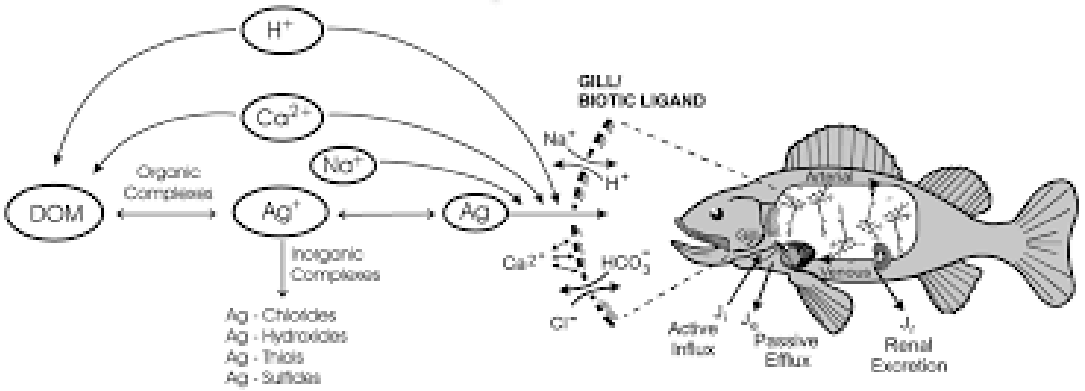
The Use of Multi-Linear Regression to Derive Water Quality Criteria for Metals

Kevin Brix, David DeForest, Lucinda Tear, Robert Santore, Adam Ryan, William Adams

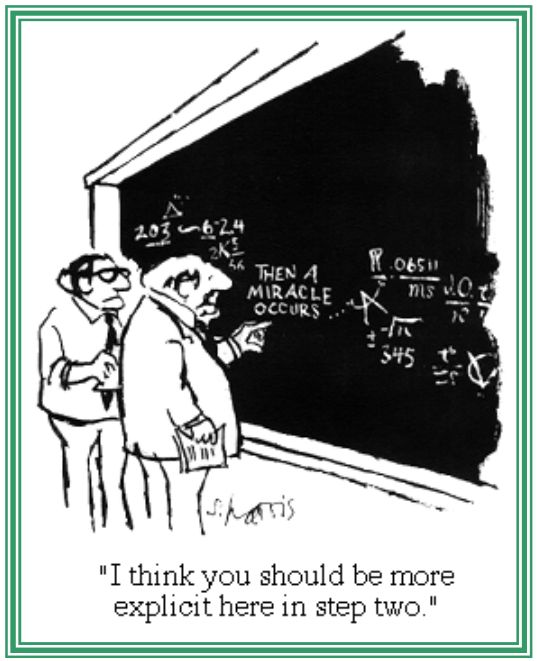
Status of BLM Implementation

- **BLMs used in European regional risk assessments**
- **USEPA derived BLM-based Cu WQC in 2007**
- **Only a few states have adopted the BLM-based Cu WQC, normally under limited conditions**
- **BLM-based WQC for other metals stalled**



Reasons for Limited BLM Implementation

- **Data limitations**
  - **Routine monitoring of water ionic composition and DOC not standard practice….yet**
- **BLM <u>perceived</u> as too complicated**
  - **Significantly more complex than current hardness-dependent WQC for metals**
- **BLM performance held to a higher standard**



"I think you should be more explicit here in step two."

Is there an alternative "intermediate" approach?

- **If the BLM is not being adopted by States, what can we do?**
- **Reduce data needs of the BLM**
- **BLM look-up tables**
- **Modify the existing hardness-dependent criteria approach to incorporate (at least conceptually) the BLM**

The Concept

- **Develop multi-linear regression models within the same hardness-based framework in practice today for most WQC for metals**
  - **Erickson et al. 1987**
    - **Acute Cu for *Pimephales promelas***
    - **LC50 = 1.0 * F_{Ionic} * F_{pH} * F_{Org} * F_{SS} * F_{Temp}**
  - **DeSchamphelaere et al. 2002**
    - **Acute Cu for *Daphnia magna***
    - **LC50 [nMCu^{2+}] = 308+(42.6*mMCa)+(41.3*pH)**
  - **Rogevich et al. 2008**
    - **Acute Cu for *Pomacea paludosa***
    - **Log LC50 = 0.54+(0.008*Age)+(0.024*DOC)+(0.12*pH)**

Methods

- **Updated existing acute and chronic data sets for Cd, Cu, Ni, Pb and Zn**
- **Identified key water quality parameters from existing BLMs**
  - **DOC, hardness, pH**
- **Developed MLRs for individual species**

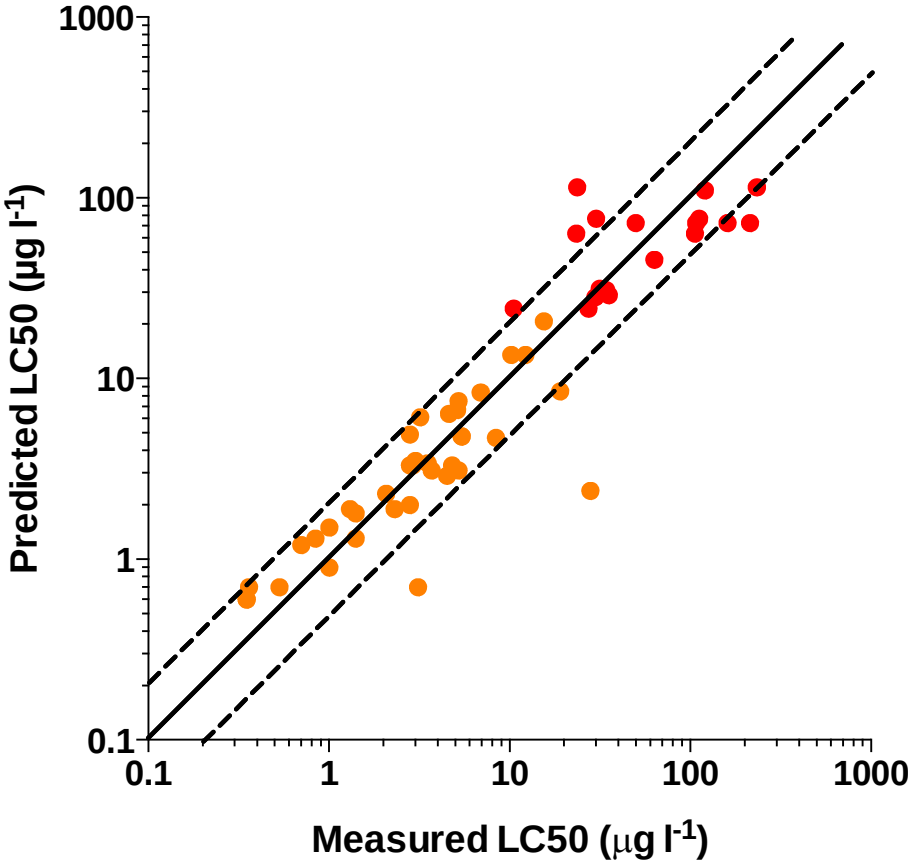
Species-Specific MLR Methods

- **ln transformed data**
  - **Hardness range: 100 mg l^{-1}**
  - **DOC Range = 5 mg l^{-1}**
  - **pH Range = 1.5**
- **For each species develop model with and without interactions among variables**
  - **ln(ECx) = ln(Hard) + ln(DOC) + pH**
  - **ln(ECx) = ln(Hard) + ln(DOC) + pH + ln(DOC)*ln(Hard) + ln(DOC)*pH**
- **For each model conduct stepwise assessment in R using Akaike's Information Criterion (AIC)**
  - **R code: stepAIC(model)**
  - **Multi-collinearity assessed using VIFs**
  - **Variable sign**

Acute Cadmium

MLR No Interactions

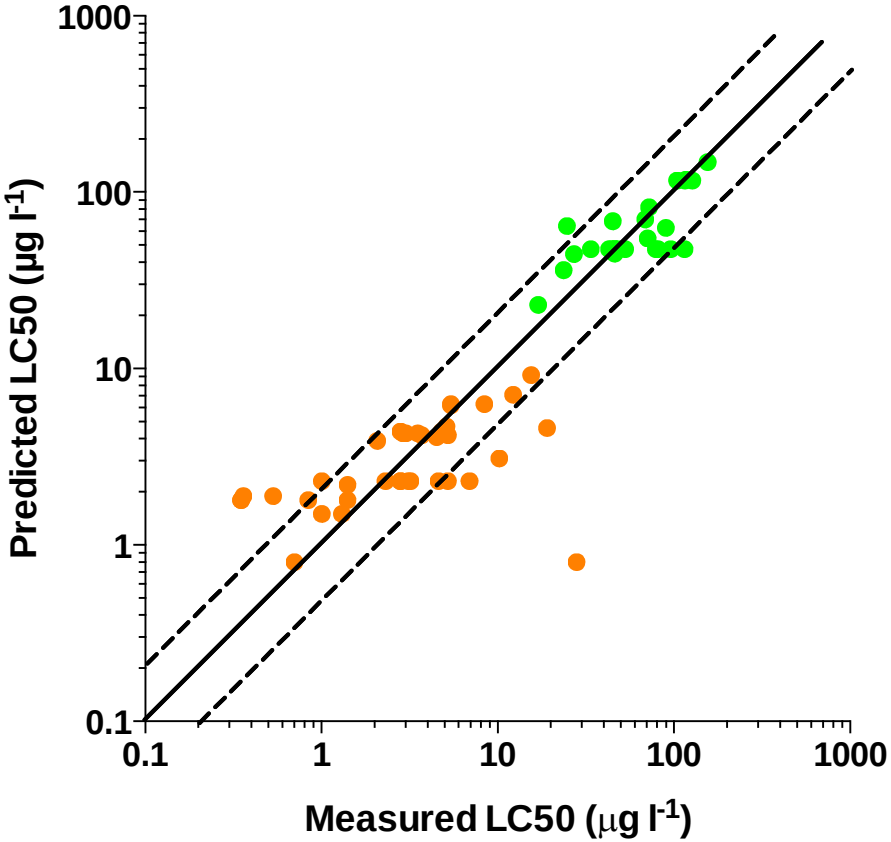
84% within factor of 2



- Ceriodaphnia dubia (Adj. r^2 = 0.29; n = 18)
- Oncorhynchus mykiss (Adj. r^2 = 0.66; n = 37)

Hardness

81% within factor of 2

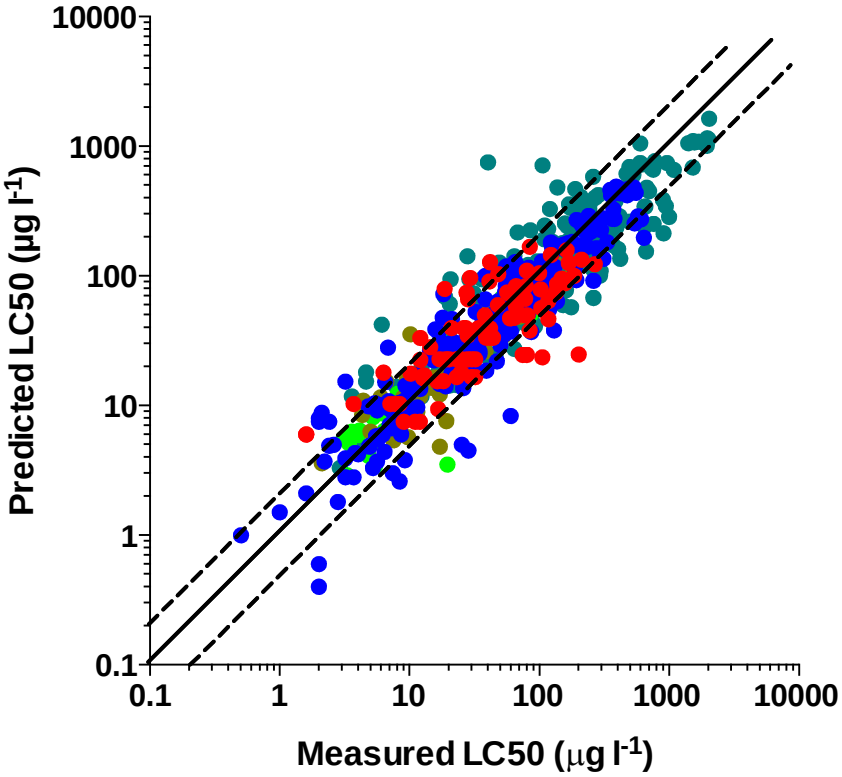


- Daphnia pulex (r^2 = 0.55; n = 27)
- Oncorhynchus mykiss (r^2 = 0.26; n = 37)

