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MOLECULAR DESCRIPTORS FAMILY ON CHROMATOGRAPHY

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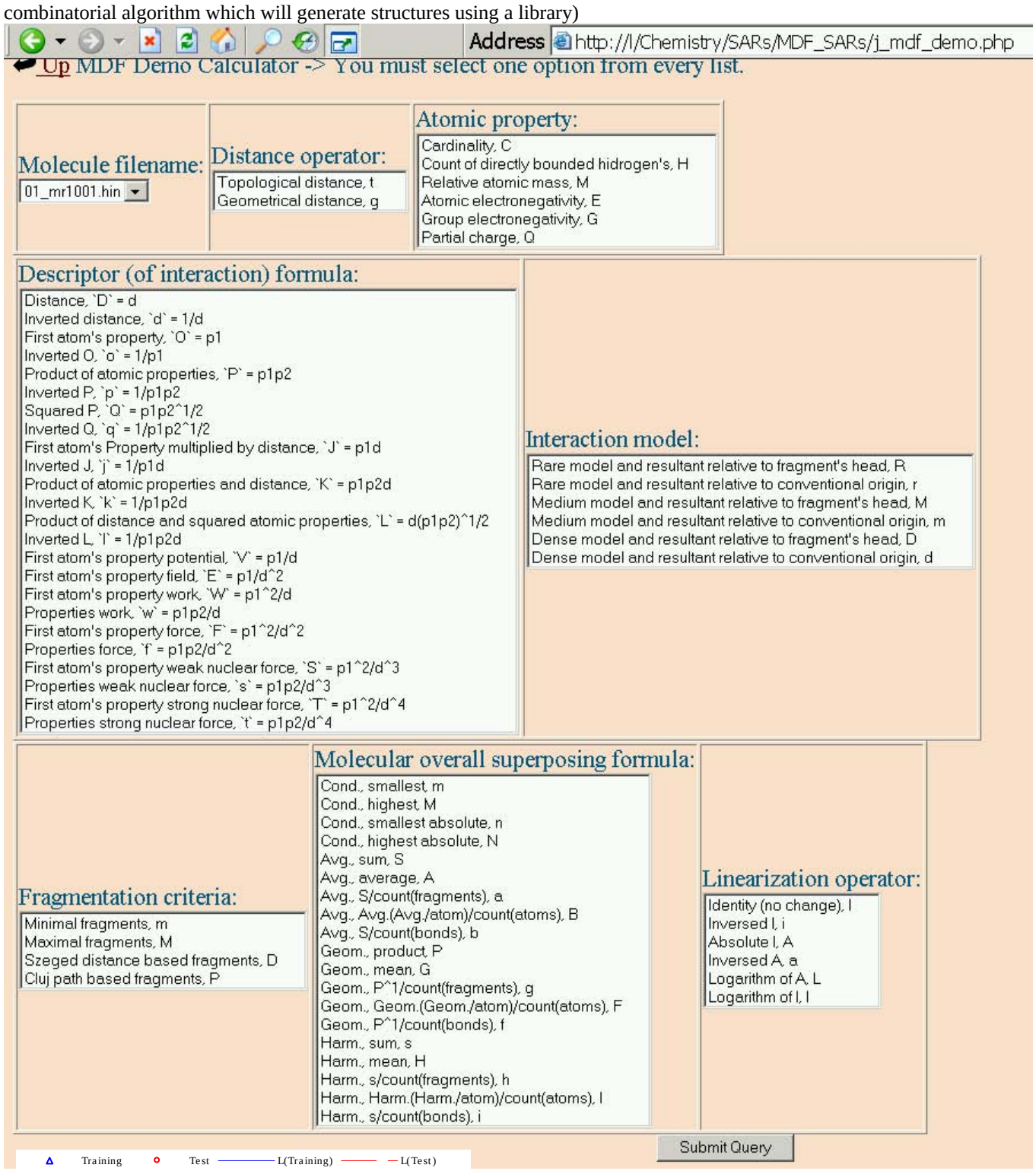
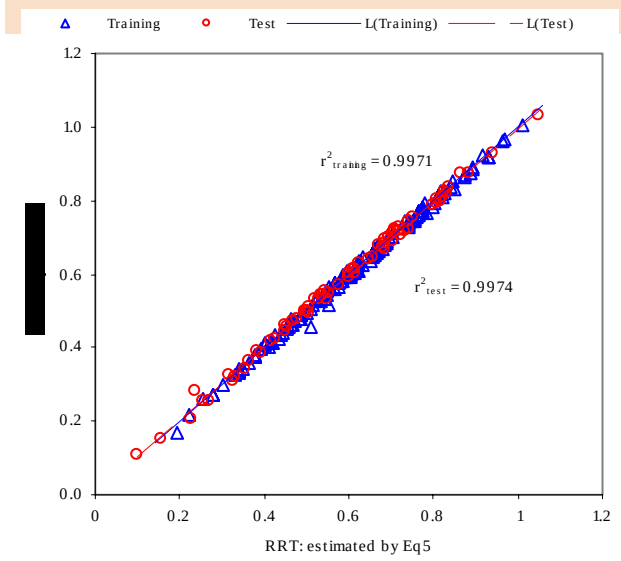
Molecular Descriptors Family is a family of structure-based molecular descriptors. It implies a molecular design on molecules which are subject of investigation. Are applied on molecules sets on which a given property are known. It provides a structure-property model for given set of molecules. The model contains a number of seven parameters for every involved descriptor. These parameters allow: ► Structure-property analysis of the given property; ►Validation of experimental measurements in relationship with compounds properties; ► Prediction of property of interest for not included compounds which are structural and/or property related with given set; ► Further developments will allow virtual synthesis of new compounds (by including a combinatorial algorithm which will generate structures using a library)





