

Table 1. 2×2 contingency table for modified Fisher's exact test.

Number of chemicals	CASRN Input set	Whole Tox21 set
Annotated with the term	13-1	735
Not annotated with the term	0	8,023

Note: A 2×2 contingency table for modified Fisher's exact test is constructed for the input set "BPAanalogue" consisting of 13 chemicals for enrichment analysis in the annotation term "bond:COH_alcohol_aromatic_phenol" in the ToxPrint substructure category. Modification of "-1" is applied to the typical Fisher's exact test to make the statistical test more conservative, resulting in a p-value of 2.59E-13.