

Electronic supplementary information-2 (ESI-2) for
“Refinement and extension of COSMO-RS-trained fragment contribution models for
predicting partition properties of C_{10–20} chlorinated paraffin congeners”

Satoshi Endo

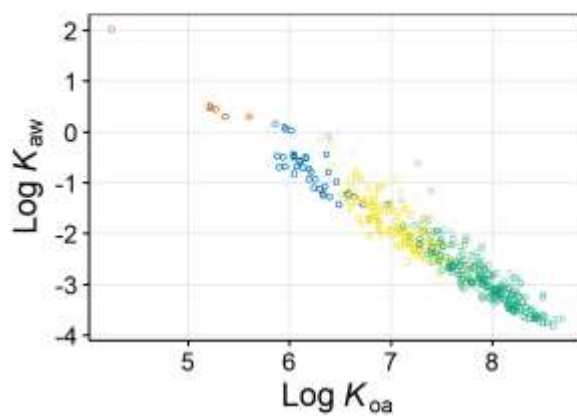
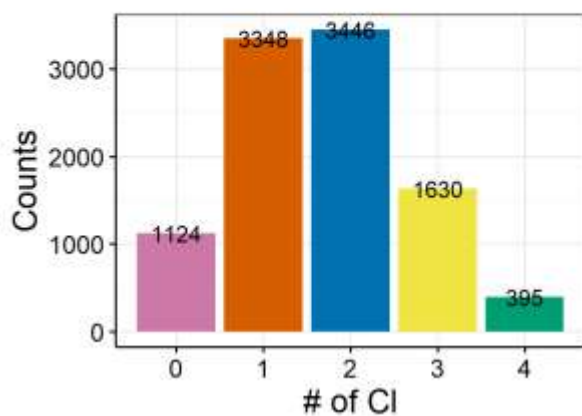
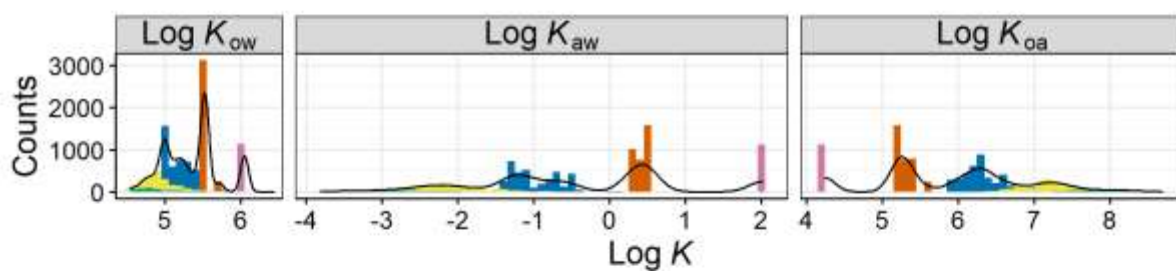
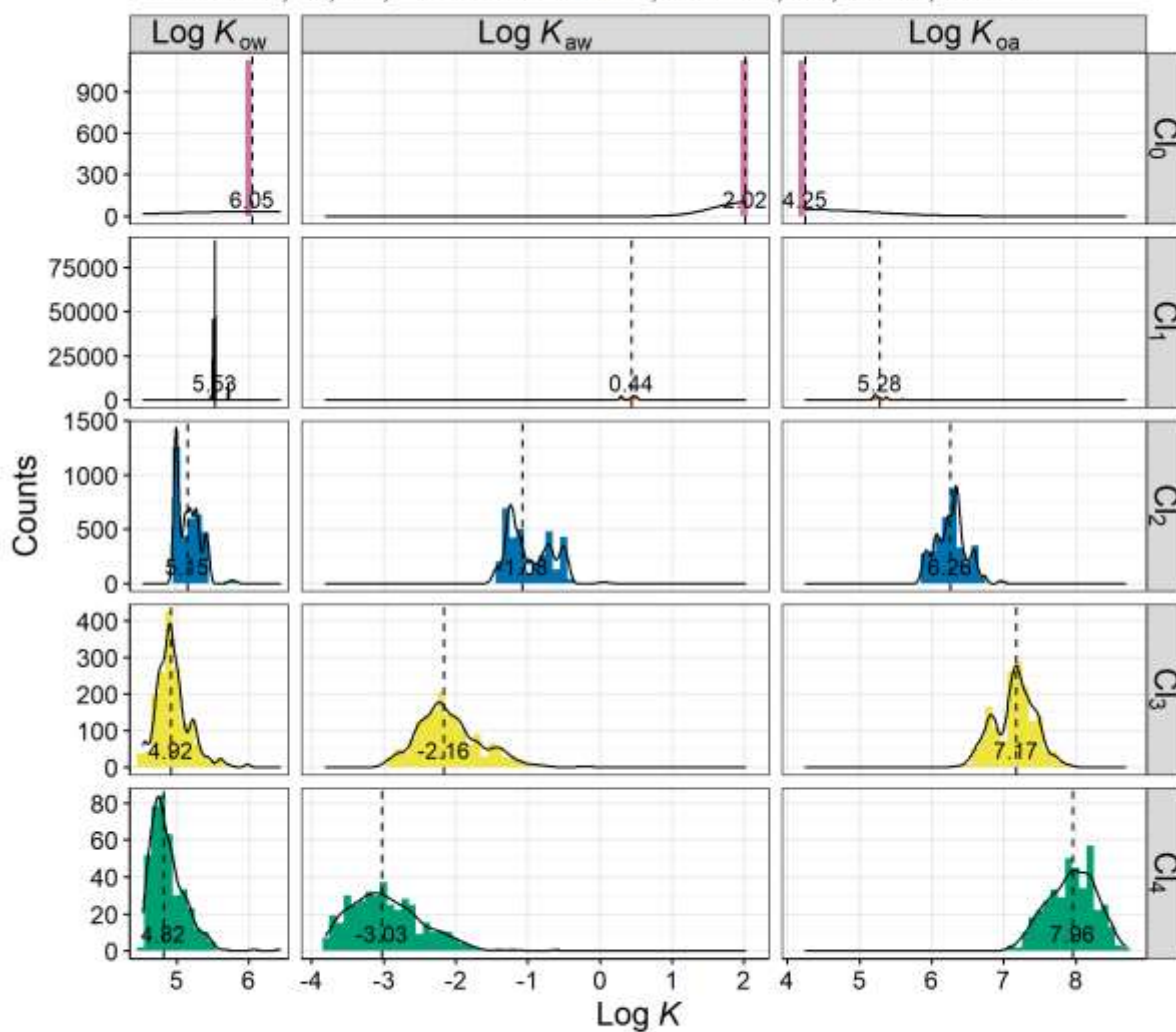
Center for Health and Environmental Risk Research, National Institute for Environmental Studies
(NIES), Onogawa 16-2, 305-8506 Tsukuba, Ibaraki, Japan

Phone: ++81-29-850-2695, endo.satoshi@nies.go.jp

**Property distributions of CP mixtures with a carbon-chain length of C_{10–20} and a chlorination degree of 30–70 wt%:
log K_{ow} , log K_{aw} , log K_{oa}**

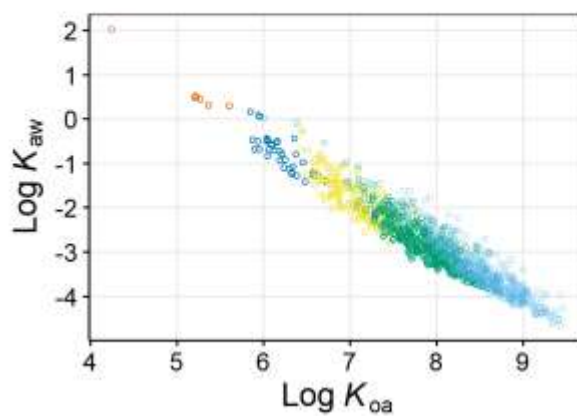
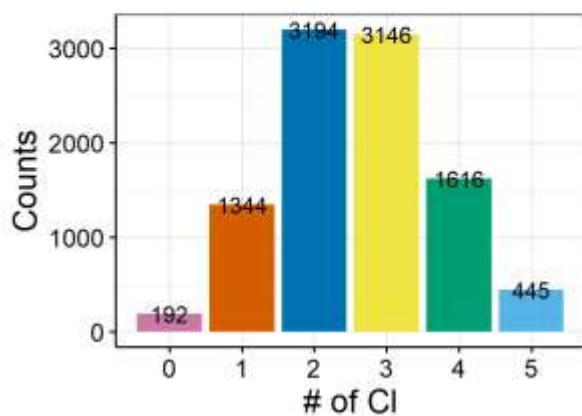
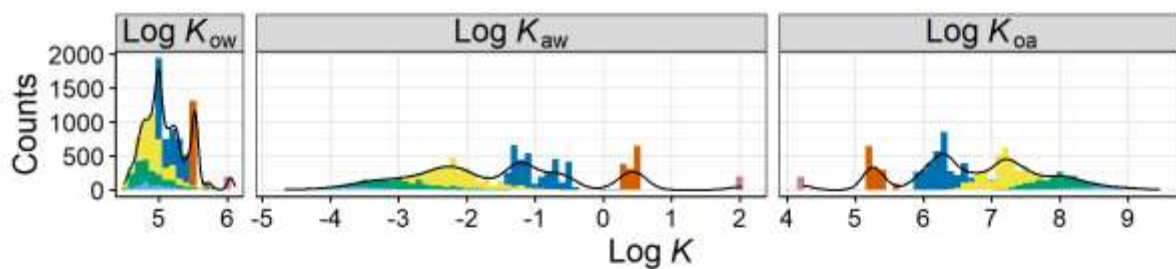
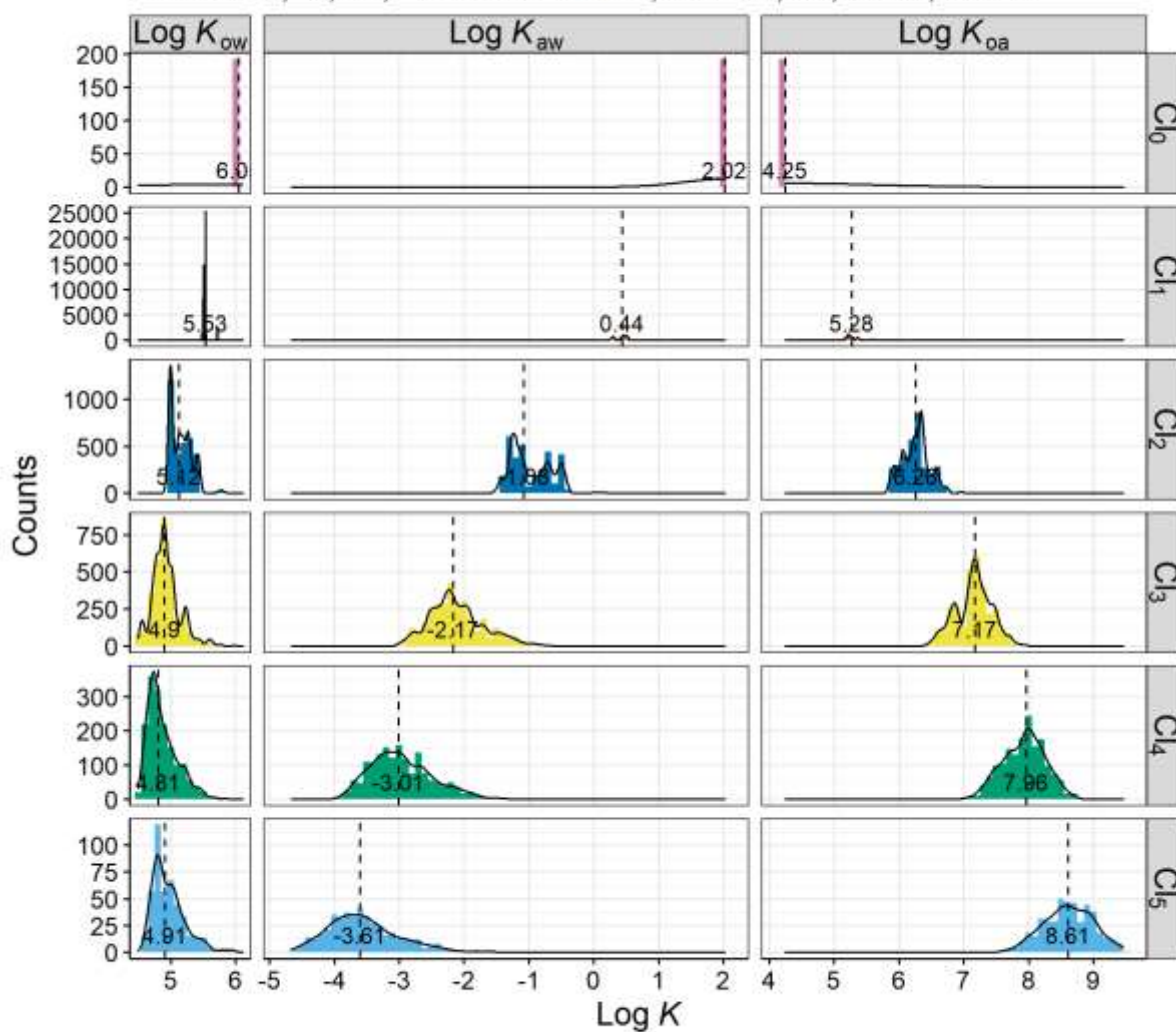
C₁₀, 30 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



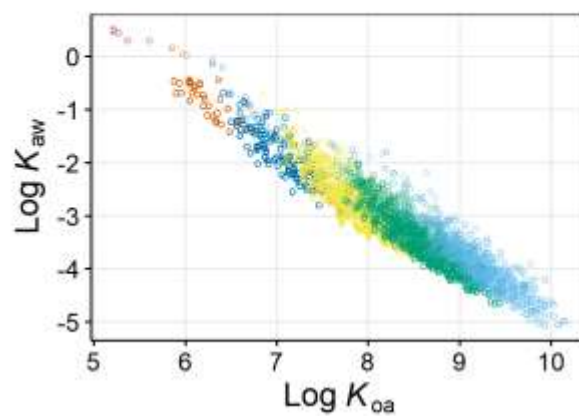
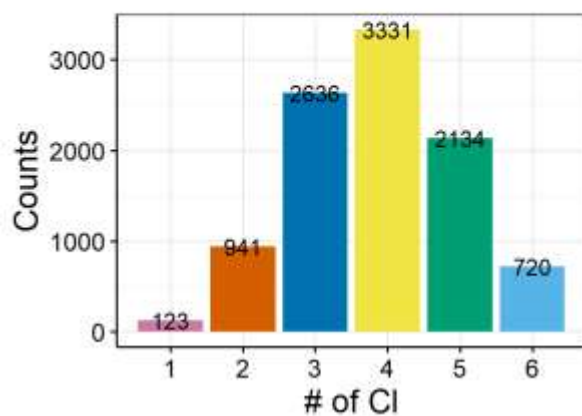
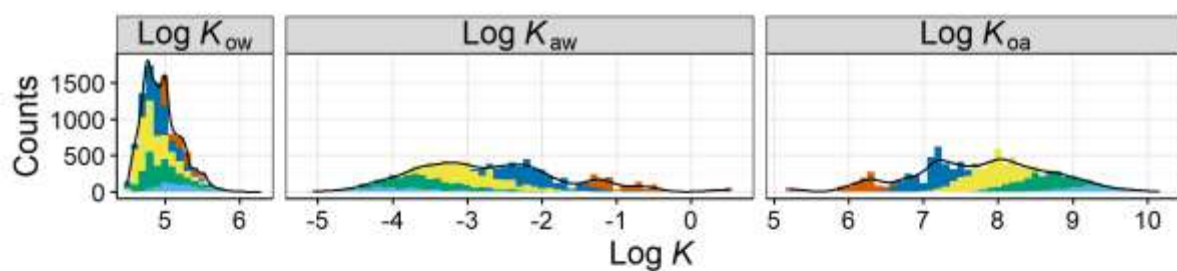
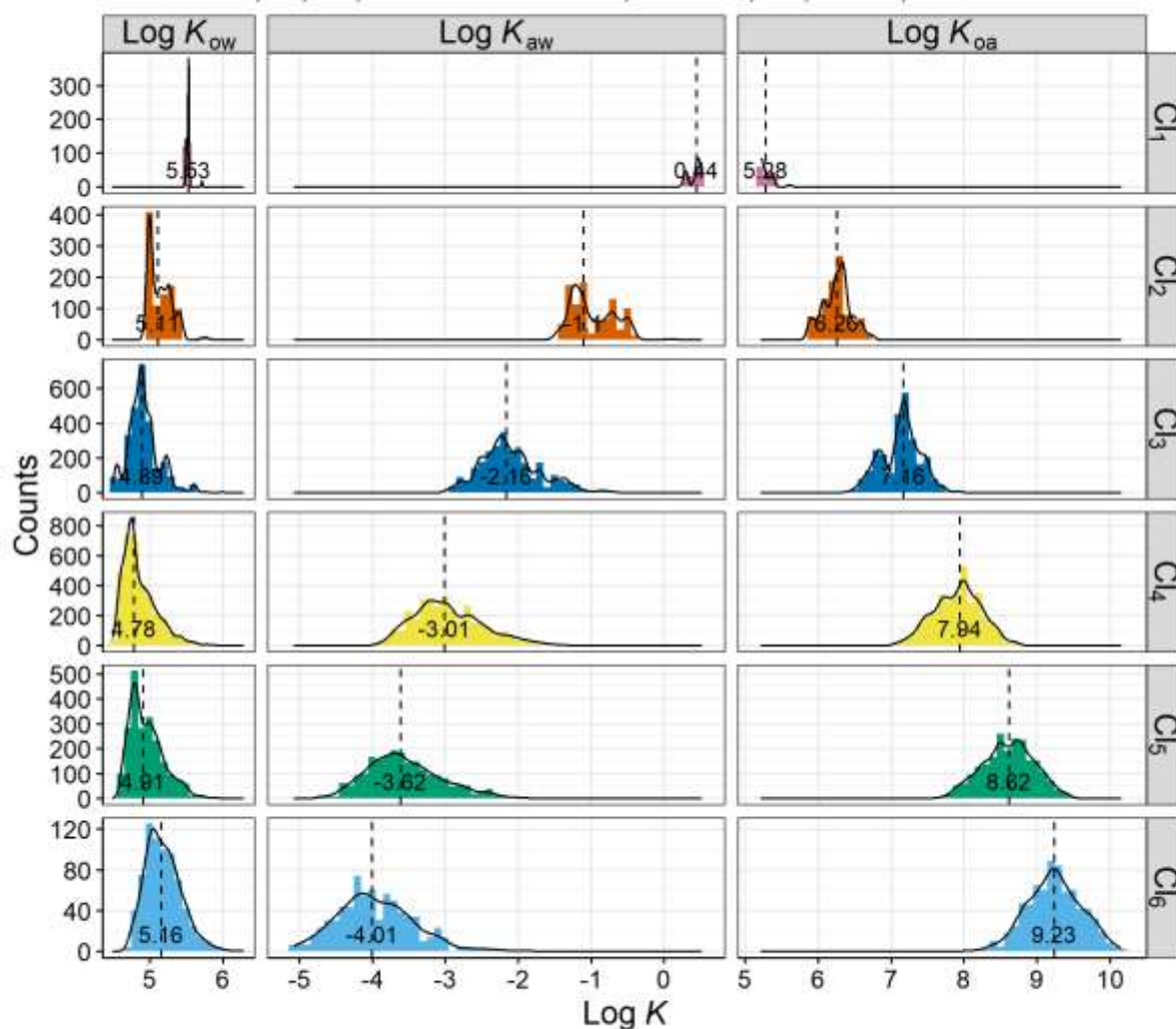
C₁₀, 40 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



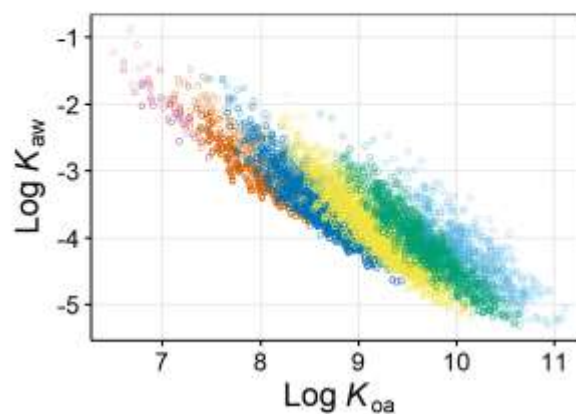
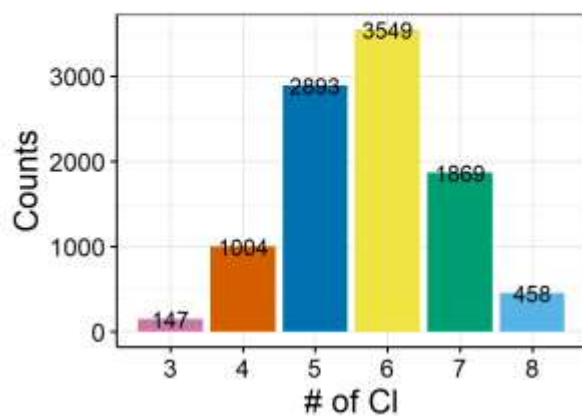
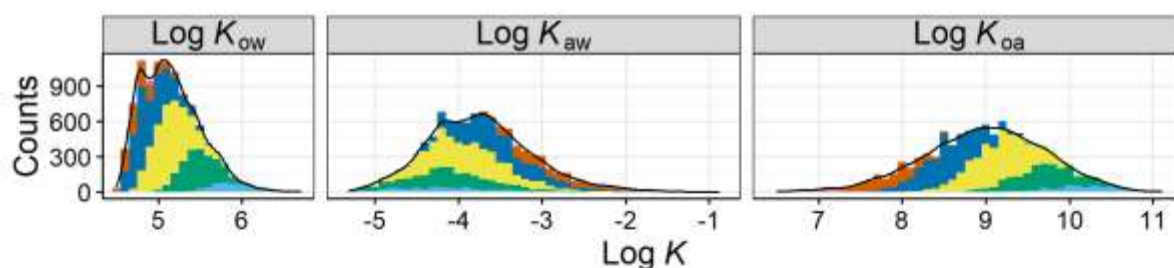
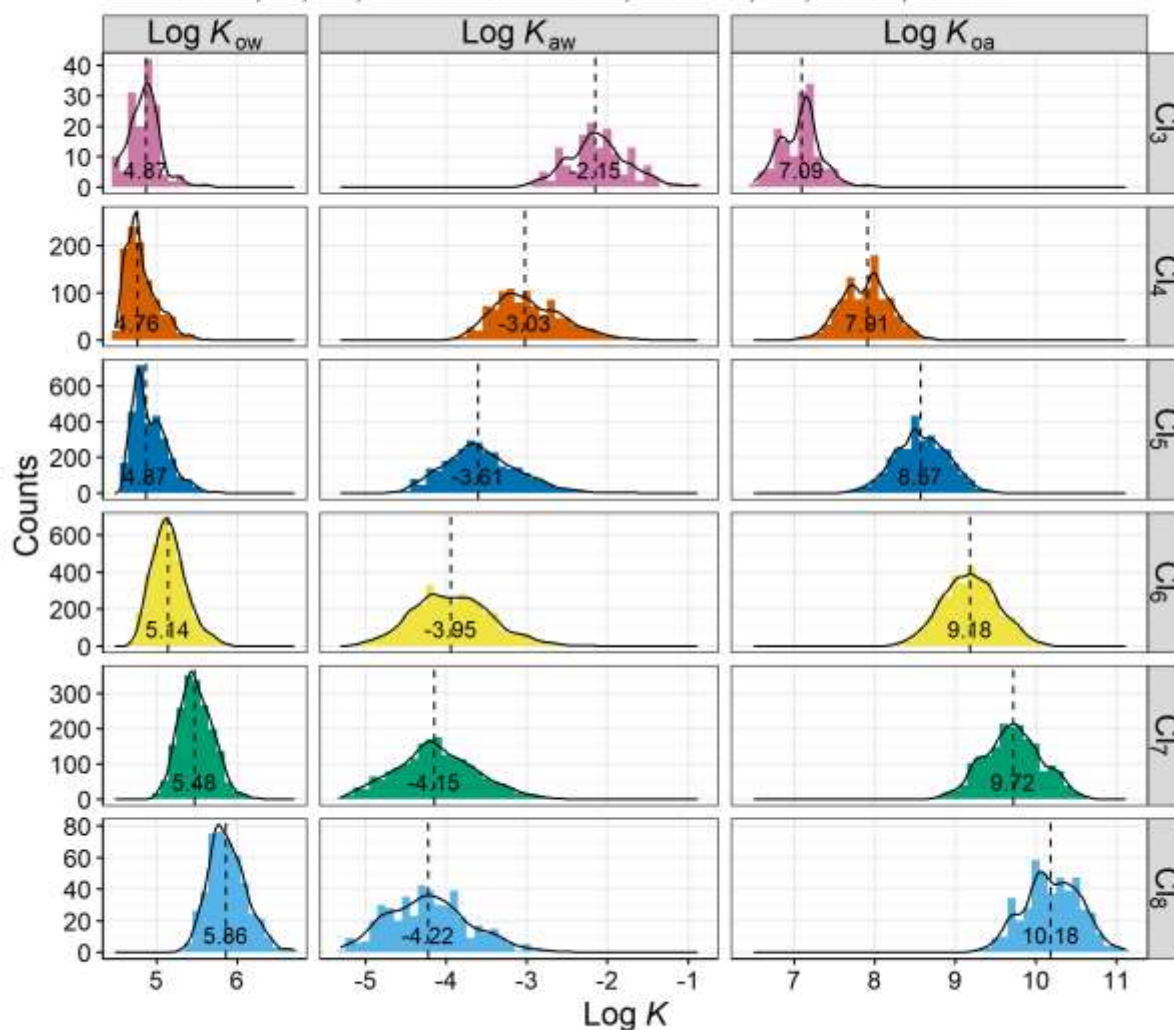
C₁₀, 50 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



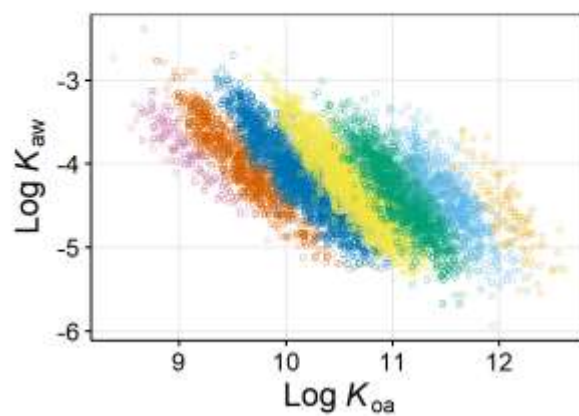
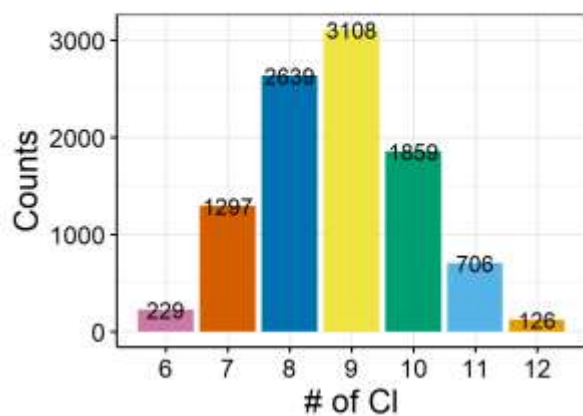
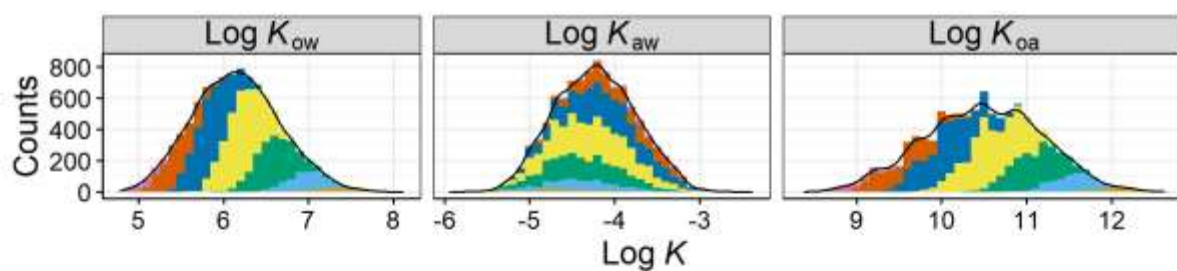
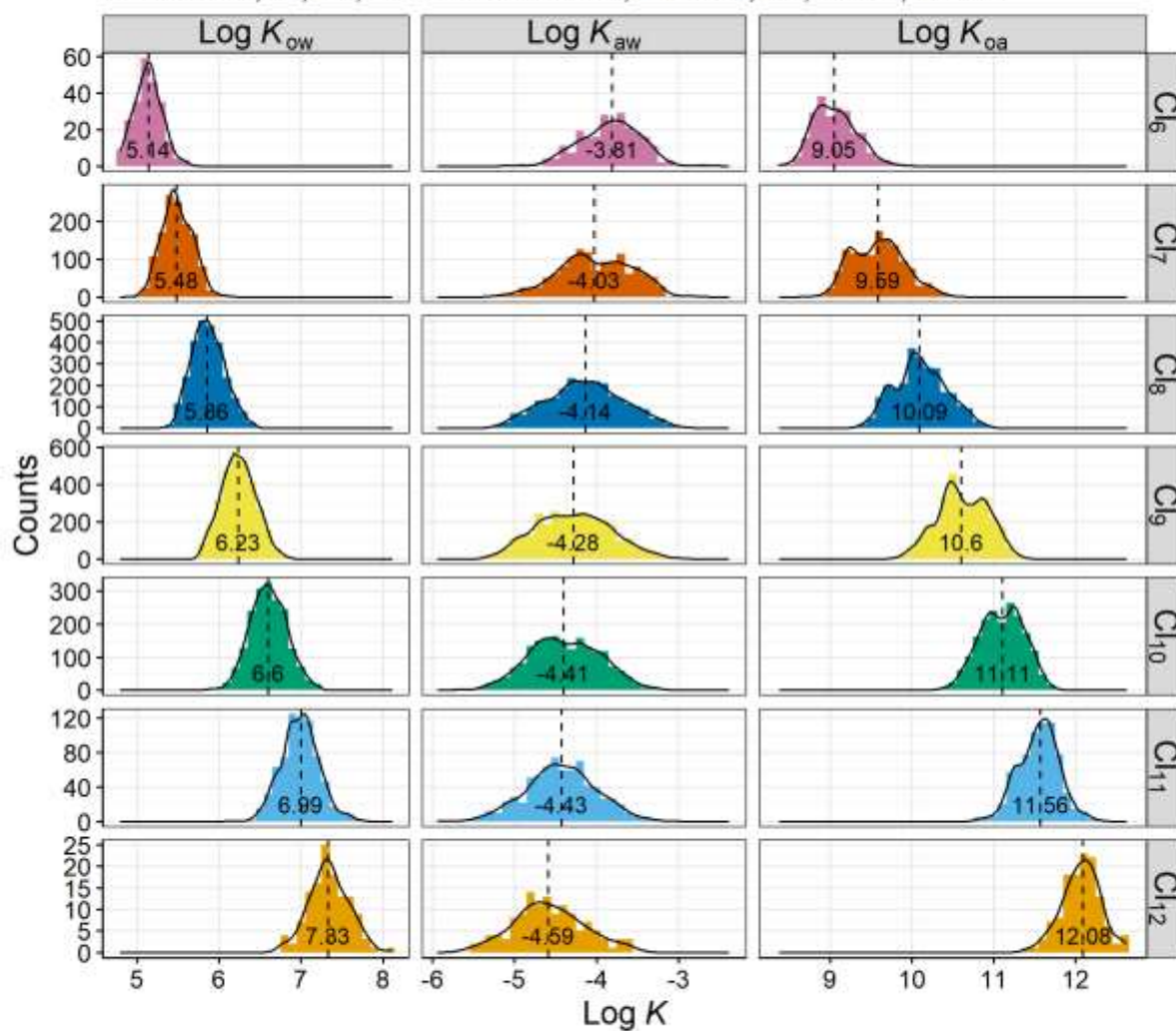
C₁₀, 60 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



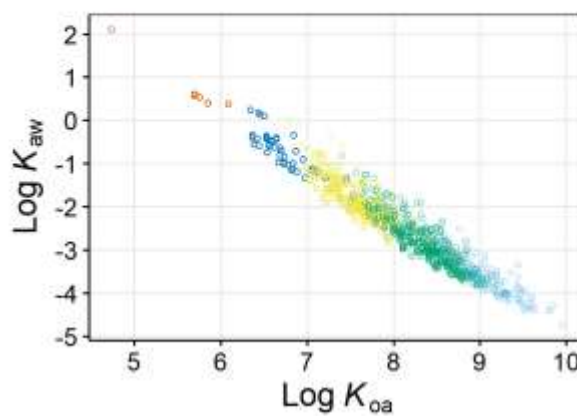
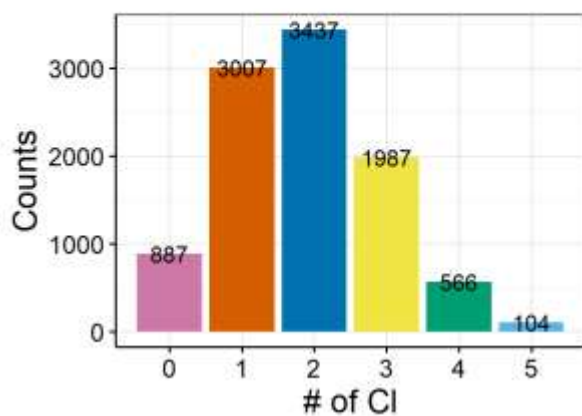
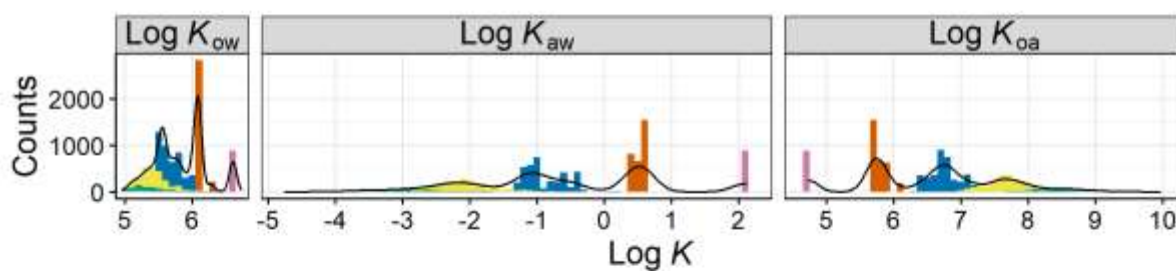
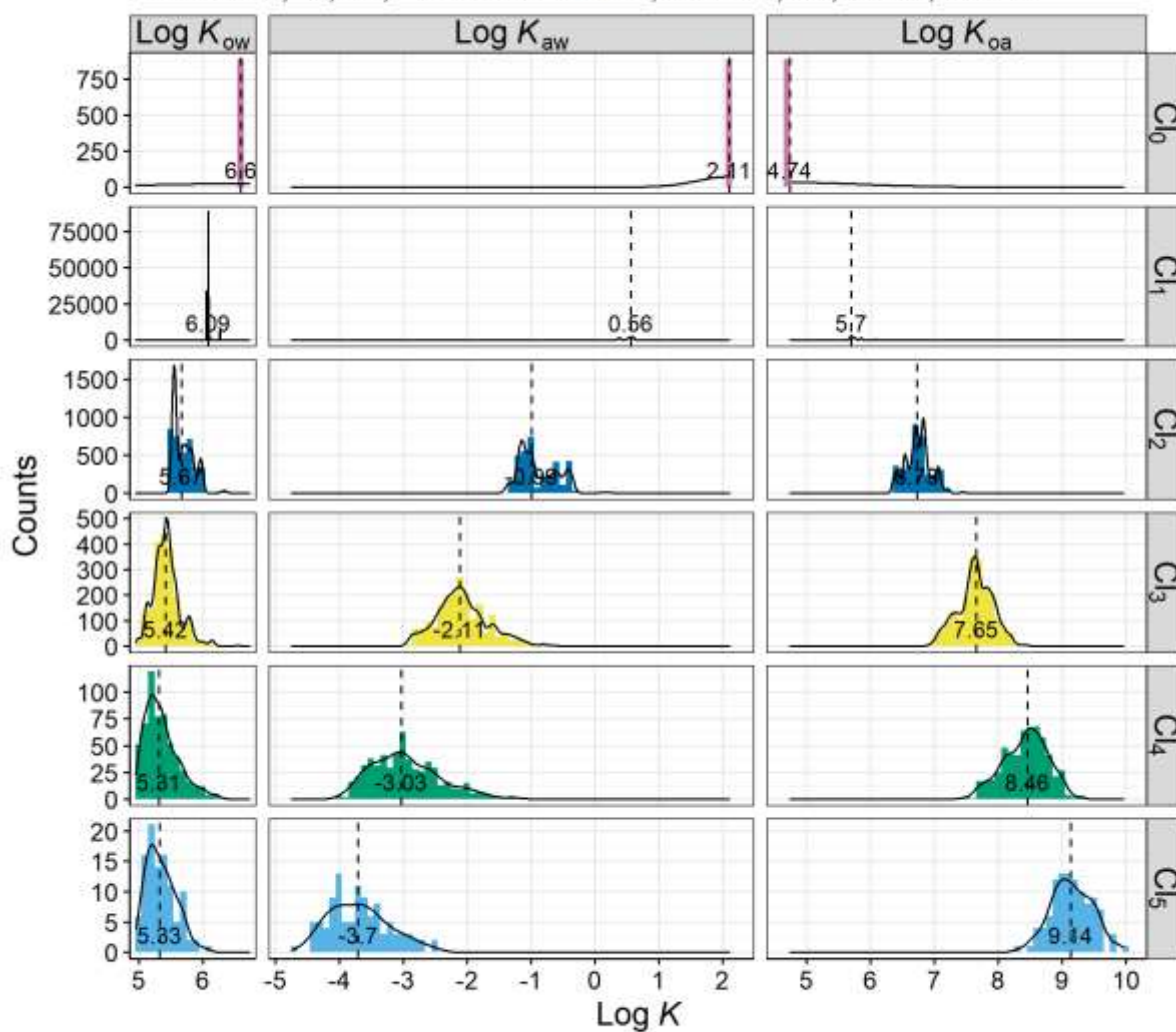
C₁₀, 70 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



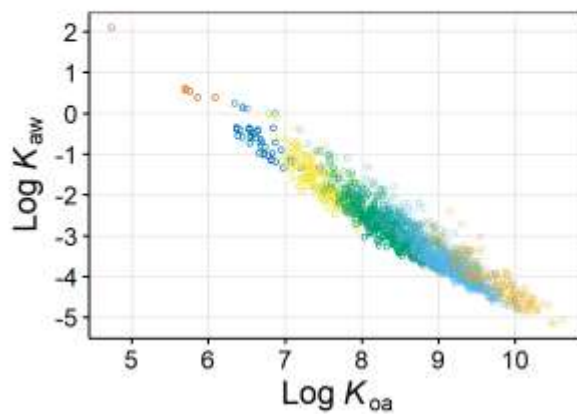
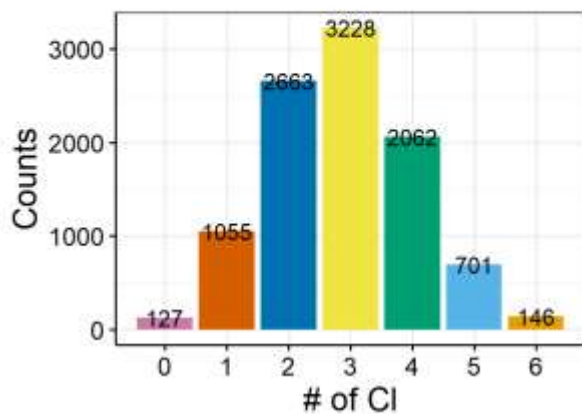
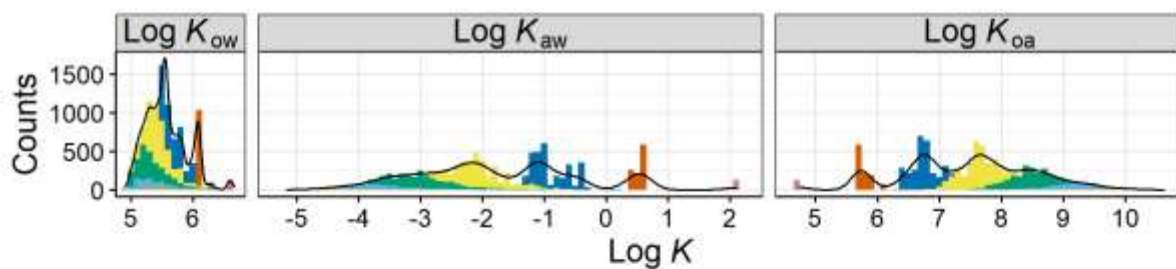
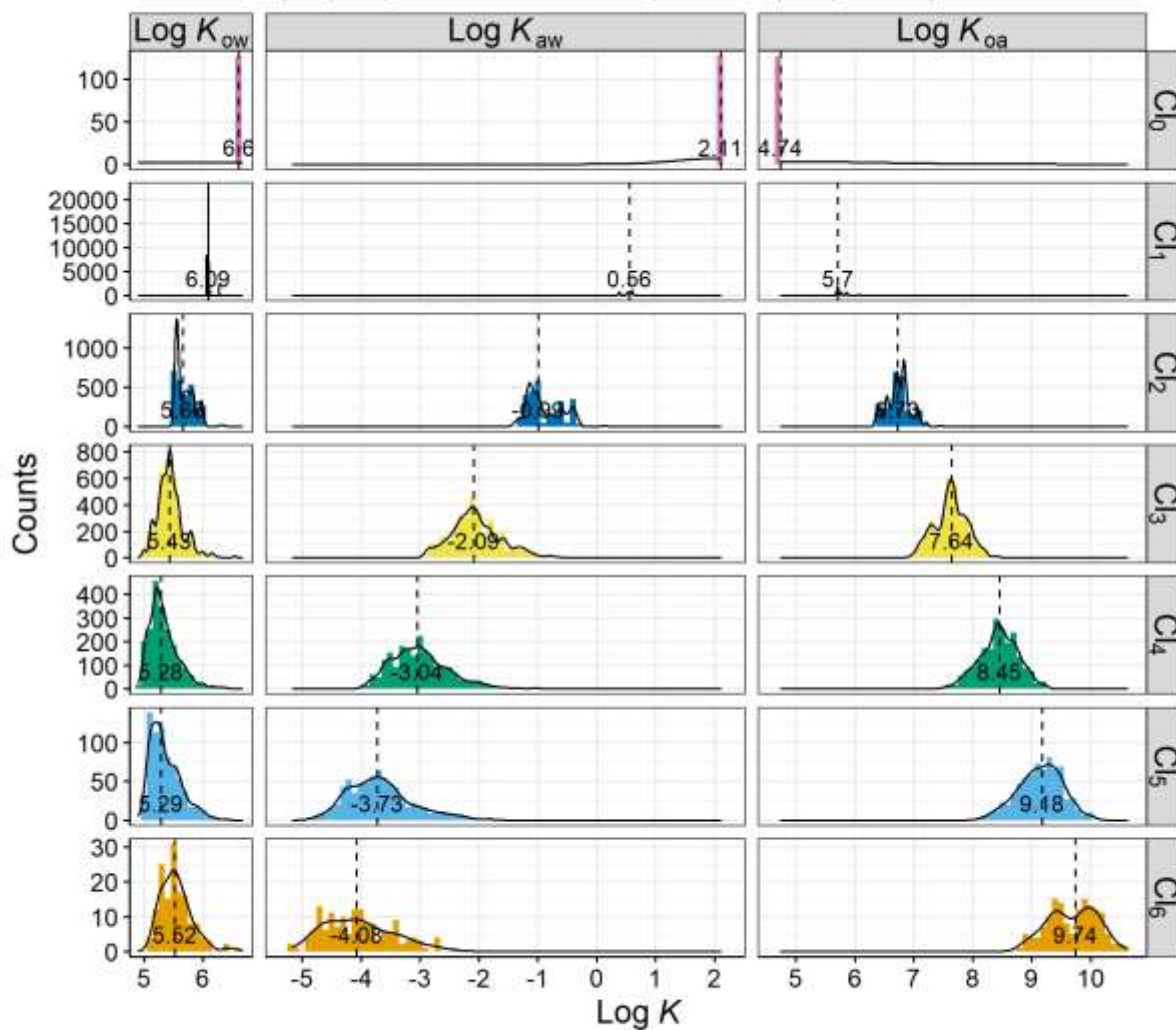
C₁₁, 30 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



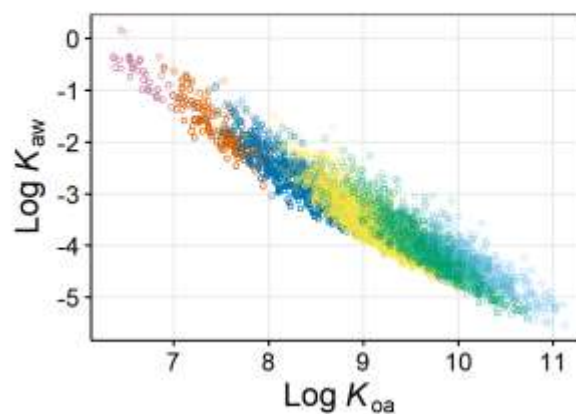
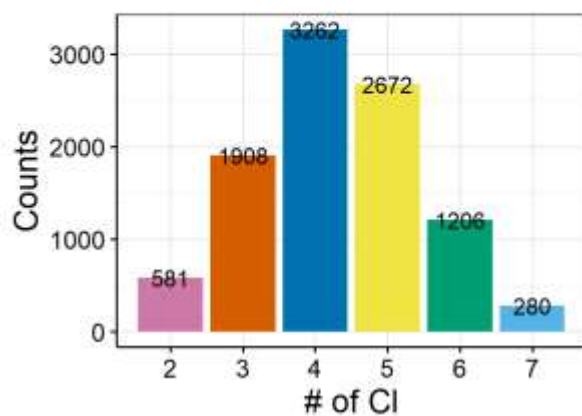
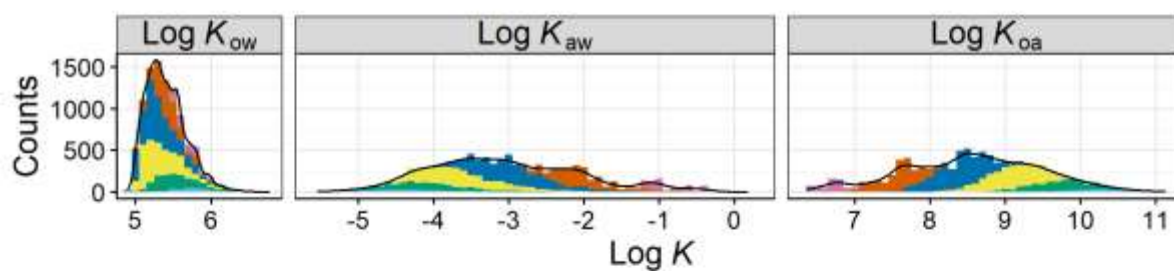
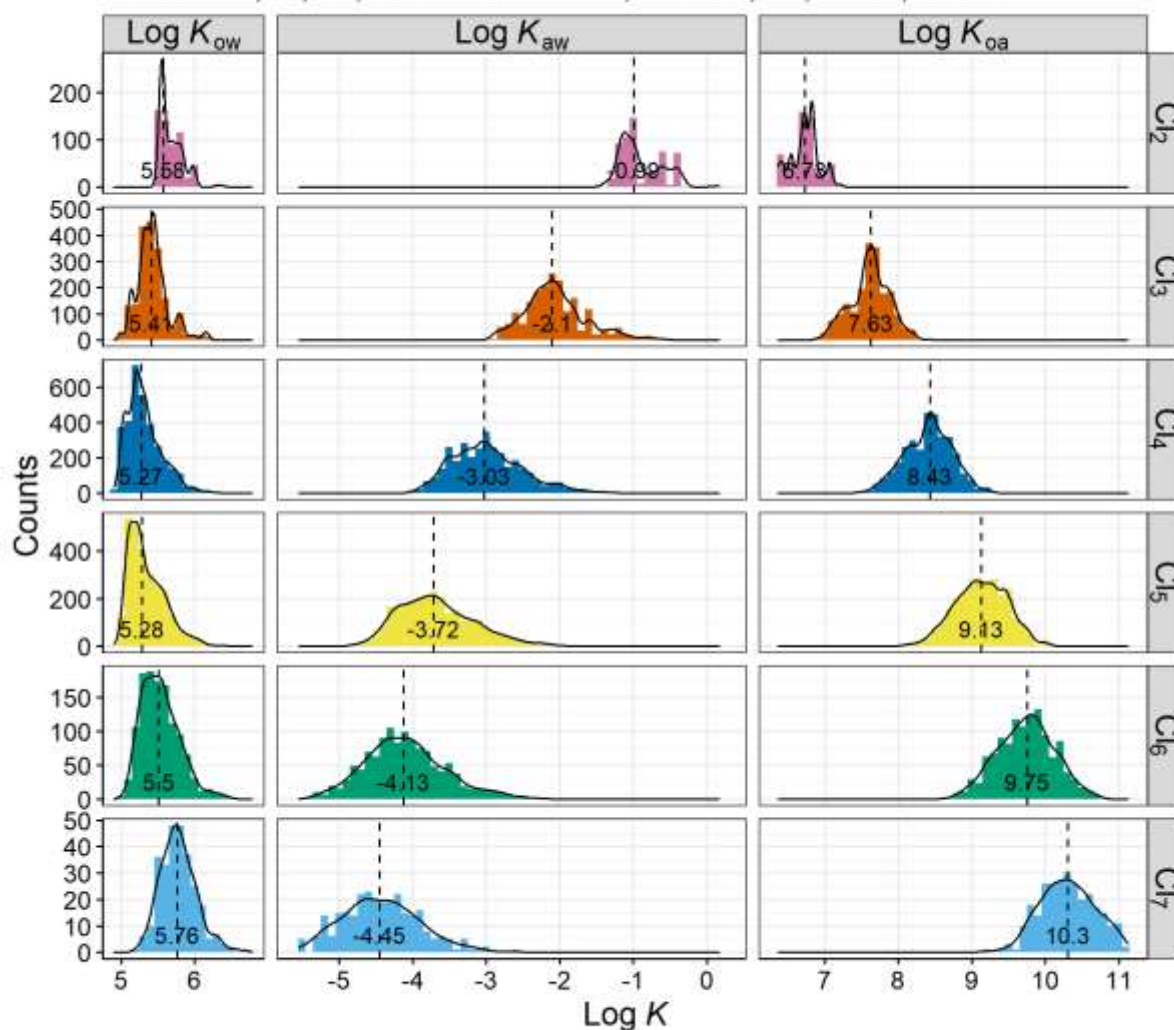
C_{11} , 40 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



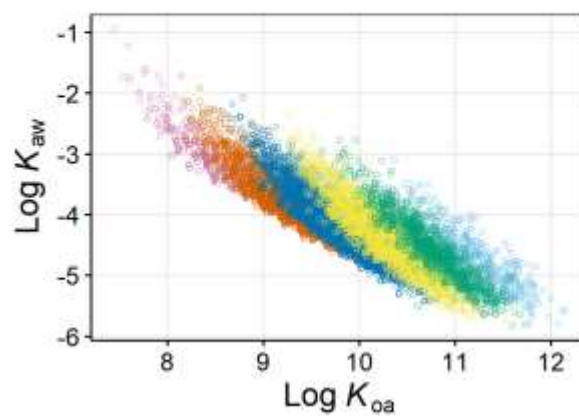
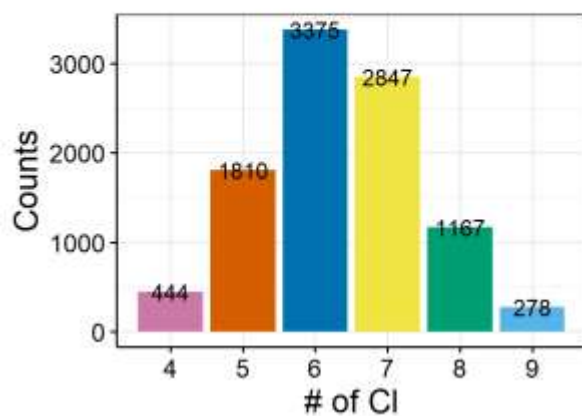
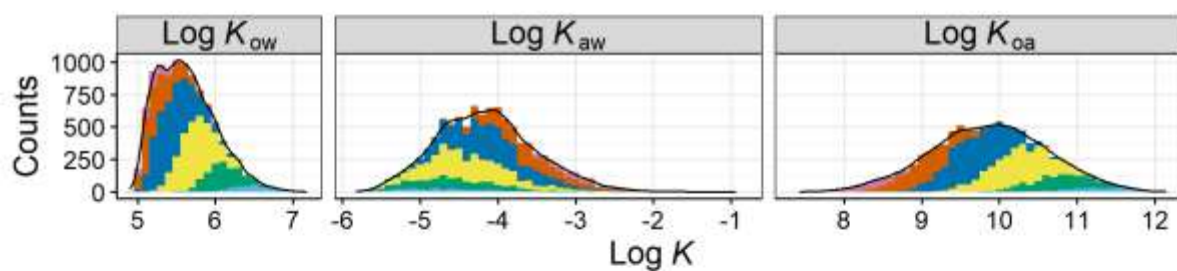
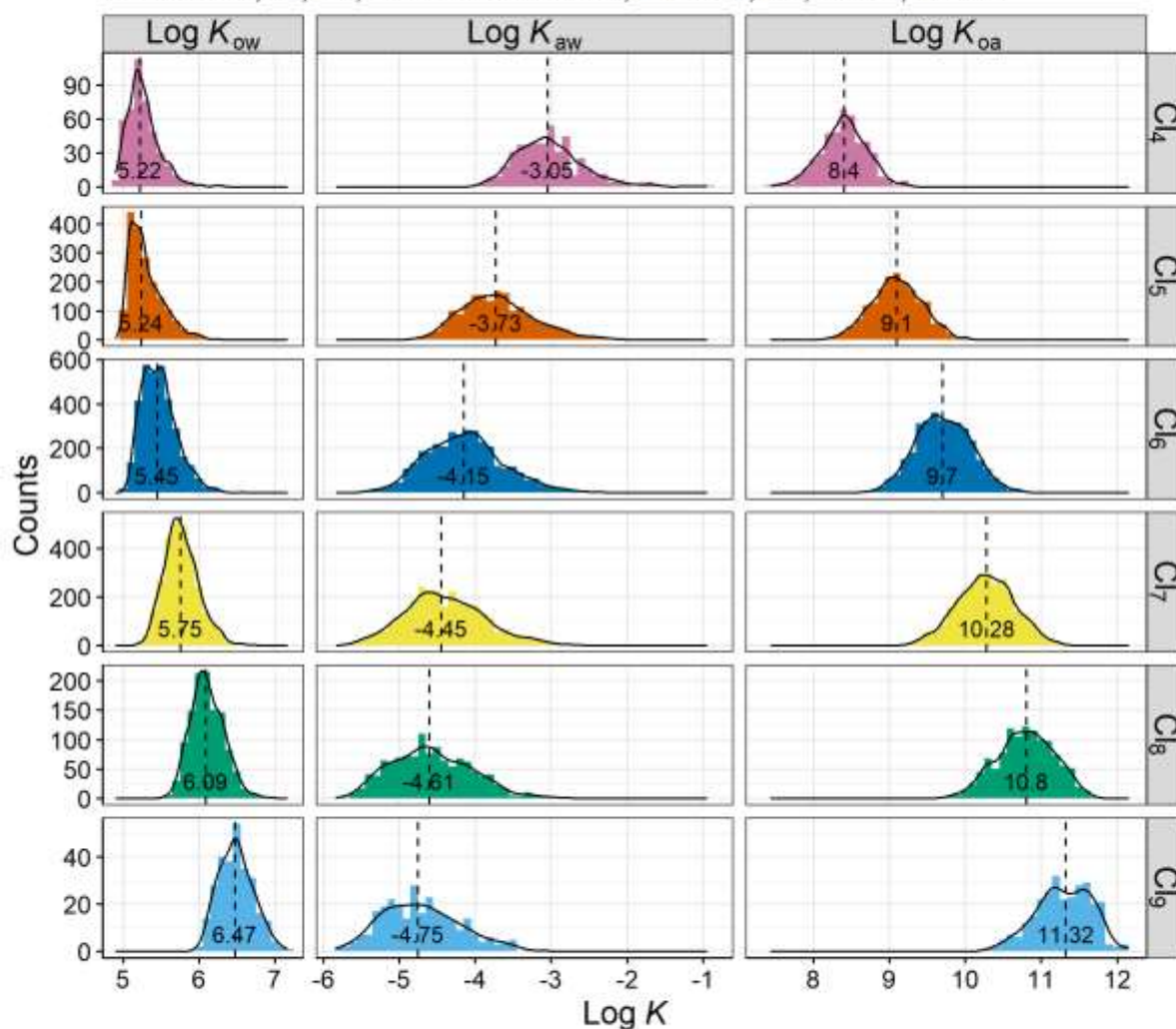
C₁₁, 50 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



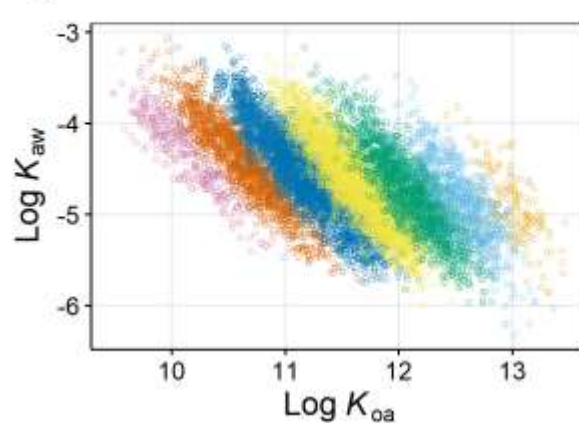
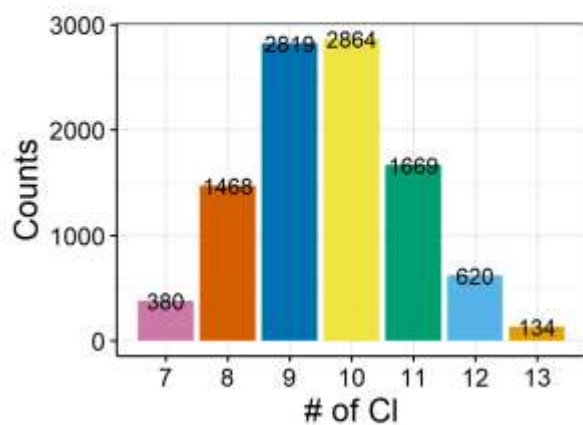
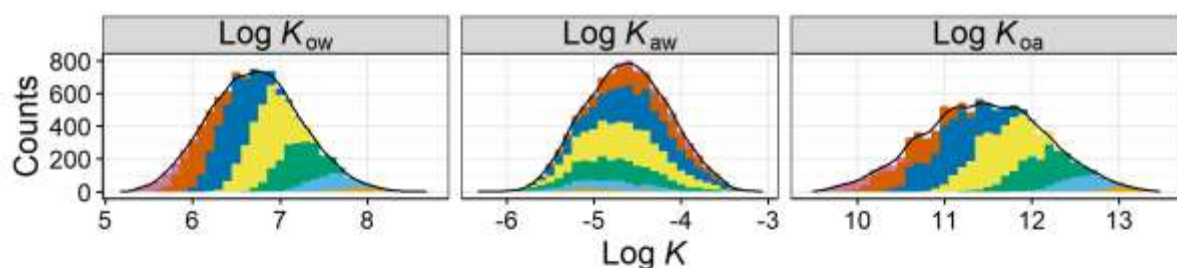
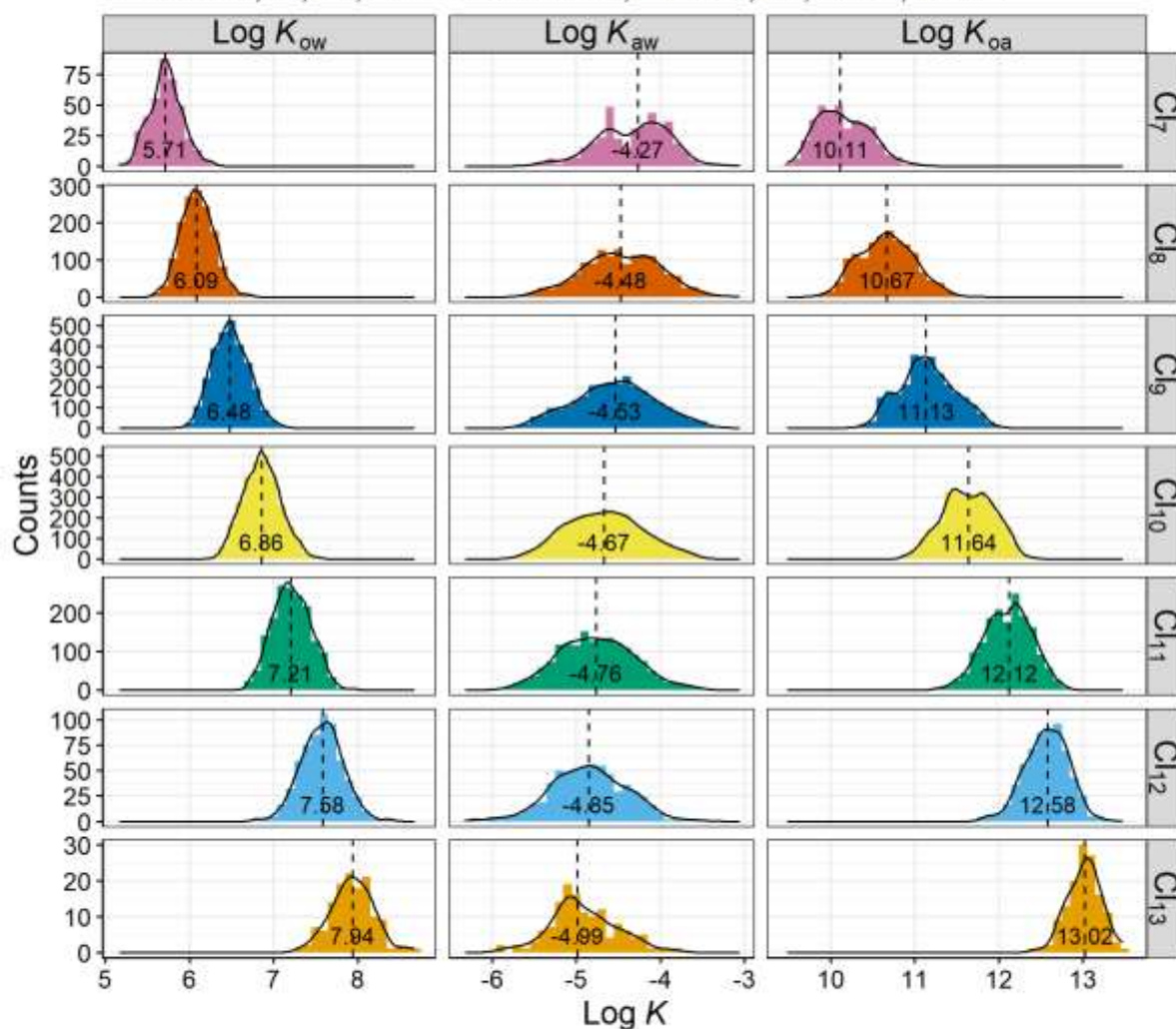
C₁₁, 60 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



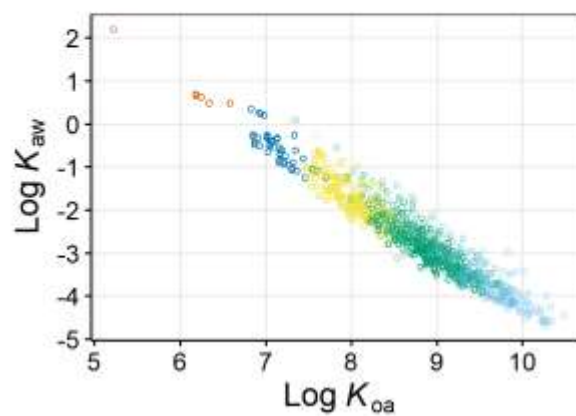
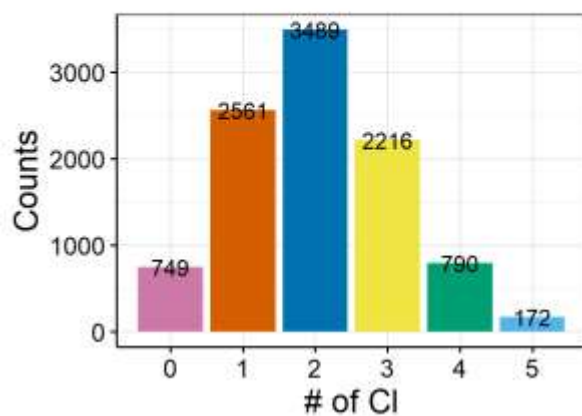
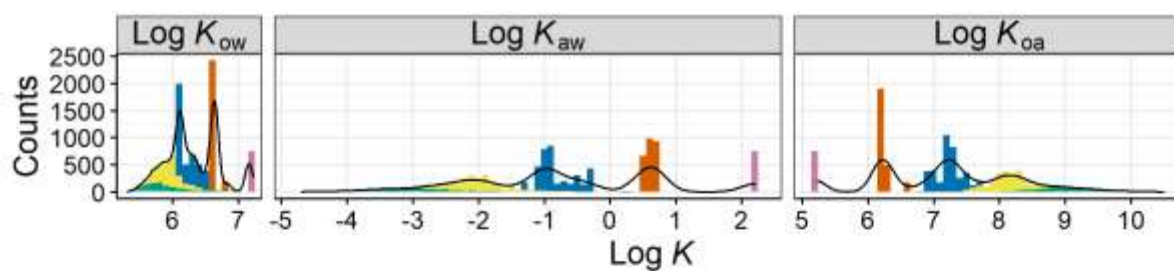
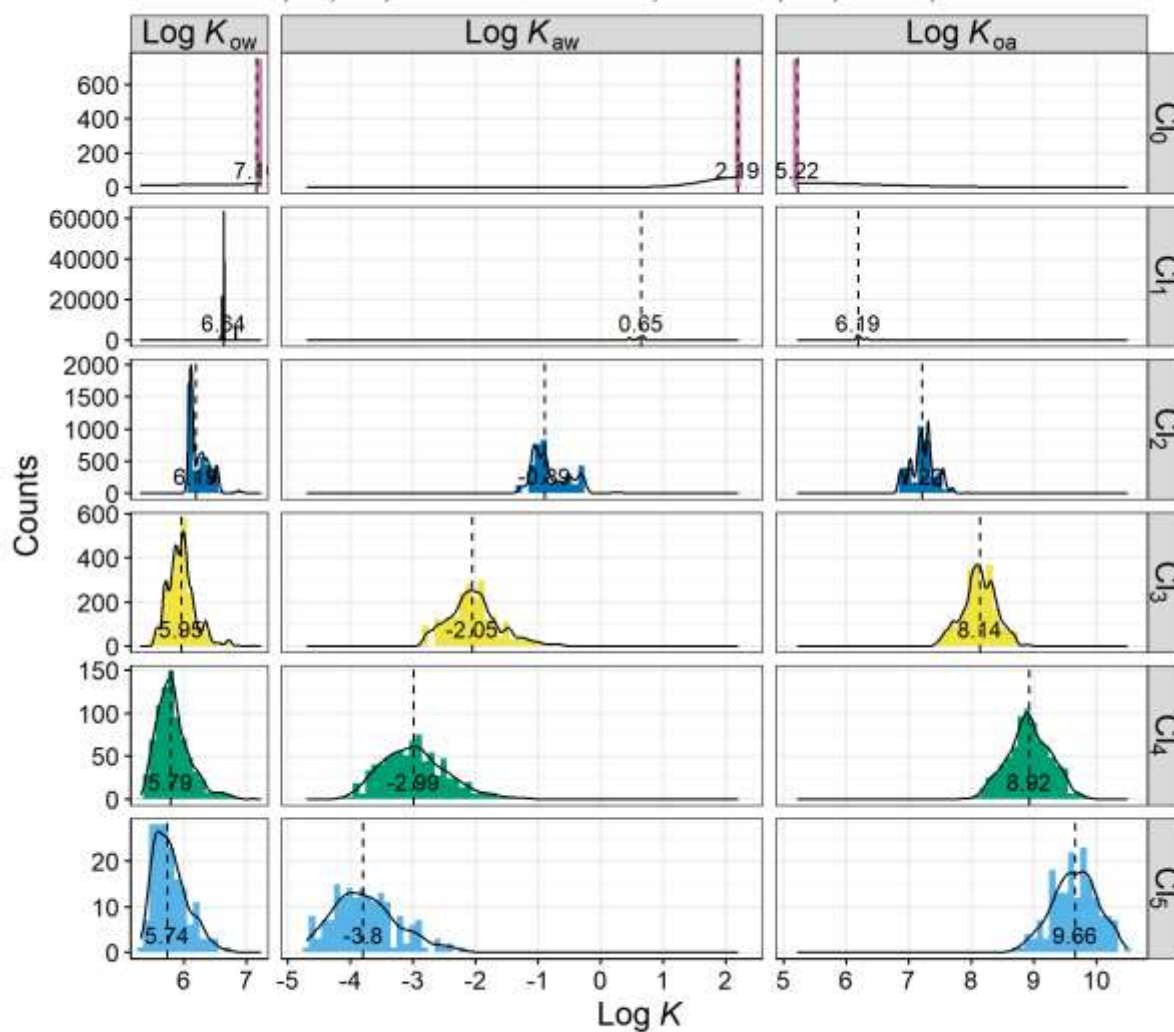
C₁₁, 70 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



