



REUTERS/Fayaz Kabli

ICIC 2012 -Markush datafeed

Brian Larner

Product specialist

Thomson Reuters

September 2012



THOMSON REUTERS

What is the biggest problem with searching markush patents?

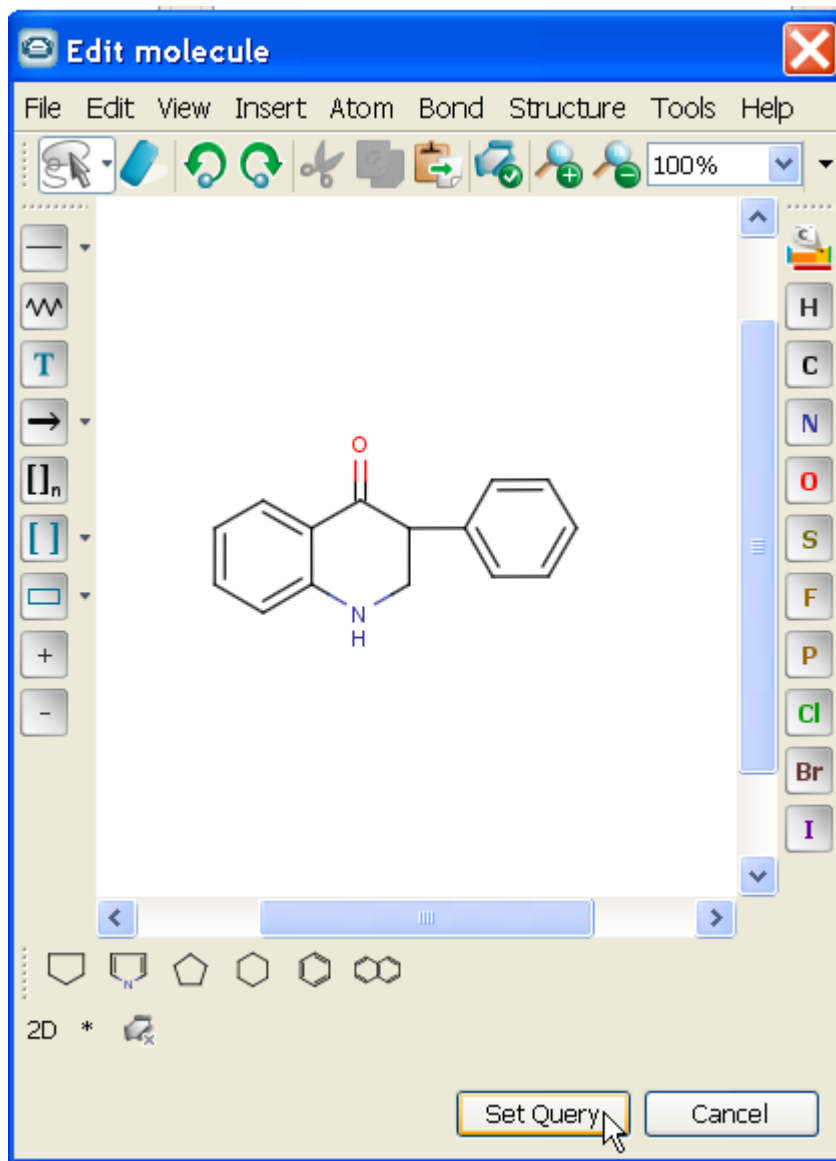
- Designing the best search to find them?
- Understanding them once you have found them?
- Finding white space around them?



