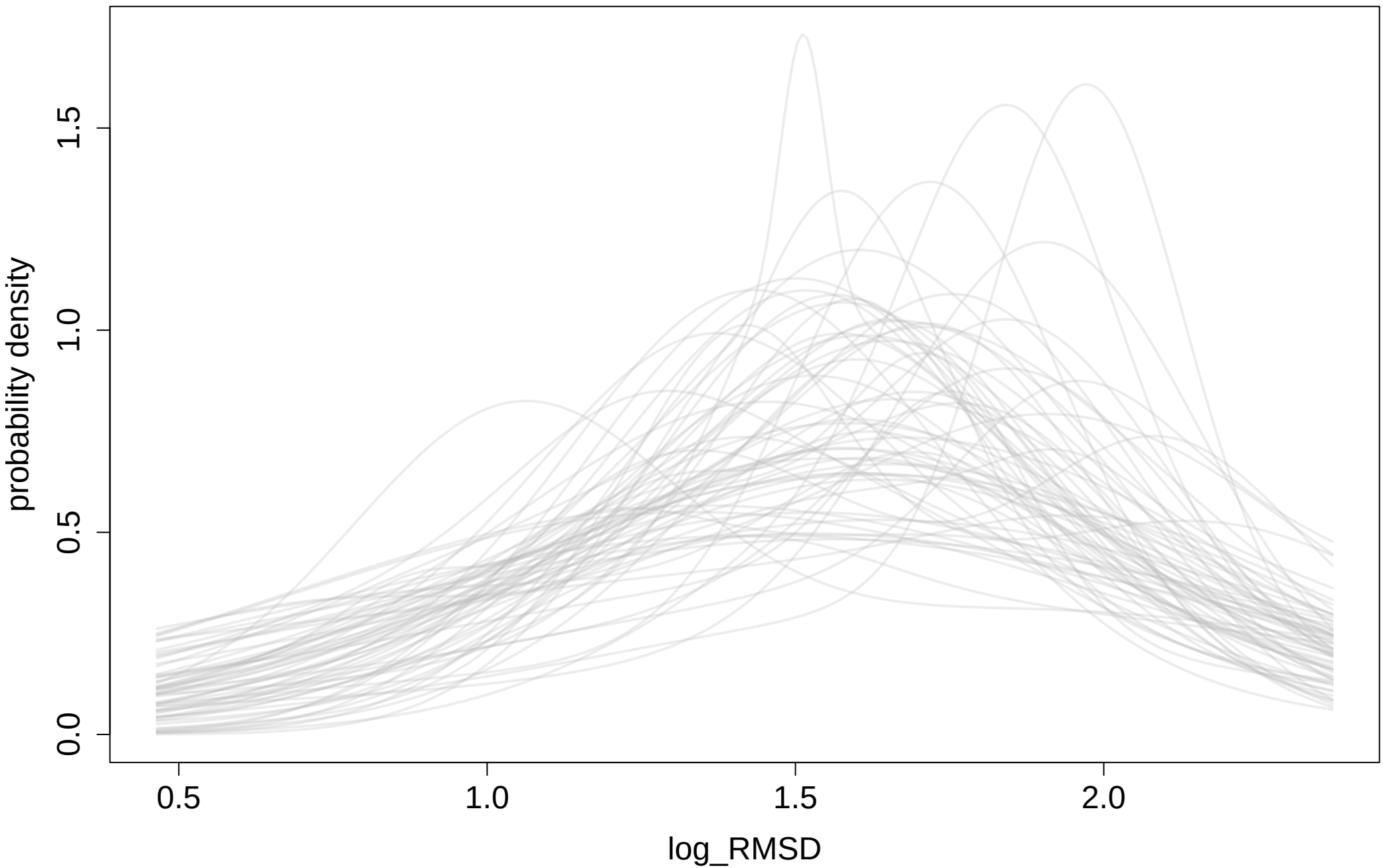
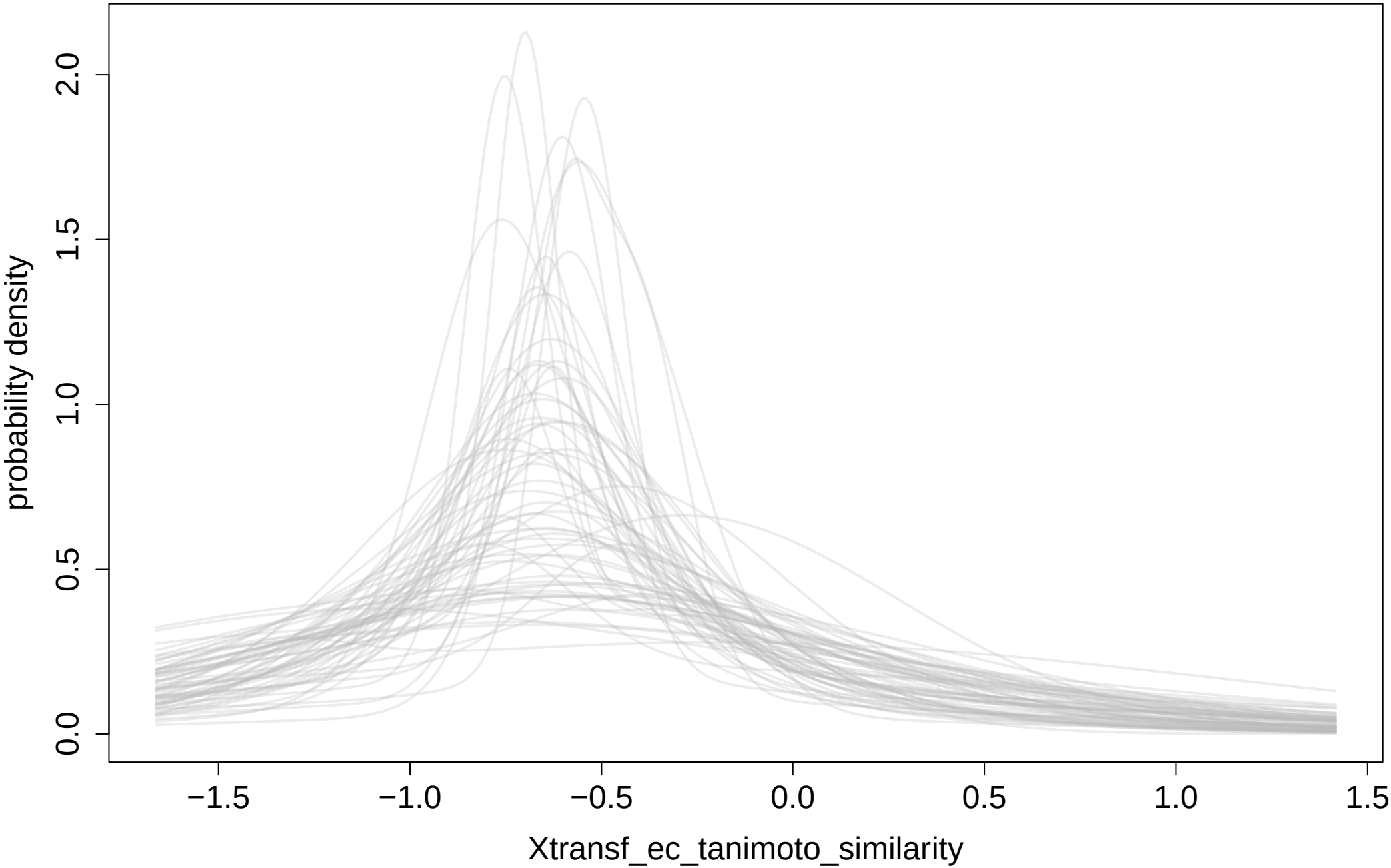
−− STATS maxD −−
min ESS = 4.92323365413773
max BMK = 1
max MCSE = 57.303652372114
all stationary: FALSE
burn: 120

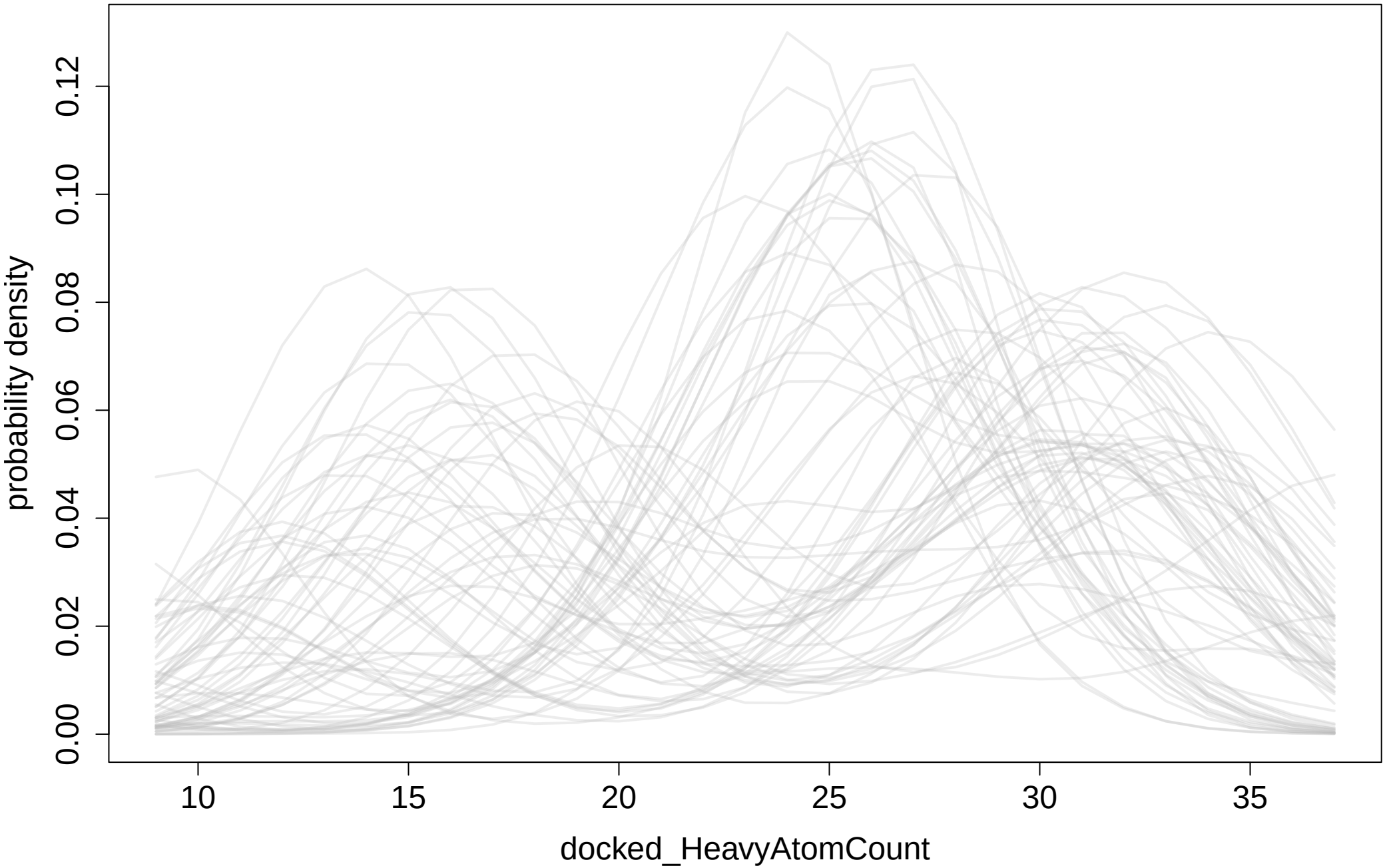
−− STATS 2D −−
min ESS = 5.05499730103278
max BMK = 0.529157187381079
max MCSE = 30.3660726896564
all stationary: FALSE
burn: 120

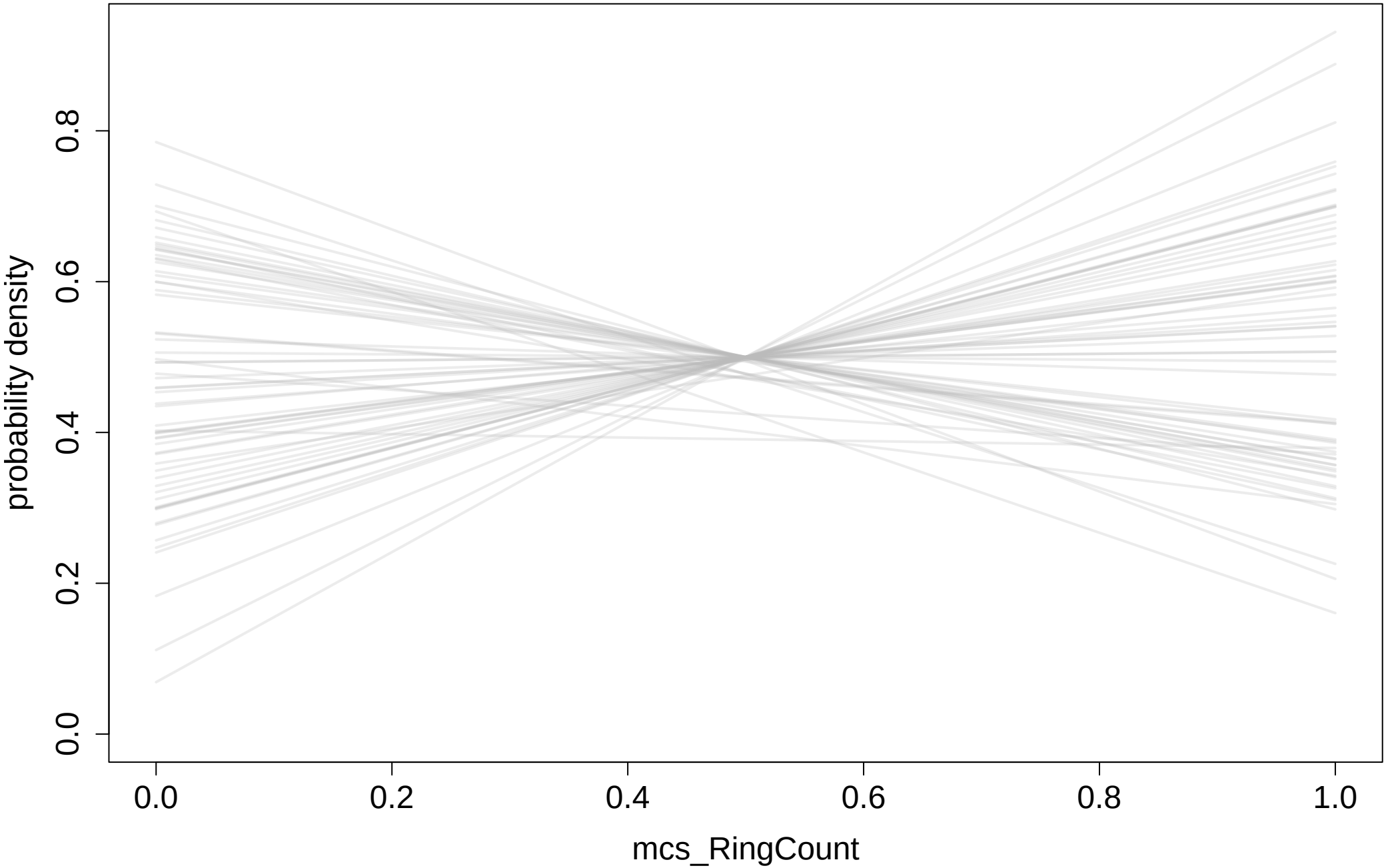
−− STATS 1D −−
min ESS = 2.2204604925031e−16
max BMK = 0.507247904893242
max MCSE = NaN
all stationary: FALSE
burn: 120

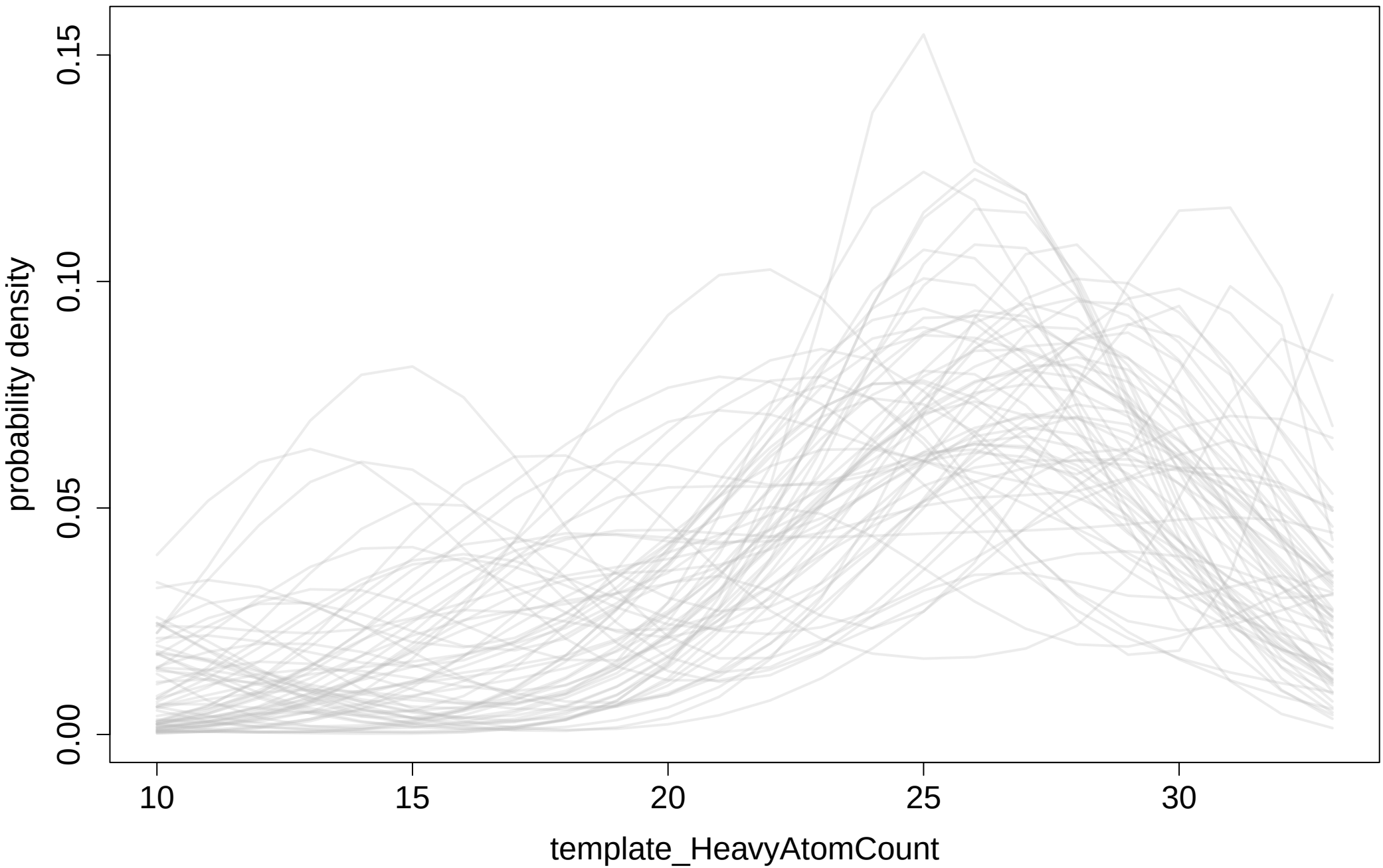
Occupied clusters: 4 of 4
LL: −98.4 +− 11.8

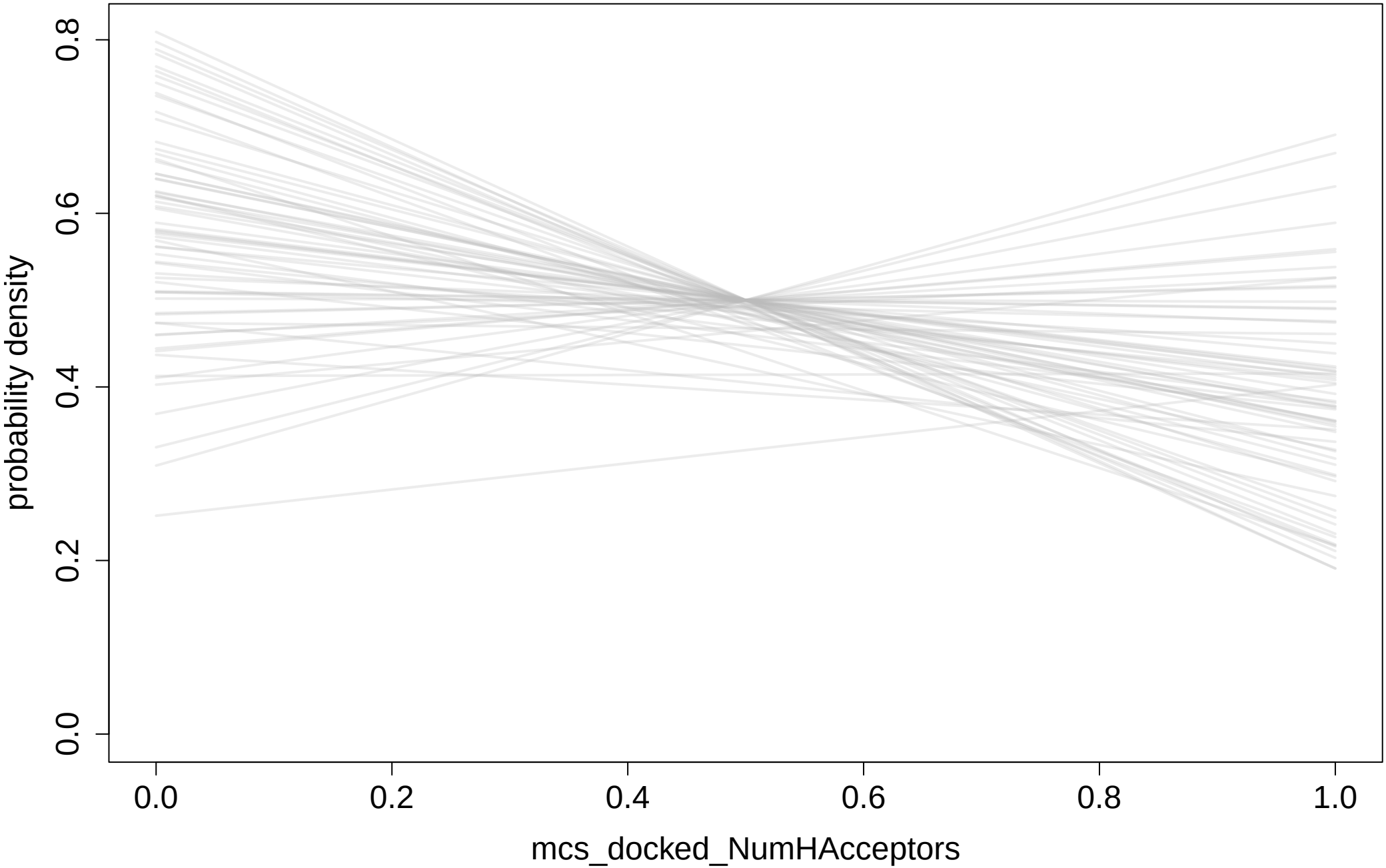

probability density
0.0
0.5
1.0
1.5
0.5
1.0
1.5
2.0
log_RMSD

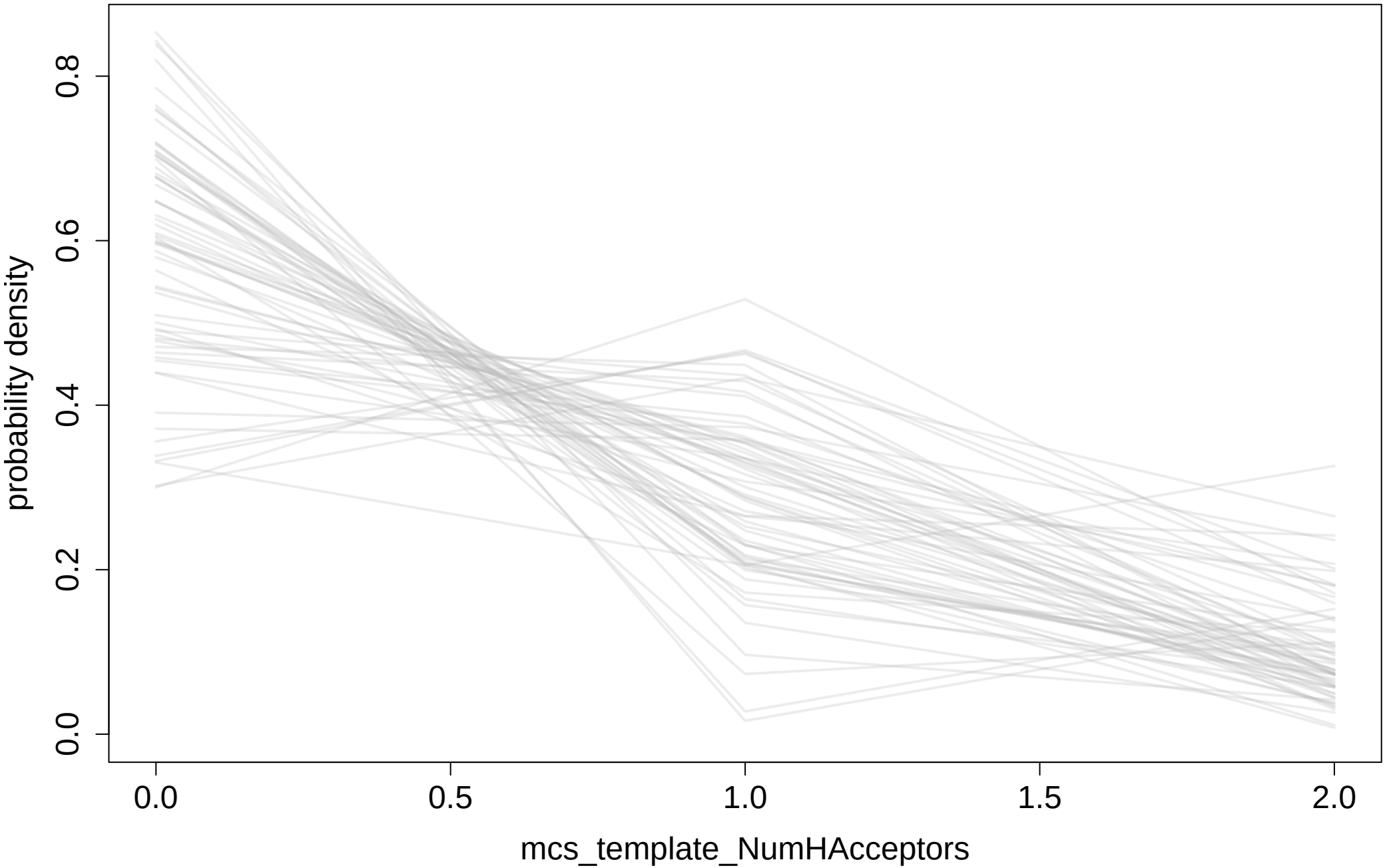

probability density
0.0
0.5
1.0
1.5
2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
Xtransf_ec_tanimoto_similarity

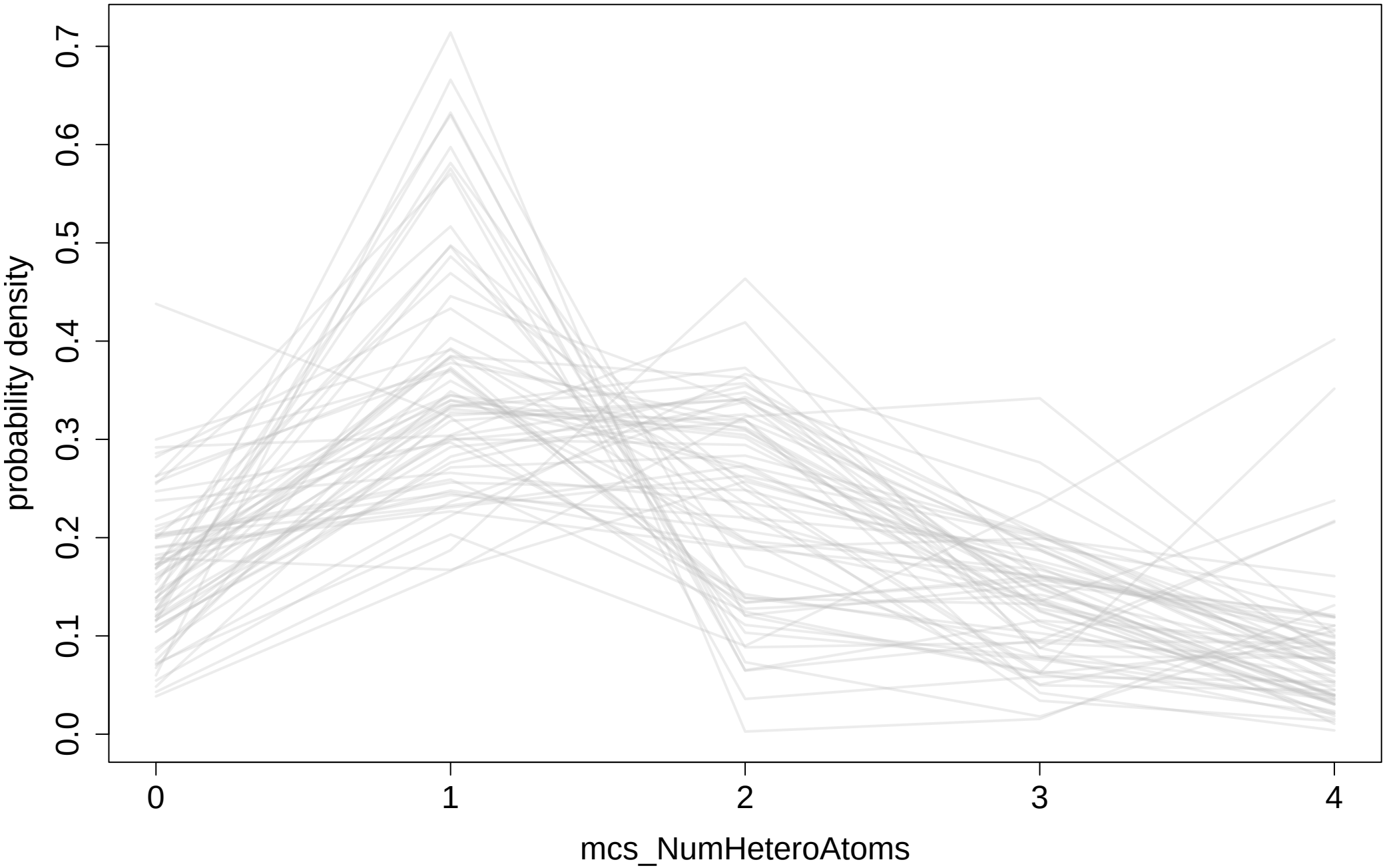

probability density
0.00
0.02
0.04
0.06
0.08
0.10
0.12
10
15
20
25
30
35
docked_HeavyAtomCount

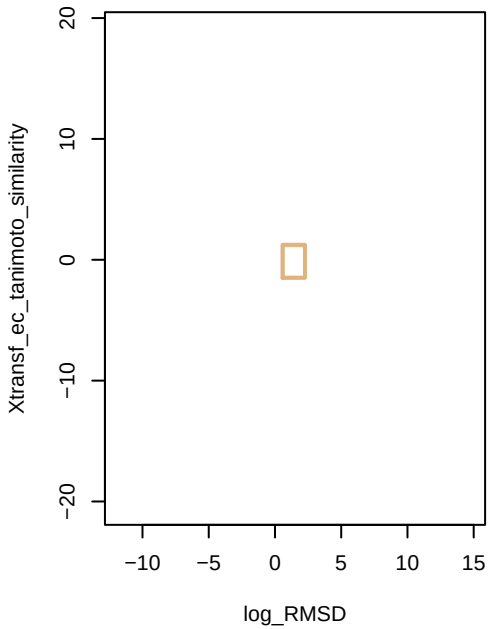

probability density
0.0
0.2
0.4
0.6
0.8
0.0
0.2
0.4
0.6
0.8
1.0
mcs_RingCount

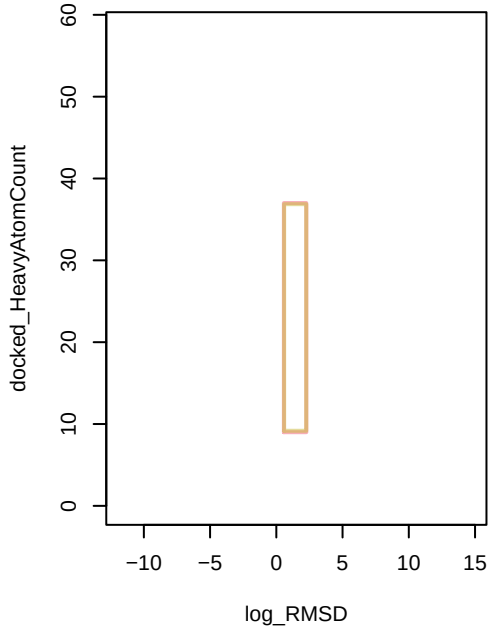

probability density
0.00
0.05
0.10
0.15
10
15
20
25
30
template_HeavyAtomCount

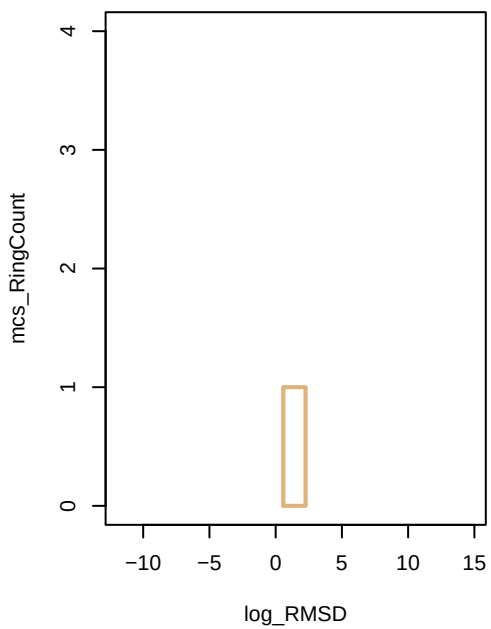

probability density
0.0
0.2
0.4
0.6
0.8
0.0
0.2
0.4
0.6
0.8
1.0
mcs_docked_NumHAcceptors

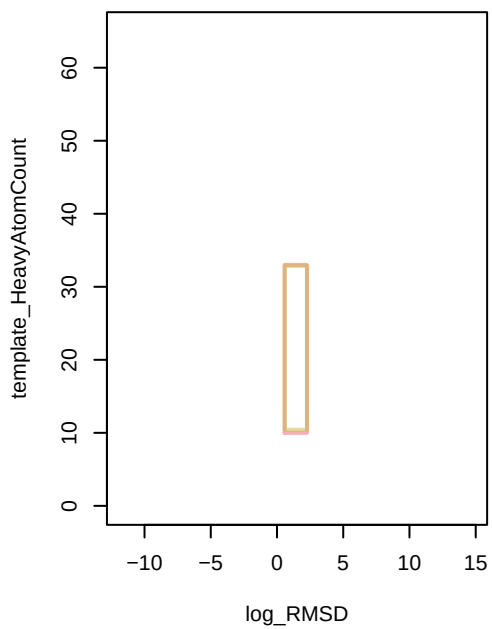

probability density
0.0
0.2
0.4
0.6
0.8
0.0
0.5
1.0
1.5
2.0
mcs_template_NumHAcceptors

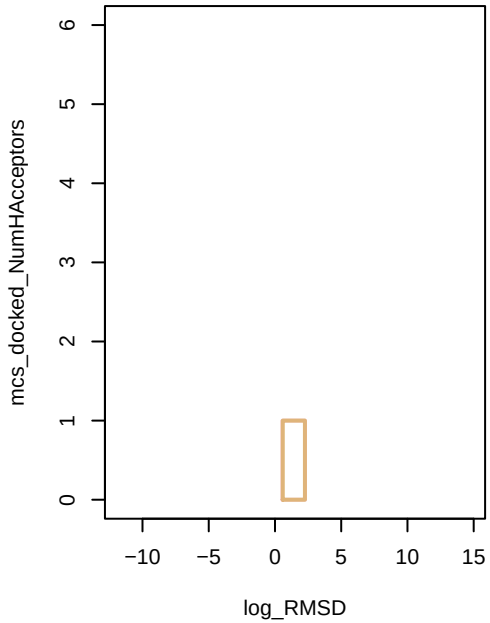

probability density
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
1
2
3
4
mcs_NumHeteroAtoms