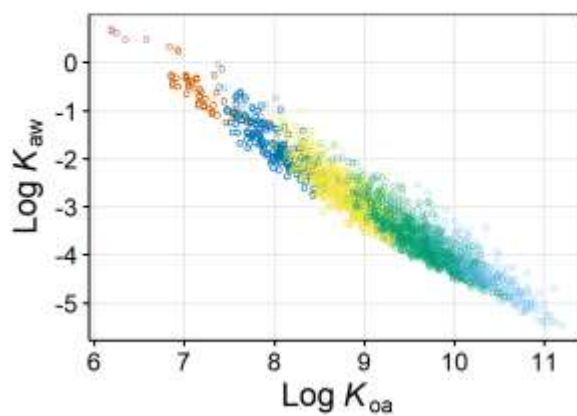
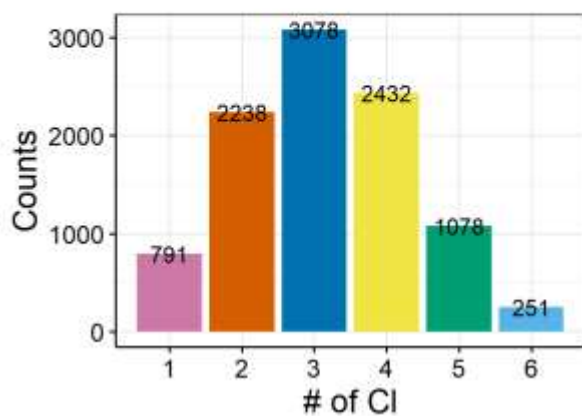
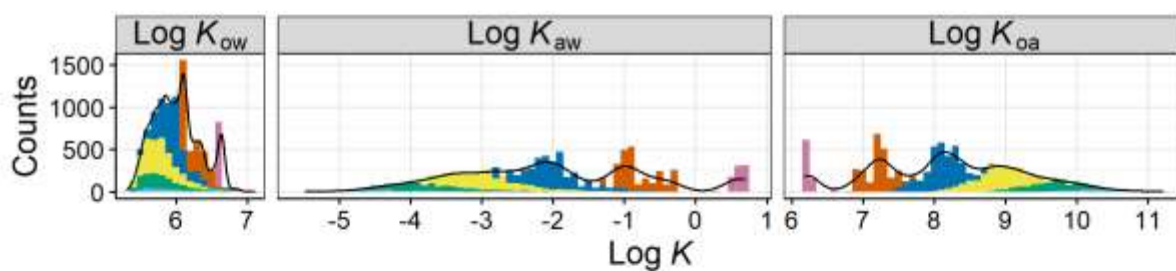
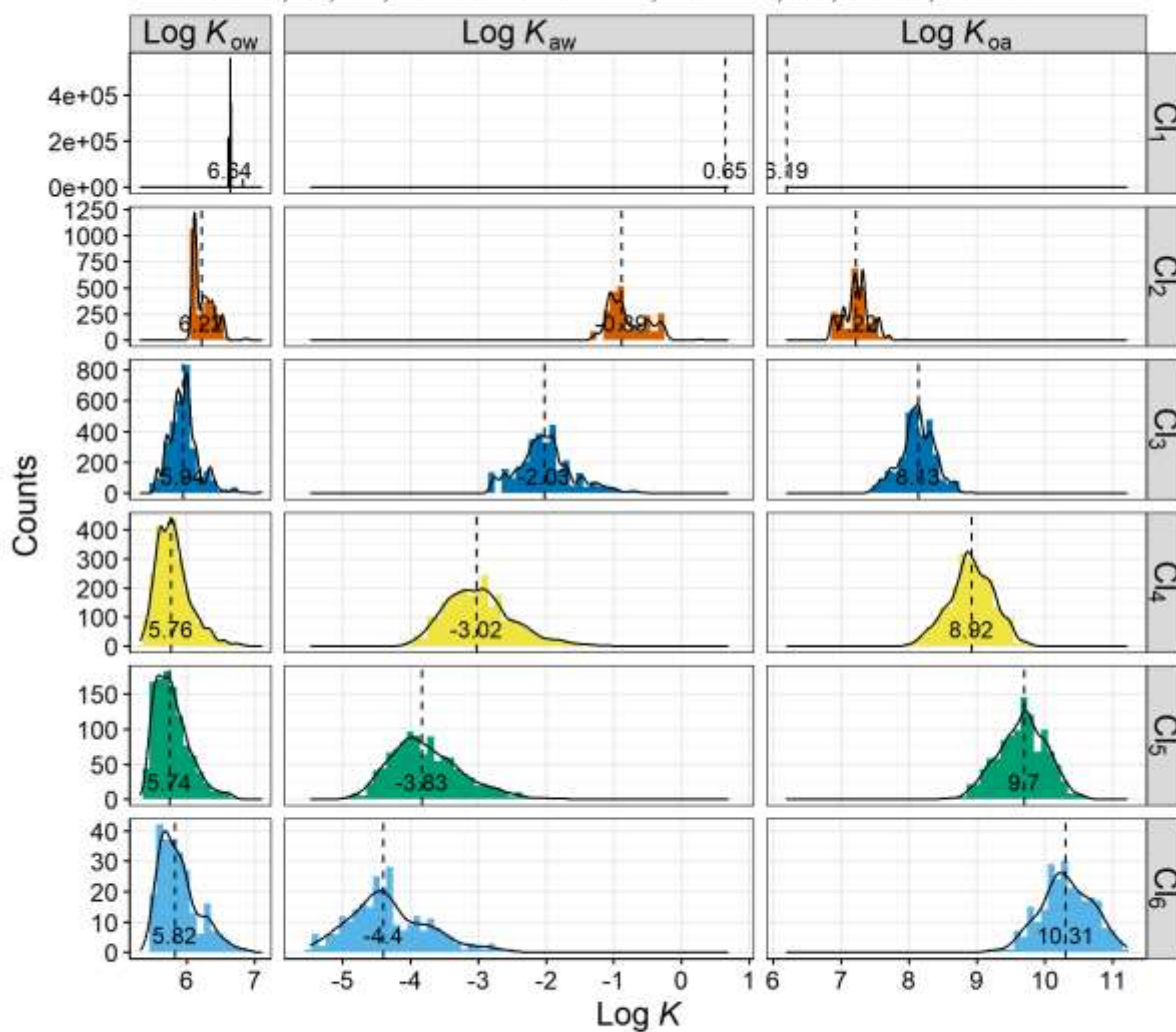
C₁₂, 30 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



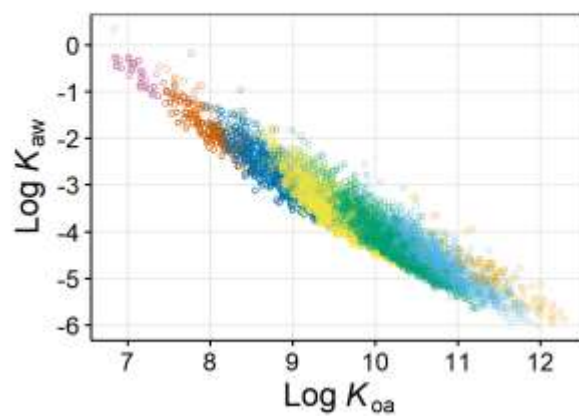
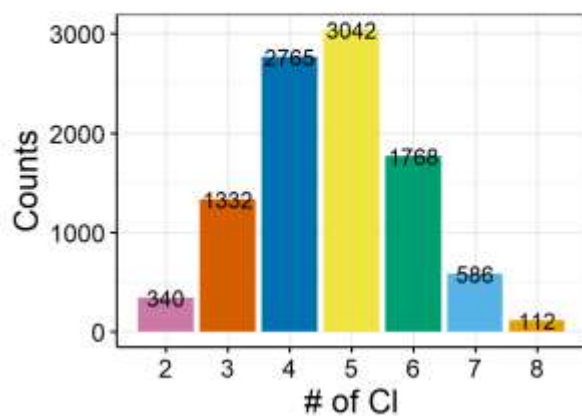
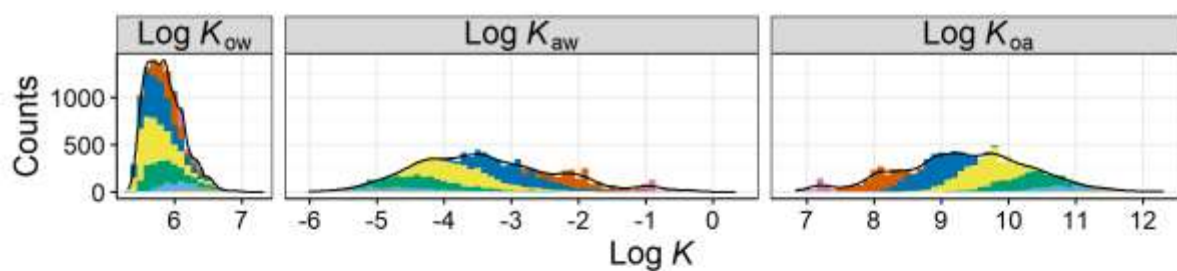
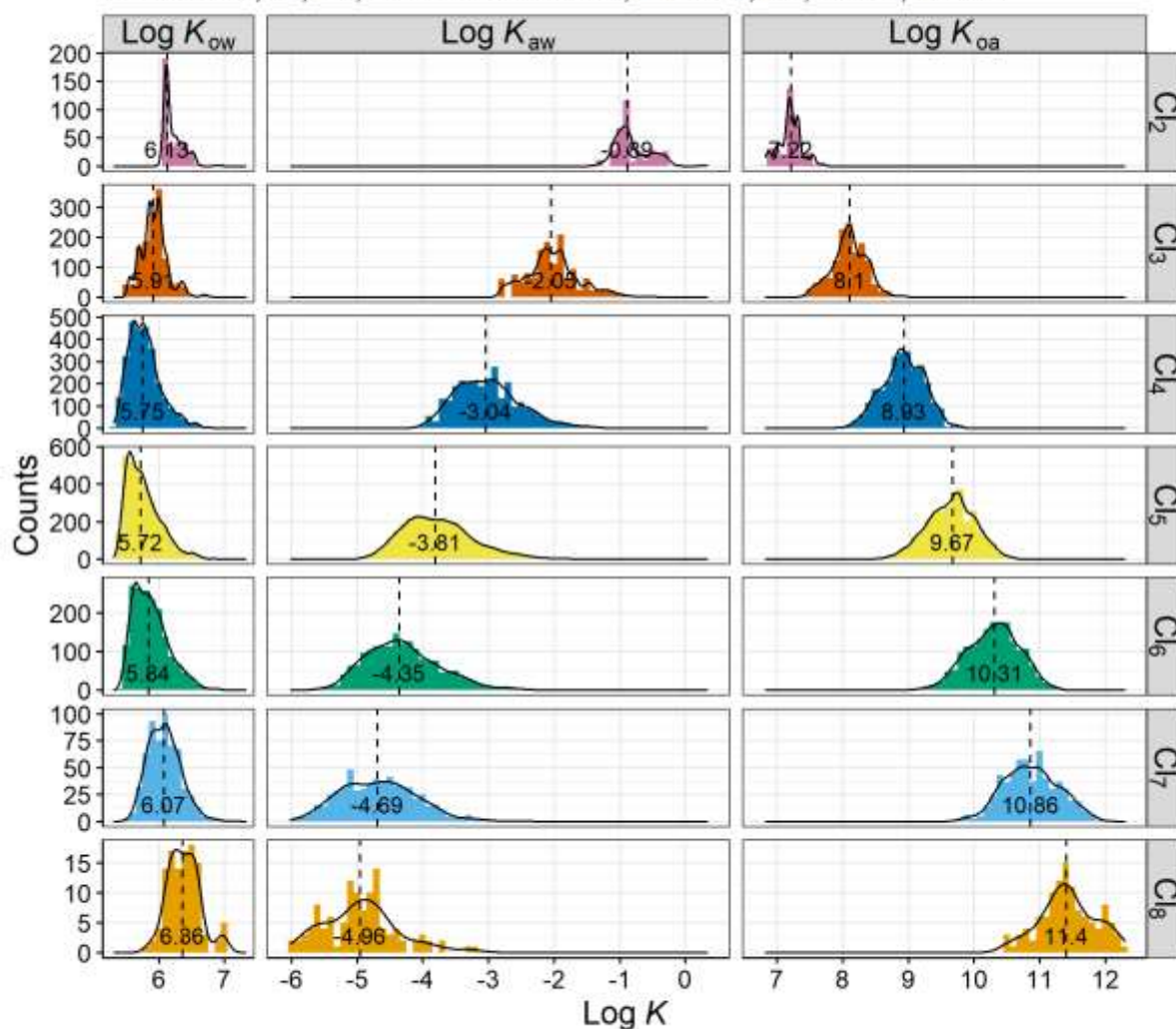
C₁₂, 40 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



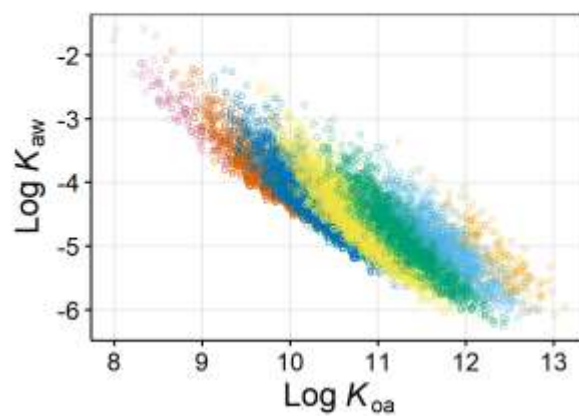
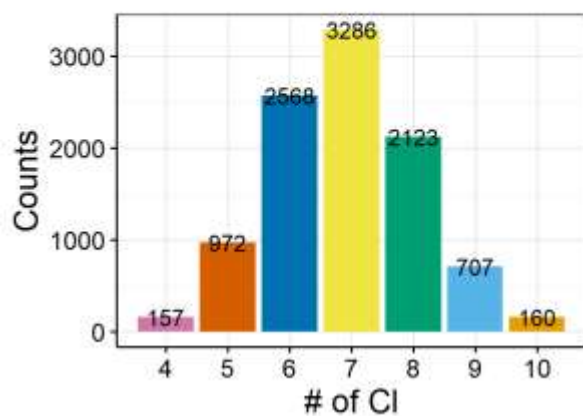
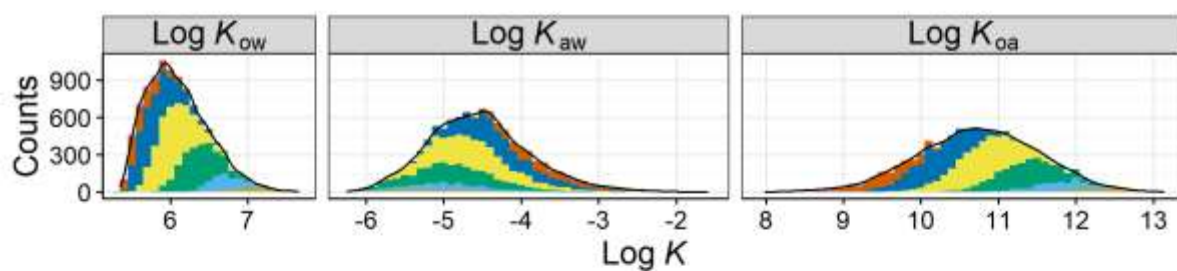
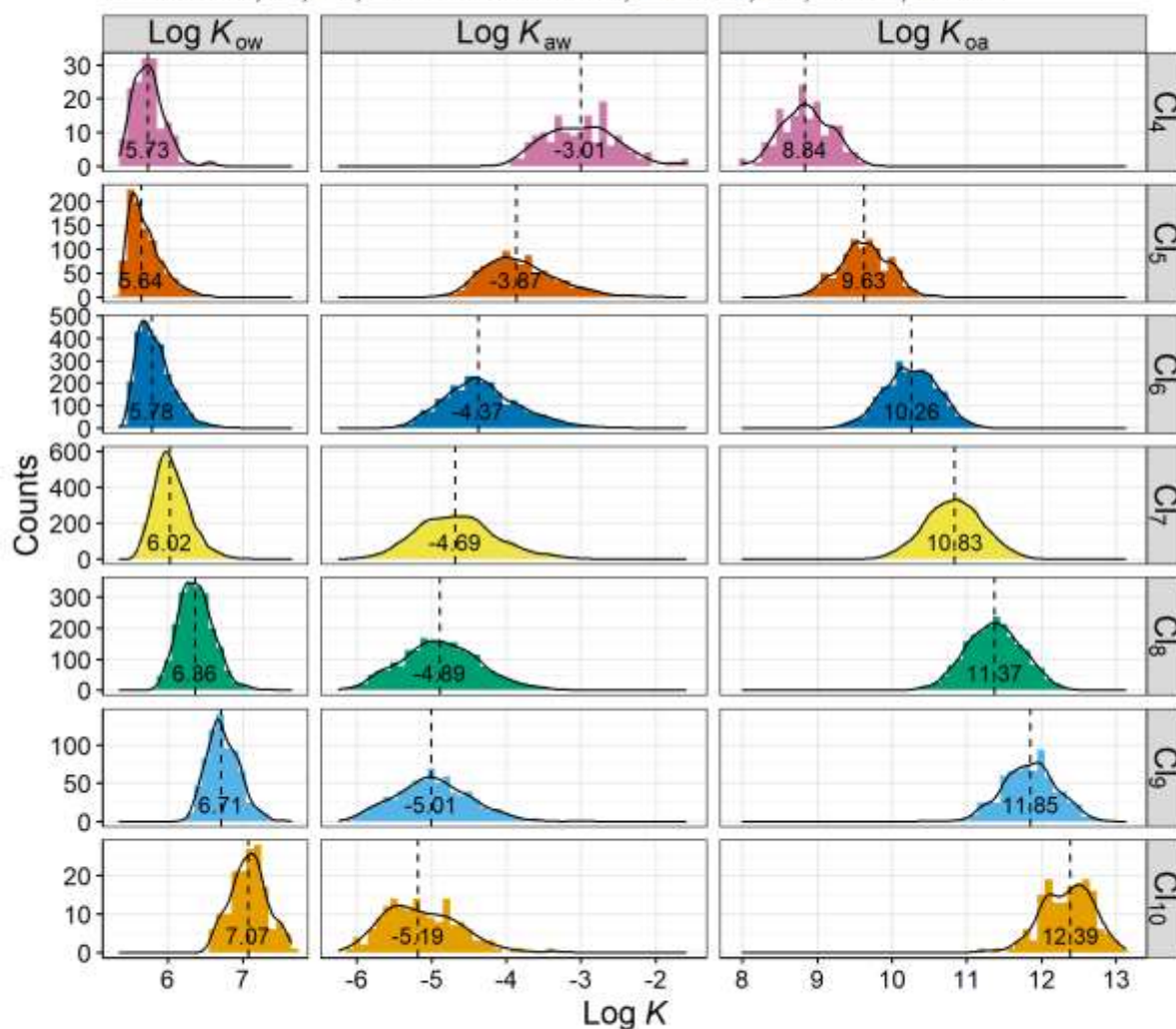
C₁₂, 50 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



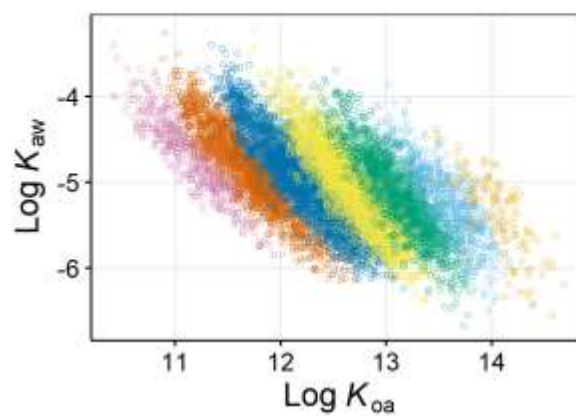
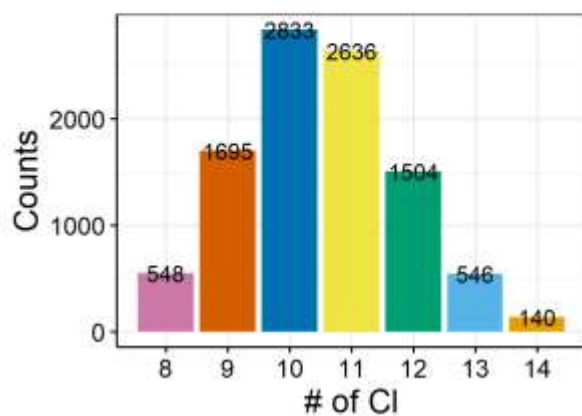
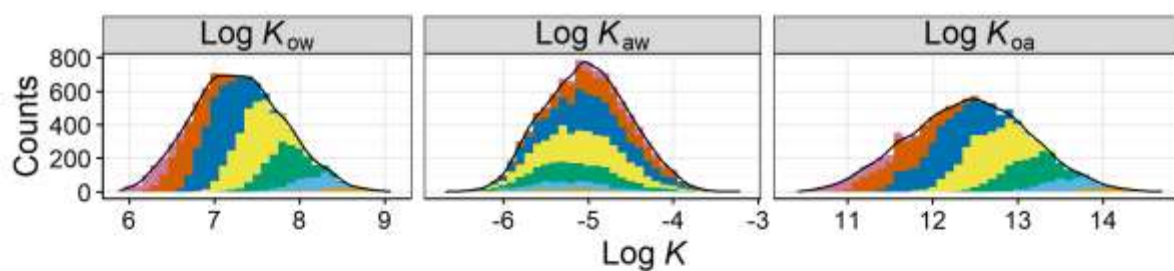
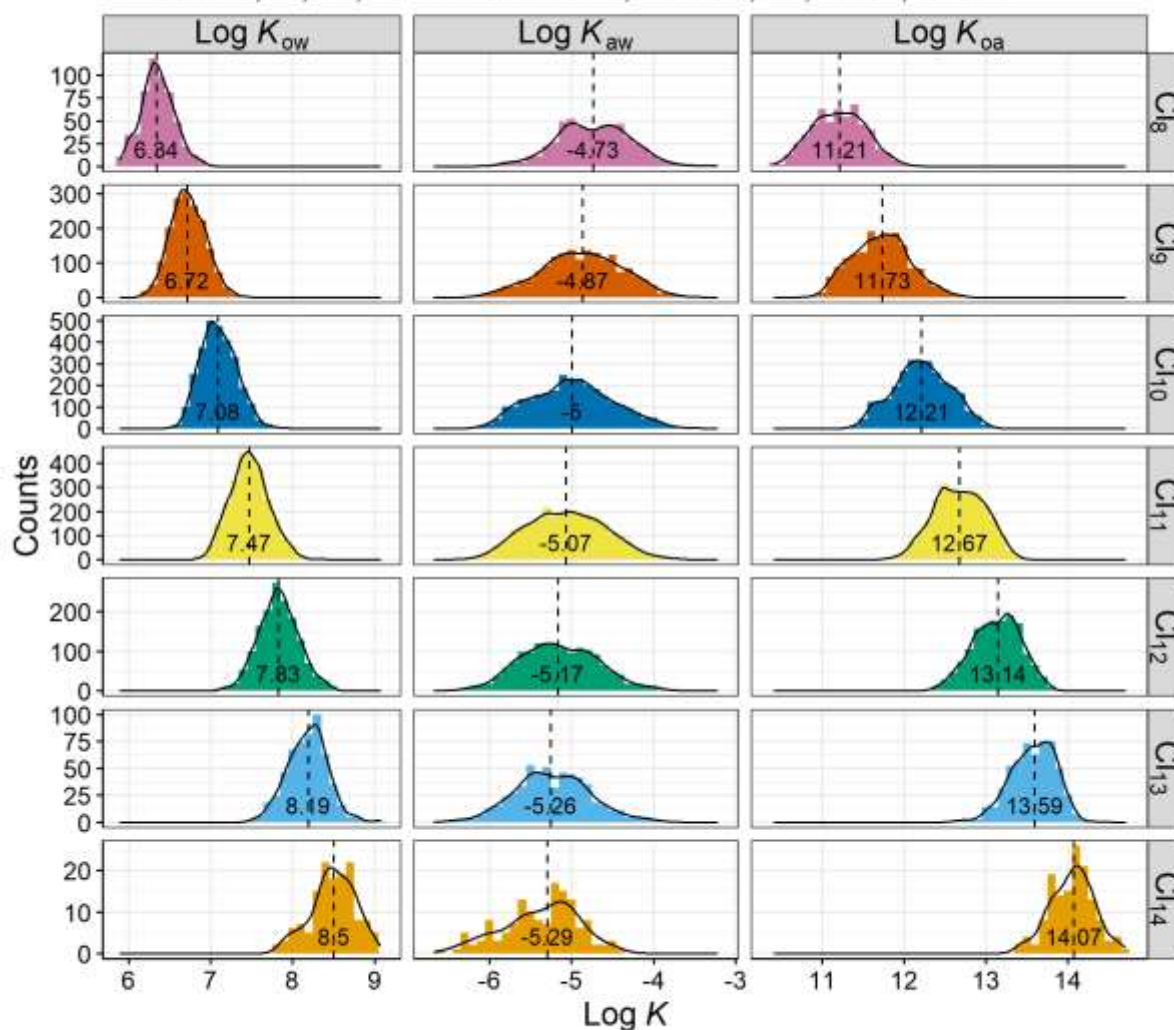
C₁₂, 60 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



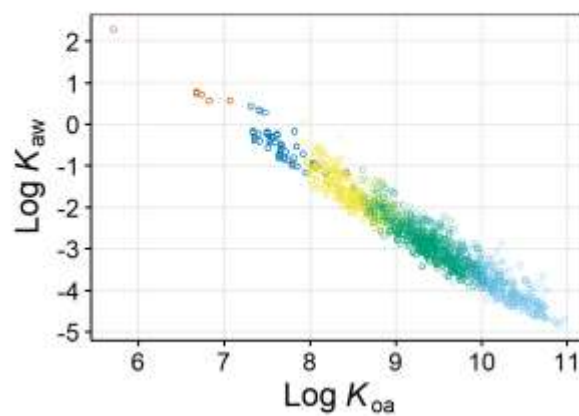
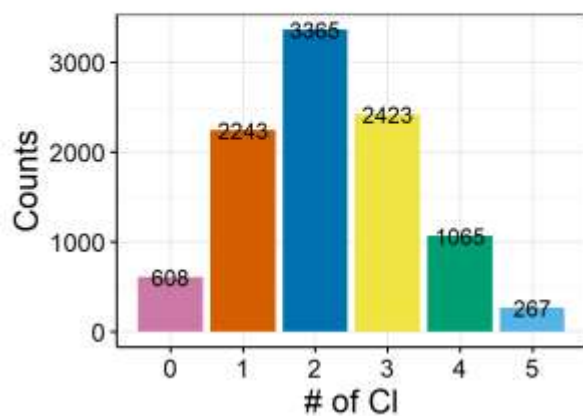
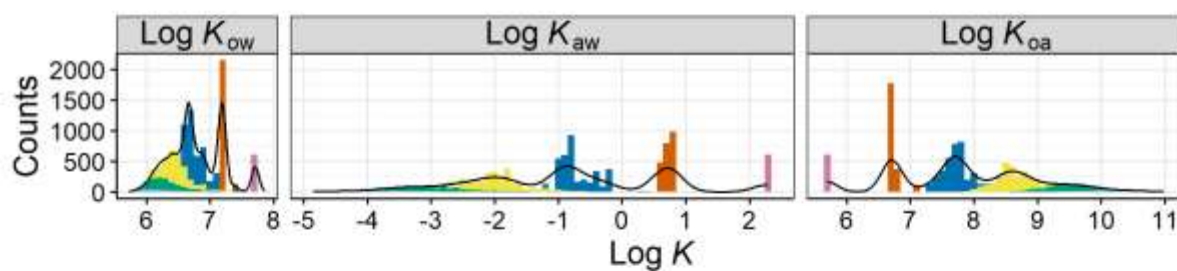
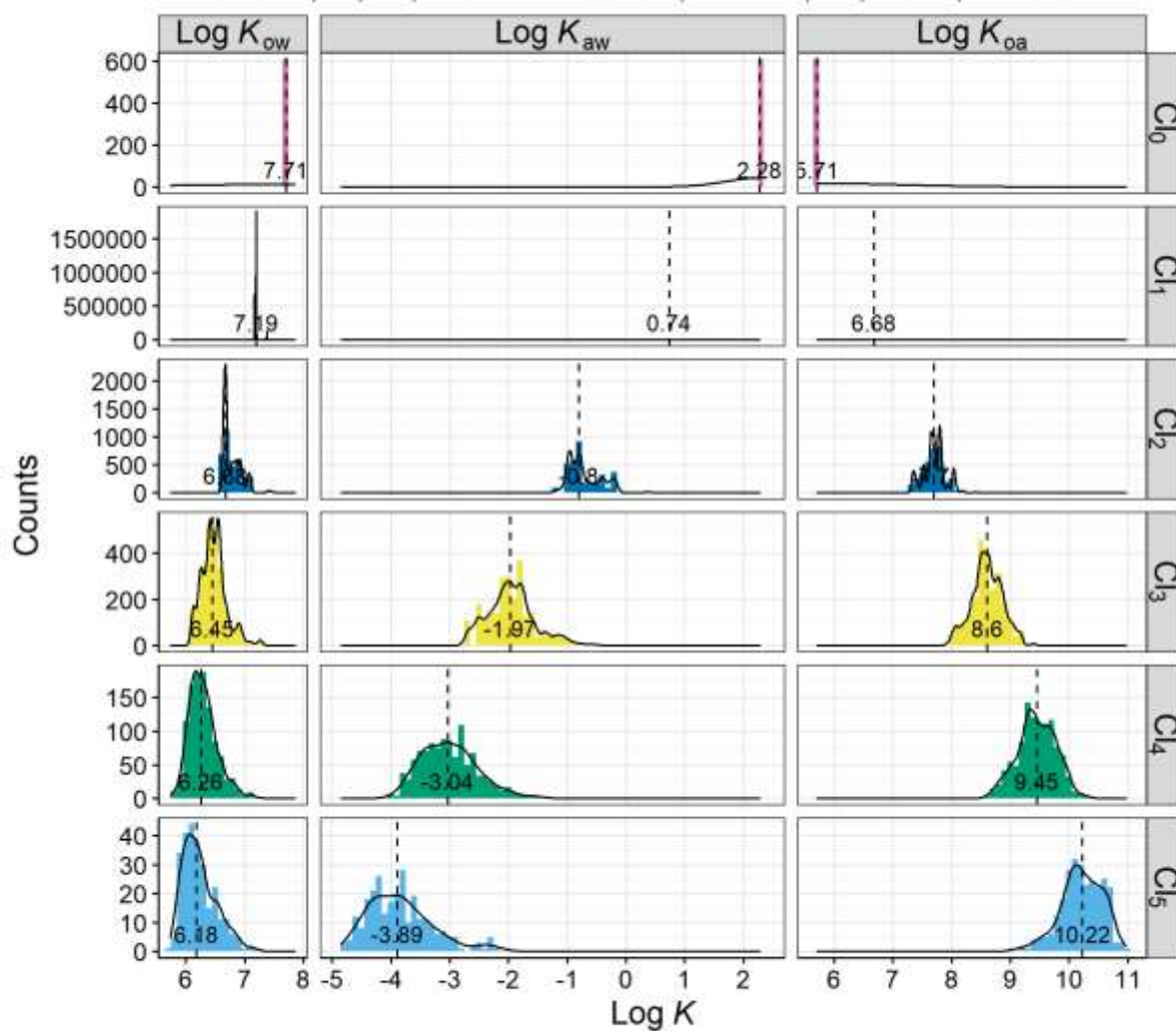
C₁₂, 70 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



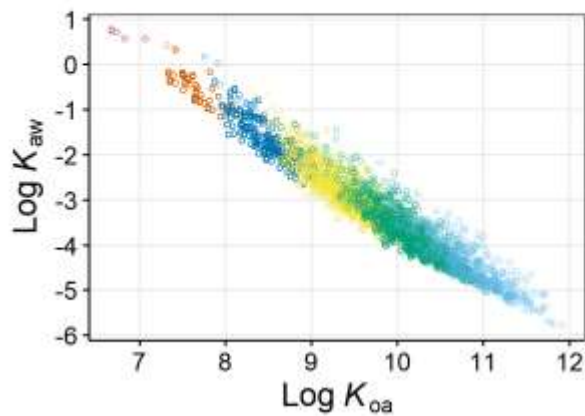
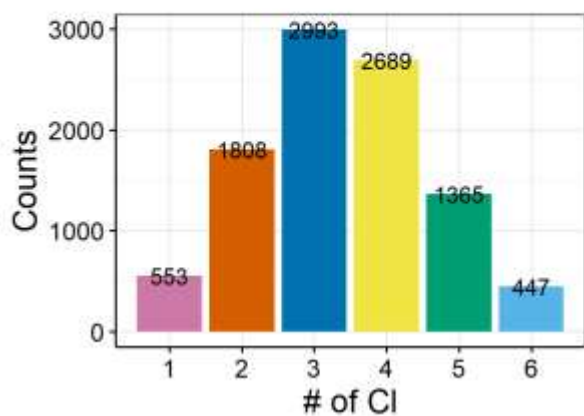
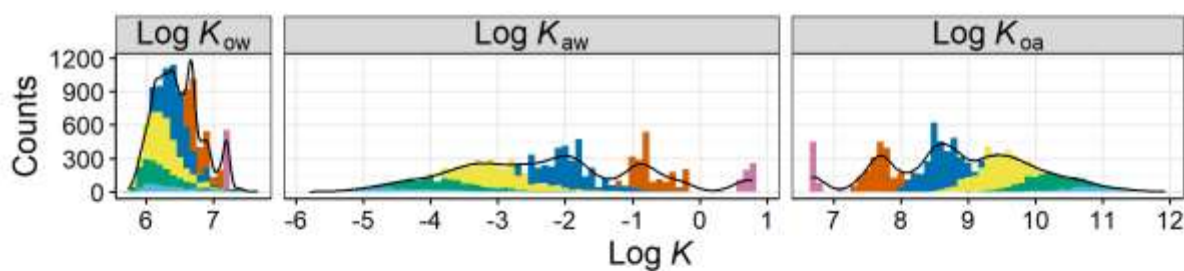
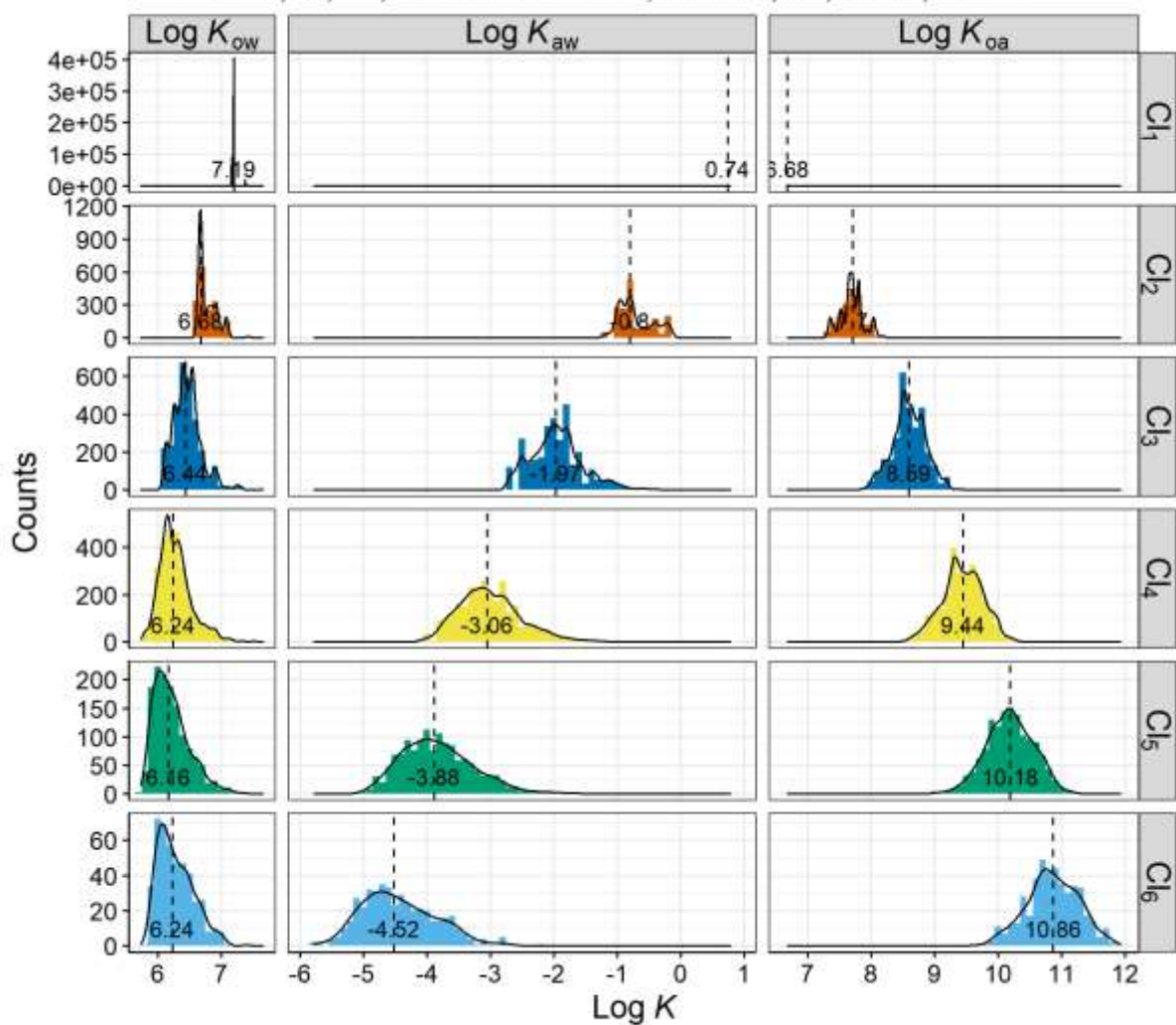
C_{13} , 30 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



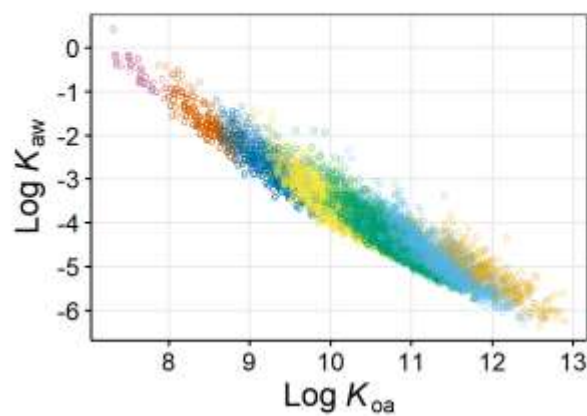
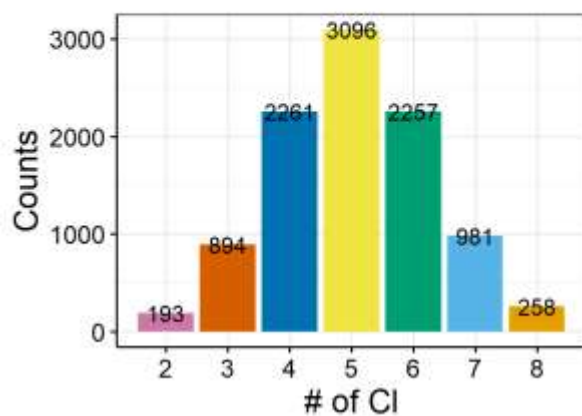
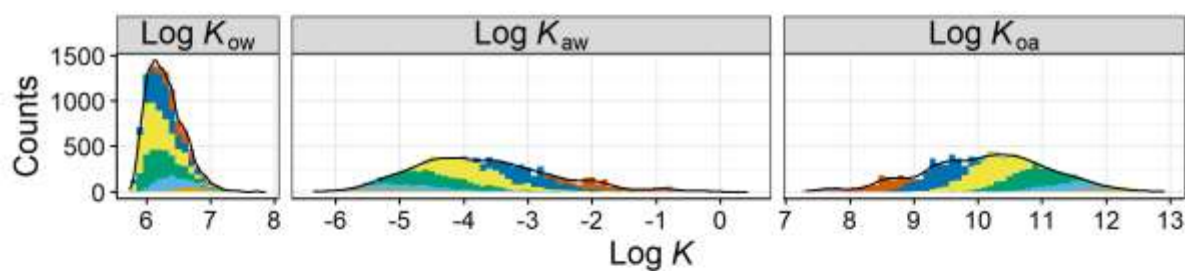
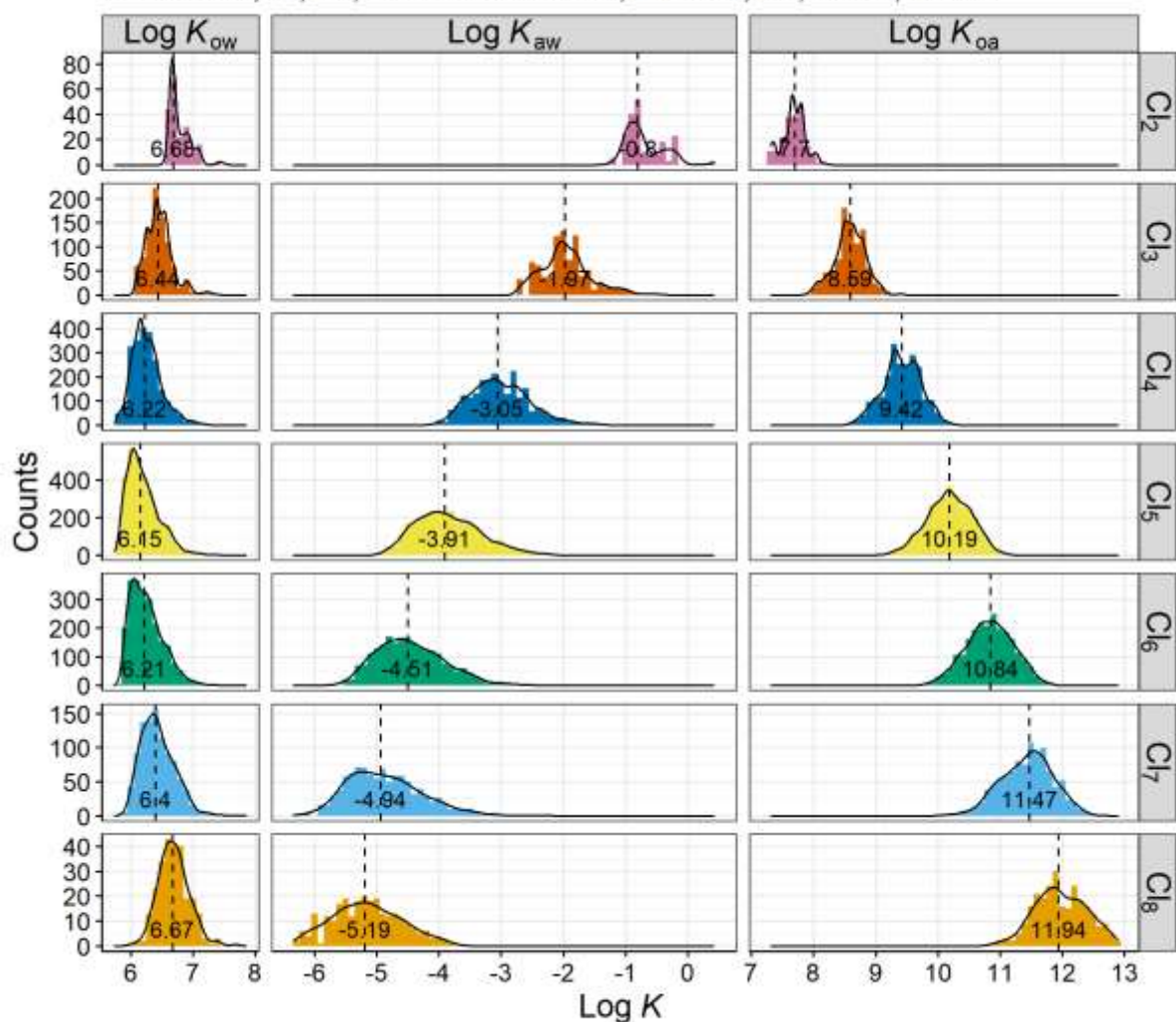
C₁₃, 40 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



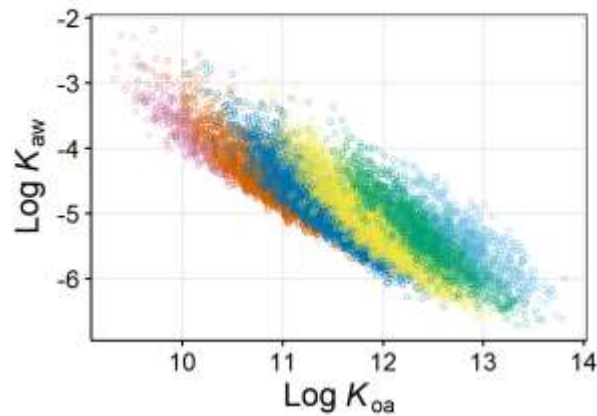
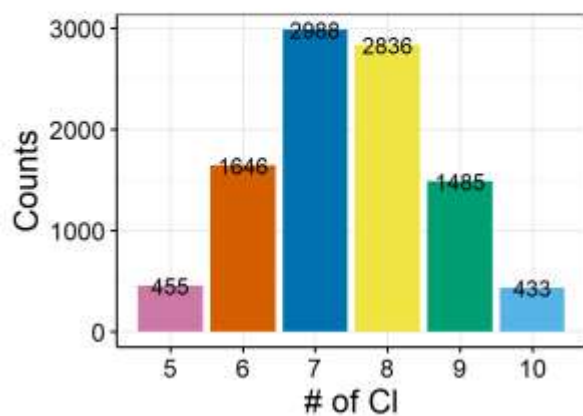
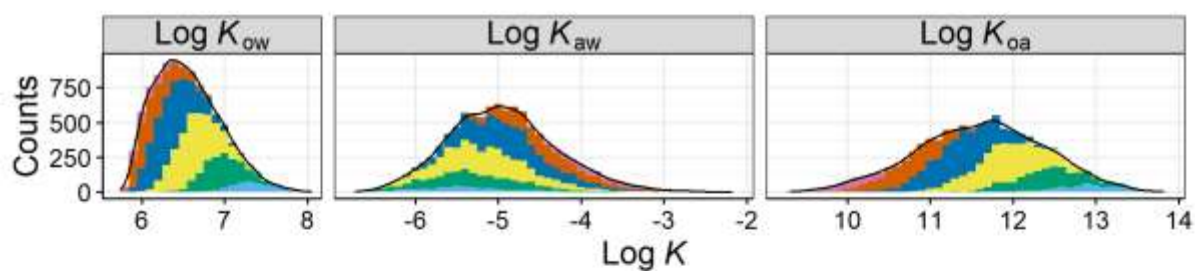
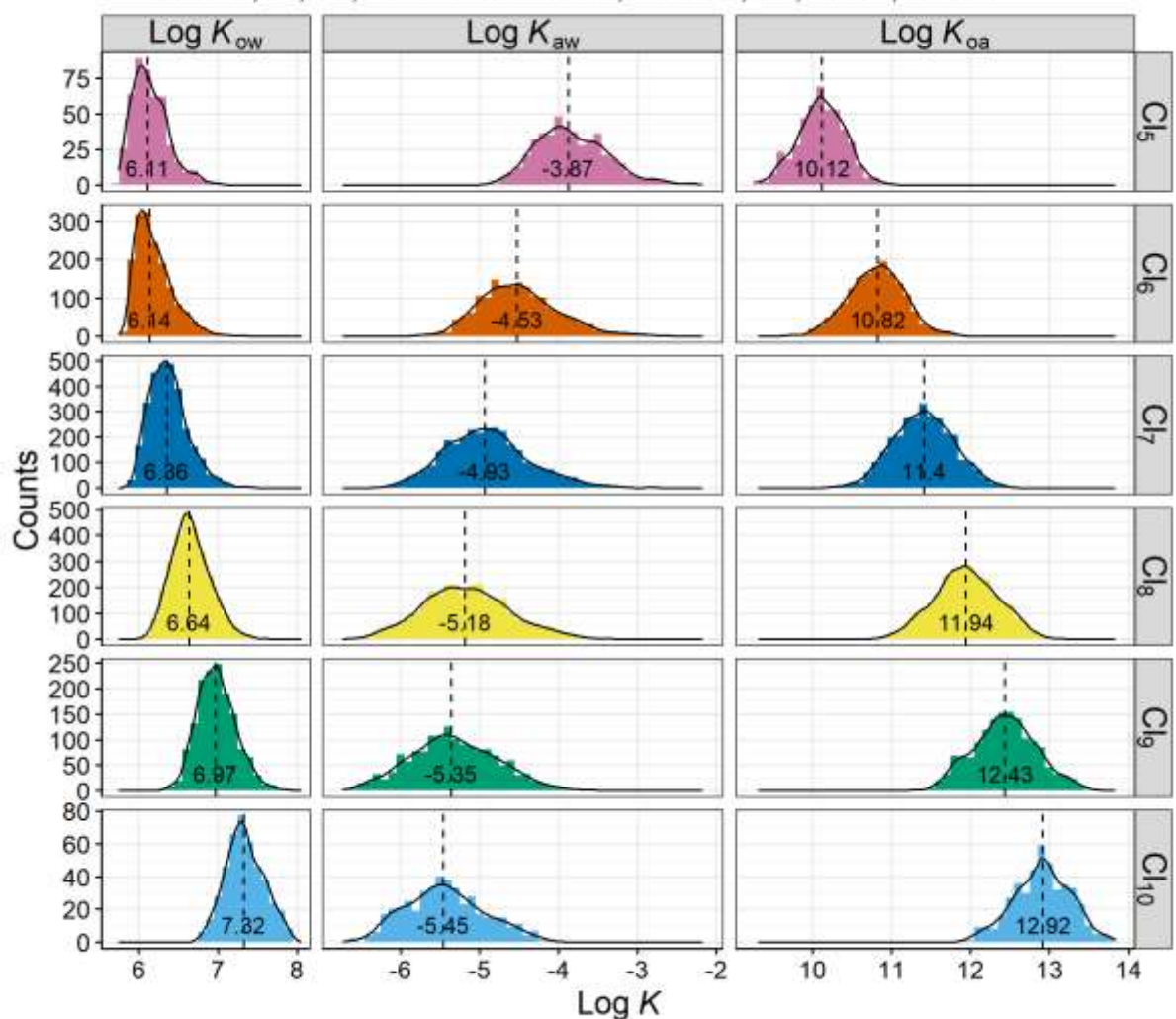
C₁₃, 50 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



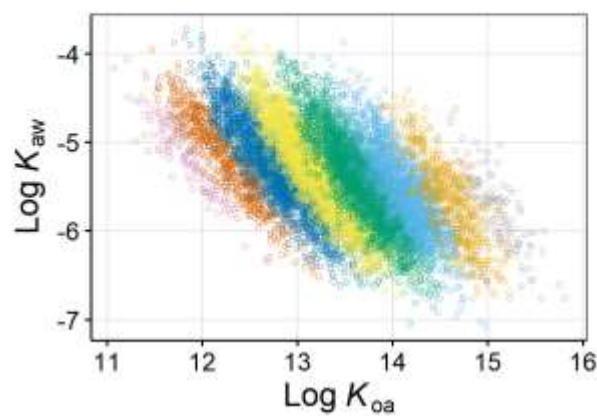
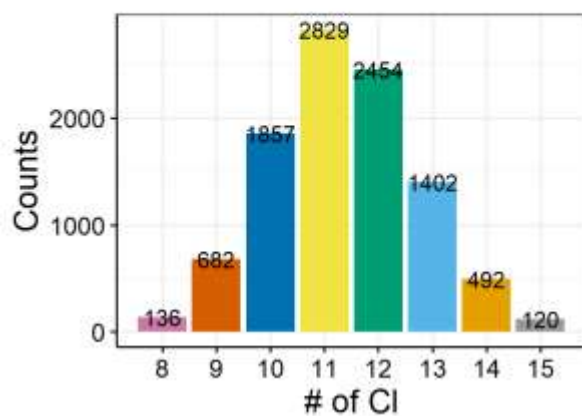
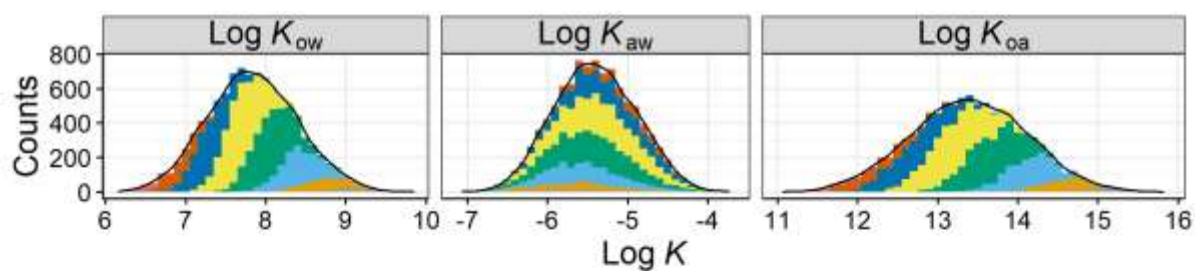
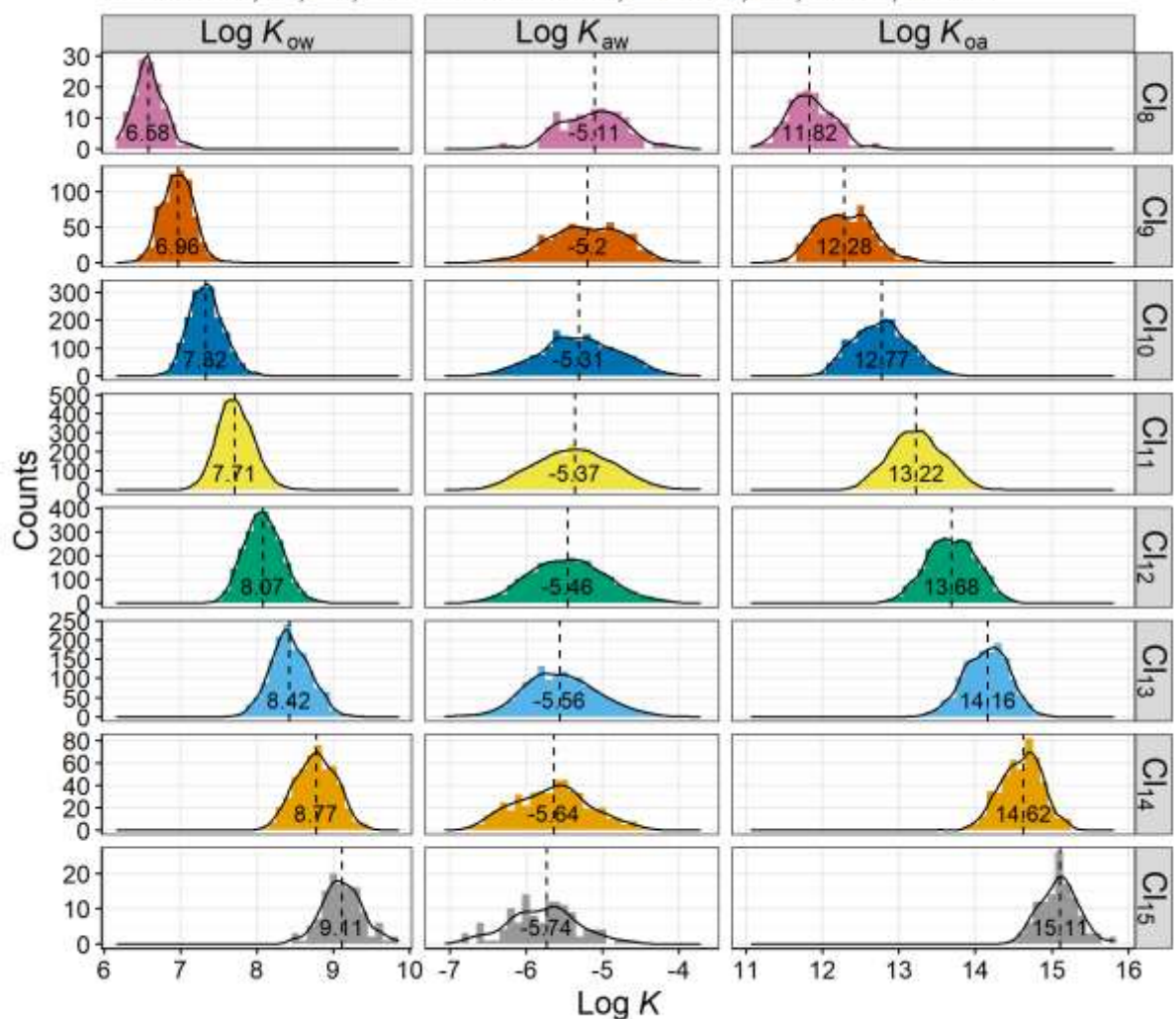
C₁₃, 60 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



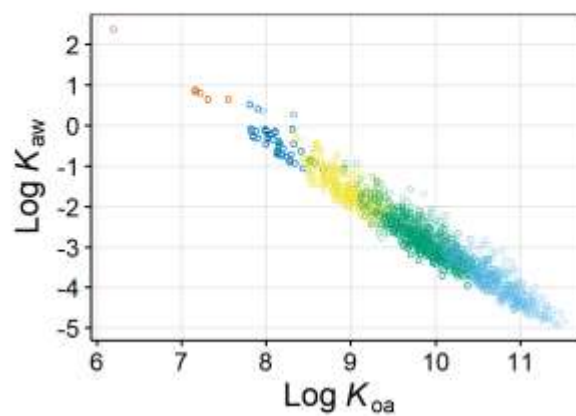
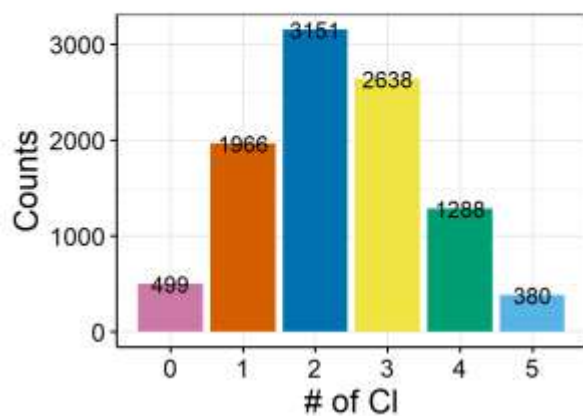
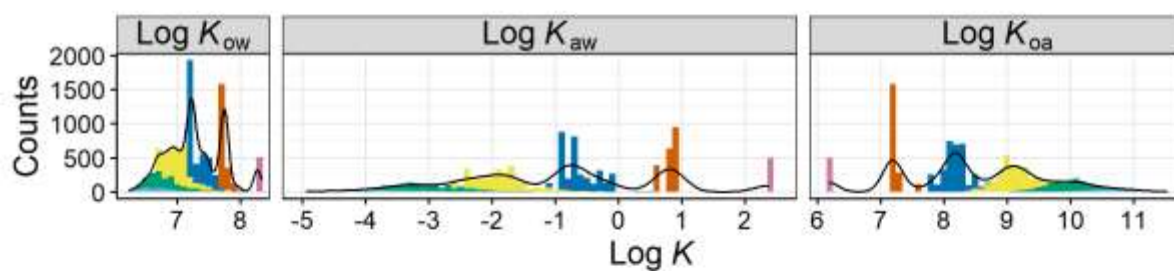
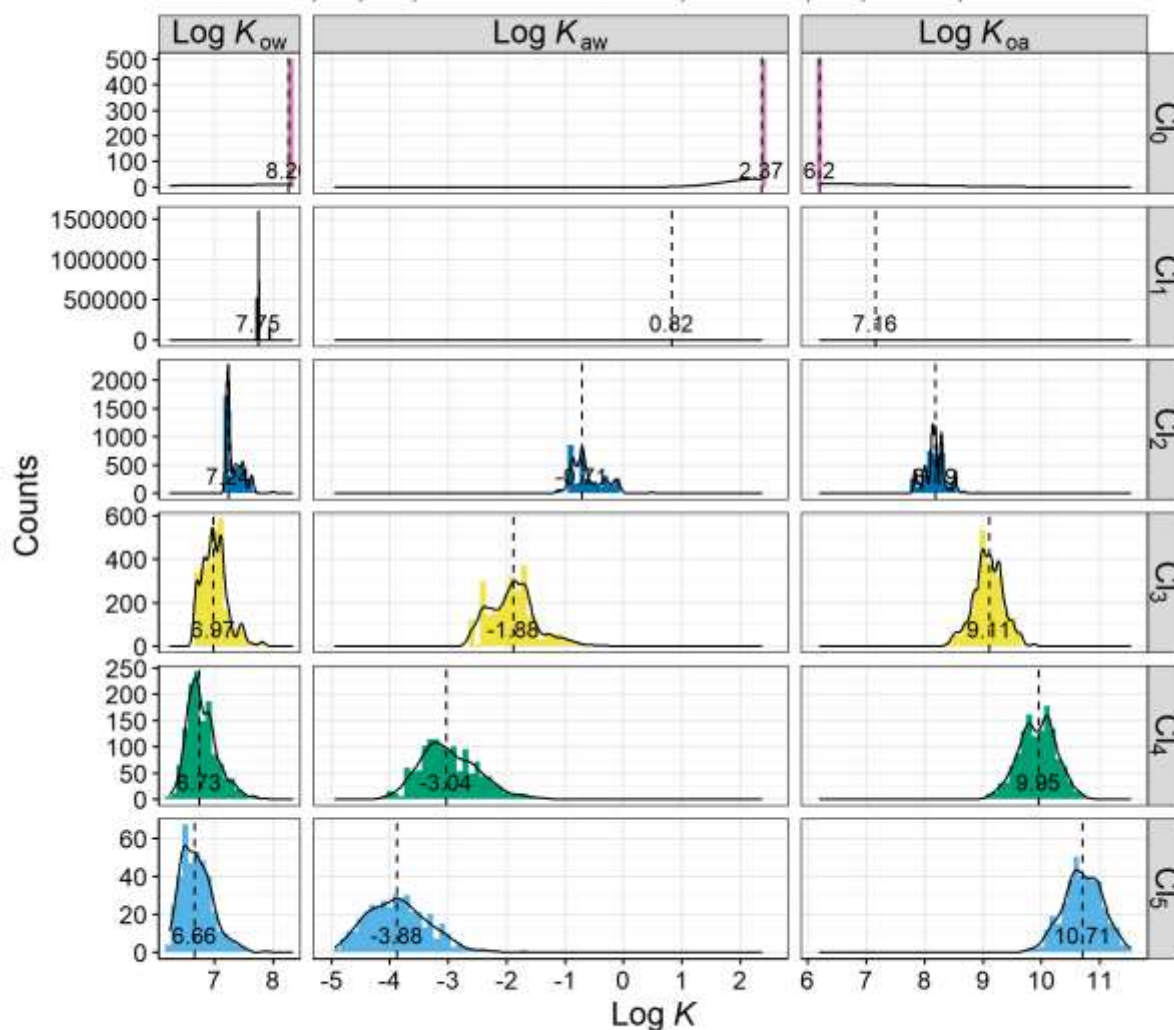
C₁₃, 70 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



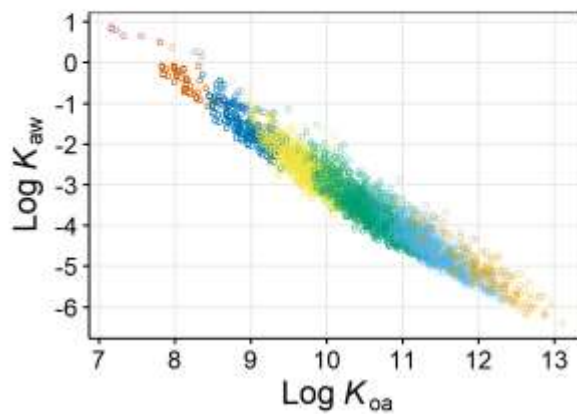
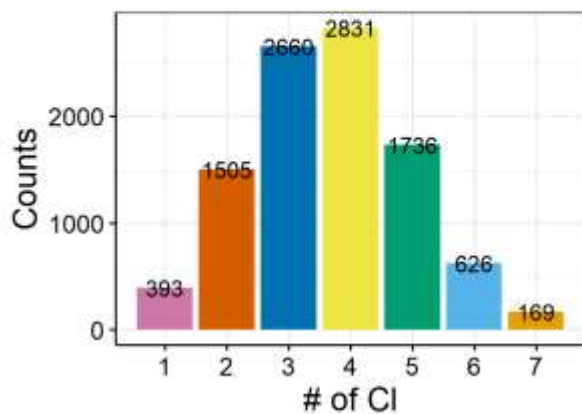
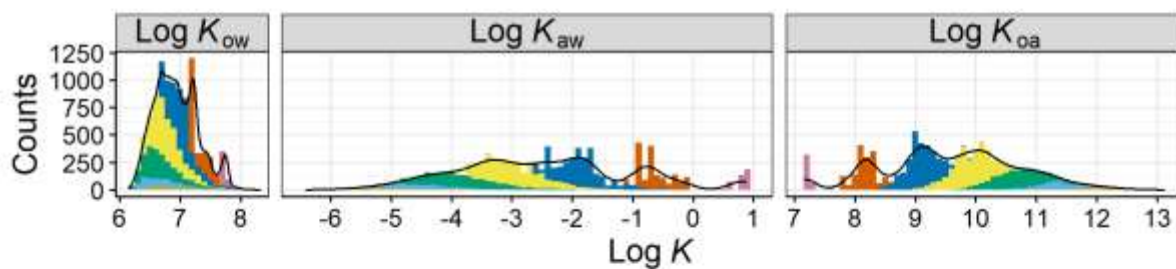
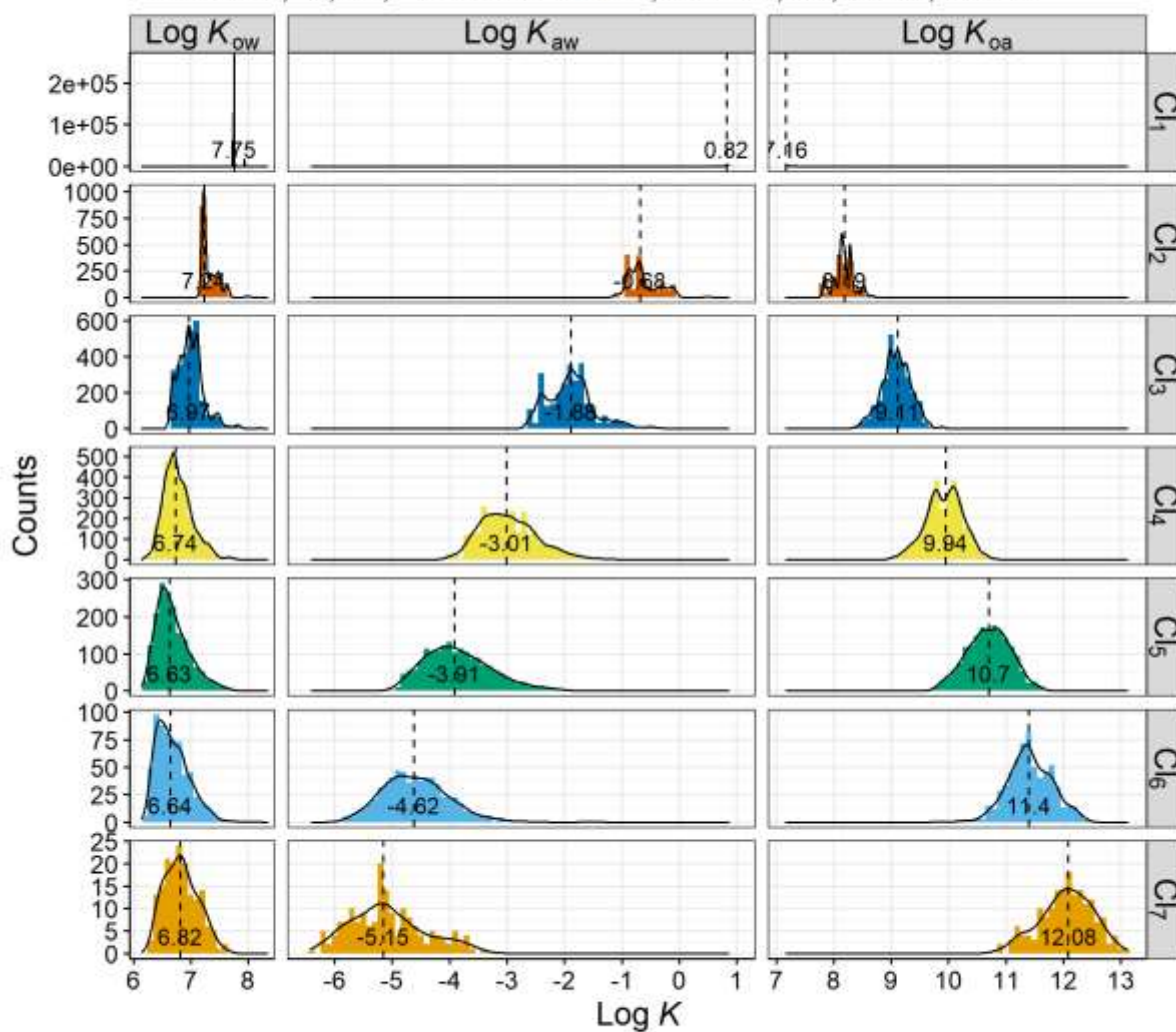
C₁₄, 30 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



