Graduate School of Pharmaceutical Sciences

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The especially advanced possibilities of complex pharmaceutical research are exploited at the Faculty of Pharmacy, University of Szeged since its different institutes represent the whole area of pharmaceutical research from the synthesis or isolation of biologically active compounds through their pharmacological or biopharmaceutical investigations to their formulation. Students can join different fields of pharmaceutical research according to their interests, at the same time gain wide-ranging knowledge on other fields as well on the available courses. The scientific parts of each program are introduced separately although they represent a single unit.

Cooperating Institutions

Faculty of Science of the University of Szeged
Department of Applied and Environmental Chemistry
Department of Colloid Chemistry
Department of Organic Chemistry
Department of Physical Chemistry
Department of Solid State and Radiochemistry

Faculty of General Medicine of the University of Szeged
Clinics and the Theoretical Institutes

Faculty of Pharmacy, Semmelweis University, Budapest

Faculty of Horticulture of the Corvinus University Budapest
Department of Medicinal and Aromatic Plants

Faculty of Science of the University of Pécs
Department of Botany and Botanical Garden

Faculty of Chemical Engineering of the Technical University Budapest
Department of Organic Chemistry
Department of Organic Chemical Technologies

Faculty of Science of the University of Debrecen
Department of Organic Chemistry

Research Institute of Ecology and Botany of the Hungarian Academy of Sciences, Vácrátót

Plant Protection Research Institute of the Hungarian Academy of Sciences, Budapest

EDUCATIONAL PROGRAMMES

1. PHARMACEUTICAL CHEMISTRY AND DRUG RESEARCH

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Research programmes

(A) Chemistry of cyclic ß-amino acids

- Development of new synthetic process for ß -amino acids.
- Synthesis of cyclic ß-amino acids from terpene derivatives.
- Functionalizations of ß-amino acids.
- Synthesis and structure studies of peptide oligomers.
- The use of difunctional synthons on enantioselective catalysis.

Supervisors: Prof. Ferenc Fülöp DSc, Zsolt Szakonyi PhD, Tamás Martinek PhD

(B) Isoquinoline chemistry

- Synthesis of new isoquinolines alkaloid analogs.
- Synthesis of di- and trifunctional tetrahydroisoquinolines.
- Synthesis and stereochemistry of isoquinoline fused heterocycles.

Supervisors: Assoc. Prof. László Lázár CSc, Prof. Ferenc Fülöp DSc

(C) Enzyme catalysed transformations

- Kinetic resolutions of amino acids, 1,2- and 1,3-aminoalcohol derivatives.
- Bakers yeast catalysed transformations of prochiral compounds.
- Dynamic kinetic resolutions, of mono- and difunctional compounds.

Supervisors: Prof. Ferenc Fülöp DSc, Enikő Forró PhD

(D) Synthesis of 1,3-heterocycles, potential pharmacons.

- Retro Diels-Alder methodology for preparation of heterocycles.
- Synthesis of 1,3-heterocycles from cyclic -amino acids and aminoalcohol derivatives.
- Application of heterocycles in enantioselective syntheses.

Supervisors: Prof. Géza Stájer DSc, Prof. Ferenc Fülöp DSc, Assoc. Prof. László Lázár CSc.

Instrumental background

The Institute possesses all the modern instruments to aid the synthetic activity. For analytical and spectroscopic characterization of compounds: Bruker Avance DRX 400 and 500 MHZ NMR spectrometer, Perkin-Elmer Paragon 1000 PC FT-IR spectrophotometer; Unicam UV2 UV/VIS spectrometer; Crompack CP-9002 GC; Varian 3900 GC with automatic sample adapter, Perkin-Elmer Autosystem XL GC; Waters HPLC with 600E type pump and 486 type detector; Jasco 870-UV type HPLC detector with Varian 2510 pump; Finnigan MAT 95 S type LC-MS, GC-MS and HRMS instrument; Perkin-Elmer 2400 elemental analyzer; Perkin-Elmer 341 polarimeter. MOE (Molecular Operating Enviroment); Gaussian C3.

