Applications

Chemistry, Biochem, Biotechnology

AMBER

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AMBER is a suite of programs that allow users to perform molecular dynamics simulations, on biomolecules.

AMBER V4.1 (1994) represents significant development over version 4.0 (1991). The differences include:

* updated forcefield for proteins and nucleic acids

* faster algorithms for simulations with water

* parallelized dynamics codes

* new algorithms for free energy simulations, including support for forcefields with polarization terms

* new graphical tools for preparing input to the dynamics programs

* powerful tools for NMR spectral simulations

* a new program for fitting point electrostatic charges from quantum data

Further information is available from http//www.amber.ucsf.edu/.

IRIX version compatibility:

AMPAC 5.0 with Graphical User Interface

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AMPAC 5.0 with Graphical User Interface is the most modern and reliable semiempirical quantum mechancial program on the market , and presently includes the SAM1, AM1, PM3, MNDo, MNDOC, and MINDO/3, semiempirical methods along with an extensive set of tools to study molecular structure and chemical reactions. M.J.S. Dewar's new SAM1 semiempirical method, which includes and explicit description of d-orbitals, now has parameters for or C, H, O, N, F, C1, Br, I, Si, P, S, and (our first transition metal) Fe. AMPAC 5.0 also includes a graphical user interface (GUI) implemented under the popular X-Windows/Motif environment for compatibility and seamless network access.

IRIX version compatibility:

AURELIA©

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AURELIA© (AUtomatic REsonance LIne Assignment) is used for the semi-automatic analysis of 2D and 3D NMR spectra. It uses X-Window™ graphics and offers two different user interfaces based on X11™ and X11/Motif™. The program features the display and plotting of spectra and spectral information, artifact reduction techniques, peak picking, cluster analysis, multiplet analysis, volume and distanced calculation, J-pattern search, spectral pattern definition and pattern match techniques. Molecular structures may be read and correlated to NMR data. Applications range from the analysis of complicated spectra of bi-molecules to the analysis of mixtures. All SGI models are supported.

IRIX version compatibility: 5.3, 5.x, 6.x

Chemistry, Biochem, Biotechnology

AbM™

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AbM™ is designed specifically for modeling of antibody structures and is capable of constructing a 3-D structure from a 1-D sequence. The program provides accurate, reliable and rapid modeling results.

AbM™ predicts the effects of site-directed mutagenesis experiments and larger modifications to the combining site. Applications using CDR replacement, humanization, introduction of catalytic activity, and metal binding sites, as well as the design of combining sites to new antigens can be approached realistically.

AbM™ is one of many software tools for bioinformatics that is available from Oxford Molecular Group.

IRIX version compatibility:

Affinity

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Affinity provides automated docking of ligands to receptors in the structure-based drug design process.

IRIX version compatibility:

Amorphous Cell

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Amorphous Cell is a comprehensive set of construction and analysis tools for predicting properties of bulk amorphous systems. You can investigate important material characteristics, such as cohesive energy density, chain packing and localized chain motions.

IRIX version compatibility:

Anaconda™

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Anaconda™ enables users to compare molecules by providing an interactive graphical method for the display and comparison of surface properties. Comparison of the structures and properties of a series of known active drug compounds can often result in the definition of the pharmacophoric pattern when the structure of the receptor is unknown. The method involves projecting the surface property of a molecule onto a sphere using the "Gnomonic projection" technique. The projection of properties and their differences can be represented as different colors on the spherical surface or as modifications to the shape of the sphere itself.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Apex-3D

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Apex-3D idenitifies pharmacophores and active conformations from a set of biologically active and inactive compounds. This information is stored as rules used to predict the activity of new compounds. Apex-3D is a DCL product, fully integrated into Insight II.

IRIX version compatibility:

Asp™

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Asp™ provides a simple solution to the problem of obtaining a quantitative measure of the similarity between two molecules. Similarity indices give a quantitative measure of the concept of bioisosterism and help guide researchers in deciding which compounds should be synthesized and submitted for biological screening.

IRIX version compatibility:

BRAGI

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BRAGI is the tool for the special purpose of interactive modeling unknown proteins from the structure of a known one. The current version has a number of features we think necessary and helpful for planning site-directed mutagenesis or designing proteins with new properties. The program package is written in such a way that it can be used almost instantly by the average scientist who is not a computer specialist. BRAGI is fully menu driven, using many well known features of OSF-MOTIF, a window like user interface. 3-D representation includes features like wireframe display of structures, chicken wire surface colored by electrostatics, ball and stick display, solids to show secondary structure and generation of ray traced images.

IRIX version compatibility:

BioMerge™

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BioMerge™ is a revolutionary solution for the enterprise wide integration and management of genome information. Biomerge supports DNA sequence analysis, queries for biological structure and functions, and other database functions. BioMerge stores public, third-party, and proprietary data in a single, industry-standard relational database from which you can launch analyses, answer queries, and generate reports for comparison and analysis. And, Biomerge supports placing analysis results directly into the database, attached to the original data, rather than scattering data in individual files throughout your company.

IRIX version compatibility: 6.3

Chemistry, Biochem, Biotechnology

Biopolymer

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Biopolymer is a graphically-oriented builder for constructing peptides, proteins, carbohydrates, and nucleic acids of canonical forms or user-defined geometrics.

IRIX version compatibility:

Bruker NMR Suite

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The Bruker NMR Suite is a set of integrated programs assisting today's chemist in practically all NMR spectroscopy applications. The NMR Suite provides a wide variety of visualization, processing and plotting functions for one and multi-dimentional spectra. In addition, it features advanced tools for the interpretation of mixtures and complex large molecule spectra. Experiment simulation based on quantum mechanical calculations may be employed for both NMR experiment planning and educational purposes.

IRIX version compatibility: 5.2, 5.3, 6.2, 6.3

C2•ADF

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C2•ADF is an interface to the well-known and validated Amsterdam Density Functional Codes. Applicatons include organic molecules, heterogeneous and homogeneous catalysts, transition-metal and heavy-element compounds, and semicondudtors.

IRIX version compatibility:

C2•Blends

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C2•Blends predicts phase diagrams, interaction parameters for liquid-liquid, polymer-polymer and polymer-additive mixtures. The C2•Blends module employs sophisticated simulation techniques to construct clusters of molecules and evaluate the structural and energetic parameters required for the prediction.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

C2•CASTEP

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C2•CASTEP is a revolutionary quantum code for the materials sciences. CASTEP enables simulation of the solid state, surface and bulk molecular structures. Properties such as energy, band structure, and charge distribution can be computed. Minimization and dynamics simulations can be carried out. CASTEP is suitable for much larger systems than conventional quantum codes.

IRIX version compatibility:

C2•Caveat

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C2•Caveat is an interactive drug design tool that can increase productivity by suggesting interesting new synthetic targets de novo. Through C2•Caveat's unique vector pair searching capabilities, all possible skeletons upon which drug candidates can be constructed can be easily identified. These new skeletons can then be optimized using the QSAR tools available in Cerius2.

IRIX version compatibility:

C2•Conformers

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C2•Conformers provides conformational search algorithms for molecular structures and the associated analysis tools. You can characterize molecular conformation and flexibility. The module generates many conformations, which can be examined individually or as clusters of similar structures. Average structures may be generated and displayed. Geometric and energetic properties can be easily plotted and evaluated.

IRIX version compatibility:

C2•Crystal Growth Workbench

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The C2•Crystal Growth Workbench is a particular set of modules within the Cerius2 environment. This integrated system combines advanced molecular modeling techniques and Computational Instruments, and is tailored to study and assist the solution of crystallization related problems, e.g.:

- Crystal shape prediction and control by rationally designed additives
- The effects of solvents, excipients and impurities on crystal shape
- Interpretation of diffraction patterns; crystal structure refinement
- Prediction of physico-chemical properties
- Prediction and control of polymorphism
- Preferential crystallization of metastable polymorphs

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

C2•Crystal Packer

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C2•Crystal Packer perofrms rigid body energy minimization under full symmetry conditions. You can optimize the packing of molecular crystals and calculate their sublimation energy. Applications include the prediction and analysis of molecular packing for pigment and drug polymorphs.

IRIX version compatibility:

C2•DBAccess

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C2•DBAccess interfaces to the ISIS corporate information standard from MDL and the flexible 3D database capabilities within MSI's Catalyst/INFO product. The C2•DBAccess module has the powerful advantage of spanning multiple database types and sources.

IRIX version compatibility:

C2•DLS

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C2•DLS predicts the structures of inorganic framework crystals from a trial model using the DLS-76 method of Baerlocher et al for geometric refinement. It is tailored for zeolite crystal structures.

IRIX version compatibility:

C2•Diffraction-Amorphous

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C2•Diffraction-Amorphous simulates non-crystalline powder and fiber diffraction patterns and radial distribution functions. Comparison with experimental data helps you to determine amorphous structure, polymer chain conformation, copolymer sequence structure and orientation.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

C2•Diffraction-Crystals

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C2•Diffraction-Crystals simulates powder, fiber and single crystal diffraction patterns from crystalline models for comparison with experimental X-ray, neutron and electron data. You can simulate diffraction in real-time while manipulating structure, providing you with a powerful method for data interpretation.

IRIX version compatibility:

C2•Diffraction-Faulted

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C2•Diffraction-Faulted simulates powder diffraction from faulted or layered structures via a user-friendly interface to the DIFFaX program of Treacy et al. Important examples of such structures include zeolites and clays.

IRIX version compatibility:

C2•Dynamics

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C2•Dynamics offers a suite of tools for molecular dynamics simulation. You can investigate the behavior of a material over a time period and study structure relaxation. A number of well-validated dynamics algorithms may be easily applied to molecules and 3-D periodic models of bulk structure. This extensive dynamics suite lets you deduce properties including diffusion, RDFs and structure factors, and velocity auto-correlation functions.

IRIX version compatibility:

C2•EXAFS

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C2•EXAFS interfaces to EXCURV92, the leading EXAFS code from Daresbury Laboratories in the UK. EXCURV92's trusted analysis and refinement techniques are fully integrated with Cerius2's modeling and graphical presentation tools.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

C2•FFE

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C2•FFE (Force Field Editor) offers enhanced functionality for the Cerius2 Open Force Field. The Force Field Editor enables you to adapt Force Fields from the Cerius2 database or create your own parameterizations. Apply previously inaccessible Force Fields from the literature to your own problems. Develop and validate in-house parameterizations. The Force Field Editor offers computational chemists the flexibility to investigate the properties of any material.

IRIX version compatibility:

C2•GA

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C2•GA provides the breakthrough technology of Genetic Algorithms to evolve a family of predictive models for use in Cerius2. C2•GA is used to develop QSAR models from receptor surface and other data, and is also useful in variable selection for field-based 3D QSAR.

IRIX version compatibility:

C2•Gaussian

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C2•Gaussian is the interface to the world's number one fully functioned quantum mechanics program. Designed in close collaboration with Gaussian Inc., C2•Gaussian allows you to apply ab initio, semi-empirical, and density functional techniques to study the energetics, structure, and chemistry of molecules and transition states. Useful features include transition state finding routines and the ability to follow reaction paths.

IRIX version compatibility:

C2•HRTEM

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C2•HRTEM simulates High Resolution Transmission Electron Microscope images and dynamical diffraction patterns from crystals, interfaces and defect structures. HRTEM represents a significant advance over previous simulation packages due to its speed and integration with structure building tools. Assists you in both the set-up and interpretation of EM experiments that investigate technologically important materials.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

C2•MFA

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C2•MFA permits field-based 3D QSAR as a complement to the Drug Discovery Workbench. Important scientiic innovations, including field evaluation using the Open Force Field, enables C2•MFA to be used as a tool in both Life and Material Sciences.

