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SciFinder^{n}

New premier CAS solutions to explore chemistry including MethodsNow, PatentPak

Veli-Pekka Hyttinen

Budapest, September 19, 2018

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ACS Chemistry for Life®

CAS Mission

To provide the world's best digital research environment to search, retrieve, analyze and link chemical information.

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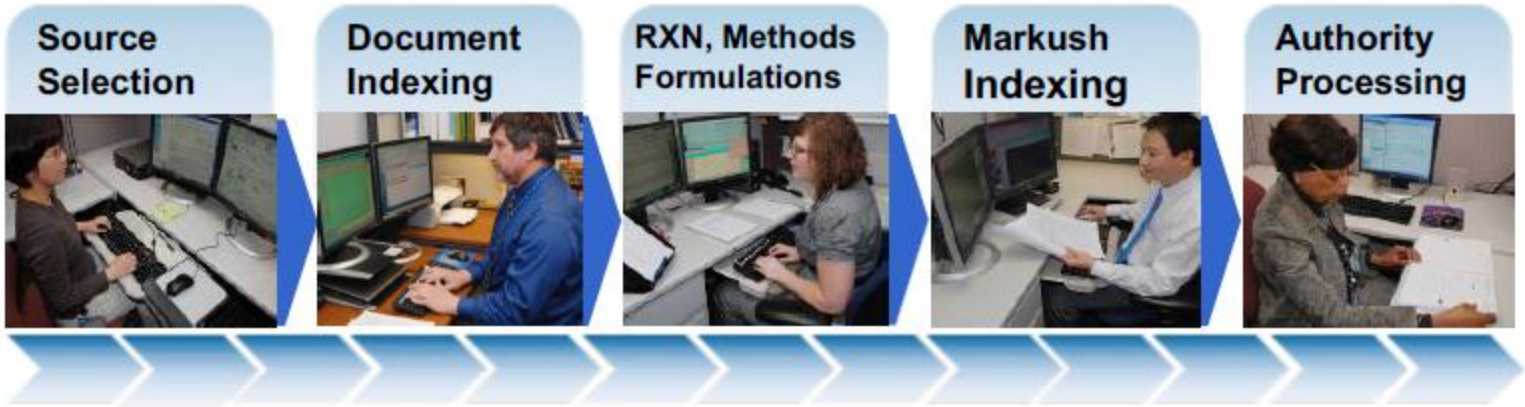
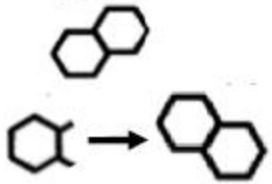
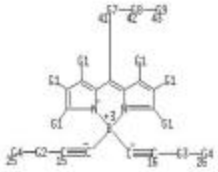
CAS indexing process



1990
Smith, M.
anthracene





Androst-4-en-3-one, 17-hydroxy-17-methyl-, (17β)-

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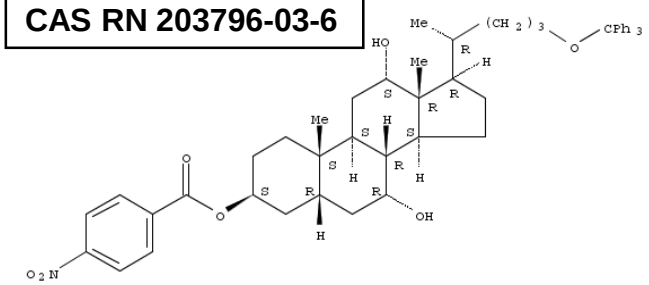
CAS scientists find the chemistry, and save you time!

Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste. Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 mmol) were dissolved in THF (50 mL) and added to the paste. The resulted mixture was stirred at ambient temperature overnight. Water (100 mL) was added and the mixture was made slightly basic by adding $NaHCO_3$ solution followed by extraction with EtOAc (3x50 mL). The combined extracts were washed with brine once and dried over anhydrous Na_2SO_4. The desired product (2.72 g, 85% yield) was obtained as white powder after SiO_2 chromatography (Et_2O/hexanes 1:2). m.p. 207-209 °C.; IR (KBr) 3434, 3056, 2940, 2868, 1722, 1608, 1529,1489, 1448, 1345 cm^{-1} ; ^1H NMR ($CDCl_3$, 300 MHz) δ 8.30-8.26 (m, 2 H), 8.21-8.16 (m, 2 H), 7.46-7.42 (m, 6 H), 7.31-7.18 (m, 9 H)5.33 (bs, 1 H), 4.02 (bs, 1 H), 3.90 (bs, 1 H), 3.09-2.97 (m, 2 H), 2.68 (td, J=14.95, 2.56 Hz, 1 H), 2.29-2.19 (m, 1 H), 2.07-1.06 (series of multiplets, 24 H), 1.01 (s, 3 H), 0.98 (d, J=6.6 Hz, 3 H), 0.70 (s, 3 H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 164.21, 150.56, 144.70, 136.79, 130.77, 64.22, 47.79, 46.79, 42.1 28.74, 27.71, 26.85, 26.3 (thioglycerol+Na^+ matrix

CAS RN 203796-03-6



Absolute stereochemistry.

