Research project offer for incoming students

Department of Clinical Pharmacy

Head: prof. dr hab. Anna Wesołowska

1. **Presentation-Objectives-Key points**

   The main topics cover the study of behavioural pharmacological properties of centrally acting molecules with potential application in treatment of psychiatric diseases, neurodegenerative disorders and epilepsy as well as pain relievers. Also, pharmacological properties of newly synthesized compounds based on molecular mechanism of ligand-receptor interaction are specified in the frame of wide structure-affinity and structure-activity relationships studies.

2.1 Research Topics

2.1 Pharmacological properties of compounds with potential antidepressant, anxiolytic and antipsychotic activity, targeted on serotonin, dopamine, $GABA_A$ and metabotropic receptors – therapeutic activity and side-effect actions

2.2 Pharmacological characteristics of compounds with potential anticonvulsant activity and GABA uptake inhibitors

2.3 Pharmacological characteristics of potential pain relievers in rodents

2.4 Vitamin D metabolism and polymorphisms of the vitamin D receptor gene in relation to structure and function of large arteries and left ventricle

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Department of Food Chemistry and Nutrition

Head: dr hab. Paweł Zagrodzki

1. **Presentation-Objectives-Key points**

   The main topics cover: 1) biochemistry of minerals (calcium, magnesium), trace elements (zinc, copper, selenium, iodine, vanadium) and heavy and toxic metals (lead, cadmium, aluminum) in food products, as well as in human body and animals; 2) antioxidant status *in vitro* and *in vivo*.

2. **Research Topics**

   2.1. Investigation on effects of various plants (amaranth, quinoa, buckwheat, rye, rutabaga) on some biochemical parameters in blood and organs in rats fed high-fat and high-fructose diet with various supplements.

   2.2. Determination of various chemical parameters in wines.

   2.3. Antioxidant activity, content of poliphenols and organic acids, and selected elements in fruit juices originated from conventional and organic cultivations.

   2.4. Investigation of oily plants with pro-healthy properties.

   2.5. Evaluation of minerals and trace elements intake via drinking water.

   2.6. Study on interaction between selenium status, thyroid metabolism, immunological system and antioxidant status in women with Hashimoto disease.

   2.7. *In vivo* models for new organic compounds of vanadium designed to support the treatment of diabetes.

   2.8. Lithium status in healthy subjects, in patients with CVD and with kidney diseases.

   2.9. The influence of trace elements on the fermentation process carried out by the wild culture of *Lactobacillus* bacteria

   2.10. The chemometric approach to biochemical studies.

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Department of Medicinal Chemistry

Head: Prof. dr hab. Maciej Pawłowski

1. **Presentation-Objectives-Key points**

   The main topics covers synthesis, study of physico-chemical, biological and pharmacological properties of biomolecules acting on CNS with potential application in the treatment of psychiatric disorders, neurodegenerative disorders and epilepsy. Structure design and structure-activity relationships of newly synthesized compounds are based on molecular mechanism of ligand-receptor interaction and supported by computer-aided methods.

2. Research Topics

2.1 Chemistry

- Chemistry of heterocycles
- Microwave-assisted synthesis
- Solid-phase organic chemistry

2.2 Medicinal Chemistry

- Design and synthesis of compounds with potential antidepressant, anxiolytic and antipsychotic activity, targeted on 5-HT_{1A}, 5-HT_{2A}, 5-HT_6, 5-HT_7, D_2 receptors
- Design and synthesis of compounds with potential antpsychotic activity targeted on GABAA receptors
- Synthesis of compounds with potential anticonvulsant activity

2.3 Analysis

- Molecular modeling: homology modeling of GPCRs, ligand docking, pharmacophore based database search
- Determination of newly synthesized compounds structure by means of spectroscopic and combustion analysis
- QSAR, prediction and determination of physic-chemical properties of organic compounds

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Department of Pharmaceutical Botany

Head: prof. dr hab. Halina Ekiert

1. **Presentation-Objectives-Key points**

   The main topics covers: establishing and maintaining medicinal plant in vitro cultures intended as a biotechnological source of therapeutically important compounds; chemical studies of fruiting bodies of higher fungi, mostly representatives of Basidiomycota, aimed at examining the contents of biologically active metabolites; establishing and maintaining in vitro cultures (so-called mycelial culture) of some chosen species of higher fungi in order to propose biotechnological methods of obtaining therapeutically important compounds.

