

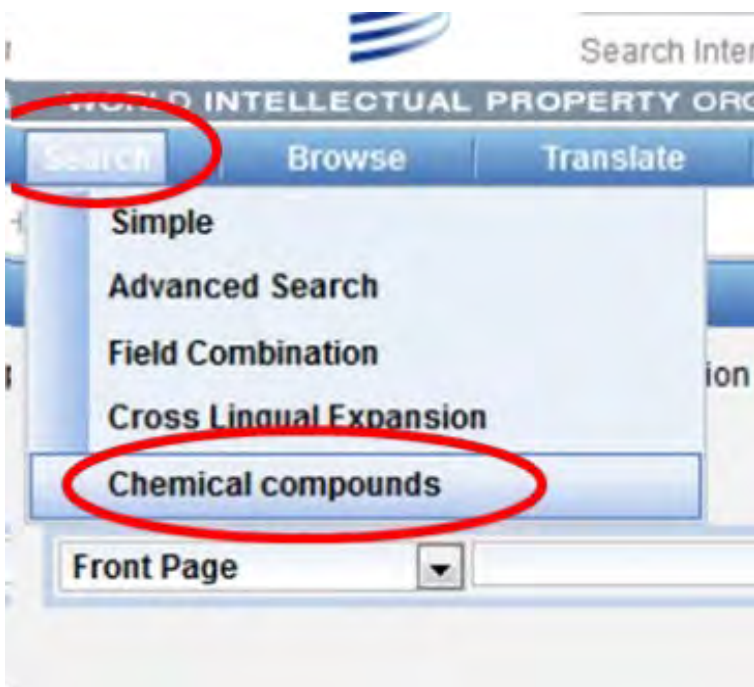
## WIPO Structure Searching I

By Rick Neifeld, Neifeld IP Law, PC

On 9/27/2016, WIPO conducted a webinar previewing the new chemical structure searching capability being programmed into PatentScope. Copied below in part I are my notes taken during the Webinar and corresponding snippets of the presenters slides. On 9/28/2016, the WIPO presenter emailed participants a list of questions posed by the participants and her answers to those questions. I provide those Q and As in part II.

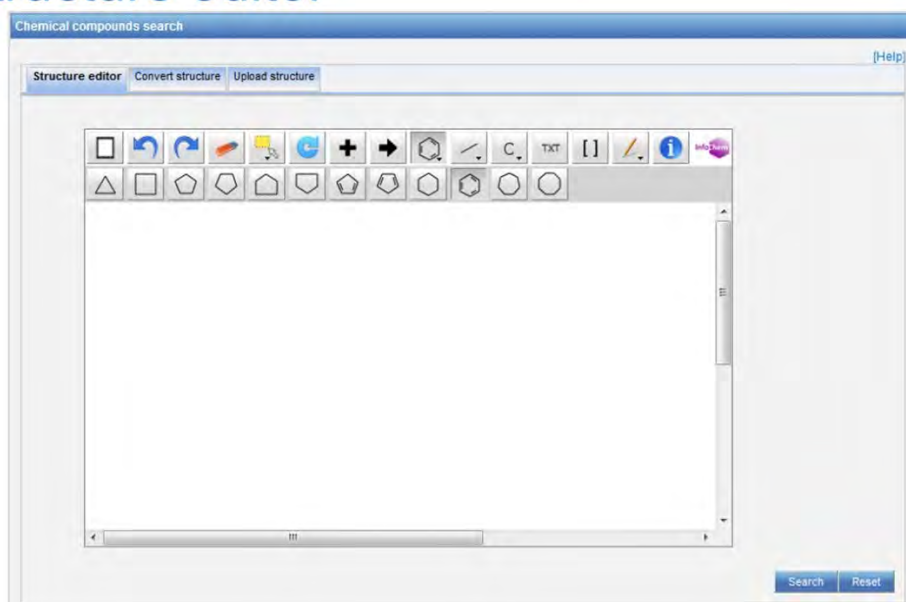
### I. Webinar Notes and Snippets

Search location: This feature will appear in the search drop-down box in PatentScope.



