

# COSMOS Database and Data Content



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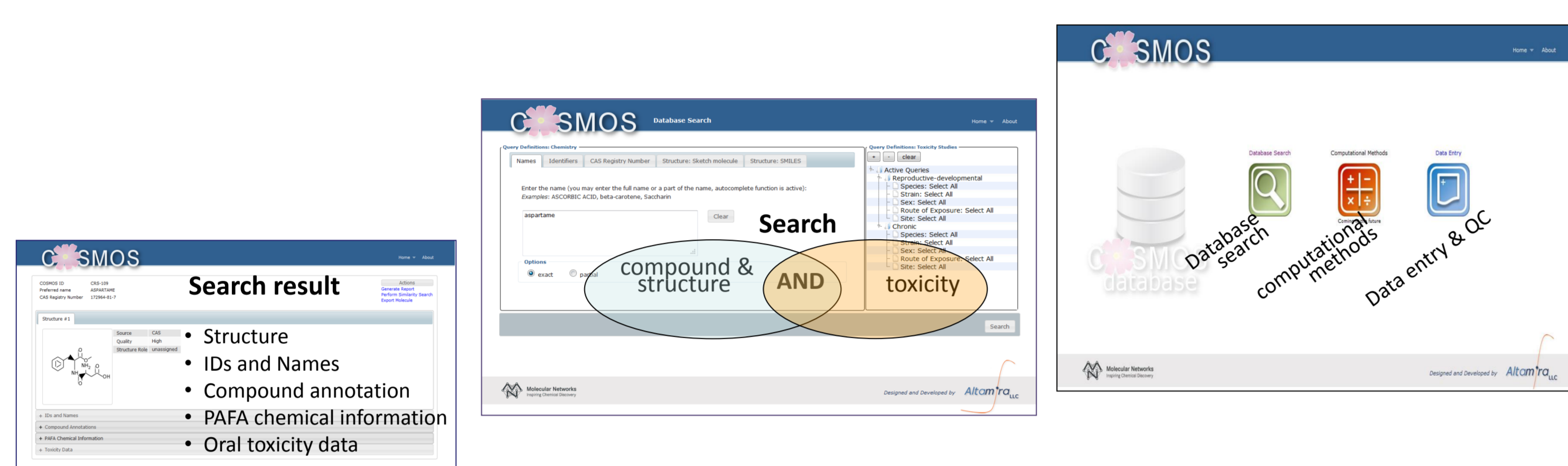
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## Introduction and Aims

The COSMOS DB contains chemical structures, compound records and biological data important for developing computational methods for repeat-dose toxicity for assessing the safety of cosmetic products. Dermal and oral absorption data to address the bioavailability issues are also included.

This poster describes the COSMOS DB and the data content housed in the database. The COSMOS DB is based entirely on open-source technology for its database and cheminformatics library. COSMOS DB provides a Data Entry System (DES) that can be used for data entry as well as in the quality control process.



Search result

Compound annotation table  
Data essential for chemistry QC

Formula	C14 H18 N2 O5
Material Type	ORGANIC
Composition Type	DEFINED FORMULA
Stereochemistry	ABSOLUTE STEREOCHEMISTRY
Double Bond	unassigned
Comments	
Use Functions	FOOD DIRECT ADDITIVE
Use Types	NON-NUTRITIVE SWEETENER/FLAVOR ENHANCER

