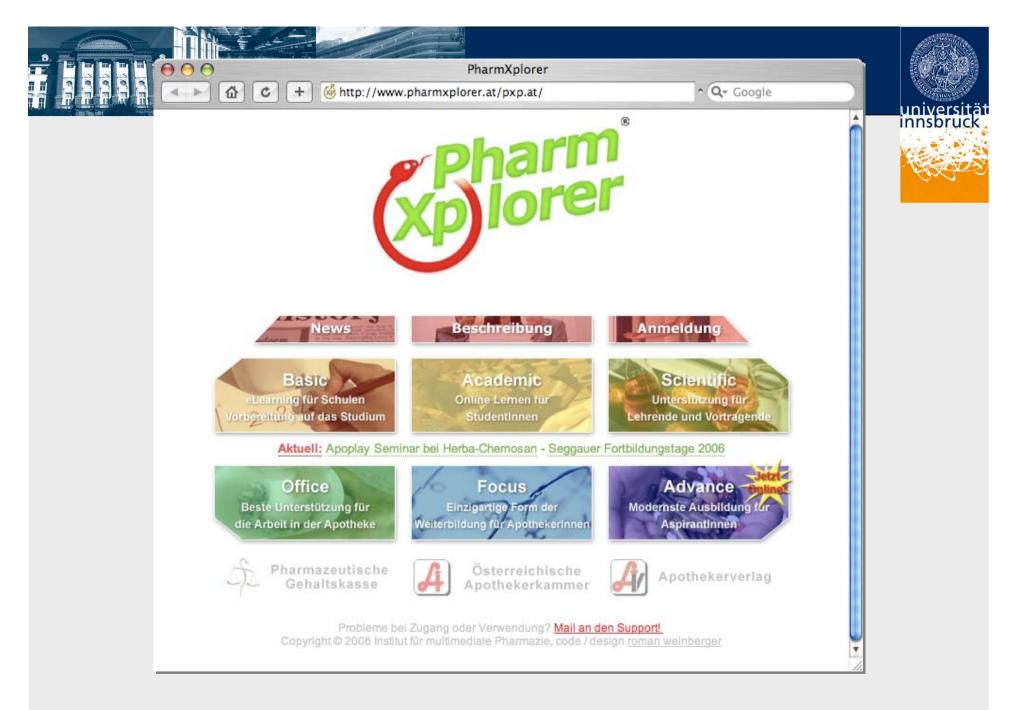


# **PharmXplorer -** An Integrated Platform For E-Learning In Pharmaceutical Sciences

**Prof. Thierry Langer Institute of Pharmacy / Pharmaceutical Chemistry** 

# Outline

- PharmXplorer: Project description
- Technical background
- Application 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, ...)
- Our experiences ...



# **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



# **The PharmXplorer Project**

- Official end of funded project: 2005
- Number of registered users: more than 4000
- Data: several Gb
- Page hits: several 100.000

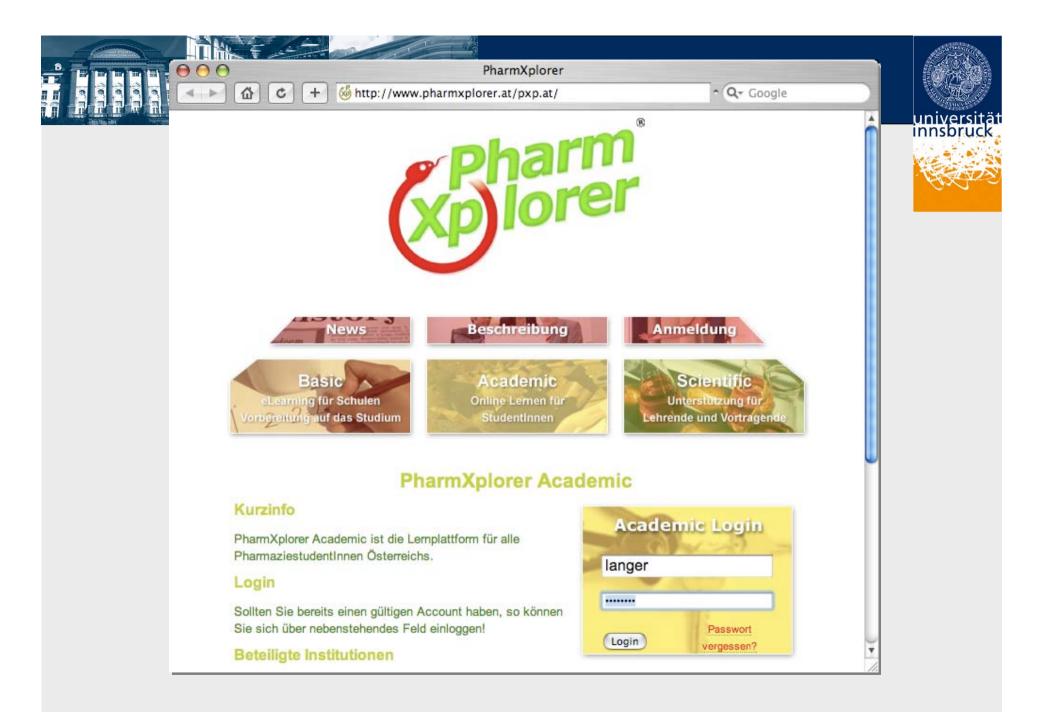


# **PharmXplorer: Technical Background**

- Distributed architecture
- Client: Generic web browser (IE, Mozilla/Firebird, Netscape, Opera, Safari, ...)
- Server
  - Operating system: Linux
  - Web server: Apache
  - Relational database: MySQL
  - Script languages: PHP, Perl, Java
  - User administration: OpenLDAP
  - Generic software development (substructure search ...)