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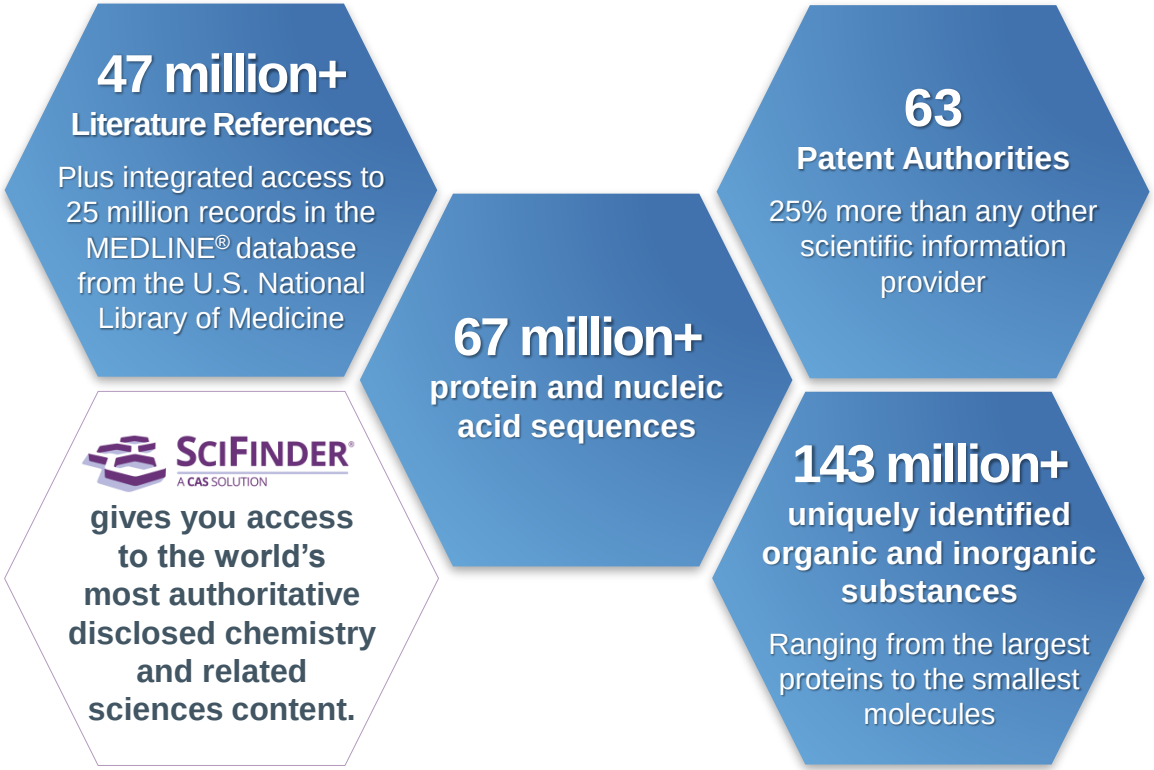
CAS analyzes the world's disclosed research to keep SciFinder the most valuable tool supporting your organization's research enterprise



Data as of March 2016

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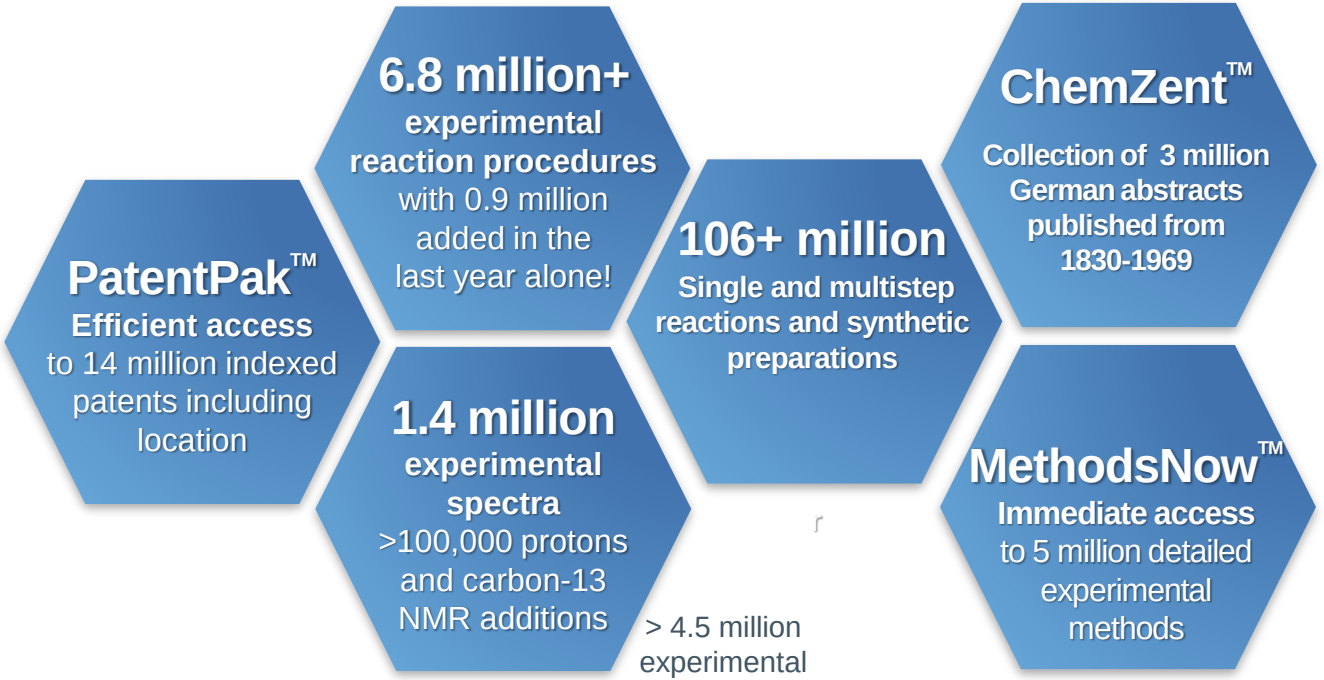
SciFinder saves you time by delivering valuable information to advance your research



