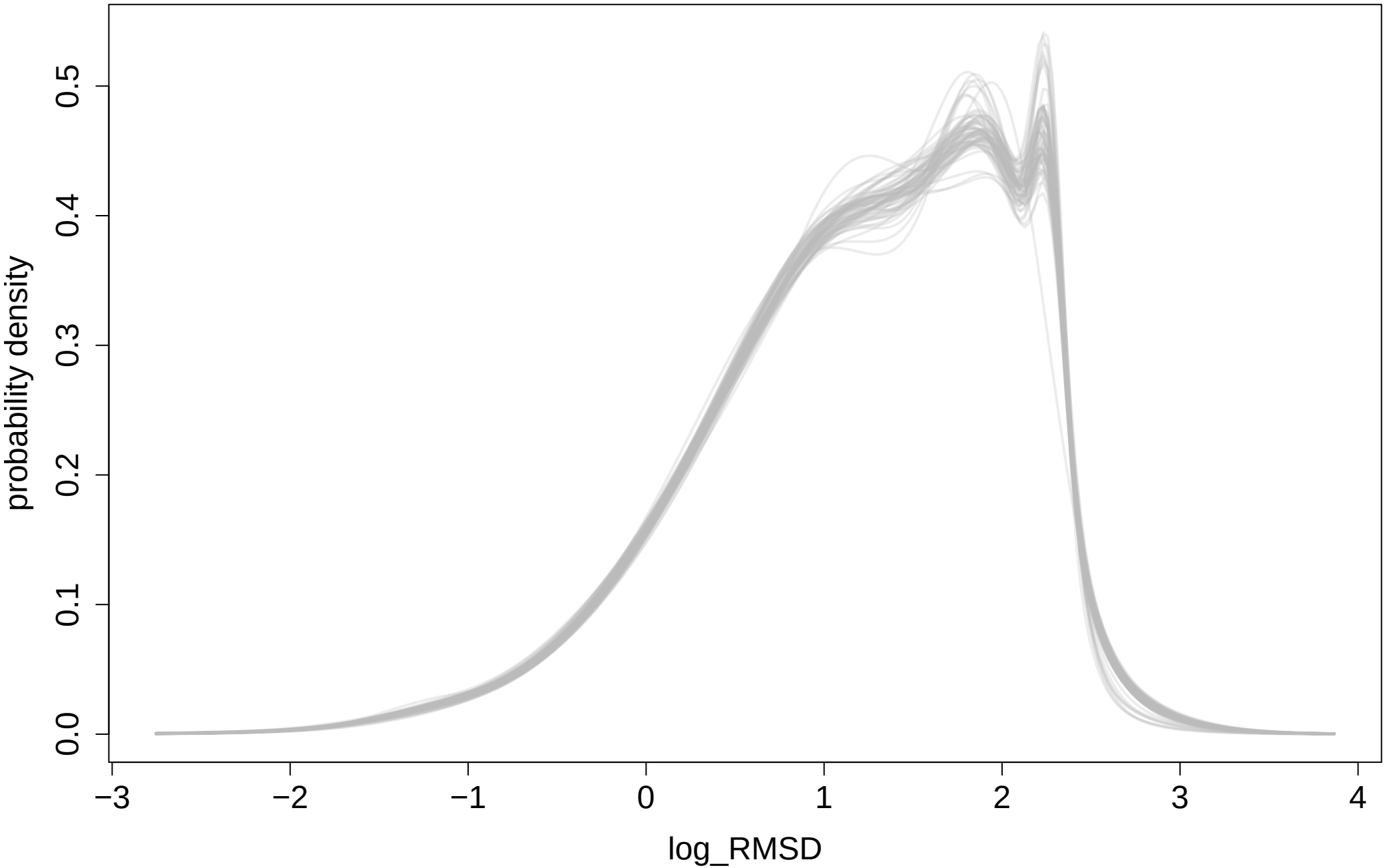
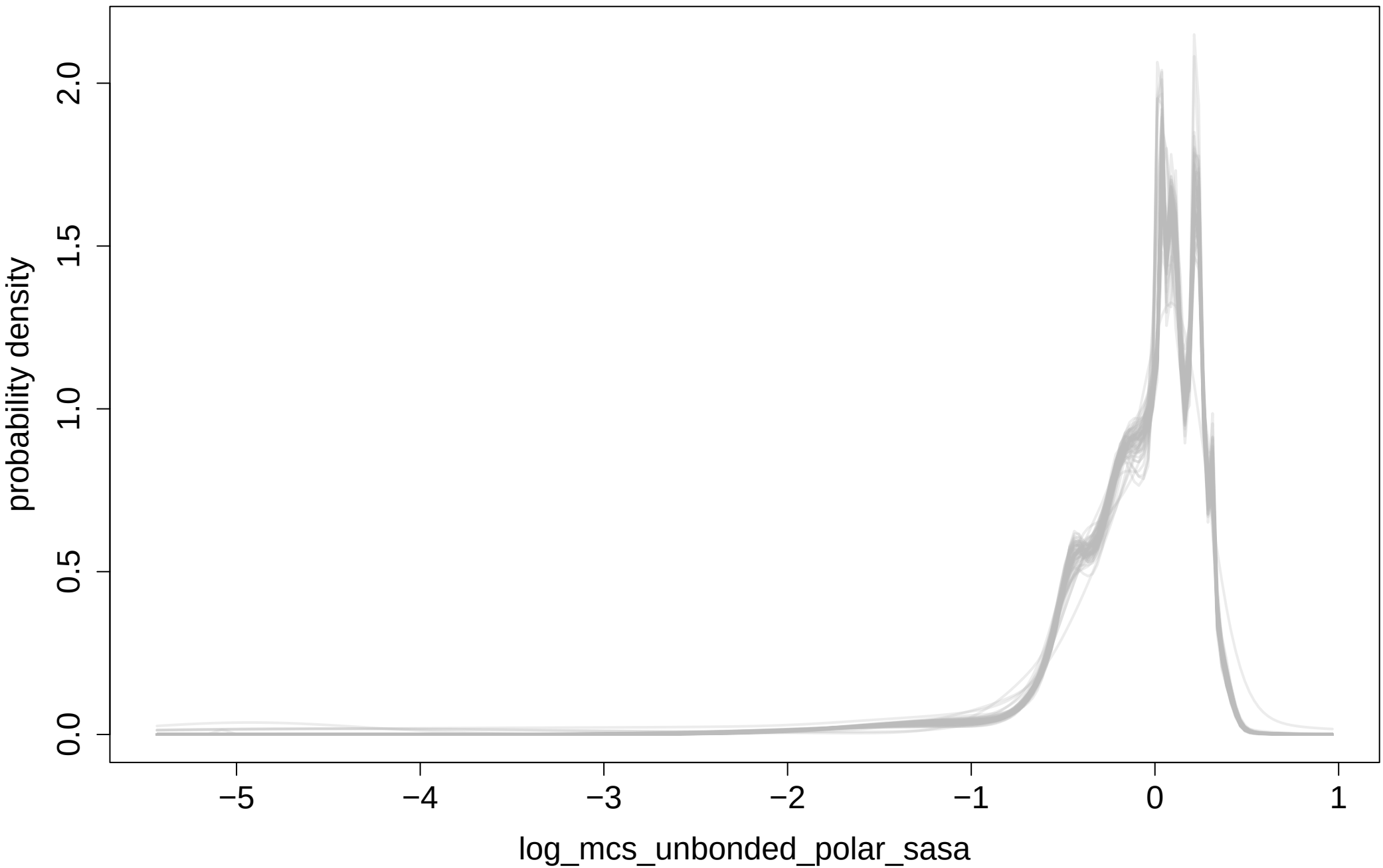
−− STATS maxD −−
min ESS = 3.37541588717936
max BMK = 0.57757194703806
max MCSE = 17.4515552973197
all stationary: FALSE
burn: 816

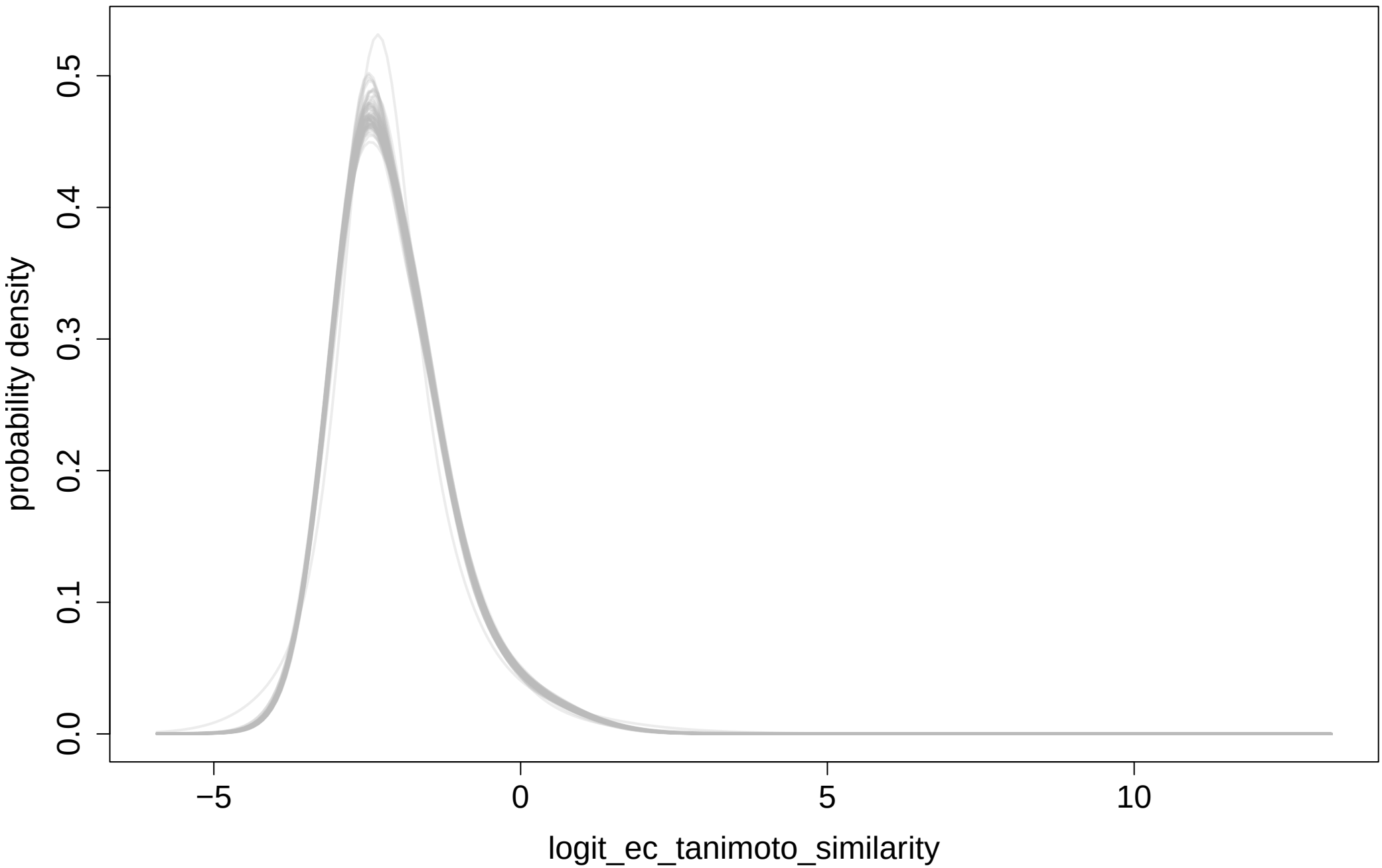
−− STATS 2D −−
min ESS = 8.78797650577303
max BMK = 0.359919775556933
max MCSE = 16.1337737541801
all stationary: FALSE
burn: 102

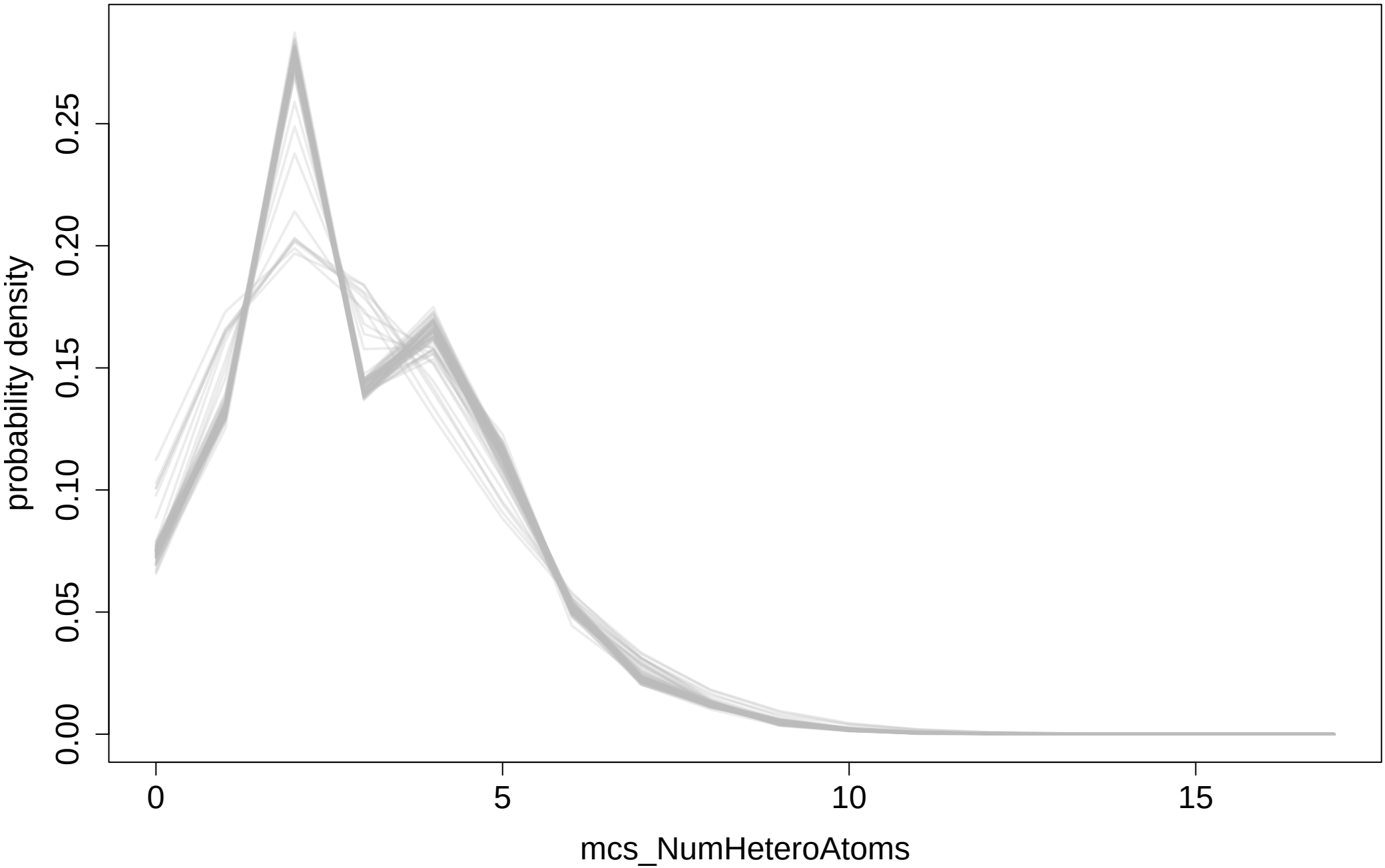
−− STATS 1D −−
min ESS = 2.2204604925031e−16
max BMK = 0.69711691648665
max MCSE = NaN
all stationary: FALSE
burn: 102

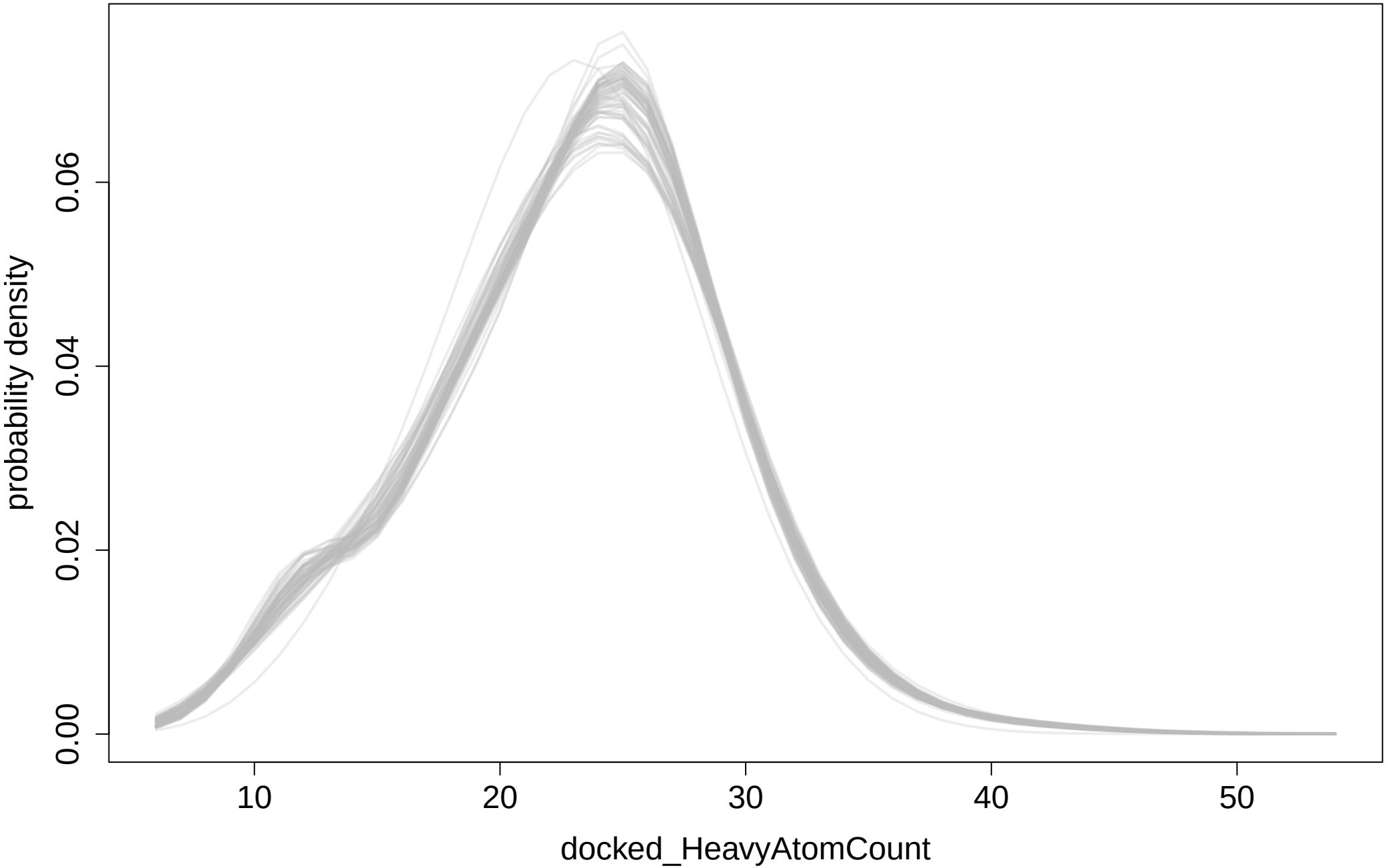
Occupied clusters: 39 of 64
LL: −77100 +− 4260

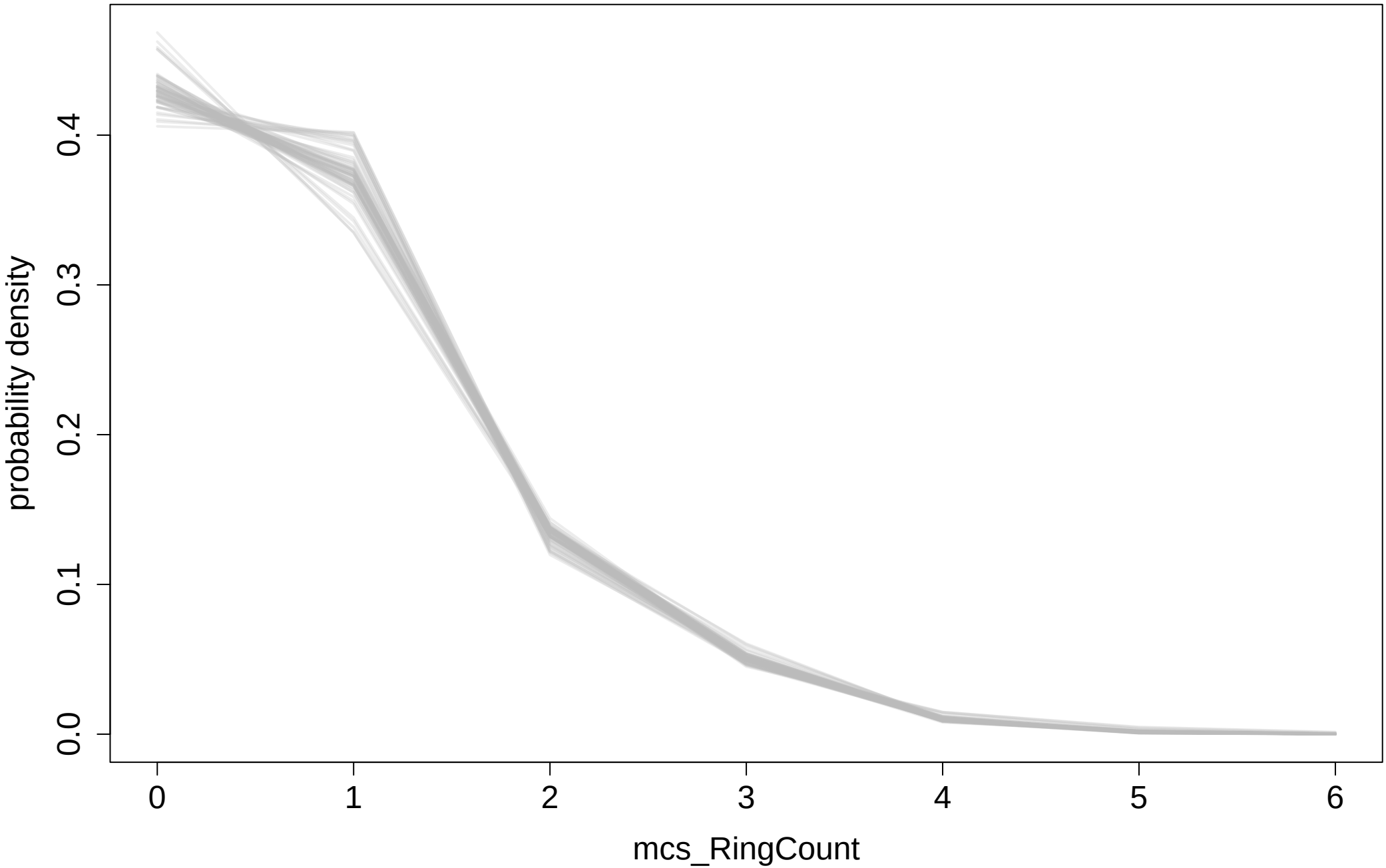

probability density
0.0
0.1
0.2
0.3
0.4
0.5
−3
−2
−1
0
1
2
3
4
log_RMSD


probability density
0.0
0.5
1.0
1.5
2.0
−5
−4
−3
−2
−1
0
1
log_mcs_unbonded_polar_sasa


probability density
0.0
0.1
0.2
0.3
0.4
0.5
−5
0
5
10
logit_ec_tanimoto_similarity


probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_NumHeteroAtoms


probability density
0.00
0.02
0.04
0.06
10
20
30
40
50
docked_HeavyAtomCount


probability density
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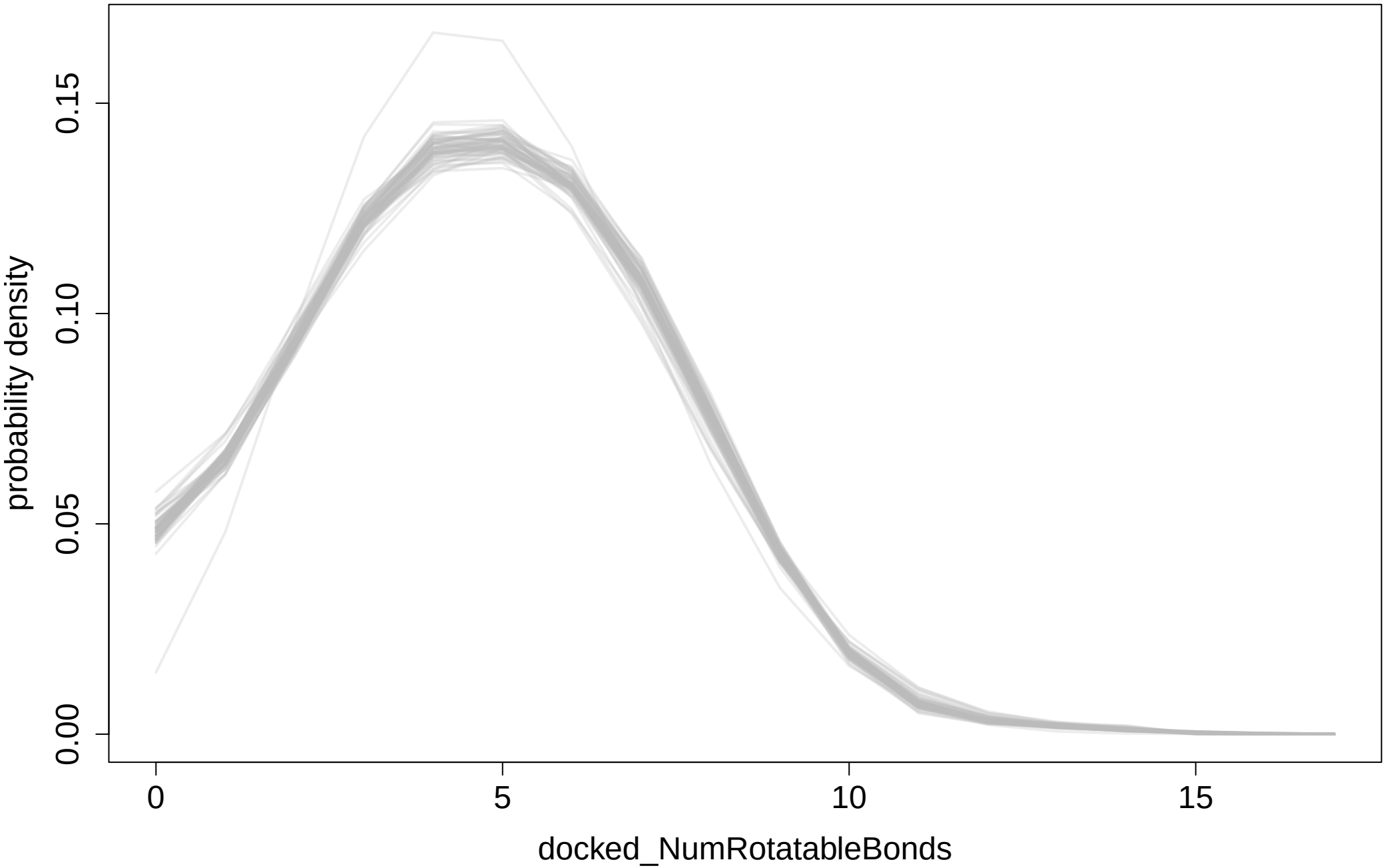
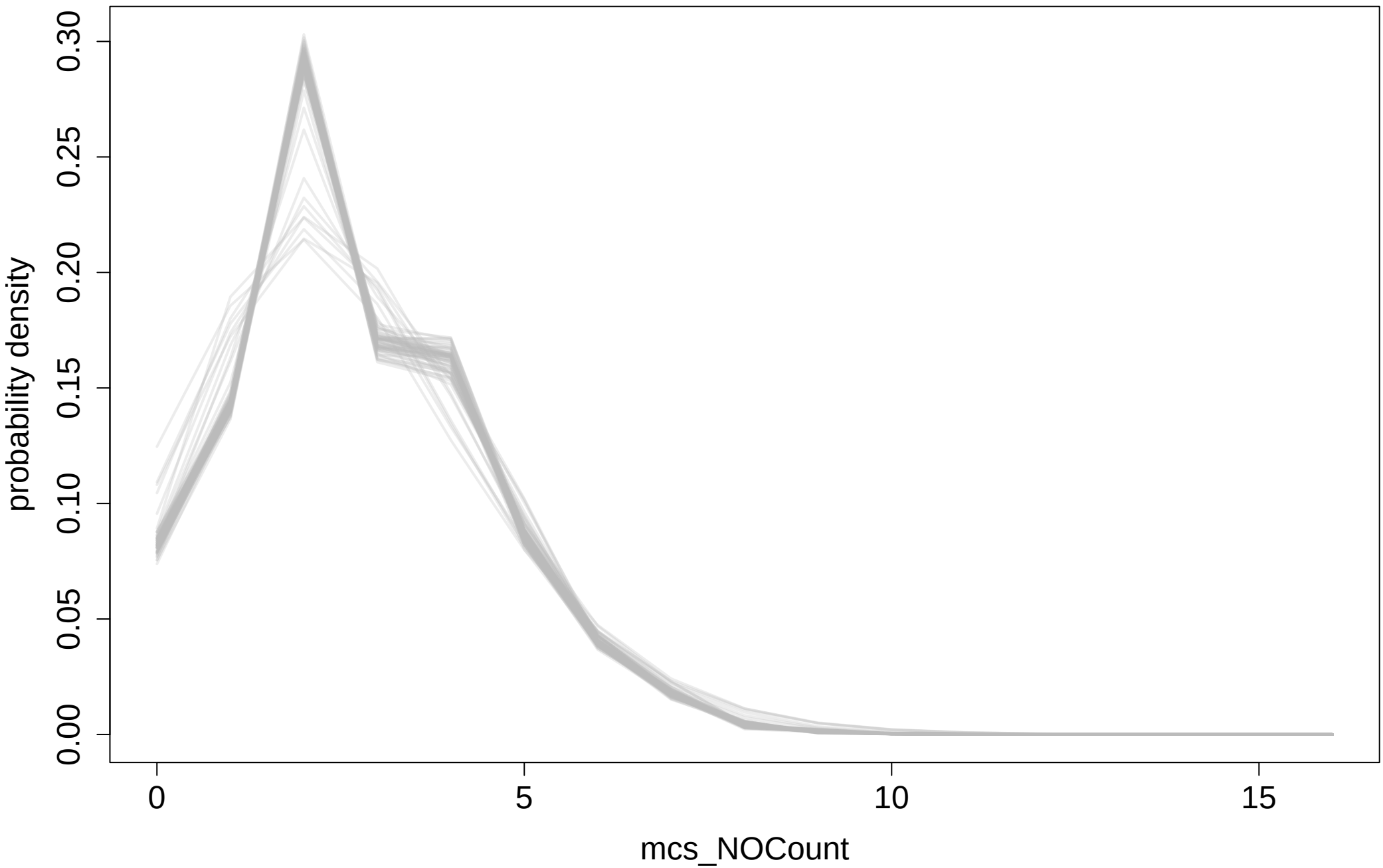
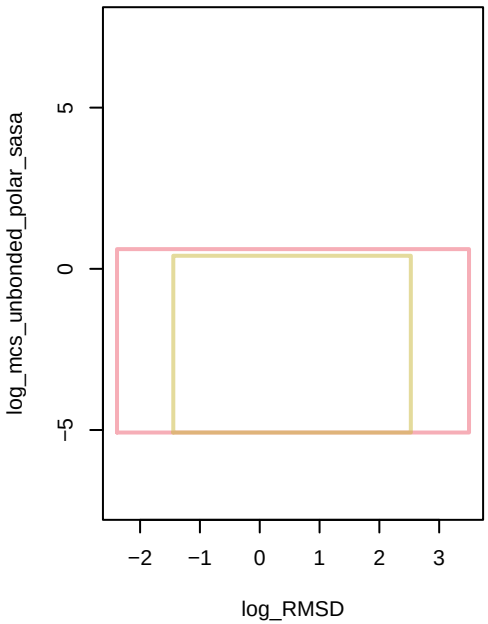
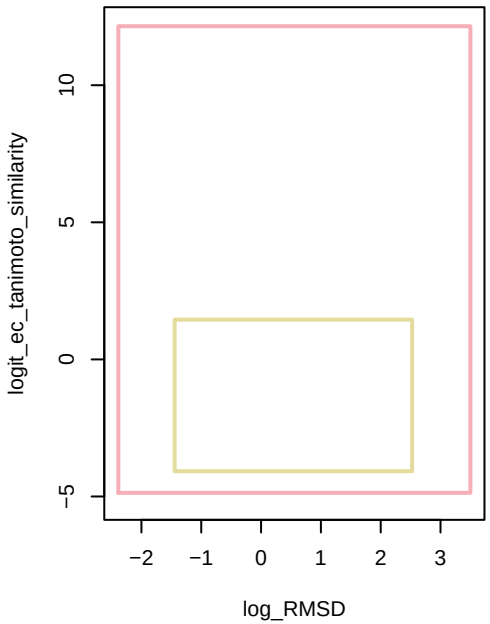
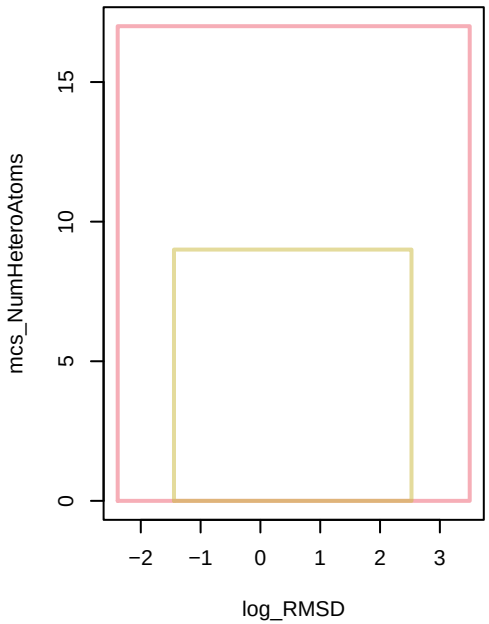
0.1
0.2
0.3
0.4
0
1
2
3
4
5
6
mcs_RingCount

