19th EuroQSAR

Knowledge Enabled Ligand Design

August 26-30, 2012

Vienna, Austria

Abstract Book

EuroQSAR 2012 Symposium Secretariat
LD Organisation sprl
Scientific Conference Producers
Rue Michel de Ghelderode 33/2
B 1348 Louvain-la-Neuve, Belgium
T: +32 10 45 47 77 F: +32 10 45 97 19
secretariat@LDOrganisation.com
www.LDOrganisation.com

www.euroqsar2012.org

Sponsored by

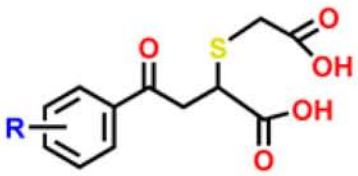
EFMC
European Federation
for Medicinal Chemistry

2-[(CARBOXYMETHYL)SULFANYL]-4-OXO-4-ARYLBUTANOIC ACIDS. PART 3. PHARMACOLOGY AND CONFORMATIONAL PREFERENCES IN DIFFERENT SOLVENTS. THE NMR/MD STUDY

Branko J. Drakulić, Željko S. Žižak, Tatjana P. Stanojković, Slavica Ristić, Dejan M. Gođevac, Ivan O. Juranić

(1,5,6) Department of Chemistry-IChTM, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia; (2,3) Institute of Oncology and Radiology of Serbia, Pasterova 14, 11000 Belgrade, Serbia; (4) Biomedical Research, R&D Institute, Galenika a.d. Batajnički Drum b.b., 11000 Belgrade, Serbia

2-[(Carboxymethyl)sulfanyl]-4-oxo-4-arylbutanoic acids (Figure) exerts antiproliferative potency toward human tumor cells *in vitro* in low micromolar to submicromolar concentrations [1].



Compounds show selective toxicity *in vitro* toward healthy human cells non-stimulated, or stimulated for growth, with selectivity indexes 2-30. So far we showed that selectivity of compounds correlate with their flexibility. Linear correlation was found between selectivity and the time needed for conformational change, as obtained by molecular dynamics simulations in explicit *n*-octanol-water as a solvent, and by applying biasing force to speed-up sampling and to map free-energy surfaces [2, 3]. Congeners having similar substitution pattern on phenyl ring, which exert high or low selectivity, have significantly different free-energy surfaces, even conformations of global minima were comparable [3]. Acute toxicity of selected compounds, *in vivo*, was obtained on mice. Remarkably, compounds that exert high selectivity *in vitro*, also show low toxicity (LD_{50} > 2g/kg), while the first signs of the toxicity of compounds having low selectivity *in vitro*, appear on 100 mg/kg. When applied intravenously as disodium salt, the major amount of the one of the most selective compound (2,4,6-tri-Et- derivative) was excreted unchanged. Conformational properties of selected compounds, in different isotropic or anisotropic solvents, were examined by the NMR and the NAMFIS analysis [4]. In non-polar solvents extended conformations predominate; while in polar solvent predominate folded conformations. DOSY-NMR spectra were used to differentiate shape of major conformers in solvents of different polarity and HBA/HBD abilities. Those results were compared with the conformational behavior of compounds obtained by molecular dynamics simulations in the model of the explicit solvents, without or with applied biasing forces. Distribution of the conformation-dependent molecular properties is discussed.

Acknowledgments: This communication is supported by the European Commission under EU FP7 project HP-SEE, http://www.hp-see.eu/. Contract number 261499. The Ministry of Education and Science of Serbia support this work under Grant 172035.

References

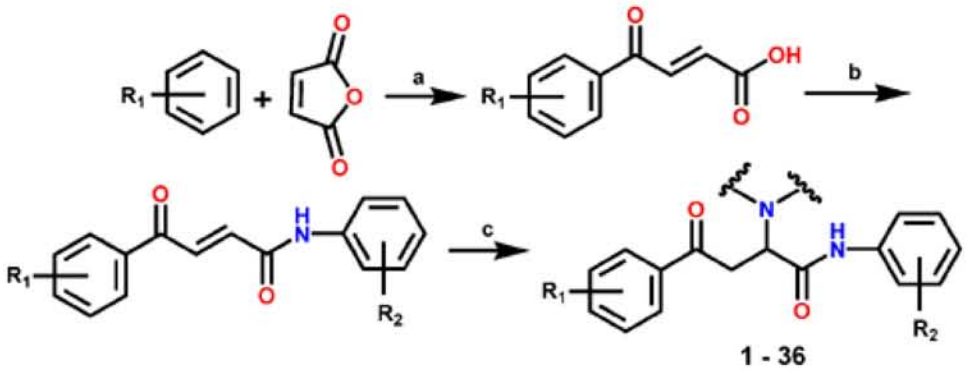
1) B.J. Drakulić, Z.D. Juranić, T.P. Stanojković, I.O. Juranić J. Med. Chem. 48 (2005) 5600-5603
2) J. Henin, G. Fiorin, C. Chipot, M.L. Klein J. Chem. Theory Comput. 6 (2010) 35-47
3) B.J. Drakulić, A. Pedrretti, M. Zloh, V. Slavnić, I.O. Juranić, M.M. Dabović, The 18th European Symposium on Quantitative Structure-Activity Relationships, Book of Abstracts, pp. 278-279, Greece, 2010
4) D.O. Cicero, G. Barbato, R. Bazzo J. Am. Chem. Soc. 117 (1995) 1027-1033