Data as of March 2016

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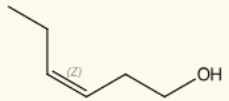
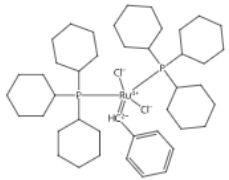
Key Substances in Patent

CAS RN
928-96-1



Analyst Markup Locations (2)
Page 14
Page 24

CAS RN
172222-30-9



Analyst Markup Locations (1)
Page 24

inlet and a septum. The monomer was degassed under vacuum for one hour. The contents of the reaction vessel was then kept under an argon atmosphere. Distilled cis-3-hexen-1-ol (0.13 grams, 1.35 mmoles, 0.16 ml) was added by syringe. Methylene chloride (40 ml) was sparged for 15 minutes with a vigorous stream of argon and then cannula transferred into the resin kettle. The monomer / solvent solution was stirred vigorously. In an argon filled drybox, ruthenium catalyst, phenylmethylene bis(tricyclohexylphosphine) dichloride (0.11 grams, 0.141 mmoles), was weighed into a septum capped glass vial and dissolved in 10 ml of methylene chloride. The catalyst solution was injected via syringe into the reaction vessel. The reaction mixture was heated and maintained at 40°C while being vigorously stirred under an argon atmosphere for 24 hours. The reaction mixture was then cooled to ambient temperature. A mixture of ethyl vinyl ether (2.92 grams, 3.9 ml, 40.4 mmoles)

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- Largest single collection of scientific method information
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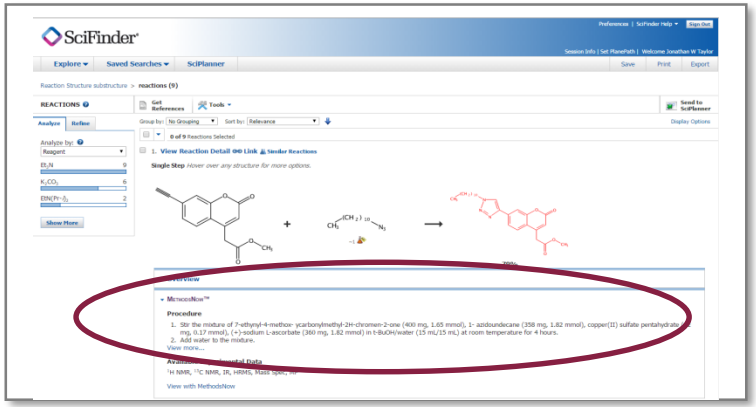
Synthetic chemist looking for great methods? They are in SciFinder.



- **Analytical methods in separate database: www.MethodsNow.com**

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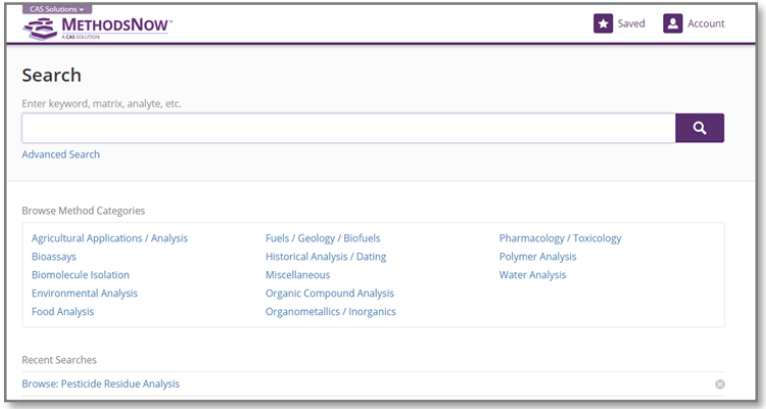

