C07D

HETEROCYCLIC COMPOUNDS (macromolecular compounds <u>C08</u>)

Definition statement

This place covers:

Organic compounds containing at least one heterocyclic ring, and with no ring comprising a steroid, saccharide or peptide moiety. Said compounds of C07D contain ring heteroatoms selected from nitrogen, oxygen, sulphur, selenium, tellurium, halogen or a combination thereof.

The compounds may also contain metal atoms, but only as the cations of heterocyclic organic acid salts, alcoholates, phenolates or mercaptides, or as chelating atoms, e.g. in porphyrins.

Preparation of such compounds, including purification, separation, stabilisation or use of additives, unless a separate place is provided elsewhere in the classification scheme.

Relationships with other classification places

In class CO7, the last place priority rule is used, i.e. in the absence of an indication to the contrary, a compound is classified in the last appropriate subclass. Hence, while individual heterocycle-containing amino acids are classified in this subclass CO7D, peptides are generally classified in subclass CO7K. Similarly, compounds containing saccharide radicals are classified in subclass CO7H, and heterocyclic steroids are classified in subclass CO7J. (Detailed instructions which compounds are considered as CO7H, CO7J or CO7K can be found in the corresponding CPC Definitions.) Heterocycles incorporating elements other than C, H, halogen, N, O, S, Se or Te are classified in subclass CO7F, but only if the metal-containing compound has a metal carbon bond or if the metal is attached to at least two different ligands. Salts, adducts or complexes formed between two or more organic compounds are classified according to all compounds forming the salts, adducts or complexes (e.g., maleic acid salts of heterocyclic compounds are also classified in CO7C).

This subclass is a structure-oriented entry for the compounds themselves and does not cover the application or use of the compounds under the subclass definition.

For classifying such information other entries exist, for example:

- Heterocyclic compounds disclosed as dyes or pigments are classified in subclass C09B.
- Compounds or compositions for preservation of bodies of humans, animals, plants, or parts
 thereof, as biocides, e.g. disinfectants, pesticides, herbicides, as pest repellents or attractants, and
 as plant growth regulators are classified in subclass A01N.
- Preparations for medical, dental, or toilet purposes or methods of using compounds for the same purposes are classified in subclass <u>A61K</u>.

Multiple classification:

Biocidal, pest repellent, or plant growth regulatory activity of chemical compounds or preparations is further classified in subclass A01P.

Therapeutic activity of chemical compounds is further classified in subclass A61P.

Uses of cosmetics or similar toilet preparations are further classified in subclass A61Q.

Oligomers are classified as low molecular compounds in C07D and as macromolecular compounds in C08.

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References

Limiting references

This place does not cover:

Macromolecular compounds	<u>C08</u>

Application-oriented references

Examples of places where the subject matter of this place is covered when specially adapted, used for a particular purpose, or incorporated in a larger system:

Pesticides	<u>A01N</u>
Biocidal activity	<u>A01P</u>
Therapeutic activity	<u>A61P</u>
Dyes and Pigments	<u>C09B</u>
Adhesives	<u>C09J</u>
Luminescent, e.g. electroluminescent or chemiluminescent materials	C09K 11/00
Use of organic compounds in semiconductors	H10K 99/00

Informative references

Food or functional food (nutraceuticals)	<u>A23L</u>
Cosmetics	A61K 8/00, A61Q
Medicinal preparations containing organic ingredients	A61K 31/00
Physical or Chemical Processes or Apparatus in General	<u>B01</u>
Catalysts	<u>B01J</u>
Generic methods and apparatus therefor used in organic chemistry, such as oxidation, reduction, addition, substitution, purification, separation, stabilisation	<u>C07B</u>
Heterocyclic organic compounds containing elements other than carbon, hydrogen, halogen, oxygen, nitrogen, sulphur, selenium or tellurium	<u>C07F</u>
Sugars	<u>C07H</u>
Steroids	<u>C07J</u>
Peptides	<u>C07K</u>
Preparation of heterocyclic organic compounds using enzymes or fermentation processes	<u>C12P</u>
Electrolytic production of organic compounds	C25B 3/00
Processes for producing compounds in which simultaneously electricity is generated	C25B 5/00
Electrophoretic production of compounds	C25B 7/00
Combinatorial libraries containing organic compounds	C40B 40/00

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Special rules of classification

In this subclass, in the absence of an indication to the contrary, a compound is classified in the last appropriate place.

Chemical compounds and their preparation are classified in the groups for the type of compound prepared. The processes of preparation are also classified in the groups for the types of reaction employed, if of interest. The compounds prepared are also classified in the groups for the types of compounds prepared, if of interest.

Salts of a compound, unless specifically provided for, are classified as that compound. Salts, adducts or complexes formed between two or more organic compounds are classified according to all compounds forming the salts, adducts or complexes. Salts, chelates, alcoholates (except Ti/ Zr), phenates involving a single ligand are classified as the parent compound (metal containing porphyrin CO7D 487/22).

Where a molecule may exist in tautomeric forms, classification is made for the form which appears latest in the scheme. Therefore, double bonds between ring members and non-ring members and double bonds between ring members themselves are considered equivalent in determining the degree of hydrogenation of the ring.