4-ARYL-4-OXO-N-PHENYL-2-AMINYLBUTYRAMIDES WITH INTERESTING AChE/BChE SELECTIVITY PROFILE

Maja D. Vitorović-Todorović, Catherine Koukoulitsa, Ivan O. Juranić, Branko J. Drakulić

(1) Faculty of Chemistry, University of Belgrade, Serbia; (2) Department of Chemistry, University of Athens, Greece; (3, 4) Department of Chemistry-IChTM, University of Belgrade, Serbia

Recent findings that acetylcholinesterase (AChE) is involved in Aβ peptide deposition and aggregation through its peripheral anionic site (PAS) [1] revoked the interest in synthesizing novel AChE reversible inhibitors with better pharmacokinetic profile than those currently available, FDA approved drugs, for the treatment of Alzheimer's disease (AD). Butyrylcholinesterase (BChE) was also proved as important target for AD, since it plays the supportive role in cholinergic neurotransmission. Recently, we reported congeric series of the twenty 4-aryl-4-oxo-*N*-phenyl-2-aminylbutyramides with varying substitution on the aroyl phenyl ring [2]. Alkyl-substituted congeners inhibited both AChE and BChE in micromolar concentrations, while chloro- or metoxy-substituted compounds were proved to be inactive. In this communication, we have investigated the influence of the amide portion of the molecule on the activity toward AChE and BChE. We systematicaly changed the amine used to obtain aroylacrylic acid amides (3,5-dimetoxyaniline, 4-isopropylaniline and cyclohexyl amine), keeping the favourable alkyl substituents on the aroyl part of the molecule. For the Michael addition to the activated double bond, four amines were used: piperidine, imidazole, morpholine and *N*-methylpiperazine (Scheme).



Scheme. Synthesis of **1-36**. Reagents: (a) $AlCl_3$; (b) $POCl_3$, THF and 3,5-dimetoxyaniline, 4-*i*Pr-aniline or cyclohexylamine; (c) piperidine, imidazole, morpholine or *N*-methylpiperazine in CH_2Cl_2/toluene. R_1= 4-*i*Pr, 2,4-di-*i*Pr or 1,2,3,4-tetrahydronaphtalenyl.

The inhibitory activity of 36 novel compounds was tested on both AChE and BChE. Compounds have shown interesting selectivity profile with piperidino and imidazolo derivatives being active toward AChE, and some morpholino and *N*-methylpiperazino derivatives being active toward BChE, both in low micromolar concentrations. Possible interactions of the compounds with AChE were investigated by docking calculations and MD simulations.

Acknowledgement: The Ministry of Education and Science of Serbia support this work, under Grant 172035. C. Koukoulitsa was recipient of Hrakleitos II scholarship. This communication is supported by the European Commission under EU FP7 project HP-SEE, http://www.hp-see.eu/. Contract number 261499.

References

1) M. Bartolini, C. Bertucci, V. Cavrini, V. Andrisano, Biochem. Pharmacol. 65 (2003) 407-416.
2) M. Vitorović-Todorović, Lj. Mandić, I. Juranić, B. Drakulić, Bioorg. Med. Chem. 18 (2010) 1181-1193.