Courses

Synthetic pharmaceutical chemistry, drug research (Prof. Gábor Bernáth DSc, Prof. Géza Stájer DSc)

The lectures give a review on the most frequently used building blocks in pharmaceutical synthesis and some of their selected applications. Methods for building up the most important skeletons and functional groups in drug molecules are demonstrated. Among the specialities the synthesis of different types of pharmaceuticals are discussed. The structure-activity relationships are pointed out with special emphasis during the discussion of different types of pharmaceuticals and their

members. Different synthesis routes are usually demonstrated for the included drugs and drug types, special synthesis routes besides commonly applicable ones.

Chemical and stereochemical basics of drug research (Prof. Ferenc Fülöp DSc and invited lecturers)

Chemical aspects of novel drug design. Pharmaceutical industry of the world. Possibilities of picking out "lead molecules" and their chemical development to drugs. Possibilities of structure modification. Pharmacological effects of related structures, homologues, isosters and isomers. Overview of stereochemical and conformational knowledge. Nomenclature, ways of representation. Conformational relationships in acyclic, cyclic and polycyclic systems. Most commonly occurring types of isomerism in drug molecules. Synthesis and separation methods of isomers. Effect of stereoisomerism on drug activity. Structure and isomerism in different drug types. Pharmacological differences between isomers.

Enantioselective syntheses (Prof. Ferenc Fülöp DSc, Assoc. Prof. László Lázár CSc and invited lecturers)

During the lectures the following topics are discussed: enzymatic enantioselective transformations (hydrolysis, reduction, oxidation etc.); application of optically pure chiral building blocks in asymmetric synthesis; enantioselective catalysts and additives; asymmetric "en"-reactions; the role of metal complexes in asymmetric syntheses; asymmetric hydrogen-transfer reactions; the origin of homogenity in nature; enantioselective syntheses in the preparation of pharmaceuticals.

Chemistry and stereochemistry of saturated heterocycles (Prof. Ferenc Fülöp DSc)

The lectures review the results up to date in the field of two or more membered saturated heterocycles (mainly six-membered O,N, N,N, O,S and N,S 1,3-heterocycles condensed with carbocycles with different ring sizes). It gives an overall picture of synthetic, stereochemical and conformational analysis methods.

Combinatorial chemistry (Prof. Ferenc Fülöp DSc and invited lecturers)

The lectures deal with the development of combinatorial chemistry and the main possibilities of application, like combinatorial syntheses on solid support (types and characteristics of solid supports). Synthesis of heterocyclic compounds on solid support. Solution phase combinatorial syntheses. Multicomponent reactions. Purification techniques. Analytics in combinatorial chemistry. Automatic synthesizers.

Basics of computer-assisted drug design (Tamás Martinek PhD and invited lecturers)

An introduction to the practical applications of theoretical methods in rational drug design is aimed. Tools of molecular modelling: computer-assisted representation of molecular structure (Z-matrix, coordinate-matrix), molecular graphics; conformational energy, energy map and its determination (ab-initio, semi-empirical methods, molecular force-field models); methods for determination of stable conformations (minimalisation techniques, molecular dynamics, DG (distance geometry), random and systematic search methods); assignment of conformation with the aid of experimental data (Rtg → X-Ray, NMR), search for conditional minimum. Quantitative structure-activity relationships (QSAR): interpretation of functional relationship between measured and calculated physical-chemical parameters and biological activity, notion of predictive force; originating functional relationships and their adaptation to experimental data (minimal square method, partial minimal square, application of neural networks, genetic algorithms); main QSAR models (Hansch-models, CoMFA, Hologram-QSAR).

2. PHARMACODYNAMICS, BIOPARMACY AND CLINICAL PHARMACY

Programme director: Prof. György Falkay DSc

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Research programmes

(A) Pharmacology of reproduction.

- Pharmacological manipulation of pregnant uterus and cervix focusing on the possible treatments of the premature labor.
- Identification and ontogeny of adrenergic receptor subtypes in the pregnant myometrium (radioligand technique, PCR, blotting assay).
- Assessing contractility and pharmacological reactivity of pregnant myometrium and placental vessels by electric field stimulation.
- Investigation of the adrenergic denervation of the pregnant uterus using electric field stimulation and superfusion technique.
- Investigation of tocolytic substances (adrenergic agonists and antagonists, oxytocin antagonists) by a post-partum rat model in vivo.

