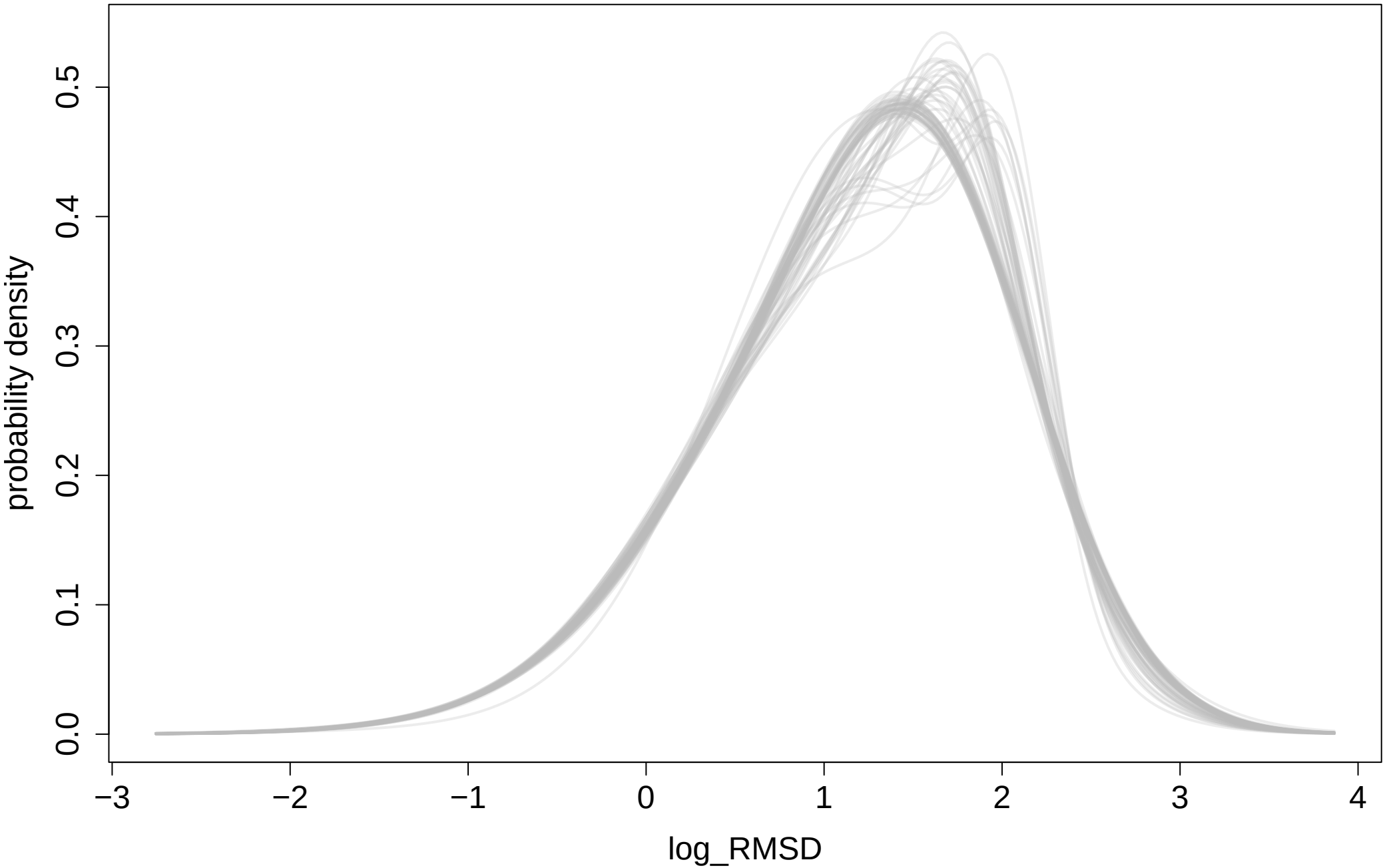
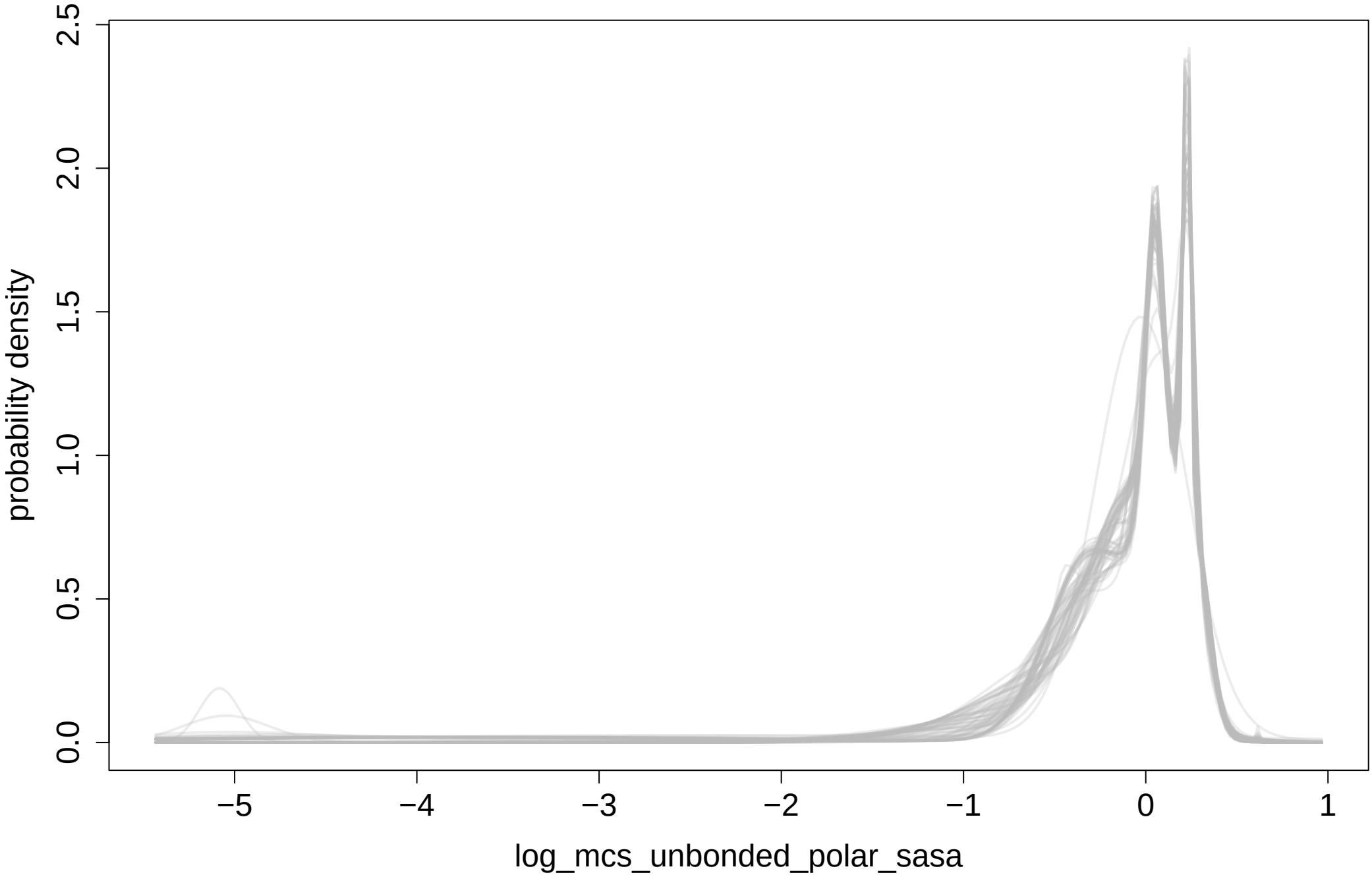
−− STATS maxD −−
min ESS = 3.65792317376021
max BMK = 0.614211489137882
max MCSE = 17.5095619003657
all stationary: FALSE
burn: 1020

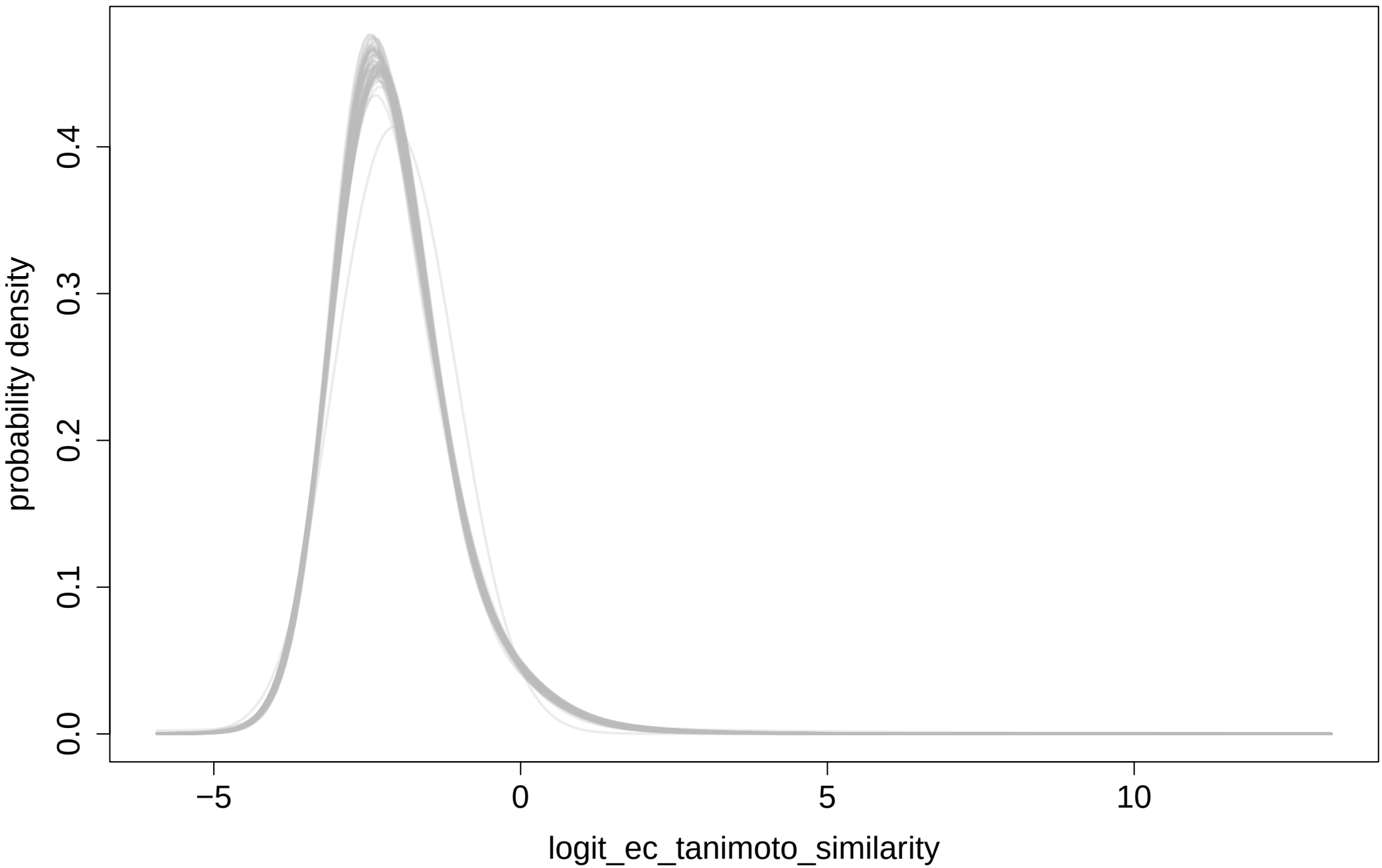
−− STATS 2D −−
min ESS = 4.92504603184206
max BMK = 0.690393971408766
max MCSE = 15.3996319224687
all stationary: FALSE
burn: 816

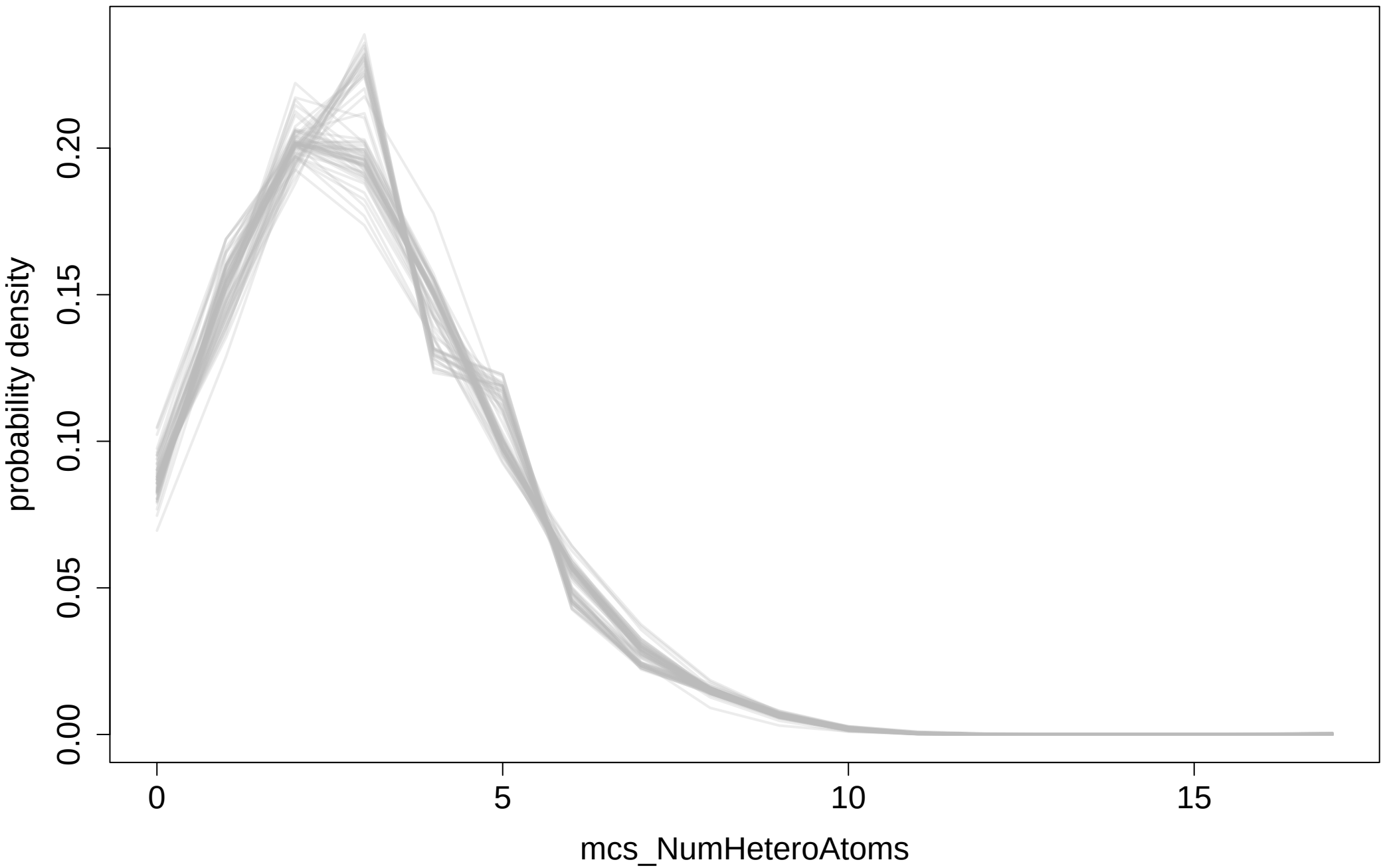
−− STATS 1D −−
min ESS = 2.2204604925031e−16
max BMK = 1
max MCSE = NaN
all stationary: FALSE
burn: 1020

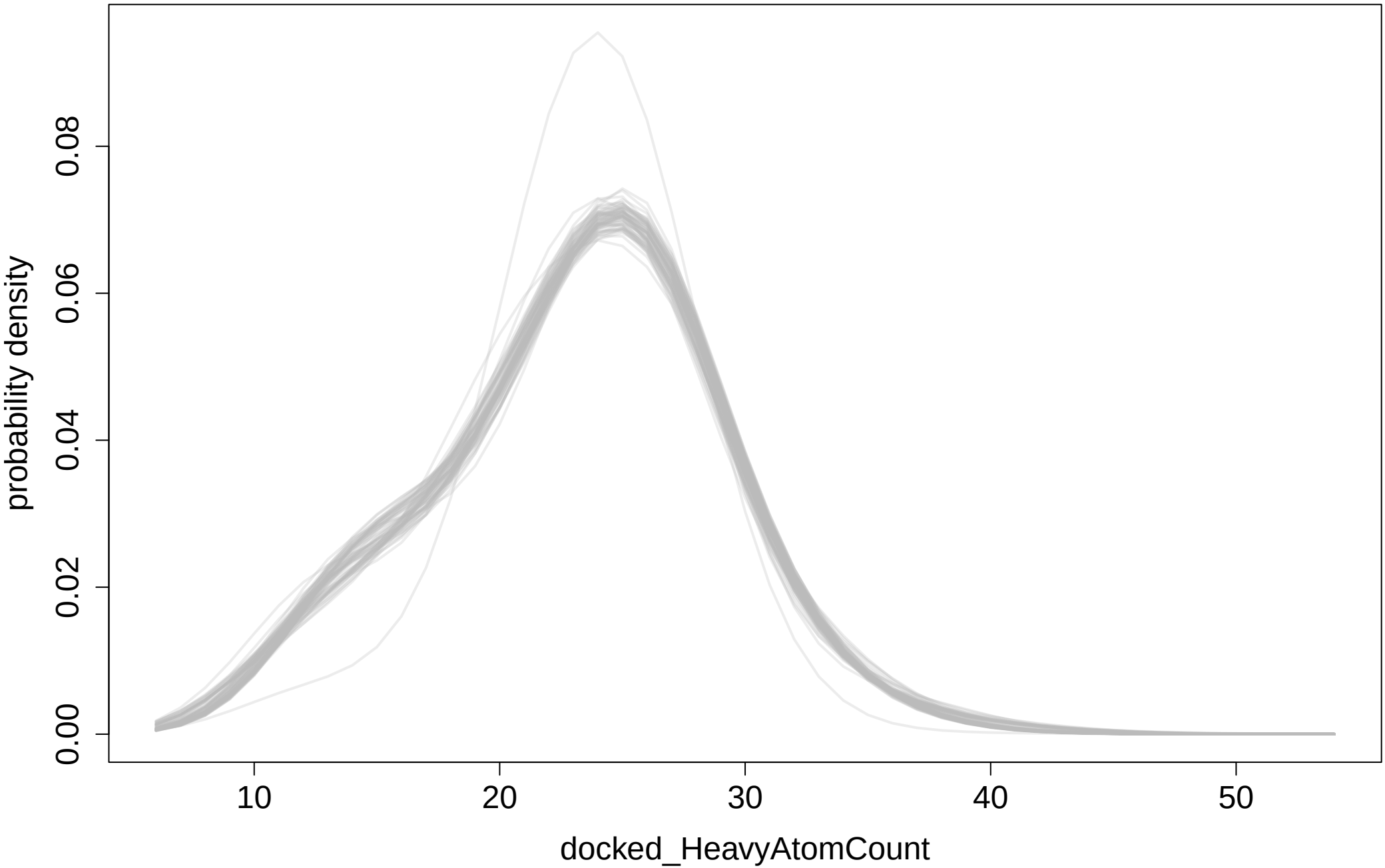
Occupied clusters: 13 of 64
LL: −90100 +− 7410

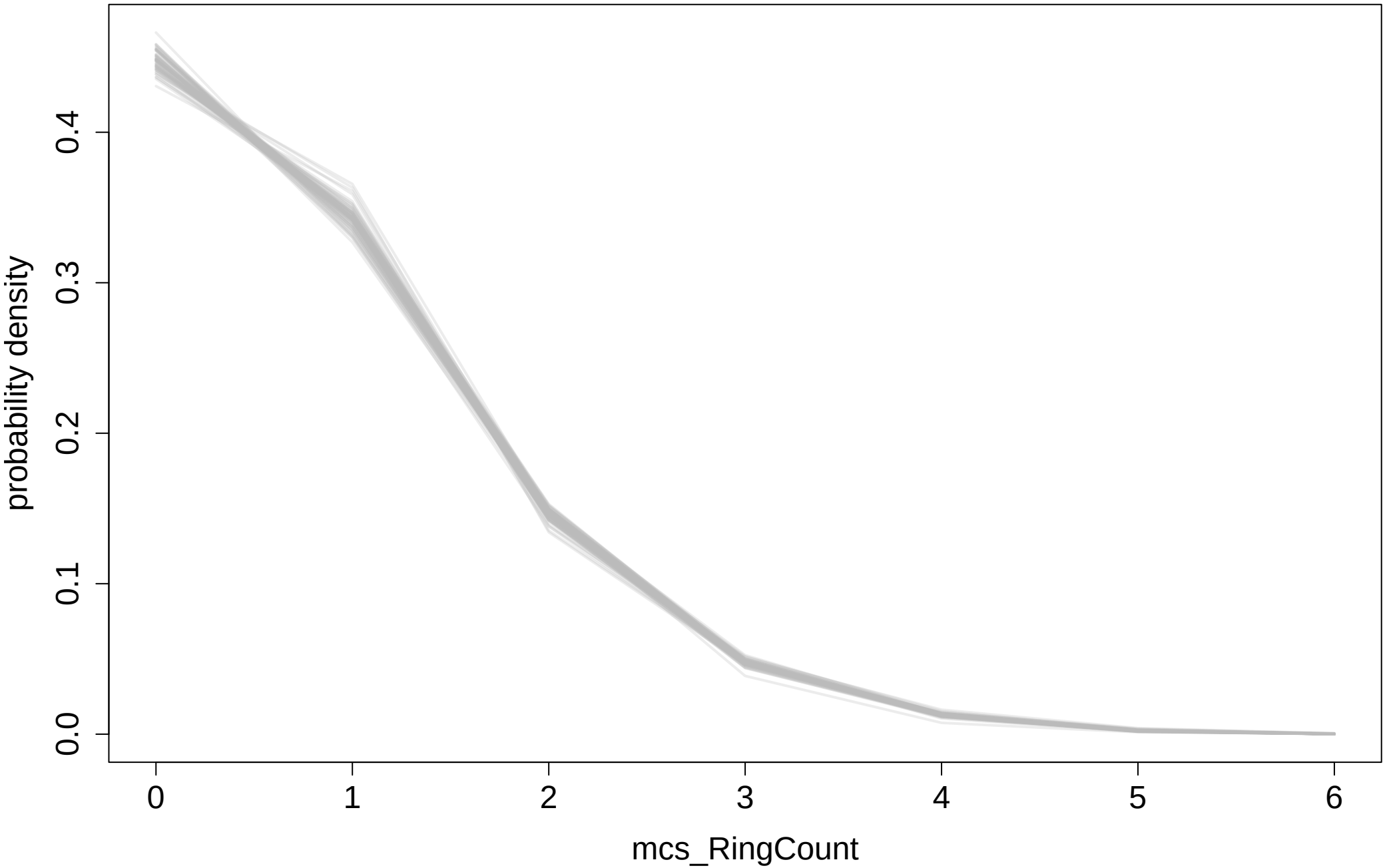

probability density
0.0
0.1
0.2
0.3
0.4
0.5
−3
−2
−1
0
1
2
3
4
log_RMSD


probability density
0.0
0.5
1.0
1.5
2.0
2.5
−5
−4
−3
−2
−1
0
1
log_mcs_unbonded_polar_sasa


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


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


probability density
0.00
0.02
0.04
0.06
0.08
10
20
30
40
50
docked_HeavyAtomCount


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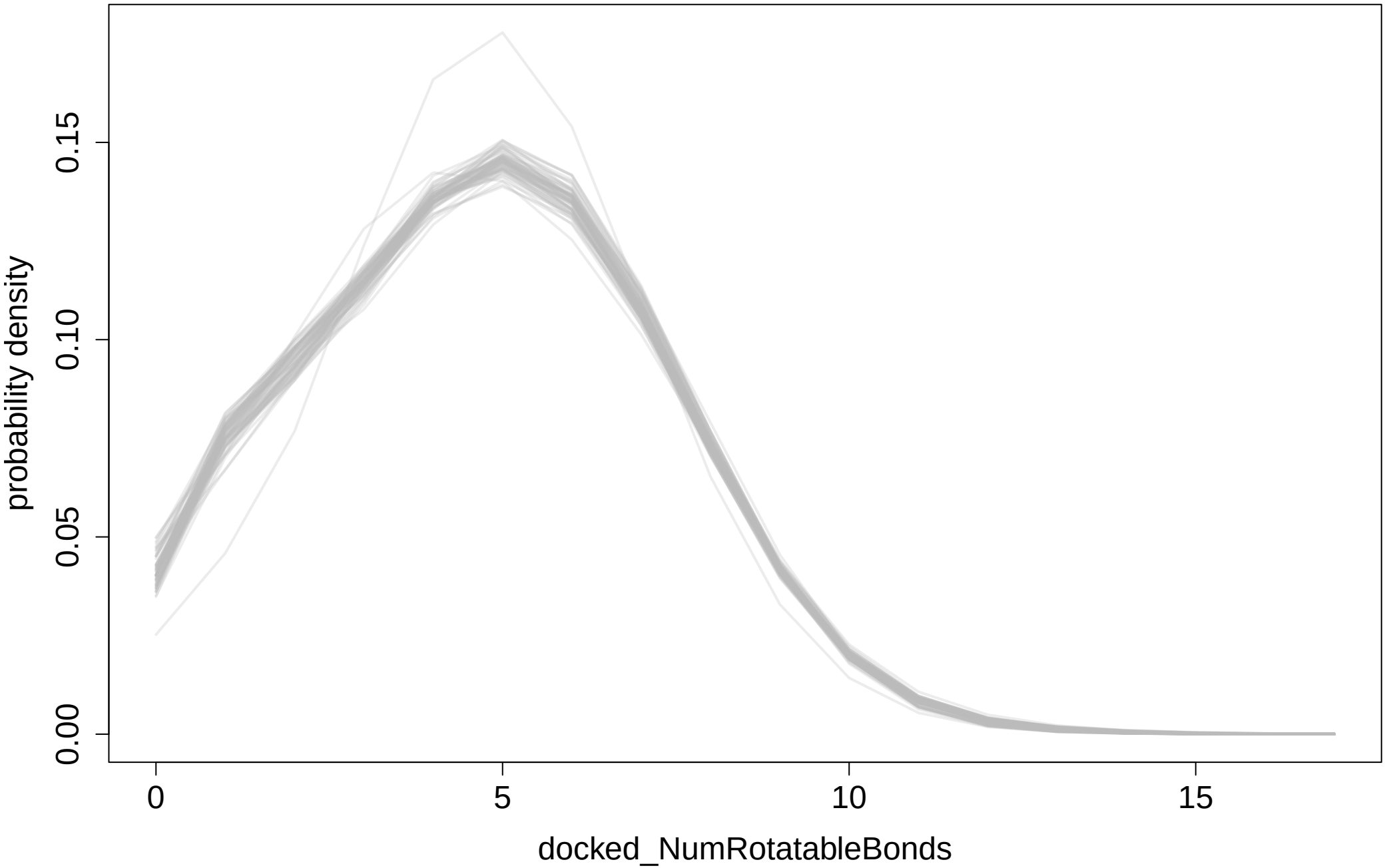
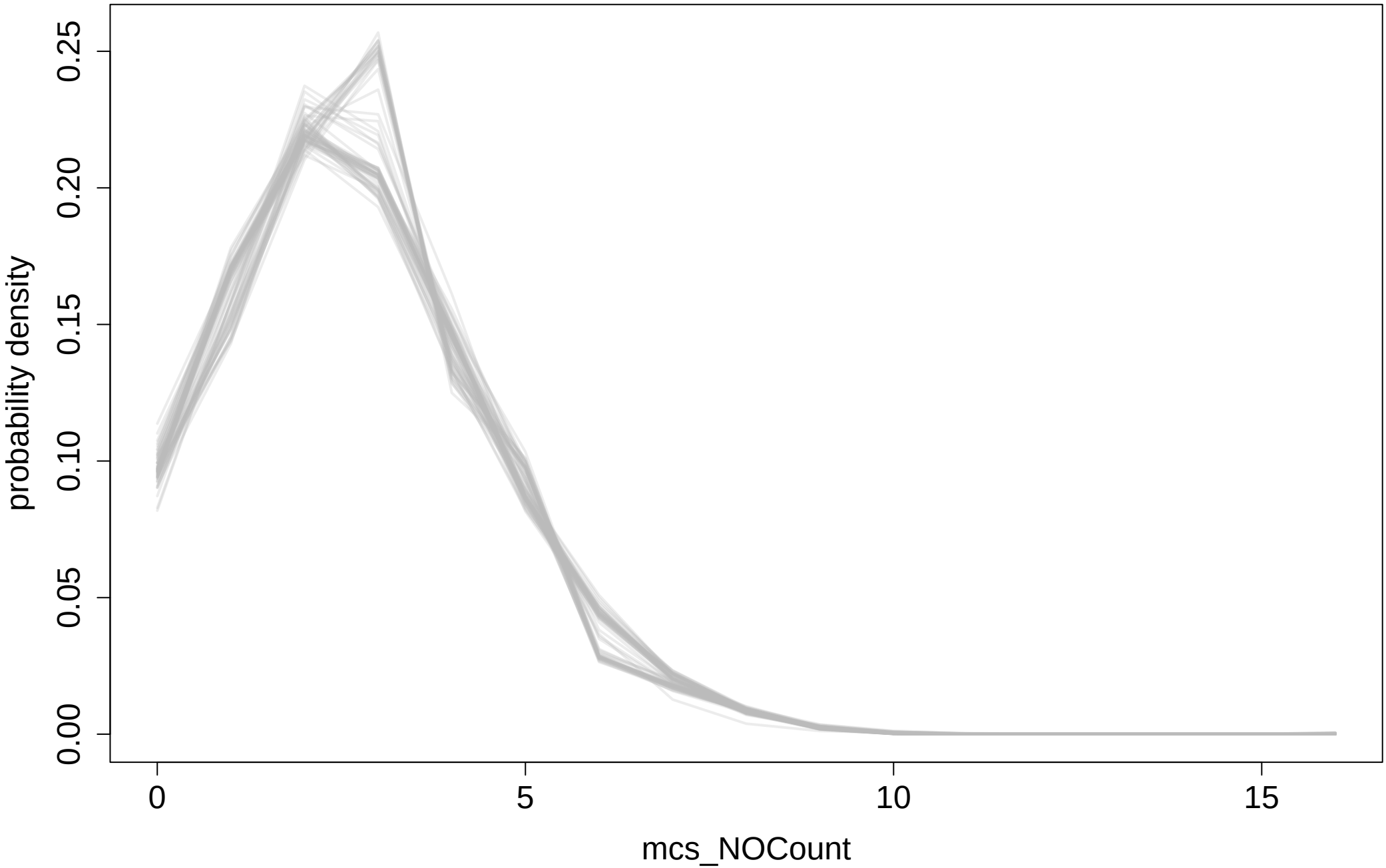
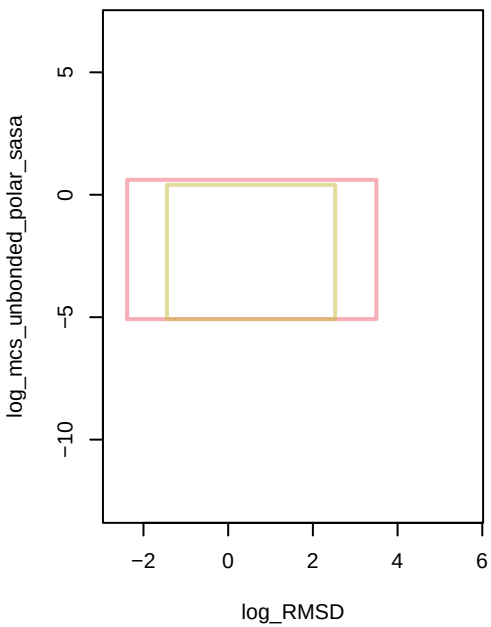
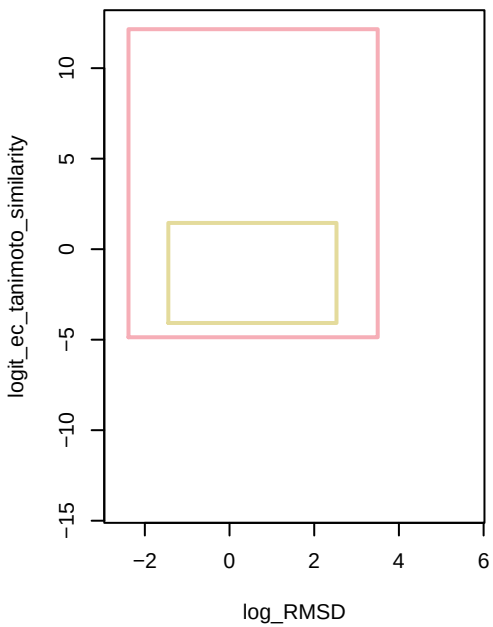
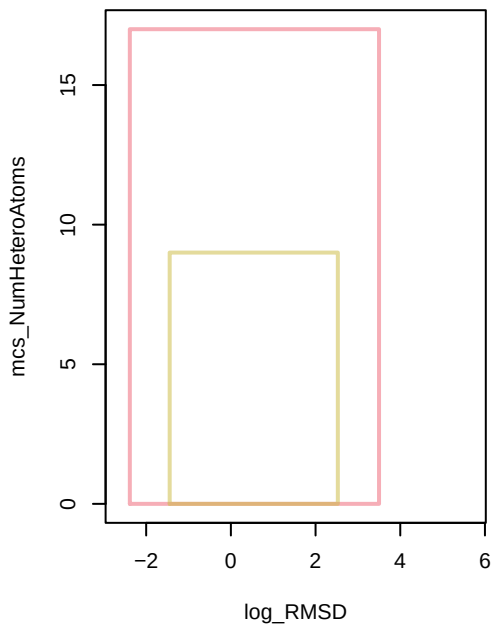
0.1
0.2
0.3
0.4
0
1
2
3
4
5
6
mcs_RingCount