Index of Abstracts

Table of Content

DRAKULIC Branko	2-[(CARBOXYMETHYL)SULFANYL]-4-OXO-4-ARYLBUTANOIC ACIDS. PART 3. PHARMACOLOGY AND CONFORMATIONAL PREFERENCES IN DIFFERENT SOLVENTS. THE NMR/MD STUDY.	P084
DRUZHILOVSKIY Dmitry	COMPUTER-AIDED ANALYSIS OF HIDDEN POTENTIAL IN TRADITIONAL INDIAN MEDICINE AYURVEDA	P065
DUCROT Pierre	A NETWORK-BASED APPROACH TO THE KINASE SELECTIVITY CHALLENGE	P055
DULIN Fabienne	IN SILICO HIGHLIGHTS OF VARROACIDE COMPOUNDS (ACHE INHIBITORS) TO PROTECT THE HONEYBEE HEALTH	P143
DULIN Fabienne	NEW ECOTOXICOLOGICAL DATA OF 24 PCBS AND RELATED SAR STUDIES	P144
ERIC Slavica	DOCKING STUDIES OF THE NOVEL DERIVATIVES OF ARYL-AMINOPYRIDINES WITH POTENTIAL ANTICANCER ACTIVITY	P010
ERIC Slavica	DOCKING OF ANTICANCER DRUGS AND MODULATORS OF THE MULTIDRUG RESISTANCE TOWARDS P-GLYCOPROTEIN	P011
ERIC Slavica	PREDICTION OF THYROID HORMONE RECEPTOR β1 ACTIVITY OF SERIES OF SUBSTANCES USING COUNTER-PROPAGATION ARTIFICIAL NEURAL NETWORKS	P012
ERIC Slavica	COMPUTATIONAL MODELS FOR PREDICTING THE TRANSPORT OF DRUG-LIKE COMPOUNDS BY P-GLYCOPROTEIN AND BREAST CANCER RESISTANCE PROTEIN	P013
EVERS Andreas	EFFICIENT IN SILICO SCAFFOLD HOPPING FOR LEAD FINDING CONSIDERING ROBUST CHEMICAL REACTIONS AND AVAILABLE REAGENTS	OC11
FALLACARA Anna Lucia	DEVELOPMENT AND OPTIMIZATION OF NEW COMPOUNDS AS ALLOSTERIC INHIBITORS OF BCR-ABL KINASE	P024
FANG Weishuo	A COMBINE MODEL GUIDED DESIGN OF NEW TAXANES WITH HIGH AFFINITY BOUND TO MICROTUBULES	P064
FERREIRA Ricardo	TOWARDS A DEEPER UNDERSTANDING OF THE MODULATION ACTIVITY AND SPECIFICITY OF P-GLYCOPROTEIN	P019
FERREIRA Ricardo	INSIGHTS ON MACROCYCLIC LATHYRANE DITERPENES AS MDR REVERSERS: STRUCTURE-ACTIVITY RELATIONSHIPS AND DOCKING STUDIES	P020
FILIMONOV Dmitry	OPEN ACCESS WEB-SERVICES FOR PREDICTING BIOLOGICAL ACTIVITY	OC24
FISCHER Thomas	STRUCTURE BASED DESIGN AND SYNTHESIS OF NOVEL MMP INHIBITORS	P133
FORSTER Mark	OPEN INNOVATION APPLIED TO AGROCHEMICAL DISCOVERY	PL09
FRACZKIEWICZ Robert	NOVEL ANTIMALARIAL DRUG CANDIDATES GENERATED IN SILICO BY ANALYSIS OF PUBLIC HTS DATA	P156
FUCHS Julian	IN SILICO IDENTIFICATION OF PRECURSORS FOR CYP PROFILING BREATH TESTS	P017
FULLE Simone	SUBSTRATE DRIVEN DESIGN OF INHIBITORS OF THE MALARIAL PROTEASE PFSUB1	P054
GALLO Grazia	HOMOLOGY MODELING OF HEPARANASE AND ITS BINDING INTERACTIONS	P160
GASTREICH Marcus	ReCore ROX U.	OC10
GOBEC Stanislav	NOVEL INHIBITORS OF TRIHYDROXYNAPHTHALENE REDUCTASE WITH ANTIFUNGAL ACTIVITY IDENTIFIED BY LIGAND-BASED AND STRUCTURE-BASED VIRTUAL SCREENING	P106
GRANDITS Melanie	MD SIMULATIONS OF RAM2 WITH RUTINOSE AS EXAMPLE FOR A PROTEIN-LIGAND INTERACTION STUDY	P085
GRECU Tudor	VIRTUAL COCRYSTAL SCREENING	P068
GREGORI-PUIGJANE Elisabet	COULD DRUGS BE USED AS PROBES?	P110
GÜTLEIN Martin	IN DEFENSE OF CROSS-VALIDATION	OC15
HARA Hideto	DEVELOPMENT OF A NOVEL MATCHED MOLECULAR PAIR METHODOLOGY, SABUN	P038
HARLAND Lee	OPEN DRUG DISCOVERY INTELLIGENCE : OPEN PHACTS AND SciBite	OC28
HARTENFELLER Markus	THE FAST AND THE PRECIOUS: REACTION DRIVEN DE NOVO DESIGN IN THE CHEMICAL SPACE OF SYNTHETICALLY ACCESSIBLE COMPOUNDS	OC12
HAWKINS Paul	POSITIVE FALSE DISCOVERY RATE: A NEW DEAL" FOR SHAPE SEARCHING?"	OC14
HENRY Thomas	MUSE+TRIPOSSCORE: A LIGAND-BASED DE NOVO DESIGN APPROACH	P081
HENZLER Angela	CONSISTENT HANDLING OF FLEXIBLE INTERACTION SITES FOR EFFICIENT STRUCTURE-BASED VIRTUAL SCREENING	OC05
HEO Lim	GALAXYWEB SERVER FOR PROTEIN STRUCTURE PREDICTION, REFINEMENT, AND OTHER APPLICATIONS	P101
HIRAYAMA Noriaki	AutoGPA: AN AUTOMATIC 3D-QSAR METHOD BASED ON GRID POTENTIAL ANALYSIS AND PHARMACOPHORE ALIGNMENT	P026
HÄRKÖNEN Henna	FROM CYCLIC PEPTIDES TO DRUG-LIKE COMPOUNDS STIMULATING KALLIKREIN-RELATED PEPTIDASE 3 (KLK3)	P157
JALAIE Mehran	DESIGINING BETTER COMPOUNDS FASTER: THE TALE OF DISCOVERING A NOVEL CLASS OF CENP-E INHIBITORS USING STRUCTURE-GUIDED PHARMACOPHORE METHODS IN COMBINATION WITH A NEW VISUALIZATION TOOL	OC03