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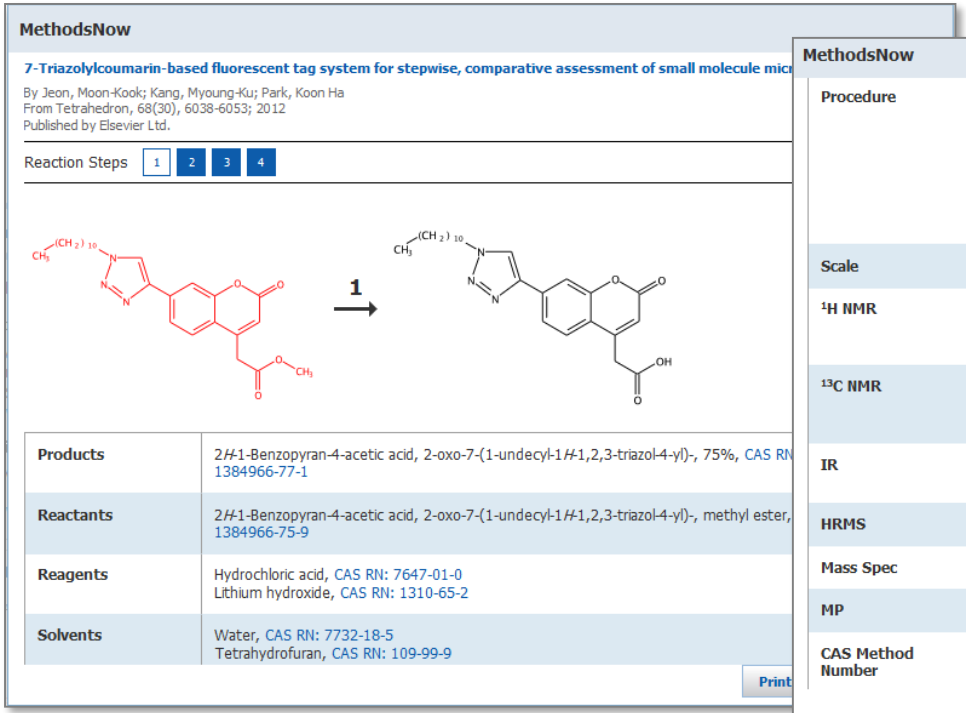
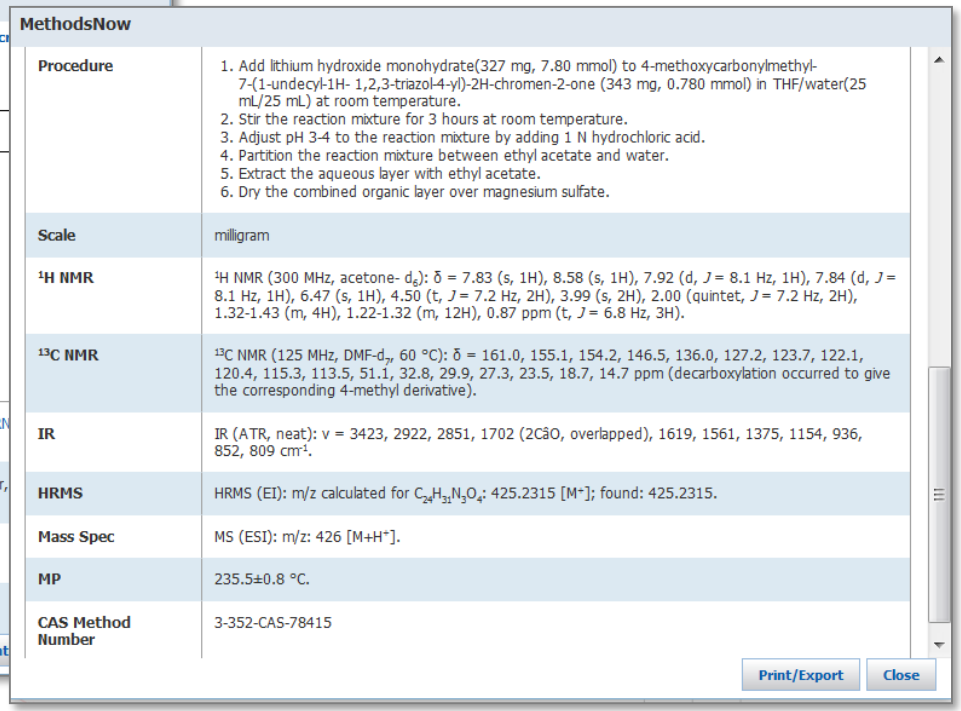
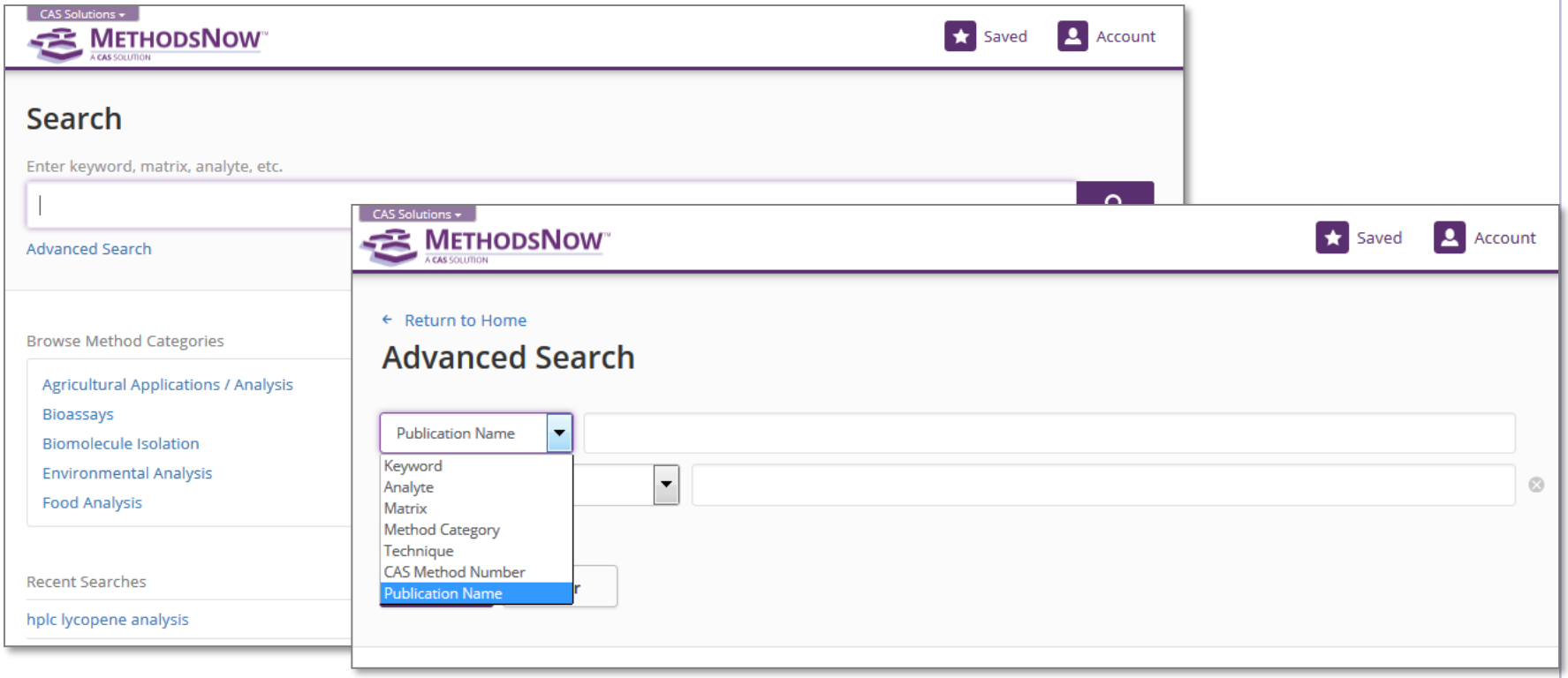
Synthesis – Step-by-step experimental protocols in SciFinder





