# Evaluation and calibration of the Product Register based Exposure Index

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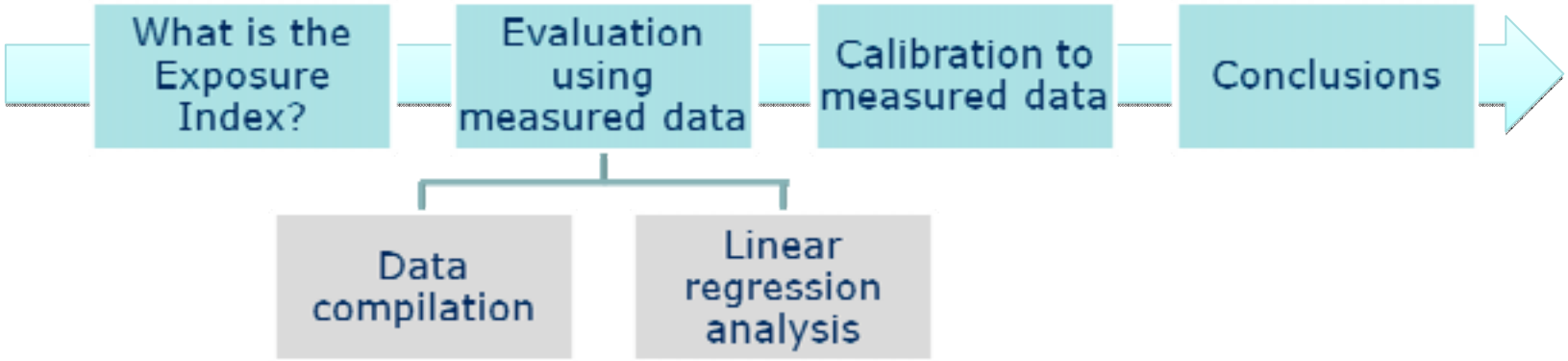
# Outline


What is the Exposure Index?
Evaluation using measured data
Calibration to measured data
Conclusions
Data compilation
Linear regression analysis

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## Product Register based Exposure Index

- Developed by the Swedish Chemicals Agency (KEMI) at the request of the Swedish EPA
- Employs information in the Product Register to rank chemicals based on emissions to various recipients (air, surface water, soil, human, sewage treatment plant (STP))
- High Exposure Index → candidate for screening program

## What is the Exposure Index?

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### The Product Register

Product "SuperPaint"

Hazard label? Yes

Consumer availability? No

Function code = A

Bransch code = C

Quantity of chemical X

Quantity of chemical Y

Quantity of chemical Z

### Key (expert judgement)

| Function Code | Branch Code | Hazard label? | Consumer available? |
|---|---|---|---|
| A = 100 | A = 100 | Yes = 1 | Yes = 10 |
| B = 1 | B = 1 | No = 10 | No = 1 |
| C = 0.01 | C = 0.01 | | |
| D = 100 | D = 10 | | |
| ... | ... | | |

Number of products containing chemical X

### Exposure Index of chemical X

$$EI = \log(9 + n_{prod}^{p}) \cdot \log\left( \sum_{i=1}^{n\,prod} F_i^f \; B_i^b \; Q_i^q \; K_i^k \; (S_i^{-1})^s \right) + C$$

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# Evaluation

- Matrix: Sewage Treatment Plant (sludge and wastewater)
- Comparison of measured concentrations of organic compounds in Swedish STPs to the corresponding EIs
- Compilation of suitable data from the environmental screening database (hosted by IVL at the request of the Swedish EPA) and from other reports and scientific publications
- Number of compounds in final datasets:
  - 51 (sludge)
  - 53 (influent)
  - 62 (effluent)

What is the Exposure Index?

