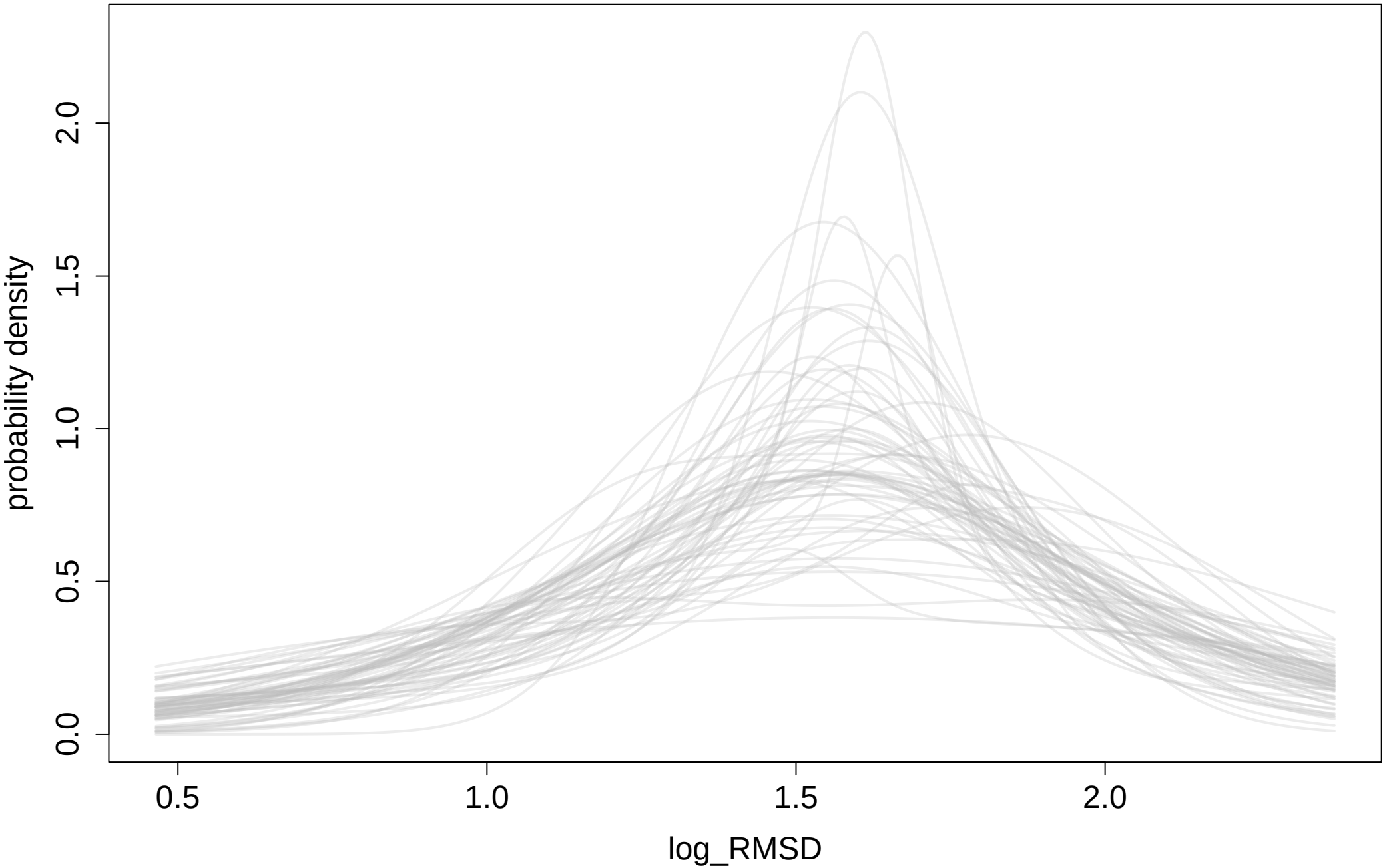
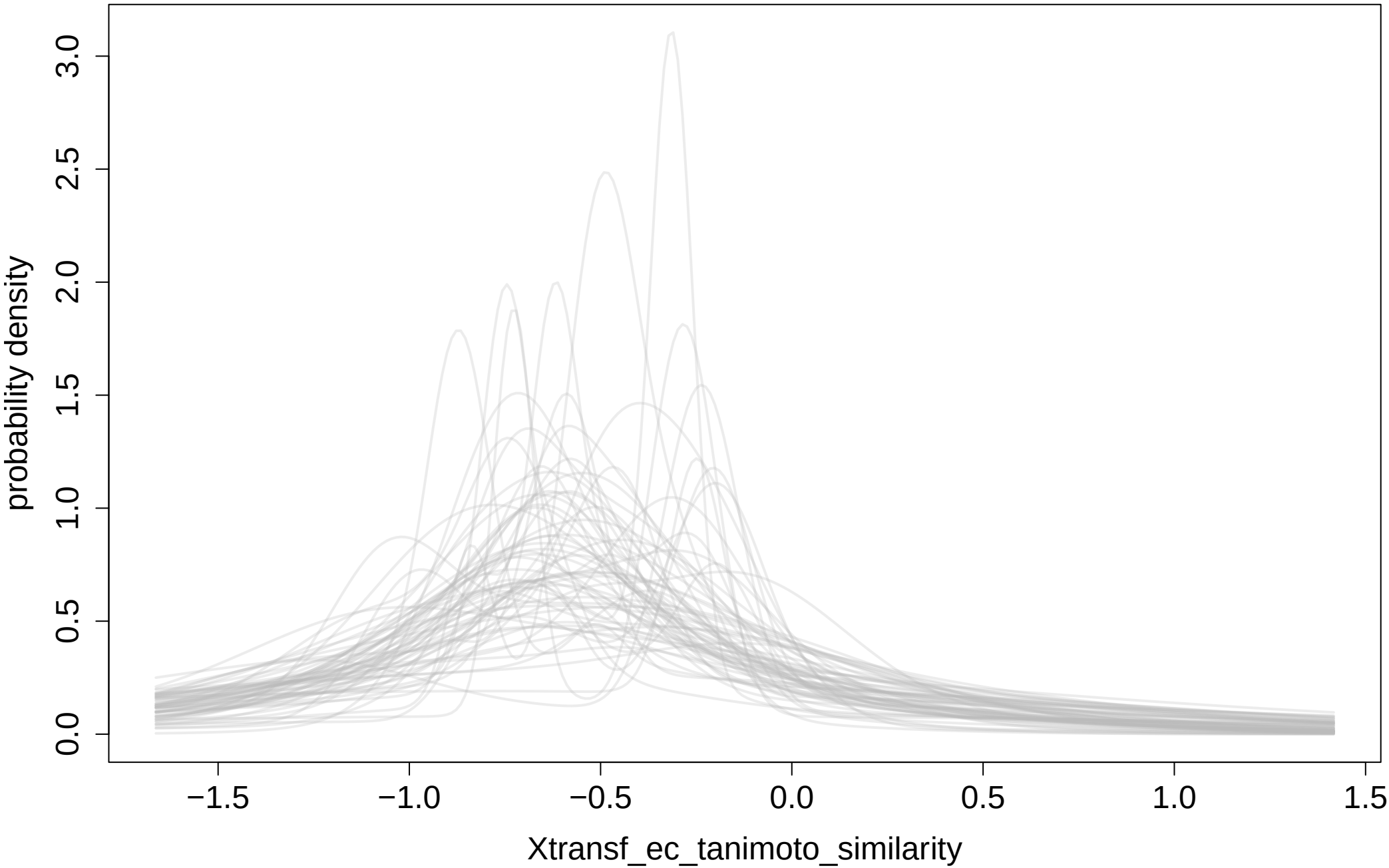
−− STATS maxD −−
min ESS = 23.1279254748828
max BMK = 1
max MCSE = 25.1871531891162
all stationary: FALSE
burn: 120

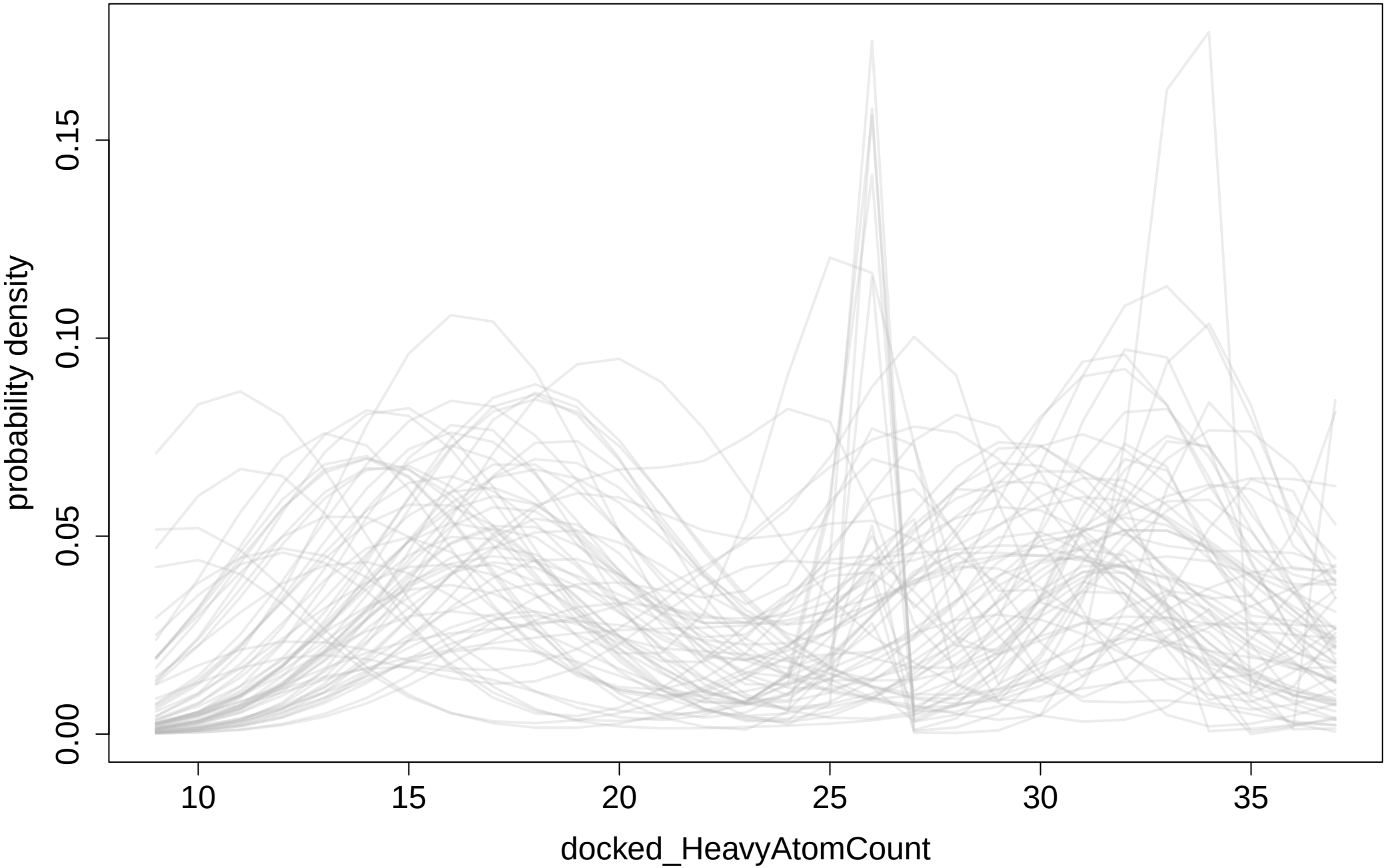
−− STATS 2D −−
min ESS = 26.3466344745808
max BMK = 0.373073700812954
max MCSE = 20.9258789470046
all stationary: FALSE
burn: 96

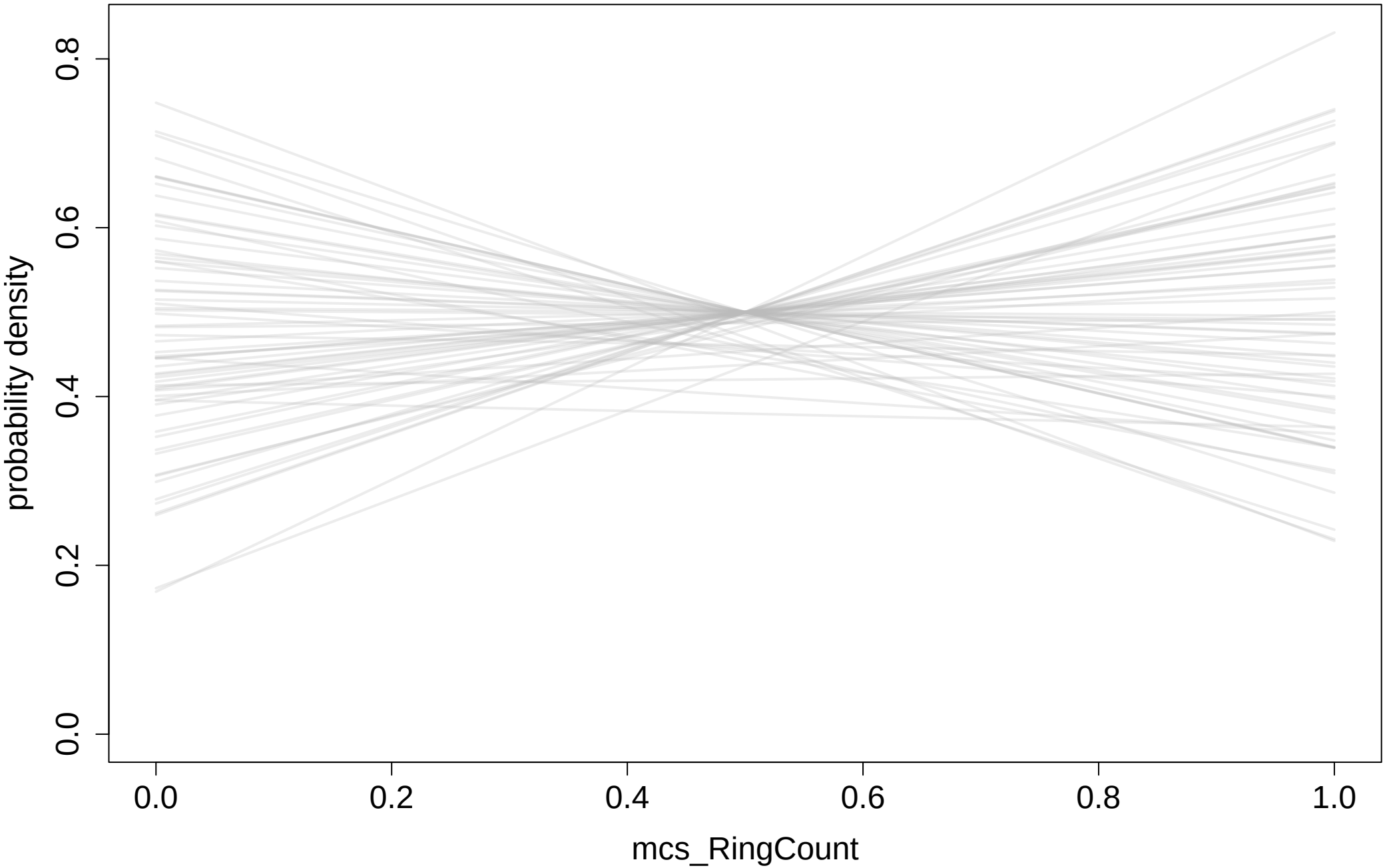
−− STATS 1D −−
min ESS = 2.2204604925031e−16
max BMK = 0.520323941140938
max MCSE = NaN
all stationary: FALSE
burn: 96

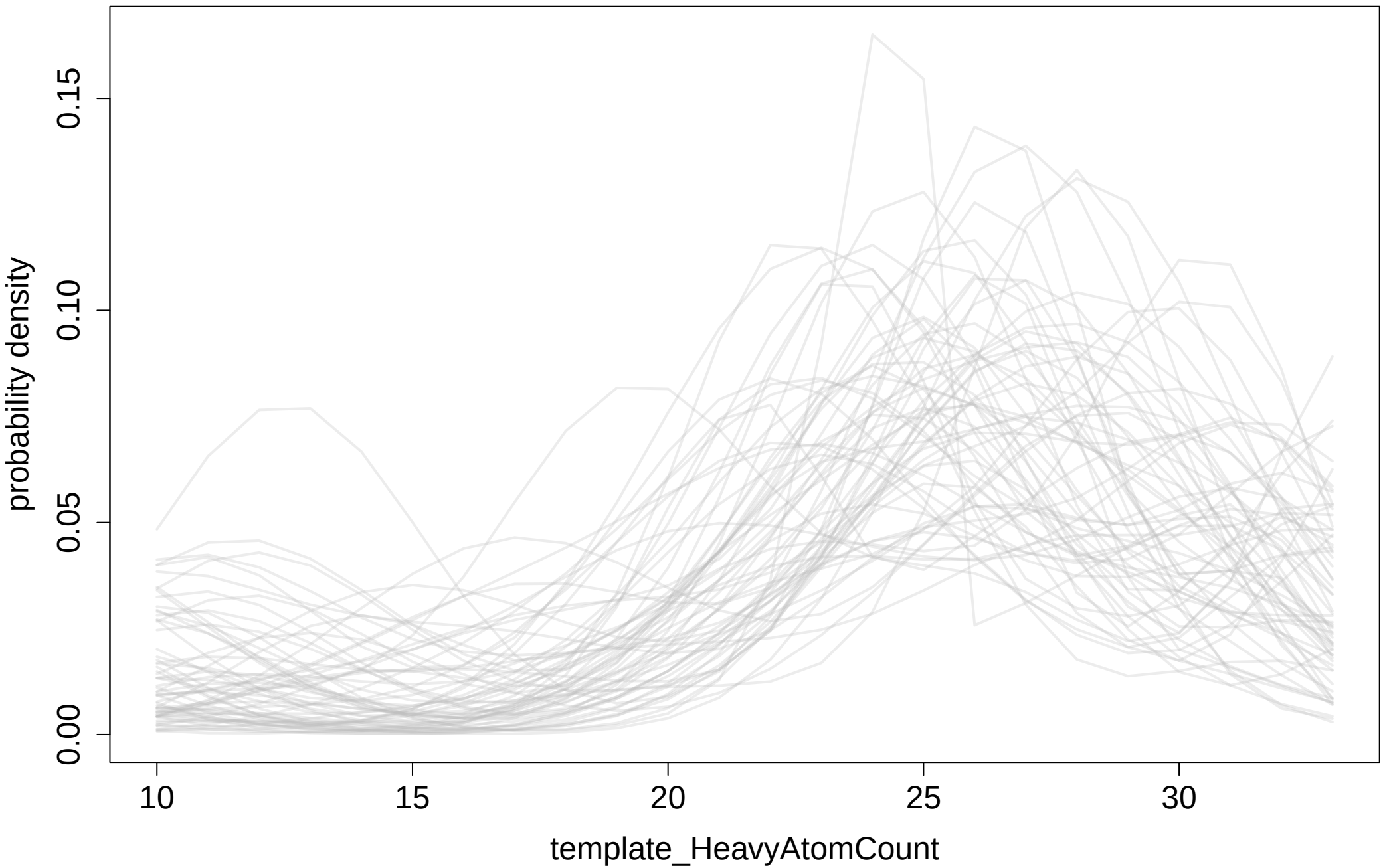
Occupied clusters: 4 of 4
LL: −86.8 +− 4.67

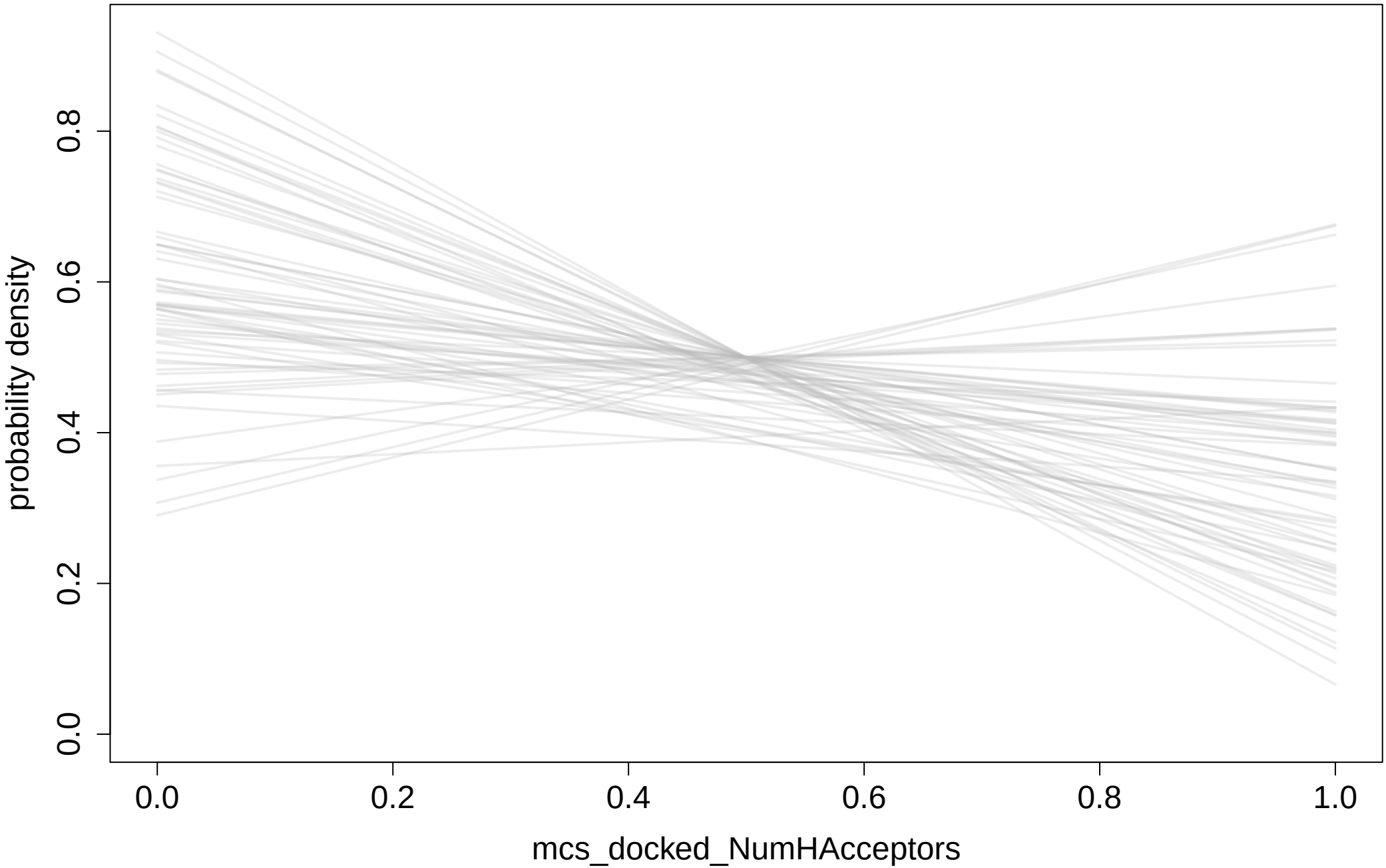

probability density
0.0
0.5
1.0
1.5
2.0
0.5
1.0
1.5
2.0
log_RMSD

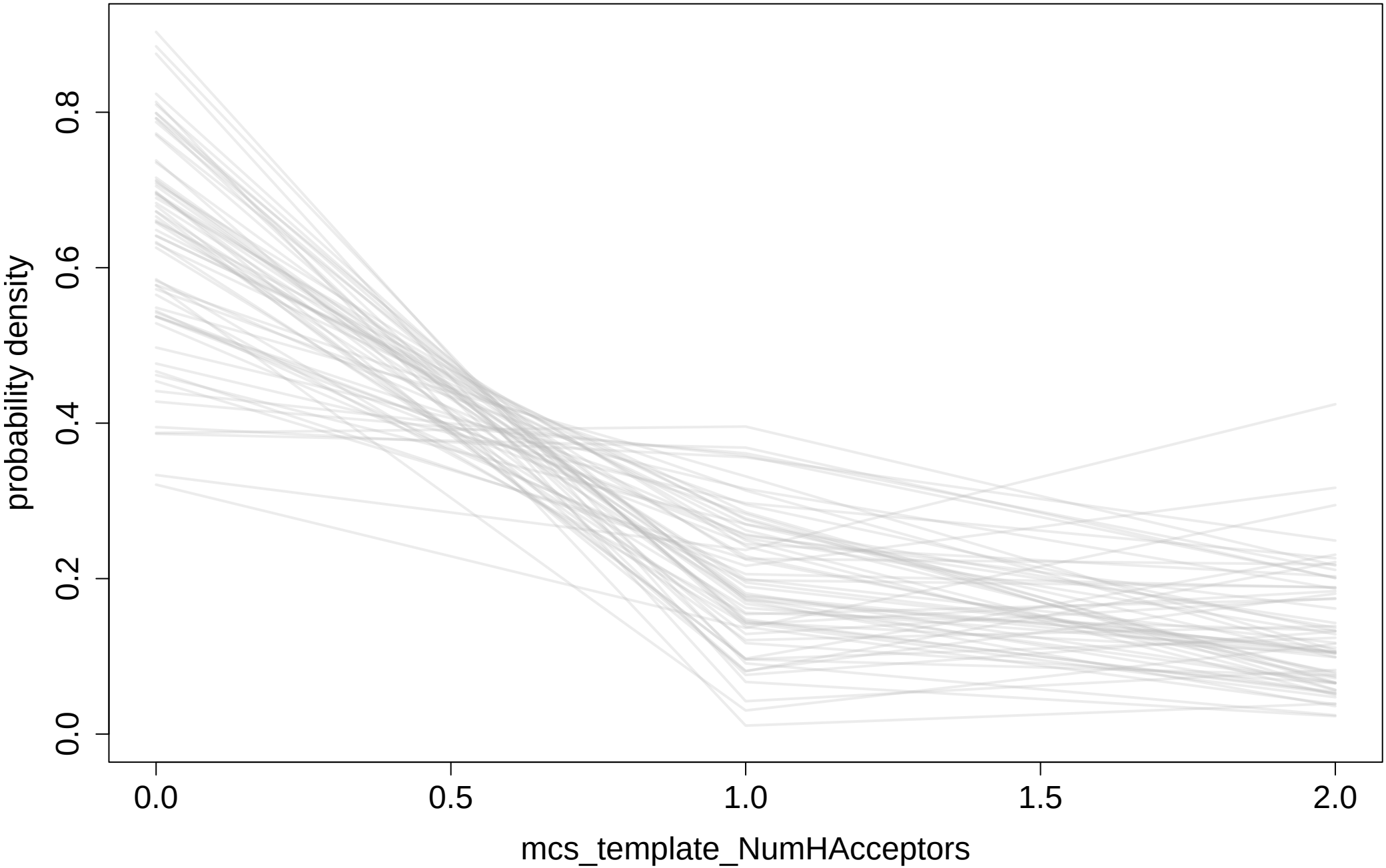

probability density
0.0
0.5
1.0
1.5
2.0
2.5
3.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
Xtransf_ec_tanimoto_similarity

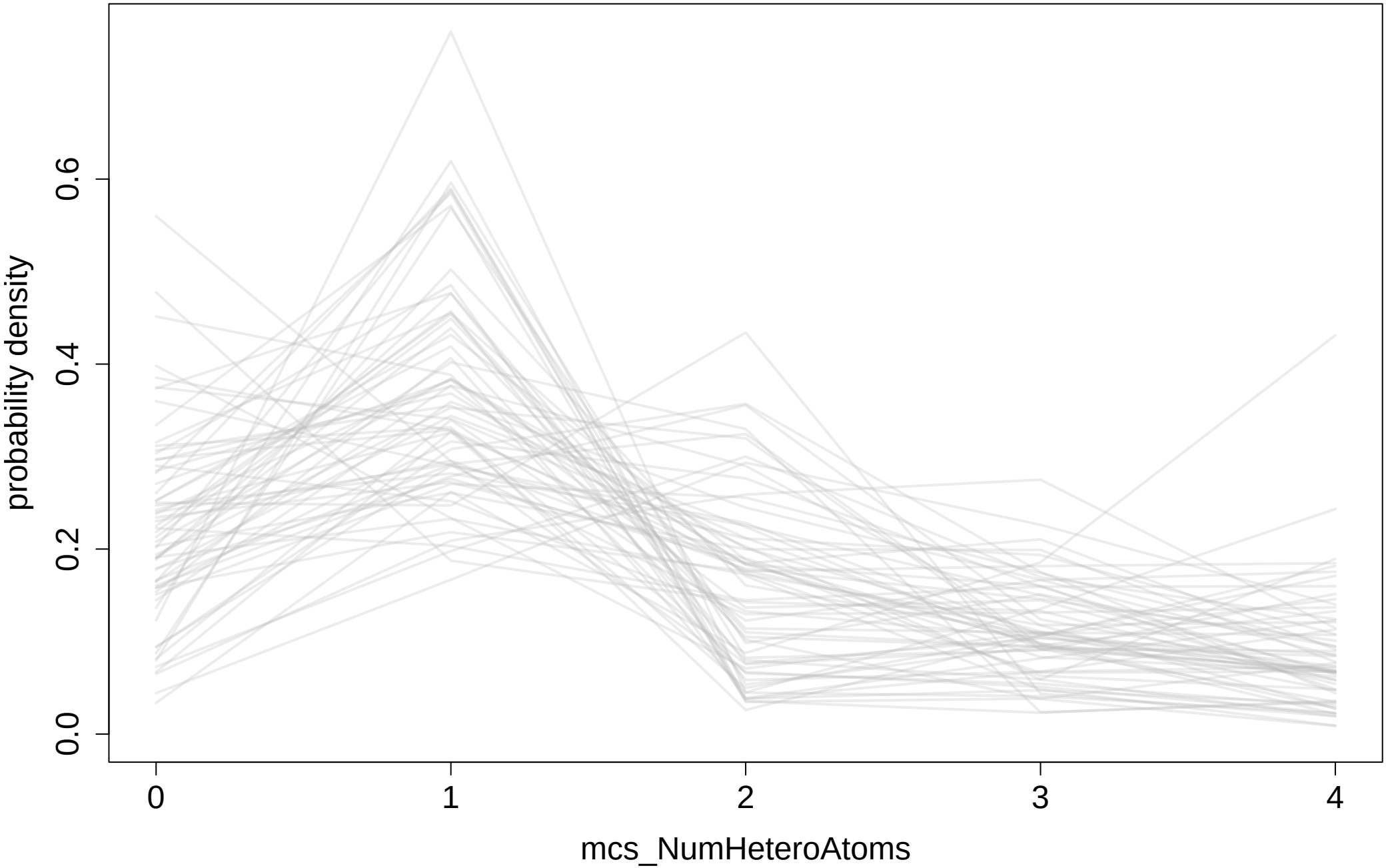

probability density
0.00
0.05
0.10
0.15
10
15
20
25
30
35
docked_HeavyAtomCount

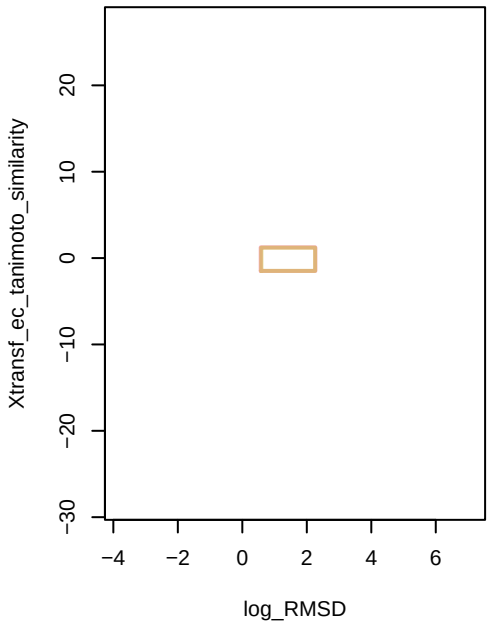

probability density
0.0
0.2
0.4
0.6
0.8
0.0
0.2
0.4
0.6
0.8
1.0
mcs_RingCount

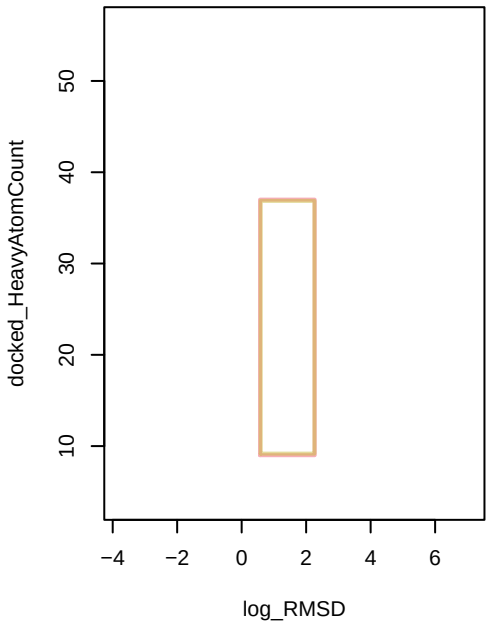

probability density
0.00
0.05
0.10
0.15
10
15
20
25
30
template_HeavyAtomCount

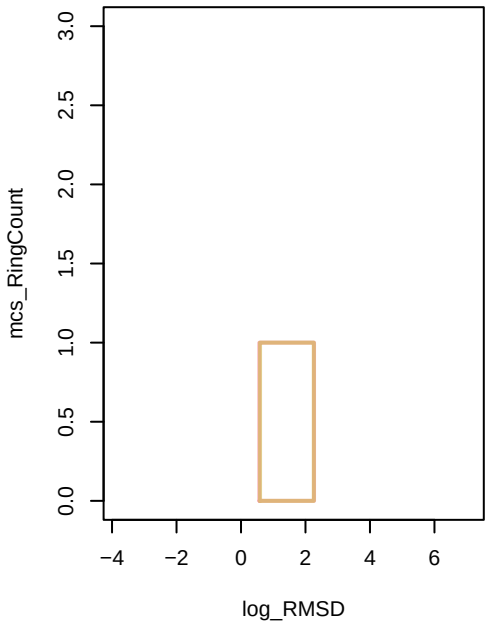

probability density
0.0
0.2
0.4
0.6
0.8
0.0
0.2
0.4
0.6
0.8
1.0
mcs_docked_NumHAcceptors

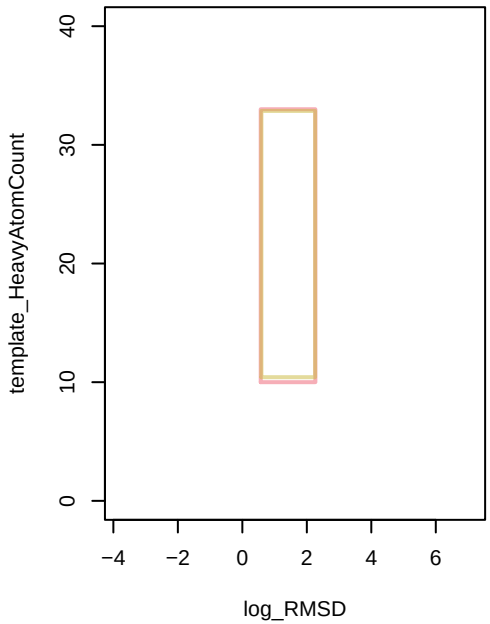

probability density
0.0
0.2
0.4
0.6
0.8
0.0
0.5
1.0
1.5
2.0
mcs_template_NumHAcceptors

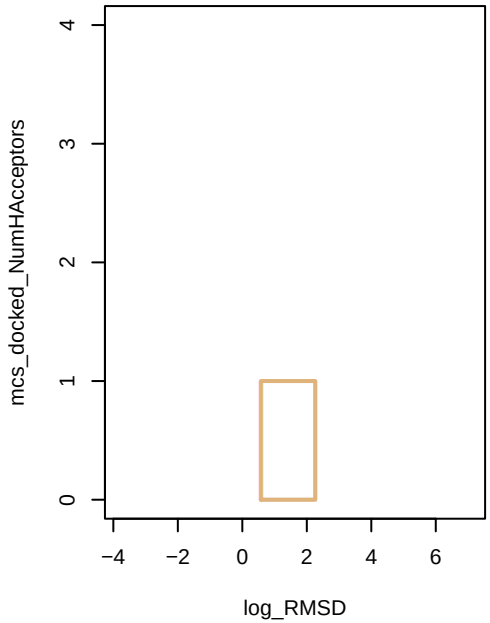

probability density
0.0
0.2
0.4
0.6
0
1
2
3
4
mcs_NumHeteroAtoms

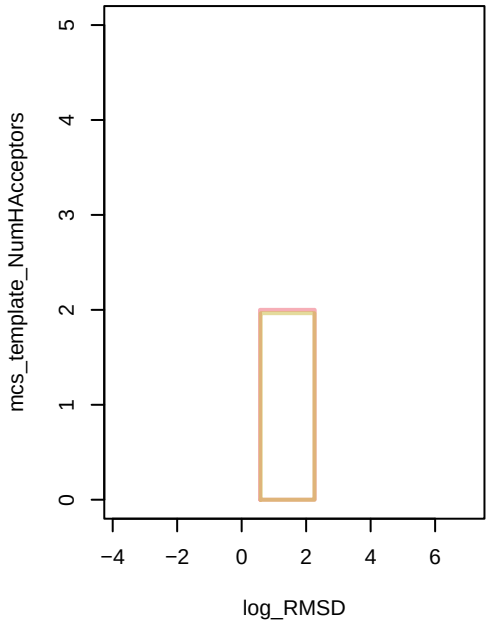

Xtransf_ec_tanimoto_similarity
20
10
0
−10
−20
−30
−4
−2
0
2
4
6
log_RMSD

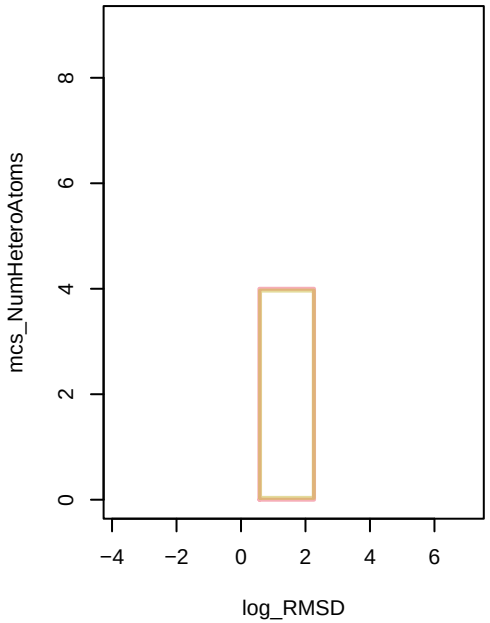

docked_HeavyAtomCount
50
40
30
20
10
−4
−2
0
2
4
6
log_RMSD

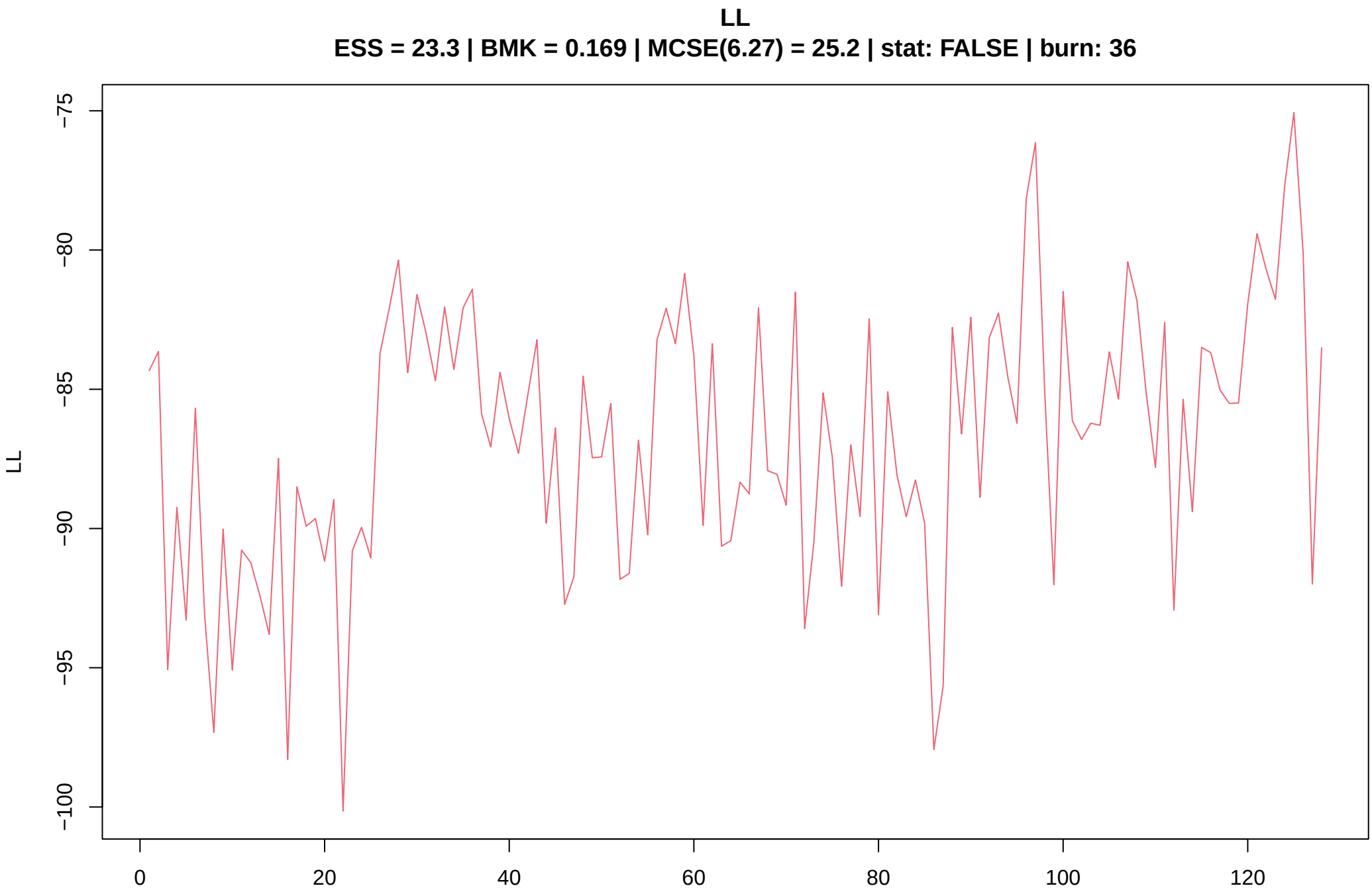

mcs_RingCount
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−4
−2
0
2
4
6
log_RMSD