MethodsNow – Analytical Scientist Interface



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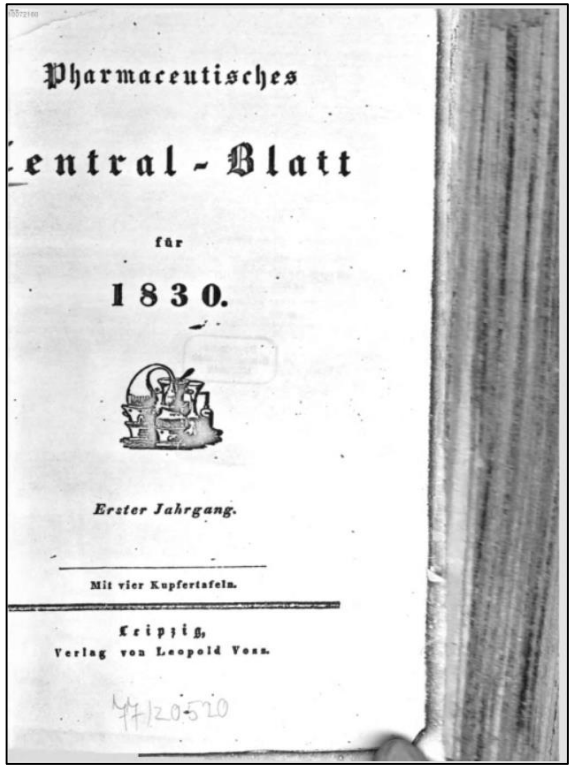
Chemisches Zentralblatt predates the introduction of Chemical Abstracts by almost 80 years

- Published German language abstracts from 1830-1969
- Chronicles the birth of chemistry as a science
  - Before 1800, chemistry was more alchemy (i.e. how to turn lead into gold) than actual science
- Searchable substance structures in 3 million machine translated abstracts


Pharmaceutisches

entral - Blatt

für

1830.

Erster Jahrgang.

Mit vier Kupfertafeln.

Leipzig,
Verlag von Leopold Voss.