Acute Copper

MLR No Interactions

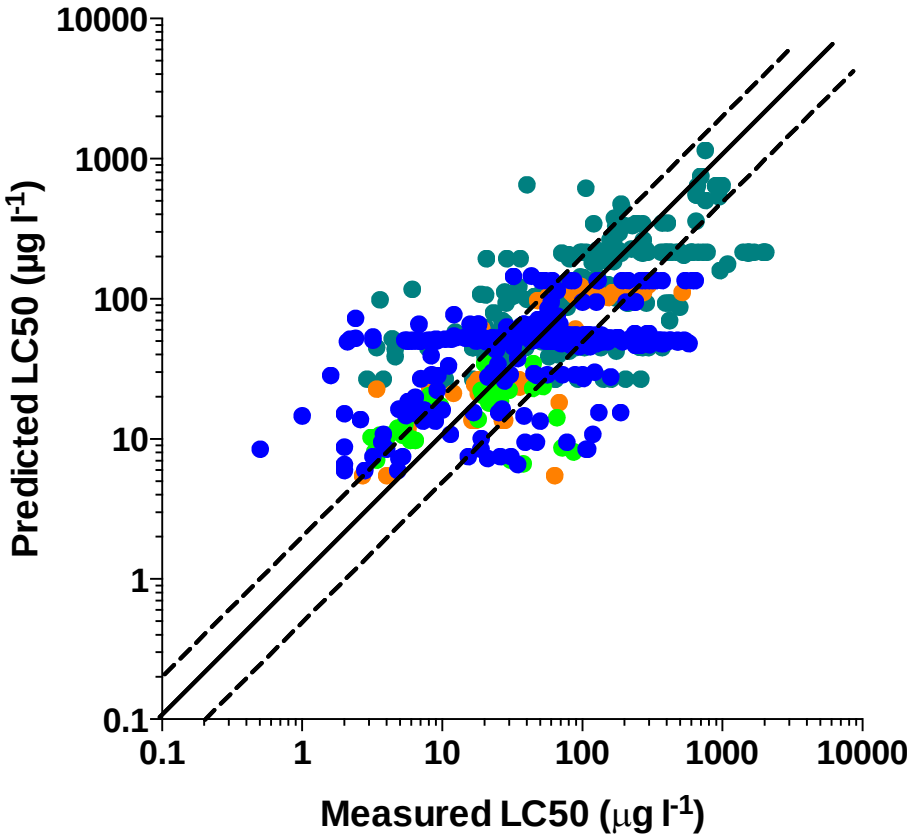
83% within factor of 2



- Ceriodaphnia dubia (Adj. r^2 = 0.63; n = 87)
- Daphnia magna (Adj. r^2 = 0.88; n = 287)
- Daphnia obtusa (Adj. r^2 = 0.82; n = 52)
- Daphnia pulex (Adj. r^2 = 0.81; n = 35)
- Pimephales promelas (Adj. r^2 = 0.76; n = 206)

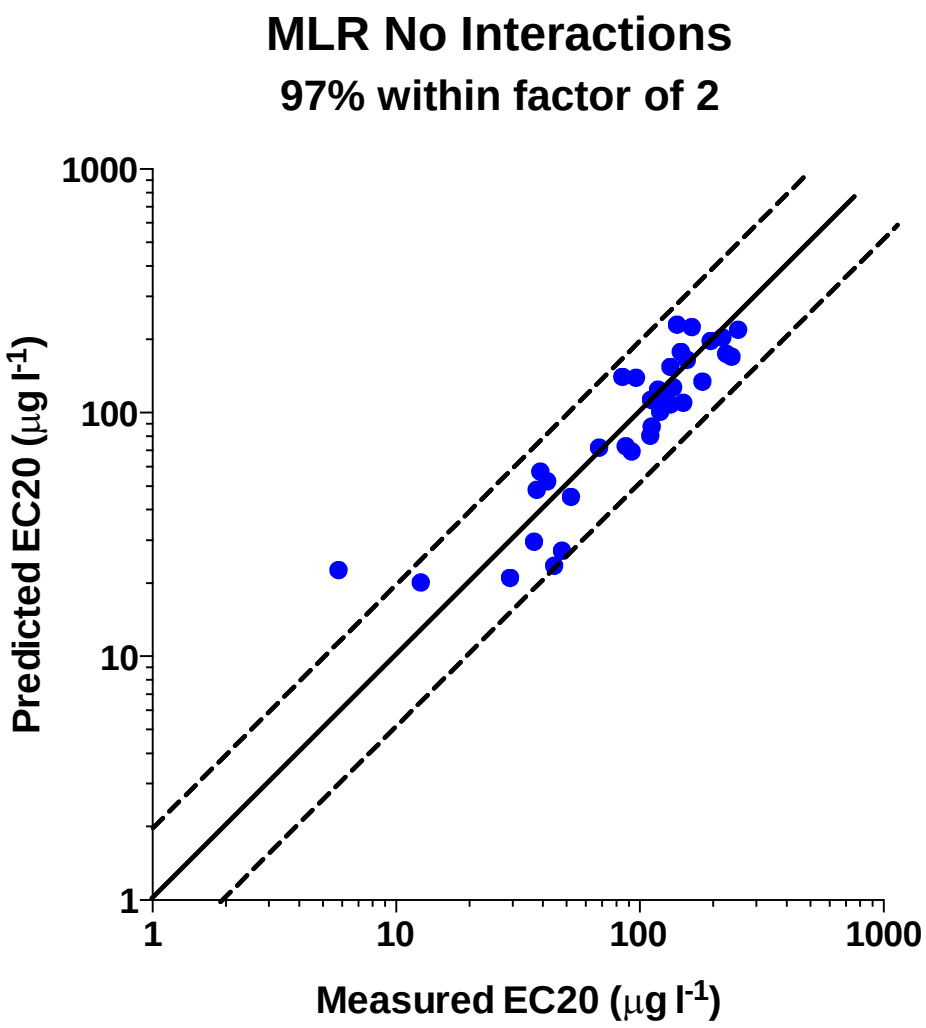
Hardness

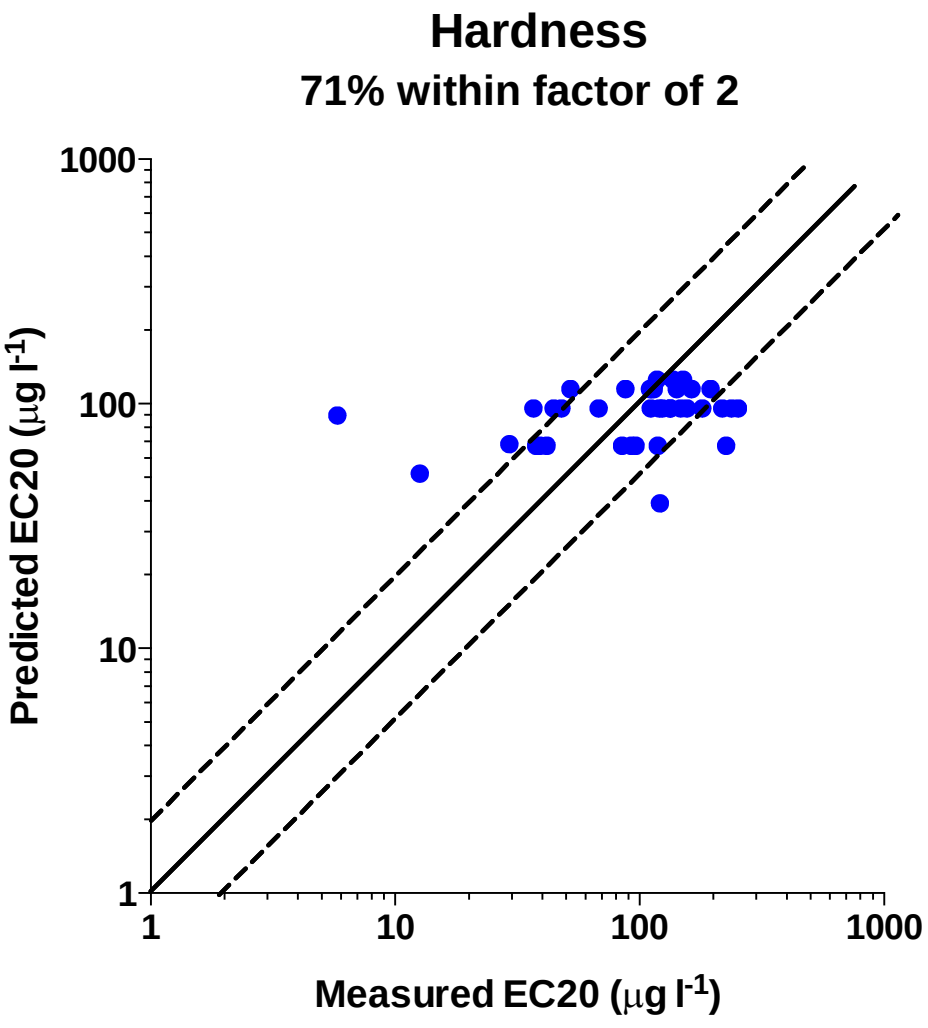
49% within factor of 2



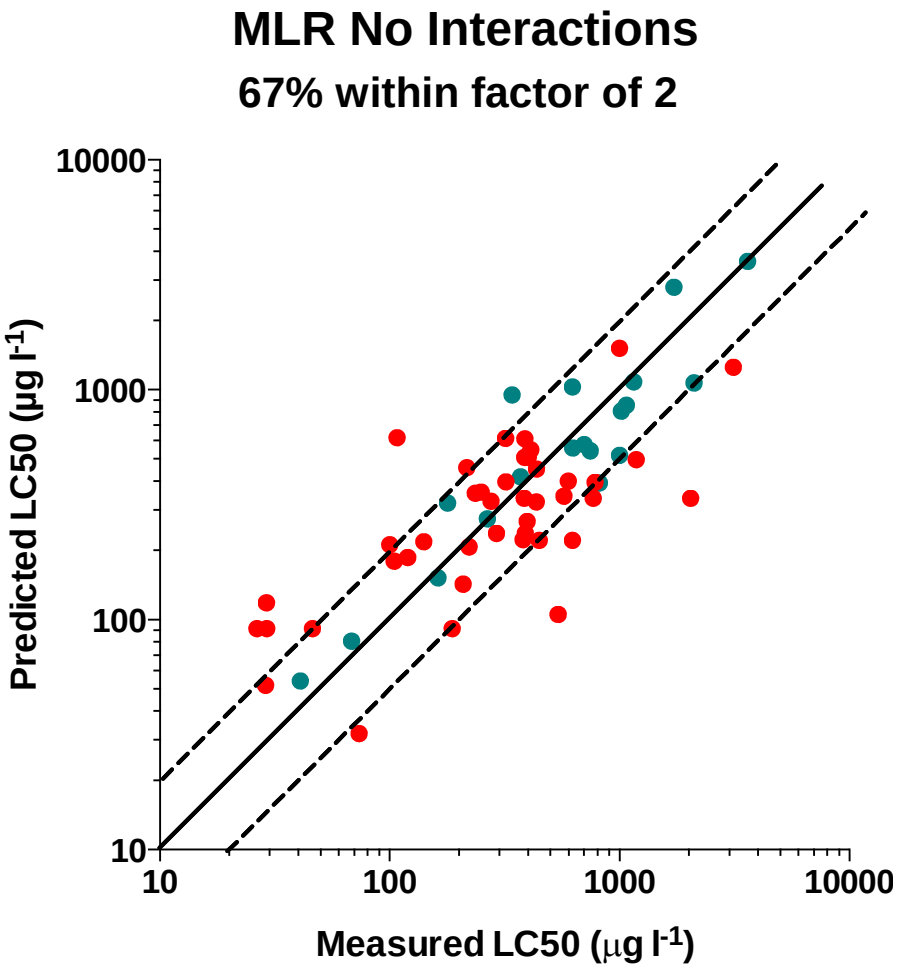
- Daphnia magna (r^2 = 0.24; n = 287)
- Daphnia pulex (r^2 = 0.19; n = 35)
- Oncorhynchus mykiss (r^2 = 0.61; n = 52)
- Pimephales promelas (r^2 = 0.35; n = 206)

