
AmicBase Drugs-Online 2011

Manual

1 Introduction

Antibiotics are essential for treatment of infectious diseases, however, no summary of world-wide licensed compounds plus their antimicrobial activities is published. AmicBase Drugs-Online 2011 is database on this topic published for free in the internet. It was created and published for information and education purposes. This database enables people concerned access to comprehensive data material in short time.

More in detail, AmicBase Drugs-Online 2011 displays information about antibiotics and antimycotics drugs, antiseptics as well as other antimicrobial compounds being licensed on the markets of United States, Japan and Europe.

AmicBase Drugs-Online 2011 informs in over 70.000 data records about kind of available drugs, their activities and microbial resistences being reported from scientific literature. It contains all data records of "AmicBase 2005 Drugs", which has been being offically marketed in the year 2005. In difference, toxicological data, resulting calculations (Therapeutic Indices) and searchable chemical structures are not given in the free online version. The database can be reached in the internet on the webpages of ReviewScience, the former company of the author of AmicBase, Dr. Alexander Pauli.

Before studying data in AmicBase Drugs-Online 2011, please, check the manual for abbreviations, classicfication of compound and microorganisms, country codes and others.

Newer Drugs being licensed since 2006 are not included in the current version of AmicBase Drugs-Online 2011. Data of such drugs will be added, if there is satisfying response from the users.

Visitors of the database AmicBase Drugs-Online 2011 are pointed to the fact, that the provided information should not be used in other ways than regulated in national laws and regulations.

Sincerely Yours
Dr. Alexander Pauli

2 Sources

The information included in the entire AmicBase (currently not available) is compiled from various literature sources.

Publication Types

Type	Count
Journal articles	2844
Patents	1878
Books	41
Doctoral theses	12
Other	17
Total	4792

Journal articles

Chemical Abstracts,

US National Library of Medicine, Medline: <http://www.igm.nlm.nih.gov/>

Patents

Deutsches Patent und Markenamt: <http://www.dpma.de>

United States Patent and Trademark Office: [US Patent Full-Text Database](#)

Compound data

US National Library of Medicine

PubChem Substance: <http://www.ncbi.nlm.nih.gov/entrez/query.fcgi>

ChemIDplus: <http://chem.sis.nlm.nih.gov/chemidplus/>

Toxicology data

Vermont Safety Information Resources, Inc.

Vermont SIRI MSDS Collection: <http://hazard.com/msds/>

Nomenclature in Microbiology

Index fungorum <http://www.indexfungorum.org/Names/Names.asp>

US National Library of Medicine, Taxonomy Browser,

<http://www.ncbi.nlm.nih.gov/Taxonomy/Browser/wwwtax.cgi?id=5073>

Pharmaceuticals

Pharmavista: <http://www.pharmavista.ch> (e-mediat AG)

3 Database Standardization

Revision of data was inevitable for a standardized presentation of the database records. These are as follows:

Unification of Language (English)

Scientific journal articles, doctoral theses or patents are written in different languages. To compare results, translation in one unique language is a precondition for the data management. However, some data obtained from Russian, Japanese, Chinese or Hungarian references are worked up without translation of test methods.

Unification of Microbial Strain Names

Scientific names of microorganisms changed in course of time. Therefore, it was inevitable to insert the actual microbial species names in order to compare the results. The older names are given in an extra database field.

Unification of Compound Names

Similar to microbial species names, the names of compounds changed in course of time and needed standardization. However, it was impossible to find a naming-system appropriate for all compounds in AmicBase. Small molecules are named according to IUPAC rules (see 'Other Names'). A usual, short name of almost every compound is given in the field 'Name'.

Unification of Inhibitory Data

The inhibitory concentration of test compounds in liquid media is given in different ways in literature. All these data are recalculated in ppm (mg/l) in order to compare results. Sometimes the volume of a test compound was given in a defined volume of growth medium. The amount in ppm of the test compound was calculated with the density of 1 in such cases.

Annotations

Due to the failure of one generally established standard testing procedure in microbiology annotations were necessary in some cases. Data about experimental conditions or inhibitory results are given among 'Annotations'.

4 Compound Categorizing

AmicBase Drugs-Online 2011 contains different categories (antiseptics, disinfectants, antibiotics, antimycotics and preservatives) of compounds, which are licensed as drugs elsewhere in the world. The compounds are classified by their chemical structure. The abbreviations, number of compounds and count of respective data records are scheduled in the following table.