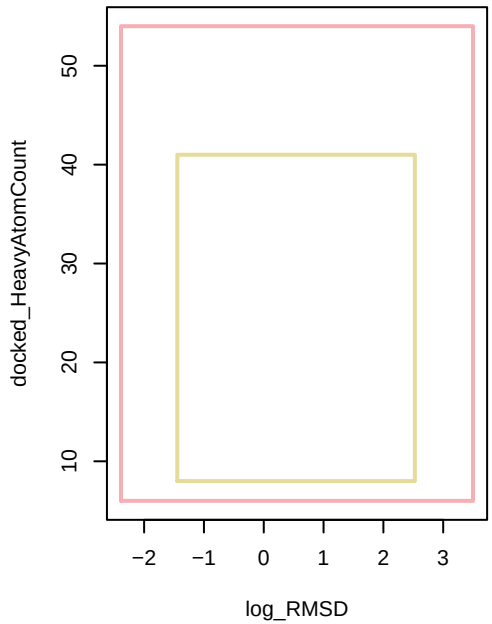

probability density
0.00
0.05
0.10
0.15
0
5
10
15
docked_NumRotatableBonds

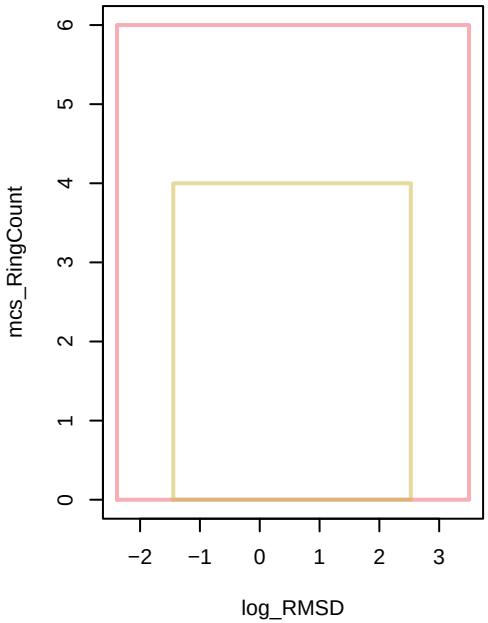

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
5
10
15
mcs_NOCount

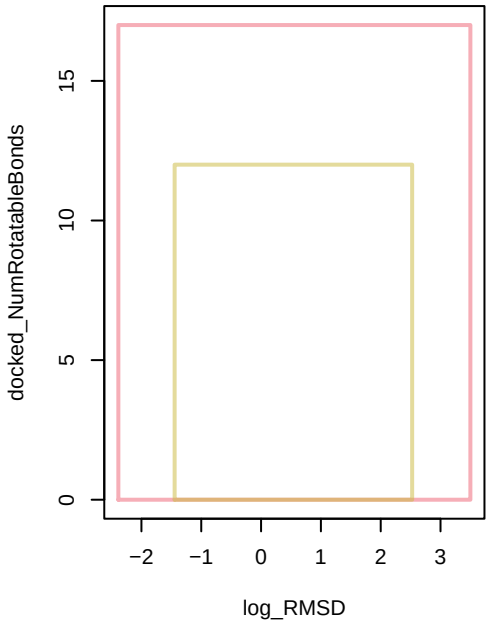

log_mcs_unbonded_polar_sasa
log_RMSD

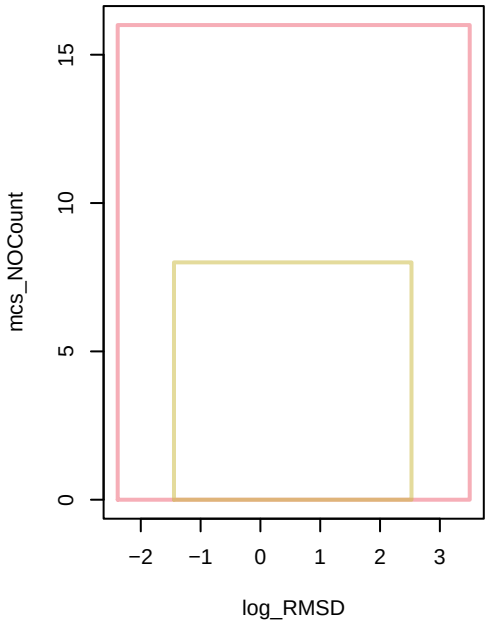

logit_ec_tanimoto_similarity
log_RMSD

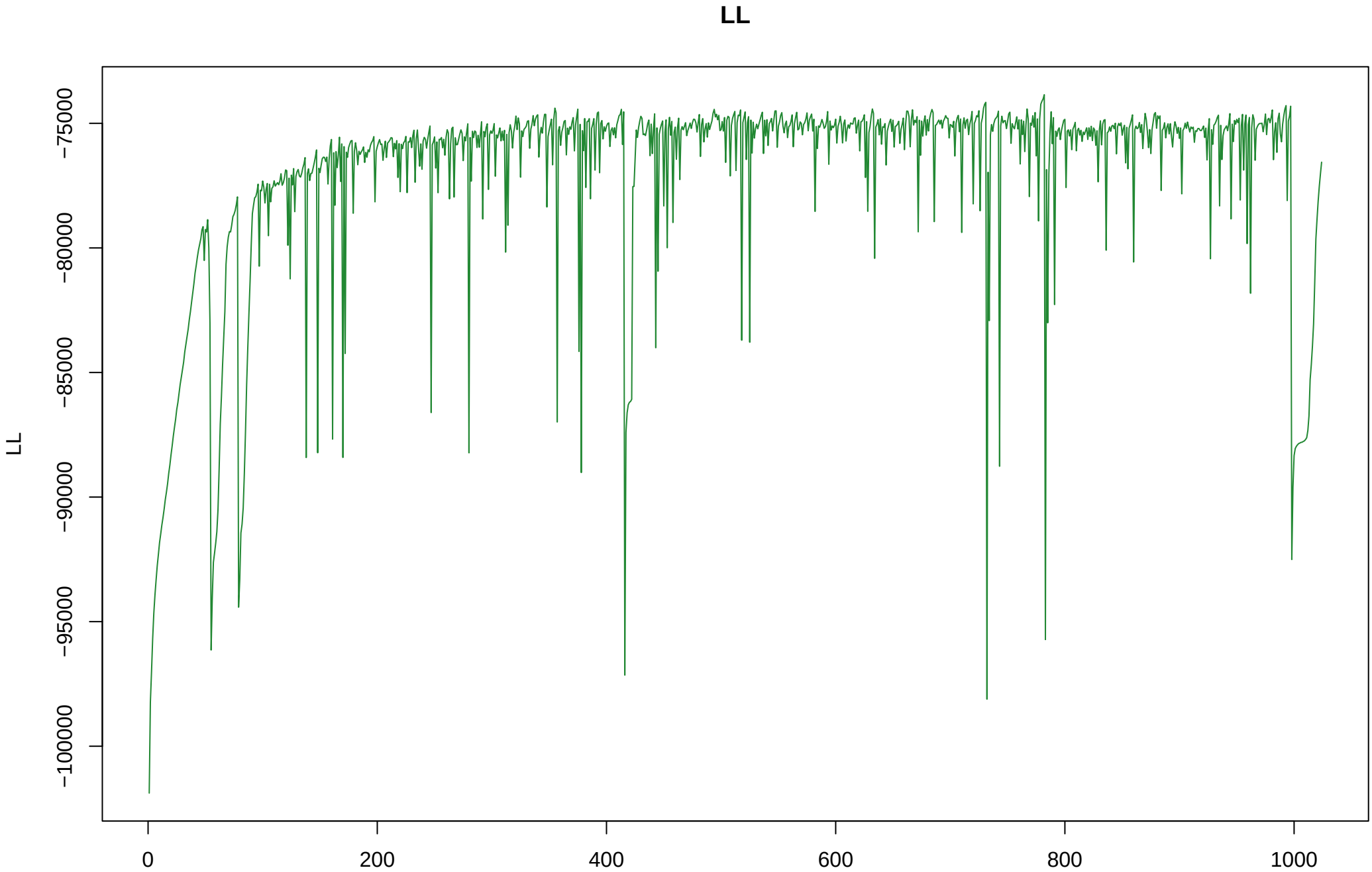

mcs_NumHeteroAtoms
log_RMSD

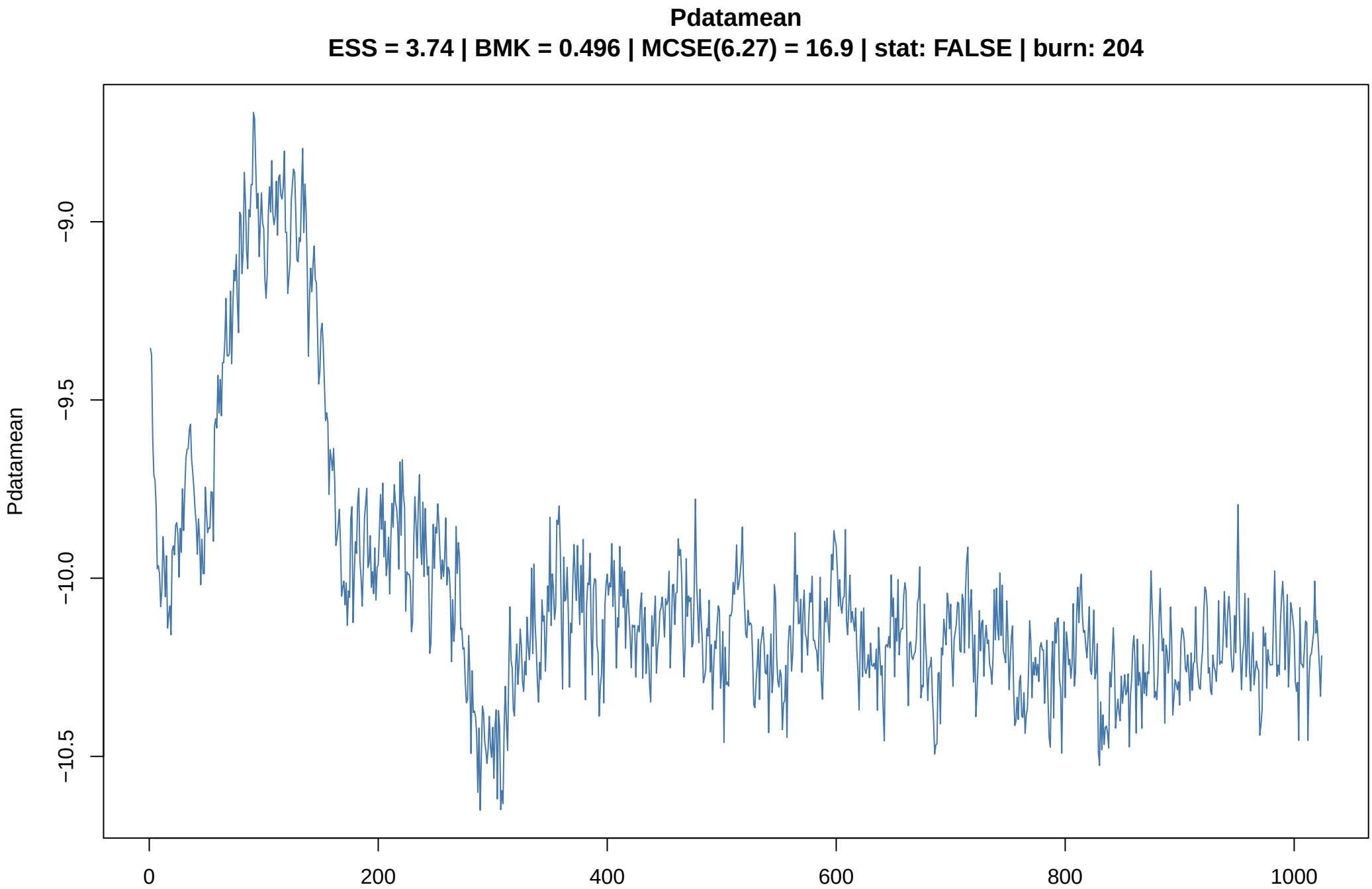

docked_HeavyAtomCount
log_RMSD

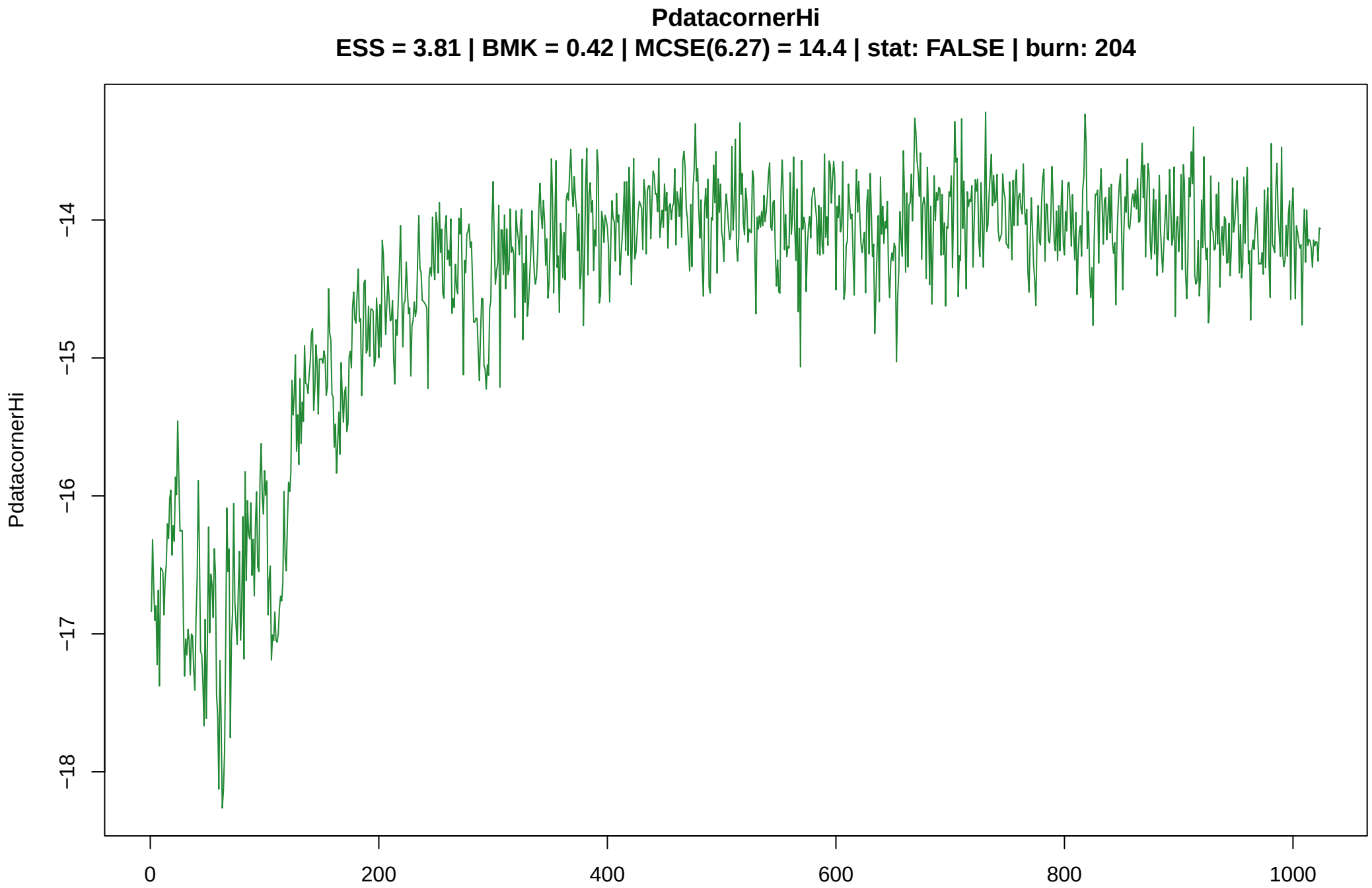

mcs_RingCount
log_RMSD

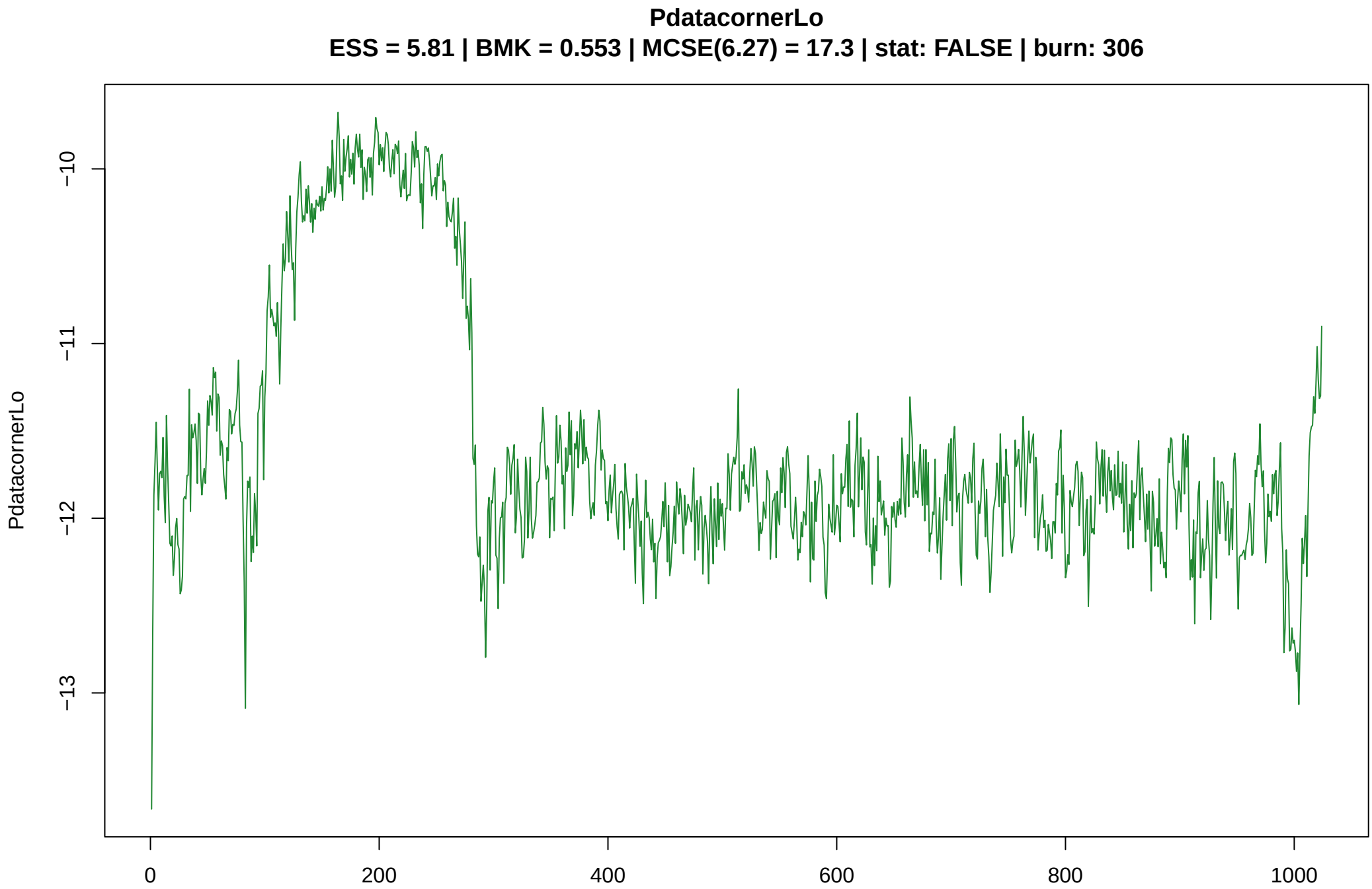

docked_NumRotatableBonds
log_RMSD

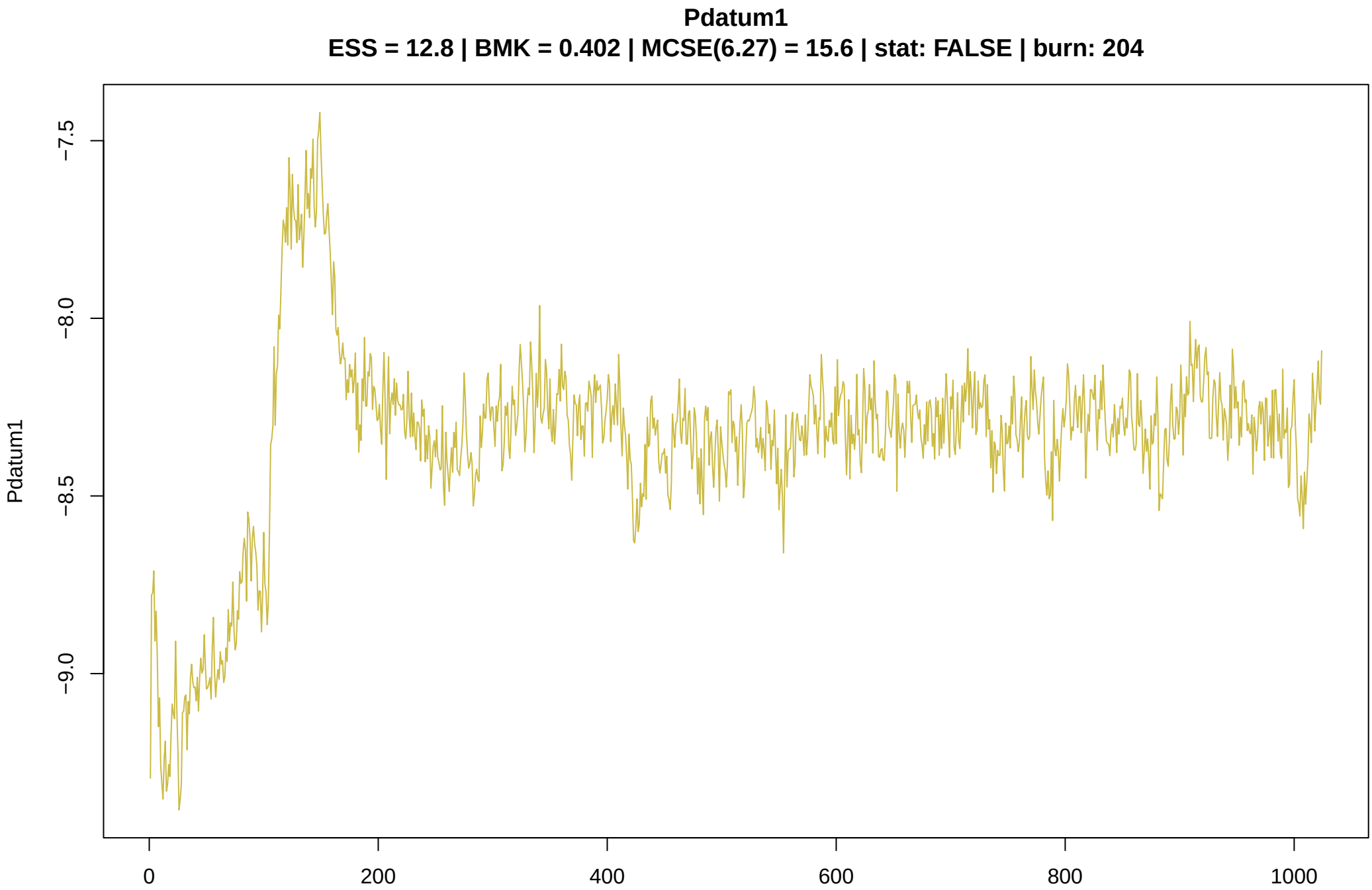

mcs_NOCount
log_RMSD

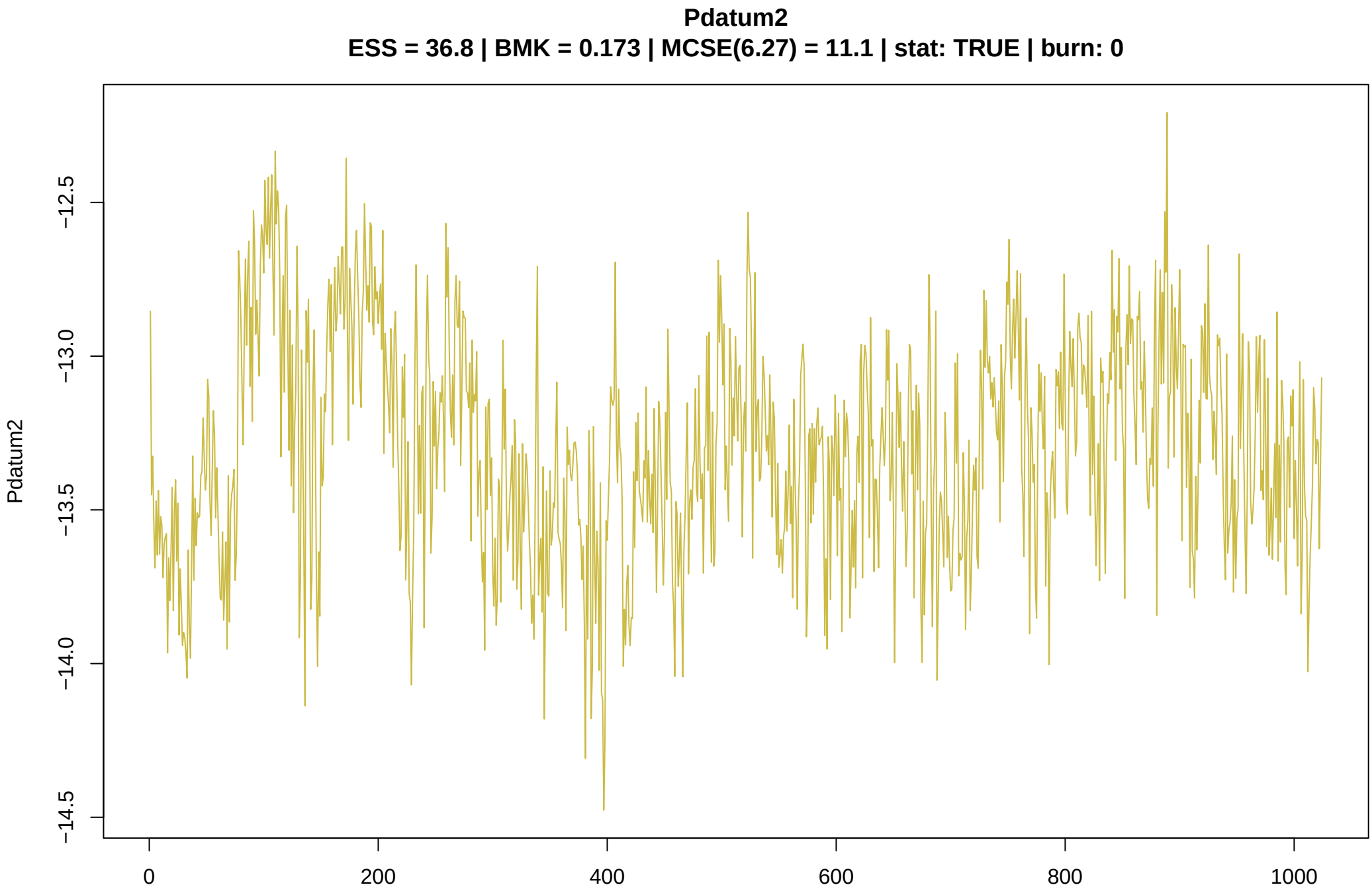

LL
LL
−75000
−80000
−85000
−90000
−95000
−100000
0
200
400
600
800
1000

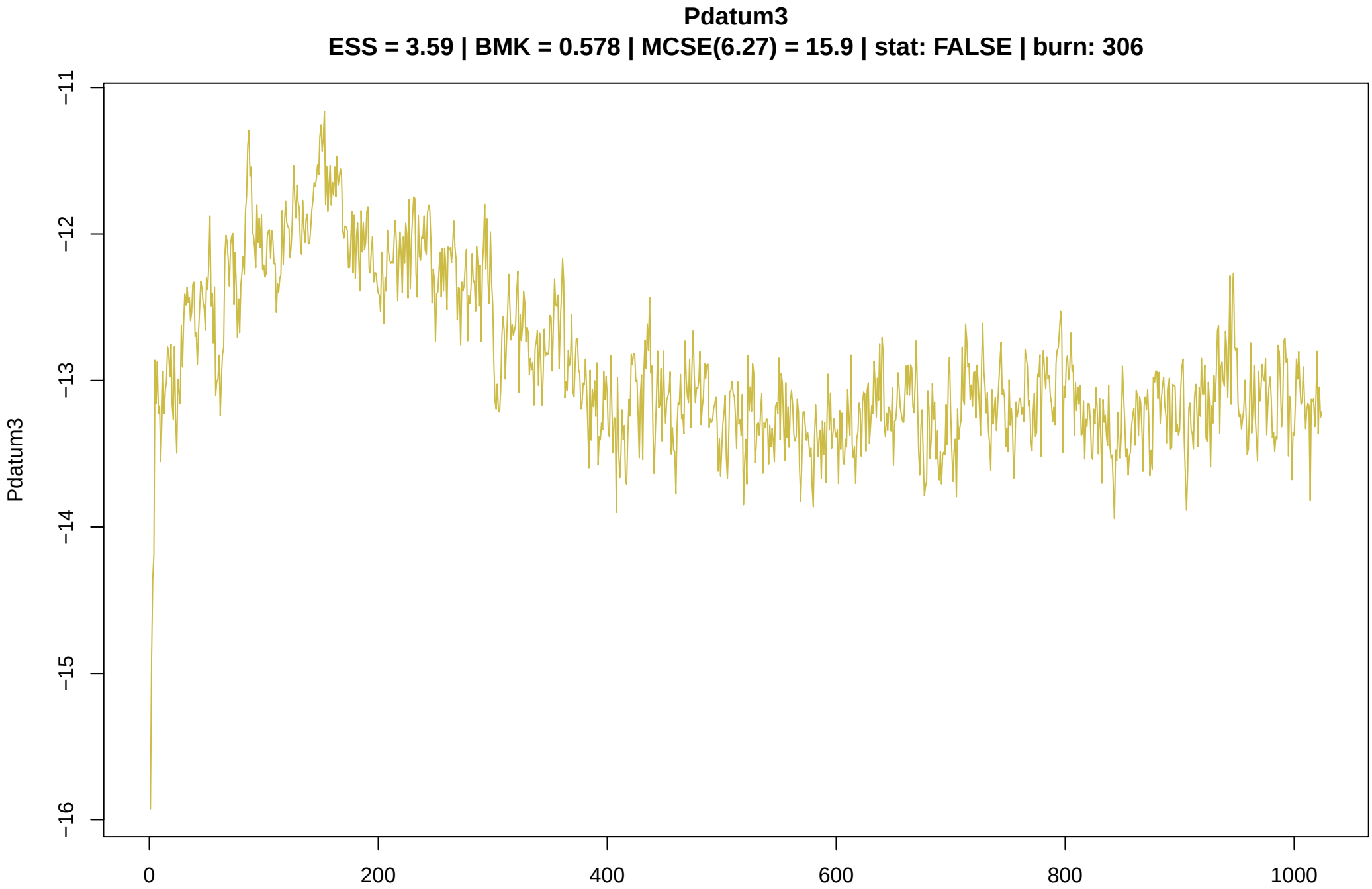

Pdatamean
ESS = 3.74 | BMK = 0.496 | MCSE(6.27) = 16.9 | stat: FALSE | burn: 204
Pdatamean
−9.0
−9.5
−10.0
−10.5
0
200
400
600
800
1000

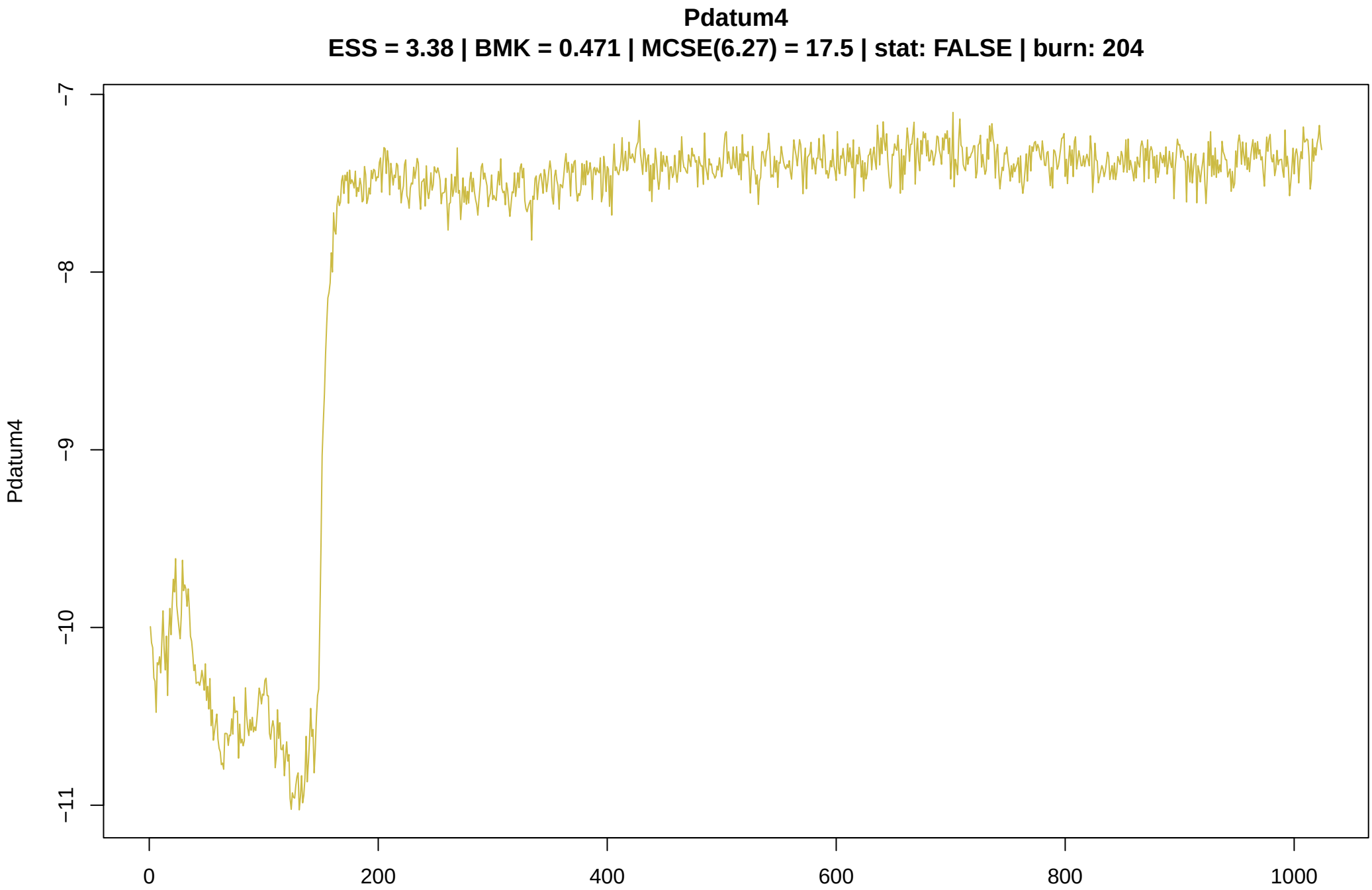

PdatacornerHi
ESS = 3.81 | BMK = 0.42 | MCSE(6.27) = 14.4 | stat: FALSE | burn: 204
PdatacornerHi
−14
−15
−16
−17
−18
0
200
400
600
800
1000

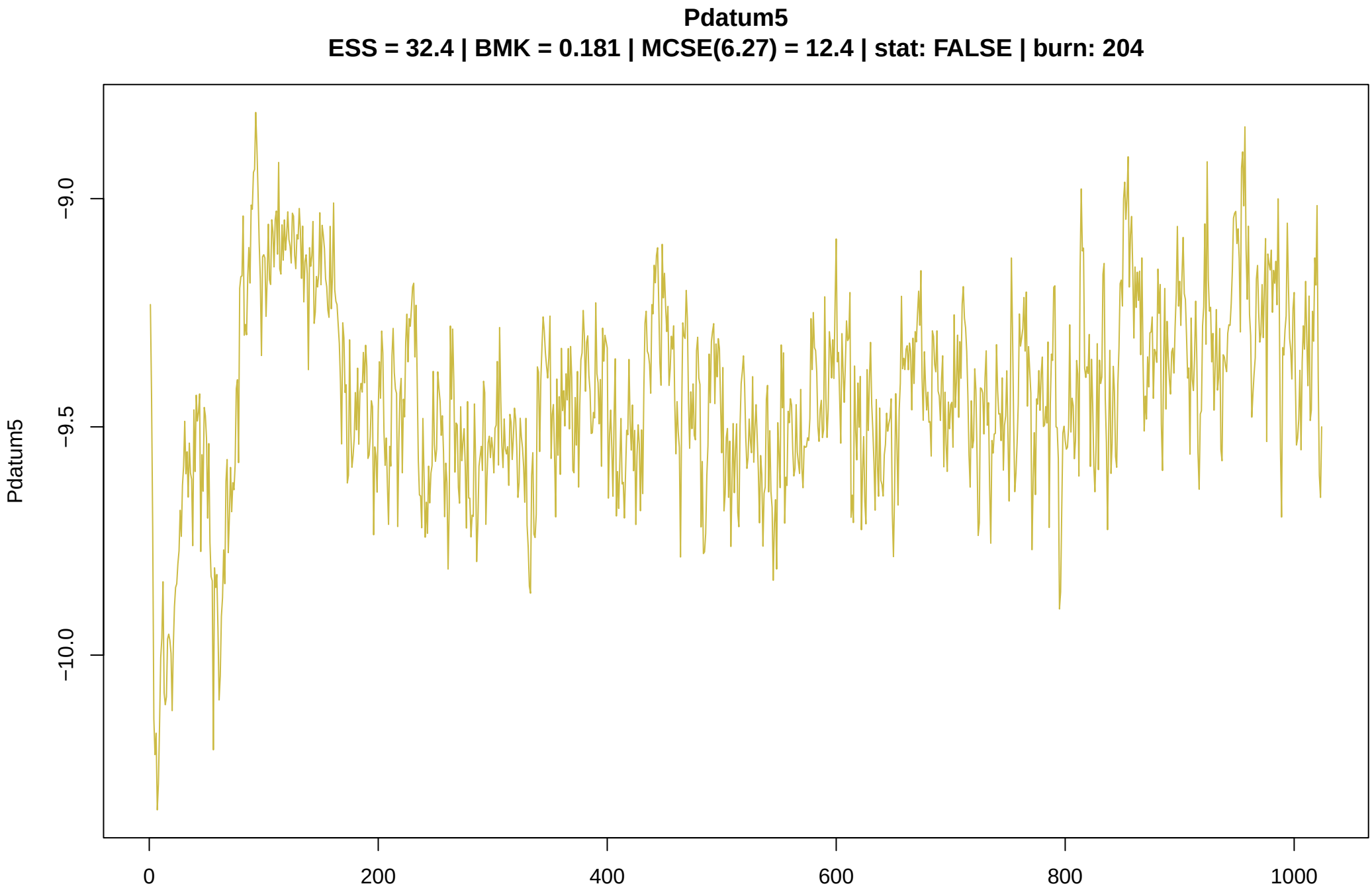

PdatacornerLo
ESS = 5.81 | BMK = 0.553 | MCSE(6.27) = 17.3 | stat: FALSE | burn: 306
PdatacornerLo
−10
−11
−12
−13
0
200
400
600
800
1000

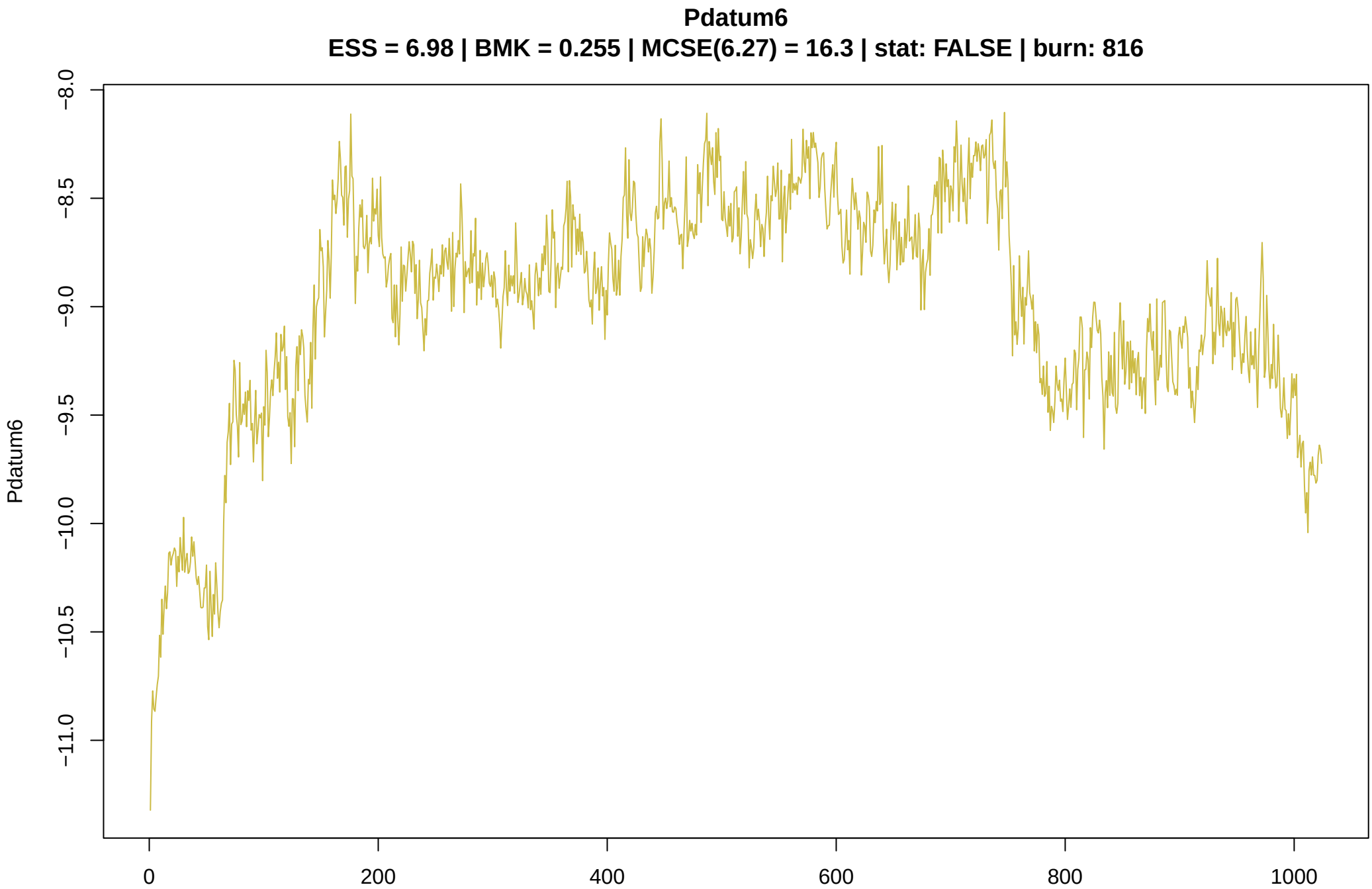

Pdatum1
ESS = 12.8 | BMK = 0.402 | MCSE(6.27) = 15.6 | stat: FALSE | burn: 204
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
200
400
600
800
1000

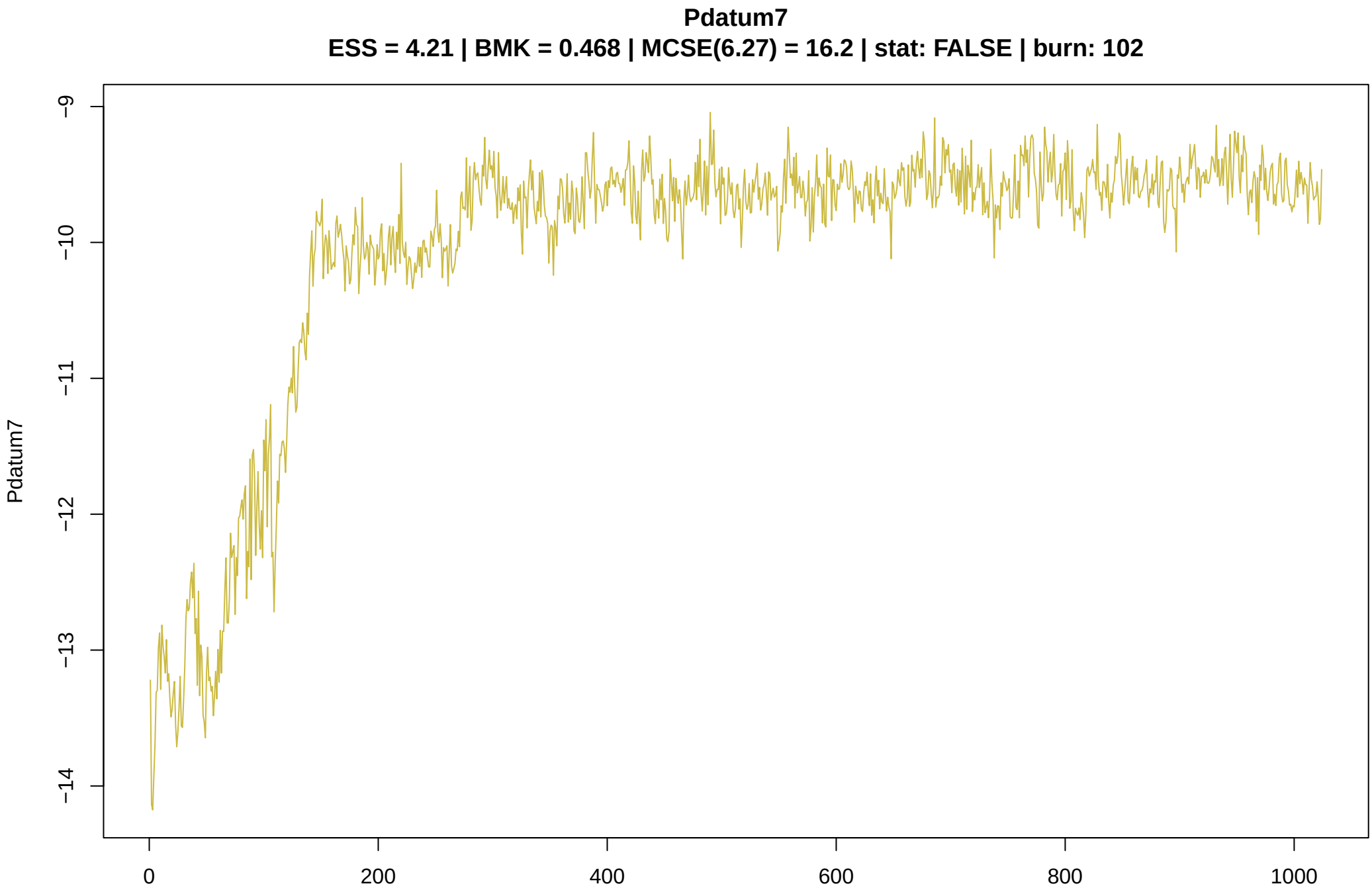

Pdatum2
ESS = 36.8 | BMK = 0.173 | MCSE(6.27) = 11.1 | stat: TRUE | burn: 0
Pdatum2
−12.5
−13.0
−13.5
−14.0
−14.5
0
200
400
600
800
1000

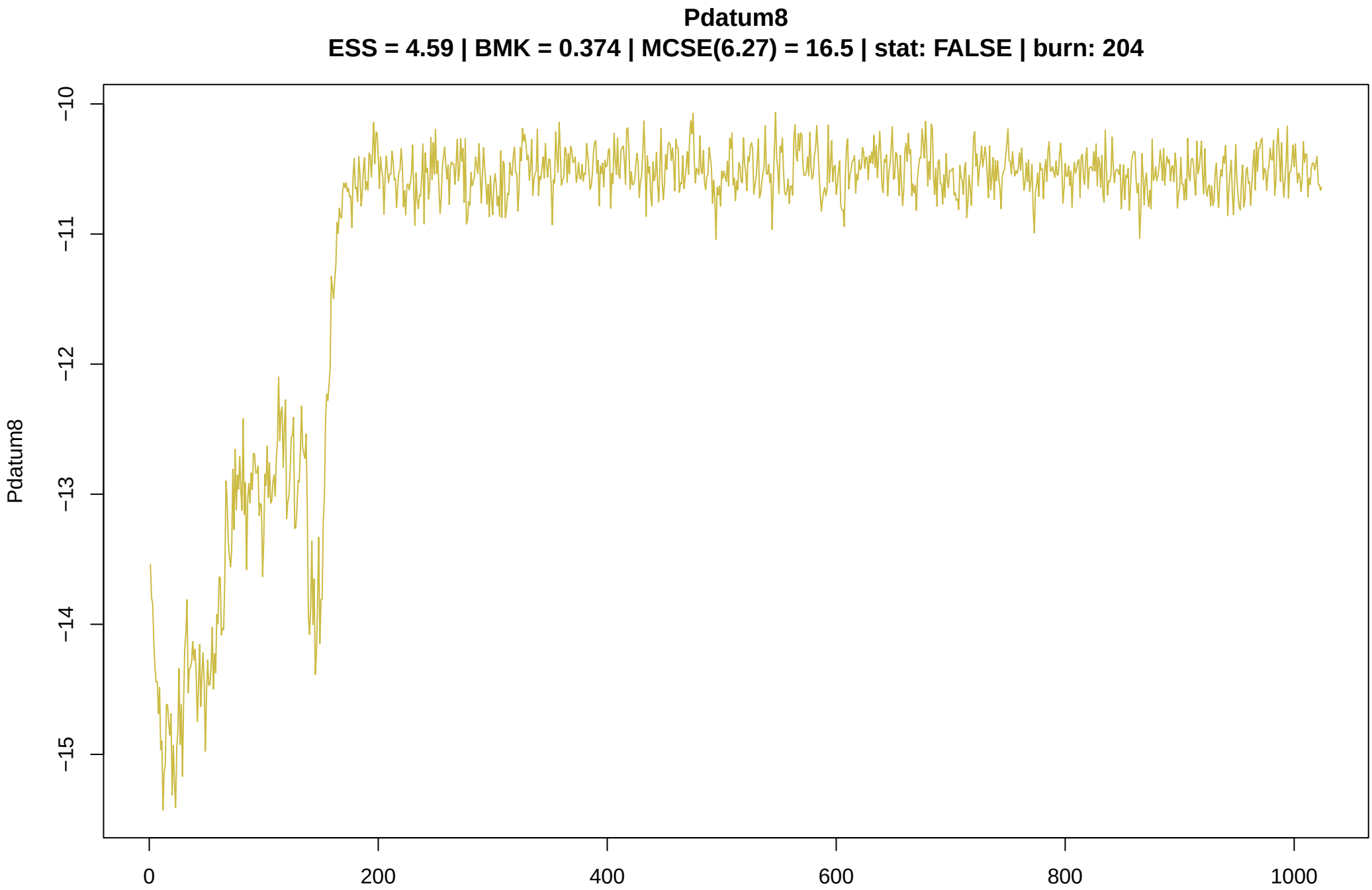

Pdatum3
ESS = 3.59 | BMK = 0.578 | MCSE(6.27) = 15.9 | stat: FALSE | burn: 306
Pdatum3
−11
−12
−13
−14
−15
−16
0
200
400
600
800
1000

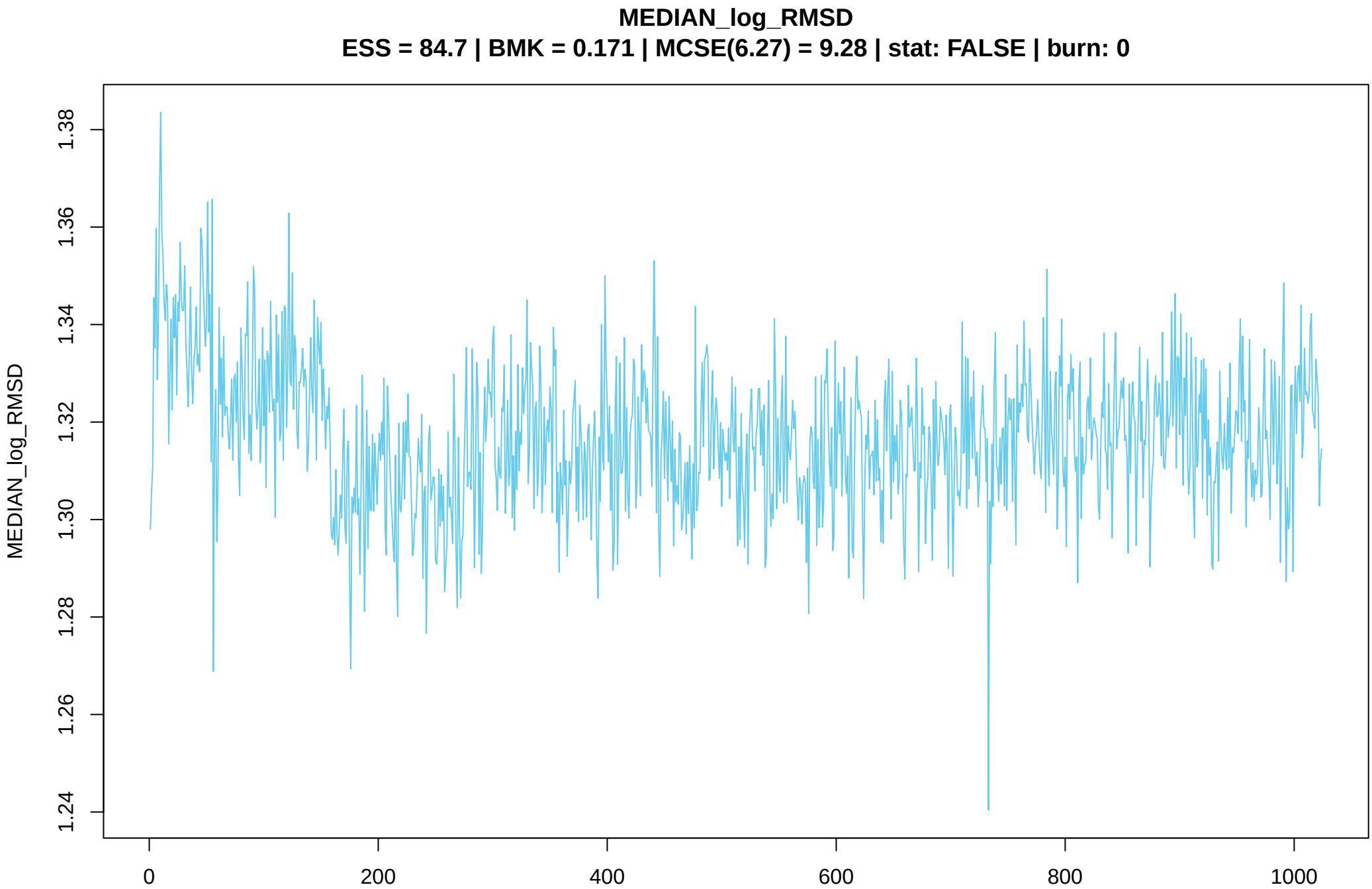

Pdatum4
ESS = 3.38 | BMK = 0.471 | MCSE(6.27) = 17.5 | stat: FALSE | burn: 204
Pdatum4
−7
−8
−9
−10
−11
0
200
400
600
800
1000

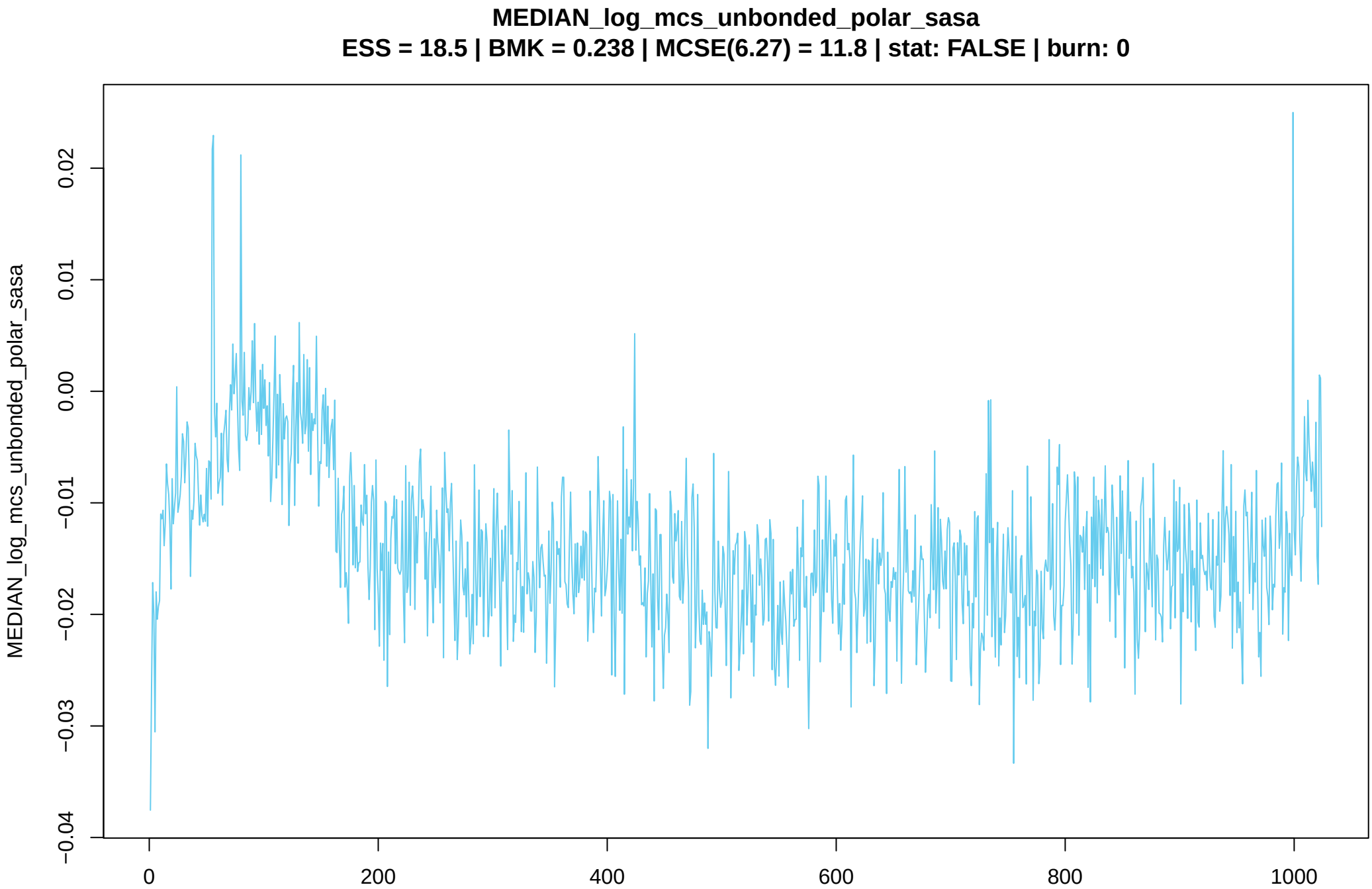

Pdatum5
ESS = 32.4 | BMK = 0.181 | MCSE(6.27) = 12.4 | stat: FALSE | burn: 204
Pdatum5
−9.0
−9.5
−10.0
0
200
400
600
800
1000

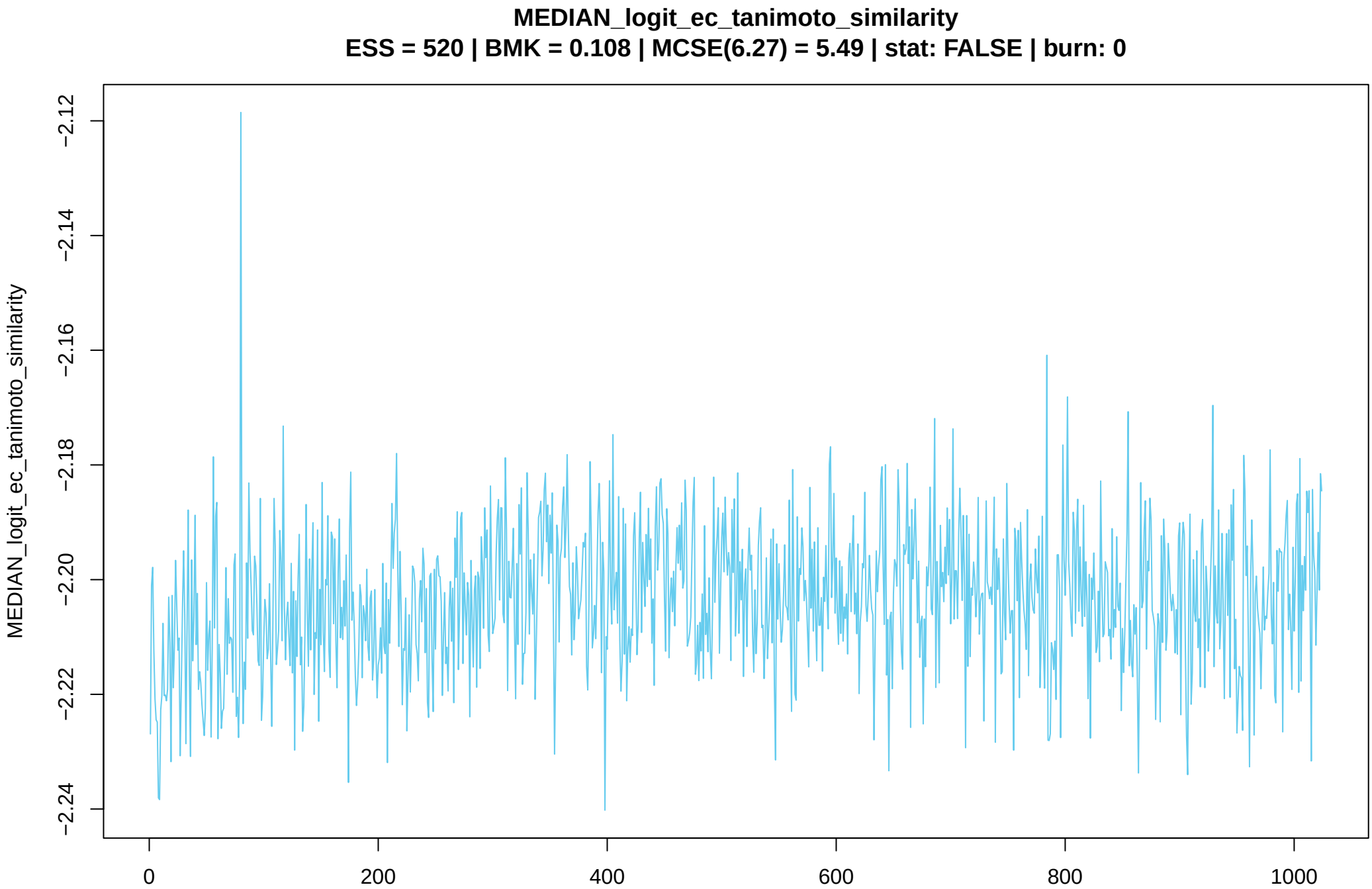

Pdatum6
ESS = 6.98 | BMK = 0.255 | MCSE(6.27) = 16.3 | stat: FALSE | burn: 816
Pdatum6
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
0
200
400
600
800
1000