# 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



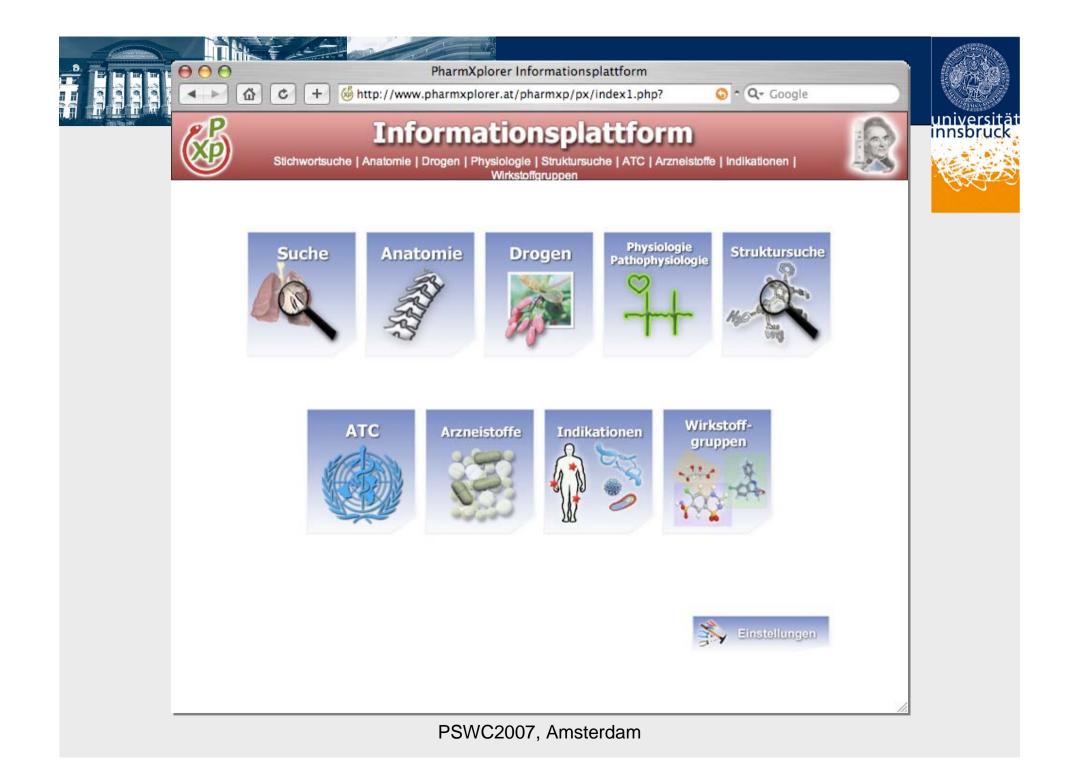


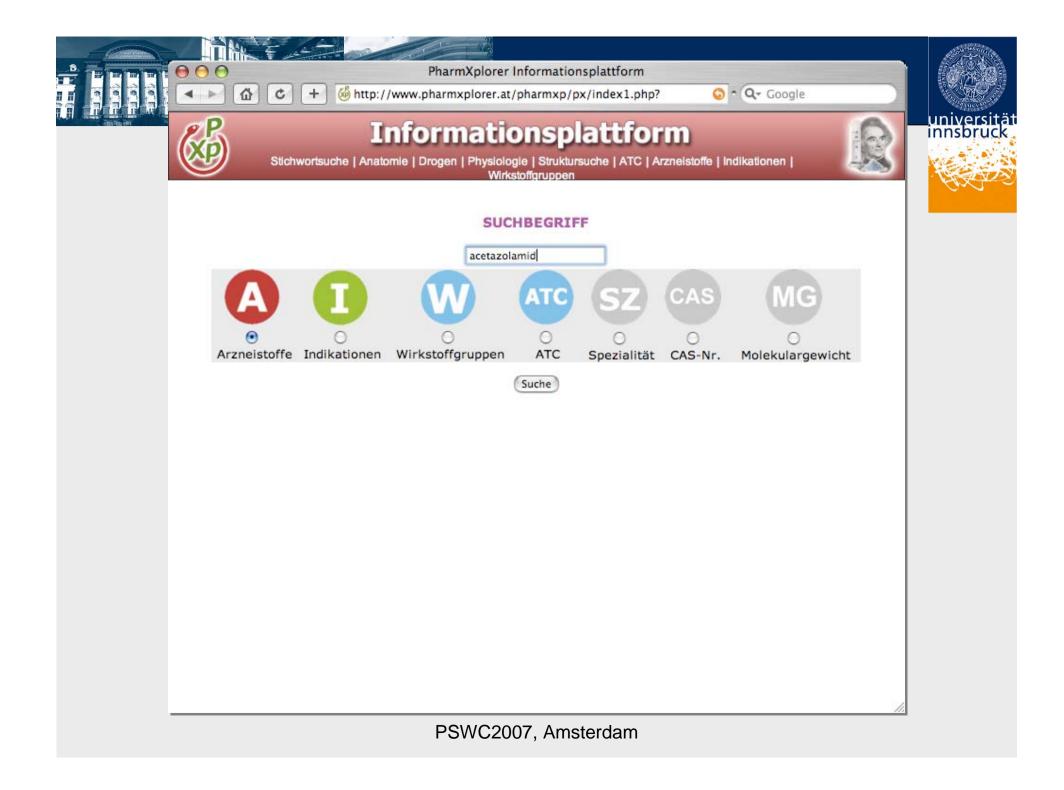


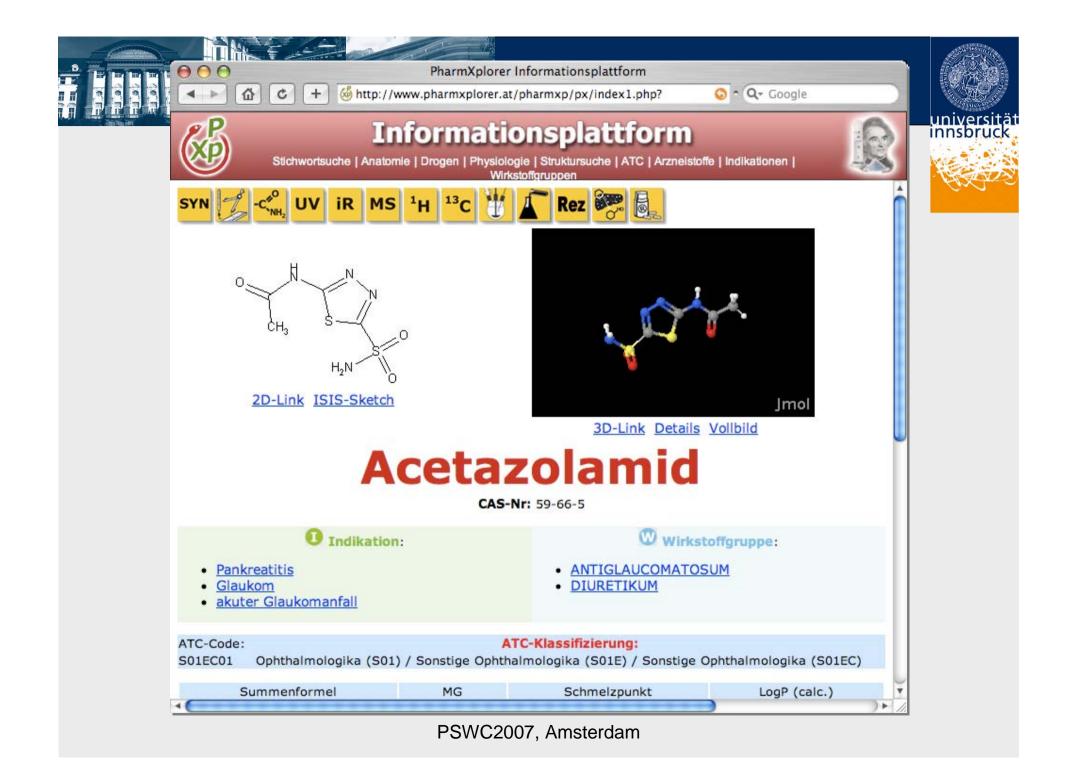
# **Application Example 1**

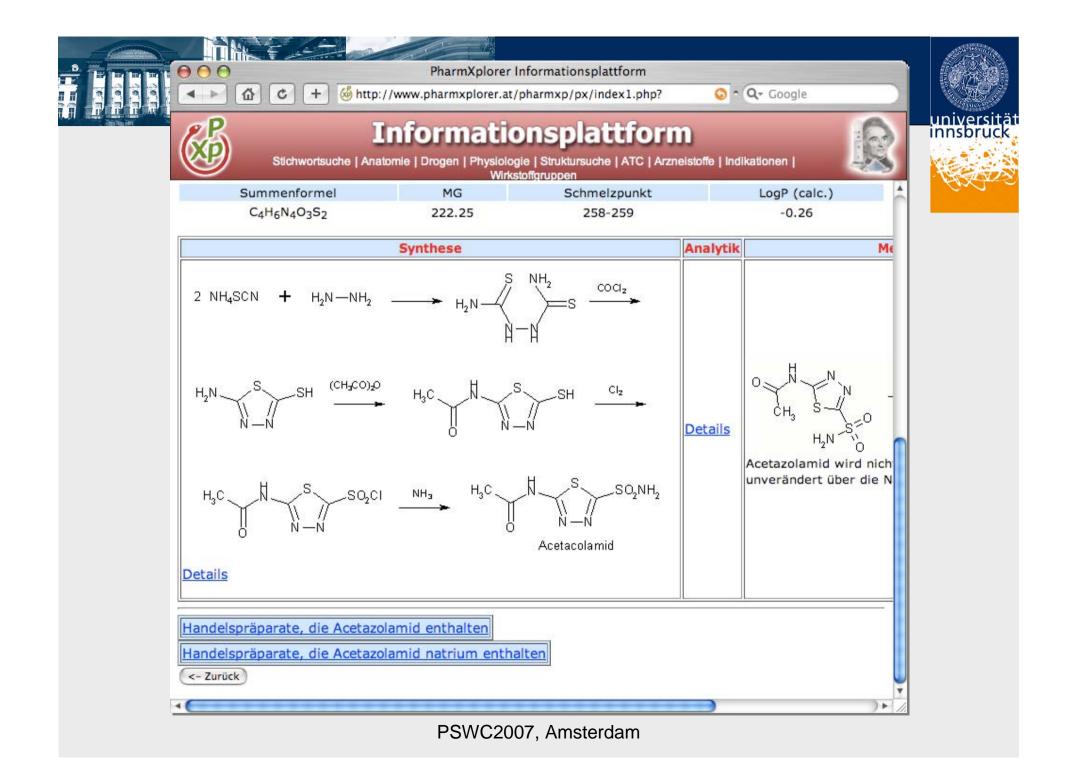
- Search for drug 'Acetazolamide'
- Retrieve all relevant information
- Display results

