

HOW TO

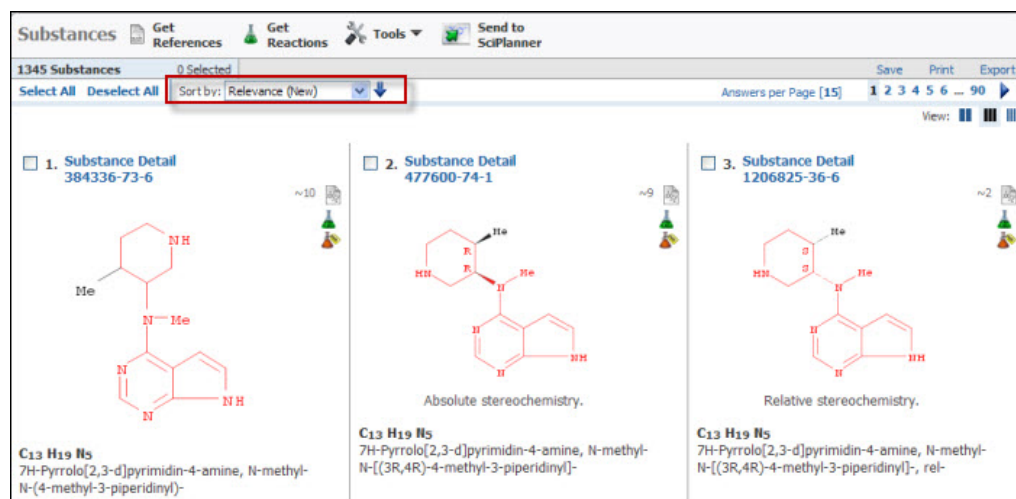
Use the New Features



Enhancements in the December 2011 SciFinder update include relevance ranking of substance answer sets, additional mass spec and NMR data for ~75,000 substances, new streamlined display formats for references and substances, and the introduction of bioactivity and target indicators to substance detail displays and substance Analyze options. With bioactivity and target indicators, you can use SciFinder to easily assess the biological relevance of substances in early stage discovery efforts.

Relevance Ranking of Substance Answer Sets

1. Structure search answer sets are now automatically sorted by relevance, so you can quickly review your answer set and access the most relevant substances first.
2. This is the default **Sort** option for structure search answers.



The screenshot displays the SciFinder interface with the following details:

- Top navigation: Substances, Get References, Get Reactions, Tools, Send to SciPlanner.
- Search results: 1345 Substances, 0 Selected.
- Sort dropdown: **Sort by: Relevance (View)** (highlighted with a red box).
- Answers per Page: [15], with options 1, 2, 3, 4, 5, 6, ..., 90.
- Three substance detail cards are shown:

Substance ID	Chemical Structure	Notes
1. Substance Detail 384336-73-6		
2. Substance Detail 477600-74-1		Absolute stereochemistry.
3. Substance Detail 1206825-36-6		Relative stereochemistry.

Bioactivity and Target Indicators

In Substance Detail Display

Quickly find the bioactivity (e.g., antibiotic, vasoconstrictor) and target (e.g., alpha-amylase, prostate-specific antigen) indicators of a specific substance or an entire substance answer set. Click the Indicator of interest to see the associated reference(s).

Return

CAS Registry Number: 28911-01-5
C₁₇ H₁₂ Cl₂ N₄
4H-[1,2,4]Triazolo[4,3-a][1,4]benzodiazepine, 8-chloro-6-(2-chlorophenyl)-1-methyl-
4H-s-Triazolo[4,3-a][1,4]benzodiazepine, 8-chloro-6-(o-chlorophenyl)-1-methyl- (8Cl); 8-Chloro-1-methyl-6-(o-chlorophenyl)-4H-s-triazolo[4,3-a][1,4]benzodiazepine; D II-18-2; Halcion; Novodorm; Songar; Triazolam; U 33030

CN1CC2=NC=NC=C2N1C3=CC=C(Cl)C=C3Cl

~1,742 References

CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study	✓	✓	✓	✓
Biological Study	✓	✓	✓	✓
Formation, Nonpreparative	✓	✓	✓	✓
Preparation	✓	✓	✓	✓
Properties	✓	✓	✓	✓
Prophetic in Patents	✓			
Reactant or Reagent	✓	✓		
Uses	✓	✓	✓	✓

