INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

CHEMISTRY AND HUMAN HEALTH DIVISION

MEDICINAL CHEMISTRY SECTION

GLOSSARY OF TERMS USED IN MEDICINAL CHEMISTRY

(IUPAC Recommendations 1998)

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Glossary of terms used in medicinal chemistry (IUPAC Recommendations 1998)

Abstract: The objective of the glossary is to provide in a single document a consistent terminology and concise definitions of terms covering the various aspects of medicinal chemistry. This was felt necessary with regard to the rapid changes occurring in medicinal chemistry and also by the need to establish international definition standards. Effectively the possibility exists that in different countries certain terms may not have the same meaning, in such a case the creation of an internationally accepted definition is particularly justified.

A Working Party belonging to the IUPAC Section on Medicinal Chemistry has therefore been assembled which prepared the present glossary. Concise but sufficiently explanatory definitions have been formulated for about one hundred commonly employed terms which can be considered of particular interest to the medicinal chemistry community. The glossary has been compiled in part from definitions proposed by the Working Party in part from earlier IUPAC glossaries and in part from well-accepted definitions taken from the literature but which were sometimes published in journals or books that may not be readily accessible.

ALPHABETICAL ORDERED ENTRIES

The glossary has been compiled in part from definitions proposed by the Working Party and in part from well-accepted definitions taken from the literature. In most cases, definitions given here are for specific areas of medicinal chemistry. Some definitions taken from the Glossary for Chemists of Terms Used in Biotechnology (Pure Appl. Chem., 1992, 64, 143–168) were also included, eventually in a slightly modified form; they are identified by an asterisk*. Others, which appear in the Glossary on Computational Drug Design (Pure Appl. Chem., 1997, 69, 1137–1152) and in Glossary for Chemists of terms used in Toxicology (Pure Appl. Chem. 1993, 65, 2003–2122), are identified by a double** and a triple*** asterisk respectively.

Active transport*

Active transport is the carriage of a solute across a biological membrane from low to high concentration that requires the expenditure of (metabolic) energy.

Address-message concept

Address-message concept refers to compounds in which part of the molecule is required for binding (address) and part for the biological action (message).

ADME

Abbreviation for Absorption, Distribution, Metabolism, Excretion. (See also Pharmacokinetics; Drug disposition).

Affinity

Affinity is the tendency of a molecule to associate with another. The affinity of a drug is its ability to bind to its biological target (receptor, enzyme, transport system, etc.) For pharmacological receptors it can be thought of as the frequency with which the drug, when brought into the proximity of a receptor by diffusion, will reside at a position of minimum free energy within the force field of that receptor.
For an agonist (or for an antagonist) the numerical representation of affinity is the reciprocal of the equilibrium dissociation constant of the ligand-receptor complex denoted \( K_A \), calculated as the rate constant for offset \( (k_{-1}) \) divided by the rate constant for onset \( (k_1) \).

**Agonist**

An agonist is an endogenous substance or a drug that can interact with a receptor and initiate a physiological or a pharmacological response characteristic of that receptor (contraction, relaxation, secretion, enzyme activation, etc.).

**Allosteric binding sites**

Allosteric binding sites are contained in many enzymes and receptors. As a consequence of the binding to allosteric binding sites, the interaction with the normal ligand may be either enhanced or reduced.

**Allosteric enzyme**

An allosteric enzyme is an enzyme that contains a region to which small, regulatory molecules ("effectors") may bind in addition to and separate from the substrate binding site and thereby affect the catalytic activity.

On binding the effector, the catalytic activity of the enzyme towards the substrate may be enhanced, in which case the effector is an activator, or reduced, in which case it is a de-activator or inhibitor.

**Allosteric regulation**

Allosteric regulation is the regulation of the activity of allosteric enzymes. (See also Allosteric binding sites; Allosteric enzymes).

**Analog**

An analog is a drug whose structure is related to that of another drug but whose chemical and biological properties may be quite different. (See also Congener).

**Antagonist**

An antagonist is a drug or a compound that opposes the physiological effects of another. At the receptor level, it is a chemical entity that opposes the receptor-associated responses normally induced by another bioactive agent.

