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Veli-Pekka Hyttinen

May 23, 2018

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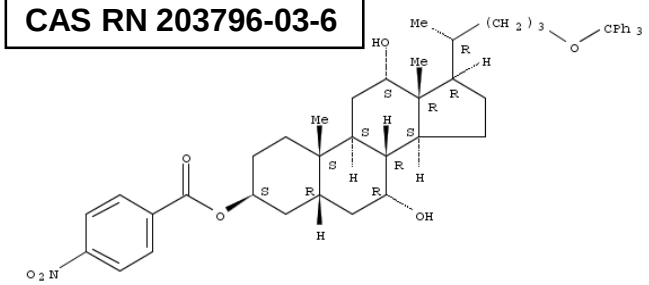
Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste. Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 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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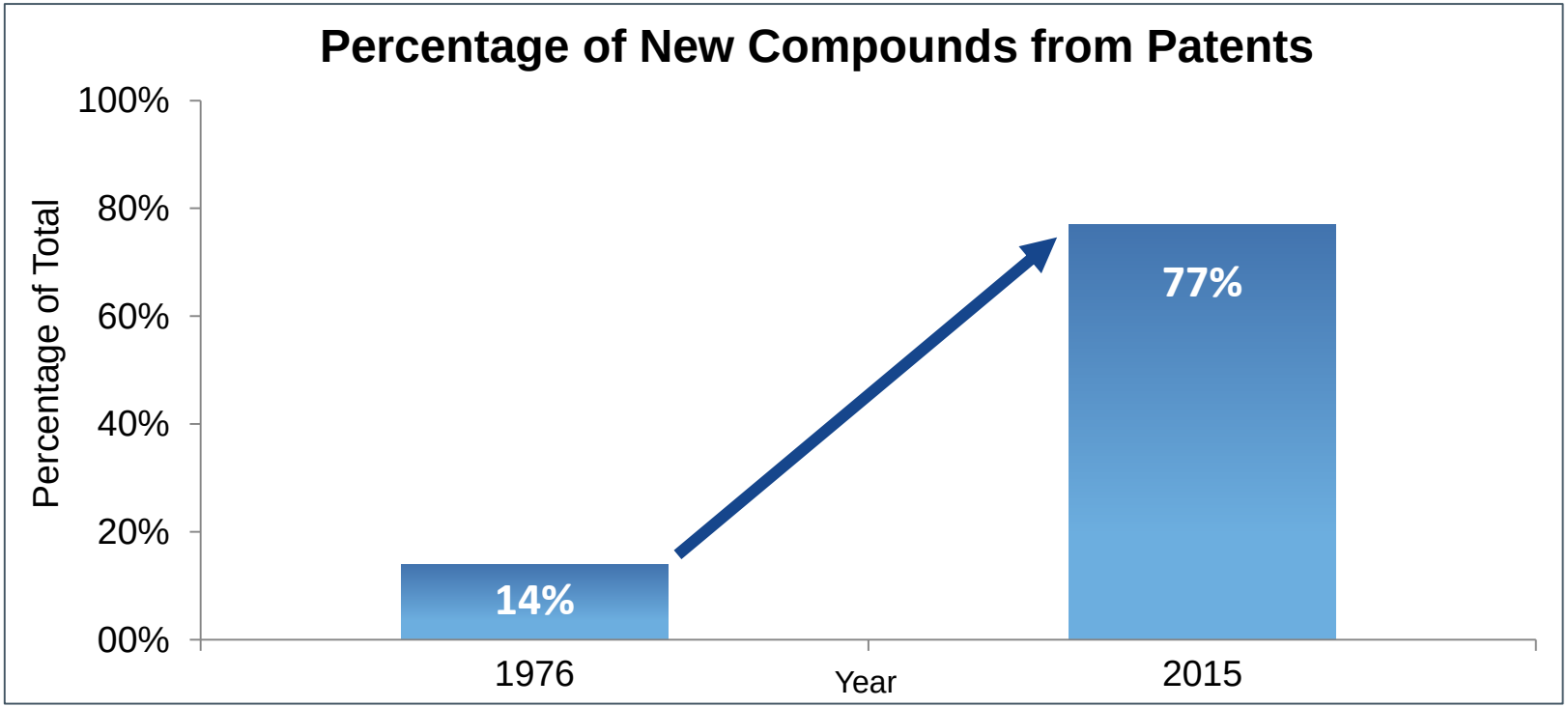

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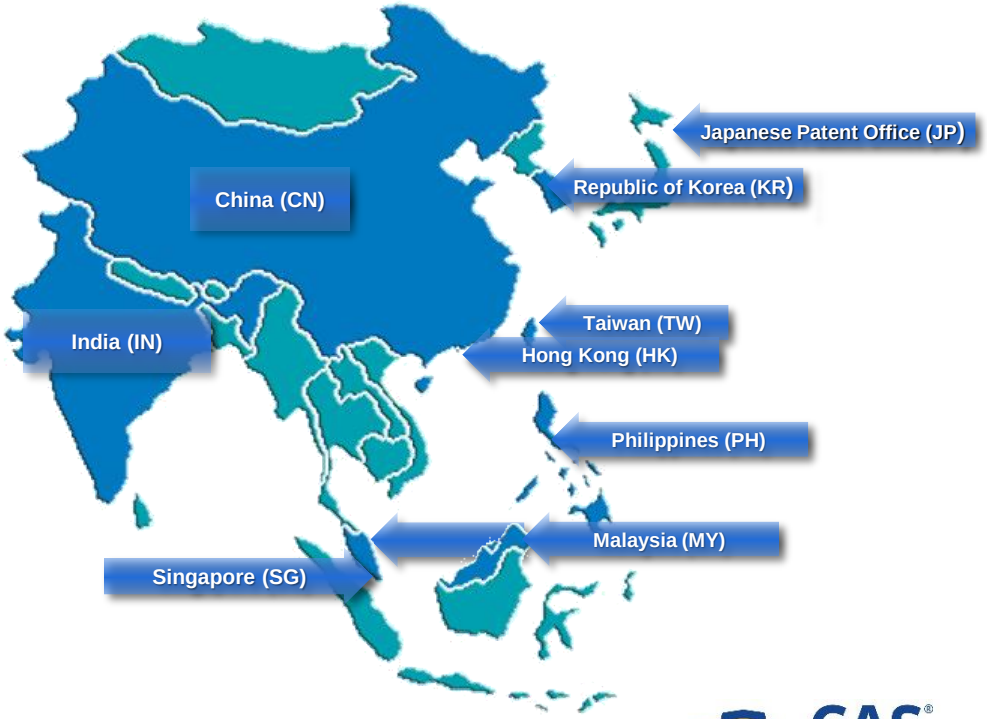