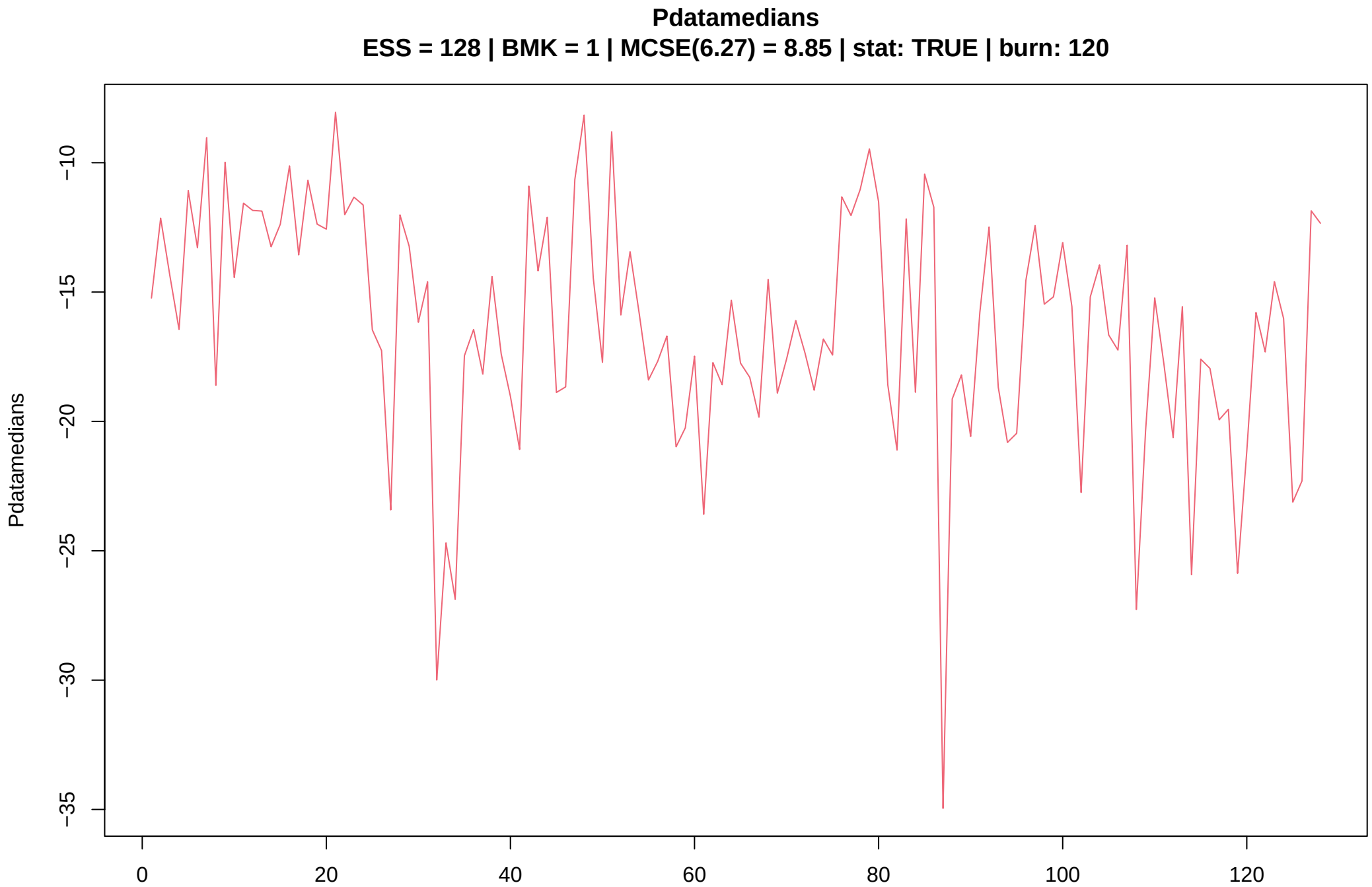

template_HeavyAtomCount
40
30
20
10
0
−4
−2
0
2
4
6
log_RMSD

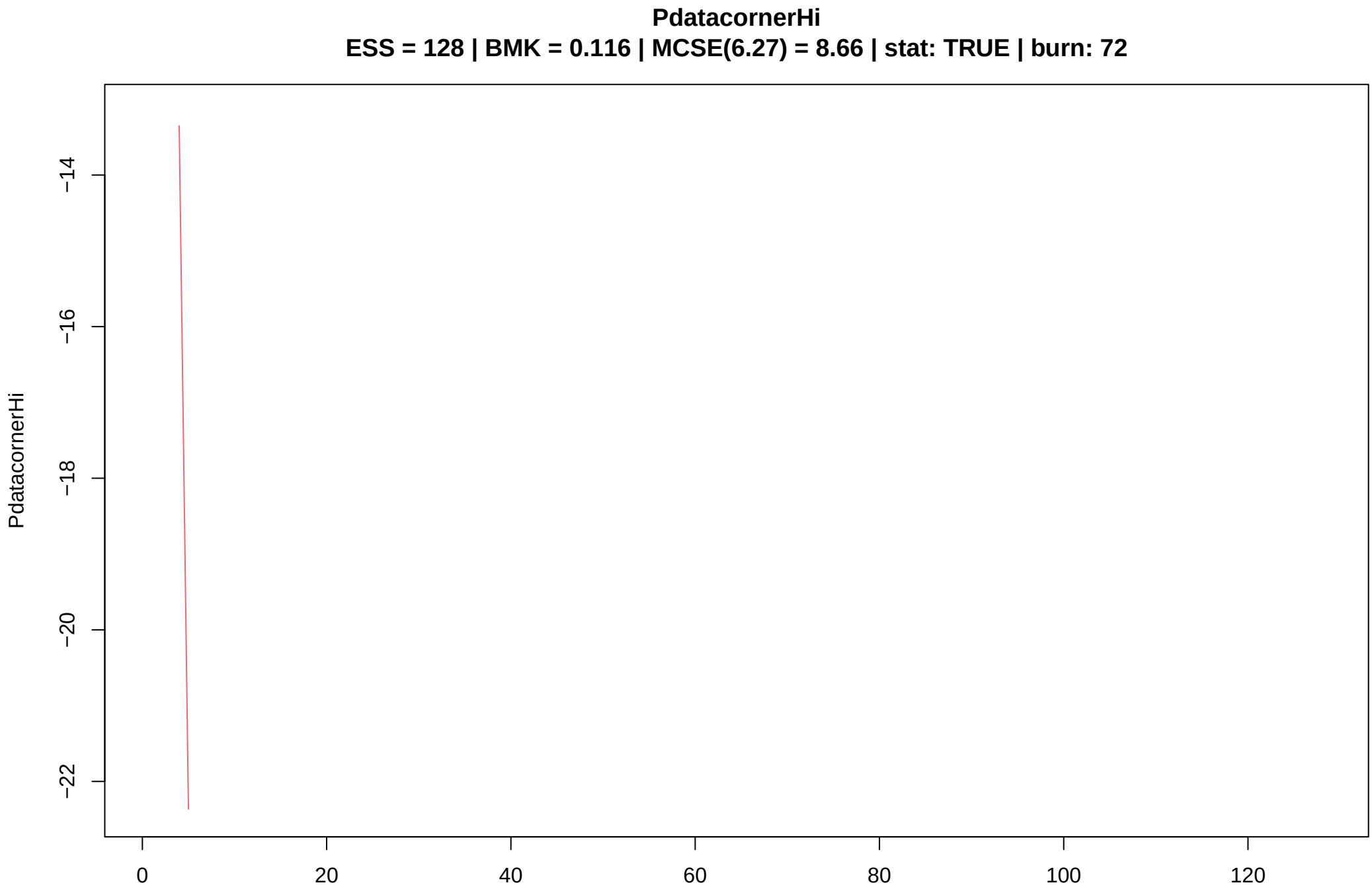

mcs_docked_NumHAcceptors
4
3
2
1
0
−4
−2
0
2
4
6
log_RMSD

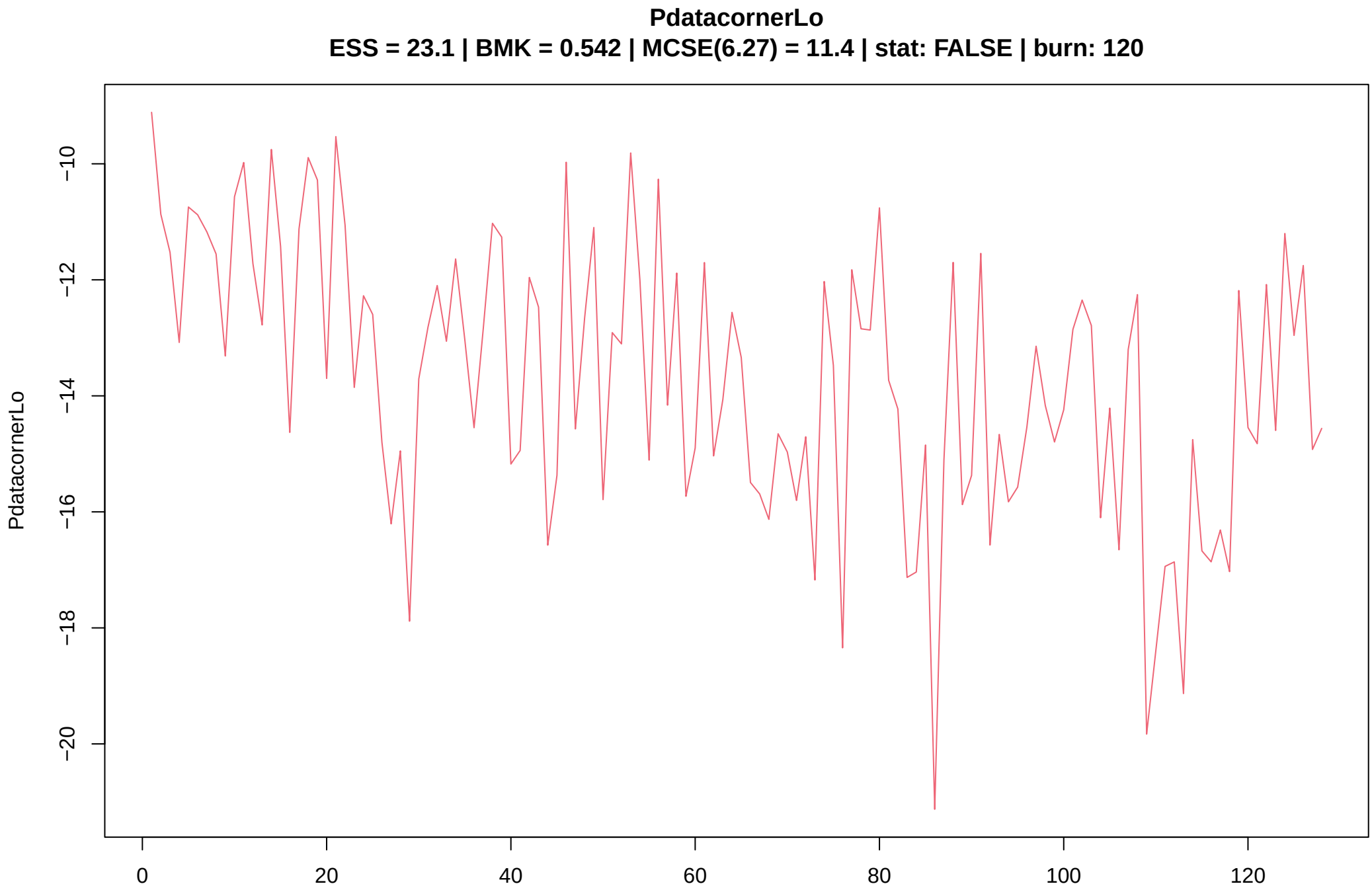

mcs_template_NumHAcceptors
5
4
3
2
1
0
−4
−2
0
2
4
6
log_RMSD

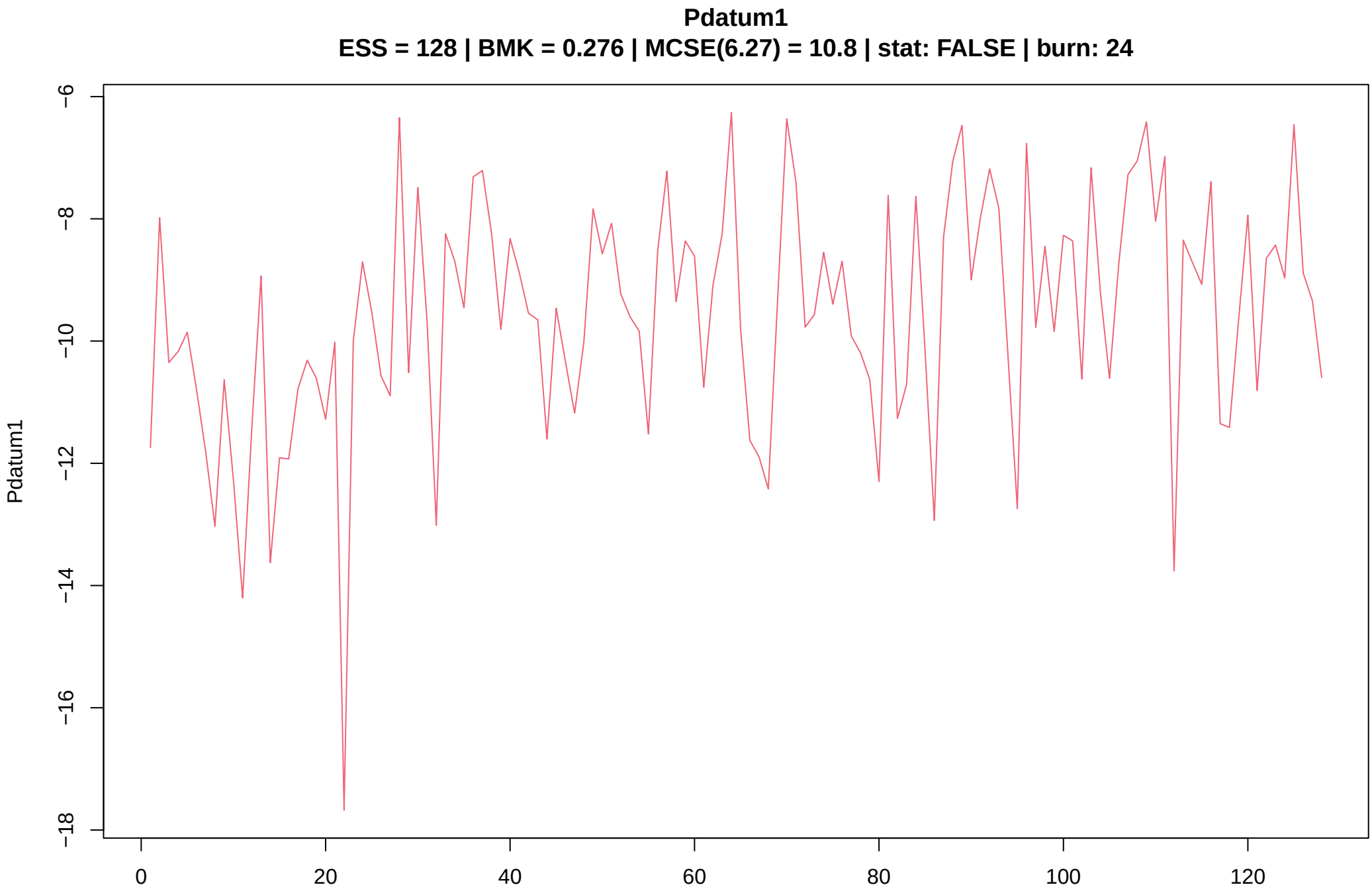

mcs_NumHeteroAtoms
8
6
4
2
0
−4
−2
0
2
4
6
log_RMSD

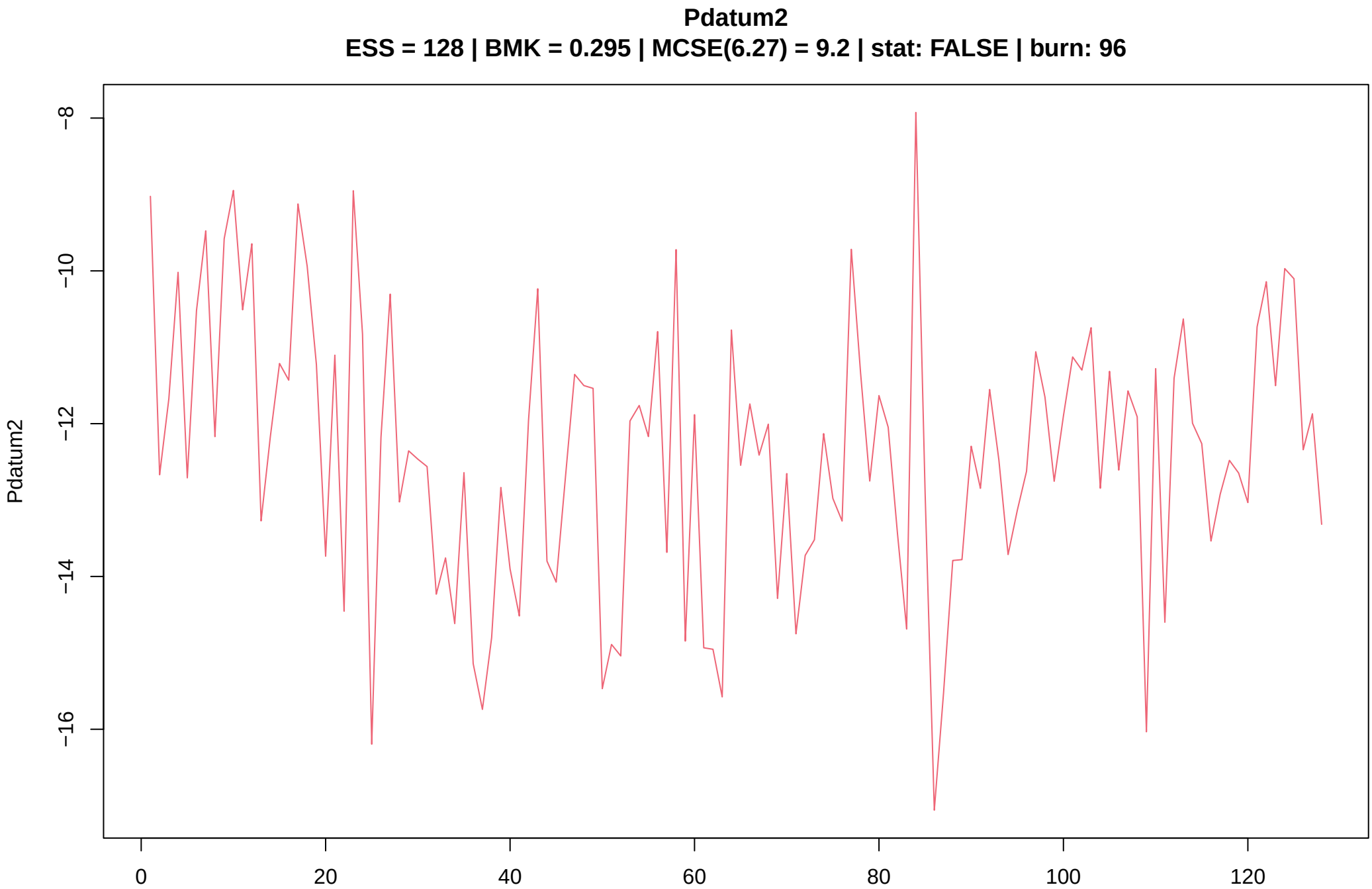

LL
ESS = 23.3 | BMK = 0.169 | MCSE(6.27) = 25.2 | stat: FALSE | burn: 36
LL
−75
−80
−85
−90
−95
−100
0
20
40
60
80
100
120

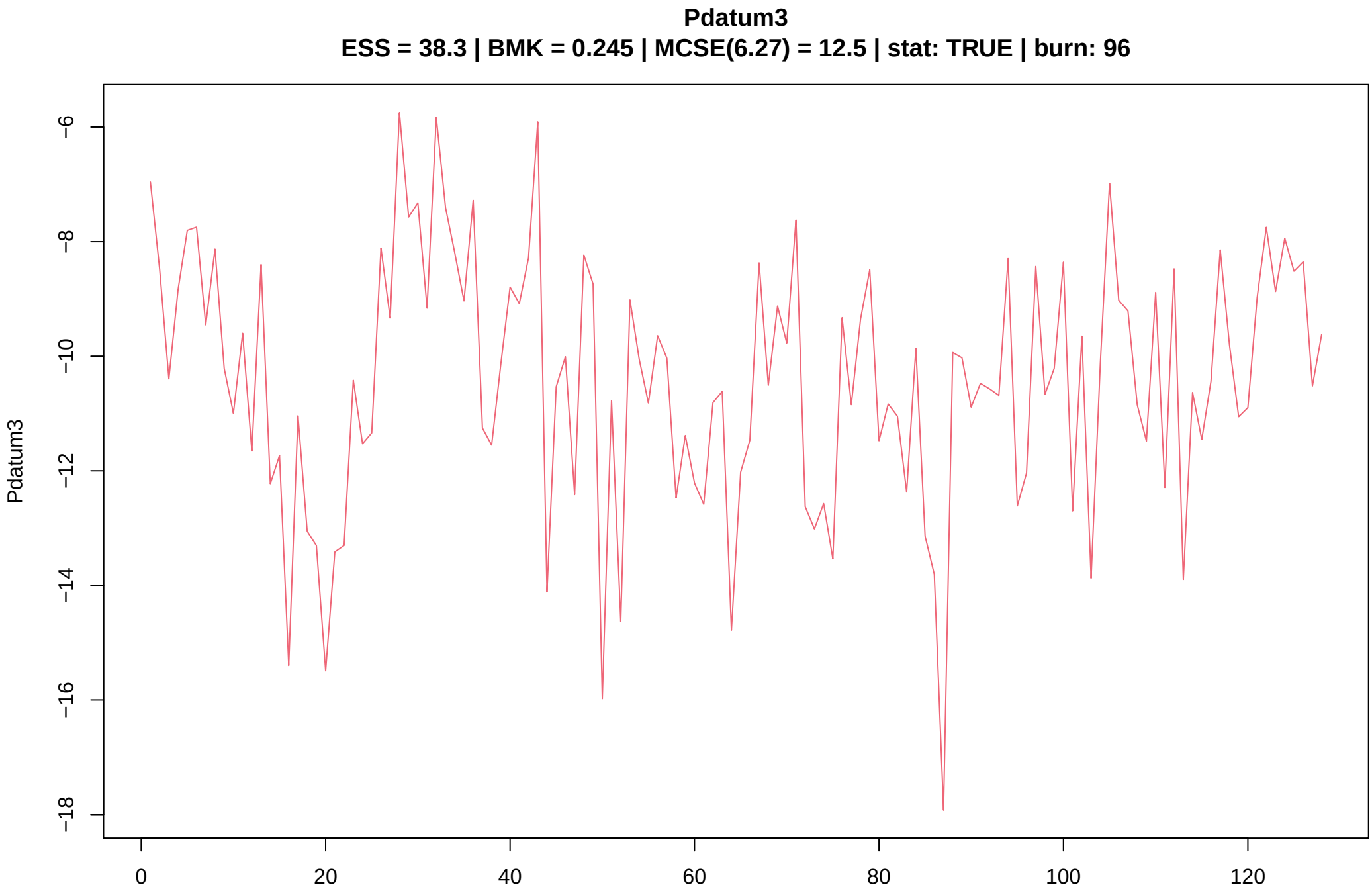

Pdatamedians
ESS = 128 | BMK = 1 | MCSE(6.27) = 8.85 | stat: TRUE | burn: 120
Pdatamedians
−10
−15
−20
−25
−30
−35
0
20
40
60
80
100
120

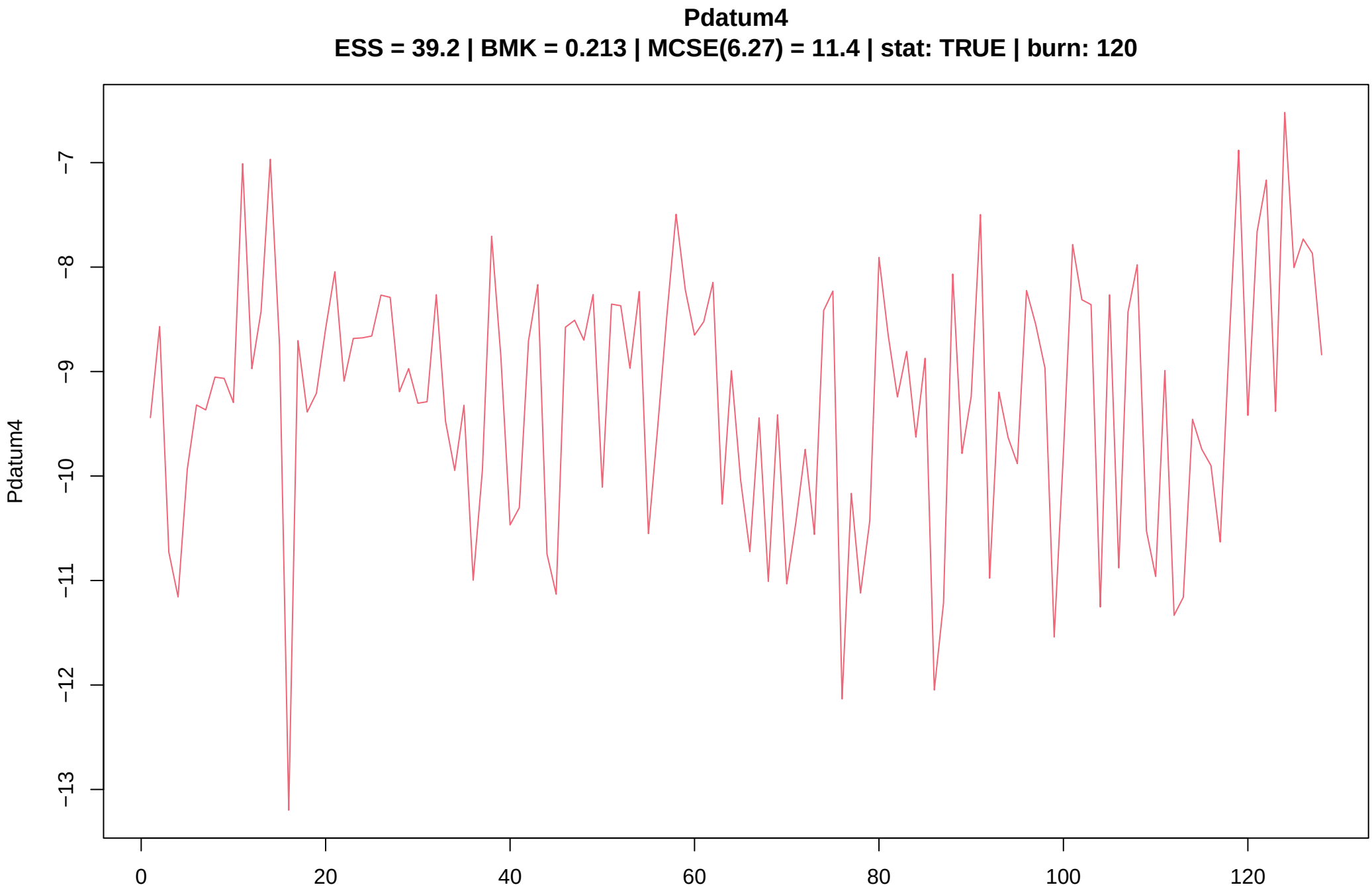

PdatacornerHi
ESS = 128 | BMK = 0.116 | MCSE(6.27) = 8.66 | stat: TRUE | burn: 72
PdatacornerHi
−14
−16
−18
−20
−22
0
20
40
60
80
100
120

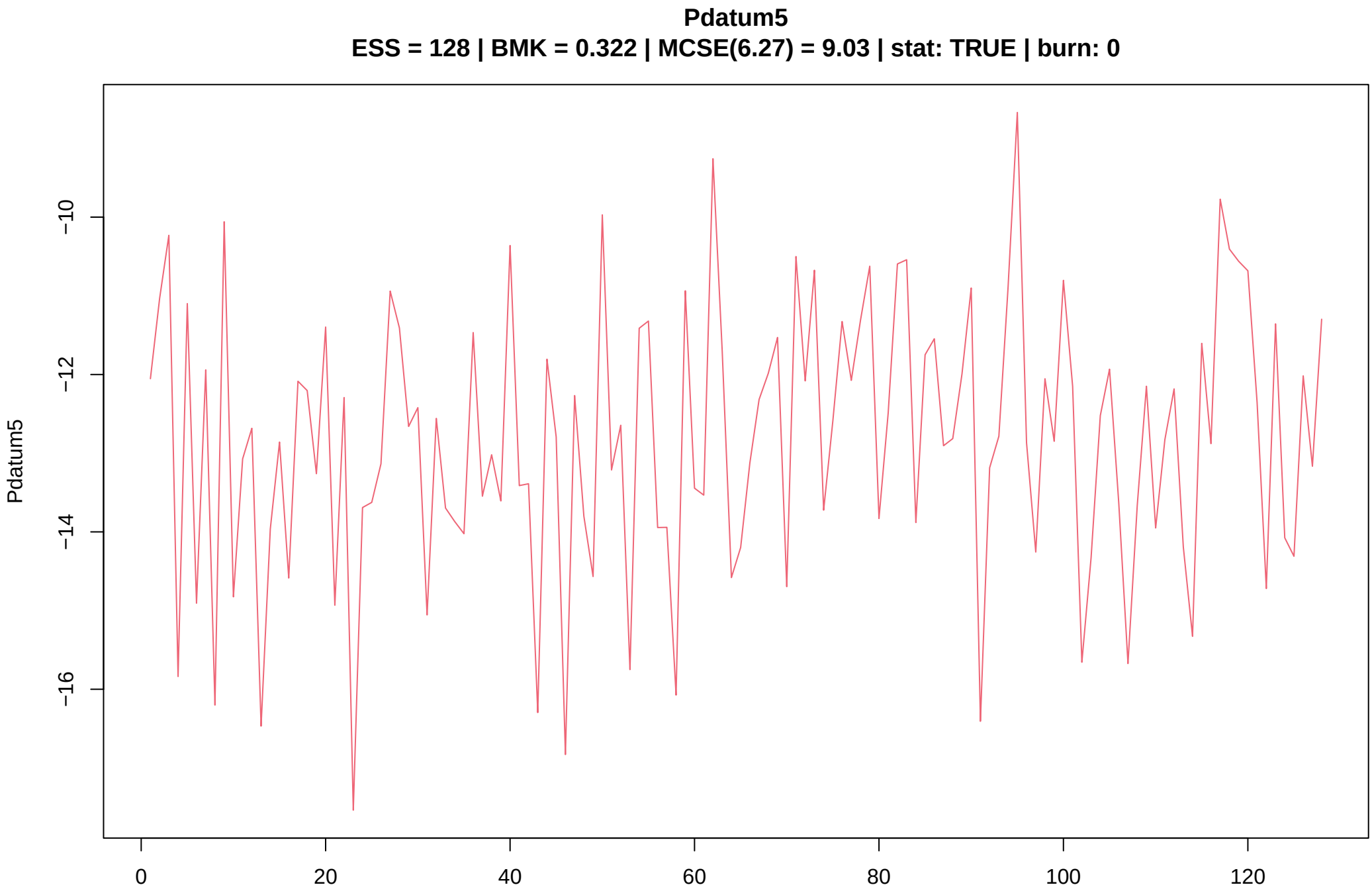

PdatacornerLo
ESS = 23.1 | BMK = 0.542 | MCSE(6.27) = 11.4 | stat: FALSE | burn: 120
PdatacornerLo
−10
−12
−14
−16
−18
−20
0
20
40
60
80
100
120

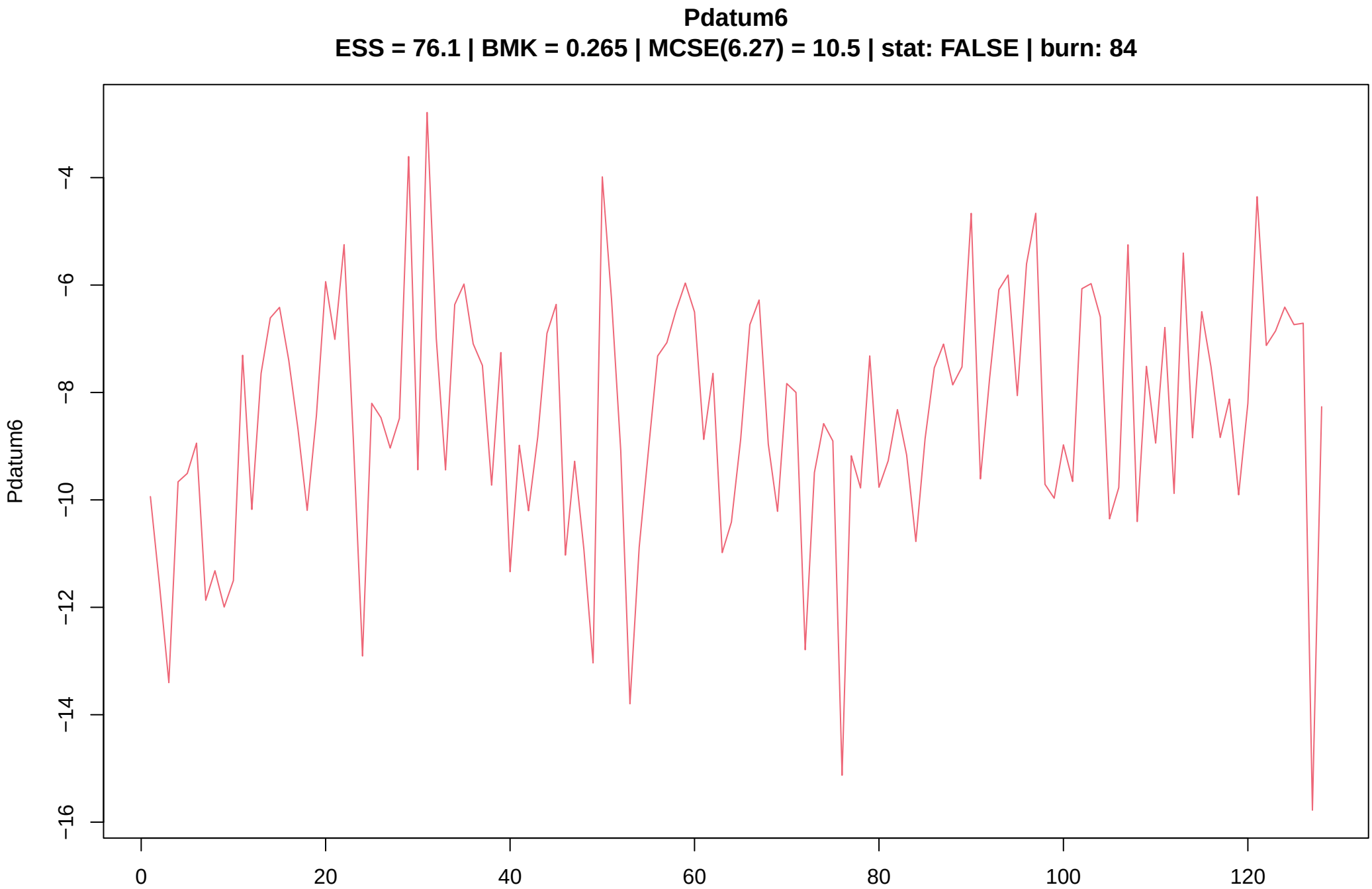

Pdatum1
ESS = 128 | BMK = 0.276 | MCSE(6.27) = 10.8 | stat: FALSE | burn: 24
Pdatum1
−6
−8
−10
−12
−14
−16
−18
0
20
40
60
80
100
120

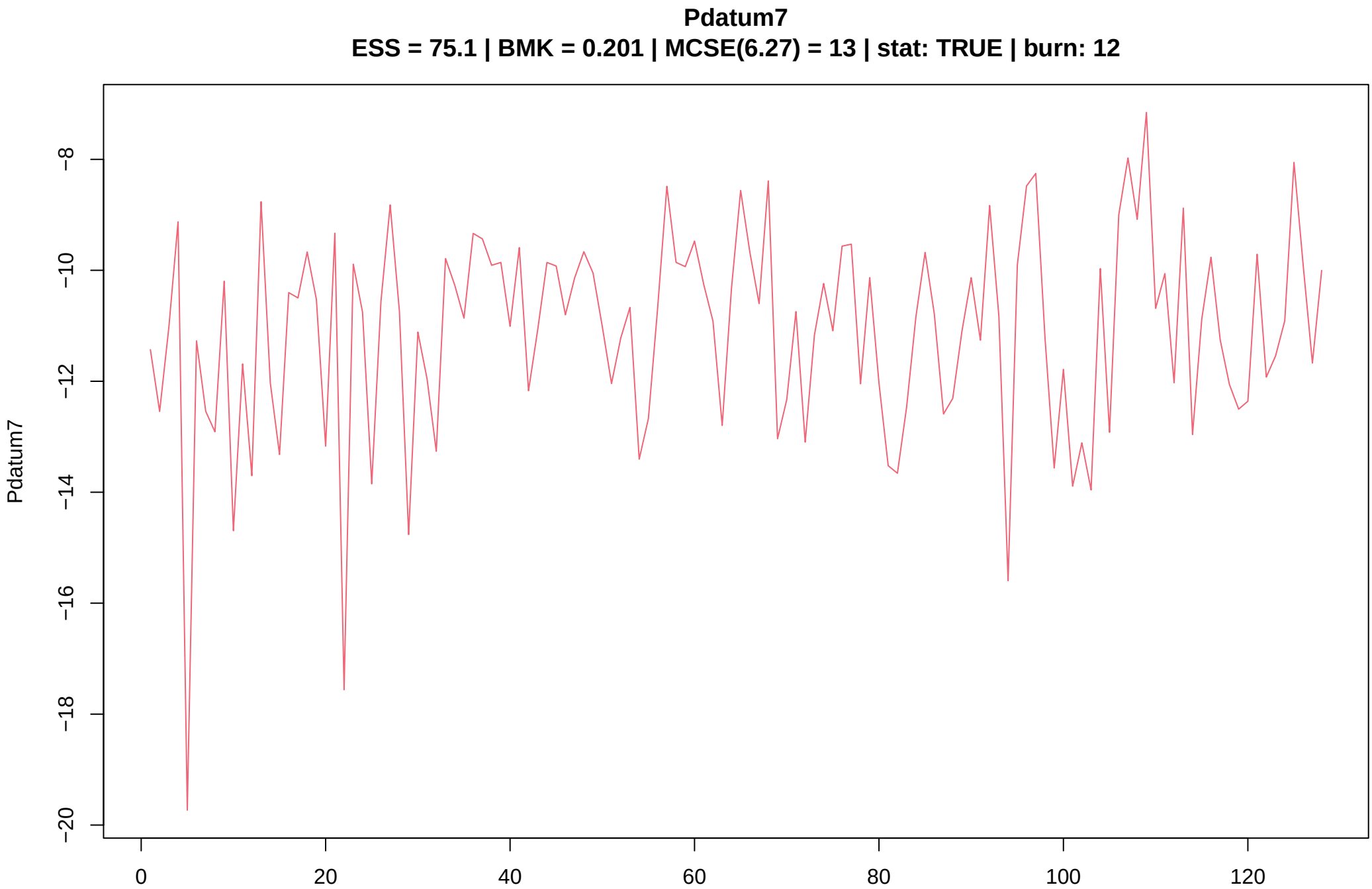

Pdatum2
ESS = 128 | BMK = 0.295 | MCSE(6.27) = 9.2 | stat: FALSE | burn: 96
Pdatum2
−8
−10
−12
−14
−16
0
20
40
60
80
100
120

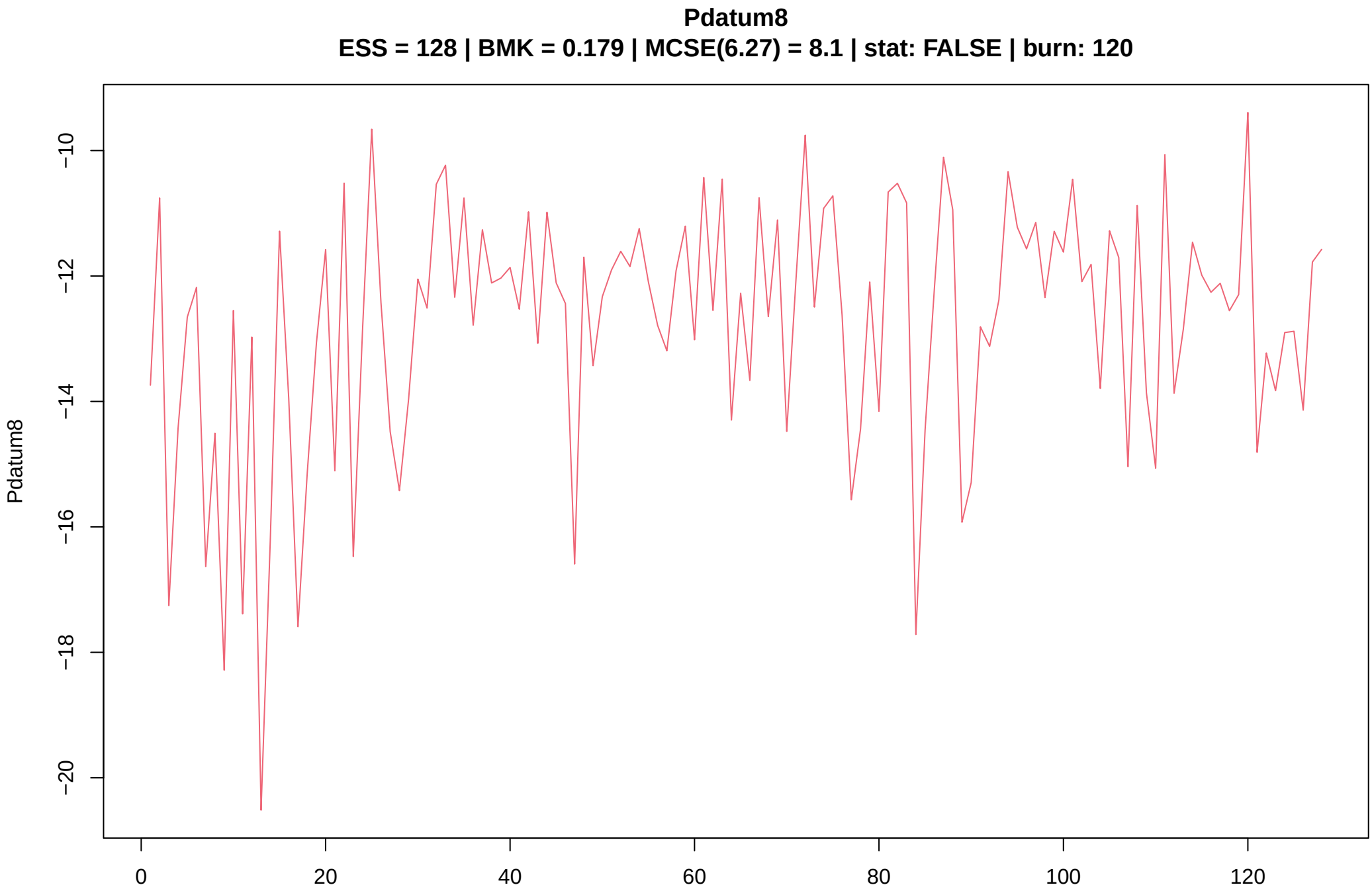

Pdatum3
ESS = 38.3 | BMK = 0.245 | MCSE(6.27) = 12.5 | stat: TRUE | burn: 96
Pdatum3
−6
−8
−10
−12
−14
−16
−18
0
20
40
60
80
100
120

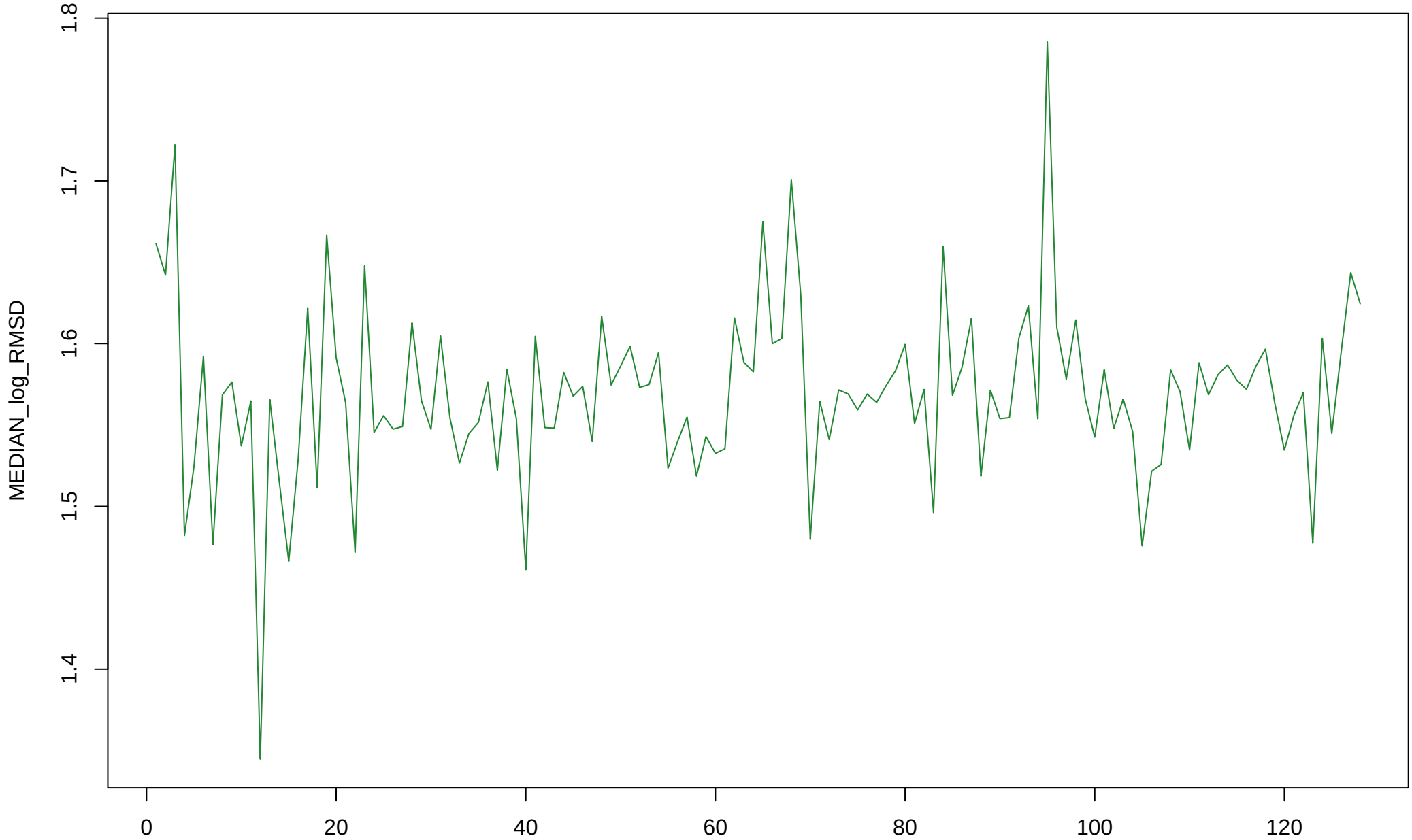

Pdatum4
ESS = 39.2 | BMK = 0.213 | MCSE(6.27) = 11.4 | stat: TRUE | burn: 120
Pdatum4
−7
−8
−9
−10
−11
−12
−13
0
20
40
60
80
100
120

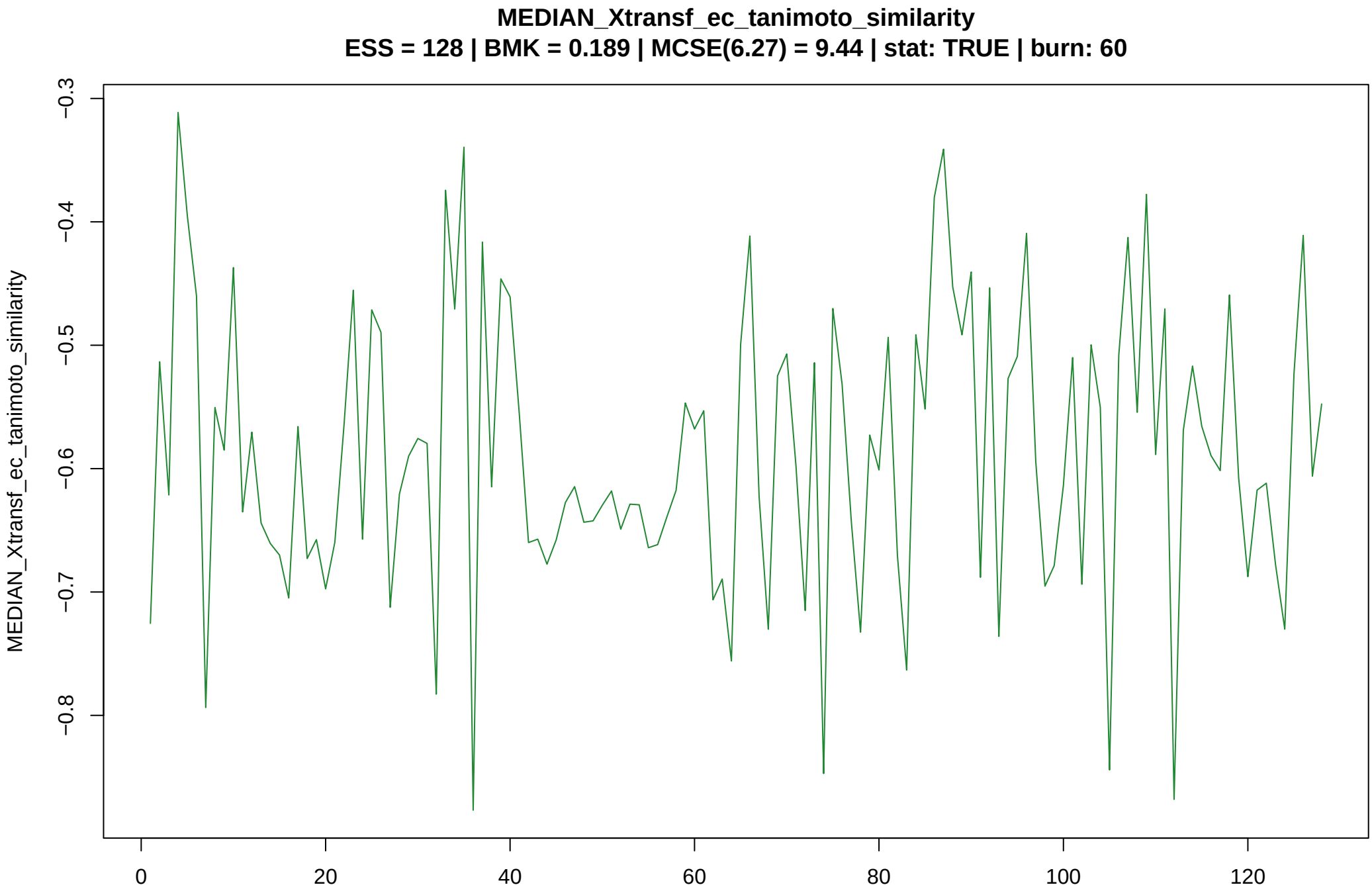

Pdatum5
ESS = 128 | BMK = 0.322 | MCSE(6.27) = 9.03 | stat: TRUE | burn: 0
Pdatum5
−10
−12
−14
−16
0
20
40
60
80
100
120

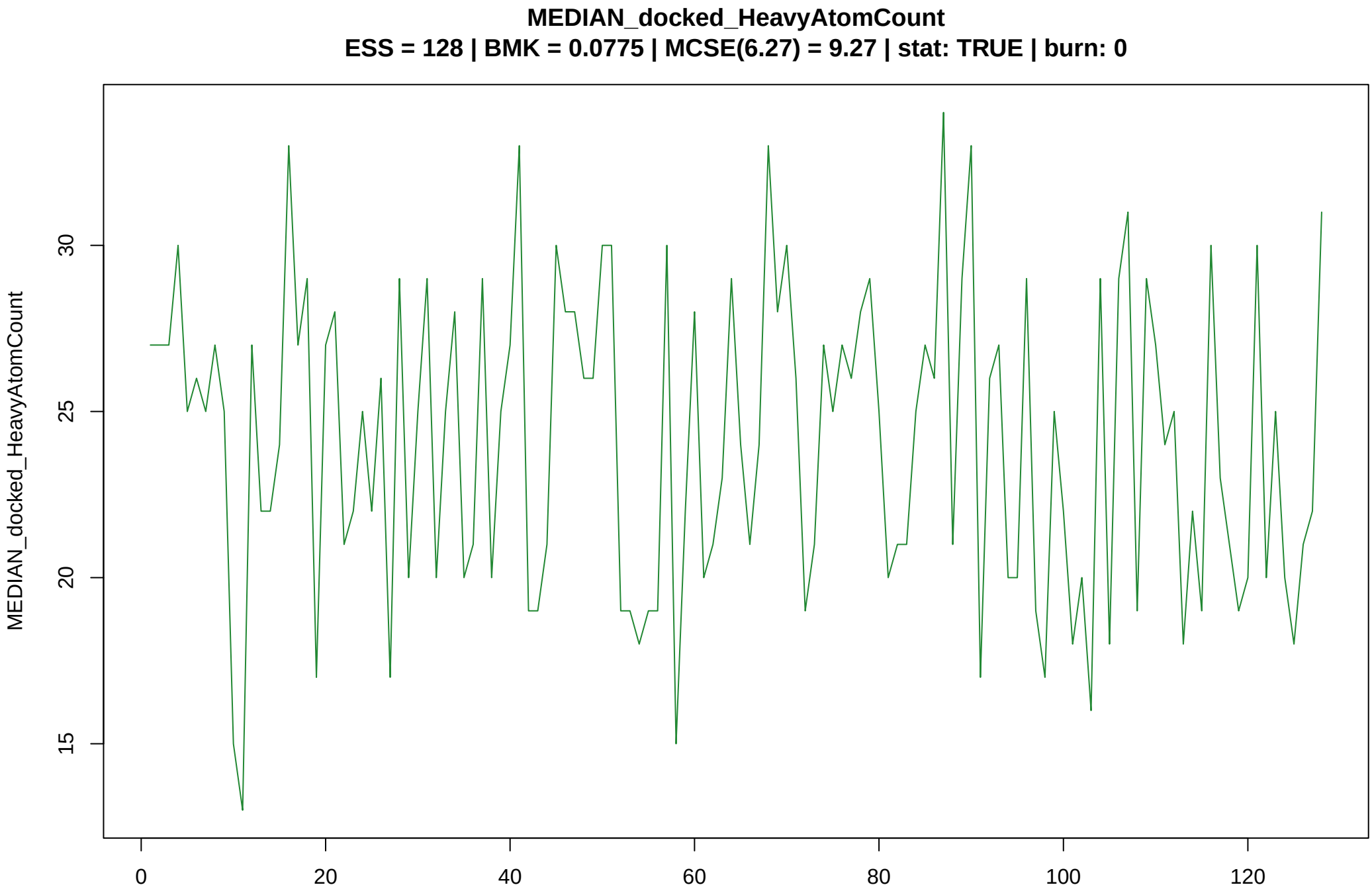

Pdatum6
ESS = 76.1 | BMK = 0.265 | MCSE(6.27) = 10.5 | stat: FALSE | burn: 84
Pdatum6
−4
−6
−8
−10
−12
−14
−16
0
20
40
60
80
100
120

