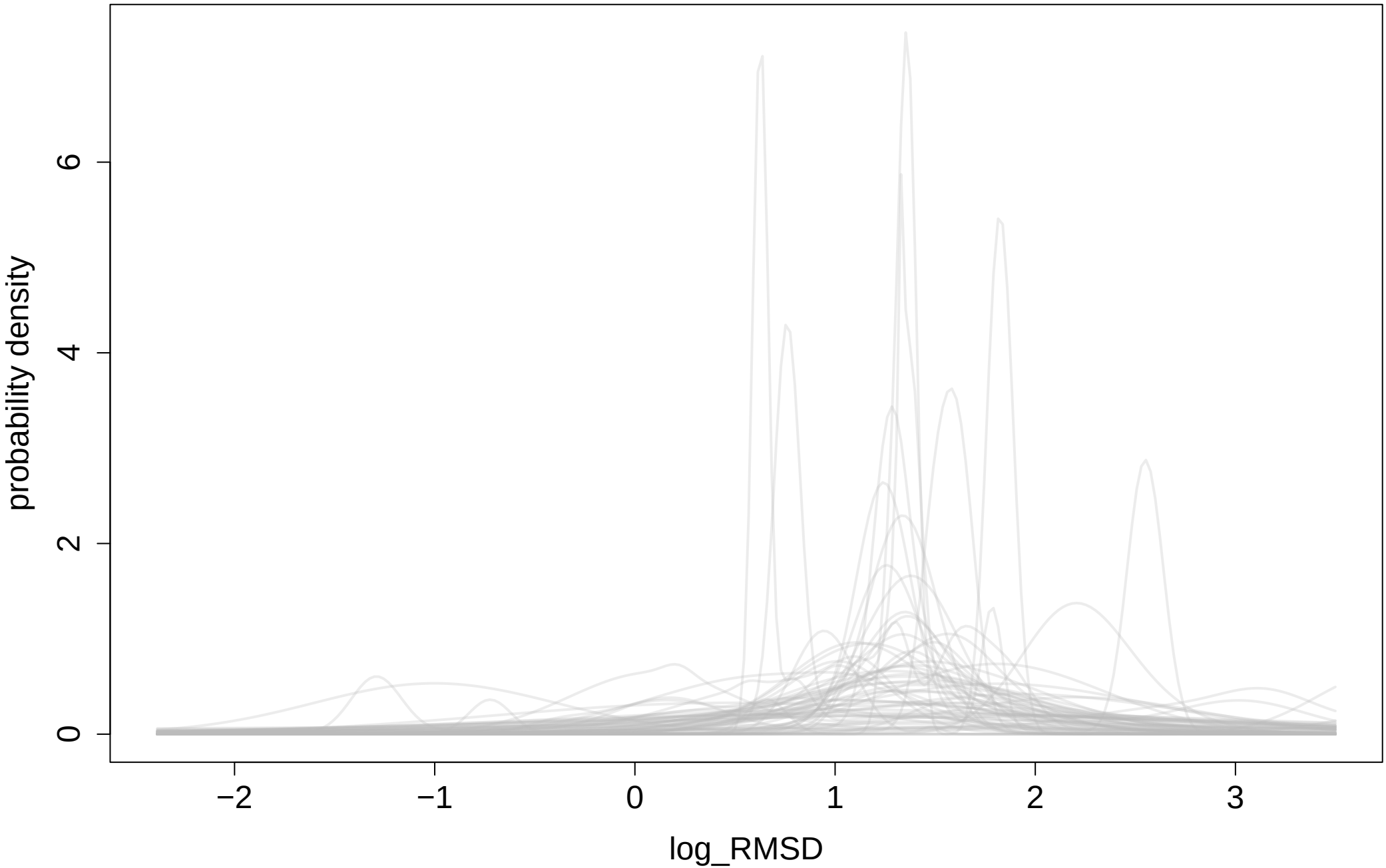
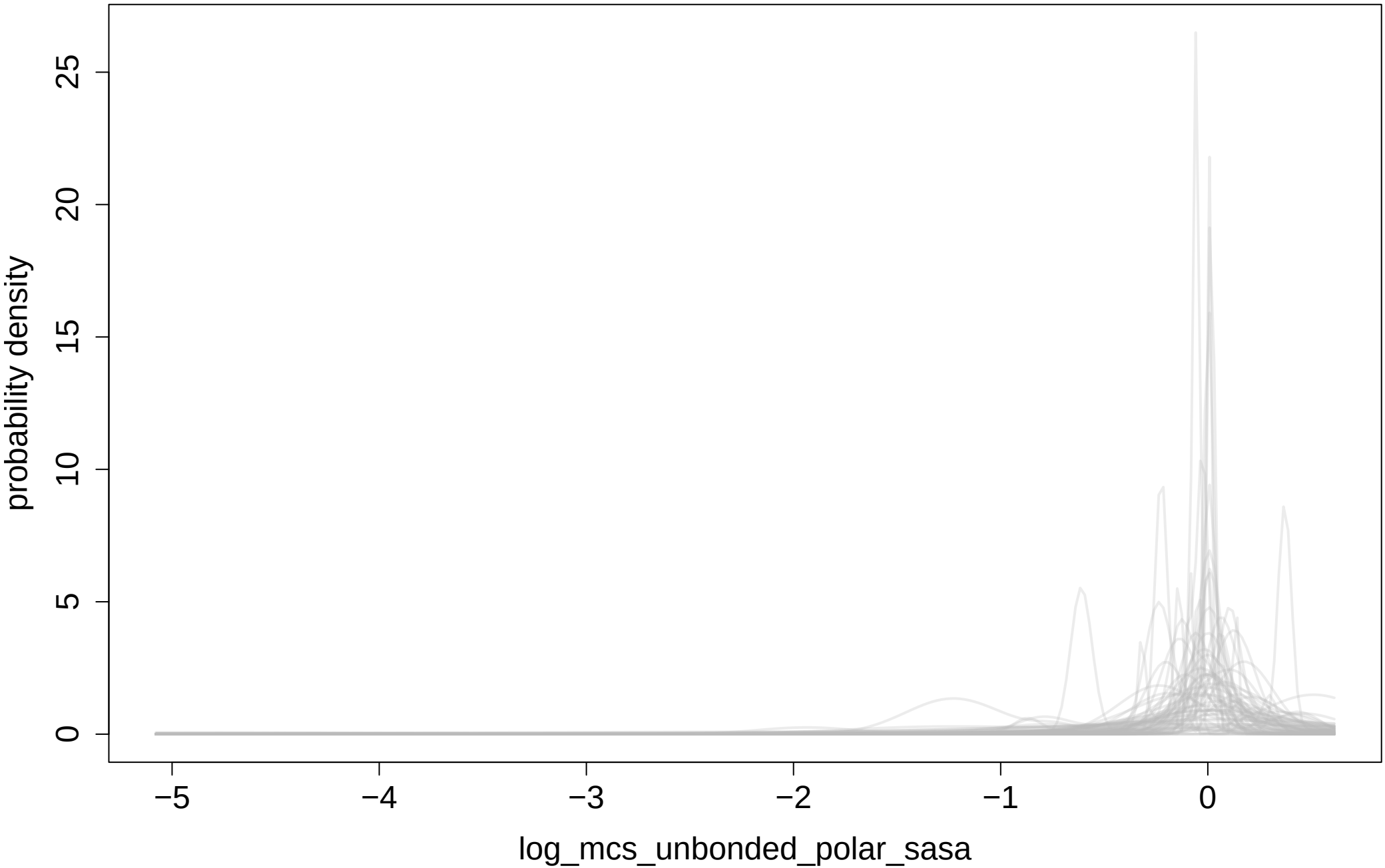
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 1
max MCSE = 4.00328574164155
all stationary: TRUE
burn: 1020

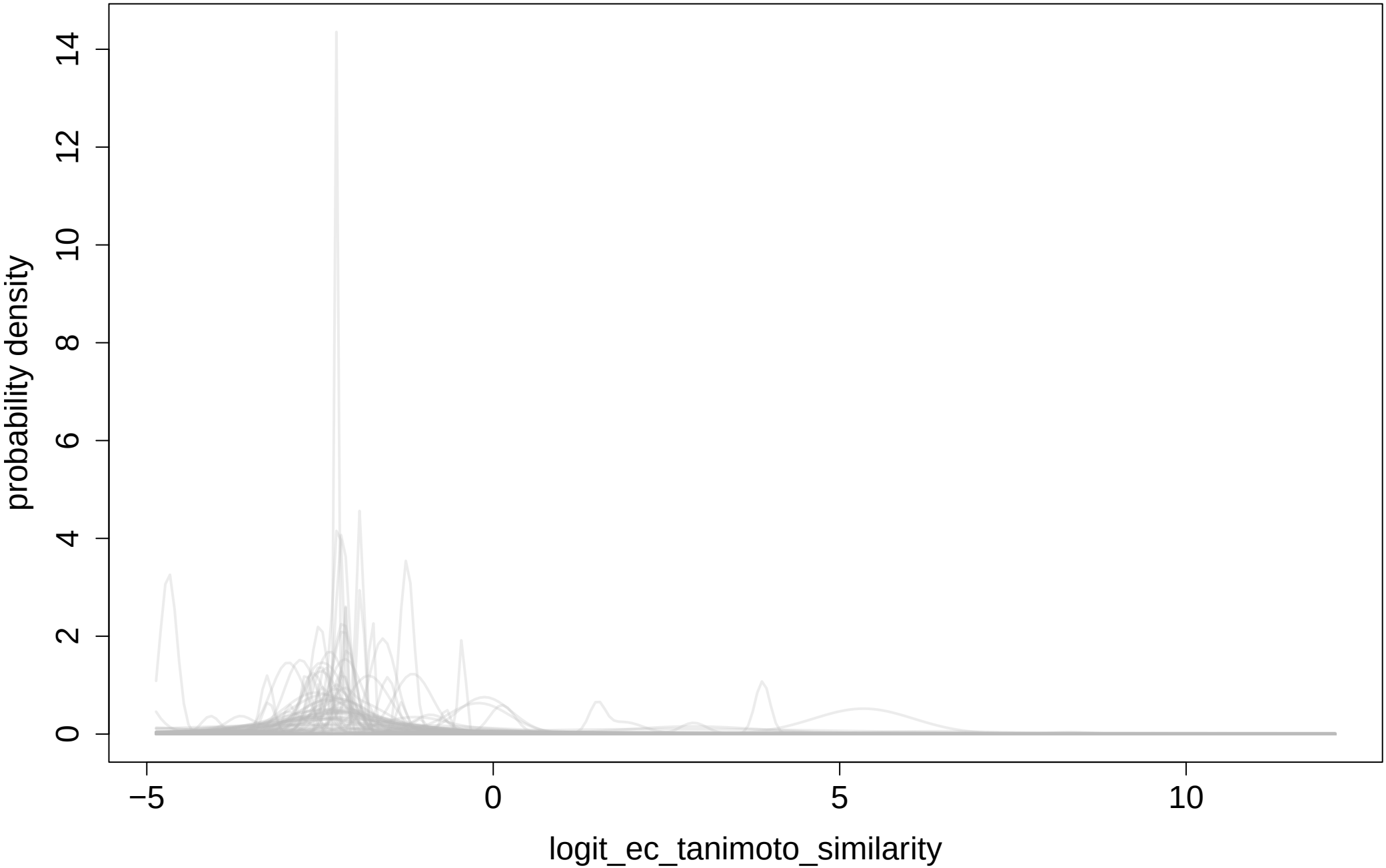
−− STATS 2D −−
min ESS = 500.936963397539
max BMK = 0.849250701829364
max MCSE = 4.13480046518136
all stationary: TRUE
burn: 816

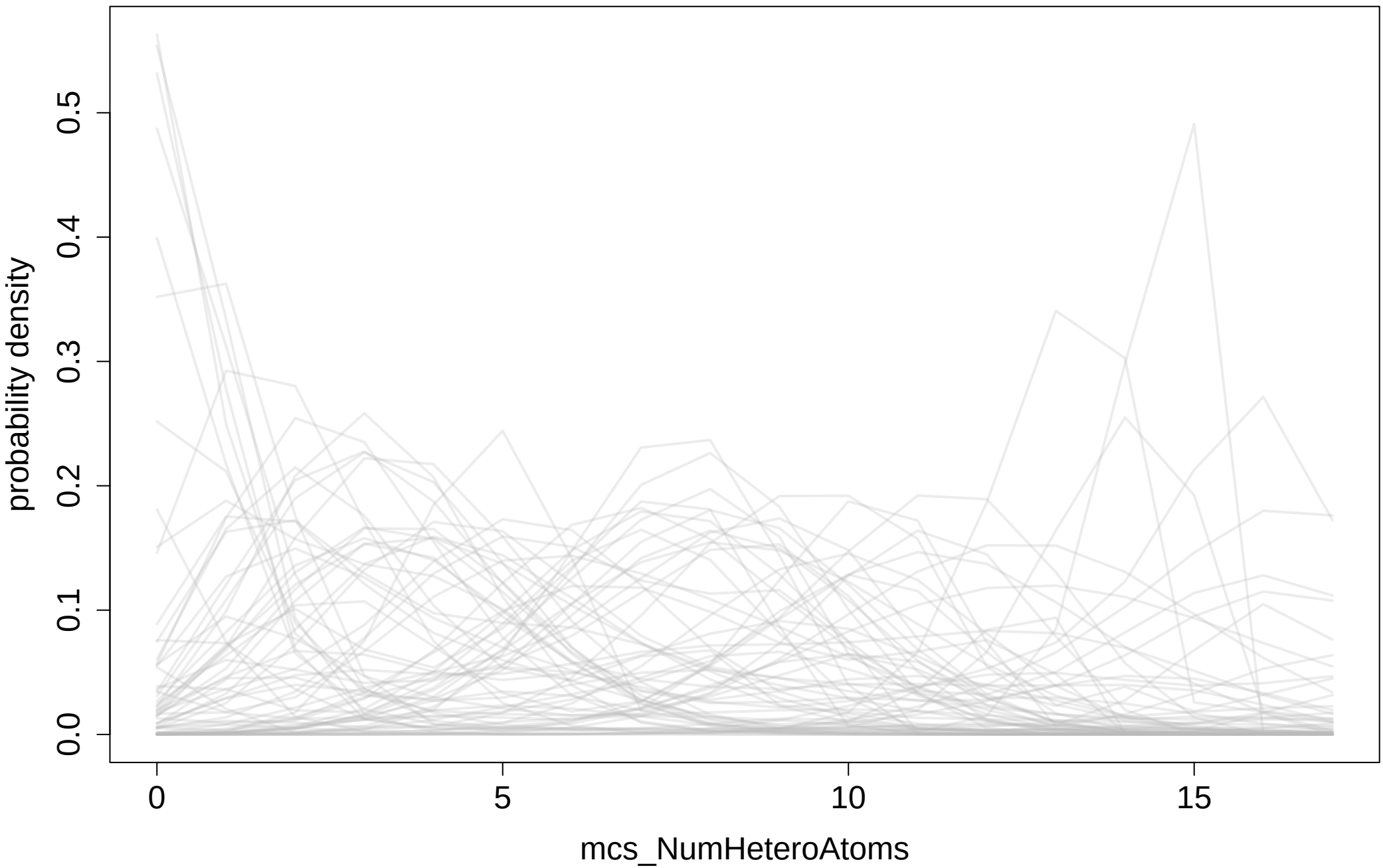
−− STATS 1D −−
min ESS = 718.074274097692
max BMK = 1
max MCSE = 4.01345244171101
all stationary: FALSE
burn: 1020

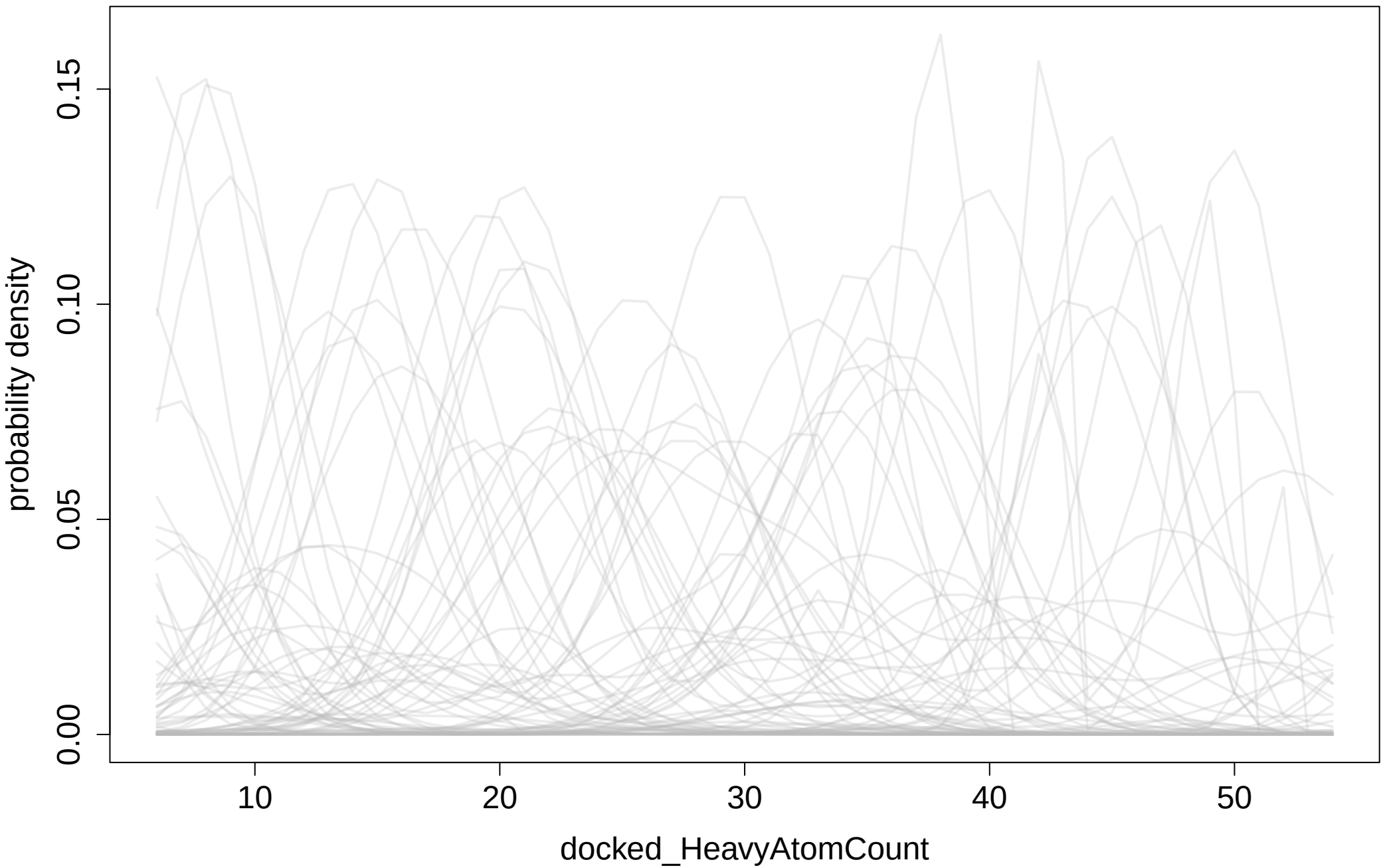
Occupied clusters: 0 of 64
LL: −Inf +− NaN

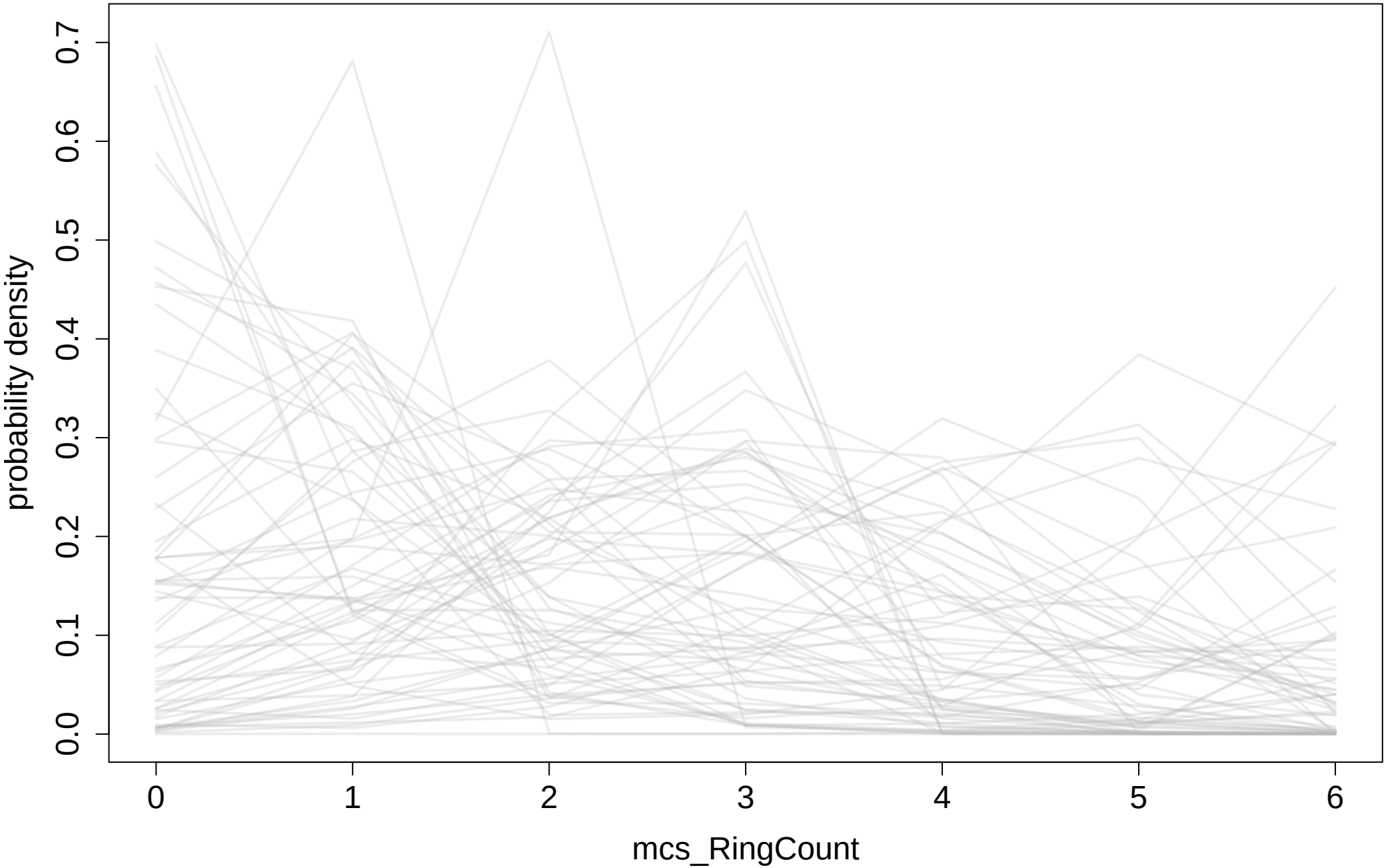

probability density
0
2
4
6
−2
−1
0
1
2
3
log_RMSD

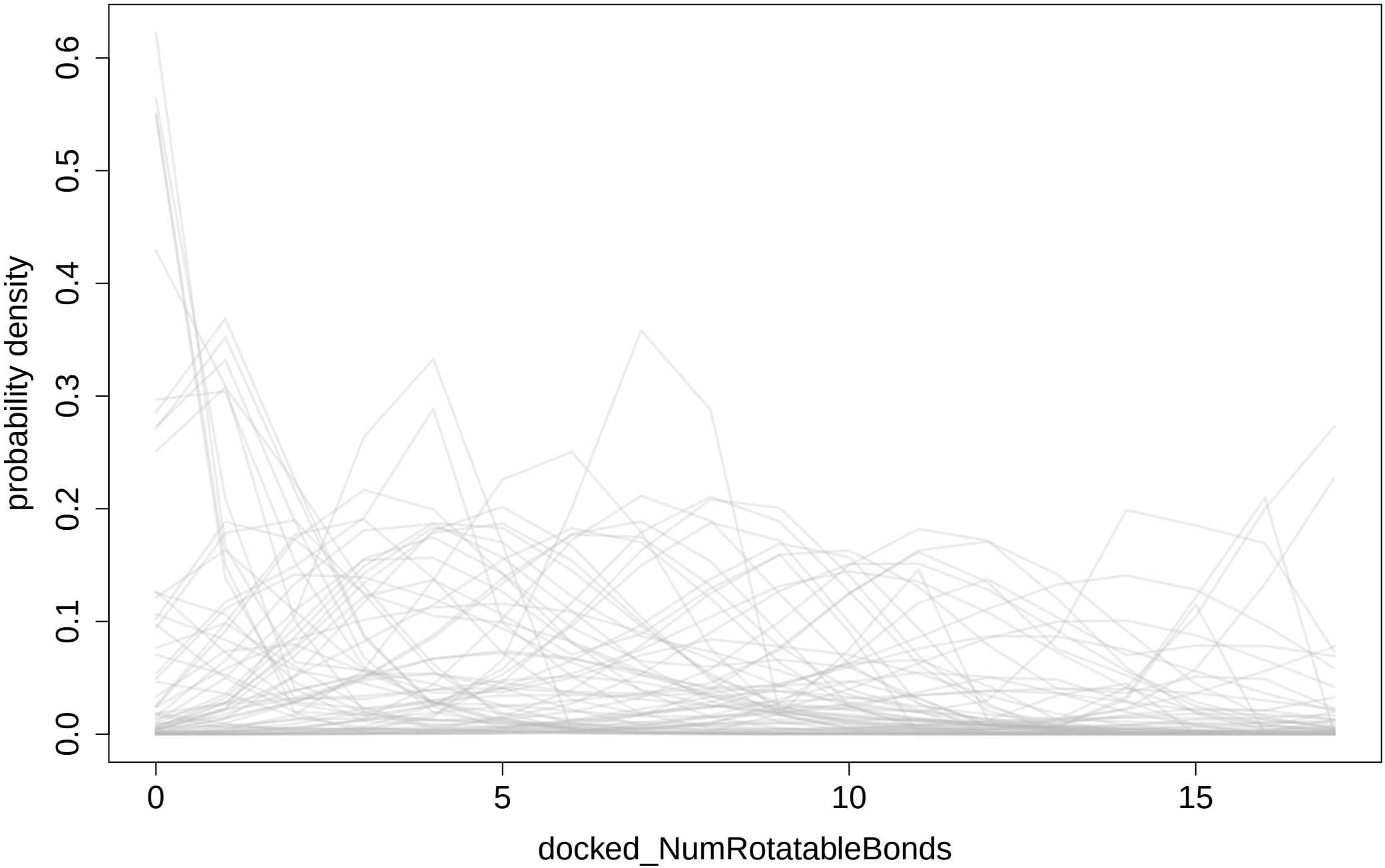

probability density
0
5
10
15
20
25
−5
−4
−3
−2
−1
0
log_mcs_unbonded_polar_sasa

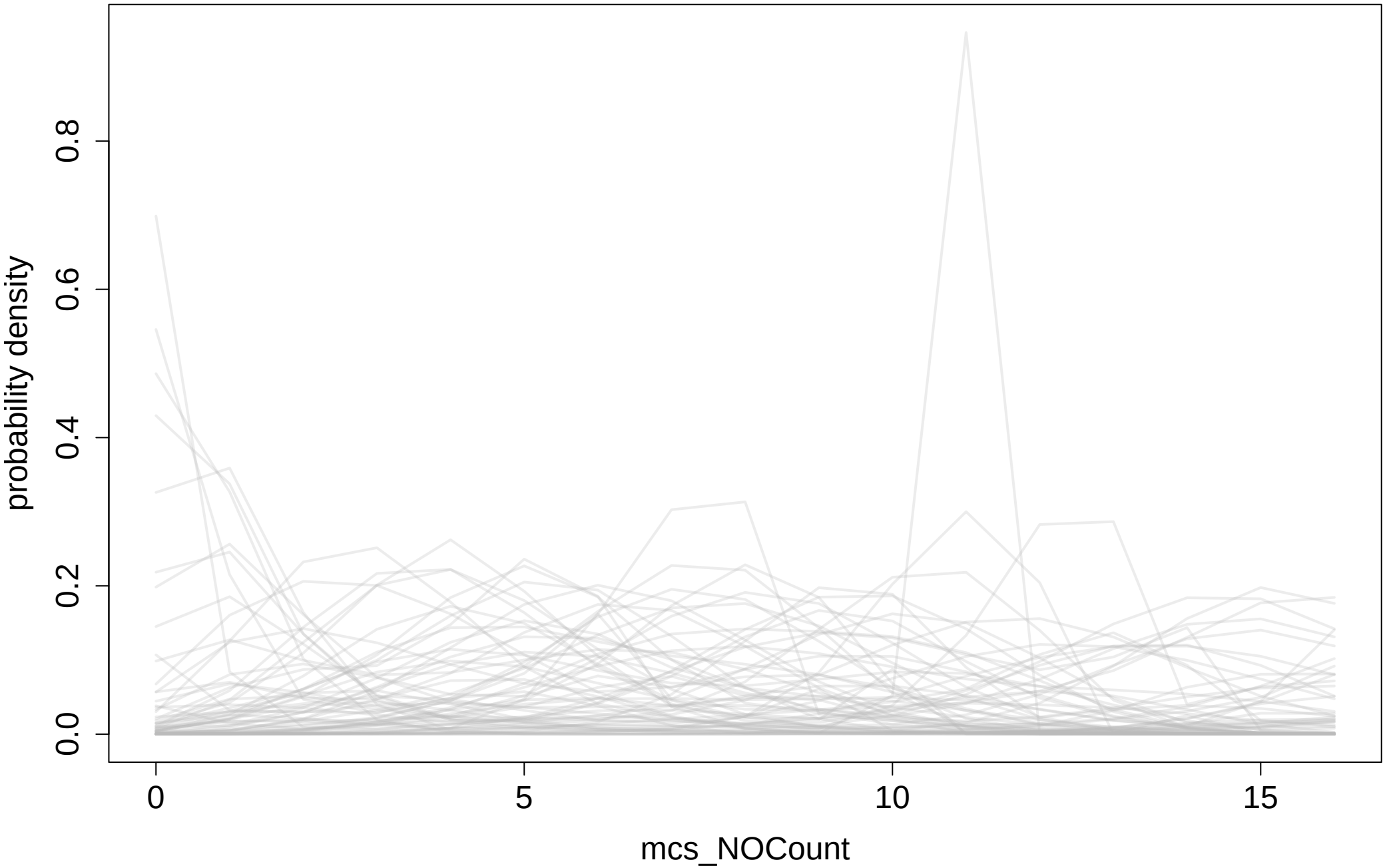

probability density
0
2
4
6
8
10
12
14
−5
0
5
10
logit_ec_tanimoto_similarity

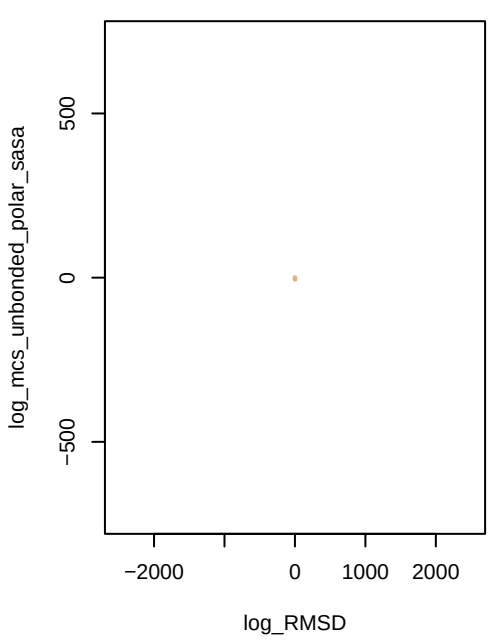

probability density
0.0
0.1
0.2
0.3
0.4
0.5
0
5
10
15
mcs_NumHeteroAtoms

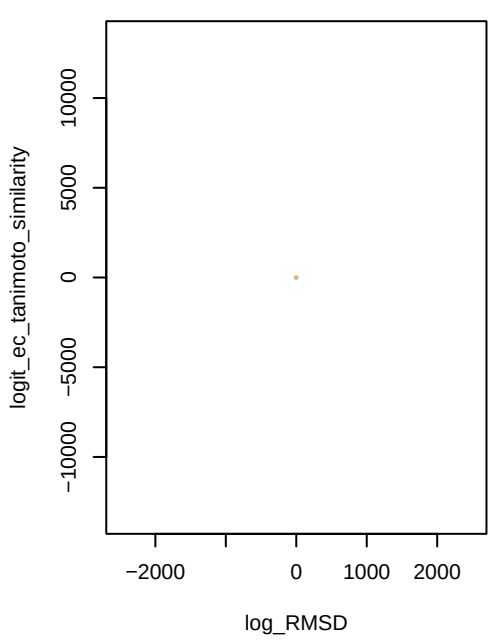

probability density
0.00
0.05
0.10
0.15
10
20
30
40
50
docked_HeavyAtomCount

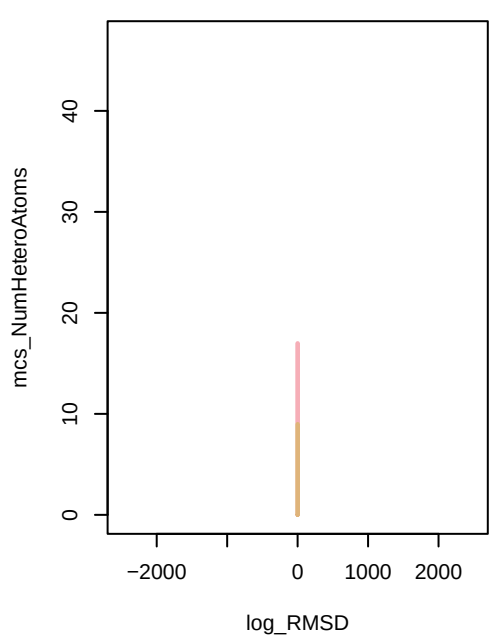

probability density
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
1
2
3
4
5
6
mcs_RingCount

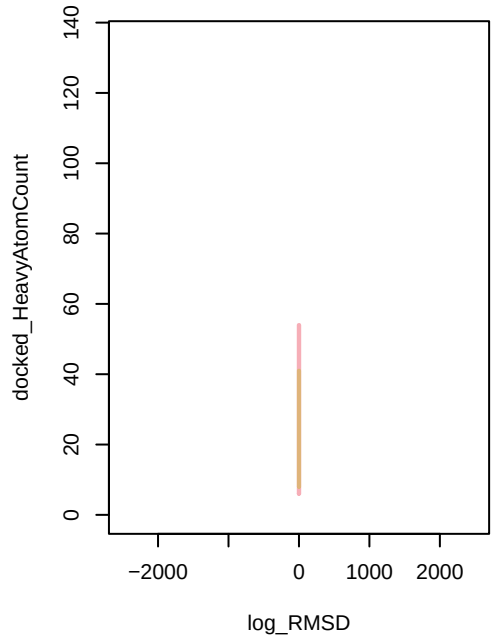

probability density
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0
5
10
15
docked_NumRotatableBonds

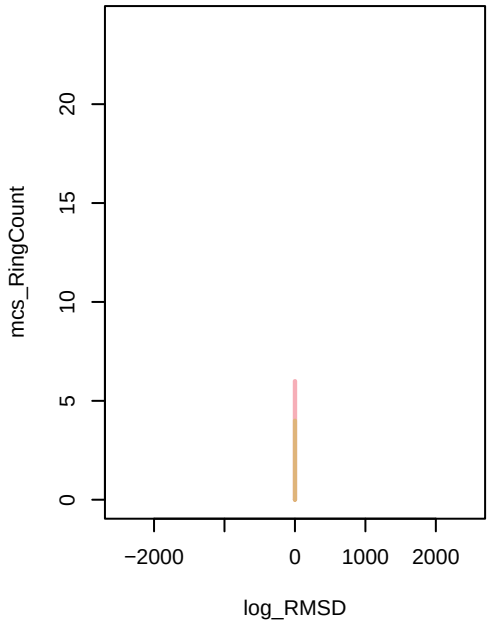

probability density
0.0
0.2
0.4
0.6
0.8
0
5
10
15
mcs_NOCount

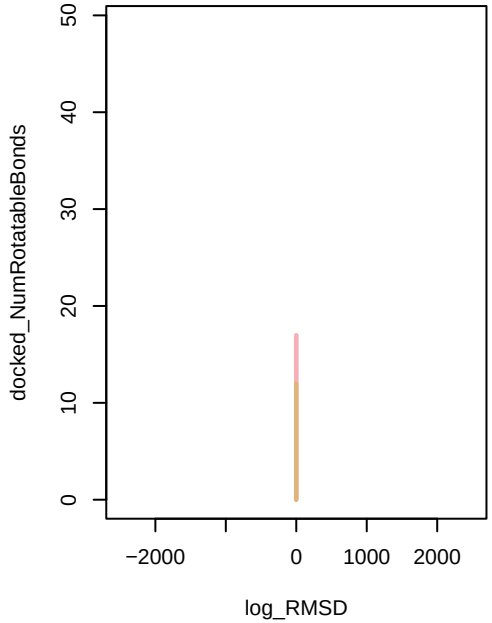

log_mcs_unbonded_polar_sasa
500
0
−500
−2000
0
1000
2000
log_RMSD

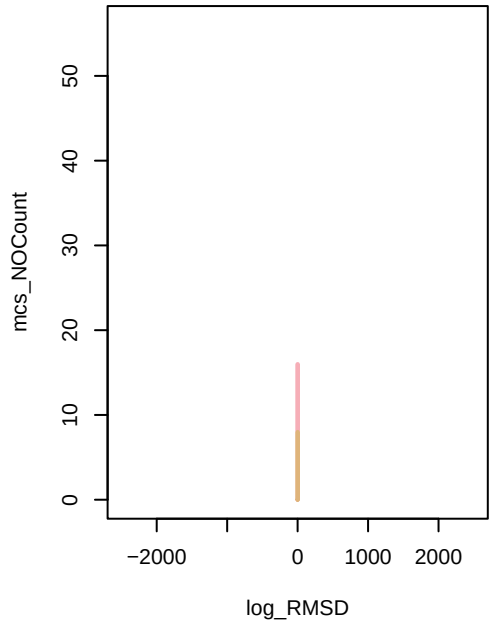

logit_ec_tanimoto_similarity
10000
5000
0
−5000
−10000
−2000
0
1000
2000
log_RMSD