The user can upload a structure or draw a structure or convert an entered structure:

## Structure editor

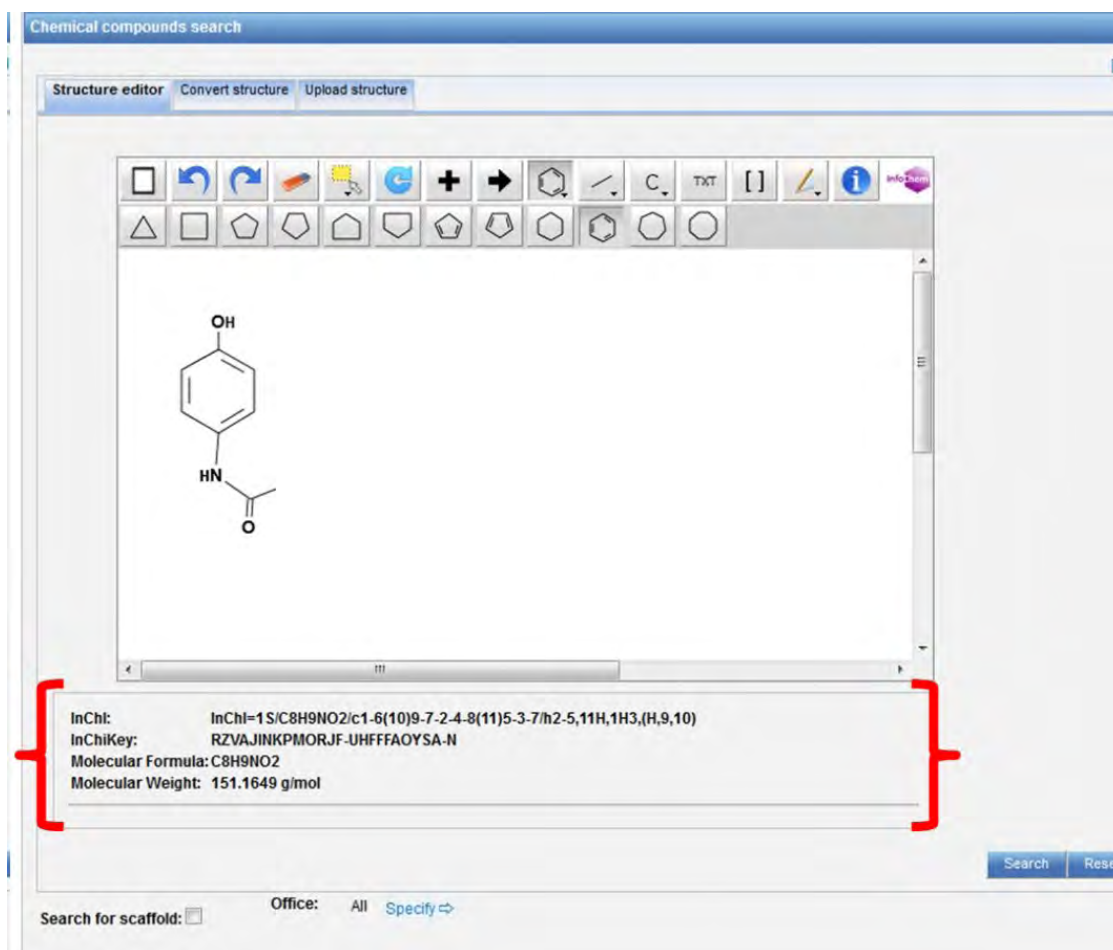


The structure editor window appears below. Note the use of the InChI standard and InChIKeys. The InChIKeys are 27 length text string resulting from applying a Hash function to the InChI representation of the molecule.

Search format allows searching by compound name, INN, InChI, SMILES formats.

Scaffold searching based upon the entered molecule is an option.

Markush groups of molecules cannot now be entered as a structure for searching.



