PRECLAV Crack Registration Code Free Download [Mac/Win] [Latest]

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PRECLAV Crack

PRECLAV is a useful software for QSPR / QSAR calculations, available from Tarko Laszlo, Center of Organic Chemistry (CCO) - Bucharest, Romanian Academy. Here are some key features of "PRECLAV": · accepts as input MOPAC93 output files · analyzes molecules with maximum 99 atoms (H, C, N, O, S, P, F, Cl, Br, I, B, Si or As) · analyzes molecules with maximum 60 heavy atoms (C, N, O, S, P, F, Cl, Br, I, B, Si or As) · analyzes maximum 500 molecules (learning set + testing set) · calculates over 1100 (global, local and grid / field) descriptors · calculates the aromaticity of chemical bonds by the TPA algorithm · computes the optimum value for probe atom distances · selects descriptors using r2 and Class functions · computes weighting factors by the Ordinary Least Squares Method · minimum number of predictors in final QSPR /QSAR: 2 · maximum number of predictors in final QSPR /QSAR: 10 · adaptable to work with user databases Limitations: · may analyse only 50 molecule databases · none time limitations What's New in This Release: · accepts as input MOPAC93 output files · new molecular descriptors · work very easy with user database Download PRECLAV now! Contact Tarko Laszlo TBC Romania NOTE: There are no Internet / Intranet links on the ODOBO server. If you want to connect from outside of Romania it is possible to do so from three locations on your own private Internet connection. In fact, the Bulgarian company SoSoft.bg (with approval from ODOBO) offers this service and it is completely free of charge. According to the 2003 census in Bulgaria, there are approximately 35 million internet users of the country. Public Internet access points (cafes, bars, government buildings) are almost available to everyone. Be sure to take advantage of it. Language Internet / Intranet and email TEL: +359 2 232 42 24 E-MAIL: Notice: The Bulgarian software developer team is not responsible for any problems you may encounter from connecting from outside of Romania, especially

PRECLAV Crack+ With Product Key PC/Windows [Updated-2022]

PRECLAV is a QSPR software for the assessment of chemical descriptors and their predictive properties. The practical applicability of PRECLAV is based on two main features: 1. PRECLAV calculates a huge number of descriptors (global, local and grid/field) and is very easy to handle. 2. It provides the user with the advantages of QSPR methods which are calculating optimized molecular descriptors (like QSAR models) and which are sampling and handling the decision boundaries of the QSPR models. Because of the enormous computation load, PRECLAV uses a modified version of the widely-known MOPAC (acronym for MOPAC by M.THIERRY, PARAMAC, MP2, NMR, QM/MM, etc.) software for most calculations. MOPAC is distributed by the Center of Organic Chemistry (CCO) of the Romanian Academy. MOVAL 3.0 for Windows MOVAL 3.0 is a three-dimensional molecular visualization software. MOVAL has improved and upgraded features that make it a more powerful

tool to visualize the results of molecular modeling calculations. These features include: * visualization of 3D spatial distribution of physicochemical descriptors; * 3D molecular surface; * 3D molecular electrostatic potential; * interactive highlighting; * description of atom-properties in a molecule; * calculation of molecular descriptors; * quantitative and qualitative correlations between the molecular properties and the computed descriptors; * automatic molecular alignment of the database structures by superposition of the 3D structures. MOVAL Description: MOVAL is a three-dimensional molecular visualization software. MOVAL has improved and upgraded features that make it a more powerful tool to visualize the results of molecular modeling calculations. These features include: * visualization of 3D spatial distribution of physicochemical descriptors; * 3D molecular surface; * 3D molecular electrostatic potential; * interactive highlighting; * description of atom-properties in a molecule; * calculation of molecular descriptors; * quantitative and qualitative correlations between the molecular properties and the computed descriptors; * automatic molecular alignment of the database structures by superposition of the 3D structures. PLATON v3.0 for Windows We are pleased to announce the availability of PLATON v3.0 (part of the Molecular Design product family), the version that brings state- 3a67dffeec