IRIX version compatibility:

C2•MMFF

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C2•MMFF provides specialist access to the Merck Molecular Force Field for accurately studying molecular systems in the life sciences. MMFF is broadly parameterized for organic and bio-organic systems and for the intermolecular interactions crucial to enzyme binding.

IRIX version compatibility:

C2•Mechanical Properties

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C2•Mechanical Properties is a comprehensive computational instrument for the prediction of bulk mechanical properties. This module works for any materials type--for example, crystalline and amorphous polymers, ceramics, semiconductors--and predicts a range of elastic moduli. Methods used include the second derivative method, constant stress minimization, constant strain minimization, and stress-strain dynamics.

IRIX version compatibility:

C2•Minimizer

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C2•Minimizer performs energy minimization of molecular and periodic structures, drawing on the technology of the C2•OFF (see below). You can predict low-energy structures using molecular mechanics calculations. Such methods will aid your understanding of molecular, crystalline and surface structure and its relationship to materials properties.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

C2•Mopac

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C2•Mopac interfaces to all the features of the popular semi-empirical quantum code Mopac6. The module also accesses Mopac7 and Mopac93. You can study the structure and energetics of molecules and transition states, computing properties such as molecular orbitals and charges.

IRIX version compatibility:

C2•Morphology

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C2•Morphology predicts and analyzes the morphology of crystals from their internal crystal structure. C2•Morphology uses the Donnay-Harker and Attachment Energy methods to display the equilibrium morphology of a given crystal structure. You can relate morphological features to structure and consider the effects of crystal growth modifying additives and solvents.

IRIX version compatibility:

C2•OFF

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C2•OFF (Open Force Field) provides molecular mechanics force fields to support Cerius2's property prediction modules. Choosing from an extensive database of force fields covering organics, polymers, zeolites, organometallics, and other materials types, simply load the force field, go to the relevent module, and run the calculation-Cerius2 takes care of the rest.

IRIX version compatibility:

C2•Polymer Properties

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C2•Polymer Properties analyzes polymer structures generated by the Amorphous Builder or Dynamics modules. You can calculate properties such as radius of gyration, end-to-end distance, order parameters, distribution of torsional states, free volume, density and Voronoi volume.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

C2•Polymorph

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C2•Polymorph predicts the polymorphs of organic molecules from the molecular structure alone. The module employs breakthrough technology from the laboratory of Professor Heinrich Karfunkel at Ciba-Geigy AG. With successful predictions on a variety of pigment and drug molecules as validation, C2•Polymorph can be used to find unknown polymorphs or as a structure determination tool integrated with techniques such as Rietveld refinement.

IRIX version compatibility:

C2•Powder Indexing

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C2•Powder Indexing completes the most comprehensive package of software modules for crystal structure determination currently available. An interface to the well-known TREOR90 indexing program, the module allows you to extract unit cell and symmetry information from powder patterns. You can use this information to assist with Rietveld refinement or crystal packing trials, or to confirm results from polymorph predictions.

IRIX version compatibility:

C2•QSAR+

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C2•QSAR+ greatly enhances QSAR analysis in the discovery and optimization of active lead compounds by providing ready access to a wide range of regression technologies. C2•QSAR+ fully integrates a variety of novel techniques using a "chemically aware" molecular spreadsheet.

IRIX version compatibility:

C2•Receptor

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C2•Receptor introduces receptor-surface modeling, a new technique for structural modeling in the absence of crystallographic data. C2•Receptor can be used in conjunction with genetic algorithms to develop predictive QSAR models, or with flexible 3D database searching to rank a collection of ’hit’ compounds by volumetric similarity.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

C2•Rietveld

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C2•Rietveld performs crystal structure refinement and quantitative phase analysis using experimental powder diffraction data and the Rietveld method. The Rietveld module is fast, interactive and easy to learn and to use. You have access to two trusted refinement programs, DBWS (Young et al) and GSAS (Von Dreele and Larson).

IRIX version compatibility:

C2•SDK

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C2•SDK is used to develop and integrate applications within the Cerius2 modeling and simulation environment, eliminating the need for you to write graphics, windowing, or systems-level code. Users also benefit from MSI's extensive library of computational and visualization subroutines.

IRIX version compatibility:

C2•Sorption

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C2•Sorption predicts the adsorption properties of molecules in microporous solids (e.g., zeolites) and on surfaces. C2•Sorption applies a "Grand Canonical Monte Carlo" simulation, using the C2•OFF for energy calculations. You can predict adsorption isotherms, binding sites, adhesion energies, diffusion paths and molecular selectivity.

IRIX version compatibility:

C2•Visualizer

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C2•Visualizer provides a comprehensive modeling environment for building, editing and visualizing models of molecular structures. Into this environment the user plugs one or more software modules, building a completely integrated package tailored to specific research needs. C•2Visualizer provides access to external or in-house databases. It allows for sketching molecular structures using the mouse, and displaying advanced graphics representations of materials. Hard copy output directed to black and white, gray-scale or color PostScript printers is straightforward. With X-terminal access and distributed network licensing, C2•Visualizer offers a fast and easy-to-use system for communicating chemical information.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

CAChe GroupServer™

Sales Department
Oxford Molecular Group, Inc.
2105 South Bascom Avenue
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Campbell, CA 95008
USA
408-879-6302 (fax)
800-876-9994 (tollfree)
webmaster@oxmol.com
http://www.oxmol.com

CAChe GroupServer™ is a suite of semi-empirical and ab initio chemistry applications optimized for Silicon Graphics R4000 and R8000 systems. CAChe GroupServer/Satellite is an intuitive client/server implementation designed for researchers outfitting entire teams, groups or departments. CAChe is used extensively to predict and visualize molecular structure and properties, elucidate reaction mechanisms, model catalysts, estimate polymer properties, predict UV/Vis and IR spectra and perform QSPR studies.

CAChe GroupServer™ is one of the many molecular modeling software capabilities available from Oxford Molecular Group.

IRIX version compatibility:

CAChe GroupServer™ and Mulliken™

Evelyn Brosnan
VP, Marketing
CAChe Scientific, Inc.
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Beaverton, OR 97076
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503-526-5099 (fax)
evelynb@cache.com

CAChe GroupServer™ is a suite of semi-empirical and ab initio chemistry applications designed to increase the capabilities and processing power of a group or entire department. Access to GroupServer software provided by CAChe Satellite, CAChe WorkSystem, or Personal CAChe connected to the GroupServer over a network; it cannot be used independently. All user interface and network software is included in Satellite and WorkSystem products and is optional with Personal CAChe. GroupServer Software includes: Molecular Mechanics, Extended Huckel, MOPAC, Zindo, Dynamics, and Tabulator. Mulliken™, the new ab initio application from the CAChe and IBM Almaden Labs collaboration, is purchased separately and can be fully integrated with a CAChe user interface.

IRIX version compatibility:

CAVEAT

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CAVEAT is an interactive drug design tool that can increase productivity by suggesting interesting, new synthetic targets de novo. Developed by Professor Paul Bartlett (University of California at Berkeley), CAVEAT generates, clusters, and scores novel structures holding three or more functional groups in positions required for biological activity. The funtional groups and their vectors can be inferred from a known ligand in its bioactive or bound conformation, or from an MCSS Functionality Map. CAVEAT rapidly searches preordered databases of likely skeletons that have been assembled from available crystal structure or modeled 3D databases, or two special databases, TRIAD and ILIAD. CAVEAT saves those structures that present the required vectors within a specified tolerance, filters out structures that have steric or chemical problems or are duplicates, clusters the remainder, and presents a representative member of each cluster. CAVEAT interfaces with Cerius2 and with QUANTA.

IRIX version compatibility:

CCD Detector System for X-Ray Crystallography

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Company Treasurer
Area Detector Systems Corporation
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Poway, CA 92064
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619-486-0444
619-486-0722 (fax)
clo@adsc-xray.com

Area Detector Systems Corporation has been manufacturing high quality area detectors for crystallography since 1983. ADSC is currently producing the Quantum line of CCD based area detectors. The Quantum 1 is a single CCD and taper module while the Quantum 4 is a multi-taper array.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

CCP4 Program Suite

S. Bailey
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Warrington, CH WA4 4AD
UK
44-1925-603-528
44-1925-603-124 (fax)
ccp4@sl.ac.uk

The CCP4 Program Suite is a dynamic collection of Fortran programs for protein crystallography, written by research workers and crystallographers in universities and other institutions. Applications include film processing (data reduction, scaling film packs, and image plates), phase determination, isomorphous replacement and anomalous scattering, (constrained and restrained) least squares refinement, solvent flattening, electron density maps, and software for the presentation of results.

IRIX version compatibility:

CET 93

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http://www.cosmic.uga.edu/pub/SGI.html

CET93 - Chemical Equilibrium with Thermal Tranport Properties, is a general program which will calculate chemical equilibrium compositions and mixture properties for any chemical system with available thermodynamic data. Generally, mixtures may include condensed and gaseous products. GET93 includes thermodynamic data for over 1100 gaseous and condensed species and thermal transport data for 151 gases. Written in FORTRAN 77 to be machine independent. PROGRAM NUMBER: LEW-16153

IRIX version compatibility: 5.x, 6.x

CFF95

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CFF95 is the most advanced Class II Force field available for molecular modeling, simulation, and analysis. CFF95 is used to optimize DNA, RNA, carbohydrates, lipids, proteins, peptides, and small-molecule models, giving a high confidence level for drug discovery, protein design, genomic theraputics, NMR spectroscopy, and X-ray crystallography.

IRIX version compatibility:

CHARMm

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CHARMm™ provides full molecular mechanics and dynamics simulations, targeted at small organics, proteins and macromelecules. Run via the QUANTA™ interface, CHARMm employs extensive conformational search methods (both stochastic and exhaustive), and incorporates a wide range of functionality, including free energy perturbation methods (FEP) and a comprehensive set of force field parameters. Developed and continually enhanced by Professor Martin Karplus (Harvard University) and collaborators, CHARMm is one of the most widely used and validated computational engines in use for molecular modeling.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

CLUSTERING Package

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CLUSTERING Package provides chemical database characterization, analog discovery, and directed structure selection for binding assays, toxicity tests, and other screens.

The Package operates on a set of structures represented in SMILES and produces clustering results in tabular format. The results are ready for manual examination as well as for output files suitable for loading into a database (for example, THOR™) or processing by an exploratory data analysis program (for example, MERLIN™).

This application provides an extremely efficient set of tools for a rigorous, yet fast, way of analyzing and calcifying the structures in a database. The application allows reclustering the database in a very short time to achieve the ultimate cluster information.

IRIX version compatibility:

CONCORD™

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Tripos, Inc.
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USA
314-647-1099
314-647-9241 (fax)
http://www.webcom.com/~tripos2/

CONCORD™ is a program for the rapid generation of high-quality 3-D organic molecular structures. Used interactively, CONCORD quickly generates structures for immediate computer graphic display. In batch mode, CONCORD provides a powerful mechanism for converting large databases of 2-D atomic connectivities into databases of 3-D chemical structures. CONCORD provides an advantageous alternative for molecular structure input using a simple, easy-to-learn chemical line notation. Structures are generated in an average of .075 Silicon Graphics® 4D/25 CPU seconds per MolFile.

IRIX version compatibility:

CONGEN™

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CONGEN™ (CONformation GENerator) is a noninteractive molecular modeling program that uses systematic conformational search to explore the energy surface of proteins (see Bruccoleri, Molecular Simulation, 10, 151-174 (1993)). It can be used on either small peptides or segments (loops) within proteins. In addition, it can perform molecular mechanics and analysis operations.