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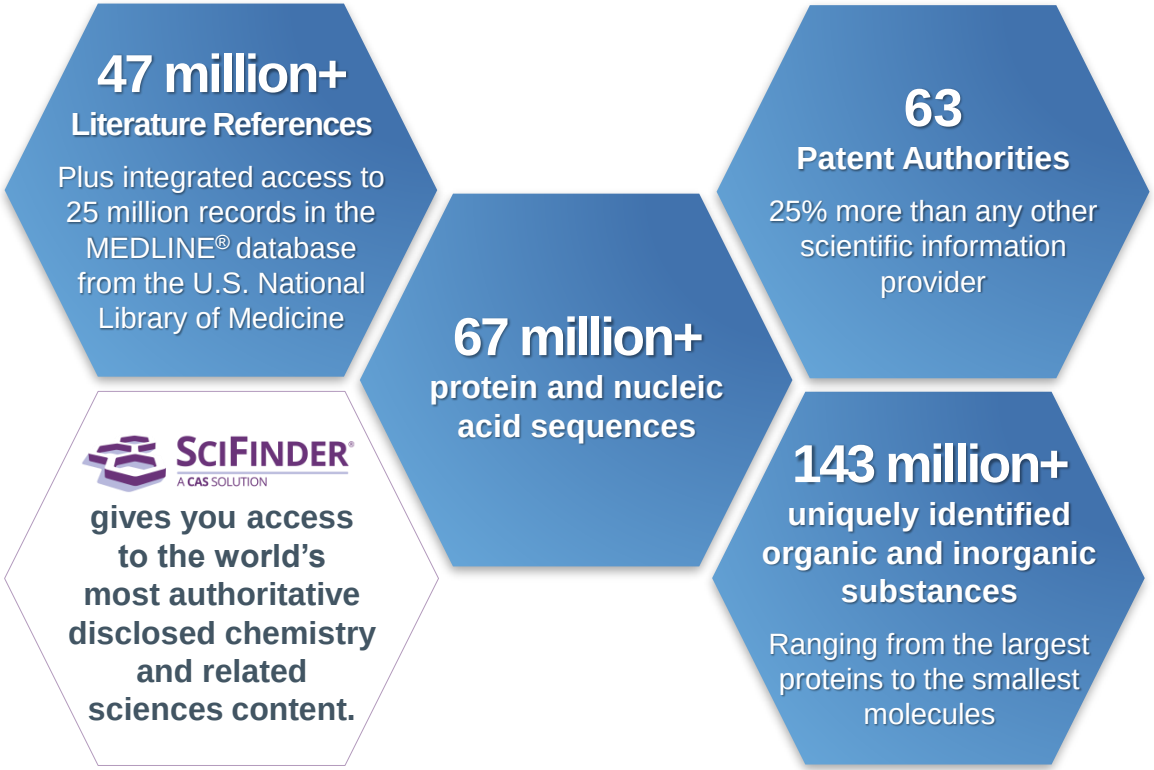

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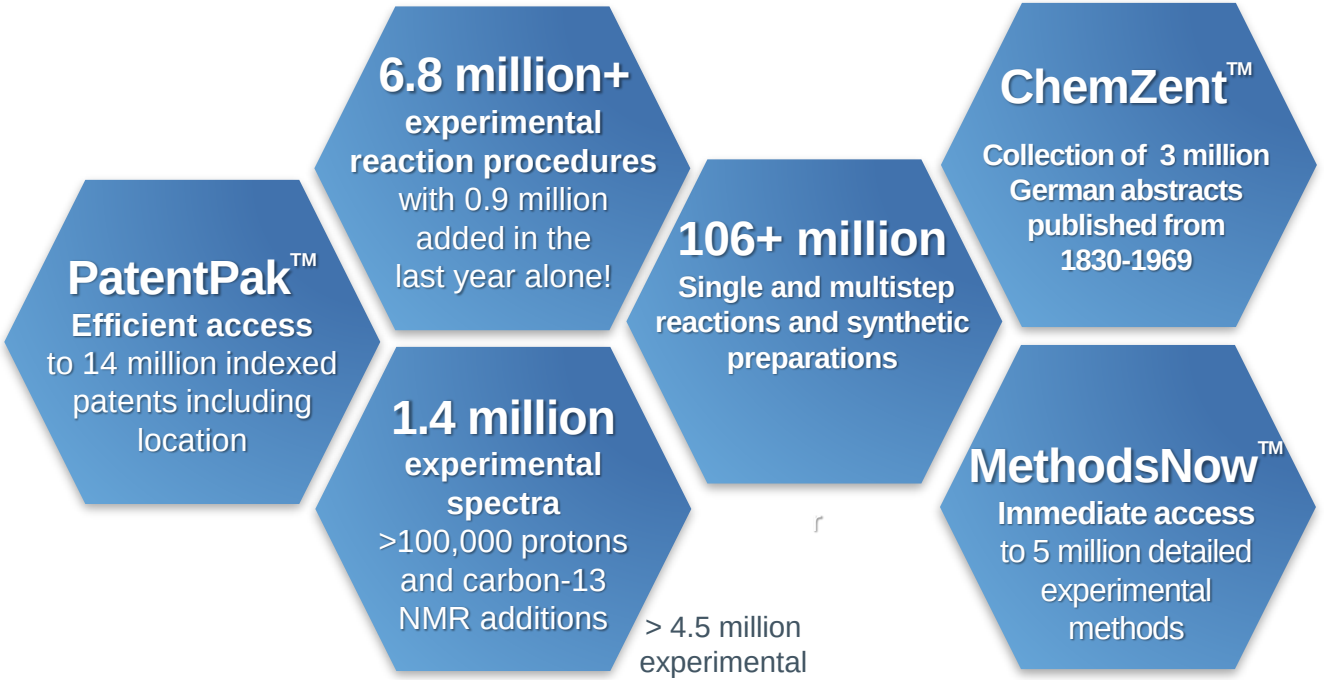