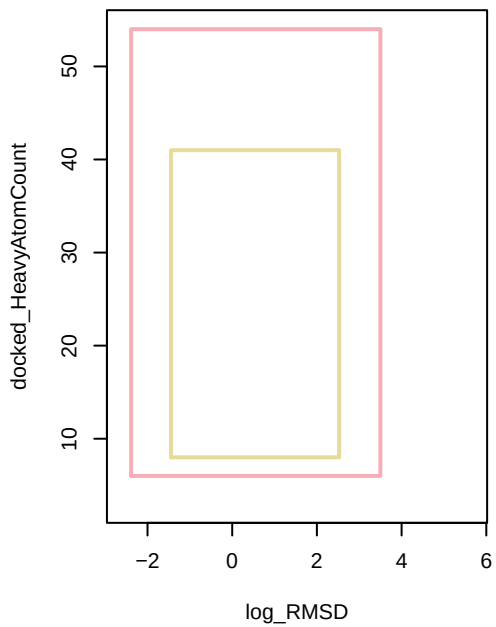

probability density
0.00
0.05
0.10
0.15
0
5
10
15
docked_NumRotatableBonds

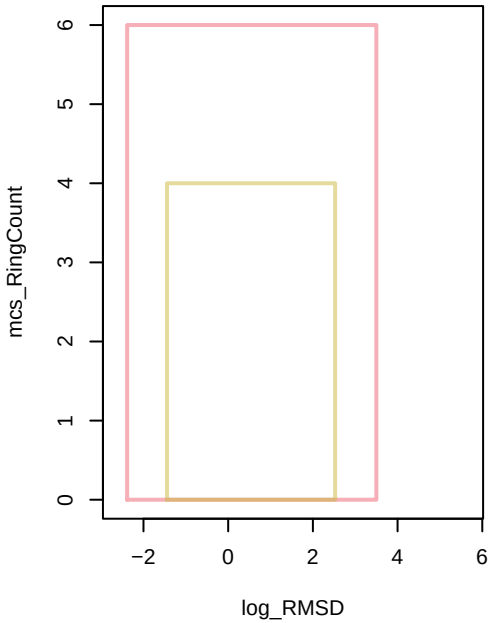

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_NOCount

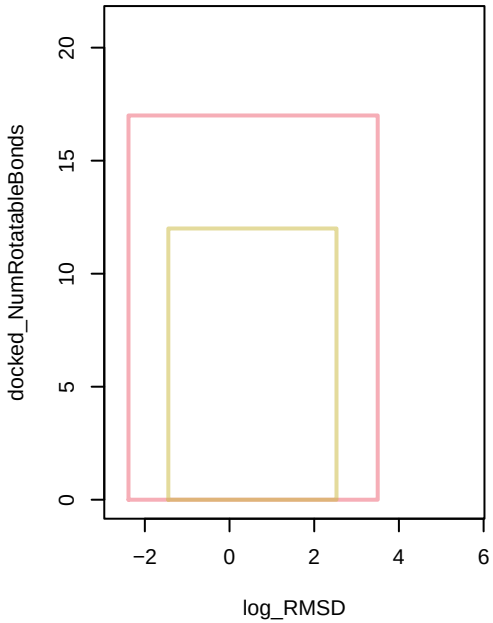

log_mcs_unbonded_polar_sasa
log_RMSD

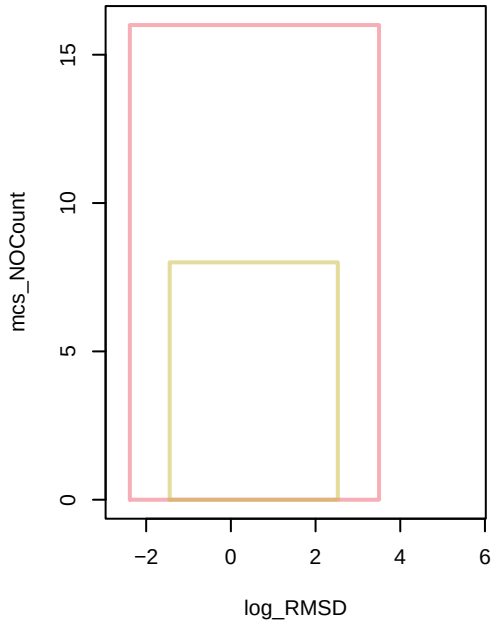

logit_ec_tanimoto_similarity
log_RMSD

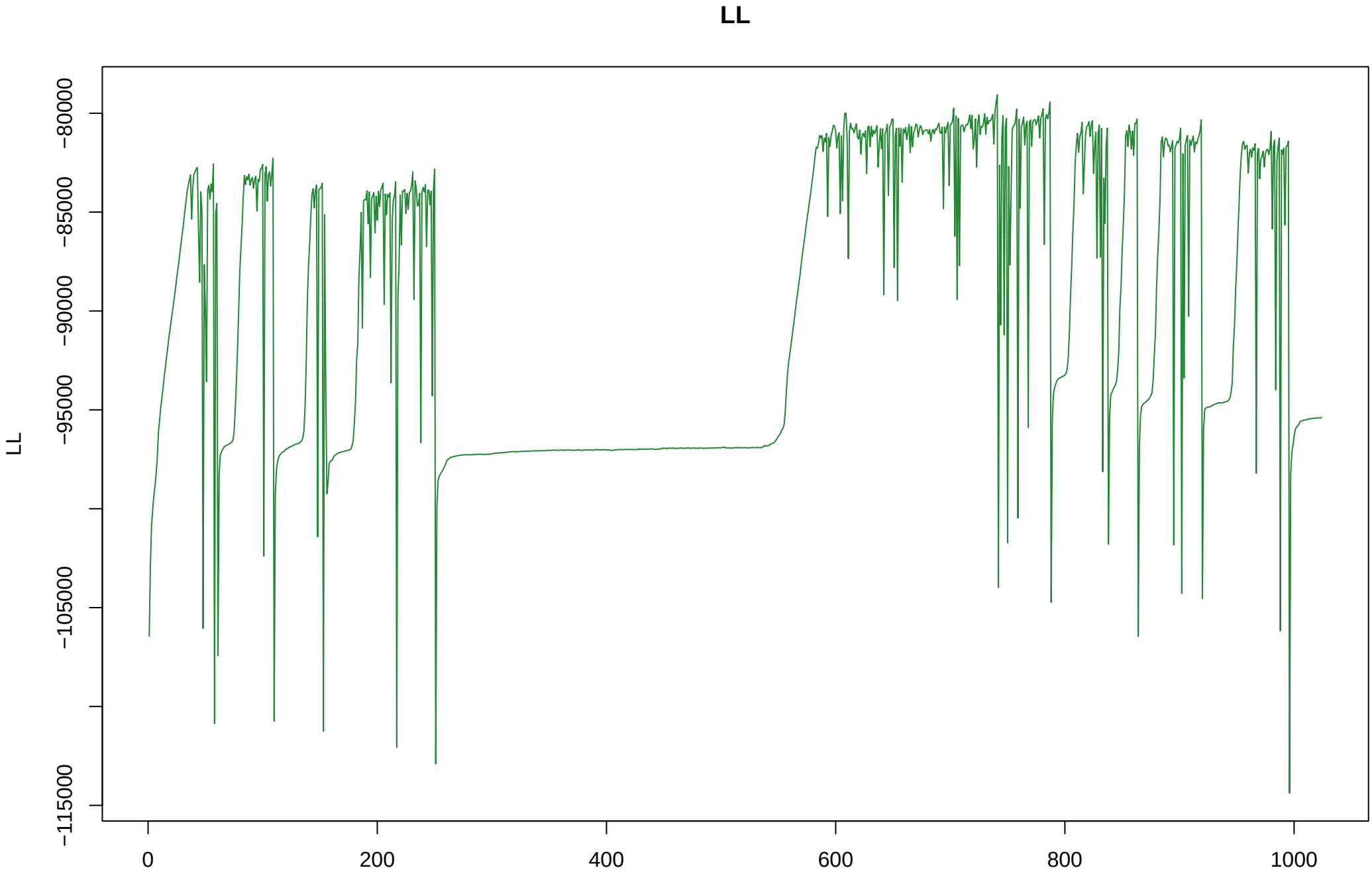

mcs_NumHeteroAtoms
log_RMSD

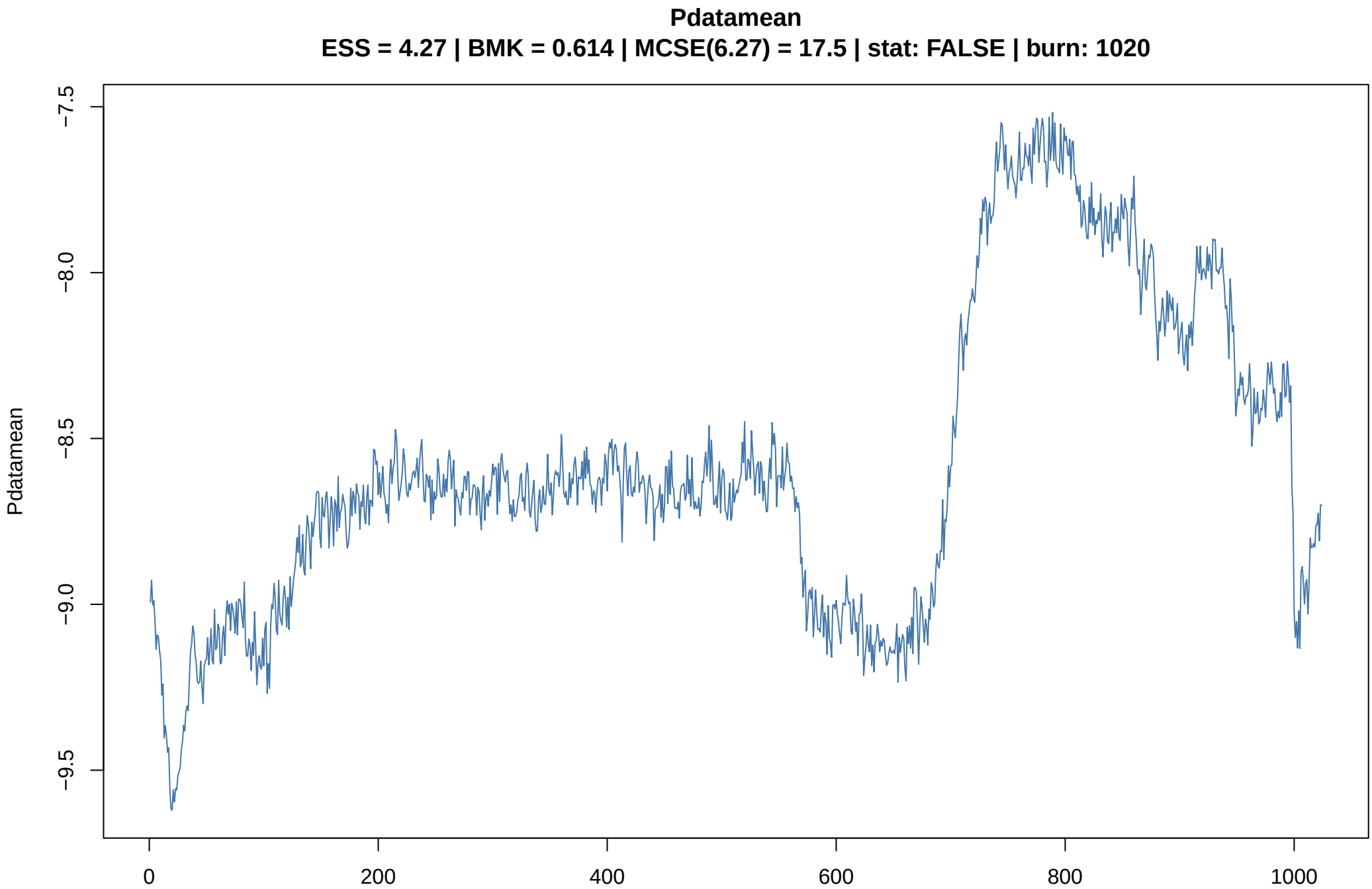

docked_HeavyAtomCount
log_RMSD

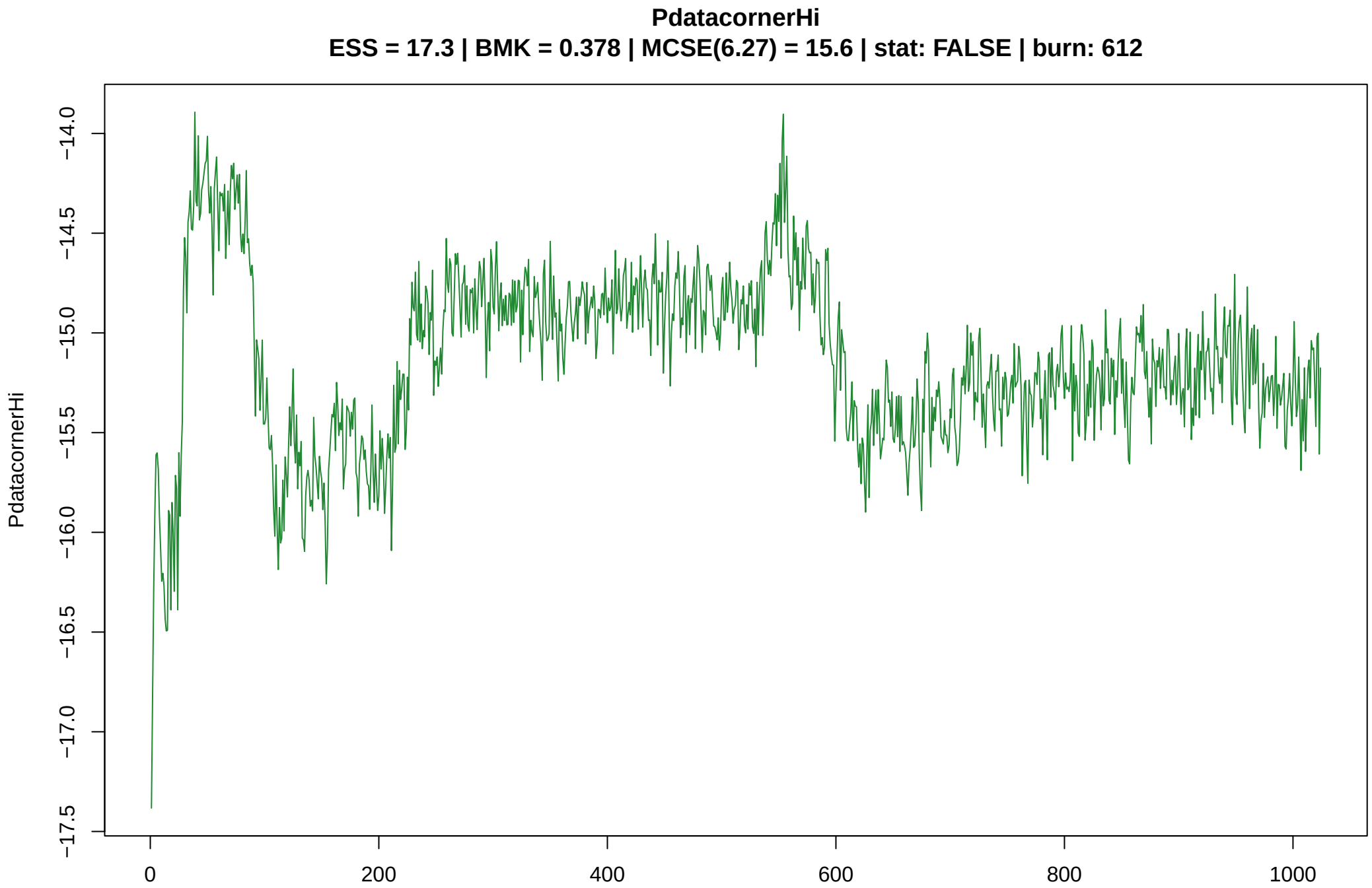

mcs_RingCount
log_RMSD

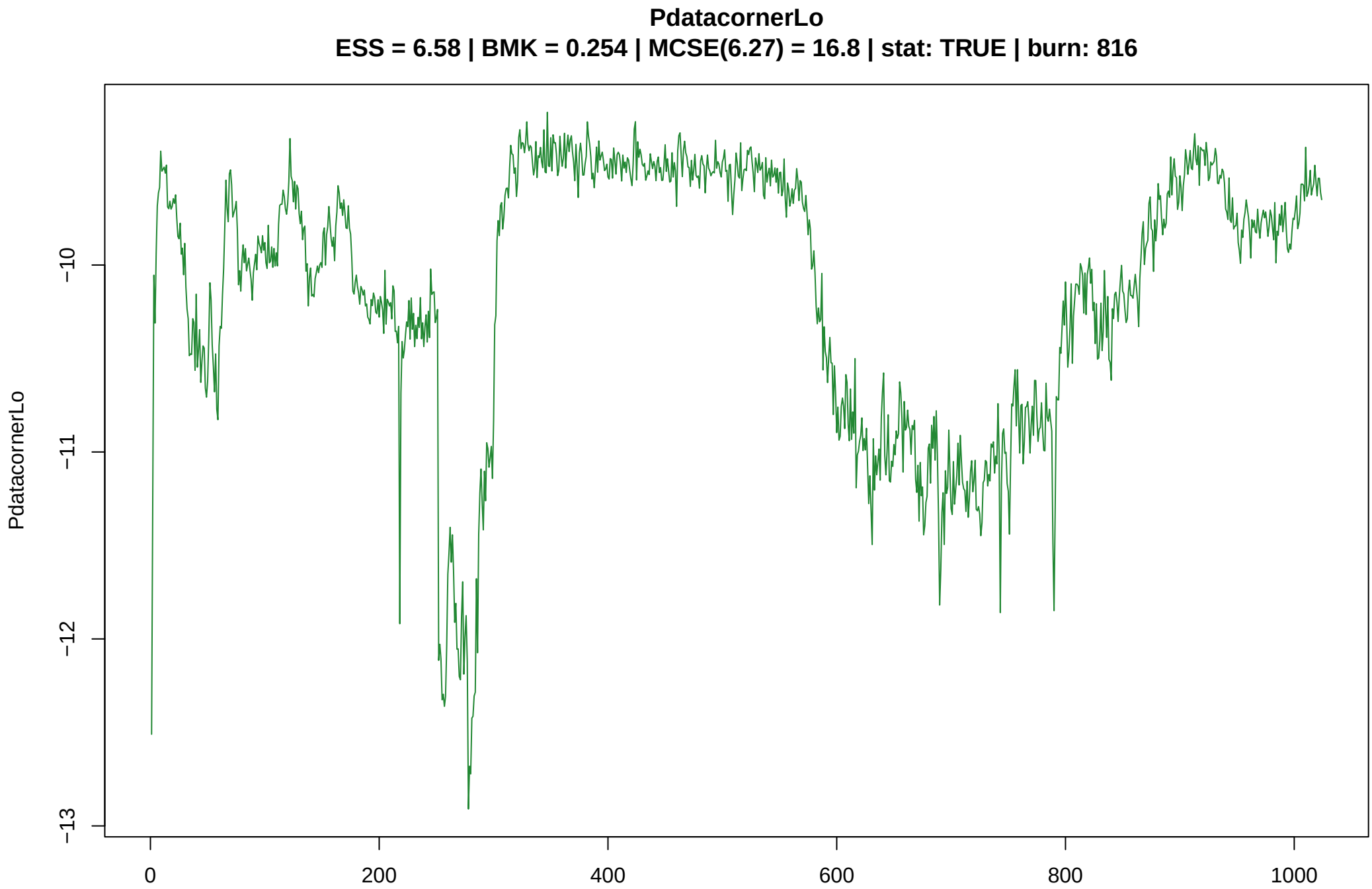

docked_NumRotatableBonds
log_RMSD

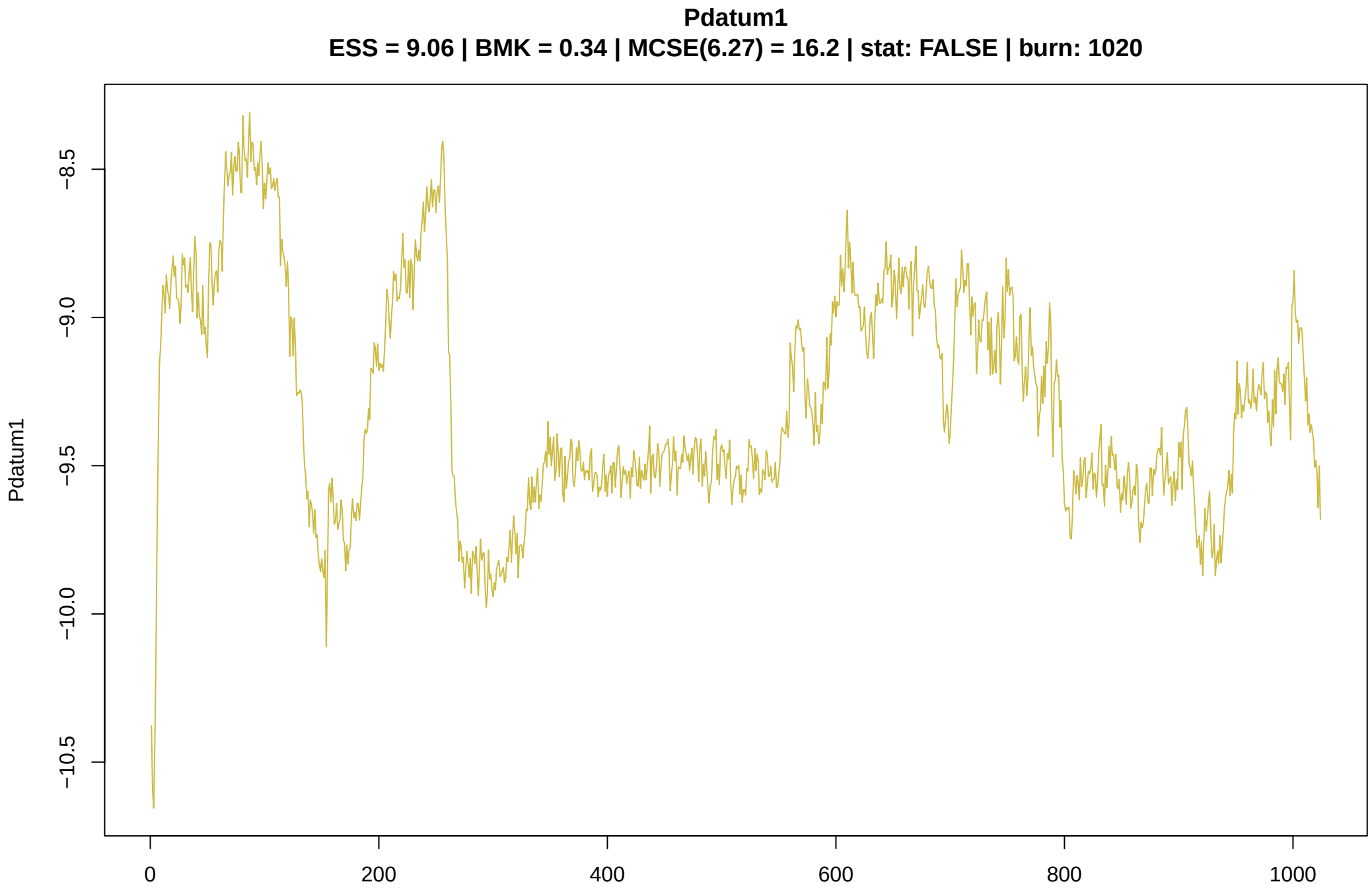

mcs_NOCount
log_RMSD

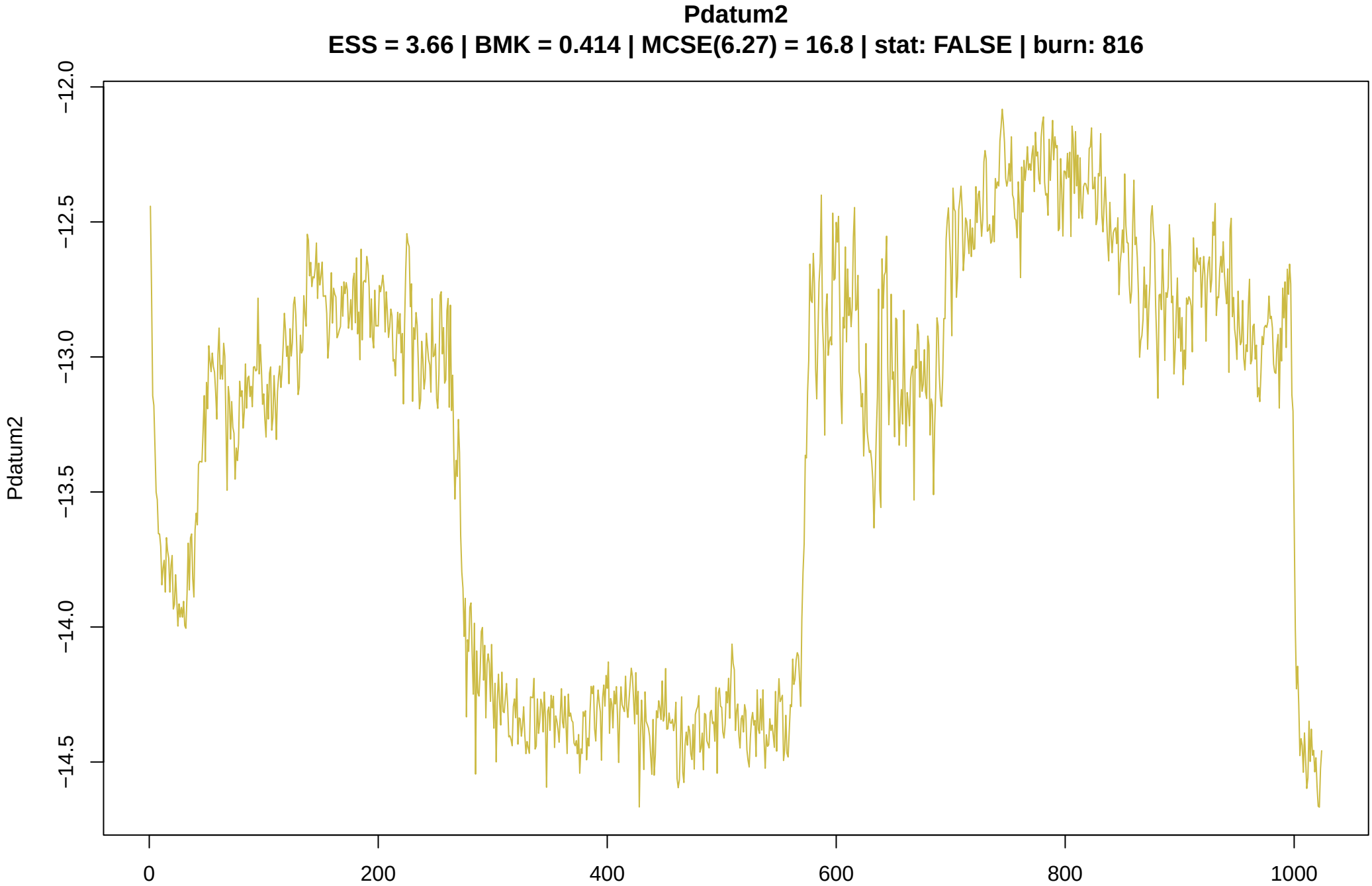

LL
LL
−80000
−85000
−90000
−95000
−105000
−115000
0
200
400
600
800
1000

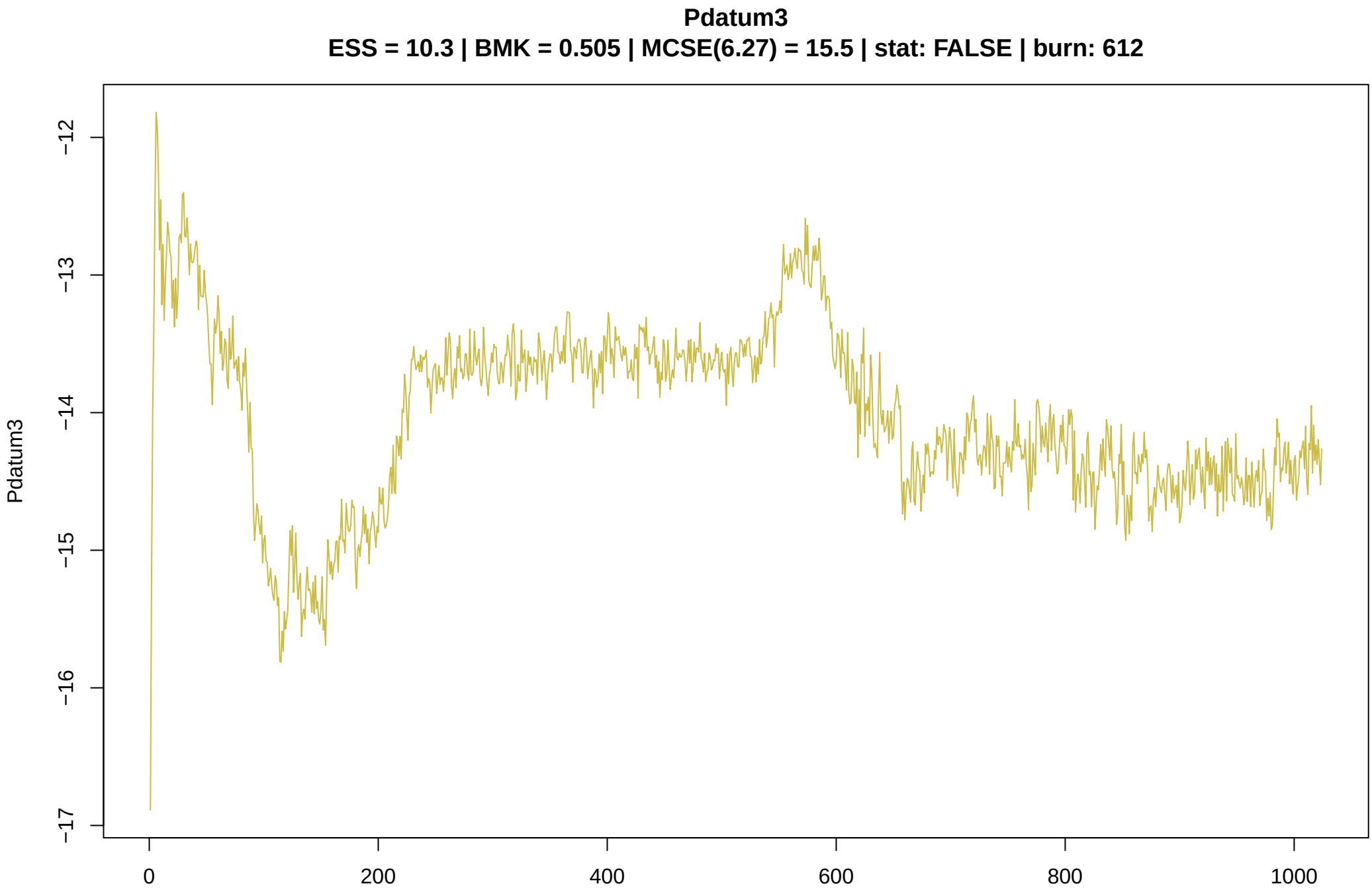

Pdatamean
ESS = 4.27 | BMK = 0.614 | MCSE(6.27) = 17.5 | stat: FALSE | burn: 1020
Pdatamean
−7.5
−8.0
−8.5
−9.0
−9.5
0
200
400
600
800
1000

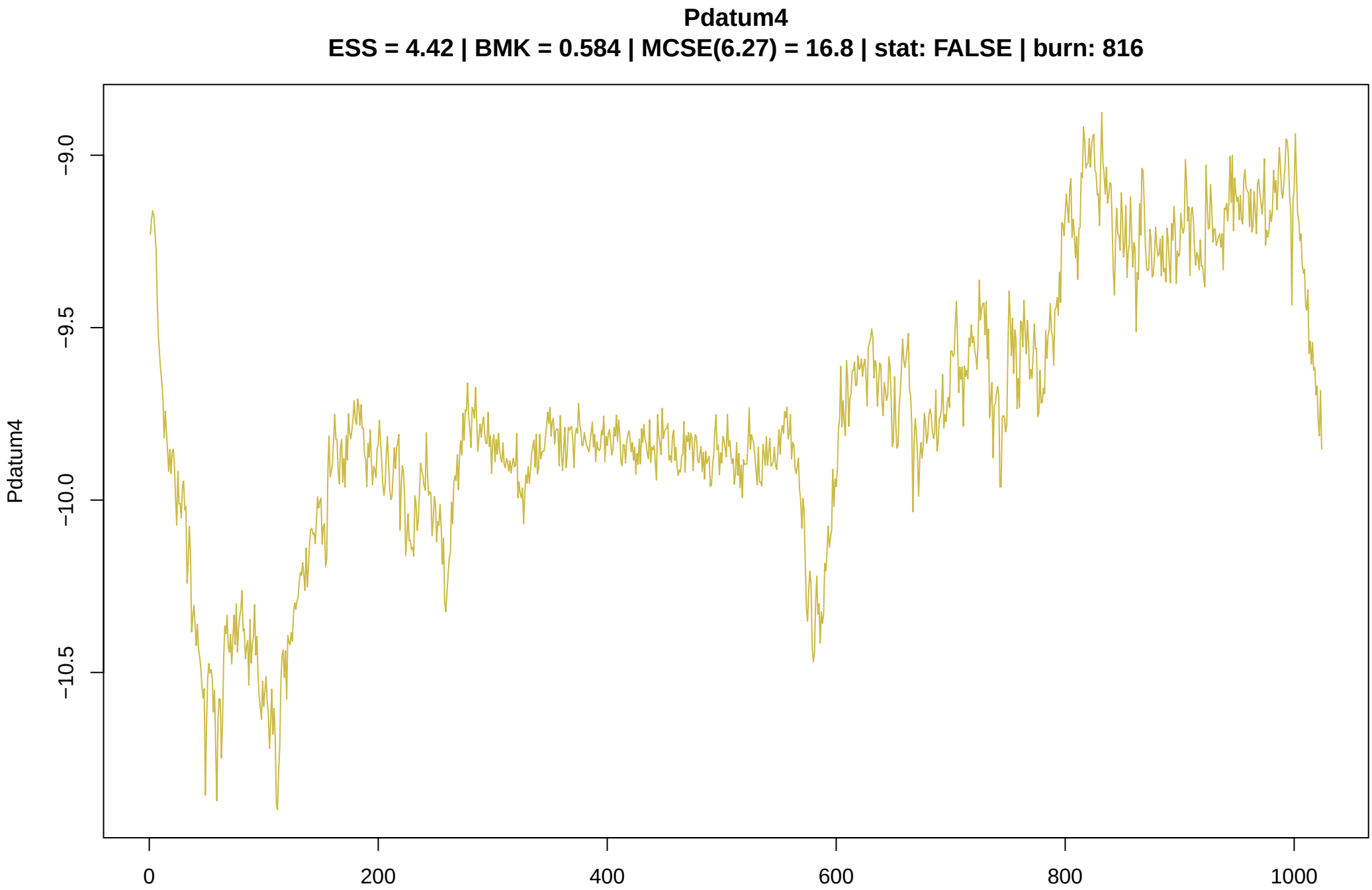

PdatacornerHi
ESS = 17.3 | BMK = 0.378 | MCSE(6.27) = 15.6 | stat: FALSE | burn: 612
PdatacornerHi
−14.0
−14.5
−15.0
−15.5
−16.0
−16.5
−17.0
−17.5
0
200
400
600
800
1000

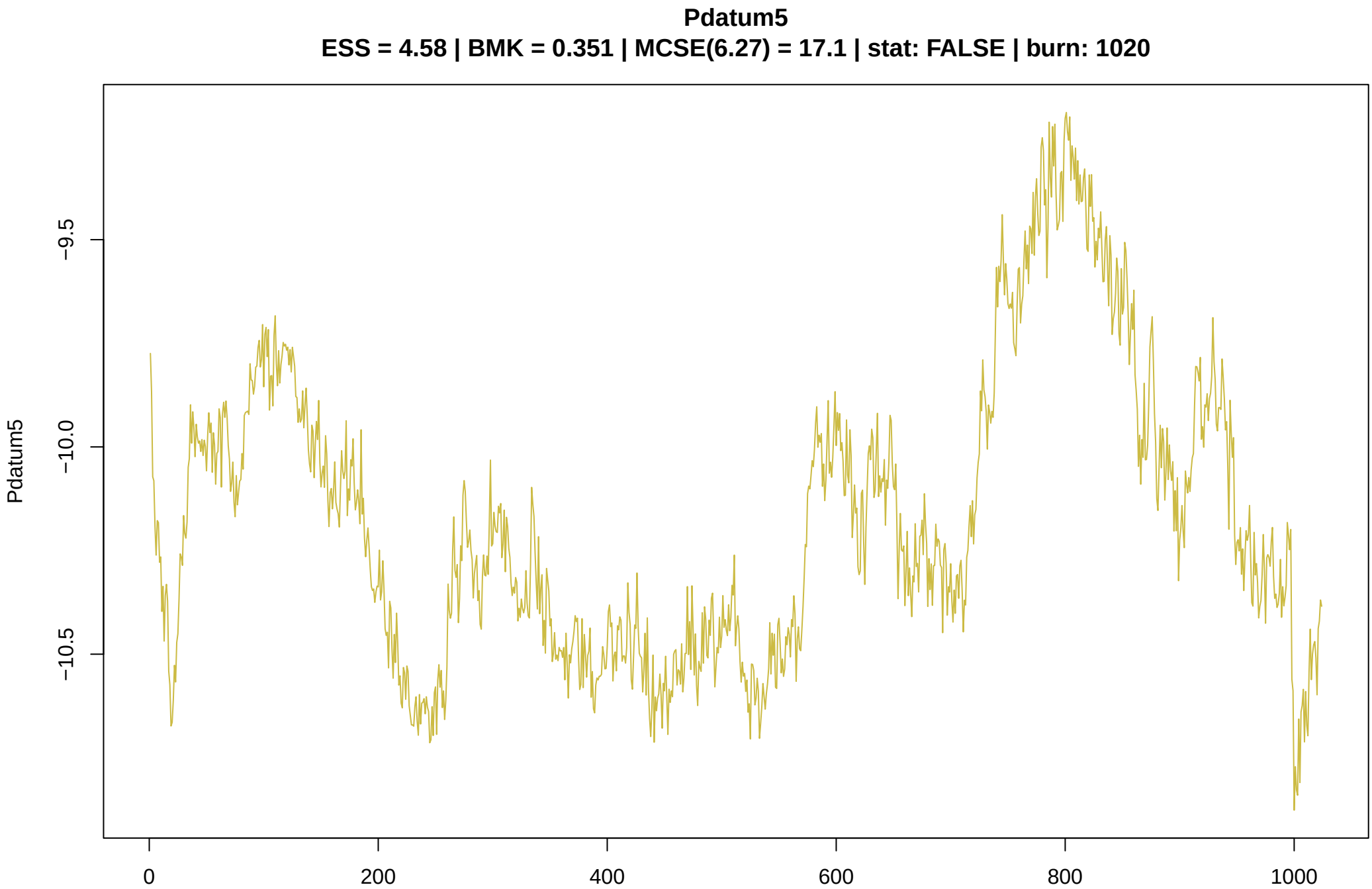

PdatacornerLo
ESS = 6.58 | BMK = 0.254 | MCSE(6.27) = 16.8 | stat: TRUE | burn: 816
PdatacornerLo
−10
−11
−12
−13
0
200
400
600
800
1000

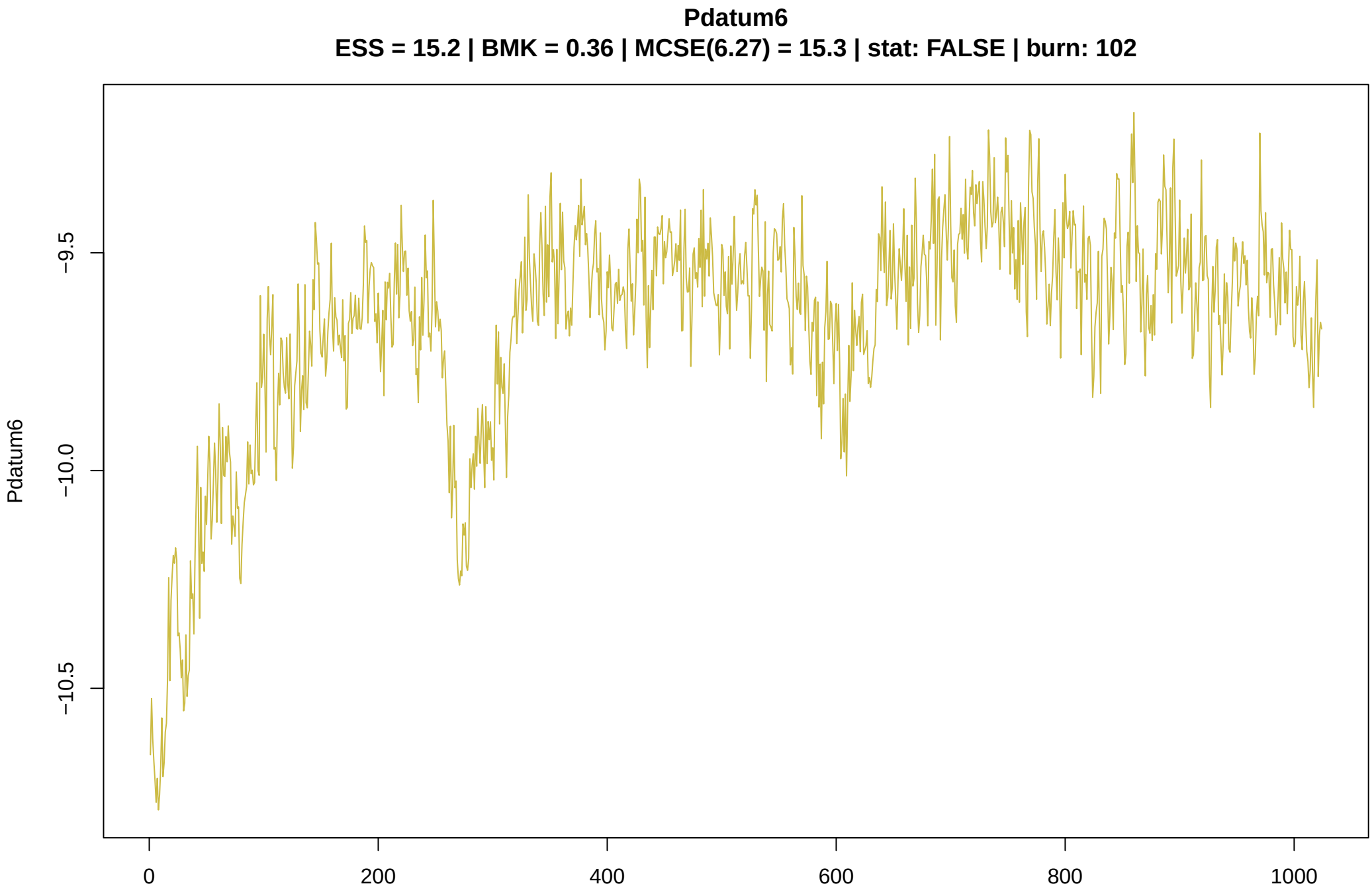

Pdatum1
ESS = 9.06 | BMK = 0.34 | MCSE(6.27) = 16.2 | stat: FALSE | burn: 1020
Pdatum1
−8.5
−9.0
−9.5
−10.0
−10.5
0
200
400
600
800
1000

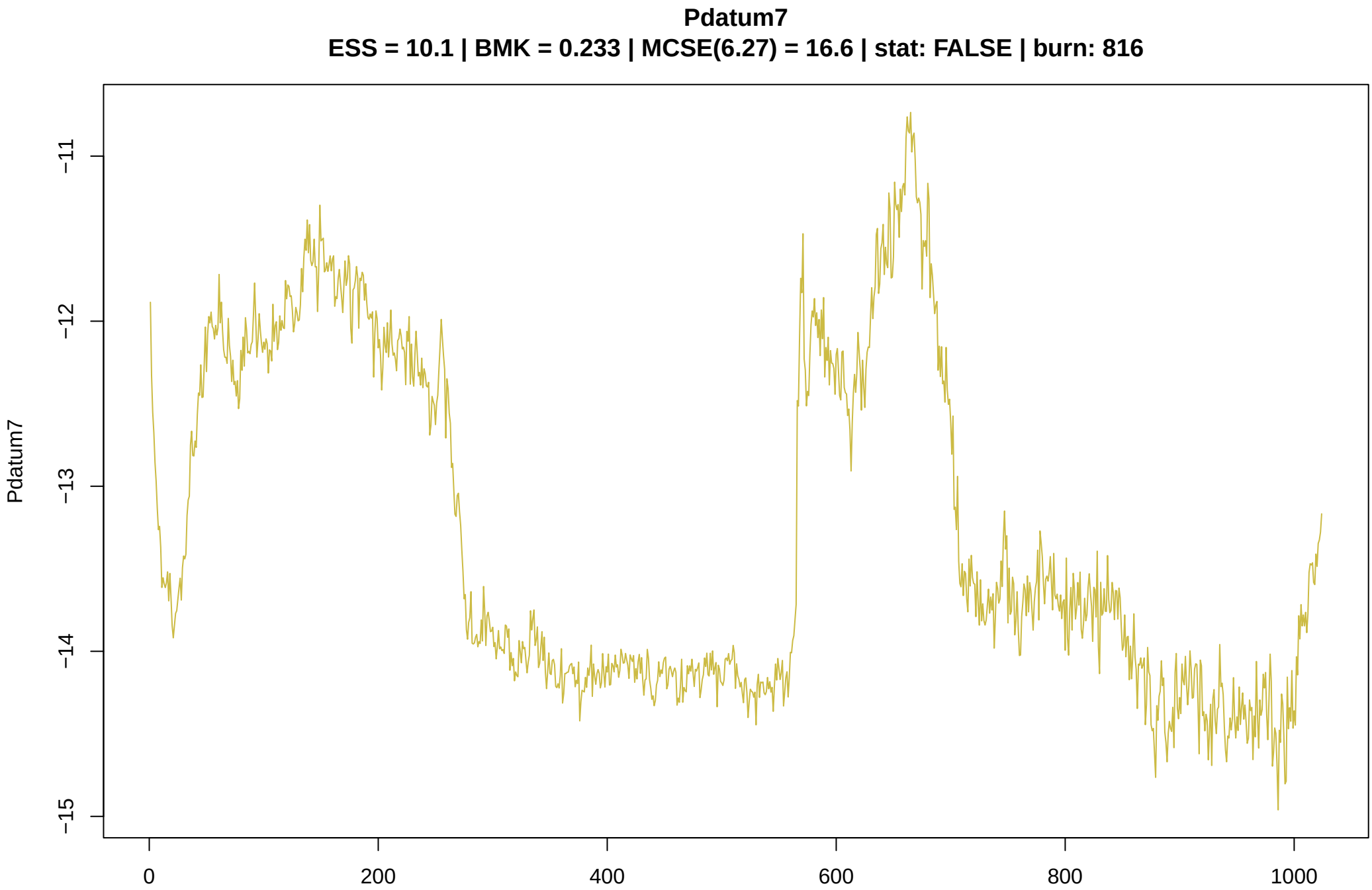

Pdatum2
ESS = 3.66 | BMK = 0.414 | MCSE(6.27) = 16.8 | stat: FALSE | burn: 816
Pdatum2
−12.0
−12.5
−13.0
−13.5
−14.0
−14.5
0
200
400
600
800
1000

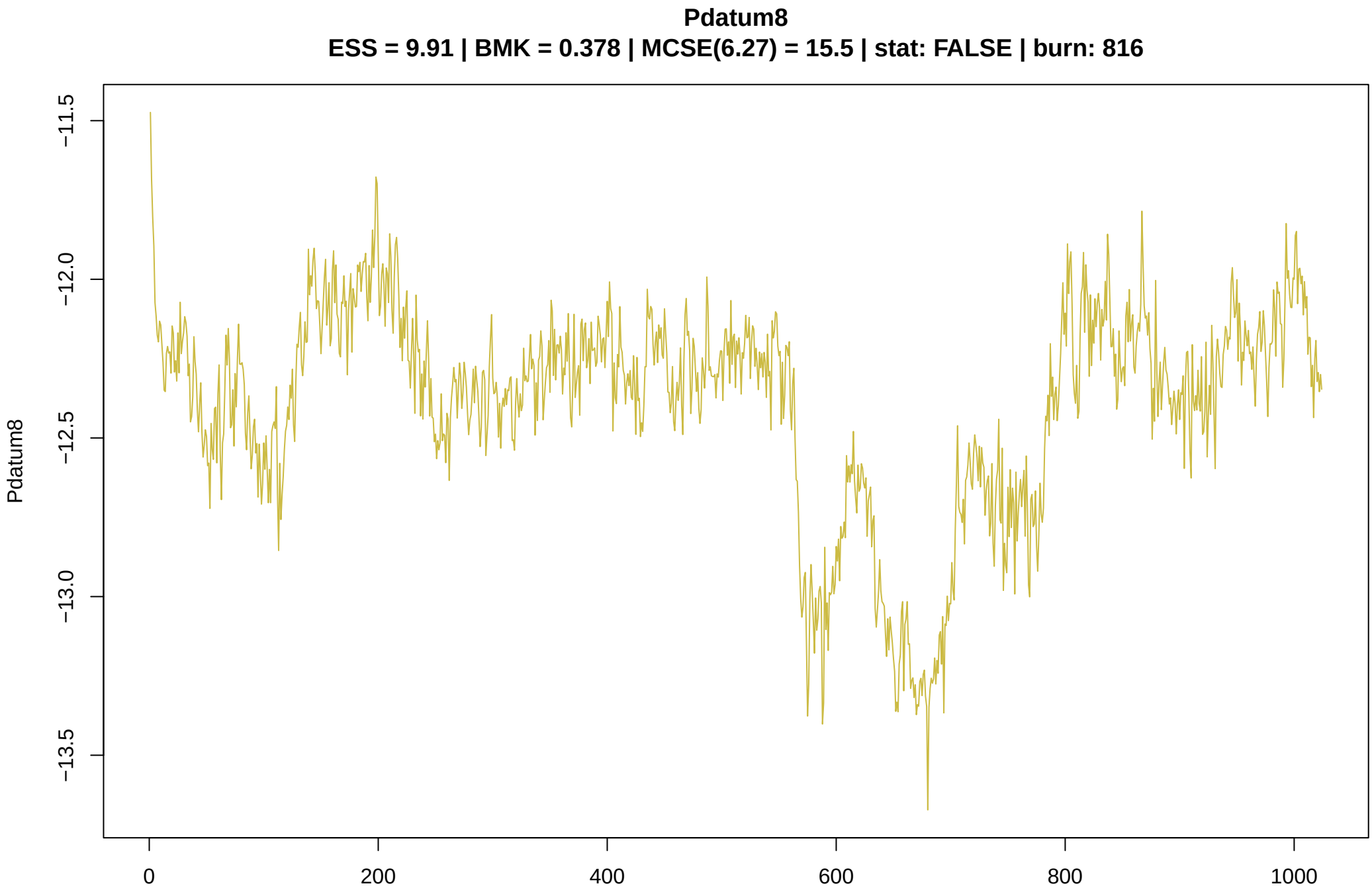

Pdatum3
ESS = 10.3 | BMK = 0.505 | MCSE(6.27) = 15.5 | stat: FALSE | burn: 612
Pdatum3
−12
−13
−14
−15
−16
−17
0
200
400
600
800
1000

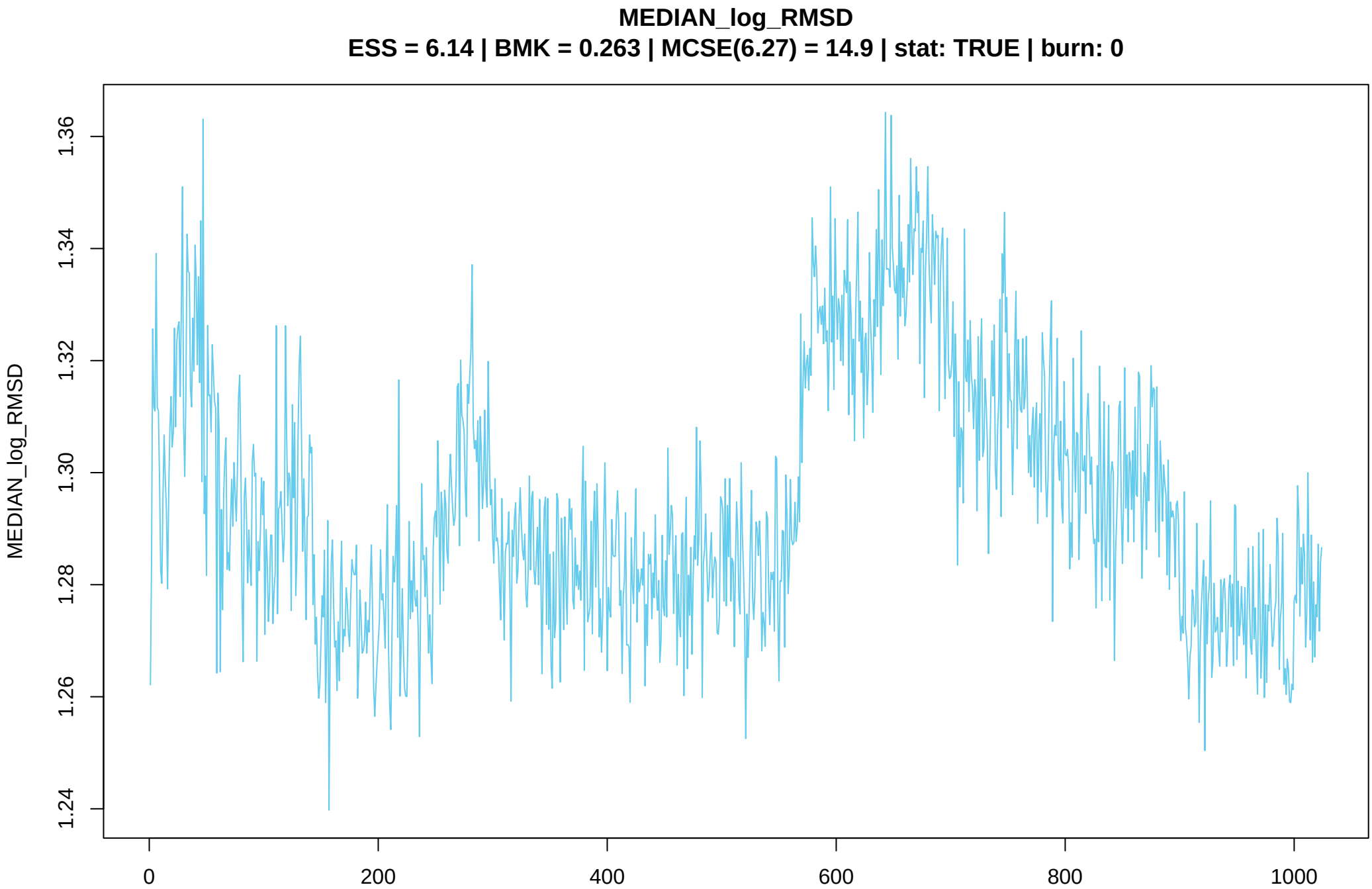

Pdatum4
ESS = 4.42 | BMK = 0.584 | MCSE(6.27) = 16.8 | stat: FALSE | burn: 816
Pdatum4
−9.0
−9.5
−10.0
−10.5
0
200
400
600
800
1000

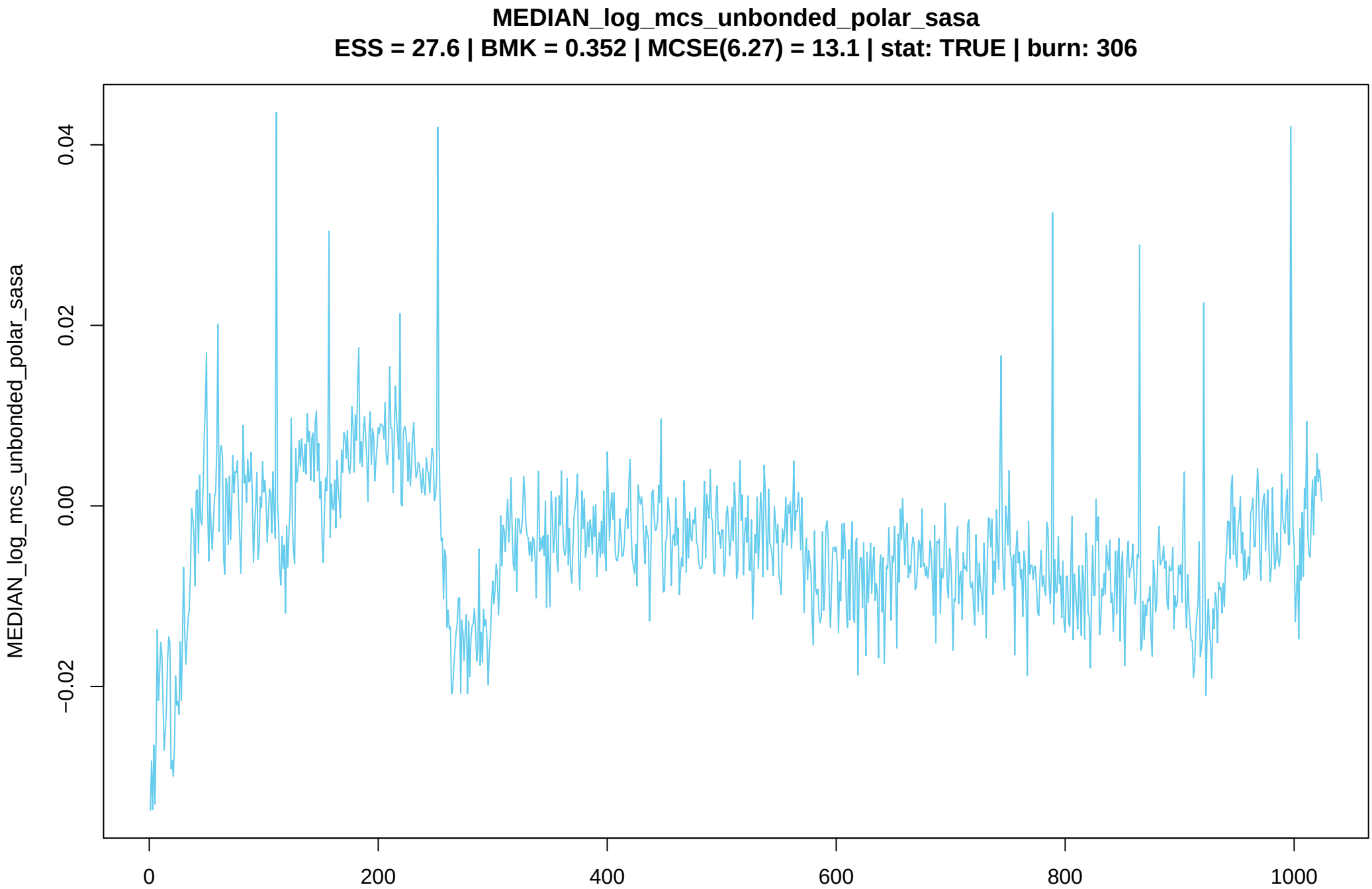

Pdatum5
ESS = 4.58 | BMK = 0.351 | MCSE(6.27) = 17.1 | stat: FALSE | burn: 1020
Pdatum5
−9.5
−10.0
−10.5
0
200
400
600
800
1000

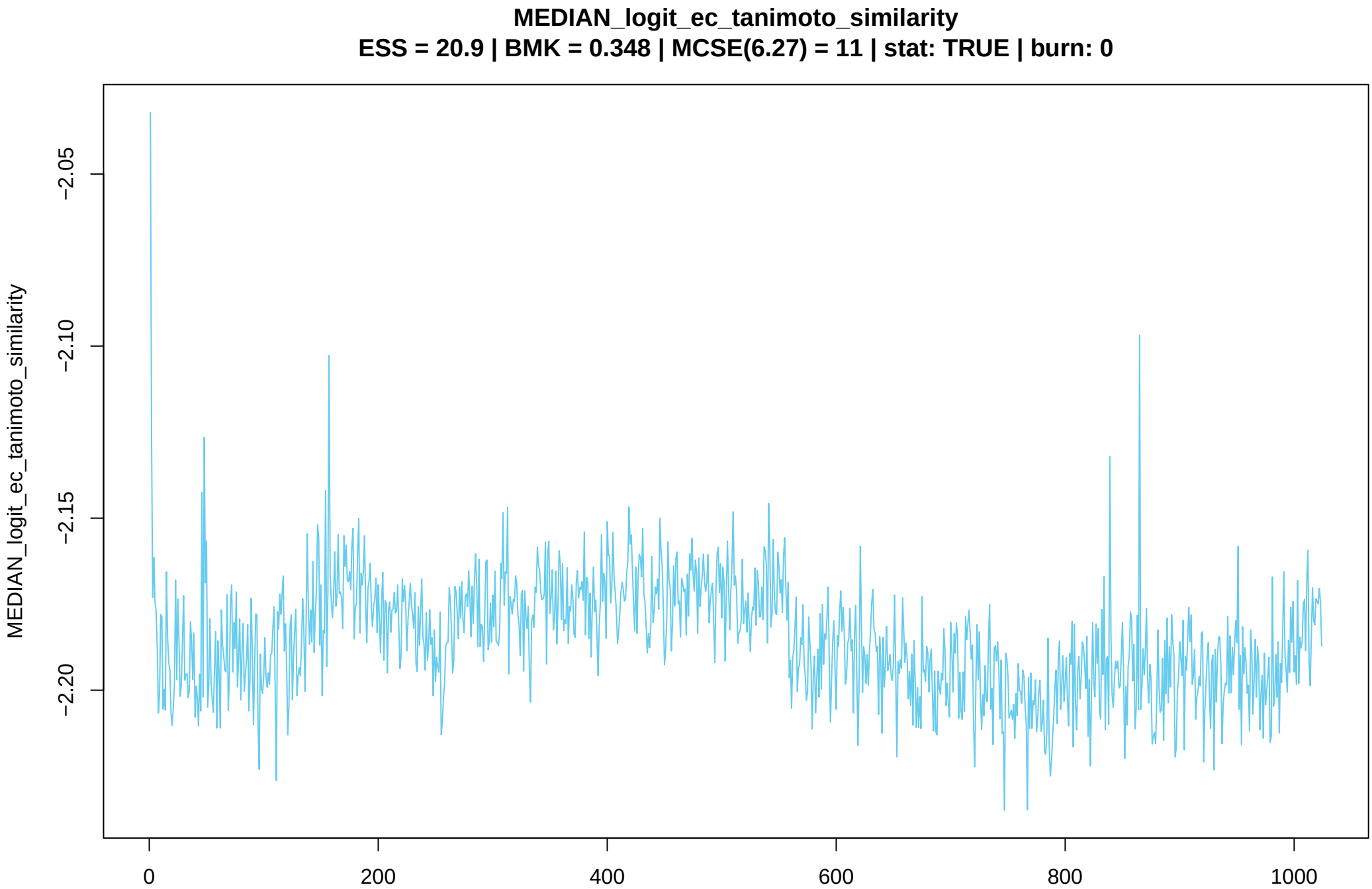

Pdatum6
ESS = 15.2 | BMK = 0.36 | MCSE(6.27) = 15.3 | stat: FALSE | burn: 102
Pdatum6
−9.5
−10.0
−10.5
0
200
400
600
800
1000