CONGEN is licensed only for research or educational usage, and the license is free of charge. This program is unsupported, but full source code, a 278-page manual, and additional tools (including graphical display) are provided.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

COSMO

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COSMO is a quantum mechanics solvation model implemented in DMol. For the first time you can accurately compute the structure and properties of molecules in a solvent environment using quantum mechanics.

IRIX version compatibility:

CRYSALIS

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CRYSALIS integrates crystal building (from unit cell data), static lattice calculations and visualization at the atomistic scale. Applications include ceramics, catalysts, fast 10N conductors, superconductors and a range of ionic and quasi-ionic oxide and halide systems.

IRIX version compatibility:

CS ChemDraw Pro™

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http://www.camsci.com/

CS ChemDraw Pro™ is the standard for chemical structure drawing programs. It provides specialized tools for drawing chemical structures, reactions and mechanisms as well as powerful general-purpose drawing and text tools, user-definable templates and full-color support. Everything about ChemDraw is designed to make chemical structure drawing as simple as possible. To add bonds and rings, just click. ChemDraw anticipates the best bond angles for you. Intelligent atom labeling makes creating even complicated labels a snap. Once drawn, structures can be copied via the clipboard to other high-end modeling packages including BIOSYM's INSIGHT II, MSI's Cerius2, and, shortly, Tripos's ALCHEMY, UNITY, and UNISON.

IRIX version compatibility:

CSEARCH

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CSEARCH is a spectrum assignment program for NMR spectroscopists. It facilitates the daily activities of an analytical department in medium to large chemical companies. It uses a Carbon-13 NMR library (60,000 compounds) of chemical structures with Carbon-13 NMR assignments. The program is capable of verifying the assignments of unknown spectra. Spectra can also be estimated from an input chemical structure. The database management capabilities of CSEARCH enable it to serve as the core of an information system focused on analytical sciences.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Cameleon™

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Cameleon™ generates multiple representations of the available protein sequence and structure data and correlates primary sequence, 3D structures and predicted properties. This information provides an understanding of the functional anatomy of the protein sequence and accurate insight into its structural characteristics.

Cameleon™ automatically aligns thousands of amino acid sequences. With Cameleon™, you can visually correlate sequences, residue properties and structure information. The program's predictive tols allow generation of aligned sequence-dependent profiles, including antigenicity, hydropathy and flexibility-all displayed by the interactive graph manager.

Cameleon™ is one of many bioinformatics software tools available from Oxford Molecular Group.

IRIX version compatibility:

Catalyst Visualizer

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Catalyst Visualizer provides an easy-to-use modeling, hypothesis generation, and structure search environment for collaborative studies by molecular modeling experts and practicing chemists. Catalyst offers excellent transfer of results to and from QUANTA and Cerius2 applications.

IRIX version compatibility:

Catalyst/Hypo

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Catalyst/Hypo helps drug discovery teams seeking active leads to prioritize synthetic work. Catalyst/Hypo is used in situations where one or more active structures are identified but no detailed structural informatin about the bioactive receptor is available. It generates 3-D hypotheses to explain the variations of activity with structure. These hypotheses can be visually inspected to help the scientist infer the chemical effects that mediate a compound's activity. The chemist can sketch a molecule and automatically get back a predicted activity based on a fit to the 3-D hypothesis; this helps to concentrate experiment on likely active compounds.

IRIX version compatibility:

Catalyst/Info

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Catalyst/Info lets the chemist find and identify structurally diverse leads by using a hypothesis as a search query against one or more databases which may contain hundreds of thousands of molecules. These databases may be company-proprietary or commercial. The hypothesis used can be either generated by Catalyst/Hypo, or constructed by hand from a crystal structure. The hypothesis can include 3-D binding features, 2-D structural constraints, and 1-D property constraints. Using 1-D, 2-D, and 3-D constraints, Catalyst/Info hit lists can be used to select compounds for assay, or to guide synthesis of new compounds. It provides a flexible, powerful, and rapid 2-D and 3-D structure and substructure search system.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Catalyst/SHAPE

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Catalyst/SHAPE idenitifies compounds that can possess similar 3D shapes with a specified 3D confirmation provided as input.

IRIX version compatibility:

Cerius2 Builder Modules

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Cerius2 Builder Modules enable the construction, display, and analysis of models of any type of molecular structure or mateial. Included are specialized builders for crystals (molecular, inorganic, and polymeric) and other periodic systems, amorphous polymers, proteins, surfaces, interfaces, and small molecules.

IRIX version compatibility:

Cerius2 Catalysis and Separations Workbench

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Cerius2 Catalysis and Separations Workbench predicts properties critical to catalysts and separating agents. These include the molecular geometry, energetics, and dynamic behavior of homogeneous catalysts; and the crystal structure, gas adsorption properties, and interaction with organic molecules of molecular sieves. Force fields such as the Universal Force Field enable the study of organometallics and inorganics. Simulation tools are integrated with structure libraries and modules to interpret diffraction, EXAFS, and HRTEM data.

IRIX version compatibility:

Cerius2 Crystal Growth Workbench

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Cerius2 Crystal Growth Workbench provides computational tools to model and investigate crystal structure and crystallization. Available methods include diffraction simulation, morphology prediction, and the simulation of surface interactions. These enable characterization of structure; prediction of crystal shape; rational design of additives to control and inhibit crystal growth; a better understanding of solvents and impurities; design of excipients and tailor-made additives; and prediction of physico-chemical properties.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Cerius2 Drug Discovery Workbench

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Cerius2 Drug Discovery Workbench is an integrated set of small molecule modeling tools incorporating over twenty computational algorithms for rational drug design. The Drug Discovery Workbench contains modules to generate, manipulate, visualize and analyze 2-D and 3-D molecular structures, conformations, and associated properties using a molecular spreadsheet paradigm; to generate, manipulate and visualize pharmacophoric and receptor pattern hypotheses; and to search for known molecules, and to design novel molecules to test mathematical and structure-activity hypotheses.

IRIX version compatibility:

Cerius2 Polymer Workbench

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Cerius2 Polymer Workbench simulates and predicts polymer properties. Building tools construct models of isolated chains or bulk polymers, either crystalline or amorphous. Simulation tools allow study of conformation, geometry, time-dependent behavior, and interactions with solvents, gas molecules and surfaces. Properties which can be predicted include solubility, adhesion, elastic moduli, phase diagrams, and fiber and power diffraction patterns.

IRIX version compatibility:

Cerius2 Polymorph Workbench

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Cerius2 Polymorph Workbench provides the first validated, commercially available computational method for predicting polymorphic crystal structures from the molecular structure of an organic compound alone. The Polymorph Predictor™ method, which is made available in an easy-to-use interface, combines an approach similar to Monte Carlo simulated annealing with sophisticated cluster analysis and energy minimization methods.

IRIX version compatibility:

Cerius2 Quantum Mechanics Workbench

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Cerius2 Quantum Mechanics Workbench integrates the entire range of QM methods. Ab initio, semi-empirical, and density functional calculations predict properties including molecular structure, energetics and charge distribution. Modeling tools help calculation set up. High quality graphics display of results assists analysis. The Workbench interfaces to three leading quantum programs Mopac, Gaussian92/DFT, and CASTEP.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Characterize

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Characterize provides a flexible framework within which to manipulate, display, interpret, and edit a wide range of analytical data. Optional modules include: Geometrics, Diffraction, IR Raman, Morphology, NMR, and EXAFS.

IRIX version compatibility:

Chemical Products Information (CPI) file

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The CPI file consists of supplier and pricing information for 418,000 chemical products built into preconfigured relational tables in ASCII format. These tables come with a tool kit for loading into Oracle, Ingress, and Rdb. The CPI file has an annual right-to-use license and can only be purchased if ACD has been licensed.

IRIX version compatibility:

Cobra™

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http://www.oxmol.com

Cobra™ is used to perform automated conformational analysis and generation of 3-D structures from 2-D information. The input information can be a SMILES string or a structure sketched using the Pimms (qv)the molecular graphics interface to Oxford Molecular's specialist molecules. Cobra performs conformational analysis by joining conformational templates from its knowledge base and contains advanced artificial intelligence techniques for identifying minimum energy conformations. Cobra can also carry out combined configurational/conformational searching, and, via input of a SMILES file, can be used in conversion of 2-D databases to 3-D.

IRIX version compatibility:

Combinatorial Chemistry Application Builder

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Monomers are partial molecules, complete with connectivity, chirality, multiple (possibly asymmetrical) connections, names, symbols, and other properties of atoms, bonds, and molecules. The Monomer Toolkit™ provides a complete programming interface to chemical structure at the monomer-level (rather than the atomic-level) of abstraction. Objects supported by the Toolkit include: Monomers, multimers, monomersets, varimers, and varimerpatterns. Languages supported by this Toolkit include CHUCKLES, CHORTLES, and CHARTS. Although the Monomer Toolkit may be used to process normal chemical information, it is particularly suitable for describing molecules and mixtures resulting from combinatorial synthesis. The Monomer Toolkit may be used to describe all reported types of combinatorial chemistry.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Comprehensive Heterocyclic Chemistry (CHC)

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CHC is a compendium of heterocyclic chemistry published in the chemical literature through 1983. The source of the information in the database is Comprehensive Heterocyclic Chemistry, 1984. The database focuses on synthesis of heterocycles, reactions of heterocyclic systems, and use of heterocycles in the synthesis of non-heterocyclic structures.

IRIX version compatibility:

Comprehensive Medicinal Chemistry-3D (CMC-3D)

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The CMC-3D database provides 3-D models and important biochemical properties for 6,500 compounds with biological activity. Developed from Pergammons Comprehensive Medicinal Chemistry, data include synonyms, drug class, log P, and pKa.

IRIX version compatibility:

ConFirm

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ConFirm is a batch conformational analysis program for the generation of coverage-based conformational models. Capable of generating conformational models for thousands of molecules every day on a single processor workstation, ConFirm can be used to explore energetically accessible flexibility in large libraries of compounds. ConFirm supports a wide array of standard file formats for compatibility with all standard modeling packages.

IRIX version compatibility:

ConSystant

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ConSystant is a utility that allows the user to interconvert chemical structure files. ConSystant allows users of software packages that manipulate chemical structures (such as molecular modeling software, chemical databases, and 2-D structure drawing) to exchange data. The current version 3.0 supports many different chemical data interchange file formats as well as several simple graphical outputs.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Consensus

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Consensus builds a 3D model of a protein from its amino acid sequence and the known structures of related proteins using distance constraints derived from the reference proteins.

IRIX version compatibility:

Converter

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Converter builds 3D structures from a 2D structure database. The resulting structures can be used in conjunction with commercial 3D database software, sch as ISIS™/3D (MDL Information Systems, Inc.).

IRIX version compatibility:

Crystal Cell

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Crystal Cell aids you in the study and characterization of crystal structure, stability and mechanical properties. Use Crystal Cell to determine crystal structures corresponding to local minima in potential energy.

IRIX version compatibility:

Current Synthetic Methodology (CSM)

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Current Synthetic Methodology is a selection of significant reactions to synthetic chemists. It consists of approximately 7,000 new reactions each year from ChemInform RXL from 1992 onwards. The focus of the database is:

1. New reagents or important modifications of known reagents.

2. Chemo-, regio-, and stereo-selective reactions

3. New synthetic methodology, emphasizing reactions of general use

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Custom Databases for High-throughput Screening

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With the inclusion in ACD of large libraries of compounds that can be readily obtained for biological testing, registering these compounds into corporate databases is now a bottleneck. To alleviate this, MDL provides a perpetual license to the chemical structure, chemical name, and CAS registry number of compounds selected on a custom basis.