**Evaluation using measured data**

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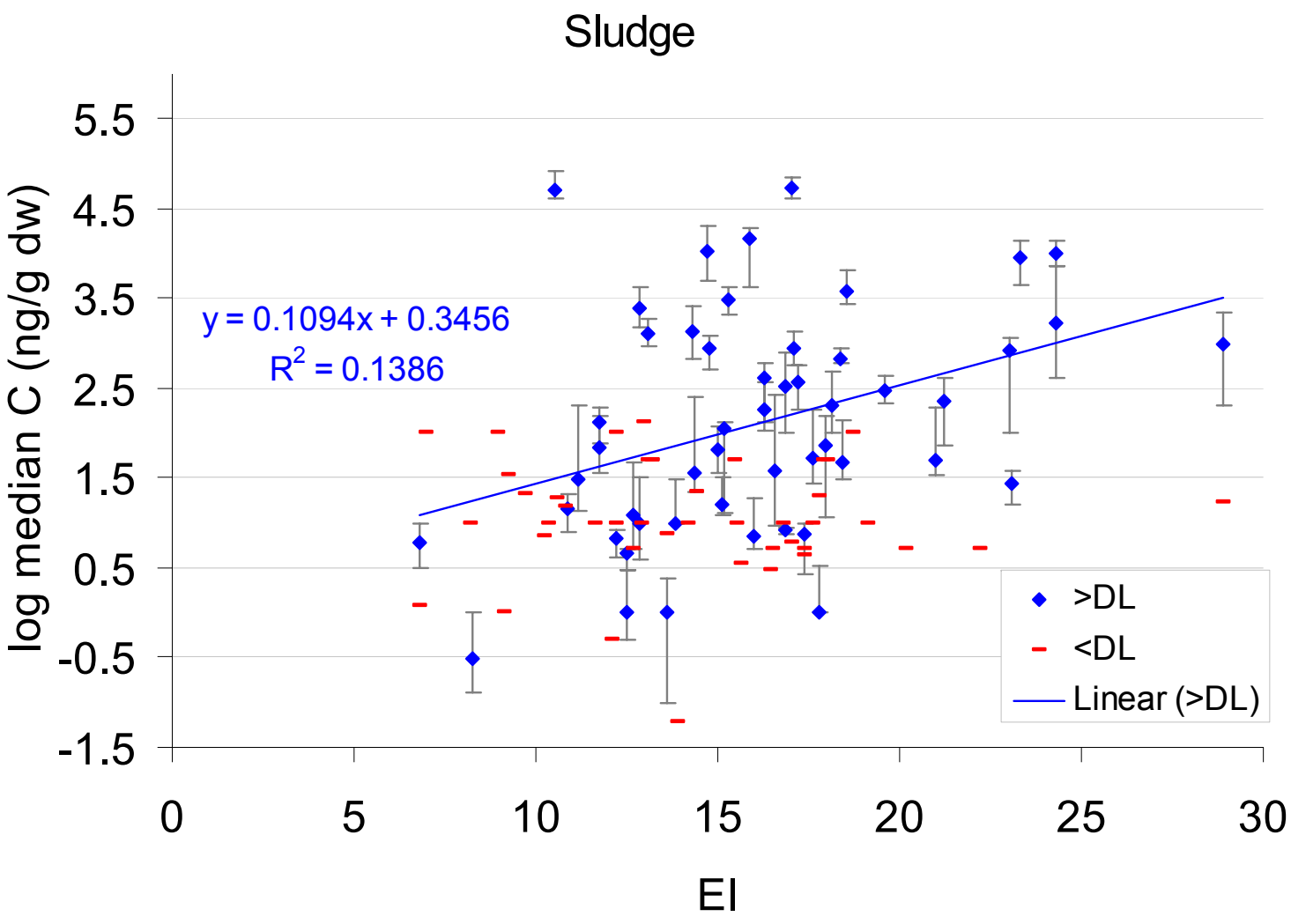

What is the Exposure Index?

