time: 4.31
LL ESS: 9.39
ESS Min. 1st Qu. Median Mean 3rd Qu. Max.
ESS 0.748 6.1 100 68.2 100 1270

logprobData

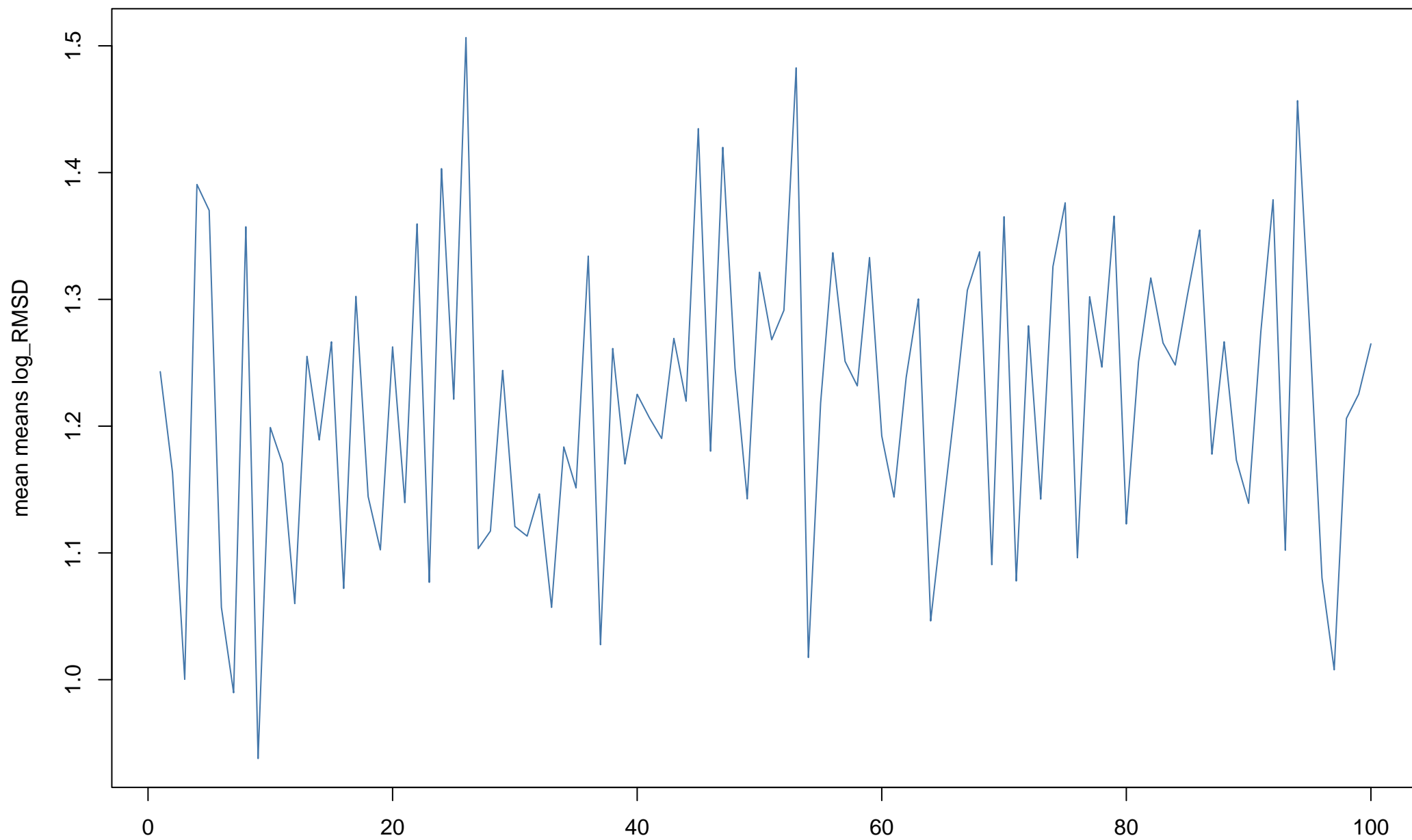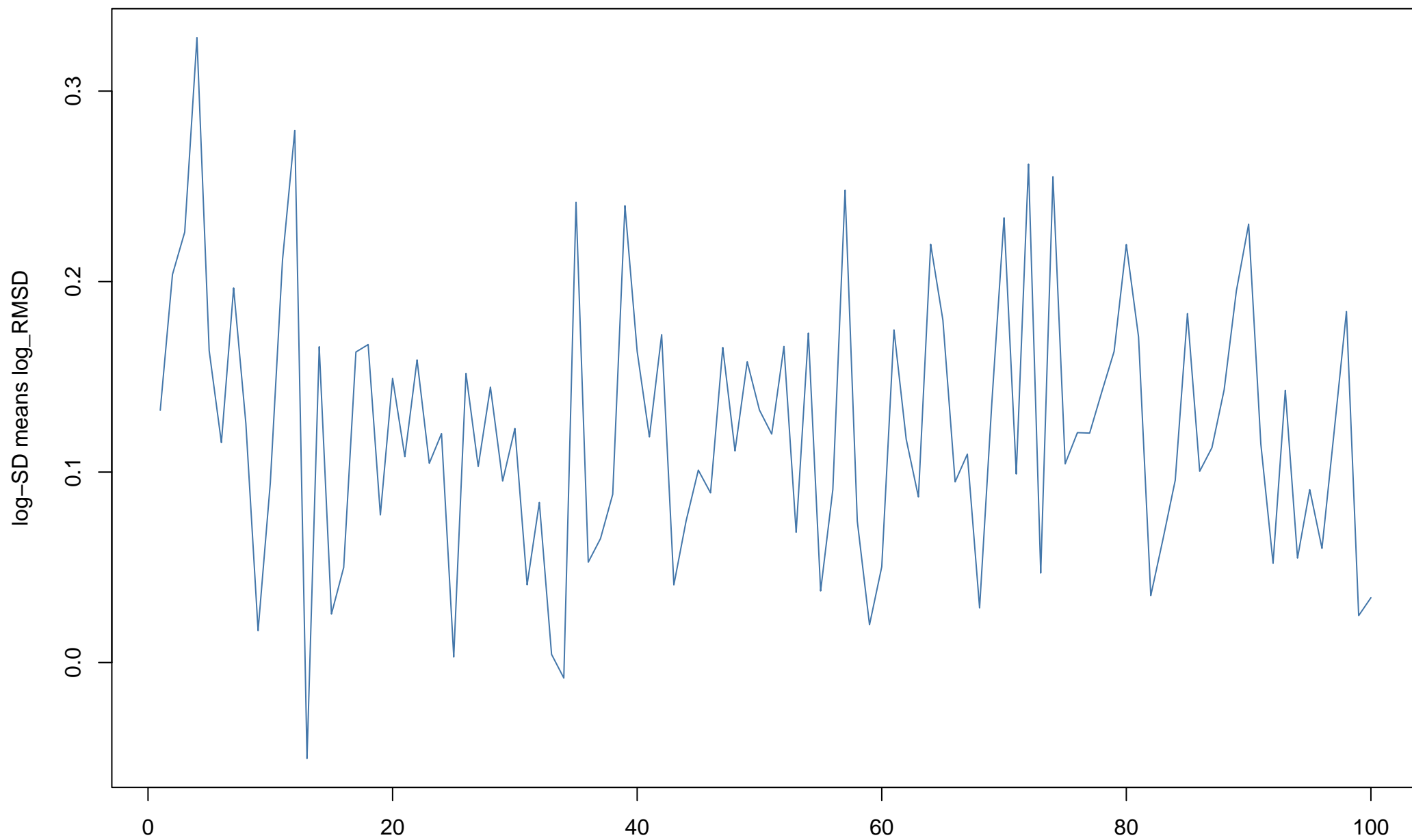**mean log−q**

