xPharm A Pharmacological Reference Work for Life Scientists

Chulalongkorn University, Thailand

Presented by: Doreen Tan Title: Product Sales Manager, Life Sciences Date: 01 Sep 2005



xPharm



The new authoritative reference work for Medicinal Pharmacology and Life Science



- 2300 <u>Agents</u>
- 600 <u>Targets</u>
- 450 Disorders
- 180 Principles

>500 expert editors around the world continuously contribute to populating and updating database



Emerging demand

xPharm

- Demand for
 - High quality and focused information
 - provided in an usable language
 - though an easily accessed resource,
 - organized in a simple, well thought through manner,
 - stored in highly functional repository
 - and connected to deep supporting material.





- All content has been created by world leading authorities in pharmacology
- Executive Editors
 - Sam J. Enna
 - David B. Bylund
- Associate Editors
 - Hanns Mohler (Targets)
 - Gary O. Rankin and Israel Hanin (Agents)
 - Frank J. Dowd (Disorders)
 - Lynn Wecker (Principles)



Editors and contributors



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Roderick Flower, Ph.D. Director of the William Harvey Research Institute, London; President of the British Pharmacological Society

Joseph Beavo, Ph.D. University of Washington, Seattle; Member of the prestigious National Academy of Sciences



Target End-users

- Pharmacologists
- Geneticists
- Molecular Biologists
- Biochemists
- Cell Biologists/Neuroscientists
- Immunologists
- Physiologists/Toxicologists
- Toxicologists
- Medicinal Chemists









- Authored by top scientists currently working in the field
- Records are written solely for xPharm by researchers
 - >500 contributors
 - Representing over 20 nations
 - Working in academic, government, and corporate institutions.
 - Data updated constantly by the primary researchers







"The drug research paradigm has moved from a compound looking for an effect to targets looking for a compound"

Dr. Jurgen Drews, Modern Drug Discovery, April 2004

- xPharm displays more detailed information about pharmacologically relevant targets
 - Classification, alternate names
 - Structural information for humans and all relevant animal models
 - Control of expression, protein partners, physiological role
 - Disease associations
 - Pharmacological regulation
 - This information is not available in any other single source







		Image: Construction Image: Construct		🥂 – ð ×			
		Pharmacological Regulation					
G • D •	💌 🖻 🐔 🔎 📩 -	As noted above, the binding of agonists to the D3 receptor is not regulated by guanine nucleotides. For the binding af additional ligands at the D3 dopamine receptor, other than those given below visit <u>http://kidb.bioc.cwru.edu/pdsp.php</u>					
D3 Dopa	amine Recepto	Dr ^{"dopamine} D3".					
Kim Neve and Day	id Sibley	Agonist / Activator / Substrate					
Click <u>here</u> to ci	() - () - E	Color	🦺 – 8 ×				
Introduction	,		·				
The D3 d	Mutant Targets						
superfam	The tGRAP mutant	recentor database (http://tgrap.uit.po/gueryform10.html) lists a number of mutants of the D3 donamine recentor					
receptors inhibit ad	The tGRAP mutant receptor database (<u>http://tgrap.uit.no/queryform10.html</u>) lists a number of mutants of the D3 dopamine receptor.						
abundant	Assays						
Nomenclature							
	-						
Superfa		obustly coupled to the inhibition of cyclic AMP accumulation unless expressed in a cell that either endogenously expresses, or has een transfected with type V adenylate cyclase <u>Robinson and Caron (1997</u>). Enhancement of [³⁵ S]GTP-gamma-S binding to					
Family	n	nembrane preparations can be employed to assess G protein-coupling. Cellular-based assays have included induction of					
Туре		mitogenesis and c-fos production, although these responses are downstream of initial second messenger generation. Electrophysiological methods that involve assessment of potassium or calcium channel activity in cells or tissue slice preparations					
	c	can also be employed.					
Subtyp	Genetically D3 receptor knockout mice have been produced by three separate groups, reviewed in <u>Sibley (1999)</u> <u>Glickstein and Schmauss</u>						
Classifi Numbe	Engineered (2001). In some cases, the D3 receptor-deficient mice have been crossed with other dopamine receptor-deficient mice, such as the D2 knockout mouse, to create mice lacking multiple dopamine receptors.						
Alterna Previou							
Comme							
		or, the D3 receptor exhibits high affinity for most antipsychotic drugs suggesting that it may be involved in					
Target Structi	psychotic <mark>disorders</mark> . However, numerous neuropathological and genetic studies have failed to provide a conclusive association between D3 receptors and schizophrenia. Nonetheless, blockade of the D3 receptor may contribute to the efficacy of some						
		s, reviewed in <u>Schwartz et al (2000)</u> .					
Protein 1							
The D3 <mark>d</mark> being ext	Other Information						
has a lar	Web Sites:						
amino ter			E	80			
9	<u>http://www.</u>	biotrend.com/pdf/dopa.pdf		相保			
	Molecule pag	ge of the Alliance for Cellular Signaling. PID for the <mark>dopamine</mark> D3 receptor is A000782: <u>http://www.afcs.org/</u>		<u>C 11</u> 2 2			
				VIER			