**Evaluation using measured data**

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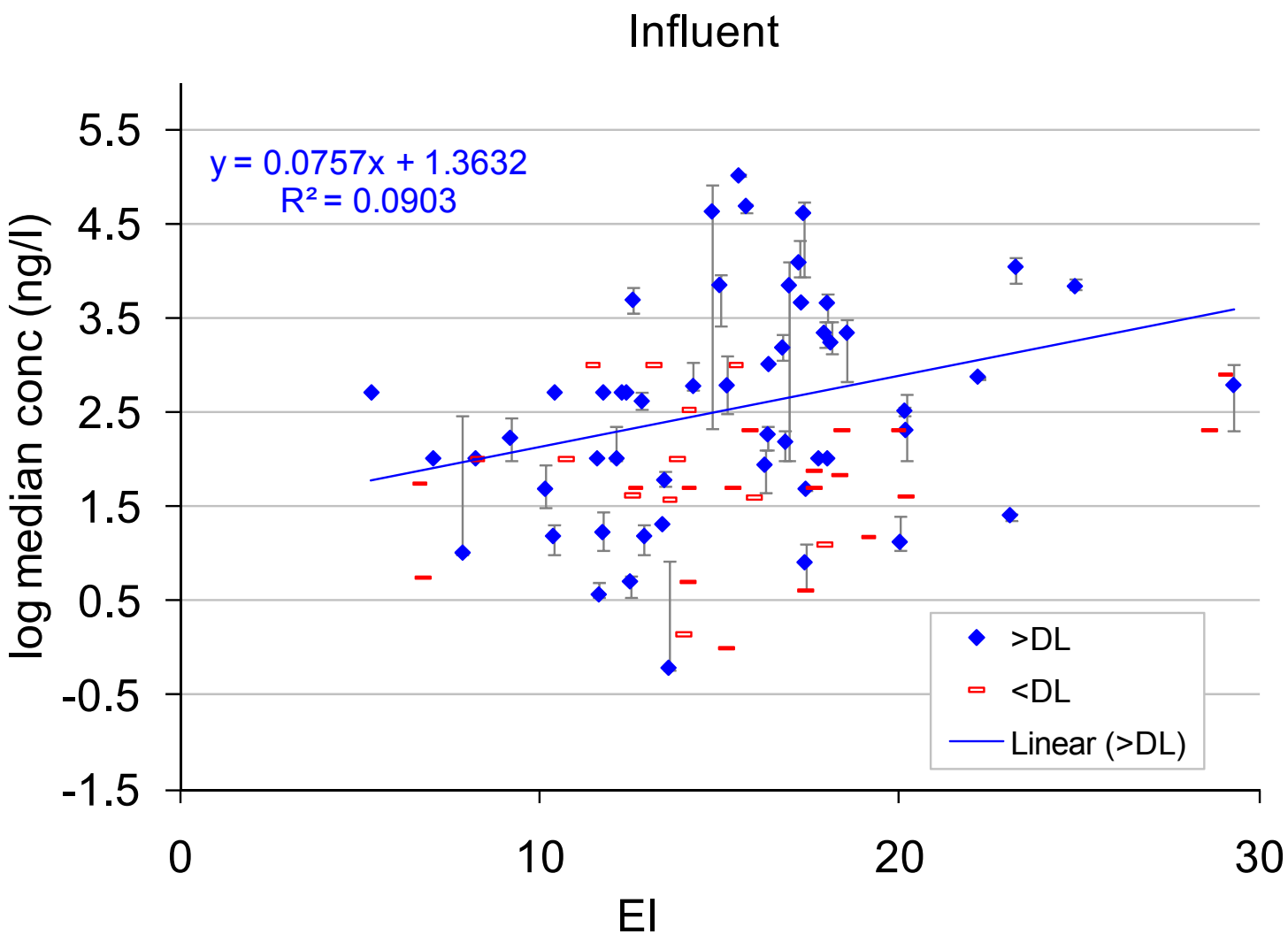

What is the Exposure Index?

**Evaluation using measured data**

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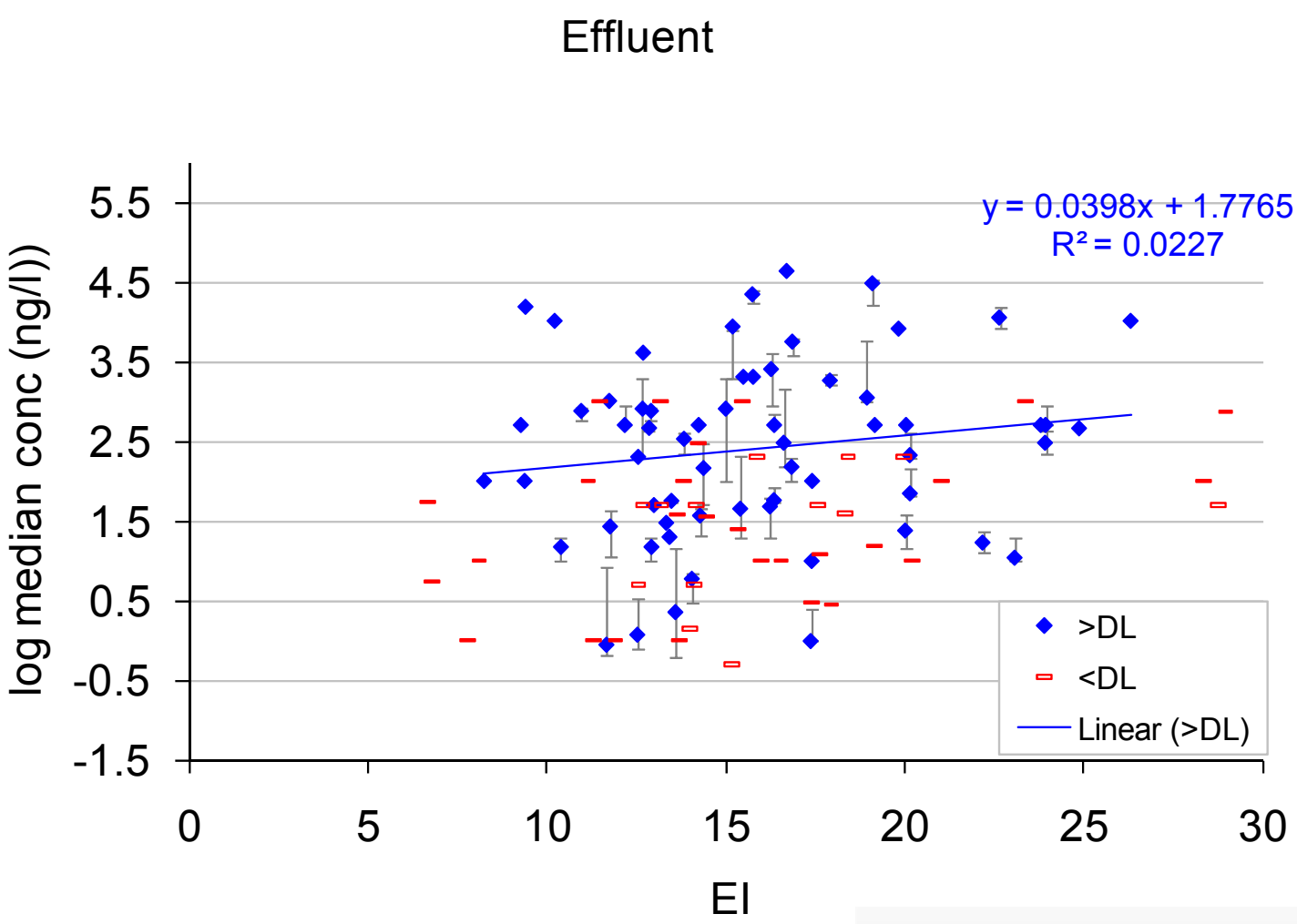