Compound Groups	Abbreviation	No. Com- pounds	No. Data Records
GROUPS I to III: Aliphatics and Aromatics	Ali-CHO-Drug, Ali-COOH-Drug, Ali-OH-Drug, Ar-COOH-Drug, Ar-COOR-Drug, Ar-OH-Drug, Ar-R-Drug, Monoterpene-Drug, Phenylpropane-Drug, Terpene related-Drug	34	5830
GROUP IV: Hetero Compounds	Hetero-Drug, Heterocycle-Drug	101	5330
GROUP V: Antibiotics and Antimycotics			
beta-Lactam antibiotics	AB-bLac-Drug	164	16422
Aminoglycosides	AB-AmGl-Drug	39	5219
Ansa-type antibiotics	AB-Ansa-Drug	5	821
Glycopeptides	AB-GiPe-Drug	13	1457
Antifungal drugs, miscellaneous	AB-Fu00-Drug	24	2553
Antifungal drugs, Azoles	AB-FuAz-Drug	34	5218
Antifungal drugs, Polyethers	AB-FuPoEn-Drug	6	2165
Macrolides	AB-Macr-Drug	33	4474
Nucleosides	AB-Nucl-Drug	1	400
Peptides	AB-Pept-Drug	20	1478
Polyethers	AB-PoEt-Drug	2	21
Quinolones	AB-Quin-Drug	33	7411
Steroides	AB-Ster-Drug	2	76
Sulfonamides	AB-Sulf-Drug	41	2539
Tetracyclines	AB-Tetr-Drug	25	3530
Not classified antibiotics	AB-0000-Drug	34	5408
Miscellaneous	Miscellaneous-Drug	1	20
Total drugs		612	70372

5 Database Fields

Characterization of Compounds

Structure: Optimized 3D-compound structure

Molname: Short compound name, common name

Other Names: further compound names, synonyms, trade names. The countries in which such drugs are sold are abbreviated using three-letter WHO country codes.

Mol-Annotation: compound annotations

Compound classification: for details of the classification system used, see 'Compounds Categorizing'. Drugs are characterized by the addition of the suffix '-drug'

Compound-Nr: Database number of test compound

CAS-Nr: Chemical Abstract Service Number

Molecular formula: Molecular formula

MW: Molecular weight in g/mol

Characterization of Microorganisms

Microorganism: Actual scientific name of a microbial species

Microorganism type: Strain type of the microorganism, e.g. ATCC strain

Publication strain name: Microorganism name used in a publication

Microorganism classification: Abbreviations of microorganism classes:

Bac = bacteria, undefined gram coloring

Bac+ = gram positive bacteria

Bac- = gram negative bacteria

fungi, yeast (without abbreviation)

MO = undefined microorganisms

Proto = protozoa (not many data records)

Characterization of Test Method

Method: Brief listing of test parameters

Method type: Abbreviation of test method

SDT: Serial dilution test: a test compound was examined on growth inhibitory properties at different concentrations in a liquid culture medium; resulting inhibitory data: MIC, MMC, and NIC.

ADIT: Agar dilution test: a test compound was examined on growth inhibitory properties at different concentrations in semi-solid agar medium – microorganisms were cultivated on agar surface; resulting inhibitory data: MIC, NIC.

ADT: Agar diffusion test: a reservoir of the test compound was given on the surface of an agar plate – microorganisms were cultivated on agar surface, growth inhibitory compounds cause a zone without growth; resulting inhibitory data: inhibition zone (mm)

VPT: Vapor phase test: vapors of a test compound were examined on growth inhibitory properties in a sealed container – microorganisms were exposed to vapors. The techniques varied often; resulting inhibitory data: inhibition zone (mm) and others.

Annotation: Annotation on test results, test conditions or compounds

Characterization of Inhibitory Data

MIC: Minimal Inhibitory Concentration in ppm: the concentration causing no growth of microorganisms – growth was determined with the naked eye.

MMC: Minimal Microbicidal Concentration in ppm: the concentration causing no growth of microorganisms – growth was determined in subcultures.

NIC: Non-Inhibitory Concentration in ppm: the concentration at which a microbial strain survived.

PC: Phenol coefficient: this calculates the inhibitory activity of a test compound relative to phenol. The phenol coefficient was used preferably in older literature. It was a measure in experiments, in which the short-time killing concentration (15 minutes) was determined.

