



FIZ CHEMIE BERLIN

Fachinformationszentrum Chemie GmbH

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# Index Terms/Controlled Terms/Roles

Beschreiben wesentliche Inhalte des Dokuments.

IT field: Kontrollierte und nicht-kontrollierte Stichwörter, Registry Nummern und Roles.

IT Coating process  
(surface; process for producing magnetic composite particles for magnetic recording medium)

Controlled  
Term (/CT)

Registry Number

Modifying Phrases

IT 7439-89-6, Iron, uses  
RL: TEM (Technical or engineered material use); USES  
(Uses)  
(acicular magnetic metal; process for producing magnetic composite particles for magnetic recording medium)

Roles  
(/RL)

# Controlled Terms /CT

Was Sie bei einer Stichwortsuche beachten sollten:

- Man verwendet so viele Synonyme wie möglich
- Man geht sicher, dass unter den Suchbegriffen auch der „Controlled Term“ ist.
- Man sucht den richtigen „Controlled Term“ im CA Thesaurus

## Beispiel:

Verschiedene Stichwörter wurden für die Suche verwendet:

**L1**            **28298**    **s (ANTICANCER OR ANTICARCINO?) (W) (AGENT OR DRUG)**

Aber der von CAS vergebene „Controlled term“ - „Antitumor Agent“ - war nicht darunter:

**L2**            **233070**    **s ANTITUMOR AGENT**

## Strategie:

1. Das CA Lexikon hilft den richtigen Begriff zu finden

=> e antitumor agents/ct

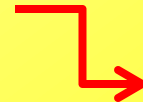
E#	FREQUENCY	AT	TERM
--	-----	--	----
E1	0	2	ANTITUMOR AGENT/CT
E2	0	3	ANTITUMOR AGENT RESISTANCE/CT
E3	222266	196	--> ANTITUMOR AGENTS/CT

=> e e3+all

E13	2786	BT2	Health products/CT
E14	33585	BT1	Drugs/CT
E15	222266	-->	Antitumor agents/CT

HNTE Valid heading during volume 126 (1997) to present.

NOTE Chemotherapeutic agents and other chemically defined natural products, such as food constituents, for the prevention or inhibition of tumors are indexed here. For nonchemical therapies, see Radiotherapy, Therapy, and headings for the specific nonchemical therapy.



**E16 77038 OLD Neoplasm inhibitors/CT**

E17	UF	Anticancer agents/CT
E18	UF	Anticancer drugs/CT
E19	UF	Anticarcinogenic agents/CT
E20	UF	Anticarcinogenic drugs/CT
E21	UF	Anticarcinogenics/CT
E22	UF	Anticarcinogens/CT
E23	UF	Antineoplastic agents/CT
E24	UF	Antineoplastic drugs/CT
E25	UF	Antineoplastics/CT
E26	UF	Antitumor agent/CT
E27	UF	Antitumor compds./CT
E28	UF	Antitumor drugs/CT
E29	UF	Antitumor medicines/CT
E30	UF	Antitumors/CT
E31	UF	Antitumors agents/CT
E32	UF	Cancer chemotherapy/CT
E33	UF	Cancer inhibitors/CT
E34	UF	Cancer therapy/CT
E35	UF	Carcinogenesis inhibitors/CT
E36	UF	Carcinostatic agents/CT
E37	UF	Carcinostatics/CT
E38	UF	Neoplasm inhibitor/CT
E39	UF	Oncolytic agent/CT
E40	UF	Synergistic neoplasm inhibitors/CT
E41	UF	Tumor growth inhibitors/CT
E42	UF	Tumor inhibitors/CT

**UF:Used For**  
Keine  
kontrollierten  
Begriffe  
(CTs)  
sondern  
Synonyme.  
Nicht  
auffindbar im  
Feld /CT

Expand im CA Lexikon mit einem „Used For Term“ führt zum eigentlichen „Controlled Term“.

*Unser Beispiel:* Ist „Anticancer drugs“ ein Controlled Term?

=> e anticancer drugs/ct

E#	FREQUENCY	AT	TERM
--	-----	--	----
E1	0	1	ANTICANCER/CT
E2	0	2	ANTICANCER AGENTS/CT
E3	0	2 -->	ANTICANCER DRUGS/CT

=> e e3+all

E13	0	-->	Anticancer drugs/CT
E14	222266	USE	Antitumor agents/CT
***** END *****			

=> e e14+all

=> e e14+all

E15 222266

--> Antitumor agents/CT

HNTE Valid heading during volume 126  
(1997) to present.

NOTE Chemotherapeutic agents and  
other chemically defined natural  
products, such as food  
constituents, for the prevention  
or inhibition of tumors are  
indexed here. For nonchemical  
therapies, see Radiotherapy,  
Therapy, and headings for the  
specific nonchemical therapy.



<b>E16</b>	<b>77038</b>	<b>OLD</b>	<b>Neoplasm inhibitors/CT</b>
E17		UF	Anticancer agents/CT
E18		UF	Anticancer drugs/CT
E19		UF	Anticarcinogenic agents/CT
E20		UF	Anticarcinogenic drugs/CT
E21		UF	Anticarcinogenics/CT
E22		UF	Anticarcinogens/CT
E23		UF	Antineoplastic agents/CT
E24		UF	Antineoplastic drugs/CT
E25		UF	Antineoplastics/CT
E26		UF	Antitumor agent/CT
E27		UF	Antitumor compds./CT
E28		UF	Antitumor drugs/CT
E29		UF	Antitumor medicines/CT
E30		UF	Antitumors/CT
E31		UF	Antitumors agents/CT
E32		UF	Cancer chemotherapy/CT
E33		UF	Cancer inhibitors/CT
E34		UF	Cancer therapy/CT
E35		UF	Carcinogenesis inhibitors/CT
E36		UF	Carcinostatic agents/CT
E37		UF	Carcinostatics/CT
E38		UF	Neoplasm inhibitor/CT
E39		UF	Oncolytic agent/CT
E40		UF	Synergistic neoplasm inhibitors/CT
E41		UF	Tumor growth inhibitors/CT
E42		UF	Tumor inhibitors/CT

2. Verwenden Sie für Ihre Suche den „Controlled Term“, „Old Controlled Terms“ und „Used For Terms“ neben weiteren Synonymen im Basic Index.