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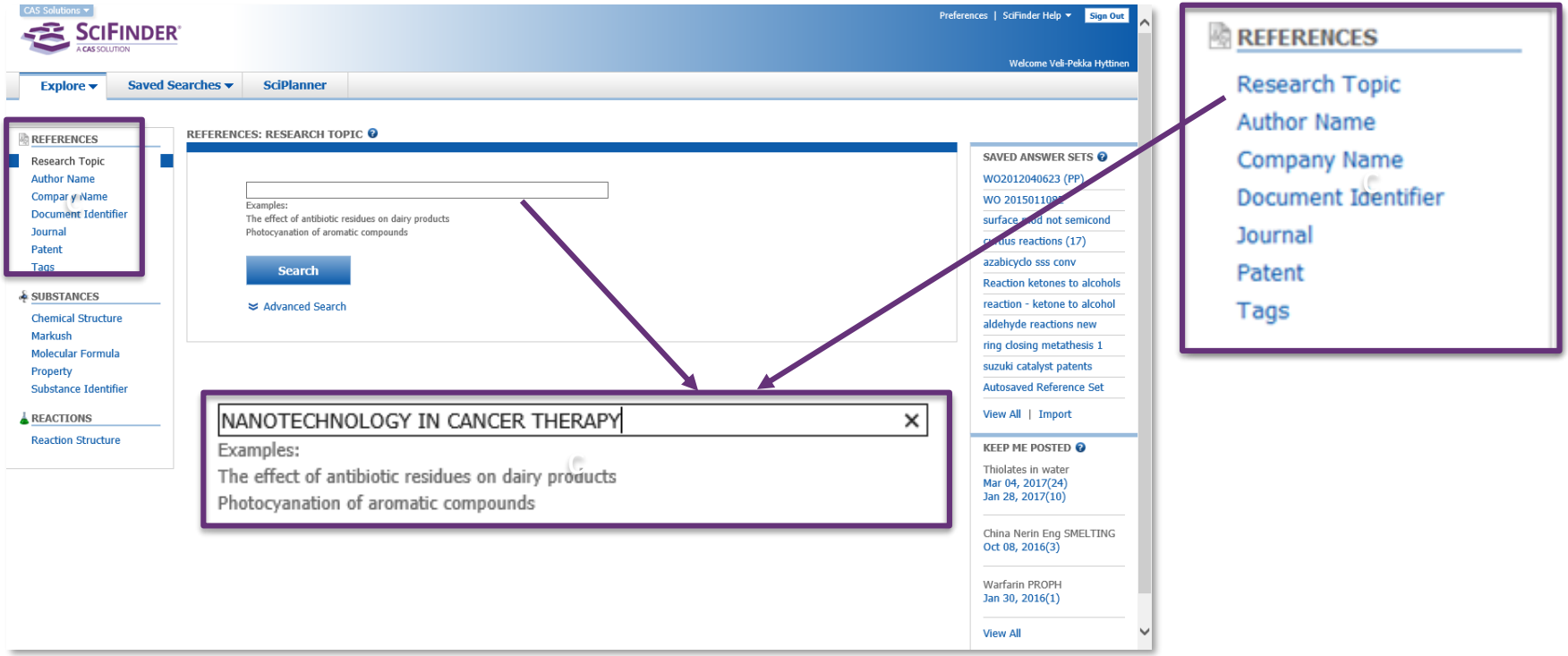

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Quick View

Development of a Rapid LC-MS/MS Method for the Quantification of Cannabidiol, Cannabidivarin, Δ9-Tetrahydrocannabivarin, and Cannabigerol in Mouse Peripheral ...

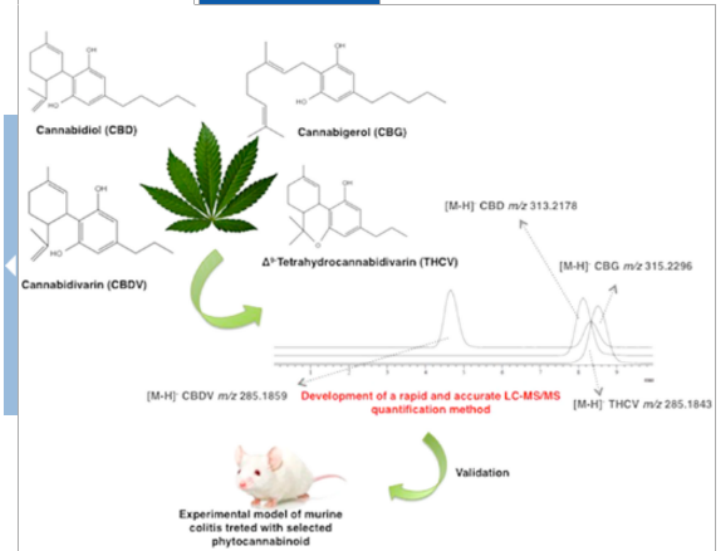
Other Sources

By Piscitelli, Fabiana; Pagano, Ester; Lauritano, Anna; Izzo, Angelo A.; Di Marzo, Vincenzo