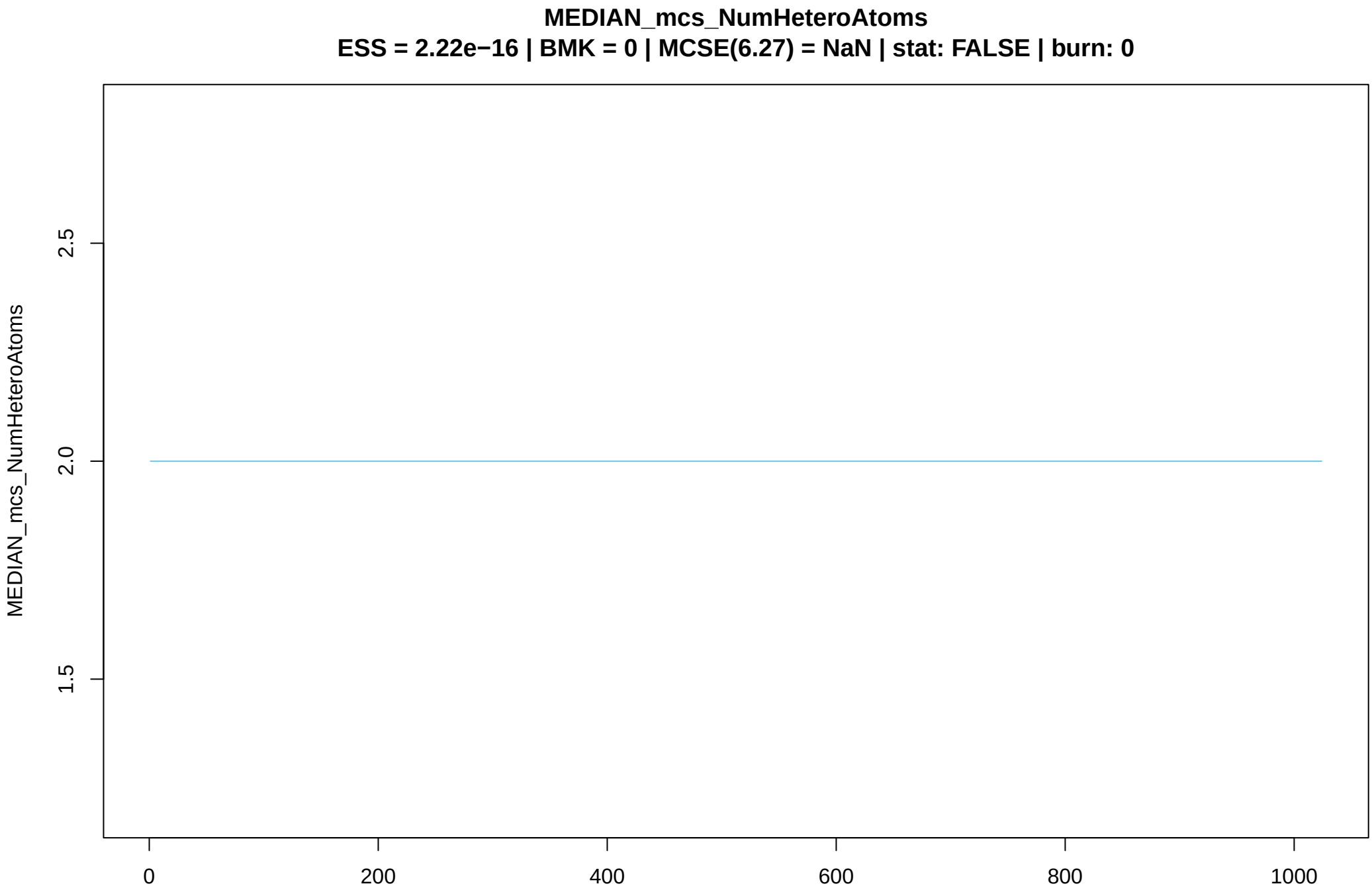

Pdatum7
ESS = 4.21 | BMK = 0.468 | MCSE(6.27) = 16.2 | stat: FALSE | burn: 102
Pdatum7
−9
−10
−11
−12
−13
−14
0
200
400
600
800
1000

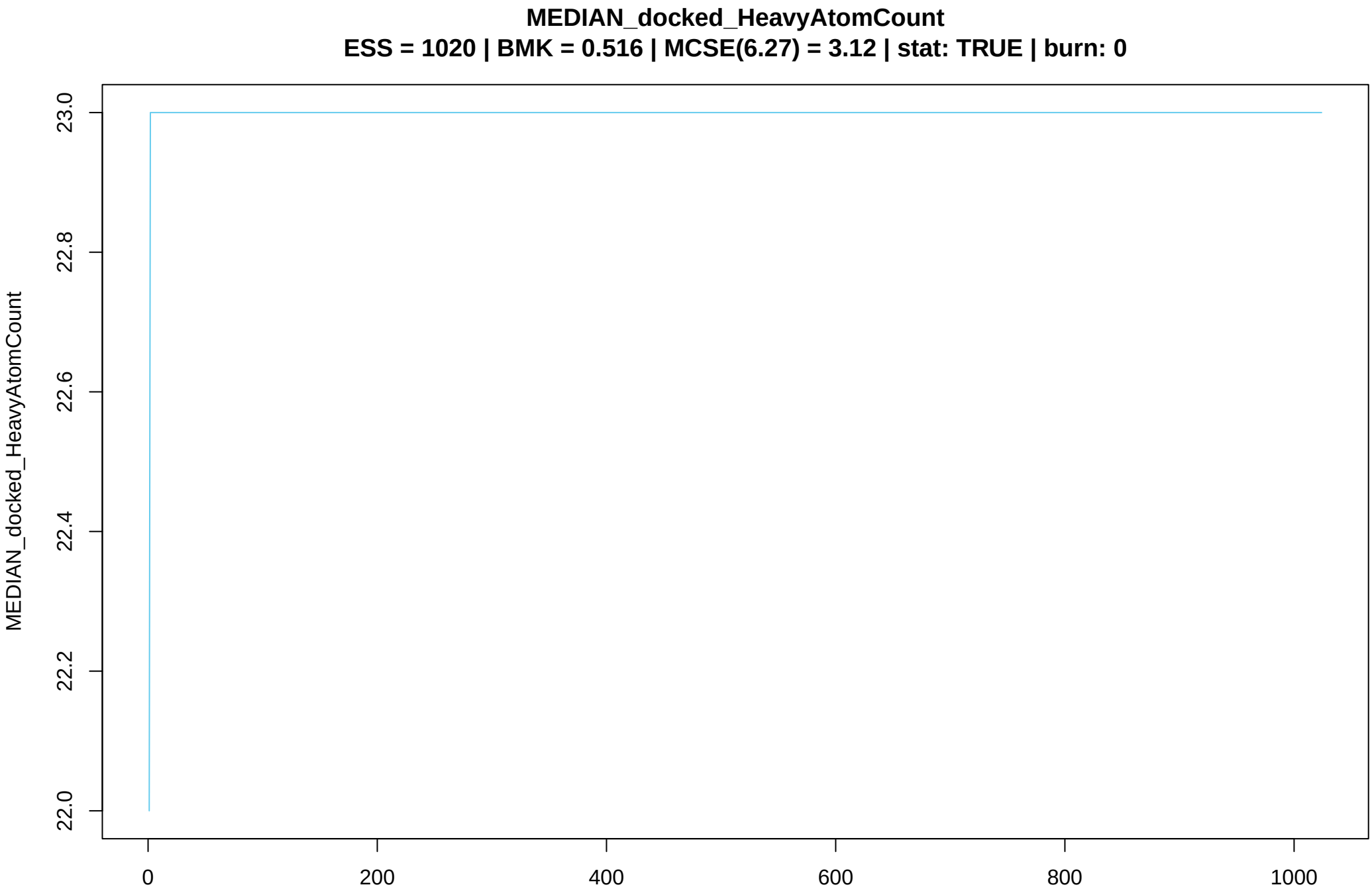

Pdatum8
ESS = 4.59 | BMK = 0.374 | MCSE(6.27) = 16.5 | stat: FALSE | burn: 204
Pdatum8
−10
−11
−12
−13
−14
−15
0
200
400
600
800
1000

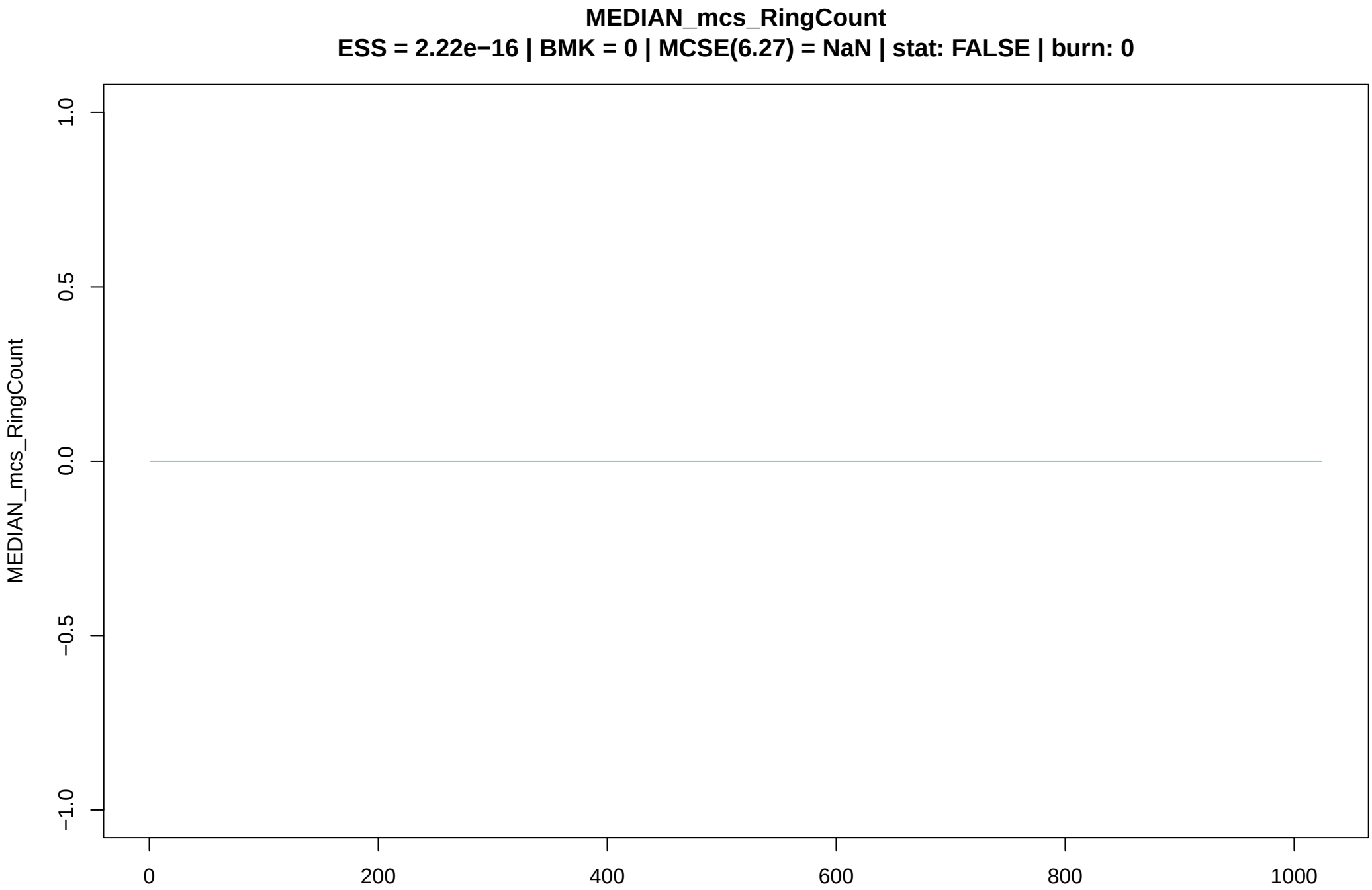

MEDIAN_log_RMSD
ESS = 84.7 | BMK = 0.171 | MCSE(6.27) = 9.28 | stat: FALSE | burn: 0
MEDIAN_log_RMSD
1.24
1.26
1.28
1.30
1.32
1.34
1.36
1.38
0
200
400
600
800
1000

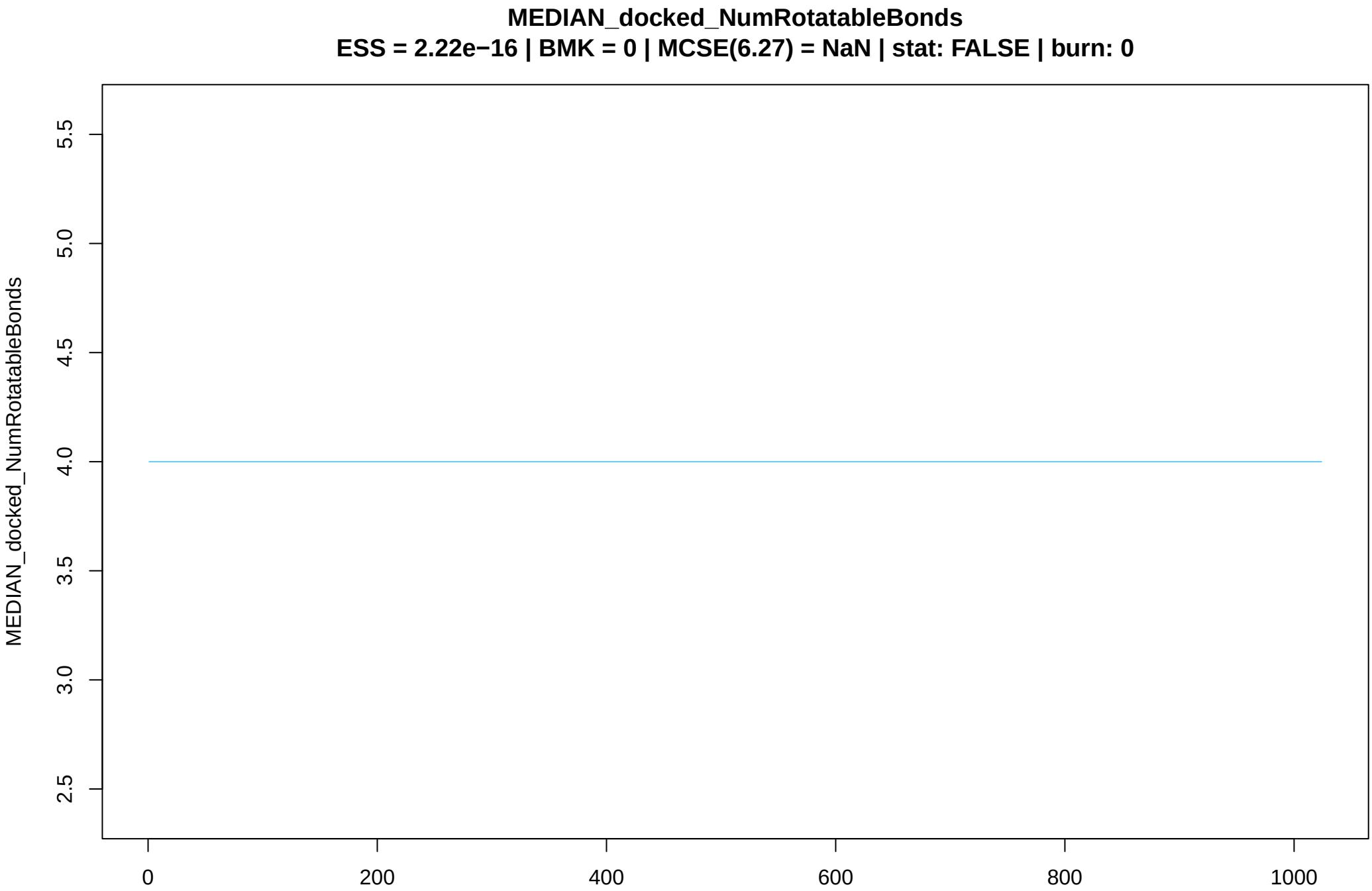

MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 18.5 | BMK = 0.238 | MCSE(6.27) = 11.8 | stat: FALSE | burn: 0
MEDIAN_log_mcs_unbonded_polar_sasa
0.02
0.01
0.00
−0.01
−0.02
−0.03
−0.04
0
200
400
600
800
1000

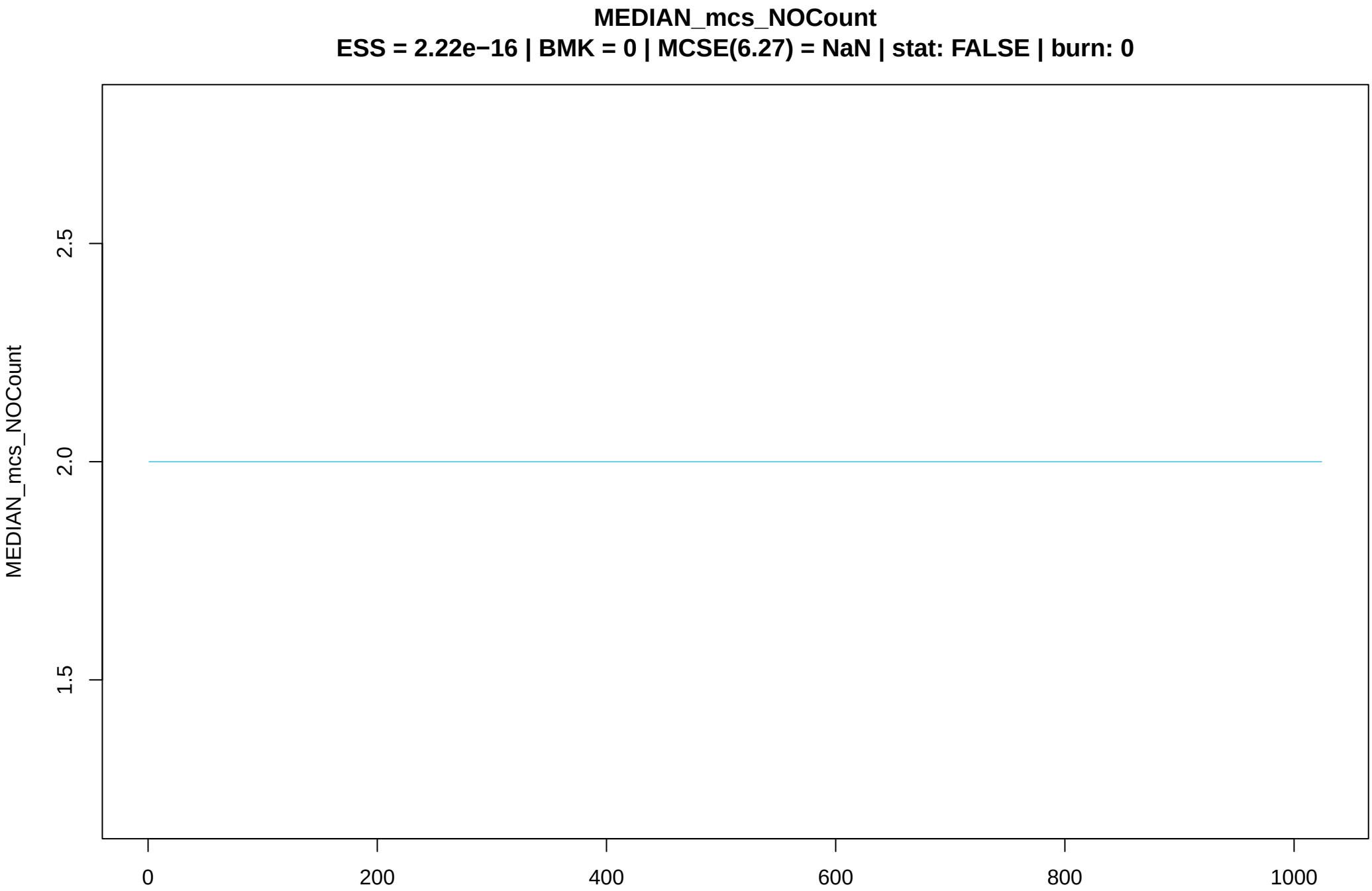

MEDIAN_logit_ec_tanimoto_similarity
ESS = 520 | BMK = 0.108 | MCSE(6.27) = 5.49 | stat: FALSE | burn: 0
MEDIAN_logit_ec_tanimoto_similarity
−2.12
−2.14
−2.16
−2.18
−2.20
−2.22
−2.24
0
200
400
600
800
1000

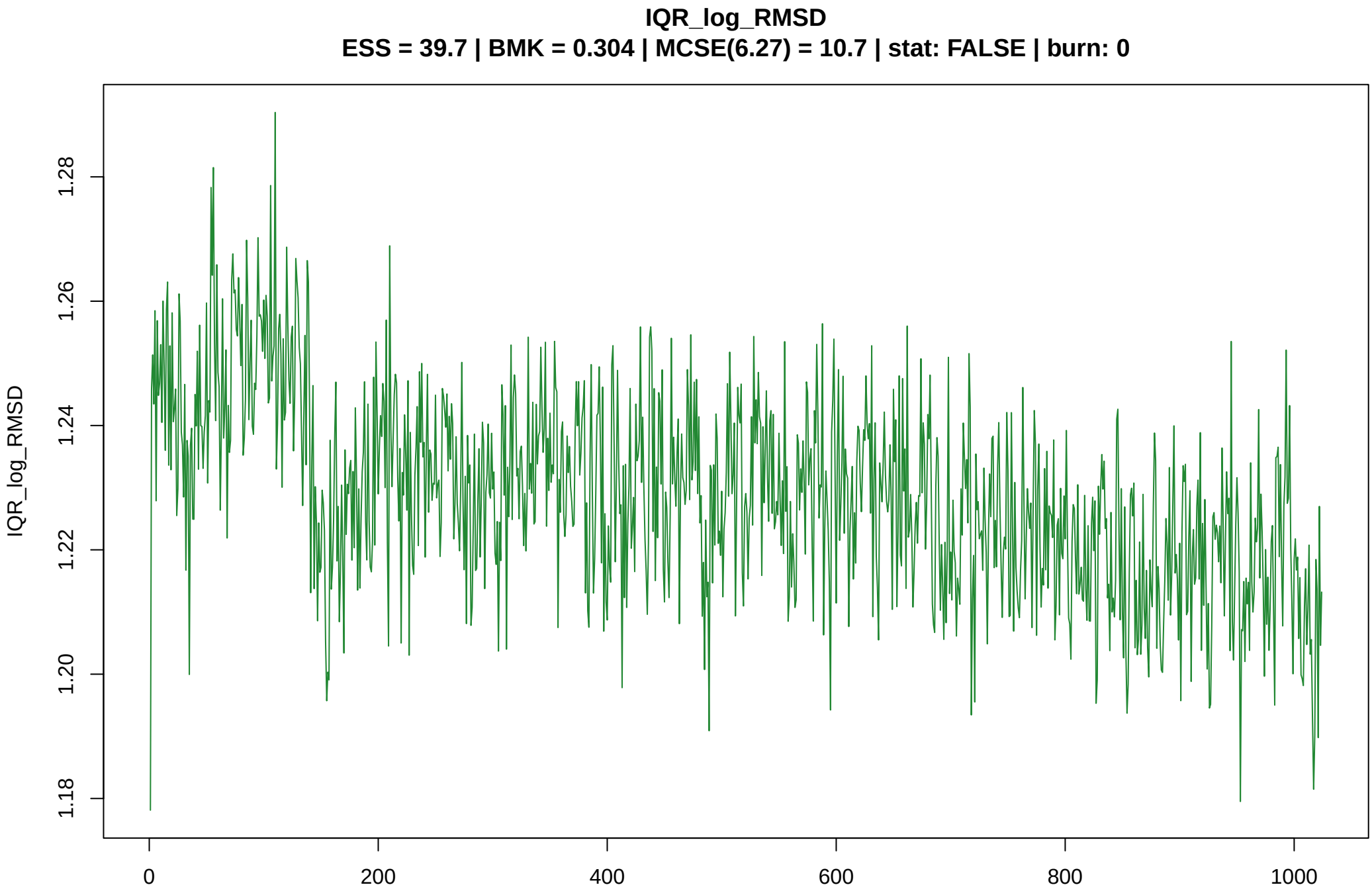

MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
1.5
2.0
2.5
0
200
400
600
800
1000

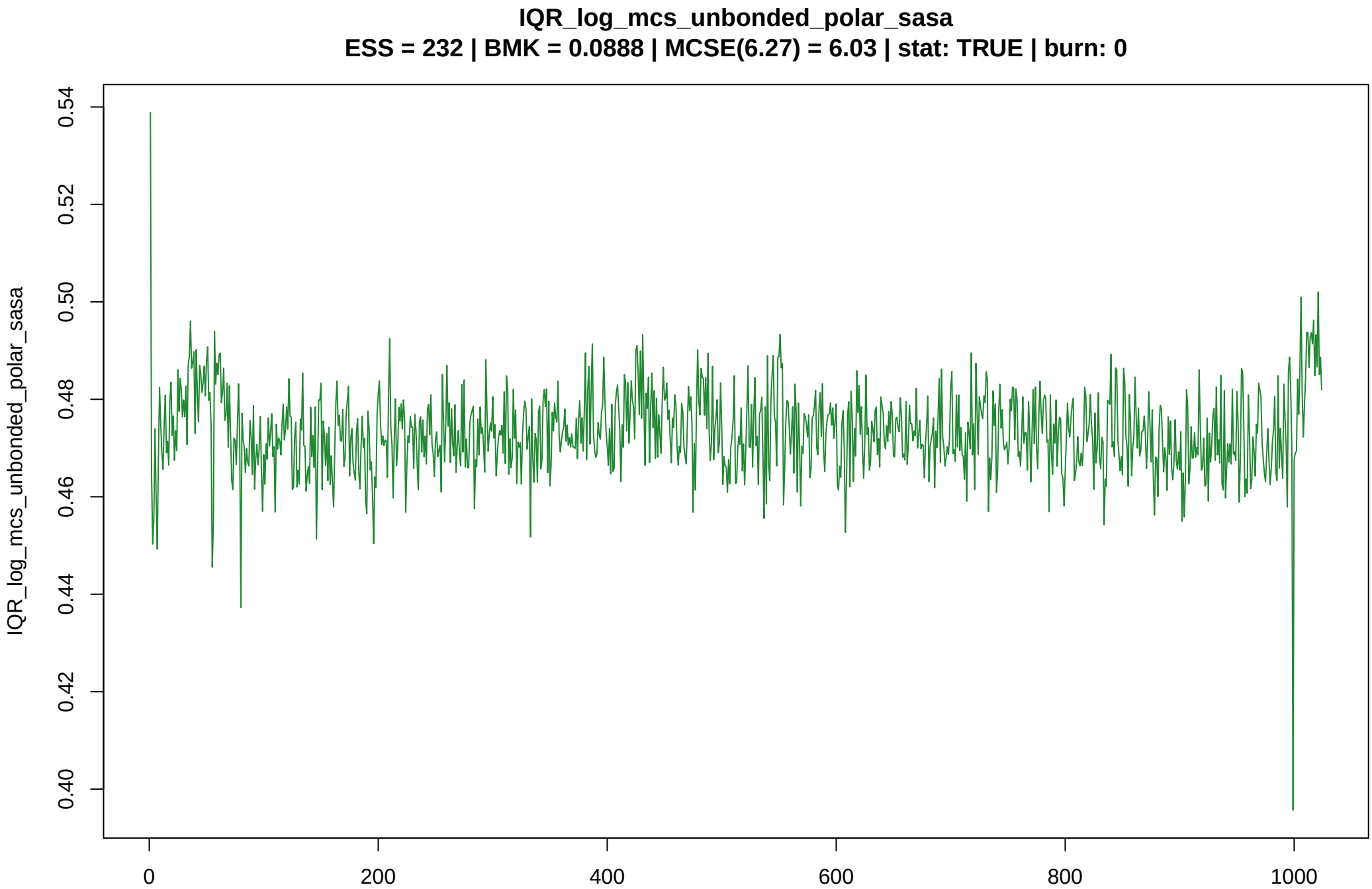

MEDIAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.516 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0
MEDIAN_docked_HeavyAtomCount
22.0
22.2
22.4
22.6
22.8
23.0
0
200
400
600
800
1000

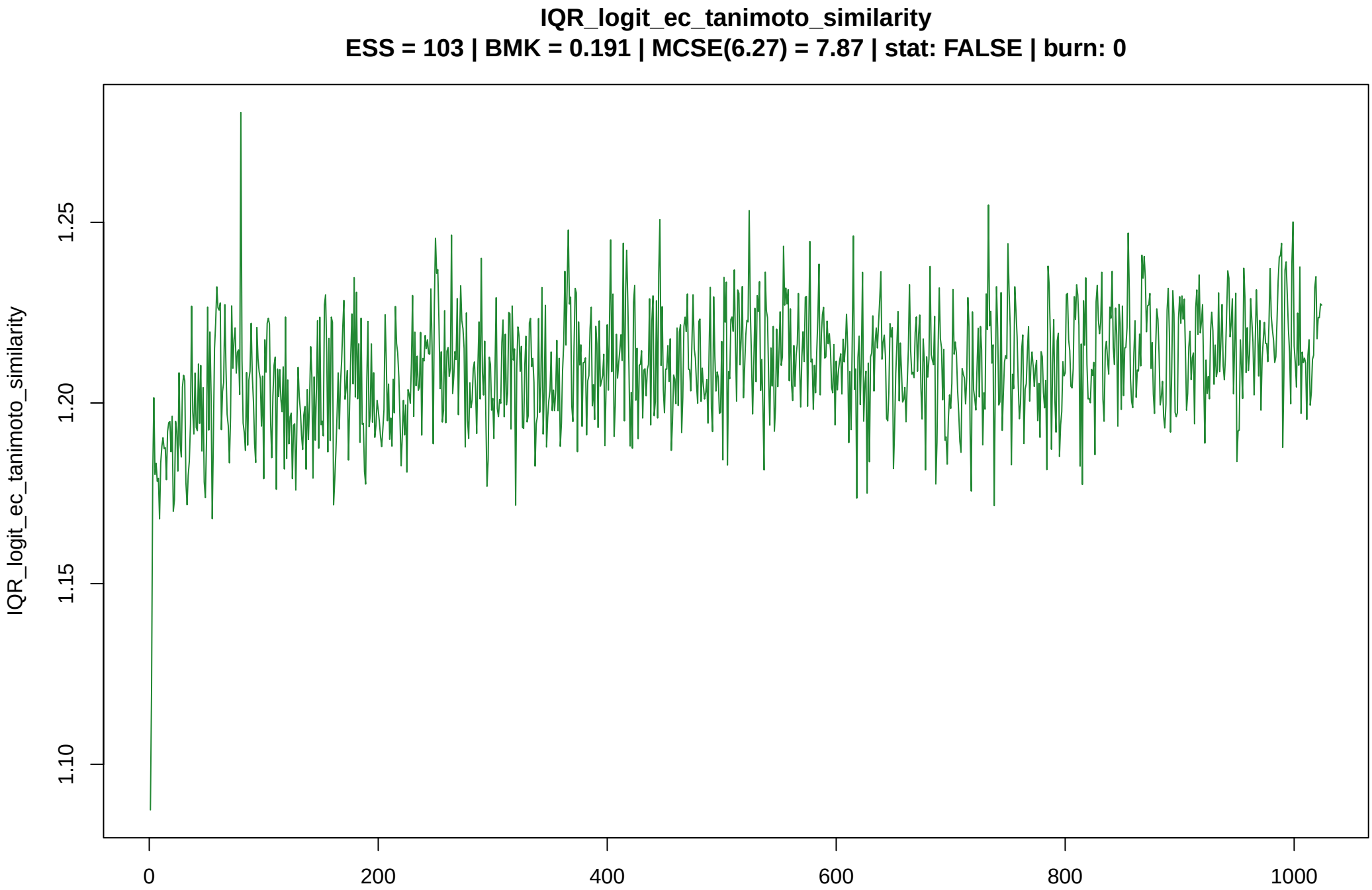

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
200
400
600
800
1000

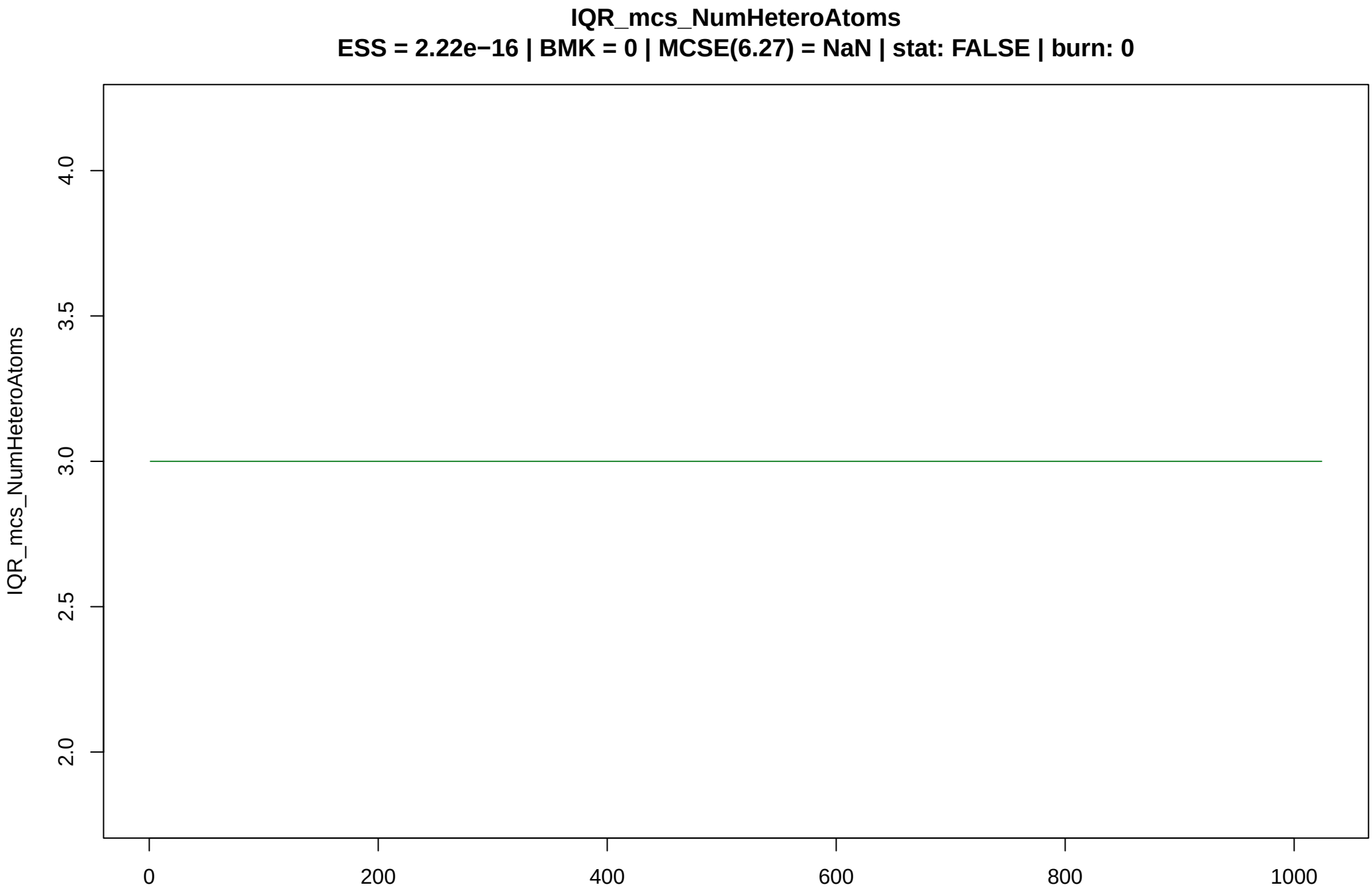

MEDIAN_docked_NumRotatableBonds
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_docked_NumRotatableBonds
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
200
400
600
800
1000

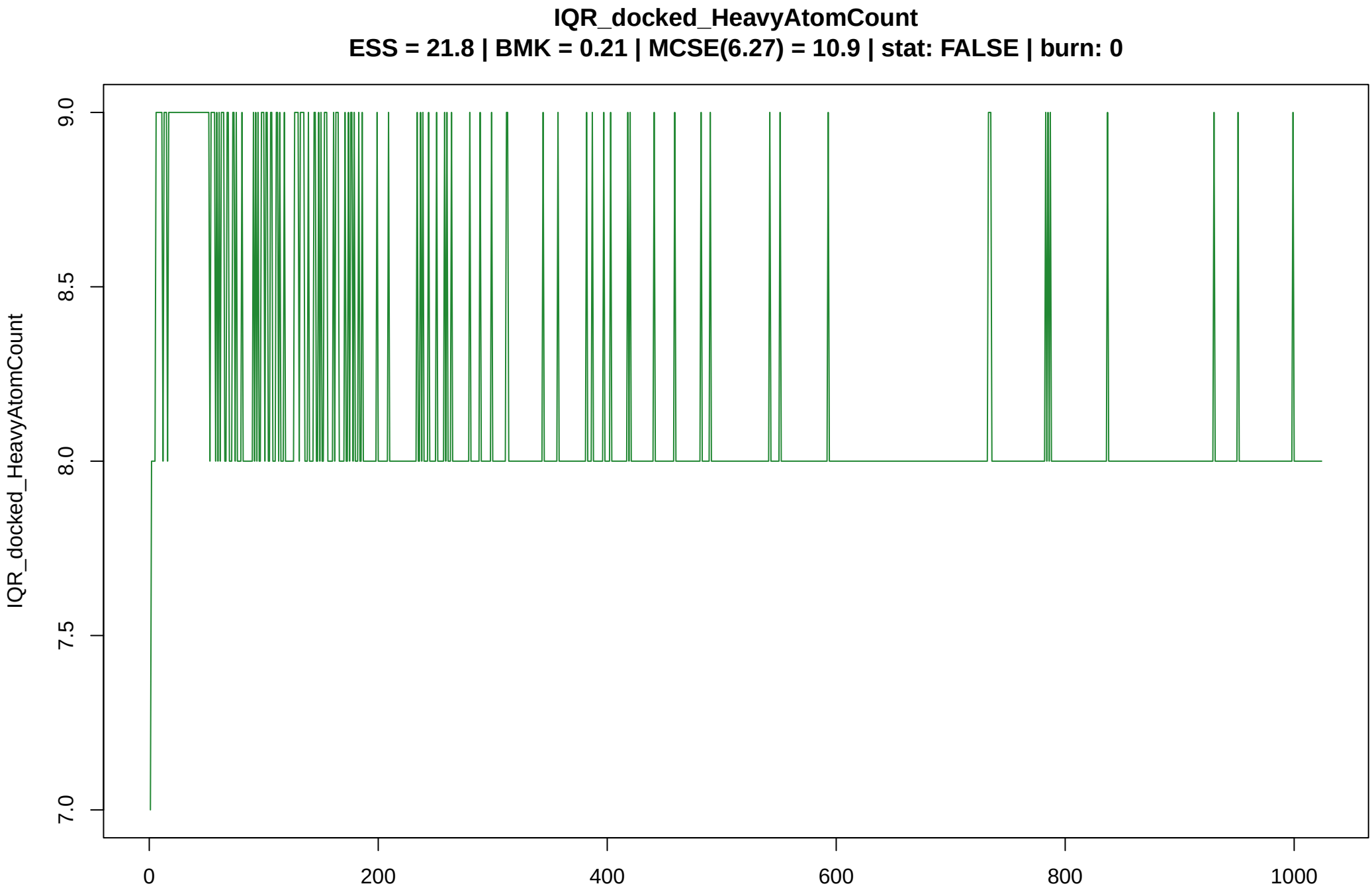

MEDIAN_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NOCount
2.5
2.0
1.5
0
200
400
600
800
1000

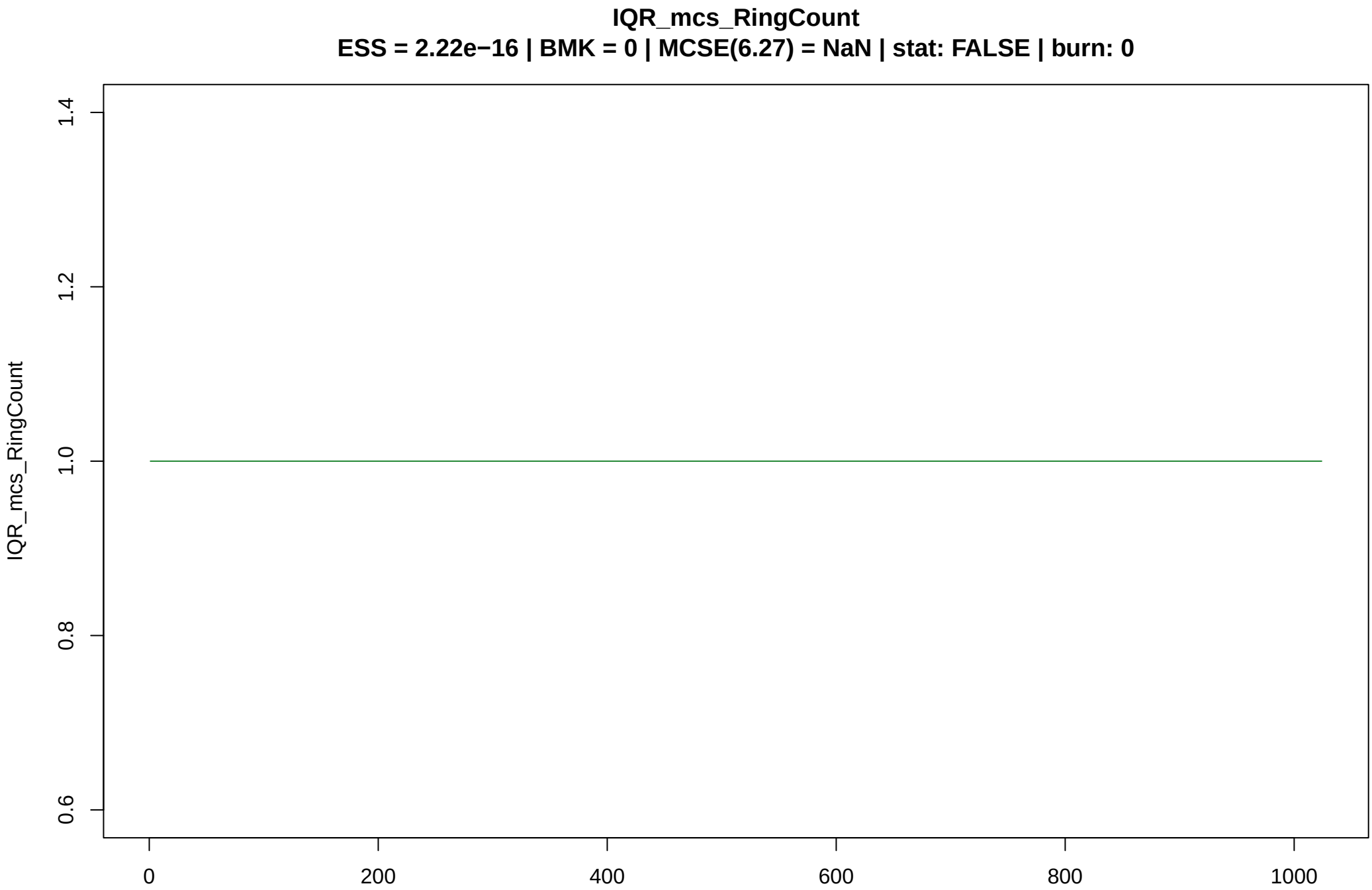

IQR_log_RMSD
ESS = 39.7 | BMK = 0.304 | MCSE(6.27) = 10.7 | stat: FALSE | burn: 0
IQR_log_RMSD
1.18
1.20
1.22
1.24
1.26
1.28
0
200
400
600
800
1000

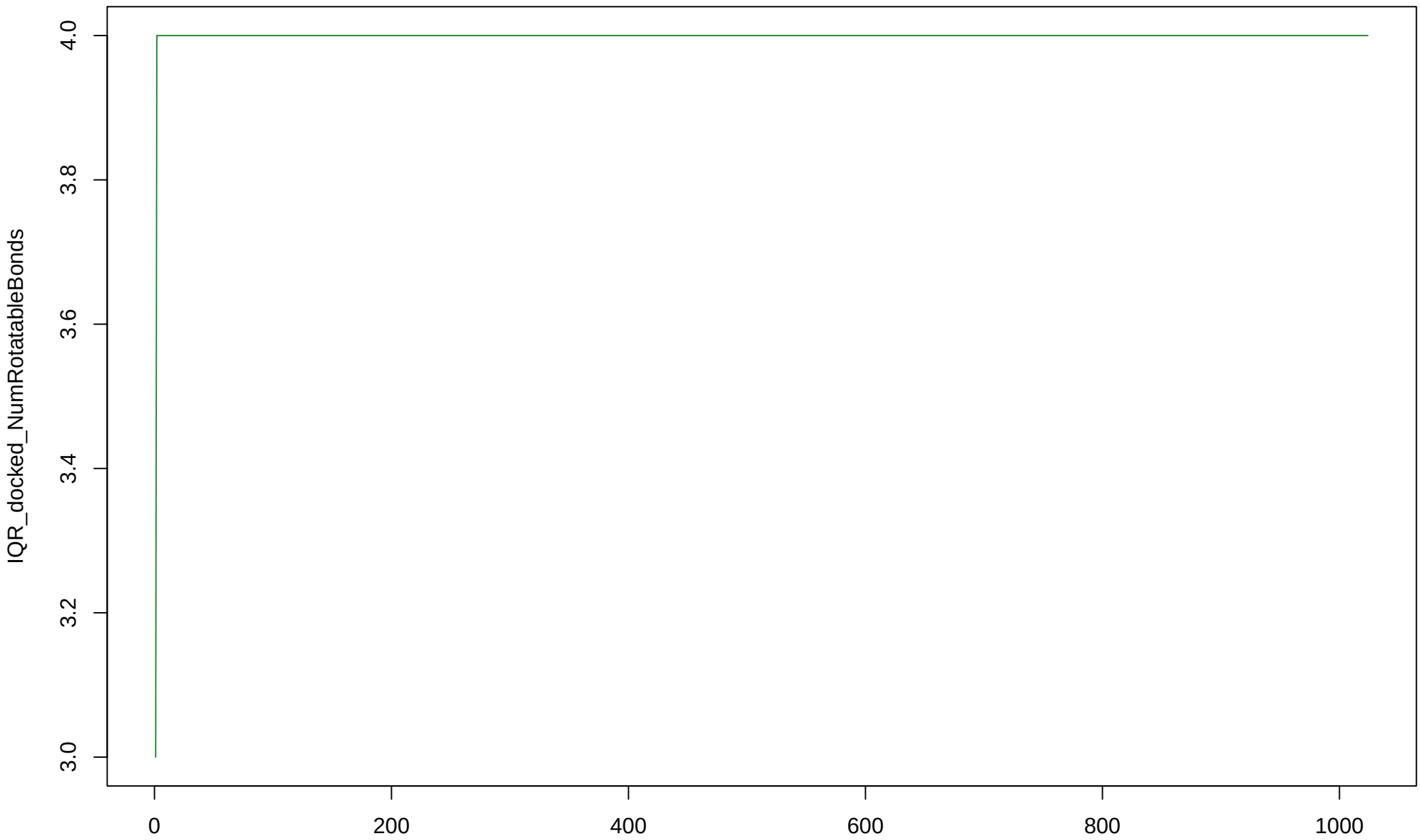

IQR_log_mcs_unbonded_polar_sasa
ESS = 232 | BMK = 0.0888 | MCSE(6.27) = 6.03 | stat: TRUE | burn: 0
IQR_log_mcs_unbonded_polar_sasa
0.40
0.42
0.44
0.46
0.48
0.50
0.52
0.54
0
200
400
600
800
1000

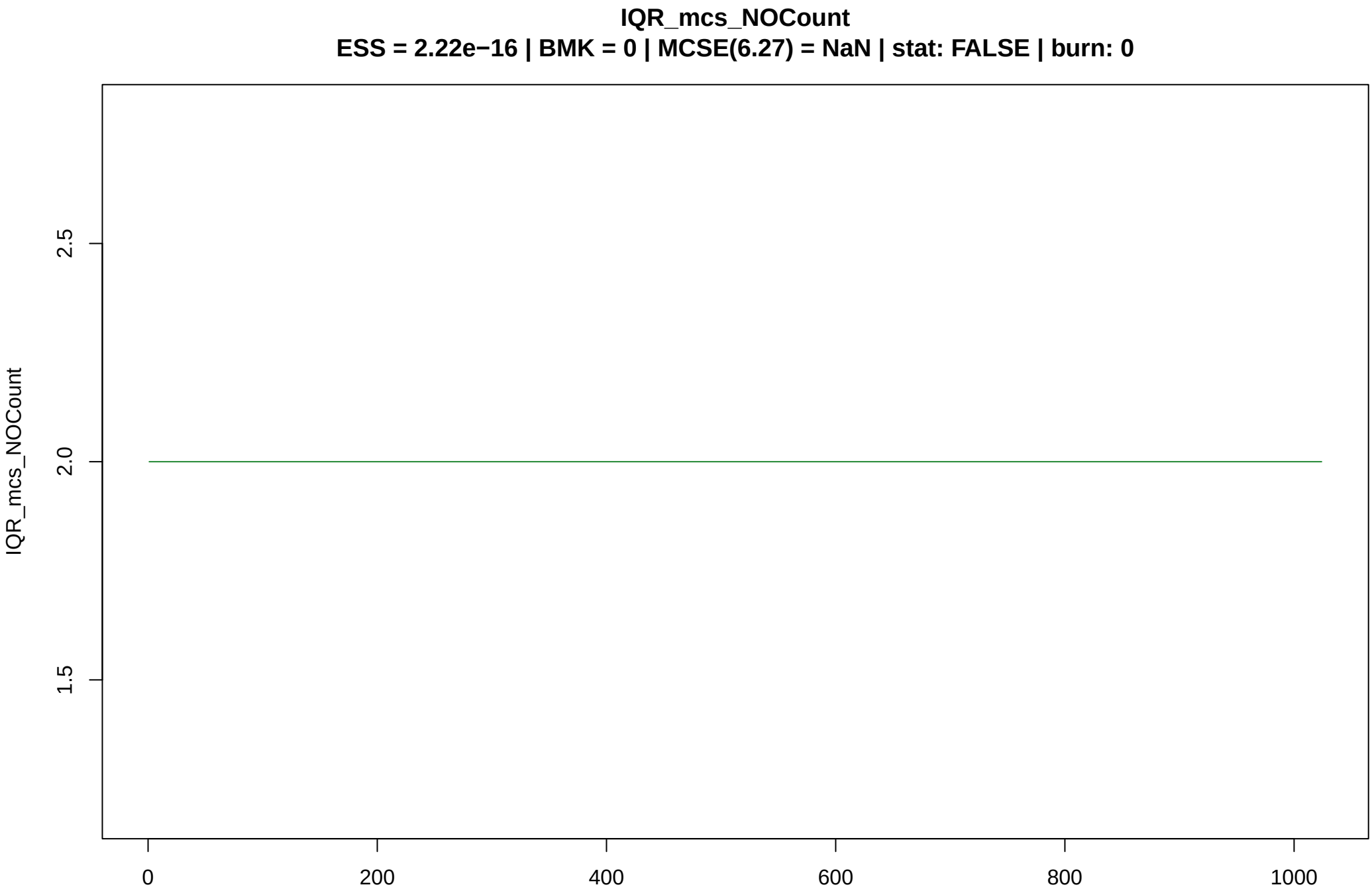

IQR_logit_ec_tanimoto_similarity
ESS = 103 | BMK = 0.191 | MCSE(6.27) = 7.87 | stat: FALSE | burn: 0
IQR_logit_ec_tanimoto_similarity
1.10
1.15
1.20
1.25
0
200
400
600
800
1000