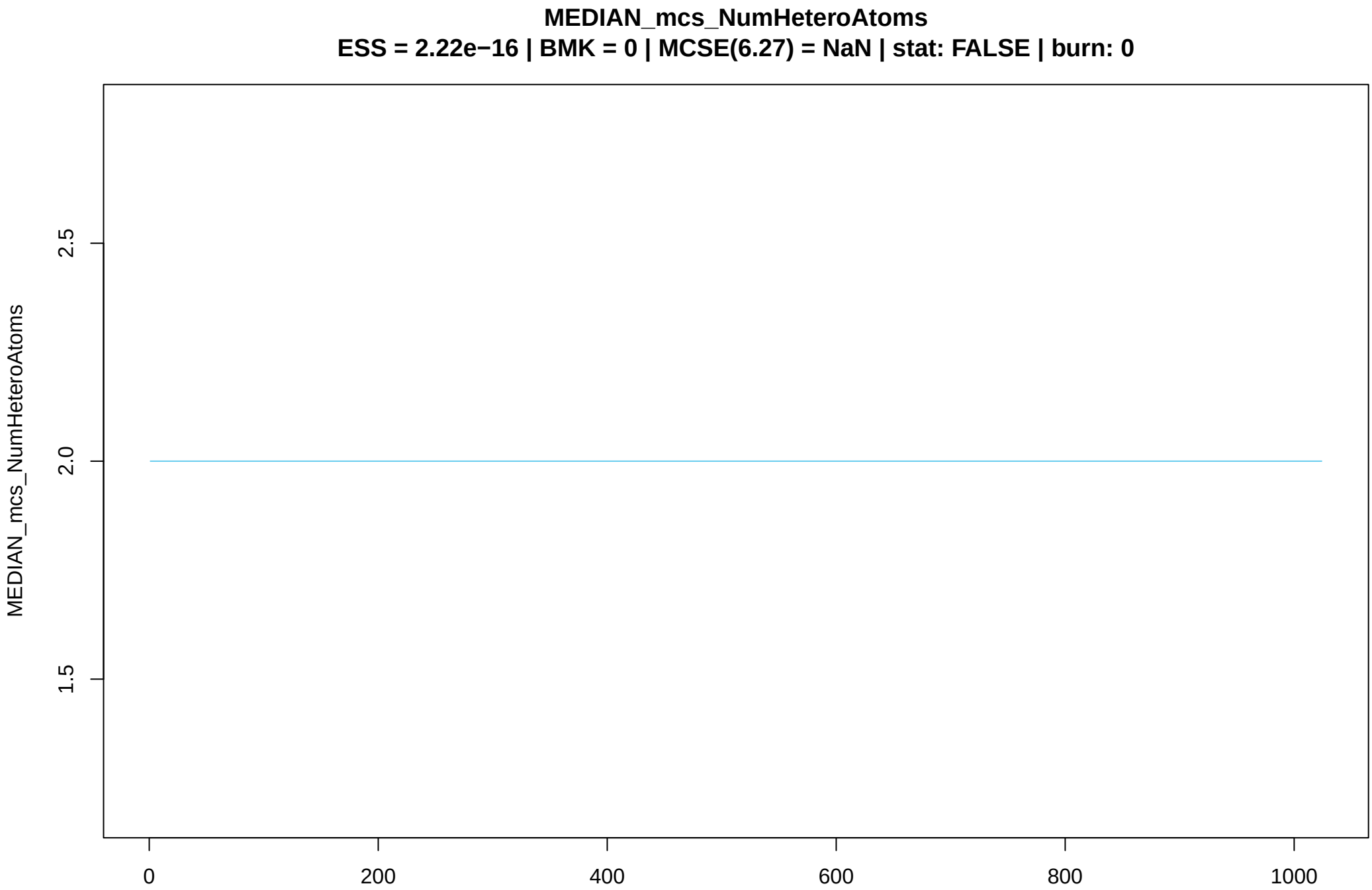

Pdatum7
ESS = 10.1 | BMK = 0.233 | MCSE(6.27) = 16.6 | stat: FALSE | burn: 816
Pdatum7
−11
−12
−13
−14
−15
0
200
400
600
800
1000

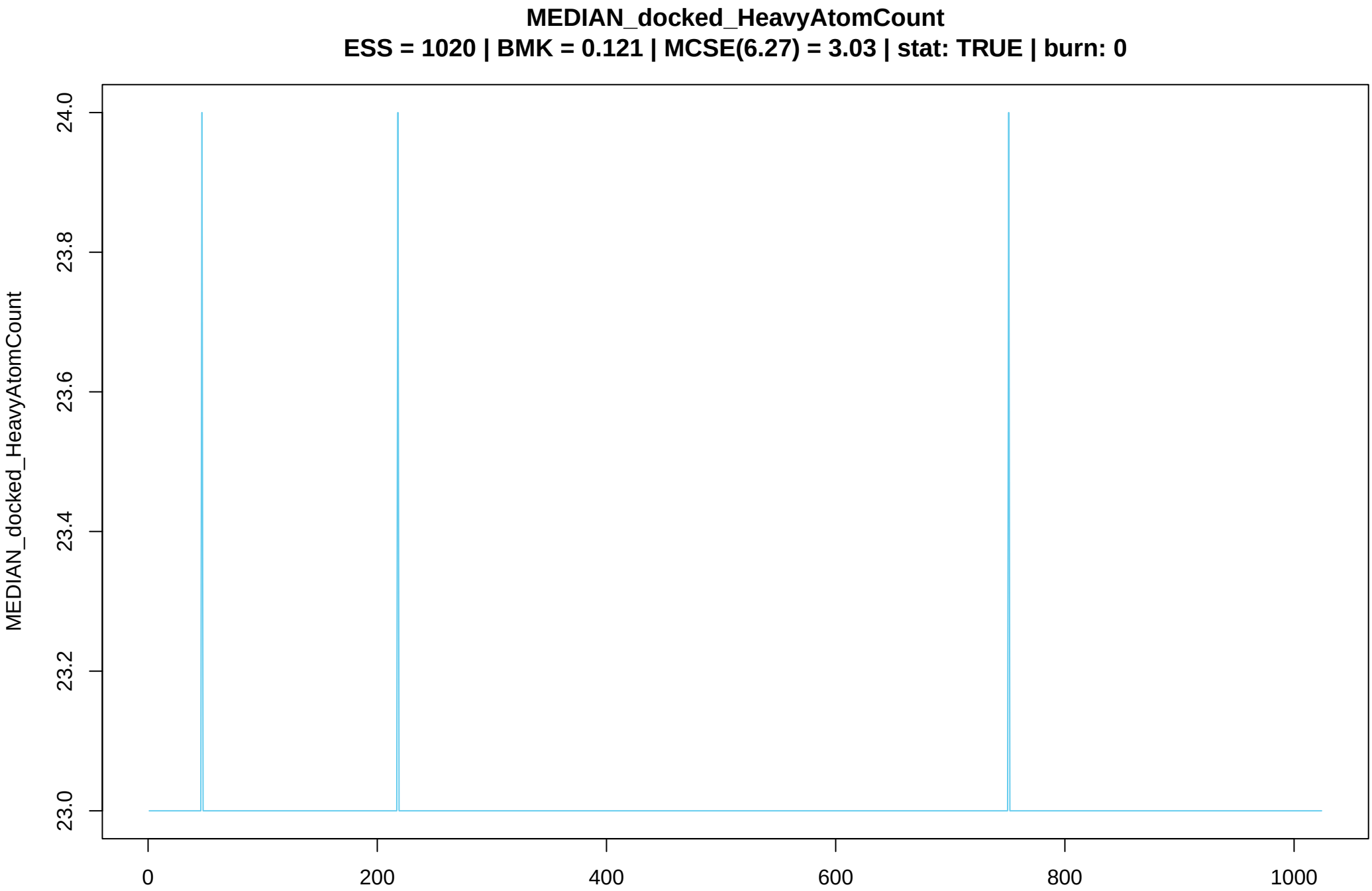

Pdatum8
ESS = 9.91 | BMK = 0.378 | MCSE(6.27) = 15.5 | stat: FALSE | burn: 816
Pdatum8
−11.5
−12.0
−12.5
−13.0
−13.5
0
200
400
600
800
1000

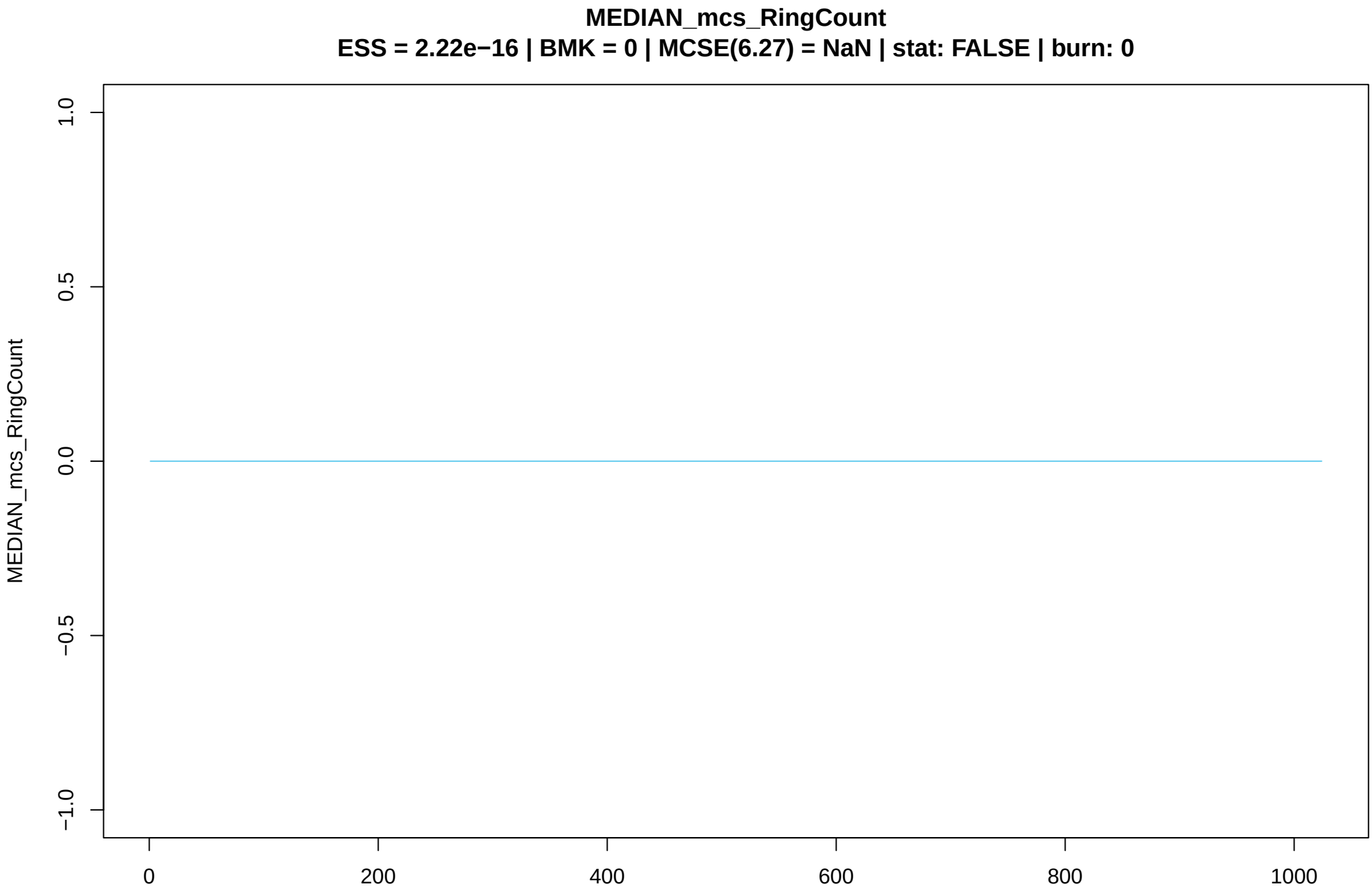

MEDIAN_log_RMSD
ESS = 6.14 | BMK = 0.263 | MCSE(6.27) = 14.9 | stat: TRUE | burn: 0
MEDIAN_log_RMSD
1.24
1.26
1.28
1.30
1.32
1.34
1.36
0
200
400
600
800
1000

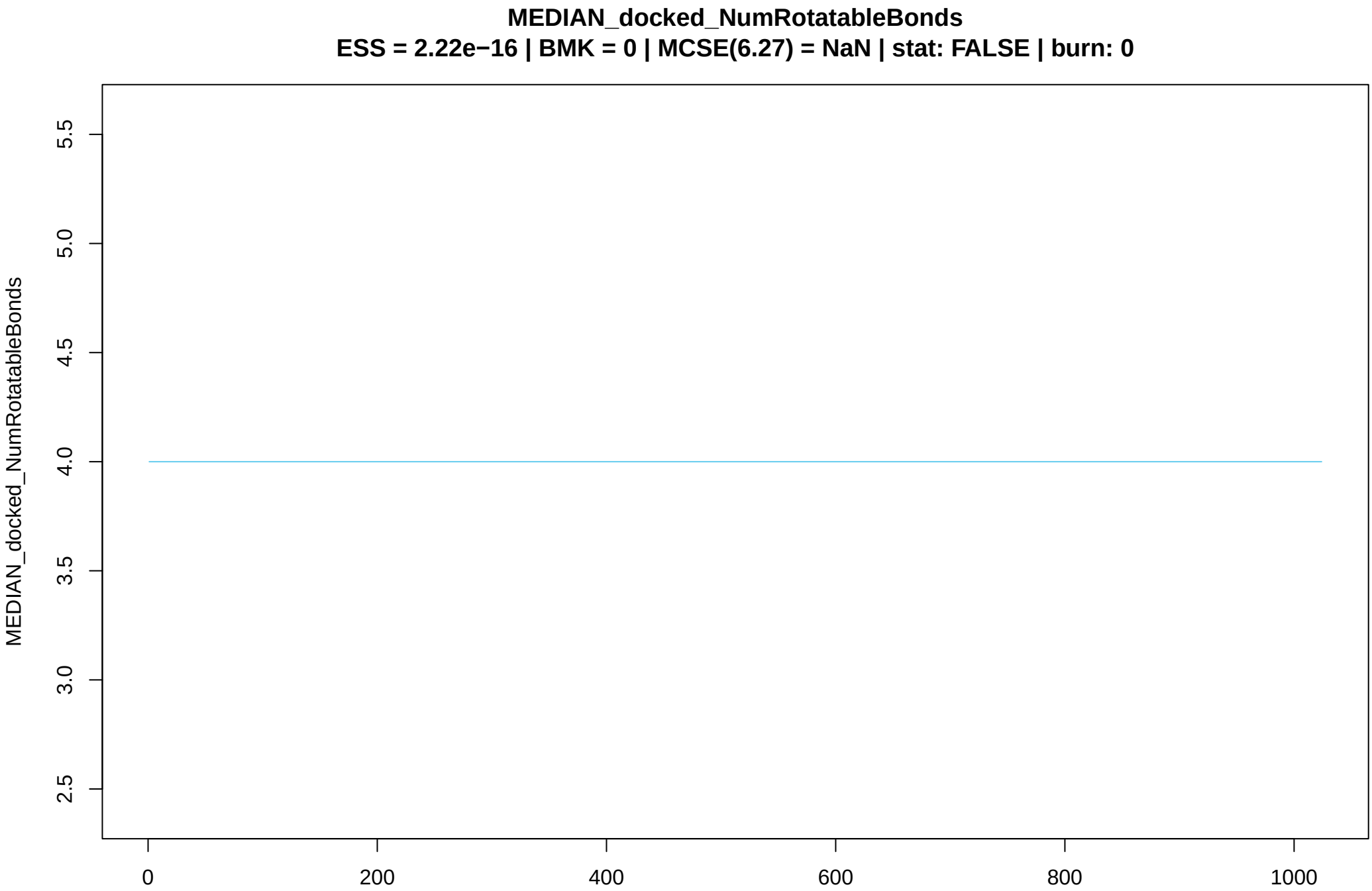

MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 27.6 | BMK = 0.352 | MCSE(6.27) = 13.1 | stat: TRUE | burn: 306
MEDIAN_log_mcs_unbonded_polar_sasa
0.04
0.02
0.00
−0.02
0
200
400
600
800
1000

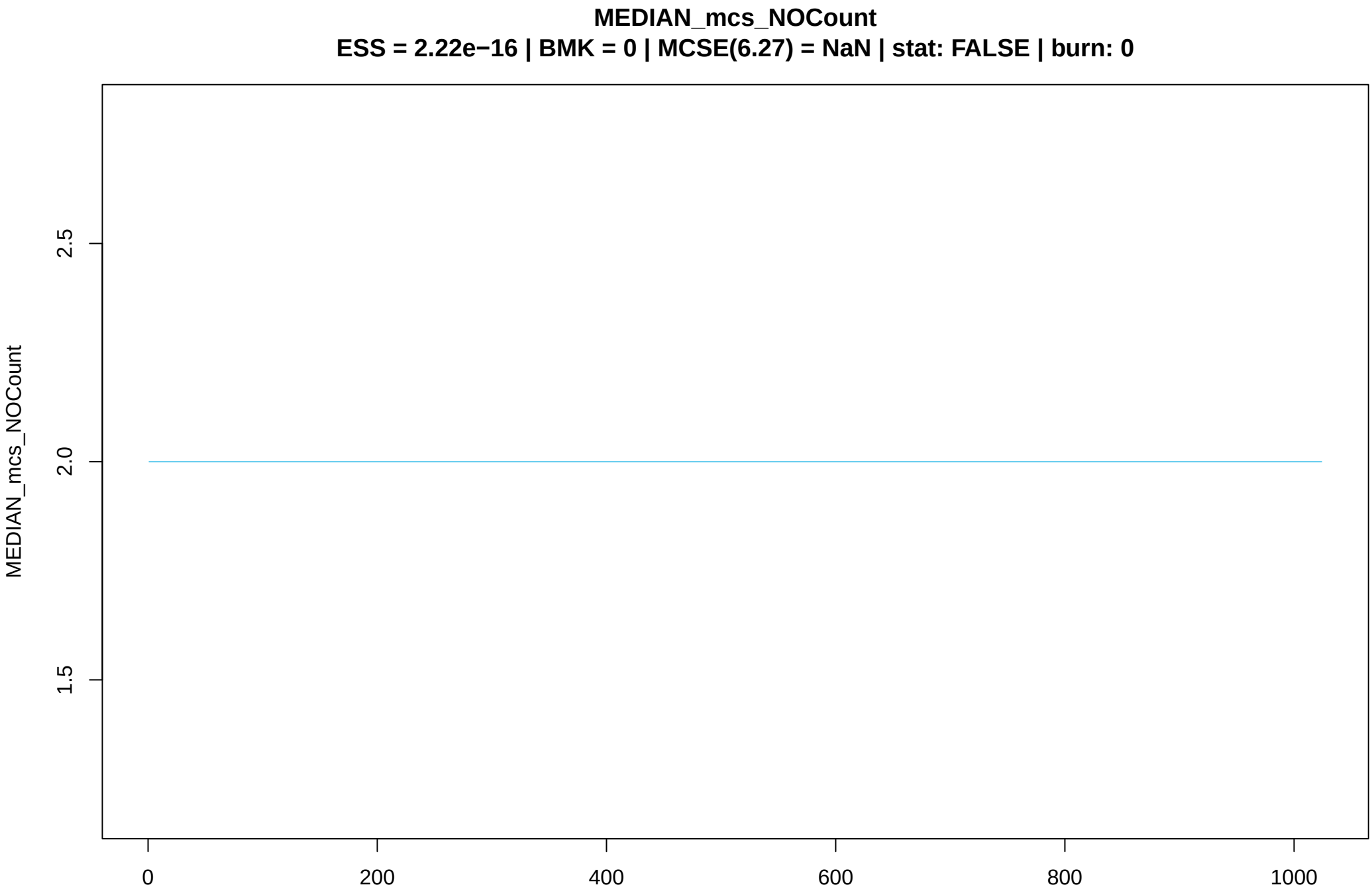

MEDIAN_logit_ec_tanimoto_similarity
ESS = 20.9 | BMK = 0.348 | MCSE(6.27) = 11 | stat: TRUE | burn: 0
MEDIAN_logit_ec_tanimoto_similarity
−2.05
−2.10
−2.15
−2.20
0
200
400
600
800
1000

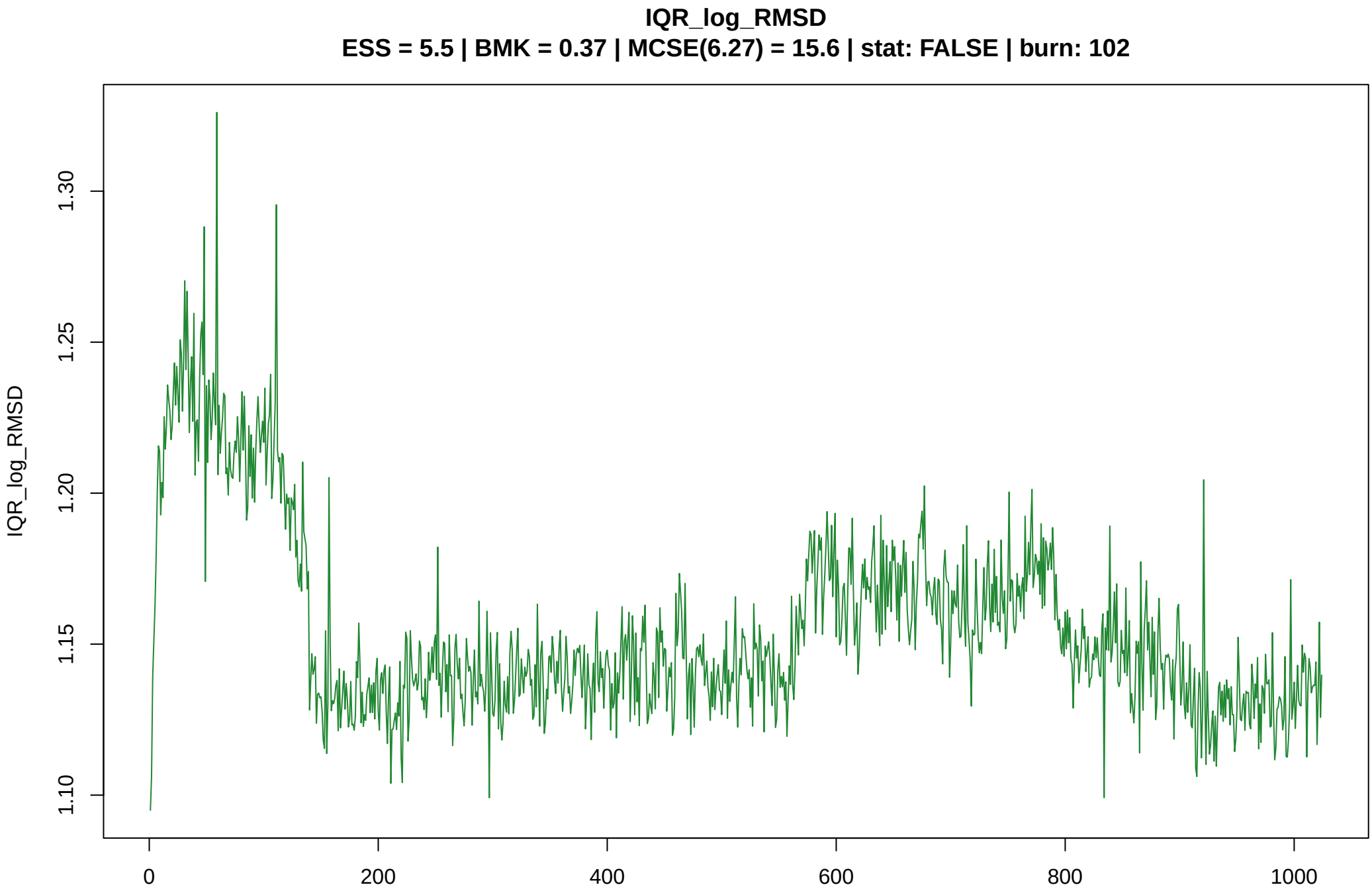

MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
1.5
2.0
2.5
0
200
400
600
800
1000

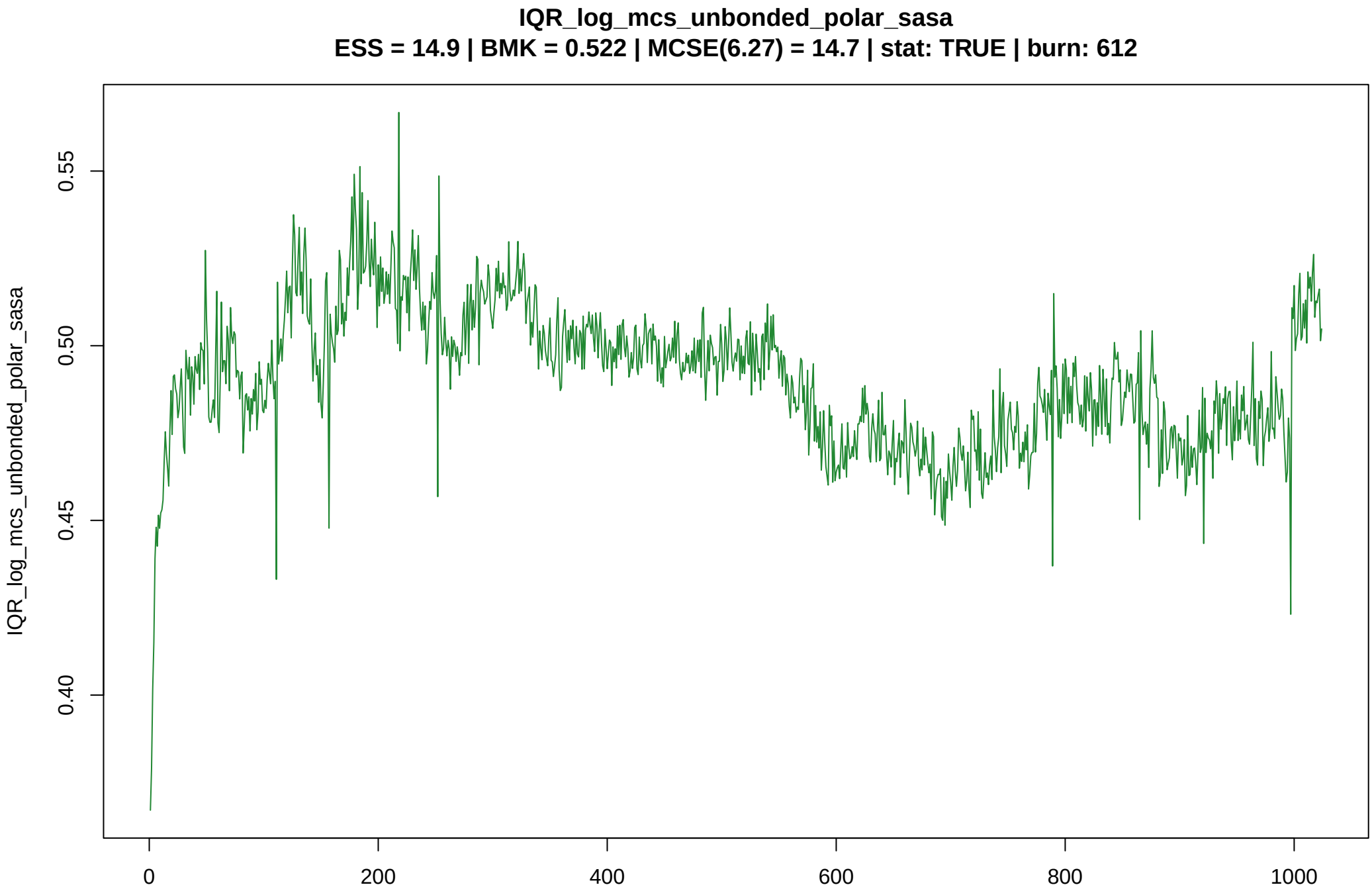

MEDIAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.121 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0
MEDIAN_docked_HeavyAtomCount
24.0
23.8
23.6
23.4
23.2
23.0
0
200
400
600
800
1000

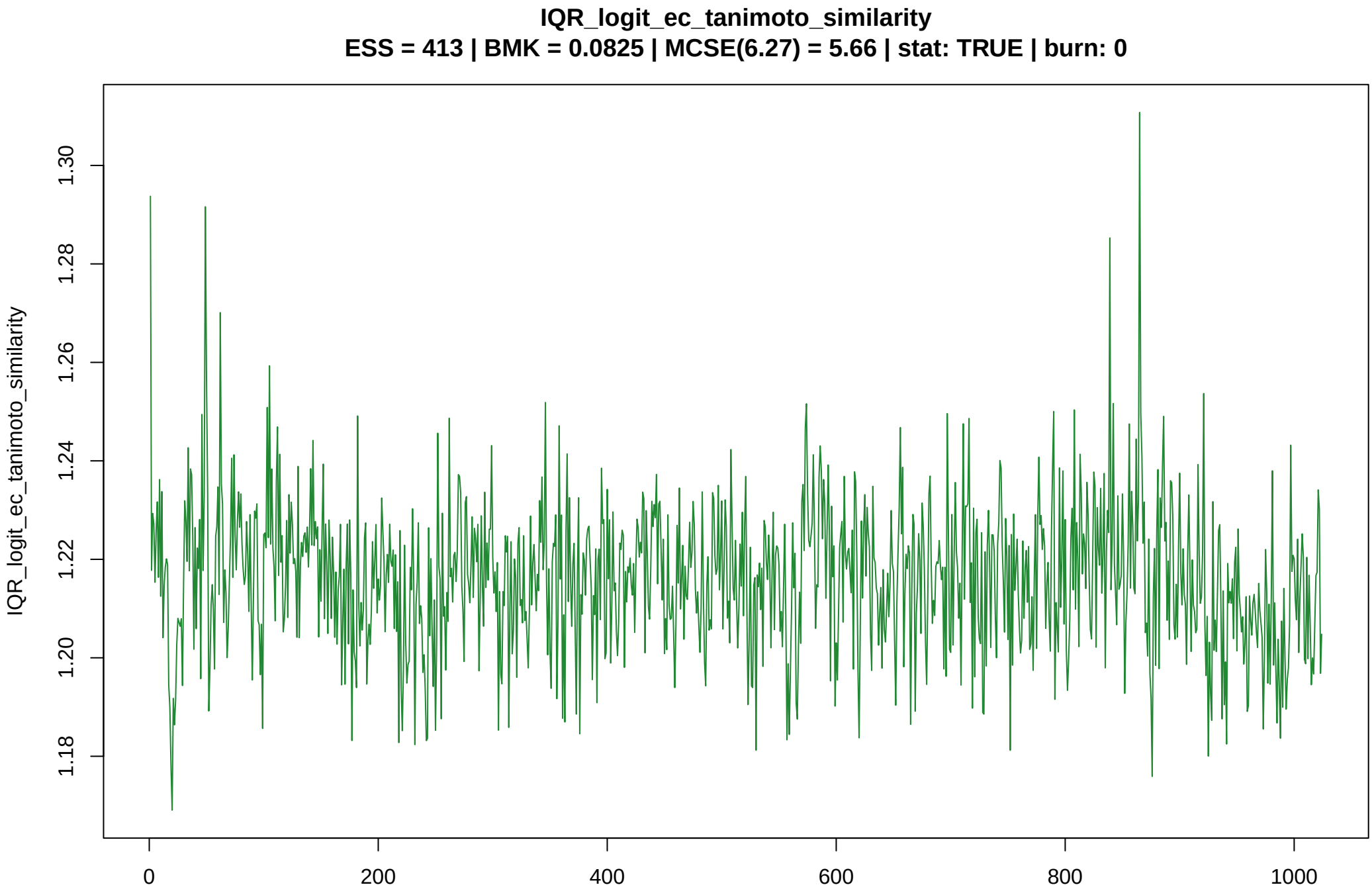

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
200
400
600
800
1000

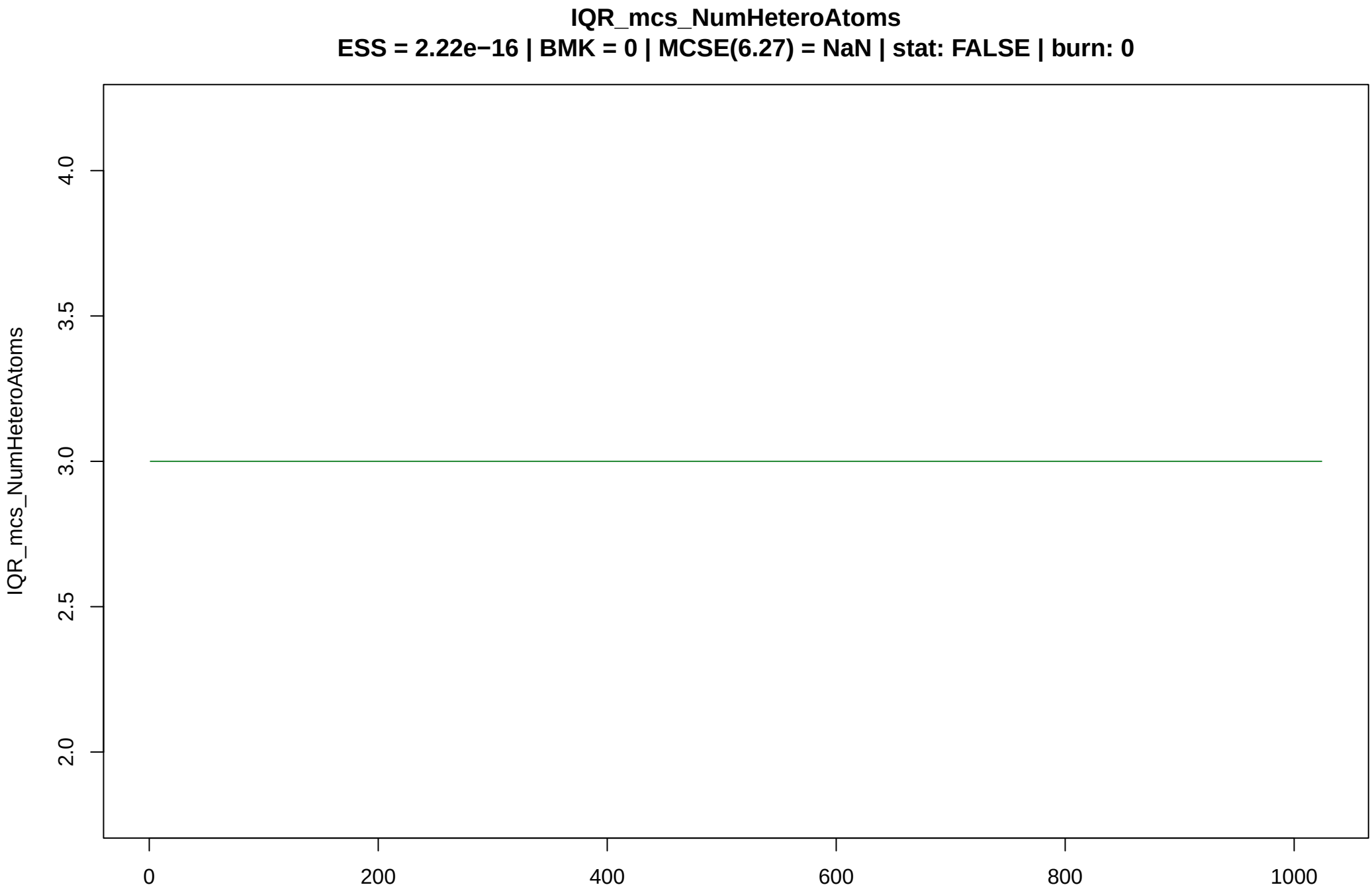

MEDIAN_docked_NumRotatableBonds
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_docked_NumRotatableBonds
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
200
400
600
800
1000

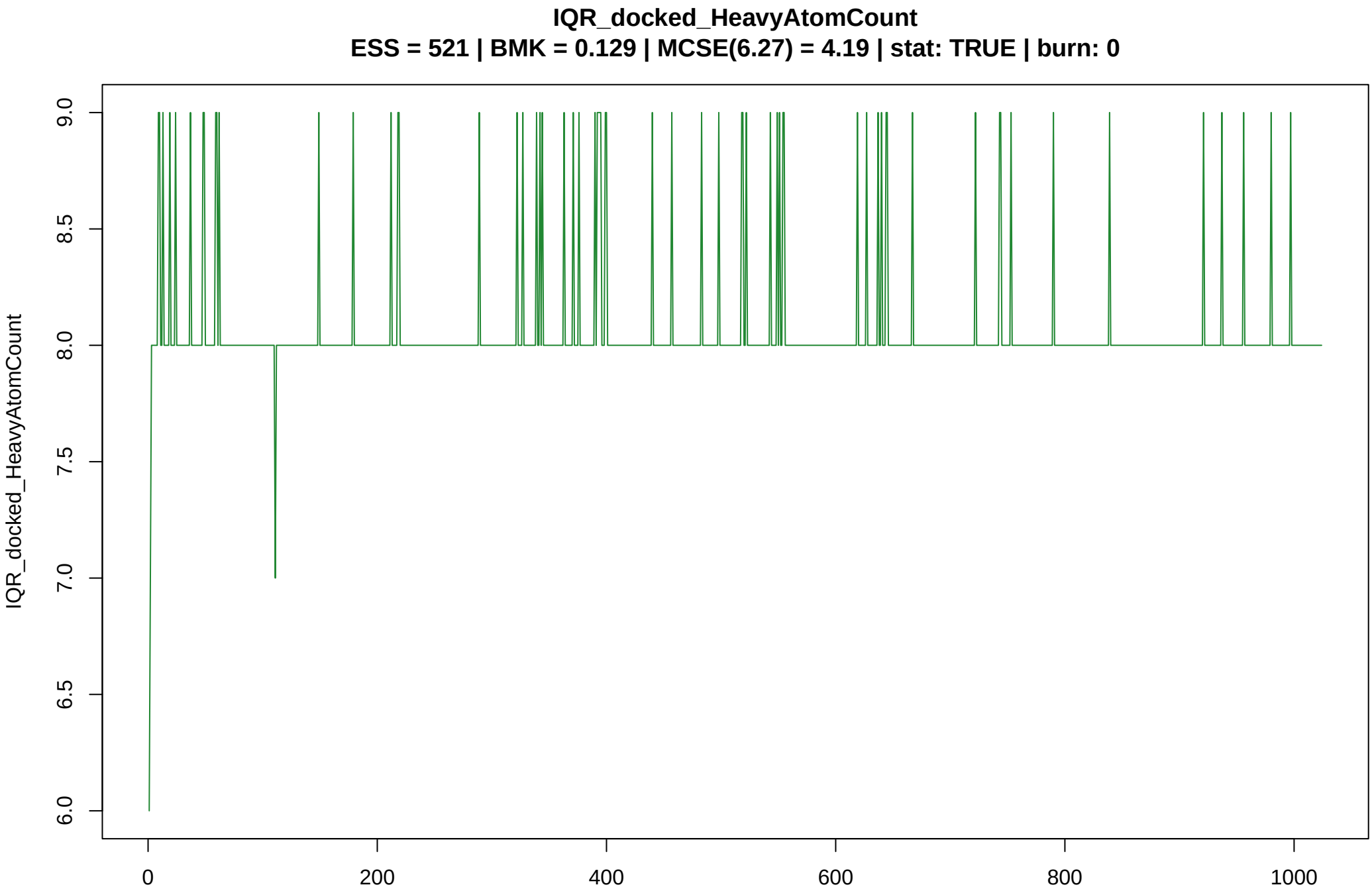

MEDIAN_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NOCount
2.5
2.0
1.5
0
200
400
600
800
1000

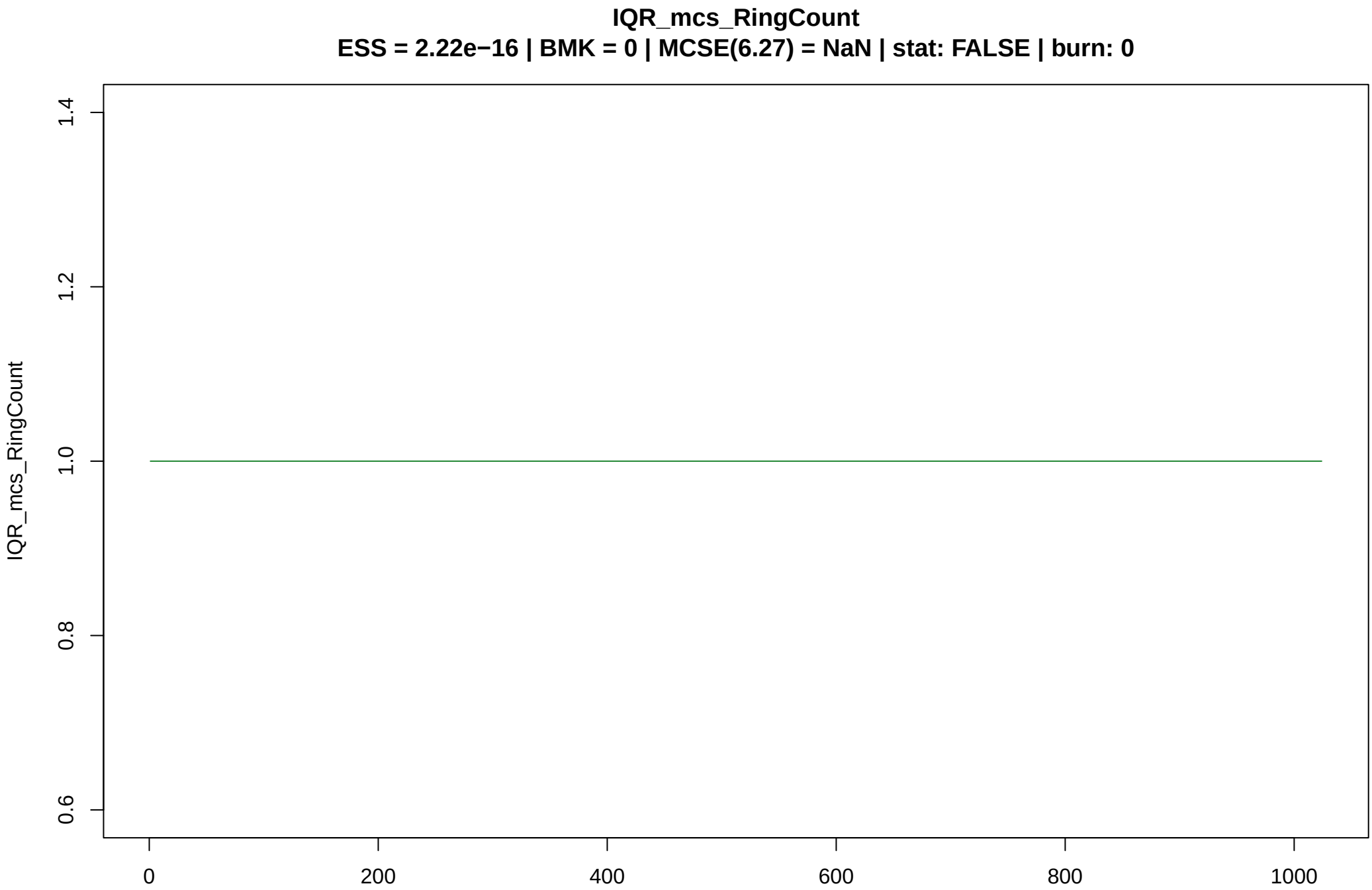

IQR_log_RMSD
ESS = 5.5 | BMK = 0.37 | MCSE(6.27) = 15.6 | stat: FALSE | burn: 102
IQR_log_RMSD
1.10
1.15
1.20
1.25
1.30
0
200
400
600
800
1000

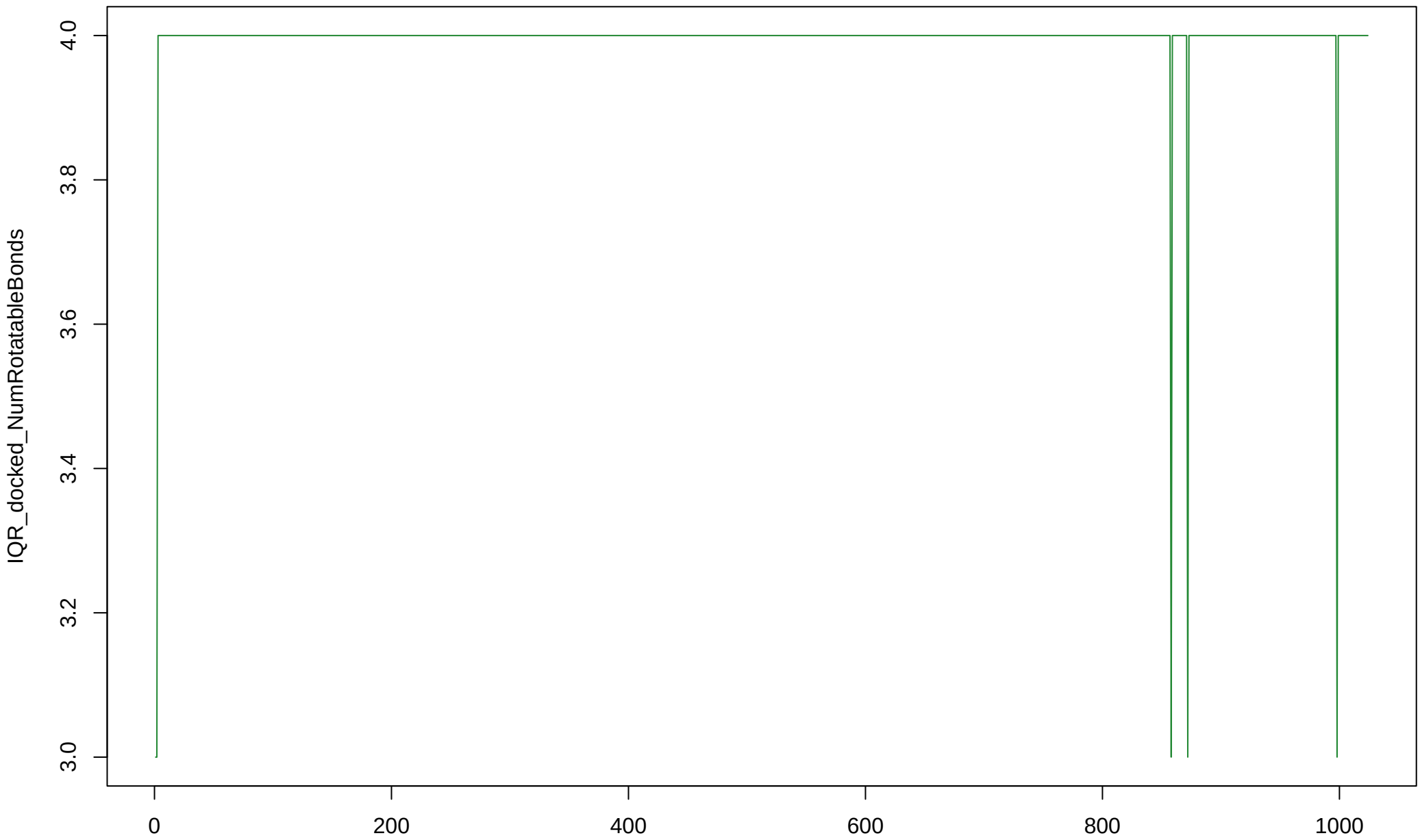

IQR_log_mcs_unbonded_polar_sasa
ESS = 14.9 | BMK = 0.522 | MCSE(6.27) = 14.7 | stat: TRUE | burn: 612
IQR_log_mcs_unbonded_polar_sasa
0.40
0.45
0.50
0.55
0
200
400
600
800
1000

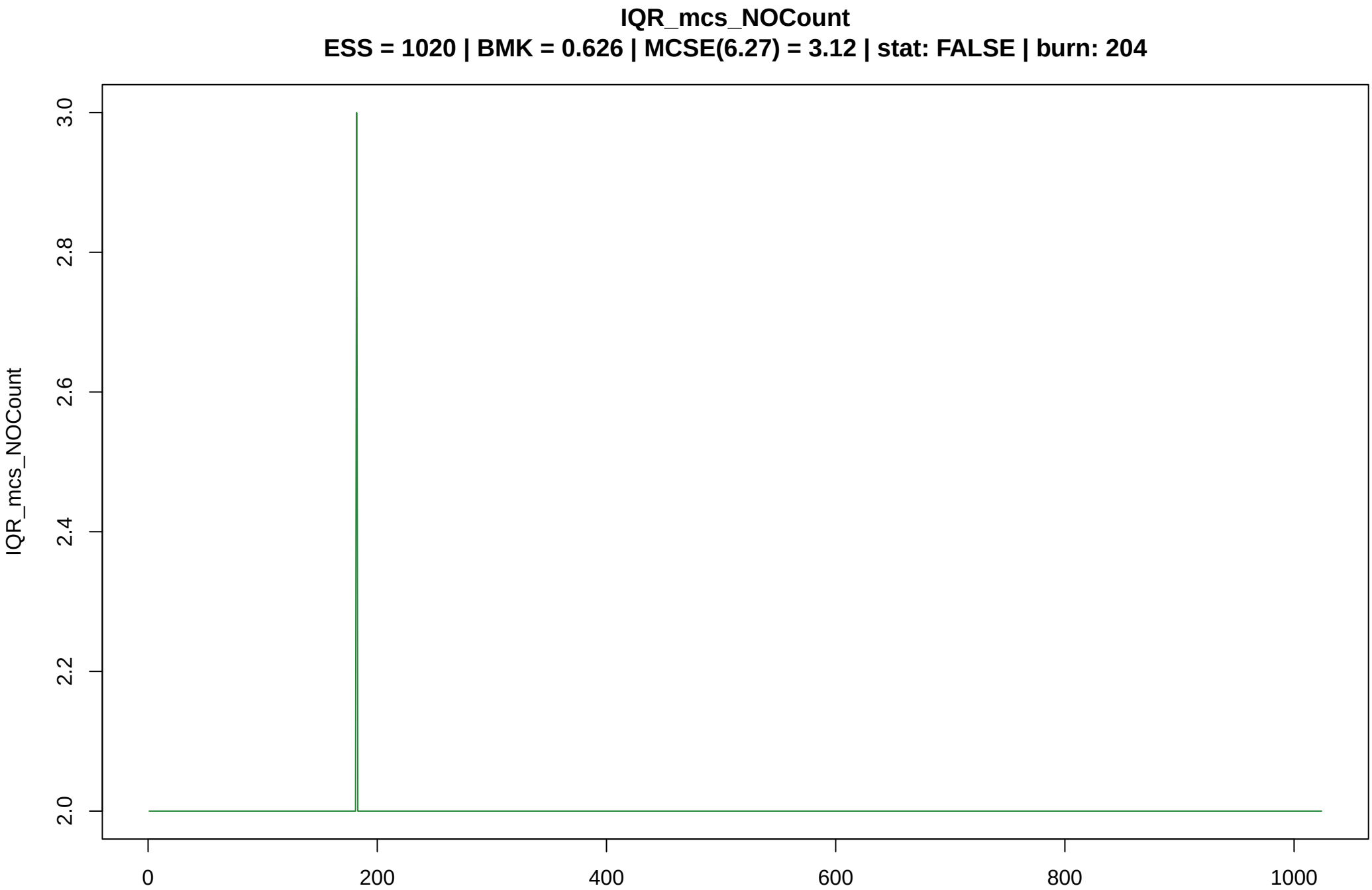

IQR_logit_ec_tanimoto_similarity
ESS = 413 | BMK = 0.0825 | MCSE(6.27) = 5.66 | stat: TRUE | burn: 0
IQR_logit_ec_tanimoto_similarity
1.18
1.20
1.22
1.24
1.26
1.28
1.30
0
200
400
600
800
1000