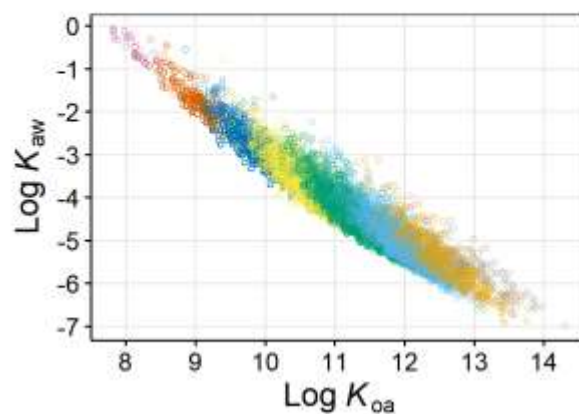
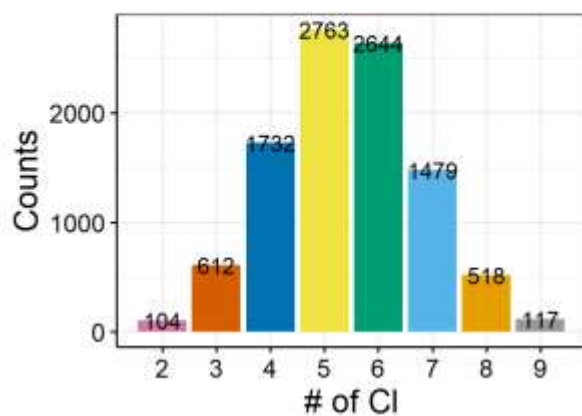
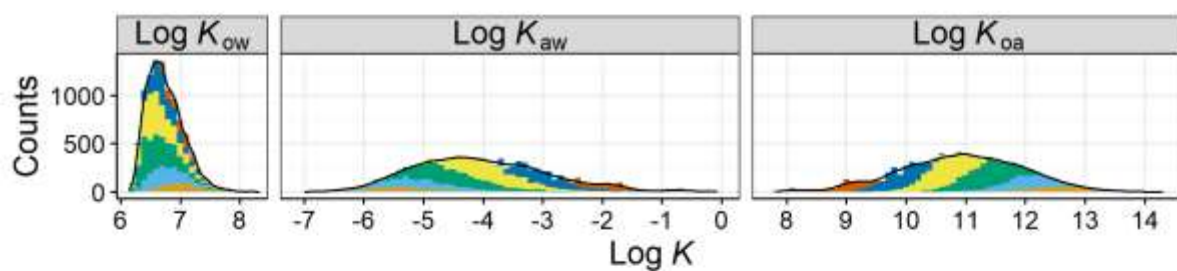
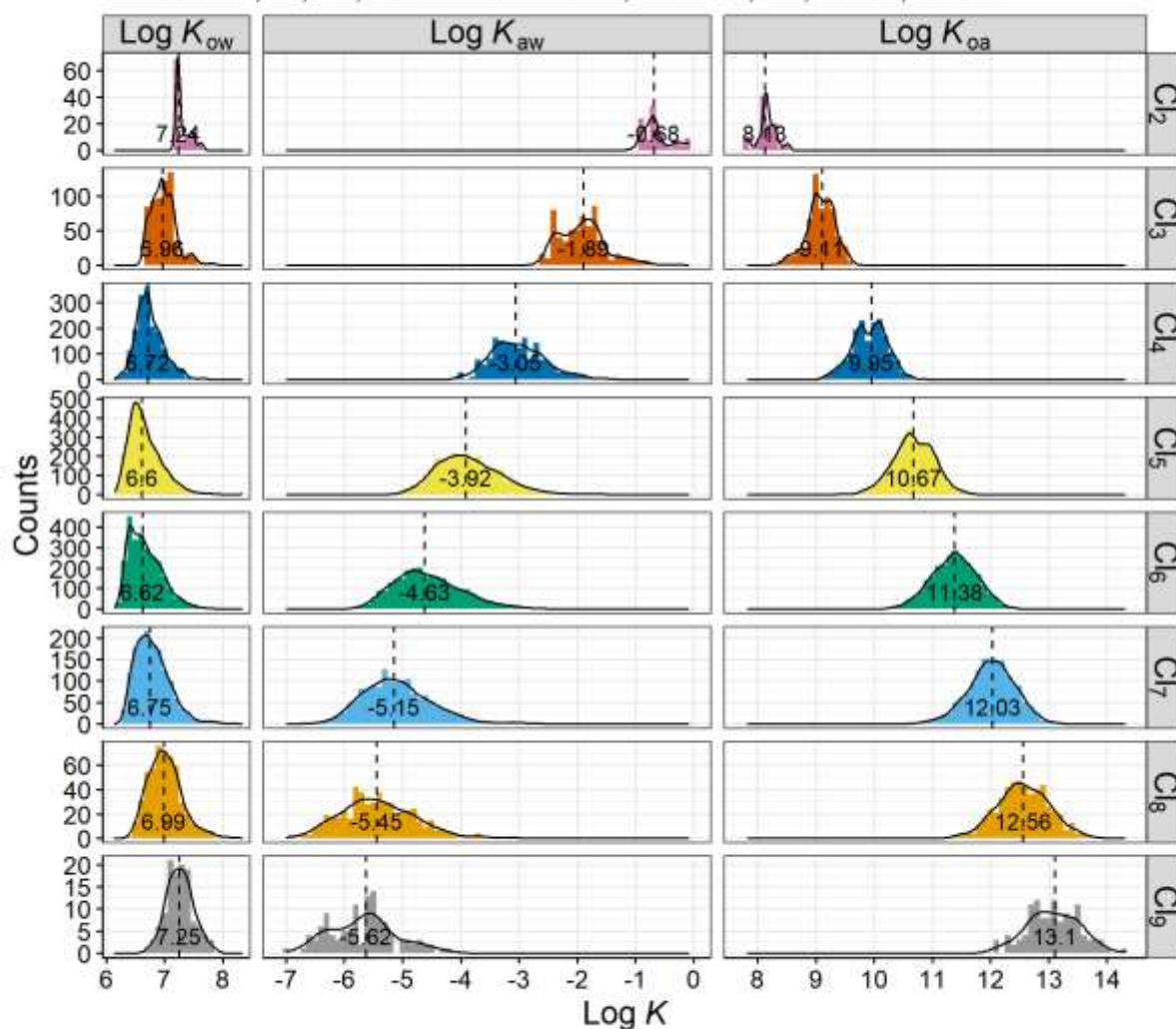
C₁₄, 40 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



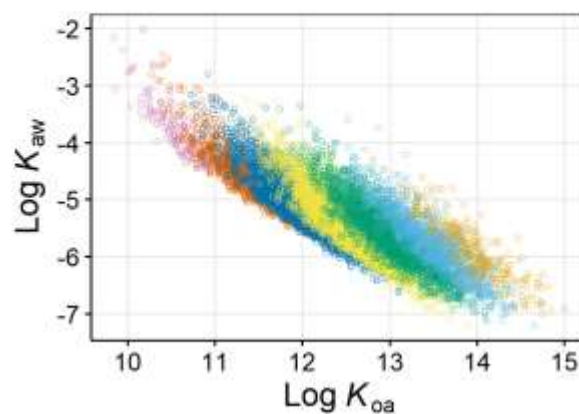
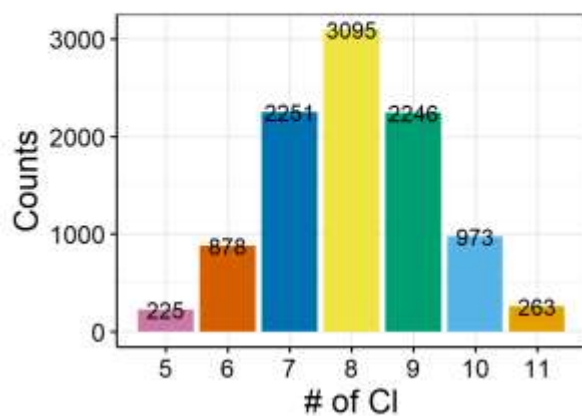
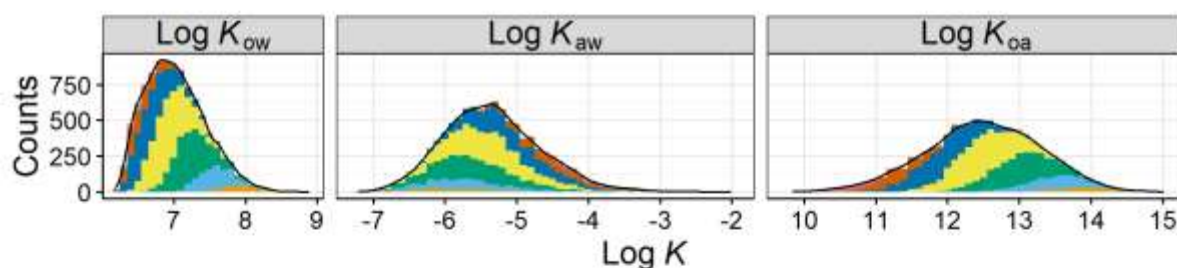
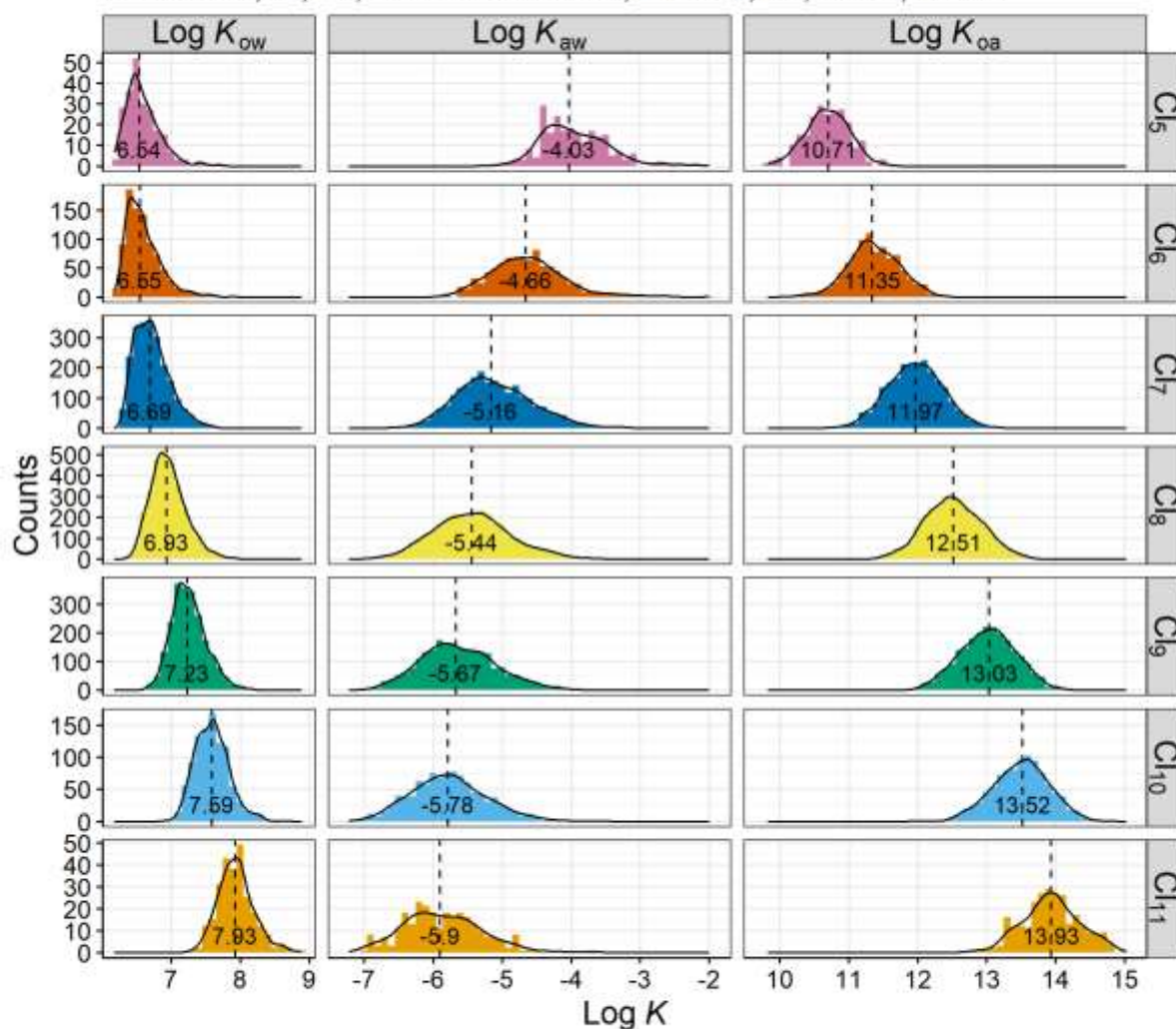
C₁₄, 50 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



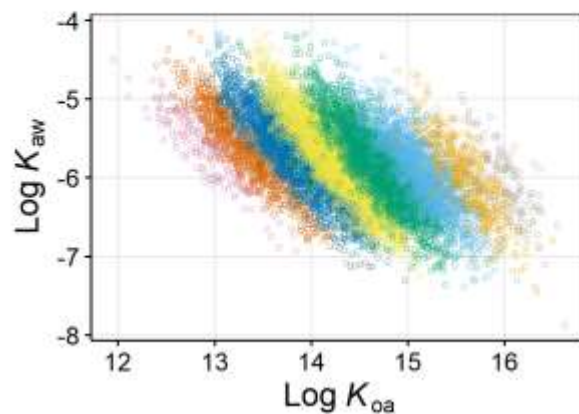
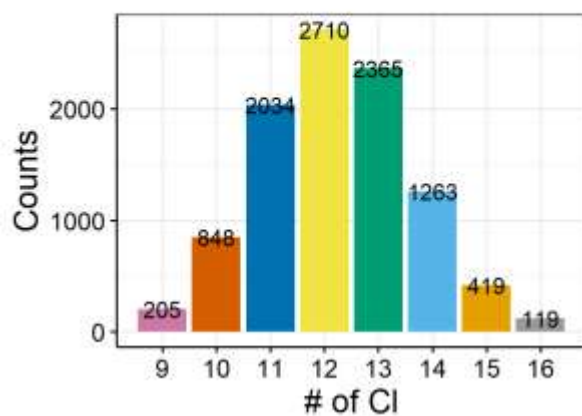
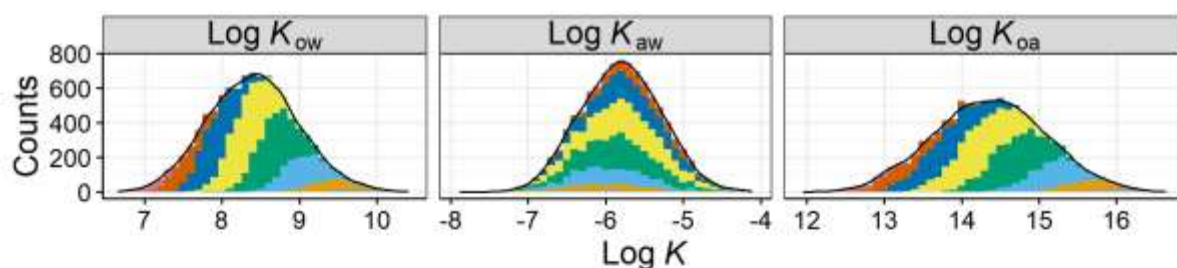
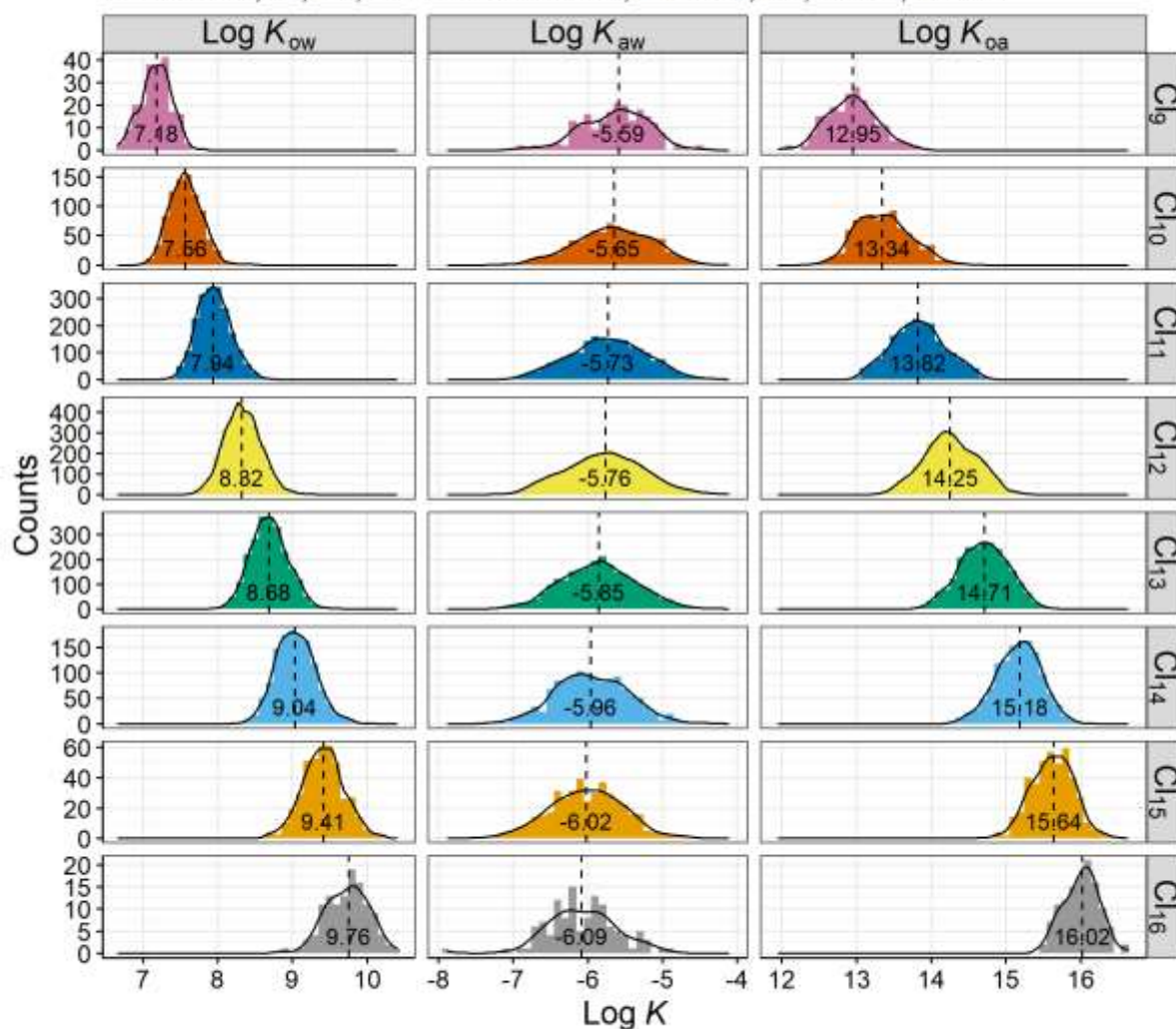
C₁₄, 60 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



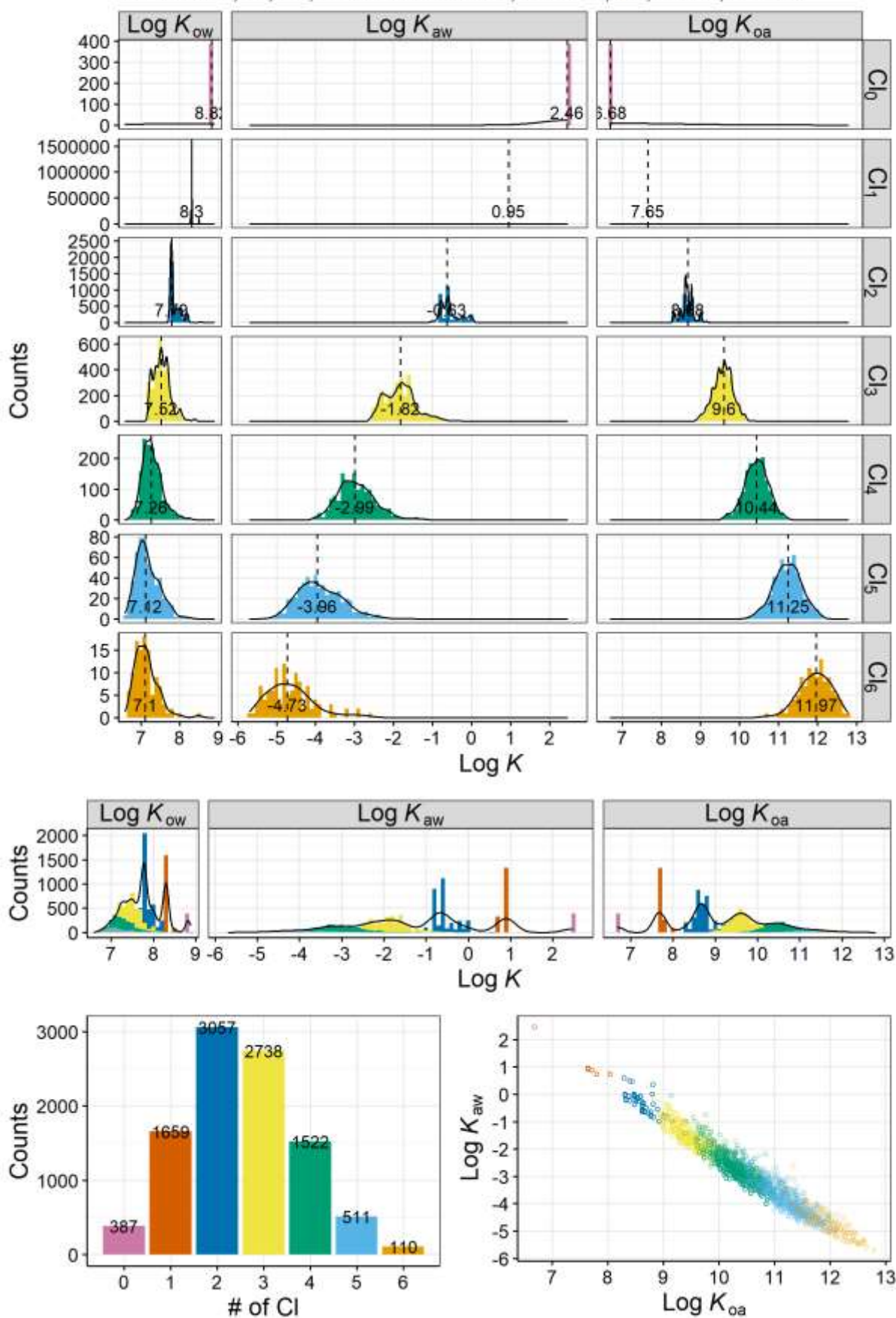
C₁₄, 70 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



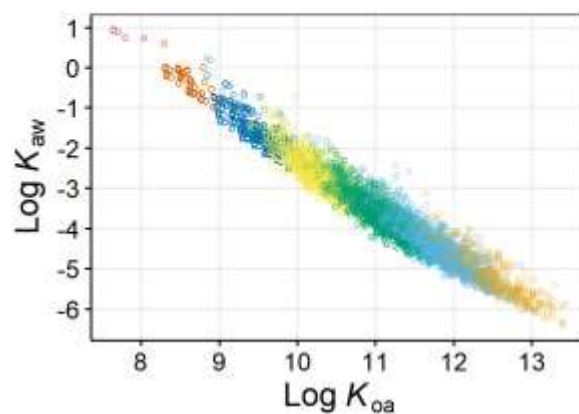
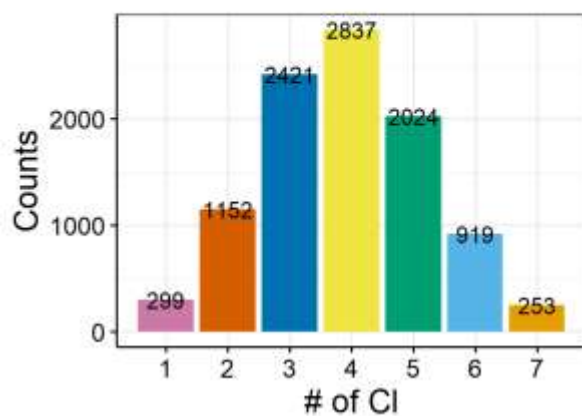
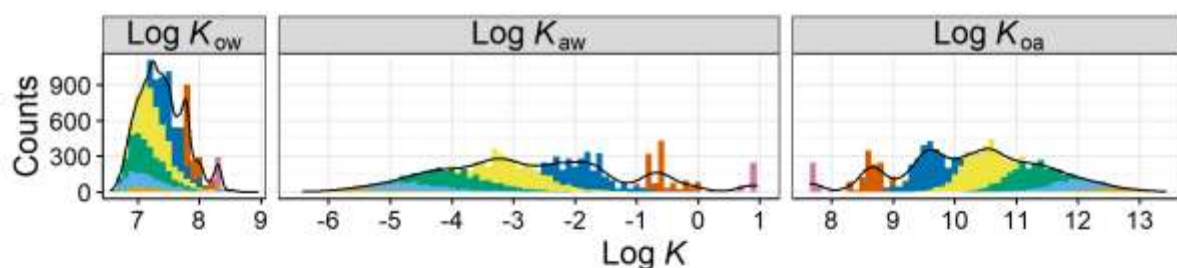
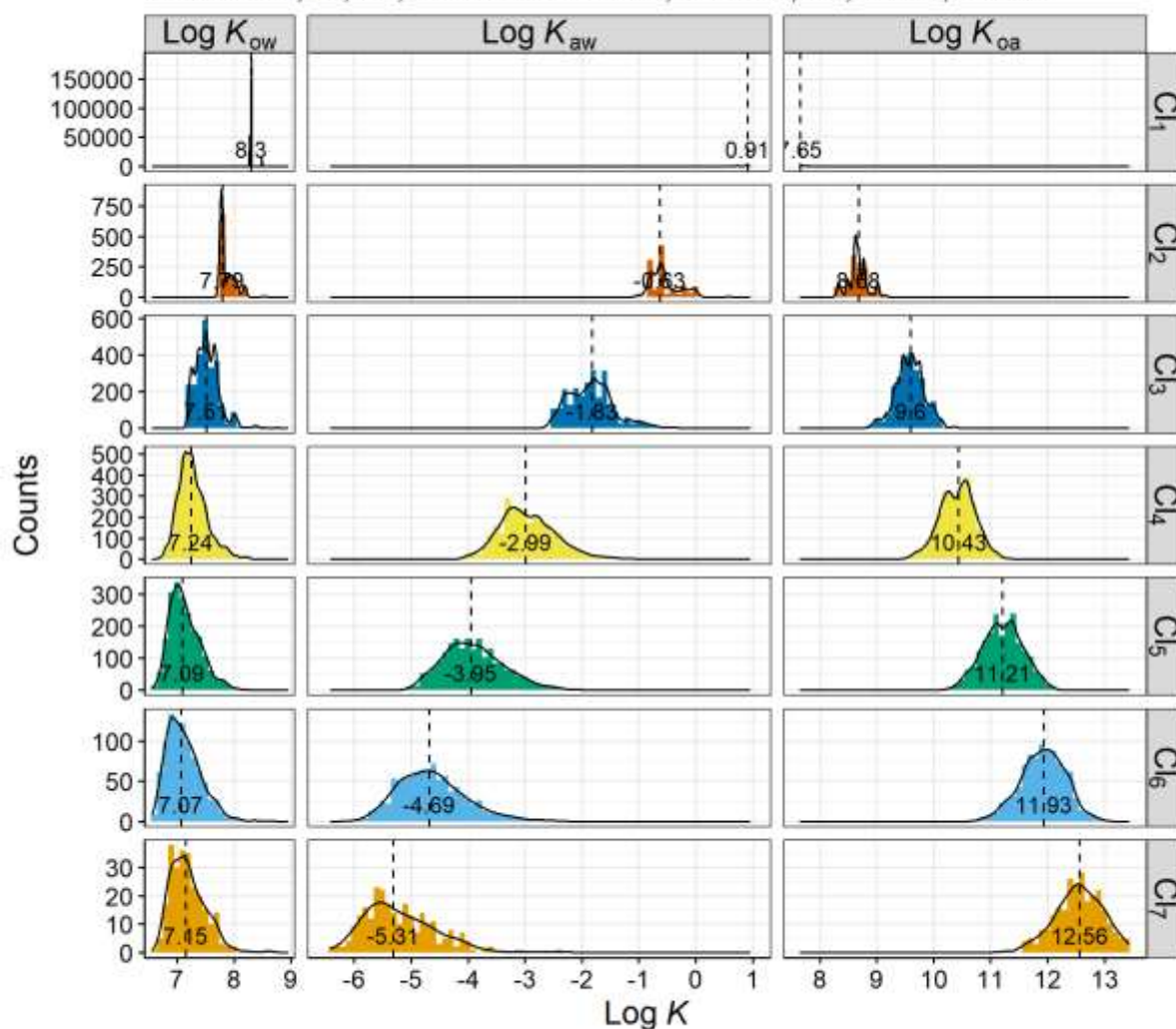
C₁₅, 30 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



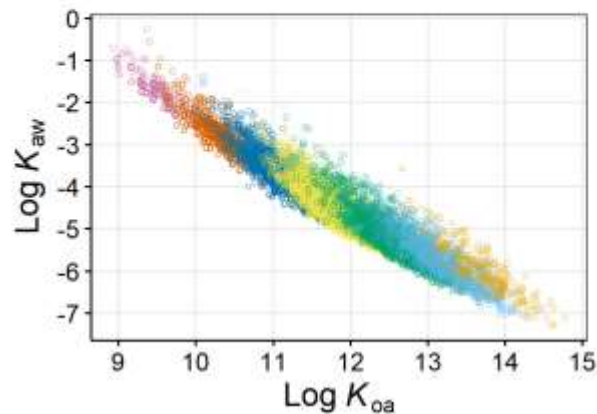
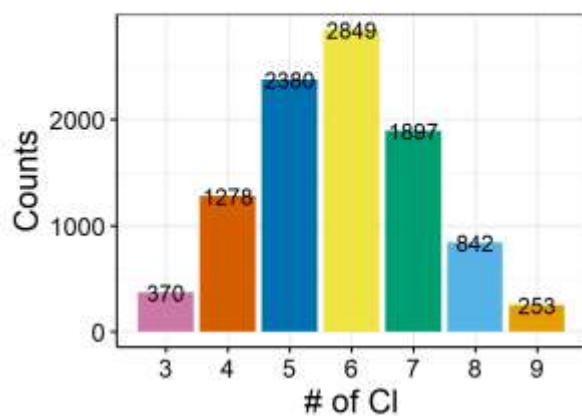
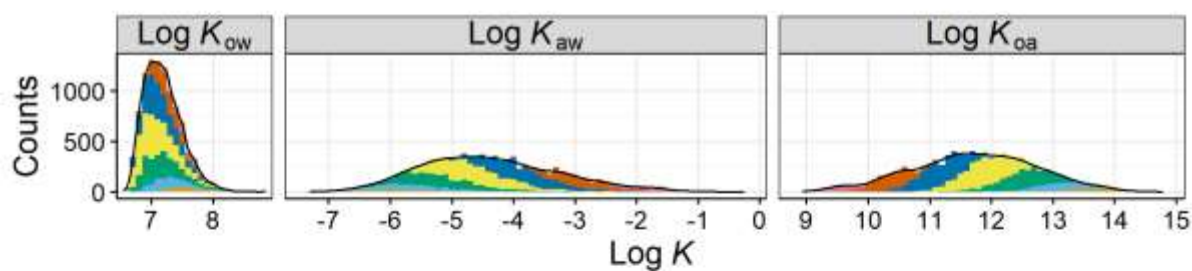
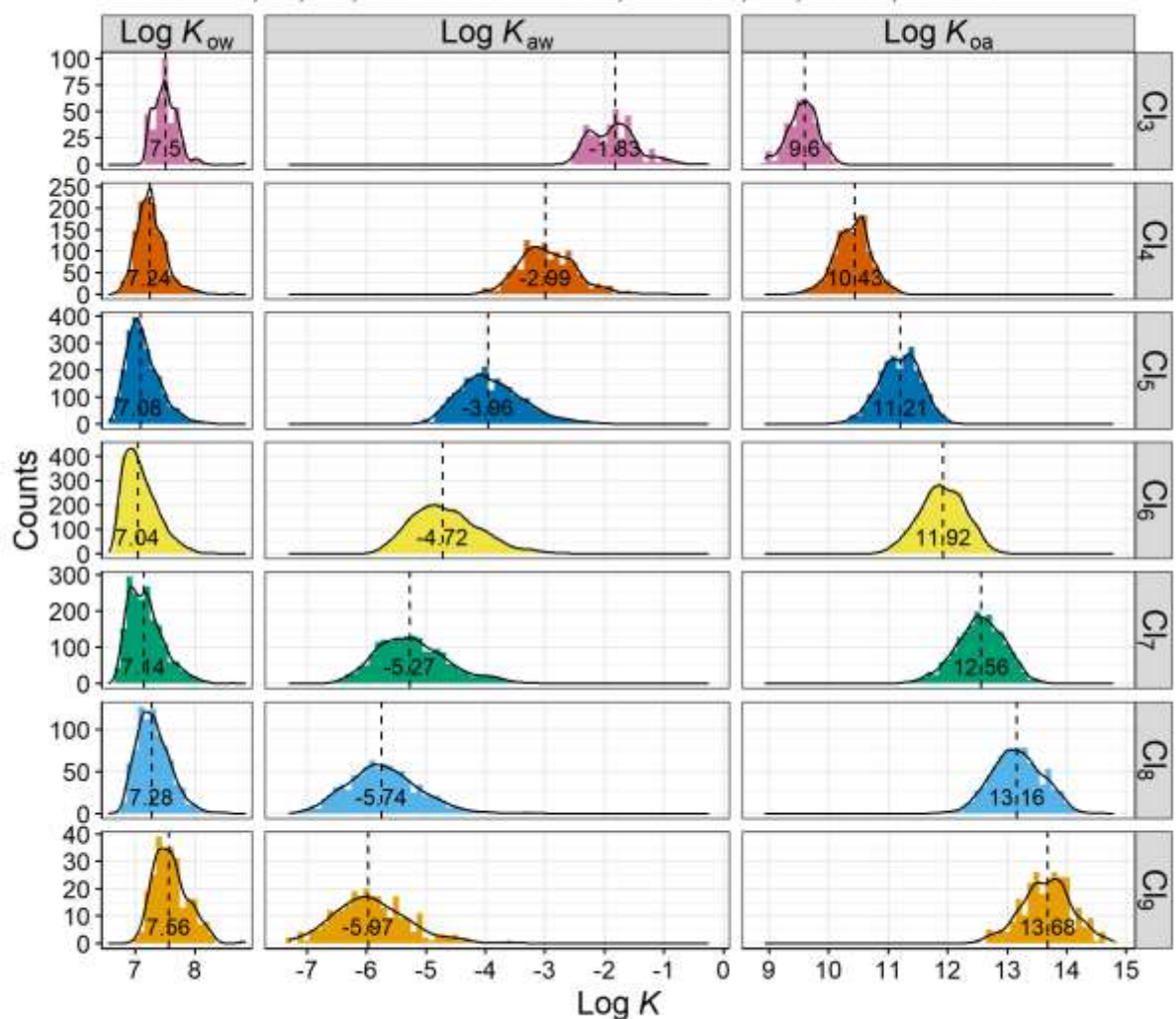
C₁₅, 40 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



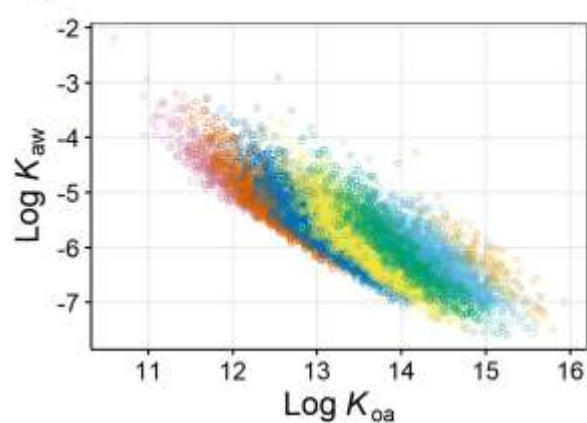
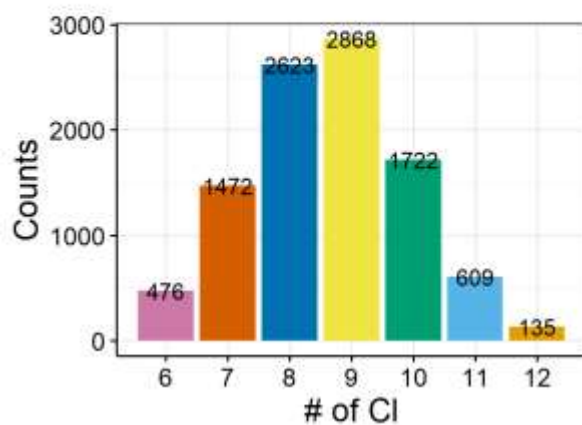
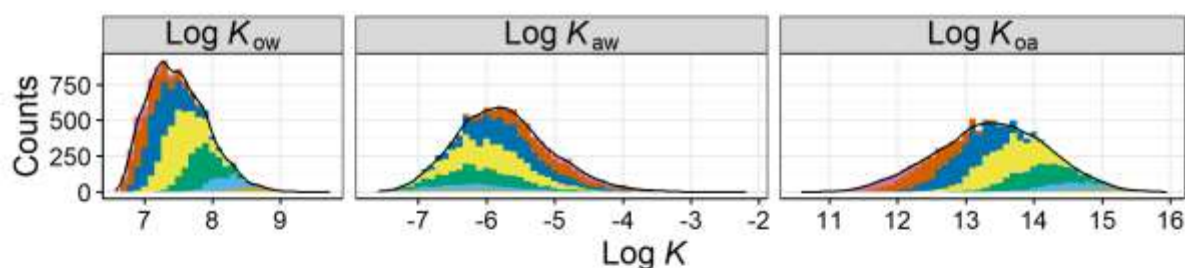
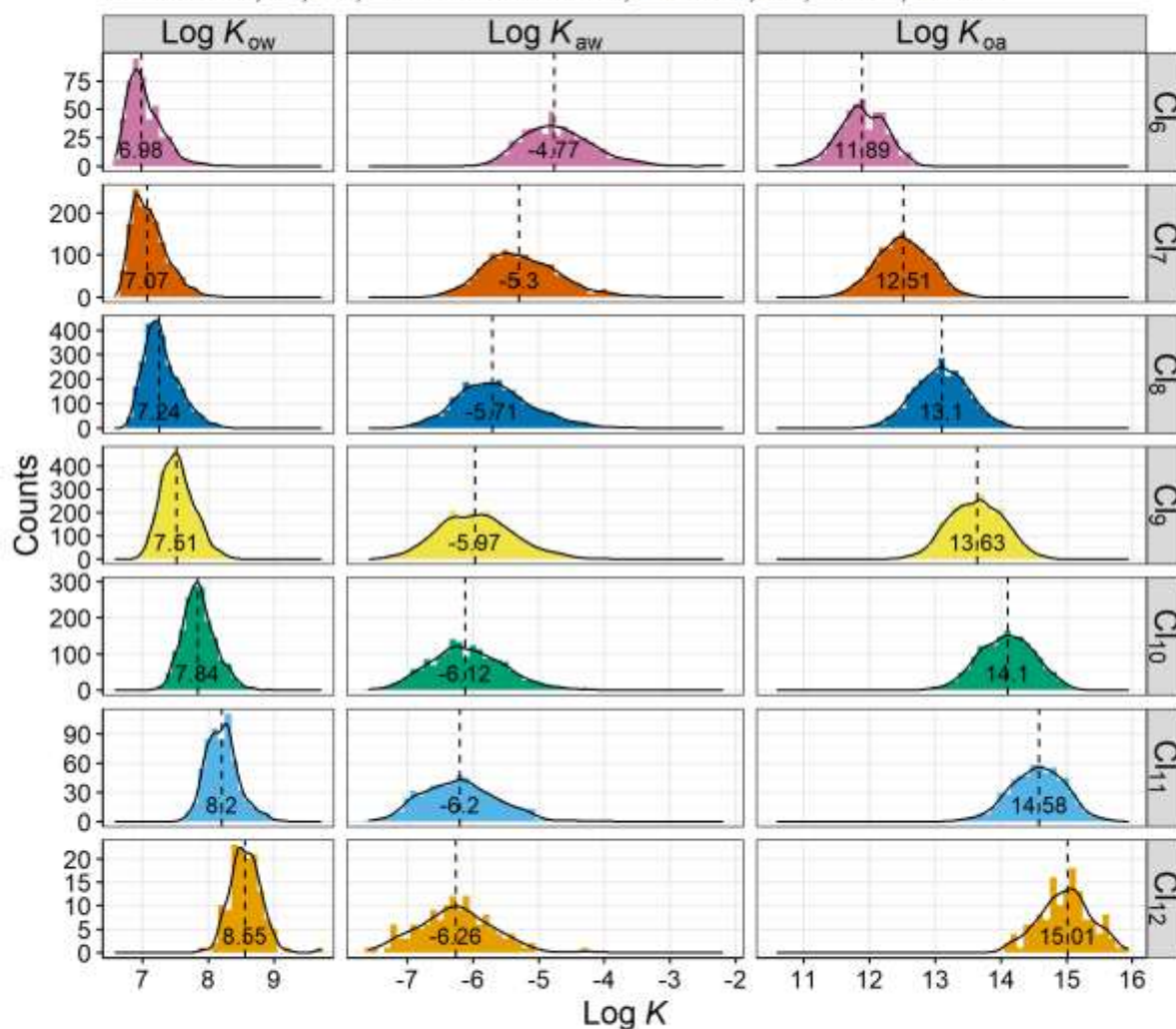
C₁₅, 50 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



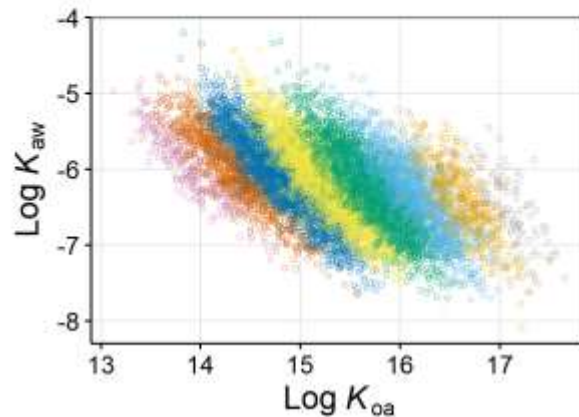
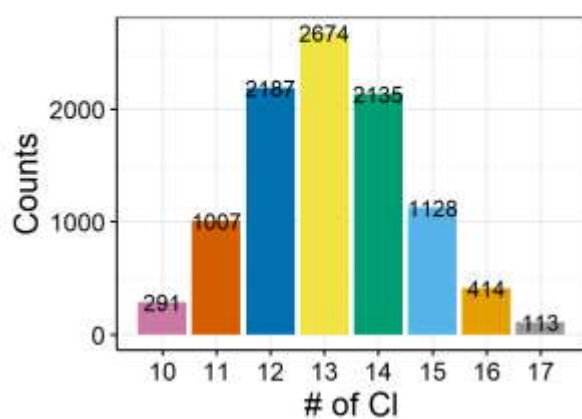
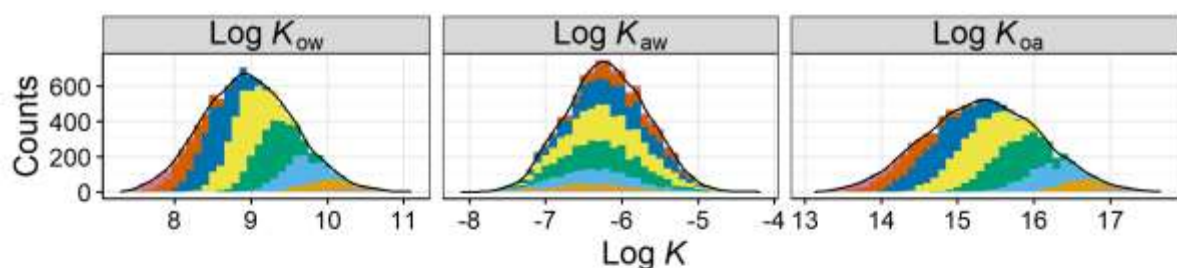
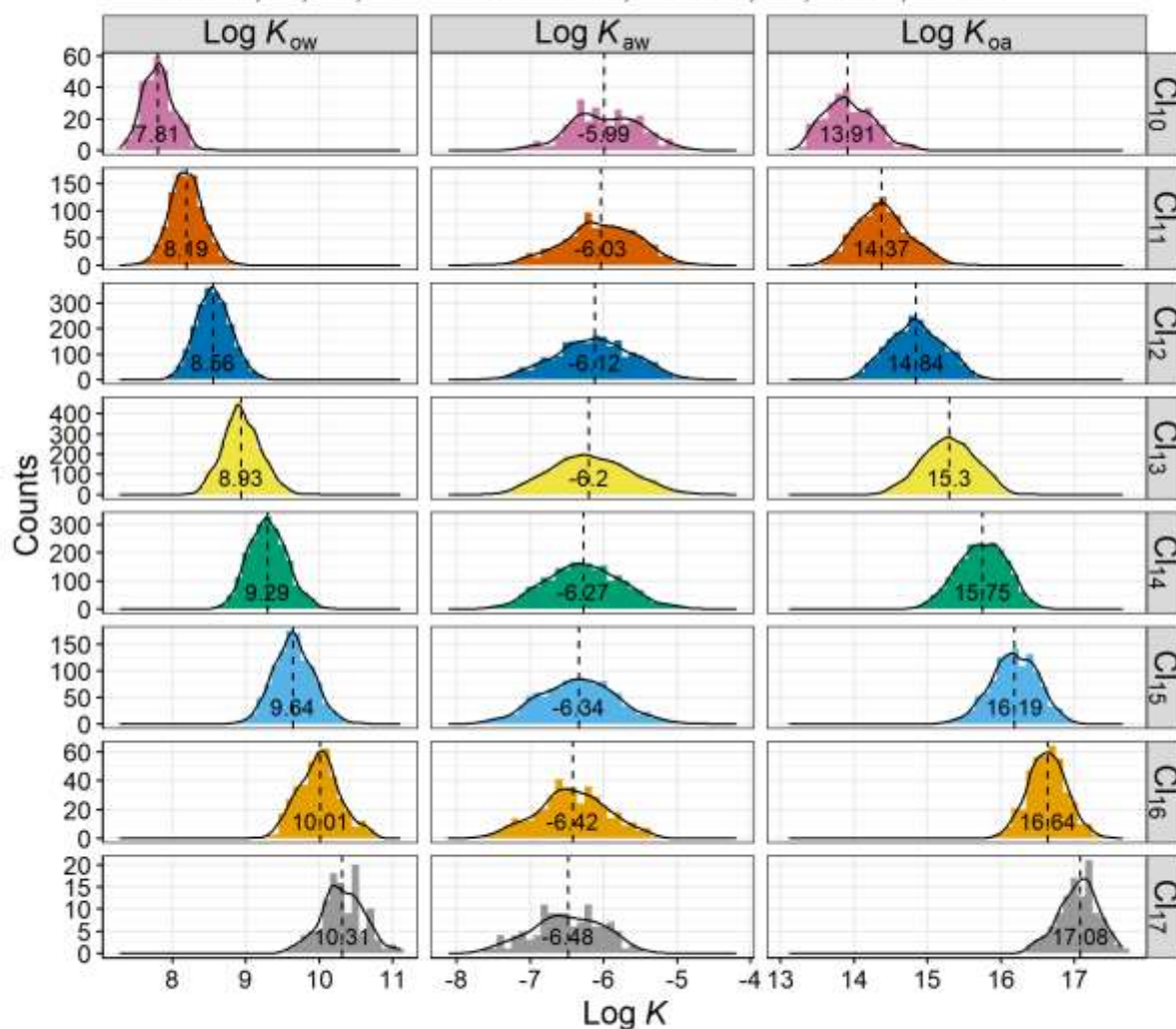
C₁₅, 60 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



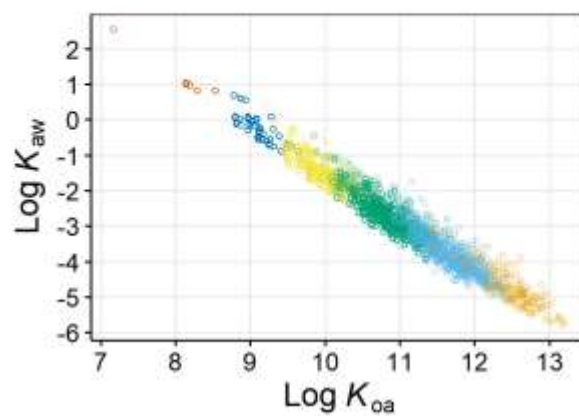
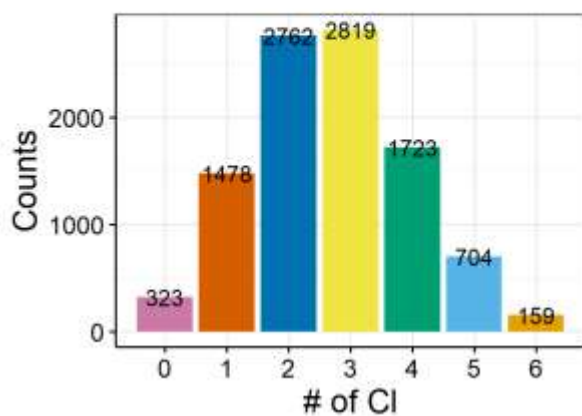
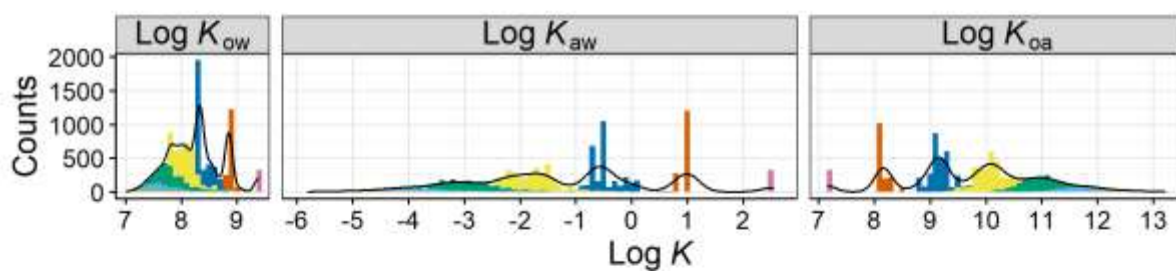
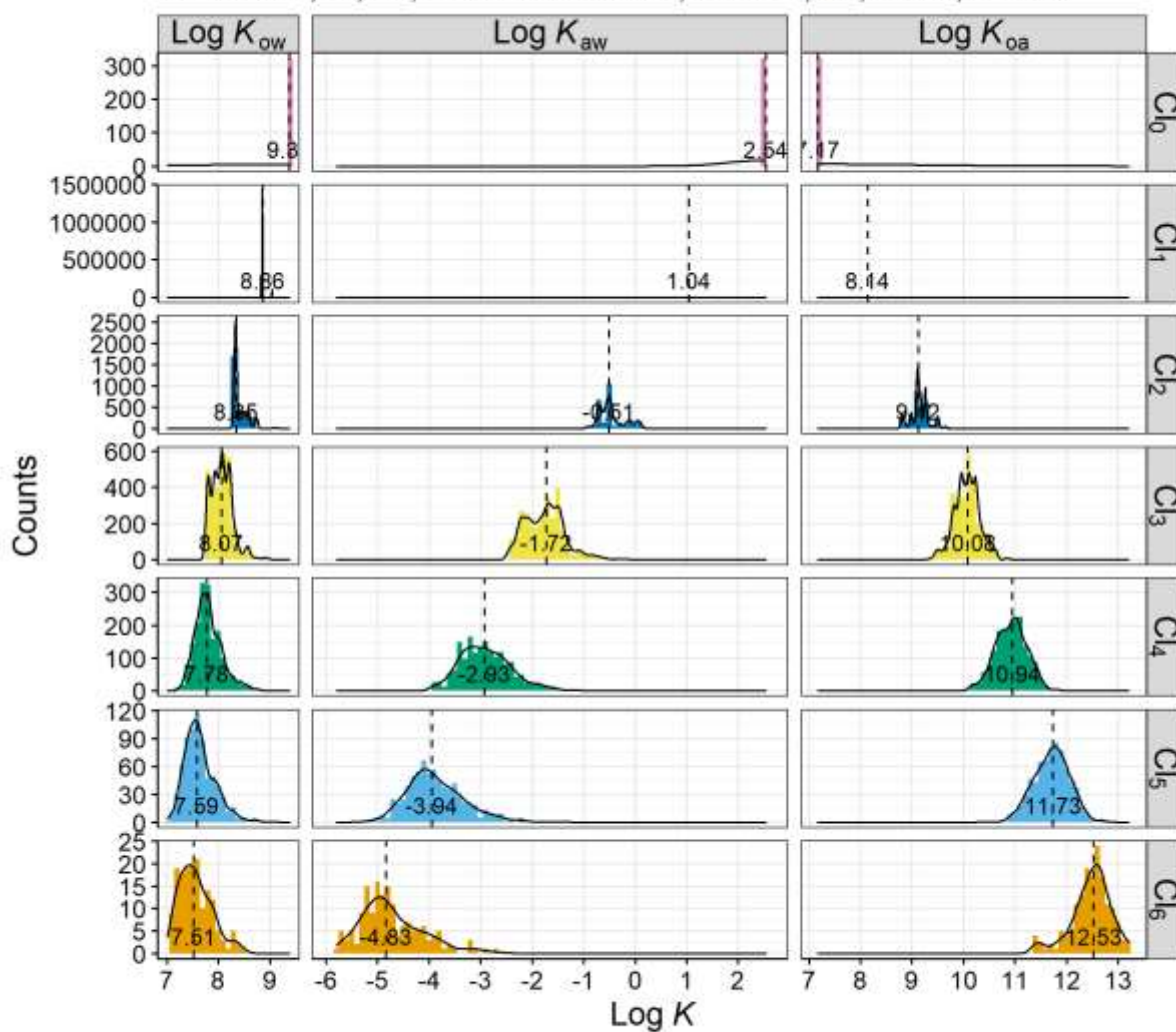
C₁₅, 70 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



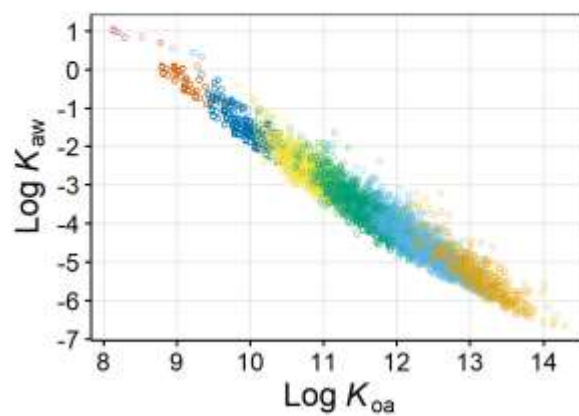
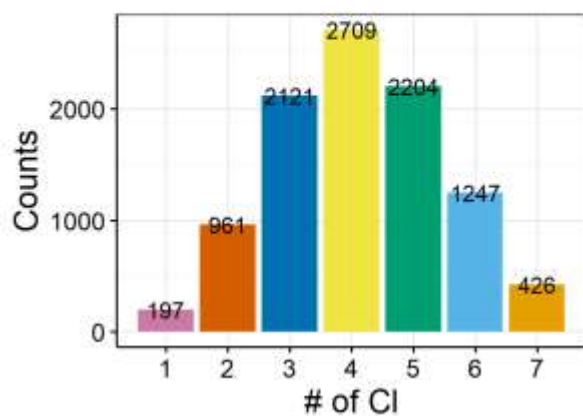
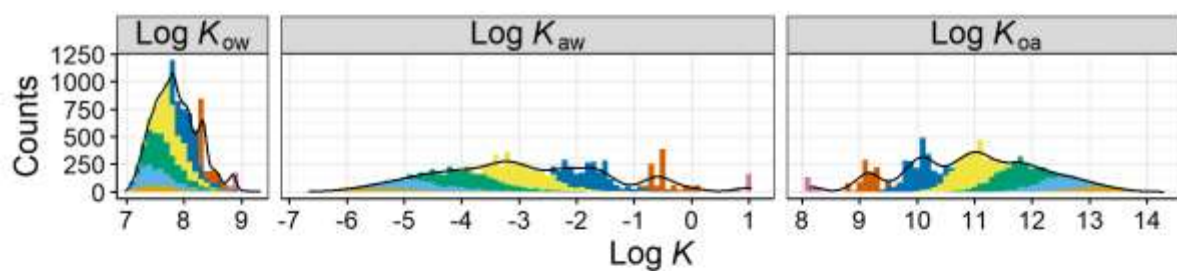
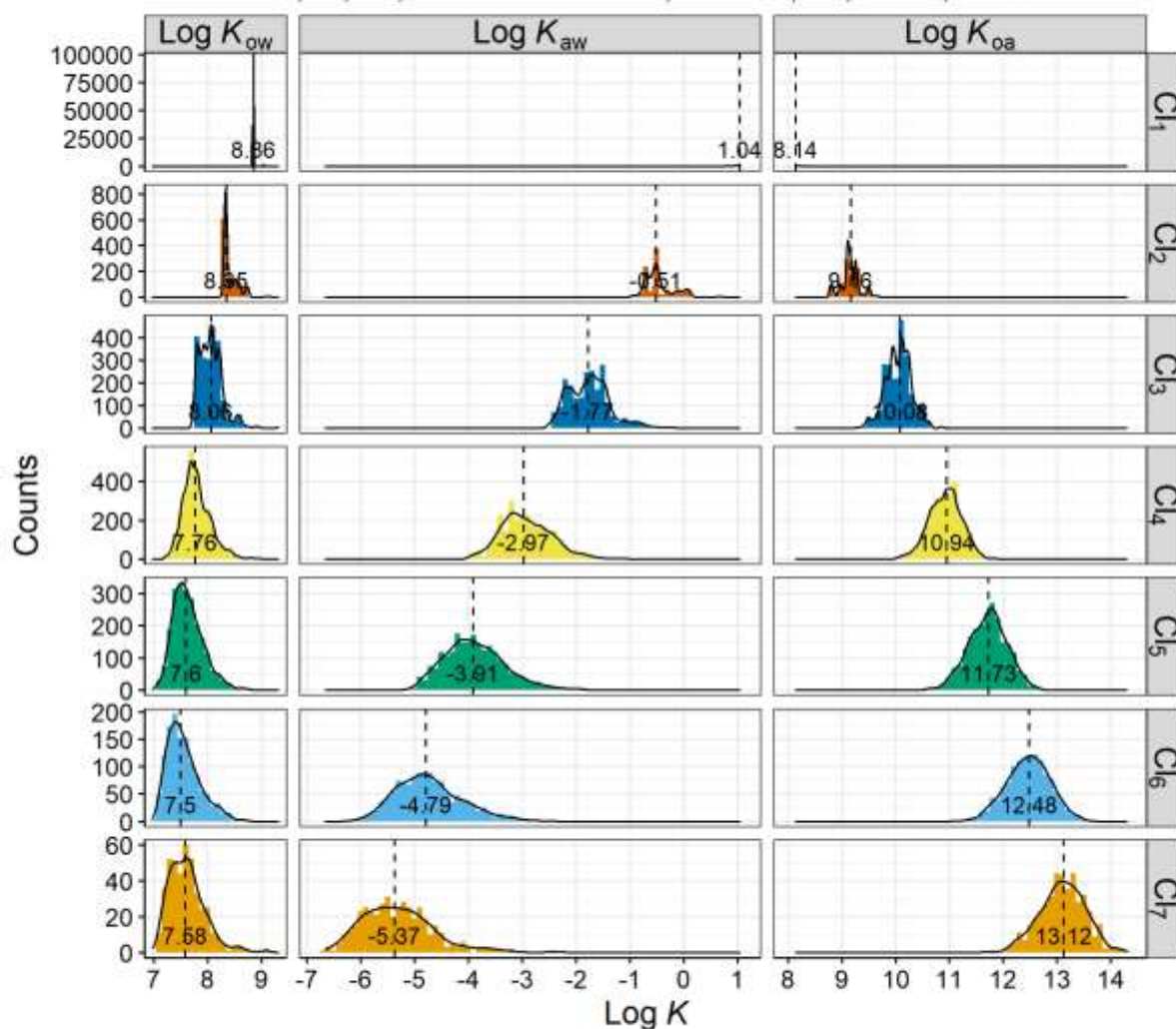
C₁₆, 30 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



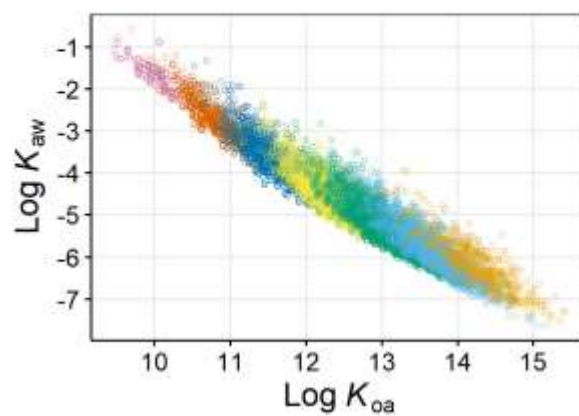
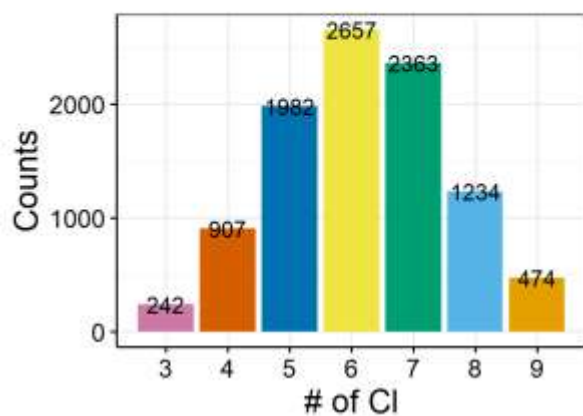
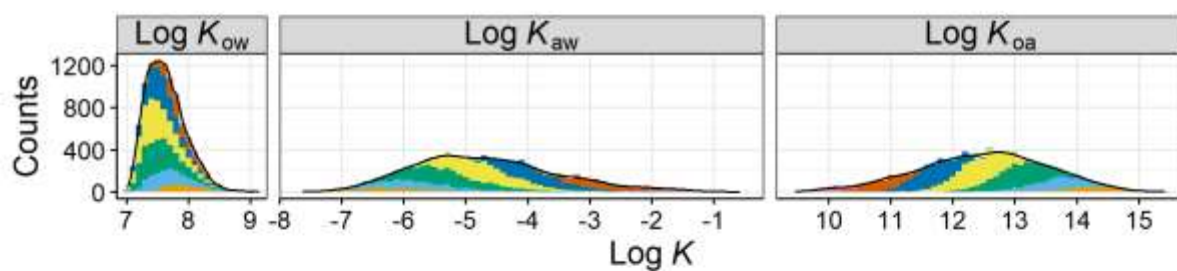
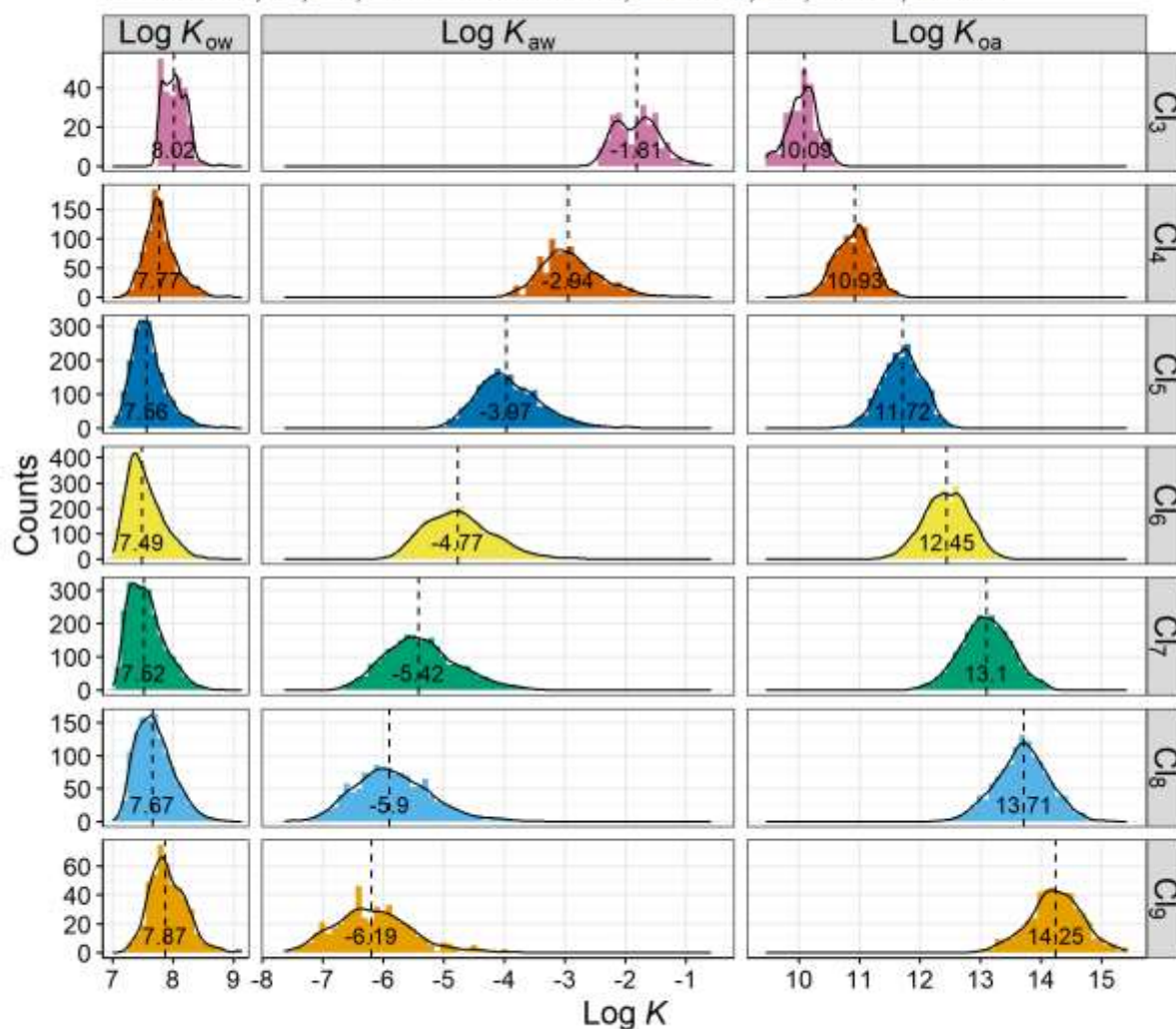
C₁₆, 40 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



