



CAS STNext E-Seminar

# NUMERIC PROPERTY SEARCHING ON CAS STNEXT®

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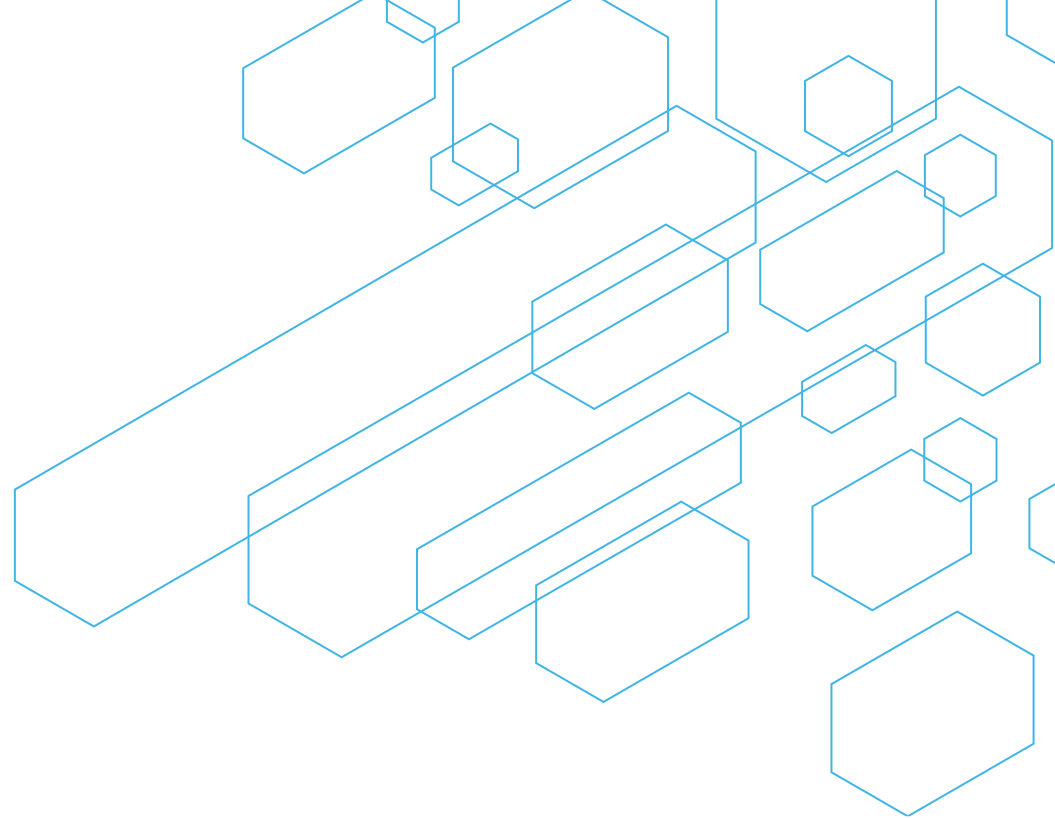
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 **FIZ Karlsruhe**  
Leibniz Institute for Information Infrastructure

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A division of the  
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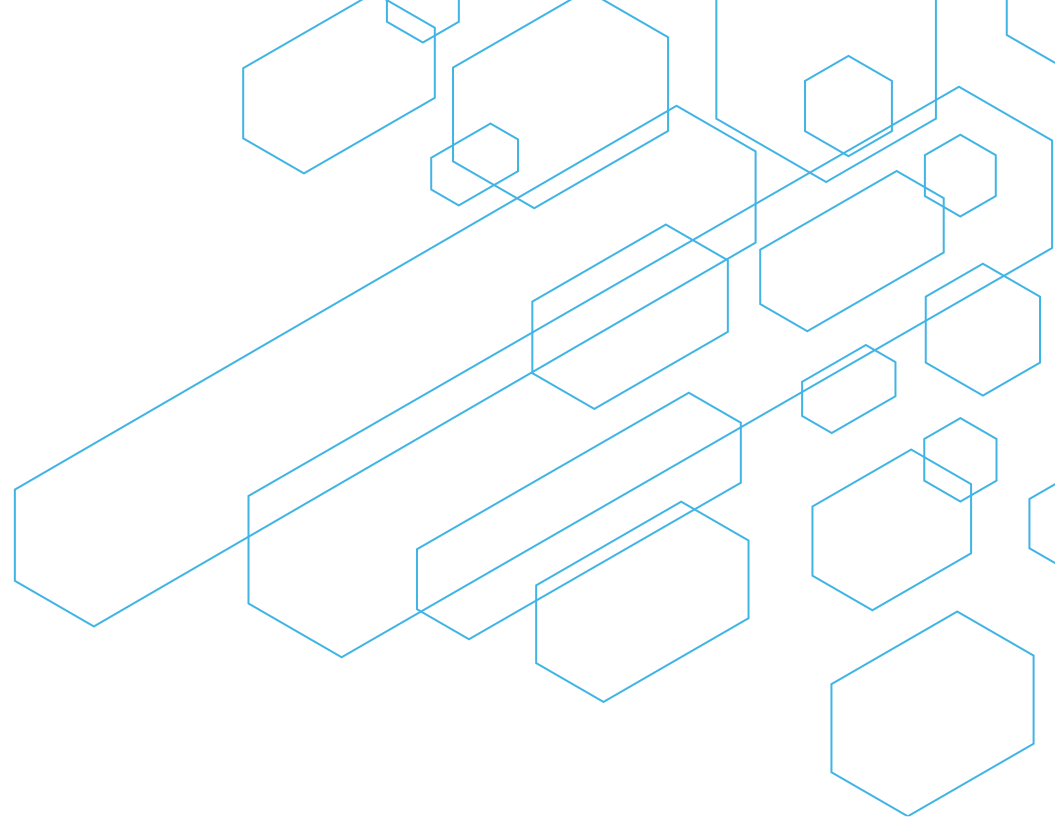
# Agenda

- Numeric properties in CAS Registry
- Overview of Numeric Property Searching (NPS)
- Databases with NPS capability
- Searchable properties
- Search examples



# Agenda

- **Numeric properties in CAS Registry**
- Overview of Numeric Property Searching (NPS)
- Databases with NPS capability
- Searchable properties
- Search examples



# Property information in CAS Registry

## Predicted Properties\*

199 M

| CODE | VALUE  | TYPE      | NOTE |
|------|--------|-----------|------|
| MW   | 208.21 | Predicted | (1)  |

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02  
(C) 1994-2024 ACD/Labs

## Experimental properties

- Experimental properties or spectra
- Tags for experimental properties or spectra
- Experimental spectra

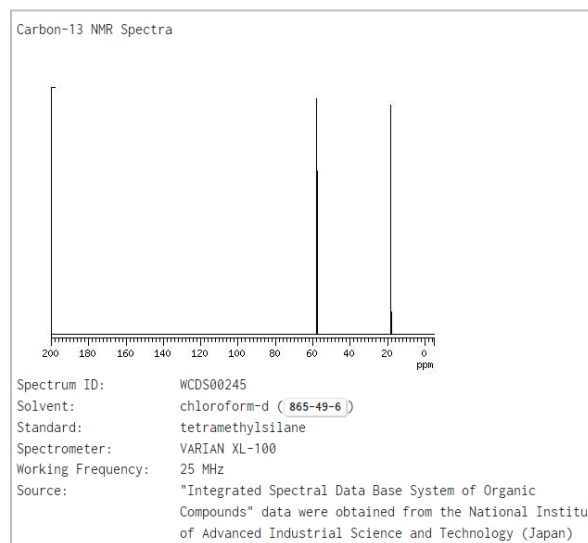
3.7 M

| Experimental Properties (EPROP) |          |                 |         |
|---------------------------------|----------|-----------------|---------|
| PROPERTY (CODE)                 | VALUE    | CONDITION       | NOTE    |
| Boiling Point (BP)              | 79 deg C | Press: 760 Torr | (1) CAS |

3.7 M

| PROPERTY                                | NOTE    |
|---|---------|
| Acid/Base Dissociation Constant (Ka/Kb) | (1) CAS |

980 K



Literature references are shown in a tabular view below the property table

\*Available for single-component organic substances

# Available property data in Registry

Check overview resources to get a proper understanding

## CAS website

<https://www.cas.org/support/training/stn/database-specific>

- Property data documentation
  - [Definitions of Properties with Searchable Data in REGISTRY](#) (PDF)
  - [Property Search Fields in CAS REGISTRY](#) (PDF)
  - [Sources of Property Data in REGISTRY](#) (PDF)
  - [STN Units System](#)
  - [Tagged Experimental Properties in REGISTRY](#) (PDF)

### Definitions of properties with experimental or predicted values in REGISTRY

| Property name | Definition  | Experimental Values Available | Predicted Values Available |
|---------------|---|-------------------------------|----------------------------|
| Density       | Mass per unit volume of a substance expressed in grams per cubic centimeter as the default units. | √                             | √                          |

...