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Results:

Following results were obtained using MDF Methodology on estimation of chromatographic parameters:

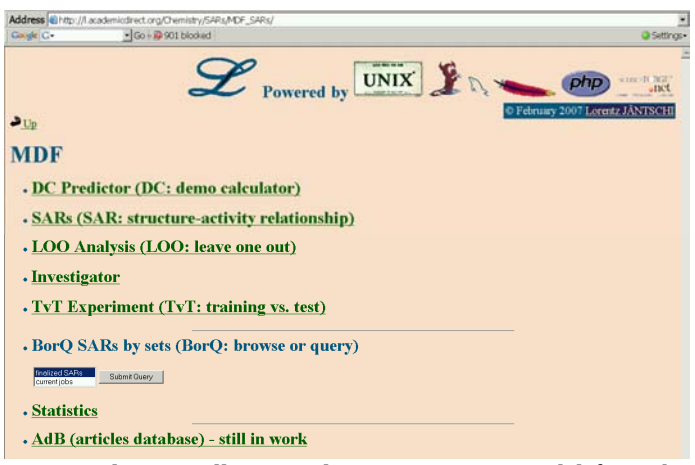
Set	Compounds	Number	Property	Equation	r^2	Ref
IChr_10	organophosphorus herbicides	10	retention index	$I_{CHR} = -3.4 + 0.32 \cdot IBPdqHg$	0.94	[7]
PCB_rrf	polychlorinated biphenyls	209	relative response factor	$R_{RF} = 6\text{-}417 \cdot imMrFHt + 2.3 \cdot iHDdFHg + 1.83 \cdot iMMMjQg - 2.510^{-3} \cdot iAMrVQg$	0.74	[6]
PCB_rrt	polychlorinated biphenyls	209	relative retention time	$R_{Rt} = -0.17 + 0.08745 \cdot iIDRwHg$	0.98	[8]

Following results were obtained using MDF Methodology on estimation of chromatographic-like parameters:

Set	Compounds	Number	Property	Equation	r^2	Ref
MR_10	cyclic organophosphorus compounds	10	molar refraction	$MR = 17 + 28 \cdot lGDmSMt - 84 \cdot lAmrfEt$	0.94	[9]
PCB_lkow	polychlorinated biphenyls	209	Octanol-Water Partition Coefficient	$\log K_{ow} = 3 - 0.4 \cdot IIDDKGg + 0.04 \cdot IHDRKEg + 0.07 \cdot aHMmjQt - 37.5 \cdot aSMMjQg$	0.74	[4]
PCB_rrt	para-substituted phenols	30	idem	$\log K_{ow} = 1 + 3.4 \cdot isDDkGg - 0.4 \cdot IMmrKQg$	0.95	[2]

MDF Methodology: ► Constructing of 3D model of the given set of molecules (structure are known); we use HyperChem software to do this. ► Optimizing of the molecular geometry if is necessary (for a "in vivo" model we can use a periodic box of water molecules surrounding the molecule subject to geometry optimization). ► Generating of Molecular Descriptors Family (a family with 131328 relatives). ► Biasing of MDF and simple linear regression with measured property (this task apply 6 types of linearization operators on MDF members rising up to 787968 their number and in same time reduces it's number through bias procedure to a number of about 100000. ► If simple linear regression between measured property and MDF members does not produce a satisfactory result, then procedure it continue with multiple linear regression (with two, three, or more MDF members as independent variables)

MDF Assessment: ► A series of assessing procedures were developed and are available (online). ► Leave-One-Out Analysis let each compound out of the set and reconstruct MDF-SPR model without it, and using this new model their property are predicted; using all predicted properties a new coefficient, called leave-one-out squared correlation coefficient. ► Training vs. Test experiment split the data set in two sets, training one and test one; use the training set for obtaining MDF-SPR model and apply the model to the test set (size of the training and test set can be choused from the interface; compounds are randomly selected into the training and test sets). ► Correlated correlations analysis apply the Steiger's Z test between two or mode models in order to see if the models express same thing (being significantly correlated or not).



MDF Features: ► Our investigated sets are available online. ► Our MDF-SPR models are available online. ► MDF Investigator application allow to select a MDF-SPR model from the database, to submit a compound (a HyperChem file containing compound 3D structure) and to predict the property based on the selected model.