Bioactivity Indicators NEW

	References
Nervous system agents (all) >> Hypnotics and Sedatives	149
Nervous system agents (all) >>> Antidepressants	47
Nervous system agents (all) >>>> Antipsychotics	27
Nervous system agents (all) >> Anxiolytics	64

Target Indicators NEW

	References
Enzymes (all) >>> Monoamine oxidase	13
Hemoproteins (all) >>> Cytochrome P 450	27
Hemoproteins (all) >>> Cytochrome P 450 3A4	38
Receptors (all) >>> GABAA receptors	48
Receptors (all) >>>> 5-HT receptors	11
Receptors (all) >>>>> Benzodiazepine	43

In Analyze Options

Use the new Analyze options to narrow an answer set to substances based on bioactivity or target indicator information of interest.

Substances 890 Substances 0 Selected

Get References Get Reactions Tools Send to SciPlanner

Select All Deselect All Sort by: Relevance (New) Answers per Page [15] 1 2 3 4 5 6 ... 60

View: [Icons]

1. Substance Detail 384336-73-6

CN1CC2=NC=NC=C2N1C3=CC=C(Cl)C=C3Cl

C₁₃ H₁₉ N₅
7H-Pyrrolo[2,3-d]pyrimidin-4-amine, N-methyl-N-(4-methyl-3-piperidinyl)-

2. Substance Detail 477600-74-1

CN1CC2=NC=NC=C2N1C3=CC=C(Cl)C=C3Cl

Absolute stereochemistry.
C₁₃ H₁₉ N₅
7H-Pyrrolo[2,3-d]pyrimidin-4-amine, N-methyl-N-[(3R,4R)-4-methyl-3-piperidinyl]-

3. Substance Detail 1206825-36-6

CN1CC2=NC=NC=C2N1C3=CC=C(Cl)C=C3Cl

Relative stereochemistry.
C₁₃ H₁₉ N₅
7H-Pyrrolo[2,3-d]pyrimidin-4-amine, N-methyl-N-[(3R,4R)-4-methyl-3-piperidinyl]-, rel-

Analysis Refine

Analyze by: [Dropdown]

- Bioactivity Indicators (New)
- Bioactivity Indicators (New)
- Commercial Availability
- Elements
- Reaction Availability
- Substance Role
- Target Indicators (New)

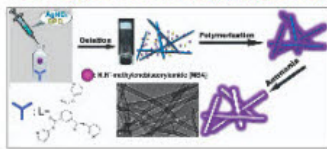
Anti-inflammatory agents (all)	314
Immune agents (pharmaceutical)	293
Respiratory system agents (all)	286
Antidiabetic agents	285
Nervous system agents (all)	285
Enzyme inhibitors (all)	20

Simplified Reference Answer Set Displays

(Table of Contents Graphics from ACS Publications)

1. Access full text and related information such as substances and citing references with simplified reference displays.
2. Preview more journal content with Table of Contents graphics from ACS Publications.

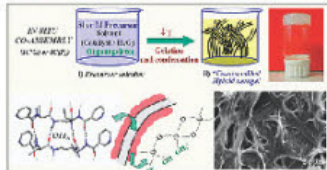
2. **Silver(I)-coordinated organogel-templated fabrication of 3D networks of polymer nanotubes** [Full Text](#)



By Chen, Kai; Tang, Liming; Xia, Yu; Wang, Yujiang
From Langmuir (2008), 24(24), 13838-13841. | Language: English, Database: CAPLUS

Organo gels comprising 3D networks of self-assembled fibers have long been employed to transcribe the fibrous structure into inorg. nanotubes; however, herein organogel has been used to access polymer nanotubes. The organogel induced by crosslinking between a tripodal ligand and Ag(I) possesses high thermal stability, which makes it suitable for in situ polymn. at elevated temp. The silver ions in the gel can attract monomeric capping agent added, responsible for the adhesion of polymd. product onto gel fibers. In situ polymn. is followed by ammonia treatment to produce polymer nanotubes that are directly organized into 3D superstructures.