=> HELP SFIELDS

**HELP SFIELDS** command displays list of property search fields including default units

REGISTRY contains property data and related information in the following search fields. Unless indicated otherwise in footnote (1), property search fields may be searched using numeric operators or ranges.

| Field Name                    | Search Field | Default Unit |
|-------------------------------|--------------|--------------|
| -----                         | -----        | -----        |
| Bioconcentration Factor       | /BCF         | none         |
| Bioconcentration Factor pH    | /BCF.PH      | none         |
| Bioconcentration Factor Temp. | /BCF.T       | deg C        |
| Boiling Point                 | /BP          | deg C        |
| Boiling Point Pressure        | /BP.P        | Torr         |
| Density                       | /DEN         | g/cm**3      |
| Density Pressure              | /DEN.P       | Torr         |
| Density Temperature           | /DEN.T       | deg C        |

# Available spectral data in Registry

Expand the /SPEC field in REGISTRY:

=> E A/SPEC 16

```
. . .
E3          0 --> A/SPEC
E4      93219  ABSORPTION/SPEC
E5       5703  BORON/SPEC
E6       5703  BORON-11 NMR SPECTRA/SPEC
E7     293252  CARBON/SPEC
E8     293252  CARBON-13 NMR SPECTRA/SPEC
E9      36215  FLUORINE/SPEC
E10     36215  FLUORINE-19 NMR SPECTRA/SPEC
E11    337466  HYDROGEN/SPEC
E12    337466  HYDROGEN-1 NMR SPECTRA/SPEC
E13     93219  IR/SPEC
E14     93219  IR ABSORPTION SPECTRA/SPEC
E15     93219  IR SPECTRA/SPEC
E16    395578  MASS/SPEC
E17    395578  MASS SPECTRA/SPEC
E18       7614  NITROGEN/SPEC
E19       7614  NITROGEN-15 NMR SPECTRA/SPEC
E20    637761  NMR/SPEC
E21    637761  NMR SPECTRA/SPEC
E22       3370  OXYGEN/SPEC
E23       3370  OXYGEN-17 NMR SPECTRA/SPEC
E24     32290  PHOSPHORUS/SPEC
E25     32290  PHOSPHORUS-31 NMR SPECTRA/SPEC
E26    337466  PROTON/SPEC
E27    337466  PROTON NMR SPECTRA/SPEC
E28       2964  RAMAN/SPEC
E29       2964  RAMAN SPECTRA/SPEC
E30       2278  SILICON/SPEC
E31       2278  SILICON-29 NMR SPECTRA/SPEC
E32    983430  SPECTRA/SPEC
```

# General search principle for properties

Identify numeric search field using expand → Perform numeric search

=> **HELP SFIELDS**

```
...
Melting Point           /MP           deg C
  Melting Point Pressure /MP.P         Torr
  Melting Point Solvent  /MP.SOL       none
```

=> **s L1 AND 150-200/MP**

```
648926 150 DEGC - 200 DEGC /MP
L3      57 L1 AND 150 DEGC - 200 DEGC /MP
```

Add conditions if desired

=> **s L3 AND HEXANE/MP.SOL**

```
648926 150 DEGC - 200 DEGC /MP
105063 HEXANE/MP.SOL
L4      4 L1 AND 150 DEGC - 200 DEGC/MP AND HEXANE/MP.SOL
```

**Numeric search options**

=> **S 150/MP**

=> **S 423.15 K/MP**

=> **S 150-200/MP**

=> **S 175+-25/MP**

=> **S MP>=150**

=> **S MP<201**

Enter **D UNIT <property>** to see the default unit for a particular field.

Enter **D UNITS ALL** or **HELP SFIELDS** to see all default units.

# Search on a more general level

## Example: Melting Point

### Answers with any experimental tag or value

**=> S L1 AND MELTING POINT/EPROPS**

L16                    171 L1 AND MELTING POINT/EPROP

### Answers with numeric values

**=> S L1 AND MP/FA**

L18                    166 L1 AND MP/FA

### Answers with experimental tag

**=> S L1 AND MELTING POINT/ETAG**

L17                    25 L1 AND MELTING POINT/ETAG



# General search principle for spectra

## Example: Carbon 13 NMR

Spectral peaks are not numerically searchable

Identify spectrum using expand in SPEC → Perform search in /SPEC field

=> **E A/SPEC 16**

```
. . .  
E7      293252      CARBON/SPEC  
E8      293252      CARBON-13 NMR SPECTRA/SPEC
```

=> **S L1 AND CARBON/SPEC**

```
L19      38 L1 AND CARBON/SPEC
```

Identifies all substances with C13-NMR spectra in the answer set.

## Identify substances with any spectrum

=> **S L1 AND SPECTRA/SPEC**

```
L25      71 L1 AND SPECTRA/SPE
```

Retrieves substances with any spectrum in L1.

# Display properties

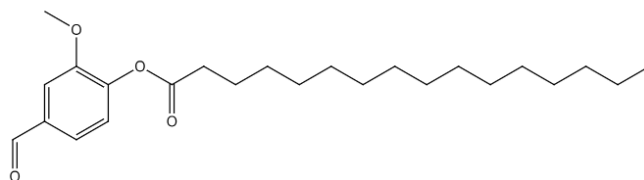
Properties can be displayed in total or by property

## Display all properties

=> D L4 IDE PROP

L4 ANSWER 1 OF 166 REGISTRY COPYRIGHT 2024 ACS ON STN  
RN 933675-28-6 REGISTRY

. . .  
CN VANILLIN PALMITATE  
MF C24 H38 O4  
. . .



### EXPERIMENTAL PROPERTIES (EPROP)

| PROPERTY (CODE)    | VALUE       | CONDITION     | NOTE    |
|--------------------|-------------|---------------|---------|
| MELTING POINT (MP) | 37-38 DEG C | SOLV: BENZENE | (1) CAS |
|                    |             | (71-43-2),    |         |
|                    |             | HEXANE        |         |
|                    |             | (110-54-3)    |         |

(1) DIKUSAR, E. A.; RUSSIAN JOURNAL OF APPLIED CHEMISTRY 2006 V79(6) P1035-1037 CAPLUS

### Predicted Properties (PPROP)

| PROPERTY (CODE)       | VALUE                 | CONDITION         |
|-----------------------|-----------------------|-------------------|
| NOTE                  |                       |                   |
| Bioconc. Factor (BCF) | 1000000.0             | pH 1 25 deg C (1) |
| Bioconc. Factor (BCF) | 1000000.0             | pH 2 25 deg C (1) |
| Bioconc. Factor (BCF) | 1000000.0             | pH 3 25 deg C (1) |
| Bioconc. Factor (BCF) | 1000000.0             | pH 4 25 deg C (1) |
| Molar Volume (MVOL)   | 393.8+/-3.0 cm**3/mol | 20 deg C (1)      |
|                       |                       | 760 Torr (1)      |
| Vapor Pressure (VP)   | 1.37E-09 Torr         | 25 deg C (1)      |

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 ((C) 1994-2024 ACD/Labs)

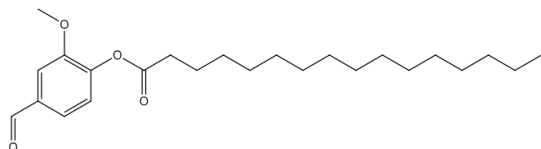
# Display properties (cont.)

Properties can be displayed in total or by property

## Display searched property only

=> D L4 RN IN MF STR HIT

L4 ANSWER 1 OF 166 REGISTRY COPYRIGHT 2024 ACS ON STN  
RN 933675-28-6 REGISTRY  
IN HEXADECANOIC ACID, 4-FORMYL-2-METHOXYPHENYL ESTER  
MF C24 H38 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HIT can't be combined with other display formats, however, it can be joined by other display fields as shown above.

QRD is an alternative, it displays IDE and HIT formats.

| CODE | VALUE       | CONDITION     | TYPE         | NOTE    |
|------|-------------|---------------|--------------|---------|
| MP   | 37-38 deg C | Solv: benzene | Experimental | (1) CAS |
|      |             | (71-43-2),    |              |         |
|      |             | hexane        |              |         |
|      |             | (110-54-3)    |              |         |

(1) Dikusar, E. A.; Russian Journal of Applied Chemistry  
2006 V79(6)  
P1035-1037 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.

