CAS REGISTRY℠: Finding CAS Registry Numbers®

When you know the Substance Name

Field	Use	Example
/CN Chemical Name	Use when you know the **complete substance name.** EXPAND first to determine if the name is in the database.	=> E BENZOIC ACID/CN => E "BICYCLO(2.2.1)HEPTANE"/CN
Basic Index	Use when you know **segments of the name** or don't know how the name segments go together.	=> S FLUOROMETHYL => S "2,2'" (W) BIPYRID? => S PYRIDINE (XW) DICARBOXY?
/CNS Chemical Name Segments	Use when you want to search for a **character string embedded in a trade name.** Use left and right truncation to search for an embedded character string.	=> S ?MYCIN?/CNS => S ?QUAT/CNS
	Use when you want to require that a **name segment is not part of a larger segment.**	=> S CHLOROPHENYL/CNS => S HEXANEDIOIC (XW) DIMETHYL/CNS
/HP Heading Parent	Use when you want to restrict the search to a **Heading Parent from a CA index name.**	=> S 1-PROPANOL/HP => S 2-PYRIDINECARBO?/HP
/INS.HP Index Name Segments - Heading Parent	Use when you want to restrict the search to **name segments from the Heading Parent** part of a CA index name.	=> S (PYRIDINE (XW) CARBONITRIL?)/INS.HP => S FLUOROMETHYL/INS.HP
/INS.NHP Index Name Segments - Non-Heading Parent	Use when you want to restrict the search to **name segments from the non-Heading-Parent** part of a CA index name.	=> S MORPHOL?/INS.NHP => S FLUOROMETHYL/INS.NHP
/ONS Other Name Segments	Use when you want to restrict the search to **name segments from names other than CA index names** such as semi-systematic names, trade names, common names, etc.	=> S VINCAM?/ONS => S (INDOLE(XW)AMIN?)/ONS

PROXIMITY FOR NAME SEGMENT SEARCHING

(L) - in the same name
(W) - adjacent and in order input
(XW) - anywhere in name in order input
(A) - adjacent
(XA) - anywhere in the name

When you know the Molecular Formula

Field	Use	Example
/MF Molecular Formula	Use when you know the **entire molecular formula** of the substance. Elements must be in Hill order with or without spaces between them.	=> S C3HCL2F5/MF => S C5H12O.C3HCL2F5/MF => S H2O4S/MF
Basic Index	Use when you want a molecular formula to retrieve **single-component substances and multi-component substances.** Elements must be in Hill order with no spaces between.	=> S C3HCL2F5 => S H2O4S
/ELF Elemental Formula	Use when you know the **elements in the formula** and want to allow the element counts to vary. Elements must be in Hill order and separated by spaces.	=> S C H CL F/ELF => S H O S/ELF
/ELS Element Symbol	Use when you want to **specify some elements** in the substance. Special symbols: M = metal, X = halogen	=> S (NB (L) PR (L) O)/ELS => S C H/ELF NOT X/ELS
Individual Element Counts, e.g., **/Fe, /C, /S**	Use when you want to specify **how many times an element occurs** in a single-component substance or in a component of a multicomponent substance. Numeric operators may be used.	=> S C H/ELF (P) 20-25/C => S 1-4/C (P) F/ELS

/PG
Periodic
Group
	Use when you want to specify **elements from a row or column in the periodic table of elements.** Use EXPAND to locate the codes.	=> S (O P OR H O P)/ELF
		    AND A1/PG
		=> S (NB (L) PR (L) O)/ELS
		    (L) LNTH/PG

/ELC
Element
Count
	Use when you want to specify the **total number of elements** in a single-component substance or in a component of a multicomponent substance. Numeric operators may be used.	=> S (C (P) X)/ELS (P)
		    2/ELC
		=> S (C (P) M (P) O)/ELS
		    (P) 4-5/ELC

/ELC.SUB
Element Count
for the entire
substance
	Use when you want to specify the **total number of unique elements in the entire substance.** Numeric operators may be used.	=> S (NB (L) PR (L) O)/ELS
		    (L) 5/ELC.SUB
		=> S (P (L) O (L) NA)/ELS
		    (L) 3-4/ELC.SUB

