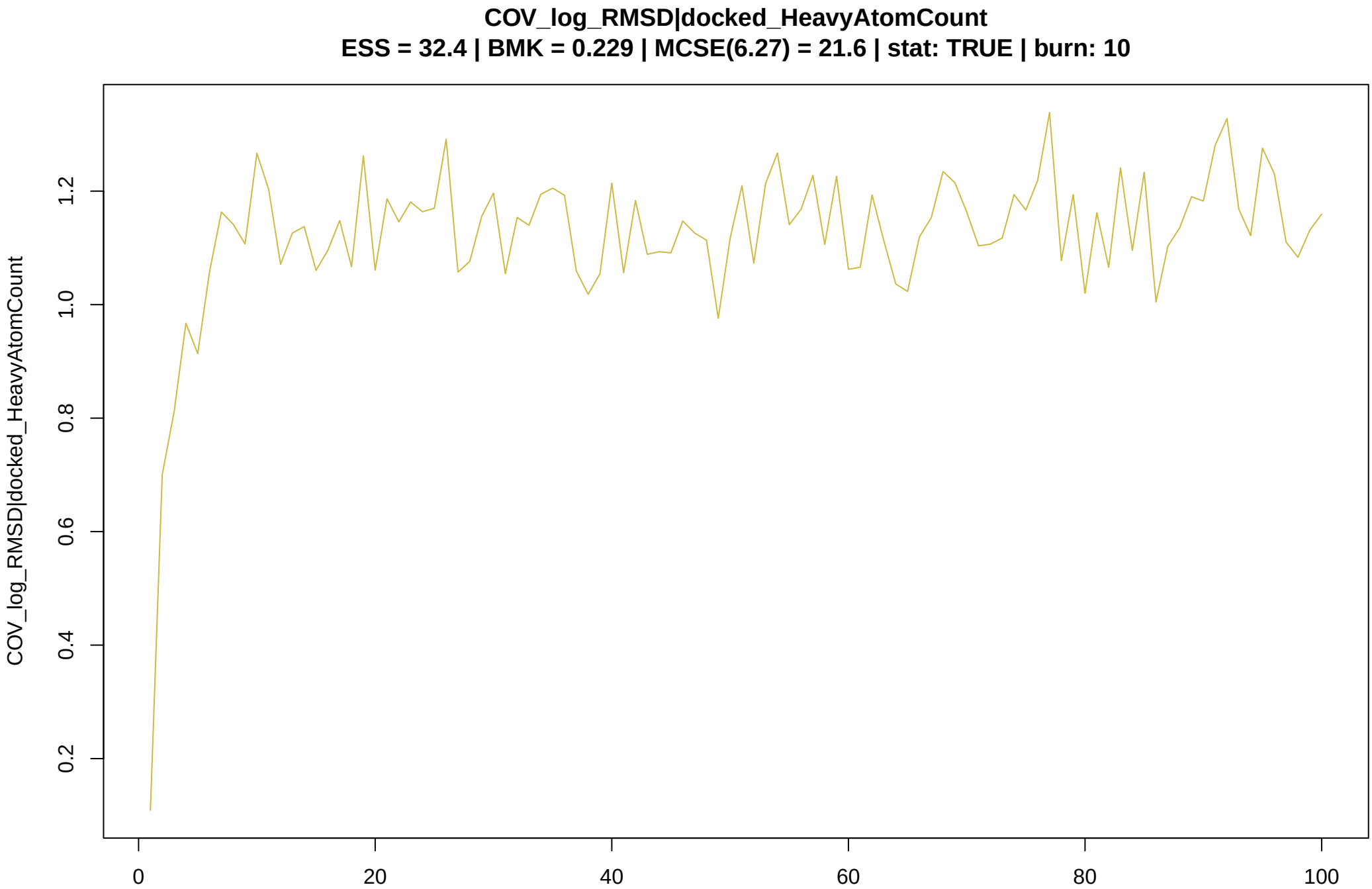

VAR_mcs_RingCount
ESS = 33.3 | BMK = 0.251 | MCSE(6.27) = 19.5 | stat: TRUE | burn: 80
VAR_mcs_RingCount
0.0
−0.1
−0.2
−0.3
0
20
40
60
80
100

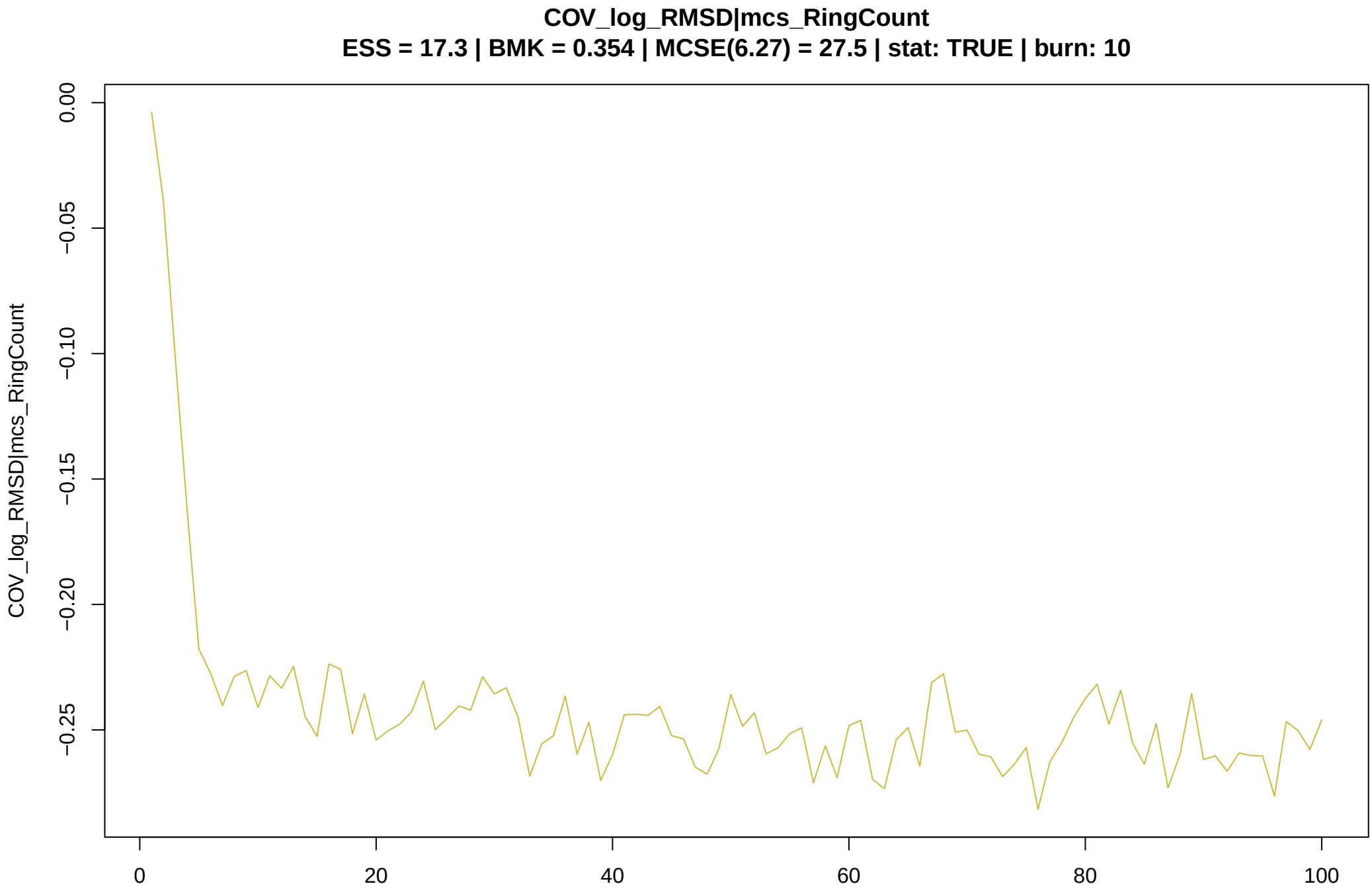

VAR_docked_NumRotatableBonds
ESS = 43.6 | BMK = 0.286 | MCSE(6.27) = 24.2 | stat: TRUE | burn: 10
VAR_docked_NumRotatableBonds
1.4
1.5
1.6
1.7
1.8
1.9
2.0
0
20
40
60
80
100