**Antimetabolite**

An antimetabolite is a structural analog of an intermediate (substrate or coenzyme) in a physiologically occurring metabolic pathway that acts by replacing the natural substrate thus blocking or diverting the biosynthesis of physiologically important substances.

**Antisense molecule**

An antisense molecule is an oligonucleotide or analog thereof that is complementary to a segment of RNA (ribonucleic acid) or DNA (deoxyribonucleic acid) and that binds to it and inhibits its normal function.
Autacoid
An autacoid is a biological substance secreted by various cells whose physiological activity is restricted to the vicinity of its release; it is often referred to as local hormone.

Autoreceptor
An autoreceptor, present at a nerve ending, is a receptor that regulates, via positive or negative feedback processes, the synthesis and/or release of its own physiological ligand. (See also Heteroreceptor).

Bioassay
A bioassay is a procedure for determining the concentration, purity, and/or biological activity of a substance (e.g., vitamin, hormone, plant growth factor, antibiotic, enzyme) by measuring its effect on an organism, tissue, cell, enzyme or receptor preparation compared to a standard preparation.

Bioisostere
A bioisostere is a compound resulting from the exchange of an atom or of a group of atoms with another, broadly similar, atom or group of atoms. The objective of a bioisosteric replacement is to create a new compound with similar biological properties to the parent compound. The bioisosteric replacement may be physicochemically or topologically based. (See also Isostere)

Bioprecursor prodrug
A bioprecursor prodrug is a prodrug that does not imply the linkage to a carrier group, but results from a molecular modification of the active principle itself. This modification generates a new compound, able to be transformed metabolically or chemically, the resulting compound being the active principle.

Biotransformation
Biotransformation is the chemical conversion of substances by living organisms or enzyme preparations.

CADD
See Computer-assisted drug design

Carrier-linked prodrug (Carrier prodrug)
A carrier-linked prodrug is a prodrug that contains a temporary linkage of a given active substance with a transient carrier group that produces improved physicochemical or pharmacokinetic properties and that can be easily removed in vivo, usually by a hydrolytic cleavage.

Cascade prodrug
A cascade prodrug is a prodrug for which the cleavage of the carrier group becomes effective only after unmasking an activating group.

Catabolism
Catabolism consists of reactions involving endogenous organic substrates to provide chemically available energy (e.g., ATP) and/or to generate metabolic intermediates used in subsequent anabolic reactions.
Catabolite
A catabolite is a naturally occurring metabolite.

Clone*
A clone is a population of genetically identical cells produced from a common ancestor. Sometimes, "clone" is also used for a number of recombinant DNA (deoxyribonucleic acid) molecules all carrying the same inserted sequence.

Codon*
A codon is the sequence of three consecutive nucleotides that occurs in mRNA which directs the incorporation of a specific amino acid into a protein or represents the starting or termination signals of protein synthesis.

Coenzyme
A coenzyme is a dissociable, low-molecular weight, non-proteinaceous organic compound (often nucleotide) participating in enzymatic reactions as acceptor or donor of chemical groups or electrons.

Combinatorial synthesis
Combinatorial synthesis is a process to prepare large sets of organic compounds by combining sets of building blocks.

Combinatorial library
A combinatorial library is a set of compounds prepared by combinatorial synthesis.

CoMFA
See Comparative Molecular Field Analysis

Comparative Molecular Field Analysis (CoMFA)**
Comparative molecular field analysis (CoMFA) is a 3D-QSAR method that uses statistical correlation techniques for the analysis of the quantitative relationship between the biological activity of a set of compounds with a specified alignment, and their three-dimensional electronic and steric properties. Other properties such as hydrophobicity and hydrogen bonding can also be incorporated into the analysis. (See also Three-dimensional Quantitative Structure-Activity Relationship [3D-QSAR]).

Computational chemistry**
Computational chemistry is a discipline using mathematical methods for the calculation of molecular properties or for the simulation of molecular behaviour.

Computer-assisted drug design (CADD)**
Computer-assisted drug design involves all computer-assisted techniques used to discover, design and optimize biologically active compounds with a putative use as drugs.
Congener***

A congener is a substance literally con- (with) generated or synthesized by essentially the same synthetic chemical reactions and the same procedures. Analogs are substances that are analogous in some respect to the prototype agent in chemical structure.

