Supplementary Information

Log-transformed concentrations

A simple log-transformed concentration, $D = \log_{10}(d)$, leaves the control out of the analysis (because $d = 0$ for the control). Therefore, the objective was then to find an appropriate transformation that includes the control data in the fit and that keeps the points evenly spaced apart. Therefore, given a vector of m concentration points (d_i, i = 1 to m, with $d_1 = 0$ being the control) we defined a transformed concentration, $D = \log(nd + 1)$, where $n = (\delta\text{-}1)/d_2$ with d_2 being the lowest non-zero dose in the experiment; $\delta = d_m/d_{m-1}$,where d_m and d_{m-1} are the last and penultimate dose points, respectively (EPA, 2012). This transformation ensured that concentration points were evenly spaced apart. Specifically, the difference between the 1st and 2nd transformed concentration ($D_2 - D_1 = \log(\delta)$) was roughly equal to the difference between the m^{th} and m-1th transformed concentration ($D_m - D_{m-1} = \log(nd_m+1) - \log(nd_{m-1}+1) \sim \log(d_m/d_{m-1}) = \log(\delta)$). We used the transformed concentration, D, to visualize the plots of all the model fits to the data.

Supplementary Figures

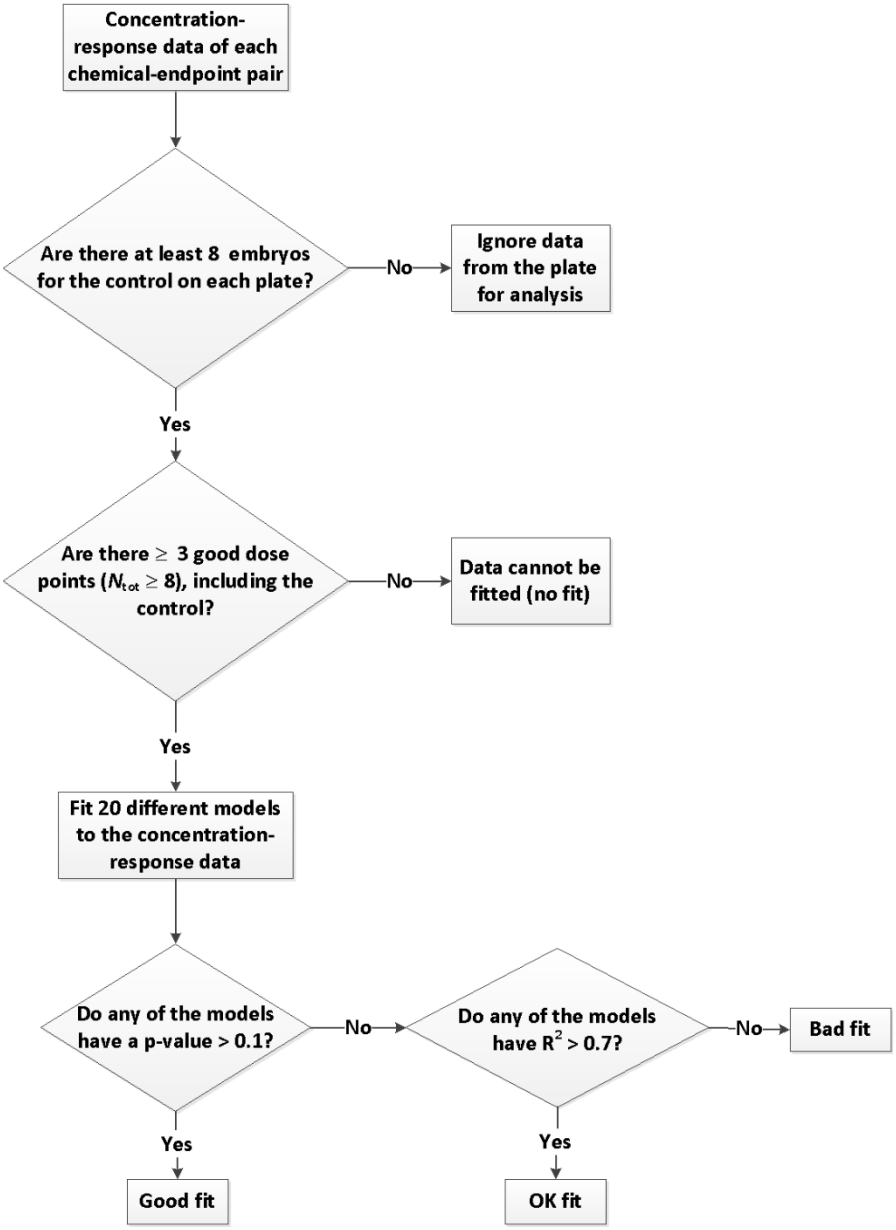

Figure S1. Workflow showing the statistical criteria applied for evaluating the data and the quality of model fits.

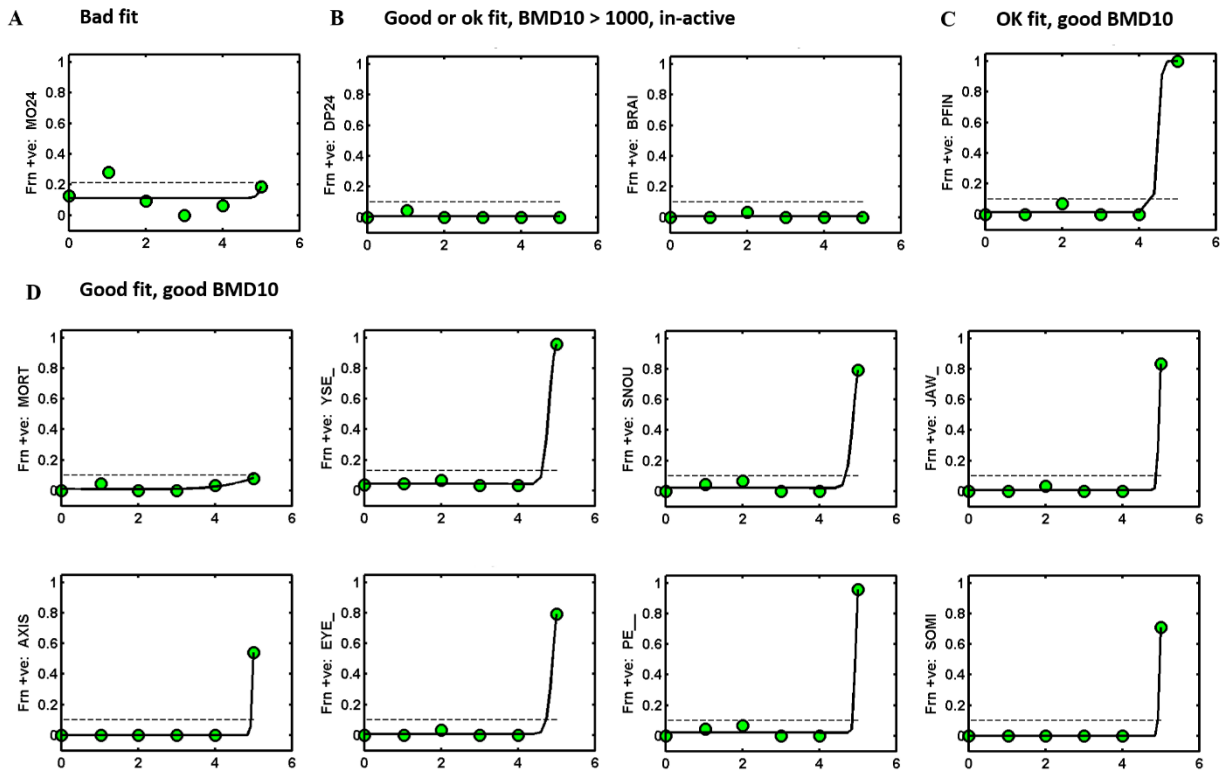

Figure S2. Concentration-response (C-R) curve-fit results showing the response probability versus scaled (log-transformed) dose of cymoxanil (TX001425) for morphology/mortality endpoints: (A) C-R curve with bad fit; (B) C-R curves with good or ok fits and BMD_{10} values > 1000 (in-active); (C) C-R curves with OK fits and good BMD_{10} values ($0 < BMD_{10} \leq 1000$). (D) C-R curves with good fits and good BMD_{10} values.