log-SD log-q
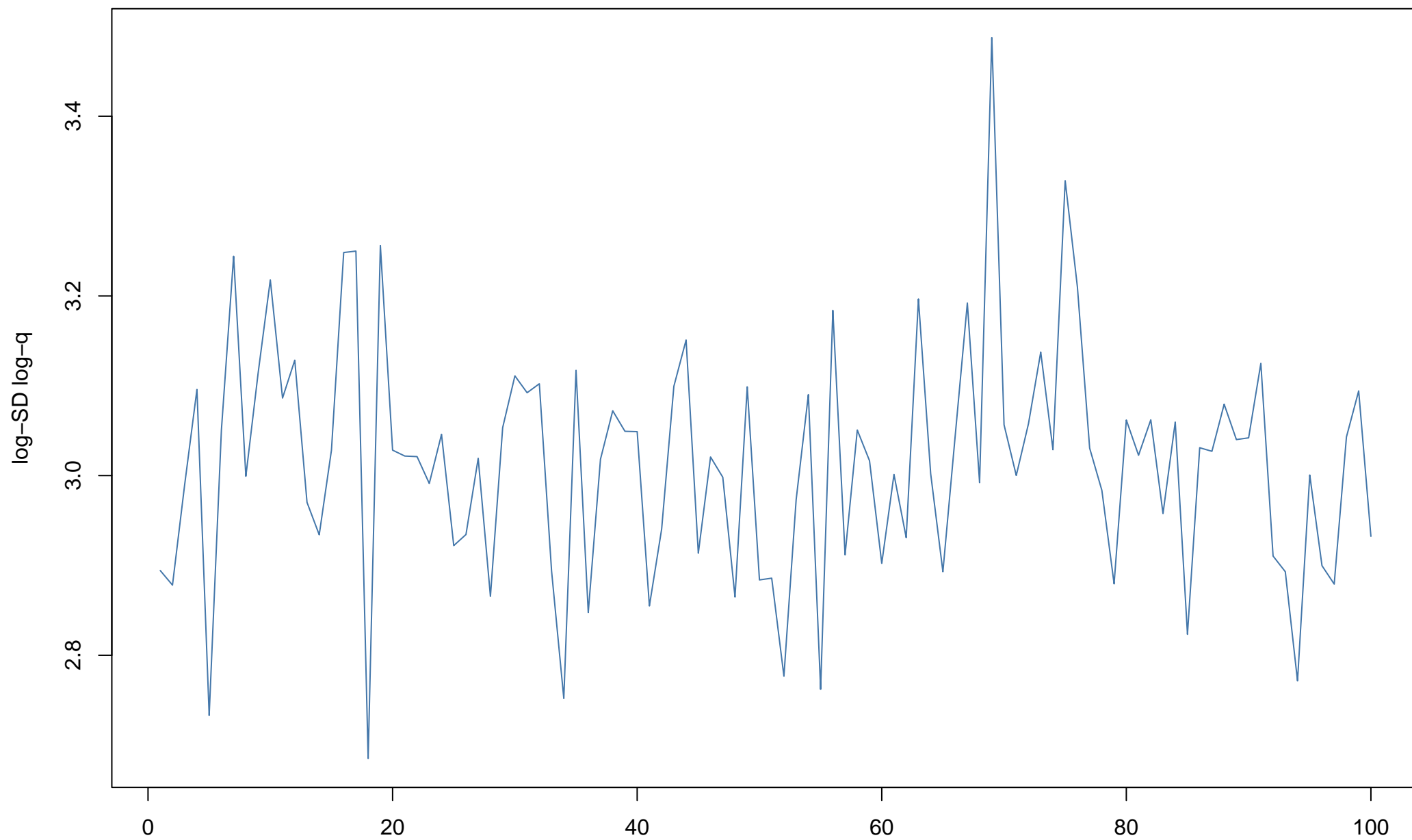
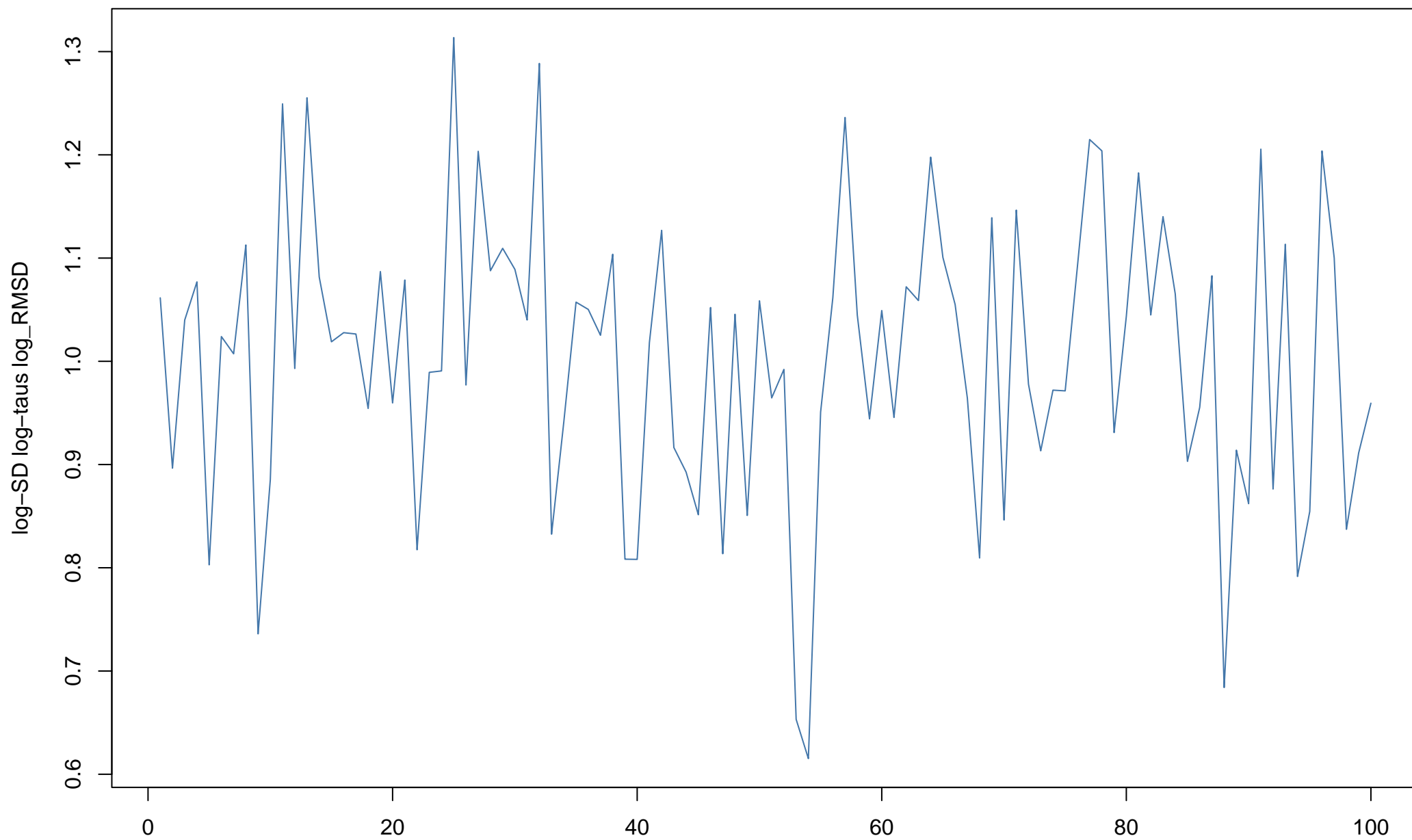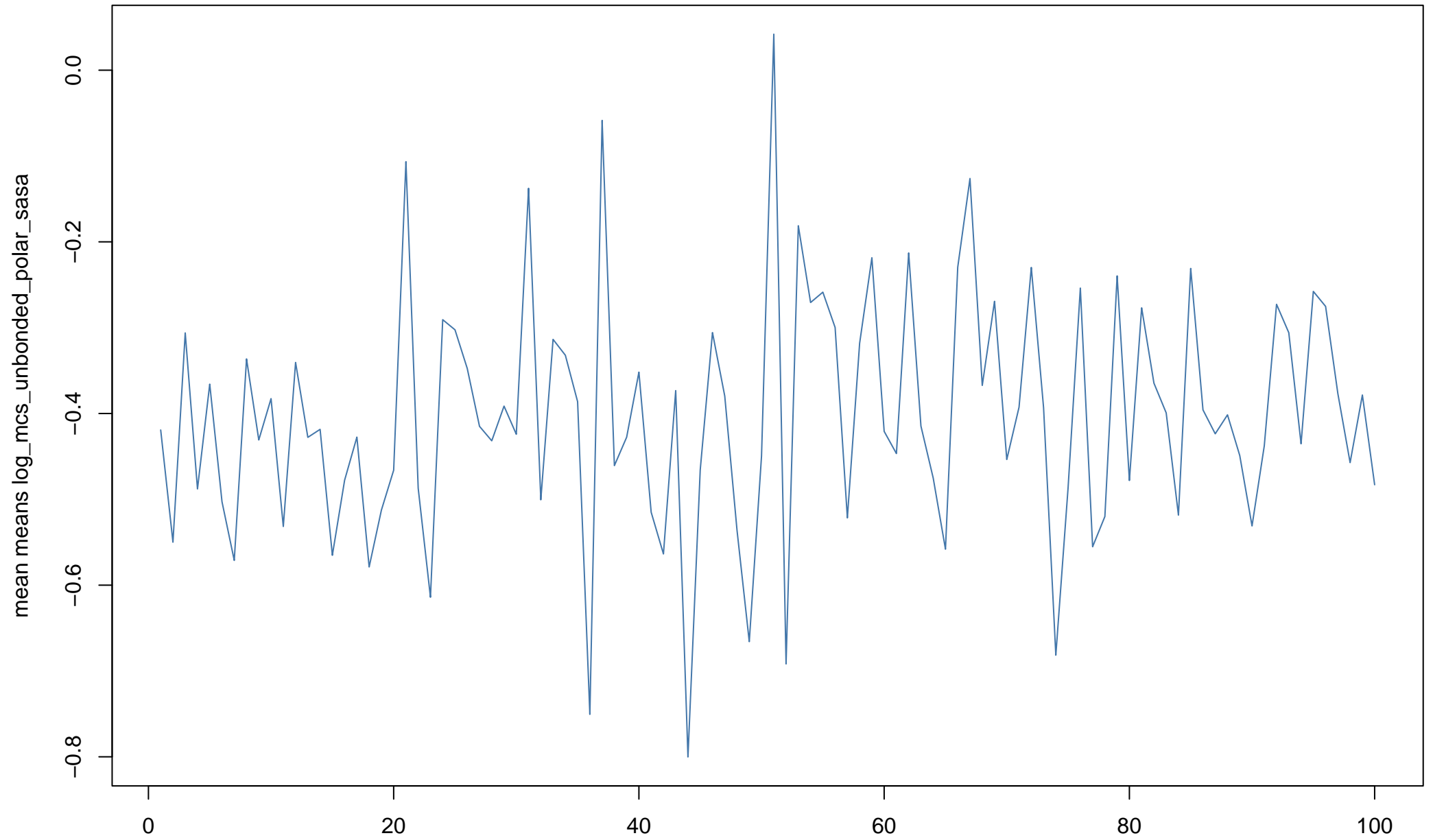**mean means log_RMSD**