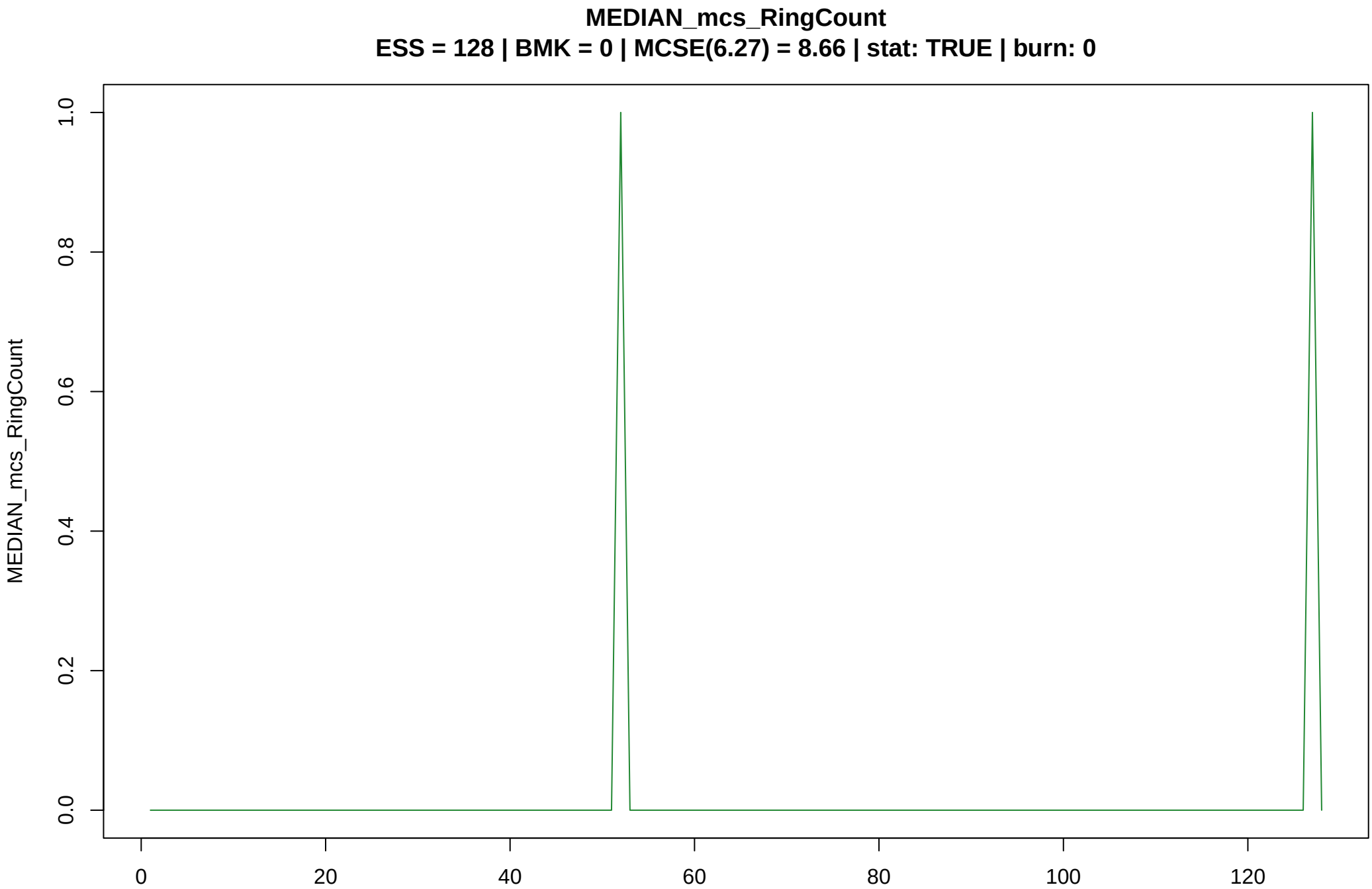

Pdatum7
ESS = 75.1 | BMK = 0.201 | MCSE(6.27) = 13 | stat: TRUE | burn: 12
Pdatum7
−8
−10
−12
−14
−16
−18
−20
0
20
40
60
80
100
120

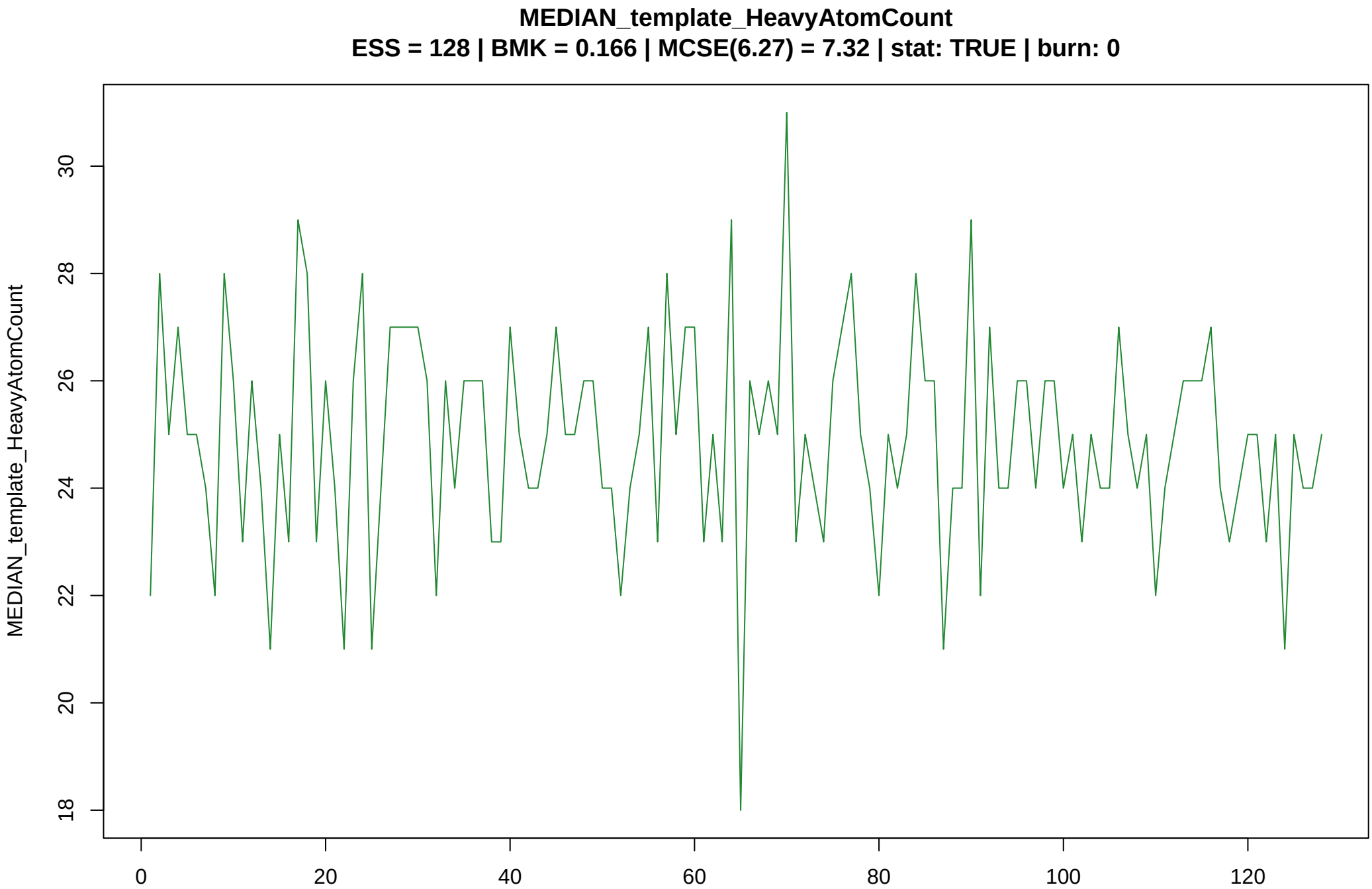

Pdatum8
ESS = 128 | BMK = 0.179 | MCSE(6.27) = 8.1 | stat: FALSE | burn: 120
Pdatum8
−10
−12
−14
−16
−18
−20
0
20
40
60
80
100
120

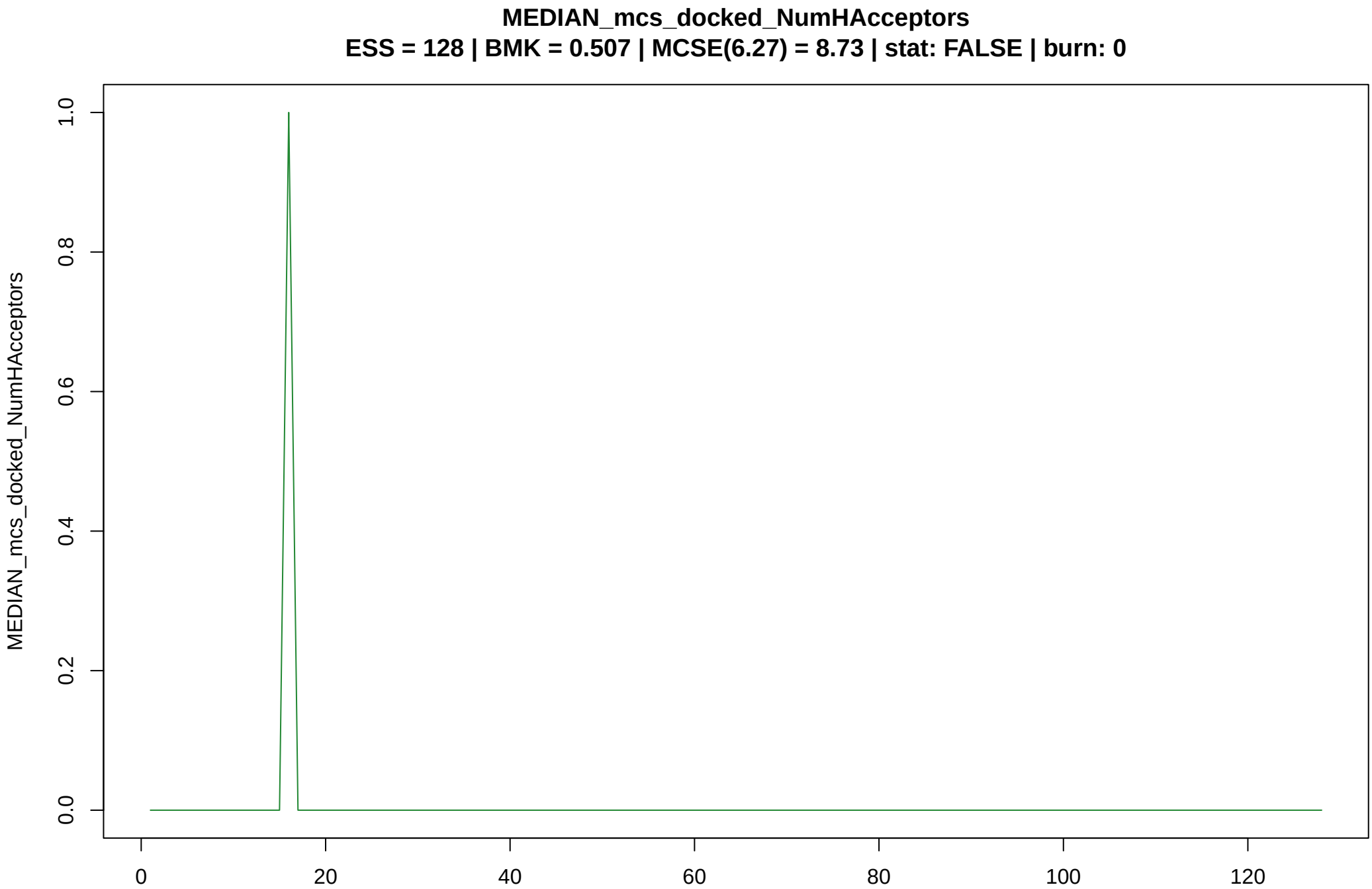

MEDIAN_log_RMSD
ESS = 56.3 | BMK = 0.172 | MCSE(6.27) = 10.9 | stat: TRUE | burn: 0
MEDIAN_log_RMSD
1.8
1.7
1.6
1.5
1.4
0
20
40
60
80
100
120

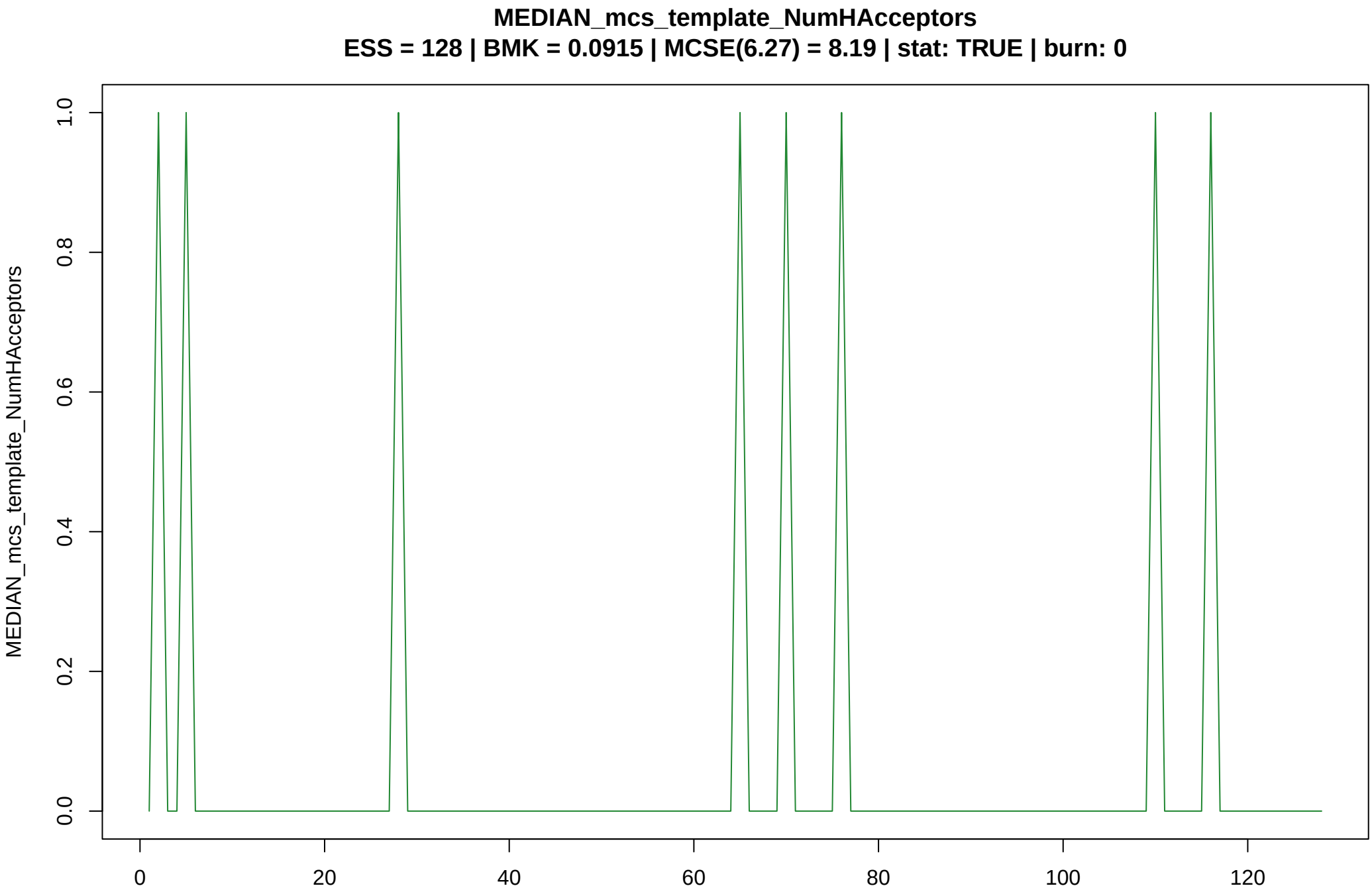

MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 128 | BMK = 0.189 | MCSE(6.27) = 9.44 | stat: TRUE | burn: 60
MEDIAN_Xtransf_ec_tanimoto_similarity
−0.3
−0.4
−0.5
−0.6
−0.7
−0.8
0
20
40
60
80
100
120

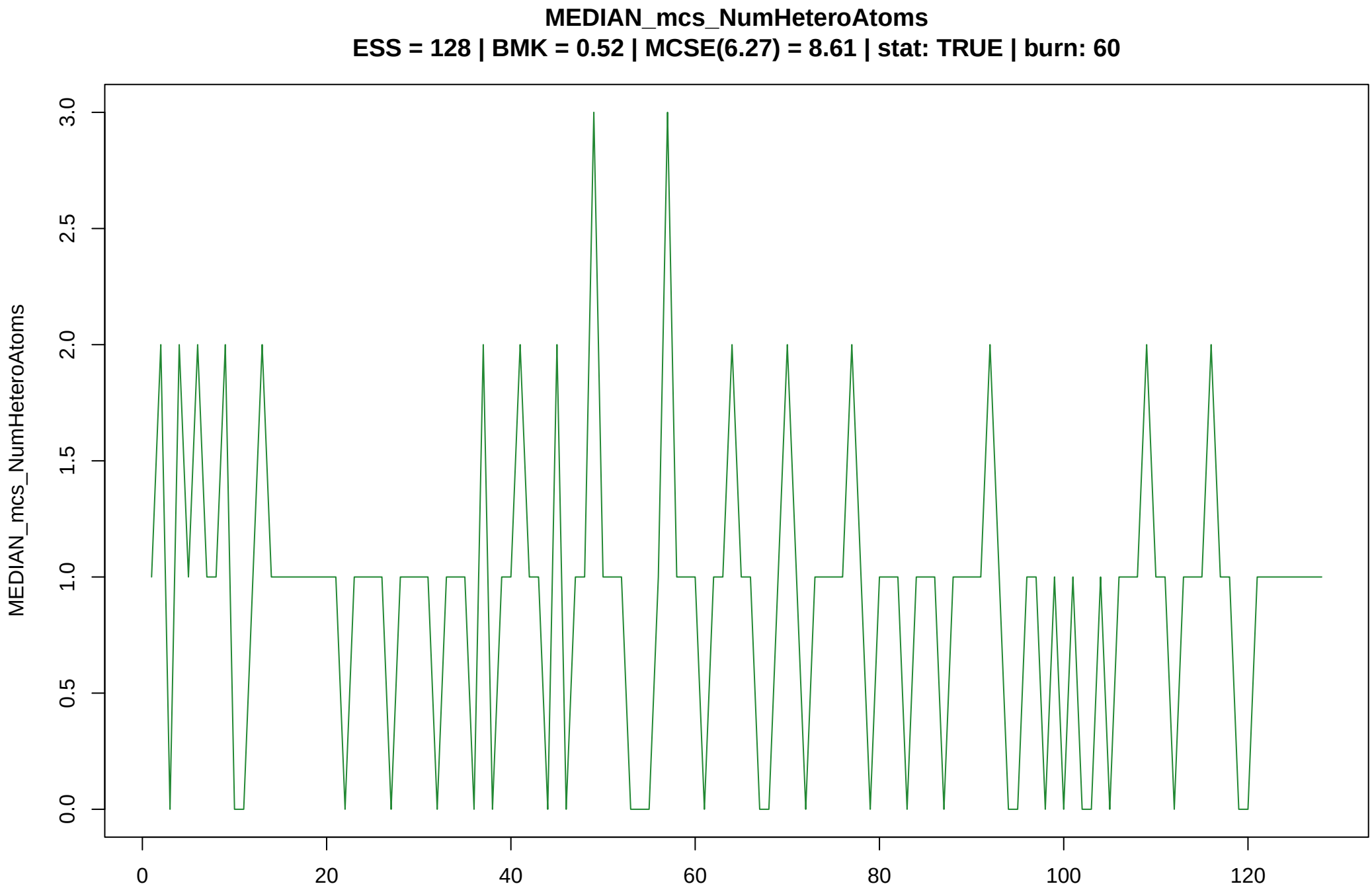

MEDIAN_docked_HeavyAtomCount
ESS = 128 | BMK = 0.0775 | MCSE(6.27) = 9.27 | stat: TRUE | burn: 0
MEDIAN_docked_HeavyAtomCount
15
20
25
30
0
20
40
60
80
100
120

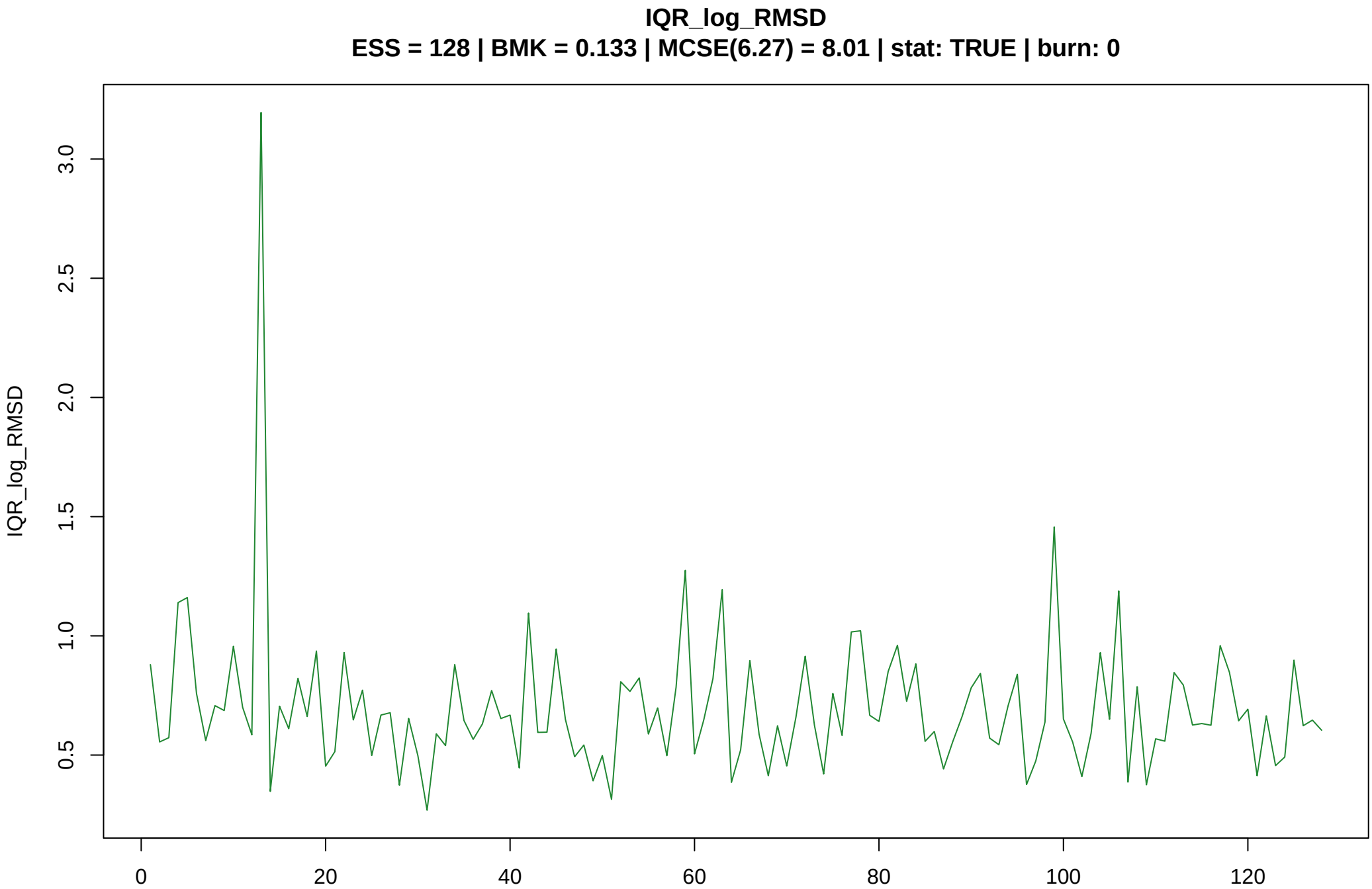

MEDIAN_mcs_RingCount
ESS = 128 | BMK = 0 | MCSE(6.27) = 8.66 | stat: TRUE | burn: 0
MEDIAN_mcs_RingCount
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

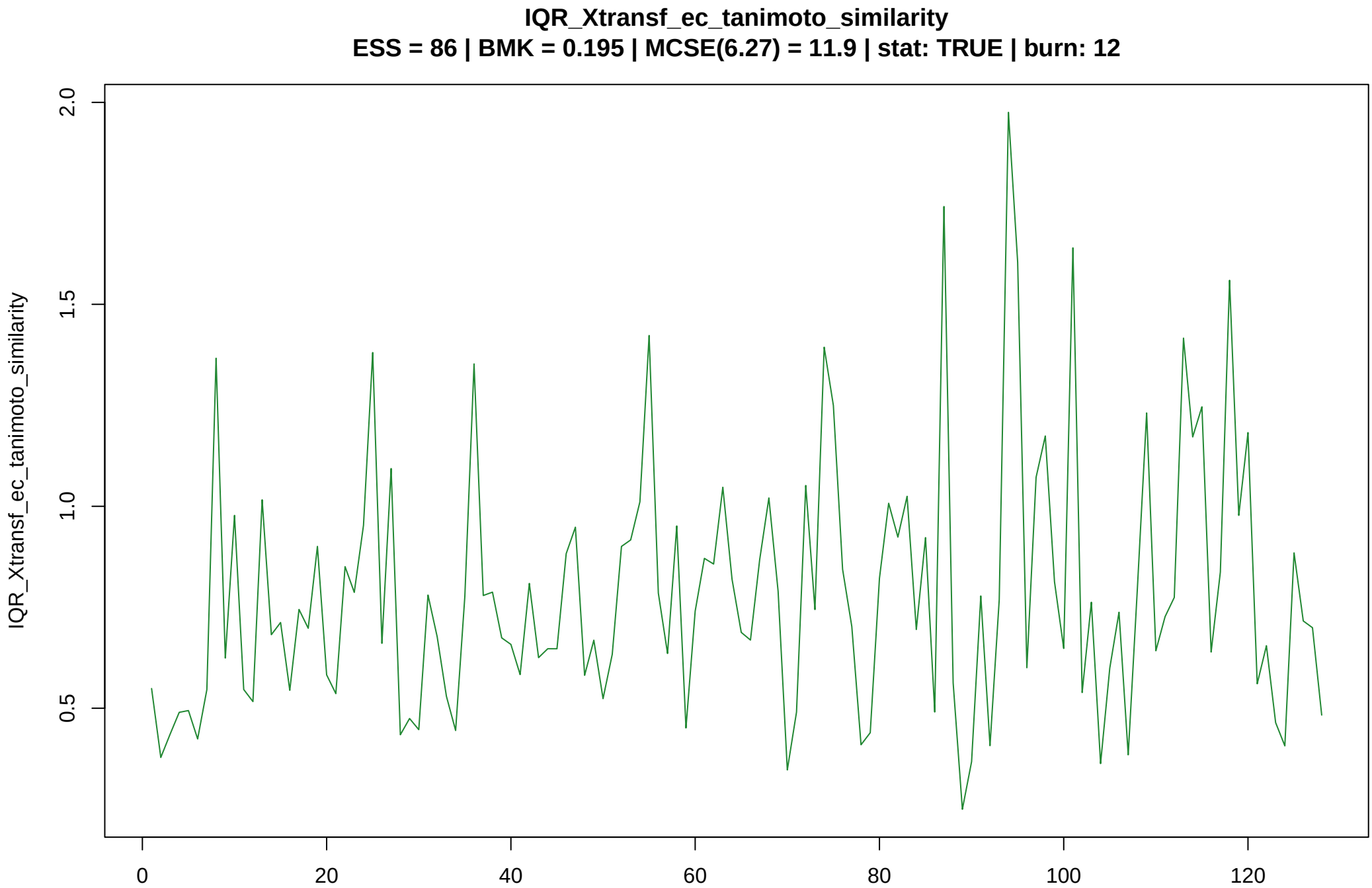

MEDIAN_template_HeavyAtomCount
ESS = 128 | BMK = 0.166 | MCSE(6.27) = 7.32 | stat: TRUE | burn: 0
MEDIAN_template_HeavyAtomCount
18
20
22
24
26
28
30
0
20
40
60
80
100
120

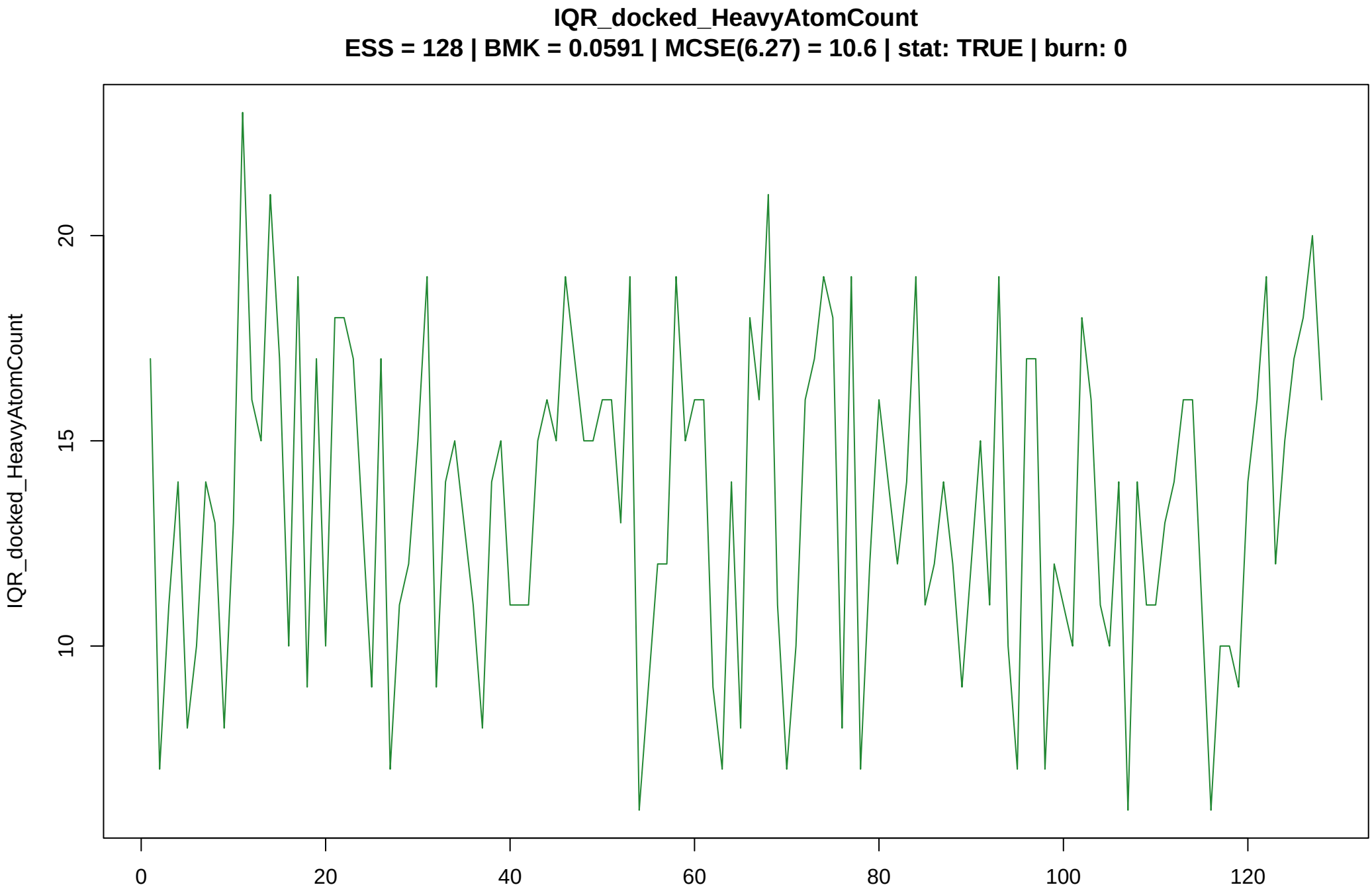

MEDIAN_mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.507 | MCSE(6.27) = 8.73 | stat: FALSE | burn: 0
MEDIAN_mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

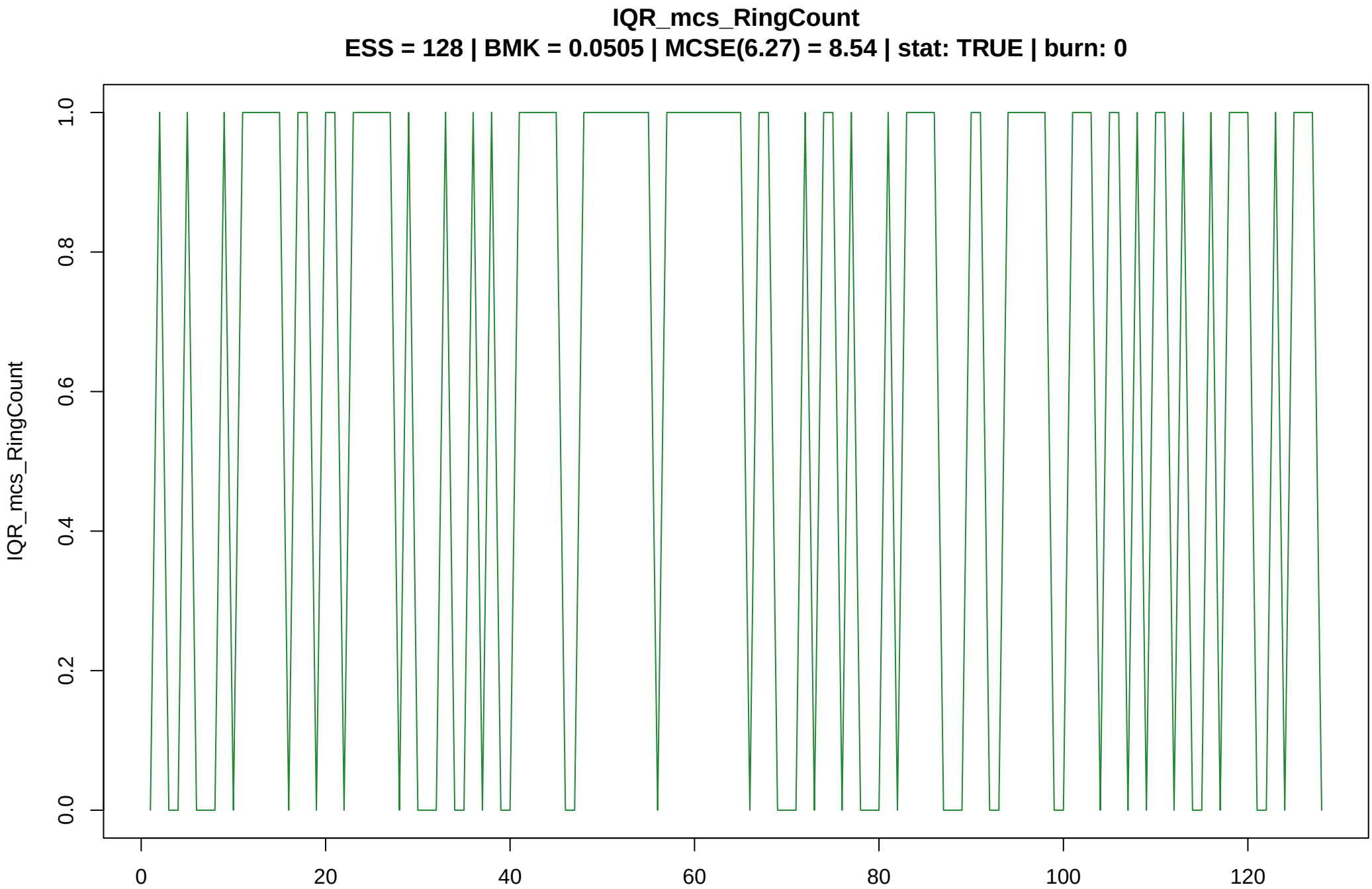

MEDIAN_mcs_template_NumHAcceptors
ESS = 128 | BMK = 0.0915 | MCSE(6.27) = 8.19 | stat: TRUE | burn: 0
MEDIAN_mcs_template_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

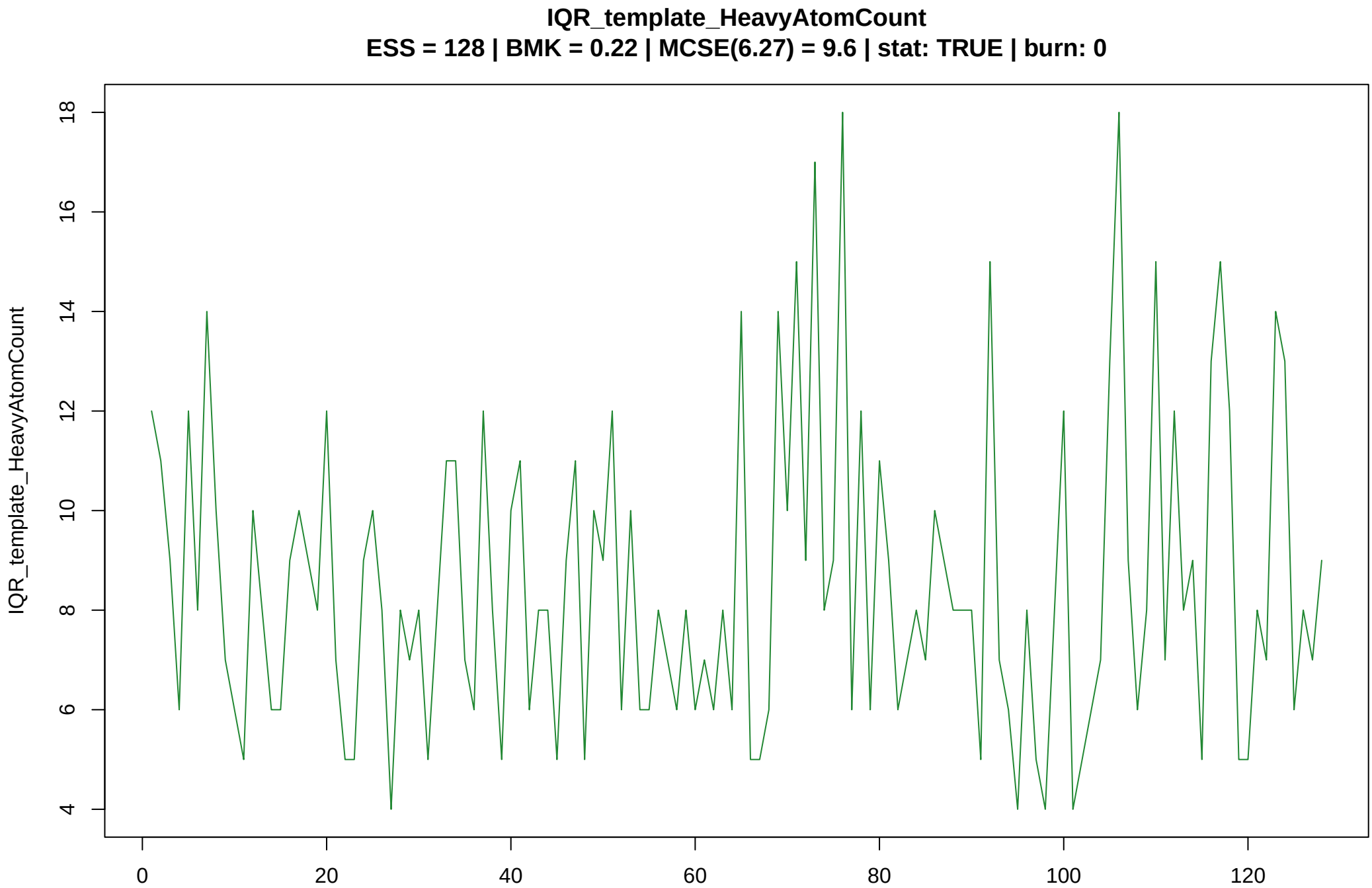

MEDIAN_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.52 | MCSE(6.27) = 8.61 | stat: TRUE | burn: 60
MEDIAN_mcs_NumHeteroAtoms
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
20
40
60
80
100
120

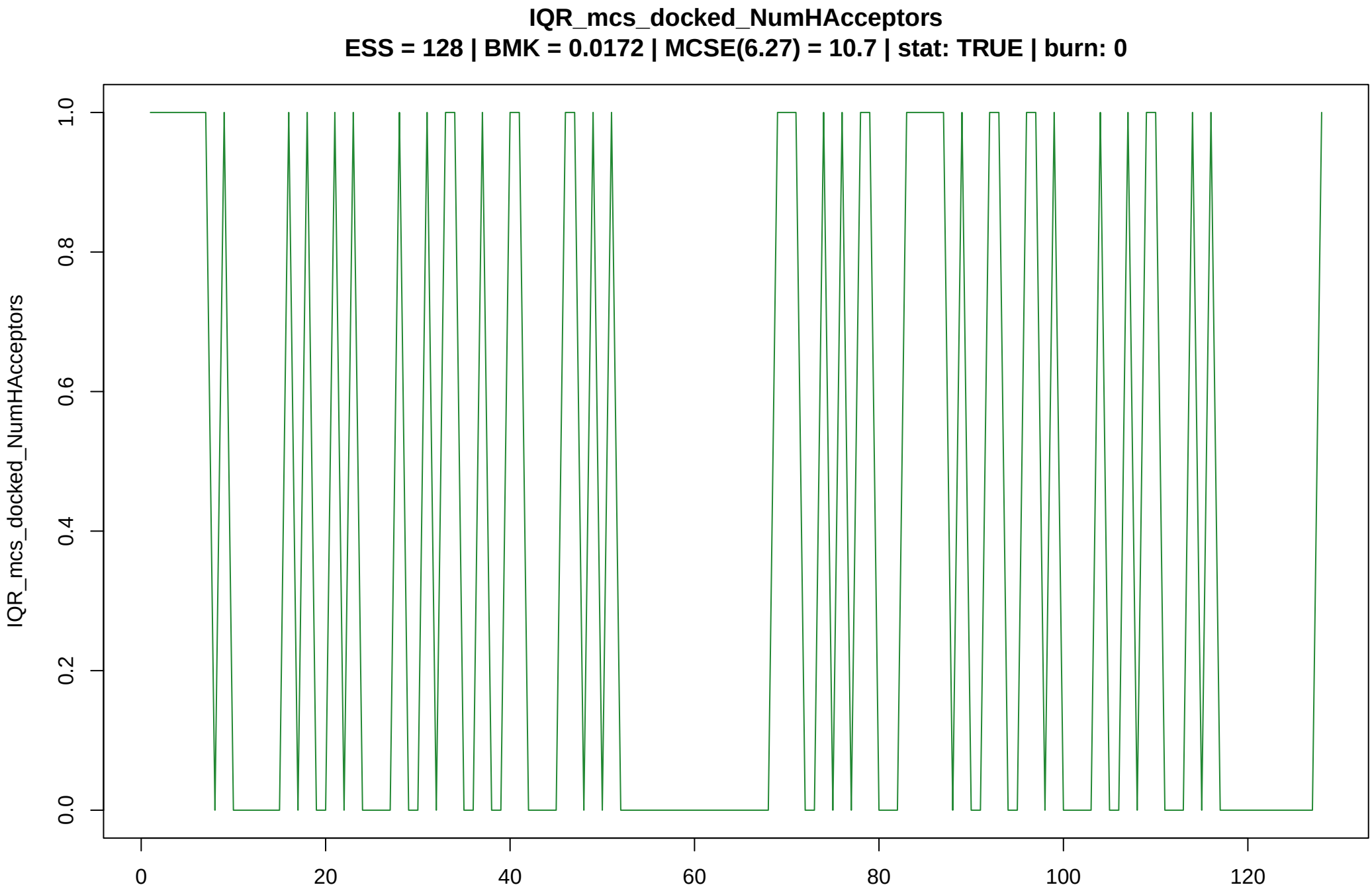

IQR_log_RMSD
ESS = 128 | BMK = 0.133 | MCSE(6.27) = 8.01 | stat: TRUE | burn: 0
IQR_log_RMSD
0.5
1.0
1.5
2.0
2.5
3.0
0
20
40
60
80
100
120

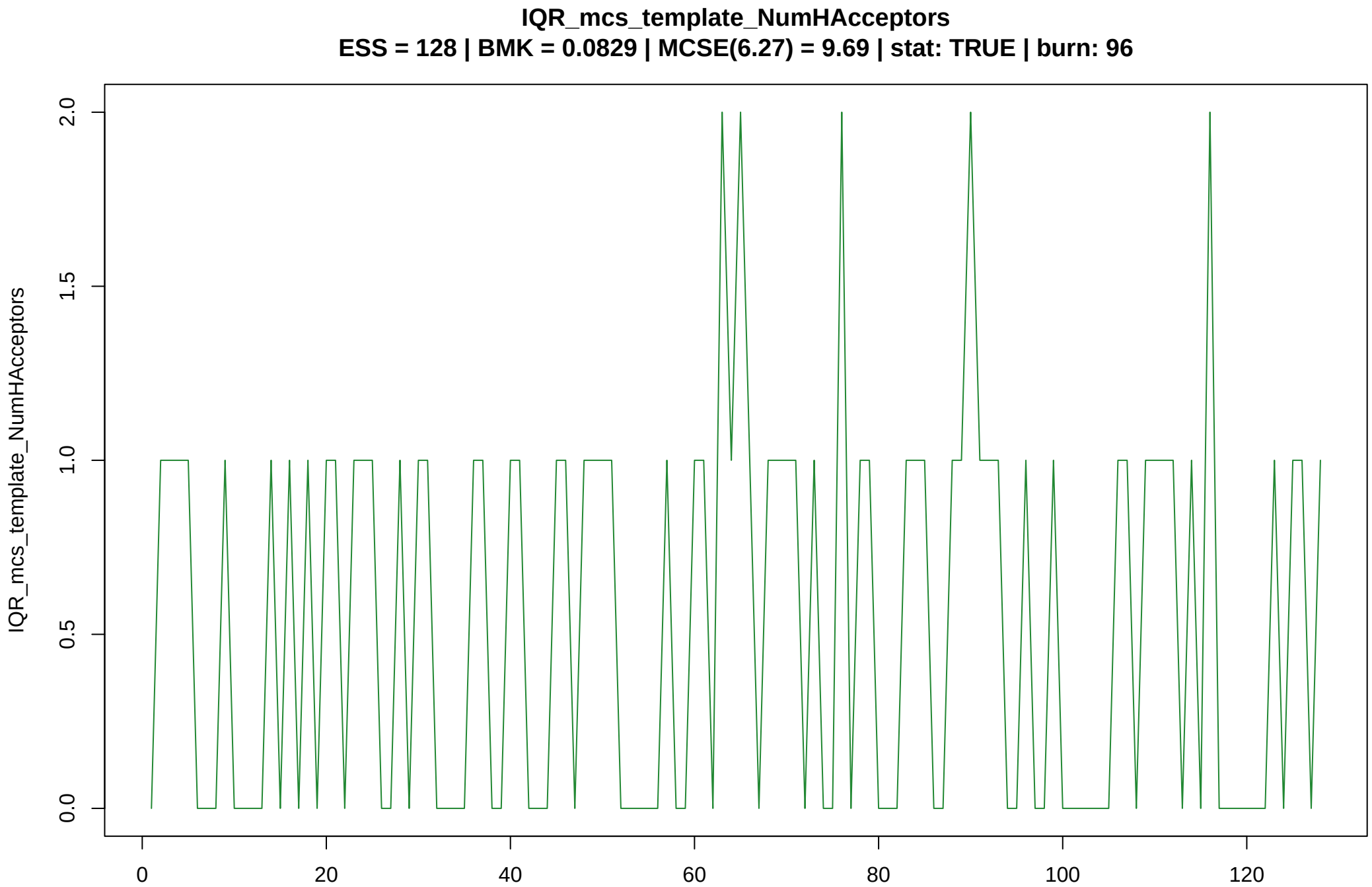

IQR_Xtransf_ec_tanimoto_similarity
ESS = 86 | BMK = 0.195 | MCSE(6.27) = 11.9 | stat: TRUE | burn: 12
IQR_Xtransf_ec_tanimoto_similarity
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120