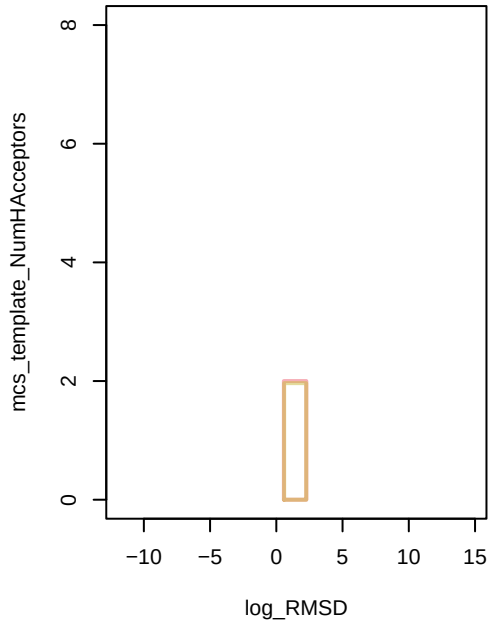

Xtransf_ec_tanimoto_similarity
20
10
0
−10
−20
−10
−5
0
5
10
15
log_RMSD

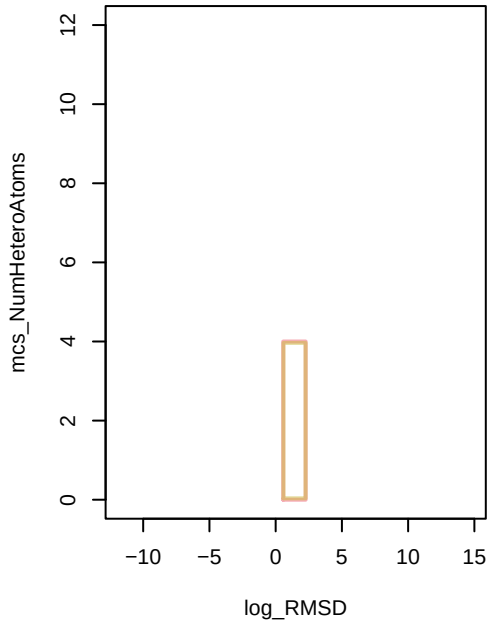

docked_HeavyAtomCount
60
50
40
30
20
10
0
−10
−5
0
5
10
15
log_RMSD

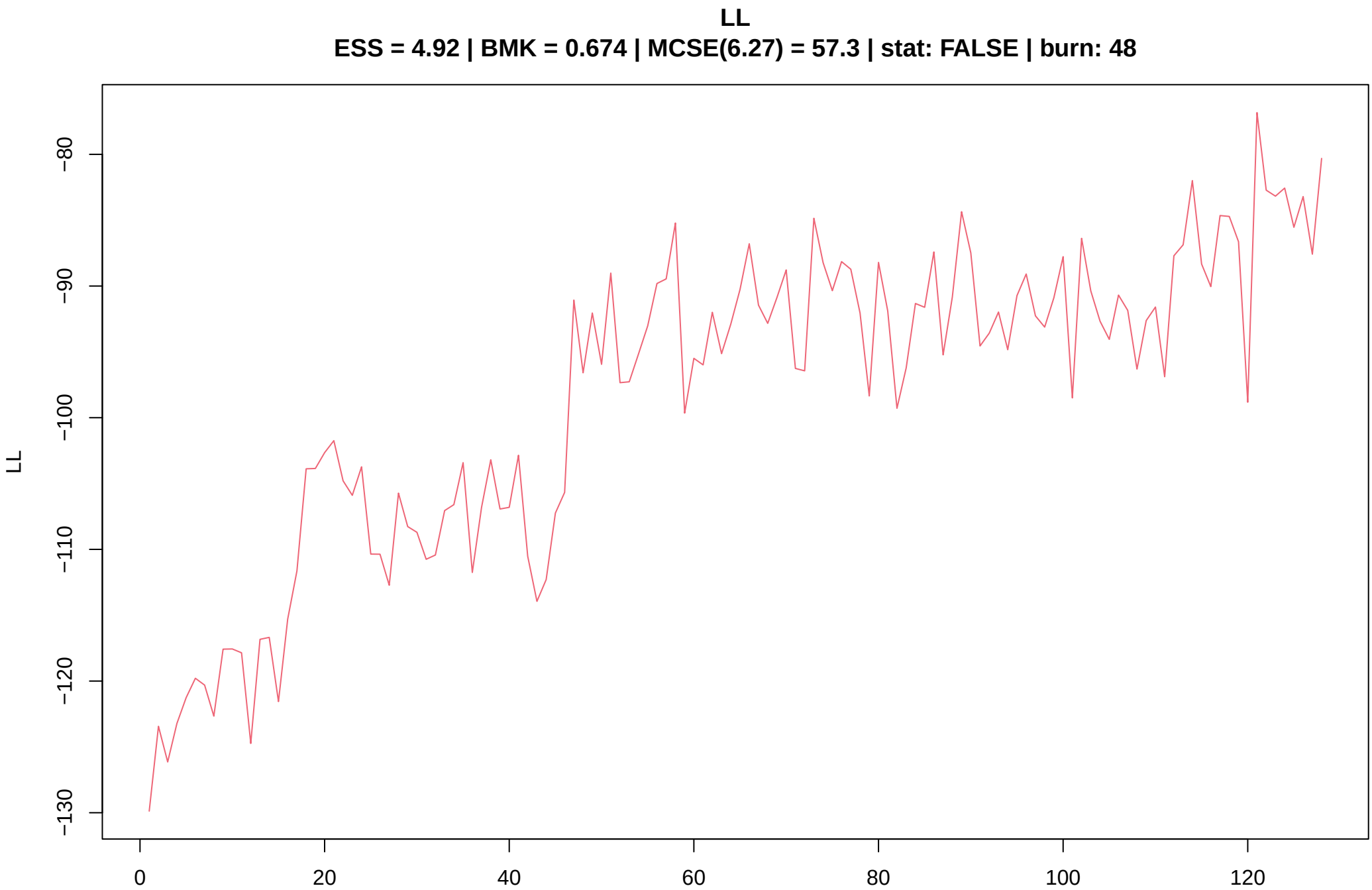

mcs_RingCount
4
3
2
1
0
−10
−5
0
5
10
15
log_RMSD

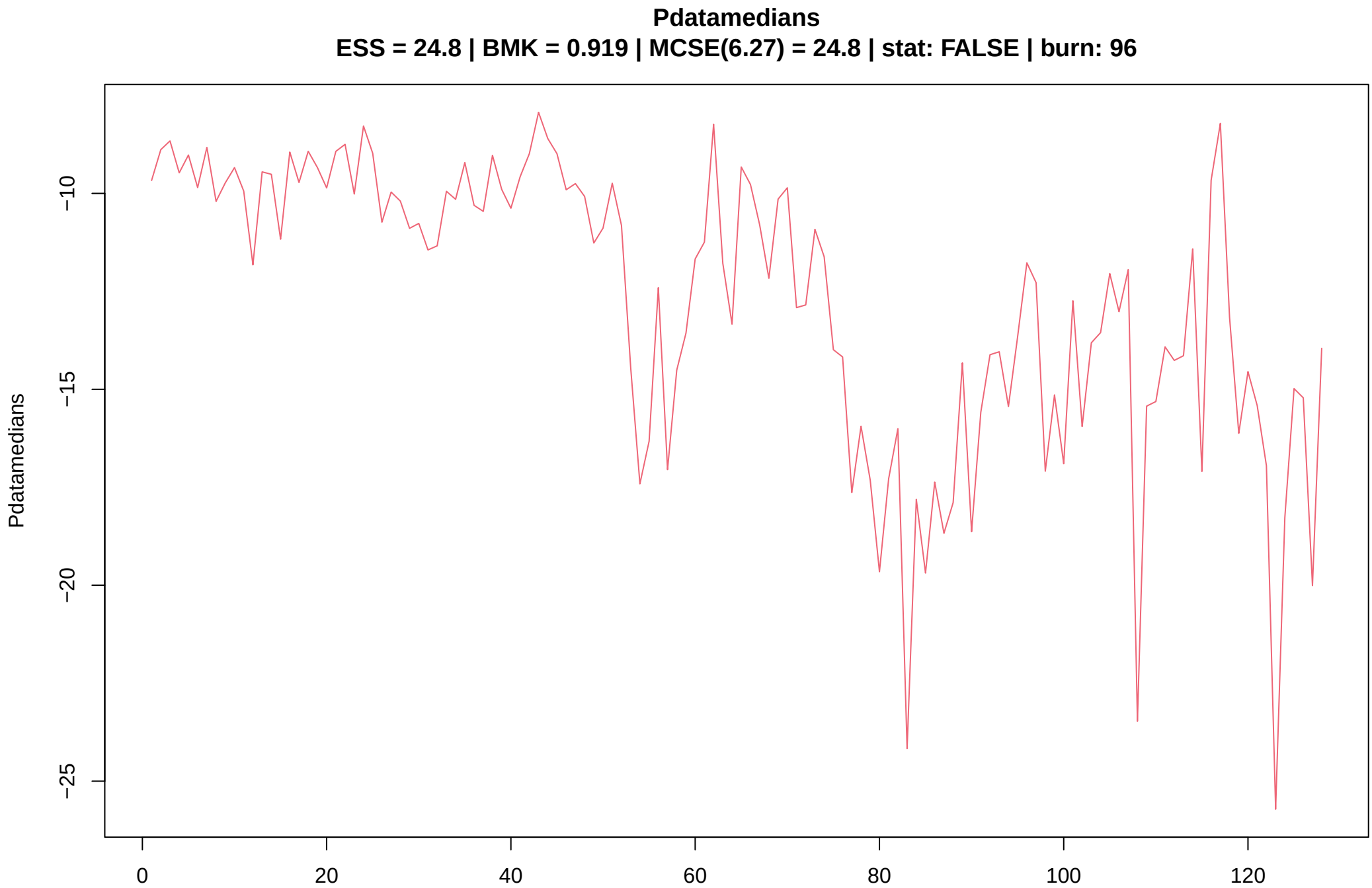

template_HeavyAtomCount
60
50
40
30
20
10
0
−10
−5
0
5
10
15
log_RMSD

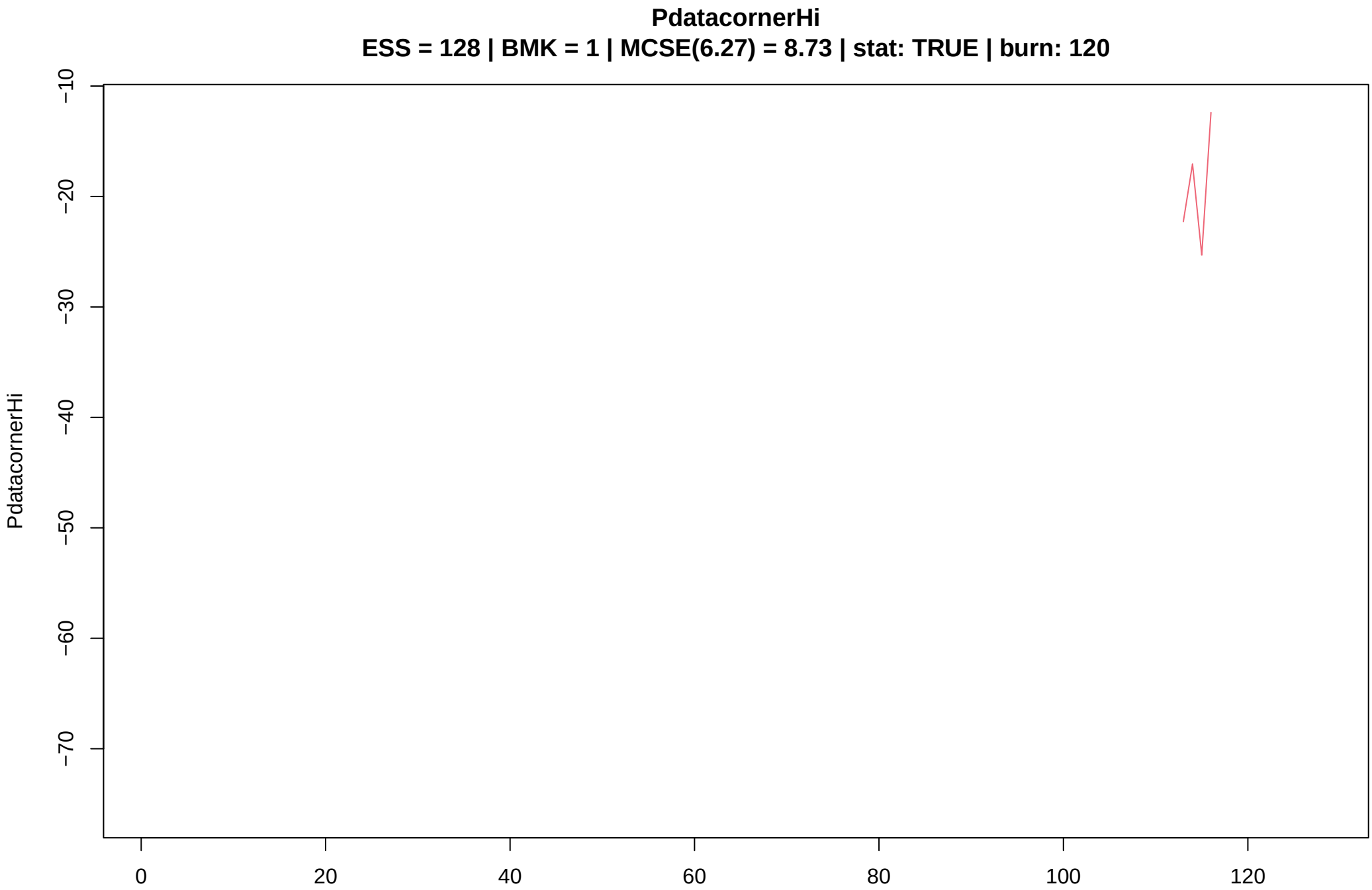

mcs_docked_NumHAcceptors
6
5
4
3
2
1
0
−10
−5
0
5
10
15
log_RMSD

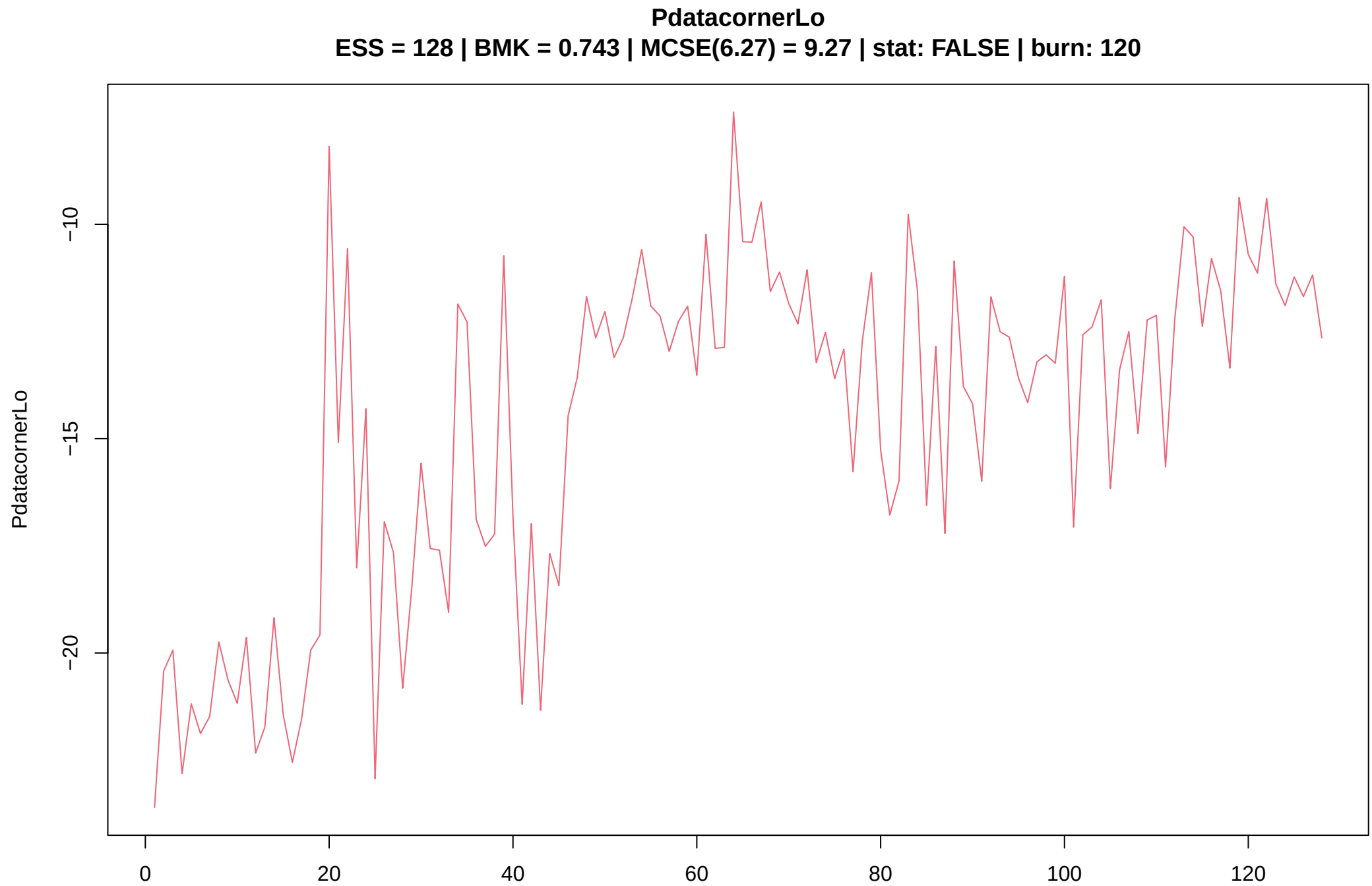

mcs_template_NumHAcceptors
8
6
4
2
0
−10
−5
0
5
10
15
log_RMSD

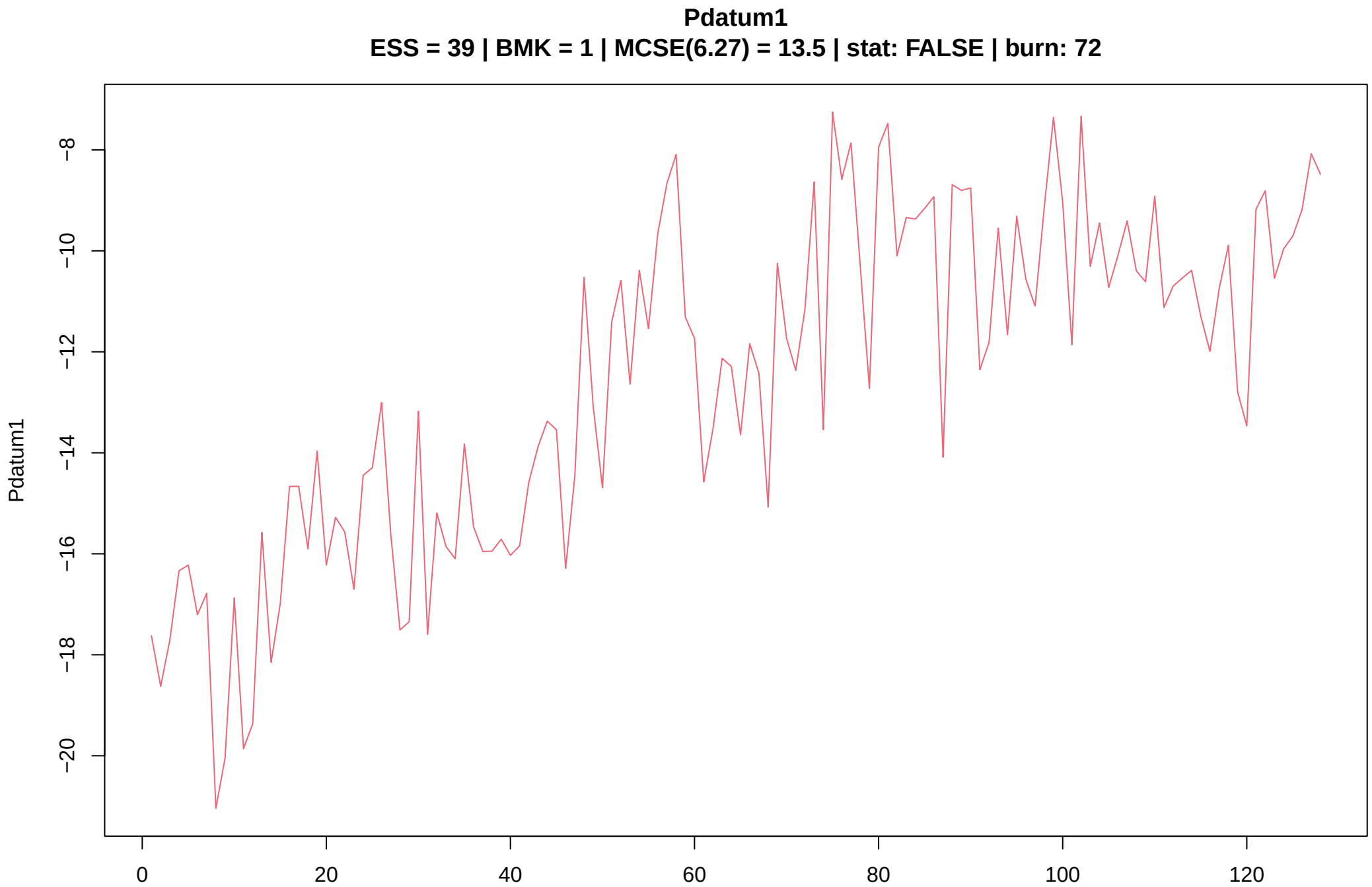

mcs_NumHeteroAtoms
12
10
8
6
4
2
0
−10
−5
0
5
10
15
log_RMSD

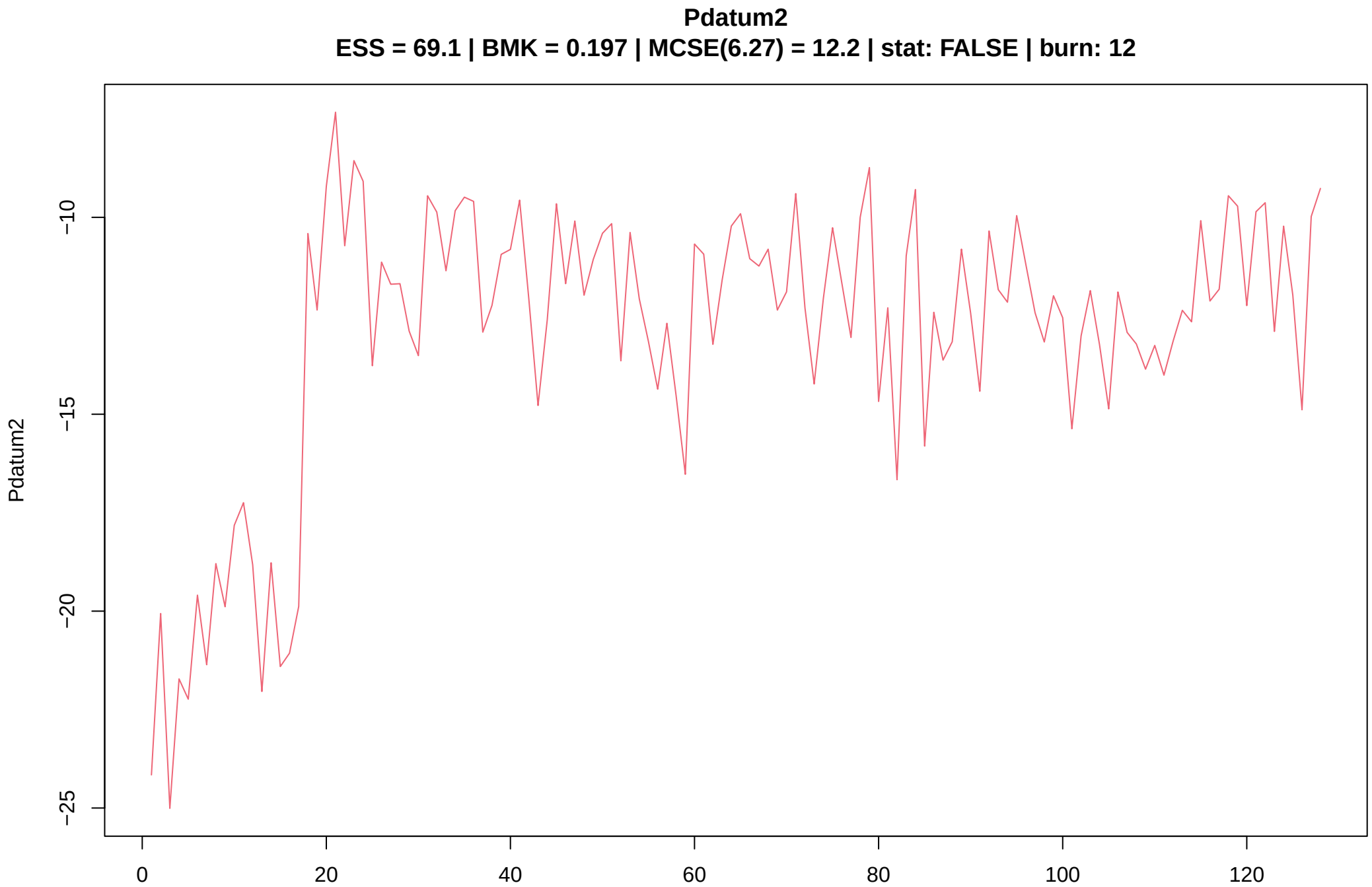

LL
ESS = 4.92 | BMK = 0.674 | MCSE(6.27) = 57.3 | stat: FALSE | burn: 48
LL
−80
−90
−100
−110
−120
−130
0
20
40
60
80
100
120

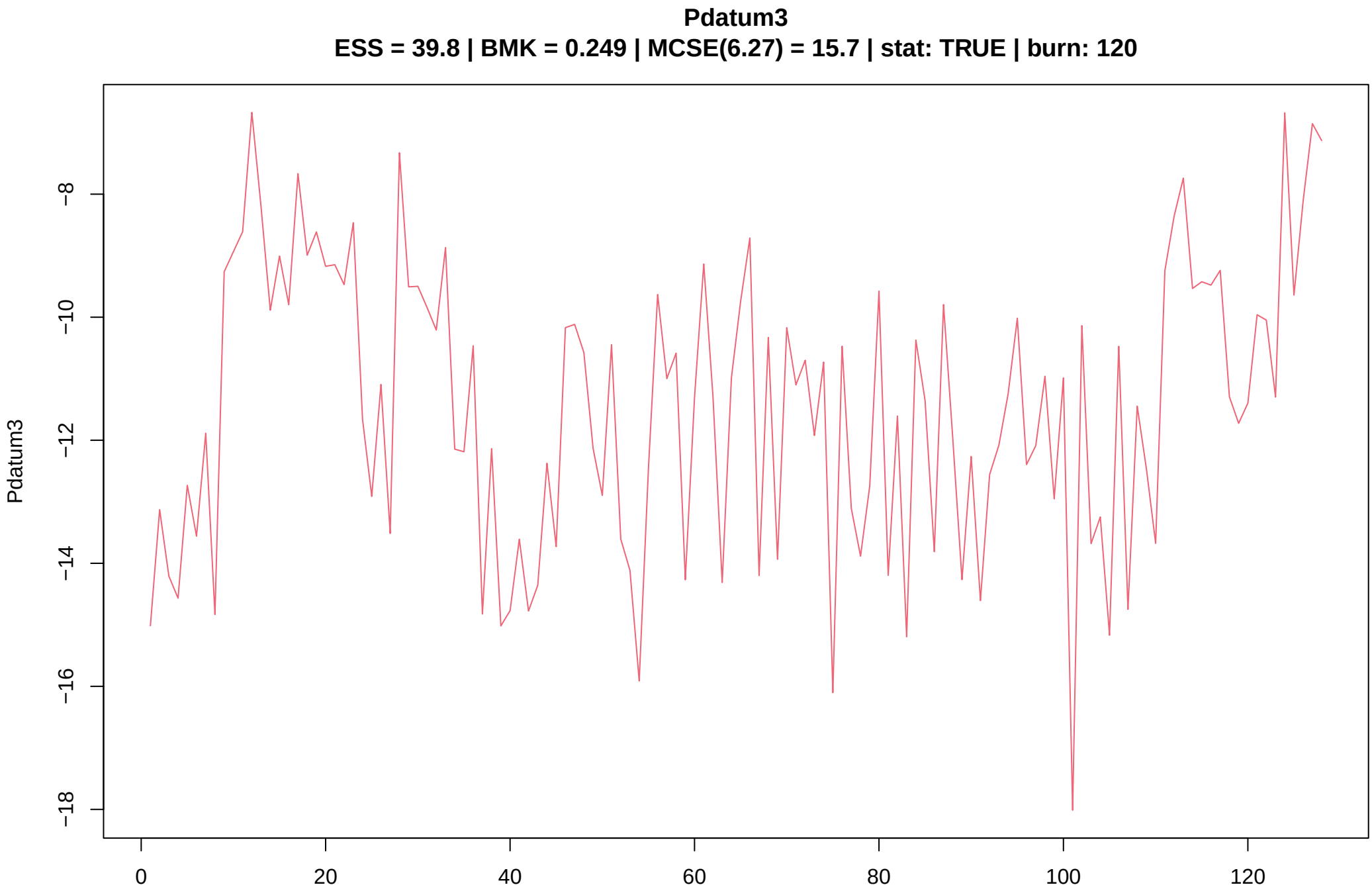

Pdatamedians
ESS = 24.8 | BMK = 0.919 | MCSE(6.27) = 24.8 | stat: FALSE | burn: 96
Pdatamedians
−10
−15
−20
−25
0
20
40
60
80
100
120

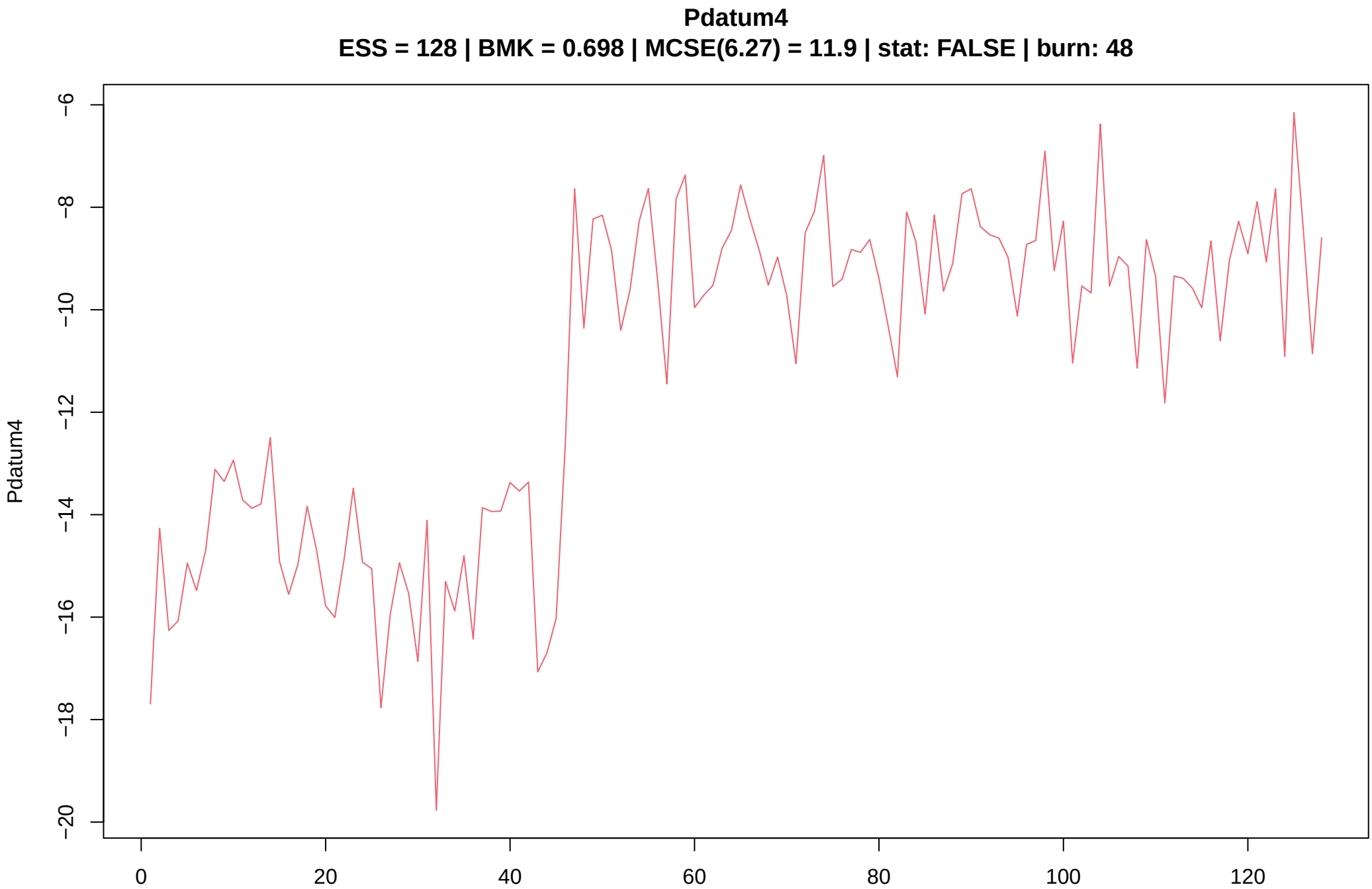

PdatacornerHi
ESS = 128 | BMK = 1 | MCSE(6.27) = 8.73 | stat: TRUE | burn: 120
PdatacornerHi
−10
−20
−30
−40
−50
−60
−70
0
20
40
60
80
100
120

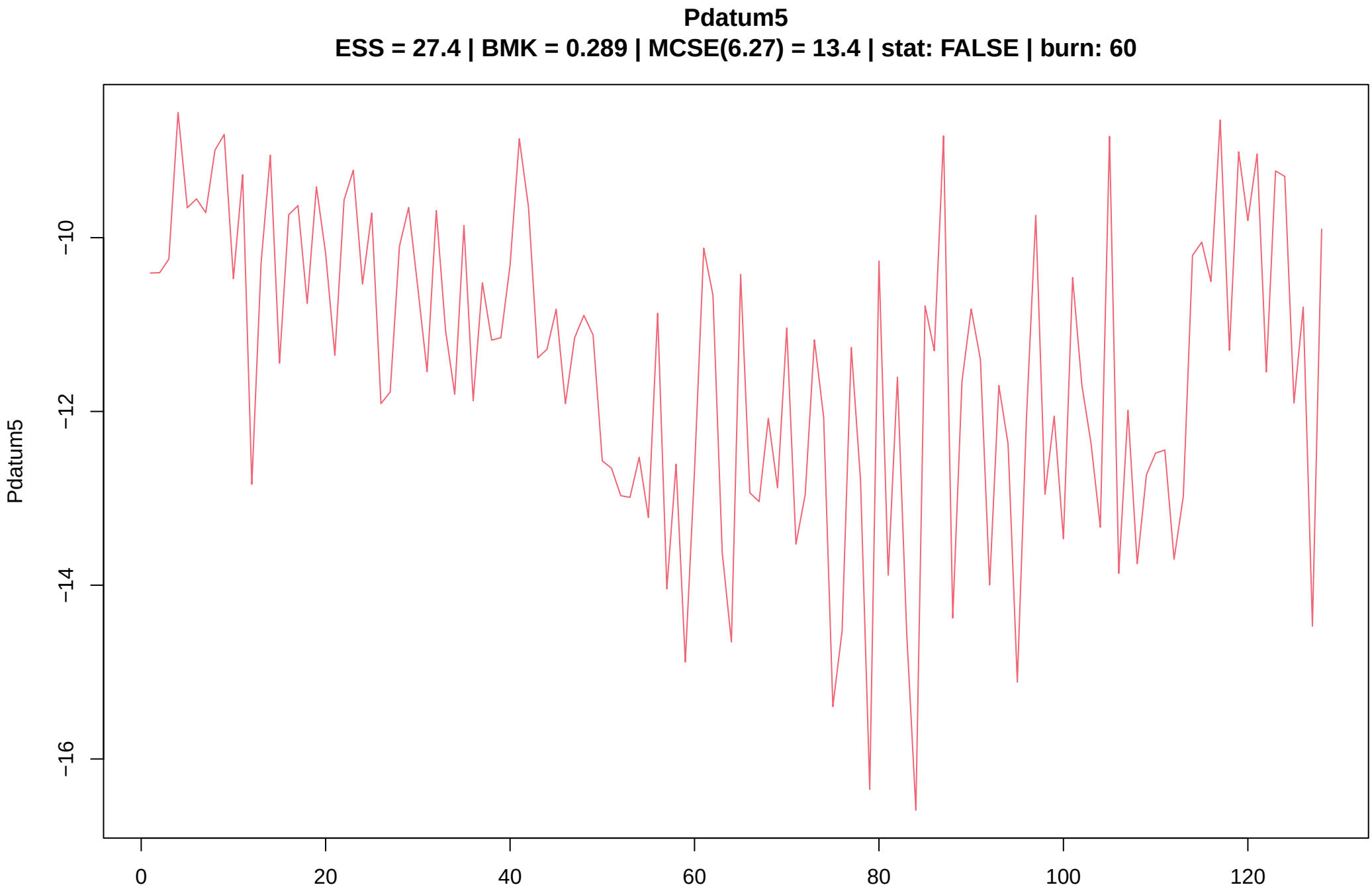

PdatacornerLo
ESS = 128 | BMK = 0.743 | MCSE(6.27) = 9.27 | stat: FALSE | burn: 120
PdatacornerLo
−10
−15
−20
0
20
40
60
80
100
120

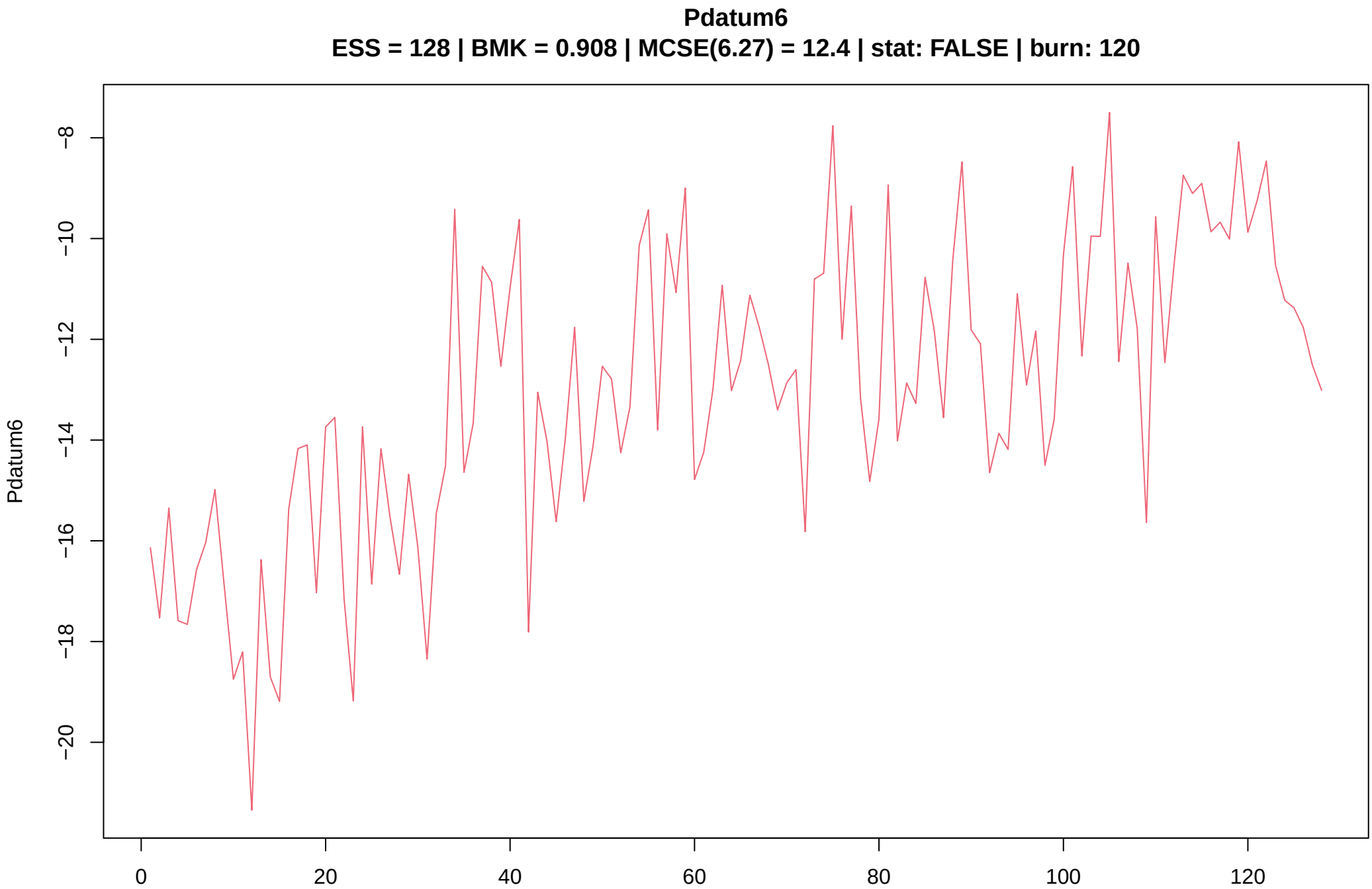

Pdatum1
ESS = 39 | BMK = 1 | MCSE(6.27) = 13.5 | stat: FALSE | burn: 72
Pdatum1
−8
−10
−12
−14
−16
−18
−20
0
20
40
60
80
100
120

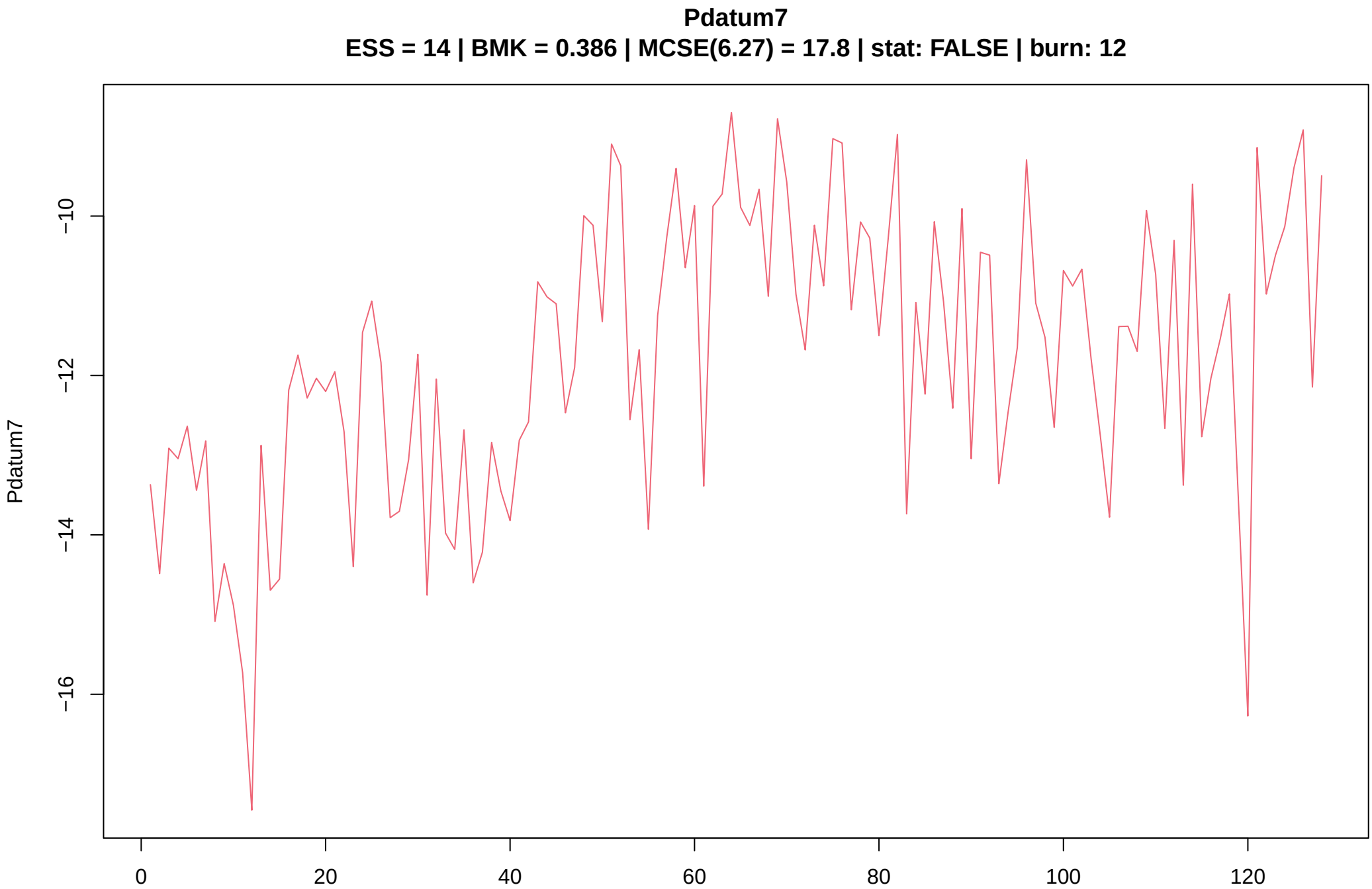

Pdatum2
ESS = 69.1 | BMK = 0.197 | MCSE(6.27) = 12.2 | stat: FALSE | burn: 12
Pdatum2
−10
−15
−20
−25
0
20
40
60
80
100
120

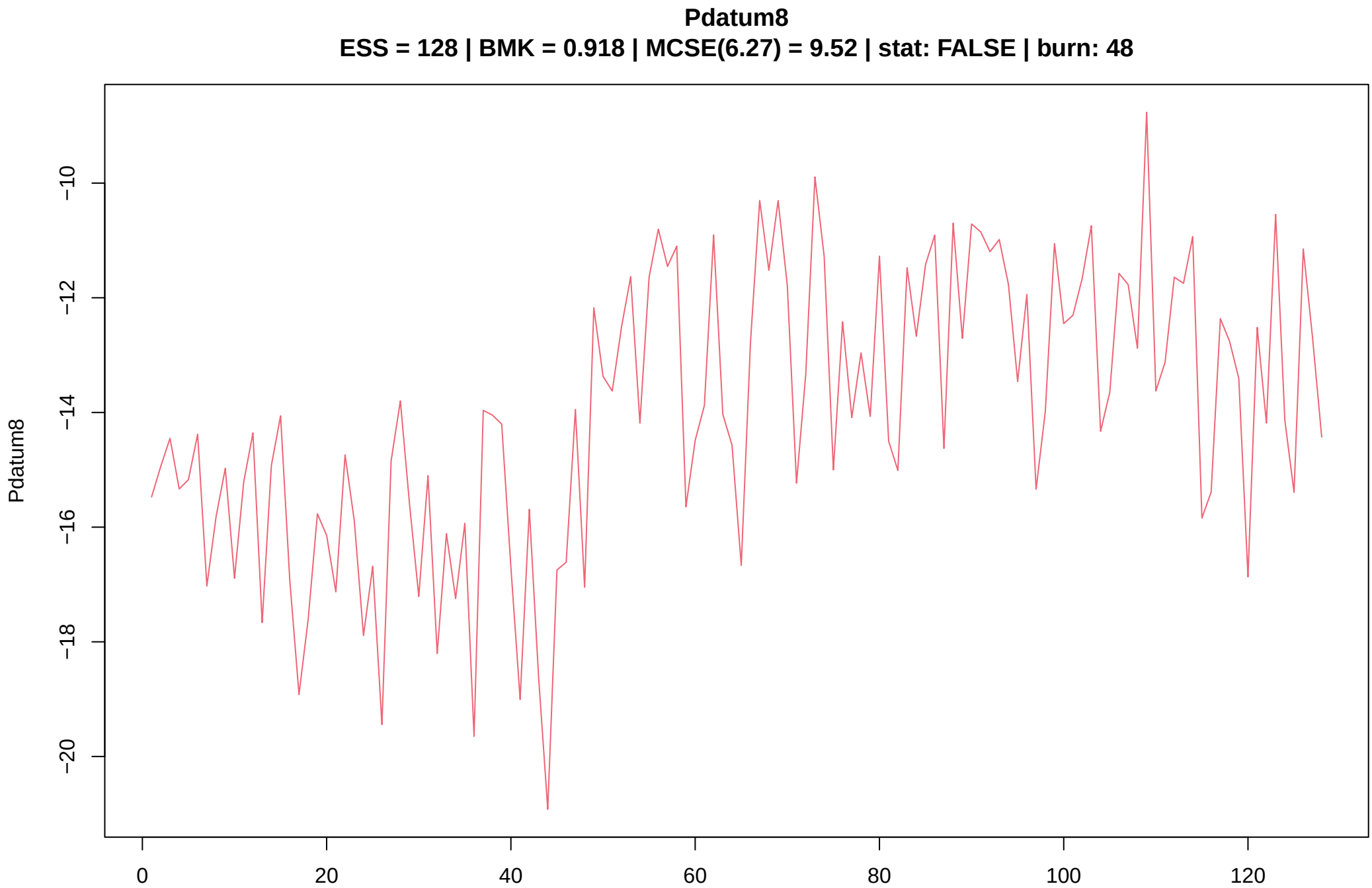

Pdatum3
ESS = 39.8 | BMK = 0.249 | MCSE(6.27) = 15.7 | stat: TRUE | burn: 120
Pdatum3
−8
−10
−12
−14
−16
−18
0
20
40
60
80
100
120

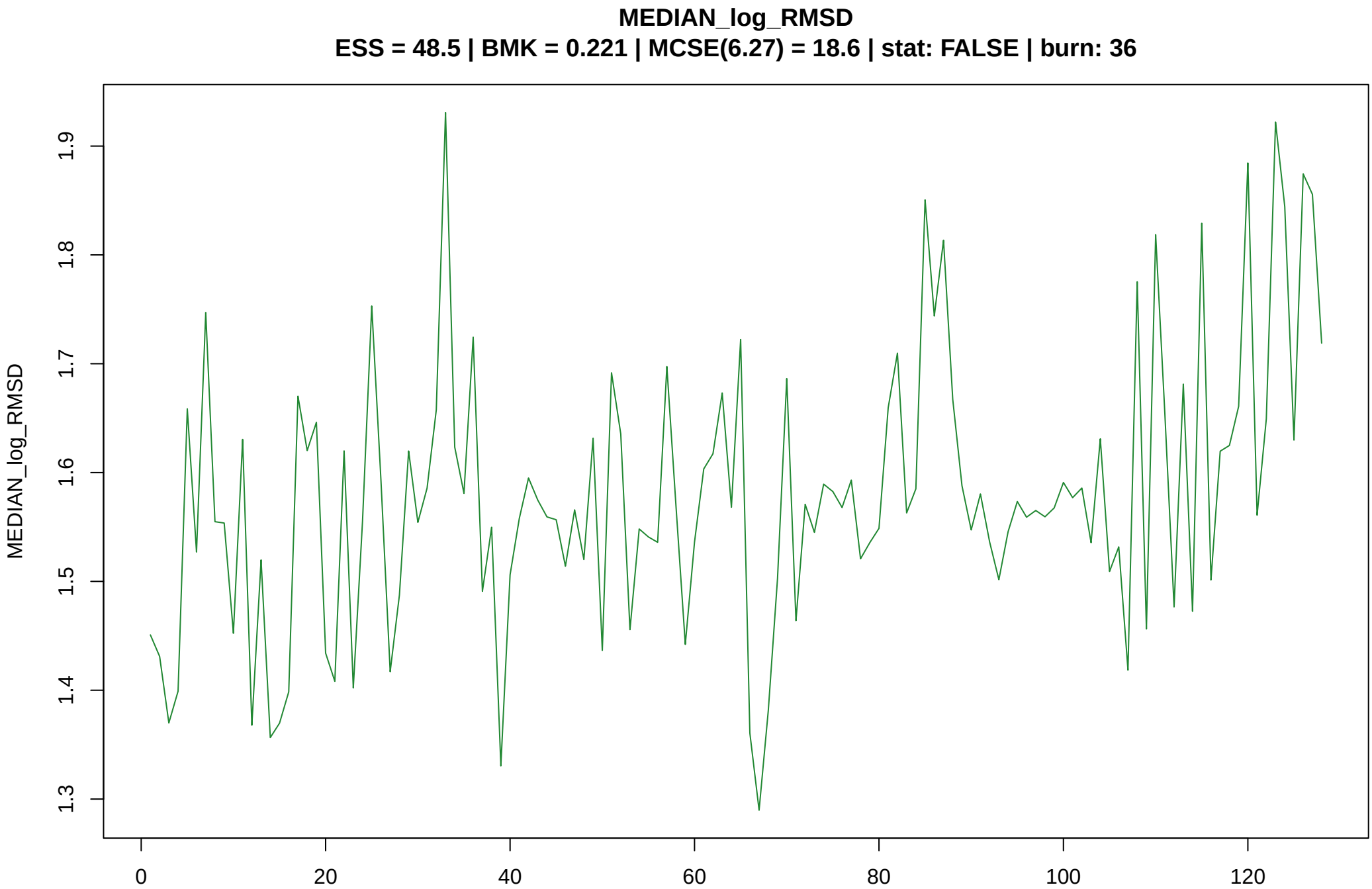

Pdatum4
ESS = 128 | BMK = 0.698 | MCSE(6.27) = 11.9 | stat: FALSE | burn: 48
Pdatum4
−6
−8
−10
−12
−14
−16
−18
−20
0
20
40
60
80
100
120

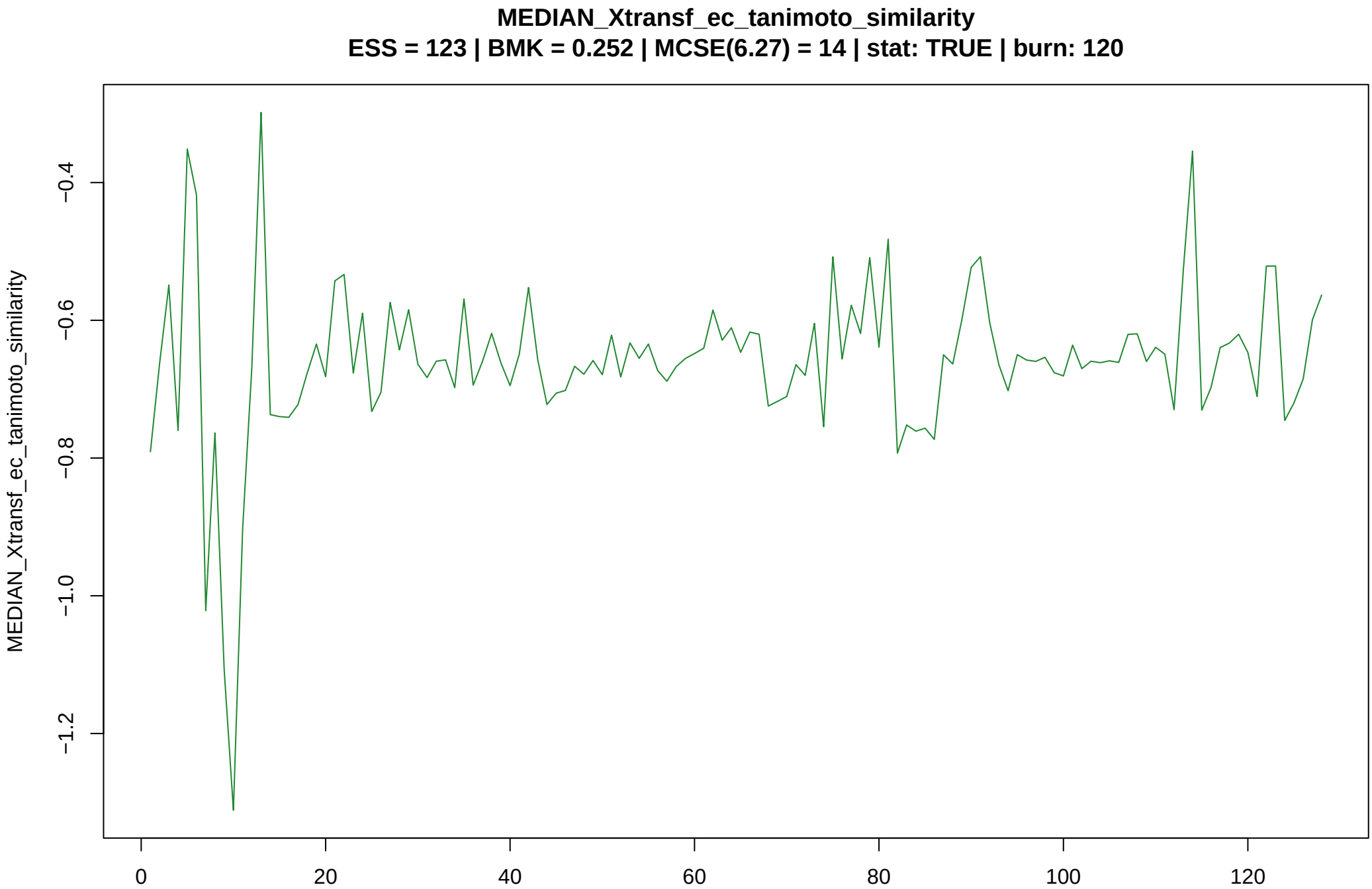

Pdatum5
ESS = 27.4 | BMK = 0.289 | MCSE(6.27) = 13.4 | stat: FALSE | burn: 60
Pdatum5
−10
−12
−14
−16
0
20
40
60
80
100
120

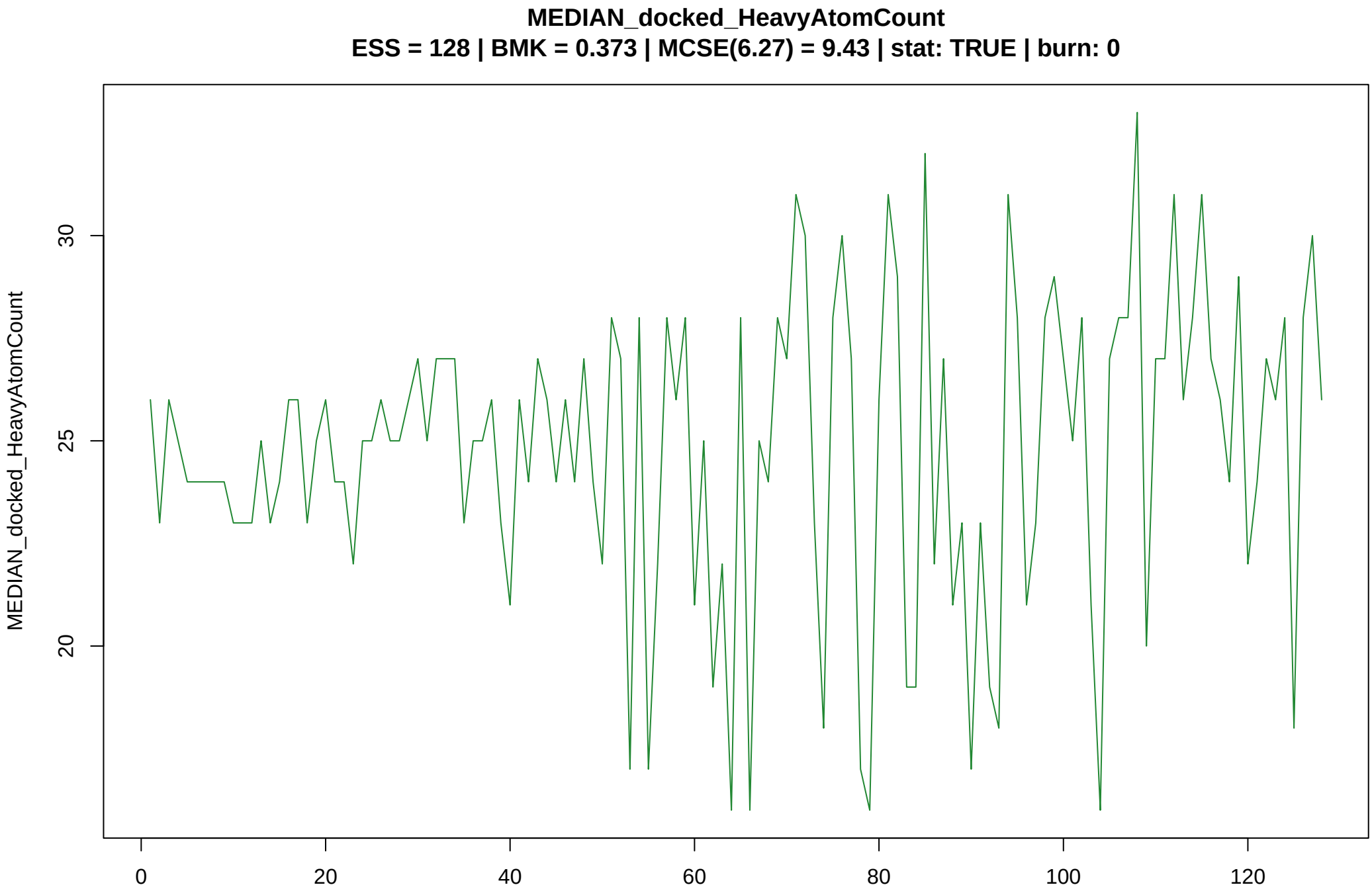

Pdatum6
ESS = 128 | BMK = 0.908 | MCSE(6.27) = 12.4 | stat: FALSE | burn: 120
Pdatum6
−8
−10
−12
−14
−16
−18
−20
0
20
40
60
80
100
120

