Welcome:

Prof Chihae Yang, MN-AM
Agenda

- Introduction – Prof Chihae Yang, MN-AM
- Update – Prof Mark Cronin, LJMU
- User Feedback
  - Dr Kyu-Bong Kim, Dankook University, S. Korea
  - Dr Bertrand Desprez, Cosmetics Europe
- Demo of the New DB and Tools (COSMOS DB v3!)
- Demo of Read-Across Tool from MN-AM
Update, On-Going and Future Plans

Mark Cronin

Liverpool John Moores University
COSMOS Project (2011-2015)

New Toxicological Databases

Threshold of Toxicological Concern (TTC)

PBPK and In Vitro – In Vivo Extrapolation

In Silico Models

www.cosmostox.eu
COSMOS DB: Freely Available and Searchable Resources for Toxicity Data

- Open-source technology
- High quality data
- Intuitive browsing of complex data
Profile of COSMOS DB Users

- Over 1800 unique registered users 2013 - 2018
- Most common users are cosmetics industries (over 70%)
Registration Profile 2013-2017

# of new registrations each year 2013-2017

Cumulative registrations 2013-2017
COSMOS DataShare Point

https://cosmosdb.eu/cosmosdb.v2
• Computational Toxicology now mainstream?

• In the sea of big data, the need for high quality, reliable and relevant (and free) information is vital

• Please use the Forum to share / make opinion, comment on use of COSMOS, opportunities etc

• Thank you to MNJAM for on-going support
New for 2018 and Beyond
Cancer Potency Database (CPDB)

1547 unique substances
47,064 records

CPDB original

NEW

Study inclusion criteria

e.g. NTP, EFSA, RepDose

CPDB Cancer TTC
(2012 Altamira)

New CPDB 2018
Cancer TTC Dataset

• Importance of curation
• Points of Departure
• TTC dataset
User Feedback – and Action!

- Apply physical chemistry to define the chemical space when using TTC workflow (Dr Heli Hollnagel, Dow)
- Provide the skin permeability database from COSMOS harvesting into COSMOS DB (Dr Helga Rothe, P&G)
- Set up a systematic way to donate data from US FDA CERES database, the grandfather of COSMOS DB (Dr. Kirk Arvidson, US FDA CFSAN)
- Will COSMOS DB provide computational tools? (many from SOT)
- Will COSMOS DB include ECHA data?
Using COSMOS DB to Support Cosmetics Europe Long Range Science Strategy (LRSS)

- 2015: COSMOS DB completed
- Now: Utilisation
- Future: Update and Further Applications
From a Database → Data Supported Chemoinformatics Platform

• New software architecture

• COSMOS DB will remain accessible

• Development of CE-ToxGPS
COSMOS DB v3

- Freely available
- Maintain and extend content
- Improved appearance and usability
- New functionalities e.g. profilers
  - DNA Binding
  - Protein Binding
  - Liver toxicity
Acknowledgements

• Cosmetics Europe (through the Long Range Science Strategy, LRSS)
• EU IMI eTox Project
• MN-AM, Nürnberg DE; Columbus OH, USA
• The European Community’s Seventh Framework Program (FP7/2007-2013) COSMOS Project under grant agreement n° 266835 and Cosmetics Europe
• Co-workers in Liverpool, elsewhere in the EU, USA
Thank You and Any Questions
Agenda

• Introduction – Prof Chihae Yang, MN-AM
• Update – Prof Mark Cronin, LJMU
• User Feedback
  – Dr Kyu-Bong Kim, Dankook University, S. Korea
  – Dr Bertrand Desprez, Cosmetics Europe
• Demo of the Next Generation (COSMOS DB v3!)
• Demo of Read-Across tool from MN-AM