



ACS Local Section
North Jersey

Analytical Characterization of Macrocyclic Peptidomimetic Compounds by NMR Spectroscopy

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Time: 12:00 pm ET via Microsoft Teams



Abstract

In an effort to develop novel therapeutics to complex biological targets, many new drug modalities that extend beyond traditional small molecule drugs have gained popularity within the drug discovery landscape. Amongst these, peptide-based drugs offer an attractive means of inhibiting protein:protein interactions of featureless protein surfaces and constitute ~10% of new drug approvals in the past 2 years. The hybrid features of peptidomimetic drugs make analytical and structural characterization using standard small molecule or protein techniques difficult, and a robust analytical toolkit is needed. Herein, we describe several NMR based applications to the characterization of conformationally constrained cyclic peptidomimetic compounds including: 1) concentration determination and purity workflows, 2) triaging of well-behaved single conformer compounds by 1D proton spectral screening, 3) qualitative structural characterization for medium throughput analysis and 4) generation of full 3D structural ensembles on well behaved drug leads. These methods have been applied to address numerous questions in the early discovery process.

Connection Information

This will be a virtual meeting hosted via Microsoft Teams. A direct link to the meeting is located [HERE](#). Further information can be found on the NMR Topical Group website (<https://www.njacs.org/nmr-spectroscopy-topical-group>). Please reach out to Tom Osborn Popp (thomas.osbornpopp@rutgers.edu) or Christine Jorge (christine.jorge@bms.com) with any questions.

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