ADT Evaluation: Agar diffusion test – evaluation field

VPT Evaluation: Vapor phase test – evaluation field

ADT and VPT yield inhibitory data other than a given amount of test compound per volume unit. Therefore, effects obtained by these methods were evaluated on a scale from 1 to 4 to obtain a ranking of compounds:

- 1 = no growth inhibitory activity
- 2 = slight growth inhibitory activity

3 = moderate growth inhibitory activity
4 = strong growth inhibitory activity

Due to the failure of concentration data within the agar medium, the results of the activity evaluation are only of limited value. Generally, the evaluation 2 to 4 indicates antimicrobial activity. When comparing the results of a series test compound being examined under the same test conditions, the evaluation 4 is given to compounds, which caused the largest inhibition zone. This evaluation method does not allow a quantitative comparison of results obtained under various test conditions.

Inhibitory zone: Size of inhibition zone (mm) caused by a test compound either by diffusion (ADT) or volatilization (VPT).

Characterization of Information Source

RefNo: Database number of reference

Author: Author(s) of reference

Title: Title of reference

Citation: Complete journal title, book title or patent publication number of reference. The publication number is the number assigned to a patent when the patent application is published.

Volume: Journal issue number of reference

Pages: Pages of reference

Year: Year of publication of reference

DocType: Type of document of reference

5.1 Data Table in AmicBase-Online

'AmicBase-Online consists of 1 table with following fields:

Data Table

Field name	Type
MOL_ID or Compound Number	Numeric
Name	Text
Other Names	Text
Mol-Annotation	Text
Molecular Formula	Text
CAS-Nr	Text
MW	Numeric
Compound Classification	Text
Microorganism Classification	Text
Microorganism	Text
Microorganism Type	Text
Publication Strain Name	Text
Method Abbreviation	Text
Method	Text
Annotation	Text
MIC	Numeric
MMC	Numeric
NIC	Numeric
PC	Numeric
Inhibitory Zone	Text
ADT Evaluation	Numeric
VPT Evaluation	Numeric
Ref-Nr	Numeric
Reference	Text
Publication Year	Numeric
DocType	Text

5.2 Country Codes in AmicBase-Online

Countries in which a drug is distributed are given next to the drug name as abbreviation in brackets, e.g. EFLORAN (CZH, CRO, SVN, YUG) means metronidazole is sold under name EFLORAN in the countries Czech Republic, Croatia, Slovenia and Yugoslavia (former).

In text searches one will be able to find a drugs by its trade name.

The abbreviations used in AmicBase present three-letter WHO country codes.