Conventional PatentScope search results list:

Results 1-10 of 13,105 for Criteria CHEM:(RZVAJINKPMORJF-UHFFFAOYSA-N) Office(s):wo Language:EN Stemming: true

prev 1 2 3 4 5 6 7 8 9 10 next Page: 1 / 1311 Go >

Refine Search CHEM:(RZVAJINKPMORJF-UHFFFAOYSA-N) Search

RSS

Analysis

Sort by: Pub Date Desc View: All List Length: 10 Machine translation

Int.Class	Appl.No	Title	Applicant	Ctr	PubDate
1. WO/2016/142349	A61K 38/45 PCT/EP2016/054816	USE OF CREATINE KINASE AND DERIVED PEPTIDES THEREOF TO RELIEF PAIN	CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE - CNRS -	WO	15.09.2016
<p>The present invention relates to the use of creatine kinase or fragments thereof which induce analgesia, and also to the use of pharmaceutical compositions comprising the same, to relief pain.</p>					
2. WO/2016/142689	G01N 33/68 PCT/GB2016/050619	TISSUE ANALYSIS BY MASS SPECTROMETRY OR ION MOBILITY SPECTROMETRY	MICROMASS UK LIMITED	WO	15.09.2016
<p>A method of analysis using mass and/or ion mobility spectrometry or ion mobility spectrometry is disclosed comprising: using a first device to generate aerosol, smoke or vapour from one or more regions of a first target of biological material; and mass and/or ion mobility analysing and/or ion mobility analysing said aerosol, smoke, or vapour, or ions derived therefrom so as to obtain first spectrometric data. The method may use an ambient ionisation method.</p>					
3. WO/2016/142691	G01N 33/68 PCT/GB2016/050621	RAPID EVAPORATIVE IONISATION MASS SPECTROMETRY ("REIMS") AND DESORPTION ELECTROSPRAY IONISATION MASS SPECTROMETRY ("DESI-MS") ANALYSIS OF SWABS AND BIOPSY SAMPLES	MICROMASS UK LIMITED	WO	15.09.2016
<p>A method is disclosed comprising providing a biological sample on a swab (900), directing a spray of charged droplets onto a surface of the swab (900) in order to generate a plurality of analyte ions, and analysing the analyte ions.</p>					
4. WO/2016/142674	G01N 33/68 PCT/GB2016/050603	CELL POPULATION ANALYSIS	MICROMASS UK LIMITED	WO	15.09.2016
<p>A method of analysis using mass spectrometry and/or ion mobility spectrometry is disclosed comprising: (a) using a first device to generate smoke, aerosol or vapour from a target in vitro or ex vivo cell population; (b) mass analysing and/or ion mobility analysing said smoke, aerosol or vapour, or ions derived therefrom, in order to obtain spectrometric data; and (c) analysing said spectrometric data in order to identify and/or characterise said target cell population or one or more cells and/or compounds present in said target cell population.</p>					

PatentScope can display the structures in the results retrieved by the search, as shown.

The screenshot displays the PatentScope interface with the 'Compound' tab selected. Below the navigation tabs, the 'Description' and 'Claims' sub-tabs are also visible. The main content area features a grid of 24 chemical structures arranged in 4 rows and 6 columns. The structures include various organic and inorganic molecules, such as amino acids, alcohols, and salts. At the bottom of the grid, the names 'Lysine Lysine' and 'Octanoic acid Octanoic acid' are listed, followed by a pagination control showing page 1 of 6.


Lysine Lysine    Octanoic acid Octanoic acid    1 2 3 4 5 6    >>>>

See the InChIKey in the refined search.