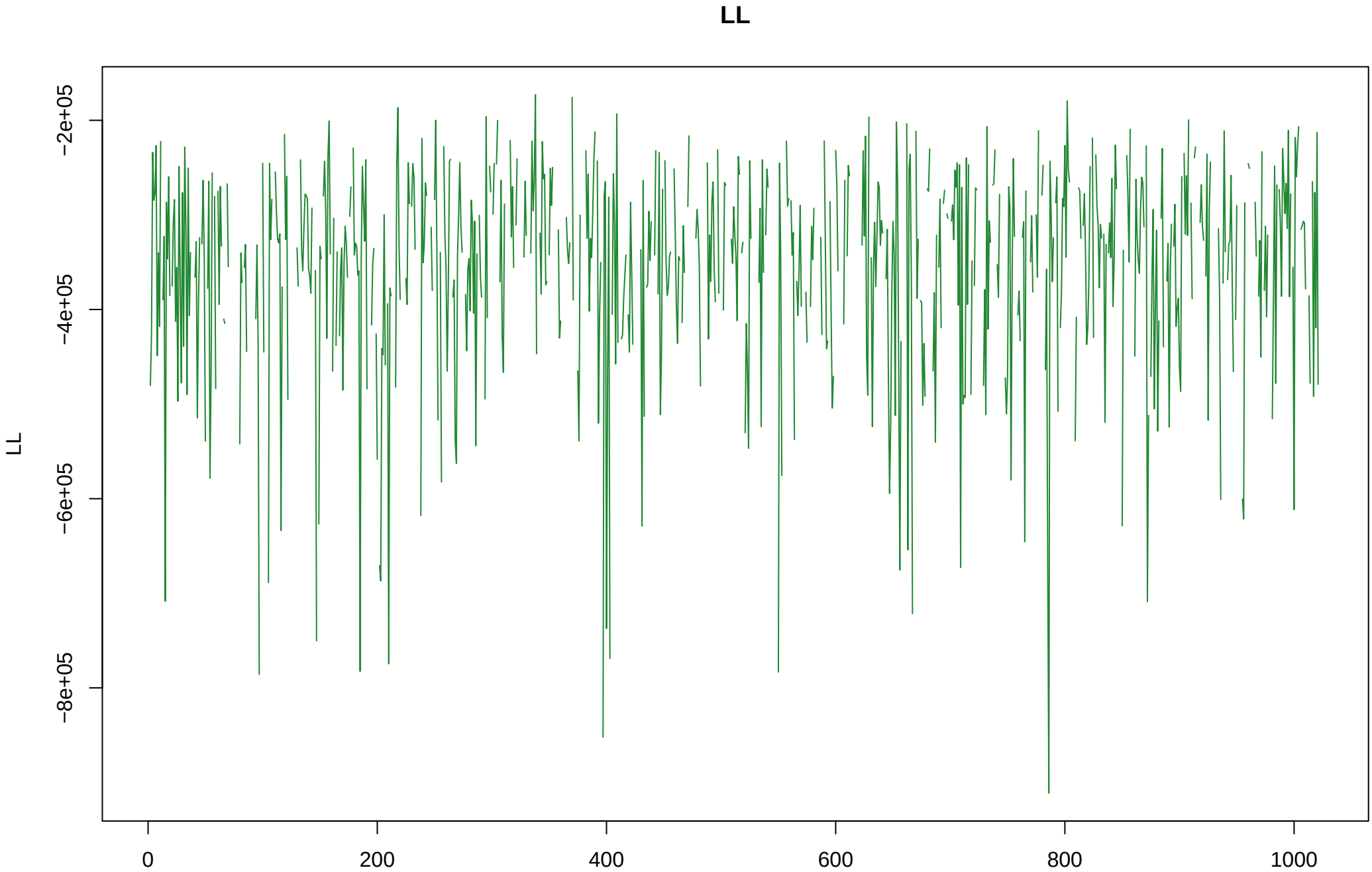

mcs_NumHeteroAtoms
40
30
20
10
0
−2000
0
1000
2000
log_RMSD

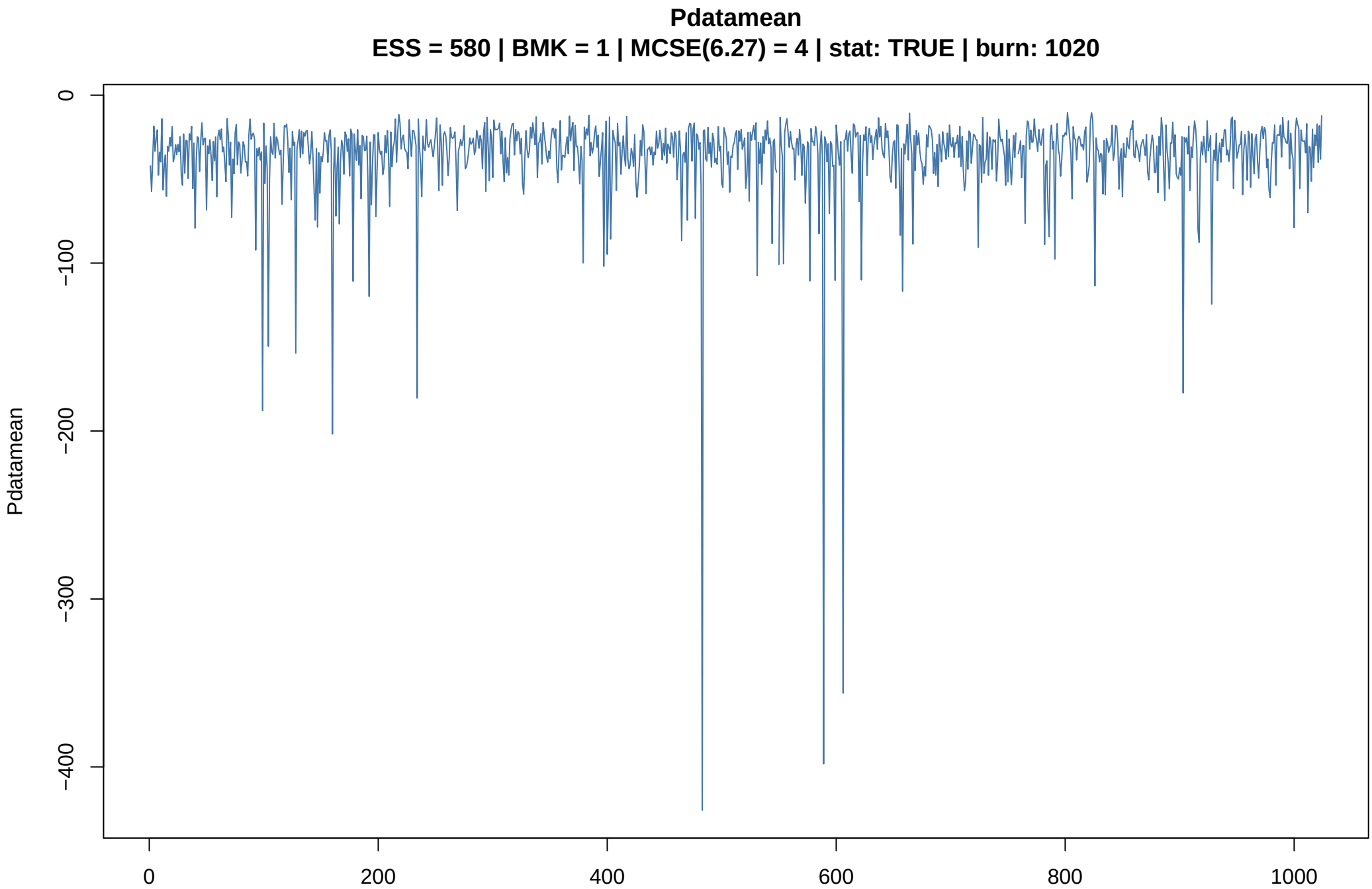

docked_HeavyAtomCount
140
120
100
80
60
40
20
0
−2000
0
1000
2000
log_RMSD

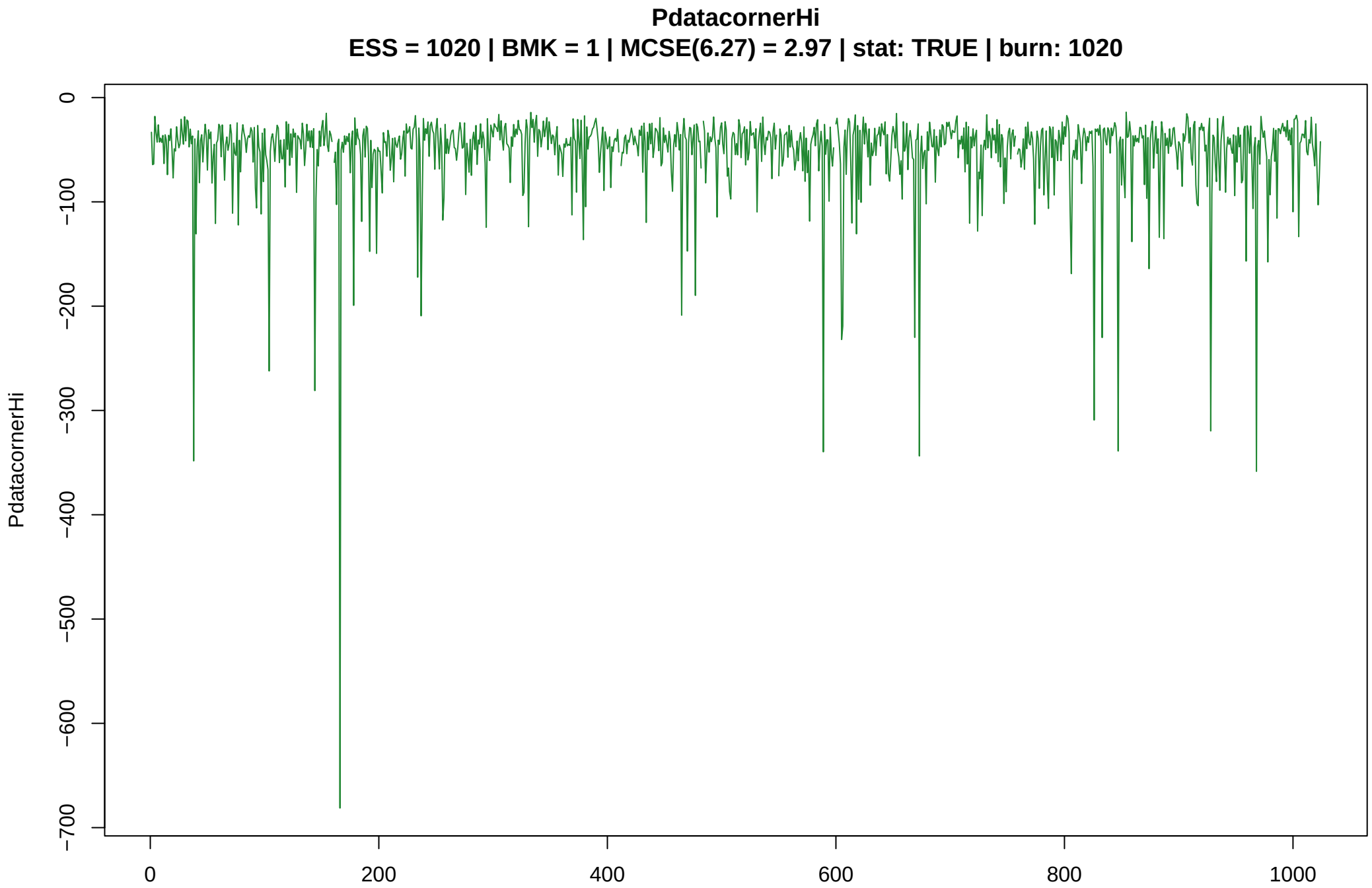

mcs_RingCount
20
15
10
5
0
−2000
0
1000
2000
log_RMSD

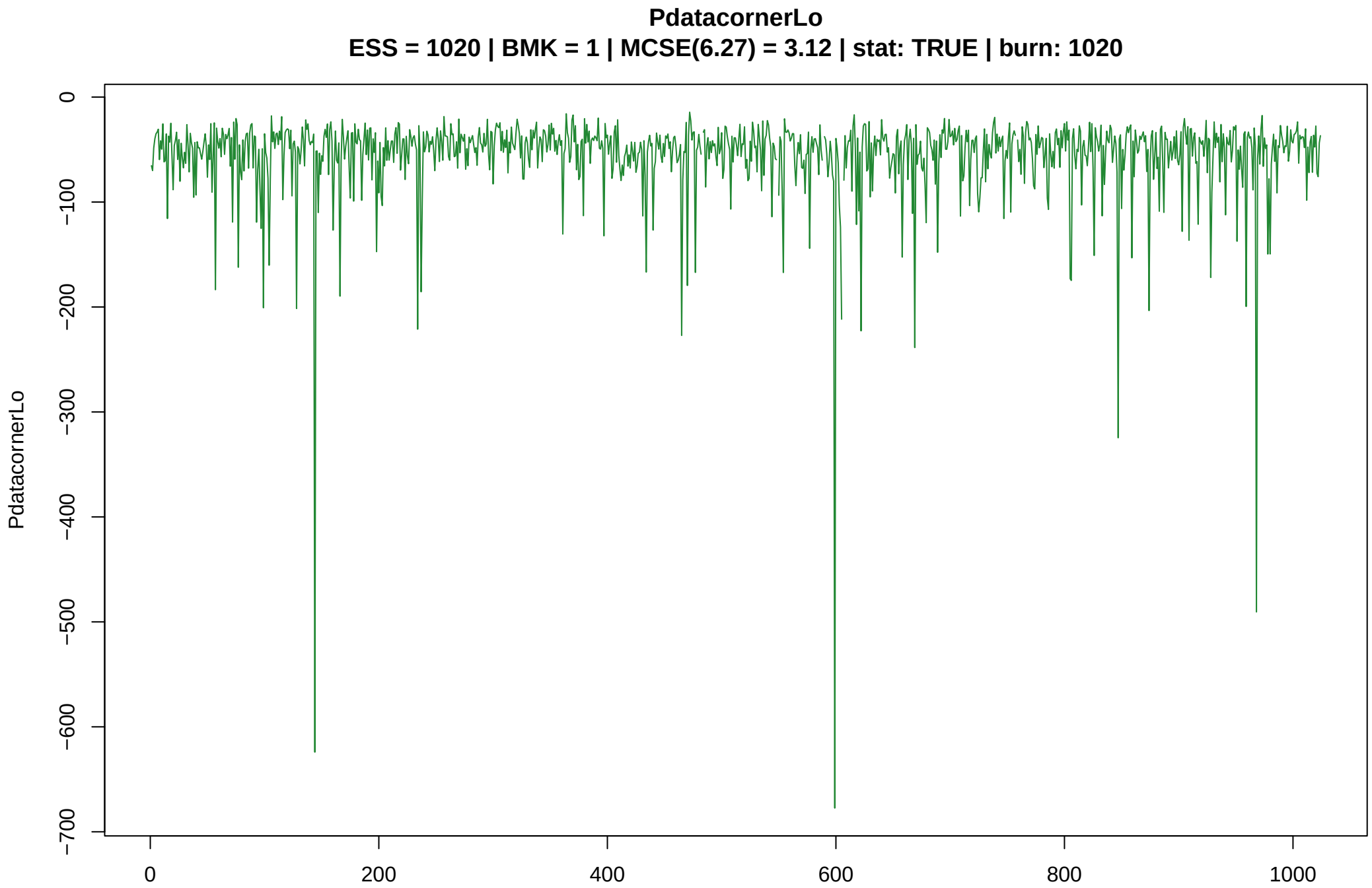

docked_NumRotatableBonds
50
40
30
20
10
0
−2000
0
1000
2000
log_RMSD

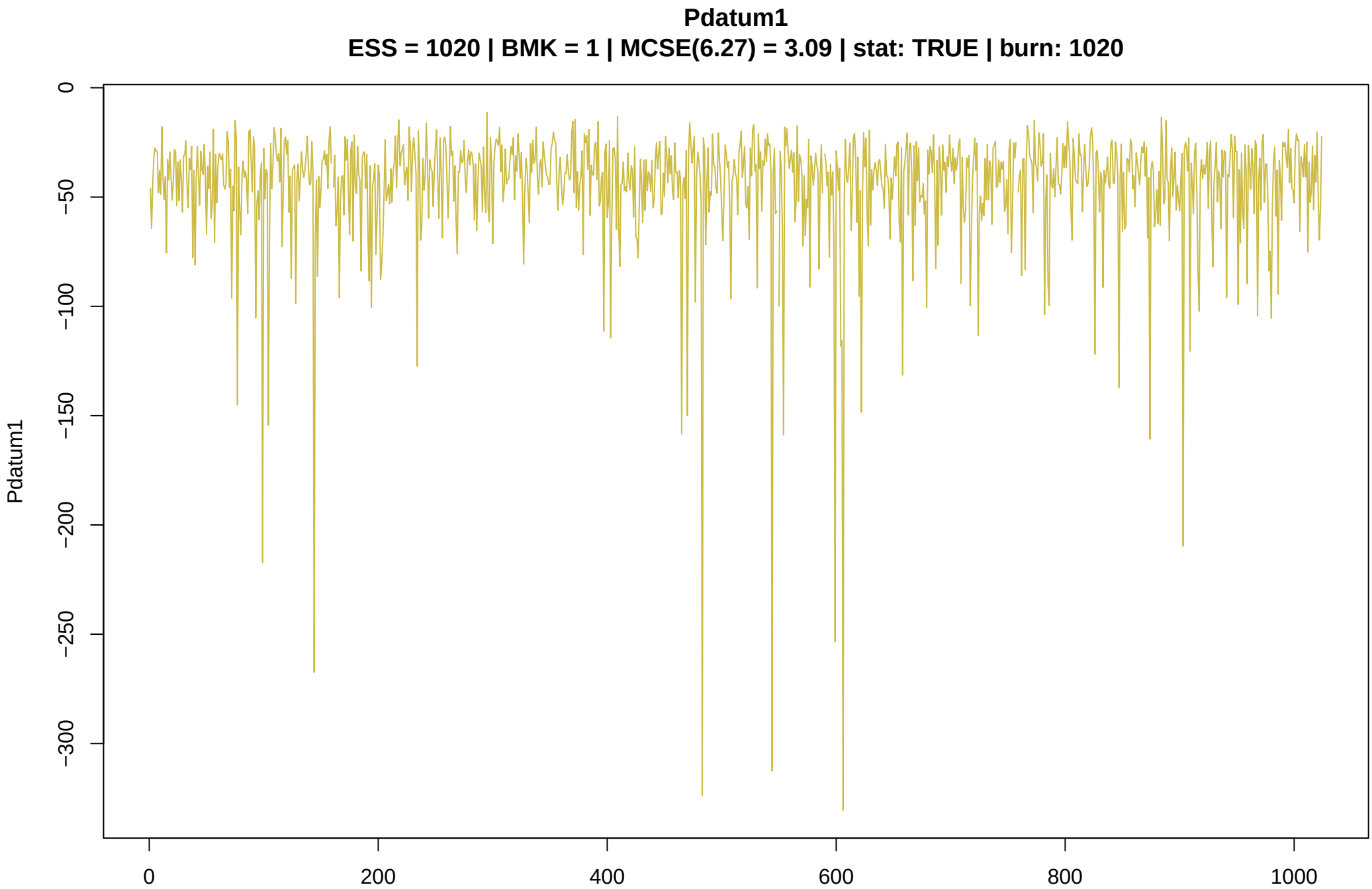

mcs_NOCount
50
40
30
20
10
0
−2000
0
1000
2000
log_RMSD

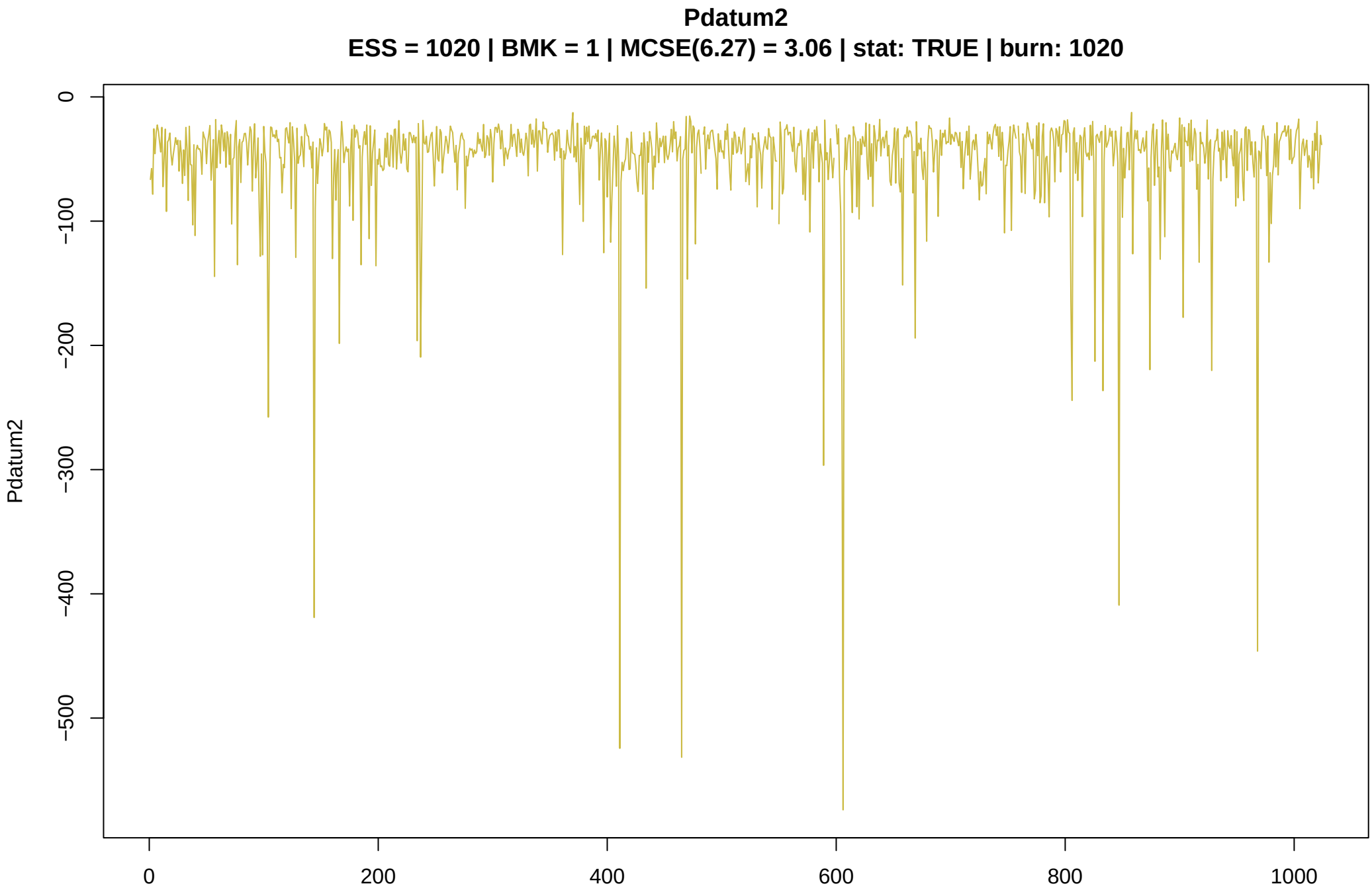

LL
LL
−2e+05
−4e+05
−6e+05
−8e+05
0
200
400
600
800
1000

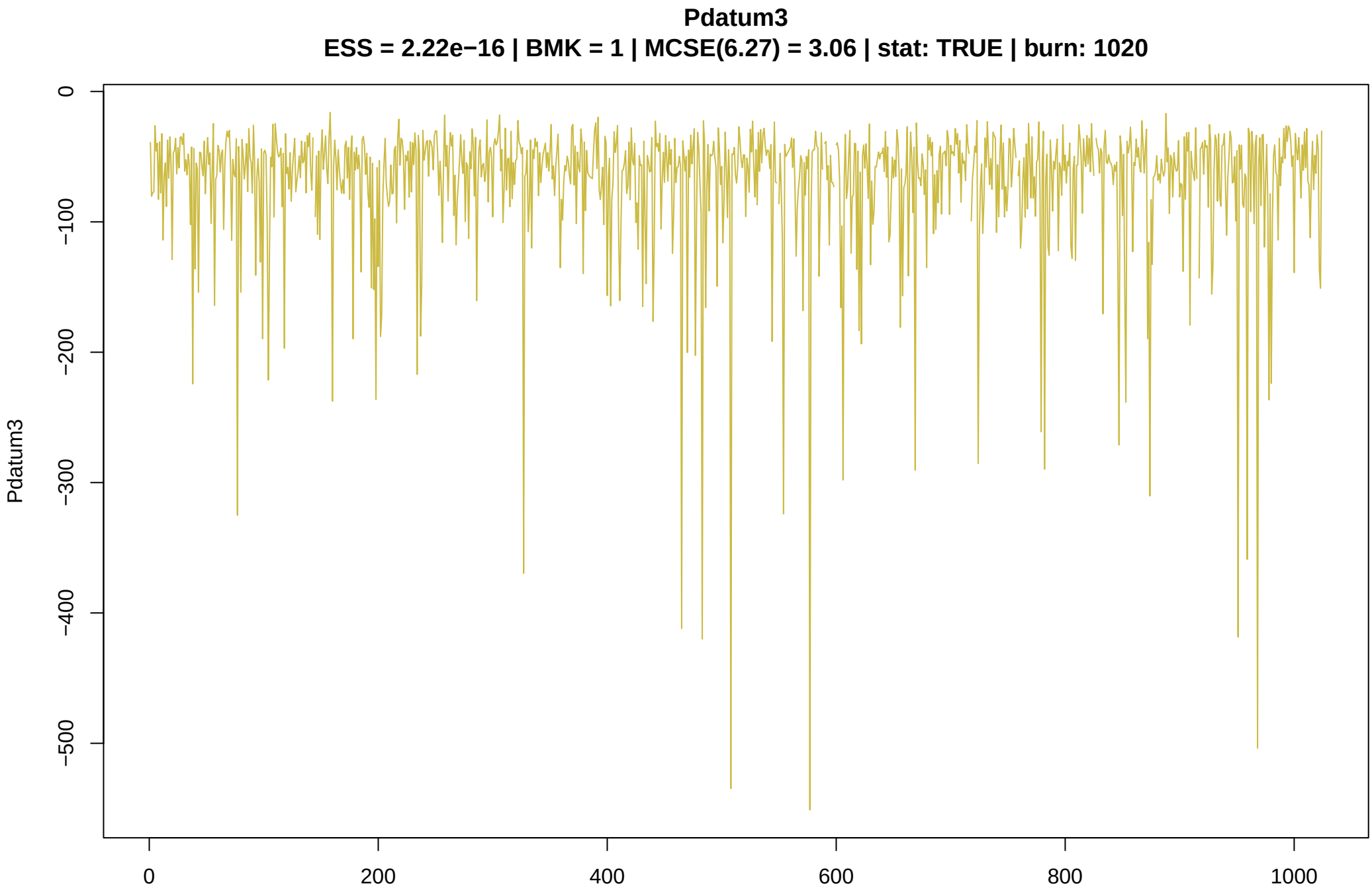

Pdatamean
ESS = 580 | BMK = 1 | MCSE(6.27) = 4 | stat: TRUE | burn: 1020
Pdatamean
0
−100
−200
−300
−400
0
200
400
600
800
1000

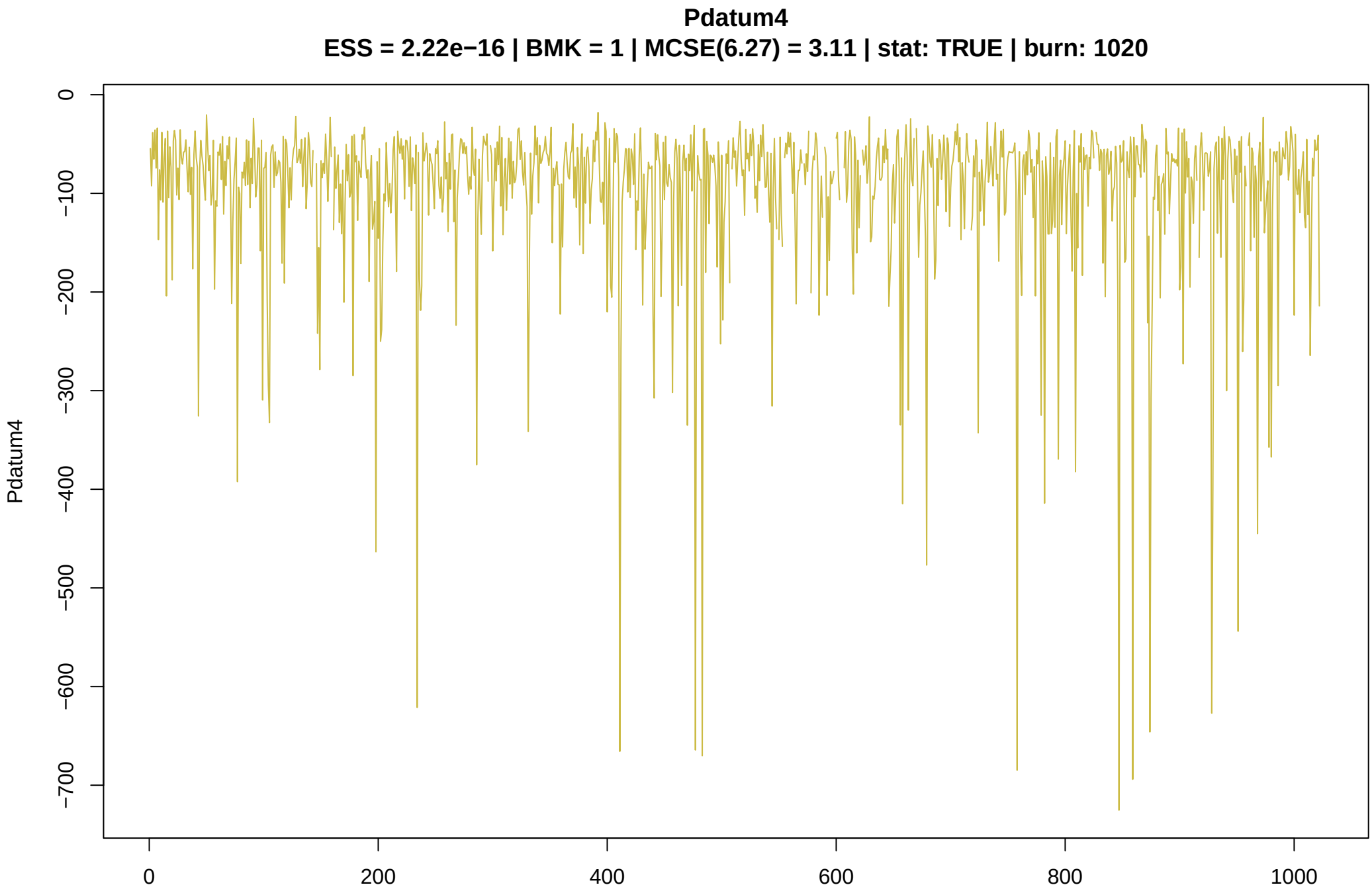

PdatacornerHi
ESS = 1020 | BMK = 1 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 1020
PdatacornerHi
0
−100
−200
−300
−400
−500
−600
−700
0
200
400
600
800
1000

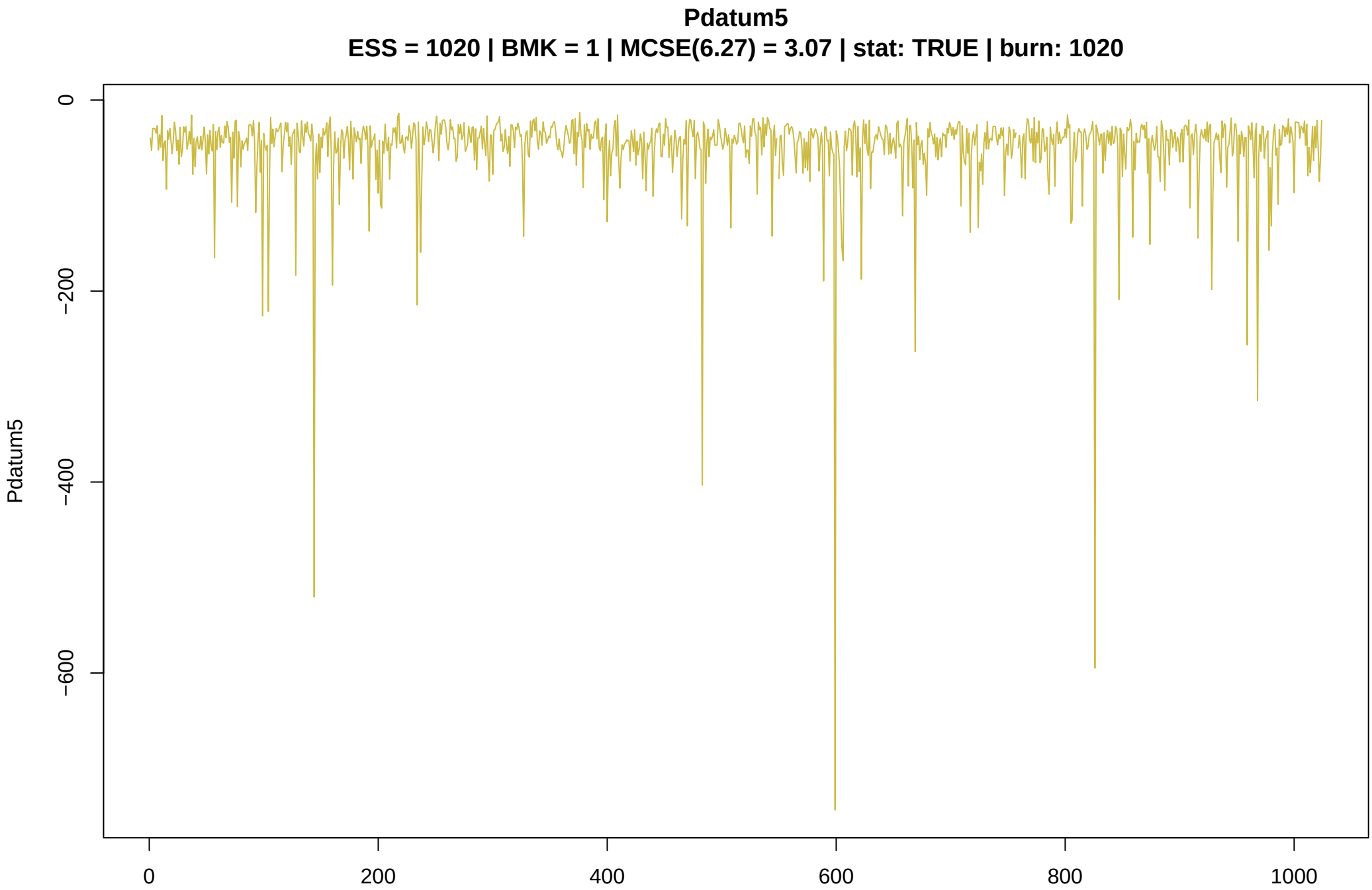

PdatacornerLo
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 1020
PdatacornerLo
0
−100
−200
−300
−400
−500
−600
−700
0
200
400
600
800
1000

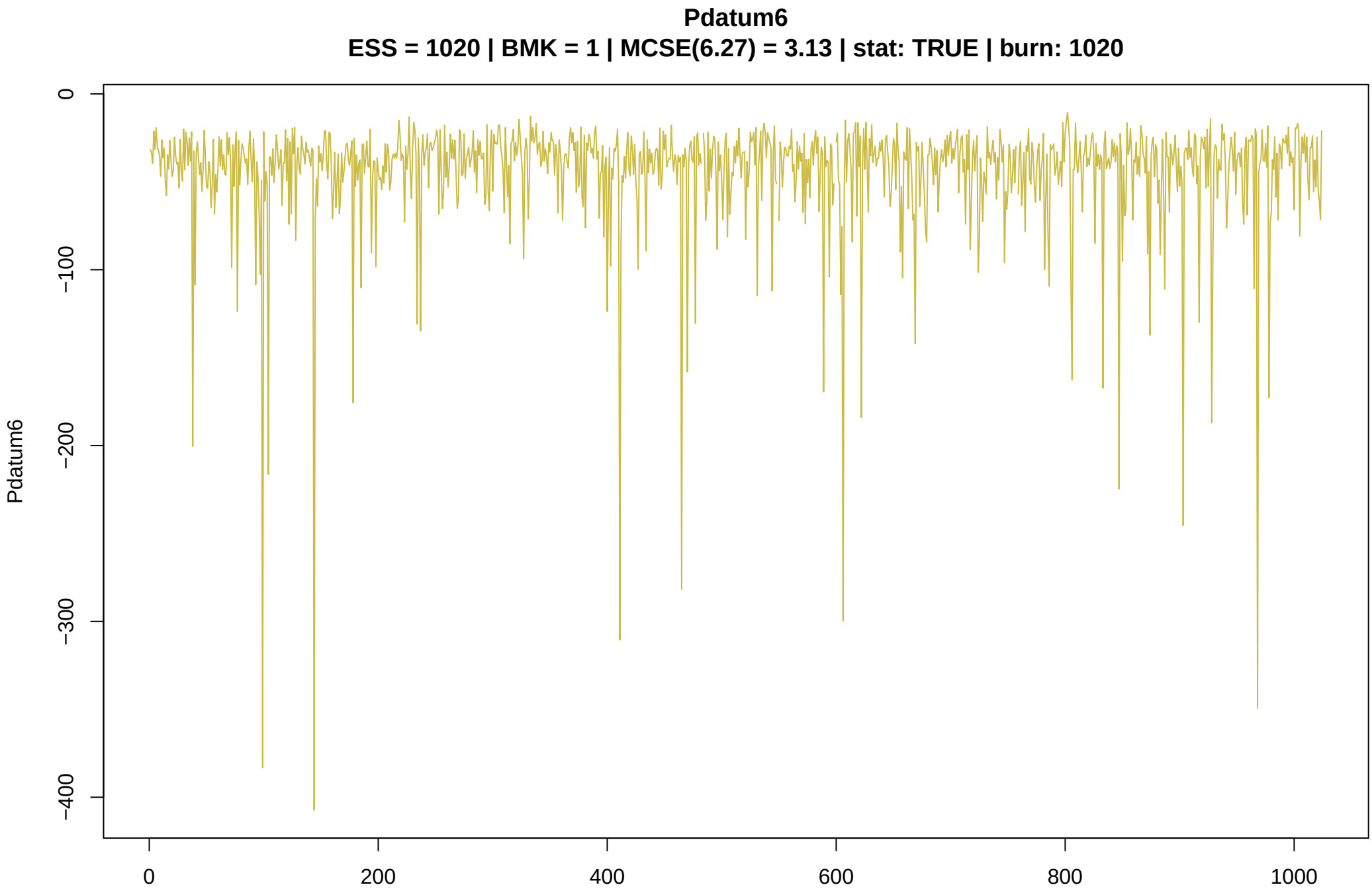

Pdatum1
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 1020
Pdatum1
0
−50
−100
−150
−200
−250
−300
0
200
400
600
800
1000

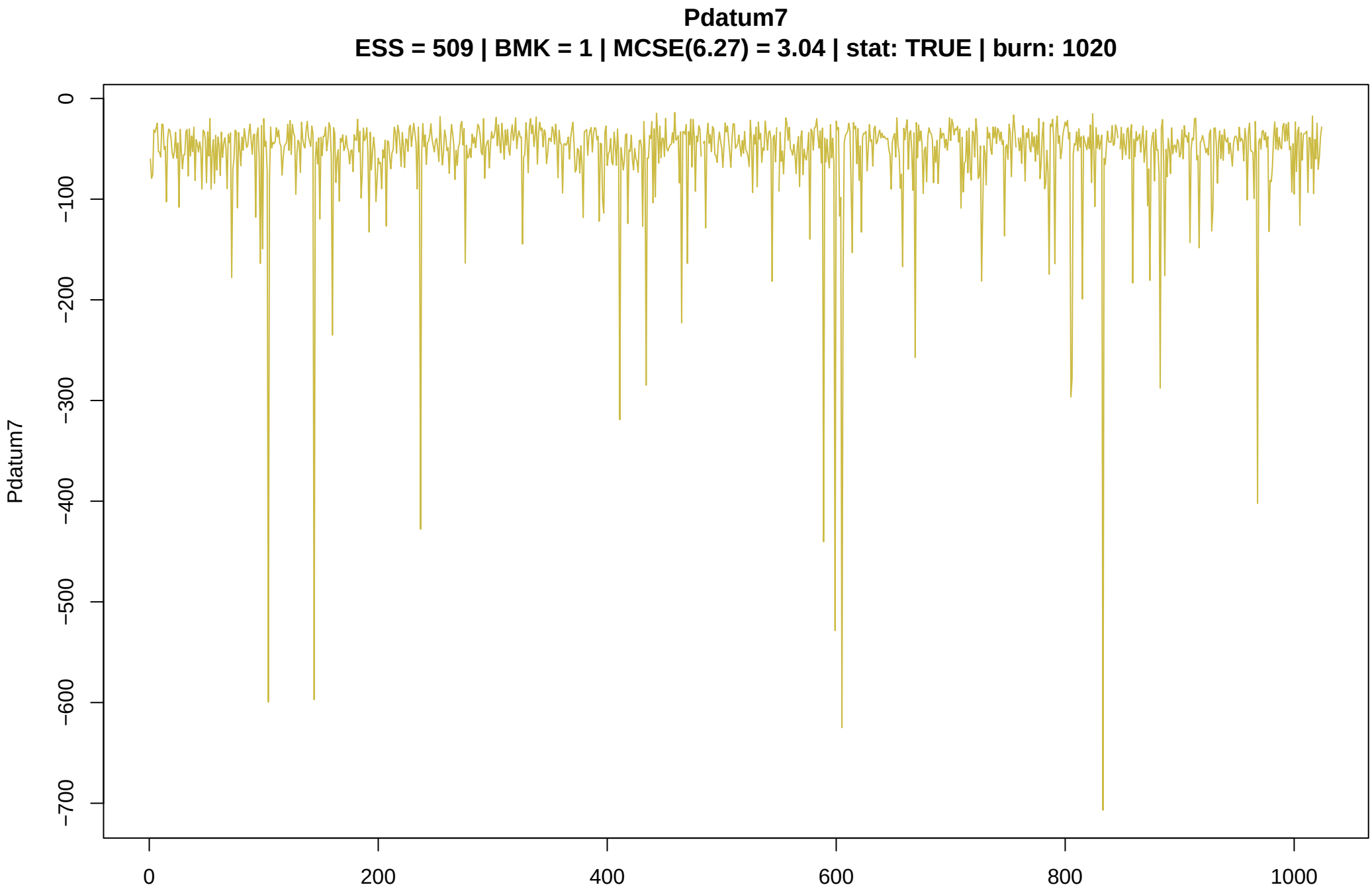

Pdatum2
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 1020
Pdatum2
0
−100
−200
−300
−400
−500
0
200
400
600
800
1000

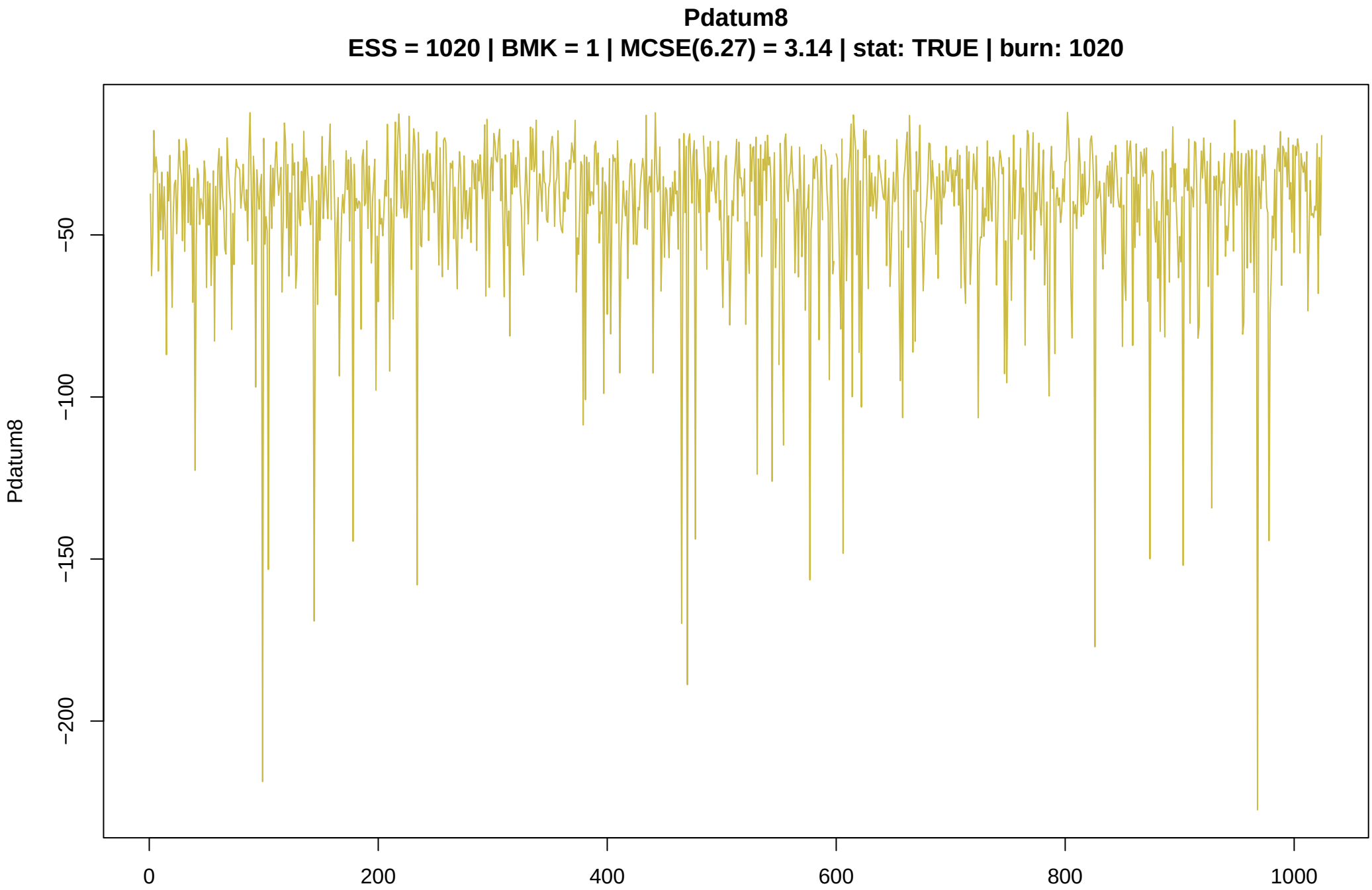

Pdatum3
ESS = 2.22e−16 | BMK = 1 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 1020
Pdatum3
0
−100
−200
−300
−400
−500
0
200
400
600
800
1000

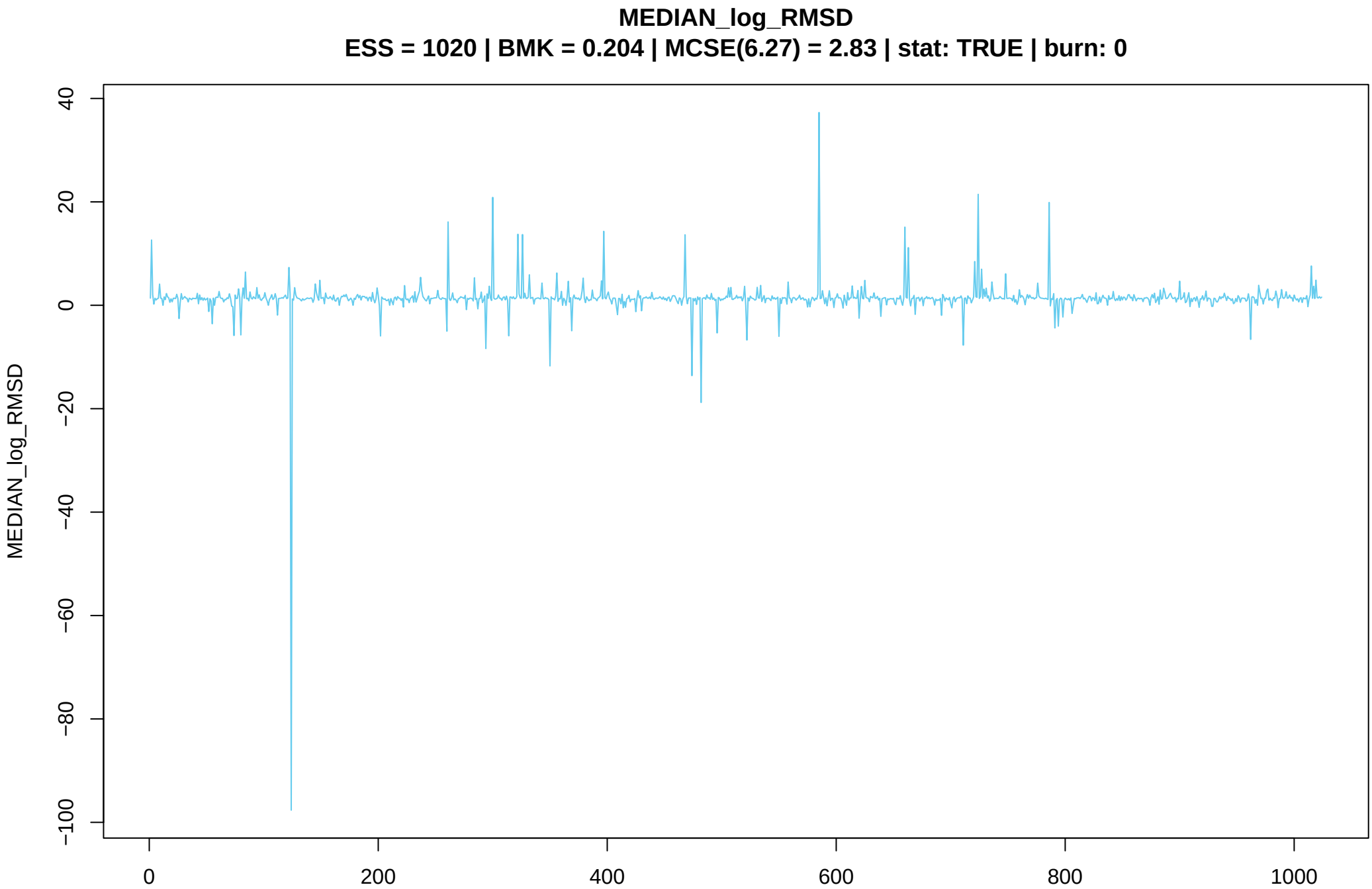

Pdatum4
ESS = 2.22e−16 | BMK = 1 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 1020
Pdatum4
0
−100
−200
−300
−400
−500
−600
−700
0
200
400
600
800
1000

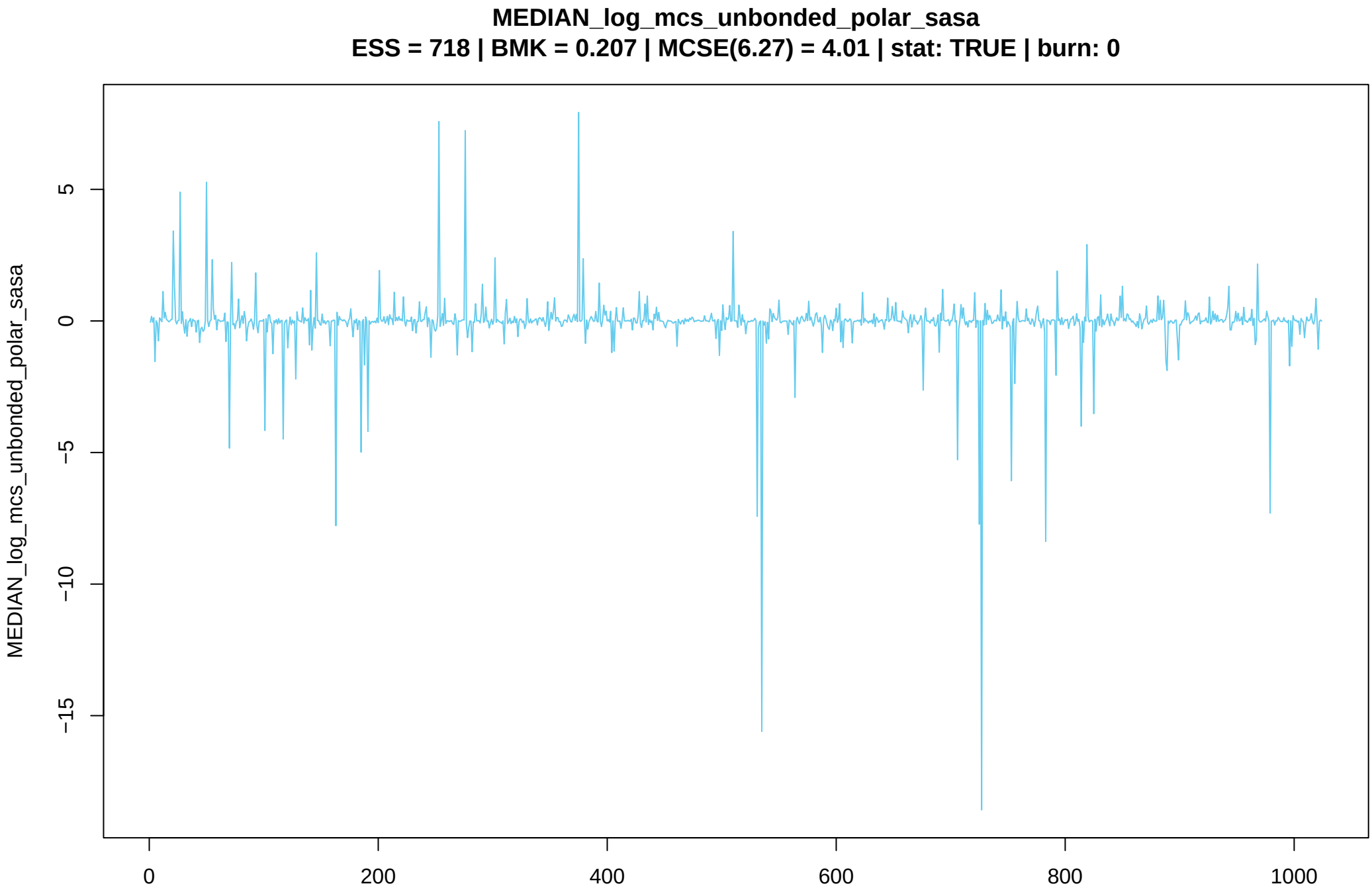

Pdatum5
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 1020
Pdatum5
0
−200
−400
−600
0
200
400
600
800
1000

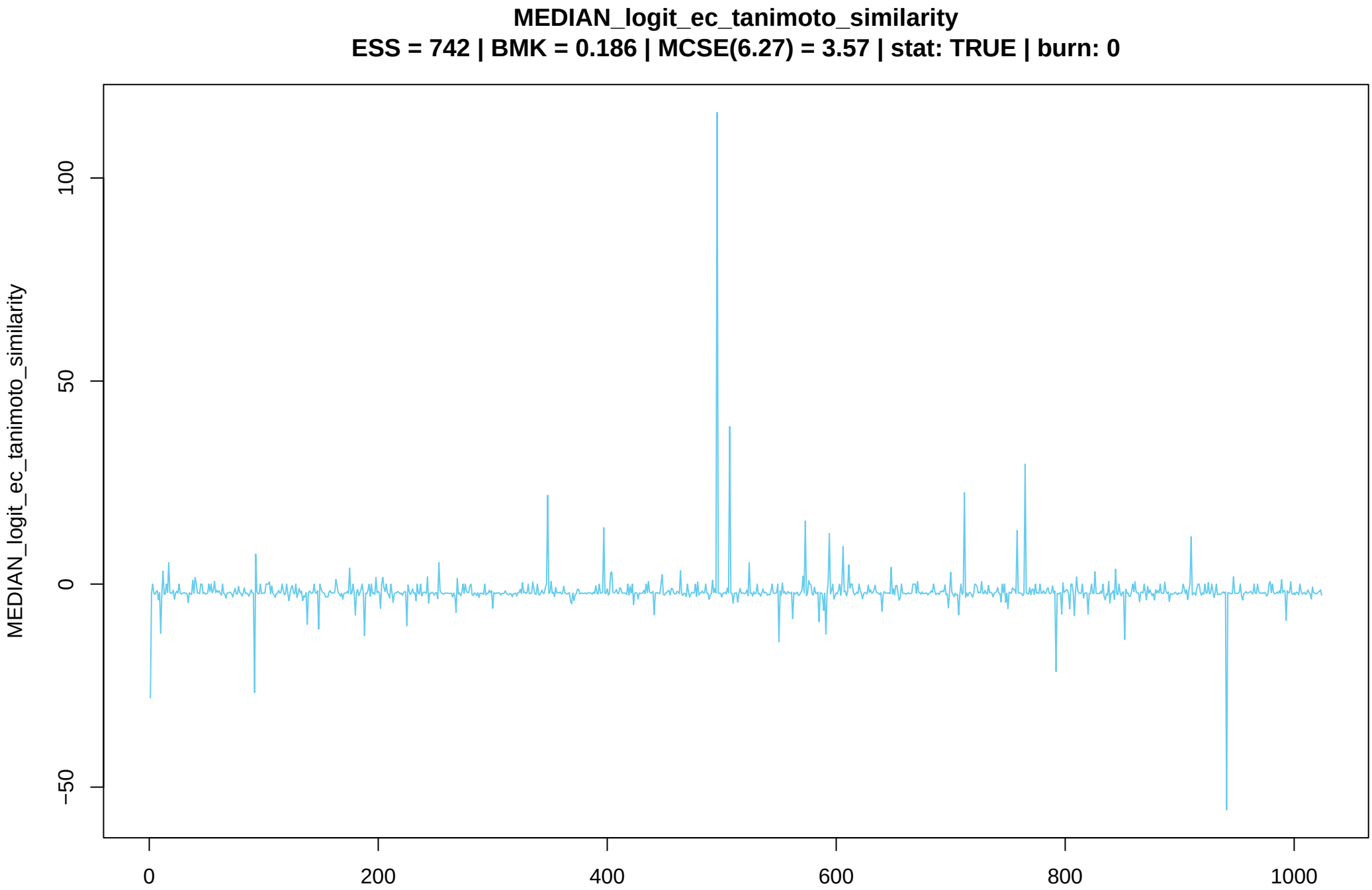

Pdatum6
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 1020
Pdatum6
0
−100
−200
−300
−400
0
200
400
600
800
1000