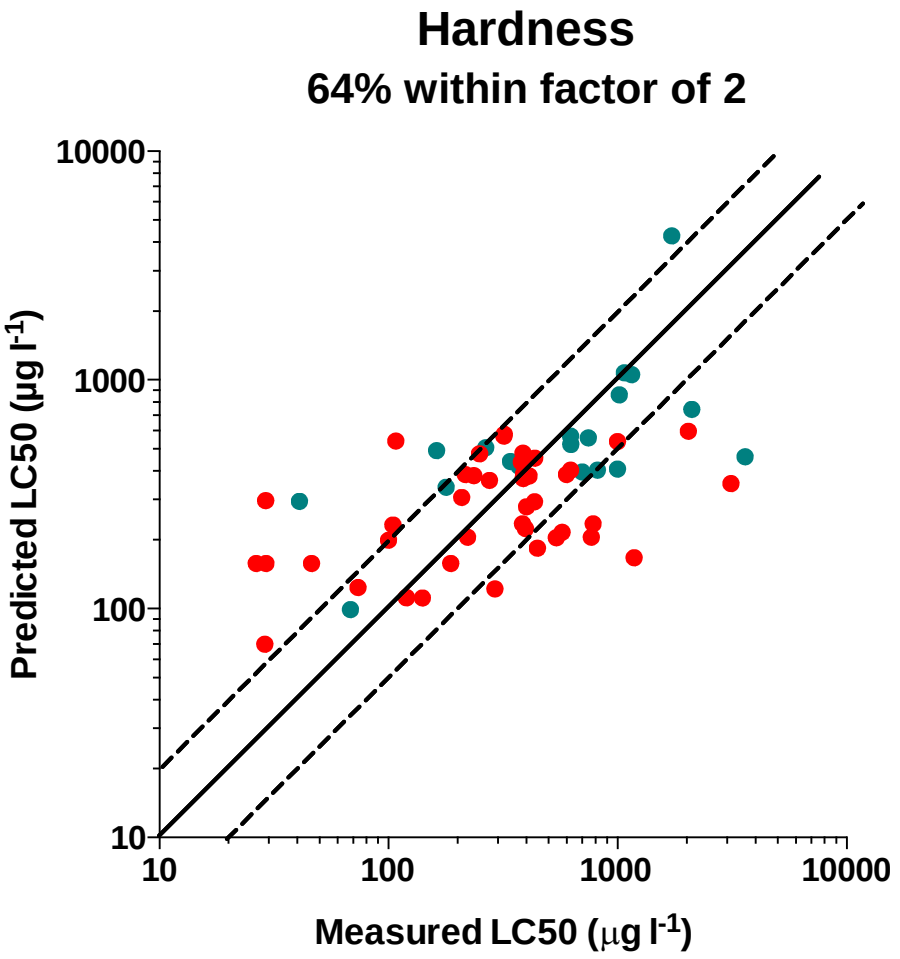
Chronic Copper





Acute Lead

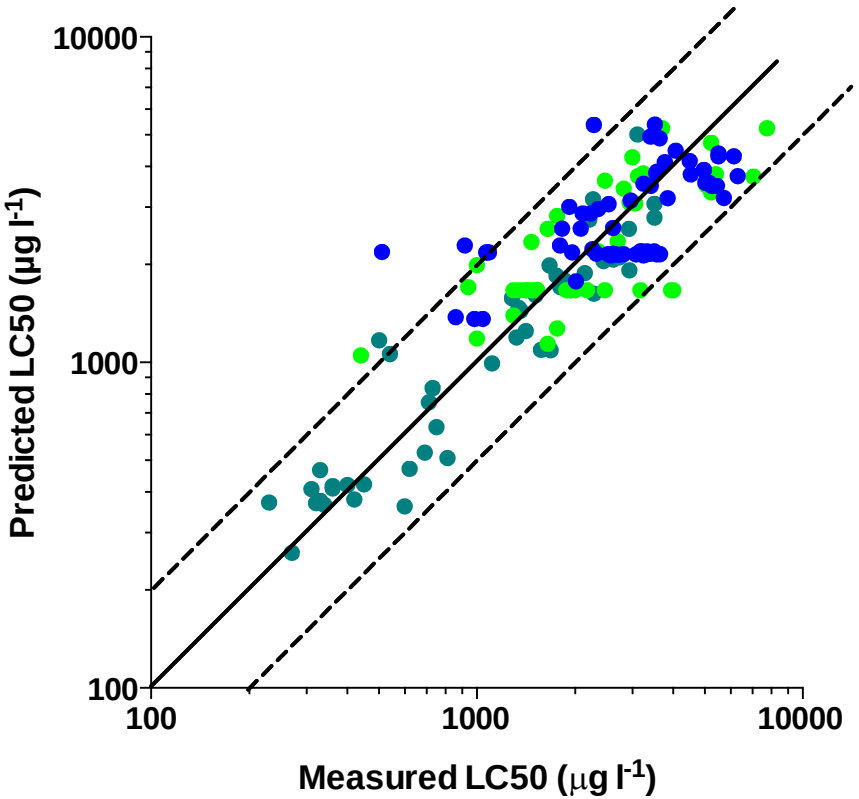

MLR No Interactions
67% within factor of 2
Predicted LC50 (µg l-1)
Measured LC50 (µg l-1)
10000
1000
100
10
10
100
1000
10000
Ceriodaphania dubia (Adj. r2 = 0.46; n = 42)
Pimephales promelas (Adj. r2 = 0.81; n = 19)


Hardness
64% within factor of 2
Predicted LC50 (µg l-1)
Measured LC50 (µg l-1)
10000
1000
100
10
10
100
1000
10000
Ceriodaphnia dubia (r2 = 0.23; n = 42)
Pimephales promelas (r2 = 0.40; n = 19)

Acute Nickel

MLR No Interactions

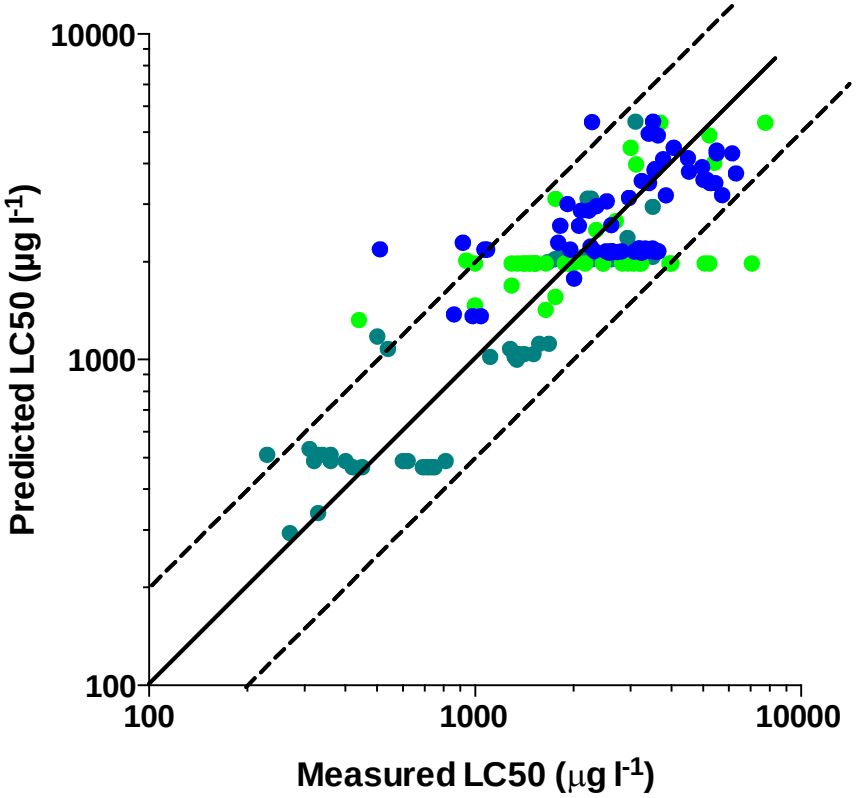
95% within factor of 2



- Daphnia magna (Adj. $r^2 = 0.38$; n = 62)
- Daphnia pulex (Adj. $r^2 = 0.54$; n = 44)
- Pimephales promelas (Adj. $r^2 = 0.87$; n = 47)