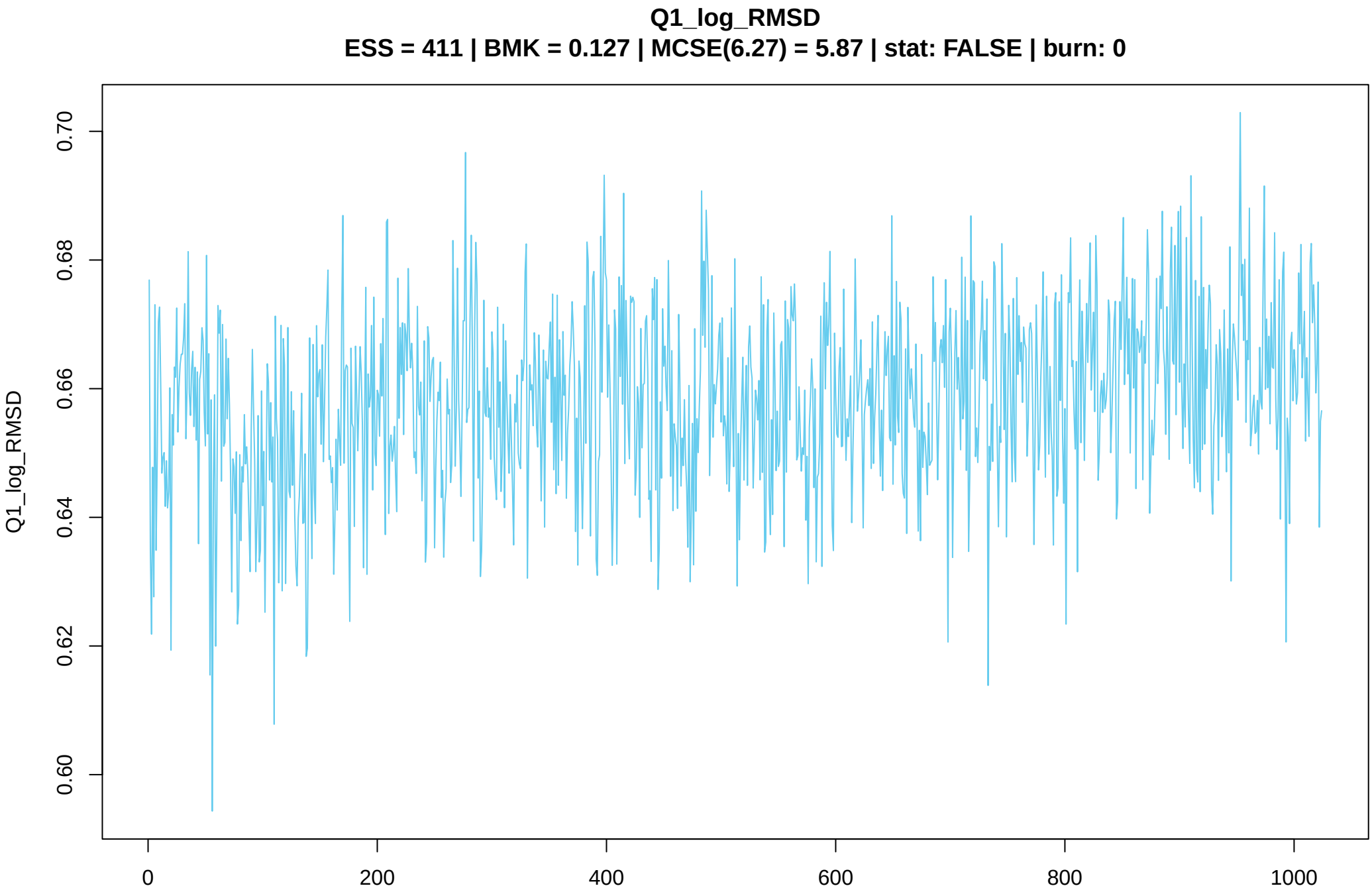

IQR_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_NumHeteroAtoms
2.0
2.5
3.0
3.5
4.0
0
200
400
600
800
1000

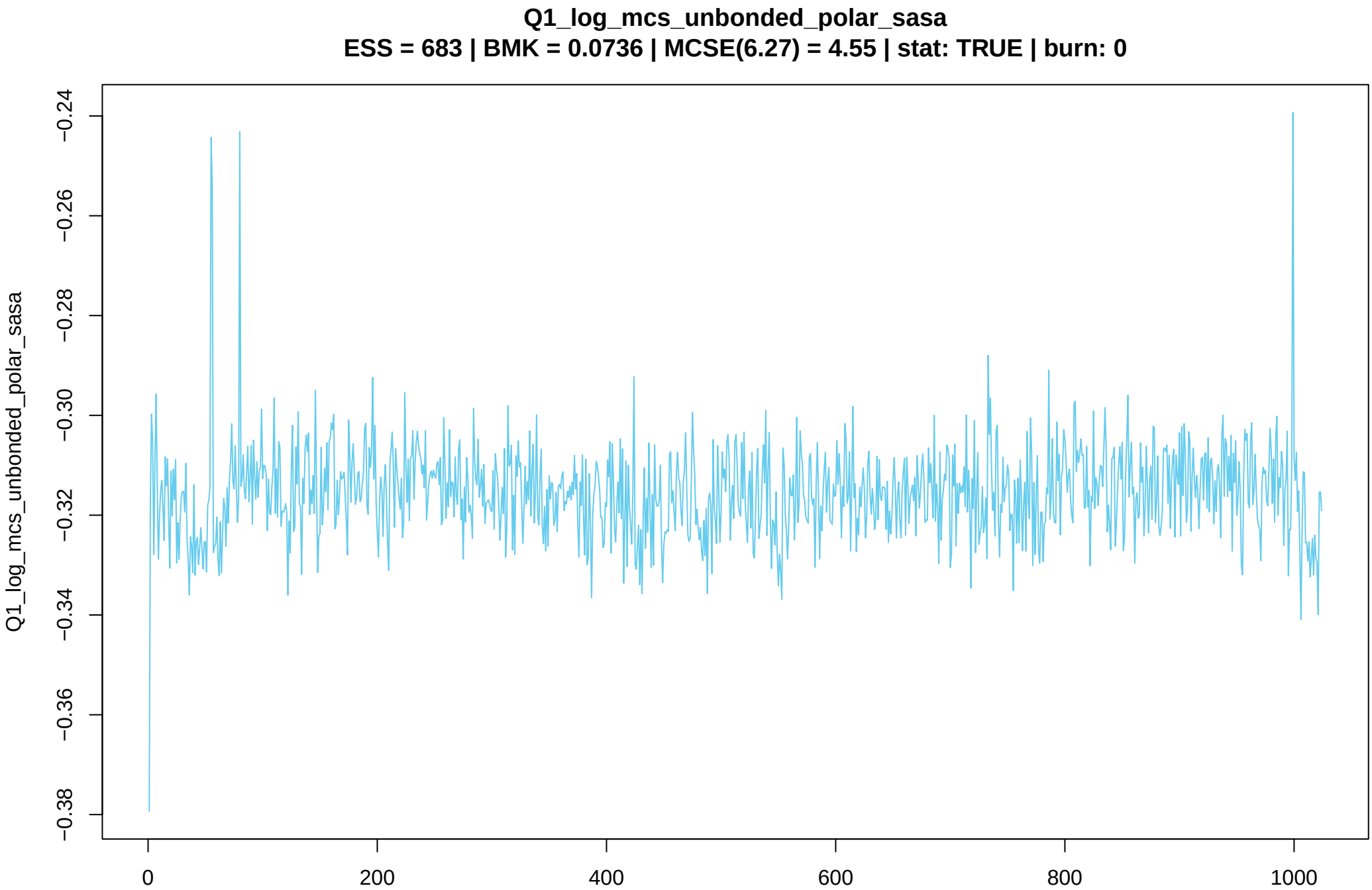

IQR_docked_HeavyAtomCount
ESS = 21.8 | BMK = 0.21 | MCSE(6.27) = 10.9 | stat: FALSE | burn: 0
IQR_docked_HeavyAtomCount
9.0
8.5
8.0
7.5
7.0
0
200
400
600
800
1000

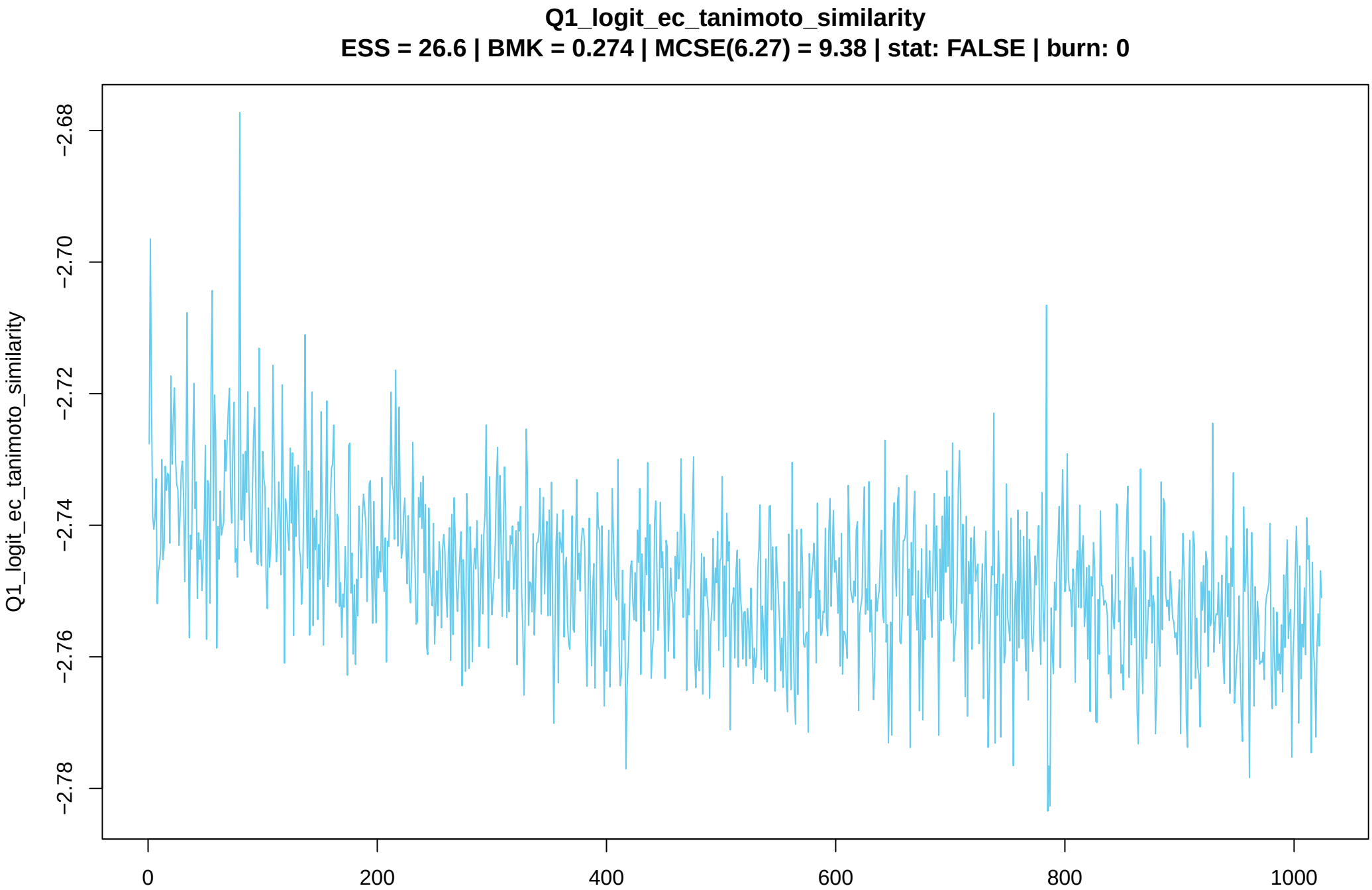

IQR_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
200
400
600
800
1000

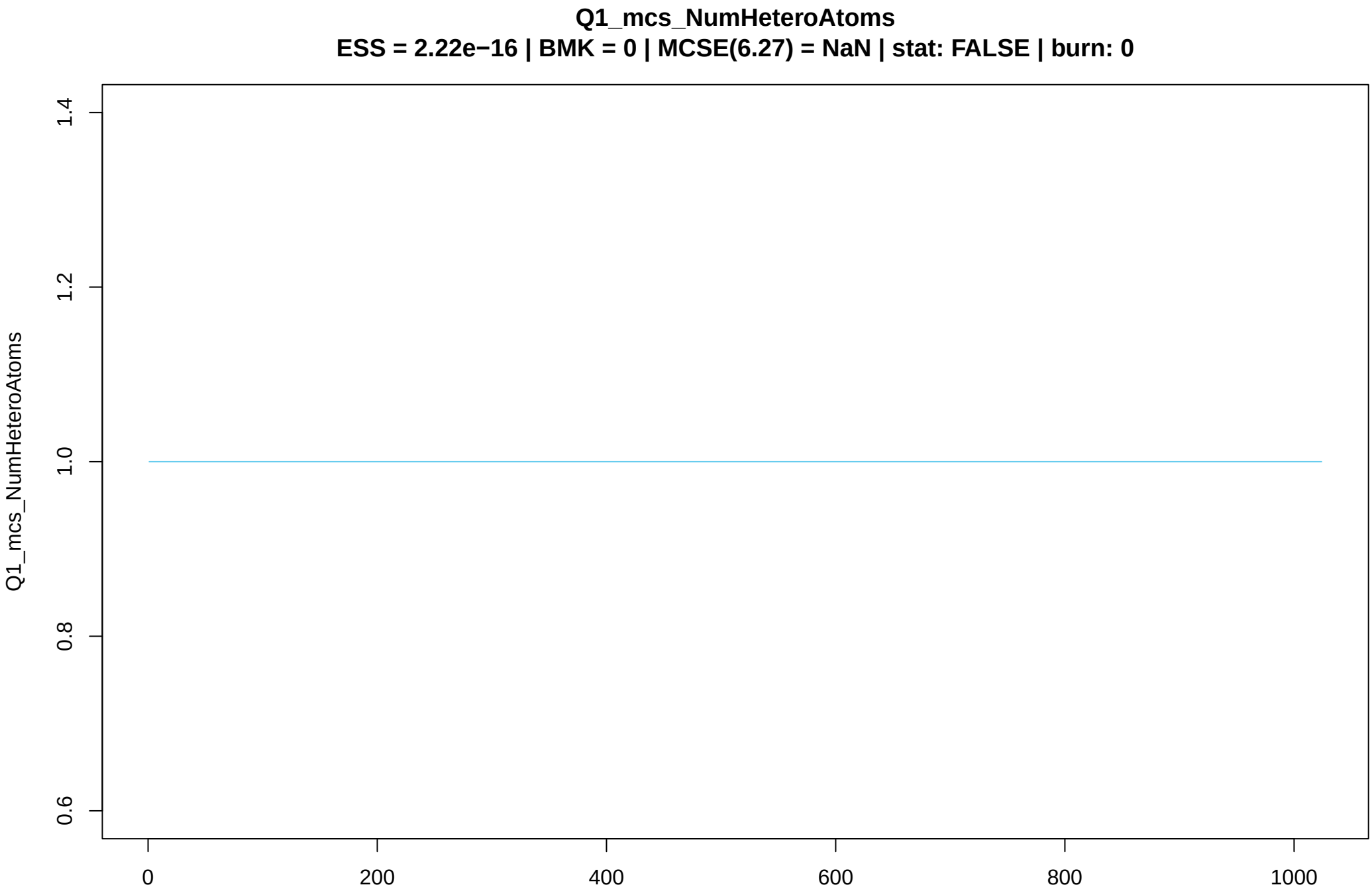

IQR_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.594 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102
IQR_docked_NumRotatableBonds
4.0
3.8
3.6
3.4
3.2
3.0
0
200
400
600
800
1000

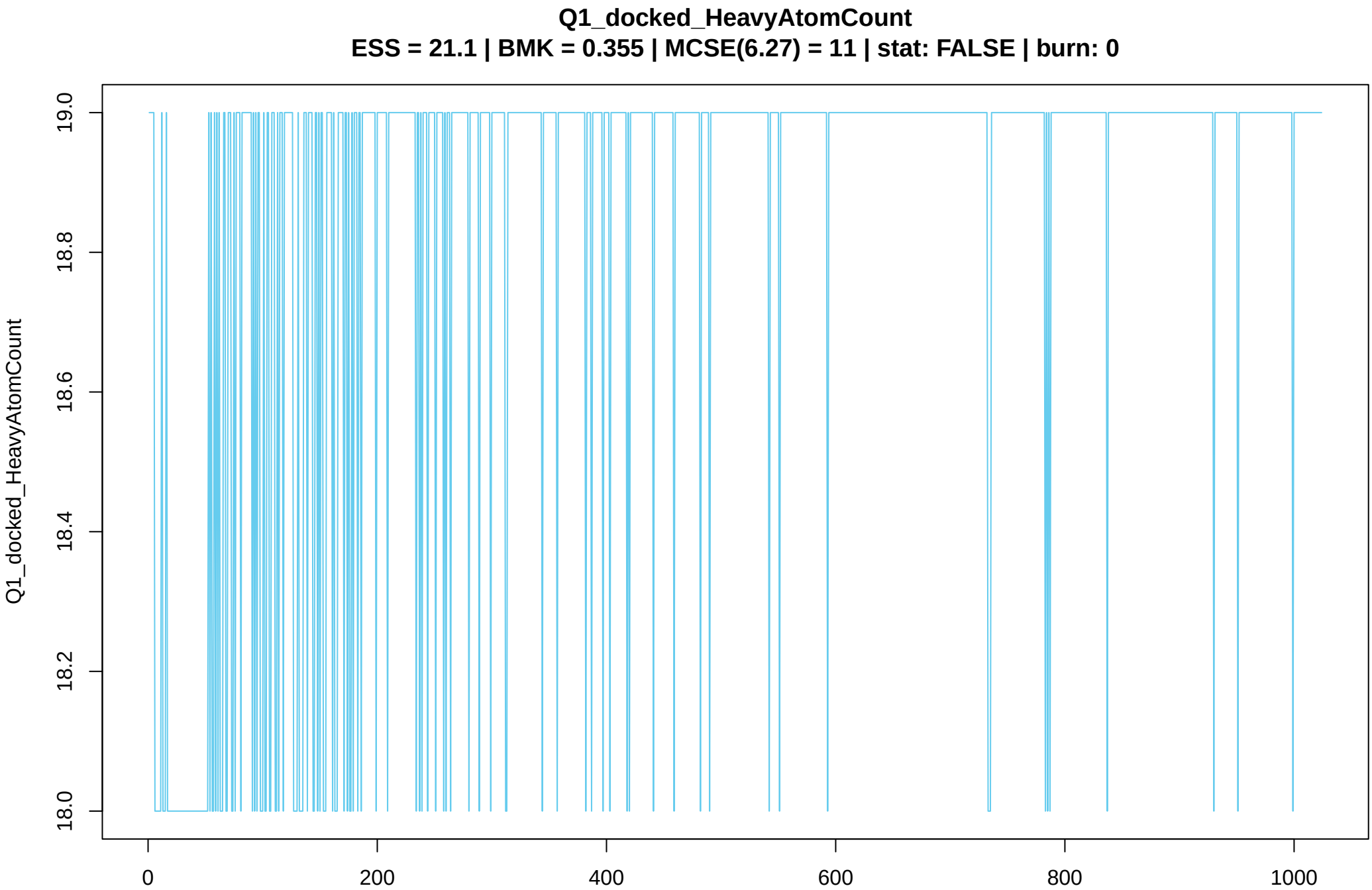

IQR_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_NOCount
2.5
2.0
1.5
0
200
400
600
800
1000

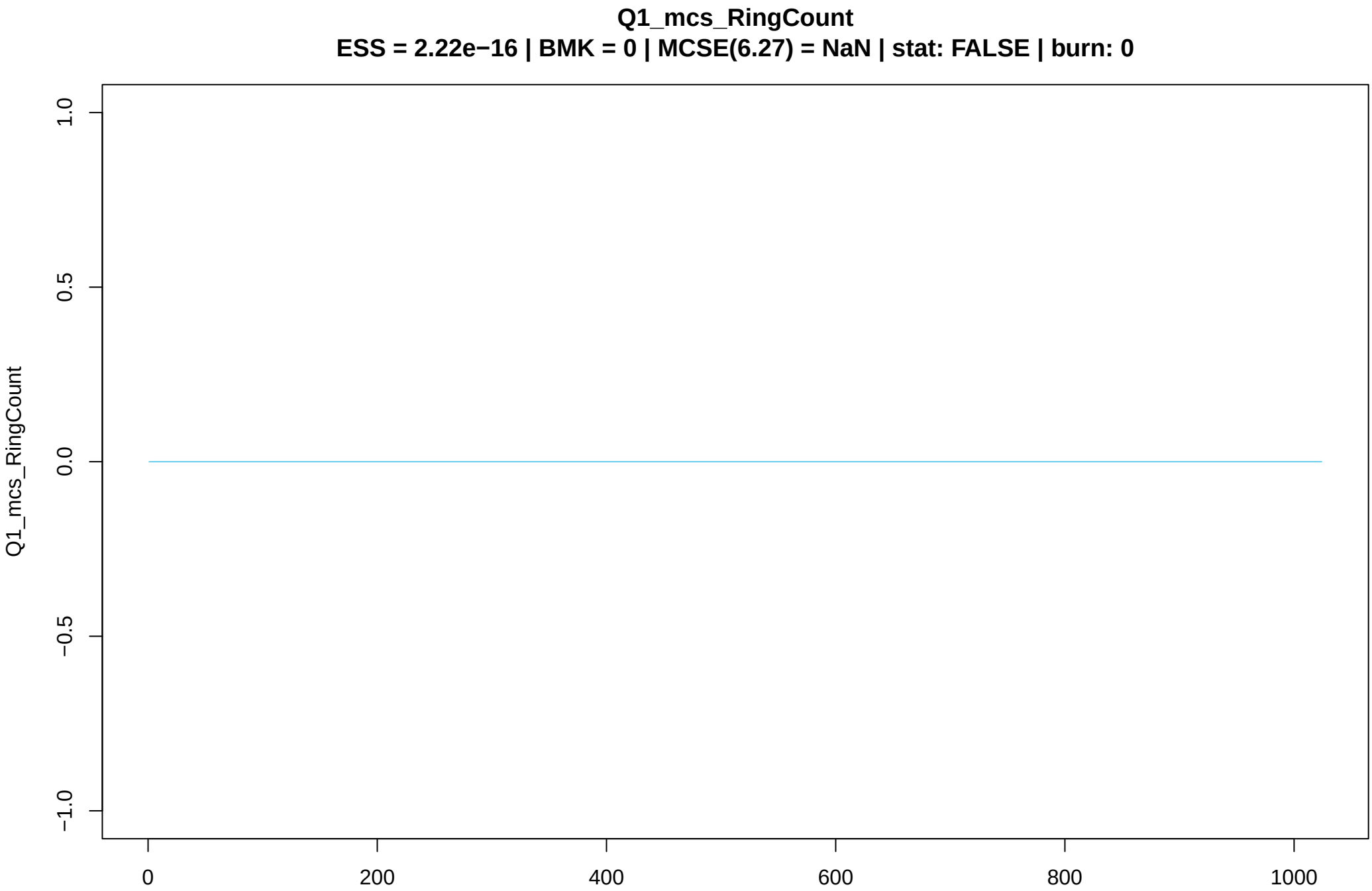

Q1_log_RMSD
ESS = 411 | BMK = 0.127 | MCSE(6.27) = 5.87 | stat: FALSE | burn: 0
Q1_log_RMSD
0.60
0.62
0.64
0.66
0.68
0.70
0
200
400
600
800
1000

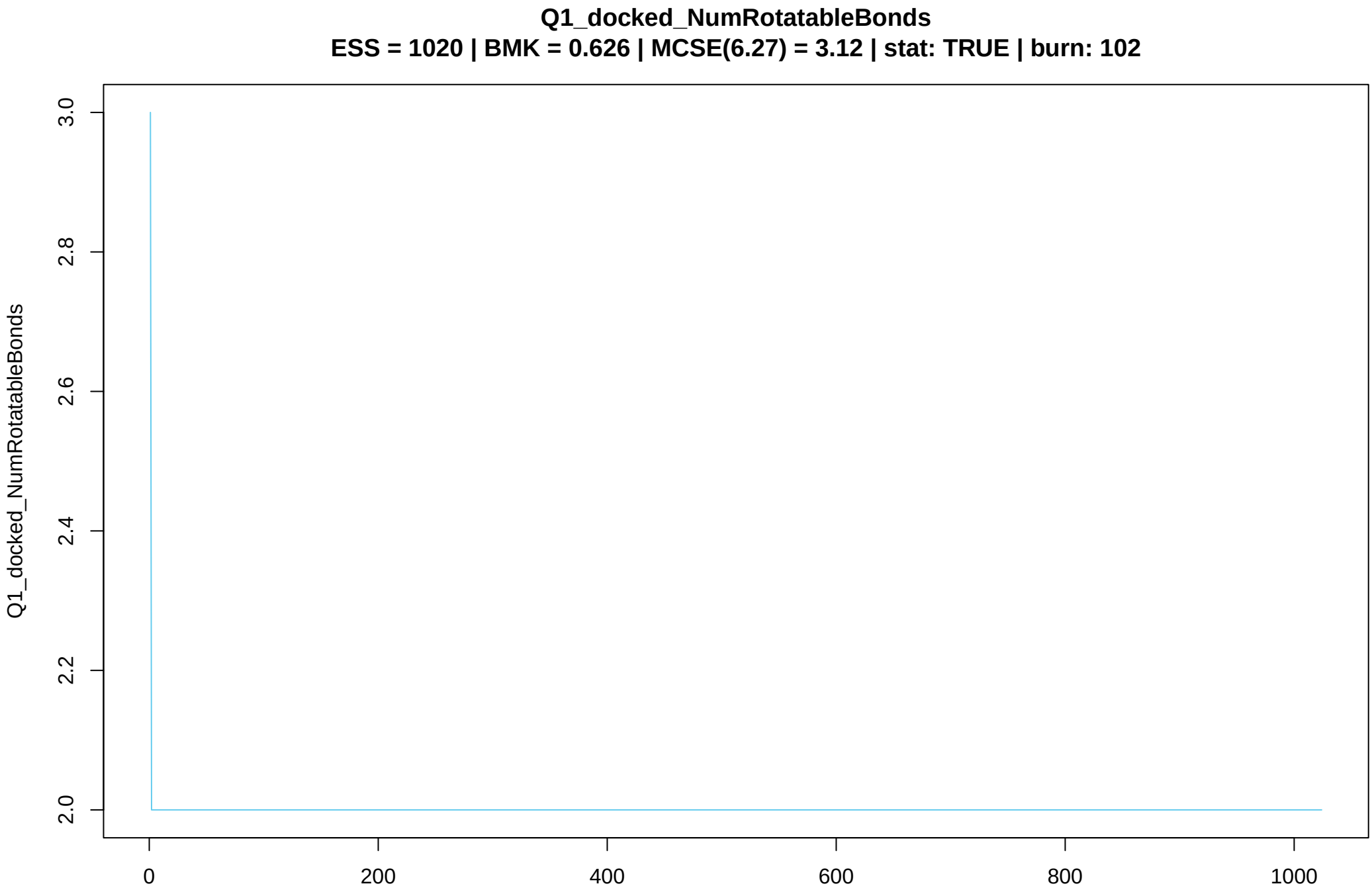

Q1_log_mcs_unbonded_polar_sasa
ESS = 683 | BMK = 0.0736 | MCSE(6.27) = 4.55 | stat: TRUE | burn: 0
Q1_log_mcs_unbonded_polar_sasa
−0.24
−0.26
−0.28
−0.30
−0.32
−0.34
−0.36
−0.38
0
200
400
600
800
1000

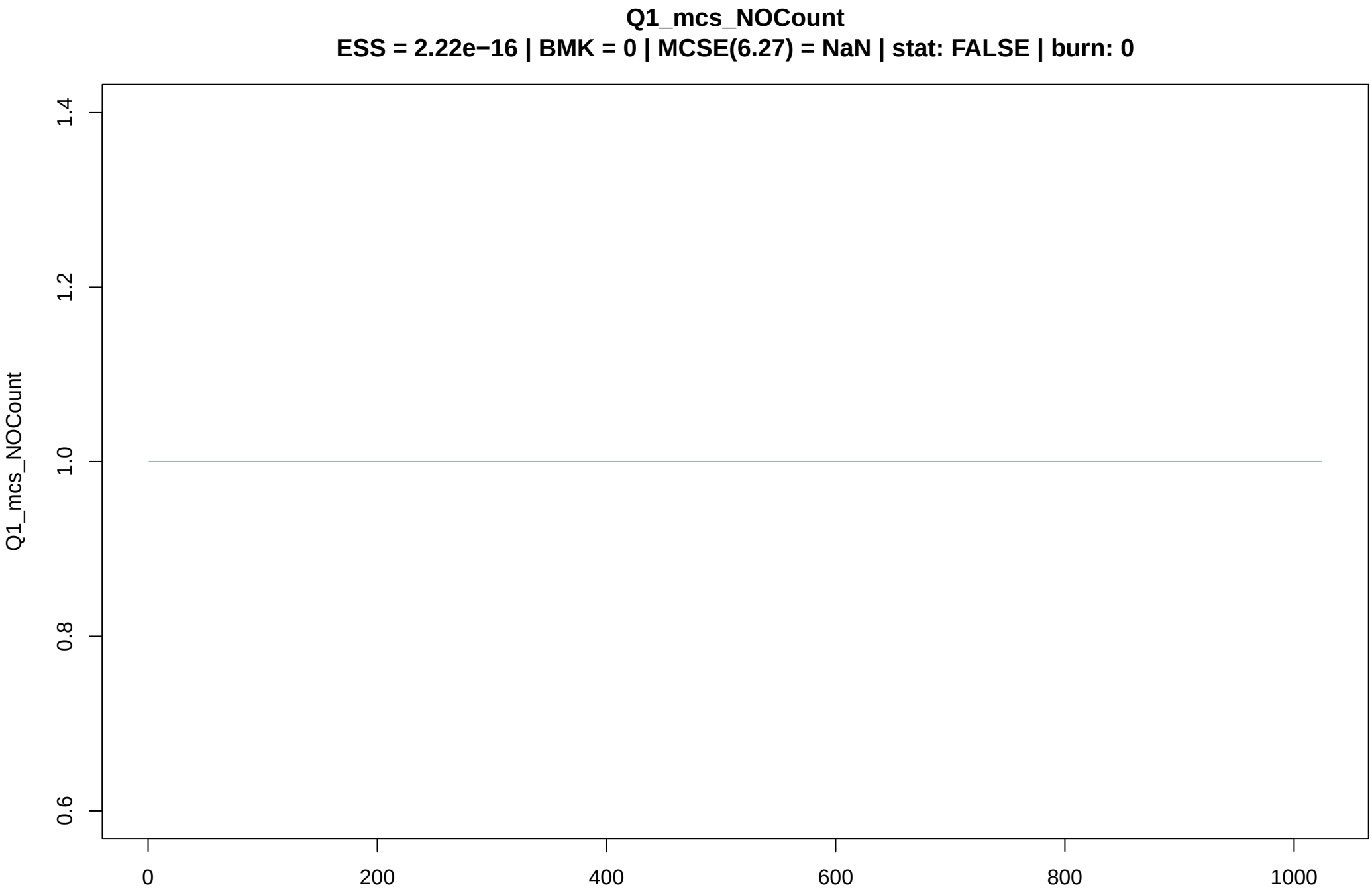

Q1_logit_ec_tanimoto_similarity
ESS = 26.6 | BMK = 0.274 | MCSE(6.27) = 9.38 | stat: FALSE | burn: 0
Q1_logit_ec_tanimoto_similarity
−2.68
−2.70
−2.72
−2.74
−2.76
−2.78
0
200
400
600
800
1000

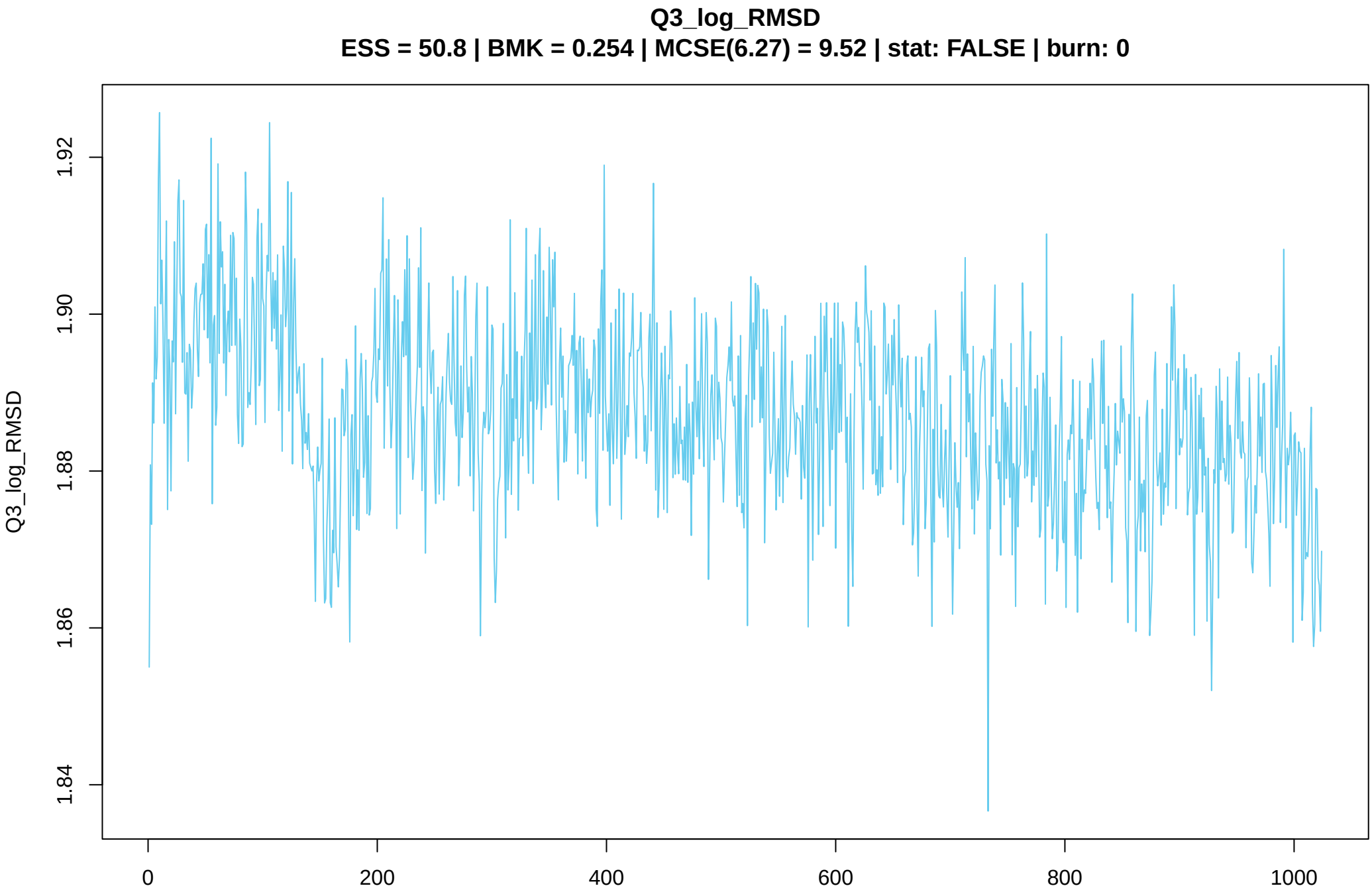

Q1_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NumHeteroAtoms
0.6
0.8
1.0
1.2
1.4
0
200
400
600
800
1000

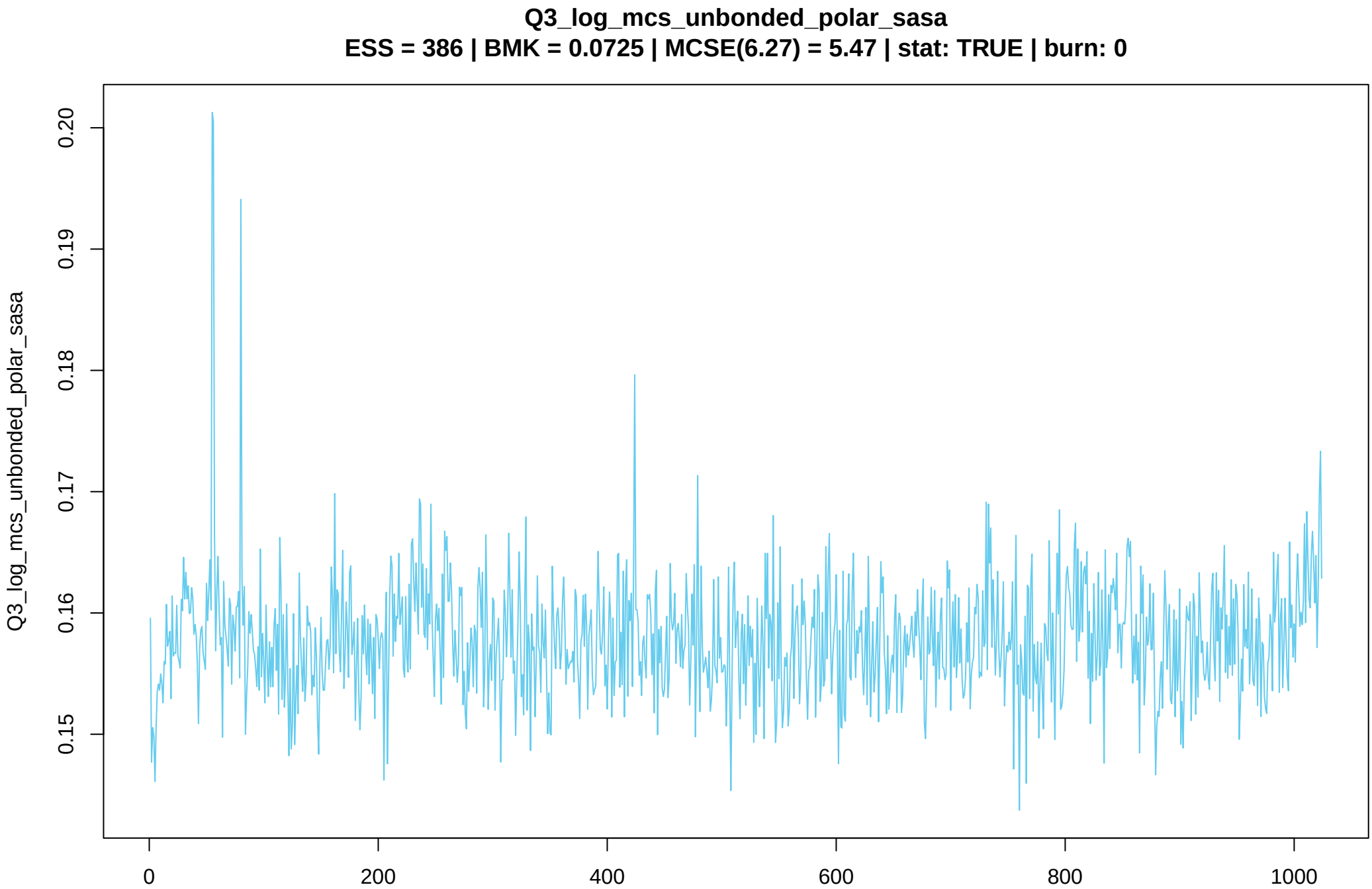

Q1_docked_HeavyAtomCount
ESS = 21.1 | BMK = 0.355 | MCSE(6.27) = 11 | stat: FALSE | burn: 0
Q1_docked_HeavyAtomCount
19.0
18.8
18.6
18.4
18.2
18.0
0
200
400
600
800
1000

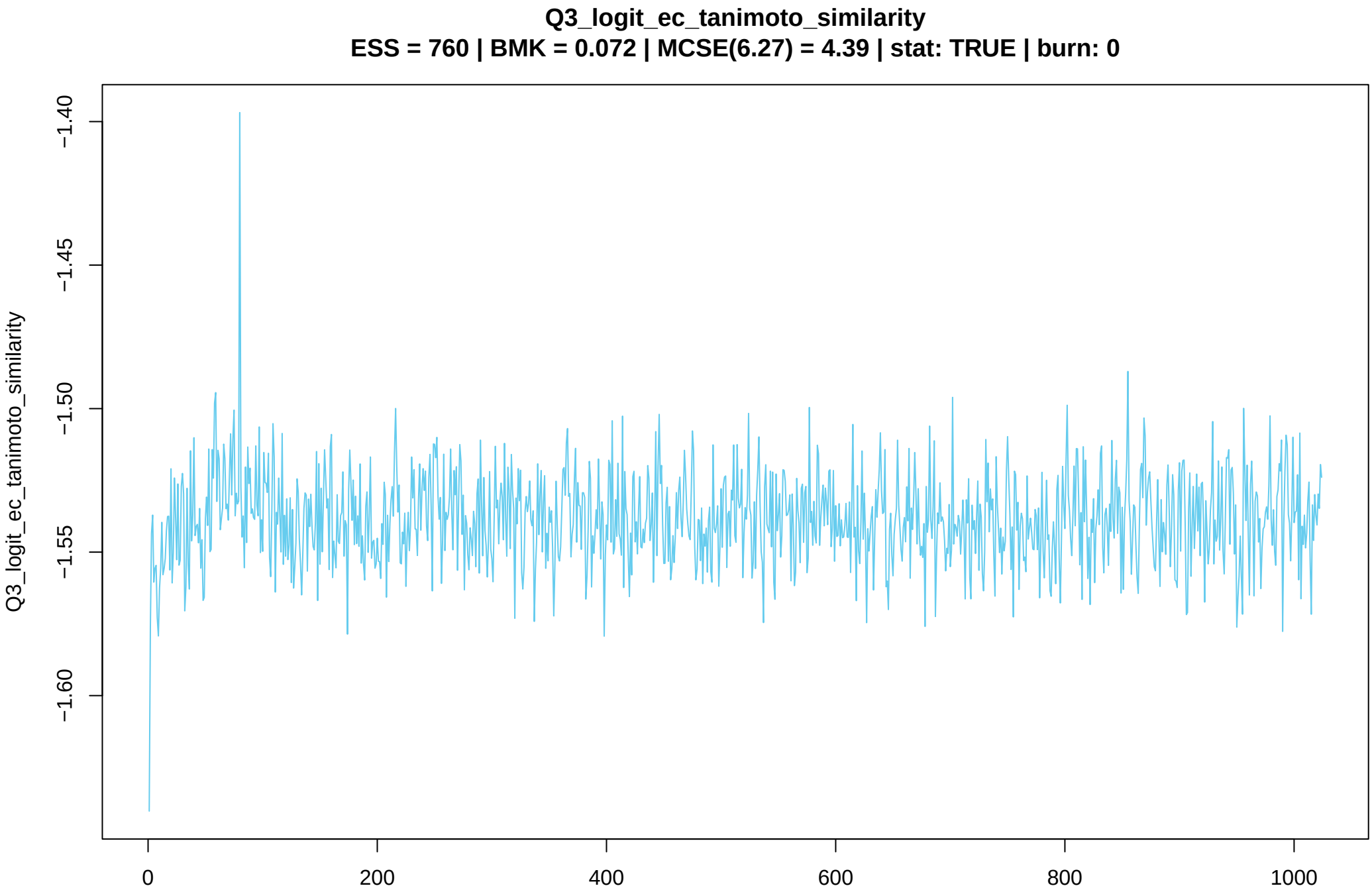

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
200
400
600
800
1000

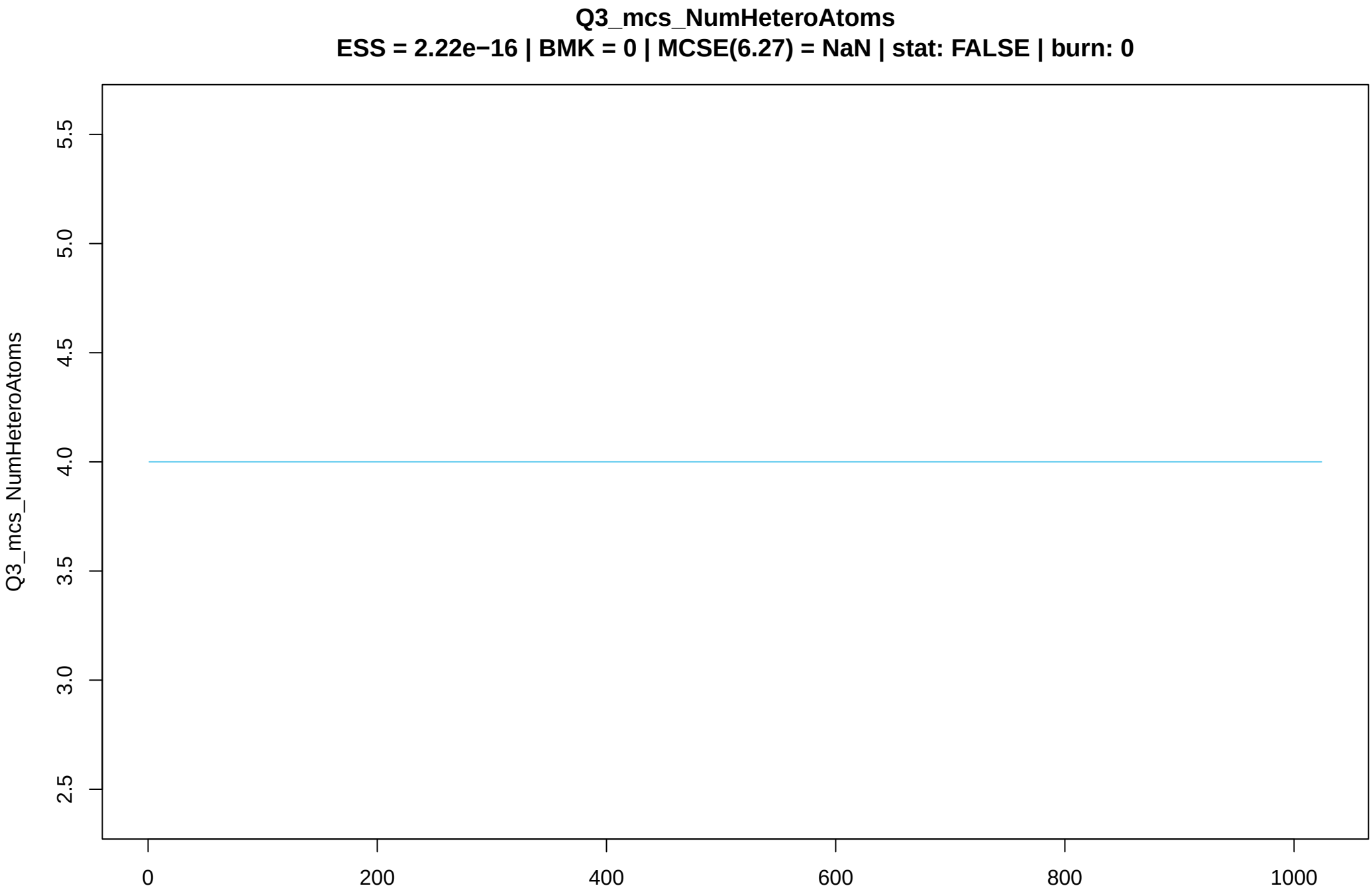

Q1_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.626 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102
Q1_docked_NumRotatableBonds
3.0
2.8
2.6
2.4
2.2
2.0
0
200
400
600
800
1000