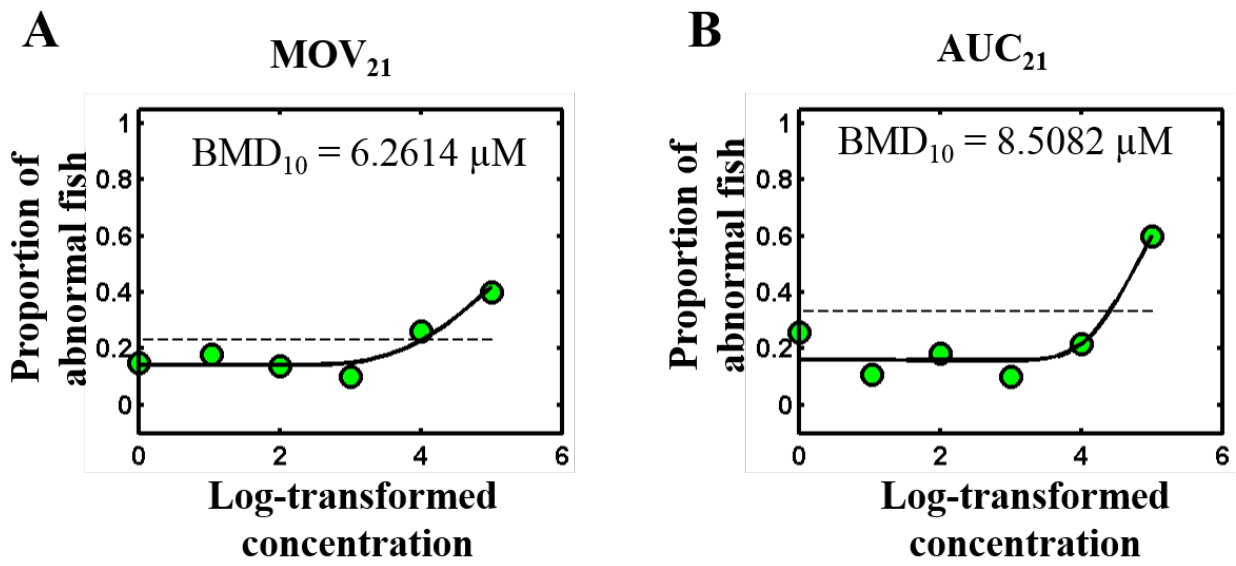

Figure S3. Proportion of abnormal fish versus log-transformed concentration plot and BMD_{10} value of flusilazole (TX000669) for the MOV_{21} (A) and AUC_{21} (B) endpoints.