# Display spectra

Spectra can be displayed in total or by spectrum

## Display all spectra

=> S L1 AND CARBON/SPEC

L19 38 L1 AND CARBON/SPEC

=> D SPEC

All available spectra diagrams for the substance are shown.

## Display spectra category

=> D SPEC.C13NMR

HELP DFIELDS shows specific spectra fields.

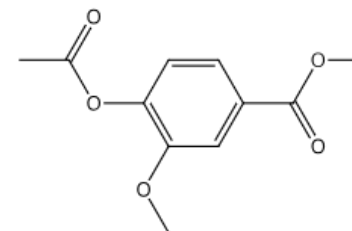
## Alternative: Display hit spectra

=> D RN IN MF STR HIT

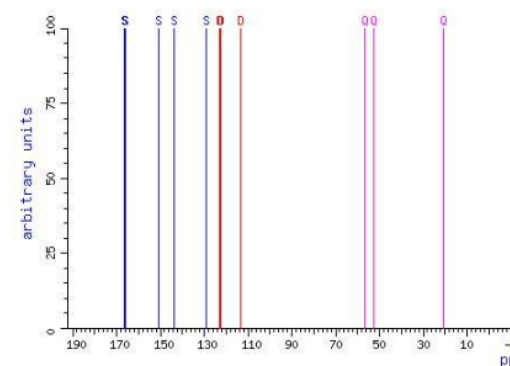
As with property displays, single fields can be combined with the HIT display.

QRD is a simple alternative, it displays IDE and HIT formats.

L4 ANSWER 10 OF 38 REGISTRY COPYRIGHT 2024 ACS on STN  
RN 35400-19-2 REGISTRY  
IN Benzoic acid, 4-(acetyloxy)-3-methoxy-, methyl ester  
MF C11 H12 O5  
CN Vanillic acid, methyl ester, acetate (7CI)  
MF C11 H12 O5



Carbon-13 NMR Spectra



Spectrum ID: CNCC-88984-585Q  
Solvent: chloroform-d (865-49-6)  
Standard: tetramethylsilane  
Source: Spectral data were obtained from Wiley Subscription Services, Inc. (US)

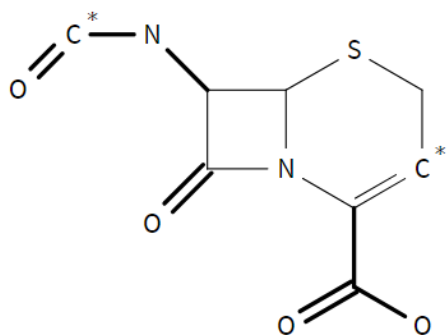
# Use Case

## Cephalosporin structure search and property filtering

Identify cephalosporins registered from 2010 on that might be used as orally active drugs and have been mentioned in patents. Display related patent families.

=> **FIL REG**

**\*\*\* Upload structure query \*\*\***



**Query structure**

C\* = Non hydrogen attachment min 3

=> **S L1 CSS FULL**

=> **S L2 AND 1/NC AND ED>=2010**

=> **S L3 AND LIPINSKI/CALC**

**LIPINSKI/CALC** is a shortcut to search the LIPINSKI rule of five, it translates to:

|           |  |
|-----------|--|
| 0-5/HD    | hydrogen donors                        |
| 0-10/HAC  | hydrogen acceptors                     |
| LOGP <= 5 | partition coefficient / hydrophobicity |
| 0-500/MW  | molecular weight                       |

=> **S L4 AND P/DT**

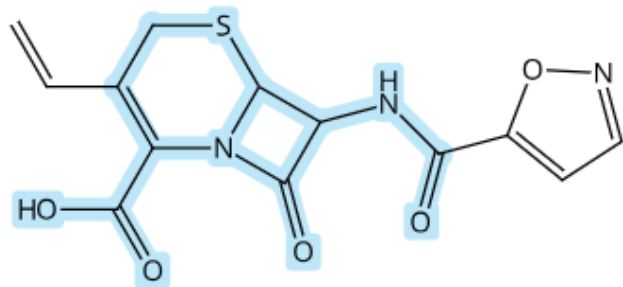
Registry allows to limit substance entries to their occurrence in specific document types such as patents.

# Use Case (cont.)

## Registry displays using QRD

=> D QRD 1-TOT

RN **3004928-09-7** REGISTRY  
ED Entered STN: 19 Nov 2023  
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-ethenyl-7-[(5-isoxazolylcarbonyl)amino]-8-oxo- (CA INDEX NAME)  
MF **C13 H11 N3 O5 S**  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

| CODE | VALUE | TYPE      | NOTE |
|------|-------|-----------|------|
| HD   | 2     | Predicted | (1)  |

This substance may exist in multiple tautomeric forms. The predicted property values in this table are calculated based upon the displayed form and may therefore differ from experimental values based on the actual tautomeric ratio at equilibrium.

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02  
(© 1994-2024 ACD/Labs)

. . .

| CODE | VALUE | TYPE      | NOTE |
|------|-------|-----------|------|
| HAC  | 8     | Predicted | (1)  |

. . .

# Use Case (cont.)

## CAplus refinements and displays

### Crossover data to CAplus, restrict to patents and and display

=> **FIL CAPLUS**

=> **S L5 AND P/DT**

=> **D BIB ABS HITIND HITPPAK 1-TOT**

L6 ANSWER 2 OF 59 CAPLUS COPYRIGHT 2024 ACS on STN

[PatentPak PDF](#) | [PatentPak PDF+](#) | [PatentPak Interactive](#)

AN 2022:2560264 CAPLUS Full-text

DN 180:246925

TI Preparation of 4',5'-dihydrocefradine

IN Zhou, Jia; Li, Fanglin; Sun, Kunjie

PA Shenzhen Sungening Bio-Medical Co., Ltd., Peop. Rep. China

UO SHENZHEN SUNGENING BIO MEDICAL

UOS SHENZHEN SUNGENING BIO MEDICAL

SO Fr. Demande, 13pp.

CODEN: FRXXBL

DT Patent

LA French

FAN.CNT 1

PPPI

| PATENT NO. | KIND | DATE     | LANGUAGE | PatentPak  |
|------------|------|----------|----------|--|
| FR 3121440 | A1   | 20221007 | French   | <a href="#">PDF</a>   <a href="#">PDF+</a>   <a href="#">Interactive</a> |

AB The present invention relates to a method of prepn. Of 4',5'-dihydrocefradine (I) starting from the (R)-(-)-2-(2,5-dihydrophenyl)glycine. The process includes stages of Boc (tert-butoxycarbonyl) protection of the amino group, redn., formation of

IT 57872-59-0P 2845098-92-0P 2845098-94-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT(Reactant or reagent) (prepn. of 4',5'-dihydrocefradine from (R)-(-)-2-(2,5-dihydrophenyl)glycine)

[PatentPak PDF](#) | [PatentPak PDF+](#) | [PatentPak Interactive](#)

PPAK

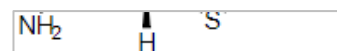
2845098-94-2P, [Pg 7](#)

**HITPPAK** shows the page links of hit substances only. Clicking this link allows to jump to the location of this hit compound in the patent full text.

# Use Case (cont.)

The markup of the indexed substance is shown in PatentPak

The preparation of the hit compound is shown in the French patent on page 7.

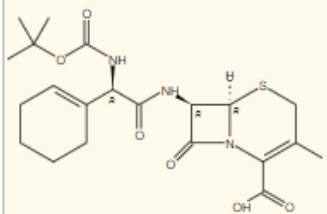


Analyst Markup Locations (2)

page 7

page 7

CAS RN 2845098-94-2

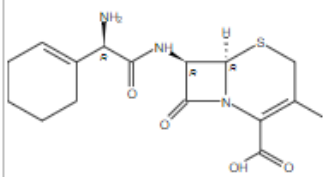


Analyst Markup Locations (2)

page 7

page 8

CAS RN 37051-00-6

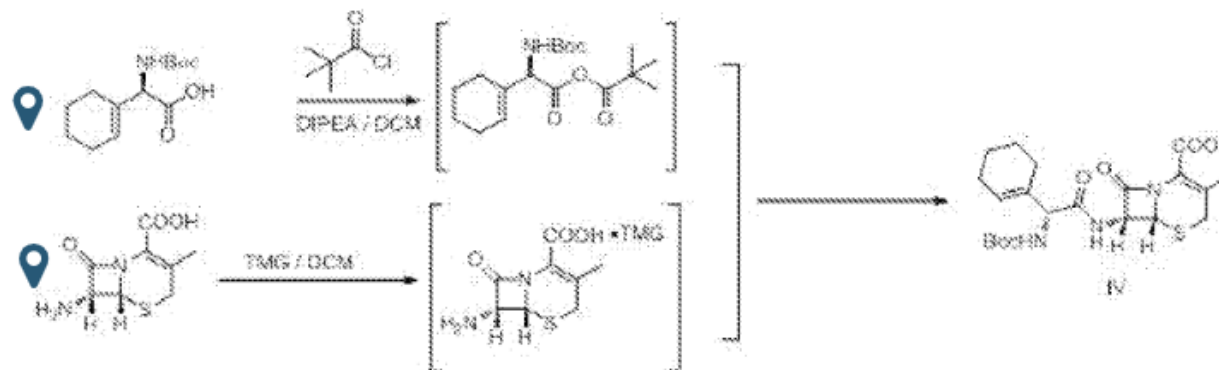


Analyst Markup Locations (2)

pour donner le composé de formule III (2,0g, rendement : 19%).