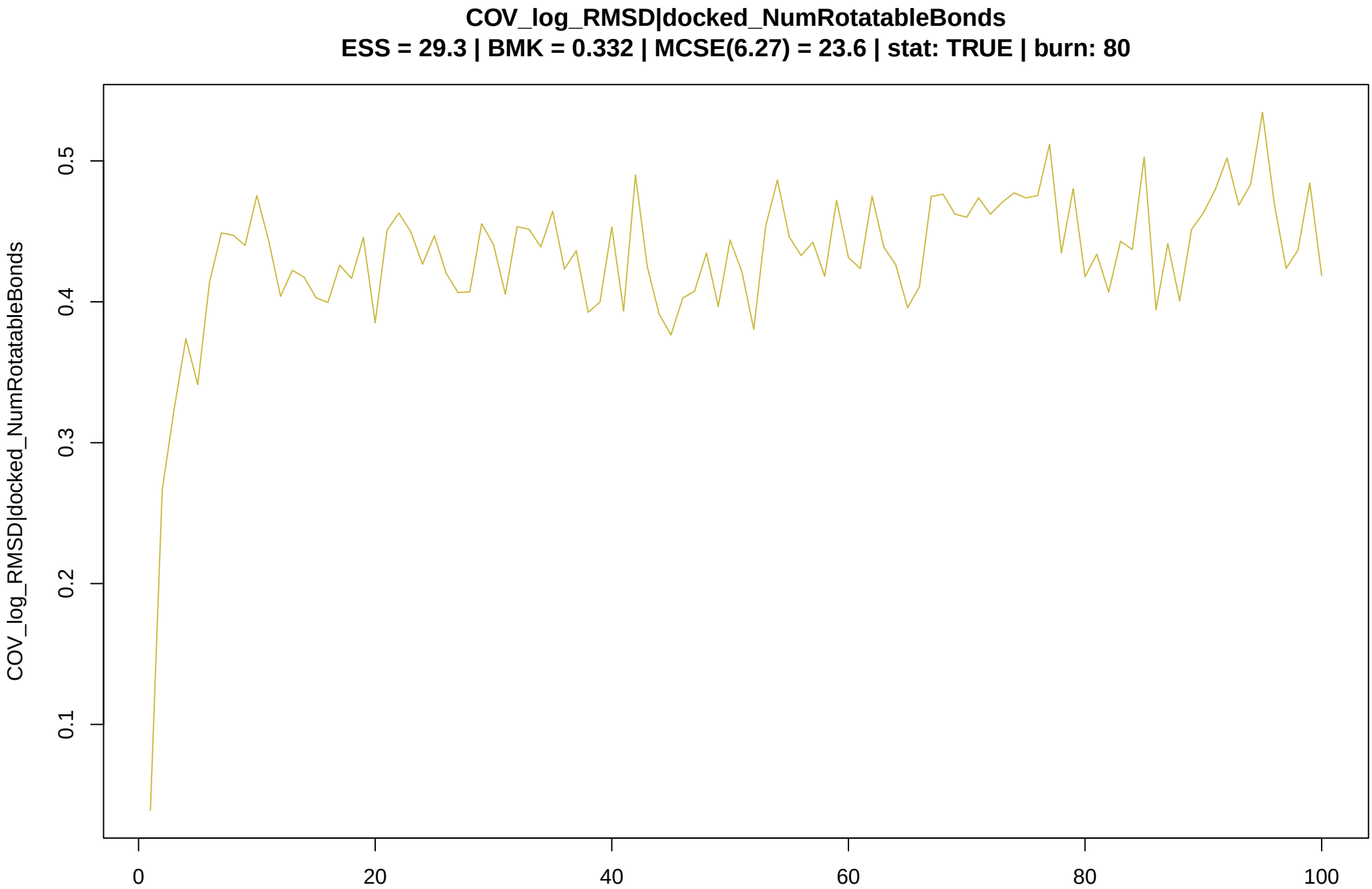

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 30.4 | BMK = 0.228 | MCSE(6.27) = 30.3 | stat: TRUE | burn: 10
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.00
−0.05
−0.10
−0.15
0
20
40
60
80
100

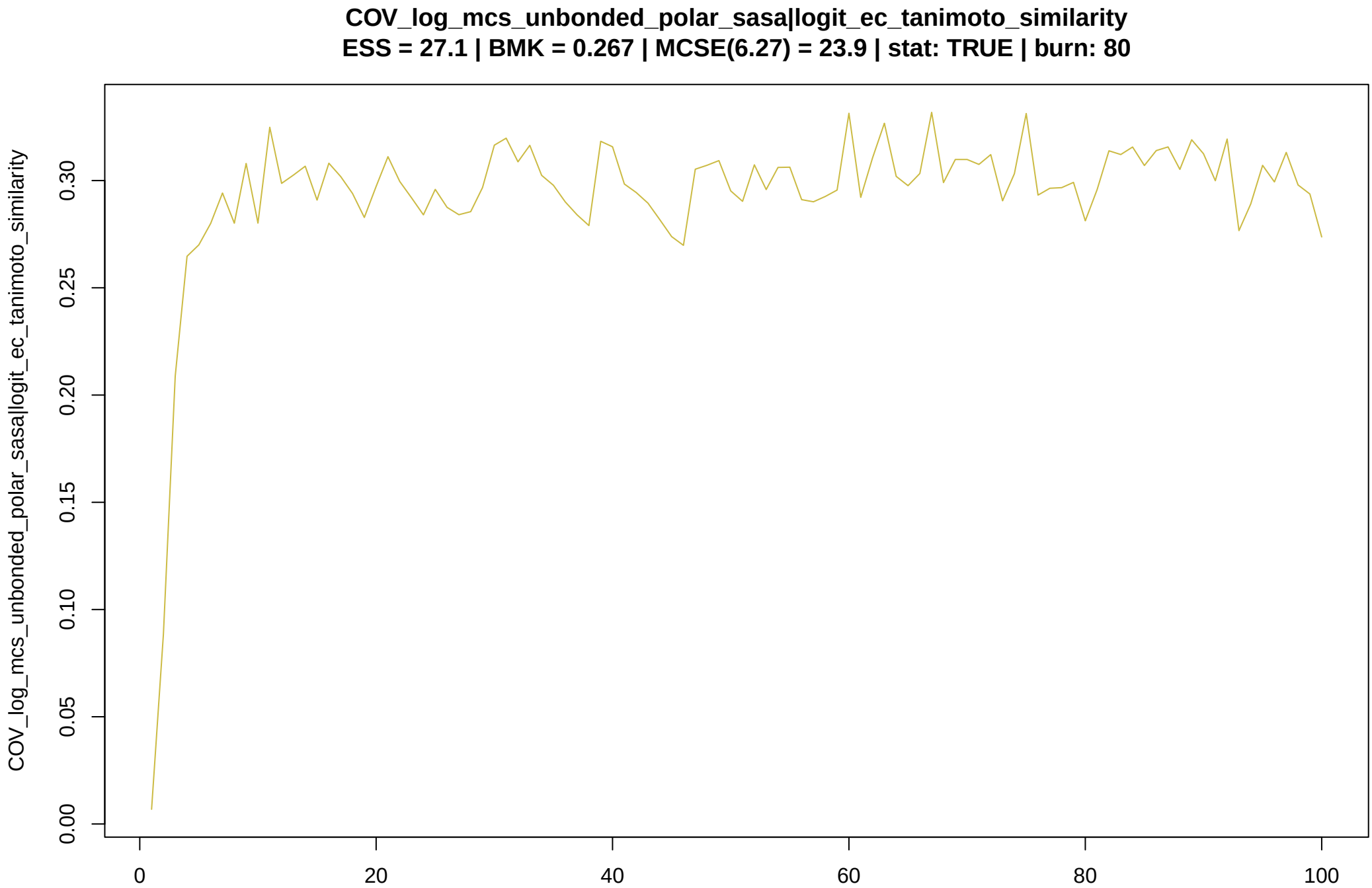

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 13.2 | BMK = 0.551 | MCSE(6.27) = 37.8 | stat: TRUE | burn: 10
COV_log_RMSD|logit_ec_tanimoto_similarity
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
0
20
40
60
80
100