Clearly congeners may be analogs or vice versa but not necessarily. The term congener, while most often a synonym for homologue, has become somewhat more diffuse in meaning so that the terms congener and analog are frequently used interchangeably in the literature.

Cooperativity

Cooperativity is the interaction process by which binding of a ligand to one site on a macromolecule (enzyme, receptor, etc.) influences binding at a second site, e.g. between the substrate binding sites of an allosteric enzyme. Cooperative enzymes typically display a sigmoid (S-shaped) plot of the reaction rate against substrate concentration. (See also Allosteric binding sites).

3D-QSAR

See Three-dimensional Quantitative Structure-Activity Relationship

De novo design**

De novo design is the design of bioactive compounds by incremental construction of a ligand model within a model of the receptor or enzyme active site, the structure of which is known from X-ray or nuclear magnetic resonance (NMR) data.

Disposition

See Drug disposition

Distomer

A distomer is the enantiomer of a chiral compound that is the less potent for a particular action. This definition does not exclude the possibility of other effect or side effect of the distomer (See also Eutomer).

Docking studies

Docking studies are molecular modeling studies aiming at finding a proper fit between a ligand and its binding site.

Double-blind study

A double-blind study is a clinical study of potential and marketed drugs, where neither the investigators nor the subjects know which subjects will be treated with the active principle and which ones will receive a placebo.

Double prodrug (or pro-prodrug)

A double prodrug is a biologically inactive molecule which is transformed in vivo in two steps (enzymatically and/or chemically) to the active species.
Drug

A drug is any substance presented for treating, curing or preventing disease in human beings or in animals. A drug may also be used for making a medical diagnosis or for restoring, correcting, or modifying physiological functions (e.g., the contraceptive pill).

Drug disposition

Drug disposition refers to all processes involved in the absorption, distribution metabolism and excretion of drugs in a living organism.

Drug latentiation

Drug latentiation is the chemical modification of a biologically active compound to form a new compound, which in vivo will liberate the parent compound. Drug latentiation is synonymous with prodrug design.

Drug targeting

Drug targeting is a strategy aiming at the delivery of a compound to a particular tissue of the body.

Dual action drug

A dual action drug is a compound which combines two desired different pharmacological actions at a similarly efficacious dose.

Efficacy

Efficacy describes the relative intensity with which agonists vary in the response they produce even when they occupy the same number of receptors and with the same affinity. Efficacy is not synonymous to Intrinsic activity.

Efficacy is the property that enables drugs to produce responses. It is convenient to differentiate the properties of drugs into two groups, those which cause them to associate with the receptors (affinity) and those that produce stimulus (efficacy). This term is often used to characterize the level of maximal responses induced by agonists. In fact, not all agonists of a receptor are capable of inducing identical levels of maximal responses. Maximal response depends on the efficiency of receptor coupling, i.e., from the cascade of events, which, from the binding of the drug to the receptor, leads to the observed biological effect.

Elimination

Elimination is the process achieving the reduction of of the concentration of a xenobiotic including its metabolism.

Enzyme

An enzyme is a macromolecule, usually a protein, that functions as a (bio) catalyst by increasing the reaction rate.

In general, an enzyme catalyzes only one reaction type (reaction selectivity) and operates on only one type of substrate (substrate selectivity). Substrate molecules are transformed at the same site (regioselectivity) and only one or preferentially one of chiral a substrate or of a racemate is transformed (enantioselectivity[special form of stereoselectivity]).

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Enzyme induction*

Enzyme induction is the process whereby an (inducible) enzyme is synthesized in response to a specific inducer molecule. The inducer molecule (often a substrate that needs the catalytic activity of the inducible enzyme for its metabolism) combines with a repressor and thereby prevents the blocking of an operator by the repressor leading to the translation of the gene for the enzyme.

Enzyme repression*

Enzyme repression is the mode by which the synthesis of an enzyme is prevented by repressor molecules.

In many cases, the end product of a synthesis chain (e.g., an amino acid) acts as a feedback corepressor by combining with an intracellular aporepressor protein, so that this complex is able to block the function of an operator. As a result, the whole operation is prevented from being transcribed into mRNA, and the expression of all enzymes necessary for the synthesis of the end product enzyme is abolished.