JELIAZKOVA Nina	AMBIT-TAUTOMER: AN OPEN SOURCE TOOL FOR TAUTOMER GENERATION	P040
JELIAZKOVA Nina	BIOCLIPSE-OPENTOX: INTERACTIVE PREDICTIVE TOXICOLOGY	P041
JELIAZKOVA Nina	TOXTREE: TOXIC HAZARD ESTIMATION BY A DECISION TREE APPROACH - THE FIRST SEVEN YEARS	P043
JONSDOTTIR Svava Osk	IDENTIFICATION OF CYTOCHROME P450 2D6, 2C9 AND 3A4 SUBSTRATES AND INHIBITORS BY QSAR MODELS BASED ON HUMAN CLINICAL DATA	P070
JORGE Salomao Doria	DESIGN, SYNTHESIS, BIOACTIVITY AND MOLECULAR MODELING STUDIES OF 5-NITRO-2-FURFURILIDENE DERIVATIVES AS POTENTIAL ANTI-T. CRUZI AGENTS	P036
JORGE Salomao Doria	2D/3D-QSAR STUDIES OF BENZOFUROXAN DERIVATIVES AS ANTI-Trypanosoma cruzi AGENTS	P025
JURIK Andreas	COMBINING BINARY QSAR AND DOCKING FOR STUDYING STRUCTURE-ACTIVITY RELATIONSHIPS OF TIAGABINE ANALOGS	P071
KACER Petr	RELATIONS STRUCTURE-ACTIVITY" AS A TOOL FOR DESIGN OF NEW PLATINUM-BASED CYTOSTATICS"	P142
KALLIOKOSKI Tuomo	AN ESTIMATION FOR THE EXPERIMENTAL UNCERTAINTY OF HETEROGENEOUS KI DATA FROM CHEMBL DATABASE	P018
KARLOV Dmitry	ON MECHANISM OF NMDA RECEPTOR ALLOSTERIC INHIBITION	P034
KASERER Teresa	PROSPECTIVE PERFORMANCE EVALUATION OF DIFFERENT VIRTUAL SCREENING TOOLS FOR COX-ACTIVITY PREDICTION	P127
KHATIB Soliman	GLABRIDIN AND OTHER FLAVONOIDS PROTECTS PON1 FROM LINOLEIC ACID HYDROPEROXIDE INHIBITION VIA A SPECIFIC INTERACTION: A FLUORESCENCE QUENCHING AND MOLECULAR DOCKING STUDY	P150
KIDRON Heidi	PREDICTION OF THE VITREAL HALF-LIFE OF DRUG-LIKE COMPOUNDS	P022
KIJKOWSKA-MURAK Urszula	TOWARDS NOVEL MORE EFFICIENT ANTIPSYCHOTIC DRUGS ACTING THROUGH 5-HT1A RECEPTOR - CASE STUDIES OF THE ARYLPIPERAZINE IMIDE DERIVATIVES	P090
KIJKOWSKA-MURAK Urszula	STRUCTURAL DETERMINANTS OF ANTAGONISTS ACTIVITY OF THE OREXIN OX1 RECEPTOR - CONSTRUCTION OF THE PHARMACOPHORE MODEL	P091
KISS Robert	MCULE.COM: AN INTEGRATED VIRTUAL SCREENING TOOLBOX ON THE WEB	P008
KITTELMANN Jörg	QSPR DESCRIPTOR DEVELOPMENT FOR PROTEIN BINDING ORIENTATION SENSITIVE ION-EXCHANGE CHROMATOGRAPHY PARAMETER PREDICTION	P104
KLEBE Gerhard	HOW VALID ARE POPULAR ASSUMPTIONS APPLIED IN COMPUTATIONAL DRUG DESIGN?	PL02
KOCH Christian	DESIGNING MHC-I STABILIZING PEPTIDES BY MULTI-MODEL CASCADED MACHINE-LEARNING	OC13
KOICHI Handa	3D-QSAR MODELS FOR HUMAN/RAT CYP3A FAMILY INHIBITORS	P009
KOKH Daria	TRAPP - A COMPUTATIONAL TOOL FOR IDENTIFICATION OF TRANSIENT BINDING POCKETS IN PROTEINS	P029
KOLB Peter	COMPUTER-AIDED DISCOVERY OF NOVEL CHEMOTYPES ADDRESSING THE CHEMOKINE RECEPTOR CXCR3	P129
KONSTANTINIDOU Markella	QSAR OF CXCR2 CHEMOKINE RECEPTOR ANTAGONISTS AS POTENT ANTI-INFLAMMATORY AGENTS	P082
KONTOYIANNI Maria	AN INTEGRATED COMPUTATIONAL STRATEGY TO PROBE LIGAND PROMISCUITY IN THE HUMAN CYTOCHROME 3A4	OC18
KOTSAMPASAKOU Eleni	STRUCTURE-ACTIVITY-SELECTIVITY RELATIONS ON DIFLUORO-PYRROLYL-PHENOL ALDOSE REDUCTASE INHIBITORS (ARIs)	P058
KRAMER Christian	USING PUBLIC DATA FOR STATISTICAL SCORING FUNCTIONS	OC25
KRIEGL Jan M.	MINING IN CORPORATE DATABASES: WHAT CAN WE LEARN FROM OUR HISTORICAL DATA ?	PL04
KRINGELUM Jens	PREDICTING POLYPHARMACOLOGY USING SEA - SUCCESS AND FAILURES	P032
KUBINYI Hugo	THE IMPACT OF QSAR ON MEDICINAL CHEMISTRY	H04
LAMPRINIDIS George	RATIONAL DRUG DESIGN: FROM VIRTUAL SCREENING TO NEW LEAD COMPOUNDS. THE CASE OF TYROSINASE INHIBITORS	P114
LE QUESTEL Jean-Yves	QUANTIFICATION OF THE STRENGTH OF HYDROGEN BONDING : FROM SIMPLE ORGANIC MOLECULES TO A DATABASE FOR USE IN DRUG DESIGN	P028
LEE Gyu Rie	PREDICTING LOOP CONFORMATIONS IN INACCURATE PROTEIN MODEL STRUCTURES	P103
LEE Sehan	G-SFED MODEL: A GENERALIZDE CONTINUUM SOLVATION MODEL FOR DRUG DISCOVERY	P045
LEPAILLEUR Alban	TOWARDS AUTOMATED DETECTION OF STRUCTURAL ALERTS FOR PREDICTIVE ECOTOXICOLOGY	P145
LIARGKOVA Thalia	USING 2D-QSAR AS A TOOL IN THE DESIGN OF BIOLOGICAL ACTIVE ENONIC COMPOUNDS	P076
LINDER Tobias	PROBING THE DYNAMICS OF THE BACTERIAL K+ CHANNEL KCSA DURING PORE	P105

