

BIONIC v3 QUICK START

PHYS-CHEM INPUT SHEET

1. Enter ID (1, 2, 3, 4 etc., etc.), Name, CAS, SMILES
2. DEFINE IOC Type – **A** for acid, **B** for base, **N** for neutral, **Q** for quaternary amine
3. IF IOC, enter pKa
4. Enter all available partitioning data – **Minimum for neutral** = log KOW,N, **Minimum for IOC** = log KOW,N + Δ OW + all other scaling factors (Δ MW, Δ SaW, Δ PW)
5. Enter whole body biotransformation rate constant (Scroll over to column Y)

WHEN FINISHED ENTERING DATA, YOU MUST CLICK ON THIS BUTTON TO PROCEED

CLICK ME to Transfer ID, Name,
CAS, SMILES to other sheets

TEST SYSTEM INPUT SHEET

1. Enter water temperature (T, °C), bulk water pH, dissolved oxygen (mg/L) and TOC (mg/L) **OR**
2. CLICK on **AutoFill button** (DEFAULT Environment)

Biota INPUT SHEET

1. Enter fish mass (kg), composition (storage lipid, membrane lipid, structural protein, serum albumin), biota pH and gill pH **OR**
2. CLICK on the **two AutoFill buttons** (Default Test Organism, Gill pH)

To generate MODEL OUTPUT

3. CLICK on CALCULATE BCFs button

CALCULATE
BCFs