## Analysis

Results 1-10 of 145 for Criteria:CHEM:(RZVAJINKPMORJF-UHFFFAOYSA-N) Office(s):all Language:EN Stemming: true

prev 1 2 3 4 5 6 7 8 9 10 next Page: 1 / 15 Go >

Refine Search: CHEM:(RZVAJINKPMORJF-UHFFFAOYSA-N) Search  

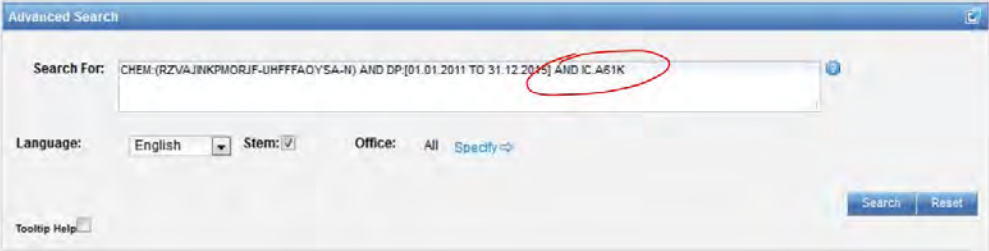
Analysis

Options  Table  Graph Options  bar  pie  Line

Countries		Main IPC		Main Inventor		Main Applicant		Pub Date	
Name	No	Name	No	Name	No	Name	No	Date	No
PCT	145	A61K	106	LIN, Yikang	3	GENENTECH, INC.	7	2010	8
		A61P	55	SREEKRISHNA, Koti	3	F. HOFFMANN-LA ROCHE AG	5	2011	7
		C07D	38	ALMEIDA PECORELLI, Susana Marques	2	NOVARTIS AG	4	2012	8
		C07K	18	BALAGUE PELAEZ, Cristina	2	ALMIRALL, S.A.	3	2013	14
		C12N	13	BYLLIND, Johan	2	GALAPAGOS NV	3	2014	5
		A01N	9	CASIMIRO CAIXADO, Carlos Alberto Eufrásio	2	MASSACHUSETTS INSTITUTE OF TECHNOLOGY	3	2015	72
		G01N	7		2	THE PROCTER & GAMBLE COMPANY	3	2016	31
		C12Q	6	CHALMERS, Derek, T.	2	ABBVIE, INC.	2		
		A23L	5	EK, Maria	2	ACTURUM REAL ESTATE AB	2		
		C07C	5	EUFRÁSIO PEDROSO, Pedro Filipe FASSIH, Ali	2	ADVANCED FIRST AID RESEARCH PTE. LTD.	2		

Structure search is combinable with other search criteria:

## Combine results with searches



The screenshot shows an "Advanced Search" window. The search query is: `CHEM:(RZVAJINKPMORJF-UHFFFAOYSA-N) AND DP:[01.01.2011 TO 31.12.2015] AND IC:A61K`. A red circle highlights the date range `[01.01.2011 TO 31.12.2015]`. Below the search box, there are options for "Language" (English), "Stem" (checked), and "Office" (All). There are "Search" and "Reset" buttons at the bottom right, and a "Tooltip Help" link at the bottom left.

To get a new results list.

Results 1-10 of 77 for Criteria: CHEM:(RZVAJNKPMORJF-UHFFFAOYSA-N) AND DP:[01.01.2011 TO 31.12.2015] AND IC:A61K Offices:all Language:EN Stemming: true

prev 1 2 3 4 5 6 7 8 next Page: 1 / 8 Go >

Refine Search: CHEM:(RZVAJNKPMORJF-UHFFFAOYSA-N) AND DP:[01.01.2011 TO 31.12.2015] AND IC:A61K Search RSS

Analysis

Options: Table Graph Options bar pie Line

Countries		Main IPC		Main Inventor		Main Applicant		Pub Date	
Name	No	Name	No	Name	No	Name	No	Date	No
PCT	77	A61K	77	LIN, Yakang	3	ALMIRALL, S.A.	3	2011	3
		A61P	36	SREEKRISHNA, Kott	3	GALAPAGOS NV	3	2012	7
		C07D	21	ALMEIDA PECORELLI, Susana Marques	2	THE PROCTER & GAMBLE COMPANY	3	2013	9
		C12N	7					2014	3
		C07K	6	BALAGUE PELAEZ, Cristina	2	F. HOFFMANN-LA ROCHE AG	2	2015	55
		A01N	4	CASIMIRO CAIXADO, Carlos Alberto Eufrazio	2	GENENTECH, INC.	2		
		A51Q	4	EUFRAÁSIO PEDRÓSÓ, Pedro Filipe	2	JOHNSON & JOHNSON CONSUMER INC.	2		
		C12P	3	FASSIH, Ali	2	KARYOPHARM THERAPEUTICS, INC.	2		
		A23L	2	GODESSART MARINA, Nuria	2				
		A61L	1	KAY, Noel	2	MCCAULEY, Dilara	2		
				LOPES, Ana Sofia da Conceição	2	NOVARTIS AG	2		
						SANDANAYAKA, Vincent, P.	2		

