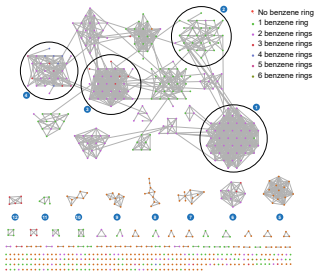
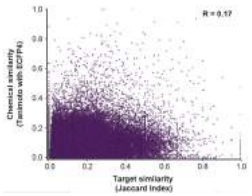
Network-centric analysis

Chemical Similarity Network (CSN)

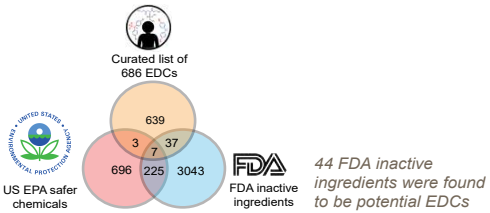


Target Similarity Network (TSN)

Lack of correlation between chemical structure and target genes of EDCs



Comparison with US EPA safer chemicals and FDA inactive ingredients



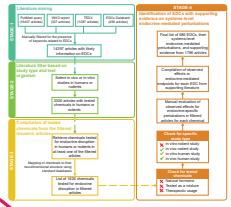
10 safer chemicals were found to be potential EDCs

44 FDA inactive ingredients were found to be potential EDCs

Identification of EDCs with published experimental evidence on endocrine disruption in humans or rodents

Literature mining

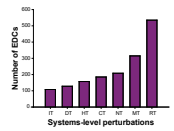
PubMed query
WHO report
TEDX
EDCs Databank



Curation of ~16000 research articles using 4-stage workflow

Compilation of curated list of 686 EDCs from 1796 published research articles

Compilation and standardization of 514 endocrine-mediated endpoints



Systems-level understanding of endocrine disruption mechanism

Dosage at which an endocrine-mediated endpoint is observed

Lowest-observed-adverse-effect level (LOAEL)
No-observed-adverse-effect level (NOAEL)

Analysis

Curation

Database

Classification

Endocrine Disrupting Chemicals (EDCs) and their biological systems-level perturbations

DEDuCT-Database of Endocrine Disrupting Chemicals and their Toxicity profiles

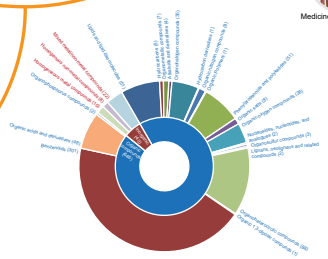
https://cb.imsc.res.in/deduct/

Additional information for EDCs:

2D and 3D chemical structure
Physicochemical properties
Molecular descriptors
Predicted ADMET properties
Experimentally inferred target genes

Classification of EDCs

Classification based on chemical properties



Classification based on Environmental source
7 broad categories
48 sub-categories

Classification based on type of supporting evidence from published literature