	GATING	
LIPINSKI Christopher A.	MYTHS AND FALLACIES ABOUT EXPLORING CHEMICAL SPACE: SAR IS THE MEDICINAL CHEMIST'S RETROSPECTIVE TOOL IN LIGAND DESIGN	OL
LIVINGSTONE David	QSAR: PAST ACHIEVEMENTS, PRESENT PROBLEMS AND FUTURE DIRECTIONS	PL05
MACCHIARULO Antonio	MOLECULAR DOCKING AND HIGH-THROUGHPUT MOLECULAR DYNAMICS TO DETECT AND ANALYZE BINDING SITE PROPERTIES OF DAF-12 ORTHOLOGS IN PARASITIC NEMATODES.	P004
MACKEY Mark	3D QSAR - WHY BE SQUARE?	P100
MAGGIORA Gerald M.	ACTIVITY CLIFFS, INFORMATION THEORY, AND QSAR	H03
MAJEKOVA Magdalena	THE USE OF ADVANCED STATISTICAL METHODS IN THE STUDY OF PYRIDOINDOLE COMPOUNDS WITH NEUROPROTECTIVE EFFECTS	P132
MANALLACK David T	A CHEMOGENOMIC ANALYSIS OF IONIZATION CONSTANTS	OC21
MANELFI Candida	CHEMICAL DOMAIN ANALYSIS OF THE COSMETICS INVENTORY OF THE COSMOS PROJECT	P139
MANIVANNAN E	COMPARATIVE QSAR MODELLING OF SULFONATED QUINAZOLINONES AND DIHYDROQUINAZOLINONES FOR ITS ANTI-INFLAMMATORY ACTION	P087
MANSOURI Kamel	MULTICRITERIA VARIABLE SELECTION FOR QSARS	P151
MARAN Uko	ELECTRONIC ORGANIZATION AND ARCHIVING OF QSAR/QSPR MODEL INFORMATION - QSARDB	P161
MARTI-SOLANO Maria	STUDY OF THE STRUCTURAL DETERMINANTS OF LIGAND BIAS AT THE SEROTONIN 2A RECEPTOR USING DOCKING AND MOLECULAR DYNAMICS SIMULATIONS	P047
MARTI-SOLANO Maria	DEVELOPMENT OF A PREDICTION TOOL OF BINDING AFFINITY PROFILES FOR ANTIPSYCHOTIC DRUG TARGETS	P048
MARTIN Yvonne C.	THE SIN OF SEDUCTION: DECEPTIVE IMAGES FROM MACROMOLECULAR CRYOCRYSTALLOGRAPHY	H05
MARTINS Filomena	PERFORMANCE OF DIFFERENT QSAR METHODOLOGIES IN THE MODELING OF ANTITUBERCULAR ACTIVITY: MULTIPLE LINEAR REGRESSIONS AND NEURAL NETWORKS	P063
MASEK Brian	RECENT ADVANCES IN QSAR	P060
MATOSIUK Dariusz	STRUCTURAL DETERMINANTS OF BRANCHED 3-(1H-IMIDAZOL-4-YL)PROPYL N-ALKYLCARBAMATES SELECTIVITY FOR THE HISTAMINE H3 OVER H4 RECEPTORS	P088
MERLOT Cedric	PREDICTING ADVERSE DRUG REACTIONS USING SYSTEMS BIOLOGY	P003
MIKROS Emmanuel	VIRTUAL SCREENING, BIOLOGICAL EVALUATIONS AND STRUCTURAL STUDIES OF NOVEL BROMODOMAIN LIGANDS	P117
MITEVA Maria	TOWARDS IN SILICO STRUCTURE-BASED ADMET PREDICTION: MECHANISTIC INSIGHTS FROM PROBING SMALL MOLECULE BINDING TO METABOLISING ENZYMES	OC17
MORREALE Francesca	DRUG DISCOVERY INSPIRED BY NATURE: A VIRTUAL SCREENING APPROACH	P021
MOSER Daniel	DESIGN OF DUAL LIGANDS USING ALIGNED PHARAMACOPHORE MODELS AND MULTI-LAYER SELF-ORGANIZING MAPS	P099
MUENSTERBERG Moritz	EVALUATION OF WATER MOLECULES IN THE ATPASE BINDING SITE OF GYRB	P030
MURGUEITIO Manuela	VIRTUAL SCREENING FOR TOLL-LIKE RECEPTOR ANTAGONISTS: A COMBINED APPROACH	P051
NARAYANA MOORTHY Hari N.S.	BINDING FEATURE ANALYSIS OF SOME PYRROLIDINE DERIVATIVES ON A-MANNOSIDASE ENZYME USING DRUG DESIGN TECHNIQUES	P116
NARAYANA MOORTHY Hari N.S.	ANALYSIS OF PREDICTIVE QSAR MODELS USING MAHALANOBIS DISTANCES	P057
NICOLAOU Christos	THE LILLY OPEN INNOVATION DRUG DISCOVERY PROGRAM	OC23
NIKOLOV Nikolai	IMPROVED TOXICITY PREDICTIONS USING A BATTERY OF QSAR MODELS	P121
NOHA Stefan	MOLECULAR DOCKING OF NATURAL PRODUCTS CHARACTERIZED AS PARTIAL ACTIVATORS OF PPAR-gamma: INFLUENCE OF CHARGES FOR MACROMOLECULE MODELING	P137
OSOLODKIN Dmitry	FLAVIVIRUS ENVELOPE PROTEINS AS A TARGET OF NOVEL ANTIVIRAL LEADS: LEAD IDENTIFICATION AND MOLECULAR DYNAMICS STUDIES	P153
PALA Daniele	INFLUENCE OF TEMPLATE STRUCTURE AND OF LIGAND-BASED OPTIMIZATION ON GPCRS HOMOLOGY MODELING: THE CASE OF THE MT2 MELATONIN RECEPTOR	P075
PALYULIN Vladimir A.	NEW BIVALENT POSITIVE AMPA RECEPTOR MODULATORS: DESIGN, SYNTHESIS AND STUDIES	P115
PANTIC Igor	GREY LEVEL CO-OCCURRENCE MATRIX (GLCM) METHOD: POTENTIAL APPLICATION IN QUANTIFYING CHROMATIN STRUCTURAL CHANGES DURING LYMPHOCYTE MIGRATION AND MATURATION IN THYMUS	P147
PANTIC Igor	QUANTIFICATION OF CHROMATIN AGE-RELATED STRUCTURAL CHANGES IN ERYTHROID PRECURSOR CELLS: GLCM COMPUTATIONAL BIOLOGY ANALYSIS	P148

