WIPO Structure Searching I

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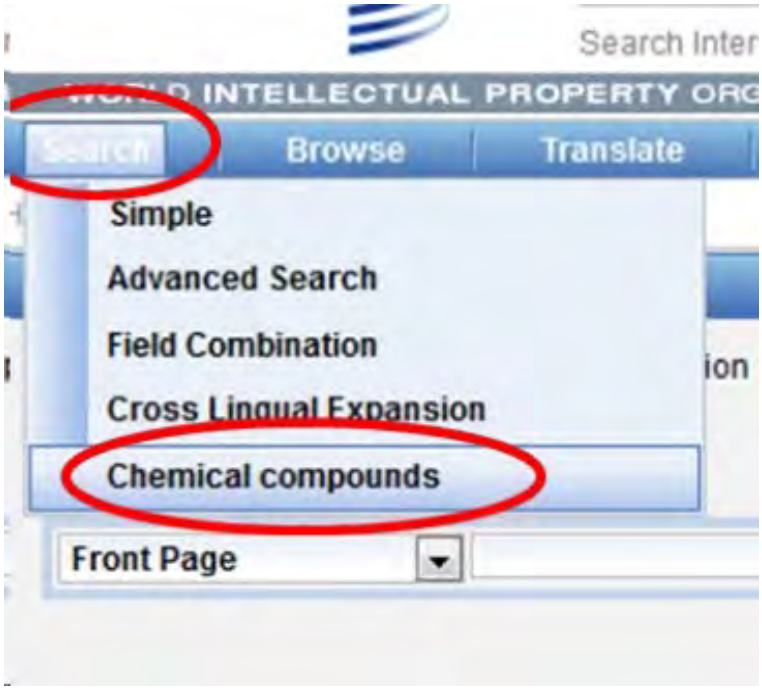
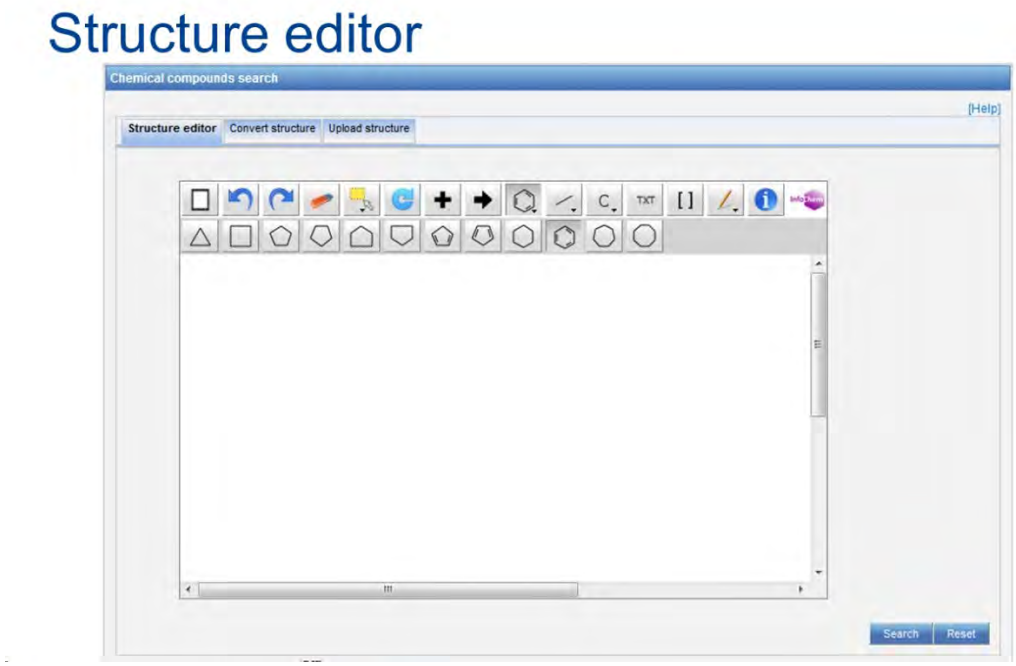
On 9/27/2016, WIPO conducted a webinar previewing the new chemical structure searching capability being programmed into PatentScope. Copied below in part I are my notes taken during the Webinar and corresponding snippets of the presenters slides. On 9/28/2016, the WIPO presenter emailed participants 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