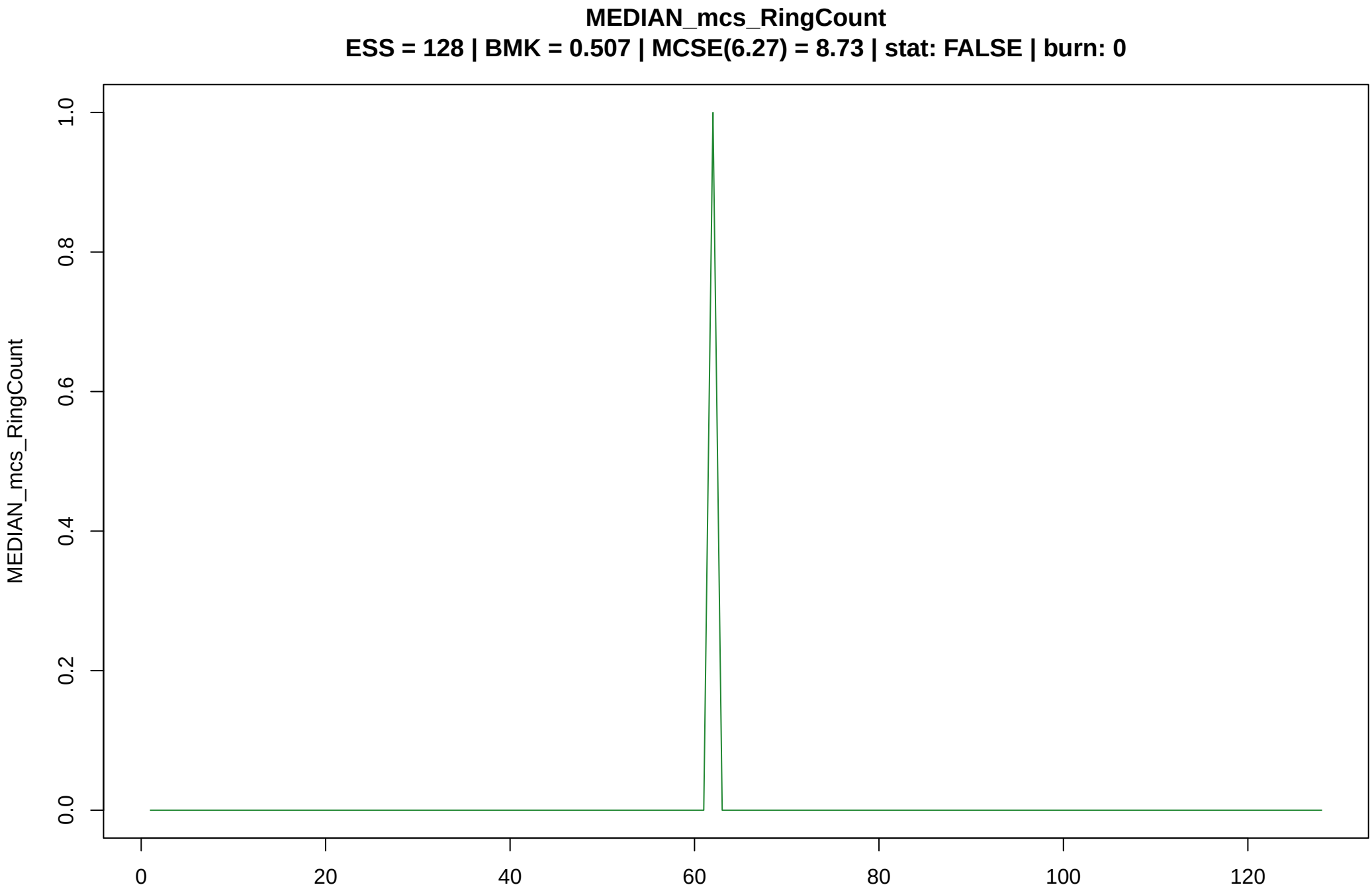

Pdatum7
ESS = 14 | BMK = 0.386 | MCSE(6.27) = 17.8 | stat: FALSE | burn: 12
Pdatum7
−10
−12
−14
−16
0
20
40
60
80
100
120

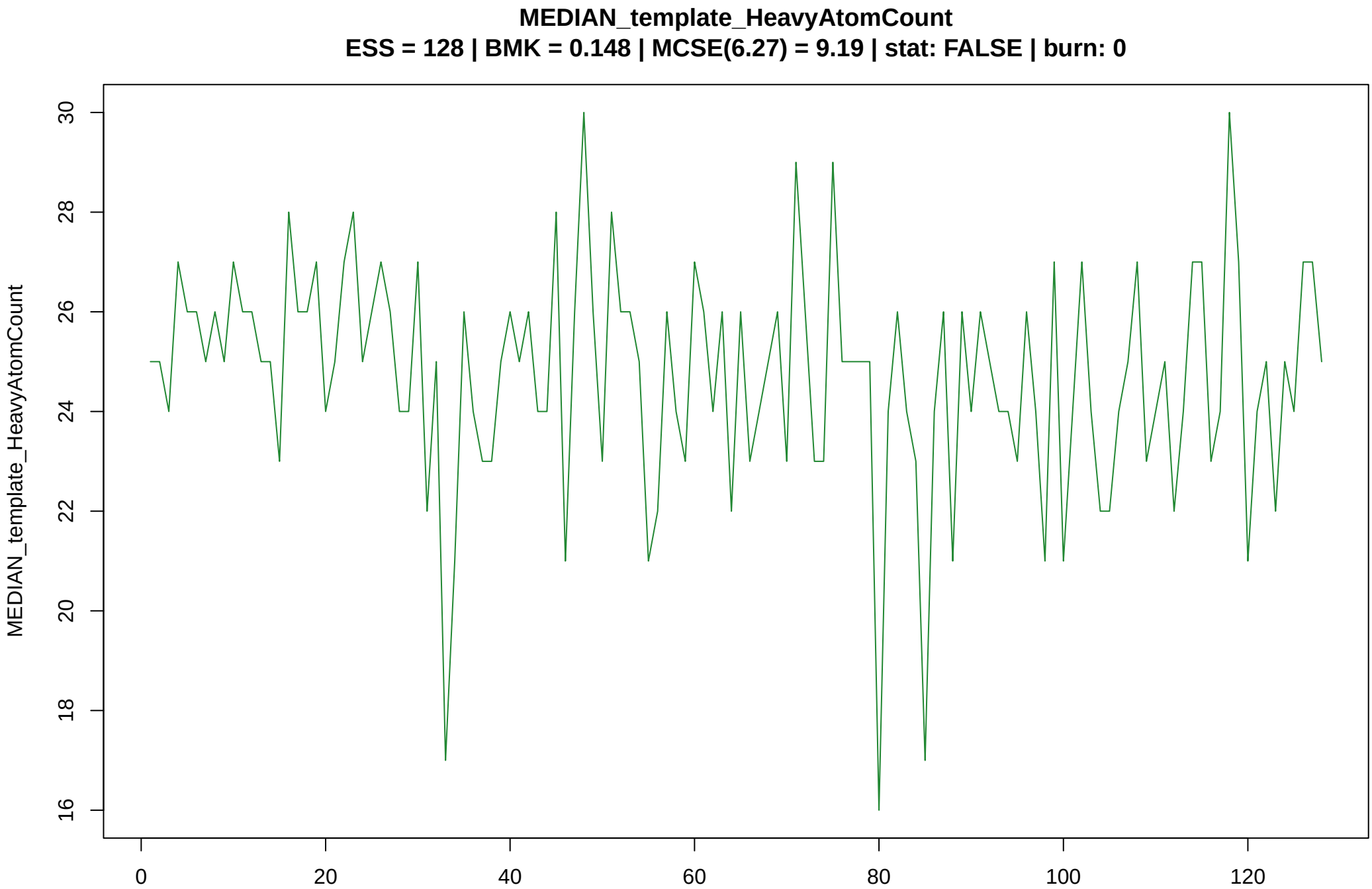

Pdatum8
ESS = 128 | BMK = 0.918 | MCSE(6.27) = 9.52 | stat: FALSE | burn: 48
Pdatum8
−10
−12
−14
−16
−18
−20
0
20
40
60
80
100
120

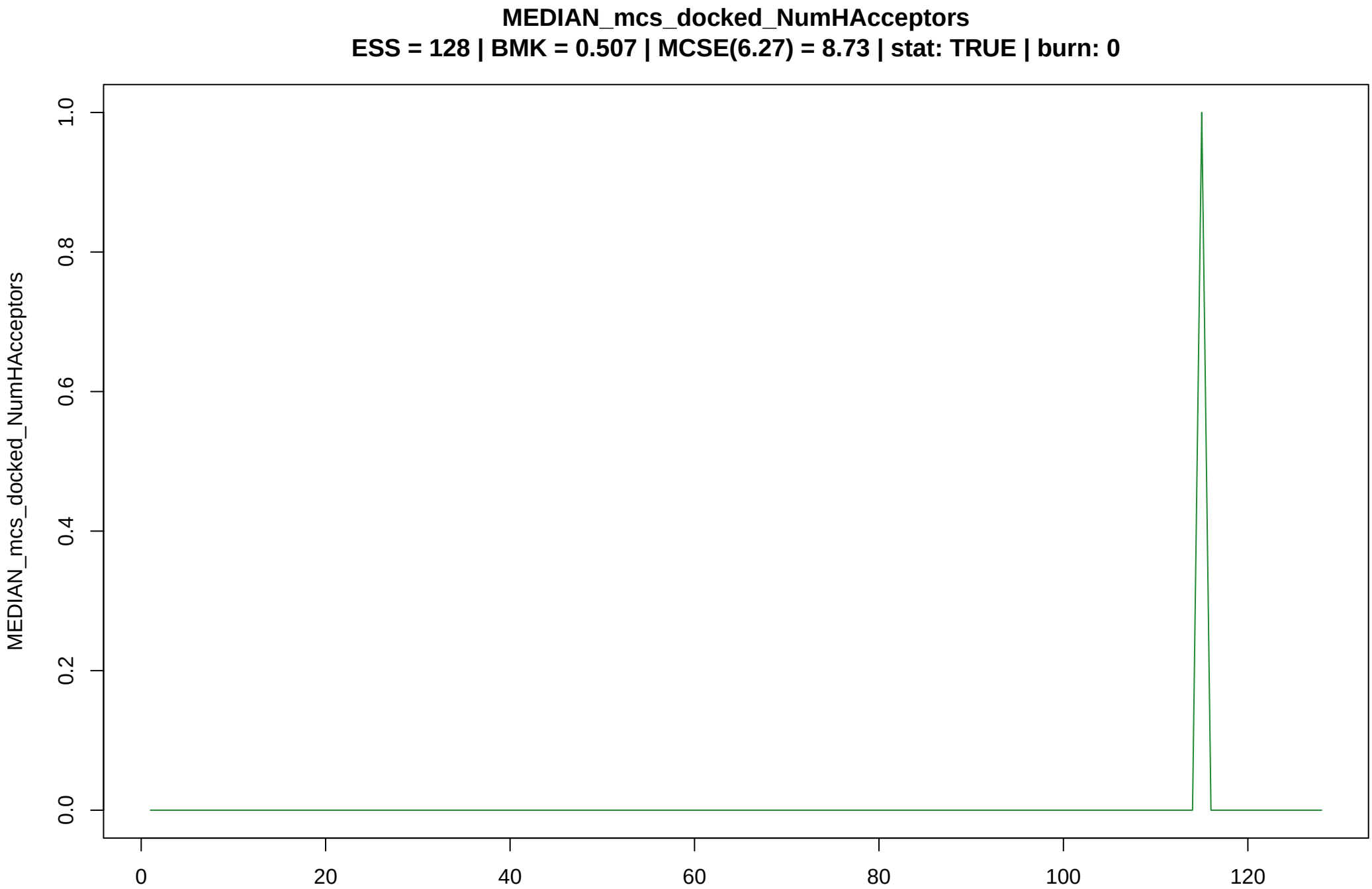

MEDIAN_log_RMSD
ESS = 48.5 | BMK = 0.221 | MCSE(6.27) = 18.6 | stat: FALSE | burn: 36
MEDIAN_log_RMSD
1.3
1.4
1.5
1.6
1.7
1.8
1.9
0
20
40
60
80
100
120

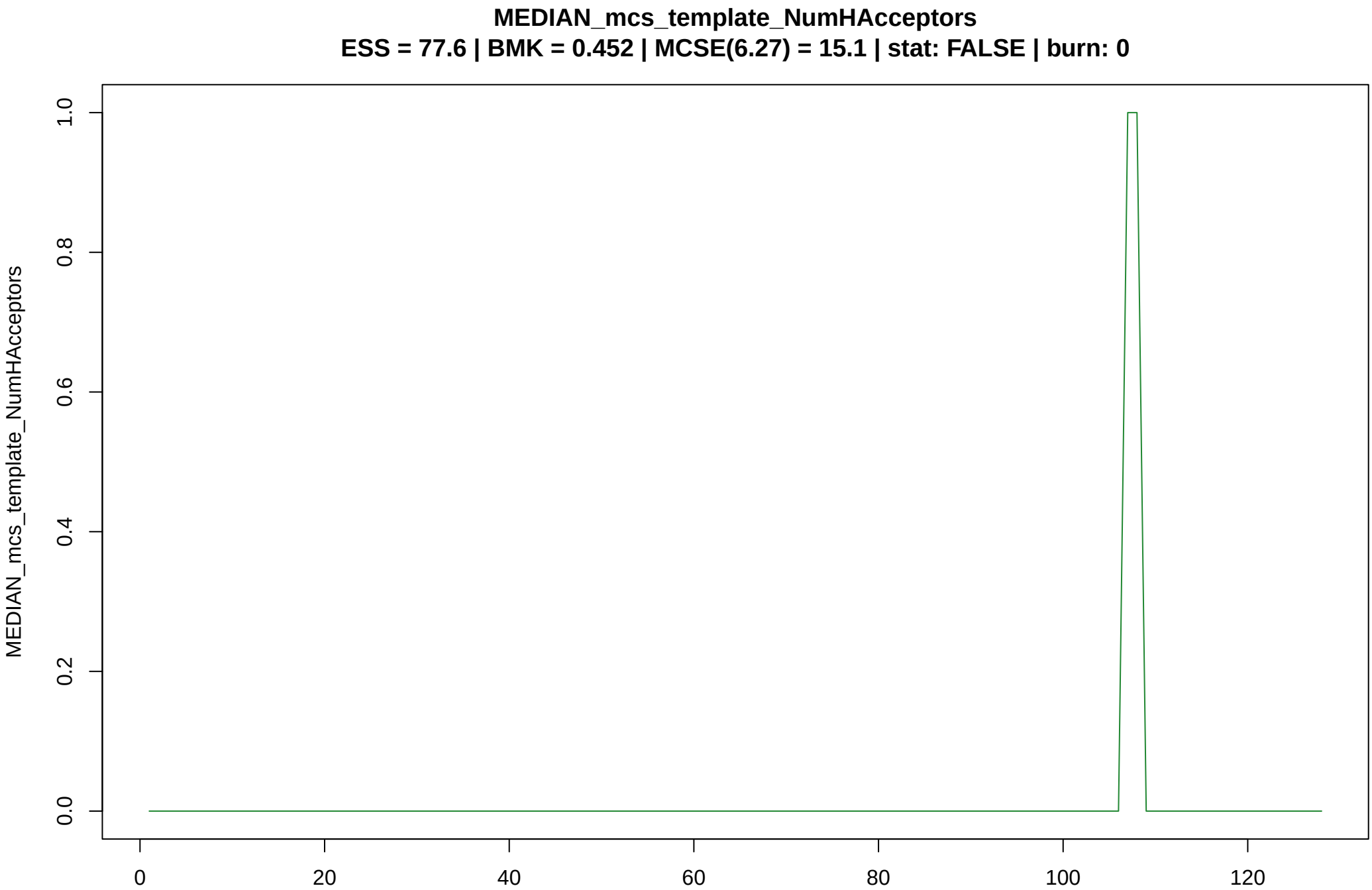

MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 123 | BMK = 0.252 | MCSE(6.27) = 14 | stat: TRUE | burn: 120
MEDIAN_Xtransf_ec_tanimoto_similarity
−0.4
−0.6
−0.8
−1.0
−1.2
0
20
40
60
80
100
120

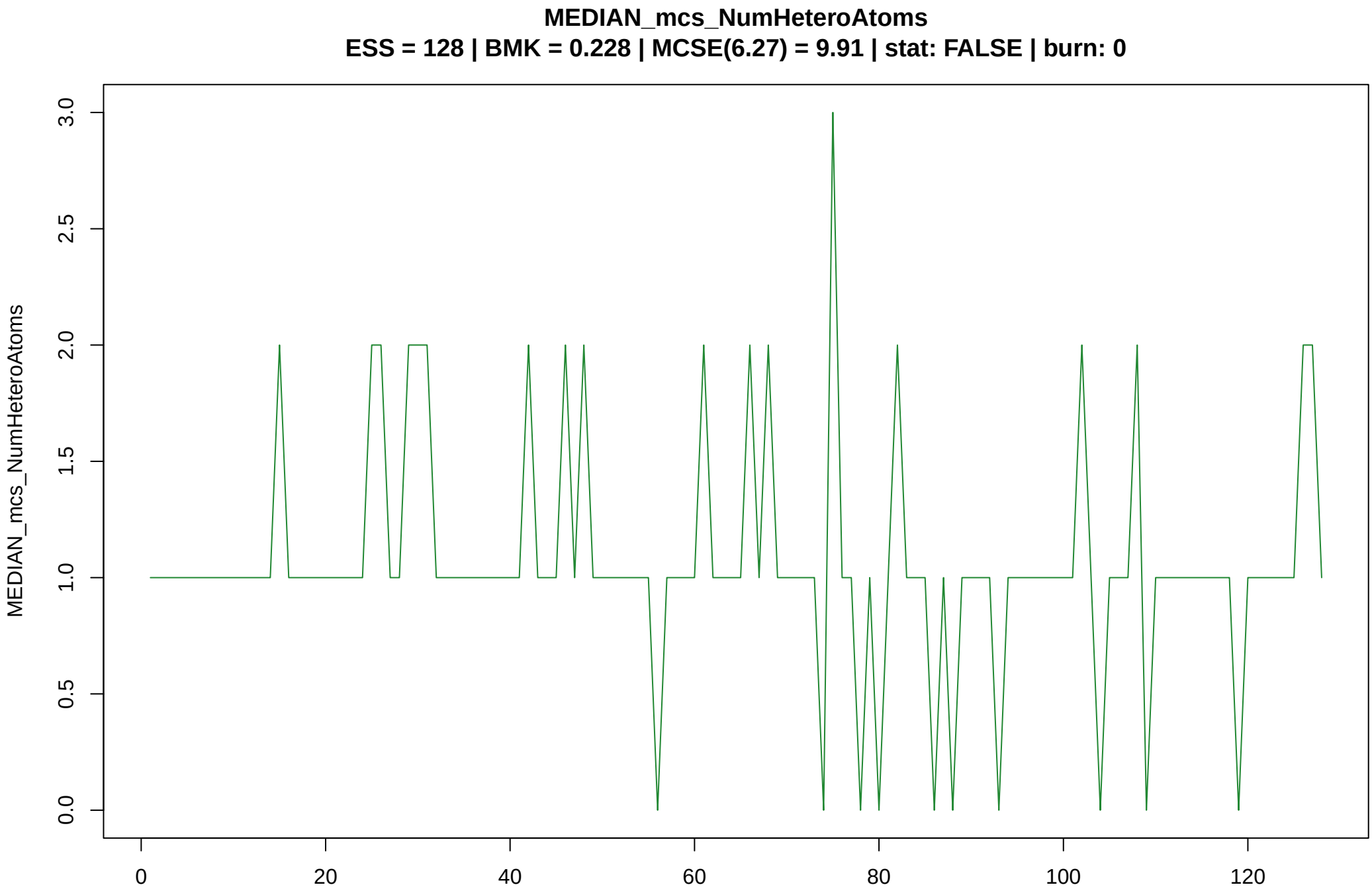

MEDIAN_docked_HeavyAtomCount
ESS = 128 | BMK = 0.373 | MCSE(6.27) = 9.43 | stat: TRUE | burn: 0
MEDIAN_docked_HeavyAtomCount
20
25
30
0
20
40
60
80
100
120

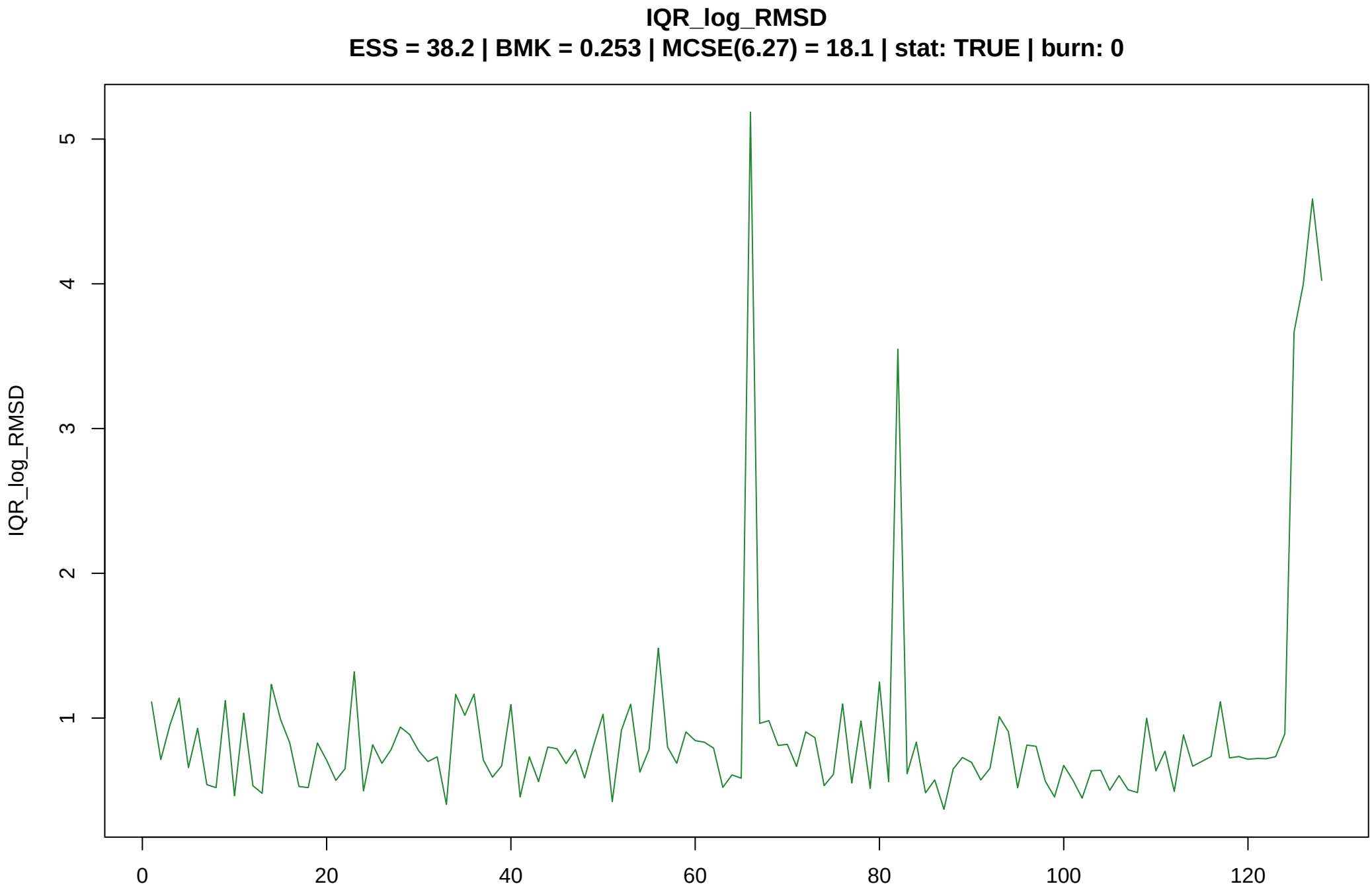

MEDIAN_mcs_RingCount
ESS = 128 | BMK = 0.507 | MCSE(6.27) = 8.73 | stat: FALSE | burn: 0
MEDIAN_mcs_RingCount
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

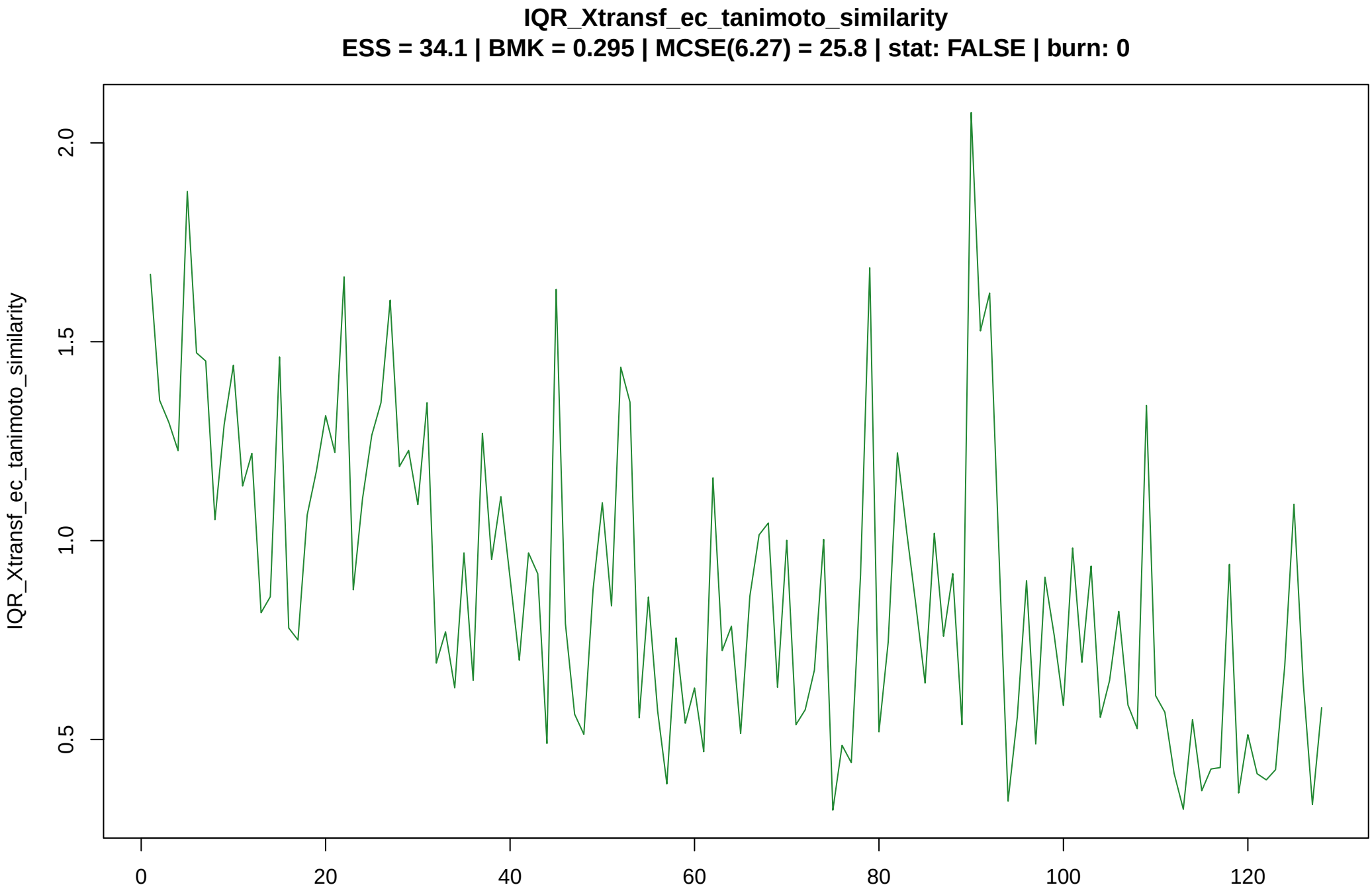

MEDIAN_template_HeavyAtomCount
ESS = 128 | BMK = 0.148 | MCSE(6.27) = 9.19 | stat: FALSE | burn: 0
MEDIAN_template_HeavyAtomCount
16
18
20
22
24
26
28
30
0
20
40
60
80
100
120

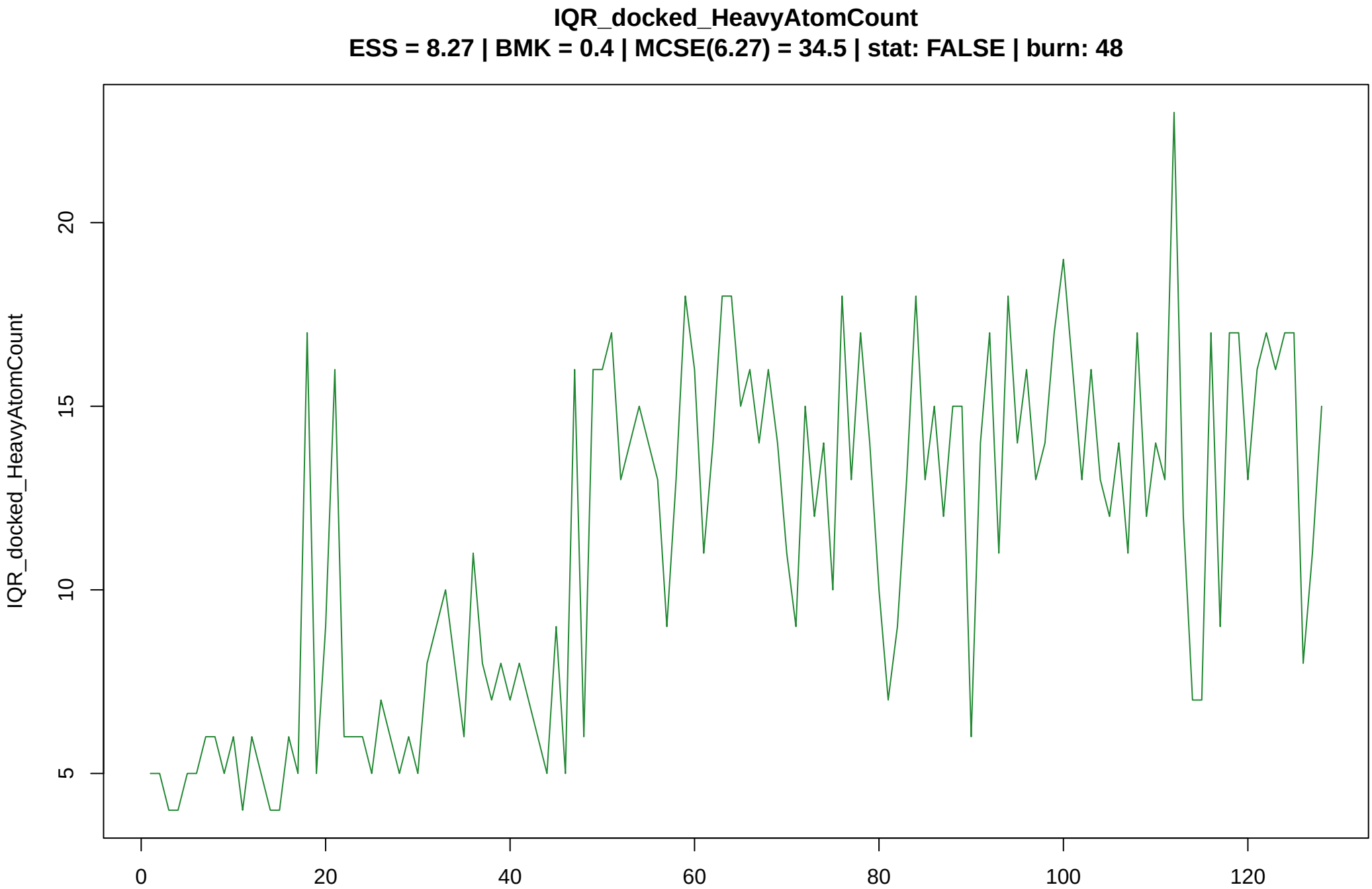

MEDIAN_mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.507 | MCSE(6.27) = 8.73 | stat: TRUE | burn: 0
MEDIAN_mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

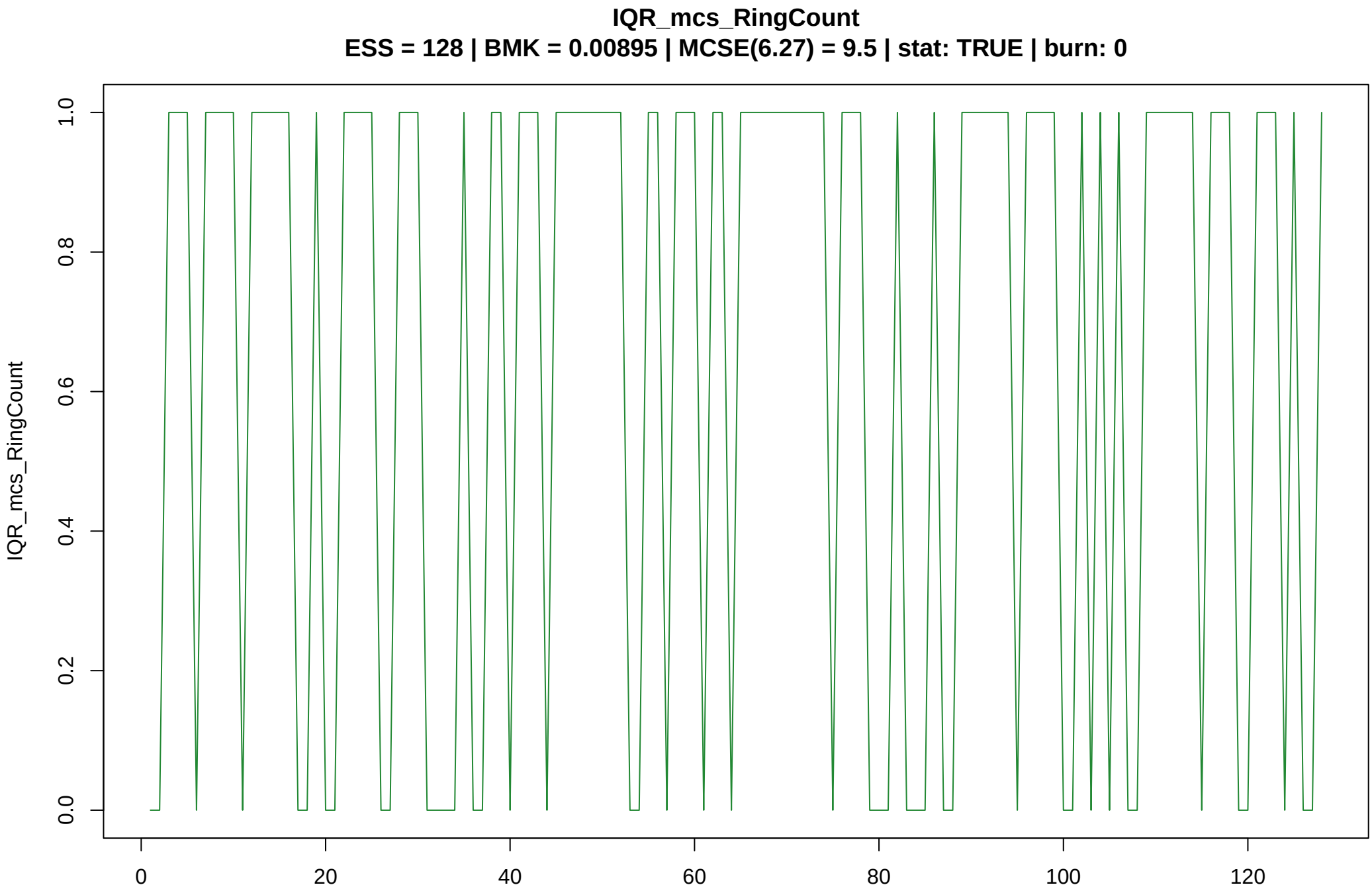

MEDIAN_mcs_template_NumHAcceptors
ESS = 77.6 | BMK = 0.452 | MCSE(6.27) = 15.1 | stat: FALSE | burn: 0
MEDIAN_mcs_template_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

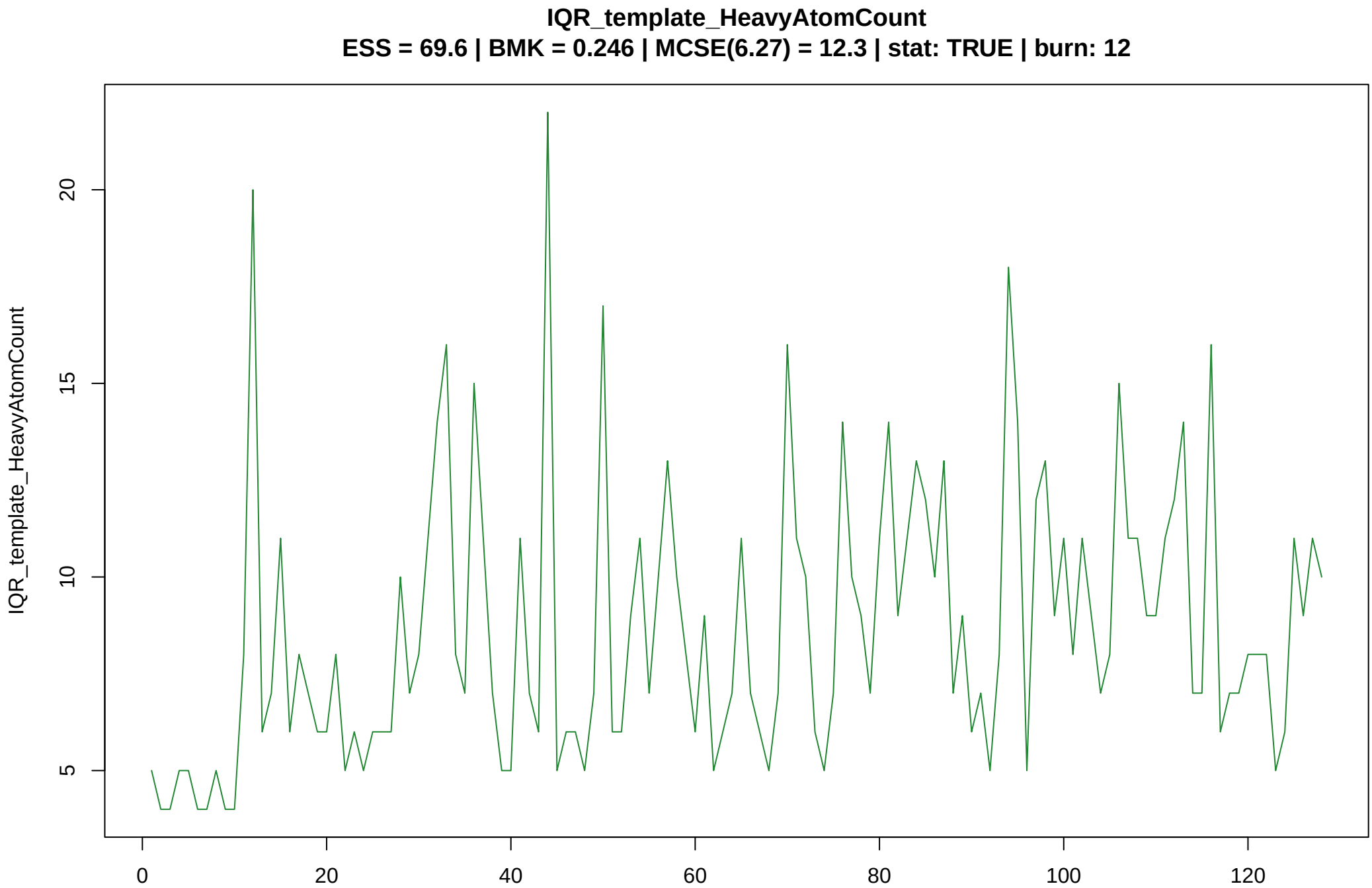

MEDIAN_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.228 | MCSE(6.27) = 9.91 | stat: FALSE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
20
40
60
80
100
120

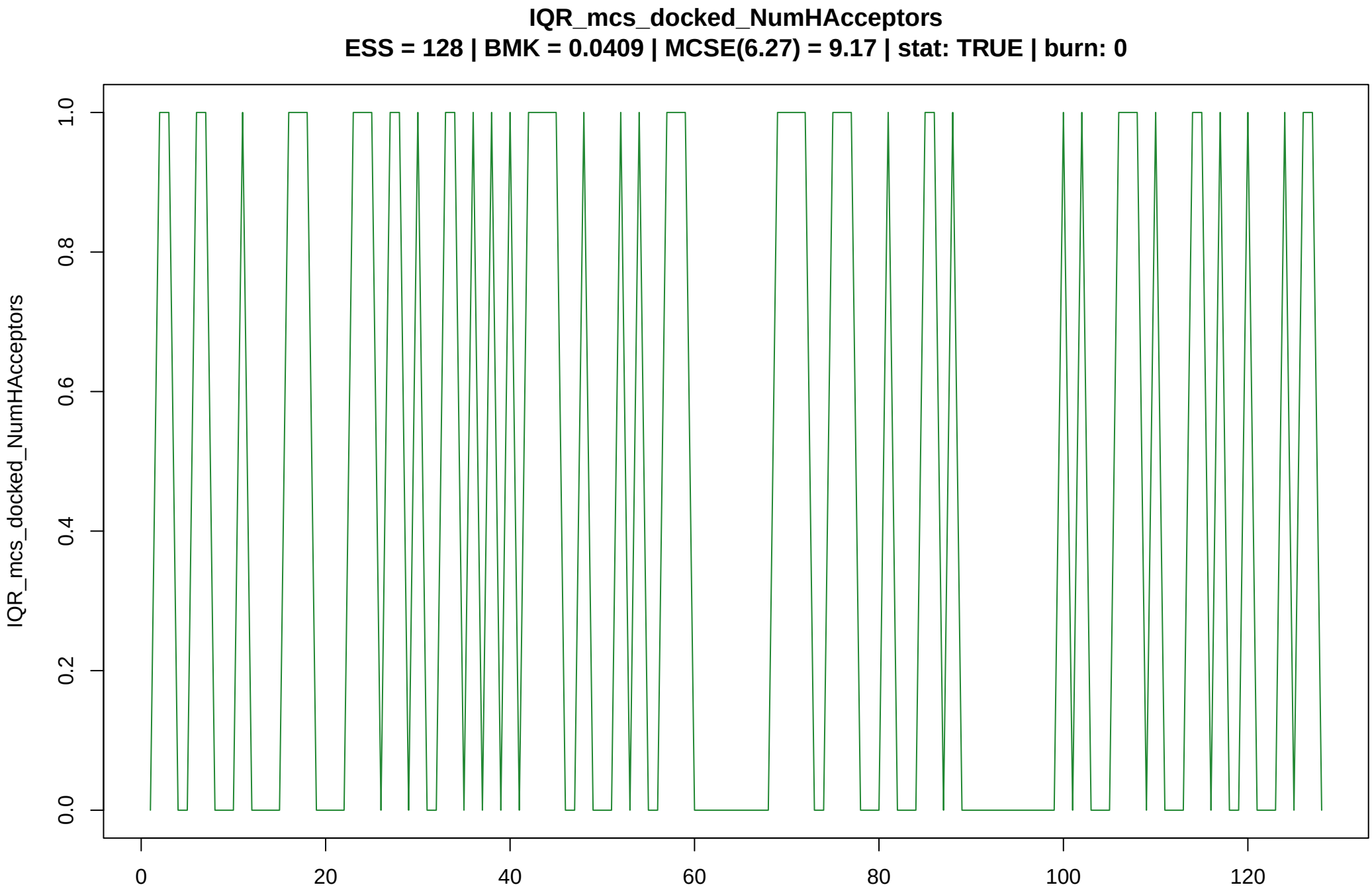

IQR_log_RMSD
ESS = 38.2 | BMK = 0.253 | MCSE(6.27) = 18.1 | stat: TRUE | burn: 0
IQR_log_RMSD
1
2
3
4
5
0
20
40
60
80
100
120

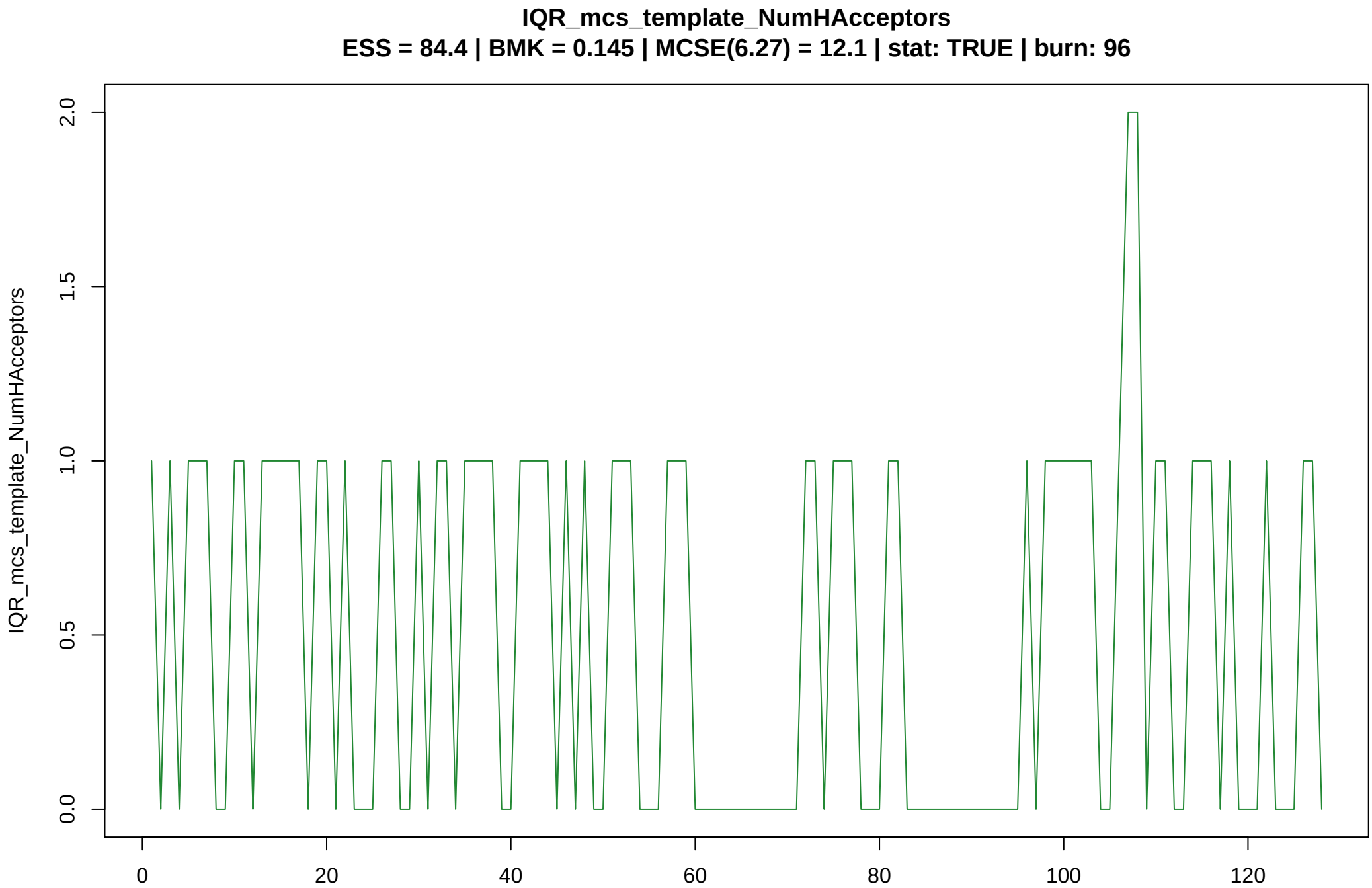

IQR_Xtransf_ec_tanimoto_similarity
ESS = 34.1 | BMK = 0.295 | MCSE(6.27) = 25.8 | stat: FALSE | burn: 0
IQR_Xtransf_ec_tanimoto_similarity
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120

