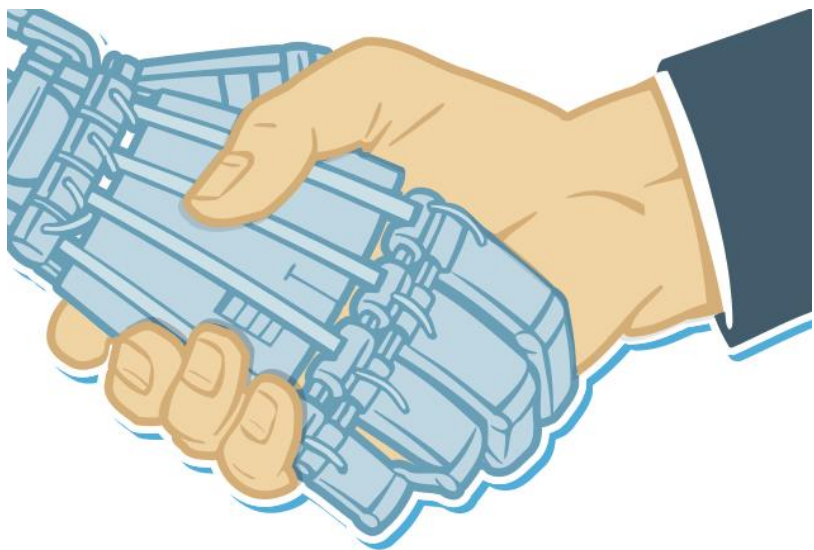


ChemCurator and Patent Curation Service

Computer-assisted chemical data extraction



- Name to Structure technology
- Structure search and representation
- Markush technology

Compounds extraction view

The screenshot displays a software interface with three main components:

- Project explorer:** Located on the left, it shows a tree view of projects including 'US20090048306A1', 'US20090270418A1', and 'US6796383_DEMO'.
- Annotated document:** The central pane shows a document with chemical synthesis procedures. Key text includes: 'mixture was quenched with NH₄Cl (aqueous saturated solution) and extracted with EtOAc. The organic layer washed with H₂O and brine, dried over Na₂SO₄, filtered, and concentrated in vacuo to yield a brown solid. The crude material was purified (hexane) to yield the desired product. LC/MS m/z 278.3 (MH+), R_t 1.88 minutes.' and 'Example 4 Ethyl 2-(5-methylbenzimidazol-2-yl)acetate'. The title compound was synthesized as described in Example 3, Method A using ethyl 2-(5-methylbenzimidazol-2-yl)acetate. LC/MS m/z 292.4 (MH+), R_t 1.60 minutes. N-(4-Cyano(3-pyridyl))-2-(5-methylbenzimidazol-2-yl)acetamide. The title compound was synthesized as described in Example 3, Method A using ethyl 2-(5-methylbenzimidazol-2-yl)acetate. LC/MS m/z 292.4 (MH+), R_t 1.71 minutes. 4-Amino-3-(5-methylbenzimidazol-2-yl)hydropyridino[3,4-b]pyridin-2-one. The title compound was synthesized as described in Example 3, Method A using N-(4-cyano(3-pyridyl))-2-(5-methylbenzimidazol-2-yl)acetamide. LC/MS m/z 292.4 (MH+), R_t 2.04 minutes. Example 5 4-(2-Morpholin-4-ylethoxy)-2-nitrophenylamine. Diisopropyl azodicarboxylate (1.1 eq) was added dropwise to a stirred solution of 4-amino-3-nitrophenol (1.0 eq), triethylamine (1.1 eq), and N,N'-dicyclohexylcarbodiimide (1.0 eq) in THF at 0°C. The mixture was allowed to warm to room temperature and the resulting mixture was stirred to warm to room temperature. The mixture was filtered and concentrated in vacuo to yield a brown solid. The crude material was purified (hexane) to yield the desired product. LC/MS m/z 278.3 (MH+), R_t 1.91 minutes.
- Compound list:** A table on the right listing extracted compounds with their structures, formulas, masses, and names.

#	Structure	Formula	Mass	Name	Comment
1					naphthyridin-4-yl 3-(... Ester in Y
2		C16H12N4O2	292.30	4-hydroxy-3-(5-methyl-1H-1,3-benzodiazol-2-yl)-1H-1,7-naphth...	OH in Y p
3		C19H11N5O	277.29	4-amino-3-(1H-1,3-benzodiazol-2-yl)-1H-1,7-naphthyridin-2-one	
4		C16H13N5O	291.31	4-amino-3-(5-methyl-1H-1,3-benzodiazol-2-yl)-1H-1,7-naphthy...	
5		C21H22N6O3	406.45	4-amino-3-[5-[2-(morpholin-4-yl)ethoxy]-1H-1,3-benzodiazol-2...	
6		C18H16N6O2	348.37	2-(4-amino-2-oxo-1H-1,7-naphthyridin-3-yl)-N,N-dimethyl-1H-1...	