From Analytical Chemistry (Washington, DC, United States) (2017), 89(8), 4749-4755. | Language: English, Database: CAPLUS

Cannabis has been known as a medicine for several thousand years across many cultures and its beneficial effects are mostly due to the presence of cannabinoids, unique natural products, whose pharmacol. is going to gain increasing interest in the scientific community. The discovery of the main psychoactive constituent of Cannabis sativa L., Δ^9-tetrahydrocannabinol (Δ^9-THC), led to the identification of at least 100 addnl. phytocannabinoids, including cannabidiol (CBD), cannabidivarin (CBDV), Δ^9-tetrahydrocannabivarin (Δ^9-THCV), and cannabigerol (CBG). These mols. are gaining growing interest for their medical properties; however, further research is needed to assess the differences in their pharmacokinetic and pharmacodymanic profiles. The aim of this study was to set up a rapid and accurate method, by using the LC-MS-IT-TOF technol., to detect and quantify CBD, CBDV, Δ^9-THCV, and CBG in biol. matrixes. Data show that the method developed here is linear in the calibration range; recoveries from mouse tissues were in the 50-60% range and sensitivity was 2 ng/mL for CBDV, 4 ng/mL for CBG and THCV, and 7 ng/mL for CBD. The method is rapid, precise and accurate, and it will represent a fundamental tool to evaluate the pharmacokinetic and pharmacodynamic properties of selected phytocannabinoids in tissues from different animal models, and develop new cannabinoid-based medicine.

Reference Images | Substance Images



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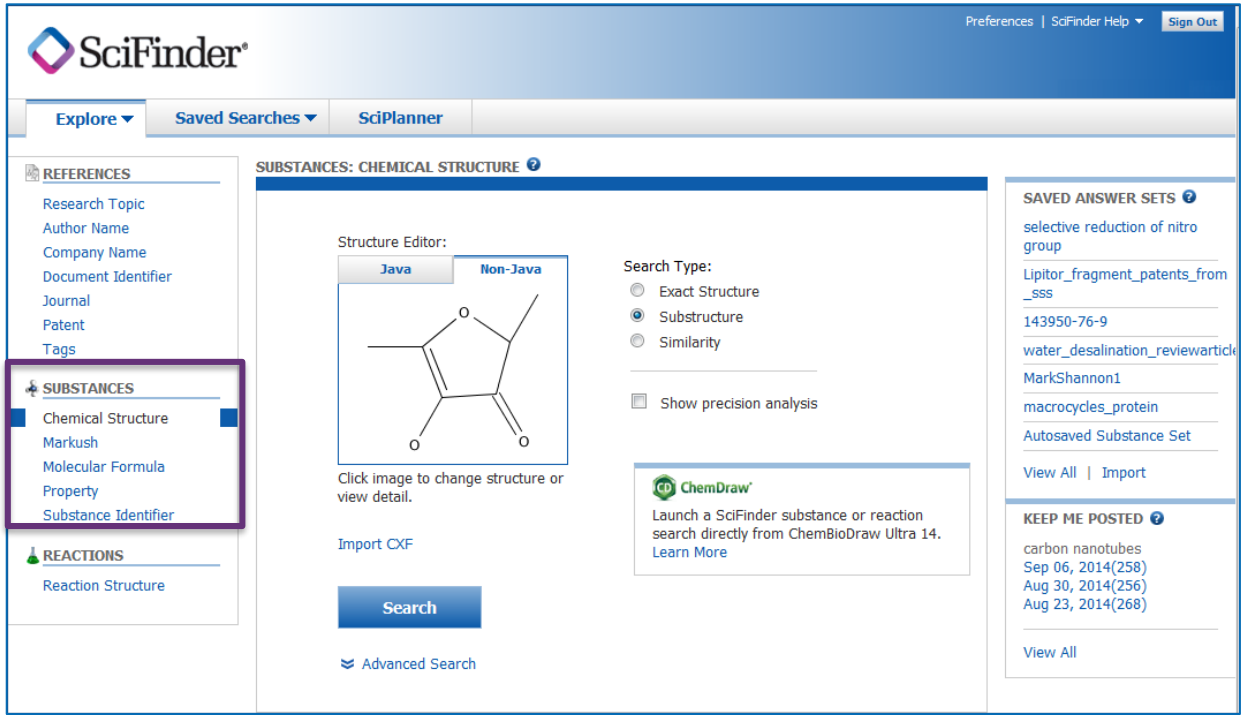
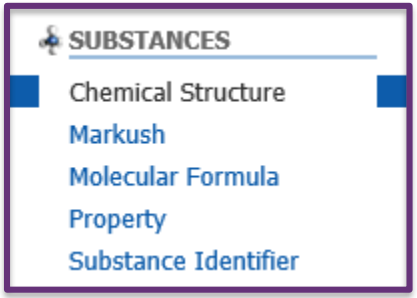
143+ million organic and inorganic small molecules, 67+ million bio sequences and 1,1+ million MARKUSH structures from patents – structures; names, molecular formulae