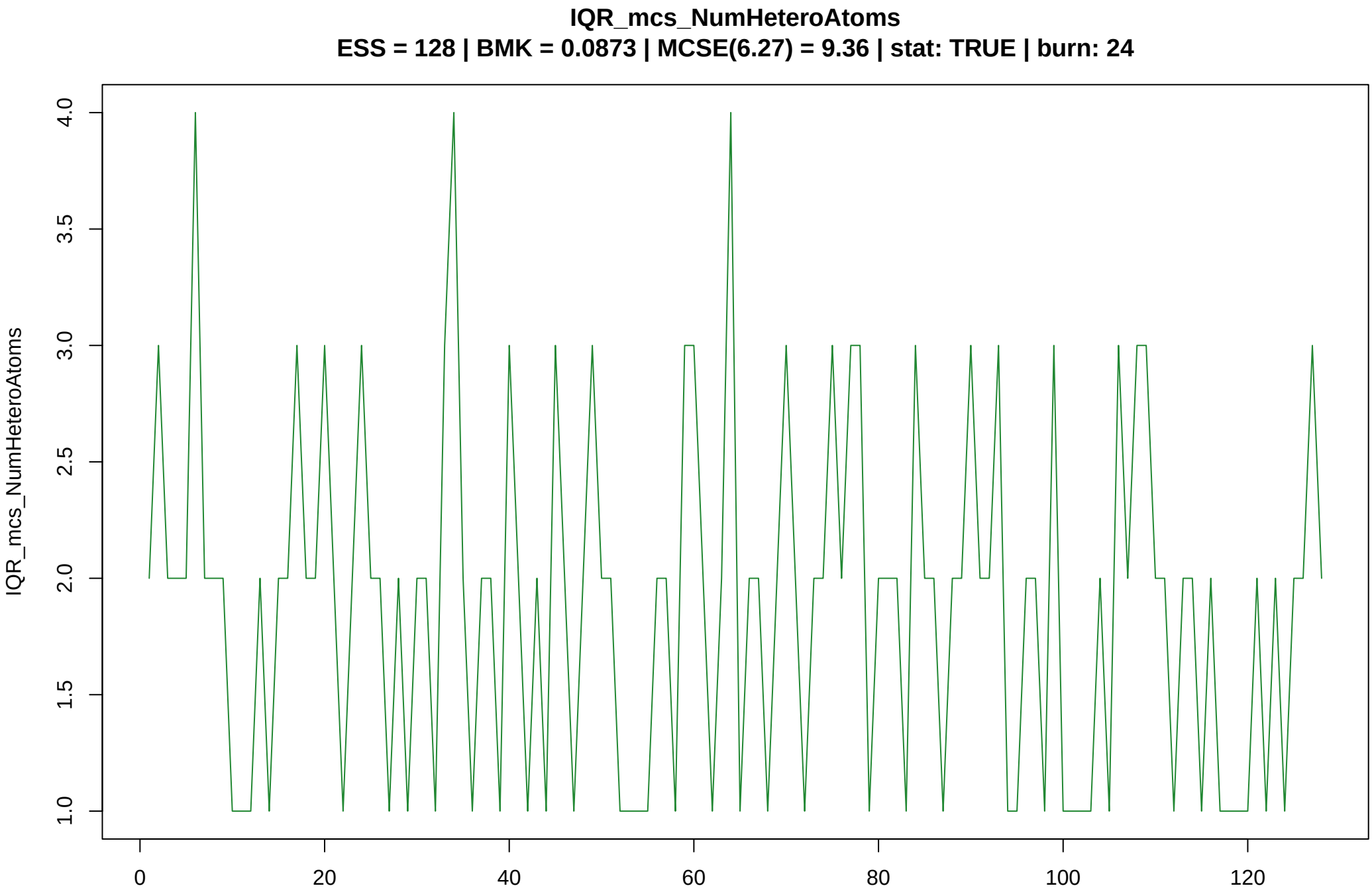

IQR_docked_HeavyAtomCount
ESS = 128 | BMK = 0.0591 | MCSE(6.27) = 10.6 | stat: TRUE | burn: 0
IQR_docked_HeavyAtomCount
10
15
20
0
20
40
60
80
100
120

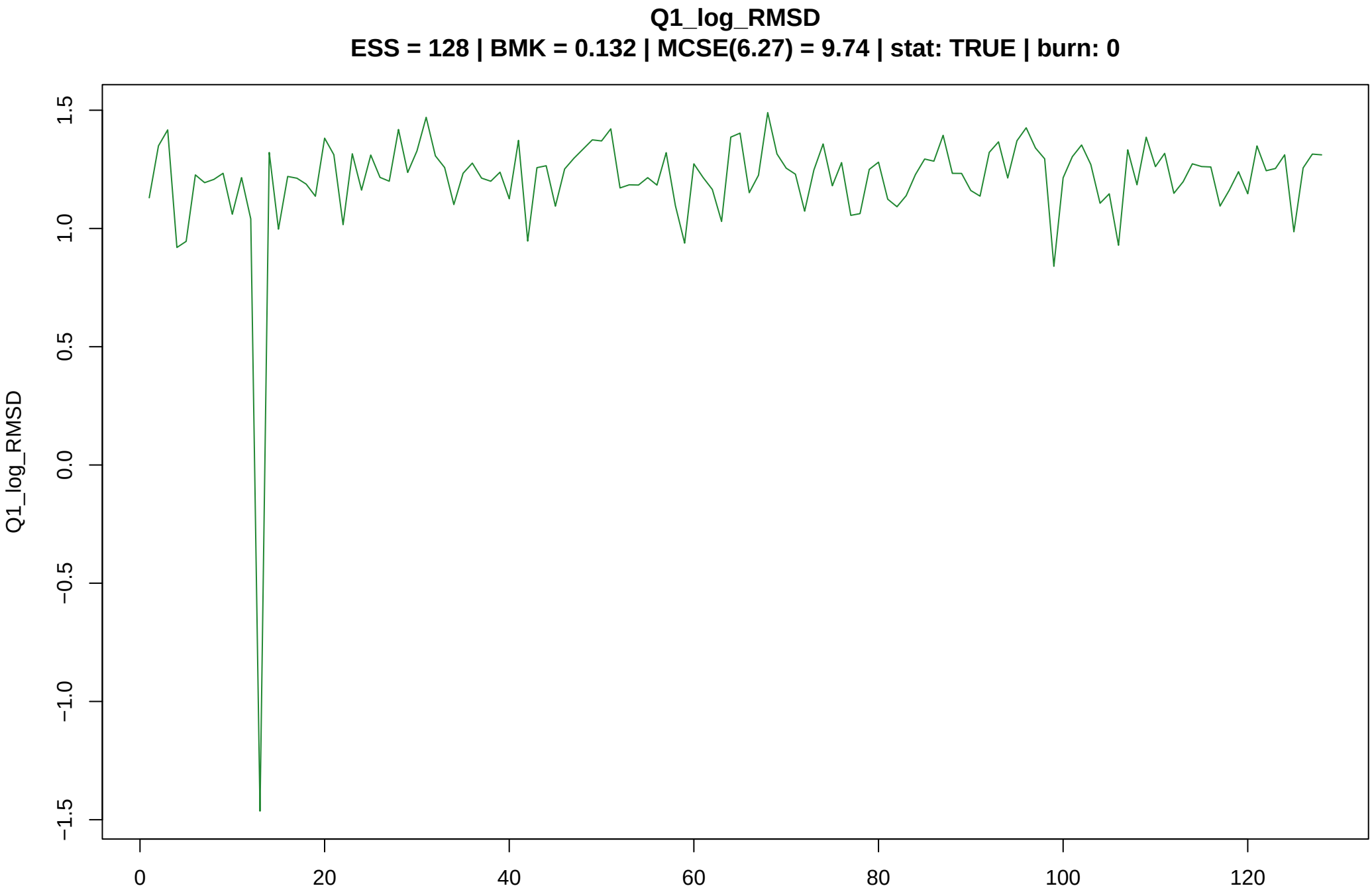

IQR_mcs_RingCount
ESS = 128 | BMK = 0.0505 | MCSE(6.27) = 8.54 | stat: TRUE | burn: 0
IQR_mcs_RingCount
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

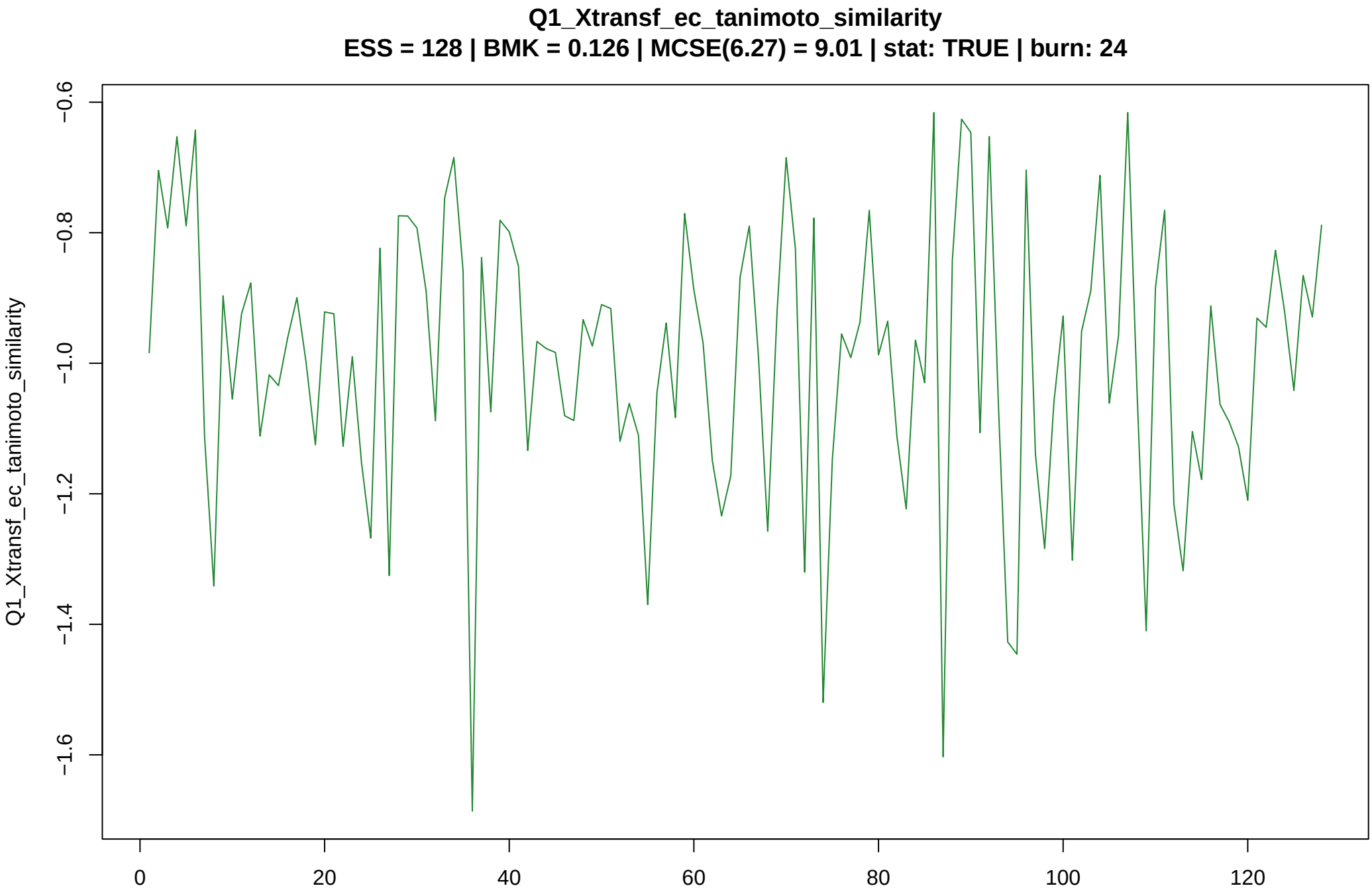

IQR_template_HeavyAtomCount
ESS = 128 | BMK = 0.22 | MCSE(6.27) = 9.6 | stat: TRUE | burn: 0
IQR_template_HeavyAtomCount
4
6
8
10
12
14
16
18
0
20
40
60
80
100
120

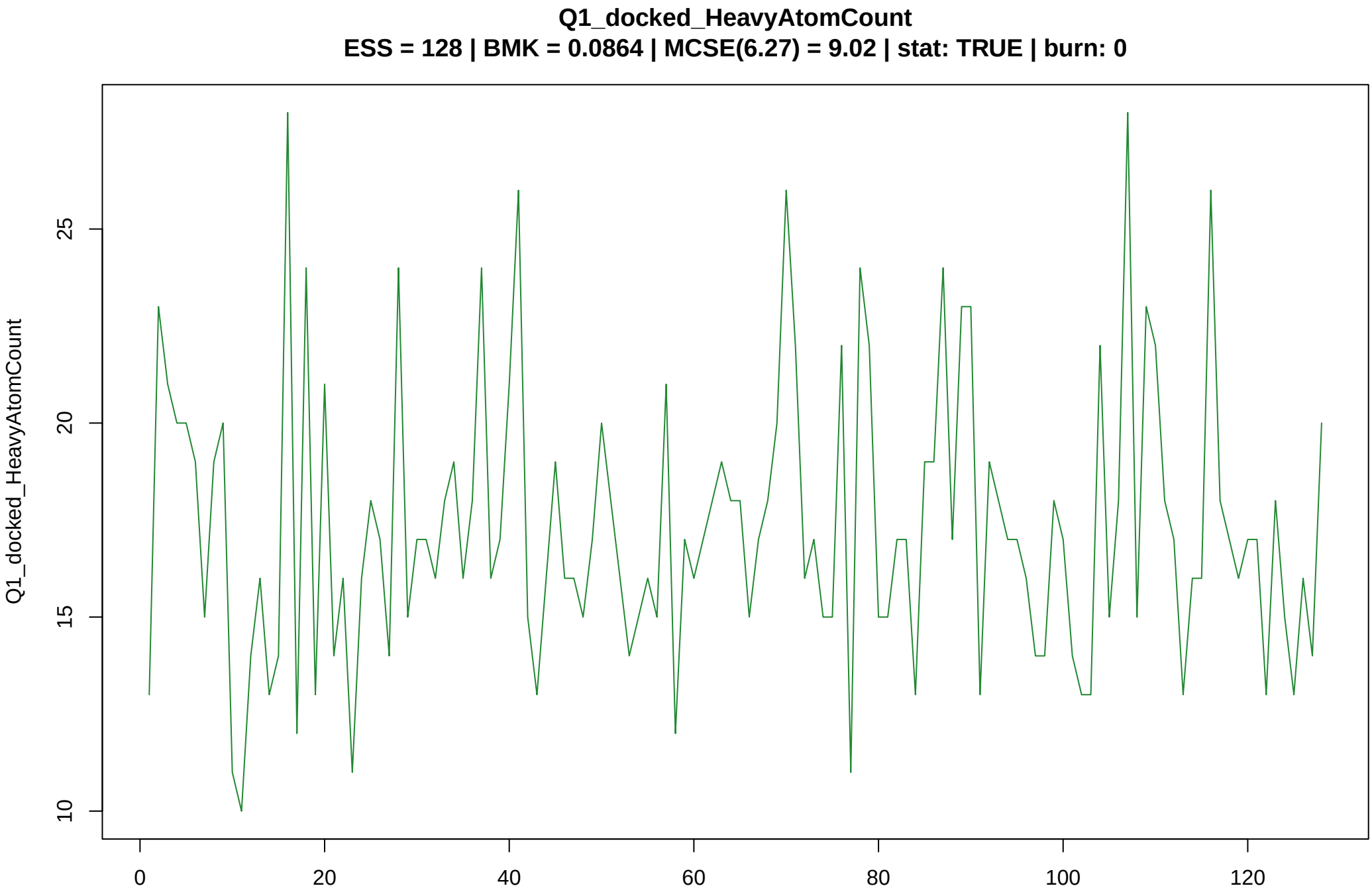

IQR_mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.0172 | MCSE(6.27) = 10.7 | stat: TRUE | burn: 0
IQR_mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

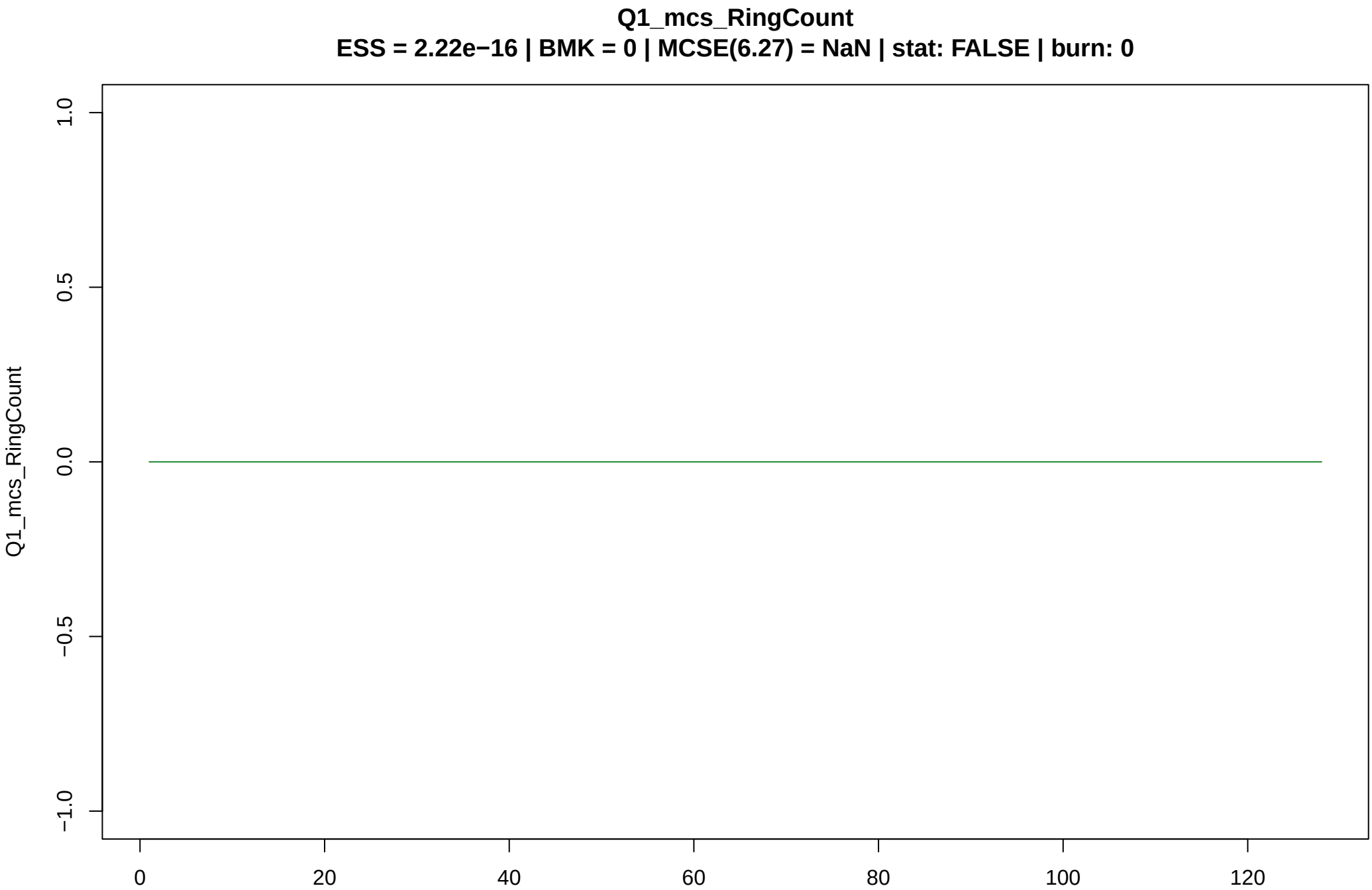

IQR_mcs_template_NumHAcceptors
ESS = 128 | BMK = 0.0829 | MCSE(6.27) = 9.69 | stat: TRUE | burn: 96
IQR_mcs_template_NumHAcceptors
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120

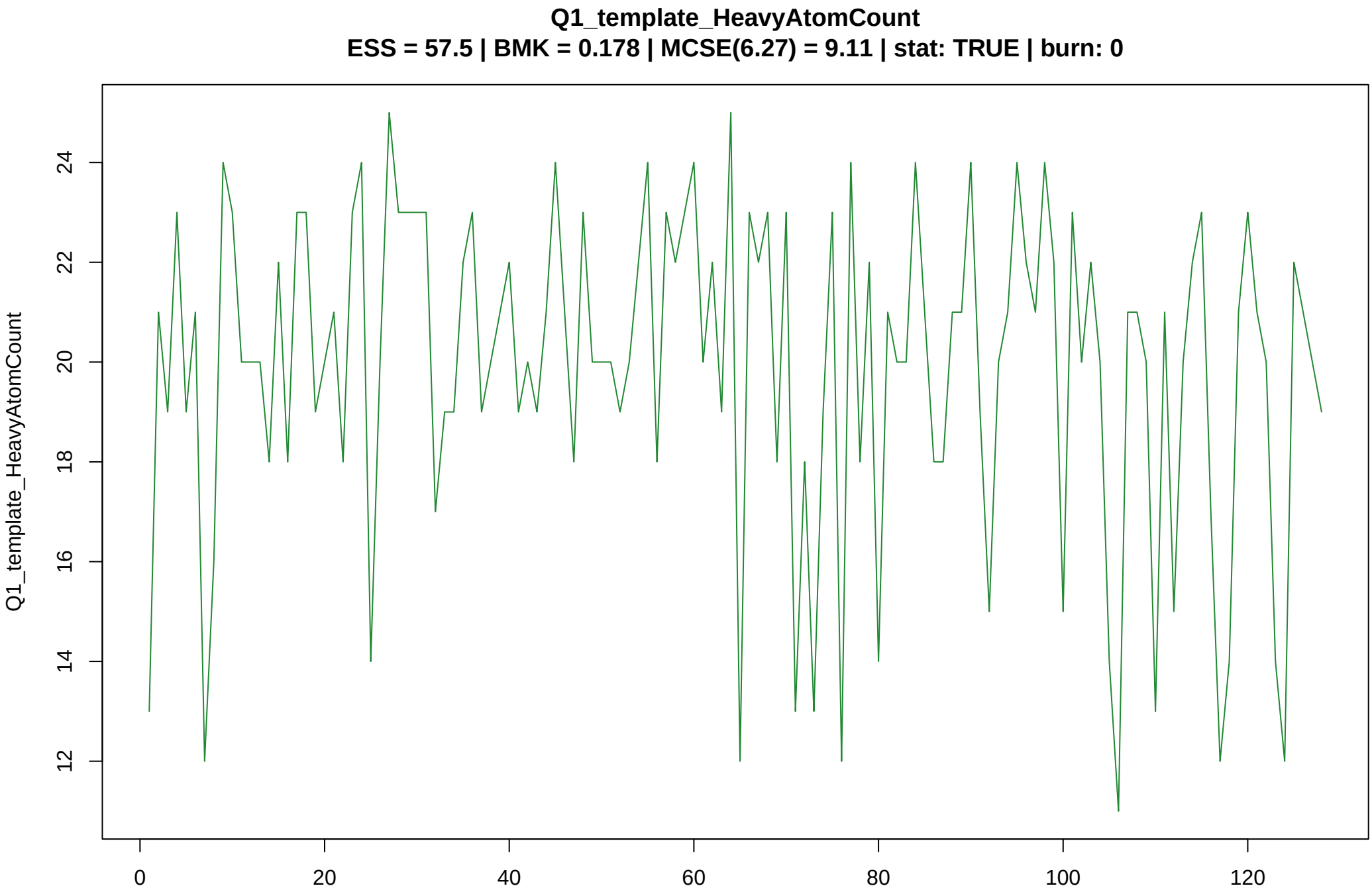

IQR_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.0873 | MCSE(6.27) = 9.36 | stat: TRUE | burn: 24
IQR_mcs_NumHeteroAtoms
1.0
1.5
2.0
2.5
3.0
3.5
4.0
0
20
40
60
80
100
120

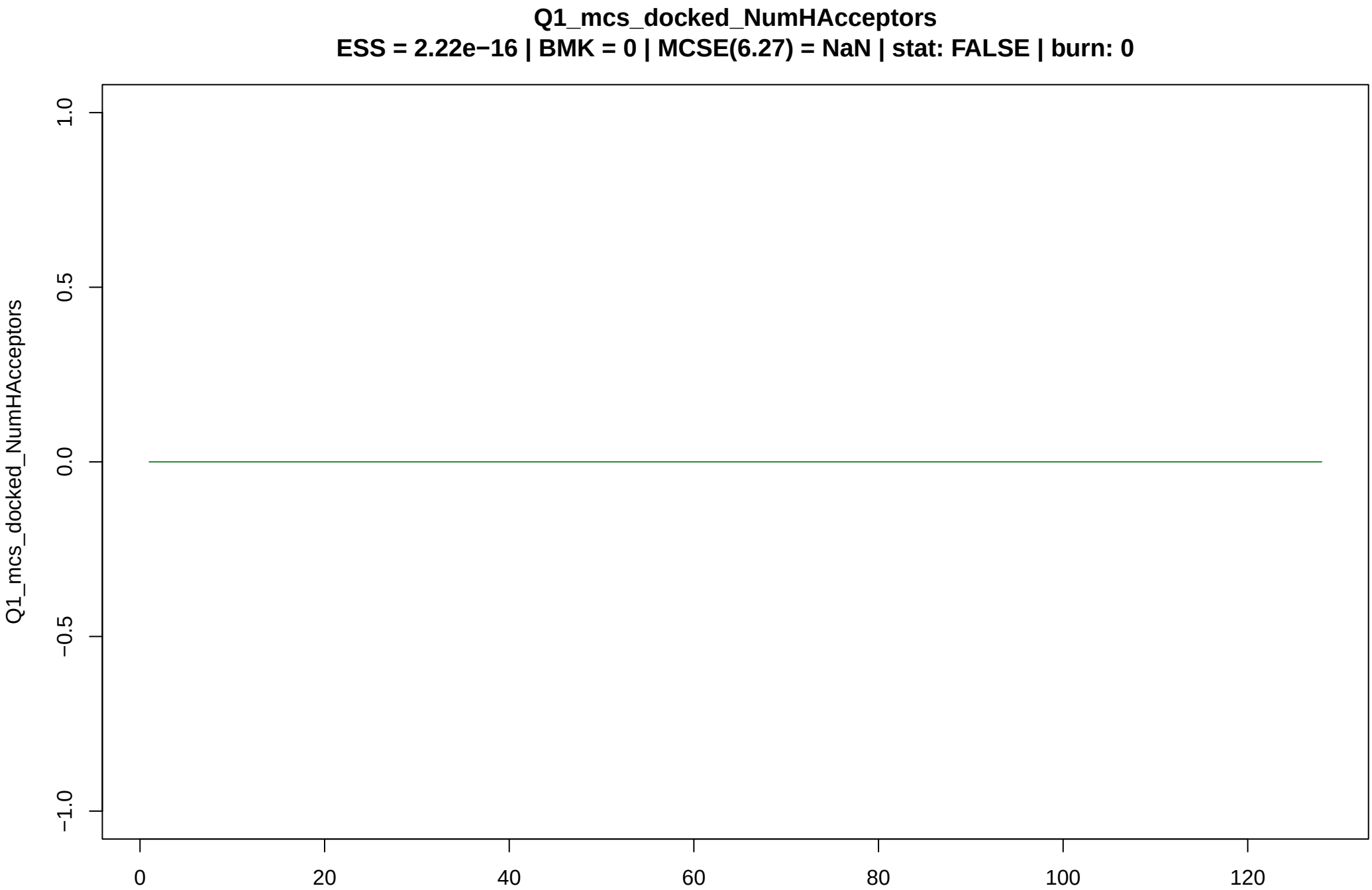

Q1_log_RMSD
ESS = 128 | BMK = 0.132 | MCSE(6.27) = 9.74 | stat: TRUE | burn: 0
Q1_log_RMSD
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
20
40
60
80
100
120

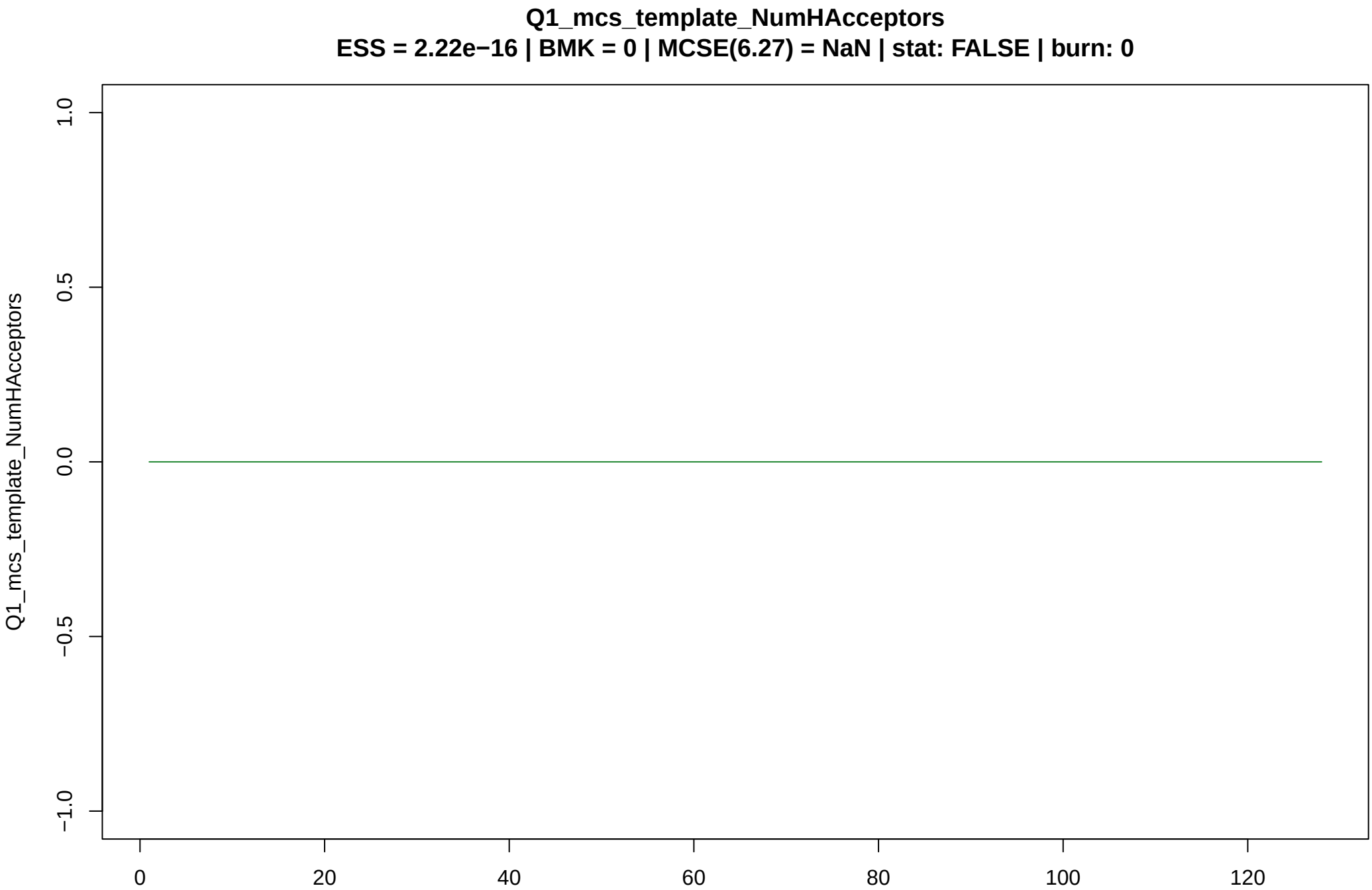

Q1_Xtransf_ec_tanimoto_similarity
ESS = 128 | BMK = 0.126 | MCSE(6.27) = 9.01 | stat: TRUE | burn: 24
Q1_Xtransf_ec_tanimoto_similarity
−0.6
−0.8
−1.0
−1.2
−1.4
−1.6
0
20
40
60
80
100
120

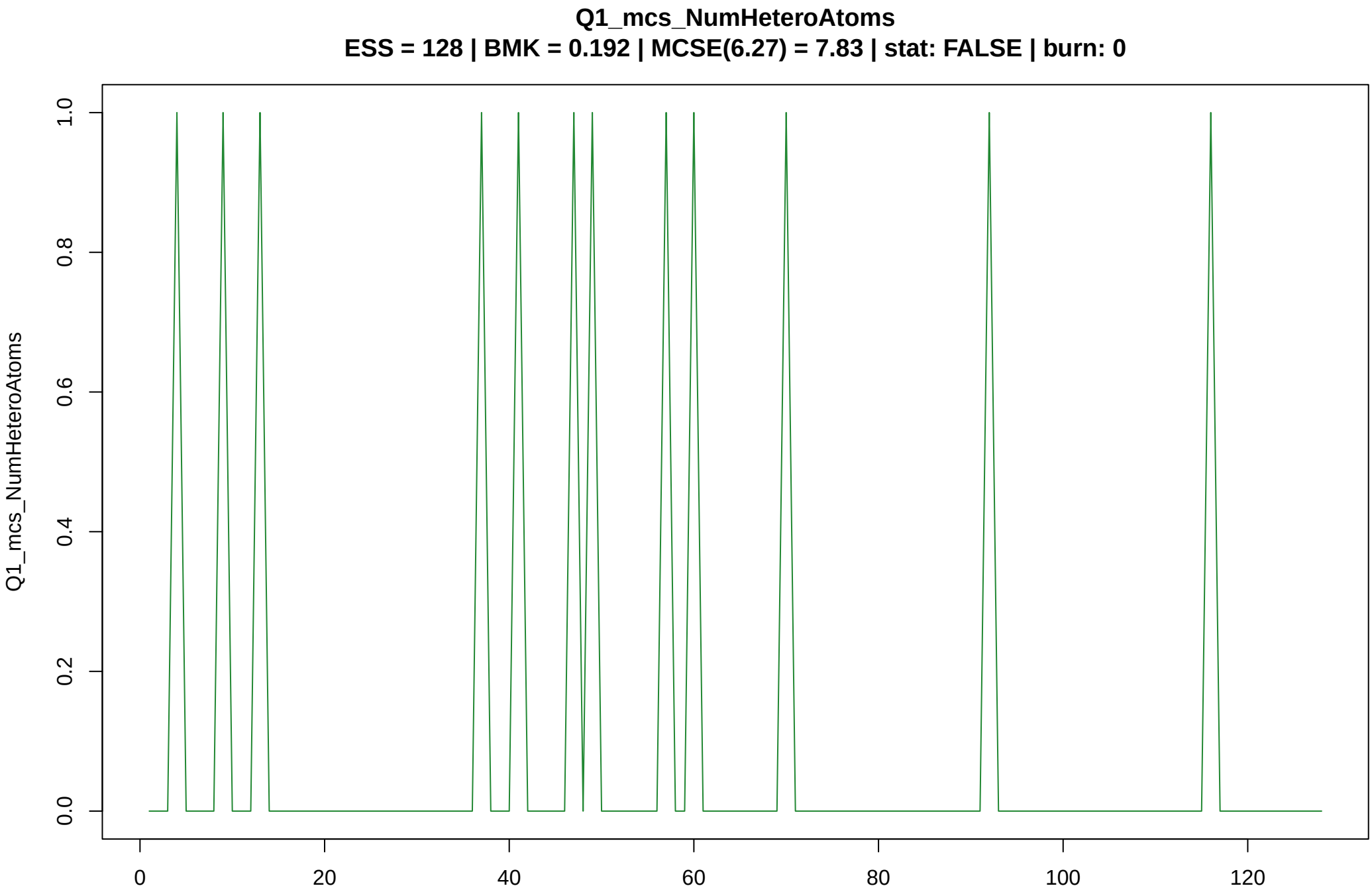

Q1_docked_HeavyAtomCount
ESS = 128 | BMK = 0.0864 | MCSE(6.27) = 9.02 | stat: TRUE | burn: 0
Q1_docked_HeavyAtomCount
10
15
20
25
0
20
40
60
80
100
120

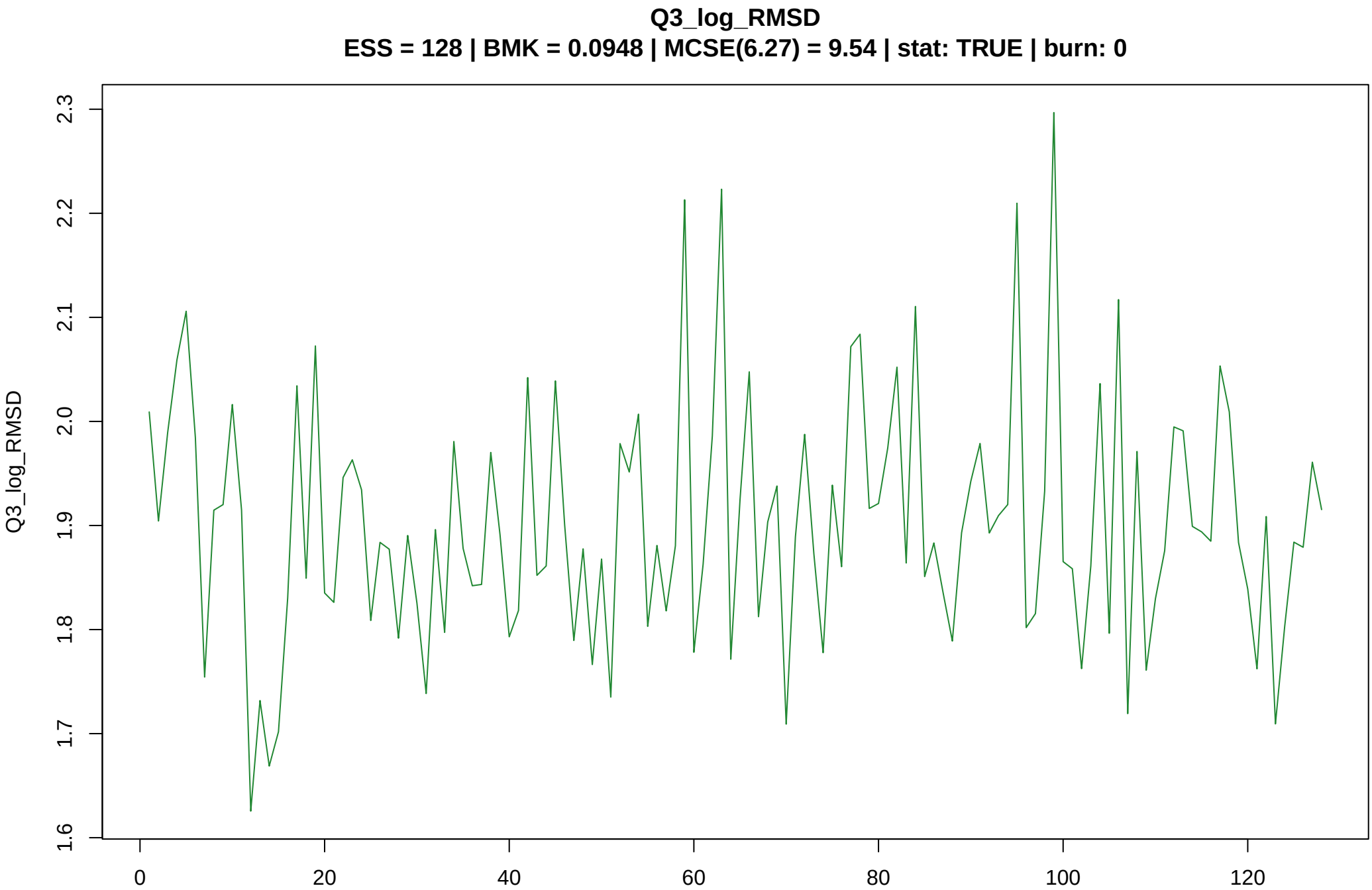

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
20
40
60
80
100
120

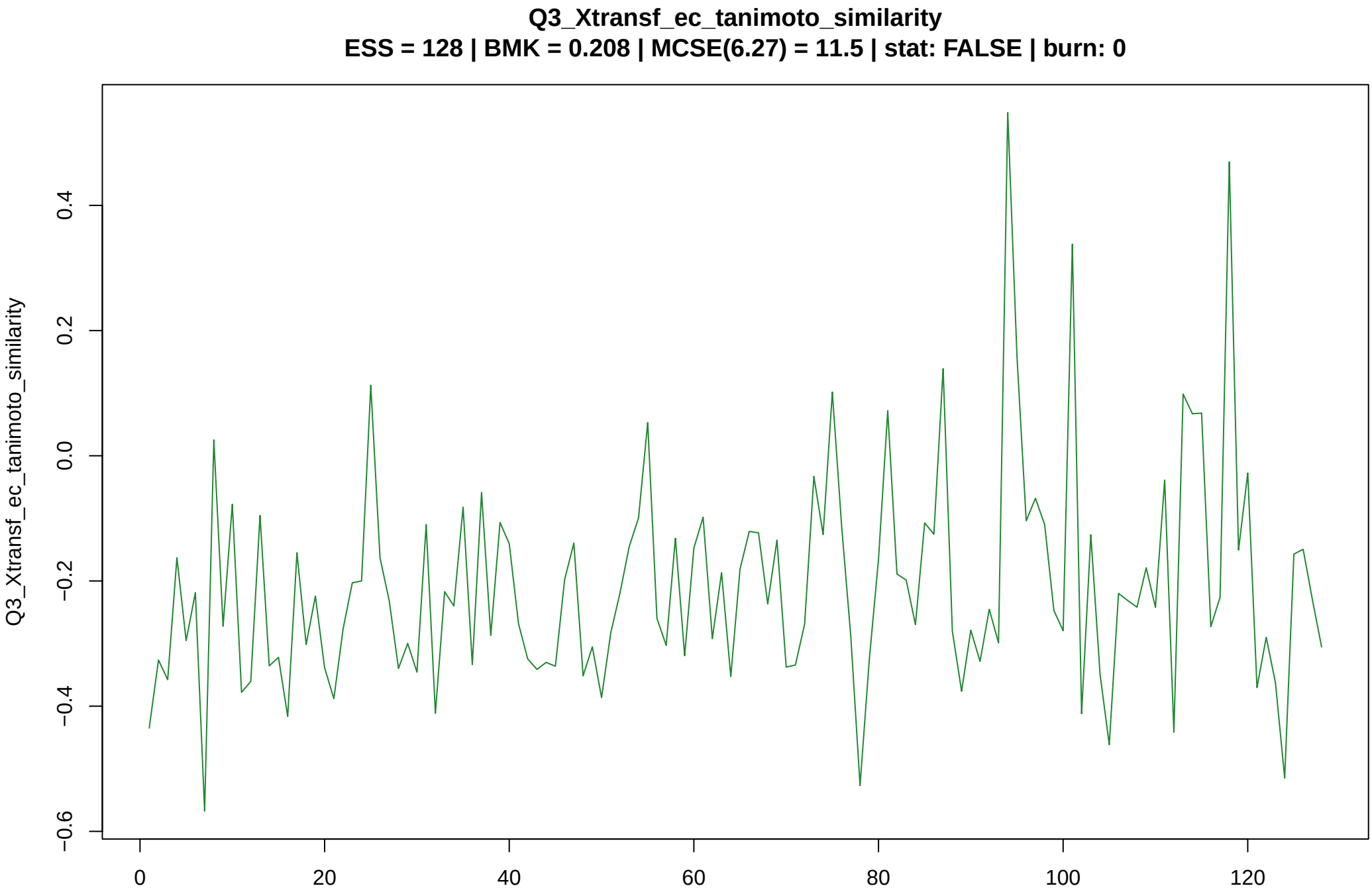

Q1_template_HeavyAtomCount
ESS = 57.5 | BMK = 0.178 | MCSE(6.27) = 9.11 | stat: TRUE | burn: 0
Q1_template_HeavyAtomCount
12
14
16
18
20
22
24
0
20
40
60
80
100
120

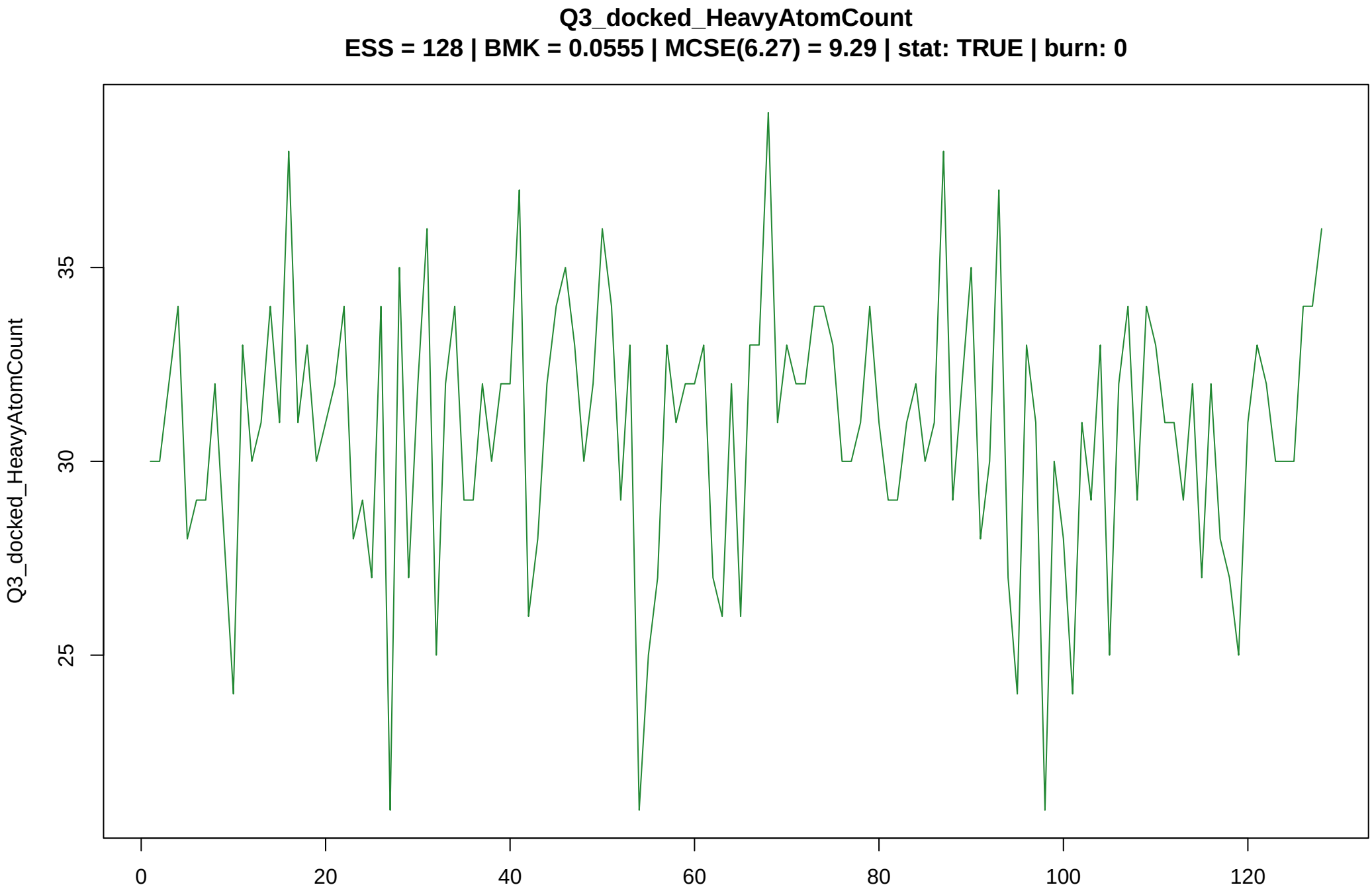

Q1_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_docked_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
20
40
60
80
100
120

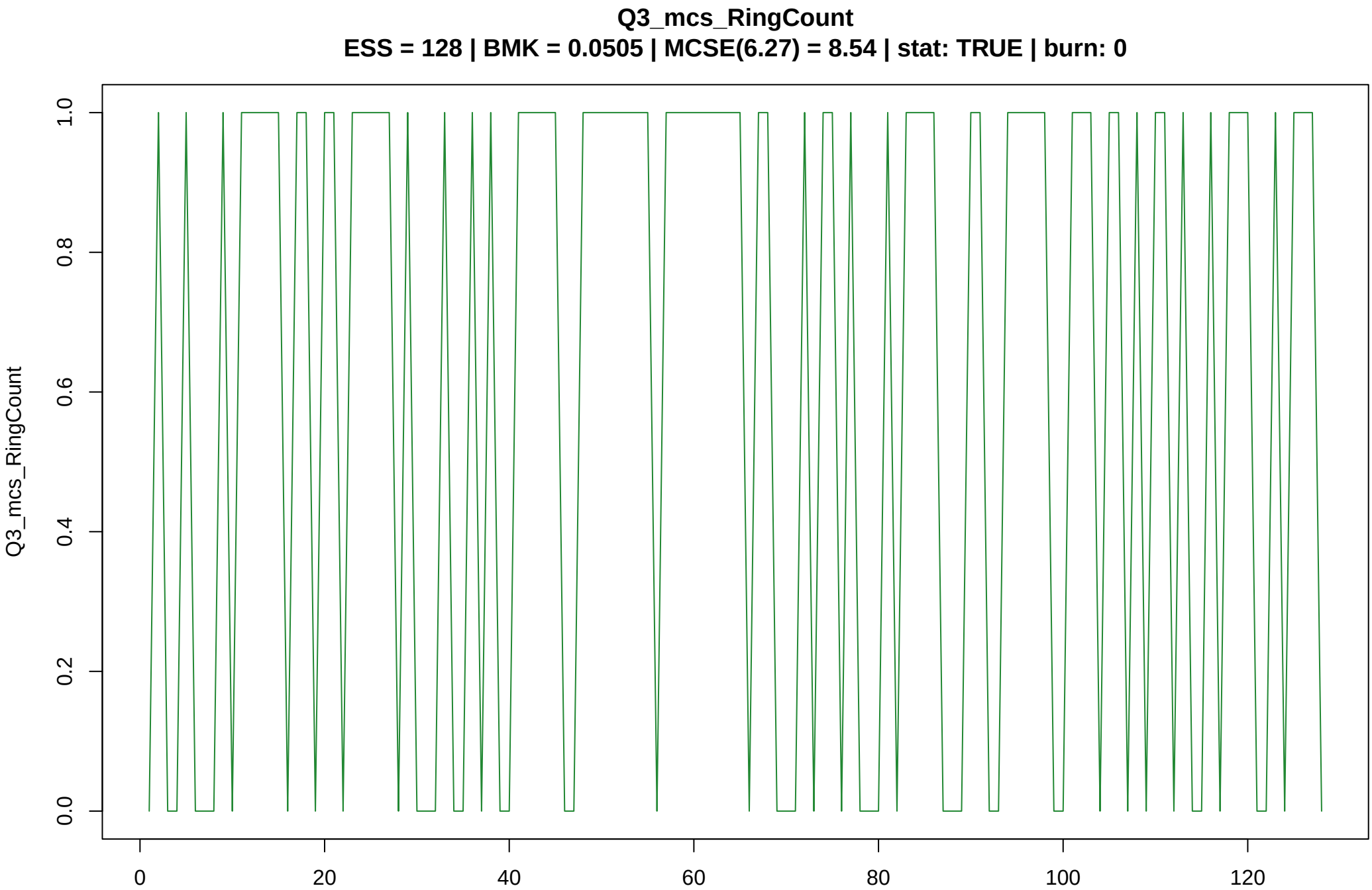

Q1_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_template_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
20
40
60
80
100
120