IRIX version compatibility:

DAYLIGHT ToolKit™

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DAYLIGHT ToolKit is a set of tools for computer implementation of chemical infrastructures. It is a set of object libraries that are used to create software modules needed for chemical applications and programs.

The ToolKit combines proven algorithms. Written in C in an object-oriented fashion, it is capable of interfacing with other languages. DAYLIGHT ToolKit is fast, easy to use, and very portable.

IRIX version compatibility:

DBAccess

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DBAccess identifies leads by using a hypothesis that may include binding features, structural and property constraints, as a search query against databases containing hundreds of thousands of molecules. DVBAccess is used to select molecules for trial or to the guide synthesis of new compounds, significantly accelerating the discovery process. DBAccess comes preloaded with the Maybridge catalog and the NCI database.

IRIX version compatibility:

DMol

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blp@msi.com
http://www.biosym.com/

DMol implements density functional theory (DFT) using both local and gradient-corrected (non-local) potentials to provide the capability to make reliable, quantitative predictions about molecular systems.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

DSolid

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DSolid is for the accurate simulation of molecular crystals and organometallics. It is an adaptation of BIOSYM's DMol program; DSolid treats extended solids through the use of periodic boundary conditions. Use DSolid for intra-molecular structure, structural properties, electron densities, homo's and lumo's, and solvent effects.

IRIX version compatibility:

DeCipher

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DeCipher is a molecular structure and dynamics analysis program. DeCipher fills a long-standing need for high-level analysis.

IRIX version compatibility:

DeCypher II®

Jim Lindelien
President/CEO
Time Logic, Inc.
880 Northwood Boulevard
Incline Village, NV 89451-8241
USA
702-833-0200
702-833-1222 (fax)
jiml@timelogic.com
http://www.timelogic.com

Time Logic, Inc. DeCypher II® Genetics Supercomputing PC yields 100x-10,000x speed gain over conventional UNIX workstaitons for massive DNA and Protein database searches. Utilizing a scalable Xilinx reconfigurable logic array processor, the DeCypher II® is the world's fastest and most affordable implementation of the Smith-Waterman sequence similarity algorithm, and runs many other algorithms. Smith-Waterman is regarded as the most sensitive genetic search algorithm available today for revealing distant, inter-species genetic simularities. Reconfigurable logic permits future algorithms to be run on the existing computaitonal array without hardware obsolescence.

IRIX version compatibility: 5.1, 5.2, 5.3, 5.x, 6.0, 6.1, 6.2

DelPhi

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DelPhi calculates electrostatic potential and solvation energy of both large and small molecules, including nucleic acids. Use DelPhi to rigorously examine the effects of charge distribution, ionic strength, and dielectric constant on the electrostatic potential of macromolecules.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Discover®

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Discover® is a molecular simulation program that uses a carefully derived empirical forcefield for performing dynamics simulations, minimization, and conformational search on molecular, aggregate or periodic systems.

IRIX version compatibility:

DryAdd

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Oxford Materials Ltd.
Chestnut Farm, Tarvin Road
Frodsham
Cheshire, WA6 6XN
UK
44-1928-735679
44-1928-735352 (fax)
j.h.exelby@oxmat.co.uk

Modeling Polymerisation and network formation in paints, coatings and adhesives, Dry-Add is based on algorithms developed and tested in ICI's paints business. Network, sequence and formula analyses allon properties of polymers and networks to be related to experiment.

IRIX version compatibility:

ESOCS (Electronic Structure of Close-packed Solids)

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ESOCS (Electronic Structure of Close-packed Solids) calculates electronic and magnetic properties of 3D periodic systems, and treats large unit cells, metals, semi-conductors and insulators. The program is most accurate for close-packed solids.

IRIX version compatibility:

EXPOD: An Expert System for Polymer Design

Takashi Nishikawa
Dir., Software Business
Mitsubishi Chemical
America, Inc.
99 W. Tasman Drive
Suite 200
San Jose, CA 95134
USA
408-232-6228
408-954-8494 (fax)

EXPOD provides comprehensive data and know-how management for designers of polymers. The porgram can accurately predict the fundamental properties of a polymer from its molecular structure using a specialized knowledge base and database. EXPOD allows a polymer designer to quickly work through design-cycles, greatly reducing development time. The program employs estimation methods stored in its knowledge base to predict fundamental properties of candidate polymers and compares calculated results with the polymer properties stored in the database. EXPOD cal also reverse-engineer polymer structures from a set of required properties. The parameter optimization module facilitates customization of EXPOD's parameter sites.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Eclipse™-NMR Spectrometer

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AID Operations Manager
JEOL USA, Inc.
11 Dearborn Road
PO Box 6043
Peabody, MA 01960
USA
508-535-5900
508-536-2205 (fax)
nmr@jeol.com
http://www.jeol.com

The Eclipse™ NMR Spectrometer, available at 270 and 400 MHz field strengths, features a Silicon Graphics workstation as the host computer. The host computer connects to the spectrometer via Ethernet. This allows any workstation connected to the network to submit samples and access data. The Eclipse can be completely automated, automation that is built-in, not added on - one mouse click can produce the requested NMR data. The Eclipse also allows full control of the parameters required to collect complex NMR experiments. The degree of flexibility offered by the Eclipse-Delta combination sets a new standard in the NMR market.

IRIX version compatibility:

Electrostatics & Brownian Dynamics Simulation

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Electrostatics & Brownian Dynamics Simulation computes electrostatics in ionic solution using the Poisson-Boltzmann equation. Such interactions are dominant in many molecular processes, especially those affecting diffusion within a molecular system. Brownian dynamics can be used to examine these diffusional processes, including rates for diffusion of ligands to active sites in enzymes or the motion of critical loops on a protein surface. An optional module in QUANTA™ allows visualization of electrostatic maps and diffusion trajectories.

IRIX version compatibility:

Extensive Computational Chemistry Environment (ECCE)

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Technical Group Leader
PNL/Battelle
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509-375-2913
509-375-6631 (fax)
dr_jones@pnl.gov
http://www.battelle.org

Extensive Computational Chemistry Environment (ECCE) is a suite of software tools built around an object-oriented chemistry data moves and an object-oriented database. The ECCE data model will facilitate the integration of multiple applications beneath a unifying graphical user interface that provides a common look-and-feel. The ECCE data model permits much greater freedom in the manipulation and viewing of data than conventional approaches. The database provides a persistent repository for information related to the chemistry data model and the computational chemistry applications.

IRIX version compatibility: 5.x, 6.x

Fast Data Finder

Arthur Thomas
Bioinformatics Tech Advsr
Paracel, Inc.
One First Street
Suite 14
Los Altos, CA 94022
USA
415-854-6504
415-854-6504 (fax)
ajt@proteus.com
http://www.paracel.com

The company’s products include hardware and software tools that can be used for building customized information services and high speed bioinformatics solutions. The hardware FDF accelerator would act as a SCSI peripheral to the SGI Host. These tools enable a client to launch an Internet-based information service within a matter of days, without having to assemble a solution piecemeal. Hardware-based, high-performance "information filters" analyze and identify the contents of textual data streams, which may include non-English text as well as protein and DNA sequences. Software tools perform data gathering, organization, archiving, and distribution through the Internet and corporate enterprise networks ("intranets").

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Fast Structure

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Fast Structure uses an approximate density functional method to calculate energy and forces, to determine equilibrium geometries in molecules and clusters.

IRIX version compatibility:

Felix 1D/2D and Felix ND

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Felix 1D/2D and Felix ND are programs for processing, displaying, and analyzing all types of high-resolution, solid-state, in vivo, one- to four-dimensional, homo-nuclear, and heteronuclear data using the same set of processing tools.

IRIX version compatibility:

Felix Assign

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Felix Assign is a unique package for computer-assisted assignment of 2D, 3D, and 4D NMR spectra of proteins and nucleic acids, which encompasses tools for semiautomatic spin system detection, identification, sequential assignment and NOE crosspeak assignment.

IRIX version compatibility:

Felix Model

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Felix Model is an option of the Felix program that provides direct interaction between experimental NOESY data, molecular structures, and back-calculated NOESY data within an integrated interface.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Flexiblend

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Flexiblend rapidly estimates polymer miscibility. Approximate, but fast, Flexiblend helps you quickly screen polymer blend candidates.

IRIX version compatibility:

GEMM

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301-402-0436
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GEMM, (Generate, Edit, and Manipulate Molecules), is an interactive molecular graphics package that has been in sue at the NIH for years. It is a convenient tool for constructing, viewing, modifying, and manipulating a molecular structure in three dimensions. The molecular structure can be any collection of small and large molecules. The program is menu-driven and most operations are self-explanatory from the description of each menu item. Thus, a bench scientist with no computer training can learn to use the package in minutes and without a manual.

IRIX version compatibility:

GMMX

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GLOBAL-MMX (GMMX) is a steric energy minimization program which uses the MMX force field and operates in batch mode. Its main purpose is to search conformational space and to list out the lowest energy unique conformations thus produced. One of the major problems in molecular modeling is known as the local minimum problem. Energy minimization routines are designed to remove from the system by proceeding downhill on the potential energy surface. Invariably such routines find the local energy minimum closest to the input geometry. This local energy minimum may not be the global energy minimum and also provides no information about the number and relative energies of other local minima on the potential energy surface. Information about the number and energies of local energy minima can be important in planning syntheses, understanding reaction mechanisms and interpreting NMR spectra. GMMX is designed to address this problem by automating the generation, minimization and comparison of conformations.

IRIX version compatibility:

GMMX v.1

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Conformational searching program using the MMX force field. GMMX searches conformational space using both bond rotation and catesian atom movement and lists the lowest unique energy conformations found. Structure input is automated and comparison of low energy structures can be done in either cartesian or torsion space. Options for constraining distances, angles or dihedrals and for monitoring distances, angles, dihedrals or PMR coupling constraints.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

GRASP

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GRASP is a visualization and analysis tool for protein and DNA structures. In addition to traditional representations, GRASP includes many novel display forms. In particular it features highly optimized algorithms for the construction and display of molecular surfaces. GRASP also contains procedures for evaluating eletrostatics, via the Poisson-Boltzmann equation, along with a wide variety of representations such as contours, vectors and field lines. Version 1.2 includes a panel interface, and a complete scripting and macro language.

IRIX version compatibility:

GROUP

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Customer Liaison Manager
Molecular Discovery
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Elms Parade
Oxford, OX OX2 9LL
UK
44-1993-830385
44-1993-830966 (fax)

GROUP is an extension of the well-known GRID method of drug design, but can detect larger and more-specific binding sites. For example, it will find all places on a biological macromolecule at which glucose could bind, and all possible orientations of the glucose at each of these sites. The output from GROUP is compatible with other molecular modeling software systems, and can be used to interpret and extend QSAR and chemometric analyses.

IRIX version compatibility:

Gaussian 94®

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Gaussian, Inc.
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412-279-2118 (fax)
info@gaussian.com

Gaussian 94® provides a framework for the practical application of proven ab initio, density functional and semi-empirical electronic structure methods to chemical investigations. Detailed examination of a molecular potential energy surface yields accurate molecular structures, properties and reaction energetics. The properties that can be evaluated include vibrational frequencies, IR and Raman intensities, multipole moments, electrostatic potentials, polarizabilities, magnetic shielding tensors, magnetic susceptibilities, elctron affinities, ionization potentials, andelectrostatic potential derived charges. These results can then be used to predict thermodynamic properties, interpret molecular spectra, elucidate reaction mechanisms, and parameterize molecular mechanics calculations.