- Compounds containing a single heterocycle are classified in the range <u>C07D 203/00</u> - <u>C07D 347/00</u> (cf. Table 1). Compounds containing two or more heterocycles, none of which are condensed among themselves nor condensed with a carbocyclic ring, and all of which are covered by the same main group, are also classified in this range.
- Heterocyclic compounds which contain rings of five or more members, wherein only nitrogen is
 present as a ring heteroatom, and wherein the ring carbon atoms are fully saturated and only
 bound to hydrogen atoms, are classified in main group <u>C07D 295/00</u>. 3-azabicyclo[3.2.2]nonanes,
 piperazines, morpholines and thiomorpholines unsubstituted on the ring carbon atoms are also
 classified here.
- Compounds containing two or more hetero rings individually covered by different
 main groups, and not part of the same condensed ring system are classified in the
 range C07D 401/00 C07D 421/00 (cf. Table 2). Compounds containing two rings of two
 different main groups are classified in the relevant subgroups, e.g. C07D 401/04, C07D 401/06,
 C07D 401/08, C07D 401/10 or C07D 401/12", depending on how they are attached. Compounds
 containing three or more rings of two or more different main groups are classified in the relevant
 subgroup, e.g. C07D 401/14.
- Where a compound contains at least one ring covered by group C07D 295/00 and at least one other hetero ring, the hetero ring covered by group C07D 295/00 is ignored and treated as an acyclic chain containing nitrogen atoms for the purposes of classification.
- Compounds containing two or more hetero rings, being part of the same condensed ring system, are classified in the range C07D 451/00 C07D 519/00 (cf. Table 3 and 4).

The following table shows how classification can change depending on substitution:

CH ₃	C07D 213/74
	C07D 405/12
N N N	C07D 241/04
	C07D 265/30
N N N	C07D 413/06
	C07D 213/22 Three occurrences of a pyridine ring in the same compound (one main group)
"	

An acyclic side-chain linked to the hetero ring is considered to be terminated by every bond to: 1) an element other than carbon 2) a carbon atom having three bonds to hetero atoms, with at the most one bond to halogen, e.g. ester or nitrile radicals. For example, the following compound is classified in C07D 203/10 and not in C07D 203/12.

Where a heterocycle is linked to a carbocycle by an acyclic chain, and both the chain and the carbocycle are further substituted by either hetero atoms or carbon atoms with three bonds to hetero

atoms, not more than one hetero atom being a halogen, the molecule is classified according to the substituents on the acyclic chain. See the following example:

is classified in group C07D 233/22, and the compound

is classified in groups CO7D 233/24 and CO7D 233/26, where X = - NH₂, - NHCOCH₃, or - COOCH₃.

C07D 451/00 - C07D 517/00 cover compounds containing one system of two or more relevant hetero rings condensed among themselves or condensed with a common carbocyclic ring system, with or without other non- condensed hetero rings. For the purpose of classification in groups C07D 451/00 - C07D 519/00, the degree of hydrogenation of the ring system is not taken into consideration. For the purpose of classification in groups C07D 451/00 - C07D 463/00, C07D 473/00 - C07D 477/00, C07D 489/00, C07D 499/00 - C07D 507/00, the wording of the groups has to be understood, in the absence of an indication to the contrary, as including ring systems further condensed with other hetero rings, either directly or through a common carbocyclic ring system, e.g. sparteine is classified in group C07D 471/22 and not in group C07D 455/02. In groups C07D 471/00, C07D 487/00, C07D 491/00 - C07D 498/00 or C07D 513/00 - C07D 517/00, the subdivision is based on the number of relevant hetero rings.

Classification of complex fused ring systems

C07D 451/00 - C07D 517/00 cover heterocyclic compounds containing one system of two or more relevant hetero rings condensed among themselves or condensed with a common carbocyclic ring system, with or without other noncondensed hetero rings. As mentioned in the Glossary of Terms under "number of relevant rings" and "relevant rings", the rings which identify the ring system are determined according to a specific manner and hierarchy of criteria.

Example

Six scissions are necessary to convert the ring system into an acyclic chain.

The relevant rings, when classified according to the aforementioned hierarchy, are the following: C_3N_2 , C_5 , C_4N_0 , C_4N_2 , C_5N , $C_{10}N_3O$.

The condensed system contains five heterorings, is bridged, and contains at least one hetero ring having nitrogen and oxygen atoms as the only ring hetero atoms.

Thus, the compound should be classified as CO7D 498/22.

Classification guidance

What is classified as a compound?

The following compounds are classified: those which are individually named or drawn in the claims; and real examples of compounds disclosed in the specification, that fall within the scope of the claims. A real example is a compound which is prepared or for which physical and/or biological data is given.

The same rules apply for compounds claimed or disclosed as reaction intermediates.

Not classified are the following: generic formulae (Markush formulae, even if they have only one variable group); list(s) of "prophetic compounds" which fall within the scope of the claims but which were not actually prepared; and compounds disclosed in the description/specification but which are not claimed as compounds per se.

