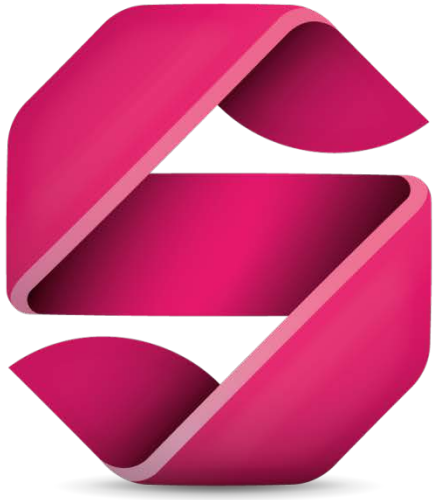
Product Update

Dr Nicholas Marchetti
Product Manager
nik.marchetti@lhasalimited.org



Sarah

nexus

Model Building for Sarah Nexus 2.0

- New functionality to enable users to build predictive models for mutagenicity
- Also allows for users to supplement the Lhasa model with their own data
- Predictions can be run using different models can be manually compared to understand the impact of the additional compounds
- The best prediction settings can be automatically determined for your chemical space

Sarah Nexus 2.0 Updates

- Changes to training set
  - Broader Training Set
  - More reliable data
  - More consistent and reliable structures
- Changes to prediction algorithm
  - Hypotheses with Connection Points
  - Hypothesis weighting when combined to give an overall prediction

Balanced accuracy has increased by 3 percentage points

Derek

nexus

Updates to Derek Nexus 5

- Significant work on the Skin Sensitisation endpoint
  - Leading to the implementation of Potency predictions for LLNA EC3
  - Classification of Sensitisers
  - Will be discussed later in the ICGM
- Derek ICH M7 Mueller Classification
  - Presents additional information to help perform expert review
  - Will be discussed later in the ICGM

Zeneth

Zeneth Update

- Zeneth 2015.1.0 Knowledge Base
  - Released 9th September 2015
  - 33 new transformations
  - 16 improved transformations
  - Summary:

Transformation Type	Number added	Total number
Oxidations	11	126
Hydrolyses	4	80
Condensations/additions	6	77
Eliminations/fragmentations	6	49
Isomerisations/rearrangements	2	31
Photochemical reactions	4	37
Total	**33**	**400**

Vitic
nexus

Vitic Nexus Updates

- Vitic Nexus 2015.1
  - In vitro genetox – 164,001 records covering 10,246 compounds
  - In vivo genetox – 10,595 records covering 2,723 compounds
  - Overall genetox – 17,322 records covering 8,932 compounds

Data sharing consortia

- Lhasa facilitate pre-competitive data sharing
- Members of these consortia contribute to these projects:
  - CIGAA (Aromatic Amines) 2015.1.0
    - 3,639 records (increase of 2307)
    - 424 compounds (increase of 124)
  - Intermediates (includes boronic acid sub-group) 2015.1.0
    - 16,971 records
    - 1,088 compounds
  - Excipients 2015.1.0
    - 2,435 records (increase of 463)
    - 975 compounds (increase of 70)

Meteor

nexus

Meteor Nexus Updates

- A hybrid machine-learnt approach to rank expert system-generated metabolites based on known metabolic reactions
  - reduces the number of “false positive” predictions
- Ability to overlay toxicity predictions directly on to the tree

Questions?

Lhasa Limited Registered Office
Granary Wharf House, 2 Canal Wharf, Leeds LS11 5PS
Registered Charity (290866)

+44 (0)113 394 6020
info@lhasalimited.org
www.lhasalimited.org

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