What about degradation and transfer between water, air and sludge?

What is the Exposure Index?

**Evaluation using measured data**

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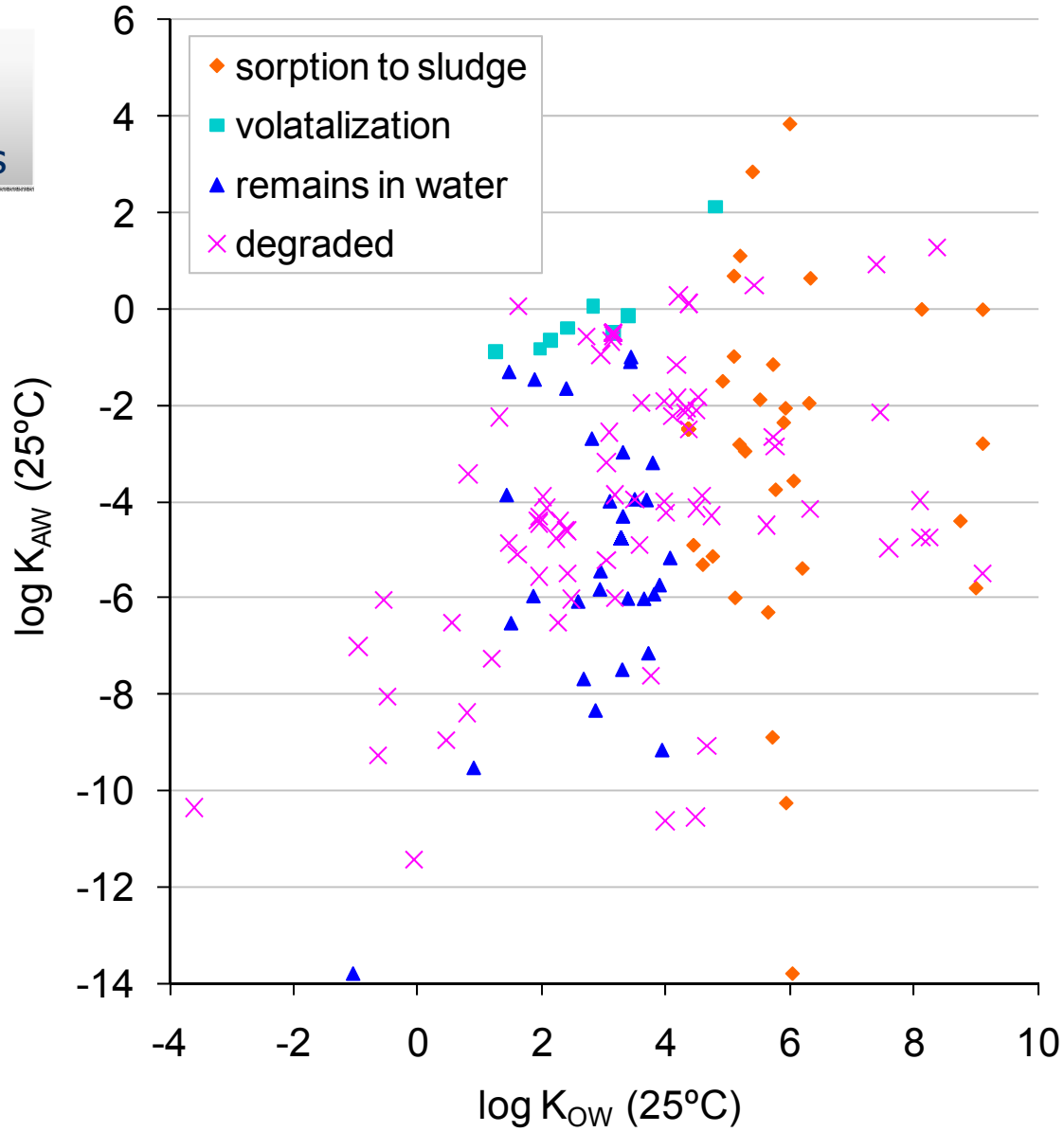
Chemical fate in STPs