Supervisors: Prof. György Falkay DSc, Róbert Gáspár PhD, István Zupkó PhD

(B) Pharmacology of sexual steroid hormones.

- Development of sexual steroids (estrogens, progestins and antiprogestins) by in vitro and in vivo methods. This project targets the elaboration of new, selective active agents.
- Investigation of effects of progestins and antiprogestins on the cervical resistance during pregnancy of the rat.

Supervisors: Prof. György Falkay DSc, Róbert Gáspár PhD, István Zupkó PhD

(C) Clinical pharmacy.

- Methods for improving rational drug use. This topic includes therapeutic drug monitoring of selected antibacterial preparations as well as assessment of interaction risk: genetic polymorphism of CYP-s.
- Pharmaceutical care models for optimizing the chronic drug administration including adherence /compliance assessment, quality of life measurement. Investigation of indicators of rational drug prescribing: problem of polypharmacy.

Supervisor: Assoc. Prof. Gyöngyvér Soós CSc

Courses

Signal transduction mechanisms (Prof. György Falkay DSc, Res. Prof. Anna Borsodi DSc)

This course includes the discussion and demonstration of the methods used in receptor research, detailed characterization of the main receptor types according to the generally accepted classification (e.g. ion channels, nuclear receptors, enzyme and G-protein coupled receptors). The emphasis is put on the possible pharmacological influence of the special receptors.

Practical pharmacology of reproduction (Prof. György Falkay DSc)

This course deals with the practical therapeutic possibilities of negative and positive family planning. The most important chapters include oral contraception, induction of ovulation, hormone replacement therapy, tocolysis and pregnancy-associated therapy. The presently used methods in assisted reproduction are additionally discussed.

Selected chapters in pharmacology (Prof. György Falkay DSc, István Zupkó PhD, Róbert Gáspár PhD)

The course discusses the most intensively developing chapters of the pharmacology in a more detailed way as it is possible in the gradual education. In the selection pharmacons or groups are favoured with new mechanism of action, which are not generally used yet. The course is given partly by invited lecturers.

Research methods in pharmaceutical care (Assoc. Prof. Gyöngyvér Soós PhD)

During the seminars relevant examples from the pharmaceutical field will be given including issues dealing with drug utilization and information and the pharmacist's professional activities.

Pharmacovigilance, pharmacoepidemiology (Assoc. Prof. Gyöngyvér Soós CSc)

Comprehensive overview about the safety problem of drug use in the every day practice.

3. PHARMACOGNOSY. CHEMICAL DIVERSITY AND UTILIZATION OF PLANTS (PHARMACOBOTANY, PHYTOCHEMISTRY, UTILIZATION OF MEDICINAL PLANTS)

Programme director: Prof. Imre Máthé DSc

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Pharmacognosy is one of the oldest sciences, which is in the most direct relation with the natural living world, especially with the plant kingdom, in medicinal treatment, and as such it strives not only to learn about and to utilize the diversity of the plant kingdom as widely as possible, but it also has an interest in its preservation and in the broadest sence with the utilisation of plants. It covers Pharmacobotany, Chemotaxonomy, Phytochemistry, Phytotherapy, Utilization of Medicinal Plants, (bio)technology as main fields. The structure of the program expresses this by its following training programmes: 1. Pharmacobotany, 2. Phytochemistry, 3. Utilization of medicinal plants (phytotherapy).

The program covers disciplines or scientific fields like Classical botany within it plant morphology, chemotaxonomy, biodiversity of medicinal plants, production biology of the active principles, plant physiology (metabolic pathways) allelochemistry, pharmacognosy, cultivation of medicinal plants, plant chemistry (phytohemistry), extraction, separation, instrumental examination of plant substances, description of preparations made from medicinal plants, their manufacturing technology (GMP), phytotherapy, some aspects of pharmacodynamics, drug research, biotechnology.

The programme is open for pharmacists, diploma chemists, biologists diploma agriculturists, medical doctors, having university degree. It is open for Hungarian and foreign students, speaking Hungarian and/or English and in special cases German languages.

