

# Quantitative Structure-Activity Relationship

[View the current Quantitative Structure-Activity Relationship InDepth page on BioPortfolio.com](http://www.bioportfolio.com/indepth/Quantitative_Structure-Activity_Relationship.html)  
([http://www.bioportfolio.com/indepth/Quantitative\\_Structure-Activity\\_Relationship.html](http://www.bioportfolio.com/indepth/Quantitative_Structure-Activity_Relationship.html))

## Recent Publications on Quantitative Structure-Activity Relationship:



- [Structural Development of Benzhydrol-Type 1'-Acetoxychavicol Acetate \(ACA\) Analogs as Human Leukemia Cell-Growth Inhibitors Based on Quantitative Structure-Activity Relationship \(QSAR\) Analysis.](#)  
*Benzhydrol-type analogs of 1'-acetoxychavicol acetate (ACA) were developed...*2nd October, 2008  
Institute of Molecular and Cellular Biosciences, The University of Tokyo.- *Chem Pharm Bull (Tokyo)*. 2008 Oct;56(10):1490-5.
- [Robust Cross-Validation of Linear Regression QSAR Models.](#)  
*A quantitative structure-activity relationship (QSAR) model is typically...*2nd October, 2008  
School of Mathematics, Physics & Information Technology, James Cook- *J Chem Inf Model*. 2008 Oct 1. ([DOI Direct Link](#))
- [Using multidimensional patterns of amino acid attributes for QSAR analysis of peptides.](#)  
*On the basis of exploratory factor analysis, six multidimensional patterns...*30th September, 2008  
College of Bioengineering, Chongqing University, 400030, Chongqing, China,- *Amino Acids*. 2008 Sep 28. ([DOI Direct Link](#))
- [Combining Ligand-Based Pharmacophore Modeling, Quantitative Structure-Activity Relationship Analysis and in Silico Screening for the Discovery of New Potent Hormone Sensitive Lipase Inhibitors.](#)  
*Hormone sensitive lipase (HSL) has been recently implicated in diabetes...*24th September, 2008  
Department of Pharmaceutical Sciences, Faculty of Pharmacy, University of- *J Med Chem*. 2008 Sep 20. ([DOI Direct Link](#))
- [Efficient removal of estrogenic activity during oxidative treatment of waters containing steroid estrogens.](#)  
*The discharge of synthetic and natural steroid estrogens from municipal...*20th September, 2008  
Eawag, Swiss Federal Institute of Aquatic Science and Technology, CH-8600,- *Environ Sci Technol*. 2008 Sep 1;42(17):6333-9.
- [CoMFA and CoMSIA 3D-QSAR analysis of DMDP derivatives as anti-cancer agents.](#)  
*Comparative molecular field analysis (CoMFA) and comparative molecular...*17th September, 2008  
- *Bioinformation*. 2008 Jun 27;2(9):384-91.
- [Development of predictive in silico model for cyclosporine- and aureobasidin-based P-glycoprotein inhibitors employing receptor surface analysis.](#)  
*P-glycoprotein (Pgp) is implicated in multiple drug resistance (MDR)...*16th September, 2008  
Department of Pharmaceutical Sciences, Faculty of Pharmacy, University of- *J Mol Graph Model*. 2008 Aug 13. ([DOI Direct Link](#))
- [QSAR analysis and specific endpoints for classifying the physiological modes of action of biocides in synchronous green algae.](#)