IRIX version compatibility:

HINT™ - Hydropathic Interaction Visualization and Analysis Tools

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eduSoft, LC
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Mercer Island, WA 98040
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206-236-5268 (fax)
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http://www.eslc.vabiotech.com

HINT™ is a novel empirical molecular modeling system with new methods for de novo ligand design and protein or nucleotide structural analysis. HINT translates the well-developed Medicinal Chemistry and QSAR formalism of LogP and hydrophobicity into an interaction model for all biomolecular systems. LogP is a thermodynamic parameter that encodes all non-covalent interactions in the biological environment as well as solvent effects and entropy. HINT visualization tools include: (1) 3D hydropathy fields useful in 3D QSAR; (2) 3D hydropathic interaction maps that are uniquely instructive for understanding biomolecular structure including substrate binding, protein folding, etc.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

HOOK

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HOOK uses a Functionality Map generated by MCSS to generate novel potential ligands that satisfy the chemical and steric requirements of a macromolecular binding site. HOOK connects pairwise functional groups to molecular skeletons from a library and fits the resulting molecule into the receptor site. HOOK orders the hits by steric fit and allows further analysis by CHARMm and QUANTA.

IRIX version compatibility:

HipHop

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HipHop is a batch molecule alignment application, which can be used with MSI or other modeling programs to provide feature-based alignment of a collection of compounds onto a pharmacophoric hypothesis. HipHop takes a collection of conformational models of molecules and a selection of chemical features as input and produces a series of molecular alignments in a variety of standard file formats. The richness of chemical features supported includes: surface-accessible hydrophobes, surface-accessible hydrogen bond donors/acceptors, charged/ionizable groups and user-defined features to cover even the most subtle chemical concepts. HipHop can also produce a collection of 3-D database queries that can be used to find chemically diverse structural templates.

IRIX version compatibility:

Homology

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Homology builds a 3D model of a protein from its amino acid sequence and the known structures of related proteins. Tools for assigning structurally conserved regions and building loops are built into the program.

IRIX version compatibility:

ISIS™/Base

David Hughes
MDL Information Systems, Inc.
14600 Catalina Street
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510-895-1313
510-483-4738 (fax)
800-635-0064 (tollfree)
isis@mdli.com
http://www.mdli.com/

ISIS™/Base provides scientists with the ability to: (1) manage, store, and retrieve chemical structures, reactions, and text stored on a local computer; and (2) in conjunction with ISIS/Host, store, search, and retrieve two- and three-dimensional molecules and reaction data and biological activity data stored in relational databases on a host computer. ISIS/Base provides a single user interface for searching and viewing data from several sources, whether stored on a local workstation or (with ISIS/Host) on a host computer on another continent. ISIS/Base allows scientists to create queries without learning the query language specific to the different database types accessible through ISIS.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

ISIS™/Draw

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ISIS™/Draw provides scientists with tools to create presentation-quality sketches of chemical structures and reactions and a wide range of other graphics, and can operate as a stand-alone application or in conjunction with ISIS/Base. Unlike a number of competing packages, ISIS/Draw recognizes the chemistry underlying the graphic representation and automatically positions atoms and chemical groups as a chemist would position them. The graphic representation can be used throughout ISIS either as presentation-quality graphics or as representations of chemical structures. As structures, graphics created under ISIS/Draw can be used with ISIS/Base as a means for effecting database searches.

IRIX version compatibility:

ISIS™/Host

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ISIS™, the Integrated Scientific Information System, provides a client-server system for sharing scientific information throughout an organization. From a personal workstation, scientists can access an organization's proprietary and commercial chemical data, reaction data, test data, etc., in relational and other local remote databases. ISIS integrates these data sources through a single user interface, and allows searches of these data sources without learning the specific language and protocol of each. ISIS/Host works in conjuction with ISIS/Base to bring information from networked host computers to the desktop. ISIS's 3-D database searching can be used in conjuction with computational chemistry software.

IRIX version compatibility:

Iditis Architect™

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Oxford Molecular Group, Inc.
2105 South Bascom Avenue
Suite 200
Campbell, CA 95008
USA
408-879-6302 (fax)
800-876-9994 (tollfree)
webmaster@oxmol.com
http://www.oxmol.com

Iditis Architect™ simplifies the complex task of validating, characterizing, and archiving proprietary 3D protein structures. The program also provides structural validation tools that have been adopted by the PDB for checking the stereochemical accuracy of all deposited structures.

Iditis Architect™ ensures that the structure is consistent and correctly formatted. The structures can then be entered into the Iditis database alongside publicly available structures allowing functional motifs and unexpected similarities within proprietary proteins to be indentified.

Iditis Architect™ is one of many bioinformatics software tools available from Oxford Molecular Group.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Iditis™

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Iditis™ organizes over 500 fields of data for each published protein structure in a series of very efficient compressed relational tables using only 60% of the hard disk space of the equivalent PDB release. The database is updated by Oxford Molecular with each release of the PDB and is the most in-depth database of protein structure data available.

The program manages the protein structure data so that all of the 3,300 proteins in the PDB can be searched simultaneously in seconds, making th research process more efficient and accurate. Iditis™ uncovers loops, motifs, and active site interactions and examines structural similarities in related protein families.

Iditis™ is one of the many bioinformatics software tools available from Oxford Molecular Group.

IRIX version compatibility:

Insight II®

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Insight II® is BIOSYM's 3D graphical environment for molecular modeling. It's powerful interface gives you a seamless flow of data between other BIOSYM programs. Use the Insight II program to create, modify, manipulate, display and analyze molecular systems and related data.

IRIX version compatibility:

Interphases

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Interphases calculates order parameters, statistical layer weights, configuration statistics, and solute distributions for monolayers and bilayers within the interphase by using a lattice model.

IRIX version compatibility:

LOOK

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415-846-3570
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char@mag.com

LOOK is a unique software tool specifically designed to bring structural insight to molecular biology. LOOK bridges the gap between the study of protein sequence and protein structure to help you understand protein function.

With LOOK you will design and analyze your experiments based on structural knowledge:

- Visualize your protein, directly from a known crystallized structure, or by homology modeling (using the SegMod accessory package)
- Identify evolutionarily conserved regions and evolutionarily correlated mutations
- Predict structural changes induced during mutagenesis experiments
- Access relevant structural information in the literature, searching by residue or region
- Perform various structural analyses, including burial/accessibility analyses and hydrophobocity determinations
- Communicate results with persuasive, insightful graphics ready for publications or slide

presentations

LOOK'sintuitive, user-friendly interface makes the full power of all of these features readily accessible to any user, making it an invaluable partner to laboratory work.

IRIX version compatibility:

LOOK-SegMod

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LOOK-SegMod (Segment Match Modeling) Homology Modeling package combines automated simplicity with a powerful and accurate algorithm, to make homology modeling accessible to modelers and non modelers alike.

The proliferation of available protein information has made more accurate structure predictions possible using homology modeling. Current homology modeling techniques, however, are time-consuming and require a high level of user involvement to adjust parameters, fix errors, and control refinements. Given a sequence alignment, SegMod is so powerful that it can accurately and automatically generate a model.

SegMod is extremely robust and completely automatic with the highest level of prediction accuracy, and flexibility. SegMod now works with LOOK interface, where LOOK's superior user interface provides easy access and a user-friendly environment.

IRIX version compatibility:

Ludi

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Ludi is a ligand design tool that suggests compounds that make specific interactions with a receptor site for de novo design and lead optimization. Ludi can also suggest new substituents and isoteric replacements for a series of active analogs.

IRIX version compatibility:

Ludi/ADC

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Lucid/ADC links the design tools of Ludi to MDL's Available Chemicals Directory, a database of 2D structures. You can access over 65,000 such structures and convert them to 3D models, accelerating your search for drug candidates.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

MAR Image Plate Scanner System for Crystallography

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Imaging plate scanner systems are used in the study of the structure of both macromolecular protein crystals and imorganic small molecular crystals. The systems are used by universities, synchrotron facilities, and pharmaceutical companies, among others. The MAR Image Plate Scanner System is a high-performance, highly automated system for the collection of crystallographic data. We are pleased to offer software for any Silicon Graphics® workstation running IRIX™ 4.0.1 or higher as the data collection and data processing platform for MAR Research Scanners.

IRIX version compatibility:

MATLAB® Chemometrics Toolbox

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The MathWorks, Inc.
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508-647-7000
508-653-2997 (fax)
efroio@mathworks.com
http://www.mathworks.com/

The MATLAB® Chemometrics Toolbox is a collection of functions for developing and evaluating the calibration matrices used in chemometric quantitive analysis. The toolbox may be used with any type of chemical or physical data. Common applications include analytical chemistry, spectroscopy and chromatography. The package provides Multiple Linear Regression routines for producing K-, P-, and Q-matrix calibrations and for establishing calibrations in using Factor Analysis (Principal Component Regression) and Partial Least Squares in latent variables. The toolbox consists of routines that implement various statiscally-based calibration methods that have become accepted as standard chemometric techniques. The Chemometric Toolbox is delivered as MATLAB M-files, enabling the user to see the algorithms and implementations, as well as to make changes or create new functions to address a particular application.

IRIX version compatibility:

MCSS

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MCSS is a de novo ligand design method. It creates a Functionality Map describing preferred binding sites and directionality of bound functional groups for the receptor. The Functionality Map can be used to design novel receptor ligands either manually or by finding skeletons to connect the functional groups. MCSS optimizes placement in the receptor using CHARMm dynamics in which each copy of the group moves independently, with no influence from the other copies of the functional group.

IRIX version compatibility:

MDL Drug Data Report (MDDR)

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The MDDR database contains structure and biological activity information for 57,000 drug candidates. Every month it is updated with new biologically active compounds as they are disclosed. The progress of these compounds are then tracked through development and clinical trials. The information in MDDR comes from patents, conferences, journals, and company communications. MDDR is valuable in helping to identify structural features which may contribute to a given biological activity, and in staying abreast of competitive discoveries. A 3-D version is available.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

MERLIN™

Yosef Taitz
Chief Executive Officer
DAYLIGHT Chemical
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MERLIN offers high-performance searching and exploratory data analysis of chemical information. MERLIN can be used with the THOR™ database. It achieves its high performance by operating entirely in memory.

MERLIN uses novel, self-optimizing software technology to provide search performance approaching the theoretical limit (for example, the substructure search function typically operates in excess of 400,000 structures per second on a UNIX® workstation).

IRIX version compatibility:

MMFF

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MMFF, an option to CHARMm, provides an independently derived force field. It was developed by Dr. Tom Halgren at Merck Research Laboratories. MMFF is parameterized using highest quality ab initio quantum mecanical potential energy surfaces. It provides accurate geometries and conformational energies for an unusually large variety of organic molecules. Featuring a novel "Buffered 7-14 Non-bonded Potential", MMFF has also yielded more predictive enzyme-ligand binding energies than alternative force fields in studies at Merck.