3. **Inorganic and Hybrid Nanofibrous Materials Templated with Organogelators** [Full Text](#)

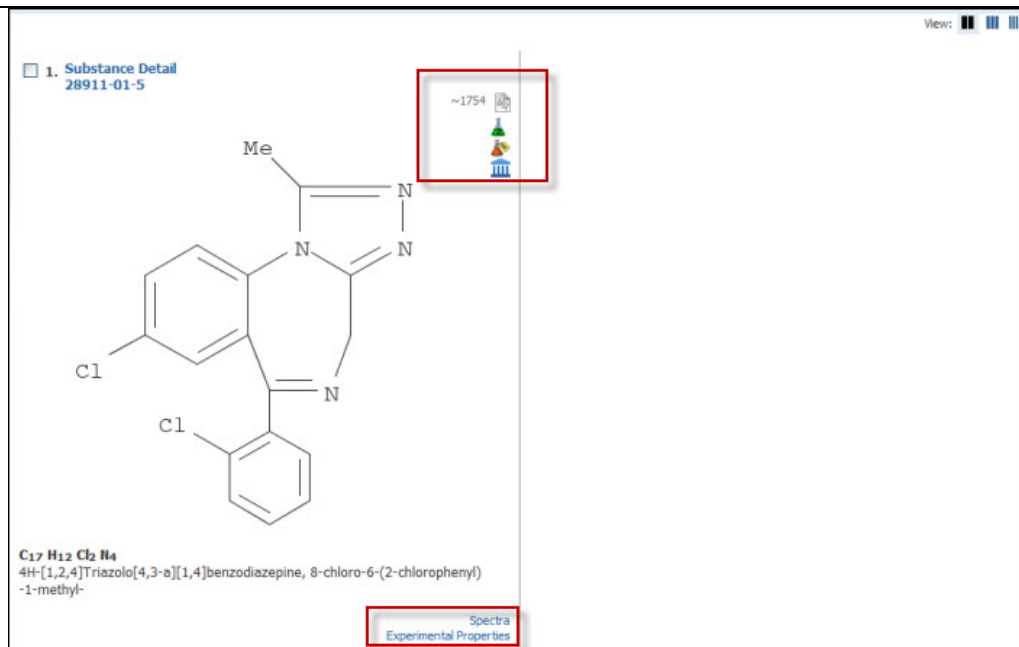


By Ulsar, Mario; Sanchez, Clement
From Chemistry of Materials (2008), 20(3), 782-820.
| Language: English, Database: CAPLUS

A review. This article presents a general overview about the designed synthesis of one-dimensional (1-D) inorg. and org.-inorg. hybrid fibrous nanostructures templated through the use of organogelator-based supramol. assemblies. The growing no. of structural families and derivs. of low-mol.-wt. organogelators (LMOGs) already used as templates for materials transcription are first presented, including a detailed compilation with relevant information about the gelation properties and the morphologies of their resulting self-assembled fibrillar networks (SAFINs). The main types of intermol. interactions responsible for the gel-phase formation and some of the principal variables governing the gelation process and controlling the obtained fibrous morphologies (fibers, rods, ribbons, helices, tubes, etc.) are also discussed. After highlighting the most important processing methodologies that are available for materials transcription through organogel templates (coassembly, post-transcription, or self-templating procedures), the manuscript presents an updated description of the different inorg. (silica-based, other metal oxides, nonoxides) and org.-inorg. hybrid fibrous materials so far templated by using these approaches. The key mechanistic aspects and different templating pathways involved in the transcription process are also discussed, concluding with a final discussion about challenging aspects or future prospects in this field.

Streamlined Substance Displays

1. Related information such as references, reactions, commercial sources, and regulatory information are now displayed next to the substance.
2. Link to the Spectra and Experimental Properties sections in the Substance Detail Display.



Additional ¹³C and ¹H NMR spectra and mass spectra

With the addition of approximately 79,000 ¹³C, ¹H NMR spectra and mass spectra from Bio-Rad, you can access and display more experimental substance property information than ever before.