What is classified as a process for the preparation of a compound?

Classified are only preparation examples of claimed processes. A process is classified in a process group if a dedicated process group exists (e.g. <u>C07D 201/00</u> or <u>C07D 301/00</u>). Where there is no process group for making a particular compound, the process is classified according to the product obtained in the claimed process.

Further classification information:

Tables 1-4 provide an overview of the main groups in <u>C07D</u>.

Structural chemical formulae for various subgroups (in particular for specific ring systems as shown in table 3 below) are available in the IPC definitions

Table 1: Overview of main groups <u>C07D 201/00</u> - <u>C07D 347/00</u>:

Only N: Number of Heteroatoms + Number of

Carbon atoms; Ring Type

C07D 201/00	Preparation of unsubstituted lactam
C07D 203/00	1N+2C; aziridine,
C07D 205/00	1N+3C; azetidine,
C07D 207/00	1N+4C; non-condensed pyrrole
C07D 209/00	1N+4C; condensed pyrrole
C07D 211/00	1N+5C; hydrogenated
C07D 213/00	1N+5C; aromatic
C07D 215/00	Quinoline
C07D 217/00	Isoquinoline
C07D 219/00	Acridine
C07D 221/00	Other condensed pyridines
C07D 223/00	1N+6C; azepane

C07D 225/00	1N+>6C; azocane and larger
C07D 227/00	Heterocyclic compounds according to more than one of groups C07D 203/00- C07D 225/00
C07D 229/00	2N+(1C or 2C)
C07D 231/00	2N+3C; 1,2-diazole,
C07D 233/00	2N+3C; 1,3-diazole non-condensed
C07D 235/00	2N+3C; condensed imidazole
C07D 237/00	2N+4C; 1,2-diazine,
C07D 239/00	2N+4C; 1,3-diazine,
C07D 241/00	2N+4C; 1,4-diazine,
C07D 243/00	2N+5C
C07D 245/00	2N+>5C
C07D 247/00	Heterocyclic compounds according to more than one of groups C07D 229/00- C07D 245/00
C07D 249/00	3N+2C; 1,2,3 or 1,2,4-triazole,
C07D 251/00	3N+3C; 1,3,5-triazine,
C07D 253/00	3N+3C; 1,2,3 or 1,2,4-triazine,
C07D 255/00	Heterocyclic rings with 3N not provided for in C07D 251/00-C07D 253/00
C07D 257/00	4N
C07D 259/00	>4N

Only N + O:

C07D 261/00	1N+1O+3C; 1,2-oxazole,
C07D 263/00	1N+1O+3C; 1,3-oxazole,
C07D 265/00	1N+1O+4C; oxazine,
C07D 267/00	1N+1O+>4C
C07D 269/00	Heterocyclic compounds according to more than one of groups C07D 229/00 - C07D 245/00
C07D 271/00	2N+1O+2C,
C07D 273/00	Heterocyclic rings with N+O not provided for in C07D 261/00 -C07D 271/00

Only N + S:

C07D 275/00	1N+1S+3C; 1,2-thiazole,
C07D 277/00	1N+1S+3C; 1,3-thiazole,
C07D 279/00	1N+1S+4C; thiazine,
C07D 281/00	1N+1S+>4C,
C07D 283/00	Heterocyclic compounds according to more than one of groups C07D 275/00- C07D 281/00

Heterocyclic compounds containing rings having N+S as the only ring heteroatoms, not provided
for by groups <u>C07D 275/00</u> - <u>C07D 283/00</u>

<u>Only N + O + S:</u>

C07D 291/00	N+O+S,

N + Se/Te (+O)(+S):

C07D 293/00	N+Se/Te(+O)(+S)
	Compounds containing polymethylene-imine rings with at least five ring members, 3-azabicyclo [3.2.2] nonane, piperazine, morpholine, or thiomorpholine rings, having only hydrogen atoms directly attached to the ring carbon atoms

Only O:

C07D 301/00	Preparation of oxirane
C07D 303/00	1O+2C; oxirane,
C07D 305/00	1O+3C; oxetane,
C07D 307/00	10+4C; furan,
C07D 309/00	1O+5C; non-condensed pyran
C07D 311/00	1O+5C; condensed pyran
C07D 313/00	1O+>5C,
C07D 315/00	Heterocyclic compounds according to more than one of groups C07D 303/00- C07D 313/00
C07D 317/00	2O+3C,
C07D 319/00	2O+4C,
C07D 321/00	Heterocyclic compounds containing rings with 2O not provided for by groups CO7D 317/00 - CO7D 319/00
C07D 323/00	>20,
C07D 325/00	Heterocyclic compounds according to more than one of groups C07D 317/00- C07D 321/00

Only O + S:

C07D 327/00	O+S.
	,

Only +Se/Te (+S):

C07D 329/00	O+Se/Te(+S),
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Only S:

C07D 331/00	1S+(2C or 3C); thiirane or thietane,

C07D 333/00	1S+4C; (tetrahydro)thiophene,
C07D 335/00	1S+5C; thiopyran,
C07D 337/00	1S+>5C,
C07D 339/00	2 S,
C07D 341/00	>2S,

Only S + Se/Te:

0070 040/00	0 0 F
C07D 343/00	S+Se/Te,
	/

Only Se or Te:

C07D 345/00	Heterocyclic compounds containing rings with Se
	or Te as only ring hetero atoms

Containing Halogen:

C07D 347/00	Heterocyclic compounds containing rings with
	halogen atoms

NOTES to Table 1:

Unless otherwise stated the parent ring is non-condensed or condensed with a carbocyclic ring or ring system.

hydrogenated derivatives are together with the parent hetero ring, with the exception of $\underline{\text{C07D 211/00}}$ and $\underline{\text{C07D 213/00}}$.