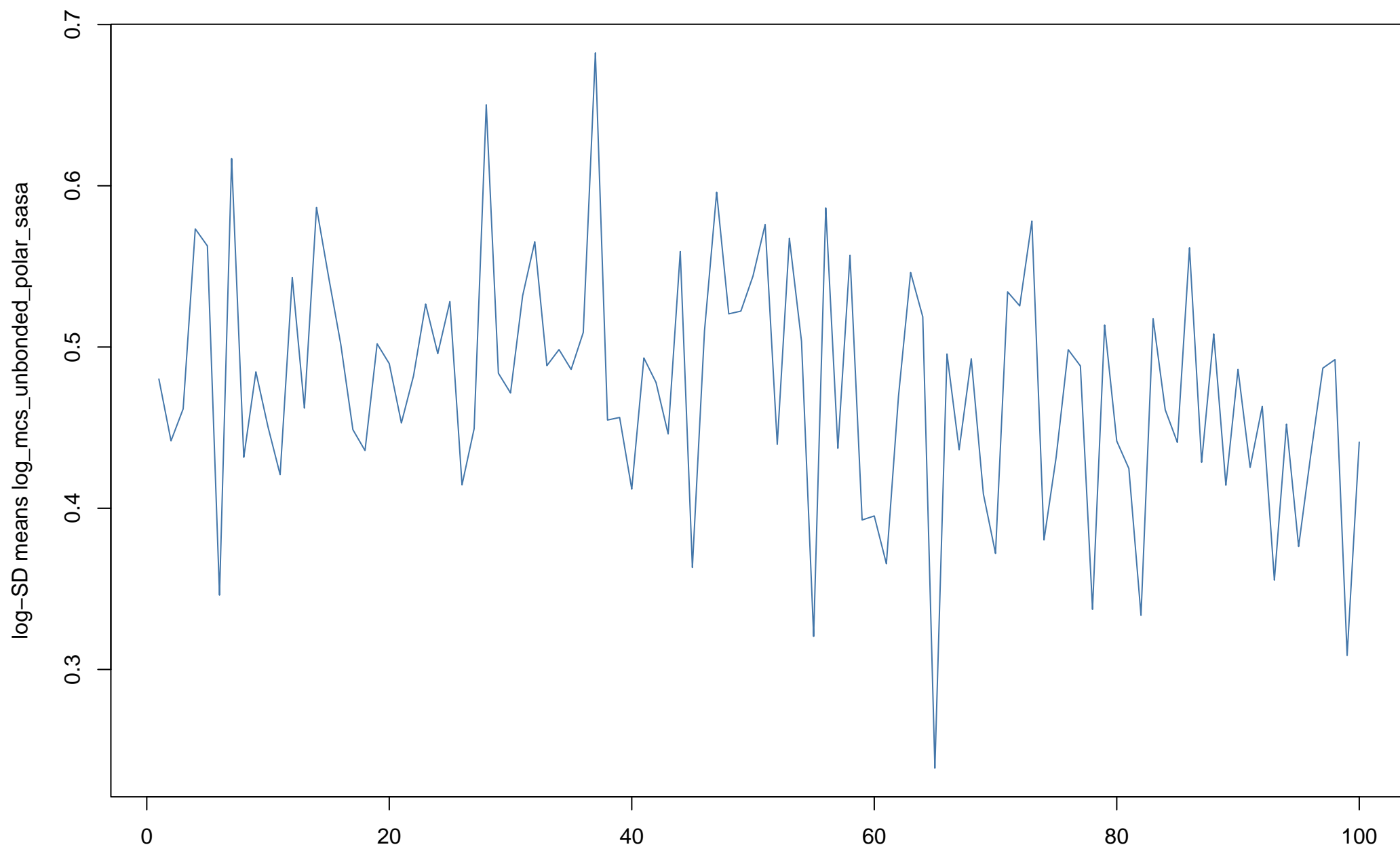**log-SD means log_RMSD**

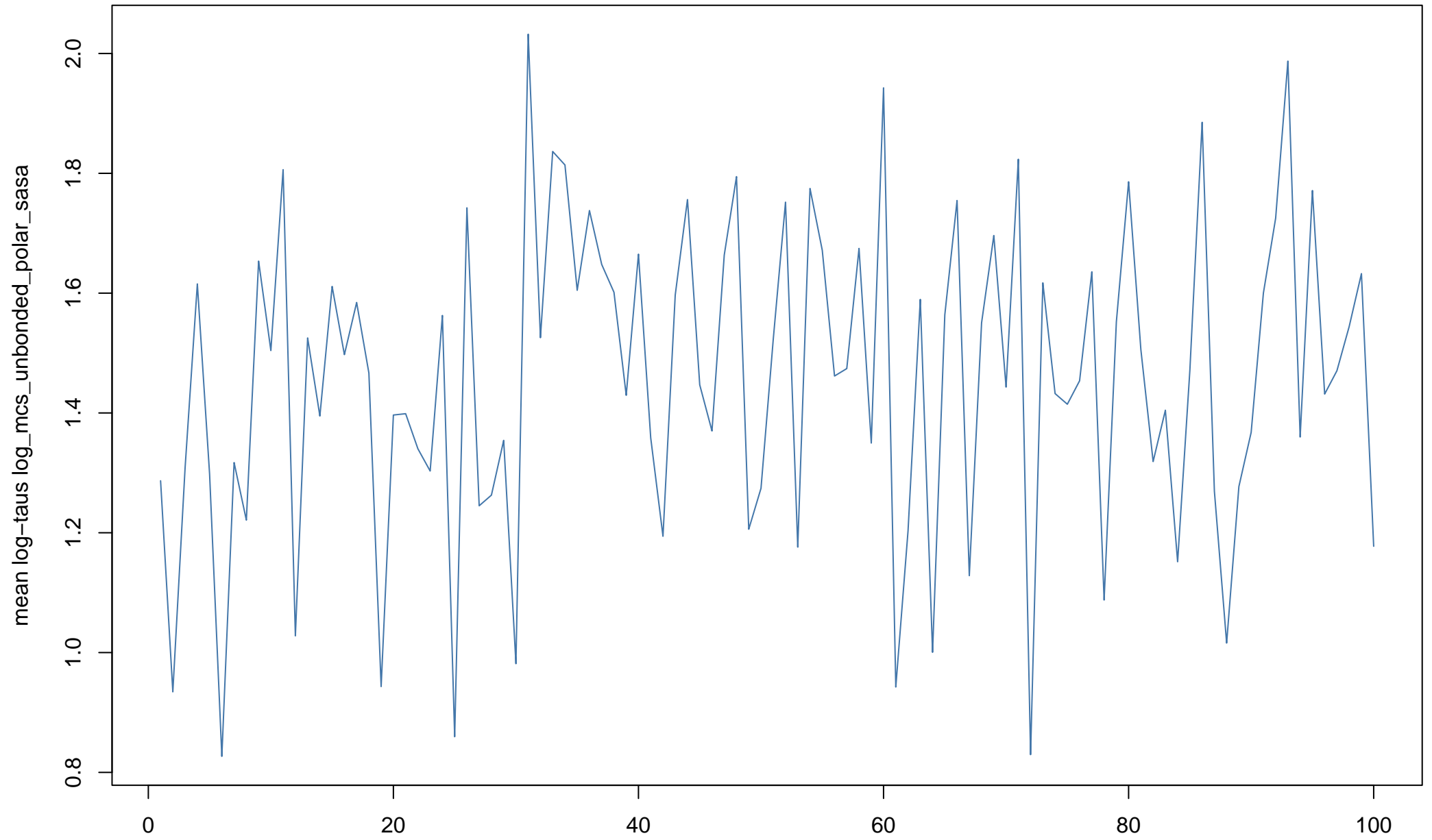**mean taus log_RMSD**
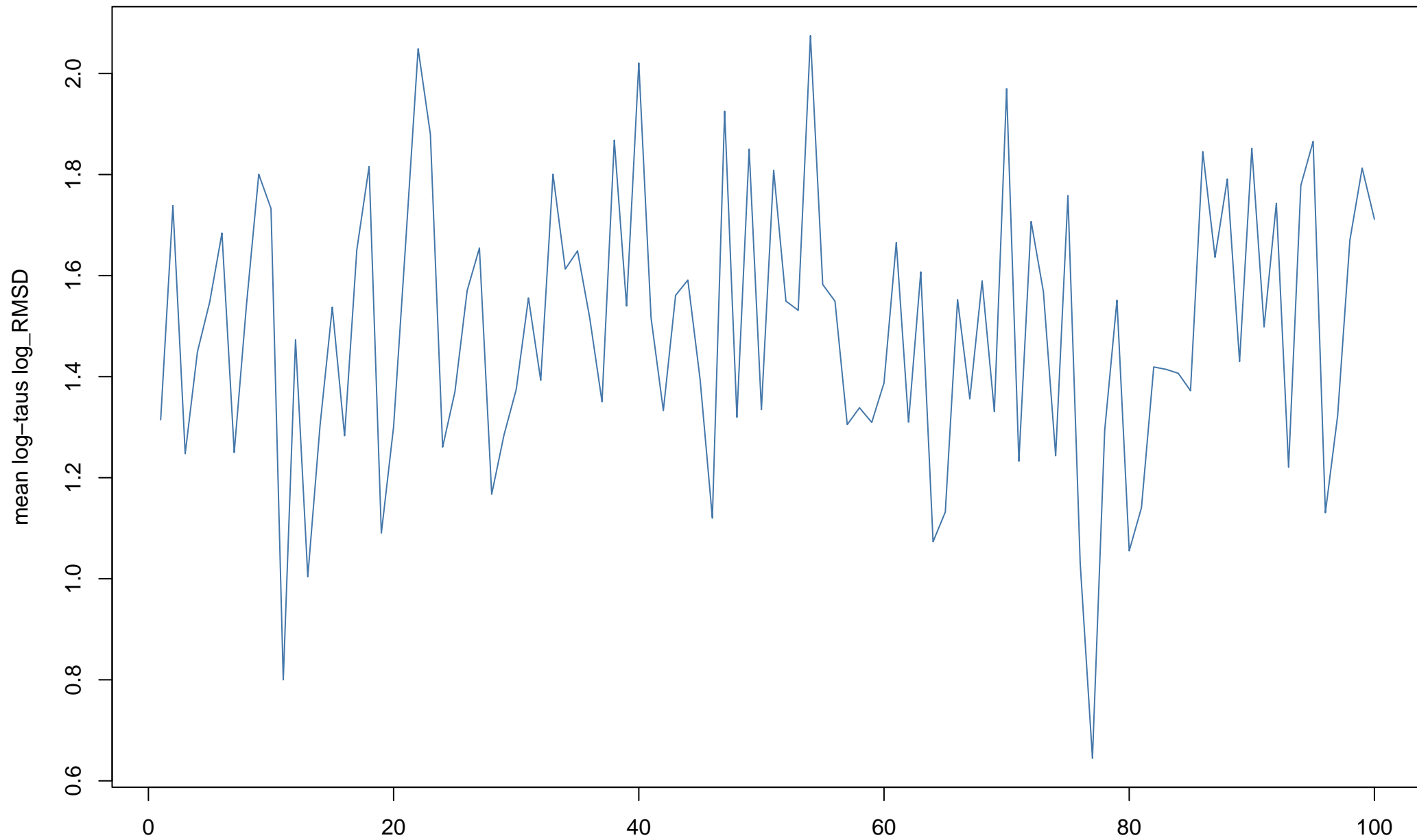
log−SD taus log_RMSD
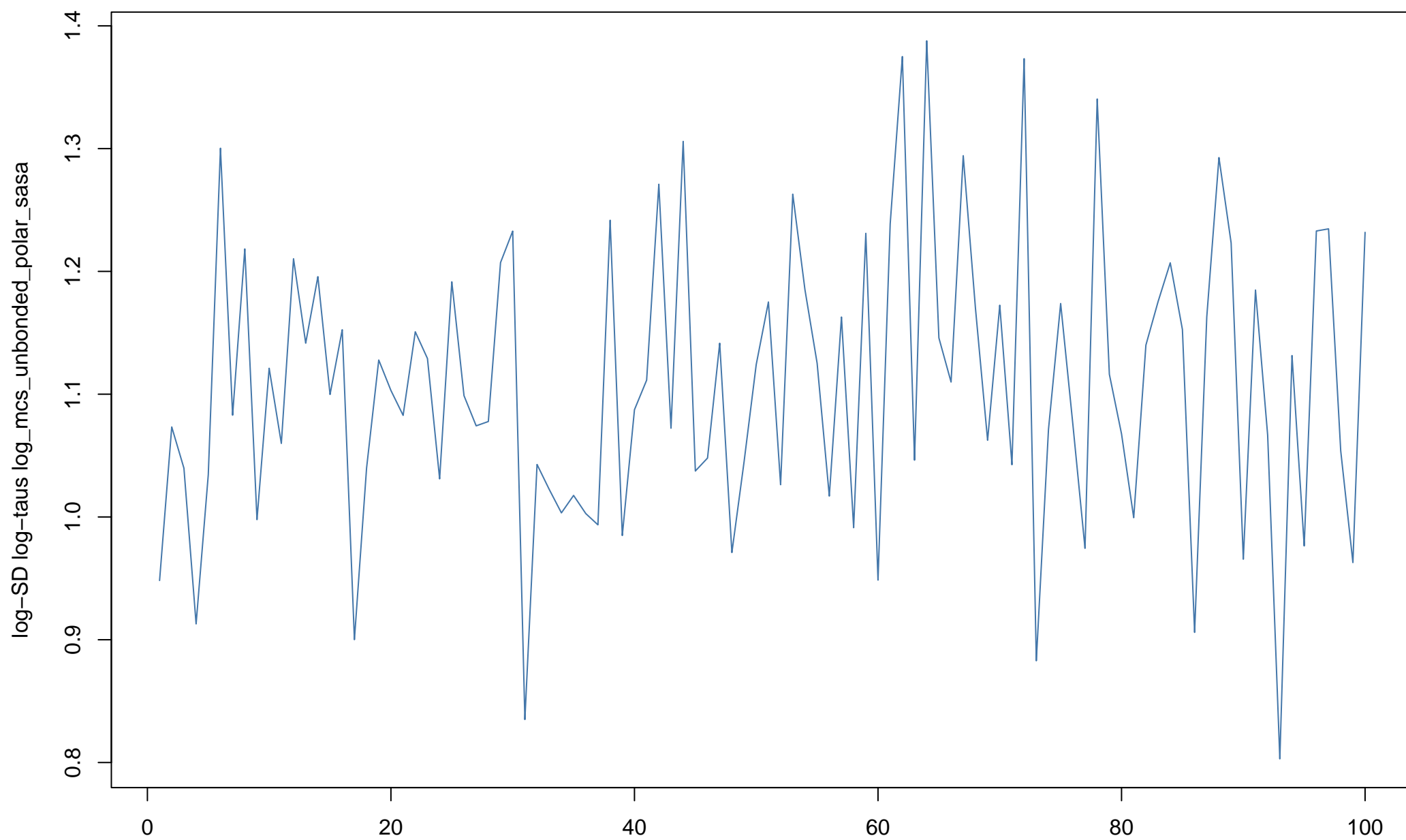
mean means log_mcs_unbonded_polar_sasa

log−SD means log_mcs_unbonded_polar_sasa
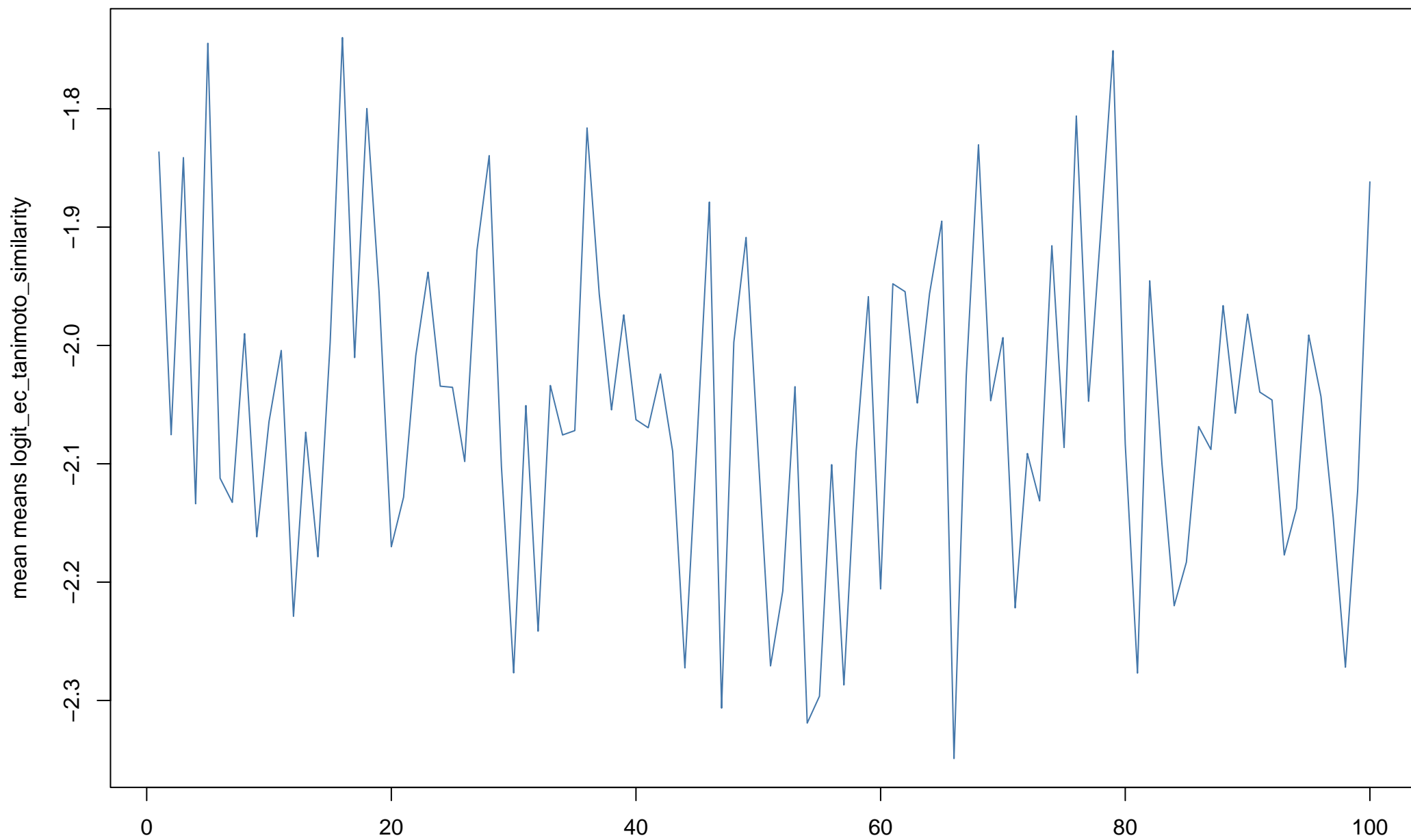
mean taus log_mcs_unbonded_polar_sasa