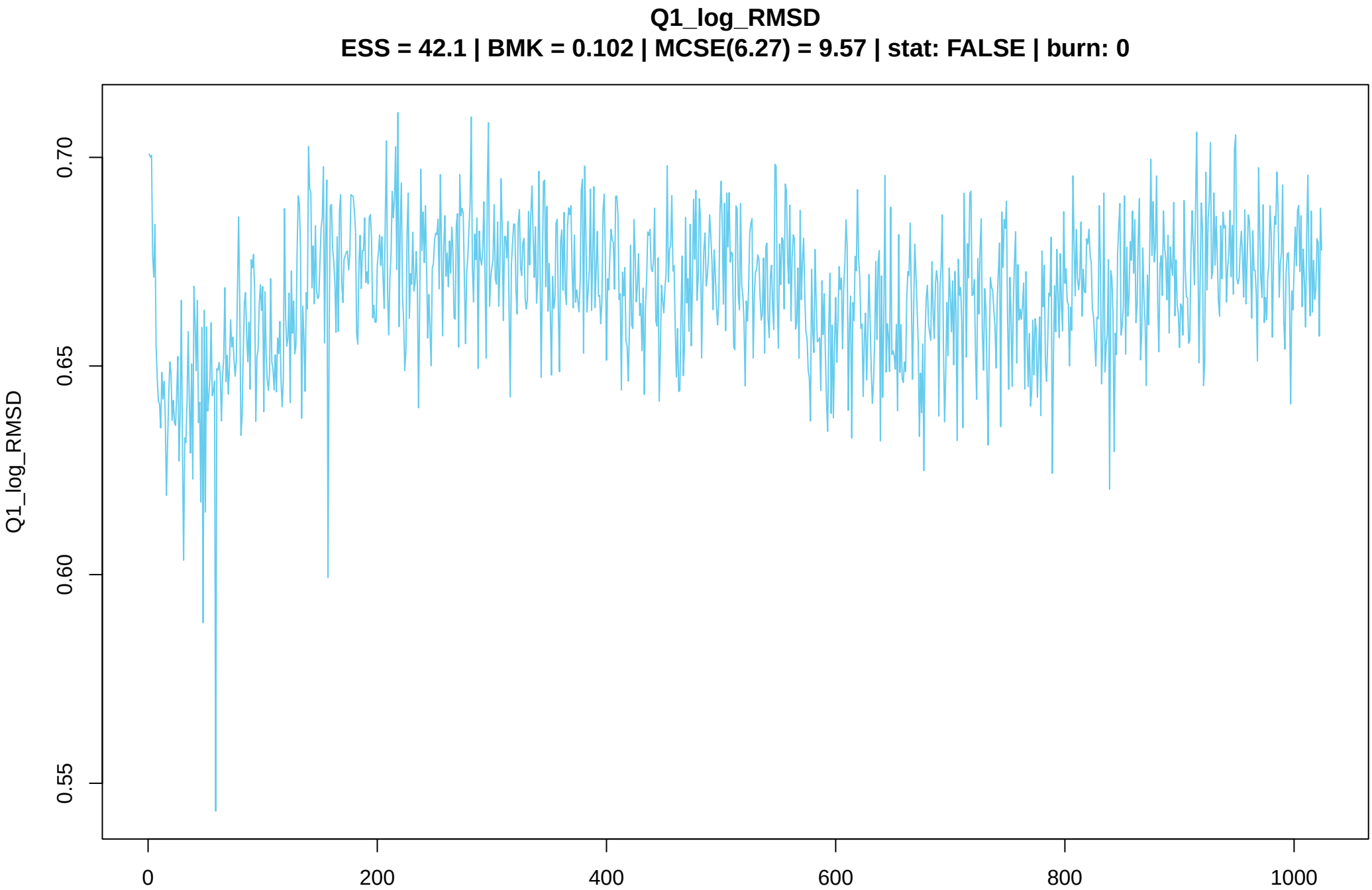

IQR_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_NumHeteroAtoms
2.0
2.5
3.0
3.5
4.0
0
200
400
600
800
1000

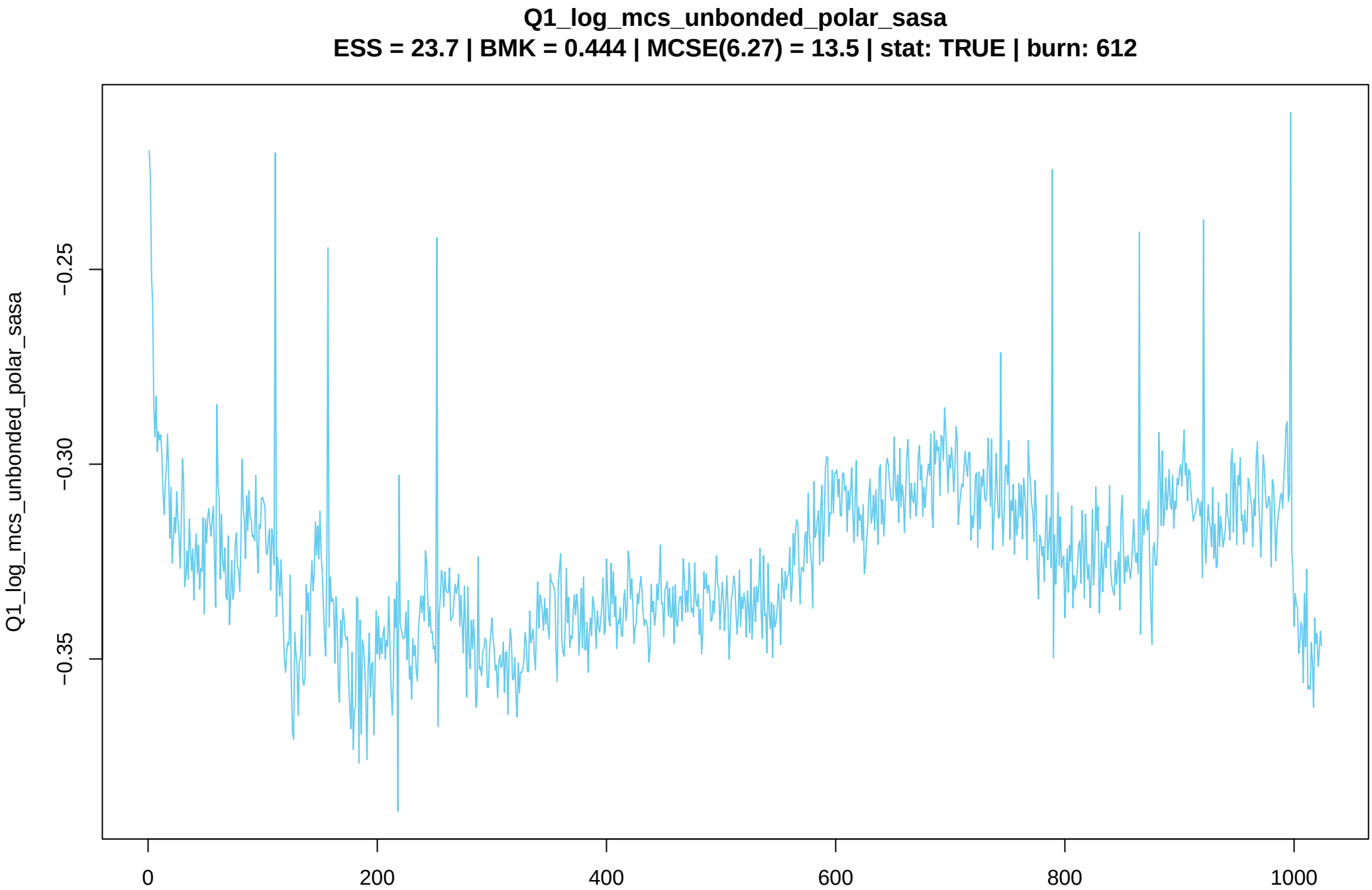

IQR_docked_HeavyAtomCount
ESS = 521 | BMK = 0.129 | MCSE(6.27) = 4.19 | stat: TRUE | burn: 0
IQR_docked_HeavyAtomCount
6.0
6.5
7.0
7.5
8.0
8.5
9.0
0
200
400
600
800
1000

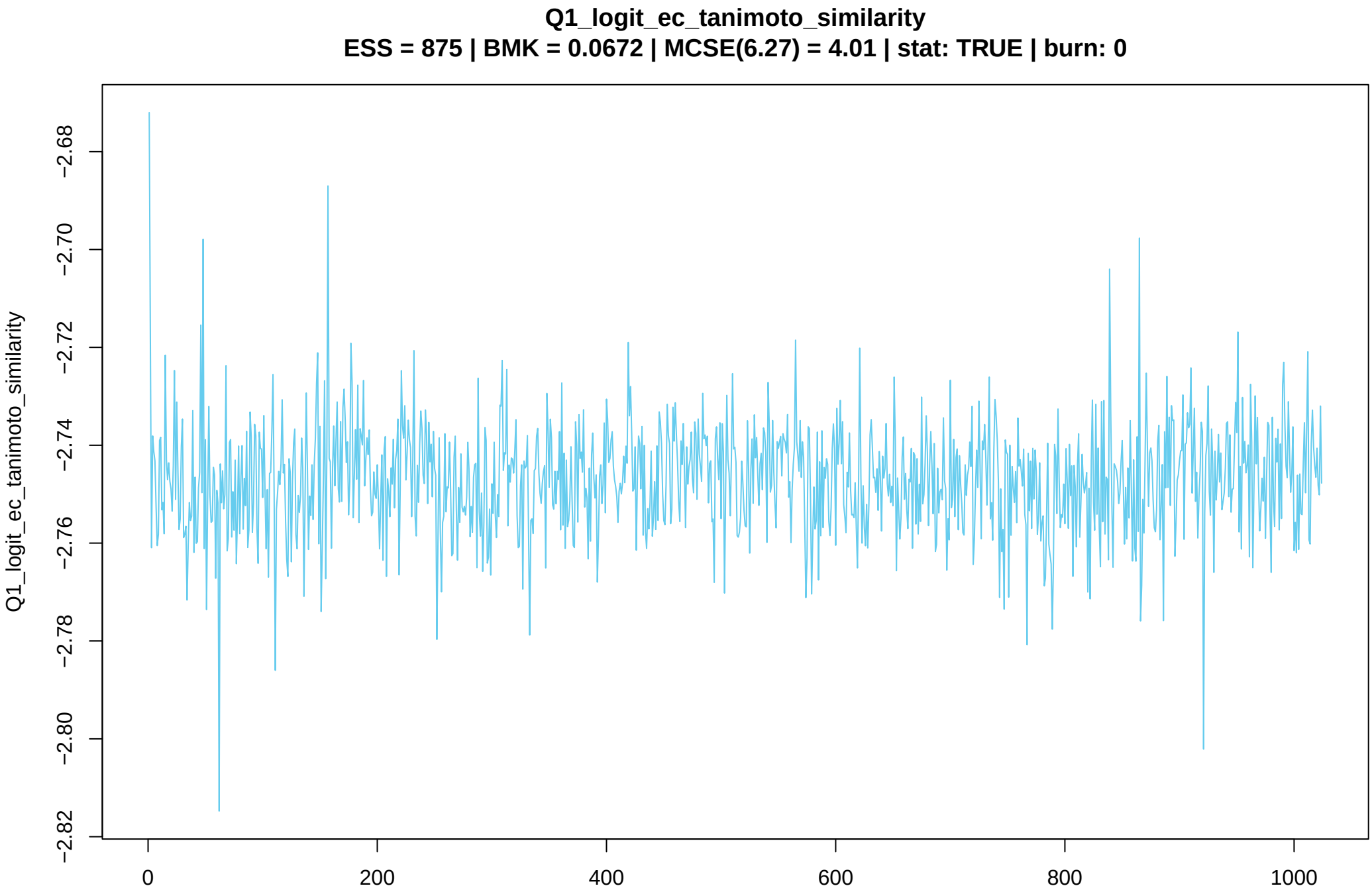

IQR_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
200
400
600
800
1000

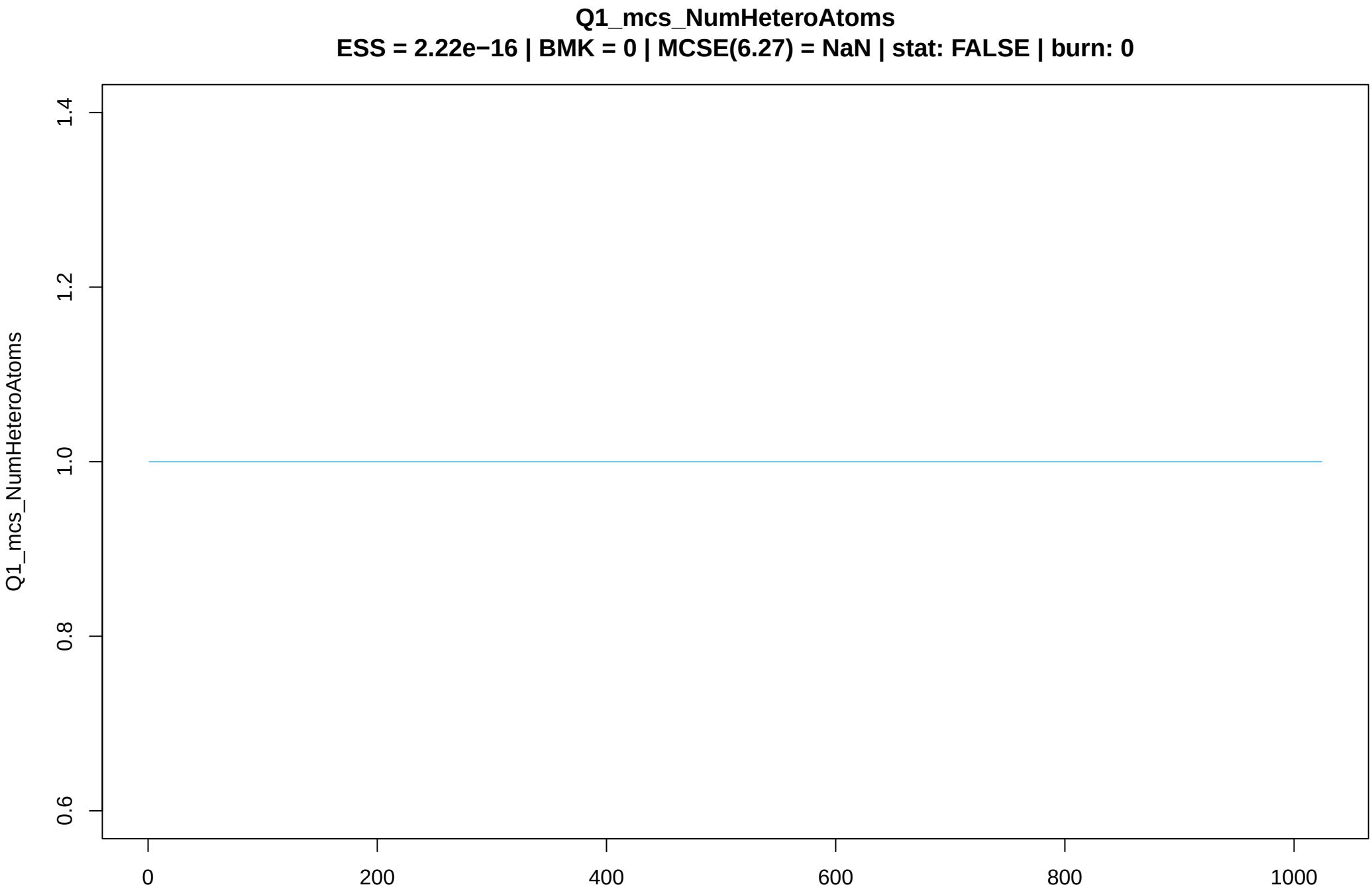

IQR_docked_NumRotatableBonds
ESS = 603 | BMK = 0.0717 | MCSE(6.27) = 3.55 | stat: TRUE | burn: 0
IQR_docked_NumRotatableBonds
4.0
3.8
3.6
3.4
3.2
3.0
0
200
400
600
800
1000

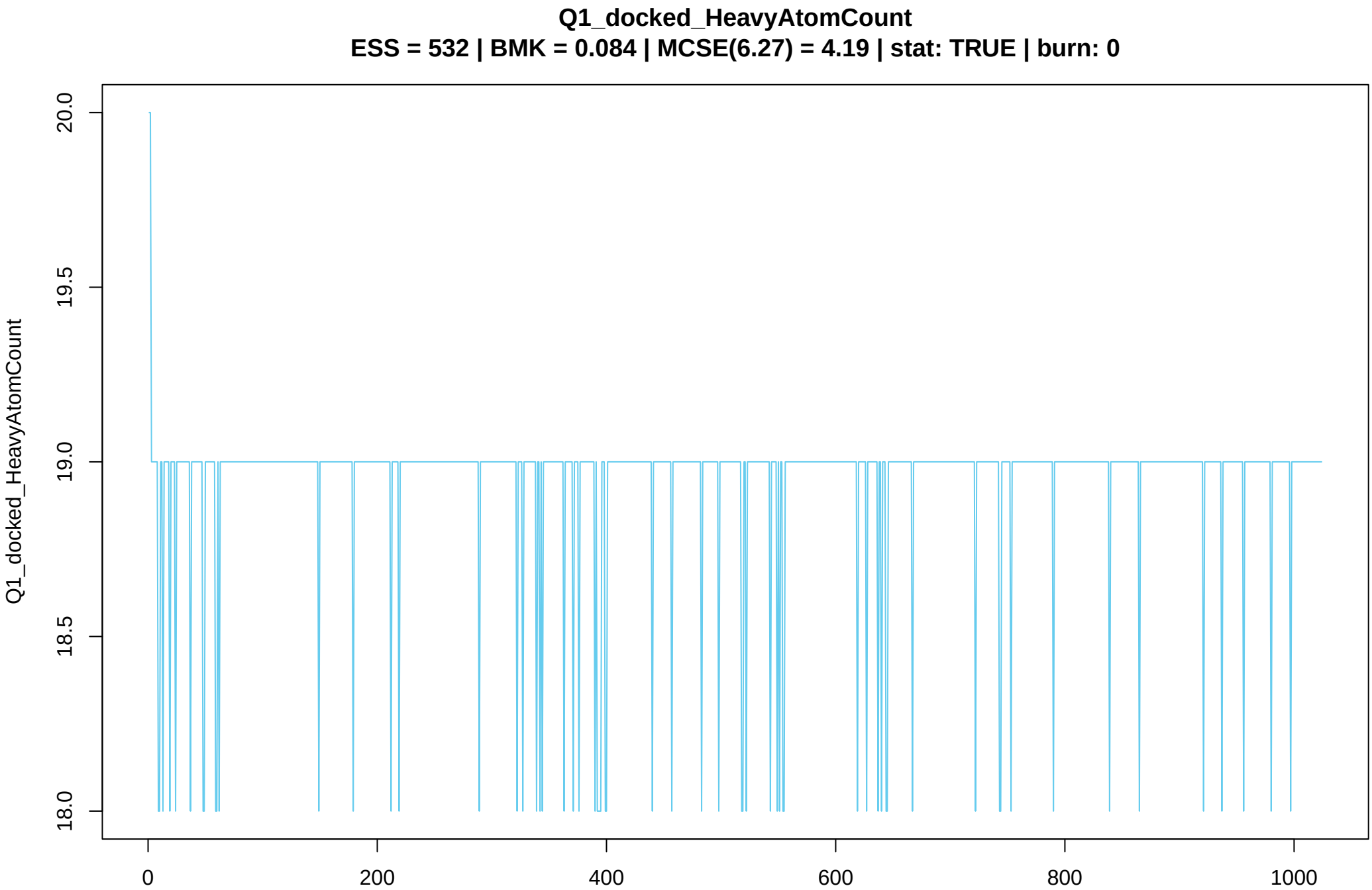

IQR_mcs_NOCount
ESS = 1020 | BMK = 0.626 | MCSE(6.27) = 3.12 | stat: FALSE | burn: 204
IQR_mcs_NOCount
3.0
2.8
2.6
2.4
2.2
2.0
0
200
400
600
800
1000

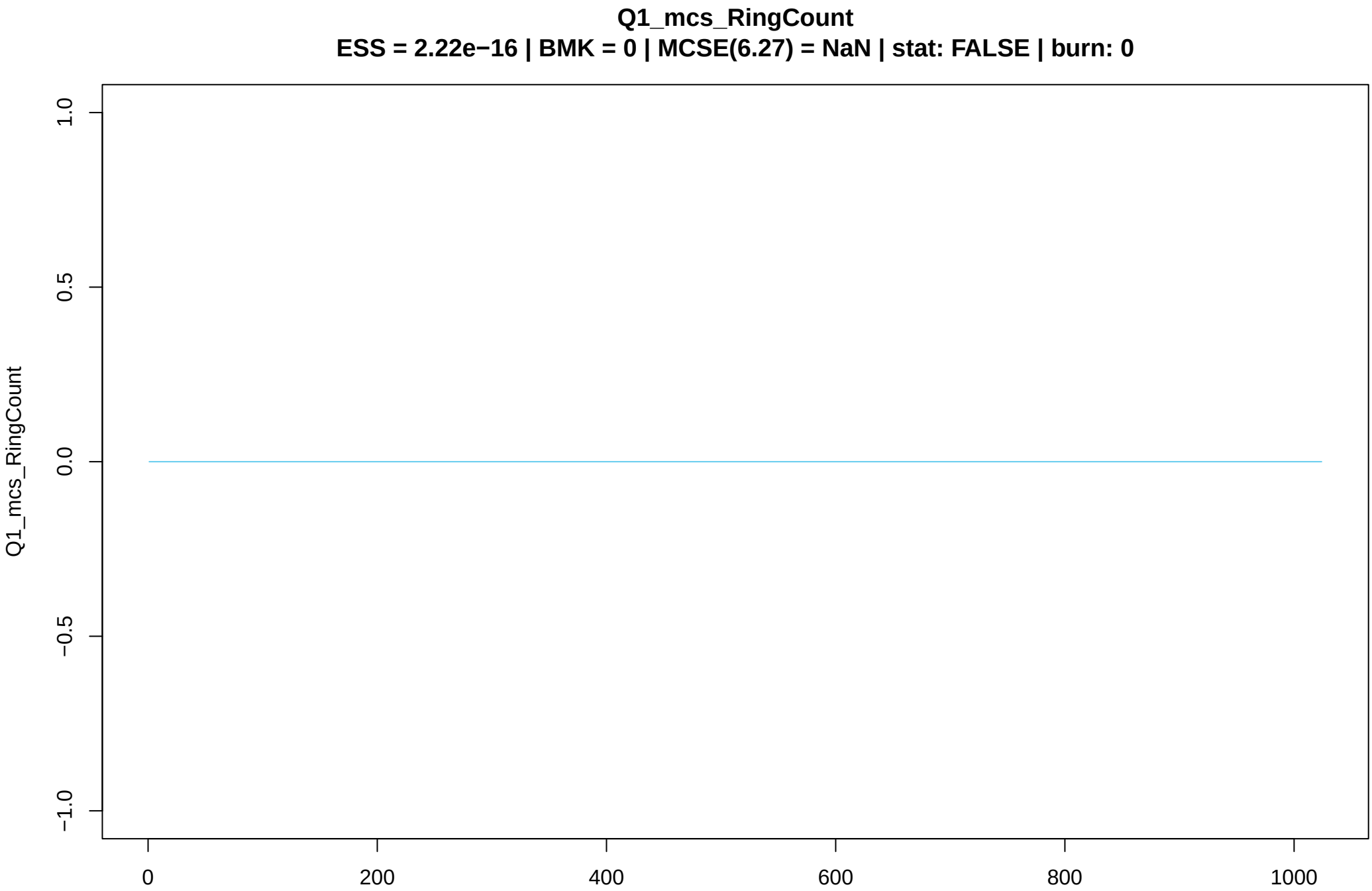

Q1_log_RMSD
ESS = 42.1 | BMK = 0.102 | MCSE(6.27) = 9.57 | stat: FALSE | burn: 0
Q1_log_RMSD
0.55
0.60
0.65
0.70
0
200
400
600
800
1000

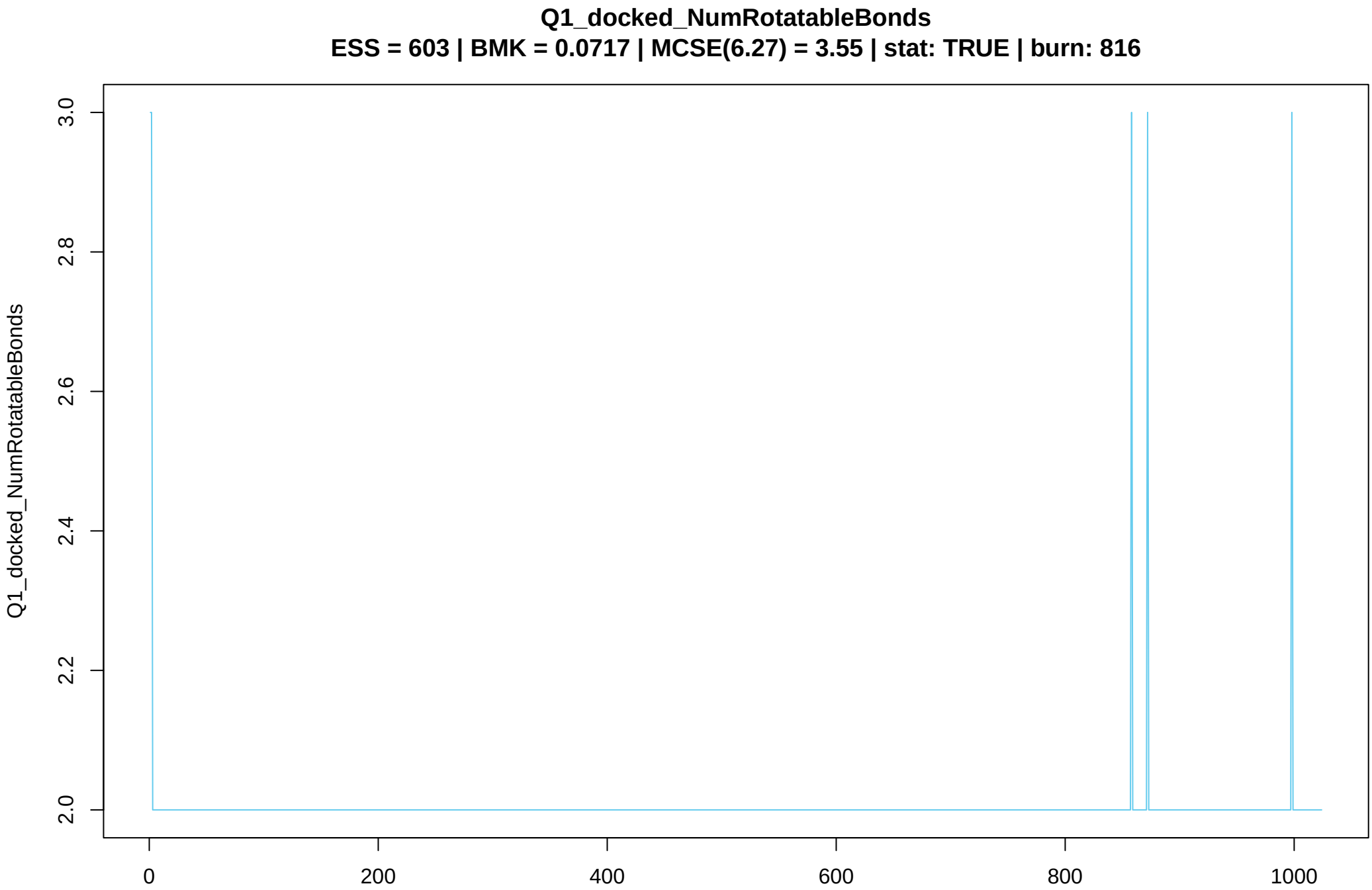

Q1_log_mcs_unbonded_polar_sasa
ESS = 23.7 | BMK = 0.444 | MCSE(6.27) = 13.5 | stat: TRUE | burn: 612
Q1_log_mcs_unbonded_polar_sasa
−0.25
−0.30
−0.35
0
200
400
600
800
1000

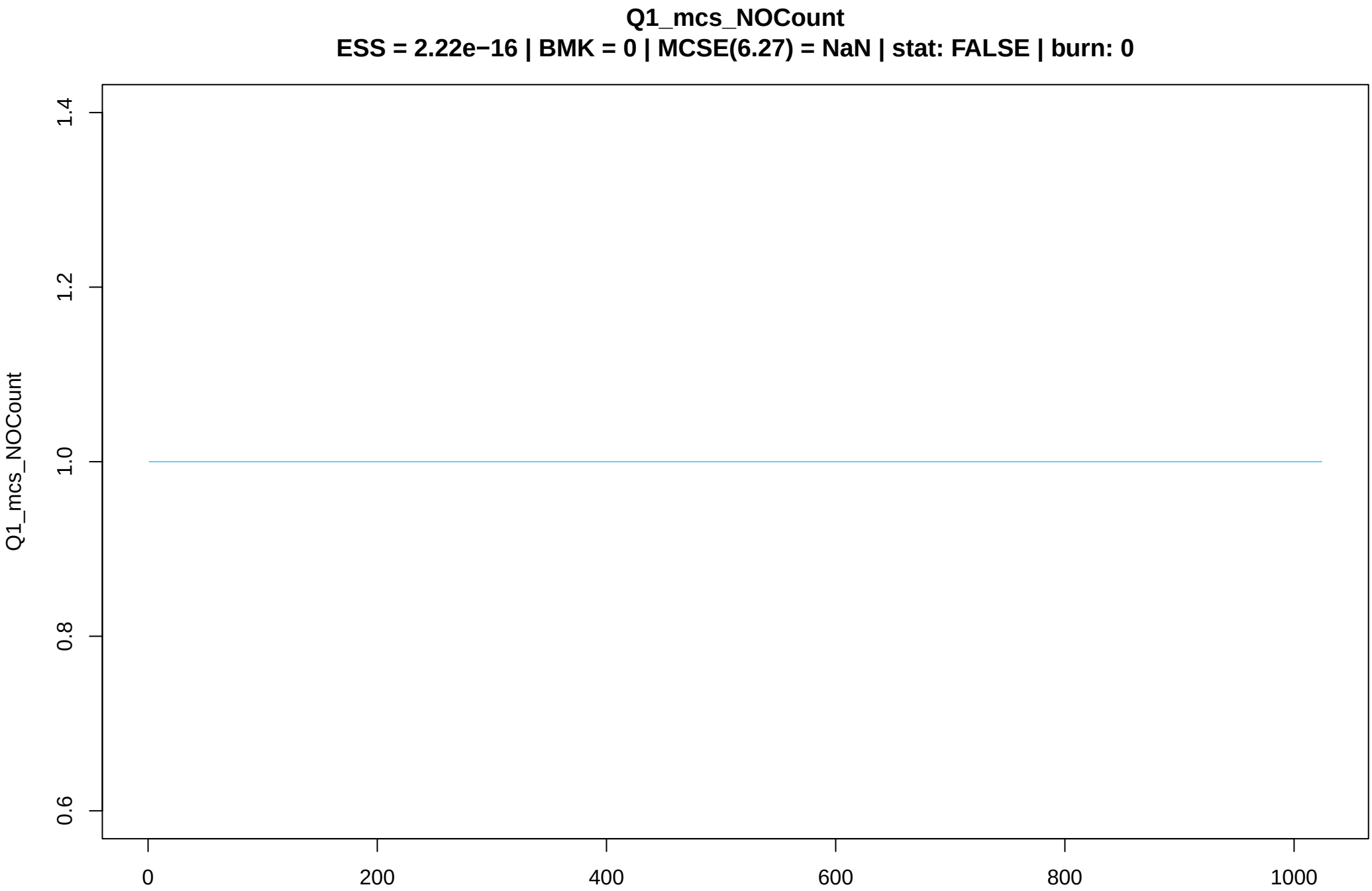

Q1_logit_ec_tanimoto_similarity
ESS = 875 | BMK = 0.0672 | MCSE(6.27) = 4.01 | stat: TRUE | burn: 0
Q1_logit_ec_tanimoto_similarity
−2.68
−2.70
−2.72
−2.74
−2.76
−2.78
−2.80
−2.82
0
200
400
600
800
1000

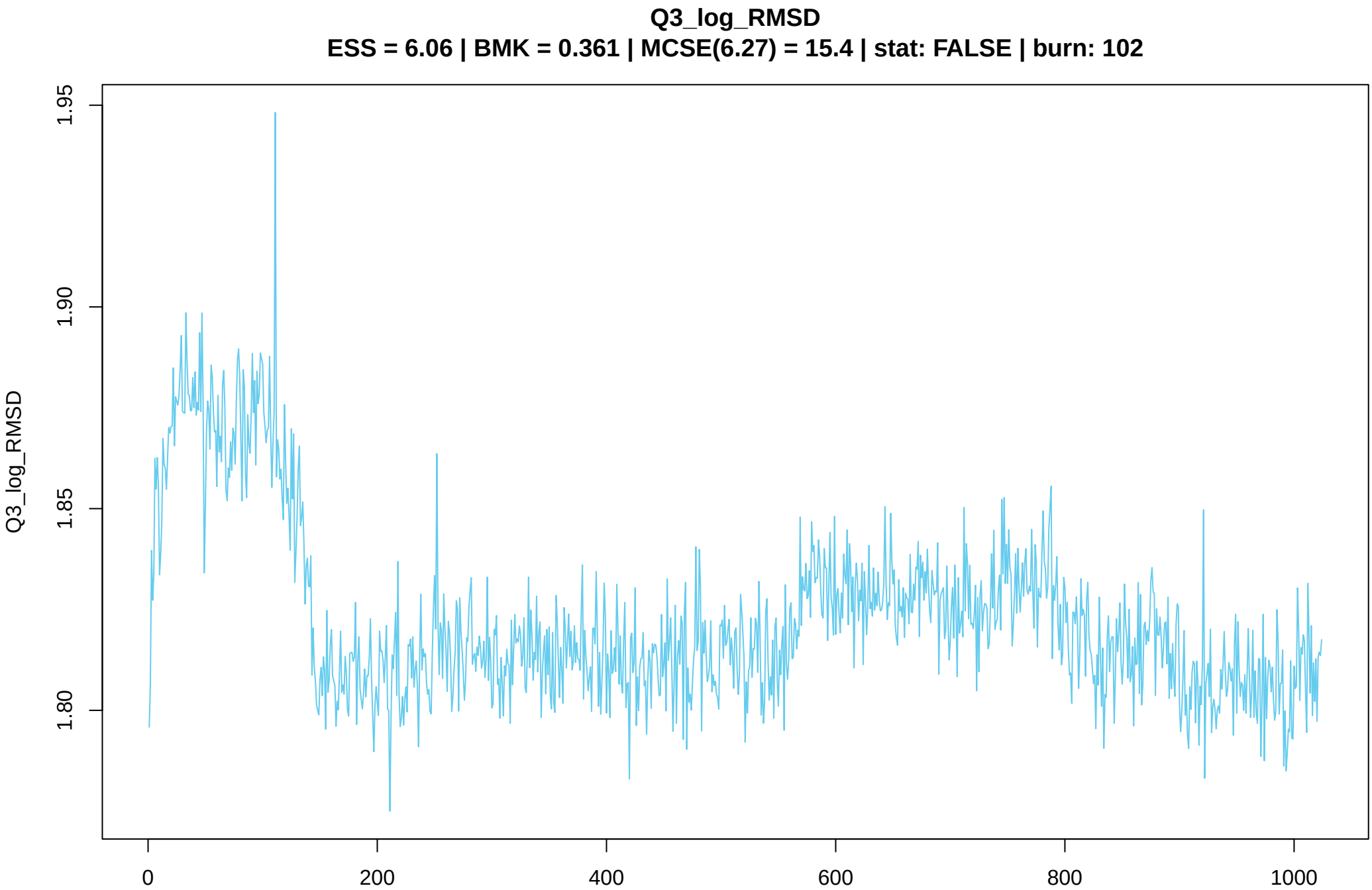

Q1_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NumHeteroAtoms
0.6
0.8
1.0
1.2
1.4
0
200
400
600
800
1000

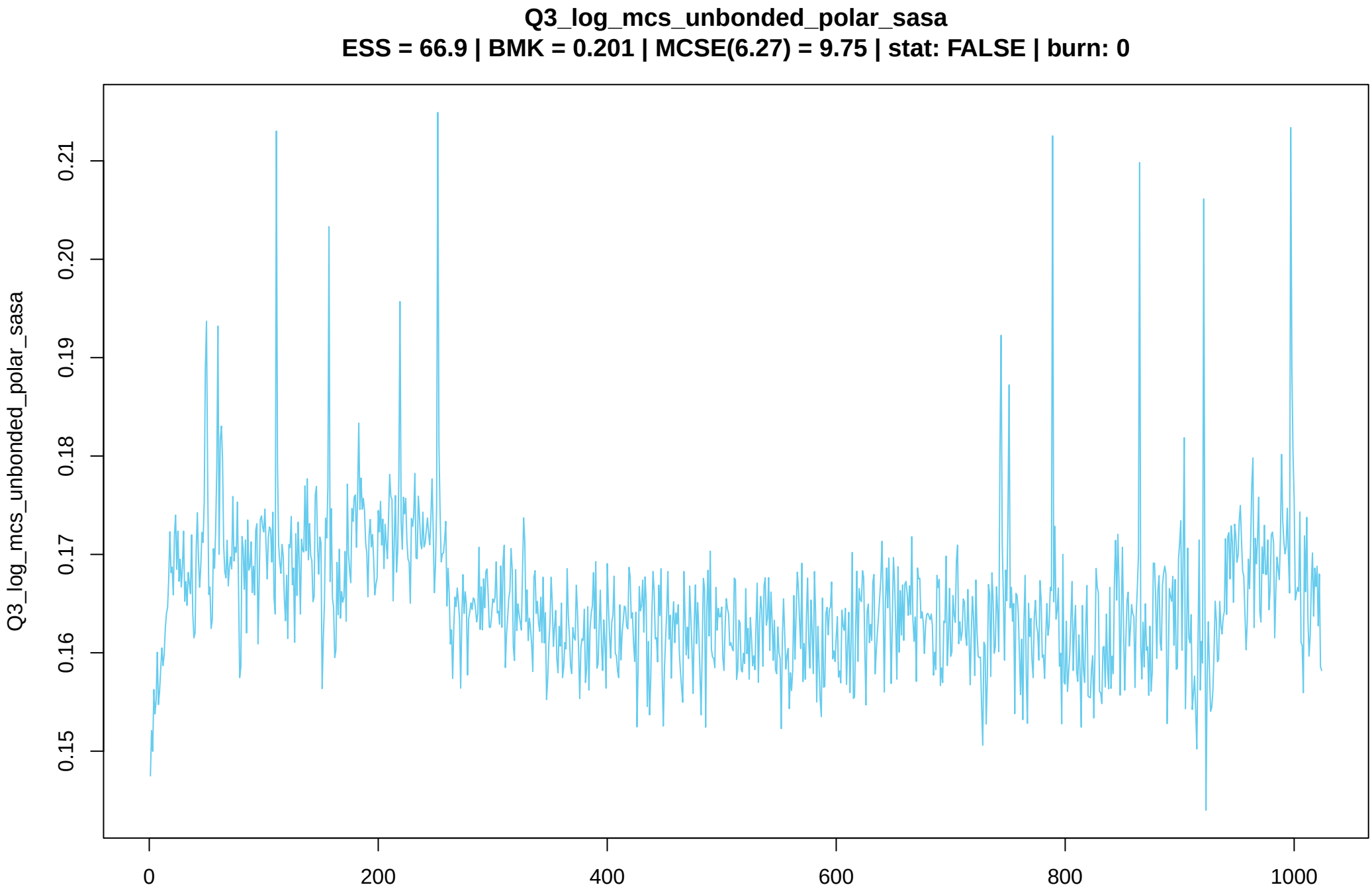

Q1_docked_HeavyAtomCount
ESS = 532 | BMK = 0.084 | MCSE(6.27) = 4.19 | stat: TRUE | burn: 0
Q1_docked_HeavyAtomCount
20.0
19.5
19.0
18.5
18.0
0
200
400
600
800
1000

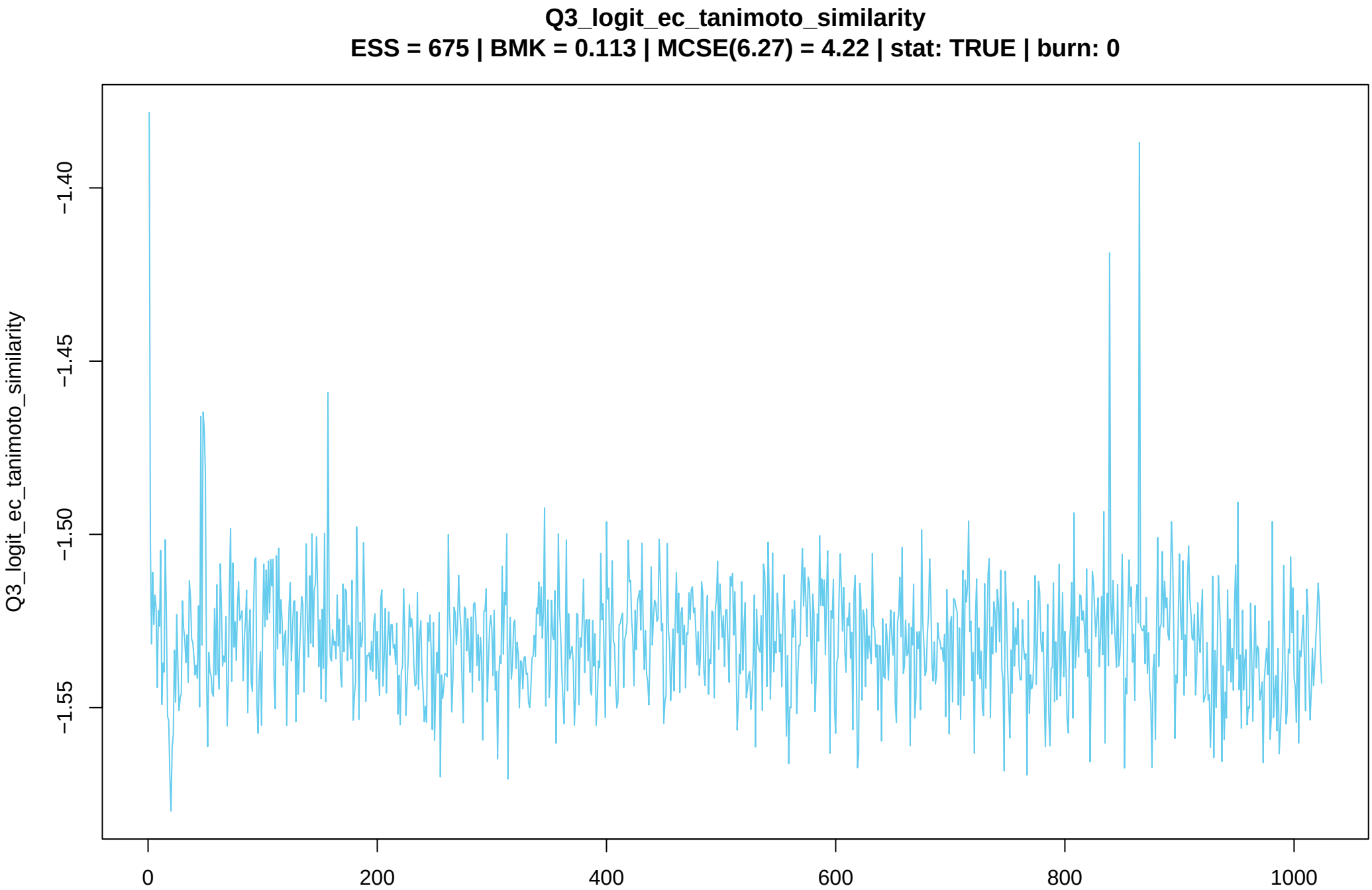

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
200
400
600
800
1000

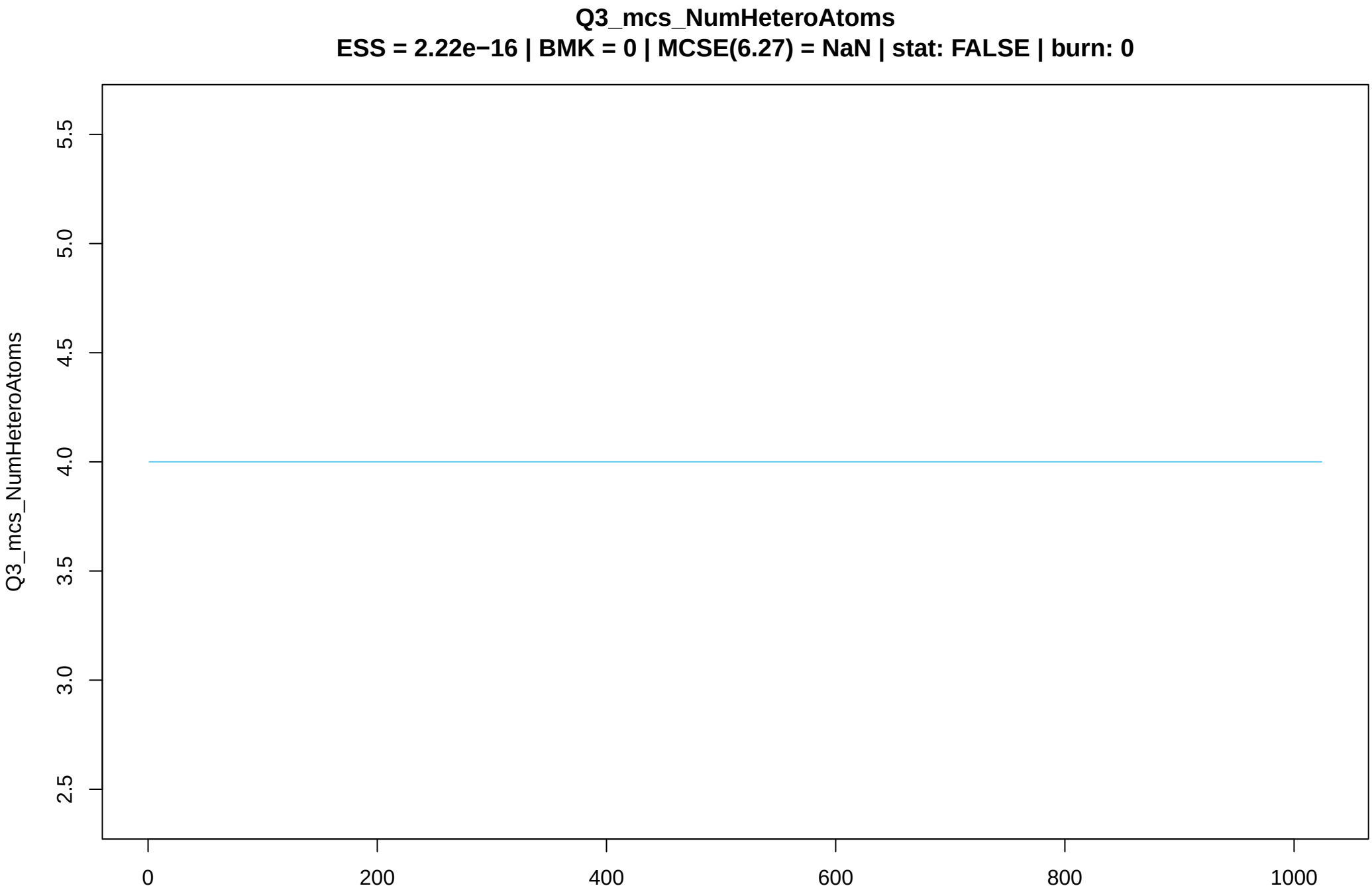

Q1_docked_NumRotatableBonds
ESS = 603 | BMK = 0.0717 | MCSE(6.27) = 3.55 | stat: TRUE | burn: 816
Q1_docked_NumRotatableBonds
2.0
2.2
2.4
2.6
2.8
3.0
0
200
400
600
800
1000