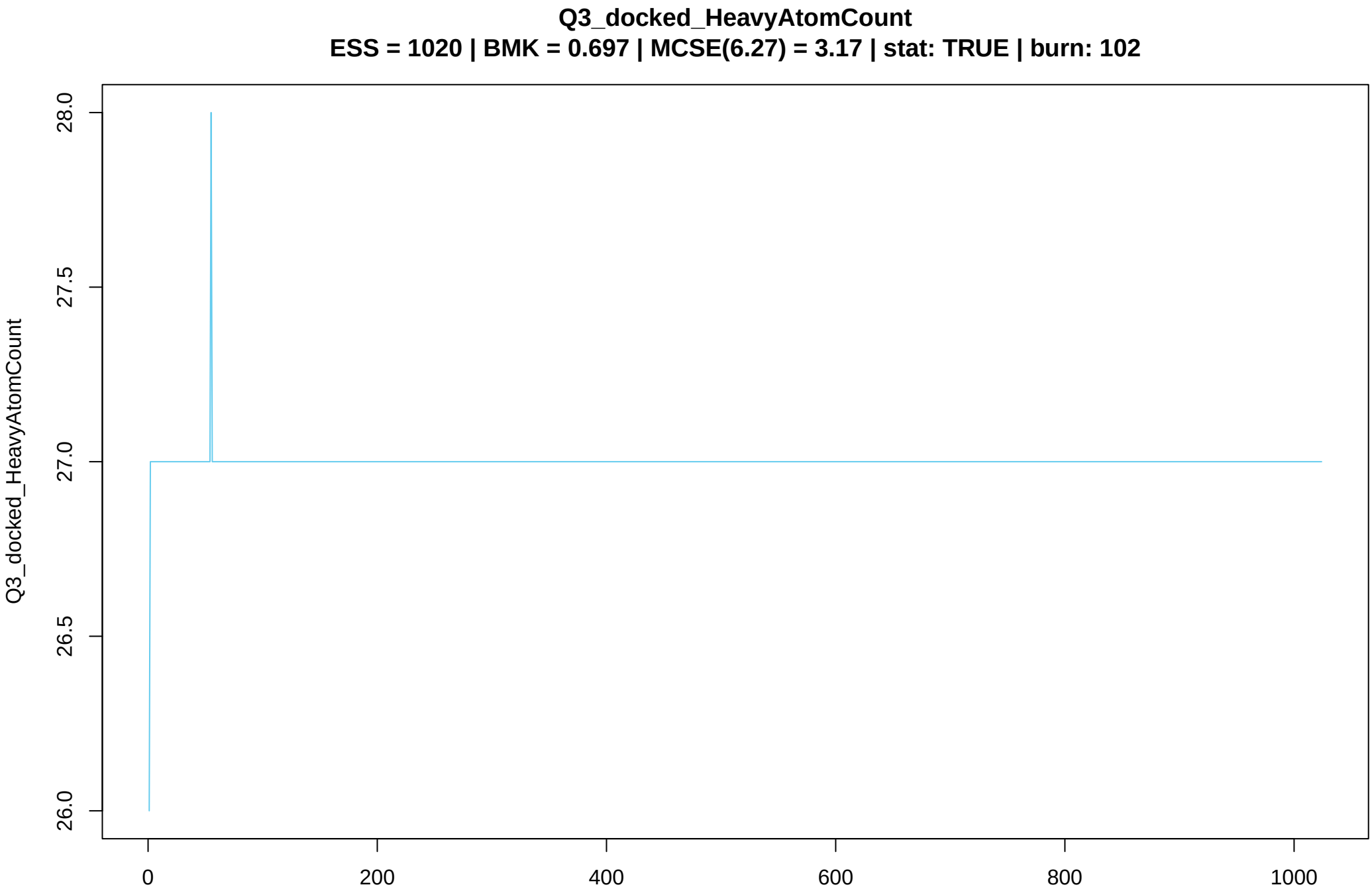

Q1_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NOCount
0.6
0.8
1.0
1.2
1.4
0
200
400
600
800
1000

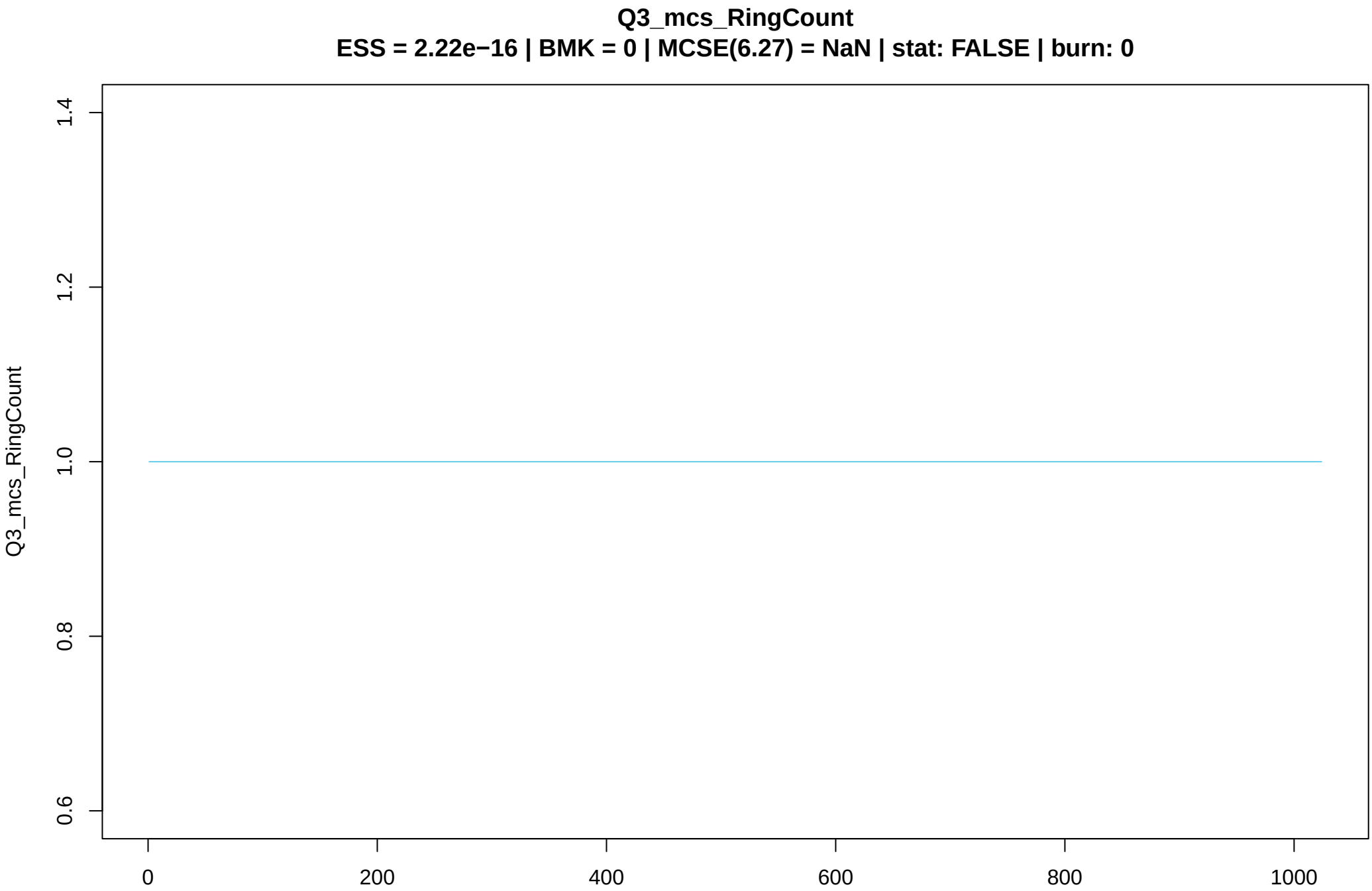

Q3_log_RMSD
ESS = 50.8 | BMK = 0.254 | MCSE(6.27) = 9.52 | stat: FALSE | burn: 0
Q3_log_RMSD
1.84
1.86
1.88
1.90
1.92
0
200
400
600
800
1000

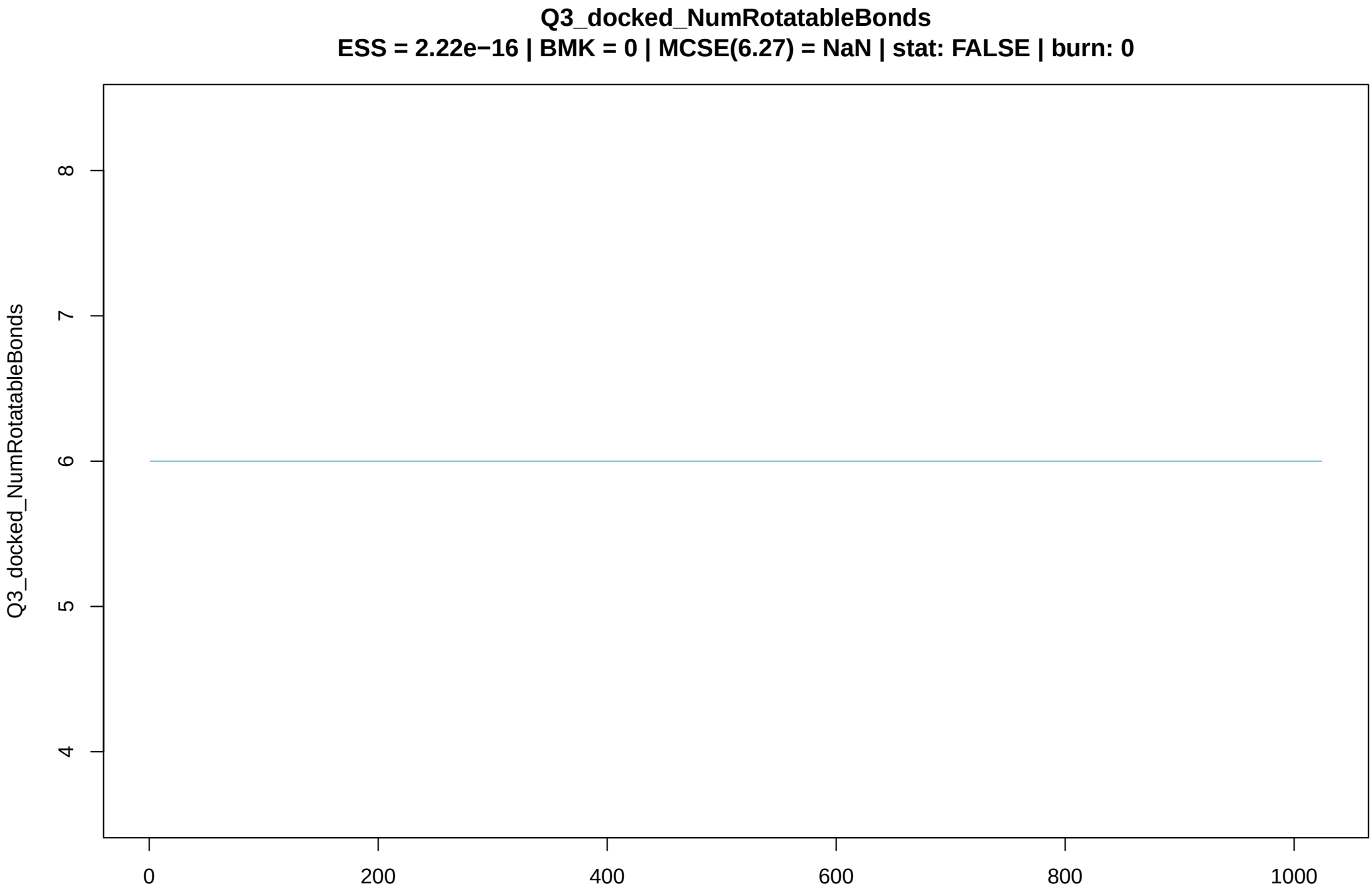

Q3_log_mcs_unbonded_polar_sasa
ESS = 386 | BMK = 0.0725 | MCSE(6.27) = 5.47 | stat: TRUE | burn: 0
Q3_log_mcs_unbonded_polar_sasa
0.15
0.16
0.17
0.18
0.19
0.20
0
200
400
600
800
1000

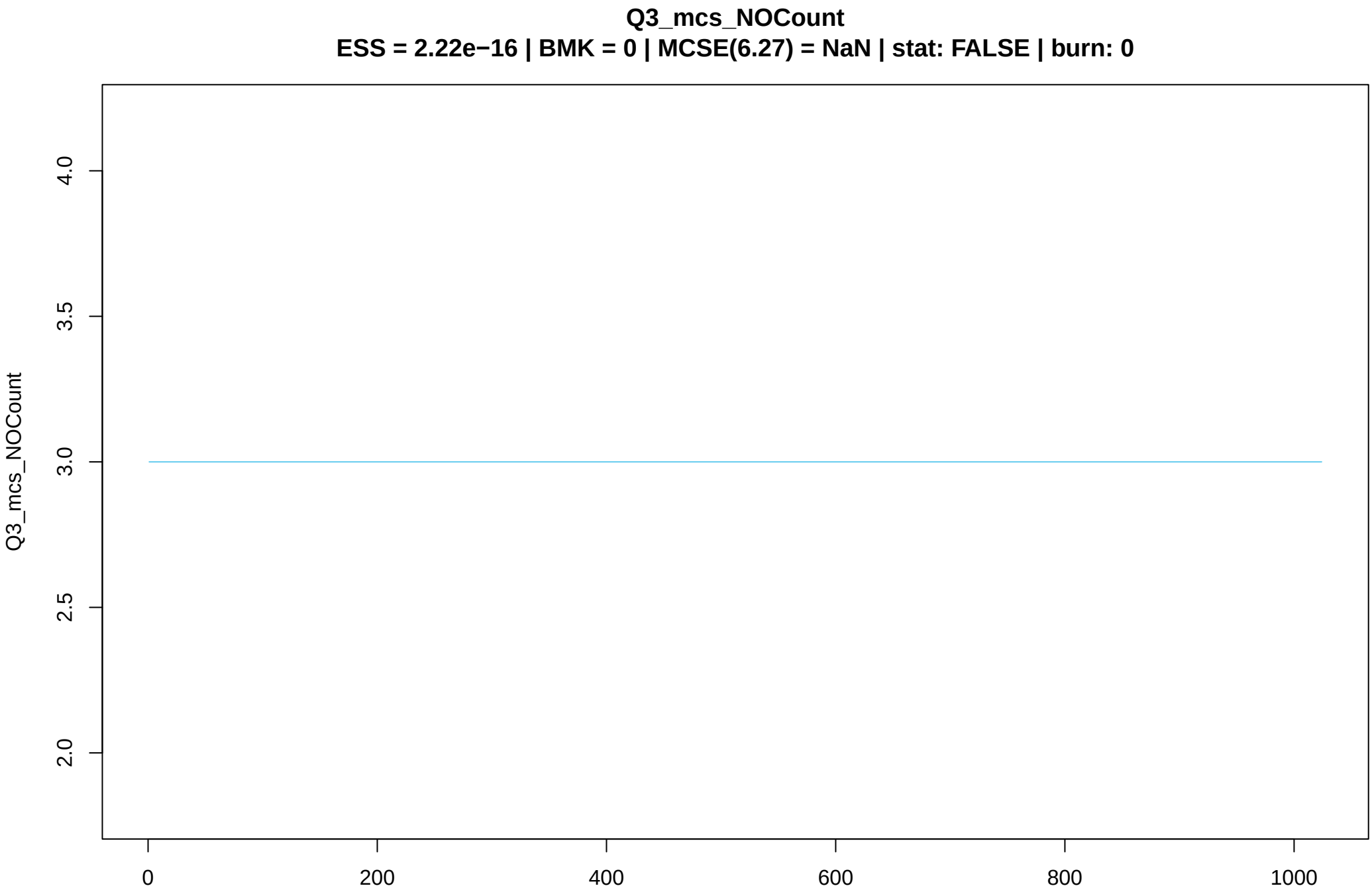

Q3_logit_ec_tanimoto_similarity
ESS = 760 | BMK = 0.072 | MCSE(6.27) = 4.39 | stat: TRUE | burn: 0
Q3_logit_ec_tanimoto_similarity
−1.40
−1.45
−1.50
−1.55
−1.60
0
200
400
600
800
1000

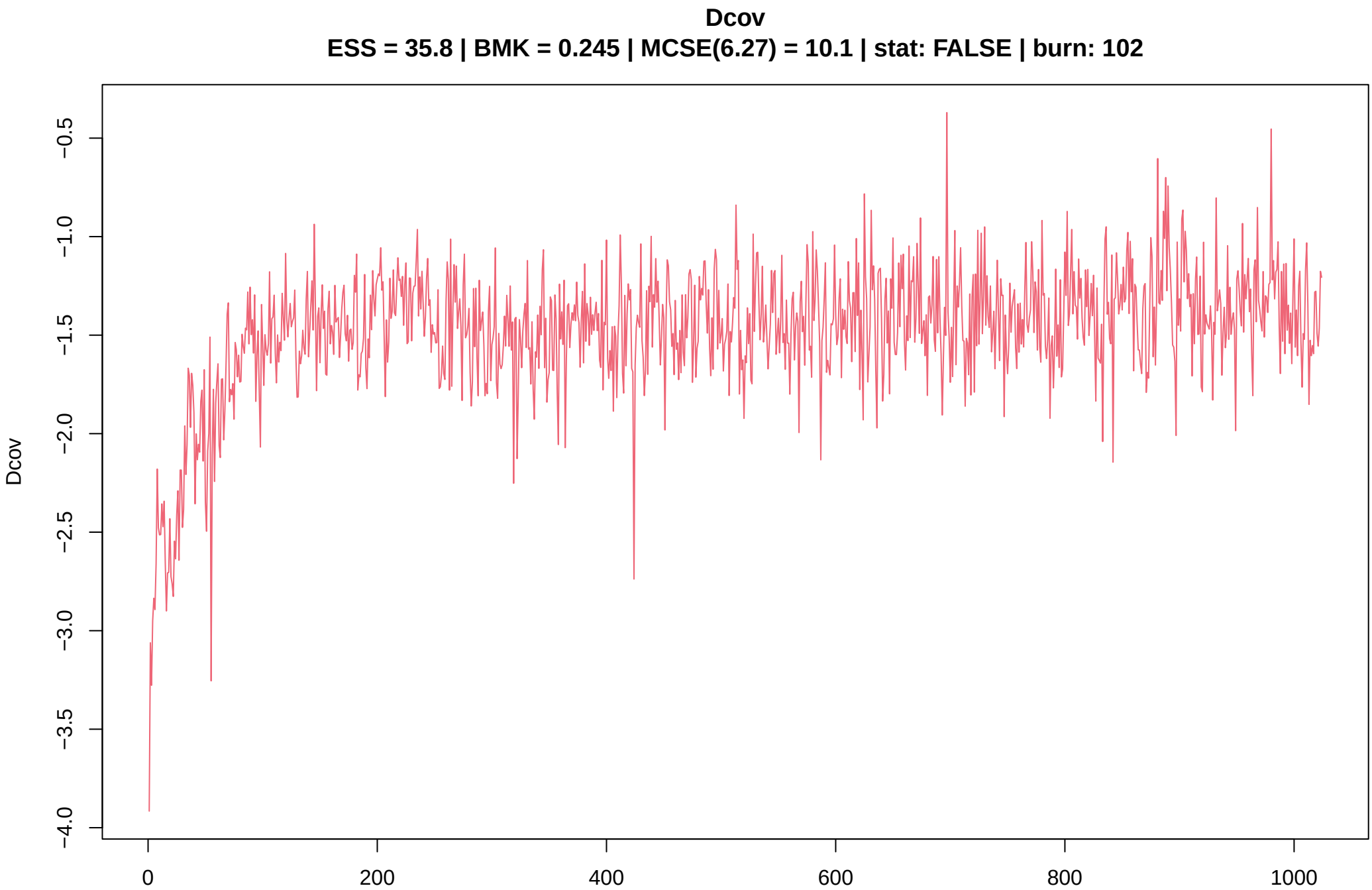

Q3_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_NumHeteroAtoms
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
200
400
600
800
1000

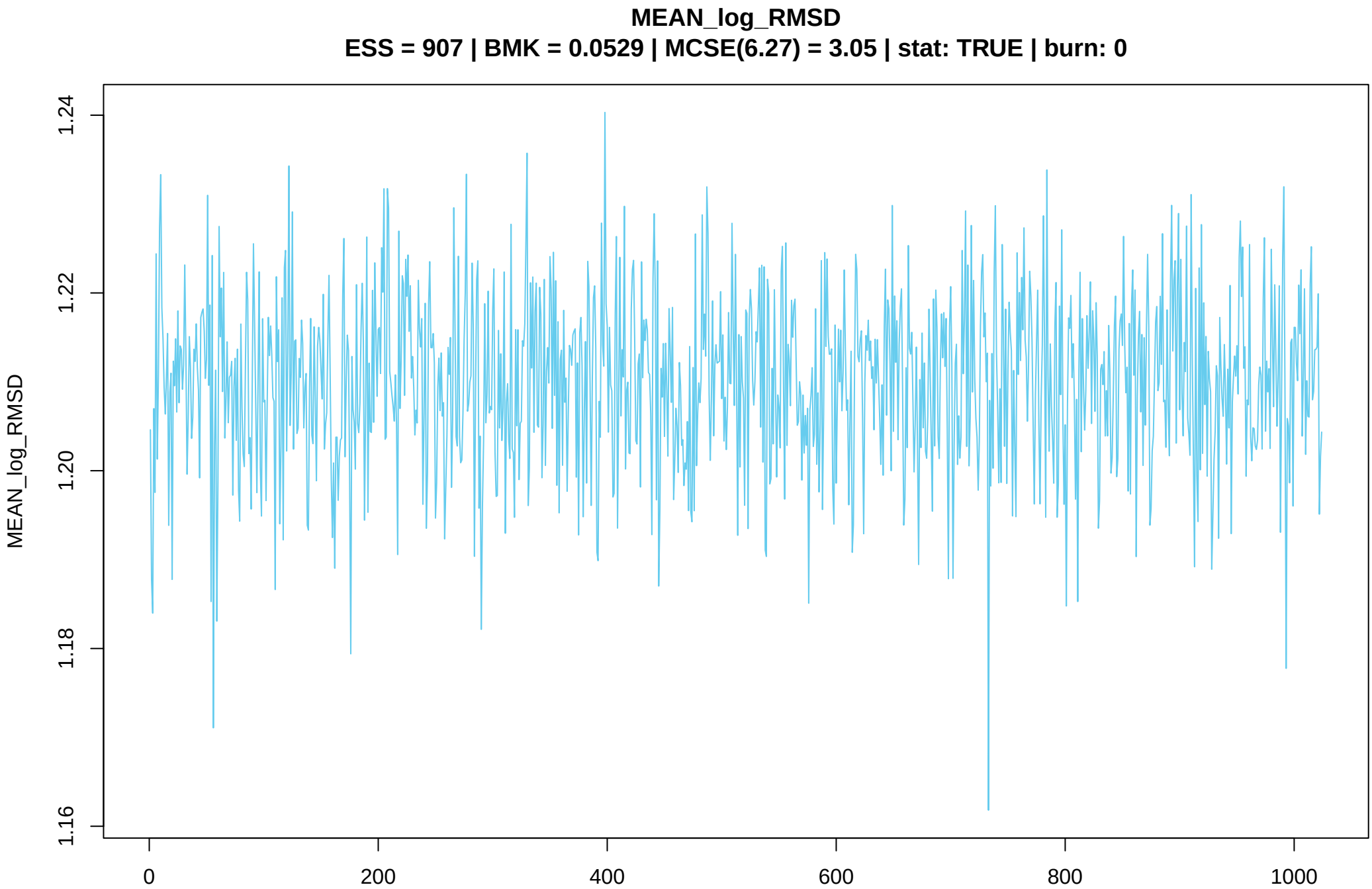

Q3_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.697 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 102
Q3_docked_HeavyAtomCount
28.0
27.5
27.0
26.5
26.0
0
200
400
600
800
1000

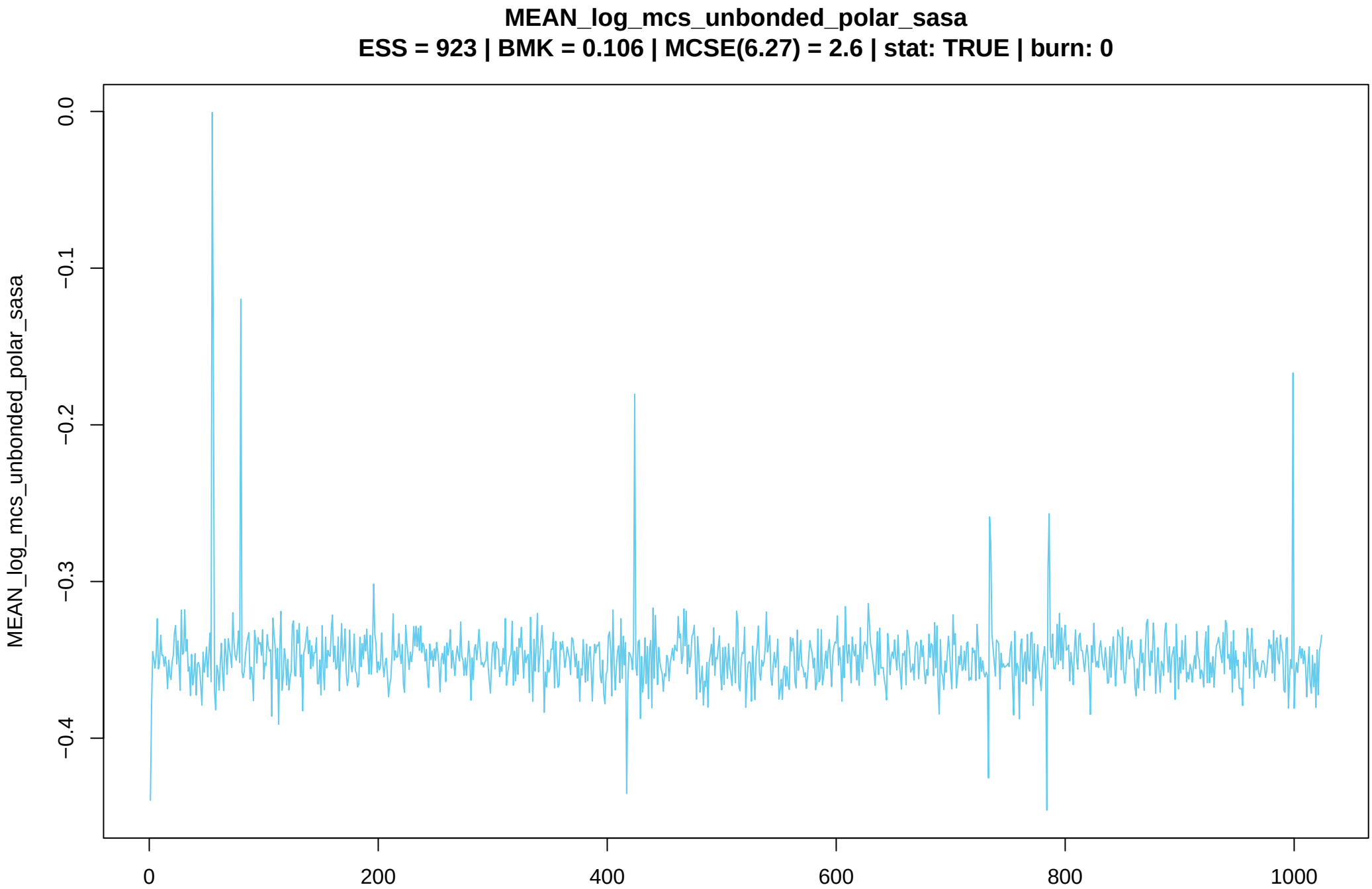

Q3_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
200
400
600
800
1000

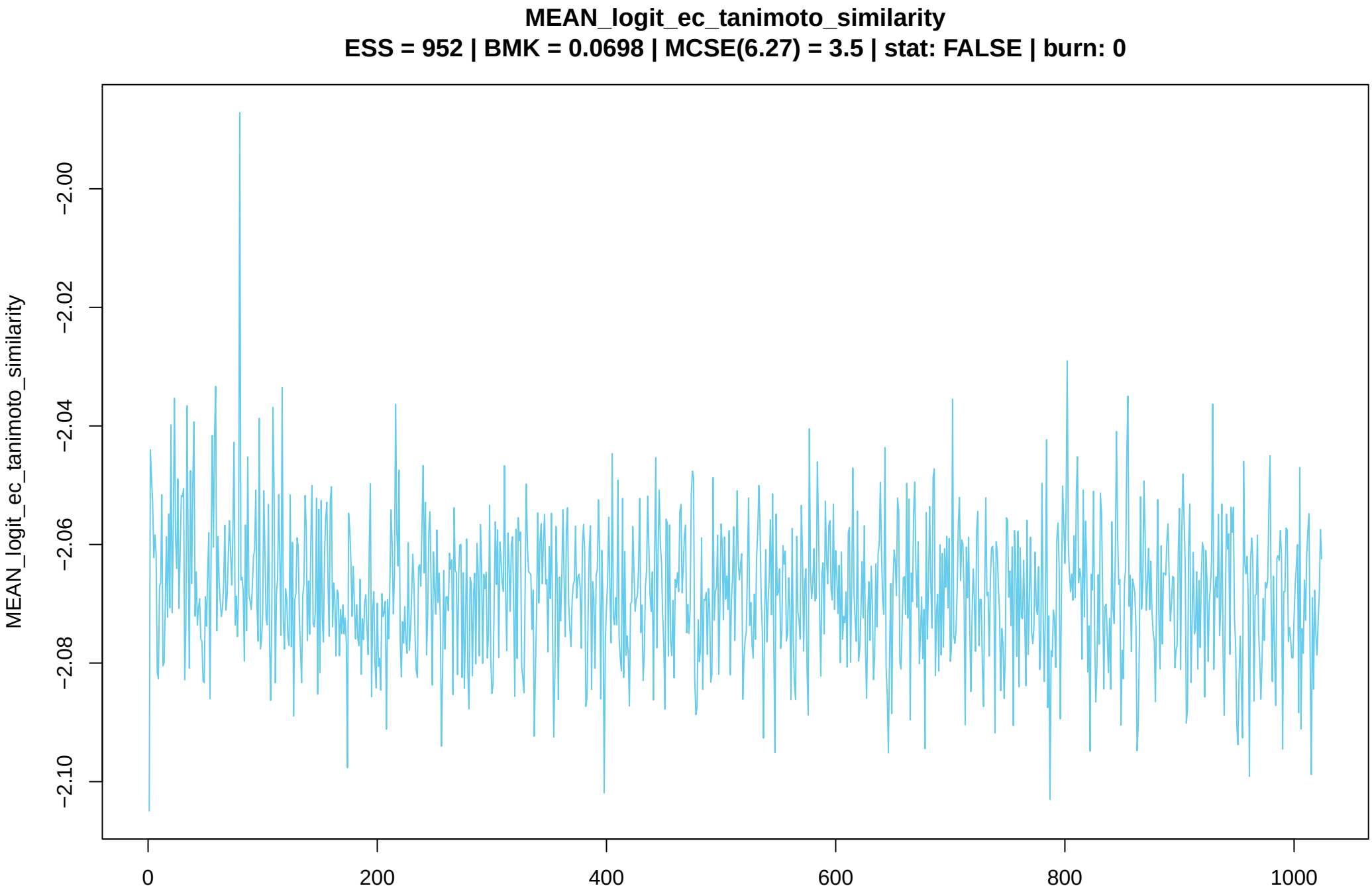

Q3_docked_NumRotatableBonds
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_docked_NumRotatableBonds
4
5
6
7
8
0
200
400
600
800
1000

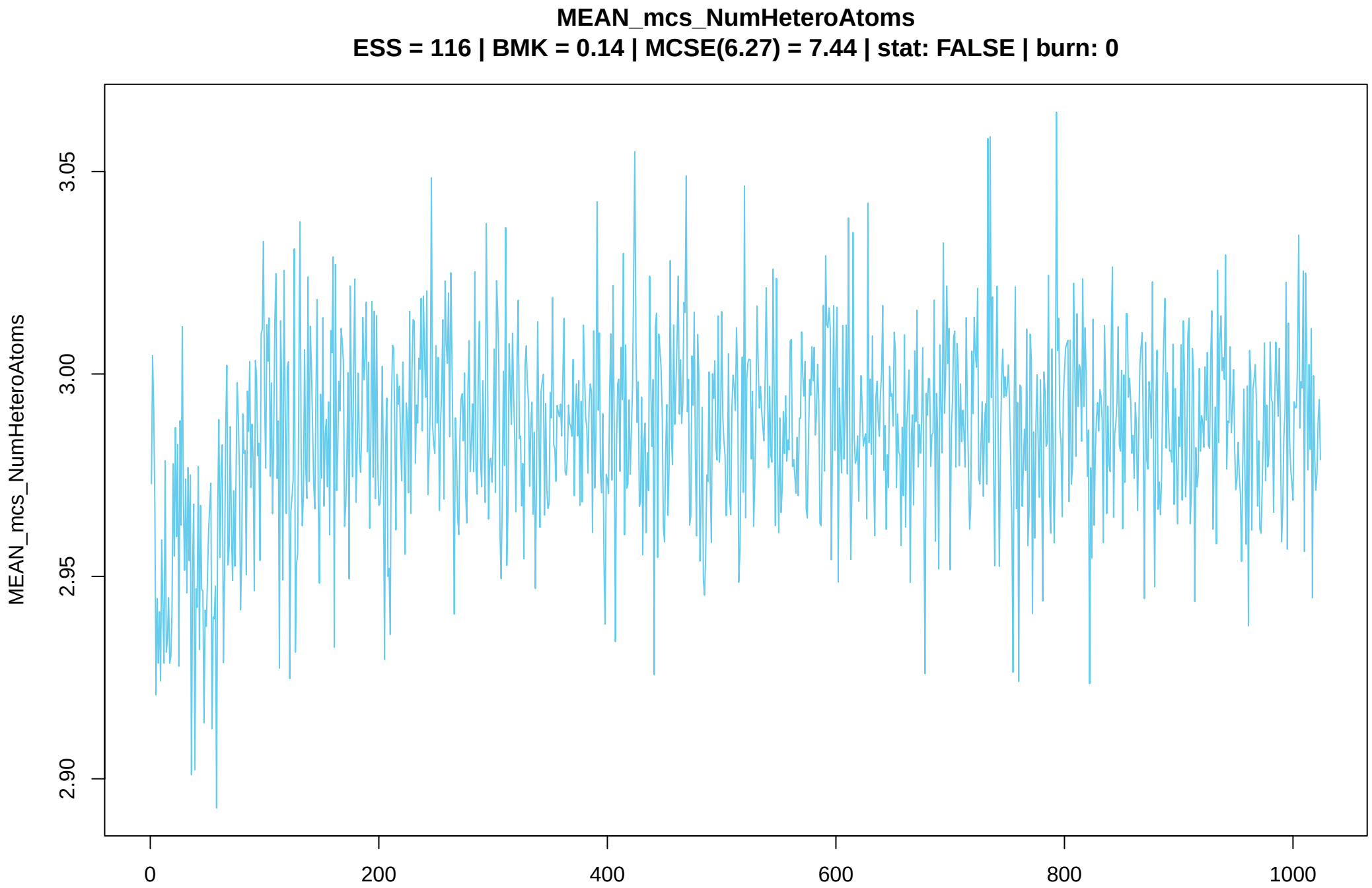

Q3_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_NOCount
2.0
2.5
3.0
3.5
4.0
0
200
400
600
800
1000

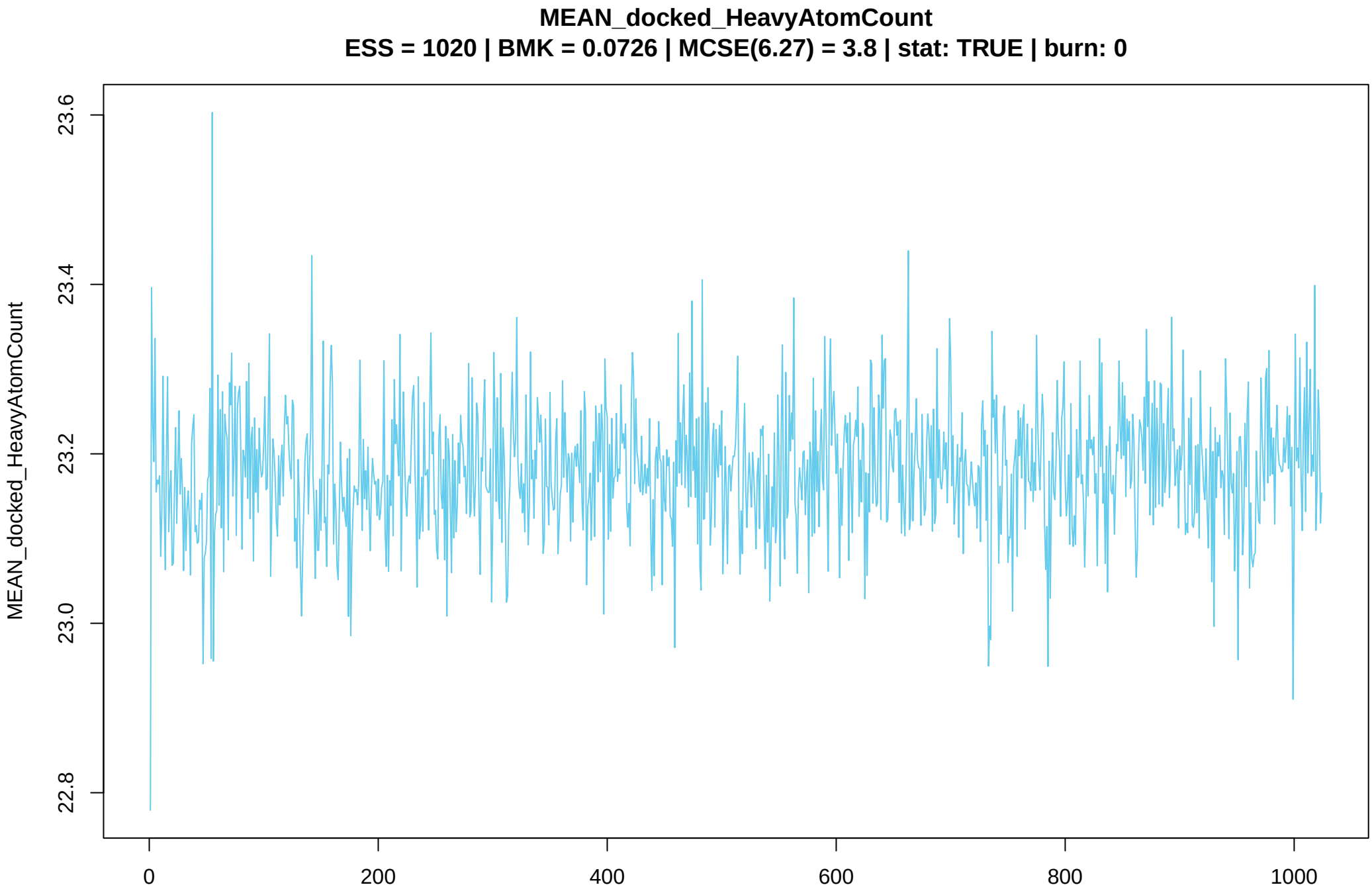

Dcov
ESS = 35.8 | BMK = 0.245 | MCSE(6.27) = 10.1 | stat: FALSE | burn: 102
Dcov
−0.5
−1.0
−1.5
−2.0
−2.5
−3.0
−3.5
−4.0
0
200
400
600
800
1000

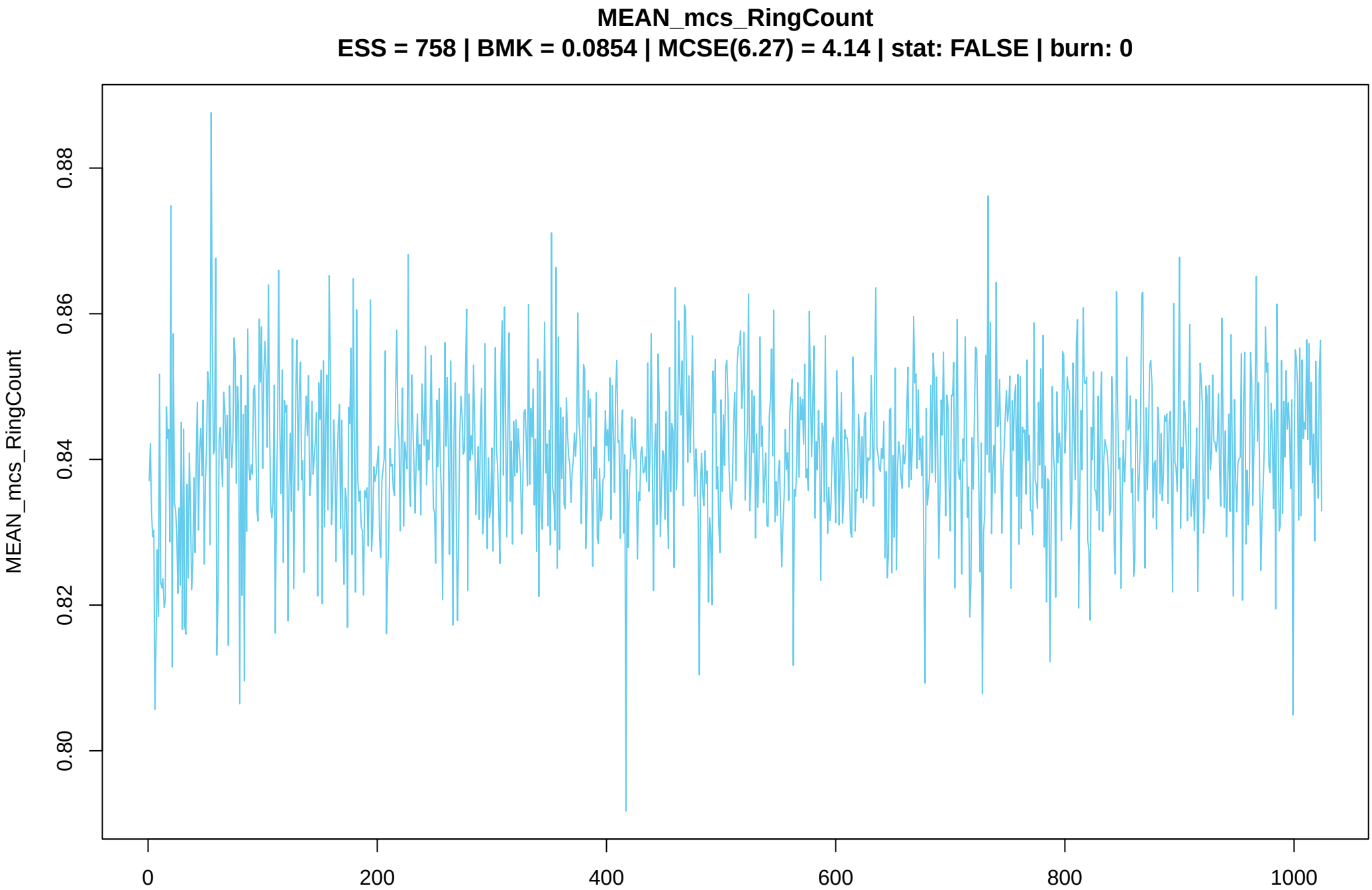

MEAN_log_RMSD
ESS = 907 | BMK = 0.0529 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.24
1.22
1.20
1.18
1.16
0
200
400
600
800
1000

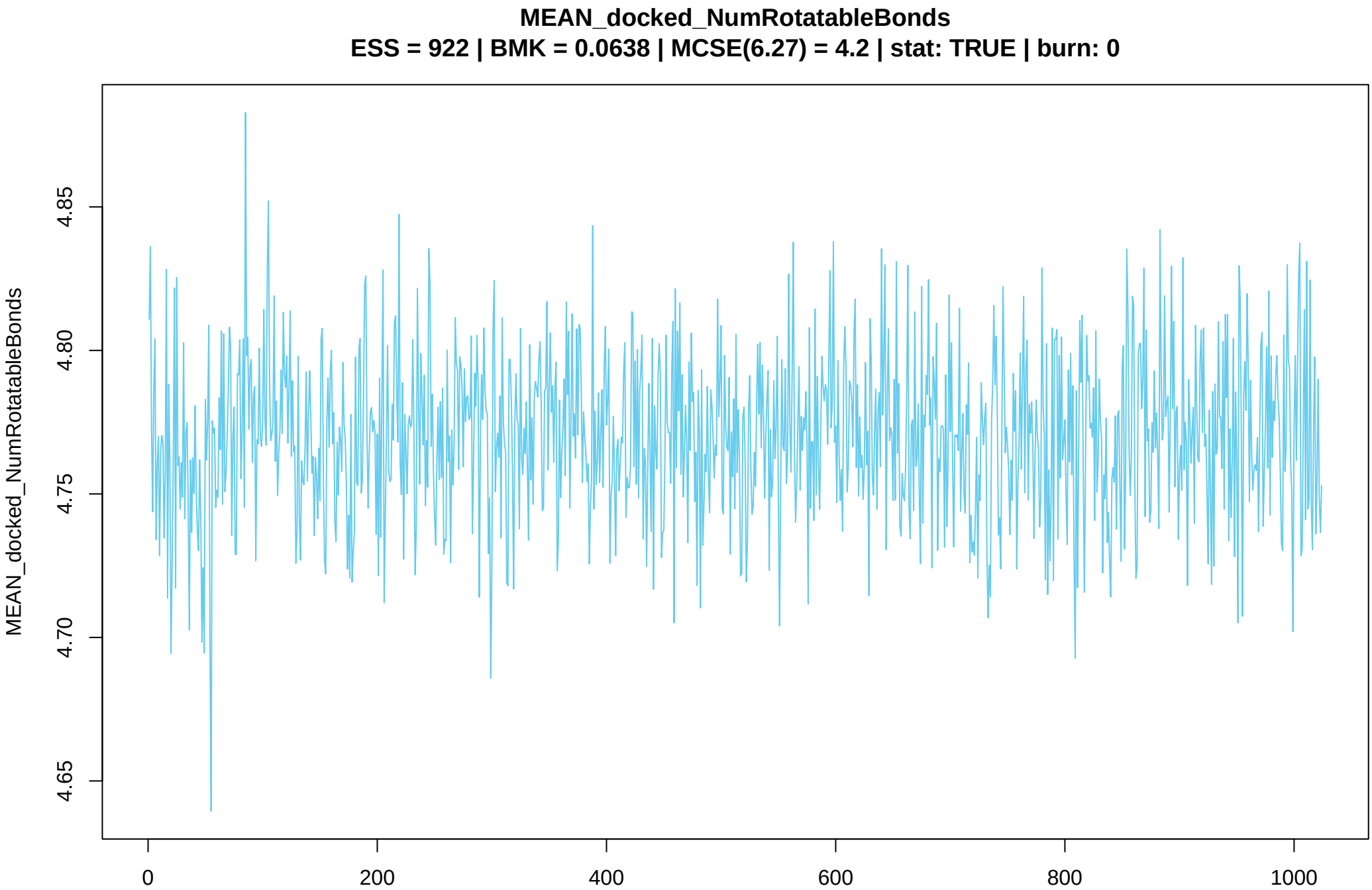

MEAN_log_mcs_unbonded_polar_sasa
ESS = 923 | BMK = 0.106 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0
MEAN_log_mcs_unbonded_polar_sasa
0.0
−0.1
−0.2
−0.3
−0.4
0
200
400
600
800
1000