=> s e15-e42/bi

```
L3      321801 "ANTITUMOR AGENTS"/BI OR ("NEOPLASM
          INHIBITORS"/BI OR "ANTICANCER
          AGENTS"/BI OR "ANTICANCER DRUGS"/BI OR
          "ANTICARCINOGENIC AGENTS"/BI OR
          "ANTICARCINOGENIC DRUGS"/BI OR
          ANTICARCINOGENICS/BI o o o
```

Oder: Verwenden Sie „Controlled“ und „Old ControlledTerms“ im Feld /CT und die „Used For Terms“ neben weiteren Synonymen im Basic Index.

=> s e15-e16 or e17-e42/bi

```
L4      321799 "ANTITUMOR AGENTS"/CT OR "NEOPLASM
          INHIBITORS"/CT OR ("ANTICANCER
          AGENTS"/BI OR "ANTICANCER DRUGS"/BI OR
          "ANTICARCINOGENIC AGENTS"/BI OR
          "ANTICARCINOGENIC DRUGS"/BI o o o
```

### 3. Schränken Sie Ihre Recherche mit im Zusammenhang stehenden Begriffen ein.

=> S L4 (L) prostate

L5 9761 L2 (L) PROSTATE

=> d hit 200

L5 ANSWER 200 OF 9761 CAPLUS COPYRIGHT 2009 ACS on STN

IT Antitumor agents

Genetic mapping

Human

Molecular association

Proliferation inhibition

(interaction of vitamin D receptor with vitamin D response element in Mullerian-inhibiting substance (MIS) in prostate cancer cells)

# Roles

Stehen neben jeder **indexierten Verbindung** und neben **Controlled Terms für Substanzklassen**

L6 ANSWER 1000 OF 1614 CAPLUS COPYRIGHT 2009 ACS on STN

IT **Esters, reactions**

**RL: RCT (Reactant); RACT (Reactant or reagent)**  
(**aliphatic**; electroredn. of aliphatic esters using lanthanide ions as mediators)

L6 ANSWER 1200 OF 1614 CAPLUS COPYRIGHT 2009 ACS on STN

IT **Esters, preparation**

**RL: SPN (Synthetic preparation); PREP (Preparation)**  
(**aliphatic**, preparation of, by esterification of alkenes with Me formate, ruthenium complex-catalyzed)

IT **554-12-1P, Methyl propionate**

**RL: SPN (Synthetic preparation); PREP (Preparation)**  
(preparation of, by reaction of ethylene with Me formate, ruthenium complex-catalyzed)

CT: Esters (L) aliphatic

# Anwendung von Roles (=> help roles)

```
=> s "esters(L)aliphatic"/ct
```

```
L13      1908 "ESTERS(L)ALIPHATIC"/CT
```

```
=> s L13 (L) spn/rl
```

```
2232676 SPN/RL
```

```
L14      231 L13 (L) SPN/RL
```

```
L14 ANSWER 30 OF 231 CAPLUS COPYRIGHT 2009 ACS on STN
```

```
IT Esters, preparation
```

```
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)
```

```
(diesters, aliphatic; stereoselective preparation of  
pyrrolylmethyl malonates via Cu(OTf)2/synthesized  
chiral trisoxazoline catalyzed Friedel-Crafts reaction  
of pyrroles with alkylidene malonates)
```

# Anwendung von Roles (=> help roles)

*Beispiel:* Suche die synthetische Herstellung aliphatischer unsubstituierter Esters mit einem Molekulargewicht von <200

=> **Fil Reg**

=> **s c h o/ELF and ester and mw<200**

L1 45317 C H O/ELF AND ESTER AND MW<200

=> **S L1 not RSD/FA**

L2 20576 L1 NOT RSD/FA

=> **Fil Caplus**

=> **s L2/spn**

L3 31918 L26/SPN

(L2 (L) SPN/RL)

*In L3 finden sich auch  
Dokumente zur Herstellung  
der Derivate aliphatischer  
Ester.*

**Besser:**

L4 27994 S (L2 (NOTL) L2/D) (L) SPN/RL

*Beispiel:* Suche nach pharmazeutischen Verabreichungsformen (Drug Delivery Systems), die mittels Nanomaterialien hergestellt werden

**Vorgehensweise:**

Suche die Suchbegriffe und verwandte Begriffe im CA Lexikon.

Kombiniere die kontrollierten Begriffe des einen Suchterms im Feld /CT mit dem zweiten Suchterm und seinen Synonymen im Basic Index.

# 1. Suchterm: Nanomaterialien

=> FILE CAPLUS

=> E NANO/CT

E#	FREQUENCY	AT	TERM
--	-----	--	----
E1	0	1	NANO-/CT
E2	0	1	NANO2/CT
E3	0		--> NANO?/CT
E4	7	5	NANOARCHAEOTA/CT
E5	4	5	NANOARCHAEUM/CT
E6	21	5	NANOARCHAEUM EQUITANS/CT
E7	19	5	NANOBACTERIUM/CT
E8	2	5	NANOBACTERIUM SANGUINEUM/CT
E9	0	11	NANOBAGRUS/CT
E10	1	11	NANOBAGRUS STELLATUS/CT
E11	256	2	NANOCAPSULES/CT
E12	0	2	NANOCAPSULES (DRUG DELIVERY SYSTEMS)/CT



Mit => E gelangt man zu nachfolgenden Begriffen im Index  
Mit => E#+all erhält man alle assoziierten Begriffe

=> E

. . .