MARKUSH DATA FEED CONTENT

- Markush from ~550,000 patent families
 - re-drawn & stored in Thomson Reuters vmn file format
 - plus 1.7m related specific compounds
 - plus the corresponding DWPI records in cXML format
 - from 26 patent issuing authorities
 - covers pharmaceutical, agrochemical and general chemistry patents
- Complete data set now available
 - DWPI Markush data back to 1987
 - All DCR structural records included (including patents with no markush structures)
 - INPI data also added
- Indexed as part of the editorial process that creates Derwent World Patents Index (DWPI) which can form part of the datafeed
 - Informative English language titles & abstracts from worldwide patents
 - Patent family listing, patent assignees





Draw the structure



THOMSON REUTERS

Instant JChem 5.3.8

File Edit View Search Data Lists Tools Window Help

1 / 2

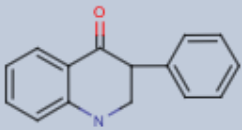
Projects [ijc-project-markush-demoset] x Welcome x Grid view for Invention:

Design Query Browse Clear Query Show All Run Query

Run Query (Ctrl+Q)

ID

vmns

Markush structure	compound number
	
Substructure	

Patents

Substructure search against the Markush dataset

Hit patent #1

Instant JChem 5.3.8

File Edit View Search Data Lists Tools Window Help

Projects [ijc-project-markush-demose] Welcome Grid view for Inventions Grid view for chemaxon_sample Form view for Inventions

Design Query Browse Entity: vmns

ID: 219

vmns

Markush structure

Go to First Row
Go to Previous Row
Go to Next Row
Go to Last Row

Browse to next hit patent

Title
New spiro-heterocyclic chromans, thiochromans and dihydroquinolines useful for treating e.g. apoptosis in cancer cells, cardiovascular disease, Alzheimer disease, Parkinson disease, depression or chronic obstructive pulmonary

Description
Spiro-heterocyclic chromans, thiochromans and dihydroquinolines of formula (I), their stereoisomers and salts are new. X=O, S(O)_n or NR; n=0 - 2; R₁, R₃, and R₄=hydrogen, alkyl, cycloalkyl, halogen, nitro, cyano, aryl, sulfonyl, aryl, alkoxy, alkoxy, carboxy, aminocarbonyl;
R₂=hydroxy, amino, aminocarbonyl, alkoxy, -O-alkenyl, -O-acyl, -O-alkylene-amino, -O-C(O)-alkylene-COOR_a, -O-C(O)-alkylene-amino, -O-C(O)-alkylene-heterocyclyl, -O-glucoside, -O-phosphoryl, -O-alkylene-phosphoryl or -O-C(O)-AA; AA=amino acid or di-peptide; R₅ R₁₀=hydrogen, alkyl

Assignees
LILLY & CO ELI
LILLY & CO ELI
CHU D T W
GALILEO PHARM INC
JAMES D R
WANG B

Novelty
Spiro-heterocyclic chromans, thiochromans, dihydroquinolines, their stereoisomers, and salts are new.

Patents
WO2006093548-A1 *
AU2005328328-A1
EP1856079-A1
IN200703515-P2
CN101163687-A
JP2008531559-W
US20080207588-A1
MX2007010328-A1
BR200520097-A2

Use
In preparation of composition useful for treating apoptosis in cancer cells (e.g. prostatic cancer, gastric cancer, breast cancer, pancreatic cancer, colorectal or esophageal cancer and airways carcinoma); diseases involving hypoxia or anoxia (e.g. atherosclerosis, myocardial infarction)

Mechanism Of Action
Lipoxygenase enzyme inhibitor. No biological data given.

Activity
Cytostatic; Respiratory-Gen.; Cardiovascular-Gen.; Antiarteriosclerotic; Cardiant; Cardiovascular-Gen.; Cerebroprotective; Vasotropic; Cardiant; Nootropic; Antidiabetic; Antiinflammatory; Gastrointestinal-Gen.; Nephrotropic; Gynecological; Antiasthmatic; Antiallergic; Antiinflammatory; Antigout; Antiarthritic; Antirheumatic; Antiarthritic; Osteopathic; Muscular-Gen.; Antiseborrheic; Dermatological; Antipsoriatic; Antiasthmatic; Respiratory-Gen.; CNS-Gen.; Tranquillizer; Antidepressant; Neuroleptic; Neuroprotective; Nootropic; Antiparkinsonian; Neuroprotective; Vulnery; Immunosuppressive; Ophthalmological. No biological data given.