The relative position of the hetero atoms in the hetero ring is given between brackets.

Table 2: Overview of main groups <u>C07D 401/00</u> - <u>C07D 421/00</u>:

C07D 401/00	Heterocyclic compounds containing two or more hetero rings, having nitrogen atoms (N) as the only ring hetero atom, at least one ring being a six-membered ring with only one nitrogen ring atom (C_5N)
C07D 403/00	Heterocyclic compounds containing two or more hetero rings, having nitrogen atoms (N) as the only ring hetero atoms, not provided for by group C07D 401/00
C07D 405/00	Heterocyclic compounds containing two or more hetero rings, at least one ring having oxygen atoms (O) as the only ring hetero atom, and at least one ring with only nitrogen (N) as the only ring heteroatom
C07D 407/00	Heterocyclic compounds containing two or more hetero rings, having oxygen atoms (O) as the only ring hetero atoms, not provided for by group C07D 405/00

C07D 409/00	Heterocyclic compounds containing two or more hetero rings, at least one ring having sulphur atoms (S) as the only ring hetero atoms
C07D 411/00	Heterocyclic compounds containing two or more hetero rings, at least one ring having oxygen and sulphur atoms (O+S) as the only ring hetero atoms
C07D 413/00	Heterocyclic compounds containing two or more hetero rings, at least one ring having nitrogen and oxygen atoms (N+O) as the only ring hetero atoms
C07D 415/00	Heterocyclic compounds containing the thiamine skeleton
C07D 417/00	Heterocyclic compounds containing two or more hetero rings, at least one ring having nitrogen and sulphur atoms (N+S) not provided by group C07D 415/00
C07D 419/00	Heterocyclic compounds containing two or more hetero rings, at least one ring having nitrogen, oxygen, and sulphur atoms (N+O+S) as the only ring hetero atoms
C07D 421/00	Heterocyclic compounds containing two or more hetero rings, at least one ring having selenium, tellurium, or halogen atoms as the only ring hetero atoms (Se/Te; halogen; (+O) (+S) (+N))

Tables 3 and 4: Overview of main groups <u>C07D 451/00</u> - <u>C07D 521/00</u>:

Table 3: Overview of specific condensed systems:

C07D 451/00	8-Azabicyclo[3.2.1]octane (tropane),) 6,7- Epoxy-8-azabicyclo[3.2.1]octane (scopolamine) and cyclic acetals; 9-Azabicyclo[3.3.1]nonane (granatane)
C07D 453/00	Quinuclidine or isoquinuclidine containing ring systems (e.g. quinine derivatives)
C07D 455/00	Quinolizine containing ring systems (e.g. berberine or emetine)
C07D 457/00	Indolo[4,3-f,g]quinoline, (e.g. Ergot alkaloids)
C07D 459/00	Benz[g] indolo[2,3-a]quinolizine (yohimbine) and lactones (reserpic acid lactone)
C07D 461/00	Indolo[3,2,1-d,e]pyrido[3,2,1-i,j] [1,5]]- naphthyridine ring systems, e.g. vincamine (dimeric indolo alkaloids CO7D 519/04)
C07D 463/00	Carbacephalosporins
C07D 473/00	Purine
C07D 475/00	Pteridine
C07D 477/00	Thienamycins (Carbapenicillins)

C07D 489/00	4aH-8,9c-Iminoethanophenanthro[4,5-b,c,d]furan ring systems, (e.g. morphine) and 6,14-carbon bridged derivatives (oripavines)
C07D 499/00	Penicillins
C07D 501/00	Cephalosporins
C07D 503/00	Oxapenicillins
C07D 505/00	Oxacephalosporins
C07D 507/00	Condensed beta-lactam ring systems, not provided for by groups C07D 463/00, C07D 477/00 or C07D 499/00 - C07D 505/00
C07D 519/02 and C07D 519/04	Ergot and Vinca alkaloids containing two or more condensed systems in the molecule

Table 4: Overview of other condensed systems:

(compounds of Table 3 take precedence)

The ring system contains as heteroatoms...