E85	0	6	NANONEIS/CT
E86	1	6	NANONEIS HASLEAE/CT
E87	0	2	NANOPARTICLE/CT
E88	0	2	NANOPARTICLE SIZE/CT
E89	44079	16	NANOPARTICLES/CT
E90	0	2	NANOPARTICLES (DRUG DELIVERY SYSTEMS)/CT
E91	0	2	NANOPARTICLES (DRUG DELIVERY SYSTEMS) (L) CONTROLLED R RELEASE/CT
E92	0	5	NANOPARTICLES (L) FERROMAGNETIC/CT
E93	0	5	NANOPARTICLES (L) NANOCCLUSERS/CT
E94	0	6	NANOPARTICLES (L) NANODROPLETS/CT
E95	0	5	NANOPARTICLES (L) NANOPOWDERS/CT
E96	0	2	NANOPARTICLES CONTROLLED-RELEASE PHARMACEUTICAL CAPSULES/CT

...

=> e nanocapsules+all/ct

E3	36674	BT3	Apparatus/CT
E4	55656	BT2	Containers/CT
E5	5415	BT1	Capsules/CT
E6	36674	BT2	Apparatus/CT
E7	1327	BT1	Nanodevices/CT
E8	44677	BT1	Nanostructures/CT
E9	256	-->	Nanocapsules/CT

HNTE Valid heading during volume 146 (2007) to present.

NOTE Nanocapsules are supramolecular objects encapsulating guest molecules. Nanocapsules for drug delivery are indexed at Drug delivery systems LT capsules.

E10	414	USE	Pharmaceutical nanocapsules/CT
E11		UF	Nanocapsule/CT
E12	414	NT1	Pharmaceutical nanocapsules/CT
E13	1296	RT	Cage compounds/CT
E14	24431	RT	Encapsulation/CT
E15	414	RT	Pharmaceutical nanocapsules/CT

Nanocapsules muß im Basic Index gesucht werden !!

=> e Nanoparticles+all/CT

E1 22423 BT1 Nanostructures/CT

E2 59797 BT1 Particles/CT

E3 44079 --> Nanoparticles/CT

HNTE Valid heading during volume 126 (1997)  
to present.

E4 OLD Particles (L) nano-/CT

E5 UF Magnetic nanoparticles/CT

E6 UF Nanoparticle/CT

E7 UF Nanoscale particle/CT

E8 UF Nanoscale particles/CT

E9 UF Nanosize particles/CT

E10 UF Nanosized particles/CT

E11 168827 RT Drug delivery systems/CT

E12 1356 RT Mesophase/CT

E13 17131 RT Nanocomposites/CT

E14 4398 RT Nanocrystalline metals/CT

E15 12656 RT Nanocrystals/CT

E16 RTCS 11-Mercaptoundecanoic acid/CT

\*\*\*\*\* END \*\*\*\*\*

=> E Nanocomposites+all/ct

E1 27204 BT1 Composites/CT

E2 17131 --> Nanocomposites/CT

HNTE Valid heading during volume 126 (1997) to present.

E3 OLD Composites (L) nano-/CT

E4 34396 RT Clusters/CT

E5 4736 RT Hybrid organic-inorganic materials/CT

E6 44079 RT Nanoparticles/CT

E7 22423 RT Nanostructures/CT

E8 2219 RT Nanotechnology/CT

E9 11800 RT Powder metallurgy/CT

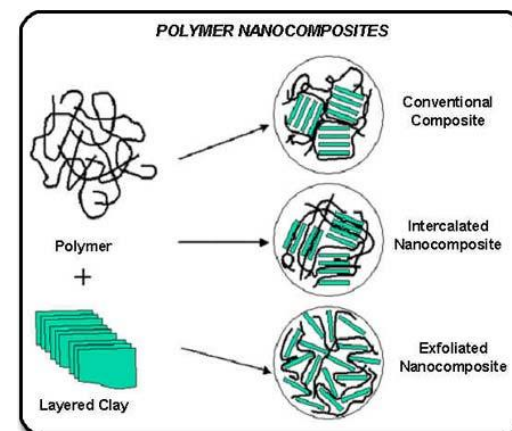
E10 RTCS Alumina/CT

E11 RTCS Cloisite 30B/CT

E12 RTCS Kunipia F/CT

E13 RTCS Silicon monocarbide/CT

\*\*\*\*\* END \*\*\*\*\*



## Suche Controlled Terms für Nanomaterials:

=> FILE HCAPLUS

=> S (NANOCOMPOSITES+PFT/CT OR NANOFIBERS+PFT,NT/CT OR NANOMACHINES+PFT,NT/CT OR NANOSPHERES+PFT,NT/CT OR NANOSTRUCTURES+PFT,NT/CT OR NANOTECHNOLOGY+PFT,NT/CT OR NANOTUBES+PFT,NT/CT OR NANOWIRES+PFT,NT/CT) OR NANOCAPSUL?

L1 179603

## Controlled Terms für Drug Delivery Systems:

=> S DRUG DELIVERY SYSTEM+ALL/CT

L2 186525

PFT = Preferred & Forbidden Terms  
(einschl.: SELF, OLD, NEW, USE,  
UF)

NT = Narrower Terms

# Suche der Begriffe im Basic Index

**=> S    NANOSTRUCTURE OR NANOCOMPOS? OR    NANOPARTIC?  
OR NANOTUBES OR NANOTECHNOLOGY OR  
NANOCAPSUL?**

**L3        298776**

**=> S    (DRUG OR DOSAGE OR PHARMACEUTIC? OR SUSTAIN? OR  
CONTROL?) (L) (RELEASE? OR DELIVER? OR TARGET? OR  
PREPAR? OR TABLET OR MICROTABLET OR CAPSULE? OR  
MICROCAPSULE OR DEPOT OR FORM?)**

**L4        1508106**

# Kombination von Controlled Terms mit Begriffen, die in der Textmodifikation stehen

=> S L1 (L) L4  
L5 3027

=> S L2 (L) L3  
L6 7077

=> S L6 not L5  
L7 6279

L1: Nano-Keywörter als Controlled Term

L2: Drug delivery als Controlled Terms

L3: Nano-Keywörter im Basic Index

L4: Drug Delivery Keywörter im Basic Index

=> d hit

L7 ANSWER 1 OF 6279 CAPLUS COPYRIGHT 2009 ACS on STN

IT **Drug delivery systems**

(targeted, contrast agent; **nanoparticles** that facilitate imaging of biol. tissue and methods of forming the same for MRI)