Eudismic ratio

Eudismic ratio is the potency of the eutomer relative to that of the distomer.

Eutomer

The Eutomer is the enantiomer of a chiral compound that is the more potent for a particular action (See also Distomer).

Genome*

A genome is the complete set of chromosomal and extrachromosomal genes of an organism, a cell, an organelle or a virus; the complete DNA (deoxyribonucleic acid) component of an organism.

Hansch analysis**

Hansch analysis is the investigation of the quantitative relationship between the biological activity of a series of compounds and their physicochemical substituent or global parameters representing hydrophobic, electronic, steric and other effects using multiple regression correlation methodology.

Hapten***

A hapten is a low molecular weight molecule that contains an antigenic determinant but which is not itself antigenic unless combined with an antigenic carrier.

Hard drug

A hard drug is a nonmetabolizable compound, characterized either by high lipid solubility and accumulation in adipose tissues and organelles, or by high water solubility.

In the lay press the term "Hard Drug" refers to a powerful drug of abuse such as cocaine or heroin.

Heteroreceptor

A heteroreceptor is a receptor regulating the synthesis and/or the release of mediators other than its own ligand (See also Autoreceptor).
Terms used in medicinal chemistry

Homo I o g u e
The term homologue is used to describe a compound belonging to a series of compounds differing from each other by a repeating unit, such as a methylene group, a peptide residue, etc.

Hormone***
A hormone is a substance produced by endocrine glands, released in very low concentration into the bloodstream, and which exerts regulatory effects on specific organs or tissues distant from the site of secretion.

Hydrophilicity**
Hydrophilicity is the tendency of a molecule to be solvated by water.

Hydrophobicity**
Hydrophobicity is the association of non-polar groups or molecules in an aqueous environment which arises from the tendency of water to exclude non polar molecules. (See also Lipophilicity).

IND
Abbreviation for Investigational New Drug.

Intrinsic activity
Intrinsic activity is the maximal stimulatory response induced by a compound in relation to that of a given reference compound (See also Partial agonist)

This term has evolved with common usage. It was introduced by Ariëns as a proportionality factor between tissue response and receptor occupancy. The numerical value of intrinsic activity (alpha) could range from unity (for full agonists, i.e., agonist inducing the tissue maximal response) to zero (for antagonists), the fractional values within this range denoting partial agonists. Ariëns' original definition equates the molecular nature of alpha to maximal response only when response is a linear function of receptor occupancy. This function has been verified. Thus, intrinsic activity, which is a drug and tissue parameter, cannot be used as a characteristic drug parameter for classification of drugs or drug receptors. For this purpose, a proportionality factor derived by null methods, namely, relative efficacy, should be used. Finally, "intrinsic activity" should not be used instead of "intrinsic efficacy". A "partial agonist" should be termed "agonist with intermediate intrinsic efficacy" in a given tissue.

Inverse agonist
An inverse agonist is a drug which acts at the same receptor as that of an agonist, yet produces an opposite effect. Also called negative antagonists.

Isosteres
Isosteres are molecules or ions of similar size containing the same number of atoms and valence electrons, e.g., O²⁻, F⁻, Ne (See also Bioisoste).
Lead discovery

Lead discovery is the process of identifying active new chemical entities, which by subsequent modification may be transformed into a clinically useful drug.

Lead generation

Lead generation is the term applied to strategies developed to identify compounds which possess a desired but non-optimized biological activity.

Lead optimization

Lead optimization is the synthetic modification of a biologically active compound, to fulfill all stereoelectronic, physicochemical, pharmacokinetic and toxicologic requirements for clinical usefulness.

Lipophilicity**

Lipophilicity represents the affinity of a molecule or a moiety for a lipophilic environment. It is commonly measured by its distribution behaviour in a biphasic system, either liquid-liquid (e.g., partition coefficient in octan-1-ol/water) or solid/liquid (retention on reversed-phase high performance liquid chromatography (RP-HPLC) or thin-layer chromatography (TLC) system). (See also Hydrophobicity).

