Zeneth®

Expert decision support software for predicting the forced degradation pathways of organic compounds
Zeneth is an expert, knowledge-based software that gives accurate forced degradation predictions. It is the only commercially available, actively maintained software of its kind.

Including features such as a comprehensive transformation library and customizable reports, Zeneth provides transparent and scientifically robust predictions.

Using a knowledge base and reasoning, Zeneth determines the most likely degradants based on structural features, conditions, and the likelihood of competing transformations.

Lhasa has been creating scientifically robust expert software to improve efficiency and aid regulatory submission for over 30 years. Lhasa develops software for toxicity, metabolic fate, purge factor calculation, and chemical degradation.

Why choose Lhasa?

Our products

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Introduction to Zeneth

Zeneth is the expert knowledge-based software for the prediction of forced degradation pathways.

The only actively maintained system for the prediction of degradation, the software is built on a knowledge base of transformations implemented by Lhasa’s scientific experts. Based on user submitted query compound(s), these highly transparent and scientifically robust predictions provide the right level of information to support a thorough review by experts.

Drawing on over 30 years of experience, Lhasa’s expert scientists implement and regularly update Zeneth transformations using public and proprietary data, ensuring vast coverage of degradation pathways. They use their expertise to analyse complex, sometimes conflicting data and provide expert reasoning rules to give you an indication of how compounds are likely to be degraded.

Used by scientists across a range of industries, Zeneth adds value in numerous stages of compound and drug discovery.
Features and benefits

Degradation Assessment
Zeneth can swiftly provide predictions for the likely degradation products of query compounds whilst taking into account the effect of different excipients and impurities within the final formulated product. Structures of common excipients, with associated impurities, are provided for easy processing alongside the query compound.

Meeting Regulatory Requirements
Numerous guidelines (ICH Q1A/B, ICH Q3A/B, ICH M7, RDC 58/2013 and RDC 53/2015) stipulate the need to understand the consequences of degradation, and focus on impurities and stability testing. The decision support that Zeneth offers can be invaluable in meeting many of these requirements.

Degradant Identification
Zeneth has comprehensive knowledge of degradation pathways which ensures structure elucidation of experimentally seen degradants. Intuitive tools allow filtering of results based on chemical formula, mass and mass difference allowing experimental data to guide predictions.

Early Screen for Toxic Degradants
Predicted degradants can be easily exported, enabling analysis of potential toxicity in Lhasa’s toxicity prediction tools; Derek Nexus and Sarah Nexus.

Expert ICH M7 Support
Under ICH M7, potential degradation products likely to be present in the final drug product should be evaluated for mutagenic potential. Zeneth’s comprehensive transformation library permits the identification of potential degradants.
### Features and benefits

#### Meaningful Predictions

In addition to structural features, Zeneth accounts for a number of reaction conditions, making its predictions consistent with the conditions that have to be tested according to the ICH guidelines: thermolytic, hydrolytic, oxidative and photolytic.

#### Advanced Warning System

Provides an instant understanding of what results might be expected when running stress tests. This additional information can increase efficiency and productivity by informing decisions, aiding the design of experiments and assisting with excipient selection.

#### Transparency

Predictions are clearly represented and contain detailed supporting evidence associated with the degradation pathway. Expert commentary, including a review of data, mechanistic rationale and explanation of the structure activity relationship are also included.

#### Customisable Reports

Zeneth incorporates a reporting framework that allows (.rtf .txt .xlsx and .sdf) file export. Report templates are fully customisable by the end user.

#### Extensive Degradation Knowledge

Drawing on over 30 years of experience, Lhasa expert scientists implement and regularly update Zeneth transformations using public and proprietary data ensuring vast coverage of degradation pathways.
How Zeneth works

Using transformations and reasoning created by Lhasa’s scientific experts, Zeneth provides you with an early indication of the potential degradation products of your query compound(s).

Following submission of your queries to Zeneth, the structures are compared to the Lhasa knowledge base, or your own knowledge base that you have created using the Zeneth Knowledge Editor. Zeneth then predicts the first generation degradants by considering:

1. The presence or absence of structural features
2. The presence or absence of conditions (light, water, oxygen, radical initiator, peroxide, metal) as well as temperature and pH
3. The relative likelihood of competing transformations

Structure of the starting material
Reaction conditions
Maximum number of steps
Likelihood threshold

Perceive structural features

Match transformations present in the knowledge base and generate degradants

Apply reasoning to determine likelihood

Discard degradants whose likelihood is below the threshold

Has the maximum number of steps been reached?

NO

YES

Display Results

- Structures of degradants displayed in a degradation tree
- Structures of intermediates displayed in reaction path
- Reaction name, comments, references and literature examples
- Likelihood displayed (colour coded)

Has all degradants been processed?

NO

YES
When asked why people choose to work with Lhasa Limited, the common responses are:

1. Over 30 years of experience in developing state-of-the-art *in silico* prediction and database systems.
2. Transparency of Lhasa systems allows trust and confidence in the science presented.
3. All science is developed in-house, providing the opportunity to discuss directly with Lhasa expert scientists.
4. Software is easy to use and well supported.
An expert rule-based system for the prediction of toxicology.

An expert rule-based system for the prediction of metabolic fate.

A tool for assessing the relative purging of mutagenic impurities.

A statistical-based system for the prediction of mutagenicity.

A chemical database and information management system.

References

  http://dx.doi.org/10.1021/mp5003976

  http://dx.doi.org/10.1021/mp400083h