IRIX version compatibility:

MOL-GRAPH™

Hiroshi Shimizu
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Japan
81-3-3344-8147
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MOL-GRAPH™ is a practical computer-aided molecular modeling, simulation, and analysis system, providing not only visualization of molecular structures but also physical properties. MOL-GRAPH consists of three systems and two options: MOL-MOLIS, a molecular orbital analysis system; MOL-CRYS, a crystal molecule analysis system (inorganic and organic molecule); MOL-FS, a full analysis system; BIO-option, a large molecule biological analysis option; MD-option, a molecular dynamics analysis option.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

MacroModel©

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MacroModel
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http://www.columbia.edu/cu/chemistry/mmod/

The MacroModel© molecular modeling software package allows the user to construct and graphically manipulate both simple and complex chemical structures, to apply molecular mechanics and dynamics techniques to evaluate the energies and geometries of molecules in vacuo or in solution, and to display and examine graphically the results of the modeling calculations. Energy calculations use MM2*, MM3*, AMBER* or OPLSA* force fields, and an analytical GB/SA continuum treatment for solvation. Energetic processes are monitored interactively by MacroModel and can include multiple simultaneous tasks. Energetic calculations may be carried out on full structures or substructures prepared with the MacroModel substructure editor.

IRIX version compatibility:

Metabolite

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Metabolite is a complete metabolism information system containing key information about metabolic transformations of xenobiotic compounds from the literature, and a registration system to input proprietary metabolism studies. Information in the database was abstracted from Biotransformation of Drugs (1977-1983), Pharmacokinetics (1986-1990), and original metabolism literature from 1990 onwards. Metabolite is released semiannually. The database provides indexing of path and scheme information for the metabolic transformations, and includes data on species, route of administration and excretion, analytical methodology, parent compound class and physiological activity.

IRIX version compatibility:

MidasPlus®

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http://cgl.ucsf.edu/midasplus.html

MidasPlus® is a molecular modeling and drug design support system. Atomic coordinate data is used to create line and surface displays of several interacting molecules while qualitatively monitoring stereochemistry. Users manipulate the resulting image by a "virtual trackball" interaction technique to provide concise control of viewing angles and positions. It is possible to view any subsegments of a model in isolation for clarification. Images can be wireframe structures with depth cueing, dot cloud solvent accessible and van der Waals surfaces, and shaded color surfaces (appropriate for publication purpose) using either Corey-Pauling-Koltun representations or "ribbon" drawing for depicting secondary protein structure.

IRIX version compatibility: 5.3, 6.2 Certified, 6.3 Certified

Chemistry, Biochem, Biotechnology

MidasPlus™

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MidasPlus is a molecular modeling and drug design support system. Atomic coordinate data issued to create line and surface displays of several interacting molecules while qualitatively monitoring stereochemistry. Users manipulate the resulting image by a "virtual trackball" interaction technique to provide concise control of viewing angles and positions. It is possible to view any sub-segment of a model in isolation for clarification. Images can be wireframe structures with depth cueing, dot cloud solevent accessible and van der Waals surfaces, and shaded color surfaces (appropriate for publication purposes) using either Corey-Pauling-Koltun representations or "ribbon" drawings for depicting protein structure.

IRIX version compatibility: 5.3, 6.2 Certified, 6.3 Certified

Miscibility

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Miscibility is a navagational aid for predicting liquid-liquid phase diagrams of polymer solutions or blends. It increases your productivity by unifying MSI's tools for phase diagram prediction and leading you through appropriate simulation strategies.

IRIX version compatibility:

Modeler

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Modeler is a batch program which quickly and automatically generates a refined homology model of a protein, given only the sequence alignment to a known 3-D protein structure, using satisfaction of spatial restraints and simulated annealing techniques. Developed by Professor Andrej Sali (now at Rockefeller University), Modeler has been shown to generate excellent models with as little as 30% homology to known structures. It is interfaced to QUANTA for set-up and analysis of the resluting homology models.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Molconn-Z - Molecular Connectivity and Topology Tools

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Molconn-Z is the latest evolution of the standard molecular connectivity, shape and information indices program for Quantitive Structure Activity Relationships. New concepts of QSAR, including the Electrotopological State, have always been introduced first in this program. In addition to the standard QSAR Chi, Kappa, etc. indices, the current release of Molconn-Z provides several new tools for applying the E-State formalism: 1) New E-State Maps that can be contoured and displayed; 2) New Atom-typr E-State Indices; and 3) New E-State Indices for hydrogen atoms. This version of Molconn-Z is designed to interface with the latest version of Sybyl (Tripos, Inc.) with a Sybyl-compatible graphical user interface.

IRIX version compatibility:

Multiwire Counter System for Protein Crystallography

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Company Treasurer
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Multiwire counter systems are used in research laboratories at both universities and pharmaceutical companies engaged in the study of the structure of macromolecular protein crystals. SDMX multiwire counter systems have proven reliability. Over 100 protein structures have been solved using our fast and particularly accurate photon-counting detector systems. We are pleased to offer software for any Silicon Graphics ® workstation IRIX™ 4.0.1 and higher) as the data collection computer platform. The programs operate as they did on previous operating systems; the visual alignment program is implemented with the Motif™ toolkit.

IRIX version compatibility:

NMR Refine/Advanced

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NMR Refine/Advanced expands the refinement capabilities found in NMR Refine/DG-II to include simulated annealing and restrained molecular mechanics and dynamics (MD Schedule), refinement of NOE intensities using hybrid-matrix approaches (IRMA), direct refinement of NOE volumes (NOE-MD), an interface to back-calculating 2D NOESY crosspeak intensities (NOE Simulate), and a spreadsheet method of analyzing NMR-related structural and dynamical molecular parameters (Query).

IRIX version compatibility:

NMR Refine/DG-II

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NMR Refine/DG-II provides an entry-level option into NMR refinement software with capabilities for generating structures from NMR-derived distance and dihedral restraints. The DG-II, Restraint Analysis, NMR Database and ProStat pulldowns combine to give the NMR spectroscopist the necessary tools for generating, analyzing and verifying high resolution structures.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

NMR Workbench

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NMR Workbench is an integrated system that combines advanced modeling methods with interactive, multi-dimensional processing and analysis of Nuclear Magnetic Resonance spectra. By providing a complete system for NMR structure determination from spectra through structure, NMR Workbench provides a streamlined process of data extraction and structure determination. This results in increased accuracy and throughput over conventional methods. The products that comprise NMR Workbench are: NMRPipe, NMR•Compass, QUANTA, NMR•Structure Determination, X-PLOR™-DG, NOESYSIM, and DISCON.

IRIX version compatibility:

NMRchitect

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NMRchitect is an integrated suite of programs for processing, displaying, and analyzing NMR data, and for generating and refining molecular structures based on the primary sequence and NMR restraints derived from experiments. Modules include: Felix 1D/2D and Felix ND, Felix Assign, Felix Model, NMR Refine/DG-II, and NMR Refine/Advanced.

IRIX version compatibility:

Networks

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Networks uses a Monte Carlo procedure and bonding algorithm for simulating the typical cross-linking or cure reactions that form gels, elastomers, adhesives and coatings.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Nucleic Acid Database

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The Nucleic Acid Database (NDB) is a relational database designed to facilitate the easy search for crystal structures of nucleic acid structures using any of the stored primary or derived structural features. This search is done by using NDBQUERY, the menu-driven interface program, with the database. This application permits a user to create reports describing any of the stored properties of any structures in the database.

A session with the program generally consists of two separate tasks: in the first part, the user defines structures which are searched for, and then, in the second part, the output options for the selected structures are chosen. A session with the program can be saved in a well-defined command file for subsequent reuse or modification.

IRIX version compatibility:

O

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Electron density map interpretation and macromolecular model building.

IRIX version compatibility:

OHS MSDS Inventory Match Database

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This file of 90,000 independently-researched MSDSs is used to match all entities in a company's chemical inventory system, and is updated quarterly. Unmatched MSDSs can be specially generated in order to provide 100% coverage. This database is used as both a research reference tool, and for regulatory compliance. A right-to-distribute license for individual MSDS is also available to chemical manufacturers.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

OHS MSDS Reference Database

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The OHS MSDS Reference Database has 48,000 MSDS for 16,000 pure substances and 32,000 mixtures. It is updated quarterly and is used by the customers of chemical companies to provide their employees immediate access to safety label information, summary safety sheets, and material safety data sheets for commonly used commercial chemical products. MDL provides consulting and programming services to help with data integration and with writing custom user interfaces.

IRIX version compatibility:

OHS MSDS on Disc

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OHS MSDS on Disc is a database of 18,000 material safety data sheets (MSDS) supplied on CD-ROM for Macs or PCs (standalone or networked) and updated quarterly. Full text of the Code of Federal Regulations is accessible with a hot key, as are summary sheets and label information for the compounds. The PC version allows users to add up to 2000 of their own MSDSs.

IRIX version compatibility:

ORGSYN

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ORGSYN contains proven high-yield synthetic methods and preparations of specific compounds of broad interest to synthetic chemists. Information in the database is abstracted from Organic Syntheses. The database has model synthetic procedures and preparations of common reagents which are independently tested and optimized. Explicit experimental details and hazard warnings are included.

IRIX version compatibility:

Omniview

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Omniview provides 2-D, 3-D and 4-D visualization and anlysis of image data for medical, industrial andgeneral purpose image processing applications with CT, MRI, Ultrasound, microscopy and other image data. Omniview includes 3D Volumetric rendering 3D polygonal surface reconstruction, display and anlysis, image segmentation tools, multiplanar reformatting, 2D and 3D measurement and statistics, convolutional filtering, texture analysis, multimodality data registration, display and anlysis, 2D and 3D trajectory analysis, dynamic (4D0 data processing and display.

IRIX version compatibility: 5.x, 6.x

Chemistry, Biochem, Biotechnology

OpenMoleN

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OpenMoleN is a comprehensive suite of integrated programs for the analysis of crystal structures of small, medium and lager molecules. The system includes all the necessary procedures to transform X-ray diffractometer data from various sources into a complete structure presentation.

A modern Motif™ style GUI and interactive graphics are provided. Many import and export facilities provide smooth access to the included most modern and most powerful procedures available today. Included are SIR, DIRDIF, ORTEP, PLUTO, PLATON, etc. The open nature of the system, provides access to the riches of crystallographic programs available in the open literature also in the future.

IRIX version compatibility:

Orbdraw

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Orbital display program for visualizing results for Mopac calculations. Display selected orbital or electron density.

IRIX version compatibility:

PCMODEL

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PCMODEL is a full-fledged molecular modeling program for designing and studying chemical structures from drugs to dyes. Chemists can input a structure (using the mouse) much as they would sketch the structure on a piece of paper. Among the many features included are a periodic table for choosing different atom types, rotation of the entire structure in 3-D, automatic addition and deletion of hydrogens and lone pairs, structure building in three dimensions, input and output to many types of computational chemistry files, and user-selectable options for pi systems, hydrogen bonding, and transition metal coordination. Data is included for oxygen, nitrogen, phosphorus, sulfur, silicon, radicals, cations, anions, and transition metals.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

PCMODELS

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PCMODELS includes CLOGP and CMR. CLOGP estimates the octanol/water partition coefficient of a compound given its structure as specified by SMILES. CMR calculates molar refractivity for a given structure by an atom-and-bond-based method. PCMODELS is an expert system. Input to PC Models can be by individual SMILES, SMILES files, or by GRINS, a graphical molecular editor. PCMODELS is a unique product that provides accurate prediction of molecular properties.

IRIX version compatibility:

PIPEPHASE™

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The PIPEPHASE™ program rigorously simulates complex piping systems for oil and gas applications. Engineers use PIPEPHASE to monitor and optimize the performance of production systems, gathering networks, transmission lines, and distribution systems, both onshore and offshore. In addition, engineers use PIPEPHASE to design new systems and troubleshoot problems in existing systems. The TACIOTE integration enables engineers to easily evaluate transient flow behaviour for single-link applications using standard PIPEPHASE input and output procedures.