- We propose the use of additional physiological endpoints in the 24h growth...* 16th September, 2008  
Eawag, Swiss Federal Institute for Aquatic Science and Technology,- Aquat Toxicol. 2008 Jul 29. ([DOI Direct Link](#))
- [Inhibition of the sarcoplasmic/endoplasmic reticulum Ca\(2+\)-ATPase by flavonoids: A quantitative structure-activity relationship study.](#)  
*Flavonoids are commonly found in fruit and vegetables and have been shown...* 13th September, 2008  
School of Biosciences, University of Birmingham, Edgbaston, Birmingham,- IUBMB Life. 2008 Sep 11. ([DOI Direct Link](#))
  - [On the interpretation and interpretability of quantitative structure-activity relationship models.](#)  
*The goal of a quantitative structure-activity relationship (QSAR) model is...* 12th September, 2008  
School of Informatics, Indiana University, Bloomington, IN, 47408, USA,- J Comput Aided Mol Des. 2008 Sep 11. ([DOI Direct Link](#))
  - [A QSAR model for predicting mutagenicity of nitronaphthalenes and methylnitronaphthalenes.](#)  
*A quantitative structure-activity relationship model for prediction of...* 9th September, 2008  
State Key Laboratory of Water Environment Simulation, School of- Bull Environ Contam Toxicol. 2008 Nov;81(5):498-502. Epub 2008 Sep 6. ([DOI Direct Link](#))
  - [3D QSAR studies of 1,3,4-benzotriazepine derivatives as CCK\(2\) receptor antagonists.](#)  
*A number of CCK(2) antagonists have been reported to play an important...* 9th September, 2008  
Department of Pharmaceutical Sciences, College of Pharmacy and Allied- J Mol Graph Model. 2008 Jul 30. ([DOI Direct Link](#))
  - [3D-QSAR studies of boron-containing dipeptides as proteasome inhibitors with CoMFA and CoMSIA methods.](#)  
*Three-dimensional quantitative structure-activity relationship (3D-QSAR)...* 6th September, 2008  
Jiangsu Simcere Pharmaceutical Research Institute, No. 699-18 Xuan Wu- Eur J Med Chem. 2008 Jul 24. ([DOI Direct Link](#))
  - [Molecule kernels: a descriptor- and alignment-free quantitative structure-activity relationship approach.](#)  
*Quantitative structure activity relationship (QSAR) analysis is...* 5th September, 2008  
School for Electrical Engineering and Computer Science, Berlin Institute- J Chem Inf Model. 2008 Sep;48(9):1868-81. Epub 2008 Sep 4. ([DOI Direct Link](#))
  - [Design of potent aspartic protease inhibitors to treat various diseases.](#)  
*In this retrospective, personal review covering our research from the late...* 4th September, 2008  
Department of Medicinal Chemistry, Center for Frontier Research in- Arch Pharm (Weinheim). 2008 Sep;341(9):523-35. ([DOI Direct Link](#))

## BioNews Results for Quantitative Structure-Activity Relationship

- [Get a Deep Insight Into the World Blood Gas & Electrolyte Analyzers Market](#)  
*Reuters: Oct 1 2008 7:22PM Matching: quantitative structure activity relationship*
- [Examine the World Imaging Agents \(Contrast Media, Radiopharmaceuticals\) Market](#)  
*Marketwire via Yahoo!: Sep 18 2008 9:23AM Matching: quantitative structure activity relationship*