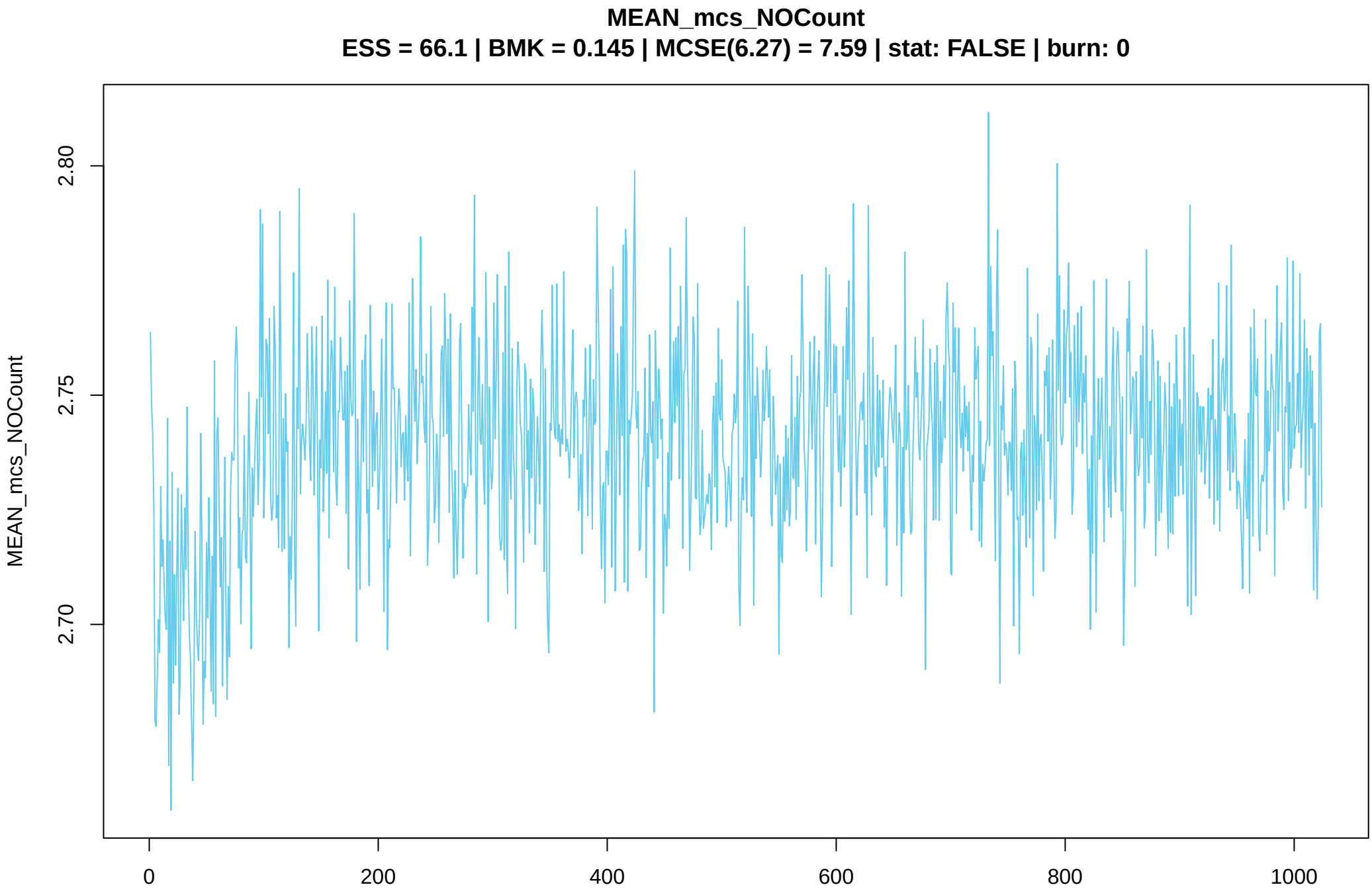

MEAN_logit_ec_tanimoto_similarity
ESS = 952 | BMK = 0.0698 | MCSE(6.27) = 3.5 | stat: FALSE | burn: 0
MEAN_logit_ec_tanimoto_similarity
−2.00
−2.02
−2.04
−2.06
−2.08
−2.10
0
200
400
600
800
1000

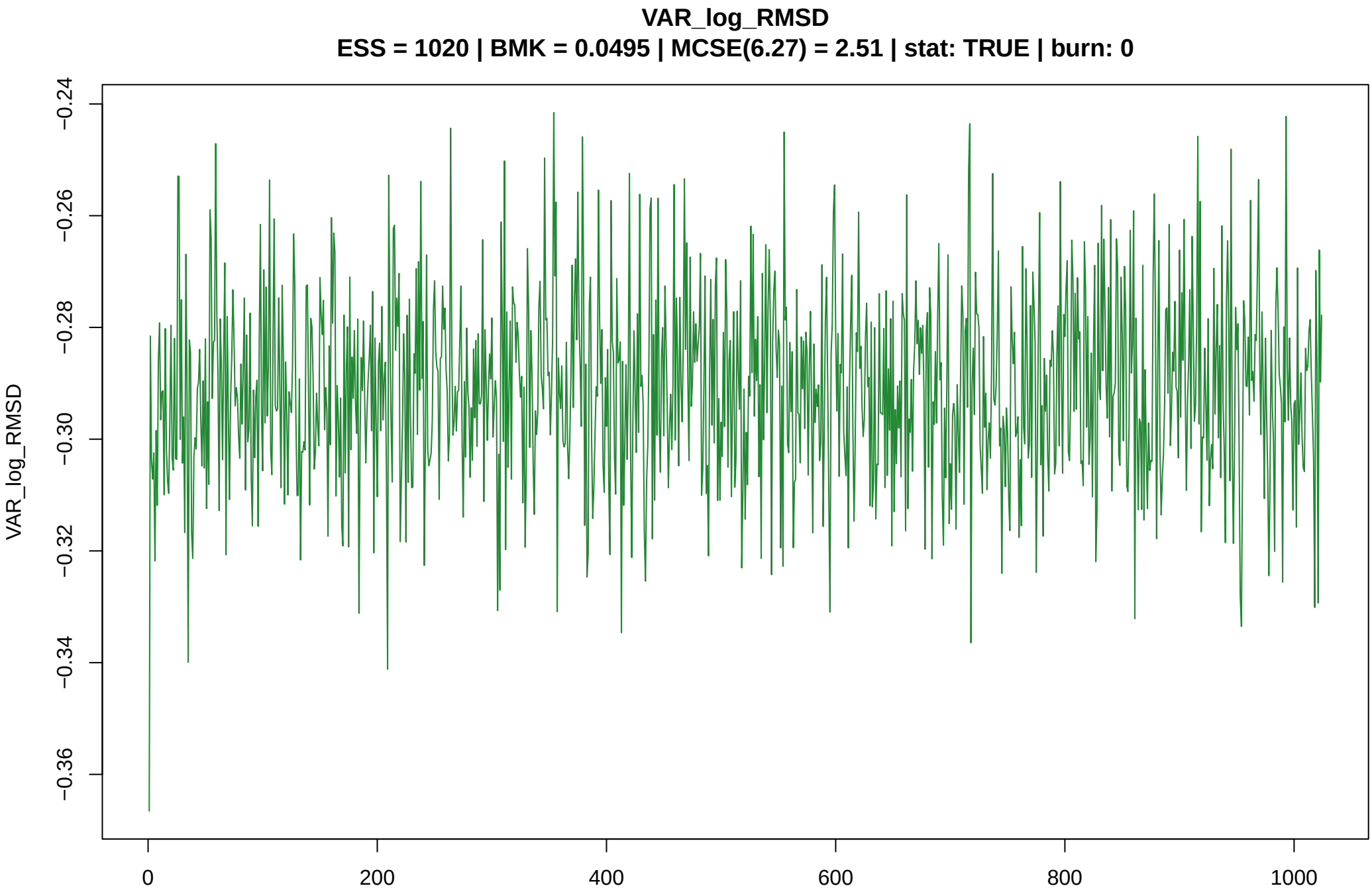

MEAN_mcs_NumHeteroAtoms
ESS = 116 | BMK = 0.14 | MCSE(6.27) = 7.44 | stat: FALSE | burn: 0
MEAN_mcs_NumHeteroAtoms
2.90
2.95
3.00
3.05
0
200
400
600
800
1000

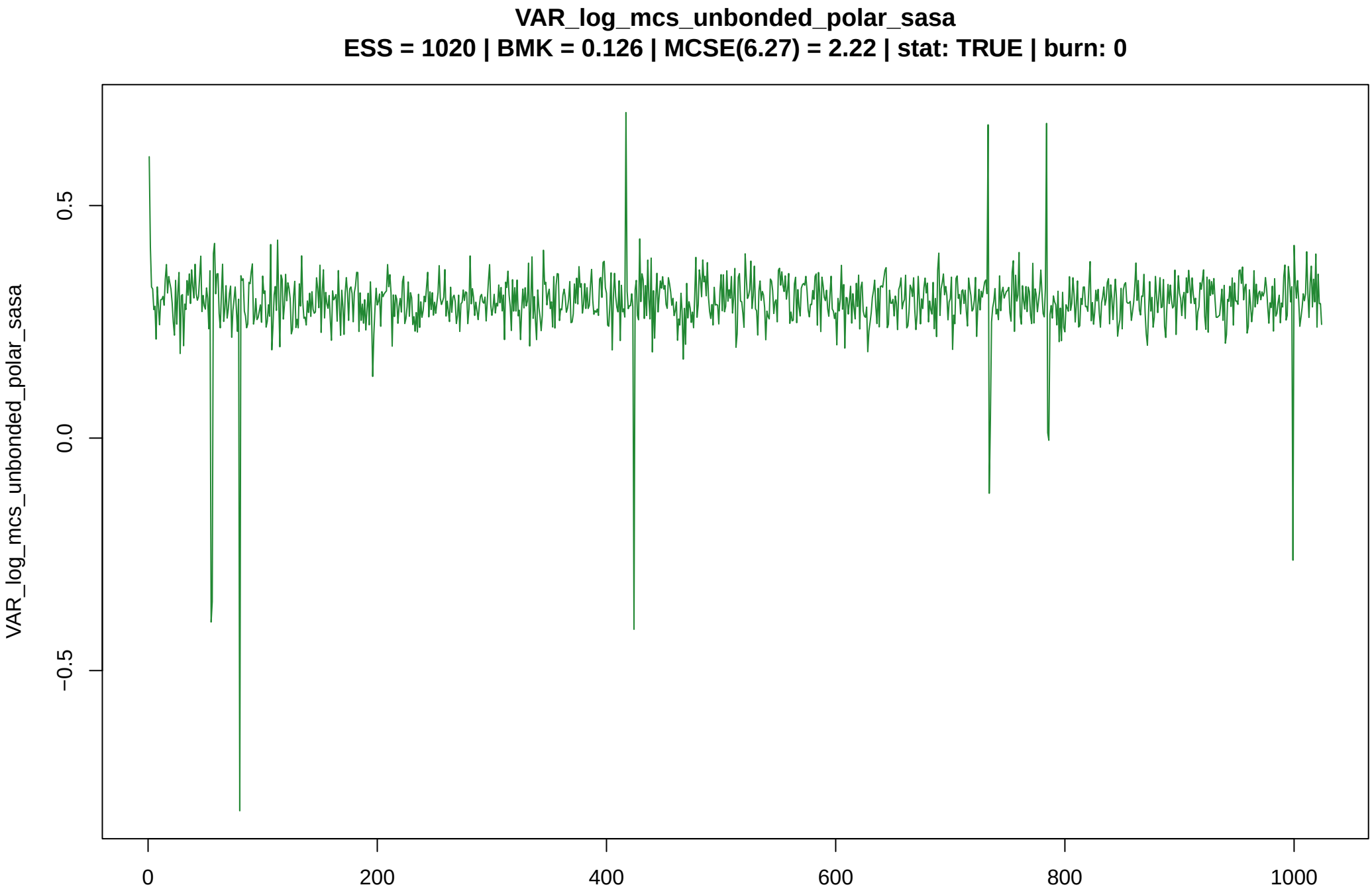

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0726 | MCSE(6.27) = 3.8 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
22.8
23.0
23.2
23.4
23.6
0
200
400
600
800
1000

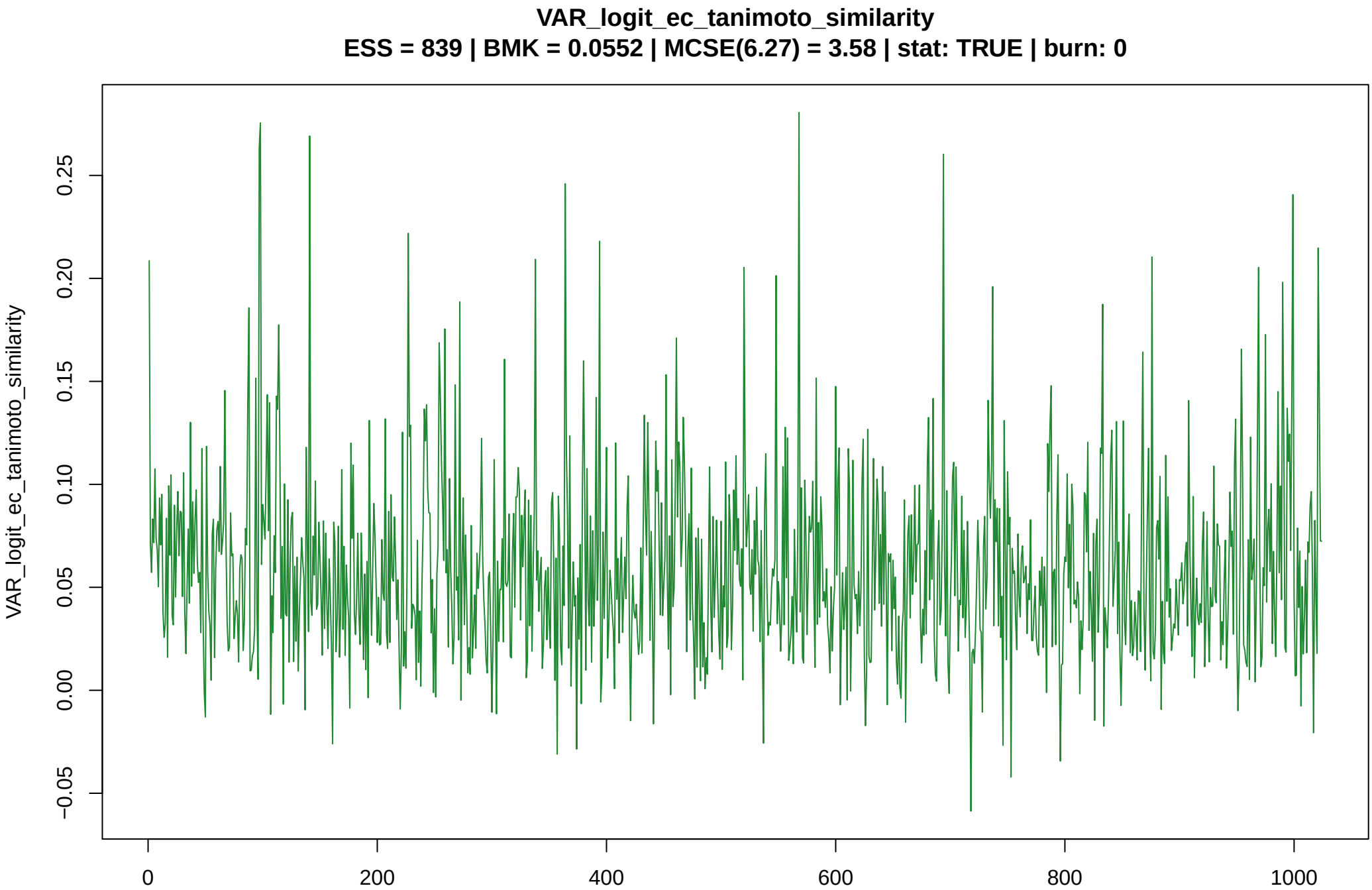

MEAN_mcs_RingCount
ESS = 758 | BMK = 0.0854 | MCSE(6.27) = 4.14 | stat: FALSE | burn: 0
MEAN_mcs_RingCount
0.80
0.82
0.84
0.86
0.88
0
200
400
600
800
1000

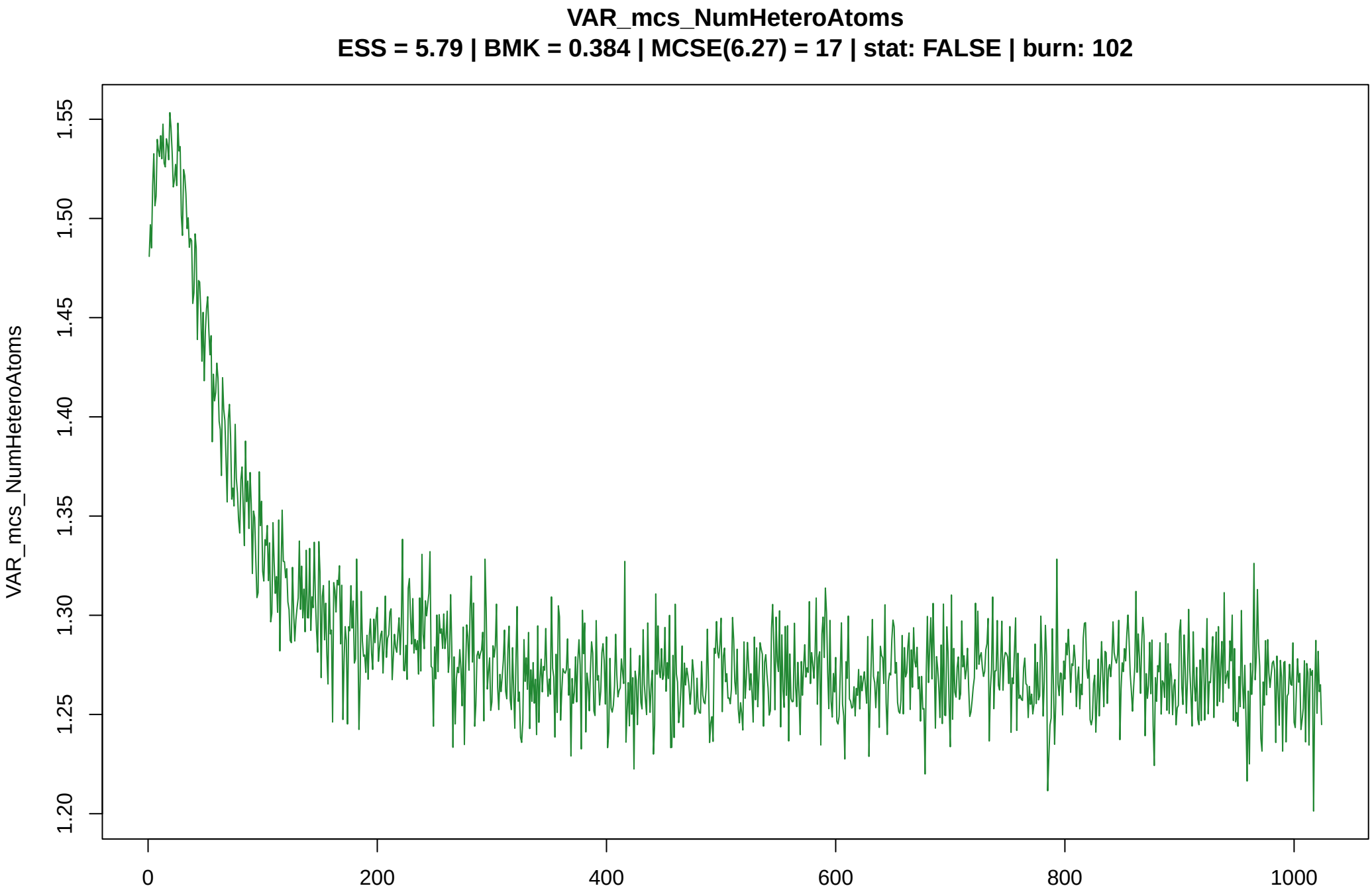

MEAN_docked_NumRotatableBonds
ESS = 922 | BMK = 0.0638 | MCSE(6.27) = 4.2 | stat: TRUE | burn: 0
MEAN_docked_NumRotatableBonds
4.65
4.70
4.75
4.80
4.85
0
200
400
600
800
1000

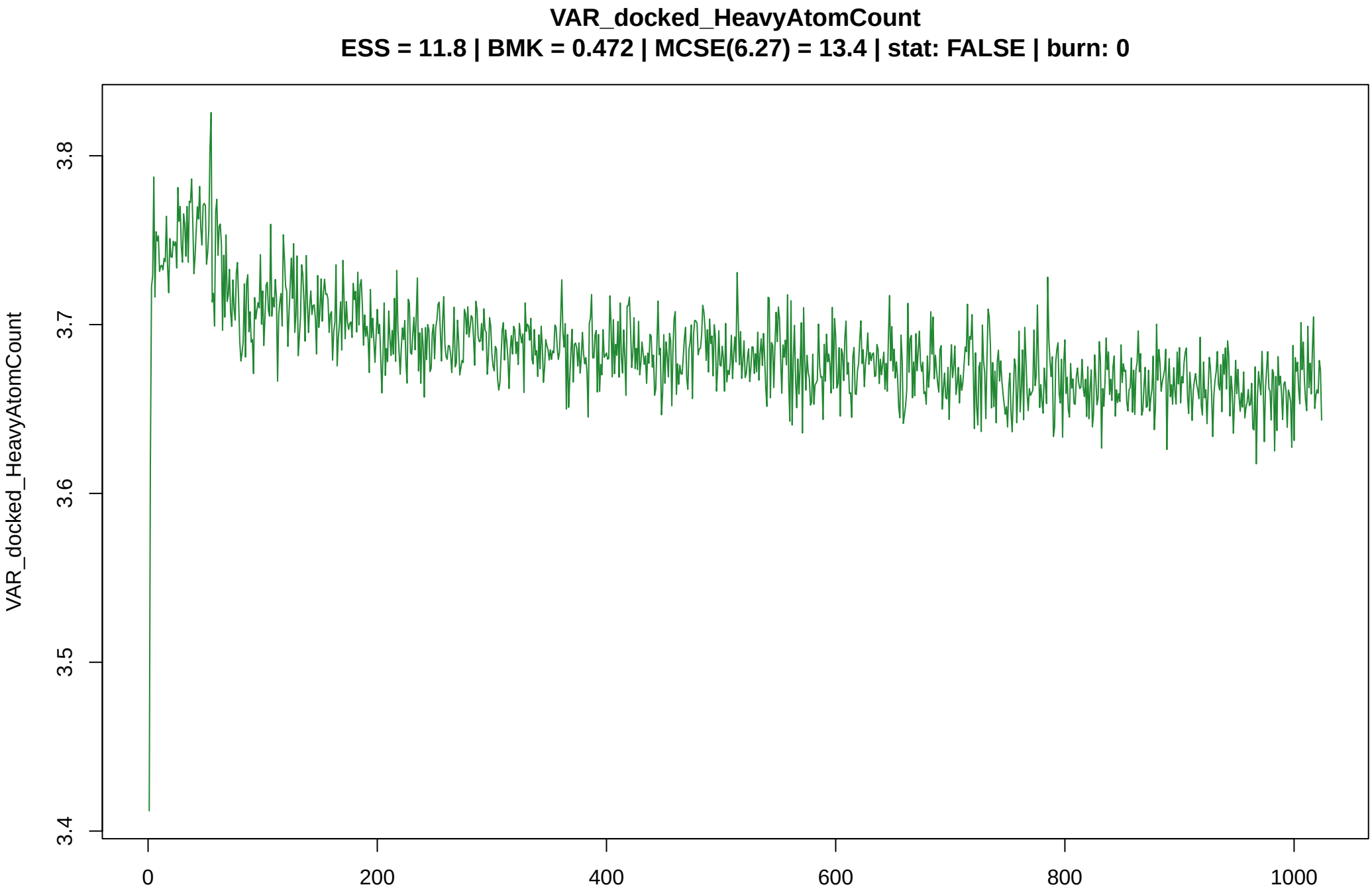

MEAN_mcs_NOCount
ESS = 66.1 | BMK = 0.145 | MCSE(6.27) = 7.59 | stat: FALSE | burn: 0
MEAN_mcs_NOCount
2.70
2.75
2.80
0
200
400
600
800
1000

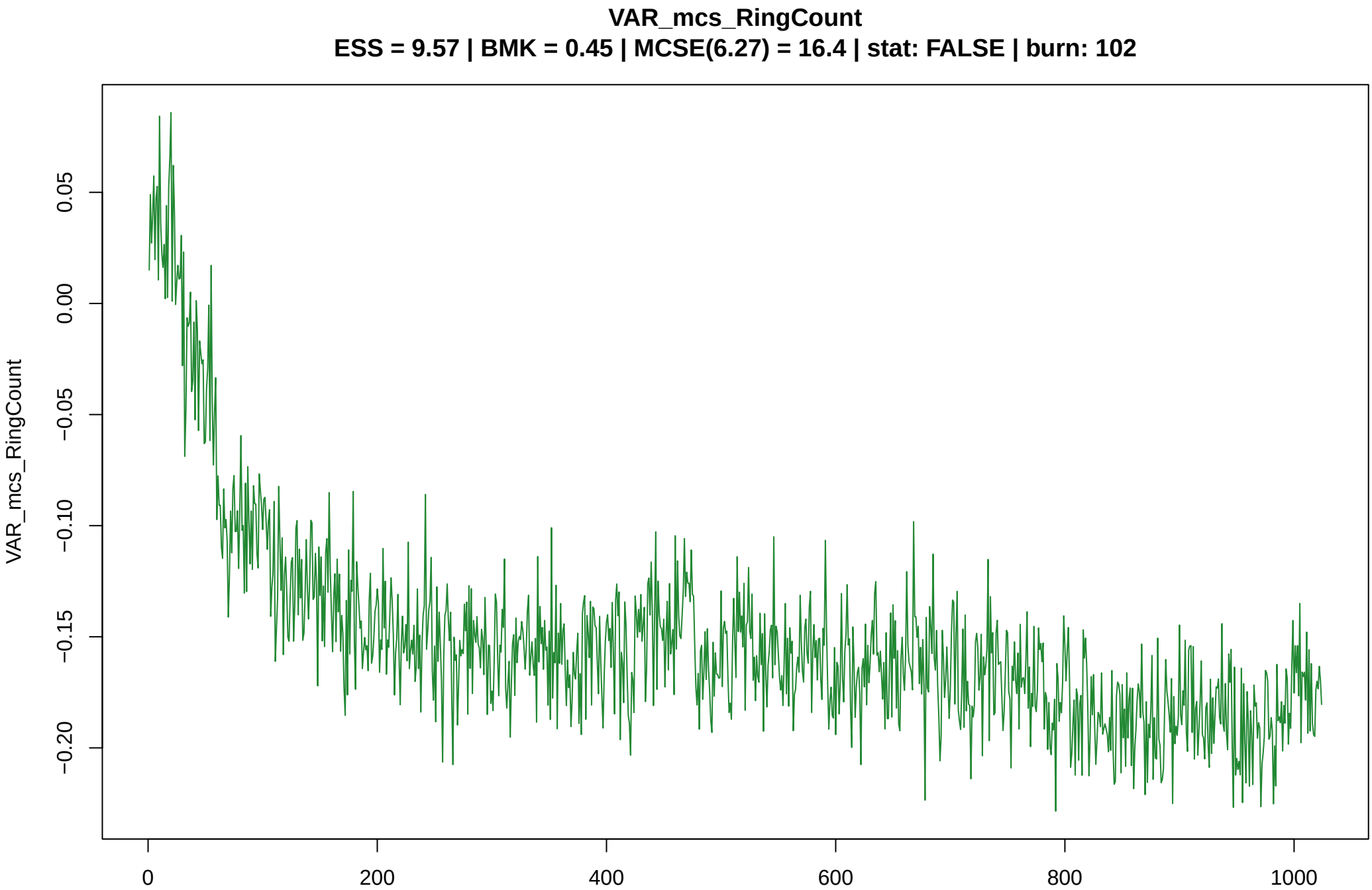

VAR_log_RMSD
ESS = 1020 | BMK = 0.0495 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0
VAR_log_RMSD
−0.24
−0.26
−0.28
−0.30
−0.32
−0.34
−0.36
0
200
400
600
800
1000

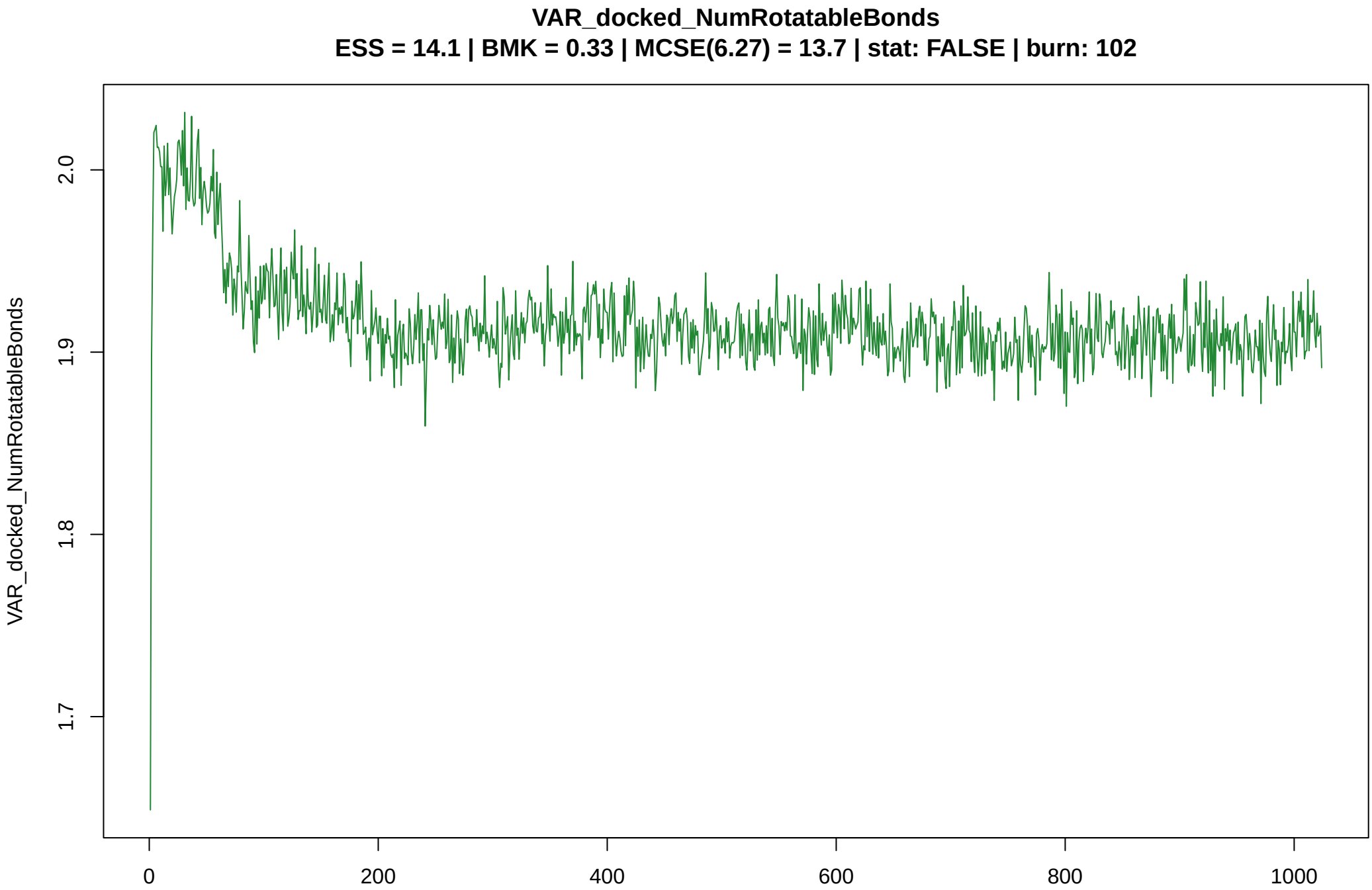

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.126 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0
VAR_log_mcs_unbonded_polar_sasa
0.5
0.0
−0.5
0
200
400
600
800
1000

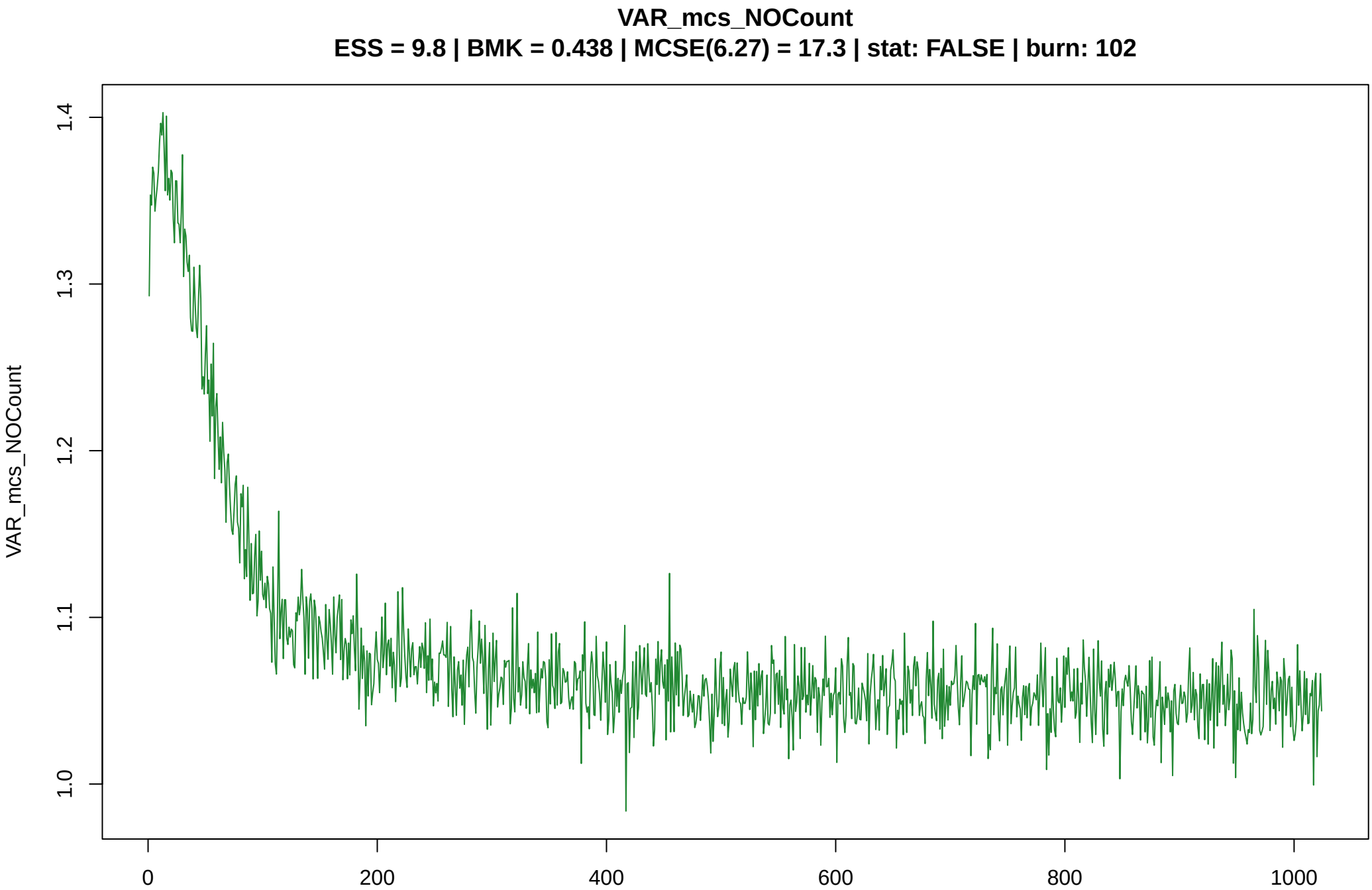

VAR_logit_ec_tanimoto_similarity
ESS = 839 | BMK = 0.0552 | MCSE(6.27) = 3.58 | stat: TRUE | burn: 0
VAR_logit_ec_tanimoto_similarity
−0.05
0.00
0.05
0.10
0.15
0.20
0.25
0
200
400
600
800
1000

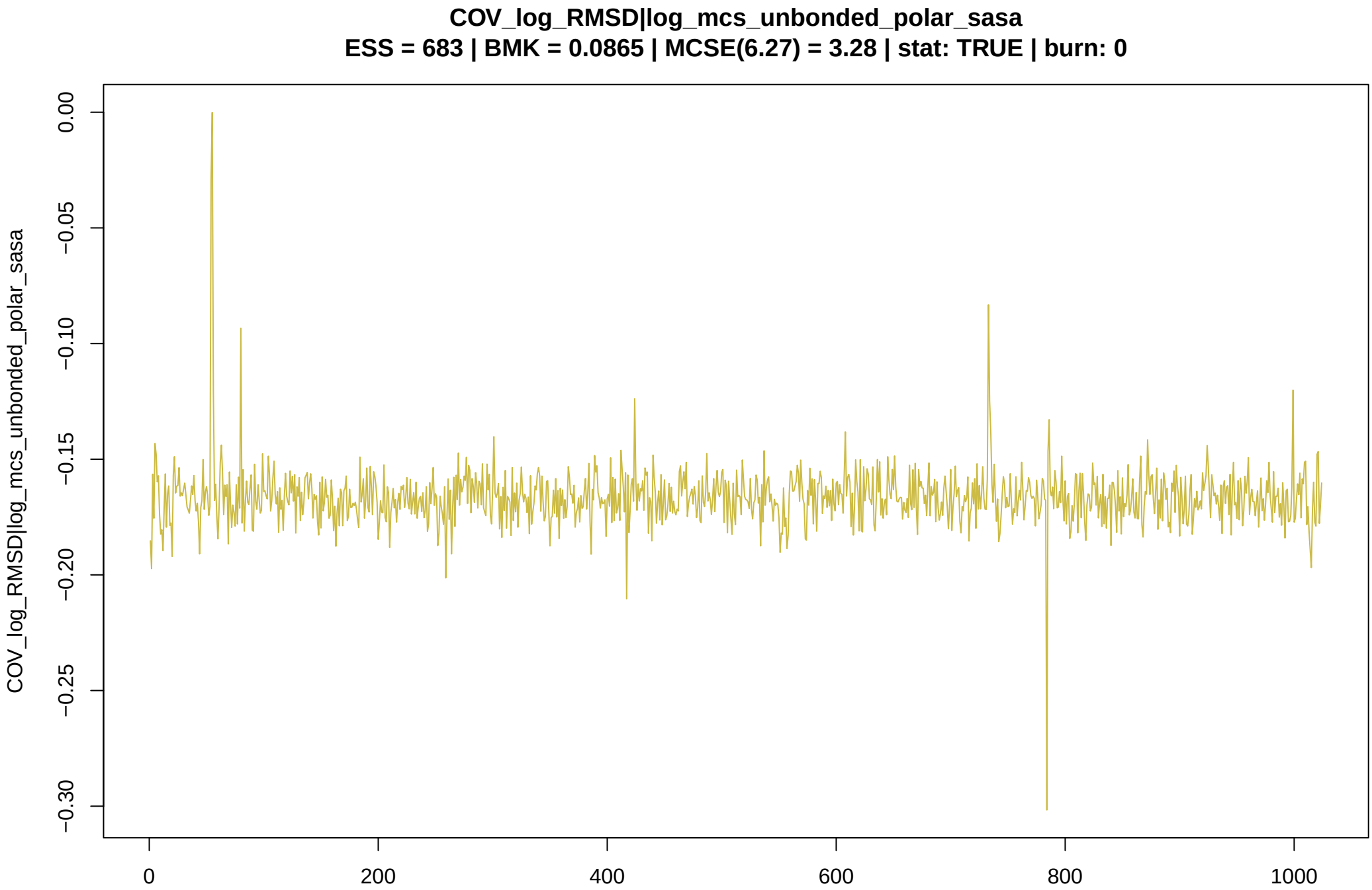

VAR_mcs_NumHeteroAtoms
ESS = 5.79 | BMK = 0.384 | MCSE(6.27) = 17 | stat: FALSE | burn: 102
VAR_mcs_NumHeteroAtoms
1.20
1.25
1.30
1.35
1.40
1.45
1.50
1.55
0
200
400
600
800
1000

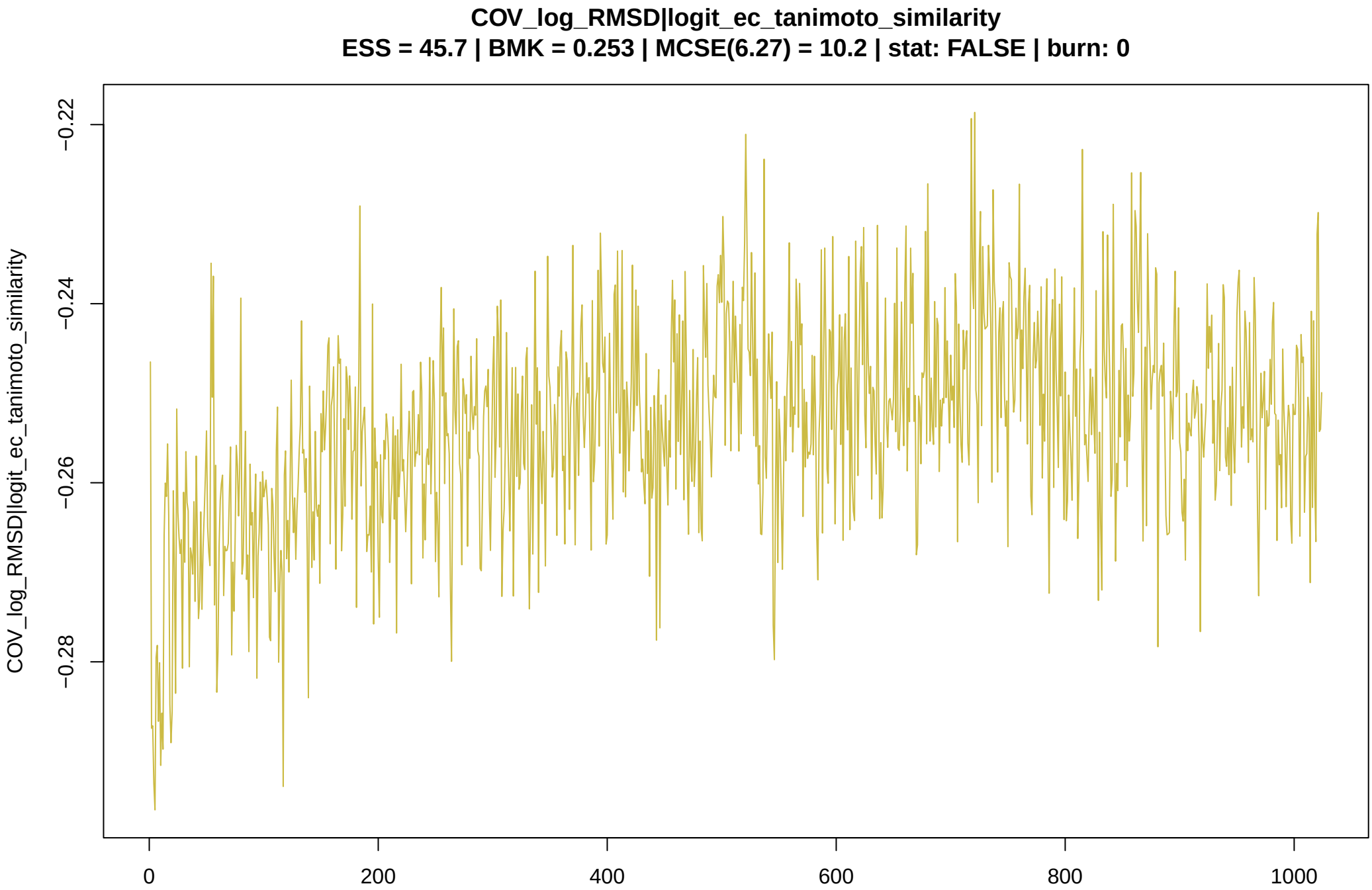

VAR_docked_HeavyAtomCount
ESS = 11.8 | BMK = 0.472 | MCSE(6.27) = 13.4 | stat: FALSE | burn: 0
VAR_docked_HeavyAtomCount
3.4
3.5
3.6
3.7
3.8
0
200
400
600
800
1000

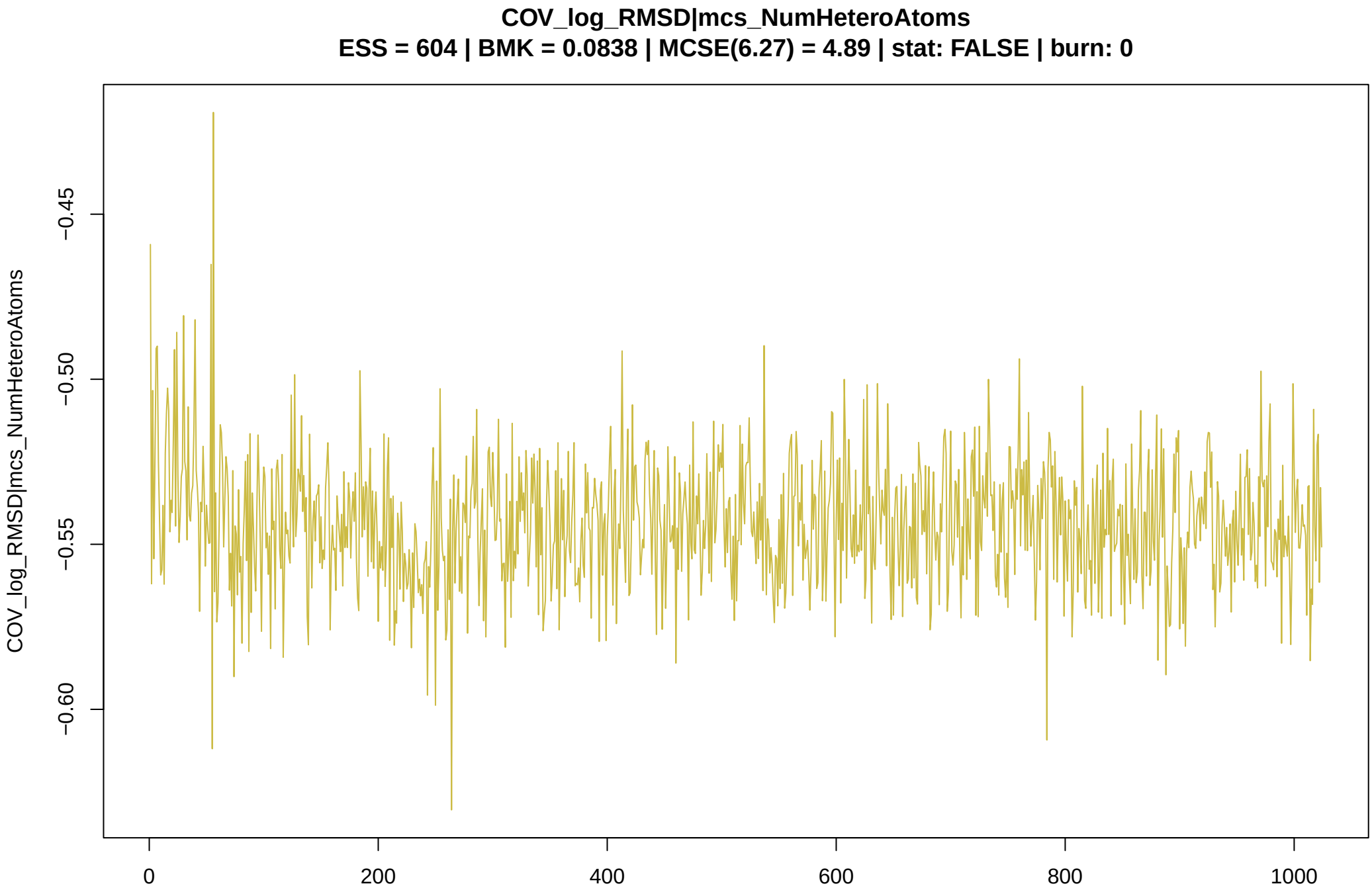

VAR_mcs_RingCount
ESS = 9.57 | BMK = 0.45 | MCSE(6.27) = 16.4 | stat: FALSE | burn: 102
VAR_mcs_RingCount
0.05
0.00
−0.05
−0.10
−0.15
−0.20
0
200
400
600
800
1000