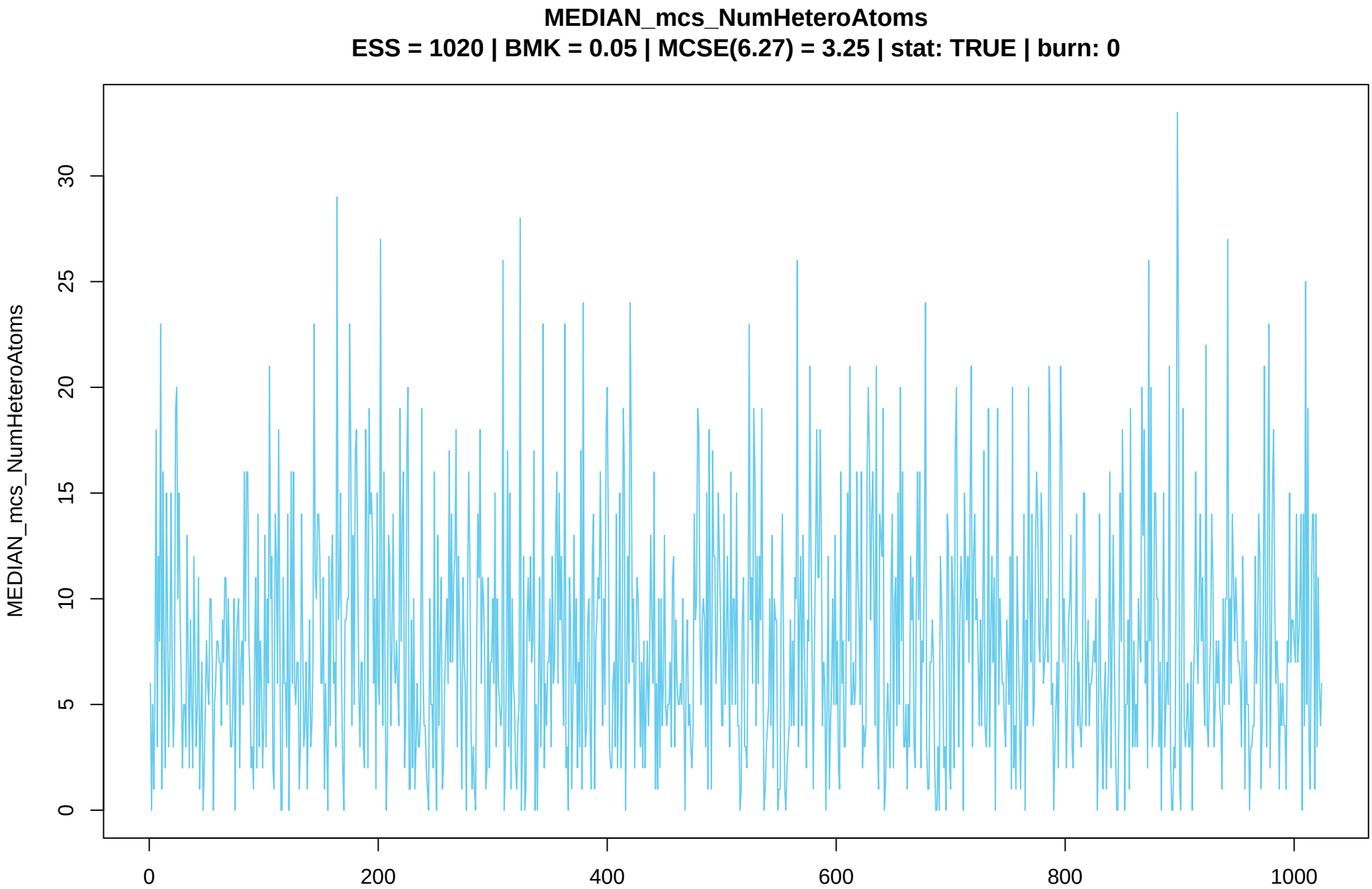

Pdatum7
ESS = 509 | BMK = 1 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 1020
Pdatum7
0
−100
−200
−300
−400
−500
−600
−700
0
200
400
600
800
1000

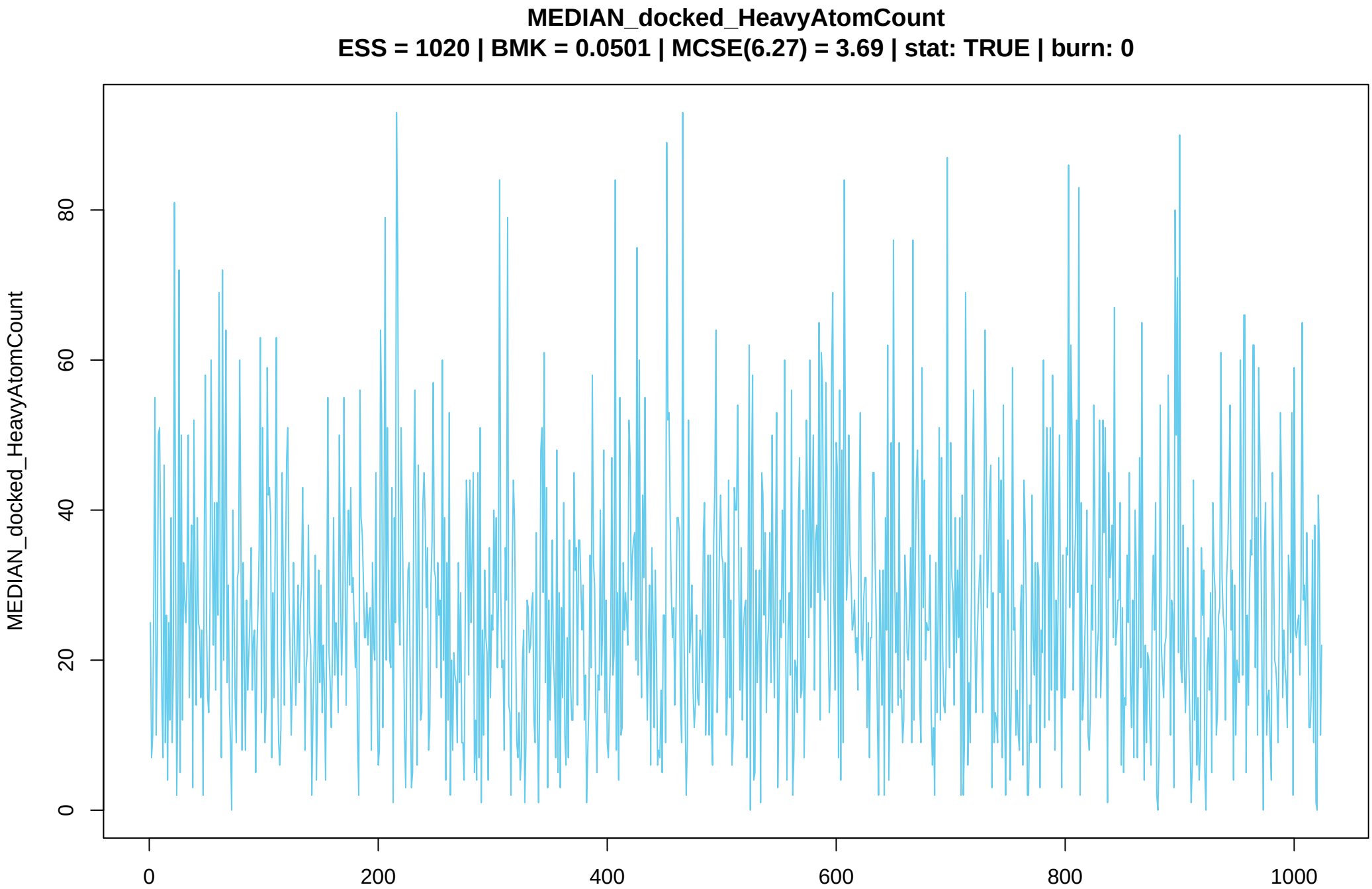

Pdatum8
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.14 | stat: TRUE | burn: 1020
Pdatum8
−50
−100
−150
−200
0
200
400
600
800
1000

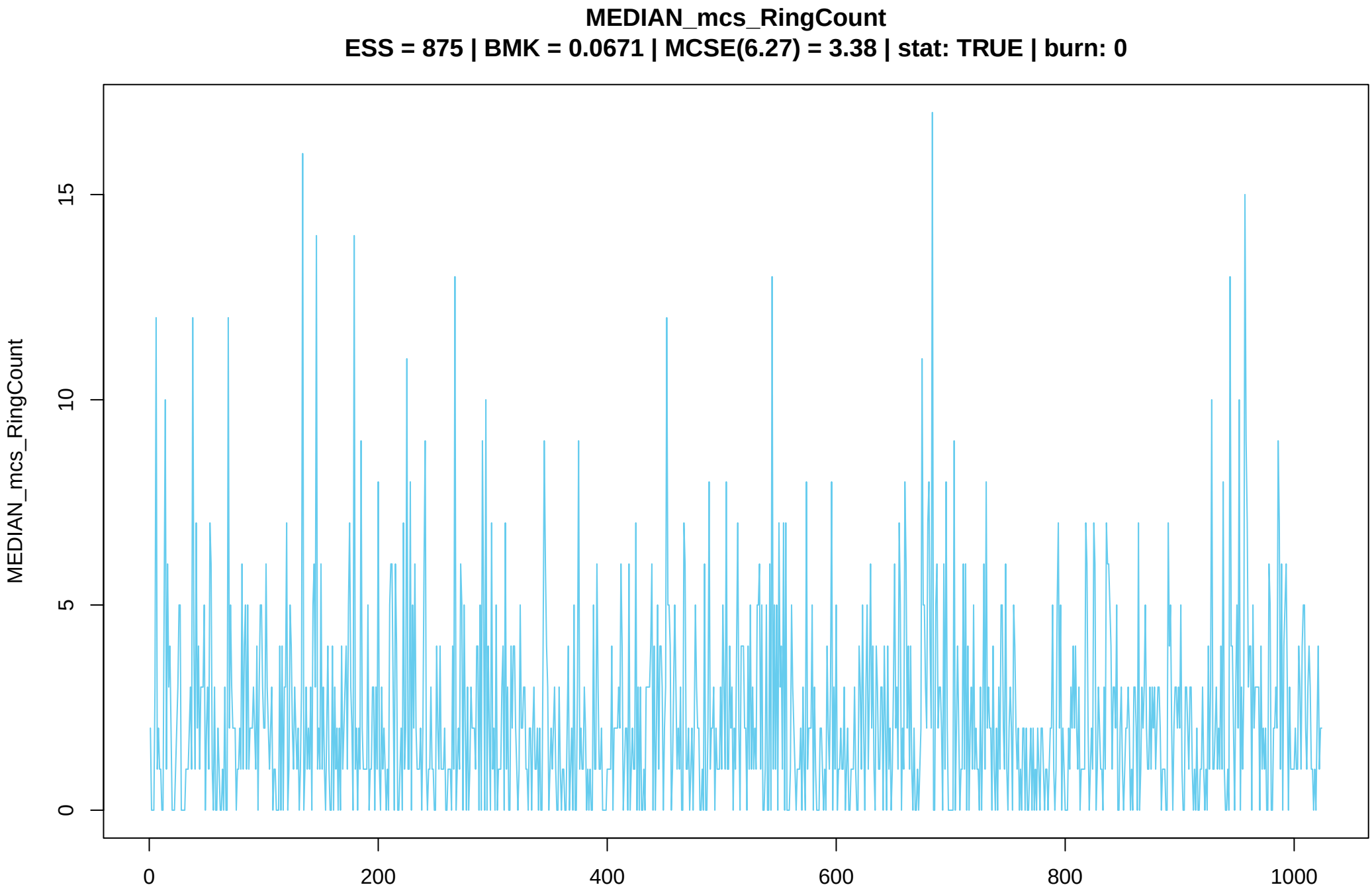

MEDIAN_log_RMSD
ESS = 1020 | BMK = 0.204 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0
MEDIAN_log_RMSD
40
20
0
−20
−40
−60
−80
−100
0
200
400
600
800
1000

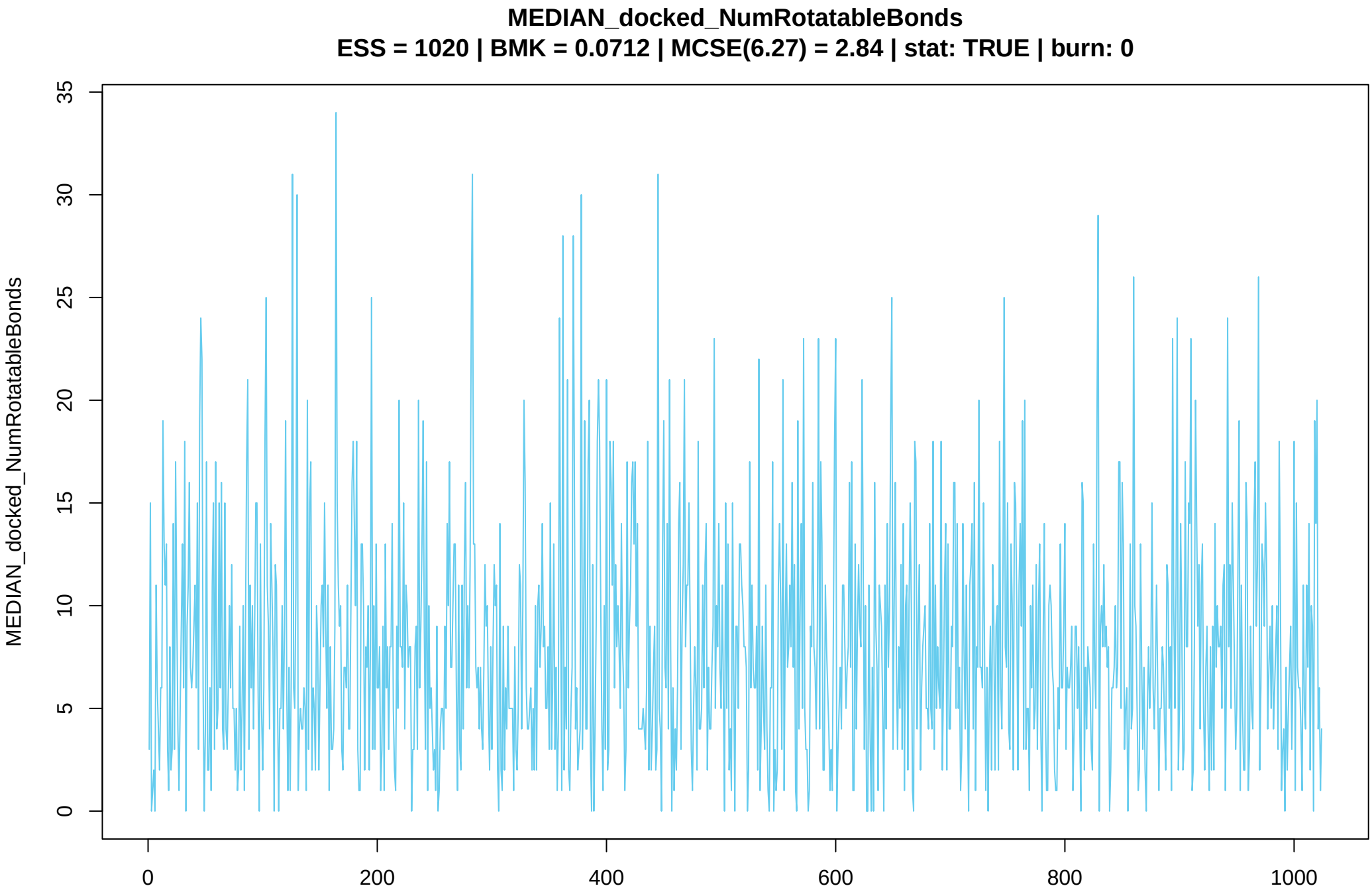

MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 718 | BMK = 0.207 | MCSE(6.27) = 4.01 | stat: TRUE | burn: 0
MEDIAN_log_mcs_unbonded_polar_sasa
5
0
−5
−10
−15
0
200
400
600
800
1000

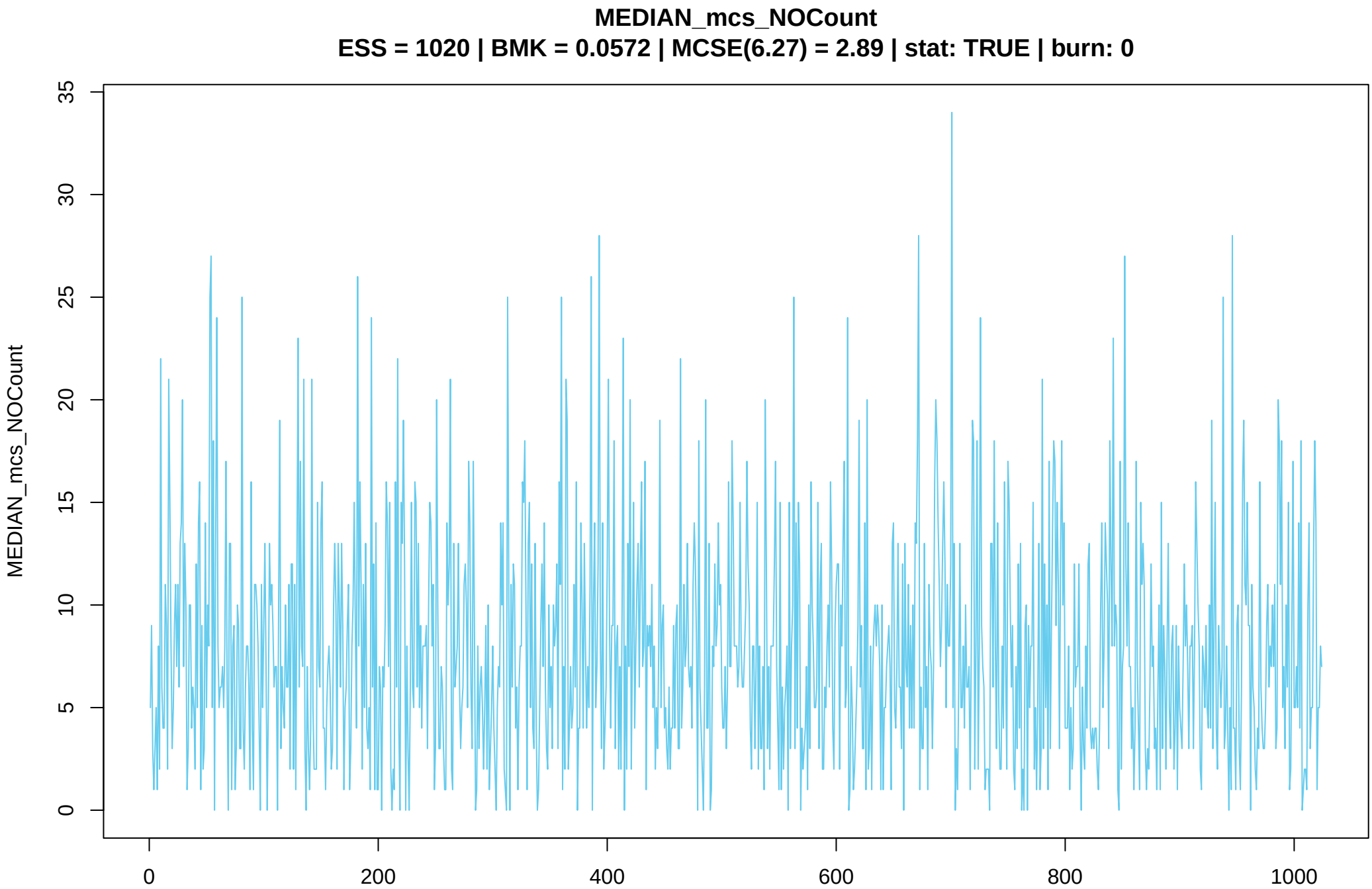

MEDIAN_logit_ec_tanimoto_similarity
ESS = 742 | BMK = 0.186 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0
MEDIAN_logit_ec_tanimoto_similarity
100
50
0
−50
0
200
400
600
800
1000

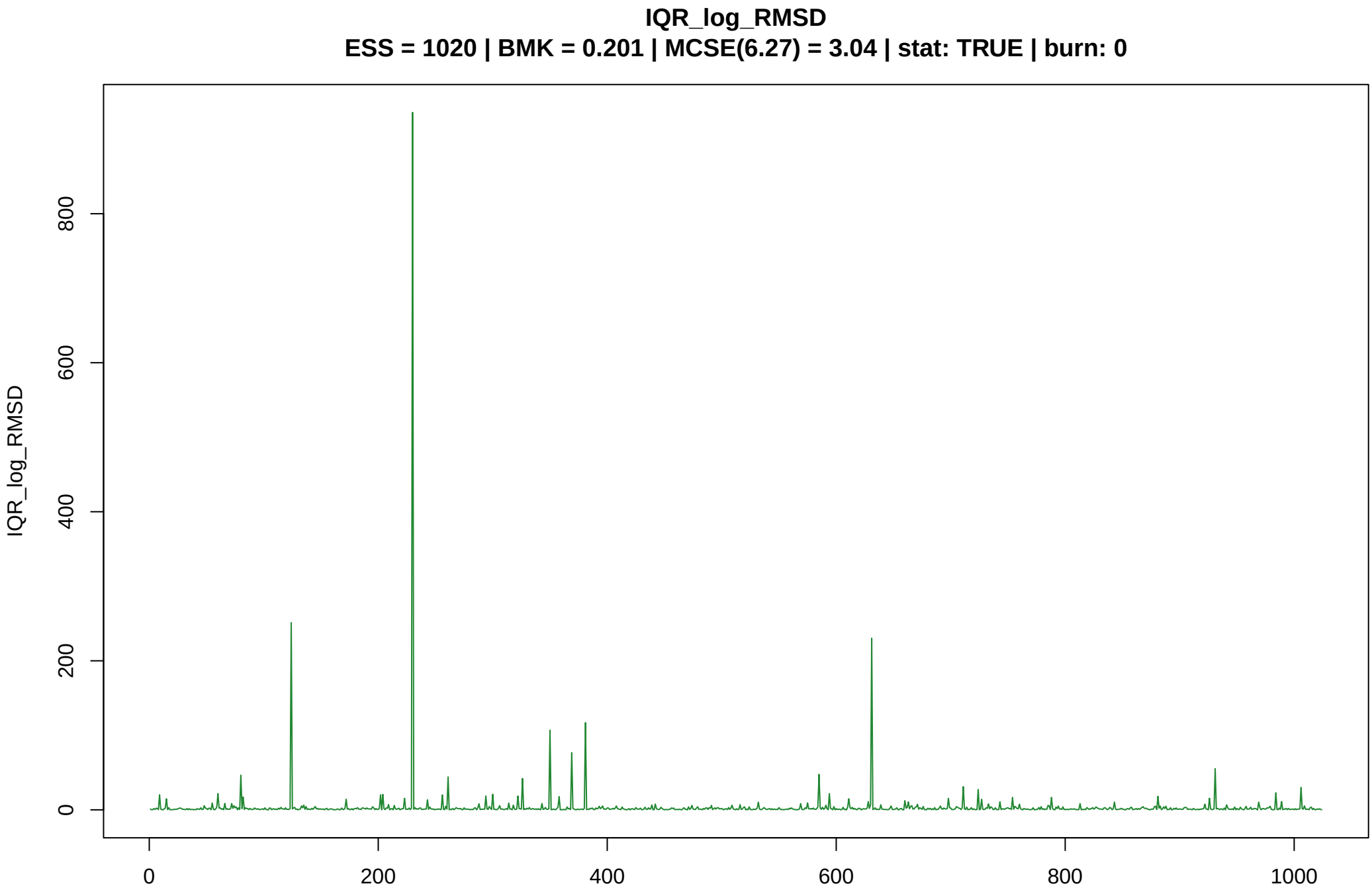

MEDIAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.05 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
0
5
10
15
20
25
30
0
200
400
600
800
1000

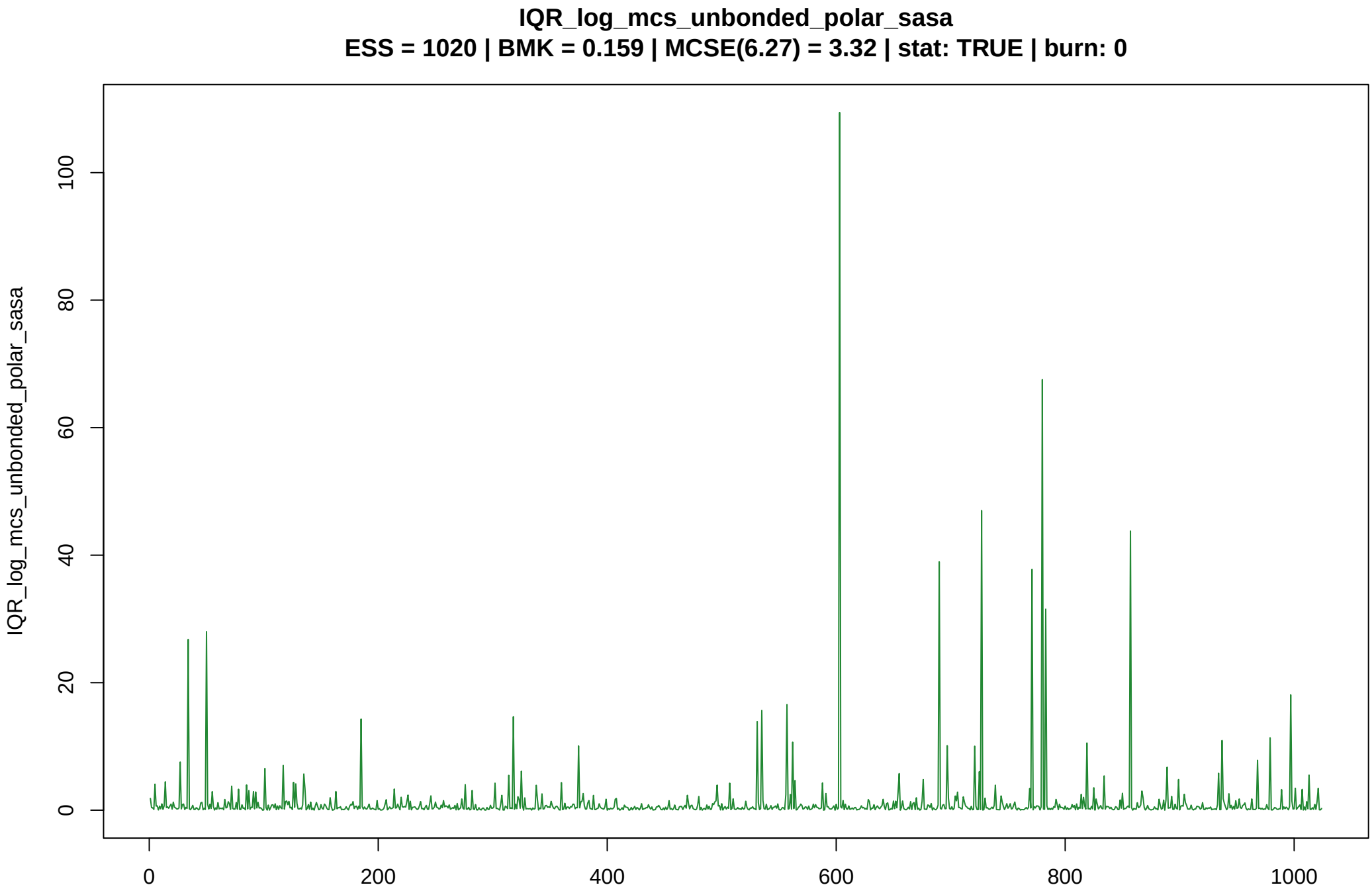

MEDIAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0501 | MCSE(6.27) = 3.69 | stat: TRUE | burn: 0
MEDIAN_docked_HeavyAtomCount
0
20
40
60
80
0
200
400
600
800
1000

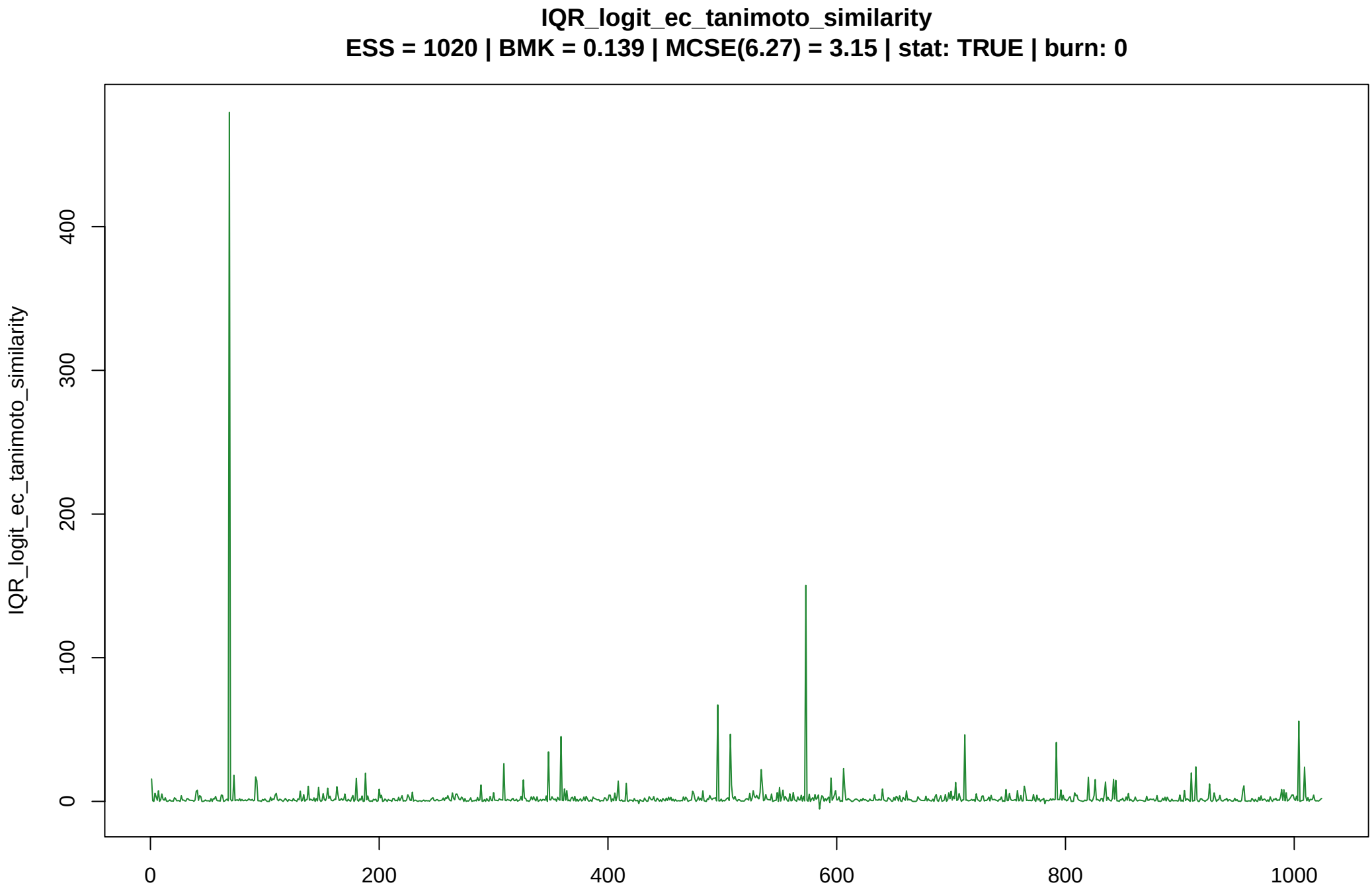

MEDIAN_mcs_RingCount
ESS = 875 | BMK = 0.0671 | MCSE(6.27) = 3.38 | stat: TRUE | burn: 0
MEDIAN_mcs_RingCount
0
5
10
15
0
200
400
600
800
1000

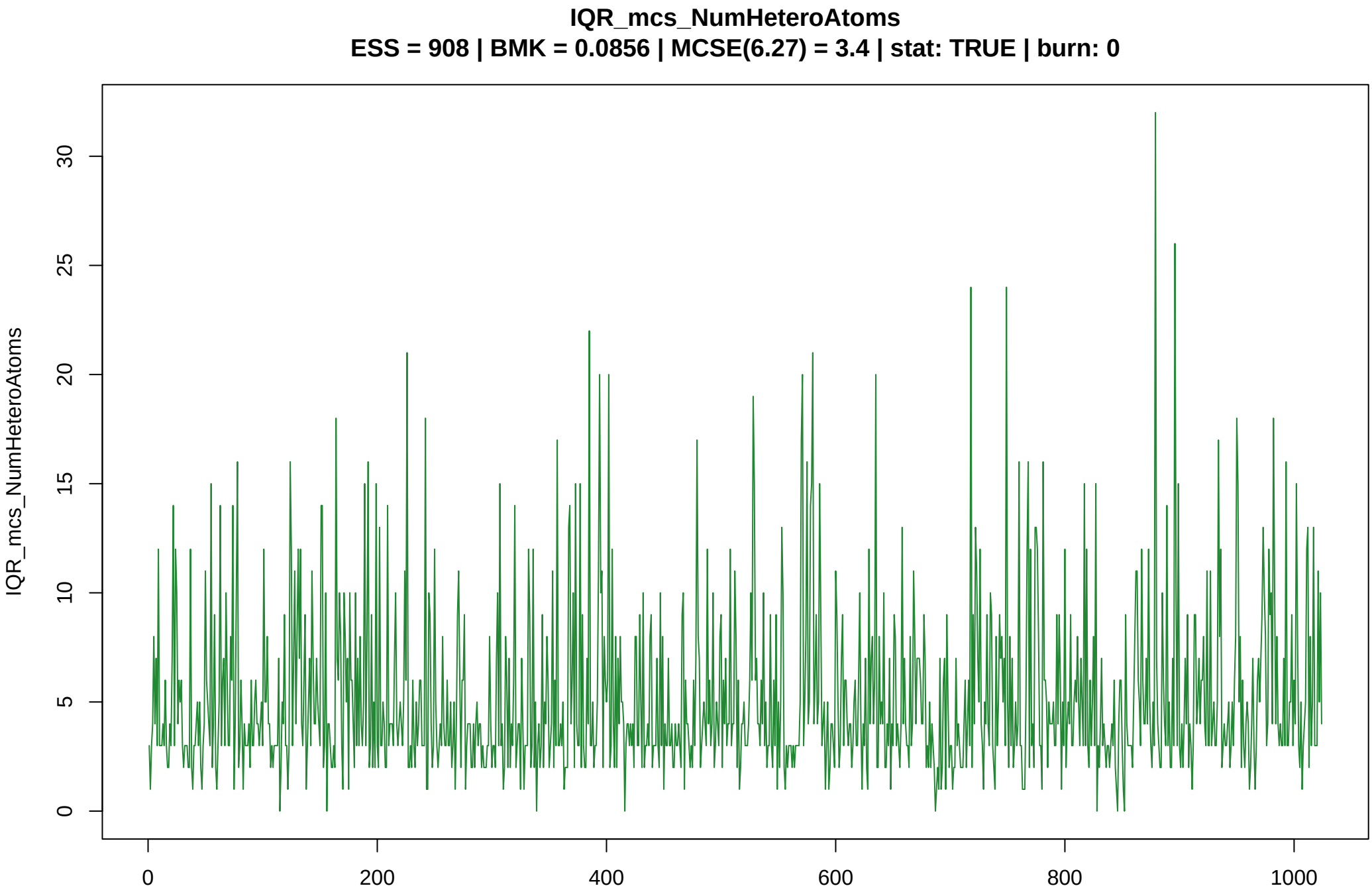

MEDIAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0712 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0
MEDIAN_docked_NumRotatableBonds
0
5
10
15
20
25
30
35
0
200
400
600
800
1000

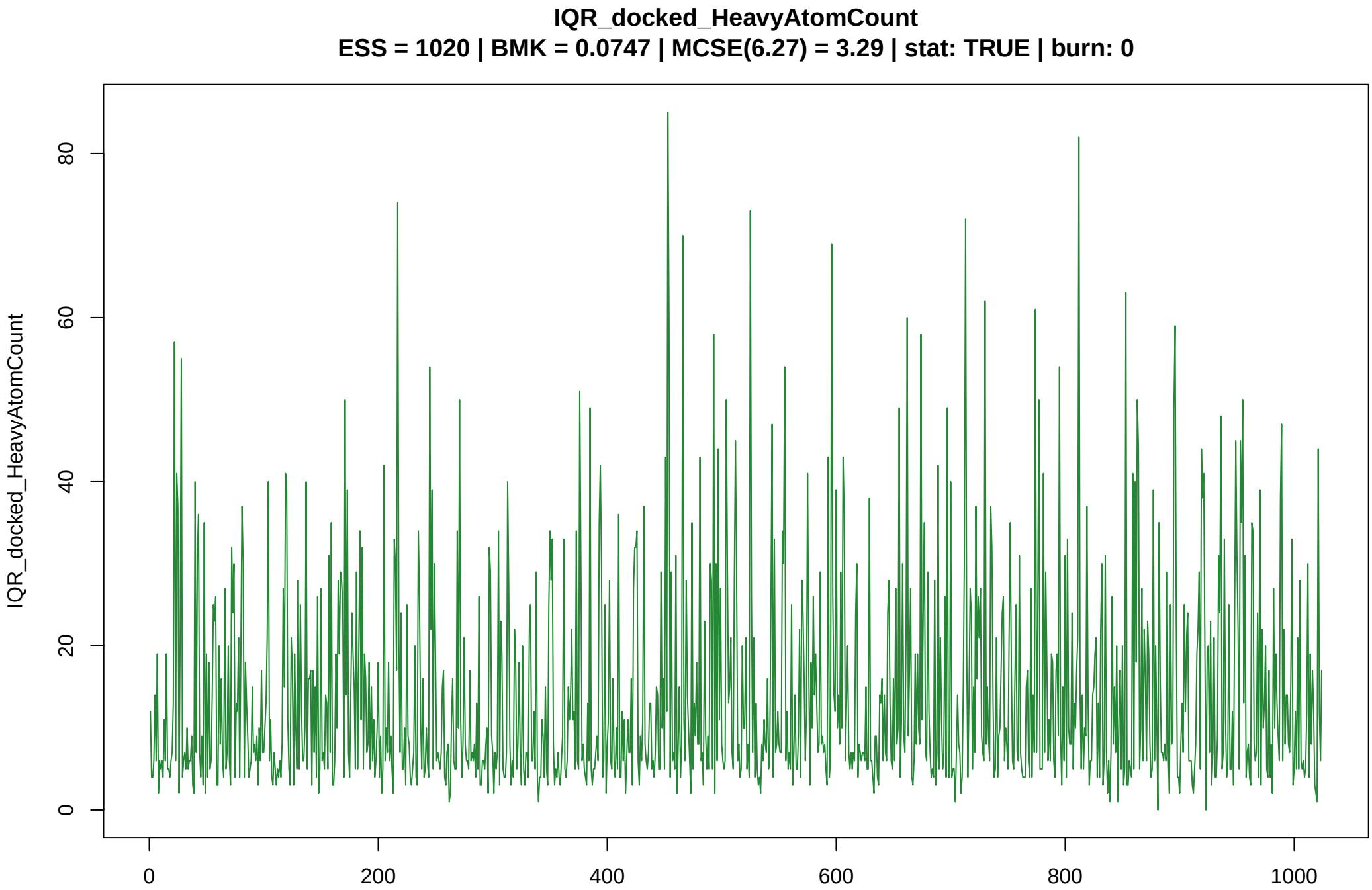

MEDIAN_mcs_NOCount
ESS = 1020 | BMK = 0.0572 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0
MEDIAN_mcs_NOCount
0
5
10
15
20
25
30
35
0
200
400
600
800
1000

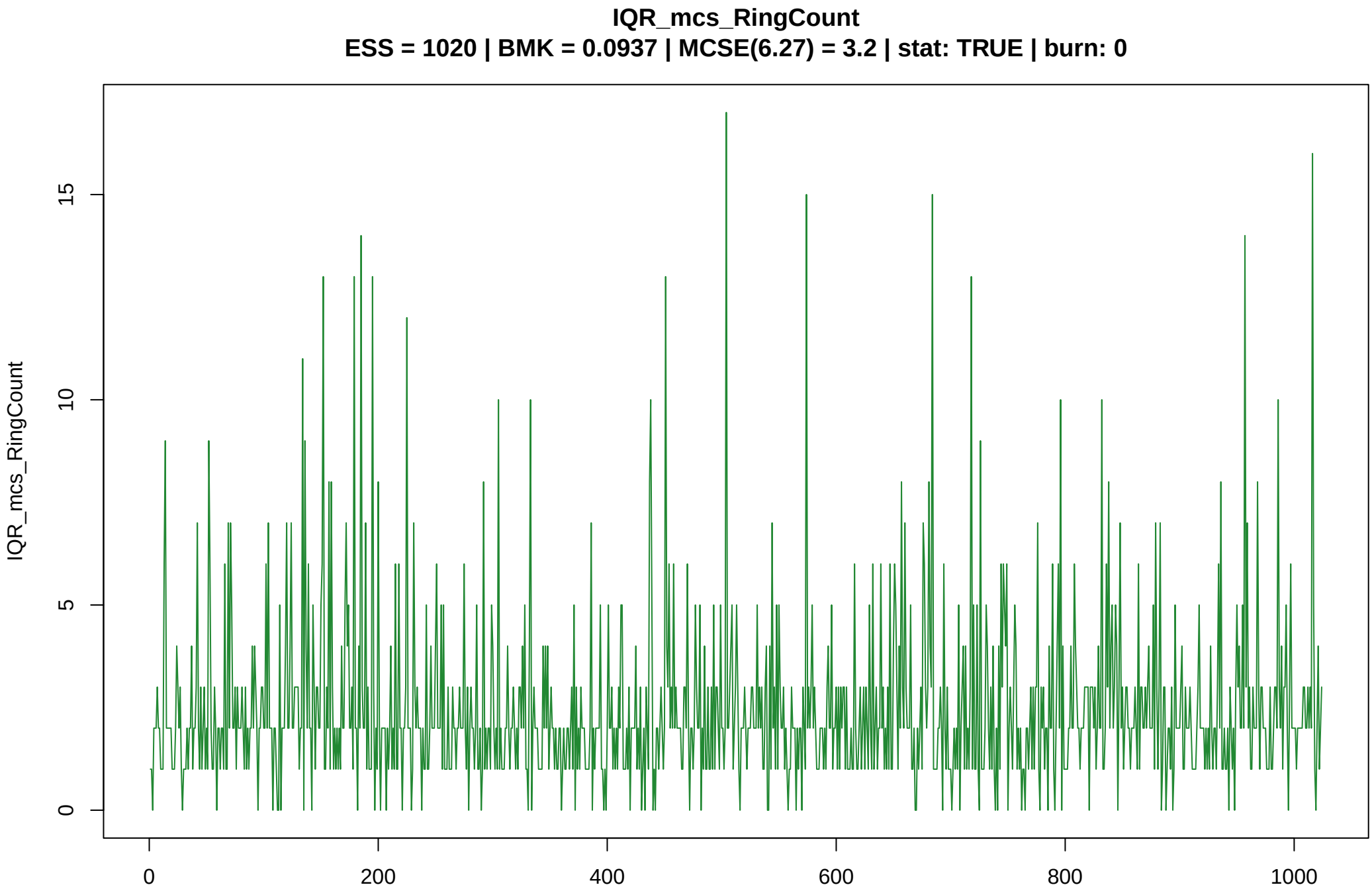

IQR_log_RMSD
ESS = 1020 | BMK = 0.201 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0
IQR_log_RMSD
0
200
400
600
800
0
200
400
600
800
1000

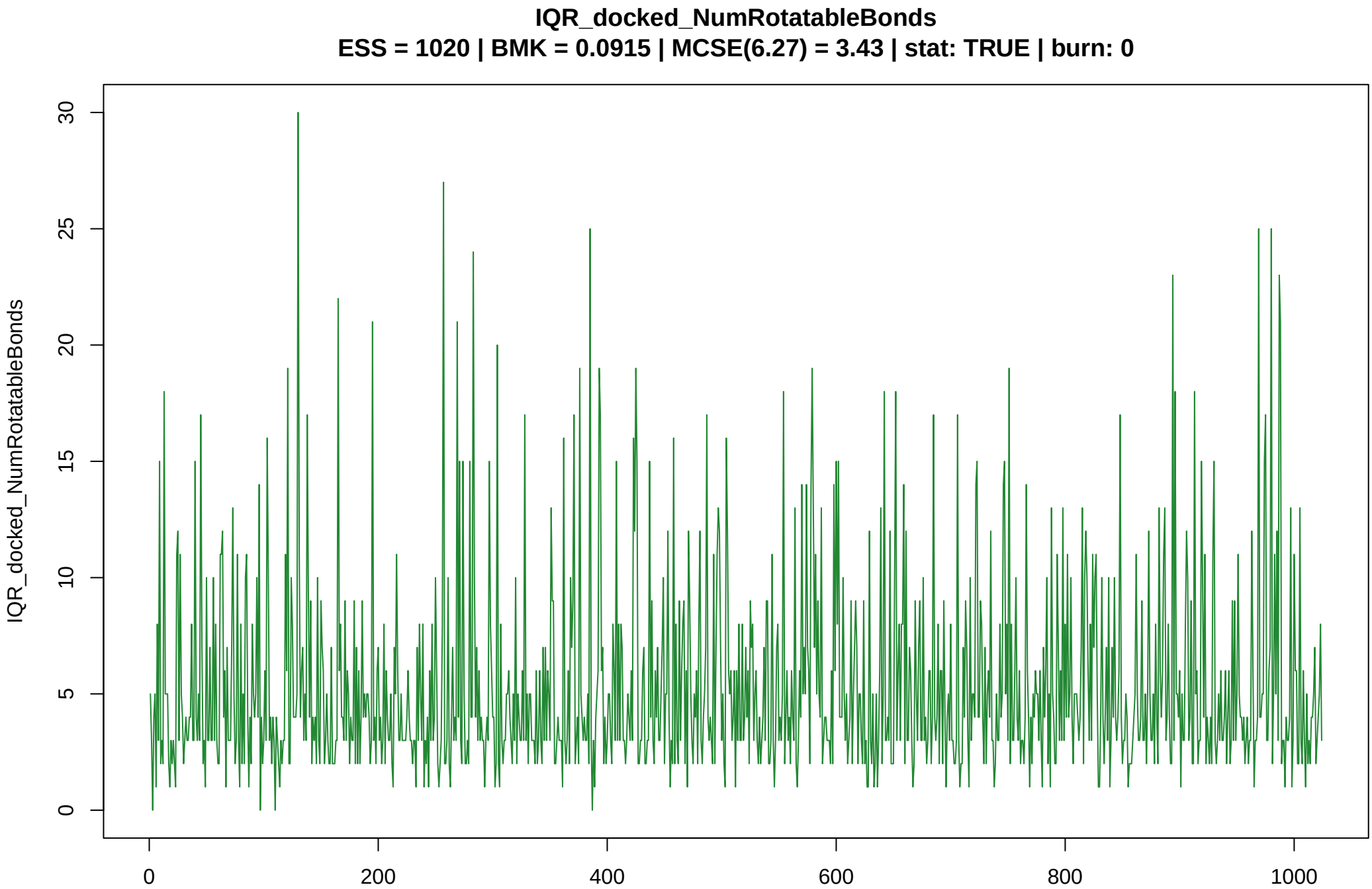

IQR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.159 | MCSE(6.27) = 3.32 | stat: TRUE | burn: 0
IQR_log_mcs_unbonded_polar_sasa
0
20
40
60
80
100
0
200
400
600
800
1000