/ATC Atom Count	Use when you want to specify the **total number of atoms** in a single-component substance or in a component of a multicomponent substance. Numeric operators may be used.	=> S C H/ELF (P) 150-200/ATC => S C CL F/ELF (P) ATC<10

/ELR.xx
Element Ratio
xx = CH CO CN
    HC HO HN
    OC OH ON
    NC NH NO
	Use when you need to specify **ratios between two elements from the group C, H, N, O.** Numeric operators may be used.	=> S C H/ELF (P) 2/ELR.HC
		=> S 143/FW (P) S/ELS (P)
		    3/ELR.CN

PROXIMITY FOR ELEMENT SEARCHING
(L) - in the entire molecular formula (searches across component formulas)
(P) - in a single-component formula or one component of a multicomponent formula

When you know the Rings

Field	Use	Example
/EA Elemental Analysis for a Ring System	Use when you know the **formulas of ALL of the small rings in a ring system.** Formulas are in Hill order and ascending ring size. Number of occurrences in a structure is optional.	=> S C5-C4N2-C6/EA => S C6-C6-C12O6/EA => S 2-4 C3S2/EA
/EAS Elemental Analysis for the Smallest Rings	Use when you know the **formulas of SOME of the small rings in a ring system.** Formulas are in Hill order. Number of occurrences in a ring system is optional.	=> S C12O6/EAS => S (2 C4N2 (S) C6)/EAS
/ES Elemental Sequence for a Ring System	Use when you know the atom sequences for **ALL of the small rings in a ring system.** Sequences are in order of ascending ring size and start with lowest alphabetical heteroatom. Number of occurrences in a structure is optional.	=> S C5-NC2NC2-C6/ES => S C6-C6-OC2OC2OC2OC2OC2 /ES => S 2-4 SCSC2/ES
/ESS Elemental Sequence for the Smallest Rings	Use when you know the **atom sequences for SOME of the small rings in a ring system.** Sequence represents the shortest path from the lowest alphabetic heteroatom to the next lowest one. Number of occurrences in a ring system is optional.	=> S OC2OC2OC2OC2OC2OC2/ESS => S (2 NC2NC2 (S) C6)/ESS
/SZ Sizes of the Rings in a Ring System	Use when you know the **sizes of ALL of the small rings in a ring system.** Sizes are in ascending order. Number of occurrences in a structure is optional.	=> S 5-6-6/SZ => S 6-6-18/SZ => S 2-4 5/SZ
/SZS Size of the Smallest Rings	Use when you know the **sizes of SOME of the small rings in a ring system.** Sizes may be specified using numeric operators. Number of occurrences in a ring system is optional.	=> S 18/SZS => S 2-3 5/SZS
/RID Ring Identifier	Use when you want to specify a **ring "shape," a ring "shape" and specific atom locations, or a ring "shape" and specific atom locations and bonding pattern.** Number of occurrences in a structure is optional.	=> S 10664/RID => S 10664.10/RID => S 10664.10.1/RID

PROXIMITY FOR RING SEARCHING
(P) - in a single-component substance or one component of a multicomponent substance
(S) - in the same ring system

When you know the Ring Elements

Field	Use	Example
/RF Ring Formula for a Ring System	Use when you know **all of the elements in a ring and their counts.** Elements are in Hill order. Number of occurrences in a structure is optional.	=> S C1902S/RF => S 1 CL2PT2/RF => S S8/RF
/RELF Ring Elemental Formula	Use when you know **all of the elements** in a ring system but not their counts. Elements are in Hill order and separated by spaces. Number of occurrences in a structure is optional.	=> S C O S/RELF => S 1 CL PT/RELF => S S/RELF
/REL Ring Element	Use when you know **some of the elements in a ring system.** Special symbols are M = metal, X = halogen, Q = non-carbon. Number of occurrences in a ring formula is optional.	=> S (15-20 C (S) O (S) S) /REL => S (M (S) X)/REL => S >8 S/REL
/RELC Ring Element Count	Use to specify the **number of unique elements in a ring system**. Numeric operators may be used.	=> S (M (S) X)/REL (S) 2/RELC => S 591/RID (S) 2-3/RELC
/RATC Ring Atom Count	Use to specify the **total number of atoms** in a ring system. Numeric operators may be used.	=> S C/RELF (S) RATC>60 => S N P/RELF (S) 7-20/RATC