[0047] C – Préparation du composé de formule IV :

[0048] [Chem.10]



- [0049] a. A une solution de composé III (2,5g, 10mmol, 1éq) et de N,N-diisopropyléthylamine (DIPEA) (20mmol) dans le dichlorométhane (DCM), du chlorure de triméthylacétyle (chlorure de pivaloyle) (1,27g, 10,5mmol, 1,05éq) a été ajouté à -40°C, puis le mélange a été agité à -25°C pendant 30 minutes.
- b. Ensuite le mélange a été ajouté à -40°C à une solution d'acide 7-aminodésacétoxycephalosporanique (7-ADCA) (2,14g, 10mmol, 1éq) et de 1,1,3,3-tétra-méthylguanidine (TMG) (1,15g, 10mmol, 1éq) dans 30 ml de DCM.

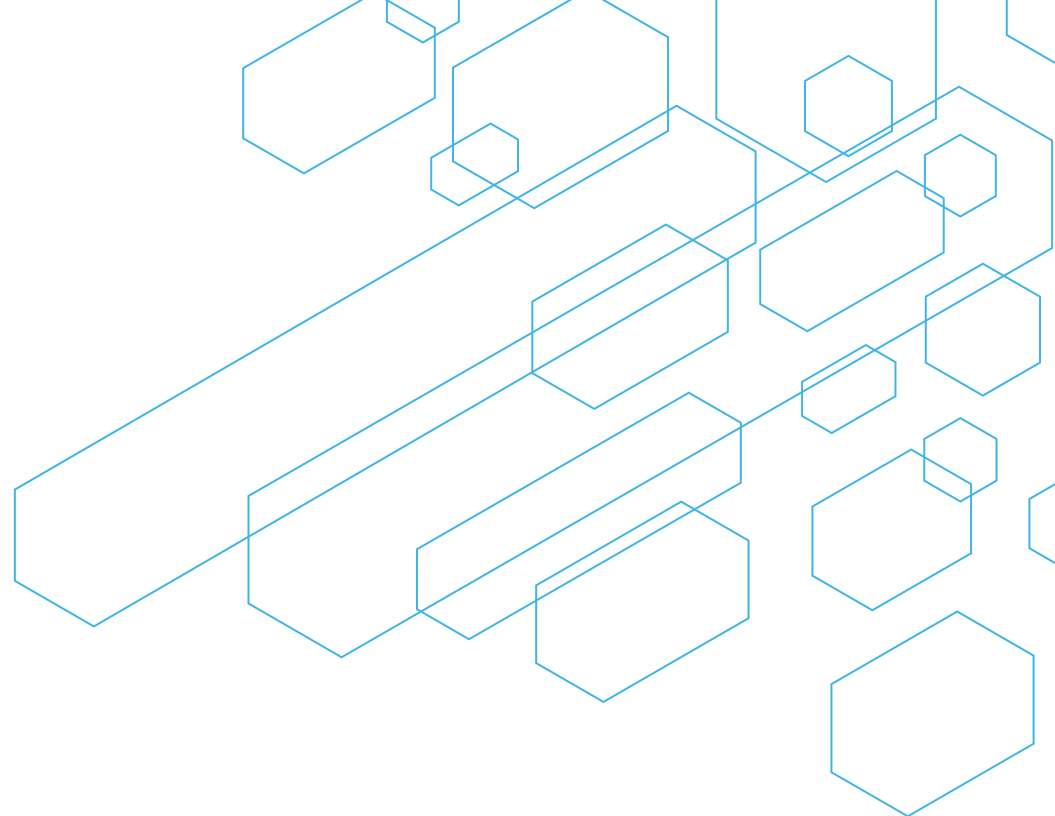


# Useful HELP messages

|                 |   |
|-----------------|---|
| HELLP SFIELDS   | List of search field codes                    |
| HELP DFIELDS    | List of display field codes                   |
| <hr/>           |   |
| HELP DUNITS     | Specifying units for display fields           |
| HELP LIPINSKI   | Searching Lipinski property parameters        |
| HELP PROPERTIES | Sources of property information in REGISTRY   |
| HELP QRD        | Query-Related Data in displays and prints     |
| HELP SNUMERIC   | Numeric fields and how to search them         |
| HELP SUNITS     | Specifying units for search fields            |
| HELP UNITS      | Where to see units for properties in REGISTRY |

# Agenda

- Numeric properties in CAS Registry
- **Overview of Numeric Property Searching (NPS)**
- Databases with NPS capability
- Searchable properties
- Search examples



# Extracting, normalizing, and indexing numeric data

- Numeric property data is captured from all English-language text fields, then made accessible for searching
- Numbers and their units within the English-language text are identified
  - About 1,800 property unit variants are identified
  - Numbers are considered from exact values, in closed ranges and open ranges
  - Numerals are detected as well in most databases
- Identified original data are normalized to base units and indexed for searching

# Searching NPS in English-language text fields

Numeric search terms can be combined with text-based search terms of interest

- Using standard text-based proximity operators
- Specifying text fields of interest, e.g. claims (/CLM)

Flexible data input options are available

- Ranges, exact values and tolerances
- A wide variety of search units

# Numeric search options

=> S 50/VOL

L1 11048 50 M\*\*3 /VOL

Search with **default units**.

=> S 50-60/VOL

L2 11338 50 M\*\*3 - 60 M\*\*3 /VOL

Search with **closed ranges**.

=> S 10-30 ML/VOL

L3 200076 10-30 ML/VOL

Search with **other units**.

=> S SIZ < 5 MM

L4 2200679 SIZ < 5 MM

Search with **open ranges**.

=> S 5 MM +-1/SIZ

L5 7603645 MM +-1/SIZ

Search with **tolerances**.

