



Medicinal Chemistry Services

Peakdale Molecular offers its customers a first class range of extensive integrated medicinal chemistry services for drug discovery. These services build on the company's core strengths of highly innovative and world-renowned chemistry, its reputation for delivering quality products to customers on time and its passion for synthetic organic chemistry when applied to biological problems.

Peakdale has built up medicinal chemistry and computational chemistry expertise across therapeutic areas and spanning the drug discovery process from hit generation to Phase I clinical studies.

Peakdale has a proven track record of success in producing robust candidates suitable for proof-of-concept testing *in vivo*. To achieve this, the company utilises its highly experienced and committed teams to deliver on project goals and ensure complete client confidentiality and protection of Intellectual Property (IP).

Our medicinal chemistry services include:

1. Hit Generation

- A unique Peakdale collection of target specific and general screening compounds
- *In silico* screening and ligand based design
- The synthesis of client driven diverse/targeted arrays

2. Hit-to-lead

- Applying QSAR analyses to generate structure-based drug design in novel patent areas
- Establishment of SAR against a target
- Optimising ligand-receptor binding and enzyme inhibition with respect to potency and selectivity

3. Lead optimisation

- The synthesis of lead optimisation arrays
- Enhancing ADMET and pharmacokinetic properties utilising *in silico* and *in vitro* ADME data

4. Scale-up of intermediates and key compounds for further biological studies

5. Scaffold-hopping to produce alternative active series with novel IP and patent exemplification to protect IP

Proven track record in drug discovery

We have added value to a variety of medicinal chemistry projects for our partners, including many of the world's leading pharmaceutical and biotechnology companies. Our medicinal chemists have contributed to drugs undergoing clinical development as well as marketed agrochemicals and pharmaceuticals.

Peakdale's medicinal chemists are listed as inventors on a variety of patents and the company has a proven track record of helping customers establish IP and clearly adding value to the drug discovery process.

Computational Chemistry Services and drug discovery

We place great emphasis on the close interaction between our medicinal chemists and our Computational Chemistry Services to ensure timely, practical hypothesis testing to meet project goals. With extensive experience across therapeutic areas, we will apply appropriate tools from our computational capabilities to solve specific problems around a project, such as selectivity, potency physical properties and early ADME. Both 2D and 3D information from known active ligands is used to construct pharmacophores which guide our synthetic chemists in the design of highly focused arrays.

QSAR models are continually refined using new biological data to identify both favourable and unfavourable regions of space, providing the construction of smaller more focussed arrays. This drug design process is used iteratively to obtain the final target profile.

Drug Discovery

All of our medicinal chemistry is driven by the demands of modern drug design, working within property space to ensure rapid progression to the desired programme objectives.

At Peakdale we offer a range of *in vitro* ADMET predictive models, delivering accurate and reproducible quality data, while maintaining a focus on efficient turnaround times to facilitate our customers' drug discovery programs. In addition to our core assays, we also offer our clients the flexibility of bespoke assay design.

Complementing our laboratory facilities, we have an *in silico* capability dedicated to virtual high throughput screening for optimisation of ADMET properties aiding rational selection of compounds for *in vitro* experiments.

By combining our *in silico* and *in vitro* expertise, we can develop QSAR models to help predict ADMET and utilise software capable of predicting common ADMET properties from 2D structures. This information is invaluable in prioritising potential synthetic targets and can be trained using *in vitro* data generated either by a client or by our own *in vitro* ADME services.

Delivering on time

With the support of a dedicated team of analysts, Peakdale ensures that customers' compounds move quickly through the discovery pipeline. Excellent project management ensures the company meets agreed aims and objectives through active tracking of project progress and close liaison with customers.

Utilise Our Expertise

Please contact us to discuss, in complete confidence, how Peakdale can add value to your drug discovery activities;

Telephone +44(0)1298 816700 Fax +44(0)1298 816701 email enquiries@peakdale.co.uk

Applying its innovative chemistry expertise and flexible resources, Peakdale Molecular supports its customers' drug discovery activities through the following products and services;

- Medicinal Chemistry
- Custom Synthesis
- Analytical Services
- Contract Research
- CADD Services
- Intermediates Catalogue
- Peakexplorer Focused Libraries
- Lead-like Compounds for Screening
- *In Vitro* ADMET Services
- Microwave Synthesis Services

Founded in 1992, Peakdale Molecular is based in Chapel-en-le-Frith in the UK, where its purpose built facilities house organic research labs, parallel synthesis labs and a kilo scale-up lab, all of which are supported by a fully equipped analytical department.

www.peakdale.com