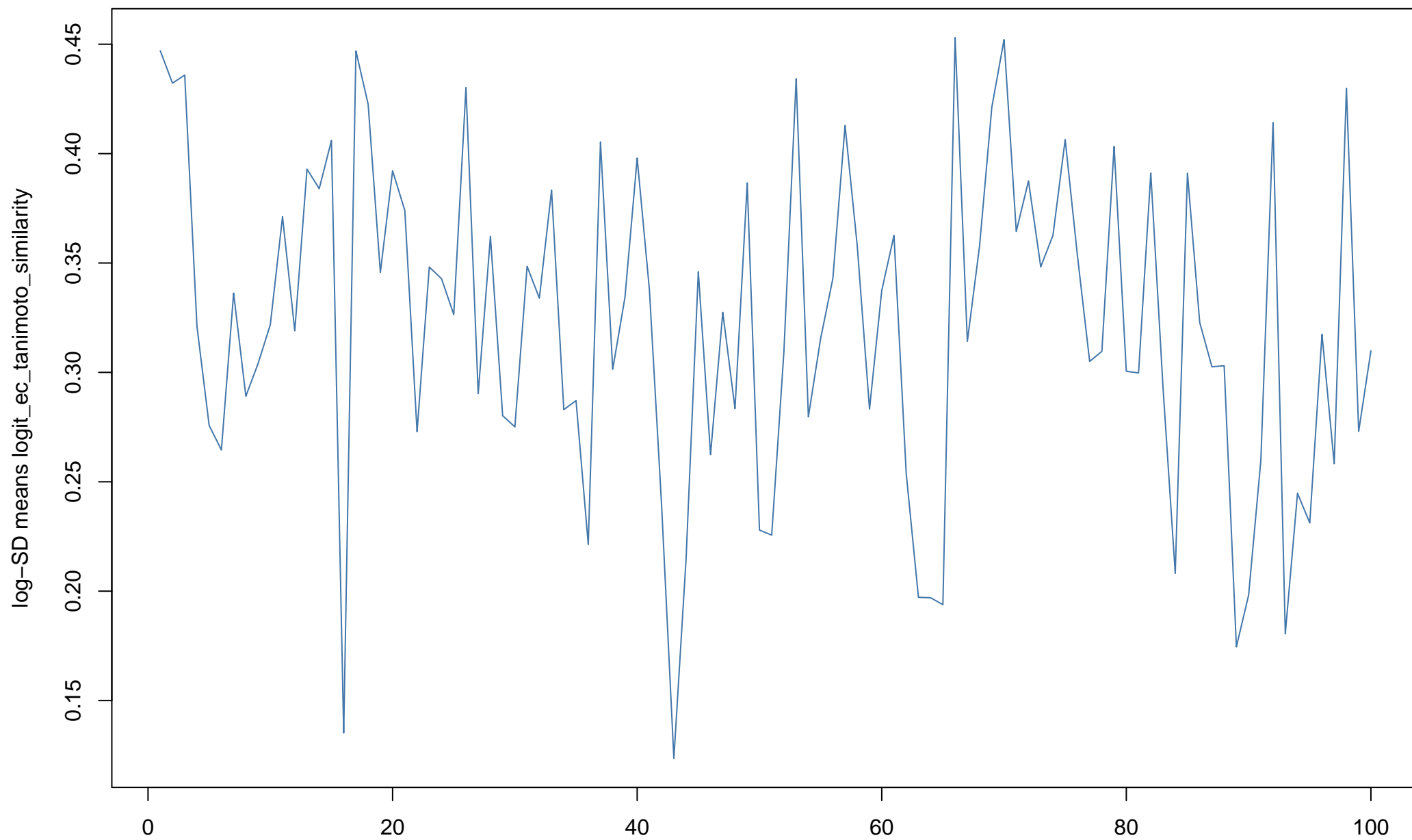**log-SD taus log_mcs_unbonded_polar_sasa**
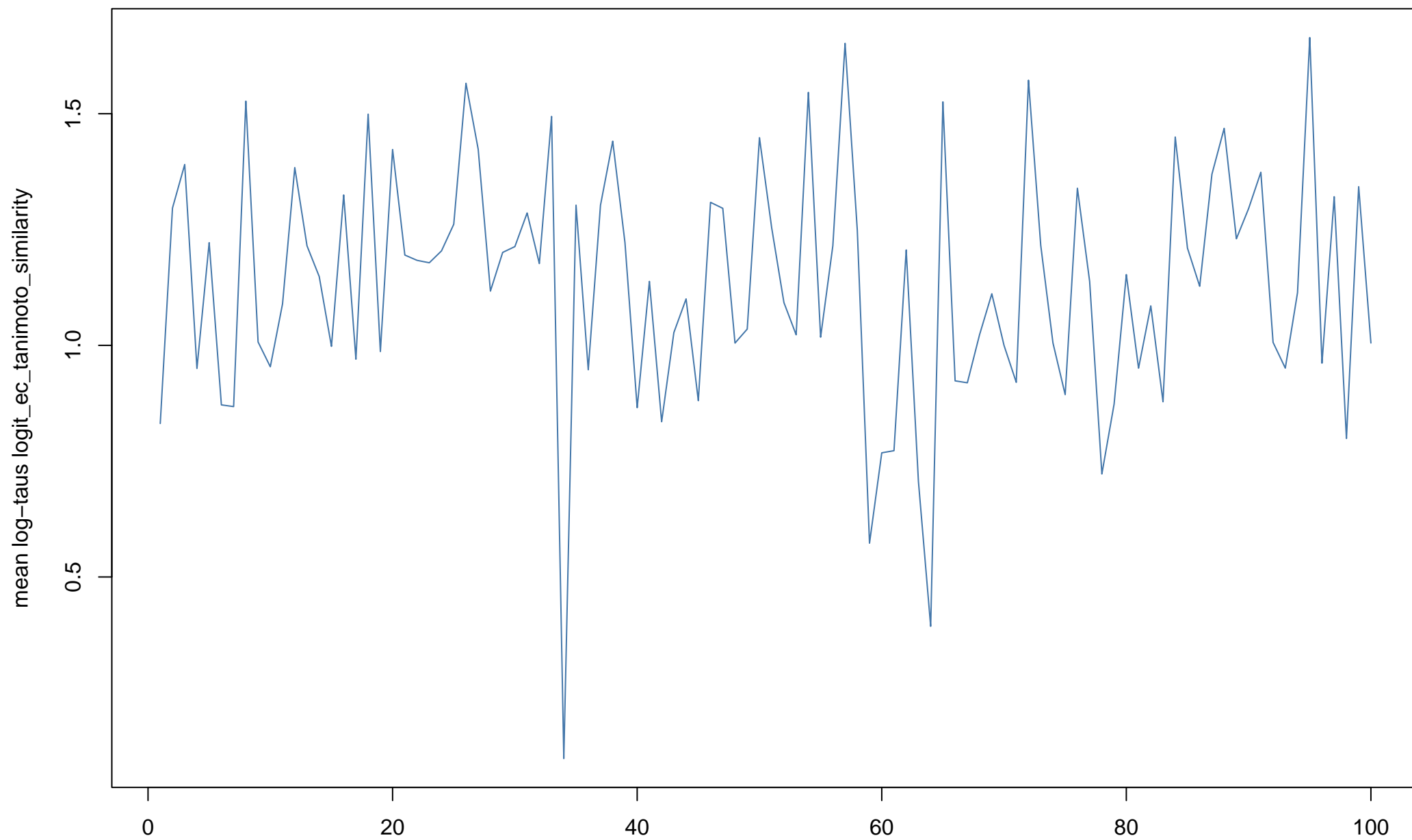
log-SD log-taus log_mcs_unbonded_polar_sasa

mean means logit_ec_tanimoto_similarity
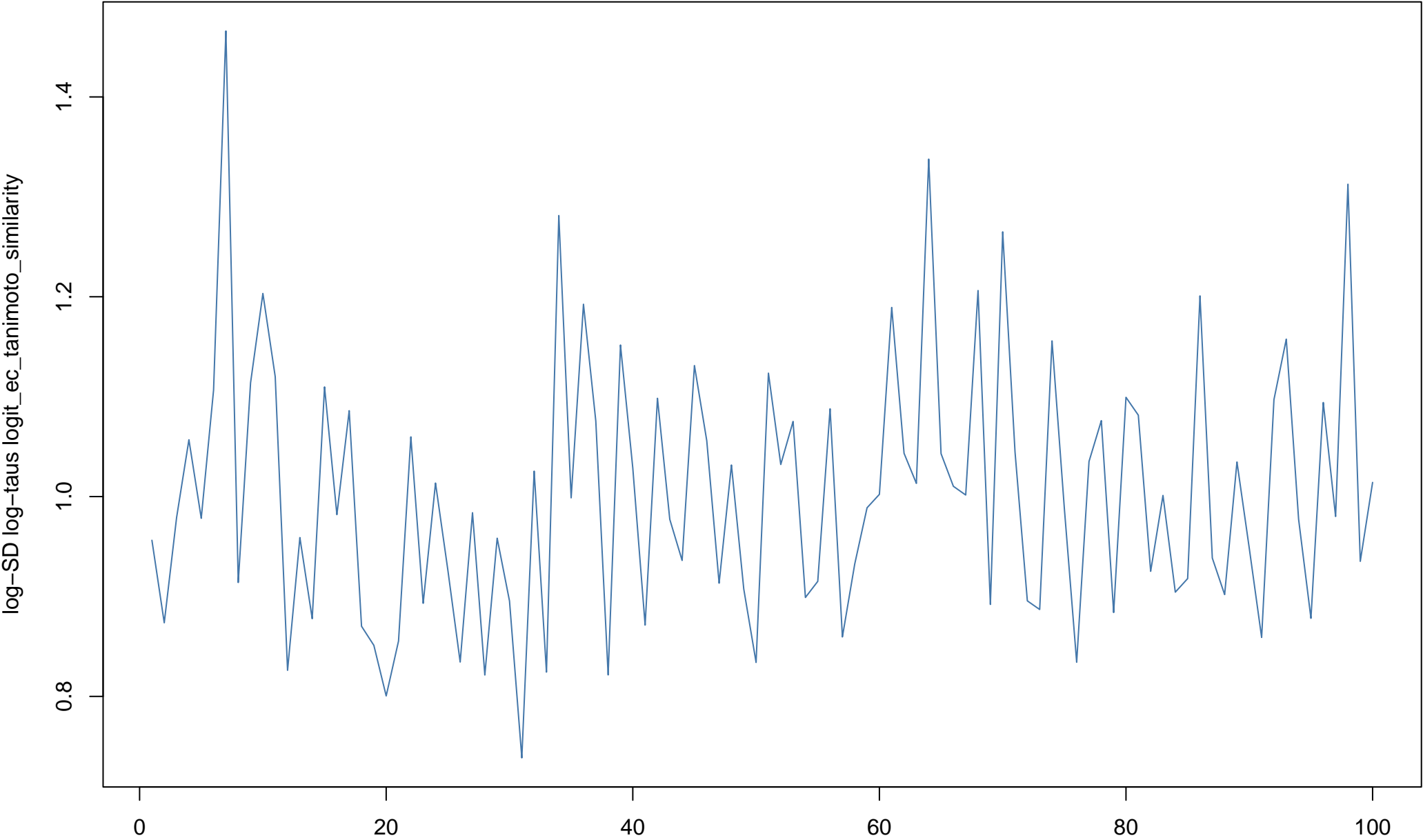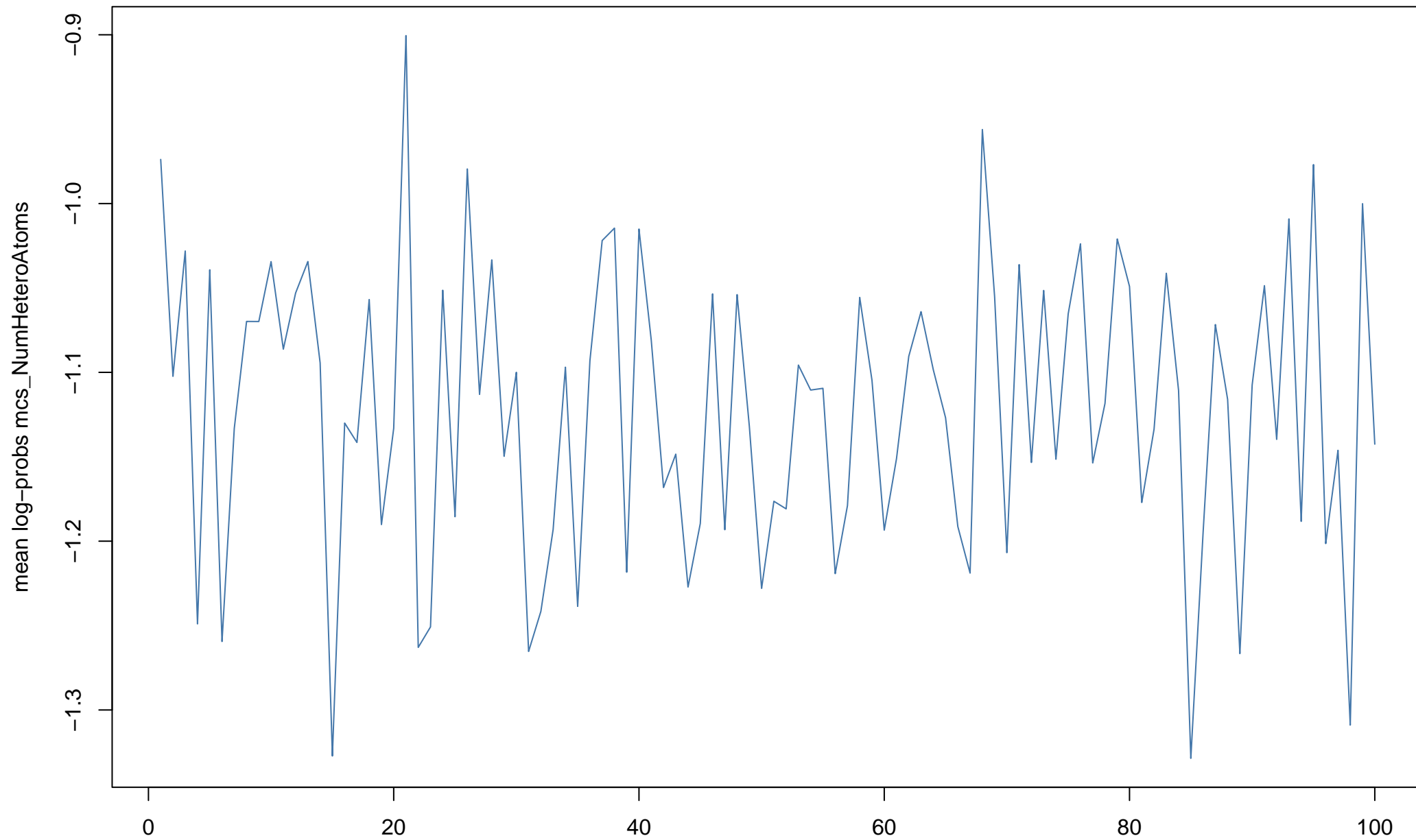
log−SD means logit_ec_tanimoto_similarity

