High quality materials innovation on your PC

Genetic function algorithms for building QSARs

Manage your materials discovery workflow

MS Modeling Datasheet

QSAR

QSAR is a workflow solution for chemicals and materials discovery. It enables research scientists to identify compounds with optimal physicochemical properties. QSAR's integration in MS Modeling provides unsurpassed access to descriptors and advanced analysis capabilities to help you to create superior materials.

'Faster materials innovation with QSAR'

Chemicals and materials industries challenges

Companies in the chemicals and materials industries are facing similar challenges. Faster innovation of novel materials, at reduced cost, with improved performance is key. Additionally, patent positions may also accelerate the search for alternative materials. It is for these reasons that companies working on materials as varied as, but not limited to, polymers, surfactants, and other soft materials, molecular/inorganic crystals, and zeolites use Quantitative Structure Activity Relationships (QSAR) techniques as an integral part of their new materials research. The use of QSAR allows the speed up of innovation and the creation of superior materials.

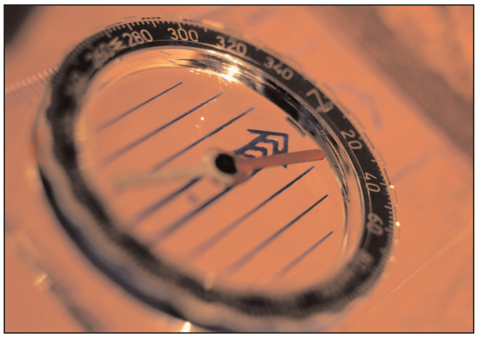
QSAR: Step into the future

QSAR brings high quality materials innovation to your PC, allowing a much broader group of researchers than previously possible access these tools. This builds on over 10 years of expertise in QSAR, bringing together the design, features, and functionality researchers in the materials chemistry industries require.

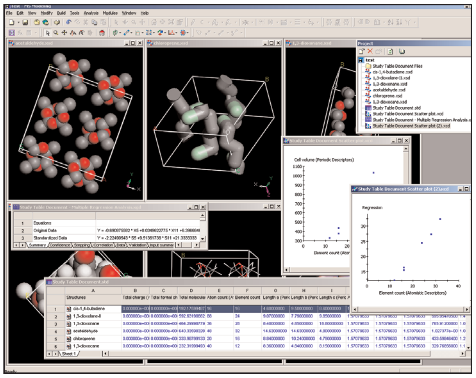
How will you work with QSAR?

QSAR can be used by individual researchers, allowing users to follow a workflow to discover novel materials. Typically you will start by obtaining molecular structures and the associated experimental data. Then structures are validated and descriptors calculated.

An initial data analysis follows, for example using a basic correlation analysis. This initial analysis may already indicate a relation between the molecular properties and experiments. From this you can proceed with model building. It is here where you, using model building/validation techniques, including hook-up to the unique genetic function approximation technique where you identify the details of your QSAR. If required you can apply data fragmenting before your models are built.



▲ *Focussed searching with QSAR*



▲ *QSAR - Materials innovation on your PC*

These candidates can now be separated in subsets, based on predicted properties. You will now have a lead group of molecules, which you may decide to synthesize or buy, if commercially available. Subsequent testing will confirm the applicability of these molecules. If needed you may use the results of these experiments to update your knowledge base and follow the above workflow, until you reach your target properties, faster.

QSAR

QSAR enables the user to manage their work in a single

MATERIALS
STUDIO

study table. It is here that your molecules are united with their properties. Descriptors provide an all-round quality set of physicochemical properties which, when interfaced with the unique genetic function approximation, give you unrivalled capabilities to calculate your QSAR. Combined with the integrated presentation and data organization and analysis capabilities, QSAR is the tool of choice for materials discovery.

The Materials Studio Advantage

QSAR is operated from within the Materials Studio® software environment. Materials Studio provides a user-friendly interface, complying with Windows® standards.

QSAR at glance

- **Study table** - provides the heart of your QSAR calculations, enabling cut/copy/paste/sorting, function definition, storing of links to structures, and flexible cell coloration
- **Data structure import** - users can import sets of materials and associated experimental data from industry standard molecular structures and data files
- **Molecule viewing capabilities** - users have the power of MS Modeling at their fingertips to draw, manipulate, and display their materials
- **Descriptors** - QSAR users may select from the following sets of build-in descriptors:

- Atomistic (charges, atoms counts etc.)
- Spatial (molecular mass, volume, surface area etc.)
- Other descriptors (fragments counts, crystal cell dimensions, polymorph etc.)
- Fast descriptors provide an extensive list of topological thermodynamic, information content, e-state and structural properties, including the Jurs descriptors
- VAMP, the semi-emperical quantum mechanics engine, provides energy, orbitals (HOMO/LUMO), multipoles etc.

Additionally, the following descriptors can be licensed:

- Forcite, allows the use of the molecular mechanics/dynamics engine and allow access to energetics (total, non-bond, and optimized structure)
- DMol^3 Descriptors allow the calcualtion of accurate electronic energies and atomistic properties such as susceptibility to nucleophilic attack using the DMol^3 quantum mechanical module.

- **Initial Data Analysis** - this unites a series of techniques to spot patterns in your data. Methods include: univariate analysis, data standardization, data transformation, correlation matrix, graphical analysis, principal components analysis, and cluster analysis and validation
- **Model Building** - here the calculation engine builds your QSAR relation. Users can choose from standard techniques such as multiple linear regression, partial least squares, or use the unique genetic function approximation.
- **Model Validation** - here you decide whether the model you have built describes your data well. In addition to each model builder's own validation, cross-validation, ANOVA and graphical validation (predicted vs. observed) is provided.
- **Model Management** - allows users to apply, import, export (xml format), copy or delete models. This also allows user to run their model when they want. Exporting models allows you to share your models with other MS Modeling users.
- **Data Fragmentation/Subsetting** - your data table can be sorted and filtered to allow you to find groups of molecules.
- **Candidate Generation - c**andidate molecules can be drawn or sets of molecules from industry standard molecular structures files can be imported.
- **Project Management** - you can save your projects at any time, allowing you to share your work with colleagues. It includes structures, models, and tables.