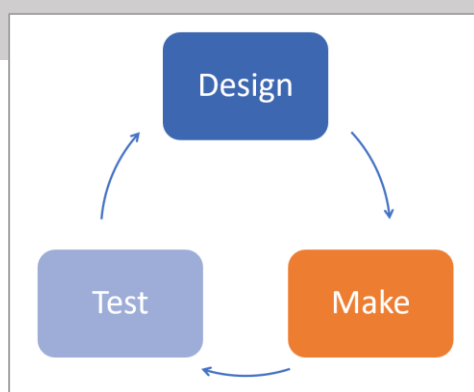


## Challenge

Artificial intelligence (AI) is a buzz word. Many of the technology scouting searches that we do at Strategic Allies Ltd (SAL) explore innovation in chemicals and related industries, so we wanted to understand how AI is being used in chemistry for molecule discovery.

We explored this hot topic by conducting a rapid landscape focusing on three key questions: - What work has been done with AI in chemistry for molecule discovery? Who is doing this work in academia and industry? Has the work been successful? SAL's clients are always looking to learn from their own and other industries, to understand who is developing new technologies and who they could partner with. Companies that can harness AI to speed up, improve, or reduce the costs associated with molecule discovery will be the key innovators in the chemicals and pharmaceuticals industries.



## The search

SAL conducted a rapid landscape using secondary research to explore the status of AI in chemistry. SAL found case studies on the use of AI in molecule discovery and identified leading academics and companies developing AI tools. To understand whether these tools are improving molecule discovery SAL identified issues with implementing AI in chemistry and looked for expert views of current progress. SAL discovered

that AI tools are applicable to a range of industries, with pharmaceutical companies being early adopters of the technology, often by partnering with some of the new AI startup companies. AI is used at all three stages of the design-make-test cycle of molecule discovery. AI can design new compounds based on known chemical, biological and physical properties, identify routes for chemical synthesis and find novel catalysts, and perform virtual screens of compound activity. AI is also being combined with robotics to speed up the bottleneck step of chemical synthesis. However, many AI tools need further validating and finessing, as AI is only as good as the training data used to develop it.

Synthesis routes for pharma drug and other molecules Chemical.AI

<b>Aim:</b> Design of chemical synthesis pathways for pharma as well as chemical engineering and new materials		<b>Outputs and success</b>	
<b>Chemists</b>	<b>AI developers</b>		
<ul style="list-style-type: none"> <li>Chemical.ai company founded in Wuhan China</li> <li>Collaborators in big pharma e.g., Wuxi Apttech, Roche</li> </ul>	<ul style="list-style-type: none"> <li>Chemical.ai, in-house IT professionals</li> </ul>	<ul style="list-style-type: none"> <li>Shortens the time needed to design a chemical synthesis route e.g., in a side-by-side comparison chemists took an average of 1.5 hours per route; versus only 8.7 minutes for AI design</li> <li>Company advertises that it has served &gt;100 pharma and CROs to expedite drug discovery</li> </ul>	
<b>Data inputs</b>			
<ul style="list-style-type: none"> <li>Probably in-house data; one of the company founders started working in cheminformatics in 2008</li> <li>Strategic partnership with Scilligence, a web-based informatics solution provider for R&amp;D, to co-develop high-efficiency data integration on Scilligence's ELN with Chemical.AI's AI-powered chemical route design systems</li> </ul>			
<b>Tools</b>			
<ul style="list-style-type: none"> <li>ChemAIRS is an AI-empowered retrosynthesis platform that designs multiple synthetic routes for specific chemicals using data mining and deep learning algorithms</li> <li>ChemAloT platform uses machine learning algorithms to support decision making in analytical chemistry e.g., during the development and optimization of chromatographic methods</li> <li>AloT automation lab (ChemAllab) combines a dry and wet lab, offering commercial chemical synthesis services</li> </ul>			
<b>Study:</b> In-house capabilities	<b>Date started:</b> 2018	<b>Chemicals discovered:</b> Pharmaceutical drugs	<b>Location:</b> China

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## Outcomes

- SAL identified academics and companies developing AI tools for all stages of the design-make-test cycle of molecule discovery
- AI in chemistry is developing, particularly in the pharmaceutical industry, but issues of data availability and how to encode molecular structures need development.