Universität Innsbruck

Pharmaceutical e-Learning at the University of Innsbruck

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Outline

- How it all began: PharmXplorer
- Current applications in teaching - examples
  - Search for a drug: e.g. Acetazolamide
  - Pharmaceutical biology: e.g. Digitalis
  - Additional features
    - General information
    - Lab exercises (mixing exercise, titration curve, ...)
    - Interactive chemistry training (nomenclature, drug synthesis, ...)
- New tools: LigandScout and ilib:diverse
- Chances and problems for the future

The PharmXplorer Project

- **bm:bwk** initiative ‘Neue Medien in der Lehre’
  Call: 2001 / Start: 2002 / Project duration: 3 years
- Consortium of the three major Austrian universities Vienna, Graz, and Innsbruck together with the Austrian Chamber of Pharmacists and the Apothekerverlag
- Funding for (wo)manpower*, no IT infrastructure
- Open source solution preferred
- Main component: “Information Platform” including a database of drugs marketed in Austria

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The PharmXplorer Project

- Official end of funded project: 2005
- Now individual use of pharmXplorer
- Local e-Learning calls at Austrian universities used to generate content
- Attempts to internationalize pharmXplorer

PharmXplorer: Content Areas

- Information - Database of marketed drugs (Austria)
- E-Learning - Modules for different levels
- Teaching - Repository for course documents
- Post graduate education
  - Special courses for pharmacists working in public pharmacy
  - Topic of the chamber of pharmacy education program
  - Education for technical staff
- Community area / discussion forum


PharmXplorer
http://www.pharmxplorer.at/pxp.at/
Google
Pharm Xplorer
News
Beschreibung
Anmeldung
Basic
eLearning für Schulen
Vorbereitung auf das Studium
Academic
Online Lernen für
StudentInnen
Scientific
Unterstützung für
Lehrende und Vortragende
Aktuell: Apoplay Seminar bei Herba-Chemosan - Seggauer Fortbildungstage 2006
Office
Beste Unterstützung für
die Arbeit in der Apotheke
Focus
Einzigartige Form der
Weiterbildung für ApothekerInnen
Advance
Jetzt Online!
Modernste Ausbildung für
AspirantInnen
Pharmazeutische Gehaltskasse
Österreichische Apothekerkammer
Apothekerverlag
Probleme bei Zugang oder Verwendung? Mail an den Support!
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Information platform

- Search for drug ‘acetazolamide’
- Retrieve all relevant information
- Display results