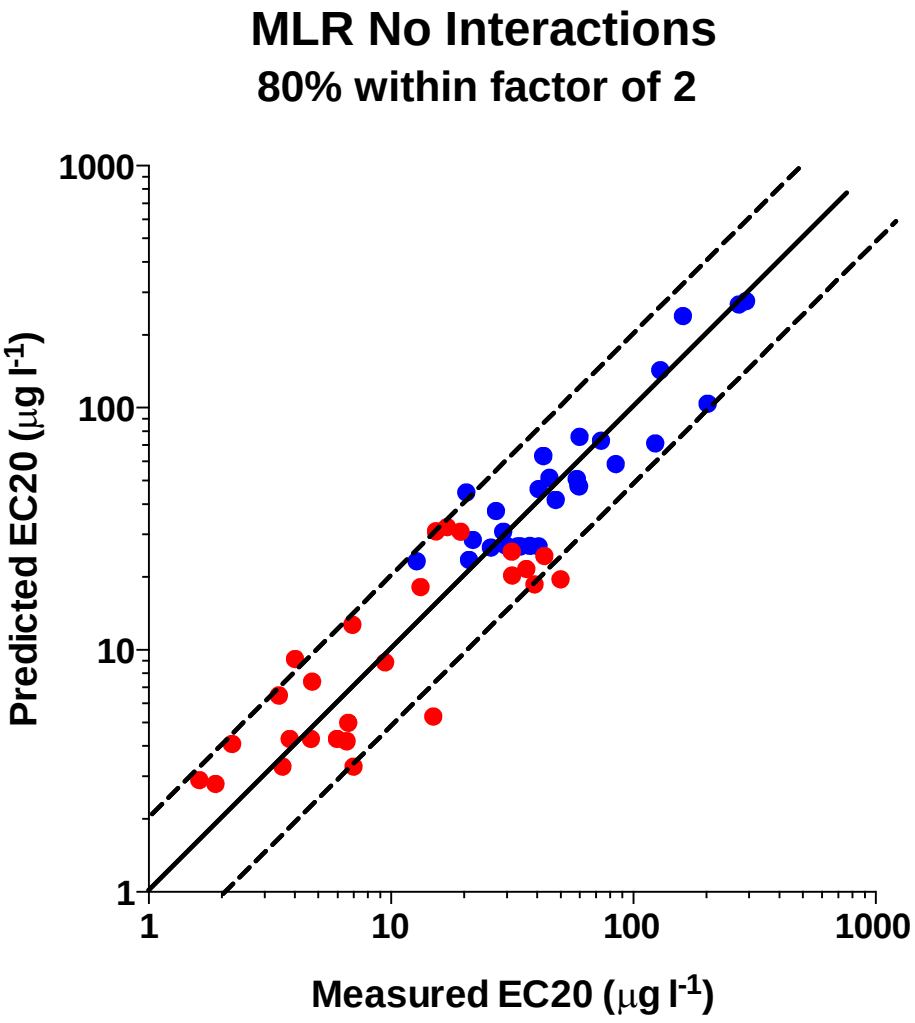
Hardness

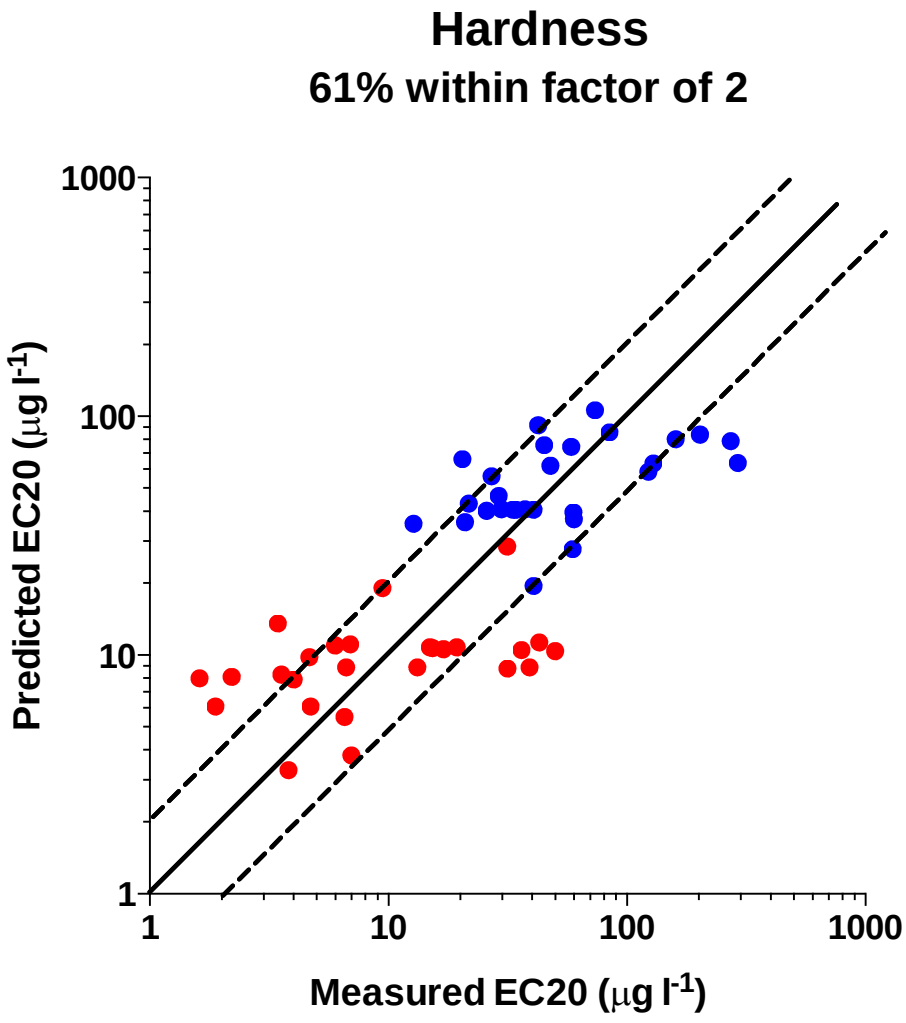
93% within factor of 2



- Daphnia magna ($r^2 = 0.39$; n = 62)
- Daphnia pulex ($r^2 = 0.32$; n = 44)
- Pimephales promelas ($r^2 = 0.80$; n = 47)

Chronic Nickel

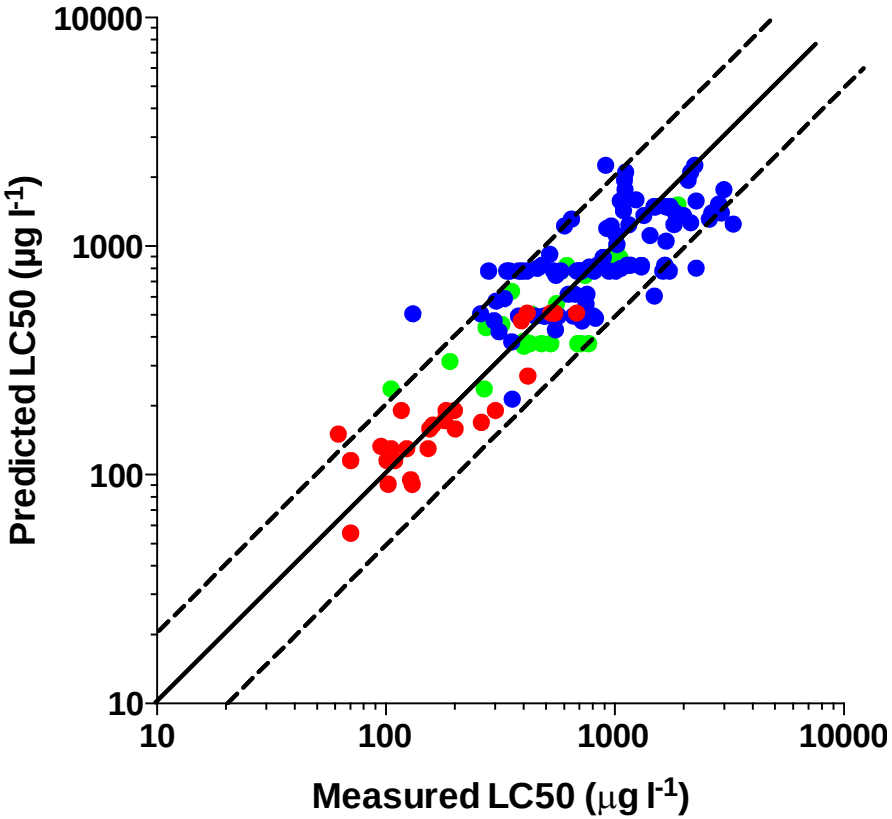




Acute Zinc

MLR No Interactions

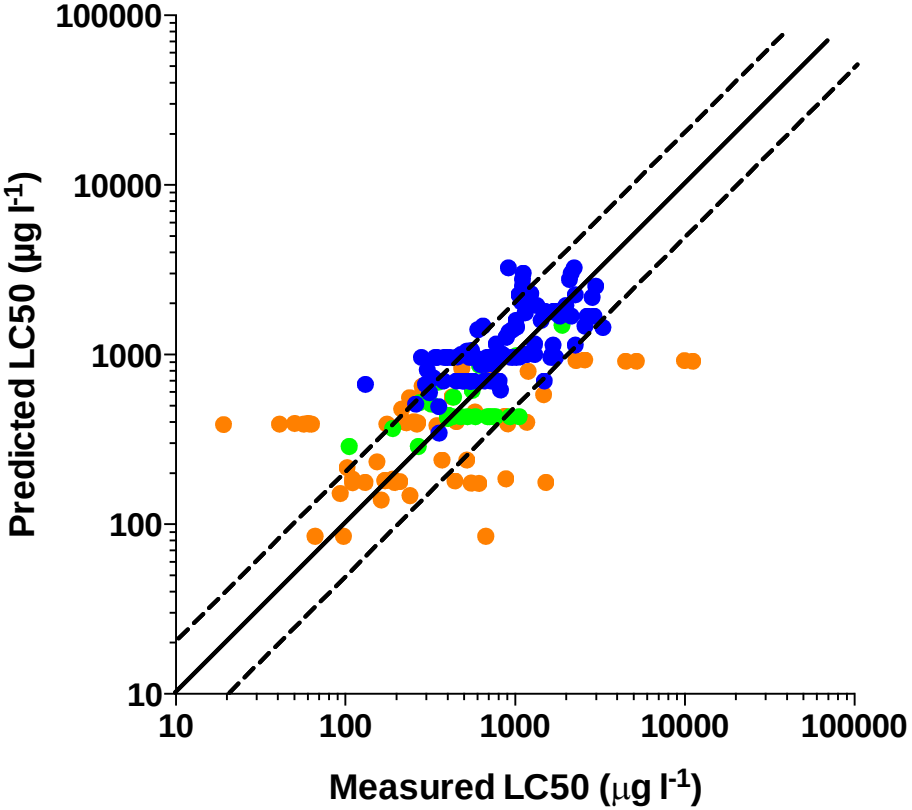
91% within factor of 2



- Ceriodaphania dubia (Adj. $r^2 = 0.78$; n = 28)
- Daphnia magna (Adj. $r^2 = 0.50$; n = 101)
- Daphnia pulex (Adj. $r^2 = 0.57$; n = 25)

Hardness

71% within factor of 2

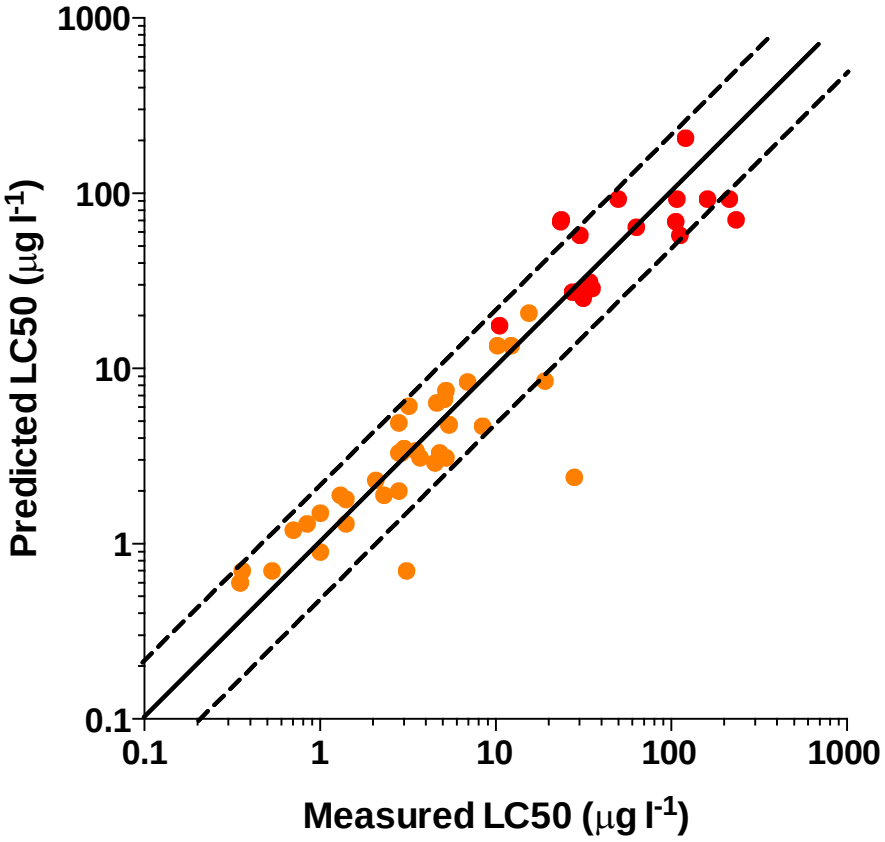


- Daphnia magna ($r^2 = 0.49$; n = 101)
- Daphnia pulex ($r^2 = 0.36$; n = 25)
- Oncorhynchus mykiss ($r^2 = 0.24$; n = 58)