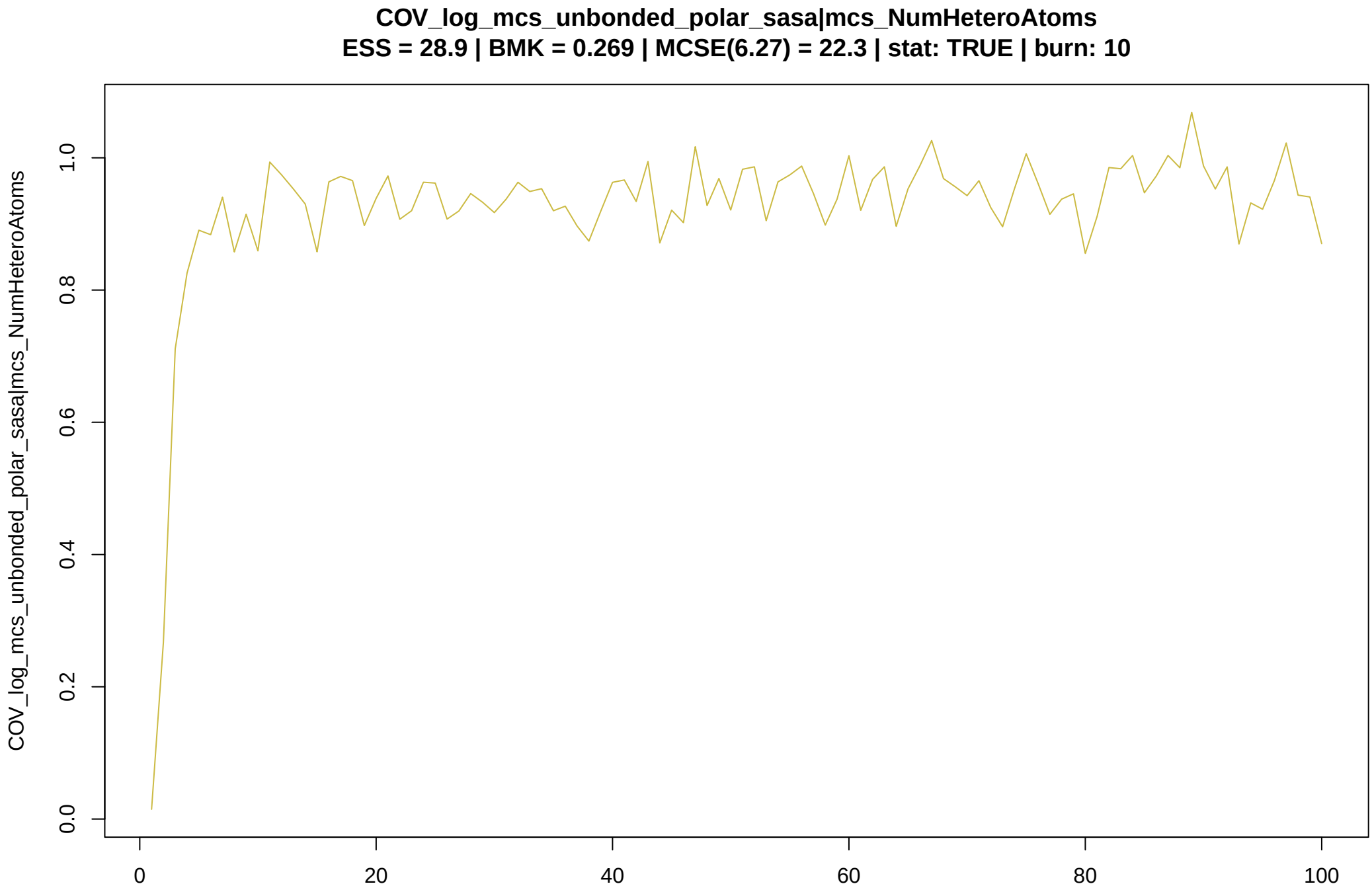

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 15.4 | BMK = 0.304 | MCSE(6.27) = 32.7 | stat: TRUE | burn: 10
COV_log_RMSD|mcs_NumHeteroAtoms
0.0
−0.1
−0.2
−0.3
−0.4
−0.5
0
20
40
60
80
100

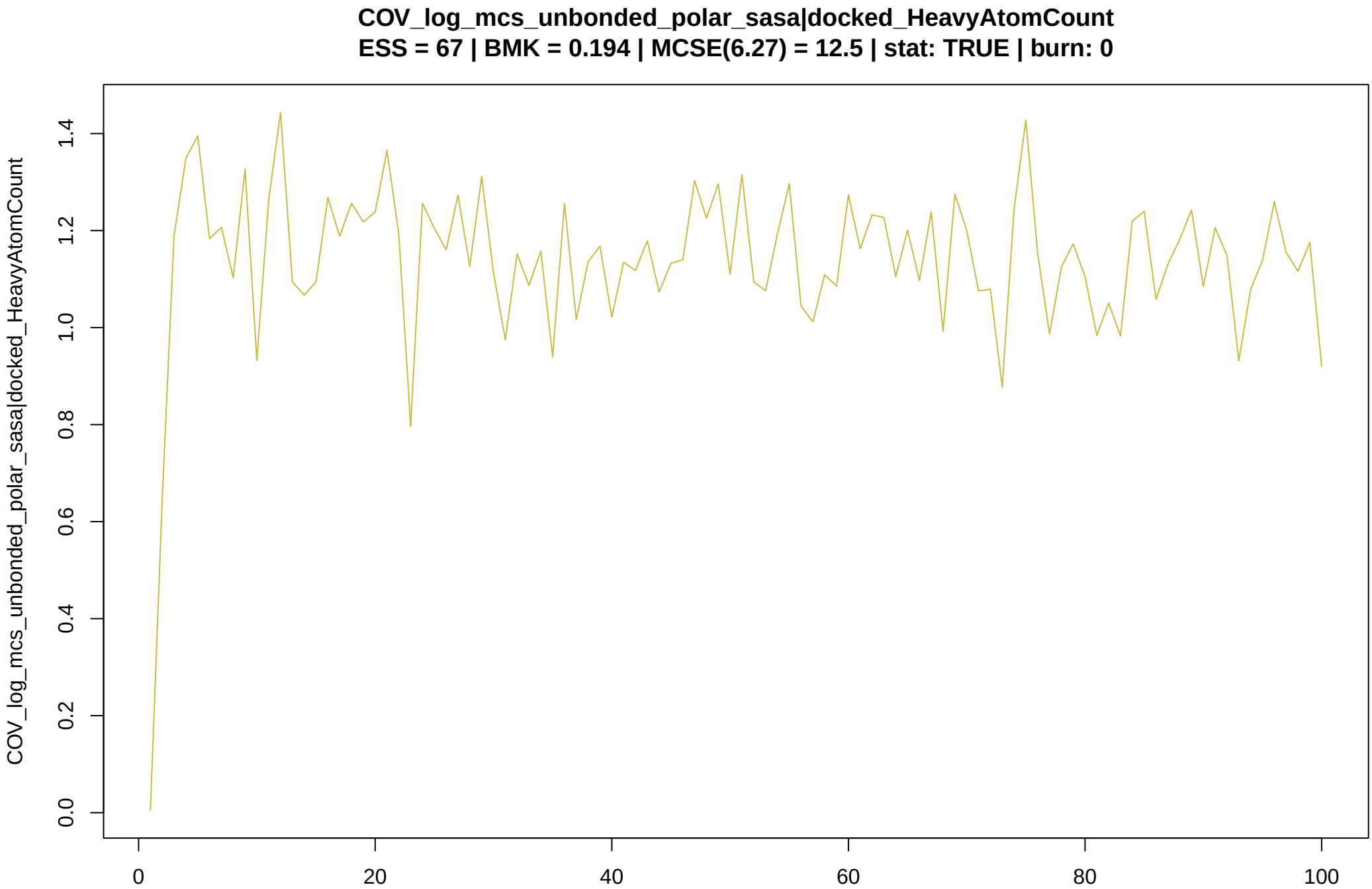

COV_log_RMSD|docked_HeavyAtomCount
ESS = 32.4 | BMK = 0.229 | MCSE(6.27) = 21.6 | stat: TRUE | burn: 10
COV_log_RMSD|docked_HeavyAtomCount
0.2
0.4
0.6
0.8
1.0
1.2
0
20
40
60
80
100

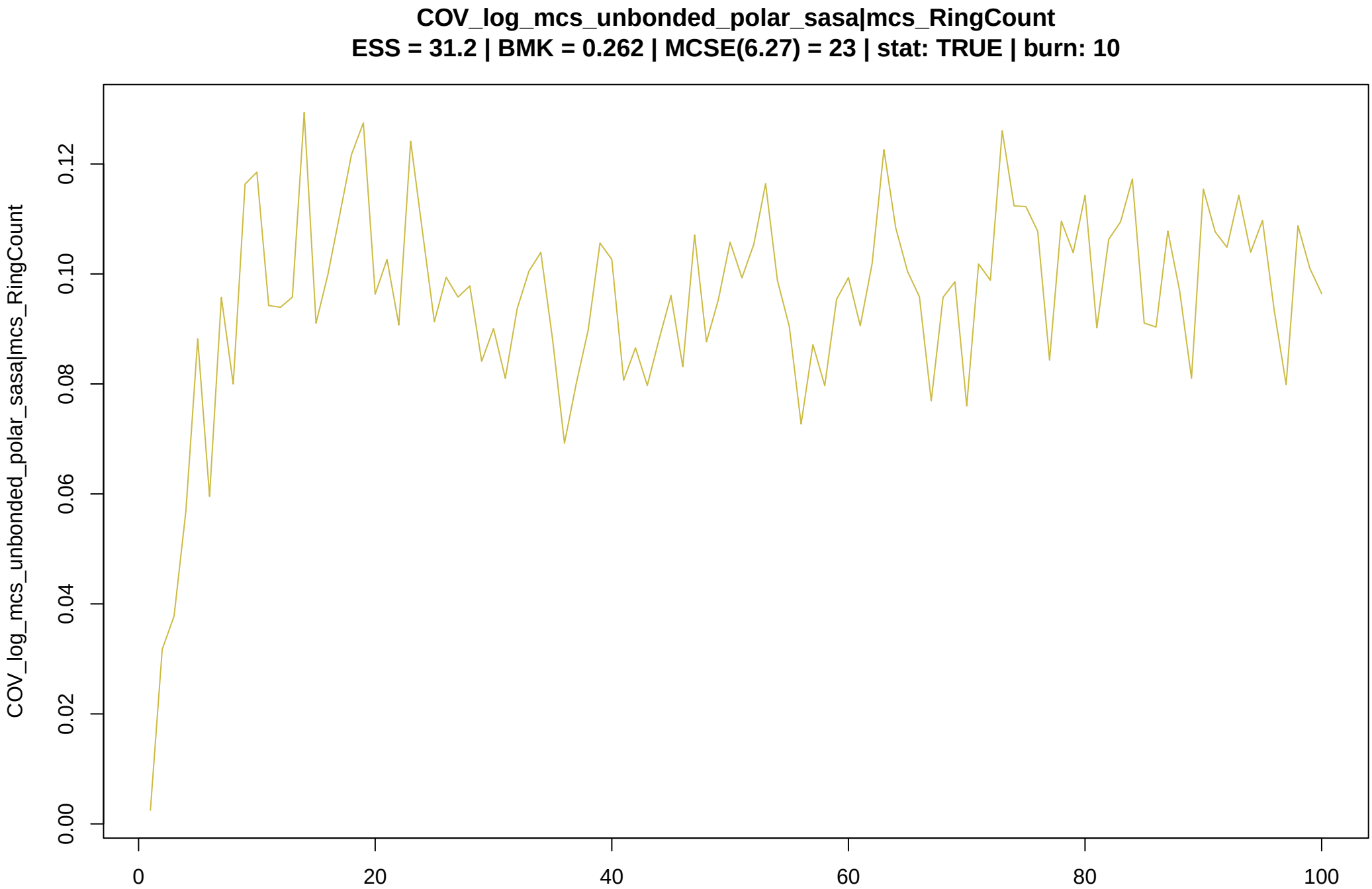

COV_log_RMSD|mcs_RingCount
ESS = 17.3 | BMK = 0.354 | MCSE(6.27) = 27.5 | stat: TRUE | burn: 10
COV_log_RMSD|mcs_RingCount
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
0
20
40
60
80
100