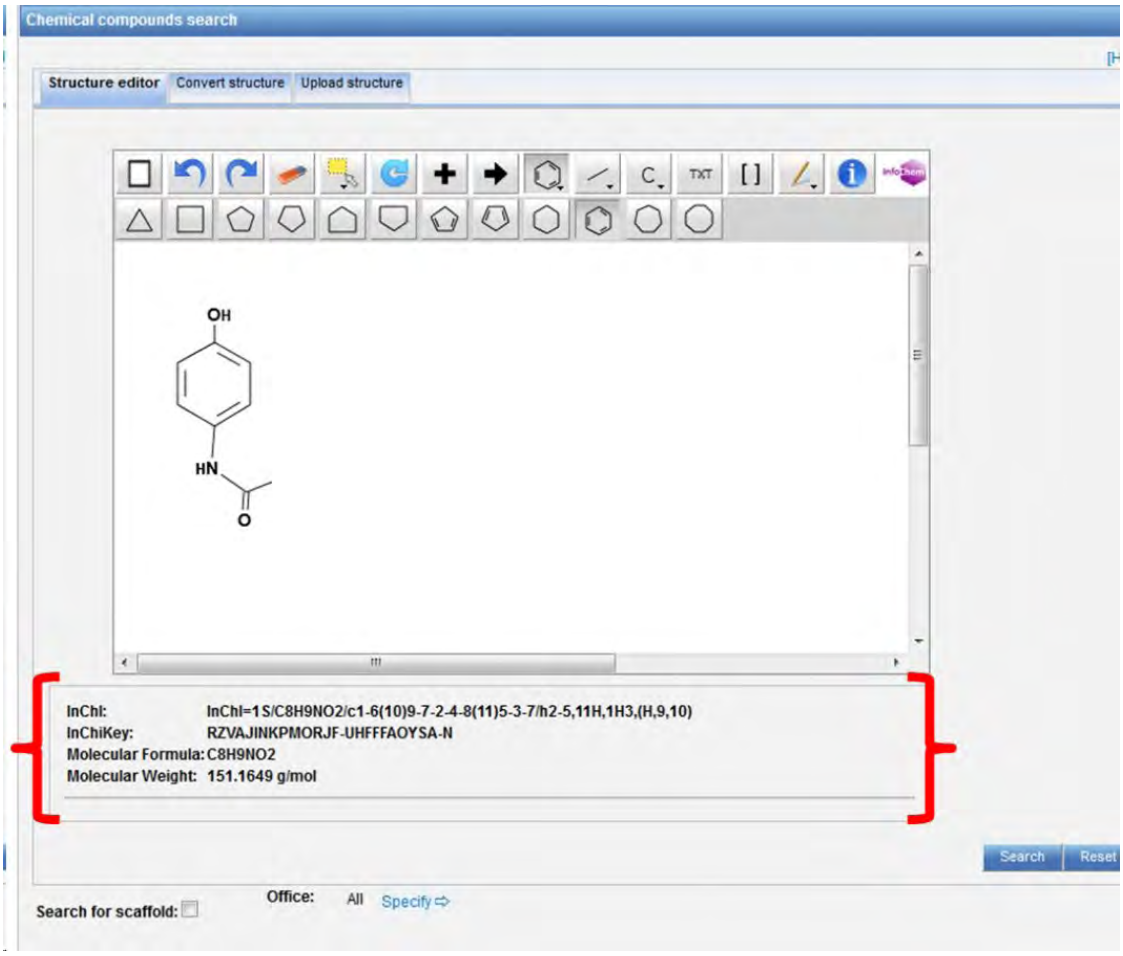
Search location: This feature will appear in the search drop-down box in PatentScope.