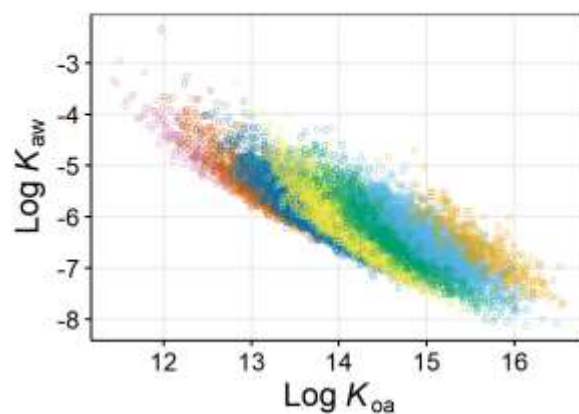
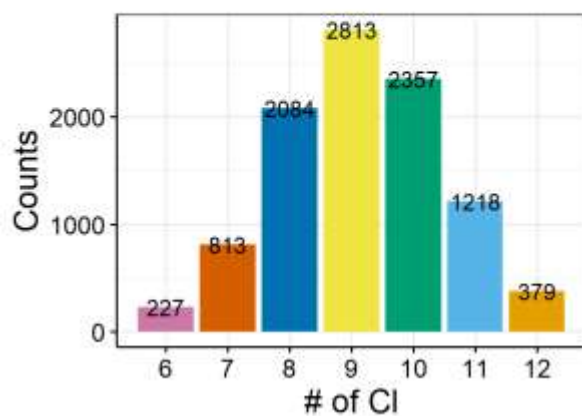
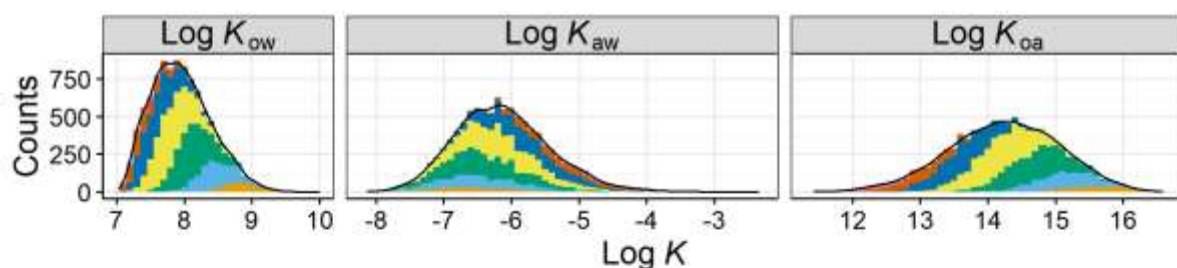
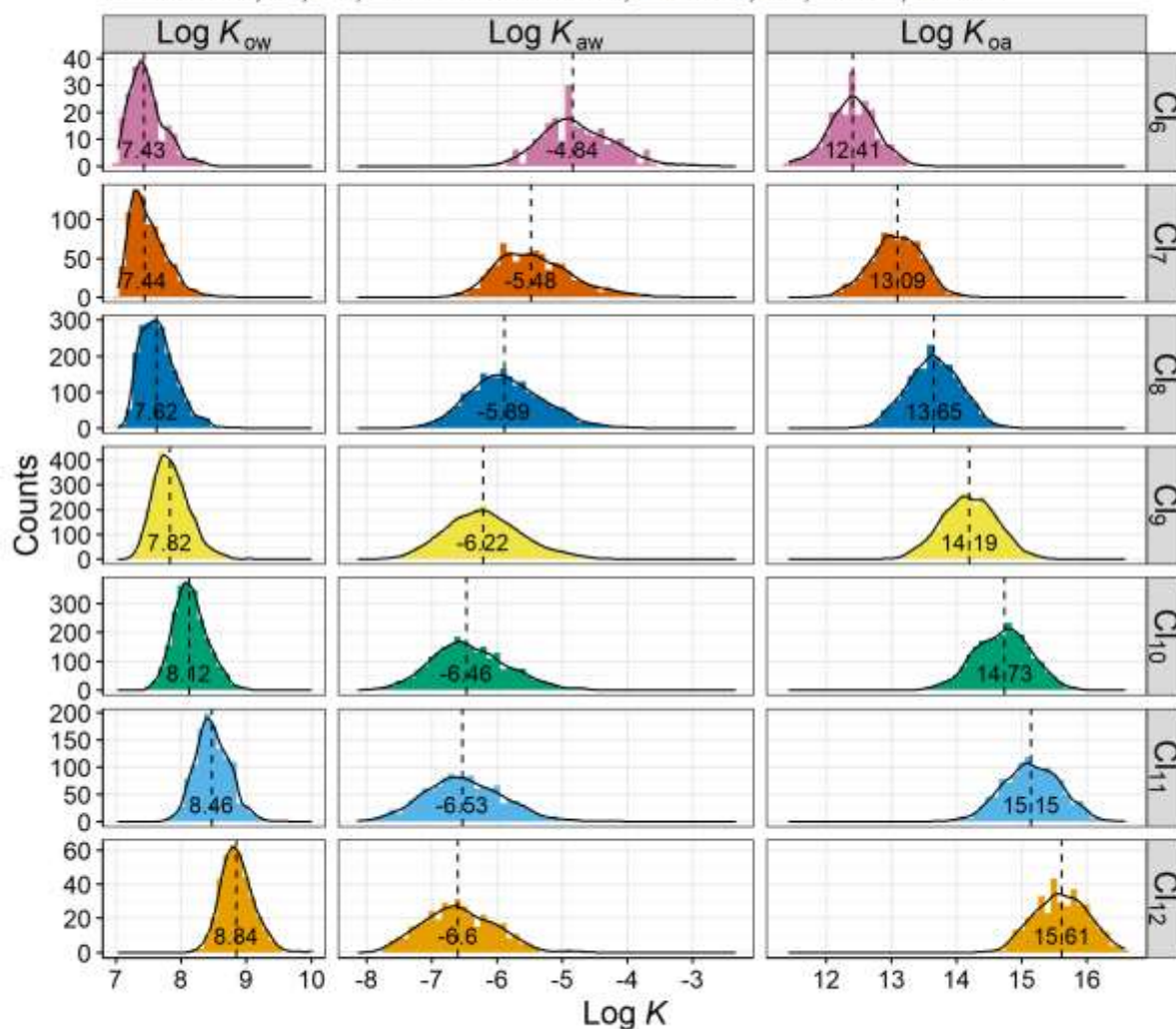
C₁₆, 50 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



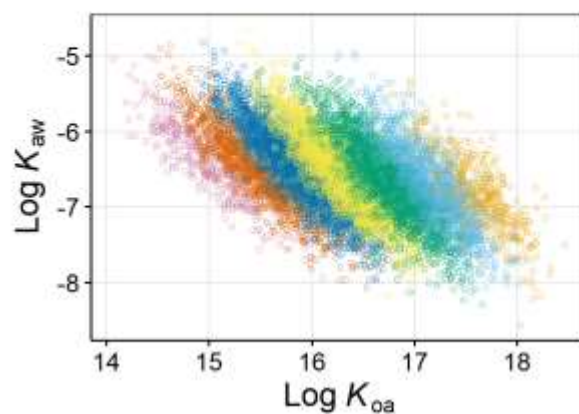
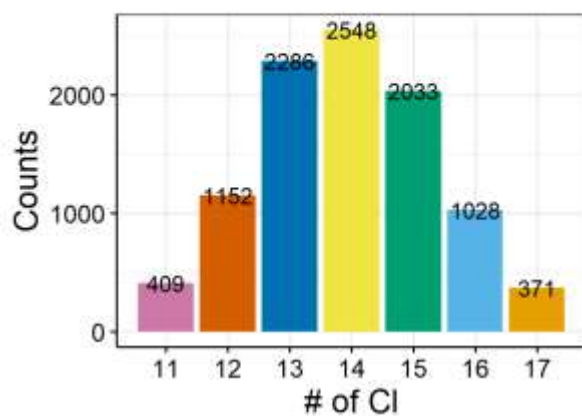
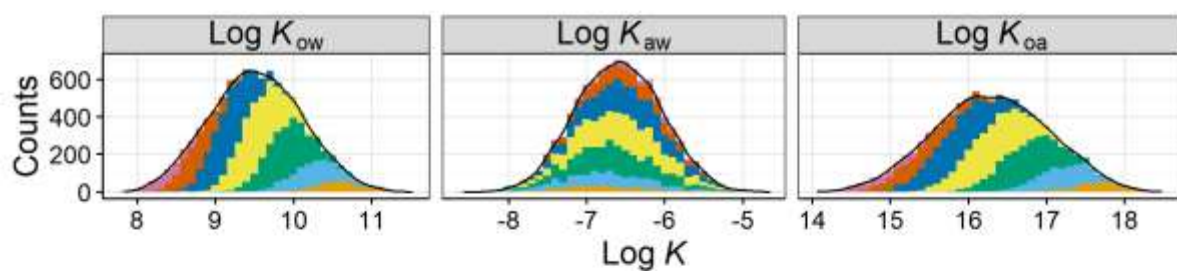
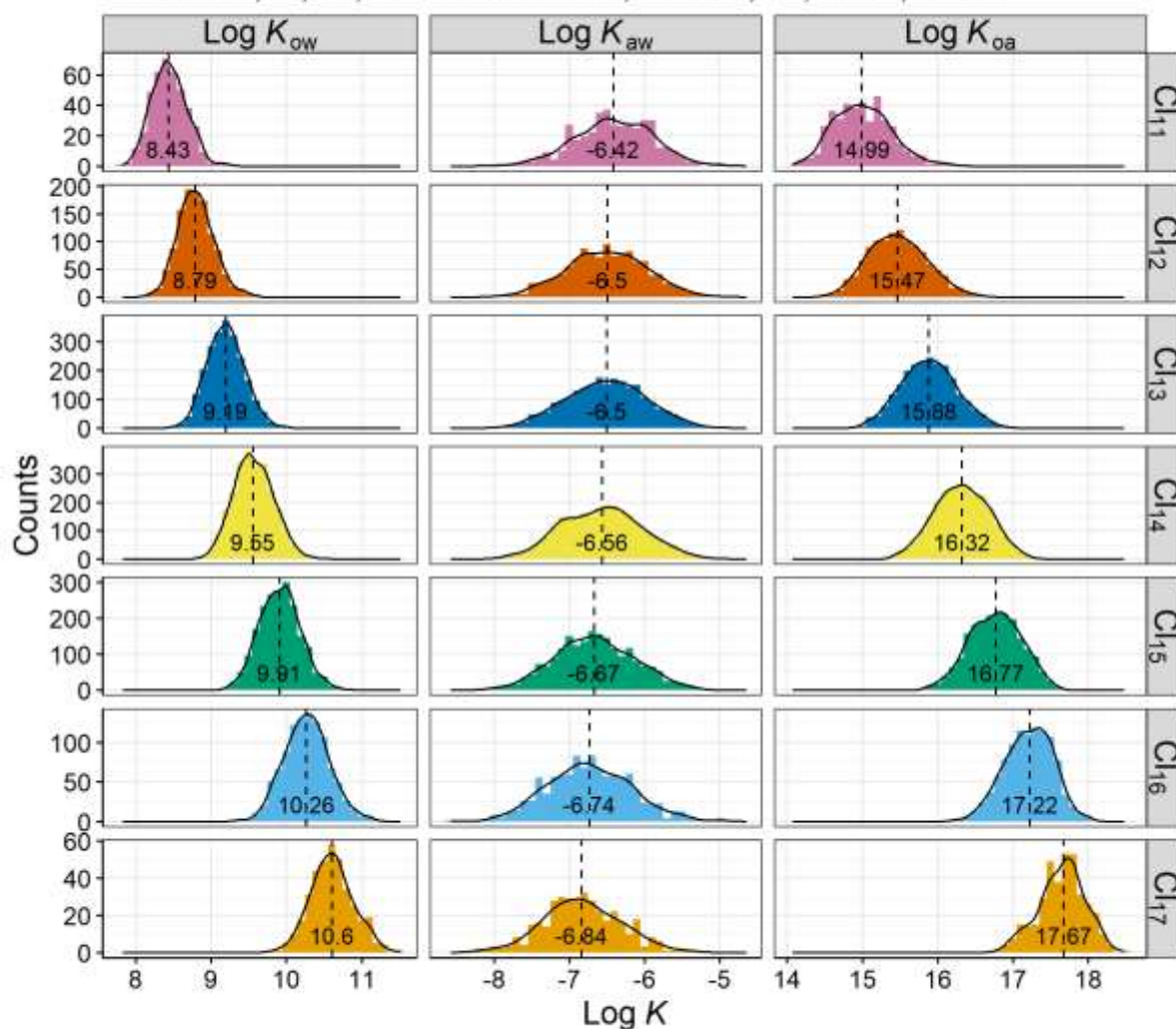
C₁₆, 60 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



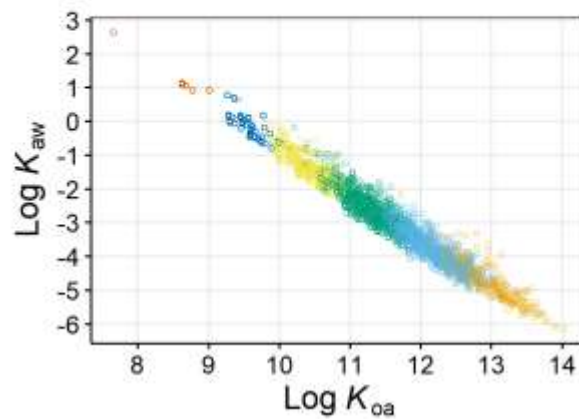
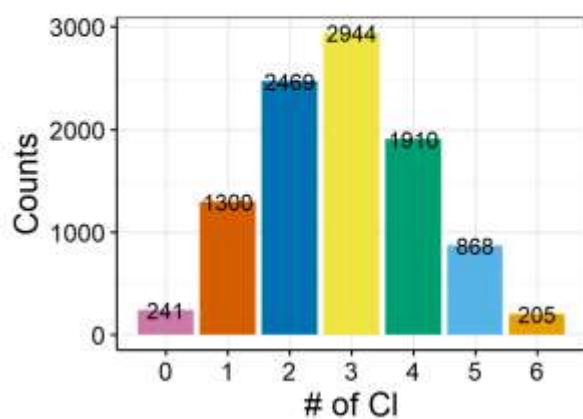
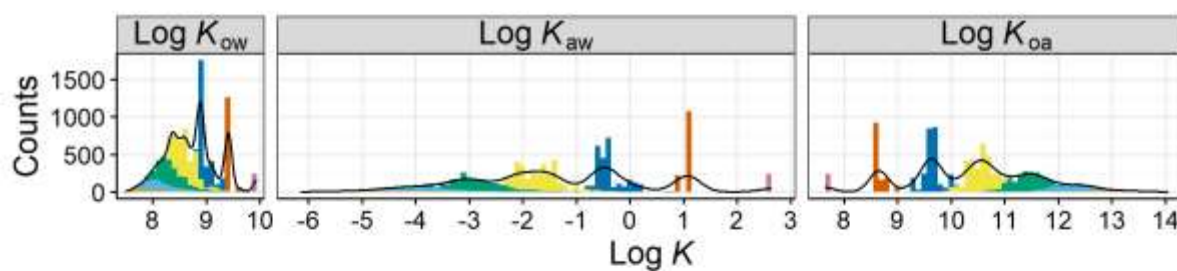
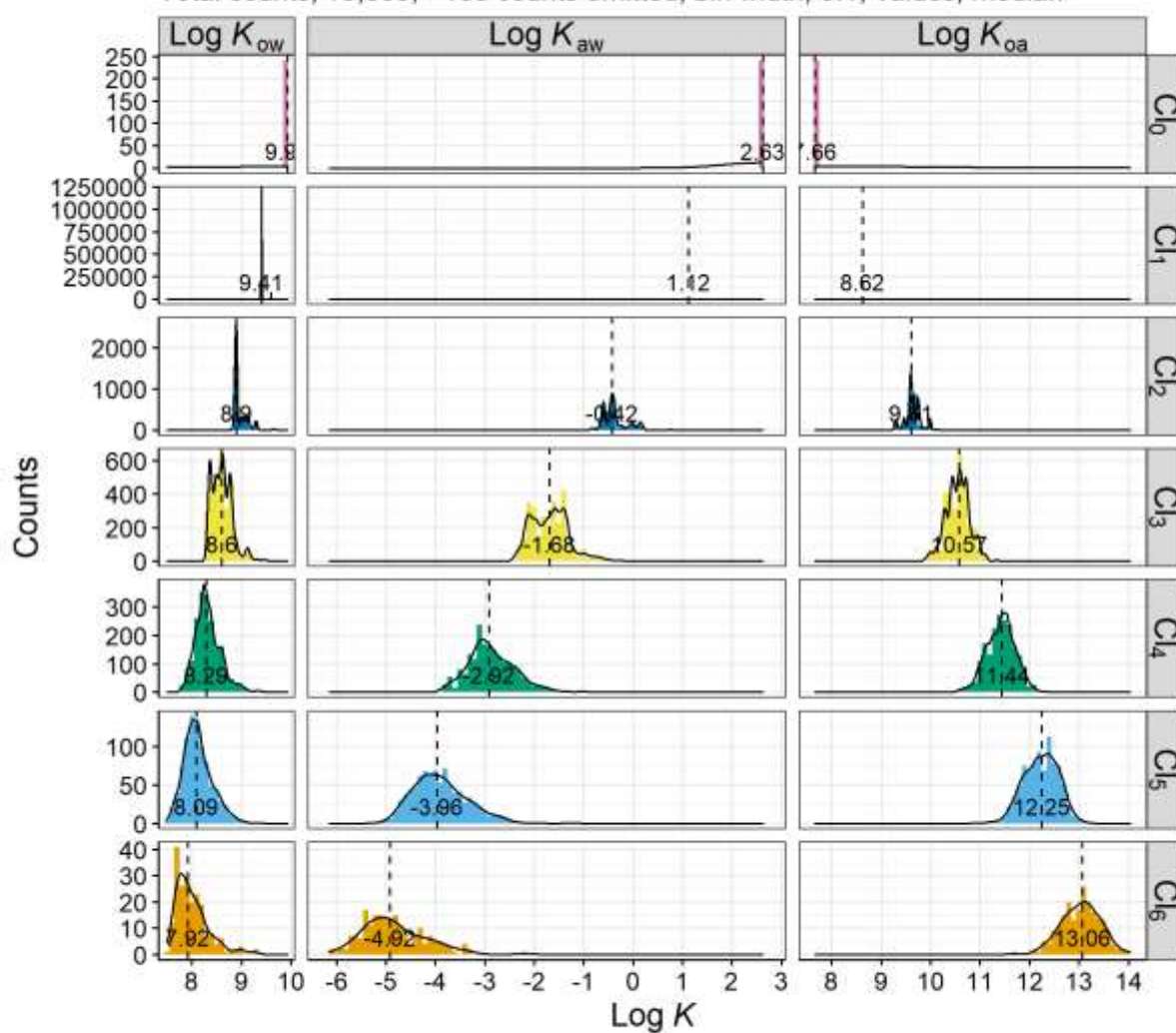
C₁₆, 70 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



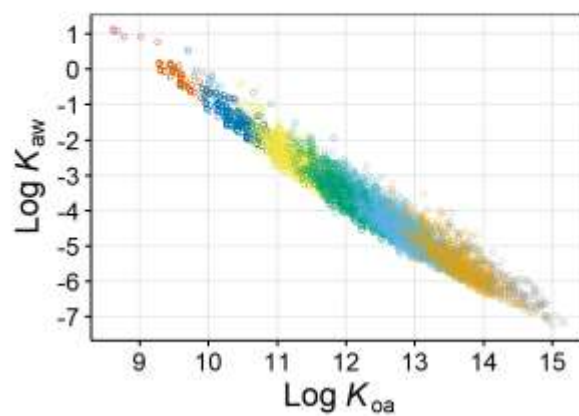
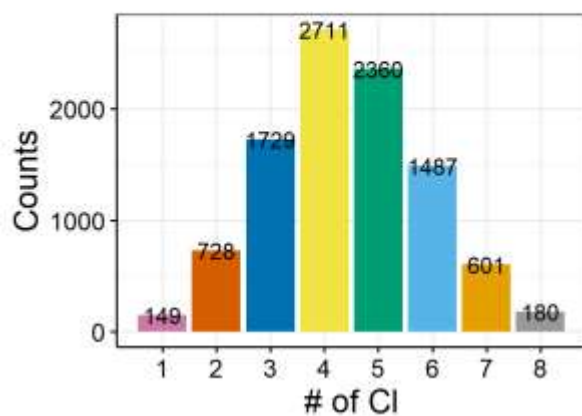
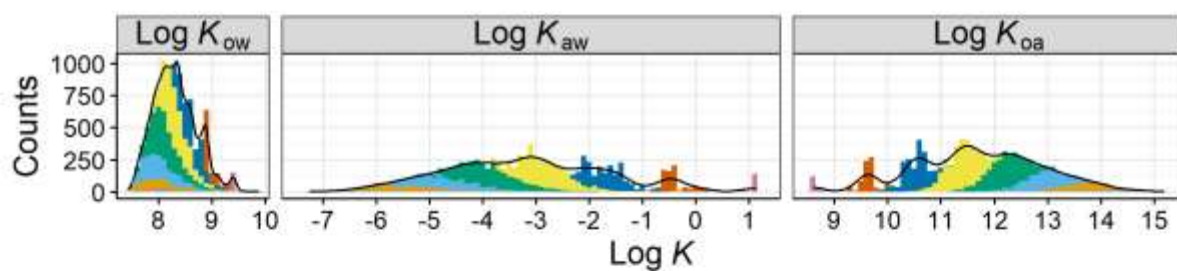
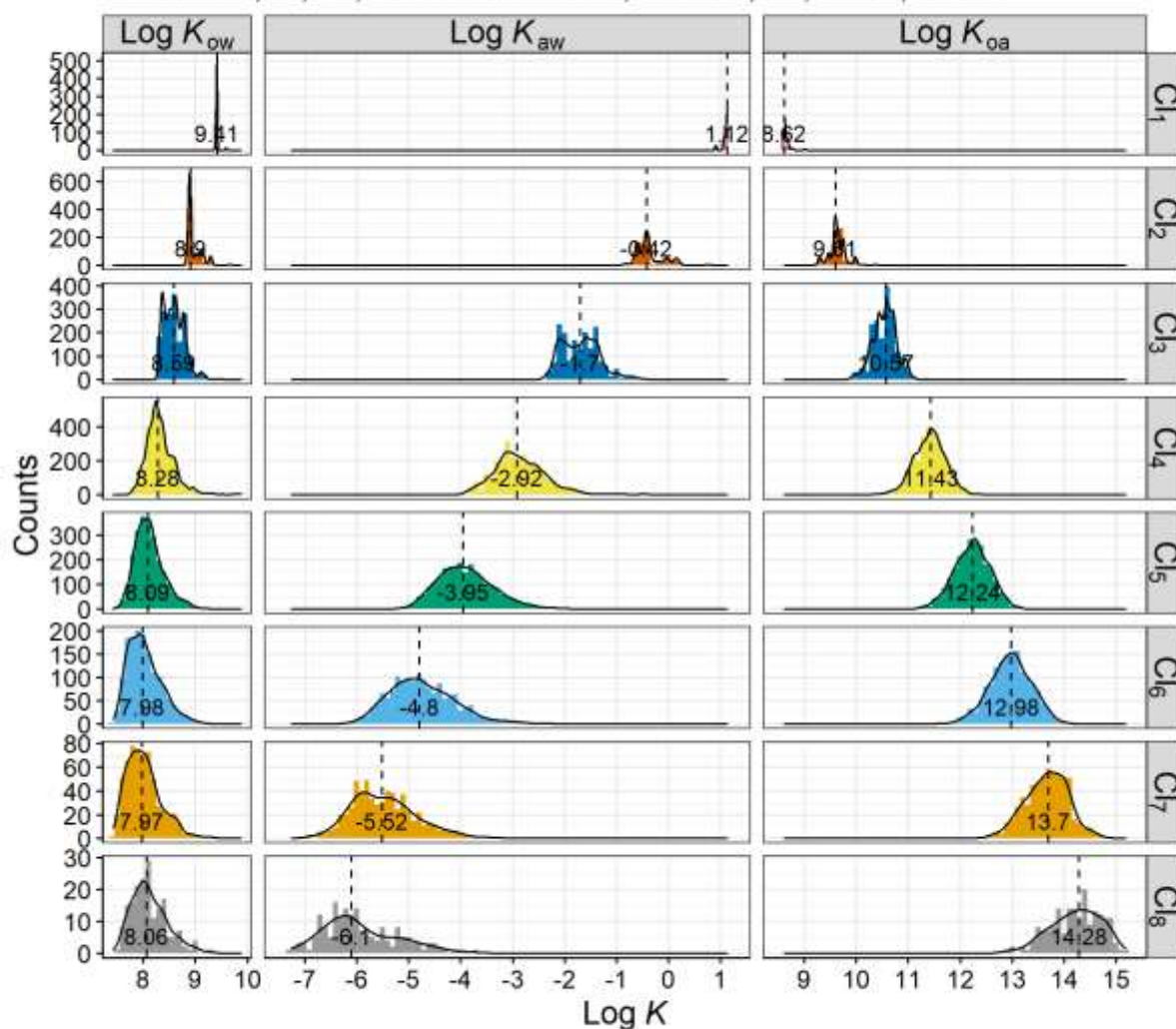
C₁₇, 30 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



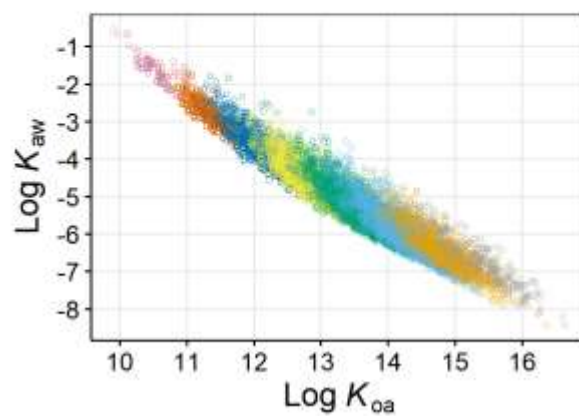
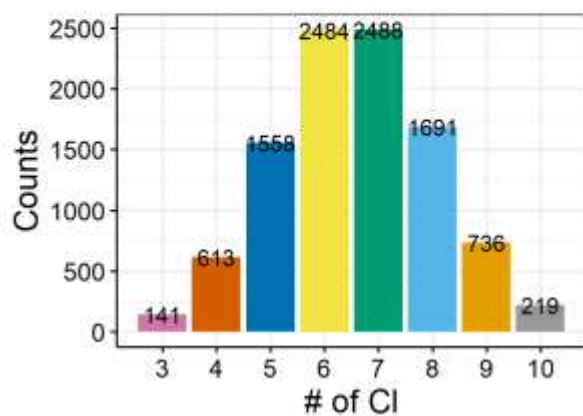
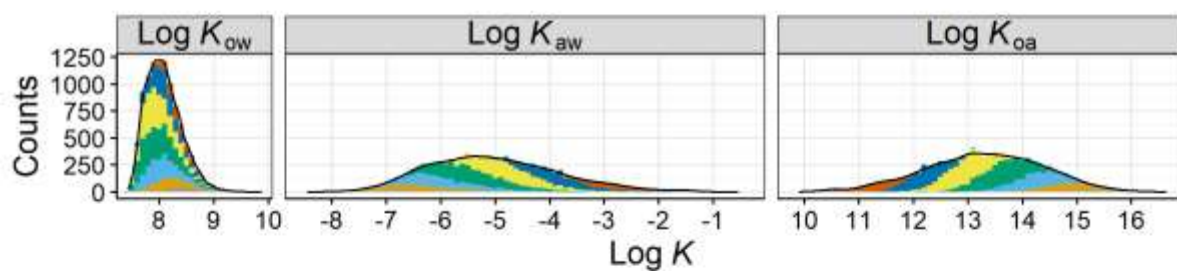
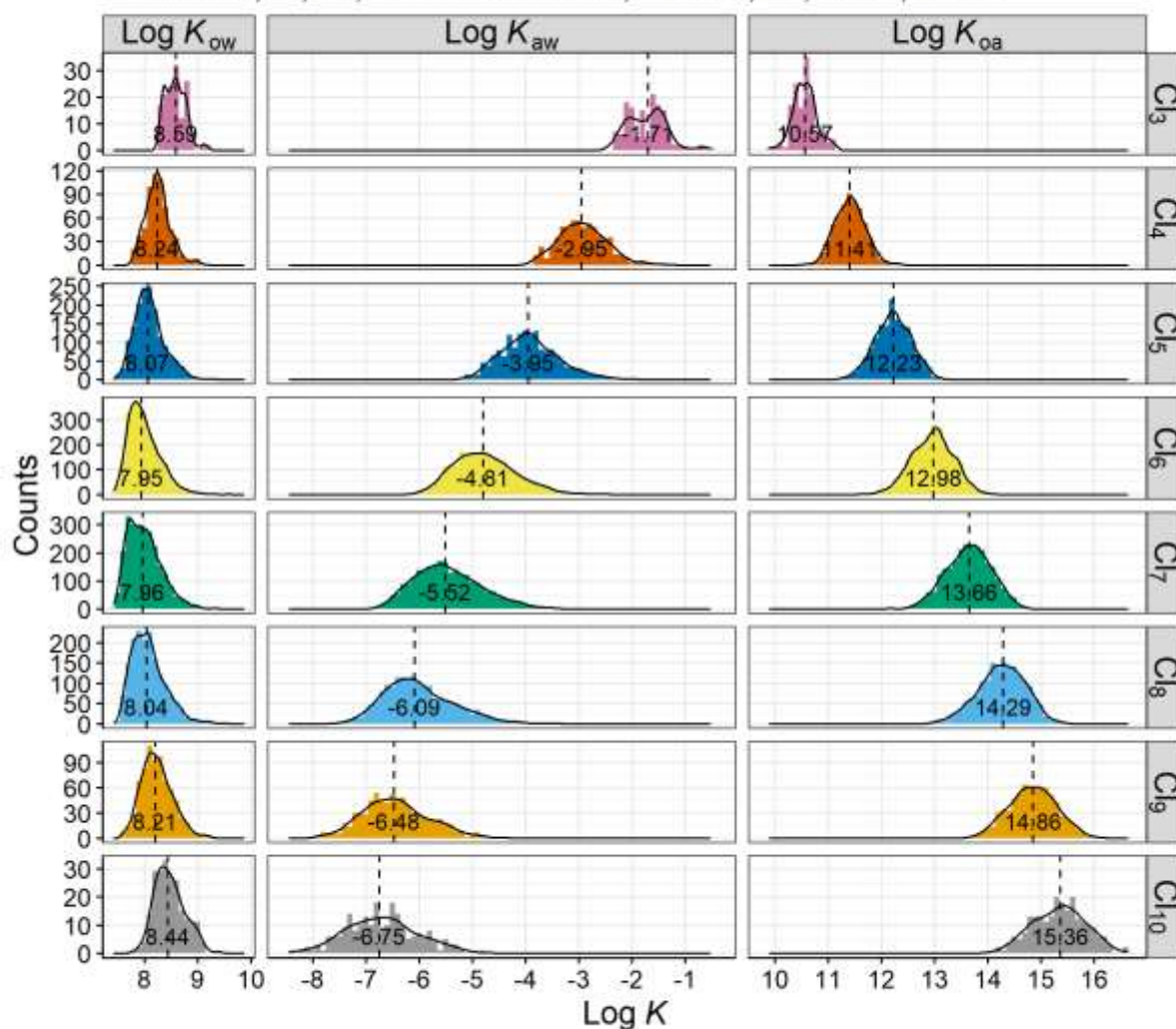
C₁₇, 40 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



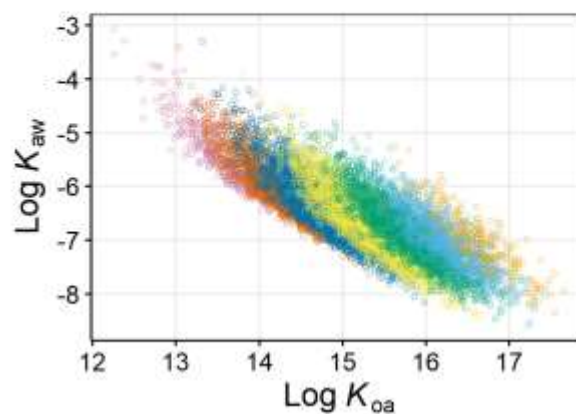
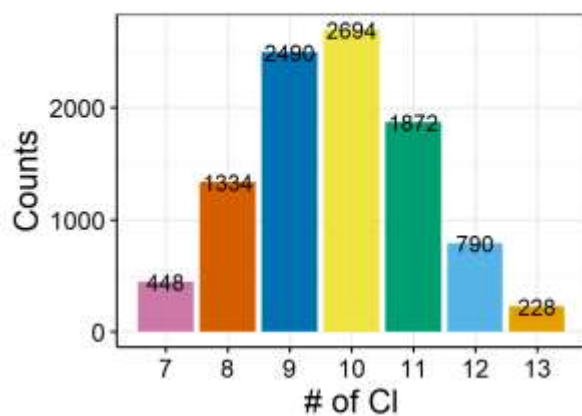
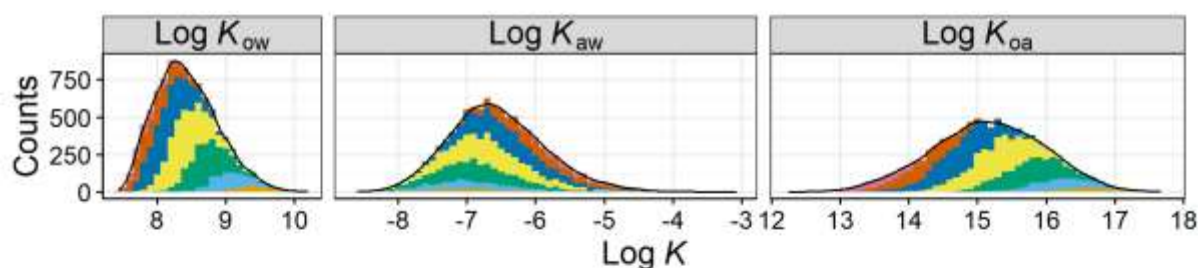
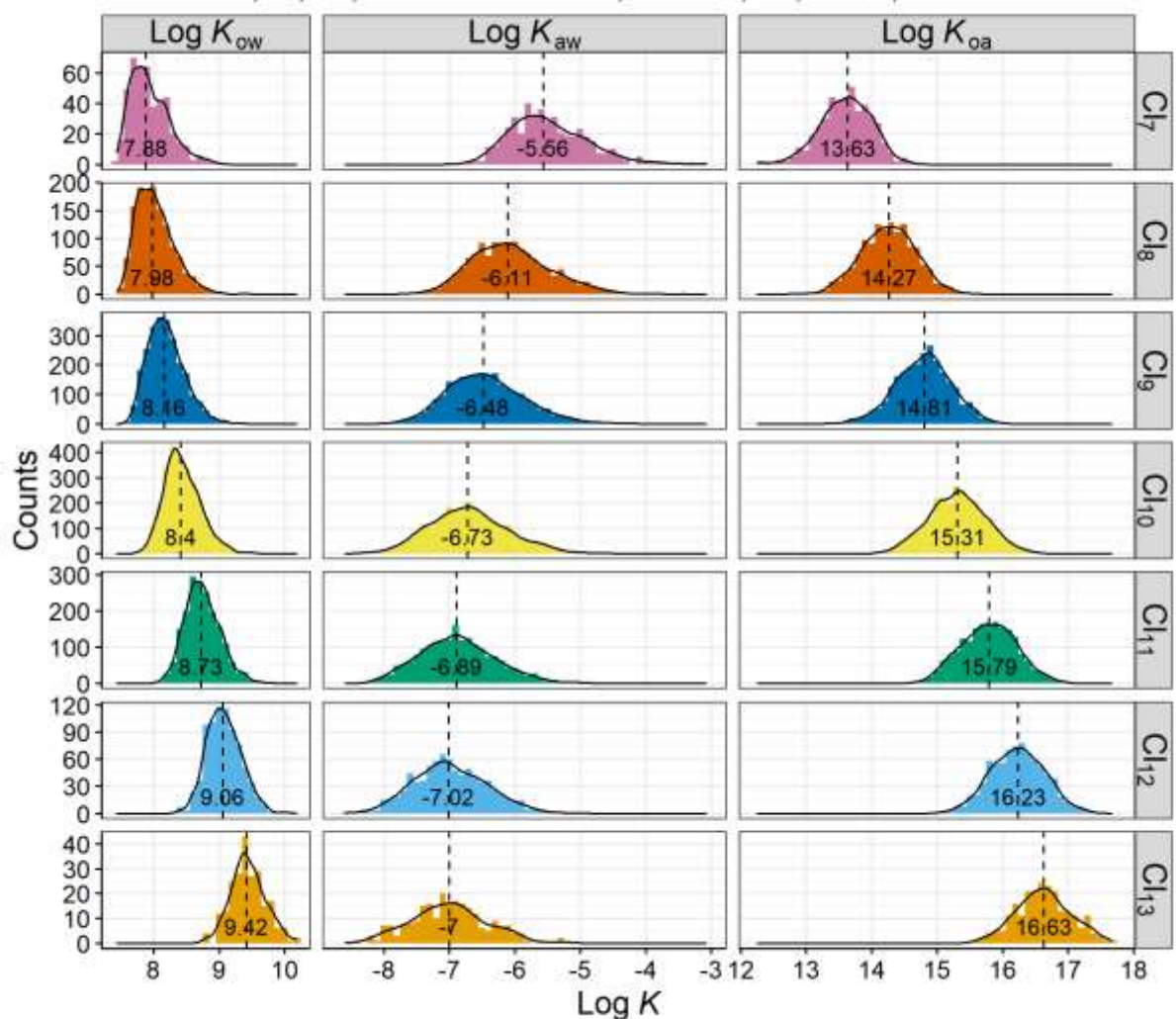
C₁₇, 50 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



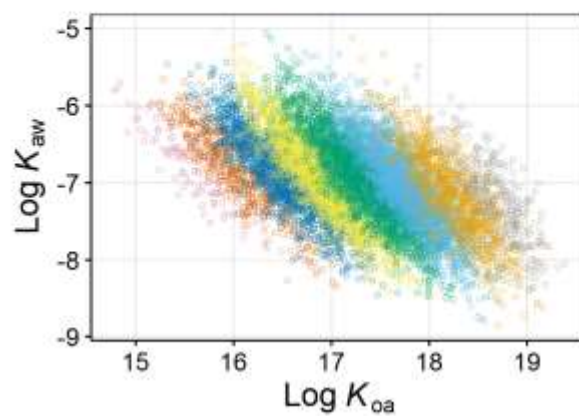
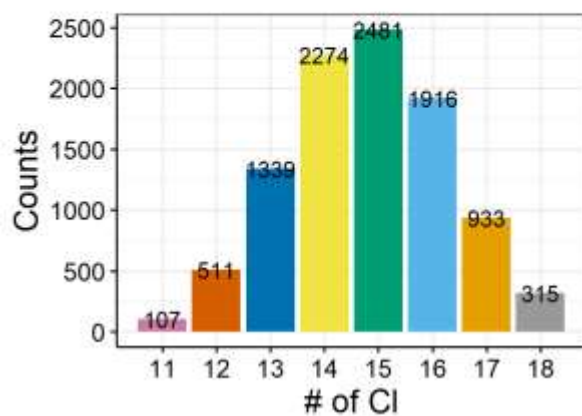
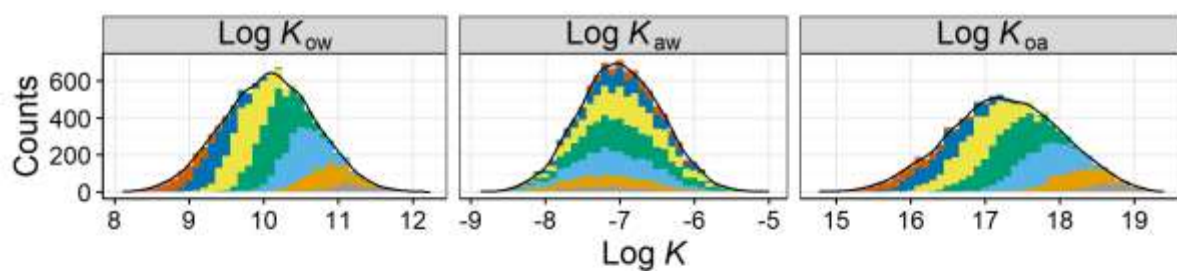
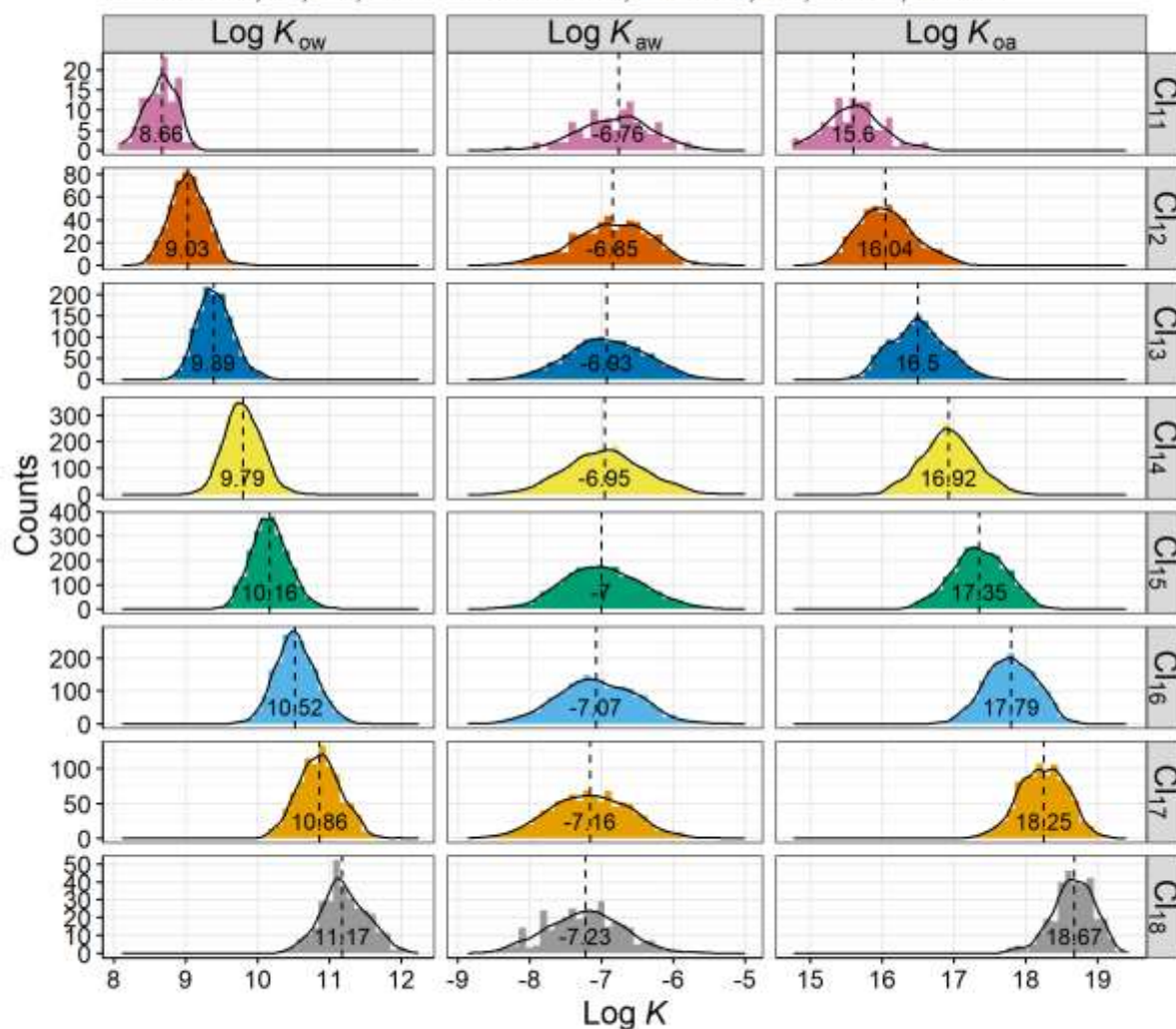
C₁₇, 60 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



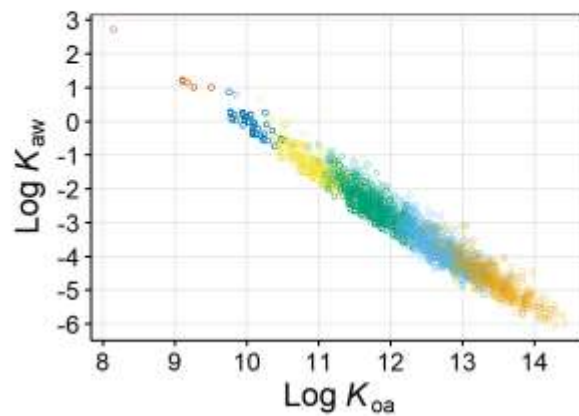
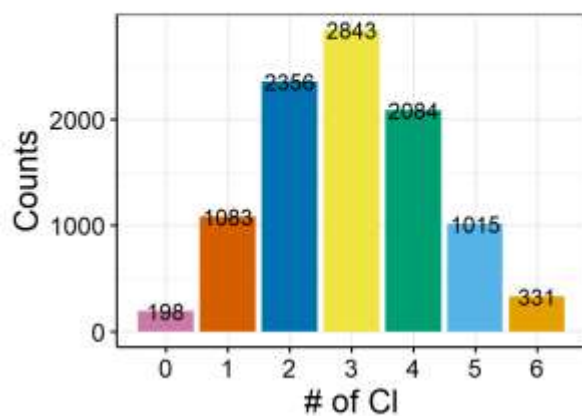
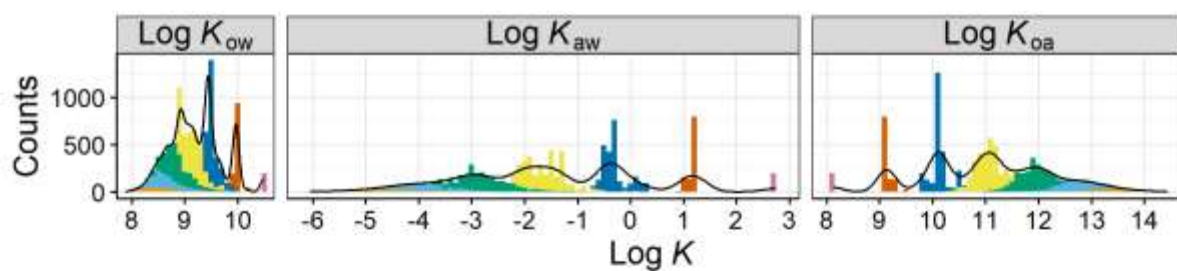
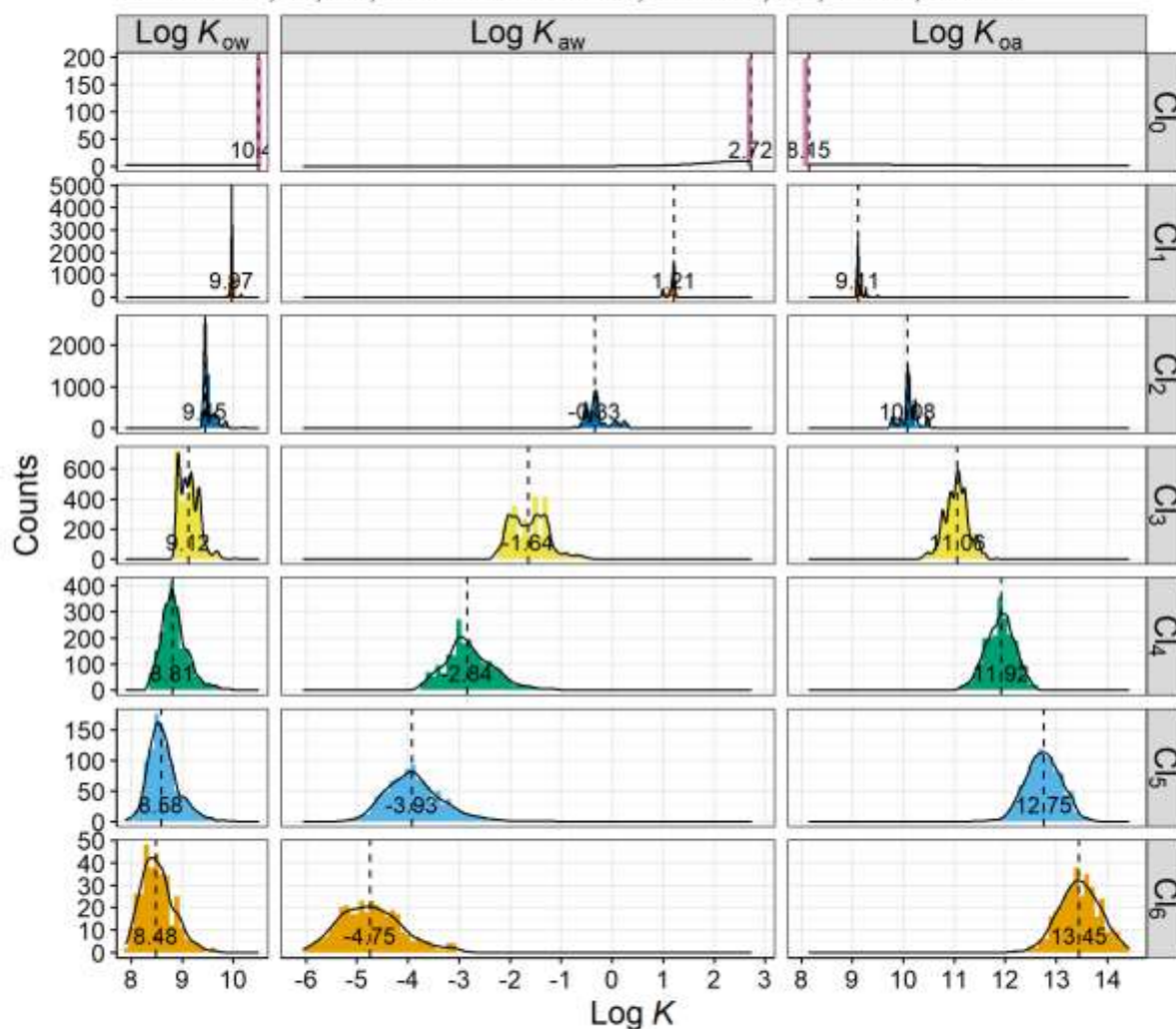
C₁₇, 70 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



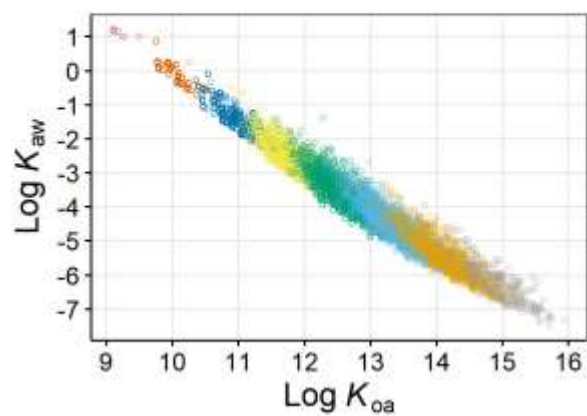
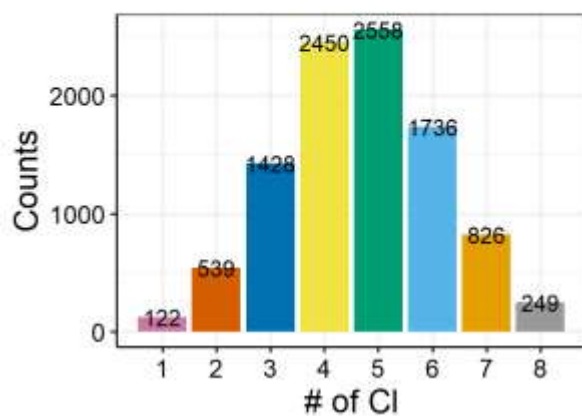
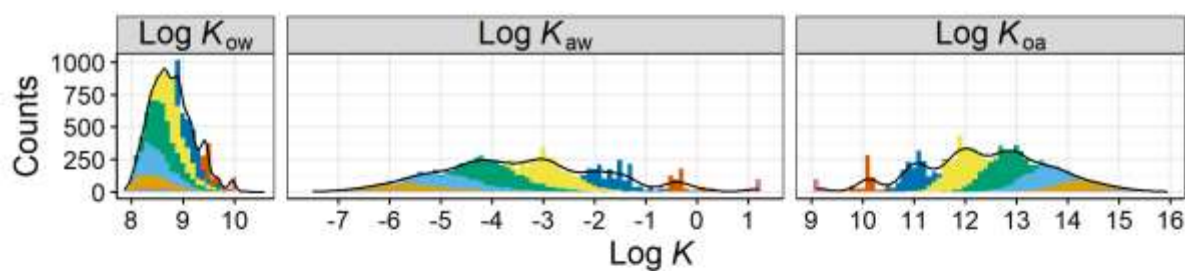
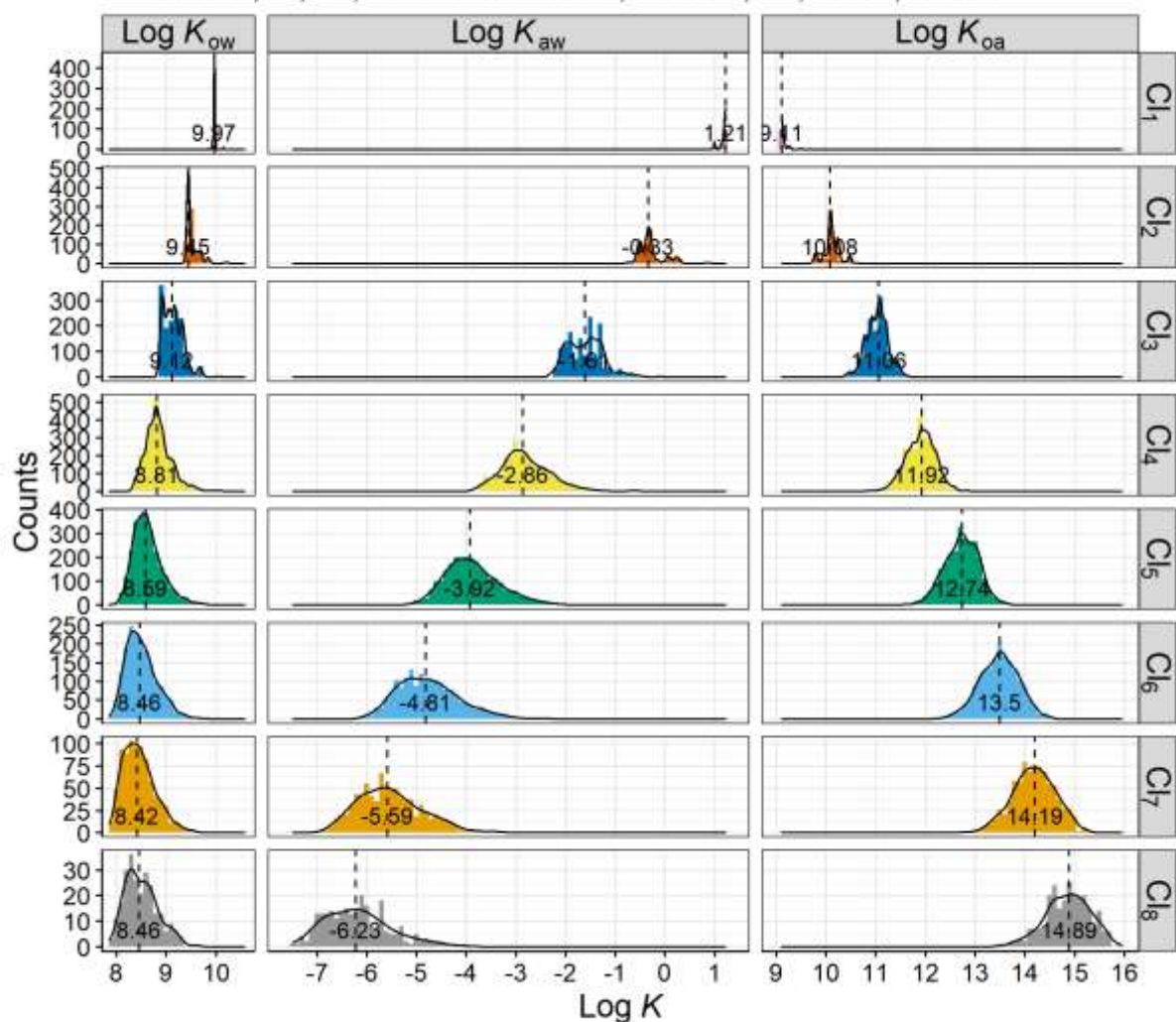
C₁₈, 30 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



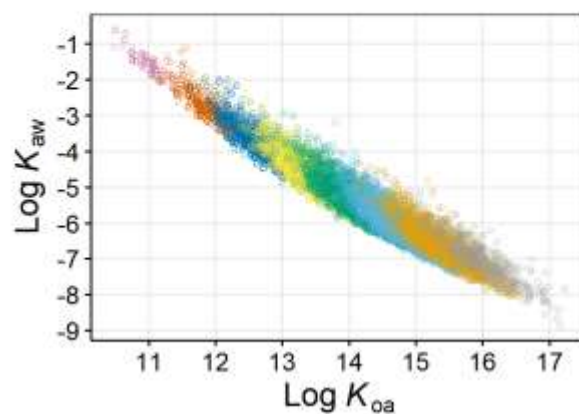
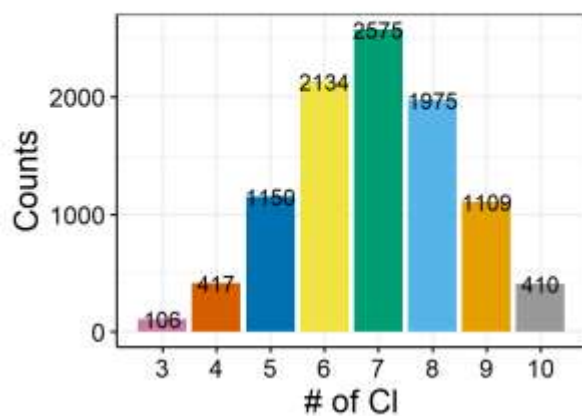
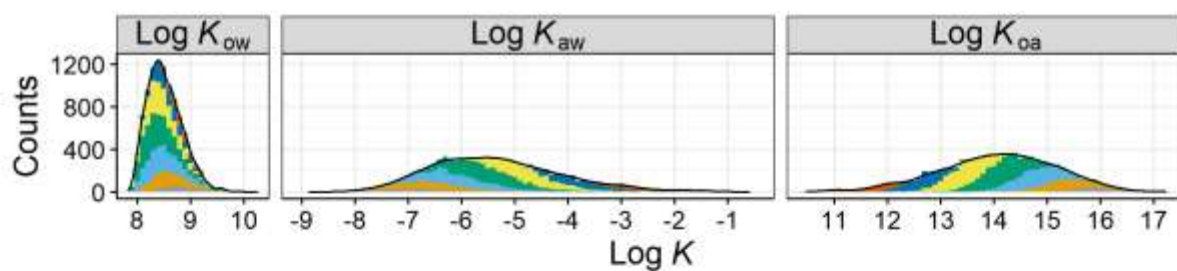
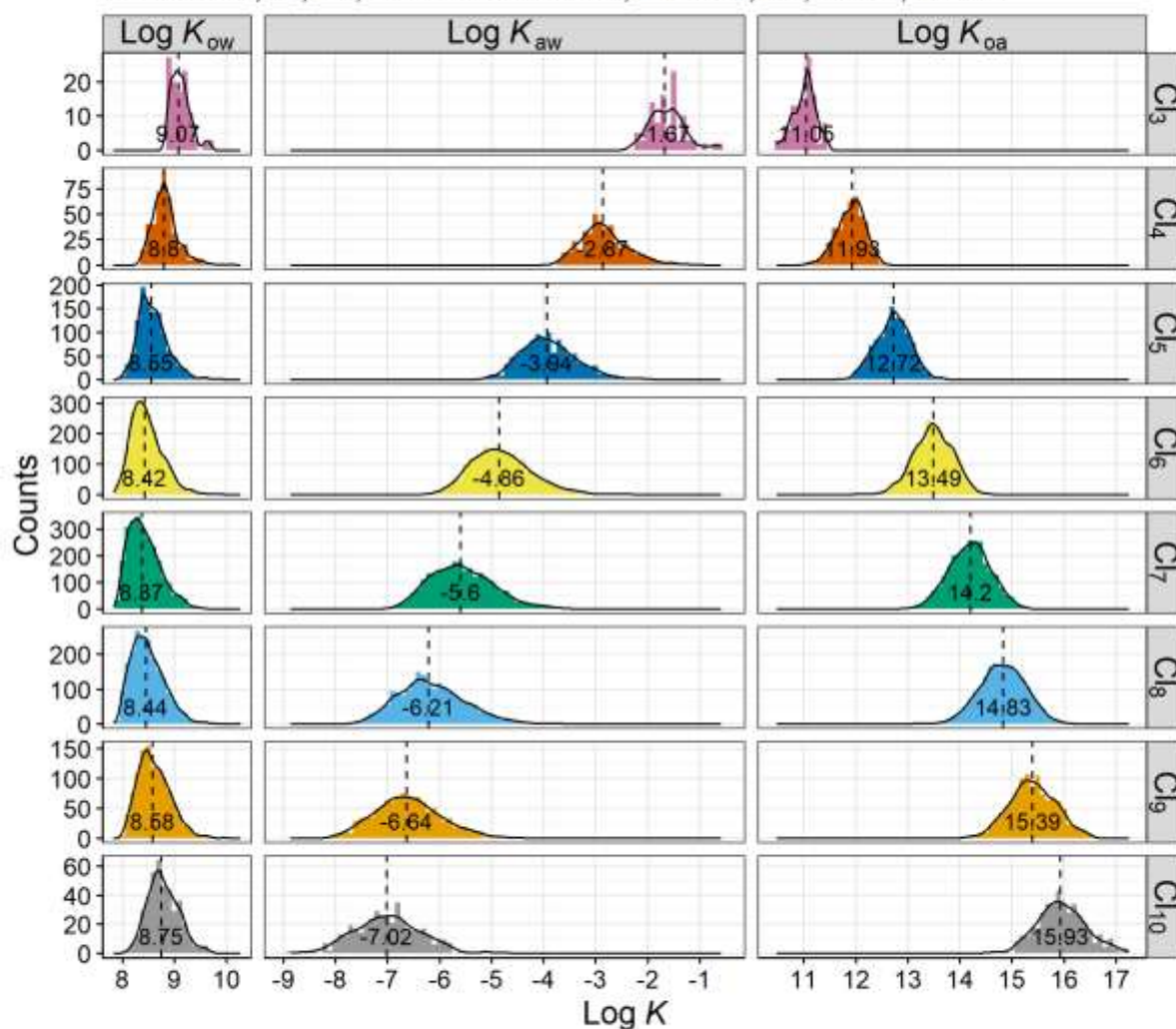
C₁₈, 40 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



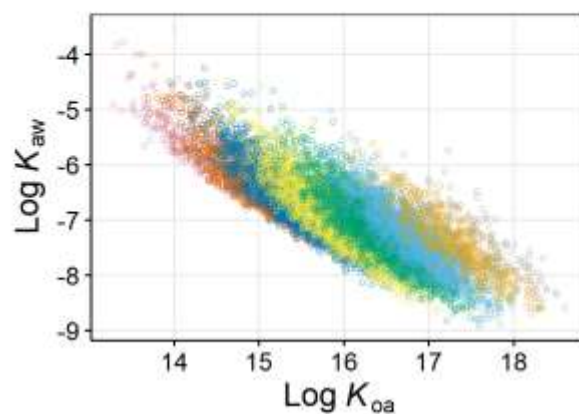
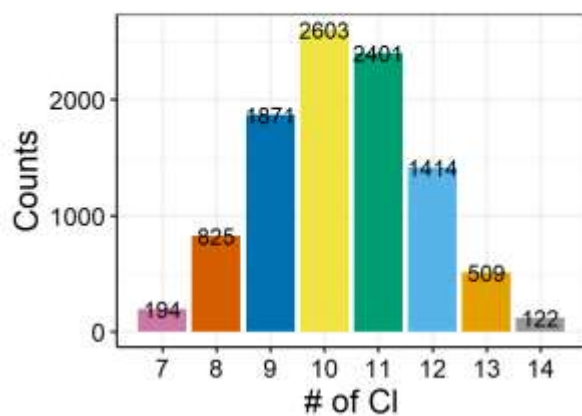
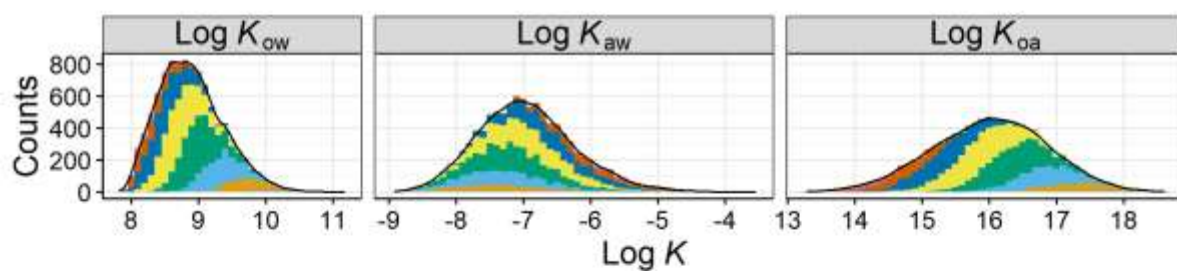
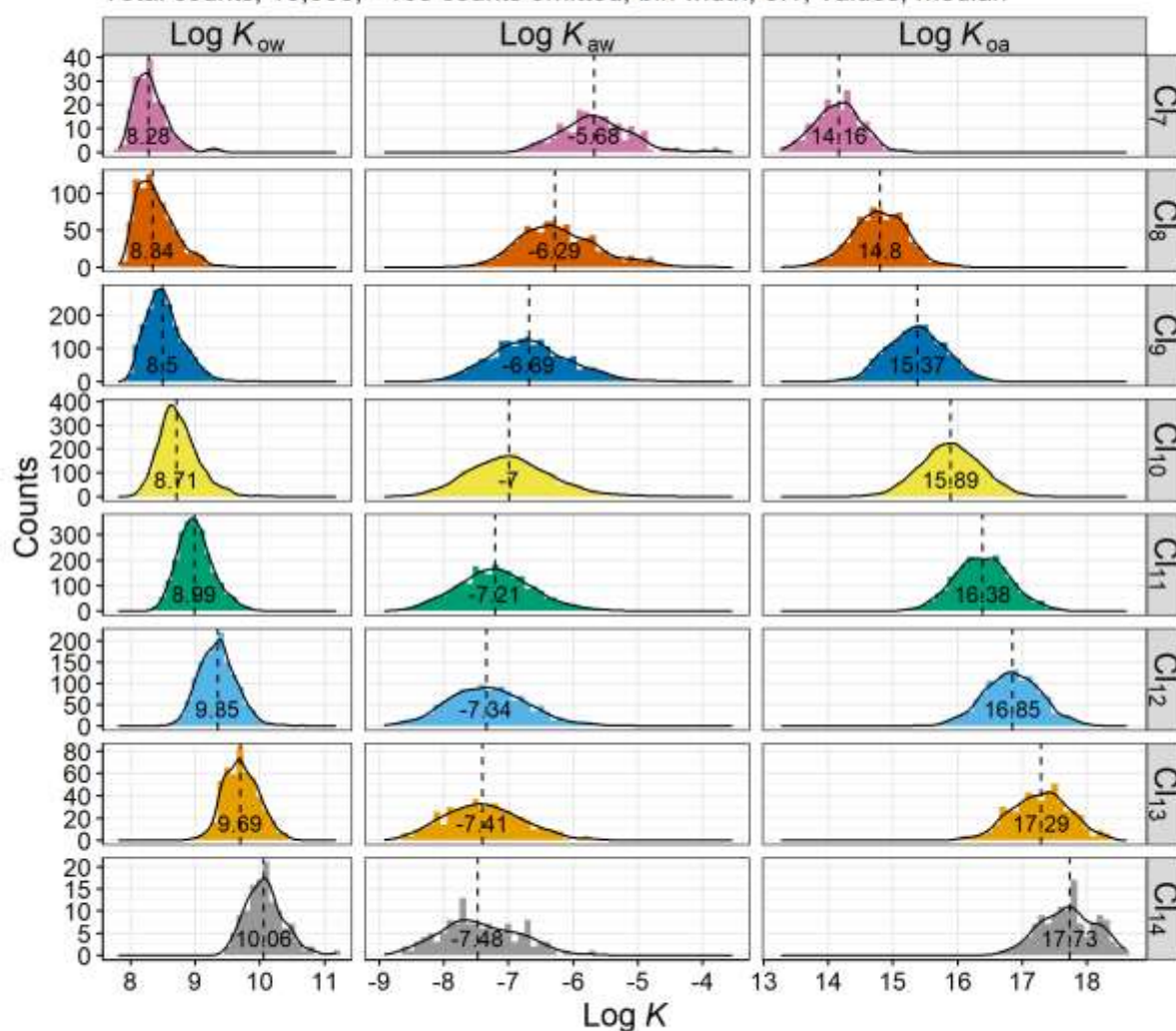
C₁₈, 50 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



