

Powerful QSAR, property prediction, and statistical analysis tool

Accelerates design and selection of single compounds and libraries for screening

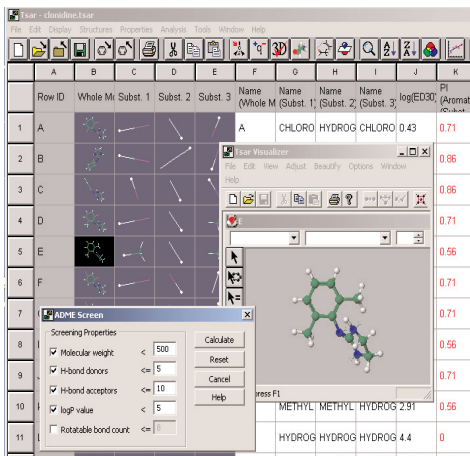
Lets you improve activity and eliminate undesirable properties in lead optimization

Integrates project data, molecular properties, and chemical structures within an easy-to-use spreadsheet

TSAR Datasheet

TSAR

Using computational tools to analyze and predict structures that are most likely to be active prior to synthesis or purchase is key to accelerating drug discovery. Tsar is a sophisticated design tool with a focus on analyzing Quantitative Structure-Activity Relationships (QSAR), which can be used throughout drug discovery, from initial compound selection for primary screening to reagent selection and creation of focused libraries for lead optimization. Tsar's easy-to-use chemical spreadsheet interface is equally accessible to medicinal chemists, computational chemists, and project team leaders.



Row ID	Whole M	Subst. 1	Subst. 2	Subst. 3	Name (Whole M)	Name (Subst. 1)	Name (Subst. 2)	Name (Subst. 3)	log(ED50)	PI (Armati)
1	A				A	CHLORO	HYDROG	CHLORO	0.43	0.71
2	B									0.86
3	C									0.86
4	D									0.71
5	E									0.56
6	F									0.71
7										0.71
8										0.56
9										0.71
10						METHYL	METHYL	HYDROG	2.91	0.56
11						HYDROG	HYDROG	HYDROG	4.4	0

▲ Automated property calculations give power to QSAR studies.

Tsar Capabilities

- **Property Prediction** - Tsar's extensive range of chemical property calculations give power to QSAR studies - you can explore different types of properties, 2D or 3D, to understand which promote activity. All properties can also be analyzed statistically to predict compound activity. In addition, the ability to screen compounds quickly for drug-like qualities of absorption, distribution, metabolism, and excretion (ADME), means faster selection.
- **Reagent Selection** - Tsar lets you select subsets of reagents by sampling reagent properties, eliminating those likely to exhibit undesirable properties (on the basis of, for example, molecular weight, logP, or

toxicity), or which do not add to diversity. You can also determine the properties of R-group combinations and use profile information to direct the design of diverse or focused libraries.

- **Selection by Product** - Tsar helps eliminate redundancy in combinatorial libraries by focusing on the product properties required. Compound selection is based on identifying combinations of R-group properties that match your target product profile.
- **Clustering and Sampling** - With Tsar, you can identify similar or diverse subsets of compounds, reducing library overlap or unnecessary screening.
- **Statistical Analysis** - Tsar offers a wide range of statistical methods for developing predictive models of activity, narrowing choices and improving decisions on which compounds to make and test. Relationships may be explained using clustering or regression methods, often using principal components or partial least squares to compress the numbers of variables. For very large datasets, Ward clustering by reciprocal nearest neighbors offers high performance.

Where activity cannot be explained by linear methods, Tsar includes a neural network for examining non-linear relationships. Large datasets can be compressed using non-linear mapping or render nets and visualized in 2D or 3D to reveal activity patterns.

FIRM analysis eases identification of unexpected relationships or data trends so that the best compounds are located for further investigation.

Effective Data Integration to Drive Decision Making

Providing access to Tsar's sophisticated QSAR capabilities can enhance teamwork. Team leaders can pull together project information for library profiling and examine computational and experimental data at the level they require.

Easy to Use

Tsar's powerful chemical spreadsheet links project data, structures, and predictions in a single view. Data trends can be visualized in a variety of formats, providing input for effective decision-making in the way you need it.

Key Capabilities:

- Automated data input
- Automated Lipinski's rule application
- Similarity/dissimilarity clustering and sampling
- Automated, powerful statistical methods, including FIRM analysis, PLS, and neural nets
- Fast retrieval of structures and associated data from Oracle
- 3D modeling alignment
- Library enumeration
- FIRM analysis

Tsar Components

- **Tsar** - A fully integrated 2D QSAR package for finding trends in data using statistical and visual analysis tools.
- **Tsar-3D** - A fully integrated 3D QSAR package adding 2D-3D conversion, 3D geometry and QM descriptions and 3D similarity to Tsar's 2D capabilities.
- **TsarBatch** - An add-on module for processing large numbers of structures in batch mode .

System Requirements

Windows NT or Windows 2000

- 36 MB free disk space for Tsar, 48 MB free disk space for Tsar-3D
- Minimum 128 MB RAM, recommended 256 MB (or greater)
- Pentium processor, recommended 266 MHz (or greater)
- Oracle client version 7.3.4, 8.0.5 or 8.1.5 if access to RS3 Discovery or Diamond Discovery databases is required, and RS3 Discovery version 1.2 or above.

Supported File Formats

- MOL2
- PDB
- CSSR
- Vamp Archive
- CAChe CSF
- UniChem
- MacroModel
- COSMIC
- MAD
- SMILES
- ASCII data



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