

CAS REGISTRYSM: 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.	=> S BENZOIC ACID/CN => S "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-OC2OC2OC2OC2OC2OC2/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.



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