Infrastructure: student laboratory for 24 persons, connection to the computer network databases, personal computers for each researcher, 3 HPLCs, 1 GC-MS, 1 GC-FID detector, densitometric, NMR access possibilities, UV-VIS, IR spectrophotometers are available etc.

Close, everyday relationship with the Research Institute of Ecology and Botany of the Hungarian Academy of Sciences where the richest plant collection in Hungary, including a special medicinal plant collection is available for field experiments.

Research programmes

- Pharmacobotany: this project group comprises questions of Botany, Plant morphology, Chemotaxonomy, Ecological chemistry and in a certain sense Cultivation of medicinal plants, etc. (Supervisors: Prof. Imre Máthé DSc, Assoc. Prof. László Tóth CSc)
- Phytochemistry: it deals with the isolation, chemical structure of active ingredients, separation technique, preparative and analytical chemistry. (Supervisors: Prof. Judit Hohmann CSc, Assoc. Prof. Mária Báthori CSc)
- Utilization of medicinal plants: it comprises subject-matter concerning the utility, processing, use of medicinal plants, spices, aromatic and other, potential medicinal plants as well as knowledge regarding phytotherapy. (Supervisor: Assoc. Prof. Erzsébet Varga CSc)

Courses

- Pharmacobotany (Assoc. Prof. László Tóth CSc)
- Chemotaxonomy (Assoc. Prof. László Tóth CSc, Prof. Imre Máthé DSc)
- Comparative phytochemistry (Assoc. Prof. László Tóth CSc, Prof. Imre Máthé DSc)
- Fundamentals in phytochemistry (Assoc. Prof. Mária Báthori CSc, Prof. Judit Hohmann CSc)
- Phytochemistry (Assoc. Prof. Mária Báthori CSc, Prof. Judit Hohmann CSc)
- Separation technique (Assoc. Prof. Mária Báthori CSc, Prof. Judit Hohmann CSc)
- Applied botany and pharmacognosy, (Assoc. Prof. Erzsébet Varga CSc, Zsuzsanna Hajdú PhD)
- Narcotics, drugs of natural origin (Prof. Kálmán Szendrei, Gábor Nagy PhD.)

4. PHARMACEUTICAL TECHNOLOGY

Programme director: Prof. István Erős DSc

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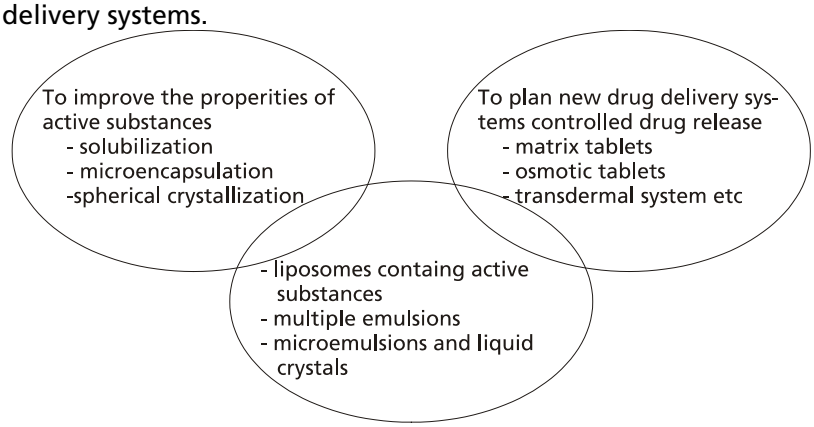
Pharmaceutical technology is one of the most dynamically developing fields of pharmaceutical sciences. Its importance lies primarily in the fact that however promising a drug is, it can be used in therapy only in an appropriate form, that is after formulation. Proper formulation is the prerequisite to bioavailability. Thus pharmaceutical technology is not only a modern, important and interesting applied science but it is also responsible for the success of therapy to a great extent.

There are two basic research directions in modern pharmaceutical technology today:

1. to improve the properties (mainly solubility) of the active ingredient,
2. to plan new drug delivery systems (therapeutic systems) with better bioavailability

Based on this, the doctoral program also consists of two major elements: the improvement of drug properties with solubilization, microencapsulation, molecular encapsulation and spherical crystallization, and the planning of new solid and semi-solid drug delivery systems.