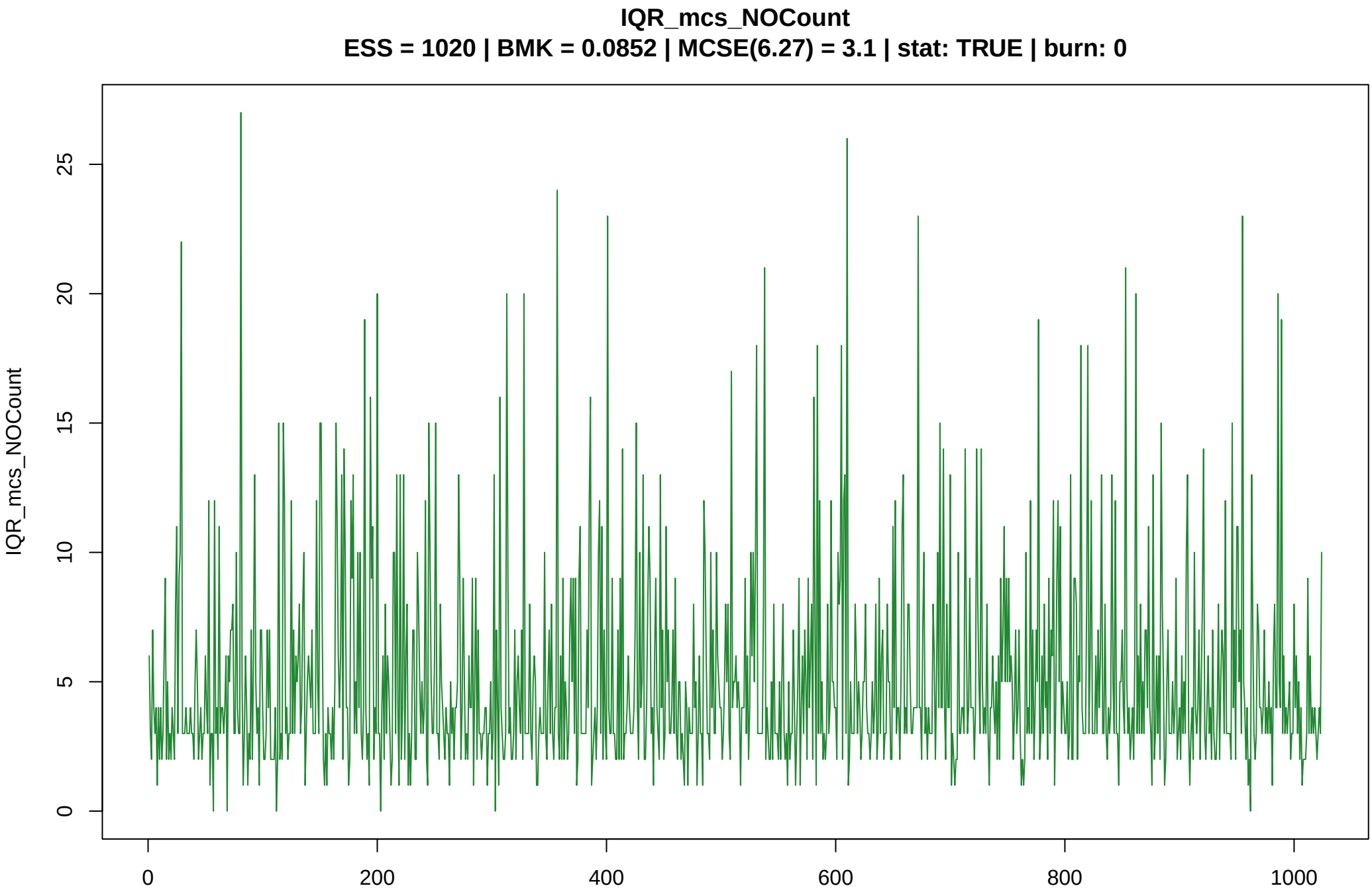

IQR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.139 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0
IQR_logit_ec_tanimoto_similarity
0
100
200
300
400
0
200
400
600
800
1000

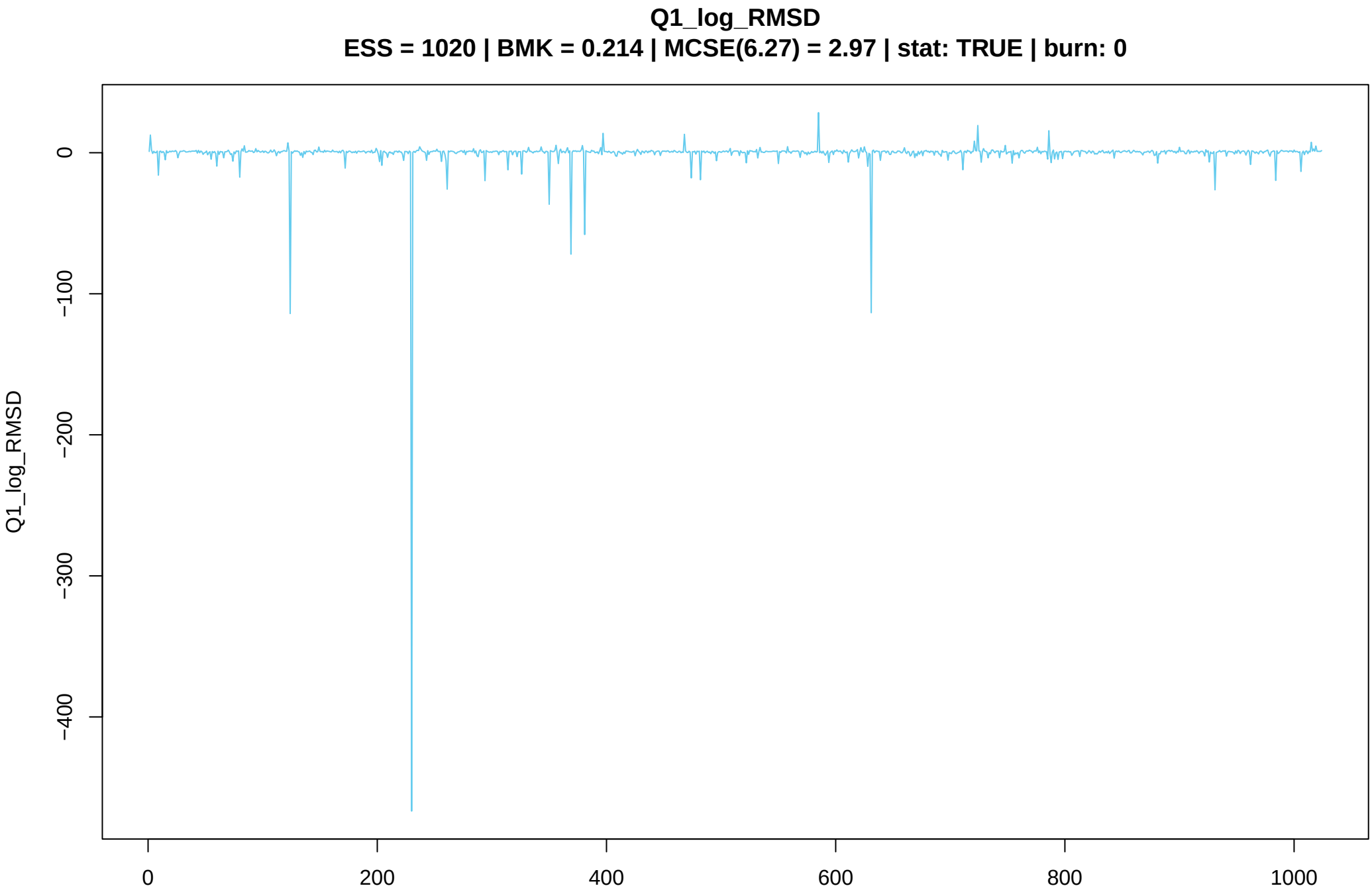

IQR_mcs_NumHeteroAtoms
ESS = 908 | BMK = 0.0856 | MCSE(6.27) = 3.4 | stat: TRUE | burn: 0
IQR_mcs_NumHeteroAtoms
0
5
10
15
20
25
30
0
200
400
600
800
1000

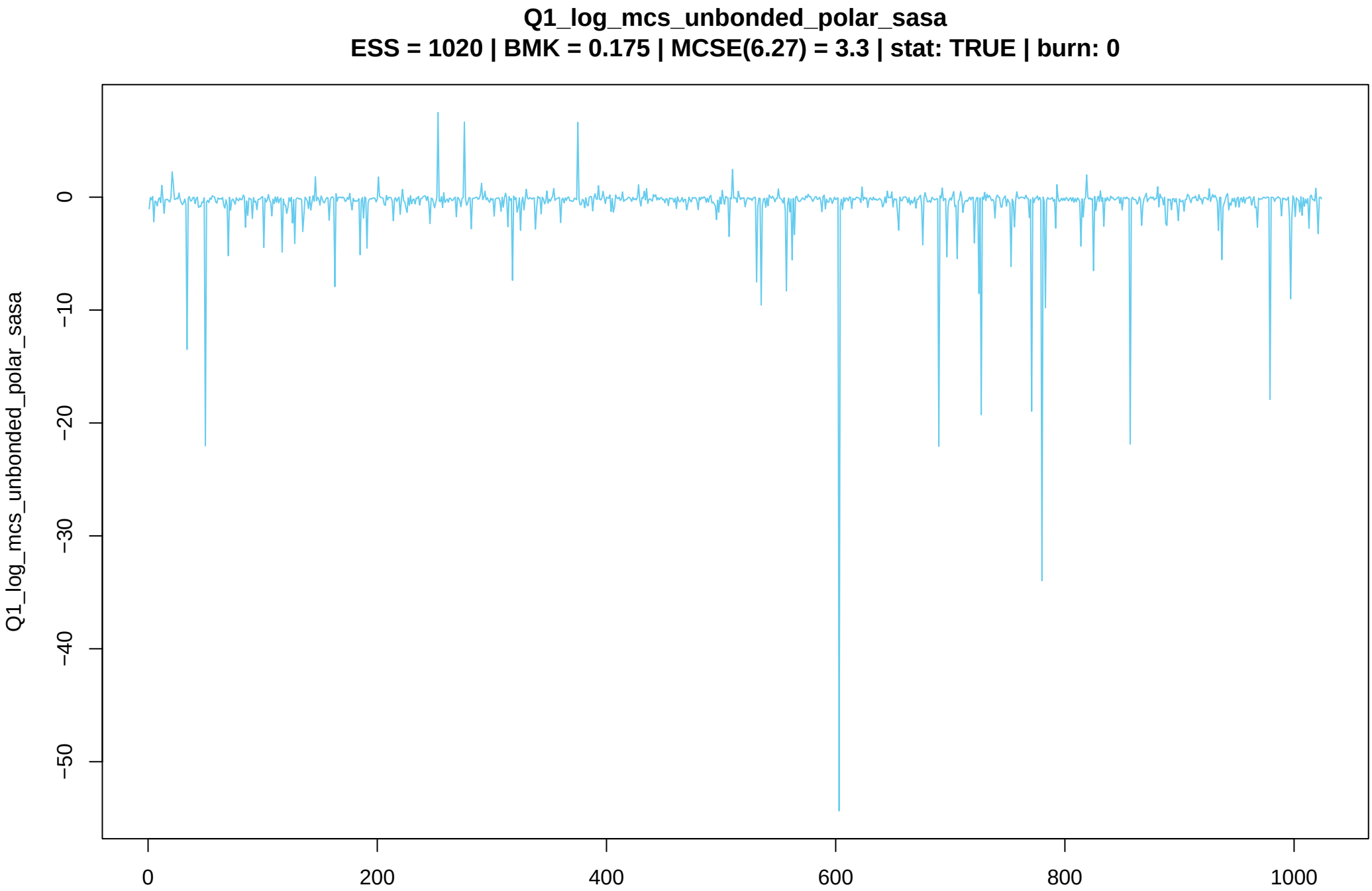

IQR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0747 | MCSE(6.27) = 3.29 | stat: TRUE | burn: 0
IQR_docked_HeavyAtomCount
0
20
40
60
80
0
200
400
600
800
1000

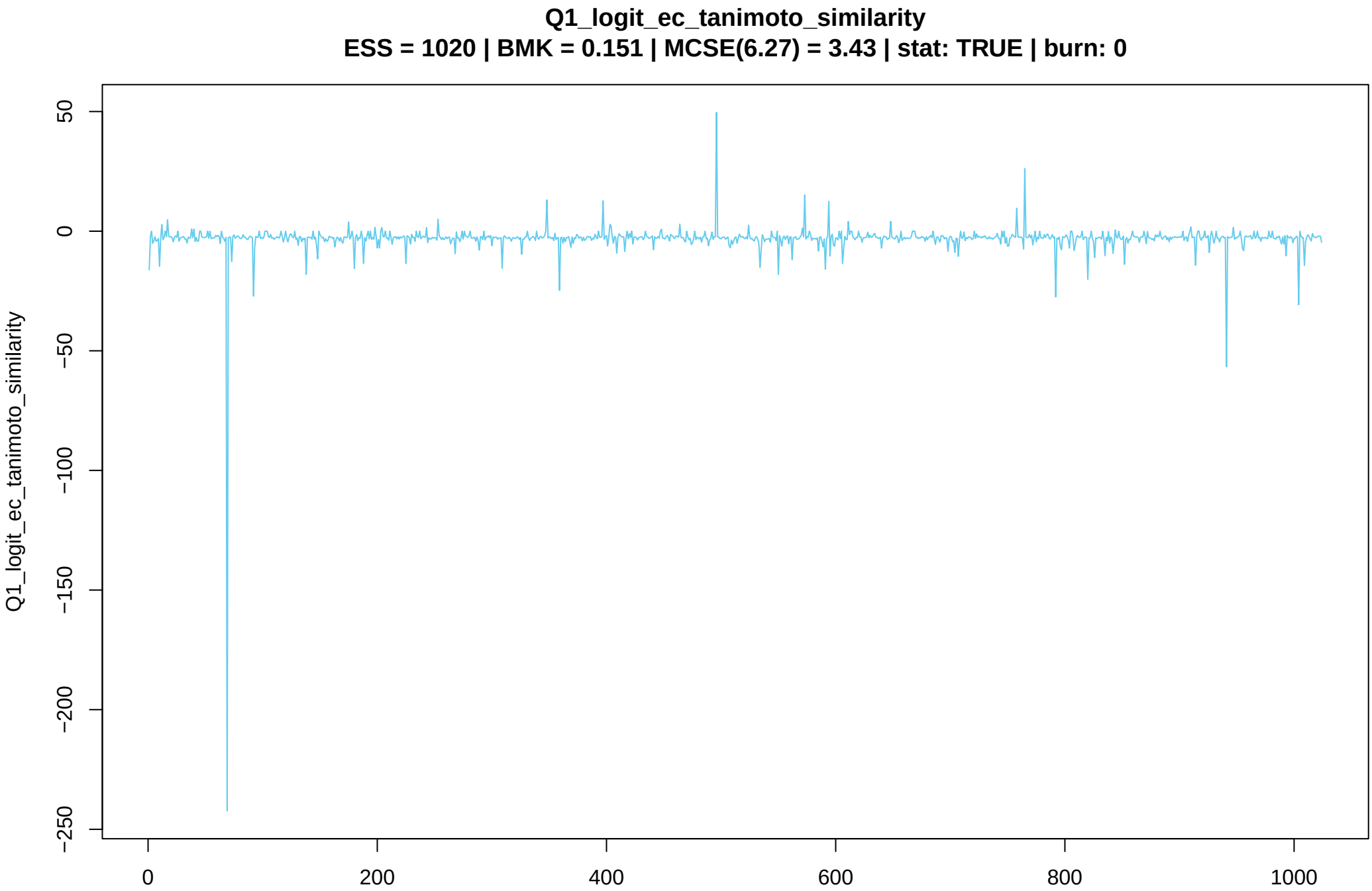

IQR_mcs_RingCount
ESS = 1020 | BMK = 0.0937 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0
IQR_mcs_RingCount
0
5
10
15
0
200
400
600
800
1000

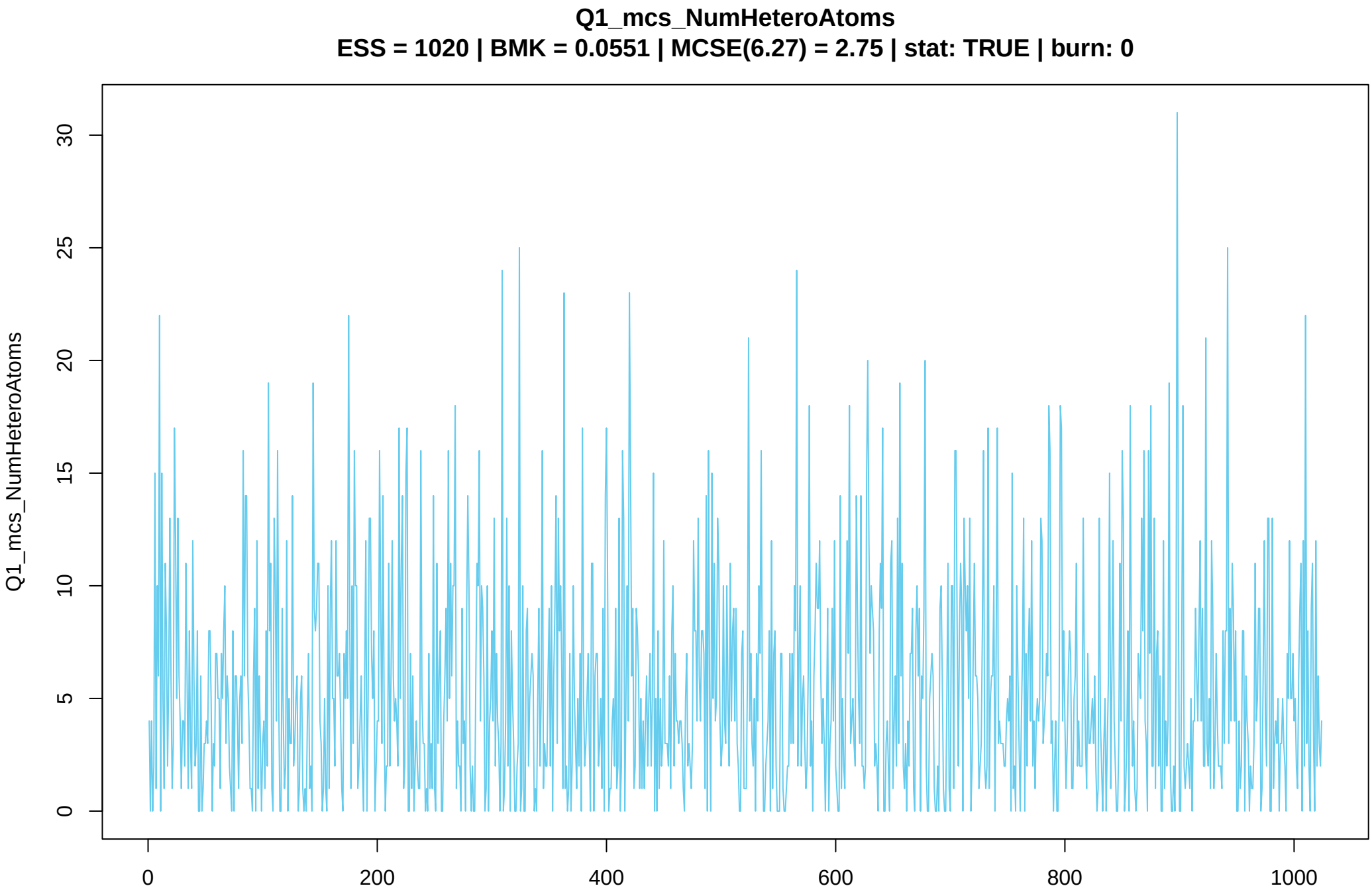

IQR_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0915 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0
IQR_docked_NumRotatableBonds
0
5
10
15
20
25
30
0
200
400
600
800
1000

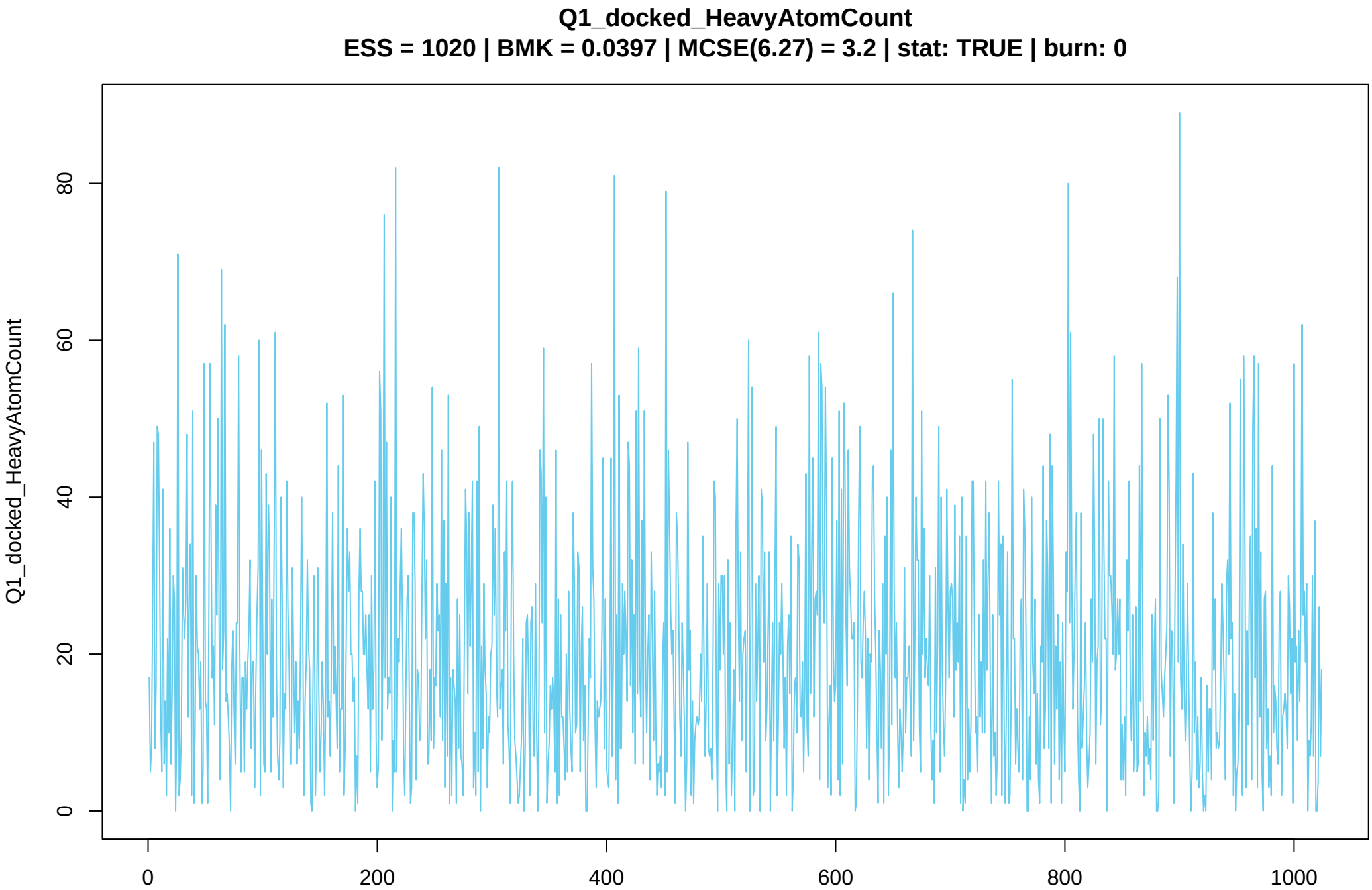

IQR_mcs_NOCount
ESS = 1020 | BMK = 0.0852 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0
IQR_mcs_NOCount
0
5
10
15
20
25
0
200
400
600
800
1000

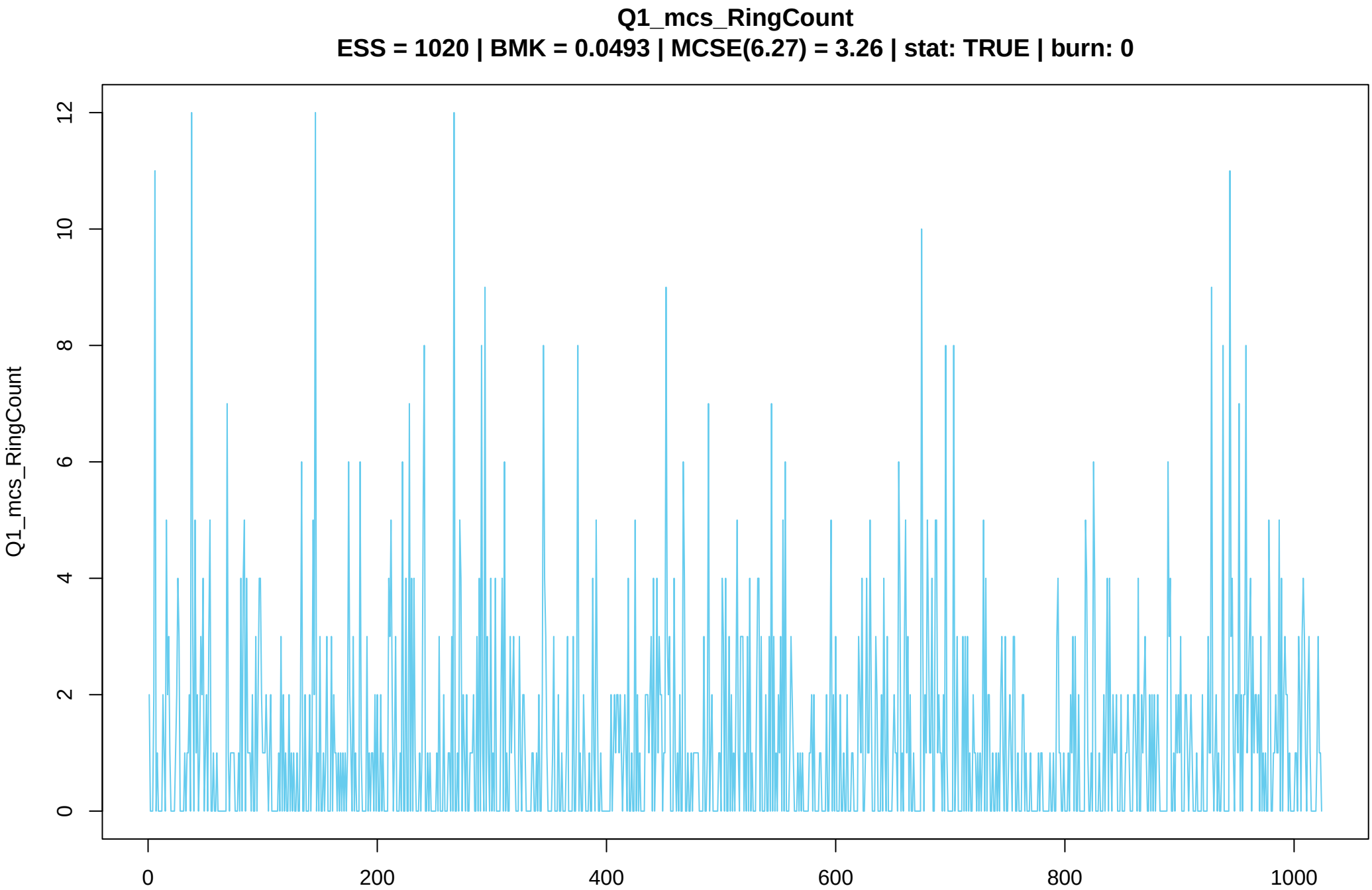

Q1_log_RMSD
ESS = 1020 | BMK = 0.214 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 0
Q1_log_RMSD
0
−100
−200
−300
−400
0
200
400
600
800
1000

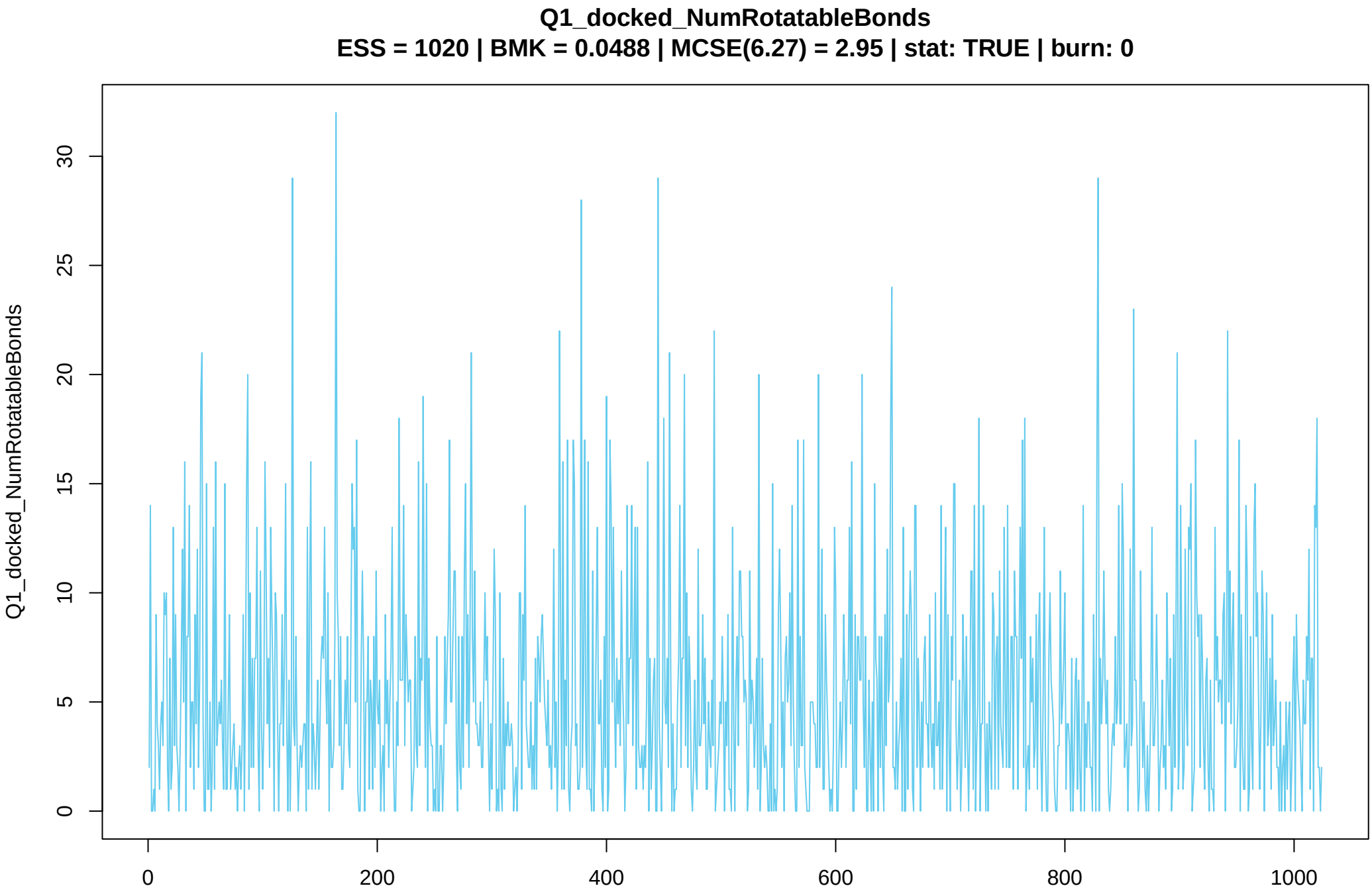

Q1_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.175 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0
Q1_log_mcs_unbonded_polar_sasa
0
−10
−20
−30
−40
−50
0
200
400
600
800
1000

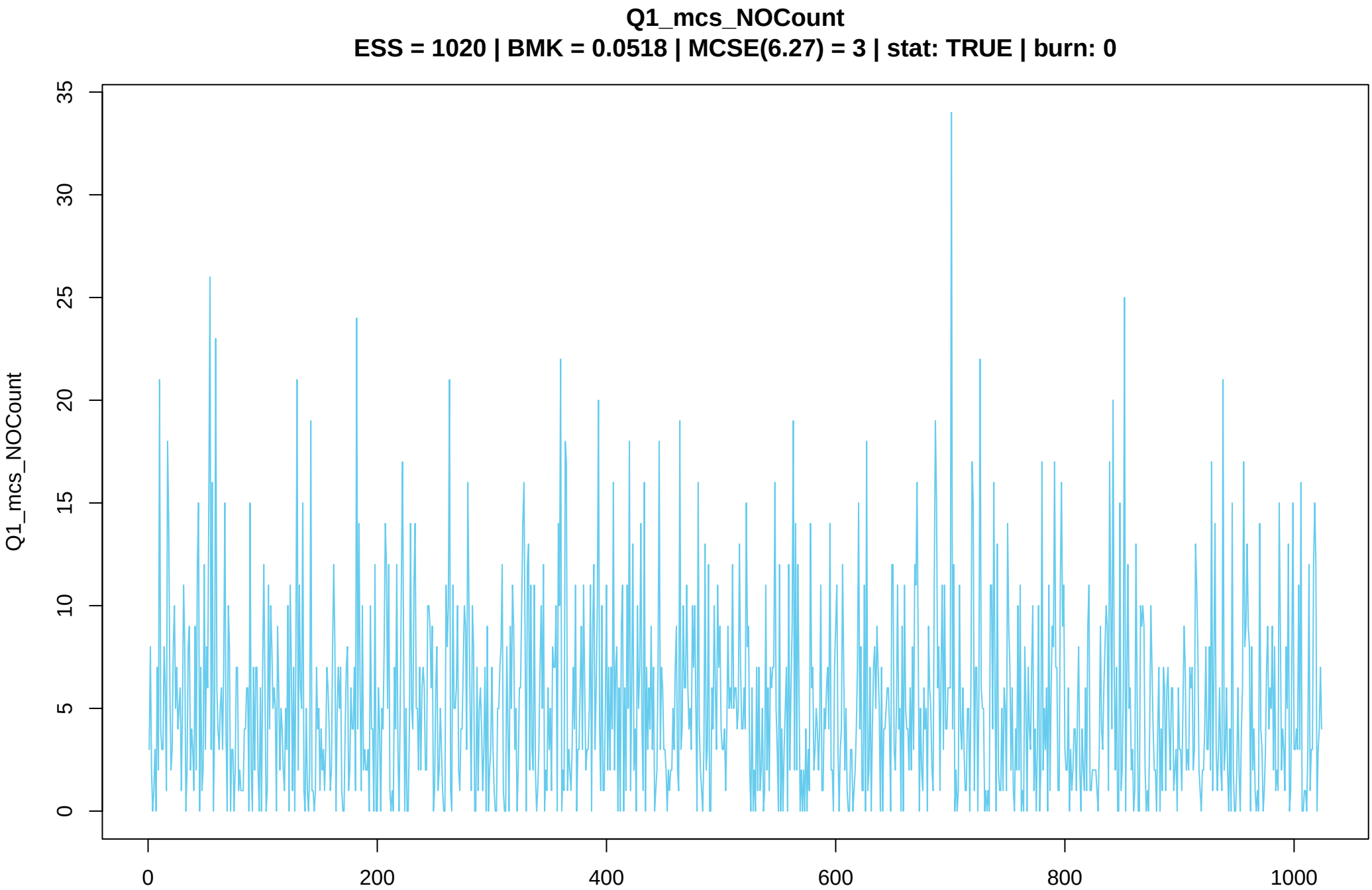

Q1_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.151 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0
Q1_logit_ec_tanimoto_similarity
50
0
−50
−100
−150
−200
−250
0
200
400
600
800
1000

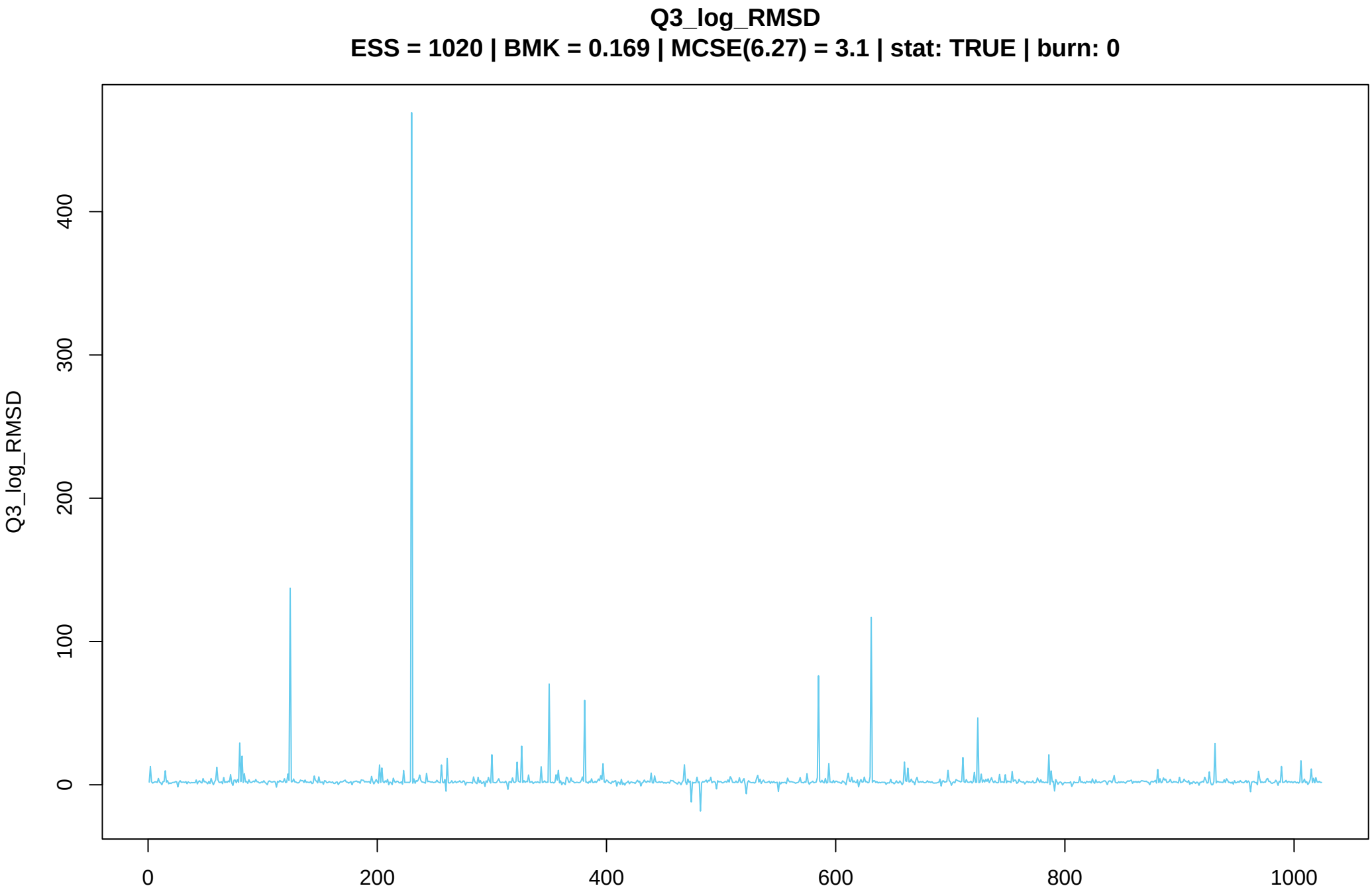

Q1_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0551 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0
Q1_mcs_NumHeteroAtoms
0
5
10
15
20
25
30
0
200
400
600
800
1000

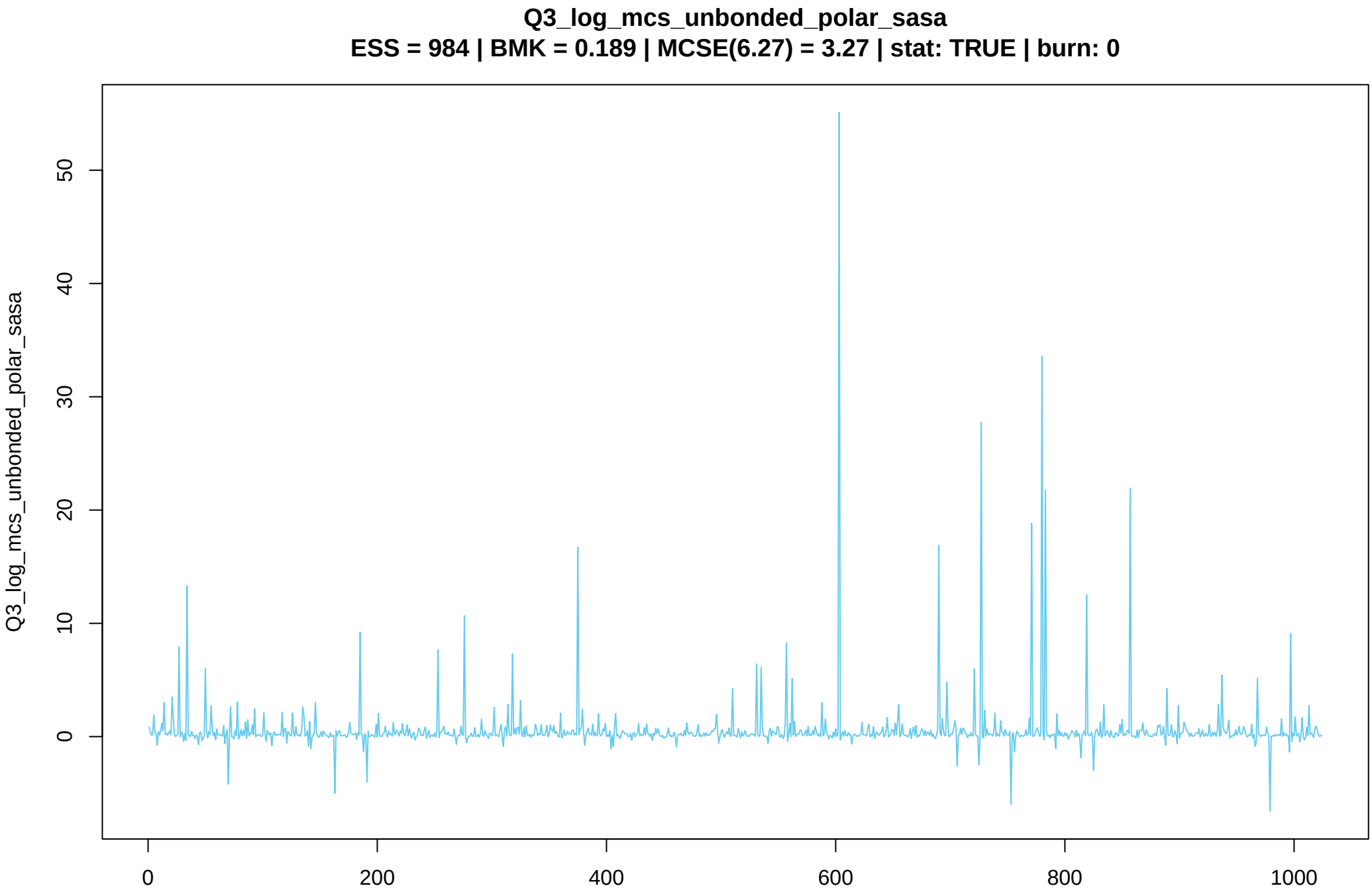

Q1_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0397 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0
Q1_docked_HeavyAtomCount
0
20
40
60
80
0
200
400
600
800
1000

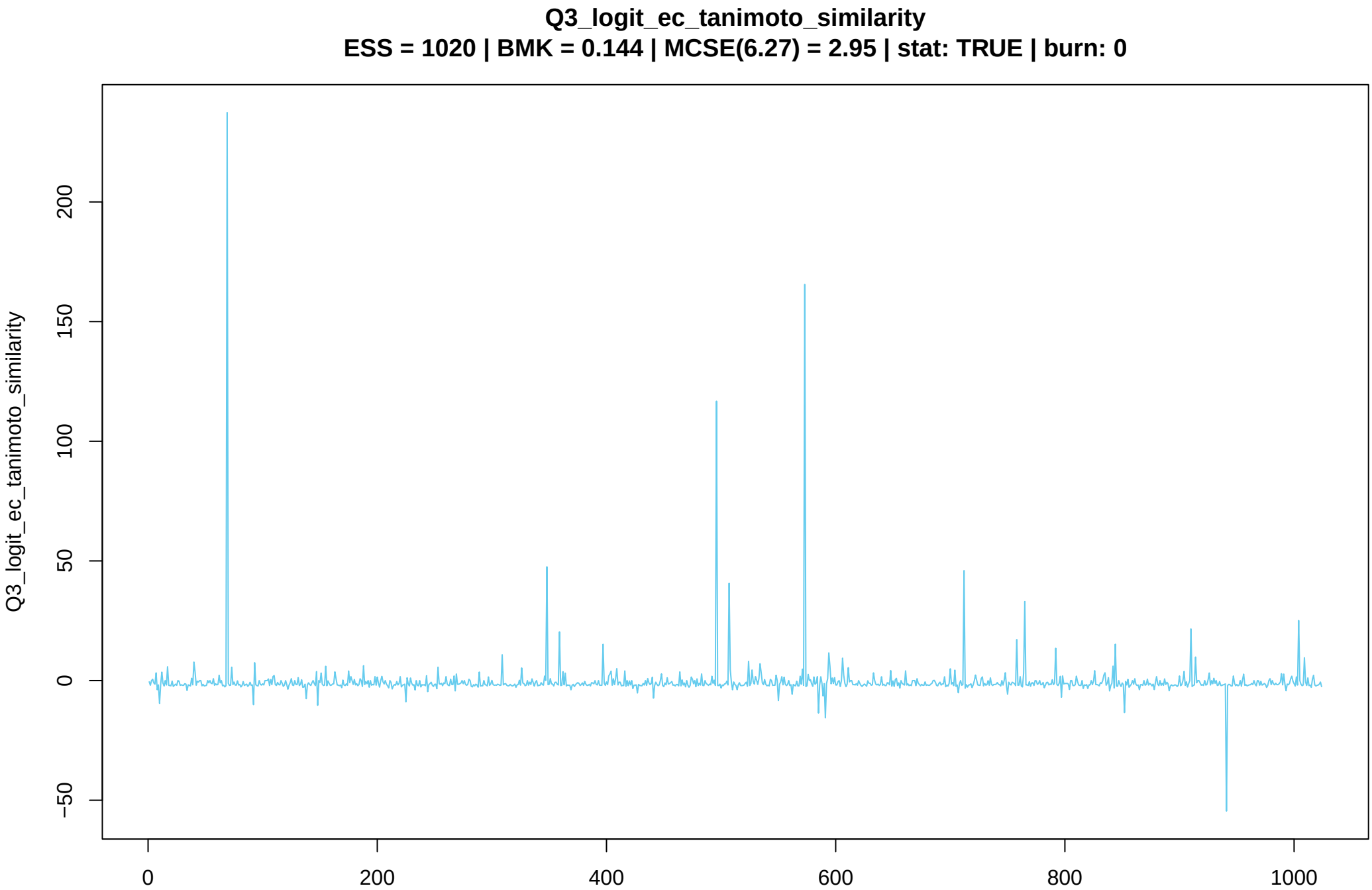

Q1_mcs_RingCount
ESS = 1020 | BMK = 0.0493 | MCSE(6.27) = 3.26 | stat: TRUE | burn: 0
Q1_mcs_RingCount
0
2
4
6
8
10
12
0
200
400
600
800
1000

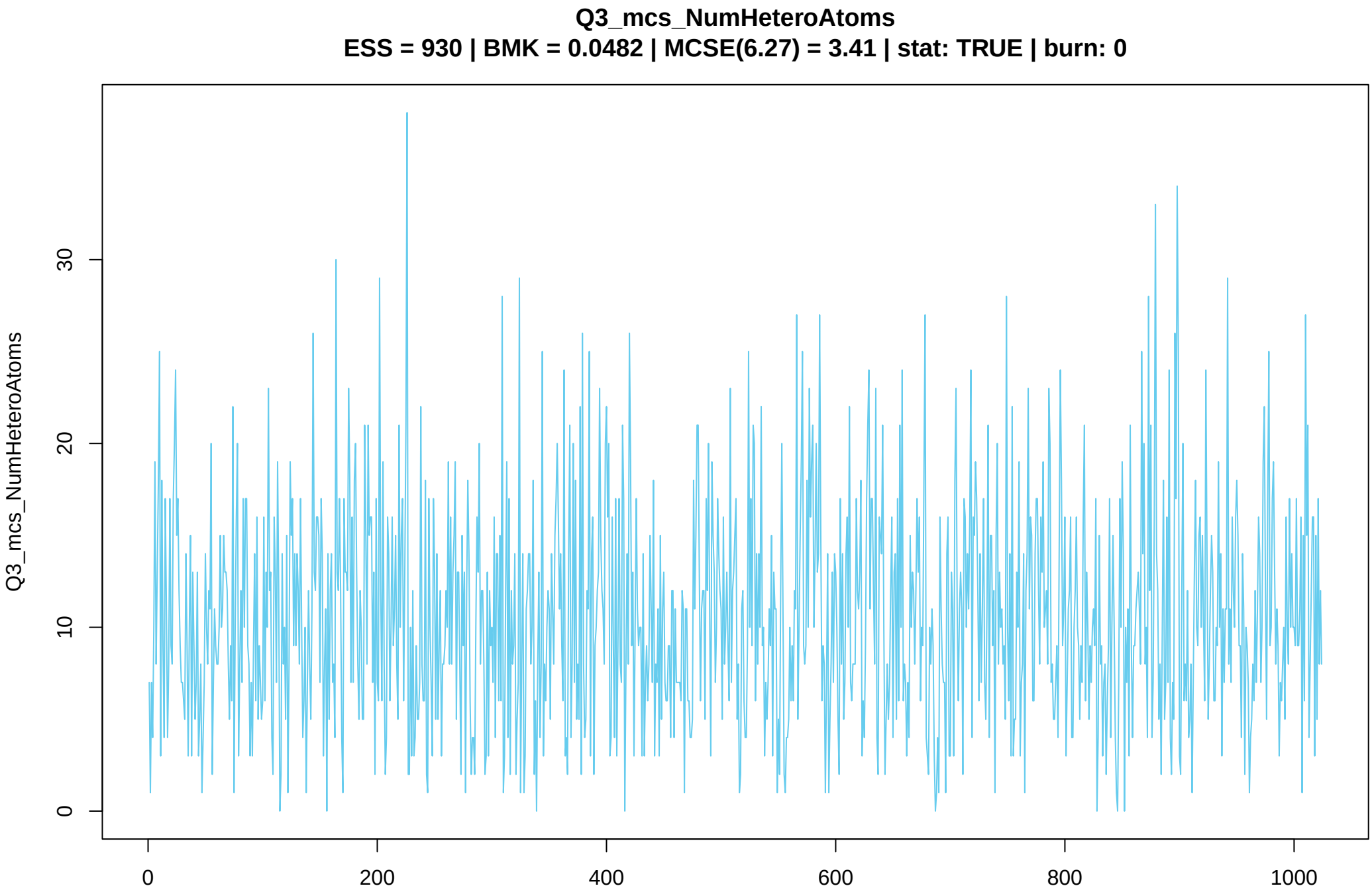

Q1_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0488 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0
Q1_docked_NumRotatableBonds
0
5
10
15
20
25
30
0
200
400
600
800
1000