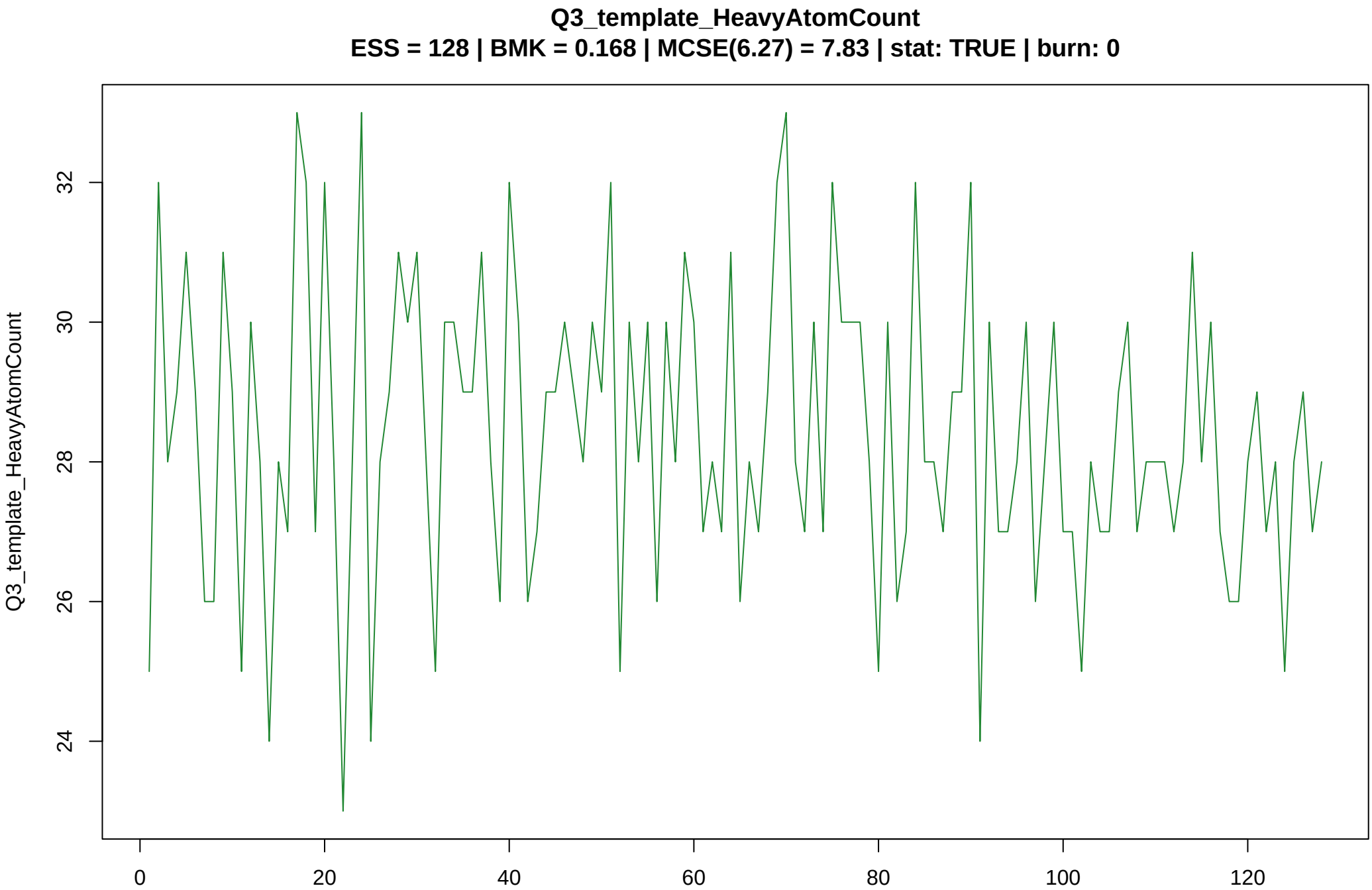

Q1_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.192 | MCSE(6.27) = 7.83 | stat: FALSE | burn: 0
Q1_mcs_NumHeteroAtoms
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

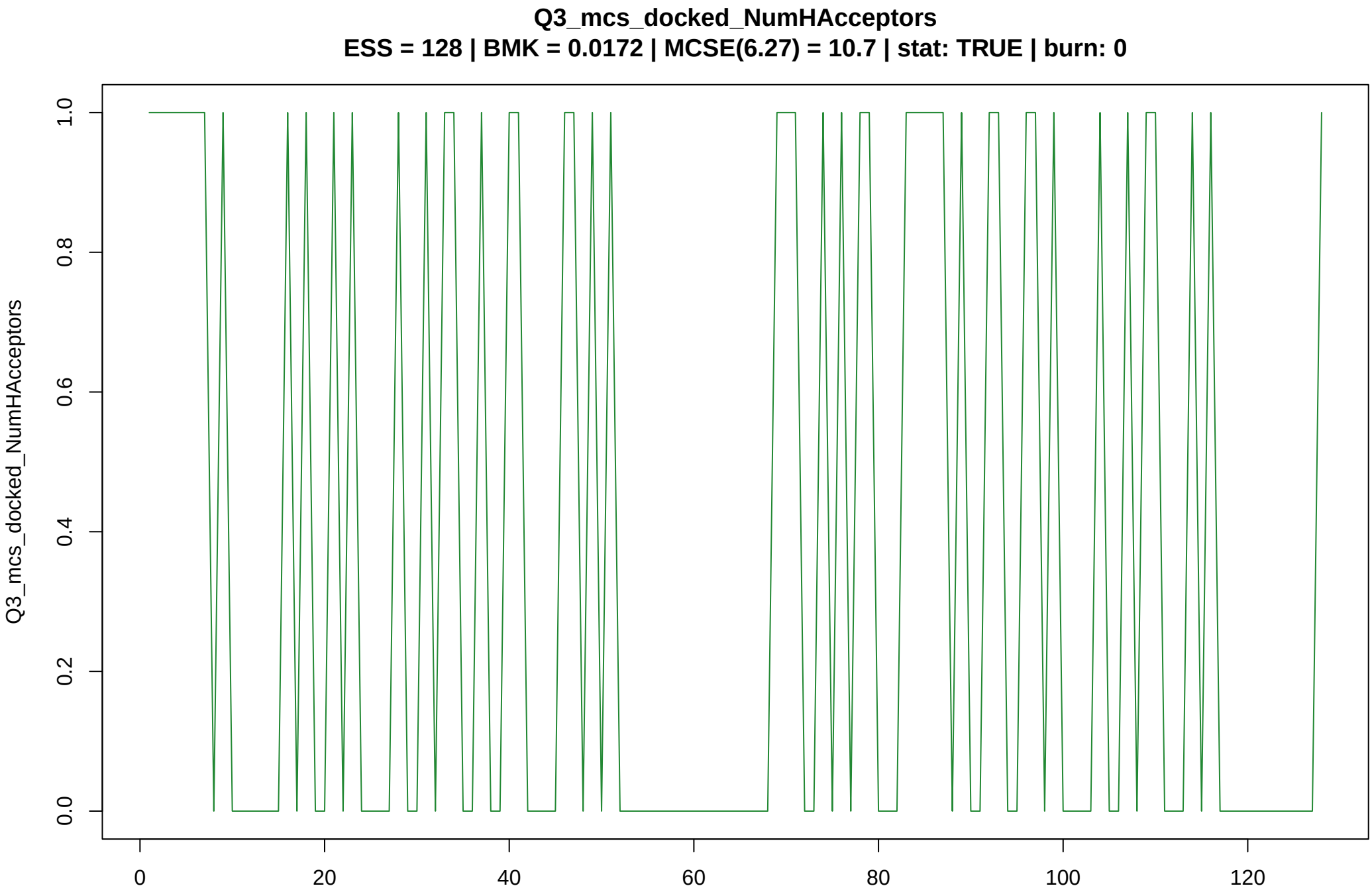

Q3_log_RMSD
ESS = 128 | BMK = 0.0948 | MCSE(6.27) = 9.54 | stat: TRUE | burn: 0
Q3_log_RMSD
1.6
1.7
1.8
1.9
2.0
2.1
2.2
2.3
0
20
40
60
80
100
120

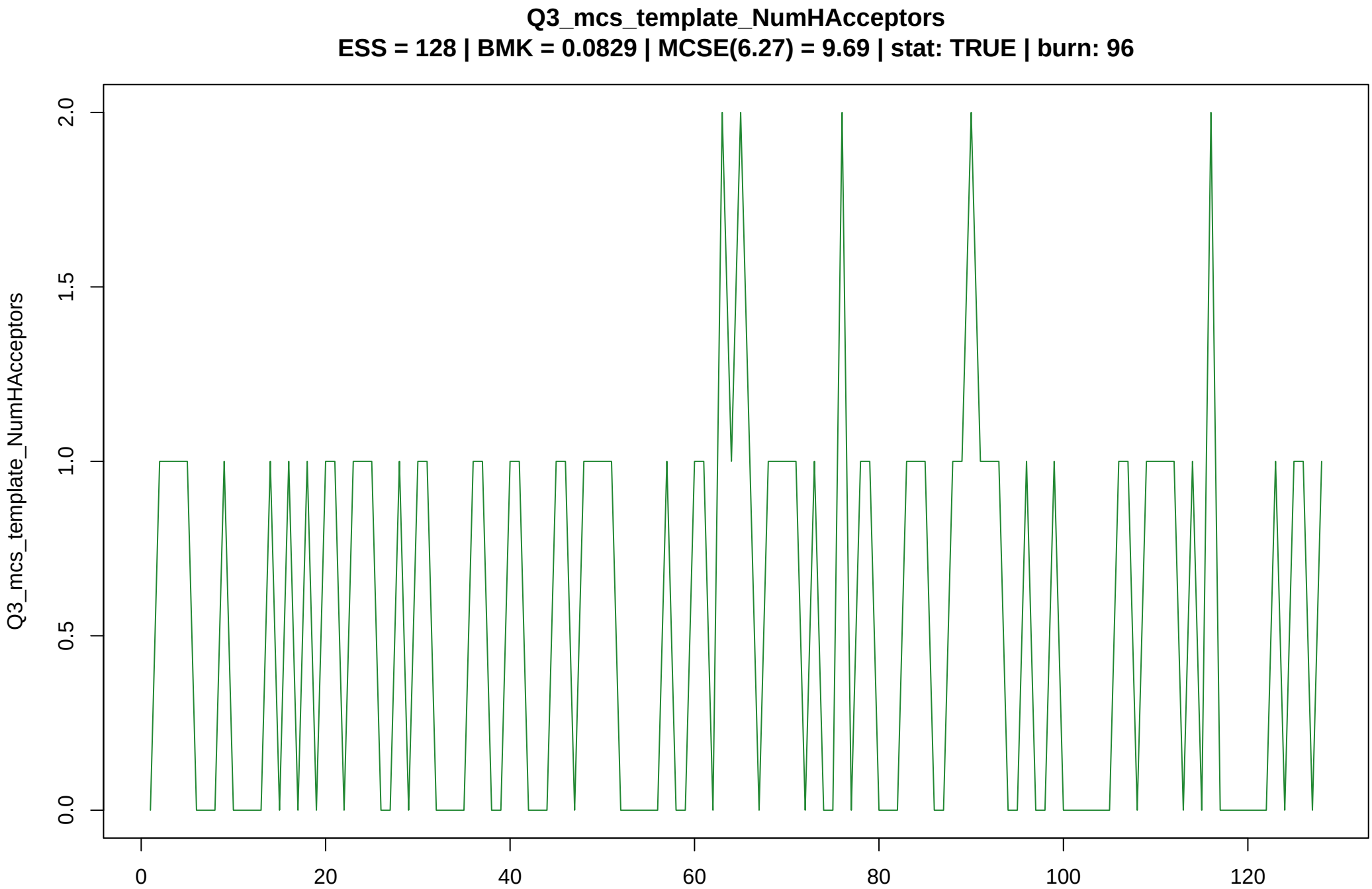

Q3_Xtransf_ec_tanimoto_similarity
ESS = 128 | BMK = 0.208 | MCSE(6.27) = 11.5 | stat: FALSE | burn: 0
Q3_Xtransf_ec_tanimoto_similarity
−0.6
−0.4
−0.2
0.0
0.2
0.4
0
20
40
60
80
100
120

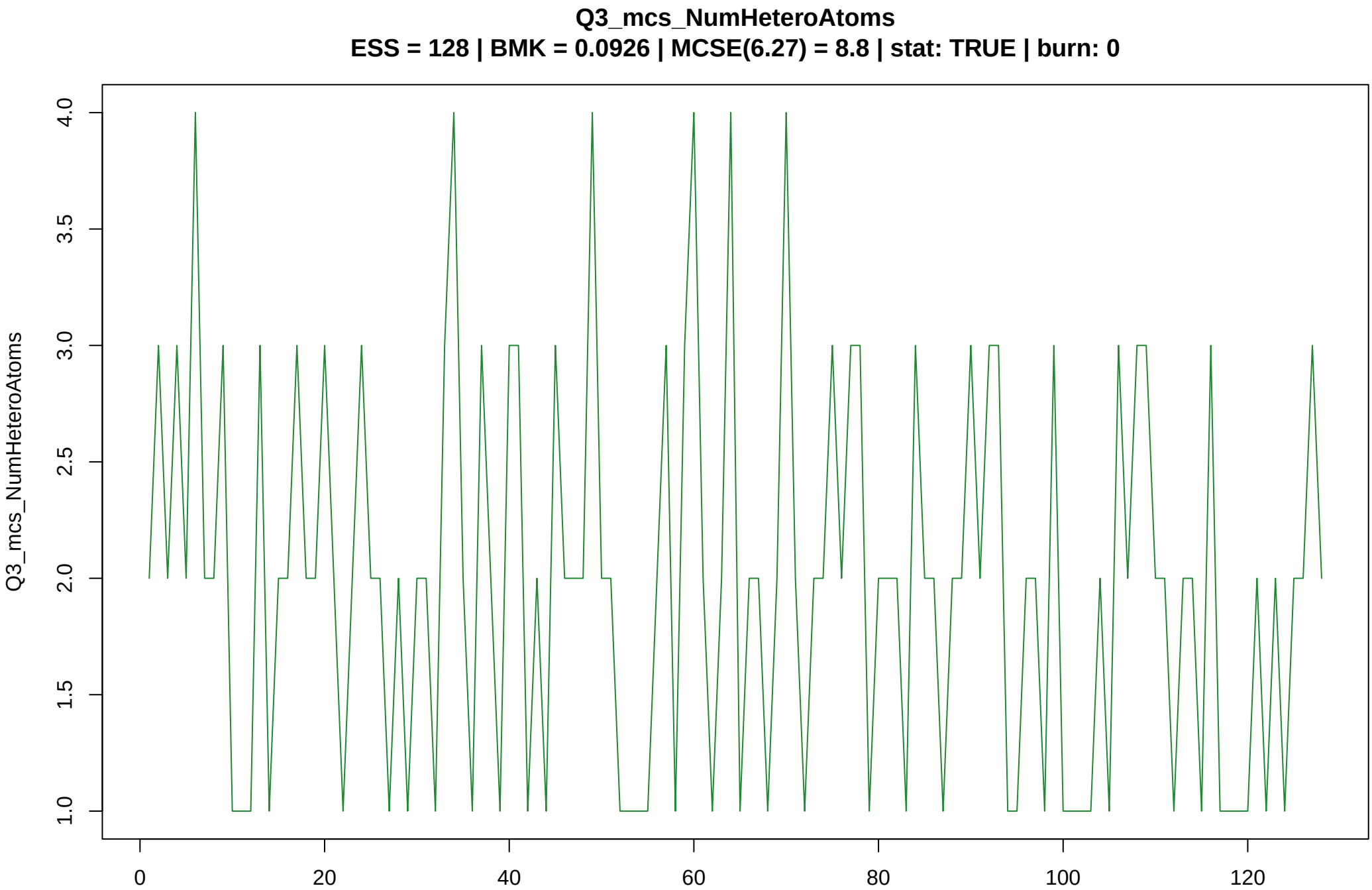

Q3_docked_HeavyAtomCount
ESS = 128 | BMK = 0.0555 | MCSE(6.27) = 9.29 | stat: TRUE | burn: 0
Q3_docked_HeavyAtomCount
25
30
35
0
20
40
60
80
100
120

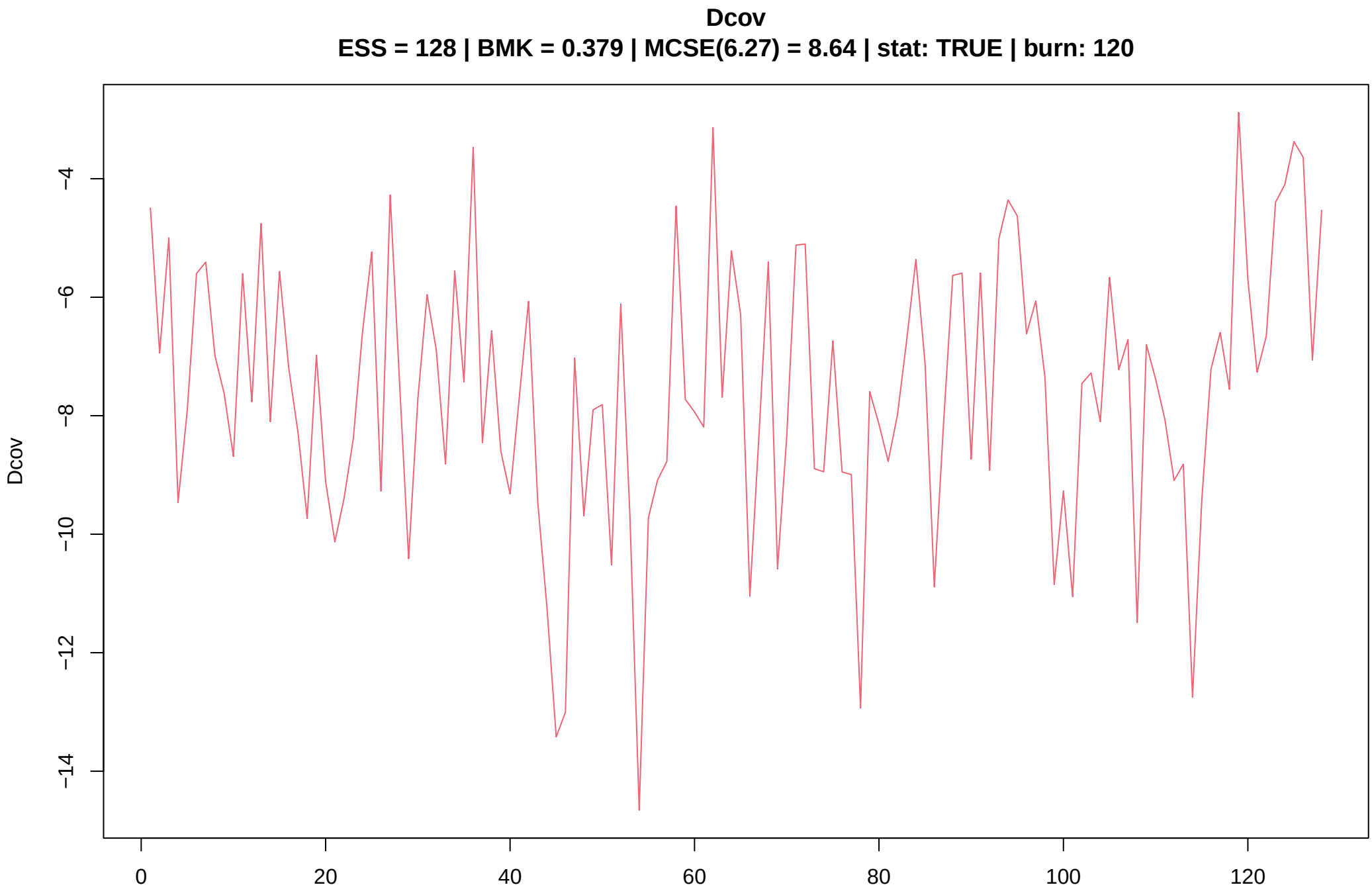

Q3_mcs_RingCount
ESS = 128 | BMK = 0.0505 | MCSE(6.27) = 8.54 | stat: TRUE | burn: 0
Q3_mcs_RingCount
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

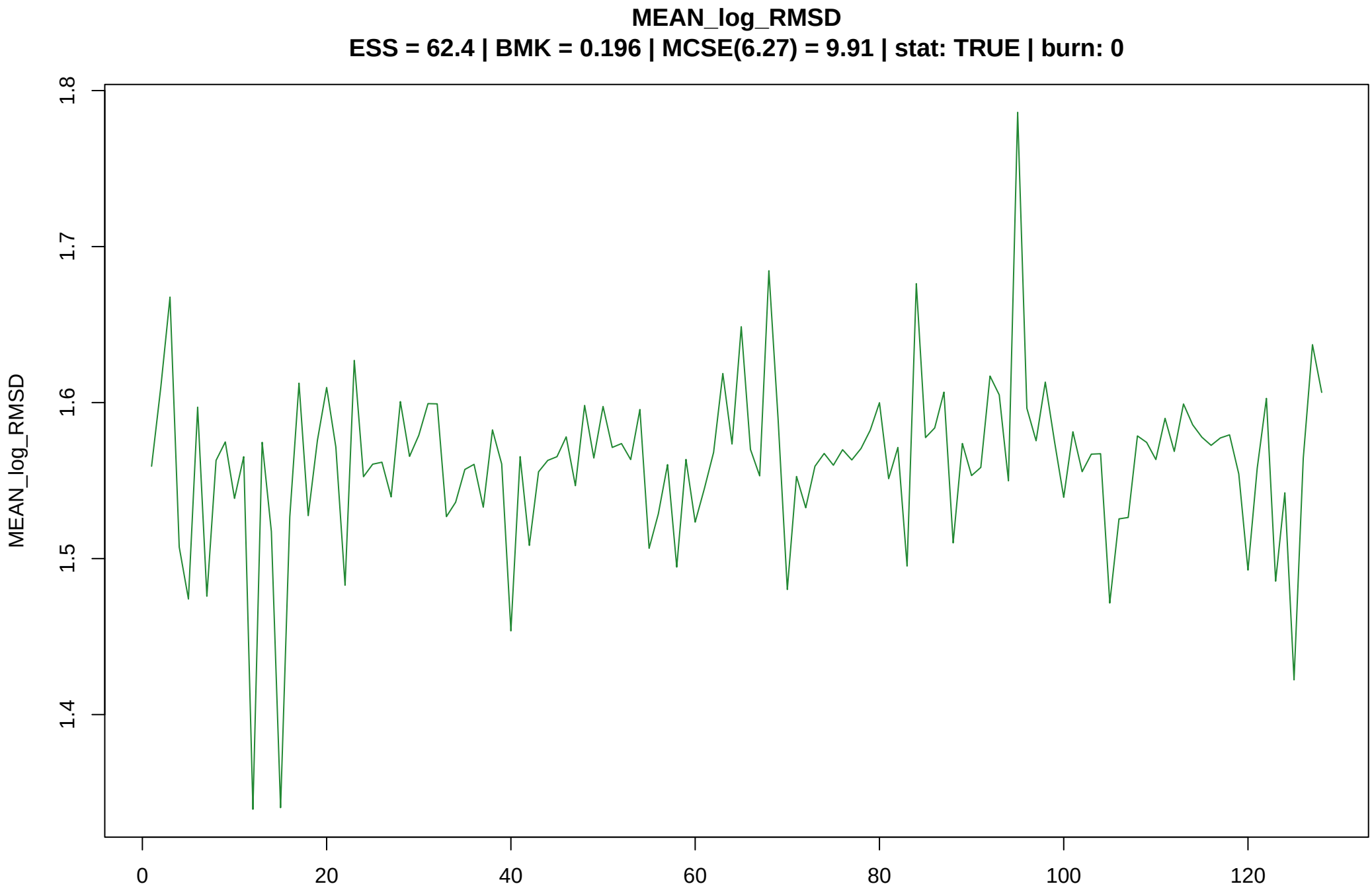

Q3_template_HeavyAtomCount
ESS = 128 | BMK = 0.168 | MCSE(6.27) = 7.83 | stat: TRUE | burn: 0
Q3_template_HeavyAtomCount
24
26
28
30
32
0
20
40
60
80
100
120

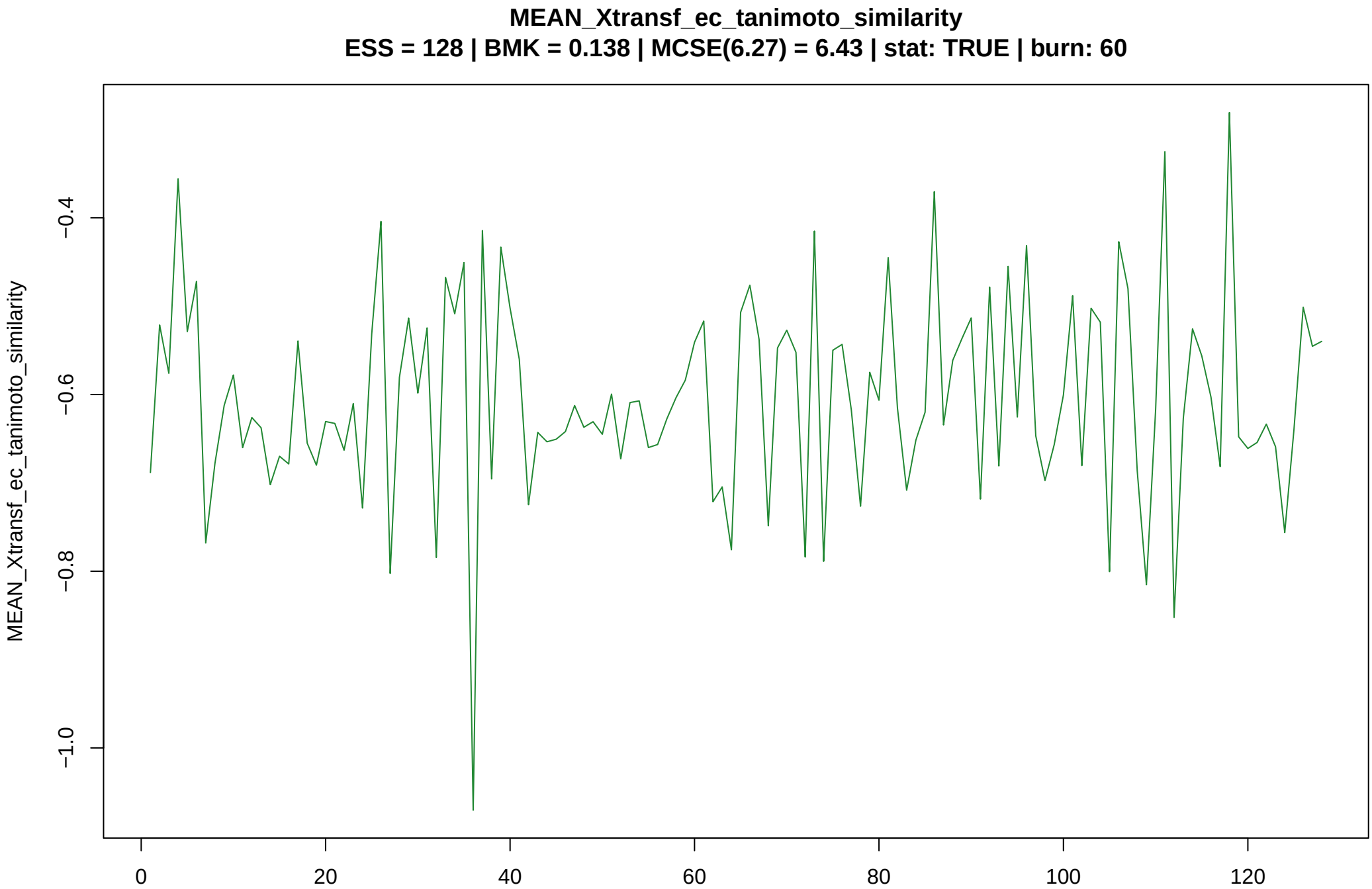

Q3_mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.0172 | MCSE(6.27) = 10.7 | stat: TRUE | burn: 0
Q3_mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

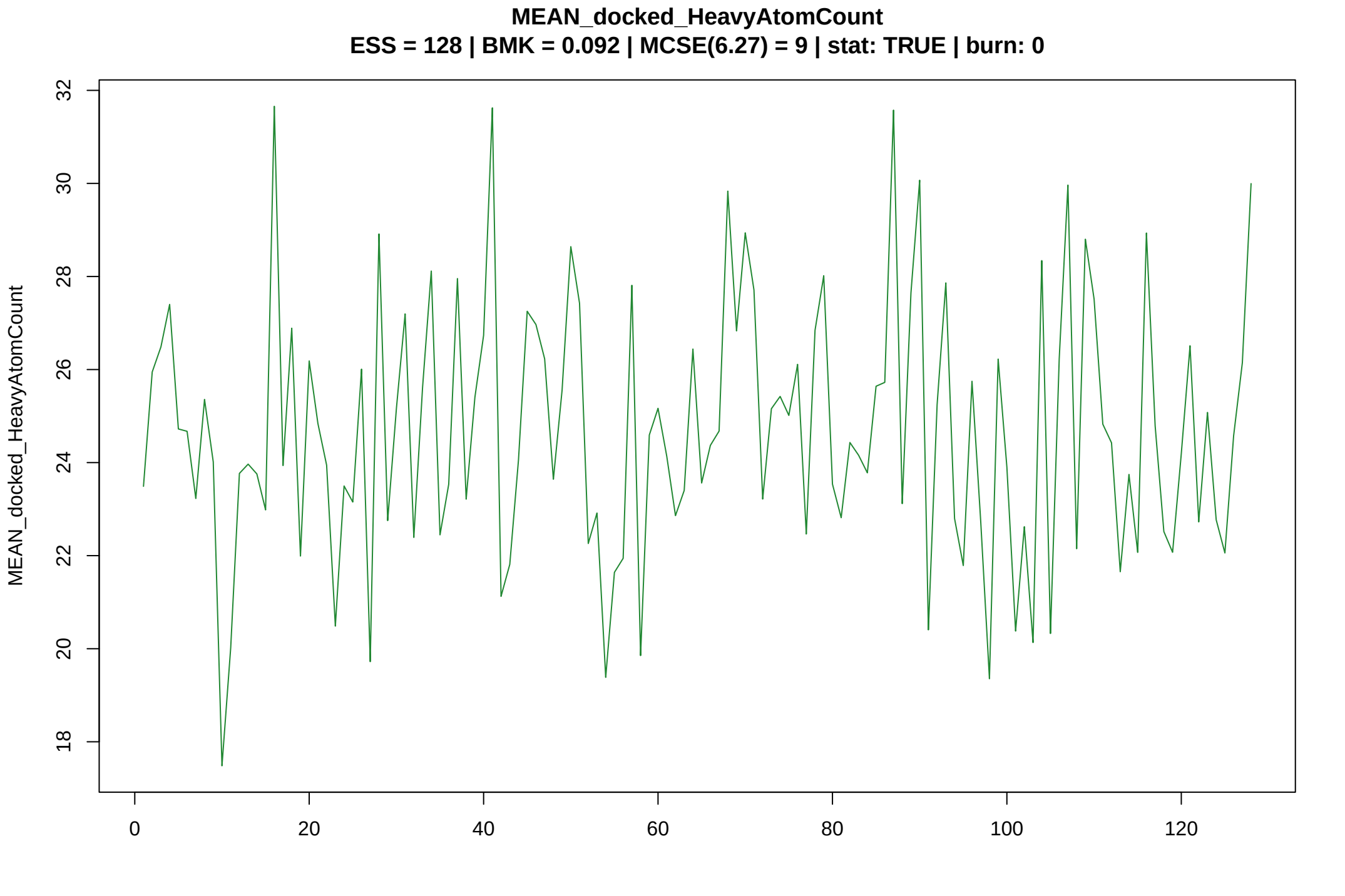

Q3_mcs_template_NumHAcceptors
ESS = 128 | BMK = 0.0829 | MCSE(6.27) = 9.69 | stat: TRUE | burn: 96
Q3_mcs_template_NumHAcceptors
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120

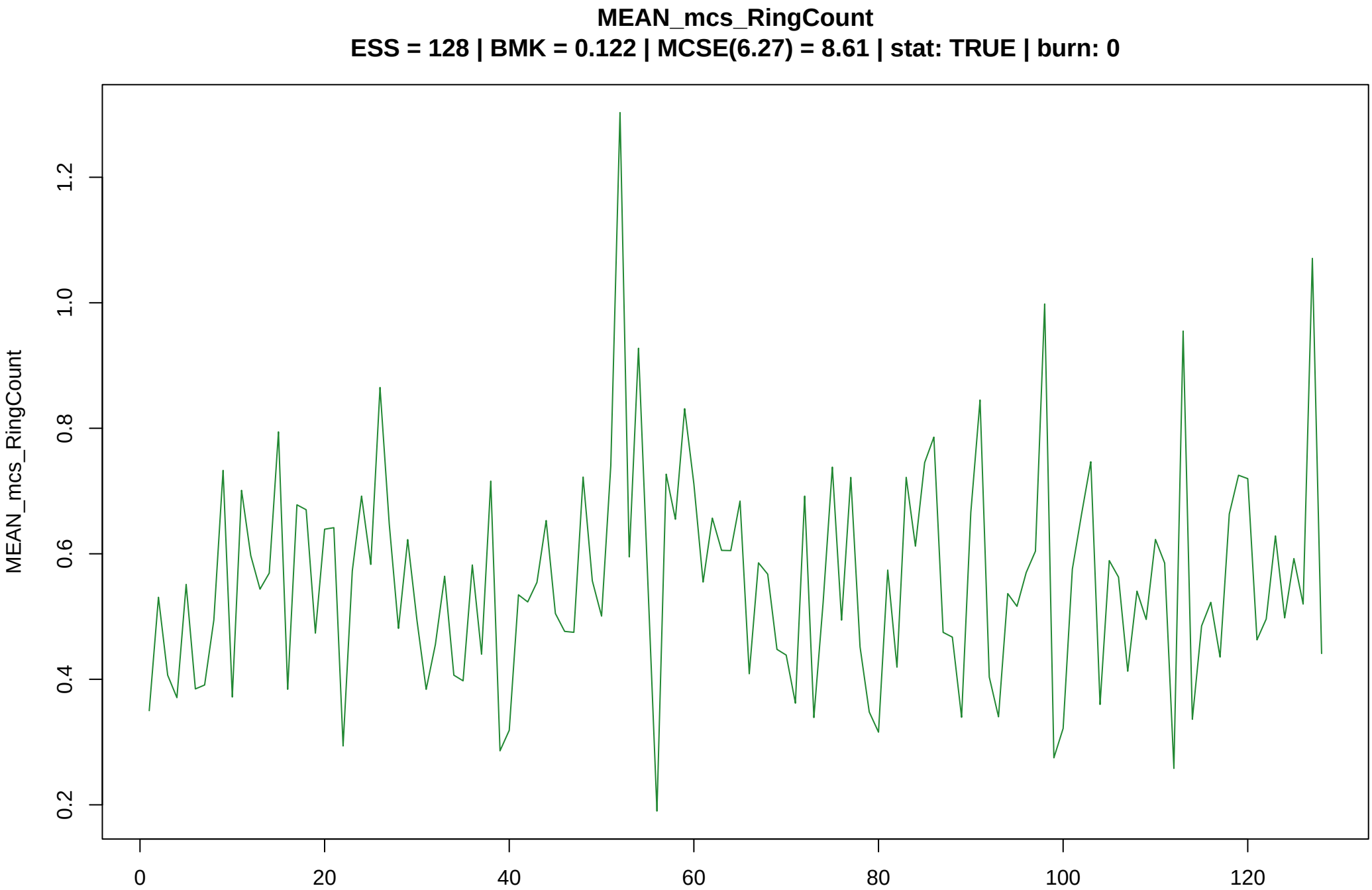

Q3_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.0926 | MCSE(6.27) = 8.8 | stat: TRUE | burn: 0
Q3_mcs_NumHeteroAtoms
1.0
1.5
2.0
2.5
3.0
3.5
4.0
0
20
40
60
80
100
120

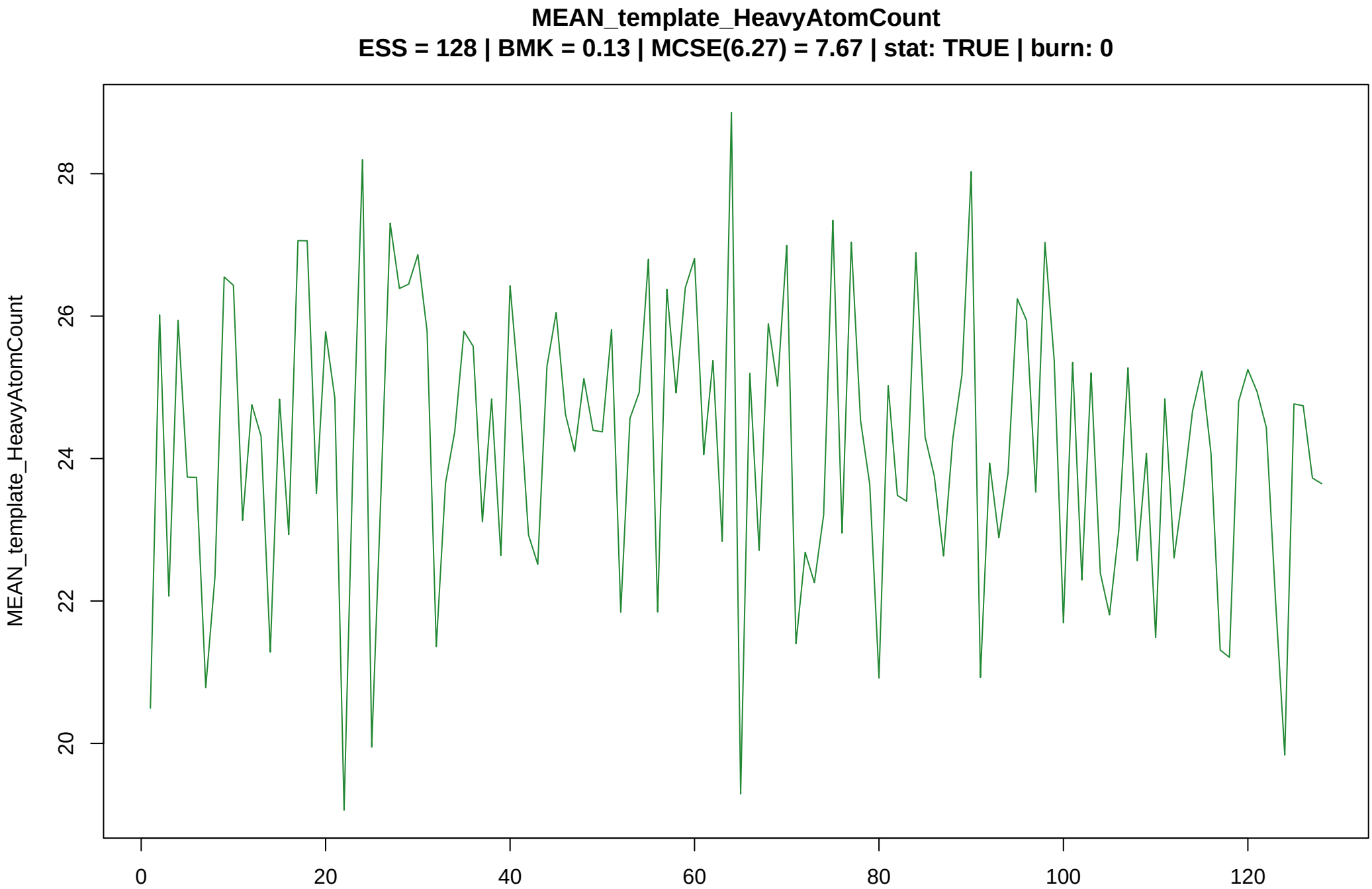

Dcov
ESS = 128 | BMK = 0.379 | MCSE(6.27) = 8.64 | stat: TRUE | burn: 120
Dcov
−4
−6
−8
−10
−12
−14
0
20
40
60
80
100
120

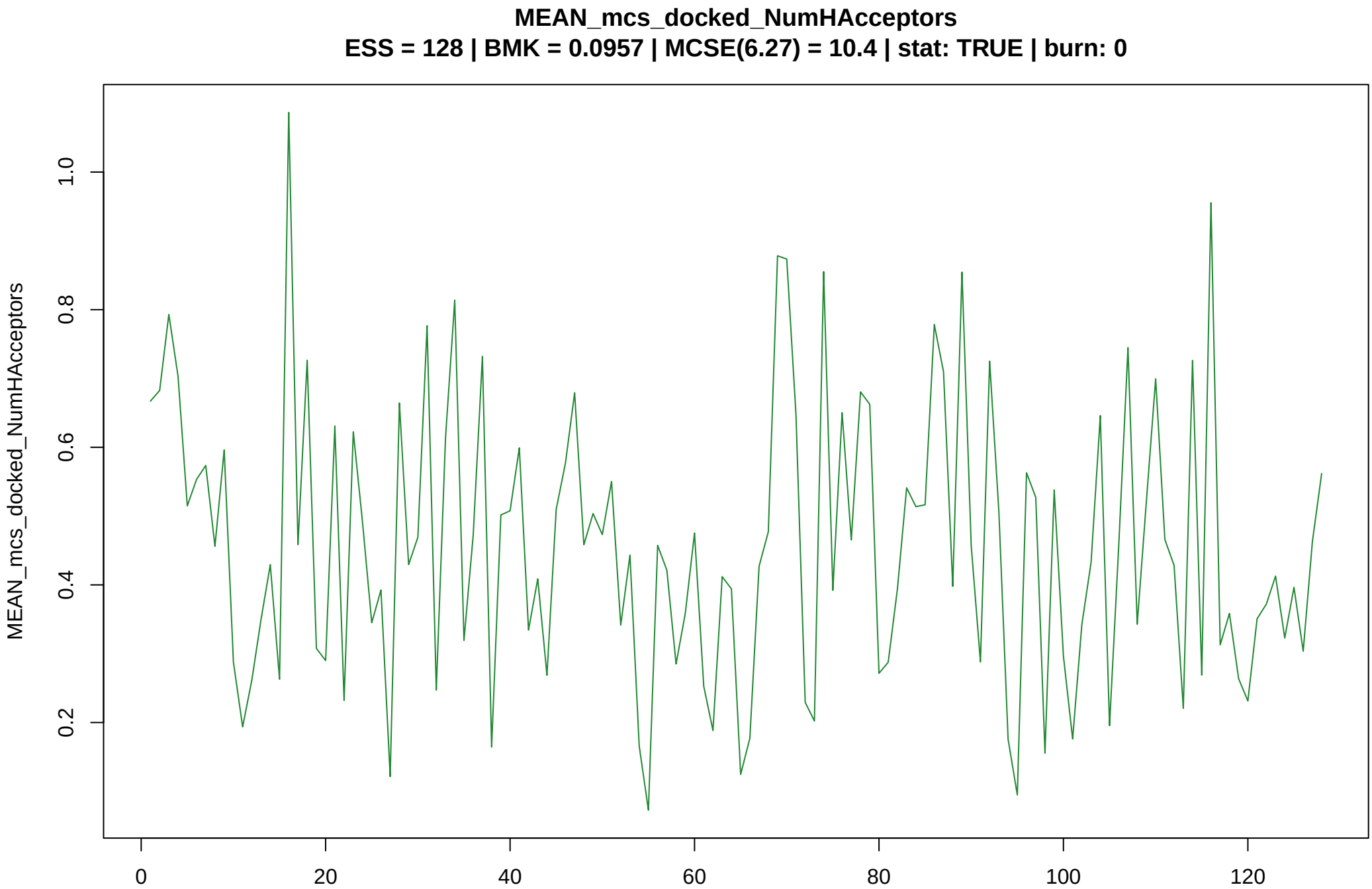

MEAN_log_RMSD
ESS = 62.4 | BMK = 0.196 | MCSE(6.27) = 9.91 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.8
1.7
1.6
1.5
1.4
0
20
40
60
80
100
120

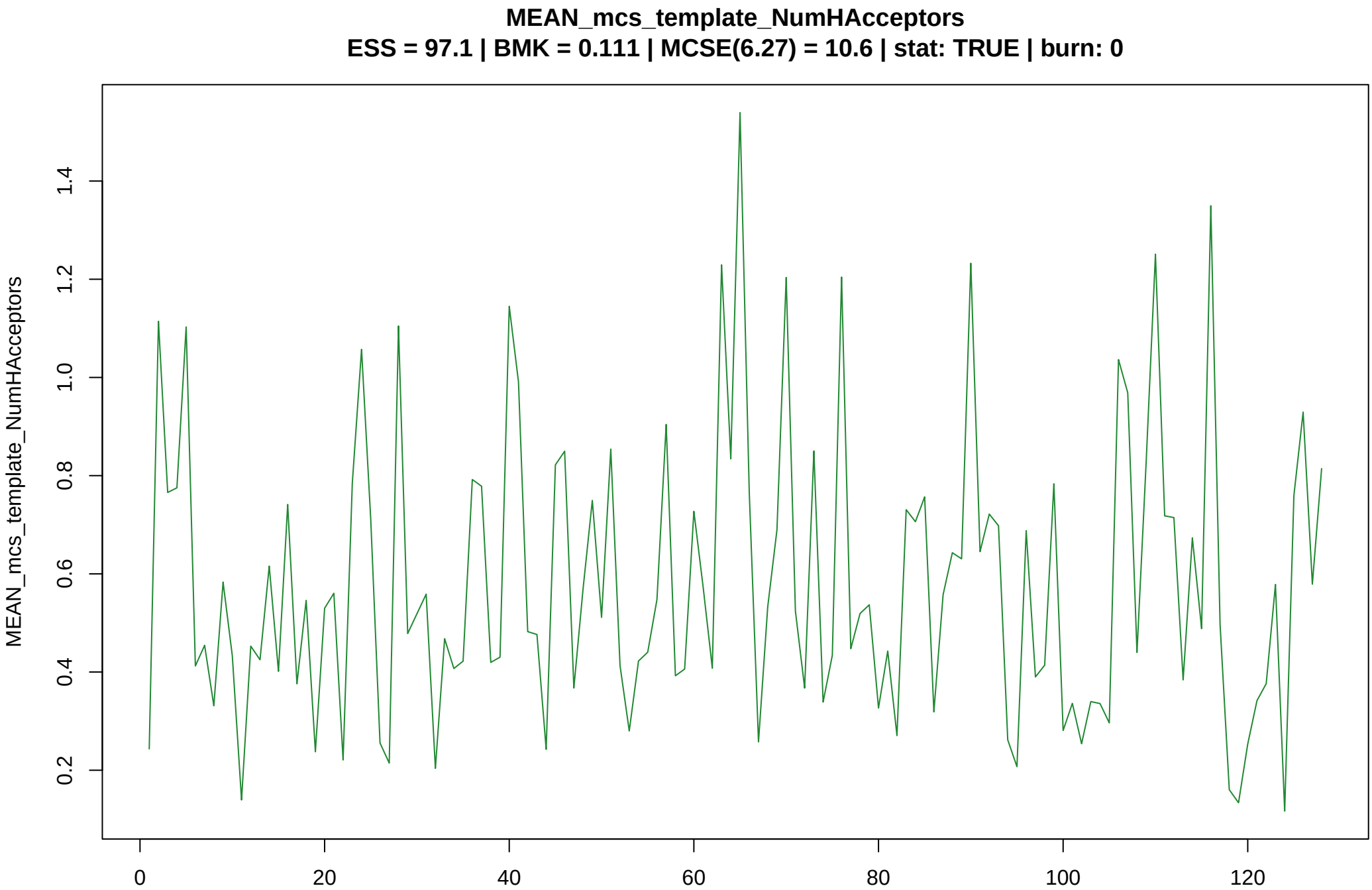

MEAN_Xtransf_ec_tanimoto_similarity
ESS = 128 | BMK = 0.138 | MCSE(6.27) = 6.43 | stat: TRUE | burn: 60
MEAN_Xtransf_ec_tanimoto_similarity
−0.4
−0.6
−0.8
−1.0
0
20
40
60
80
100
120