PANTIC Igor	RELATIONSHIP BETWEEN CHROMATIN STRUCTURE AND NUCLEAR ENVELOPE CIRCULARITY IN MOUSE THYMUS LYMPHOCYTES: IMMUNOPHYSIOLOGY VIEWPOINT	P149
PASTOR Manuel	EXPLORING THE APPLICABILITY OF STRUCTURAL MASKING STRATEGIES IN THE eTOX PROJECT	P050
PETTIFER Steve	UTOPIA DOCUMENTS	OC27
PINTO Marta	CLASSIFICATION MODELS FOR ABC TRANSPORTERS SUBSTRATES	P141
PIPPEL Martin	PARADOCKS - AN OPEN SOURCE FRAMEWORK FOR MOLECULAR MODELLING	P066
PLASENCIA Guillem	IN VIVO ADME/DMPK PARAMETER PREDICTION	P130
POLL Bernhard	PRIORIZATION OF DOCKING POSES VIA MOLECULAR DYNAMICS SIMULATIONS AND MM/GBSA-CALCULATIONS TO PREDICT THE NATIVE BINDING MODE OF THIENO[2,3-b]PYRIDINES IN PLASMODIAL GLYCOGEN SYNTHASE KINASE-3 (PfGSK-3)	P027
POSO Antti	DECOMPOSING DRUG ACTION MECHANISMS INTO RELATIONSHIPS OF CHEMICAL STRUCTURE WITH GENOME WIDE DRUG RESPONSES	P140
POULSEN Anders	STRUCTURE-BASED DESIGN OF MACROCYCLIC KINASE INHIBITORS LEADING TO THE CLINICAL CANDIDATES SB1317, SB1518 & SB1578	P152
PUNGPO Pornpan	THE KEY STRUCTURAL FEATURES OF AZANAPHTHOQUINONE ANNELATED PYRROLE DERIVATIVE AS ANTI-CANCER AGENTS BASED ON THE RATIONAL DRUG DESIGN APPROACHES	P109
RADCHENKO Eugene	PREDICTION OF PHARMACOKINETIC PARAMETERS FOR DIVERSE DRUG COMPOUNDS	P014
RAKERS Christin	INSIGHTS INTO SULFOTRANSFERASE FLEXIBILITY USING MOLECULAR DYNAMICS	P131
REINISCH Jens	AUTOMATIC ALIGNMENT, DRUG-SIMILARITY AND MOLECULAR FIELD ANALYSIS BASED ON THE SURFACE POLARIZATION CHARGE DENSITIES	P072
ROBAA Dina	STRUCTURE-BASED DESIGN OF PRMT6 INHIBITORS	P079
ROGNAN Didier	RECEPTOR-LIGAND PHARMACOPHORES: A NOVEL STRUCTURE-BASED SCREENING WEAPON FOR LIGAND PROFILING AND DISCOVERY OF PROTEIN-PROTEIN INTERFACE INHIBITORS	OC02
SAFANYAEV Alexander	PREDICTION OF ENVIRONMENTAL POLLUTANTS BINDING AFFINITIES TO ARYL HYDROCARBON RECEPTOR	P080
SALO Heikki	STRUCTURE-BASED VIRTUAL SCREENING OF HUMAN SIRT3 INHIBITORS	P023
SANDER Thomas	DATAWARRIOR - UNDERSTANDING DRUG DISCOVERY DATA	P135
SARBU Costel	COMPREHENSIVE QSPR ANALYSIS OF SOLVENTS USING FUZZY CLUSTERING	P001
SASAKI Shunta	DEVELOPMENT OF SUBSTITUENT CONVERSION DATABASE AND SEARCHING SYSTEM BASED ON ChEMBLdb FOR MEDICINAL CHEMISTS	P037
SAYLE Roger	SMALLWORLD: EFFICIENT MAXIMUM COMMON SUBGRAPH SEARCHING OF LARGE DATABASES	P126
SEDDIK Amir	PROBING THE SUBSTRATE SELECTIVITY OF THE SEROTONIN AND DOPAMINE TRANSPORTER BY STRUCTURE-BASED DESIGN	P163
SHANMUGASUNDARAM Veer	STRUCTURE-BASED DESIGN OF COVALENT INHIBITORS: REALITY OR WISHFUL THINKING	OC16
SHIN Woong-Hee	GALAXYDOCK: A FLEXIBLE RECEPTOR-LIGAND DOCKING PROGRAM FOR HIGH ACCURACY PREDICTION	P102
SLYNKO Inna	IDENTIFICATION OF PRK1 KINASE INHIBITORS BY VIRTUAL SCREENING AND BINDING FREE ENERGY CALCULATIONS	P052
SOLIMAN Salwa	USING STRUCTURE-BASED PHARMACOPHORE AND DOCKING MODELS TO GAIN INSIGHT INTO STRUCTURAL BINDING OF HUMAN ARYL SULFOTRANSFERASE 1A1	P067
SOSKIC Milan	BINDING INTERACTIONS OF INDOLE DERIVATIVES WITH β- CYCLODEXTRIN	P073
SPITZMÜLLER Andreas	IN SILICO PREDICTION OF THE TARGET SPACE RELEVANT TO MALARIA	OC26
SRIVASTAVA Sanjay	ENHANCEMENT OF CORPORATE HTS LIBRARY COLLECTION BY PLATE BASED SELECTION	P113
STEUDLE Alexander	ON- AND OFF-TARGET PREDICTION USING 2D AND 3D MOLECULAR SIMILARITY	P089
STIERAND Katrin	THE INTERNET AS SCIENTIFIC KNOWLEDGE BASE: NAVIGATING THE CHEM-BIO SPACE	P120
TAKAHASHI Yoshimasa	EXPLORING FOR MOLECULAR FRAMEWORK OF DRUGS USING EVOLUTIONARY COMPUTATION	P123
TAVARES DO AMARAL Antonia	SIMULATION OF CONFORMATIONAL CHANGE OF OHR FROM XYLELLA FASTIDIOSA BY MOLECULAR DYNAMICS AND EXPERIMENTAL VALIDATION	P061
TAVARES DO AMARAL Antonia	INSIGHTS INTO THE MECHANISM OF ACTION FOR A CYSTEINE PROTEASE INHIBITOR SELECTED BY VIRTUAL SCREENING	P062
TEIJEIRA Marta	APPLICATION OF R-GROUP QSAR FOR CONSENSUS MODELING OF A2B ADENOSINE ANTAGONISTS	P122