IRIX version compatibility:

PRISM

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PRISM predicts polymer blend miscibility based on the chemical composition of the chains in the blend. Also use PRISM to compute distribution functions, scattering functions, and approximate equations of state for homo- and copolymer melts, blends and solutions.

IRIX version compatibility:

PRO/II®

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The PRO/II® process simulator provides vigorous mass and energy balances for a variety of unit operations enabling the design of a simple or complex process. Your design can contain any number of unit operations, components, streams, or recycles which you can simulate with ease and efficiency. PRO/II increases the understanding of your process, how it works, how it can work better, and when to schedule shutdowns, make process changes, and implement revamps. It allows your design to be optimized, thereby increasing engineering productivity and ultimately producing a more efficient plant, on line sooner, and at lower costs.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Phase Diagram

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Phase Diagram offers researchers the ability to calculate liquid-liquid phase diagrams for polymer solutions and blends with the aid of only limited experimental information.

IRIX version compatibility:

Pilot

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Pilot is the solution oriented self-help tool for Insight II. Pilot provides interactive training sessions, guiding you to practical modeling solutions and showing you how to easily navigate Insight II.

IRIX version compatibility:

Plane Wave

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Plane Wave provides electronic and structural information on solid state systems at the atomic level. It calculates variational self-consistent solutions to density-functional equations for solids that are subject to 3-D periodic boundary conditions, such as insulating and semiconducting systems.

IRIX version compatibility:

PolyDraw

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Modeling the drawing process in polymer fibres and films as a function of draw rate, temperature, entanglement spacing, molecular weight, poly draw is based on published algorithms from Dr. Y. Termonia visualization of the draw process and stree. Straw curves are included.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

PolyNMR

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PolyNMR allows the researcher to construct and analyze a range of homo-and copolymers in order to gain valuable insights into the interpretation of NMR spectra, and evaluate a computer model against real-world observation.

IRIX version compatibility:

Polymerizer

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Polymerizer is an interactive program designed to build 3-D models of polymers with structures that are accurate representations of real molecules, giving you a number of construction and analysis strategies.

IRIX version compatibility:

Profiles-3D

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Profiles-3D tackles the inverse protein folding problem by finding distant relationships between proteins, and testing the validity of models or preliminary structures derived from experimental data or modeling studies.

IRIX version compatibility:

Protein Workbench

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Protein Workbench provides a rich set of tools for protein structure determination, analysis, and refinement. With an integrated interface to the Brookhaven Database, structures can be browsed, extracted, and compared with ease. There is a range of tools for homology modeling. These include secondary structure prediction capabilities, multiple sequence alignment, flexible motif, and pattern matching. Other features new to Protein Workbench involve analysis tools to determine "protein health" of predicted structures.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

QSPR

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QSPR provides very rapid methods for predicting the properties of a wide range of thermoplastic materials by use of group additivity methods.

IRIX version compatibility:

QUANTA

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QUANTA provides a powerful and comprehensive modeling environment for 2-D and 3-D modeling, simulation, and analysis of macromolecules and small organics. Functionality includes structural and similarity analysis tools, cluster analysis, and flexible fitting. Advanced and customizable graphics display assists understanding of even the most complex molecular systems. Simulation and analysis results are presented as clear plots and graphs. With access to all standard formats, and interfaces to CHARMm, X-PLOR, X-PLOR-DG, Modeler, and multiple third party QM/MM codes, QUANTA offers a complete solution for visualization and investigation of molecules in the life sciences.

IRIX version compatibility:

QuanteMM

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QuanteMM combines quantum mechanical and froce field methods, allowing you to use accurate first-principles methods to study cluster models while taking the surrounding environment fully into account. Large and complex systems can be studied with high accuracy.

IRIX version compatibility:

REACCS-JSM

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REACCS-JSM contains new methods for organic synthesis abstracted from the primary chemical and patent literature from 1980 onwards. The database is an electronic version of Derwent's Journal of Synthetic Methods. The focus of the database is novel functional group and ring chemistry, protecting group chemistry, and heterocyclic chemistry. The database is updated with approximately 3,000 new reactions each year.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

RIS

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RIS gives researchers the ability to calculate the conformational properties of polymer chains with ease and speed, while accounting for the detailed chemical structure of the chain.

IRIX version compatibility:

RS3 Discovery™

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408-879-6302 (fax)
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http://www.oxmol.com

RS3 Discovery™ is a petented ORACLE-based information amnagement system which offers fast, cost-effective, relational structure searching. Among the key advantages of RS3 Discovery™ is its optimal architecture for high-throughput screening (HTS) applications which allows the user to integrate chemical structure management, biological data storage-activity analysis.

RS3 Discovery™ is delivered in a client/server architecture, providing higher performance and productivity at lower cost.

In addition to offering RS3 Discovery™, Oxford Molecular Group is the leading worldwide developer of integrated molecular design software, including software for rational drug design (Tsar, Asp, Vamp, Cobra, Anaconda, AMBER) and software for molecular modeling (Personal CAChe, CAChe WorkSystem, CAChe GroupServer and UniChem). POWER AMBER, POWER Vamp and CAChe GroupServer have been optimized for Silicon graphics systems based on the MIPS® R8000 microprocessor.

IRIX version compatibility:

Reaction Patterns

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Reaction Patterns is used for the visualization, interpretation and analysis of chemical reactivity and reactions. It encompasses tools for the integration and development of kinetic models, the analysis of quantum mechanical energy surfaces through vibrational modes, and molecular reaction tendencies.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Ribbons 3.0©

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Ribbons 2.2© is an effective tool for the visual analysis of macromolecules and for presentation graphics. Crystallographers and molecular modelers can view solid shaded molecular structures or animation sequences in real-time. The program features a variety of styles of ribbon diagrams for both proteins and nucleic acids. Atoms, bonds, and surfaces can also be included. The ribbons are colored in segments defined by their individual residues. The colors can be interactively changed to reflect various chemical and structural properties.

IRIX version compatibility:

SAINT

Susan Byram
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Siemens Industrial
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608-276-3041
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SAINT integrates raw data frames or images from Siemens two-dimensional detectors (HI-STAR, SMART CDD, X1000, X100) used to collect single crystal X-ray diffraction data extremely rapidly. It provides exceptionally accurate 3-D integrated intensities of each reflection by using Modified Kabsch profiling and absorption and time decay corrections. Output is provided in SHELXTL™ format for use in small molecule structure determination, and in biological macromolecule least-squares refinement.

IRIX version compatibility:

SCULPT

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SCULPT is recognized as the industry's leading desktop interactive molecular modeler for the chemists and biologist. The innovations in SCULPT bring high-end graphics and molecular simualtions to the researcher's desktop.

SCULPT's three-dimensional graphics are based on a revolutionary paradigm that allows molecular structures to execute more than 100 times faster then comparative products. As a result, molecular mechanics run in real-time allowing users to interactively twist, tug, tether, and overlay molecules on desktop computers. SCULPT effectively combines the power of a computer with the hands-on feel of bending and twisting a physical model.

IRIX version compatibility: 5.2, 5.x, 6.x

SHELXTL™ Crystal Structure Determination Package

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SHELXTL™ is a complete, proprietary suite of programs for the determination of crystal structures from X-ray or neutron data. It includes space group determination, direct methods, Patterson search, rotation/translation search, full matrix least squares refinement, interactive color graphics for structure solution, and output of final plots (including thermal ellipsoids) for publication, 3-D color graphics, preparation of manuscripts and tables for publication, poster preparation, and powder pattern generation. Calculations are valid for all space groups, in all orientations, and there is no effective limit on the number of reflections per structure.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

SYBYL®

Michael Sullivan
.Communications Manager
Tripos, Inc.
1699 South Hanley Road
St. Louis, MO 63144
USA
314-647-1099
314-647-9241 (fax)
http://www.webcom.com/~tripos2/

SYBYL® is comprehensive, integrated, 3-D molecular visualization, design, and analysis software that enhances the research productivity of scientists in chemical, pharmaceutical, biotechnological, and other fields.

Researchers can easily use the innovative Molecular Spreadsheet™ with its "live chemistry" environment to enhance their daily productivity in analytical information processing (SYBYL/NMR TRIAD), chemical information processing (SYBYL/UNITY), and molecular visualization, design, and analysis. Additional SYBYL modules include Advanced Computation, CoMFA/QSAR, Dynamics, and Biopolymer.

IRIX version compatibility:

SYBYL/UNITY

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SYBYL/UNITY is a powerful integrated software package that provides comprehensive searching that is as simple as sketching a query. TRIPOS developed SYBYL/UNITY with the guidance of nine chemical and pharmaceutical companies, key database suppliers, and leading collaborators to ensure accuracy and utility.

Its proven features give scientists:

- The tools for storing and registering 2-D and 3-D chemical structures
- 2-D and 3-D molecular database searching combined with molecular modeling
- Access to databases supplied in the UNITY format.

IRIX version compatibility:

SYNthesis LIBrary™

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Distributed Chemical Graphics/Columbia University
1326 Carol Road
Meadowbrook, PA 19046
USA
212-854-5143
212-678-9039 (fax)
carol@still3.chem.columbia.edu
http://www.columbia.edu/cu/chemistry/mmod/

SYNLIB™ (SYNthesis LIBrary) is a chemical reaction retrieval computer program through which laboratory scientists can rapidly search databases of chemical reaction information. SYNLIB is easy to use and requires minimal computer expertise on the part of the chemist. A facile sketchpad method is used for building chemical structure diagrams. Chemical substructure searches can be combined with constraints (conditions, strategic bond formation or breakage, etc.). SYNLIB is available for the complete family of Silicon Graphics workstations; the SYNLIB Master Library of 86,000 reactions is updated semiannually to all subscribers.

IRIX version compatibility:

Search/Compare

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Search/Compare performs advanced systematic conformational searches, generates and compares volumes, and performs molecular superimposition.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Sketcher

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Sketcher provides an intuitive method for drawing organic molecules in 2-D with automatic 3-D conversion. Building complex ring systems and specifying stereochemistry is made very straightforward.

IRIX version compatibility:

Solids Adjustment

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Solids Adjustment is designed for editing crystal or cluster structures, for developing derivative structures, and for visualizing aspects of these structures, such as symmetry interrelationships, particular coordination environments, or polyhedra.

IRIX version compatibility:

Solids Builder

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Solids Builder constructs crystal structure models, metal or alloy structures, surfaces, interfaces, and structure intergrowths.

IRIX version compatibility:

Solids Docking and Sorption

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Solids Docking and Sorption provides a straightforward way to probe the interactions of single molecules or groups of molecules with a matrix, locate preferred structural arrangements, and predict key thermodynamic data.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Solids Embed

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Solids Embed applies the power of quantum methods to a cluster model, but with the influence of the discrete or periodic environment taken explicitly into account, allowing very large and complex systems to be studied.

IRIX version compatibility:

Solids Simulation

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Solids Simulation performs optimizations of bulk and surface structures, and crystal dynamics simulations of ionic solids.

IRIX version compatibility:

Spartan™ Version 4.0

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Wavefunction's revolutionary molecular modeling software, SPARTAN™ is quite simply a versatile tool used by chemists to do chemistry. SPARTAN ™ 4.0 couples powerful computational methods (molecular mechanics, semi-empirical, ab initio, density functional) with exceptional visualization into one convenient and affordable package. What really strikes people about SPARTAN™ is how easy it is to use. Ideal for both commercial and academic chemists, SPARTAN™ is available on all SGI platforms.

IRIX version compatibility: 5.x, 6.1, 6.2 Certified, 6.3 Certified

Structure Image

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Structure Image is a program for simulating and interpreting electron diffraction patterns and high resolution lattice images, accommodating a range of input parameters.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Structure Refine

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Structure Refine is a program for refining and completing crystal structures based on powder or single crystal diffraction data.