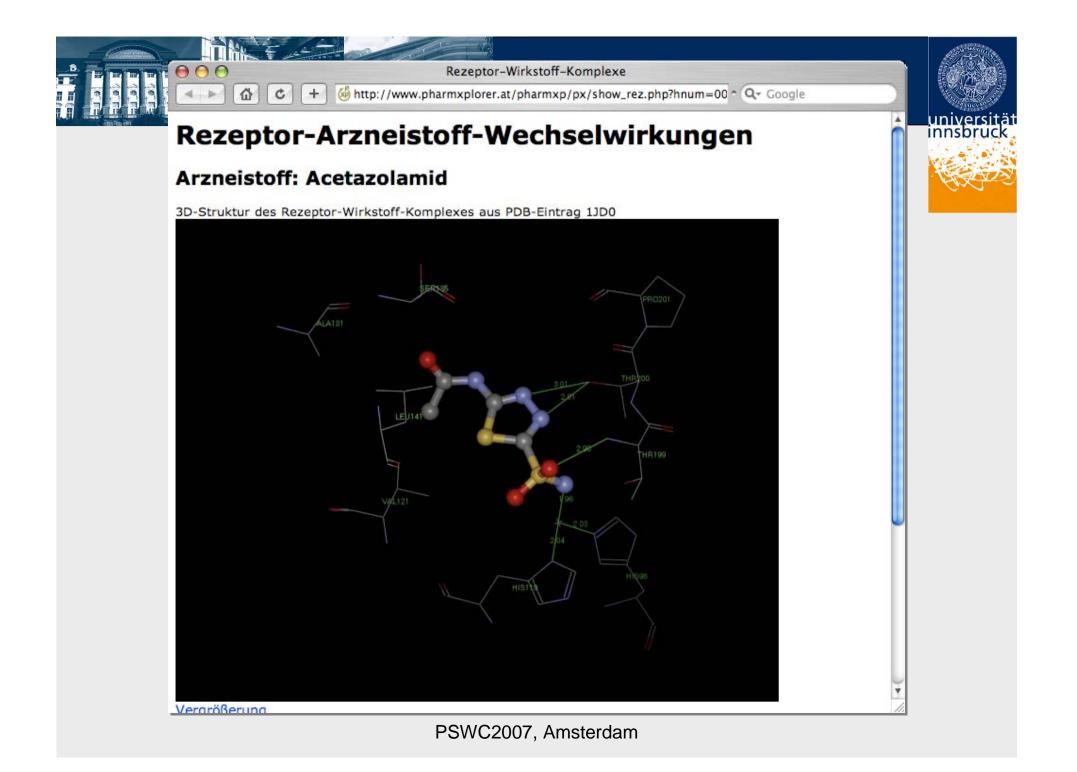










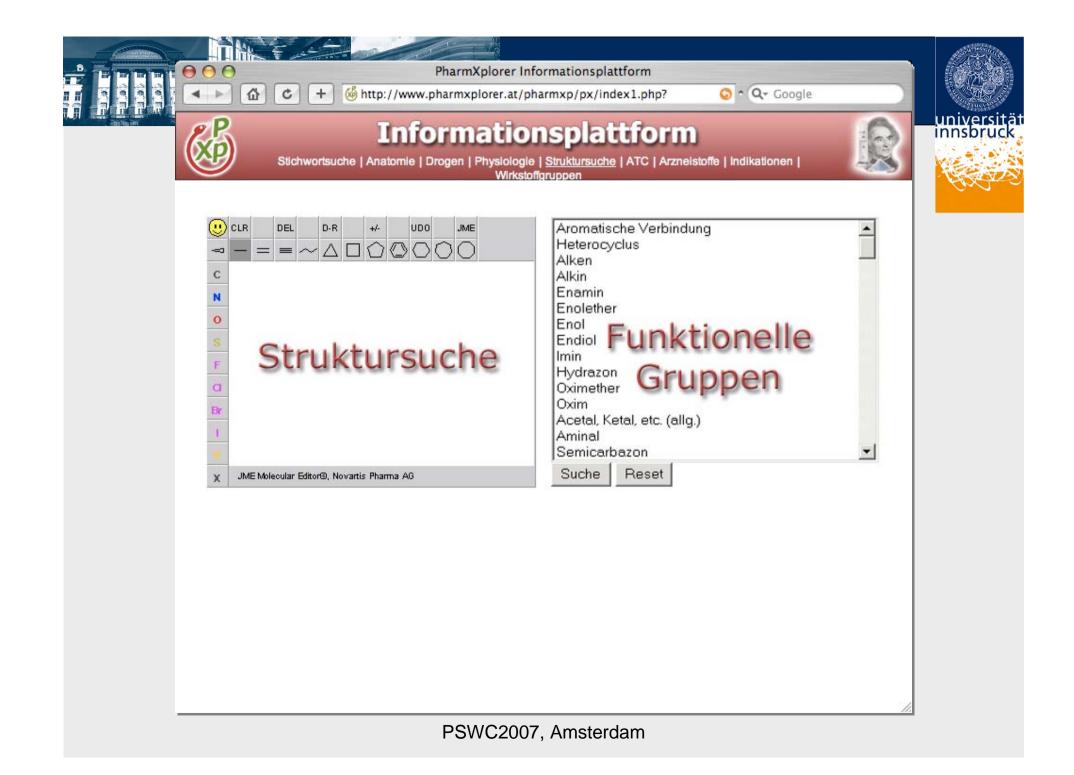


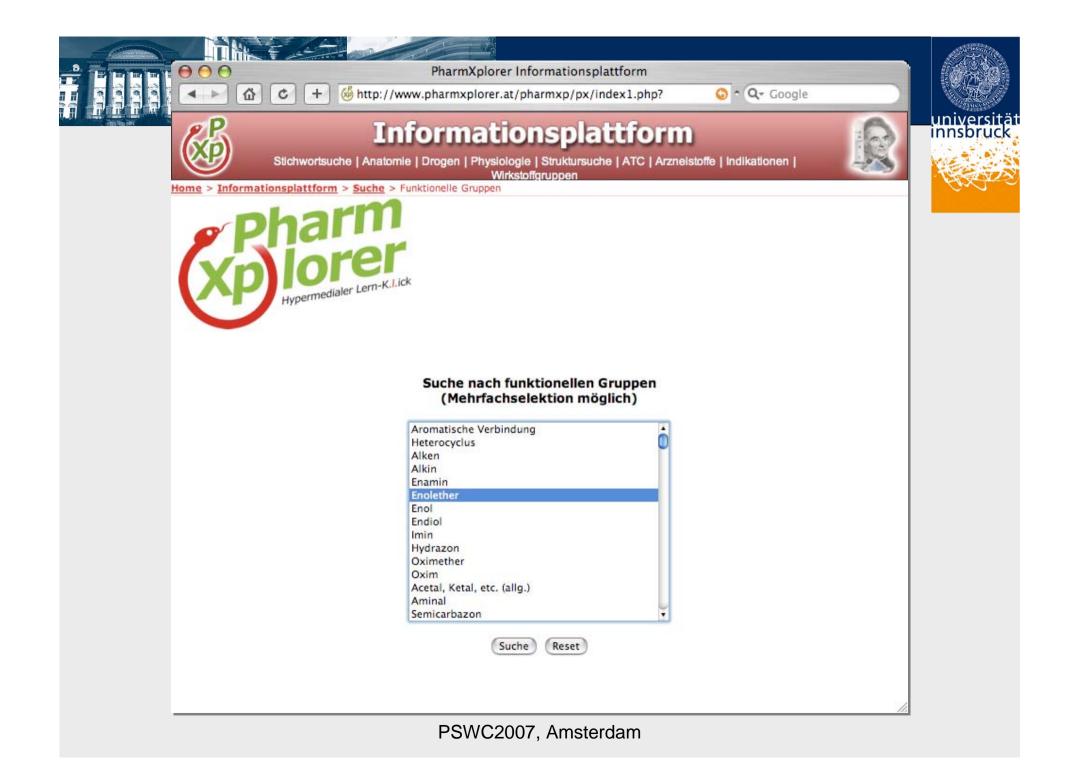


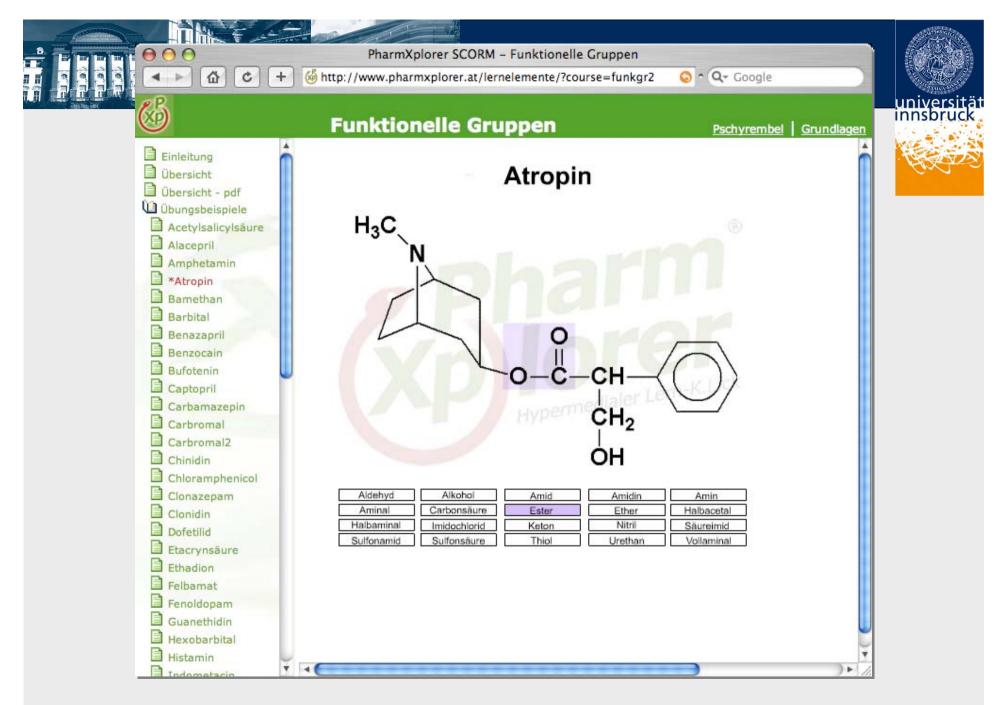


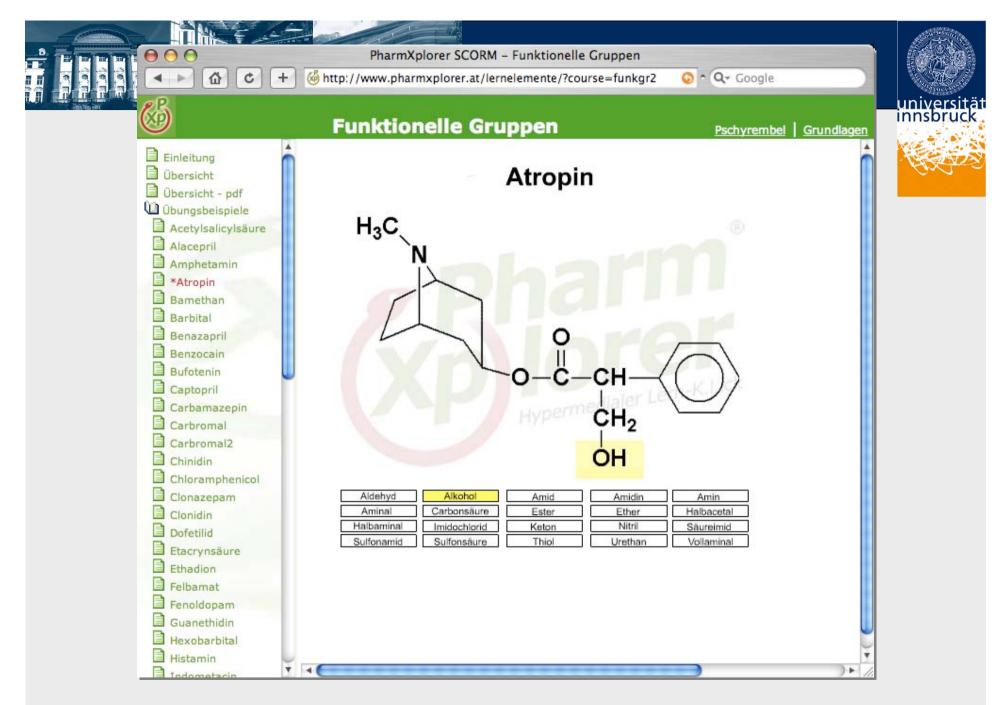
## Substructure Search & Functional Groups

- 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 <u>http://merian.pch.univie.ac.at/~nhaider/cheminf/fgtable.pdf</u>











## **Other Search Methods ...**

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





Bearbeiten einschalten

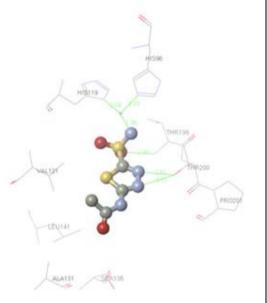
## Wirkstoffgruppen

Nervensystem Respirationstrakt Sinnesorgane Herz-Kreislaufsystem Niere Verdauungstrakt Hormone Neurotransmitter und Mediatoren Chemotherapeutica und Antibiotica Vitamine Immunsystem Dermotherapeutica Zytostatica Kontrastmittel Enzyme Spurenelemente Urogenitalsystem

## Wirkstoffgruppen

Hier finden Sie Details zu verschiedenen, nach Kategorien geordneten Wirkstoffgruppen.

Zur Auswahl verwenden Sie bitte die linke Kategorieleiste.





Bearbeiten einschalten

### Wirkstoffgruppen

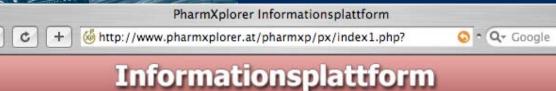
## Niere

Nervensystem Respirationstrakt Sinnesorgane Herz-Kreislaufsystem \* Niere Verdauungstrakt Hormone Neurotransmitter und Mediatoren Chemotherapeutica und Antibiotica Vitamine Immunsystem Dermotherapeutica Zytostatica Kontrastmittel Enzyme Spurenelemente Urogenitalsystem

## **Diuretica - Übersicht**

Diuretica sind Arzneistoffe, die zu einer erhöhten Harnausscheidung führen. Damit ist meistens auch eine erhöhte Salzausscheidung verbunden. Streng genommen unterscheidet man zwischen Saluretica (Salz- und Wasserausscheidende ...