Useful



- Information on Disorders is organized for bench scientists to aid grant applications and business proposals
 - Classifications according to WHO and CDC where appropriate
 - Epidemiology: who gets the disease, the size of this population.
 - Consequences, pathophysiology: what happens if the disease is not treated
 - Standard and experimental therapies: what is known about pharmacological intervention and the mechanisms of therapeutics
 - Animal models: for basic study and toxicological tests
 - Sources of funding



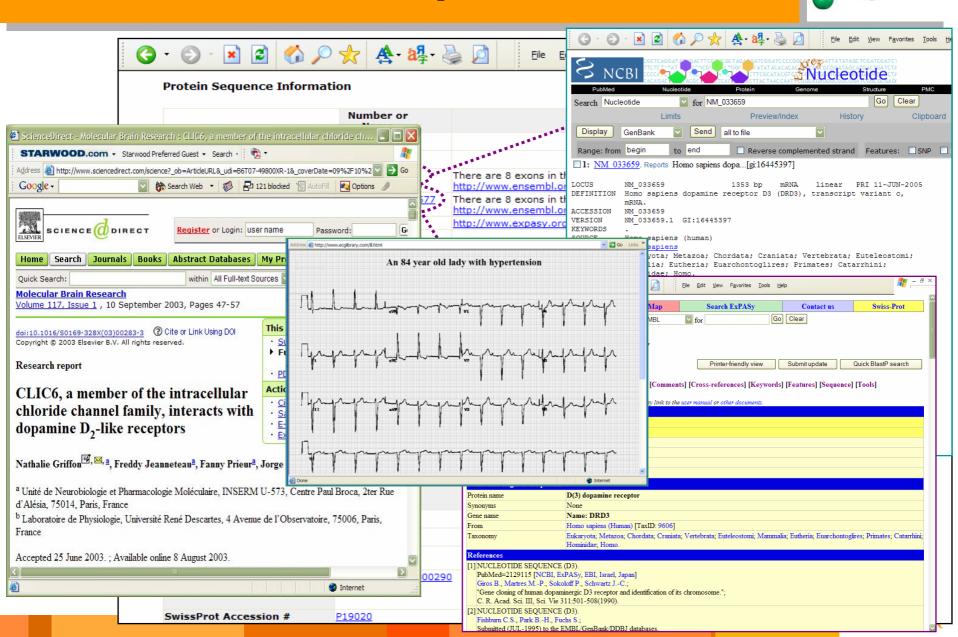




- More pharmacology content than any other online product
- More current and extensive than a print reference work
- Complementary database to bioactivity, drug pipeline and biomedical databases
- External links to:
 - Genetic database
 - Protein database
 - Literature
 - Vendors and funding sources



Extensive & Comprehensive



xPharm

A Growing Resource



- Existing records are updated quarterly
- Breaking news can be added immediately
- New records added continuously
 - Subject to editorial approval