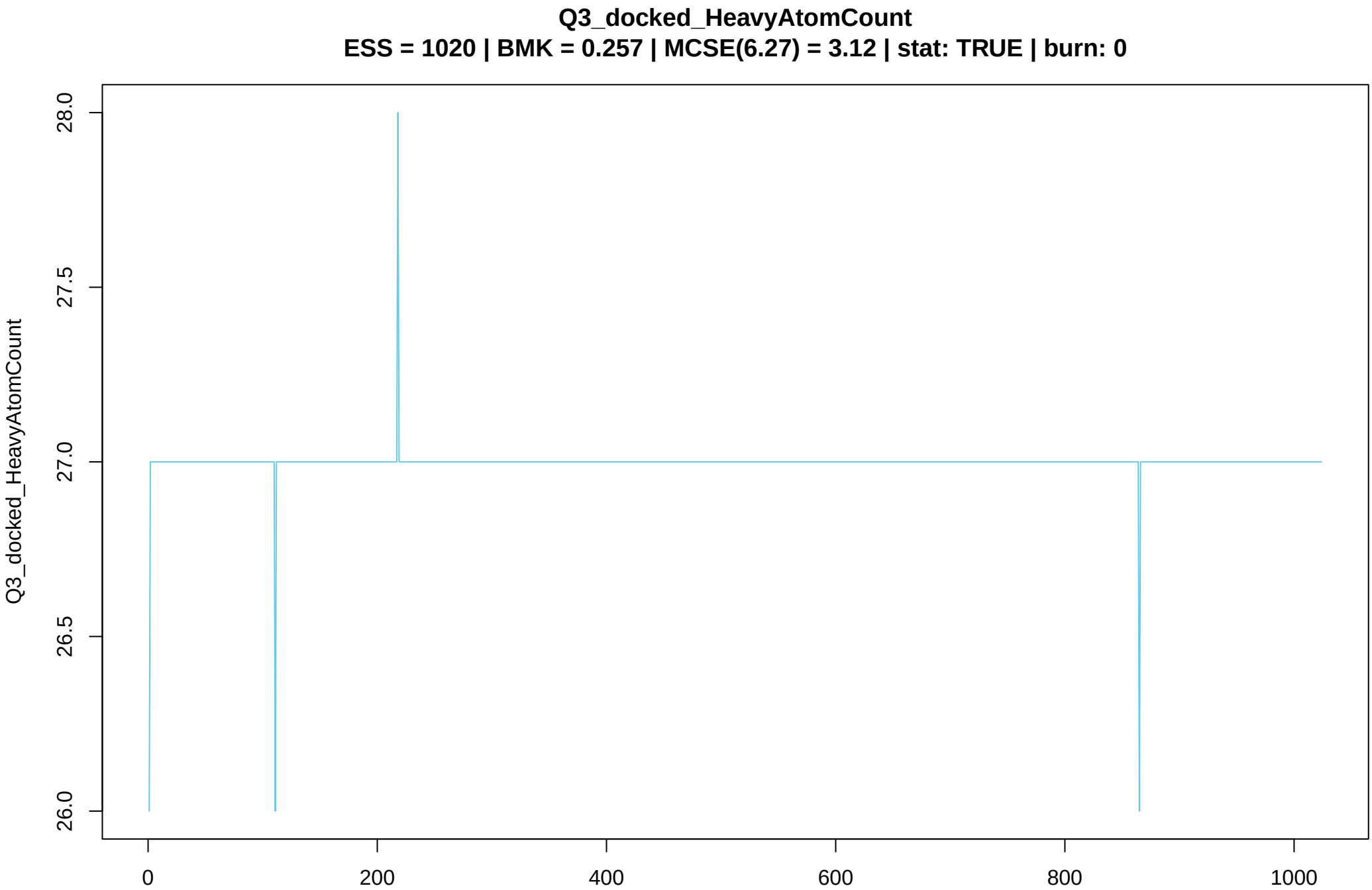

Q1_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NOCount
0.6
0.8
1.0
1.2
1.4
0
200
400
600
800
1000

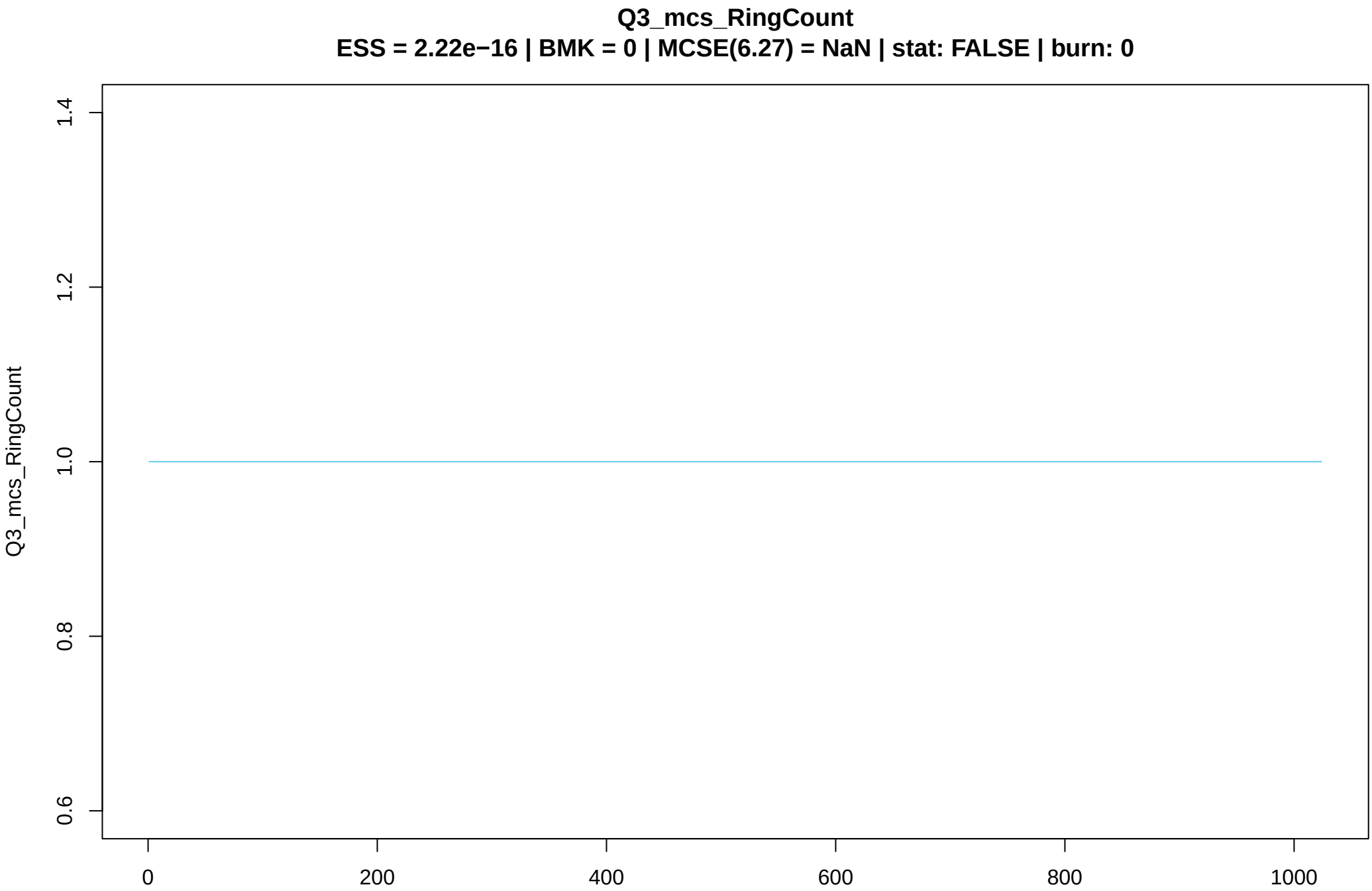

Q3_log_RMSD
ESS = 6.06 | BMK = 0.361 | MCSE(6.27) = 15.4 | stat: FALSE | burn: 102
Q3_log_RMSD
1.80
1.85
1.90
1.95
0
200
400
600
800
1000

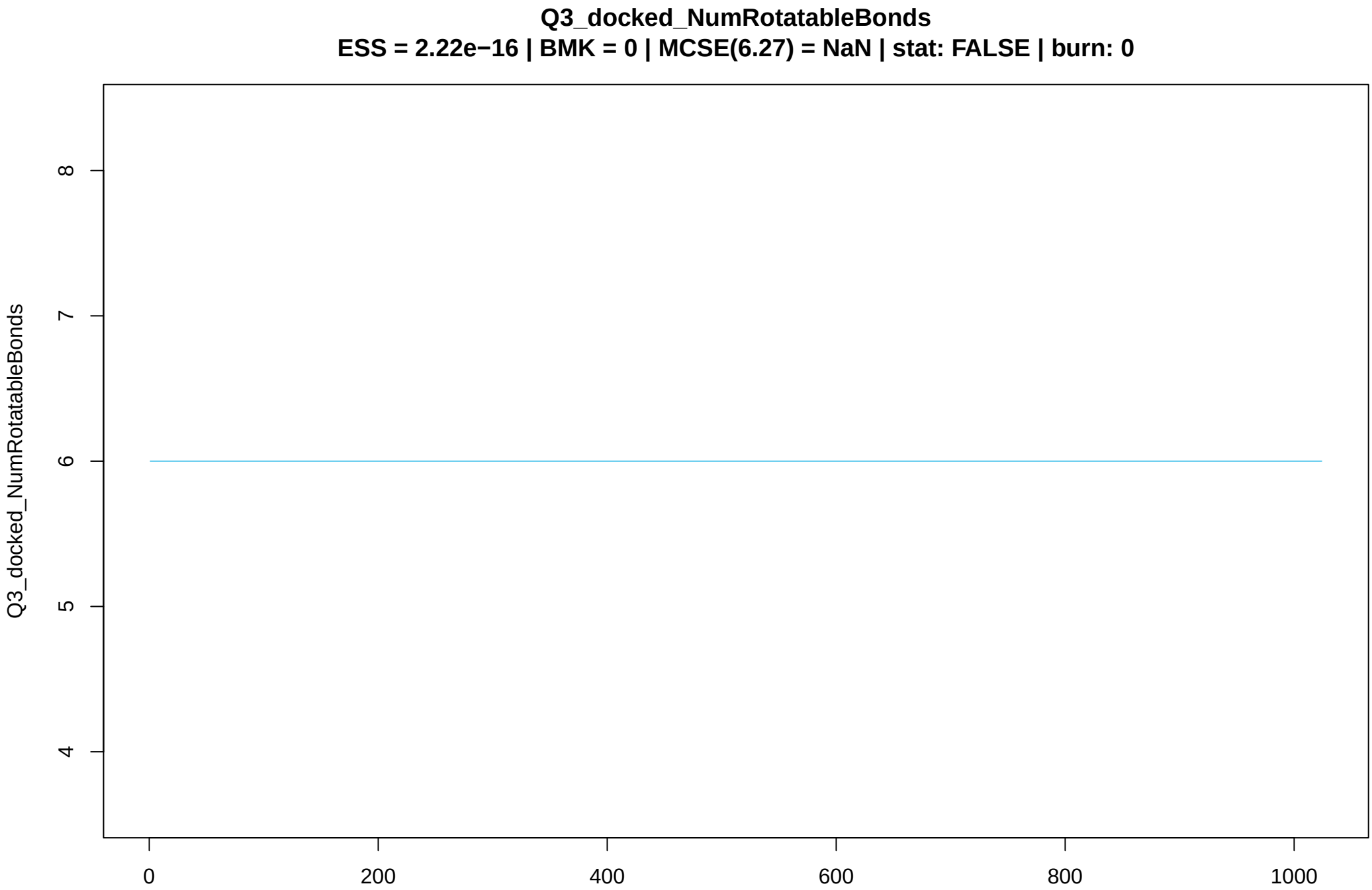

Q3_log_mcs_unbonded_polar_sasa
ESS = 66.9 | BMK = 0.201 | MCSE(6.27) = 9.75 | stat: FALSE | burn: 0
Q3_log_mcs_unbonded_polar_sasa
0.15
0.16
0.17
0.18
0.19
0.20
0.21
0
200
400
600
800
1000

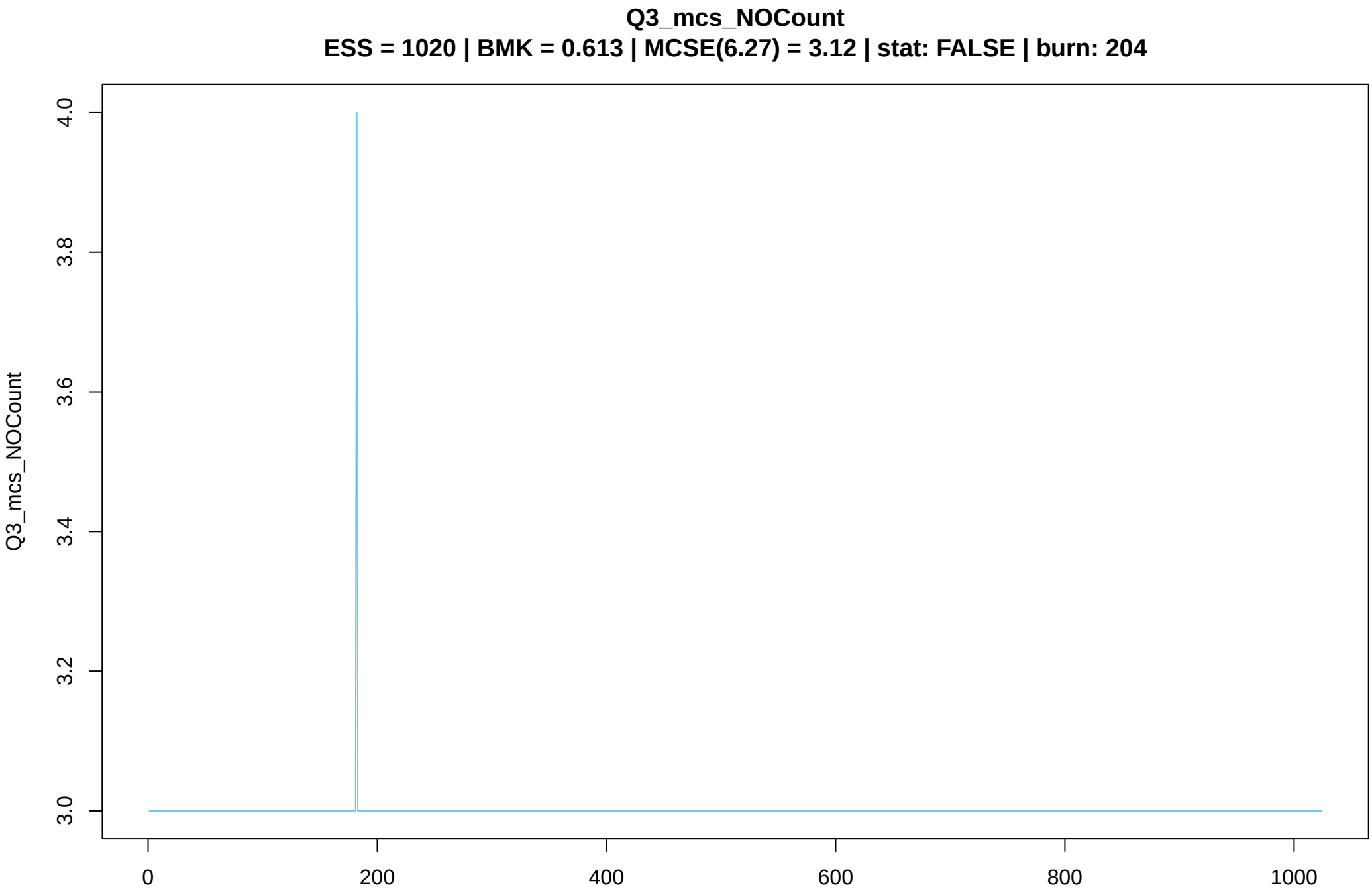

Q3_logit_ec_tanimoto_similarity
ESS = 675 | BMK = 0.113 | MCSE(6.27) = 4.22 | stat: TRUE | burn: 0
Q3_logit_ec_tanimoto_similarity
−1.40
−1.45
−1.50
−1.55
0
200
400
600
800
1000

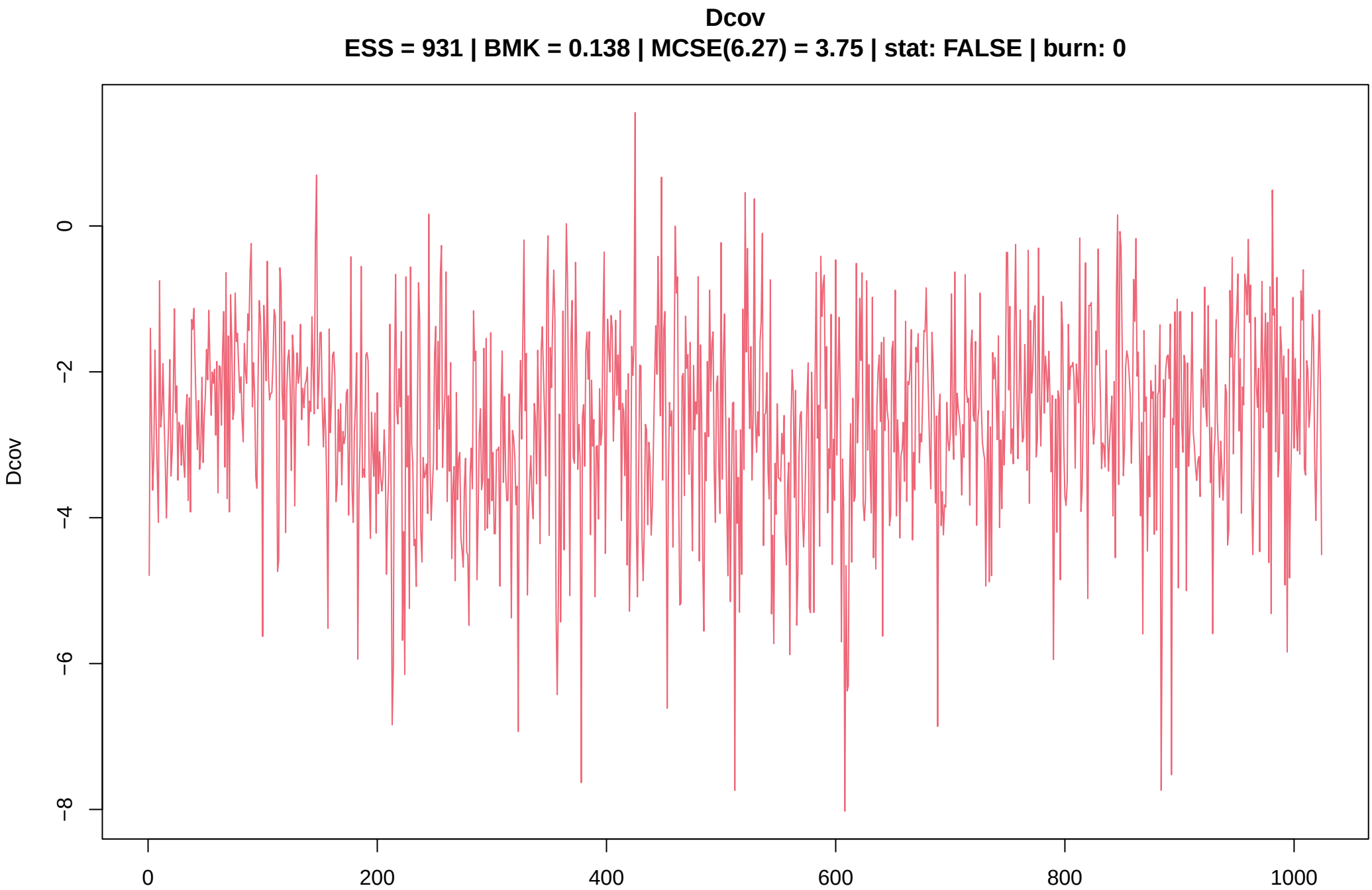

Q3_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_NumHeteroAtoms
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
200
400
600
800
1000

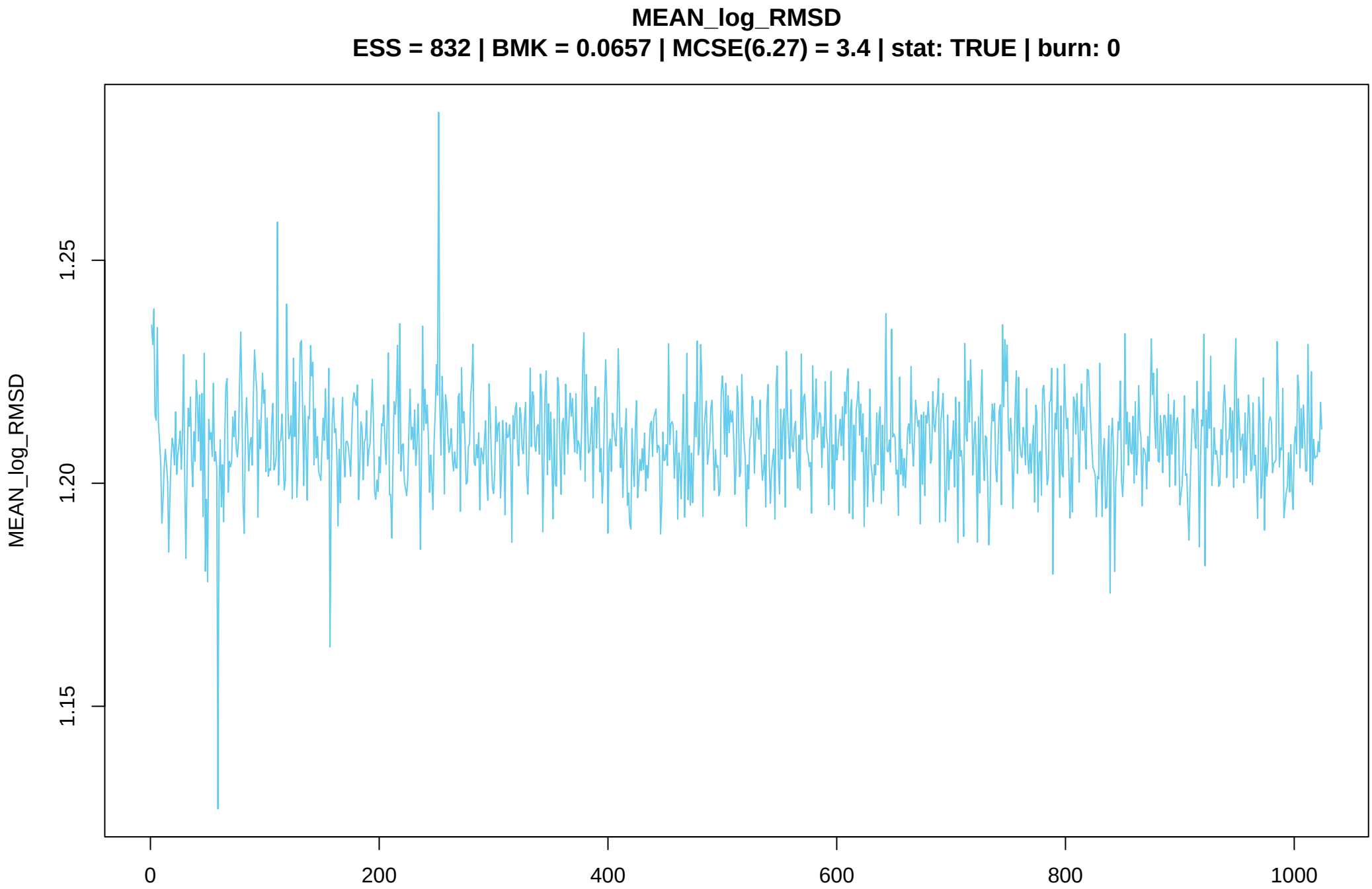

Q3_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.257 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0
Q3_docked_HeavyAtomCount
28.0
27.5
27.0
26.5
26.0
0
200
400
600
800
1000

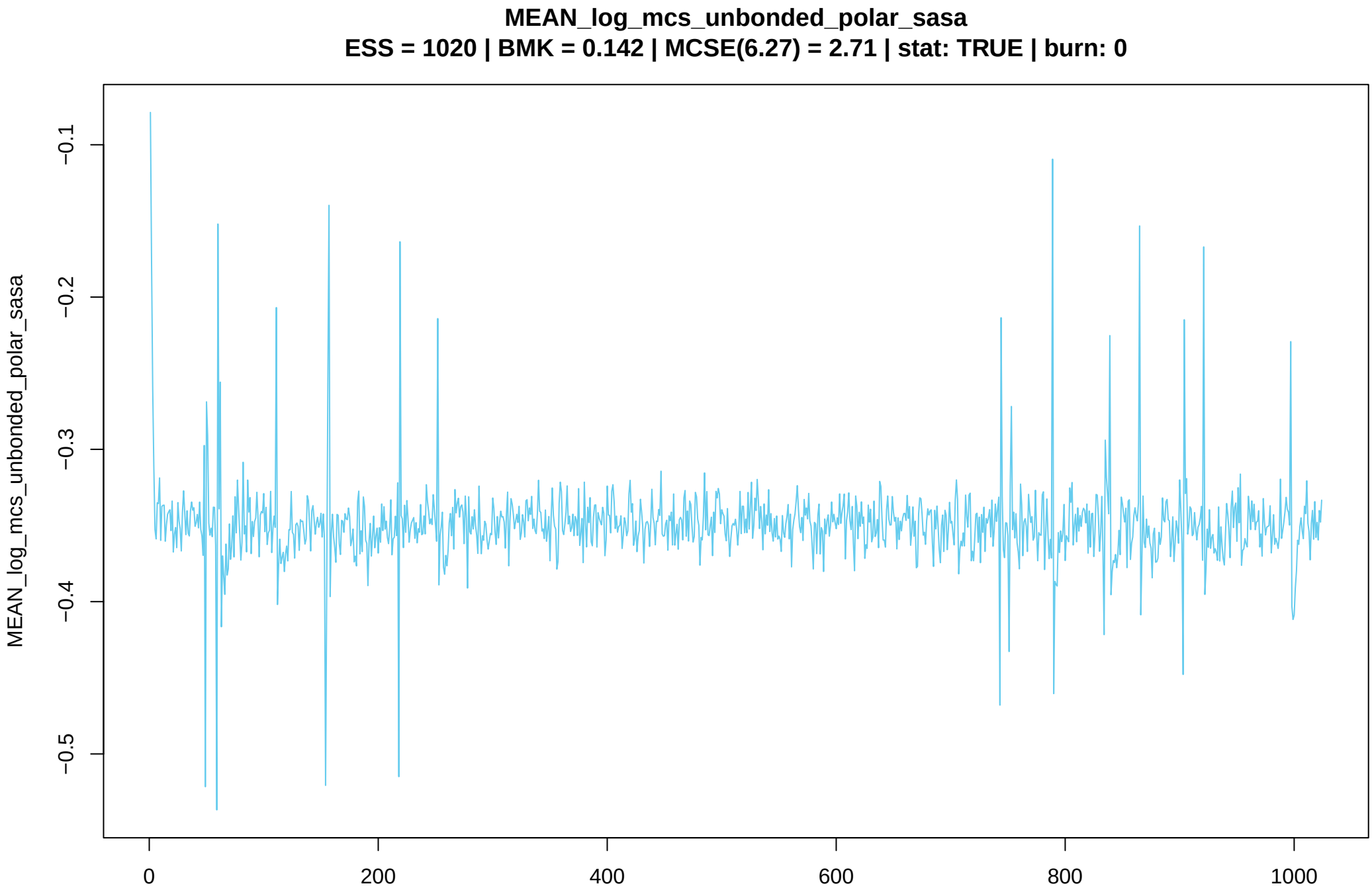

Q3_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
200
400
600
800
1000

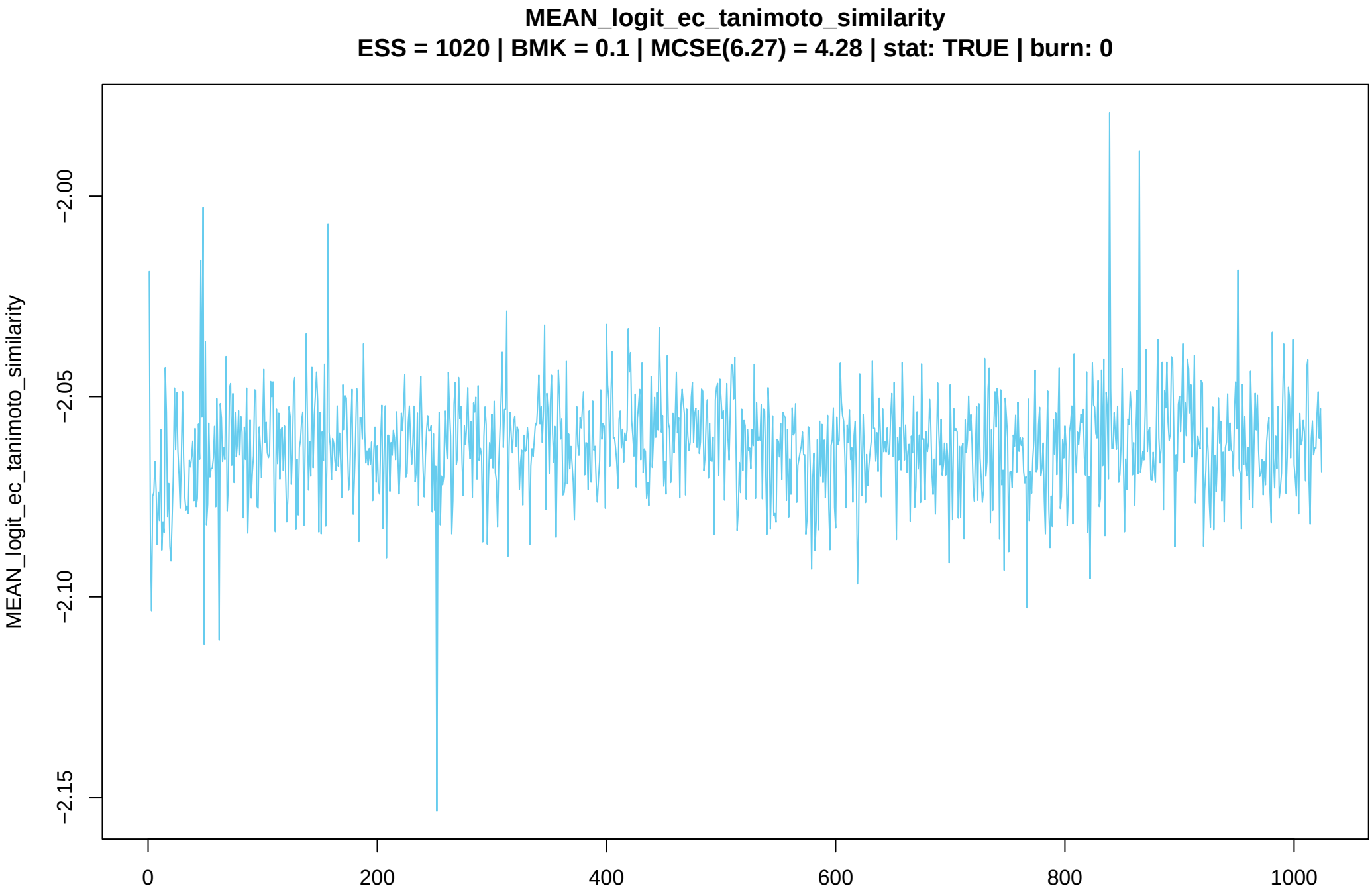

Q3_docked_NumRotatableBonds
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_docked_NumRotatableBonds
4
5
6
7
8
0
200
400
600
800
1000

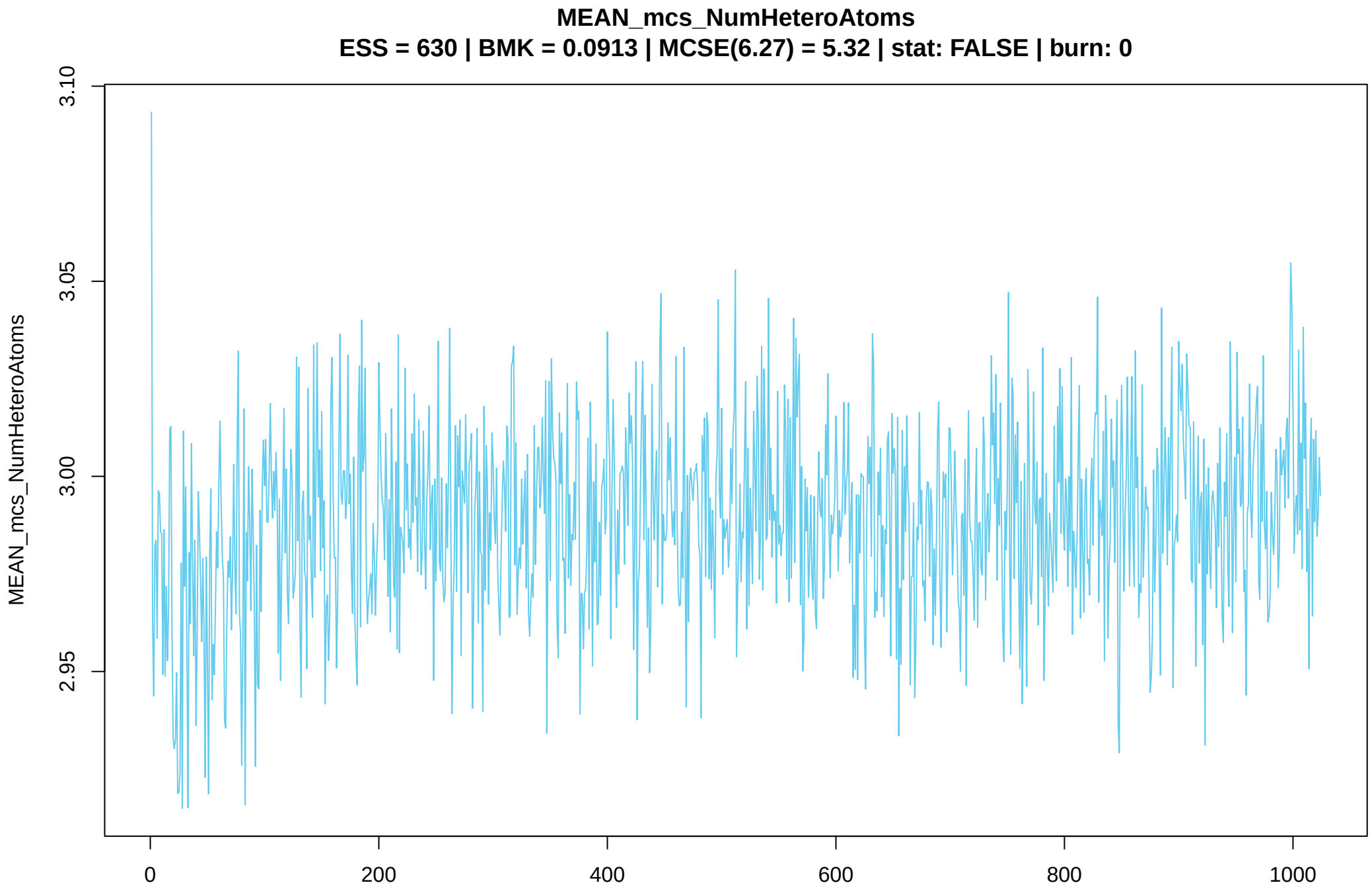

Q3_mcs_NOCount
ESS = 1020 | BMK = 0.613 | MCSE(6.27) = 3.12 | stat: FALSE | burn: 204
Q3_mcs_NOCount
4.0
3.8
3.6
3.4
3.2
3.0
0
200
400
600
800
1000

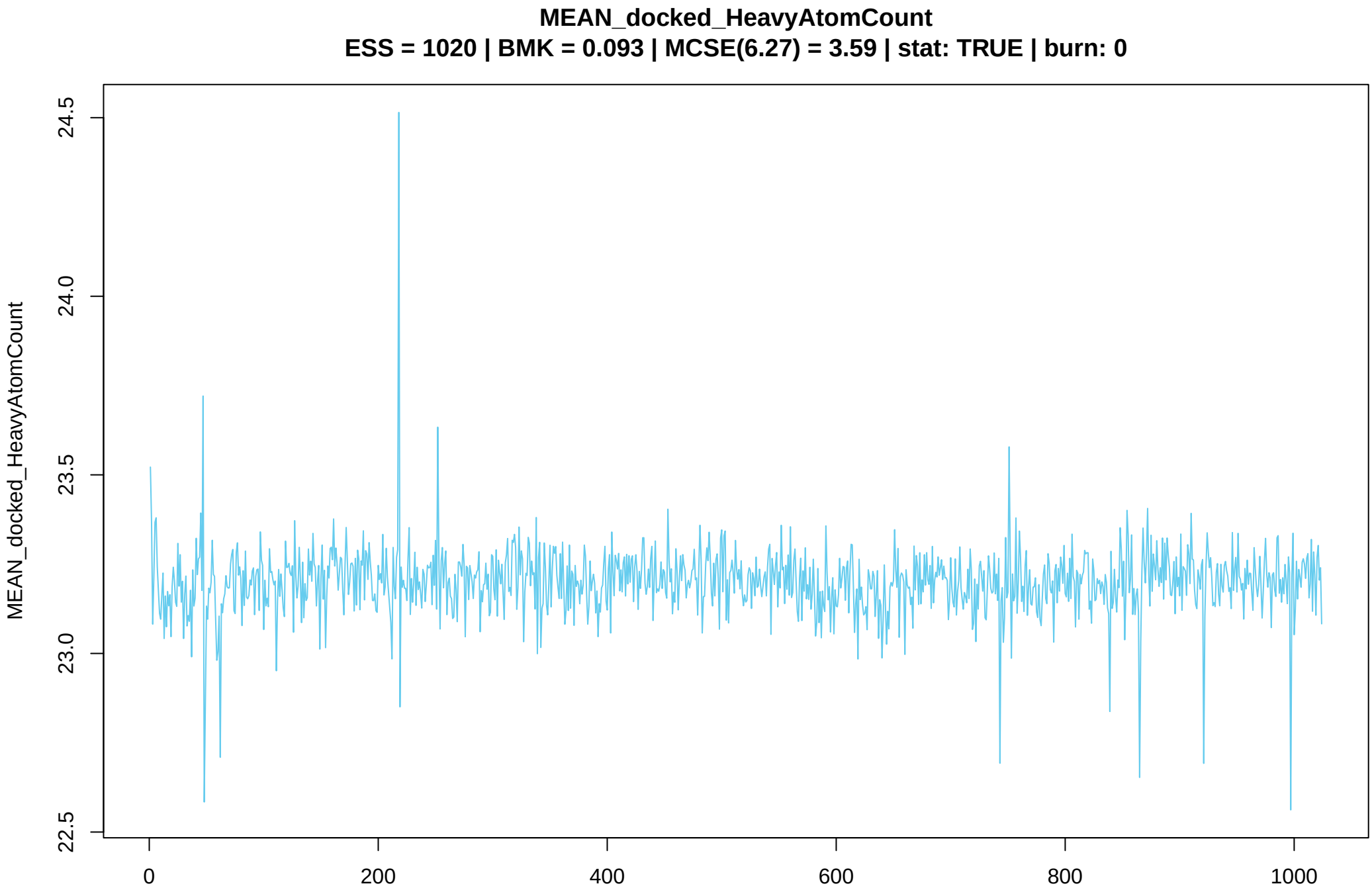

Dcov
ESS = 931 | BMK = 0.138 | MCSE(6.27) = 3.75 | stat: FALSE | burn: 0
Dcov
0
−2
−4
−6
−8
0
200
400
600
800
1000

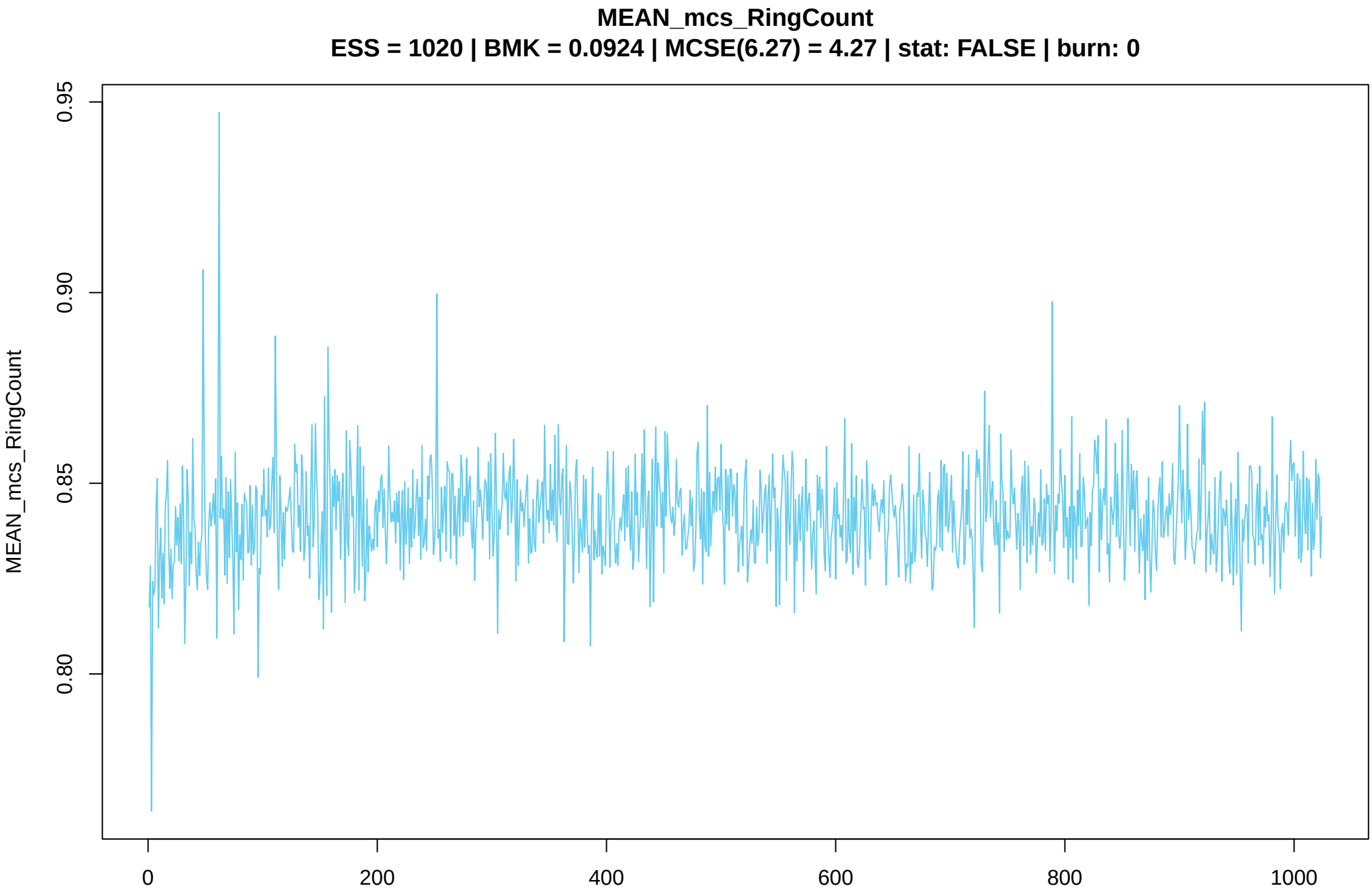

MEAN_log_RMSD
ESS = 832 | BMK = 0.0657 | MCSE(6.27) = 3.4 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.15
1.20
1.25
0
200
400
600
800
1000

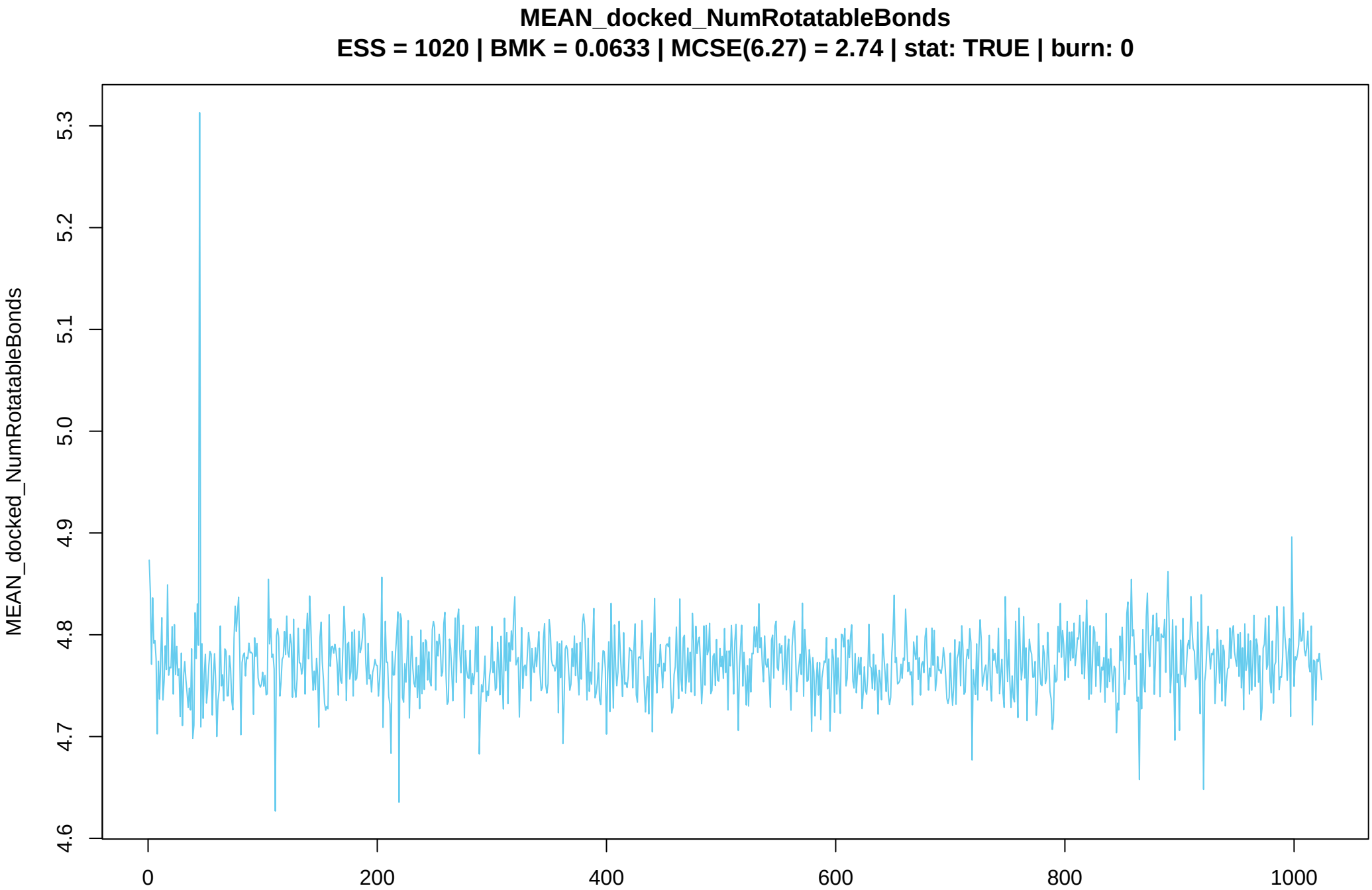

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.142 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0
MEAN_log_mcs_unbonded_polar_sasa
−0.1
−0.2
−0.3
−0.4
−0.5
0
200
400
600
800
1000