- Aldosteronantagonisten [DELETE]
- Cycloamidine [DELETE]
- Osmodiuretica [DELETE]
- Schleifendiuretica [DELETE]
- Thiazidanaloga [DELETE]





Stichwortsuche | Anatomie | Drogen | Physiologie | Struktursuche | ATC | Arzneistoffe | Indikationen |

Wirkstoffgruppen

Bearbeiten einschalten

奋

00

### Wirkstoffgruppen

Nervensystem

## Zytostatica

Respirationstrakt Sinnesorgane Herz-Kreislaufsystem Niere Verdauungstrakt Hormone Neurotransmitter und Mediatoren Chemotherapeutica und Antibiotica Vitamine Immunsystem Dermotherapeutica \* Zytostatica Kontrastmittel Enzyme Spurenelemente Urogenitalsystem

Antineoplastika

Antineoplastika sind Arzneimittel gegen Tumoren, die keine hormonelle Wachstumsabhängigkeit zeigen. Generell hemmen alle Antineoplastika das Wachstum von schnell proliferierenden Geweben. Da die meisten Tumoren eine sehr hohe Zellteilungsrate ...

- Alkylantien [DELETE]
- Angiogenese-Hemmstoffe [DELETE]
- Antimetaboliten [DELETE]
  - Folsäure-Antagonisten [DELETE]
  - Purin-Antagonisten [DELETE]
  - Pyrimidin-Antagonisten [DELETE]
- Enzyme [DELETE]
- Enzyminhibitoren [DELETE]
- Mitosehemmstoffe [DELETE]
- Monoklonale Antikörper [DELETE]
- Photosensibilisierer [DELETE]
- Retinoid Rezeptor Modulatoren [DELETE]
- Topoisomerase Hemmstoffe [DELETE]
- Zytostatische Antibiotika [DELETE]

#### Endokrine Zytostatika

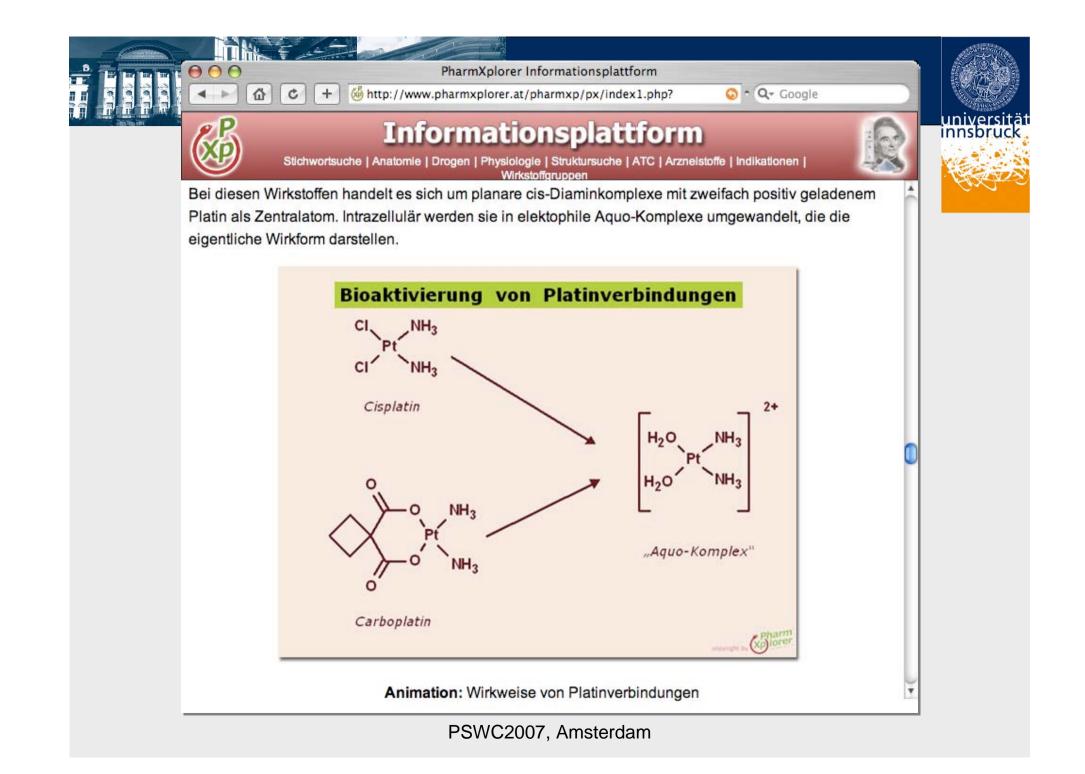
Endokrinen Zytostatika sind Arzneimittel gegen Tumoren, die hormonelle Wachstumsabhängigkeit zeigen. Bei derartigen Tumoren ist oft eine spezifische Hormontherapie möglich. Zum Einsatz kommen: Physiologische Hormone Hormon-Analoga ...