Acute Cadmium

MLR with Interactions

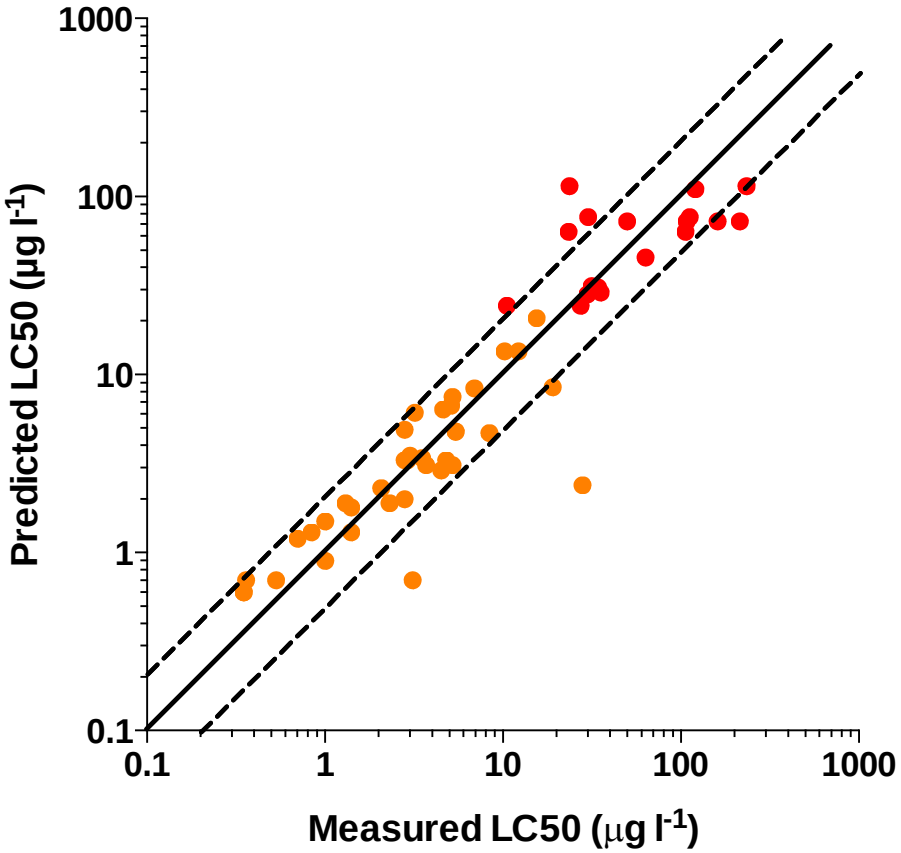
87% within factor of 2



- Ceriodaphnia dubia (Adj. $r^2 = 0.27$; n = 18)
- Oncorhynchus mykiss (Adj. $r^2 = 0.66$; n = 37)

MLR No Interactions

84% within factor of 2

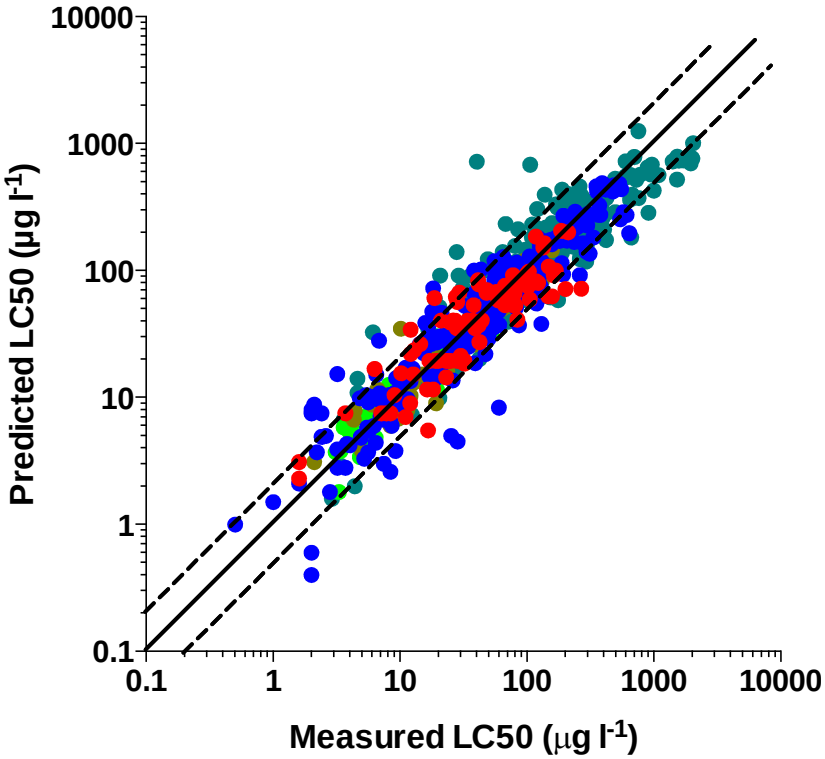


- Ceriodaphnia dubia (Adj. $r^2 = 0.29$; n = 18)
- Oncorhynchus mykiss (Adj. $r^2 = 0.66$; n = 37)

Acute Copper

MLR with Interactions

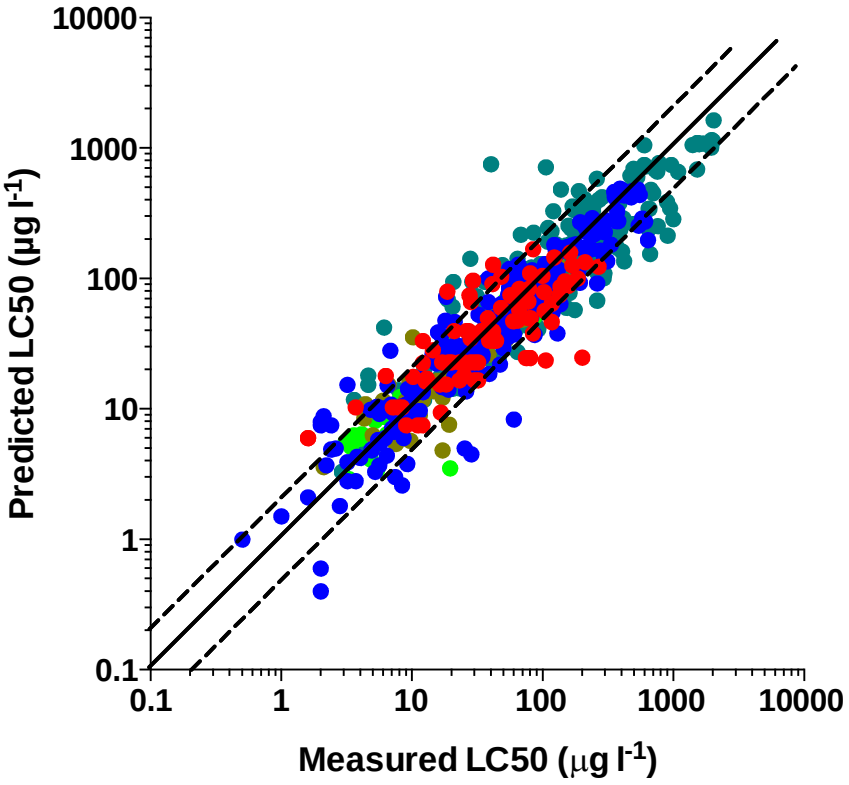
86% within factor of 2



- Ceriodaphnia dubia (Adj. r^2 = 0.78; n = 87)
- Daphnia magna (Adj. r^2 = 0.88; n = 287)
- Daphnia obtusa (Adj. r^2 = 0.89; n = 52)
- Daphnia pulex (Adj. r^2 = 0.92; n=35)
- Pimephales promelas (Adj. r^2 = 0.93; n = 206)

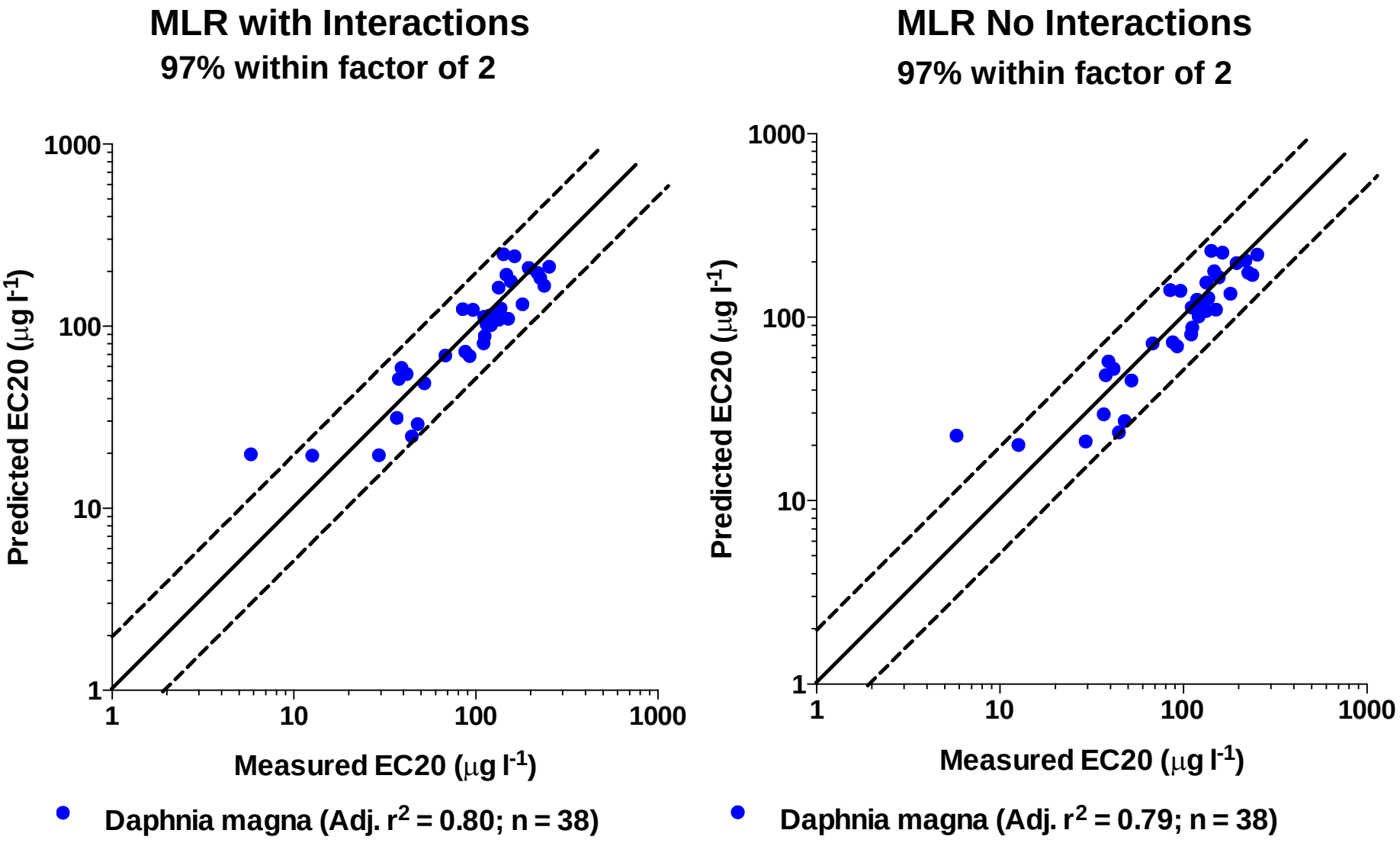
MLR No Interactions

83% within factor of 2



- Ceriodaphnia dubia (Adj. r^2 = 0.63; n = 87)
- Daphnia magna (Adj. r^2 = 0.88; n = 287)
- Daphnia obtusa (Adj. r^2 = 0.82; n = 52)
- Daphnia pulex (Adj. r^2 = 0.81; n = 35)
- Pimephales promelas (Adj. r^2 = 0.76; n = 206)