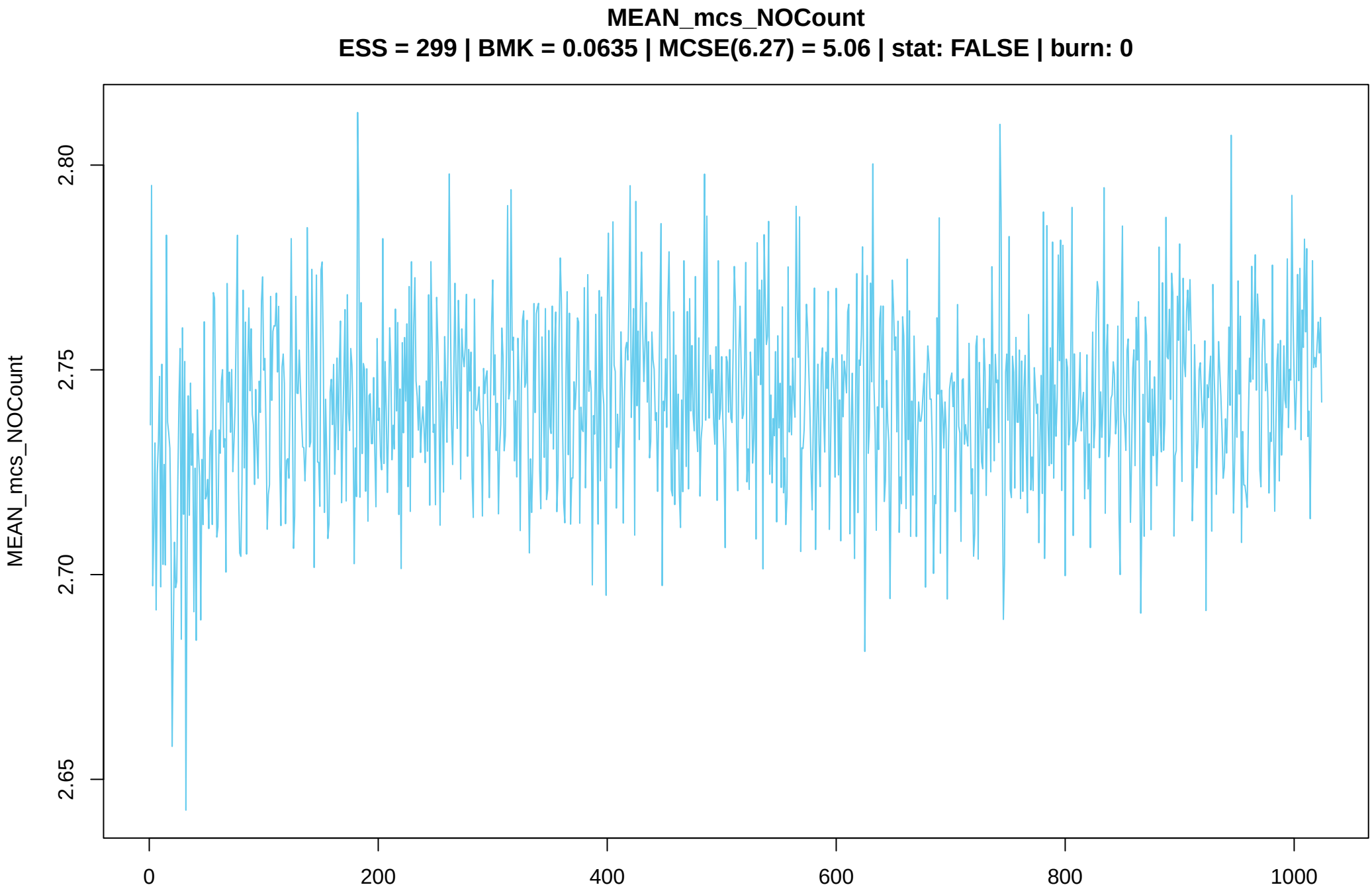

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.1 | MCSE(6.27) = 4.28 | stat: TRUE | burn: 0
MEAN_logit_ec_tanimoto_similarity
−2.00
−2.05
−2.10
−2.15
0
200
400
600
800
1000

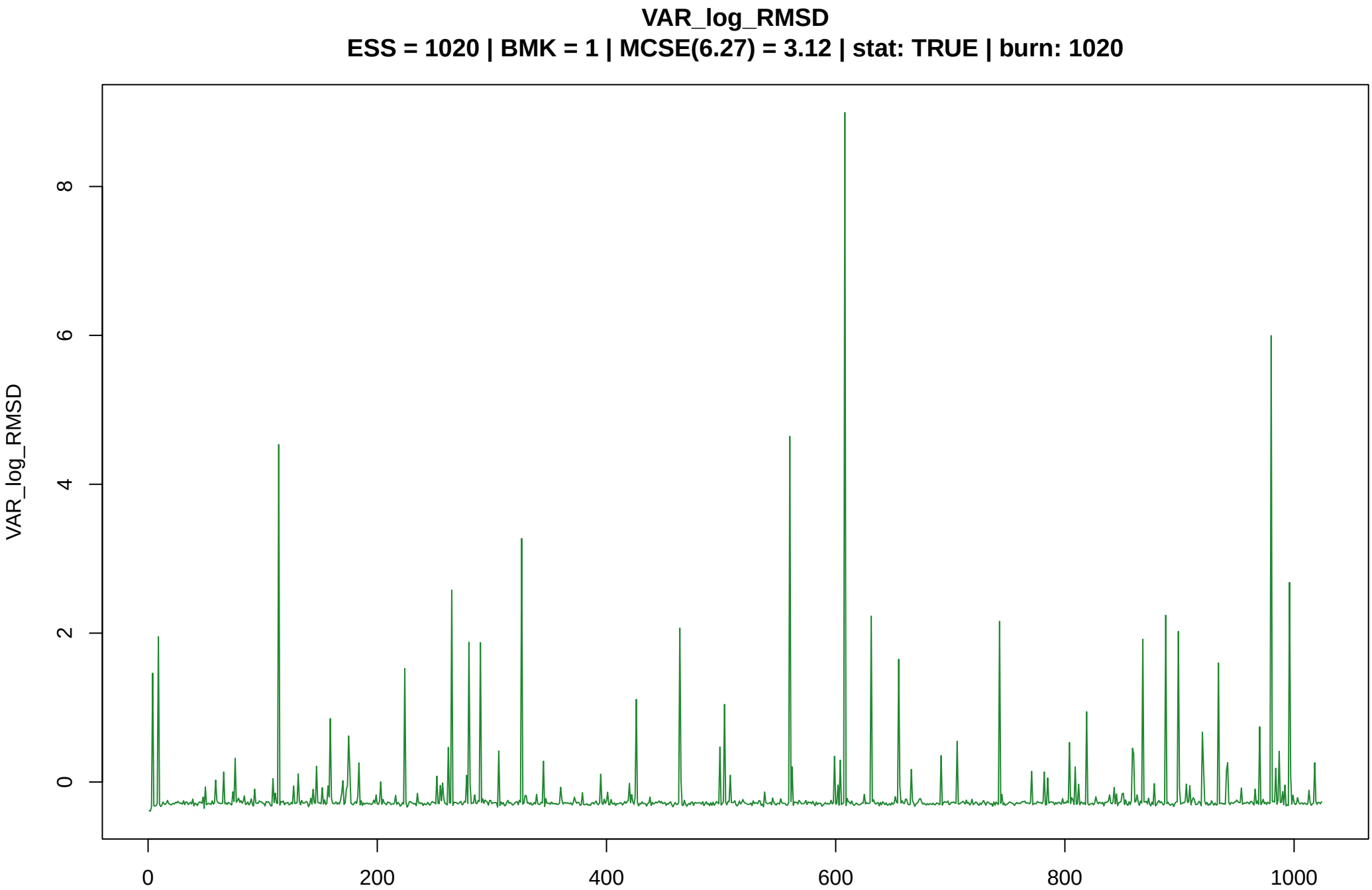

MEAN_mcs_NumHeteroAtoms
ESS = 630 | BMK = 0.0913 | MCSE(6.27) = 5.32 | stat: FALSE | burn: 0
MEAN_mcs_NumHeteroAtoms
3.10
3.05
3.00
2.95
0
200
400
600
800
1000

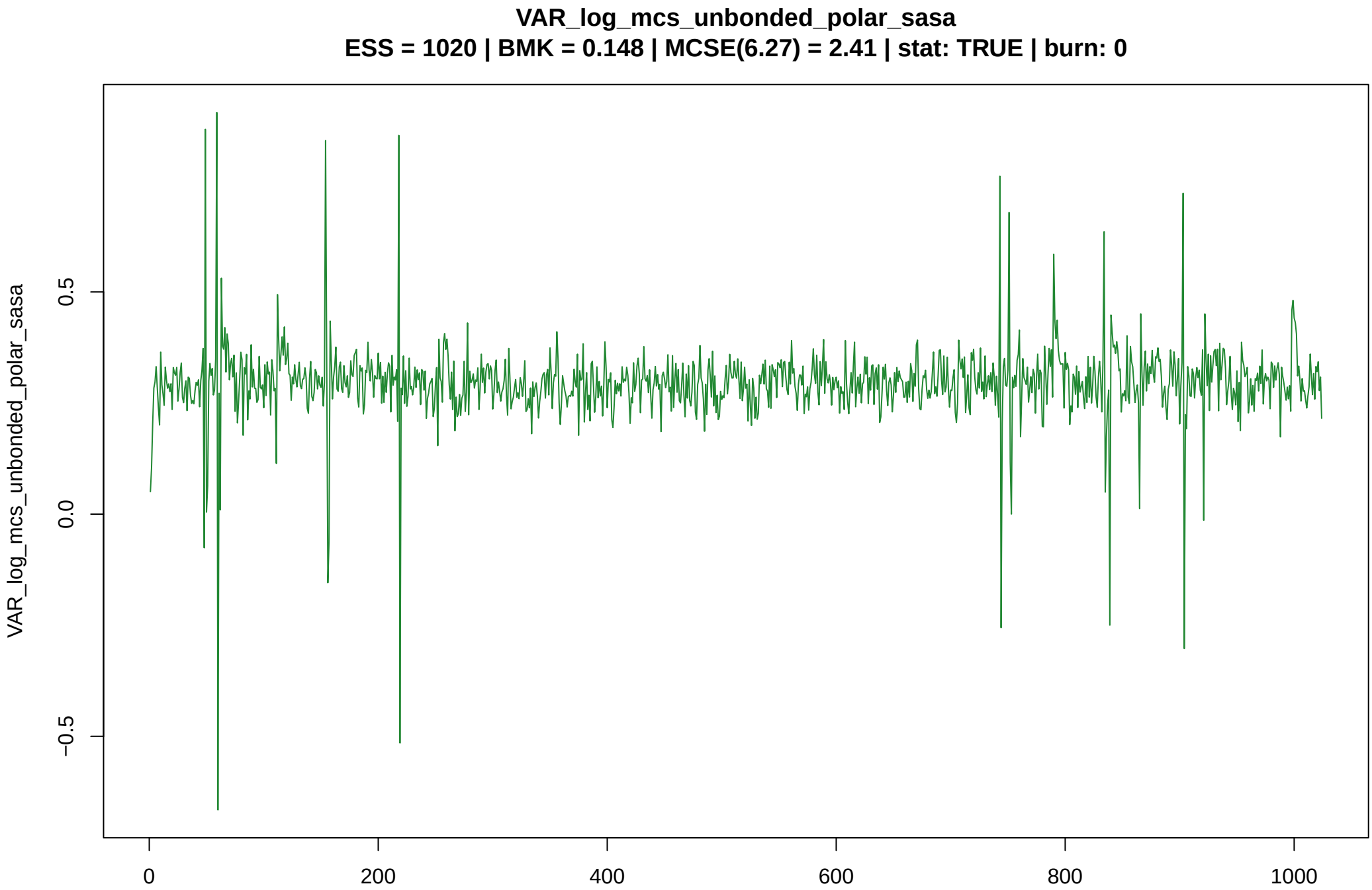

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.093 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
22.5
23.0
23.5
24.0
24.5
0
200
400
600
800
1000

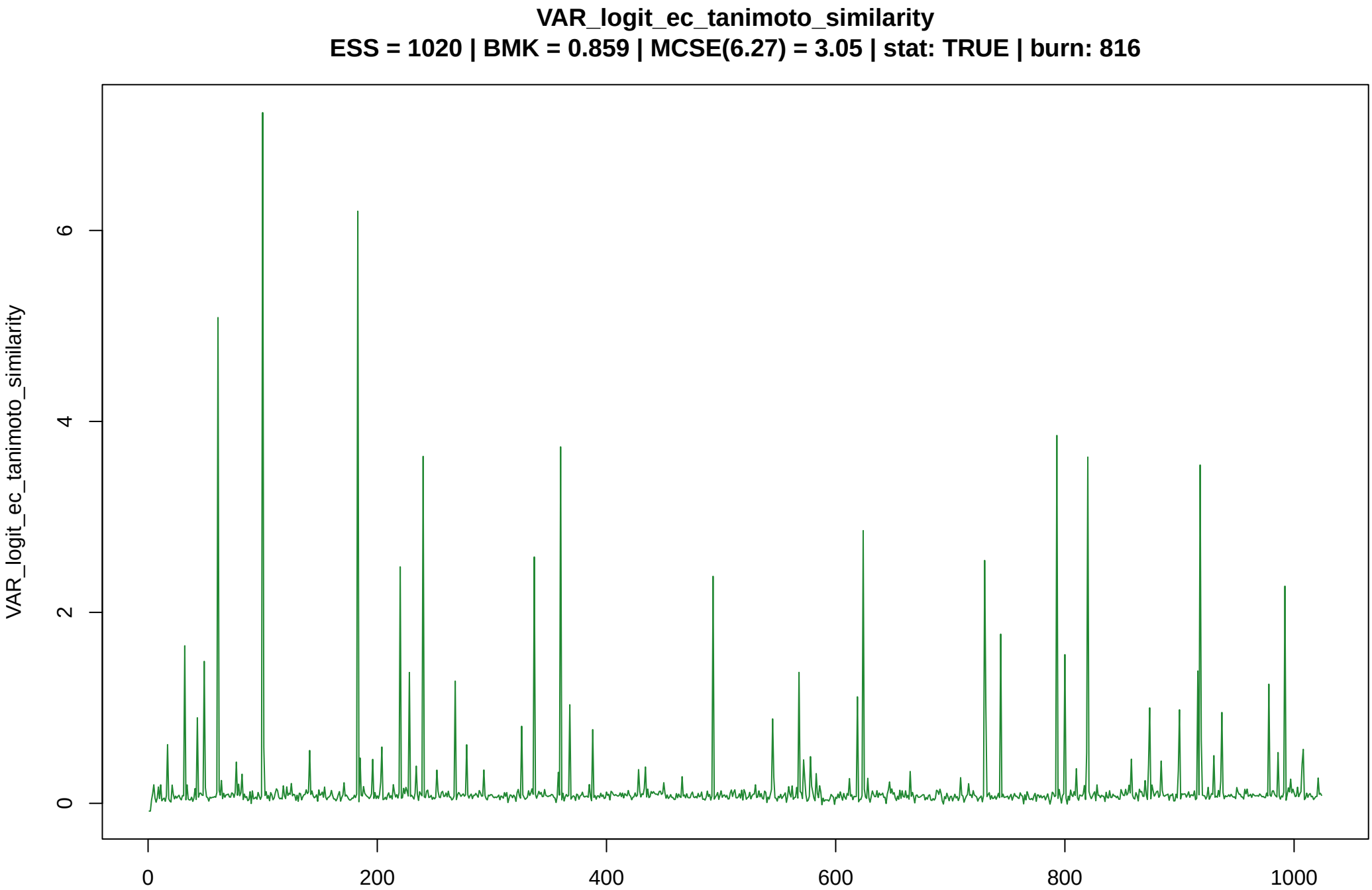

MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0924 | MCSE(6.27) = 4.27 | stat: FALSE | burn: 0
MEAN_mcs_RingCount
0.80
0.85
0.90
0.95
0
200
400
600
800
1000

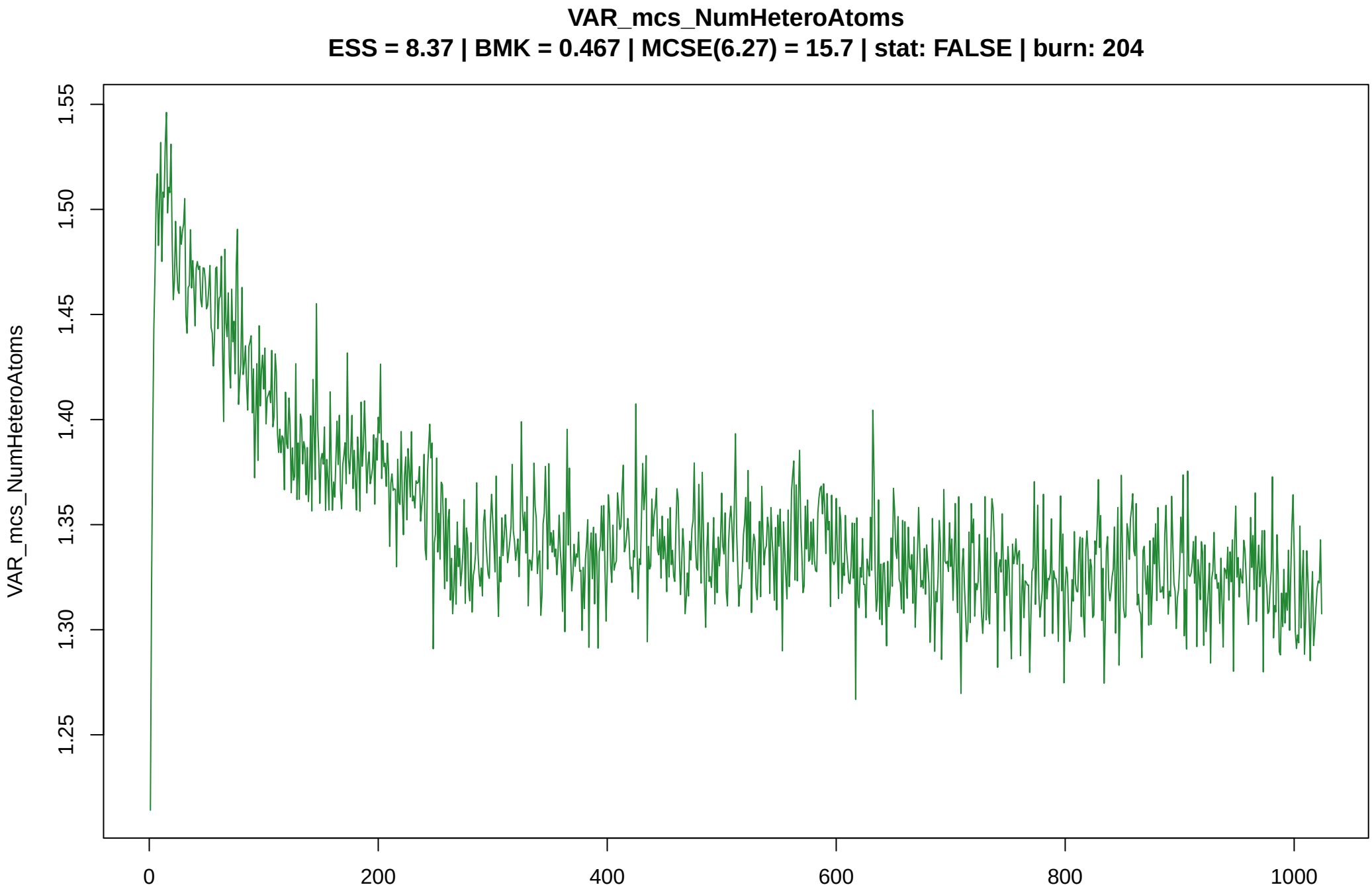

MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0633 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0
MEAN_docked_NumRotatableBonds
4.6
4.7
4.8
4.9
5.0
5.1
5.2
5.3
0
200
400
600
800
1000

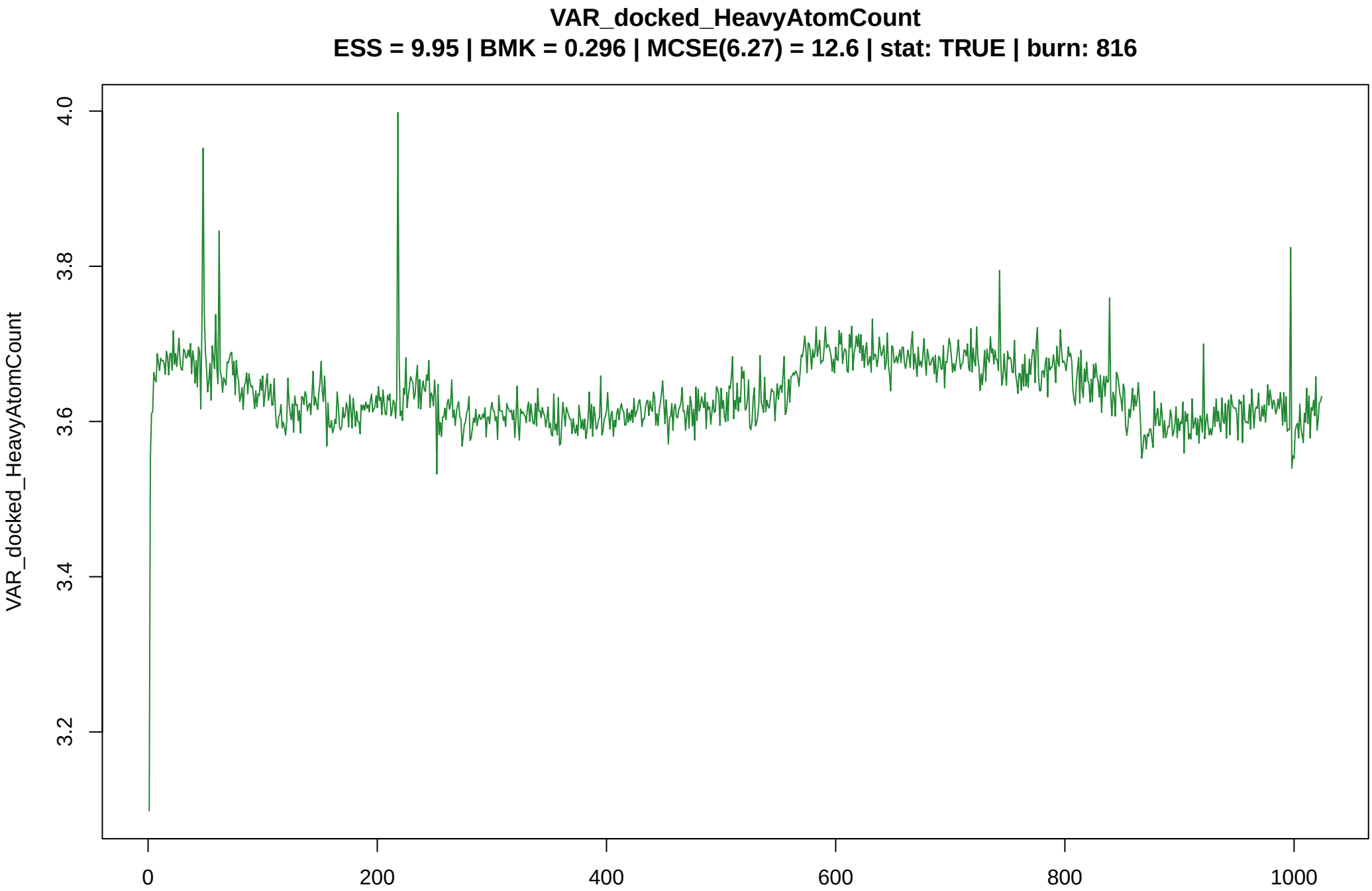

MEAN_mcs_NOCount
ESS = 299 | BMK = 0.0635 | MCSE(6.27) = 5.06 | stat: FALSE | burn: 0
MEAN_mcs_NOCount
2.65
2.70
2.75
2.80
0
200
400
600
800
1000

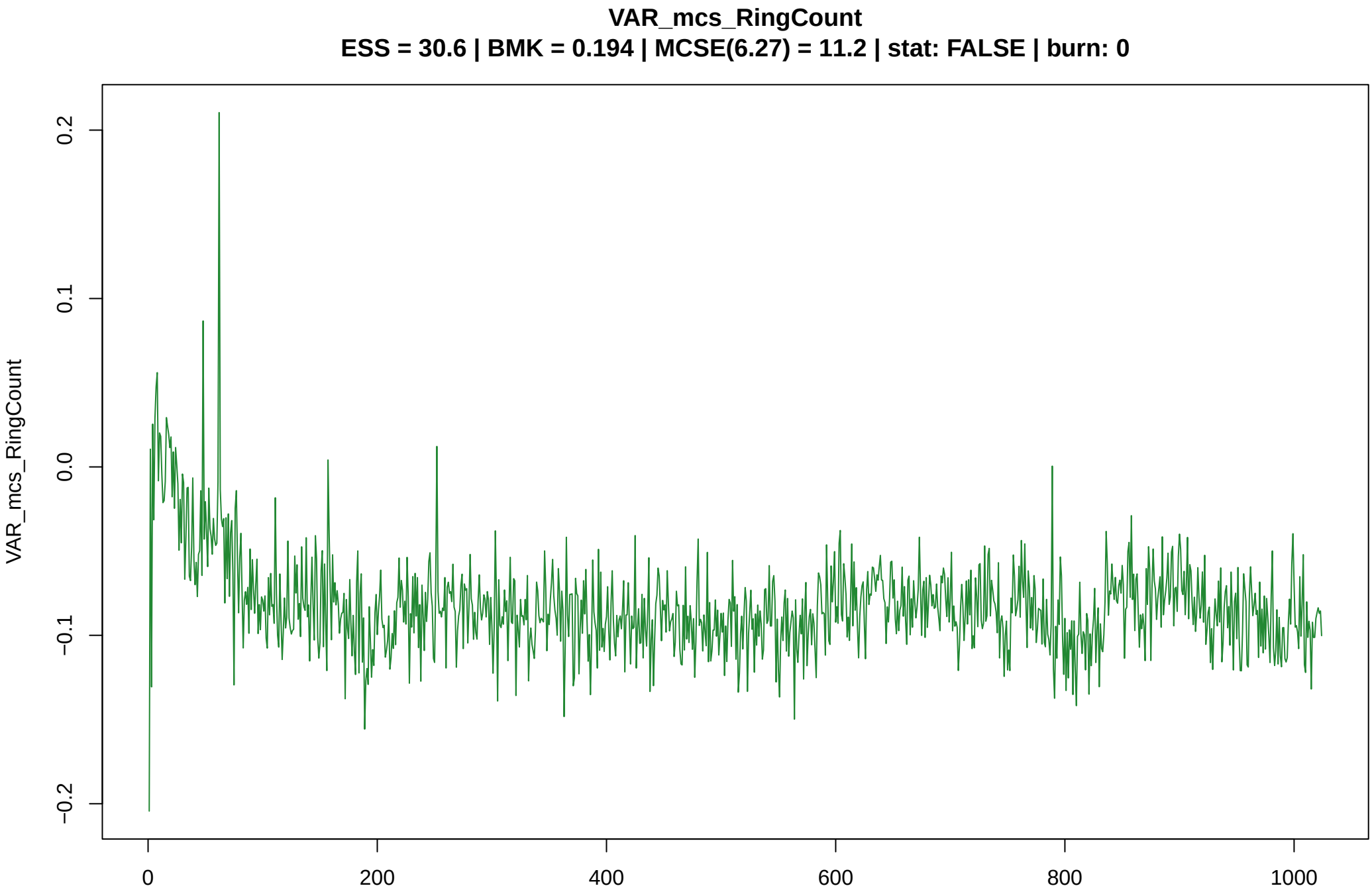

VAR_log_RMSD
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 1020
VAR_log_RMSD
0
2
4
6
8
0
200
400
600
800
1000

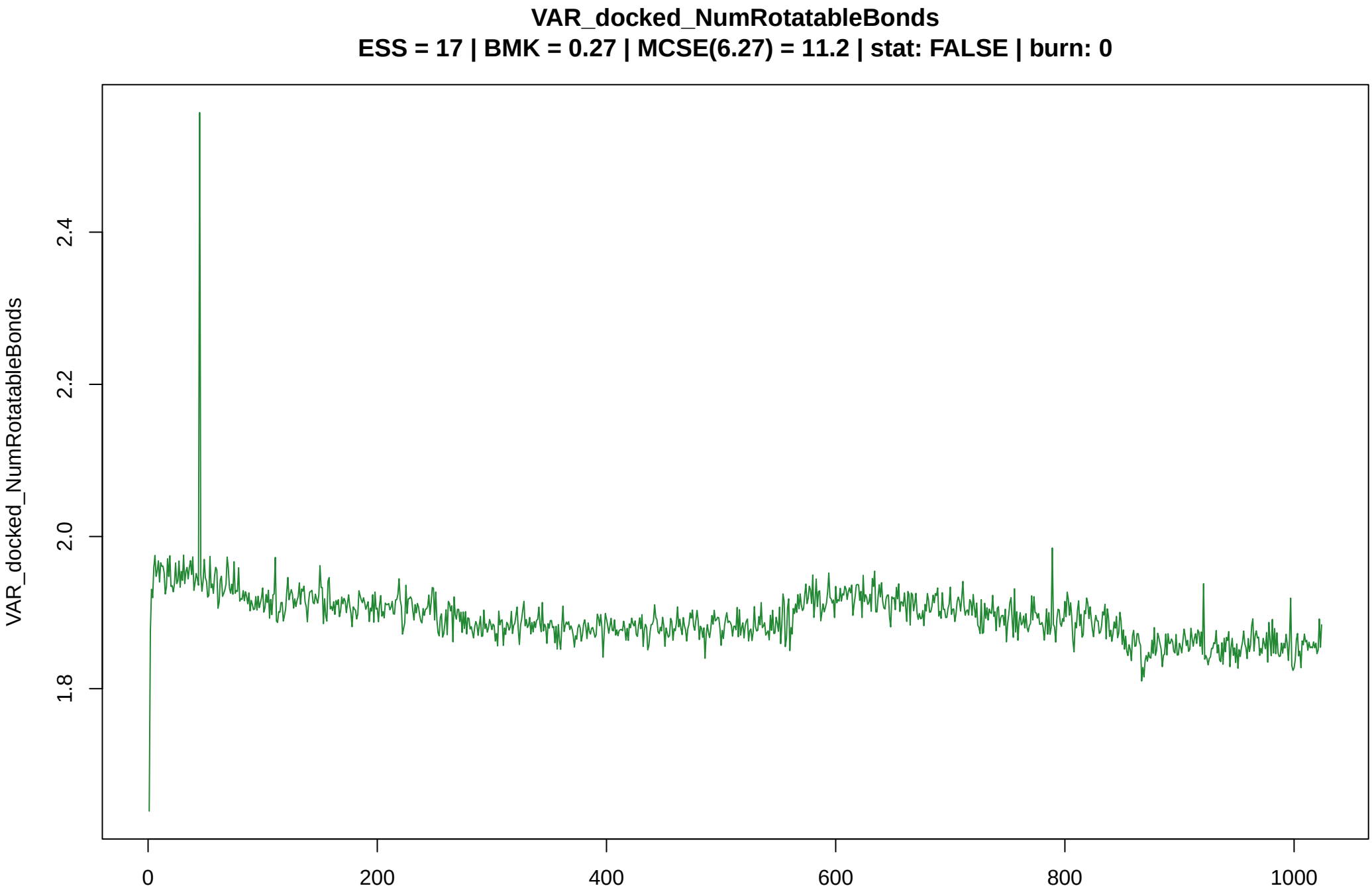

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.148 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0
VAR_log_mcs_unbonded_polar_sasa
0.5
0.0
−0.5
0
200
400
600
800
1000

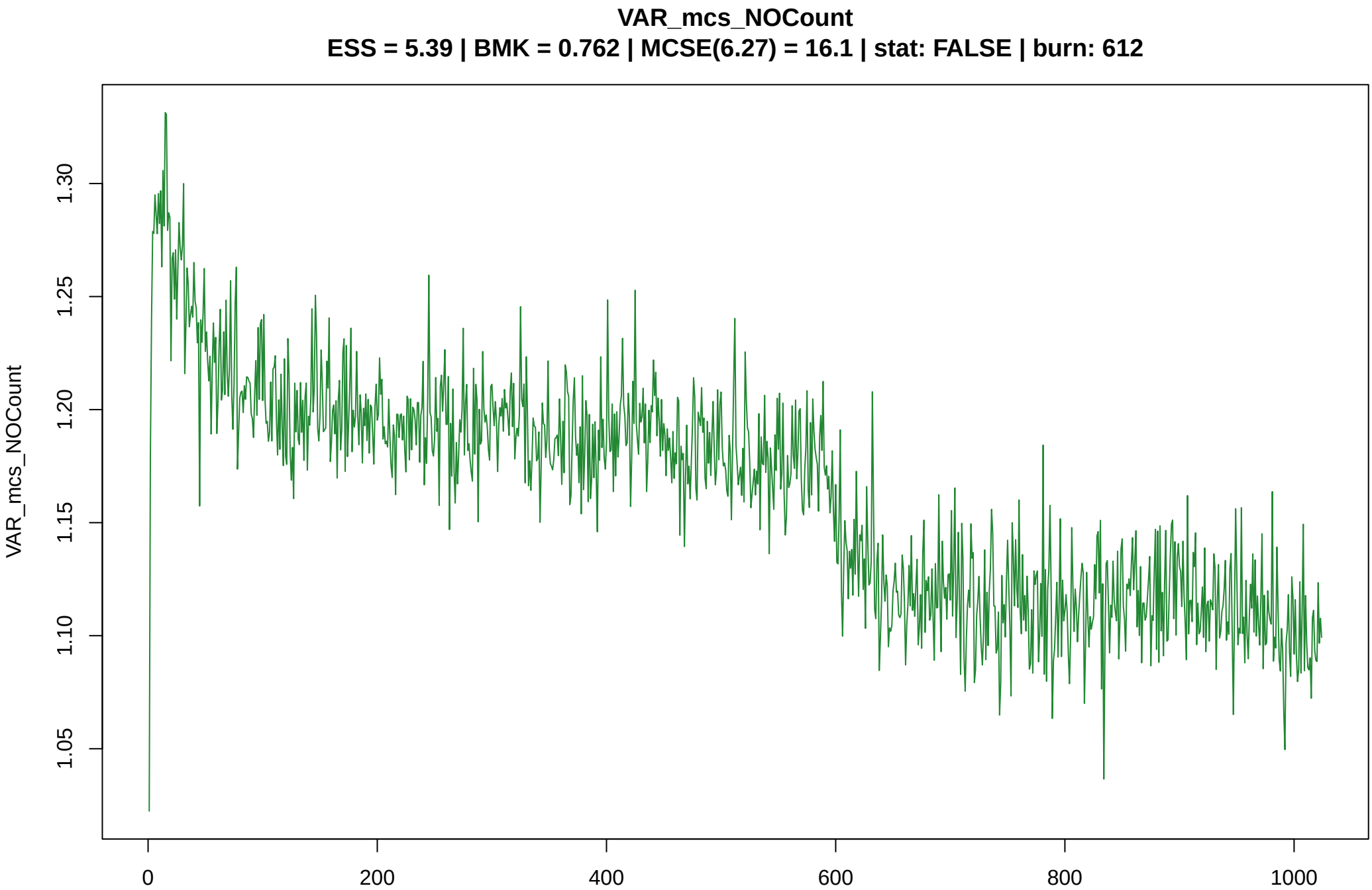

VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.859 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 816
VAR_logit_ec_tanimoto_similarity
0
2
4
6
0
200
400
600
800
1000

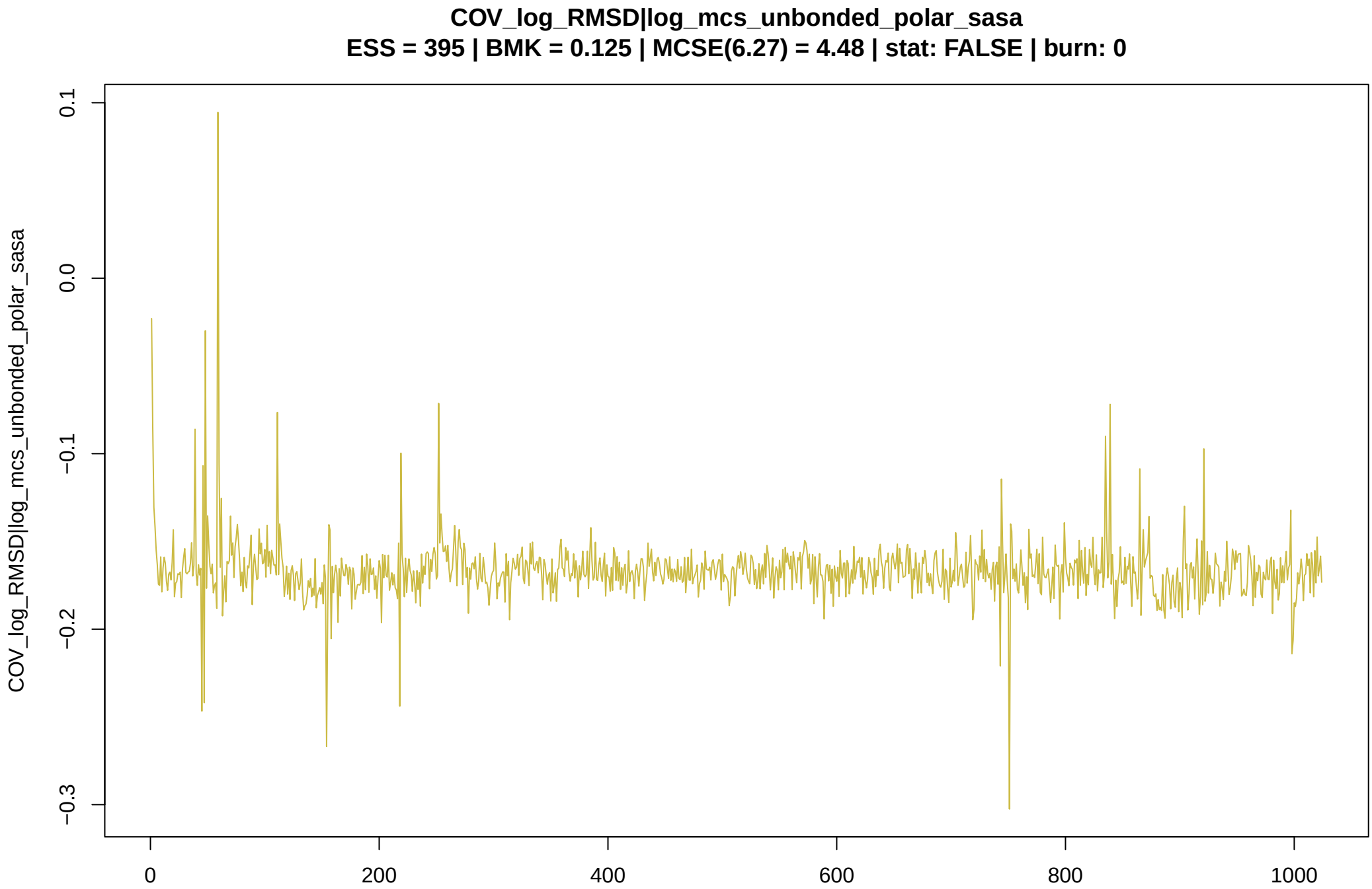

VAR_mcs_NumHeteroAtoms
ESS = 8.37 | BMK = 0.467 | MCSE(6.27) = 15.7 | stat: FALSE | burn: 204
VAR_mcs_NumHeteroAtoms
1.25
1.30
1.35
1.40
1.45
1.50
1.55
0
200
400
600
800
1000

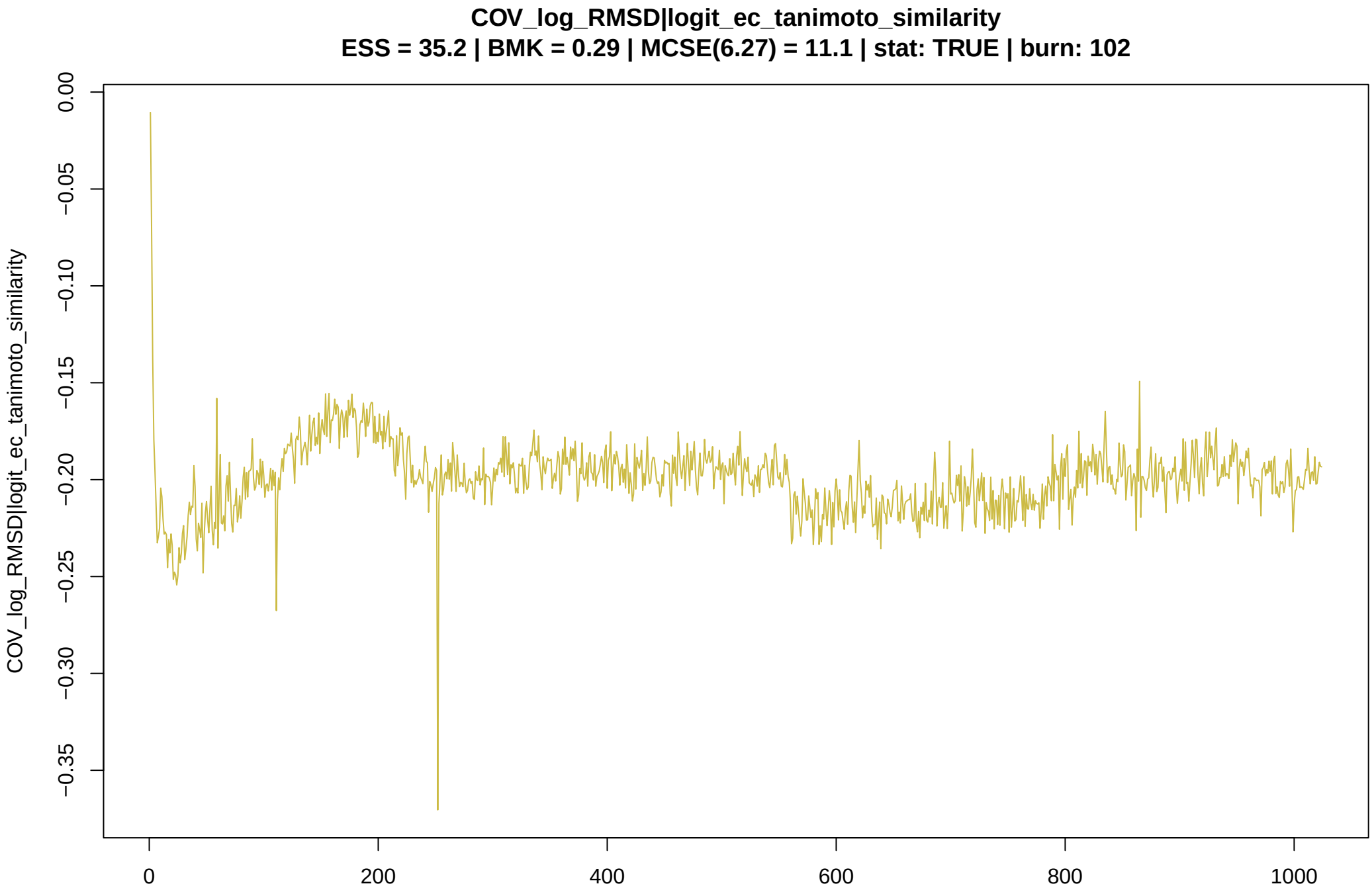

VAR_docked_HeavyAtomCount
ESS = 9.95 | BMK = 0.296 | MCSE(6.27) = 12.6 | stat: TRUE | burn: 816
VAR_docked_HeavyAtomCount
4.0
3.8
3.6
3.4
3.2
0
200
400
600
800
1000

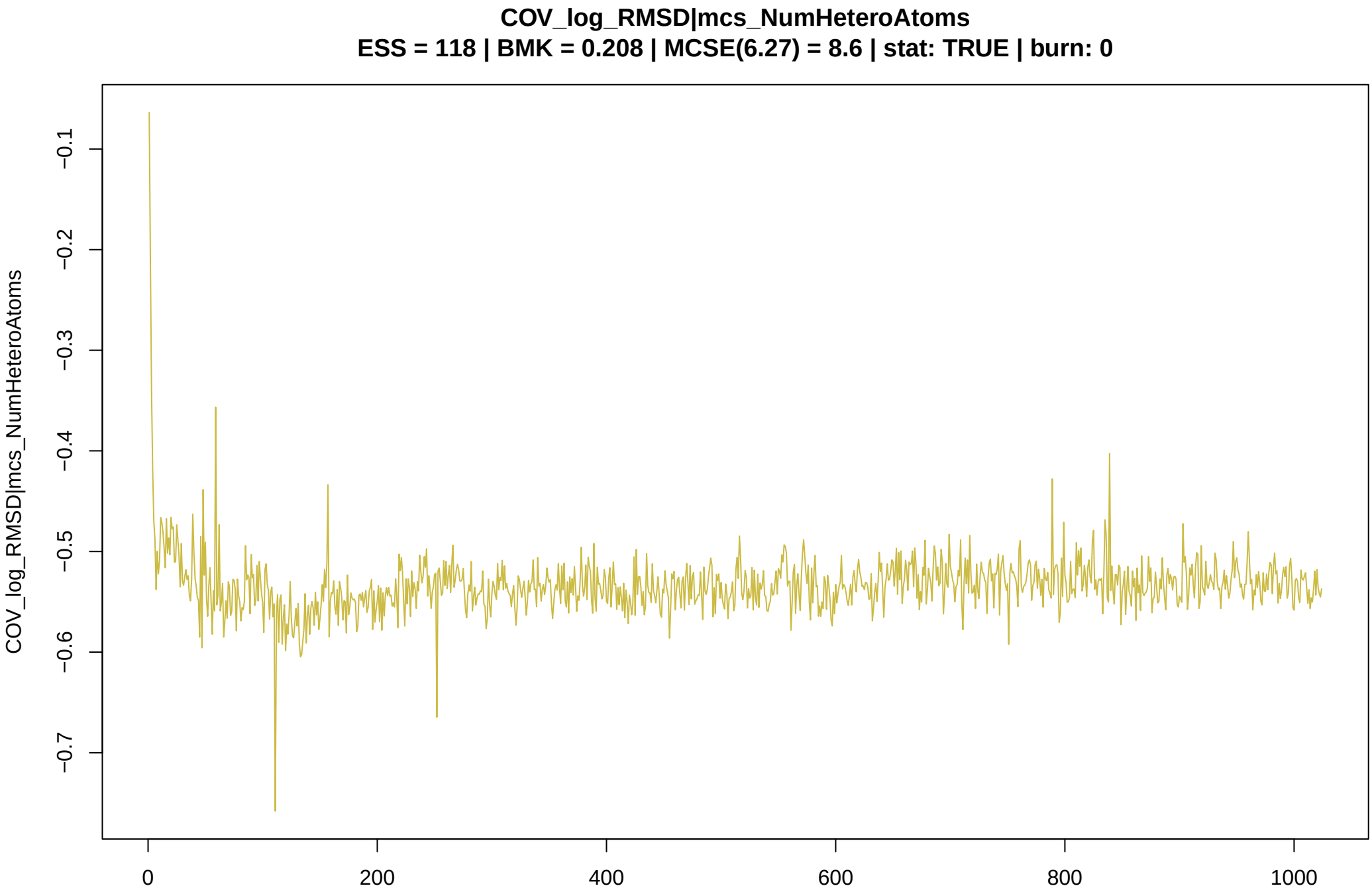

VAR_mcs_RingCount
ESS = 30.6 | BMK = 0.194 | MCSE(6.27) = 11.2 | stat: FALSE | burn: 0
VAR_mcs_RingCount
0.2
0.1
0.0
−0.1
−0.2
0
200
400
600
800
1000