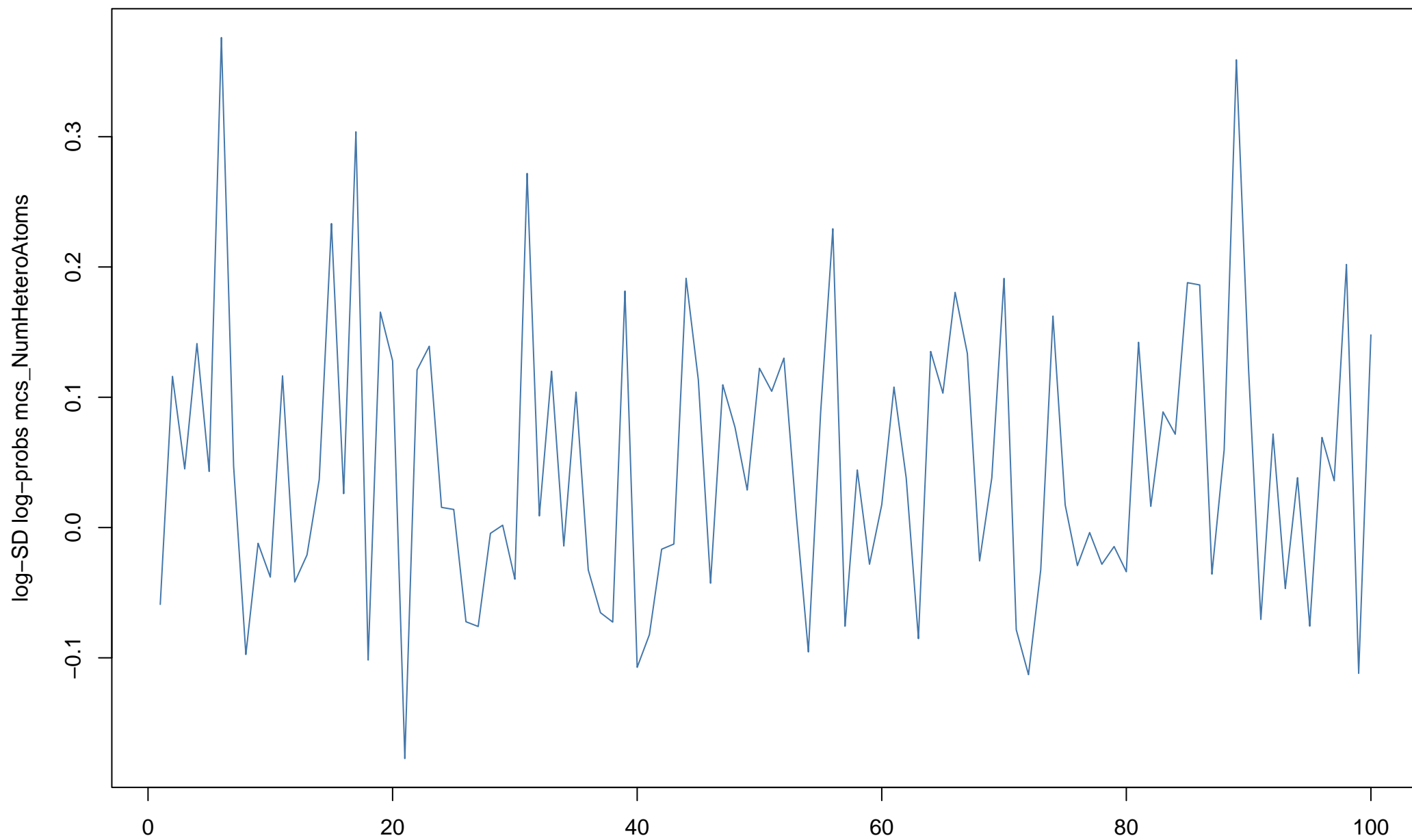**mean taus logit_ec_tanimoto_similarity**

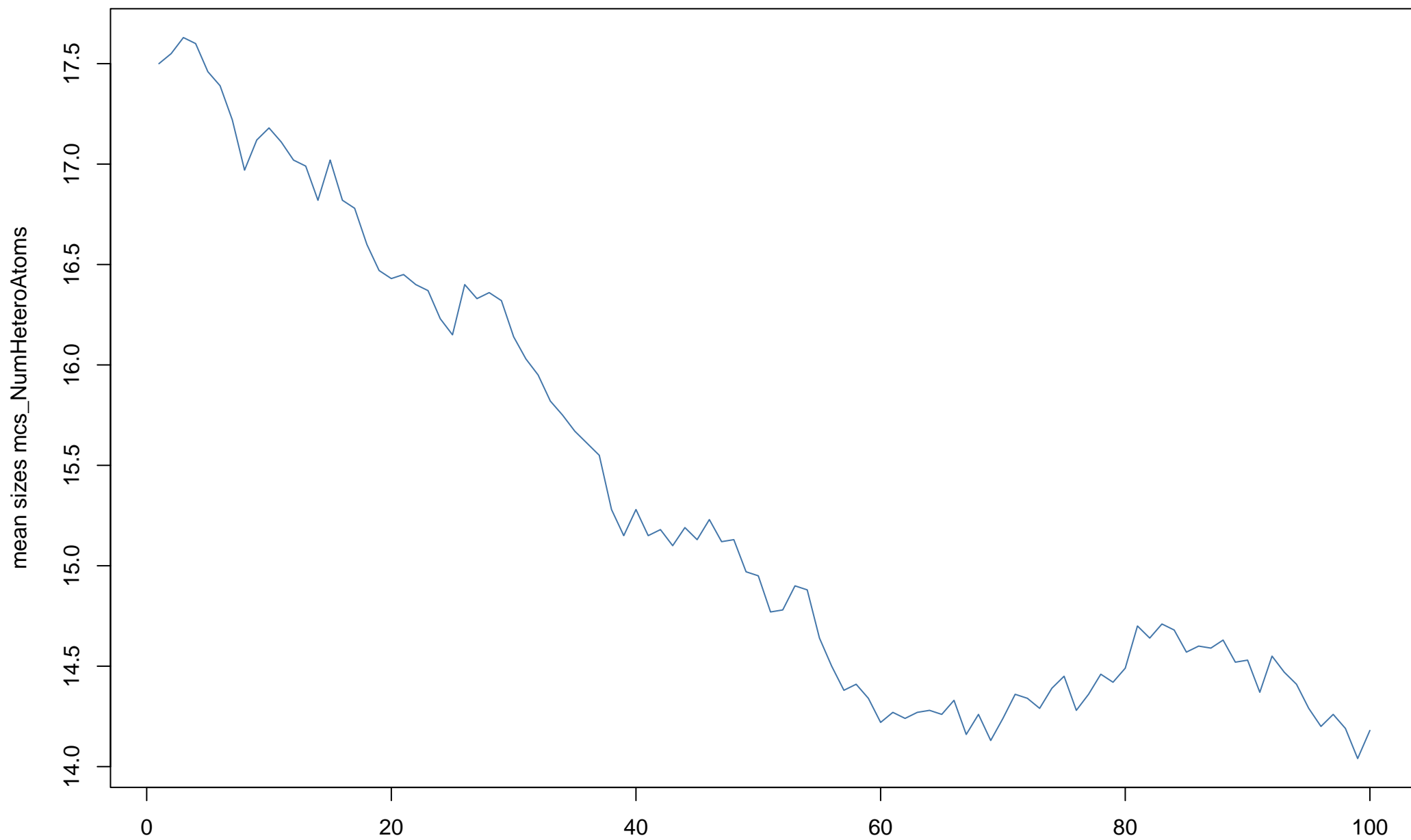**log−SD taus logit_ec_tanimoto_similarity**