Hier sind NANO-Keywörter nicht als Controlled Term indexiert

# Welche Substanzen wurden als Nanomaterialien hier verwendet?

=> S L6 or L5

L8 9306

=> S L25 and NANO/RL

L26 918

=> D scan

L26 918 ANSWERS CAPLUS COPYRIGHT 2009 ACS on STN

IT 7631-86-9, Aerosil 200, biological studies

RL: THU (Therapeutic use); **NANO (Nanomaterial)**; BIOL  
(Biological study); USES (Uses)

(colloidal; sodium diclofenac containing  
**nanocapsule** xerogel microparticles with controlled  
release)



# CA Section Codes /CC

CC 29-13 (Organometallic and Organometalloidal Compounds)  
Section cross-reference(s): 22, 75, 73, 76

=> s 22/CC, SX

Section codes werden im Feld /CC  
gesucht.

Cross-reference section codes  
werden im Feld /SX gesucht.

=> help sections

## Biochemistry (BIO/FS)

1. Pharmacology
2. Mammalian Hormones
3. Biochemical Genetics
4. Toxicology
5. Agrochemical Bioregulators
6. General Biochemistry
7. Enzymes
8. Radiation Biochemistry
9. Biochemical Methods
10. Microbial, Algal, and Fungal Biochemistry
11. Plant Biochemistry
12. Nonmammalian Biochemistry
13. Mammalian Biochemistry
14. Mammalian Pathological Biochemistry
15. Immunochemistry
16. Fermentation and Bioindustrial Chemistry
17. Food and Feed Chemistry
18. Animal Nutrition
- ...

# Der Section Code Thesaurus

=> E 2/CC

E#	FREQUENCY	AT	TERM
--	-----	--	----
E1	0	1	1987-1991/CC
E2	0	1	1992/CC
<b>E3</b>	<b>779651</b>	<b>6</b>	<b>--&gt; 2/CC</b>

Sektionsnummern haben sich über die Jahre verändert!



=> E E17+HIS,NOTE

E25	72728	-->	2 HORMONE PHARMACOLOGY, 1972-1981/CC
E26	9346	OLD	4 HORMONES AND RELATED SUBSTANCES, 1970-1971/CC
E27	12502	OLD	4 HORMONES, 1967-1969/CC
E28	13903	OLD	58 HORMONES, 1963-1966/CC
E29	2373	OLD	72 HORMONES AND RELATED SUBSTANCES, 1962 ONLY/CC
E30	437923	CUR	2 MAMMALIAN HORMONES, 1982 TO PRESENT/CC

\*\*\*\*\* END\*\*\*

=> E E18+HIS,NOTE

E31	437923	-->	2 MAMMALIAN HORMONES, 1982 TO PRESENT/CC
E32	72728	OLD	2 HORMONE PHARMACOLOGY, 1972-1981/CC
E33	9346	OLD	4 HORMONES AND RELATED SUBSTANCES, 1970-1971/CC
E34	12502	OLD	4 HORMONES, 1967-1969/CC
E35	13903	OLD	58 HORMONES, 1963-1966/CC
E36	2373	OLD	72 HORMONES AND RELATED SUBSTANCES, 1962 ONLY/CC

NOTE THIS SECTION COVERS THE BIOCHEMISTRY,  
PHYSIOLOGY, PHARMACOLOGY, TOXICOLOGY, ANALYSIS,  
STRUCTURE, PROPERTIES, ISOLATION, PURIFICATION,  
TISSUE DISTRIBUTION, METABOLISM, AND MECHANISMS  
OF MAMMALIAN HORMONES, HORMONAL RECEPTORS, AND  
HORMONE-LIKE SUBSTANCES. THE MOLECULAR GENETICS  
OF HORMONES IS ALSO PLACED HERE. NONMAMMALIAN  
HORMONES IN NONMAMMALIAN SYSTEMS ARE COVERED IN  
SECTIONS 5 OR 12, PLANT HORMONES ARE PLACED IN  
SECTIONS 5 OR 11, AND HORMONE FORMULATIONS ARE  
IN SECTION 63. HORMONES IN PATHOLOGY AND IN



HNOTE SUBJECT WAS COVERED IN BROADER BIOLOGICAL  
CHEMISTRY SECTIONS 11A-11H DURING 1912-1961, AND  
11 BIOLOGICAL CHEMISTRY, 1907-1911 PRIOR TO  
1912.

\*\*\*\*\* END\*\*\*

# Suche mit dem Section Code

Hinweis: Verwenden Sie Wörter aus dem Sektionsnamen anstelle der Code-Nummer.

=> **S L5 AND HORMONE?/CC, SX**

L8 5773 L5 AND HORMONE?/CC, SX

=> **D SCAN**

L8 5773 ANSWERS HCAPLUS COPYRIGHT 2003 ACS

CC 2-0 (Mammalian **Hormones** )

Section cross-reference(s): 6

TI The dance of the clams: twists and turns in the family

C GPCR homodimer

ST review **G protein coupled receptor**

conformation **signaling**

# Screens (structure filters)

**Filter werden in zwei Situationen benötigt:**

- Wenn eine Suche die Systemgrenzen für die Struktursuche übersteigt.
- Zum Einschränken der Suche in Registry auf:
  - Z.B.: “no isotopes”, “no substances with rings”, “only polymers”



# Filter (Screens), die Strukturelemente definieren

- Kleine Strukturfragmente
  - Beispiel: C-CH<sub>2</sub>-C
- Anzahl bestimmter Elemente
  - Beispiel: 2 or more nitrogens
- Anzahl vorhandener Ringe
  - Beispiel: 3 or more rings
- Strukturmodifikationen
  - Beispiel: presence of a tautomer

