SUPPORTING INFORMATION

Consideration of predicted small-molecule metabolites in computational toxicology

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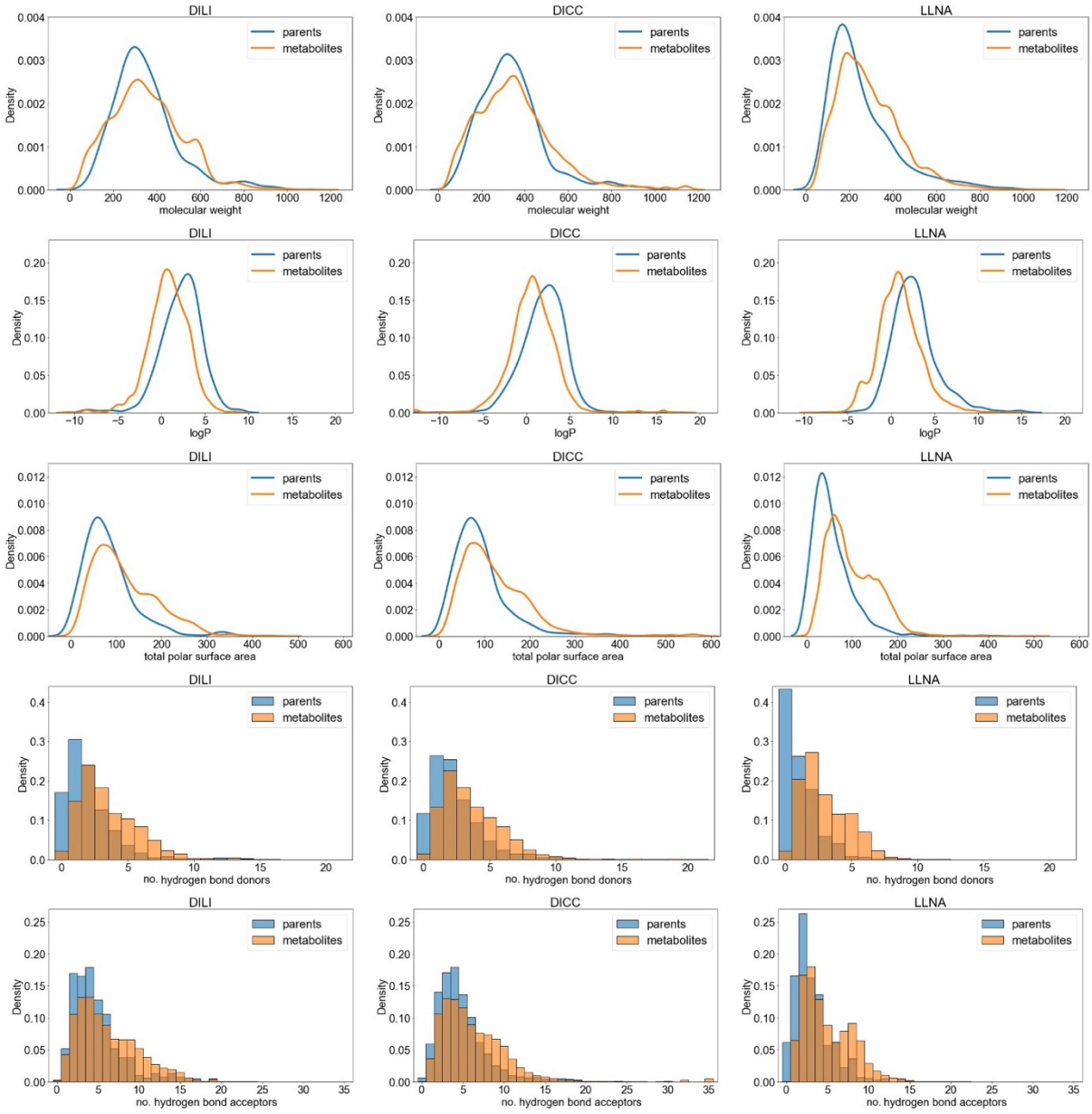

Figure S1. Comparison of the physicochemical properties of the parent compounds (blue) and predicted metabolites (orange) represented in the DILI, DICC and LLNA data sets.