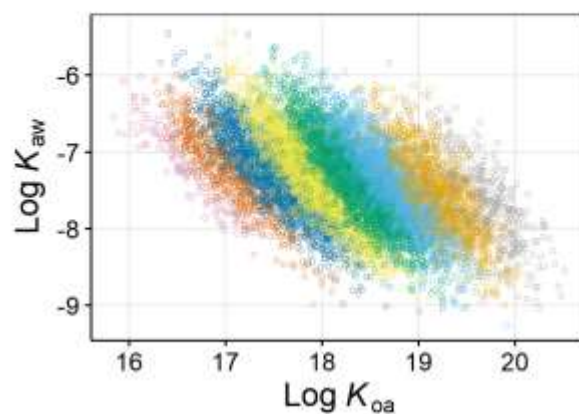
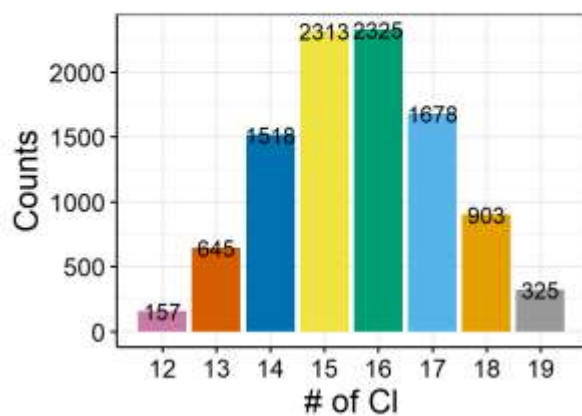
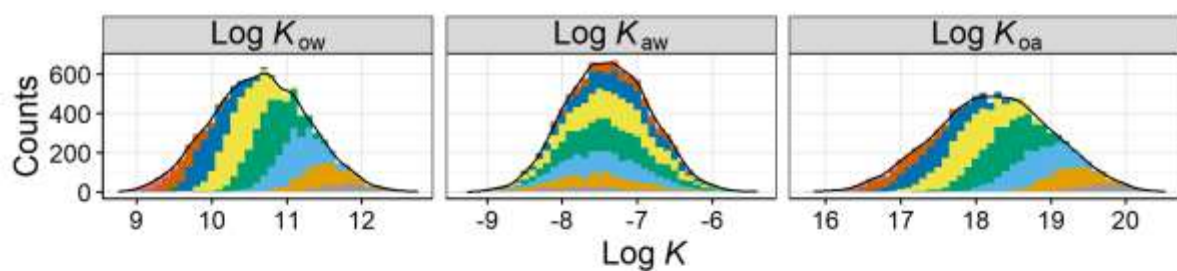
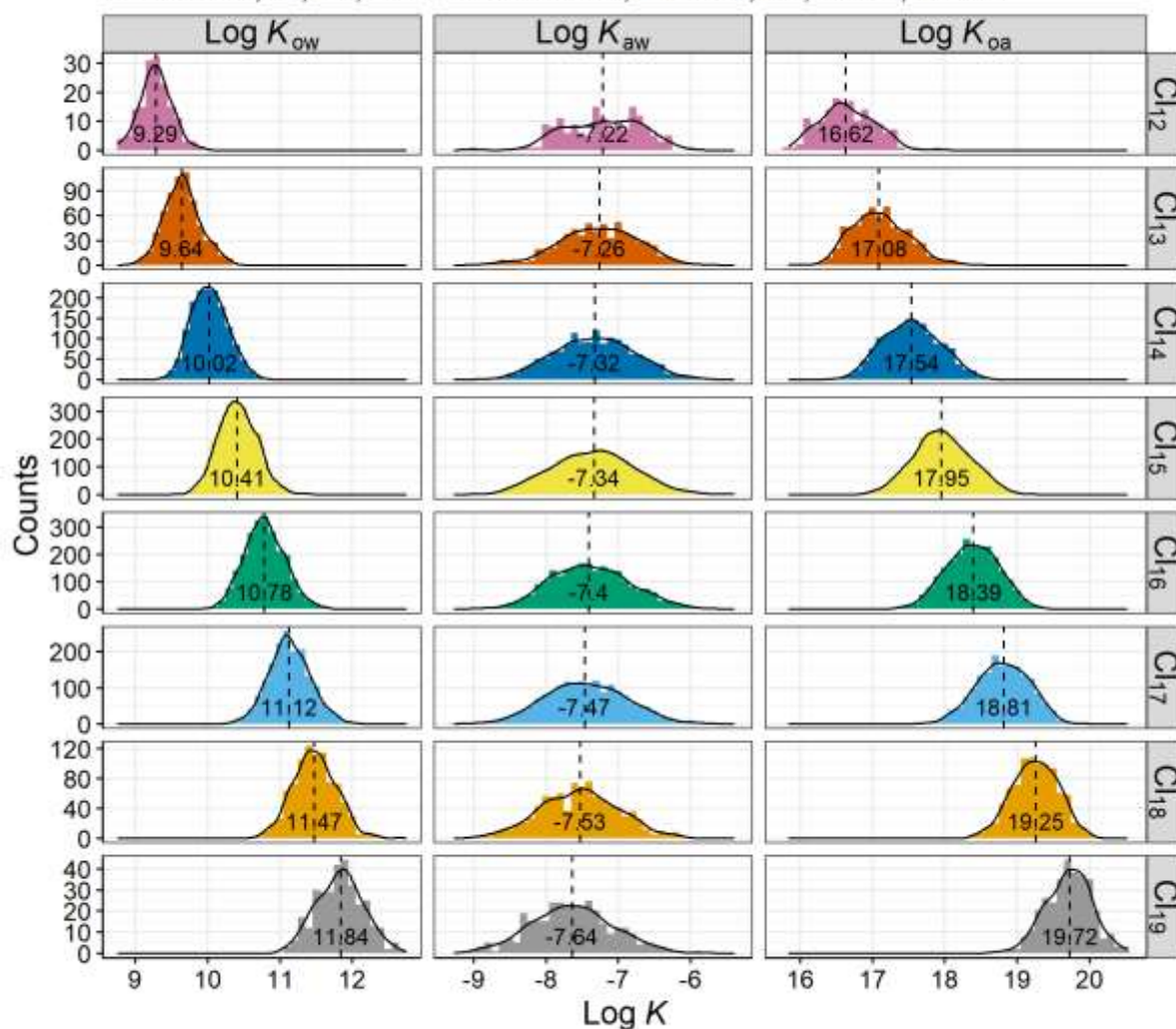
C₁₈, 60 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



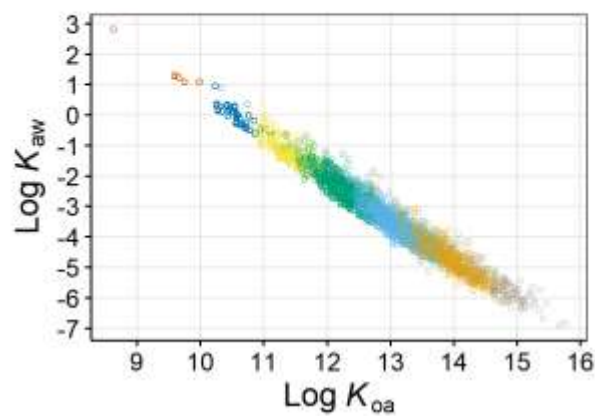
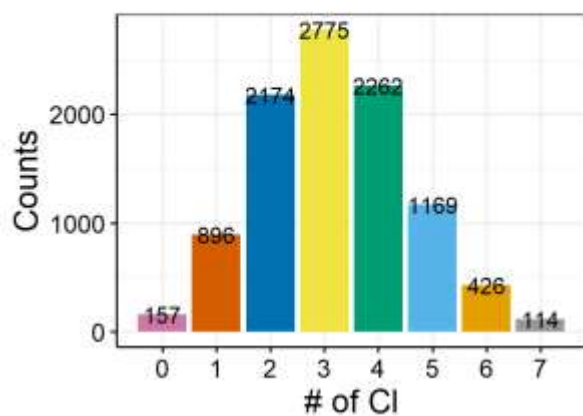
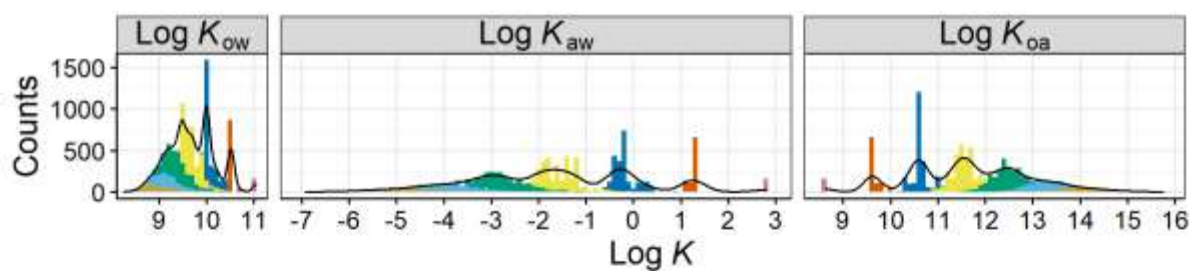
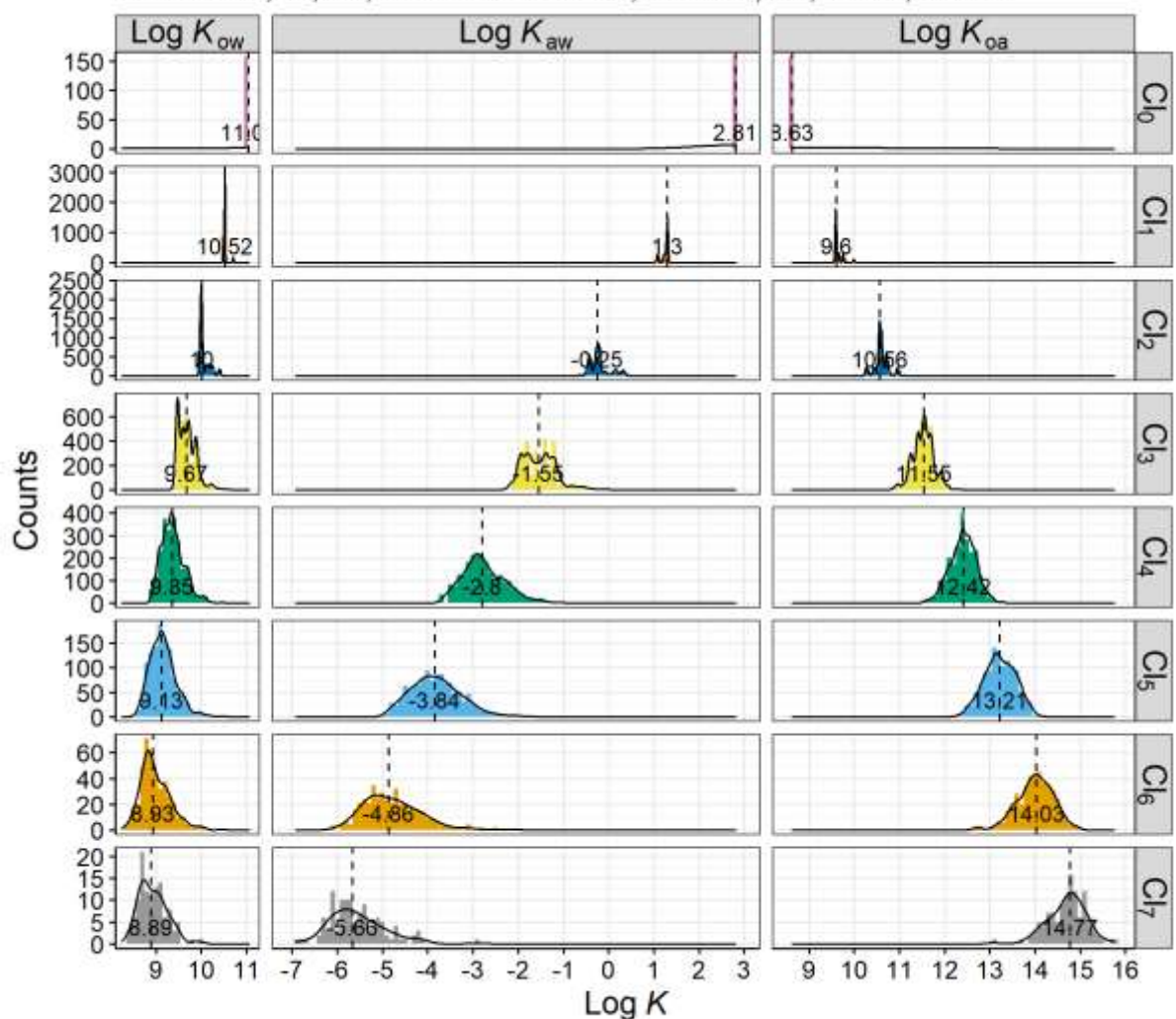
C₁₈, 70 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



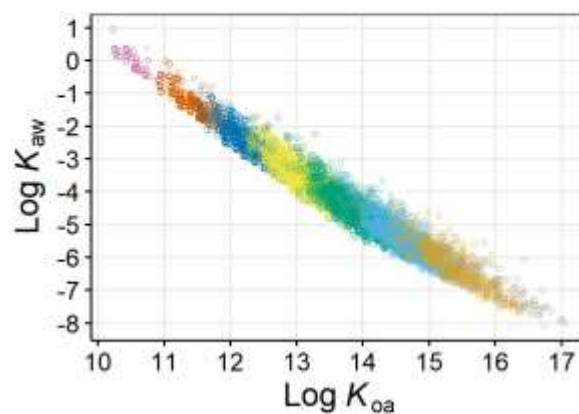
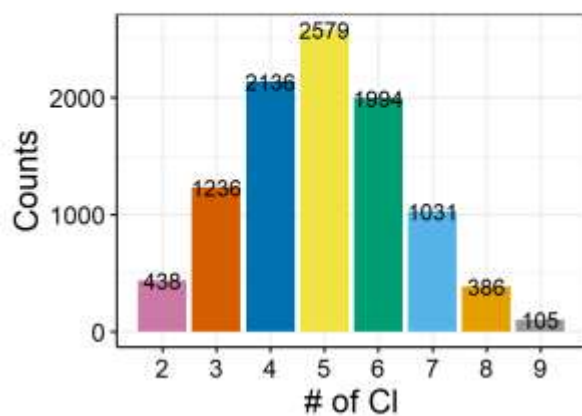
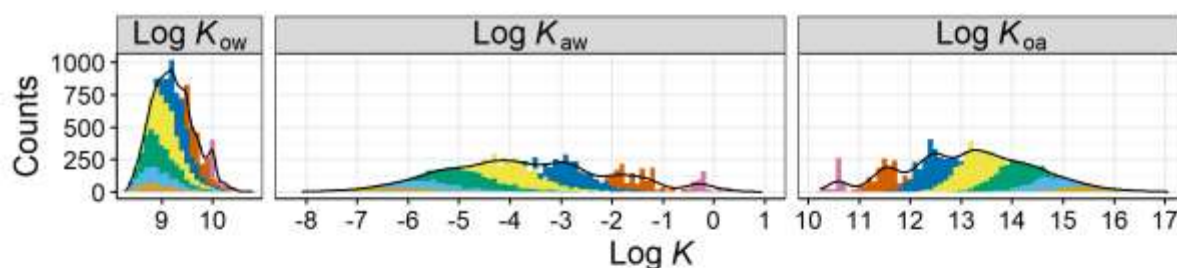
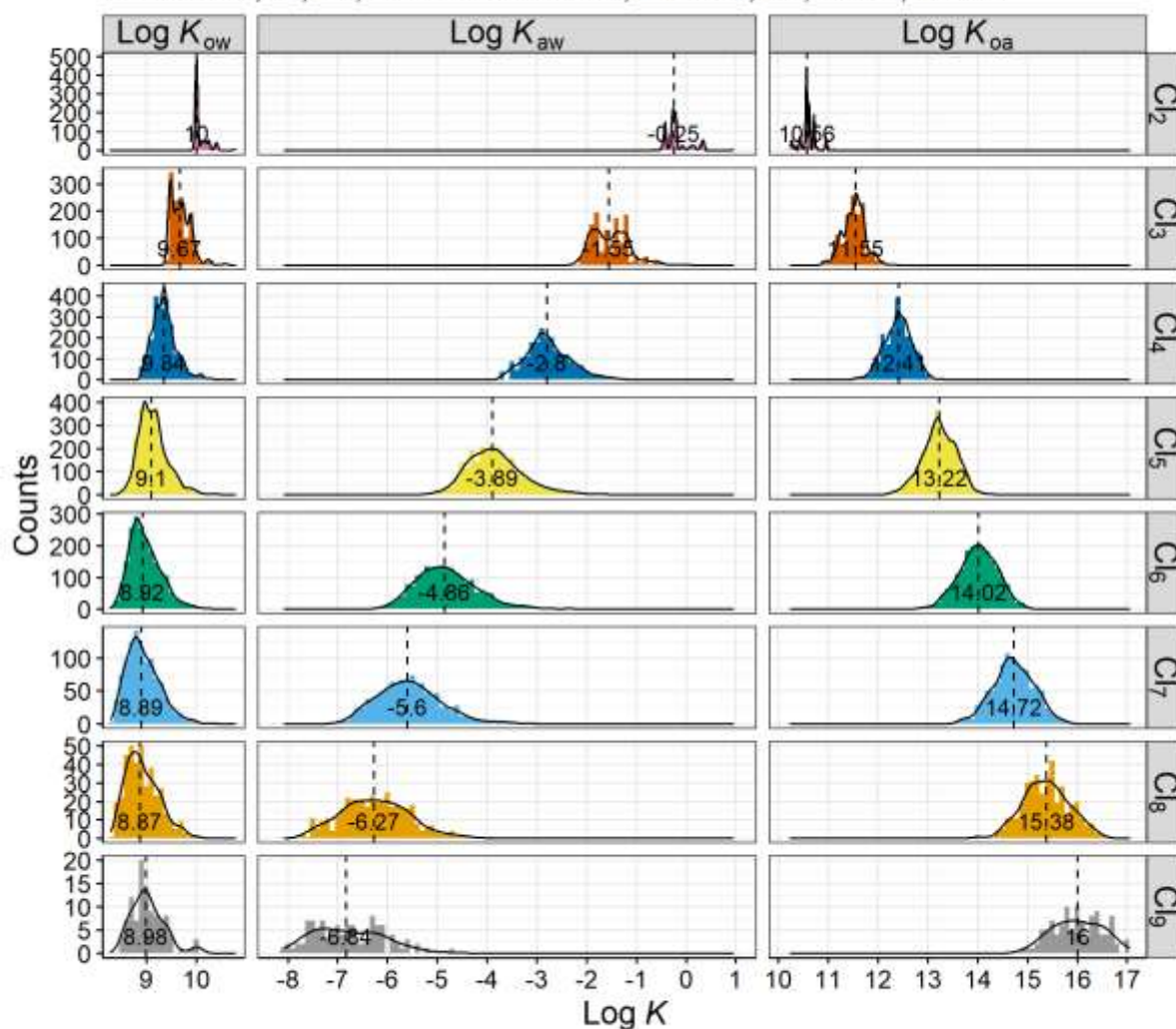
C₁₉, 30 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



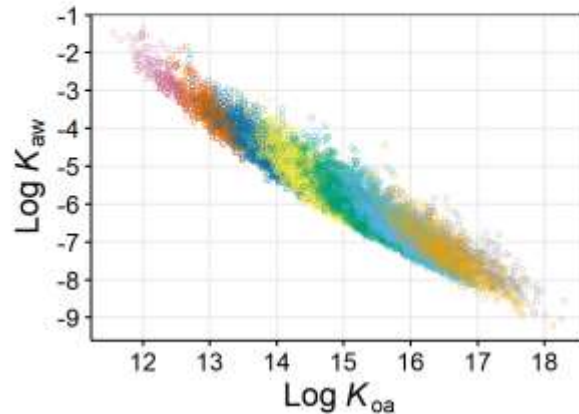
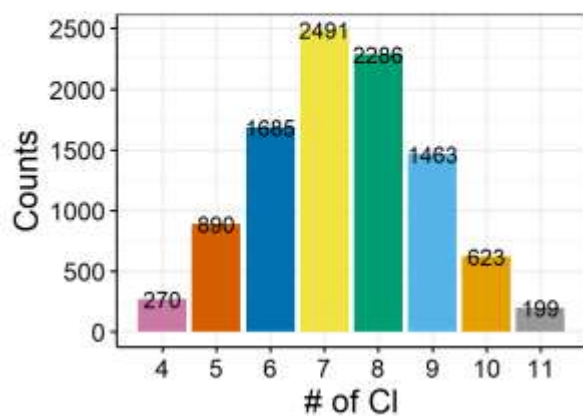
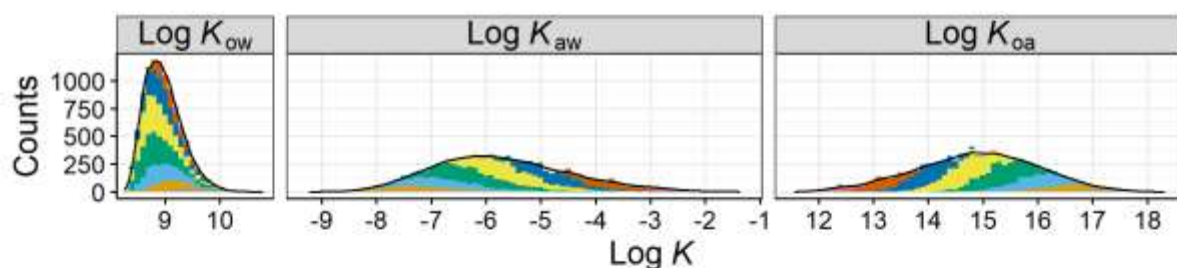
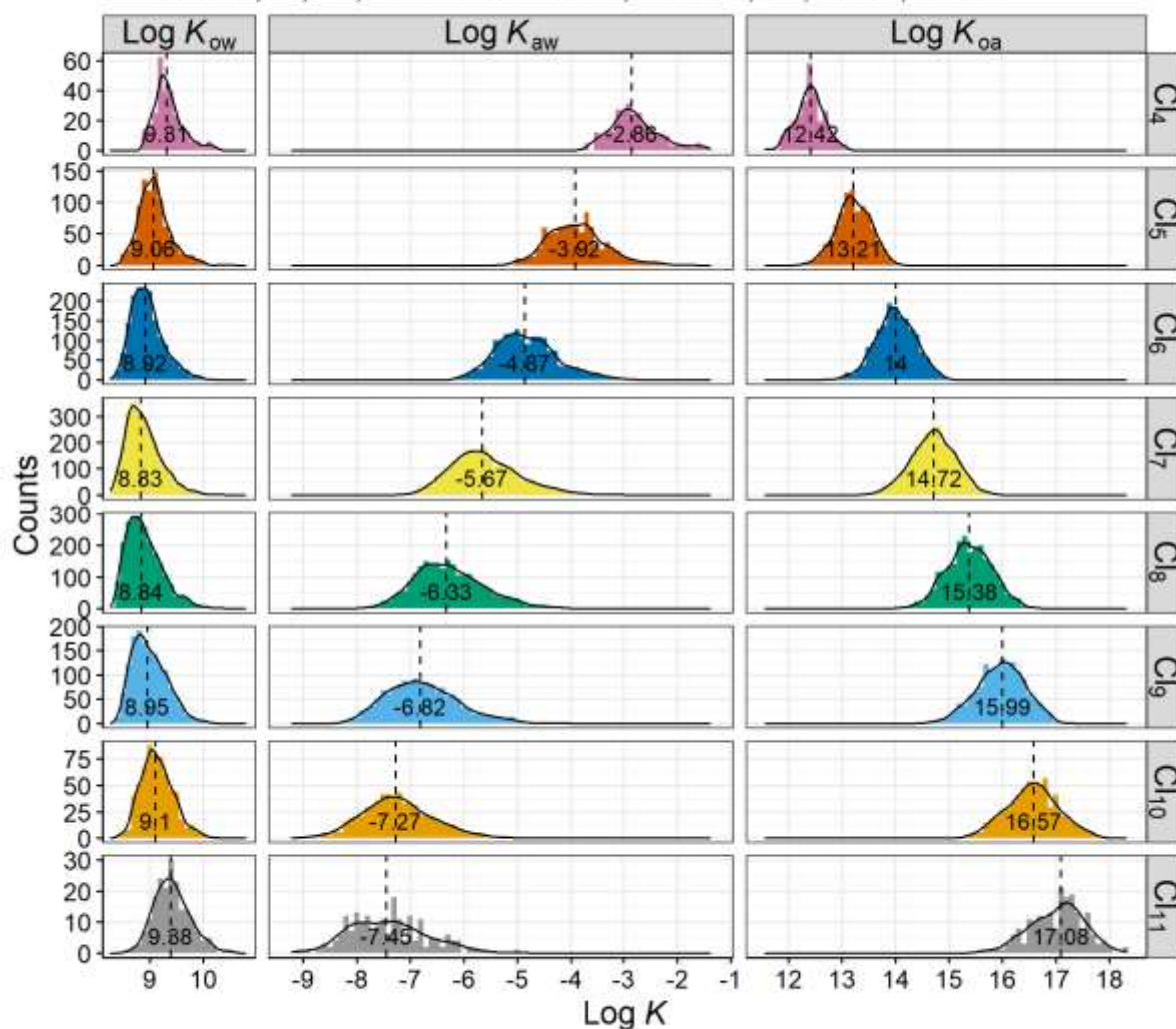
C₁₉, 40 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



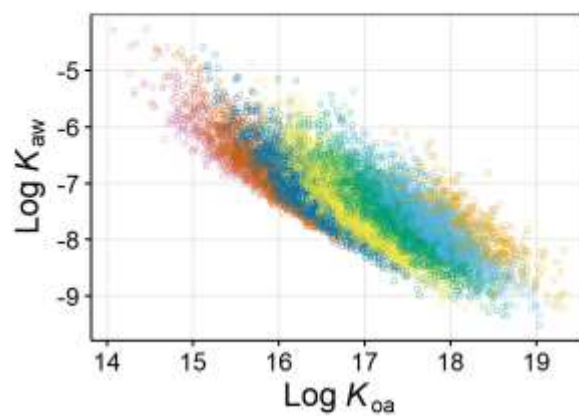
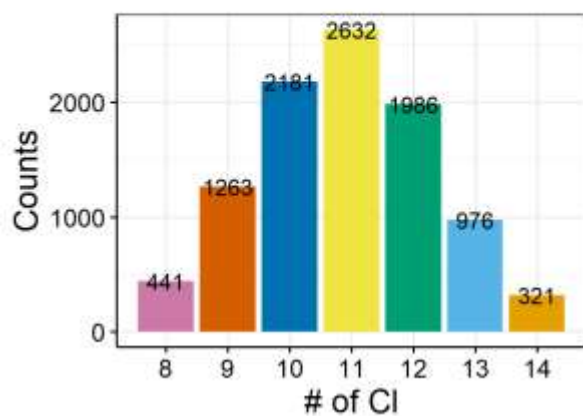
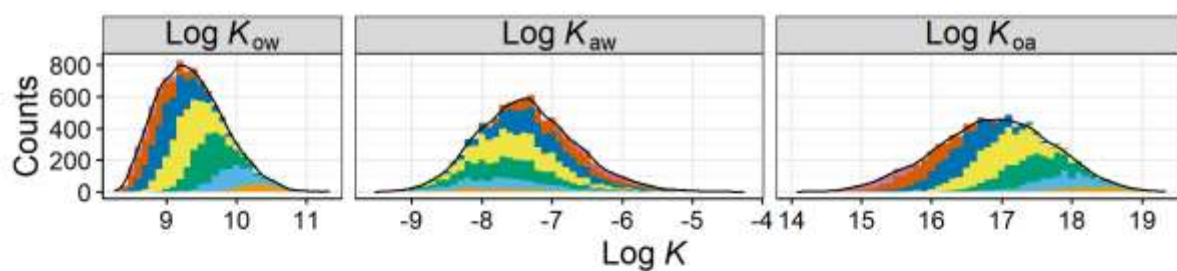
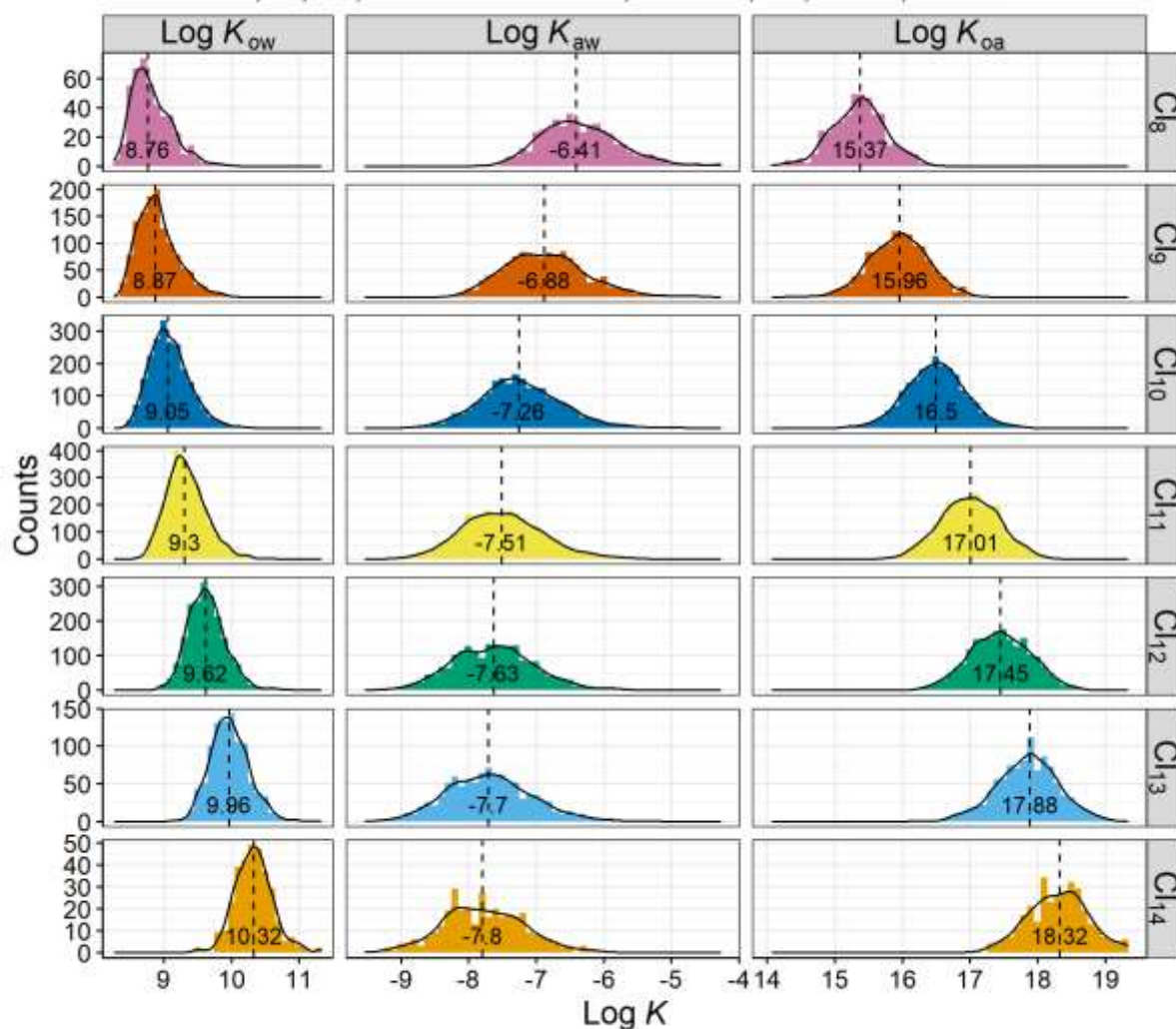
C₁₉, 50 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



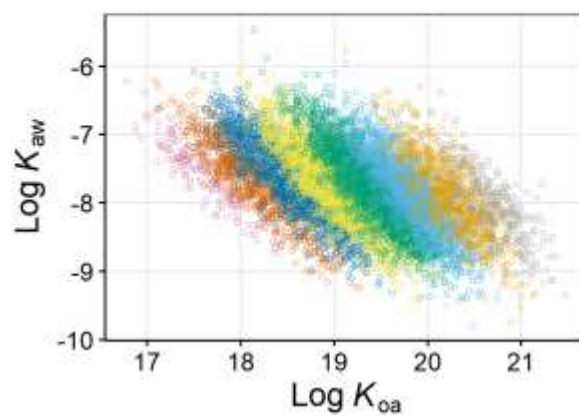
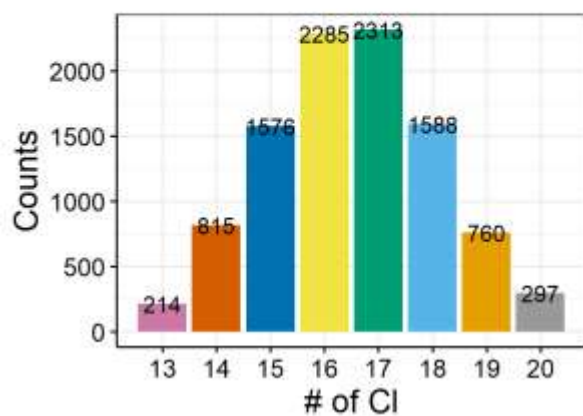
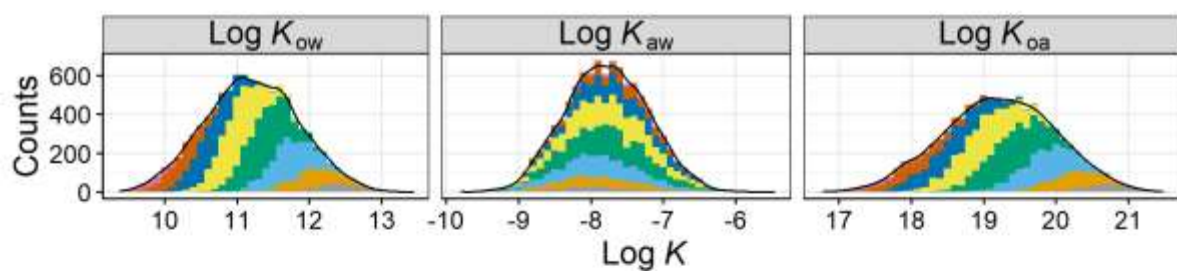
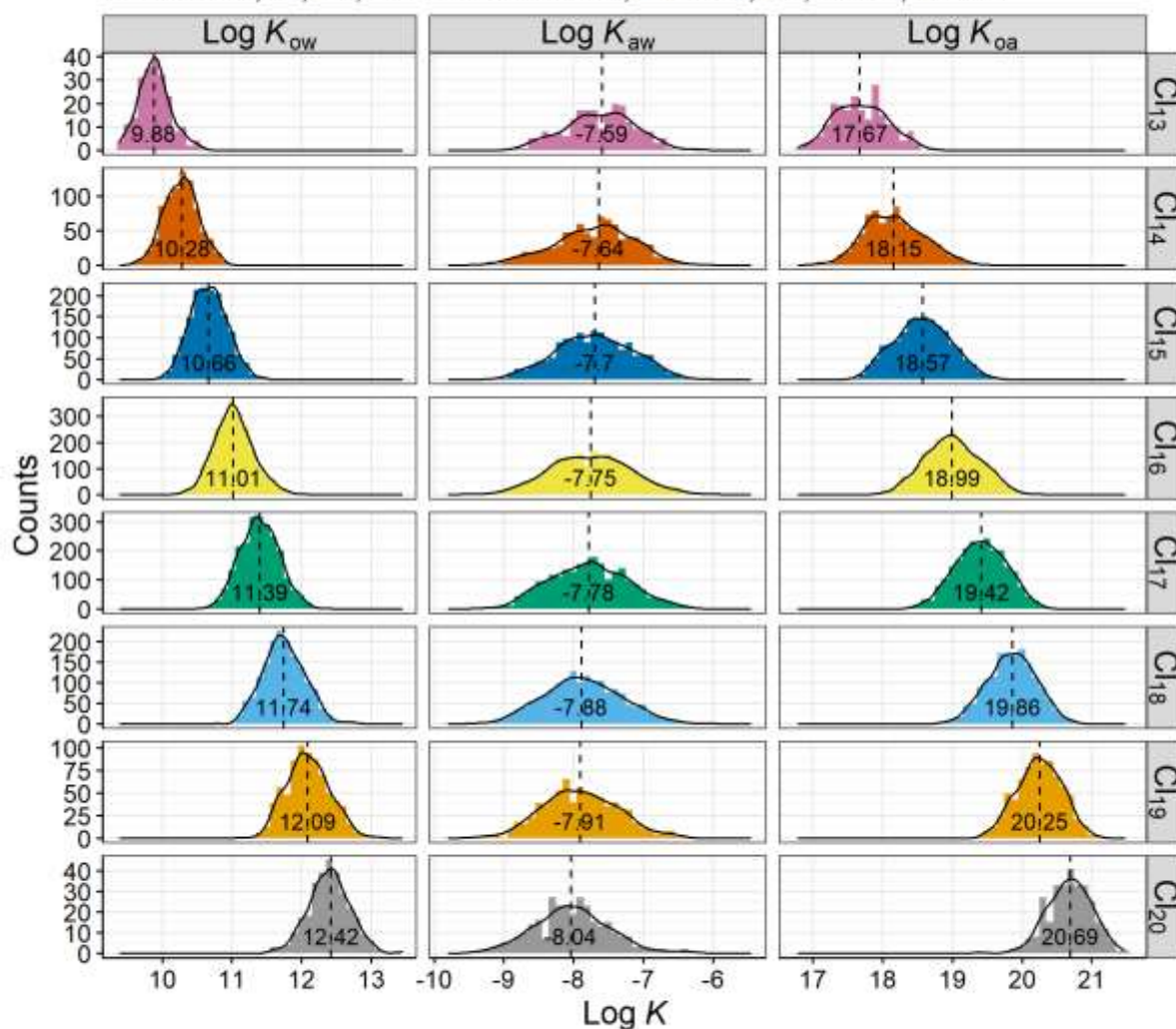
C₁₉, 60 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



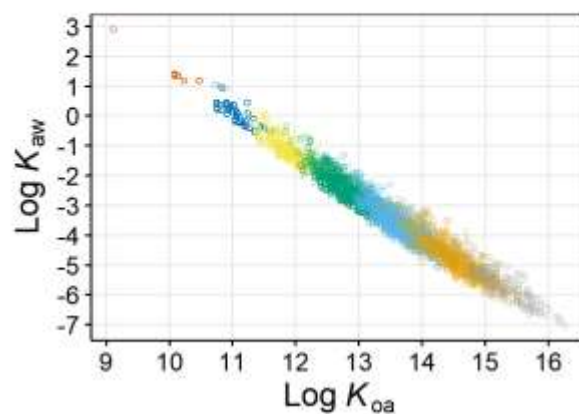
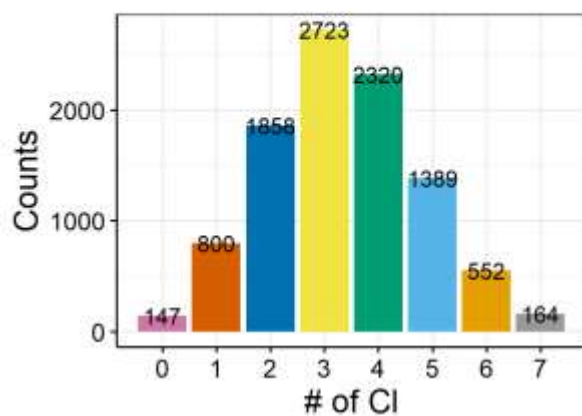
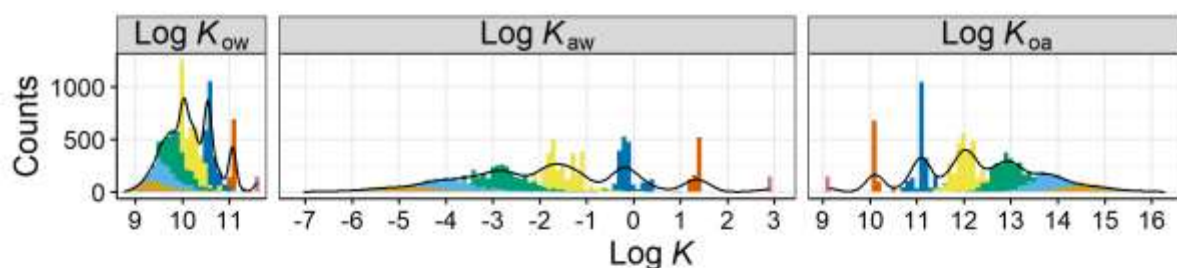
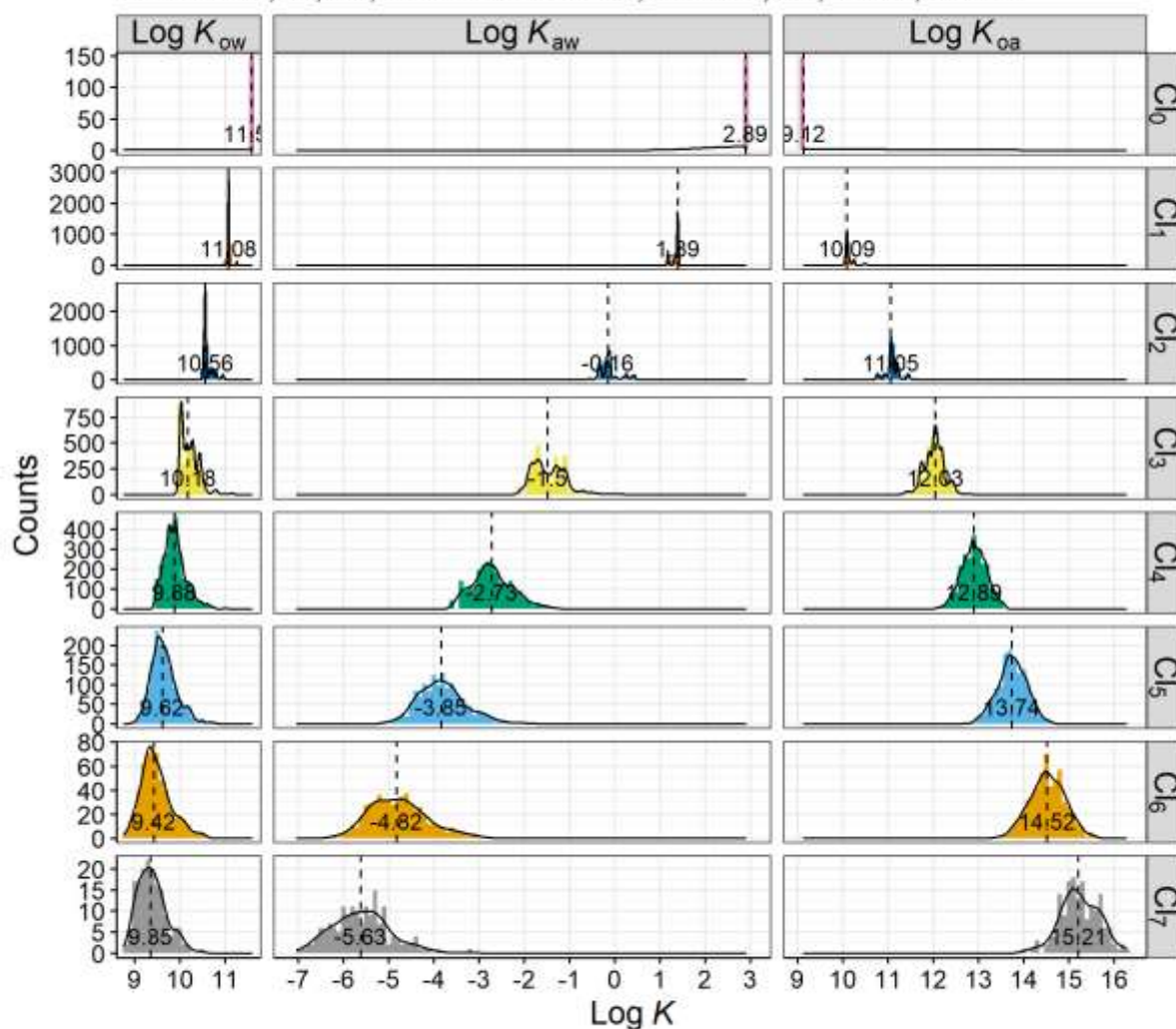
C₁₉, 70 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



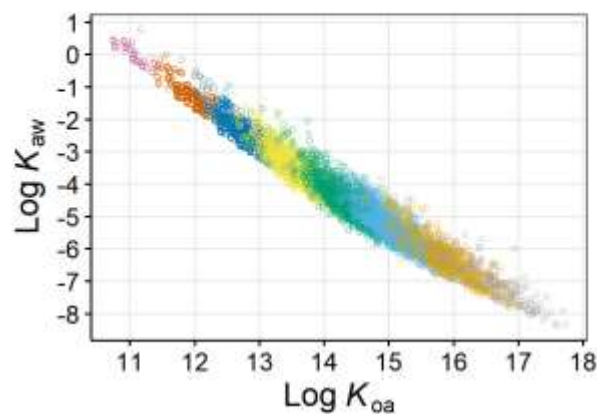
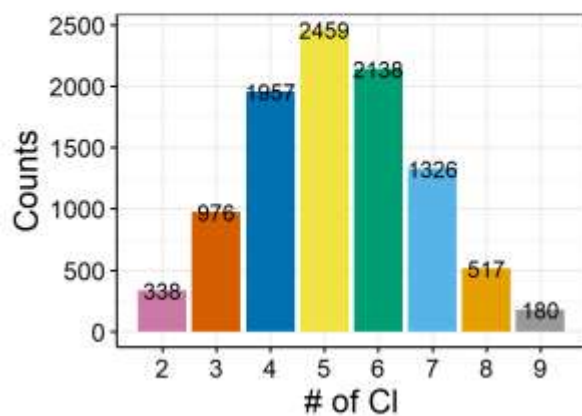
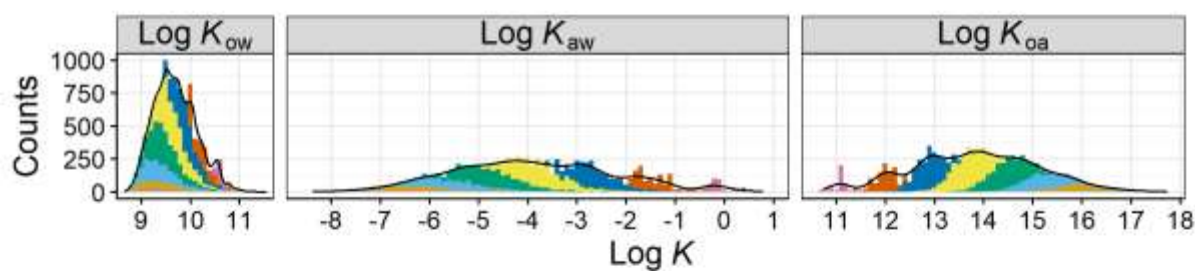
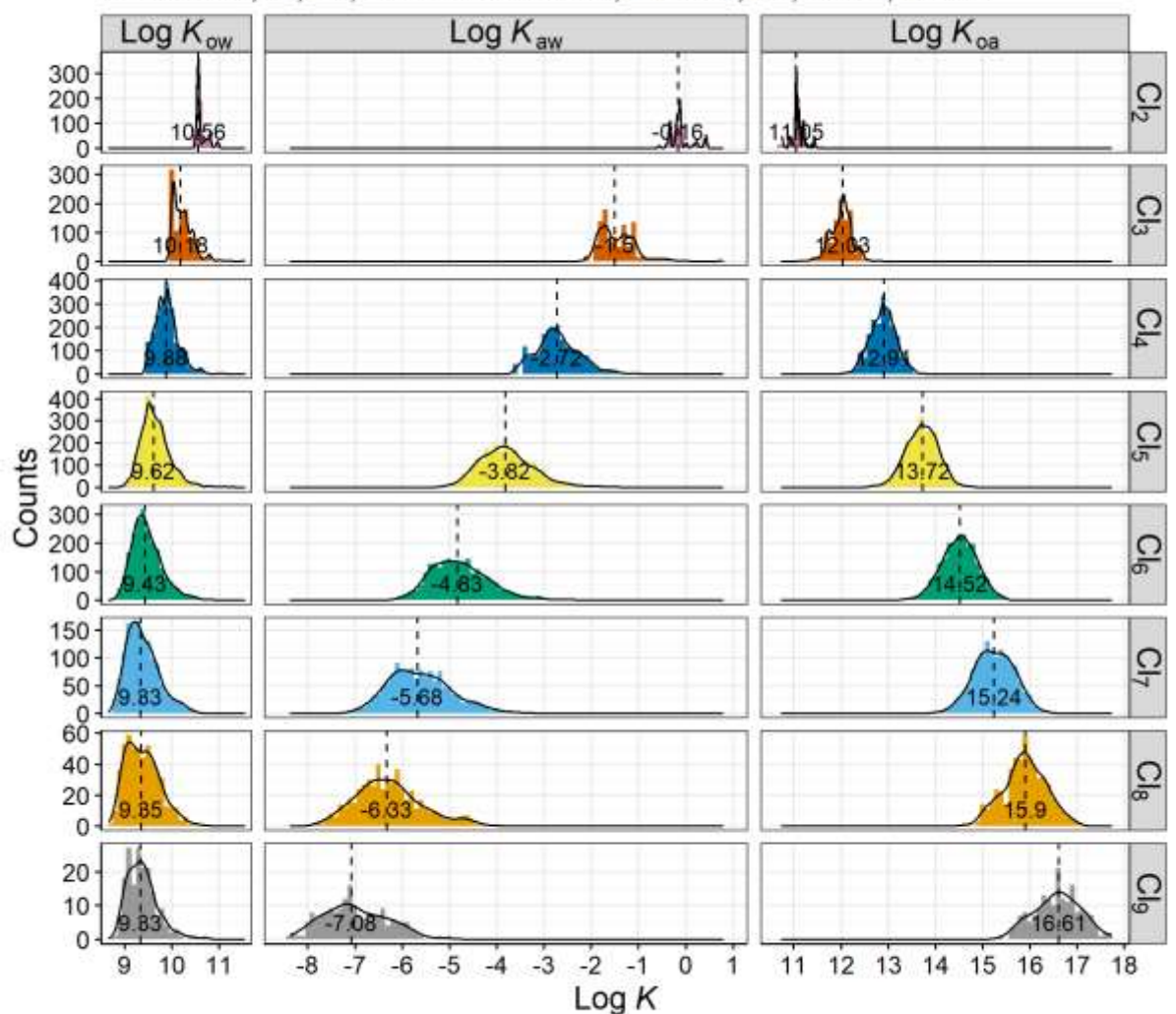
C₂₀, 30 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



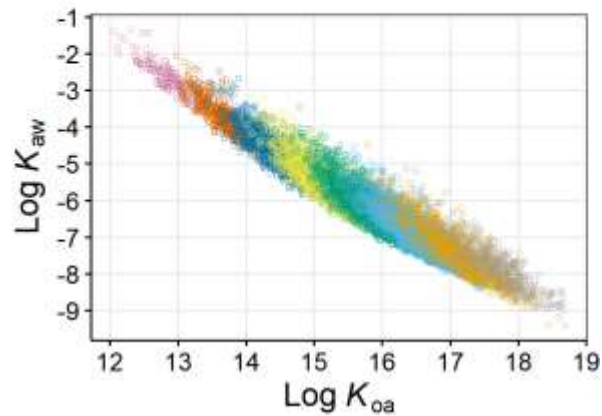
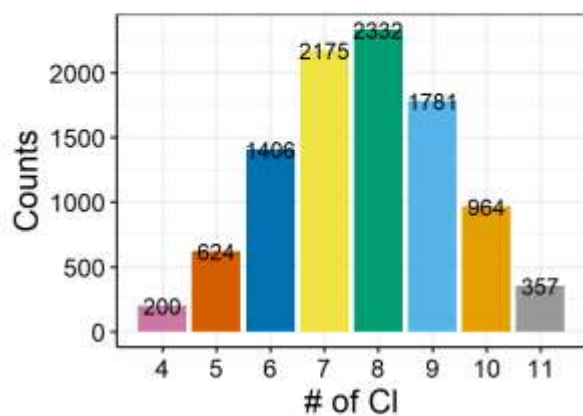
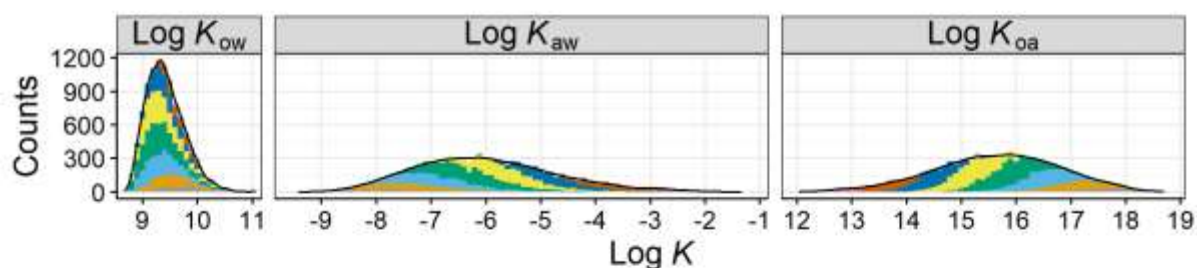
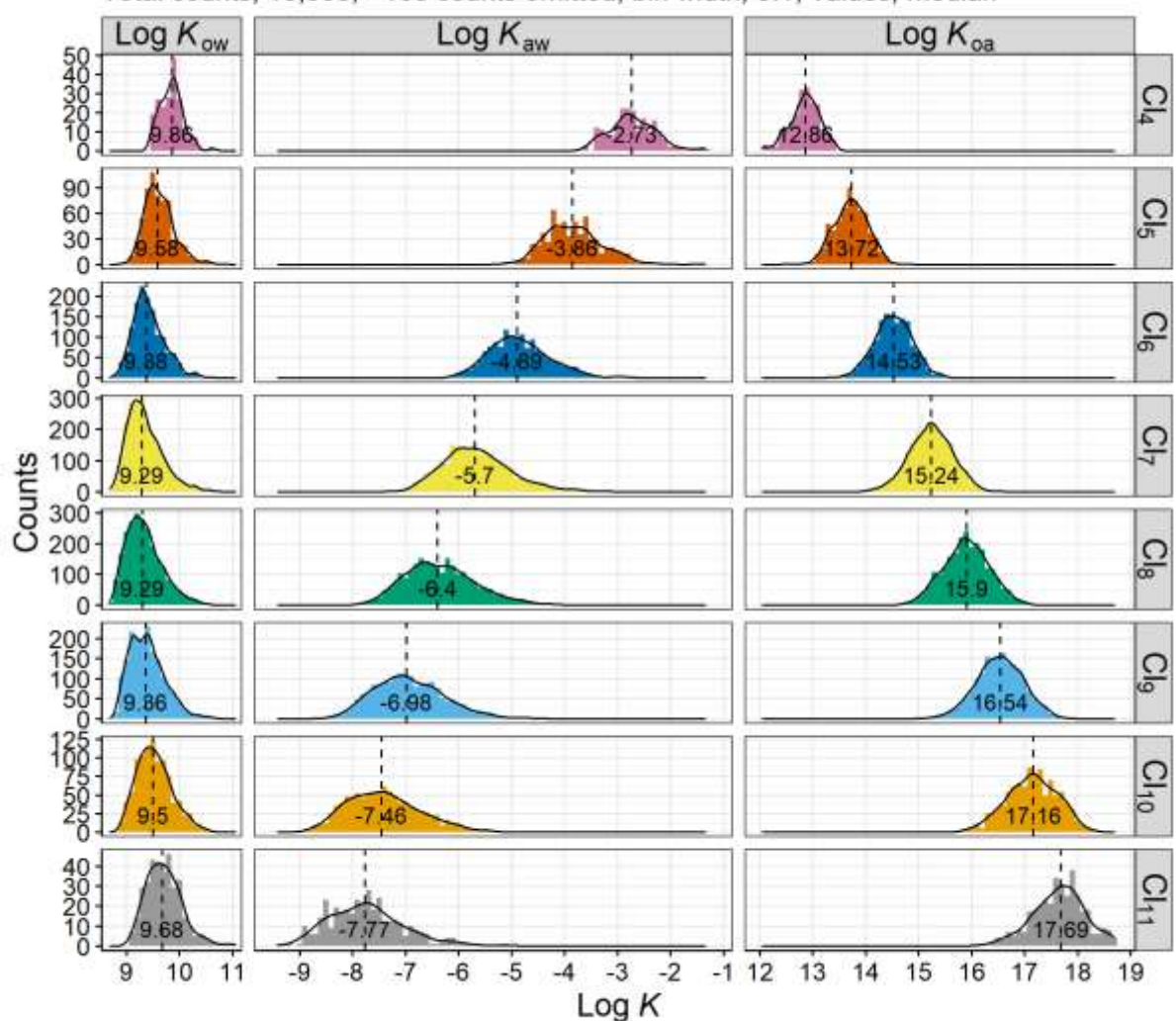
C₂₀, 40 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



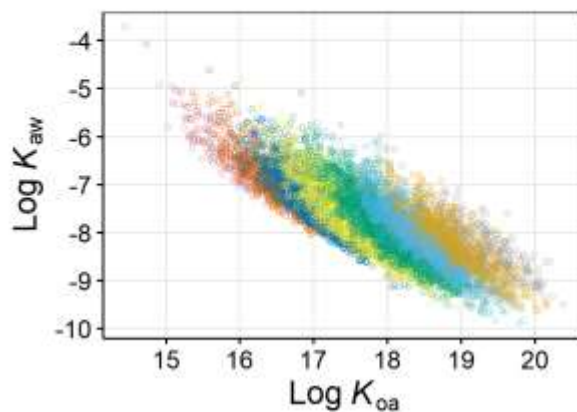
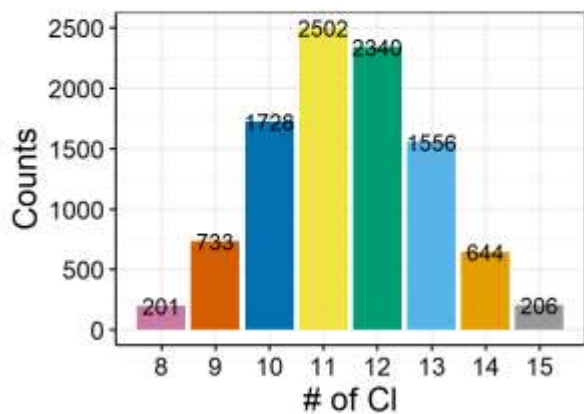
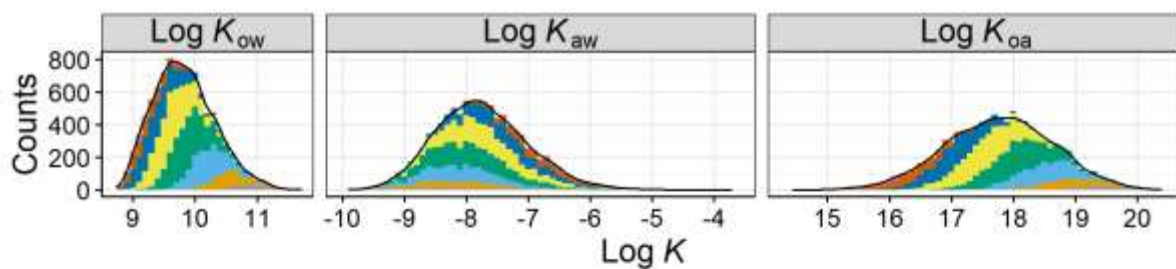
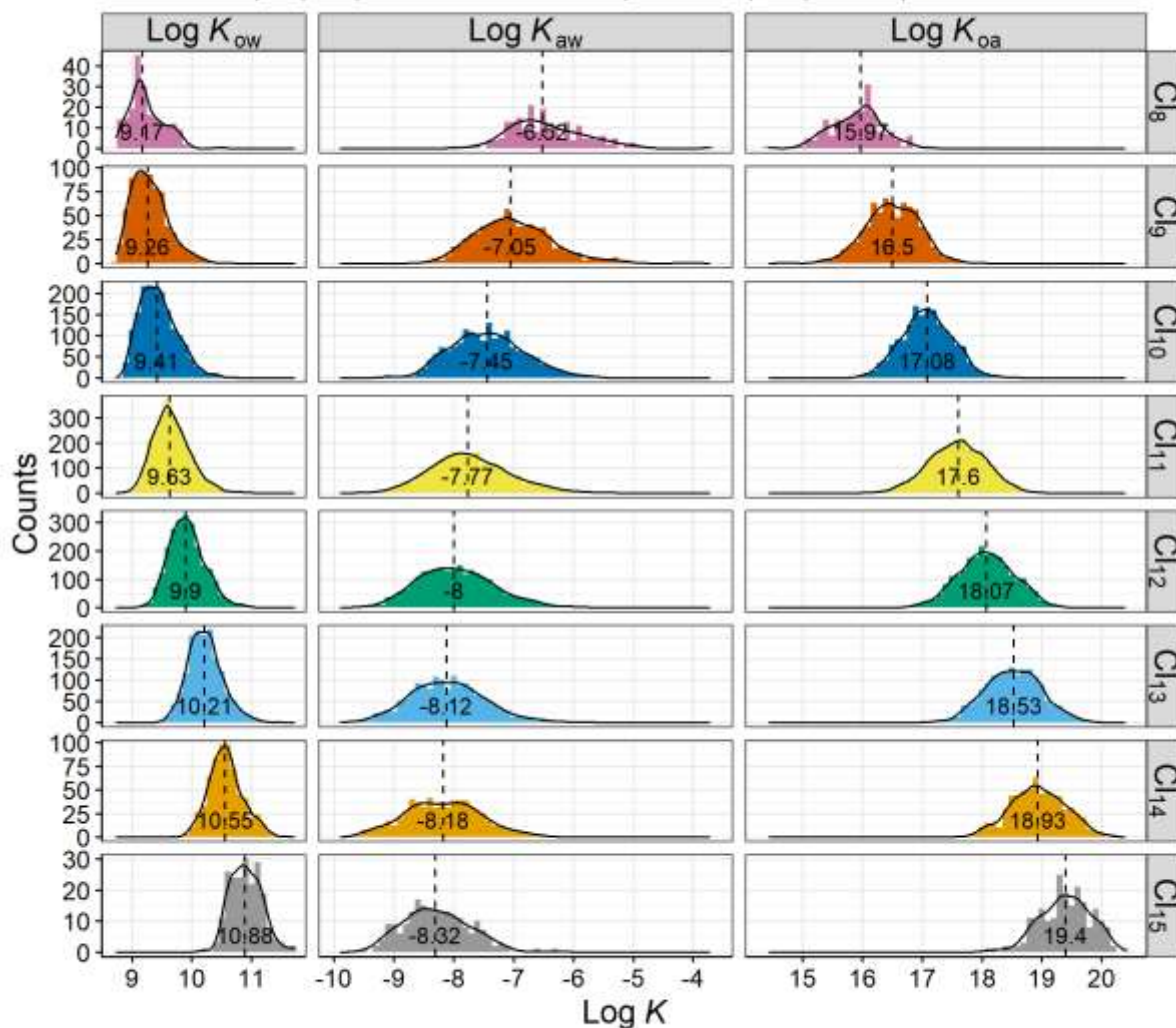
C₂₀, 50 wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



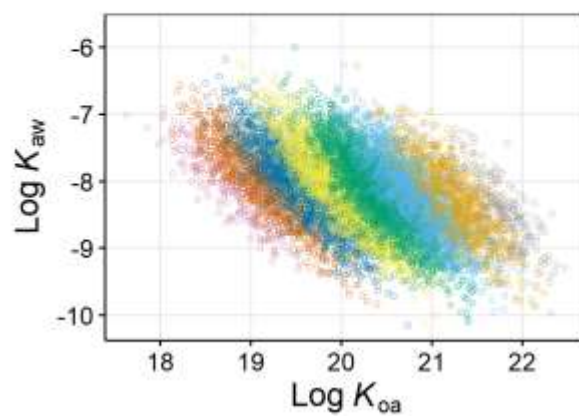
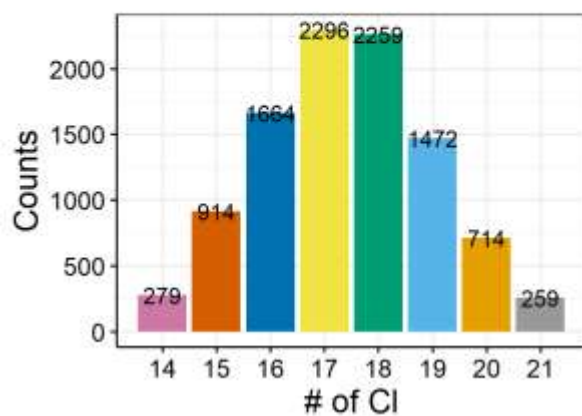
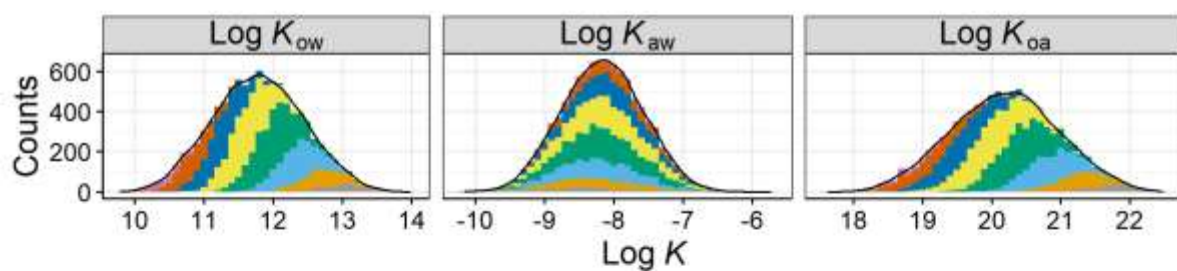
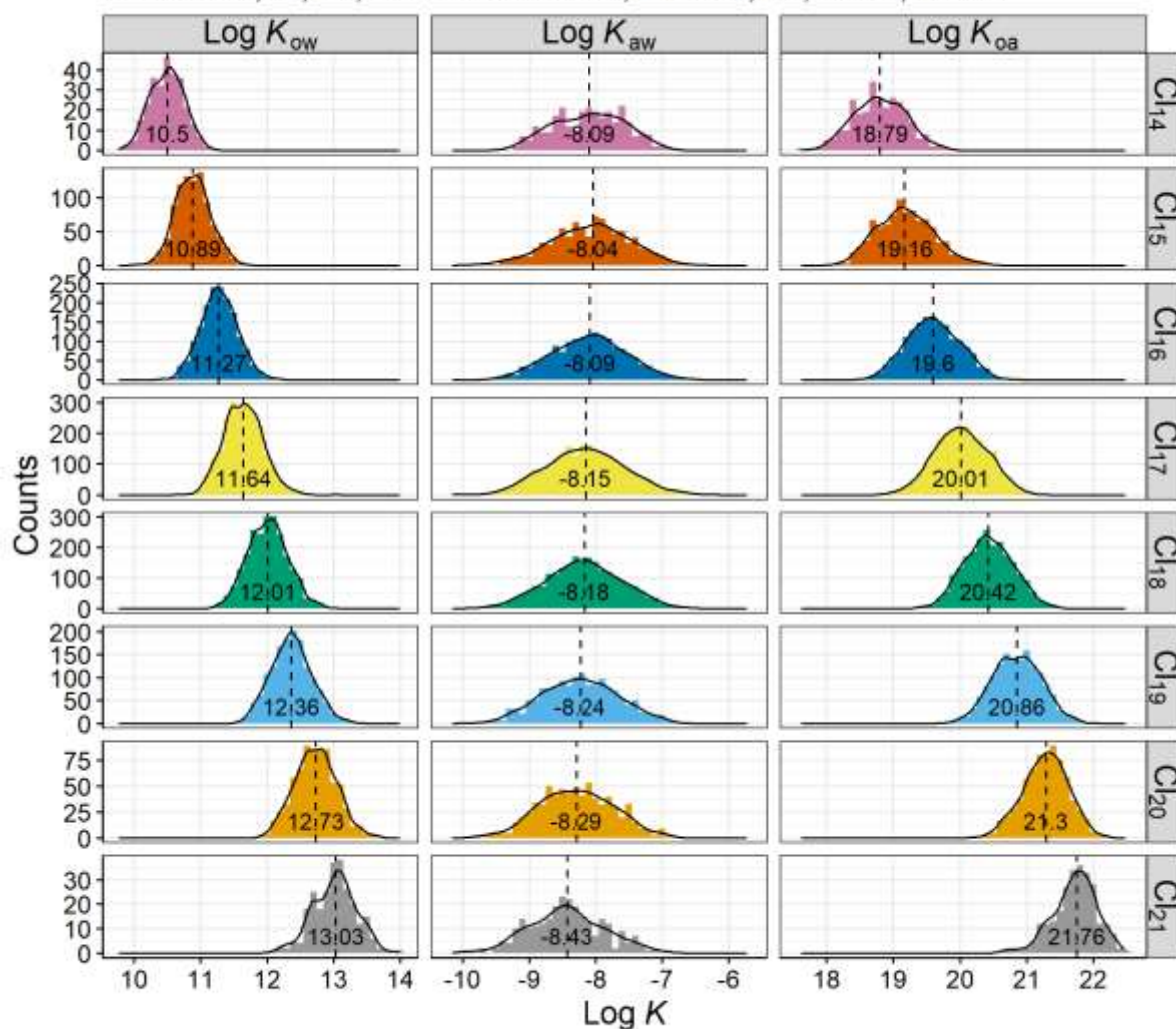
C₂₀, 60 wt% Cl