# Filter (Screens), die keine Strukturelemente definieren

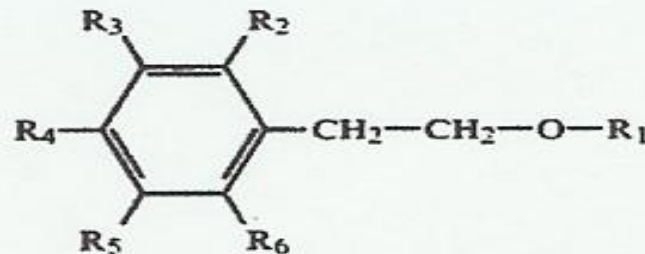
- Substanzklassen (Legierungen, Polymere, etc.)
- Substanzen mit mehr als eine Komponente
- Substanzen, die auch im File CASREACT aufgenommen wurden

# STN Express schlägt einige Filter automatisch vor

We claim:

1. A method of preparing a substituted phenethanol ether, comprising the step of reducing a corresponding substituted phenylglyoxal acetal by reacting said acetal with hydrogen in the presence of an acid catalyst and a metal catalyst.

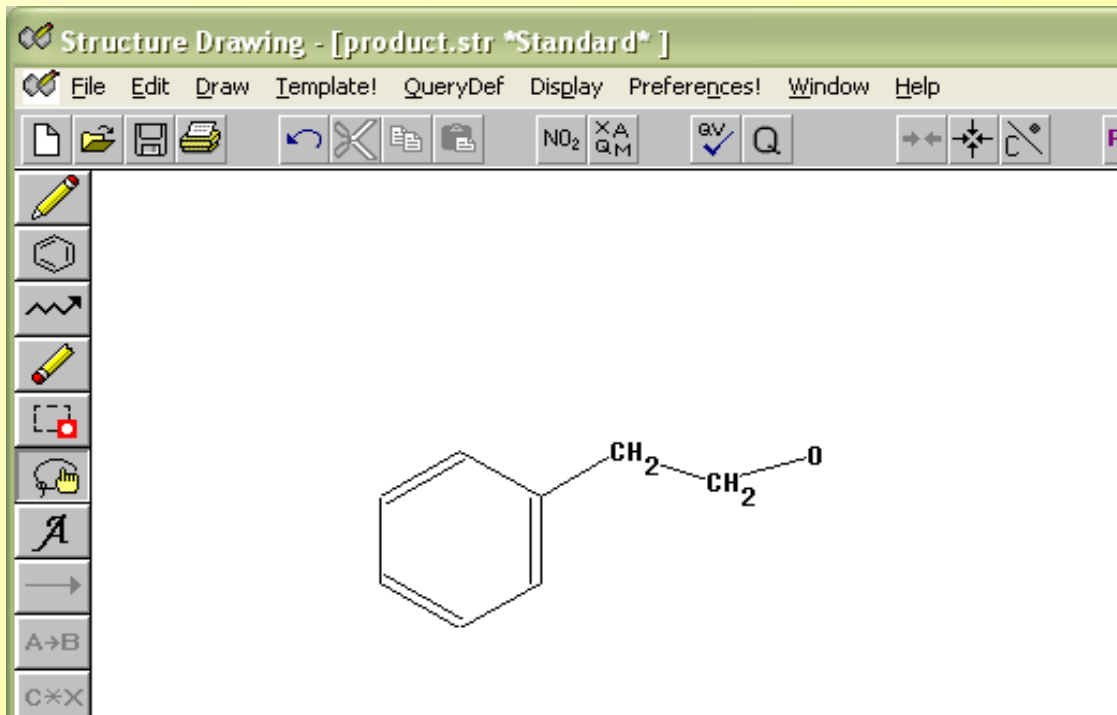
2. The method according to claim 1 wherein the phenethanol ether is of the formula



wherein  $R_1$  is a primary or a secondary alkyl group and  $R_2$ ,  $R_3$ ,  $R_4$ ,  $R_5$  and  $R_6$ , are independently hydrogen, an alkyl group, an unsubstituted or a substituted aryl group, a hydroxy group, an alkoxy group, an unsubstituted or a substituted aryloxy group, a halogen, a carboxylic acid group, a carboxylic acid derivative group, an acyloxy group, an aroyloxy group, an amino group, an alkyl substituted amino group, a substituted or an unsubstituted aryl substituted amino group.

In diesem Patent wurde eine sehr verallgemeinerte Struktur beansprucht.

# Folgende Struktur wird in STN Express gezeichnet



# Suche in Registry - sample search

=> FILE REGISTRY

=> S L1

SAMPLE SEARCH INITIATED 00:24:03 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 28953 TO ITERATE

3.5% PROCESSED 1000 ITERATIONS 50 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

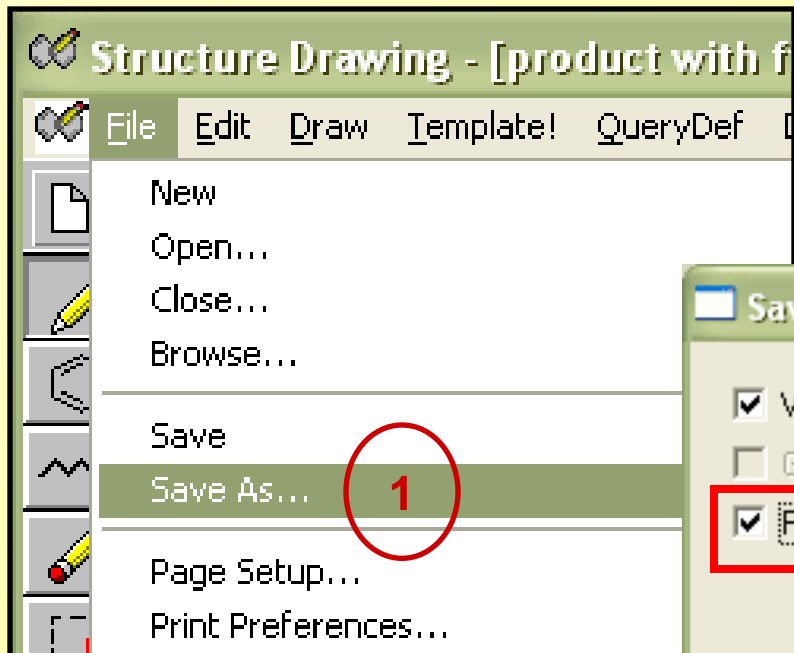
FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 568902 TO 589218