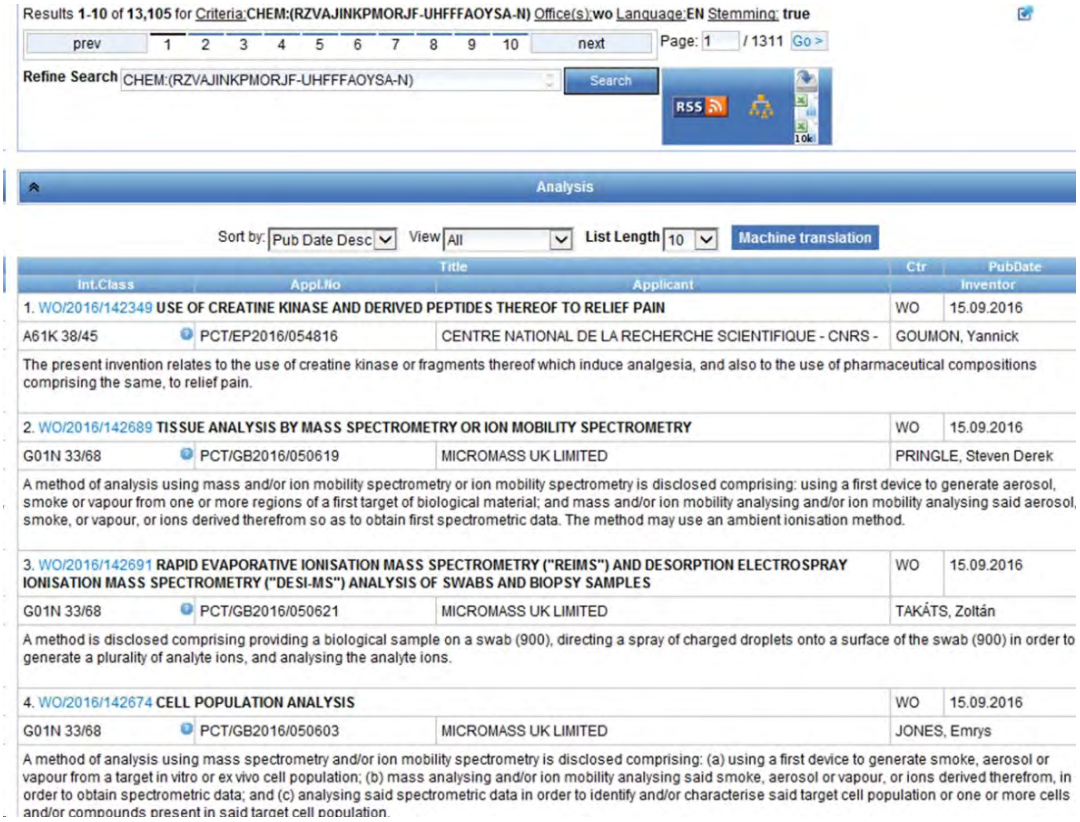
The user can upload a structure or draw a structure or convert an entered structure:



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

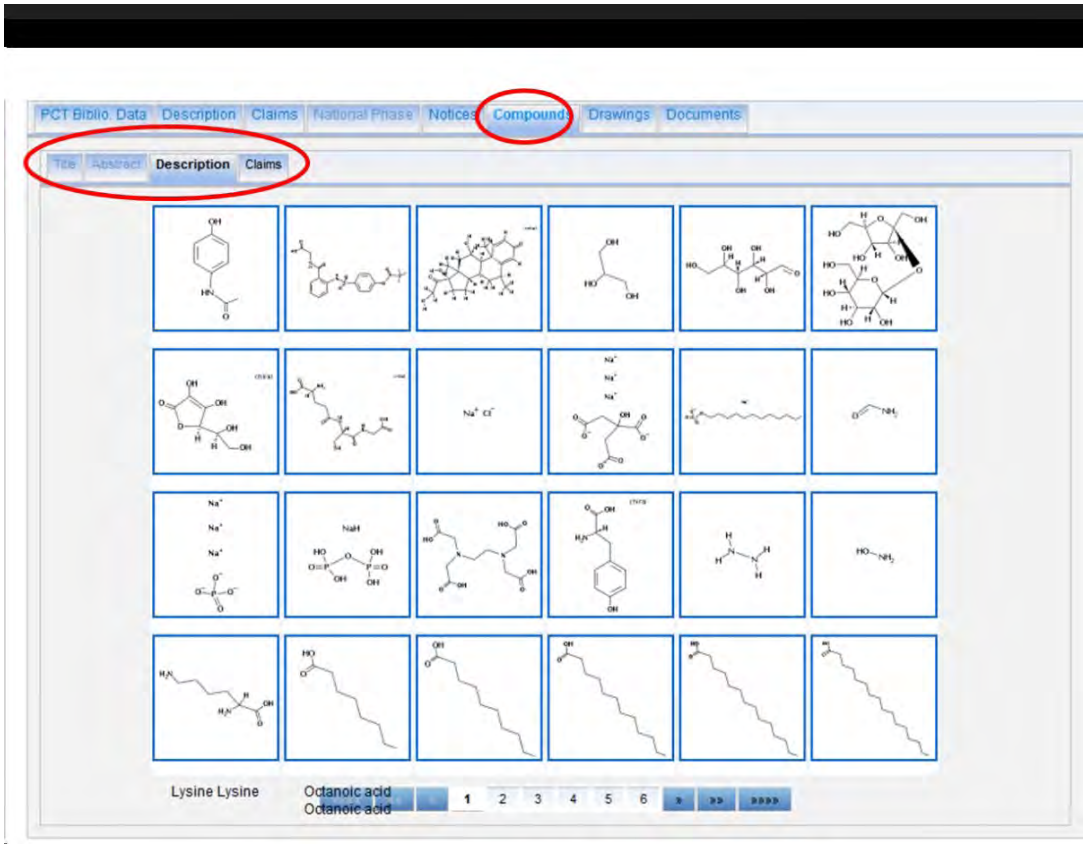
RSS

Analysis

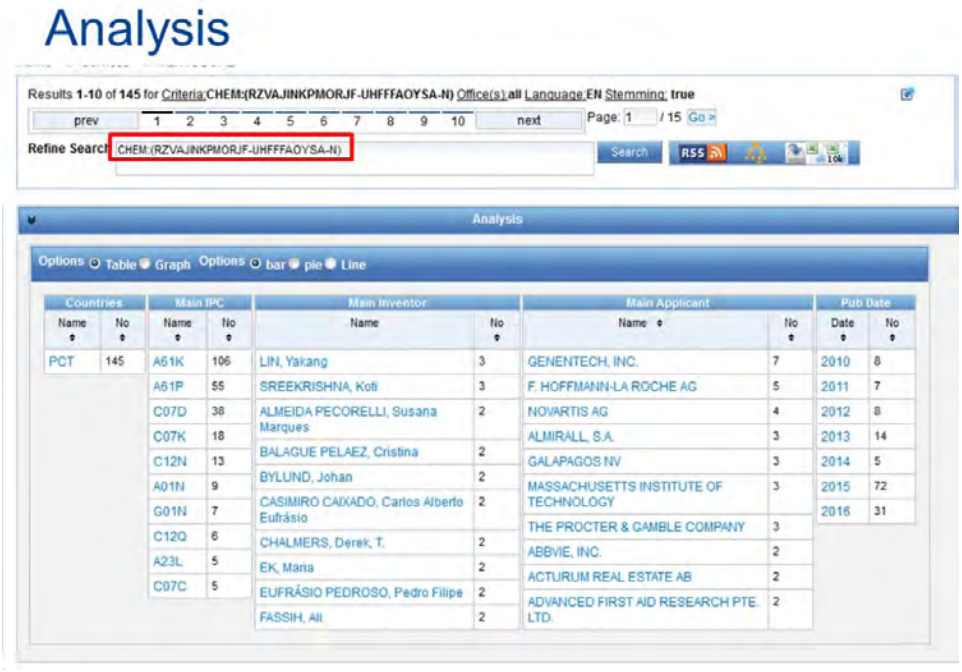
Sort by: Pub Date Desc View All List Length 10 Machine translation

Int.Class	Appl.No	Applicant	Ctr	PubDate
1. WO/2016/142349 **USE OF CREATINE KINASE AND DERIVED PEPTIDES THEREOF TO RELIEF PAIN**			WO	15.09.2016
A61K 38/45	PCT/EP2016/054816	CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE - CNRS -		GOUMON, Yannick
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.				
2. WO/2016/142689 **TISSUE ANALYSIS BY MASS SPECTROMETRY OR ION MOBILITY SPECTROMETRY**			WO	15.09.2016
G01N 33/68	PCT/GB2016/050619	MICROMASS UK LIMITED		PRINGLE, Steven Derek
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.				
3. WO/2016/142691 **RAPID EVAPORATIVE IONISATION MASS SPECTROMETRY ("REIMS") AND DESORPTION ELECTROSPRAY IONISATION MASS SPECTROMETRY ("DESI-MS") ANALYSIS OF SWABS AND BIOPSY SAMPLES**			WO	15.09.2016
G01N 33/68	PCT/GB2016/050621	MICROMASS UK LIMITED		TAKÁTS, Zoltán
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.				
4. WO/2016/142674 **CELL POPULATION ANALYSIS**			WO	15.09.2016
G01N 33/68	PCT/GB2016/050603	MICROMASS UK LIMITED		JONES, Emrys
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.				