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



C₂₀, 70 wt% CI

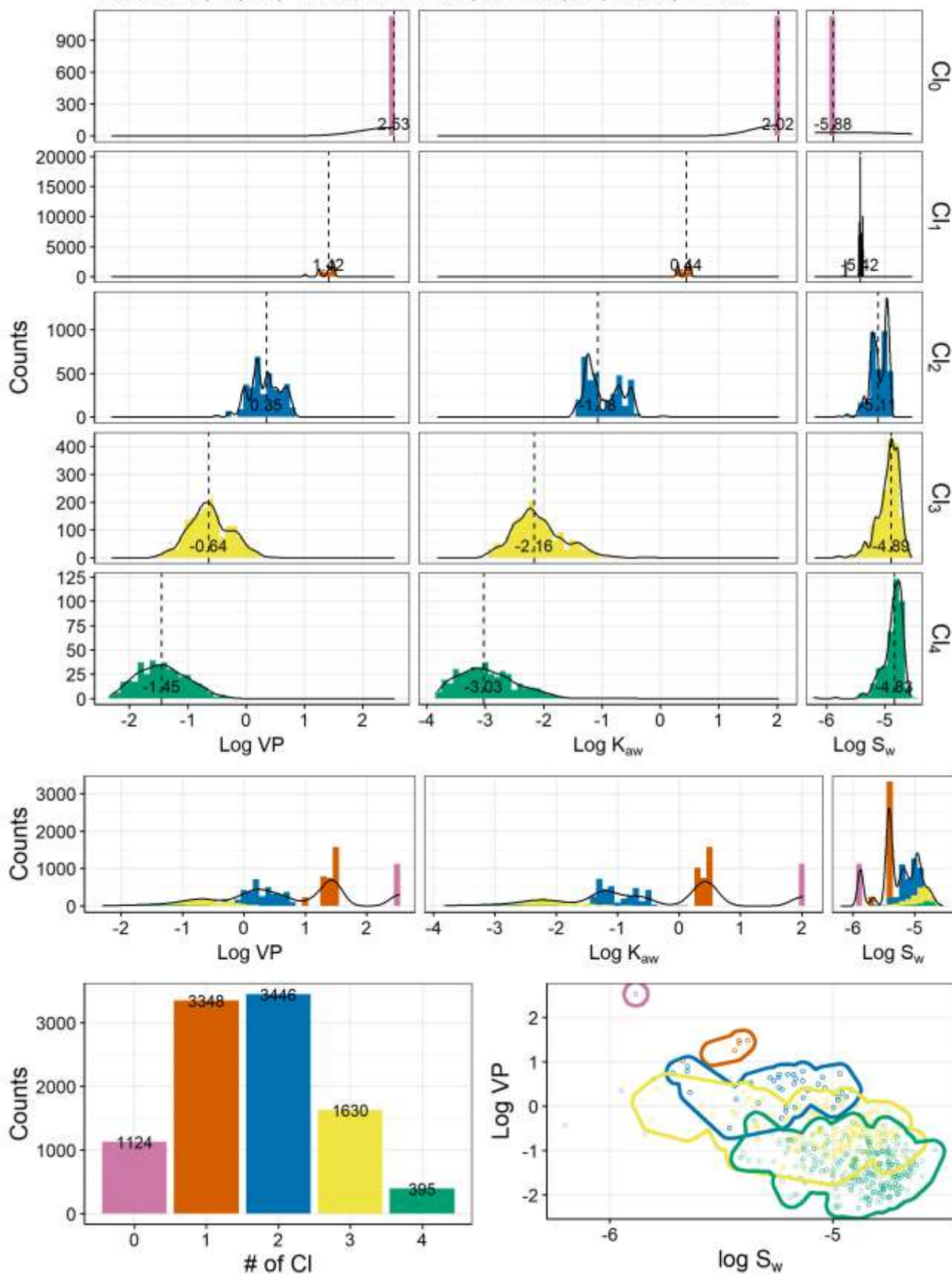
Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



**Property distributions of CP mixtures with a carbon-chain length of C_{10–20} and a chlorination degree of 30–70 wt%:
log VP, log K_{aw} , log S_w**

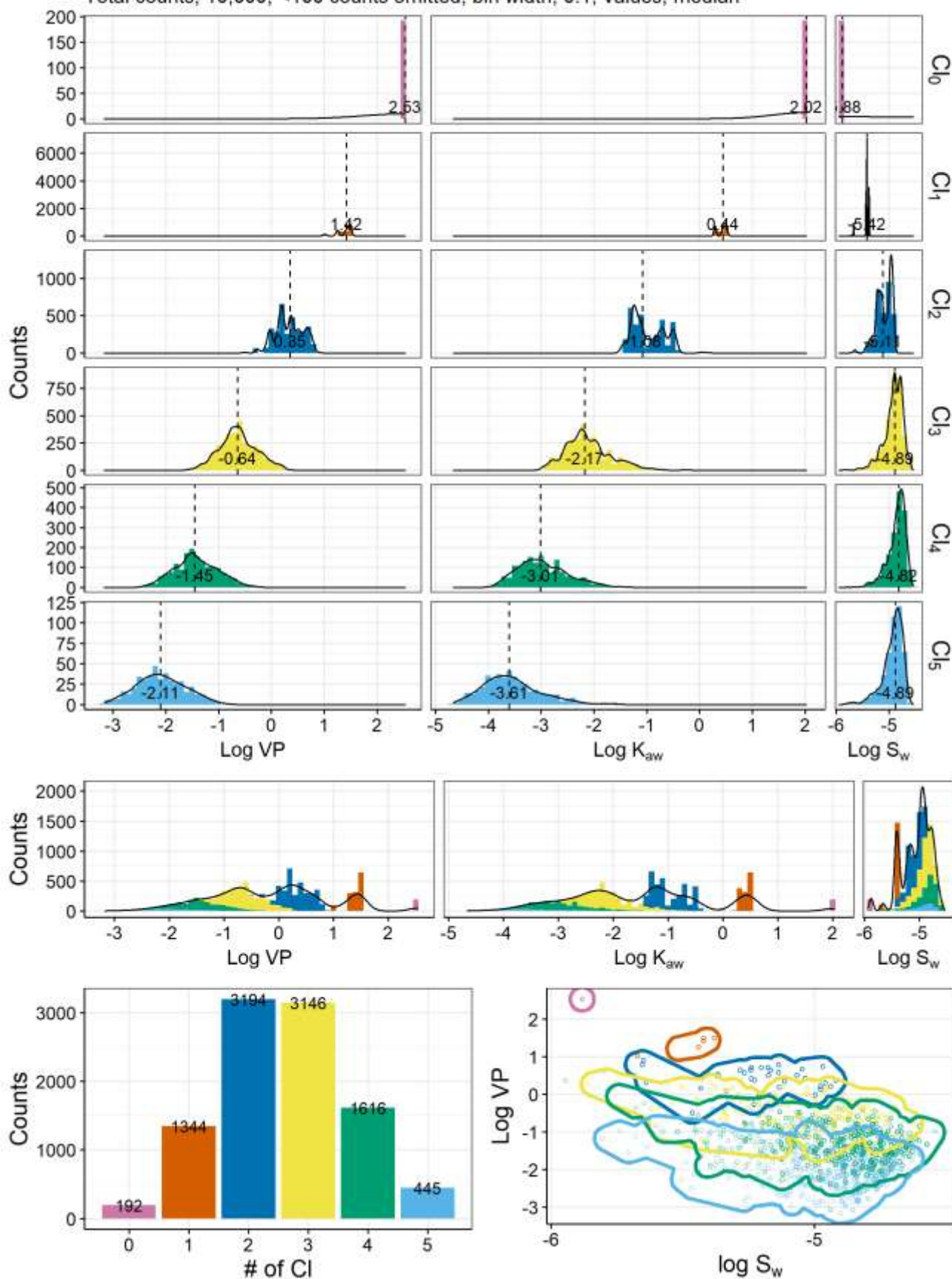
C10, 30wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



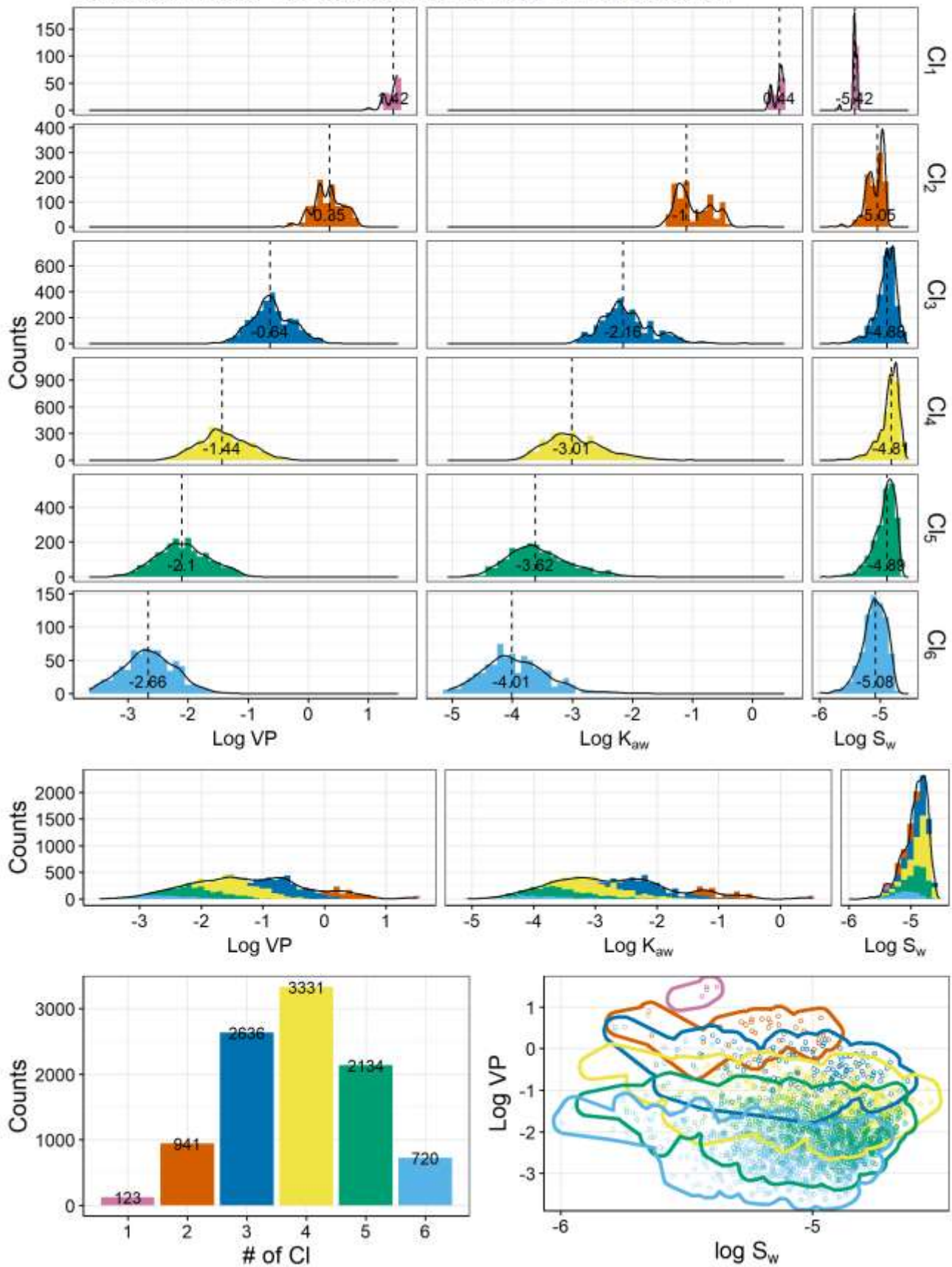
C10, 40wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



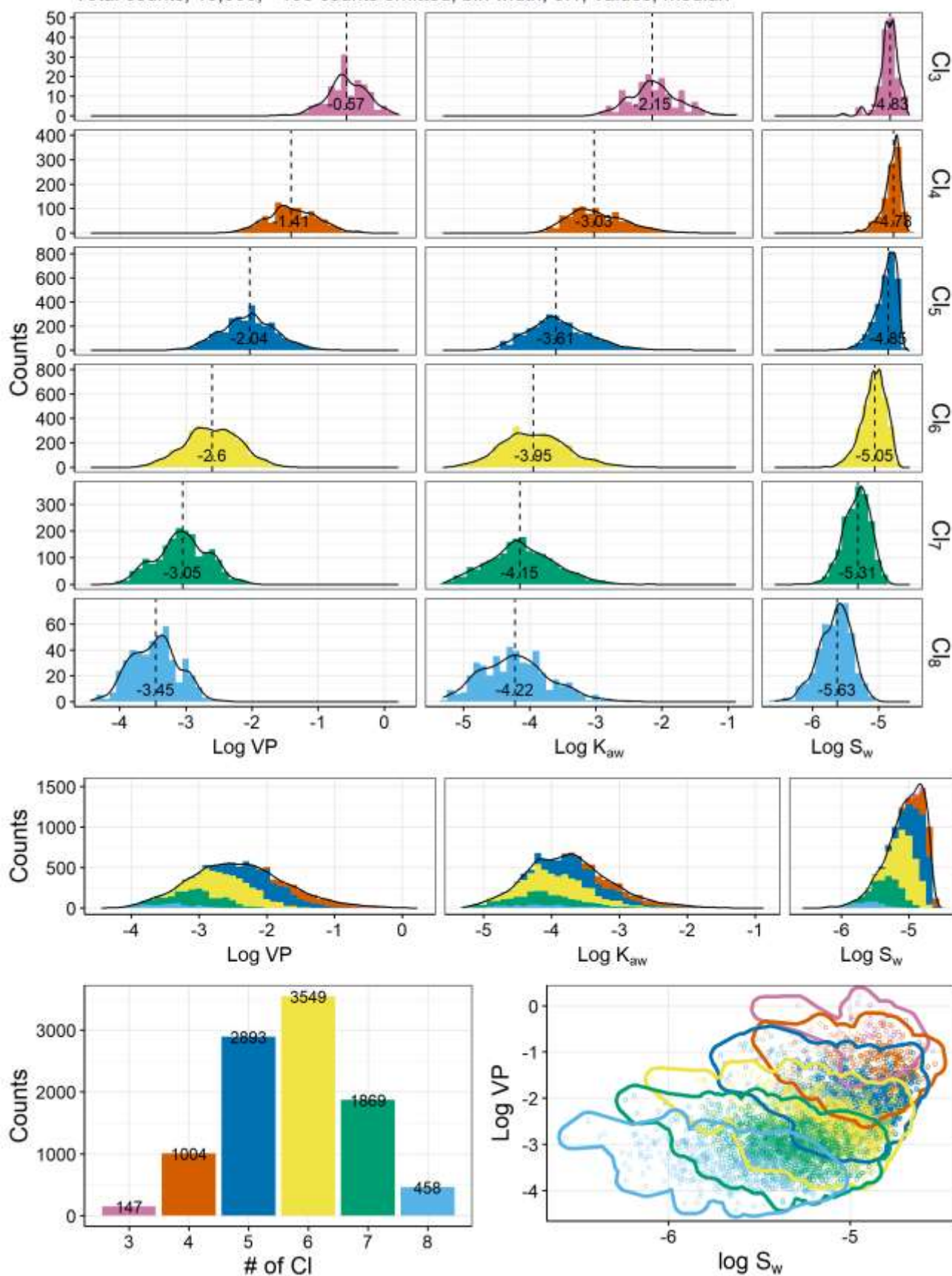
C10, 50wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



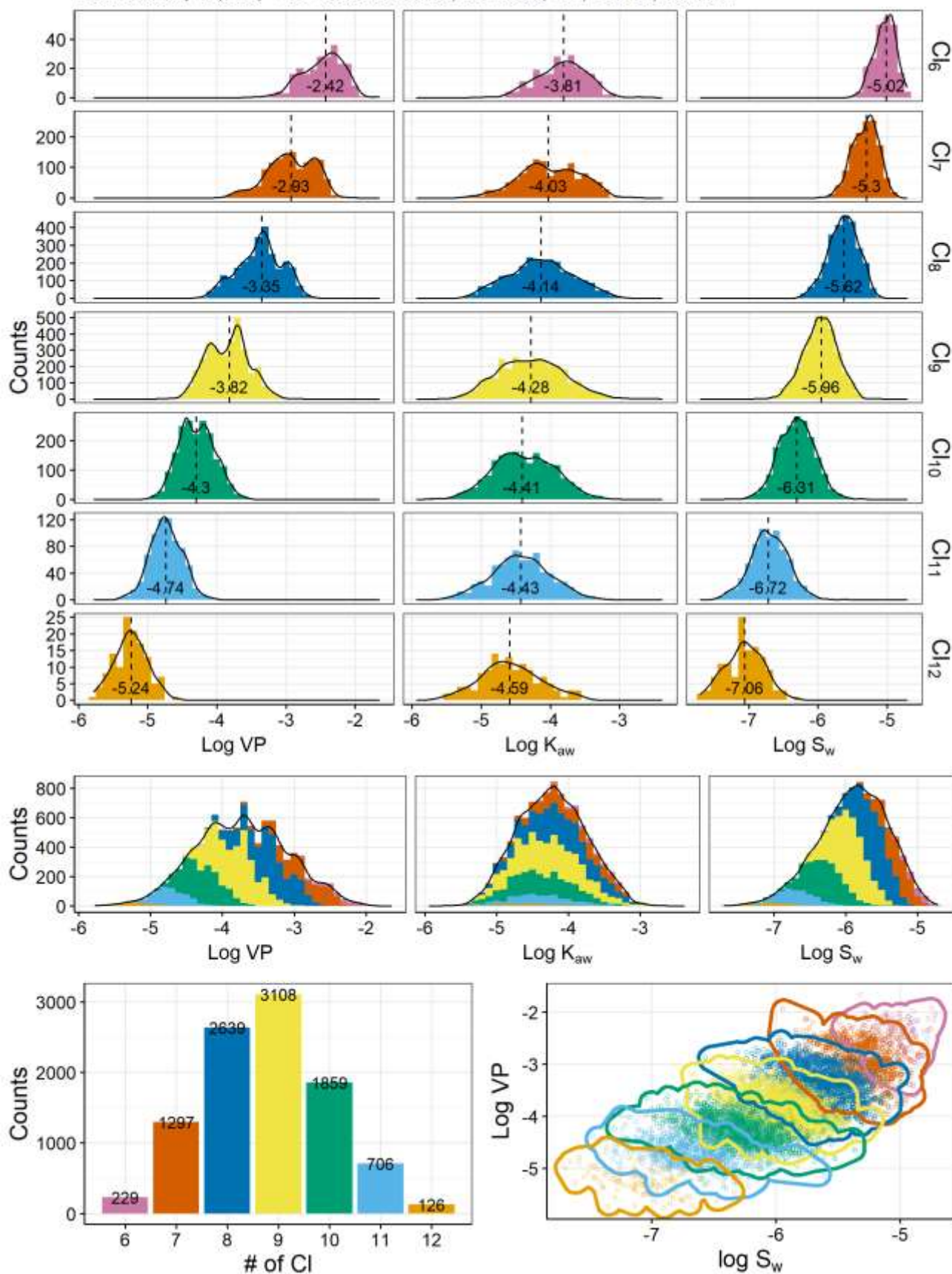
C10, 60wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



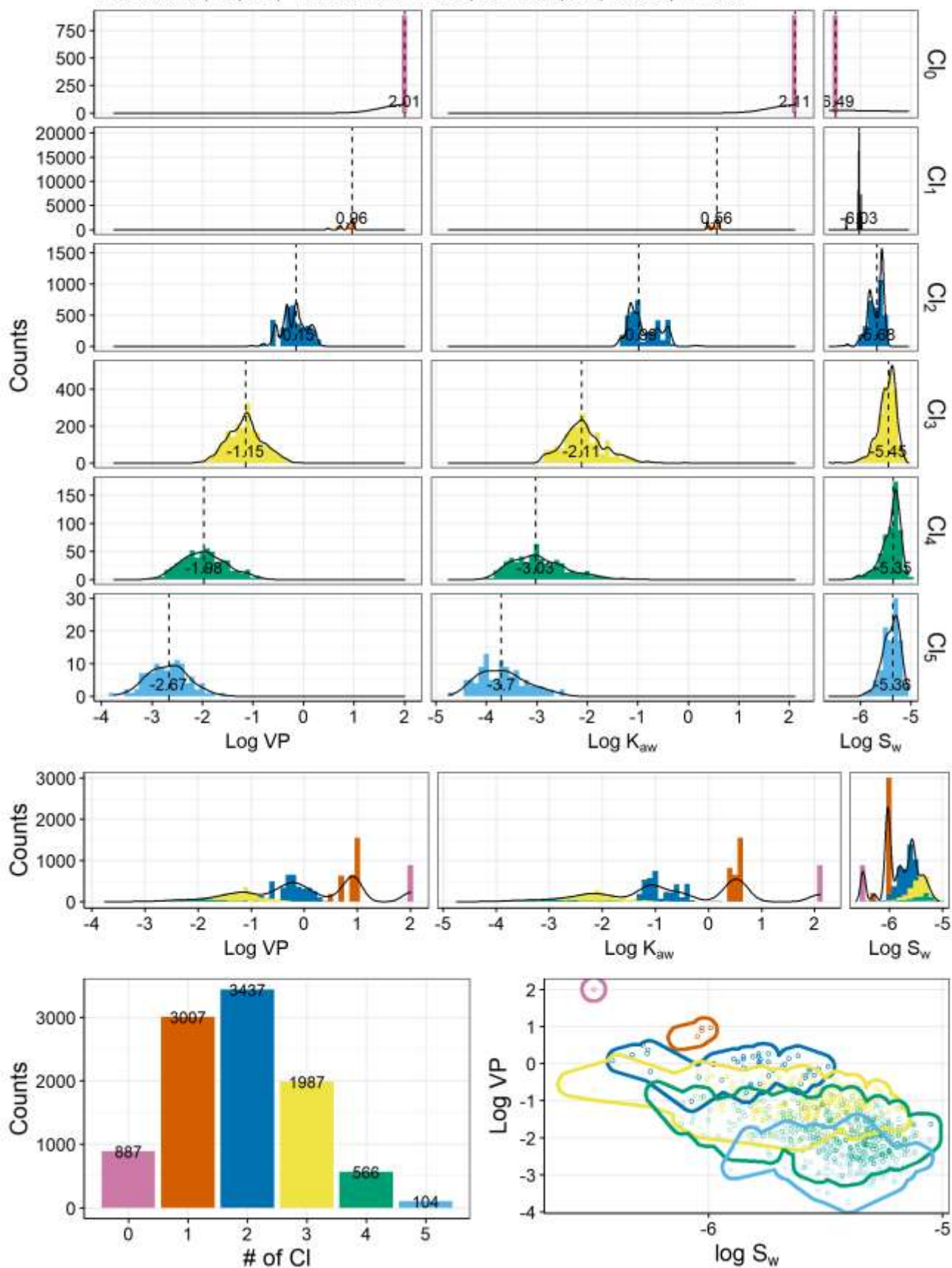
C10, 70wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



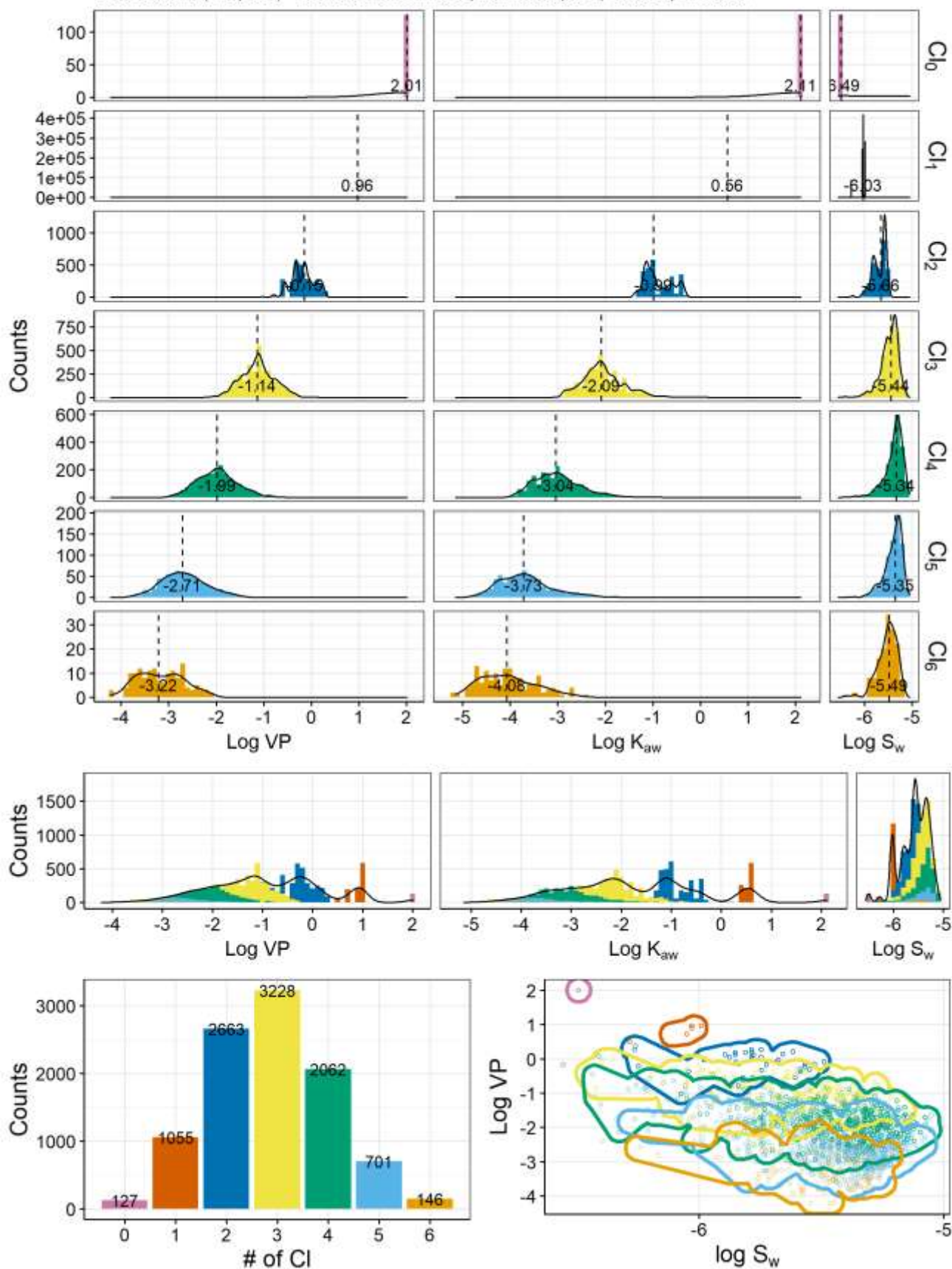
C11, 30wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



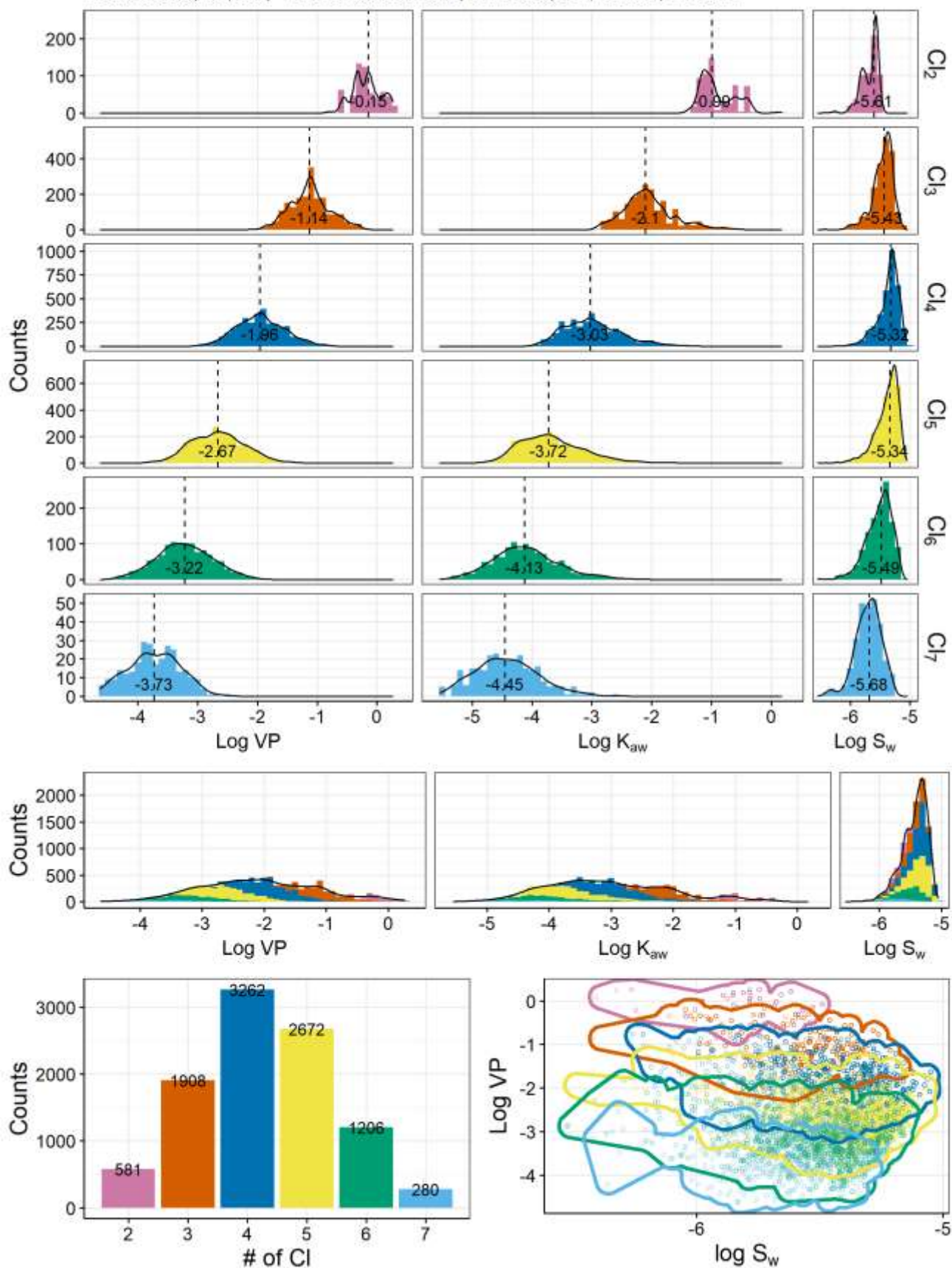
C11, 40wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



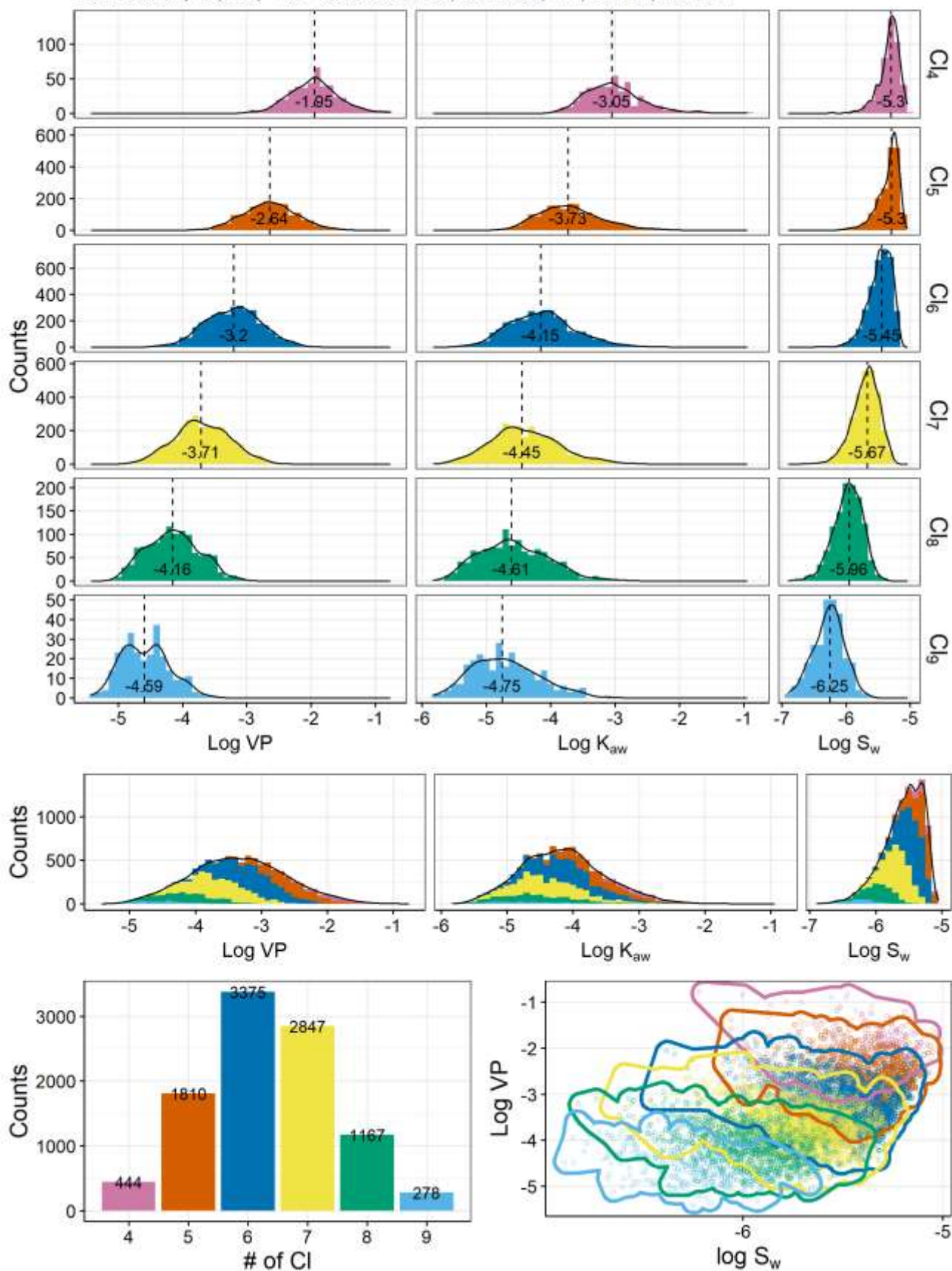
C11, 50wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



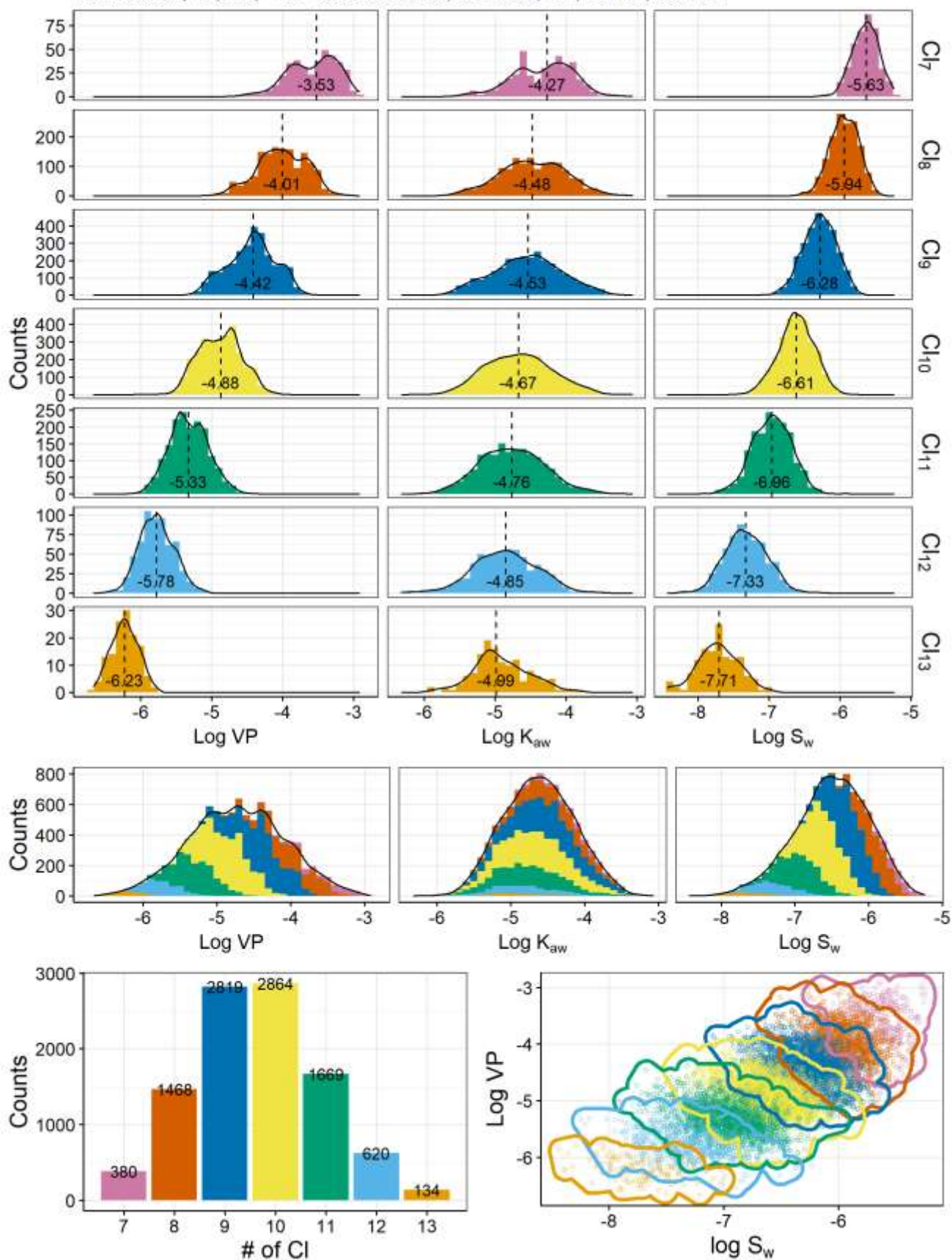
C11, 60wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



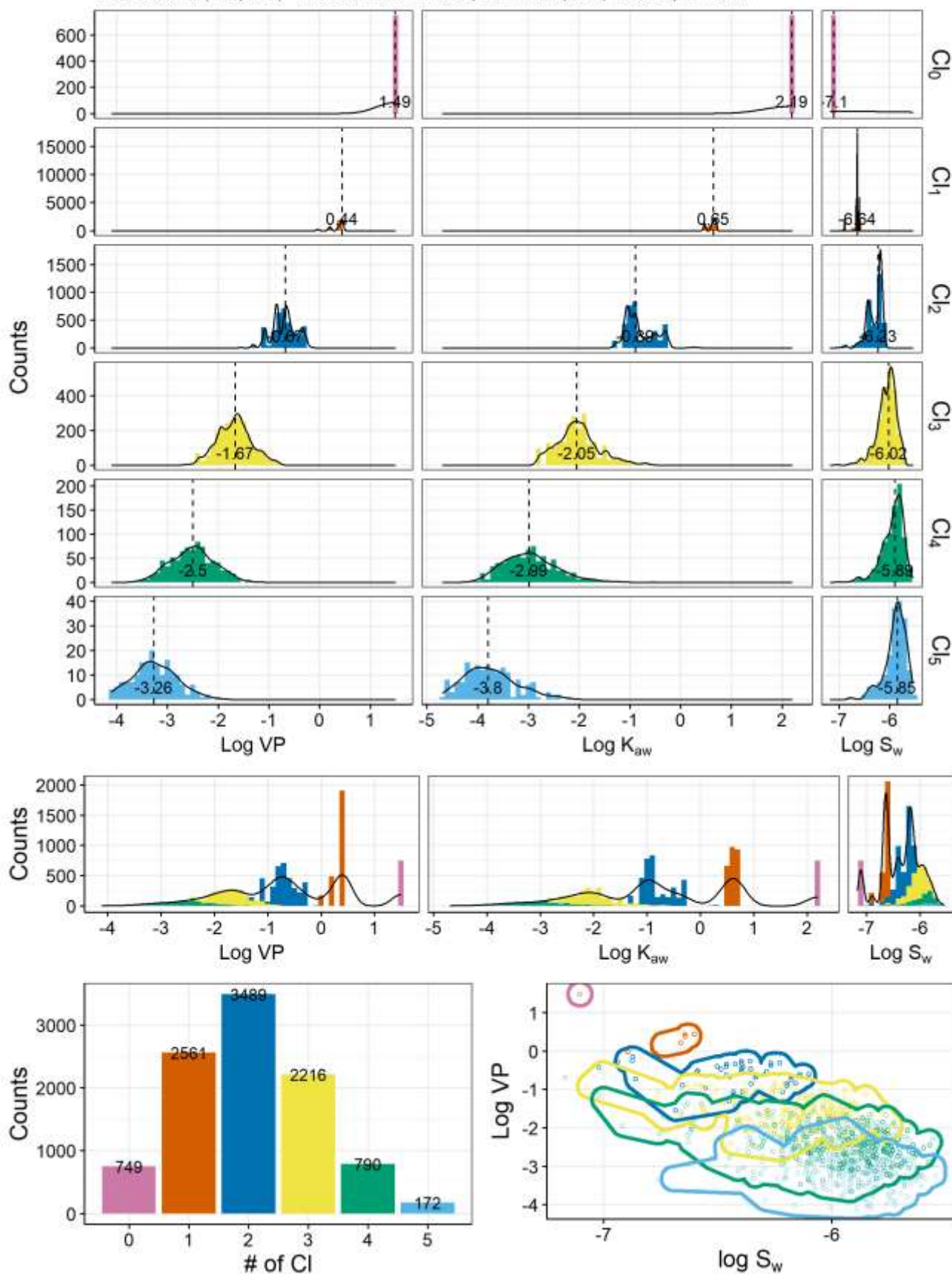
C11, 70wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



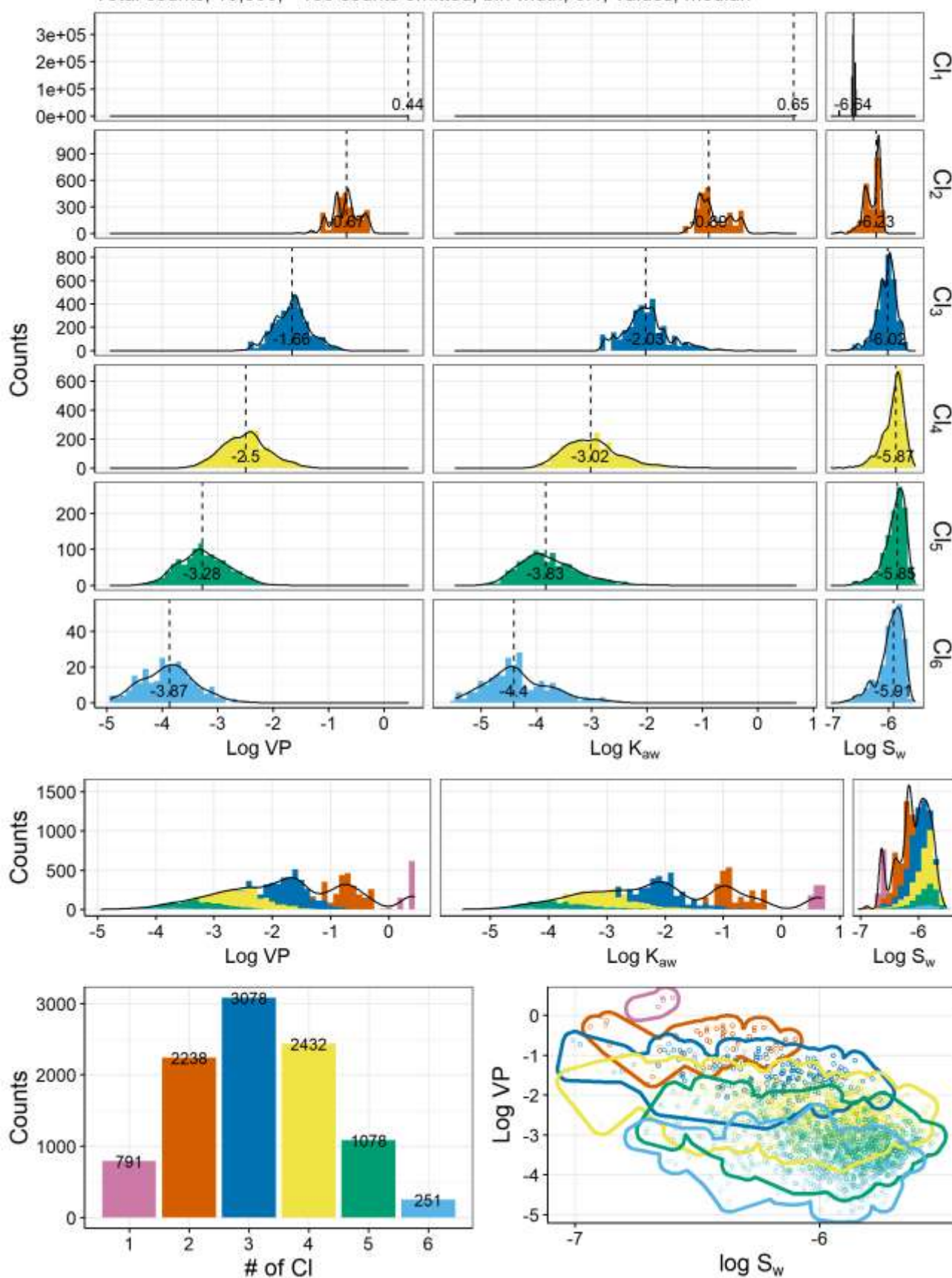
C12, 30wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



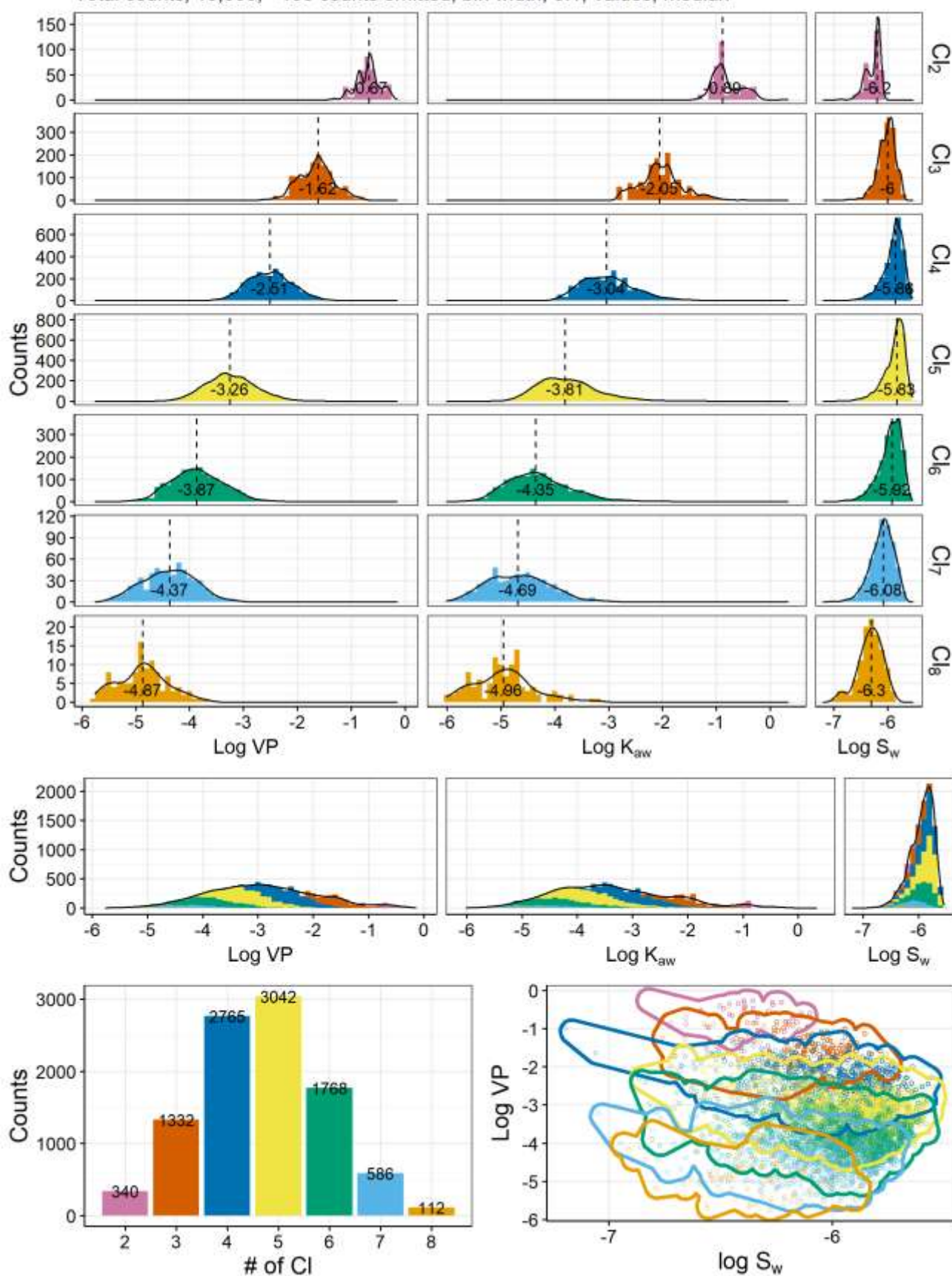
C12, 40wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



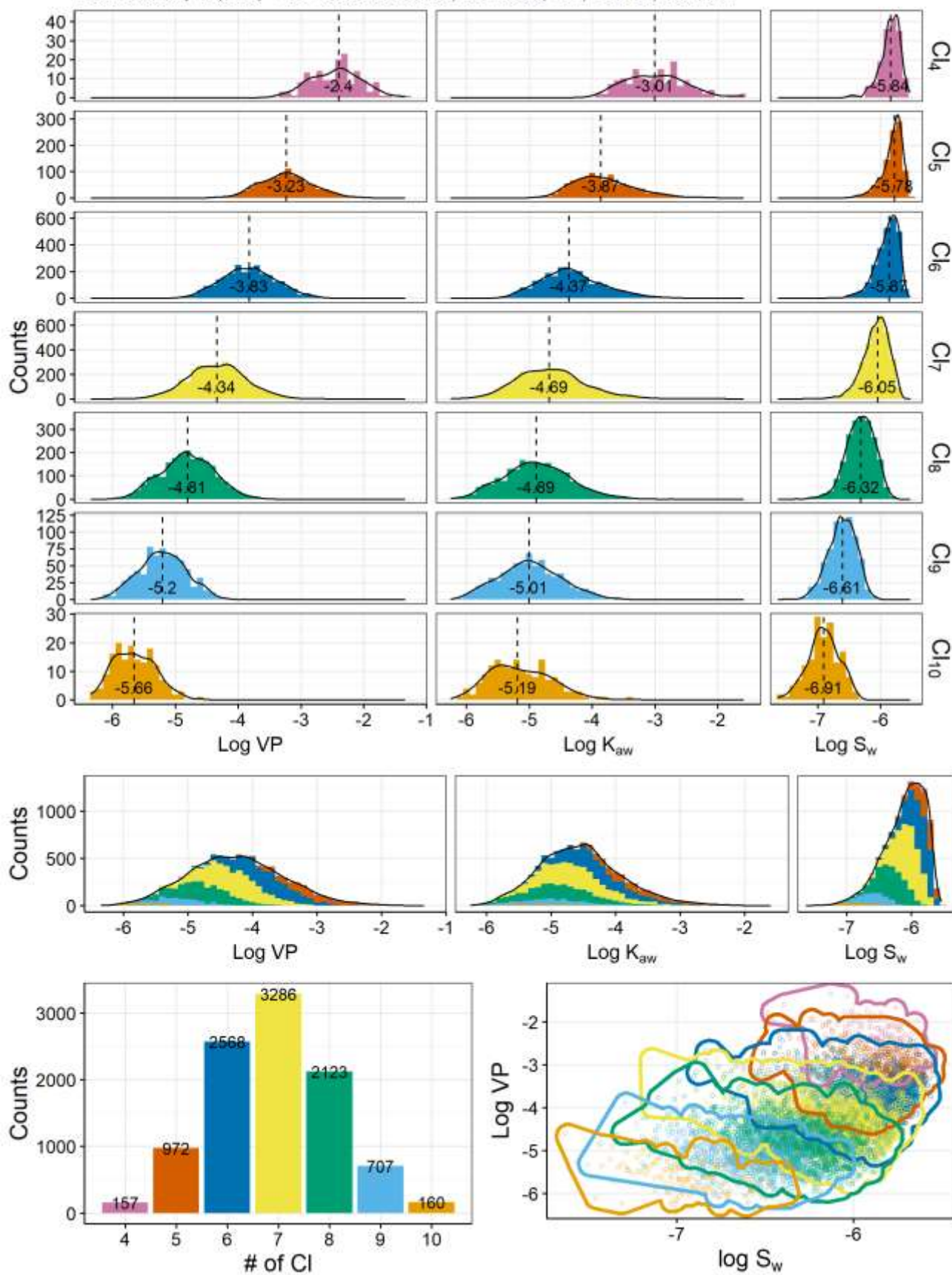
C12, 50wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



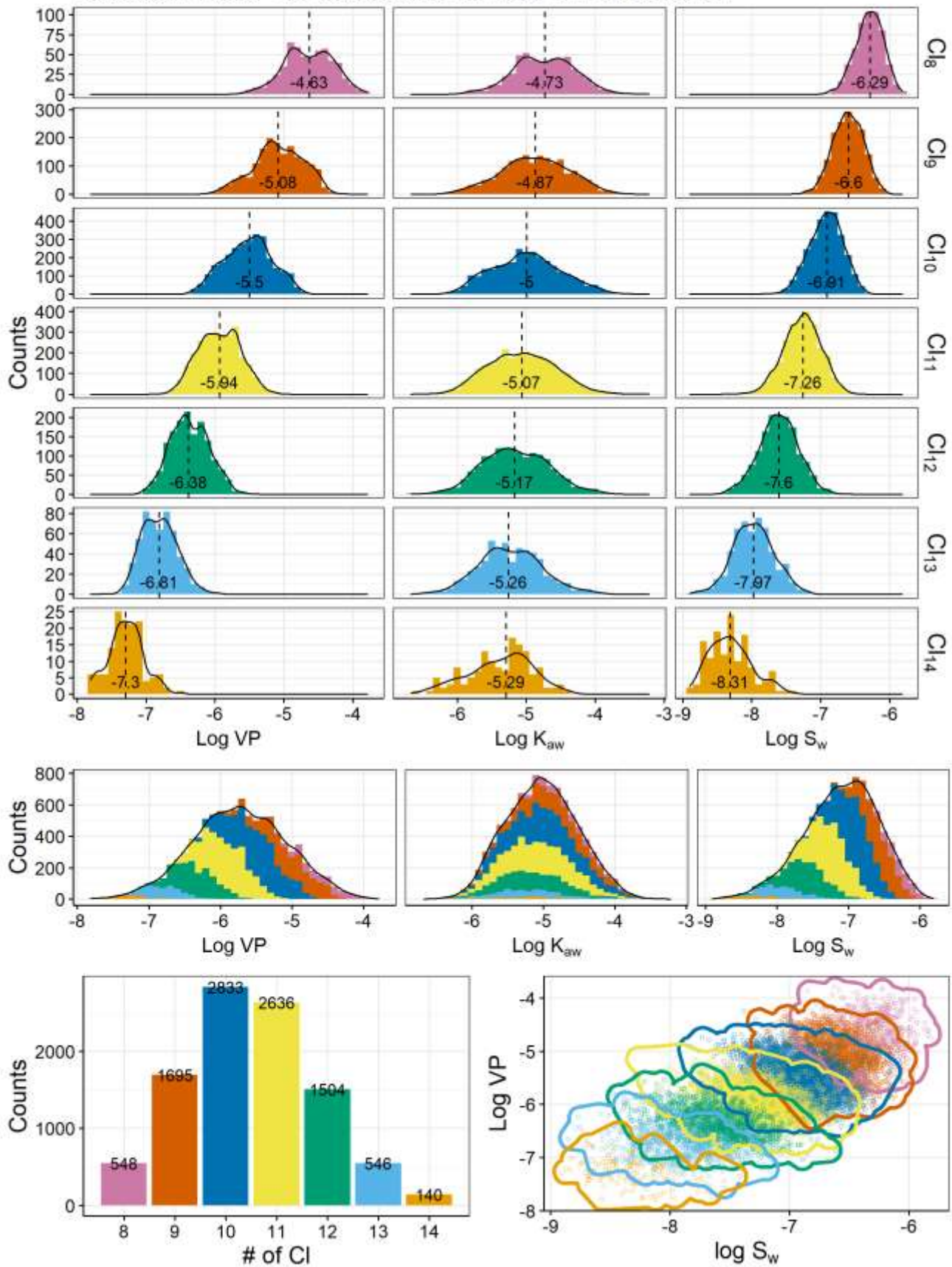
C12, 60wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



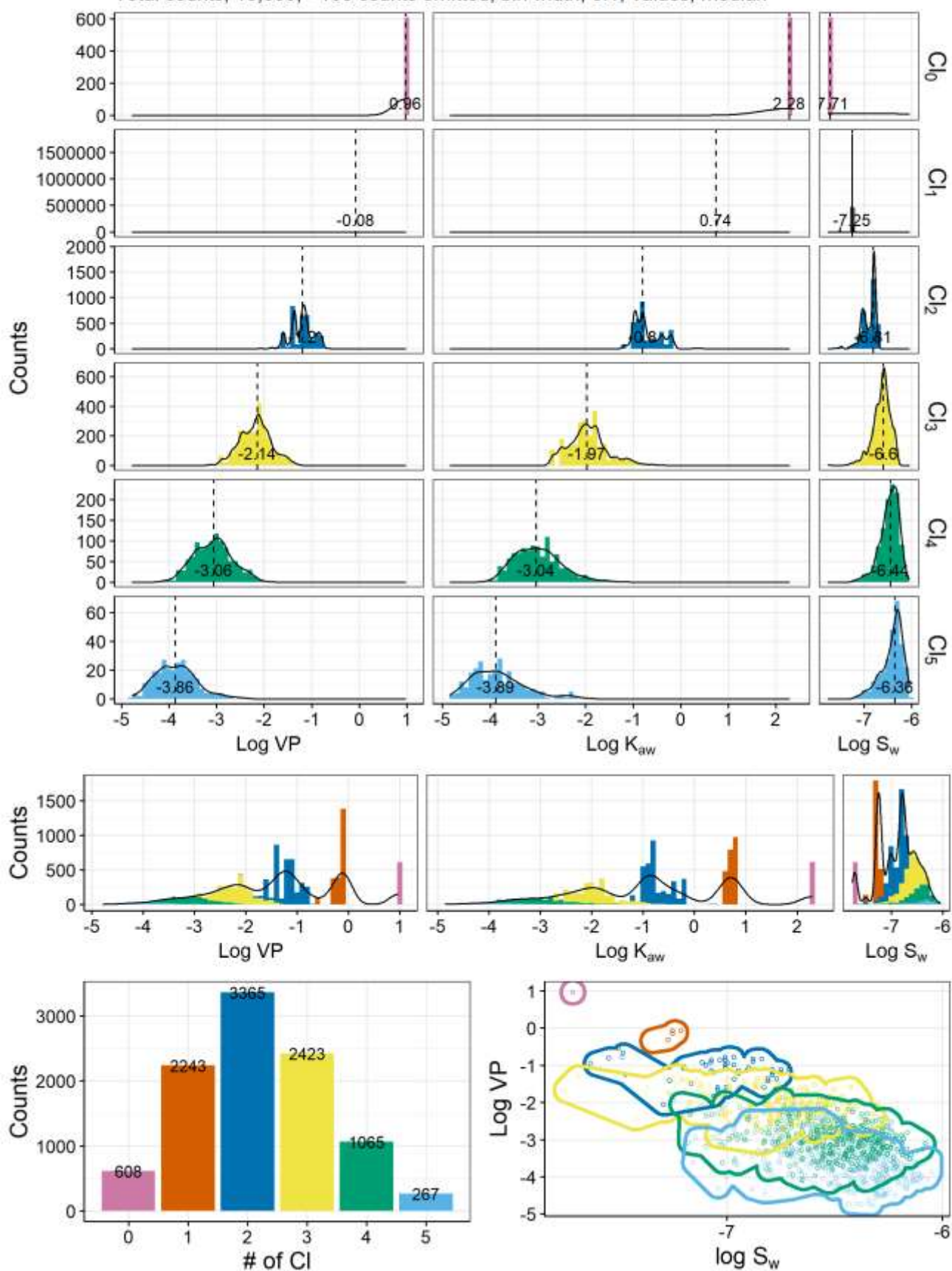
C12, 70wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



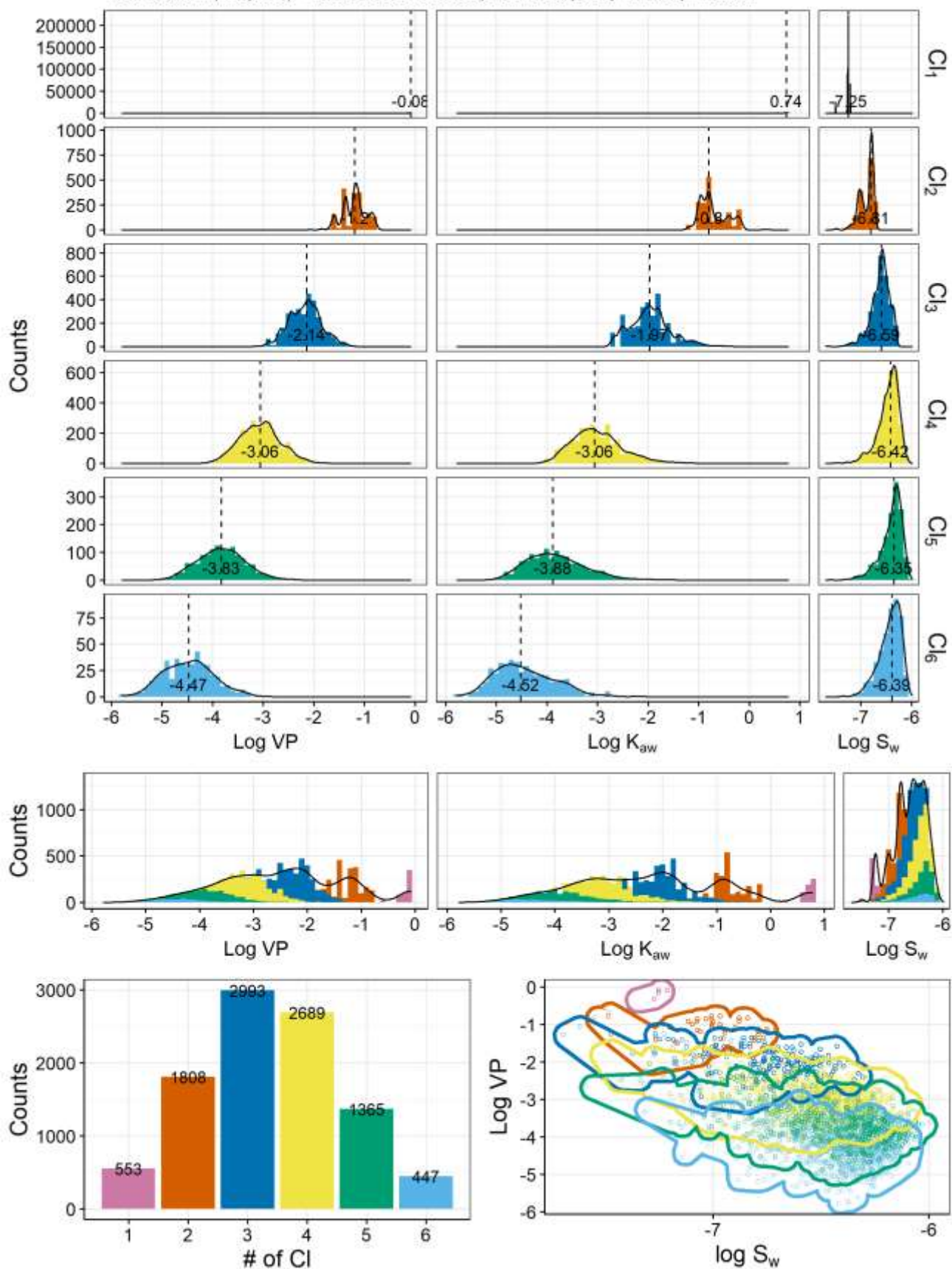
C13, 30wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



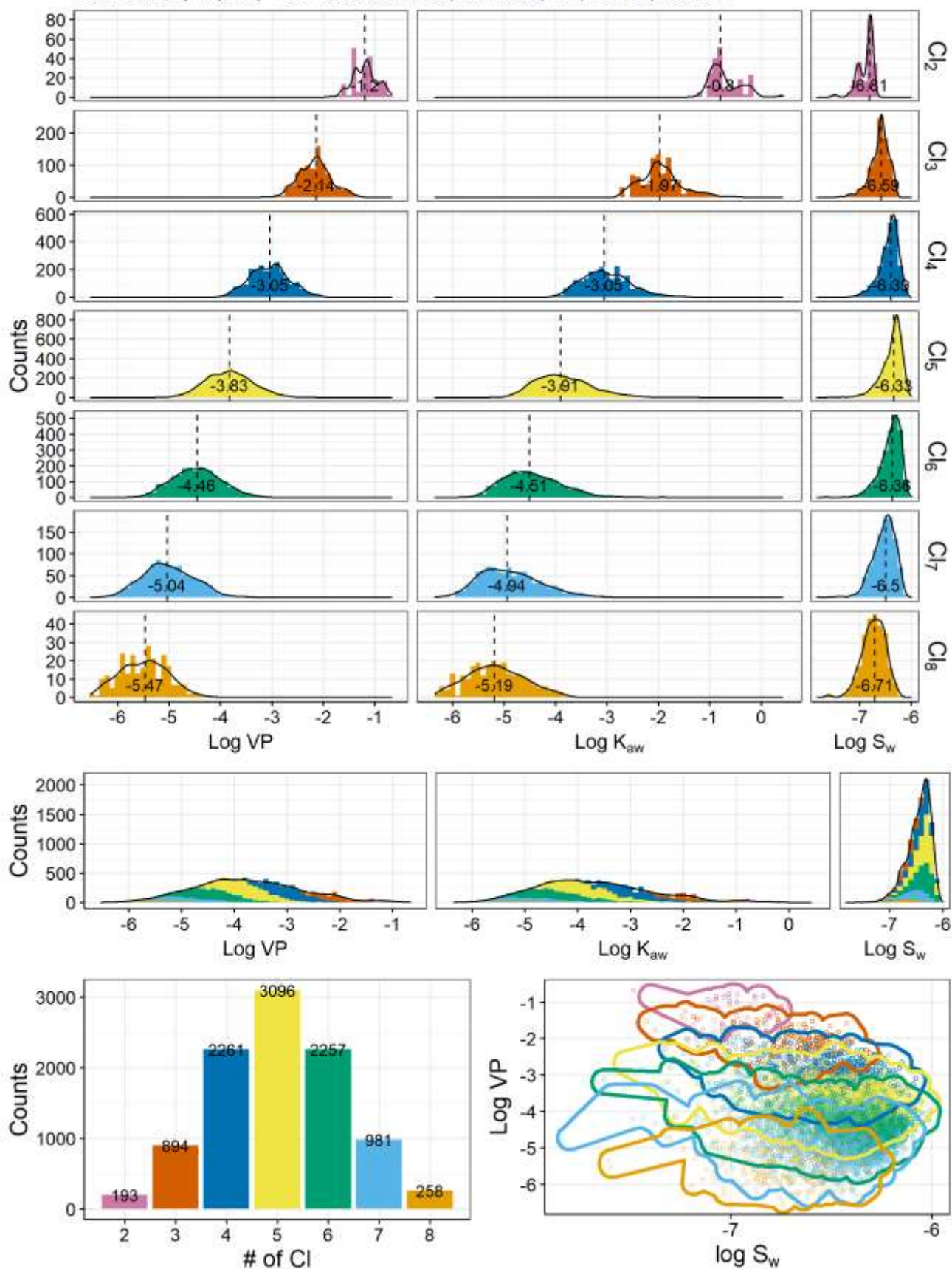
C13, 40wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