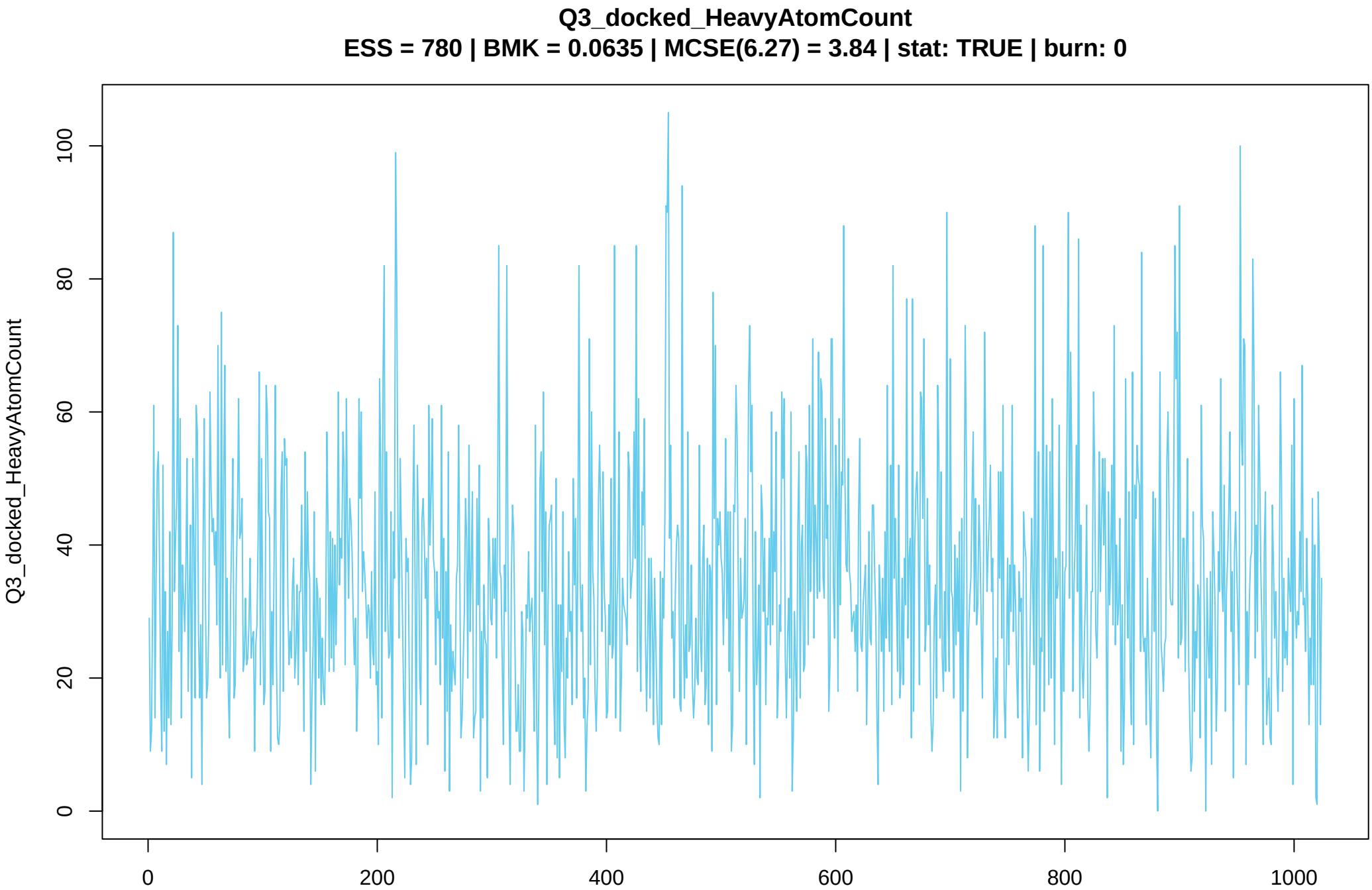

Q1_mcs_NOCount
ESS = 1020 | BMK = 0.0518 | MCSE(6.27) = 3 | stat: TRUE | burn: 0
Q1_mcs_NOCount
0
5
10
15
20
25
30
35
0
200
400
600
800
1000

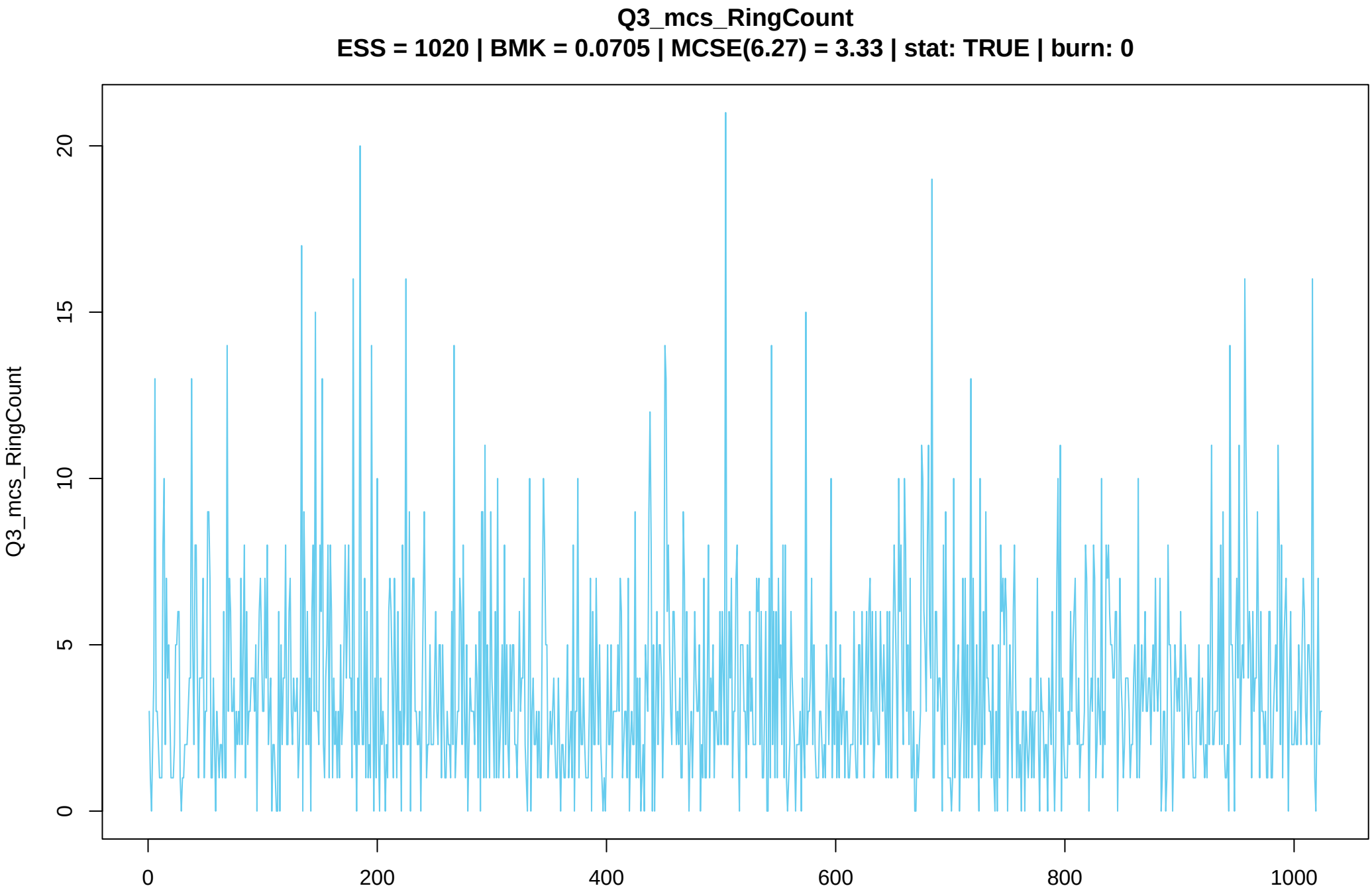

Q3_log_RMSD
ESS = 1020 | BMK = 0.169 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0
Q3_log_RMSD
0
100
200
300
400
0
200
400
600
800
1000

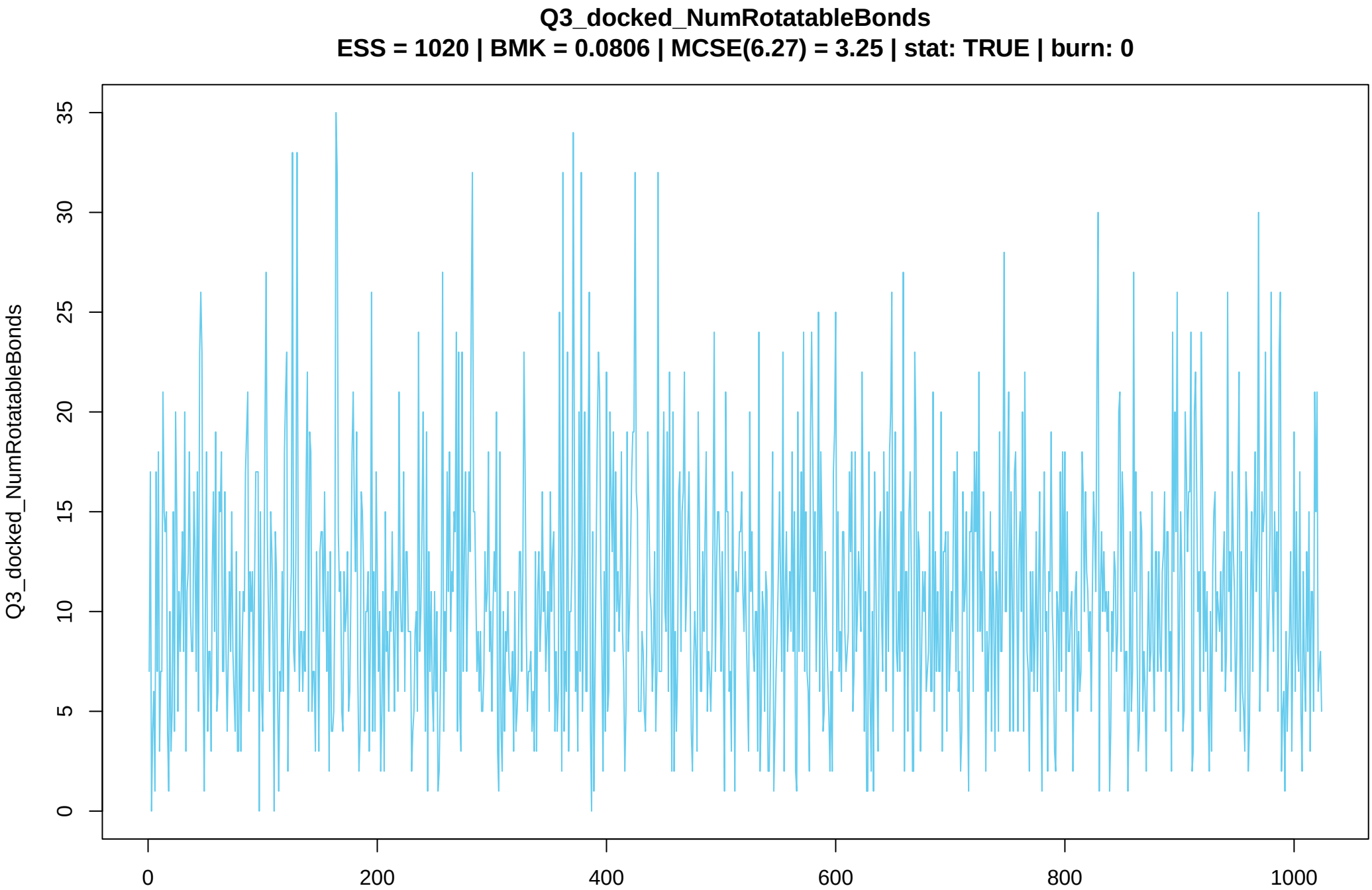

Q3_log_mcs_unbonded_polar_sasa
ESS = 984 | BMK = 0.189 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0
Q3_log_mcs_unbonded_polar_sasa
0
10
20
30
40
50
0
200
400
600
800
1000

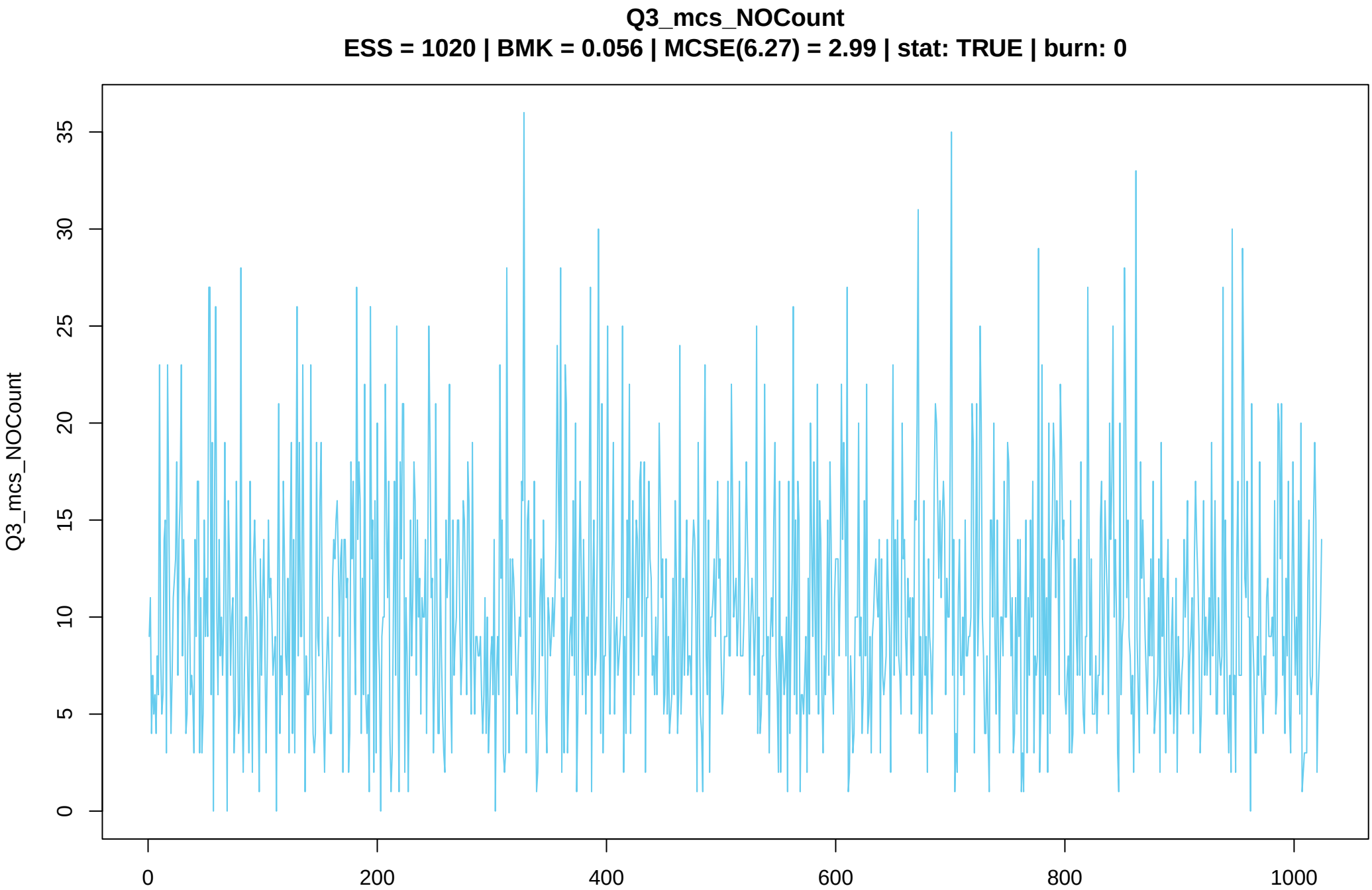

Q3_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.144 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0
Q3_logit_ec_tanimoto_similarity
−50
0
50
100
150
200
0
200
400
600
800
1000

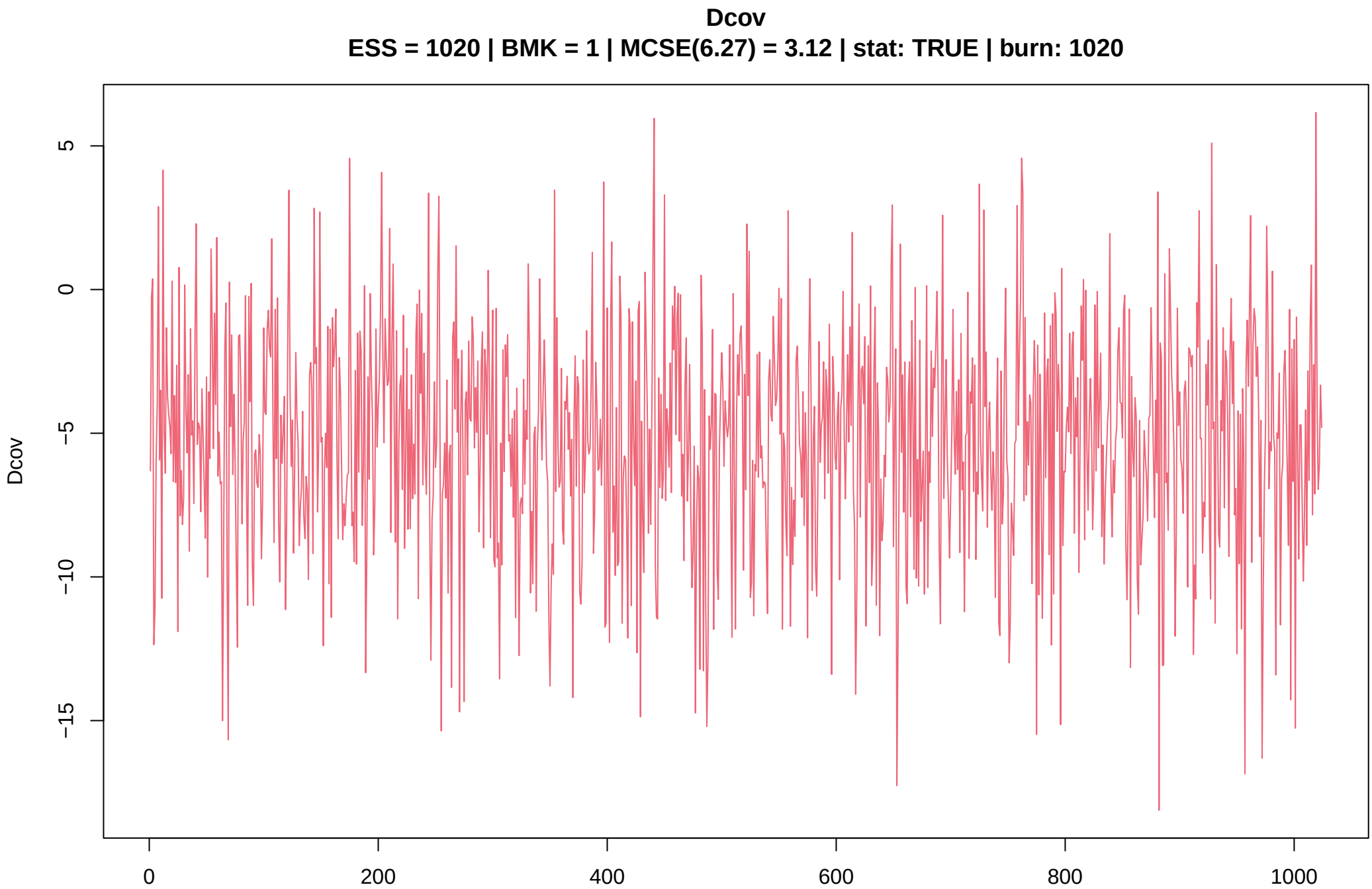

Q3_mcs_NumHeteroAtoms
ESS = 930 | BMK = 0.0482 | MCSE(6.27) = 3.41 | stat: TRUE | burn: 0
Q3_mcs_NumHeteroAtoms
0
10
20
30
0
200
400
600
800
1000

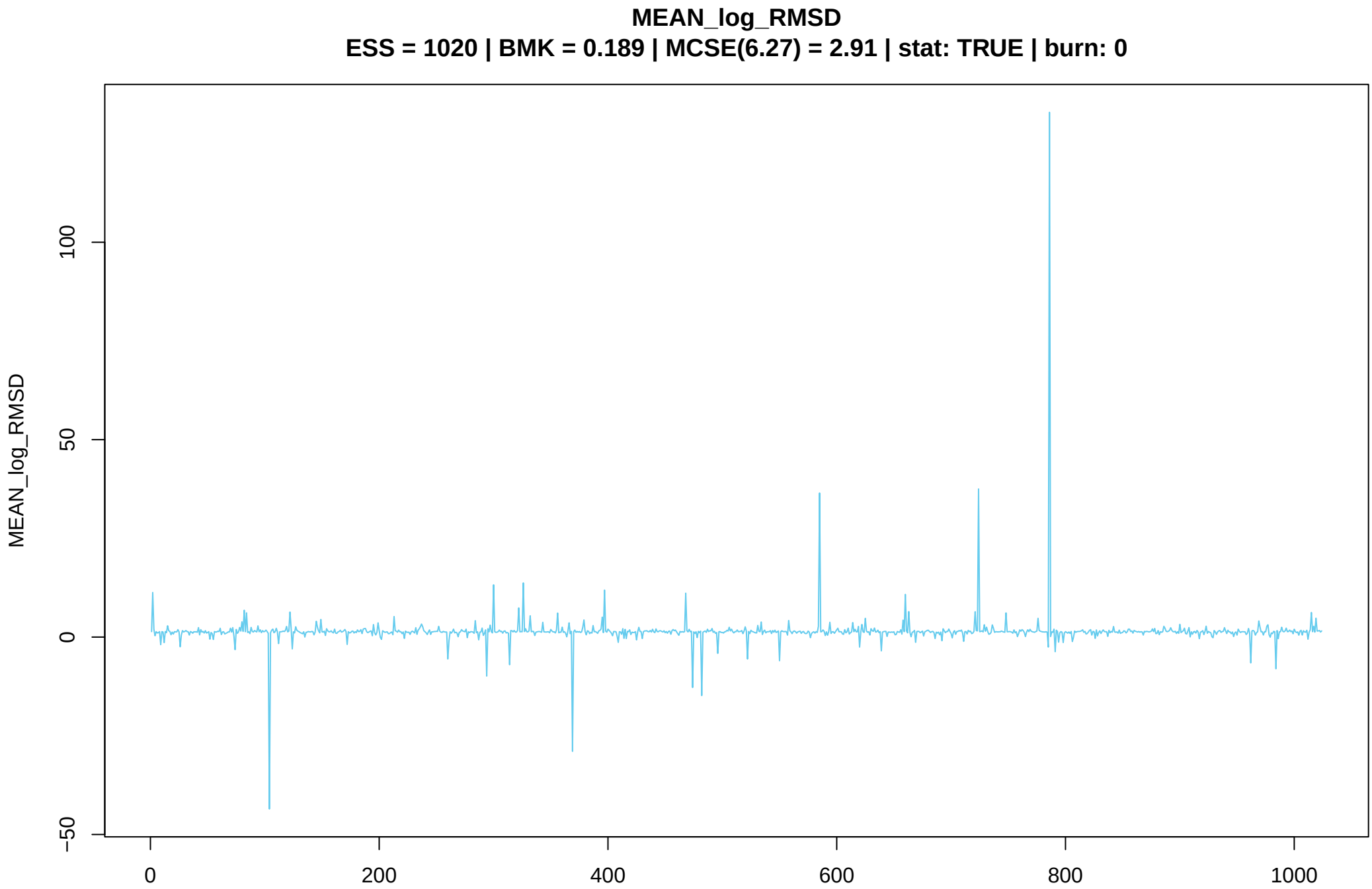

Q3_docked_HeavyAtomCount
ESS = 780 | BMK = 0.0635 | MCSE(6.27) = 3.84 | stat: TRUE | burn: 0
Q3_docked_HeavyAtomCount
0
20
40
60
80
100
0
200
400
600
800
1000

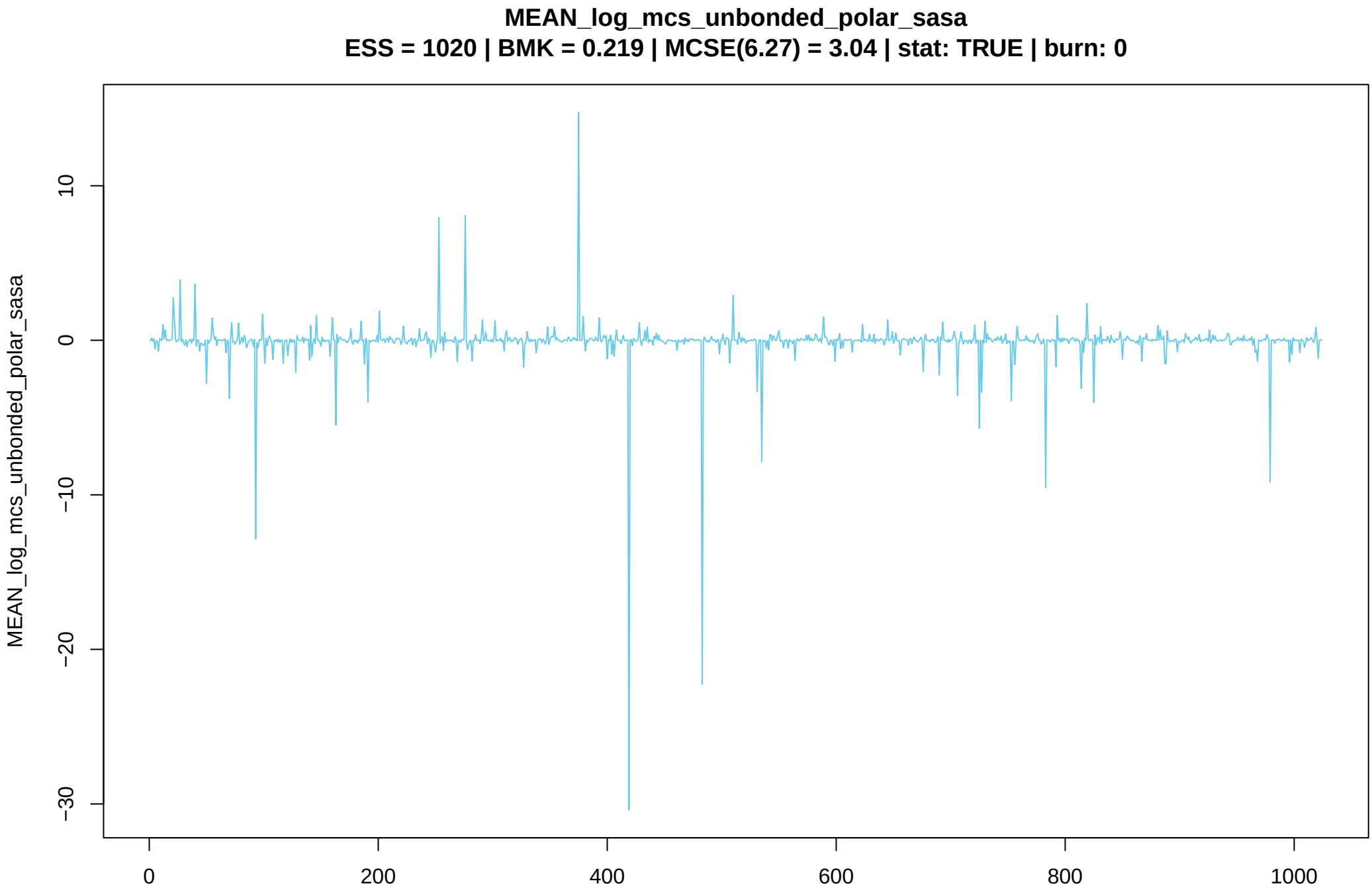

Q3_mcs_RingCount
ESS = 1020 | BMK = 0.0705 | MCSE(6.27) = 3.33 | stat: TRUE | burn: 0
Q3_mcs_RingCount
0
5
10
15
20
0
200
400
600
800
1000

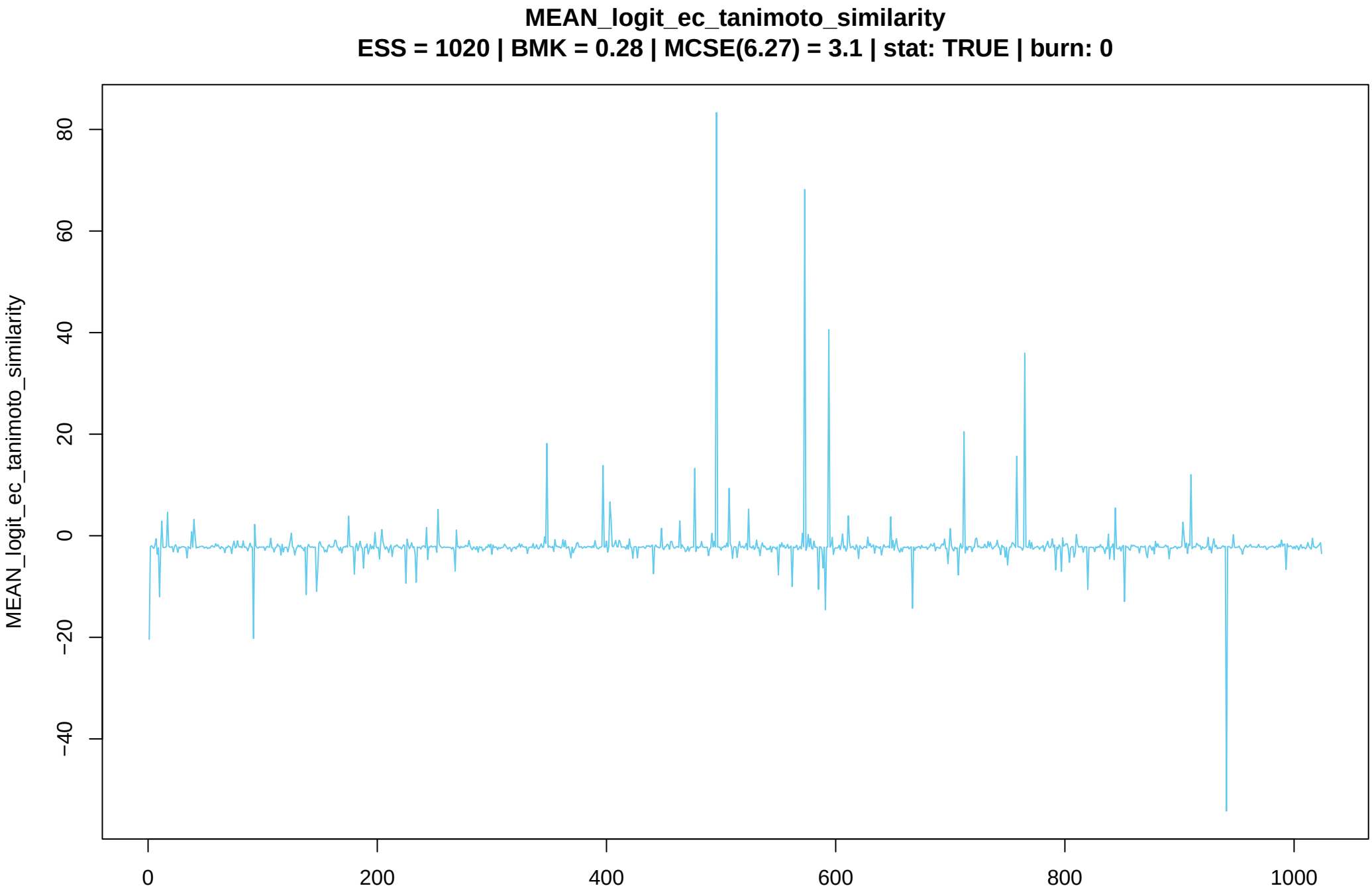

Q3_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0806 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0
Q3_docked_NumRotatableBonds
0
5
10
15
20
25
30
35
0
200
400
600
800
1000

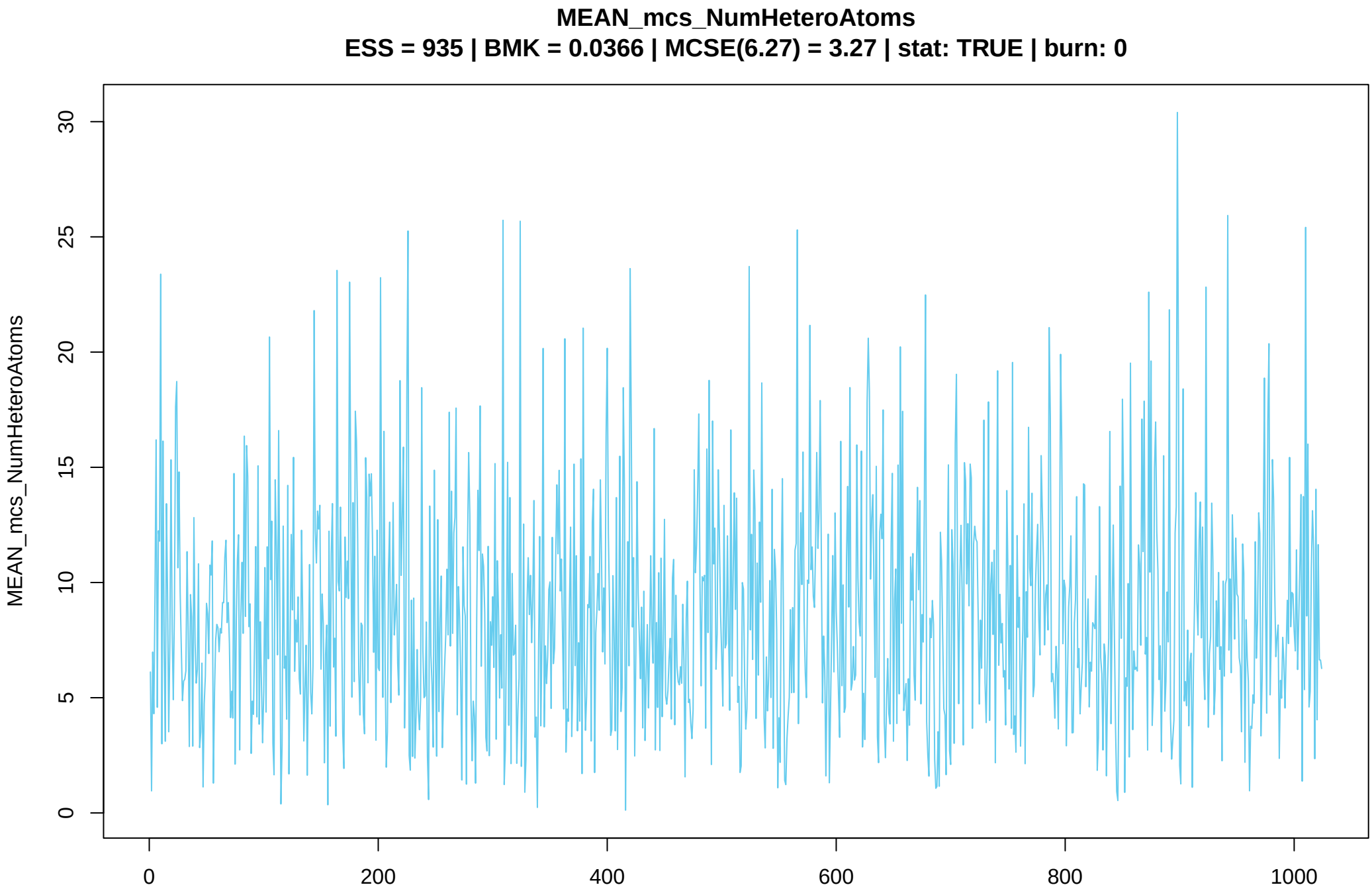

Q3_mcs_NOCount
ESS = 1020 | BMK = 0.056 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 0
Q3_mcs_NOCount
0
5
10
15
20
25
30
35
0
200
400
600
800
1000

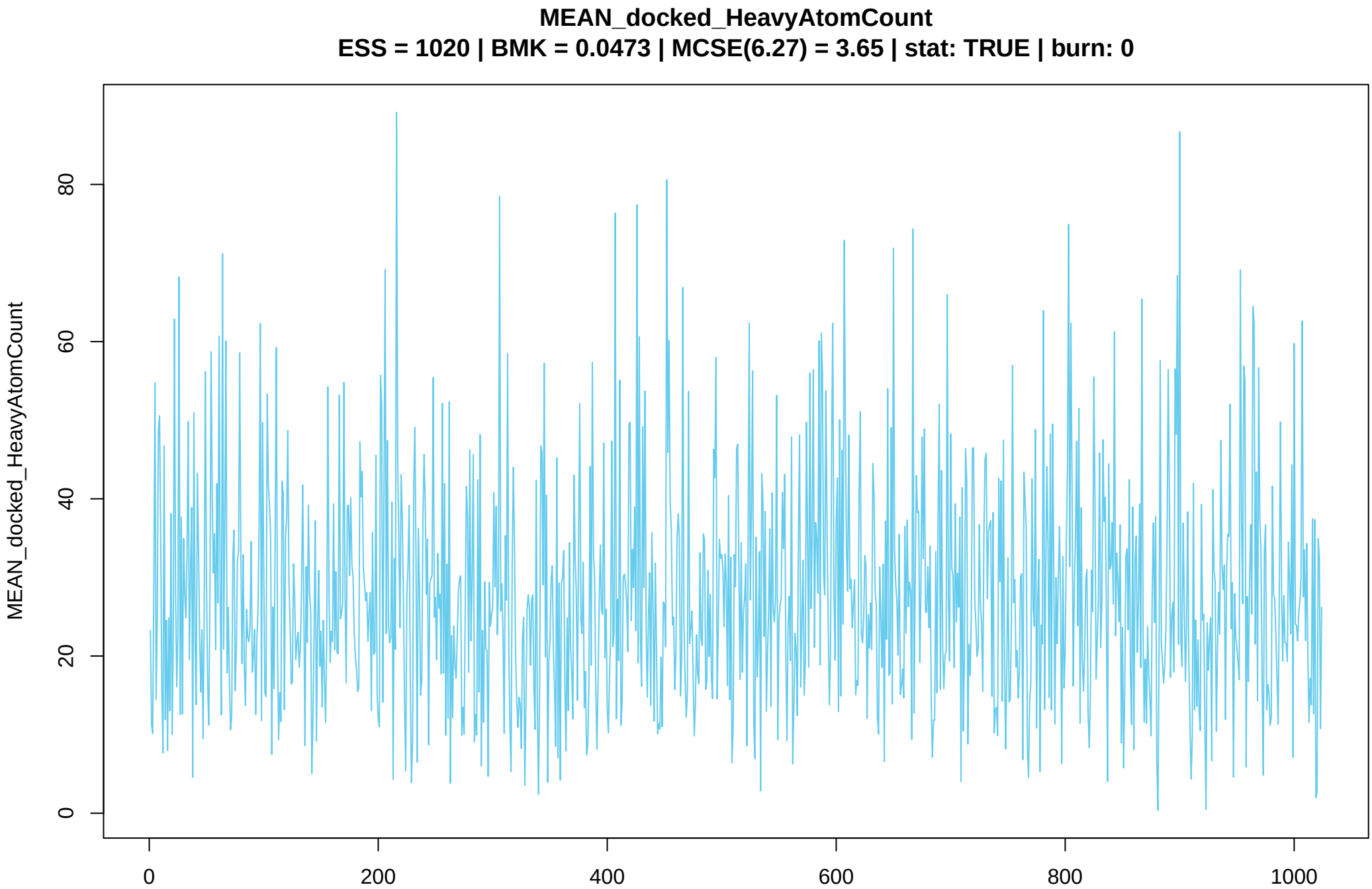

Dcov
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 1020
Dcov
5
0
−5
−10
−15
0
200
400
600
800
1000

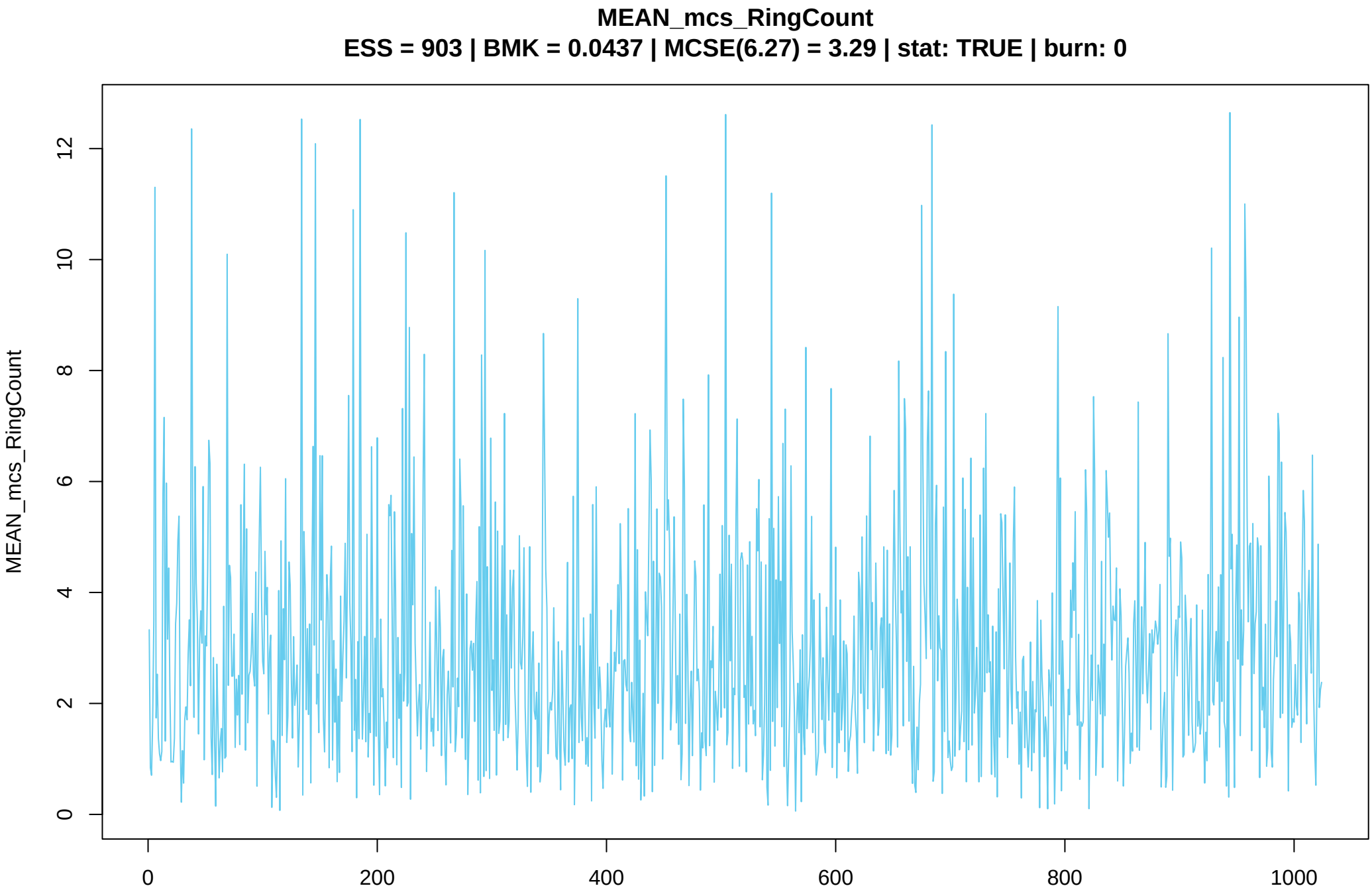

MEAN_log_RMSD
ESS = 1020 | BMK = 0.189 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0
MEAN_log_RMSD
−50
0
50
100
0
200
400
600
800
1000

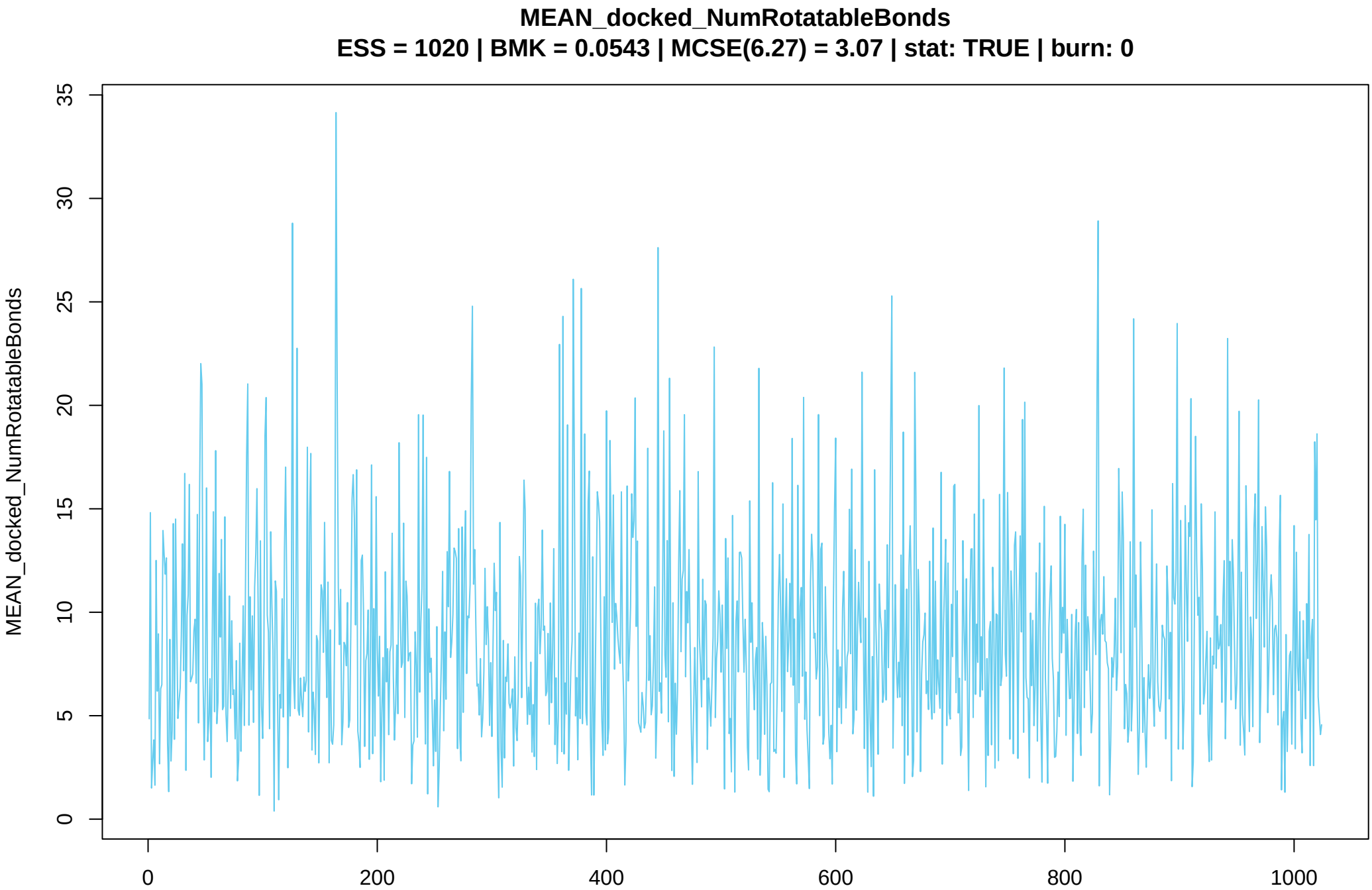

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.219 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0
MEAN_log_mcs_unbonded_polar_sasa
10
0
−10
−20
−30
0
200
400
600
800
1000

