

Searching ring systems in CAS REGISTRYSM

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Did you know you can use ring search terms in REGISTRY to help you answer questions about rings?

These terms are especially useful for:

- Specifying general information about rings that often appears in patent claims, for example, a heterocycle containing three nitrogen atoms
- Creating subsets for ring searches that exceed system limits when run as a substructure search

The following information provides an overview of searching ring systems based on information that you know about the rings.

Terminology

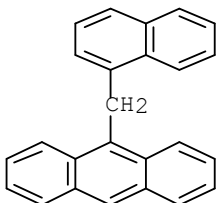
Let's start by clarifying terms used to generate ring search data in REGISTRY:

- Ring systems
- Smallest set of smallest rings (SSSR)
- Hill system order
- Multicomponent substances

Ring systems and smallest set of smallest rings

To explain ring systems and SSSR, let's use this substance as an example:

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RN 79760-50-2 REGISTRY
CN Anthracene, 9-(1-naphthalenylmethyl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
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This substance contains two ring systems:

- The upper ring system is named naphthalene.
- The lower ring system is named anthracene.

The SSSR for the naphthalene ring system is simply the set of two 6-membered C6 rings. The 10-membered C10 envelope ring is not counted.

The SSSR for the anthracene ring system is the set of three 6-membered C6 rings. The 14-membered C14 and the two 10-membered C10 envelope rings are not counted.

Hill system order

Hill system order is used to represent ring system formulas. The rules for carbon-containing substances are:

- Number of carbons first
- All other elements in alphabetical order

For substances not containing carbon, elements are placed in alphabetical order. The substance above consists of two rings: C10 and C14. Hydrogens are not included.

Multicomponent substances

Multicomponent substances are substances that consist of more than one component. For example, the mixture of aspirin, phenacetin, and caffeine is structured in REGISTRY as a multicomponent substance. The Ring System Data (RSD) is associated with each component.

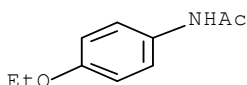
=> D STR RSD

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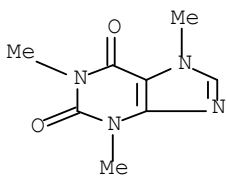
Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1 in CM 1 1 in CM 3
C3N2-C4N2	NCNC2-NCNC3	5-6	C5N4	333.446.43	1 in CM 2

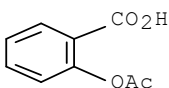
CM 1



CM 2



CM 3



Searching for ring systems completely defined by the specified small rings

The following table provides an overview of how you can search for ring systems consisting only of the specified rings. Using these fields can be very helpful if you need to do a broad sweep of the database to locate substances that contain all possible ring systems composed of a set of small rings.

When you know about all the small rings in a ring system	Do this...	In this search field...	Examples
Elemental ring formulas	Arrange formulas in Hill system order and ascending ring size. Precede by number of occurrences, if available.	/EA (Elemental Analysis of a Ring System)	S C5-C4N2-C6/EA S 2-4 C3S2/EA
Atom sequences	Arrange in order of ascending ring size and start with lowest alphabetical heteroatom. Precede by number of occurrences, if available.	/ES (Elemental Sequences for a Ring System)	S C5-NC2NC2-C6/ES
Ring sizes	Arrange in ascending order. Precede by number of occurrences, if available.	/SZ (Sizes of the Rings in a Ring System)	S 6-6-18/SZ S 2-4 5/SZ

Example 1

Locate substances containing only the rings defined as follows:

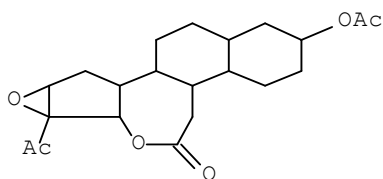
- 2 carbons and 1 oxygen
- 5 carbons
- Two rings of 6 carbons
- 6 carbons and 1 oxygen

=> **S C20-C5-C6-C6-C60/EA**

L1 114 C20-C5-C6-C6-C60/EA

=> **D STR**

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Searching for ring systems partially defined by the specified small rings

Searches in the /SZ, /EA, and /ES fields retrieve only ring systems containing the specified set of small rings. They do not retrieve ring systems in which those small rings are part of larger ring systems. Use the following search fields if you wish to allow other rings in the ring system.