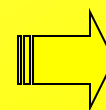
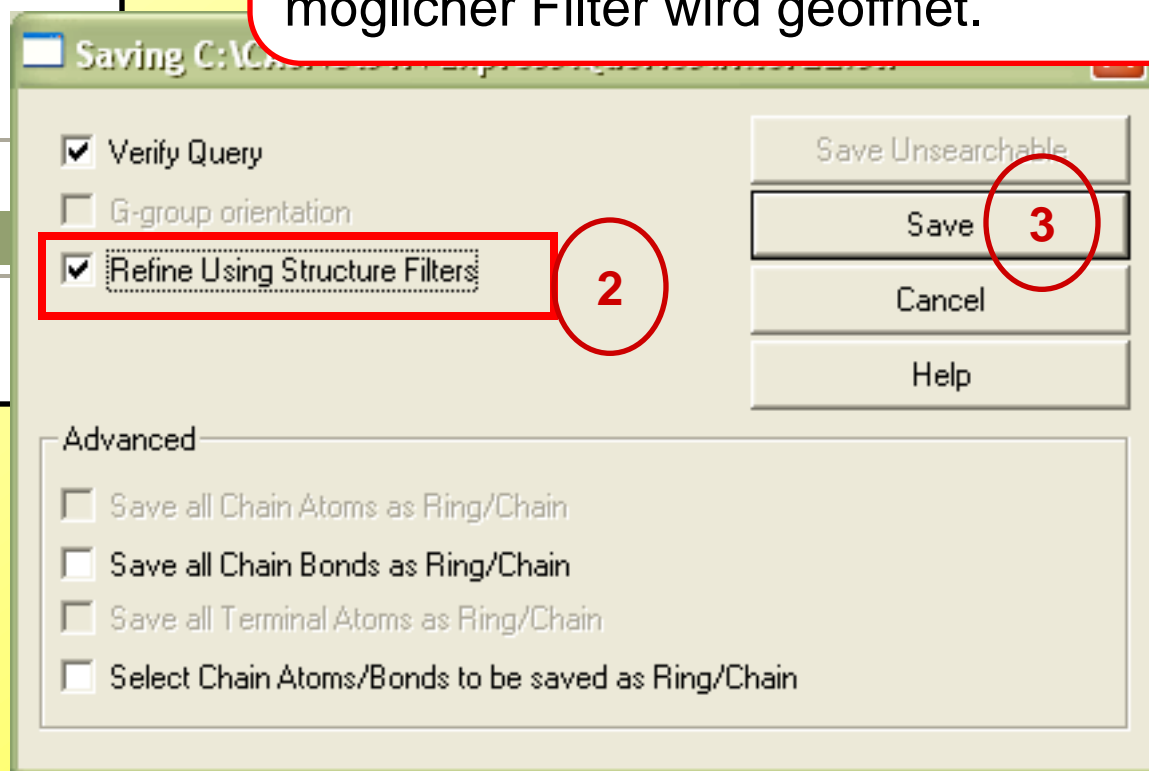
PROJECTED ANSWERS: 32802 TO 37842

L2 50 SEA SSS SAM L1

# Besser: Beim Abspeichern der Struktur "Refine Using Structure Filters" auswählen.



Refine Using Structure Filters ermöglicht die Auswahl geeigneter Filter für die Struktursuche. Die Liste möglicher Filter wird geöffnet.



# STN Express schlägt Filter vor oder man sucht sich geeignete Filter aus der Filter Liste aus.

Refine Using Structure Filters

AND NOT Remove Remove All Help

Filter List:

- 1 or more C-CH3
- 2 or more C-CH3
- 3 or more C-CH3
- 4 or more C-CH3
- C=CH2
- CH-triplebond-C
- C-CH2-C
- C-CH=C
- C-CH(C)-C

Selected Filters and Screens:

- » AND C-CH2-C

» Automatically selected by software

Remove Custom Screen

Add Custom Screen =>

Reanalyze Query

View Command File

Cancel Save

2050 - Alloy

2049 - Coordination Compound

2053 - Manual Registration

2052 - Mineral

2051 - Mixture

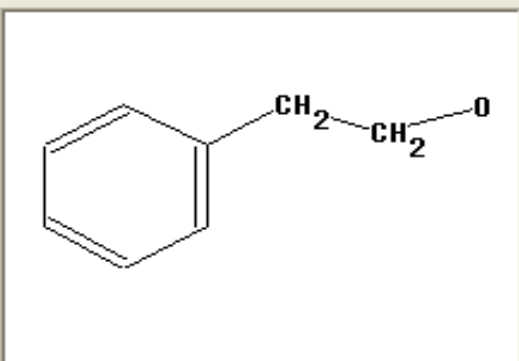
2043 - Polymer

2067 - Homopolymer or copolymer

2068 - Polymer that is a structure

2069 - Polymer that is a structure

2070 - Polymer that is a structure



# Beim Herunterladen der Struktur in Registry werden die ausgewählten Filter automatisch auf die Struktur gesetzt

```
=> .....Testing the current file..... screen  
ENTER SCREEN EXPRESSION OR (END):end
```

```
=> screen 1006  
L3      SCREEN CREATED
```

```
=>  
Uploading C:\CASNC\STN Express\Queries\product with  
filter.str  
L4      STRUCTURE UPLOADED
```

```
=> que L4 AND L3
```

```
L5      QUERY CREATED
```

```
=> S L5
```

Erfolgt automatisch beim "upload" in Registry. Die erzeugte Query muss nur noch gesucht werden.