C07D 471/00	only nitrogen atoms, with at least one (hydro) pyridine, not provided for by Table 3
C07D 487/00	only nitrogen atoms, not provided for by Table 3 and by C07D 471/00
C07D 491/00	at least one ring containing only oxygen atoms and at least one ring containing only nitrogen atoms, not provided for by C07D 451/00, C07D 459/00, C07D 463/00, C07D 477/00 or C07D 489/00
C07D 493/00	only oxygen atoms
C07D 495/00	at least one ring containing only sulphur atoms
C07D 497/00	at least one ring containing only oxygen and sulphur atoms
C07D 498/00	at least one ring containing only nitrogen and oxygen atoms
C07D 513/00	at least one ring containing only nitrogen and sulphur atoms (penicillin C07D 499/00; cephalosporin C07D 501/00)
C07D 515/00	at least one ring containing only nitrogen, oxygen and sulphur atoms
C07D 517/00	at least one ring containing selenium, tellurium or halogen atoms, with or without other hetero atoms
C07D 519/00	two or more condensed systems in the molecule not provided for by C07D 453/00 or C07D 455/00
C07D 521/00	unspecified hetero rings

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Glossary of terms

In this place, the following terms or expressions are used with the meaning indicated:

Acyclic	The absence of a ring structure. Acyclic chains may be linear or branched.	
Bridged	Where two condensed rings share at least three adjacent ring members:	
Carbocyclic	Where all ring members in a ring are carbon atoms.	
Condensed	Where at least two rings share at least one ring member.	
Condensed ring system	A ring system in which all rings are condensed among themselves, i.e. a ring system wherein the scission of a single connection between two ring atoms cannot result in the division of the ring system into separate entities. Two or more hetero rings are considered part of the same condensed ring system if they are condensed among themselves or to a common carbocycle or carbocyclic system.	
Heterocyclic	Wherein at least one ring member in a molecule containing a ring of atoms is not a carbon atom. For the purposes of classification in this subclass, a narrower definition applies wherein heteroatoms may only be chosen from nitrogen, oxygen, sulphur, selenium, tellurium or halogen.	
Number of relevant rings	In a condensed ring system, this equals the minimum number of scissions necessary to convert the ring system into an acyclic chain, a scission being the disconnection of two bonded atoms, without regard for the bond order.	
Ortho-condensed	Where two condensed rings share two adjacent ring atoms in common. A ring system is deemed ortho-condensed if each ring shares only one face with any other ring, and no ring has two adjacent shared faces:	
Peri-condensed	Where three rings in a condensed ring system share a single ring atom in common:	

Relevant rings	These are the rings which account for all the bonds in a condensed system. In order to prevent ambiguity in classifying a condensed ring system, the rings which identify the ring system are determined according to the following hierarchy of criteria: the rings with the lowest number of members; the rings with the highest number of hetero atoms as ring members; the rings with the lowest number of members shared between rings; the rings with the last place in the classification scheme.	
Rings	Rings are considered as heterocycles only if they contain at least one atom selected from halogen, N, O, S, Se or Te as a ring member. Heterocyclic rings may be present as distinct entities or condensed, either with carbocycles or among themselves.	
Spiro-condensed	Where two condensed rings share only one atom in common:"free" "frozen"	
[x,y]-condensed	The letters in the square brackets refer to the sides around the heterocyclic ring with "a" for the side 1,2; "b" for the side 2,3; etc. For example: $ \begin{array}{cccccccccccccccccccccccccccccccccc$	

C07D 201/16

Separation or purification

Definition statement

This place covers:

Separation or purification of unsubstituted lactams.

References

Informative references

Separation of inorganic salts	<u>C01</u>

C07D 211/20

with hydrocarbon radicals, substituted by singly bound oxygen or sulphur atoms

Definition statement

This place covers:

Heterocyclic compounds containing hydrogenated pyridine rings, not condensed with other rings, with only hydrogen or carbon atoms directly attached to the ring nitrogen atom, having no double bonds between ring members or between ring members and non-ring members, with hydrocarbon radicals substituted by singly bound oxygen or sulphur atoms attached to ring carbon atoms.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

The singly bound oxygen or sulphur atoms are bound to the same carbon	C07D 211/30
atom	

C07D 213/28

Radicals substituted by singly-bound oxygen or sulphur atoms

Definition statement

This place covers:

Heterocyclic compounds containing six-membered rings, not condensed with other rings, with one nitrogen atom as the only ring hetero atom, having three double bonds between ring members or between ring members and non-ring members, having no bond between the ring nitrogen atom and a non-ring member or having only hydrogen or carbon atoms directly attached to the ring nitrogen atom, with hydrocarbon radicals substituted by singly-bound oxygen or sulphur atoms attached to ring carbon atoms.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

The singly bound oxygen or sulphur atoms are bound to the same carbon	C07D 213/44
atom	

C07D 215/20

Oxygen atoms

Definition statement

This place covers:

Heterocyclic compounds containing quinoline or hydrogenated quinoline ring systems, having no bond between the ring nitrogen atom and a non-ring member or having only hydrogen atoms or carbon atoms directly attached to the ring nitrogen atom, with oxygen atoms directly attached to ring carbon atoms.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

Quinophthalone dyes C09B 25/00

C07D 219/08

Nitrogen atoms

Definition statement

This place covers:

Heterocyclic compounds containing acridine or hydrogenated acridine ring systems, with nitrogen atoms directly attached to carbon atoms of the ring system.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

Acridine dyes C09B 15/00

C07D 221/08

Aza-anthracenes

Definition statement

This place covers:

Aza-anthracenes other than acridines (dibenzo[b,e]pyridine).