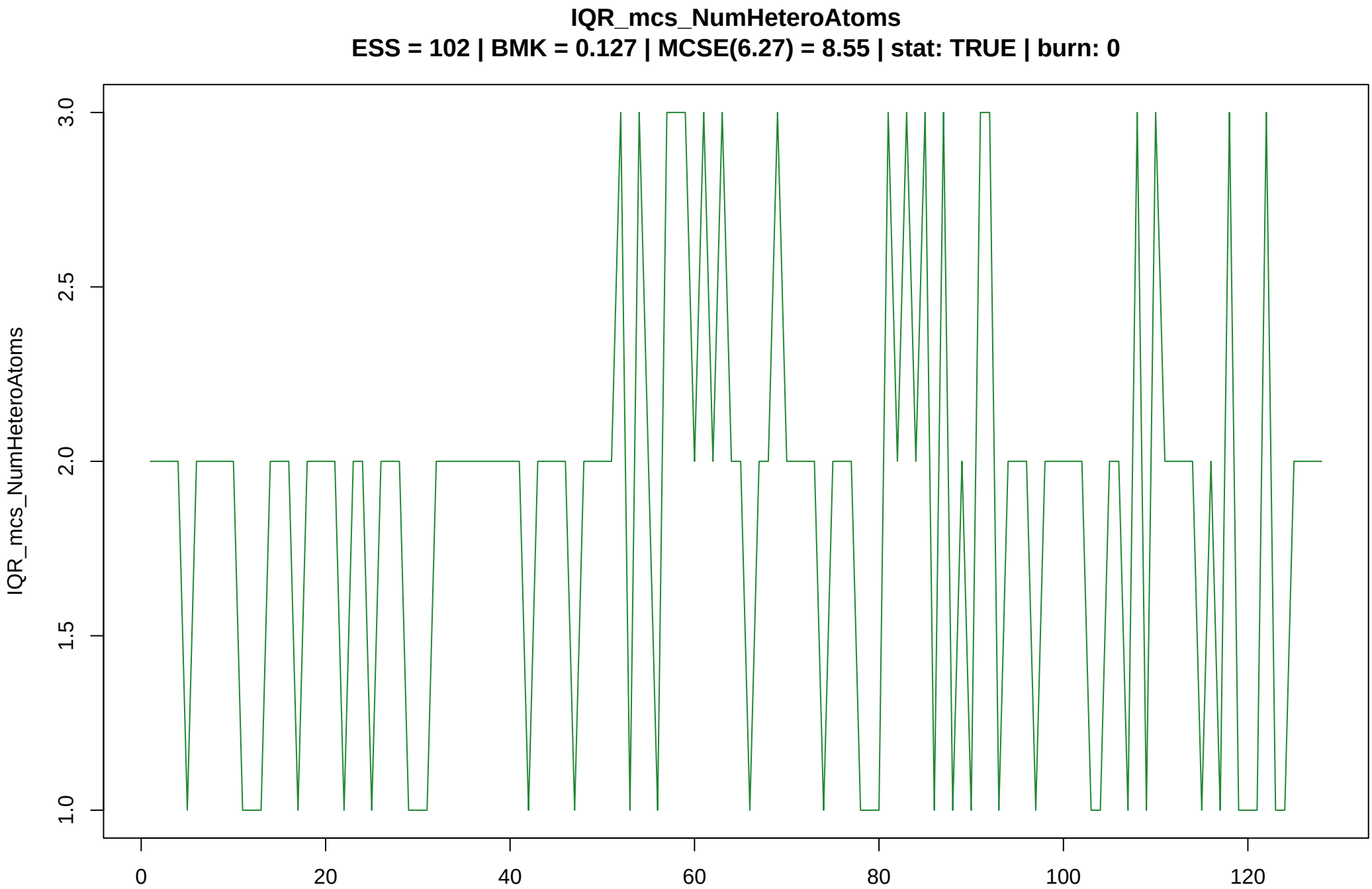

IQR_docked_HeavyAtomCount
ESS = 8.27 | BMK = 0.4 | MCSE(6.27) = 34.5 | stat: FALSE | burn: 48
IQR_docked_HeavyAtomCount
5
10
15
20
0
20
40
60
80
100
120

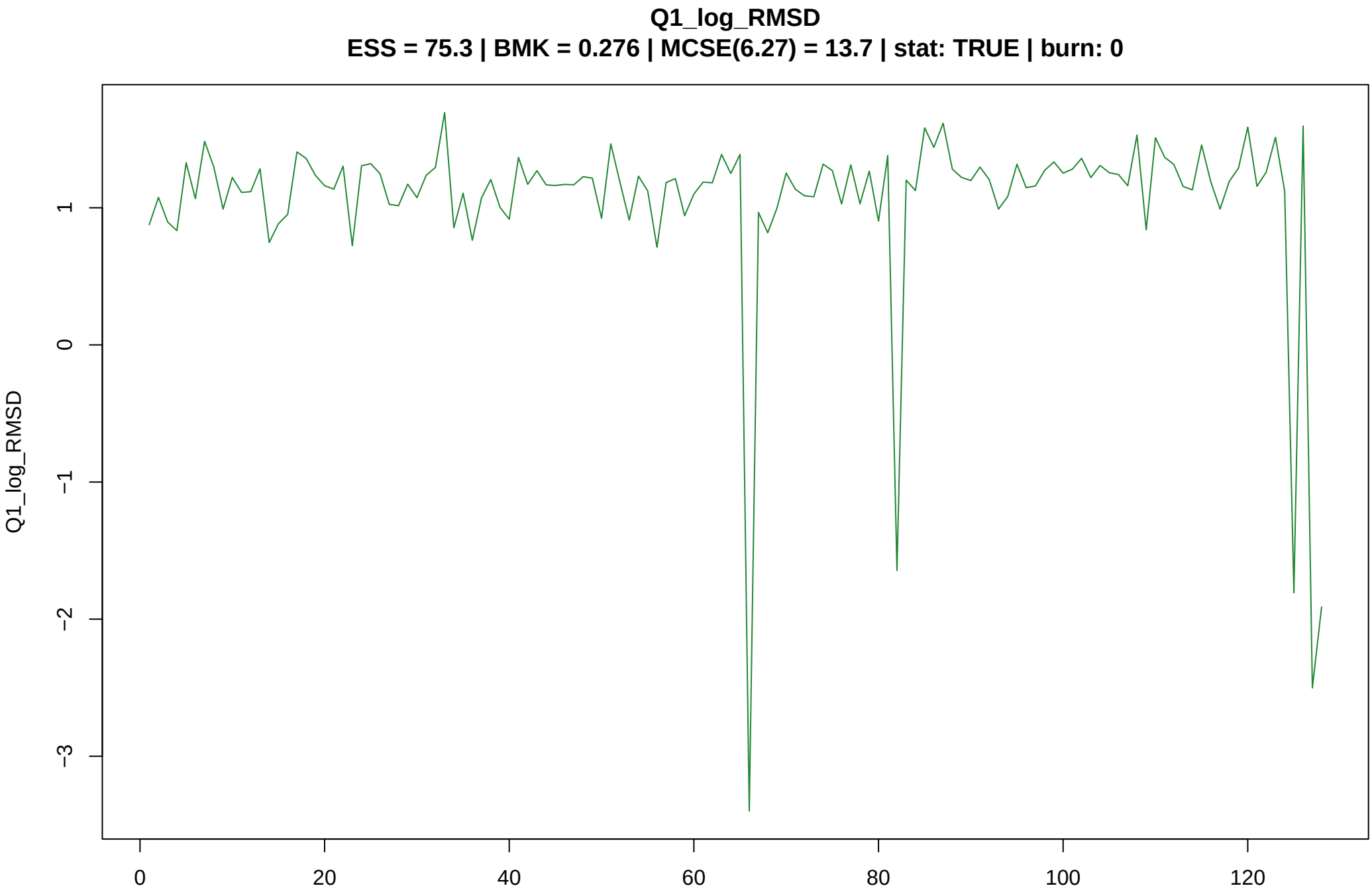

IQR_mcs_RingCount
ESS = 128 | BMK = 0.00895 | MCSE(6.27) = 9.5 | stat: TRUE | burn: 0
IQR_mcs_RingCount
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

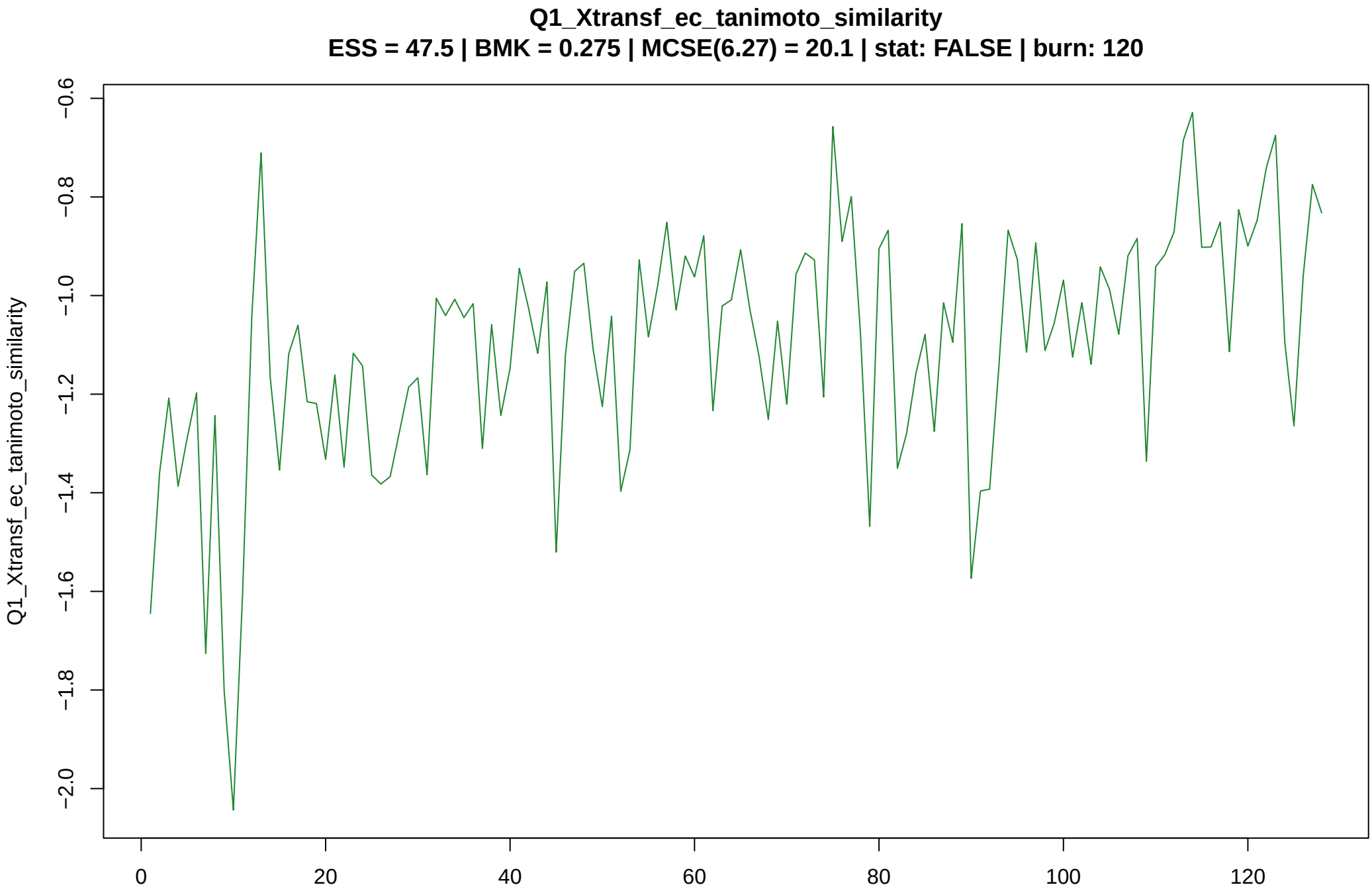

IQR_template_HeavyAtomCount
ESS = 69.6 | BMK = 0.246 | MCSE(6.27) = 12.3 | stat: TRUE | burn: 12
IQR_template_HeavyAtomCount
5
10
15
20
0
20
40
60
80
100
120

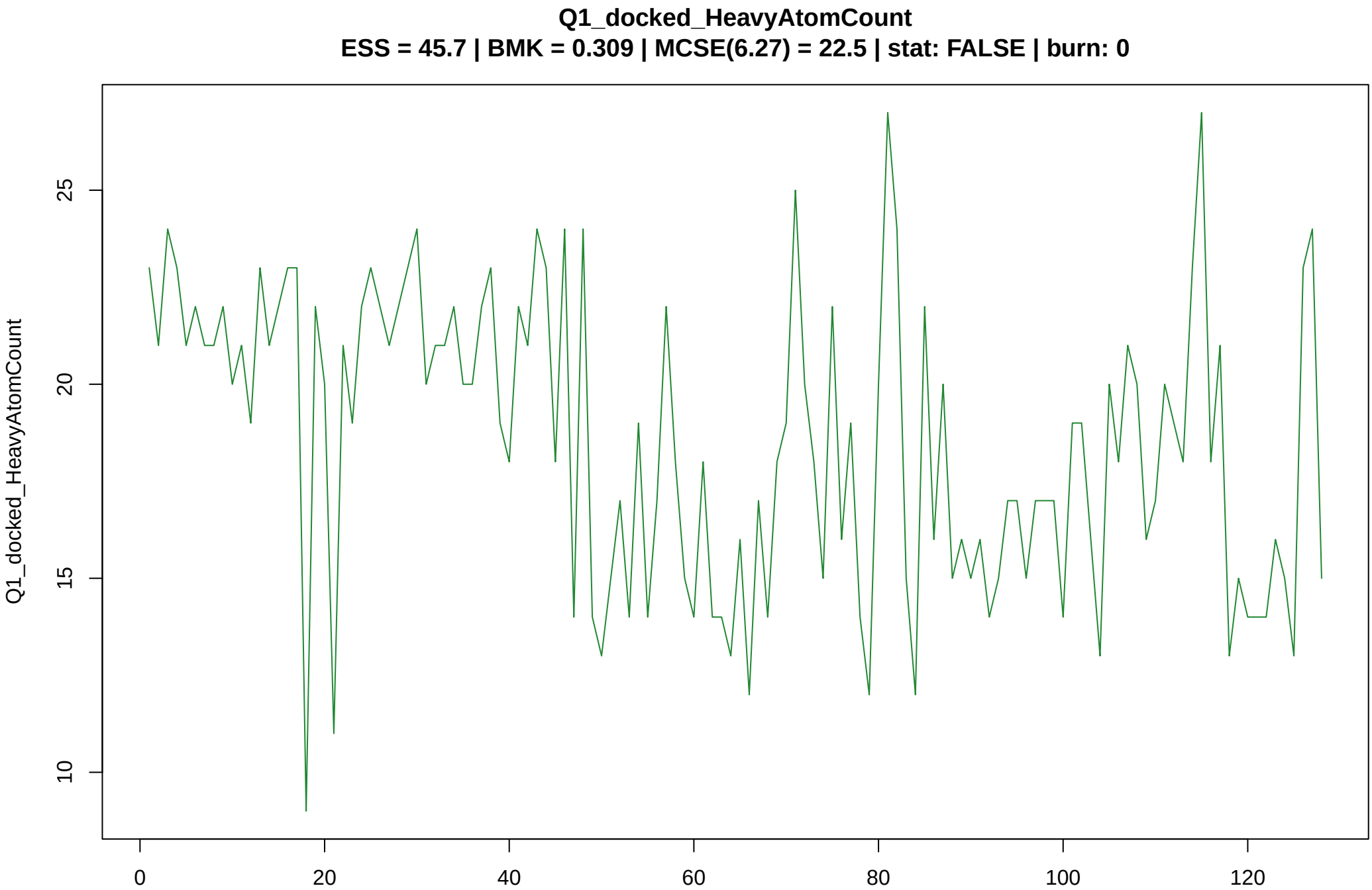

IQR_mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.0409 | MCSE(6.27) = 9.17 | stat: TRUE | burn: 0
IQR_mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

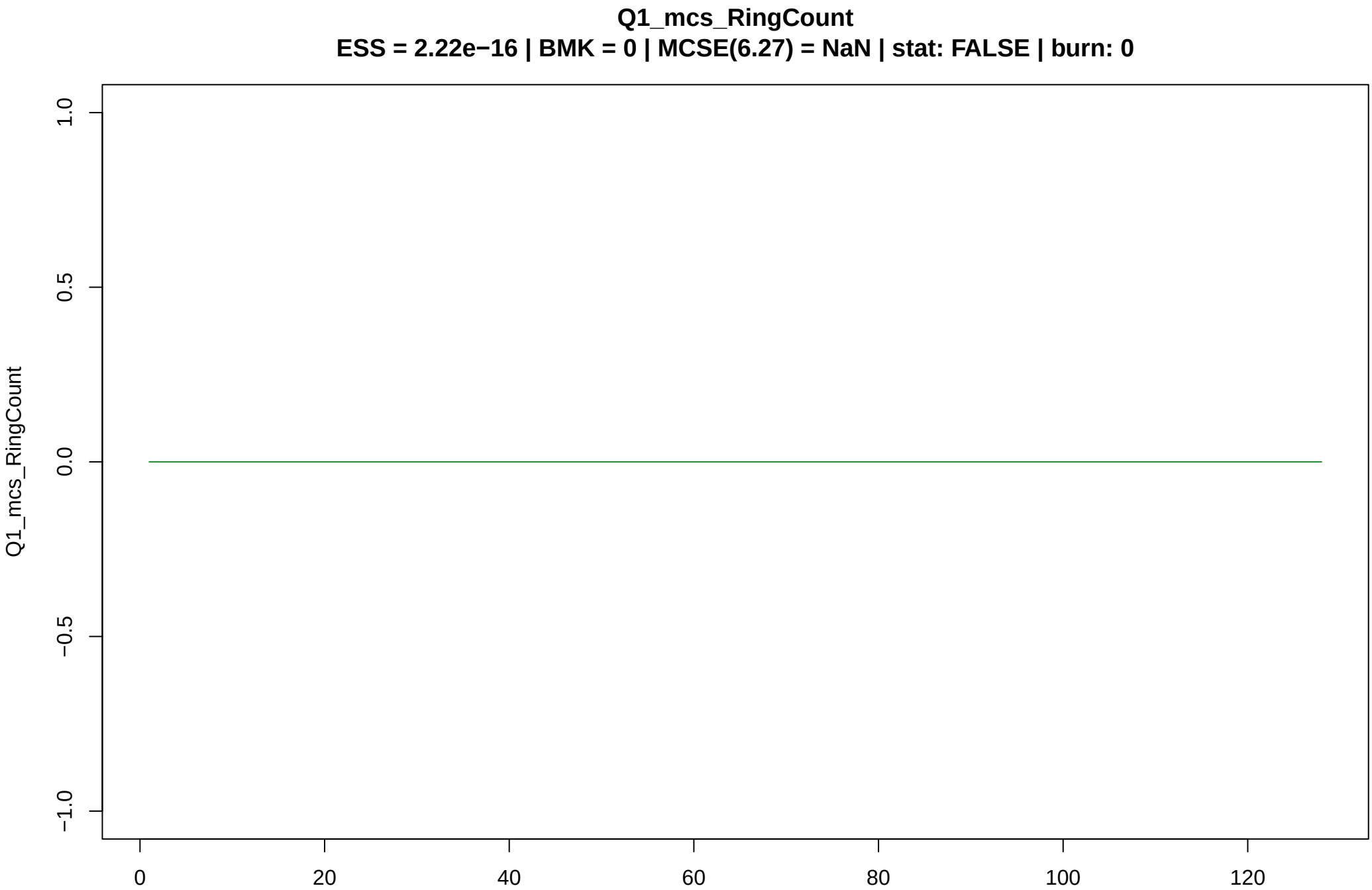

IQR_mcs_template_NumHAcceptors
ESS = 84.4 | BMK = 0.145 | MCSE(6.27) = 12.1 | stat: TRUE | burn: 96
IQR_mcs_template_NumHAcceptors
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120

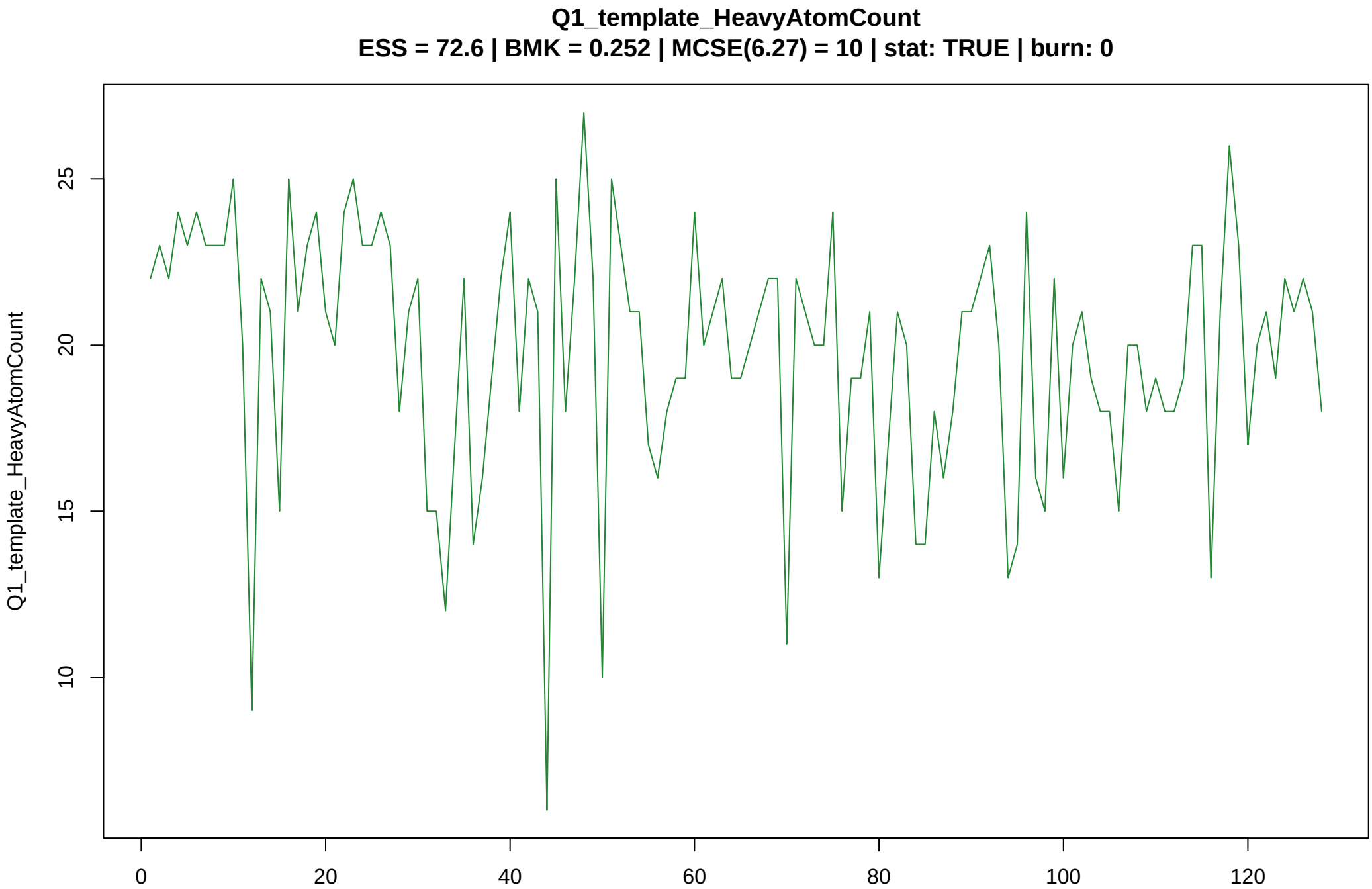

IQR_mcs_NumHeteroAtoms
ESS = 102 | BMK = 0.127 | MCSE(6.27) = 8.55 | stat: TRUE | burn: 0
IQR_mcs_NumHeteroAtoms
1.0
1.5
2.0
2.5
3.0
0
20
40
60
80
100
120

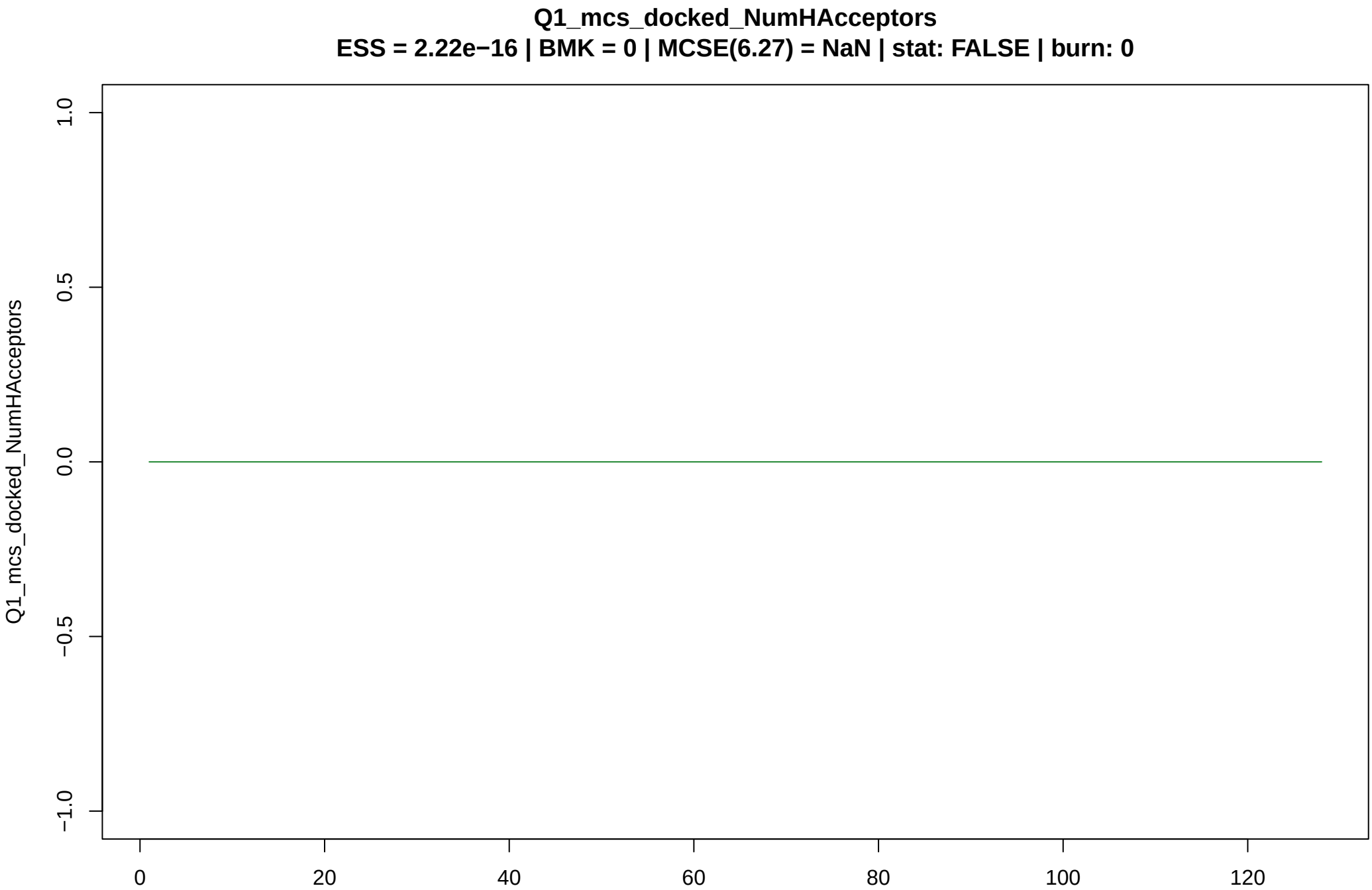

Q1_log_RMSD
ESS = 75.3 | BMK = 0.276 | MCSE(6.27) = 13.7 | stat: TRUE | burn: 0
Q1_log_RMSD
1
0
−1
−2
−3
0
20
40
60
80
100
120

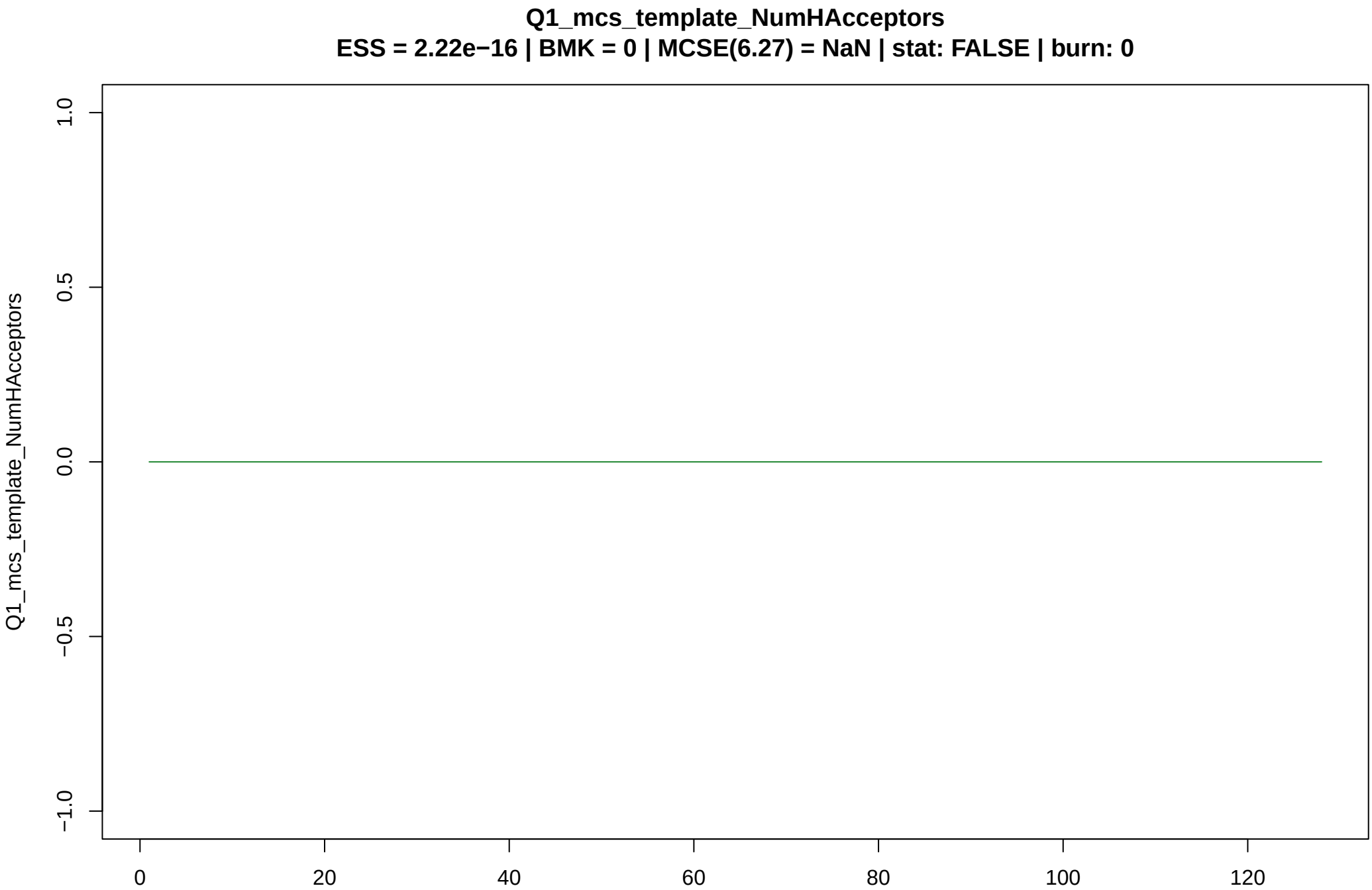

Q1_Xtransf_ec_tanimoto_similarity
ESS = 47.5 | BMK = 0.275 | MCSE(6.27) = 20.1 | stat: FALSE | burn: 120
Q1_Xtransf_ec_tanimoto_similarity
−0.6
−0.8
−1.0
−1.2
−1.4
−1.6
−1.8
−2.0
0
20
40
60
80
100
120

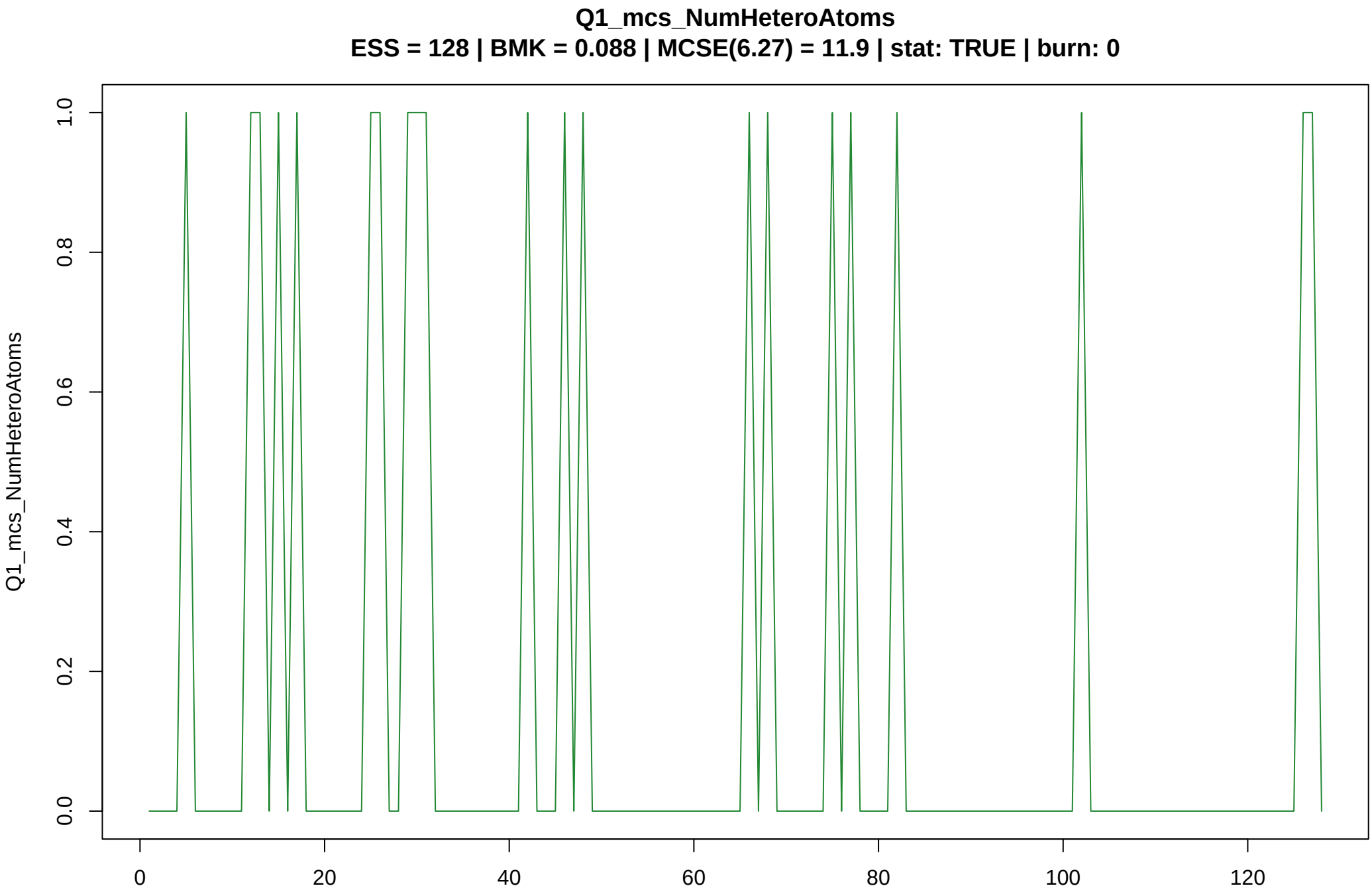

Q1_docked_HeavyAtomCount
ESS = 45.7 | BMK = 0.309 | MCSE(6.27) = 22.5 | stat: FALSE | burn: 0
Q1_docked_HeavyAtomCount
10
15
20
25
0
20
40
60
80
100
120

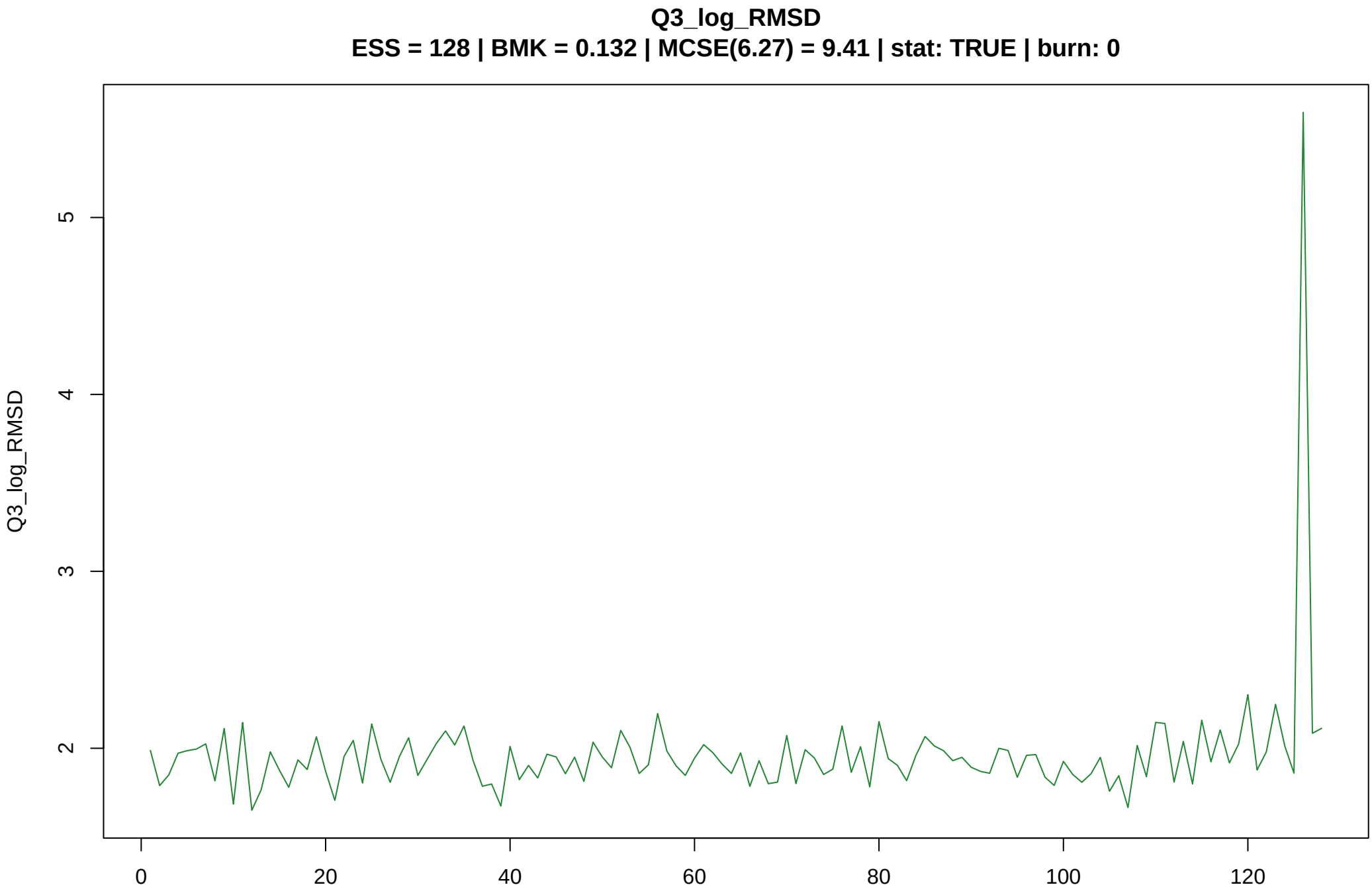

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
20
40
60
80
100
120

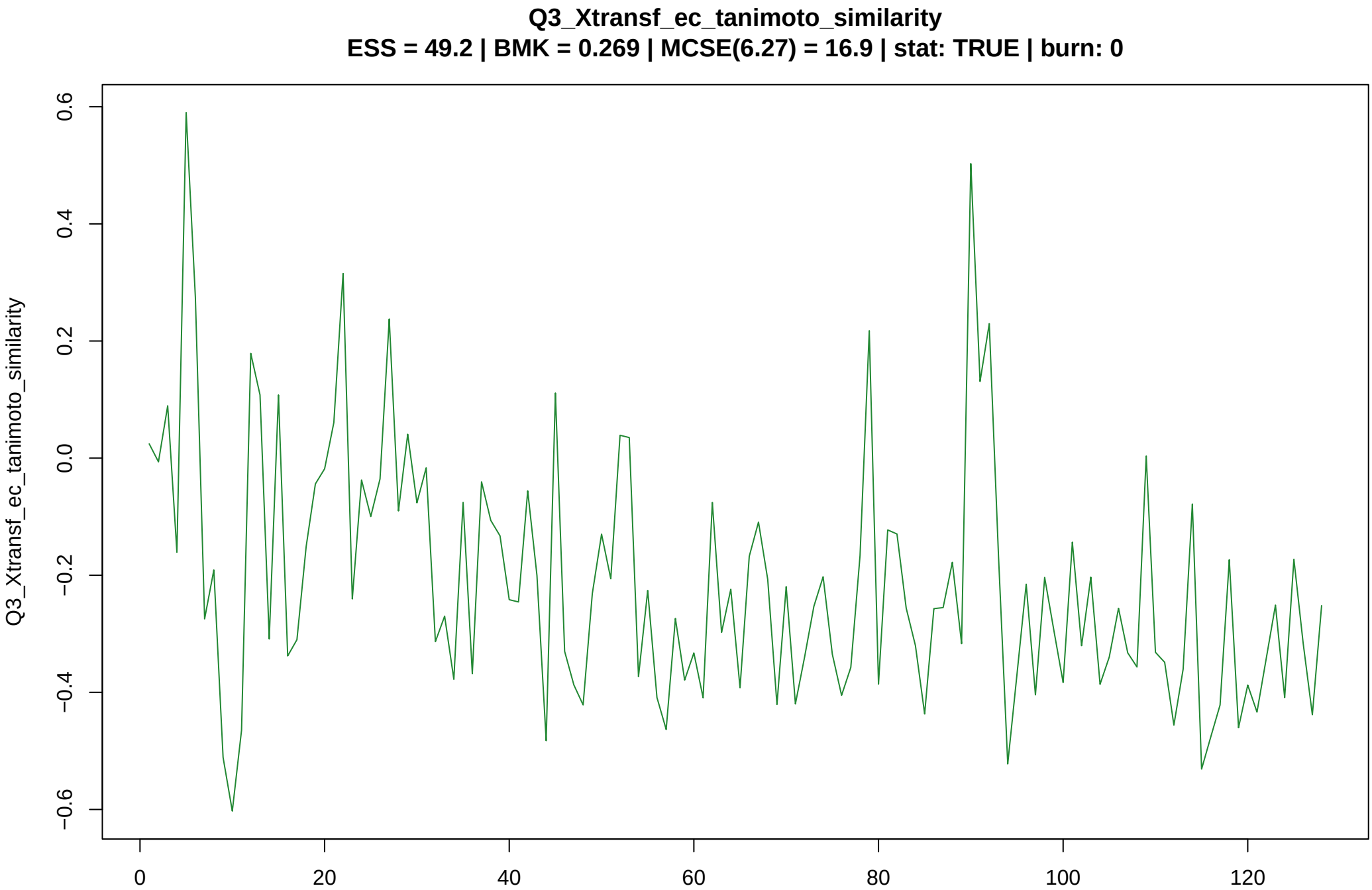

Q1_template_HeavyAtomCount
ESS = 72.6 | BMK = 0.252 | MCSE(6.27) = 10 | stat: TRUE | burn: 0
Q1_template_HeavyAtomCount
10
15
20
25
0
20
40
60
80
100
120

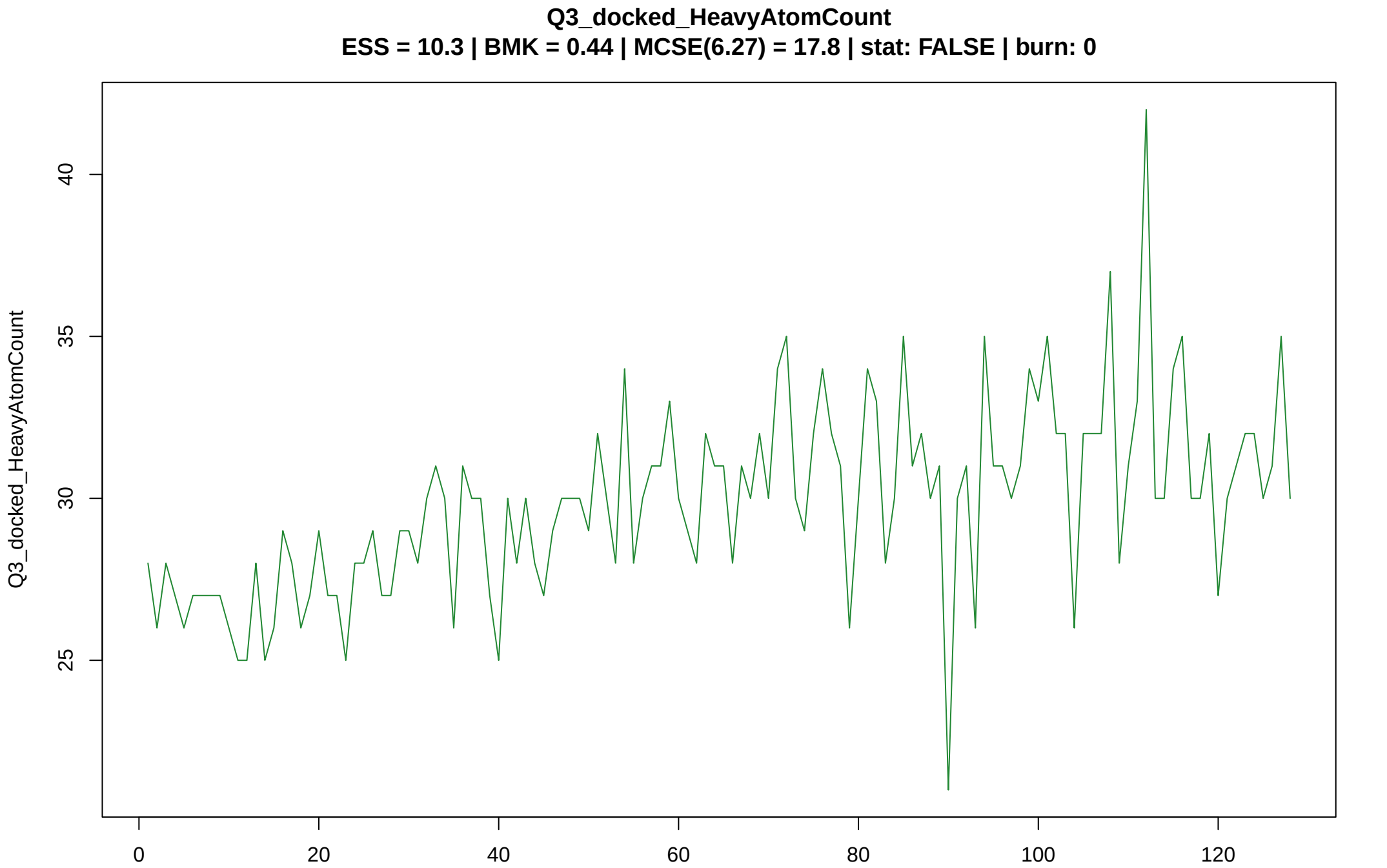

Q1_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_docked_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
20
40
60
80
100
120

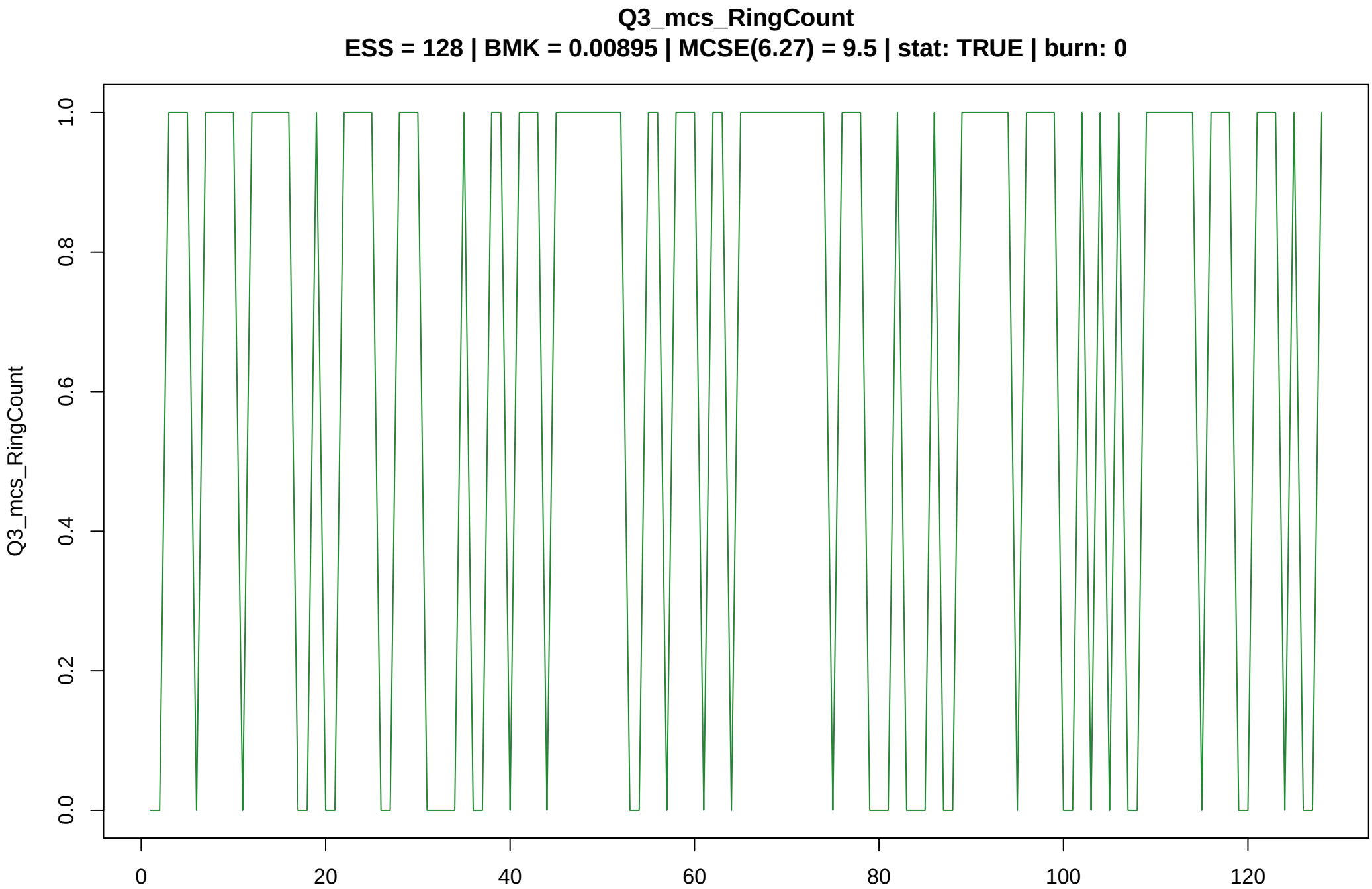

Q1_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_template_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
20
40
60
80
100
120