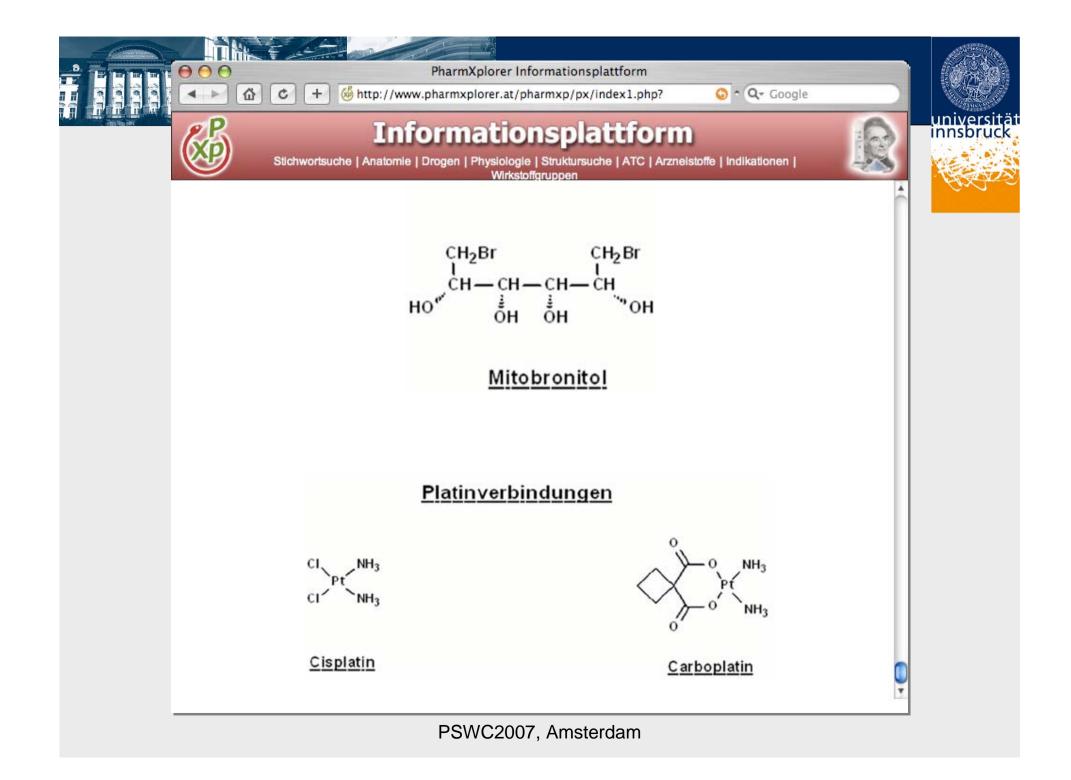
- Hormonantagonisten [DELETE]
  - Antiandrogene [DELETE]
    - Androgenrezeptorantagonisten [DELETE]
  - Antiestrogene [DELETE]
    - Aromatasehemmer [DELETE]
    - Estrogenrezeptorenblocker [DELETE]
- Hormone [DELETE]



## Wirkmechanismus

Alkylantien binden mit einer kovalenten Bindung an die DNS und andere Zellbestandteile. Die Alkylierung der DNA ist dabei von entscheidender Bedeutung; sie führt zur Vernetzung von DNA-Ketten (Cross-link-Bildung), abnormer Basenpaarung, Spaltung von DNA-Ketten und führt letztlich zu einer Hemmung der Zellteilungsvorgänge. Die cytotoxische Wirkung der Alkylantien ist bei den rasch proliferierenden Zellen