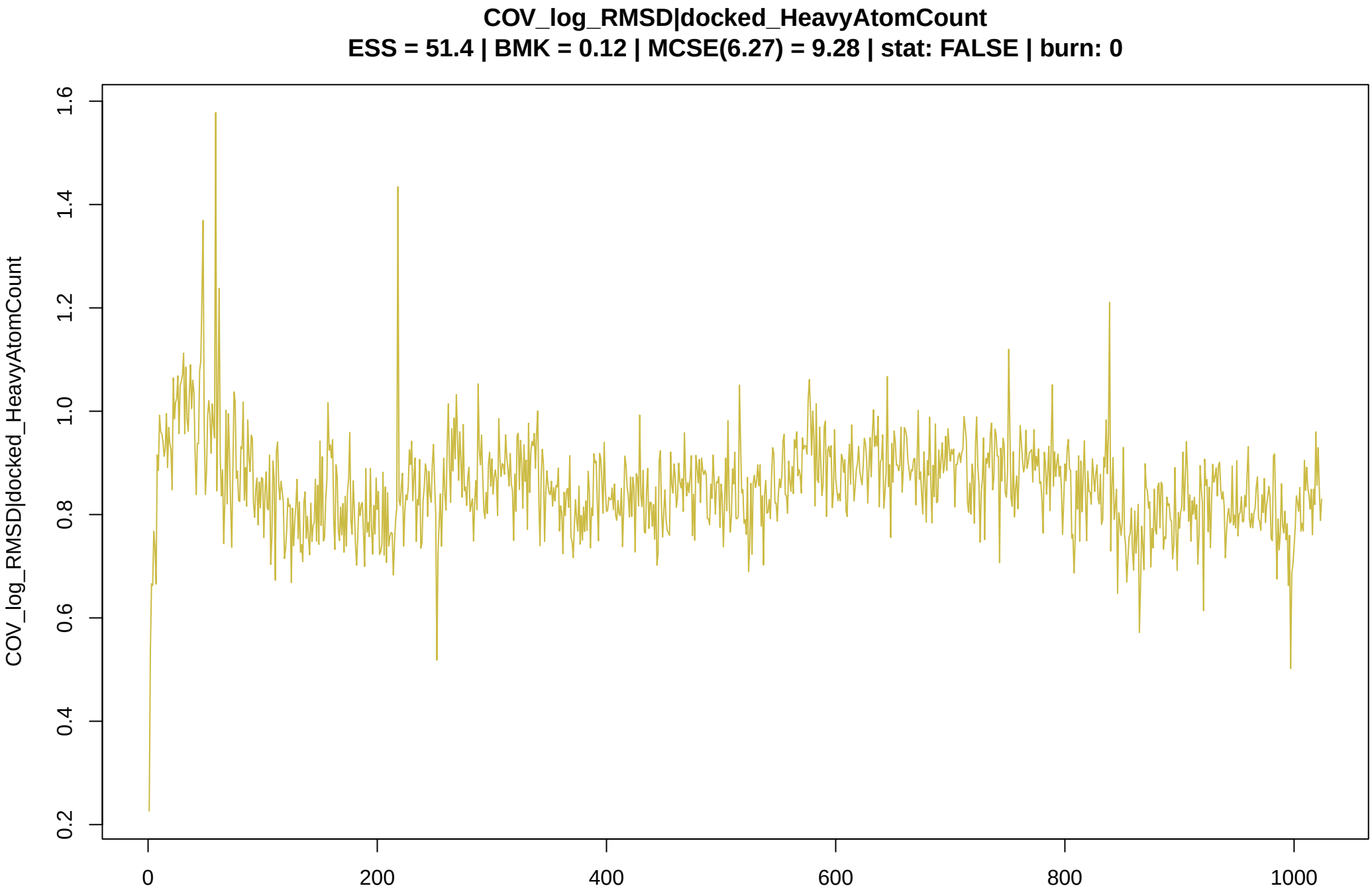

VAR_docked_NumRotatableBonds
ESS = 17 | BMK = 0.27 | MCSE(6.27) = 11.2 | stat: FALSE | burn: 0
VAR_docked_NumRotatableBonds
1.8
2.0
2.2
2.4
0
200
400
600
800
1000

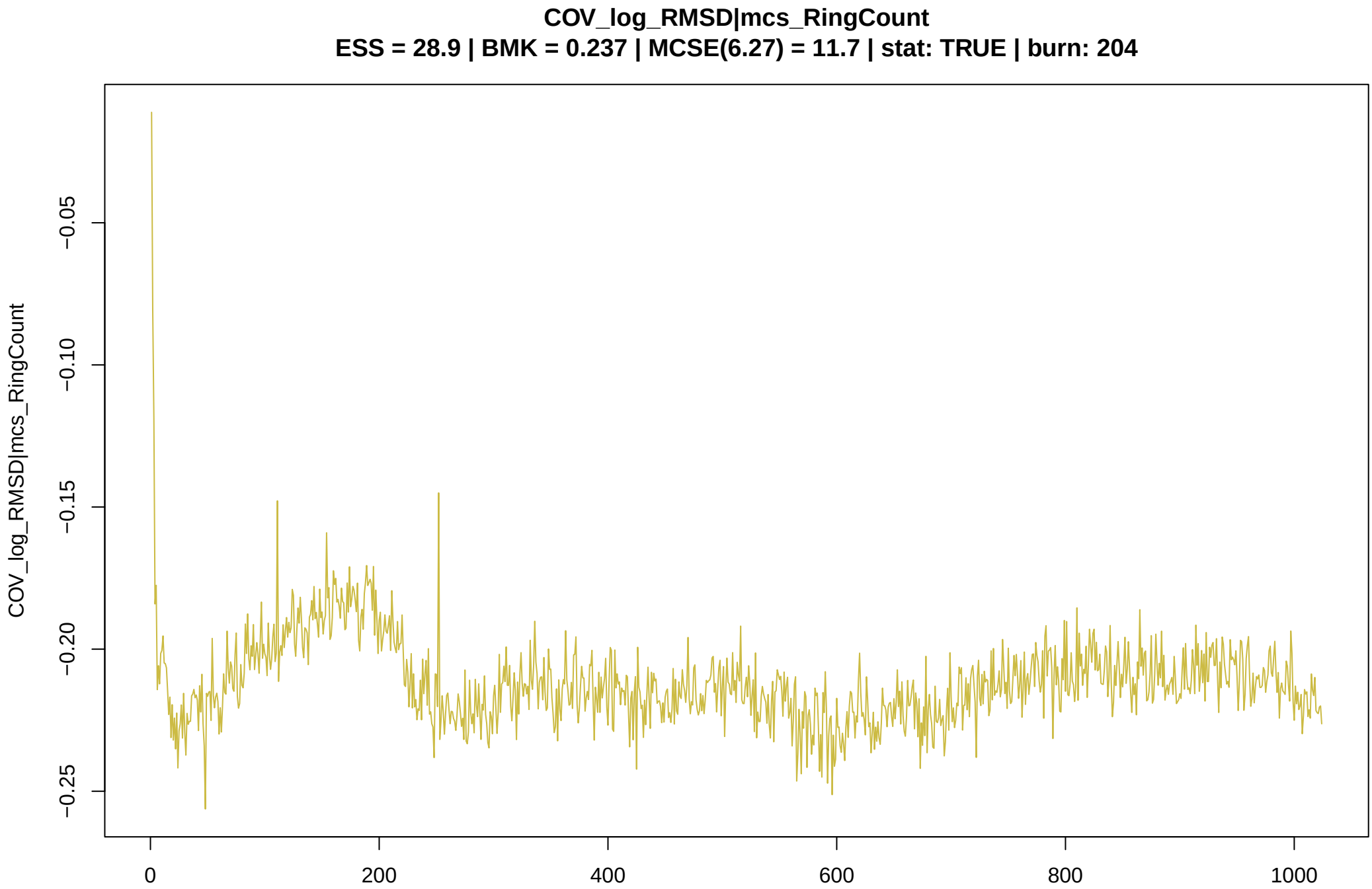

VAR_mcs_NOCount
ESS = 5.39 | BMK = 0.762 | MCSE(6.27) = 16.1 | stat: FALSE | burn: 612
VAR_mcs_NOCount
1.05
1.10
1.15
1.20
1.25
1.30
0
200
400
600
800
1000

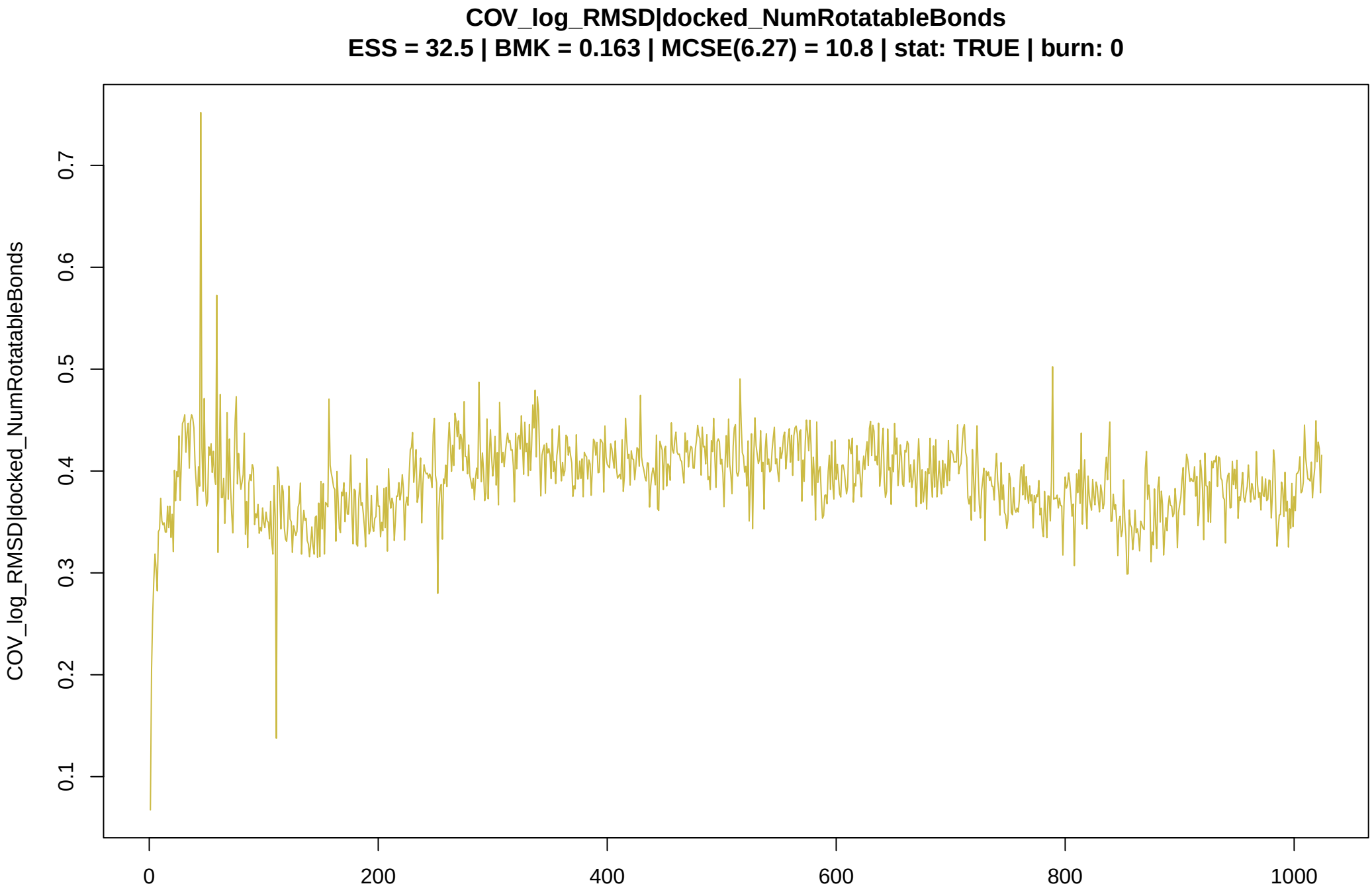

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 395 | BMK = 0.125 | MCSE(6.27) = 4.48 | stat: FALSE | burn: 0
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.1
0.0
−0.1
−0.2
−0.3
0
200
400
600
800
1000

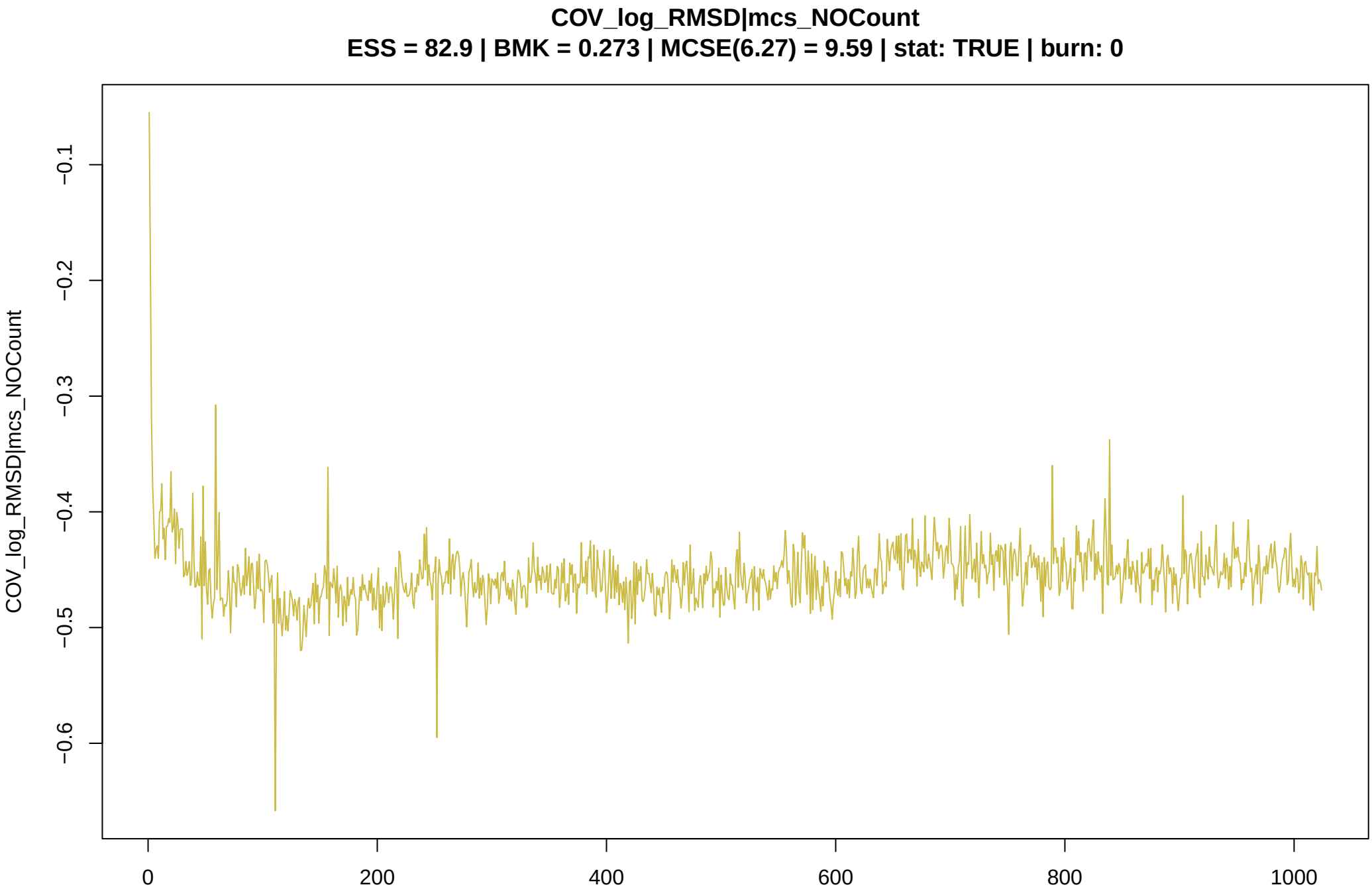

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 35.2 | BMK = 0.29 | MCSE(6.27) = 11.1 | stat: TRUE | burn: 102
COV_log_RMSD|logit_ec_tanimoto_similarity
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
−0.35
0
200
400
600
800
1000

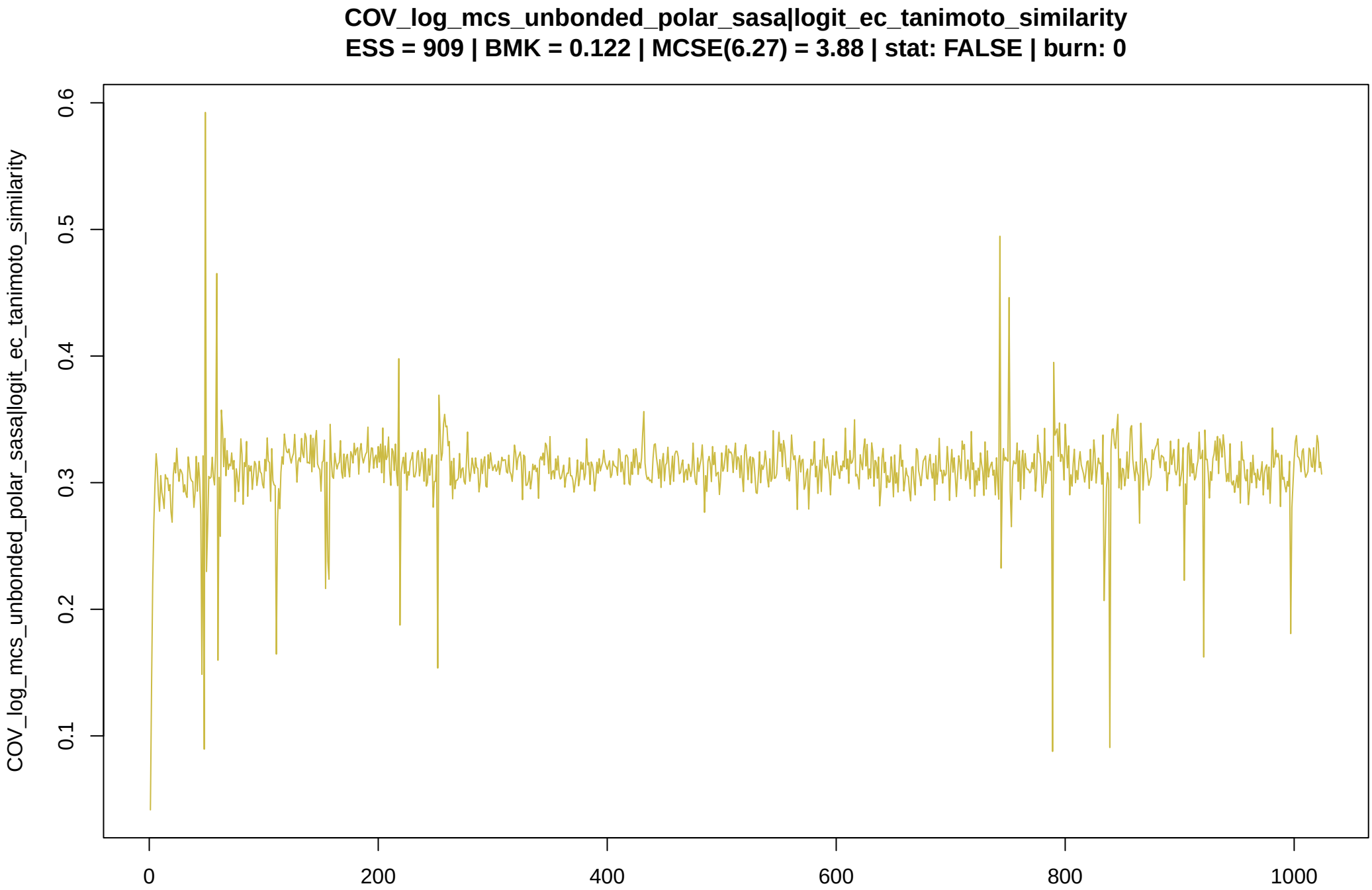

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 118 | BMK = 0.208 | MCSE(6.27) = 8.6 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
0
200
400
600
800
1000

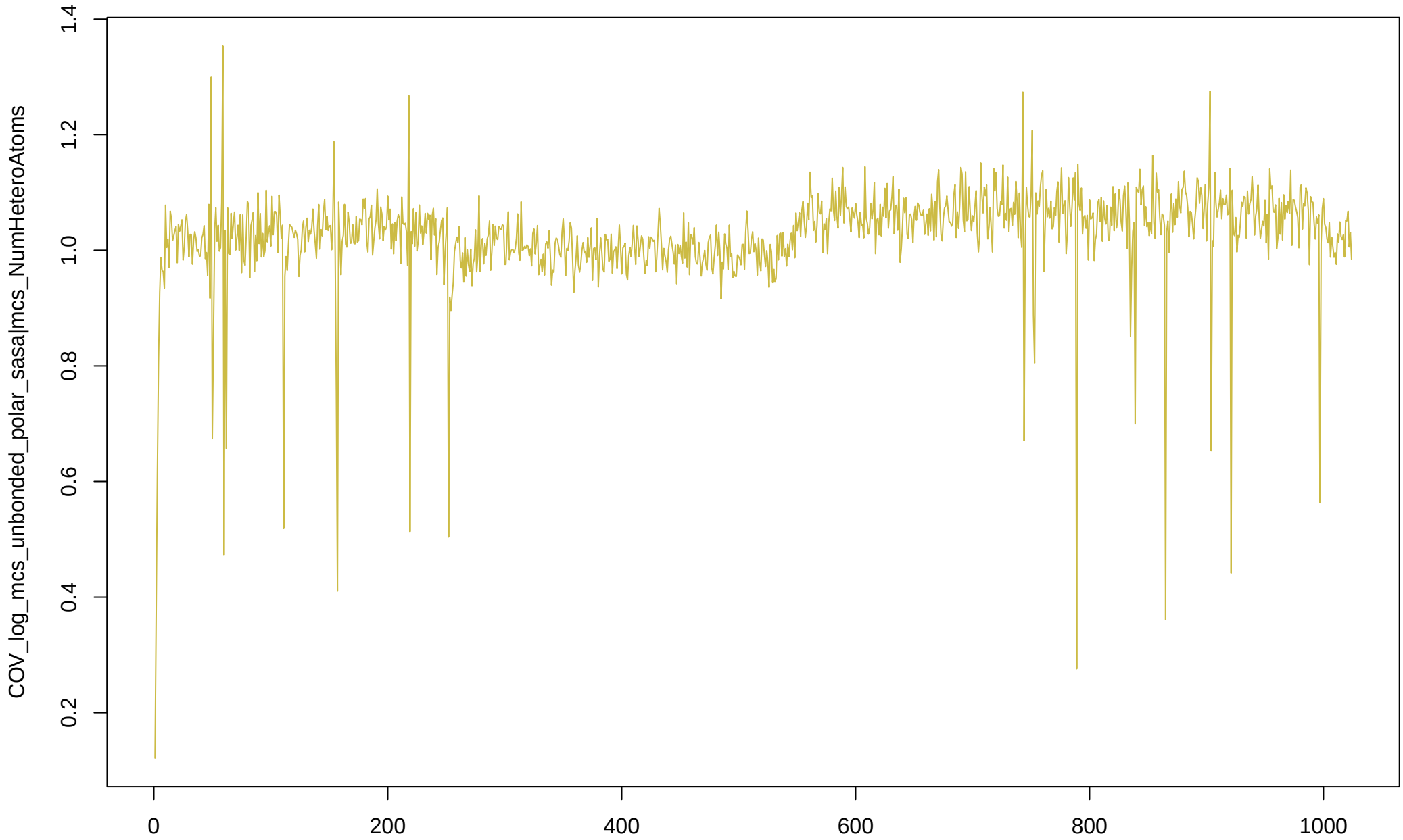

COV_log_RMSD|docked_HeavyAtomCount
ESS = 51.4 | BMK = 0.12 | MCSE(6.27) = 9.28 | stat: FALSE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
200
400
600
800
1000

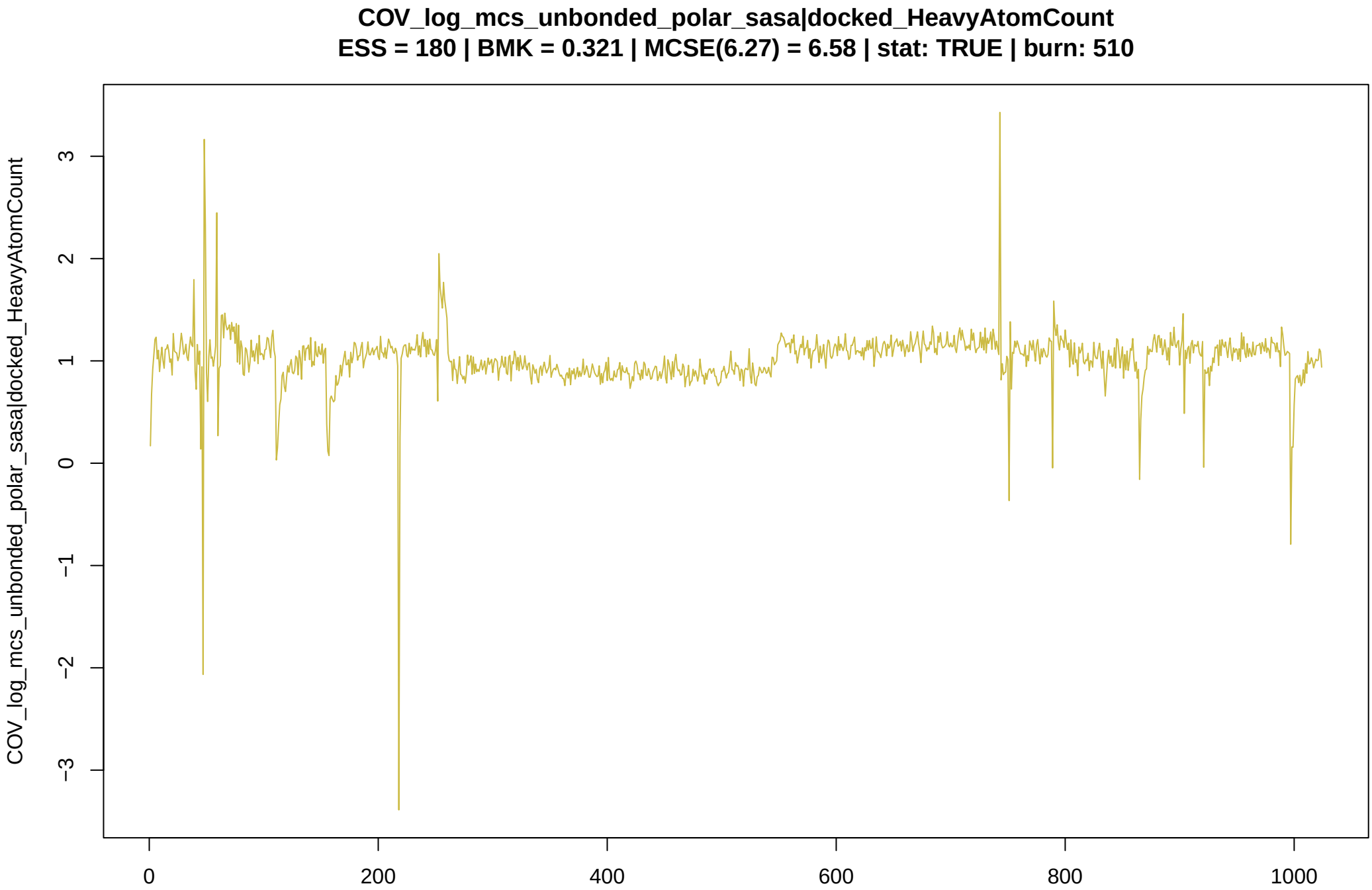

COV_log_RMSD|mcs_RingCount
ESS = 28.9 | BMK = 0.237 | MCSE(6.27) = 11.7 | stat: TRUE | burn: 204
COV_log_RMSD|mcs_RingCount
−0.05
−0.10
−0.15
−0.20
−0.25
0
200
400
600
800
1000

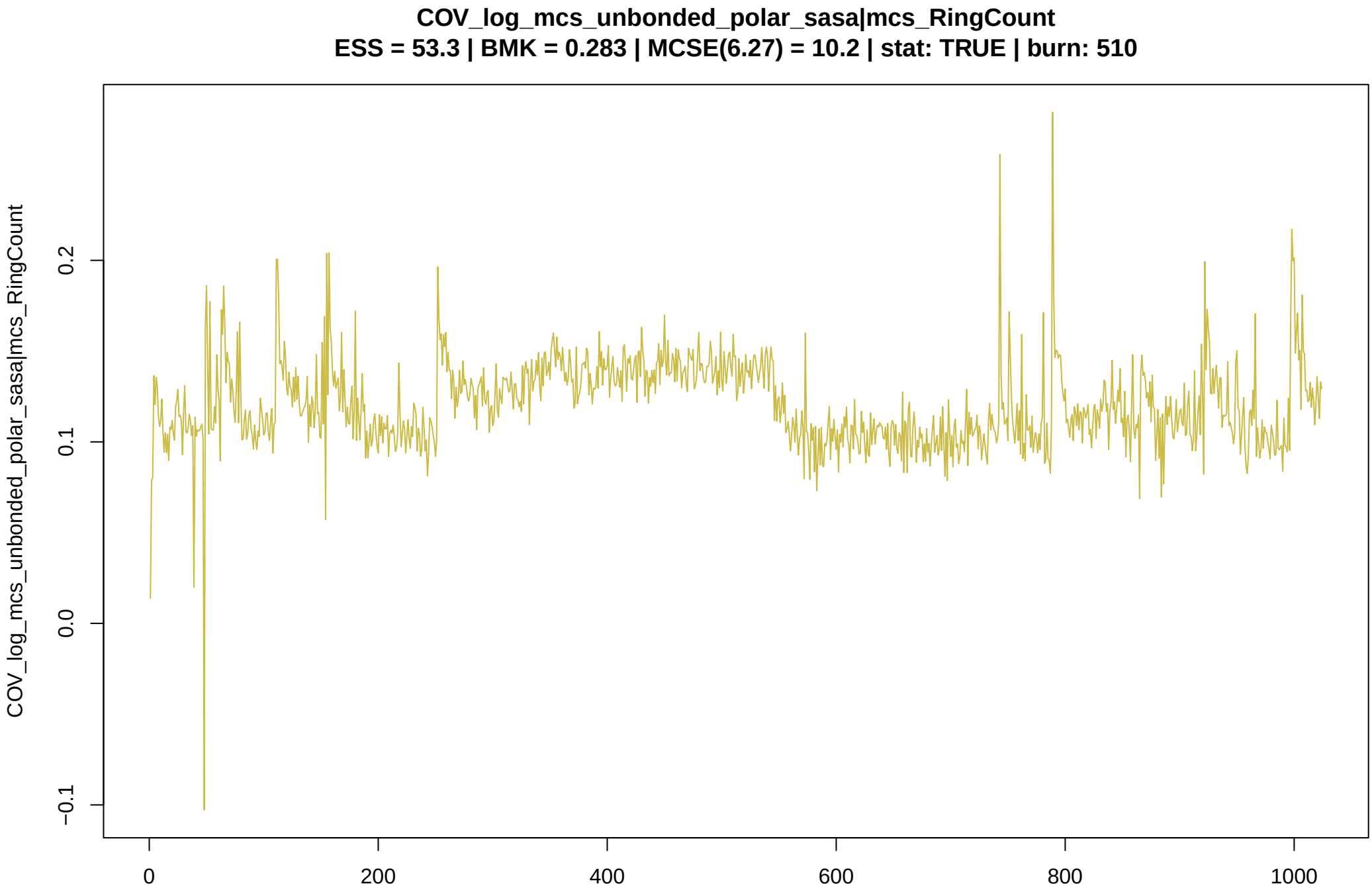

COV_log_RMSD|docked_NumRotatableBonds
ESS = 32.5 | BMK = 0.163 | MCSE(6.27) = 10.8 | stat: TRUE | burn: 0
COV_log_RMSD|docked_NumRotatableBonds
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
200
400
600
800
1000

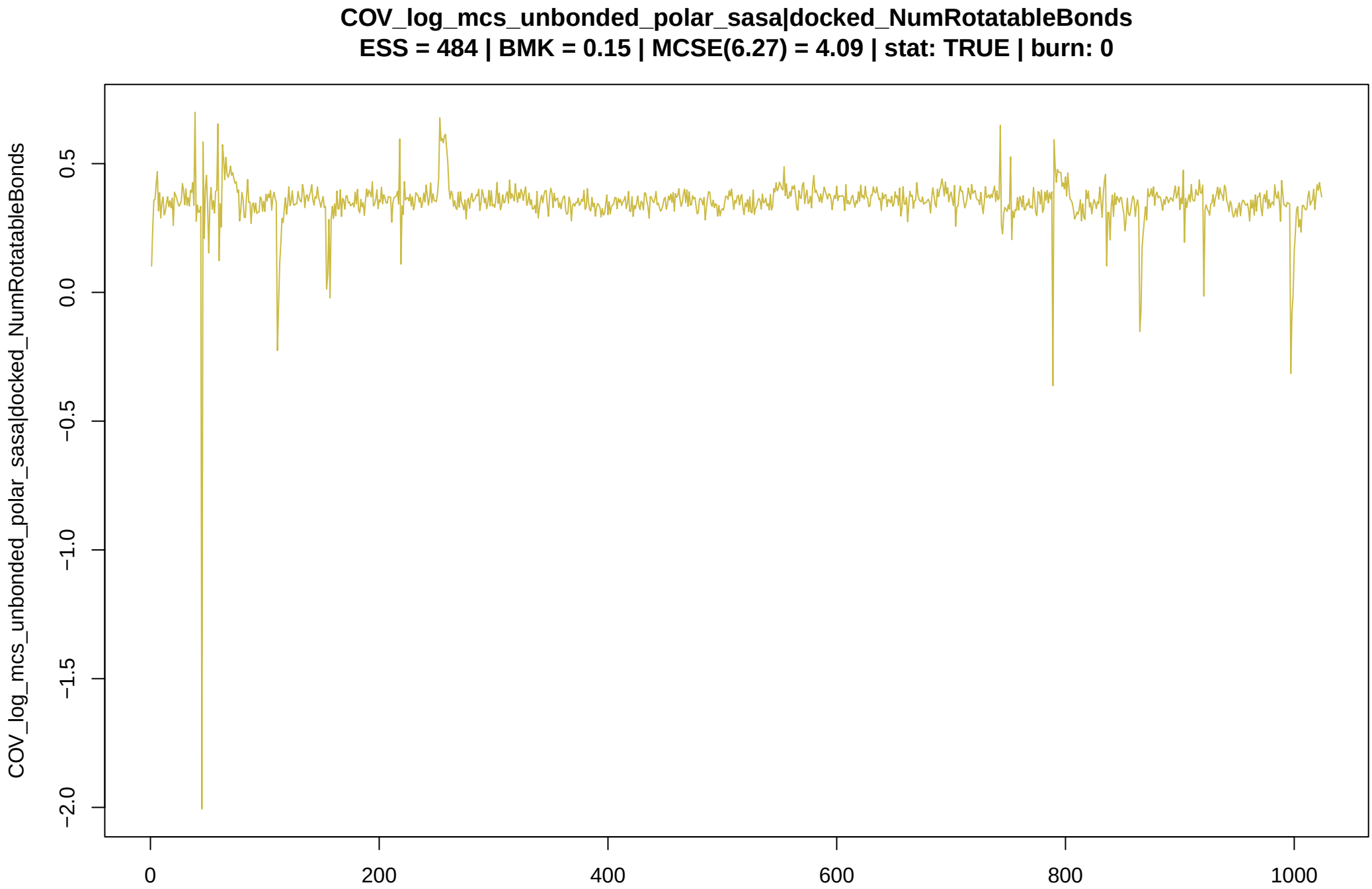

COV_log_RMSD|mcs_NOCount
ESS = 82.9 | BMK = 0.273 | MCSE(6.27) = 9.59 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NOCount
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
0
200
400
600
800
1000

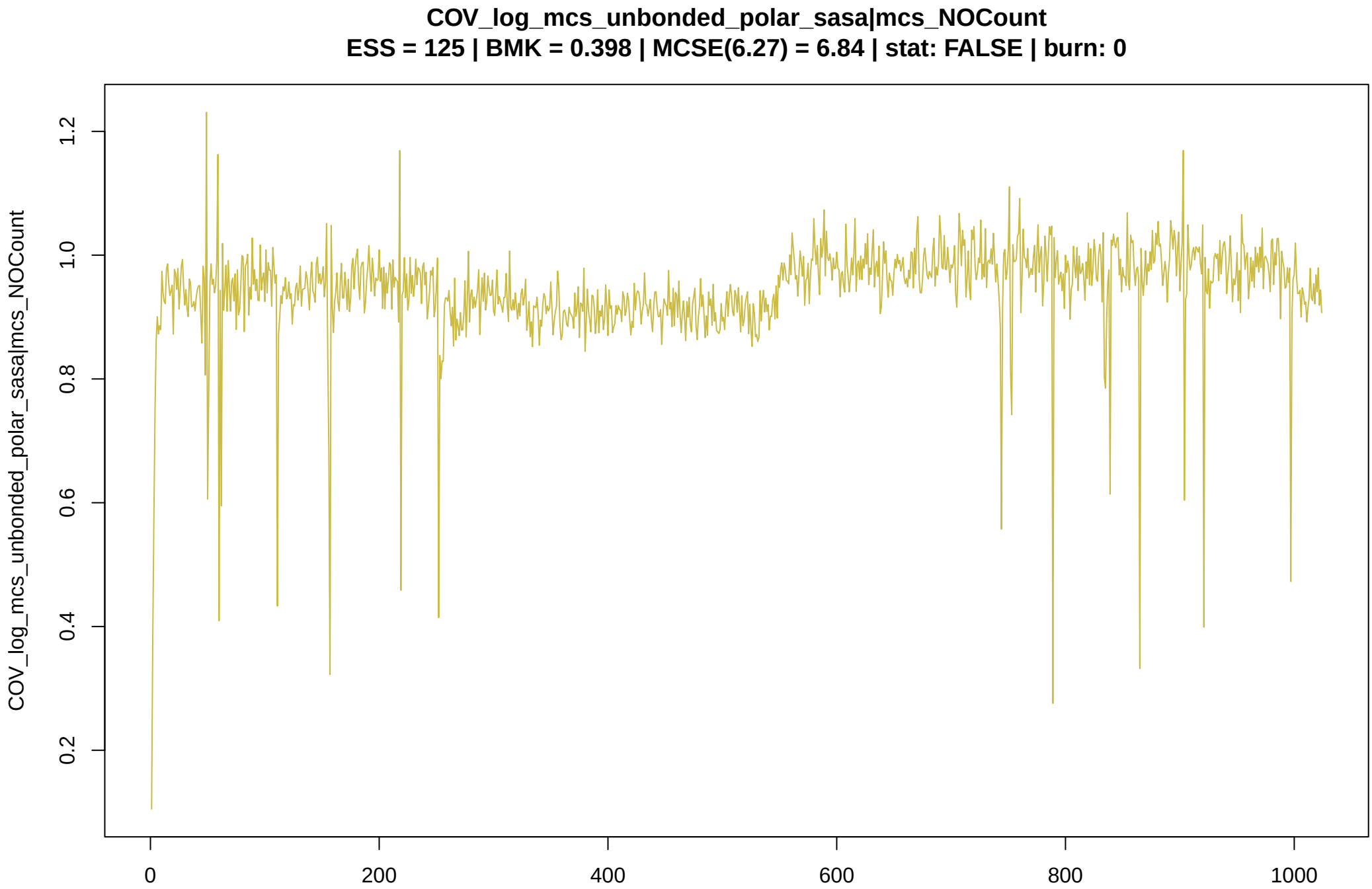

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 909 | BMK = 0.122 | MCSE(6.27) = 3.88 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0.1
0.2
0.3
0.4
0.5
0.6
0
200
400
600
800
1000

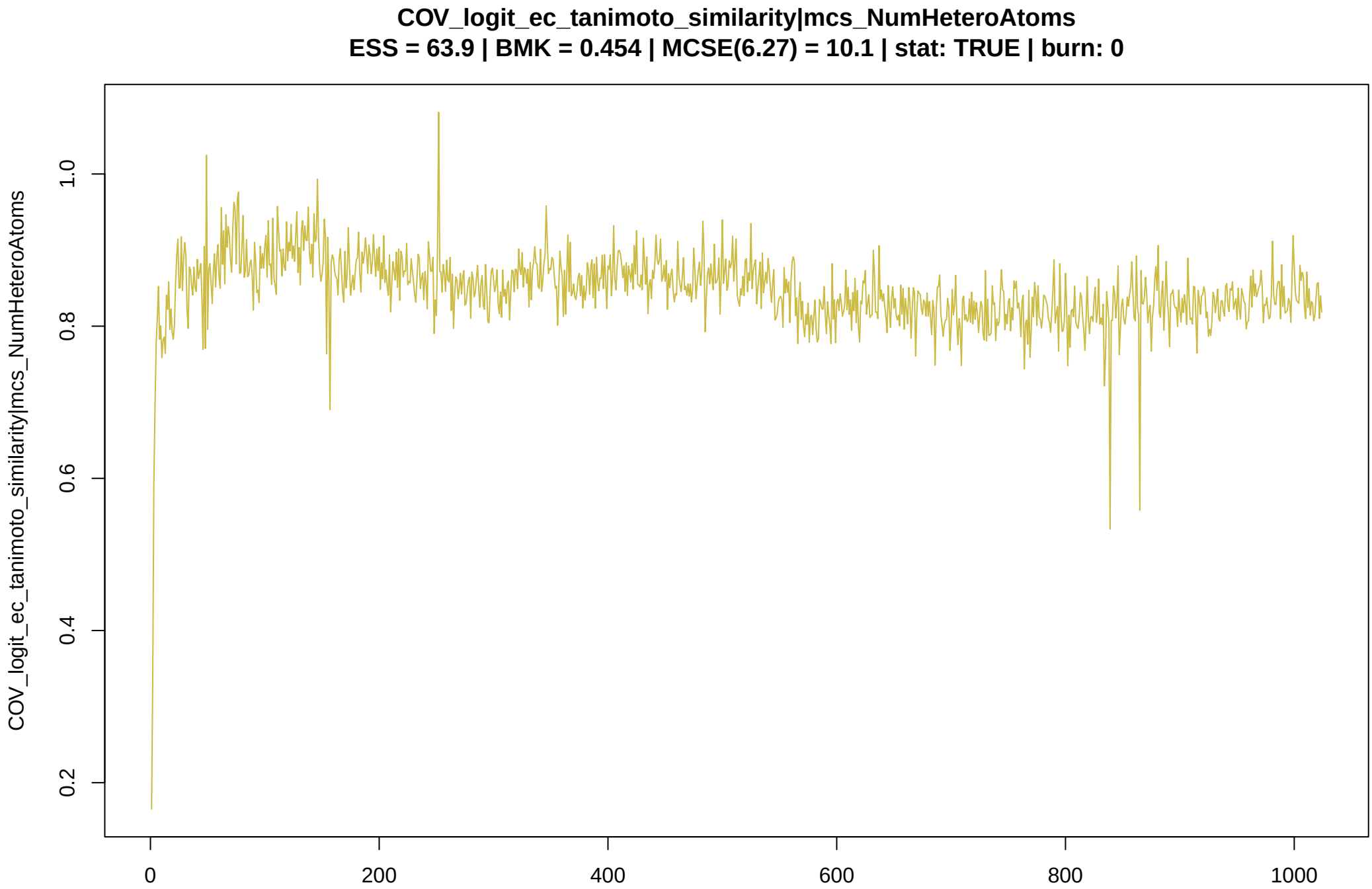

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 211 | BMK = 0.404 | MCSE(6.27) = 6.44 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
200
400
600
800
1000

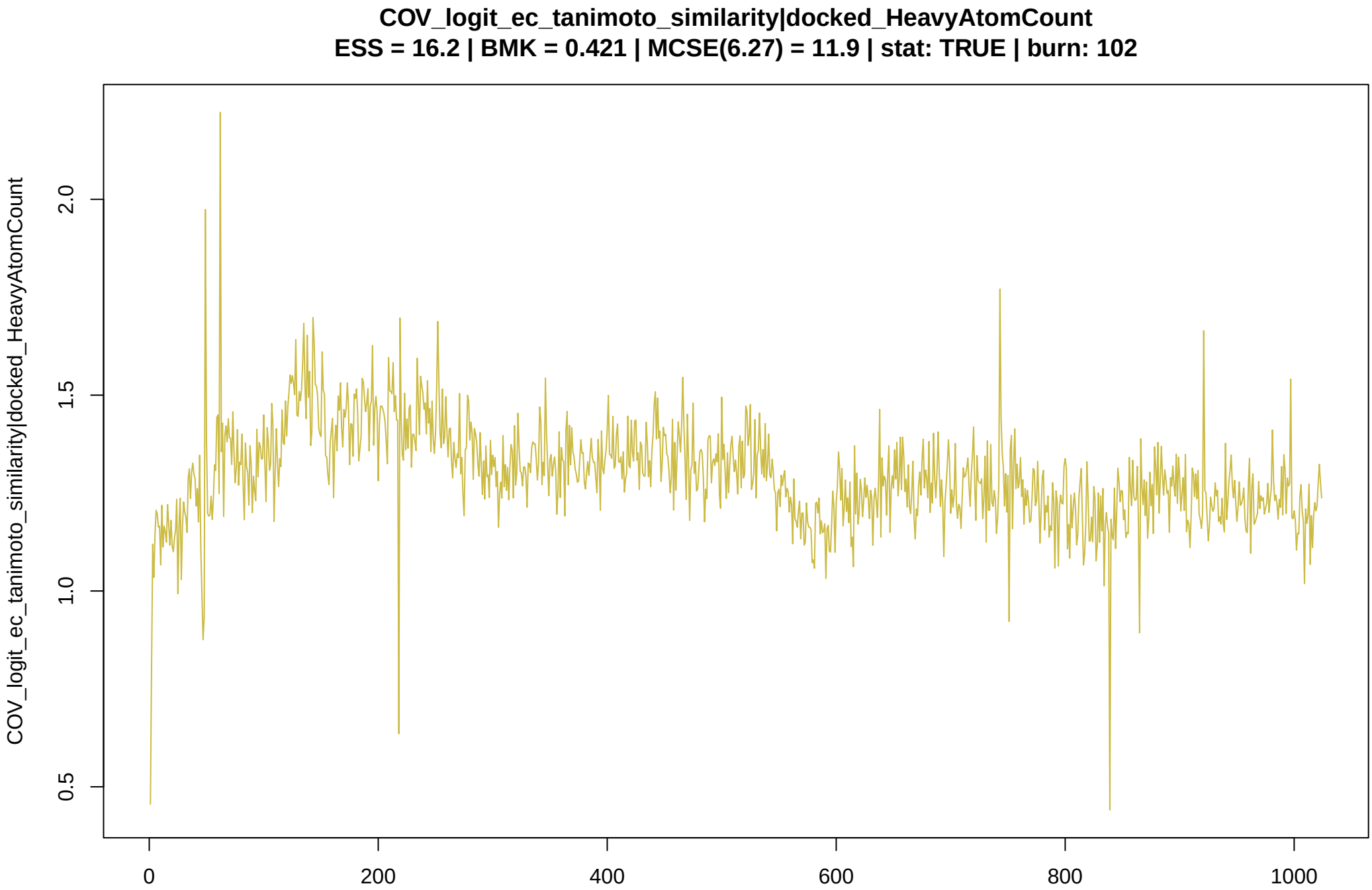

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 180 | BMK = 0.321 | MCSE(6.27) = 6.58 | stat: TRUE | burn: 510
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
3
2
1
0
−1
−2
−3
0
200
400
600
800
1000

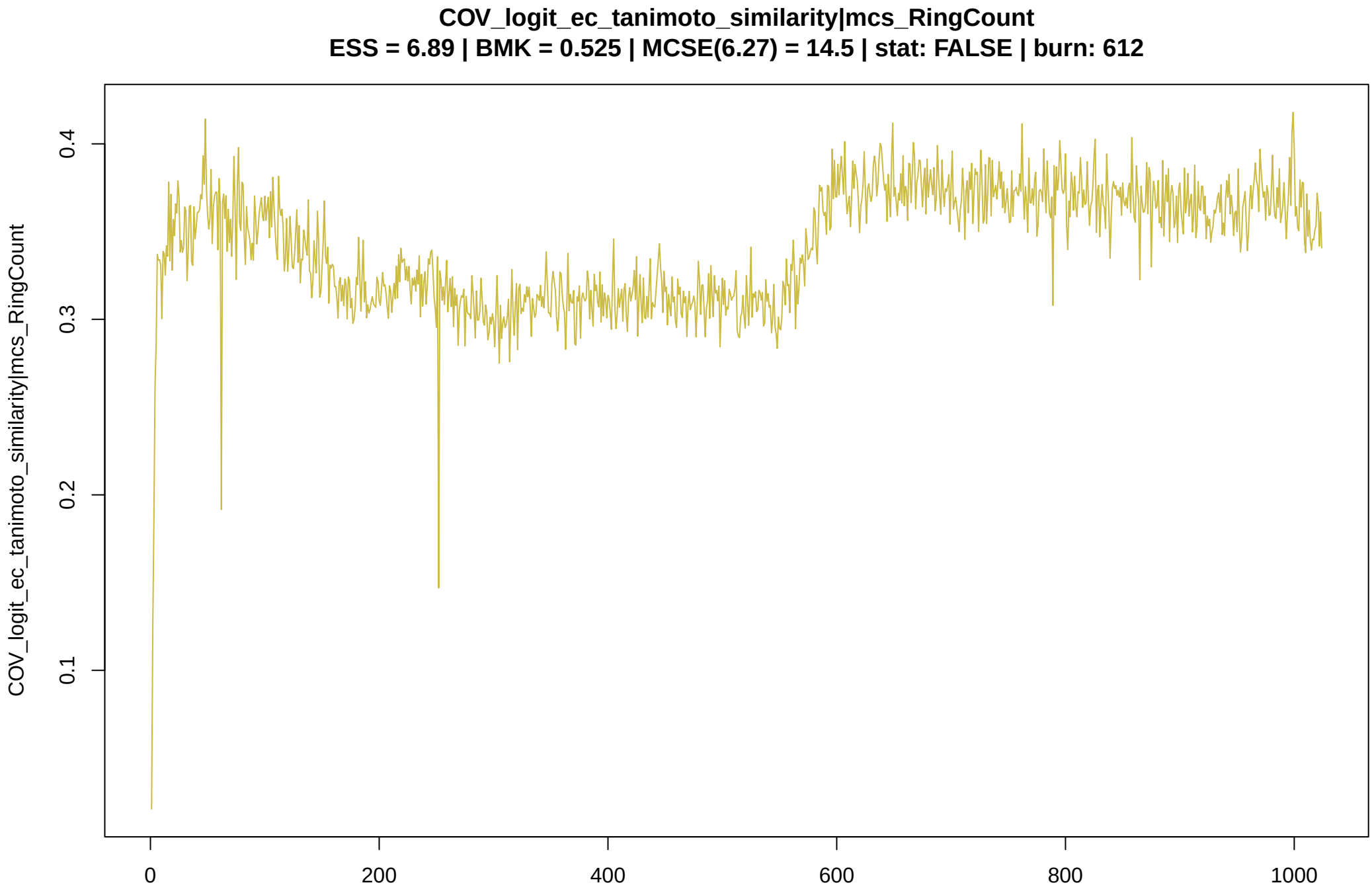

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 53.3 | BMK = 0.283 | MCSE(6.27) = 10.2 | stat: TRUE | burn: 510
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−0.1
0.0
0.1
0.2
0
200
400
600
800
1000