# Struktursuche - sample search

=> S L5

SAMPLE SEARCH INITIATED 00:35:24 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 16518 TO ITERATE

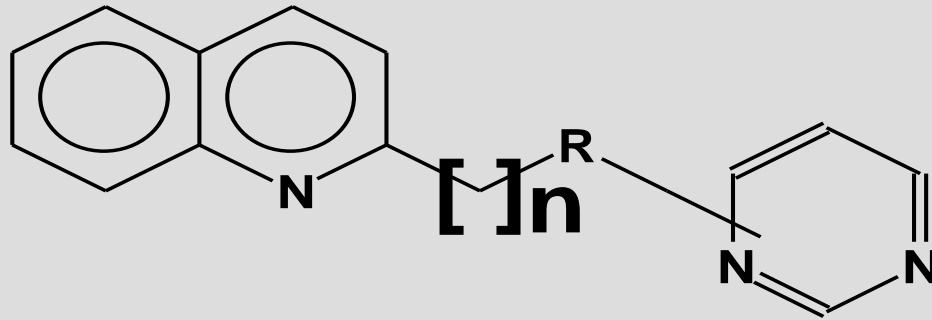
6.1% PROCESSED          1000 ITERATIONS          50 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*  
                              BATCH        \*\*COMPLETE\*\*  
PROJECTED ITERATIONS:        322671 TO        338049  
PROJECTED ANSWERS:            32509 TO        37527

L6                            50 SEA SSS SAM L4 AND L3

# Verwendung Element spezifischer Filter.

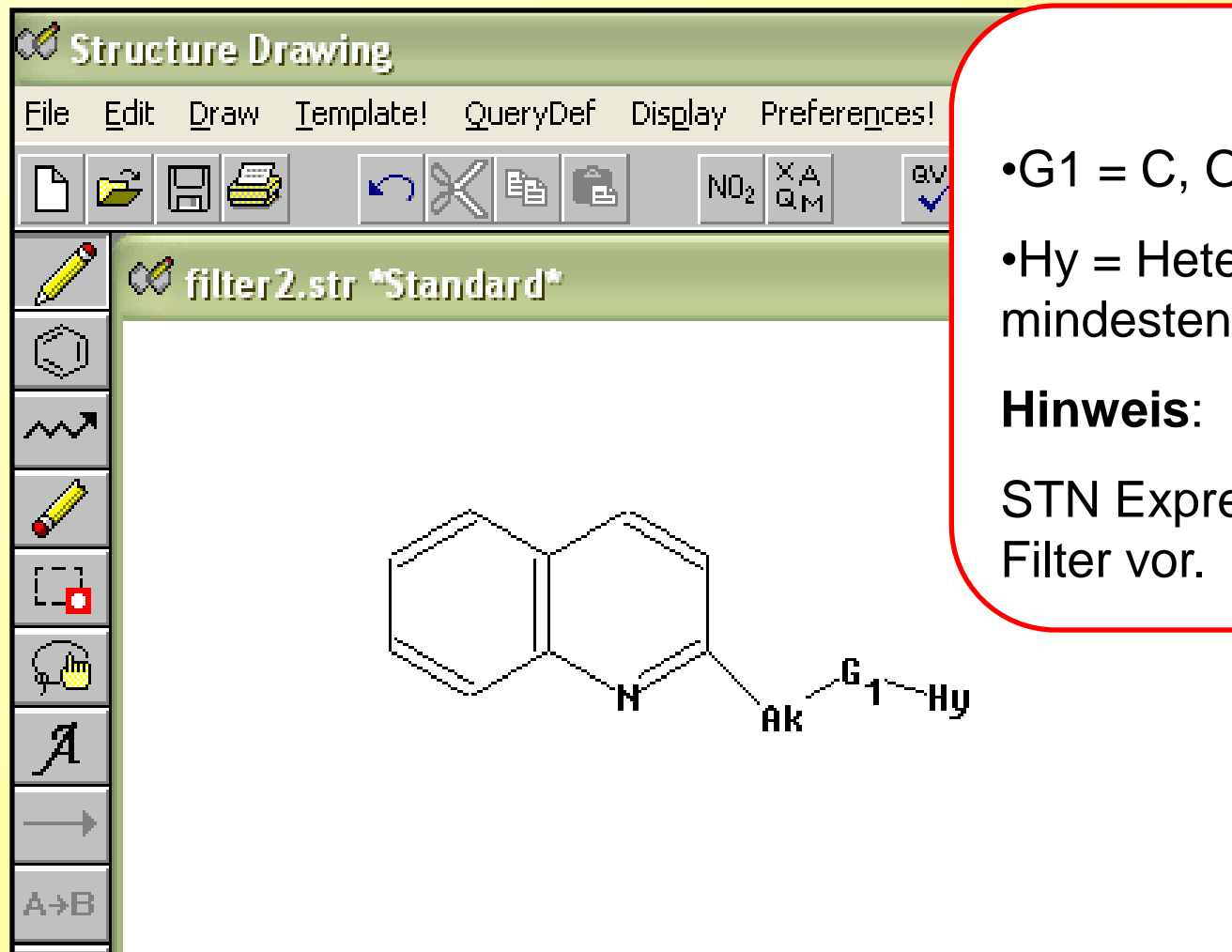
What is claimed is:



$n = 1-20$

$R = N, O, S, C$

# STN Express Struktur



•G1 = C, O, N, S

•Hy = Heterozyklus mit mindestens 2 Stickstoff

**Hinweis:**

STN Express schlägt keine Filter vor.