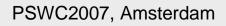


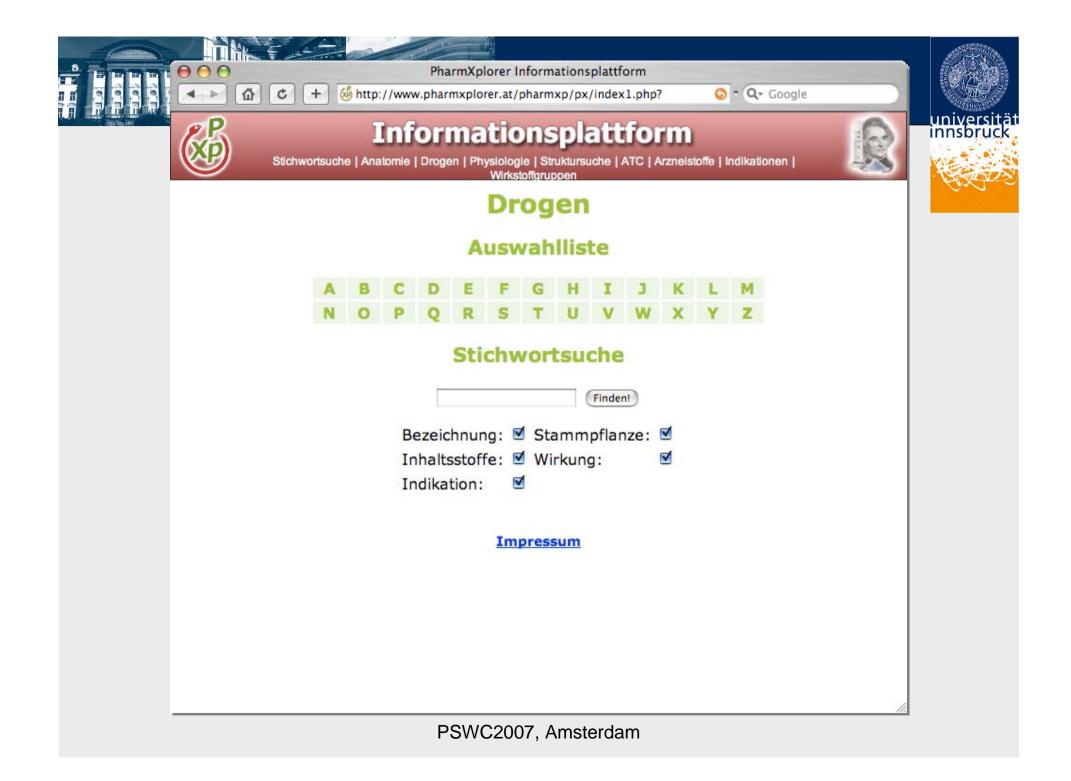


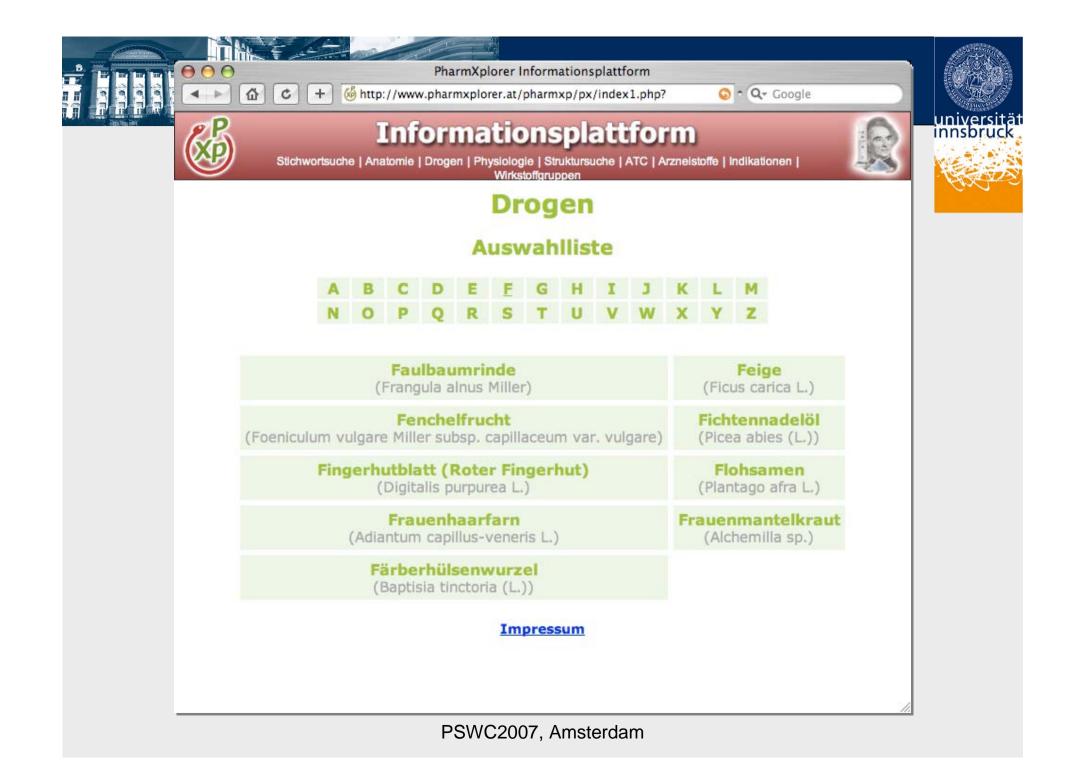


# More Application Examples ...

- Phytochemistry
- Natural Products
- Drugs originating from natural products





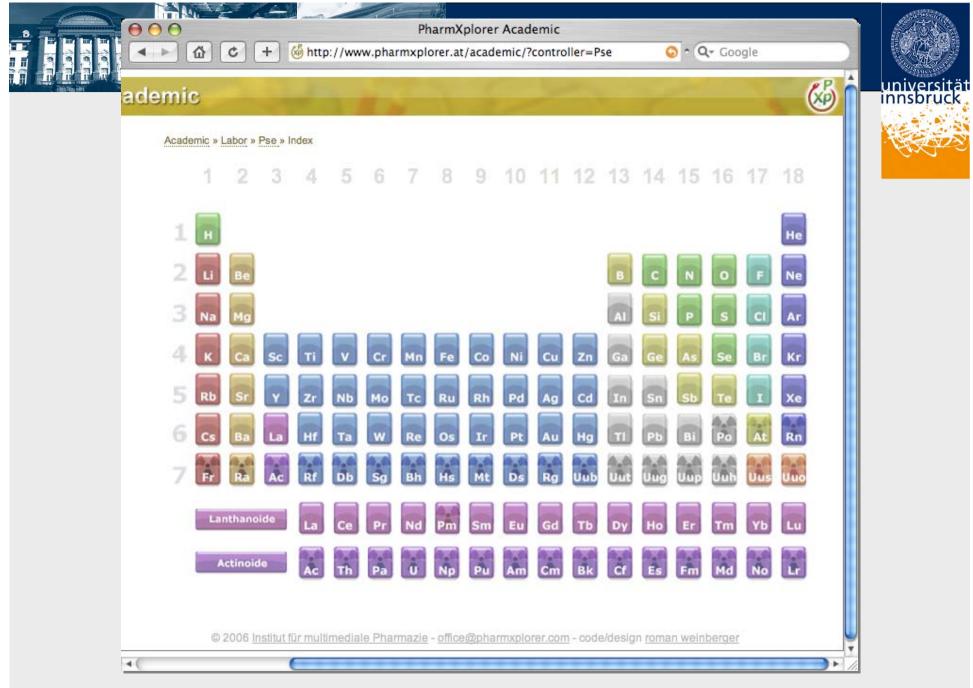


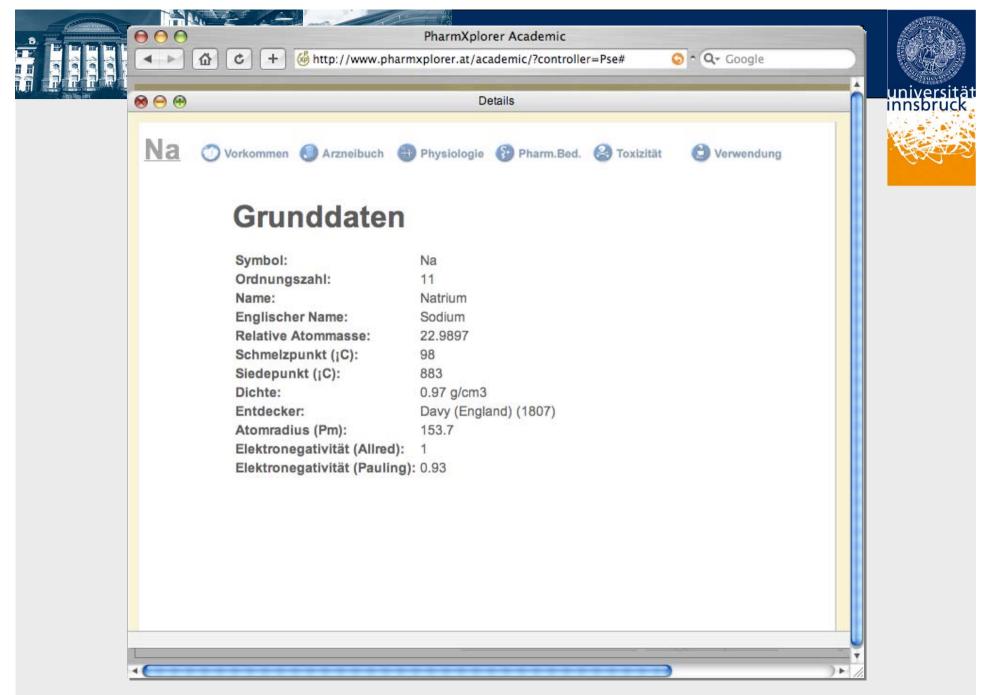




# **Additional Features**

- 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

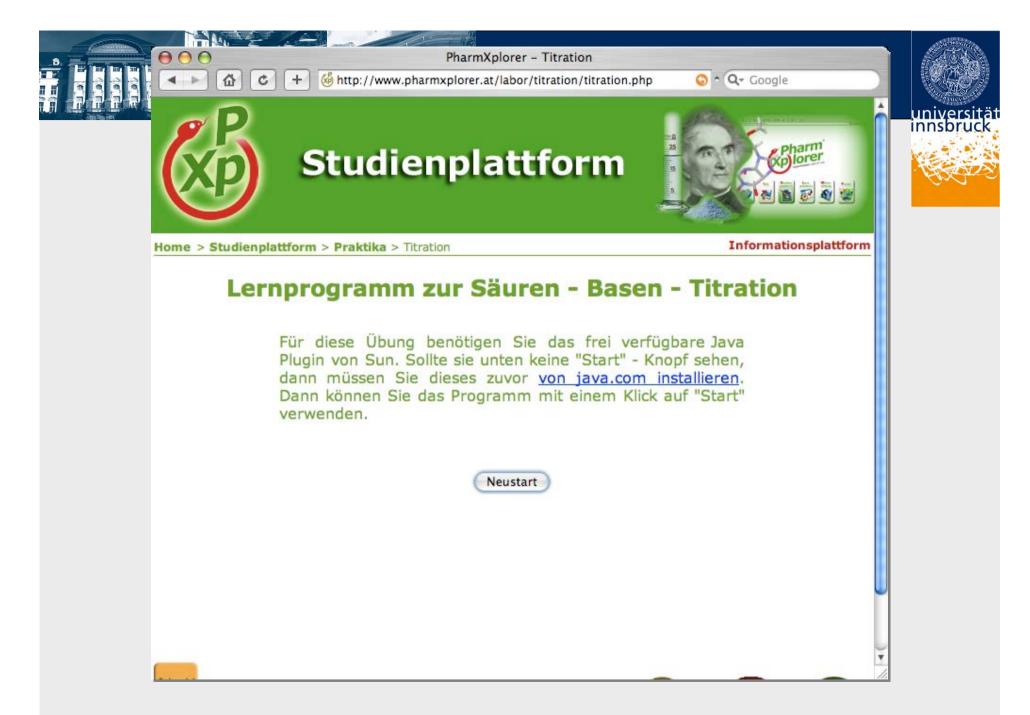


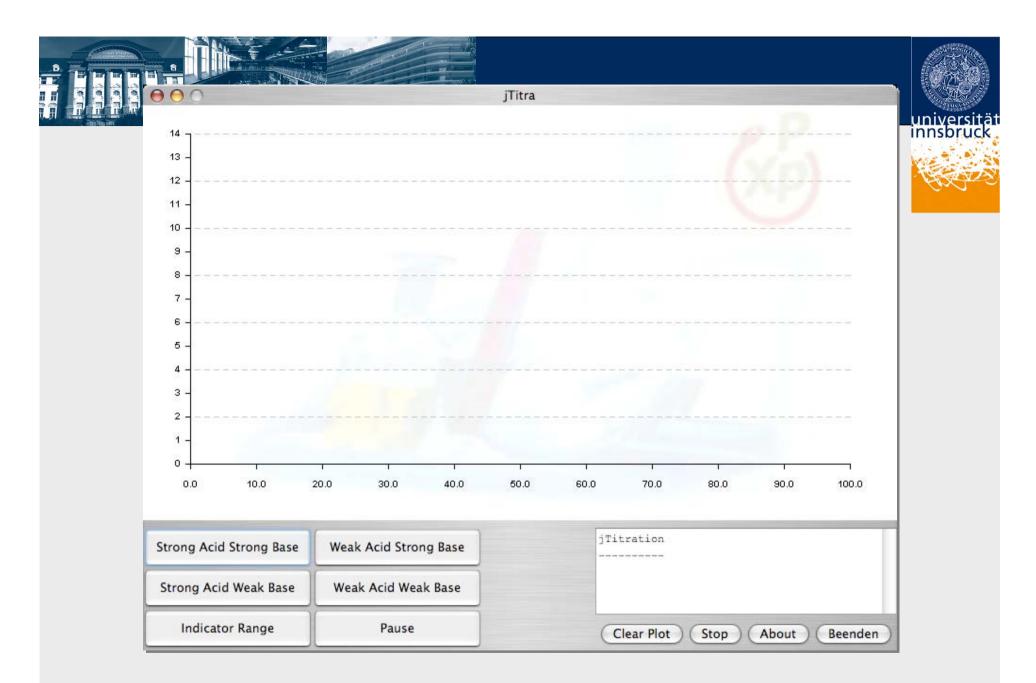


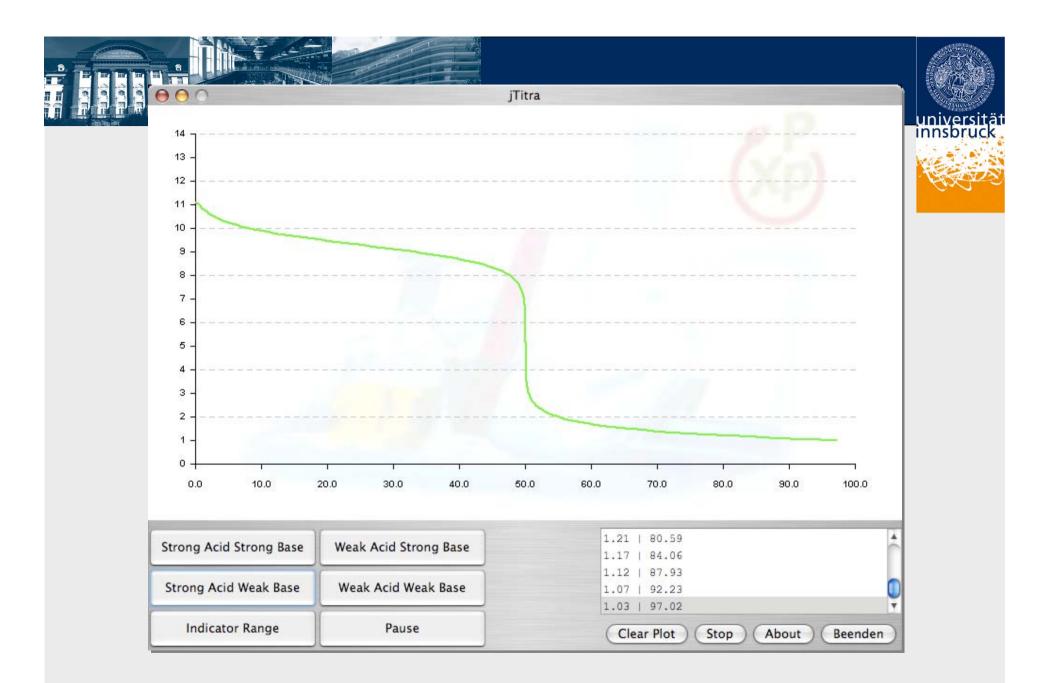
	O O   PharmXplorer - Mischungskreuz   Image: Contract of the state of the sta					
	Studienplattform					
	Home > Sudienplattform > Praktika > Mischungskreuz			Informationsplattform		
	Navigation	Berechnen einer Mischun				
	Einleitung *Berechnung Sicherheit	Konzentrationseinheit?	Massen %			