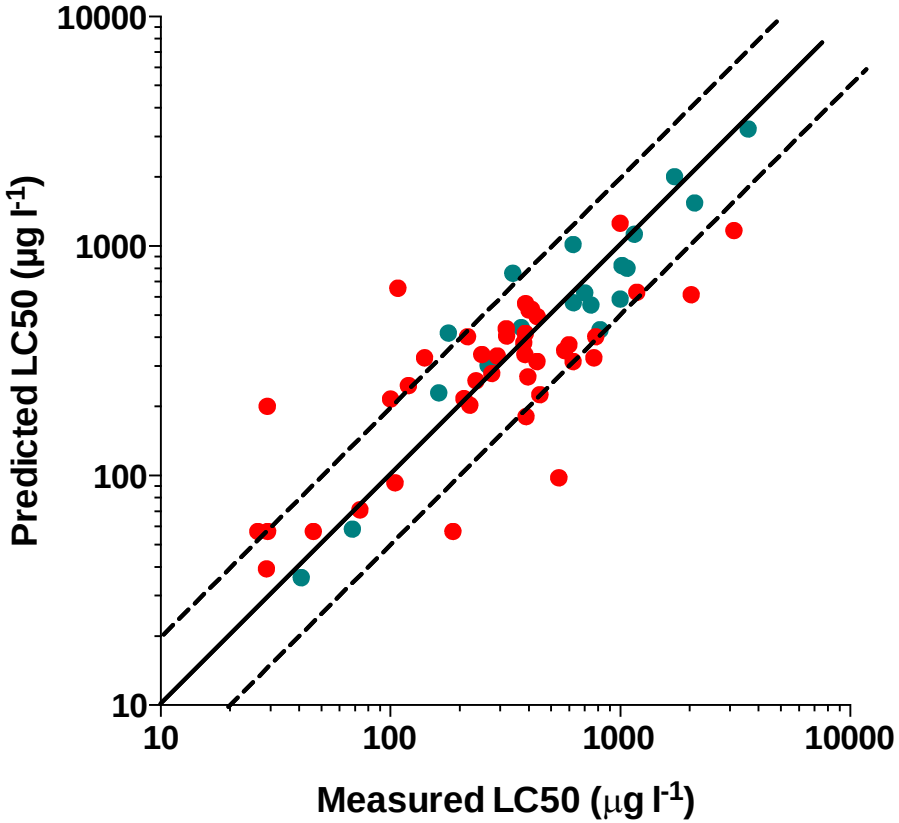
Chronic Copper



Acute Lead

MLR with Interactions

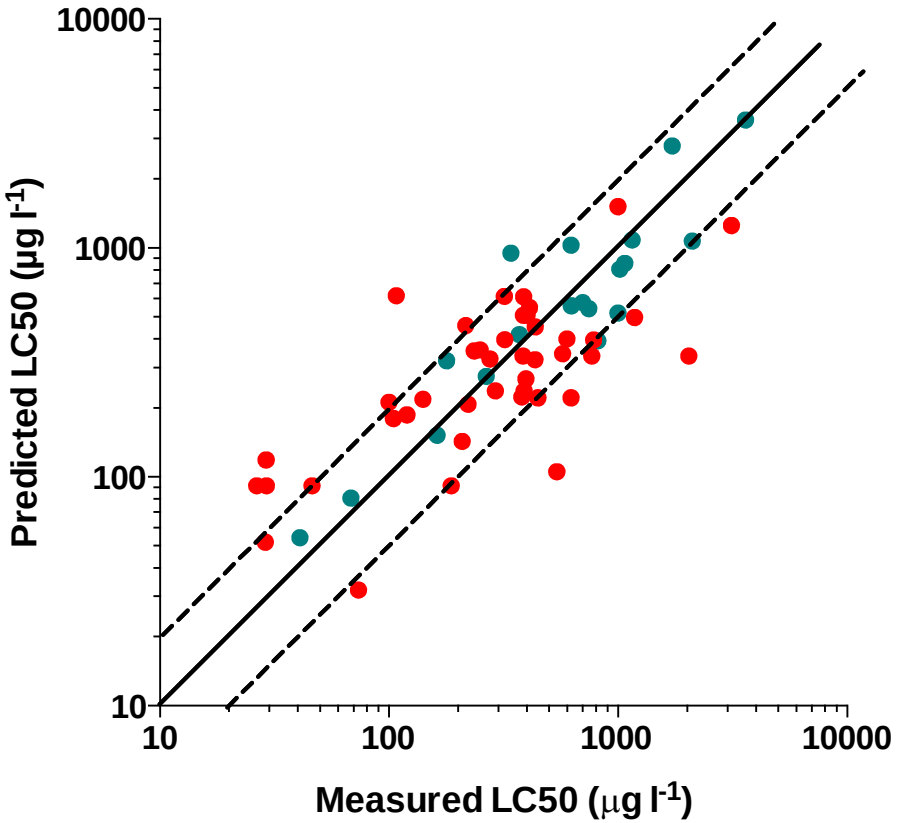
72% within factor of 2



- Ceriodaphnia dubia (Adj. $r^2 = 0.52$, n = 42)
- Pimephales promelas (Adj. $r^2 = 0.83$; n = 19)

MLR No Interactions

67% within factor of 2

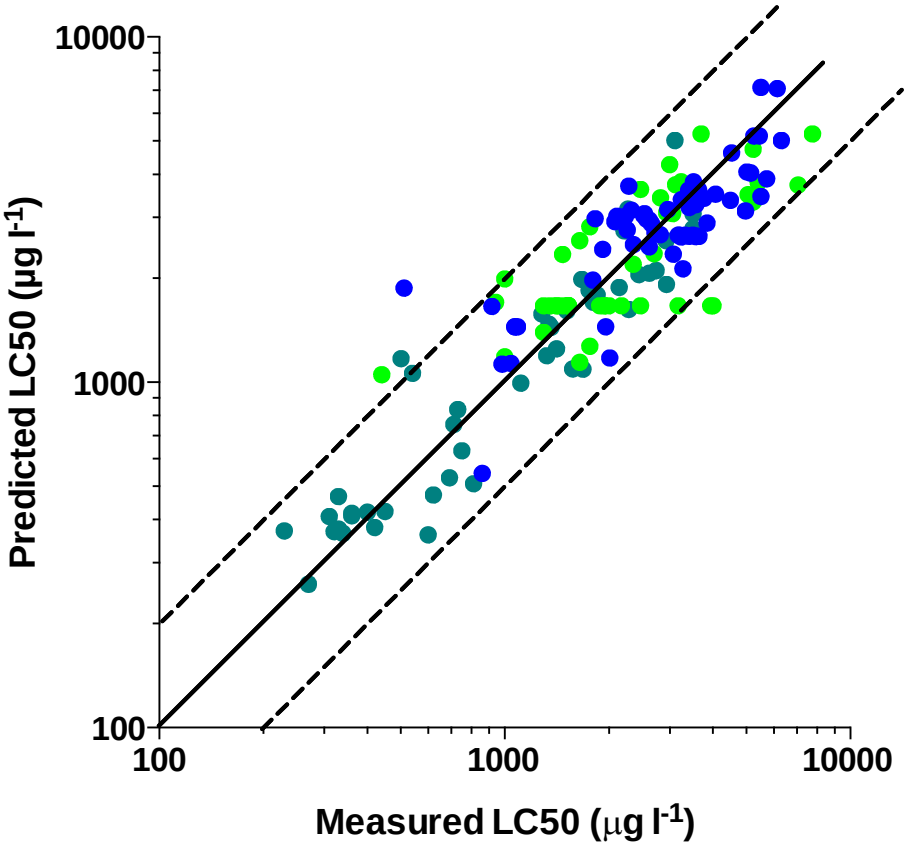


- Ceriodaphania dubia (Adj. $r^2 = 0.46$; n = 42)
- Pimephales promelas (Adj. $r^2 = 0.81$; n = 19)

Acute Nickel

MLR with Interactions

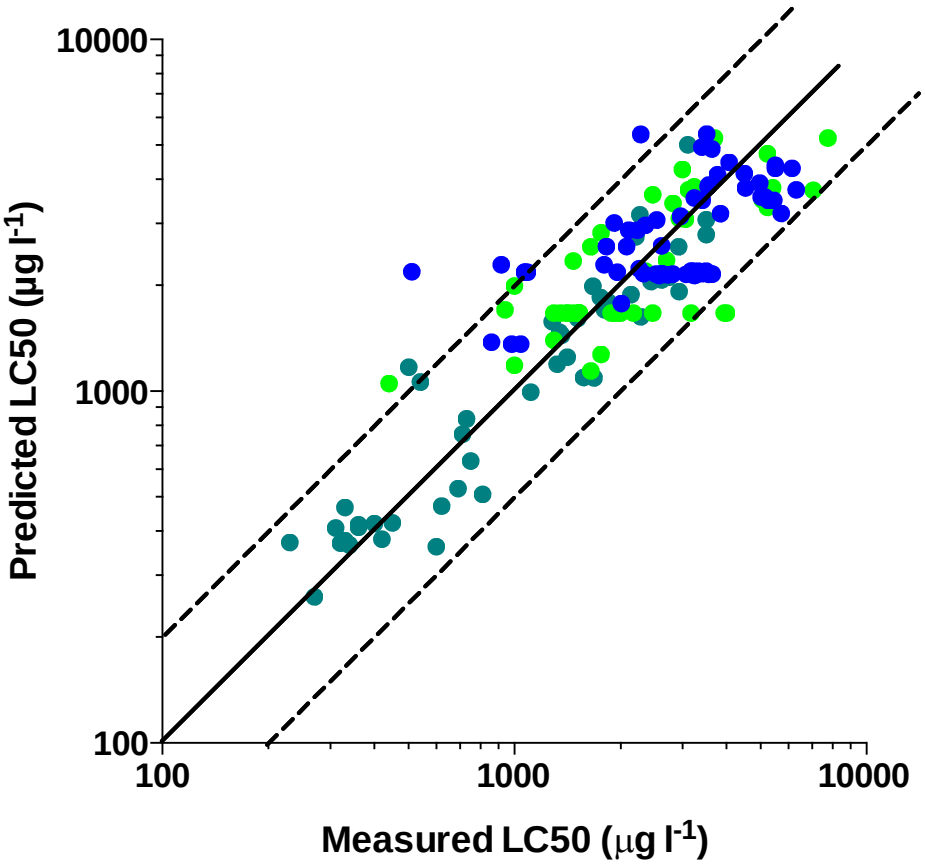
97% within factor of 2



- Daphnia magna (Adj. $r^2 = 0.64$; n = 62)
- Daphnia pulex (Adj. $r^2 = 0.54$; n = 44)
- Pimephales promelas (Adj. $r^2 = 0.87$; n = 47)

MLR No Interactions

95% within factor of 2

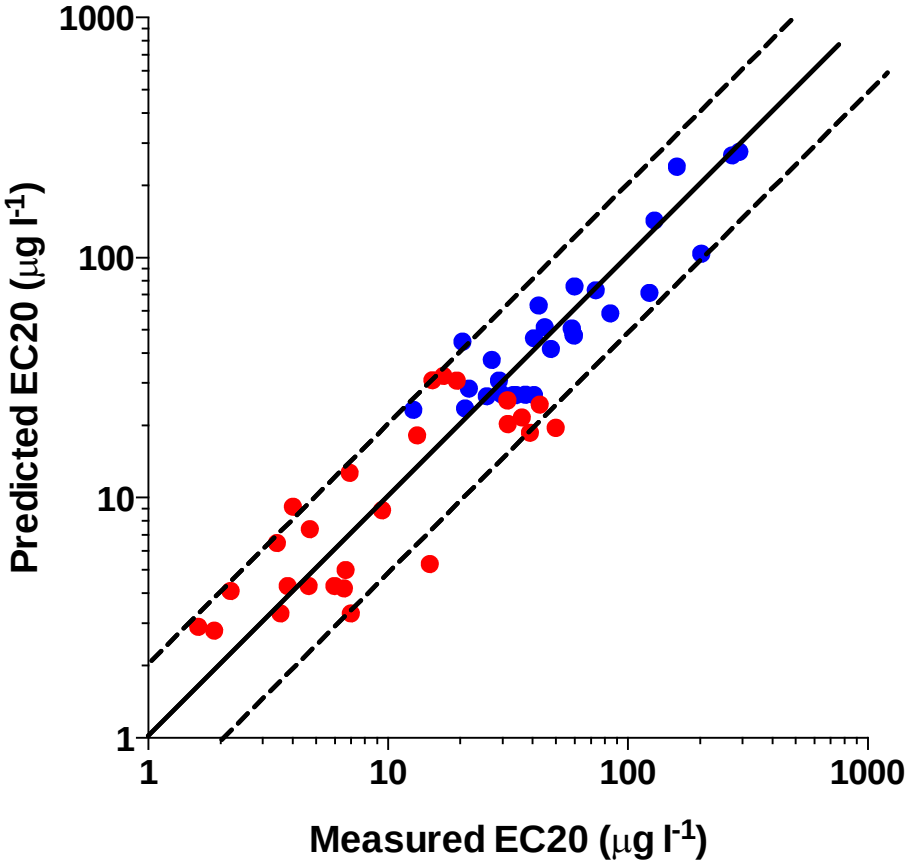


- Daphnia magna (Adj. $r^2 = 0.38$; n = 62)
- Daphnia pulex (Adj. $r^2 = 0.54$; n = 44)
- Pimephales promelas (Adj. $r^2 = 0.87$; n = 47)