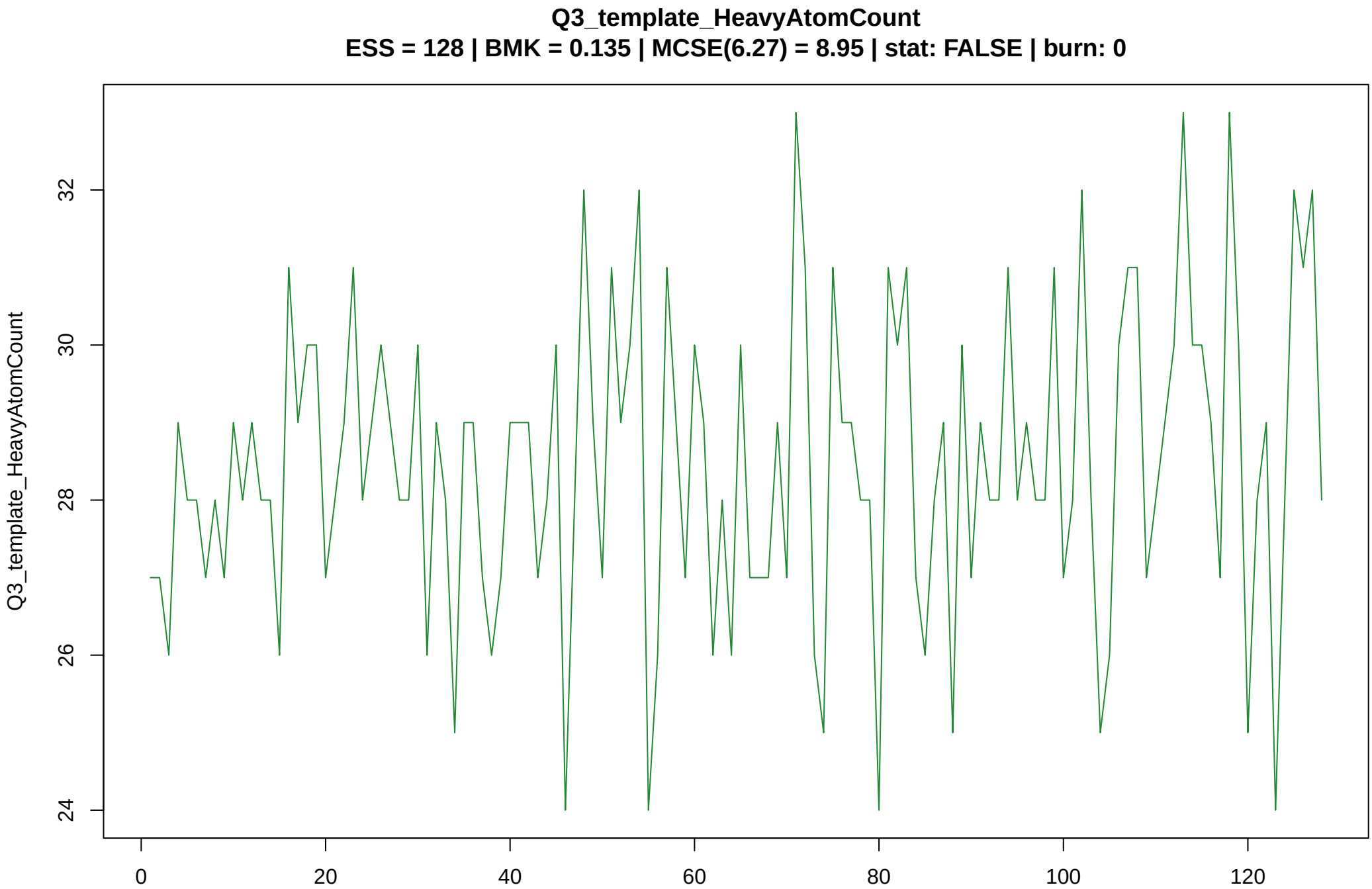

Q1_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.088 | MCSE(6.27) = 11.9 | stat: TRUE | burn: 0
Q1_mcs_NumHeteroAtoms
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

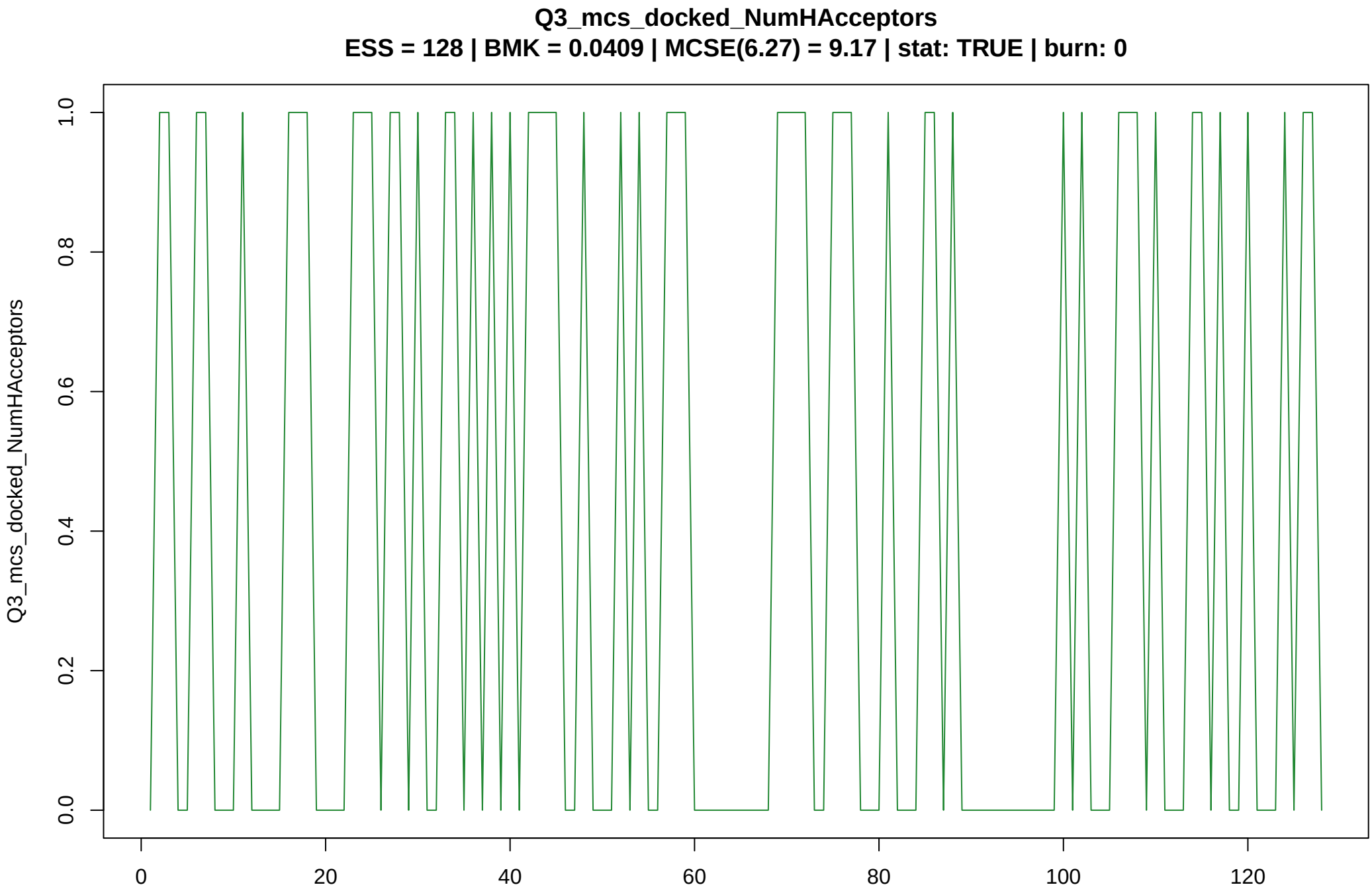

Q3_log_RMSD
ESS = 128 | BMK = 0.132 | MCSE(6.27) = 9.41 | stat: TRUE | burn: 0
Q3_log_RMSD
2
3
4
5
0
20
40
60
80
100
120

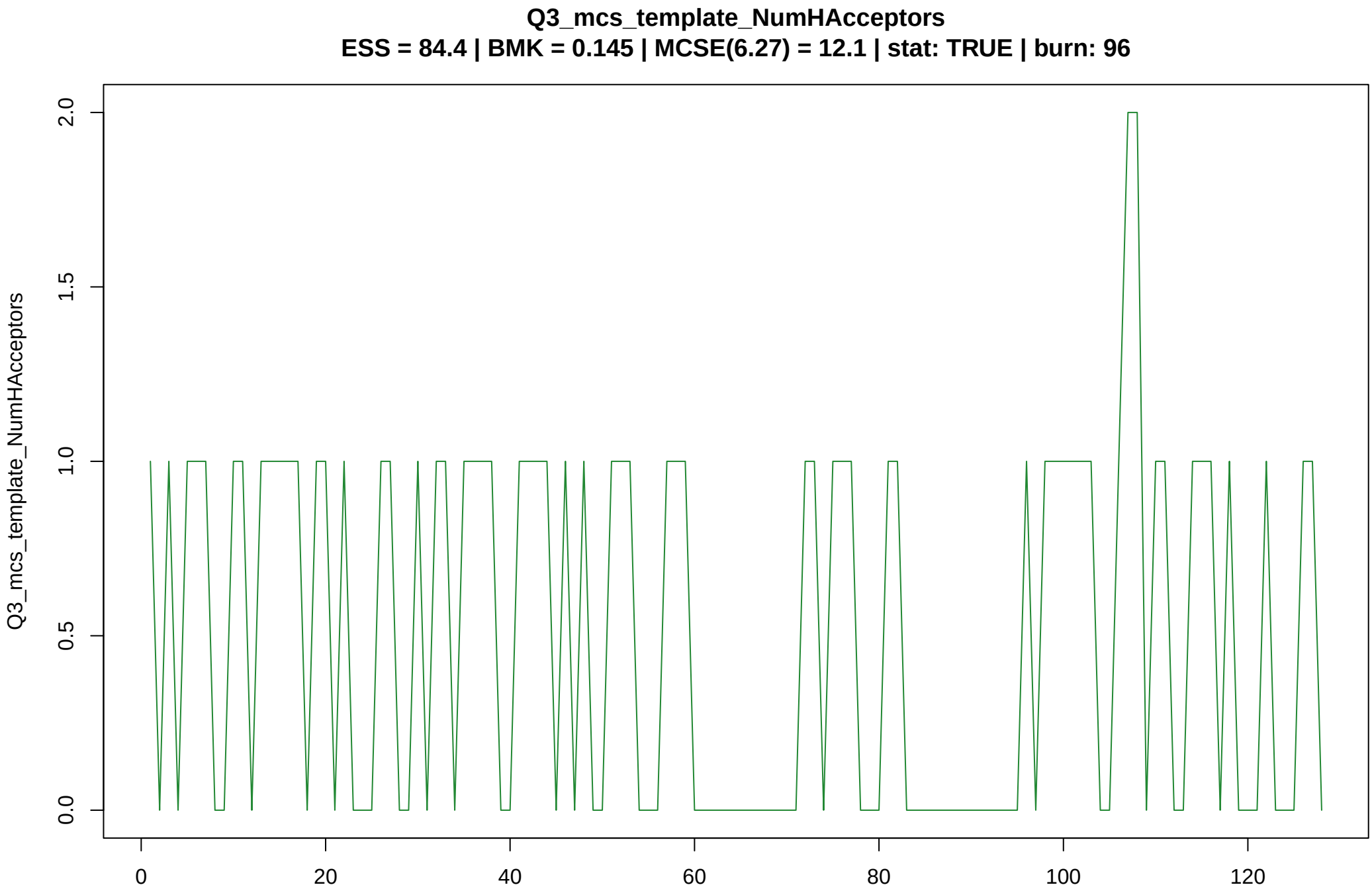

Q3_Xtransf_ec_tanimoto_similarity
ESS = 49.2 | BMK = 0.269 | MCSE(6.27) = 16.9 | stat: TRUE | burn: 0
Q3_Xtransf_ec_tanimoto_similarity
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
0
20
40
60
80
100
120

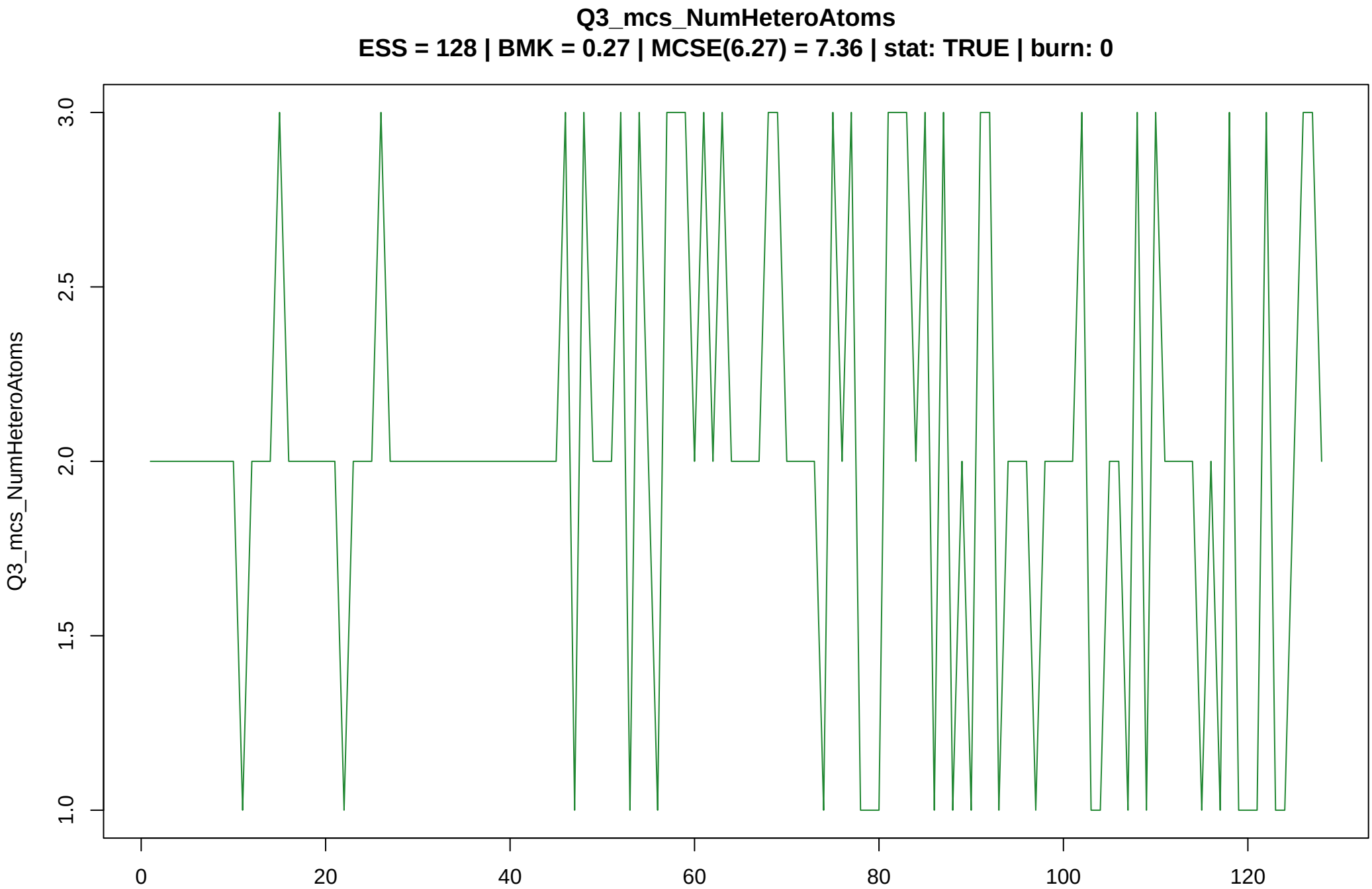

Q3_docked_HeavyAtomCount
ESS = 10.3 | BMK = 0.44 | MCSE(6.27) = 17.8 | stat: FALSE | burn: 0
Q3_docked_HeavyAtomCount
25
30
35
40
0
20
40
60
80
100
120

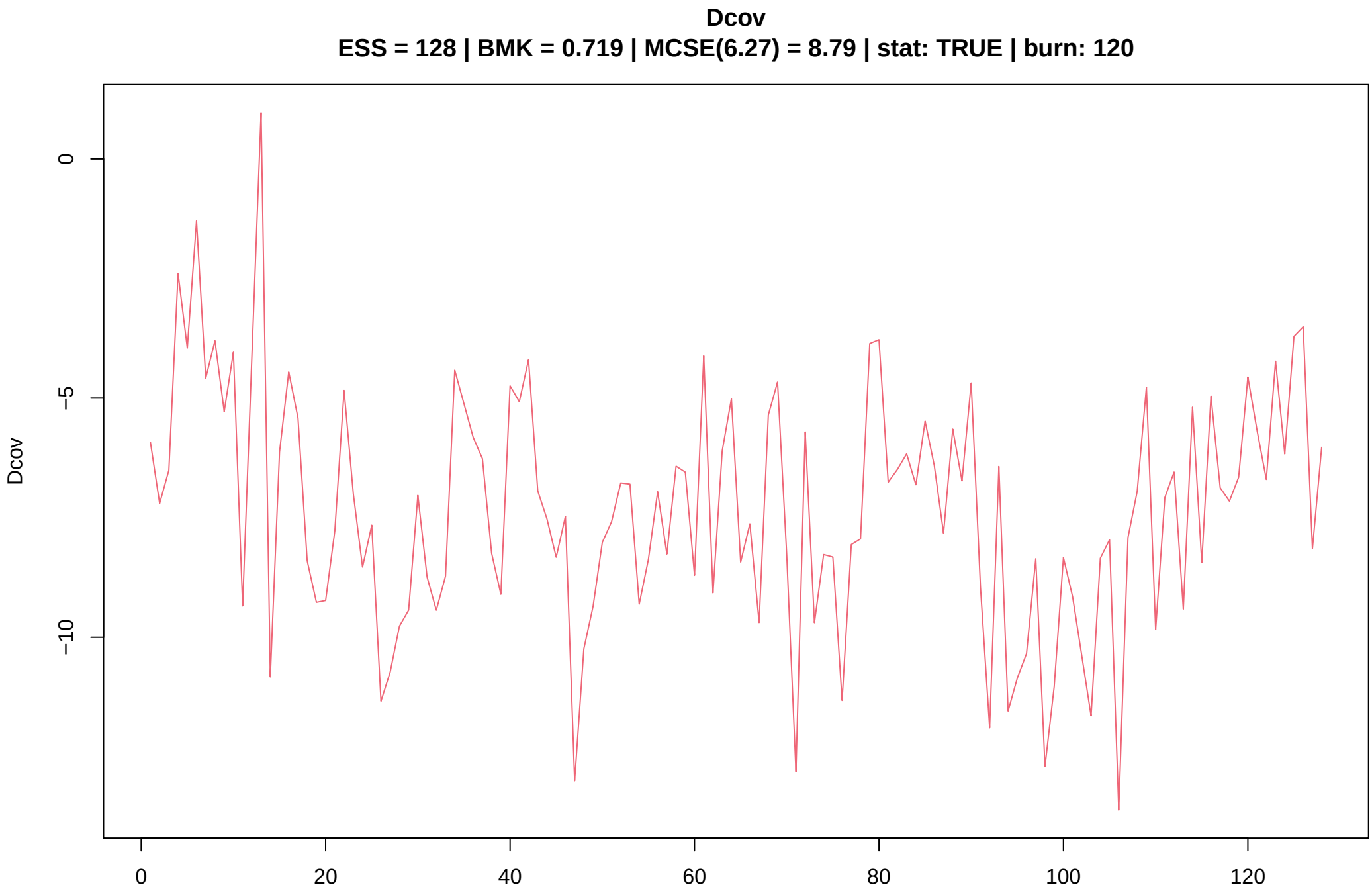

Q3_mcs_RingCount
ESS = 128 | BMK = 0.00895 | MCSE(6.27) = 9.5 | stat: TRUE | burn: 0
Q3_mcs_RingCount
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

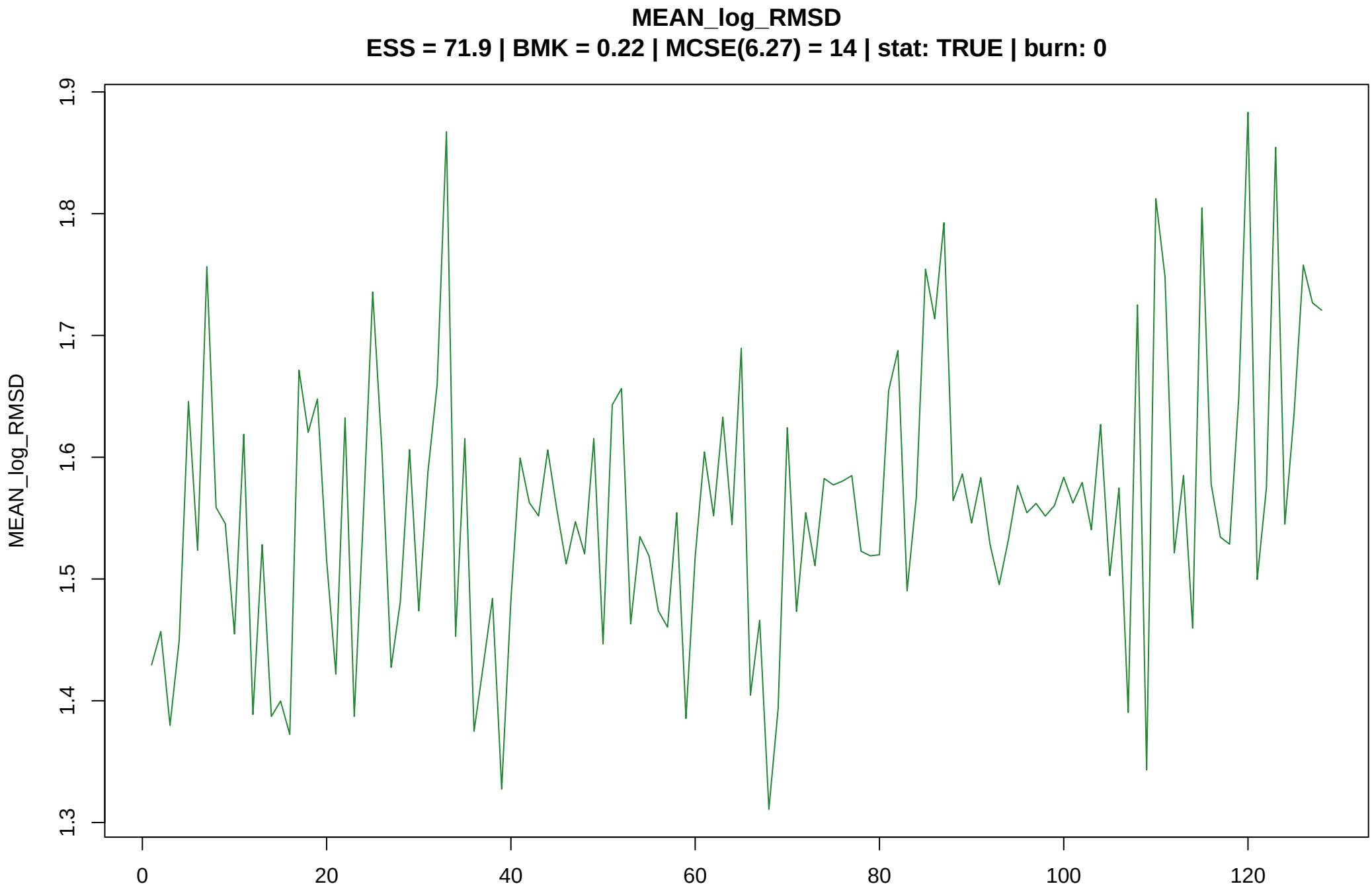

Q3_template_HeavyAtomCount
ESS = 128 | BMK = 0.135 | MCSE(6.27) = 8.95 | stat: FALSE | burn: 0
Q3_template_HeavyAtomCount
24
26
28
30
32
0
20
40
60
80
100
120

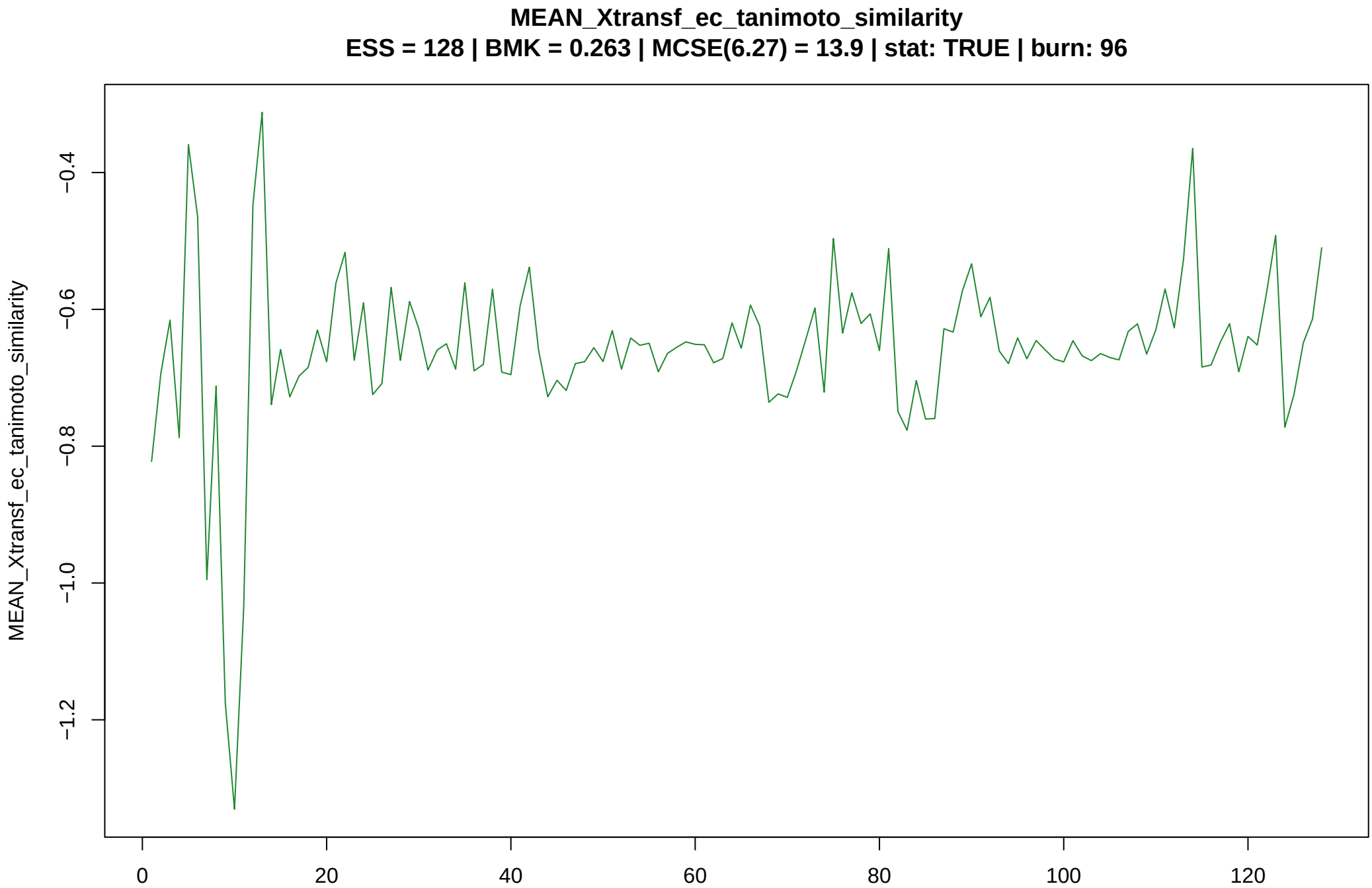

Q3_mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.0409 | MCSE(6.27) = 9.17 | stat: TRUE | burn: 0
Q3_mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

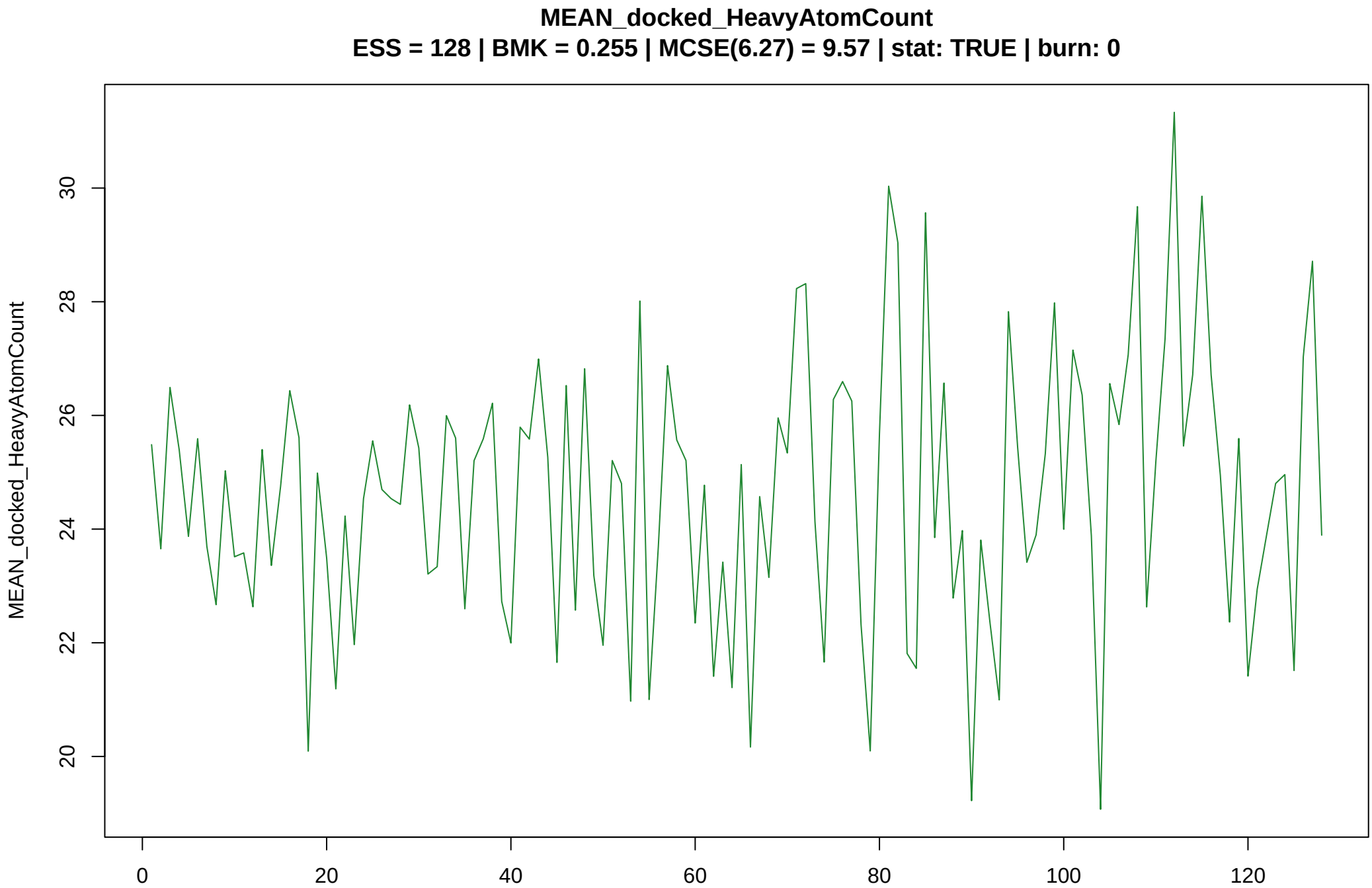

Q3_mcs_template_NumHAcceptors
ESS = 84.4 | BMK = 0.145 | MCSE(6.27) = 12.1 | stat: TRUE | burn: 96
Q3_mcs_template_NumHAcceptors
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120

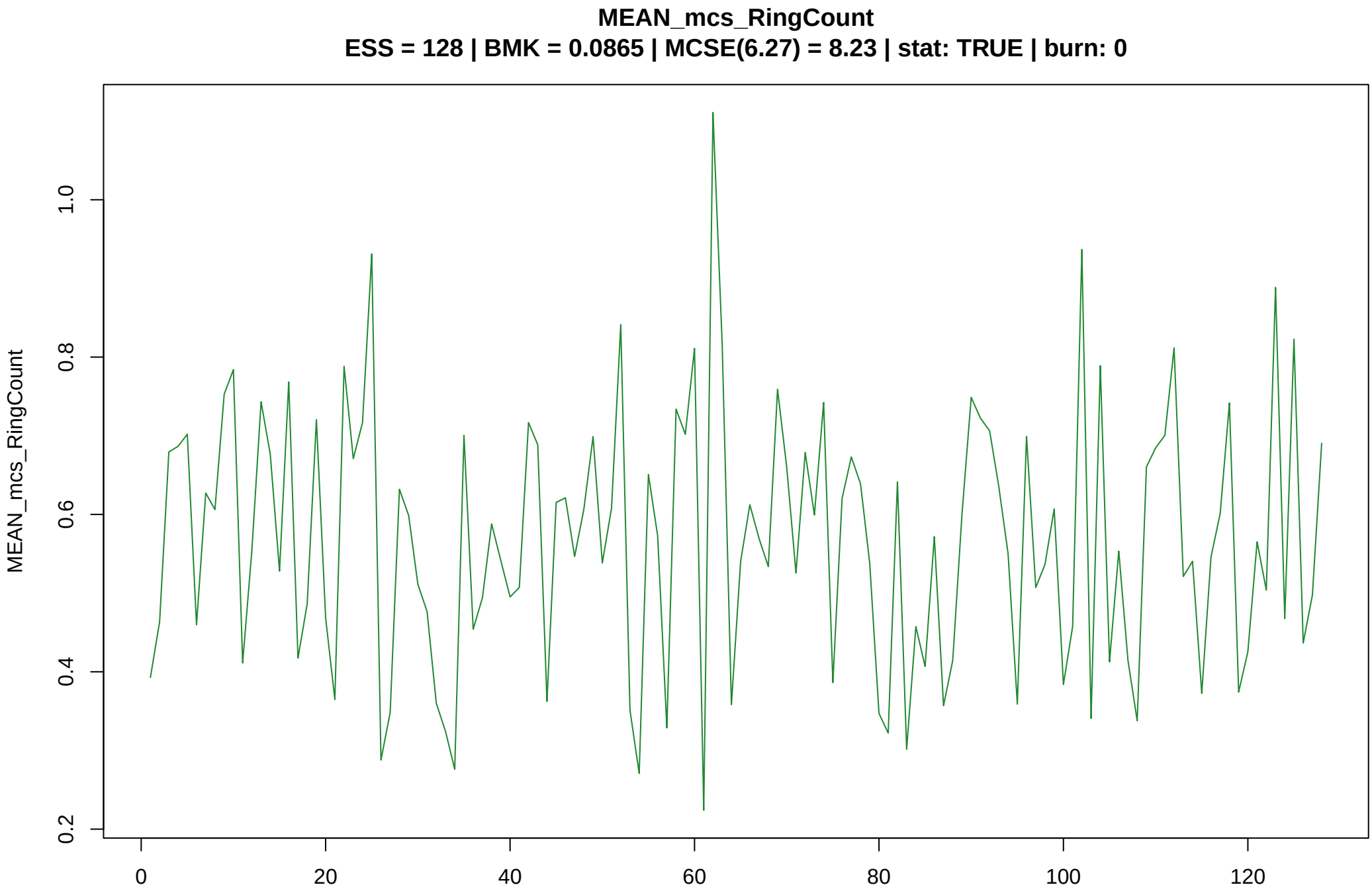

Q3_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.27 | MCSE(6.27) = 7.36 | stat: TRUE | burn: 0
Q3_mcs_NumHeteroAtoms
1.0
1.5
2.0
2.5
3.0
0
20
40
60
80
100
120

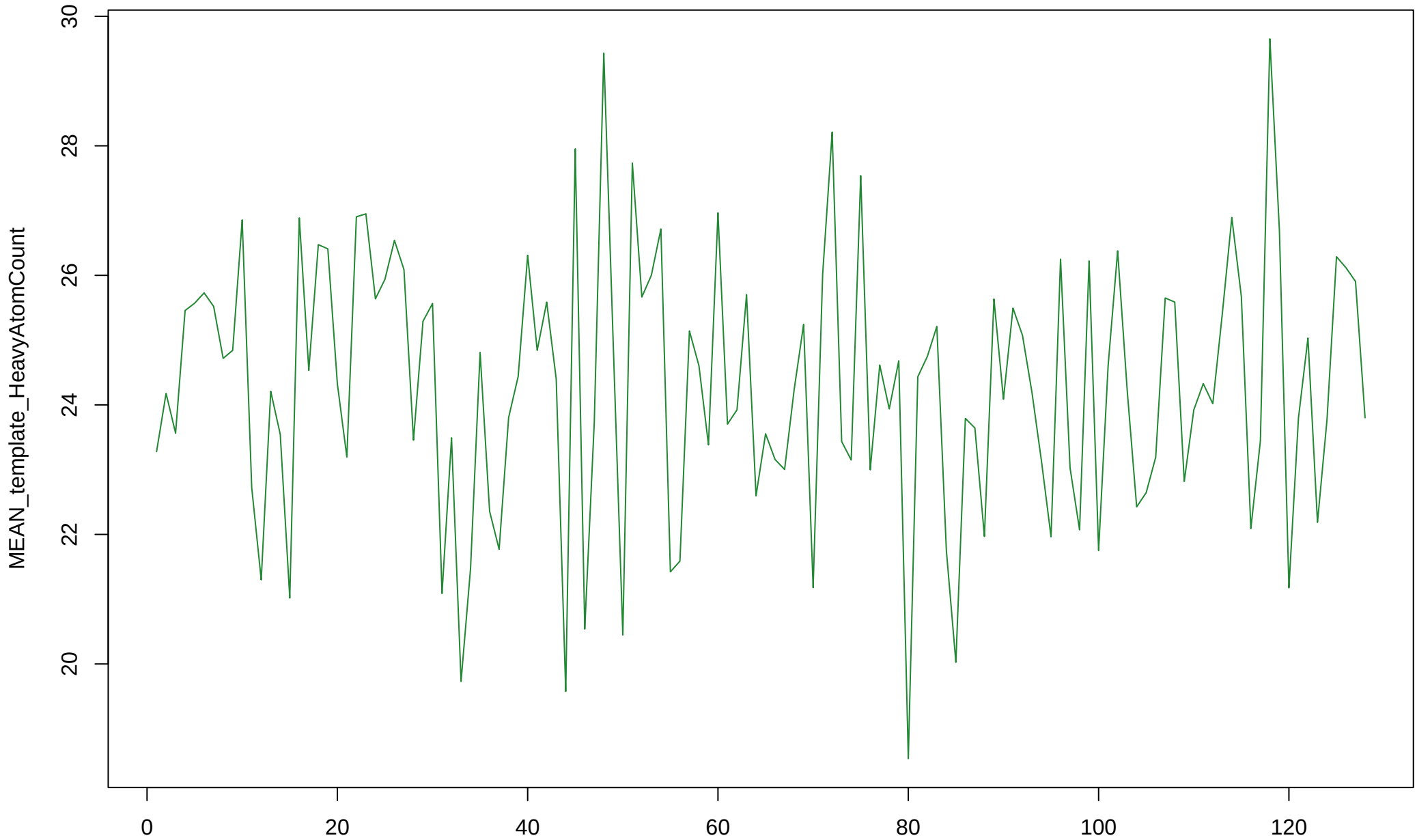

Dcov
ESS = 128 | BMK = 0.719 | MCSE(6.27) = 8.79 | stat: TRUE | burn: 120
Dcov
0
−5
−10
0
20
40
60
80
100
120

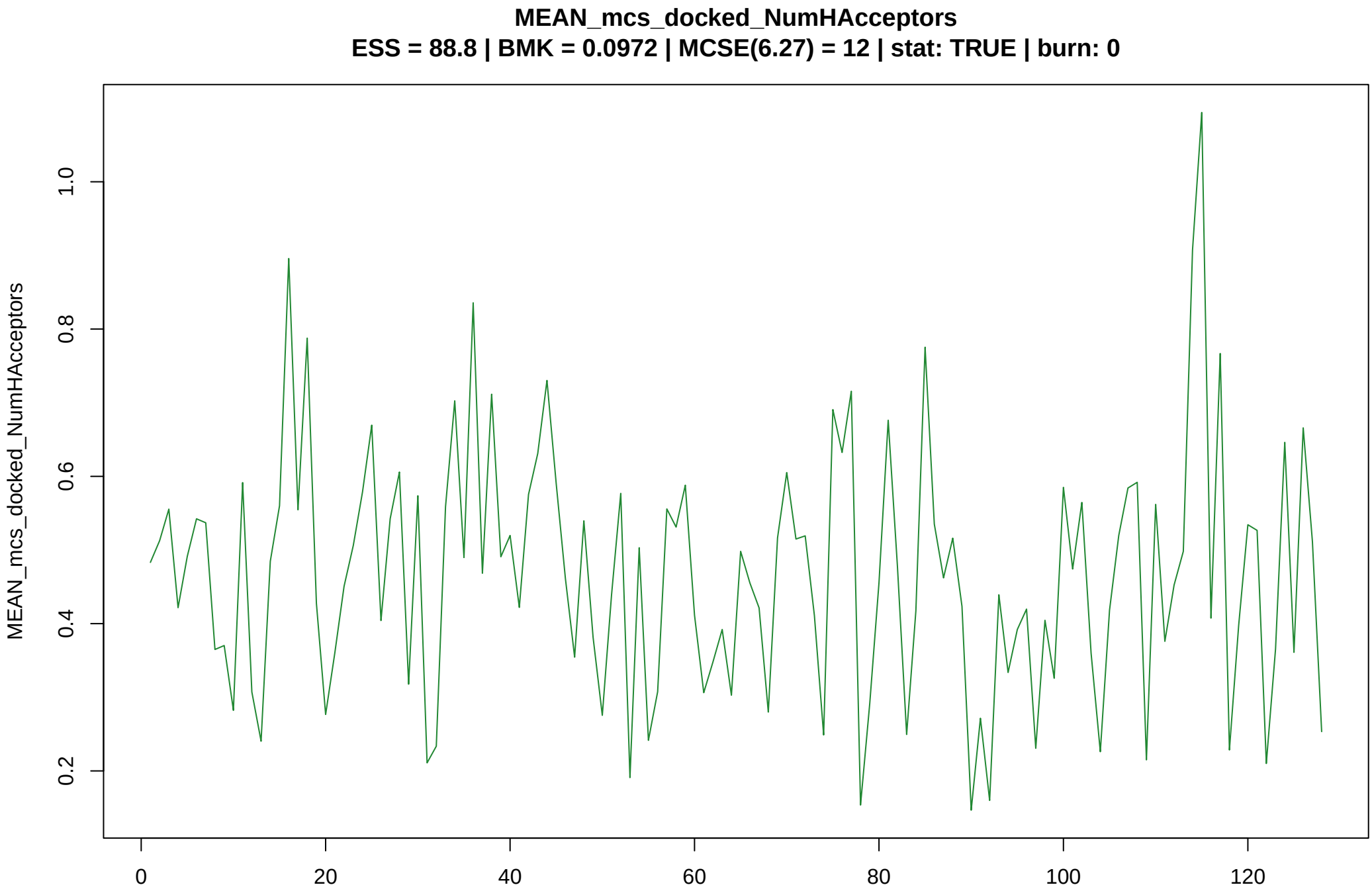

MEAN_log_RMSD
ESS = 71.9 | BMK = 0.22 | MCSE(6.27) = 14 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.3
1.4
1.5
1.6
1.7
1.8
1.9
0
20
40
60
80
100
120

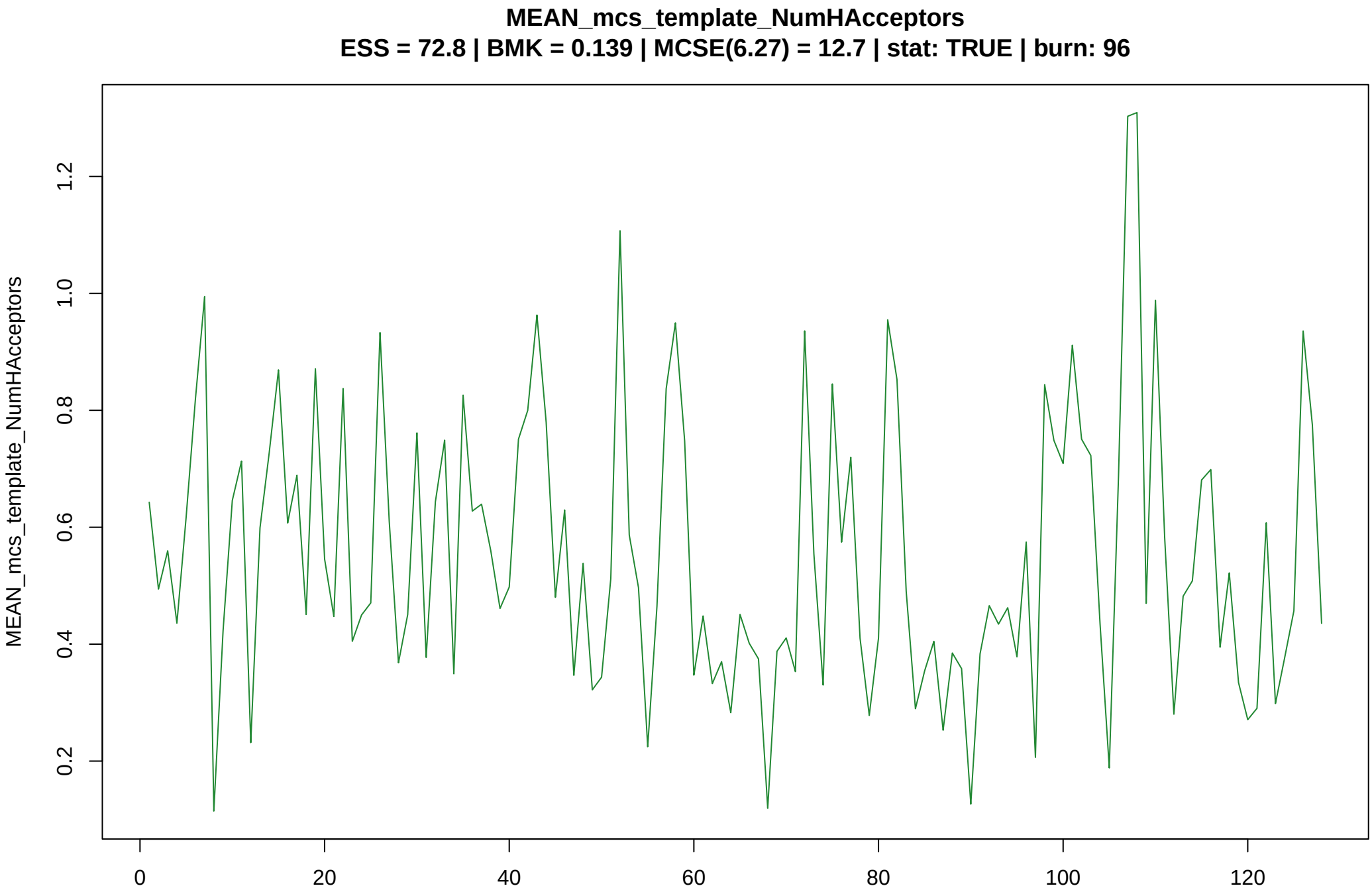

MEAN_Xtransf_ec_tanimoto_similarity
ESS = 128 | BMK = 0.263 | MCSE(6.27) = 13.9 | stat: TRUE | burn: 96
MEAN_Xtransf_ec_tanimoto_similarity
−0.4
−0.6
−0.8
−1.0
−1.2
0
20
40
60
80
100
120