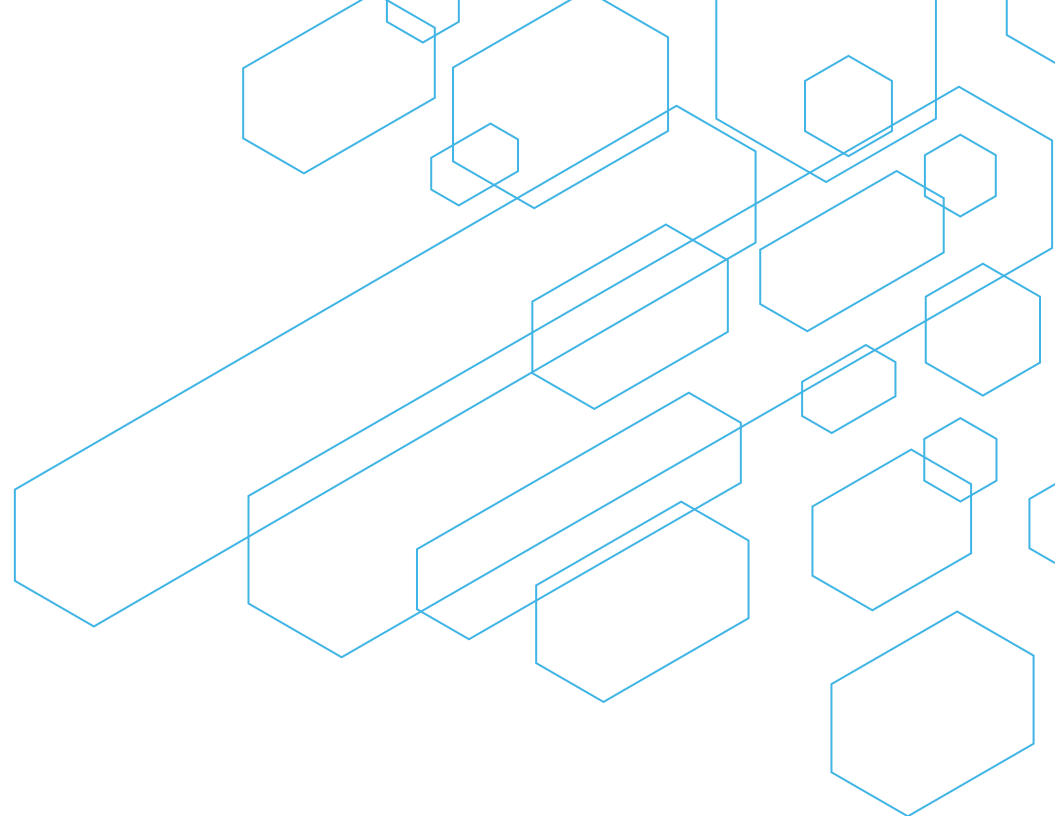
=> S 5 MM +-5%/SIZ

L6 666228 5 MM +- 5%/SIZ

Search with **tolerances in %**

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- Overview of Numeric Property Searching (NPS)
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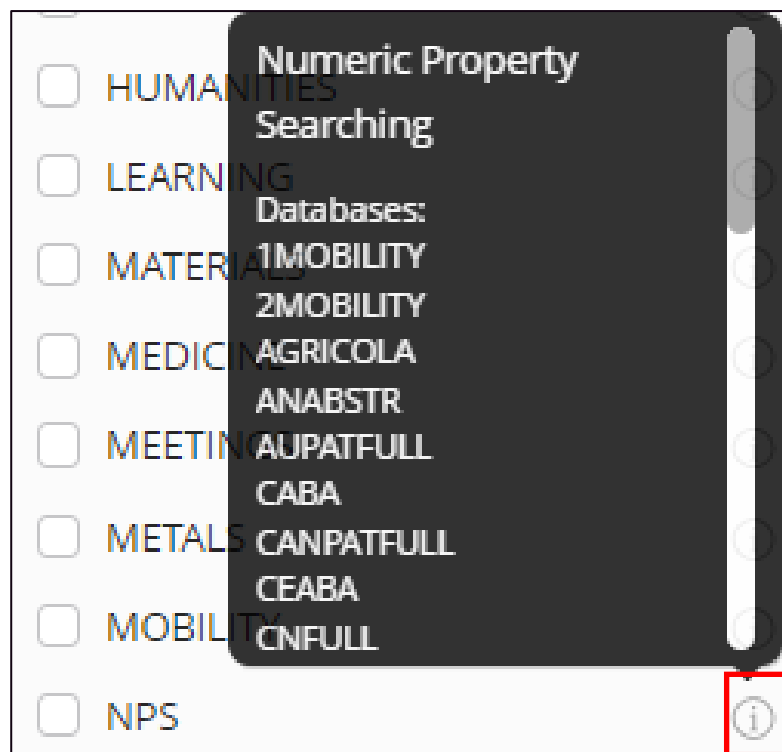
# CAS STNext databases that offer Numeric Property Search feature

```
=> D CLUSTER NPS
```

| CLUSTER NAME | CLUSTER DEFINITION  |
|--------------|---|
| NPS          | 1MOBILITY 2MOBILITY AGRICOLA ANABSTR AUPATFULL CABA<br>CANPATFULL CEABA CNFULL COMPENDEX DEFULL EPFULL<br>FRFULL FSTA GBFULL INFULL INSPEC JPFULL KRFULL NTIS<br>PCTFULL PQSCITECH RAPRA RDISCLOSURE RUFULL TEMA TULSA<br>TULSA2 TWFULL USPATFULL USPAT2 WPIDS WPINDEX WPIX<br>Numeric Property Searching |

Note: To display a list of all databases with Numeric Property Searching capability, type **D CLUSTER NPS**.

# CAS STNext databases that offer Numeric Property Search feature

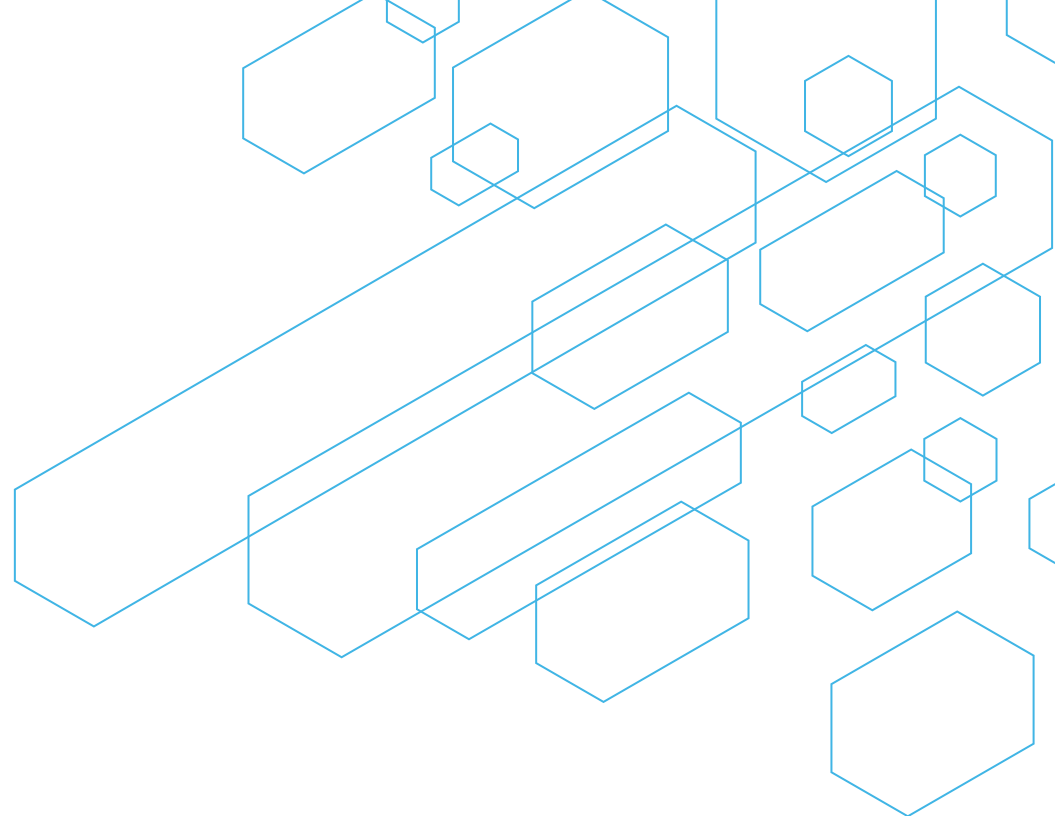


Note: Alternatively, click on the information icon next to the NPS cluster in the Databases tab.



# Agenda

- Overview of Numeric Property Searching (NPS)
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- **Searchable properties**
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# Indexed properties

| Field Code | Property                      | Base Unit              | Symbol            |
|------------|-------------------------------|------------------------|-------------------|
| AOS        | Amount of substance           | Mol                    | mol               |
| BIR        | Bit Rate                      | Bit / Second           | bit/s             |
| BIT        | Stored Information            | Bit                    | bit               |
| CAP        | Capacitance                   | Farad                  | F                 |
| CDN        | Current Density               | Ampere / Square Meter  | A/m <sup>2</sup>  |
| CMOL       | Molarity, Molar Concentration | Mol / Liter            | mol/L             |
| CON        | Electrical Conductance        | Siemens                | S                 |
| DB         | Decibel                       | Decibel                | dB                |
| DEG        | Degree                        | Degree                 | °                 |
| DEN        | Density, Mass Concentration   | Kilogram / Cubic Meter | kg/m <sup>3</sup> |
| DEQ        | Dose Equivalent               | Sievert                | Sv                |
| DOS        | Dosage                        | Milligram / Kilogram   | mg/kg             |
| DV         | Viscosity, dynamic            | Pascal x Second        | Pa s              |
| ECH        | Electric Charge               | Coulomb                | C                 |
| ECD        | Electric Charge Density       | Coulomb / Square Meter | C/m <sup>2</sup>  |
| ECO        | Electrical Conductivity       | Siemens / Meter        | S/m               |
| ELC        | Electric Current              | Ampere                 | A                 |
| ELF        | Electric Field                | Volt / Meter           | V/m               |
| ENE        | Energy                        | Joule                  | J                 |
| ERE        | Electrical Resistivity        | Ohm x Meter            | ohm m             |
| FOR        | Force                         | Newton                 | N                 |