Chronic Nickel

MLR with Interactions

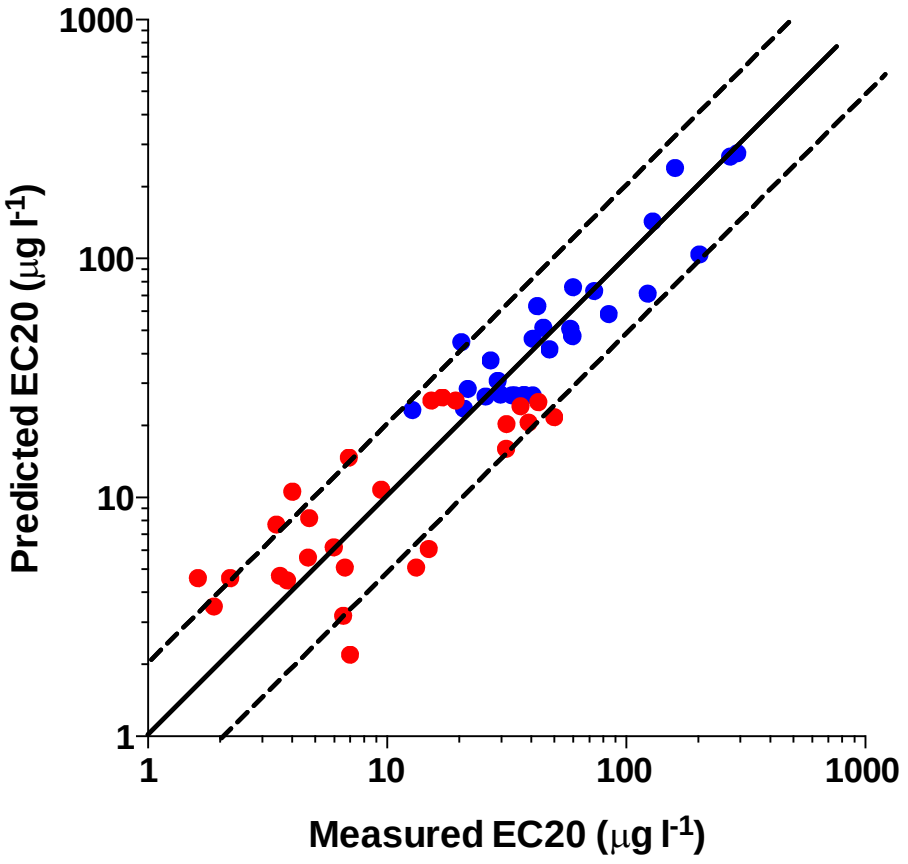
89% within factor of 2



- Ceriodaphnia dubia (Adj. r^2 = 0.65; n = 26)
- Daphnia magna (Adj. r^2 = 0.81; n = 28)

MLR No Interactions

80% within factor of 2

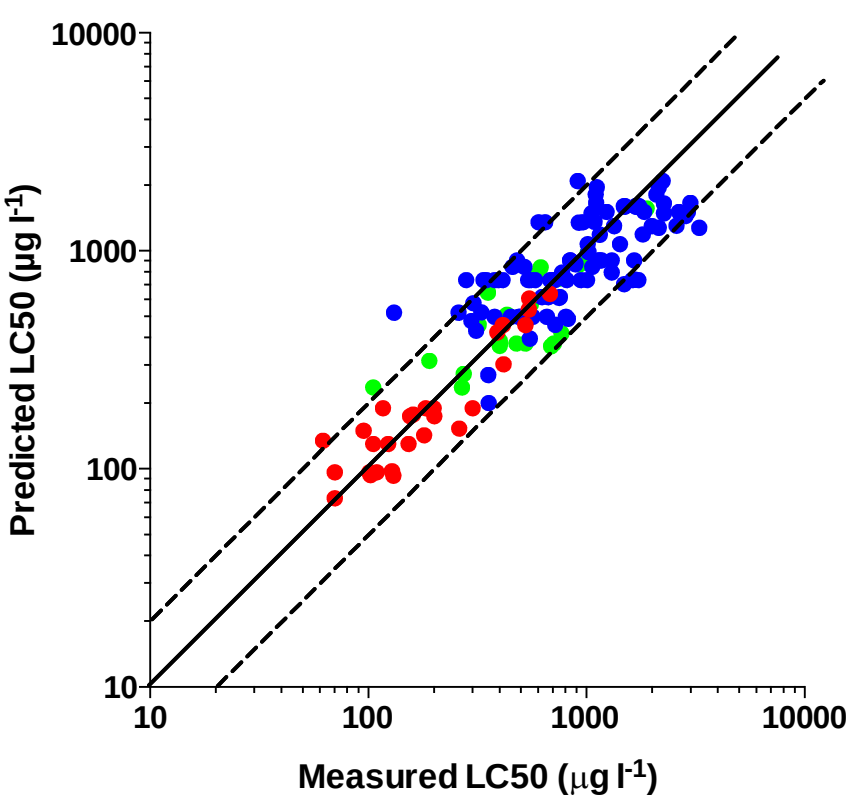


- Ceriodaphnia dubia (Adj. r^2 = 0.54; n = 26)
- Daphnia magna (Adj. r^2 = 0.81; n = 28)

Acute Zinc

MLR with Interactions

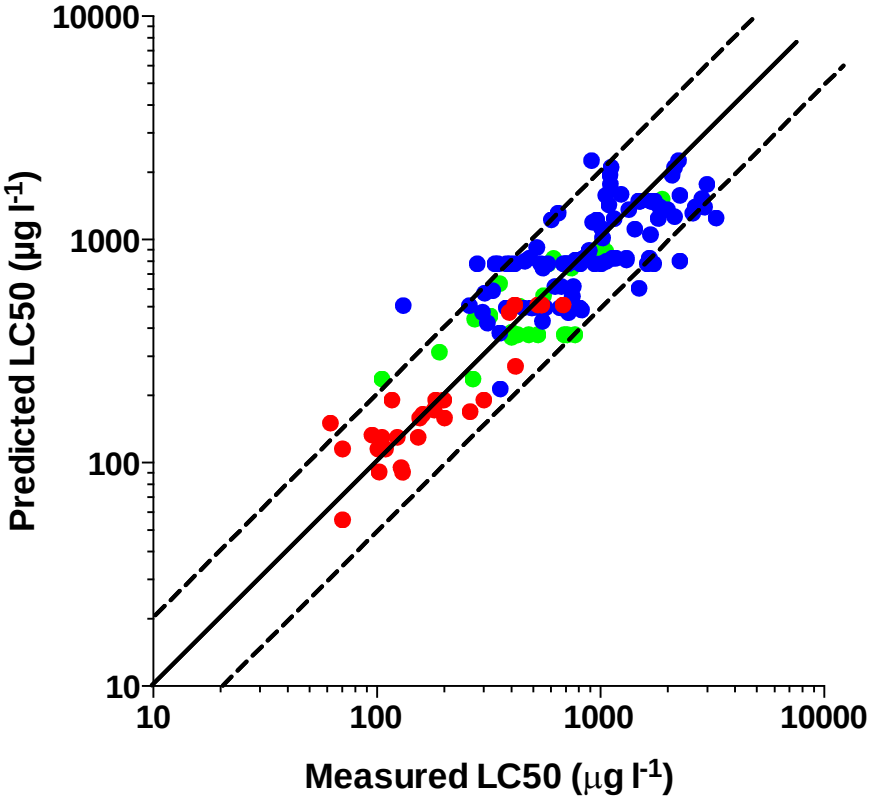
92% within factor of 2



- Ceriodaphnia dubia (Adj. r^2 = 0.79; n = 28)
- Daphnia magna (Adj. r^2 = 0.52; n = 101)
- Daphnia pulex (Adj. r^2 = 0.57; n = 25)

MLR No Interactions

92% within factor of 2



- Ceriodaphania dubia (Adj. r^2 = 0.78; n = 28)
- Daphnia magna (Adj. r^2 = 0.50; n = 101)
- Daphnia pulex (Adj. r^2 = 0.57; n = 25)

Pooled Models

- Analogous to hardness normalization procedure
- Log normalized data within species
  - $\ln(x/\text{geomean}(x_1 \ldots x_n))$
- Pool log-normalized data to create all-species data set
- Develop ANCOVA models without interactions among variables and with interactions between species and variables
- Conduct ANCOVA using “sum” contrasts
  - Tests for differences between specifies-specific coefficients and mean coefficient for each parameter