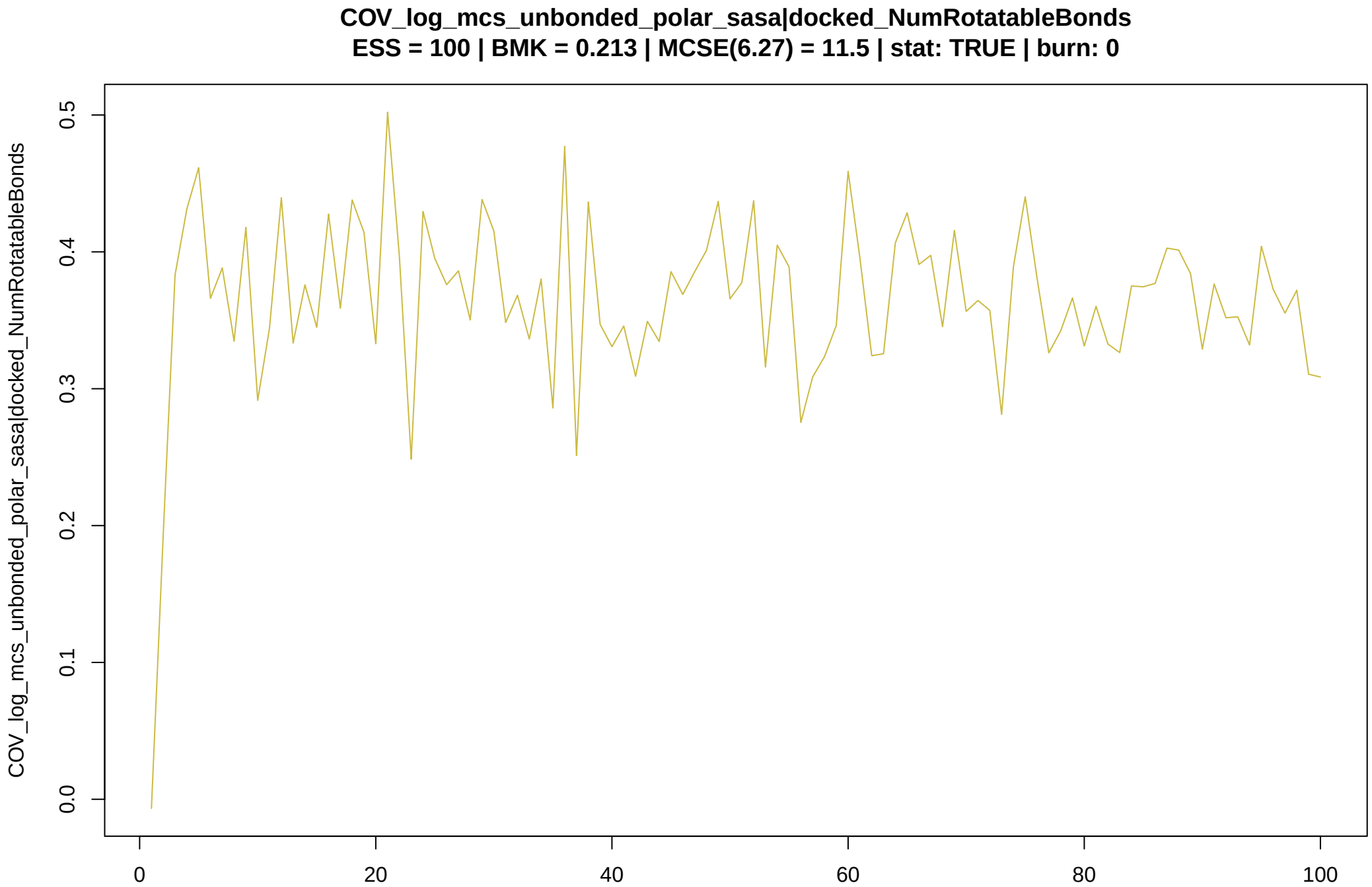

COV_log_RMSD|docked_NumRotatableBonds
ESS = 29.3 | BMK = 0.332 | MCSE(6.27) = 23.6 | stat: TRUE | burn: 80
COV_log_RMSD|docked_NumRotatableBonds
0.1
0.2
0.3
0.4
0.5
0
20
40
60
80
100

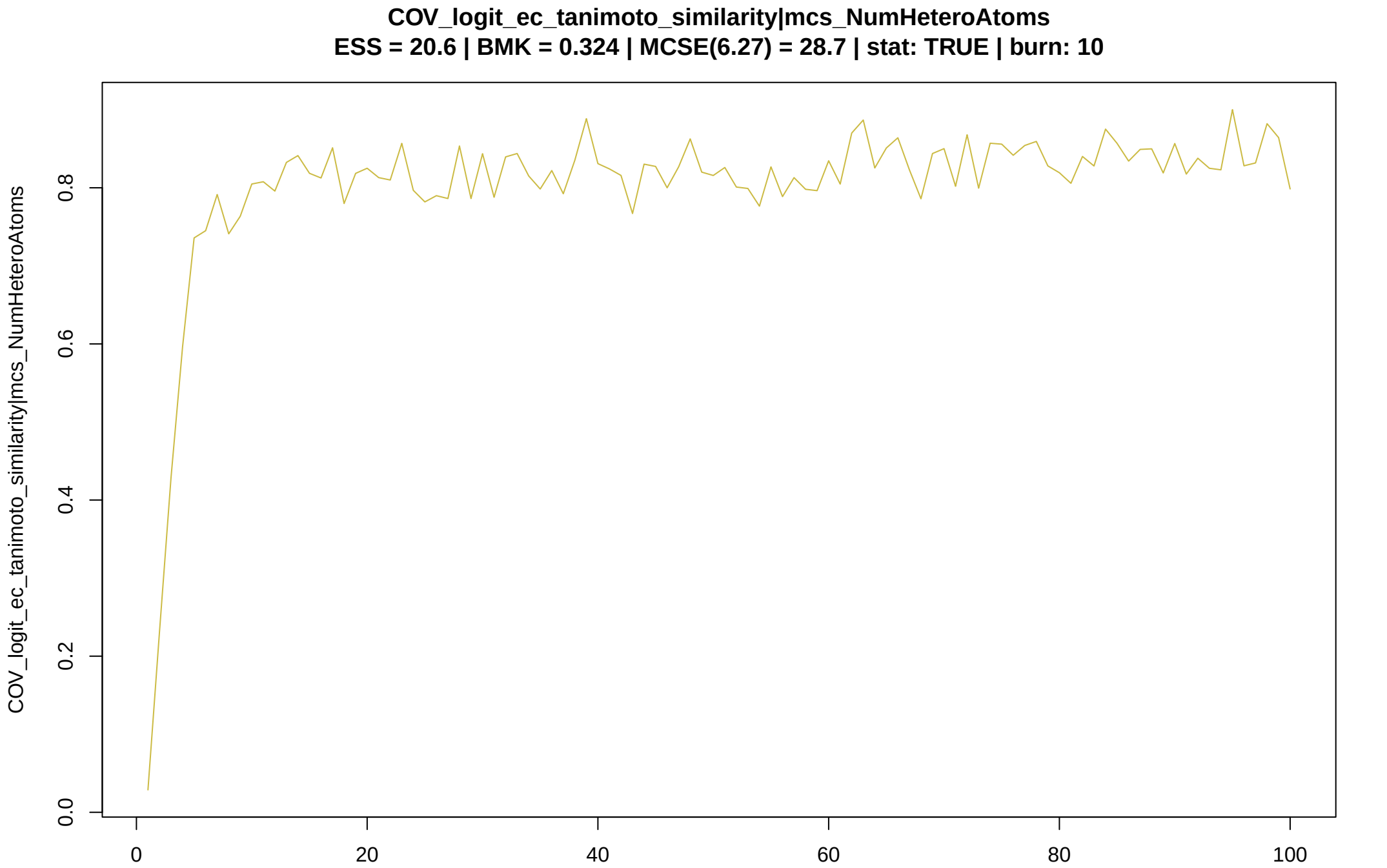

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 27.1 | BMK = 0.267 | MCSE(6.27) = 23.9 | stat: TRUE | burn: 80
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
20
40
60
80
100