TEIXEIRA Cátia	INTEGRATING CoMFA/CoMSIA AND MOLECULAR DOCKING APPROACHES FOR A SERIES OF PEPTIDYL-BASED VINYL SULFONES, PLASMODIUM FALCIPARUM CYSTEINE PROTEASE INHIBITORS	P086
TEMML Veronika	INHIBITION MODES OF QUINONE COMPOUNDS ON 5-LIPOXYGENASE	P125
THOMPSON Stuart	GAS PHASE CALCULATION OF SOLUTION PHASE INTERACTION FREE ENERGIES	P069
TIIKKAINEN Pekka	ESTIMATING ERROR RATES IN BIOACTIVITY DATABASES	P094
TODESCHINI Roberto	NEW TRENDS AND PERSPECTIVES IN QSAR MODELLING	PL07
TOLBERT Bob	OPEN INNOVATION AT OPENEYE: A DECADE OF PRACTICE	OC22
TOSCO Paolo	A NOVEL VIRTUAL SCREENING PARADIGM VIA UNSUPERVISED ITERATIVE ALIGNMENT AND COSMOsar3D DESCRIPTORS	P128
TROMELIN Anne	EXPLORING SUBTLE MOLECULAR INTERACTIONS INVOLVED BETWEEN AROMA COMPOUNDS AND FOOD MEDIUMS USING QSPR APPROACH	P035
TROPSHA Alexander	QSAR WITHOUT BORDERS	H01
TSAREVA Daria	USING OPEN DATA FOR DEVELOPMENT OF CLASSIFICATION MODELS OF TRPV1 ANTAGONISTS	P049
TU Meihua	MEDICINAL CHEMISTRY DESIGN PRINCIPLES FOR LIVER TARGETING	P002
URNIAZ Rafal	ALIGNMENT DEPENDENT STUDY OF AMPAr QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP MODELS	P154
VALENCIA Antoni	QSAR MODELING FOR THE MUTAGENIC POTENTIAL OF DRUG IMPURITIES WITH SYMMETRY	P119
VALLIANATOU Theodosia	ANALYSIS OF PPAR-α/γ ACTIVITY BY COMBINING 2-D QSAR AND MOLECULAR SIMULATION	P074
VARNEK Alexandre	GENERATIVE TOPOGRAPHIC MAPS: UNIVERSAL TOOL FOR DATA VISUALIZATION, DATASETS COMPARISON AND STRUCTURE-ACTIVITY MODELING	OC09
VESELINOVIC Aleksandar	CORAL: QUANTITATIVE STRUCTURE - ACTIVITY RELATIONSHIP MODELS FOR ESTIMATING REACTIVATION OF SARIN INHIBITED ACETLYCHOLINESTERASE BY OXIMES	P039
VIDLER Lewis	DISCOVERY OF NOVEL SMALL MOLECULE INHIBITORS OF BRD4 USING A STRUCTURE-BASED VIRTUAL SCREENING APPROACH	OC04
VITOROVIC-TODOROVIC Maja	4-ARYL-4-OXO-N-PHENYL-2-AMINYLBUTYRAMIDES WITH INTERESTING AChE/BChE SELECTIVITY PROFILE	P096
VON KORFF Modest	ABOUT THE CALCULATION OF COMPLEXITY AND SELF-SIMILARITY FOR CHEMICAL STRUCTURES IN DRUG DISCOVERY	P134
VULPETTI Anna	FLUORINE LOCAL ENVIRONMENT: FROM SCREENING TO DRUG DESIGN	PL06
VUORINEN Anna	DISCOVERY OF XENOBIOTICS DISRUPTING CORTICOSTEROID HOMEOSTASIS BY PHARMACOPHORE MODELING AND VIRTUAL SCREENING	P124
WANG Renxiao	MY STRUGGLE WITH BINDING DATA	PL08
WARR Wendy	DATA MATTERS. THE DISCOVERY OF NEW KNOWLEDGE	H02
WATANABE Yoshiaki	THE DISCOVERY OF HIGHLY ACTIVE AND SELECTIVE α2C ADRENOCEPTOR ANTAGONISTS AND THE ANALYSIS OF THE LIGAND-RECEPTOR INTERACTIONS USING THE HOMOLOGY MODEL	P005
WEINSTEIN Harel	WHY THE KNOWLEDGE REQUIRED FOR LIGAND DESIGN OF TRANSMEMBRANE PROTEIN TARGETS GOES WELL BEYOND THE BINDING SITE	PL03
WICH Louis	GARField: A GRAPH-ACTIVITY RELATIONSHIP FIELD BROWSER	P118
WIRTH Matthias	SWISS BIOISOSTERE - A DATABASE OF MOLECULAR REPLACEMENTS	P107
WISSEL Gloria	MRP2 INHIBITORS MODELLED BY NON-LINER QSAR AND APPLIED TO VIRTUAL SCREENING	P112
WOLBER Gerhard	IMPROVING 3D PHARMACOPHORE PERCEPTION AND VIRTUAL SCREENING BY INCREASED GEOMETRIC ACCURACY	OC01
YALCIN Ismail	COMMON FEATURE PHARMACOPHORE GENERATION OF BACTERIAL AdeABC EFFLUX PUMP INHIBITORS	P078
YAP Chun Wei	PaDEL-DDPREDICTOR: SOFTWARE TO CALCULATE PD/PK/T PROPERTIES	P159
YILMAZ Serap	PHARMACOPHORE MODELLING OF SOME FUSED HETEROCYCLIC COMPOUNDS AS HIV-1 REVERSE TRANSCRIPTASE INHIBITORS	P083
YOU Hwan	GA-SVM FOR CLASSIFICATION OF COMPOUNDS ABSORBED BY HEPATIC IMPORTERS	P044
YUTA Kohtaro	NEW APPROACH FOR QSAR AND QSTR TREND ANALYSIS ON LARGE SAMPLE DATA SET BY THE KY-METHODS	P077