2. **Research Topics**

   2.1 Medicinal plant biotechnology with elements of phytochemistry

   Studies on endogenous accumulation of plant metabolites, especially phenolic acids, coumarins, flavonoids, schisandra lignans, sulfur metabolites, under different in vitro culture conditions

   - Quantitative analysis of metabolites
   - Isolation and purification of main metabolites

   Comparative phytochemical studies of plants growing in vivo

   Biotransformations of exogenous substrates, especially bioconversions of simple phenolic compounds, e.g. hydroquinone, tyrosine, p-hydroxybenzoic acid into arbutin

   - Optimization of biotransformations conditions
   - Quantitative analysis of biotransformations products
   - Isolation and purification of biotransformations products

   2.2 Mycochemistry

   - Quantitative analysis of different groups of metabolites e.g. non-hallucinogenic indole compounds, phenolic acids, sterols, fatty acids, polysaccharides in fruiting bodies extracts

   2.3 Biotechnology of higher fungi

   Studies on endogenous accumulation of fungi metabolites under different in vitro culture conditions

   - Quantitative analysis of metabolites
   - Isolation and purification of main metabolites

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Department of Physicochemical Drug Analysis

Head: Prof. dr hab. Barbara Malawska

1. **Presentation-Objectives-Key points**

   The main topics covers synthesis, study of physicochemical, biological and pharmacological properties of biomolecules acting on CNS with potential application in the treatment of neurodegenerative disorders and epilepsy. Structure design and structure-activity relationships of newly synthesized compounds are based on molecular mechanism of ligand-receptor interaction and supported by computer-aided methods.

2. **Research Topics**

   2.1 Chemistry

   - Chemistry of heterocycles
   - Microwave-assisted synthesis
   - Chiral organic synthesis

   2.2 Medicinal Chemistry

   - Design and synthesis of compounds with potential anticholinesterases activity
   - Design and synthesis of compounds with potential anticonvulsant activity targeted on GABA transporter
   - Design and synthesis multifunctional ligands targeting neurodegenerative processes

   2.3 Analysis

   - Determination of physicochemical properties of newly synthesized compounds using chromatographic and electrophoresis methods and their prediction by use different software
   - Molecular modeling: virtual screening, ligand docking, pharmacophore models

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Department of Pharmacokinetics and Physical Pharmacy

Deputy Head: dr hab. Elżbieta Wyska, prof. UJCM

1. **Presentation-Objectives-Key points**

   The main topics cover pharmacokinetics and pharmacodynamics of anti-inflammatory drugs in animal models of sepsis, pharmacokinetics of new chiral compounds with antiepileptic properties, and evaluation of new bioceramic materials in *in vitro* and *in vivo* conditions. Concentrations of drugs in media, different body fluids and tissues are measured by HPLC with different detection modes, such as UV, fluorescence, electrochemical, or MS/MS detection. Markers of drug response are measured using HPLC or ELISA. Cytokine gene expression in tissues is assessed by real-time RT-PCR. Advanced modeling techniques are used for data analysis and simulations.

2. **Research Topics**

2.1 Pharmacokinetics and pharmacodynamics of drugs that modulate cAMP levels in LPS-induced model of sepsis in rats

- Animal experiments and development of analytical methods
- Assessment of different markers of drug response
- Development of pharmacokinetic-pharmacodynamic models for quantitative data analysis and predictions

2.2 Pharmacokinetics of new chiral aminoalkanol derivatives

- Studies on pharmacokinetics and tissue distribution of chiral aminoalkanol derivatives in rats
- Enantioselective HPLC method development and validation
- Physiological modeling of plasma and tissue concentrations versus time data

2.3 Kinetics of drug release from new bioceramic materials in vitro and in vivo

- Influence of biomaterial composition on kinetics of drug release
- Studies on drug release from studied biomaterials in different media
- In vivo studies on rats
- Application of mathematical models for data analysis

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Department of Pharmacodynamics

Head: Prof. dr hab. Barbara Filipek

1. **Presentation-Objectives-Key points**

   Scientific activities were focused on evaluation of the cardiovascular activity, anticonvulsant, antidepressant and anxiolytic properties, antioxidant and analgesic activity, local anaesthetic and anti-inflammatory properties of new compounds with expected biological activity.

2. **Research Topics**

2.1. In vivo models

- Investigations of the antiarrhythmic, antihypertensive and alfa-adrenoceptor blocking activity of novel compounds
- Evaluation of the local anesthetic, analgesic and anti-inflammatory activities
- Studies of the potential antidepressant and anxiolytic activity
- Evaluation of the anticonvulsant activity
- Evaluation of pharmacological properties of new GABA uptake inhibitors
- Evaluation of the sedative or stimulatory activity
- Evaluation of the pharmacological properties of new histamine H3 and H4 ligands
- Investigations of the antioxidant activity

2.2. In vitro tests

- Alfa-sympatholytic activity in isolated vascular smooth muscle (rat tail artery and thoracic aorta)
- Alfa-sympatholytic acticity in the isolated rabbit spleen
- Spasmolytic activity in the isolated guinea pig ileum and rabbit ileum
- Antihistaminic properties in the isolated guinea pig ileum
- Influence on isolated heart according to Langendorff
- Influence on the ventricular arrhythmias associated with coronary artery occlusion and reperfusion in the non-working isolated perfused rat heart

2.3. Studies on the relationships between structure of new compounds and their pharmacological activity

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Department of Pharmaceutical Technology and Biopharmaceutics

Head: Prof. dr hab. Reneta Jachowicz

1. **Presentation-Objectives-Key points**

   The proposed research topics concern the qualitative and quantitative characteristics of the phenomena associated with the penetration of water into the polymeric matrices together with the structural characteristics. Its essence is to develop and apply a set of mainly non-invasive imaging techniques, which will characterize the pharmaceutical controlled release systems in a complementary way. The applied methods will allow to characterize the hydrating matrices in micro- and meso-scale. Simultaneously with technological research studies computational and modeling tasks will be completed. Objectives include multivariate modeling with heuristic, statistical and mathematical approaches to find relationships between composition of pharmaceutical formulations and their selected properties. Data-mining and predictive modeling will be employed simultaneously for automatic knowledge acquisition and processing. Integration of description of qualitative and quantitative composition plus technological parameters of the manufacturing process will guarantee complete multi-scale modeling.