Medicinal chemistry

Medicinal chemistry is a chemistry-based discipline, also involving aspects of biological, medical and pharmaceutical sciences. It is concerned with the invention, discovery, design, identification and preparation of biologically active compounds, the study of their metabolism, the interpretation of their mode of action at the molecular level and the construction of structure-activity relationships.

Metabolism*

The term metabolism comprises the entire physical and chemical processes involved in the maintenance and reproduction of life in which nutrients are broken down to generate energy and to give simpler molecules (catabolism) which by themselves may be used to form more complex molecules (anabolism).

In case of heterotrophic organisms, the energy evolving from catabolic processes is made available for use by the organism.

In medicinal chemistry the term metabolism refers to the biotransformation of xenobiotics and particularly drugs. (See also Biotransformation; Xenobiotic).

Metabolite

A metabolite is any intermediate or product resulting from metabolism.

Me-too drug

A me-too drug is a compound that is structurally very similar to already known drugs, with only minor pharmacological differences.

Molecular graphics**

Molecular graphics is the visualization and manipulation of three-dimensional representations of molecules on a graphical display device.
Molecular modeling**

Molecular modeling is a technique for the investigation of molecular structures and properties using computational chemistry and graphical visualization techniques in order to provide a plausible three-dimensional representation under a given set of circumstances.

Mutagen***

A mutagen is an agent that causes a permanent heritable change (i.e., a mutation) into the DNA (deoxyribonucleic acid) of an organism.

Mutual prodrug

A mutual prodrug is the association in a unique molecule of two, usually synergistic, drugs attached to each other, one drug being the carrier for the other and vice versa.

NCE

See New Chemical Entity.

NDA

Abbreviation for New Drug Application.

New Chemical Entity.

A new chemical entity (NCE) is a compound not previously described in the literature.

Non-classical isostere

Same meaning as Bioisostere.

Nucleic acid*

A nucleic acid is a macromolecule composed of linear sequences of nucleotides that perform several functions in living cells, e.g., the storage of genetic information and its transfer from one generation to the next DNA (deoxyribonucleic acid), the expression of this information in protein synthesis (mRNA, tRNA) and may act as functional components of subcellular units such as ribosomes (rRNA).

RNA (ribonucleic acid) contains D-ribose, DNA contains 2-deoxy-D-ribose as the sugar component.

Nucleoside*

A nucleoside is a compound in which a purine or pyrimidine base is bound via a N-atom to C-1 replacing the hydroxy group of either 2-deoxy-D-ribose or of D-ribose, but without any phosphate groups. (See also nucleotide).

The common nucleosides in biological systems are adenosine, guanosine, cytidine, and uridine (which contain ribose) and deoxyadenosine, deoxyguanosine, deoxycytidine and thymidine (which contain deoxyribose).

Nucleotide

A nucleotide is a nucleoside in which the primary hydroxy group of either 2-deoxy-D-ribose or of D-ribose is esterified by orthophosphoric acid. (See also nucleoside).
Oligonucleotide

An oligonucleotide is an oligomer resulting from a linear sequence of nucleotides.

Oncogene

An oncogene is a normal cellular gene which, when inappropriately expressed or mutated, can transform eukaryotic cells into tumour cells.

Orphan drug

An orphan drug is a drug for the treatment of a rare disease for which reasonable recovery of the sponsoring firm's research and development expenditure is not expected within a reasonable time. The term is also used to describe substances intended for such uses.

Partial agonist

A partial agonist is an agonist which is unable to induce maximal activation of a receptor population, regardless of the amount of drug applied (See also Intrinsic activity).

Pattern recognition

Pattern recognition is the identification of patterns in large data sets using appropriate mathematical methodologies.

Peptidomimetic

A peptidomimetic is a compound containing non-peptidic structural elements that is capable of mimicking or antagonizing the biological action(s) of a natural parent peptide. A peptidomimetic does no longer have classical peptide characteristics such as enzymatically scissile peptidic bonds. (See also peptoids).

Peptoid

A peptoid is a peptidomimetic that results from the oligomeric assembly of N-substituted glycines.

Pfeiffer's rule

Pfeiffer's rule states that in a series of chiral compounds the eudismic ratio increases with increasing potency of the eutomer.