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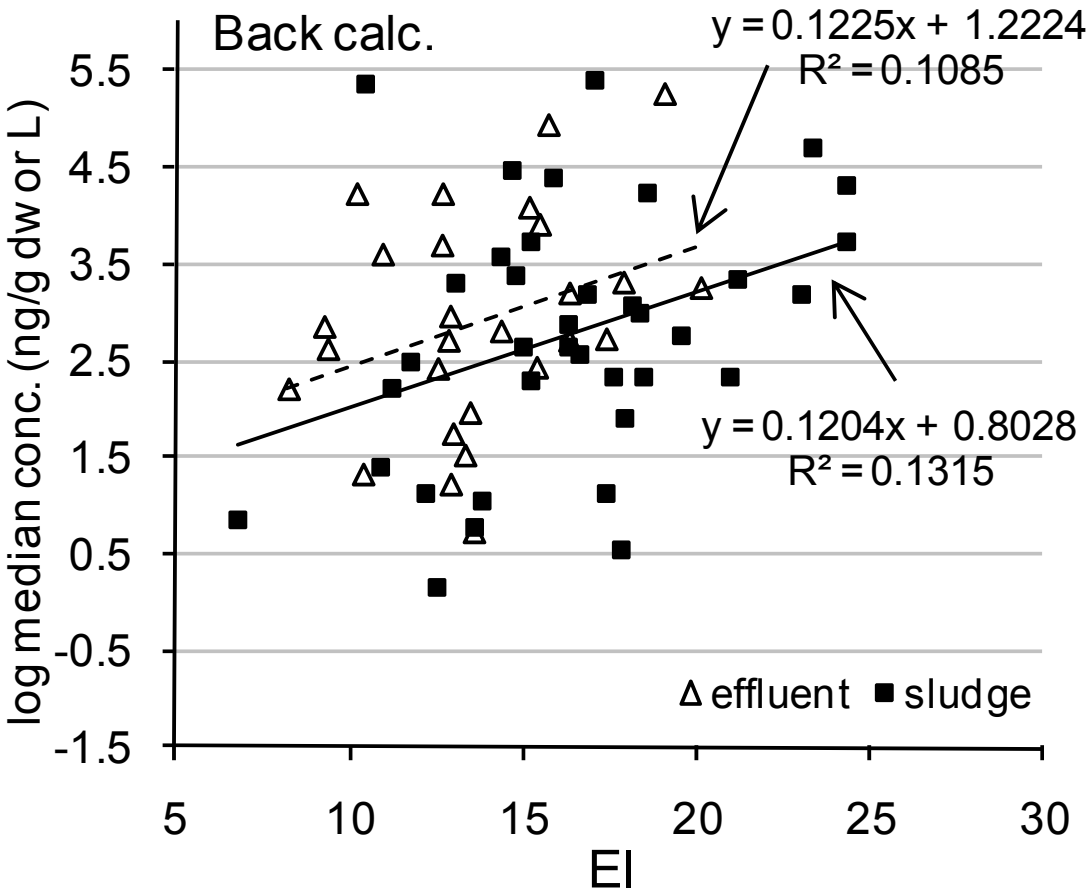
The concentrations are corrected for fate in the STPs




Sludge

n = 36, p = 0.027

Effuent

n= 27, p = 0.09

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# Calibration

- The original equation had a limited power to rank emission levels to STPs
- Could a different weighting of the six variables (quantity, function, bransch, hazard label, consumer availability, number of products containing compound) improve the result?