2. **Research Topics**

   2.1 **Technological tasks**

   - Matrix polymeric dosage forms.
   - Solid particles for pulmonary delivery.
   - Transdermal delivery systems.

   2.2 **Analytical tasks**

   - Dissolution studies in combination with Magnetic Resonance Imaging for recording water transport within the matrix dosage forms.
   - Development of reference techniques for elucidation of phenomena occurring in the polymeric matrices during hydration e.g. DSC, IR, etc.
   - Structural analyses of hydrated polymeric matrices.

   2.3 **Modeling and computational tasks**

   - Heuristic modeling: artificial neural networks, genetic algorithms, fuzzy logic.
   - Statistical modeling and optimization.
   - Sensitivity analysis.
   - Chemoinformatics.
   - Linux environment and bash programming.
   - Grid computing.
   - Parallel computations.

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Department of Social Pharmacy

Head: dr hab. Agnieszka Skowron

1. **Presentation-Objectives-Key points**

   The Department of Social Pharmacy focuses on the research topics concerning: pharmacy practice, pharmaceutical care, patient counseling, medicines usage, drug related problems, drug information, patient education, smoking cessation.
   The aim of our research programs is to support the development of the pharmacy profession in Poland towards the implementation of pharmaceutical care in community pharmacies and to provide evidence for the impact of pharmaceutical care on economic and clinical outcomes.
   Our research activities consist of observational as well as intervention studies.

2. **Research Topics**

   2.1 <u>Pharmaceutical care in hypertension and diabetes</u>
   - Pharmacoeconomic analysis of pharmaceutical care
   - Analysis of the drug-related problems identified during pharmaceutical care process

   2.2 <u>Smoking cessation</u>
   - Monitoring the outpatient smoking-cessation programme (in cooperation with the community pharmacies),

   2.3 <u>Counseling in community pharmacy</u>

   - Use of simulated patients (mystery shoppers) methodology to assess the clinical and communication skills of community pharmacists
   - Analysis of the drug-related problems identified during pharmaceutical consultation

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Department of Social Pharmacy
Unit of Pharmacoepidemiology and Pharmacoeconomics

Head: dr hab. Sebastian Polak

1. **Presentation-Objectives-Key points**

   Unit of Pharmacoepidemiology and Pharmacoeconomics carries out research in the field drugs safety assessment at the various level of drug development. The applied methods include in silico realized mathematical modeling and simulation, in vitro - in vivo extrapolation, epidemiological and pharmacoepidemiological studies. The main objective is to provide tools for early toxicity prediction at the population level. More details can be found at www.tox-portal.net

2. **Research Topics**

2.1 Health Technology Assessment

- Systematic reviews and metaanalysis
- Cost analysis in hospital pharmacy
- Quality of life analysis in diabetes and hypertension

2.2 Computational toxicology

- Early toxicity prediction,
- QSAR modeling,
- Soft computing paradigm application for drugs toxicity prediction

2.3 In vitro – in vivo extrapolation in toxicology

- Proarrhythmic activity of drugs
- Drugs cardiotoxicity
- Mathematical modeling and simulation at the population level

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Department of Technology and Biotechnology of Drugs

Head: prof. dr hab. Katarzyna Kieć-Kononowicz

1. Presentation-Objectives-Key points

Computer aided drug design
Synthesis of biologically active compounds
Biotechnological aspects in search for new drugs

2. Research Topics

2.1 **Computer aided drug design**

- Basic in molecular modeling of 3D structures of drugs and potential drugs
- Basic in prediction of ADME-Tox properties (blood-brain barrier permission, toxicity risk, phospholipidosis, drug ability)

2.2 **Practice in labs of organic chemistry**

- Synthesis of new biologically active compounds including classical and microwave aided methods
- Evaluation of purity and identity of synthesized compounds using basic analytical and spectral methods
- Estimation of physicochemical properties using planar chromatography

2.3 **Biotechnological aspects in search for new drugs.**

- Experimental studies *in vitro* on biotransformation of biologically active compounds
- Studies in silico on biotransformation of biologically active compounds
- Compounds screening against intrinsic and overexpressed efflux pumps of procariotes e.g. *Staphylococcus aureus* and eucariotes e.g. different cancer cells
- Genotoxicity and cytotoxicity of the biologically active compounds

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