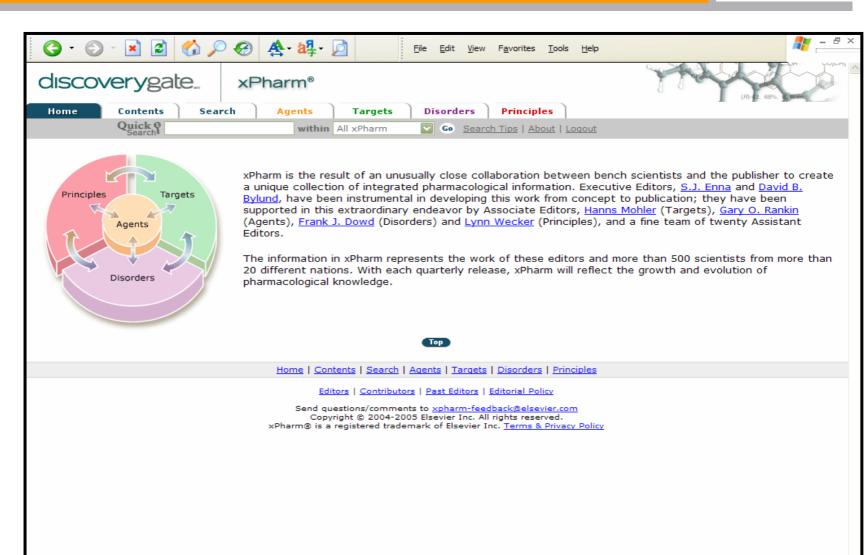


- Home Page access easy for non specialists. "Browsing of the table of Table of Contents was easy to use" – User
- Support for basic and advanced queries
- Answers pharmacology questions with focused results. (not found in journal articles, e.g. those on PubMed, or in current database offerings)
- Discover common pharmacological elements from disparate records.



www.xPharm.com





Easy to browse ToC

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discoverygate...

Home

xPharm Contents

Targets Disorders Principles

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Contents

Quick 9

agent Classes by Target

Agents Targeting Receptors

Agents Targeting Enzymes Ectonucleotidase Inhibitors

Isomerase Agents

Oxidoreductase Agents Transferase Agents

DNA-Interacting Agents

Alkylating Agents

Spindle Poisons

Docetaxel

Paclitaxel

Vinblastine Vincristine

Vinorelbine Lipid Interacting Agents Agents Targeting Proton Pumps

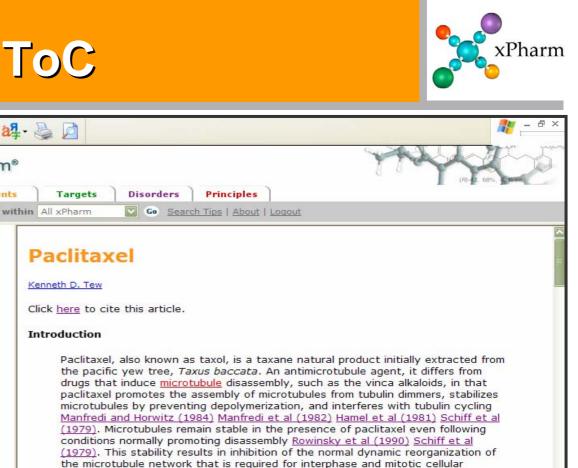
Agents by Therapeutic Use

Intercalating Agents

Platinum Derivatives

Agents Targeting Hydrolases

Agents Targeting Ion Channels Agents Targeting Transporters



Nomenclature

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Search

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Agents

Name of the Clinical Form	Paclitaxel	
Synonyms	Paclitaxel; Taxol; anzatax; bms 181339; genexol; hunxol; intaxel; nsc 125973; paxene; yewtaxan; taxol	
Chemical Names	(2S,5R,7S,10R,13S)-10,20-Bis(acetoxy)-2-benzoyloxy-1,7- dihydroxy-9-oxo-5,20-epoxytax-11-en-13-yl	

Simply point and click to drill to details.

functions Rowinsky et al (1990).