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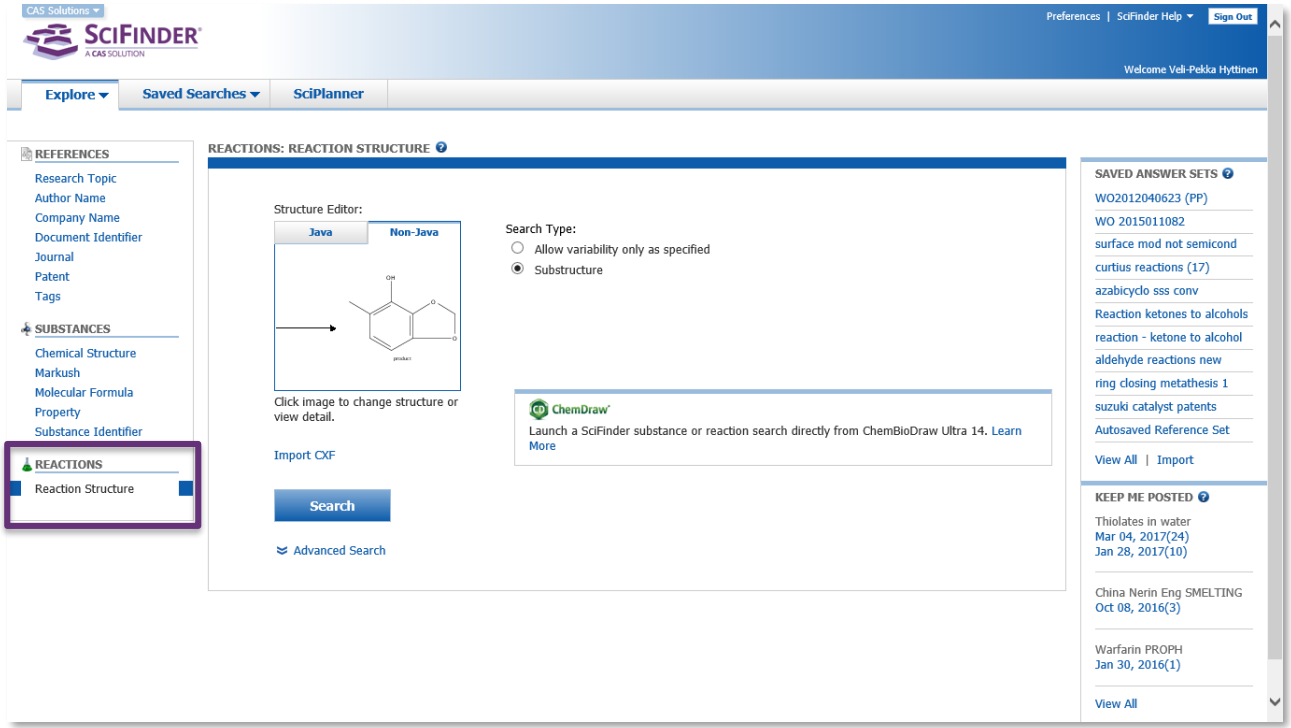

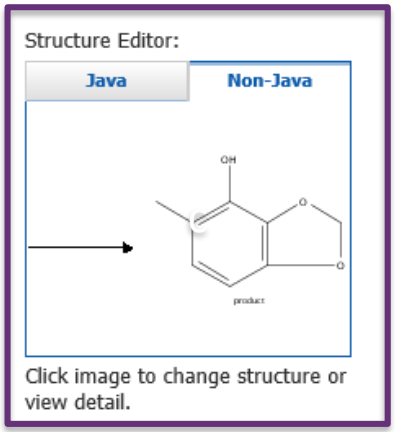

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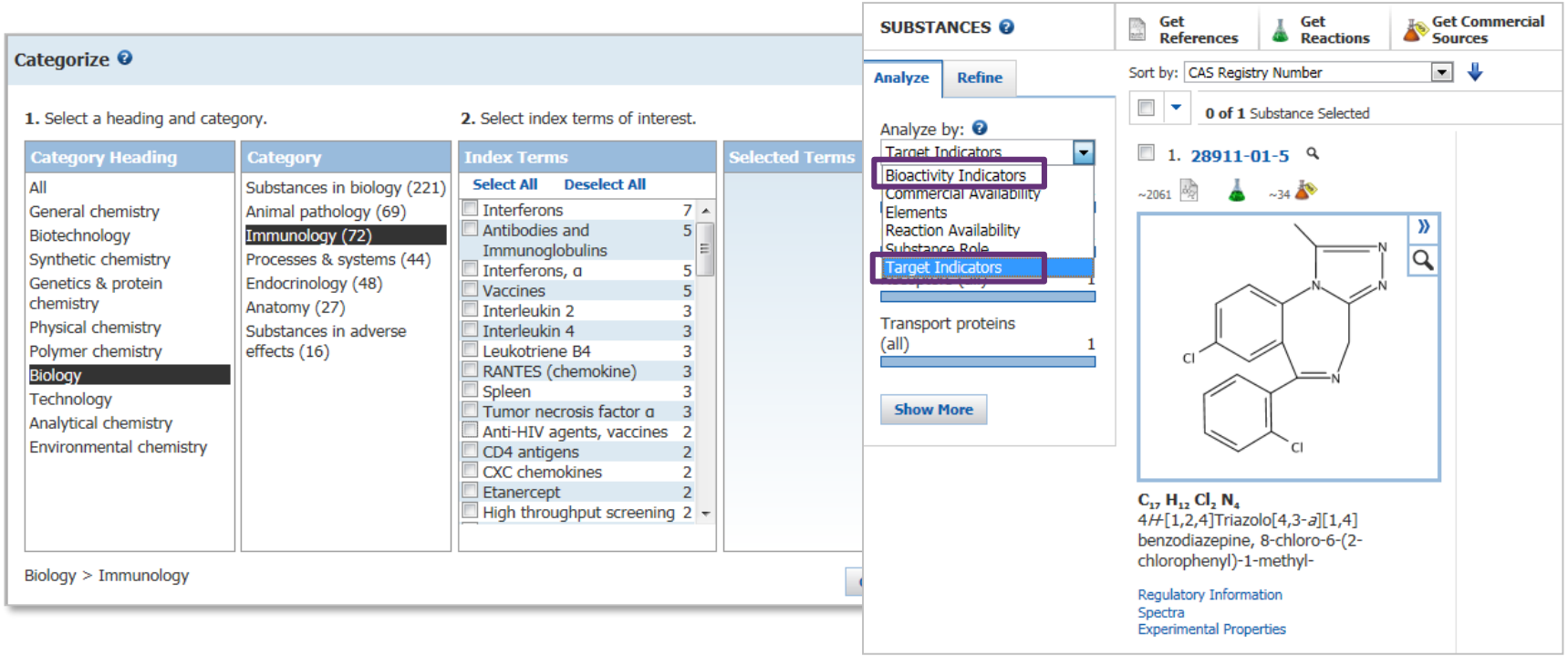