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

Acridine <u>C07D 219/00</u>

C07D 233/62

with triarylmethyl radicals attached to ring nitrogen atoms

Definition statement

This place covers:

Heterocyclic compounds containing 1,3-diazole or hydrogenated 1,3-diazole rings, not condensed with other rings, having two double bonds between ring members or between ring members and non-ring members, with only hydrogen atoms or radicals containing only hydrogen and carbon atoms attached to ring carbon atoms, with triarylmethyl radicals attached to ring nitrogen atoms.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

Triarylmethane dyes C09B 11/26

C07D 233/88

Nitrogen atoms, e.g. allantoin

Definition statement

This place covers:

Heterocyclic compounds containing 1,3-diazole or hydrogenated 1,3-diazole rings, not condensed with other rings, having two double bonds between ring members or between ring members and non-ring members, with nitrogen atoms directly attached to ring carbon atoms.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

The nitrogen atom is part of a nitro radical	C07D 233/91
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C07D 239/42

One nitrogen atom (nitro radicals C07D 239/30)

Definition statement

This place covers:

Heterocyclic compounds containing 1,3-diazine or hydrogenated 1,3-diazine rings, not condensed with other rings, having three or more double bonds between ring members or between ring members and non-ring members, with one nitrogen atom directly attached to ring carbon atoms.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

Benzenesulfonamido-pyrimidines	C07D 239/69
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C07D 239/46

Two or more oxygen, sulphur or nitrogen atoms

Definition statement

This place covers:

Heterocyclic compounds containing 1,3-diazine or hydrogenated 1,3-diazine rings, not condensed with other rings, having three or more double bonds between ring members or between ring members and non-ring members, with two or more nitrogen atoms directly attached to ring carbon atoms.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

Benzenesulfonamido-pyrimidines	C07D 239/69
Benzenesunonamido-pyrimidines	C01D 239/09

C07D 277/50

Nitrogen atoms bound to hetero atoms

Definition statement

This place covers:

Heterocyclic compounds containing 1,3-thiazole or hydrogenated 1,3-thiazole rings, not condensed with other rings, having two or three double bonds between ring members or between ring members and non-ring members, with nitrogen atoms bound to hetero atoms, directly attached to ring carbon atoms.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

The nitrogen atom is part of a nitro radical	C07D 277/58
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C07D 295/10

substituted by doubly bound oxygen or sulphur atoms

Definition statement

This place covers:

Heterocyclic compounds containing polymethylene-imine rings with at least five ring members, 3-azabicyclo [3.2.2] nonane, piperazine, morpholine or thiomorpholine rings, having only hydrogen atoms directly attached to the ring carbon atoms, with hydrocarbon radicals substituted by doubly bound oxygen or sulphur atoms attached to ring nitrogen atoms.

References

Informative references

Acylated ring nitrogen atoms	C07D 295/16
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C07D 303/10

in which the oxirane rings are condensed with a carbocyclic ring system having three or more relevant rings

Definition statement

This place covers:

Compounds containing oxirane rings, with hydrocarbon radicals, substituted by halogen atoms, nitro radicals or nitroso radicals, in which the oxirane rings are condensed with a carbocyclic ring system having three or more relevant rings.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

Steroids	<u>C07J</u>
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C07D 307/42

Singly bound oxygen atoms

Definition statement

This place covers:

Heterocyclic compounds containing five-membered rings having one oxygen atom as the only ring hetero atom, not condensed with other rings, having two or three double bonds between ring members or between ring members and non-ring members, with hydrocarbon radicals substituted by singly bound oxygen atoms attached to ring carbon atoms.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

The singly bound oxygen atoms are bound to the same carbon atom	C07D 307/46
3, ,3	

C07D 307/66

Nitrogen atoms

Definition statement

This place covers:

Heterocyclic compounds containing five-membered rings having one oxygen atom as the only ring hetero atom, not condensed with other rings, having two or three double bonds between ring members or between ring members and non-ring members, with nitrogen atoms directly attached to ring carbon atoms.

References

Informative references

The nitrogen atom is part of a nitro radical	C07D 307/70
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C07D 309/14

Nitrogen atoms not forming part of a nitro radical

Definition statement

This place covers:

Heterocyclic compounds containing six-membered rings having one oxygen atom as the only ring hetero atom, not condensed with other rings, having no double bonds between ring members or between ring members and non-ring members, with nitrogen atoms not forming part of a nitro radical directly attached to ring carbon atoms.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

The nitrogen atom is part of a nitro radical	C07D 309/08
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C07D 311/18

substituted otherwise than in position 3 or 7

Definition statement

This place covers:

Benzo[b]pyrans, not hydrogenated in the carbocyclic ring, with oxygen or sulphur atoms directly attached in position 2, not hydrogenated in the hetero ring, substituted otherwise than in position 3 or 7.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

The benzo[b]pyrans are substituted in position 4 by oxygen or sulphur	C07D 311/42
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C07D 333/36

Nitrogen atoms

Definition statement

This place covers:

Heterocyclic compounds containing five-membered rings having one sulphur atom as the only ring hetero atom, not condensed with other rings, not substituted on the ring sulphur, with nitrogen atoms directly attached to ring carbon atoms.