First Issue: Note, the name changed several times before 1856

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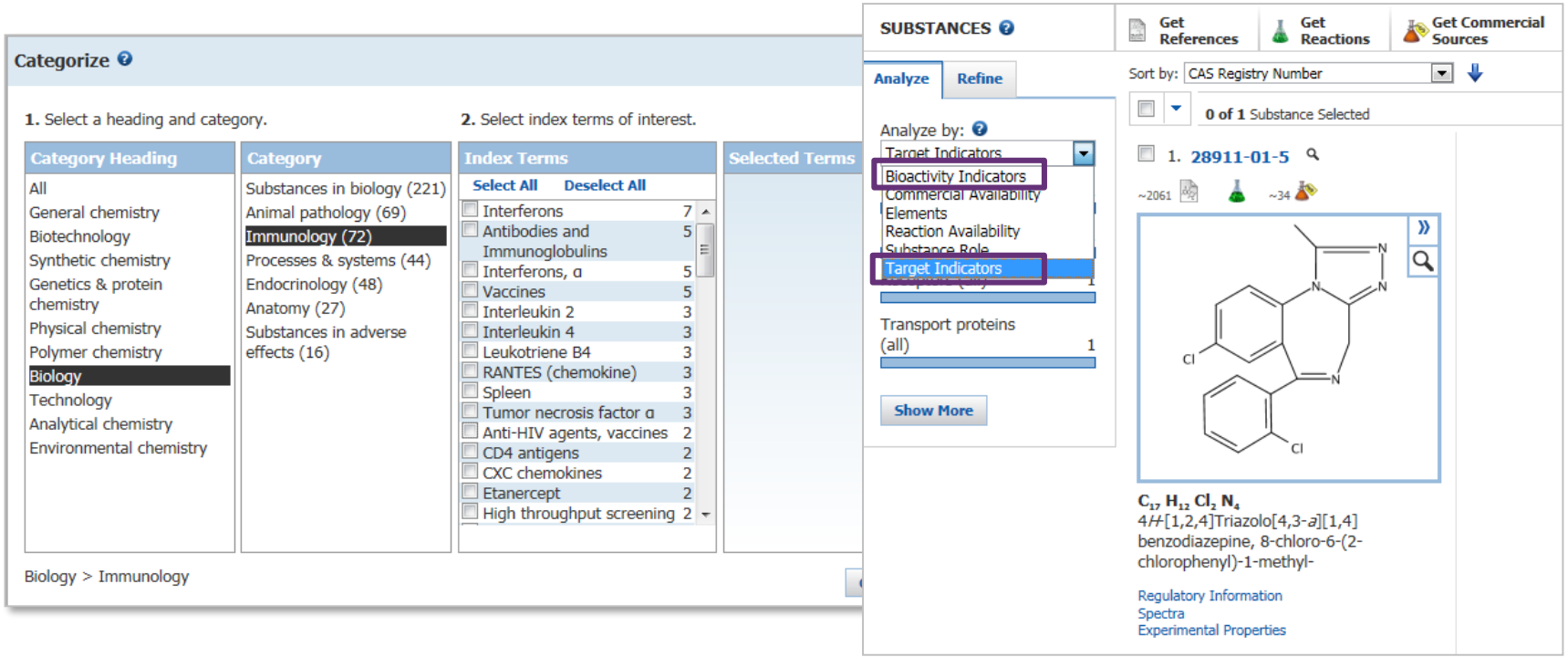
Categorize and analyze options make it easy to find relevant information



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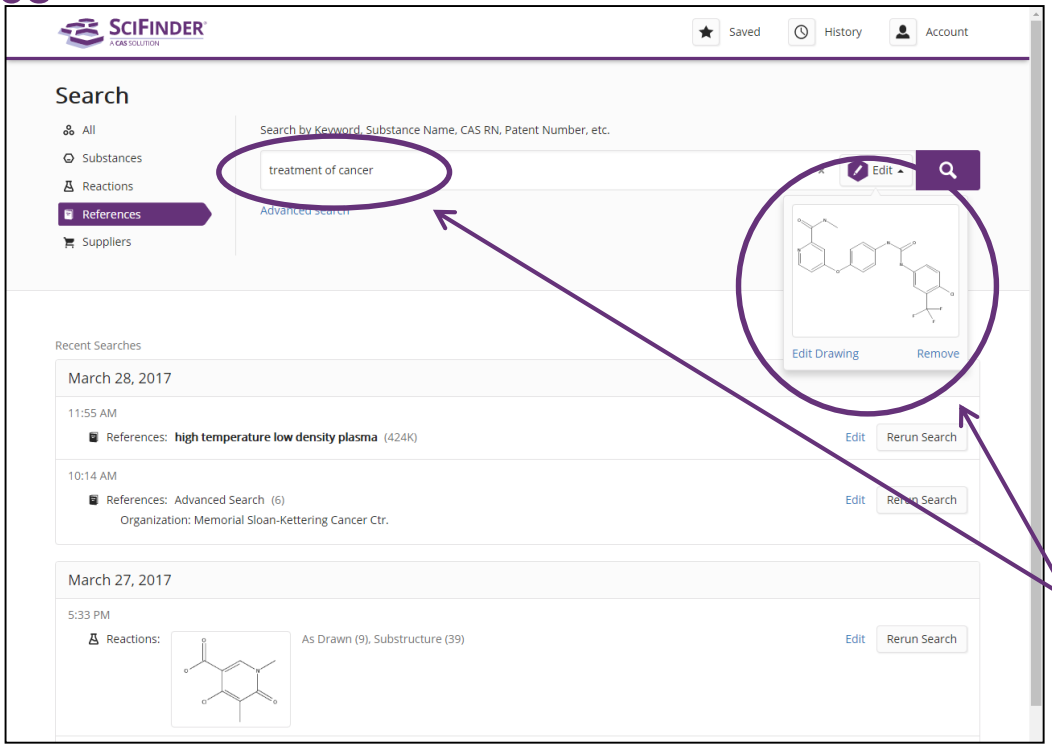
SciFinder-n Get to actionable results more quickly with a streamlined new interface