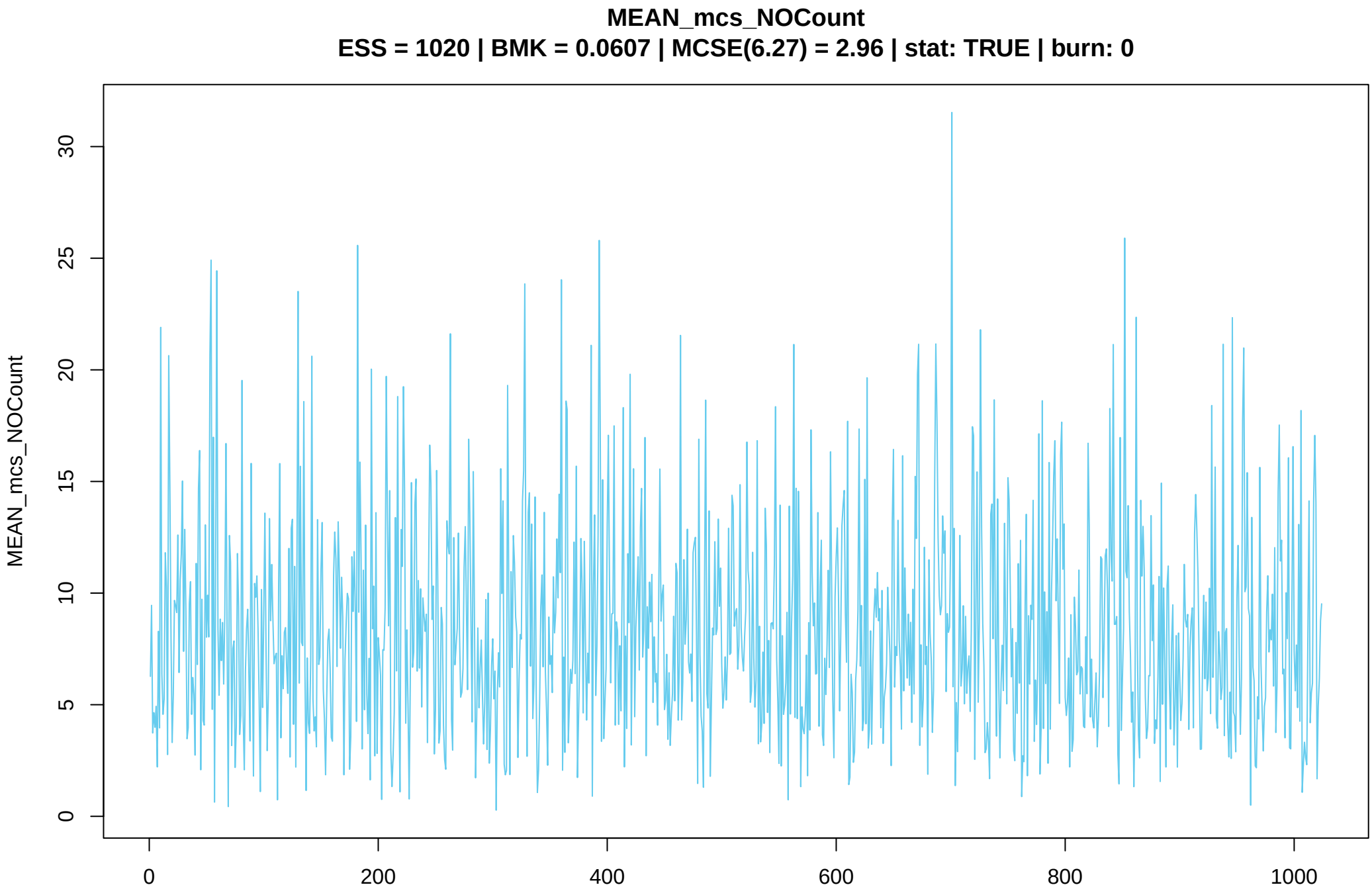

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.28 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0
MEAN_logit_ec_tanimoto_similarity
80
60
40
20
0
−20
−40
0
200
400
600
800
1000

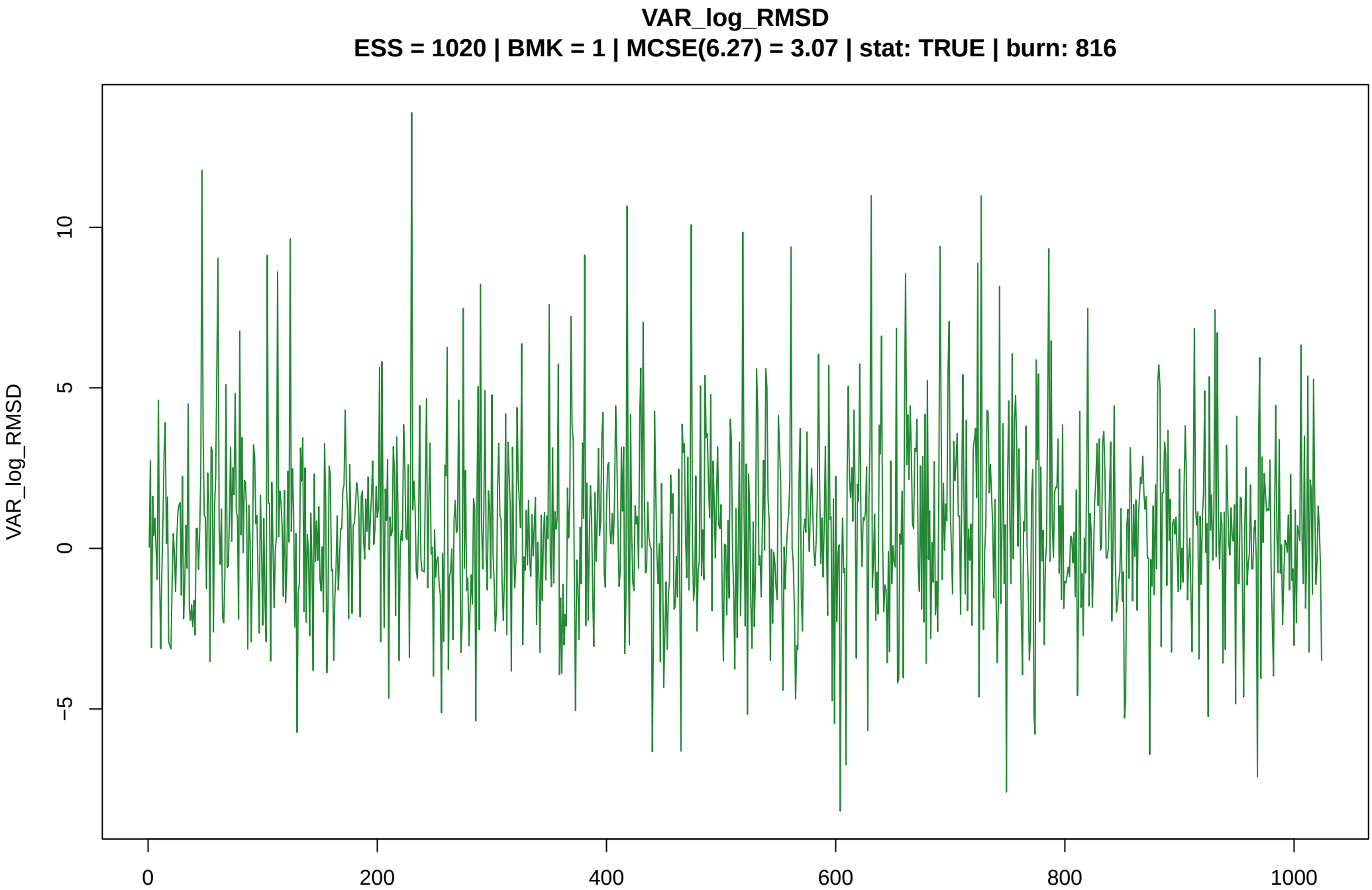

MEAN_mcs_NumHeteroAtoms
ESS = 935 | BMK = 0.0366 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
0
5
10
15
20
25
30
0
200
400
600
800
1000

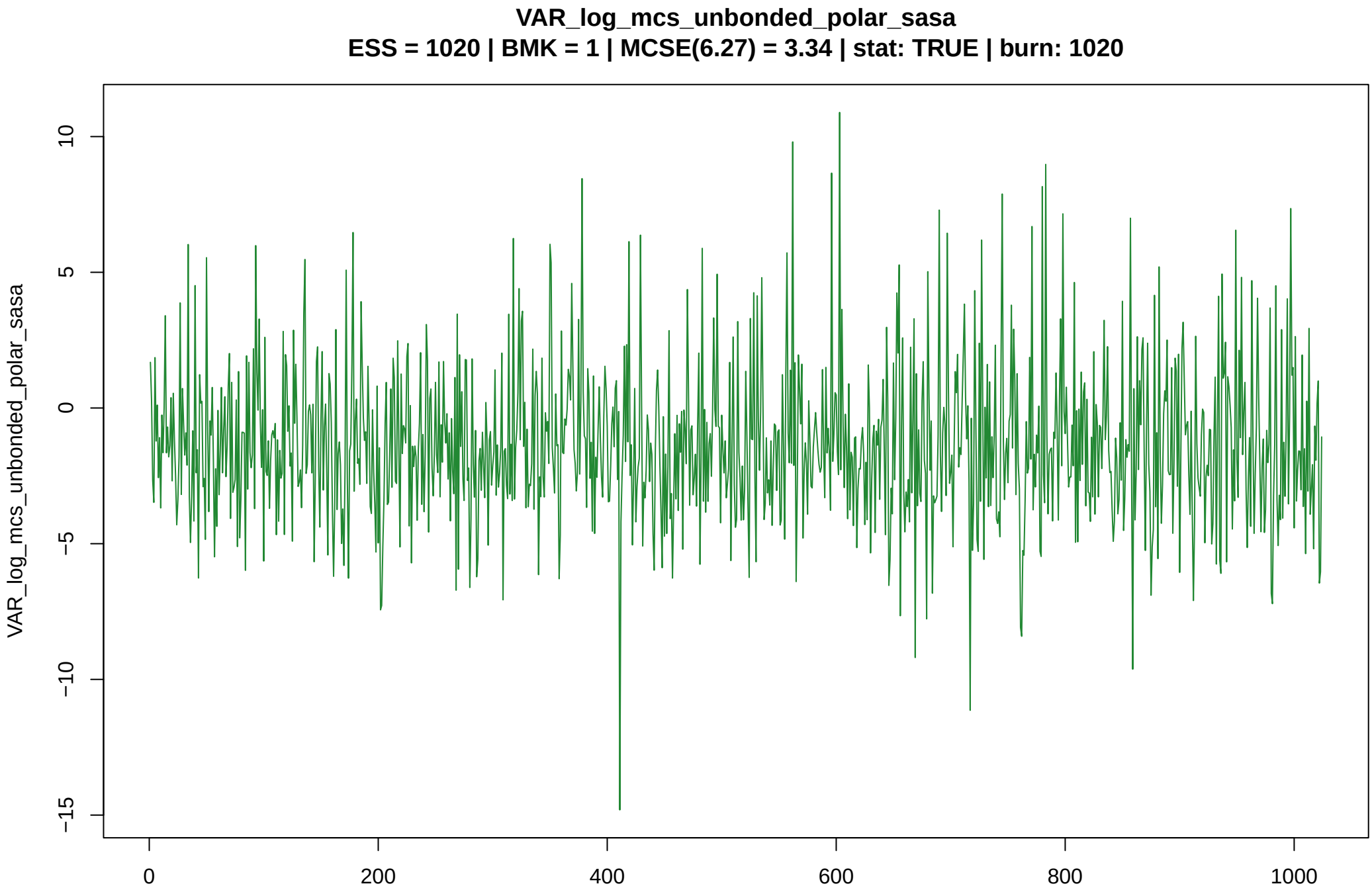

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0473 | MCSE(6.27) = 3.65 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
0
20
40
60
80
0
200
400
600
800
1000

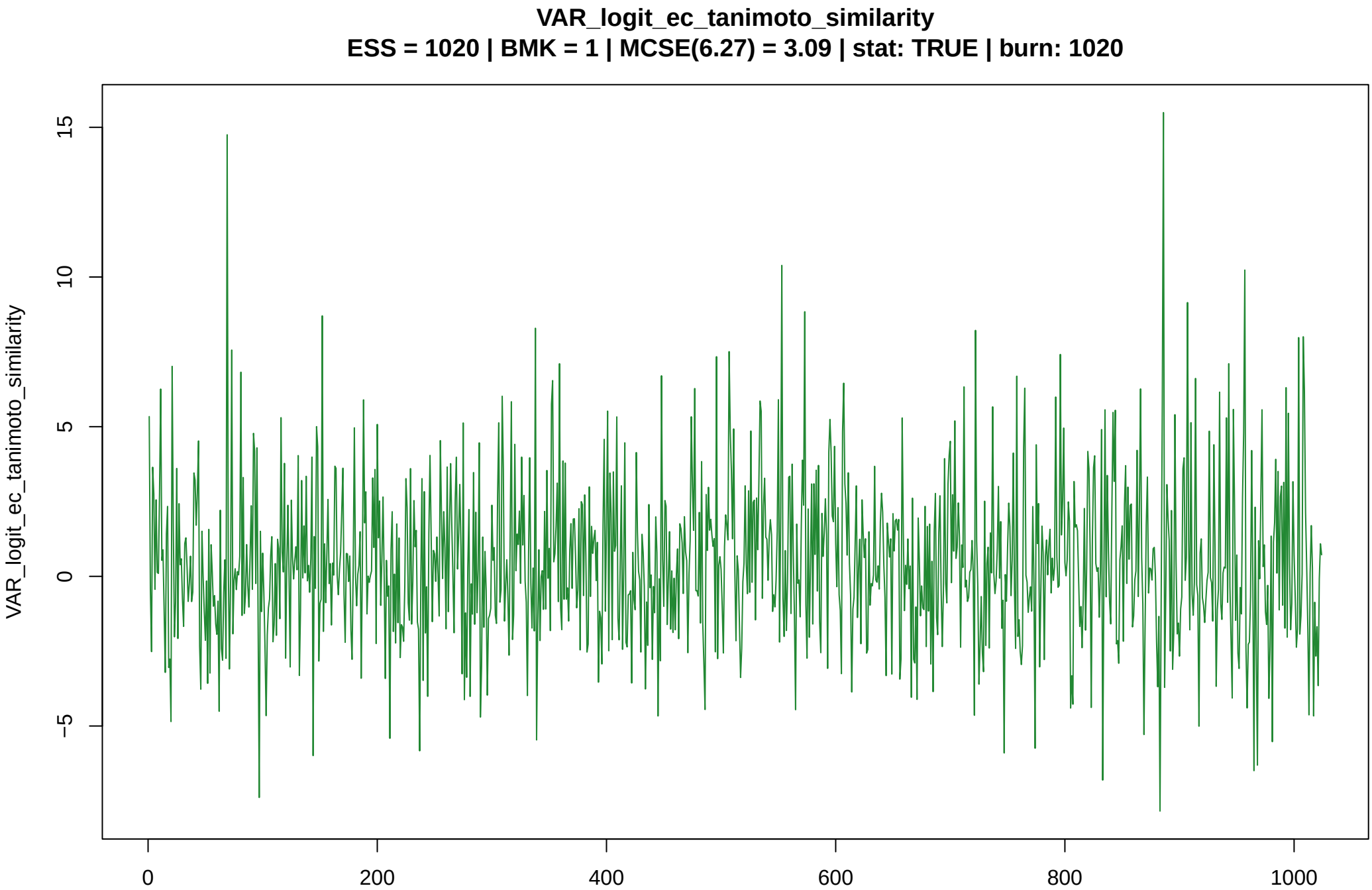

MEAN_mcs_RingCount
ESS = 903 | BMK = 0.0437 | MCSE(6.27) = 3.29 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0
2
4
6
8
10
12
0
200
400
600
800
1000

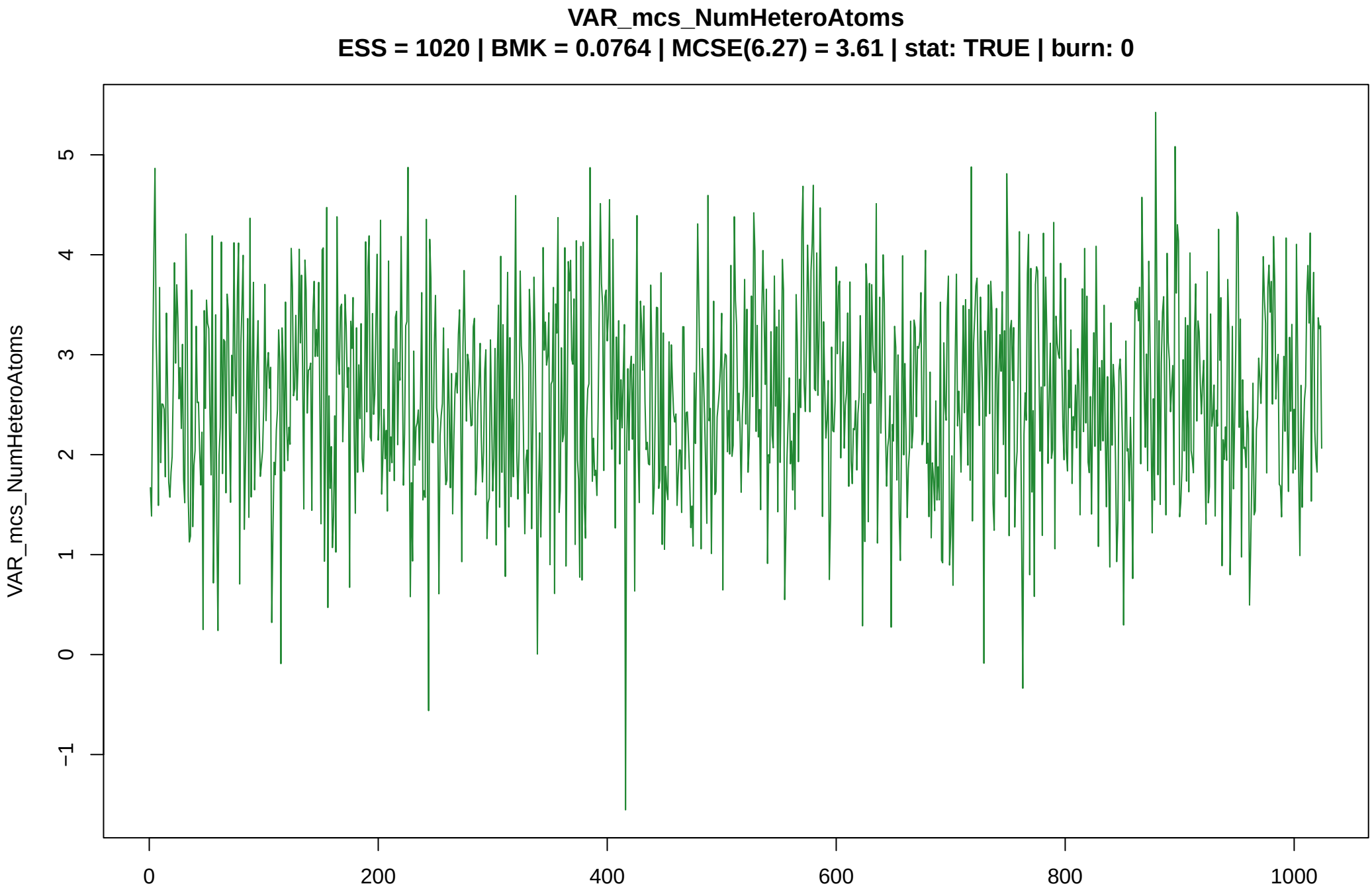

MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0543 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0
MEAN_docked_NumRotatableBonds
0
5
10
15
20
25
30
35
0
200
400
600
800
1000

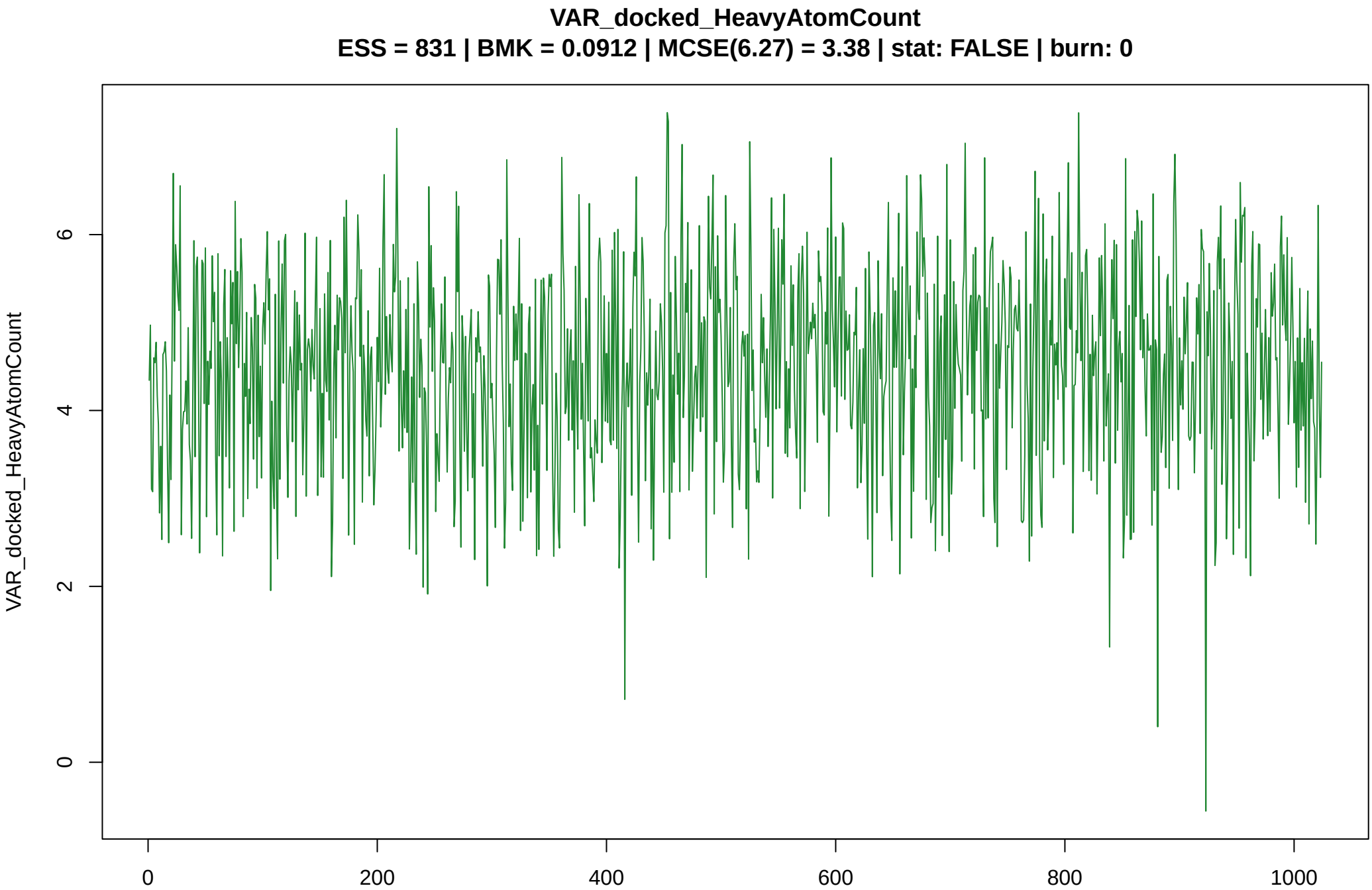

MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0607 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0
MEAN_mcs_NOCount
0
5
10
15
20
25
30
0
200
400
600
800
1000

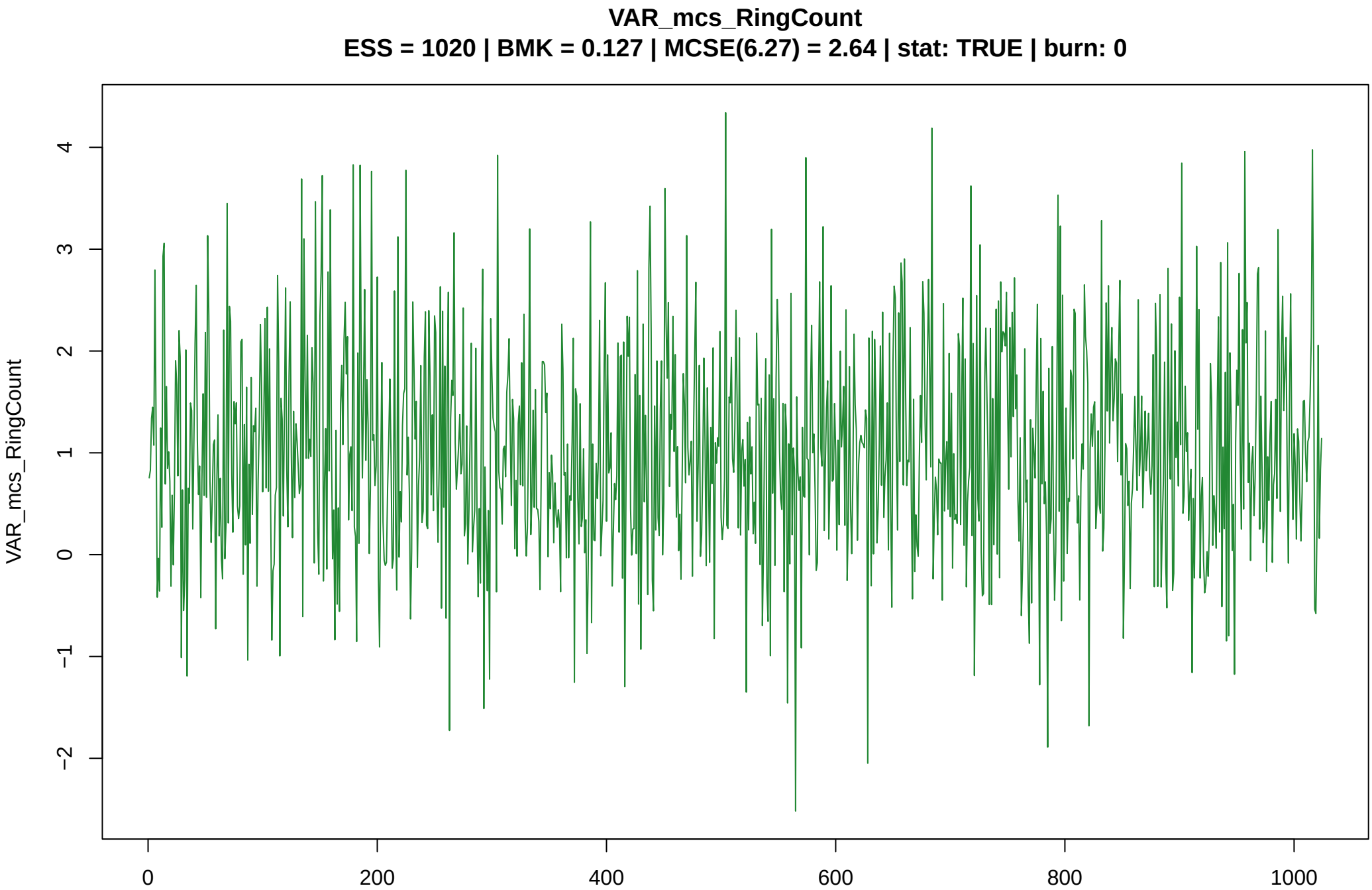

VAR_log_RMSD
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 816
VAR_log_RMSD
10
5
0
−5
0
200
400
600
800
1000

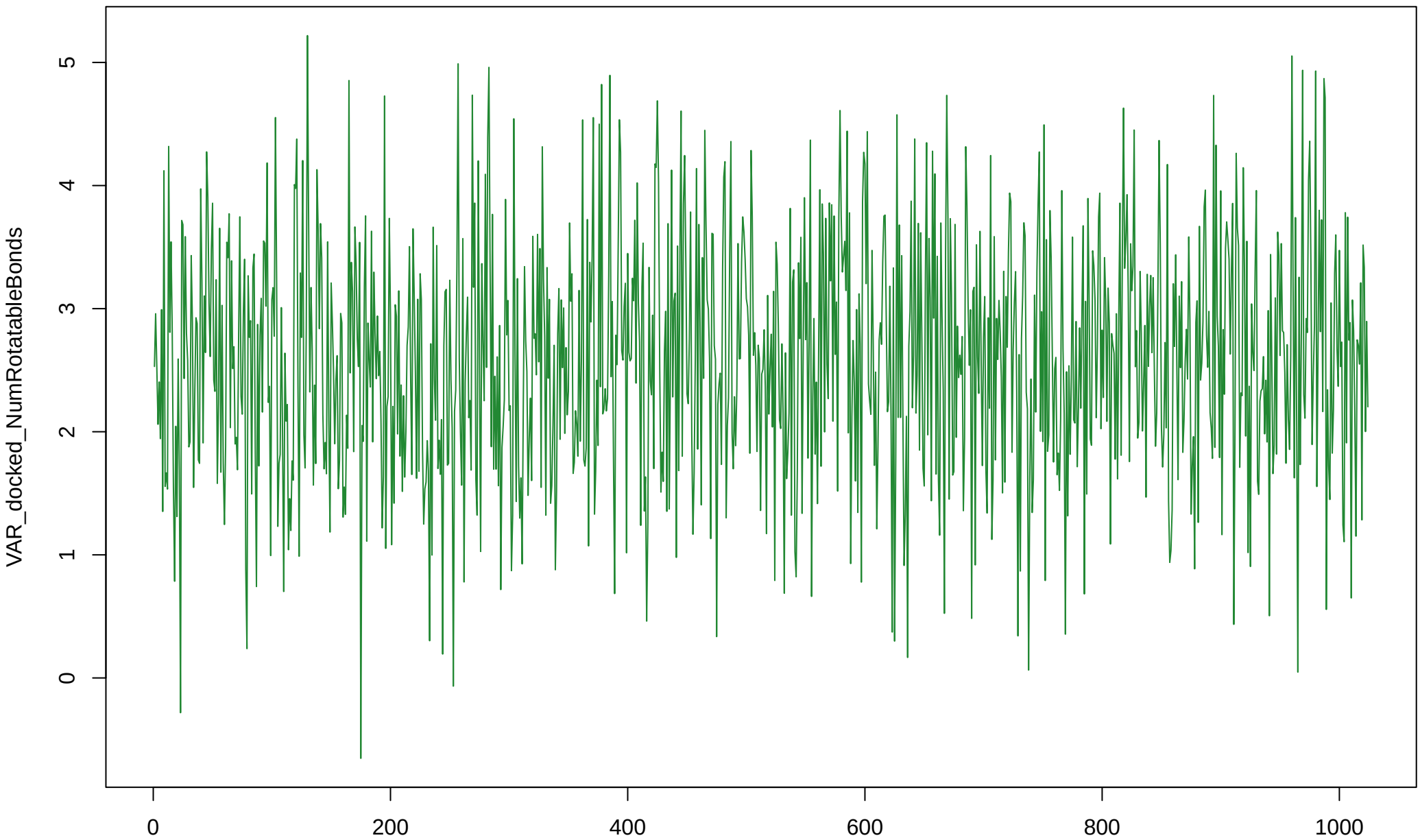

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 1020
VAR_log_mcs_unbonded_polar_sasa
10
5
0
−5
−10
−15
0
200
400
600
800
1000

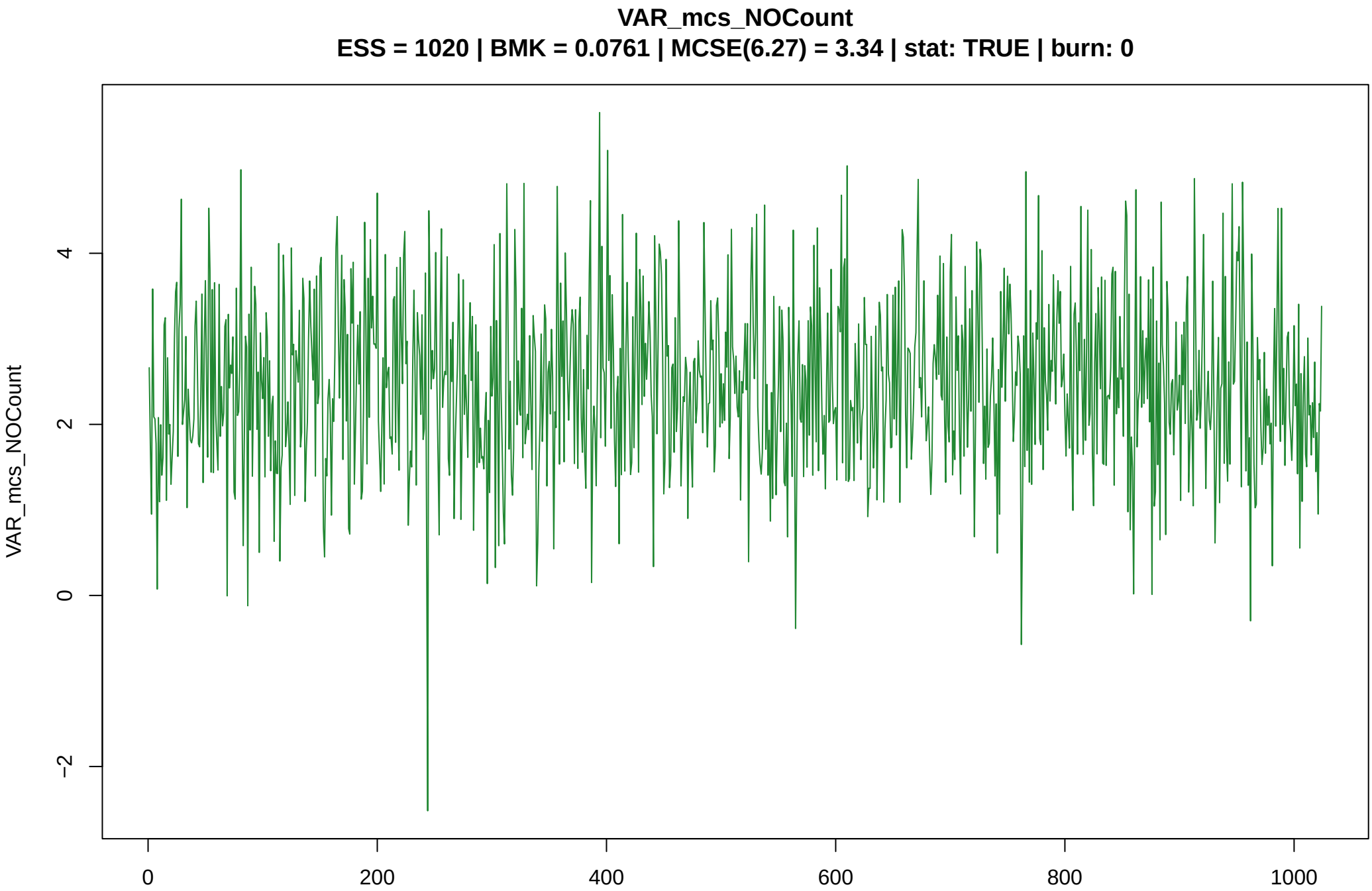

VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 1020
VAR_logit_ec_tanimoto_similarity
15
10
5
0
−5
0
200
400
600
800
1000

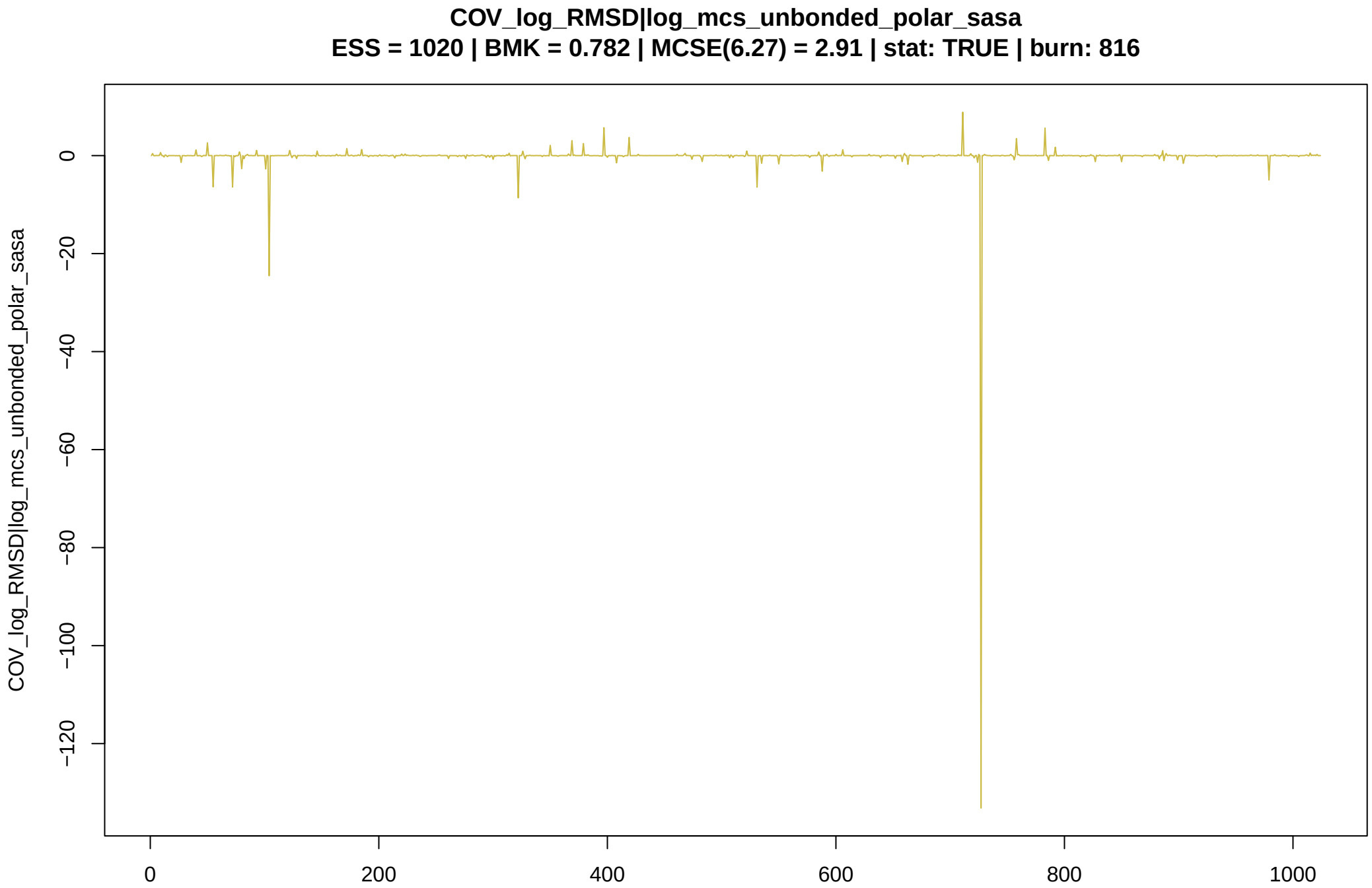

VAR_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0764 | MCSE(6.27) = 3.61 | stat: TRUE | burn: 0
VAR_mcs_NumHeteroAtoms
−1
0
1
2
3
4
5
0
200
400
600
800
1000

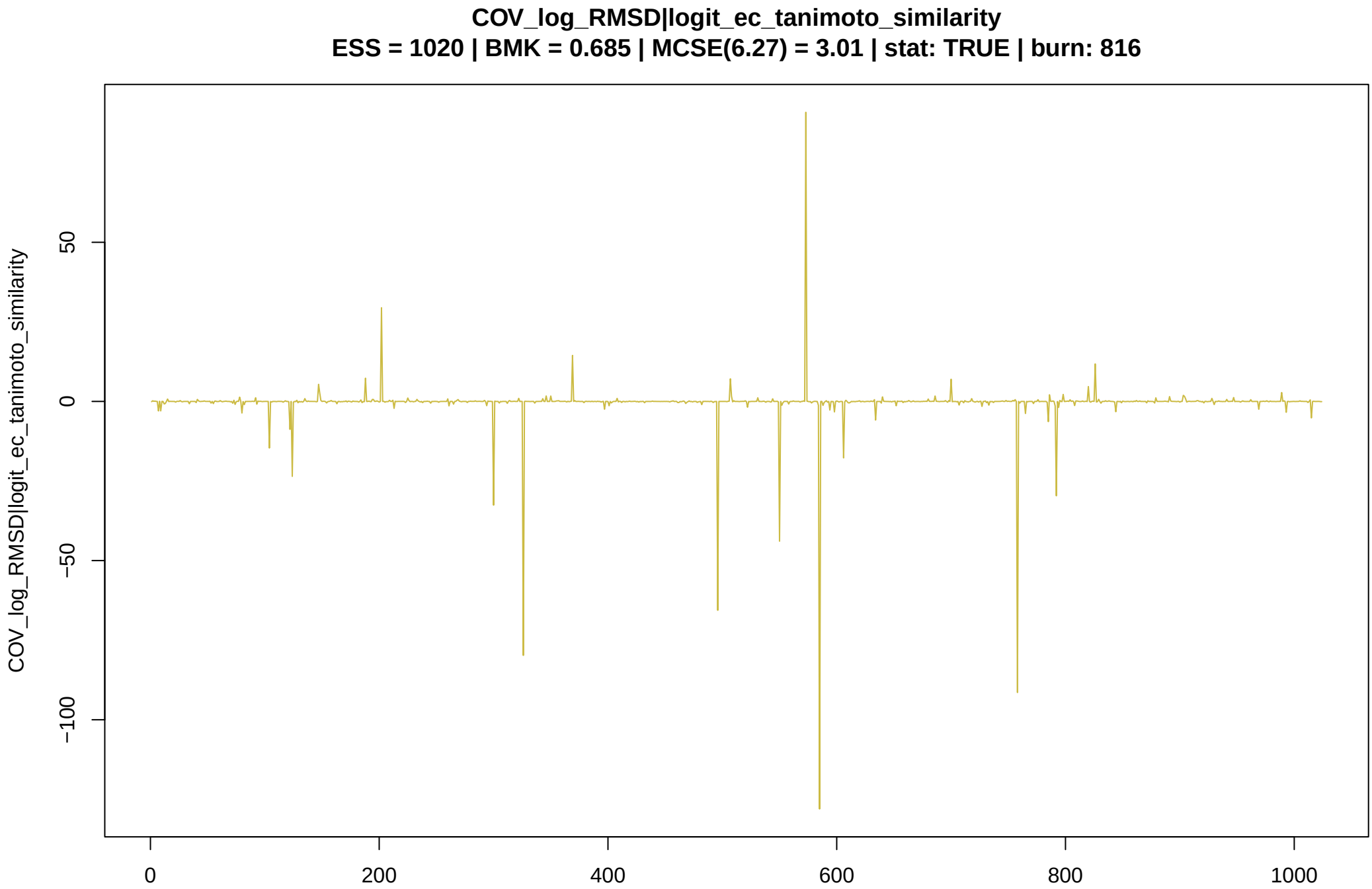

VAR_docked_HeavyAtomCount
ESS = 831 | BMK = 0.0912 | MCSE(6.27) = 3.38 | stat: FALSE | burn: 0
VAR_docked_HeavyAtomCount
0
2
4
6
0
200
400
600
800
1000

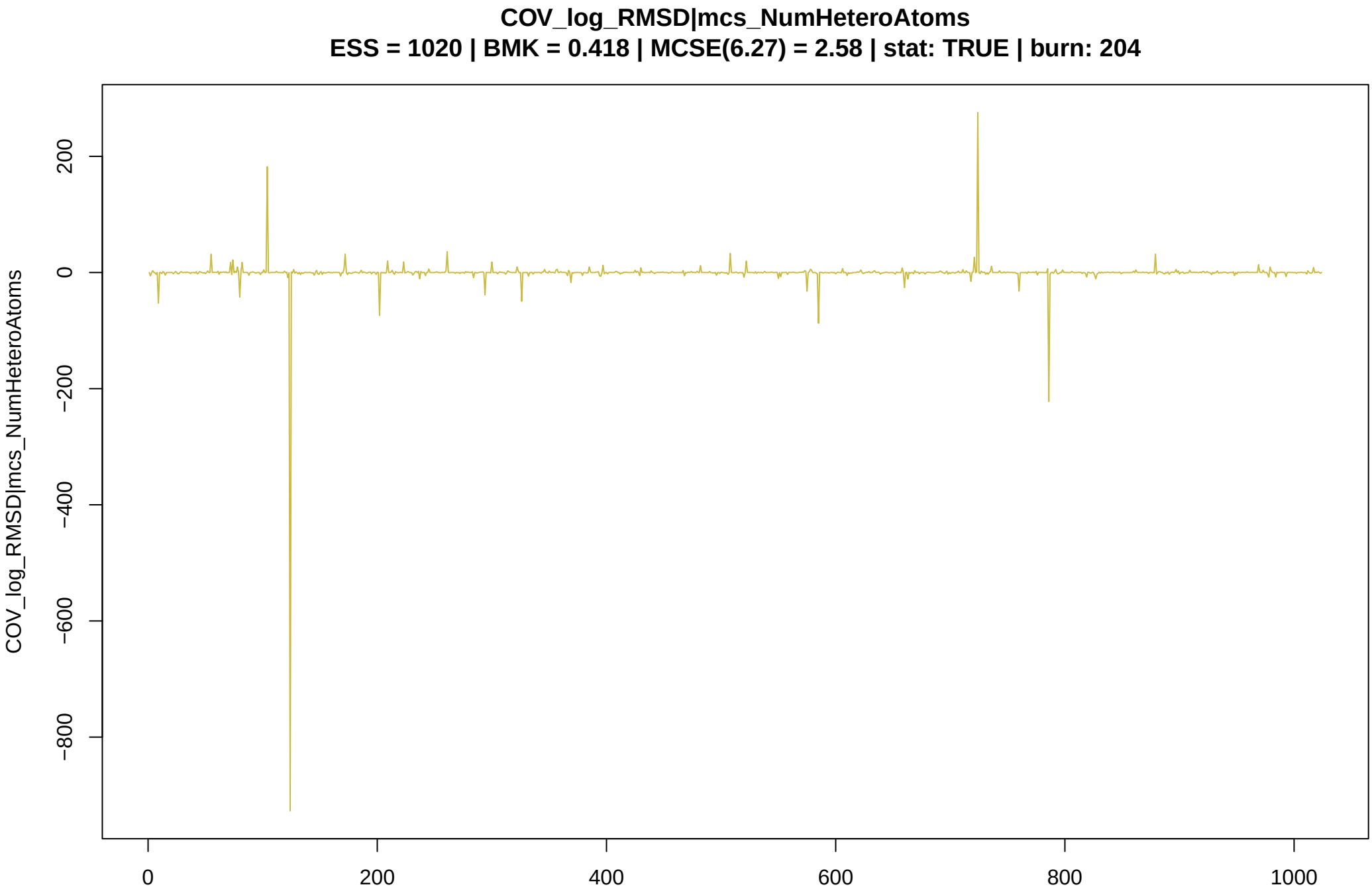

VAR_mcs_RingCount
ESS = 1020 | BMK = 0.127 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0
VAR_mcs_RingCount
4
3
2
1
0
−1
−2
0
200
400
600
800
1000