References

Informative references

The nitrogen atom is part of a nitro or nitroso radical	C07D 333/42
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C07D 471/04

Ortho-condensed systems

Definition statement

This place covers:

Heterocyclic compounds containing nitrogen atoms as the only ring hetero atoms in the condensed system, at least one ring being a six-membered ring with one nitrogen atom, in which the condensed system contains two hetero rings and is ortho-condensed.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

Carbacephalosporins	C07D 463/00
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C07D 487/04

Ortho-condensed systems

Definition statement

This place covers:

Heterocyclic compounds containing nitrogen atoms as the only ring hetero atoms in the condensed system, in which the condensed system contains two hetero rings and is ortho-condensed.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

Carbapenams, e.g. thienamycins	C07D 477/00
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C07D 491/14

Ortho-condensed systems

Definition statement

This place covers:

Heterocyclic compounds containing in the condensed ring system both one or more rings having oxygen atoms as the only ring hetero atoms and one or more rings having nitrogen atoms as the only ring hetero atoms, in which the condensed system contains three hetero rings and is orthocondensed.

References

Informative references

Alkylenedioxy derivatives of dibenzo[a, g]quinolizines, e.g. berberine	C07D 455/03
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C07D 491/18

Bridged systems

Definition statement

This place covers:

Heterocyclic compounds containing in the condensed ring system both one or more rings having oxygen atoms as the only ring hetero atoms and one or more rings having nitrogen atoms as the only ring hetero atoms, in which the condensed system contains three hetero rings and is bridged.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

3-Oxa-9-azatricyclo[3.3.1.0<2,4>]nonane ring systems, e.g. scopolamine

C07D 451/00

C07D 499/21

with a nitrogen atom directly attached in position 6 and a carbon atom having three bonds to hetero atoms with at the most one bond to halogen, e.g. an ester or nitrile radical, directly attached in position 2

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with the following groups: a nitrogen atom at the 6-position; and a carbon atom having three bonds to heteroatoms at the 2-position.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/28

with modified 2-carboxyl group

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with the following groups: a nitrogen atom at the 6-position; and a modified 2-carboxyl group at the 2-position.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/30

Acid anhydride

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with the following groups: a nitrogen atom at the 6-position; and an acid anhydride at the 2-position.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/32

Esters

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with the following groups: a nitrogen atom at the 6-position; and an ester at the 2-position.

C07D 499/34

Thio-acid; Esters thereof

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with the following groups: a nitrogen atom at the 6-position; and a thioacid (or ester thereof) at the 2-position.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/36

O-esters

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with the following groups: a nitrogen atom at the 6-position; and an O-ester of a thioacid at the 2-position.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/38

S-esters

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with the following groups: a nitrogen atom at the 6-position; and an S-ester of a thioacid at the 2-position.

The structure shown below is one example of a compound encompassed by this place

C07D 499/40

Amides; Hydrazides; Azides

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with the following groups: a nitrogen atom at the 6-position; and an amide, hydrazide, or azide at the 2-position.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/42

Compounds with a free primary amino radical attached in position 6

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with a free primary amino group at the 6-position.

C07D 499/46

with acyclic hydrocarbon radicals or such radicals substituted by carbocyclic or heterocyclic rings, attached to the carboxamido radical

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted by either an unsubstituted acyclic hydrocarbon group or an acyclic hydrocarbon group substituted by carbocyclic or heterocyclic rings.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/48

with a carbon chain, substituted by hetero atoms or by carbon atoms having three bonds to hetero atoms with at the most one bond to halogen, e.g. ester or nitrile radicals, attached to the carboxamido radical

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted by a carbon chain substituted by heteroatoms.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/50

substituted in beta-position to the carboxamido radical

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted by a carbon chain substituted by heteroatoms at the beta-position.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/52

by oxygen or sulfur atoms

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted by a carbon chain substituted by an oxygen or sulfur atom at the beta-position.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/54

by nitrogen atoms

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted by a carbon chain substituted by nitrogen atom(s) at the beta-position.

C07D 499/56

by carbon atoms having three bonds to hetero atoms with at the most one bond to halogen

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted by a carbon chain substituted by a carbon atom having three bonds to heteroatoms at the beta-position.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/58

substituted in alpha-position to the carboxamido radical

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted at the alpha-position.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/60

by oxygen atoms

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted at the alpha-position by oxygen atom(s).

The structure shown below is one example of a compound encompassed by this place.

C07D 499/62

by sulfur atoms

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted at the alpha-position by sulfur atom(s).

The structure shown below is one example of a compound encompassed by this place.

C07D 499/64

by nitrogen atoms

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted at the alpha-position by nitrogen atom(s).

C07D 499/66

with alicyclic rings as additional substituents on the carbon chain

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted at the alpha-position by nitrogen atom(s) and alicyclic ring(s).