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# Calibration

- Exponents were introduced in the equation
- Monte Carlo simulations:
  - 1000 combinations of exponent values (randomly sampled from within a specified range)
  - For each combination, the new EIs were plotted against the measured concentrations
  - And the correlation coefficient of the linear regression was recorded.

$$EI = \log(9 + n_{prod}^{p}) \cdot \log\left( \sum_{i=1}^{n\,prod} F_i^{f} B_i^{b} Q_i^{q} K_i^{k} (S_i^{-1})^{s} \right) + C$$

What is the Exposure Index? | Evaluation using measured data | **Calibration to measured data**

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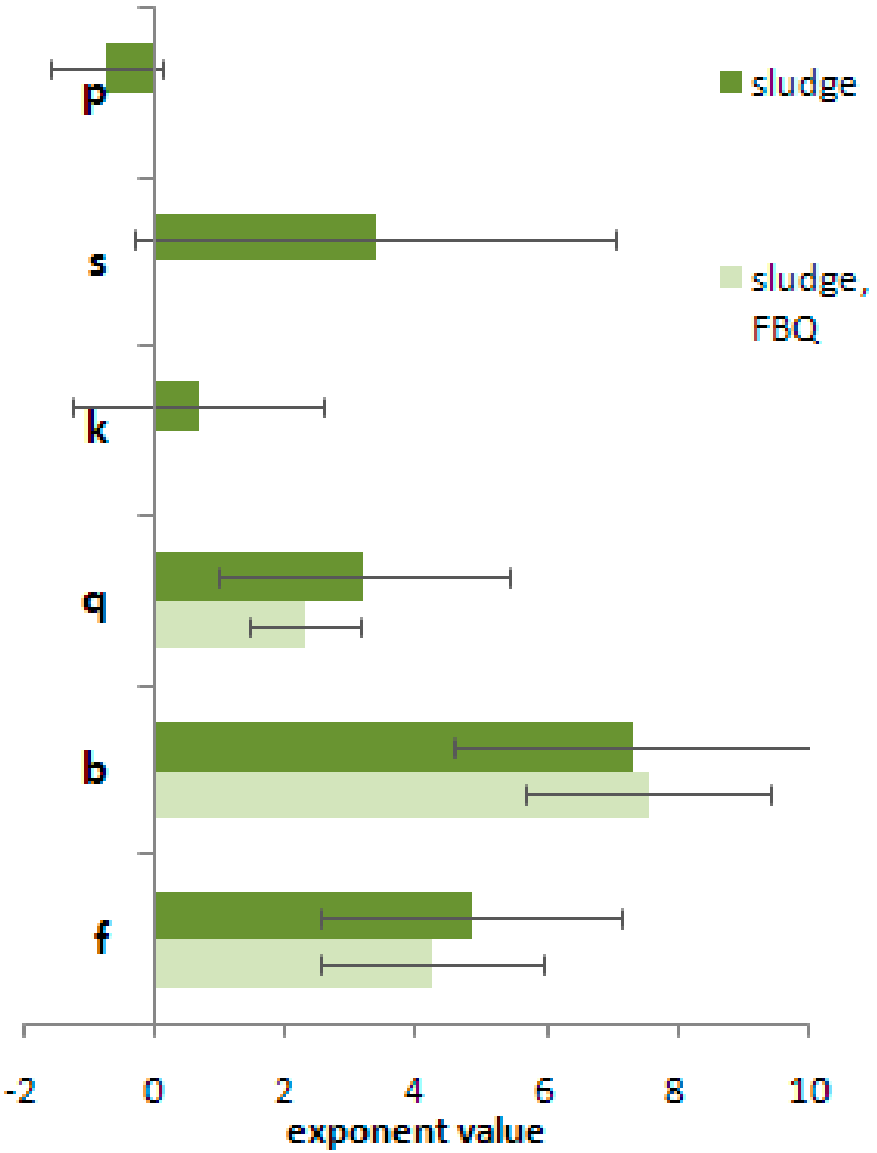
Sludge back calculated concentrations

20 best combinations

Average exponent values




**Best $r^2$ = 0.209**

**Original $r^2$ = 0.13**

What is the Exposure Index? | Evaluation using measured data | **Calibration to measured data**