PAFA Chemical Information

Toxicity Data

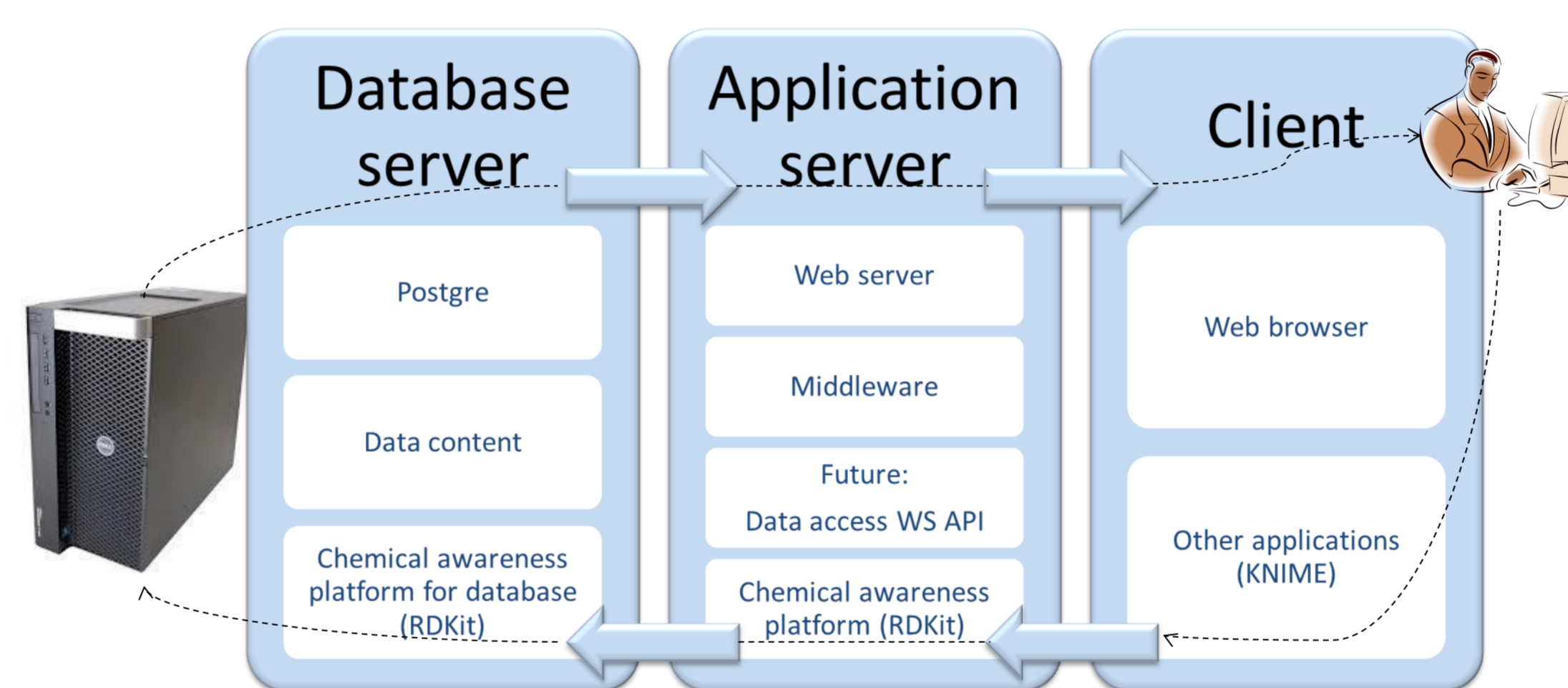
Chronic toxicity data: study and test level information

Study	Study ID	Study Name	Study Type	Study Status	Study Date	Study Location	Study Contact	Study Comments
US FDA CFSAN PAFA	COS-100-019-000-1-1572-159	US FDA CFSAN PAFA	Reproductive developmental toxicity	Completed	2012	US	US FDA CFSAN PAFA	
US FDA CFSAN PAFA	COS-100-019-000-1-1572-159	US FDA CFSAN PAFA	Reproductive developmental toxicity	Completed	2012	US	US FDA CFSAN PAFA	
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US FDA CFSAN PAFA	COS-100-019-000-1-1572-159	US FDA CFSAN PAFA	Reproductive developmental toxicity	Completed	2012	US	US FDA CFSAN PAFA	

Treatment level effects information

Treatment	Dose	Effects	Effects/Toxicity	Effects/Toxicity	Effects/Toxicity	Effects/Toxicity	Effects/Toxicity	Effects/Toxicity	Effects/Toxicity
1000.0 mg/kg bw/day	Other	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain
1000.0 mg/kg bw/day	Other	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain
1000.0 mg/kg bw/day	Other	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain
1000.0 mg/kg bw/day	Other	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain
1000.0 mg/kg bw/day	Other	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain
1000.0 mg/kg bw/day	Other	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain
1000.0 mg/kg bw/day	Other	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain
1000.0 mg/kg bw/day	Other	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain
1000.0 mg/kg bw/day	Other	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain
1000.0 mg/kg bw/day	Other	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain	Weight gain