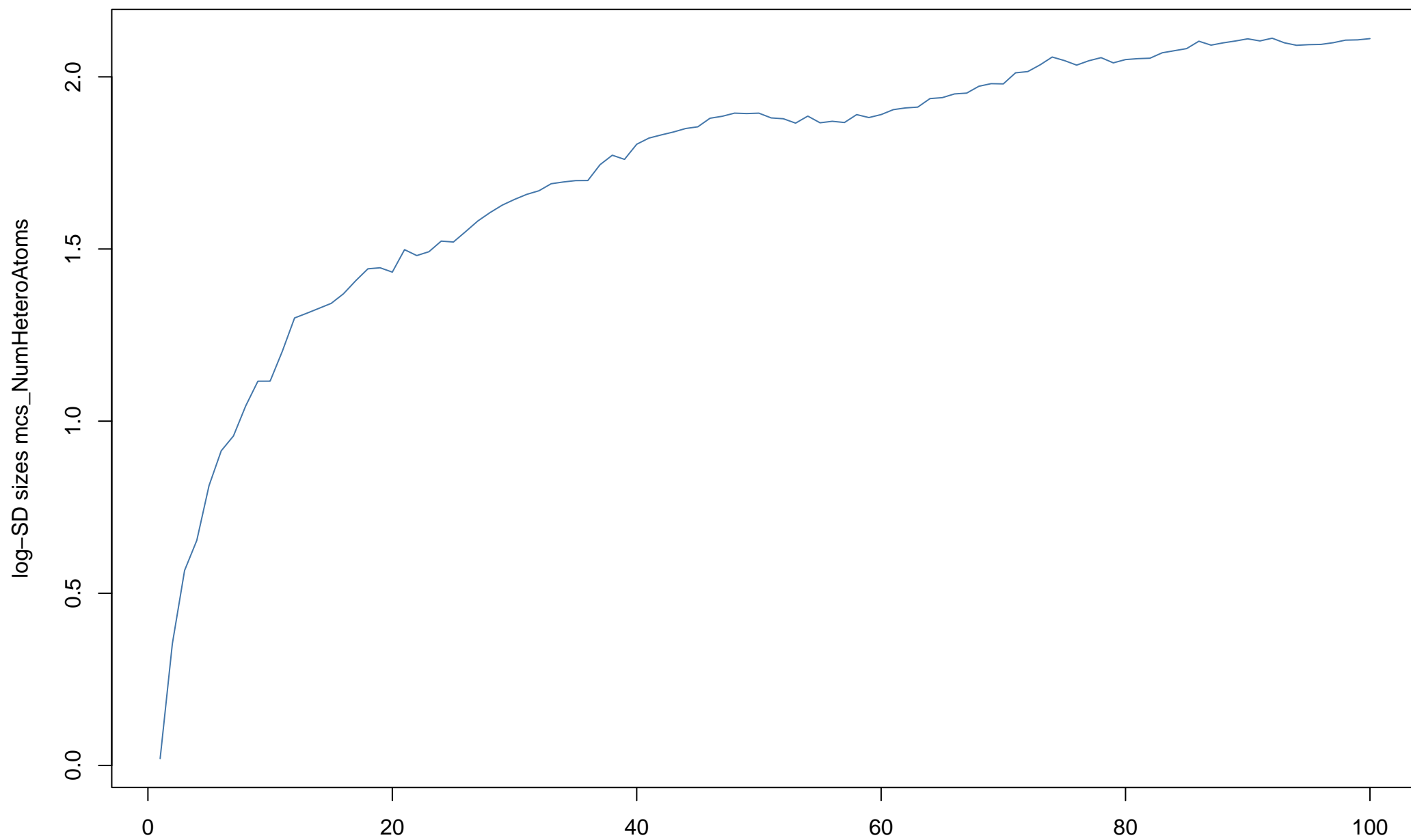**mean probs mcs_NumHeteroAtoms**

log−SD probs mcs_NumHeteroAtoms
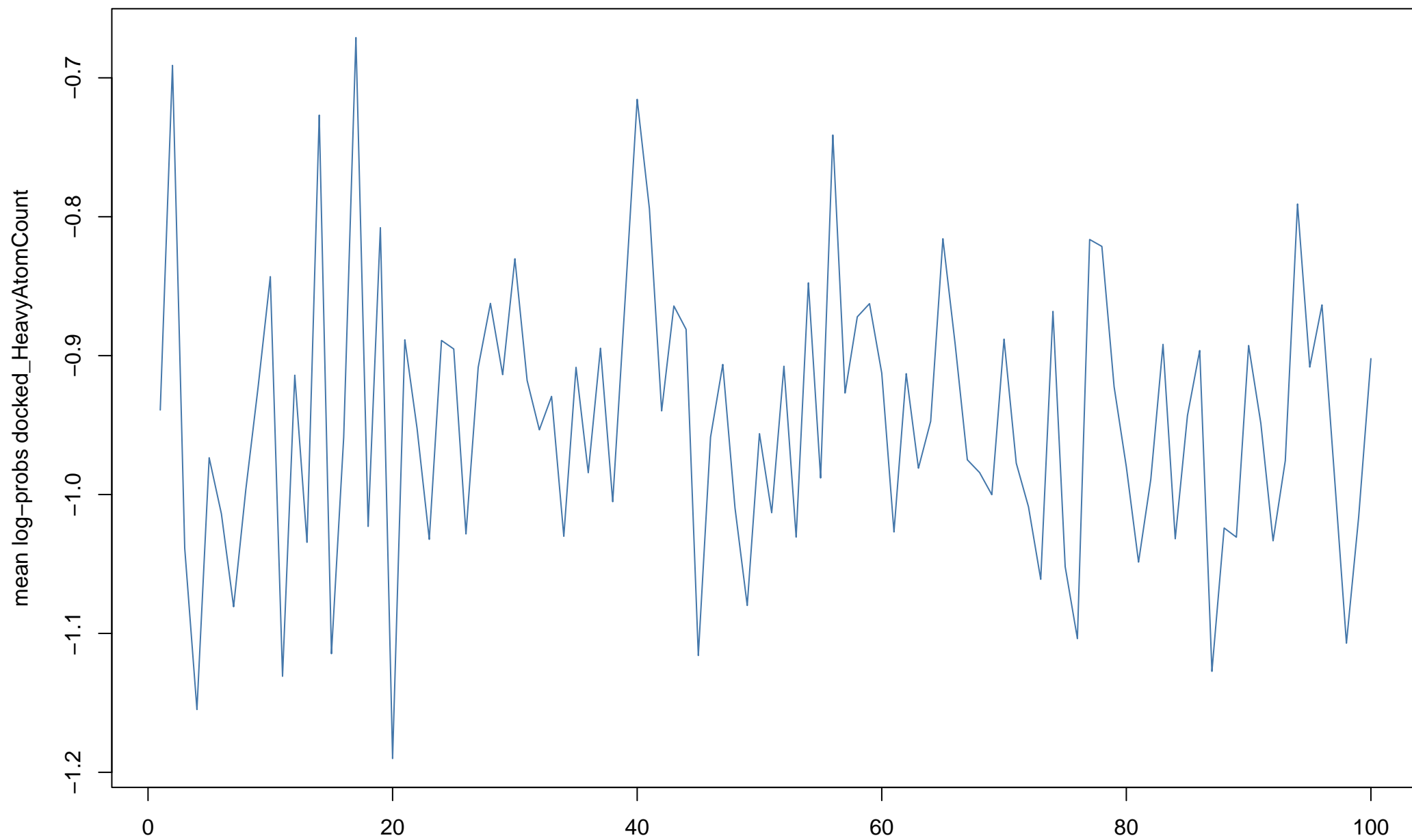
mean sizes mcs_NumHeteroAtoms
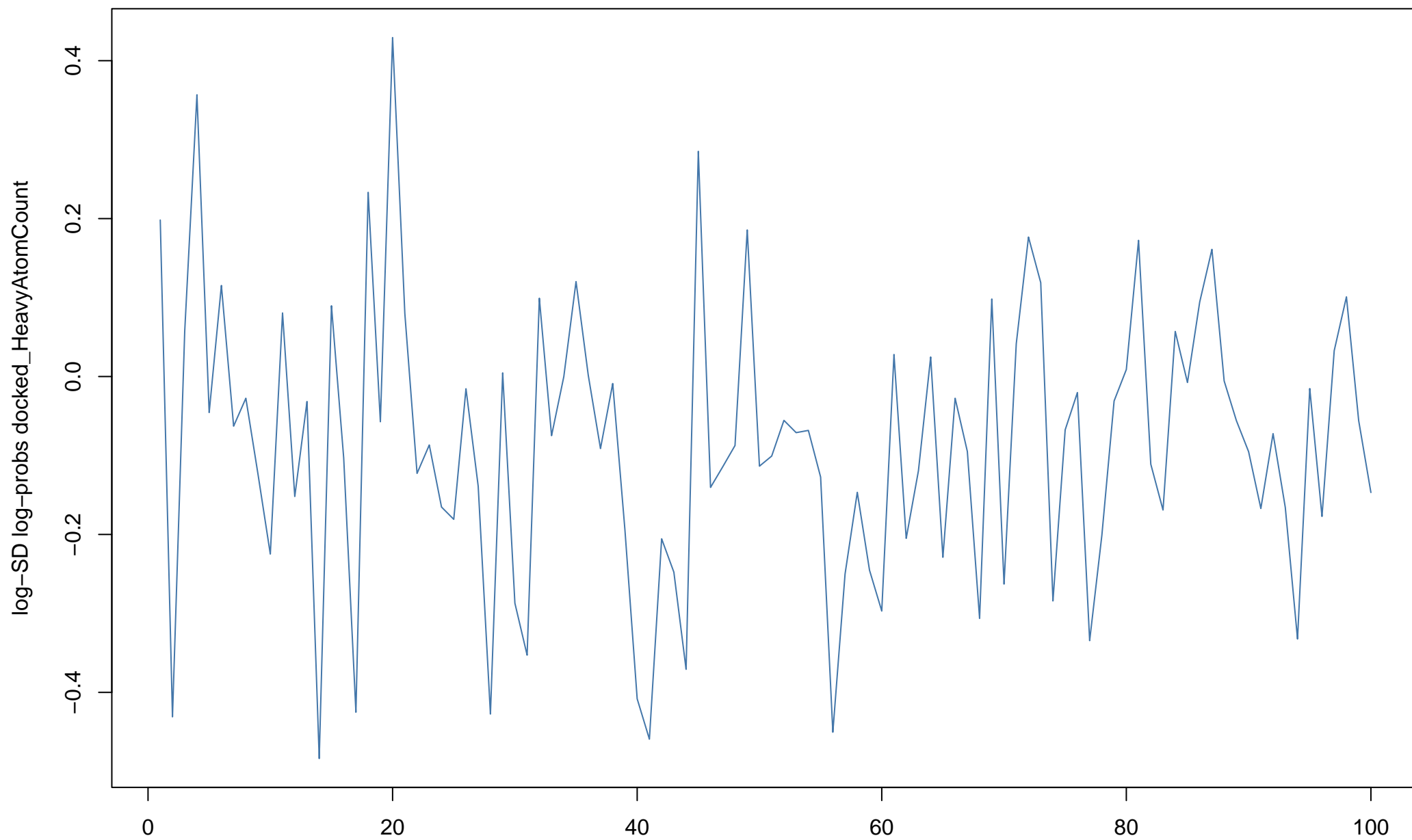
log−SD sizes mcs_NumHeteroAtoms
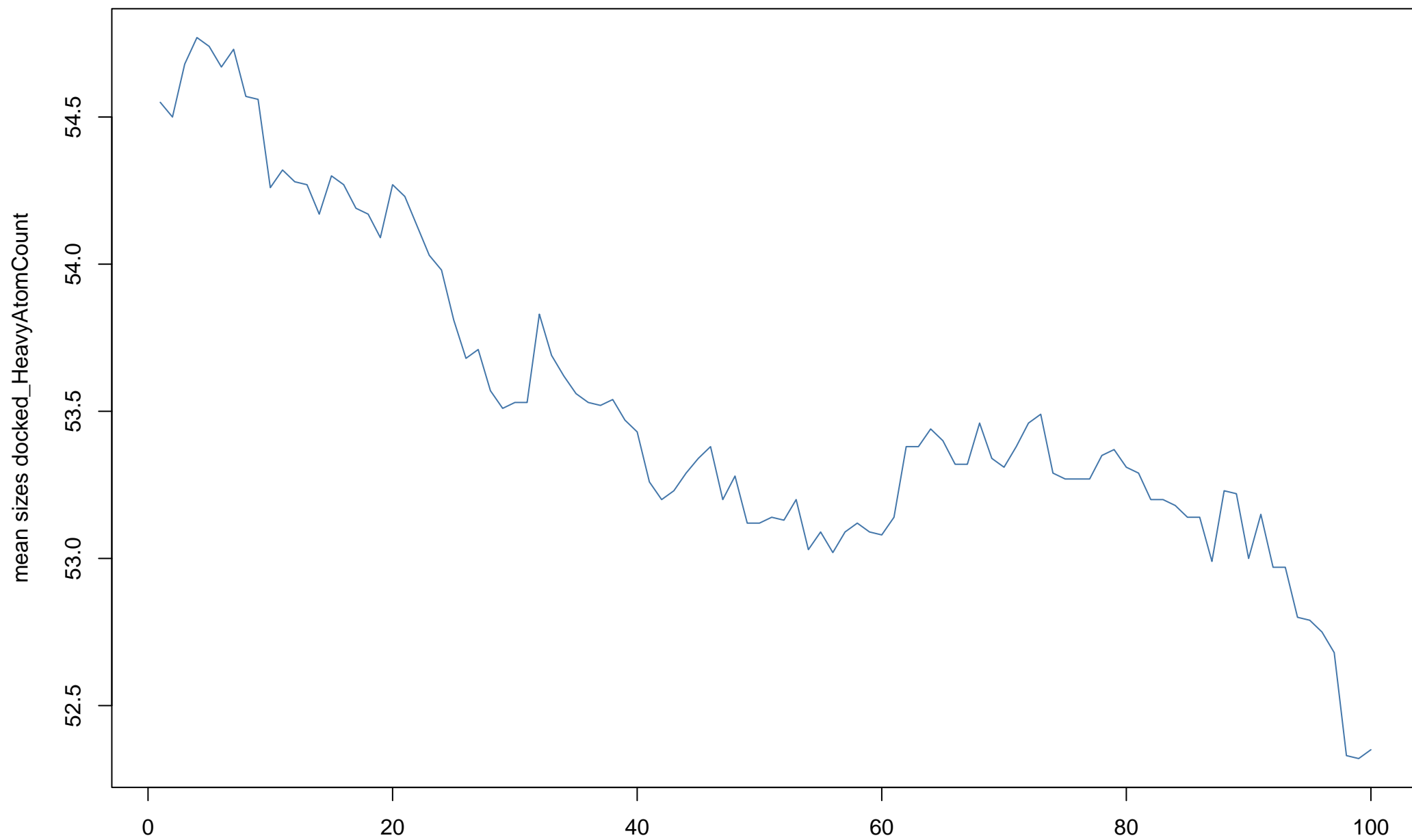
log−SD sizes mcs_NumHeteroAtoms