Pharmacokinetics

Pharmacokinetics refers to the study of absorption, distribution, metabolism and excretion (ADME) of bioactive compounds in a higher organism. (See also Drug disposition).

Pharmacophore (pharmacophoric pattern)

A pharmacophore is the ensemble of steric and electronic features that is necessary to ensure the optimal supramolecular interactions with a specific biological target structure and to trigger (or to block) its biological response.

A pharmacophore does not represent a real molecule or a real association of functional groups, but a purely abstract concept that accounts for the common molecular interaction capacities of a group of compounds towards their target structure. The pharmacophore can be considered as the largest common denominator shared by a set of active molecules. This definition
discards a misuse often found in the medicinal chemistry literature which consists of naming as pharmacophores simple chemical functionalities such as guanidines, sulfonamides or dihydroimidazoles (formerly imidazolines), or typical structural skeletons such as flavones, phenothiazines, prostaglandins or steroids.

Pharmacophoric descriptors

Pharmacophoric descriptors are used to define a pharmacophore, including H-bonding, hydrophobic and electrostatic interaction sites, defined by atoms, ring centers and virtual points.

Placebo

A placebo is an inert substance or dosage form which is identical in appearance, flavor and odour to the active substance or dosage form. It is used as a negative control in a bioassay or in a clinical study.

Potency***

Potency is the dose of drug required to produce a specific effect of given intensity as compared to a standard reference.

Potency is a comparative rather than an absolute expression of drug activity. Drug potency depends on both affinity and efficacy. Thus, two agonists can be equipotent, but have different intrinsic efficacies with compensating differences in affinity.

Prodrug

A prodrug is any compound that undergoes biotransformation before exhibiting its pharmacological effects. Prodrugs can thus be viewed as drugs containing specialized non-toxic protective groups used in a transient manner to alter or to eliminate undesirable properties in the parent molecule. (See also Double prodrug).

QSAR

See Quantitative Structure-Activity Relationships

Quantitative Structure-Activity Relationships (QSAR)**

Quantitative structure-activity relationships are mathematical relationships linking chemical structure and pharmacological activity in a quantitative manner for a series of compounds. Methods which can be used in QSAR include various regression and pattern recognition techniques.

Receptor*

A receptor is a molecule or a polymeric structure in or on a cell that specifically recognizes and binds a compound acting as a molecular messenger (neurotransmitter, hormone, lymphokine, lectin, drug, etc.).

Receptor mapping**

Receptor mapping is the technique used to describe the geometric and/or electronic features of a binding site when insufficient structural data for this receptor or enzyme are available. Generally the active site cavity is defined by comparing the superposition of active to that of inactive molecules.
Second messenger
A second messenger is an intracellular metabolite or ion increasing or decreasing as a response to the stimulation of receptors by agonists, considered as the "first messenger". This generic term usually does not prejudge the rank order of intracellular biochemical events.

Site-specific delivery
Site-specific delivery is an approach to target a drug to a specific tissue, using prodrugs or antibody recognition systems.

Soft drug
A soft drug is a compound that is degraded in vivo to predictable non-toxic and inactive metabolites, after having achieved its therapeutic role.

SPC
See Structure-property correlations

Structure-activity relationship (SAR)
Structure-activity relationship is the relationship between chemical structure and pharmacological activity for a series of compounds.

Structure-based design**
Structure-based design is a drug design strategy based on the 3D structure of the target obtained by X-ray or NMR.

Structure-property correlations (SPC)**
Structure-property correlations refers to all statistical mathematical methods used to correlate any structural property to any other property (intrinsic, chemical or biological), using statistical regression and pattern recognition techniques.

Systemic***
Systemic means relating to or affecting the whole body.

Teratogen***
A teratogen is a substance that produces a malformation in a foetus.

Three-dimensional Quantitative Structure-Activity Relationship (3D-QSAR)
A three-dimensional quantitative structure-activity relationship is the analysis of the quantitative relationship between the biological activity of a set of compounds and their spatial properties using statistical methods.

Topliss tree**
A Topliss tree is an operational scheme for analog design.
Transition-state analog
A transition-state analog is a compound that mimics the transition state of a substrate bound to an enzyme.

Xenobiotic***
A xenobiotic is a compound foreign to an organism (xenos [greek] = foreign).