Index of Authors

FONTAINE	F.	P130	HAHN	S.	P099
FORSTER	M.	PL09	HALM	M.-P.	P143, P144
FRACZKIEWICZ	R.	P156	HAN	S.	OC16
FRANKE	L.	P094	HANDA	K.	P009
FRANTI	M.	P113	HANNONGBUA	S.	P109
FUCHS	J. E.	P017	HANSON	J.	P053
FULLE	S.	P054	HARA	H.	P038
FURUTA	Y.	P005	HARDER	T.	P120
GABORIAUD-COLAR	N.	P117	HÄRKÖNEN	H. H.	P157
GAGO	F.	P064	HARLAND	L.	OC28
GALLO	G.	P160	HARPSØE	K.	P128
GARCIA-SERNA	R.	OC26	HARTENFELLER	M.	OC12
GARRIGUES	T.	P042	HAWKINS	P.	OC14
GASPAR	H.	OC09	HAYES	C.	OC18
GASTEIGER	J.	P139	HE	Y.	P159
GASTREICH	M.	OC10	HEGAZY	G.	P092
GAUTHIER	A.	P113	HEISS	E. H.	P137
GAWANDE	D.	P065	HELMA	C.	OC15
GEDECK	P.	OC25, P018	HENRICH	S.	P029
GEMTIO	L.	P112	HENRY	T.	P081
GEOGHEGAN	K.	OC16	HENZLER	A. M.	OC05
GIAGINIS	C.	P074	HEO	L.	P101
GIANNINI	G.	P160	HERT	J.	P110
GIEGERICH	C.	PL01	HESSLER	G.	OC11, PL01
GIOIELLO	A.	P004	HICKEY	M.	OC03
GOBEC	S.	P106	HIRAYAMA	N.	P026
GODEVAC	D. M.	P084	HIRONO	S.	P009
GOEL	R. K.	P065	HISS	J.	OC13
GOETHALS	O.	P158	HOELDER	S.	OC04
GOH	K. C.	P152	HOFMANN	B.	P099
GOMES	J. R. B.	P086	HOGNER	A.	OC20
GOMES	P.	P086	HONMA	T.	P037
GONZALEZ-ÁLVAREZ	I.	P042	HRDA	M.	P142
GOTO	J.	P026	HUANG	B.	OC03
GOUDA	H.	P009	HUBBUCH	J.	P104
GRACE	C. R.	P162	HUBER	R. G.	P017
GRANDITS	M.	P085	HUNTER	B.	P138
GRANT	A.	P126	HUNTER	C. A.	P068, P069
GRATON	J.	P028	IBIS	G.	OC01
GRECU	T.	P068	ILIC	K.	P011, P013
GREGORI-PUIGJANE	E.	P110	IMAGAWA	J.-I.	P005
GRESE	T.	OC23	IMAI	Y. N.	P038
GRIGORIEV	V. V.	P115	IRWIN	J.	P110
GUICHARD	E.	P035	IVANOV	S.	OC24, P065
GUY	R.K.	P162	JAIN	A. N.	P089
GÜNAY	Z.	P006, P007	JALAIE	M.	OC03
GÜTLEIN	M.	OC15	JARHO	E.	P023
HADJIPAVLOU-LITINA	D.	P076, P082	JARZEMBEK	K.	P031