Chemical structure 2: Spiro-heterocyclic chroman derivative with substituents R₁, R₂, R₃, R₄, R₅, R₆, R₇, R₈, R₉, R₁₀, R₁₁, R₁₂, R₁₃, R₁₄, R₁₅, R₁₆, R₁₇.

Chemical structure 3: Spiro-heterocyclic chroman derivative with substituents R₁, R₂, R₃, R₄, R₅, R₆, R₇, R₈, R₉, R₁₀, R₁₁, R₁₂, R₁₃, R₁₄, R₁₅, R₁₆, R₁₇.

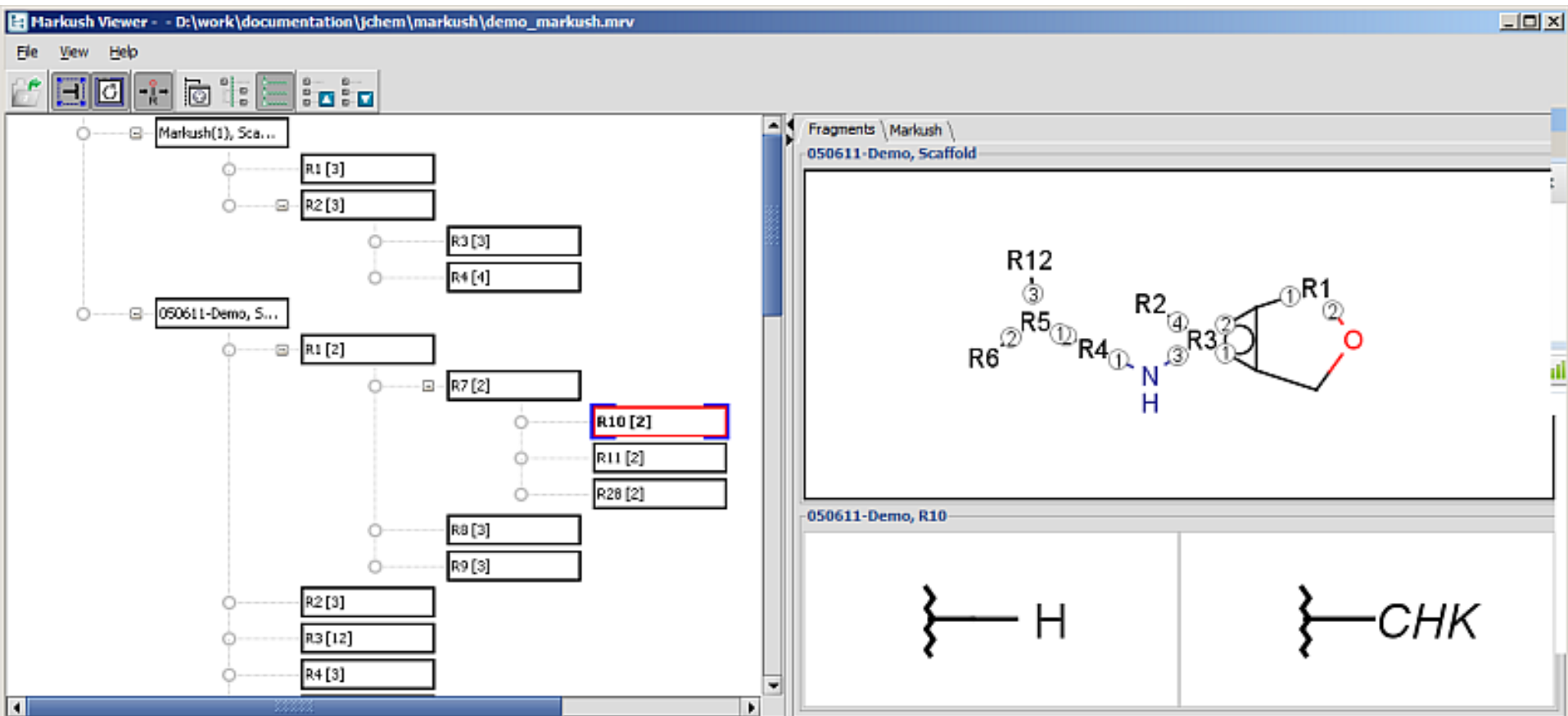
The screenshot displays the Instant JChem 5.3.8 application window. The main workspace shows a chemical structure of a 3-aryl-3-methyl-quinoline-2,4-dione derivative, highlighted in blue to indicate it is a 'Hit Markush'. The structure features a quinoline core with a methyl group at position 3 and various substituents labeled R1 through R8. A text box overlay on the left states: "Hit Markush - blue area indicates where the query occurs within the hit".