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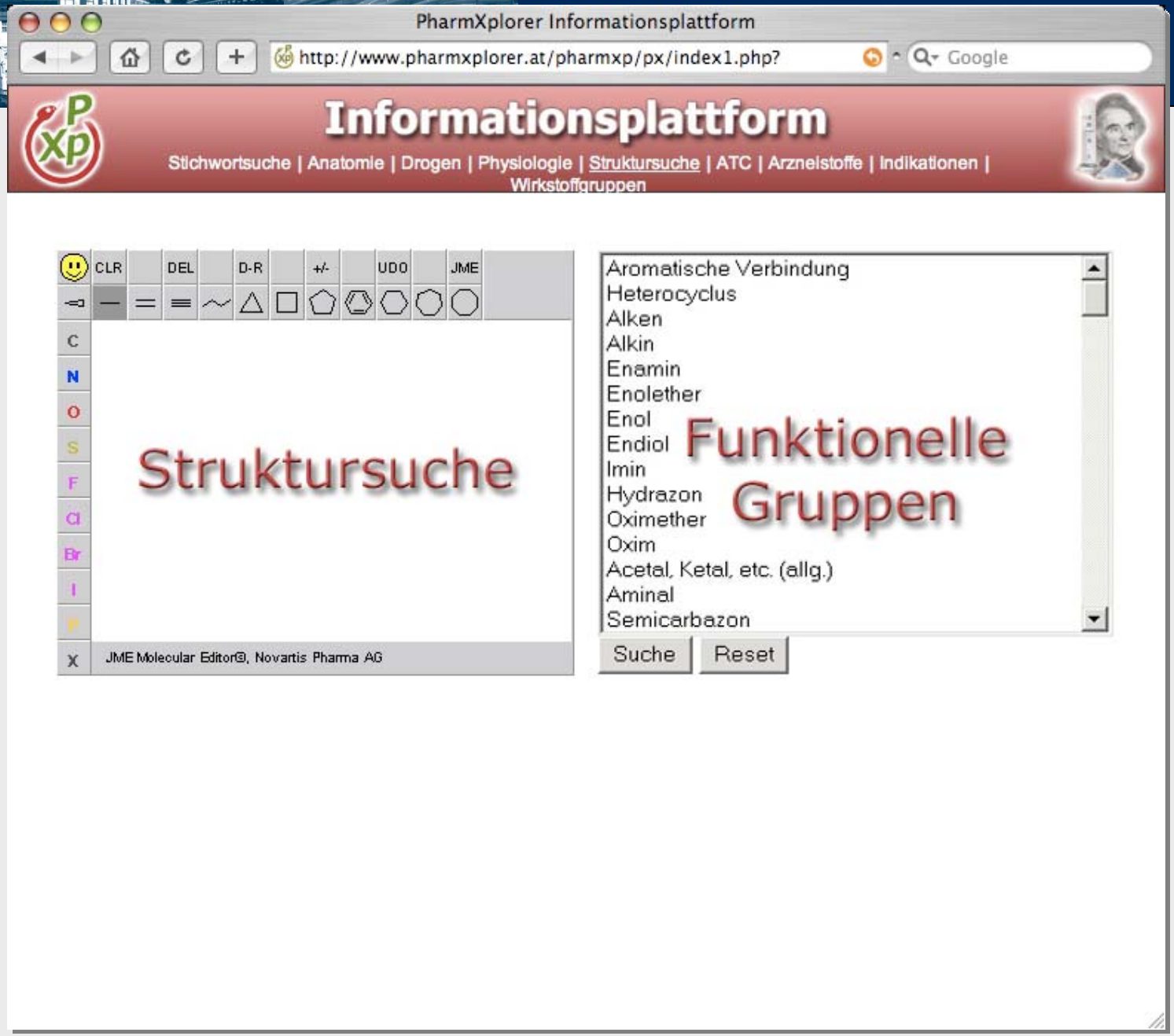
Substructure Search & Functional Groups