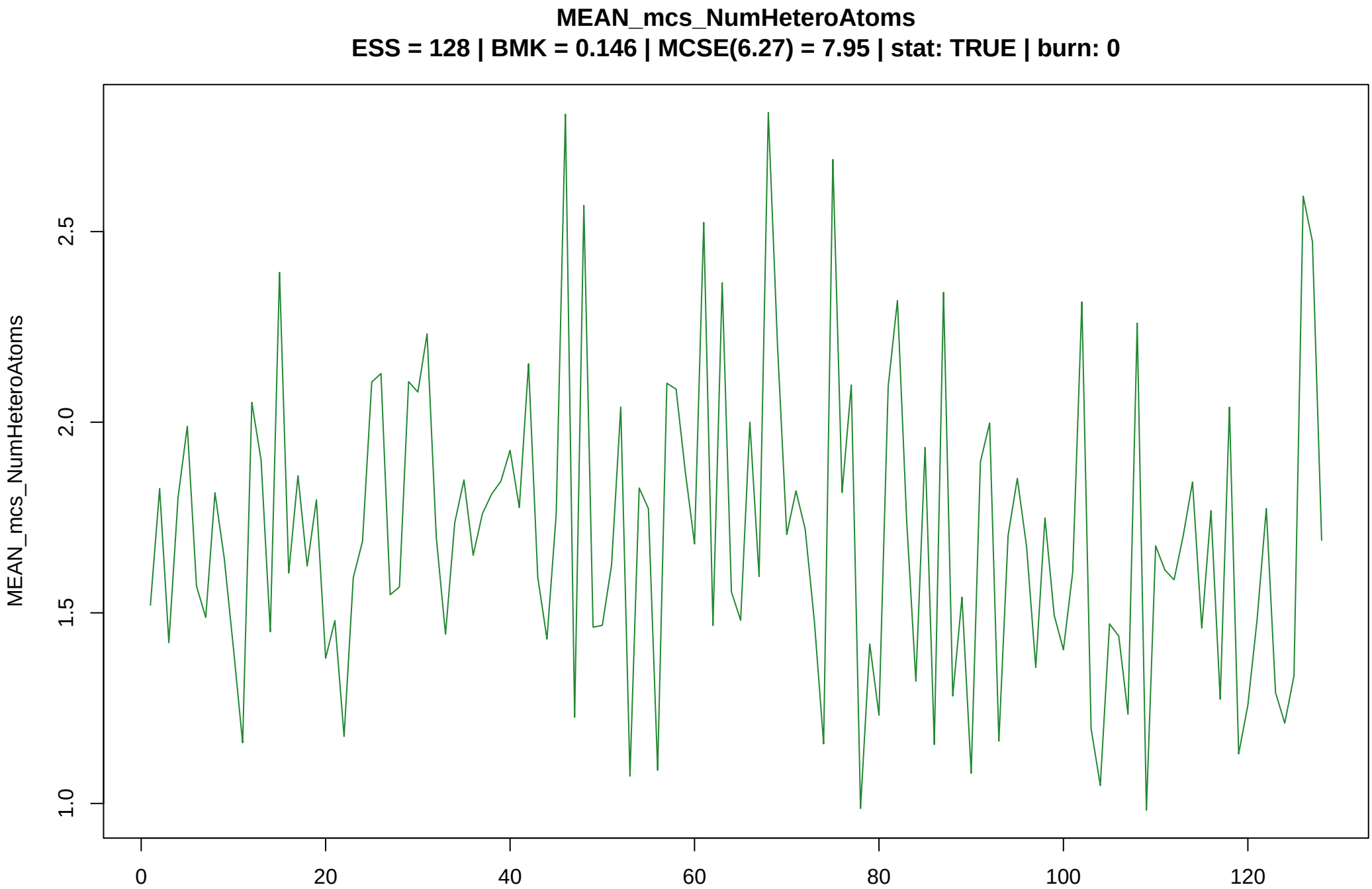

MEAN_docked_HeavyAtomCount
ESS = 128 | BMK = 0.255 | MCSE(6.27) = 9.57 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
20
22
24
26
28
30
0
20
40
60
80
100
120

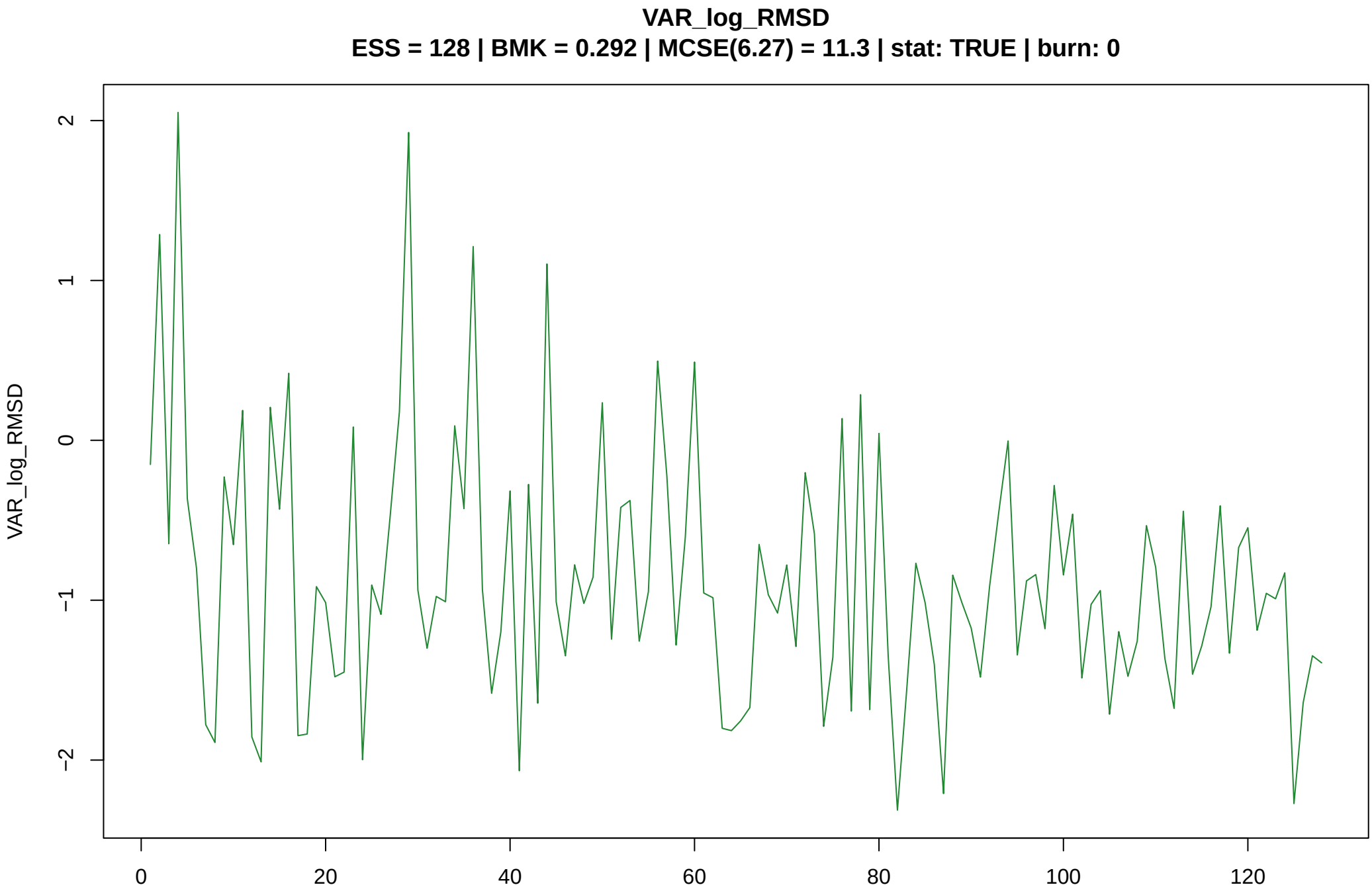

MEAN_mcs_RingCount
ESS = 128 | BMK = 0.0865 | MCSE(6.27) = 8.23 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

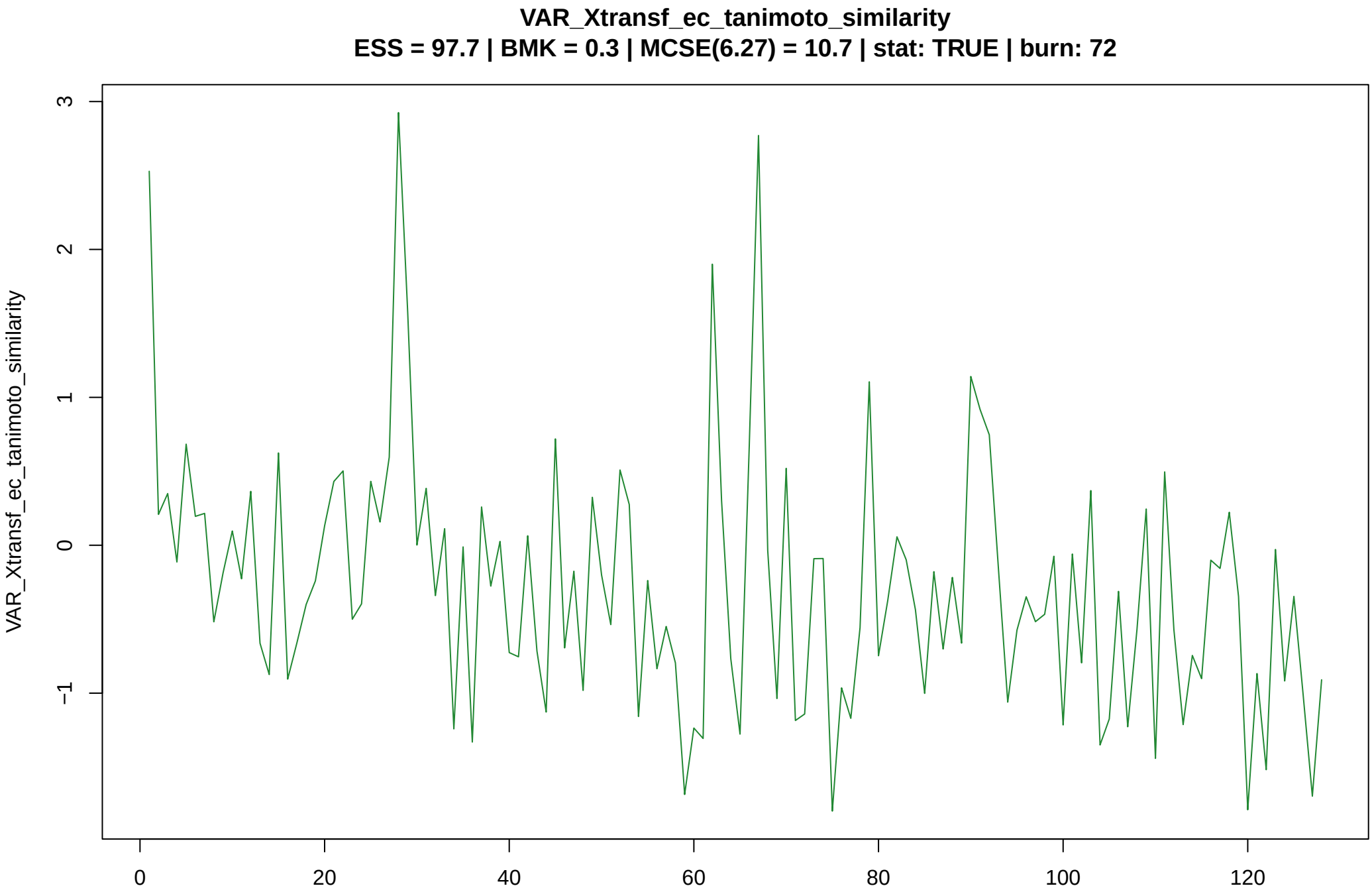

MEAN_template_HeavyAtomCount
ESS = 105 | BMK = 0.125 | MCSE(6.27) = 8.9 | stat: TRUE | burn: 0
MEAN_template_HeavyAtomCount
30
28
26
24
22
20
0
20
40
60
80
100
120

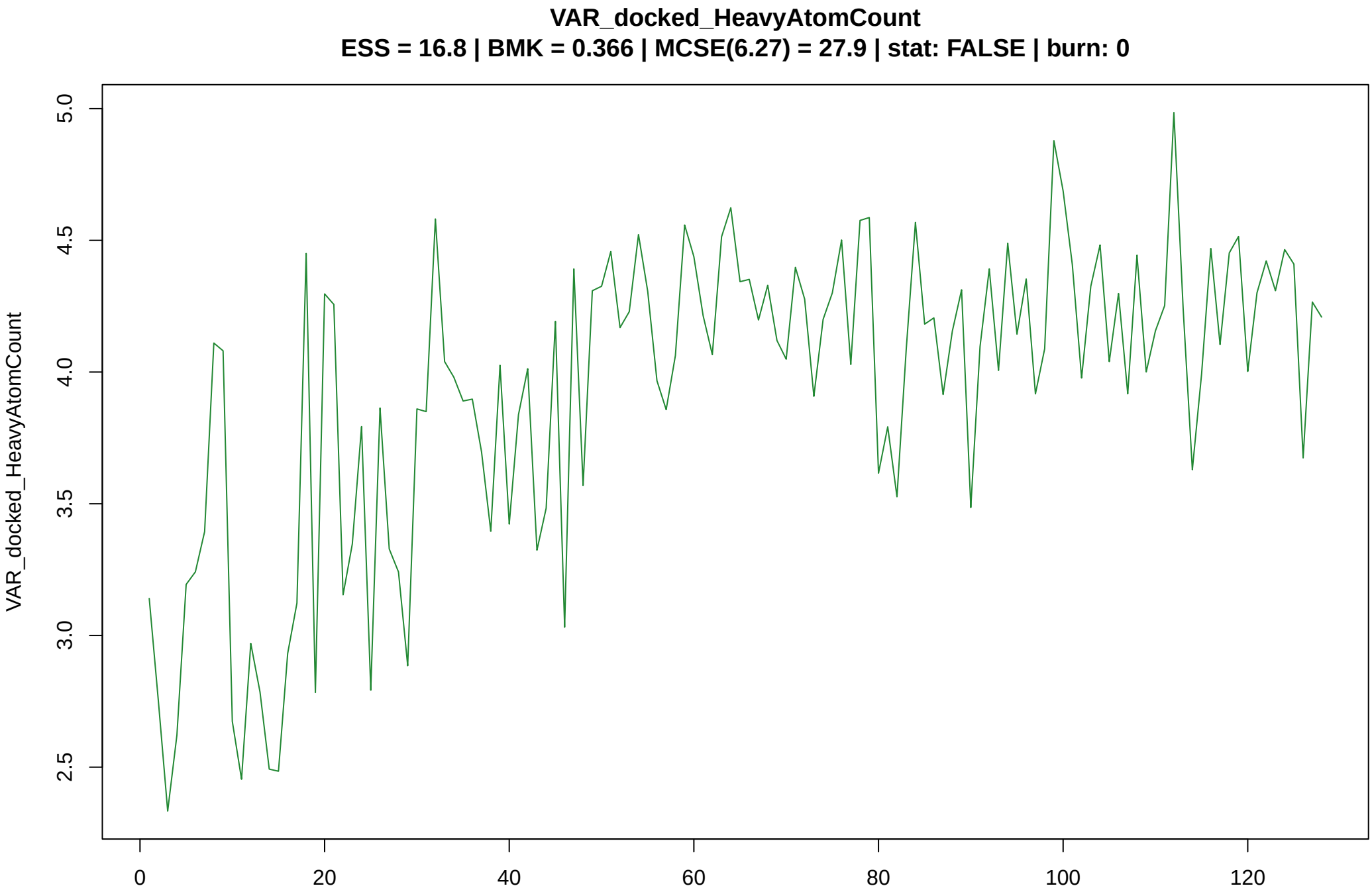

MEAN_mcs_docked_NumHAcceptors
ESS = 88.8 | BMK = 0.0972 | MCSE(6.27) = 12 | stat: TRUE | burn: 0
MEAN_mcs_docked_NumHAcceptors
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100
120

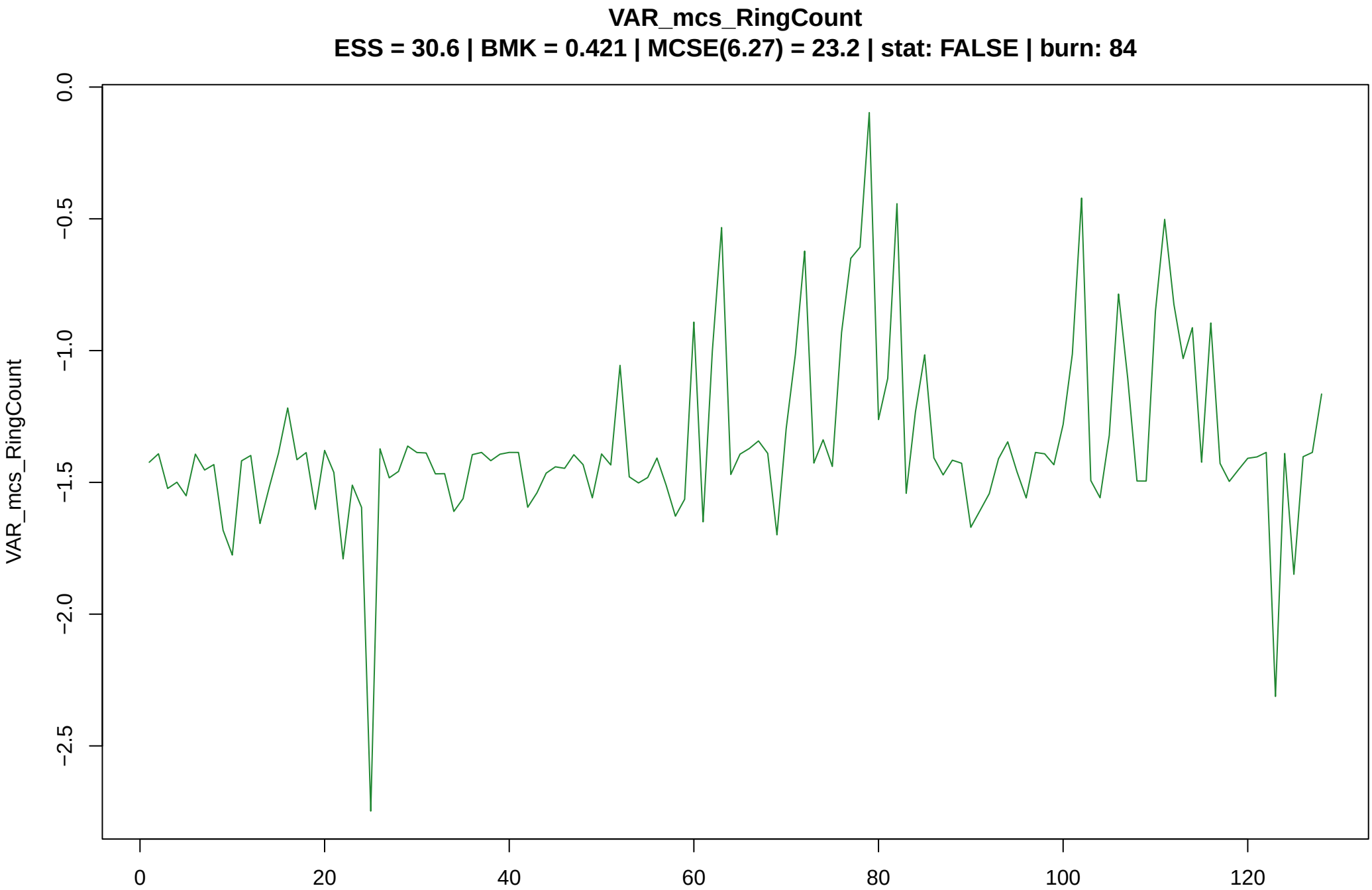

MEAN_mcs_template_NumHAcceptors
ESS = 72.8 | BMK = 0.139 | MCSE(6.27) = 12.7 | stat: TRUE | burn: 96
MEAN_mcs_template_NumHAcceptors
0.2
0.4
0.6
0.8
1.0
1.2
0
20
40
60
80
100
120

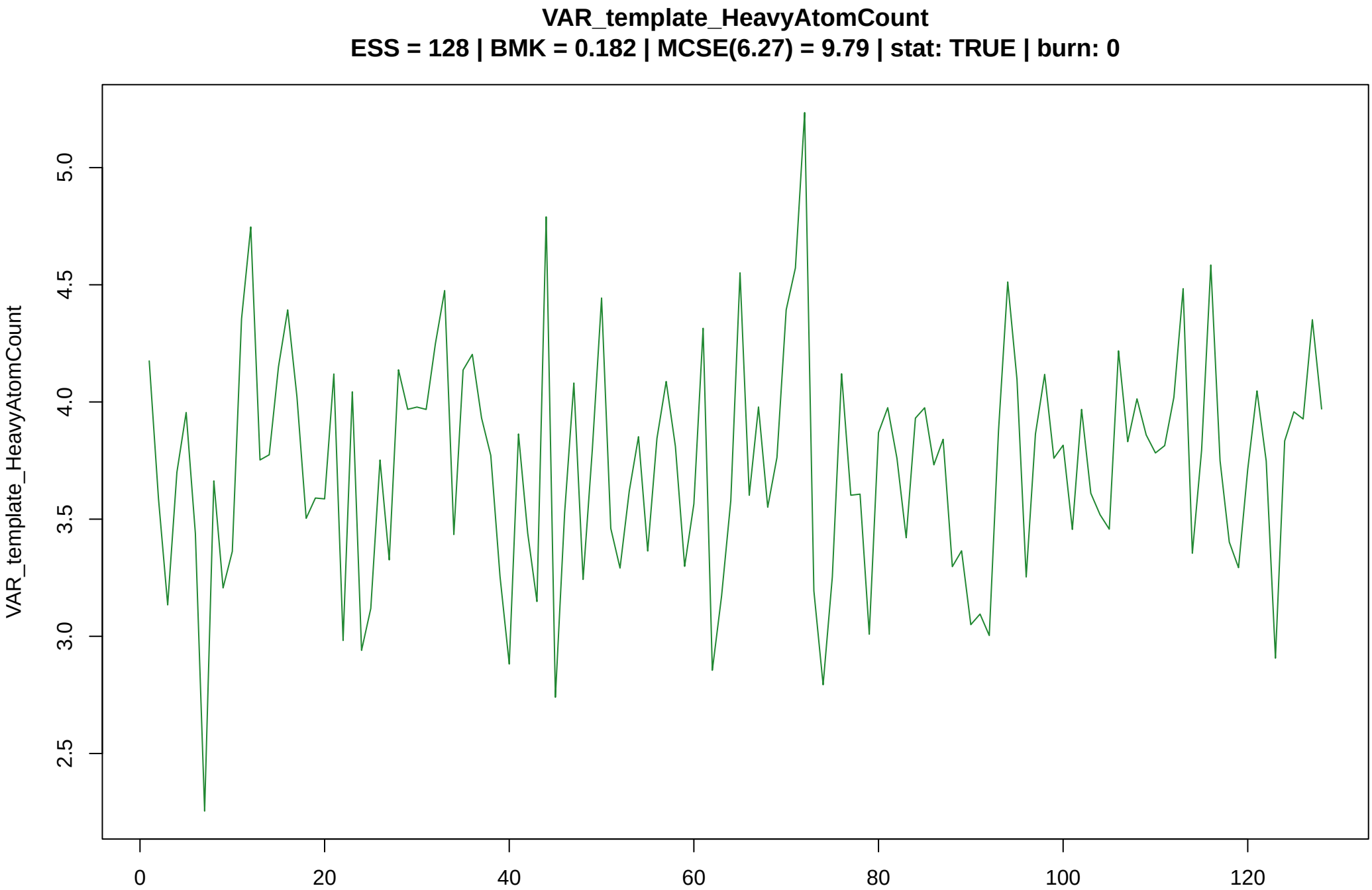

MEAN_mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.146 | MCSE(6.27) = 7.95 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120

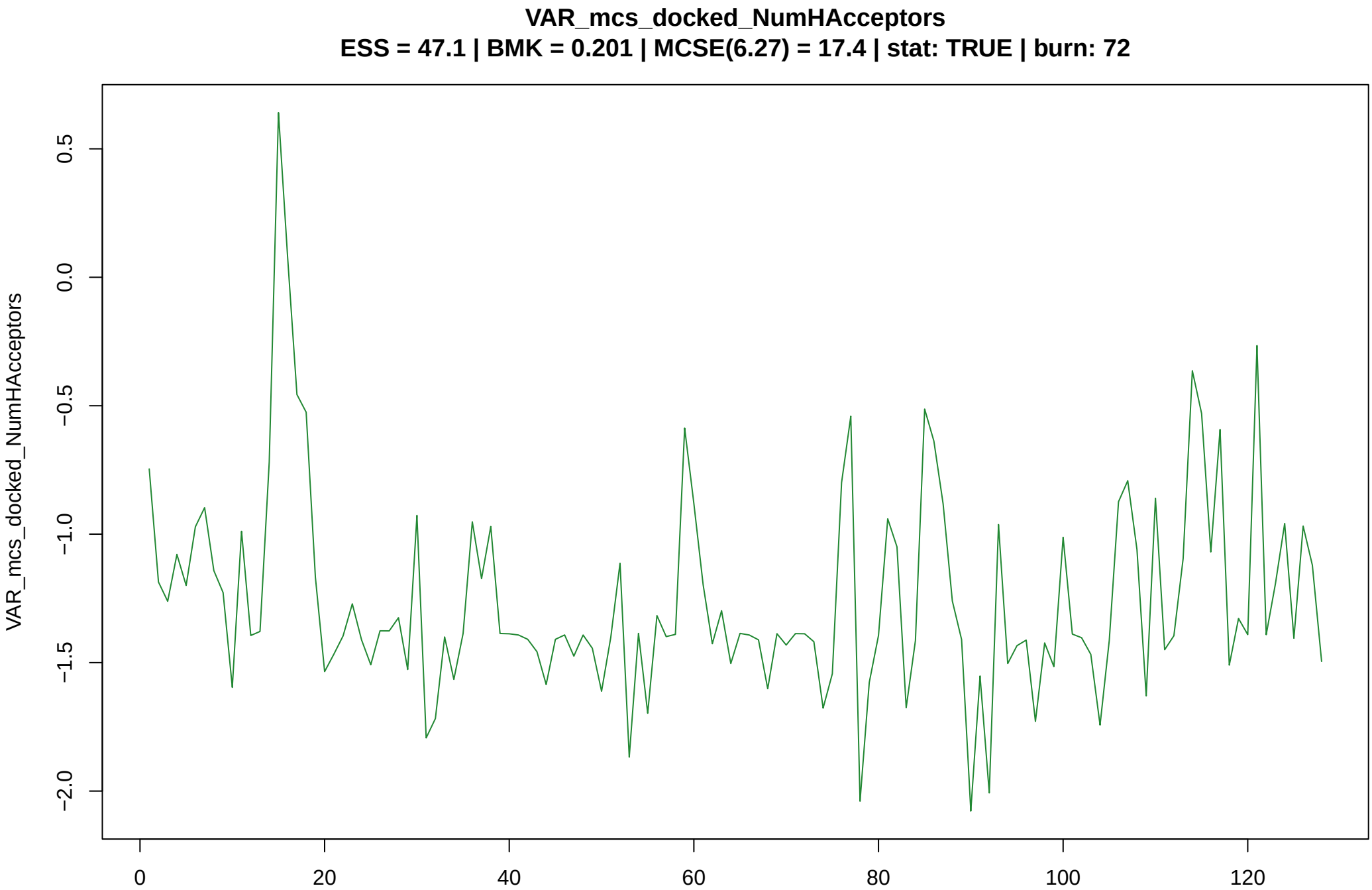

VAR_log_RMSD
ESS = 128 | BMK = 0.292 | MCSE(6.27) = 11.3 | stat: TRUE | burn: 0
VAR_log_RMSD
2
1
0
−1
−2
0
20
40
60
80
100
120

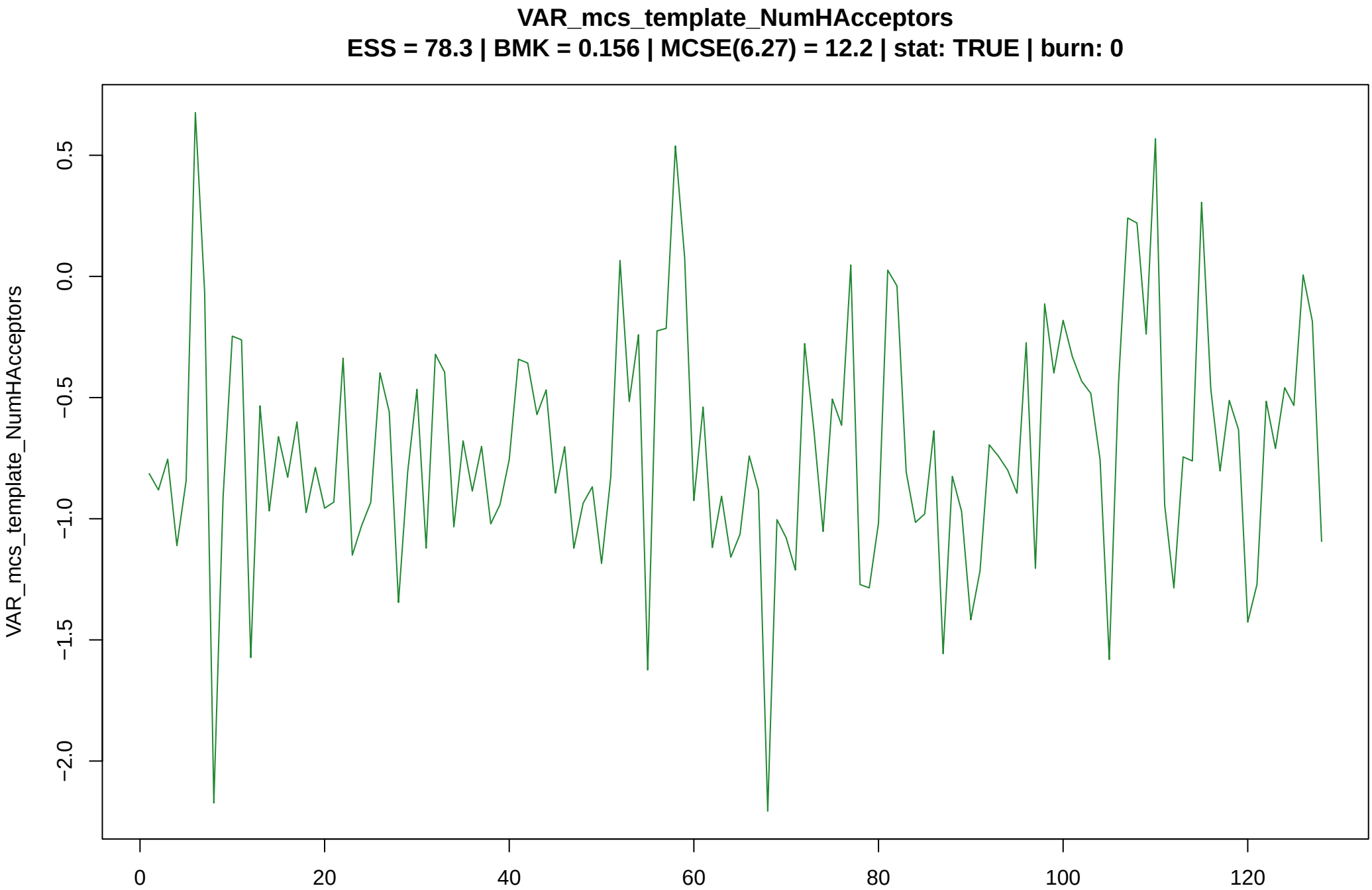

VAR_Xtransf_ec_tanimoto_similarity
ESS = 97.7 | BMK = 0.3 | MCSE(6.27) = 10.7 | stat: TRUE | burn: 72
VAR_Xtransf_ec_tanimoto_similarity
3
2
1
0
−1
0
20
40
60
80
100
120

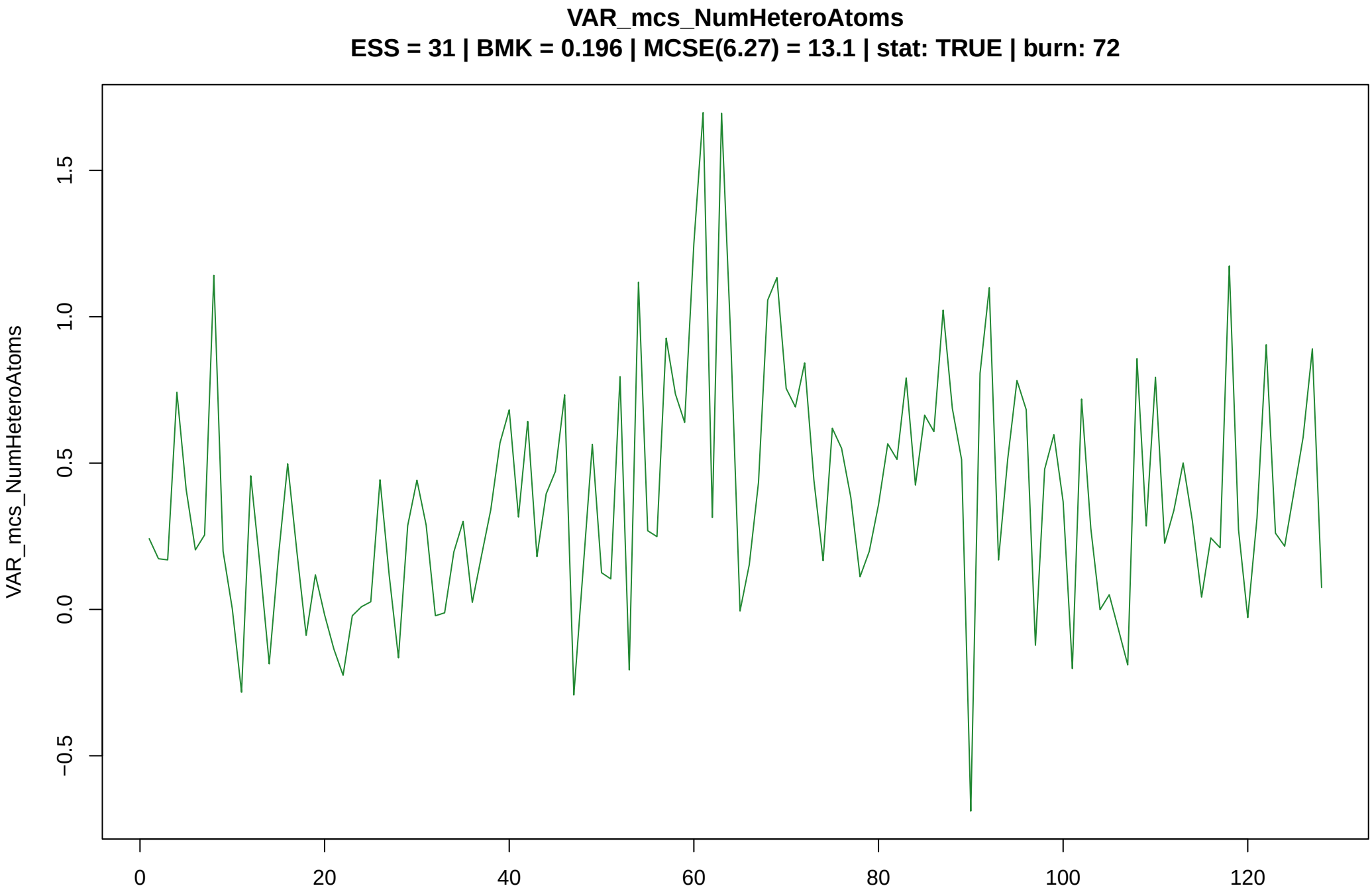

VAR_docked_HeavyAtomCount
ESS = 16.8 | BMK = 0.366 | MCSE(6.27) = 27.9 | stat: FALSE | burn: 0
VAR_docked_HeavyAtomCount
5.0
4.5
4.0
3.5
3.0
2.5
0
20
40
60
80
100
120

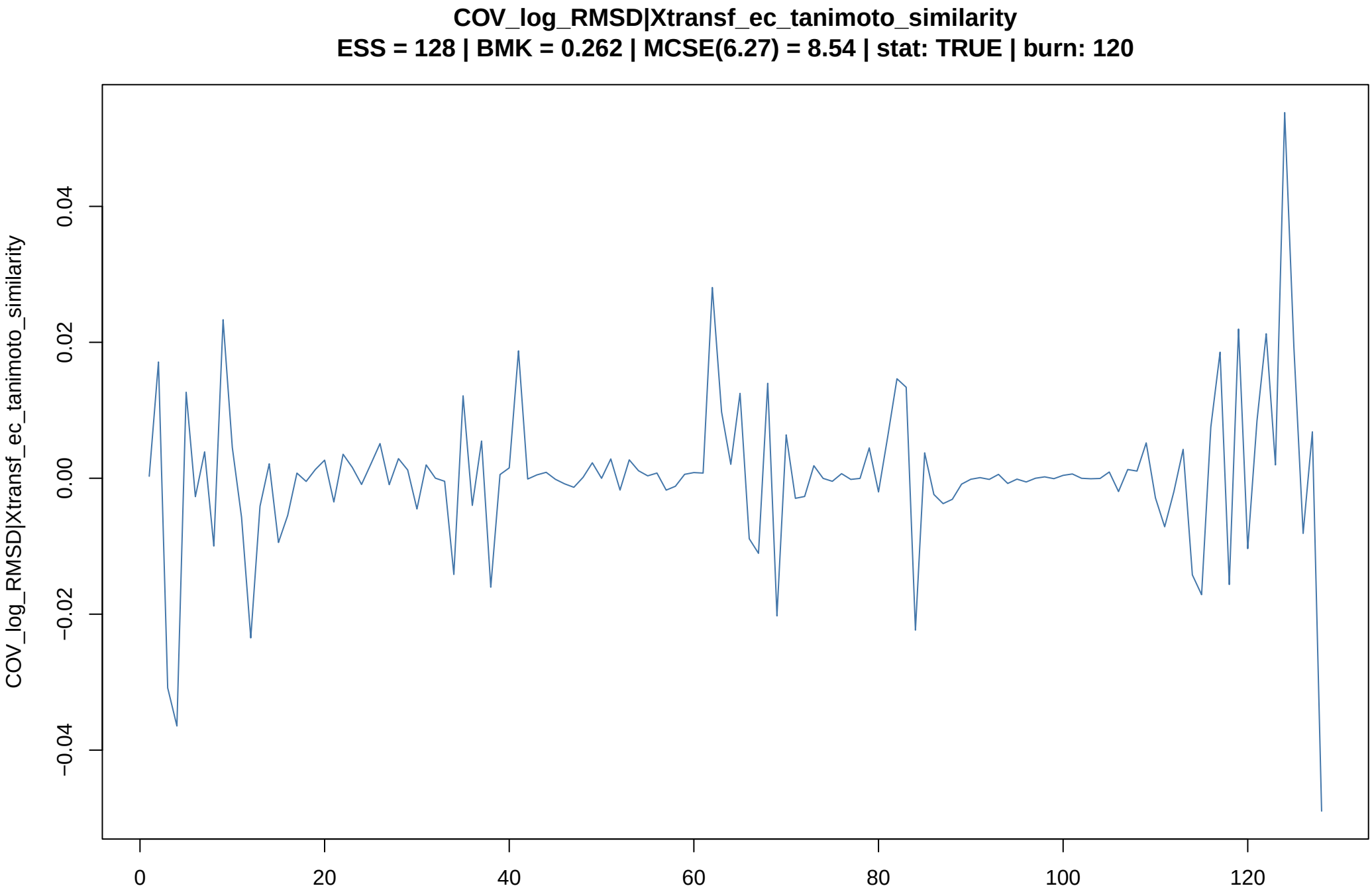

VAR_mcs_RingCount
ESS = 30.6 | BMK = 0.421 | MCSE(6.27) = 23.2 | stat: FALSE | burn: 84
VAR_mcs_RingCount
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
0
20
40
60
80
100
120

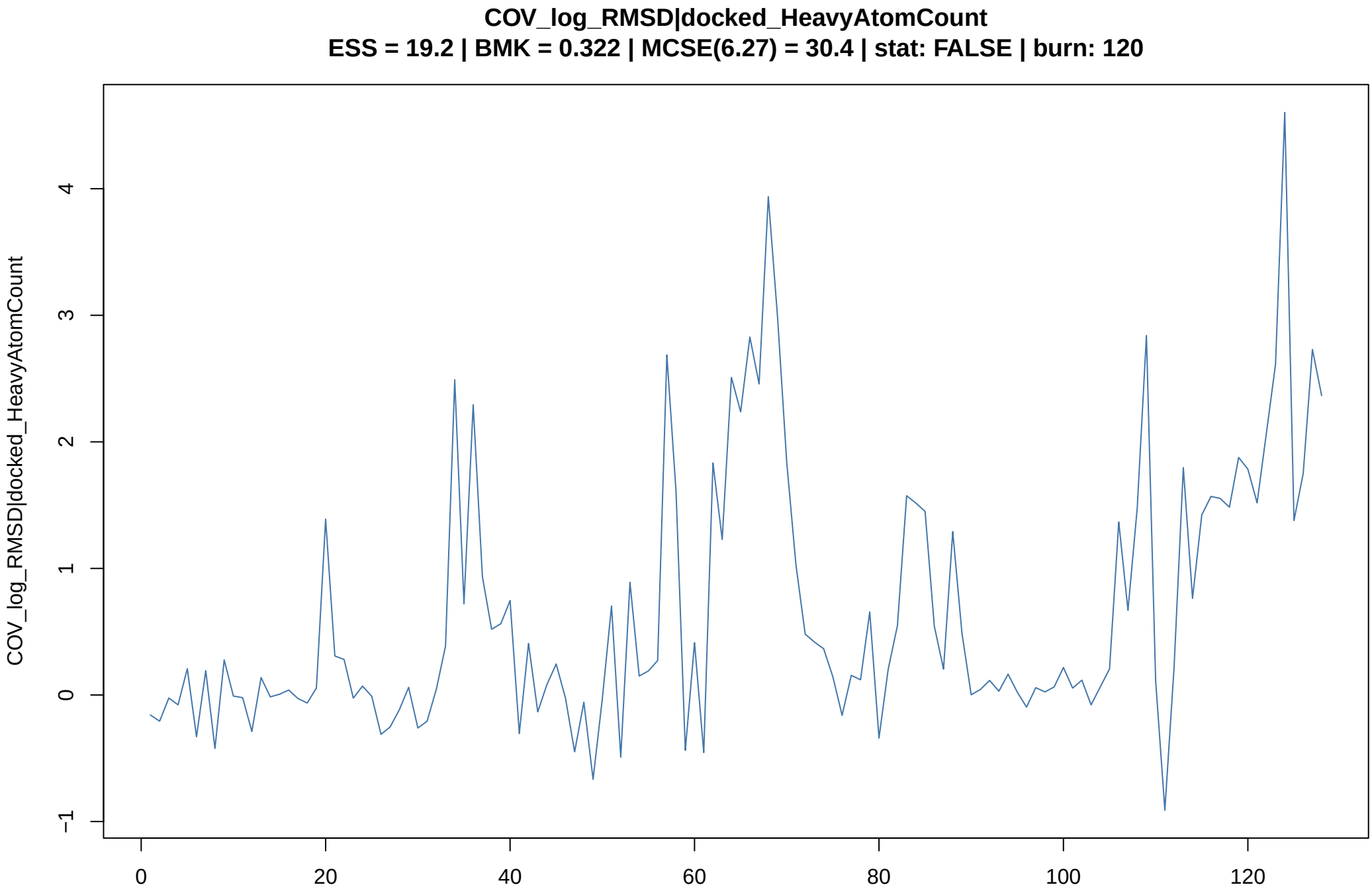

VAR_template_HeavyAtomCount
ESS = 128 | BMK = 0.182 | MCSE(6.27) = 9.79 | stat: TRUE | burn: 0
VAR_template_HeavyAtomCount
2.5
3.0
3.5
4.0
4.5
5.0
0
20
40
60
80
100
120

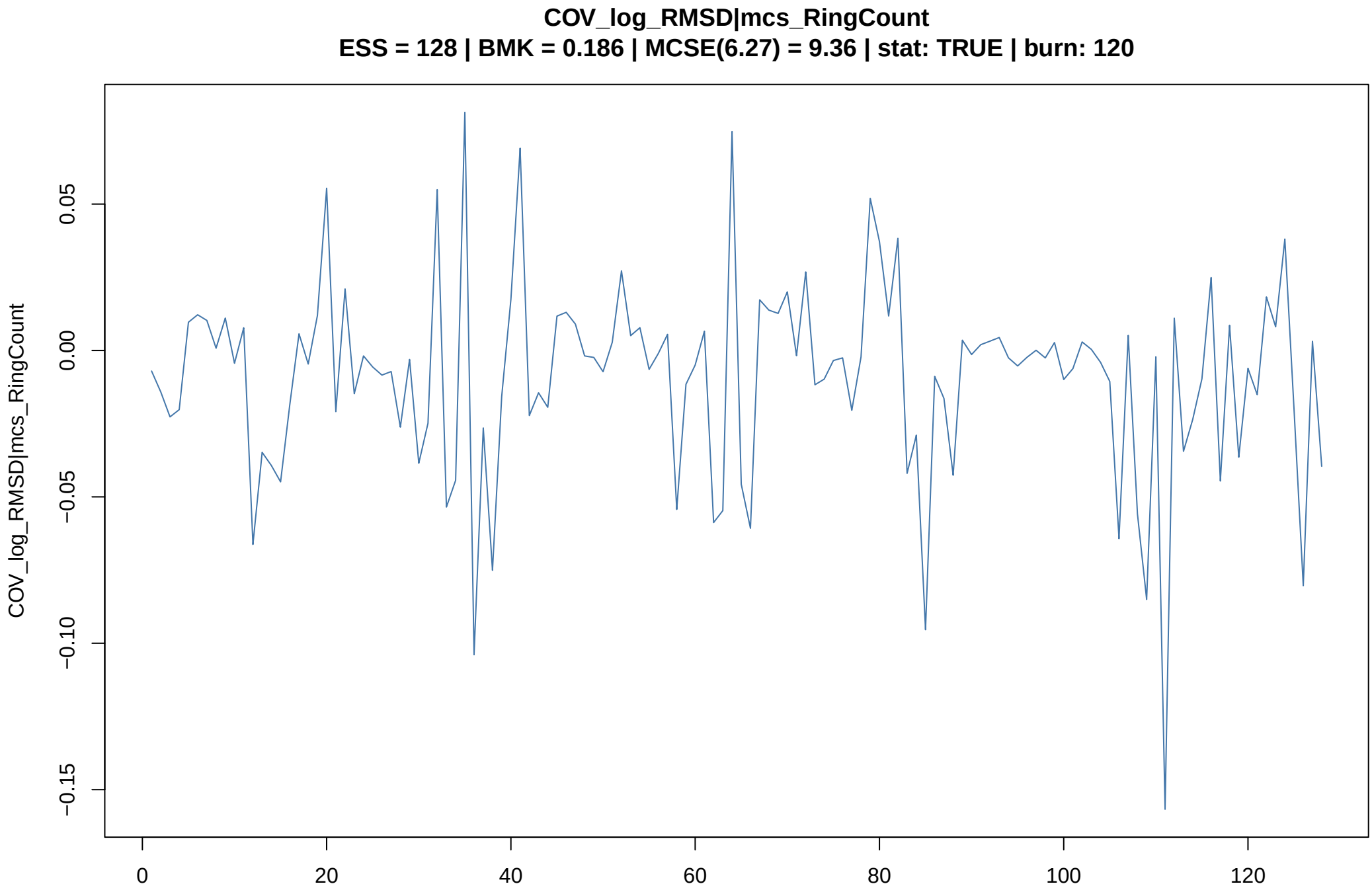

VAR_mcs_docked_NumHAcceptors
ESS = 47.1 | BMK = 0.201 | MCSE(6.27) = 17.4 | stat: TRUE | burn: 72
VAR_mcs_docked_NumHAcceptors
0.5
0.0
−0.5
−1.0
−1.5
−2.0
0
20
40
60
80
100
120

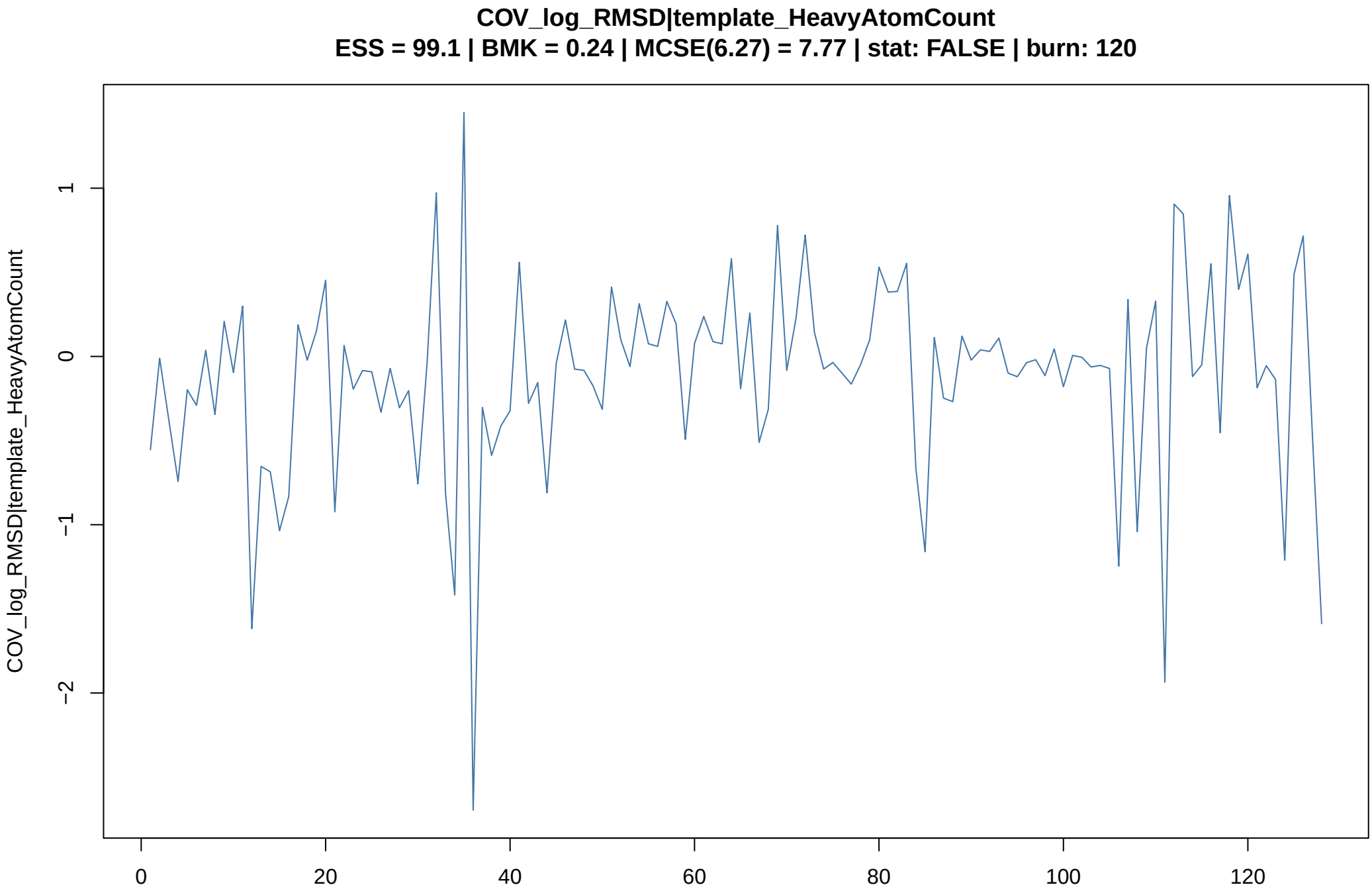

VAR_mcs_template_NumHAcceptors
ESS = 78.3 | BMK = 0.156 | MCSE(6.27) = 12.2 | stat: TRUE | burn: 0
VAR_mcs_template_NumHAcceptors
0.5
0.0
−0.5
−1.0
−1.5
−2.0
0
20
40
60
80
100
120