# Indexed properties (cont.)

| Field Code | Property                        | Base Unit           | Symbol            |
|------------|---------------------------------|---------------------|-------------------|
| FRE        | Frequency                       | Hertz               | Hz                |
| IU         | International Unit              | none                | IU                |
| KV         | Viscosity, kinematic            | Square Meter/Second | m <sup>2</sup> /s |
| LEN        | Length                          | Meter               | m                 |
| LUMI       | Luminous Intensity              | Candela             | cd                |
| LUME       | Luminous Emittance, Illuminance | Lux                 | lx                |
| LUMF       | Luminous Flux                   | Lumen               | lm                |
| M          | Mass                            | Kilogram            | kg                |
| MCH        | Mass to Charge Ratio            | none                | m/z               |
| MFR        | Mass Flow Rate                  | Kilogram/Second     | kg/s              |
| MFD        | Magnetic Flux Density           | Tesla               | T                 |
| MM         | Molar Mass, Molecular Weight    | Gram / Mol          | g/mol             |
| MOLS       | Molality of Substance           | Mol / Kilogram      | mol/kg            |
| MVR        | Melt Volume Rate                | none                | g/10 min          |
| NUC        | Nutrition Content               | none                | g/100 kcal        |
| PER        | Percent                         | none                | %                 |
| PERA       | Permittivity, Absolute          | Farad / Meter       | F/m               |
| PERR       | Permittivity, Relative          | None                | None              |
| PHV        | ph Value                        | pH                  | pH                |
| POW        | Power                           | Watt                | W                 |
| PPM        | Parts per million               | None                | None              |
| PRES       | Pressure                        | Pascal              | Pa                |
| RAD        | Radioactivity                   | Becquerel           | Bq                |

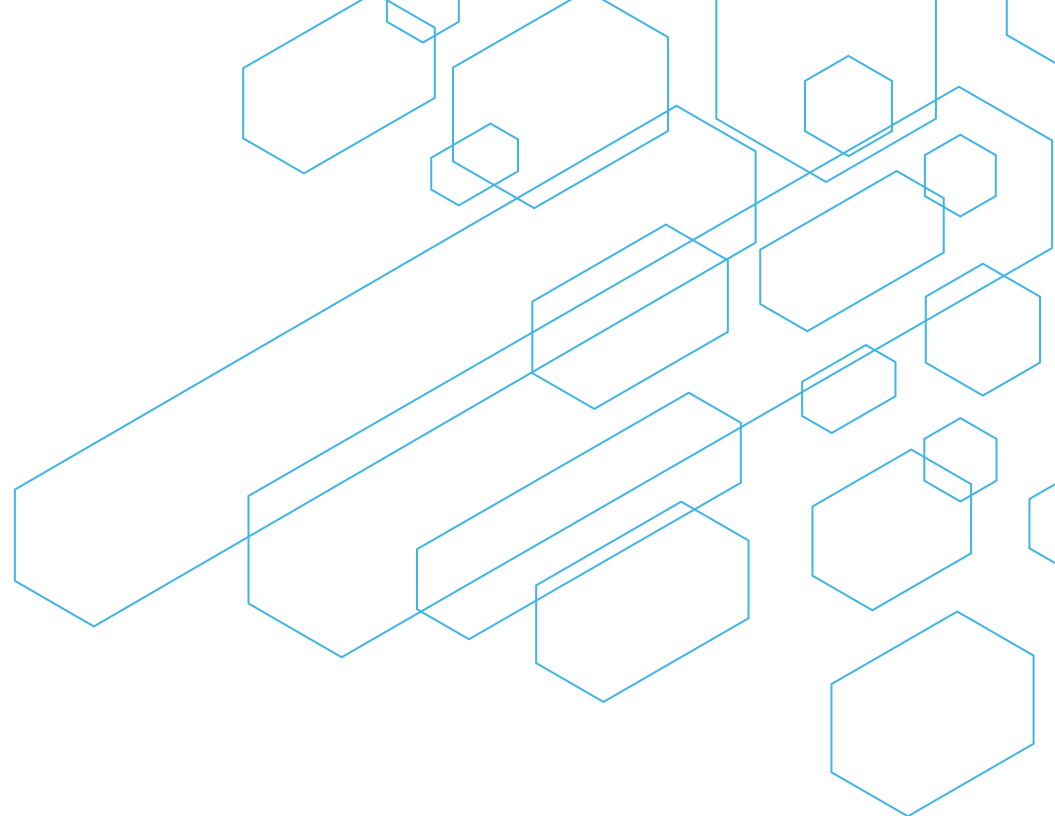
# Indexed properties (cont.)

| Field Code | Property                         | Base Unit             | Symbol            |
|------------|----------------------------------|-----------------------|-------------------|
| RES        | Electrical Resistance            | Ohm                   | Ohm               |
| RI         | Refractive Index                 | None                  | None              |
| RSP        | Rotational Speed                 | Revolution / Minute   | rpm               |
| SAR        | Area                             | Square Meter          | m <sup>2</sup>    |
| SOL        | Solubility                       | Gram / 100 gram       | g/100g            |
| STSC       | Surface Tension, Spring Constant | Joule/ Square Meter   | J/m <sup>2</sup>  |
| TCO        | Thermal Conductivity             | Watt / Meter x Kelvin | W/m K             |
| TEMP       | Temperature                      | Kelvin                | K                 |
| TIM        | Time                             | Second                | s                 |
| VEL        | Velocity                         | Meter / Second        | m/s               |
| VELA       | Velocity, angular                | Radian / Second       | rad/s             |
| VLR        | Volumetric Flow Rate             | Cubic Meter / Second  | m <sup>3</sup> /s |
| VOL        | Volume                           | Cubic Meter           | m <sup>3</sup>    |
| VOLT       | Voltage                          | Volt                  | V                 |
| WAC        | Water Activity                   | None                  | None              |

Type **HELP NPS** in specific database to learn which properties are searchable in that database.

# Agenda

- Overview of Numeric Property Searching (NPS)
- Databases with NPS capability
- Searchable properties
- Search examples



# Search example - Liquid Nitrogen pressure

Find U.S. patents and published applications where the pressure of liquid nitrogen is kept below 25 psi.

```
=> FILE USPATFULL USPAT2
```

```
=> S (LIQUID (W) NITROGEN) (5A) 0-25 PSI/PRES
```

```
L1          463 FILE USPATFULL
```

```
L2          160 FILE USPAT2
```

```
TOTAL FOR ALL FILES
```

```
L3          623 (LIQUID (W) NITROGEN) (5A) 0-25 PSI/PRES
```

- USPATFULL has information pertaining to the first published publications of U.S. patents and applications.
- USPAT2 has information pertaining to the latest publications of U.S. patents and applications.

# Liquid nitrogen pressure displays

L3 ANSWER 1 OF 623 USPATFULL on STN

DETD . . . certainly possible within the definition as set forth, “cryogenesis” and similar derivatives thereof are not limited to temperatures associated with liquid nitrogen at 1 atm or of about  $-80^{\circ}$  C.

L3 ANSWER 2 OF 623 USPATFULL on STN

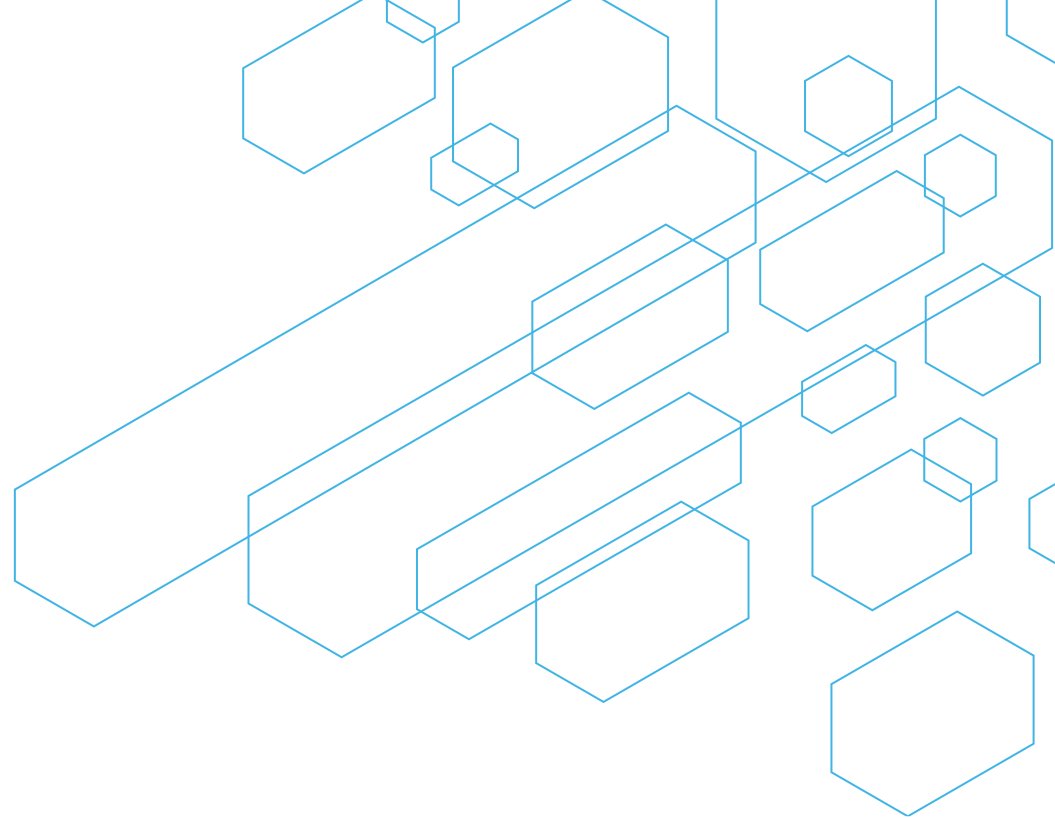
DETD . . . is as follows: aluminum cassette holder rack (compatible with CS750 freezer bags), cryostorage cassettes for 750 mL bags, low pressure (22 psi) liquid nitrogen tank, refrigerator, thermocouple sensor (ribbon type for bags), and CryoStore CS750 Freezing bags (OriGen Scientific).

