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VLAD KHOLODOVYCH, Ph.D.

TRAINING AND EDUCATION

2011 - pres.	Scientific Stuff (Rutgers: IS&T, HPC - RWJMS), Newark, NJ
2002 - 2011	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	Stipendiary Award of the Ukrainian National Academy of Sci., Ukraine
1998-1999	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***

R. Fekete, M. Bainbridge, J.F. Baizabal-Carvallo, A. Rivera, B. Miller, P.C. Du, V. Kholodovych, S. Powell, W. Ondo Exome sequencing in familial corticobasal degeneration // *Parkinsonism and Related Disorders* 2013, 19(11), 1049-1052.

D.R. Lewis, V. Kholodovych, M.D. Tomasini, D. Abdelhamid, L.K. Petersen, W.J. Welsh, K.E. Uhrich, P.V. Moghe In silico design of anti-atherogenic biomaterials // *Biomaterials* 2013, 34(32), 7950-7959.

I. Sushko, S. Novotarskyi, R. Korner, A.K. Pandey, M. Rupp, W. Teetz, S. Brandmaier, A. Abdelaziz, V.V. Prokopenko, V.V. Tanchuk, R. Todeschini, A. Varnek, G. Marcou, P. Ertl, V. Potemkin, M. Grishina, J. Gasteiger, C. Schwab, I.I. Baskin, V.A. Palyulin, E.V. Radchenko, W.J. Welsh, V. Kholodovych, D. Chekmarev, A. Cherkasov, J. Aires-de-Sousa, Q.-Y. Zhang, A. Bender, F. Nigsch, L. Patiny, A. Williams, V. Tkachenko,

I.V. Tetko Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information // *Journal of Computer-Aided Molecular Design* 2011, 25(6), 533-554.

A.V. Gubskaya, T.O. Bonates, V. Kholodovych, P. Hammer, W.J. Welsh, R. Langer, J. Kohn Logical analysis of data in structure-activity investigation of polymeric gene delivery // *Macromolecular Theory and Simulations* 2011, 20(4), 275-285.

N. Thakkar, V. Pirrone, S. Passic, S. Keogan, W. Zhu, V. Kholodovych et al. Persistent interactions between biguanide-based compound NB325 and CXCR4 result in prolonged inhibition of human immunodeficiency virus type 1 infection // *Antimicrobial Agents and Chemotherapy* 2010, 54(5), 1965-1972.

D. Chekmarev, V. Kholodovych, S. Kortagere, W.J. Welsh, S. Ekins Predicting inhibitors of acetylcholinesterase by regression and classification machine-learning approaches with combinations of molecular descriptors // *Pharmaceutical Research* 2009, 26(9), 2216-2224.

Y.S. Lin, K. Yasuda, M. Assem, C. Cline, J. Barber, C.W. Li, V. Kholodovych et al. The major human pregnane X receptor (PXR) splice variant, PXR.2, exhibits significantly diminished ligand-activated transcriptional regulation // *Drug Metabolism and Disposition* 2009, 37(6), 1295-1304.

N. Thakkar, V. Pirrone, S. Passic, W. Zhu, V. Kholodovych, W.J. Welsh et al. Specific interactions between the viral coreceptor CXCR4 and the biguanide-based compound NB325 mediate inhibition of human immunodeficiency virus type 1 infection // *Antimicrobial Agents and Chemotherapy* 2009, 53(2), 631-638.

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

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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. Kholodovich 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. Kholodovich, 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. Kholodovich Reactions of titanium alkoxides with N,N,N',N''-tetrakis(trimethylsilyl)amide of diimidophosphenic 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.

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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 n etwork *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.