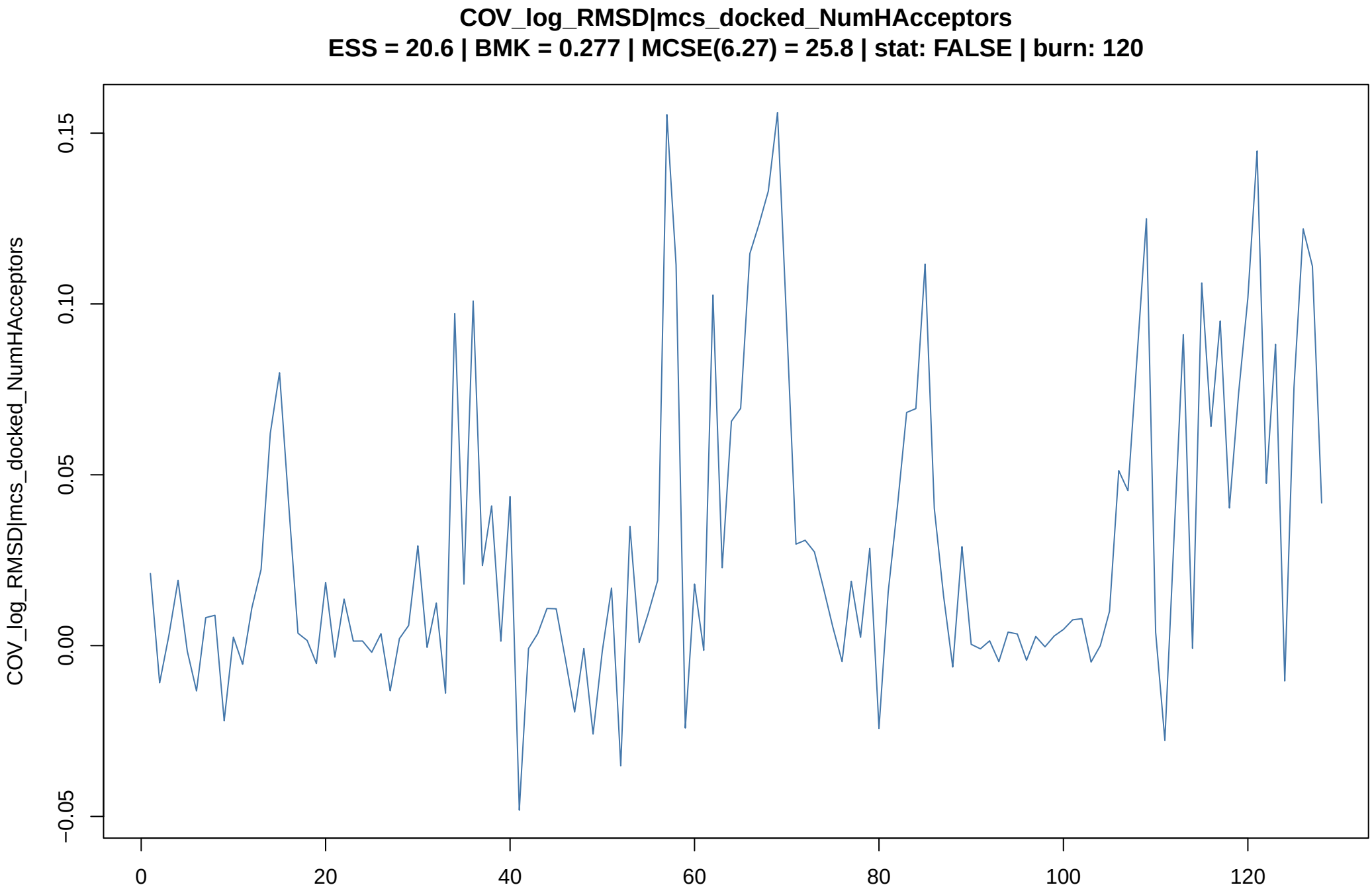

VAR_mcs_NumHeteroAtoms
ESS = 31 | BMK = 0.196 | MCSE(6.27) = 13.1 | stat: TRUE | burn: 72
VAR_mcs_NumHeteroAtoms
−0.5
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120

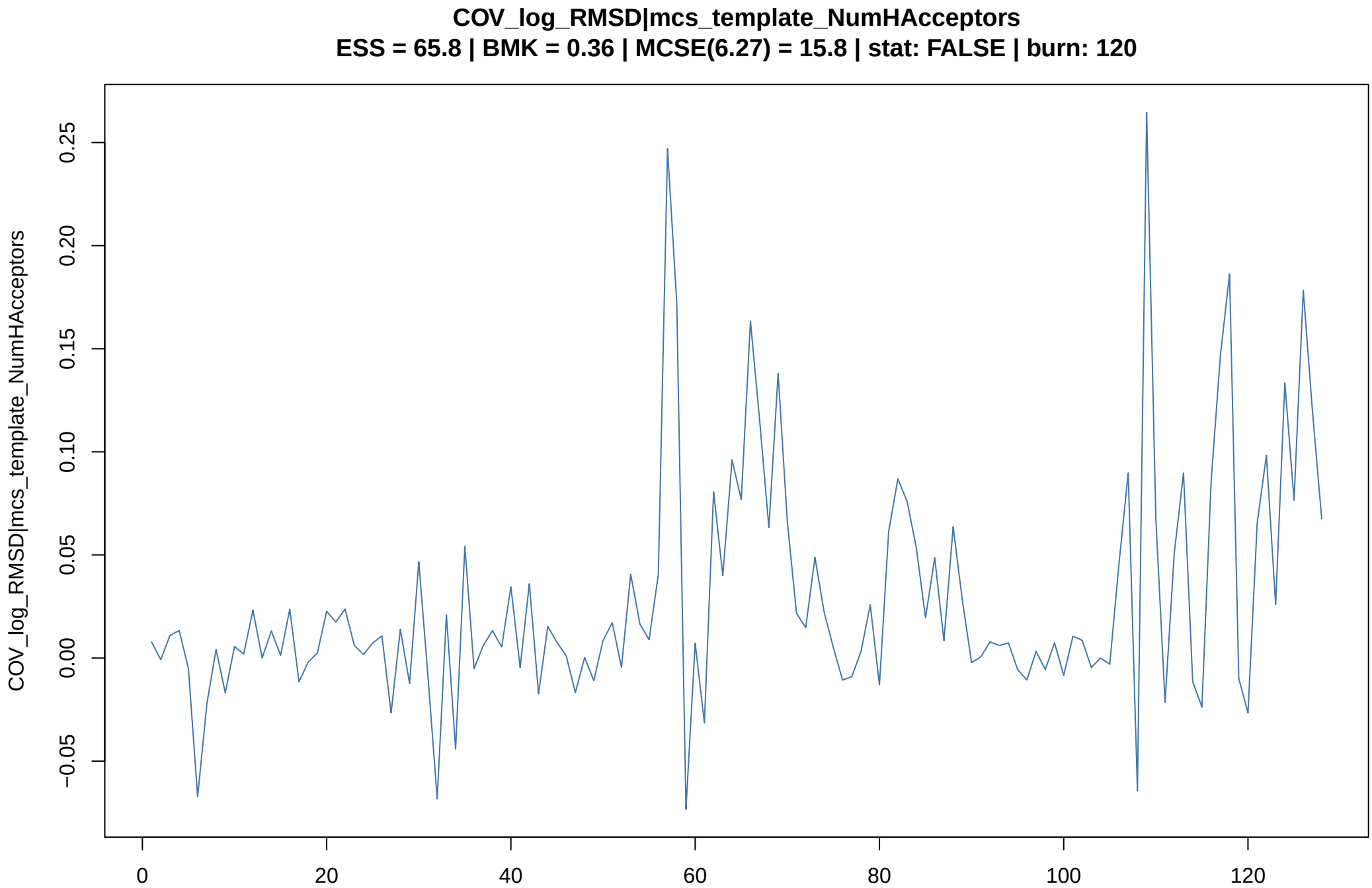

COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 128 | BMK = 0.262 | MCSE(6.27) = 8.54 | stat: TRUE | burn: 120
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
0.04
0.02
0.00
−0.02
−0.04
0
20
40
60
80
100
120

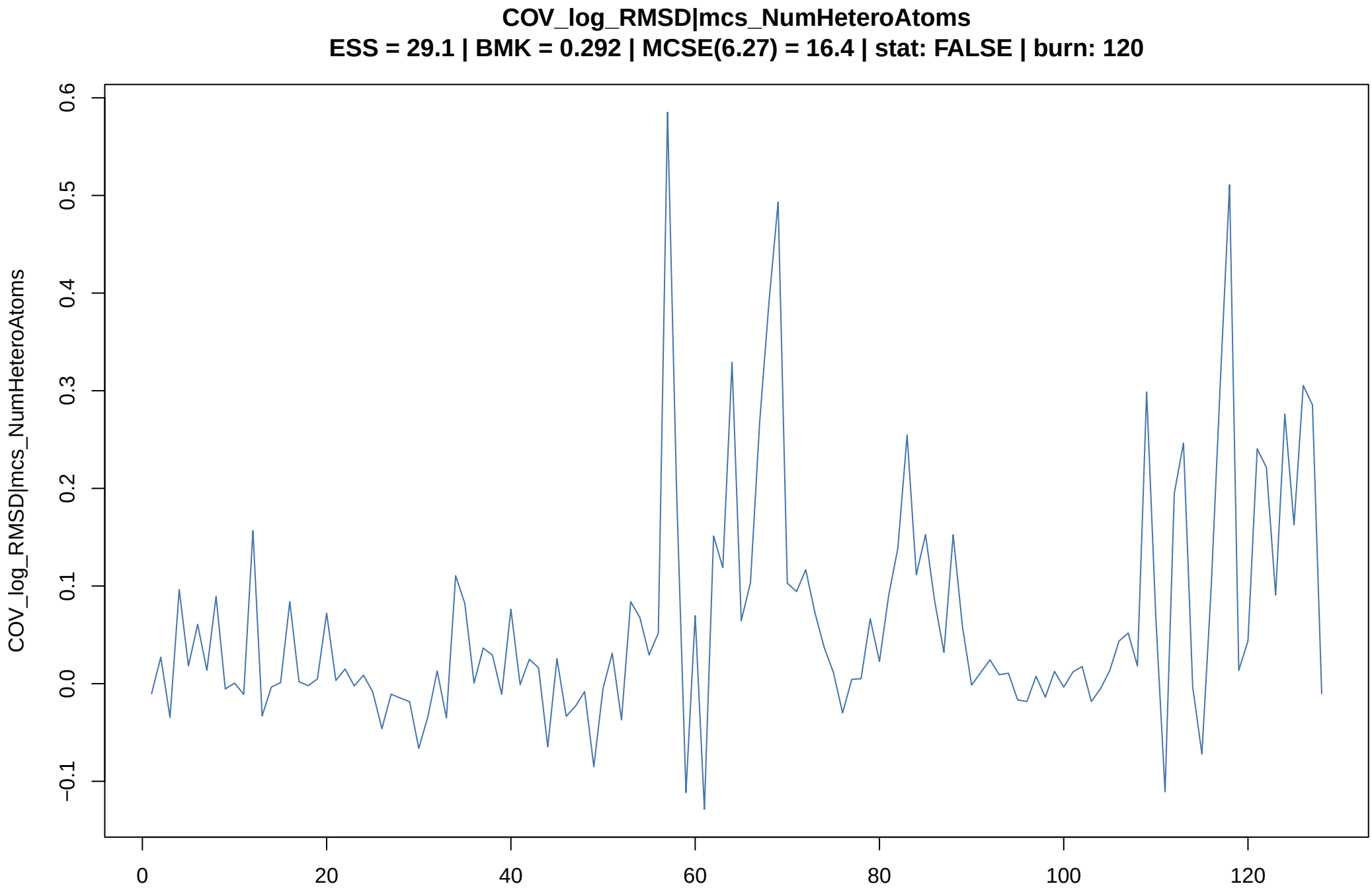

COV_log_RMSD|docked_HeavyAtomCount
ESS = 19.2 | BMK = 0.322 | MCSE(6.27) = 30.4 | stat: FALSE | burn: 120
COV_log_RMSD|docked_HeavyAtomCount
−1
0
1
2
3
4
0
20
40
60
80
100
120

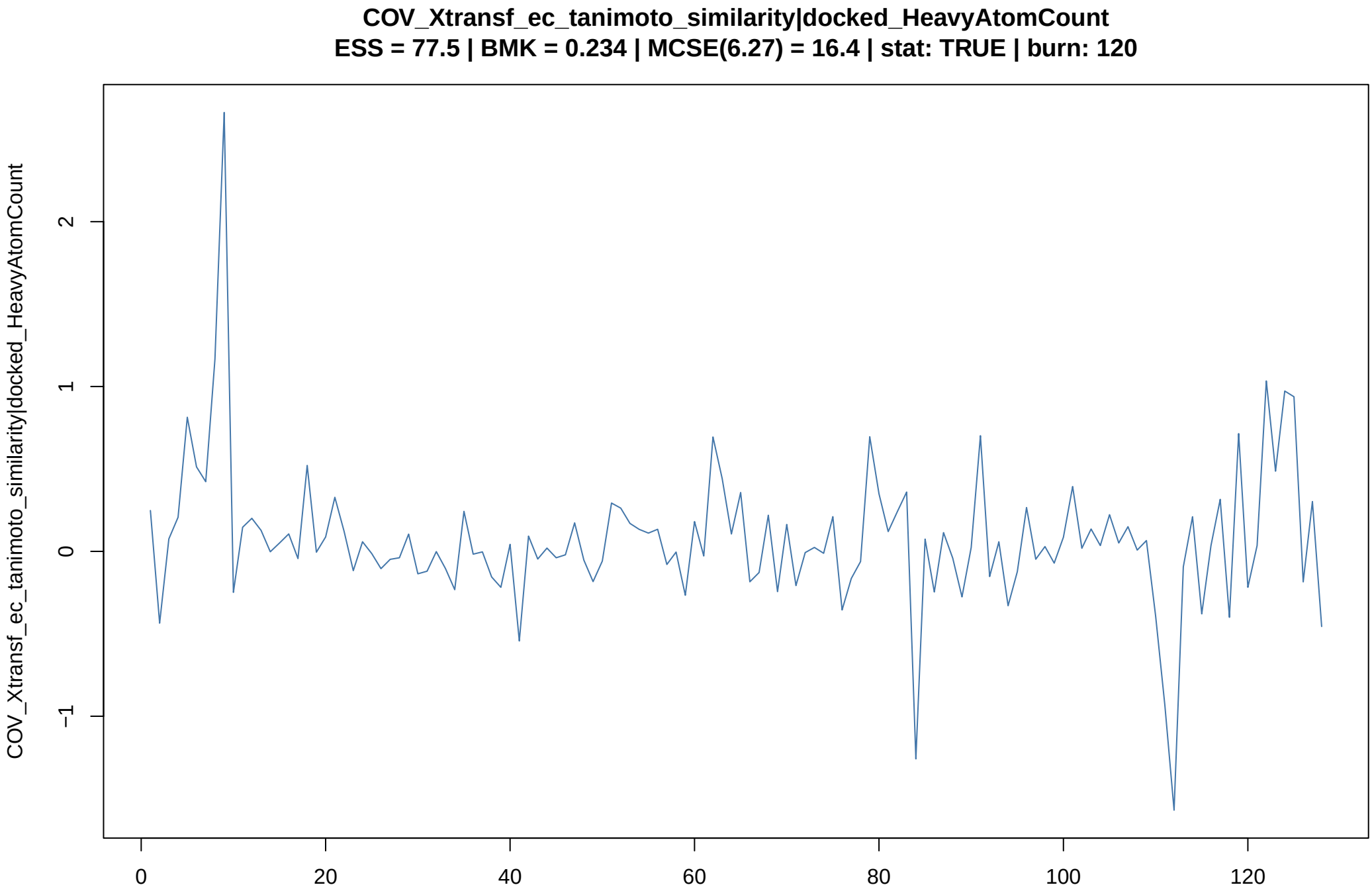

COV_log_RMSD|mcs_RingCount
ESS = 128 | BMK = 0.186 | MCSE(6.27) = 9.36 | stat: TRUE | burn: 120
COV_log_RMSD|mcs_RingCount
0.05
0.00
−0.05
−0.10
−0.15
0
20
40
60
80
100
120

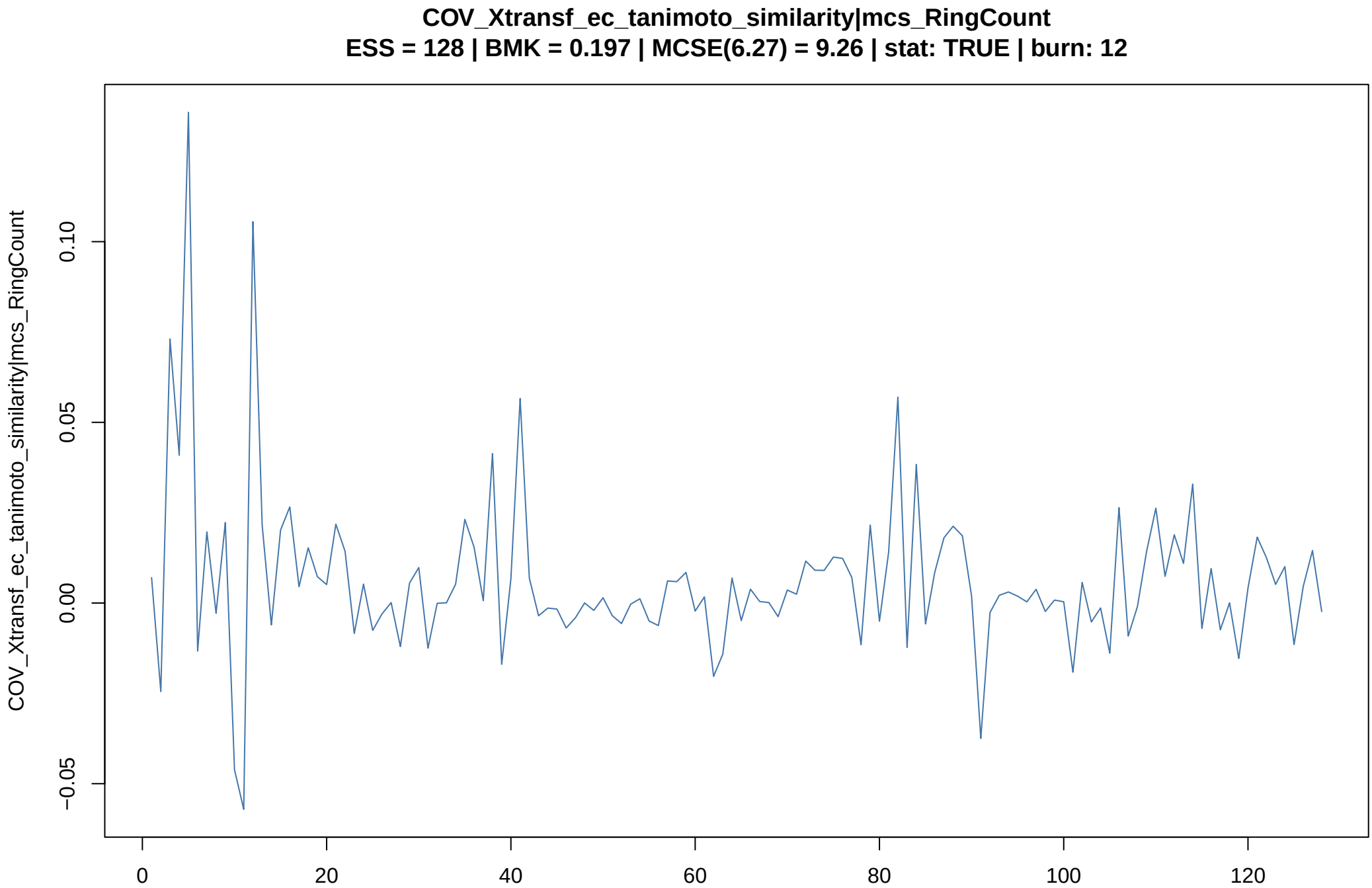

COV_log_RMSD|template_HeavyAtomCount
ESS = 99.1 | BMK = 0.24 | MCSE(6.27) = 7.77 | stat: FALSE | burn: 120
COV_log_RMSD|template_HeavyAtomCount
1
0
−1
−2
0
20
40
60
80
100
120

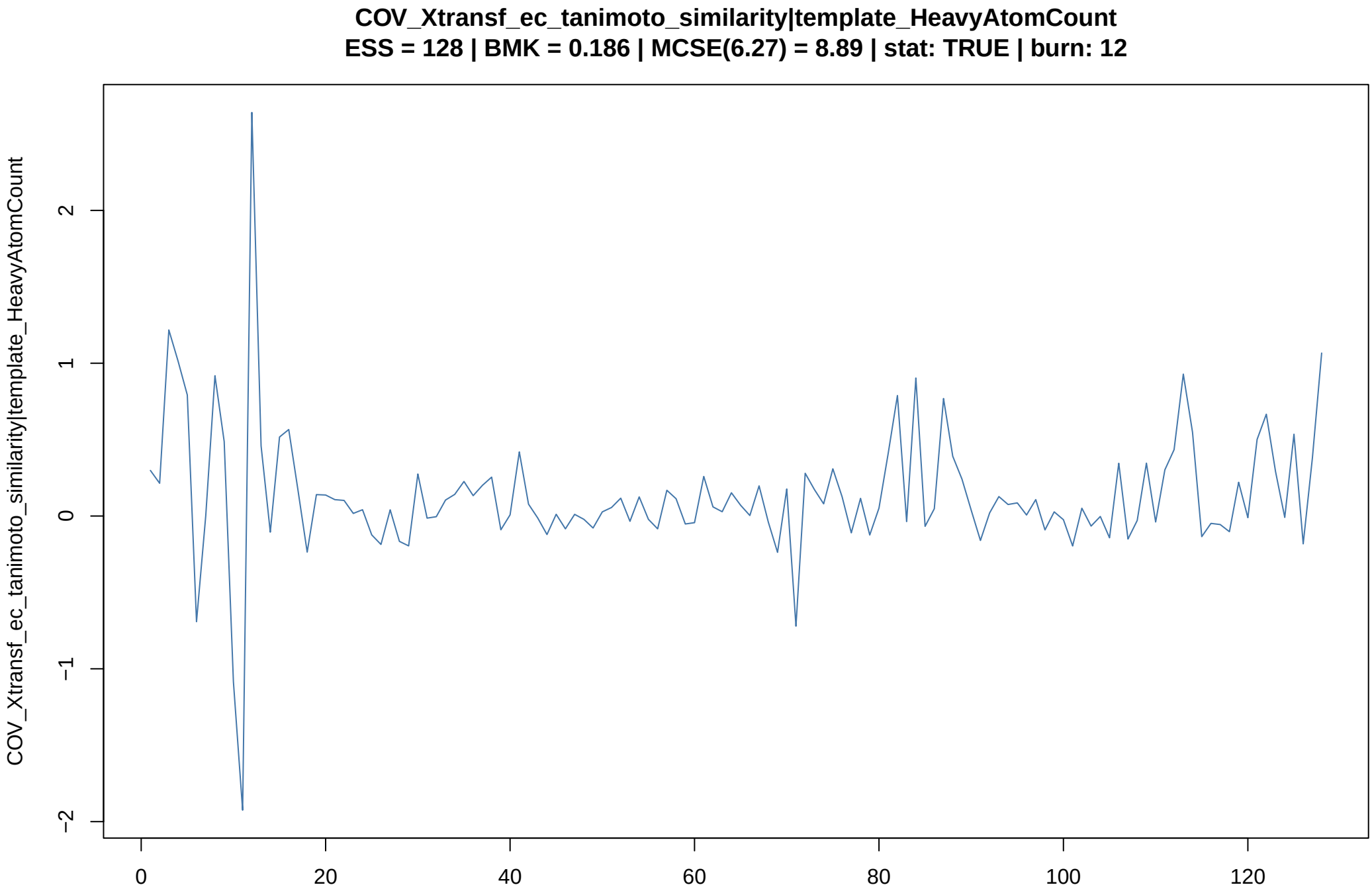

COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 20.6 | BMK = 0.277 | MCSE(6.27) = 25.8 | stat: FALSE | burn: 120
COV_log_RMSD|mcs_docked_NumHAcceptors
0.15
0.10
0.05
0.00
−0.05
0
20
40
60
80
100
120

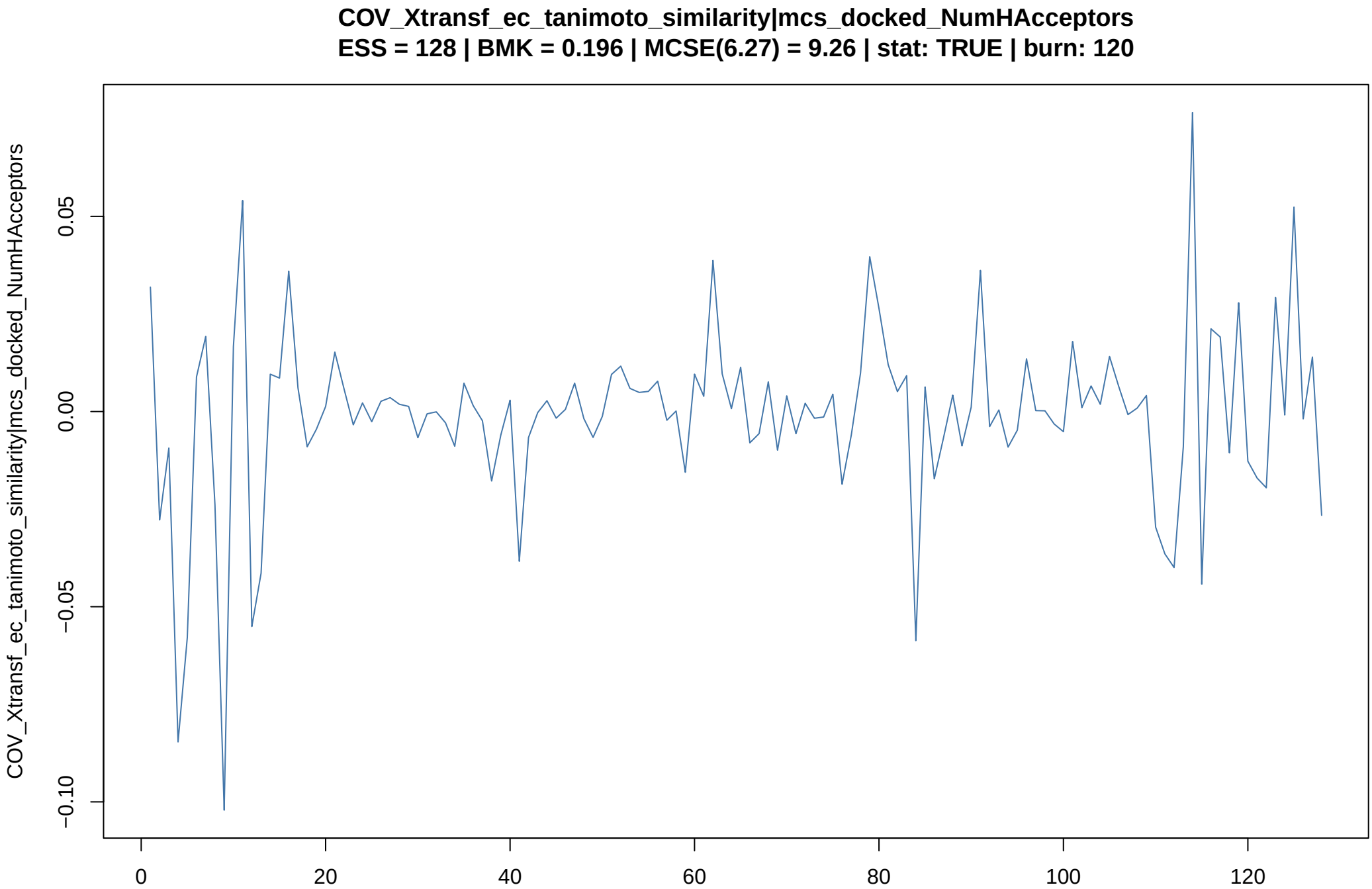

COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 65.8 | BMK = 0.36 | MCSE(6.27) = 15.8 | stat: FALSE | burn: 120
COV_log_RMSD|mcs_template_NumHAcceptors
0.25
0.20
0.15
0.10
0.05
0.00
−0.05
0
20
40
60
80
100
120

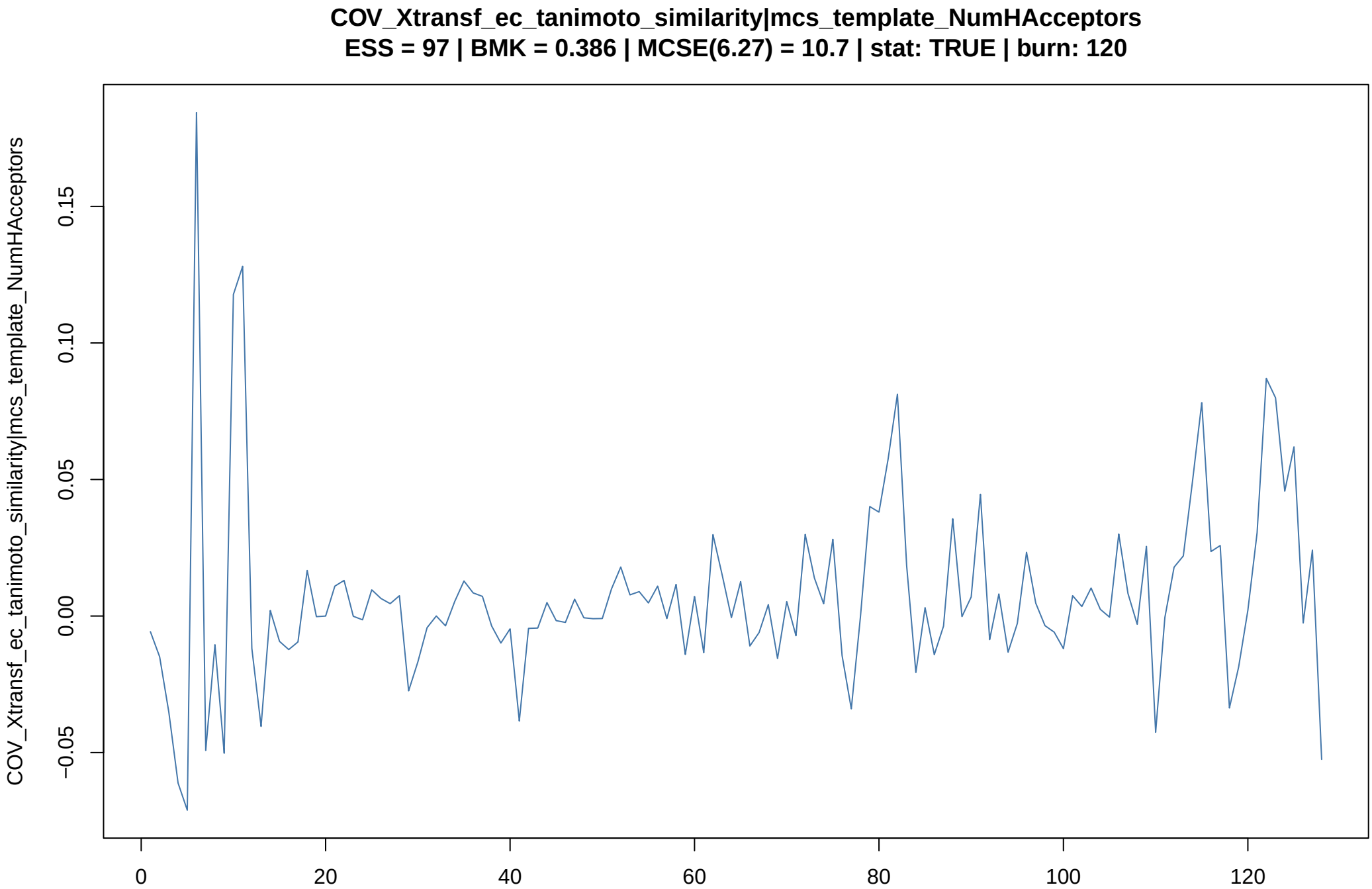

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 29.1 | BMK = 0.292 | MCSE(6.27) = 16.4 | stat: FALSE | burn: 120
COV_log_RMSD|mcs_NumHeteroAtoms
0.6
0.5
0.4
0.3
0.2
0.1
0.0
−0.1
0
20
40
60
80
100
120

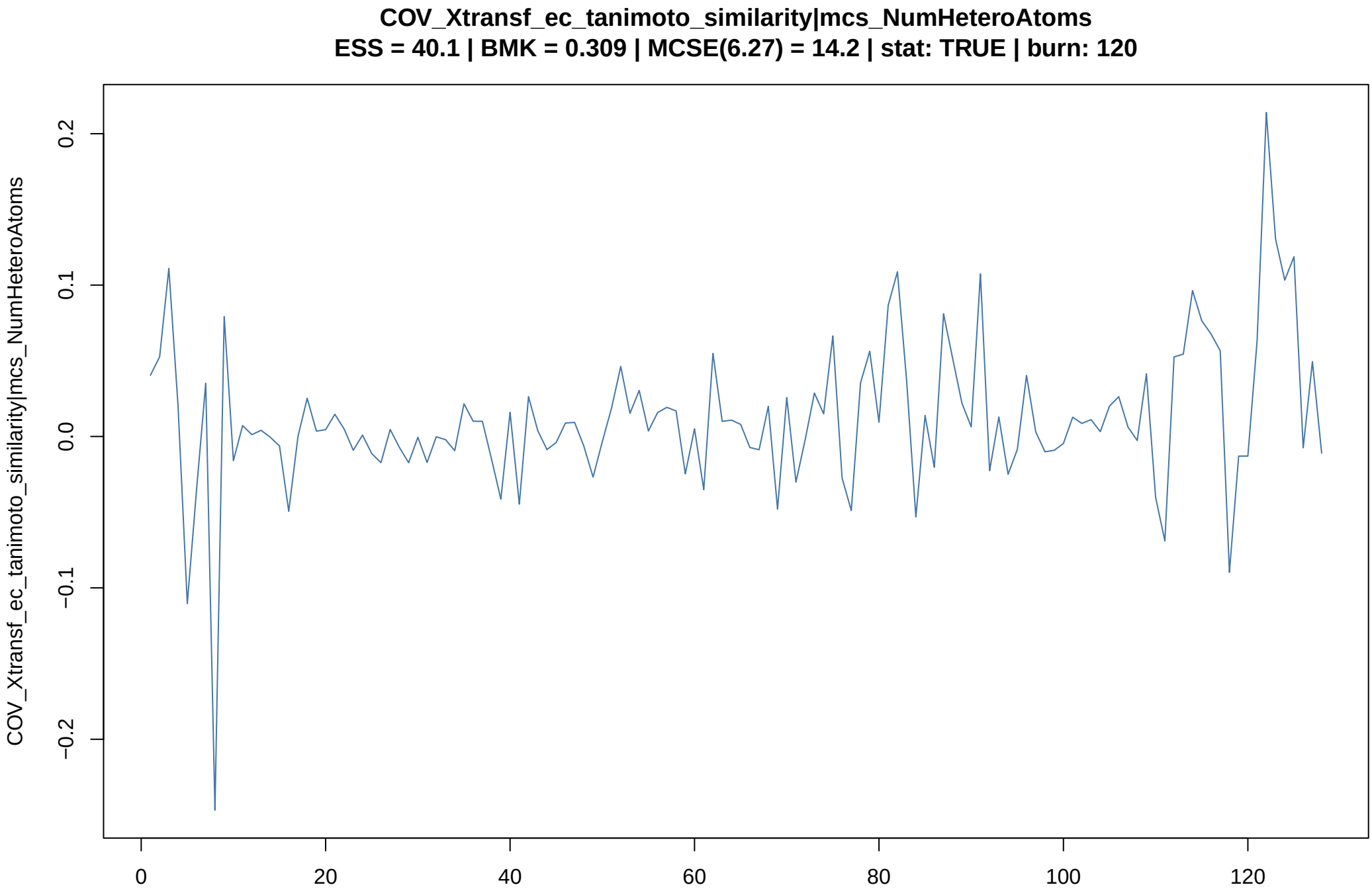

COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 77.5 | BMK = 0.234 | MCSE(6.27) = 16.4 | stat: TRUE | burn: 120
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
2
1
0
−1
0
20
40
60
80
100
120

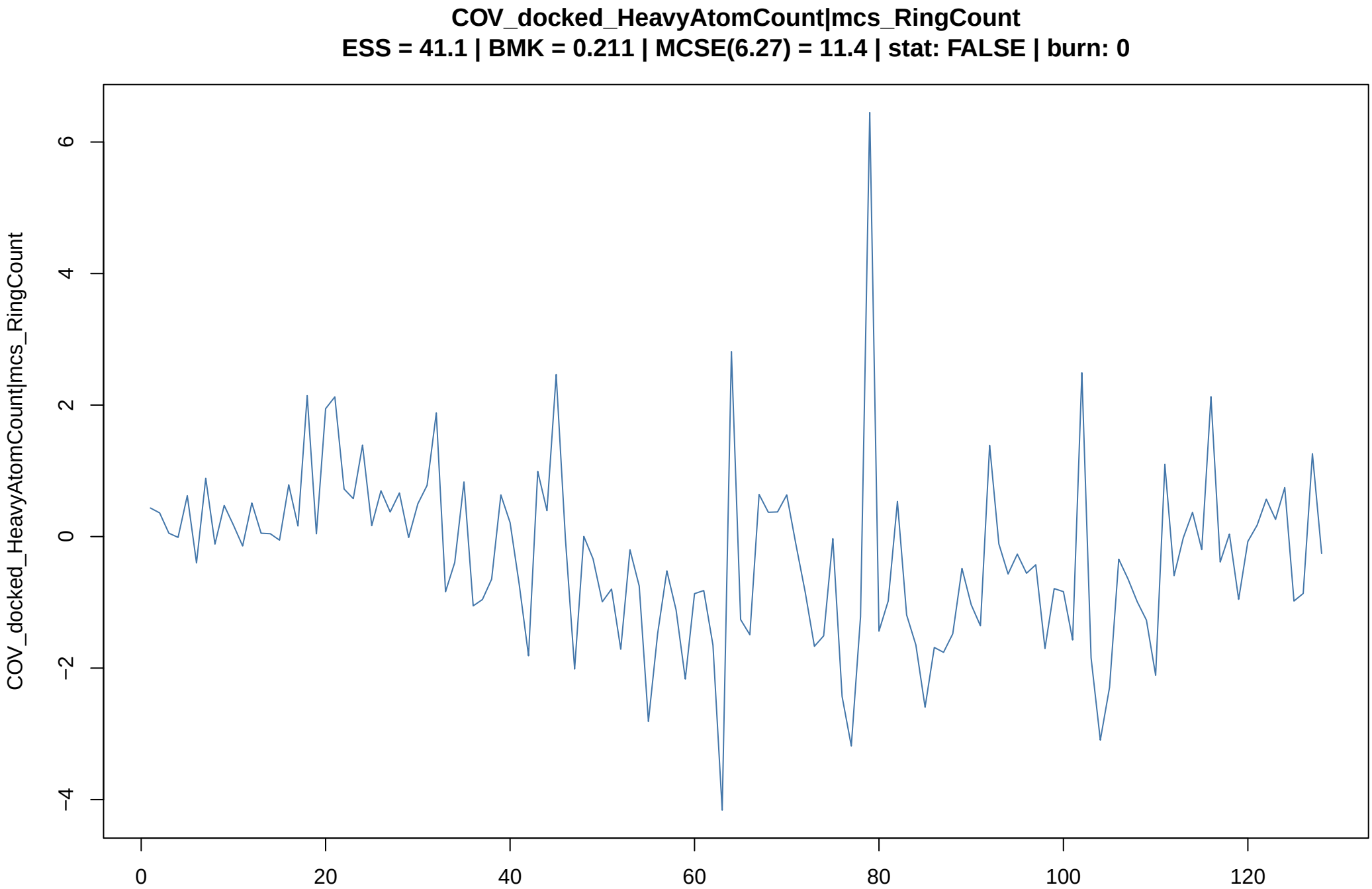

COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 128 | BMK = 0.197 | MCSE(6.27) = 9.26 | stat: TRUE | burn: 12
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
0.10
0.05
0.00
−0.05
0
20
40
60
80
100
120

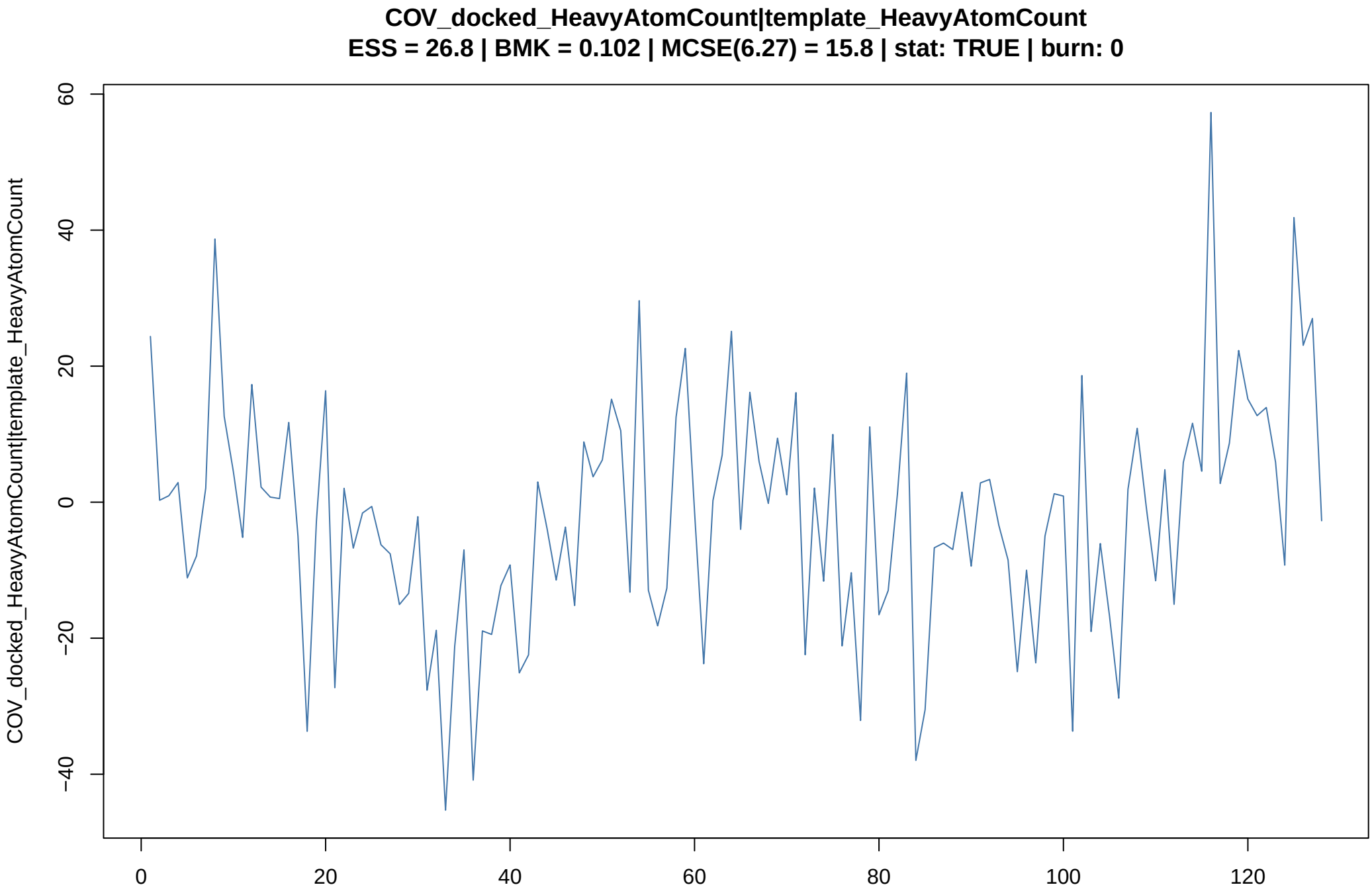

COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 128 | BMK = 0.186 | MCSE(6.27) = 8.89 | stat: TRUE | burn: 12
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
2
1
0
−1
−2
0
20
40
60
80
100
120

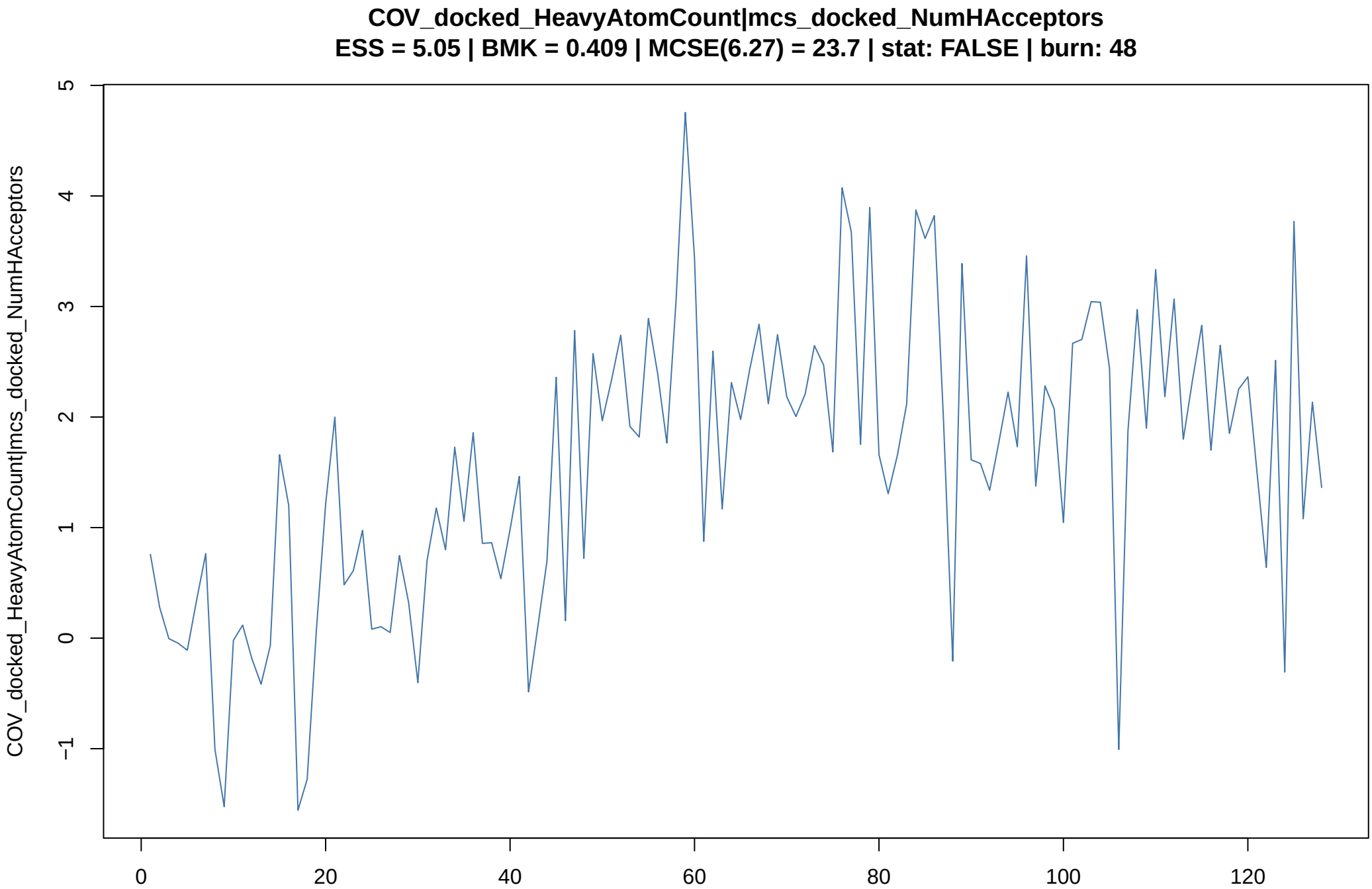

COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.196 | MCSE(6.27) = 9.26 | stat: TRUE | burn: 120
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
0.05
0.00
−0.05
−0.10
0
20
40
60
80
100
120