IRIX version compatibility:

Structure Solve

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Structure Solve solves crystal structures based on powder diffraction and potentials data. Rather than trying to solve the crystallographic phase problem directly, Structure Solve attempts circumvention by seeking structure solutions in direct, rather than reciprocal space.

IRIX version compatibility:

Synapse™

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Synapse™ is a knowledge-based molecular design system assisting in the analysis and design of improved chemical products. Using Synapse, scientists and engineers specify constraints on macroscopic physical properties such as vapor pressure, solubility, boiling point, and viscosity. Synapse then generates the molecular structures of candidate chemicals satisfying those constraints. These candidates are assembled atom by atom using either an exhaustive search engine or an interactive, graphical approach. This means that Synapse can suggest new, novel chemical products.

IRIX version compatibility:

Synthia

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Synthia provides rapid estimates of polymer properties using empirical and semi-empirical methods. Its key advantage is the use of connectivity indices allowing predictions for a broad range of polymers.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

THOR™

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THOR is a high-performance, fully distributed chemical information database system for UNIX®. It operates via a client/server mechanism. A single program (THOR Server) is responsible for maintaining databases on a given machine. Programs that access THOR databases can be run on a different machine (for example, a UNIX workstation) from the THOR Server (for example, a VAX™ mainframe), allowing either centralized or distributed database access.

THOR provides fully distributed, platform-independent, chemical database tools. The data access time is constant, regardless of the size of the the database (from 100 to 10 million structures), and the look-up time does not exceed 200 ms.

IRIX version compatibility:

The Available Chemicals Directory (ACD)

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510-483-4738 (fax)
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The Available Chemicals Directory (ACD) provides chemists with an efficient way to find supplier and pricing information for both research-grade and bulk chemicals. ACD includes 171,000 chemical substances representing 418,000 individual chemical products from 218 suppliers, making it the largest structure-searchable database of commercially available chemicals. It contains information on purities, forms and product grades, units, and prices. It also includes the address and phone for suppliers and their distributors. Licensed on an annual right-to-use basis, ACD is available in either MDL format or industry-standard ASCII format.

IRIX version compatibility:

The ChemInform Reaction Library (ChemInform RXL)

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ChemInform RXL is a collection of 480,000 novel syntheses and preparative methods in organic chemistry from 1946 onwards. The reactions are selected to answer a wide range of questions pertinent to combinatorial and discreet synthesis, including the role of steric interactions, substituent effects, structural effects and functional group compatibility.

ChemInform RXL is updated with approximately 50,000 reactions annually, and covers the following areas of chemistry:

1. New reactions, including enzymatic or microbial processes
2. Applications of known methods to the synthesis of new compounds
3. Improved synthetic methods and application of new reagent
4. Syntheses of natural products of general importance
5. Use of novel organo-element compounds and catalysts in synthesis

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

The Reference Library of Synthetic Methodology

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The Reference Library is a collection of 170,000 innovative and significant reactions in the synthetic literature from 1946 to 1990. The focus is on novelty of methodology, and the best reaction has been selected to represent a specific methodology.

IRIX version compatibility:

Tsar™

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Oxford Molecular Group, Inc.
2105 South Bascom Avenue
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Campbell, CA 95008
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408-879-6302 (fax)
800-876-9994 (tollfree)
webmaster@oxmol.com
http://www.oxmol.com

Tsar™ is an integrated system for the identification of Quantitative Structure Activity Relationships (QSAR). The system allows medicinal chemists, statisticians and modellers to read molecular structures and activity data into a spreadsheet. From within the spreadsheet users have access to many of the latest univariate and multivariate statistical techniques, including neural network algorithms for developing QSARs.

Tsar also enables users to calculate molecular and substituent properties to create additional data for QSAR analysis.

IRIX version compatibility:

TurboNMR

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TurboNMR uses ab initio quantum chemistry to predict NMR chemical shifts, enabling the prediction of and comparison to NMR shielding anisotropies from solid-state NMR and magnetic relaxation experiments.

IRIX version compatibility:

Turbomole

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Turbomole is a Hartree-Fock-based program that uses direct/semi-direct approaches for self-consistent field (SCF) and perturbation theory (MP2) calculations for calculation molecular properties, such as electrostatic potentials, molecular moments, and polarizabilities.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

UniChem

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webmaster@oxmol.com
http://www.oxmol.com

UniChem is a complete, easy-to-use molecular modeling package that provides a single, graphical interface to a variety of powerful quantum mechanics programs. Researchers may easily apply advanced theoretical methods to understand complex molecular systems such as drug molecules, proteins, agrochemicals, polymers, catalysts, and advanced materials.

The UniChem system consists of a workstation-based graphical interface and SGI/Cray Research supercomputer-basd ismulation codes, including MND093, DGauss, and CADPAC. UniChem also provides interfaces to a number of third party codes, such as GAUSSIAN™ 94. The graphical interface provides facilities to build molecules, import molecules in variety of formats, and visulaize and analyze results.

UniChem is one of the high-performance computational chemistry software tools available from Oxford Molecular Group.

IRIX version compatibility:

Vamp©

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Vamp© is a sophisticated semi-empirical quantum mechanics package, which is input compatible with MOPAC. Vamp has been optimized to be highly numerically stable and extremely fast. Vamp is the only semi-empirical program with the Natural Atomic Orbital/Point Charge (NAO/PC) model for molecular electrostatic properties. The system can be used to calculate accurate dipole, quadrupole and higher moments and high quality Molecular Electrostatic Potentials (MEPs).

Vamp can be used to:

- Search and optimize transition states.
- Calculate spectroscopic properties, including ESR, NMR, IR and RAMAN frequencies.
- Solvent effects and solvatochromic shifts.
- Simulation of environments.

IRIX version compatibility:

Vibrate

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Owner
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Normal mode vibrational display program for visualizing the output of a Mopac or Gaussian calculation. Animates the display of selected normal mode. Structure can be rotated while viewing the vibration.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

Viscoelasticity

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Viscoelasticity estimates the dynamic mechanical response of dilute polymer solutions using both random coil and RIS models.

IRIX version compatibility:

Wisconsin Sequence Analysis Package™

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The Wisconsin Package™ contains over 120 interrelated software programs for molecular biologists. Developed and distributed by Genetics Computer Group, Inc., the Wisconsin Package enables researchers to analyze DNA and protein sequences by editing, mapping, comparing, and aligning them. Included programs facilitate RNA secondary structure prediction and DNA fragment assembly. In addition, the major genetic databases GenBank™, EMBL, PIR, and SWISS-PROT are distributed with the software and are fully accessible with the database searching and manipulation programs. Documented source code is a standard feature of the Wisconsin Package.

IRIX version compatibility: 5.3, 6.2 Certified

X-PLOR™

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X-PLOR™ is a macromolecular structure determination program that integrates NMR spectral and X-ray diffraction data with molecular mechanics, dynamics, and energy minimization, to aid in the solution of three-dimensional molecular structures. X-PLOR, developed in Axel Brunger's laboratory at Yale University, is considered by many researchers to be the leading software for structure determination and is currently used in over 400 laboratories worldwide.

IRIX version compatibility:

X-PLOR™

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203-432-5067
203-432-6946 (fax)
brunger@laplace.csb.yale.edu

X-PLOR™ is a program for structure determination and refinement of 3-D macromolecular structures based on crystallographic diffraction data or nuclear magnetic resonance data in solution.

IRIX version compatibility:

Chemistry, Biochem, Biotechnology

X-RAY Crystallography Workbench

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X-RAY Crystallography Workbench is an integrated system that combines advanced modeling methods with interactive processing of crystallographic data from multiple sources. Crystallography Workbench is comprised of X-GEN for data processing, QUANTA/X-ray, which provides tools to go from first map to final model, and X-PLOR for structure refinement. Crystallography Workbench enables crystallographers to achieve new levels of productivity in determining structures for related systems such as mutant proteins, bound ligands from crystal soaking or co-crystallization experiments, and macromolecules with covalently bonded cofactors.

IRIX version compatibility:

XMASS™

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http://bruker.com/

Xmass® is a complete package for the processing and analysis of mass spectrometric data designed to work with Bruker FTMS and TOF spectrometers. The Xmass program is a sophisticated processing package that can perform all the basic processing functions: calibration, peak picking, report generation, algebraic functions, and text labelling. In addition, more advanced functions such as linear prediction and Fourier noise filtering are standard in Xmass. A mass analysis package for determining molecular formulae and a biological analysis package for peptides and proteins are also available.

IRIX version compatibility: 5.3, 5.x, 6.x

XVision

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info@sco.com
http://www.sco.com

XVision--Connect Windows PCs to UNIX-based applications with XVision - the world's first smart PC X server. XVision extends the functionality of Windows PCs by providing display management capabilities for UNIX-based applications while adhering to the X Windows standard.

- Automatically configures itself to each unique PC configuration and network for maximum performance.
- Provides X Windows, Microsoft Windows and terminal emulation -- all in one package.
- Supports 18 major TCP/IP protocols as well as IPX/SPX. XVision is available for Windows, Windows NT and remote users.

IRIX version compatibility:

XWIN-NMR™

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http://bruker.com/

XWIN-NMR™ is a software package which processes and displays data acquired on Nuclear Magnetic Resonance Spectrometers manufactured by Bruker and other vendors. It is the same software delivered with Bruker spectrometers to acquire and process the data, thus providing a seamless transition between data acquisition and off-line processing. Designed under the Motif and X-11 windowing systems XWIN-NMR makes extensive use of menus, buttons, and gadgets to provide a user-friendly, yet powerful user interface which allows complete control of display and plot layout. XWIN-NMR can process, display, and plot 1-D, 2-D, and 3-D NMR and MRI data.

IRIX version compatibility: 5.2, 5.3

Chemistry, Biochem, Biotechnology

Xsight

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Xsight integrates all of the major computational techniques for macromolecular crystallography. You can analyze and interpret X-ray data, build models of protein structures and relate them to electron density, refine structure against X-ray data, analyze structures for symmetry, and visualize and validate strategies.

IRIX version compatibility:

ZINDO

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ZINDO is a semi-empirical molecular-orbital program for studying the spectroscopic properties of molecules, including transition-metal complexes, applicable to a wide range of molecules, including organic, inorganic, polymer and organometallic compounds.

IRIX version compatibility:

bioteX

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bioteX is a suite of programs used for the collection, data reduction and interpretation of imaging plate detector data. It is used by both protein and small molecule crystallographers, chemists and biochemists. Cell indexing, parameter refinement, reflection integration and processing, graphical display and results presentation are handled in an easy-to-use Motif™ interface. The novice may easily collect and process data effectively, while the experienced user has all the flexibility required to complete difficult tasks.

IRIX version compatibility:

d* TREK

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TREK is a system of programs for collecting and processing images from a single crystal diffraction experiment for any and all crystals, goniometers, detectors and sources. d* TREK is modular, device-independent, customizable and adoptable to any experimental hardware.

IRIX version compatibility: 5.3, 6.2, 6.x, Pre 5.x

Chemistry, Biochem, Biotechnology

teXsan

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teXsan is a software package to be used for the analysis of small molecule, single crystal, X-ray diffraction data. This package is mainly used by crystallographers and chemists who are involved in the elucidation of molecular structure from experimental X-ray data. Data reduction, structure solution, model refinement, graphical display, and results presentation are all handled in an easy-to-use Motif™ menu environment.

IRIX version compatibility: Pre 5.x