AFGHANISTAN	CHAD	GEO	LEB	OMA
AFG	CHA	GERMANY	LESOTHO	PACIFIC ISLANDS
ALBANIA	CHILE	DEU	LES	PTT
ALB	CHI	GHANA	LIBERIA	PAKISTAN
ALGERIA	CHINA	GHA	LIB	PAK
ALG	CHN	GREECE	LIBYAN A. J.	PANAMA
ANGOLA	COLOMBIA	GRE	LIY	PAN
ANG	COL	GREENLAND	LITHUANIA	PAPUA NEW GUINEA
ANTIGUA & BARBUDA	COMOROS	GRN	LTU	PNG
ANI	COM	GRENADA	LUXEMBOURG	PARAGUAY
ARGENTINA	CONGO	GRA	LUX	PAR
ARG	CNG	GUADELOUPE	MACAO	PERU
ARMENIA	COSTA RICA	GUA	MAC	PER
ARM	COR	GUAM	MACEDONIA, THE FORMER YUGOSLAV REP.	PHILIPPINES
AUSTRALIA	COTE D'IVOIRE	GUM	MADAGASCAR	PHL
AUS	IVC	GUATEMALA	MAD	POLAND
AUS	CROATIA	GUT	MALAWI	POL
AUSTRIA	CRO	GUINEA	MAL	PORTUGAL
AUT	CUBA	GUI	MALAYSIA	POR
AZERBAIJAN	CUB	GUINEA-BISSAU	MAA	PUERTO RICO
AZE	CYP	GUB	MAA	PUR
BAHAMAS	CZECH REPUBLIC	GUYANA	MAA	QATAR
BAH	CZH	GUY	MALDIVES	QAT
BAHRAIN	CZECHOSLOVAKIA (former)	HAITI	MAV	REPUBLIC OF KOREA
BAA	CZE	HAI	MAL	KOR
BANGLADESH	DEM. P. REP. KOREA	HONDURAS	MAI	REUNION
BAN	KRD	HON	MALTA	REU
BARBADOS	DENMARK	HONG KONG	MAT	ROMANIA
BAR	DEN	HOK	MARTINIQUE	ROM
BELARUS	DJIBOUTI	HUNGARY	MAR	RUSSIAN FEDERATION
BLR	DJI	HUN	MAURITANIA	RUS
BELGIUM	DOMINICA	ICELAND	MAU	RWA
BEL	DOM	ICE	MAURITIUS	RUW
BELIZE	DOMINICAN REPUBLIC	INDIA	MAS	RUW
BLZ	DOR	IND	MEXICO	SAMOA
BENIN	EAST TIMOR	INDONESIA	MEX	SMA
BEN	EAT	INO	MEX	SAN MARINO
BERMUDA	ECUADOR	IRAN, ISLAMIC REP.	MOLDOVA, REP. OF	SMR
BER	ECU	IRA	MDA	SAO TOME & PRINCIPE
BHUTAN	EGYPT	IRAQ	MONGOLIA	STP
BHU	EGY	IRQ	MOG	SAUDI ARABIA
BOLIVIA	EL SALVADOR	IRELAND	MOROCCO	SAA
BOL	ELS	IRE	MOR	SENEGAL
BOSNIA & HERZEGOVINA	EQUATORIAL GUINEA	ISRAEL	MOZAMBIQUE	SEN
BIH	EGG	ISR	MOZ	SEYHELLES
BOTSWANA	ESTONIA	ITALY	MYANMAR	SEY
BOT	ETHIOPIA	ITA	BUR	SIERRA LEONE
BRAZIL	ETH	JAMAICA	NAMIBIA	SIL
BRA	FJI	JAM	NAM	SINGAPORE
BRUNEI	FIJ	JAPAN	NEP	SIN
DARUSSALAM	FINLAND	JPN	NETHERLANDS	SLOVAK REPUBLIC
BRU	FIN	JORDAN	NET	SVK
BULGARIA	FRANCE	JOR	NETHERLANDS	SLOVENIA
BUL	FRA	KAZAKHSTAN	ANTILLES	SVN
BURKINA FASO	FRG	KAZ	NEA	SOLOMON ISLANDS
BFA	FRP	KENYA	NEW CALEDONIA	SOL
CAMBODIA	GABON	KEN	NEC	SOMALIA
KAM	GAB	KIRIBATI	NEW ZEALAND	SOM
CAMEROON	GAMBIA	KIR	NEZ	SOUTH AFRICA
CAE	GAM	KUWAIT	NICARAGUA	SOA
CANADA	GEORGIA	KUW	NIC	SPAIN
CAN		KYRGYZSTAN	NIGER	SPG
CAPE VERDE		LAO, P.D.R.	KYR	SRI LANKA
CAV		LAO	NIGERIA	SRL
CENTRAL AFRICAN REP.		LATVIA	NIE	ST LUCIA
CAF		LVA	NORWAY	SAL
		LEBANON	NOR	ST VINCENT
			OMAN	

SAV	TAJIKISTAN	TUN	URU	WEST BANK AND
ST. KITTS AND NEVIS	TJK	TURKEY	US VIRGIN ISLANDS	GAZA
STK	TANZANIA, UNITED	TUR	VUS	WBG
SUDAN	REP. OF	TURKMENISTAN	USA	YEMEN
SUD	TAN	TKM	USA	YES
SURINAME	THAILAND	UGANDA	USSR (former)	YUGOSLAVIA (former)
SUR	THA	UGA	SSR	YUG
SWAZILAND	TOGO	UKRAINE	UZBEKISTAN	ZAIRE
SWZ	TOG	UKR	UZB	ZAI
SWEDEN	TONGA	UNITED ARAB	VANUATU	ZAMBIA
SWE	TON	EMIRATES	VAN	ZAM
SWITZERLAND	TRINIDAD AND	UAE	VENEZUELA	ZIMBABWE
SWI	TOBAGO	UNITED KINGDOM	VEN	Z
SYRIAN A. REP.	TRT	UNK	VIET NAM	
SYR	TUNISIA	URUGUAY	VTN	

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Author:

Dr. Alexander Pauli

Fürther Str. 13

D-90513 Zirndorf,

Germany

<http://www.reviewscience.com>