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### TRAINING AND EDUCATION

- 2002 - 2004 Post-Doctoral Research Associate, (**RWJMS-UMDNJ**),  
Piscataway, NJ
- 2001 Post-Doctoral Research Associate, Department of Chemistry,  
University of Missouri St.Louis (**UMSL**), St.Louis, Missouri, USA
- 1998 Ph.D., Bioorganic Chemistry, Chemistry of Physiologically Active  
Compounds, Institute of Bioorganic & Petrochemistry, Ukrainian  
National Academy of Sciences, Kiev, Ukraine  
Thesis: "Computational modeling, synthesis and biological tests of  
peptide immunomodulators"
- 1993 M.S. in Chemistry, Department of Chemistry of Natural  
Compounds,  
Kiev State University, Kiev, Ukraine

### RECENT AND CURRENT SCIENTIFIC PROJECTS

- Development of a new computational tools for a rational drug design and QSAR (shape signatures, neural networks and pattern recognition technique)
- Rational design for biomaterials and biodegradable polymers (QSAR, molecular dynamics, *de novo* design)
- Pregnane X receptor (PXR): modeling and design of species-specific ligands (homology modeling, molecular dynamics, pharmacophore search, high-throughput screening, docking, QSAR)
- Cannabinoid receptor inhibitors: elucidation of the mechanism of action (QSAR CoMFA/COMSIA, pharmacophore modeling, conformational search)
- Alzheimer's and Parkinson's diseases: modeling of amyloid fibril formation and its spatial organization (molecular dynamics)
- Na, K-ATPase modeling, and the design of novel inhibitors - congestive heart failure (homology and pharmacophore modeling, conformational search, *de novo* drug design, docking, 3-D database search)

### TEACHING EXPERIENCE

- 2002-present Lecturer/Instructor, Structural Bioinformatics I, Structural Bioinformatics II and Fundamentals of Bioinformatics Informatics Institute, UMDNJ, Piscataway/Newark, NJ

## HONORS

2003	Research Achievement Award, UMDNJ, NJ
2002	Research Achievement Award, UMDNJ, NJ
2002-2003	Young Investigator Award, UMDNJ, NJ
1999-2000 Ukraine	Stipendiary Award of the Ukrainian National Academy of Sci., Ukraine
1998-1999 Ukraine	Stipendiary Award of the Ukrainian National Academy of Sci., Ukraine

## MEMBERSHIP

- American Chemical Society (ACS)
- New York Academy of Science (NYAS)

## PUBLICATIONS

- **BOOK CHAPTERS**

CHAPTER 37. Densities of amorphous and crystalline polymers

**V. Kholodovych and W.J. Welsh**

"Physical Properties of Polymers Handbook ", 2nd Edition, ed. by J. E. Mark,  
Springer Science & Business Media, LLC: New York, 2007.

CHAPTER 54. Thermal-oxidative stability and degradation of polymers

**V. Kholodovych and W.J. Welsh**

"Physical Properties of Polymers Handbook ", 2nd Edition, ed. by J. E. Mark,  
Springer Science & Business Media, LLC: New York, 2007.

- **PEER-REVIEWED ARTICLES**

**V. Kholodovych, A.V. Gubskaya, M. Bohrer, N. Harris, D. Knight, J. Kohn,  
W.J. Welsh**

Prediction of biological response for large combinatorial libraries of  
biodegradable polymers: Polymethacrylates as a test case // *Polymer* 2008,  
49(10), 2435-2439.

**S. Ekins, V. Kholodovych, N. Ai, M. Sinz, J. Gal, L. Gera, W.J. Welsh, K.  
Bachmann, S. Mani** Computational discovery of novel low micromolar human  
pregnane X receptor antagonists // *Molecular Pharmacology* 2008, DOI:  
10.1124/mol.108.049437.

**D.S. Chekmarev, V. Kholodovych, K.V. Balakin, Y. Ivanenkov, S. Ekins, W.J.  
Welsh** Shape signatures: New descriptors for predicting cardiotoxicity in silico //  
*Chemical Research in Toxicology* 2008, 21(6), 304-1314.

**V.V. Kovalishyn, V. Kholodovych, I.V. Tetko, W.J. Welsh** Volume learning algorithm significantly improved PLS model for predicting the estrogenic activity of xenoestrogens // *Journal of Molecular Graphics and Modelling* 2007, 26, 591–594.

**A.V. Gubskaya, V. Kholodovych, D. Knight, J. Kohn, W.J. Welsh** Prediction of fibrinogen adsorption for biodegradable polymers: Integration of molecular dynamics and surrogate modeling // *Polymer* 2007, 48, 5788-5801.