Markush extraction view

The screenshot displays the Markush extraction view software interface. The main window is titled "US6756383_DEMO" and shows a document with chemical text and structures. A "Markush" window is open on the right, displaying a "Scaffold" and a grid of chemical structures. A "Checker View" window is open at the bottom left, showing "There are no problems found." A "Selected structures" window is open at the bottom center, showing a chemical structure and the text "alkyl-NH₂". An "Example structures" window is open at the bottom right, showing a grid of chemical structures. Several callout boxes are overlaid on the image:

- Annotated document**: A purple box pointing to a highlighted section of text in the main document: "R¹ and R² join to form a 6 membered substituted or unsubstituted ring comprising at least one O, N, or S atom."
- Structure checker**: A purple box pointing to the "Checker View" window.
- Markush editor**: A purple box pointing to the "Markush" window, which shows a grid of chemical structures and a "Scaffold" window.
- Selected structures**: A purple box pointing to the "Selected structures" window, which shows a chemical structure and the text "alkyl-NH₂".
- Example structures**: A purple box pointing to the "Example structures" window, which shows a grid of chemical structures.

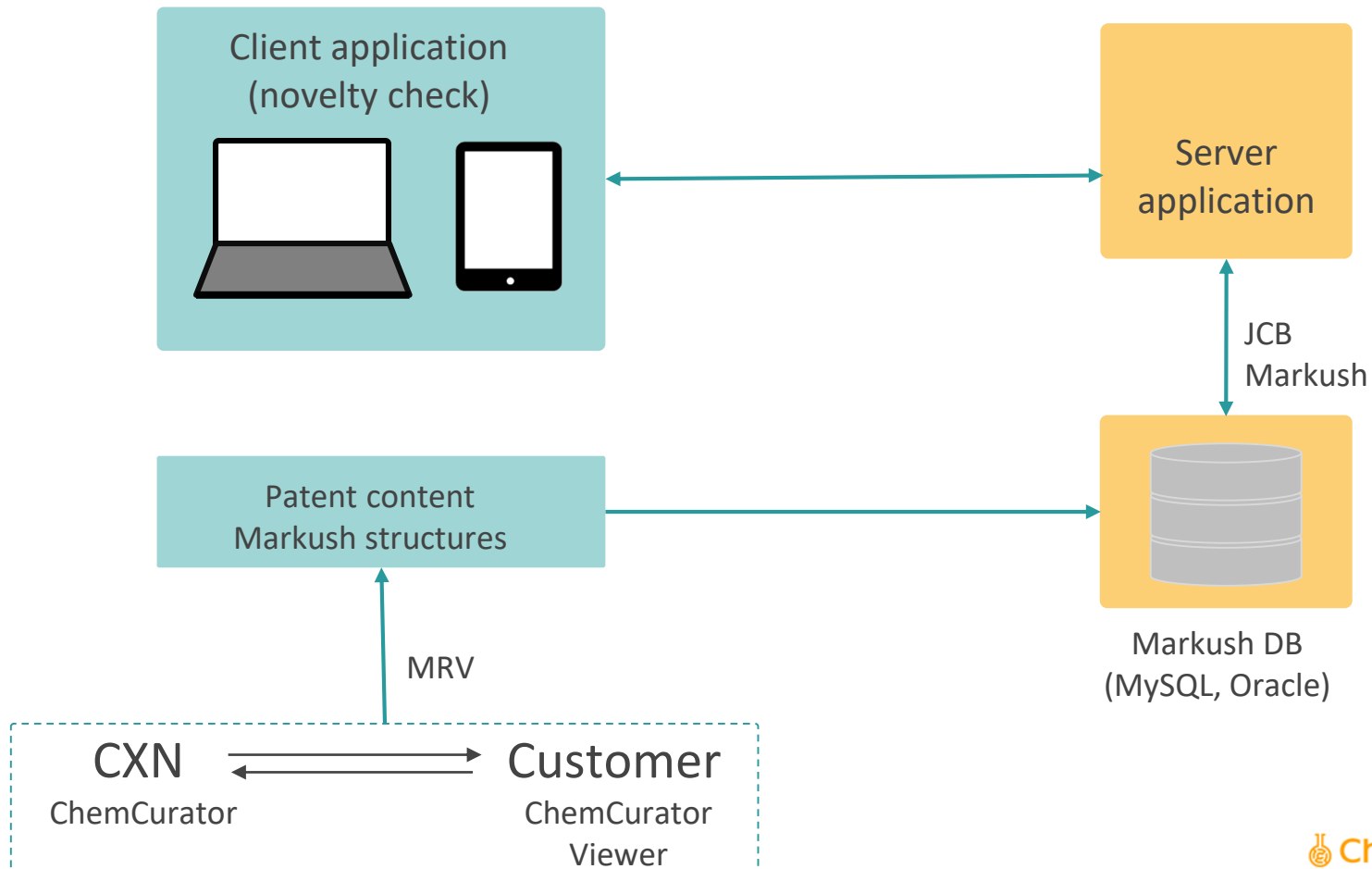
Patent curation service

High quality Markush structures extracted from project related patents or patent drafts by ChemAxon experts

Analysis of the claimed chemical space

Major use cases

- In-house novelty check
- Double check of patent drafts
- Use expert opinion in legal cases





THANK YOU