Research programmes:

(A) Improvement of the properties of drugs with incorporation in micro- and nanoforms, the planning of new colloidal drug delivery systems

- solubilization of new drugs,
- microencapsulation of drugs,
- production of nanoparticles from drugs,
- production of liposomes, incorporation of drugs in liposomes,
- production of drug delivery systems with complex emulsion base,
- production of drug delivery systems with microemulsion and liquid crystal base.

Supervisors: Prof. I Erős DSc, E. Csányi. PhD

(B) Research-development in the field of tablets and coated tablets
- technological improvement of granulation and pelleting preceding tabletting
- improvement of the flow properties of powders and gradulated products by means of coating the crystals and granules and with the use of additives
- morphological, rheological and thermoanalytical examination of treated and untreated crystals and granules
- examination of the effect of the coating on encapsulation
- research of the energy conditions of tablet pressing
- development of new coating methods
- improvement of drug dissolution
- providing controlled drug delivery with the help of technological means

Supervisors: Assoc. Prof. K. Hódi CSc, P. Kása PhD, G. Regdon PhD.

(C) Improvement of the properties of solid drugs with spherical crystallization and confection
- Investigation of the thermic behaviour of crystalline materials (DTA, DSC, DDSC examinations)
- Examination of the circumstances and results of spherical crystallization, introduction of confectioning in the formulation of solid dosage forms

Supervisors: Prof. P. Révész CSc, Z. Aigner PhD

(D) Novel aspects of quality assurance in the development of medicinal products: determination of key process parameters for control and validation. Analysis of the impact of regulatory measures on the development, application and consumption of medicines.

Supervisor: Prof. Tamás Paál CSc.

Courses

The optional courses advertised by the Institute are partly related to the research fields investigated in our Institute (e.g. pharmaceutical rheology, stability of disperse and coherent systems, modern solid and colloidal drug delivery systems), and partly to the main directions of development of pharmaceutical technology (e.g. therapeutic systems). The primary principle in organizing optional courses has been (so far) to enable the students to collect the necessary credit points by the end of the second year so that they can devote all their energy to writing their thesis and publications during the last year.

We took care to provide the student with the possibility to continue his/her student research topic and to make use of the methodology and expertise in approach already acquired, and another consideration was that the work load of the assistant consultants should be uniform, if possible.

Pharmaceutical rheology (I. Erős, E. Csányi, K. Hódi)

A two-semester course, with 15 x 2 hours per semester. The rheological properties of major dosage forms (colloidal solutions, emulsions, suspensions, creams, gels, ointments, powders), modern examinations methods (e.g. creep test, elasticity measurement) and the rheological aspects of important technological operations (mixing, grinding, pressing) are presented in the lectures.

Stability and stabilization of disperse and coherent systems (I. Erős,. P. Révész,. K. Hódi, Z. Aigner)

The course lasts for 1 semester, 15 x 3 hours. The most important topics of the lectures are: thermodynamic and kinetic stability, stability of the dispersity degree on and distribution, stability and stabilization of composed preparations, decomposition-selective analytical methods, HPLC, DSC, execution of accelerated stability examinations, determination of expiry.

Relationship between pharmaceutical technology and therapeutic effect (I. Erős, K. Hódi, P. Révész)

It is a two-semester course, 15 x 3 hours per semester. The following major topics are dealt with during the course: the LADMER system, technological possibilities of prolonged release, technological possibilities of controlled release, technological solutions of targeting drugs, technological solutions of pulsatile release, therapeutic systems for systemic use (infusion systems, transdermal therapeutic systems, oral therapeutic systems, rectal therapeutic systems, implantable pumps), therapeutic systems for local use (ocular therapeutic systems, uterine therapeutic systems), biological computers.

5. PHARMACEUTICAL ANALYSIS

Programme director: Prof. György Dombi CSc

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Research programmes

(A) NMR Spectroscopy

- Development of experiments in 2D NMR spectroscopy.
- Structure elucidation of small organic molecules (terpenes, steroids, peptides, etc.).
- Multinuclear spectroscopy of organometallic and complex compounds
- Solid state NMR spectroscopy.
- Theoretical calculation of spectral parameters

Supervisors: Prof. György Dombi CSc, Péter Forgó PhD

(B)Atomabsorption spectroscopy

- Determination of trace elements in biological systems (bones, body fluids, etc.)
- Metals in pharmaceutical preparations
- Spectroscopy of environmental samples
- Statistical evaluation of spectroscopic data

Supervisors: György Dombi CSc

(C) Chemometry

- Calculation of spectroscopic data.
- Development of algorithms on molecular similarity
- Data compression, data mining, expert programs.