## High level architecture of COSMOS DB v1.0



## Data Content

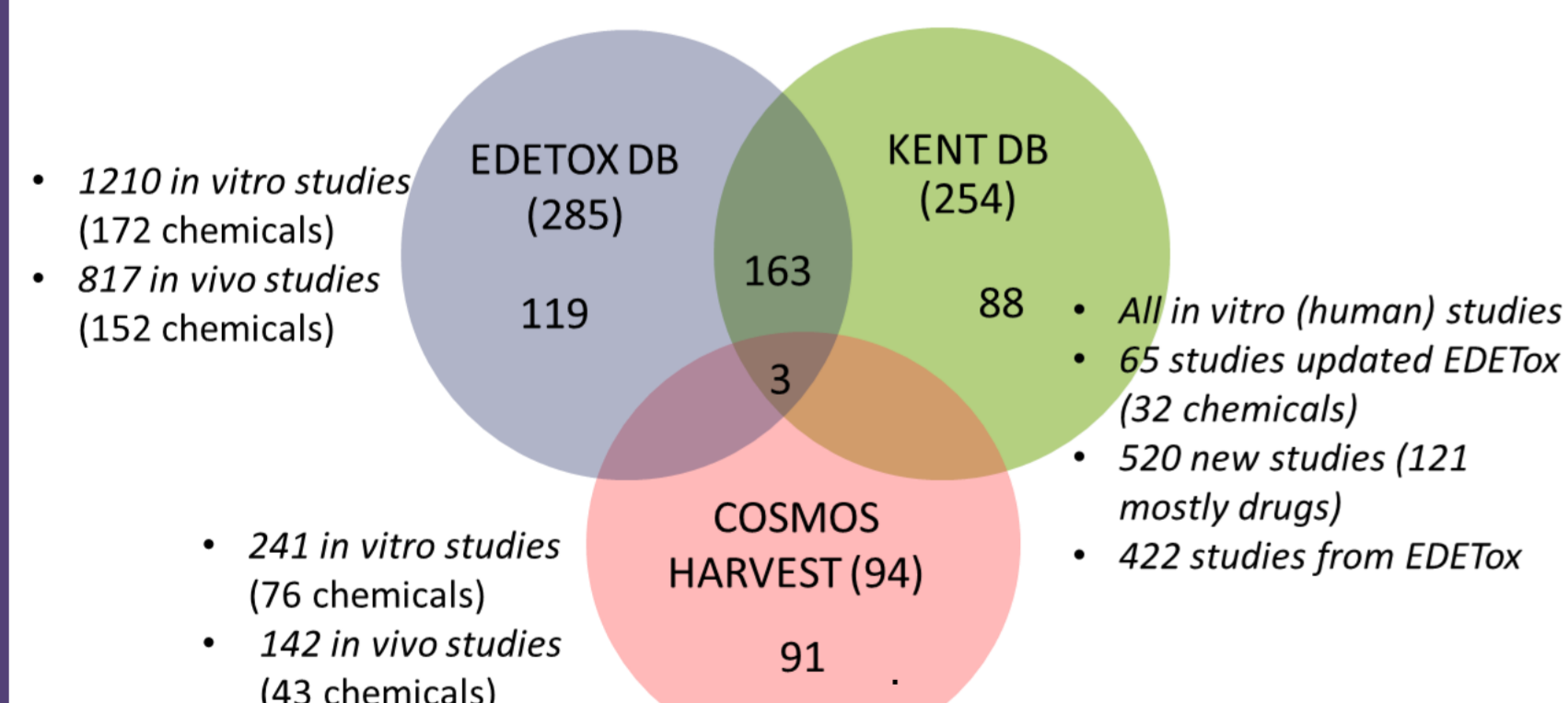
- Chemistry
  - COSMOS Cosmetics Inventory
  - Tox21 inventory [3]
  - US FDA CFSAN CERES public content
- Oral toxicity data\*
  - US FDA PAFA
  - US FDA CERES (selected public data)
  - COSMOS oRepeatDose ToxDB
    - US EPA ToxRefDB
    - EU SCCS
    - EU ECHA substance registration database
    - US NTP
- Dermal absorption data
- Oral absorption data