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Key Substances in Patent

CAS RN 7440-38-2D

As

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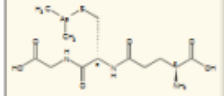
CAS RN 69819-86-9



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page 19
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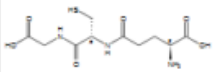
CAS RN 70-18-8



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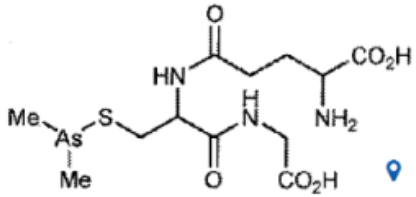
[0005] The present invention provides novel crystalline forms of organic arsenical compounds having anti-cancer properties. In certain embodiments, the present invention provides a crystalline form of a compound having a structure of formula (I) (darinaparsin)



(I)

[0006] wherein the crystalline form has a melting point greater than or equal to 185 °C. In some embodiments, the crystalline form has a melting point in the range of about 185-200 °C. In some embodiments, the crystalline form has a melting point in the range of about 187-200 °C, e.g., 187-197 °C. In some embodiments, the crystalline form has a melting point in the range of about 190-200 °C. In other embodiments, the invention provides a crystalline form of a compound having a structure of formula (I) (darinaparsin) wherein the crystal form has an X-ray-powder diffraction pattern comprising characteristic peaks
more of the following angles: about 16.6°, about 17.4°, ab

[0007] In some embodiments, the X-ray powder diffra
a compound having a structure of formula (I) (darinaparsi
expressed in terms of 2θ, at one or more of the following angles: about 14.4°, about 19.3°, about 22.0°, about 23.3° and about 25.0°. In some embodiments, the X-ray powder diffraction pattern of the crystalline form of a compound having a structure of formula (I) (darinaparsin) has

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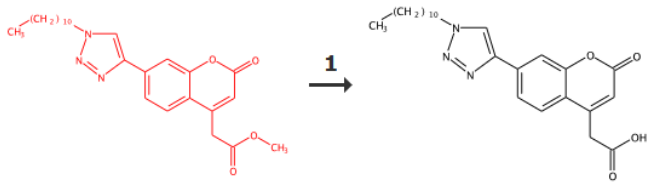
MethodsNow

7-Triazolylcoumarin-based fluorescent tag system for stepwise, comparative assessment of small molecule micr

By Jeon, Moon-Kook; Kang, Myoung-Ku; Park, Koon Ha
From Tetrahedron, 68(30), 6038-6053; 2012
Published by Elsevier Ltd.

Reaction Steps 1 2 3 4



Products	2*H*-1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1*H*-1,2,3-triazol-4-yl)-, 75%, CAS RN 1384966-77-1
Reactants	2*H*-1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1*H*-1,2,3-triazol-4-yl)-, methyl ester, 1384966-75-9
Reagents	Hydrochloric acid, CAS RN: 7647-01-0 Lithium hydroxide, CAS RN: 1310-65-2
Solvents	Water, CAS RN: 7732-18-5 Tetrahydrofuran, CAS RN: 109-99-9

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MethodsNow

Procedure	1. Add lithium hydroxide monohydrate(327 mg, 7.80 mmol) to 4-methoxycarbonylmethyl-7-(1-undecyl-1H- 1,2,3-triazol-4-yl)-2H-chromen-2-one (343 mg, 0.780 mmol) in THF/water(25 mL/25 mL) at room temperature. 2. Stir the reaction mixture for 3 hours at room temperature. 3. Adjust pH 3-4 to the reaction mixture by adding 1 N hydrochloric acid. 4. Partition the reaction mixture between ethyl acetate and water. 5. Extract the aqueous layer with ethyl acetate. 6. Dry the combined organic layer over magnesium sulfate.
Scale	milligram
^{1}H NMR	^{1}H NMR (300 MHz, acetone- d_6): δ = 7.83 (s, 1H), 8.58 (s, 1H), 7.92 (d, *J* = 8.1 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 6.47 (s, 1H), 4.50 (t, *J* = 7.2 Hz, 2H), 3.99 (s, 2H), 2.00 (quintet, *J* = 7.2 Hz, 2H), 1.32-1.43 (m, 4H), 1.22-1.32 (m, 12H), 0.87 ppm (t, *J* = 6.8 Hz, 3H).
^{13}C NMR	^{13}C NMR (125 MHz, DMF-d_7, 60 °C): δ = 161.0, 155.1, 154.2, 146.5, 136.0, 127.2, 123.7, 122.1, 120.4, 115.3, 113.5, 51.1, 32.8, 29.9, 27.3, 23.5, 18.7, 14.7 ppm (decarboxylation occurred to give the corresponding 4-methyl derivative).
IR	IR (ATR, neat): ν = 3423, 2922, 2851, 1702 (2C=O, overlapped), 1619, 1561, 1375, 1154, 936, 852, 809 cm^{-1}.
HRMS	HRMS (EI): m/z calculated for $C_{24}H_{31}N_3O_4$: 425.2315 [M$^+$]; found: 425.2315.
Mass Spec	MS (ESI): m/z: 426 [M+H$^+$].
MP	235.5±0.8 °C.
CAS Method Number	3-352-CAS-78415

