

High quality materials innovation on your PC

Neural Networks for building models with non-linear relationships

Accurate quantum mechanical descriptors for describing reactions

Materials Studio Datasheet

# QSAR PLUS

QSAR Plus is a workflow solution for chemicals and materials discovery. It builds on the base tools available in QSAR and extends them to include a neural networks model building method and accurate quantum mechanical descriptors. QSAR Plus enables research scientists to identify compounds with optimal physicochemical properties. Integration in Materials Studio® provides unsurpassed access to descriptors and advanced analysis capabilities to help you to create superior materials.

## 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 Plus allows the speed up of innovation and the creation of superior materials.

## How will you Work with QSAR Plus?

QSAR Plus can be used by individual researchers, allowing users to follow a workflow to discover novel materials. Typically molecular structures are first obtained along with 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. Here, using model building/validation techniques, including hook-up to the unique genetic function approximation technique or neural networks method, details of your QSAR can be identified. If

required you can apply data fragmenting before your models are built.

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 Plus enables the user to manage their work in a single 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. QSAR Plus extends the properties available to include highly accurate energies and reactivity indices calculated using quantum mechanical techniques. Combined with the integrated presentation and data organization and analysis capabilities, QSAR Plus is the tool of choice for materials discovery.

Structure	Structure Name	Conformer #	HOMO	LUMO
1	Concsoo E-a-1	6.20000000	-8.94020000	0.06080700
2	Concsoo E-b-2	4.30000000	-8.31429000	0.30540200
3	Concsoo E-c-3	7.50000000	-8.84775000	0.08362300
4	Concsoo E-d-4	6.30000000	-8.61083000	0.01704100
5	Concsoo E-e-5	2.70000000	-8.66426000	0.08183300
6	Concsoo E-f-6	4.00000000	-8.66496000	0.06704400
7	Concsoo E-g-7	2.00000000	-8.66020000	0.07342600
8	Concsoo E-h-8	4.50000000	-8.65868000	0.08168100
9	Concsoo E-i-9	4.50000000	-8.66060000	0.08492000
10	Concsoo E-j-10	9.60000000	-8.66760000	0.07103600
11	Concsoo E-k-11	-8.66367000	0.07612100	

▲ The study table is the heart of QSAR, from here structures can be added, edited, descriptors calculated, models built, and finally physical properties predicted.

## The Materials Studio Advantage

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

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## QSAR at a Glance

- **Study table** - provides the heart of your QSAR Plus 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 Materials Studio at their fingertips to draw, manipulate, and display their materials
- **Descriptors** - QSAR Plus users may select from the following sets of built-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 Descriptors, the semi-empirical quantum mechanics engine, provides energy, orbitals (HOMO/LUMO), multipoles etc
  - DMol<sup>3</sup> Descriptors are derived quantum mechanically to provide very accurate electronic energies, charges and other properties. They also provide atomistic properties such as susceptibility to attack from electrophiles, nucleophiles, or free radicals, hence encoding the reactivity of atoms as descriptors. Besides these novel descriptors, the DMol<sup>3</sup> Descriptors can be used to optimize both molecules and periodic systems giving precise 3D molecular structures for use as input to other descriptor engines.

Additionally, the following descriptors can be licensed:

- Forcite allows the use of the molecular mechanics/dynamics engine and allows access to energetics (total, non-bond, and optimized structure).
- **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 more sophisticated algorithms:

- GFA, a genetic algorithm with a term to penalise models that are overfitting. It uses Friedman's lack-of-fit (LOF) error measure to control the number of terms in the model whilst minimizing the least-squares error. GFA should be used when the dataset contains more descriptors than samples as it chooses the best descriptors. The GFA also supports models which include higher order polynomials and spline functions, allowing the creation of non-linear models and the use of spline terms for automatic outlier removal
- Neural Networks, sophisticated algorithms based on the way the human brain works, allow building of models with non-linear relationships and are also more tolerant of noise and outliers than other model building algorithms. The implementation in QSAR Plus is a back-propagated neural network which also allows descriptors to be chosen as both response and predictor variables. This allows the generation of non-linear PCA and PLS like calculations.
- **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, outlier analysis, 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 Materials Studio users
- **Data Fragmentation/Subsetting** - your data table can be sorted and filtered to allow you to find groups of molecules
- **Candidate Generation** - candidate molecules can be drawn or sets of molecules from industry standard molecular structures files can be imported. An analog builder is also included for markush library enumeration
- **Project Management** - you can save your projects at any time, allowing you to share your work with colleagues. It includes structures, models, and tables.



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