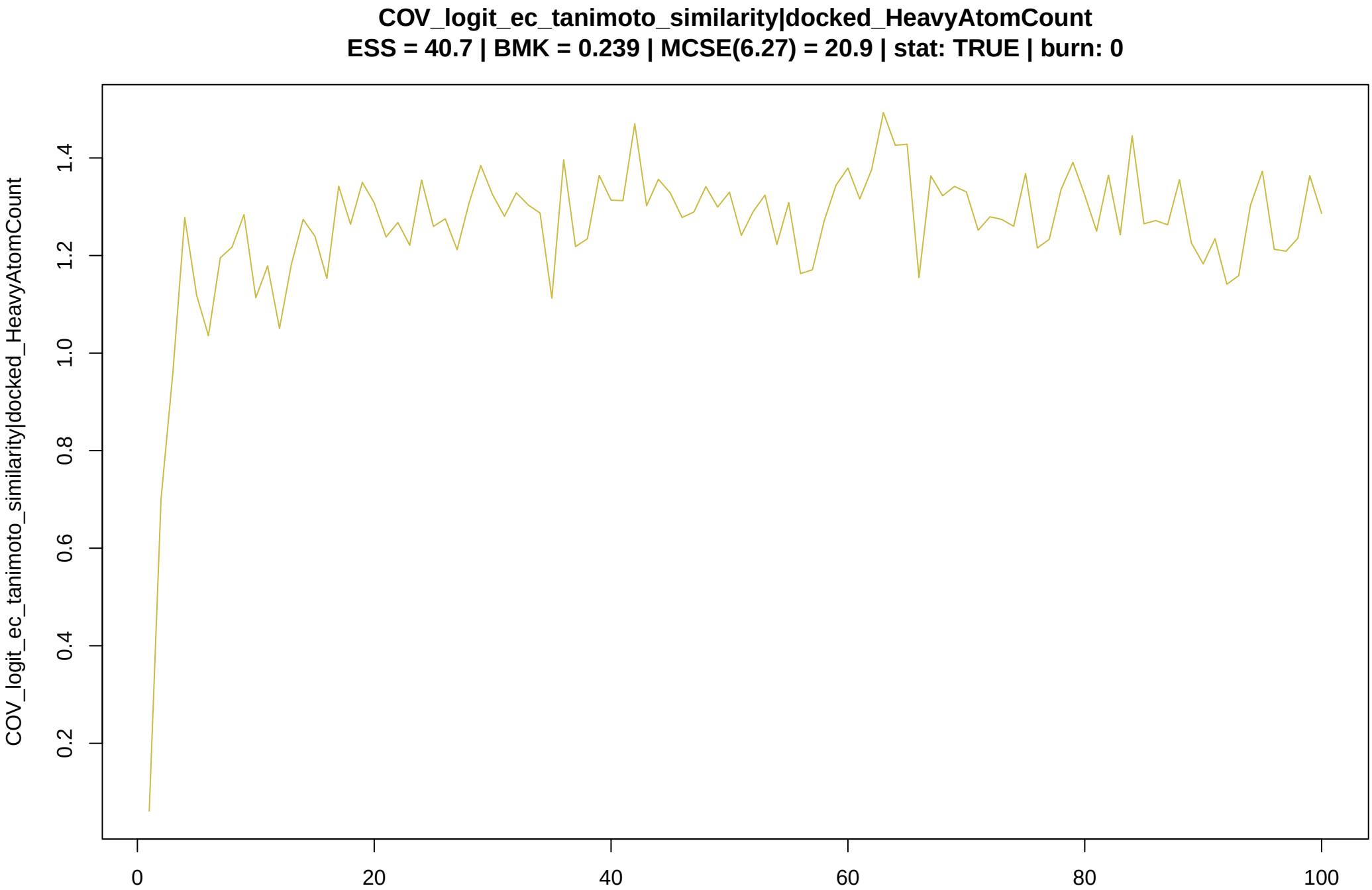

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 28.9 | BMK = 0.269 | MCSE(6.27) = 22.3 | stat: TRUE | burn: 10
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100

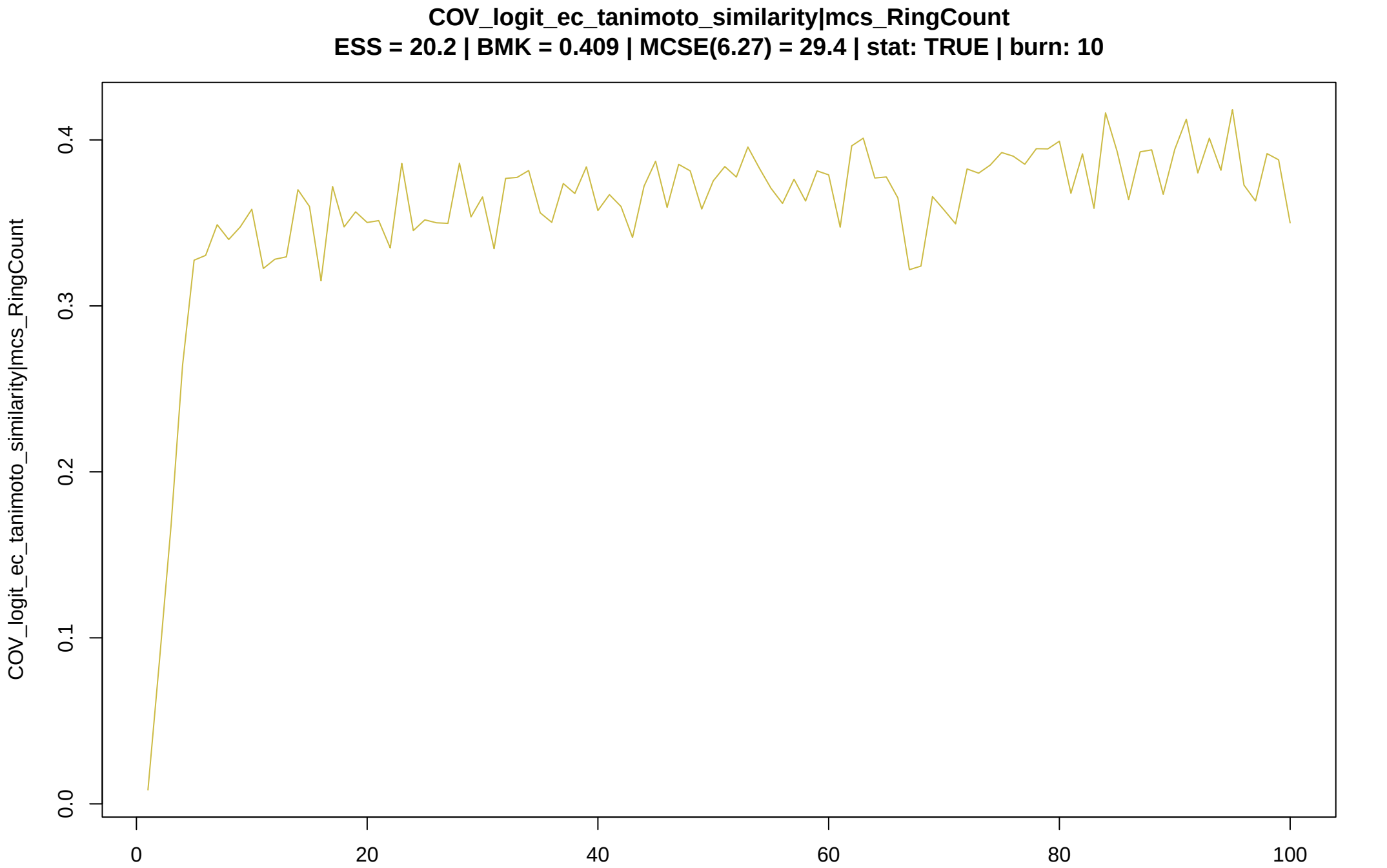

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 67 | BMK = 0.194 | MCSE(6.27) = 12.5 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
20
40
60
80
100