Streamlined search navigation saves you clicks

Immediately run past searches



More conveniently search structures and text

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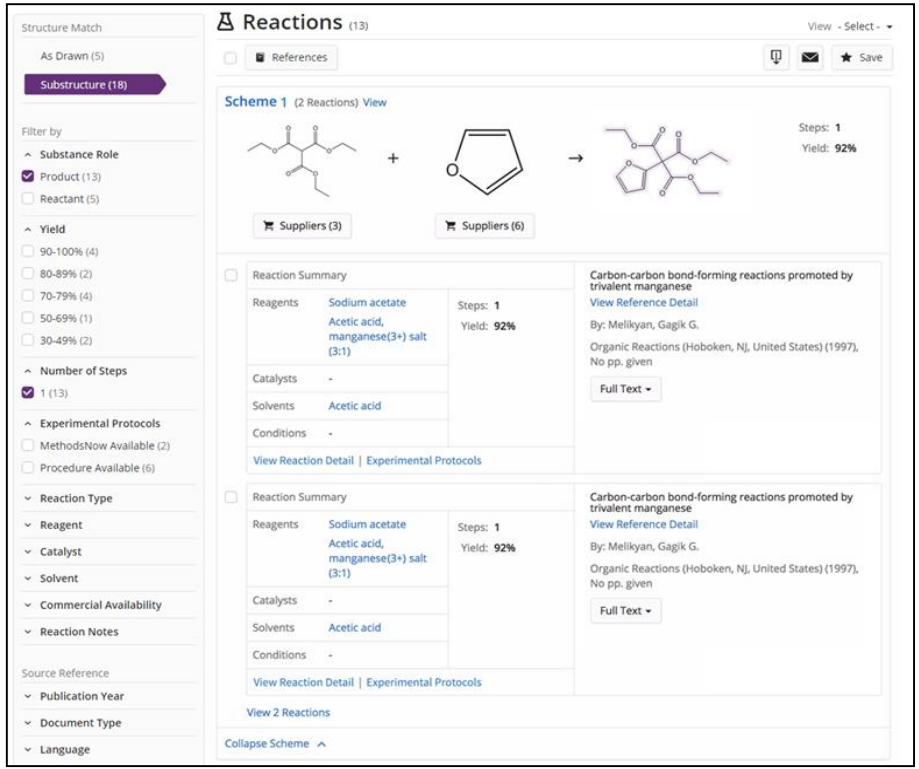
Powerful filtering capabilities allow rapid focus



Intuitive information layouts fosters quick comprehension

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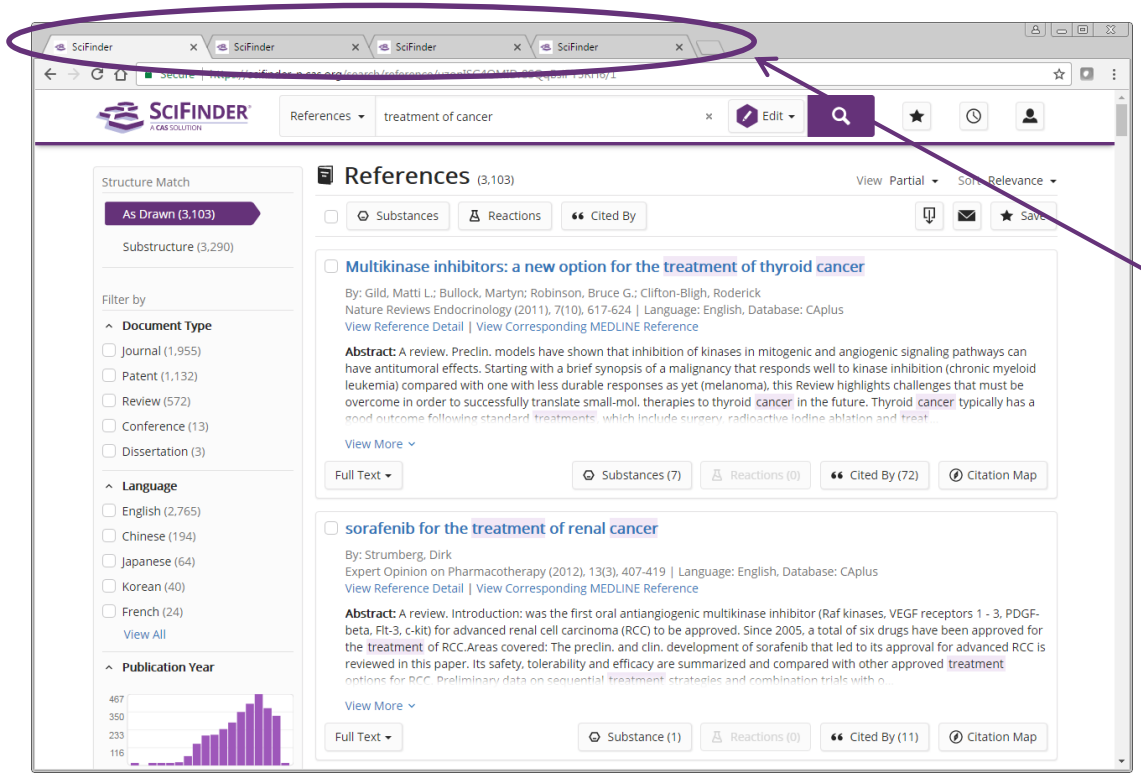
One idea can lead you to another - SciFinder^{n} has you covered!



