

## NexMR and Chemspace to expand the chemical space of photoinducible small molecules for ultrafast NMR screening

23<sup>th</sup> January 2024 – NexMR AG, a high-performance Nuclear Magnetic Resonance (NMR) company, and Chemspace LLC, a leading platform for small molecule drug discovery, are delighted to announce that they have entered a strategic collaboration. This partnership aims to develop fragment libraries compatible with photoinduced hyperpolarized NMR, accelerating NMR measurements over 10,000-fold and enabling screening with cheap benchtop NMR spectrometers. This collaboration will also expand the known chemical space of photoinducible small molecules and ultimately supercharge the REAL space with photoinduced hyperpolarized NMR.

The first library resulting from this collaboration, **NMhare™**, will be released in versions of 500 and 1,000 fragments, covering a diverse chemical and pharmacophoric space. The library is pre-dosed with the appropriate photoinduction kit to boost the recording of NMR experiments at an ultrafast pace and low sample concentration. Chemspace will supply the fragment molecules from its vast catalog, and NexMR will dope the fragments with its photoinduction kits. In the next phase of this collaboration, NexMR and Chemspace will continue developing new photoinducible libraries and methodologies for smooth and quick hit-to-lead optimization by exploring the REAL space.

Chemspace's platform, encompassing REAL and Freedom Spaces, boasts over 2.3 trillion accessible molecules. It provides the ideal platform for efficient hit finding and exploration – from uncovering previously unknown starting points for your discovery projects to rapid hit expansion and optimization using cutting-edge technologies in Computational Chemistry, Bioinformatics, and Machine Learning.

NexMR's photoinduction technology enables ultrafast NMR-based fragment screening, even at low micromolar target and fragment concentration. NexMR develops machine learning algorithms predicting the condition to trigger photoinduced hyperpolarization of individual small molecules. NexMR ultrafast screening technology is implementable on high-field NMR instruments (see **Cryolight™**) and low-field NMR such as benchtop NMR spectrometers.

Olga Tarkhanova, CEO at Chemspace, commented: "I am thrilled to announce our groundbreaking collaboration with NexMR, marking a pivotal moment in our mission to revolutionize drug discovery. This partnership merges our expansive small molecule catalog with NexMR's advanced photoinduction NMR technology, setting a new benchmark in the industry."

"We are looking forward to strengthening the collaboration with Chemspace," added Félix Torres, CEO of NexMR. "This collaboration will fuel the development of a large photoinducible fragment catalog thanks to the large synthetically accessible chemical space developed by Chemspace. Combining REAL and FREEDOM space with our ultrafast NMR technologies will supercharge hit-to-lead campaigns."

For media inquiries, please contact:

### **NEXMR AG**

Dr. Félix Torres Hubiche, CEO

Email: [ftorres@nexmr.com](mailto:ftorres@nexmr.com)

### **CHEMSPACE LLC**

Dr. Olga Tarkhanova, CEO

Email: [o.tarkhanova@chem-space.com](mailto:o.tarkhanova@chem-space.com)



### **ABOUT NEXMR**

NexMR AG is an innovative technology company dedicated to revolutionizing fragment-based drug discovery. Leveraging advanced nuclear magnetic resonance (NMR) techniques, NexMR provides efficient solutions for fragment screening and lead optimization. Their cutting-edge platform enables researchers to accelerate the development of novel therapeutics. For more information, visit <https://www.nexmr.com>.

### **ABOUT CHEMSPACE**

Chemspace LLC is a leading provider of end-to-end services covering every facet of the Drug Discovery process up to pre-clinical studies. Implementation of advanced technologies enables the identification, delivery, testing, and optimization of the exact molecule the client needs from the trillions accessible. Chemspace hosts the largest online catalog of small molecules: building blocks, fragments, screening compounds, reagents, and intermediates. We also provide sourcing and procurement services. Our main goal is to deliver high-quality products to our customers to speed up their research projects. For more information, visit <https://chem-space.com>.