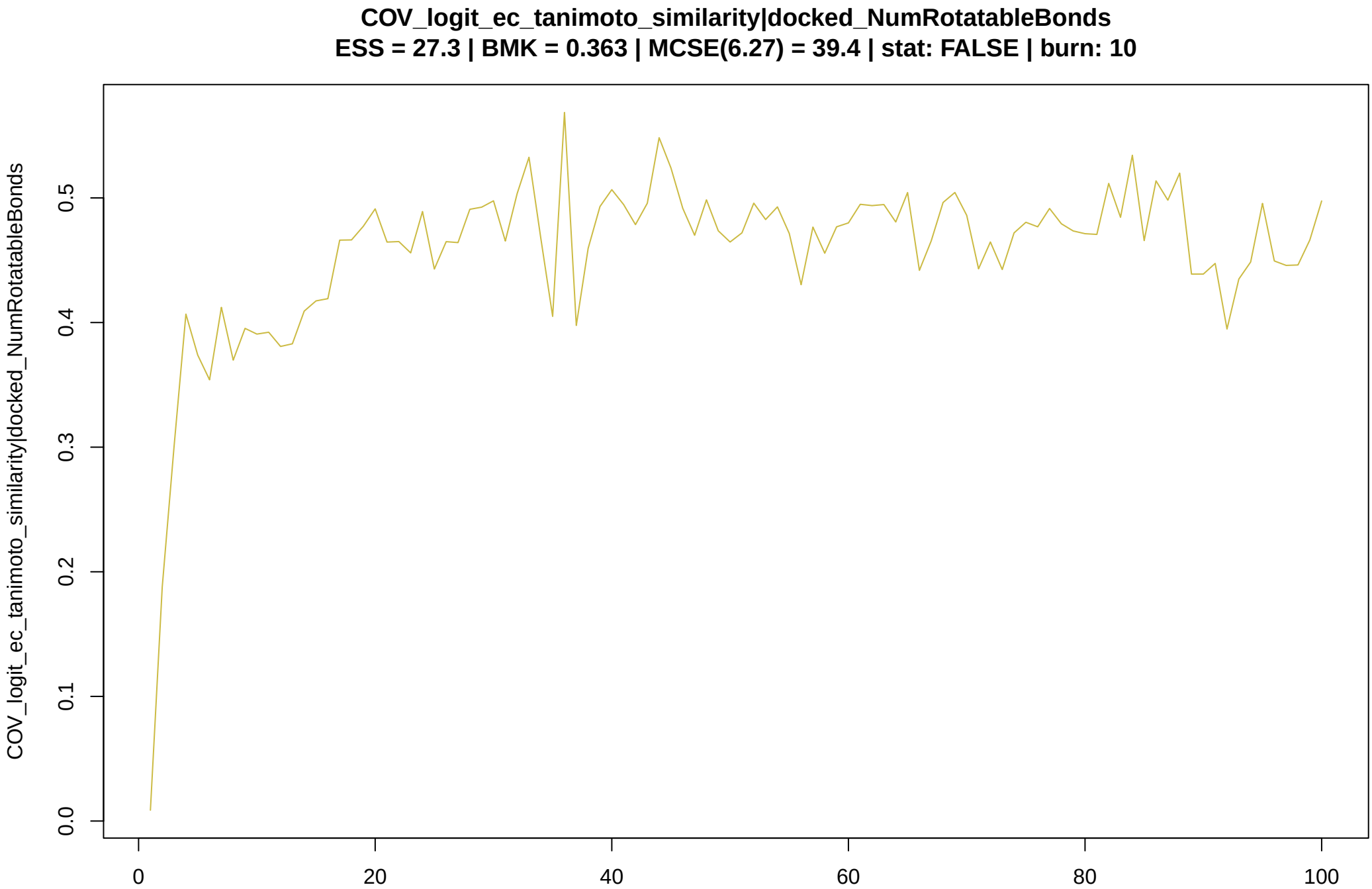

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 31.2 | BMK = 0.262 | MCSE(6.27) = 23 | stat: TRUE | burn: 10
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0
20
40
60
80
100

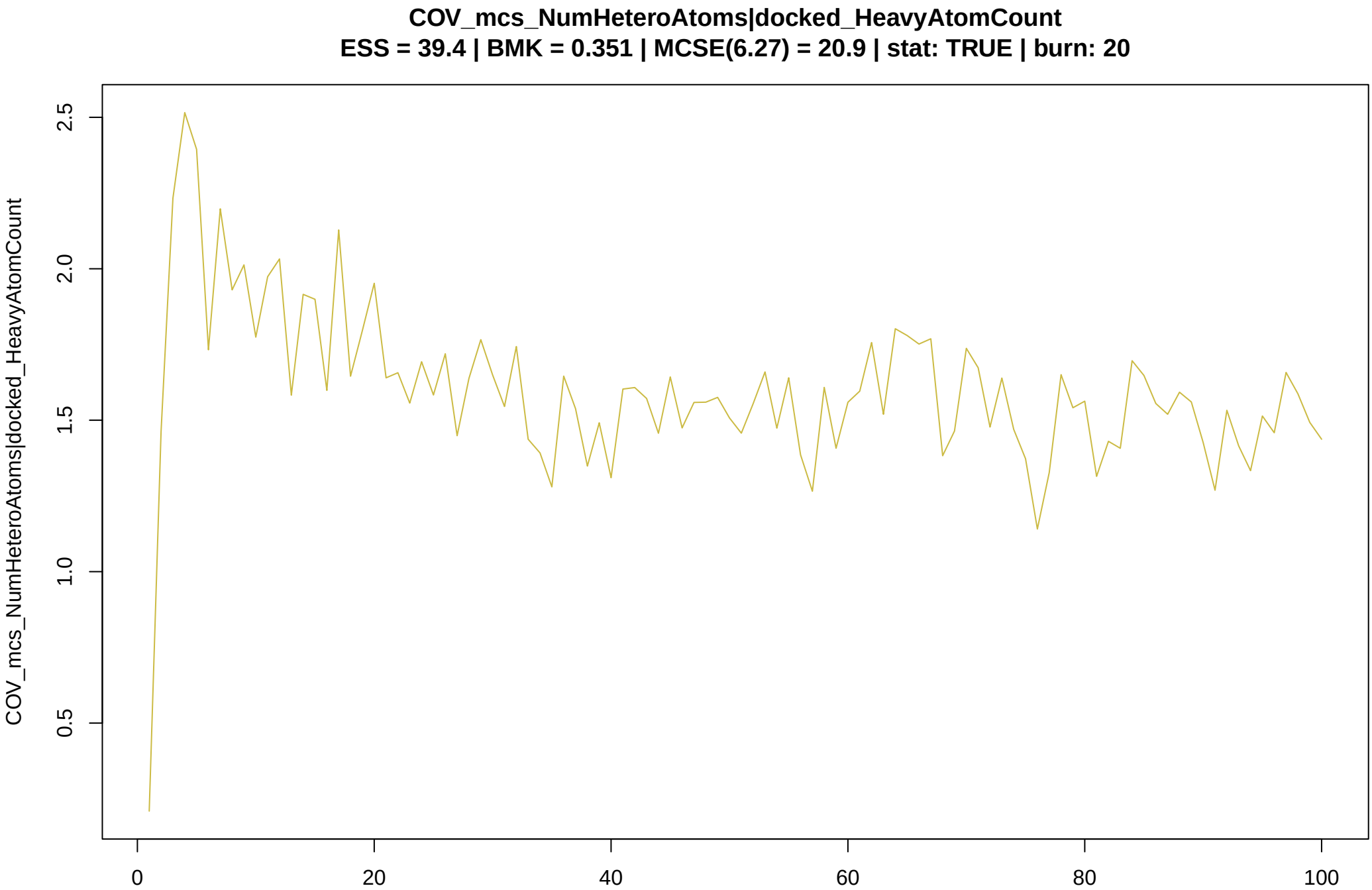

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 100 | BMK = 0.213 | MCSE(6.27) = 11.5 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
0.0
0.1
0.2
0.3
0.4
0.5
0
20
40
60
80
100