## Quantitative Structure-Activity Relationship Patents:

- 7169927- [Indole-amide derivatives and their use as glycogen phosphorylase inhibitors](#)
- 7244843- [Modulators of serotonin receptors](#)
- 7247736- [Method of identifying inhibitors of DHODH](#)
- 7253165- [Benzisoxazolyl-, pyridoisoxazolyl-and benzthienyl-phenoxy derivatives useful as D.sub.4 antagonists](#)
- 7253180- [Pre-organized tricyclic integrase inhibitor compounds](#)
- 7265102- [Substituted pyrazoles](#)
- 7276613- [Retro-anandamides, high affinity and stability cannabinoid receptor ligands](#)
- 7283239- [Method for generating a formula for calculating mottling of a paint film, and a quantification method of the mottling](#)
- 7285683- [Bicyclic and tricyclic cannabinoids](#)
- 7304050- [Antibacterial agents](#)
- 7304053- [Substituted heterocyclic compounds for treating multidrug resistance](#)
- 7241905- [Dioxin analogues and methods and kits for searching out dioxins-decomposing organisms or enzymes or dioxin-decomposing enzyme genes](#)
- 7241799- [Cannabimimetic indole derivatives](#)
- 7235521- [Previns as specific inhibitors and therapeutic agents for botulinum toxin B and tetanus neurotoxins](#)
- 7173027- [Receptor selective cannabimimetic aminoalkylindoles](#)
- 7176236- [Water-soluble etoposide analogs and methods of use thereof](#)
- 7176314- [Inflammation modulators](#)
- 7183313- [Keto cannabinoids with therapeutic indications](#)
- 7186700- [.beta.-L-2'-deoxynucleosides for the treatment of resistant HBV strains and combination therapies](#)
- 7188055- [Method, system, and computer program for displaying chemical data](#)
- 7189737- [Cocaine receptor binding ligands](#)
- 7196103- [Indole derivatives as factor Xa inhibitors](#)
- 7208521- [Selective inhibitors of the urokinase plasminogen activator](#)
- 7230027- [Anti-first-pass effect compounds](#)
- 7309703- [Substituted pyrazoles](#)
- 7317027- [Azaindole-derivatives as factor Xa inhibitors](#)
- 7388011- [Substituted pyrazoles](#)
- 7393533- [H3L envelope protein immunization methods and H3L envelope passive protection methods](#)
- 7393842- [Pyrazole analogs acting on cannabinoid receptors](#)
- 7393850- [Substituted pyrazoles](#)
- 7416524- [System, method and computer program product for fast and efficient searching of large chemical libraries](#)
- 7417046- [Substituted pyrazoles](#)
- 7419968- [Methods for treating therapy-resistant tumors](#)
- 7421347- [Identifying oligonucleotides for in vitro recombination](#)
- 7422733- [Linkable sialyl Lewis X analogs](#)
- 7429591- [Substituted pyrazoles](#)
- 7378419- [9-amino-podophyllotoxin derivatives, method for the production thereof and pharmaceutical compositions containing said derivatives](#)

- 7375079- [Previns as specific inhibitors and therapeutic agents for botulinum toxin B and tetanus neurotoxins](#)
- 7371810- [Tachykinin peptides, precursor peptides thereof and genes encoding the same](#)
- 7320786- [Photodynamic therapy treatment for eye disease](#)
- 7329651- [Cannabimimetic ligands](#)
- 7332494- [Method for treating allergies using substituted pyrazoles](#)
- 7332515- [Indole-amid derivatives which possess glycogen phosphorylase inhibitory activity](#)
- 7335688- [Bicyclic cannabinoid agonists for the cannabinoid receptor](#)
- 7347984- [Mammalian agmatinase inhibitory substance](#)
- 7354931- [Heterocyclic retinoid compounds](#)
- 7356416- [Method and system for automated inference creation of physico-chemical interaction knowledge from databases of co-occurrence data](#)
- 7358259- [HCV inhibitors and methods of using them](#)
- 7358361- [Biophosphonate compounds and methods for bone resorption diseases, cancer, bone pain, immune disorders, and infectious diseases](#)
- 7430477- [Methods of populating data structures for use in evolutionary simulations](#)

\*\*\*

Resources from the [NCBI](#) used in this document, [NCBI's standard disclaimer applies](#).

Nothing in this document should be used in place of personal medical advice from your own qualified medical practitioner. See BioPortfolio.com [User Agreement](#)

Send comments and feedback to:

Peter Barfoot Managing Director, BioPortfolio Ltd.

UK Tel: (+44) 1300 321501

USA Voicemail and Fax: (+1) 415 680 2472

[Peter Barfoot peter.barfoot@bioportfolio.com](mailto:peter.barfoot@bioportfolio.com)

All rights reserved. All other trademarks recognized.

BioPortfolio Limited is registered in England & Wales at Wessex Barn, Dorchester Road, Frampton, Dorset, DT2 9NB, UK. No.3312883 VAT No. GB 744 6483 10

Copyright 1997-2008 - BioPortfolio Limited.