PROXIMITY FOR RING ELEMENT SEARCHING
(P) - in a single-component substance or one component of a multicomponent substance
(S) - in the same ring system

When you know Alloy Information

Field	Use	Example
/NC Number of Components	Use to specify the **total number of substance components.** Numeric operators may be used.	=> S 88-99-3/CRN AND NC=3
/MAC Material Composition	Use when you know an **alloy composition.** Numeric operators may be used for the numeric composition.	=> S 85-90 CO/MAC AND MO <5/MAC
/RC Relative Composition	Use when you know the **relative composition of an alloy.** Components are cited in order of decreasing percentage composition.	=> S CO.MO/RC

When you know how many Rings you want

Field	Use	Example
/NRRS Number of Rings in a Ring System	Use to specify the **number of rings in a ring system.** Numeric operators may be used.	=> `S C/RELF (S) NRRS>20` => `S N P/RELF (S) 2/NRRS`
/NRS Number of Ring Systems	Use to specify the **total number of ring systems in a substance.** Numeric operators may be used.	=> `S 2-4 C3-S2/EA AND 2/NRS`
/CNRS Component Number of Ring Systems	Use to specify the **total number of ring systems** in a single-component substance or in one component of a multicomponent substance. Numeric operators may be used.	=> `S C6-C6-C12/EA (P) 2/CNRS`
/NR Number of Smallest Rings	Use to specify the **total number of smallest rings in a substance**. Numeric operators may be used.	=> `S M/REL AND 5-9/NR`
/CNR Component Number of Smallest Rings	Use to specify the **total number of smallest rings** in a single-component substance or in one component of a multicomponent substance. Numeric operators may be used.	=> `S M/REL (P) 5-9/CNR`
RSD/FA	Use to specify **at least one ring system** in the substance.	=> `S C H/ELF AND RSD/FA`
NO RSD/FA	Use to specify **no rings** in the substance.	=> `S C H/ELF AND NO RSD/FA`

PROXIMITY FOR RING COUNT SEARCHING
(P) - in a single-component substance or one component of a multicomponent substance
(S) - in the same ring system

When you know the CAS Registry Number

Field	Use	Example
/CRN Component Registry Number	Use to retrieve all multicomponent substances for which you know the **CAS Registry Number of one component.**	=> `S 88-99-3/CRN`
/RN CAS Registry Number	Use to retrieve a record for a **CAS Registry Number**. Registry Numbers may also be searched in the Basic Index.	=> `S 57-88-5/RN` => `S 57-88-5`

When you know a Broad Substance Class

Field	Use	Example
/CI Substance Class Identifier	Use to retrieve **broad classes of substances.** Use EXPAND to locate the terms.	=> `S 88-99-3/CRN AND POLYMER/CI` => `S CO AND NI AND ALLOY/CI`
/DEF Definition	Use when you know part of the **definition associated with substances of unknown or variable composition on regulatory lists.**	=> `S DINUCLEAR PHENOL?/DEF`
/FS File Segment	Use to isolate **broad file segments:** protein sequences, nucleotide sequences, stereosearch, etc.	=> `S L1 AND PROTEIN/FS` => `S L1 AND STEREOSEARCH/FS`
/PCT Polymer Class Term	Use to retrieve **classes of polymers.** Use EXPAND to locate terms.	=> `S PHENOLIC RESIN/PCT`

When you want to know Availability, Updates, and Databases

Field	Use	Example
/ED Entry Date	Use if you want to restrict your search to **newly added substances.** Numeric operators or ranges may be used.	=> `S C F/ELF AND ED>=20070100`
/FA Field Availability	Use when you want to determine if a **field is present** in an answer set. EXPAND to locate the terms.	=> `S L1 NOT CN/FA`
/LC Locator	Use to locate the **STN database or regulatory list** in which a substance is found. Use EXPAND to locate the terms.	=> `S ?CILLIN?/CNS AND TSCA/LC`
/UP Update Date	Use to retrieve **newly added substances or those with updated records.** Numeric operators or ranges may be used.	=> `S C H/ELF AND UP>=20080100`

For more information

Refer to the REGISTRY Database Summary Sheet at www.cas.org.