L3 ANSWER 5 OF 623 USPATFULL on STN

DETD . . . weighed into a disposable aluminium boat and loaded into the sublimation chamber. The system was sealed and pumped down to 50 milliTorr before liquid nitrogen was added to the cold trap. The system continued to evacuate throughout the deposition process. The sublimation chamber was heated. . .

# Dosage vs. mass

- The base unit for Dosage is mg/kg
- The base unit for Mass is kg
- If a dosage is described by weight (i.e., mg), search by Mass, **not dosage!**
  - Search with /M search qualifier, **NOT /DOS**
- Consider keyword search *dose?* or *dosage?* around Mass search





# Searching dosage by mass

CLM What is claimed is:

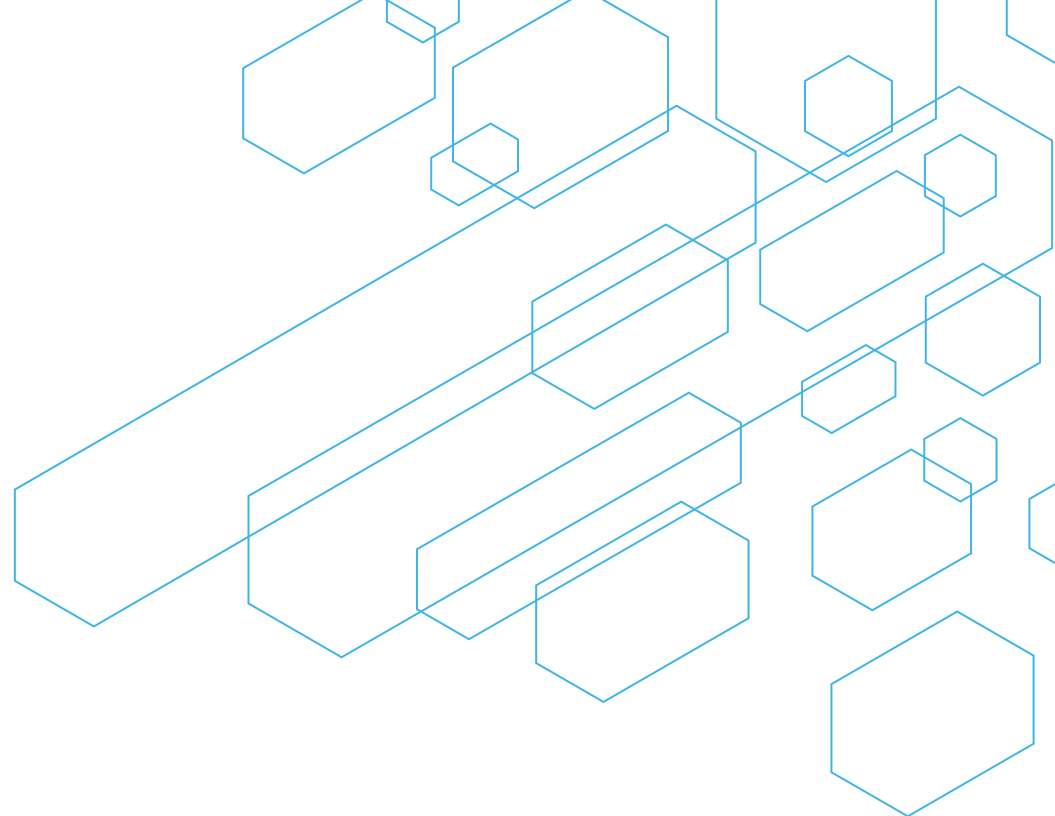
. . . doses and maintenance doses of the pharmaceutical composition are administered to the human subject as follows: (i) a first loading **dose** equivalent to about **100** mg of the antisense oligonucleotide; (ii) a second loading **dose** equivalent to about **100** mg of the antisense oligonucleotide, wherein the second loading dose is administered 14 days after the first loading dose; (iii) a third loading **dose** equivalent to about **100** mg of the antisense oligonucleotide, wherein the third loading dose is administered 28 days after the first loading dose; and (iv) a first maintenance **dose** equivalent to about **100** mg of the antisense oligonucleotide, wherein the first maintenance dose is administered 1 month after the third loading dose.

L6 ANSWER 5 OF 252540 USPATFULL on STN

DETD . . . with a suitable pharmaceutically acceptable carrier to form a liquid composition suitable for injection thereof into a subject. The unit **dosage** form typically comprises from about **10** ng to about 10 grams of the compound or salt. When the compound or salt is substantially water-insoluble, a sufficient. . .

# Using .EX with NPS

- .EX will remove open ended ranges from search
- Although these records may be 'legally valid', they may be less interesting
- Add .EX to search qualifier
  - S 97-103/TEMP.EX



# .EX Example

=> FILE USPATFULL

...

=> S 97-103 C/TEMP (3A) (MELTING(W)POINT OR MP)

941959 97-103 C/TEMP

773999 MELTING

185 MELTINGS

774031 MELTING

(MELTING OR MELTINGS)

5698002 POINT

2836920 POINTS

6301638 POINT

(POINT OR POINTS)

160339 MP

22500 MPS

179029 MP

(MP OR MPS)

L1 29047 97-103 C/TEMP (3A) (MELTING(W)POINT OR MP)

=> S 97-103 C/TEMP.EX (3A) (MELTING(W)POINT OR MP)

518899 97-103 C/TEMP.EX

773999 MELTING

185 MELTINGS

774031 MELTING

(MELTING OR MELTINGS)

5698002 POINT

2836920 POINTS

6301638 POINT

(POINT OR POINTS)

160339 MP

22500 MPS

179029 MP

(MP OR MPS)

L2 7147 97-103 C/TEMP.EX (3A) (MELTING(W)POINT OR MP)

=> S L1 NOT L2

L3 21900 L1 NOT L2

# Display of unique hits

=> D KWIC 1-2

L3 ANSWER 1 OF 21900 USPATFULL on STN

DETD . . . to a temperature of at least 5° C. above the melting point, for example, at least 6° C. above the **melting point**, at least 7° C. above the **melting point**, at least 8° C. above the **melting point**, at least 9° C. above the **melting point**, or at least 10° C. above the melting point of the thermally activatable laminating material. In some examples, activation of the thermally activatable laminating. . .