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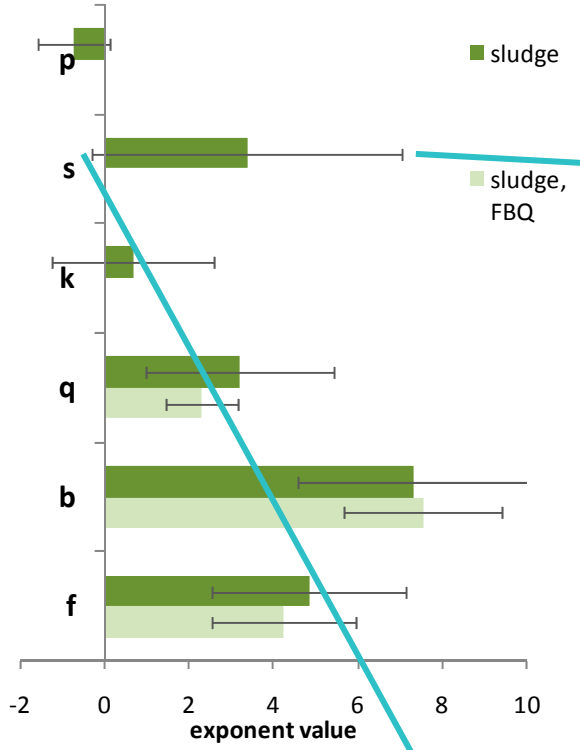


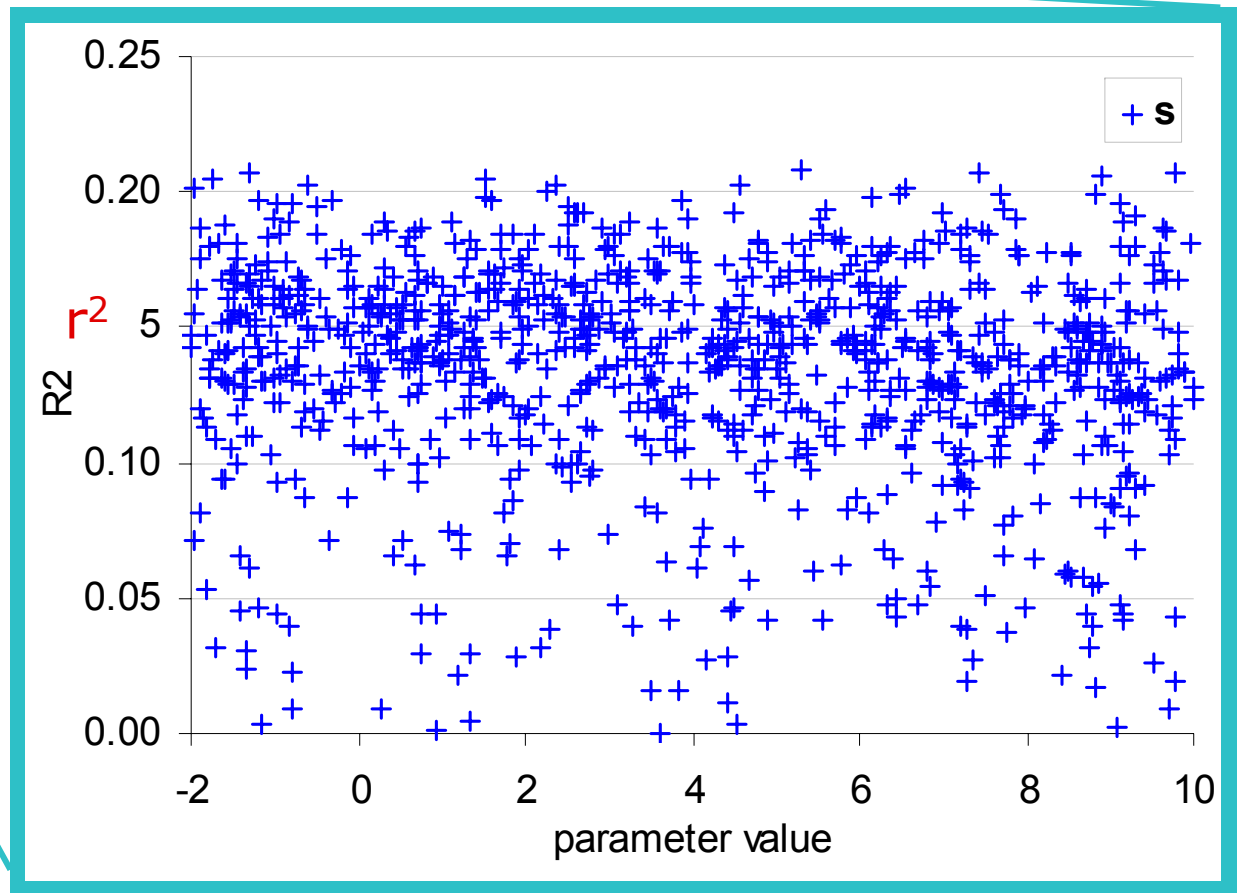

What is the Exposure Index? | Evaluation using measured data | **Calibration to measured data**

