Harmonic Pharma presents
SAFETY BY DESIGN®

ADEBIOTECH CAMPUS

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Harmonic Pharma at a glance

- **CREATION DATE AND LOCATION** : June 2009 in Campus ARTEM at Nancy, France
- **TEAM** : engineers in computational science ; senior management with complementary backgrounds from the pharmaceutical R&D field
- **EXPERTISE** : computational toxicology ; computational investigation of activity of chemicals
- **NETWORK** : experts in toxicology & regulatory affairs, data mining and analysis ; experts in biological assays

Campus ARTEM

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Harmonic Pharma at a glance

- **VISION** : For a world with safer chemicals
- **MISSION** : by applying SAFTEY BY DESIGN® integrating computational approaches
- **VALUES** :
  - To improve cost-effectiveness of testing,
  - To protect human health and environment
  - To reduce the number and suffering of test animals

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Harmonic Pharma's activity

- Harmonic Pharma has developed innovative computational solutions that combine predictive toxicology, mechanism of action (MoA) investigation, and data modeling of small molecules.

Compound toxicity profiling

- QSAR statistical toxicity models addressing more than twenty endpoints
- Compliant with regulatory requirements
- Prioritize the most promising compounds at an early stage
- Substitute marketed compounds for more compliant ones

Compound activity profiling

- Polypharmacological profiling to decipher biomolecular targets and MoA
- Objectivation of natural extracts
- Drug/chemical repurposing for novel use and new markets

Data modeling & analysis approach

- Unique spherical harmonic (SH) 3D representation of chemicals to visualize and compare molecules
- SH hierarchical clustering to select promising subgroups inside a chemical dataset
- Cluster based 3D meta-molecules as templates to guide chemical design

SAFETY BY DESIGN®

A new solution of **services** and **software** for toxicity prediction and characterization of activity of chemical substances

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SAFETY BY DESIGN® : Services

- Analyze with experts the safety of your molecules to make strategic choices and meet the regulatory needs.
  - Investigate the potential genotoxicity of API impurities/intermediates according to the ICHM7 regulation.
  - Evaluate the potential skin sensitization of chemical substances – e.g. ingredients, reaction intermediates, and APIs – and get an aid to select relevant assays
  - Quickly and accurately assign chemicals into specific exposure categories : the Occupational Exposure Band (OEB) classes

Reports reviewed and signed by an expert toxicologist (ERT)

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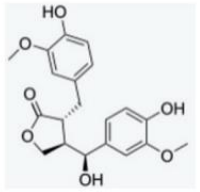
SAFETY BY DESIGN® Software : Activity

- Example of objectivation of a natural extracts from wood biomass

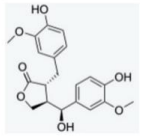
LBS®
A natural extract from the active biomass of wood...

LBS® Natural Extract Powder



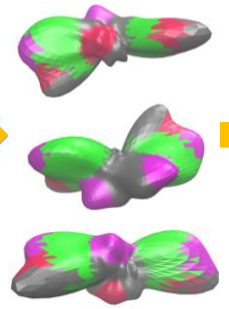
HydroxyMataiResinol (HMR) major component

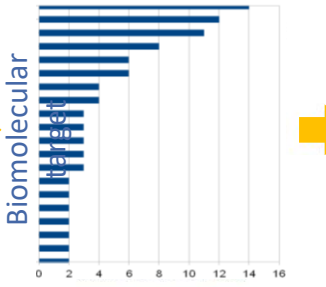
Spherical harmonic based representation	Proprietary db of 20,000 compounds	Polypharmacology 20 identified targets	Example of outcome



HydroxyMataiResinol HMR) major component

Query molecule to be investigated : synthetic or natural compound.