L3 ANSWER 2 OF 21900 USPATFULL on STN

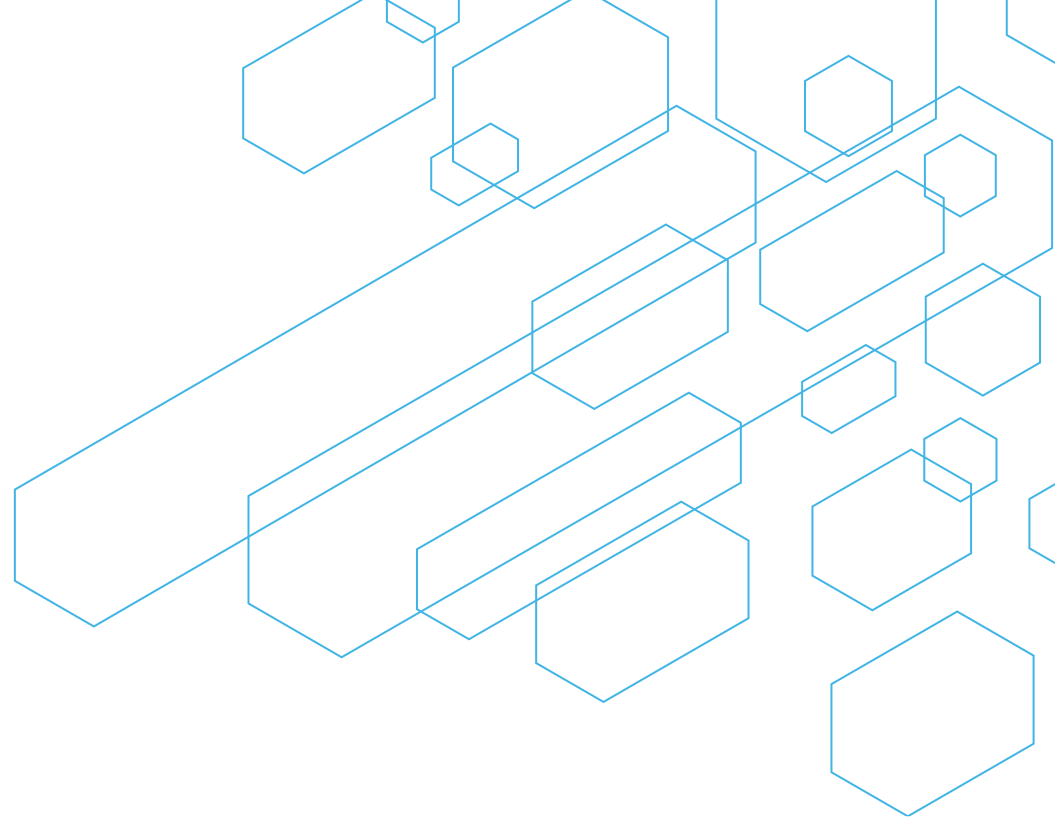
DETD . . . bonds, making a high melt, narrow cut and hard paraffin wax. The wax is a very hydrophobic material. It has **melting points** in general above 35° C. or more. More specifically, the melt points of the wax are above 55° C. It has a measured water. . .

CLM What is claimed is:

. . . wax, slick wax, or ethylene stearamide, bis-stearamide synthesis wax, carnauba wax, natural organic and organic synthesized wax that have a **melting point** of at least 35° C. or above, or/and biomaterials or their derivatives such as sweet rice flour, soy wax, soy protein isolate (SPI) particles,. . .

# Tolerances

- Tolerances can be searched with +/-
- Tolerances can be searched with %
- Tolerances can be SET for a specific search field



# Tolerances example in INSPEC

```
=> FILE INSPEC
```

```
=> S 150 KV/VOLT.EX (5A) (POLYSILOXANE? OR SILICON?)
```

```
3696 150 KV/VOLT.EX
```

```
3217 POLYSILOXANE?
```

```
879135 SILICON?
```

```
L1          3 150 KV/VOLT.EX (5A) (POLYSILOXANE? OR SILICON?)
```

```
=> S 150+-15 KV/VOLT.EX (5A) (POLYSILOXANE? OR SILICON?)
```

```
5877 150+-15 KV/VOLT.EX
```

```
3217 POLYSILOXANE?
```

```
879135 SILICON?
```

```
L2          6 150+-15 KV/VOLT.EX (5A) (POLYSILOXANE? OR SILICON?)
```

```
=> S L2 NOT L1
```

```
L3          3 L2 NOT L1
```

# INSPEC Tolerance displays

=> D KWIC 1-3

L3 ANSWER 1 OF 3 INSPEC COPYRIGHT 2024 IET on STN.

AB This study presents numerical electric field distribution of conventional glass, RTV (Room Temperature Vulcanizing) silicone rubber coated glass and **silicone** rubber insulator strings used for **154** kV transmission systems. 2D axisymmetric electric field simulations were performed by using a commercially available software based on Finite Element. . .

L3 ANSWER 2 OF 3 INSPEC COPYRIGHT 2024 IET on STN.

AB Describes the design of high voltage **silicon** hexafluoride switchgear for voltages to **145** kV. A specification of the 145 kV 3000 ampere switchgear is presented and procedures in design, in subassembly and in. . .

L3 ANSWER 3 OF 3 INSPEC COPYRIGHT 2024 IET on STN.

AB Nitrogen ions accelerated by a potential of 130-**140** kV were implanted in **silicon** heated to  $T_i=700-1100^\circ\text{C}$ . The ion current density was  $1-5 \mu\text{A}/\text{cm}^2$  and the dose did not exceed  $5 \times 10^{17} \text{ cm}^{-2}$ . The methods. . .

All of these records were unique captures by introducing the tolerance.

# Searching with Tolerances

- You can search tolerances manually
  - By number **S 150+-15 KV/VOLT**
  - By percentage **S 150 +- 10% KV/VOLT**
- You can set tolerances to a particular property
  - By number **SET TOLERANCE VOLT=15 PERM**
  - By percentage **SET TOLERANCE VOLT=10% PERM**



# Searching with Tolerances

=> S 150+-15 KV/VOLT

L4 16494 150+-15 KV/VOLT

=> S 150+-10% KV/VOLT

L5 16494 150+-10% KV/VOLT

=> SET TOLERANCE VOLT=15

SET COMMAND COMPLETED

=> S 150 KV/VOLT

L6 16494 150 KV +-15 /VOLT

=> SET TOLERANCE VOLT=10%

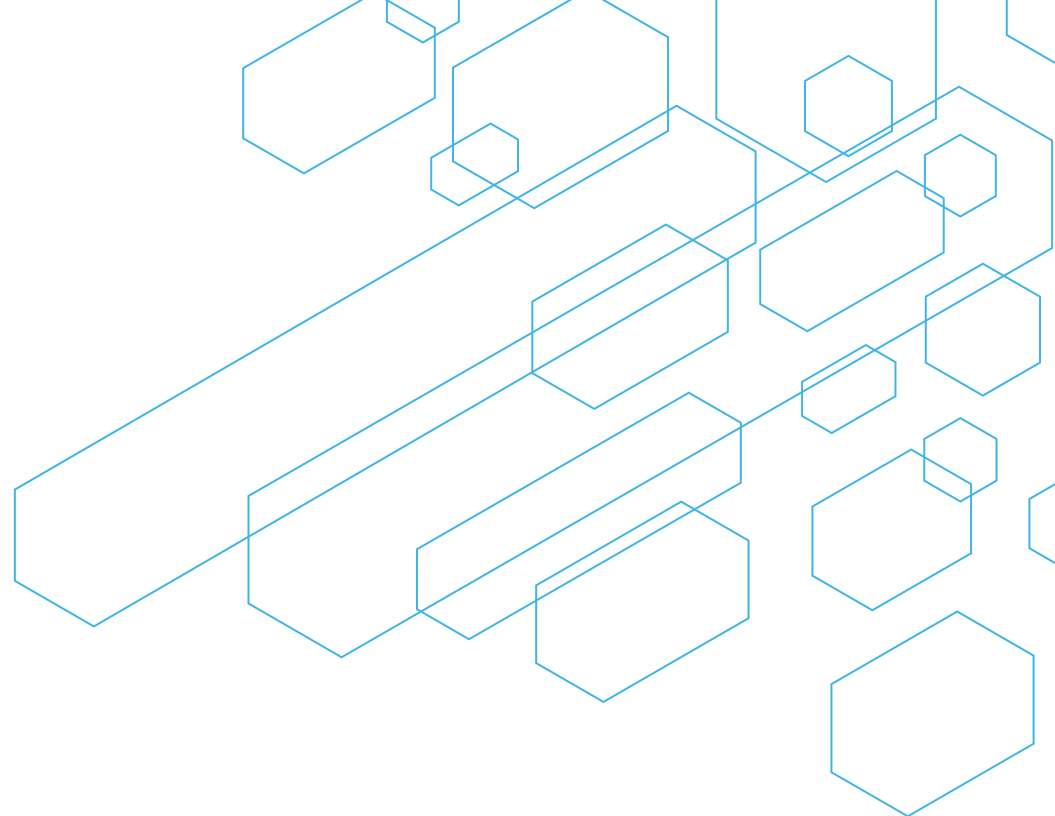
SET COMMAND COMPLETED

=> S 150 KV/VOLT

L7 16494 150 KV +-10% /VOLT

# Summary

- Numeric property search (NPS) can greatly increase quality of numeric searches
- Up to 59 properties, about 1800 units recognized
- Can be used in conjunction with keyword searching
- Exact, closed-range, open-range and tolerance searching possible



Between problems  
and progress  
are connections  
that matter



## CONTACT

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