Sort by: Pub Date Desc View: All List Length: 10 Machine translation

Int. Class	Appl. No	Title	Applicant	Int.	PubDate
1. WO/2015/181055		COMBINATION		WO	03.12.2015
A61K 45/06	PCT/EP2015/061312	ALMIRALL, S.A.		GODESSART MARINA, Nuria	
The present invention provides a pharmaceutical composition which comprises (a) a compound which is an inhibitor of phosphoinositide 3-kinase delta or a pharmaceutically acceptable salt and/or solvate thereof, and (b) a corticosteroid.					
2. WO/2015/181053		MEDICAL USE		WO	03.12.2015
A61K 45/06	PCT/EP2015/061308	ALMIRALL, S.A.		GODESSART MARINA, Nuria	

RTY



Example: Prozac

## Example: fluoxetine hydrochloride

- Its chemical formula is  $C_{17}H_{19}ClF_3NO$
- the first highly specific serotonin uptake inhibitor. It is used as an antidepressant and often has a more acceptable side-effects profile than traditional antidepressants.
- Synonyms: Prozac, Sarafem

Comparison of structure and text searches indicates shows that typically less results are retrieved using the structure search than merely name searches.

WIPO has indexed structures in English and German language PCT publications. WIPO plans to expand from PCT to other database collections that WIPO has stored and other languages.

Q & A:

Scope of indexing - Entire PCT collection.

Will search tool be modified to include Markush searching. No current plans.

Slides will be available after Friday at:

[www.wipo.int/patentscope/en/webinar/index.html](http://www.wipo.int/patentscope/en/webinar/index.html)

End of Webinar.

## II. Q & As

This part provides the participants questions and WIPO presenters answers sent to participants of the webinar, after the fact.

1. Typically, how many structures are revealed in an patent for an INN drug?  
It is difficult to compute. The system has no limit in terms of maximum number of chemical structures recognized by a document.
2. Means "CAS name" "CAS number"?  
CAS numbers are recognized due to their syntax and indexed as is.
3. Is it possible to upload structures from ChemDraw? if we get inchi from the chemdraw or chemsketch. is it possible to search by simply pasting it in chemical search?  
Yes, the CDX format not supported for file loading
4. Can generic formulae for polymers containing parameters such as n an m for the repeating units be searched?  
No, only exact structures that can be represented by an Inchi
5. Will alerting on structures be available?  
In theory yes (RSS)
6. How far back in time will PCT/US be chemically indexed?  
PCT 1978 and US 1990 (to be confirmed according to the greenbook format)

7. Is it limited to small molecules or can I search for (small) proteins too?  
Only exact structures that can be represented by an Inchi
8. Structure search for compound where only chemical name is given in patent..is that patent also get picked in the search?  
Yes
9. How does this affect drafting and filing applications - is there a size requirement for proper data capture?  
the clearer the embedded images are the better. min 300dpi
10. Do you get the FDA data from the Orange Book?  
no from Infochem SW
11. You have a library of pre-stored chemical structures?  
Probably what is needed for the conversion to Inchikeys. This is a black box for WIPO delivered by Infochem
12. Are the data annotated with InChI or InChIkeys or do you use the Inchi and Inchi keys to generate IUPAC names and search with the names.  
annotated with Inchikeys
13. OK so the trivial name is also indexed as an InChI string or InChiKey?  
yes

End of Q and As.