**S. Ekins, C. Chang, S. Mani, M.D. Krasowski, E.J. Reschly, M. Iyer, V. Kholodovych, N. Ai, W.J. Welsh, M. Sinz, P.W. Swaan, R. Patel, K. Bachmann** Human pregnane X receptor antagonists and agonists define molecular requirements for different binding sites // *Molecular Pharmacology* 2007, 72, 592–603.

**J.R. Smith, V. Kholodovych, D. Knight, W.J. Welsh, J. Kohn** QSAR models for the analysis of bioresponse data from combinatorial libraries of biomaterials // *QSAR & Combinatorial Science* 2005, 24(1), 99-113.

**J.R. Smith, V. Kholodovych, D. Knight, J. Kohn, W.J. Welsh** Predicting fibrinogen adsorption to polymeric surfaces in silico: a combined method approach // *Polymer* 2005, 46(12), 4296-4306.

**Y. Peng, S.M. Keenan, Q. Zhang, V. Kholodovych, W.J. Welsh** 3D-QSAR comparative molecular field analysis on opioid receptor antagonists: Pooling data from different studies // *Journal of Medicinal Chemistry* 2005, 48(5), 1620-1629.

**V. Kholodovych, J.R. Smith, D. Knight, S. Abramson, J. Kohn, W.J. Welsh** Accurate predictions of cellular response using QSPR: A feasibility test of rational design of polymeric biomaterials // *Polymer (Feature article)* 2004, 45(22), 7367-7379.

**P.V. Paranjpe, Y. Chen, V. Kholodovych, W. Welsh, S. Stein, P.J. Sinko** Tumor-targeted bioconjugate based delivery of camptothecin: design, synthesis and in vitro evaluation // *Journal of Controlled Release* 2004, 100(2), 275-292.

**M.M. Tabb, V. Kholodovych, F. Grün, C. Zhou, W.J. Welsh, B. Blumberg** Polychlorinated biphenyls inhibit the human xenobiotic response mediated by the steroid and xenobiotic receptor (SXR) // *Environmental Health Perspectives* 2004, 112(2), 163-169.

**J.R. Smith, D. Knight, J. Kohn, K. Rasheed, N. Weber, V. Kholodovych, W.J. Welsh** Using surrogate modeling in the prediction of fibrinogen adsorption onto polymer surfaces // *Journal of Chemical Information and Computer Sciences* 2004, 44, 1088-1097.

**W.J. Welsh, R. Zauhar, V. Kholodovych, K. Nagarajan, N. Ai** Predicting human and environmental toxicity of chemicals based on their shape and

electrostatic features // *Chemical Research in Toxicology* 2003, 16(12), 1666-?????.

**V. Kholodovych, V. Kovalishyn, I.V. Tetko, W.J. Welsh** A new approach for 3D-QSAR studies based on the volume learning artificial neural network, Book of Proceedings of the Artificial Neural Networks in Engineering Conference (ANNIE 2002), C.H. Dagli, A.L. Buczak, J. Ghosh, M.J. Embrechts, O. Ersoy, S.W. Kercel (Eds), ASME PRESS, New York, NY 2002, vol. 12, 2002, 459-464.

**V.K. Kibirev, V. Kholodovych, A.A. Gershkovich** Peptidomimetics as low molecular weight inhibitors of thrombin // *Current R&D Highlights* 2001, 23(3), 4-16.

**V. Kholodovych, S.E. Mogilevich, A.I. Luik** Computer-aided prediction of antitumor activity of cisplatin derivatives using methods of artificial intelligence// *Experimental Oncology* 2000, 22 suppl. 2, 11-15.

**A.I. Luik, V.V. Prokopenko, V.Yu. Tanchuk, V. Kholodovych, I.V. Semeniuta** Common properties of pharmacological agonists and antagonists of surface membrane receptors // *Biomedical Chemistry (Vopr. Med. Khim.)* 1999, 45(6), 514-24.

**V.V. Kovalishyn, I.V. Tetko, A.I. Luik, V.V. Kholodovych, A.E.P. Villa, D.J. Livingstone** Neural network studies 3. Variable selection in the cascade-correlation learning architectures // *Journal of Chemical Information and Computer Sciences* 1998, 38(4), 651-659.

**A.I. Luik, V.V. Prokopenko, V.Yu. Tanchuk, V.V. Kholodovych** Common properties of physiologically active substances influencing external cellular membrane receptors // *Drugs (Liky)* 1998, 6, 62-67.

**V.V. Kholodovych, D.I. Kara, A.A. Gershkovich, L.V. Karabut, V.K. Kibirev, I.V. Klimenko, A.I. Korneliuk** Application of the new donor-acceptor pairs for intramolecular fluorescence energy transfer substrates (IFETS) for thrombin and trypsin. // *Russian J. Bioorganic Chem.* 1997, 24 (3), 179-185.

**V.V. Kholodovych** Use of the computer simulation method of complementary amino acids base on a genetic code algorithm for the search for new peptide compounds belonging to tuftsin-like activity // *Ukr. Biokhim. Zh.* 1997, 69 (5-6), 203-8.

