**PRESS RELEASE**
FOR IMMEDIATE RELEASE – April 29, 2021

## OneAngstrom and Molecular Forecaster announce the first integration of the FITTED Suite as a new SAMSON application for state-of-the-art protein-ligand docking.

GRENOBLE, France and MONTRÉAL, Québec, Canada – April 29, 2021 – OneAngstrom (1A), the developers of SAMSON, the open molecular design platform, and Molecular Forecaster (MFI), a leading scientific software and consulting company accelerating various elements of the drug discovery pipeline, announce the release of the FITTED Suite as a new SAMSON application for state-of-the-art protein-ligand docking that integrates five Molecular Forecaster tools:

- FITTED (Flexibility Induced Through Targeted Evolutionary Description) is a unique, fully automated docking software that intelligently recognizes the flexibility of macromolecules, the presence of bridging "displaceable" water molecules, covalent functional groups, and proton shifts upon metal coordination. FITTED is based on a genetic algorithm with an emphasis on balancing speed and accuracy. Third-party studies attest to its success and demonstrate its application to metalloenzymes, kinases, nucleic acids, NHRs, GPCRS, and more.

- PREPARE (Protein Rotamers Evaluation and Protonation based on Accurate Residue Energy) automates protein preparation by cleaning up frequent liabilities, by optimizing various physicochemical properties, and by orienting water molecules.

- PROCESS (Protein Conformational Ensemble System Setup) generates modified protein files for FITTED.

- SMART (Small Molecule Atom-typing and Rotatable Torsion assignment) characterizes small molecules for FITTED.

- CONVERT (Conformational Optimization of Necessary Virtual Enantiomers, Rotamers and Tautomers) transforms 2D small molecules into accurate 3D representations.

"Our goal with the SAMSON platform is to democratize access to molecular modeling and enable enterprises and research groups to build personalized solutions that help them achieve their scientific and business objectives," said Stephane Redon, CEO of OneAngstrom. "Molecular Forecaster has developed an impressive suite of premium drug discovery tools, and we are thrilled that the release of the FITTED Suite will give SAMSON users access to Molecular Forecaster's recognized expertise and technology."

"Our partnership with OneAngstrom is guided by the needs of our users. The integration of our predictive modeling algorithms within SAMSON provides chemists the opportunity to perform high-quality simulations while having hands-on setup, analysis, and manipulation at their fingertips," said Josh Pottel, CEO of Molecular Forecaster. "The beautiful SAMSON interface, the complementary design tools, and the ease of installation and update make this partnership ideal for us and for our users."

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