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Roberto Todeschini and Viviana Consonni Molecular Descriptors for Chemoinformatics Volume I: Alphabetical Listing Second, Revised and Enlarged Edition

Course programme - chemoinformatics
The course objectives are to introduce participants to different chemoinformatics chemoinformatics in drug research: Molecular Molecular descriptors

Can we learn to distinguish between drug-like
Jul 23, 1998 Chem. , 1998, 41 (18), pp 3314 3324 In a computer experiment on generating a drug-like library of size 100 from a set of Journal of Medicinal Chemistry 2014 57 (14), 5845-5859 Roberto Todeschini , Viviana Consonni , Victor E. Kuz'min , Richard Molecular Pharmaceutics 2012 9 (10), 2875-2886.

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2011 Chemoinformatics as a Theoretical Chemistry Discipline; Varnek 2011 Method of Continuous Molecular Fields in the One-Class Classification of Rate Constants of S(N)2 Reactions by the Multicomponent QSPR Method Bioorganic and Medicinal Chemistry, Pergamon .. 35- 41 DOI.

Half.com: molecular descriptors for
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Molecular descriptors for chemoinformatics:
Editor(s): Roberto Todeschini, Viviana Consonni. Published Online: 12 FEB 2010. Print ISBN: 9783527318520. Online ISBN: 9783527628766. DOI: 10.1002/9783527628766

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Methods and Principles in Medicinal Chemistry Vol. 42. Todeschini, Roberto / Consonni, Viviana. Molecular Descriptors for. Chemoinformatics. Volume I: Alphabetical Listing /. Volume II: Appendices, References. 2009. ISBN: 978-3- 527-31852-0. Vol. 41 . 2. Preparing and Filtering Compound Databases for Virtual.

Chemoinformatics a new name for an old problem?
Chemoinformatics a new name for an include new molecular descriptors and in chemoinformatics include new molecular descriptors and

Structure/response correlations and
Apr 20, 2002 Application of the Novel 3D Molecular Descriptors to QSAR/QSPR Studies. Viviana Consonni , Roberto Todeschini ,* Manuela Pavan , and Paola aim of matching 3D-molecular geometry, atom relatedness, and chemical information. Comments on the Definition of the Q Parameter for QSAR Validation.

Molecular descriptors | roberto todeschini - academia.edu
The volume aims to allow the reader to nd data and descriptors and 11 2 The Use of Quantum Mechanics Derived Descriptors in Computational 29 Viviana Consonni and Roberto Todeschini 3.1. .. Chemoinformatics-Based Categories . . 322 12 Chemometric Methods and Theoretical Molecular Descriptors in

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An introduction to chemoinformatics | andrew r
An Introduction to Chemoinformatics. Authors: Leach, Andrew R., the calculation of molecular descriptors and the construction of mathematical models.

- 2015.4
204, 9783527318520, Molecular Descriptors For Chemoinformatics - Two Volume Set, 2009, 2, CNY, 3,384.00, Roberto Todeschini and Viviana Consonni and

Pharmacological classification and activity
May 29, 2012 2.4. Molecular Descriptors. Todeschini R., Consonni V. Molecular Descriptors for Chemoinformatics: Volume I: Alphabetical Listing/Volume II:

Three-dimensional qsar using the k-nearest
Jul 23, 2005 developed based on principles of the k-nearest neighbor method combined with Thus, kNN-MFA method represents a good alternative to CoMFA-like methods. Roberto Todeschini , Viviana Consonni , Victor E. Kuz'min , Richard Cramer Journal of Medicinal Chemistry 2014 57 (12), 4977-5010.

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Oct 9, 2014 Dragon molecular descriptors were used for the QSAR model classification method was calibrated on 25 molecular descriptors and gave Davide Ballabio 3, Viviana Consonni 3 and Roberto Todeschini 3 . the principle of keeping 20% of chemicals from each class as a test set. .. 1998, 41, 195 207.

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3 DISCUSSION. ChemoPy contains a selection of molecular descriptors to analyse, classify and compare complex molecular network. They facilitate to

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