	Theorie u. Grenzen Links Kontakt	Konzentration der Lösung A (höher konzentriert):				
			Gewünschte Konzentration?			
		Konzentration der Lösung B (tiefer konzentriert):				
		Gewünschte Menge der Mischung/Verdünnung:	100	Mengeneinheit? Gramm 🛟		
		(Berechnen) (Reset)				

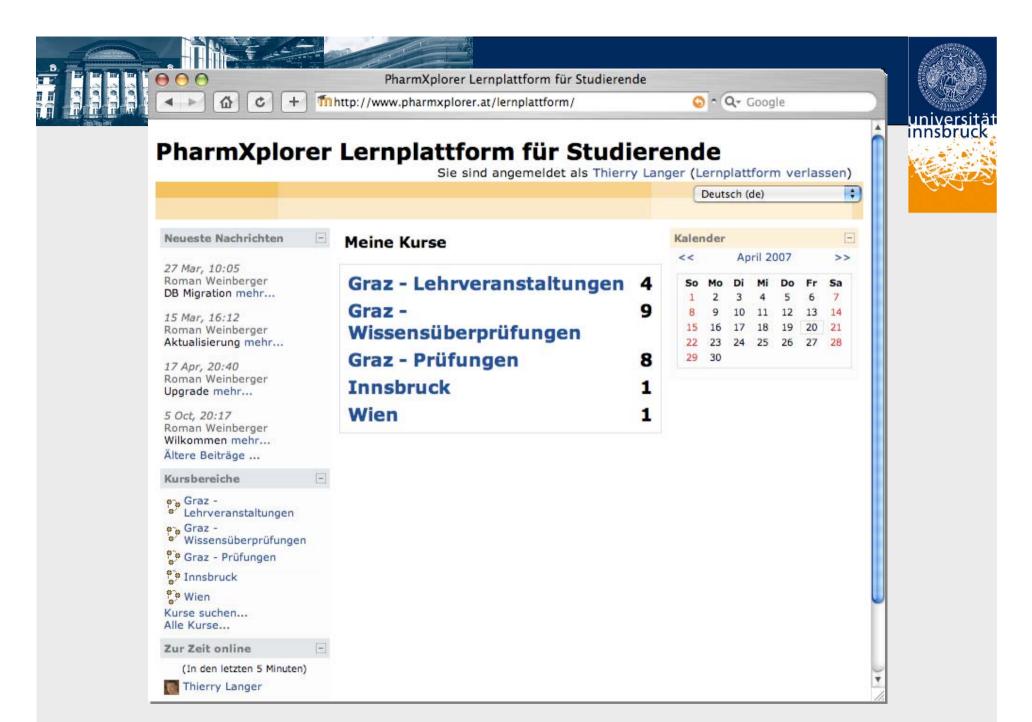
	O O   PharmXplorer - Mischungskreuz   Image: Contract of the state of the sta					
		universität				
	Home > Sudienplattform > Praktika > Mischungskreuz			Informationsplattform		
	Navigation	Berechnen einer Mischun				
	Einleitung *Berechnung Sicherheit	Konzentrationseinheit?	Massen %			
	Theorie u. Grenzen Links Kontakt	Konzentration der Lösung A (höher konzentriert):	86			
			Gewünschte Konzentration?	34		
		Konzentration der Lösung B (tiefer konzentriert):	10			
		Gewünschte Menge der Mischung/Verdünnung:	100	Mengeneinheit? Gramm		
		Berechnen Reset				