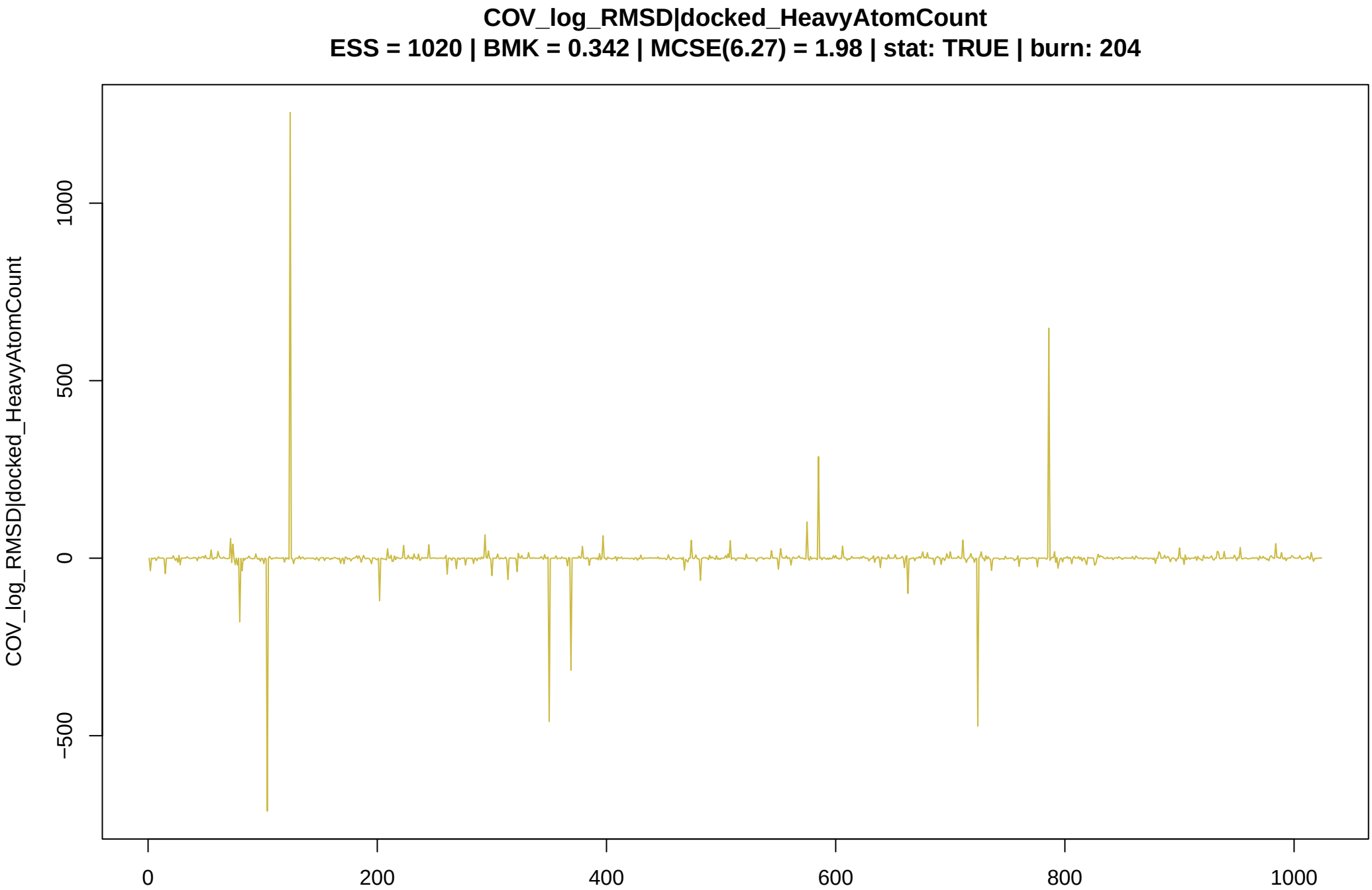

VAR_docked_NumRotatableBonds
ESS = 915 | BMK = 0.0852 | MCSE(6.27) = 3.84 | stat: TRUE | burn: 0
VAR_docked_NumRotatableBonds
0
1
2
3
4
5
0
200
400
600
800
1000

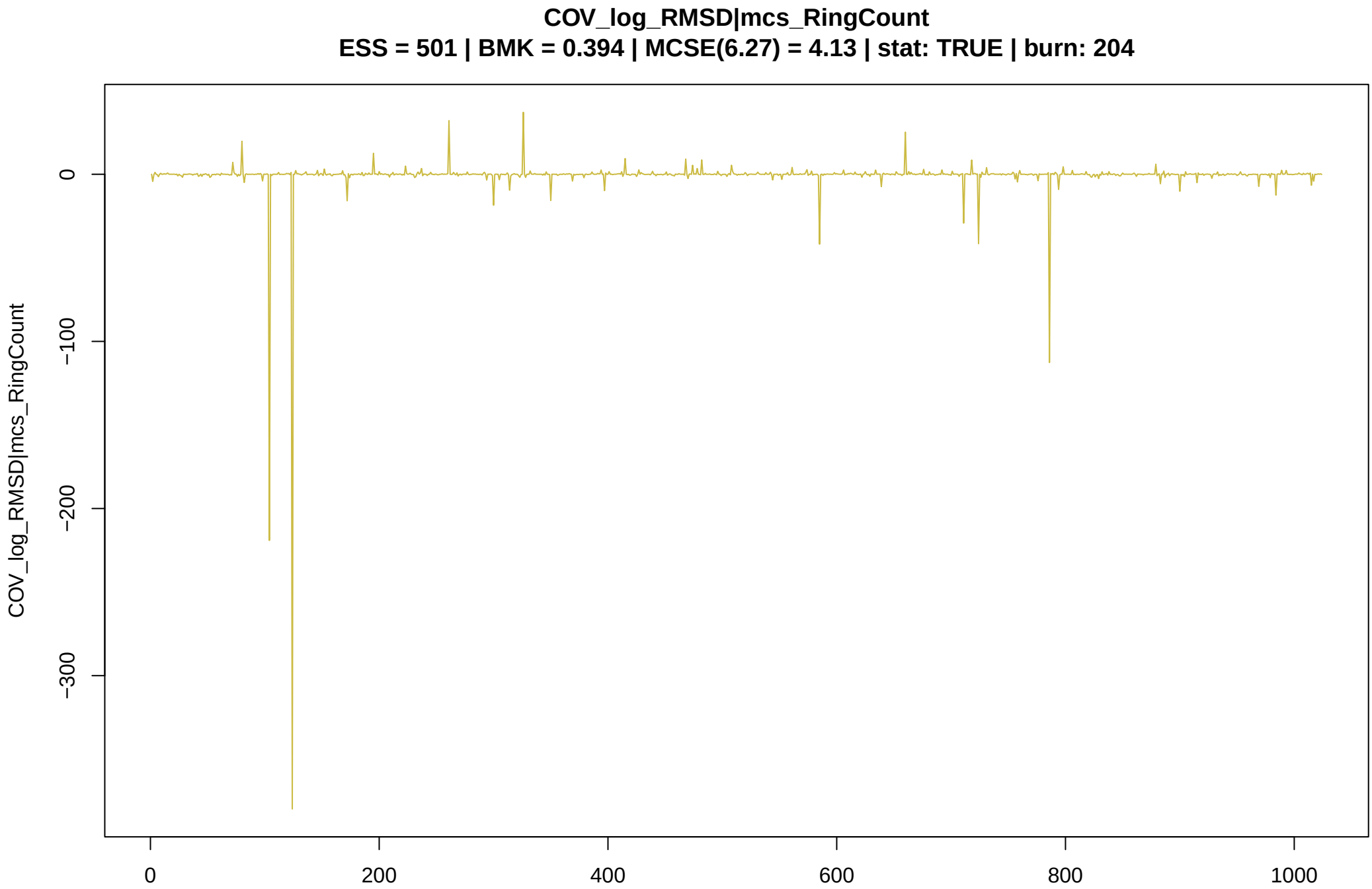

VAR_mcs_NOCount
ESS = 1020 | BMK = 0.0761 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 0
VAR_mcs_NOCount
4
2
0
−2
0
200
400
600
800
1000

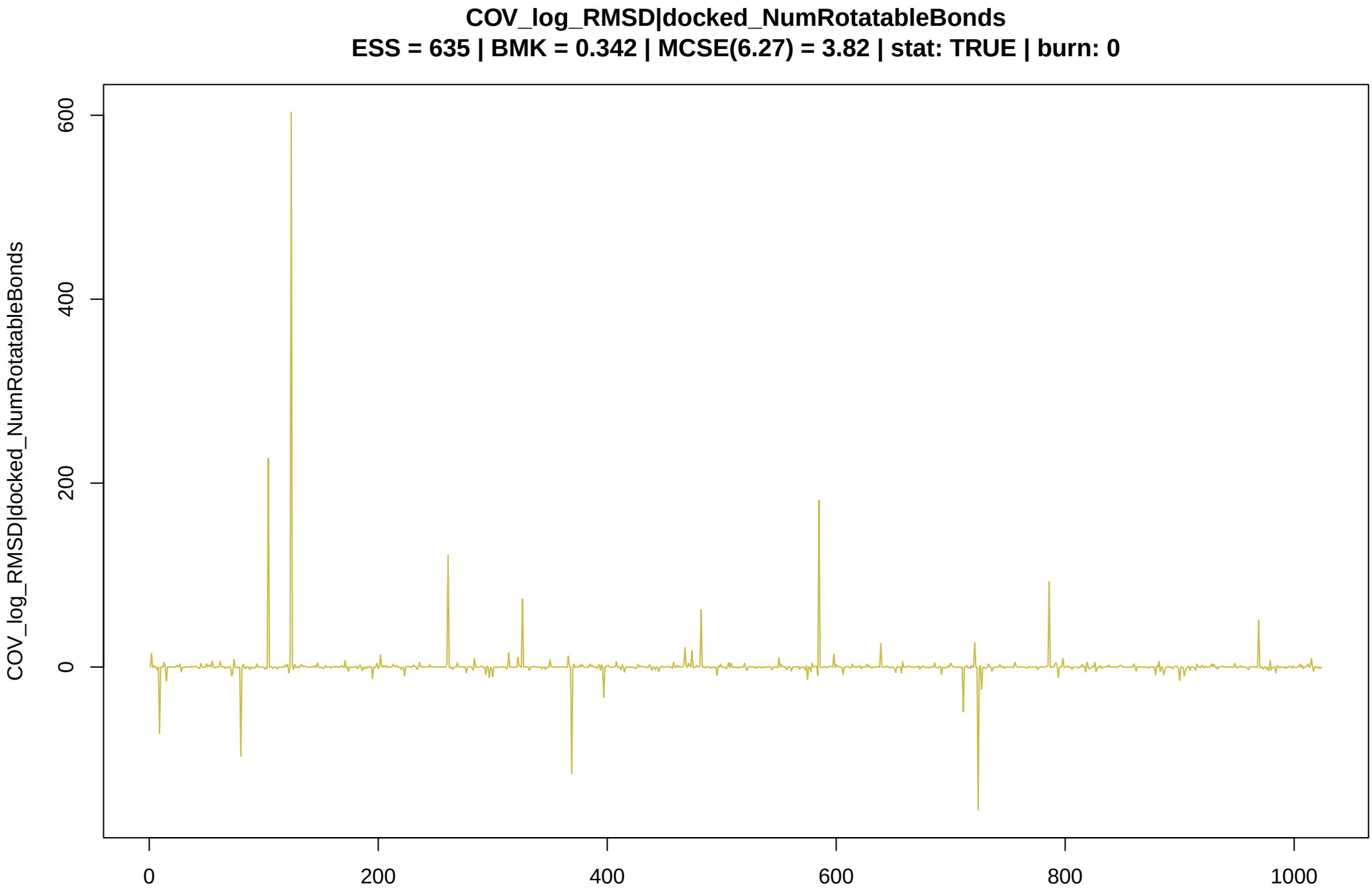

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.782 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 816
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0
−20
−40
−60
−80
−100
−120
0
200
400
600
800
1000

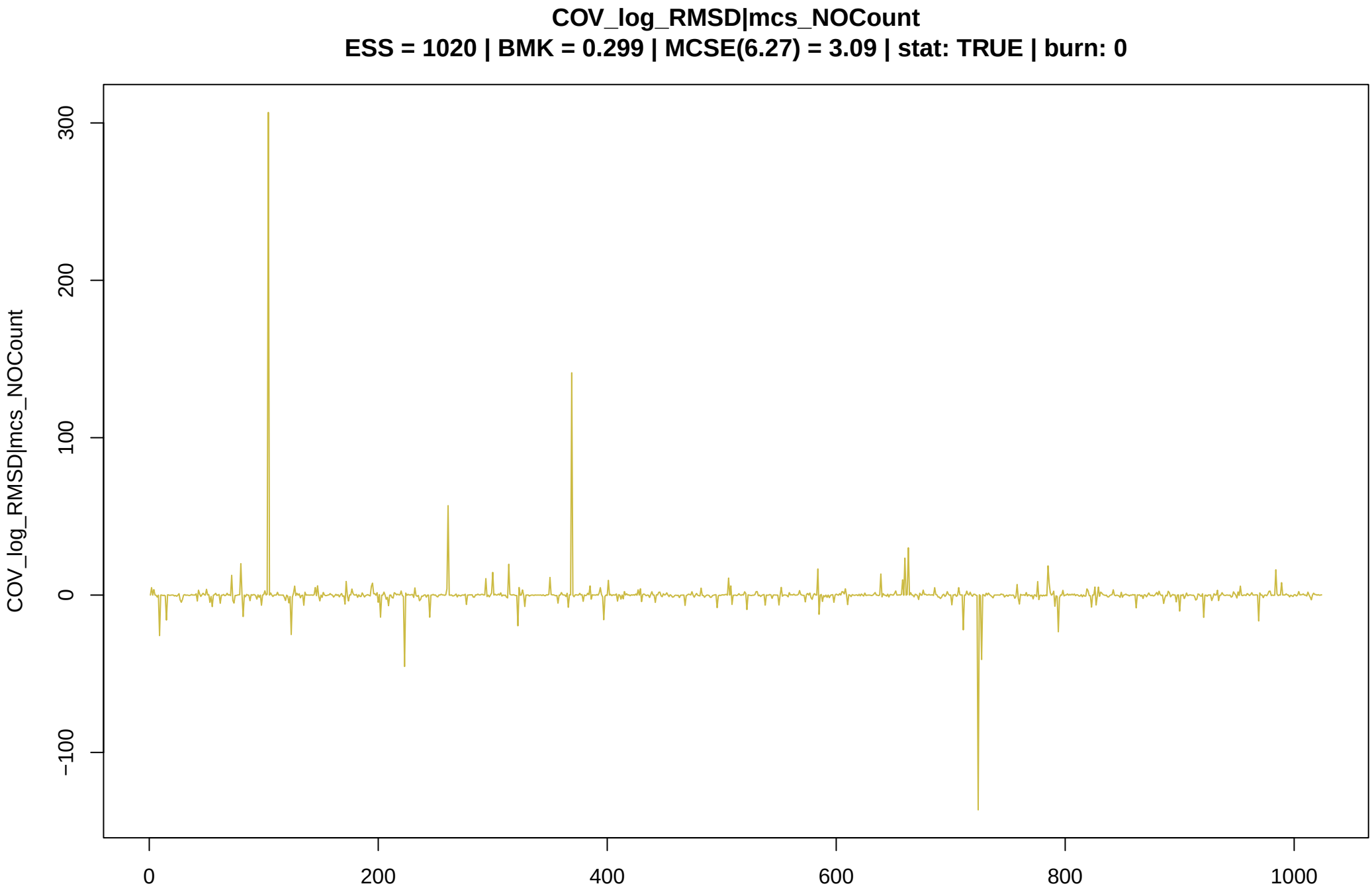

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.685 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 816
COV_log_RMSD|logit_ec_tanimoto_similarity
50
0
−50
−100
0
200
400
600
800
1000

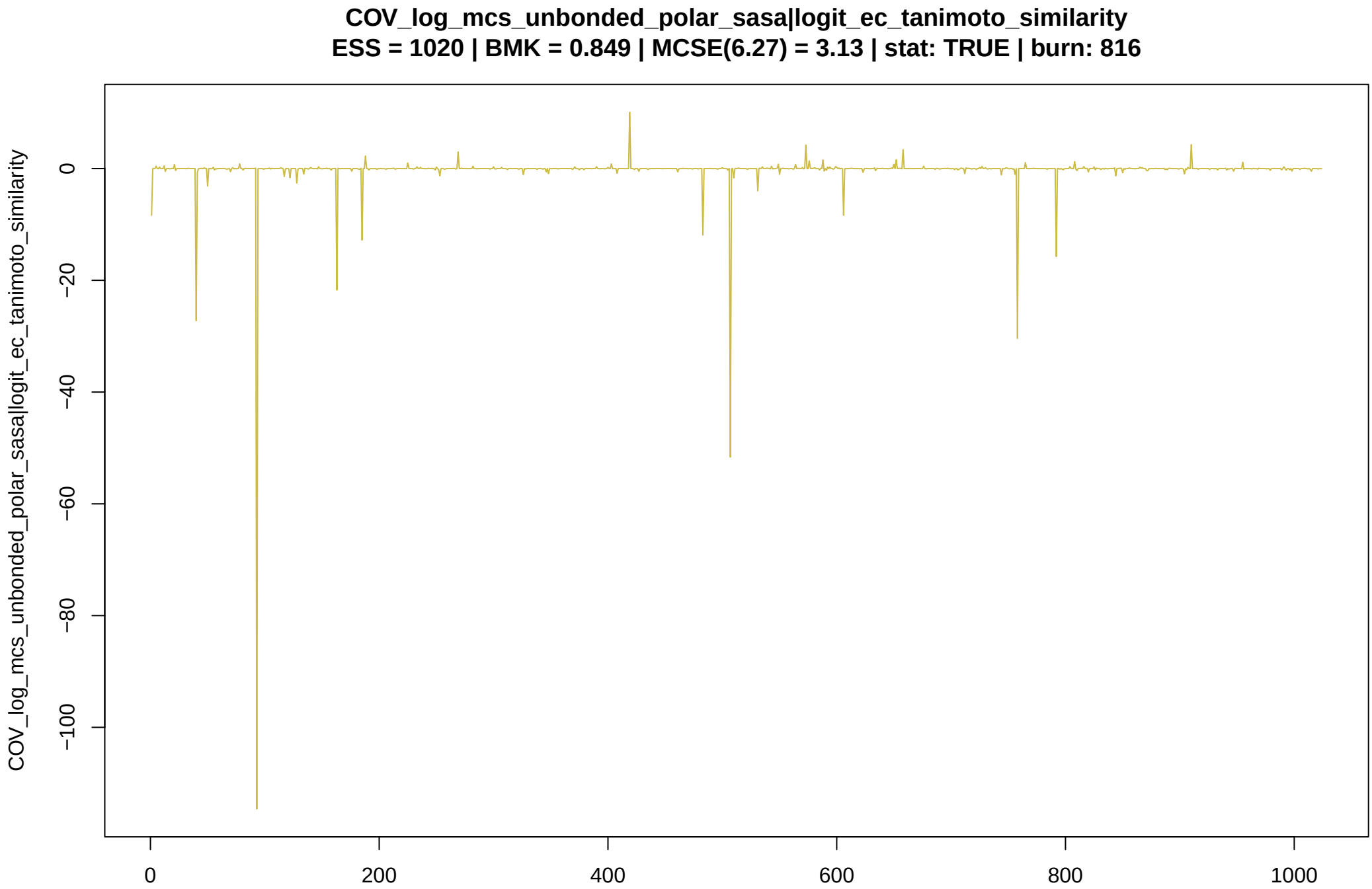

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.418 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 204
COV_log_RMSD|mcs_NumHeteroAtoms
200
0
−200
−400
−600
−800
0
200
400
600
800
1000

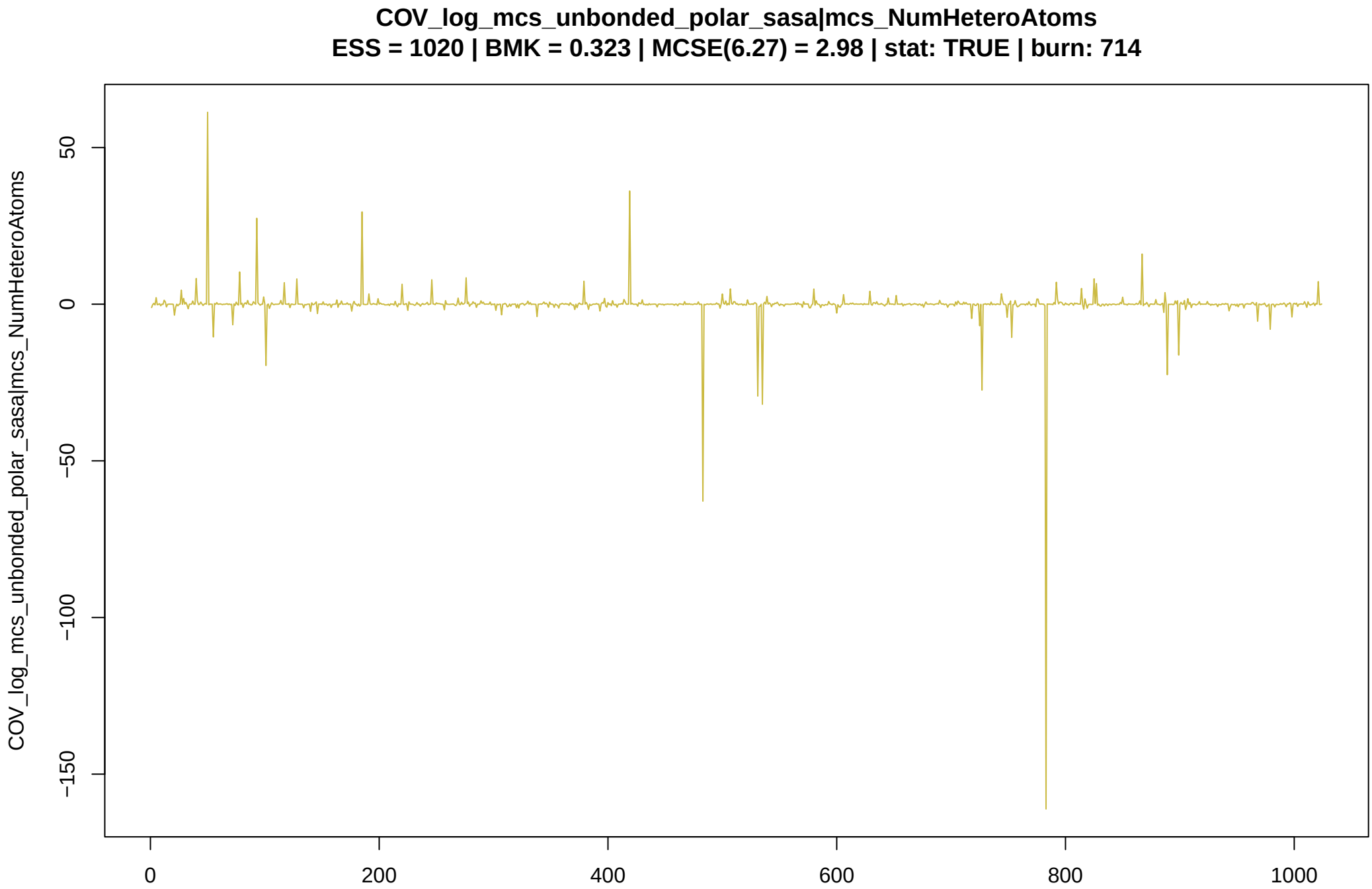

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.342 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 204
COV_log_RMSD|docked_HeavyAtomCount
1000
500
0
−500
0
200
400
600
800
1000

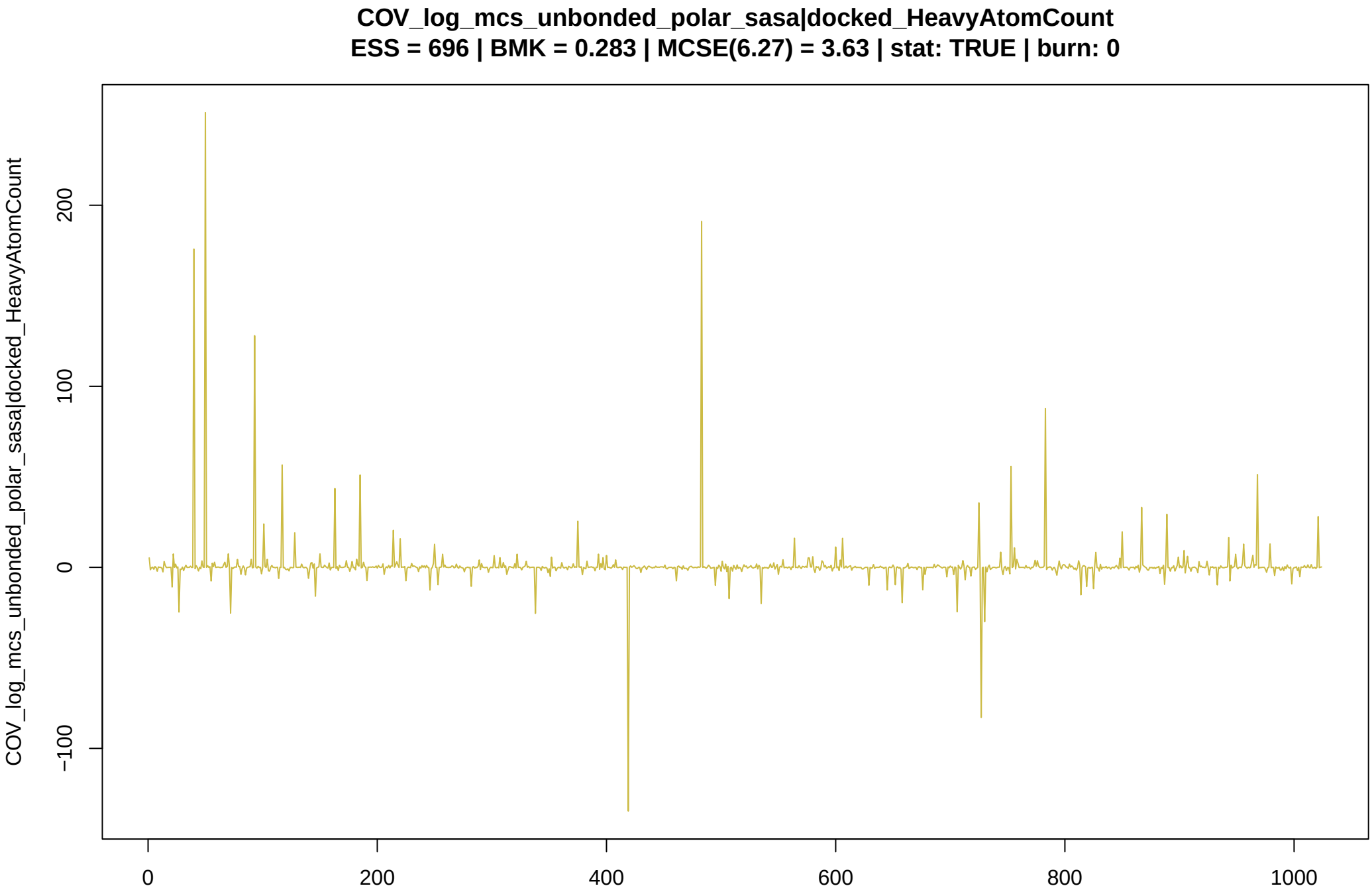

COV_log_RMSD|mcs_RingCount
ESS = 501 | BMK = 0.394 | MCSE(6.27) = 4.13 | stat: TRUE | burn: 204
COV_log_RMSD|mcs_RingCount
0
−100
−200
−300
0
200
400
600
800
1000

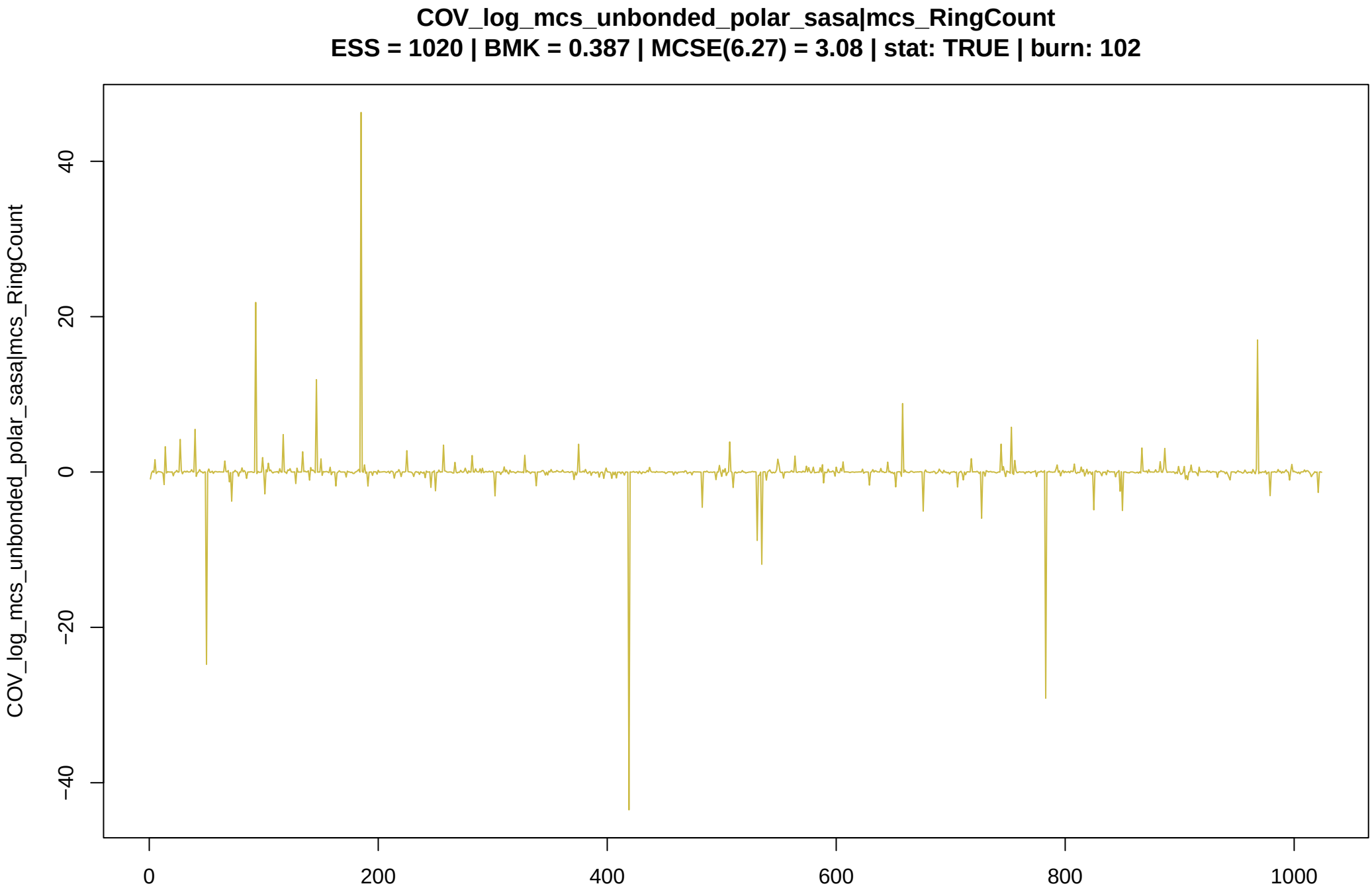

COV_log_RMSD|docked_NumRotatableBonds
ESS = 635 | BMK = 0.342 | MCSE(6.27) = 3.82 | stat: TRUE | burn: 0
COV_log_RMSD|docked_NumRotatableBonds
600
400
200
0
0
200
400
600
800
1000

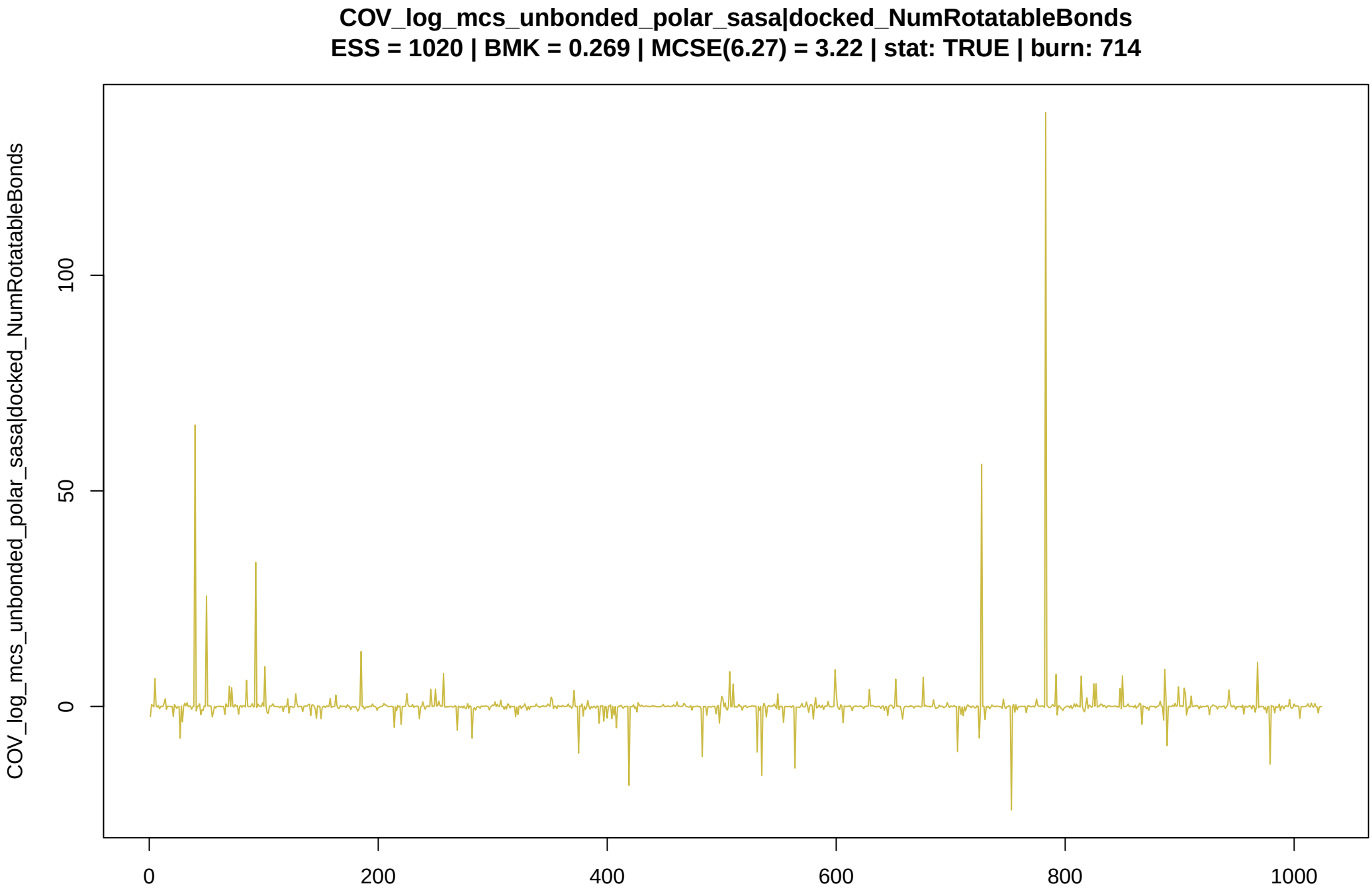

COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.299 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NOCount
300
200
100
0
−100
0
200
400
600
800
1000

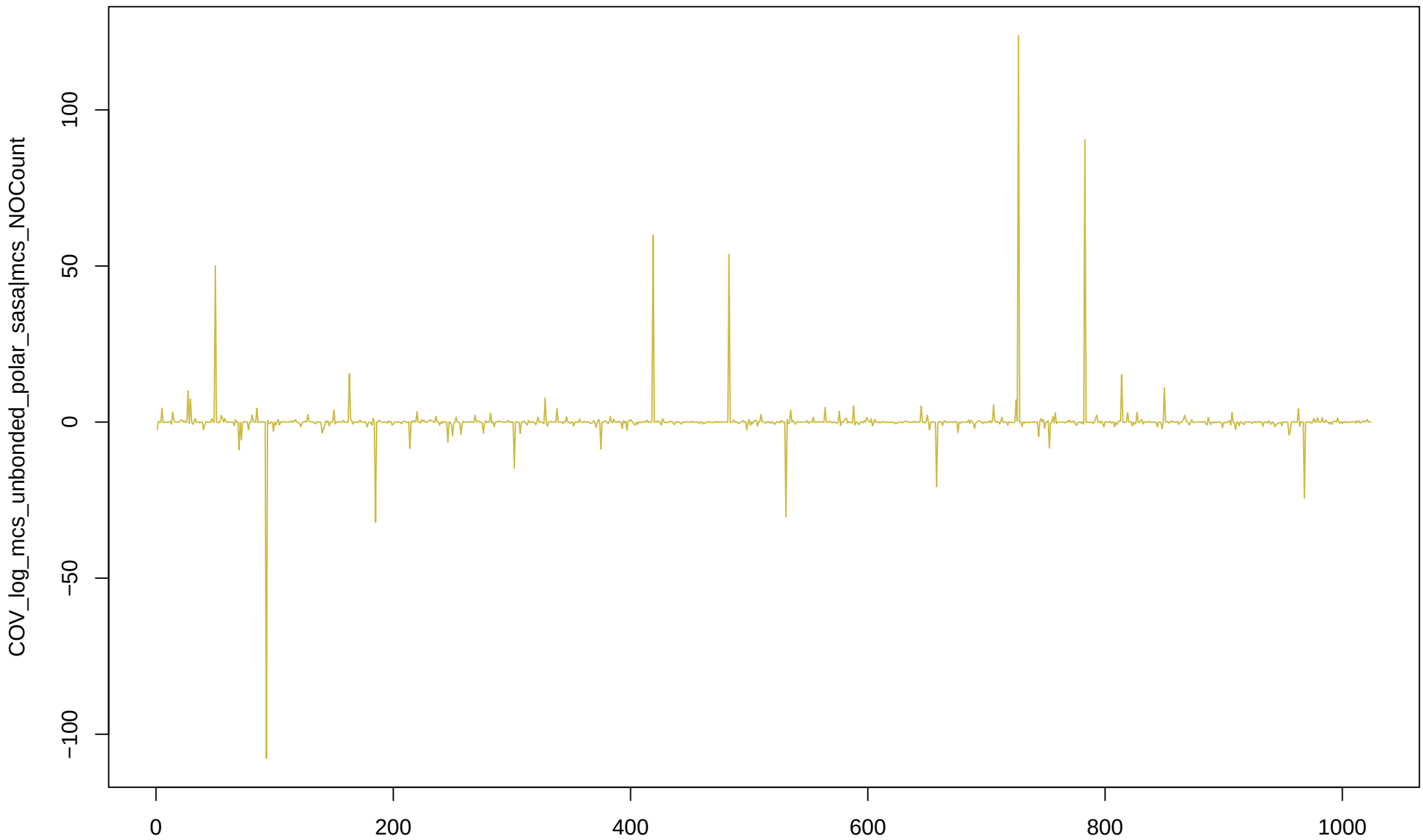

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.849 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 816
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0
−20
−40
−60
−80
−100
0
200
400
600
800
1000

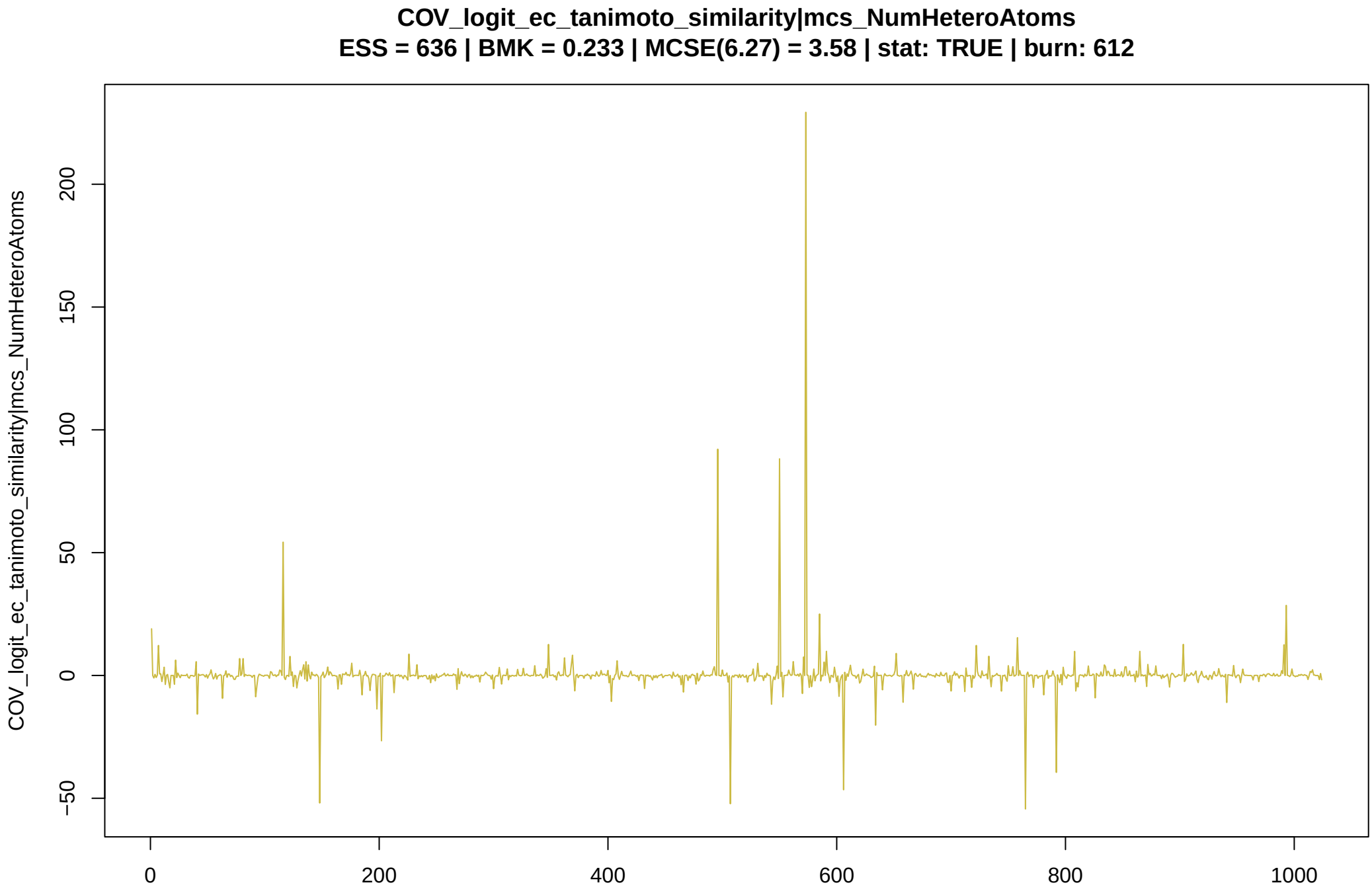

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.323 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 714
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
50
0
−50
−100
−150
0
200
400
600
800
1000

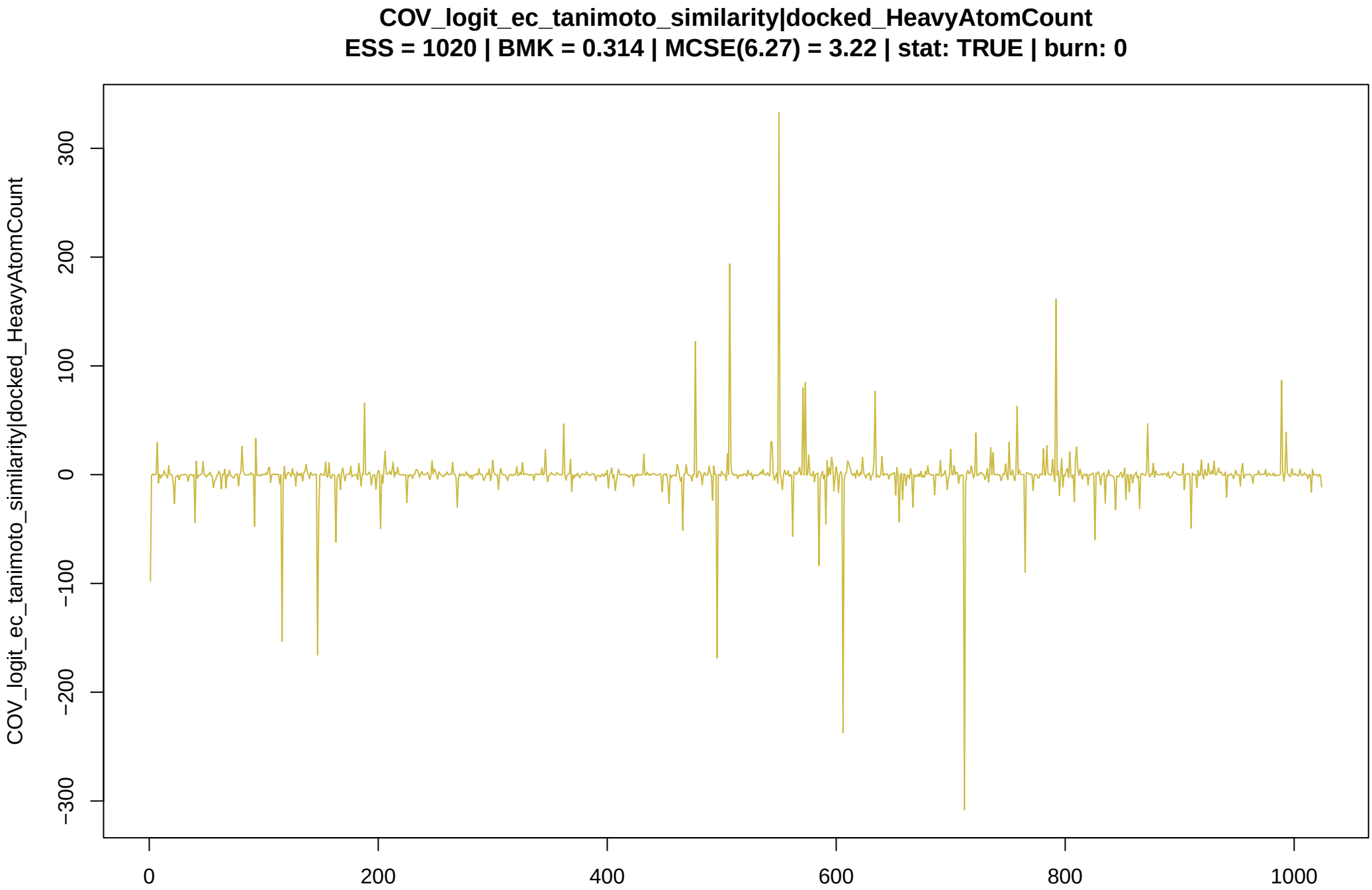

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 696 | BMK = 0.283 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
200
100
0
−100
0
200
400
600
800
1000

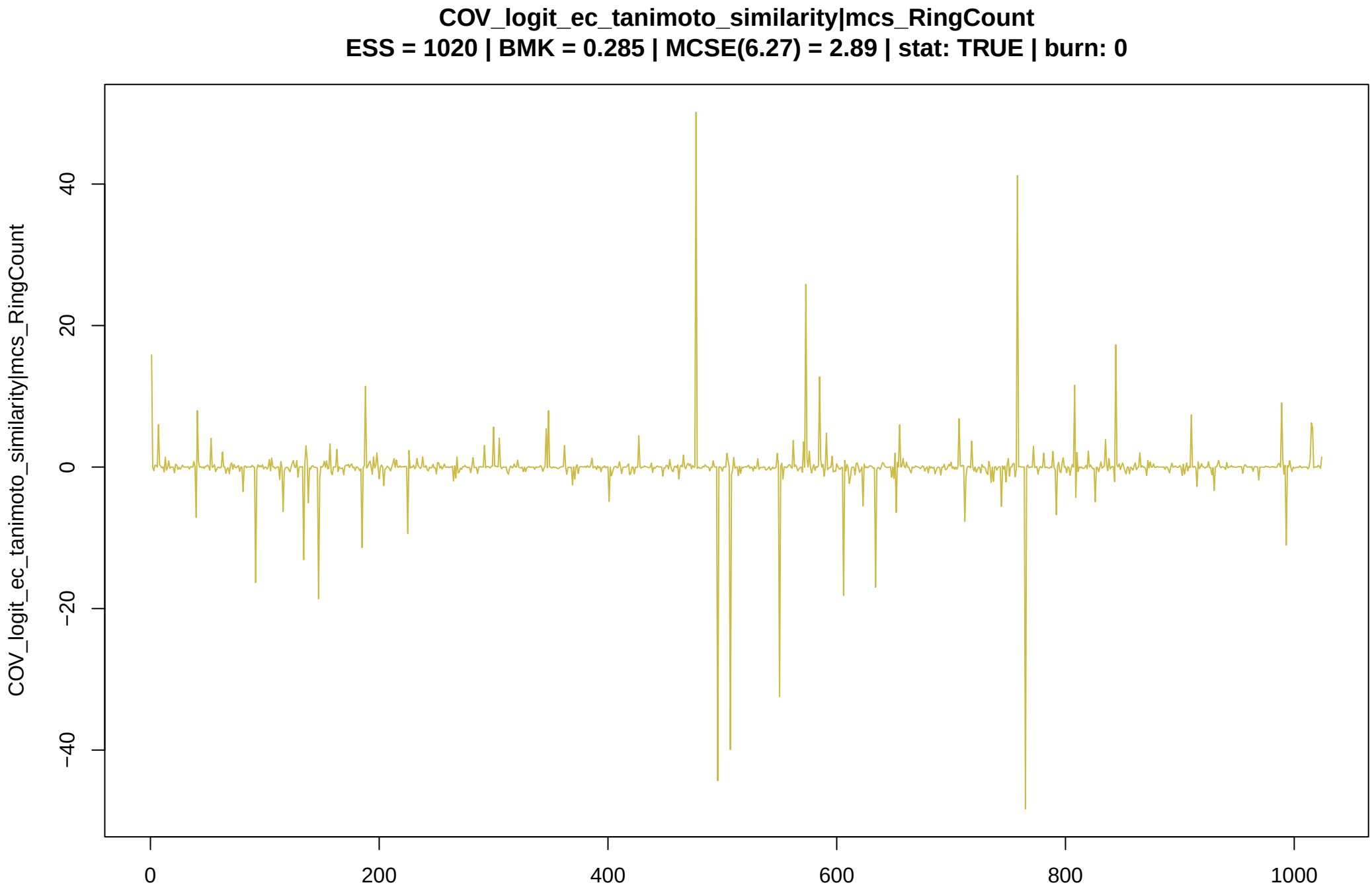

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.387 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 102
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
40
20
0
−20
−40
0
200
400
600
800
1000