**V.V. Kholodovych, V.Yu. Tanchuk, V.V. Kovalishin, I.V. Tetko, S.A. Poyarkova, L.A. Metelitsa, A.I. Luik** Application of topological indexes for immunomodulating activity prediction of new peptide compounds // *Theor. Experimental Chem.* 1997, 33(2), 100-104.

**A.A. Gershkovich, V.V. Kholodovych** Fluorogenic substrates for proteases based on intramolecular fluorescence energy transfer (IFETS) // *Journal of Biochemical and Biophysical Methods* 1996, 33 (3), 135-162.

**A.A. Gershkovich, V.V. Kholodovych, D.I. Kara, V.K. Kibirev** The design of new fluorogenic substrates for thrombin // *Thrombosis and Haemostasis* 1995, 73(6), 926-?????.

**A.I. Brusilovets, E.B. Rusanov, V.V. Kholodovych** Reactions of titanium alkoxides with N,N,N',N''-tetrakis(trimethylsilyl)amide of diimidophosphonic acid // *Journal of General Chemistry (Zhurnal Obshchei Khimii)* 1989, 59(9), 2149-2150.

- **PUBLISHED ABSTARCTS**

**L.J. Pothier, V. Kholodovych, W.J. Welsh, S.M. Decatur** The effects of amino acid substitutions on ABeta16-22 dimer stability as studied by molecular dynamics simulations and infrared spectroscopy // *Biophysical Journal* 2007, 560.

**Y. Peng, S.M. Keenan, Q. Zhang, V. Kholodovych, W.J. Welsh** 3D-QSAR comparative molecular field analysis on opioid receptor antagonists: Pooling data from different studies // *Abstracts of Papers of the American Chemical Society* 2004, 228, U526.

**V. Kholodovych, M.M. Tabb, N.C.Y. Wang, C.C. Zhou, F. Grun, B. Blumberg, W.J. Welsh** Regulation of the clearance mechanism of environmental pollutants and xenobiotic chemicals by the pregnane X receptor (PXR): Structural requirements and species to species extrapolation // *Abstracts of Papers of the American Chemical Society* 2004, 227, U1058

**W.J. Welsh, R. Zauhar, V. Kholodovych, K. Nagarajan, N. Ai** Predicting human and environmental toxicity of chemicals based on their shape and electrostatic features // *Chemical Research in Toxicology* 2003, 16(12), 1666.

**W.J. Welsh, R. Zauhar, V. Kholodovych, K. Nagarajan, N. Ai** Predicting human and environmental toxicity of chemicals based on their shape and electrostatic features // *Abstracts of Papers of the American Chemical Society* 2003, 226, U320

**S.M. Keenan, R.K. Delisle, W.J. Welsh, V. Kholodovych, S. Paula, W.J. Ball** Method for the discovery of novel Na, K-ATPase inhibitors for the therapeutic treatment of cardiovascular diseases and conditions // *FASEB Journal* 17 (5): A903-A903 Part 2 Suppl. S MAR 17 2003.

**S.M. Keenan, R.K. Delisle, W.J. Welsh, V. Kholodovych, S. Paula, W.J. Ball** Method for the discovery of novel Na, K-ATPase inhibitors for the therapeutic treatment of cardiovascular diseases and conditions // *Abstracts of Papers of the American Chemical Society* 2003, 225, U760.

**V. Kholodovych, W.J. Welsh** Determination of structural requirements for activation of the clearance mechanism of environmental pollutants and xenobiotic chemicals by the pregnane xenobiotic receptor (PXR): Species to species extrapolation. *EPA: Endocrine Disrupters* (October 2002) Research Triangle Park, North Carolina.

**I.V. Tetko, V.V. Kovalishyn, S.-J. Yu, V. Kholodovych, W.J. Welsh** A Comparison of the volume learning artificial neural networks with traditional 3D QSAR approaches for modeling of cannabinoid and estrogens receptors. *Euro QSAR 2002* (September 2002), Bournemouth, UK.

**V. Kholodovych, V. Kovalishyn, I. Tetko, W.J. Welsh** A new approach for 3D-QSAR studies based on the volume learning artificial neural network *ANNIE 2002* (November 2002), Smart Engineering System Design, St. Louis, Missouri

**V. Kholodovych, W.J. Welsh, V. Kovalishyn, I.V. Tetko** Utility of informatics in drug discovery, 4th Annual RWJMS Research Day Symposium (March 2002), UMDNJ, New Brunswick, New Jersey

**V. Kholodovych, V.V. Kovalishyn, V.V. Prokopenko, A.I. Luik** Search of common features in groups of cellular receptors' agonists and antagonists 5th Congress of Theoretically Oriented Chemists *WATOC'99* (August 1999), London, UK.