Supervisors: Prof. György Dombi CSc, Assoc. Prof. Imre Bálint CSc

Instrumental background

The Institute possess a BRUKER AVANCE DRX 500 NMR spectrometer, equipped with multinuclear probeheads, gradient coils, variable temperature units, solid state unit (CP/MAS) and corresponding computers, software etc.; a Prekin Elmer 420 atomabsorption spectrometer with 17 lamps for different elements, flame and graphite furnace atomization.

Courses

NMR spectroscopy (Prof. György Dombi CSc, Péter Forgó PhD)

The lectures give a review on the basic physical background of the NMR spectroscopy (nuclear spin, magnetic moment, Larmor precession, Bloch equations, etc.). Spectral information concerning chemical structure (chemical shift, indirect coupling constant, relaxation times, etc.). One pulse experiments. Fourier spectroscopy. Multipulse experiments. Assignment of 1D and 2D spectra. Special methods: gradient spectroscopy, oriented systems, direct couplings, Overhauser effect, solid state spectroscopy. MRI, and microscopy. Experimental methods (recording spectra).

Spectroscopy (Prof. György Dombi CSc and invited lecturers)

Physical aspects of optical spectroscopy. Concentration determination and statistical errors. Fourier spectroscopy. Absorption spectroscopy (MW, IR, Raman, NIR, UV-VIS, AA, X-ray). Emission spectroscopy (flame photometry, fluorescence). Mass spectrometry. NMR spectroscopy. Diffraction and light scattering.

Basics of chemometry (Assoc. Prof. Imre Bálint CSc and invited lecturers)

An introduction to the practical applications of theoretical and mathematical methods in chemistry, and biology. Molecular modelling, molecular similarity. Ab-initio, semi-empirical methods, molecular force-field models, minimum-search. Simulation of experimental data and converting them to structural information.

Representative dissertations (title, *author*, supervisor, year)

Lipase-catalysed kinetic resolution of 2-substituted cycloalkanols, *Enikő Forró*, Ferenc Fülöp, 2000.

Conformational studies of bioactive saturated heterocycles by NMR spectroscopy and molecular modelling, *Tamás Martinek*, Ferenc Fülöp, 2001.

Synthesis and structure of (bi)cycloalkane-fused heterocycles. Pharmacokinetic study of a new anxiolytic, *József Szúnyog*, Géza Stájer, 2003.

Syntheses and transformations of α-aminobenzylnaphthol derivatives, *István Szatmári*, Ferenc Fülöp, László Lázár, 2004.

The roles of α1-adrenergic receptor subtypes in the regulation of uterine contractility – molecular pharmacological investigations, *Eszter Ducza*, György Falkay, 2002.

Examination of the contractility of human placental blood vessels in vitro, *Béla Resch*, György Falkay, 2003.

Neural regulation of uterine contractility in the rat: the role of adrenergic and sensory nerves, *Anna Klukovits*, György Falkay, 2004.

Pharmacodynamics of β2-adrenergic agonists and subtype-selective α1A-adrenoceptor antagonists on the pregnant rat uterus in vitro, *Attila Mihályi*, Anna Borsodi, 2004.

Ecdysteroids isolated from *Silene italica* ssp. *nemoralis*, *Pongrácz Zita*, Mária Báthori, 2003.

Study of compactibility behaviour of Avicels in direct compression, *M. M. Siaan*, István Erős, Klára Hódi, 1999.

Spherical crystallization of drug materials for direct tablet making, *Göcző Hajnalka*, Piroska Révész, 2002.

Examination of the structural and permeability properties of liposomes stabilized by neutral polymers, *György Dékány*, István Erős, 2002.

Quality development of semisolid dermal drug delivery systems, *Erzsébet Csányi*, István Erős, 2003.