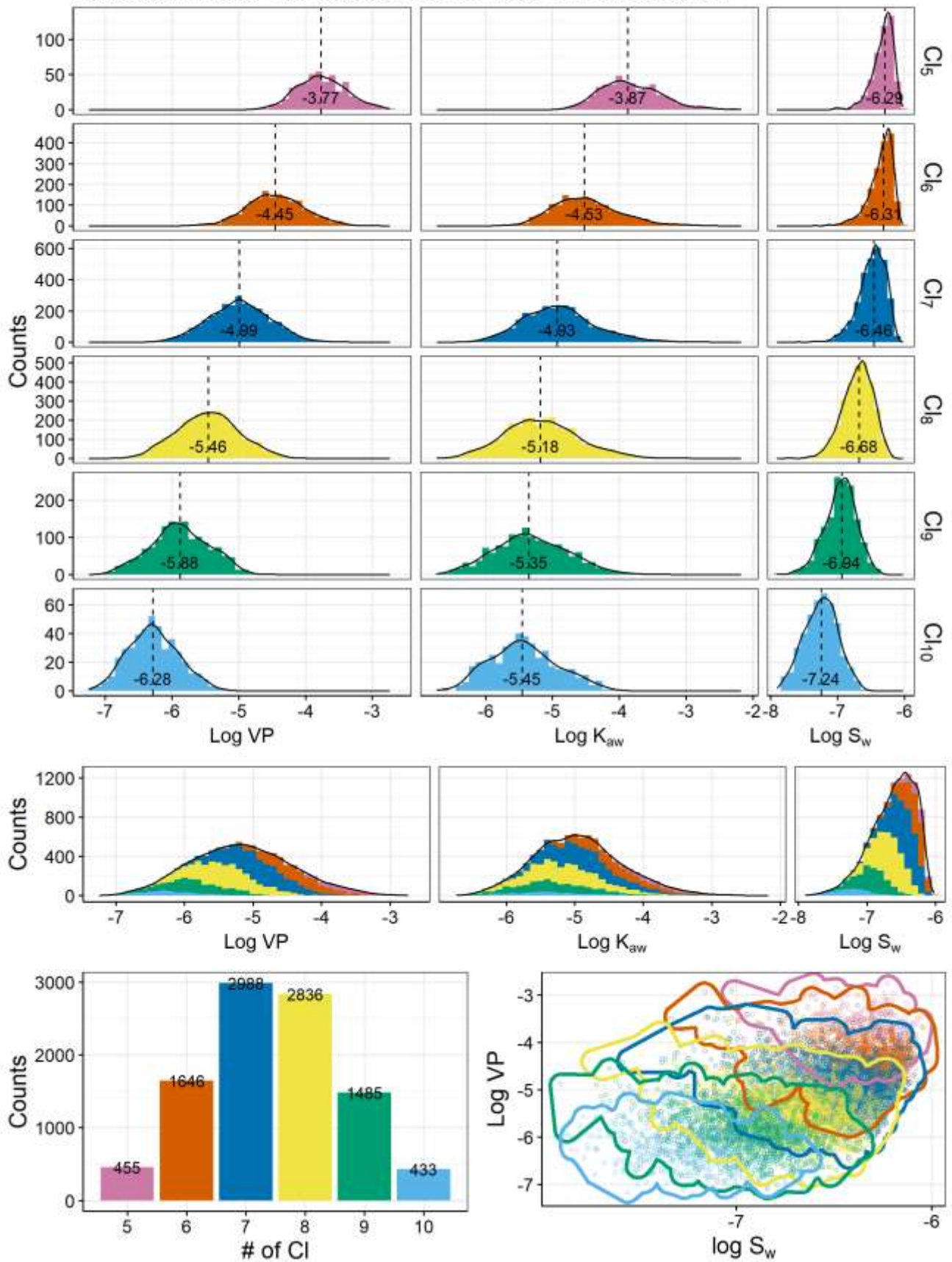
C13, 50wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



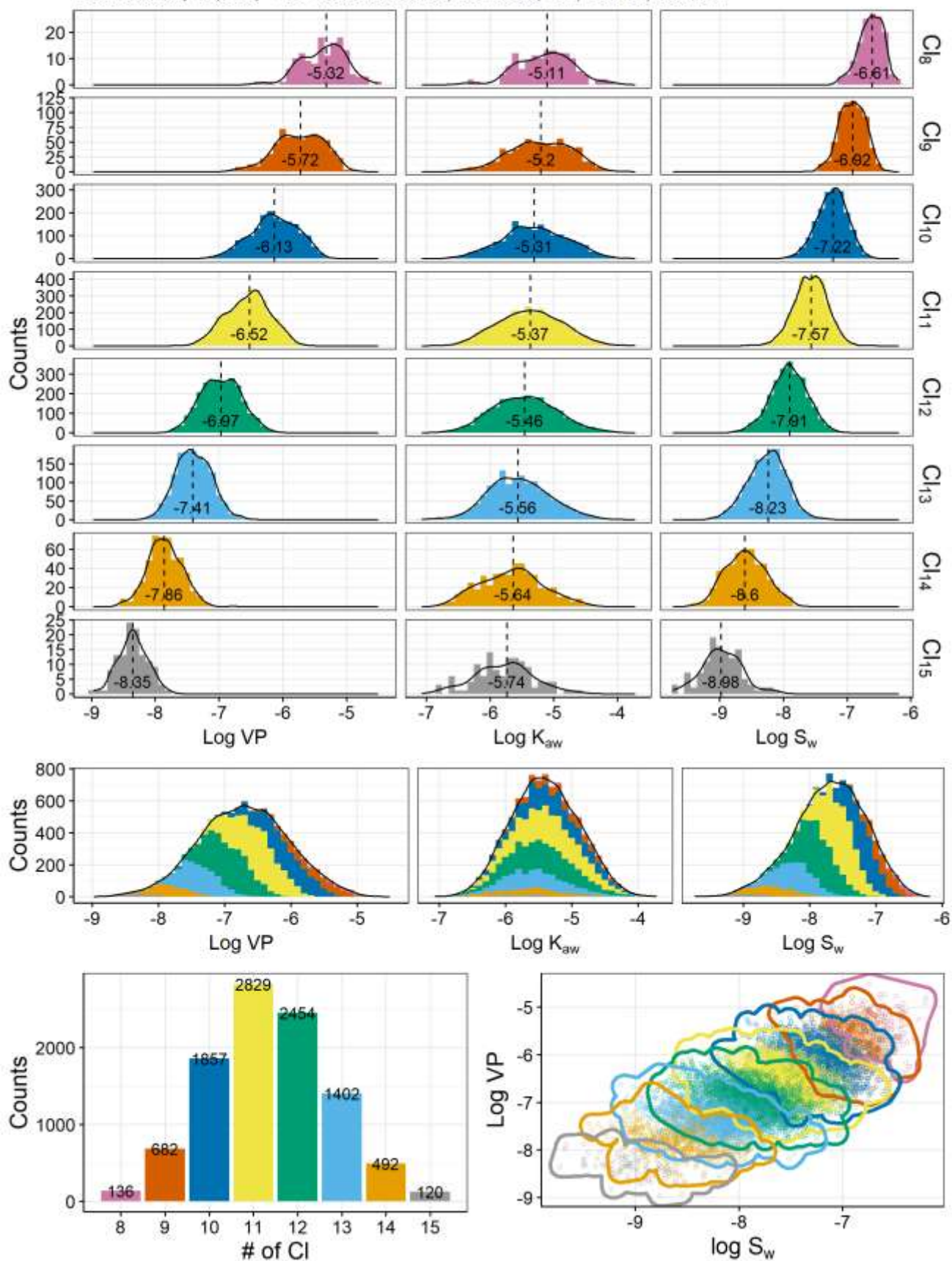
C13, 60wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



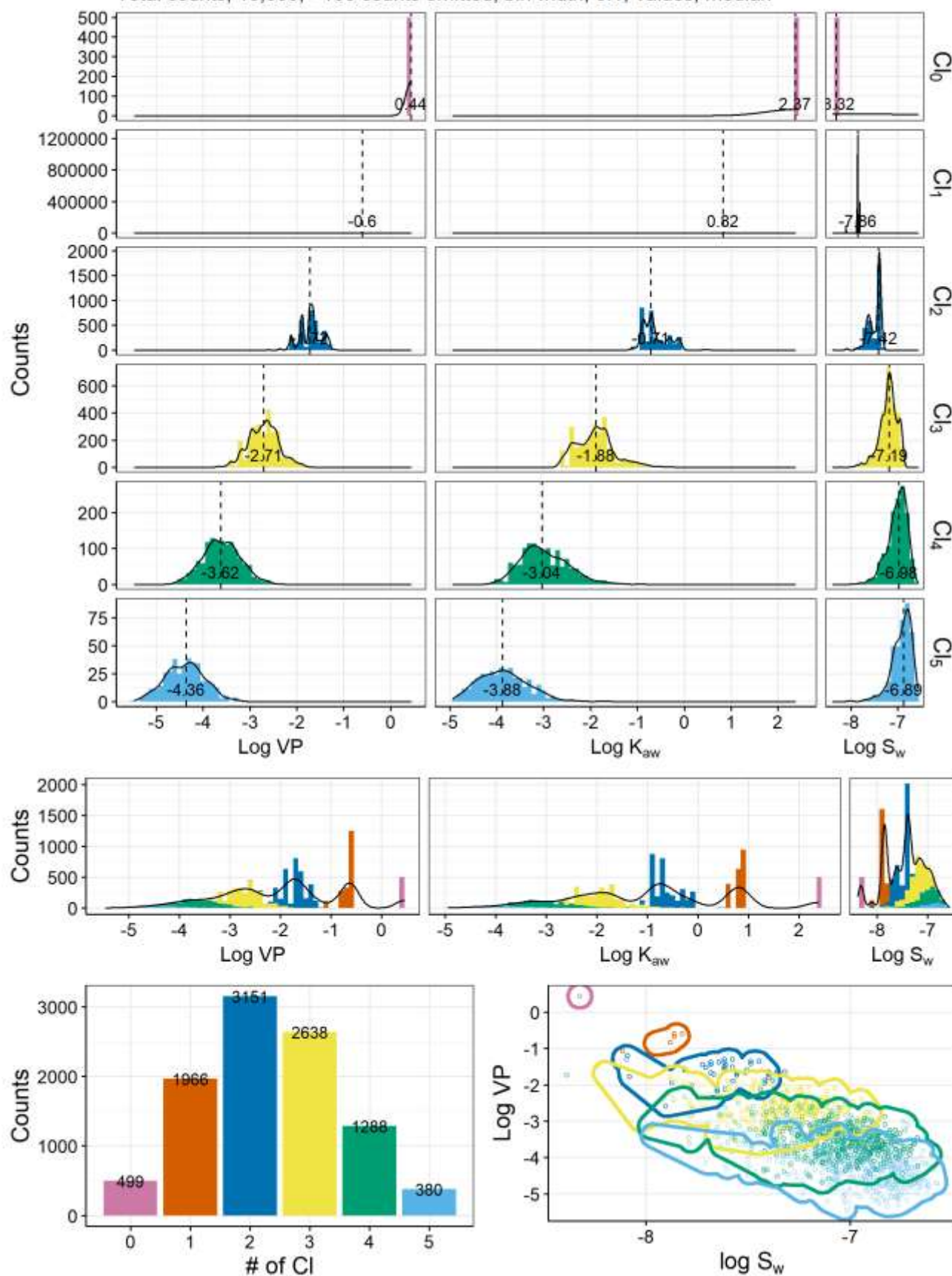
C13, 70wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



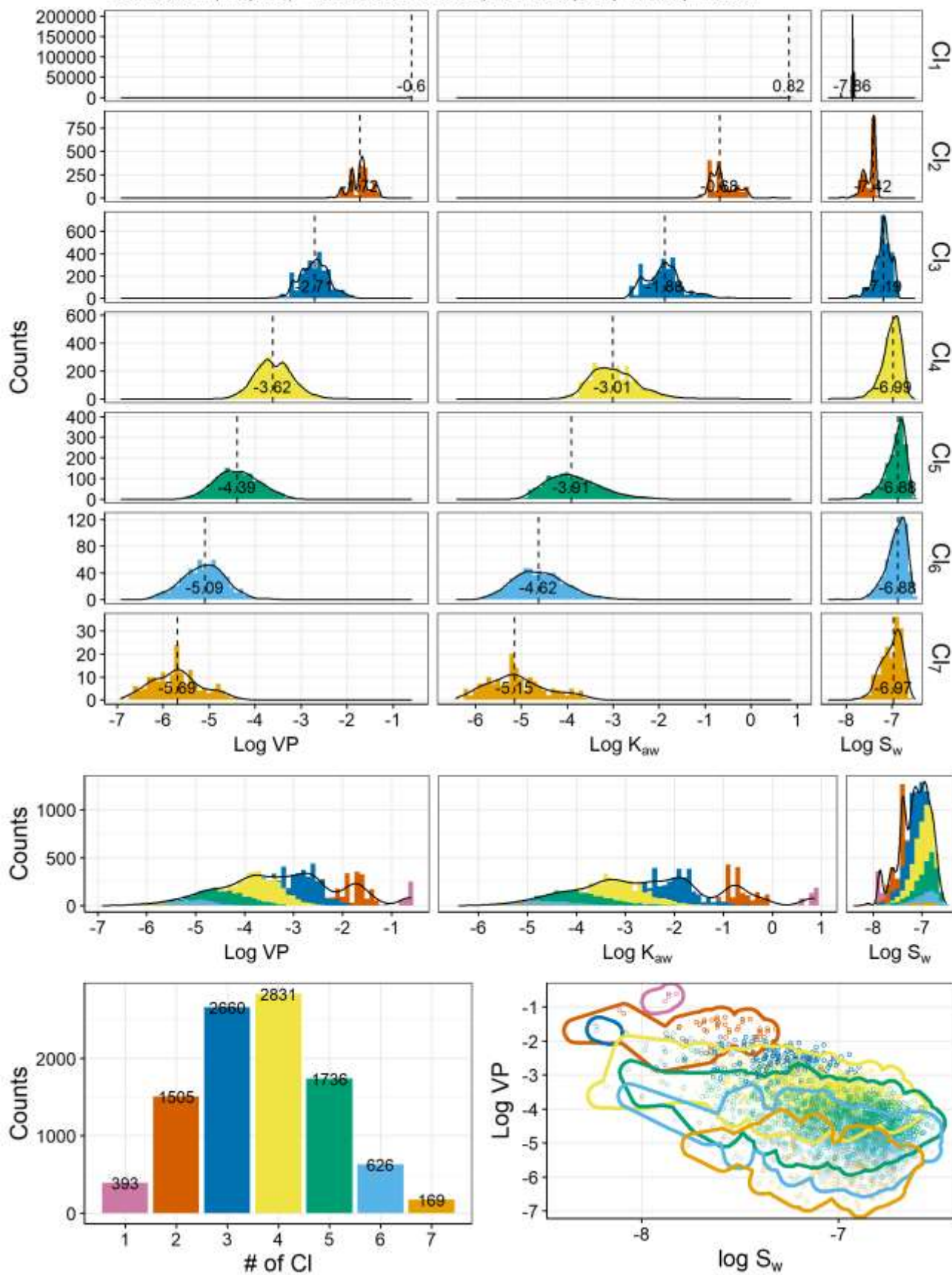
C14, 30wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



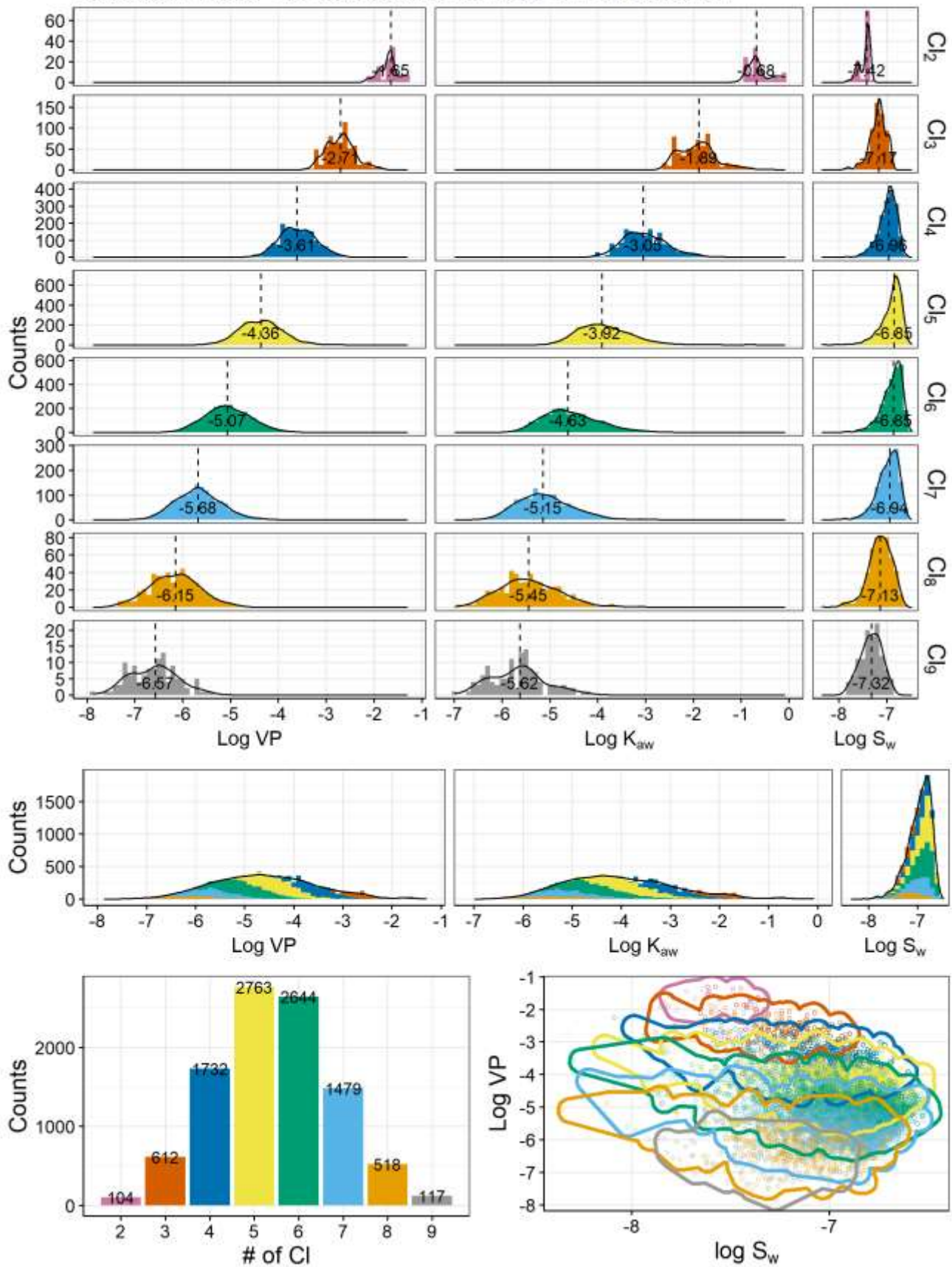
C14, 40wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



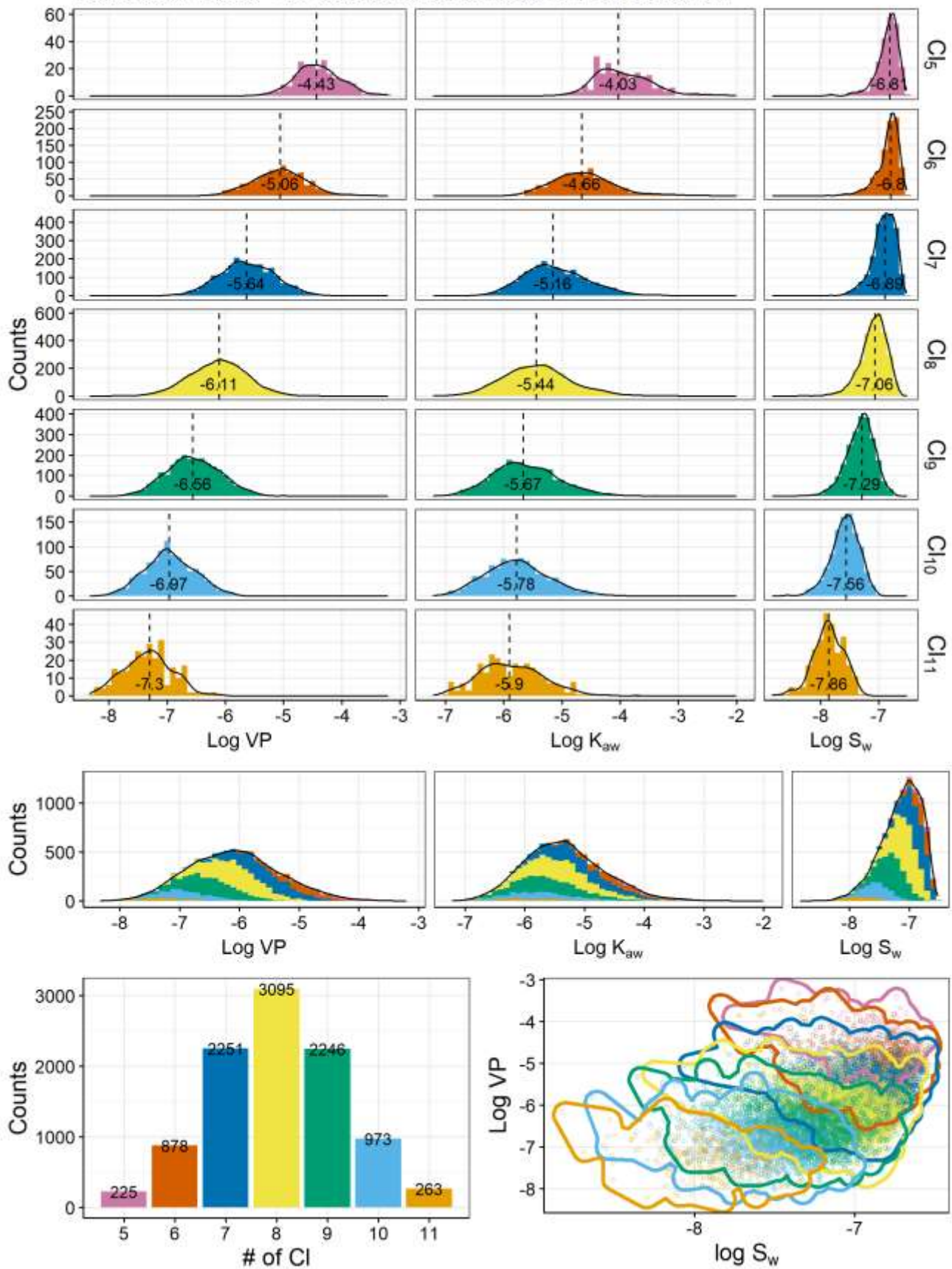
C14, 50wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



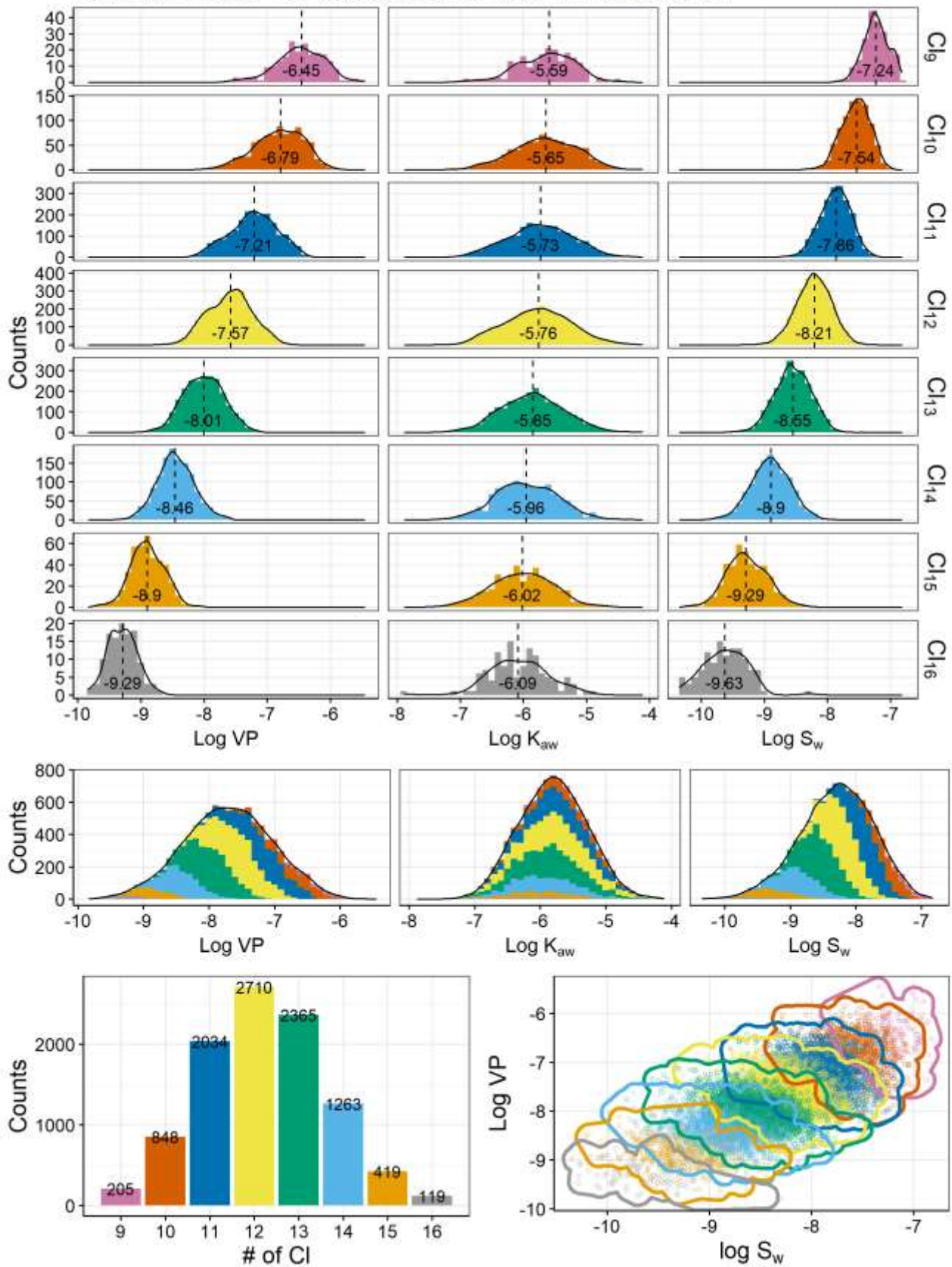
C14, 60wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



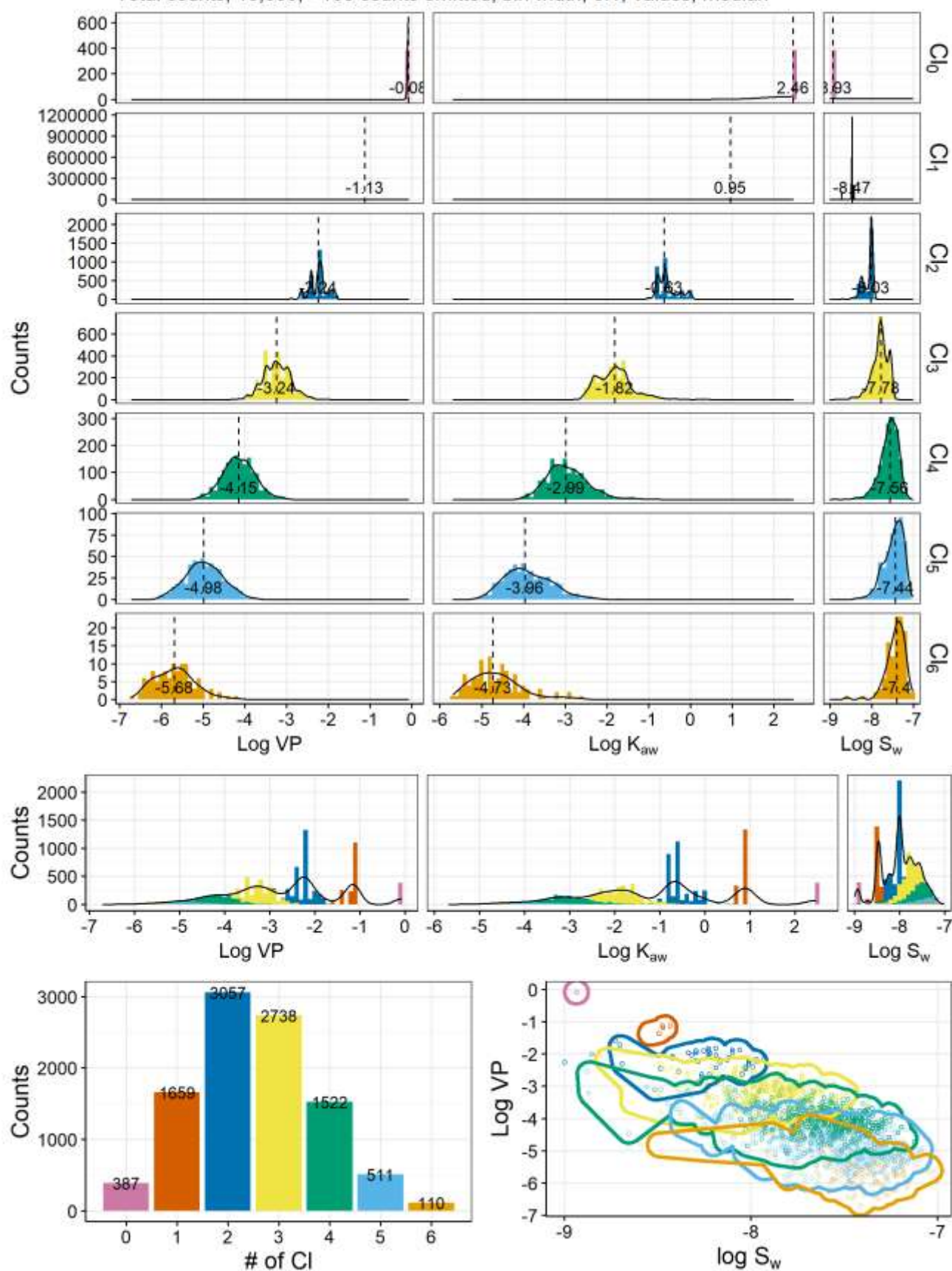
C14, 70wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



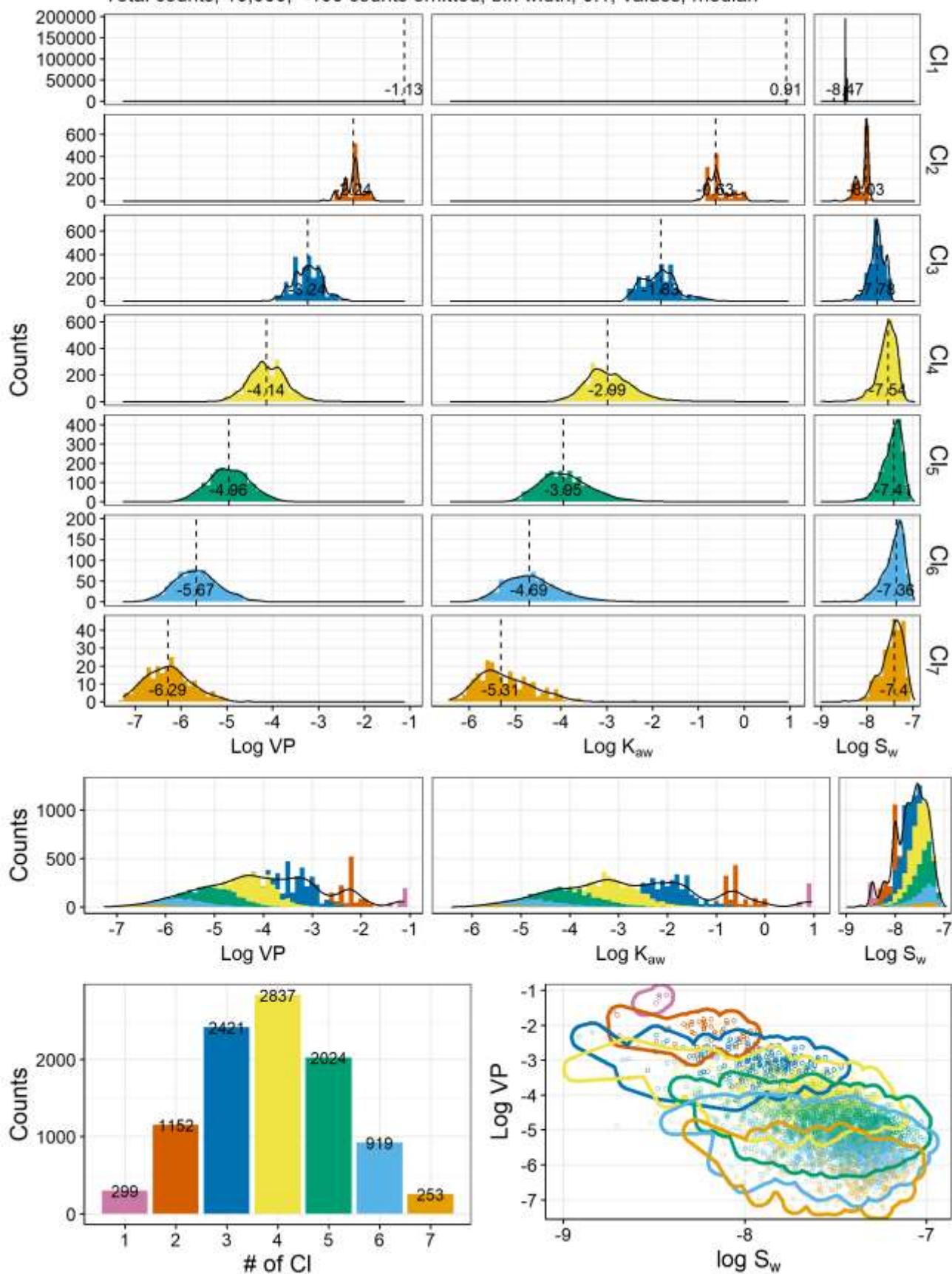
C15, 30wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



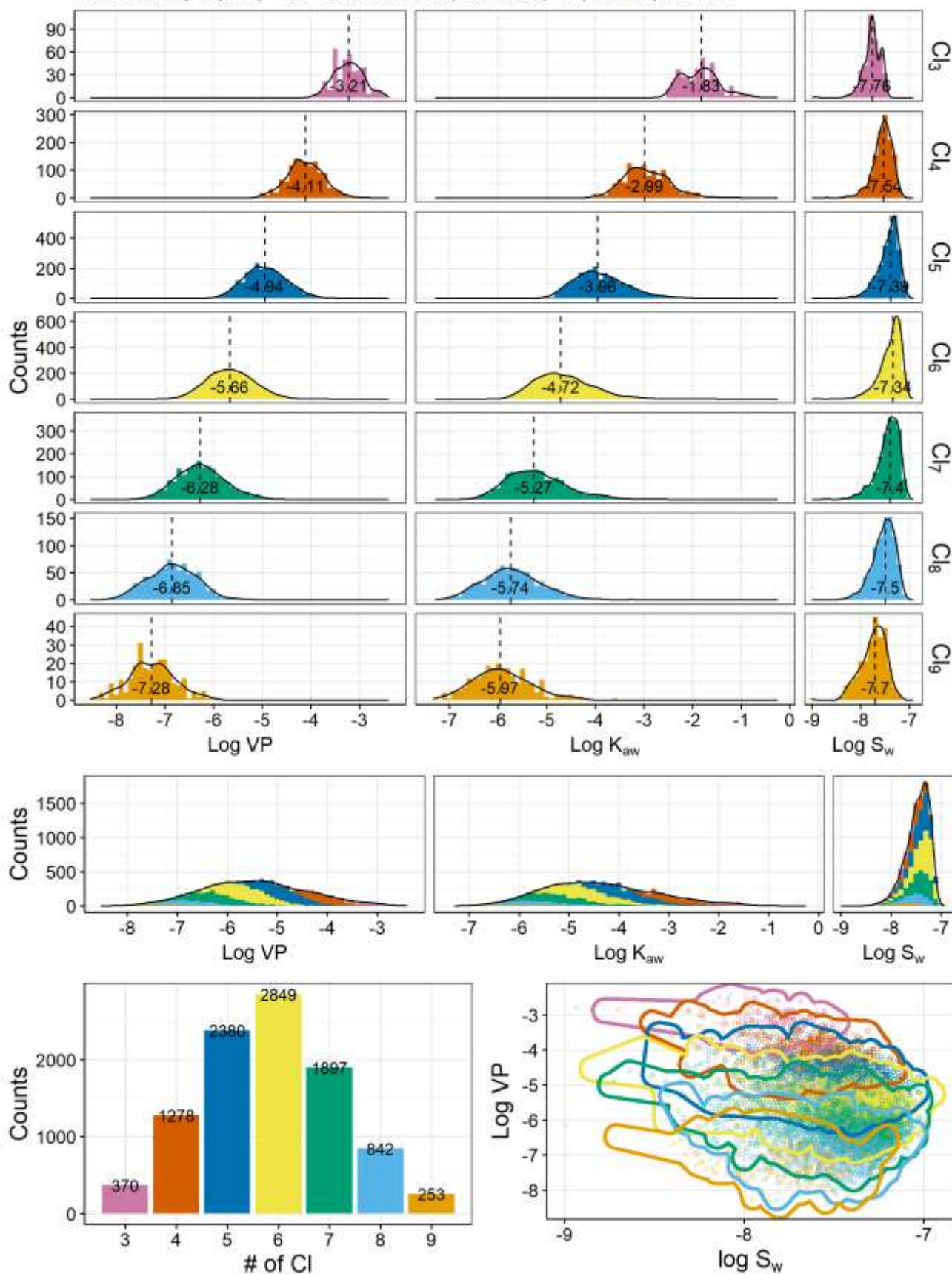
C15, 40wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



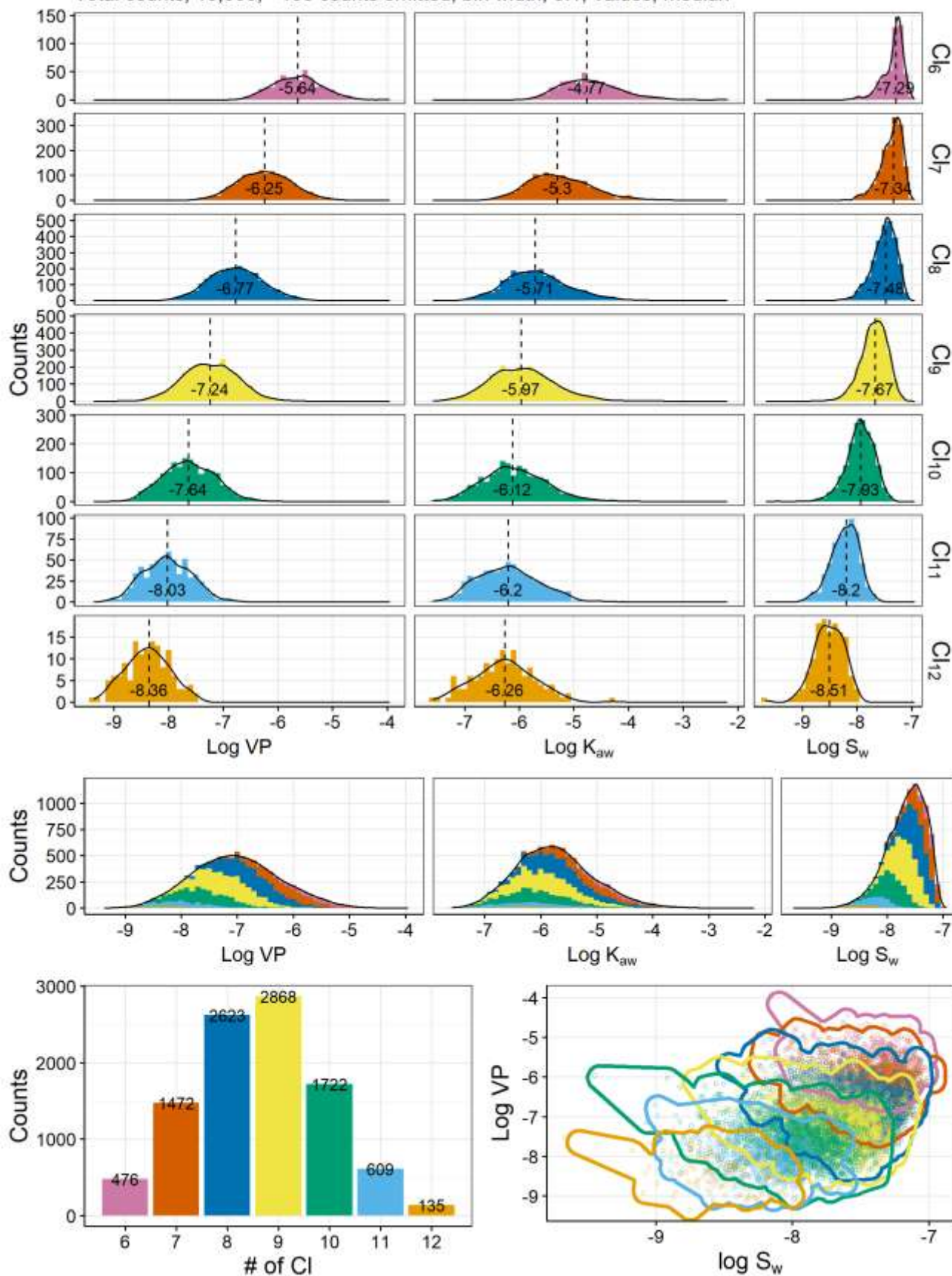
C15, 50wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



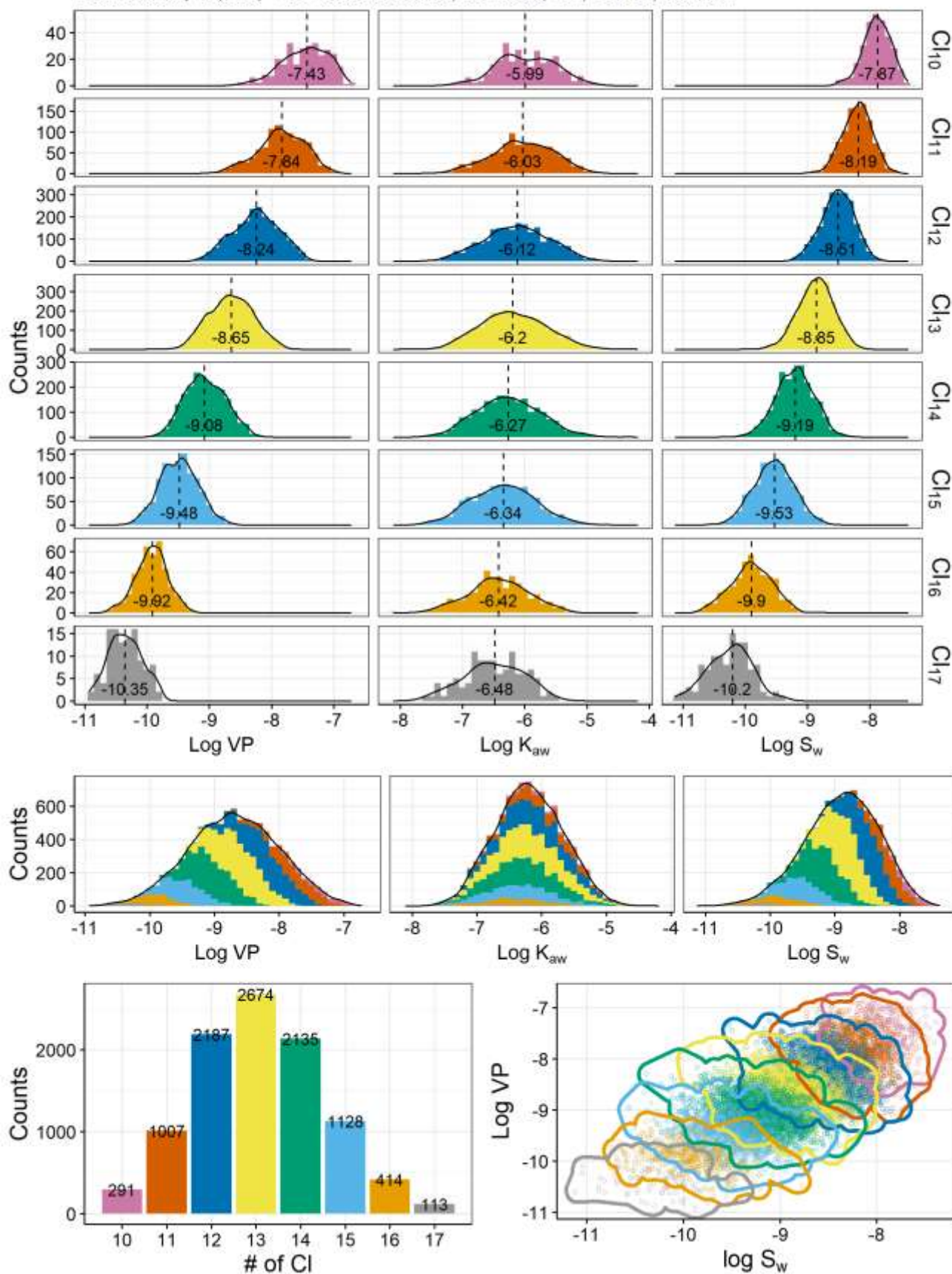
C15, 60wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



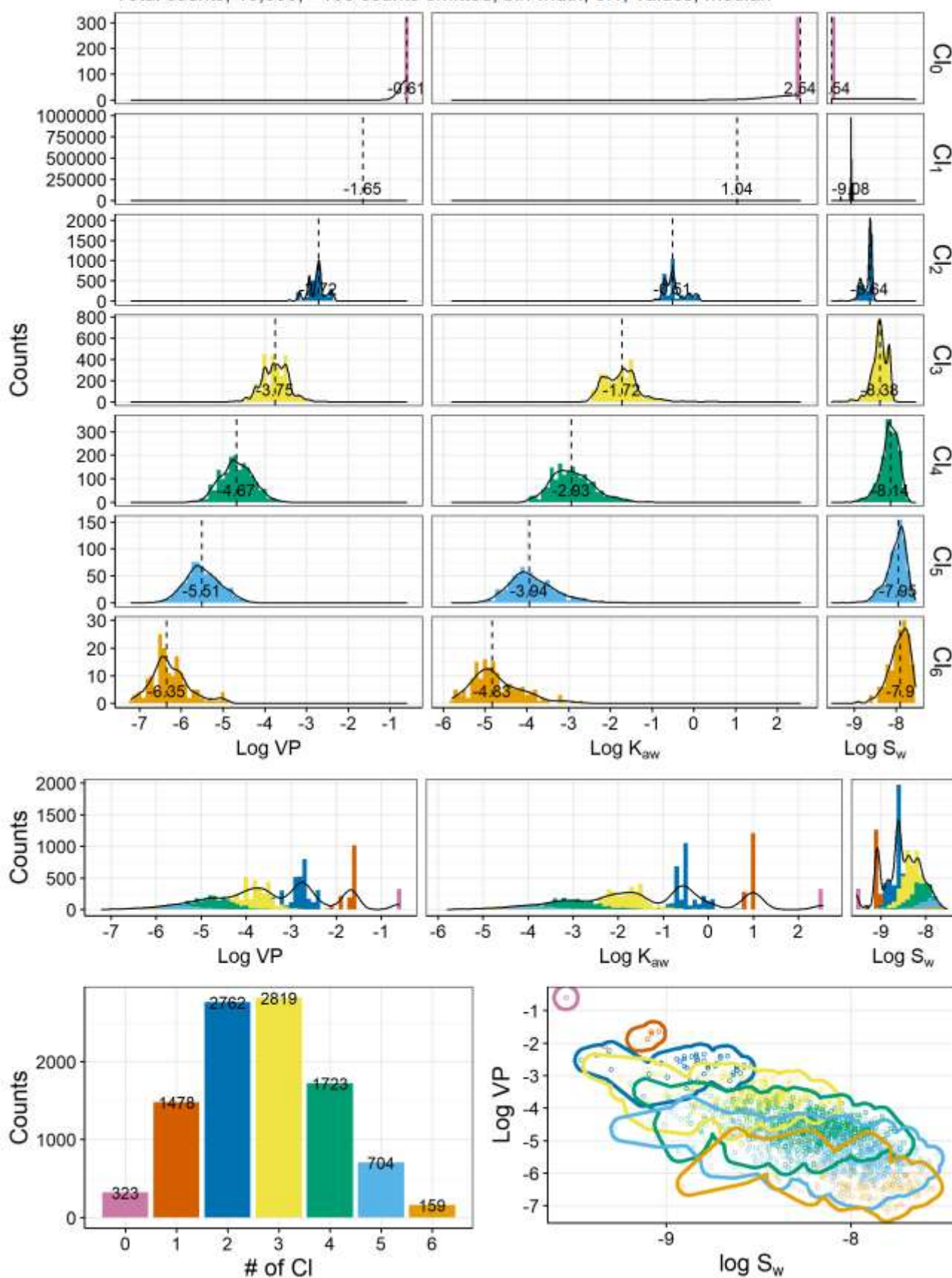
C15, 70wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



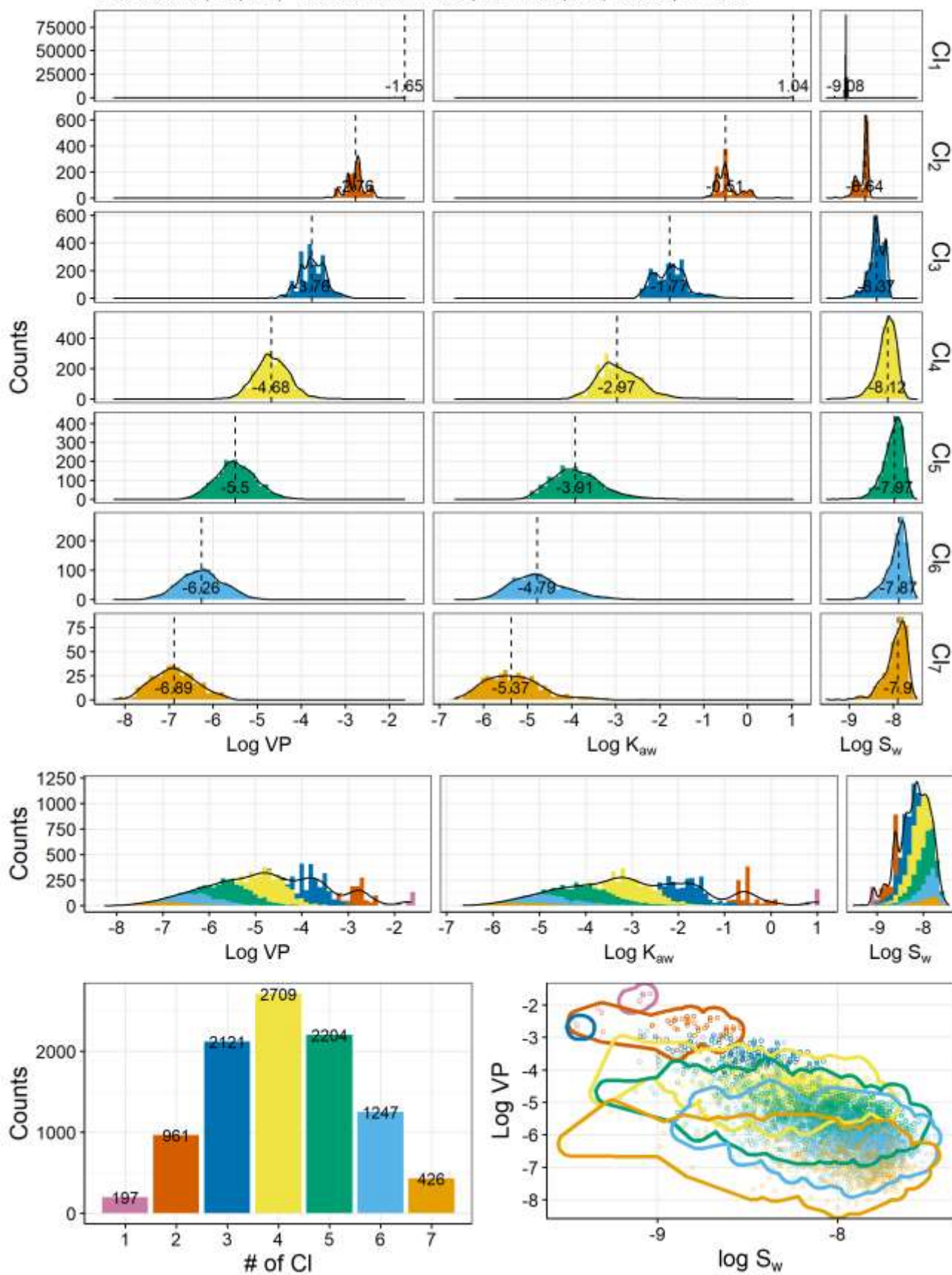
C16, 30wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



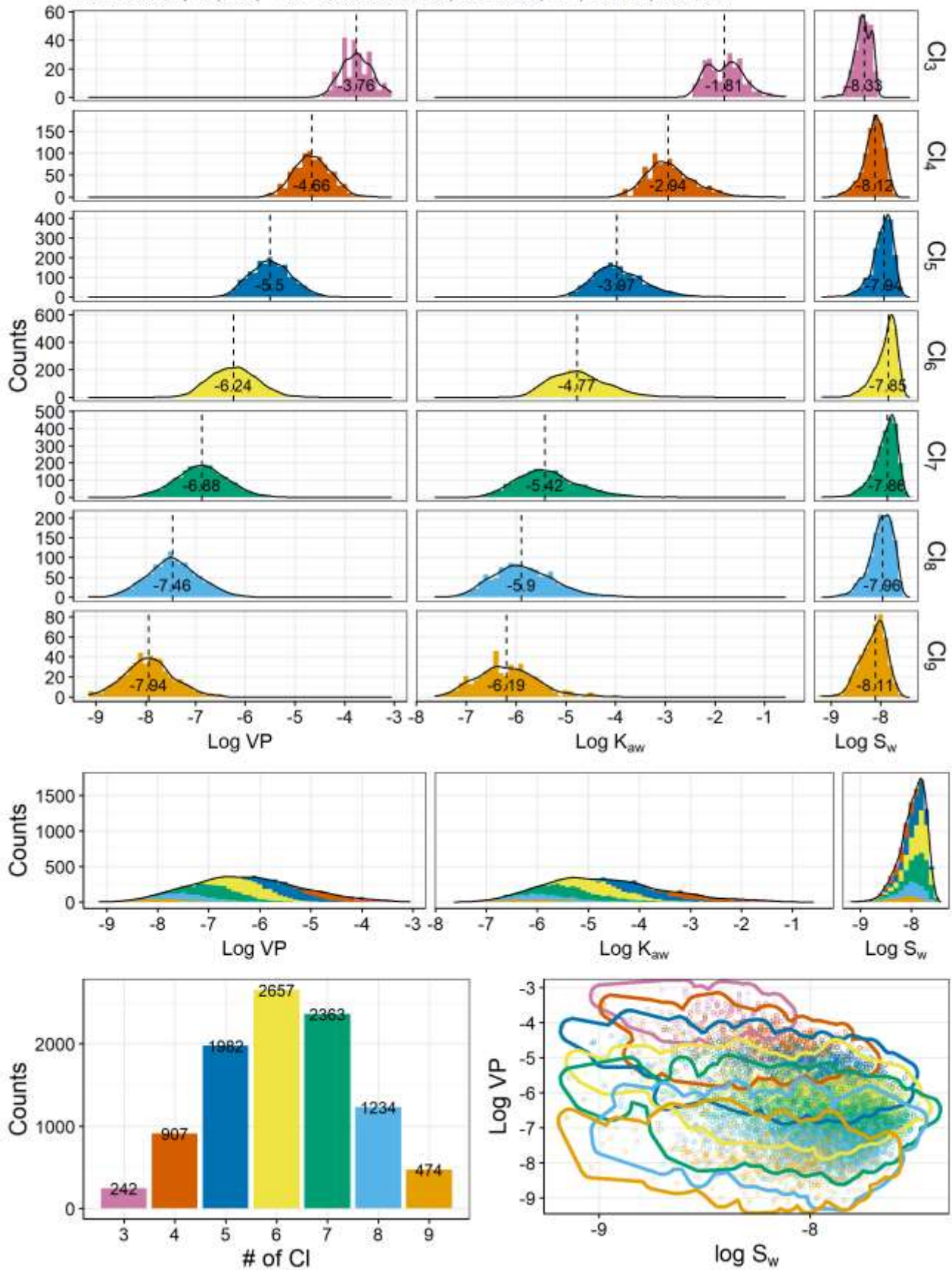
C16, 40wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



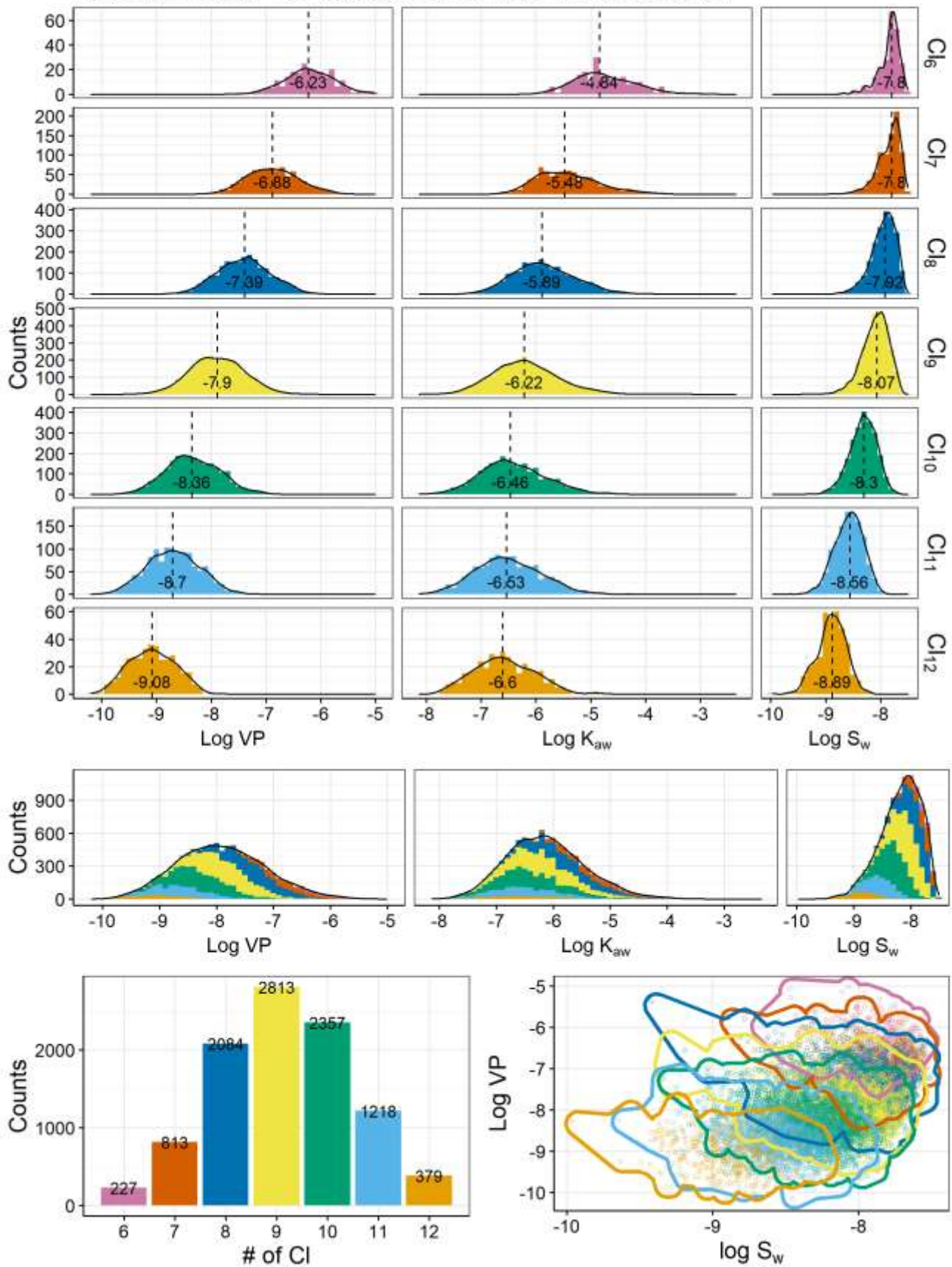
C16, 50wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



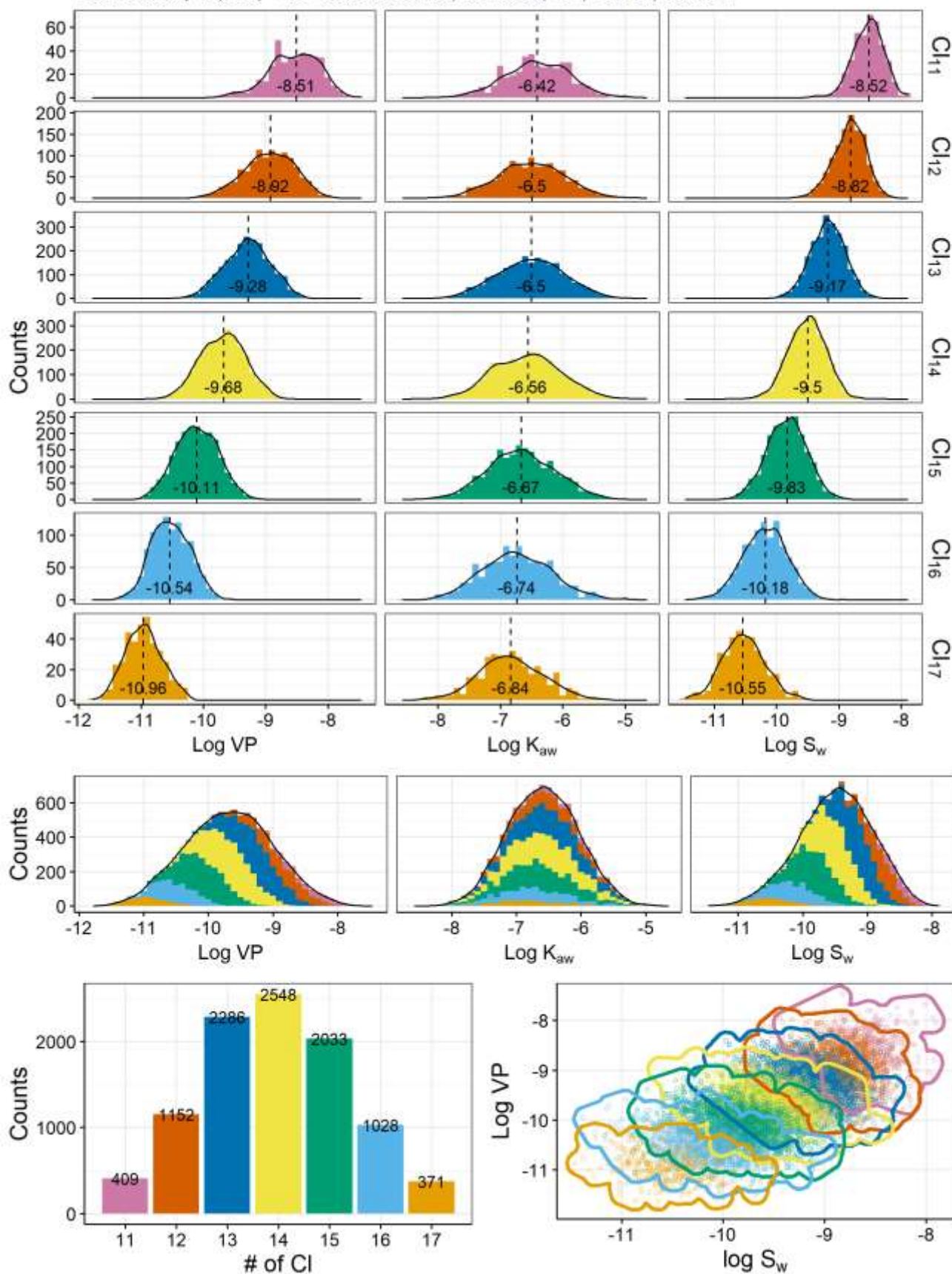
C16, 60wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



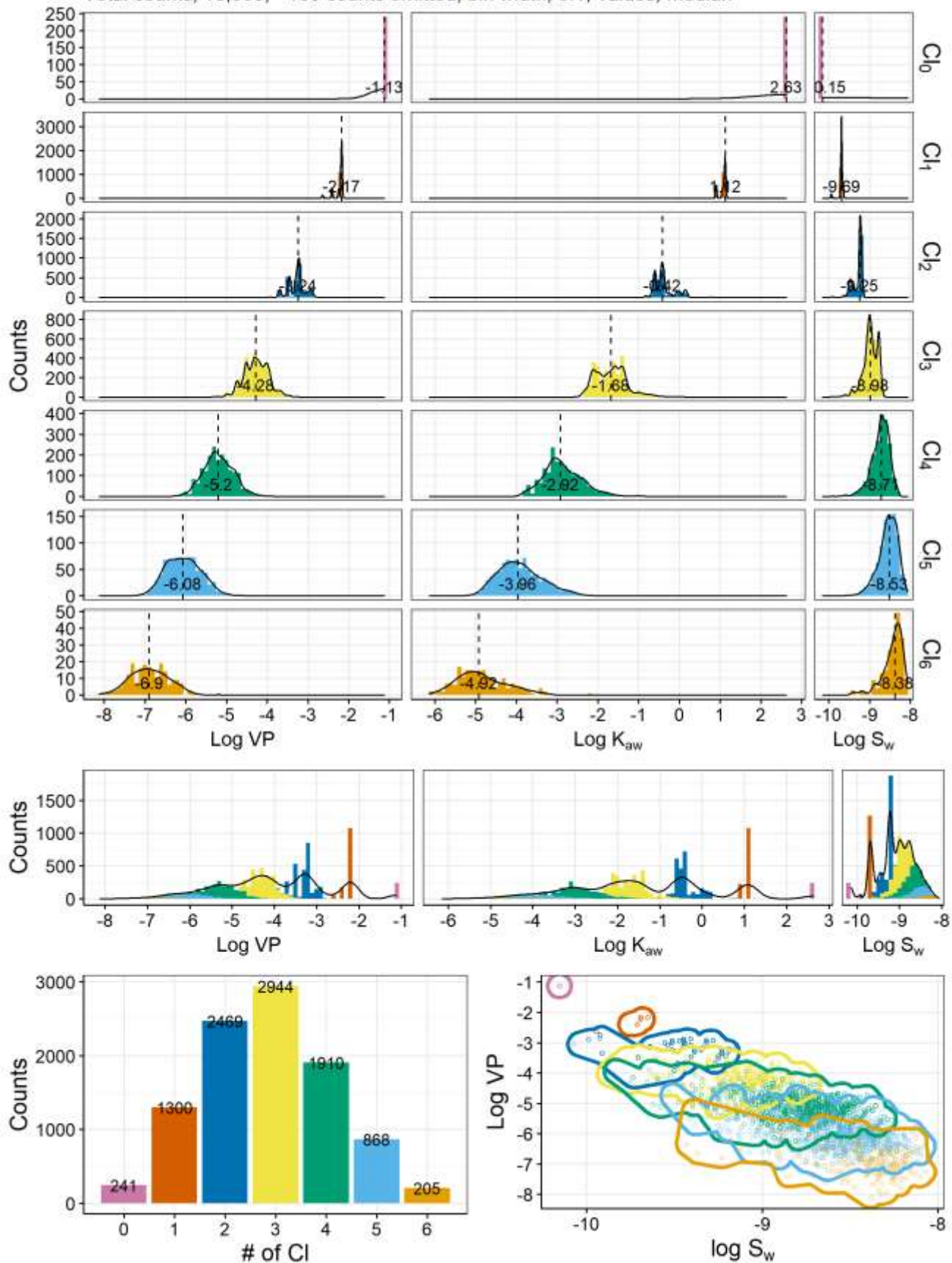
C16, 70wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