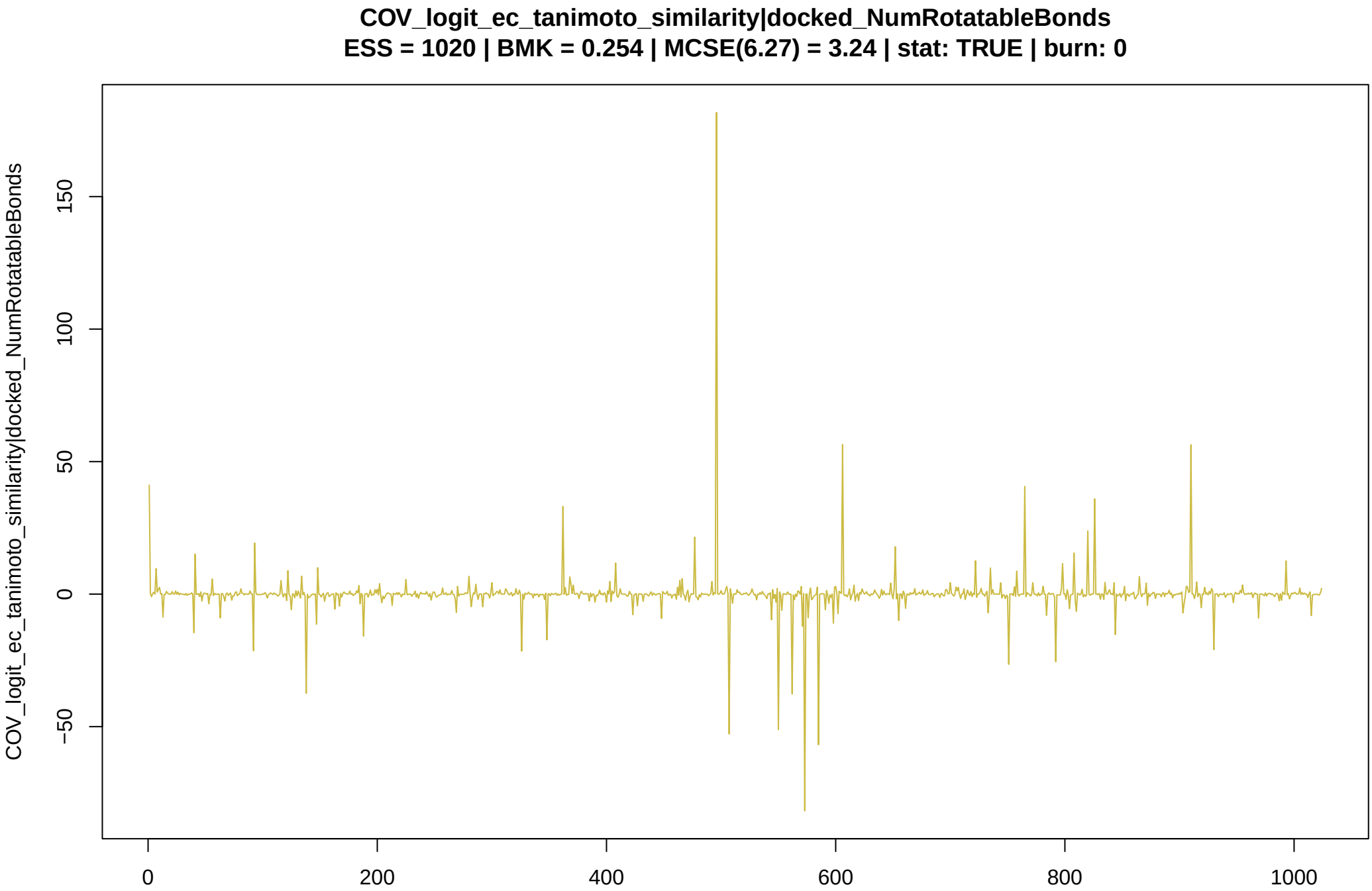

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.269 | MCSE(6.27) = 3.22 | stat: TRUE | burn: 714
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
0
50
100
0
200
400
600
800
1000

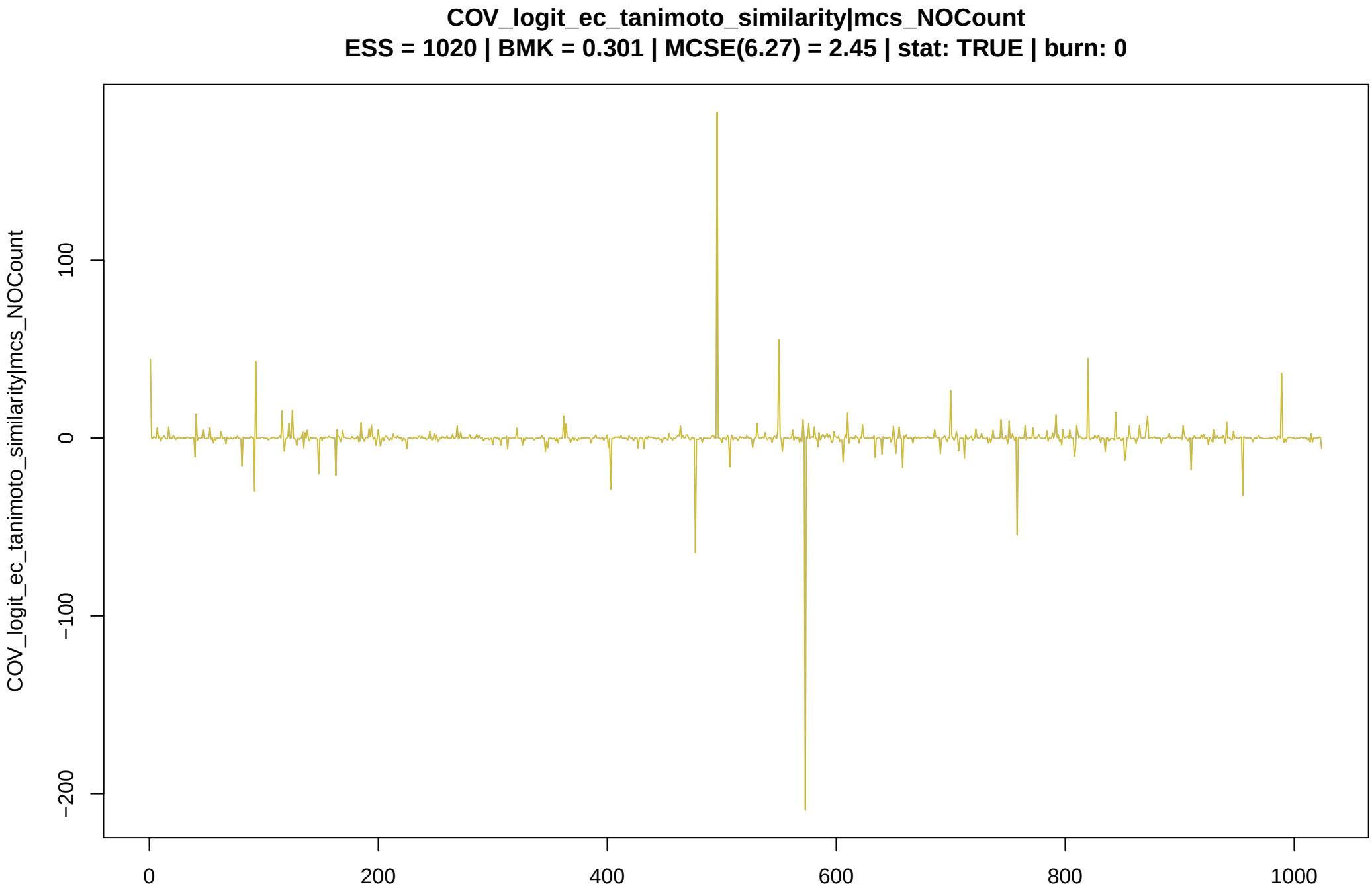

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.341 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 102
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
100
50
0
−50
−100
0
200
400
600
800
1000

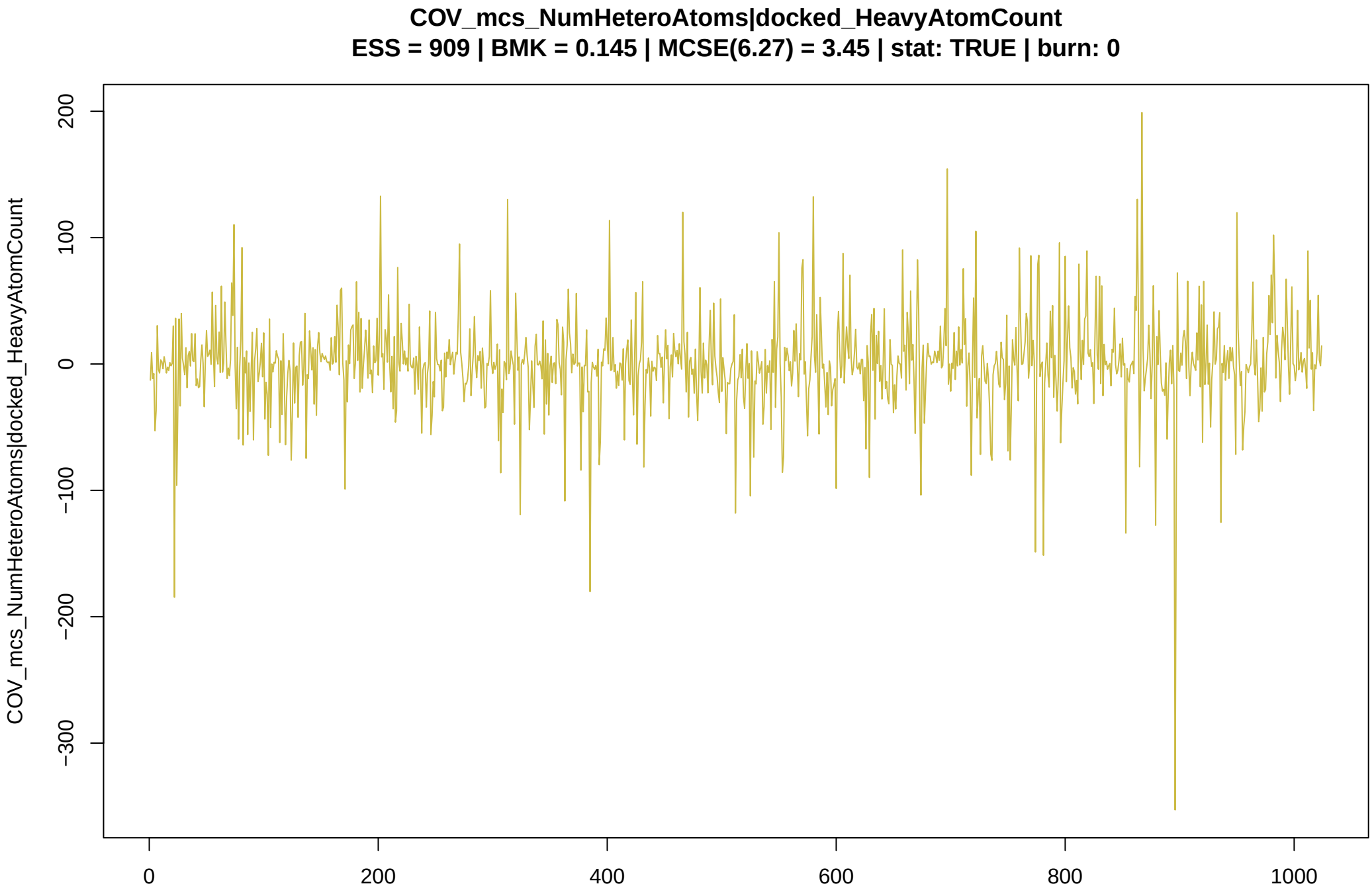

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 636 | BMK = 0.233 | MCSE(6.27) = 3.58 | stat: TRUE | burn: 612
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
200
150
100
50
0
−50
0
200
400
600
800
1000

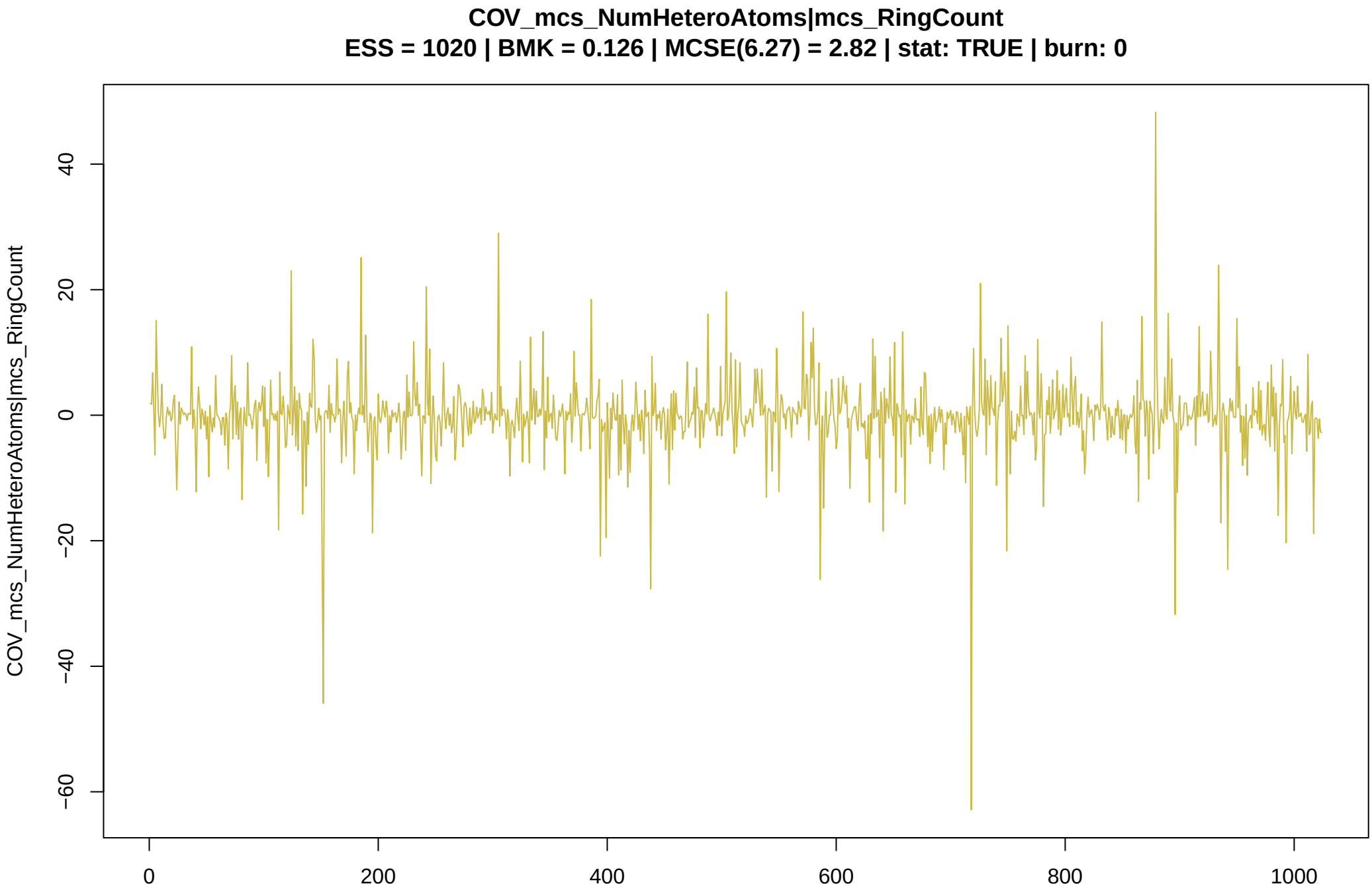

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.314 | MCSE(6.27) = 3.22 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
300
200
100
0
−100
−200
−300
0
200
400
600
800
1000

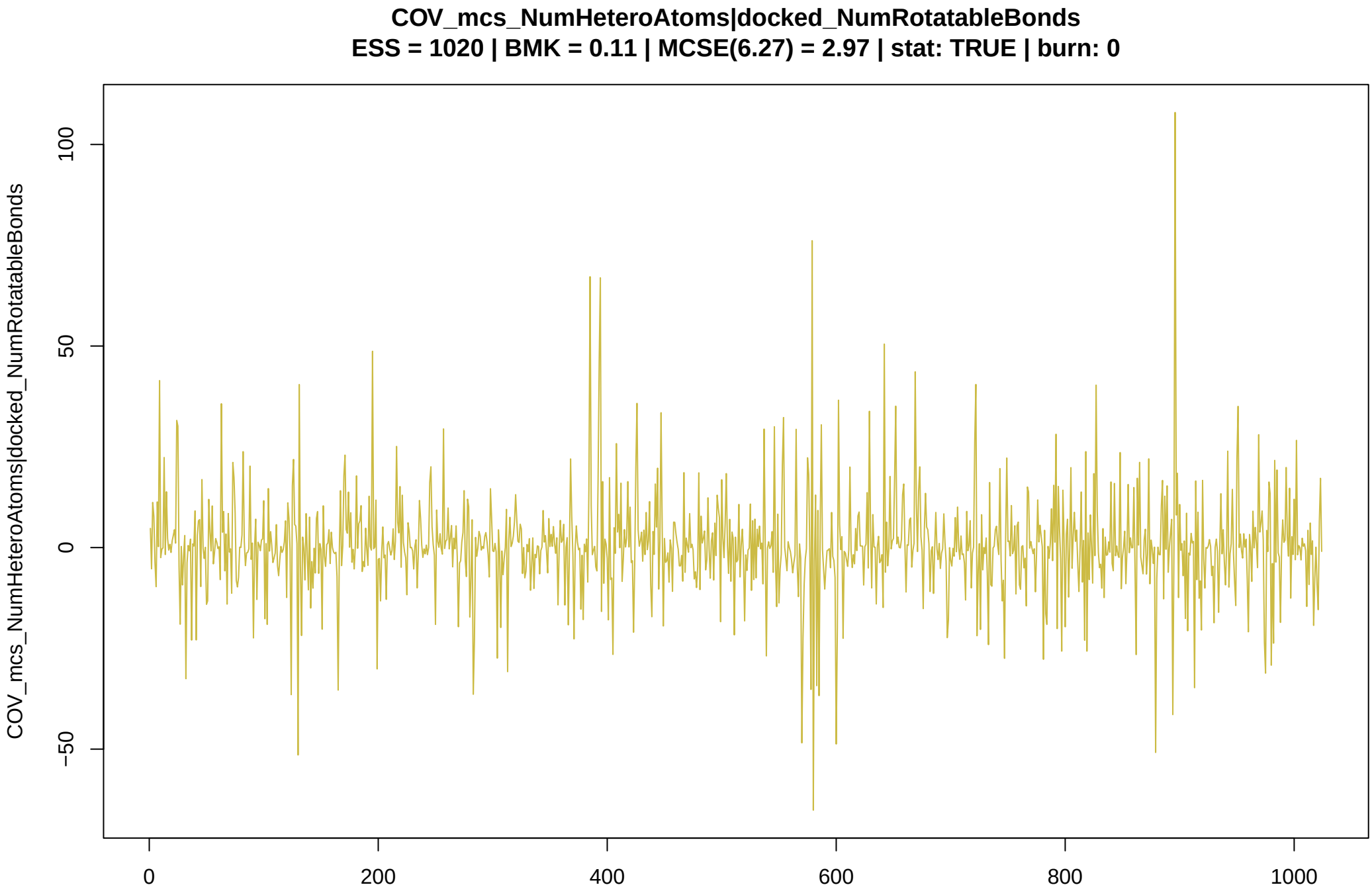

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.285 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_RingCount
40
20
0
−20
−40
0
200
400
600
800
1000

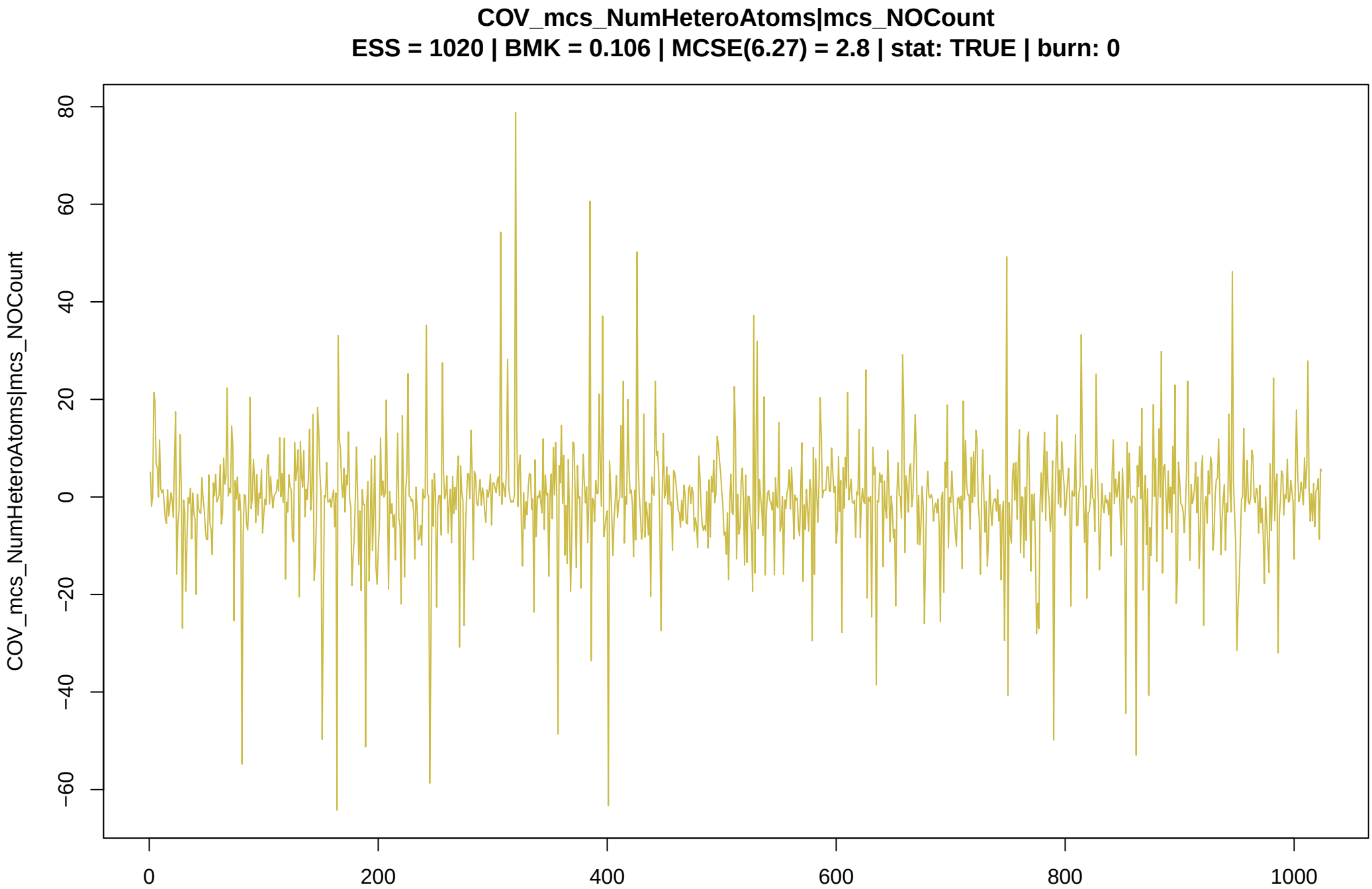

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.254 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
150
100
50
0
−50
0
200
400
600
800
1000

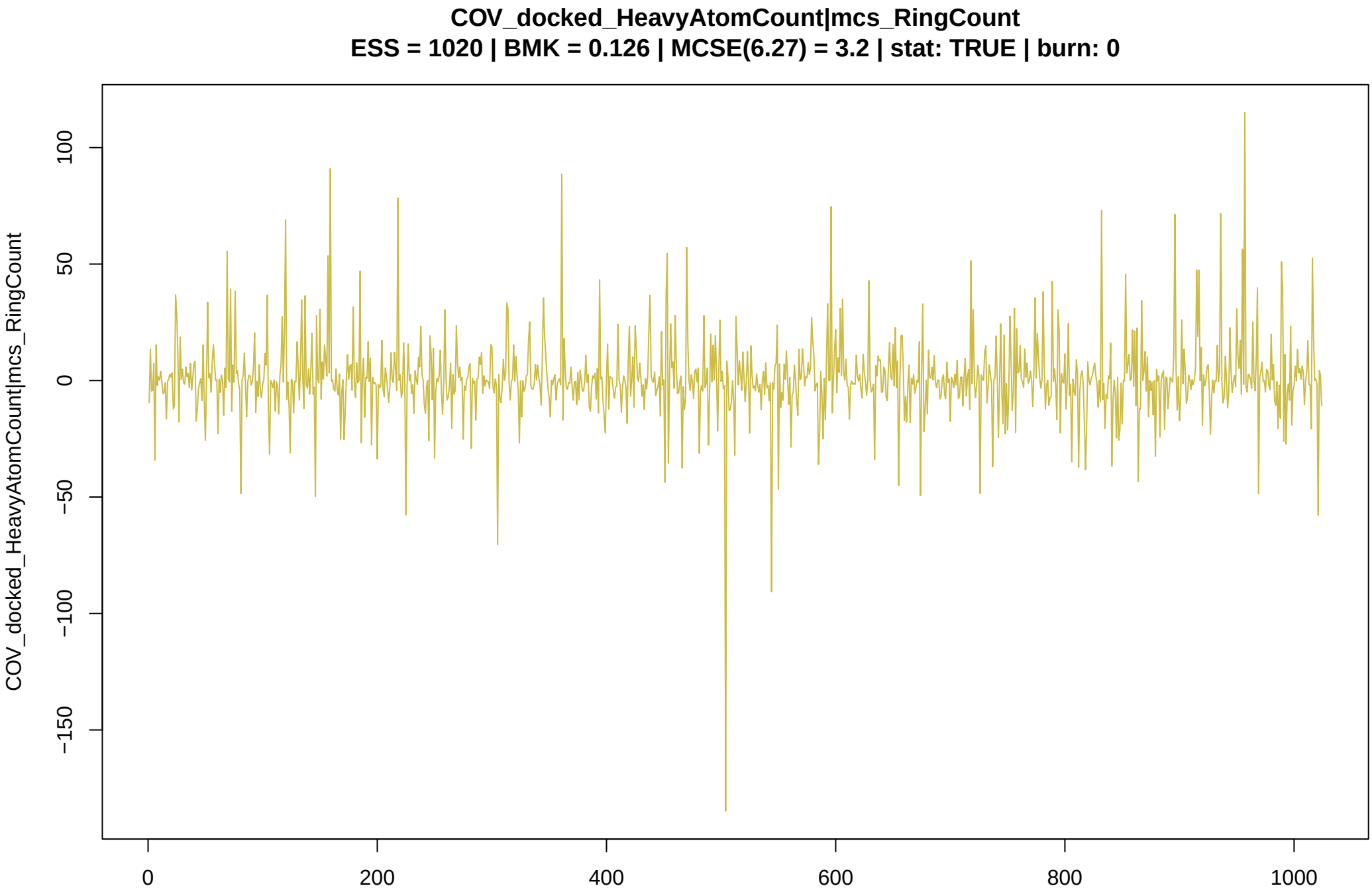

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.301 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NOCount
100
0
−100
−200
0
200
400
600
800
1000

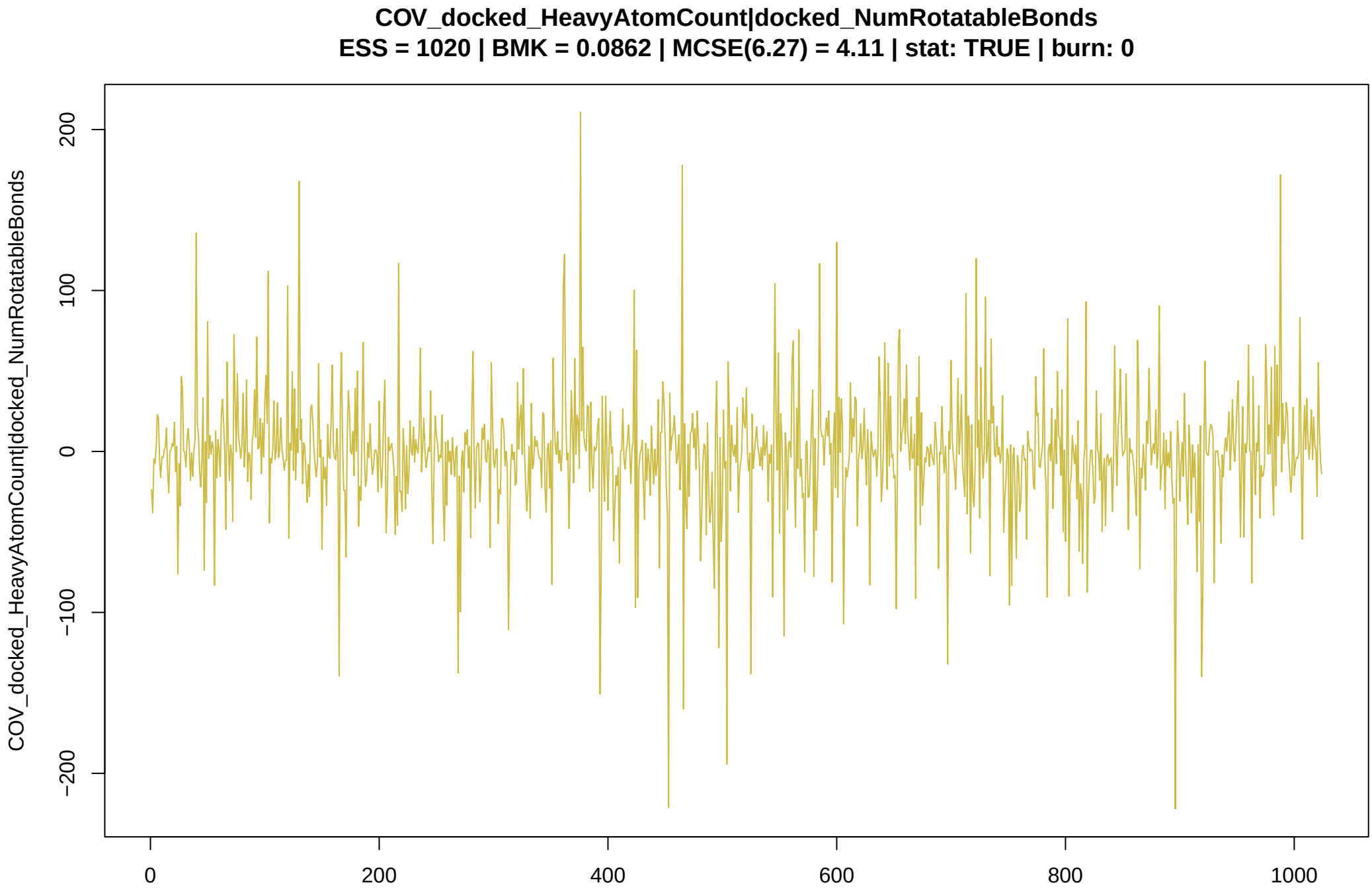

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 909 | BMK = 0.145 | MCSE(6.27) = 3.45 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
200
100
0
−100
−200
−300
0
200
400
600
800
1000

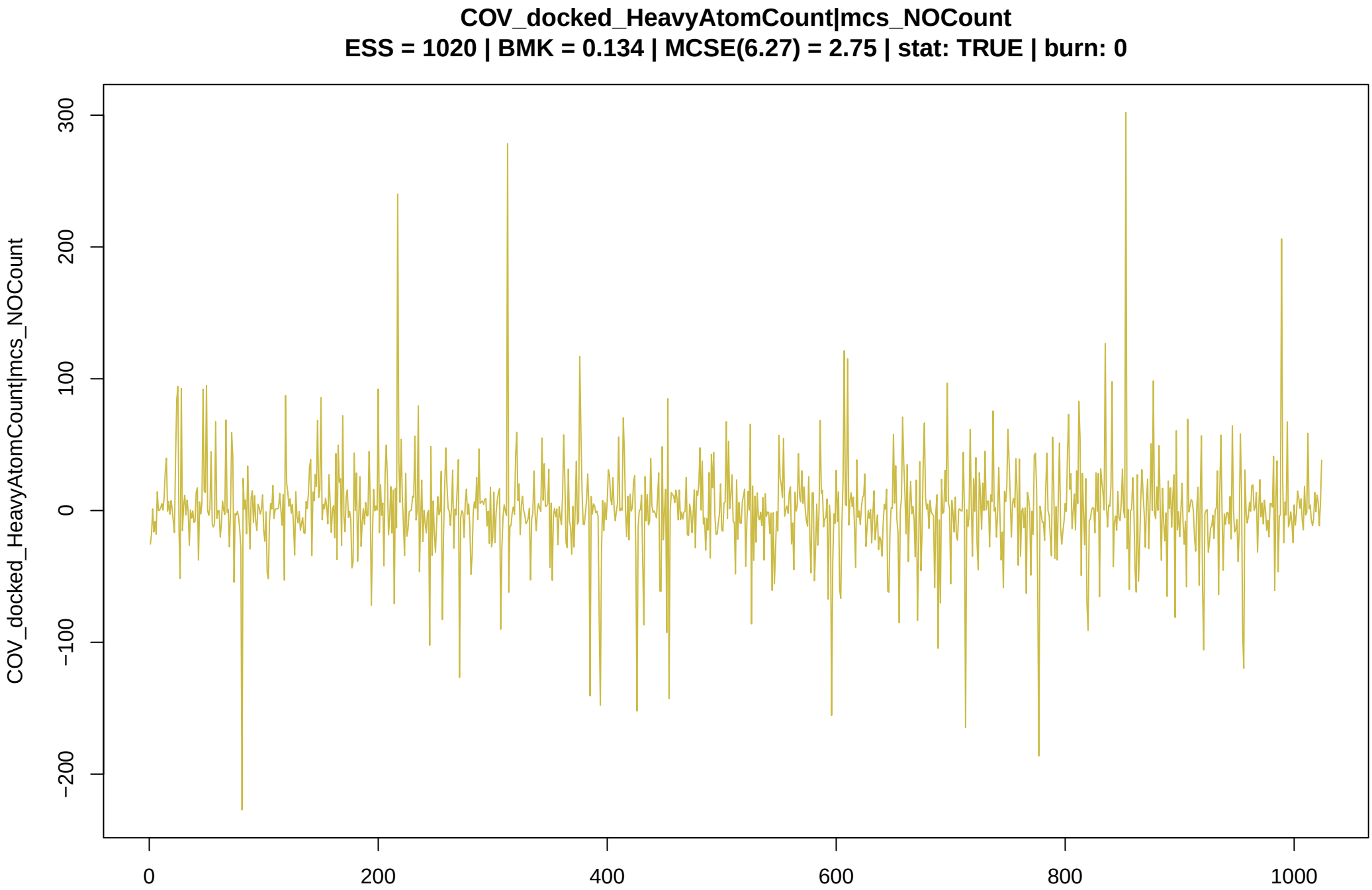

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.126 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|mcs_RingCount
40
20
0
−20
−40
−60
0
200
400
600
800
1000

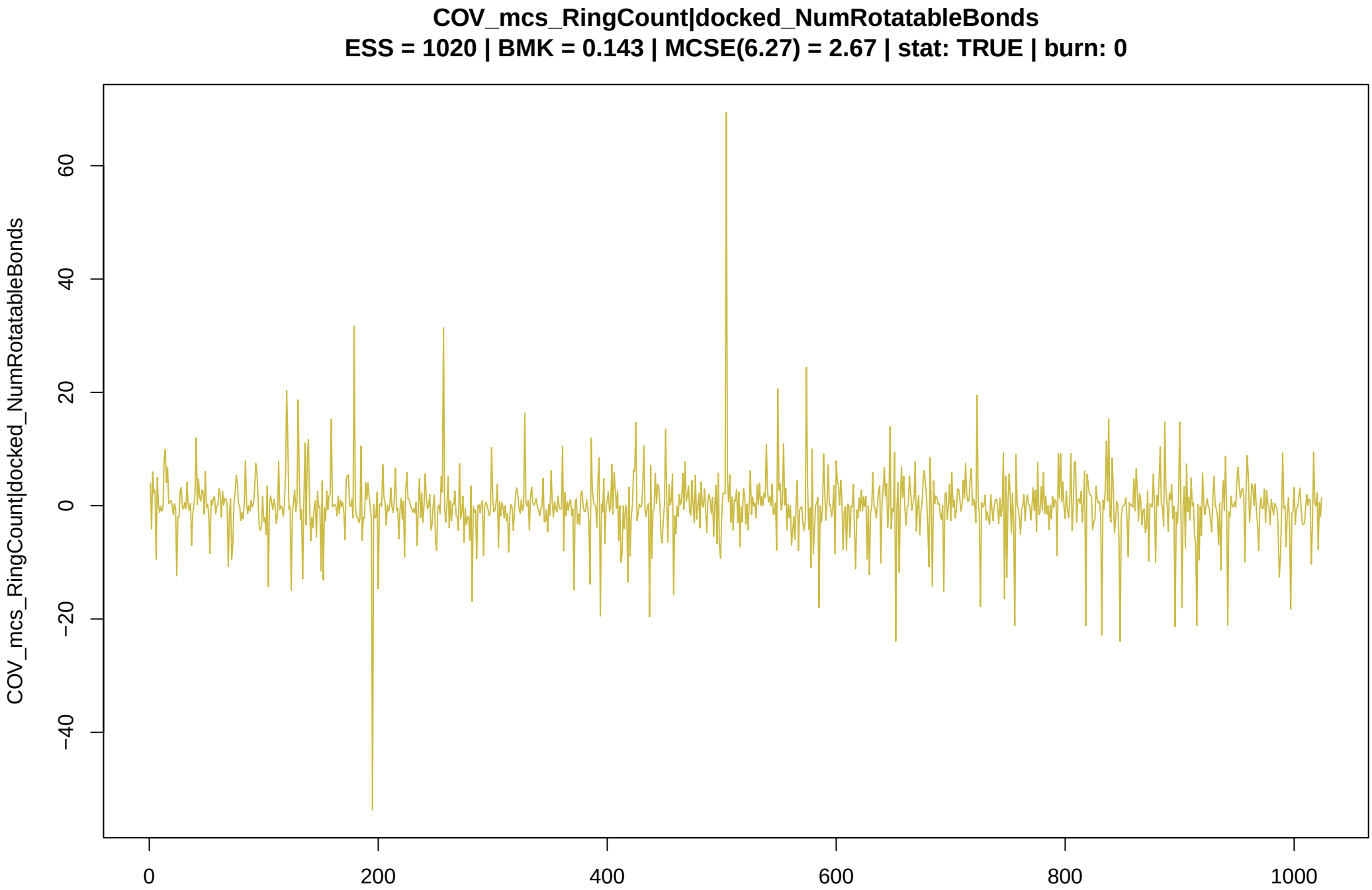

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.11 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
100
50
0
−50
0
200
400
600
800
1000

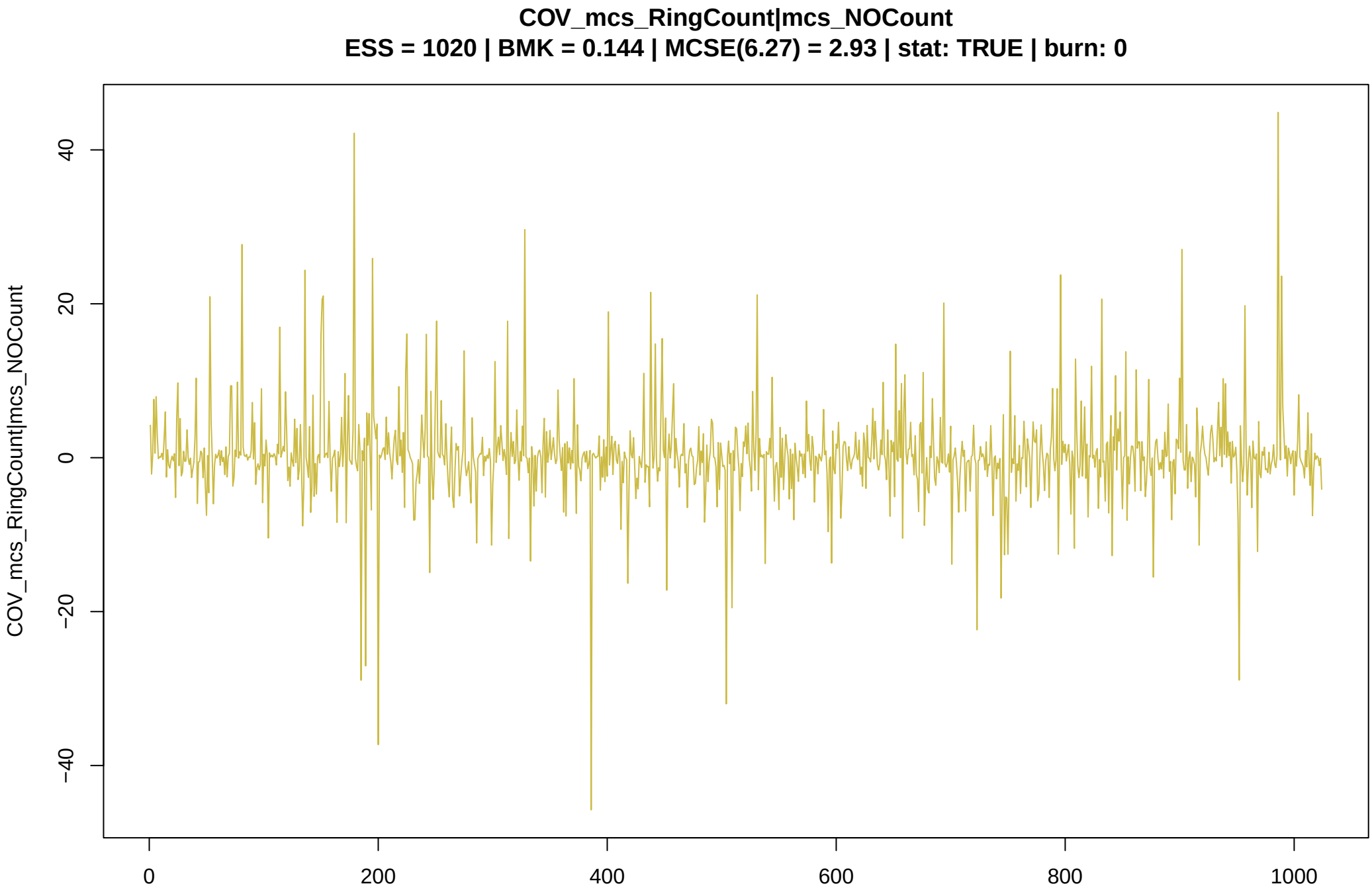

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.106 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|mcs_NOCount
80
60
40
20
0
−20
−40
−60
0
200
400
600
800
1000

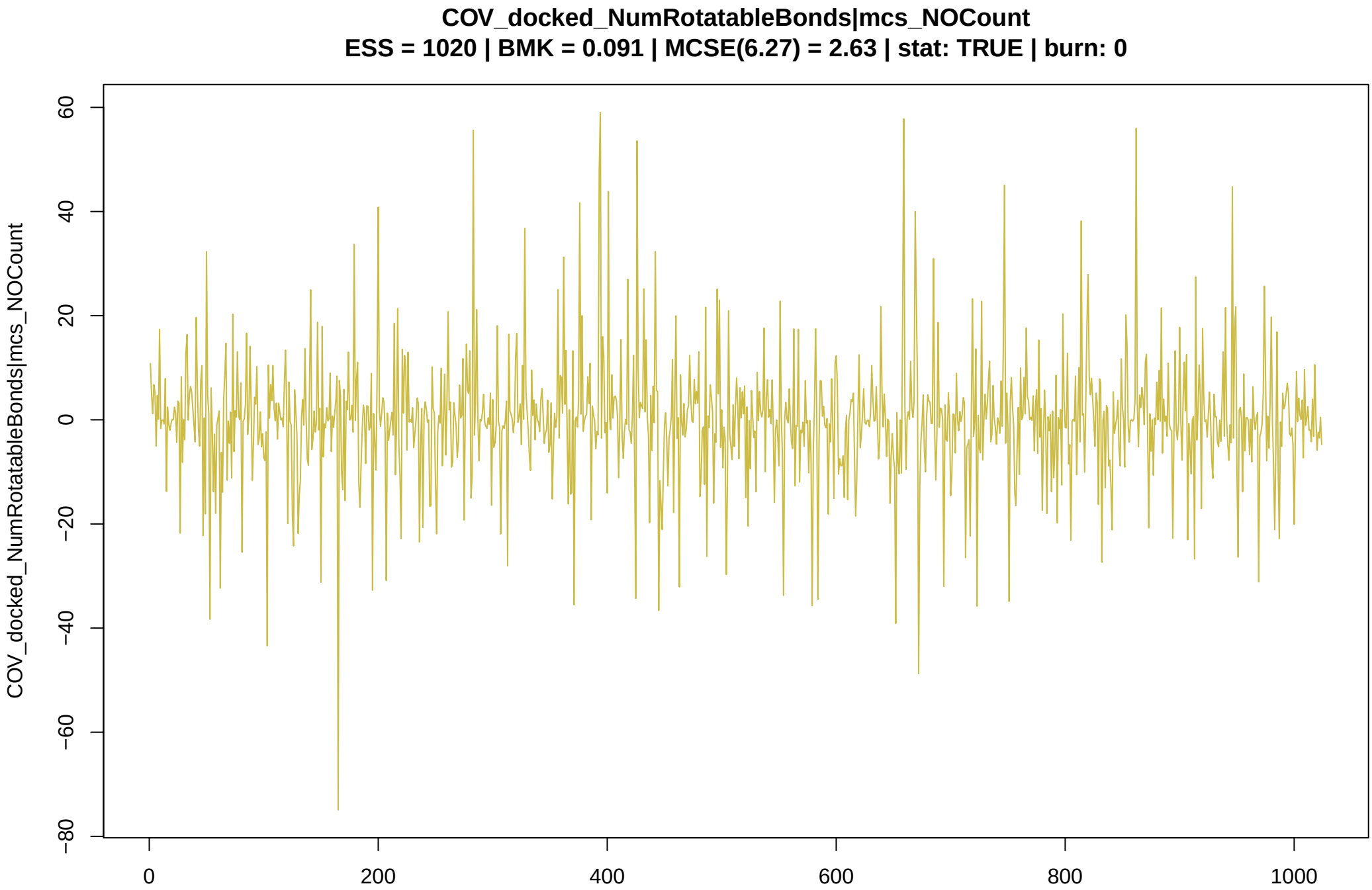

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.126 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
100
50
0
−50
−100
−150
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0862 | MCSE(6.27) = 4.11 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
200
100
0
−100
−200
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.134 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_NOCount
300
200
100
0
−100
−200
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.143 | MCSE(6.27) = 2.67 | stat: TRUE | burn: 0
COV_mcs_RingCount|docked_NumRotatableBonds
60
40
20
0
−20
−40
0
200
400
600
800
1000


COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.144 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_NOCount
40
20
0
−20
−40
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.091 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0
COV_docked_NumRotatableBonds|mcs_NOCount
60
40
20
0
−20
−40
−60
−80
0
200
400
600
800
1000