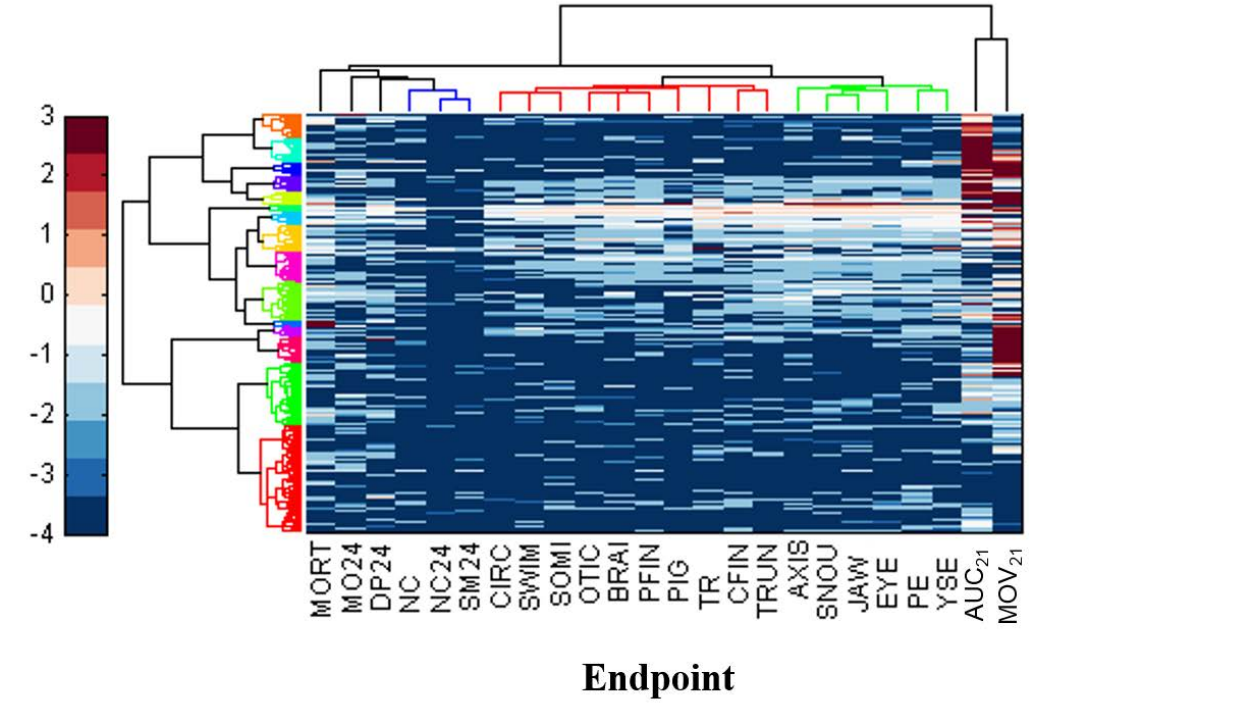

Figure S4. Hierarchical clustering result based on the BMD_{10} values of all zebrafish chemical-endpoint pairs. Heat map color bar represents $-\log_{10}(BMD_{10})$ values.