- **List of 20 newly identified putative target(s)**
- **Hypothesis of new mechanisms of action based on those new targets**
- **New insights towards novel uses of your compounds**

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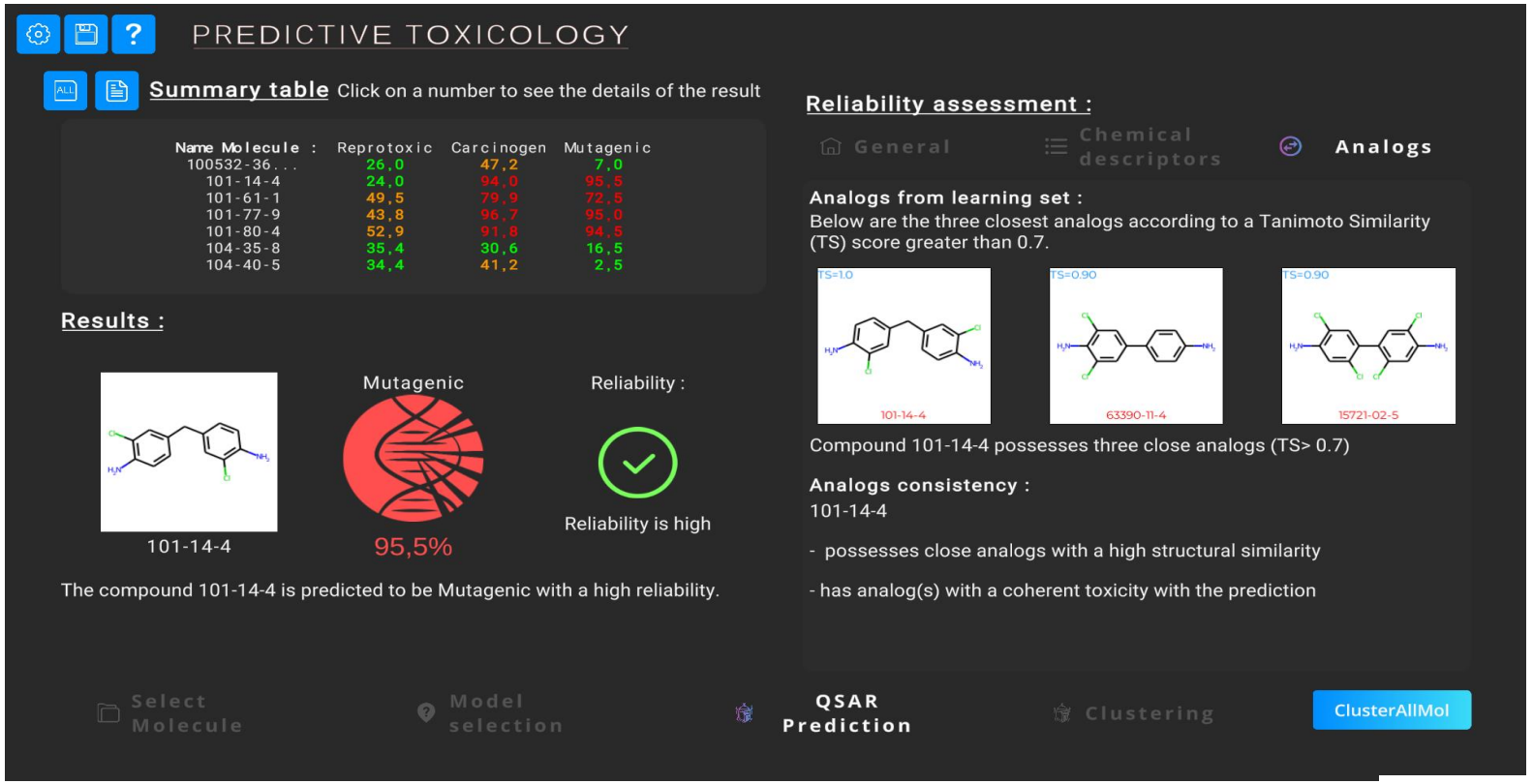
SAFETY BY DESIGN® Software : Toxicity

- Select molecules → Select QSAR Models → Predict toxicity & Generate synthetic reports