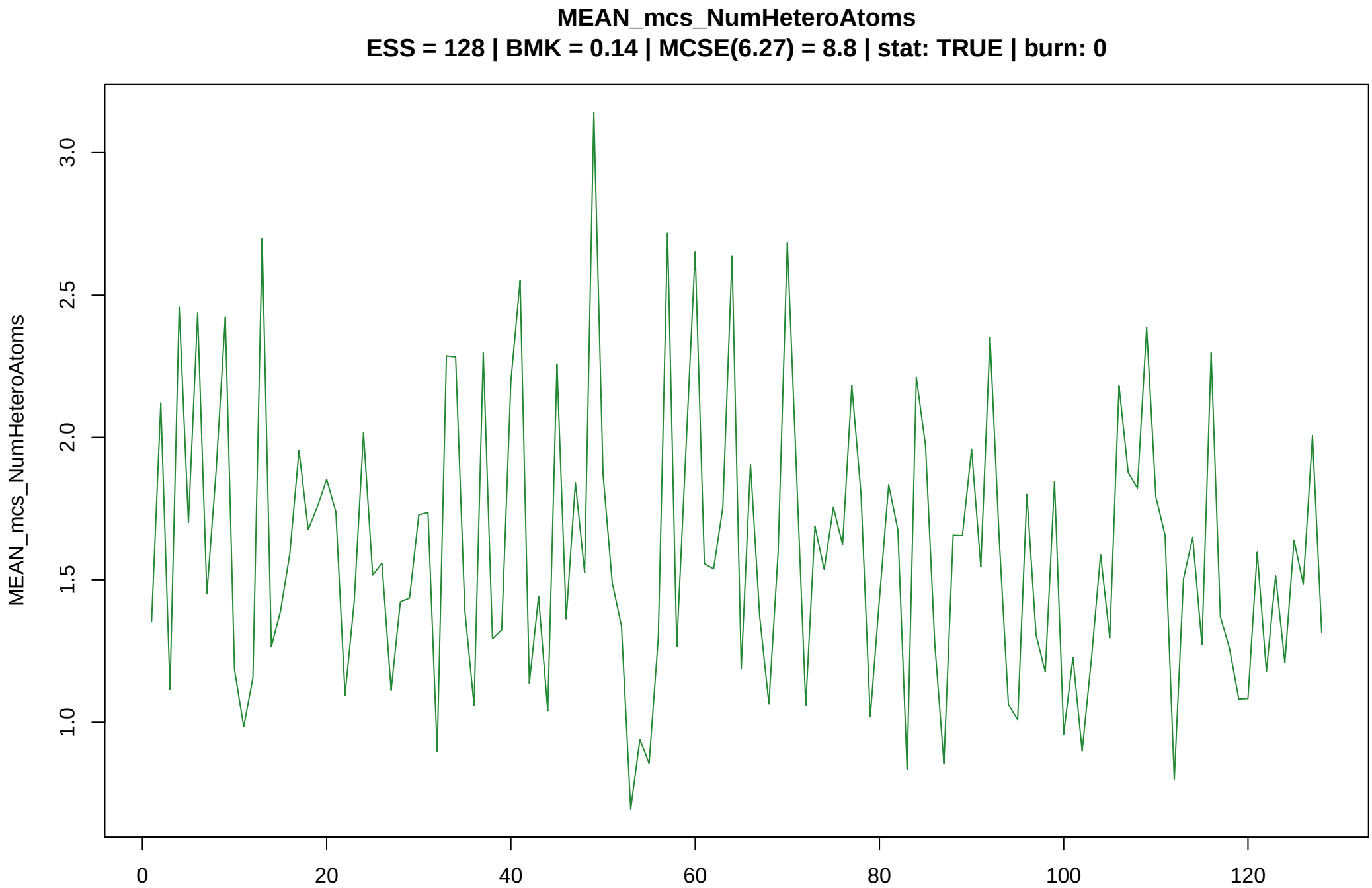

MEAN_docked_HeavyAtomCount
ESS = 128 | BMK = 0.092 | MCSE(6.27) = 9 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
18
20
22
24
26
28
30
32
0
20
40
60
80
100
120

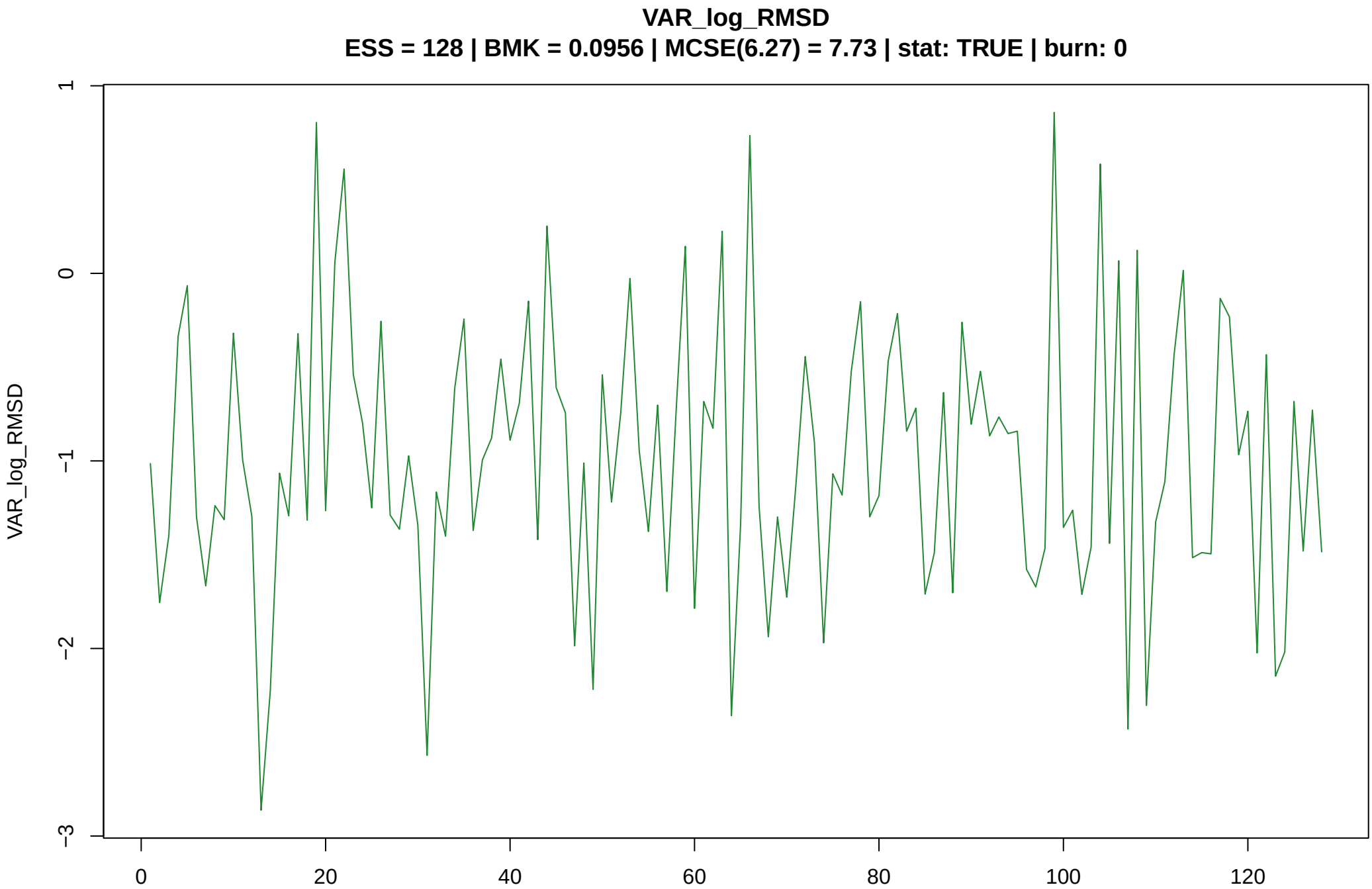

MEAN_mcs_RingCount
ESS = 128 | BMK = 0.122 | MCSE(6.27) = 8.61 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.2
0.4
0.6
0.8
1.0
1.2
0
20
40
60
80
100
120

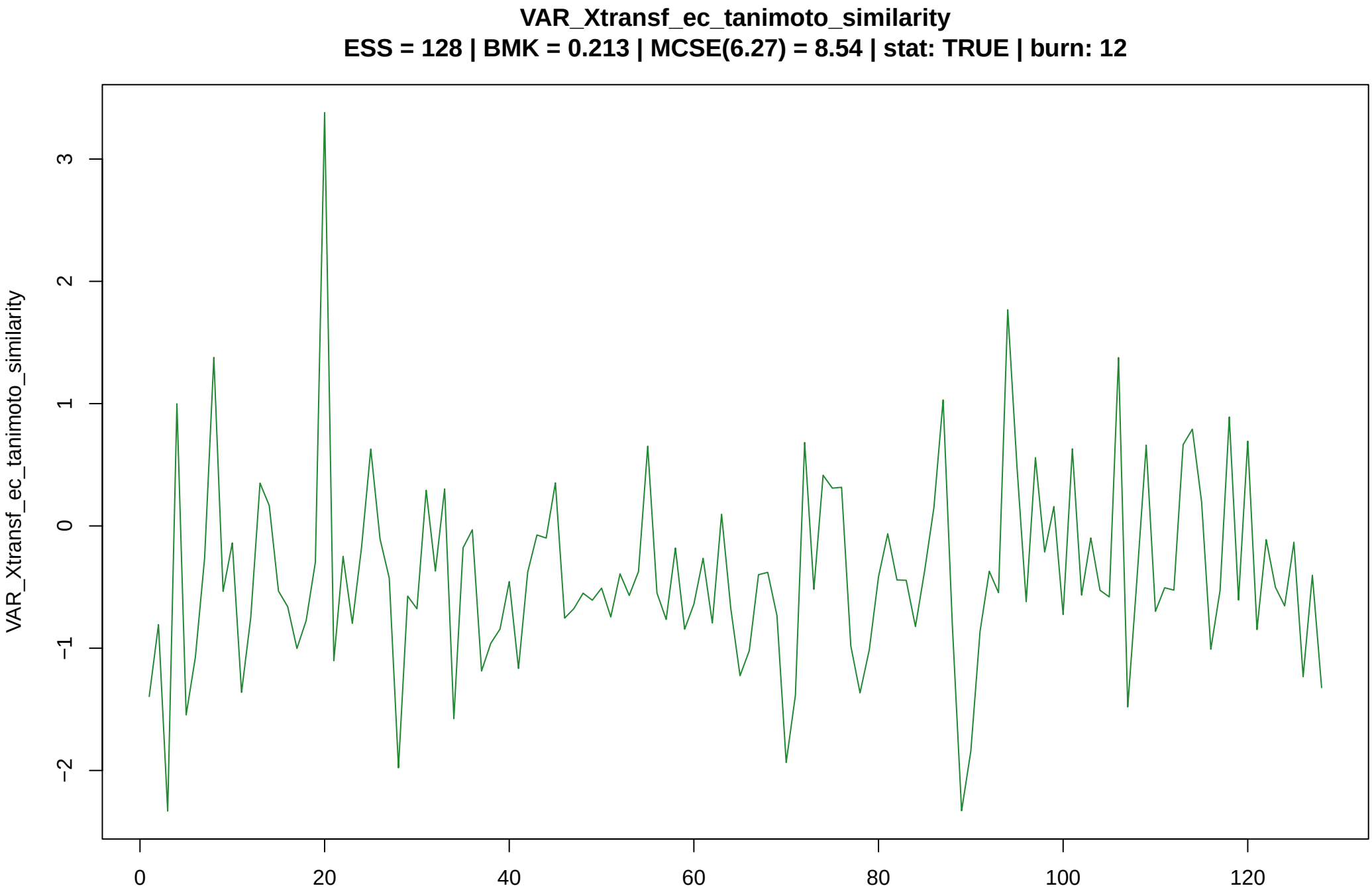

MEAN_template_HeavyAtomCount
ESS = 128 | BMK = 0.13 | MCSE(6.27) = 7.67 | stat: TRUE | burn: 0
MEAN_template_HeavyAtomCount
20
22
24
26
28
0
20
40
60
80
100
120

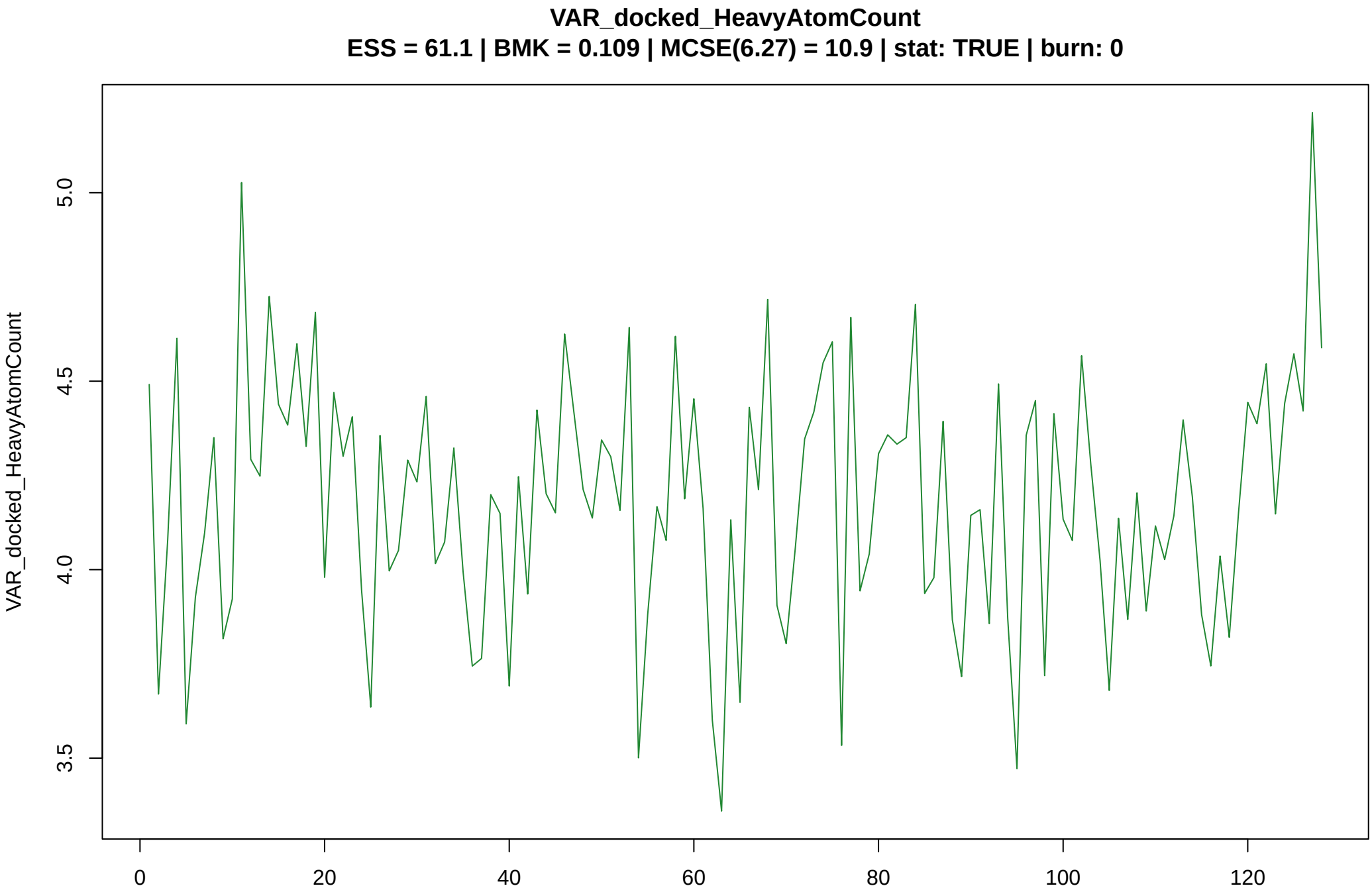

MEAN_mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.0957 | MCSE(6.27) = 10.4 | stat: TRUE | burn: 0
MEAN_mcs_docked_NumHAcceptors
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

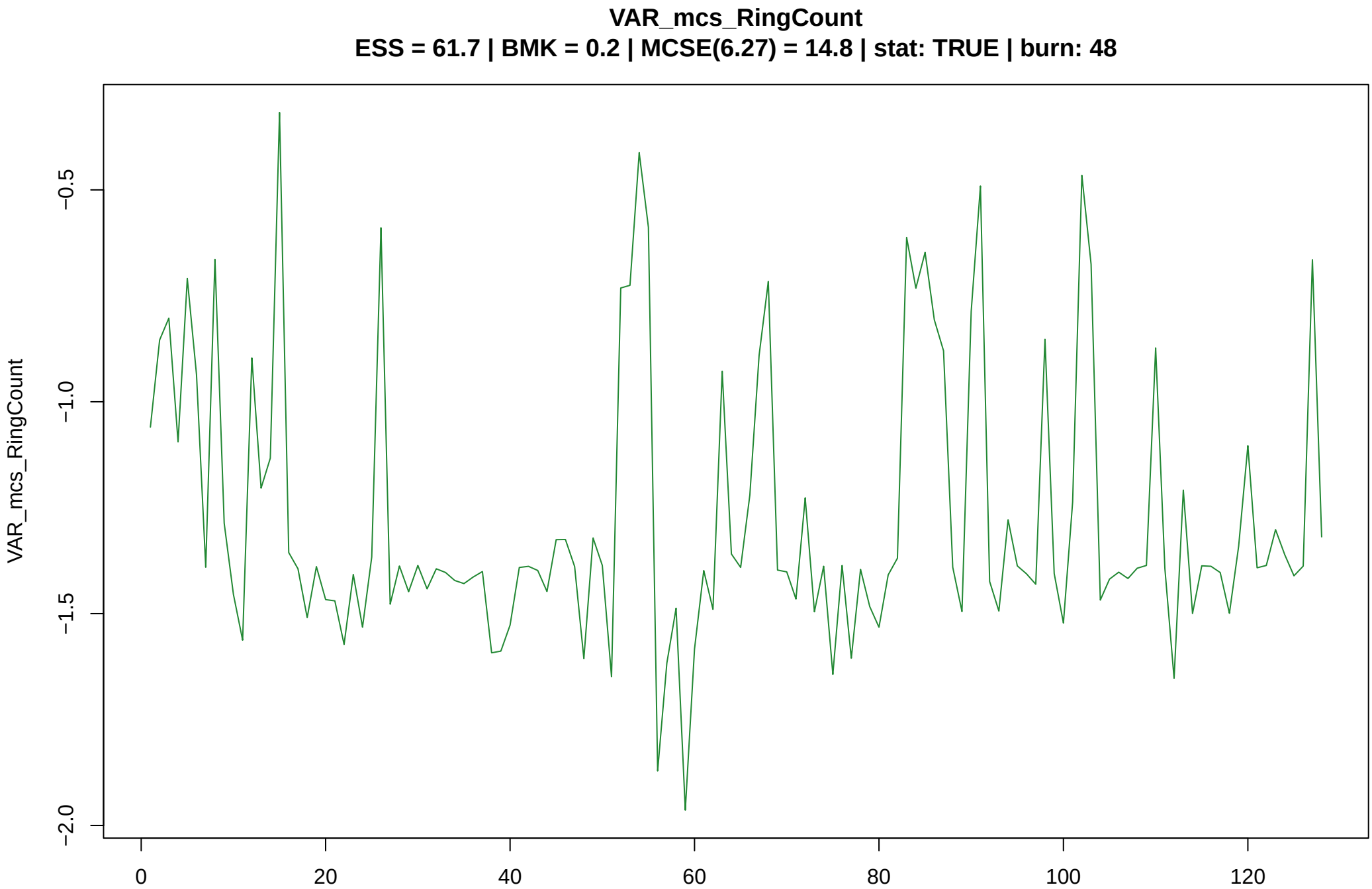

MEAN_mcs_template_NumHAcceptors
ESS = 97.1 | BMK = 0.111 | MCSE(6.27) = 10.6 | stat: TRUE | burn: 0
MEAN_mcs_template_NumHAcceptors
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
20
40
60
80
100
120

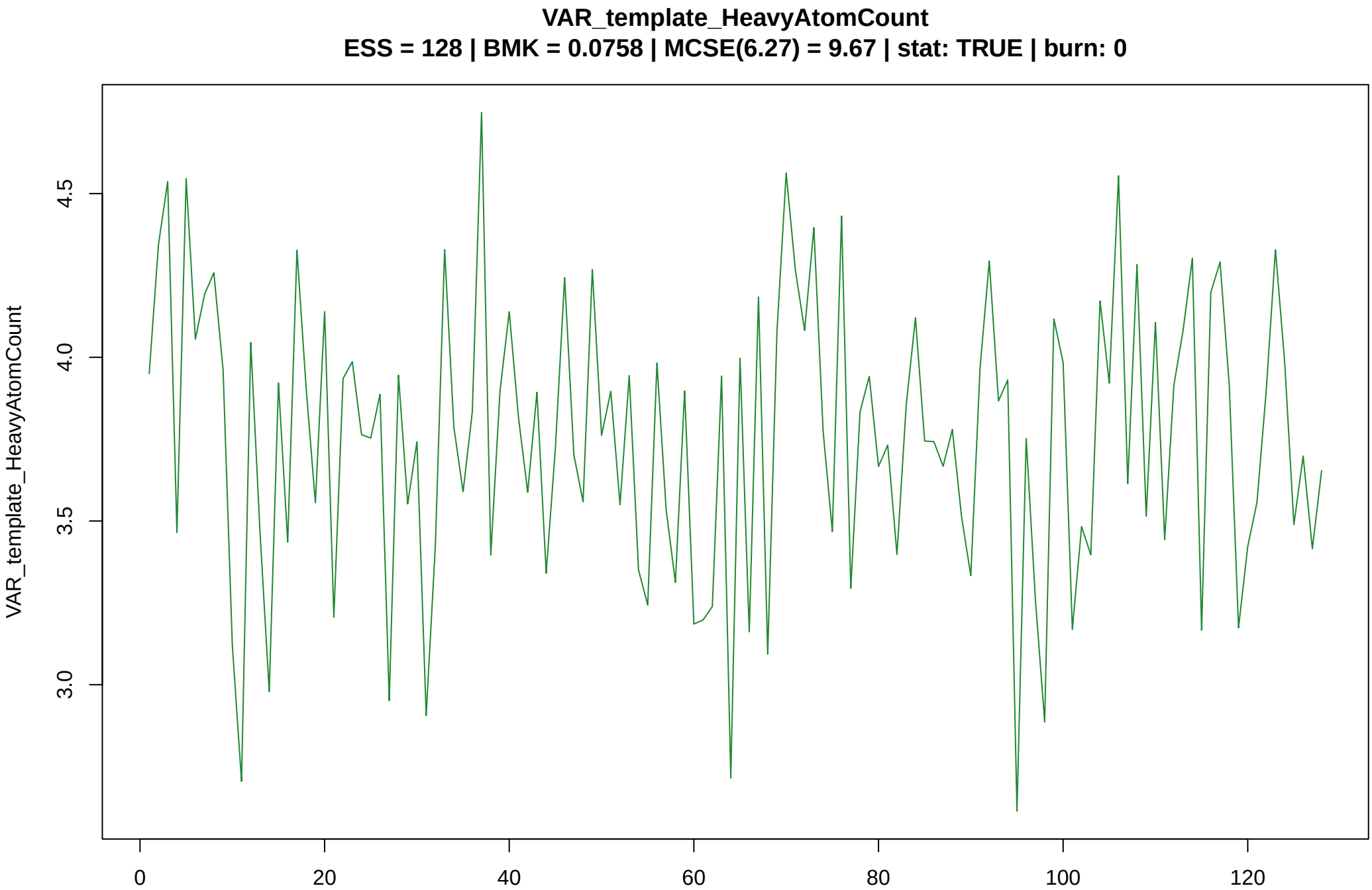

MEAN_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.14 | MCSE(6.27) = 8.8 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
1.0
1.5
2.0
2.5
3.0
0
20
40
60
80
100
120

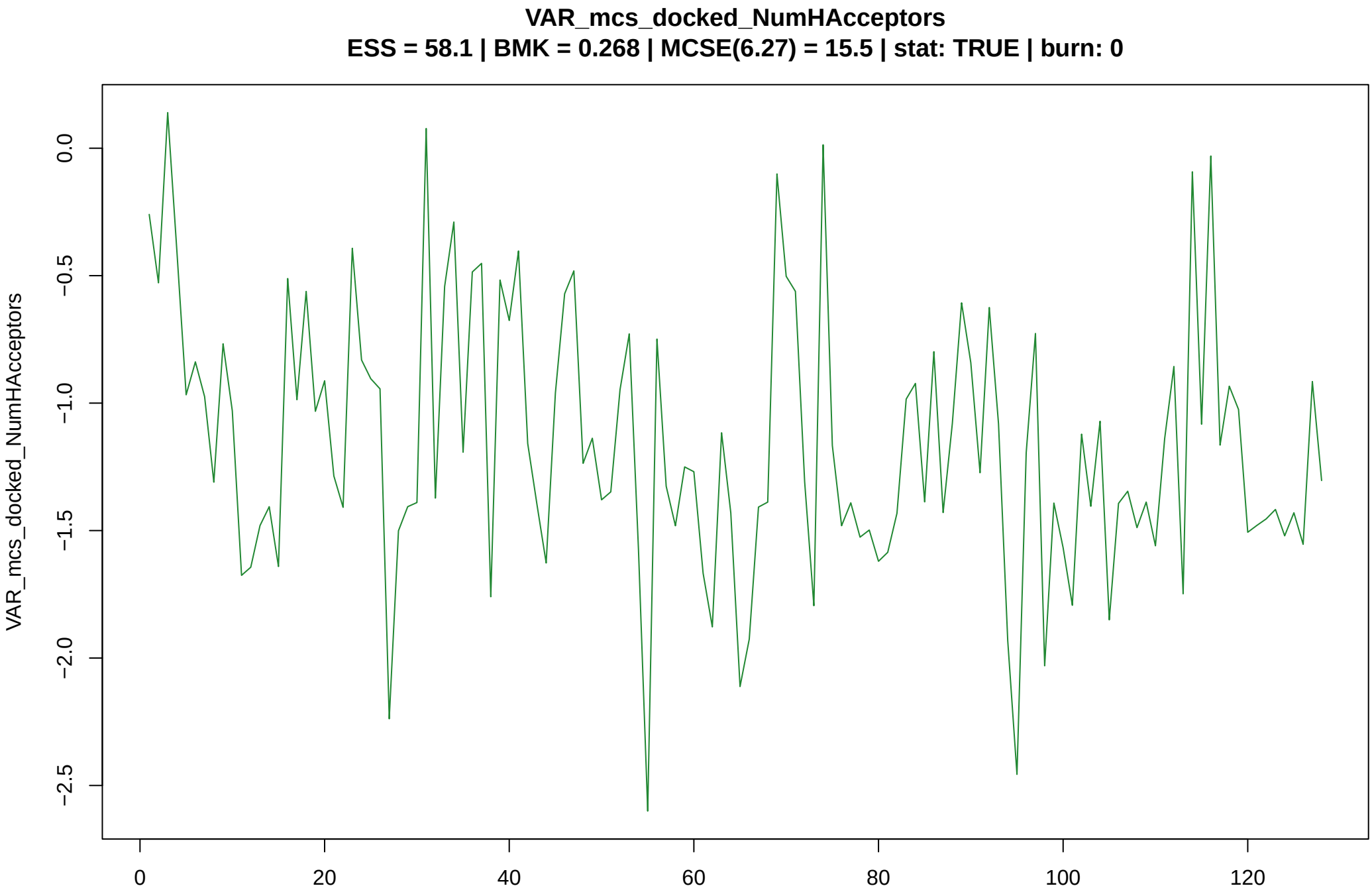

VAR_log_RMSD
ESS = 128 | BMK = 0.0956 | MCSE(6.27) = 7.73 | stat: TRUE | burn: 0
VAR_log_RMSD
1
0
−1
−2
−3
0
20
40
60
80
100
120

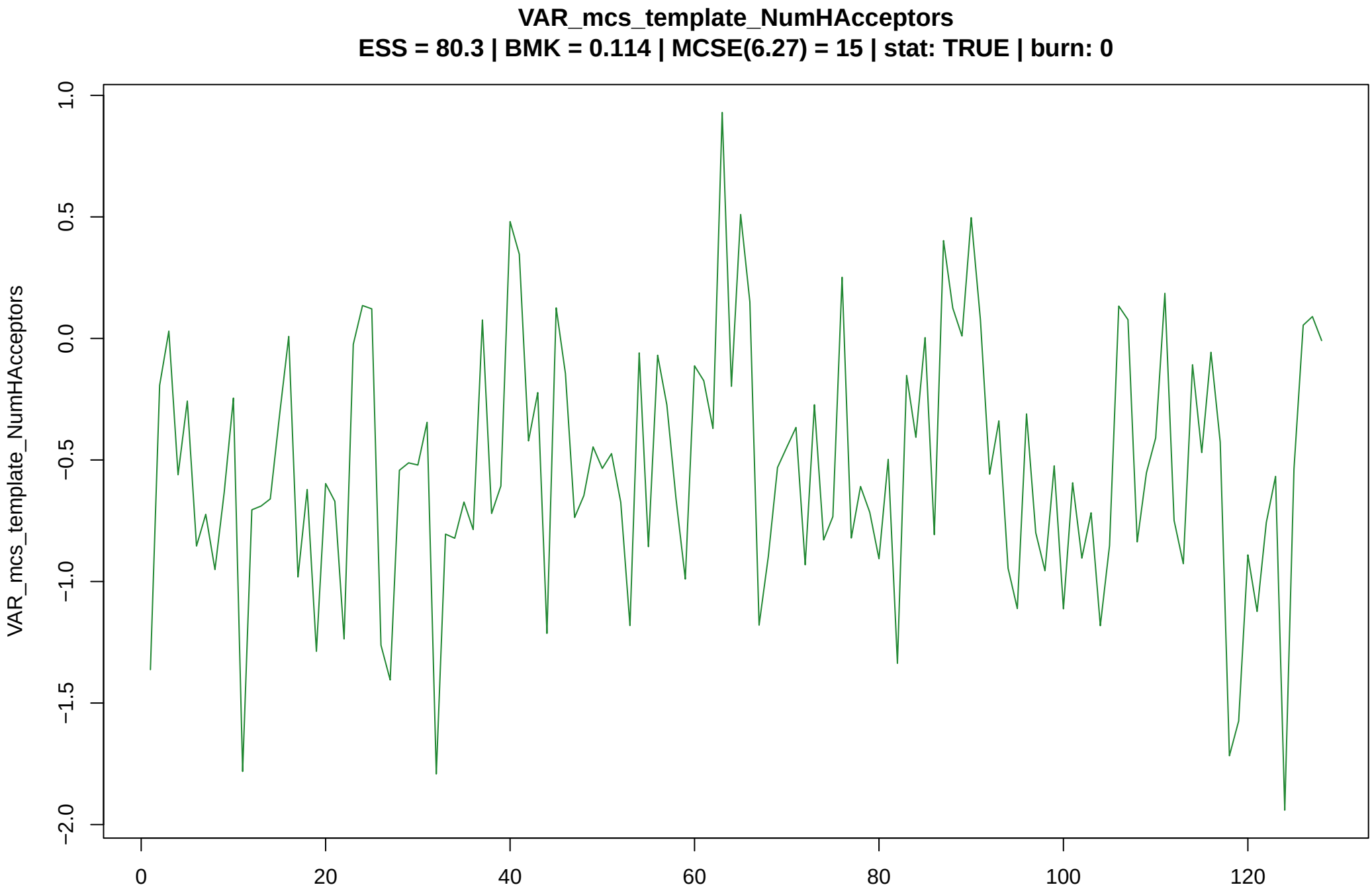

VAR_Xtransf_ec_tanimoto_similarity
ESS = 128 | BMK = 0.213 | MCSE(6.27) = 8.54 | stat: TRUE | burn: 12
VAR_Xtransf_ec_tanimoto_similarity
3
2
1
0
−1
−2
0
20
40
60
80
100
120

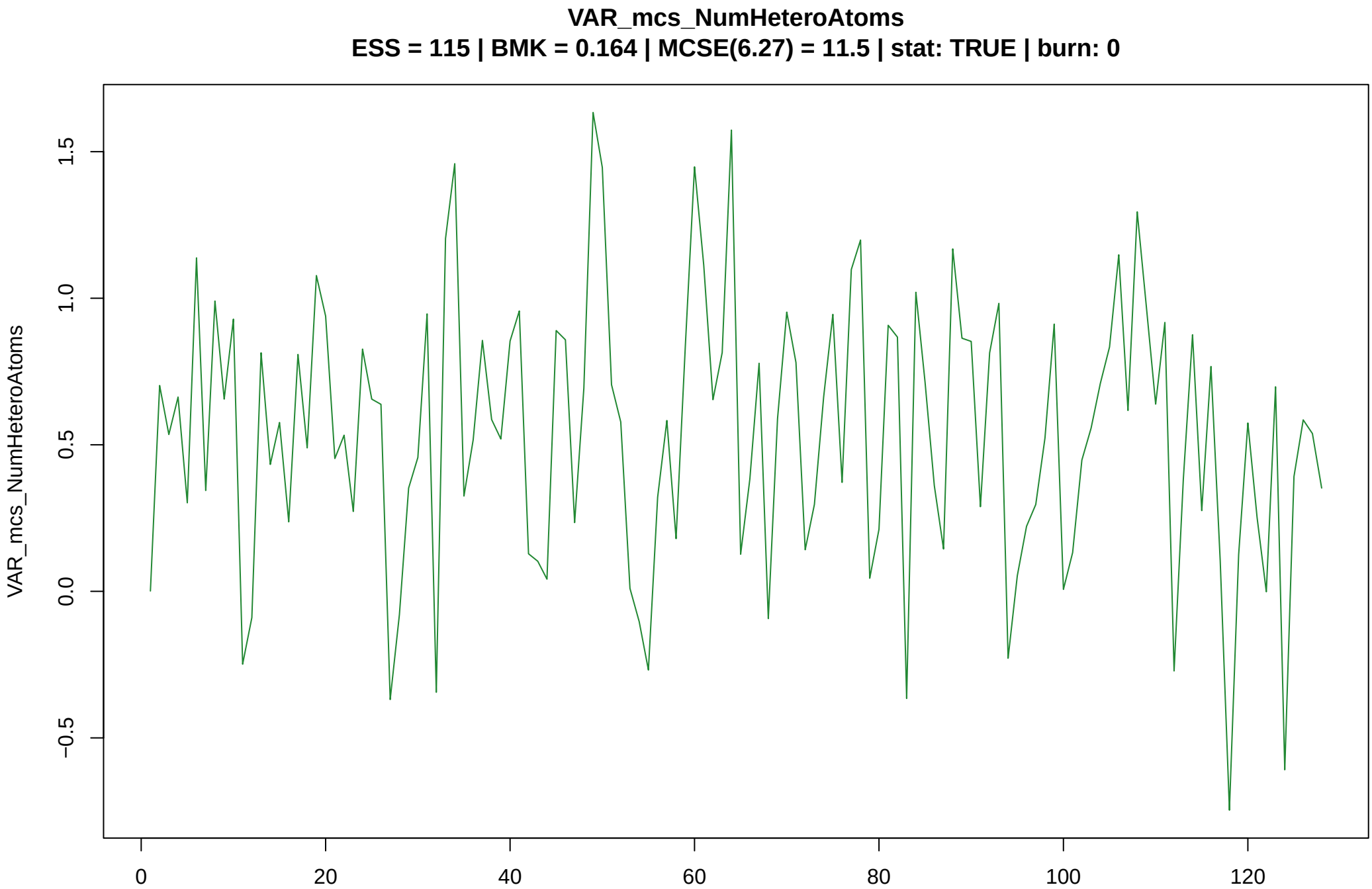

VAR_docked_HeavyAtomCount
ESS = 61.1 | BMK = 0.109 | MCSE(6.27) = 10.9 | stat: TRUE | burn: 0
VAR_docked_HeavyAtomCount
3.5
4.0
4.5
5.0
0
20
40
60
80
100
120

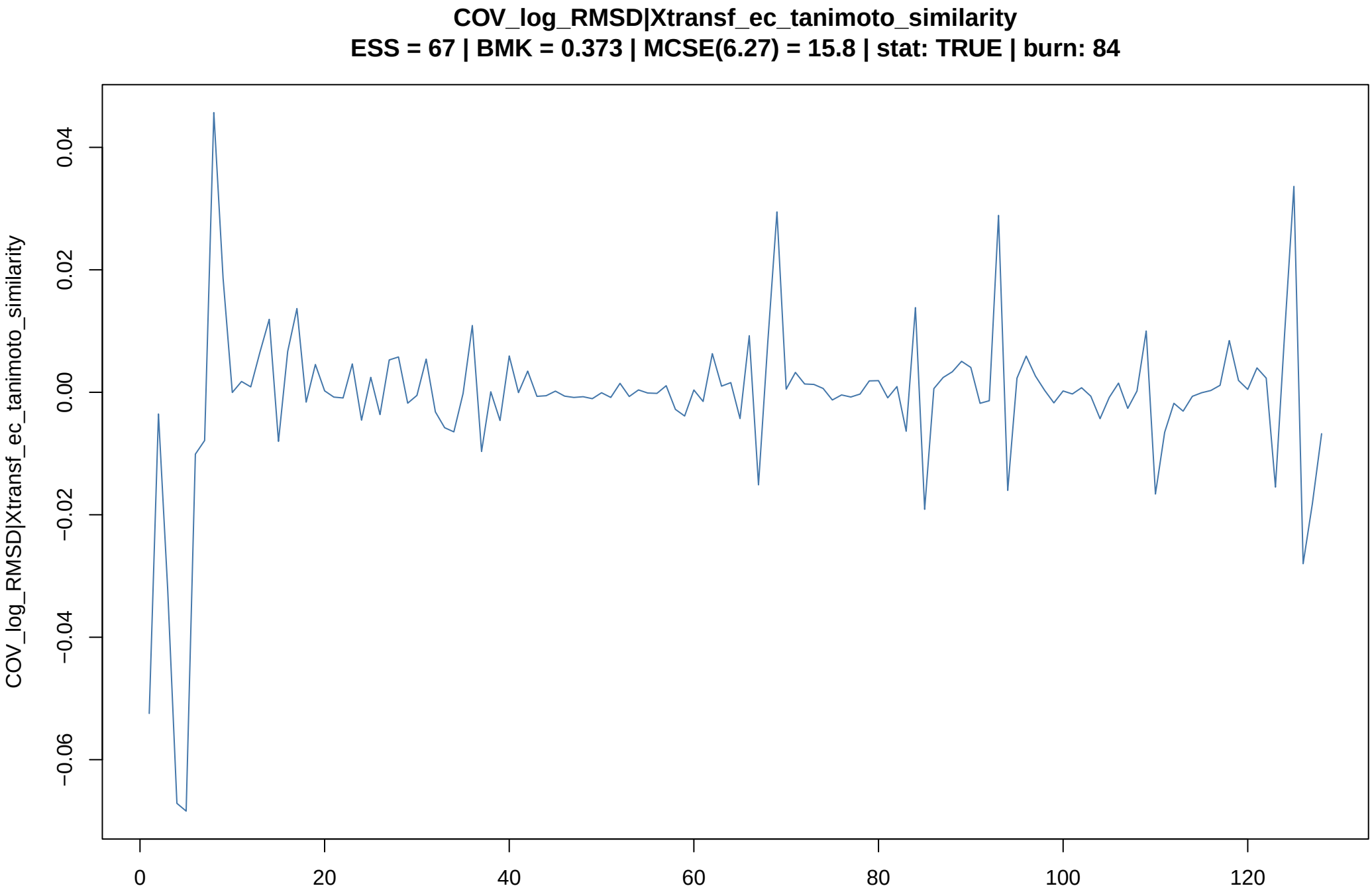

VAR_mcs_RingCount
ESS = 61.7 | BMK = 0.2 | MCSE(6.27) = 14.8 | stat: TRUE | burn: 48
VAR_mcs_RingCount
−0.5
−1.0
−1.5
−2.0
0
20
40
60
80
100
120

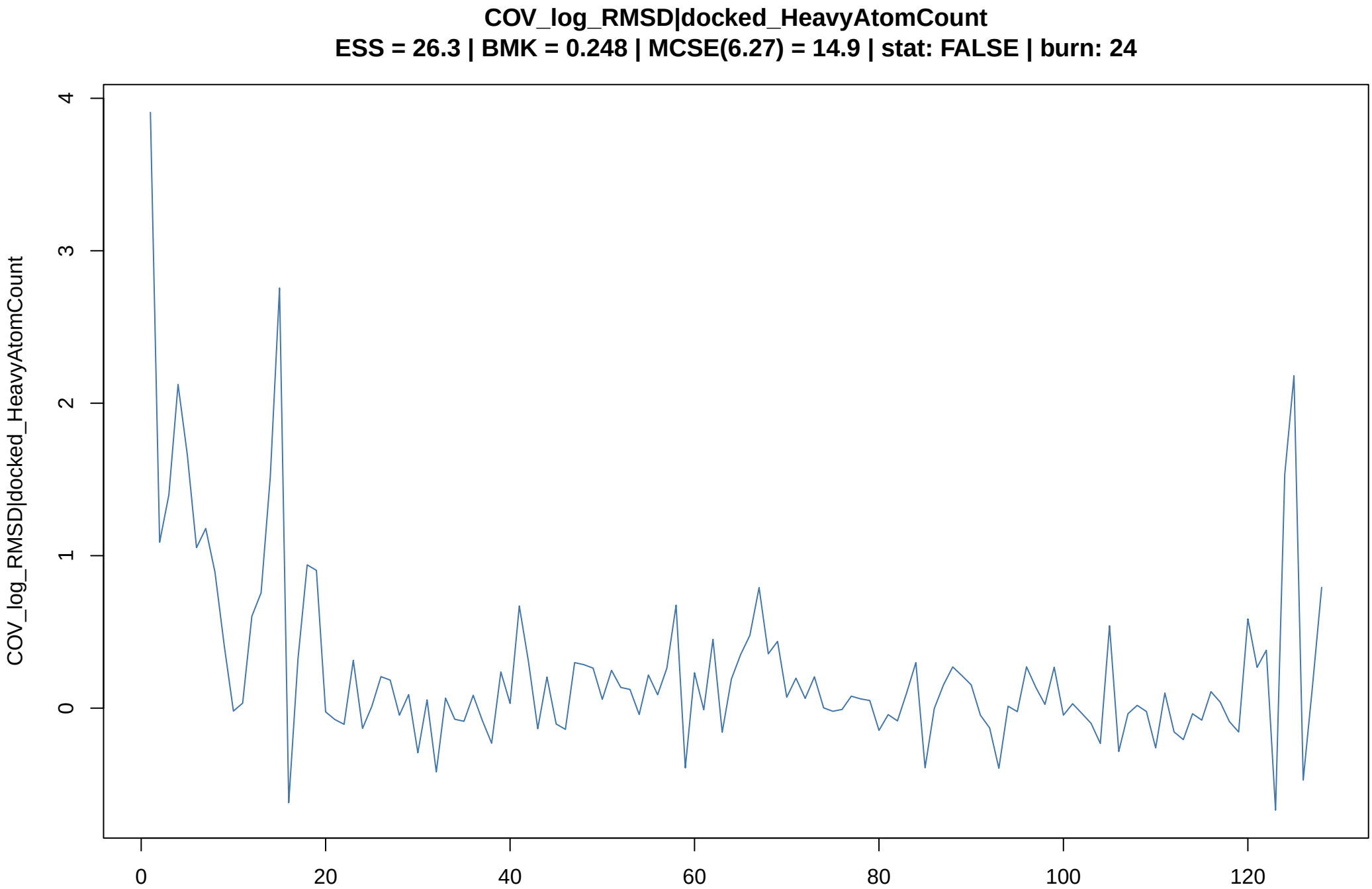

VAR_template_HeavyAtomCount
ESS = 128 | BMK = 0.0758 | MCSE(6.27) = 9.67 | stat: TRUE | burn: 0
VAR_template_HeavyAtomCount
3.0
3.5
4.0
4.5
0
20
40
60
80
100
120

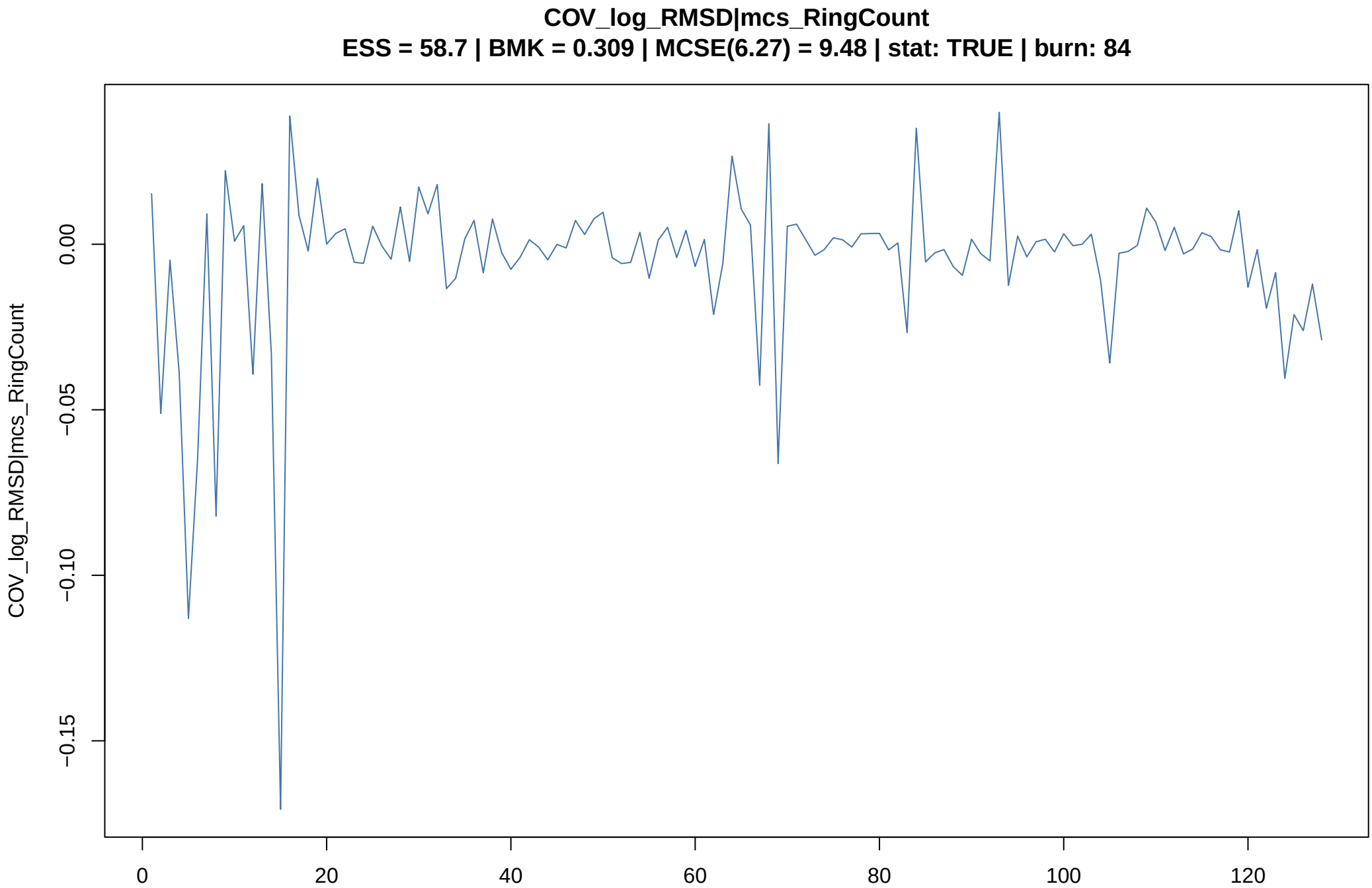

VAR_mcs_docked_NumHAcceptors
ESS = 58.1 | BMK = 0.268 | MCSE(6.27) = 15.5 | stat: TRUE | burn: 0
VAR_mcs_docked_NumHAcceptors
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
0
20
40
60
80
100
120