Simultaneous searches can be performed in new browser/windows

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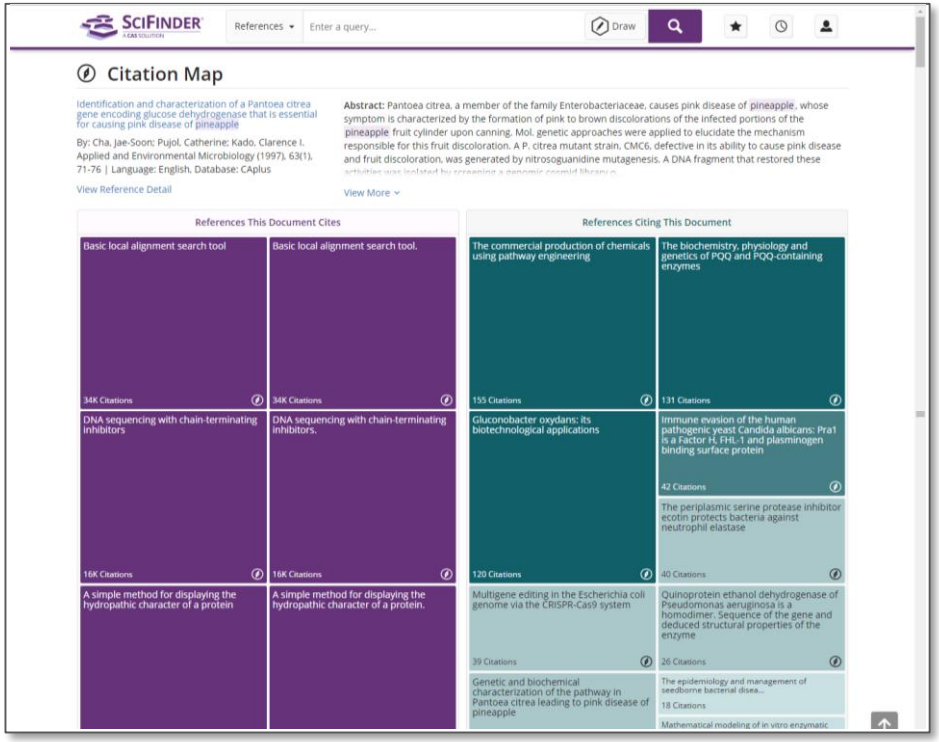
SciFinder-n Citation Mapping helps you understand where to go next in your literature review



Interactive map allows speedy identification of important research (maybe even that one paper you wouldn't otherwise find!)

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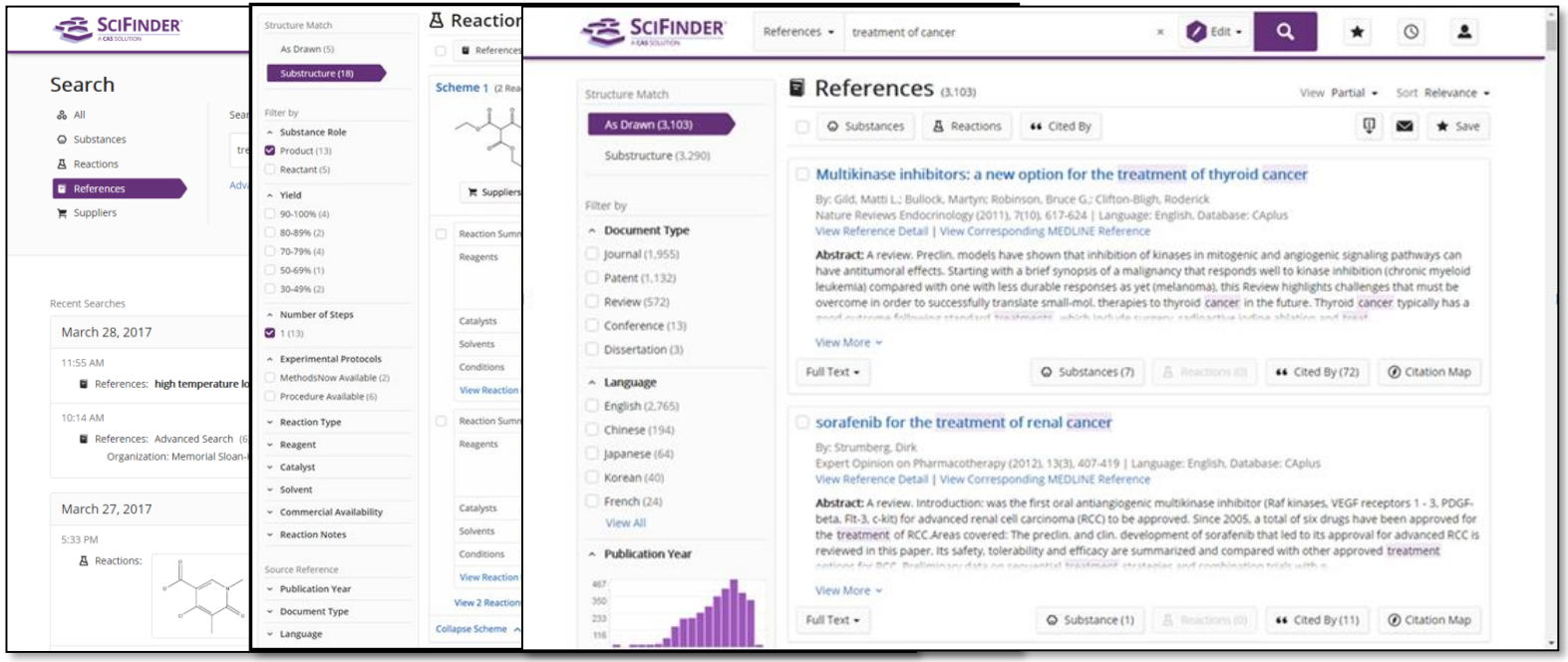
A product portfolio that emphasizes investment in AI and scalability – with a focus on speed and cost



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Questions?

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Every day at CAS hundreds of scientists analyze the world's disclosed scientific discoveries and, leveraging the latest technologies, infuse insights to deliver answers.

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