When you know about some of the smallest rings	Do this...	In this search field...	Examples
Elemental ring formulas	Arrange formulas in Hill system order and ascending ring size. Precede by number of occurrences, if available.	/EAS (Elemental Analysis for Some of the Smallest Rings)	S C12O6/EAS S 2 C4N2/EAS
Atom sequences	Arrange in order of ascending ring size, starting with lowest alphabetical heteroatom. Precede by number of occurrences, if available.	/ESS (Elemental Sequences for Some of the Smallest Rings)	S 2 NC2NC2/ESS
Ring sizes	Arrange in ascending order. Precede by number of occurrences, if available.	/SZS (Size of Some of the Smallest Rings)	S 18/SZS S 2-3 5/SZS

Proximity for ring searching:

- (P) – In a single-component substance or one component of a multicomponent substance
- (S) – In the same ring system

Example 2

Locate ring system containing at least:

- 3-membered ring
- ring containing 5 carbons
- two rings containing 6 carbons
- ring containing 6 carbons and 1 oxygen

=> **S 3/SZS (S) (C5(S)2 C6(S)C6O)/EAS**

2459109 3/SZS

2897608 C5/EAS

5336200 2/EAS.CNT

39556949 C6/EAS

3004045 2 C6/EAS

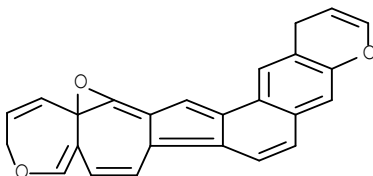
(2/EAS.CNT (T) C6/EAS)

58647 C6O/EAS

L1 179 3/SZS (S) (C5(S)2 C6(S)C6O)/EAS

=> **D STR 2**

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Searching ring elements for a ring system

You can also describe and search the ring systems simply in terms of the elements of which they are composed.

When you know...	Do this...	In this search field...	Examples
All ring elements and their counts	Arrange elements in Hill system order. Precede with the number and a space, if you know the number of occurrences.	/RF (Ring Formula)	S C19O2S/RF S S8/RF
All ring elements but not their counts	Arrange the elements in Hill system order and separate by spaces.	/RELF (Ring Elemental Formula)	S C O S/RELF S 1 CL PT/RELF
Some of the elements in a ring system	Enter element symbols for the elements, including M = any metal, X = any halogen, Q = any non-carbon atom. If available, include a count of the number of occurrences and a space before the element.	/REL (Ring Element)	S 2-3 M/REL S (M(S)X)/REL S >8 S/REL
Number of unique ring elements	Enter a number or use numeric operators.	/RELC (Ring Element Count)	S 7/RELC
Total number of ring atoms	Enter a number or use numeric operators.	/RATC (Ring Atom Count)	S 18/RATC S C/RELF(S)RATC>60

Proximity for ring element searching:

- (P) – In a single-component substance or one component of a multicomponent substance
- (S) – In the same ring system

Example 3

Locate ring systems that:

- Contain 7-10 ring atoms and 3 ring nitrogens in the same ring system
- Any number of ring carbons and sulfurs

=> **S 7-10/RATS (S) 3 N/REL (P) C S/RELF**

14641717 7-10/RATC

13926968 3/REL.CNT

29575715 N/REL

3749873 3 N/REL

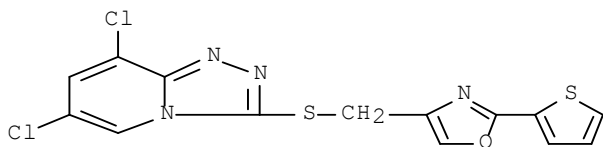
(3/REL.CNT (T) N/REL)

2225238 C S/RELF

L1 37709 7-10/RATC (S) 3 N/REL (P) C S/RELF

=> **D 3 STR**

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Searching ring counts

You can also search the number of ring systems or smallest rings.

When you know...	Search in this field...	Example
Total number of ring systems in a substance	/NRS (Number of Ring Systems)	S 7/NRS
Number of ring systems in a single component of a substance	/CNRS (Number of Ring Systems in a Single Component)	S 3-4/CNRS
Total number of smallest rings in a substance	/NR (Number of Smallest Rings)	S M/REL AND 5-9/NR
Number of smallest rings in a single component of a substance	/CNR (Number of Smallest Rings in a Single Component)	S 7/CNR
Number of smallest rings in a ring system	/NRRS (Number of Rings in a Ring System)	S C/RELF(S) NRRS>20
To require at least one ring system	RSD/FA	S L1 AND RSD/FA
To specify no rings in the substance	NO RSD/FA	S L1 AND NO RSD/FA

Proximity for ring count searching:

- (P) – In a single-component substance of the same component of a multicomponent substance
- (S) – In the same ring system

Example 4

Find ring systems that contain:

- One metal
- 5-6 rings

=> **S M/REL AND 5-6/NR**

1931091 M/REL
6982706 5-6/NR

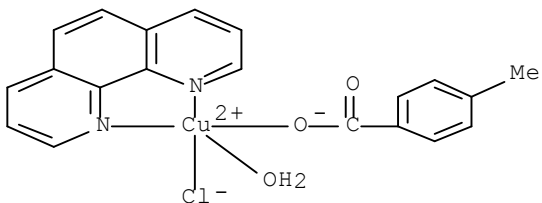
L1 353519 M/REL AND 5-6/NR

=> **D RSD STR**

L1 ANSWER 1 OF 353519 REGISTRY COPYRIGHT 2009 ACS on STN

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C2CuN2-C5N-	CuNC2N-NC5-	5-6-6-6	C12CuN2	2946.25.1	1
C5N-C6	NC5-C6				



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