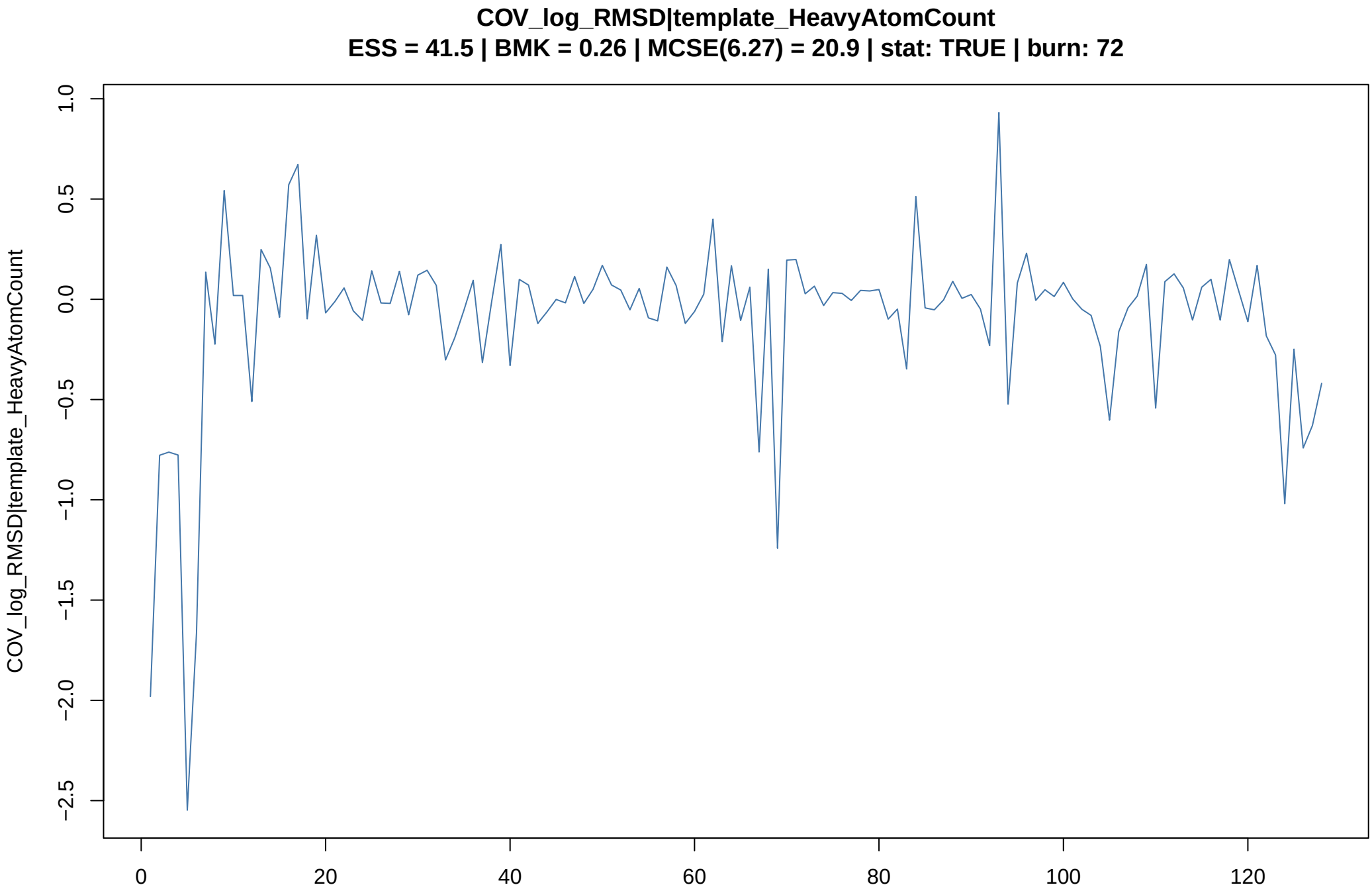

VAR_mcs_template_NumHAcceptors
ESS = 80.3 | BMK = 0.114 | MCSE(6.27) = 15 | stat: TRUE | burn: 0
VAR_mcs_template_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
0
20
40
60
80
100
120

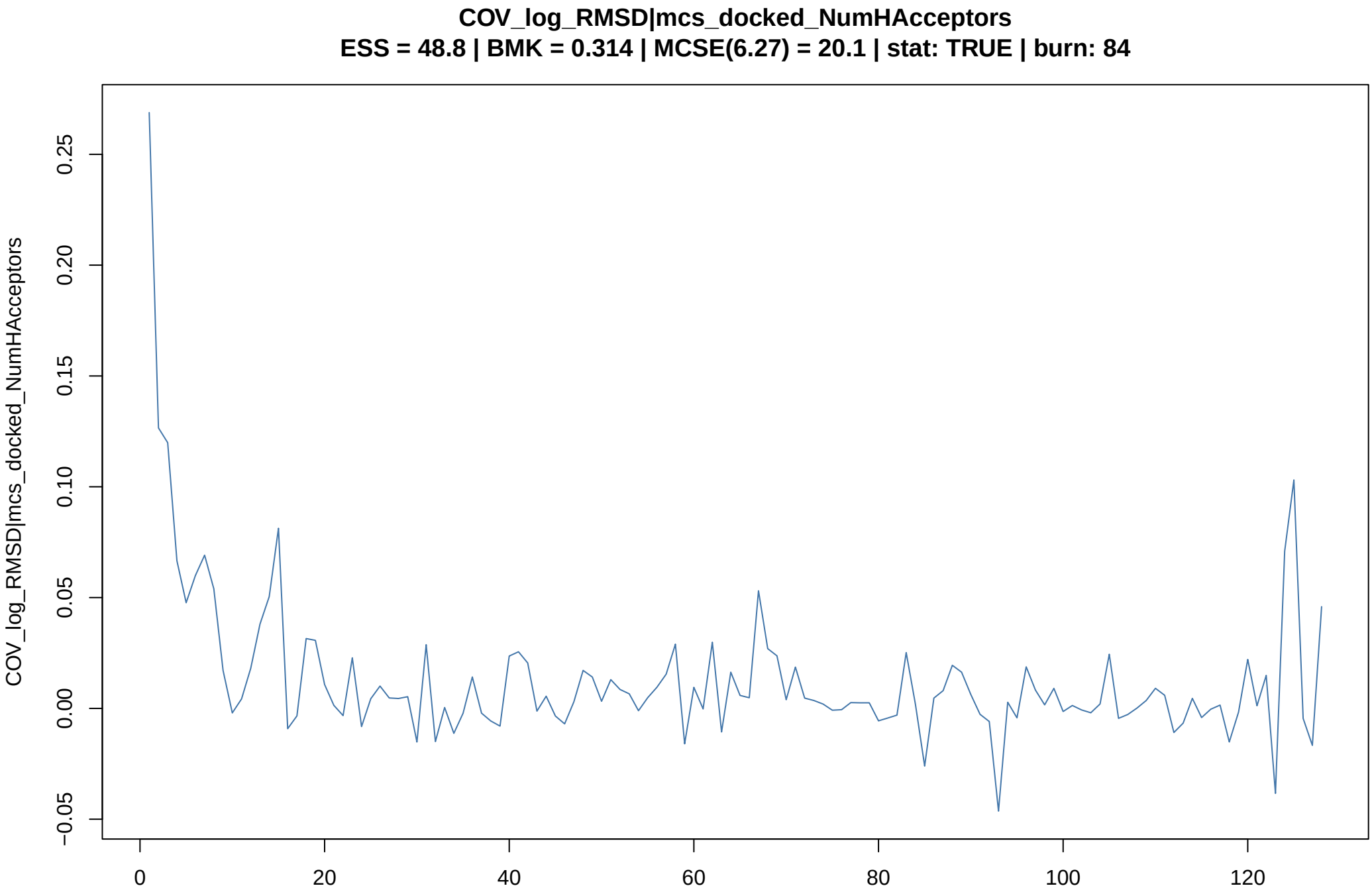

VAR_mcs_NumHeteroAtoms
ESS = 115 | BMK = 0.164 | MCSE(6.27) = 11.5 | stat: TRUE | burn: 0
VAR_mcs_NumHeteroAtoms
−0.5
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120

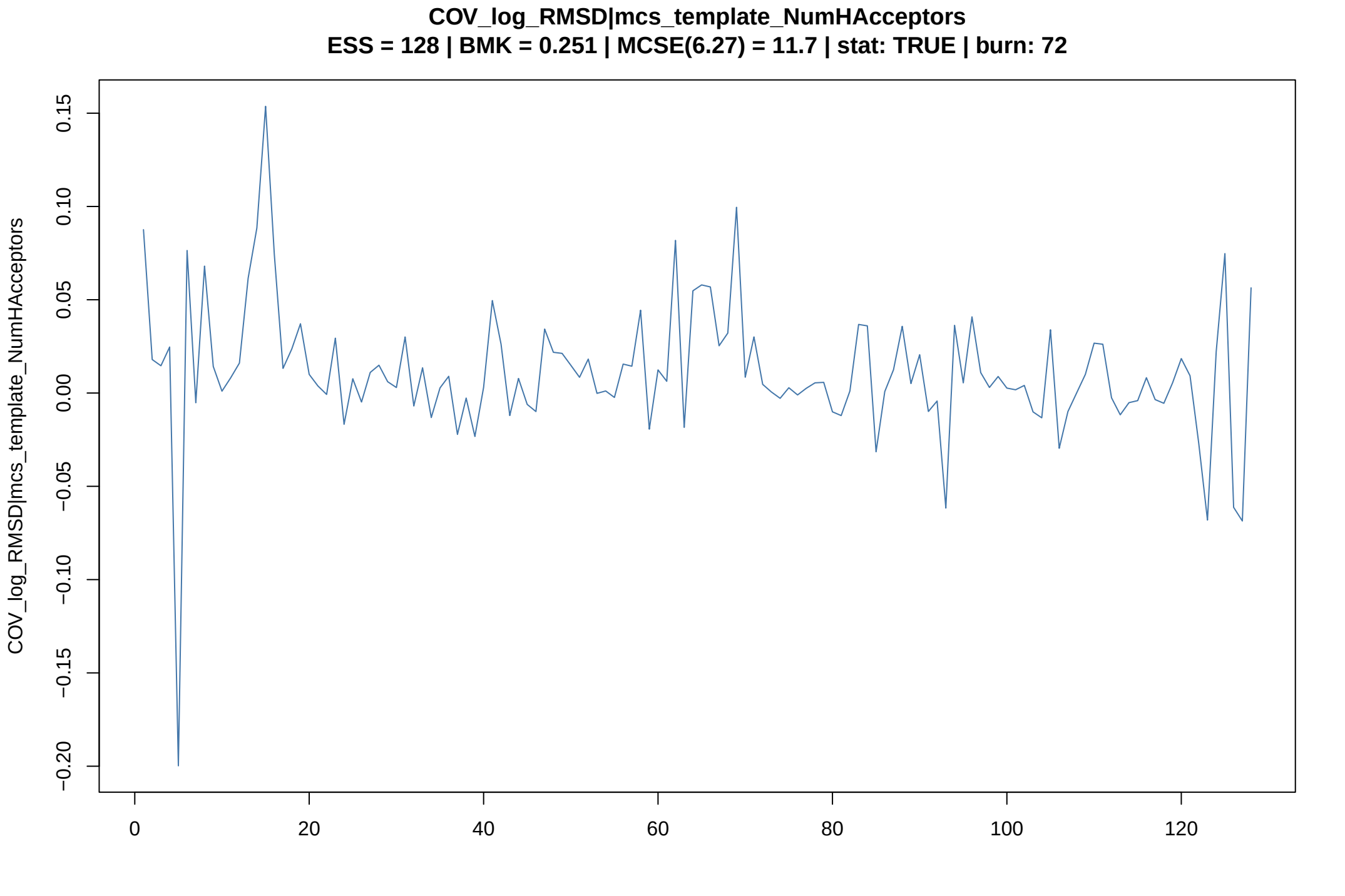

COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 67 | BMK = 0.373 | MCSE(6.27) = 15.8 | stat: TRUE | burn: 84
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
0.04
0.02
0.00
−0.02
−0.04
−0.06
0
20
40
60
80
100
120

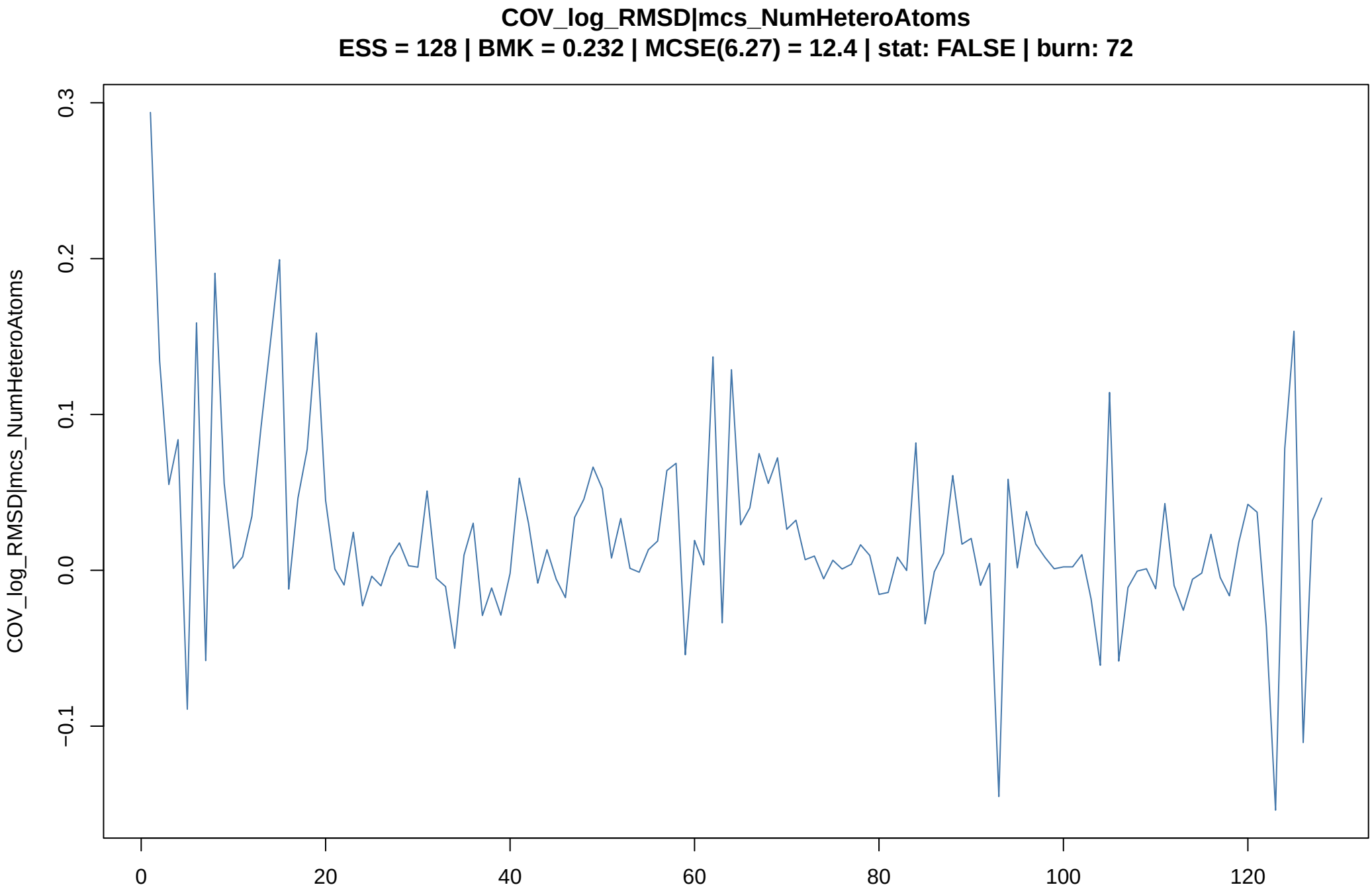

COV_log_RMSD|docked_HeavyAtomCount
ESS = 26.3 | BMK = 0.248 | MCSE(6.27) = 14.9 | stat: FALSE | burn: 24
COV_log_RMSD|docked_HeavyAtomCount
0
1
2
3
4
0
20
40
60
80
100
120

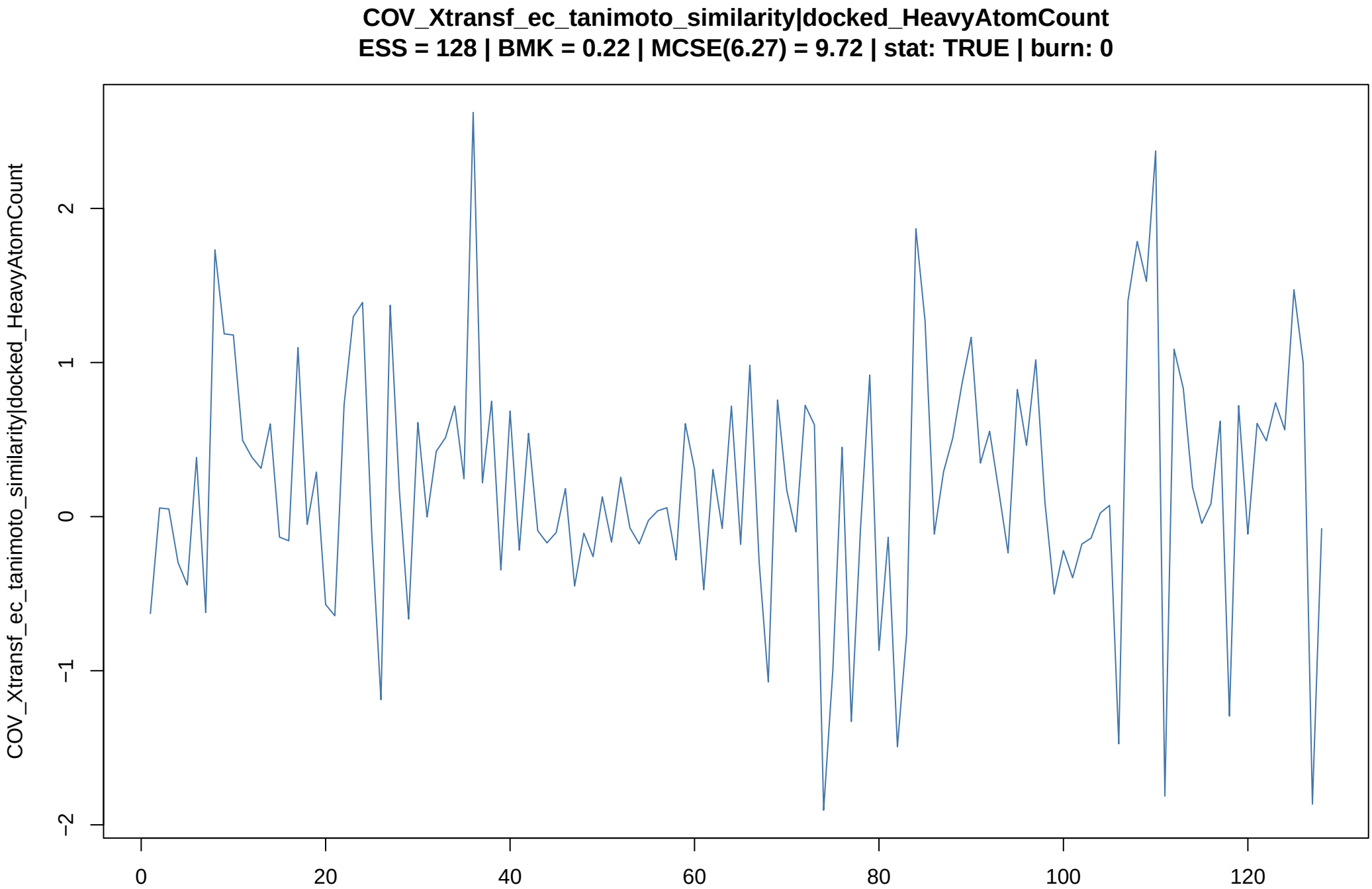

COV_log_RMSD|mcs_RingCount
ESS = 58.7 | BMK = 0.309 | MCSE(6.27) = 9.48 | stat: TRUE | burn: 84
COV_log_RMSD|mcs_RingCount
0.00
−0.05
−0.10
−0.15
0
20
40
60
80
100
120

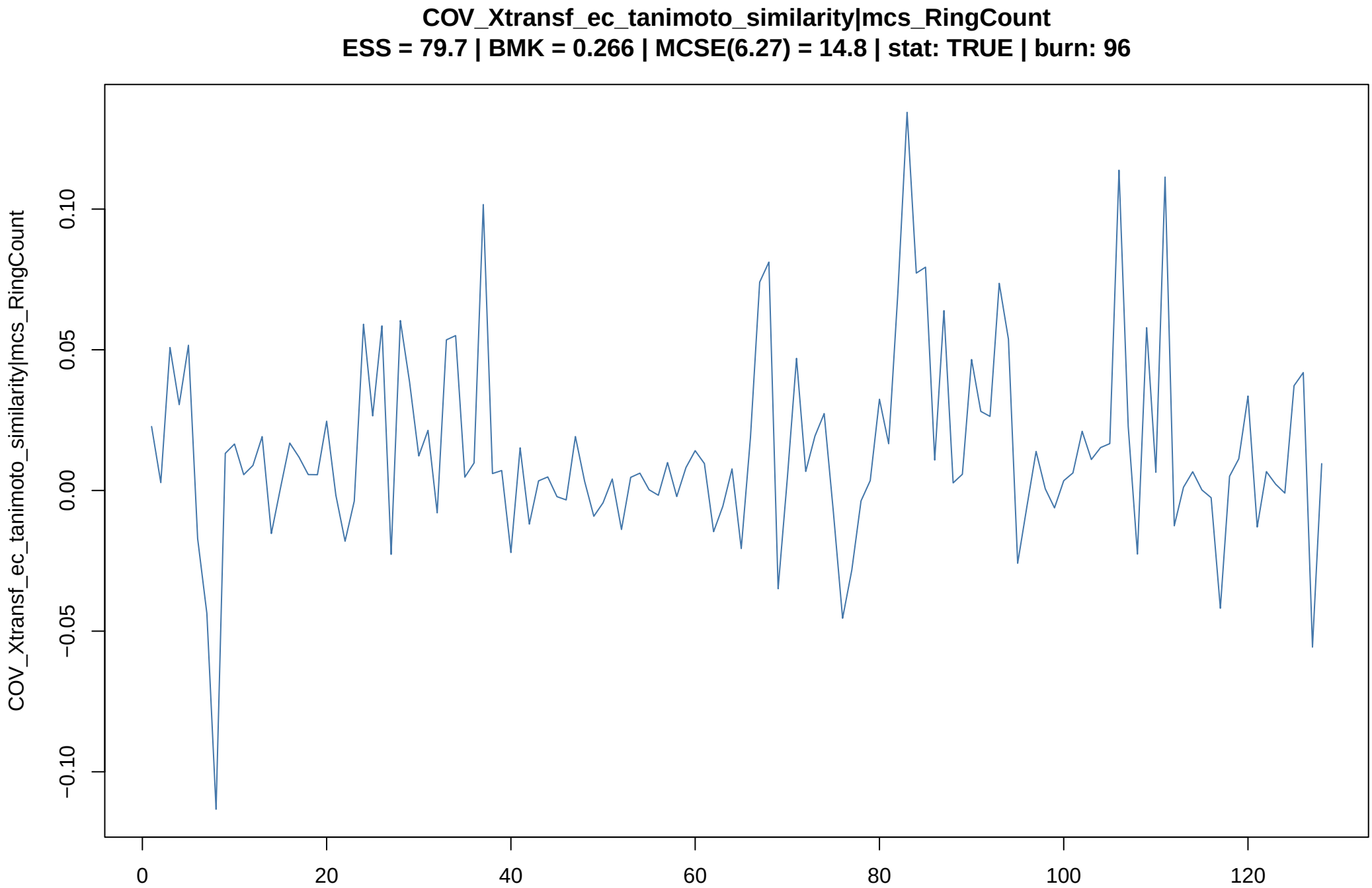

COV_log_RMSD|template_HeavyAtomCount
ESS = 41.5 | BMK = 0.26 | MCSE(6.27) = 20.9 | stat: TRUE | burn: 72
COV_log_RMSD|template_HeavyAtomCount
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
0
20
40
60
80
100
120

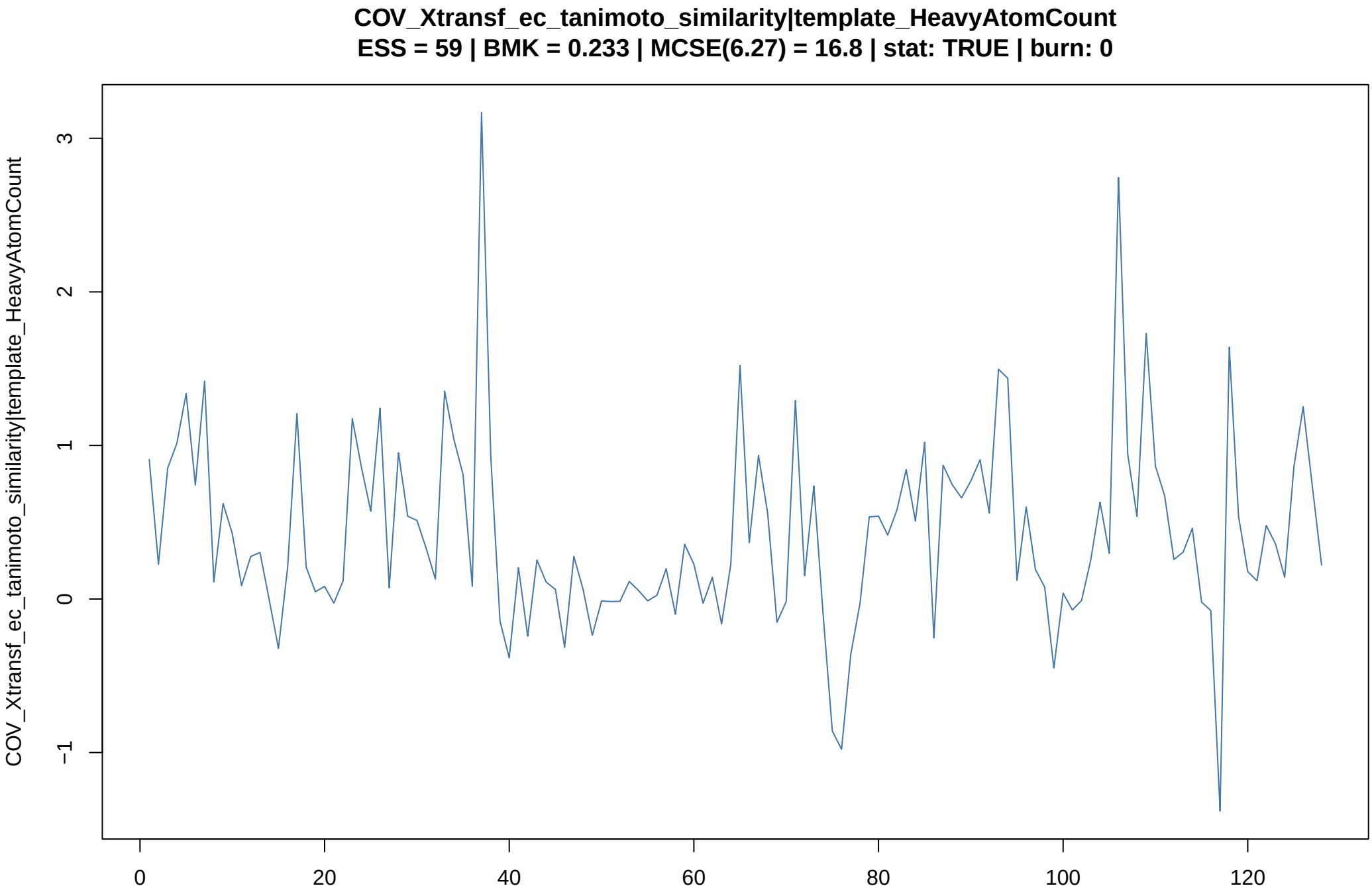

COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 48.8 | BMK = 0.314 | MCSE(6.27) = 20.1 | stat: TRUE | burn: 84
COV_log_RMSD|mcs_docked_NumHAcceptors
0.25
0.20
0.15
0.10
0.05
0.00
−0.05
0
20
40
60
80
100
120

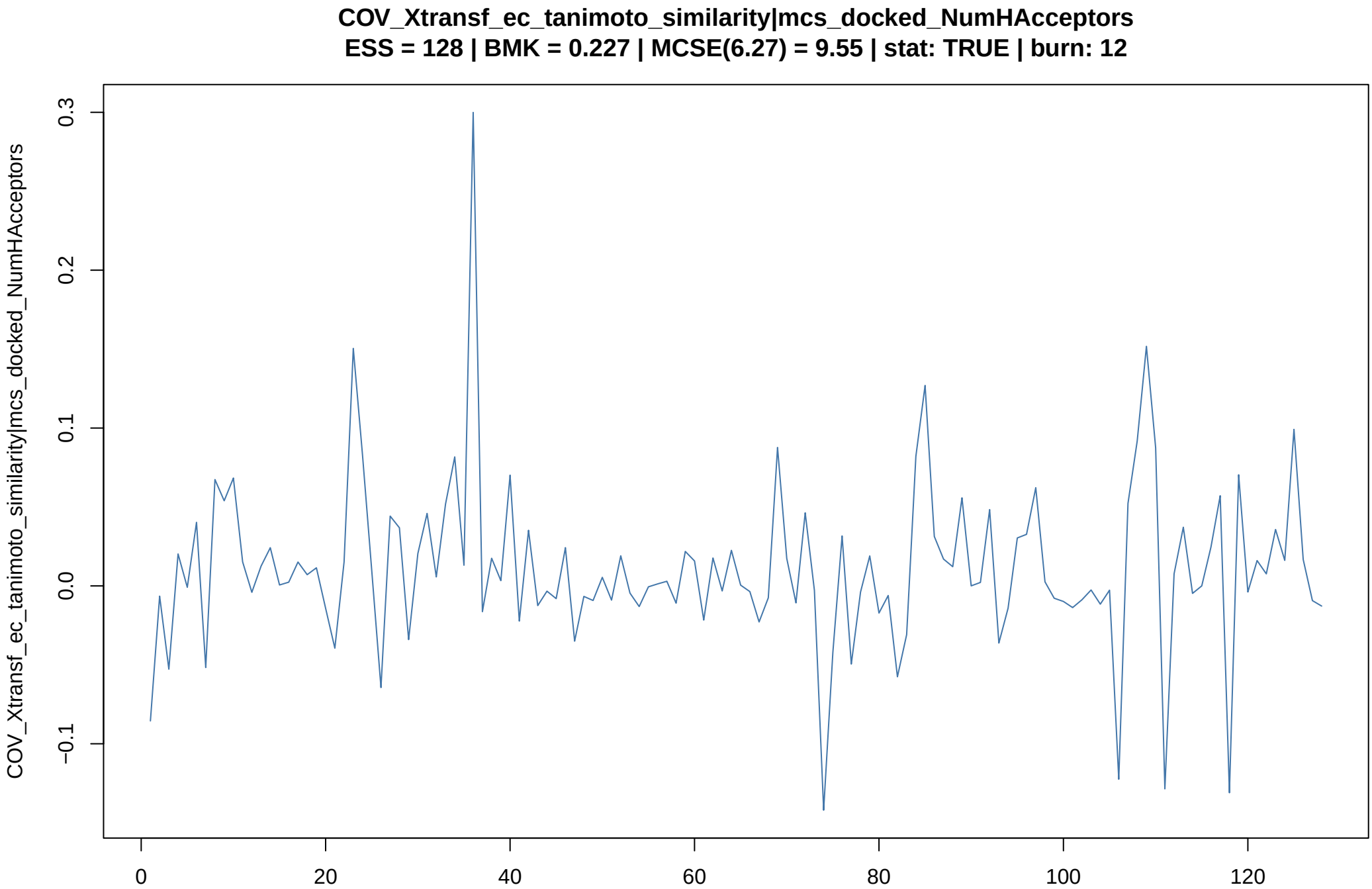

COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 128 | BMK = 0.251 | MCSE(6.27) = 11.7 | stat: TRUE | burn: 72
COV_log_RMSD|mcs_template_NumHAcceptors
0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
−0.20
0
20
40
60
80
100
120

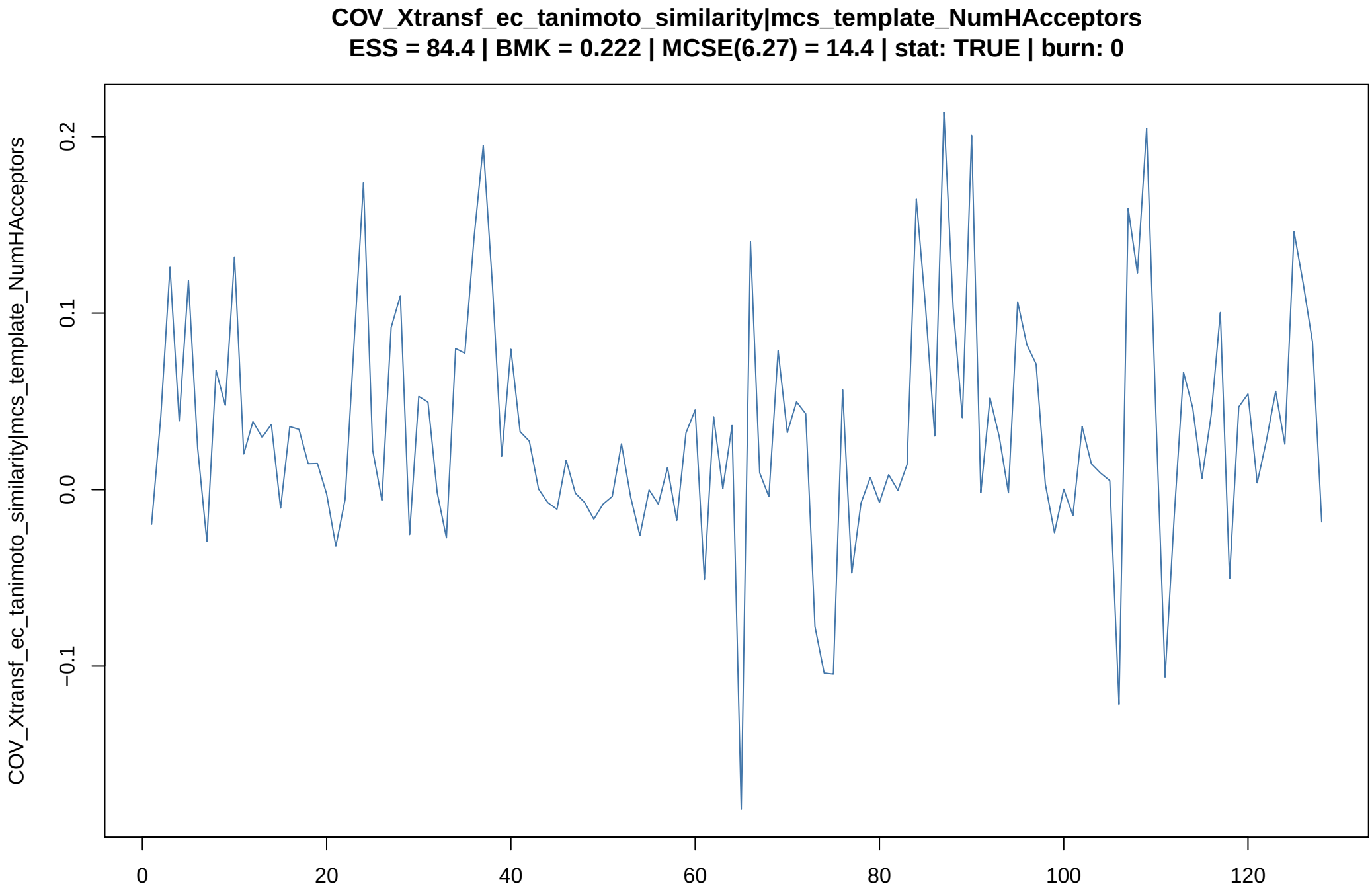

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.232 | MCSE(6.27) = 12.4 | stat: FALSE | burn: 72
COV_log_RMSD|mcs_NumHeteroAtoms
0.3
0.2
0.1
0.0
−0.1
0
20
40
60
80
100
120

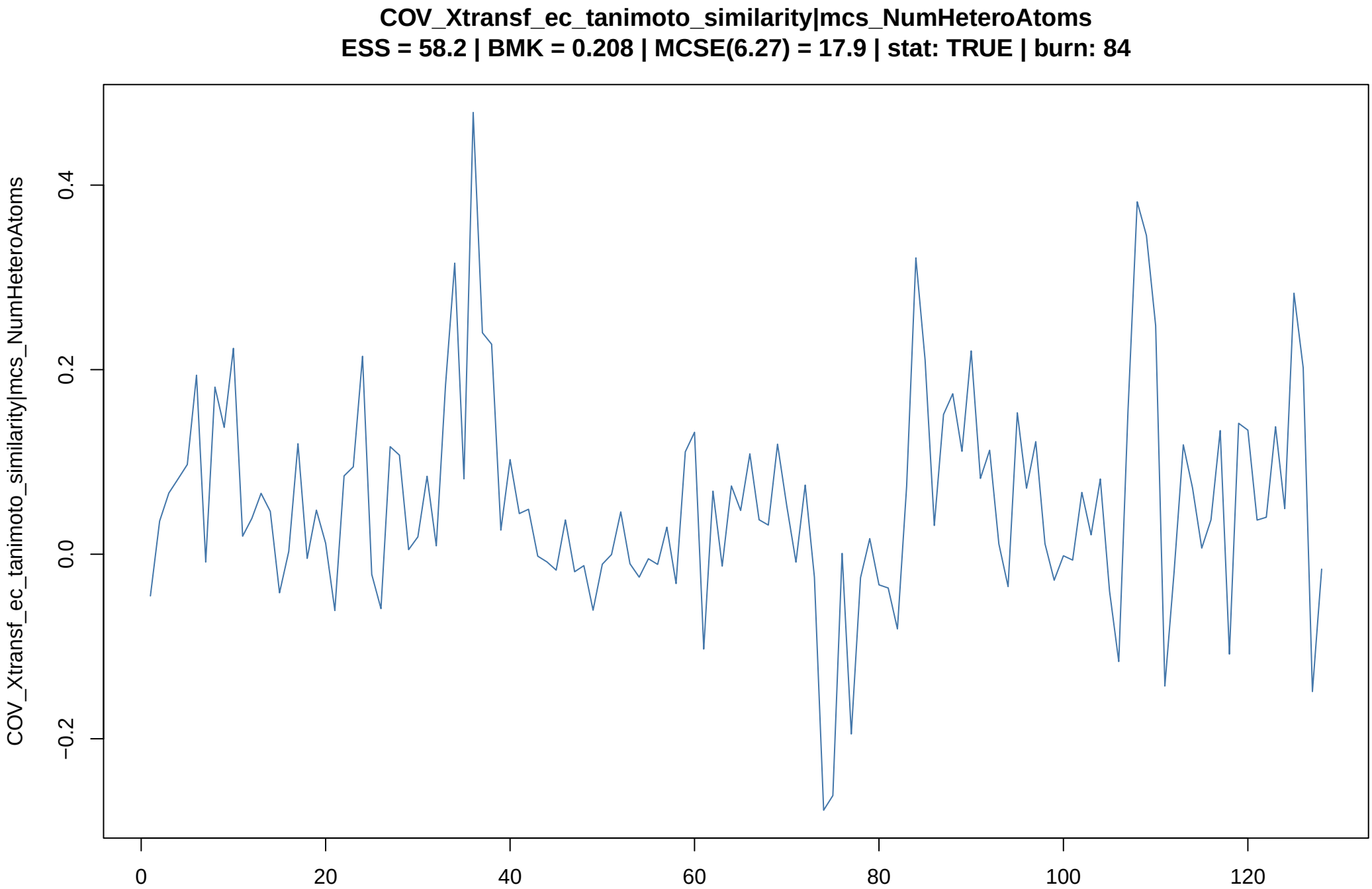

COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 128 | BMK = 0.22 | MCSE(6.27) = 9.72 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
2
1
0
−1
−2
0
20
40
60
80
100
120

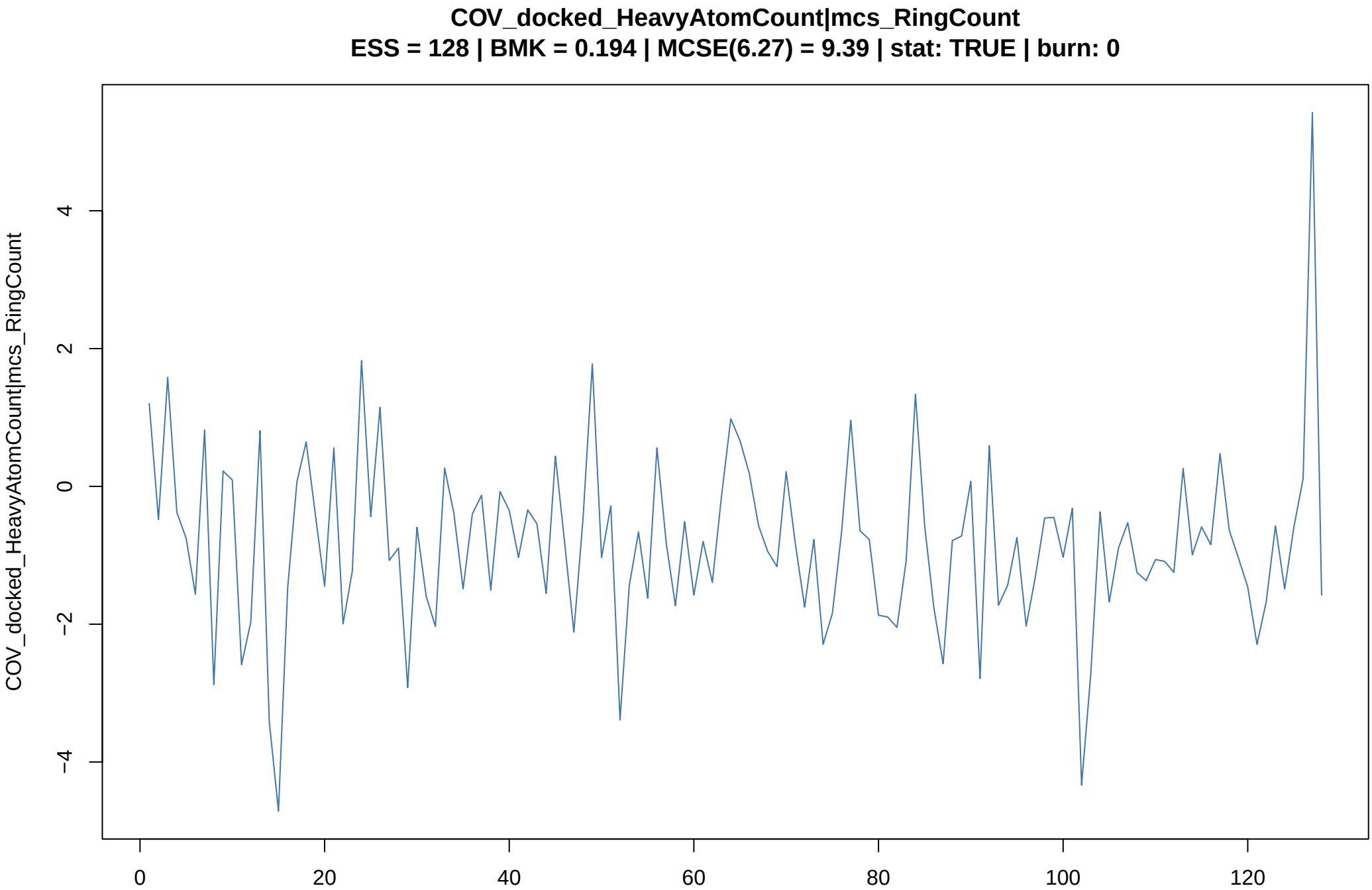

COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 79.7 | BMK = 0.266 | MCSE(6.27) = 14.8 | stat: TRUE | burn: 96
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
0.10
0.05
0.00
−0.05
−0.10
0
20
40
60
80
100
120

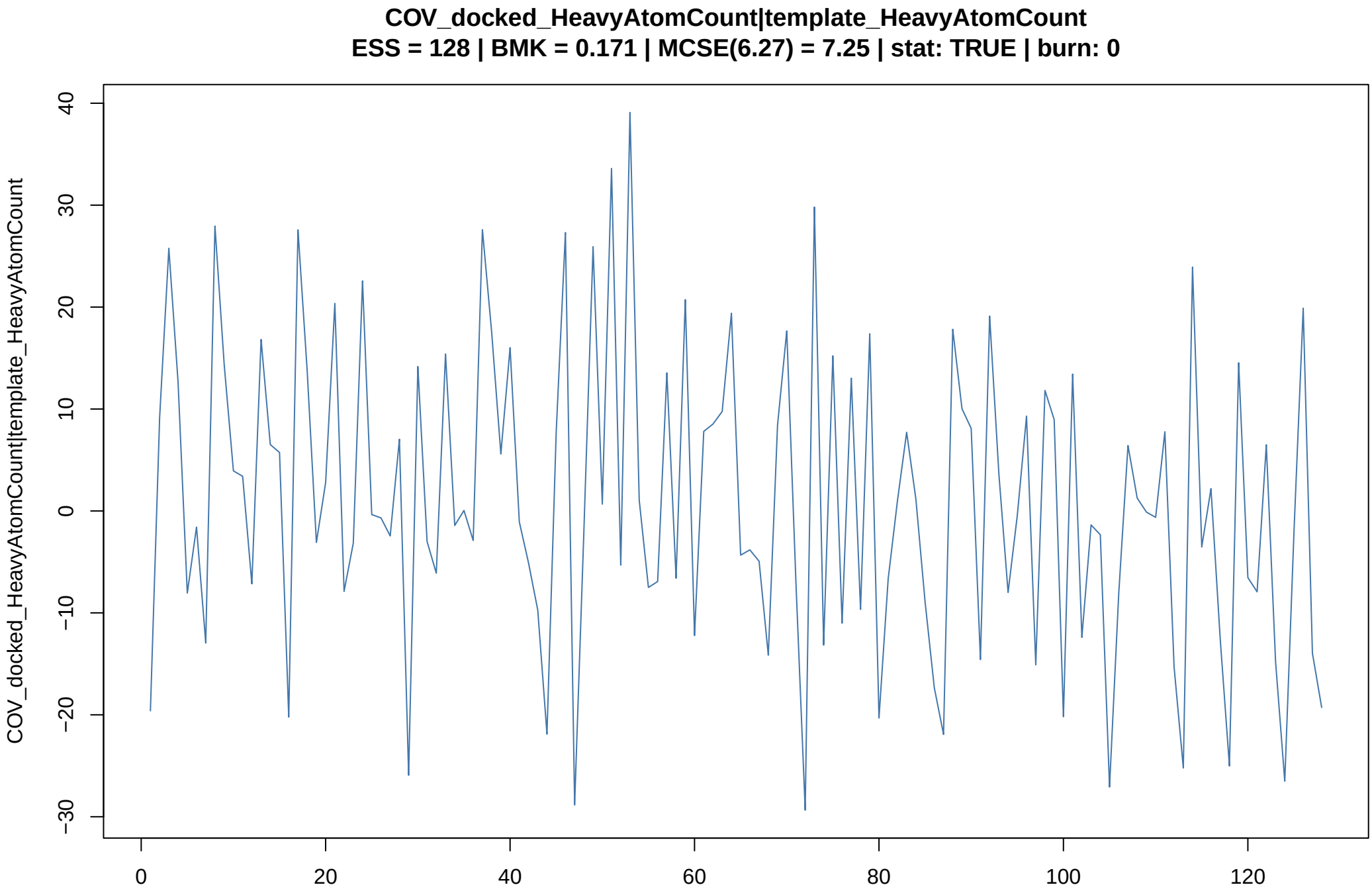

COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 59 | BMK = 0.233 | MCSE(6.27) = 16.8 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
3
2
1
0
−1
0
20
40
60
80
100
120

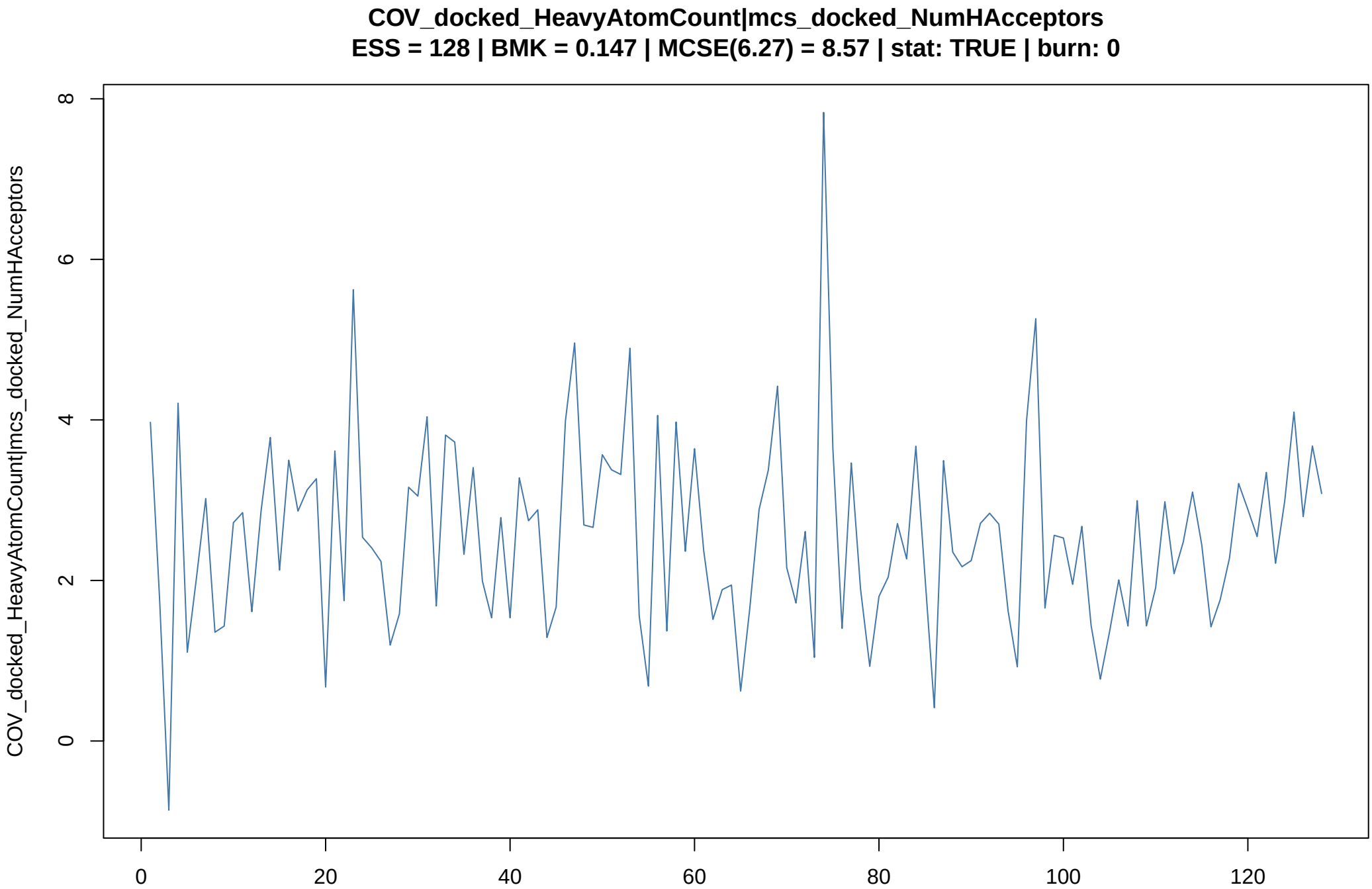

COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.227 | MCSE(6.27) = 9.55 | stat: TRUE | burn: 12
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
0.3
0.2
0.1
0.0
−0.1
0
20
40
60
80
100
120