The structure shown below is one example of a compound encompassed by this place.

C07D 499/68

with aromatic rings as additional substituents on the carbon chain

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted at the alpha-position by nitrogen atom(s) and aromatic ring(s).

The structure shown below is one example of a compound encompassed by this place.

C07D 499/70

with hetero rings as additional substituents on the carbon chain

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted at the alpha-position by nitrogen atom(s) and heterocyclic ring(s).

The structure shown below is one example of a compound encompassed by this place.

C07D 499/72

by carbon atoms having three bonds to hetero atoms

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-aza-bicyclo[3.2.0] ring system is substituted at the 6-position with a carboxylic acid-acylated amino group, further substituted at the alpha-position of the carboxamide group by carbon atoms having three bonds to heteroatoms.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/74

with carbocyclic rings directly attached to the carboxamido radical

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted by carbocyclic ring(s) directly attached to the carboxamide group.

C07D 499/76

with hetero rings directly attached to the carboxamido radical

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted at the 6-position by a carboxylic acid-acylated amino group, further substituted by heterocyclic ring(s) directly attached to the carboxamide group.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/78

Compounds with an amino radical, acylated by carbonic acid, or by nitrogen or sulfur analogues thereof, attached in position 6

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with a carbonic acid-acylated amino group or a nitrogen or sulfur analogue thereof at the 6-position.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/80

Compounds with a nitrogen-containing hetero ring, attached with the ring nitrogen atom in position 6

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with a nitrogen-containing ring attached with a ring nitrogen atom at the 6-position.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/86

with only atoms other than nitrogen atoms directly attached in position 6 and a carbon atom having three bonds to hetero atoms with at the most one bond to halogen, e.g. an ester or nitrile radical, directly attached in position 2

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with substituents other than nitrogen atoms directly attached to position 6 and a carbon atom having three bonds to heteroatom(s) at position 2.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/861

with a hydrocarbon radical or a substituted hydrocarbon radical, directly attached in position 6

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with a hydrocarbon group or a substituted hydrocarbon group at position 6 and a carbon atom having three bonds to heteroatom(s) at position 2.

C07D 499/865

with hetero atoms or with carbon atoms having three bonds to hetero atoms with at the most one bond to halogen, e.g. an ester or nitrile radical, directly attached in position 6

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with heteroatom(s) or carbon atoms having three bonds to heteroatom(s) at the 6-position.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/87

Compounds being unsubstituted in position 3 or with substituents other than only two methyl radicals attached in position 3, and with a carbon atom having three bonds to hetero atoms with at the most one bond to halogen, e.g. an ester or nitrile radical, directly attached in position 2

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system in position 3 is unsubstituted or substituted with groups other than 2 methyl groups and position 2 is substituted with a carbon atom having three bonds to heteroatom(s).

The structure shown below is one example of a compound encompassed by this place.

C07D 499/881

with a hydrogen atom or an unsubstituted hydrocarbon radical, attached in position 3

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system with a double bond is in between positions 2 and 3, in which position 2 is substituted with a carbon atom having three bonds to heteroatoms(s), and in which position 3 is substituted with a hydrogen atom or an unsubstituted hydrocarbon group.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/883

with a substituted hydrocarbon radical attached in position 3

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system with a double bond is in between positions 2 and 3, in which position 2 is substituted with a carbon atom having three bonds to heteroatom(s), and in which position 3 is substituted with a substituted hydrocarbon group.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/887

with a hetero atom or a carbon atom having three bonds to hetero atoms with at the most one bond to halogen, e.g. an ester or nitrile radical, directly attached in position 3

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system with a double bond is in between positions 2 and 3, in which position 2 is substituted with a carbon atom having three bonds to heteroatom(s), and in which position 3 is substituted with a heteroatom or a carbon atom having three bonds to heteroatom(s).

C07D 499/893

with a hetero ring or a condensed hetero ring system, directly attached in position 3

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system with a double bond is in between positions 2 and 3, in which position 2 is substituted with a carbon atom having three bonds to heteroatom(s), and in which position 3 is substituted with a heterocyclic ring or a condensed heterocyclic ring.

The structure shown below is one example of a compound encompassed by this place.

C07D 499/897

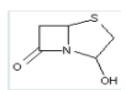
Compounds with substituents other than a carbon atom having three bonds to hetero atoms with at the most one bond to halogen, directly attached in position 2

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is substituted with a group other than a carbon atom having three bonds to heteroatom(s) at the 2-position.

The structure shown below is one example of a compound encompassed by this place.



C07D 499/90

further condensed with carbocyclic rings or ring systems

Definition statement

This place covers:

Heterocyclic compounds in which a 4-thia-1-azabicyclo[3.2.0]heptane ring system is further condensed with a carbocyclic ring or a ring system.

C07D 521/00

Heterocyclic compounds containing unspecified hetero rings

Special rules of classification

This group is only used for the classification of compounds the chemical structure of which is not specified, i.e. only in those cases where the compounds cannot be classified in any of groups: C07D 201/00 - C07D 519/00.