



REPRESENTING THE MOLECULAR BASIS OF EXPOSOMIC RESEARCH

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Background

Recent definitions of the concept of the exposome include endogenous processes within the body, biological responses of adaptation to environment, and socio-behavioral factors beyond assessment of exposures¹. Research in generating and utilizing exposomes requires an understanding and representation of molecular constituents involved in direct biological pathway alterations as well as mutagenic and epigenetic mechanisms of environmental influences on the phenome. This research project was an initial evaluation of the Chemical Entities of Biological Interest (ChEBI)² ontology for exposomic research purposes.

Research Methodology

We considered two types of exposures: (1) Air pollutant species by reviewing hazardous air pollutants literature from the Environmental Protection Agency³, and species identified within the Pediatric Research using Integrated Sensor Monitoring Systems (PRISMS) project⁴; and (2) Poisons (therapeutic and non-therapeutic) from U.S. national and state reports⁵. Some of these species interact with body are directly, others react with other chemicals within the body or environment leading to the formation of harmful agents. We mapped a sample of 224 unique air pollutant species and thousands of poisonous chemical substances (Figure 1) to ChEBI for its evaluation. The evaluation method used consisted of analyzing what information ChEBI provided on each species, and determining whether the information provided by ChEBI was sufficient to support exposomic research.

Conclusions

We found particulate matter was the most frequently referenced and studied species in all of the sources. ChEBI did not have a concept for particulate matter, although the constituents of particulate matter mapped to ChEBI. In addition to a name and a unique Identifier, ChEBI provides IUPAC names, synonyms, relationships, registry numbers, database cross-references, structural diagrams and additional information in the form of an ontology. It consists of four sub-ontologies that provide the chemical species' molecular structures, biological roles, applications and subatomic particles². The biological role classifies entities based on their role within a biological context. These roles include antimicrobial, hormonal, enzymatic and bio-membranal actions. Relationships between species provide information on existing and potential interactions

Exposure Species	ChEBI ID	ChEBI Name
Ozone	CHEBI:25812	ozone
Carbon Monoxide	CHEBI:17245	carbon monoxide
Sulfur Dioxide	CHEBI:18422	sulfur dioxide
Nitrogen Dioxide	CHEBI:33101	nitrogen dioxide
Benzene	CHEBI:16716	benzene
Formaldehyde	CHEBI:16842	formaldehyde
Toluene 2,4-diisocyanate	CHEBI:53556	toluene 2,4-diisocyanate
Carbon Dioxide	CHEBI:16526	carbon dioxide
Volatile Organic Compound	CHEBI:134179	volatile organic compound
Black Carbon	CHEBI:82297	carbon black
Eicosanoids	CHEBI:23899	icosanoid
oxycodone	CHEBI:7852	oxycodone

The screenshot shows the ChEBI entry for oxycodone. It includes a chemical structure diagram, the ChEBI name 'oxycodone', the ChEBI ID 'CHEBI:7852', a definition: 'A semisynthetic opioid of formula C₁₈H₂₅NO₃ that is derived from thebaine. It is a moderately potent opioid analgesic, generally used for relief of moderate to severe pain.', and a note that this entity has been manually annotated by the ChEBI Team. There are also links for 'Supplier Information' and 'Download'.

Figure 1: Example exposure chemical species with their ChEBI ID and Name. Details of 'Oxycodone' on ChEBI.

between different chemicals. It provides a knowledge base of reactions with different species and biological membranes or disease, and even go as far as understanding the effects on severity of disease. This molecular basis of exposure is beneficial to biomedical research as fills gaps in chemistry and its modulation in health and disease, for designing novel pharmaceutical agents, as well as short-term and long-term management of poisonous episodes. The information on chemical species provided within ChEBI can be very. While this is an initial review of ChEBI, it is a promising resource for semantic harmonization of chemical species data as well as a knowledge base for reasoning in the PRISMS project, and for the eventual development of a molecular taxonomy for disease.

References

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