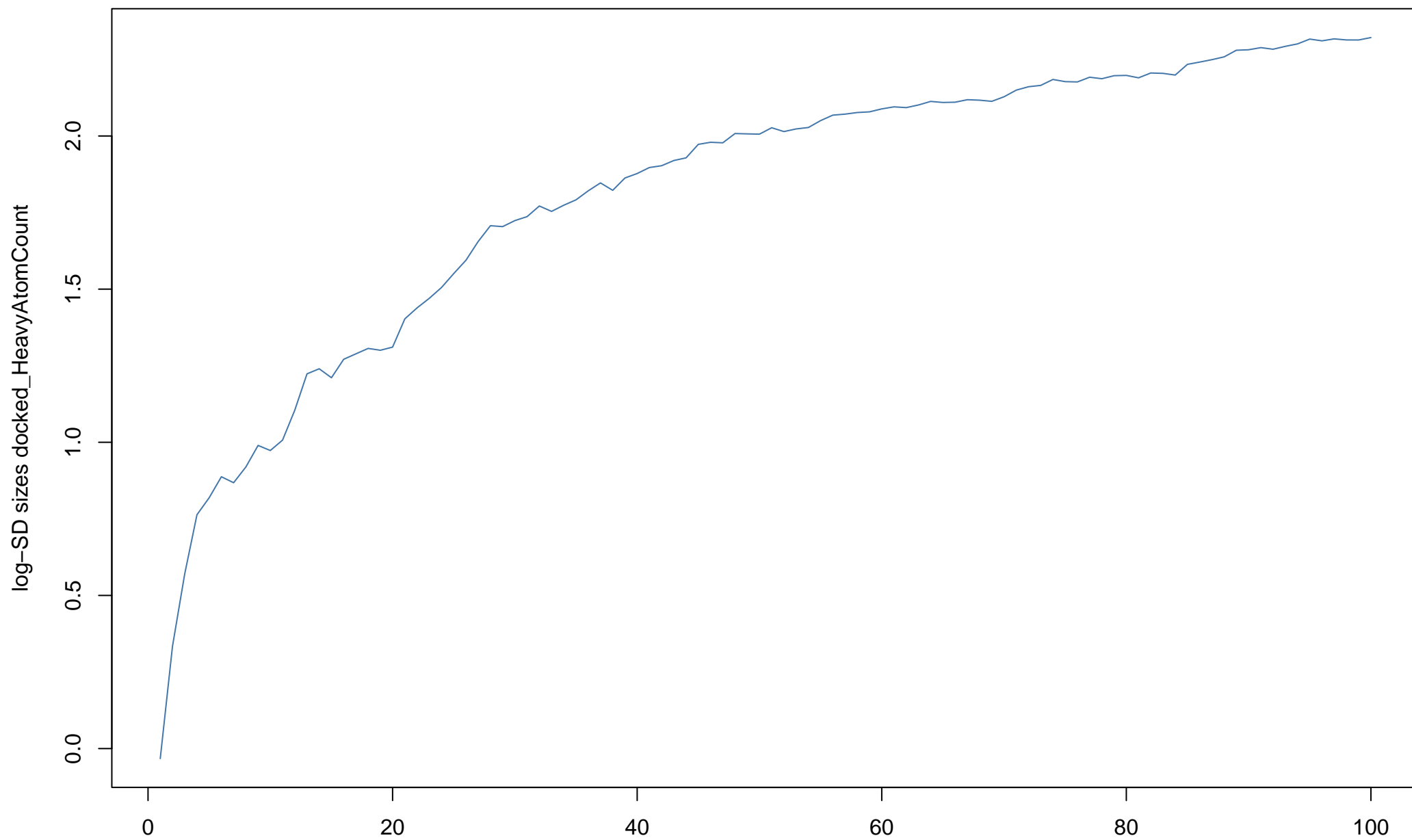mean probs docked_HeavyAtomCount

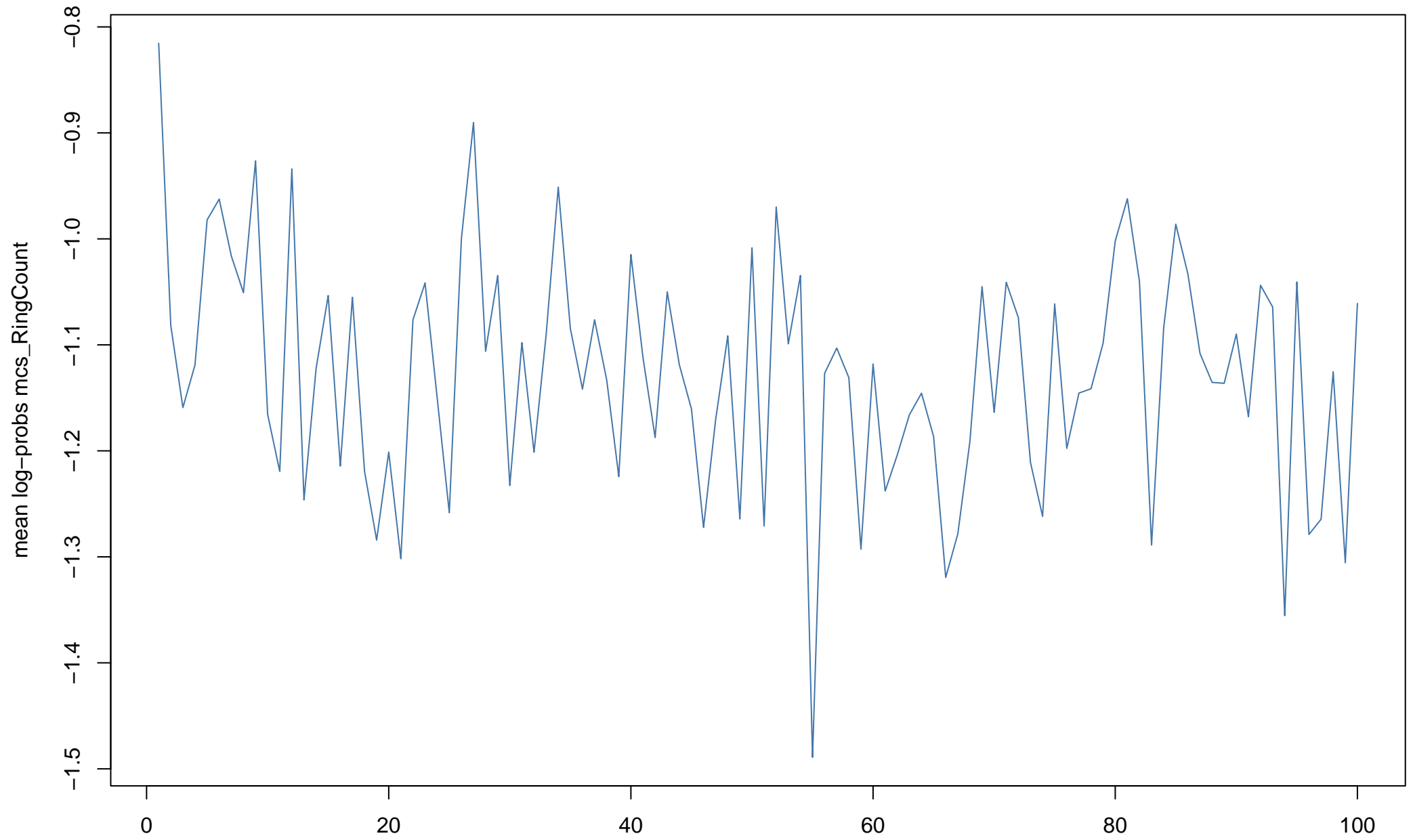log−SD probs docked_HeavyAtomCount

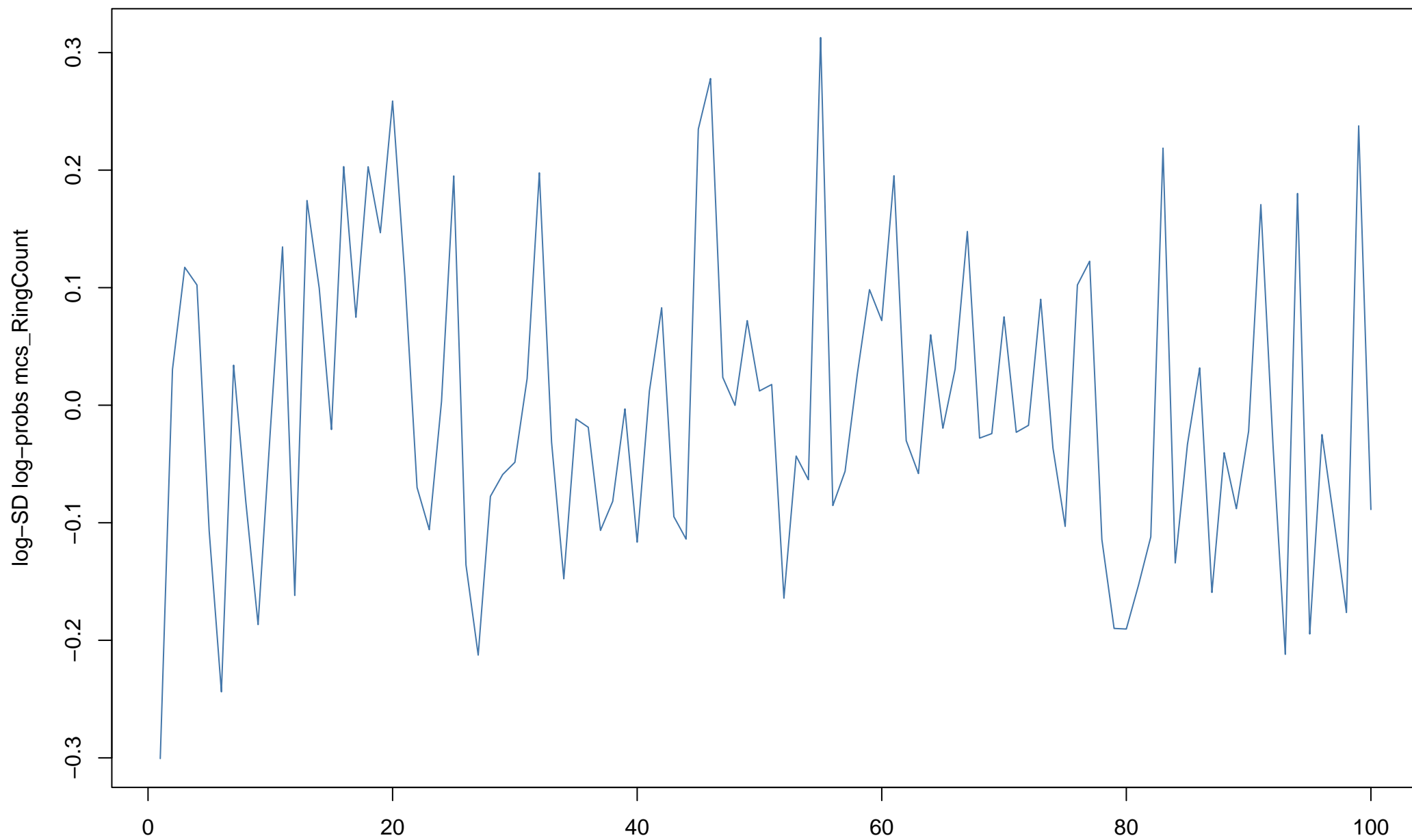**mean sizes docked_HeavyAtomCount**

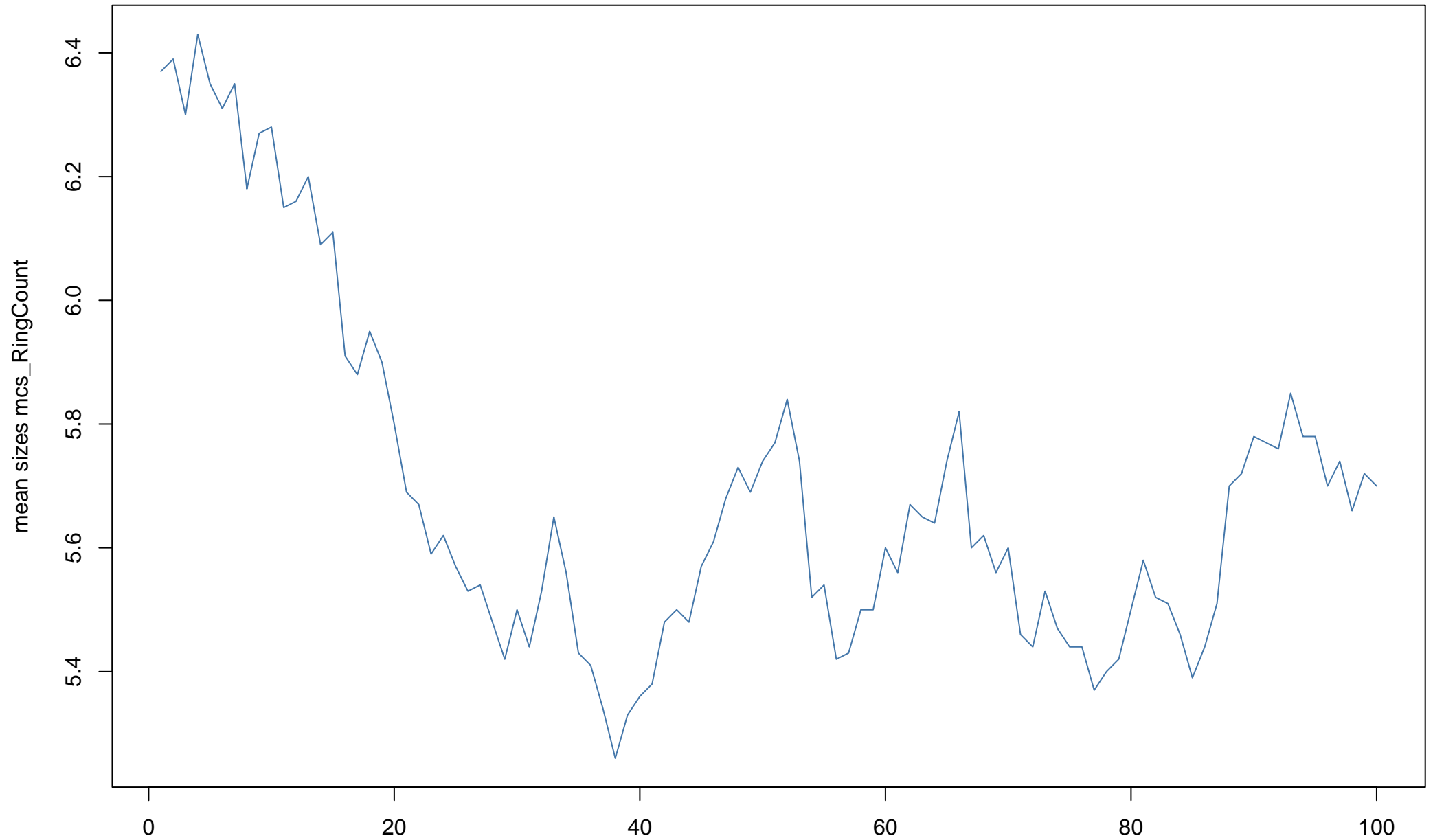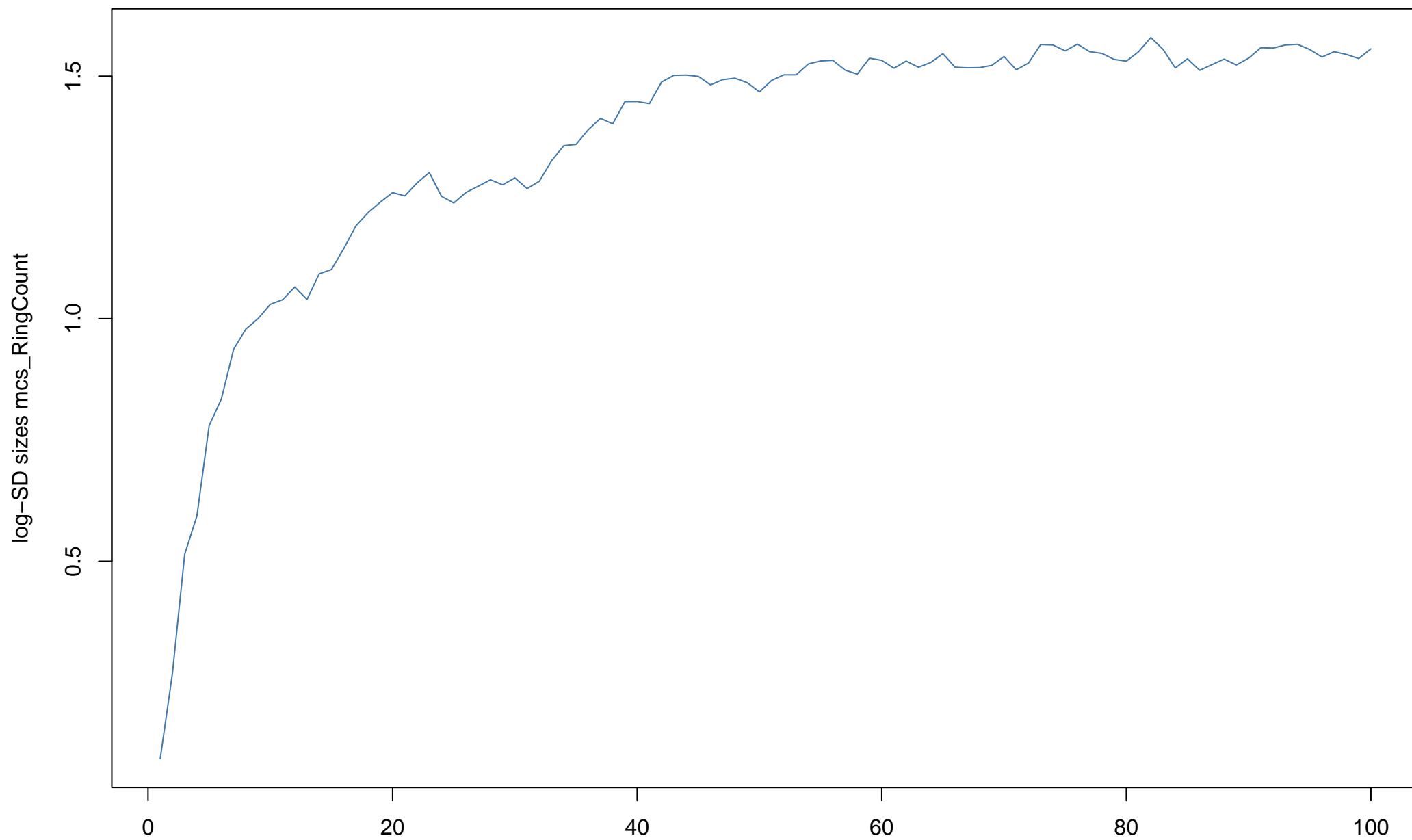**log−SD sizes docked_HeavyAtomCount**