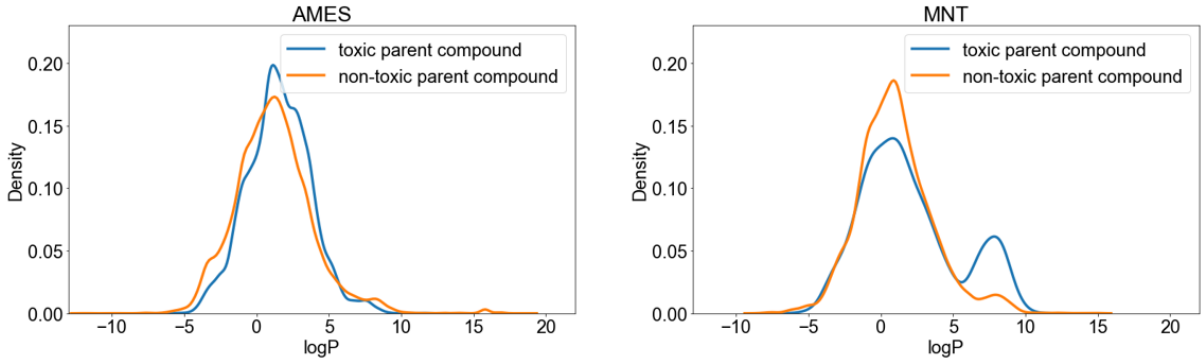

Figure S2. Distribution of the logP values for the metabolites from toxic (blue) and non-toxic (orange) parent compounds in the AMES and MNT data sets.

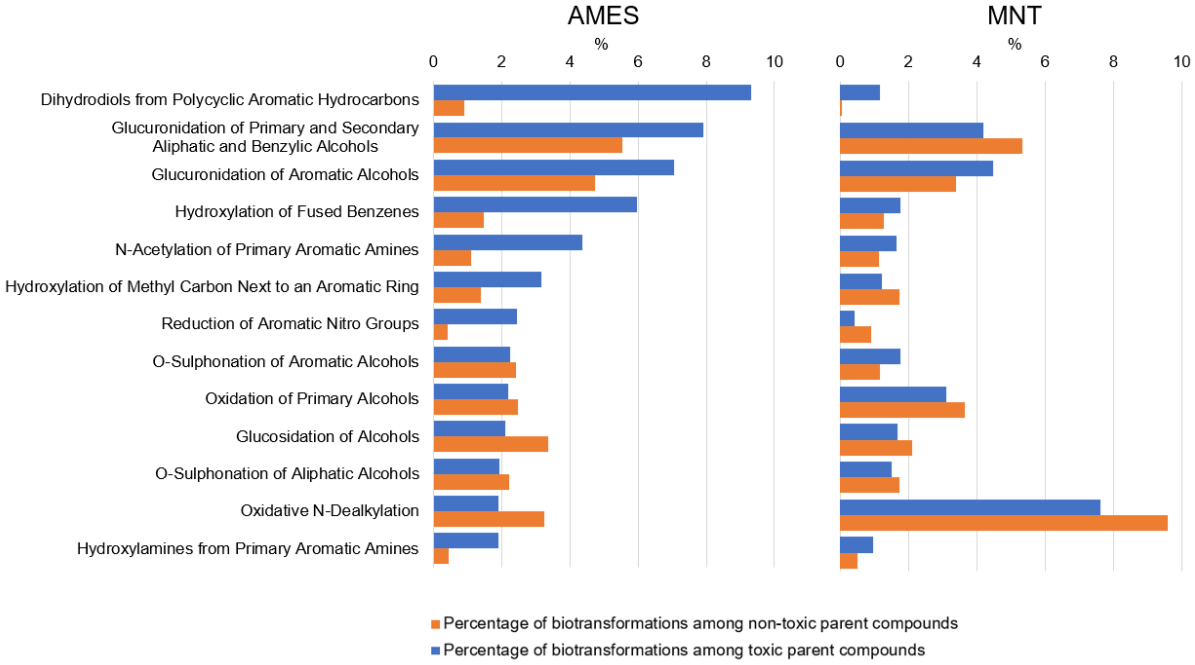

Figure S3. Percentage of occurrence of a subset of biotransformations between toxic (blue) and non-toxic (orange) compounds. The selected subset are the 15 biotransformations most often observed for toxic compounds in AMES. Although some biotransformations appear more often in one of the activity classes, these ratios are different between endpoints.