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Principles



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Search in selected Field Index

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discoverygate xr	Pharm®			
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	Basic Chemistry			
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	Contraindications			
	Adverse Effects			
	Agent-Agent Interactions			
	Preclinical Research			
	Other Research Information Other Information			
	Websites			
	Further Reading			
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	Home Contents Search Agents	Targets Disorders	Principles	
	Editors Contributors Pas	t Editors Editorial Pol	licy	
	Send questions/comments to xr			
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xPharm BROWSE & SEARCH EXAMPLES



Browsing for Disorder – Familial Hypercholesterolemia

20

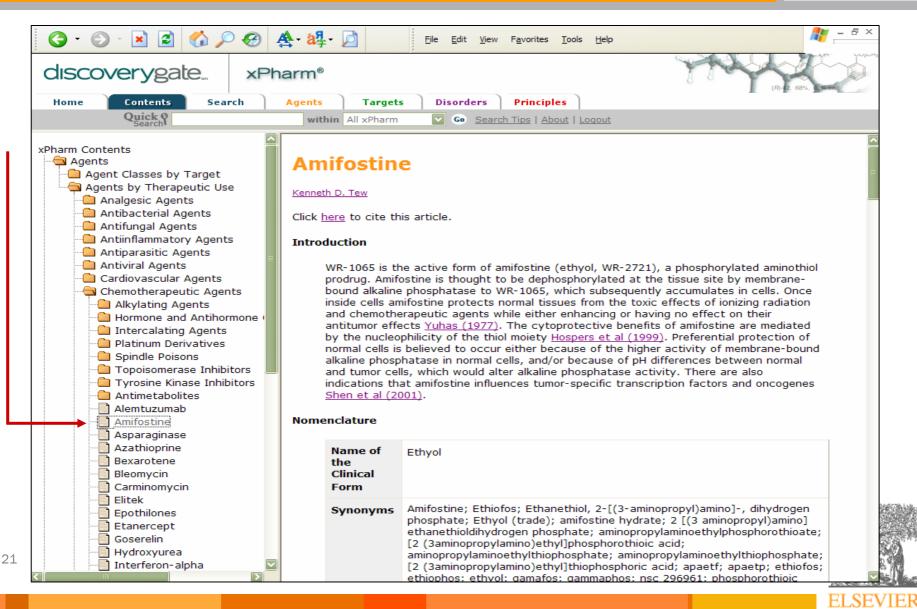


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discoverygate xPharm	(R)-12, 68%, 635-88
Home Contents Search Age	Targets Disorders Principles within All xPharm Search Tips About Logout
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xPharm Contents 	Familial Hypercholesterolemia
	Anna Maio
Blood Lipid Disorders	Click <u>here</u> to cite this article.
Hypertriglyceridemia	Introduction
 Blood and Bone Marrow Disorders Heart Disease Vascular Disorders Central Nervous System Disorders Endocrine Disorders Gastrointestinal Disease Genetic Errors in Metabolism Genitourinary Disorders Immune System and Inflammatory Disorders Infectious Diseases Musculo-Skeletal Disorders Neoplastic Disorders 	 Familial hypercholesterolemia is a type of primary hyperlipidemia in which serum low-density lipoprotein cholesterol (LDL-C) levels are elevated. Familial hypercholesterolemia is a monogenic, autosomal dominant disorder caused by defects in the gene that encodes for the low-density lipoprotein (LDL) receptor. This results in reduced clearance and an elevation of circulating LDL-C levels. Definition Familial hypercholesterolemia is defined by elevated low-density lipoprotein cholesterol (LDL-C) due to a genetic disorder. Familial hypercholesterolemia may be defined as heterozygous or homozygous. In all types of familial hypercholesterolemia, serum LDL-C is usually greater than 190 mg/dl.
 Ocular Disorders Otolaryngological Disorders Peripheral Nerve Disorders Pulmonary Disorders Renal Disorders Principles 	Classification In the Fredrickson-Levy-Lees classification of hyperlipoproteinemias, familial hypercholesterolemia is classified as type IIa based on the criteria that serum low- density lipoprotein cholesterol (LDL-C) is elevated usually without changes in serum levels of other lipoproteins <u>Fredrickson et al (1967a) Fredrickson et al (1967b)</u> <u>Fredrickson et al (1967c) Fredrickson et al (1967d) Fredrickson et al (1967e) Levy et al (1966)</u> . Familial hypercholesterolemia can also be defined according to the
	pattern of genetic inheritance as heterozygous (serum LDL-C > 250 mg/dl) or homozygous (serum LDL-C > 500 mg/dl). Consequences

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Browsing for Agent - Amifostine







Example 1:

What agents give edema as a side effect?