\* details are available at poster: COSMOS toxicity data curation (C. Yang et al)

## Dermal Absorption Data

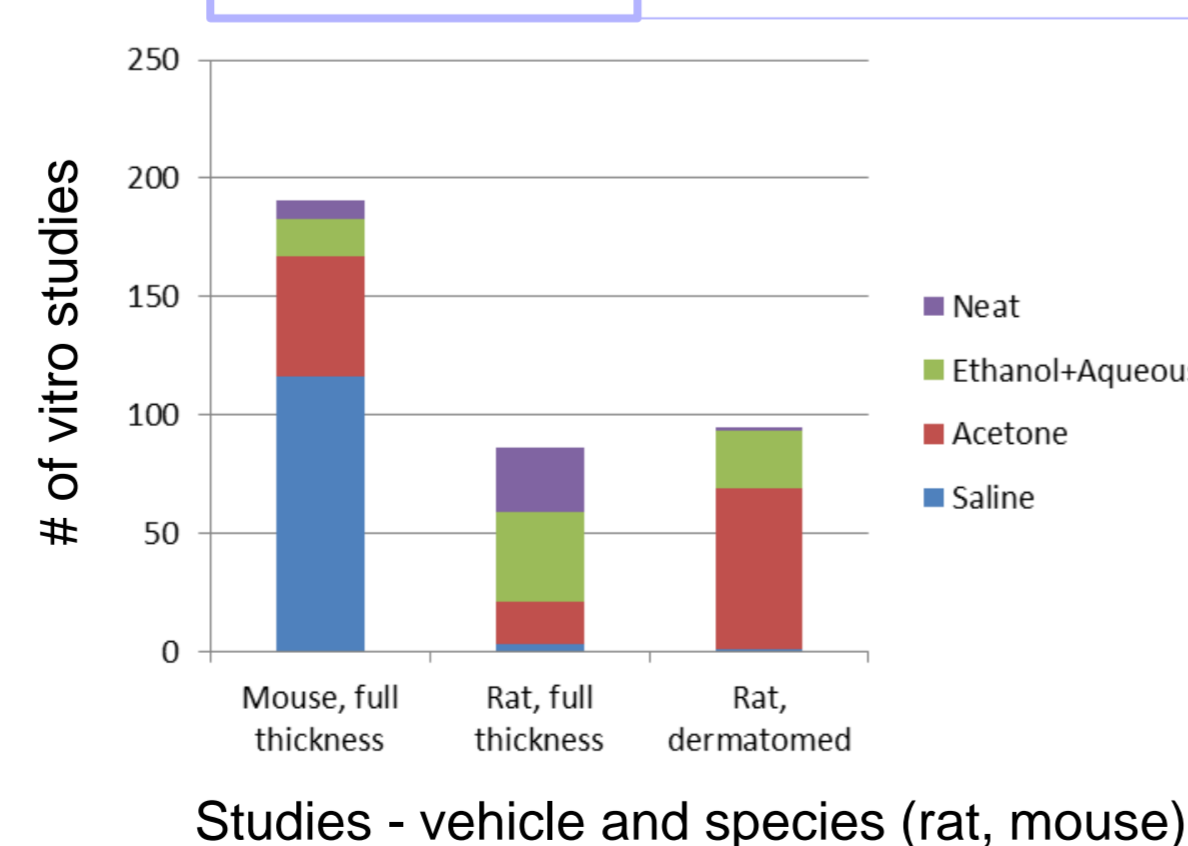
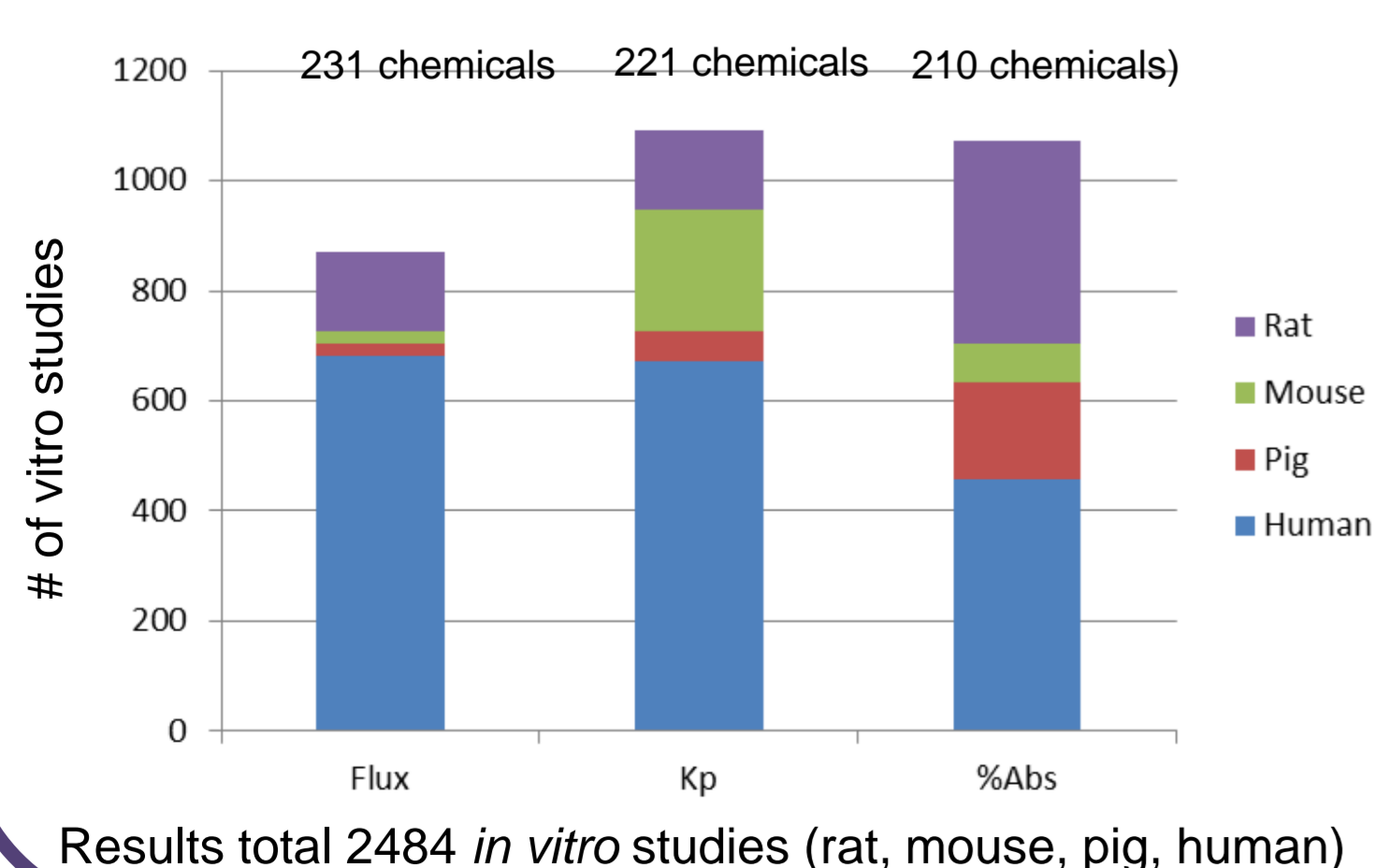
### Data sources