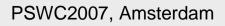


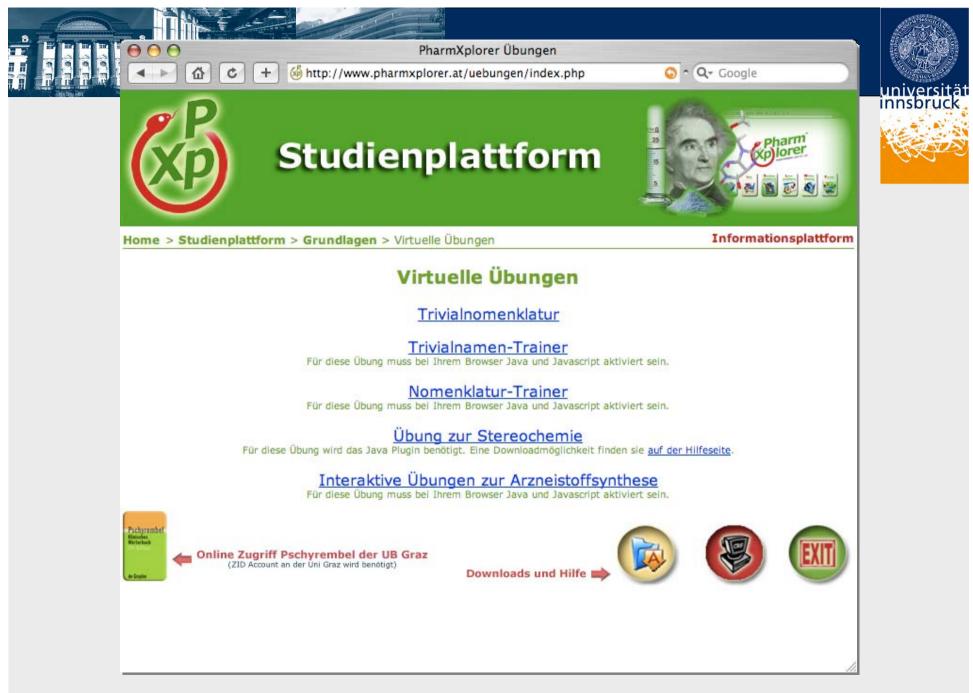


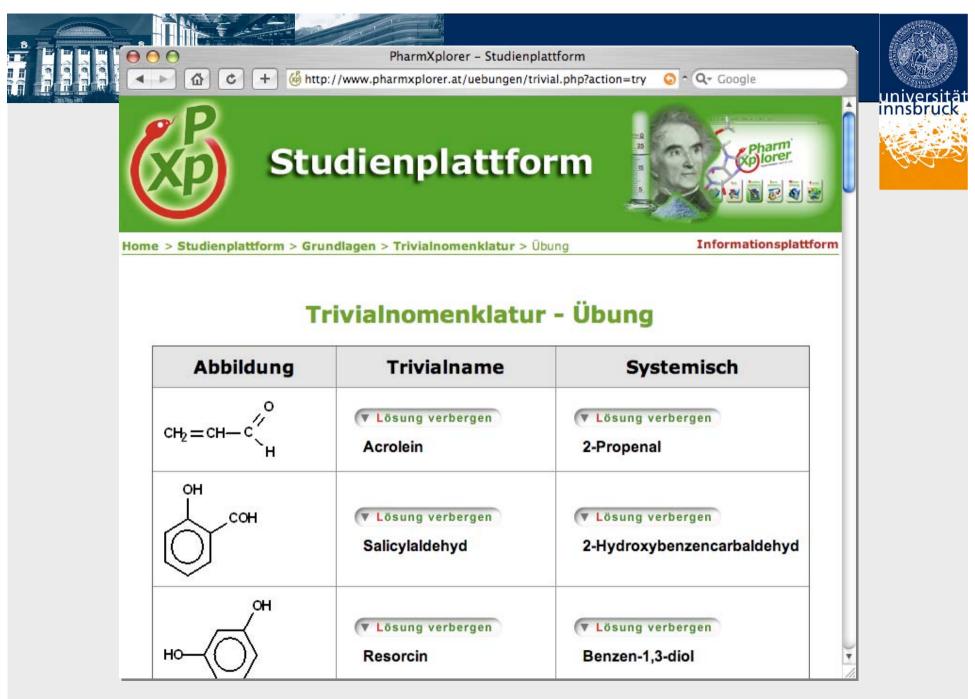


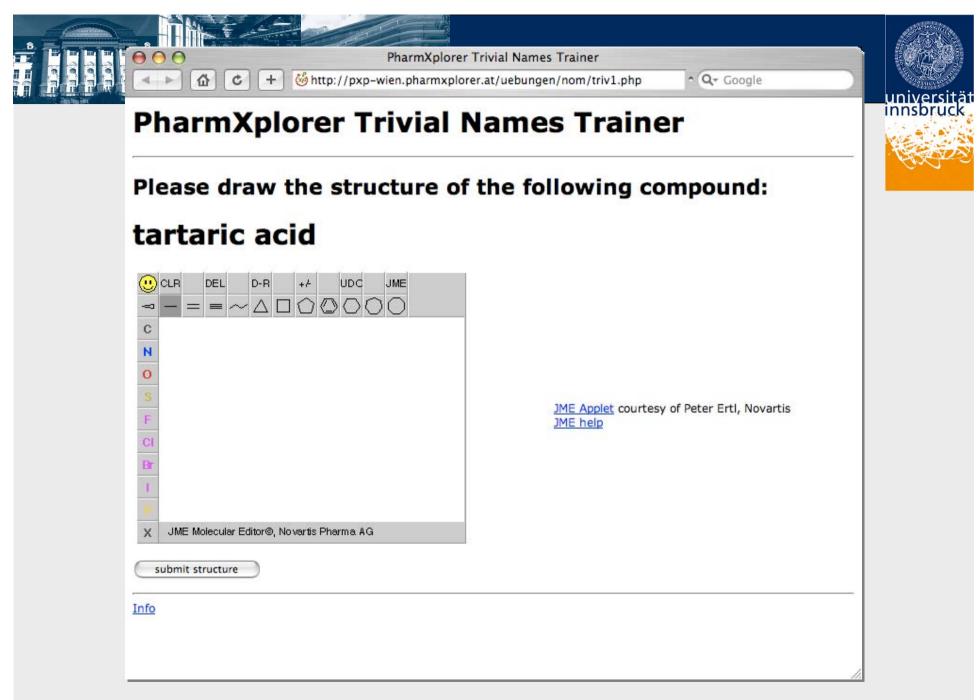
## **Interactive Training Elements**

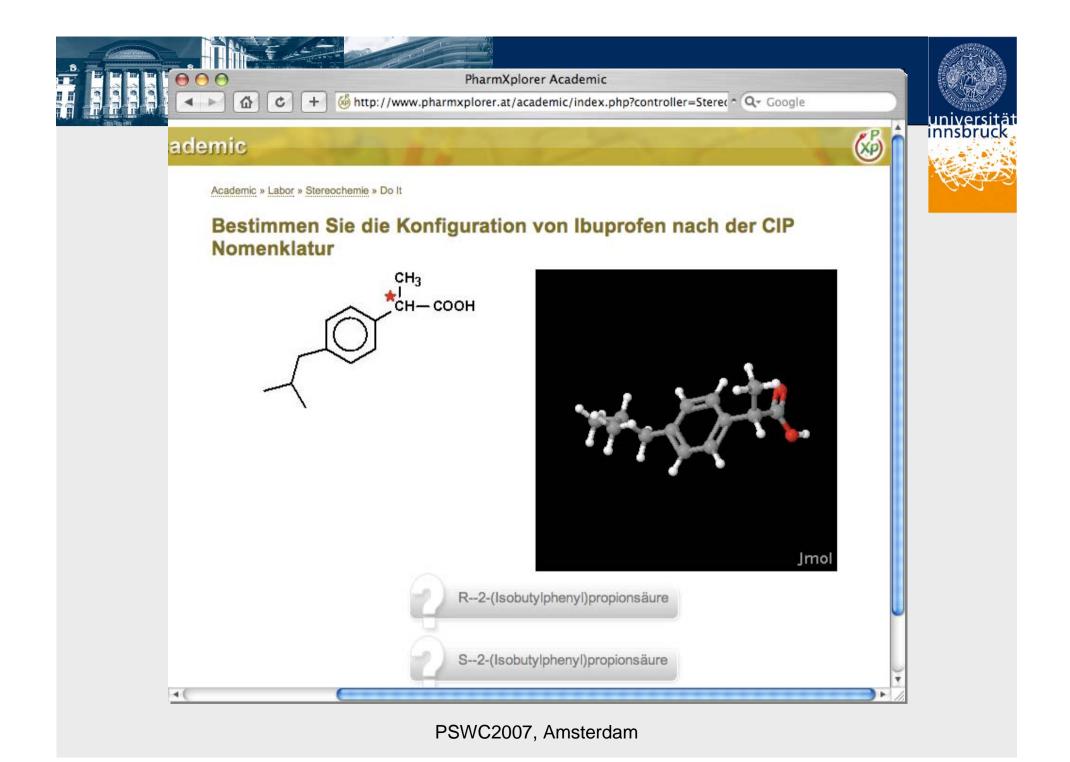
- Chemical nomenclature
  - Determine the name for a given structure formula
  - Draw a formula for a given name
- Stereo chemistry training
  - Determine the absolute stereo chemistry of chiral atoms
- Drug synthesis training
  - Find the reagent for a specific reaction
  - Draw the educts or the product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

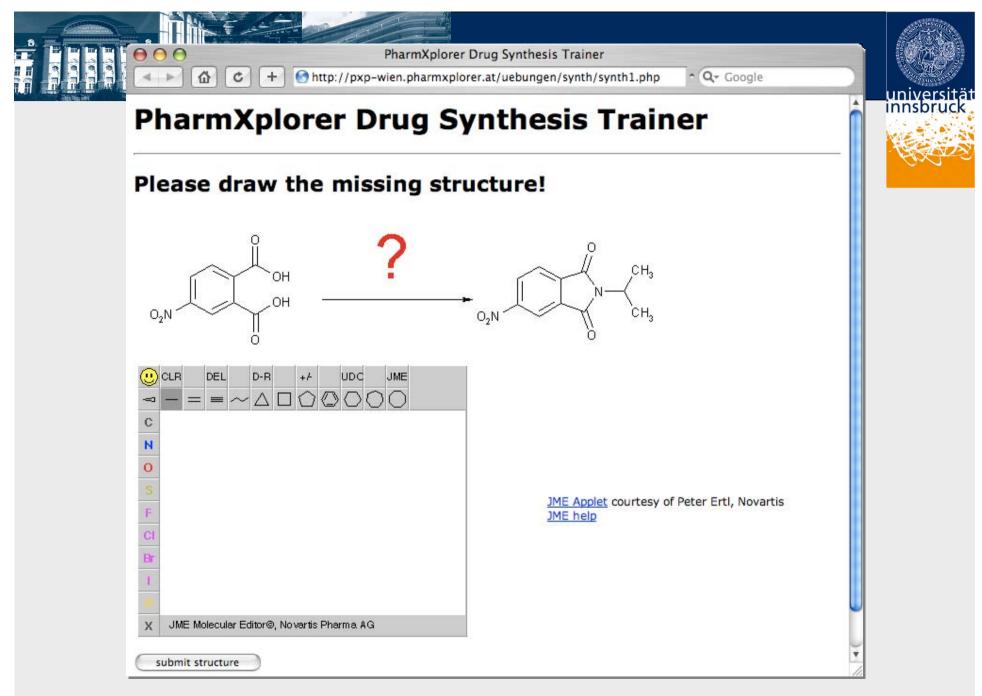












### There are much more features ...

- 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

# **Our Experiences**

- 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



#### Acknowledgements

- Prof. Klaus Schweiger, Graz
- Prof. Norbert Haider, Wien
- Dr. Daniela Schuster, Innsbruck
- Roman Weinberger, Graz
- bm:bwk for initial funding
- Apothekerverlag for sharing data

# www.pharmxplorer.com