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

- Published German language abstracts from 1830-1969
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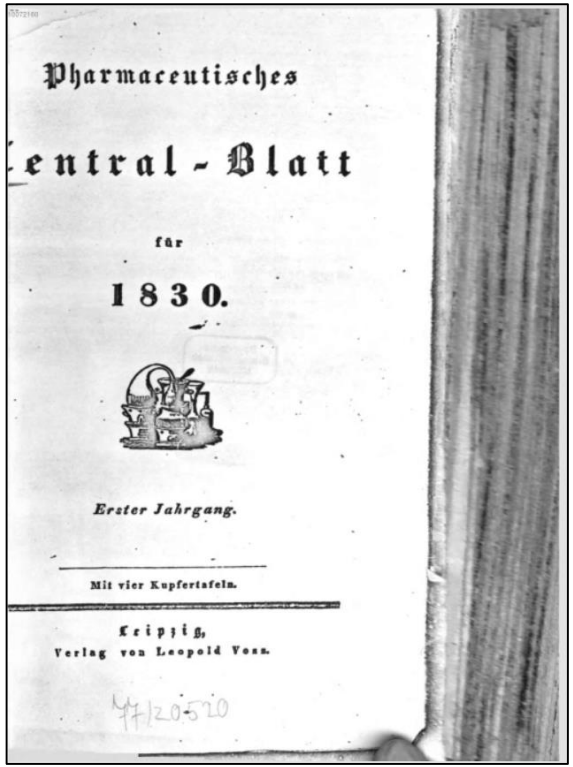
Pharmaceutisches

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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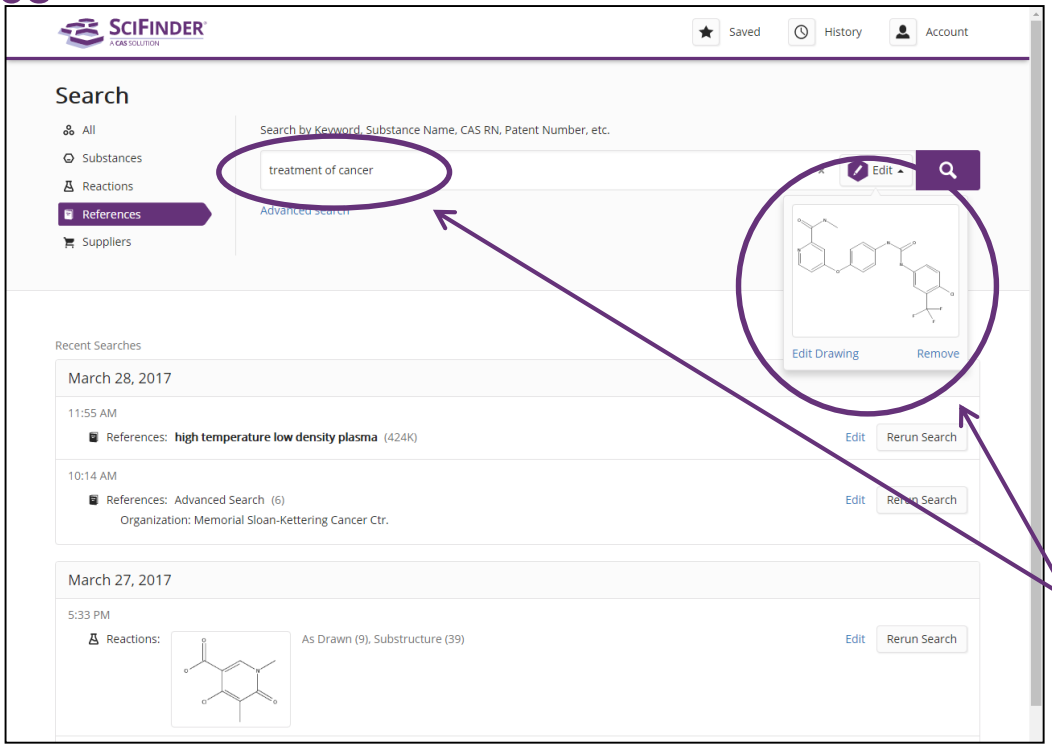

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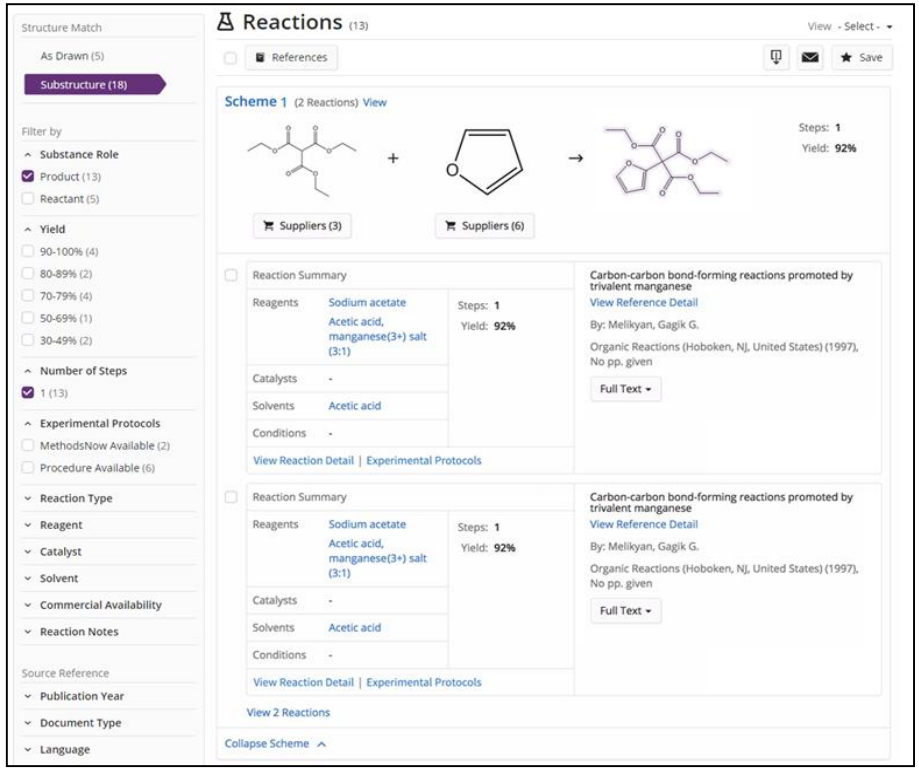