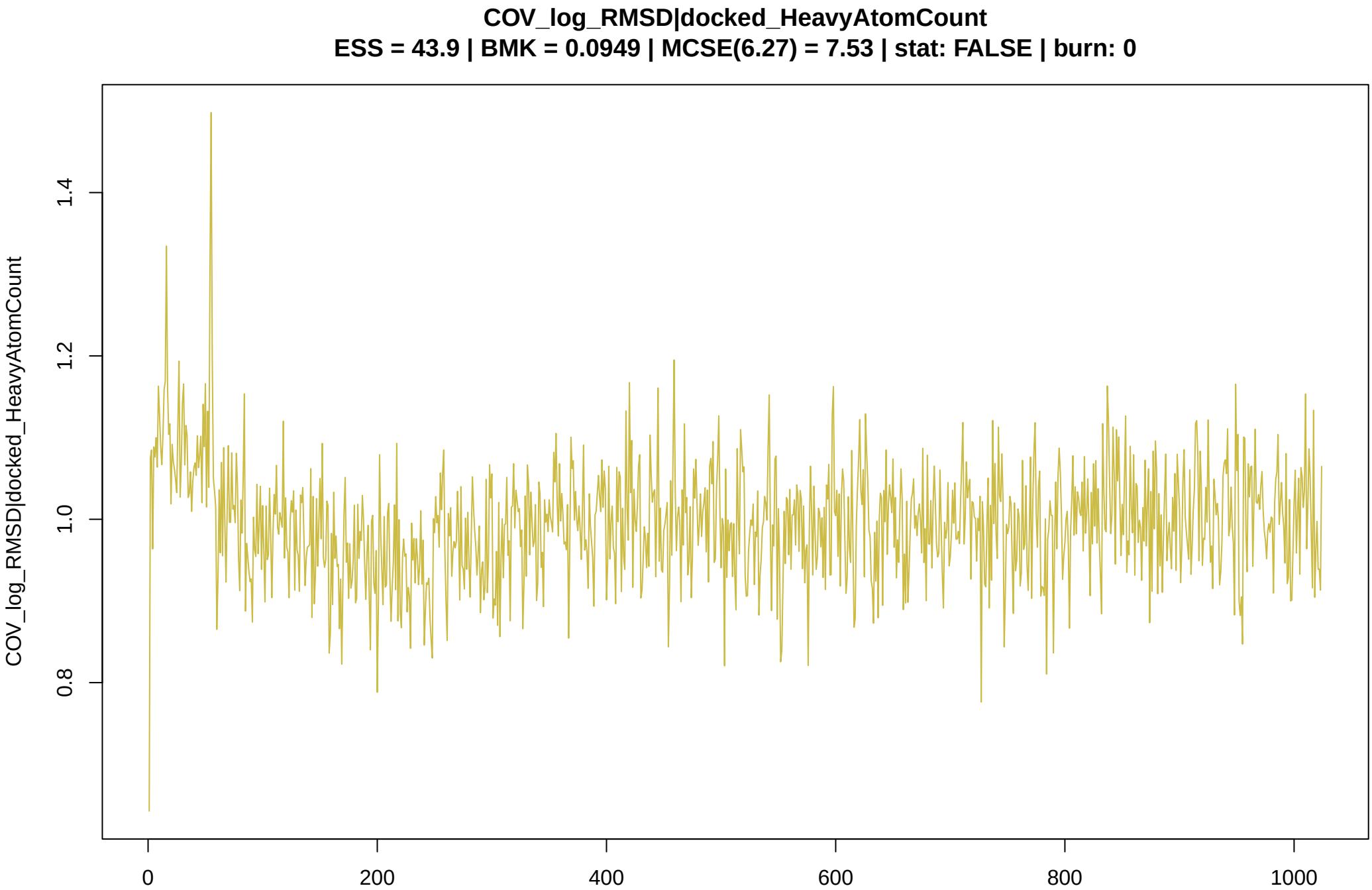

VAR_docked_NumRotatableBonds
ESS = 14.1 | BMK = 0.33 | MCSE(6.27) = 13.7 | stat: FALSE | burn: 102
VAR_docked_NumRotatableBonds
2.0
1.9
1.8
1.7
0
200
400
600
800
1000

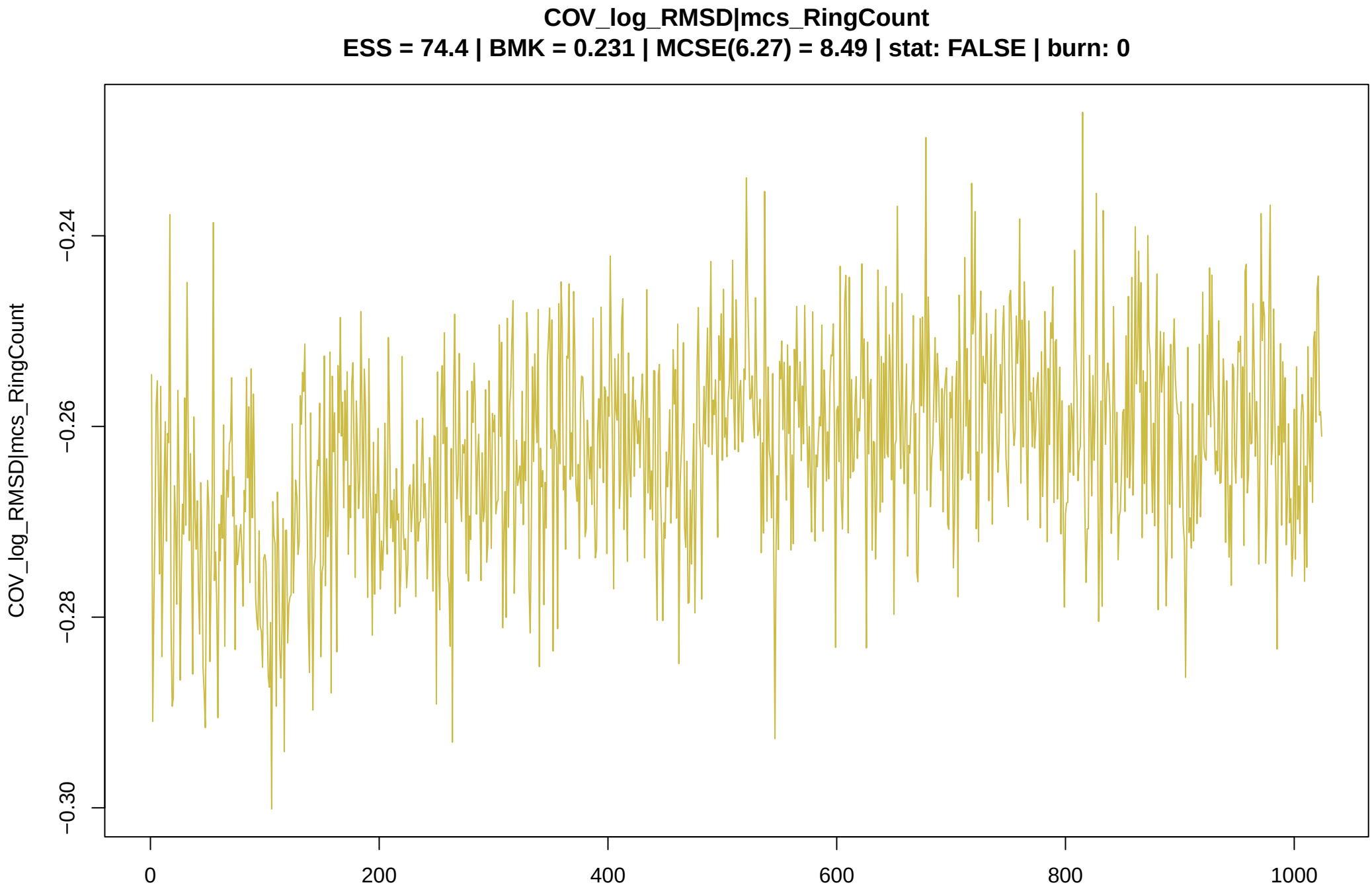

VAR_mcs_NOCount
ESS = 9.8 | BMK = 0.438 | MCSE(6.27) = 17.3 | stat: FALSE | burn: 102
VAR_mcs_NOCount
1.0
1.1
1.2
1.3
1.4
0
200
400
600
800
1000

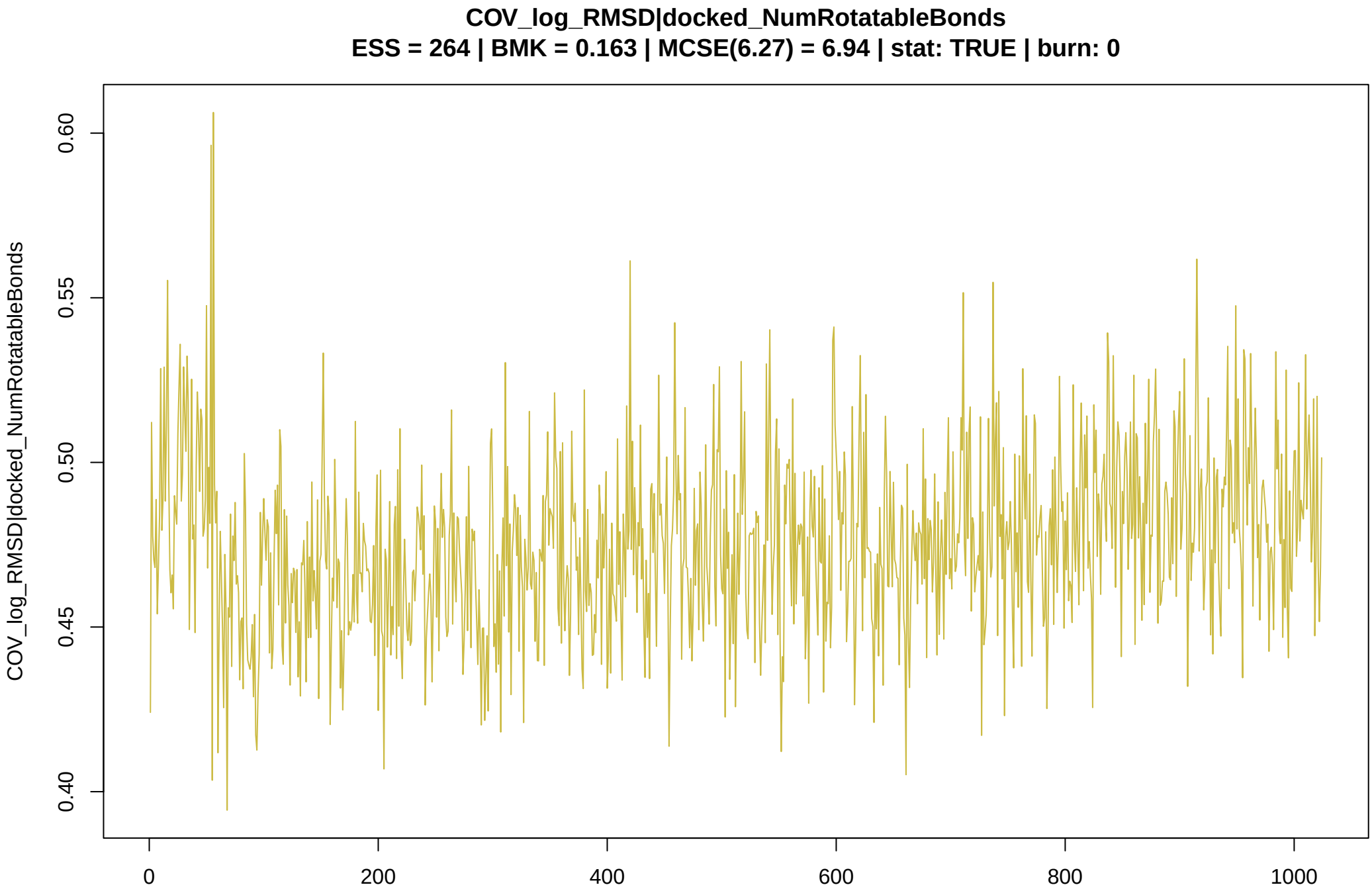

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 683 | BMK = 0.0865 | MCSE(6.27) = 3.28 | stat: TRUE | burn: 0
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
0
200
400
600
800
1000

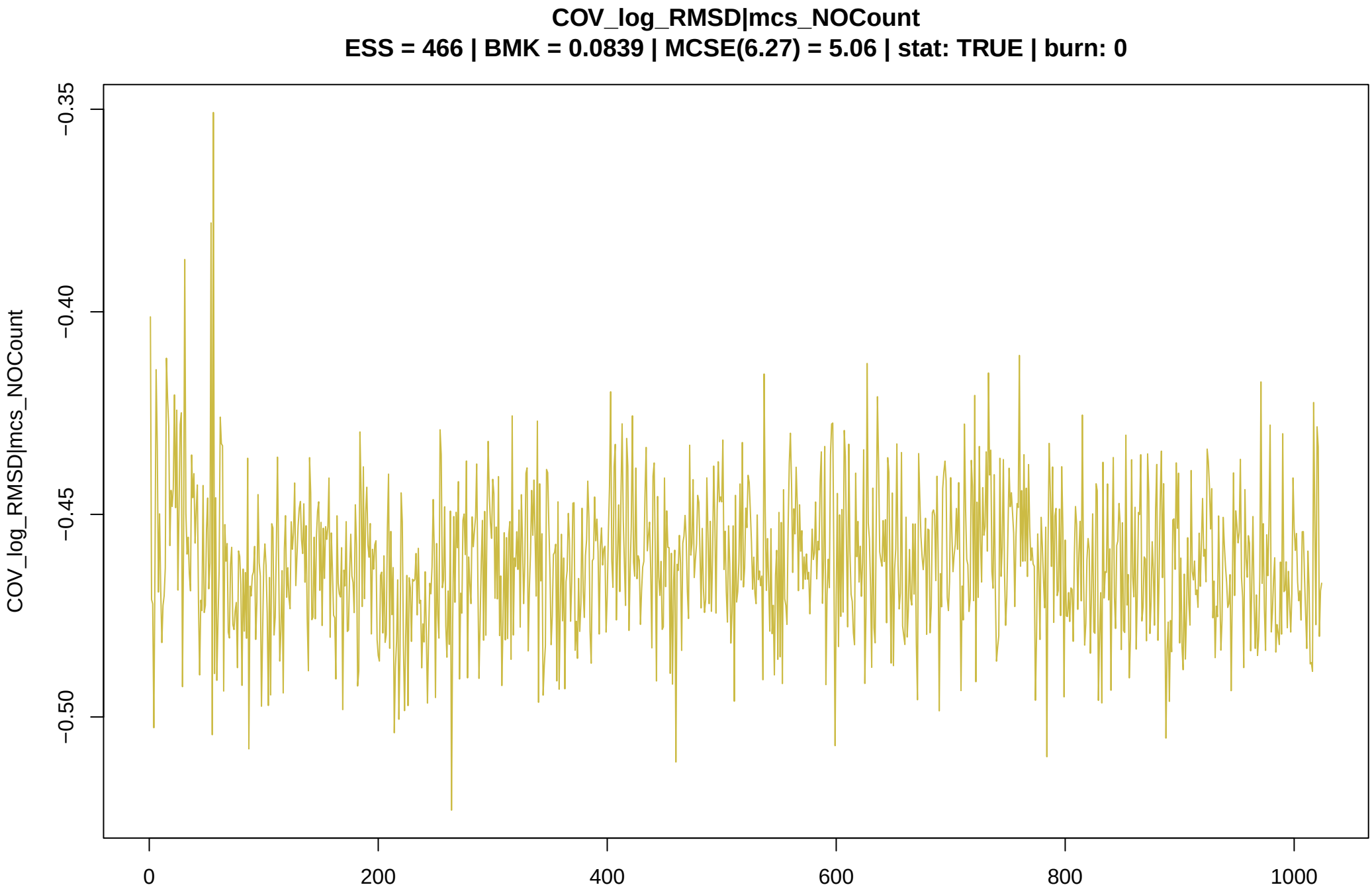

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 45.7 | BMK = 0.253 | MCSE(6.27) = 10.2 | stat: FALSE | burn: 0
COV_log_RMSD|logit_ec_tanimoto_similarity
−0.22
−0.24
−0.26
−0.28
0
200
400
600
800
1000

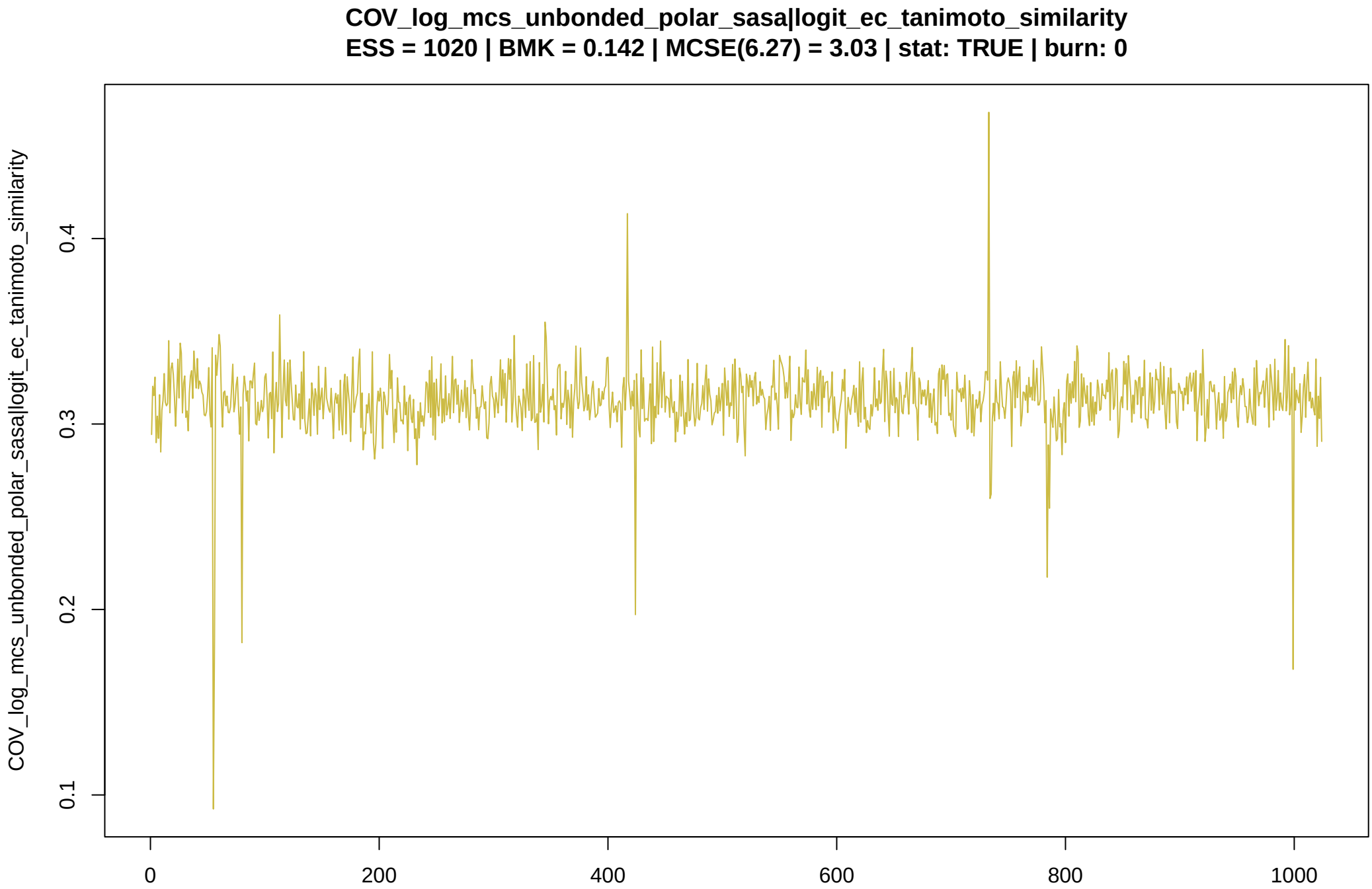

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 604 | BMK = 0.0838 | MCSE(6.27) = 4.89 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.45
−0.50
−0.55
−0.60
0
200
400
600
800
1000

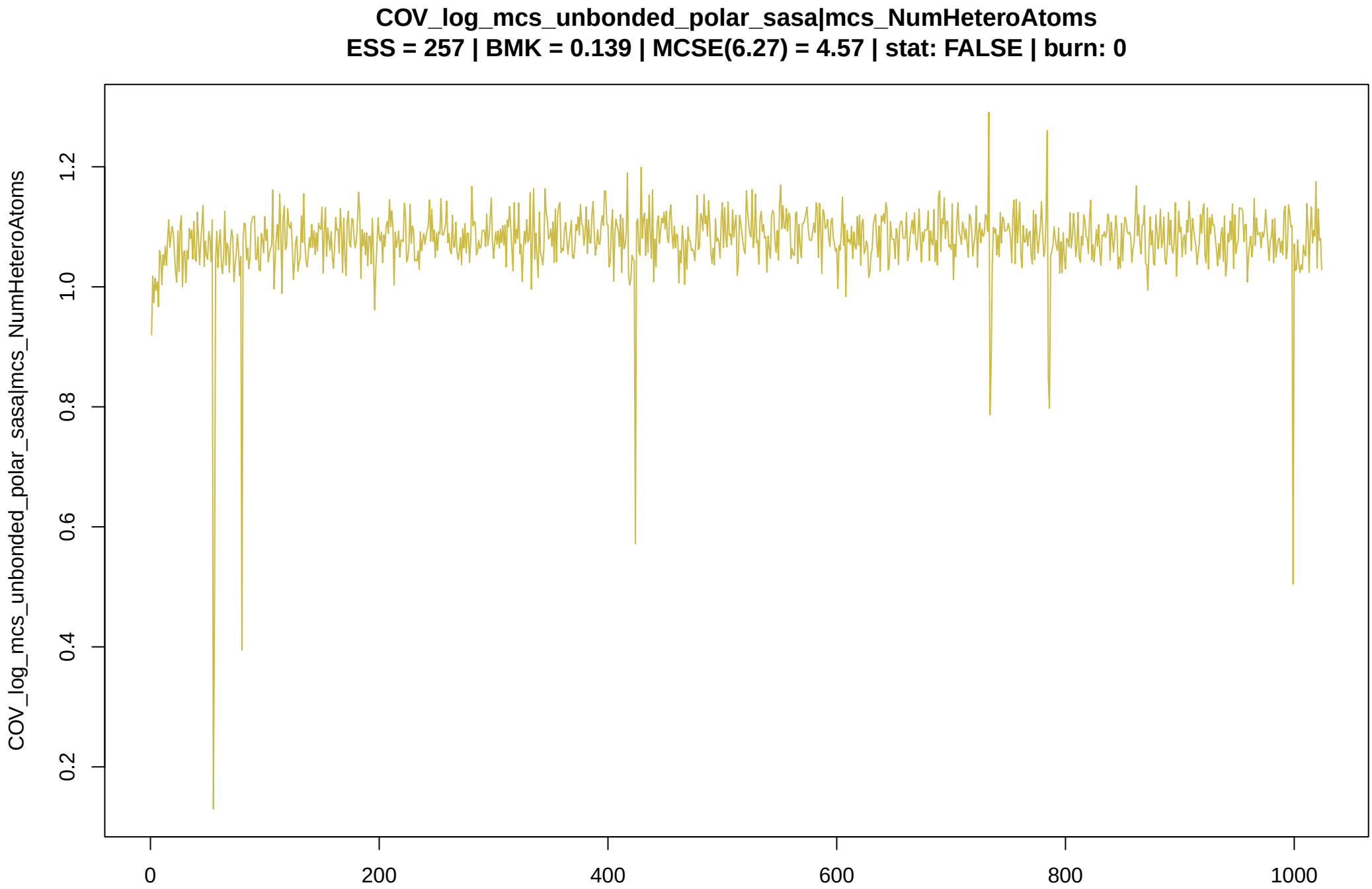

COV_log_RMSD|docked_HeavyAtomCount
ESS = 43.9 | BMK = 0.0949 | MCSE(6.27) = 7.53 | stat: FALSE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
0.8
1.0
1.2
1.4
0
200
400
600
800
1000

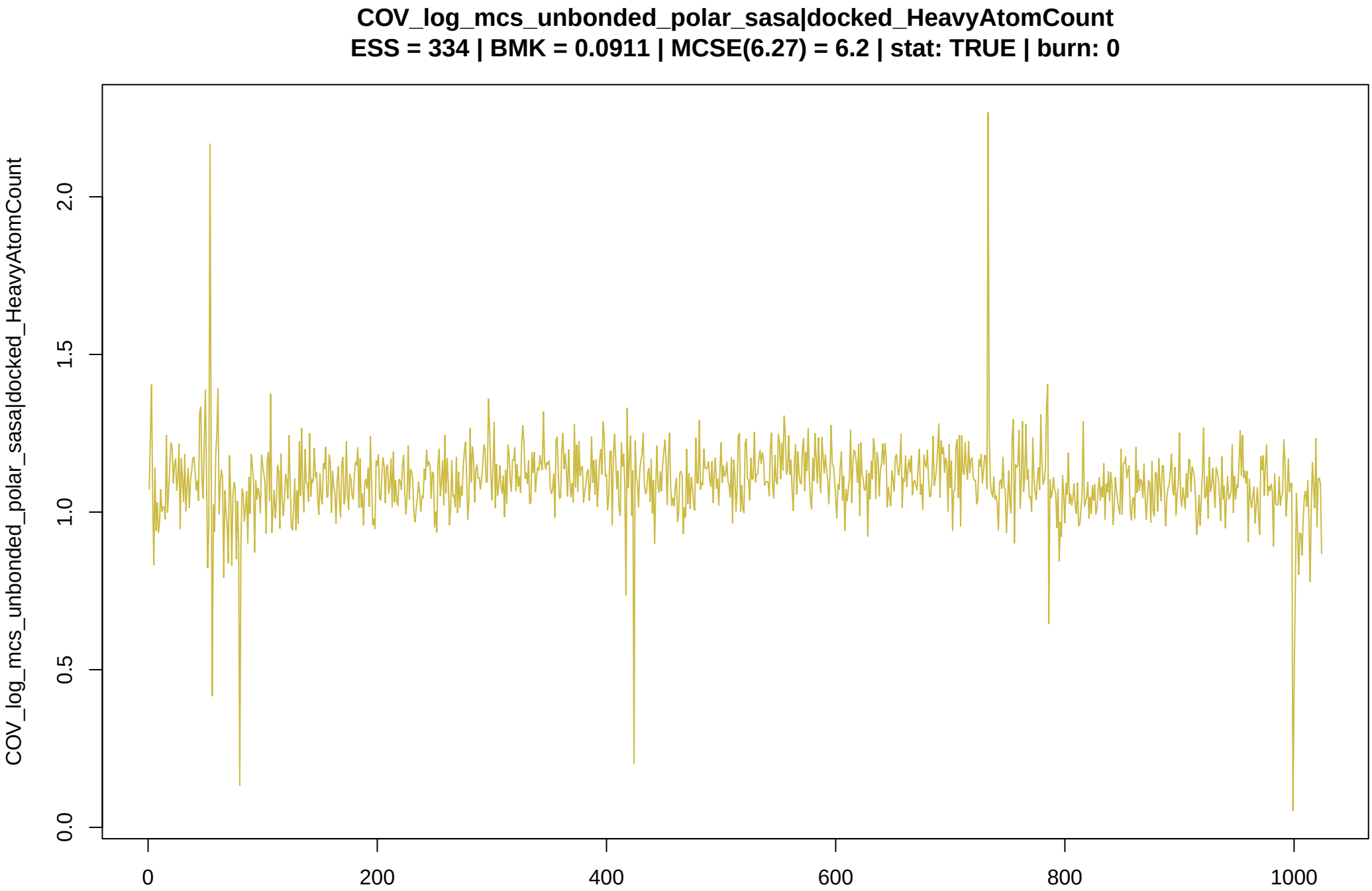

COV_log_RMSD|mcs_RingCount
ESS = 74.4 | BMK = 0.231 | MCSE(6.27) = 8.49 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.24
−0.26
−0.28
−0.30
0
200
400
600
800
1000

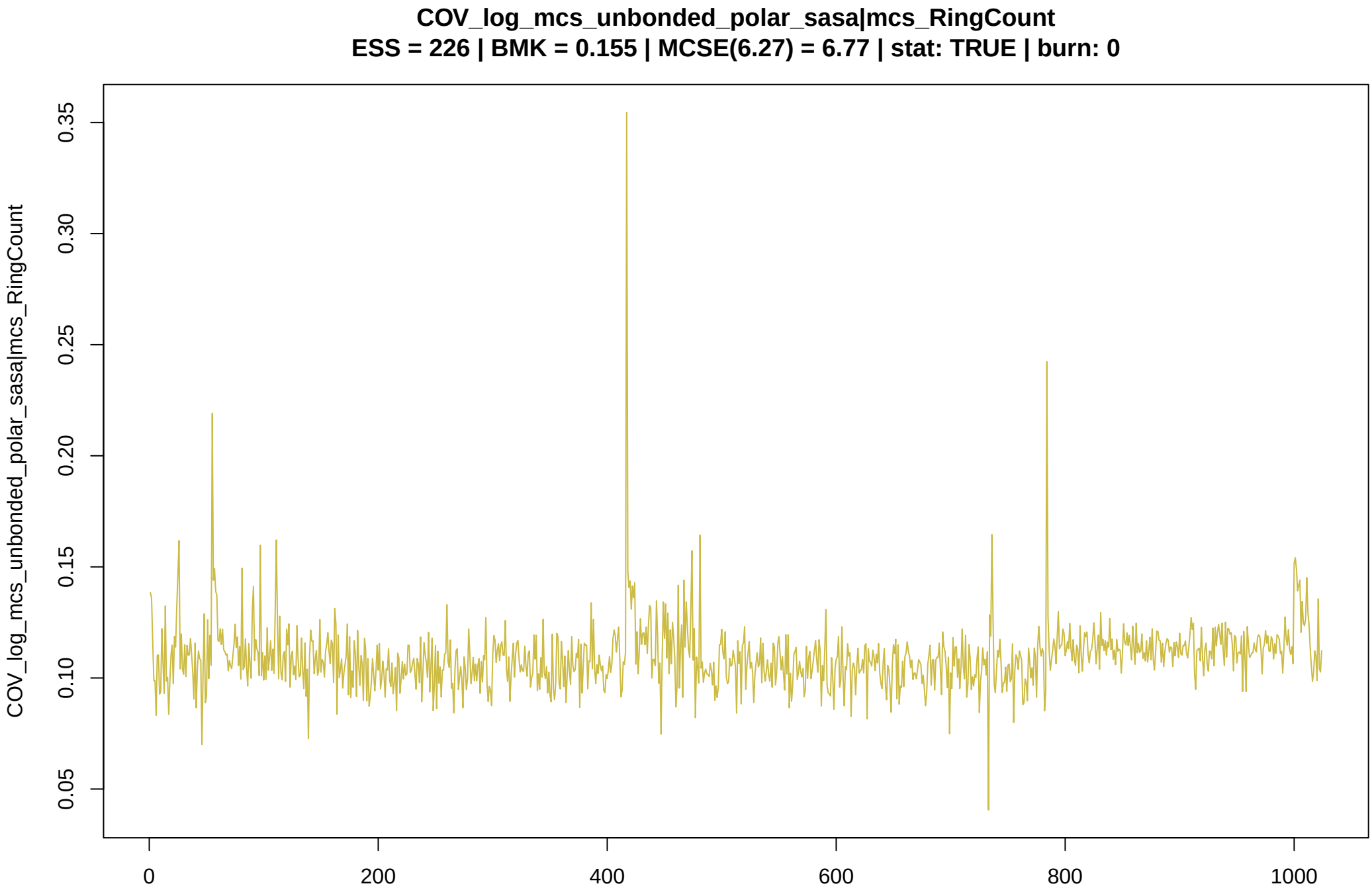

COV_log_RMSD|docked_NumRotatableBonds
ESS = 264 | BMK = 0.163 | MCSE(6.27) = 6.94 | stat: TRUE | burn: 0
COV_log_RMSD|docked_NumRotatableBonds
0.40
0.45
0.50
0.55
0.60
0
200
400
600
800
1000

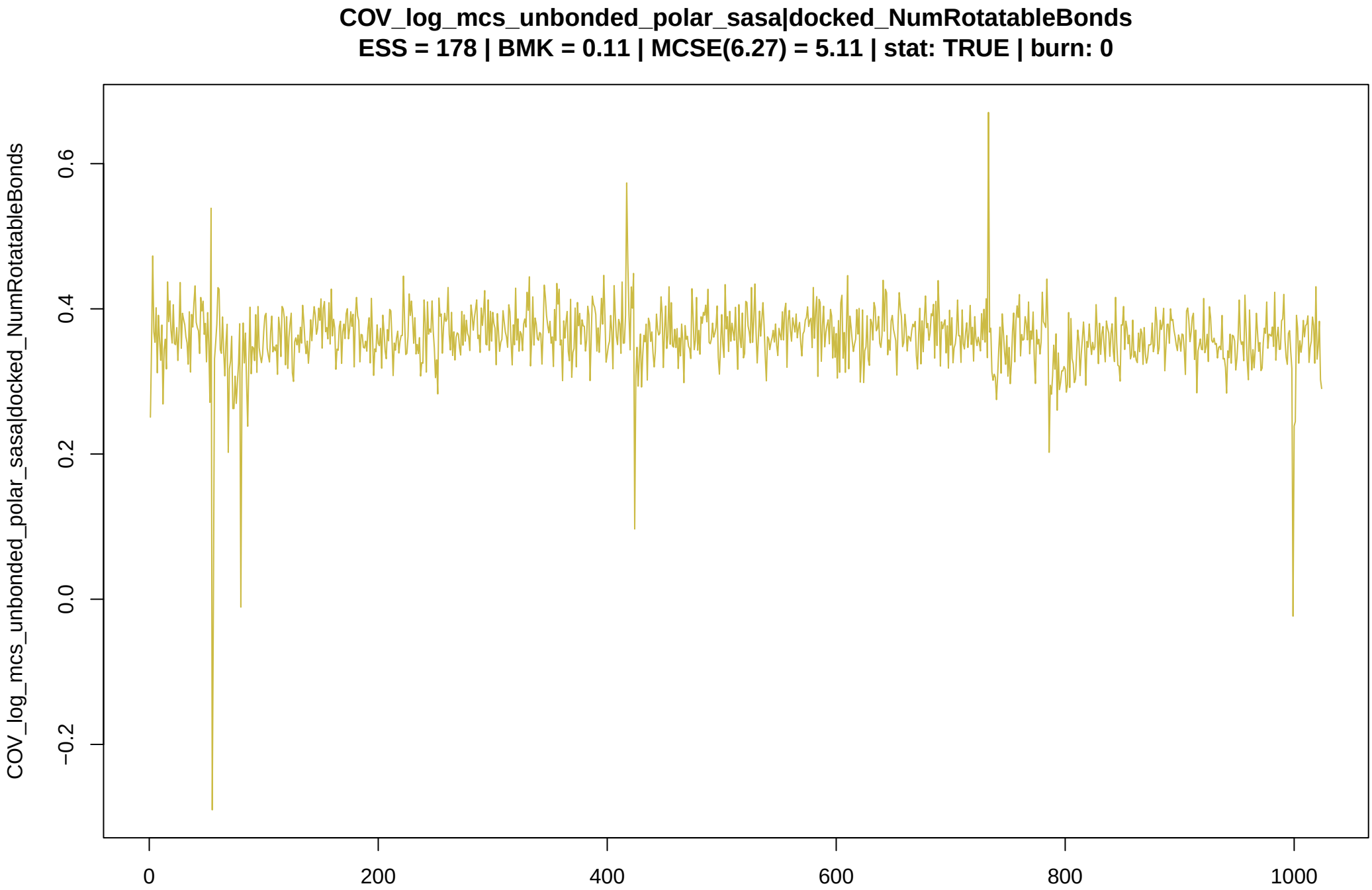

COV_log_RMSD|mcs_NOCount
ESS = 466 | BMK = 0.0839 | MCSE(6.27) = 5.06 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NOCount
−0.35
−0.40
−0.45
−0.50
0
200
400
600
800
1000

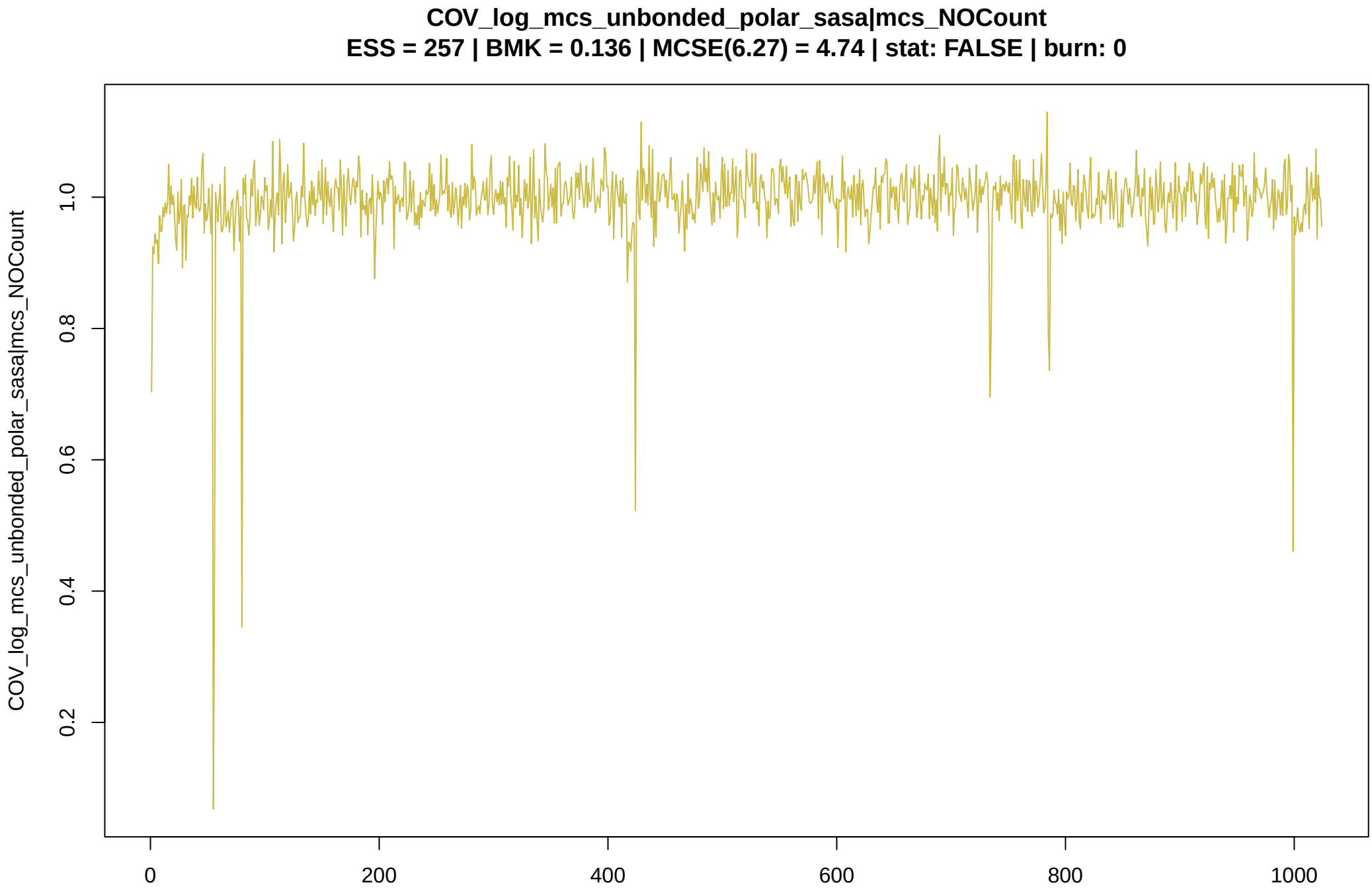

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.142 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0.1
0.2
0.3
0.4
0
200
400
600
800
1000

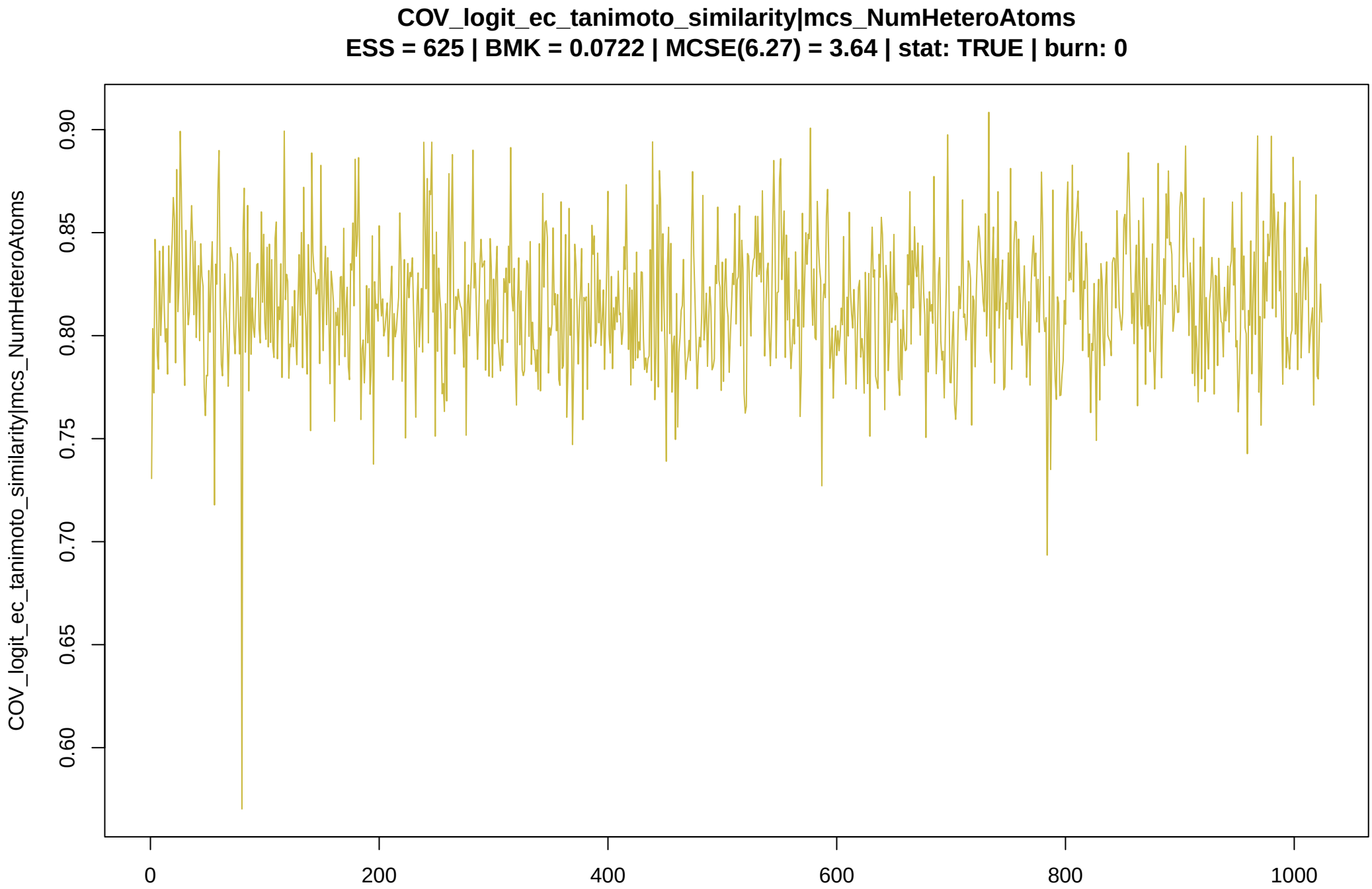

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 257 | BMK = 0.139 | MCSE(6.27) = 4.57 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.2
0.4
0.6
0.8
1.0
1.2
0
200
400
600
800
1000

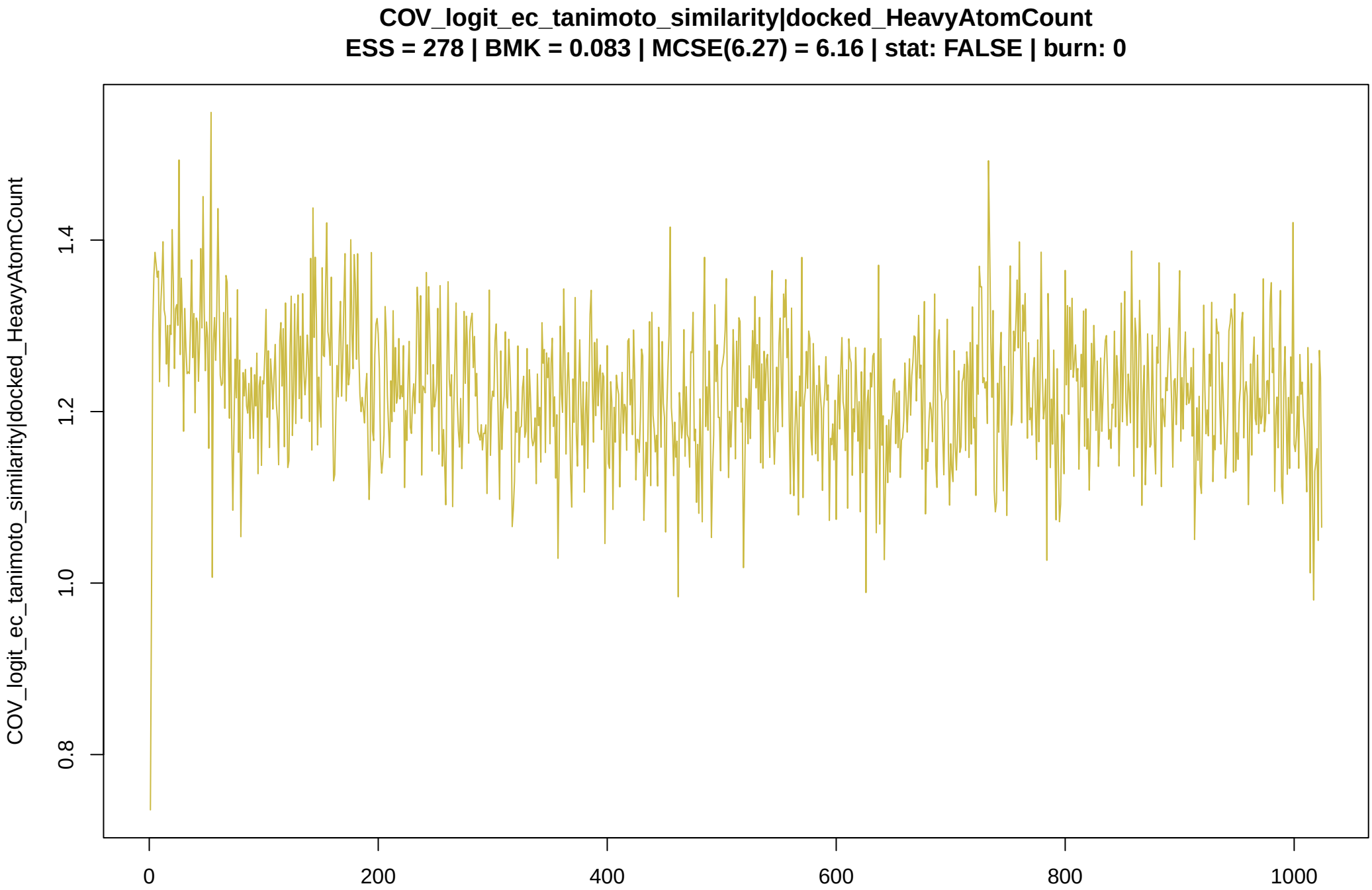

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 334 | BMK = 0.0911 | MCSE(6.27) = 6.2 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0.0
0.5
1.0
1.5
2.0
0
200
400
600
800
1000

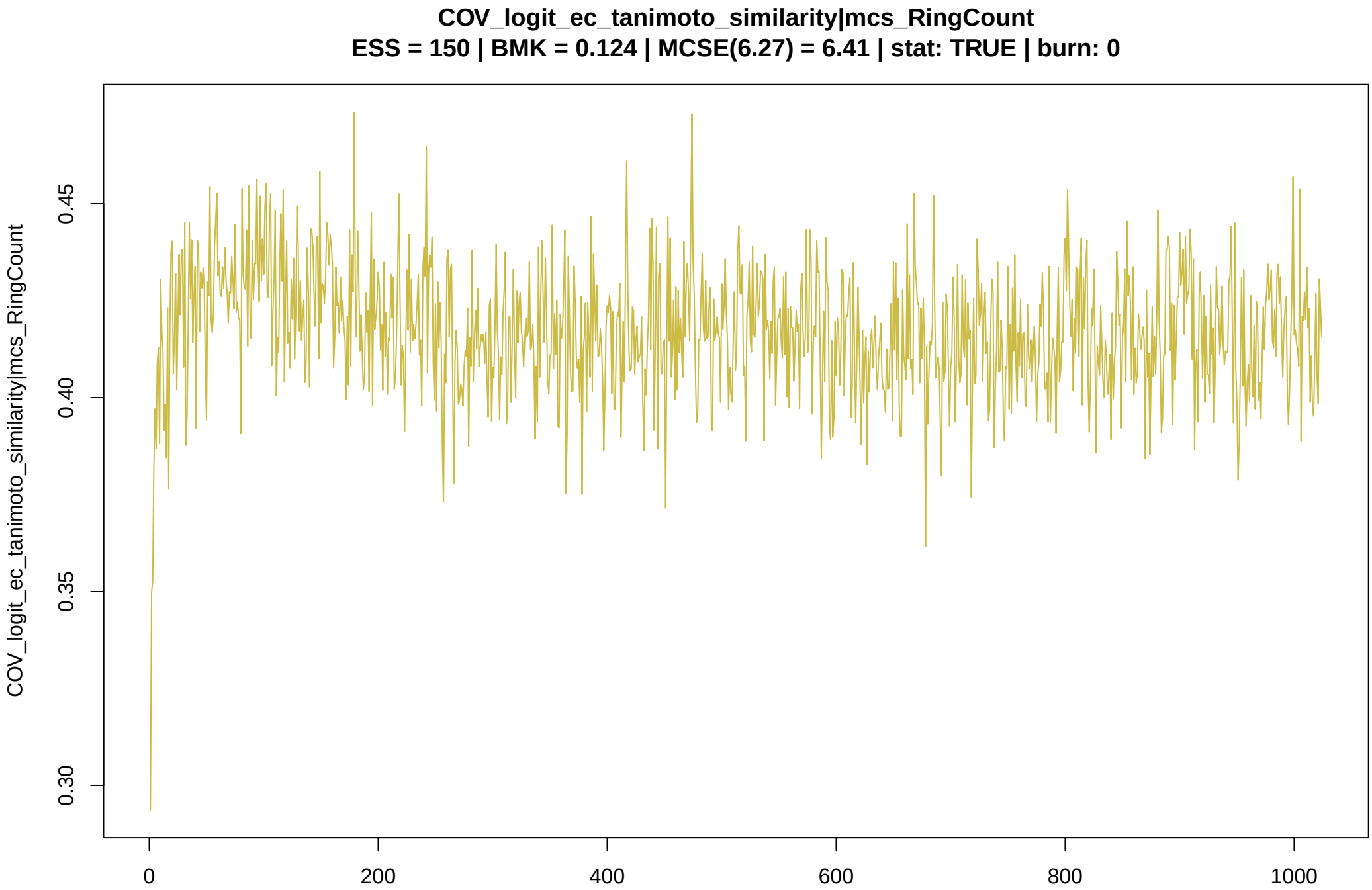

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 226 | BMK = 0.155 | MCSE(6.27) = 6.77 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0
200
400
600
800
1000

