Cheminformatics

For more than twenty five years Specs has built up an extensive knowledge and experience in the field of Cheminformatics.

Cheminformatics

Our Lead Development department uses a combination of open source, proprietary and in-house developed software to evaluate millions of structures each year. This enables Specs to make various selections from diverse to drug-like and targeted libraries for lead discovery and optimization programs. Our vast knowledge of cheminformatics services is available to all third parties who seek to expedite their compound selection process, either from the Specs compound repository or from other suppliers.

Selection and analysis

Specs has gained extensive experience in selecting compounds from large databases. Every year we continue to analyse millions of structures for novelty, diversity, drug- and lead-likeness, physicochemical properties and pharmacological relevance. We routinely compare and analyse large sets of compounds using a multitude of techniques to construct tailor-made libraries, for instance diversity based, focussed-, targeted- or fragment-based libraries in early screening campaigns, hit follow-up and hit-to-lead programs. By continuously training and developing our software we are able to significantly enhance hit ratios as was successfully validated in several screening campaigns of universities and institutes around the world.

Drug- and Lead-like compounds

Specs is continuously evaluating property and structural guidelines to ensure drug-like chemistry. New methods of calculations and evaluation of these properties lead to compounds which are easier to optimize and less likely to fail in a later stage. Structural guidelines such as PAINS and REOS, will make sure the right compounds get the attention needed and increases the changes to develop the next drug.

Cheminformatics

Chemical diversity

Chemical diversity of a compound library remains an important parameter for every successful drug discovery program. Diversity analysis can be based on a multitude of descriptors and statistical methods. Evenly important is the added diversity to in-house libraries. Being a reliable partner, Specs has a track record analysing customer libraries to add diverse compounds and enlarge the chemical space.

Hit follow-up

Hit follow-up libraries are an important part of every screening project and usually starts with analogue searches. This can be extended to third party databases, which in combination with our procurement services is a very powerful tool for follow-up libraries. Specs has a proven track record in applying various (Q)SAR methods to enhance hit ratios in hit follow-up and hit-to-lead programs.

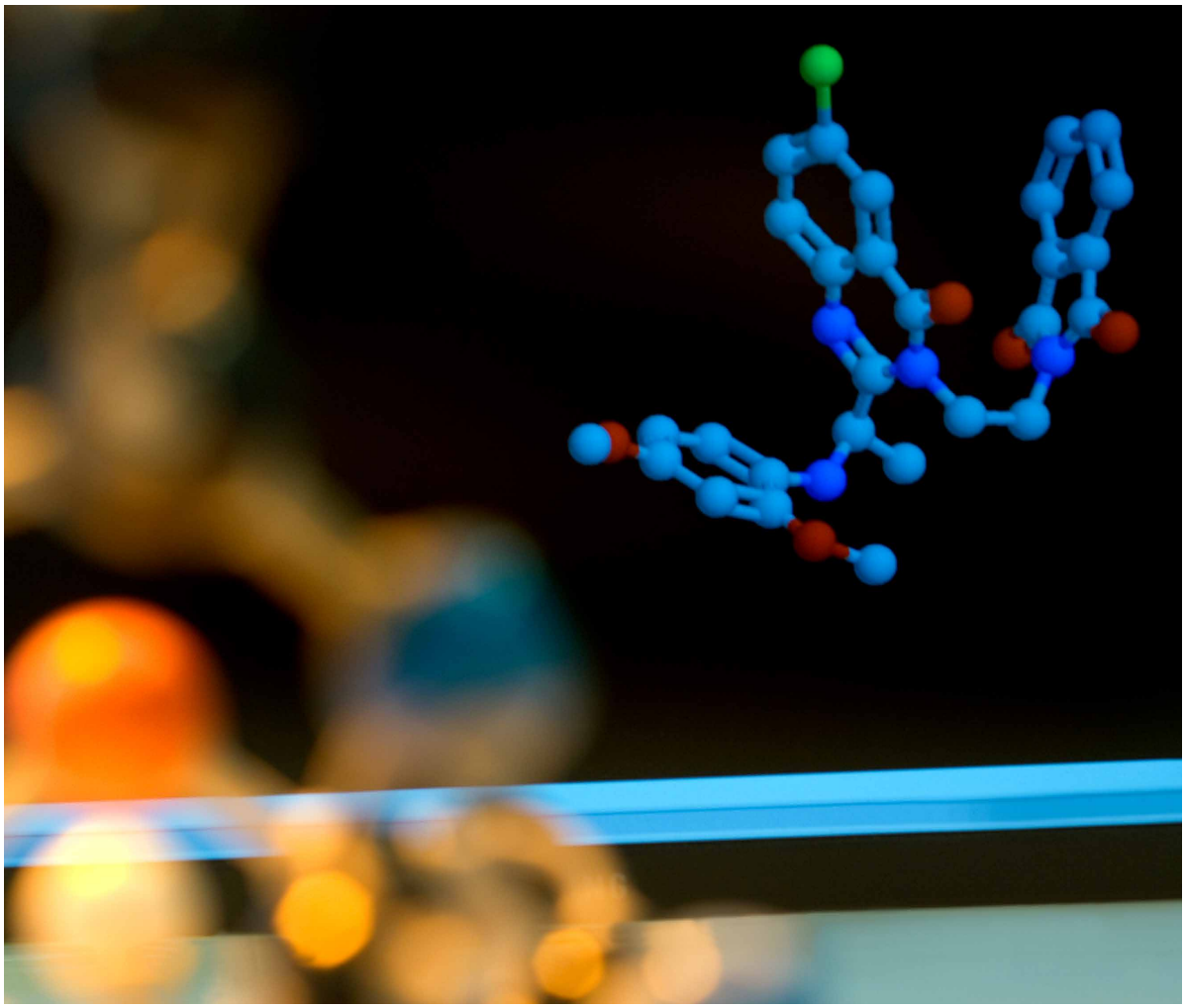
Focused Libraries

QSAR methods can also be used to build models against specific targets and predict activity of compounds from stock or other sources. Activity information is extracted from proprietary and open sources and discussed with our customers to tailor-fit their specific needs. In-house results of customer screening campaigns can also be used to train and validate these methods.

Compound Libraries

Using our decades-long experience in Cheminformatics we have analysed the Specs Compound repository and designed several focused compound libraries, which are available as pre-plated sets.

- World Diversity Set
- Kinase Targeted Library
- Fragment Library



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