Complete hydrogen bond description for QSAR, Drug Design and ADMET on your desk by means of the program HYBOT-PLUS/HYBOT 3D

Dear colleagues,

Twenty years researches in the field of intermolecular interactions gave us the possibility to create the commercial available program package *HYBOT-PLUS/HYBOT 3D* which has principal advantages compare with previous versions.

HYBOT-PLUS/HYBOT 3D program package contains the largest in the word the data bases of thermodynamic parameters of H-binding; the data bases of enthalpy, free energy and overall H-bond factors; the program for H-bond factor prediction for any organic compound.

HYBOT calculates: nineteen 2-D molecular descriptors connected with structure, electrostatic and hydrogen bond interactions; ten new original 3-D H-bonding molecular descriptors; volume-related, electrostatic and hydrogen binding parameters for each atom in a molecule; H-bond enthalpy of complexation between any organic molecules.

Platforms: Windows-95/98/NT/2000; UNIX/LINUX; command line version which can be compiled under any computer platforms. Client-server application is under developing.

Application: The calculation of all descriptors online for 100 first molecules is free (*http://www.ibmh.msk.su/molpro/webhybot*). Further use of the program package is realized in framework of license on short-term, long-term or permanent application. ***The essential academic discount !***

The detailed information about *HYBOT* and other our programs, its application and references *see* *http://www.ibmh.msk.su/molpro/*

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We are ready to discuss any kind of scientific or business cooperation!

Prof. Dr. Oleg Raevsky