- Developed and implemented by Norbert Haider (University of Vienna), based on open source software and own code (**checkmol / matchmol**)
- Molecules (standard input formats - SD, MOL2, etc) are interpreted and classified according to well defined heuristic rules
- More than 200 functional groups covered by now http://merian.pch.univie.ac.at/~nhaider/cheminf/fgtable.pdf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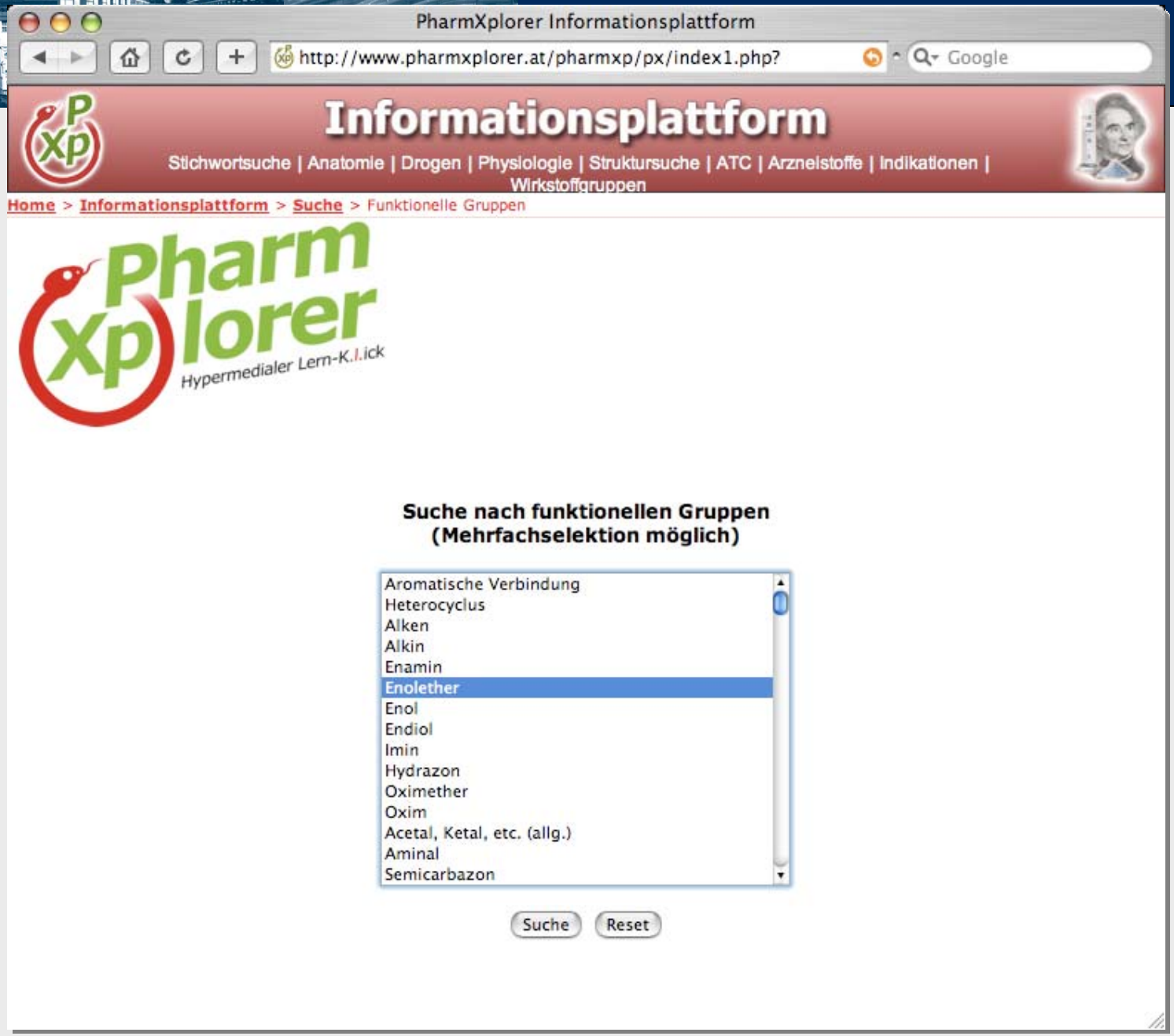
Strukturesuche
JME Molecular Editor©, Novartis Pharma AG
Aromatische Verbindung
Heterocyclus
Alken
Alkin
Enamin
Enolether
Enol
Endiol
Imin
Hydrazon
Oximether
Oxim
Acetal, Ketal, etc. (allg.)
Aminal
Semicarbazon
Funktionelle Gruppen
Suche
Reset


PharmXplorer Informationsplattform
http://www.pharmxplorer.at/pharmxp/px/index1.php?
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Informationsplattform
Stichwortsuche | Anatomie | Drogen | Physiologie | Strukturesuche | ATC | Arzneistoffe | Indikationen | Wirkstoffgruppen
Home > Informationsplattform > Suche > Funktionelle Gruppen
Pharm Xplorer
Hypermedialer Lern-K.I.ick
Suche nach funktionellen Gruppen
(Mehrfachselektion möglich)
Aromatische Verbindung
Heterocyclus
Alken
Alkin
Enamin
Enolether
Enol
Endiol
Imin
Hydrazon
Oximether
Oxim
Acetal, Ketal, etc. (allg.)
Aminal
Semicarbazon
Suche
Reset

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Other Search Methods ...

- Classification of drug compounds
  - Therapeutic classification ...
  - Organ that is affected by the drug ...
  - Mode of action ...

More Application Examples ...

- Phytochemistry
- Natural Products
- Drugs originating from natural products

Additional Features

- General chemical information
  - Periodic system of elements
- Useful items for laboratory work
  - Mixing calculations
  - Titration curves
- Self evaluation modules for specific courses
  - Check the knowledge of enrolled students
  - Can be used for on-line examinations

Interactive Training Elements

- Chemical nomenclature
  - Determine the name for a given structure formula
  - Draw a formula for a given name
- Stereo chemistry training
  - Determine the absolute stereo chemistry of chiral atoms
- Drug synthesis training
  - Find the reagent for a specific reaction
  - Draw the educts or the product of a specific reaction

There are much more features ...