Example 2:

What targets does Alzheimer's disease affect?



Agents with edema S/E



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edema within Adverse Ef			
AND within - Any Field -	Targets-Pharmacodynamics		
AND within - Any Field -			
Include Principles	Imatinib mesylate predominantly targets Abl tyrosine kinase and its oncogenic fusion form Bcr-Abl by compe inhibiting ATP binding at the active site. It also has high affinity for the ATP binding pockets of c-Kit and PC tyrosine kinases.		
Display: Record Name for each search	larget Name(s):		
Description Introduction Nomenclature Basic Chemistry Human Pharmacokinetics Targets-Pharmacodynamics Therapeutics Indications			
Contraindications Adverse Effects Agent-Agent Interactions	Targets-Pharmacodynamics		
Preclinical Research Other Research Information	Apraclonidine is a non-selective alpha-1 and alpha-2 adrenoceptor agonist.		
Other Information Websites Further Reading	Target Name(s):		
	Alpha-1 Adrenoceptors Alpha-2 Adrenoceptors		
	3 Interferon alpha-2h		



Example 1:

What agents give edema as a side effect?

Example 2:

What targets does Alzheimer's disease affect?



Targets related to Alzheimer's Disease

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xPharm ARTICLE EXAMPLES



ARTICLES



- Paralens (panadol)
- <u>xPharm editors</u>
- <u>Viral Replication</u>
- Breast Cancer
- Monoamine oxidase







- xPharm is a growing resource, content is reviewed and updated frequently by recognized pharmacologists; and it is authoritative
- xPharm contains greater detail and more information on targets and disorders than any other single online resource
- The emphasis on experimental pharmacology (new agents, new targets)
- Easy to use- no training necessary
- xPharm is the ideal source to get answers to pharmacological questions
- Offers unlimited web-based access to users in an academic institution.



Thank you!



- Questions?
- Product Sales Manager: Doreen Tan
- Personal 14-day evaluation available at http://www.mdl.com
- Further questions, please visit <u>http://www.mdl.com/products/knowledge/x</u> <u>pharm/index.jsp;</u>
- or email <u>D.Tan@elsevier.com</u>



XPharm COMMON QUESTIONS



Common questions on xPharm



- Q: Is xPharm only about approved drugs?
 A: No. xPharm's emphasis is on experimental drugs about which pharmacological activity is known. The detailed information that is provided is pre-clinical, and agents with known toxicity in whole animals may be included because of their experimental utility for life scientists. However, approved drugs are included where their pharmacology is representative of a whole class of compounds.
- **Q:** When will xPharm be complete?

A: Never: this is a living database that will evolve with the growth of research in specific areas of target development and therapeutics. The xPharm database will be updated quarterly, with breaking news updated constantly.



Common questions on xPharm



 Q: Why are there only a couple of thousand agents in xPharm, and more than 100,000 in MDDR?

A: xPharm is not intended as an exhaustive catalog of NCE's. One can select an agent in xPharm according to its biological properties and then search for all similar compounds in MDDR.

Q: What is the difference between xPharm and MDDR?

A: MDDR is a database designed for chemists. It has 132,000 compounds and for some of these, the molecular target(s) and the therapeutic use(s) are named. By contrast, xPharm is intended primarily for life scientists providing detailed information about molecular targets, and about the diseases they are related to with links to representative examples of agent classes. Thus, xPharm and MDDR provide complementary views of pharmacological information intended for different audiences.



xPharm

PRICING MODEL FOR ACADEMICS & GOVERNMENT INSITUTIONS





Population Band*		2005 Subscription US\$			
Lower limit	Upper limit	DiscoveryGate	xPharm	Patent Chemistry Database	
1	50	27,657	8,018	8,627	
51	250	34,213	10,023	10,783	
251	500	39,961	12,528	13,479	

* For academics, population band refers to the number of faculty members + post-doc students in the relevant life science disciplines. E.g.. Pharmacy dept for xPharm.

** For government institutions, population size takes into account the number of relevant life science FTEs, including contractors.