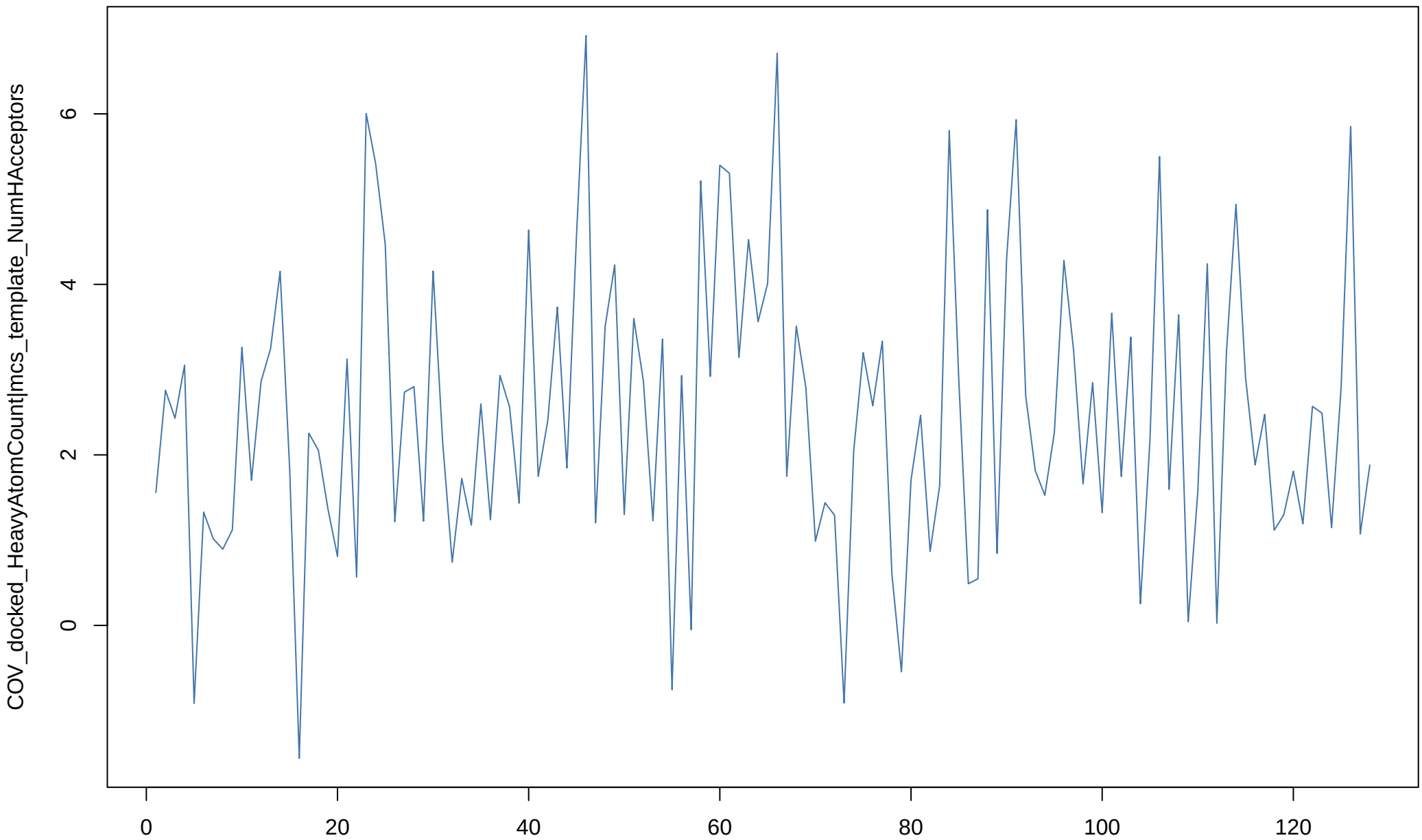

COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 84.4 | BMK = 0.222 | MCSE(6.27) = 14.4 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
0.2
0.1
0.0
−0.1
0
20
40
60
80
100
120

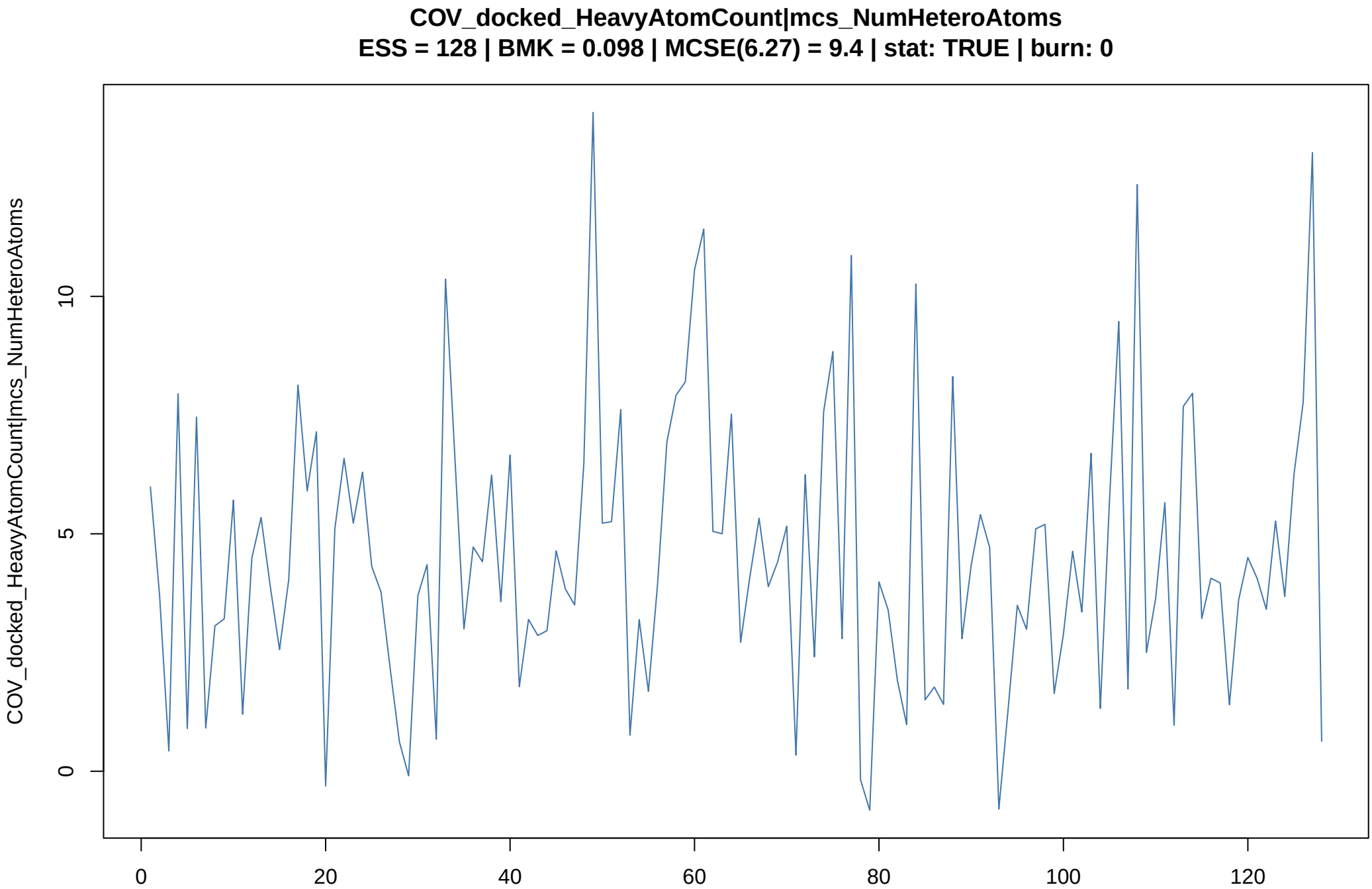

COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 58.2 | BMK = 0.208 | MCSE(6.27) = 17.9 | stat: TRUE | burn: 84
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.4
0.2
0.0
−0.2
0
20
40
60
80
100
120

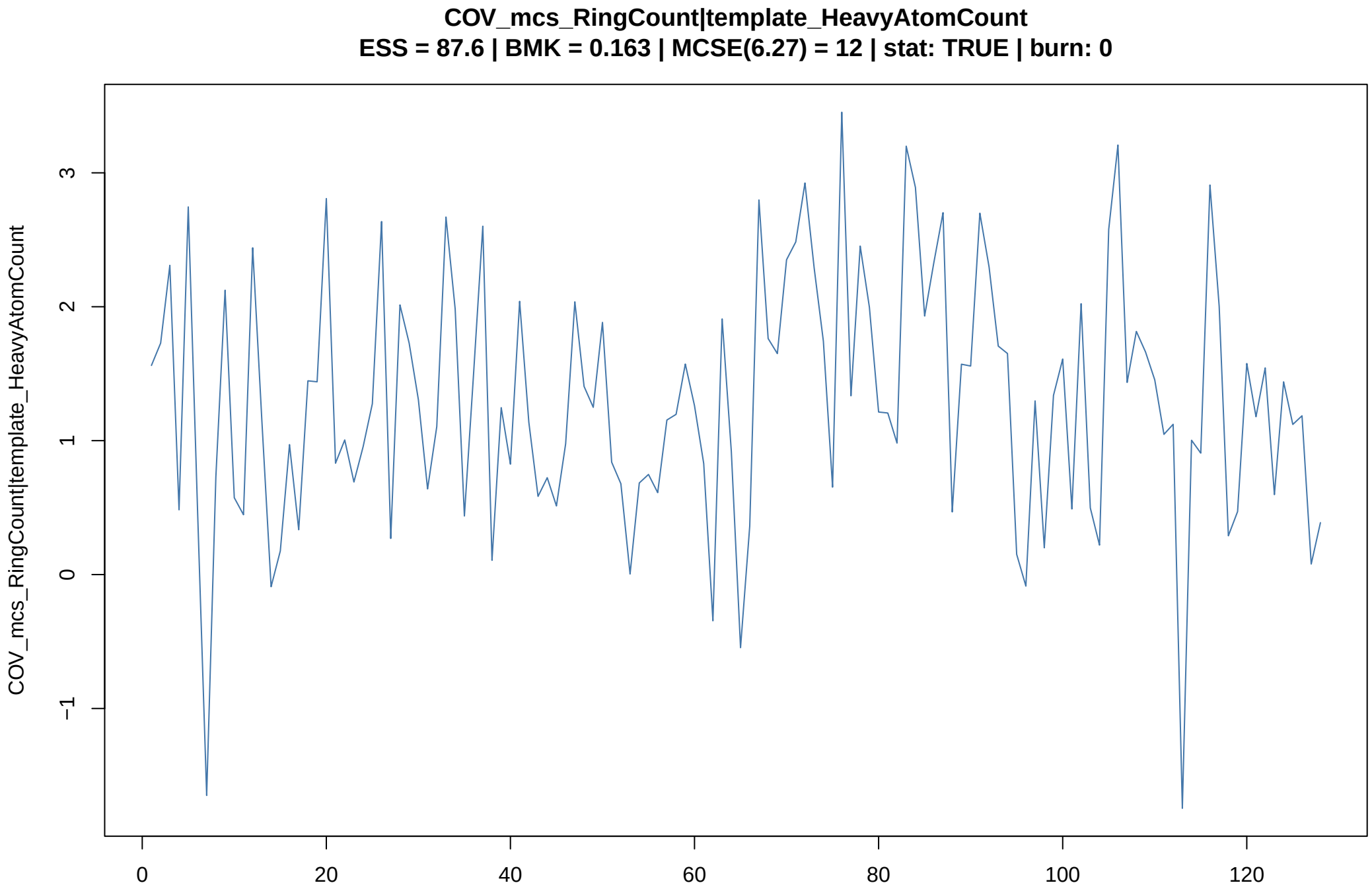

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 128 | BMK = 0.194 | MCSE(6.27) = 9.39 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
4
2
0
−2
−4
0
20
40
60
80
100
120

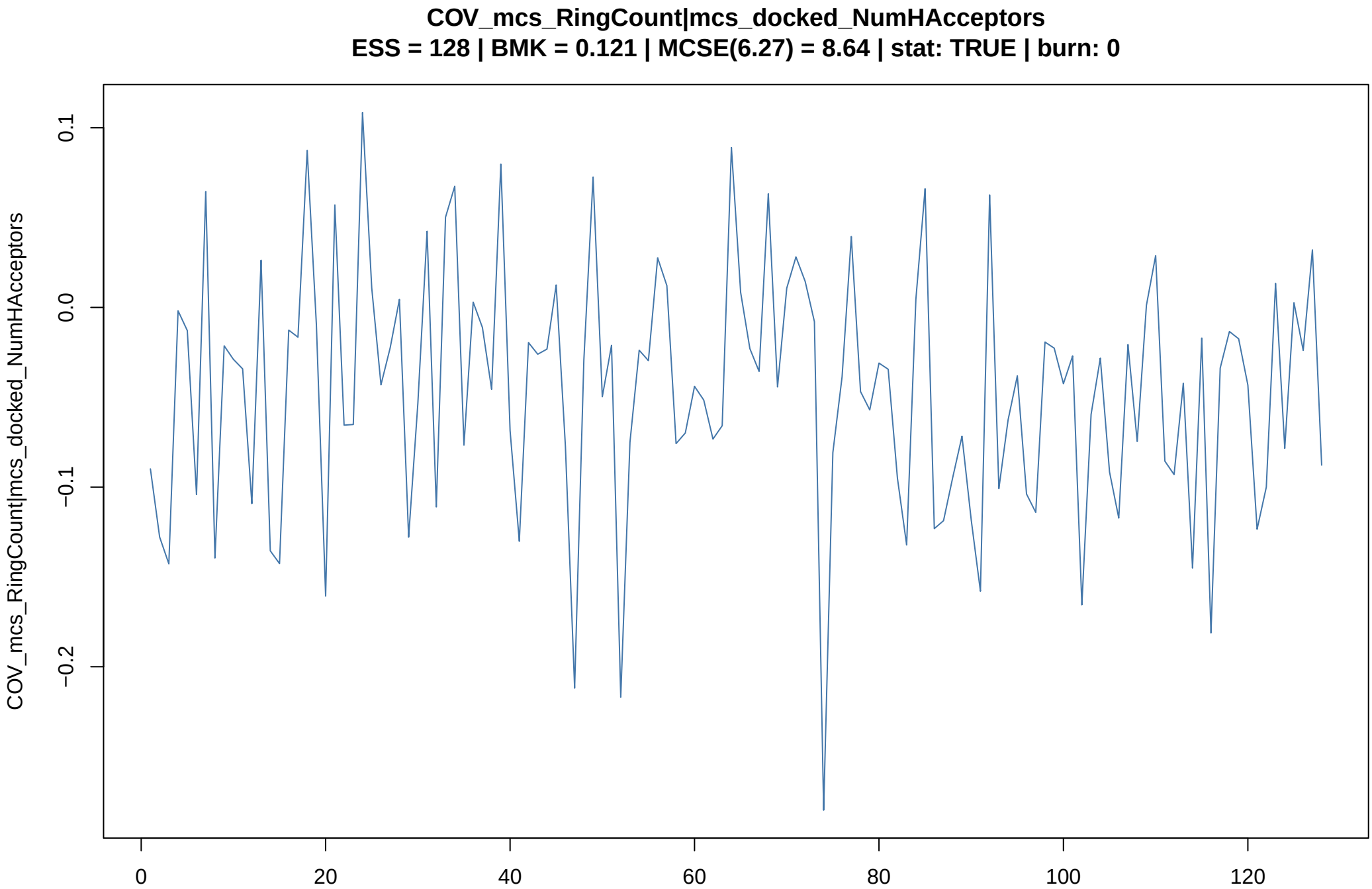

COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 128 | BMK = 0.171 | MCSE(6.27) = 7.25 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|template_HeavyAtomCount
40
30
20
10
0
−10
−20
−30
0
20
40
60
80
100
120

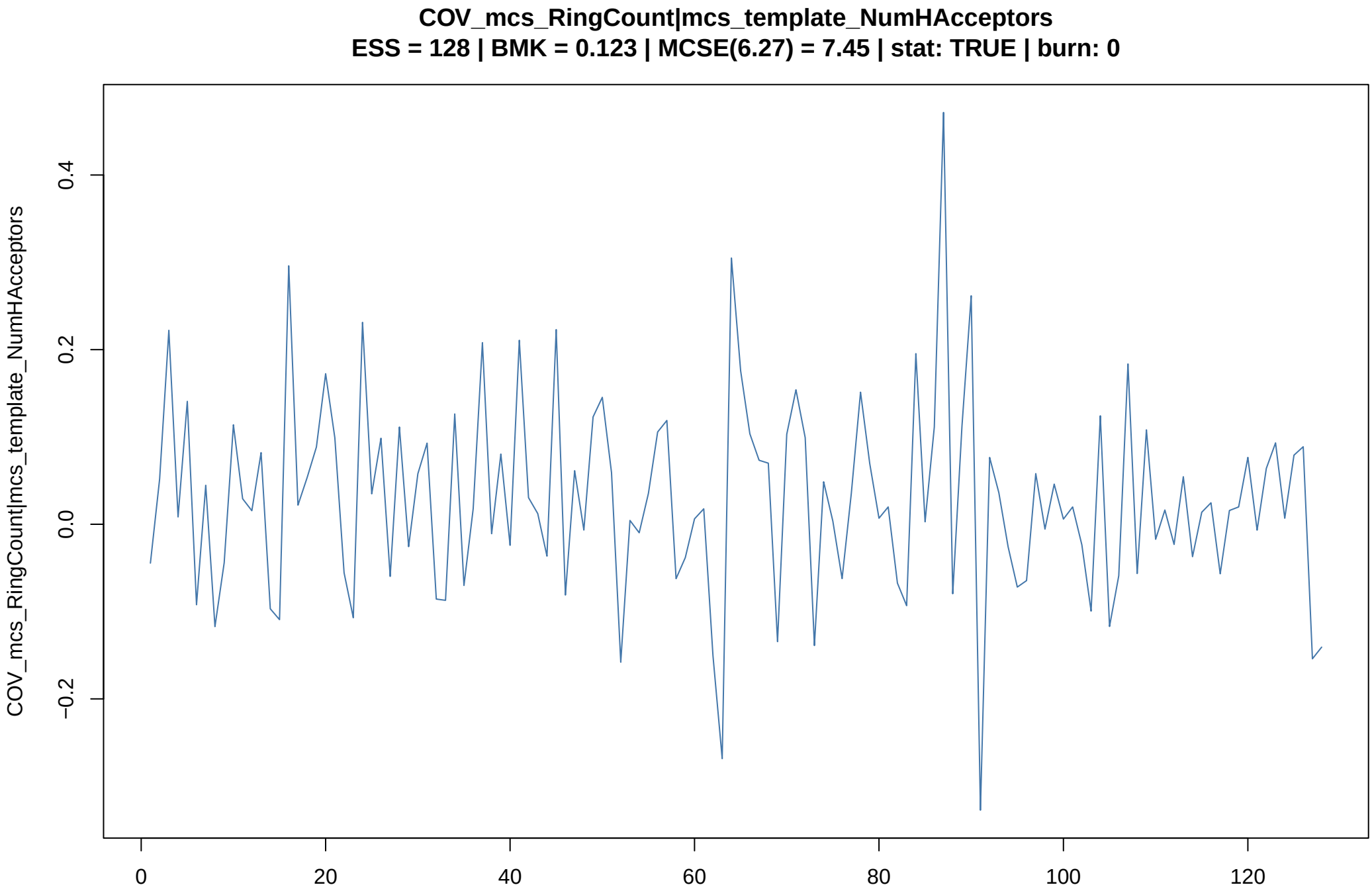

COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.147 | MCSE(6.27) = 8.57 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
0
2
4
6
8
0
20
40
60
80
100
120

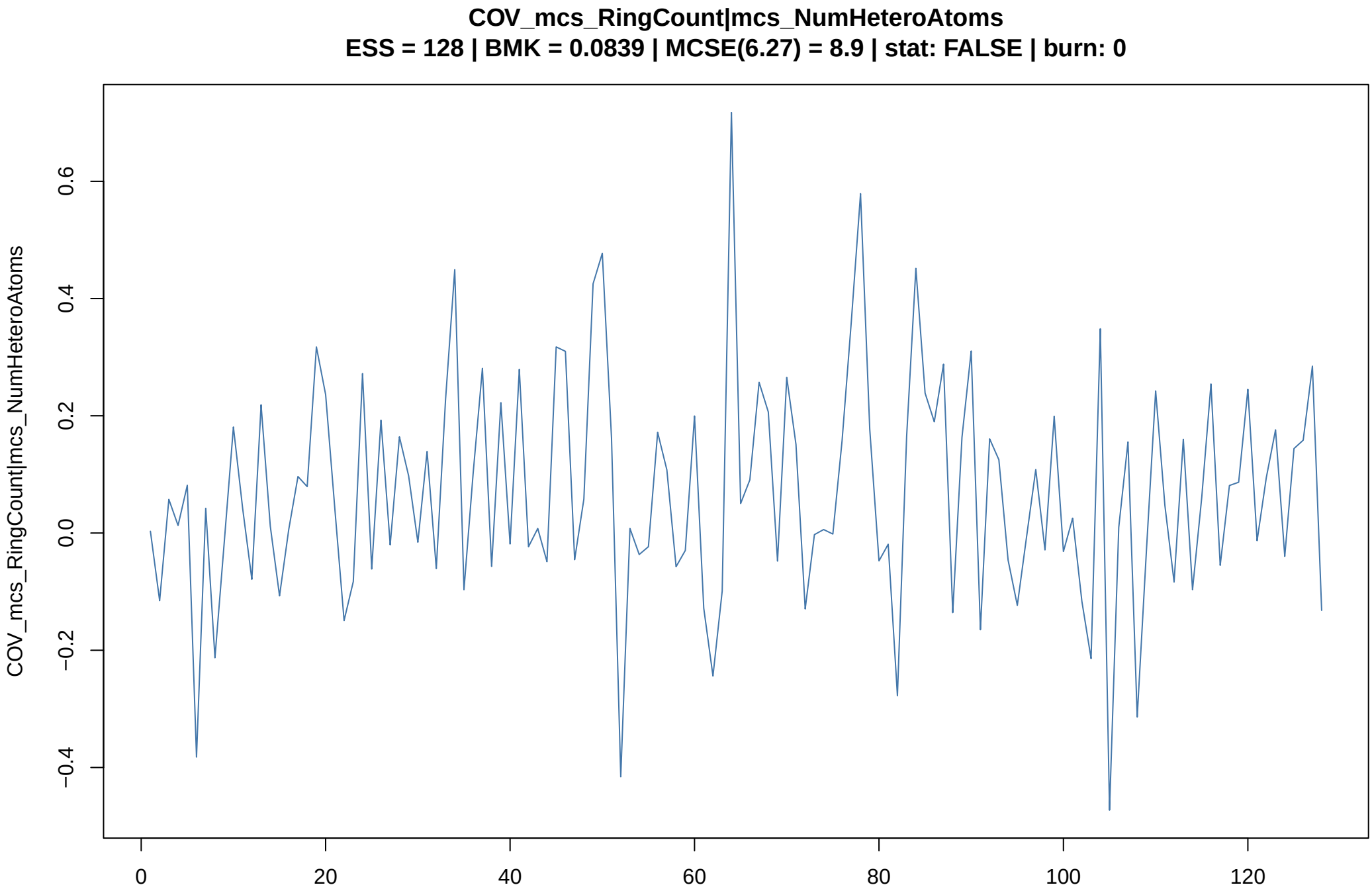

COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 128 | BMK = 0.0694 | MCSE(6.27) = 10 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
0
2
4
6
0
20
40
60
80
100
120

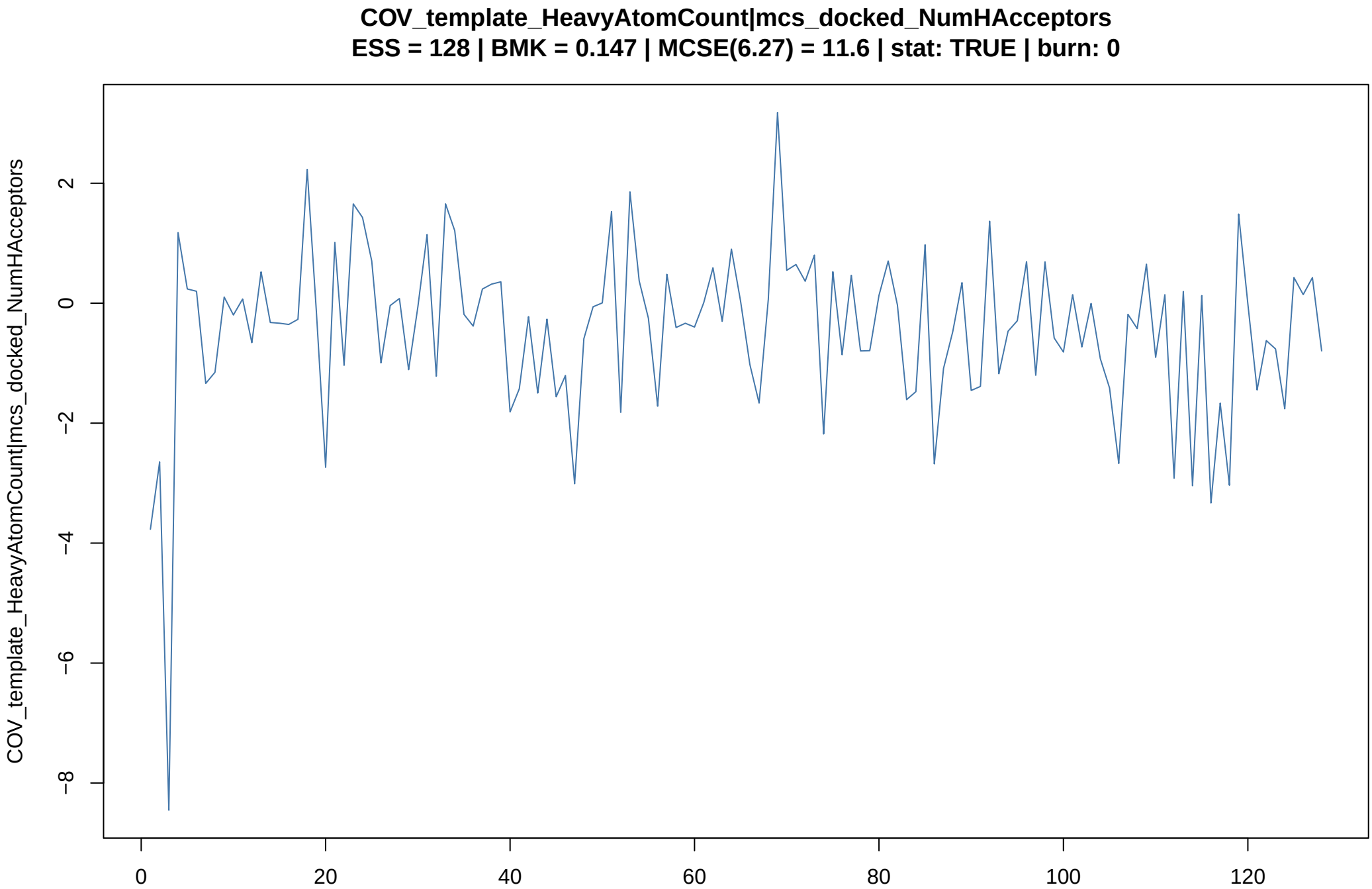

COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.098 | MCSE(6.27) = 9.4 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
0
5
10
0
20
40
60
80
100
120

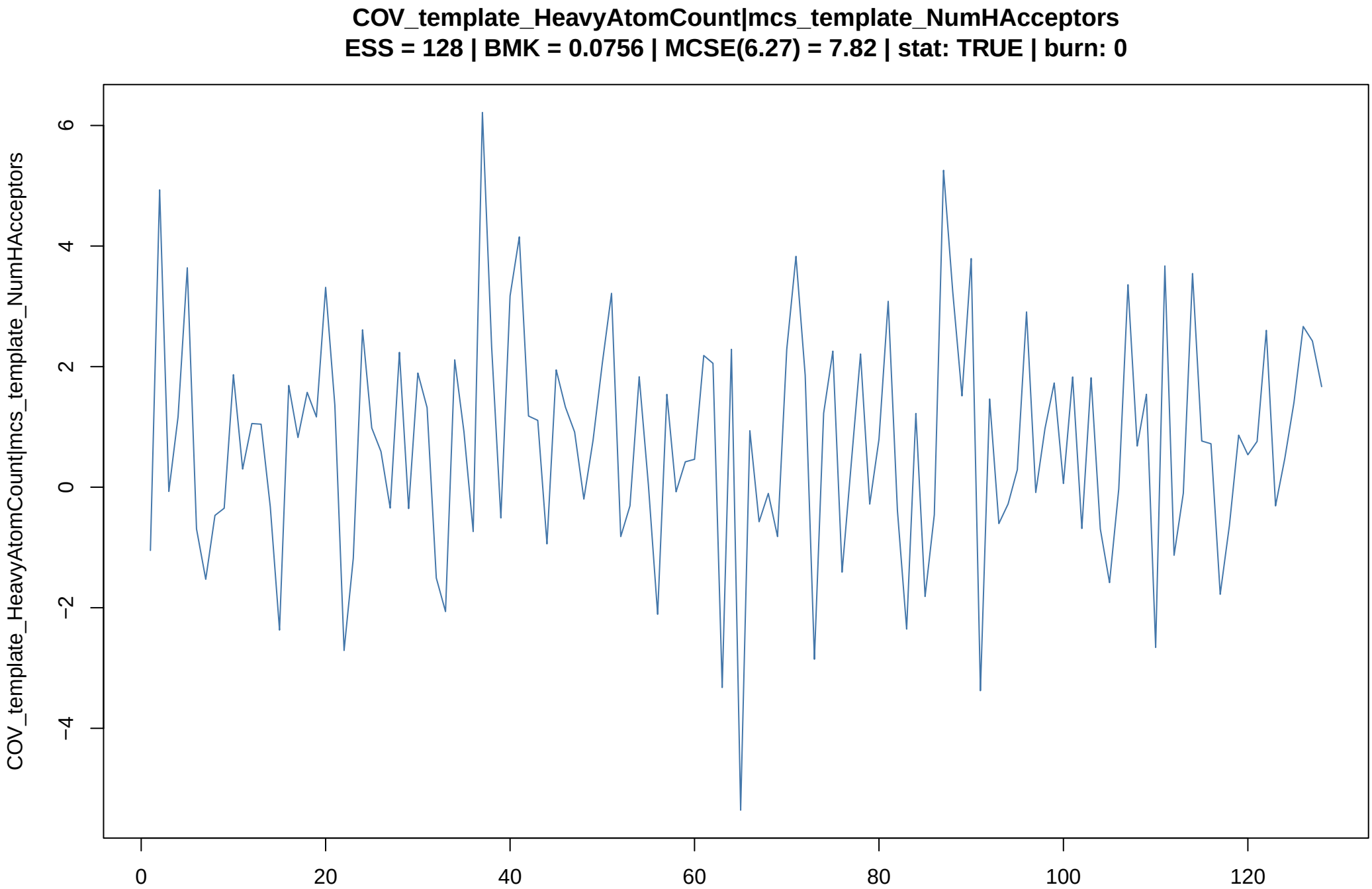

COV_mcs_RingCount|template_HeavyAtomCount
ESS = 87.6 | BMK = 0.163 | MCSE(6.27) = 12 | stat: TRUE | burn: 0
COV_mcs_RingCount|template_HeavyAtomCount
−1
0
1
2
3
0
20
40
60
80
100
120

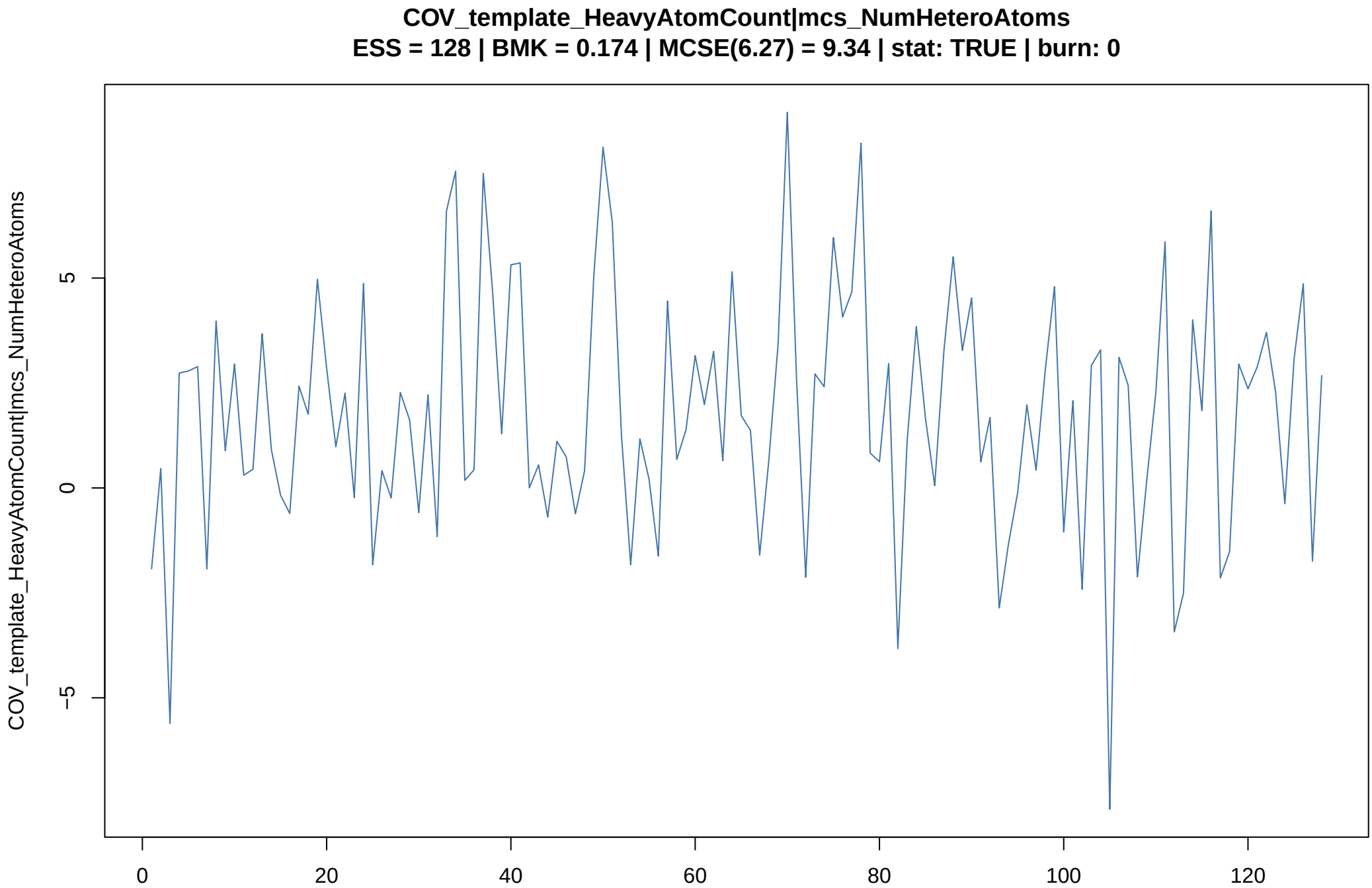

COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.121 | MCSE(6.27) = 8.64 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_docked_NumHAcceptors
0.1
0.0
−0.1
−0.2
0
20
40
60
80
100
120

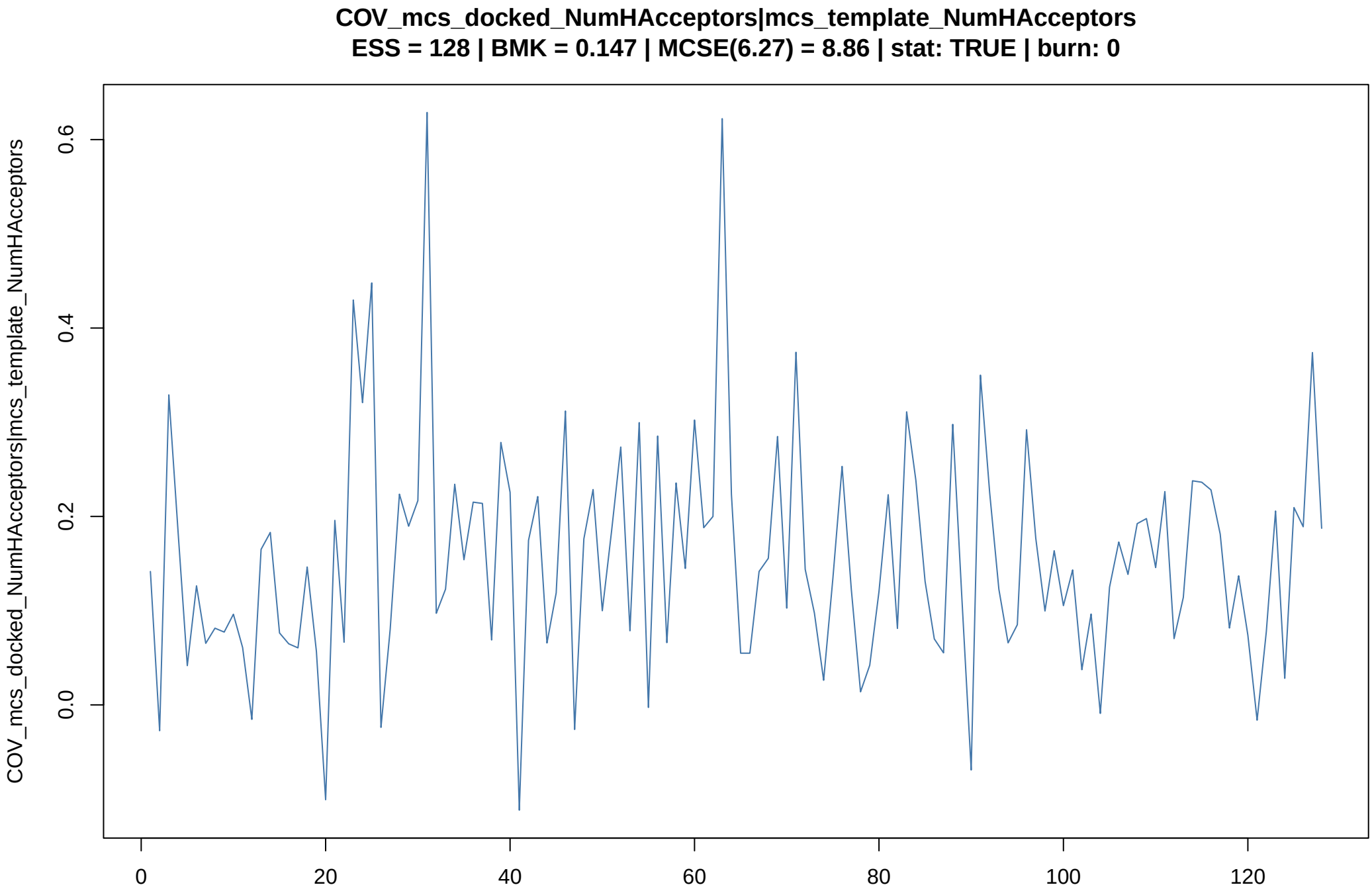

COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 128 | BMK = 0.123 | MCSE(6.27) = 7.45 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_template_NumHAcceptors
0.4
0.2
0.0
−0.2
0
20
40
60
80
100
120

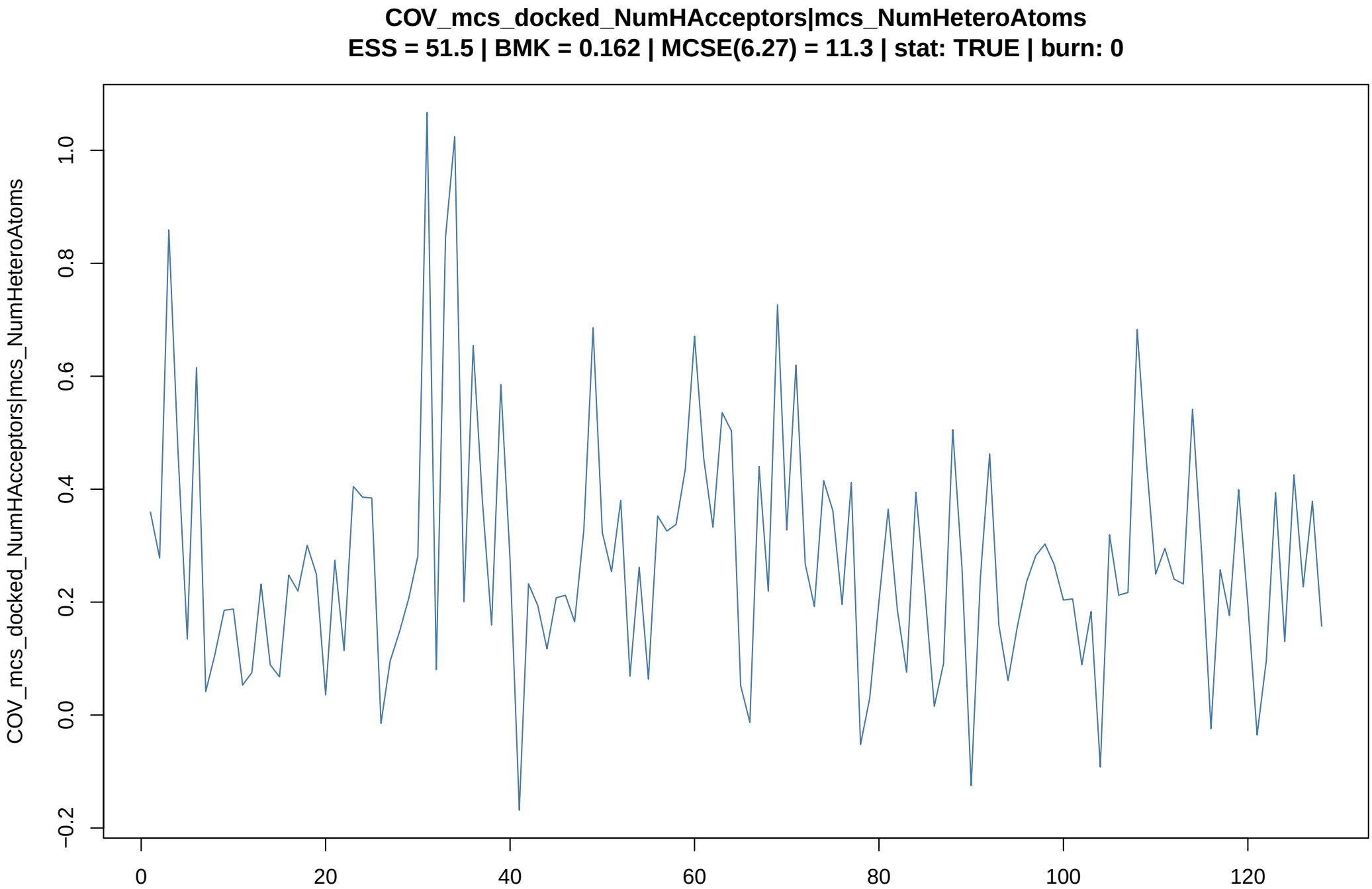

COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.0839 | MCSE(6.27) = 8.9 | stat: FALSE | burn: 0
COV_mcs_RingCount|mcs_NumHeteroAtoms
−0.4
−0.2
0.0
0.2
0.4
0.6
0
20
40
60
80
100
120

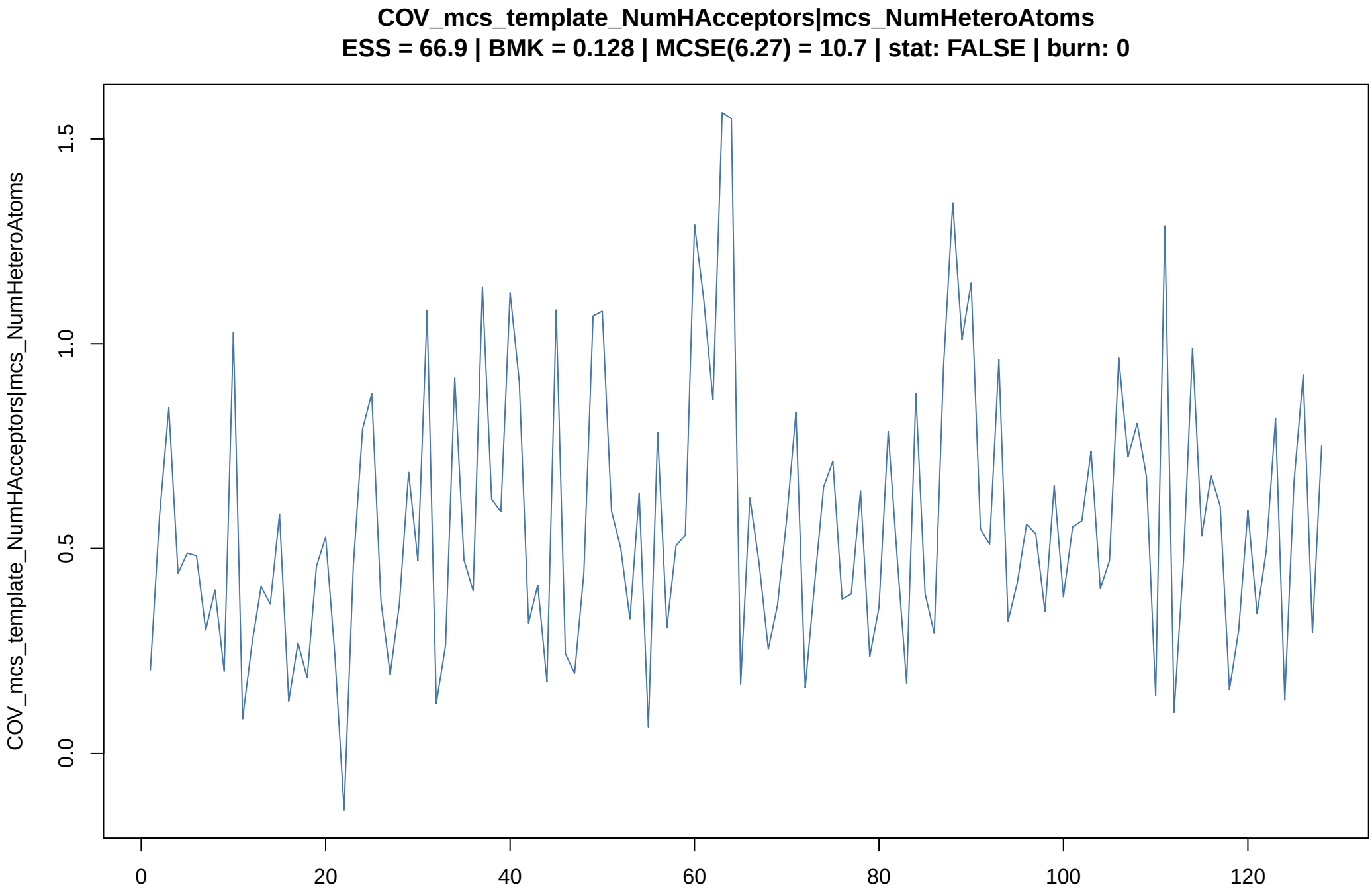

COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.147 | MCSE(6.27) = 11.6 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
2
0
−2
−4
−6
−8
0
20
40
60
80
100
120


COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 128 | BMK = 0.0756 | MCSE(6.27) = 7.82 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
6
4
2
0
−2
−4
0
20
40
60
80
100
120


COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.174 | MCSE(6.27) = 9.34 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
5
0
−5
0
20
40
60
80
100
120


COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 128 | BMK = 0.147 | MCSE(6.27) = 8.86 | stat: TRUE | burn: 0
COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
0.0
0.2
0.4
0.6
0
20
40
60
80
100
120


COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 51.5 | BMK = 0.162 | MCSE(6.27) = 11.3 | stat: TRUE | burn: 0
COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
0
20
40
60
80
100
120


COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 66.9 | BMK = 0.128 | MCSE(6.27) = 10.7 | stat: FALSE | burn: 0
COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120