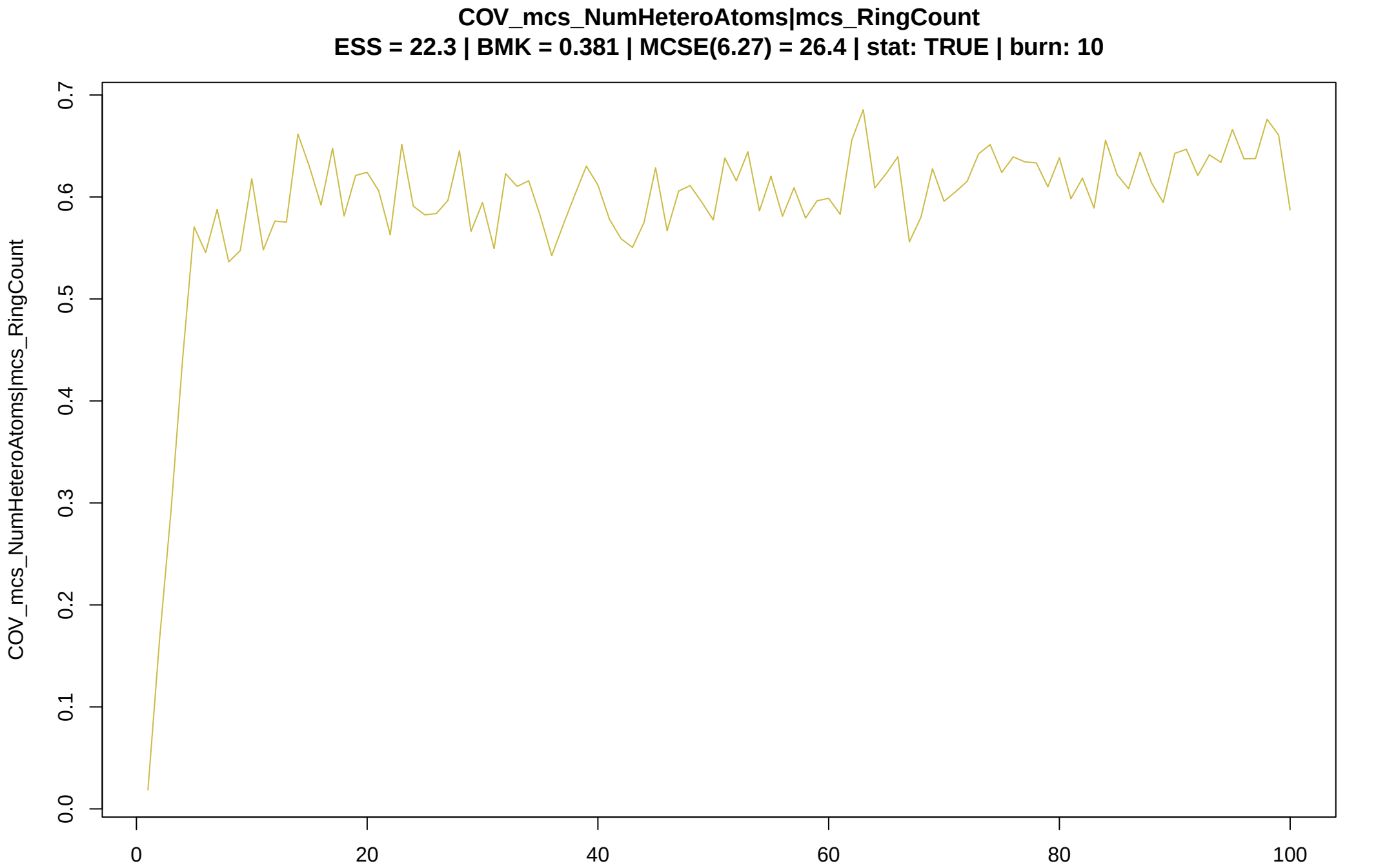

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 20.6 | BMK = 0.324 | MCSE(6.27) = 28.7 | stat: TRUE | burn: 10
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.0
0.2
0.4
0.6
0.8
0
20
40
60
80
100

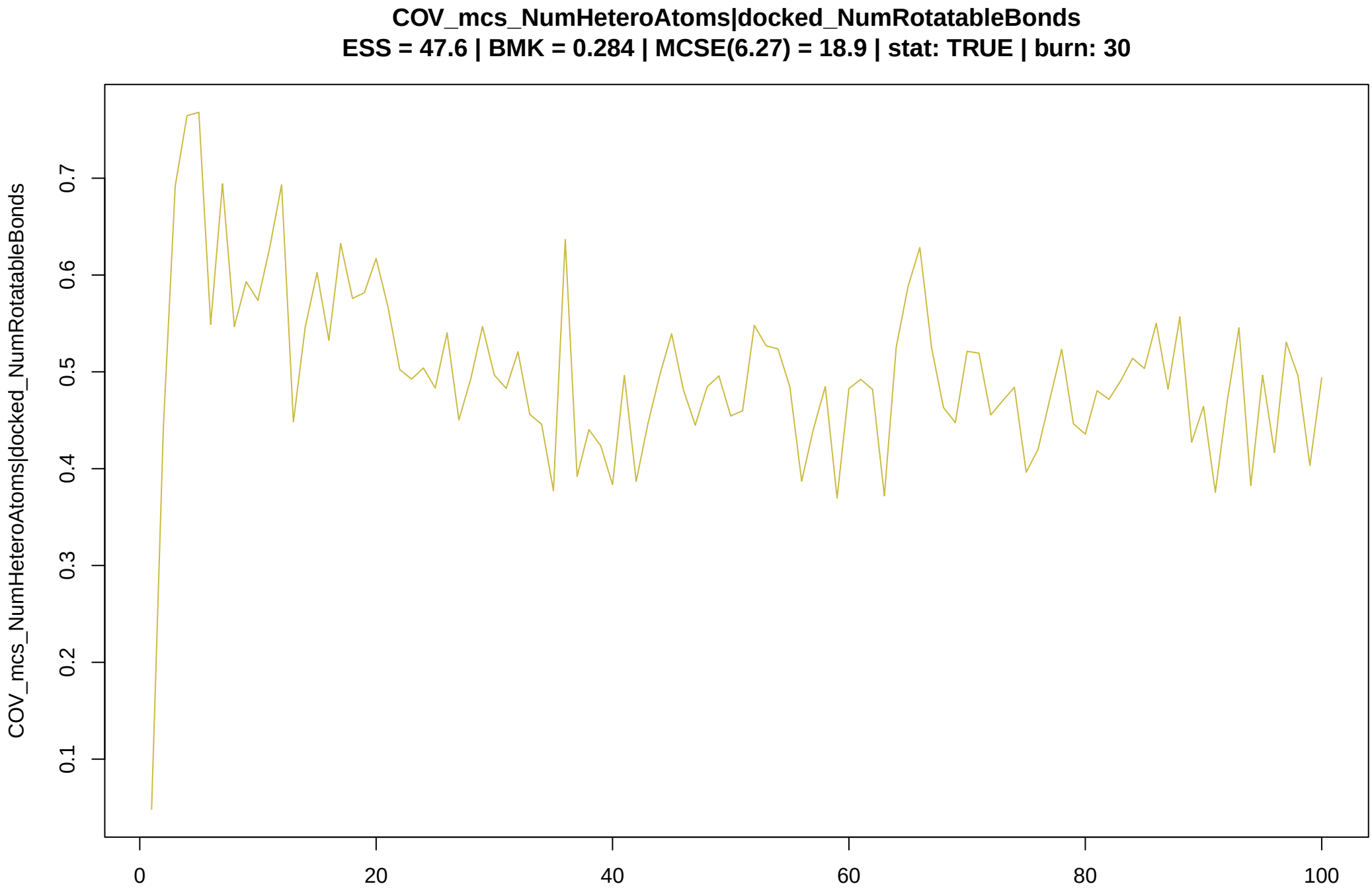

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 40.7 | BMK = 0.239 | MCSE(6.27) = 20.9 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
20
40
60
80
100

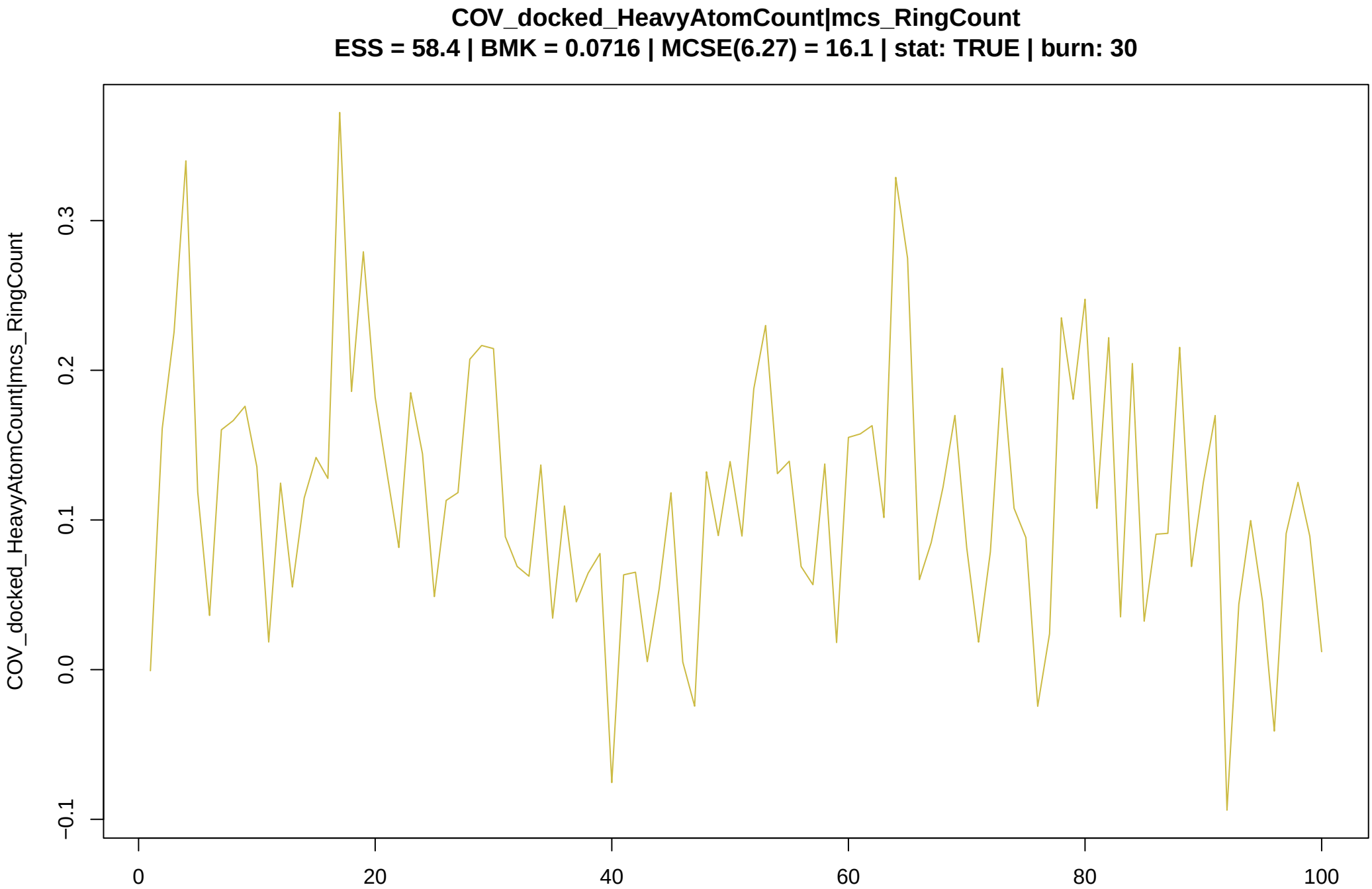

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 20.2 | BMK = 0.409 | MCSE(6.27) = 29.4 | stat: TRUE | burn: 10
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.0
0.1
0.2
0.3
0.4
0
20
40
60
80
100