mean probs mcs_RingCount
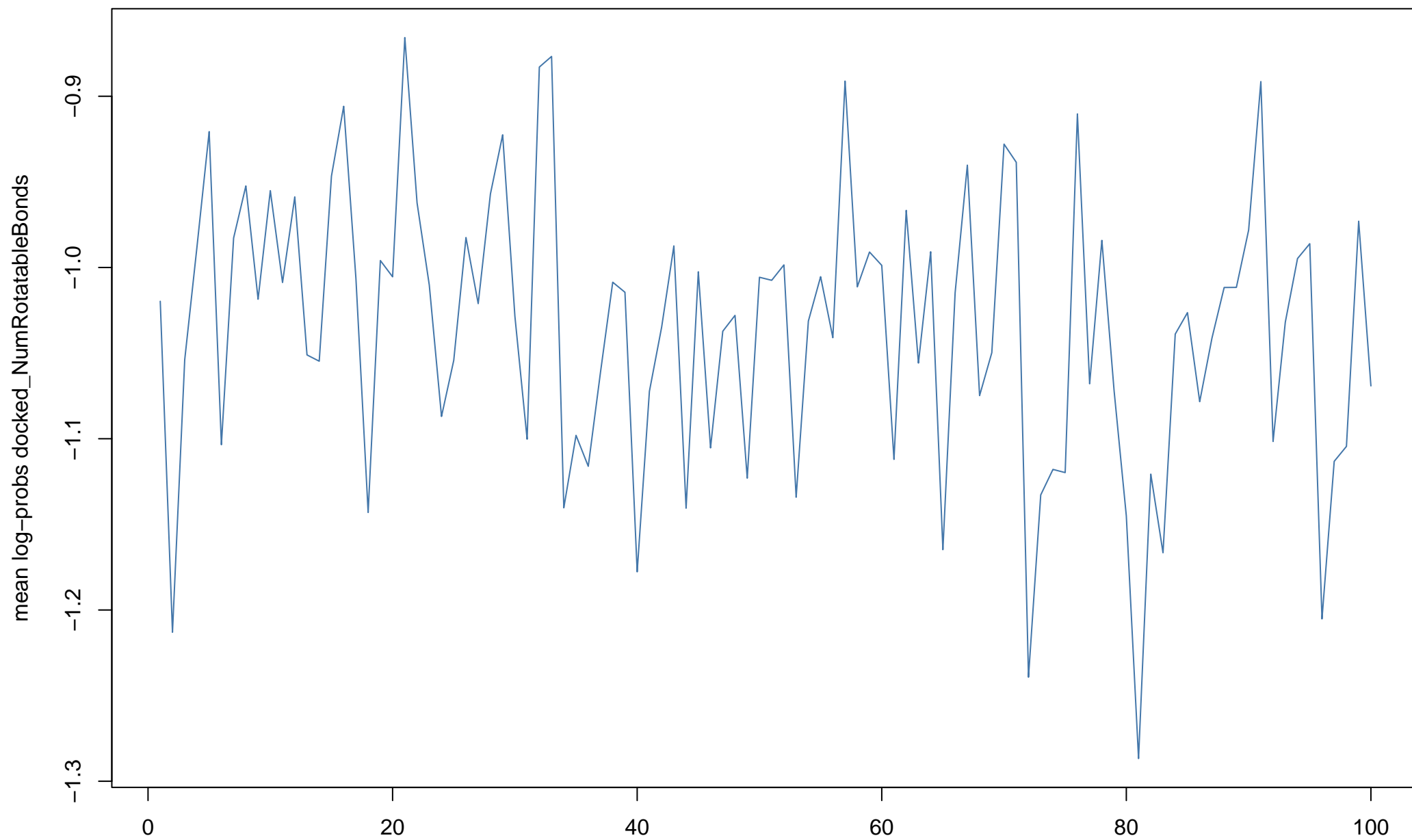
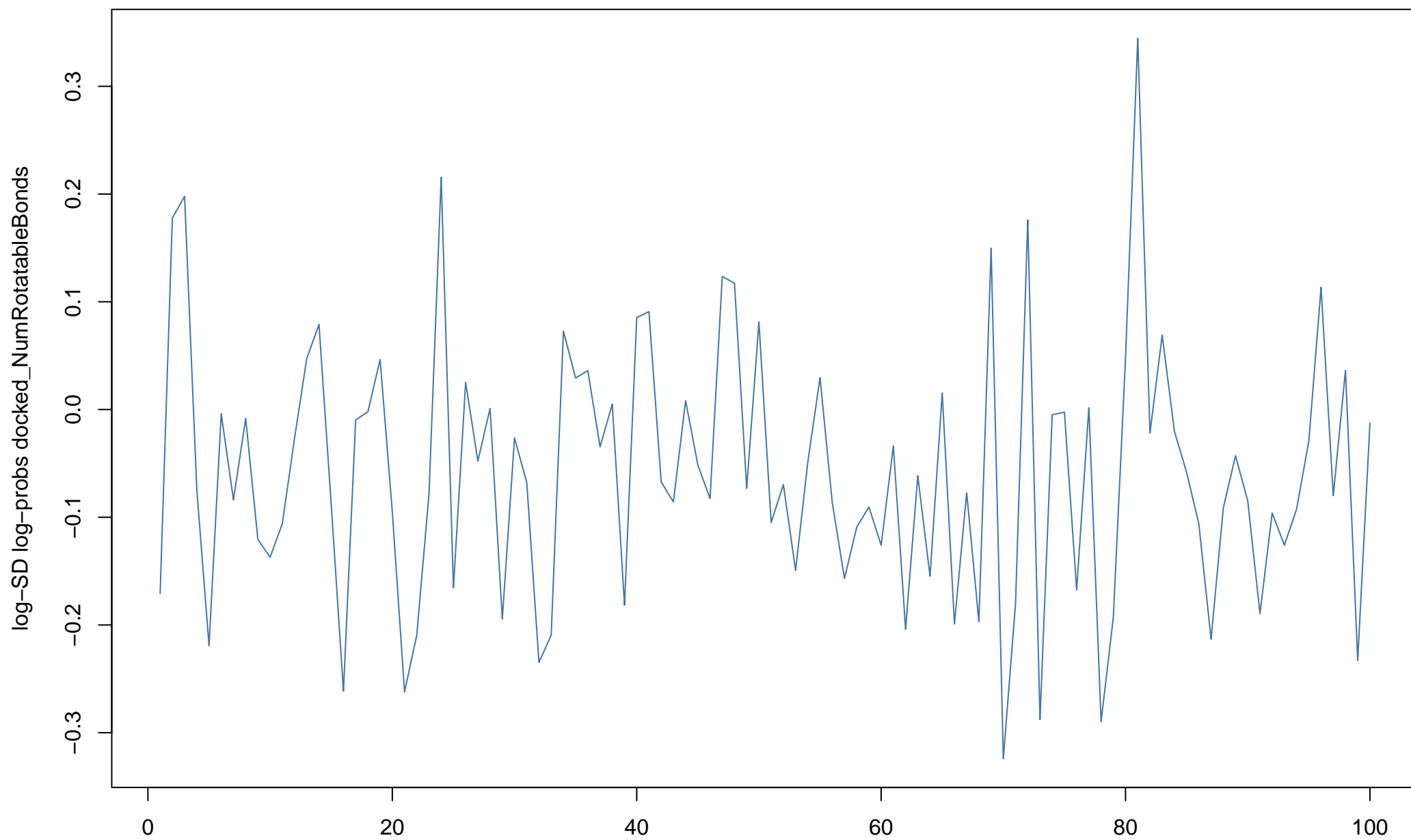**log−SD probs mcs_RingCount**

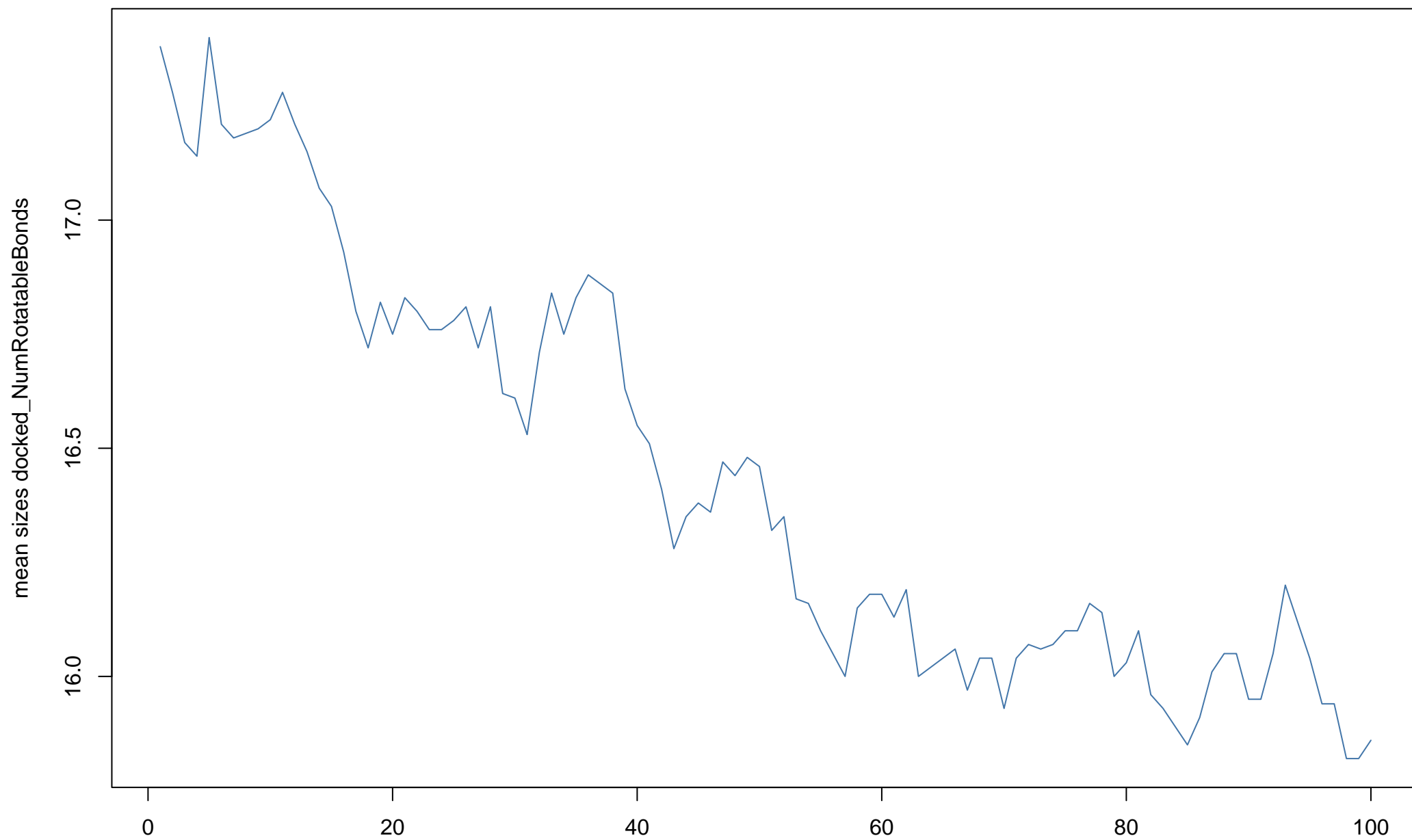**mean sizes mcs_RingCount**

log−SD sizes mcs_RingCount

mean probs docked_NumRotatableBonds

log−SD probs docked_NumRotatableBonds

mean sizes docked_NumRotatableBonds

log−SD sizes docked_NumRotatableBonds