On the right side, a panel titled "Enumerate a Markush structure" provides detailed information for the selected hit (ID 3):

- Title:** Enumerate a Markush structure
- Description:** 3-Aryl-3-methyl-quinoline-2,4-dione compounds of formula (I) their salts are new. R1-R4 = H, OH, halo, nitro, amino, 1-4C haloalkyl, CN, 1-4C alkyl, 2-4C alkenyl, 2-4C alkynyl, azido, acylamino, 6-14C aryl, 1-4C alkoxy, aryloxy, benzyloxy, piperidinyl, N-methyl piperidinyl or heterocyclic; and X, Y1 = H, halo, nitro, (cyclic) amino, piperazinyl, carboxyl, alkylsulfinyl, haloalkyl, CN, alkyl, alkenyl, alkynyl, azido, acylamino, sulfonyl, aminosulfonyl, aryl, alkoxy, heterocyclic, acyloxy, alkylthionyl, arylthionyl, alkylloxycarbonyl, aryloxycarbonyl, aralkyloxycarbonyl or carbamoyl (where ureido or amidino groups substituted by 1-4C alkyl, 6-14C aryl, 1-4C alkynyl, 2-4C alkenyl, 2-4C alkenyl).
- Assignees:** KOREA RES INST CHEM TECHNOLOGY, CHO H, CHOI J, JUNG D, JUNG Y, KANG S, KONG I.
- Novelty:** 3-Aryl-3-methyl-quinoline-2,4-dione compounds (I) their salts are new.
- Activity:** Nootropic; CNS-Gen.; Neuroprotective; Tranquillizer; Antidepressant; Neuroleptic; Antimanic; Anticonvulsant; Antimigraine; Antiaddictive; Anorectic; Eating-Disorders-Gen.; Hypnotic.
- Patents:** US20060084676-A1 *, EP1650190-A1, JP2006117667-A, KR2006054045-A, KR825040-B1, US7592457-B2.
- Mechanism Of Action:** 5-Hydroxy tryptamine (5-HT)-6 serotonin receptor inhibitor. (I) were tested for 5HT-6 serotonin receptor inhibitory activity in insect cell. The median inhibitory concentration of 5,7-dichloro-3-methyl-3-phenyl-1H-quinoline-2,4-dione was 1.5 μM.

At the bottom, a text box states: "Each record contains valuable English language DWPI (Drug-World Patent Index) information including patent status, activity, and mechanism of action." The interface also shows a menu bar (File, Edit, View, Search, Data, Lists, Tools, Window, Help) and a toolbar with various icons for file operations and chemical structure manipulation.

CHEMAXON MARKUSH VIEWER



050611-Demo nesting view



Previous

Next

Instant JChem 5.3.8

File Edit View Search Data Lists Tools Window Help

Projects [ijc-project-markush-demoset] x Welcome x Grid view for Inventions x Grid view for chemaxon_sample x Form view for Inventions x

Design Query Browse Entity: vmns

ID: 3

vmns: Markush structure

R6

Enumerate a Markush structure

Enumeration options:

- ☐ Full enumeration
- ☒ Random enumeration
- ☐ Markush reduction according to the hit

Max structures: 10

☒ Output to file

Rows: 2

Columns: 3

☐ Show R-groups

☐ Colouring

Enumerate

Full enumeration of this structure produces 4698509682954150 (~ 10¹⁶) structures

10 structures enumerated

Enumerated structures can be exported to sdf, smiles, mrv etc. formats

R7

R2 R7 R8 R8

2

Close



THANK YOU

Q&A

steve.hajkowski@thomsonreuters.com



THOMSON REUTERS