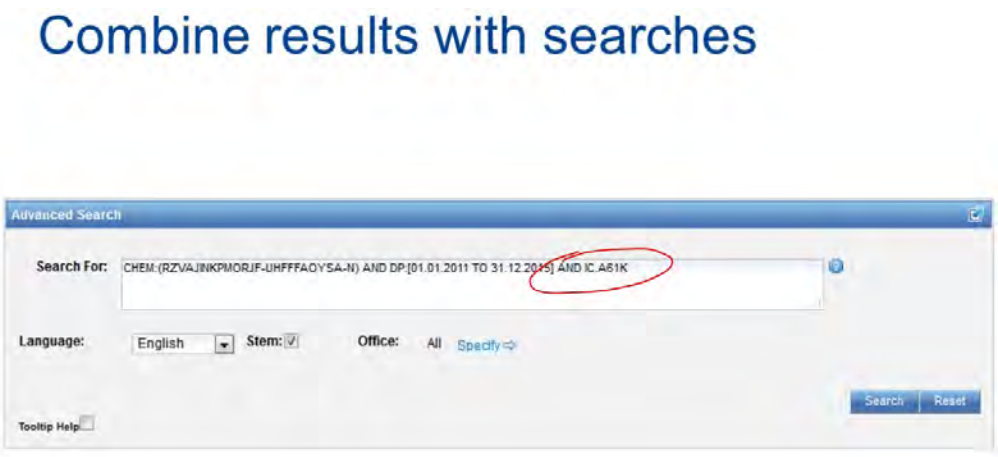
PatentScope can display the structures in the results retrieved by the search, as shown.



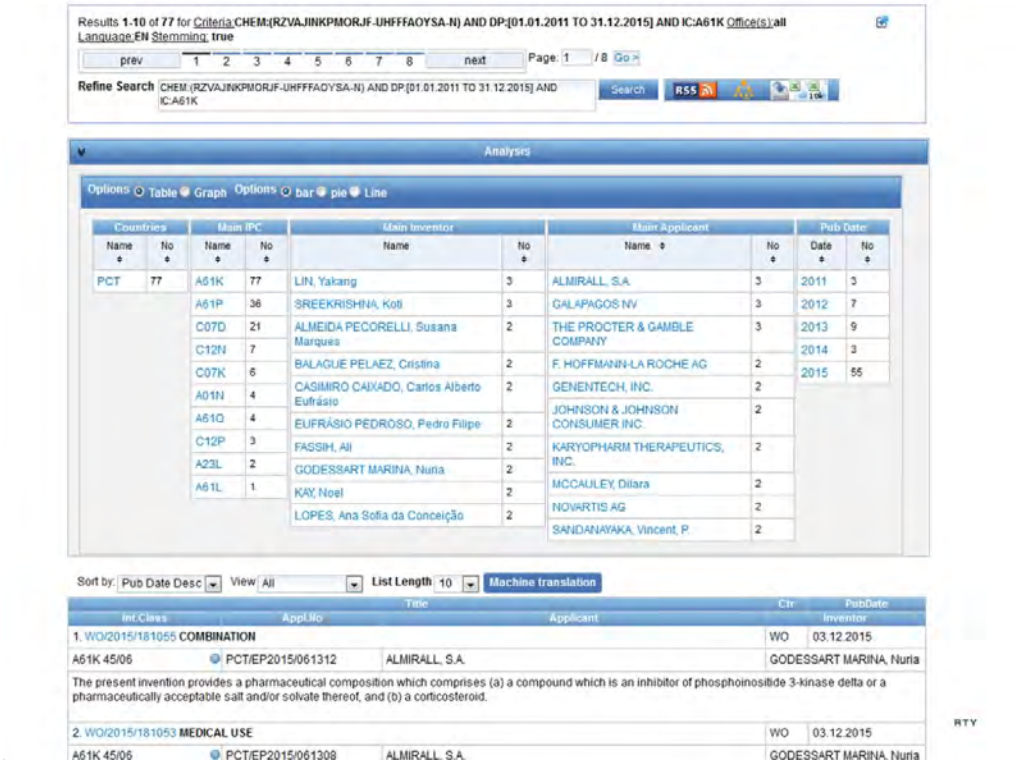
See the InChIKey in the refined search.



Structure search is combinable with other search criteria:



To get a new results list.



Example: Prozac

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

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 IiUPAC names and search with the names.
annotated with InchiIkeys

13. OK so the trivial name is also indexed as an InChI string or InChiKey?
yes

End of Q and As.