PRECLAV Crack Full Product Key

PRECLAV is a package of software products for: - QSAR/QSPR analysis by implementing different analytical methods - Enumeration of probes in chemical structures - Development and evaluation of multivariate models PRECLAV can provide a powerful knowledge base, to reduce the need of manual calculations or screen large libraries of compounds. It can help in finding trends or relations in a mass of chemical structures, especially to predict the biological activity of a compound (QSAR). A user is expected to provide a small number of descriptors with relevant information. More experienced users can develop their own methods, select molecular descriptors and their weights from a database. COMPUTER GENERATED DESCRIPTORS (QSPR): PRECLAV has built-in software for: - Generating of descriptors, both global and local - Generating of optimal probe atom distances - Weighting factors for descriptors, if needed - Determining weighting factors for molecules, if needed PRECLAV descriptors can be: - Generation of absorption, fluorescence, electronic circular dichroism, fluorescence anisotropy, electronic circular polarization, fluorescence quantum yield and lifetime, electronic line width, NMR chemical shifts and spin-spin coupling constants - Generation of topological connectivity indices (TCIs), graph invariants (GI) and their sub-classes - Generation of charge, ionization and electron affinity indices - Generation of radiochemical descriptors - Generation of quantum-chemical descriptors such as molecular hardness, global softness, molecular electrophilicity index, global electrophilicity index, atomic hardness, atomic softness and their sub-classes - Generation of molecular descriptors, for example molecular branching index, molecular surface index, PSA, PLS, TPSA, GATS and GATS2 - Calculation of molecular field analysis descriptors and their sub-classes - Calculation of values of molecular field theory descriptors and their sub-classes - Calculation of total field index - Calculation of molecular weight - Calculation of pharmacophore fingerprints - Calculation of 2D-QSAR descriptors - Calculation of molecular descriptors based on MACCS keys - Calculation of one and two dimensional descriptors - Calculation of ICF and IEF - Calculation of molar refractivity, polarizability and electronegativity - Calculation of QS

What's New in the PRECLAV?

PRECLAV aims to develop the activities of local (or grid) chemical descriptors. For this purpose, a wide range of development and evaluation of different molecular descriptors and QSPR/QSAR models was performed. Based on the experience gained, PRECLAV has already developed the possibility to calculate the chemical reactivity of organic molecules in terms of: - Half-life (hour) (t1/2) - Covalent bond dissociation energy (BDE) (Kcal/mol) - Electronegativity (χ) (C-F) - Ionization potential (I) (electronvolts) - Electrophilicity index (ω) (dimensionless) - Electronegativity of nucleophilicity (ENA) (dimensionless) The user interface of PRECLAV is a software that performs all operations for the calculation of half-life (t1/2) and covalent bond dissociation energy (BDE). Additionally, the software contains a broad range of options for calculation of other descriptors, and the QSPR/QSAR models of the training set. From the very outset it should be noted that the results that appear in this paper are from models whose construction, training, test and selection methods have been described in detail in a series of works. The models are based on a training set (first generation) composed of 1065 organic molecules and finally tested in a cross-validation set of 114 organic molecules. The calculation of half-life (or t1/2) using PRECLAV is dependent on the energy required to overcome the chemical reaction. This energy depends on the chemical reactivity (chemical reactivity index or chemical index). The chemical reactivity index (or chemical index) is based on the following descriptors: ionization potential (I), electronegativity (χ), electrophilicity (ω) and the TPA aromaticity (tpa). TPA is a simple and reliable measure of the aromaticity of a system, a property that can be obtained from the calculated TPA values. Additionally, the covalent bond dissociation energy and chemical reactivity index (chemical index) can be calculated using a final universal equation. The descriptor that is most often used to calculate the chemical reactivity index (or chemical index) is

the ionization potential (I). Indeed, there is a linear relationship between the chemical reactivity index and the ionization potential (

System Requirements:

Recommended: Game Version: 1.0.7 Processor: Intel Core 2 Duo or AMD Athlon 64 Memory: 3 GB RAM Graphics: GeForce GTX 400 Series or Radeon HD 2600 Series or Intel HD Graphics 4000 DirectX: Version 9.0 Network: Broadband Internet connection Hard Drive: 15 GB available space Sound Card: DirectX 9.0 compliant Additional Notes: DVD playback support not required STEAM DRM: YesA few weeks back, a picture appeared on Google+, showing