Cu Acute WQC

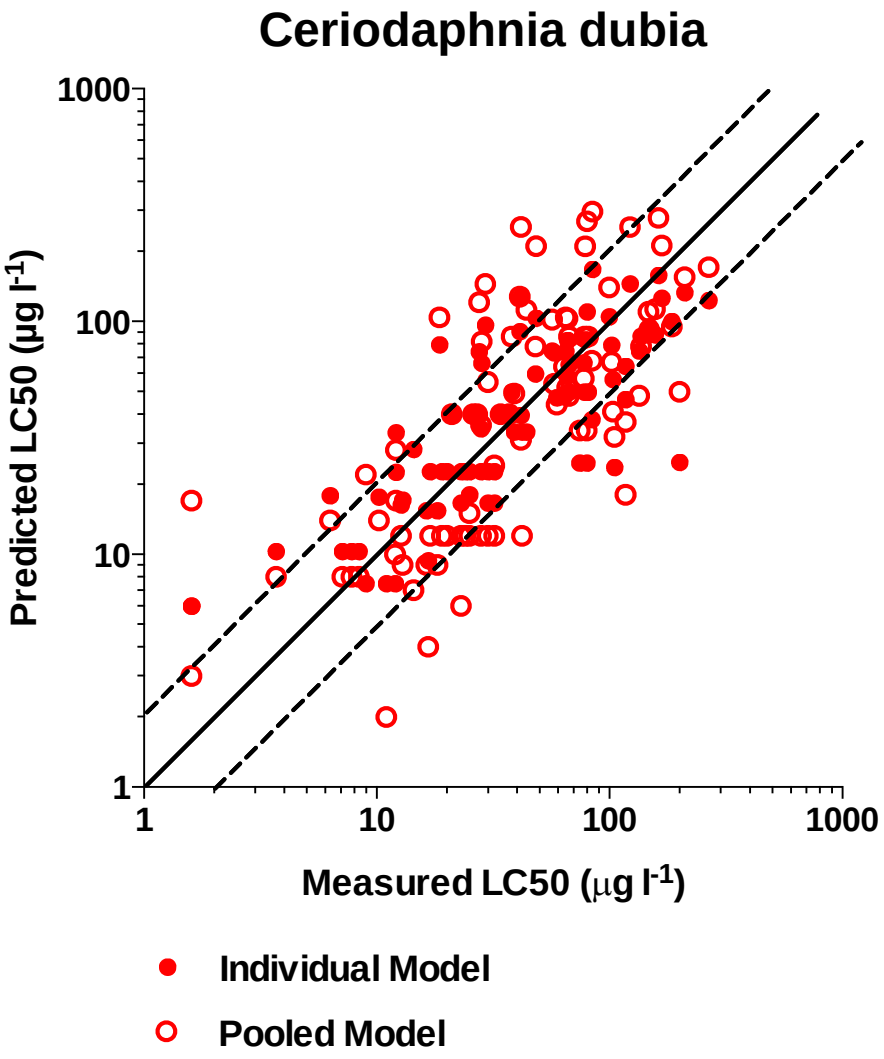
Hardness

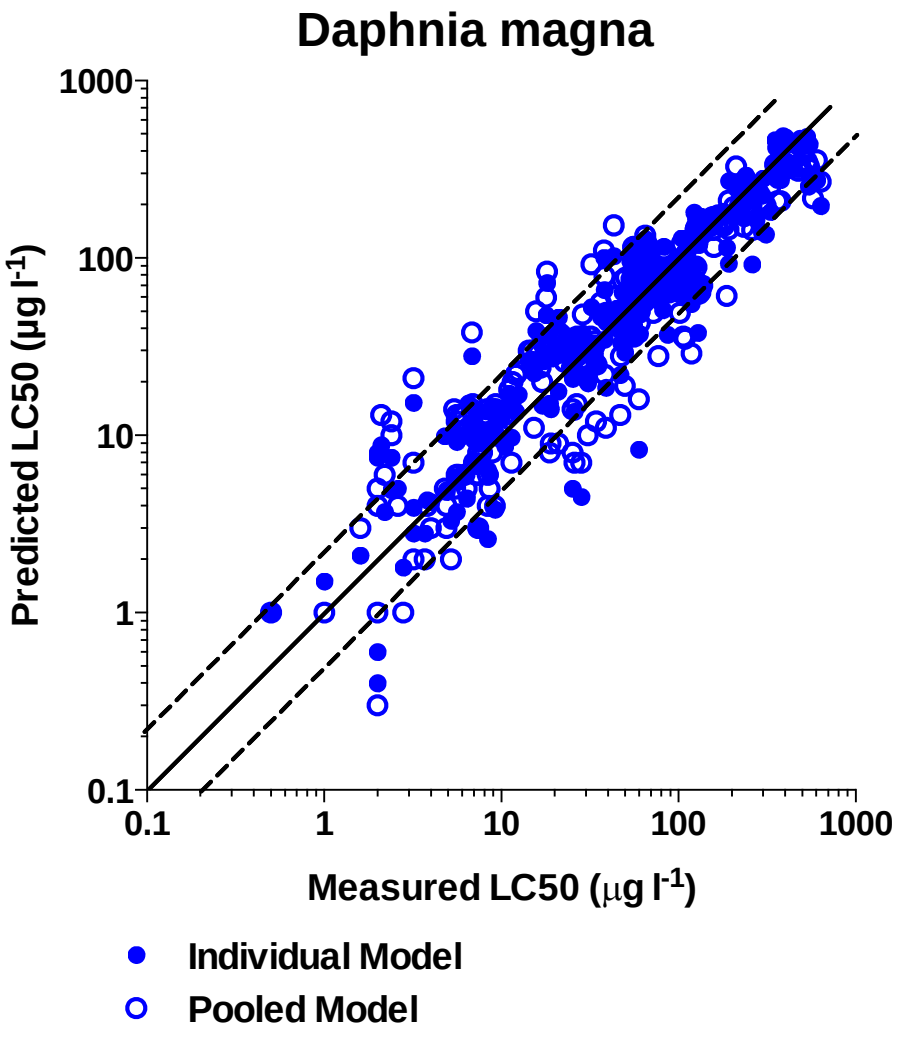
CMC = exp[-1.7+0.9422*ln(Hard)]

MLR – No Interactions

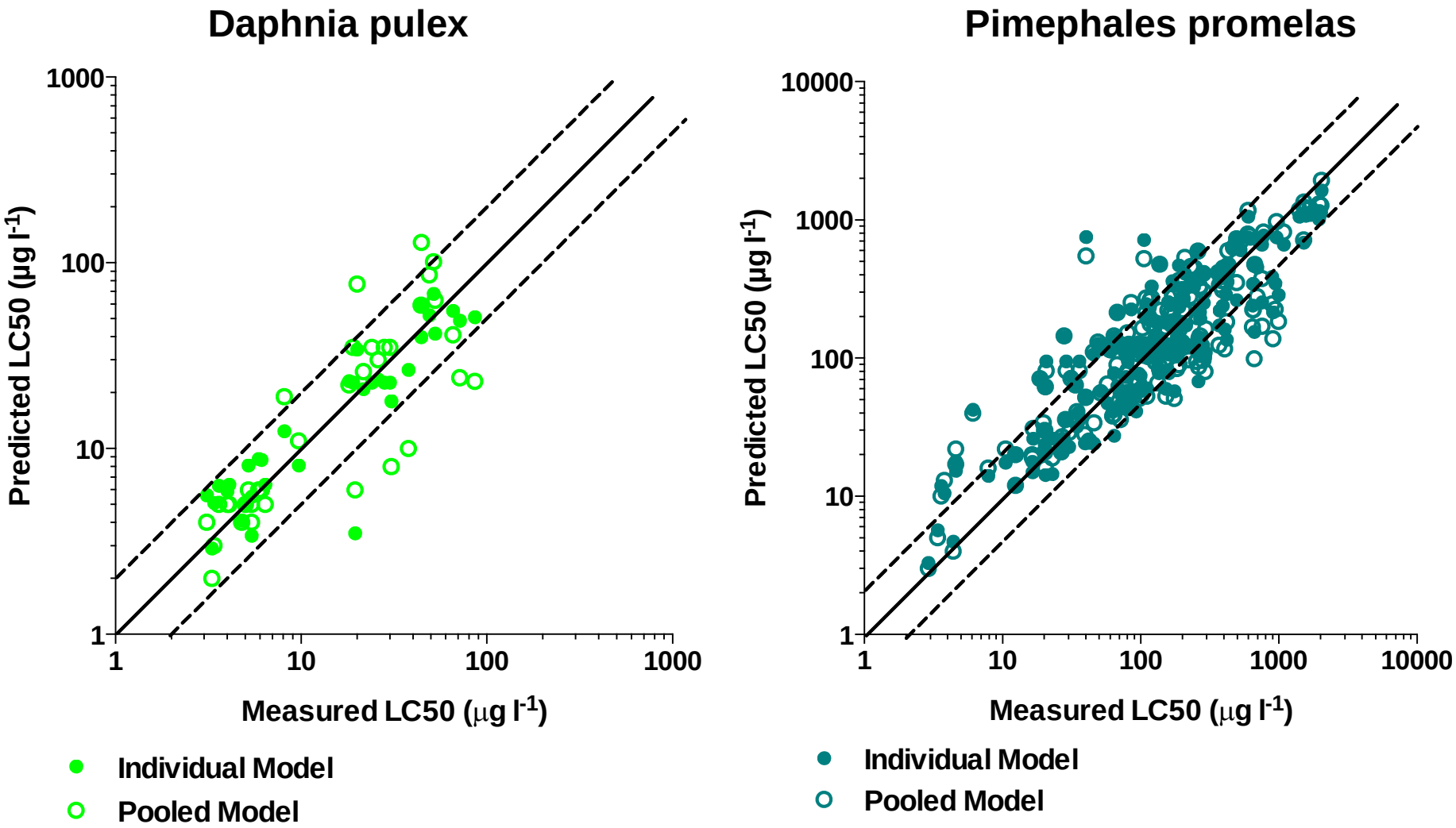
CMC = exp[-15.07+0.7748*ln(DOC)+7.102*ln(pH)+0.5839*ln(Hard)]

Comparison of Individual vs. Pooled Model – Acute Cu



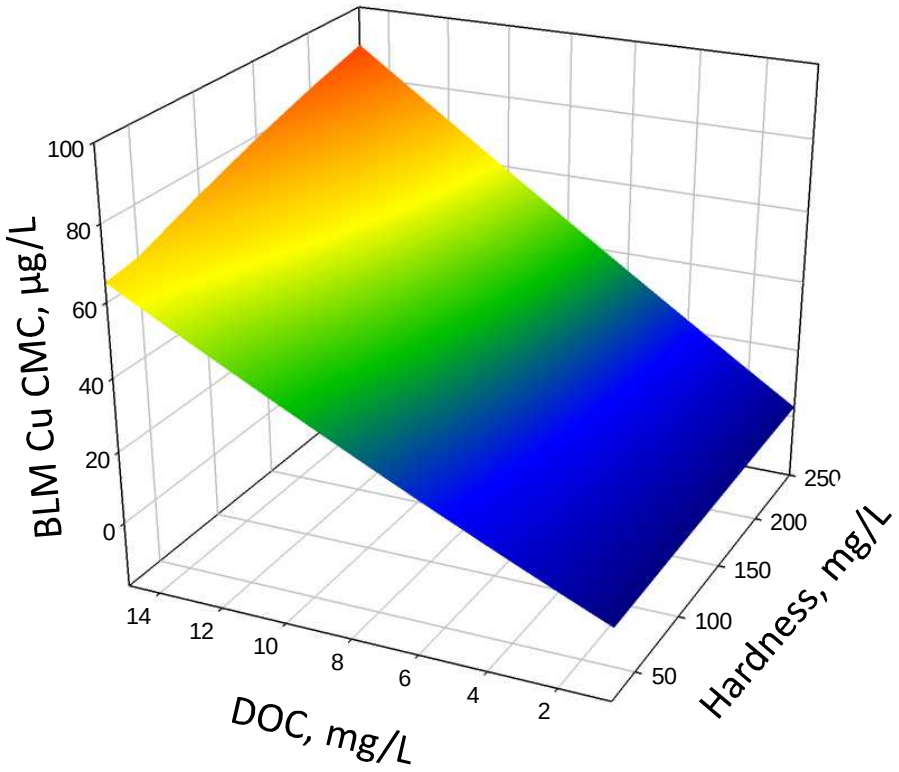


Comparison of Individual vs. Pooled Model – Acute Cu

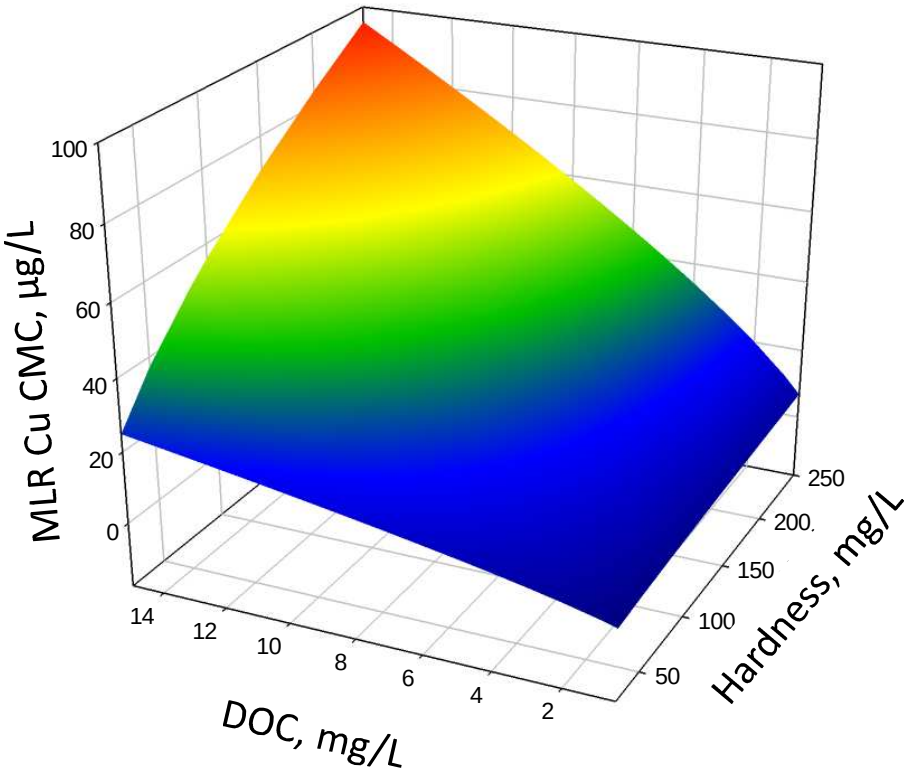


Comparison of BLM- and MLR-based Acute Cu WQC at pH 7.5

BLM



MLR



Conclusions

- **Species-specific MLRs, when based on water quality variables identified by the BLM, perform as well the BLM and generally better than hardness only models**
- **Inclusion of interaction terms provides modest improvement in MLR performance**
- **Final pooled MLR for acute Cu generally consistent with BLM, though there are important differences**
- **Overall, MLR approach appears to be promising alternative for metals to BLM-based WQC**
- **Similar models have been developed for Cd, Pb, Ni and Zn**