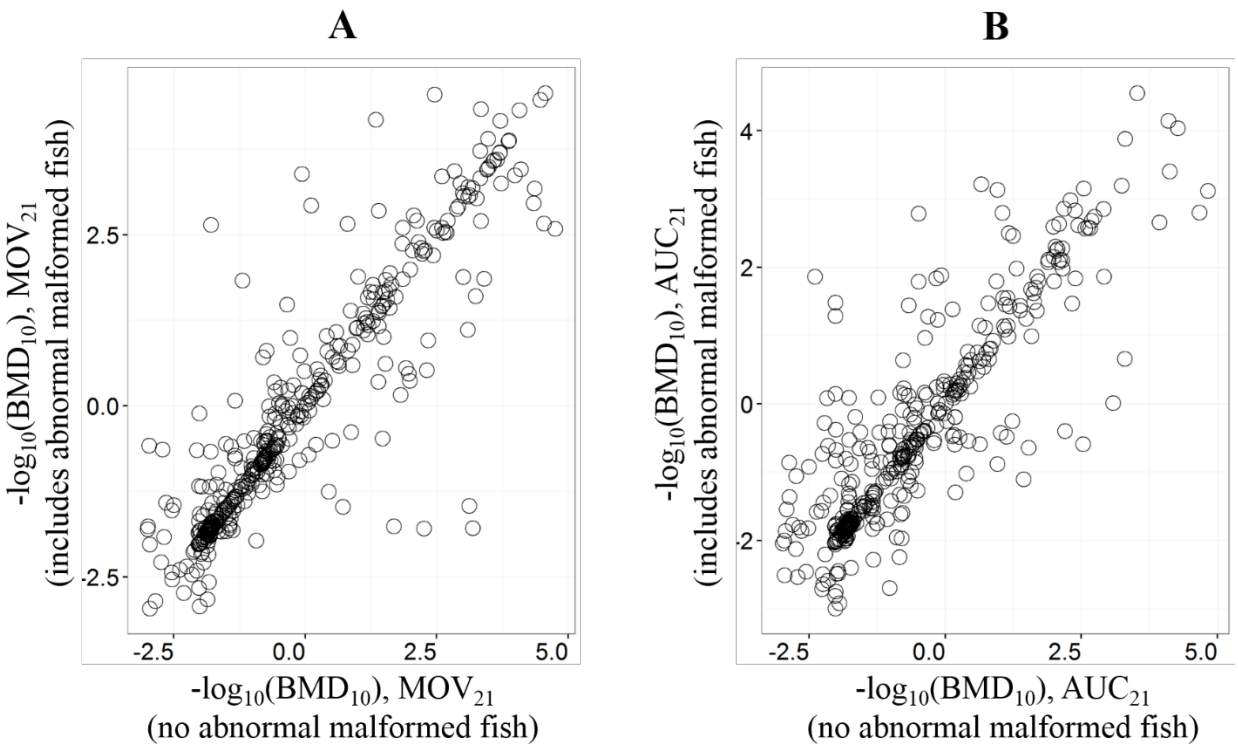

Figure S5. Comparison between the BMD_{10} values obtained with and without abnormally behaving malformed fishes for the MOV_{21} (A) and AUC_{21} (B) endpoints.

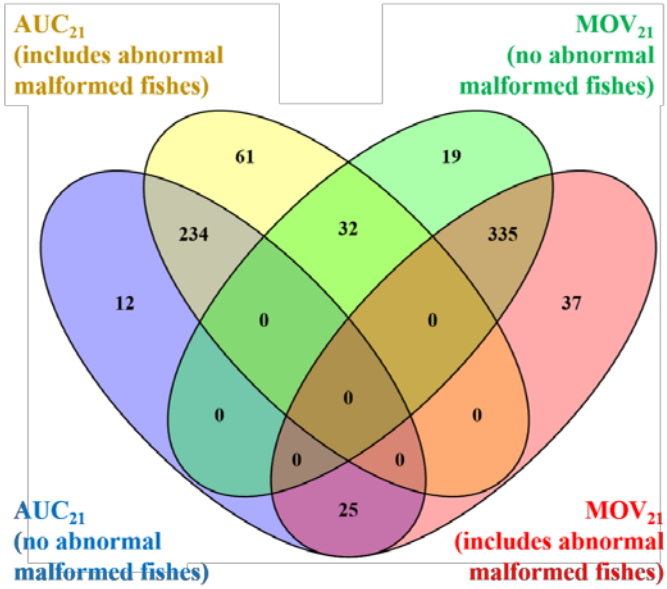

Figure S6. Venn diagram showing the number of chemicals that were most active through the behavioral endpoints when BMD10 values were calculated with and without abnormally behaving malformed fishes. Diagram created using Venny v. 2.1 (http://bioinfogp.cnb.csic.es/tools/venny/)