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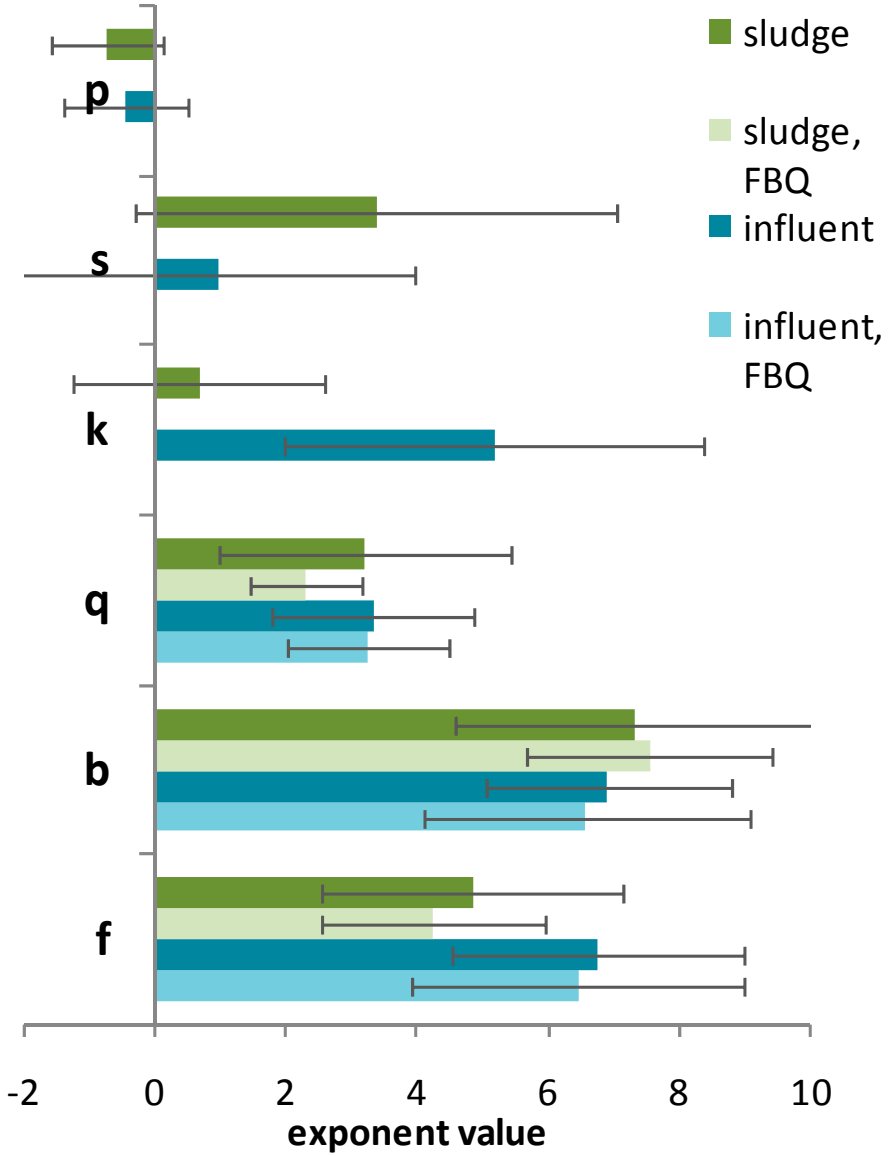
The same parameters are significant in both datasets



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# Conclusions

- Original EI equation limited use for predicting exposure levels in STPs ($r^2$ 0.08 to 0.13)
- Most likely due to mathematical format and assignment of values to parameters
- Calibration did not improve performance to any larger extent ($r^2$ values ~0.2)
- Parameters number of products (P), hazard label (S) and consumer availability (K) had no influence
- Exposure Index parameters cannot fully explain emission levels observed in STPs → another (unknown) parameter is required

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# Suggestions for future work

**Improve evaluation datasets (limited potential)**

- Selection of representative concentrations
- Mid-range EIs were overrepresented → inclusion of more low/high EI compounds

**Improve Exposure Index algorithm**

- Identify the ”unknown parameter(s)”
- Refine assignment of high/medium/low levels to the function and branch parameters – consider physical chemical properties
- Change mathematical form of the Exposure Index equation

# Thank you for listening

Also thanks to: **Katarina Hansson** for providing the Excel version of the IVL database, **Cajsa Wahlberg** at Stockholm Vatten, **Nicklas Paxeus** and **Fredrik Davidsson** at Gryaab (Göteborg) for providing data, **Jon Arnot** for help with the selection of physical chemical properties, **Knut Breivik** (NILU) for literature tips and **Jan-Olov Persson** (Statistiska forskningsgruppen, Stockholms Universitet) for advice regarding statistics.

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