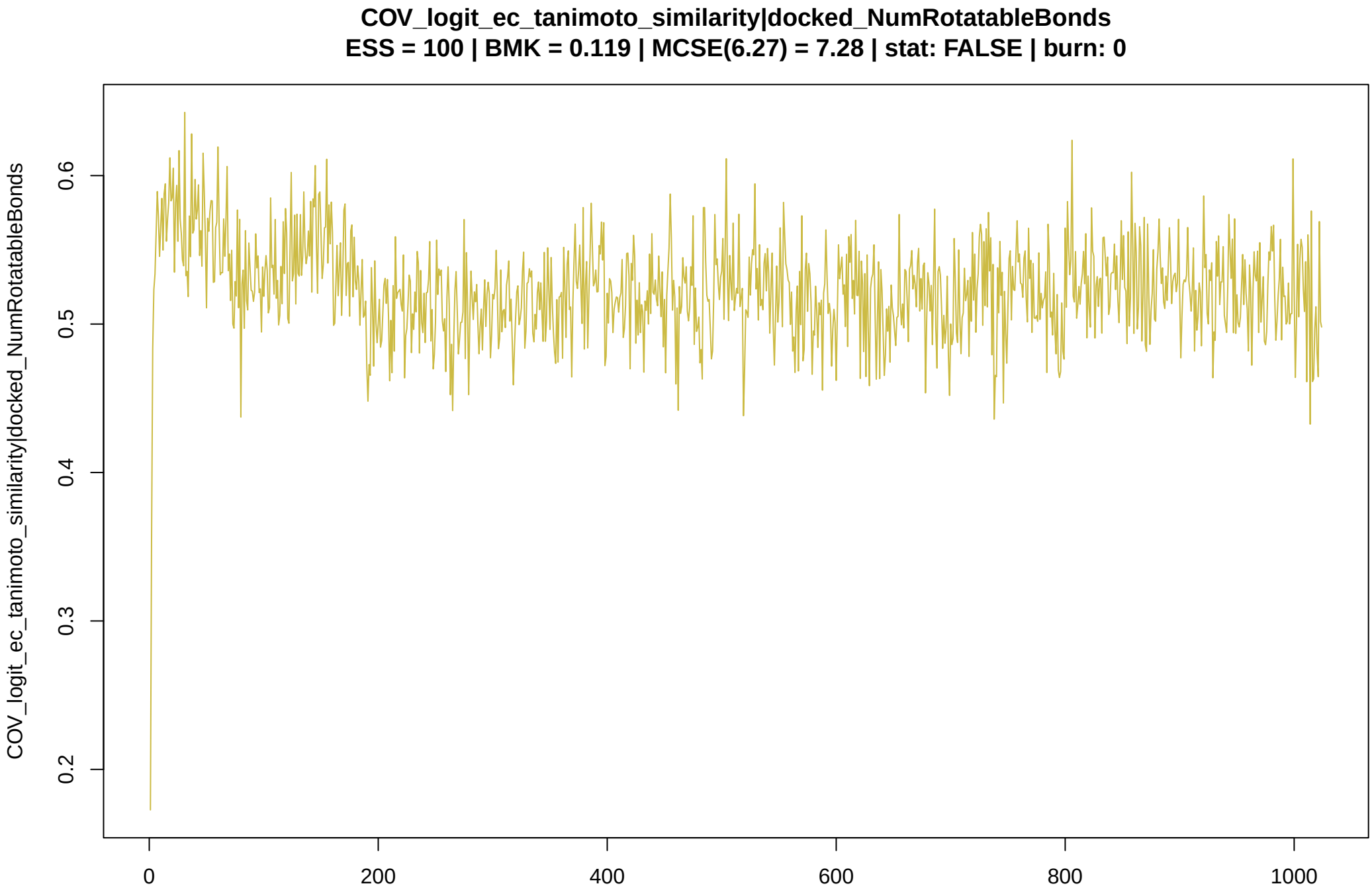

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 178 | BMK = 0.11 | MCSE(6.27) = 5.11 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
0.6
0.4
0.2
0.0
−0.2
0
200
400
600
800
1000

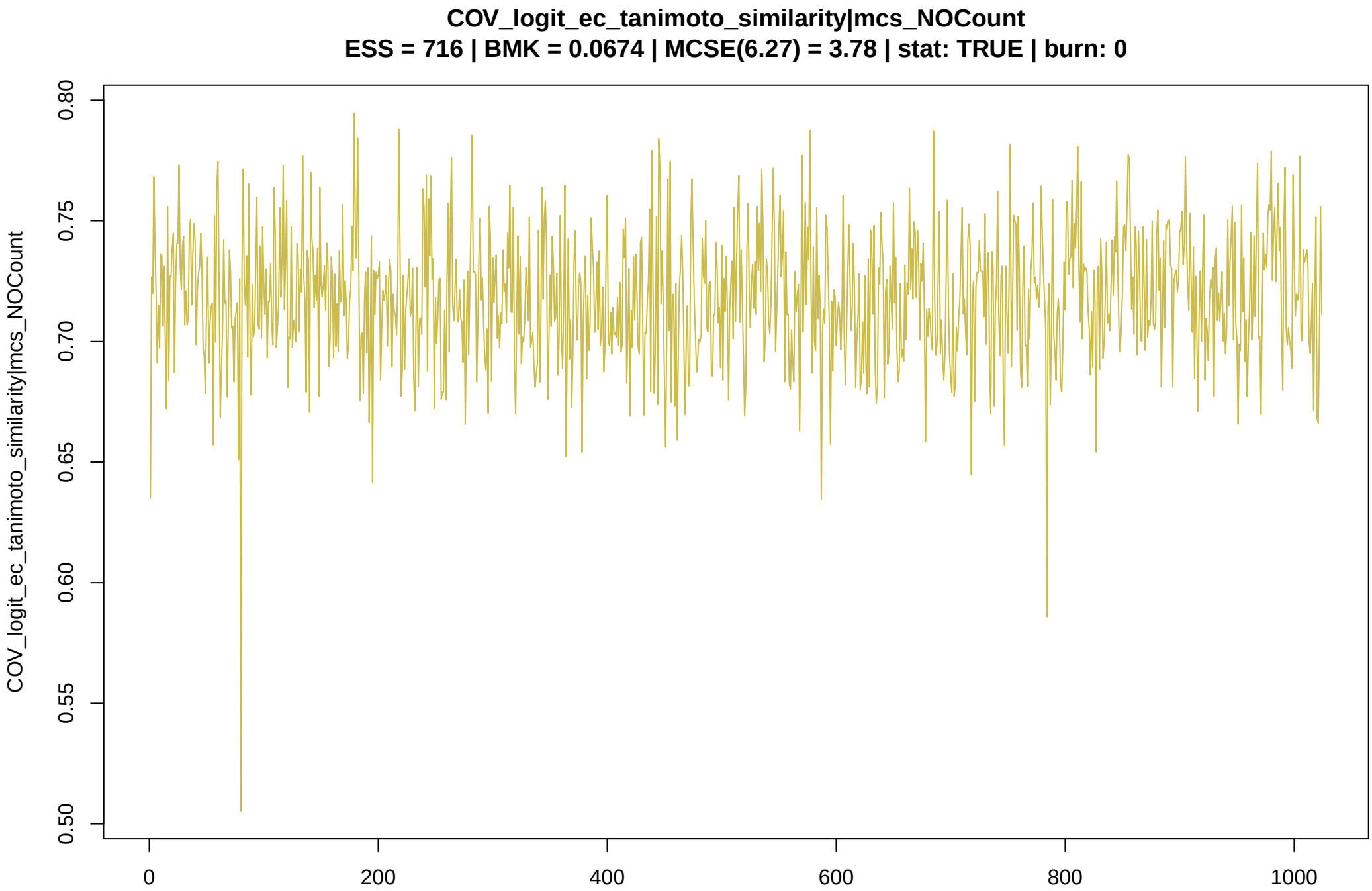

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 257 | BMK = 0.136 | MCSE(6.27) = 4.74 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
0.2
0.4
0.6
0.8
1.0
0
200
400
600
800
1000

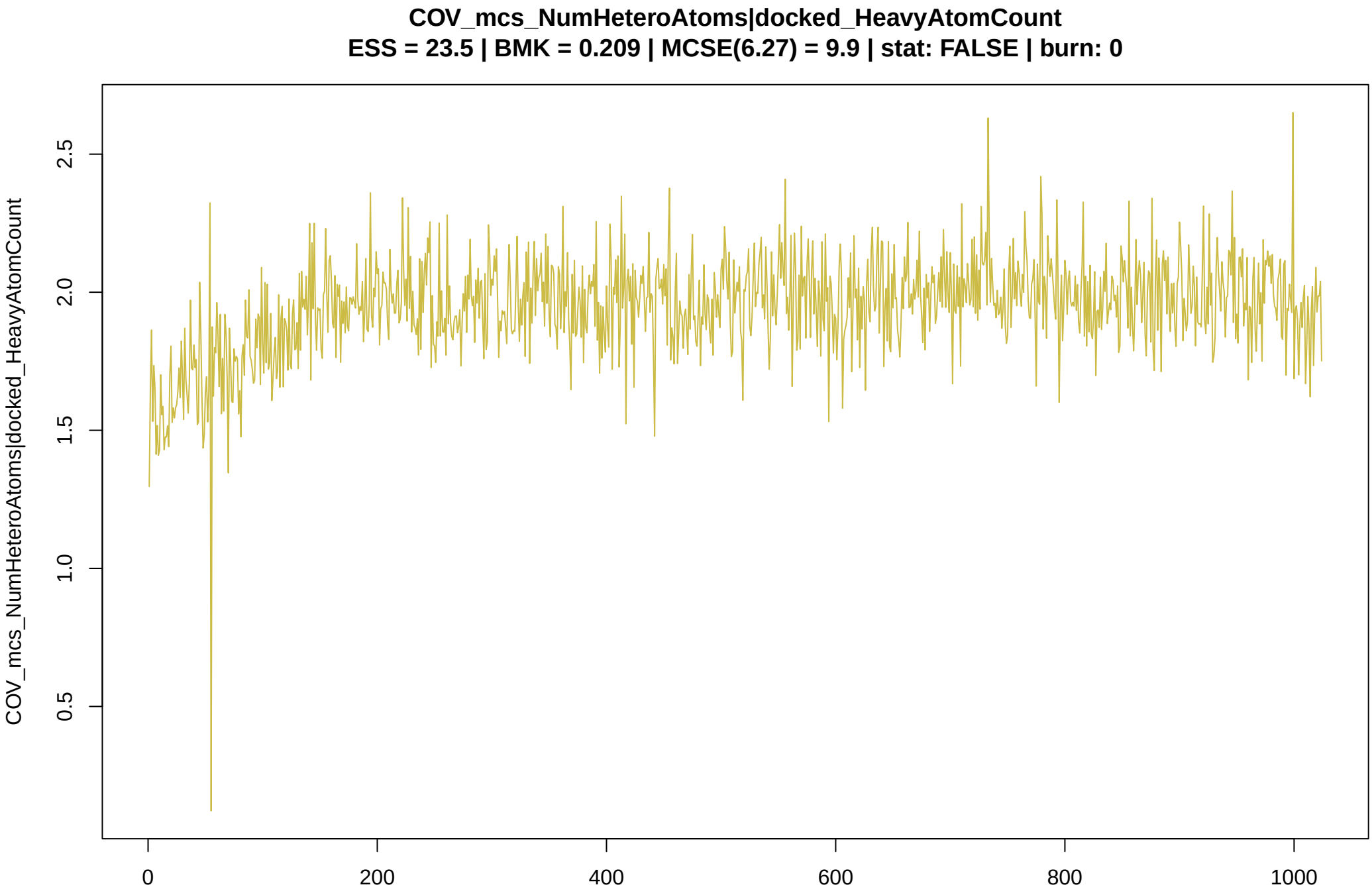

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 625 | BMK = 0.0722 | MCSE(6.27) = 3.64 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.60
0.65
0.70
0.75
0.80
0.85
0.90
0
200
400
600
800
1000

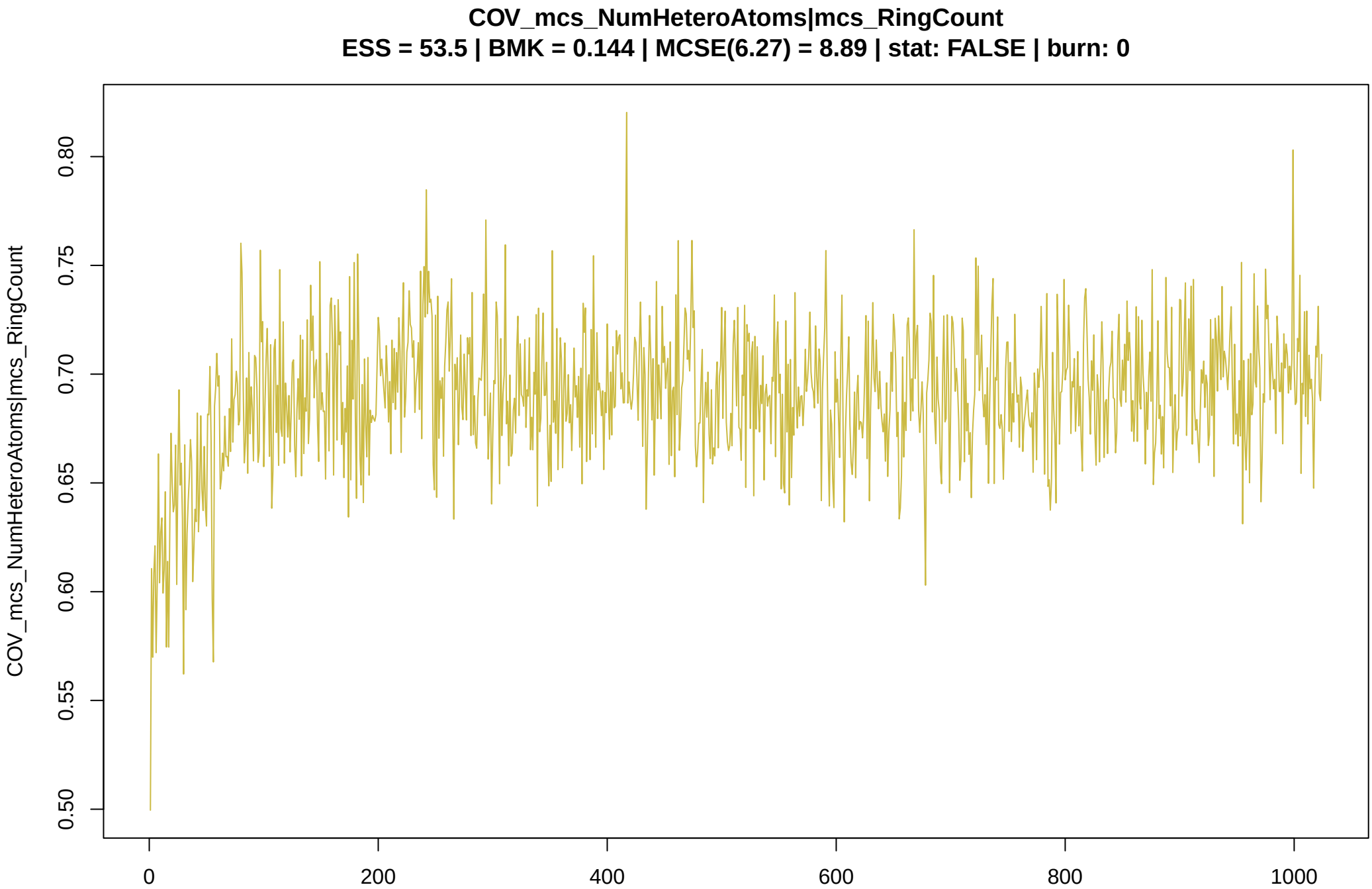

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 278 | BMK = 0.083 | MCSE(6.27) = 6.16 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
0.8
1.0
1.2
1.4
0
200
400
600
800
1000

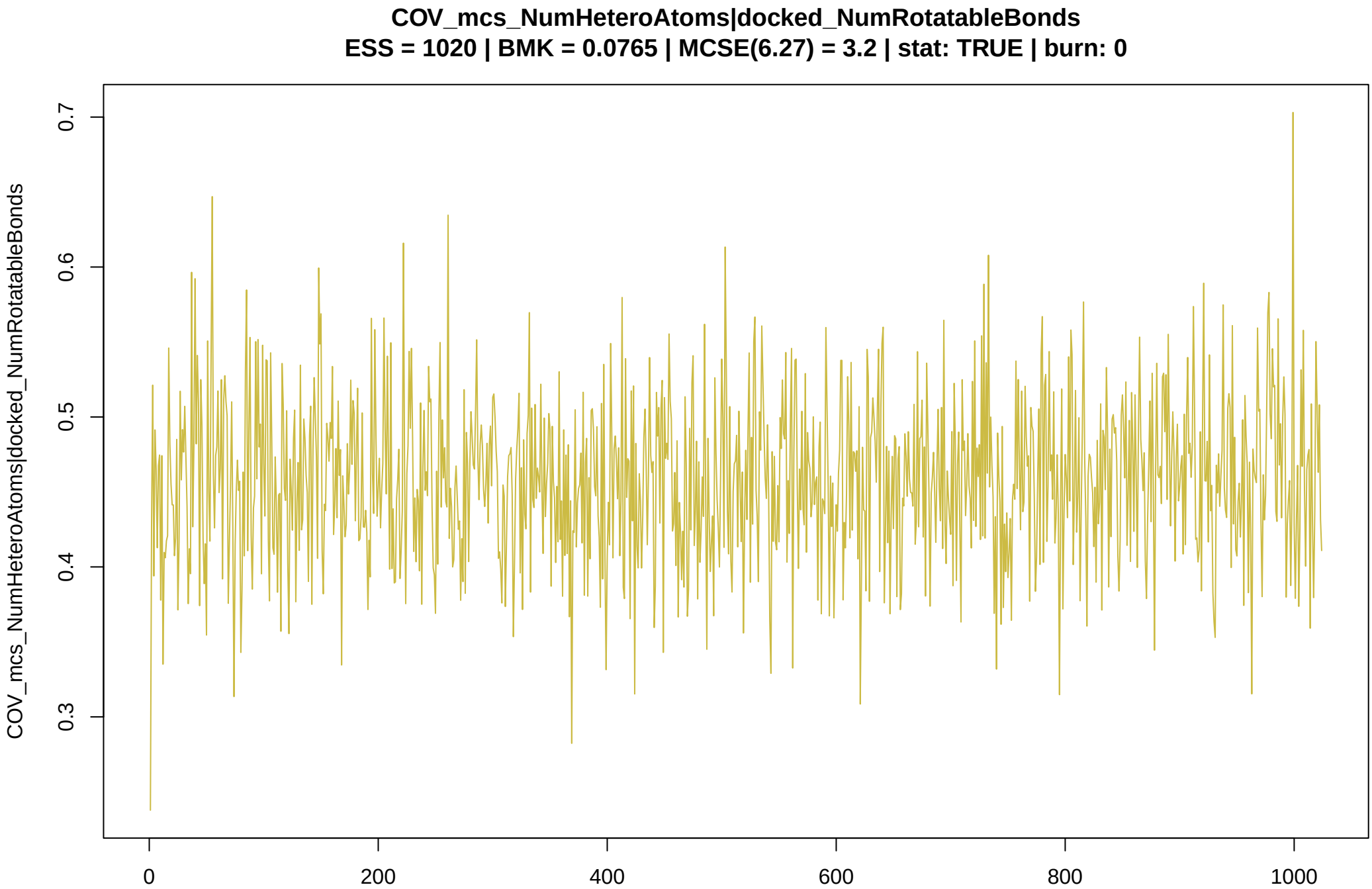

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 150 | BMK = 0.124 | MCSE(6.27) = 6.41 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.30
0.35
0.40
0.45
0
200
400
600
800
1000

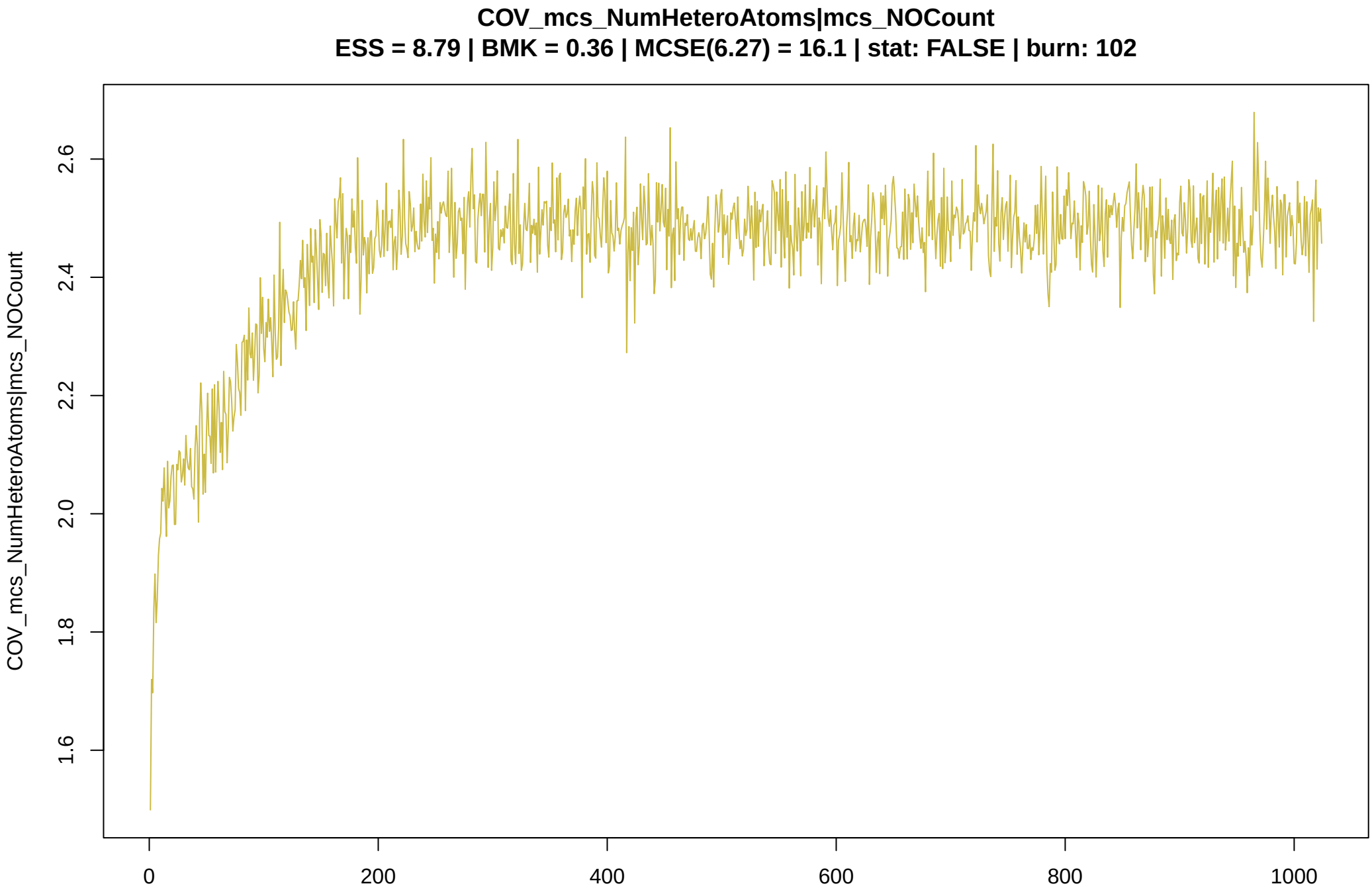

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 100 | BMK = 0.119 | MCSE(6.27) = 7.28 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
0.2
0.3
0.4
0.5
0.6
0
200
400
600
800
1000

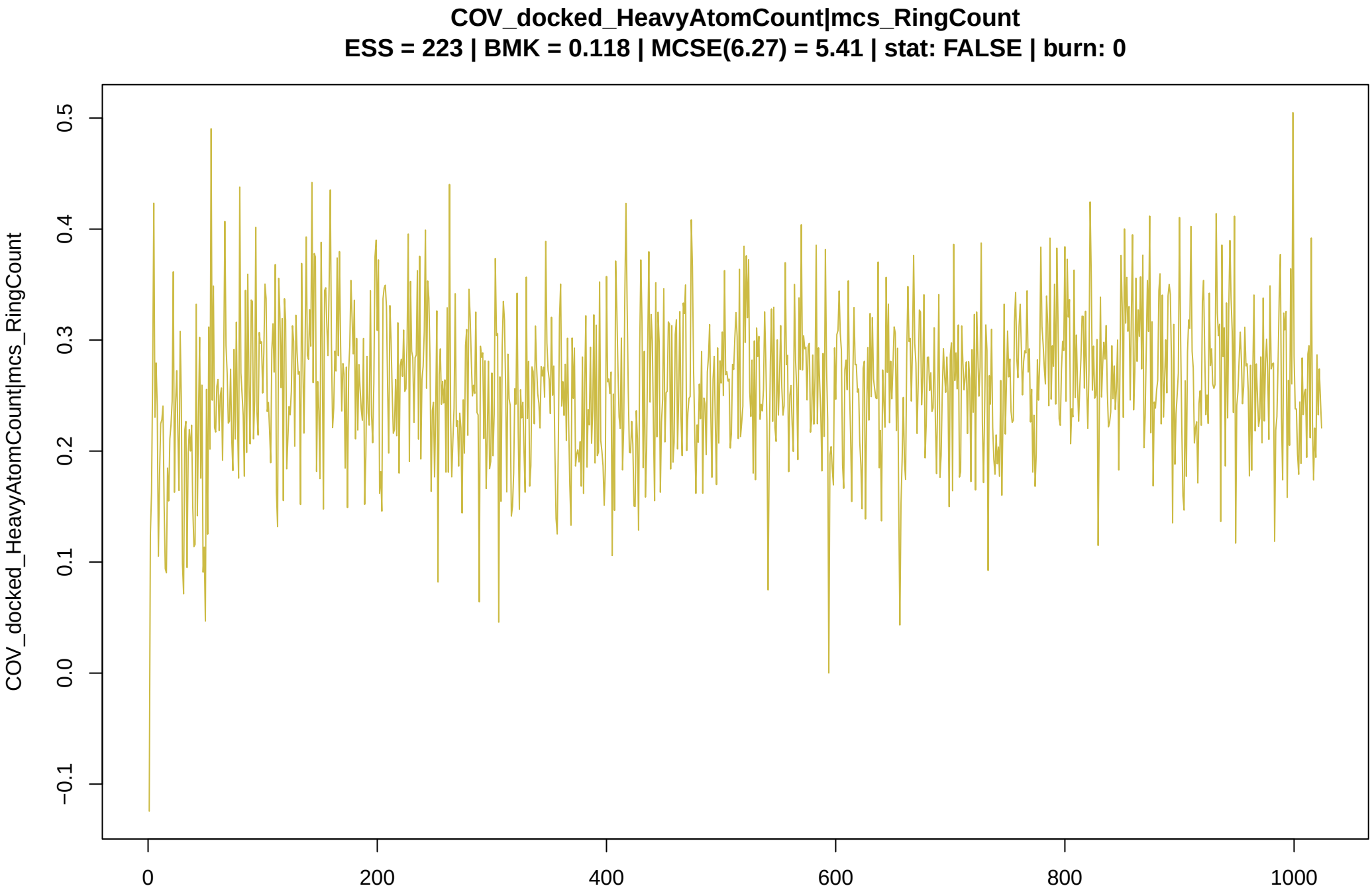

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 716 | BMK = 0.0674 | MCSE(6.27) = 3.78 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NOCount
0.50
0.55
0.60
0.65
0.70
0.75
0.80
0
200
400
600
800
1000

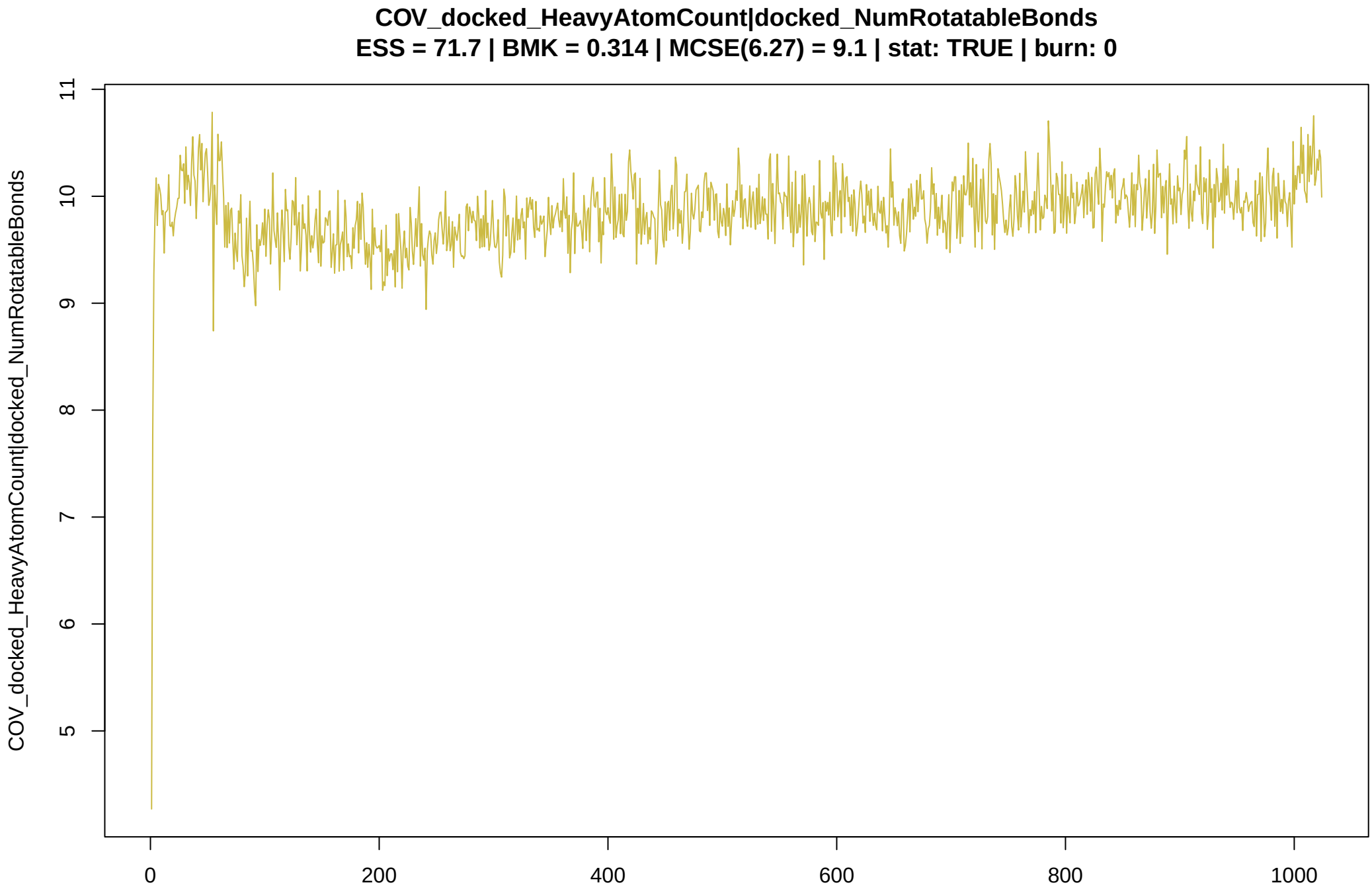

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 23.5 | BMK = 0.209 | MCSE(6.27) = 9.9 | stat: FALSE | burn: 0
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
0.5
1.0
1.5
2.0
2.5
0
200
400
600
800
1000

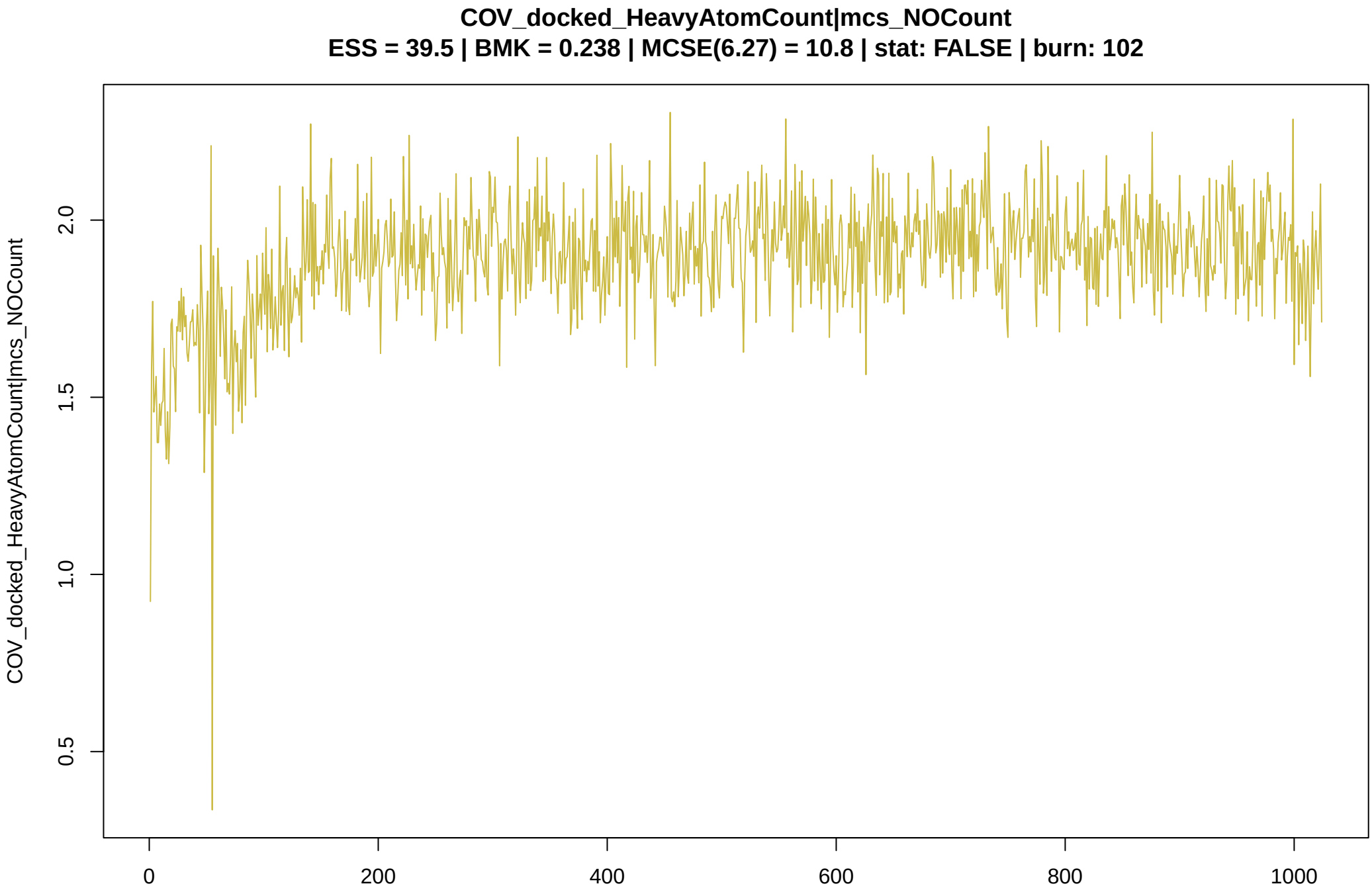

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 53.5 | BMK = 0.144 | MCSE(6.27) = 8.89 | stat: FALSE | burn: 0
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.50
0.55
0.60
0.65
0.70
0.75
0.80
0
200
400
600
800
1000

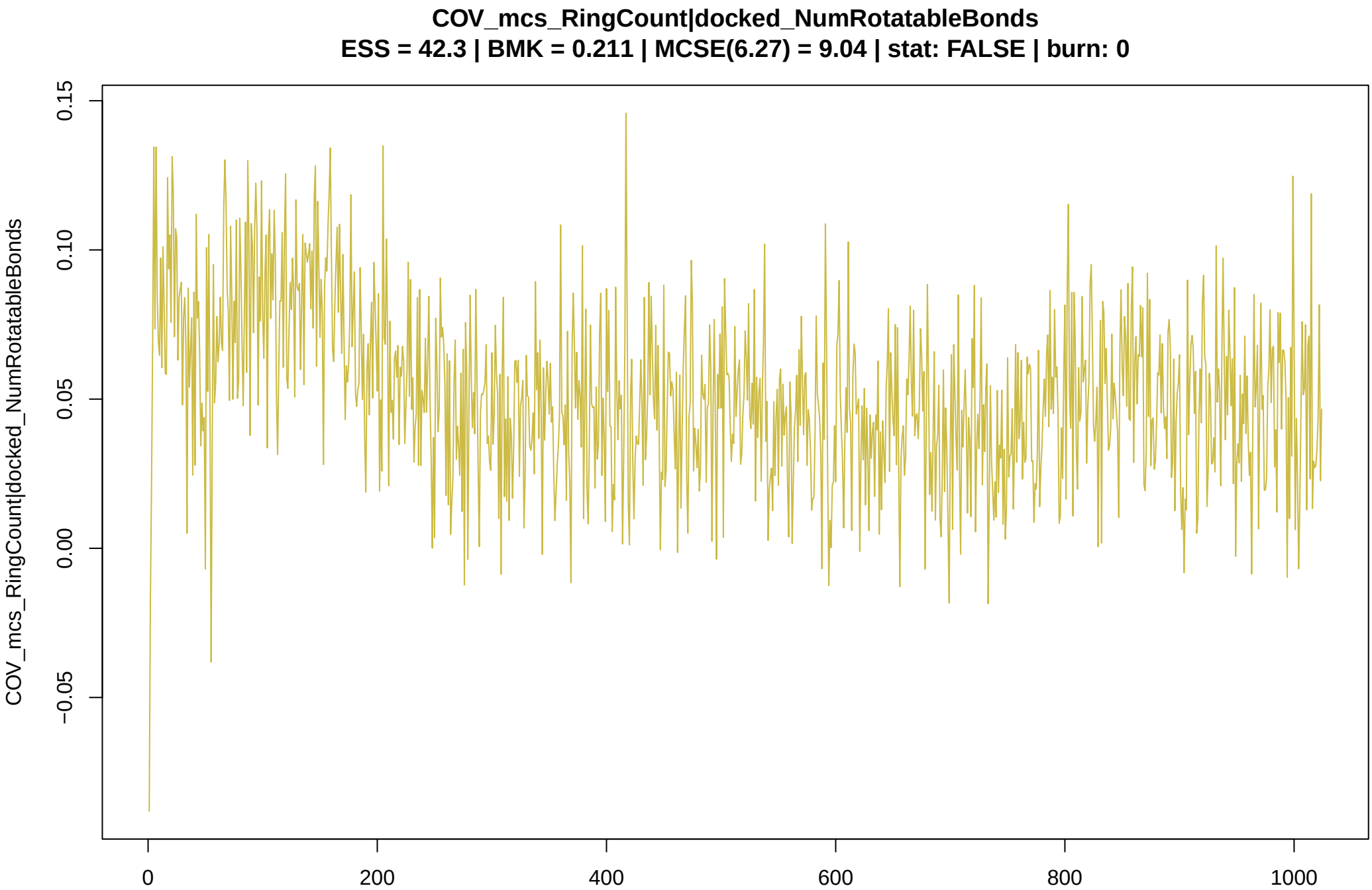

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0765 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
0.3
0.4
0.5
0.6
0.7
0
200
400
600
800
1000

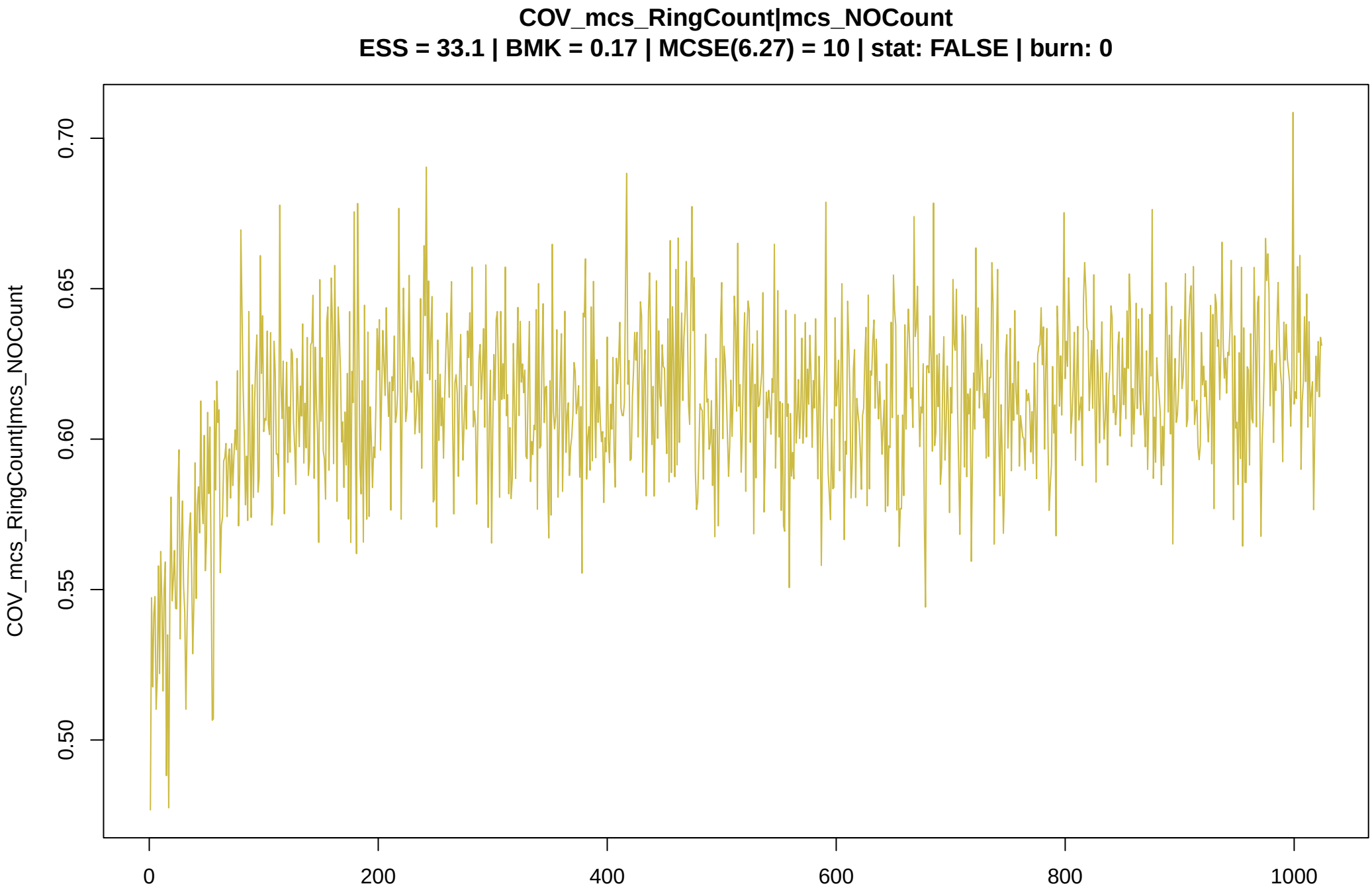

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 8.79 | BMK = 0.36 | MCSE(6.27) = 16.1 | stat: FALSE | burn: 102
COV_mcs_NumHeteroAtoms|mcs_NOCount
1.6
1.8
2.0
2.2
2.4
2.6
0
200
400
600
800
1000

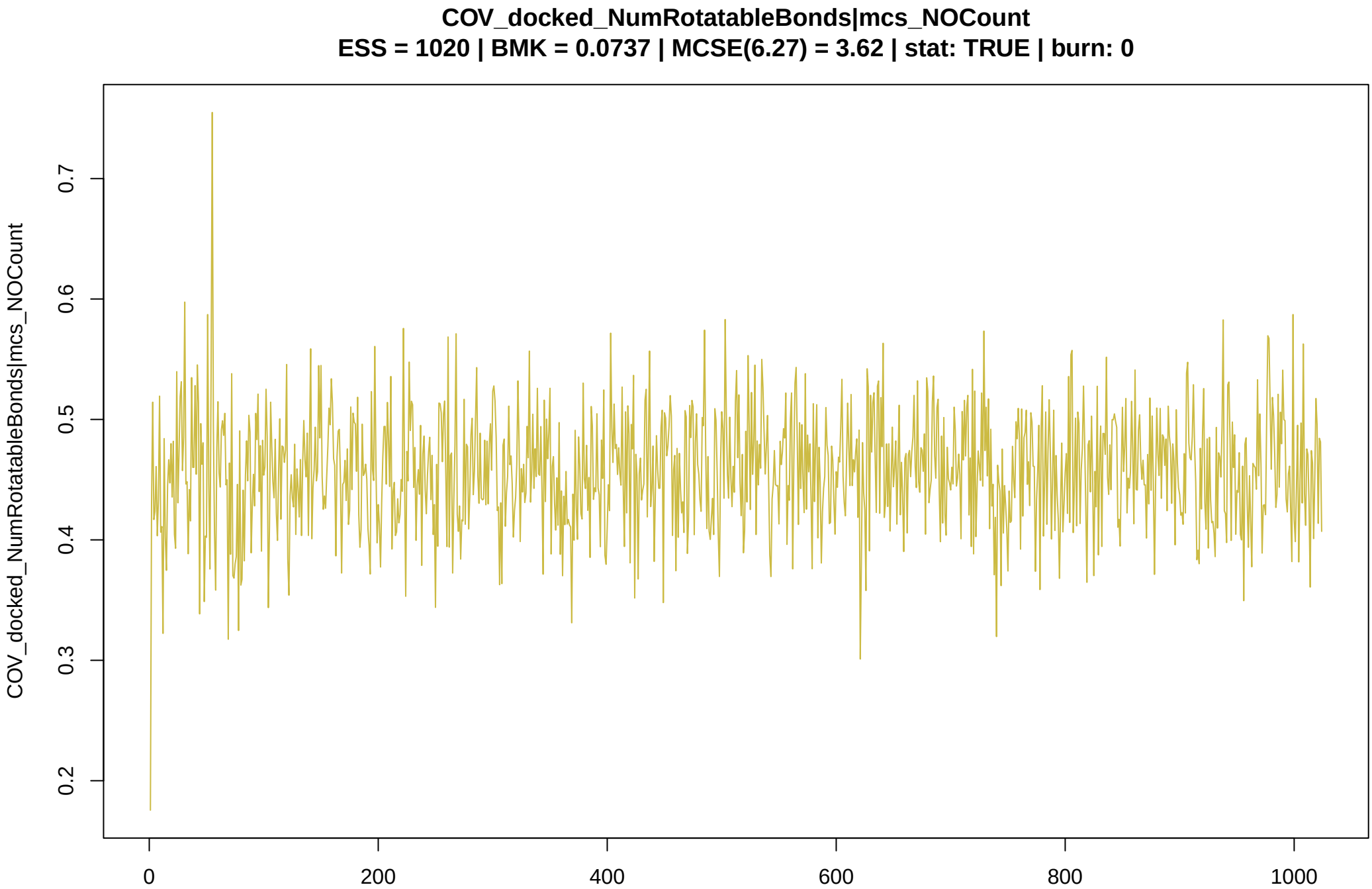

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 223 | BMK = 0.118 | MCSE(6.27) = 5.41 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
−0.1
0.0
0.1
0.2
0.3
0.4
0.5
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 71.7 | BMK = 0.314 | MCSE(6.27) = 9.1 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
5
6
7
8
9
10
11
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 39.5 | BMK = 0.238 | MCSE(6.27) = 10.8 | stat: FALSE | burn: 102
COV_docked_HeavyAtomCount|mcs_NOCount
0.5
1.0
1.5
2.0
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 42.3 | BMK = 0.211 | MCSE(6.27) = 9.04 | stat: FALSE | burn: 0
COV_mcs_RingCount|docked_NumRotatableBonds
0.15
0.10
0.05
0.00
−0.05
0
200
400
600
800
1000


COV_mcs_RingCount|mcs_NOCount
ESS = 33.1 | BMK = 0.17 | MCSE(6.27) = 10 | stat: FALSE | burn: 0
COV_mcs_RingCount|mcs_NOCount
0.50
0.55
0.60
0.65
0.70
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0737 | MCSE(6.27) = 3.62 | stat: TRUE | burn: 0
COV_docked_NumRotatableBonds|mcs_NOCount
0.2
0.3
0.4
0.5
0.6
0.7
0
200
400
600
800
1000