This file contains supporting information for "Evaluating the environmental hazard of industrial chemicals from data collected during the REACH registration process”, by Gustavsson B. M., Hellhof A., Backhaus T.

Supporting Information

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Group** | **Number of chemicals** | **Max [nmol/l]** | **Min [nmol/l]** | **Median [nmol/l]** | **Mean [nmol/l]** | **Best Fit** | **b0** | **b1** | **50% [nmol/l]** | **5% [nmol/l]** |
| Industrial Chemical | 2244 | 4166667.0 | 2.4E-03 | 237.8 | 16732.9 | LogNormal | 0.317 | 202.61 | 202.611 | 1.123 |
| Pharmaceutical | 142 | 3332.5 | 2.9E-05 | 7.0 | 149.4 | LogNormal | 0.259 | 5.23 | 5.230 | 0.009 |
| Pesticide | 298 | 57921.6 | 9.9E-06 | 4.5 | 761.2 | LogNormal | 0.255 | 4.57 | 4.572 | 0.007 |
| Priority Pollutant | 31 | 19427.8 | 6.8E-04 | 0.9 | 1034.0 | LogLogistic | -0.688 | 0.87 | 0.873 | 0.012 |
| Biocide | 76 | 46929.6 | 1.3E-04 | 0.6 | 948.5 | LogLogistic | -0.433 | 0.59 | 0.595 | 0.0007 |

**Supporting Table 1:** Extended summary of data of for the 6 different regulatory classes. Best fit names the model with the lowest MSE as fitted using the ‘drc 25-12’ package. Fitted models are LogNormal, LogLogistic and Weibul. b0 and b1 describes the regression parameters for a fit to nmol/L data. 50% and 5% describe the midpoint of the fitted curve as well as the lower 5% percentile.

LogNormal:

LogLogistic:

Weibull:

|  |  |  |
| --- | --- | --- |
|  | **p adj** | **Significance** |
| Industrial Chemical - Biocide | <0.001 | \* |
| Industrial Chemical - Pesticide | <0.001 | \* |
| Industrial Chemical - Pharmaceutical | <0.001 | \* |
| Industrial Chemical – Priority Pollutant | <0.001 | \* |
| Pesticide – Biocide | <0.001 | \* |
| Pesticide – Priority Pollutant | 0.444 |  |
| Pharmaceutical – Biocide | 0.002 | \* |
| Pharmaceutical – Pesticide | 0.992 |  |
| Pharmaceutical - Priority Pollutant | 0.645 |  |

**Supporting Table 2:** Results from Tukey’s significance test. The table shows that 6 out of the 9 pair-wise groups have significant differences (p<0.05). The test has been performed on log-transformed environmental thresholds.

|  |  |  |
| --- | --- | --- |
|  | **p adj** | **Significance** |
| 10-100-1-10 | <0.001 | \* |
| 100-1000-1-10 | 0.003 | \* |
| 1000-10000-1-10 | 0.578 |   |
| 10000-100000-1-10 | 1.000 |   |
| 100000-1000000-1-10 | 0.064 |   |
| 1000000-10000000-1-10 | 0.134 |   |
| 10000000-100000000-1-10 | 0.962 |   |
| 100-1000-10-100 | 0.347 |   |
| 1000-10000-10-100 | <0.001 | \* |
| 10000-100000-10-100 | <0.001 | \* |
| 100000-1000000-10-100 | <0.001 | \* |
| 1000000-10000000-10-100 | <0.001 | \* |
| 10000000-100000000-10-100 | 0.141 |   |
| 1000-10000-100-1000 | 0.016 | \* |
| 10000-100000-100-1000 | <0.001 | \* |
| 100000-1000000-100-1000 | <0.001 | \* |
| 1000000-10000000-100-1000 | <0.001 | \* |
| 10000000-100000000-100-1000 | 0.375 |   |
| 10000-100000-1000-10000 | 0.040 | \* |
| 100000-1000000-1000-10000 | 0.000 | \* |
| 1000000-10000000-1000-10000 | 0.001 | \* |
| 10000000-100000000-1000-10000 | 0.738 |   |
| 100000-1000000-10000-100000 | 0.050 | \* |
| 1000000-10000000-10000-100000 | 0.151 |   |
| 10000000-100000000-10000-100000 | 0.978 |   |
| 1000000-10000000-100000-1000000 | 1.000 |   |
| 10000000-100000000-100000-1000000 | 1.000 |   |
| 10000000-100000000-1000000-10000000 | 1.000 |   |

**Supporting Table 3:** Tukey test of significance. The table shows that 14 out of the 28 pair-wise groups have significant differences. The test has been performed on log-transformed environmental thresholds.