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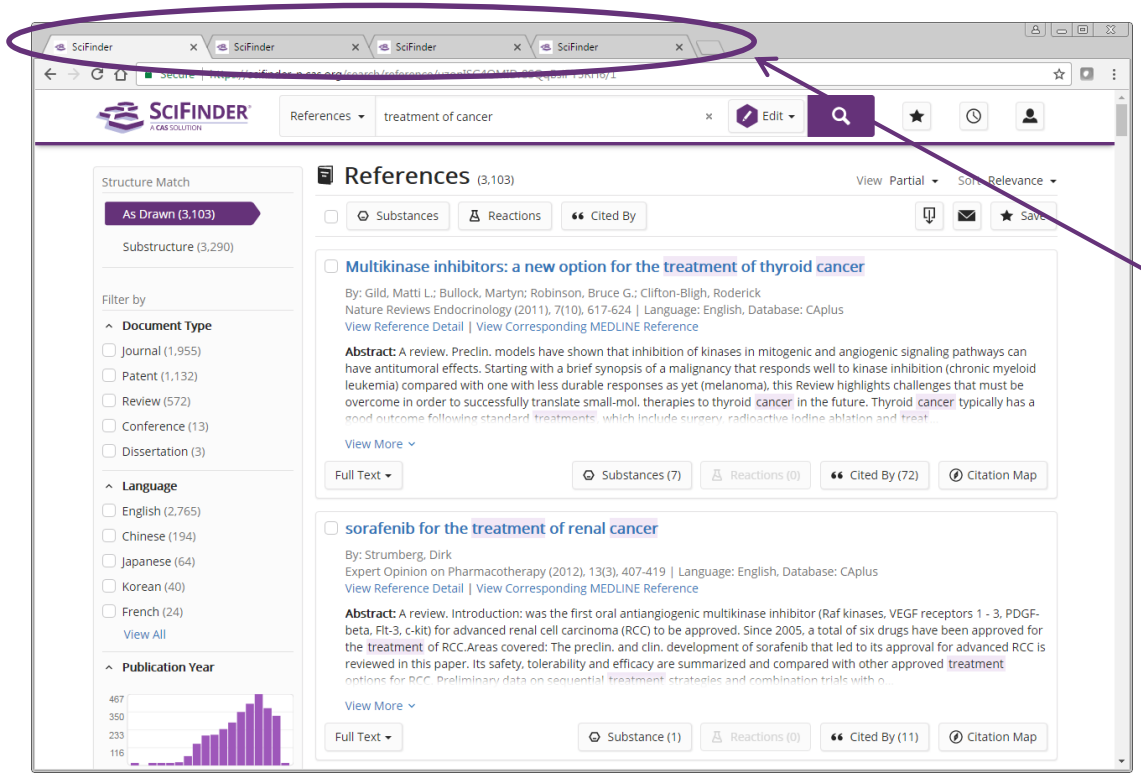

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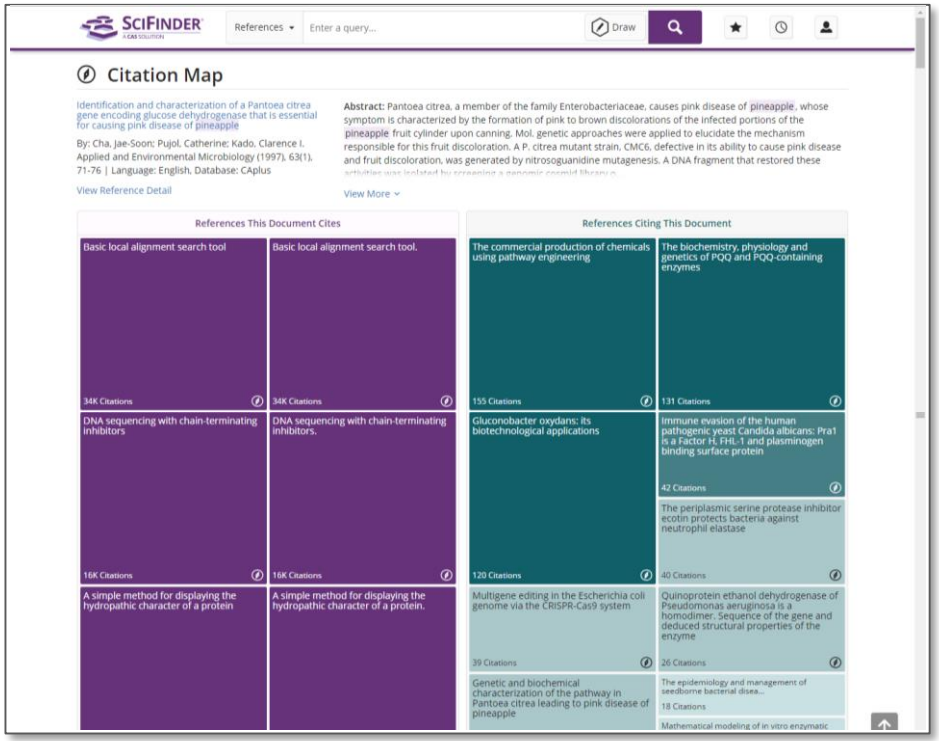

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