# Lösung: Element Count Filter

- Stehen für die häufig vorkommenden Elemente zur Verfügung
  - C, N, O, P, S, Si
  - Cl, Br, F, I
- Für die Variablen
  - X = Halogen
  - M = Metall
- Filter können eingeschlossen werden - **AND**
- Filter können ausgeschlossen werden - **NOT**

# Auswahl des Element Count Filters

Refine Using Structure Filters

AND NOT Remove Remove All Help

Filter List: Selected Filters and Screens:

(Any sized ring/ring system)-NH2  
4 or more C  
6 or more C  
8 or more C  
10 or more C  
12 or more C  
14 or more C  
16 or more C  
18 or more C

AND 3 or more N  
AND 8 or more C

» Automatically selected by software

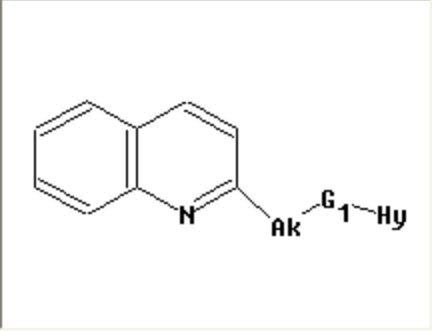
Remove Custom Screen  
Add Custom Screen =>  
Reanalyze Query  
View Command File  
Cancel Save

2050 - Alloy  
2049 - Coordination Compound  
2053 - Manual Registration  
2052 - Mineral  
2051 - Mixture  
2043 - Polymer  
2067 - Homopolymer or copolymer  
2068 - Polymer that is a structure  
2069 - Polymer that is a structure  
2070 - Polymer that is a structure

1

2

3

C1=CN2C=CC=CC=C12AkG1Hy

# Struktursuche mit ausgewählten Screens.

```
=> .....Testing the current file..... screen  
ENTER SCREEN EXPRESSION OR (END):end
```

```
=> screen 1994 AND 1944
```

```
L3      SCREEN CREATED
```

```
=>
```

```
Uploading C:\CASNC\STN Express\Queries\filter2.str  
L4      STRUCTURE UPLOADED
```

```
=> que L4 AND L3
```

```
L5      QUERY CREATED
```

```
=> S L5
```

# Sample Search

=> S L5

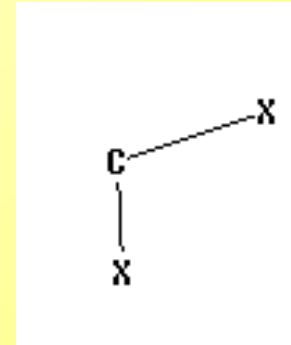
SAMPLE SEARCH INITIATED 00:58:54 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 13248 TO ITERATE

7.5% PROCESSED 1000 ITERATIONS 3 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 258070 TO 271850  
PROJECTED ANSWERS: 416 TO 1172

L6 3 SEA SSS SAM L4 AND L3

Beispiel: Folgende Carbene werden gesucht



Struktur zeichnen  
und über „Query  
Definition“ – „Other  
Node Attributes“ die  
Valenz von „2“ auf  
das C-Atom setzen

**Other Node Attributes**

Charge:

Valency:

Any  
 Specific  
 Abnormal

Isotope:  Any (1 to 255):   
 Specific  
 Abnormal



L1            STRUCTURE UPLOADED

=> s L1

SAMPLE SEARCH INITIATED 14:31:21

SAMPLE SCREEN SEARCH COMPLETED -    264677 TO ITERATE

0.8% PROCESSED            2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*INCOMPLETE\*\*

BATCH        \*\*INCOMPLETE\*\*

PROJECTED ITERATIONS:            5263409 TO    5323671

PROJECTED ANSWERS:                    0 TO            0

Und was jetzt ?????

# Struktur unter Verwendung des geeigneten Filters abspeichern

**Refine Using Structure Filters**

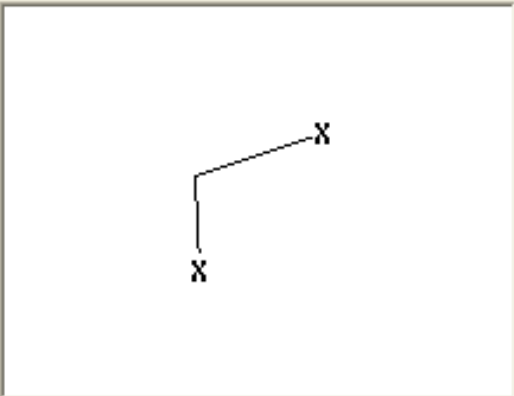
AND NOT Remove Remove All Help

Filter List: Selected Filters and Screens:

- 5 or more rings
- Presence of an isotope
- Presence of a charge
- Presence of an element with an abnormal valency
- Presence of a delocalized charge
- Presence of one or more deuterium
- Presence of one or more tritium or higher hydrogen isotope
- Presence of an isotope at an unknown location
- Presence of a tautomer

AND Presence of an element with an abnormal valency

» Automatically selected by software



Remove Custom Screen

Add Custom Screen =>

Reanalyze Query

View Command File

Cancel Save

- 2050 - Alloy
- 2049 - Coordination Compound
- 2053 - Manual Registration
- 2052 - Mineral
- 2051 - Mixture
- 2043 - Polymer
- 2067 - Homopolymer or copolymer
- 2068 - Polymer that is a structure
- 2069 - Polymer that is a structure
- 2070 - Polymer that is a structure

L3 STRUCTURE UPLOADED

=> que L2 AND L3

L4 QUE L2 AND L3

=> s L4

SAMPLE SEARCH INITIATED 14:30:29

SAMPLE SCREEN SEARCH COMPLETED - 75316 TO ITERATE

2.7% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 1489965 TO 1522675

PROJECTED ANSWERS: 0 TO 0

=> s L4 ful

L5 60 SEA SSS FUL L2 AND L3

=> s L5 and 1/NC

L6 38 L28 AND 1/NC

=> d

L6 ANSWER 1 OF 38 REGISTRY COPYRIGHT 2009 ACS on STN  
RN 1181864-66-3 REGISTRY  
ED Entered STN: 09 Sep 2009  
CN INDEX NAME NOT YET ASSIGNED  
MF C Br F  
SR CA  
LC STN Files: CAPLUS

Br — 8 1 C — F

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)