- EDETox database: University of Newcastle [4]
- EDETox update and new studies: University of Kent donation [5]
- COSMOS partners' harvesting of cosmetics ingredients
  - ~163 (of total 464 chemicals) are found in the COSMOS Cosmetics Inventory
  - compiling data on skin metabolites is in progress



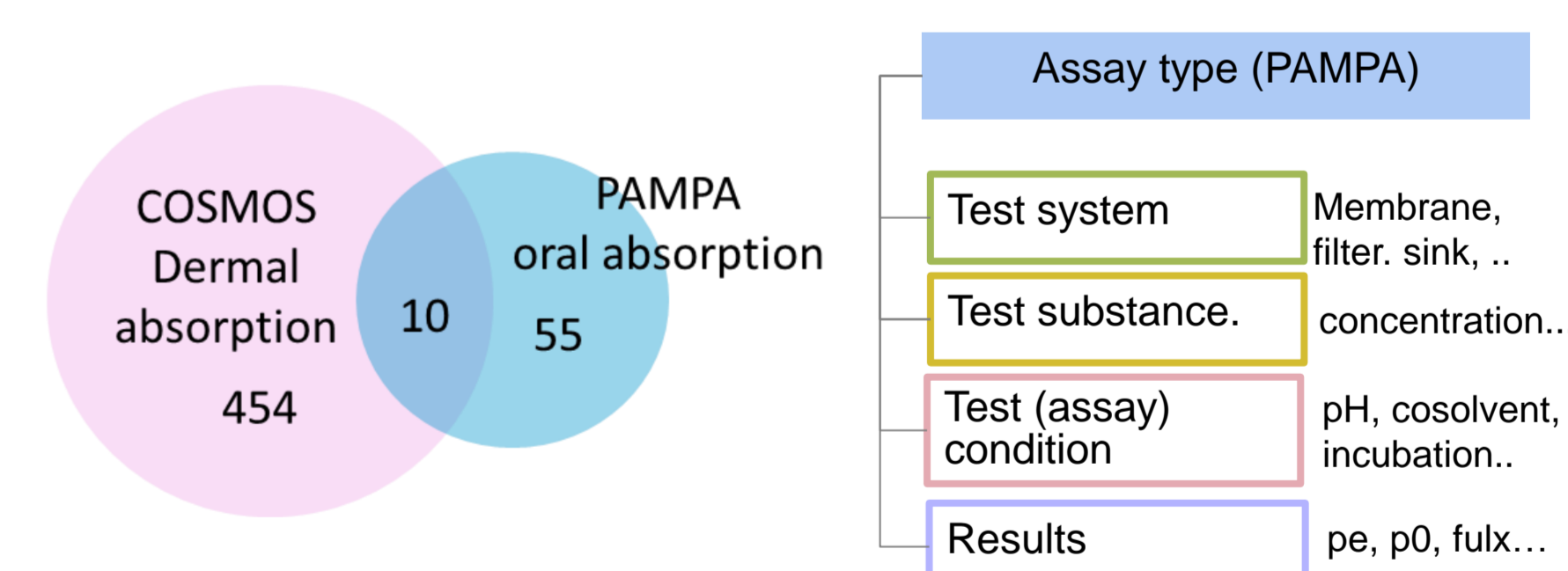
### Data content

Study Type (in vivo, in vitro)	
Test system	animal: species, strain
Test system	skin: skin/membrane type, site
Test substance	concentration, volume, loading, labeling, analytical
Test condition	diffusion cell type, temp, disk size, diffusion, equilibration
Test condition	vehicle, receptor fluid
Results	absorption, recovery



## Oral Absorption Data

- To be able to classify compounds for oral and dermal absorption\*, a systematic literature search has been conducted for oral and intestinal absorption.
- A dataset of human oral absorption has been compiled from these literature data, whilst more thorough harvesting of *in vitro* PAMPA assay are in progress.



\* more details on related poster: QSAR models for chronic toxicity endpoints (S. Kovarich et al)

## Next Steps

- Conduct structure QC for COSMOS modelling set through COSMOS DES
- Import all oral repeat-dose toxicity data and dermal absorption data to COSMOS DB after quality control review sessions.
- Import COSMOS dermal and oral absorption data to COSMOS DB after QC.
  - QC sessions for dermal database in progress as part of TTC effort with ILSI Europe.

## References

- CosIng database <http://ec.europa.eu/consumers/cosmetics/cosing/> European Commission, Health and Consumers.
- PCPC inventory: Compilation of Ingredients Used in Cosmetics in the United States, 1st Edition, JE Bailey, Ed. The Personal Care Products Council, Washington D.C. 20036-4702.
- Tox21 Inventory. [http://www.epa.gov/nct/dsstox/sdf\\_tox21s.html](http://www.epa.gov/nct/dsstox/sdf_tox21s.html)
- EDETOX, University of Newcastle. <http://research.ncl.ac.uk/edetox/theedetoxdatabase.html>
- Eleftherios G. Samaras, Jim E. Riviere, Taravat Ghafourian. International Journal of Pharmaceutics Volume 434, Issues 1–2, 15 September 2012, Pages 280–291, 2012. "The effect of formulations and experimental conditions on *in vitro* human skin permeation—Data from updated EDETOX database"

[www.cosmostox.eu](http://www.cosmostox.eu)

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