

DWPIM (Derwent Markush Resource)

Subject Coverage	 Organic and organometallic compounds Inorganic compounds, polymers, peptides and partially defined structures 					
File Type	Markush Structures					
Access	The file is only availab	le on ST	Next			
Features	Alerts (SDIs) Monthly, weekly or with each update (2 updates per week) (every update is the default)			ek)		
	CAS Registry Number [®] Identifiers		Page Images		STN [®] AnaVist™	
	Keep & Share		SLART		STN Easy®	
	Learning Database		Structures	\checkmark		
Record Content	 Markush structures from approx. 890,000 Derwent World Patents Index (DWPI) documents 					
File Size	More than 2.3 million records (08/2020)					
Coverage	1961 to date					
Updates	Twice-weekly					
Language	English					
Database Producer	Clarivate Analytics (UK) Limited Friars House, 160 Blackfriars Rd. London SE1 8EZ United Kingdom Copyright Holder: Clarivate Analytics					
Sources	For patents included in Derwent World Patents Index, DWPI Markush includes indexed structures from claims, examples, disclosure					
User Aids	 Derwent Markush Resource on STN – Reference Manual Building and Searching Structures on STN Online Helps (HELP DIRECTORY lists all help messages available) STNGUIDE 					
Clusters	File currently not available in clusters.					
Pricing	Enter HELP COST at an arrow prompt.					
Related Databases	WPIDS/WPINDEX/WPIX					

Search and Display Field Codes

Search Field Name	Search Code	Search Examples	Display Codes
Accession Number	/AN	S 9925-IWL05/AN	AN
Entry Date	/ED	S 20151029/ED	ED
Markush Descriptor	/MDE	S S/MDE S SINGLE SPECIFIC STRUCTURE/MDE	MDE
Substance Descriptor (default)	/SDM	S N/SDM S NATURAL POLYMERS/SDM	SDM
Update Date	/UP	S UP=NOV 2017	UP

DISPLAY and PRINT Formats

Any combination of formats may be used to display or print answers. Multiple codes must be separated by spaces or commas, e.g., D L1 1-5 AN ED. The fields are displayed or printed in the order requested.

Hit-term highlighting is available for all fields. Highlighting must be ON during SEARCH to use the HIT, KWIC, and OCC formats.

Format	Content	Examples
AN ED MDE (1) PNK (1) SDM	Accession Number Entry Date Markush Descriptor Patent Number/Kind Code Substance Descriptor	D AN D ED D MDE D PNK D SDM
ALL (FULL)	AN, SDM, STR, ED, UP (ASB is default) (complete Markush structure)	D ALL
IÀLL (IFULL)	ALL, indented with text labels (complete Markush structure)	D IALL
ASB (STD, IDE)	Assembled hit structure including parts of the MARKUSH structure that match the query structure	D ASB
IASB (ISTD)	ASB, indented with text labels	D IASB
BRIEF	ASB plus definitions for unmatched G-groups that are visible in the assembled display	D BRIEF
SCAN TRIAL (TRI, SAMPLE, SAM)	SDM, ASB, ED, UP (random display, no answer numbers) SDM, ASB, ED, UP	D SCAN D TRIAL
HIT KWIC OCC	Hit term(s) and field(s) Up to 50 words before and after hit term(s) (KeyWord-In-Context) Number of occurrences of hit term(s) and field(s) in which they occur	D HIT D KWIC D OCC

(1) Custom display only.

Structure Searching

Terms	Search Examples
L-numbers of structures built using the STRUCTURE editor in STNext	SEARCH L1 SSS SAM S L1 SSS FULL

Types of Structure Searching

Туре	Definition	Search Code	Search Examples
Substructure (default) Closed Substructure	Search for substances which match the query. Substitution is allowed at all open positions. Additional components may be retrieved. Search for substances which match the query exactly. Substitution is allowed at positions opened by CONNECT. Additional components may be retrieved.	SSS CSS	SEARCH L1 SSS S L2 OR L3 SSS S L7 SSS SEARCH L1 CSS S L2 NOT L3 CSS S L4 OR L5 CSS

Scopes of Structure Searching

Scope	Definition	Search Code	Search Examples
Full Sample (default)	Search 100% of the file Search a fixed 10% of the file (a maximum of 50 records displayed)	FUL SAM	S L5 OR L8 SSS S L6 SSS SAM

Limiting Search Codes

Only an L-number for an answer set created in DWPIM may be limited.

Search Field	Search Code	Search	Display
Name		Examples	Codes
Answers completely iterated	/COM	S L4/COM	Not displayed
Answers incompletely iterated	/INC	S L4/INC	Not displayed

SELECT, ANALYZE, and SORT Fields

The SELECT command is used to create E-numbers containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field in an answer set.

The SORT command is used to rearrange the search results in either alphabetic or numeric order of the specified field(s).

Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
Accession Number	AN	Y (default)	Y
Entry Date	ED	Y	Y
Markush Descriptor	DE	Y	Y
Patent Number/Kind Code	PNK	Y	Y
Substance Descriptor	SDM	Y	Y
Update Date	UP	Y	Y

Crossover from DWPIM to WPIX, WPIDS, or WPINDEX

The crossover from DWPIM results to WPIX, WPIDS or WPINDEX is established by performing a search of the respective DWPIM L-number in WPIX respectively WPIDS or WPINDEX.

=> FIL DWPIM => S *L*-number search type (e.g. L1 sss ful) => FIL WPIX => s *L*-number => d *L*-number

The assembled display is the default display in WPIX. The commands for the assembled, brief and full hit structure in WPIX are as follows:

=> d *L-number* ahitstr => d *L-number* bhitstr => d *L-number* fhitstr

Crossover of Compounds from WPIX, WPIDS, or WPINDEX to DWPIM

Markush compounds from WPIX, WPIDS or WPINDEX records can be extracted and displayed in DWPIM by applying the transfer command. It is important to note that this step requires a reassignment of compound suffix MCN to AN.

The workflow is described in the following:

Fil DWPIM Tra *L-number WPIX record [range]* MCN /AN Example: Tra L1 1-3 MCN /AN

SAMPLE Record

DISPLAY ALL

AN 2091-38502 DWPIM SDM B: Pharmaceuticals, Agrochemicals; V: Simple organic compounds; Y: Mixtures



G-GROUP 1

H <mark>C</mark> XX

G-GROUP 2

H C XX

ED	20180409
UP	20180409

DISPLAY BRIEF

- AN 2091-38502 DWPIM SDM B: Pharmaceuticals, Agrochemicals; V: Simple organic compounds; Y:
- Mixtures



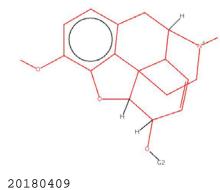
G-GROUP 1

H C XX

ED 20180409 UP 20180409

6 DWPIM DISPLAY ASB

AN 2091-38502 DWPIM SDM B: Pharmaceuticals, Agrochemicals; V: Simple organic compounds; Y: Mixtures



ED 20180409 UP 20180409

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