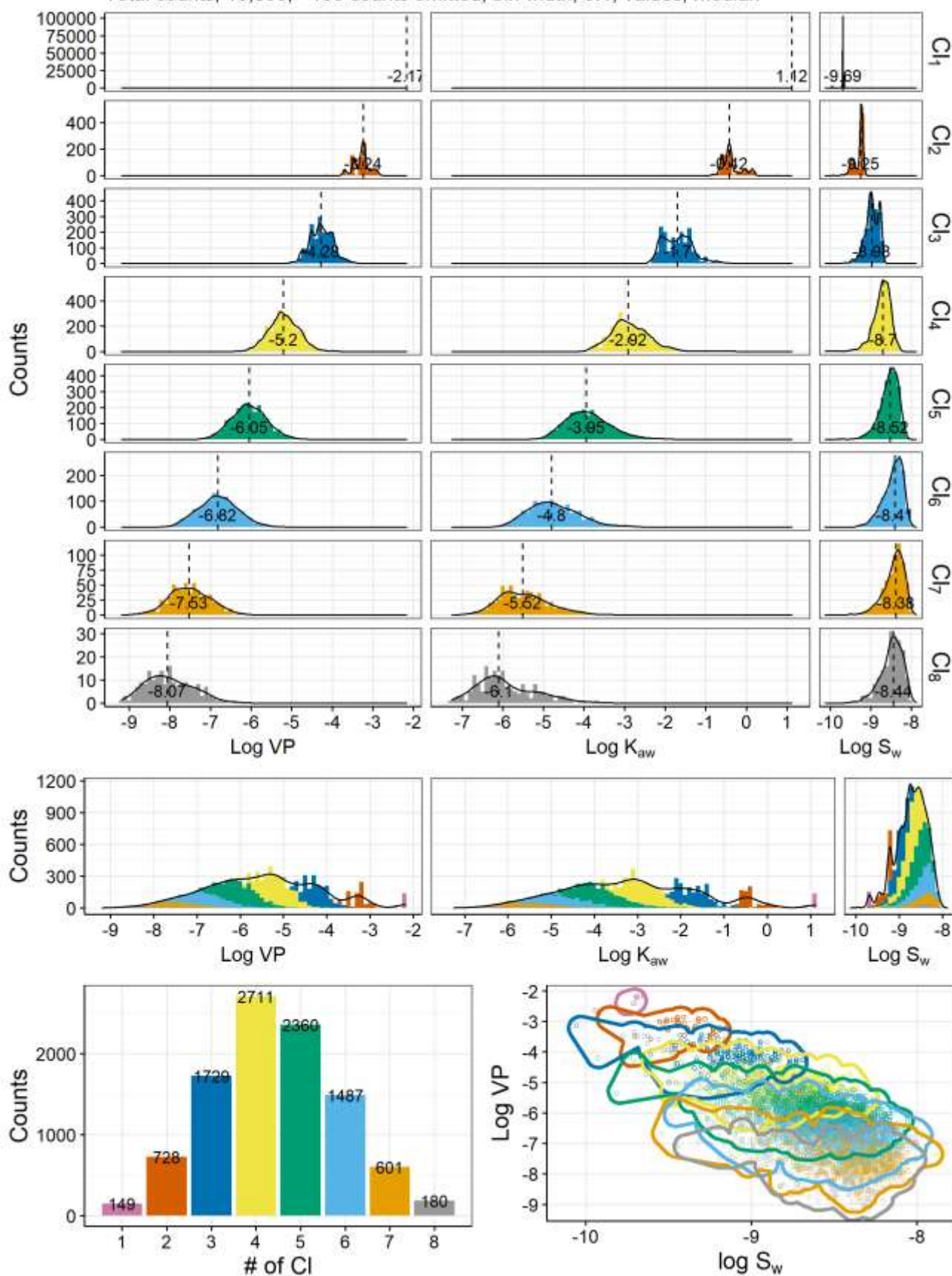
C17, 30wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



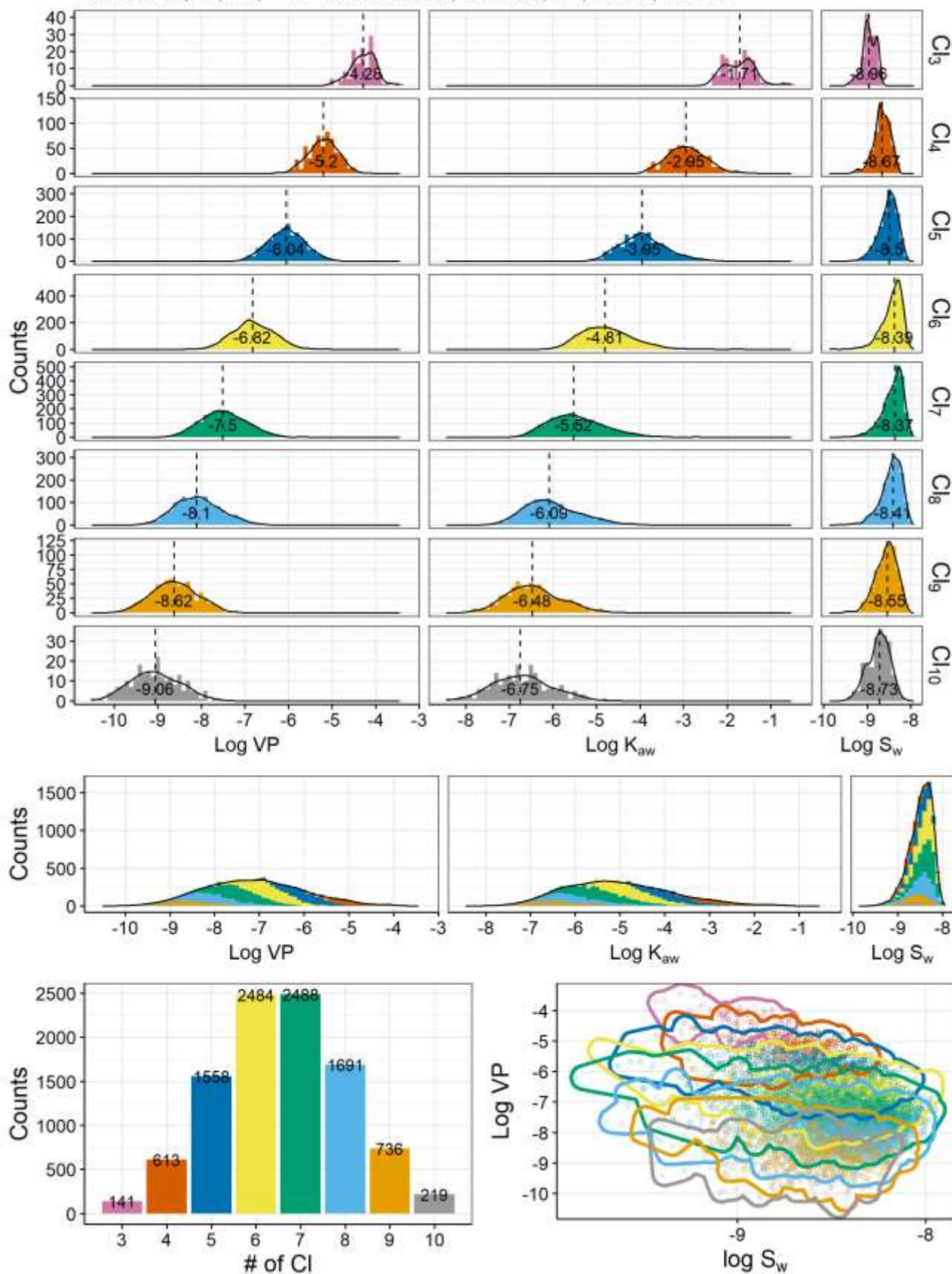
C17, 40wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



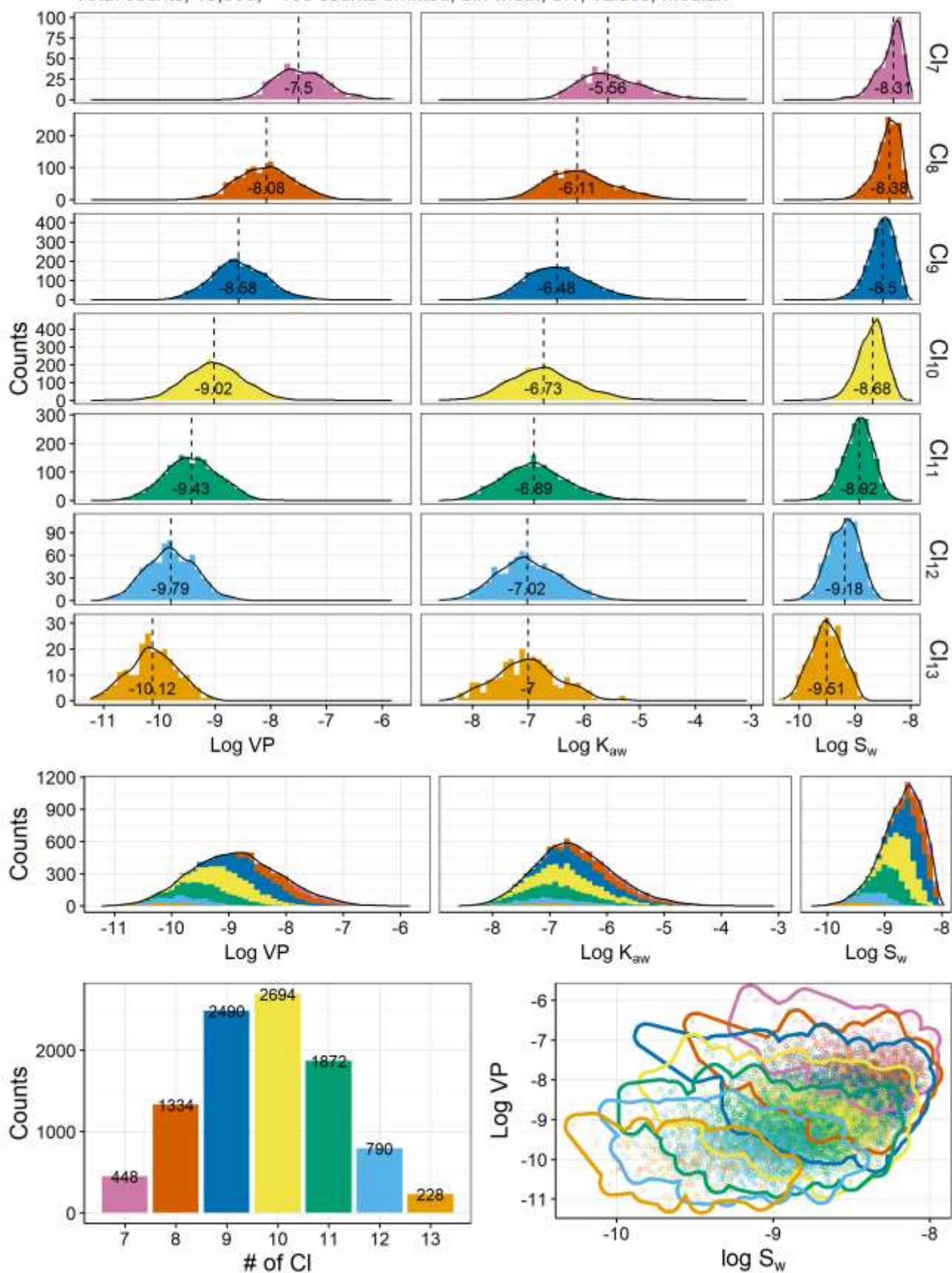
C17, 50wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



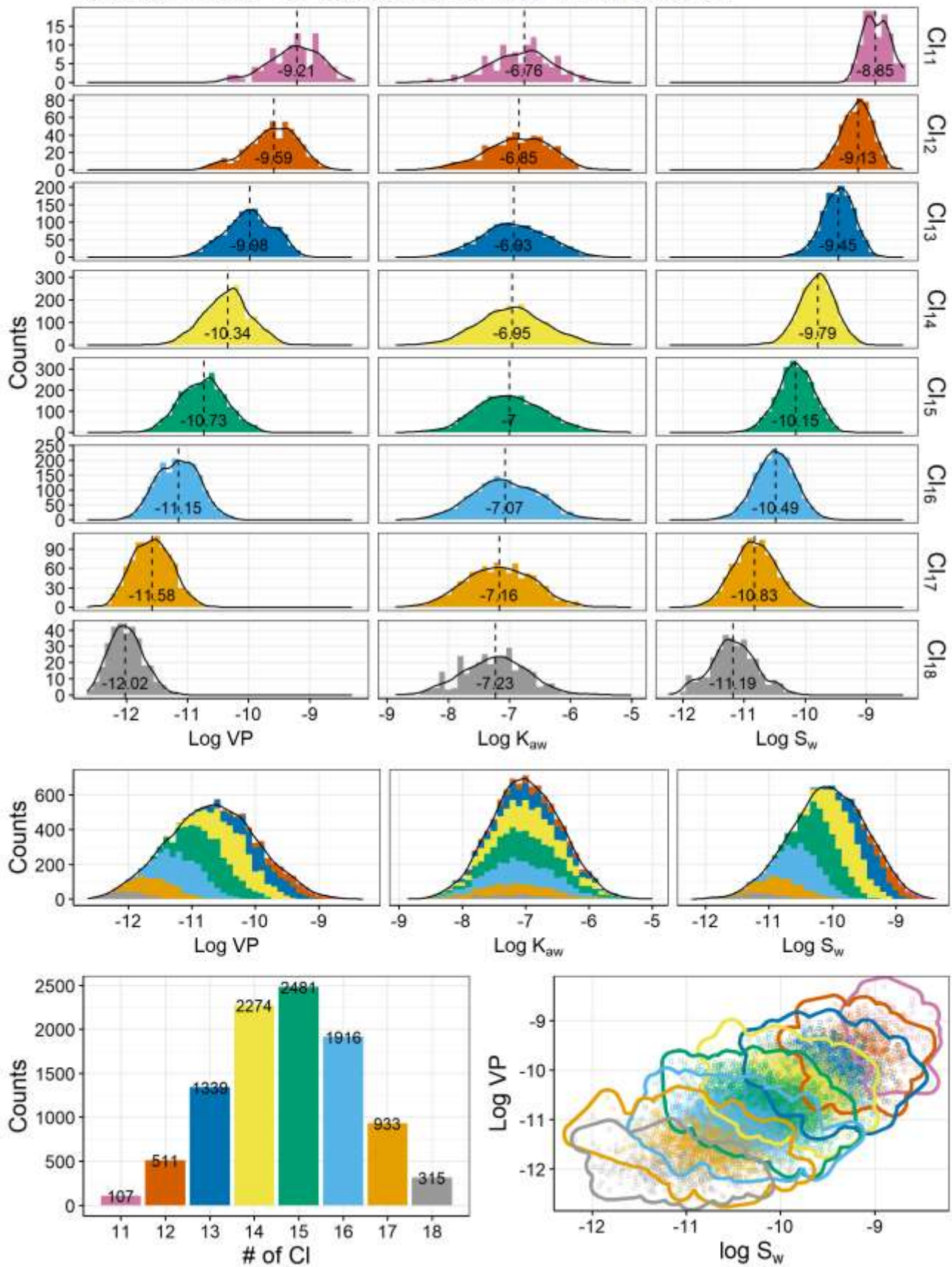
C17, 60wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



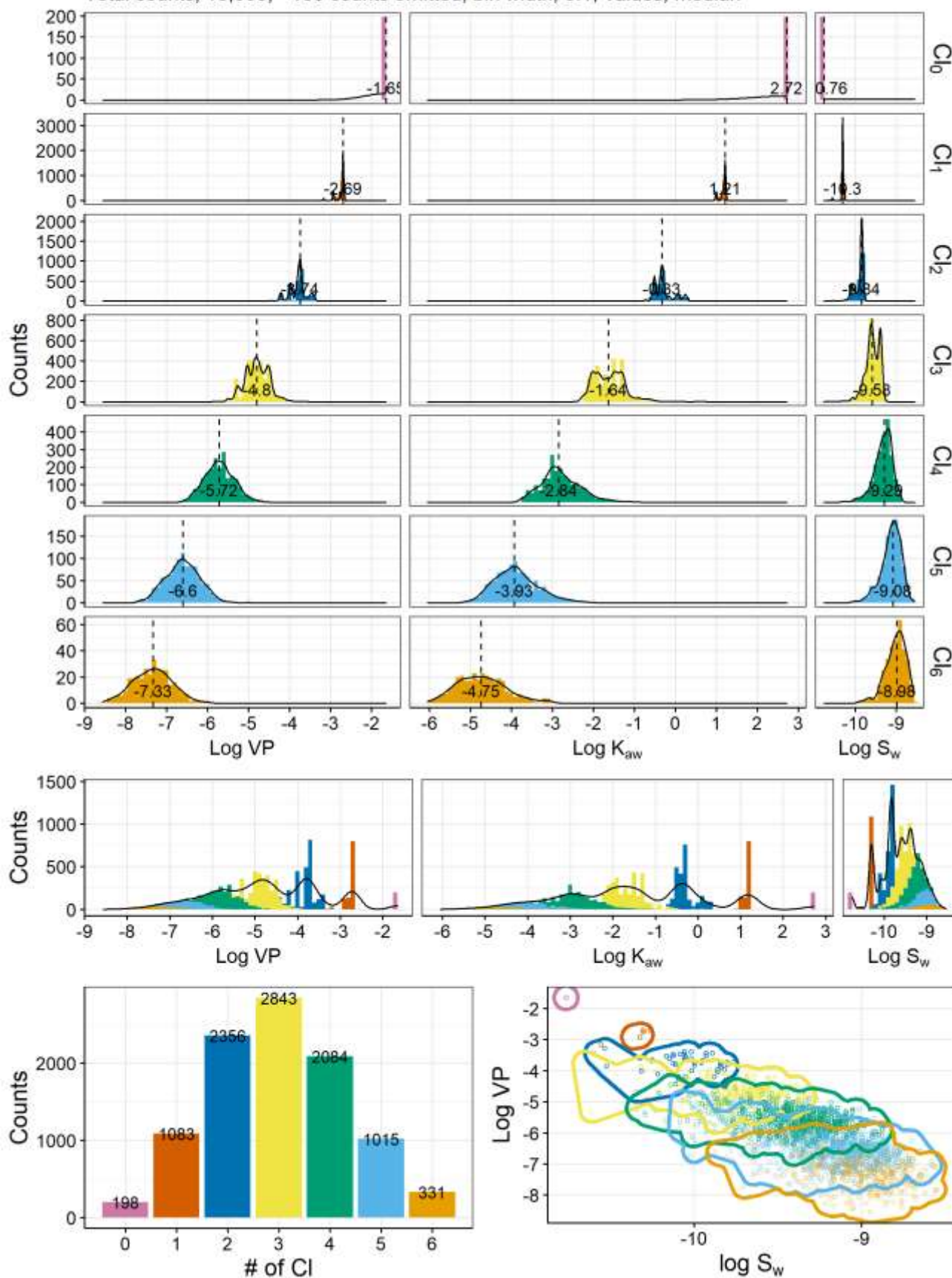
C17, 70wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



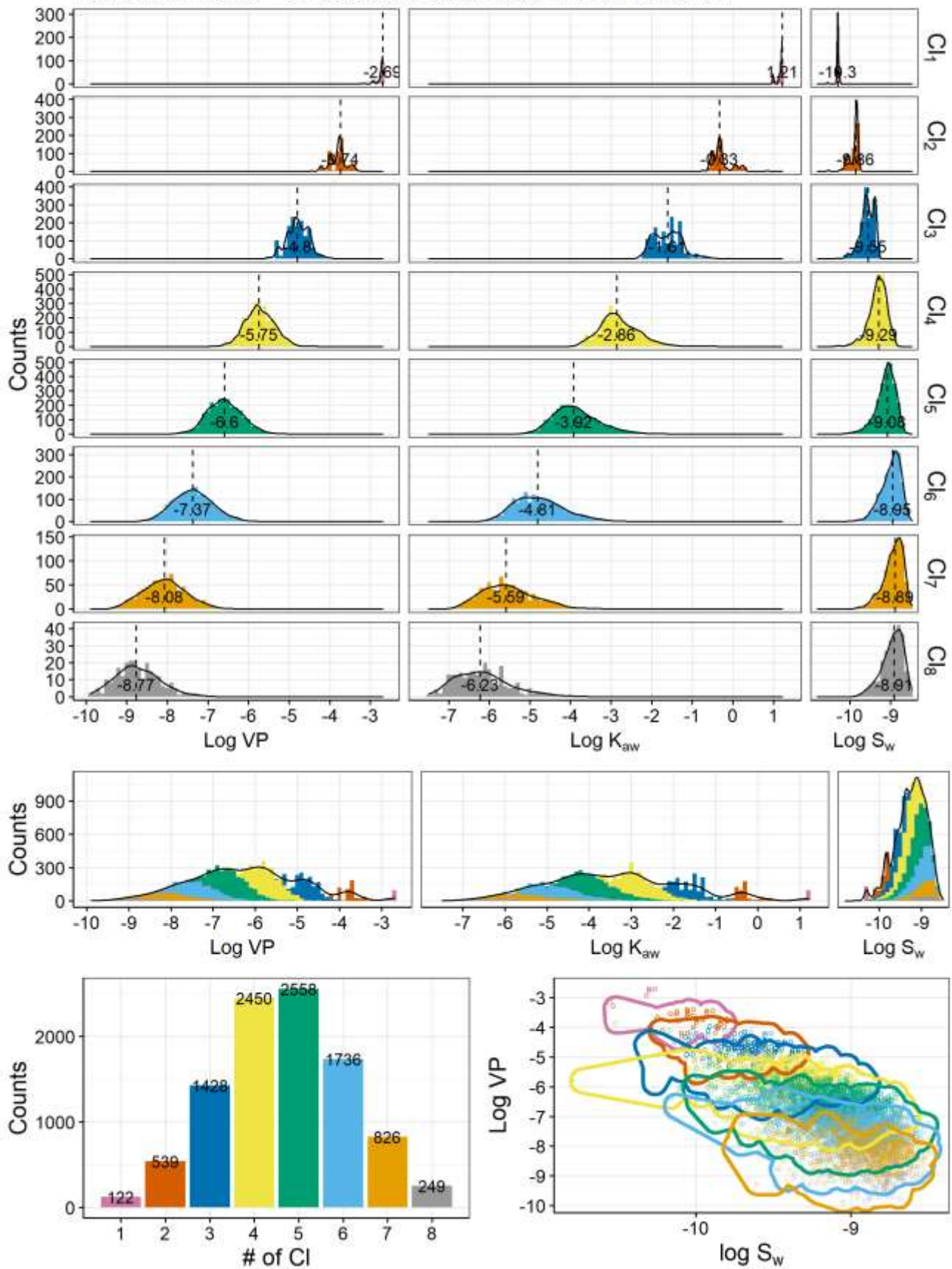
C18, 30wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



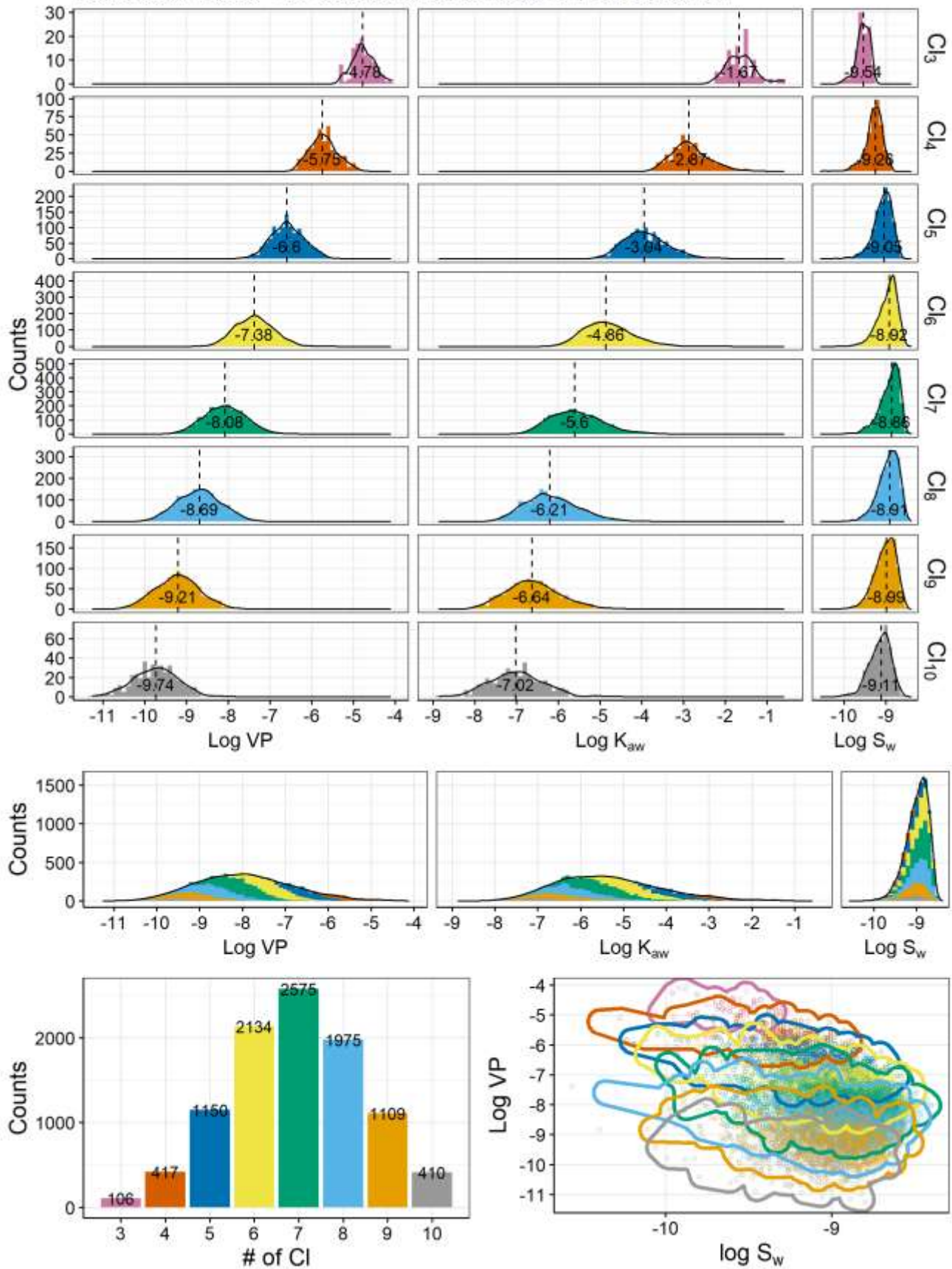
C18, 40wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



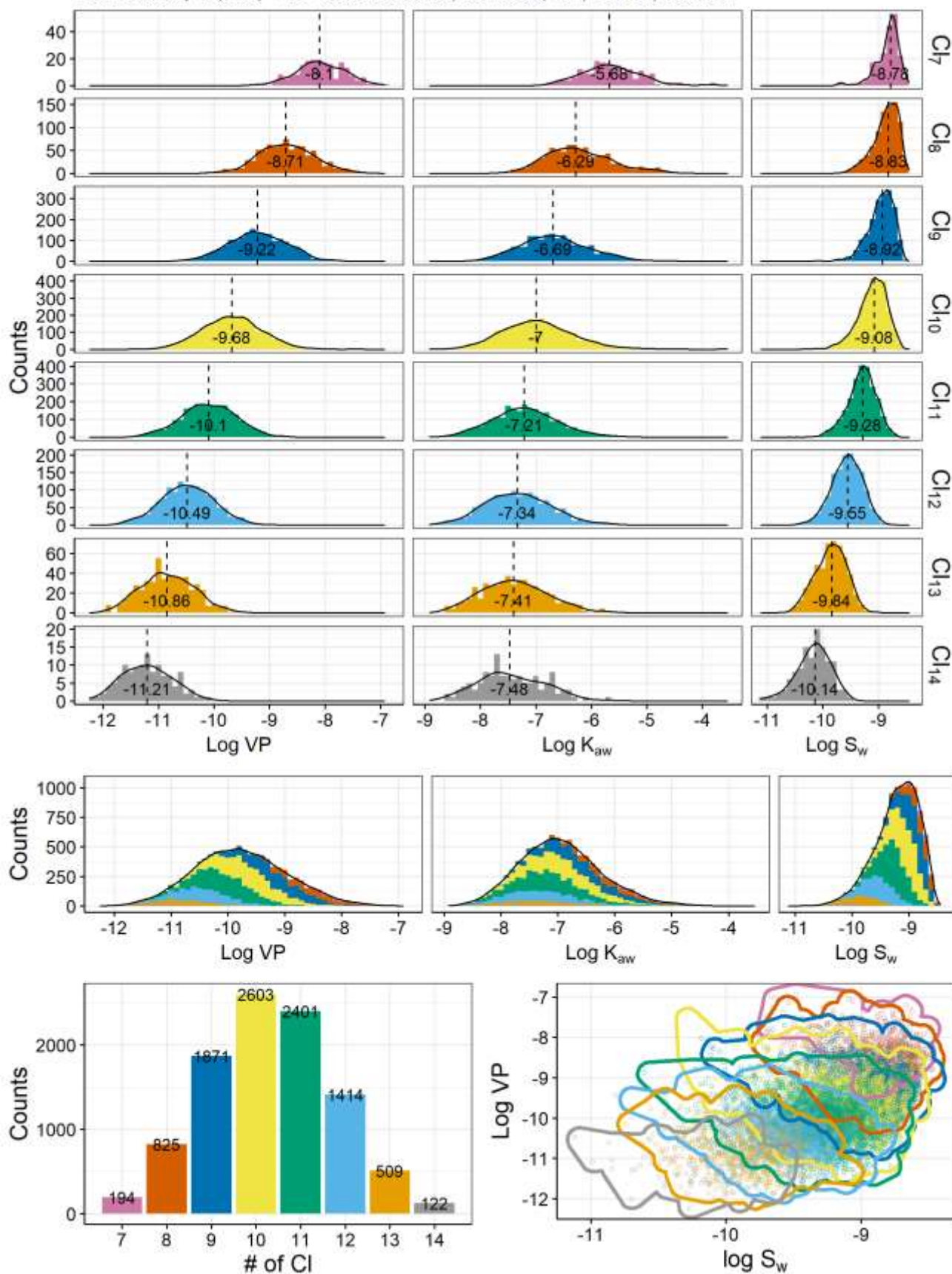
C18, 50wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



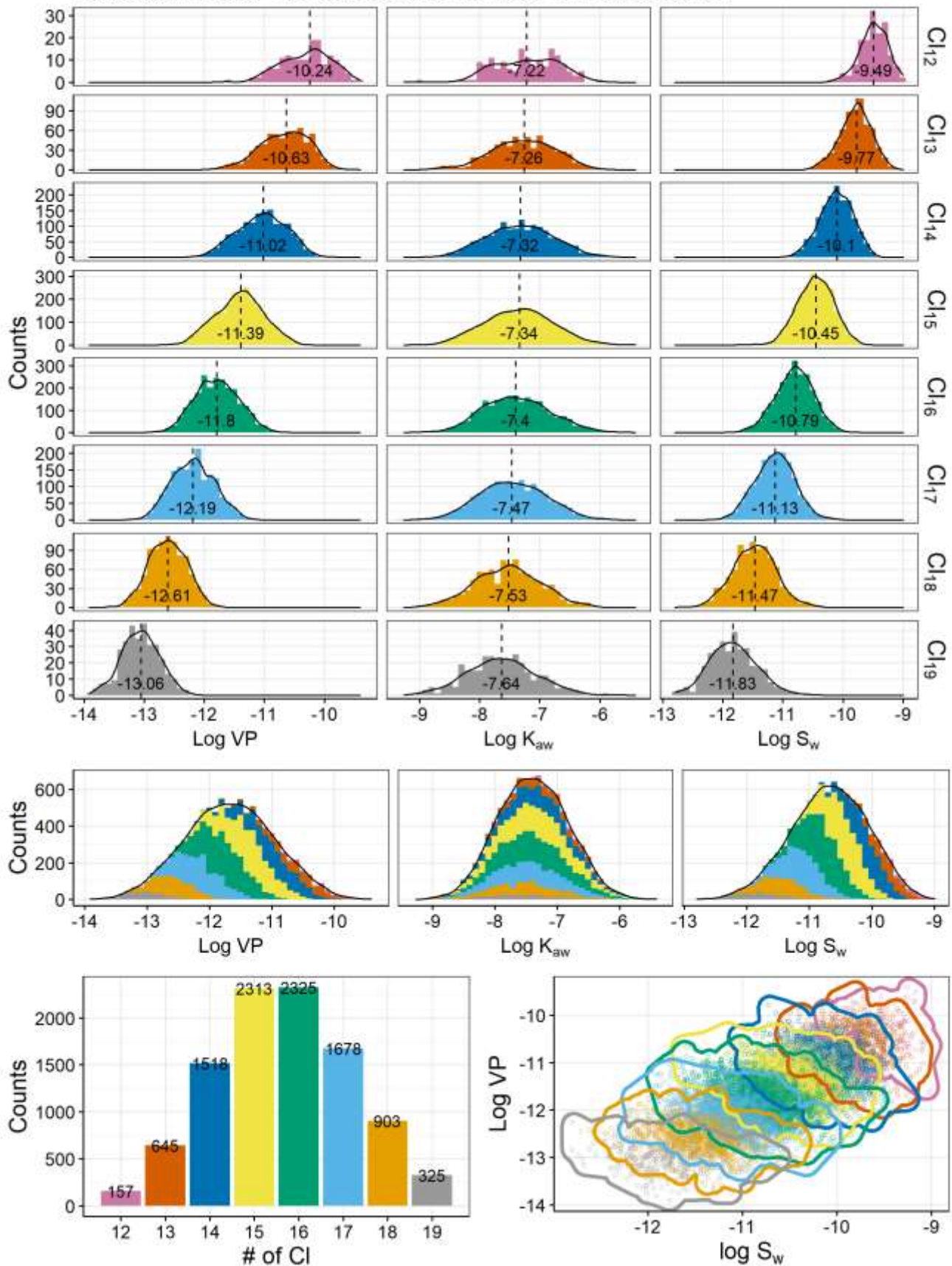
C18, 60wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



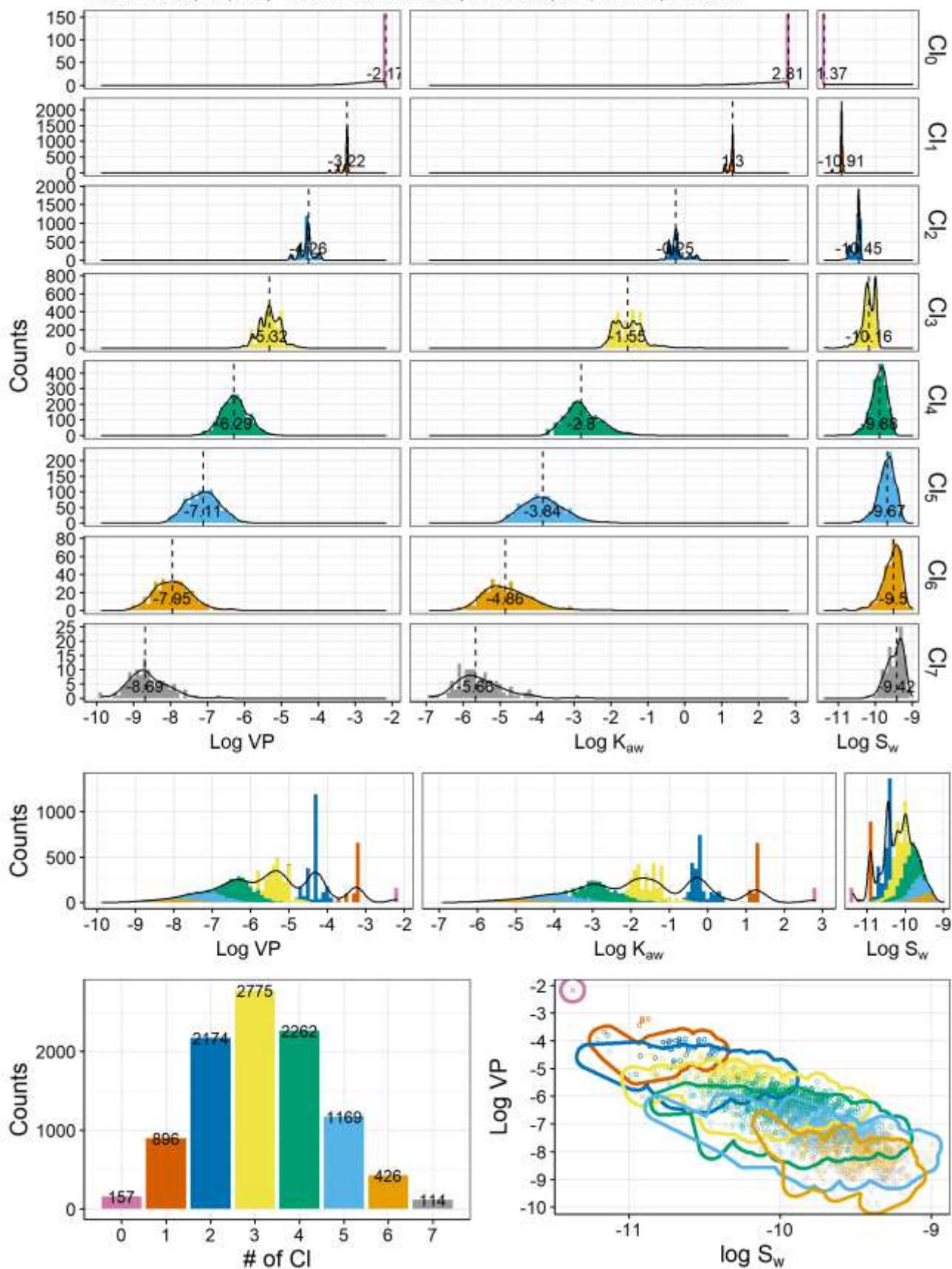
C18, 70wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



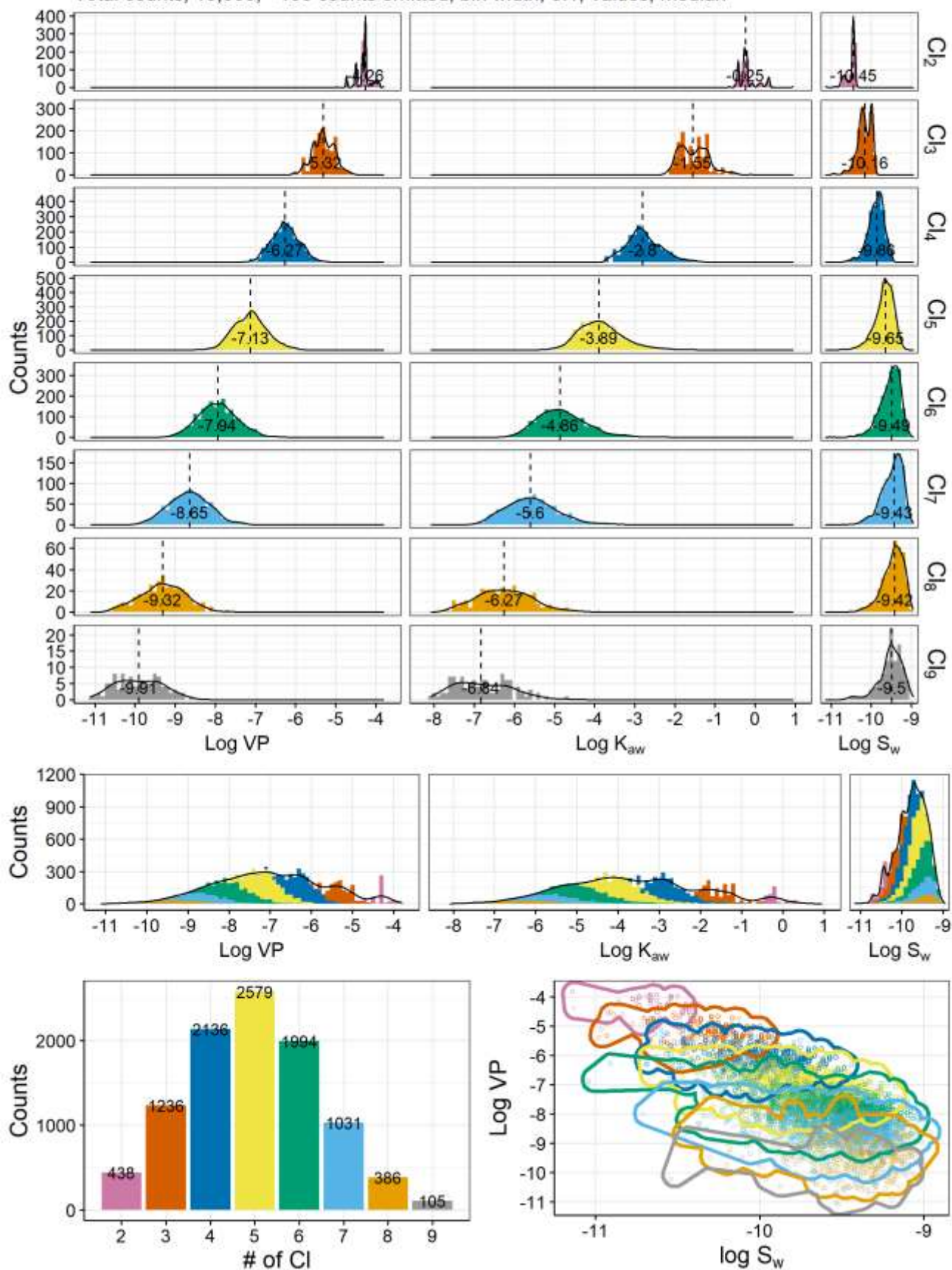
C19, 30wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



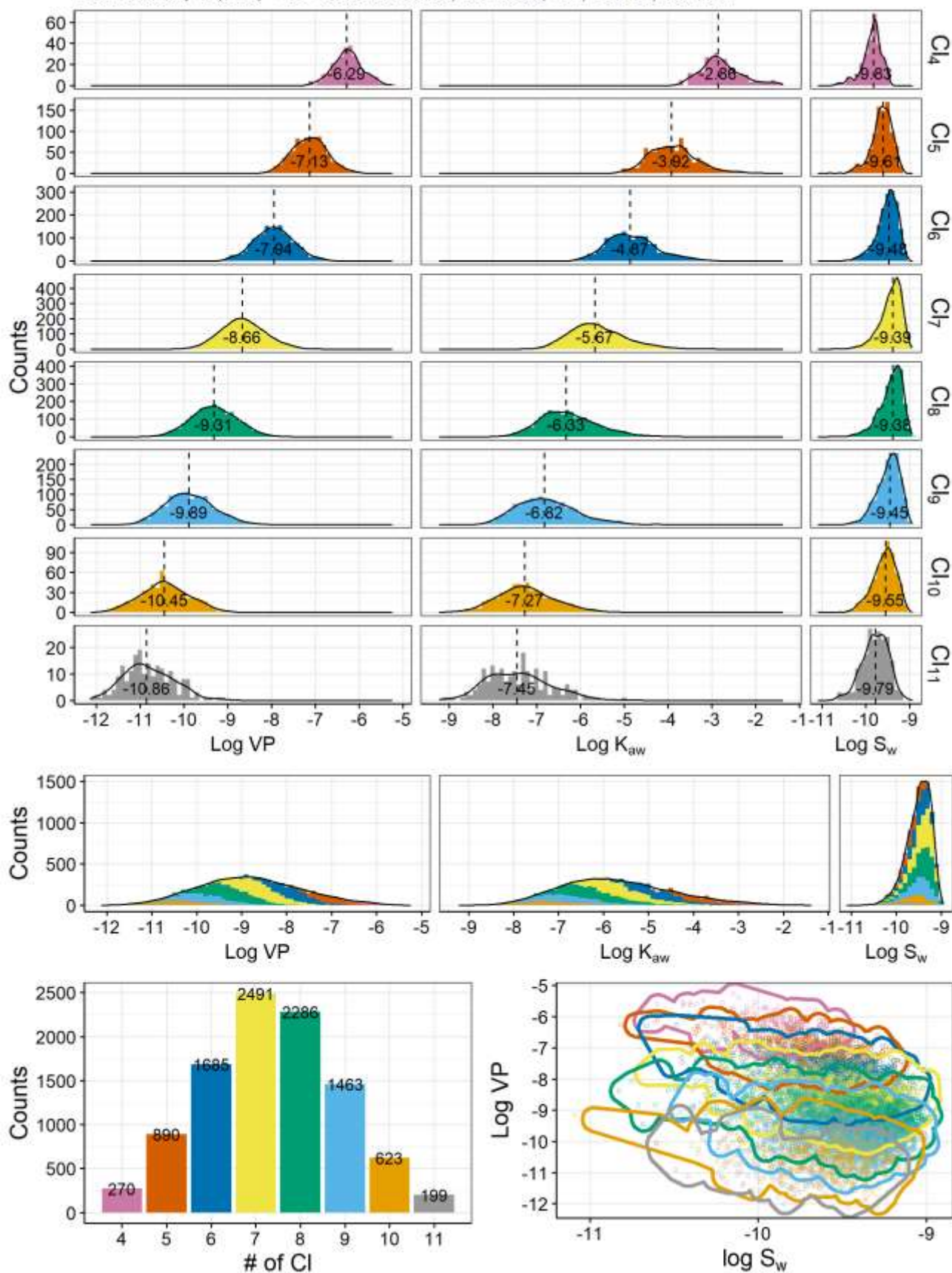
C19, 40wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



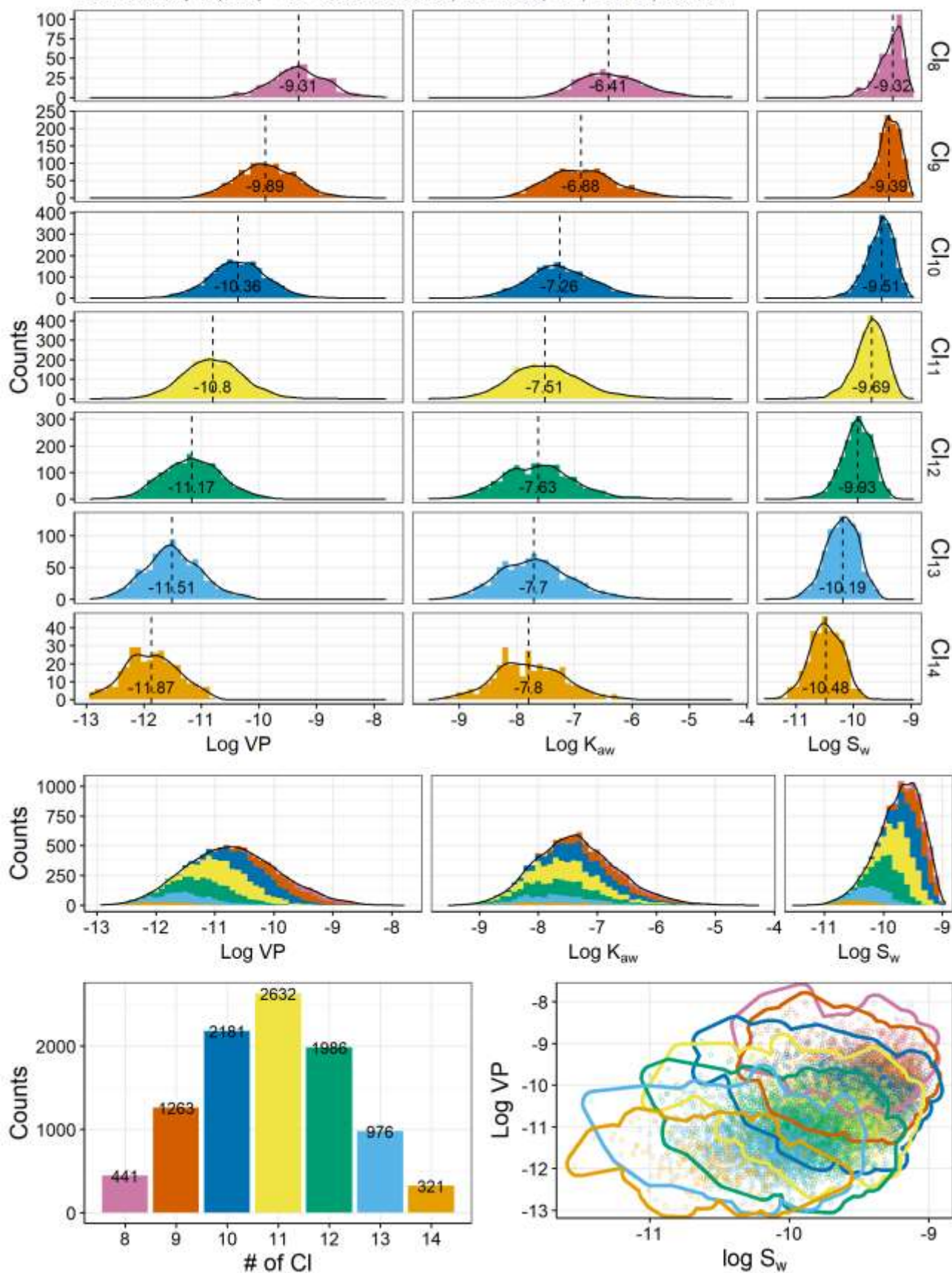
C19, 50wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



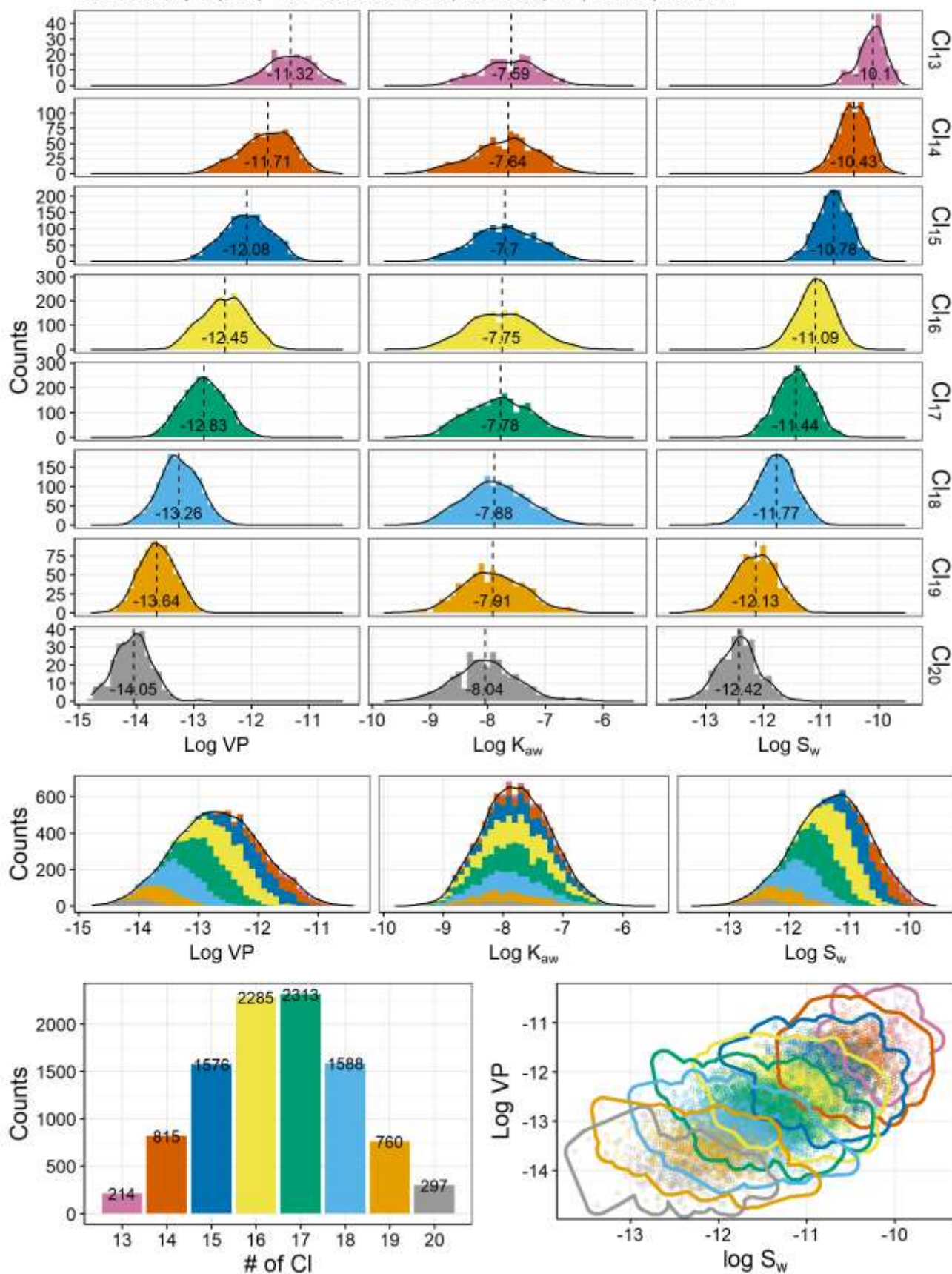
C19, 60wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



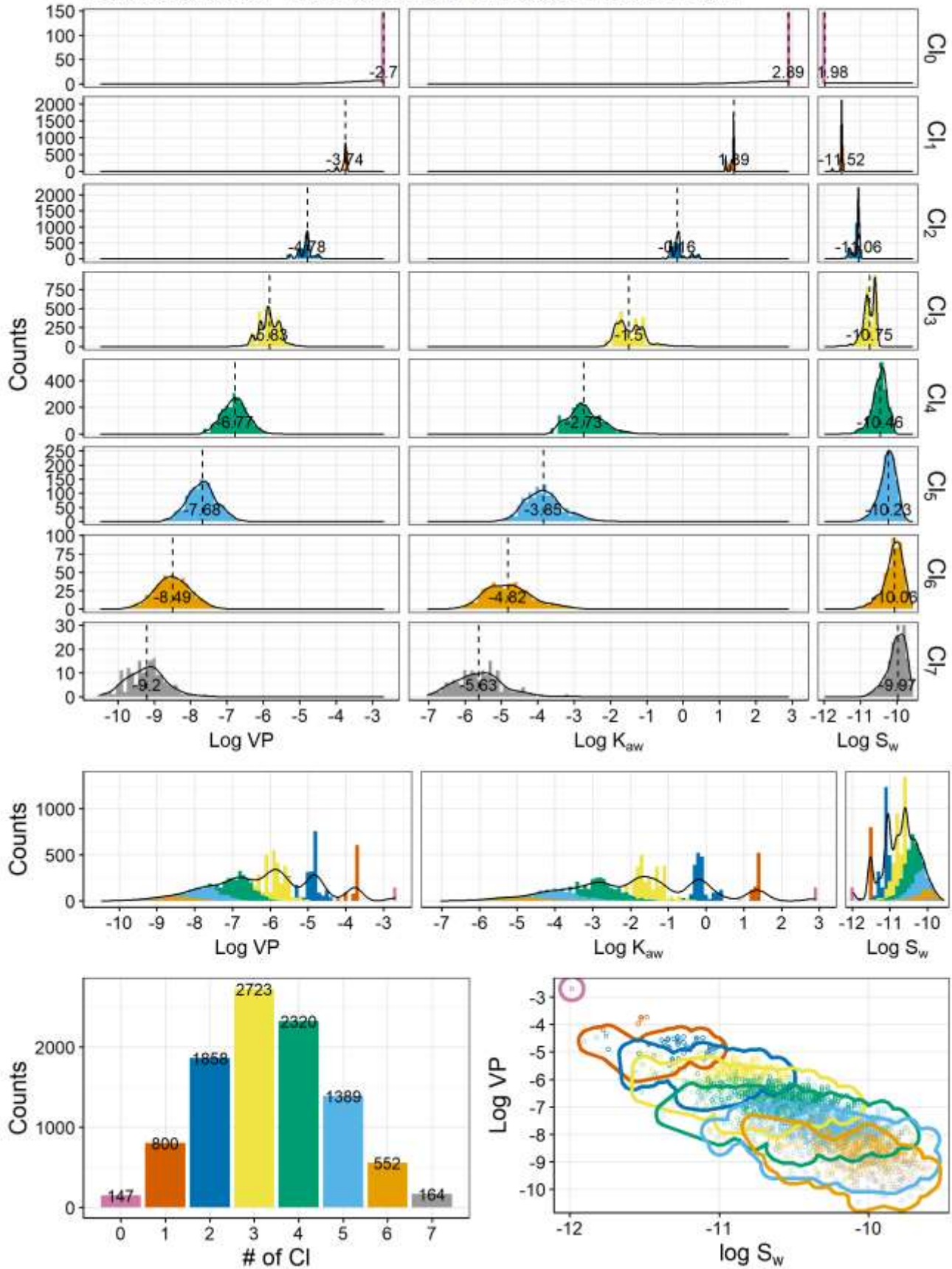
C19, 70wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



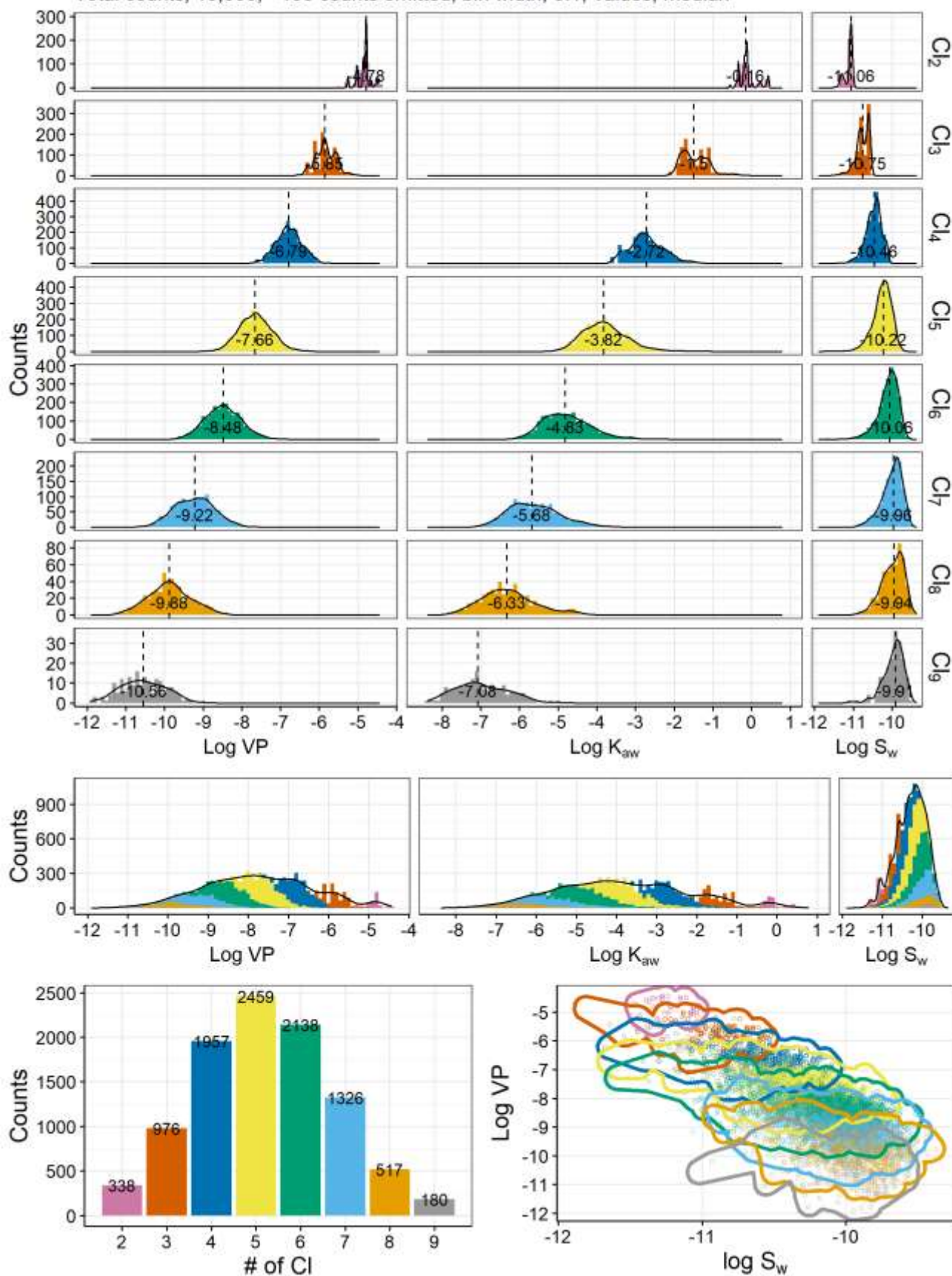
C20, 30wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



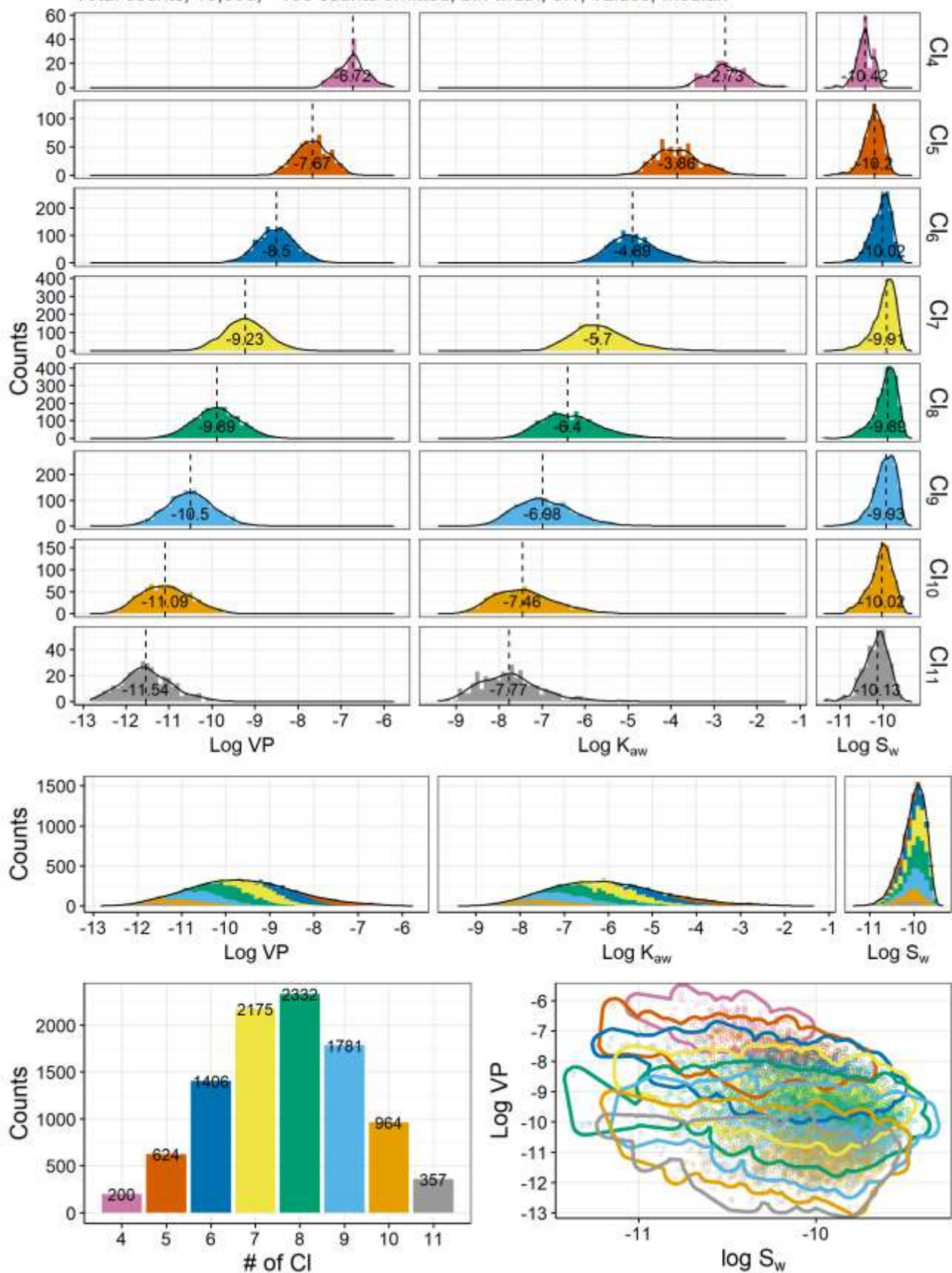
C20, 40wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



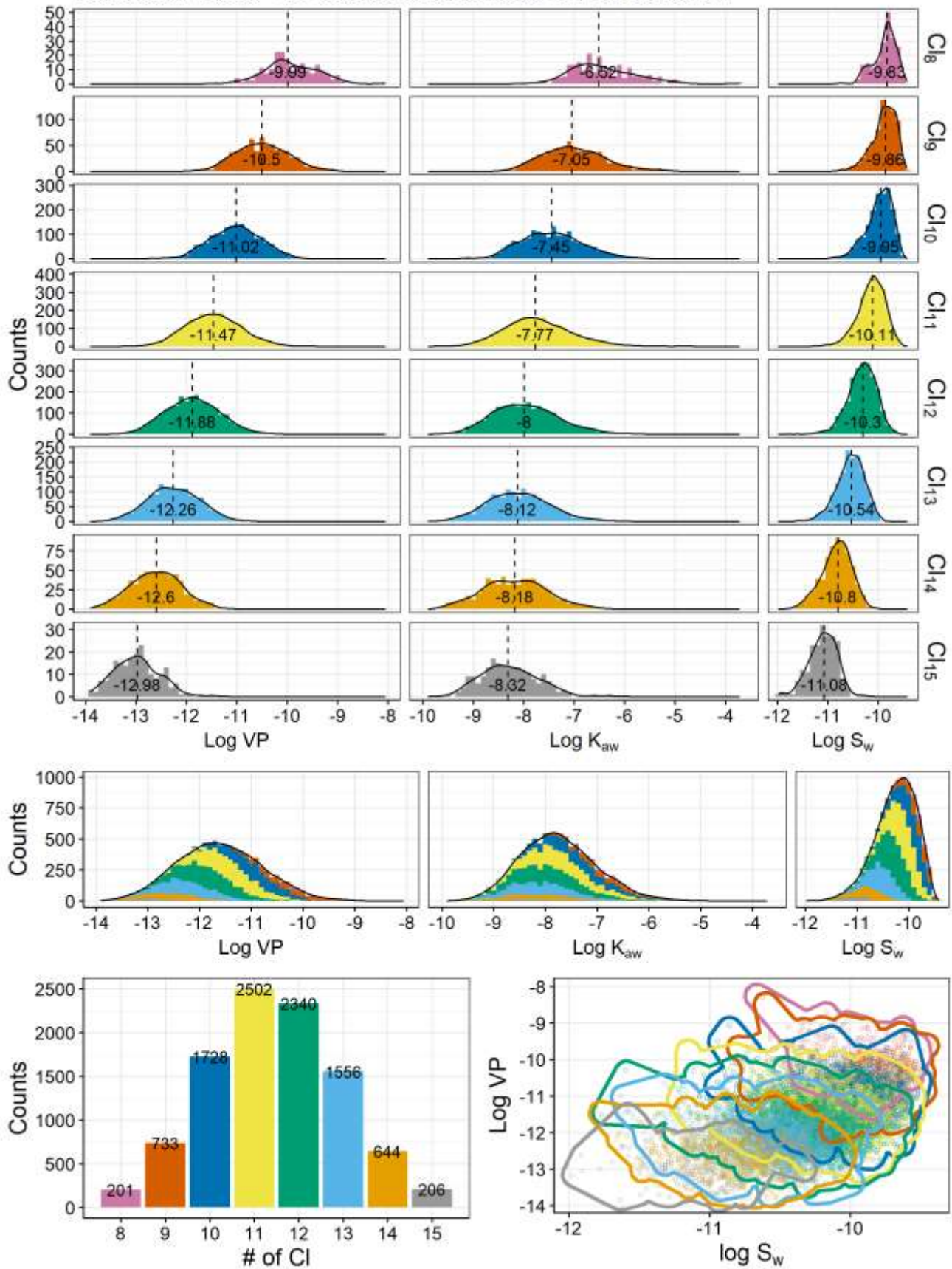
C20, 50wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



C20, 60wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median



C20, 70wt% CI

Total counts, 10,000; <100 counts omitted; bin width, 0.1; values, median