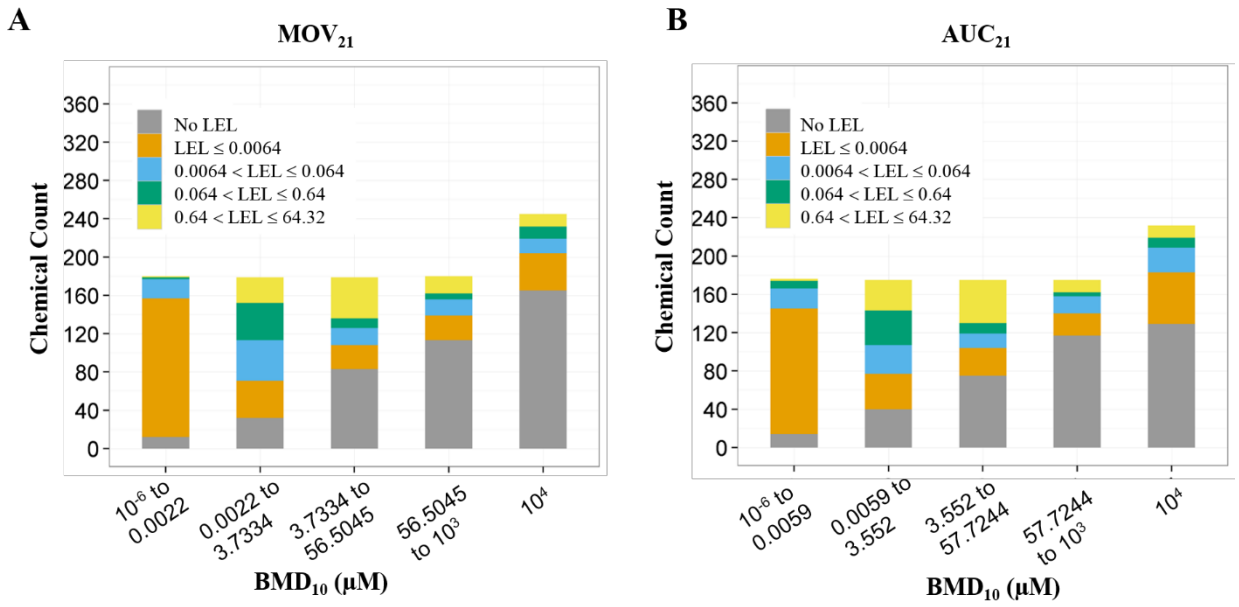

Figure S7. Number of chemicals in each quartile range of BMD_{10} values and their LEL range for the two most sensitive endpoints: (A) MOV_{21} (963 chemicals) and (B) AUC_{21} (934 chemicals). The inactive chemicals based on LEL are indicated as 'No LEL' and based on BMD_{10} values are indicated as $BMD_{10} = 10^4$.

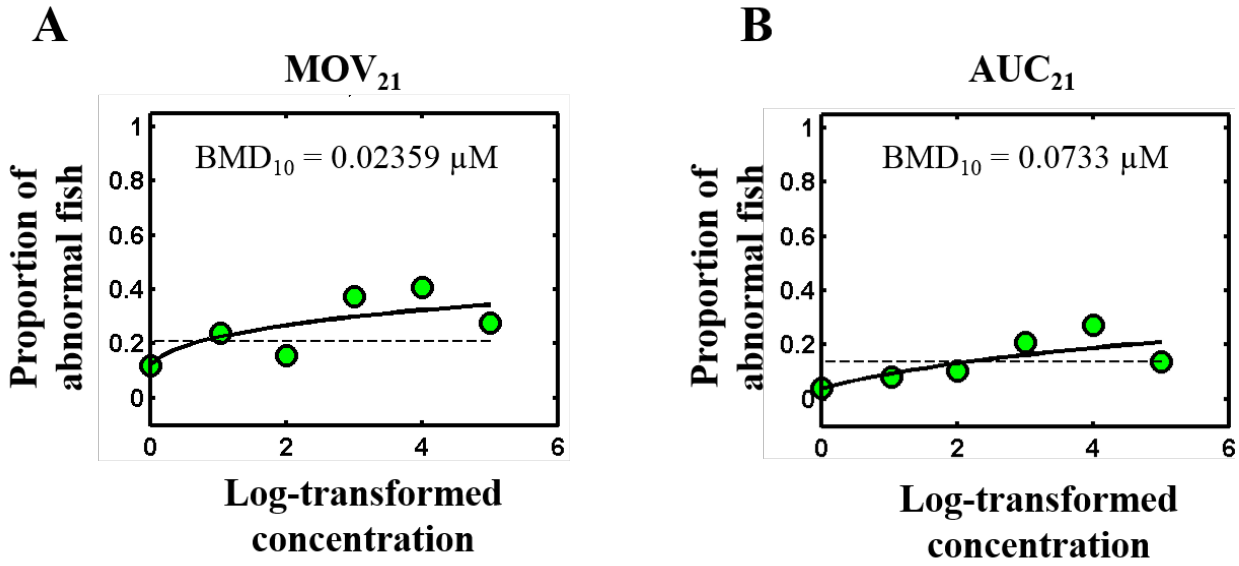

Figure S8. Concentration-response plots for the chemical Quinoline (TX002359) based on MOV_{21} (A) and AUC_{21} (B) endpoints. The chemical ranking changed from 7 to 89 when the MOV_{21} and AUC_{21} BMD_{10} values were added to the *in vitro* ToxCast AC_{50} values in the ToxPi chemical ranking analysis.