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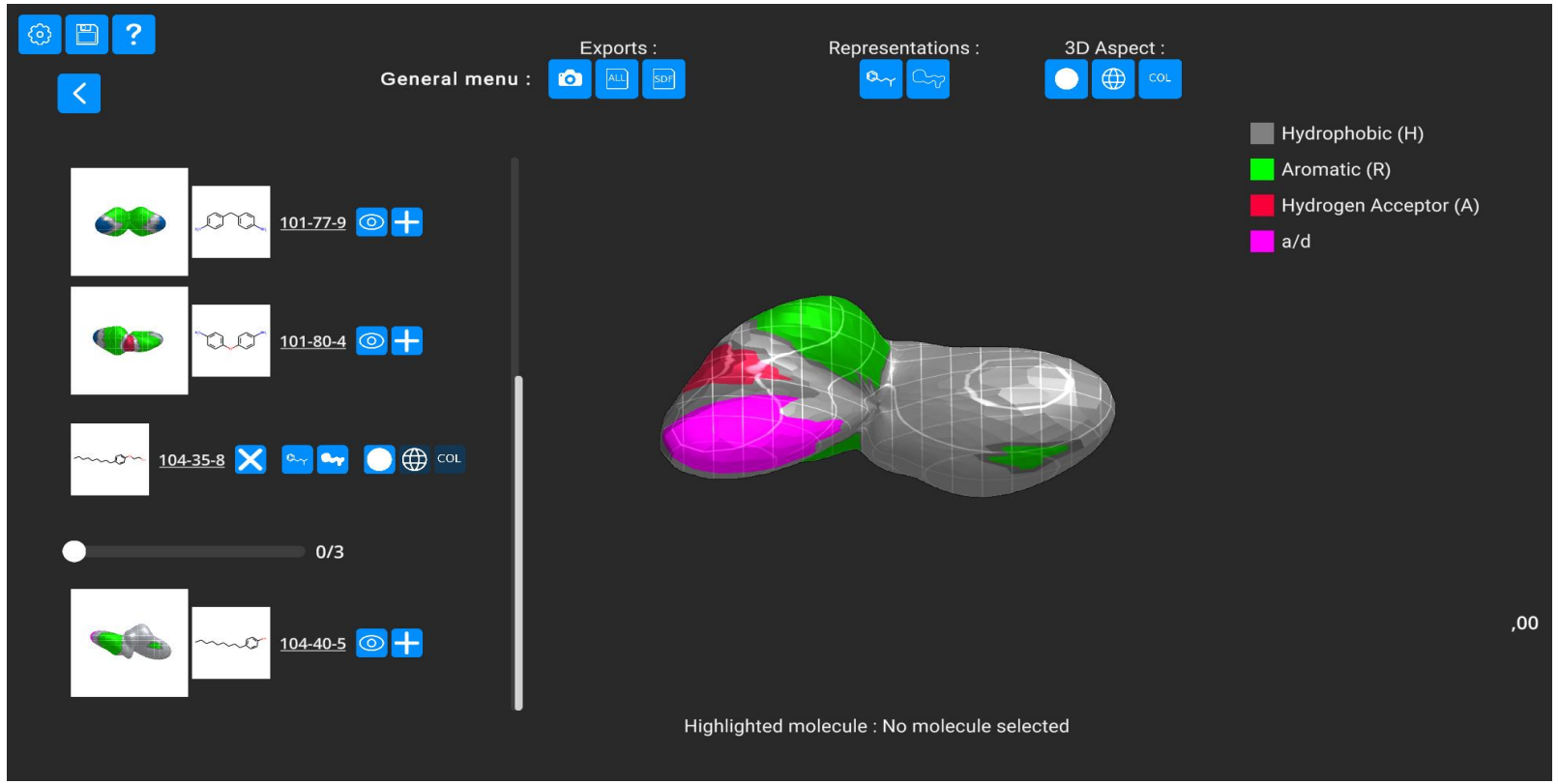
SAFETY BY DESIGN® Software : Toxicity

- Visualize toxicity into chemical clusters → Visualize and compare molecules and Generate representative meta-molecules for any cluster



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SAFETY BY DESIGN® : Overall

- A new solution of services and software for toxicity prediction and characterization of activity of chemical substances to :
  - Meet evolving regulatory needs
  - Improve the cost-effectiveness of testing
  - Reduce the number and suffering of test animals

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THANK YOU !

contact us at
contact@harmonicpharma.com

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