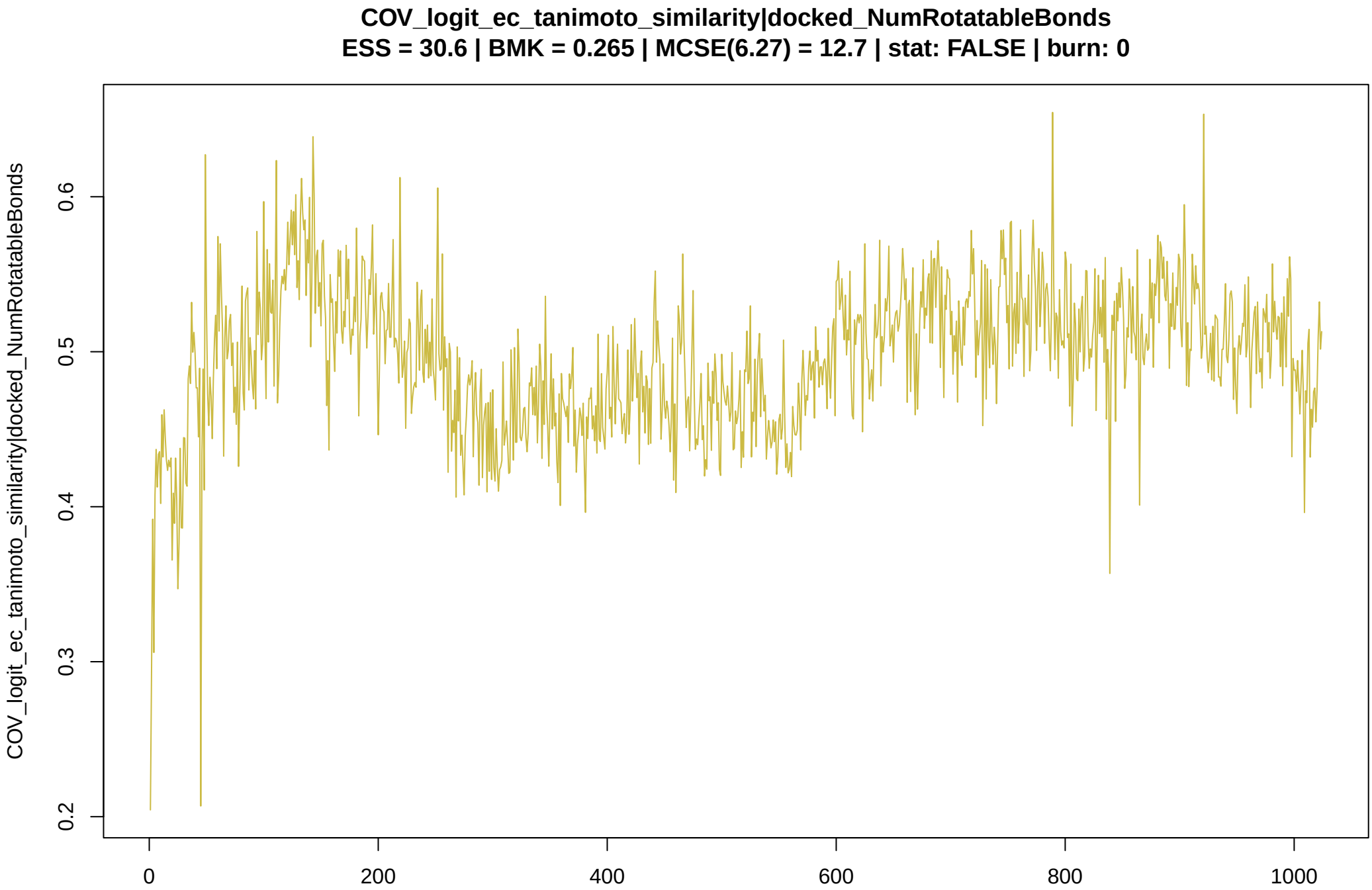

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 484 | BMK = 0.15 | MCSE(6.27) = 4.09 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
0.5
0.0
−0.5
−1.0
−1.5
−2.0
0
200
400
600
800
1000

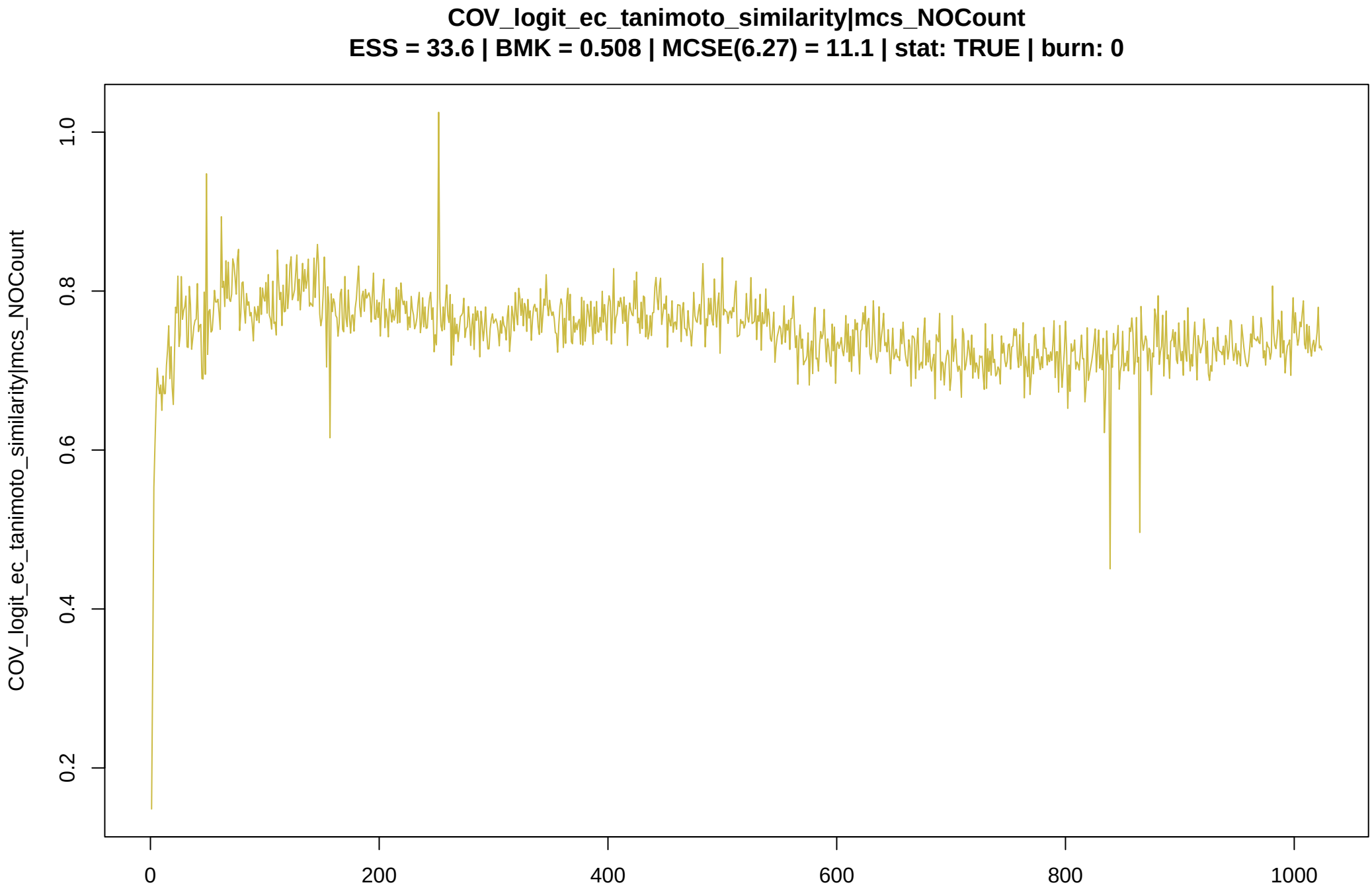

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 125 | BMK = 0.398 | MCSE(6.27) = 6.84 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
0.2
0.4
0.6
0.8
1.0
1.2
0
200
400
600
800
1000

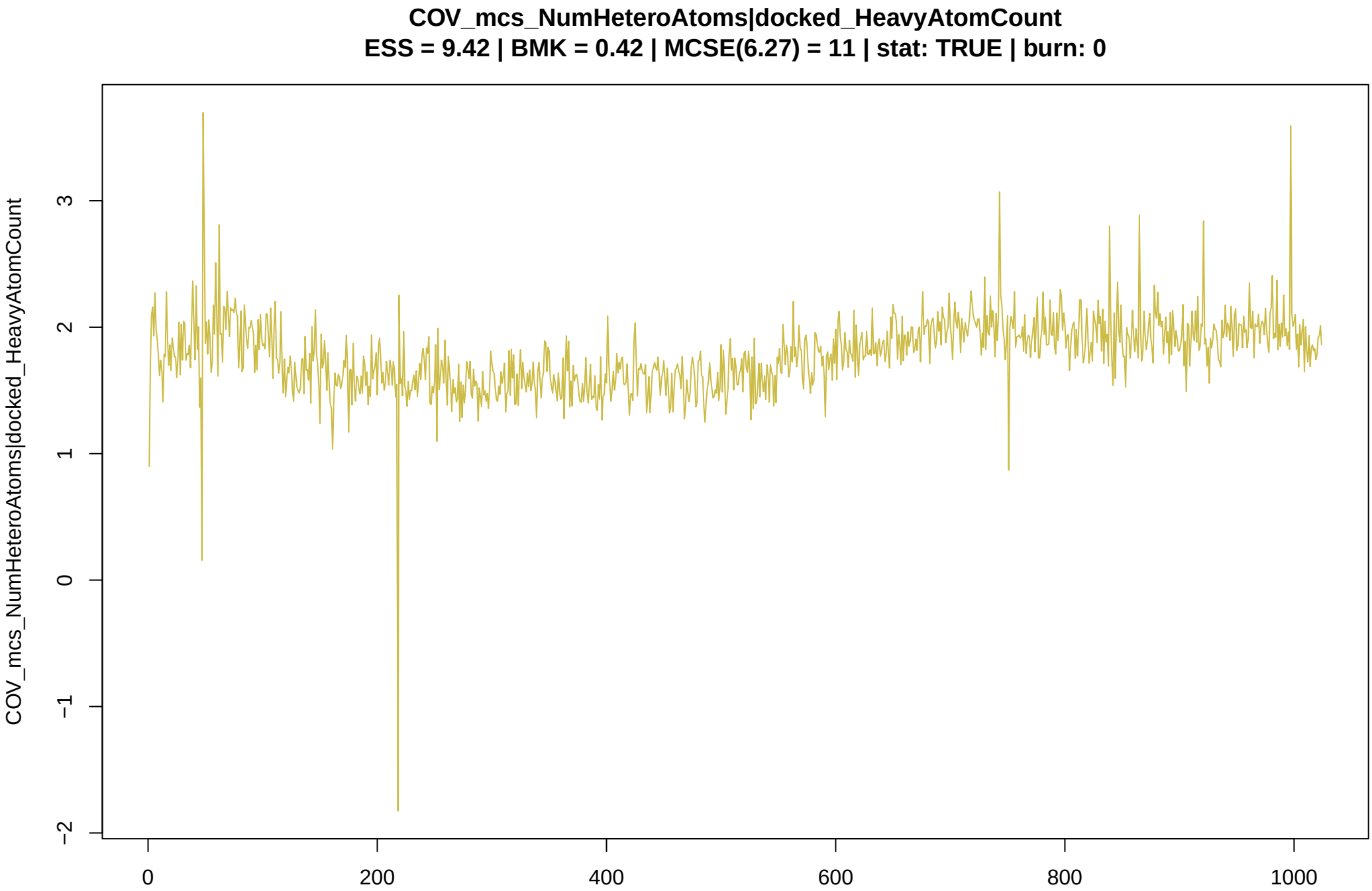

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 63.9 | BMK = 0.454 | MCSE(6.27) = 10.1 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.2
0.4
0.6
0.8
1.0
0
200
400
600
800
1000

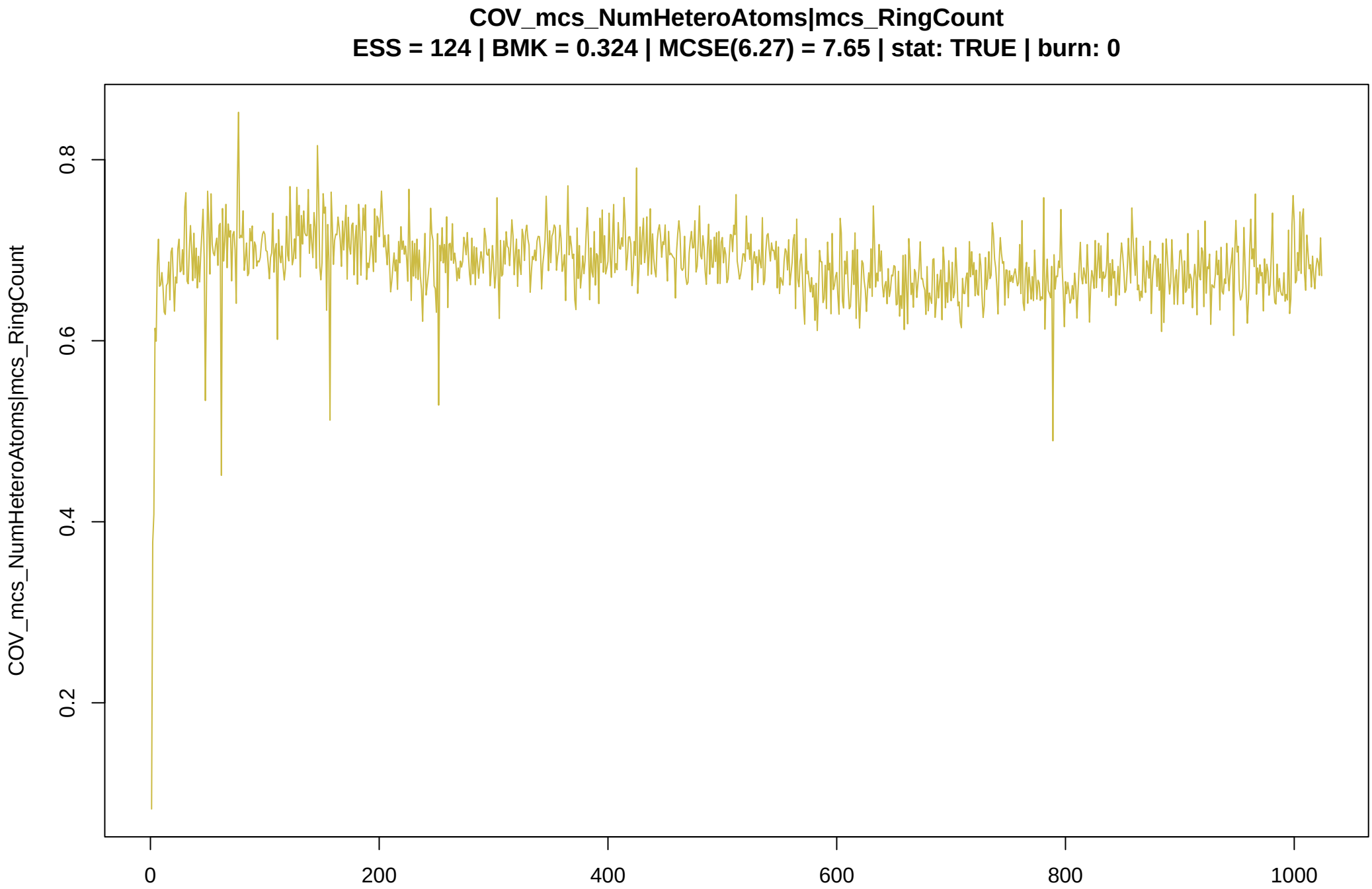

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 16.2 | BMK = 0.421 | MCSE(6.27) = 11.9 | stat: TRUE | burn: 102
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
0.5
1.0
1.5
2.0
0
200
400
600
800
1000

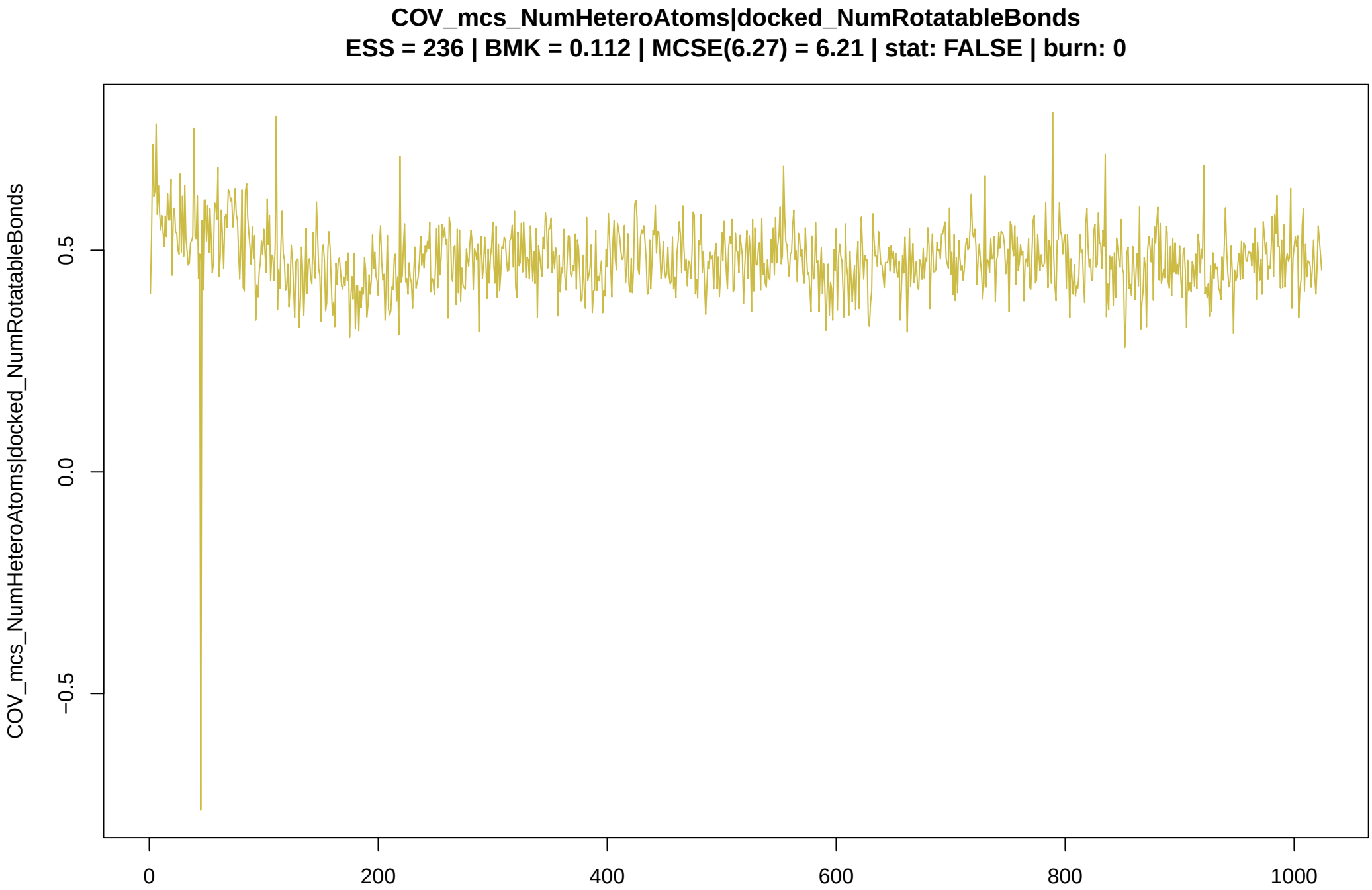

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 6.89 | BMK = 0.525 | MCSE(6.27) = 14.5 | stat: FALSE | burn: 612
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.1
0.2
0.3
0.4
0
200
400
600
800
1000

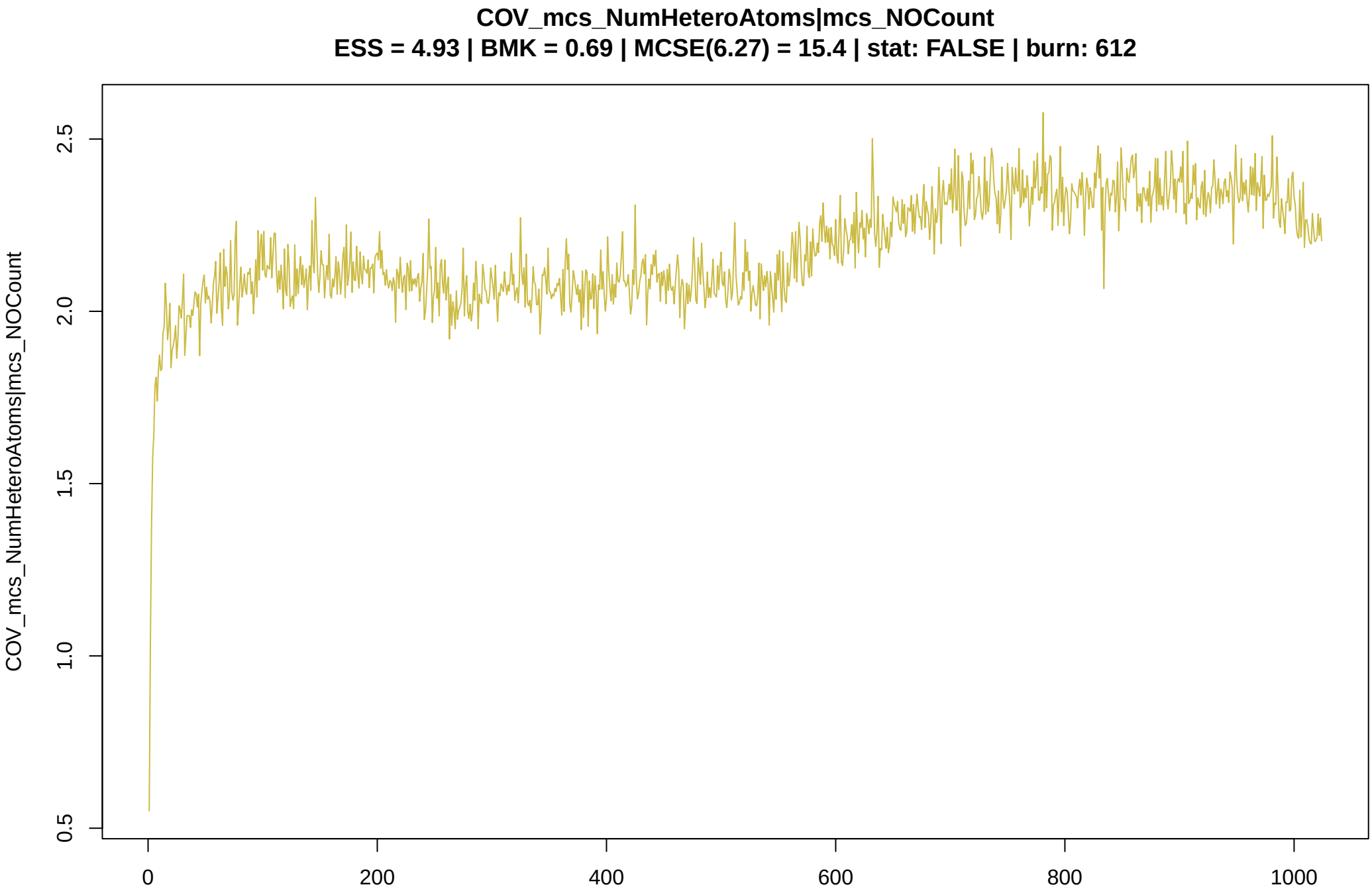

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 30.6 | BMK = 0.265 | MCSE(6.27) = 12.7 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
0.2
0.3
0.4
0.5
0.6
0
200
400
600
800
1000

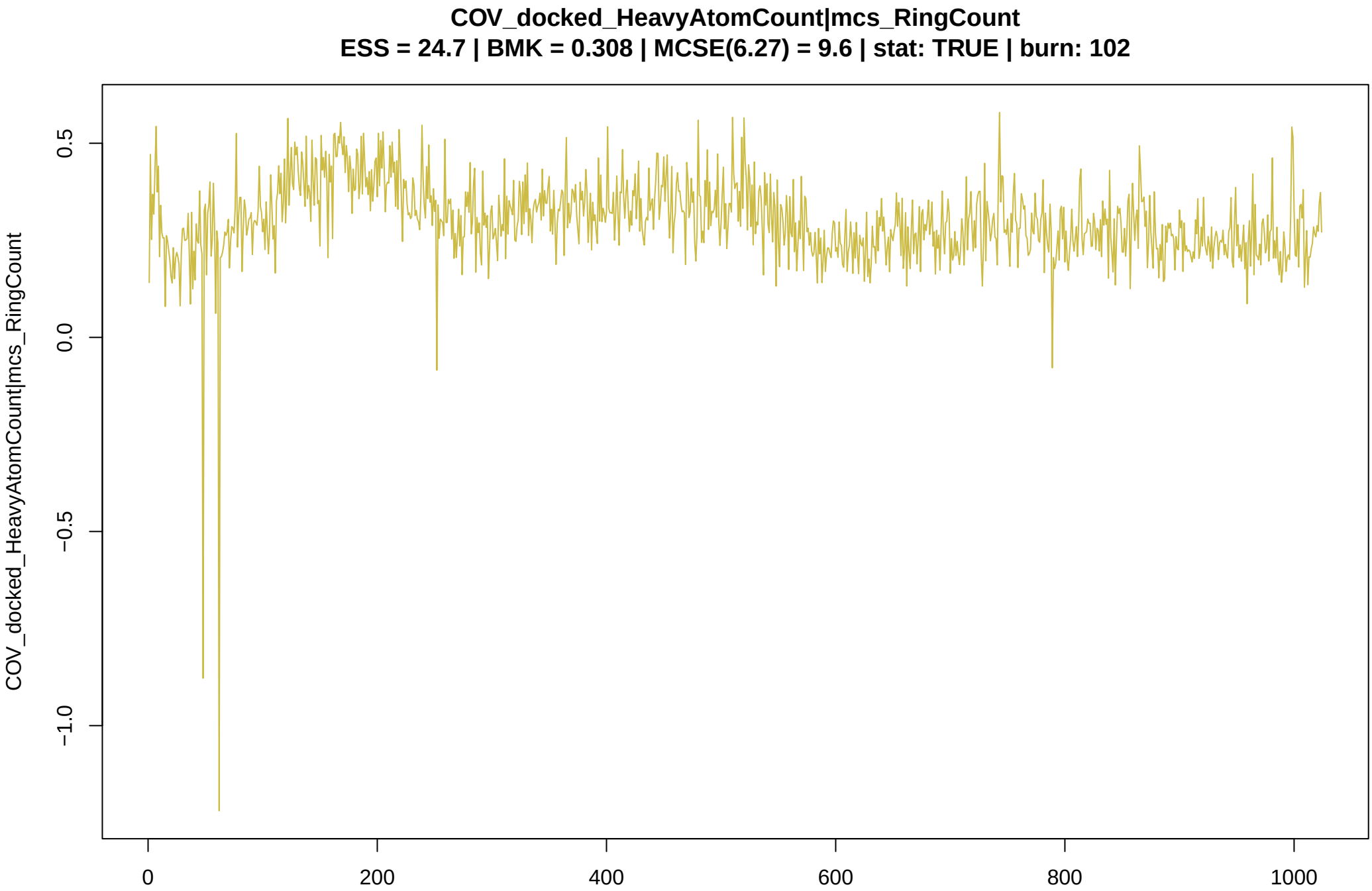

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 33.6 | BMK = 0.508 | MCSE(6.27) = 11.1 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NOCount
0.2
0.4
0.6
0.8
1.0
0
200
400
600
800
1000

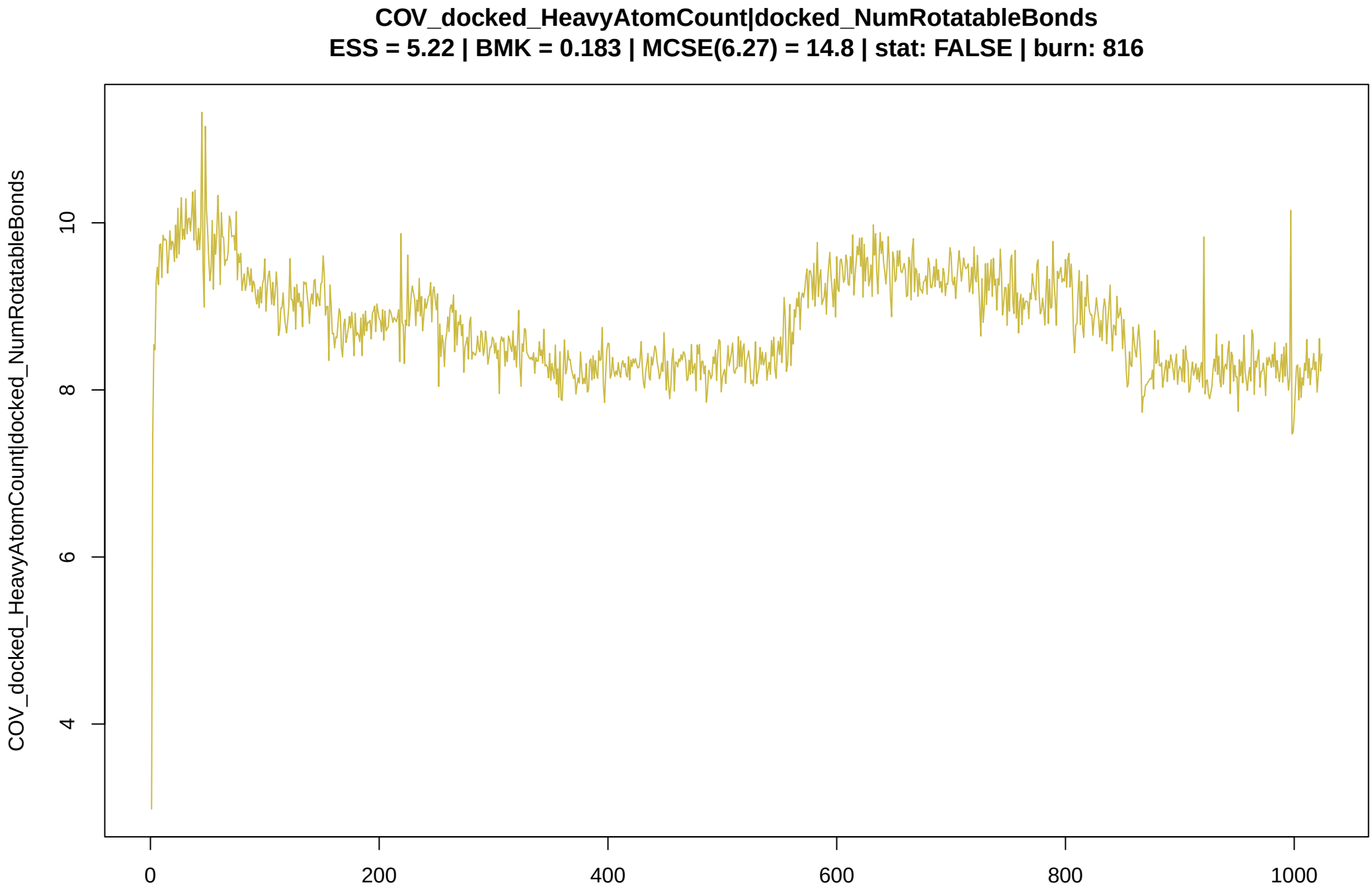

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 9.42 | BMK = 0.42 | MCSE(6.27) = 11 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
3
2
1
0
−1
−2
0
200
400
600
800
1000

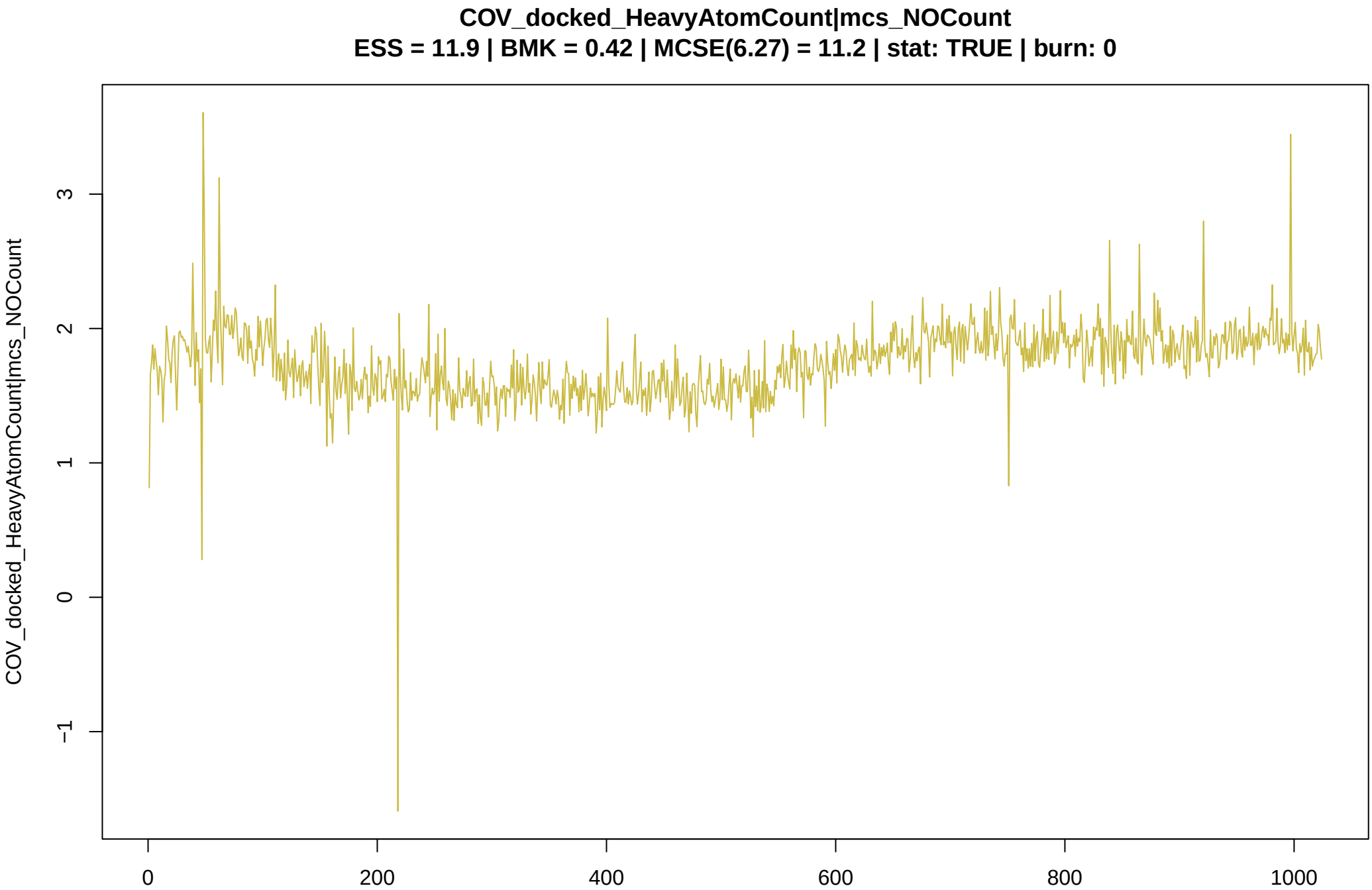

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 124 | BMK = 0.324 | MCSE(6.27) = 7.65 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.2
0.4
0.6
0.8
0
200
400
600
800
1000

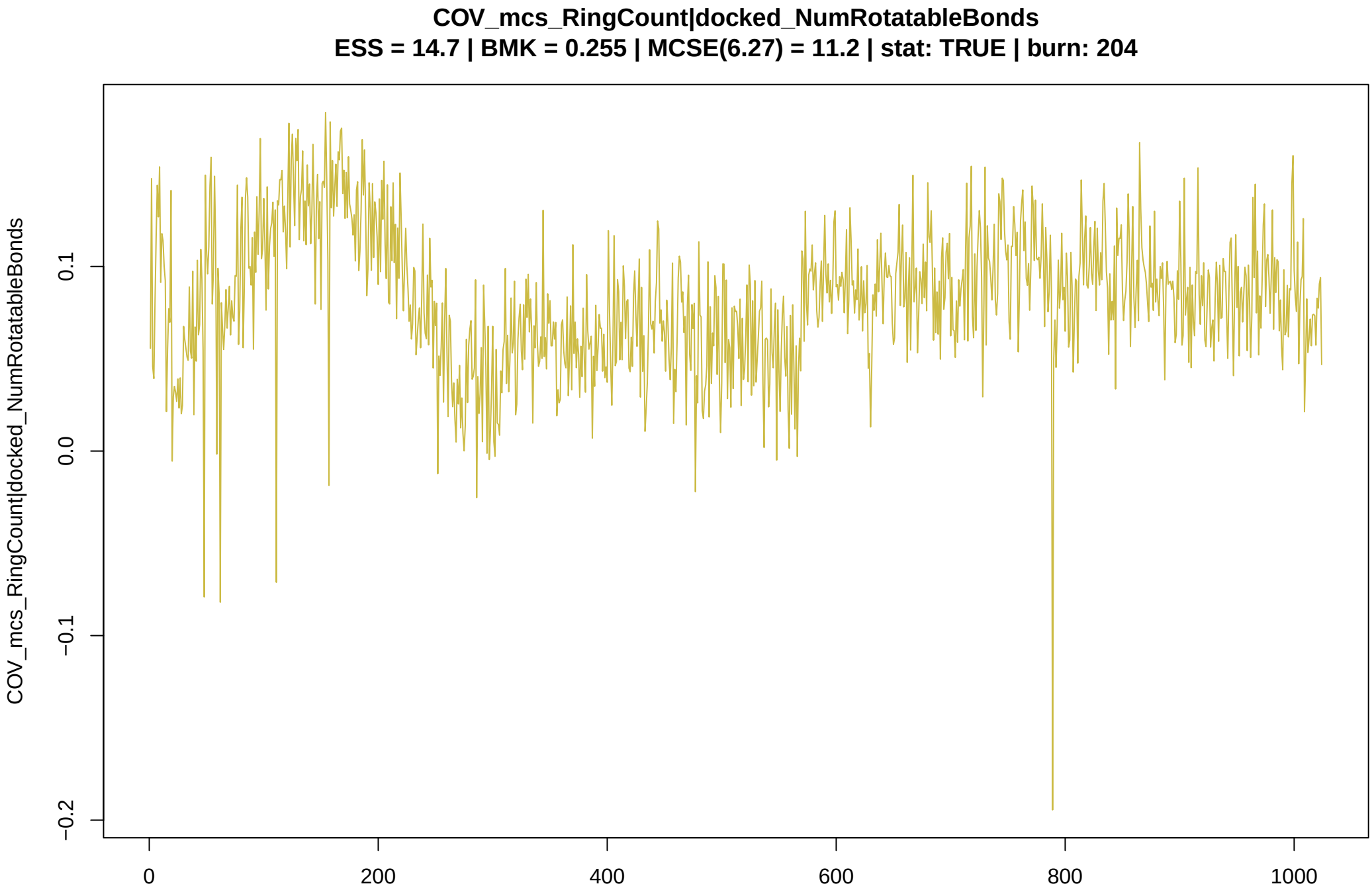

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 236 | BMK = 0.112 | MCSE(6.27) = 6.21 | stat: FALSE | burn: 0
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
0.5
0.0
−0.5
0
200
400
600
800
1000

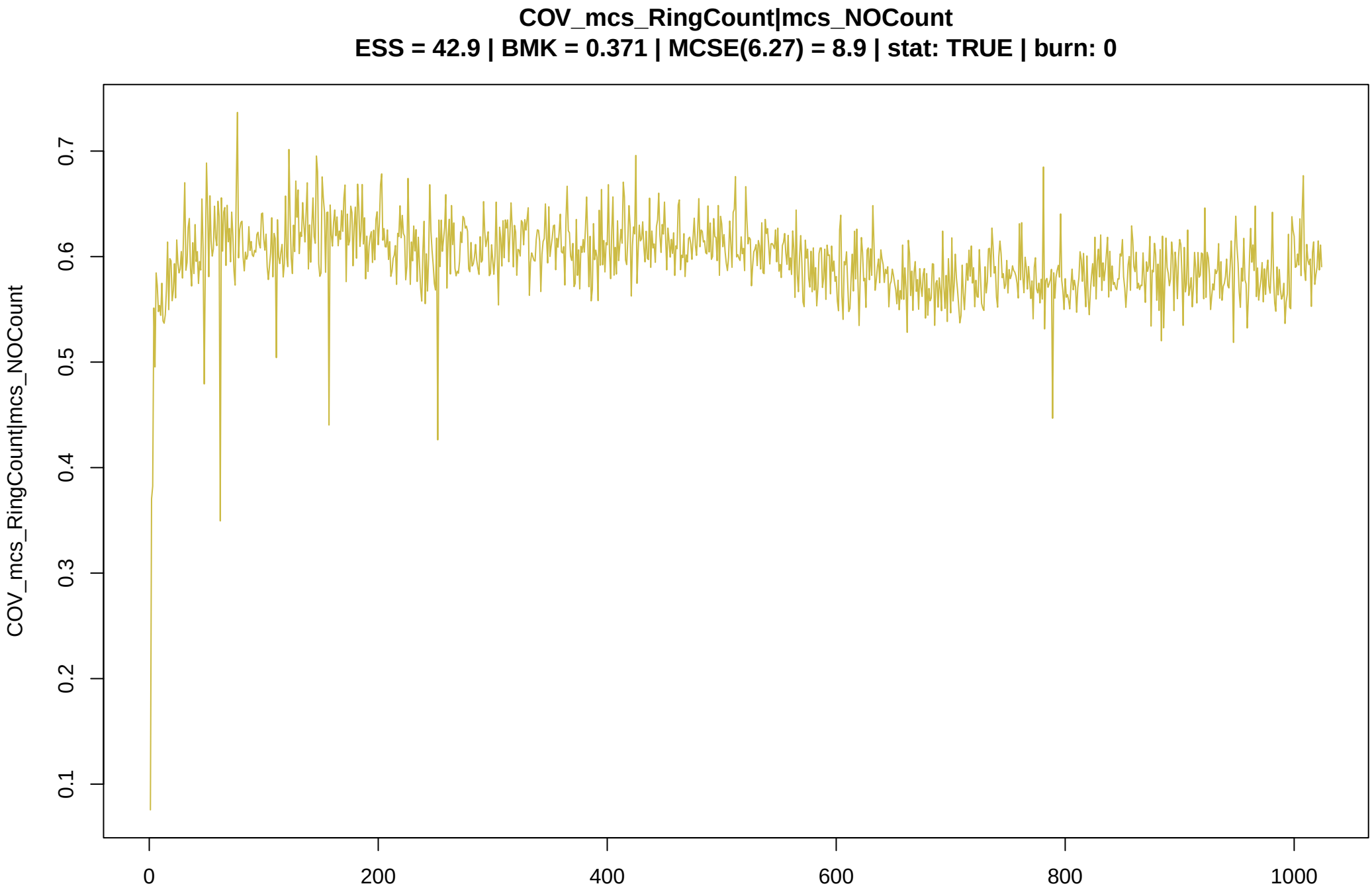

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 4.93 | BMK = 0.69 | MCSE(6.27) = 15.4 | stat: FALSE | burn: 612
COV_mcs_NumHeteroAtoms|mcs_NOCount
0.5
1.0
1.5
2.0
2.5
0
200
400
600
800
1000

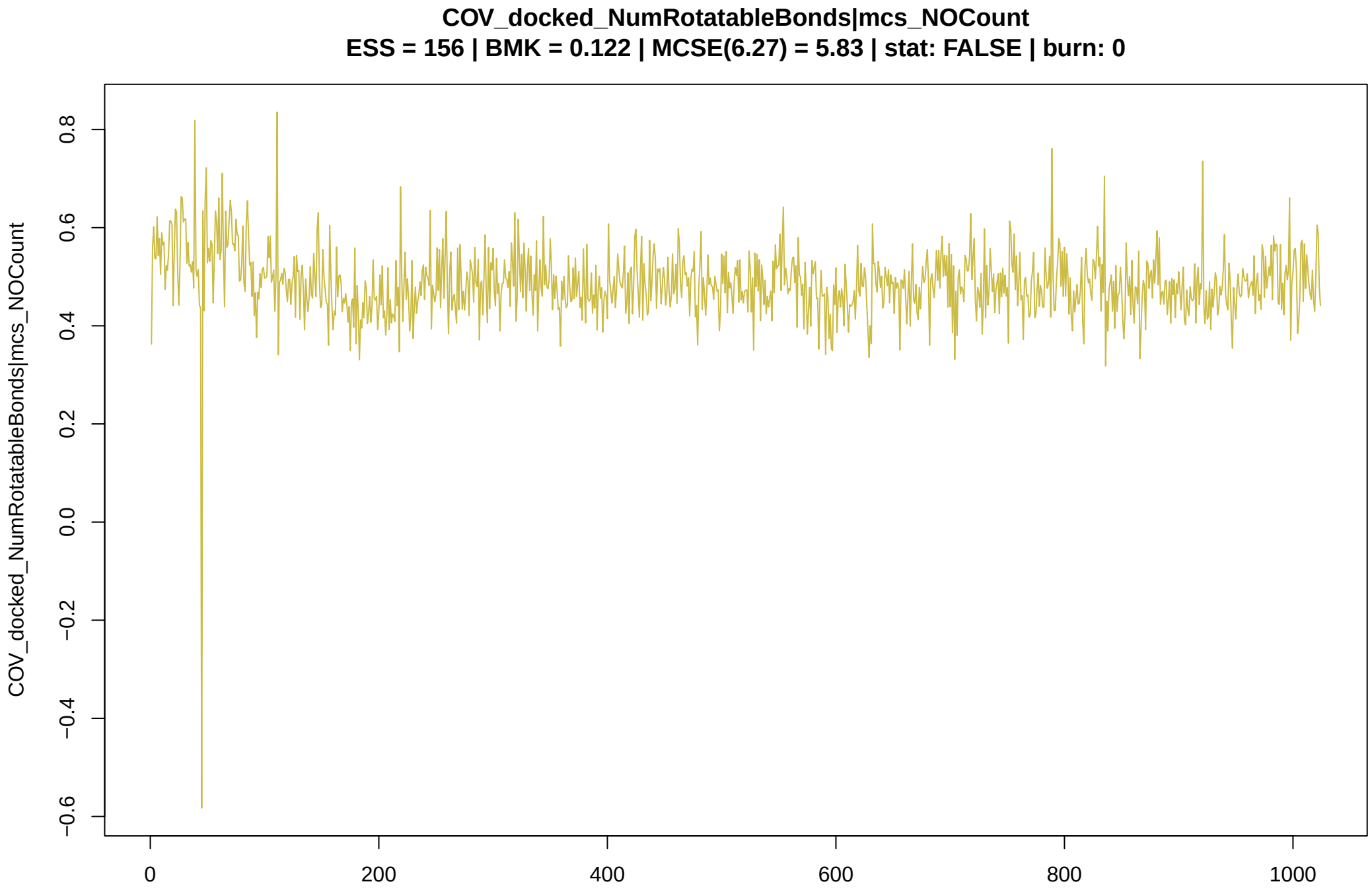

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 24.7 | BMK = 0.308 | MCSE(6.27) = 9.6 | stat: TRUE | burn: 102
COV_docked_HeavyAtomCount|mcs_RingCount
0.5
0.0
−0.5
−1.0
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 5.22 | BMK = 0.183 | MCSE(6.27) = 14.8 | stat: FALSE | burn: 816
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
4
6
8
10
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 11.9 | BMK = 0.42 | MCSE(6.27) = 11.2 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_NOCount
3
2
1
0
−1
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 14.7 | BMK = 0.255 | MCSE(6.27) = 11.2 | stat: TRUE | burn: 204
COV_mcs_RingCount|docked_NumRotatableBonds
0.1
0.0
−0.1
−0.2
0
200
400
600
800
1000


COV_mcs_RingCount|mcs_NOCount
ESS = 42.9 | BMK = 0.371 | MCSE(6.27) = 8.9 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_NOCount
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 156 | BMK = 0.122 | MCSE(6.27) = 5.83 | stat: FALSE | burn: 0
COV_docked_NumRotatableBonds|mcs_NOCount
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
0
200
400
600
800
1000