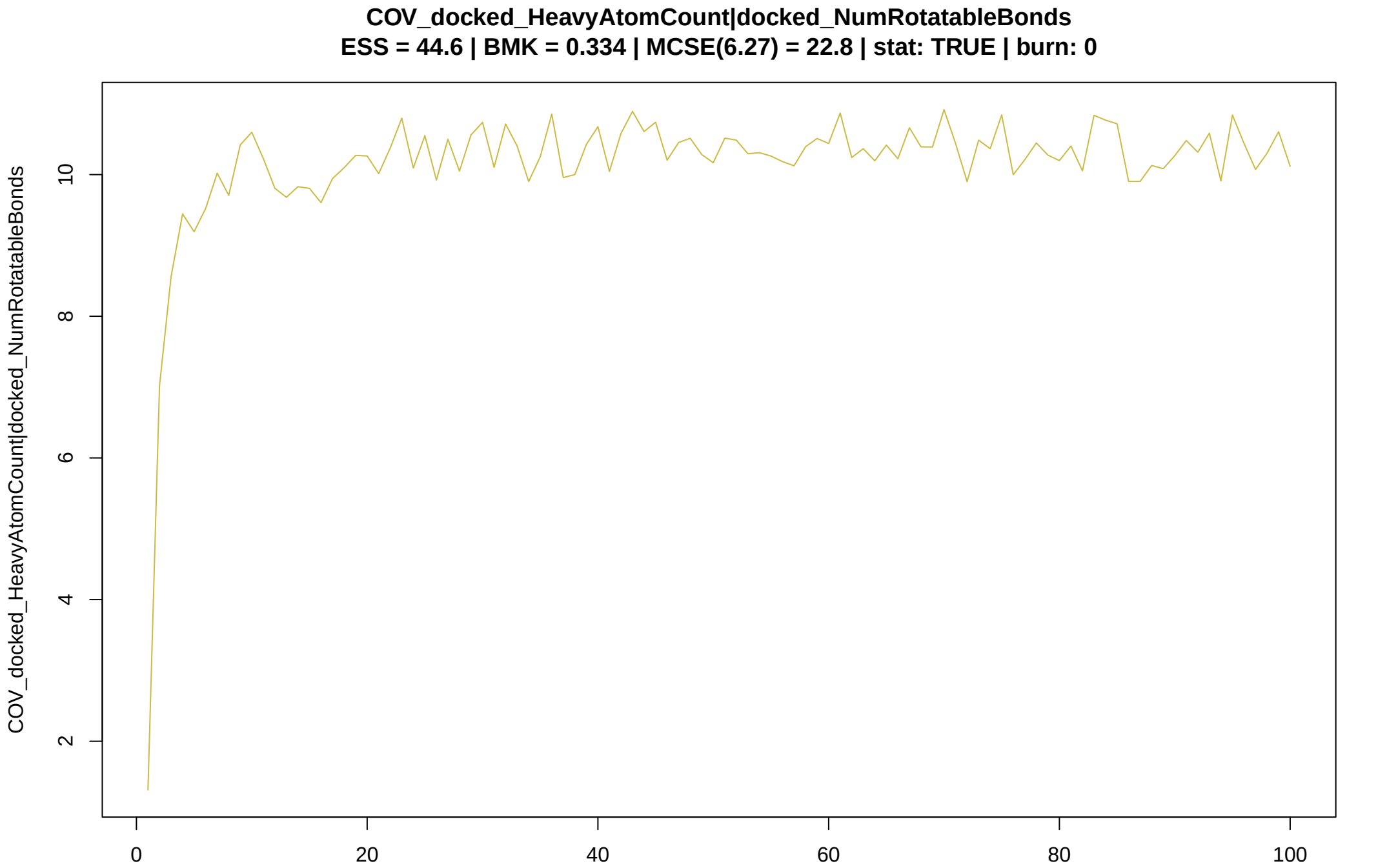

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 27.3 | BMK = 0.363 | MCSE(6.27) = 39.4 | stat: FALSE | burn: 10
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
0.0
0.1
0.2
0.3
0.4
0.5
0
20
40
60
80
100

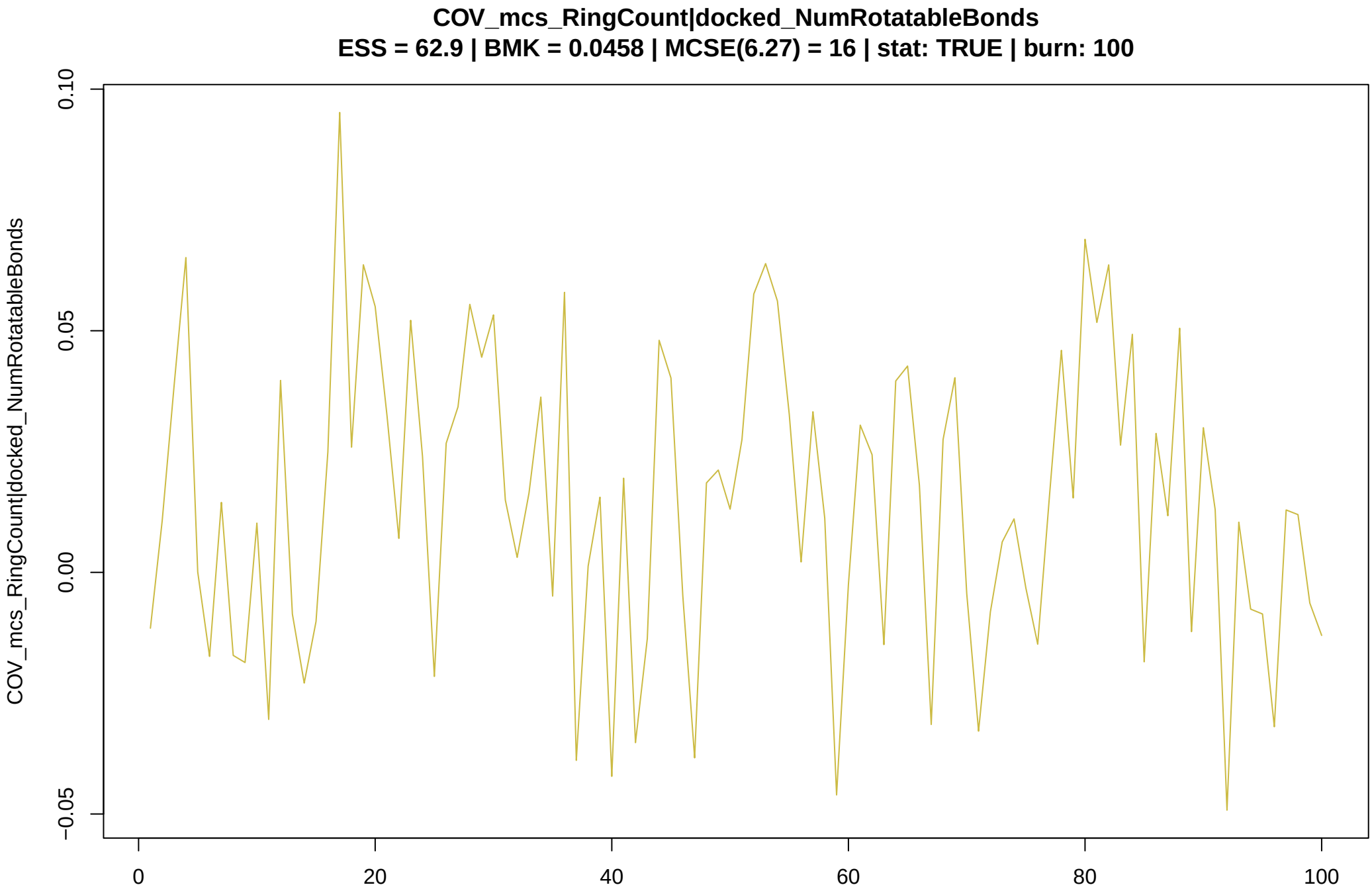

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 39.4 | BMK = 0.351 | MCSE(6.27) = 20.9 | stat: TRUE | burn: 20
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100


COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 22.3 | BMK = 0.381 | MCSE(6.27) = 26.4 | stat: TRUE | burn: 10
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
20
40
60
80
100


COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 47.6 | BMK = 0.284 | MCSE(6.27) = 18.9 | stat: TRUE | burn: 30
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
20
40
60
80
100


COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 58.4 | BMK = 0.0716 | MCSE(6.27) = 16.1 | stat: TRUE | burn: 30
COV_docked_HeavyAtomCount|mcs_RingCount
−0.1
0.0
0.1
0.2
0.3
0
20
40
60
80
100


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 44.6 | BMK = 0.334 | MCSE(6.27) = 22.8 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
2
4
6
8
10
0
20
40
60
80
100


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 62.9 | BMK = 0.0458 | MCSE(6.27) = 16 | stat: TRUE | burn: 100
COV_mcs_RingCount|docked_NumRotatableBonds
0.10
0.05
0.00
−0.05
0
20
40
60
80
100