



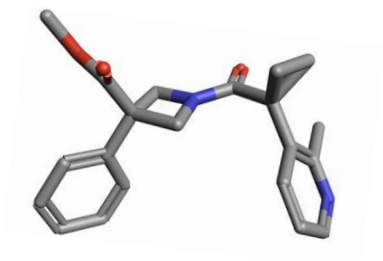
LCC'S MOLECULES OF THE MONTH

Lead-like Virtual Library of 3D-Fragments

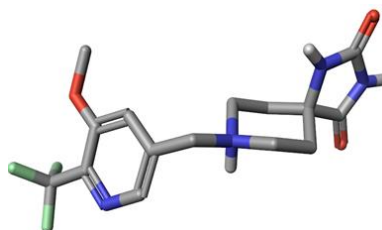
In order to create a Ro4 lead-like virtual library that is **drug-like**, **novel**, **diverse**, **3D-rich**, and **enantiomerically pure**, LCC collaborated with one of the best-in-class cheminformatics companies (Cresset). This set of > 5,000,000 compounds is now available for virtual screening, while the team prepares to tackle the synthesis of the hits, with a success rate > 90%.



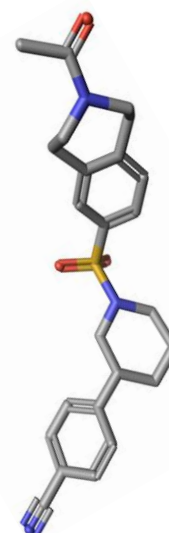
Acylation of A1626



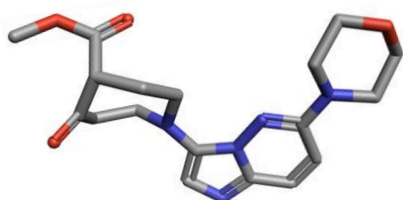
Alkylation of A10804



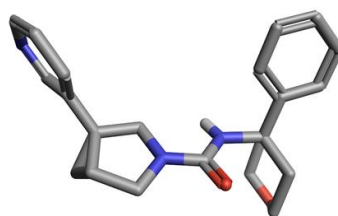
Sulfonamide formation on A0384



SnAr of A10153



Urea formation on A8662



Library's **properties overview**: **MW = 370** (160 to 420), **cLogP = 3** (-3 to 4), **PSA = 70** (20 to 140),
f-sp³ = 0.5 (0.1 to 1.0), **QED = 0.85** (0.2 to 1.0)

The lead-like library is part of **LCC's private chemical space** and only available to selected clients under CDA. To explore the library's full range of properties and/or access it, please contact us at sales@liverpoolchirochem.com.

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