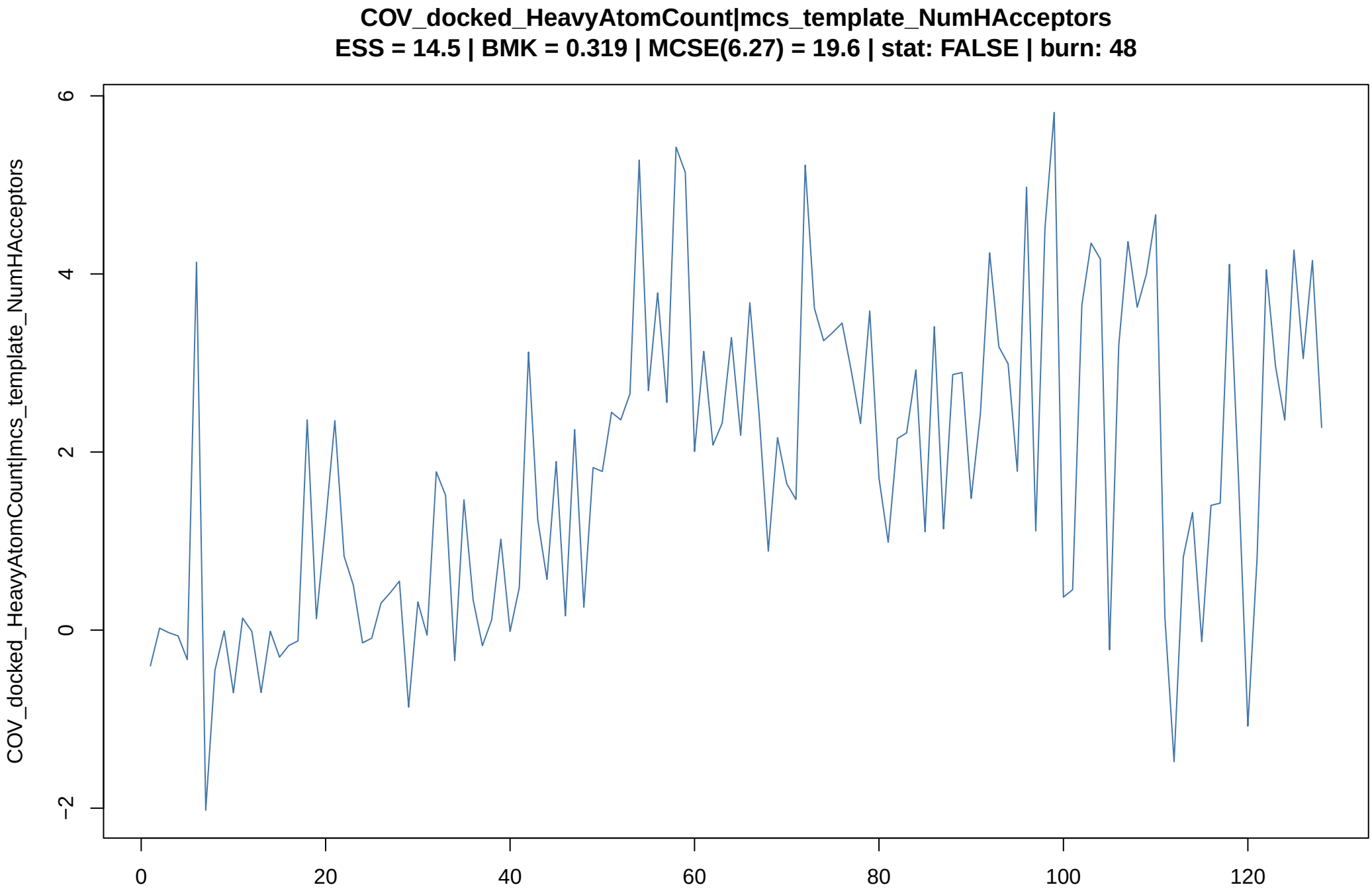

COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 97 | BMK = 0.386 | MCSE(6.27) = 10.7 | stat: TRUE | burn: 120
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
−0.05
0.00
0.05
0.10
0.15
0
20
40
60
80
100
120

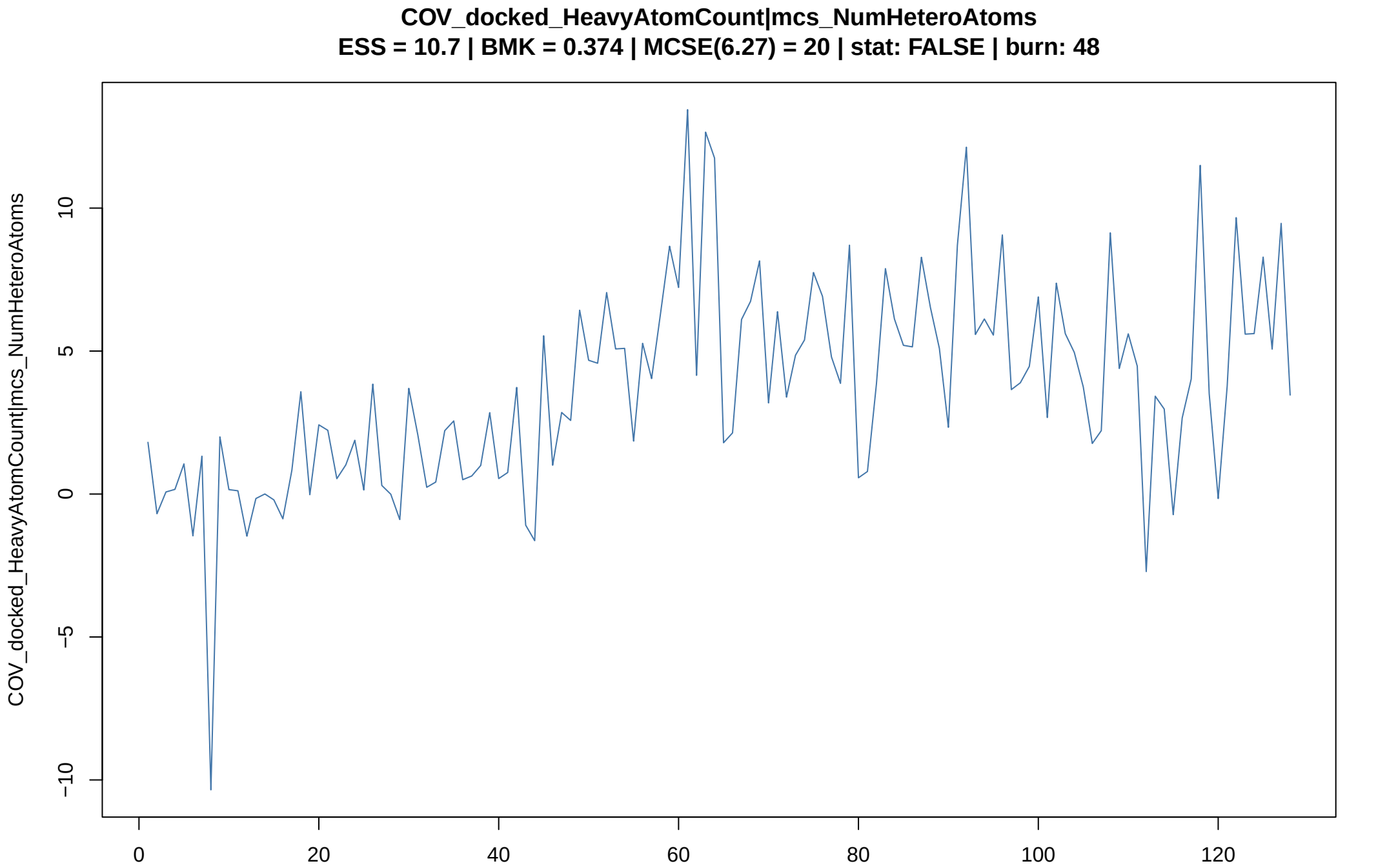

COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 40.1 | BMK = 0.309 | MCSE(6.27) = 14.2 | stat: TRUE | burn: 120
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.2
0.1
0.0
−0.1
−0.2
0
20
40
60
80
100
120

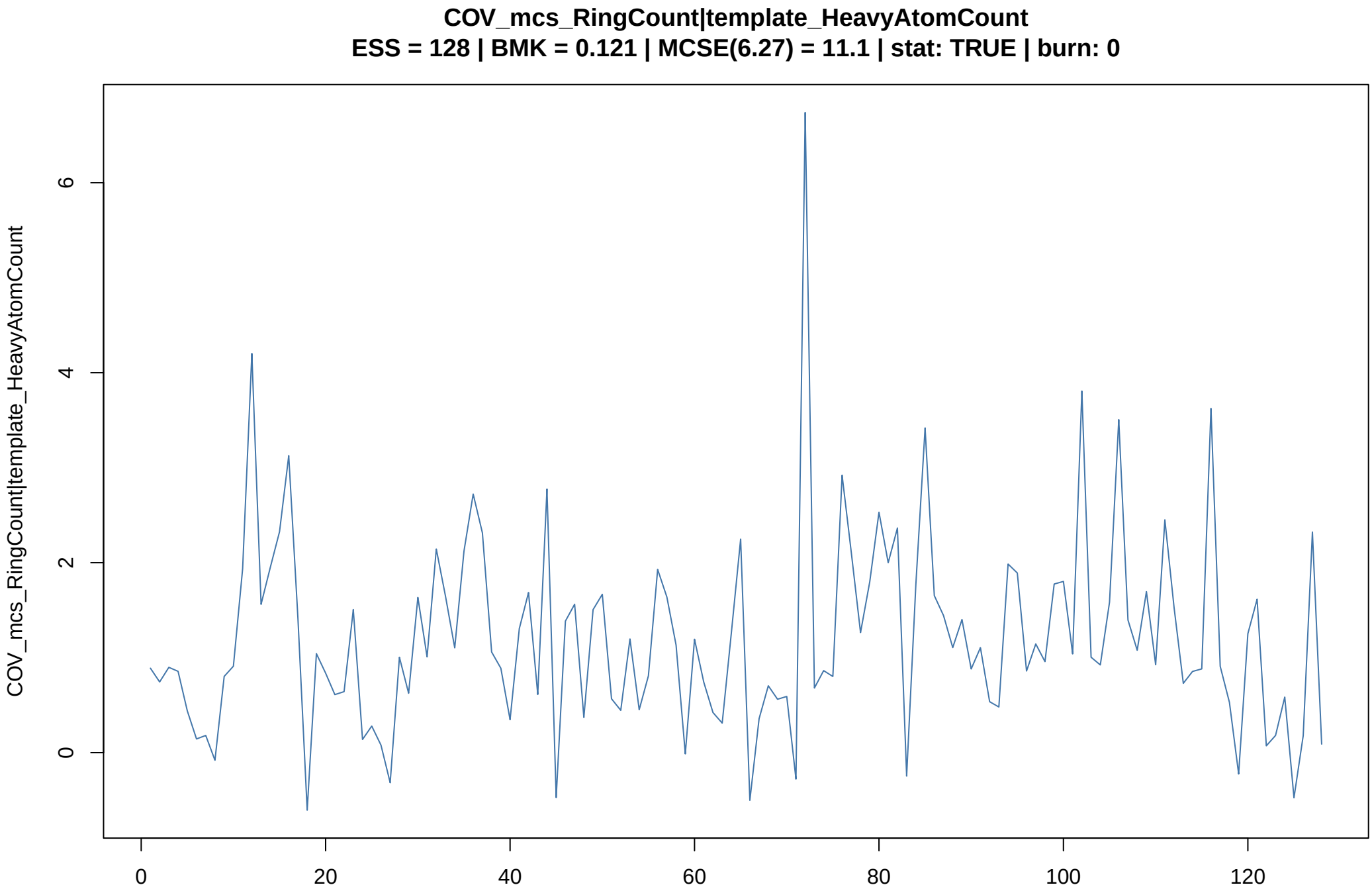

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 41.1 | BMK = 0.211 | MCSE(6.27) = 11.4 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
6
4
2
0
−2
−4
0
20
40
60
80
100
120

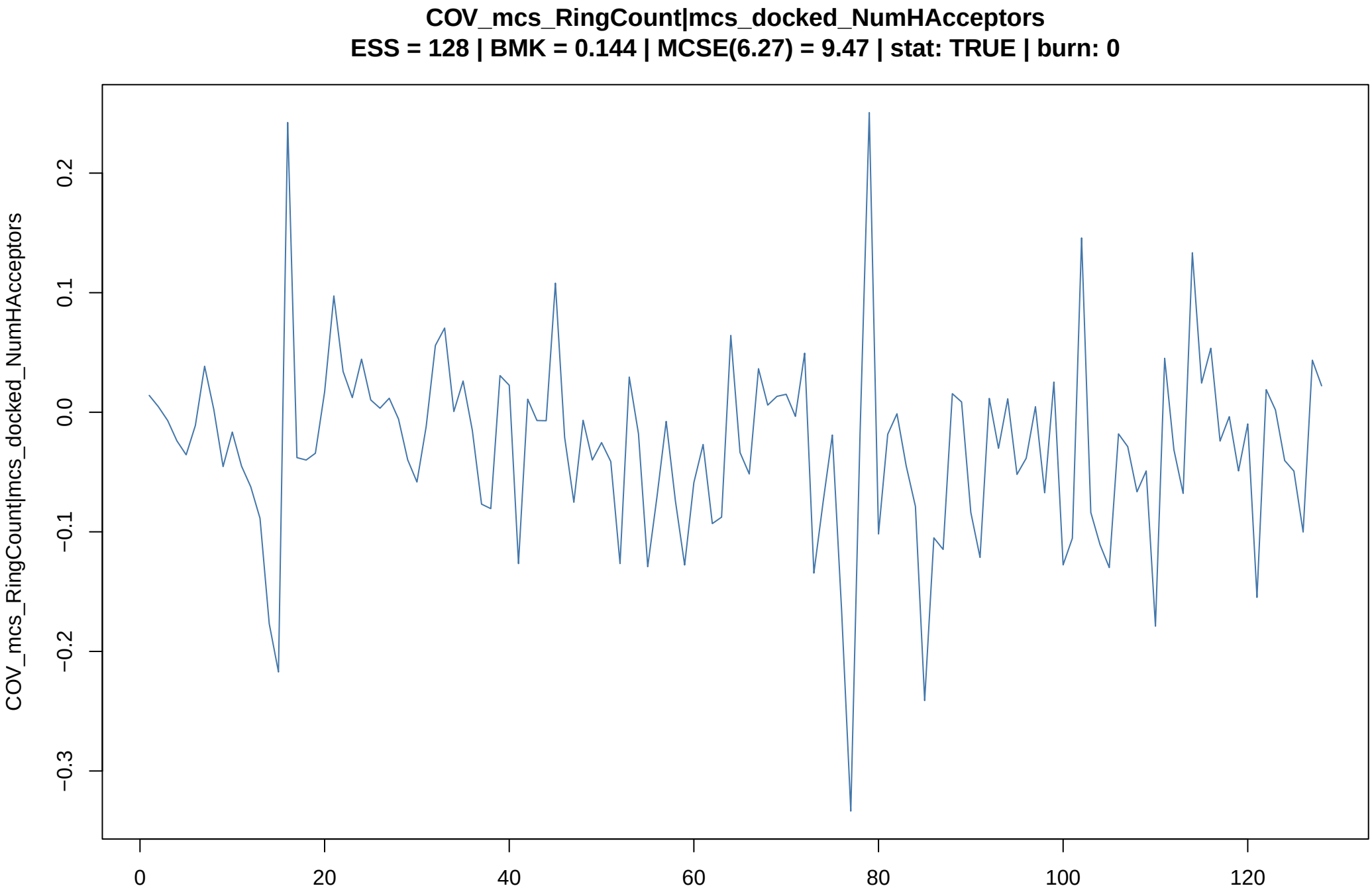

COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 26.8 | BMK = 0.102 | MCSE(6.27) = 15.8 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|template_HeavyAtomCount
60
40
20
0
−20
−40
0
20
40
60
80
100
120

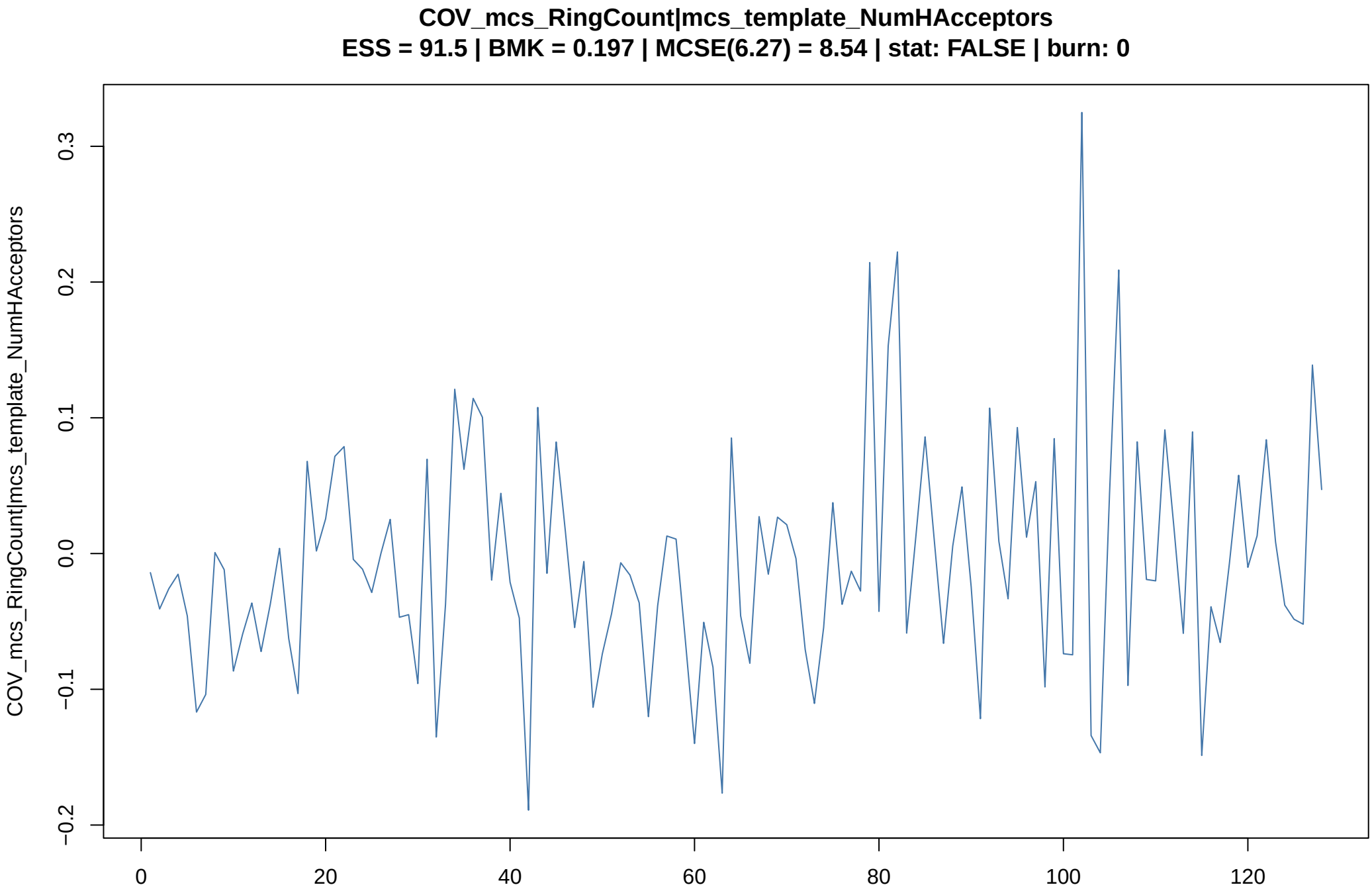

COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 5.05 | BMK = 0.409 | MCSE(6.27) = 23.7 | stat: FALSE | burn: 48
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
5
4
3
2
1
0
−1
0
20
40
60
80
100
120

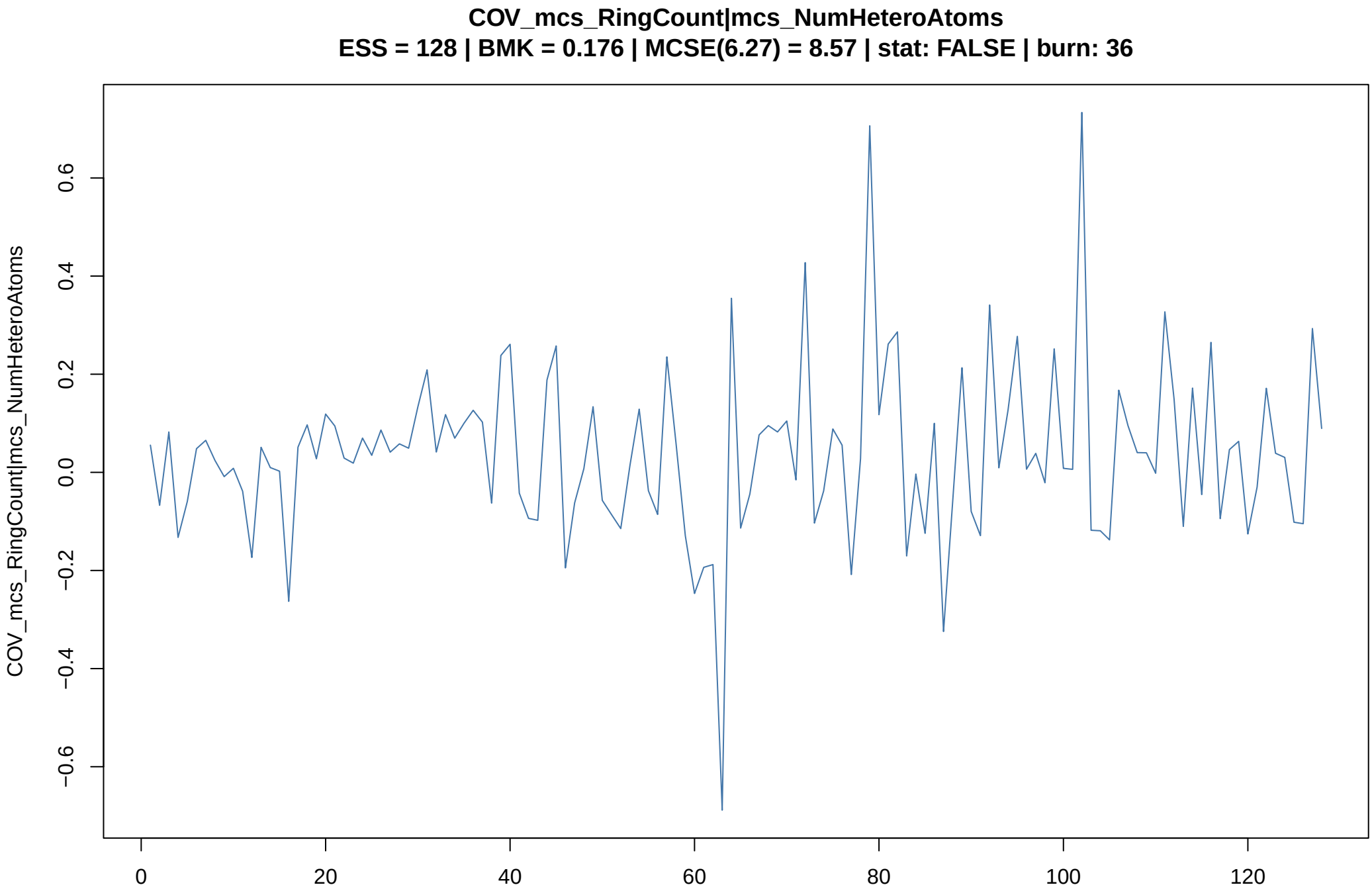

COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 14.5 | BMK = 0.319 | MCSE(6.27) = 19.6 | stat: FALSE | burn: 48
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
6
4
2
0
−2
0
20
40
60
80
100
120

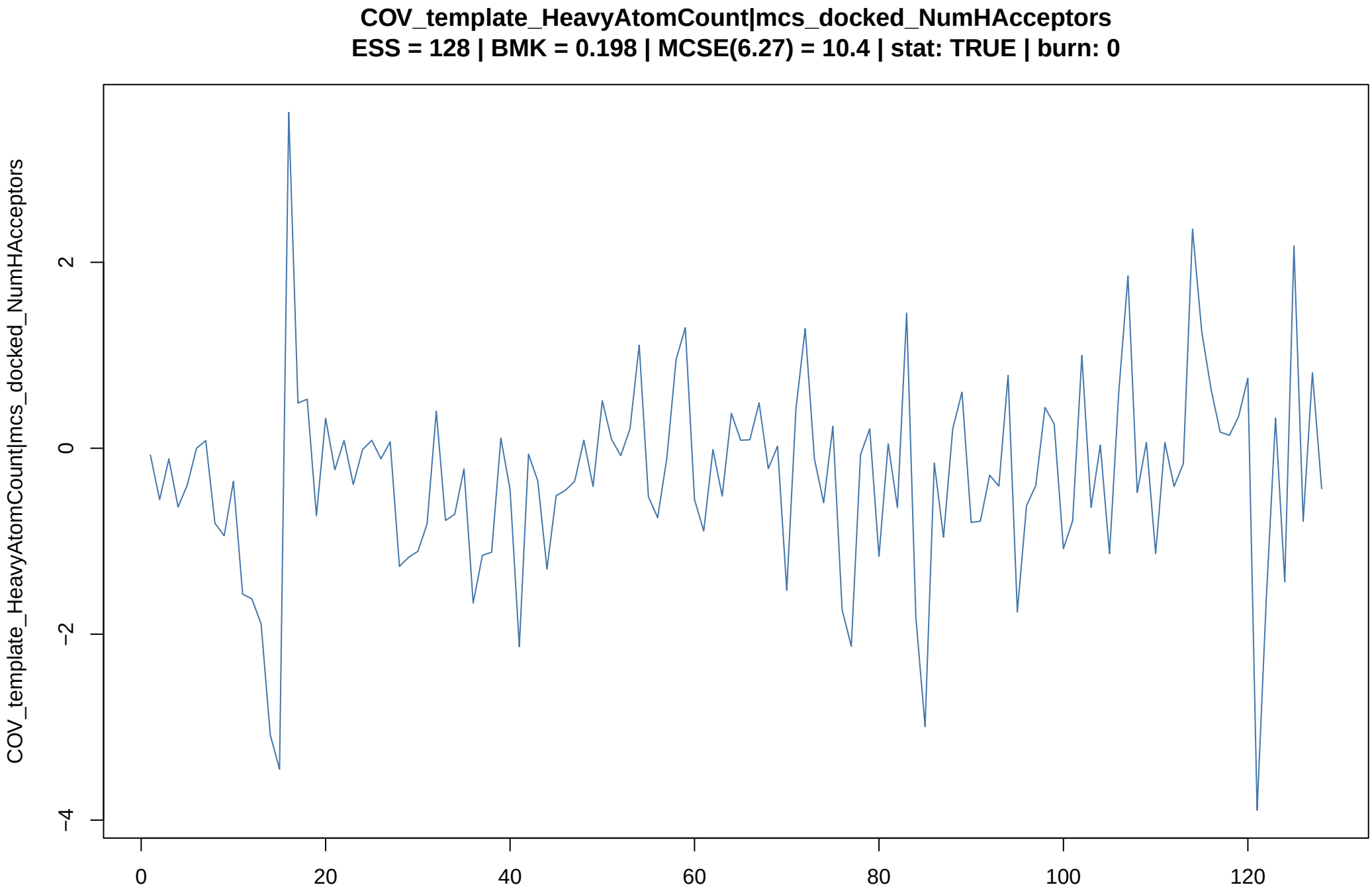

COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 10.7 | BMK = 0.374 | MCSE(6.27) = 20 | stat: FALSE | burn: 48
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
10
5
0
−5
−10
0
20
40
60
80
100
120

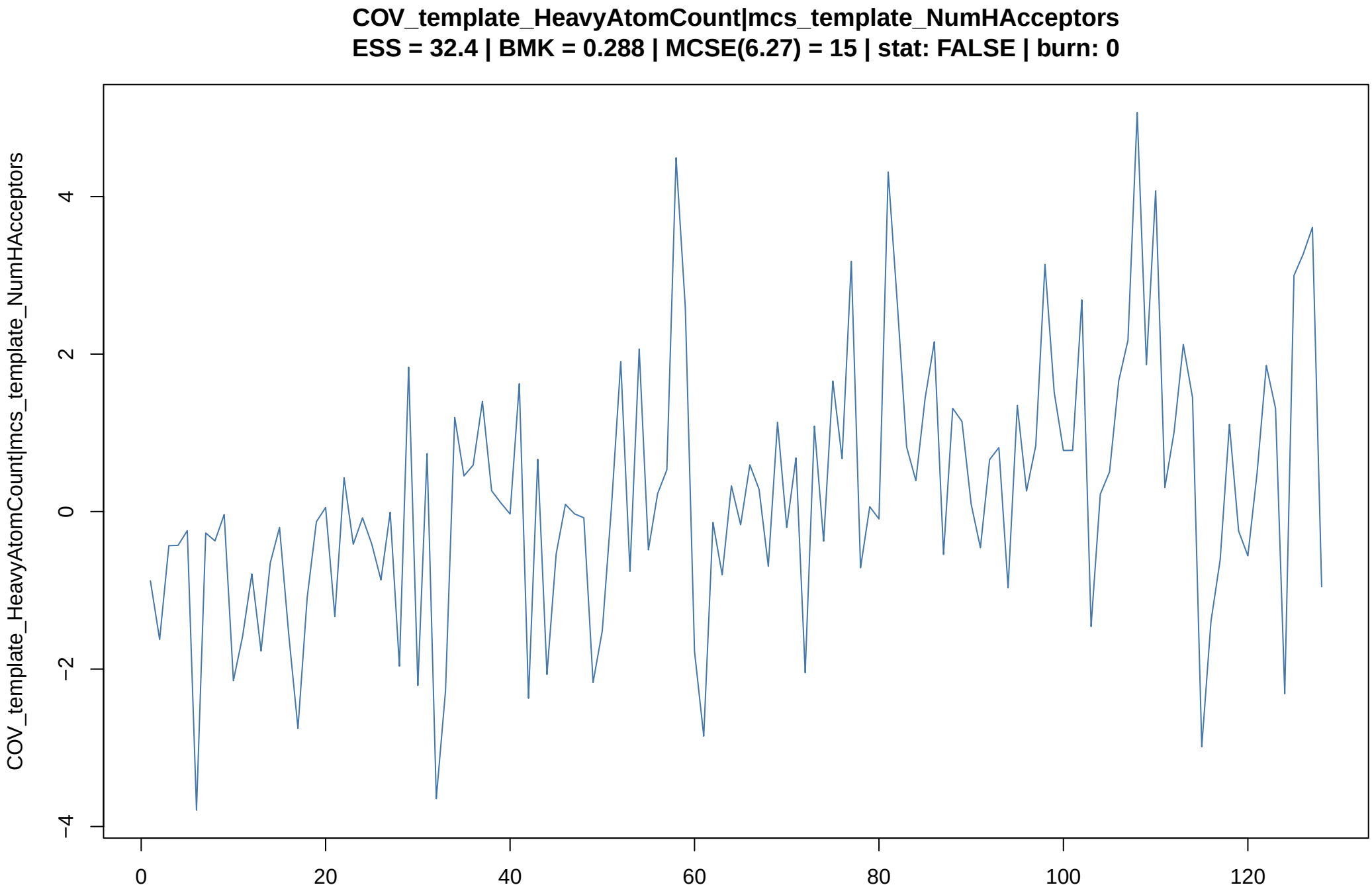

COV_mcs_RingCount|template_HeavyAtomCount
ESS = 128 | BMK = 0.121 | MCSE(6.27) = 11.1 | stat: TRUE | burn: 0
COV_mcs_RingCount|template_HeavyAtomCount
0
2
4
6
0
20
40
60
80
100
120

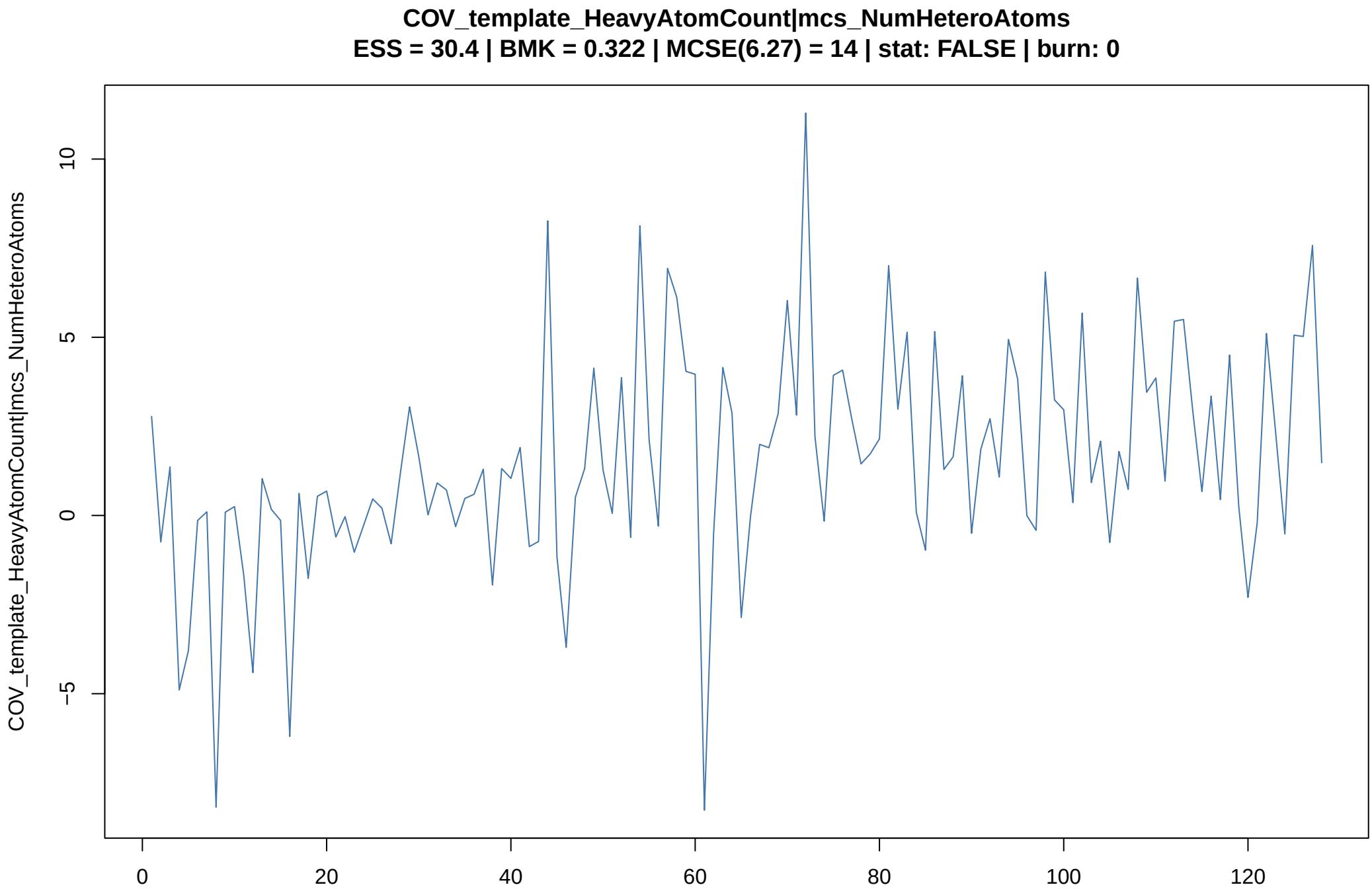

COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.144 | MCSE(6.27) = 9.47 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_docked_NumHAcceptors
0.2
0.1
0.0
−0.1
−0.2
−0.3
0
20
40
60
80
100
120

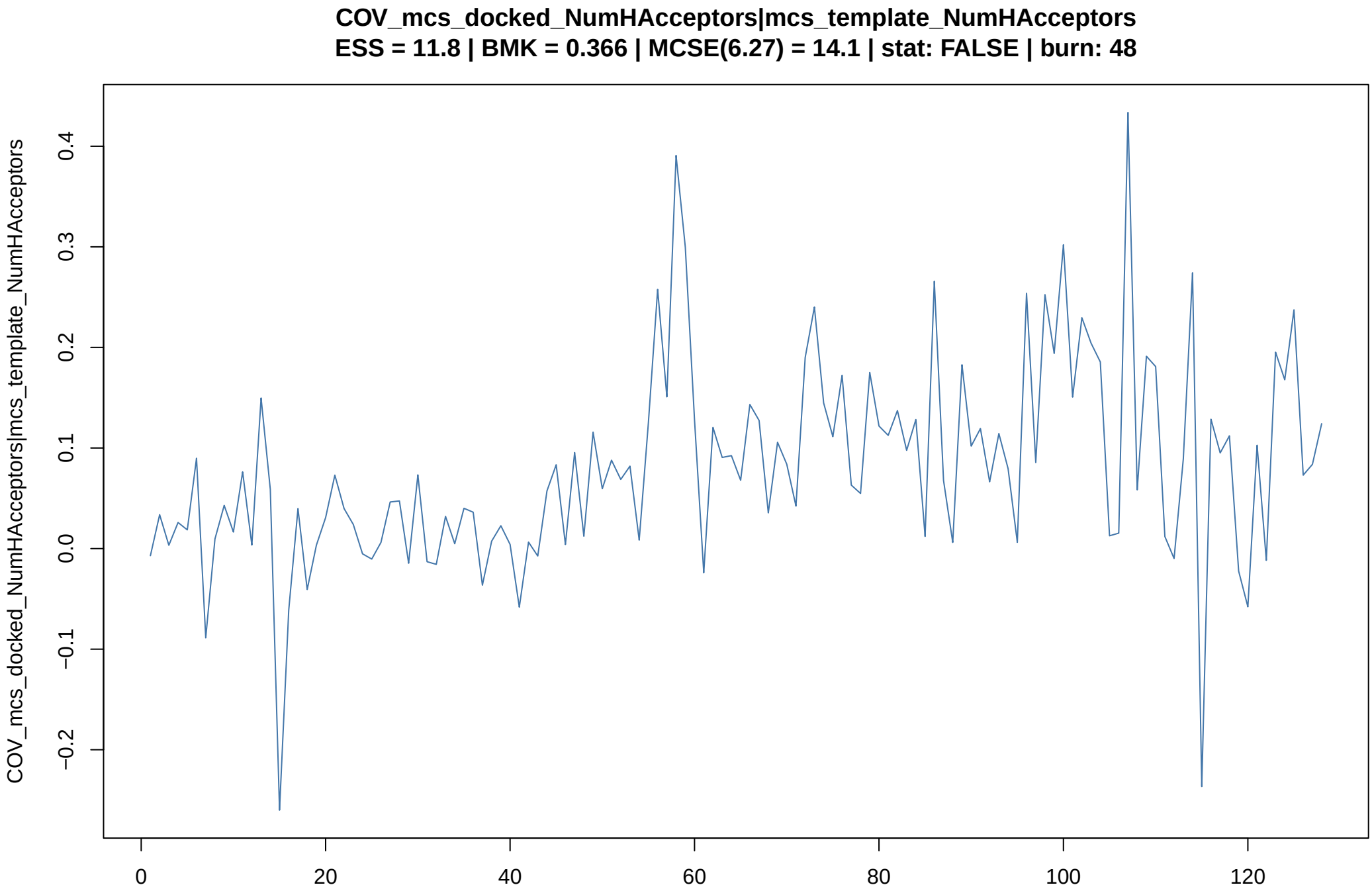

COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 91.5 | BMK = 0.197 | MCSE(6.27) = 8.54 | stat: FALSE | burn: 0
COV_mcs_RingCount|mcs_template_NumHAcceptors
0.3
0.2
0.1
0.0
−0.1
−0.2
0
20
40
60
80
100
120

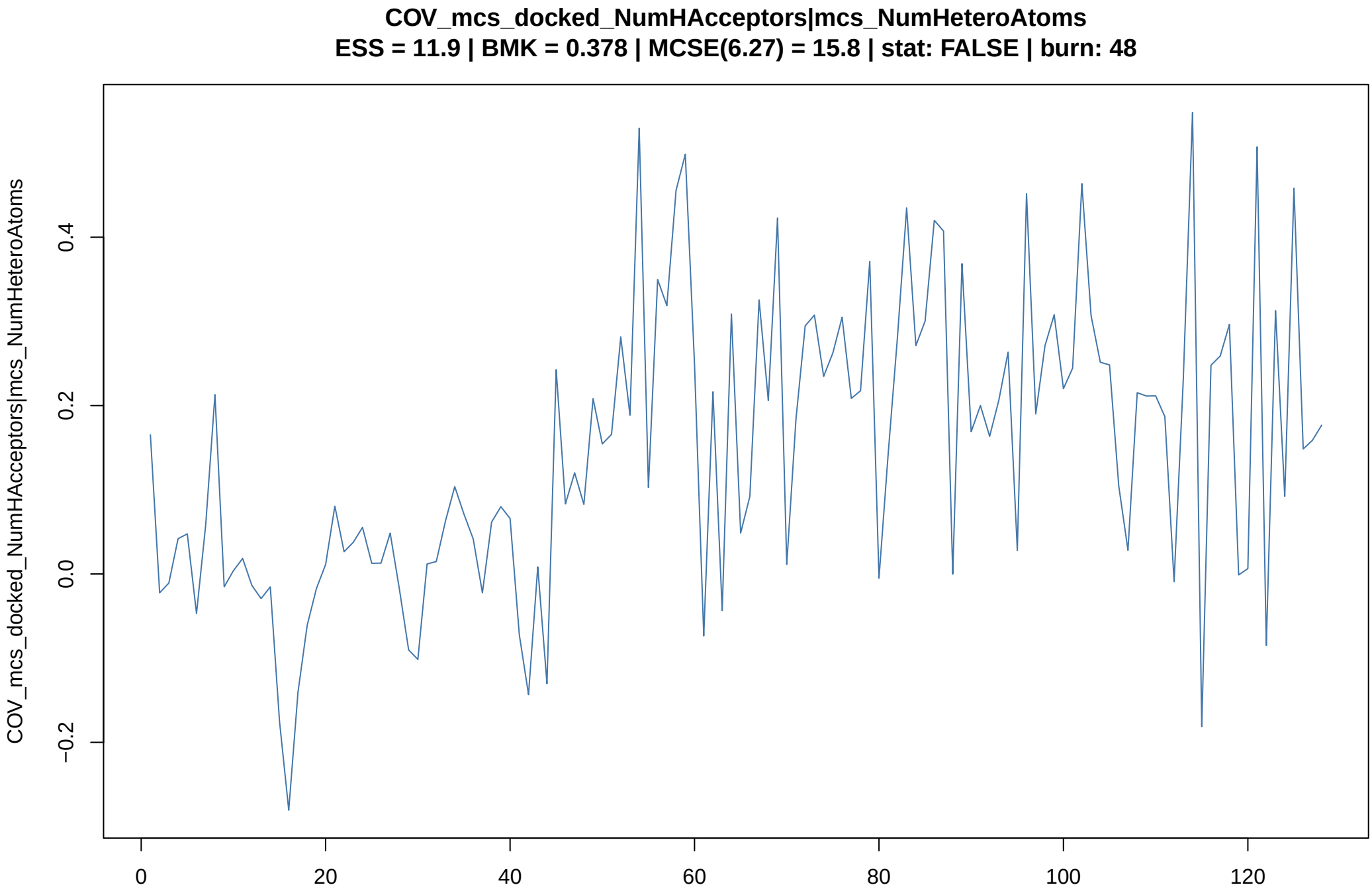

COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 128 | BMK = 0.176 | MCSE(6.27) = 8.57 | stat: FALSE | burn: 36
COV_mcs_RingCount|mcs_NumHeteroAtoms
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
0
20
40
60
80
100
120

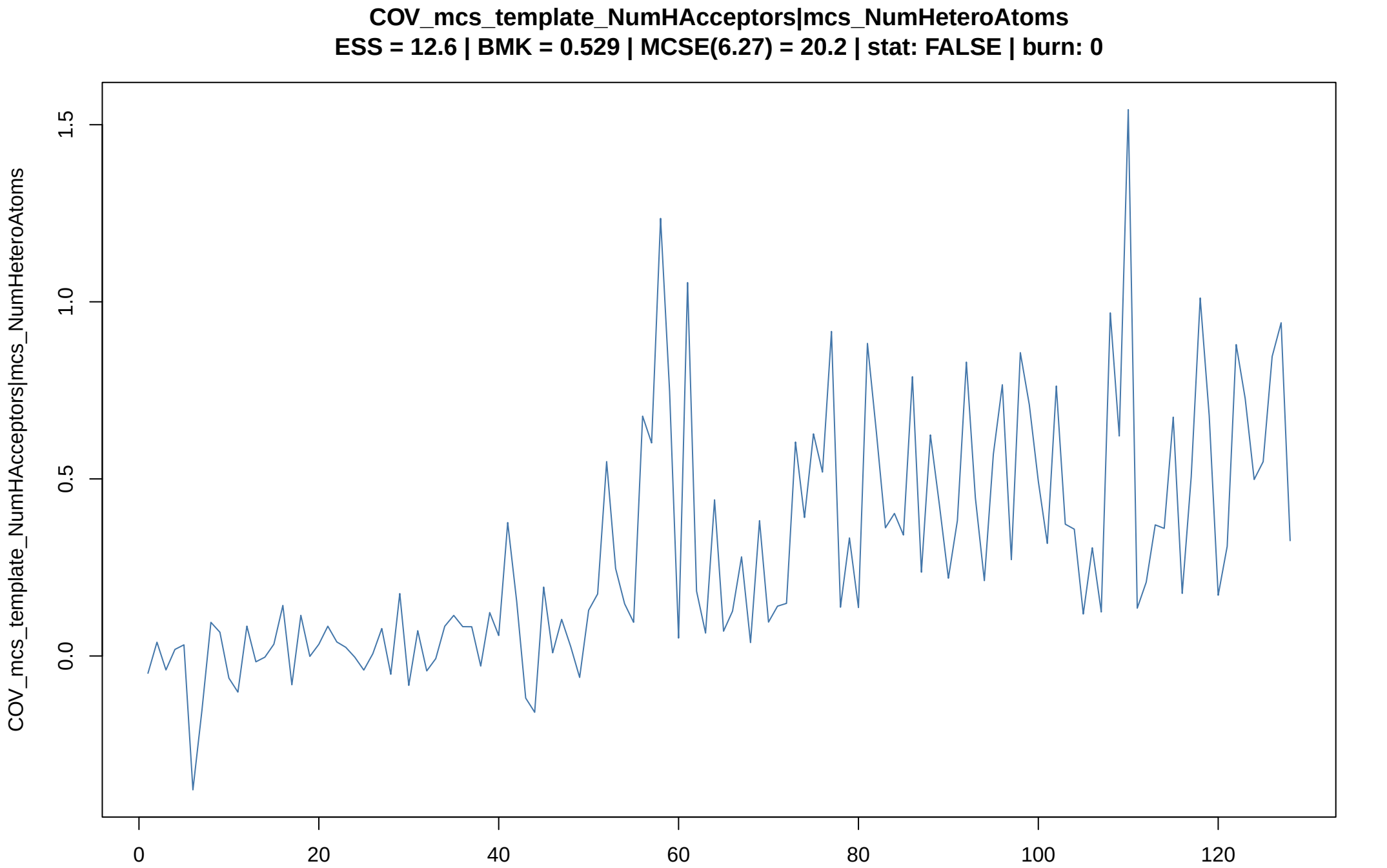

COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 128 | BMK = 0.198 | MCSE(6.27) = 10.4 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
2
0
−2
−4
0
20
40
60
80
100
120


COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 32.4 | BMK = 0.288 | MCSE(6.27) = 15 | stat: FALSE | burn: 0
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
−4
−2
0
2
4
0
20
40
60
80
100
120


COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 30.4 | BMK = 0.322 | MCSE(6.27) = 14 | stat: FALSE | burn: 0
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
10
5
0
−5
0
20
40
60
80
100
120


COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 11.8 | BMK = 0.366 | MCSE(6.27) = 14.1 | stat: FALSE | burn: 48
COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
−0.2
−0.1
0.0
0.1
0.2
0.3
0.4
0
20
40
60
80
100
120


COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 11.9 | BMK = 0.378 | MCSE(6.27) = 15.8 | stat: FALSE | burn: 48
COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
−0.2
0.0
0.2
0.4
0
20
40
60
80
100
120


COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 12.6 | BMK = 0.529 | MCSE(6.27) = 20.2 | 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