1. Supplementary data

**Supplementary File 1. Compounds.** Excel file with additional information on the 33 compounds used in the computational analysis, including the number of gene profiles per compound taken from the Open TG-GATEs database.

**Supplementary File 2. GO – compounds associations.** Excel file that provides the original and filtered results from the GO-based gene set enrichment analysis across compounds and model systems. The files has a “readme” sheet that explains its content.

**Supplementary File 3. MeSH – compound associations.** Excel file that provides the original and filtered results from the literature annotation co-occurrence analysis. The files has a “readme” sheet that explains its content.

**Supplementary File 4. GO – MeSH associations.** An Excel file that provides all pair-wise associations selected across model systems. The files has a “readme” sheet that explains its content.