- PDF documents from lectures originating from the three major Austrian universities
- Links to recent literature covering hot news from pharmaceutical development
- More than 400 animated graphics
- Video clips of standard laboratory techniques
- Interactive training elements
- Regular updates

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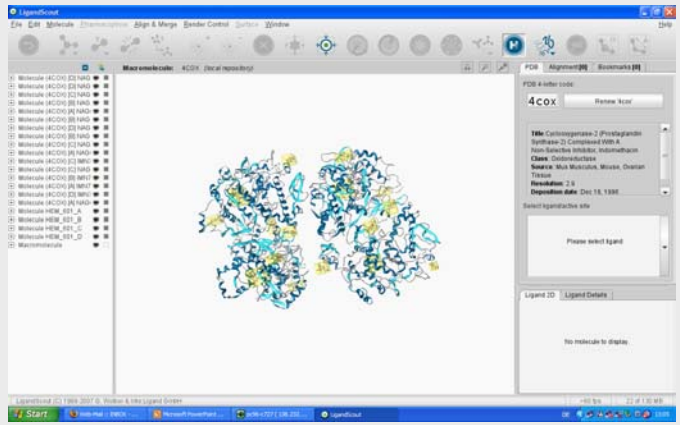
Our Experiences with PharmXplorer

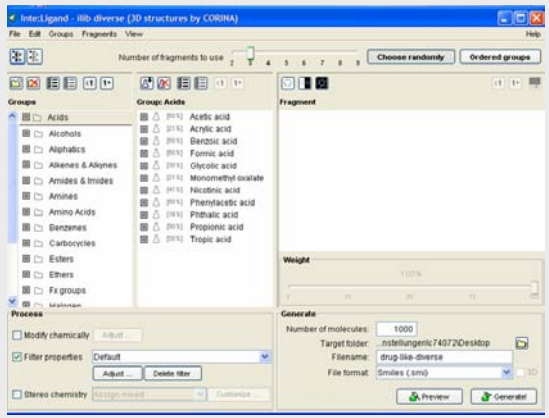
- We use pharmXplorer in the pharmaceutical chemistry curriculum
- Students need to perform ‘upfront’ studies
- During the lectures, discussion is stimulated
- Examination results are significantly better since we started to use this platform
- Students are getting more involved
- High acceptance among students!

New e-learning tools for pharmaceutical / medicinal chemistry

- LigandScout
  - pharmaceutical chemistry
  - pharmacology
  - computational tools in drug discovery and development



- Ilib:diverse
  - organic chemistry
  - pharmaceutical chemistry
  - computational tools in drug discovery and development



Vienna, 25.9.2007

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LigandScout exercises

- COX: ASS mode of action 1pth (mode-of-action)
- Reverse transcriptase: 1lw0, 1fk9 (comparison)
- Competitive / mechanism-based inhibitors
- Determination of compound-target interactions (with solution!)
- Binding site architecture vs. drug structure (aldose reductase)
- Rationalization of structure-activity relationships
- Introduction to molecular modeling – learn industrial research techniques

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Ilib:diverse exercises

- Understand combinatorial chemistry (example: esters)
- Generate virtual libraries based on defined reaction mechanisms
- Playful introduction to chemistry, descriptors, and compound properties
- Work with software that is also part of industrial syntheses

Focus for future e-learning projects

- Student number raises
- Basics (from school) as e-learning courses
- E-tests for selection of best students

- Funding for the generation of e-content???

- ! E-courses are time- and work-intensive (if they are to be done properly including forums, online discussions, networking…) and can not replace face-to-face teaching!
- ! E-courses are no mean to reduce teaching costs at universities!

Other challenges…

- Funding
- Infrastructure
  - Enough computer labs for the students
  - Software
  - Contacts (teachers, tutors, students)

- Keeping content up-to-date
- One pharmacy – one e-learning platform?
- Language issues

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www.pharmxplorer.com

www.inteligand.com

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Acknowledgements

Thank you for your attention!