Center for Eukaryotic Structural Genomics

Technology Dissemination Report

CESG Tech Report No.	014
Title	PINE (Probabilistic Inference Network of Evidence)
Research Unit	NMR Spectroscopy
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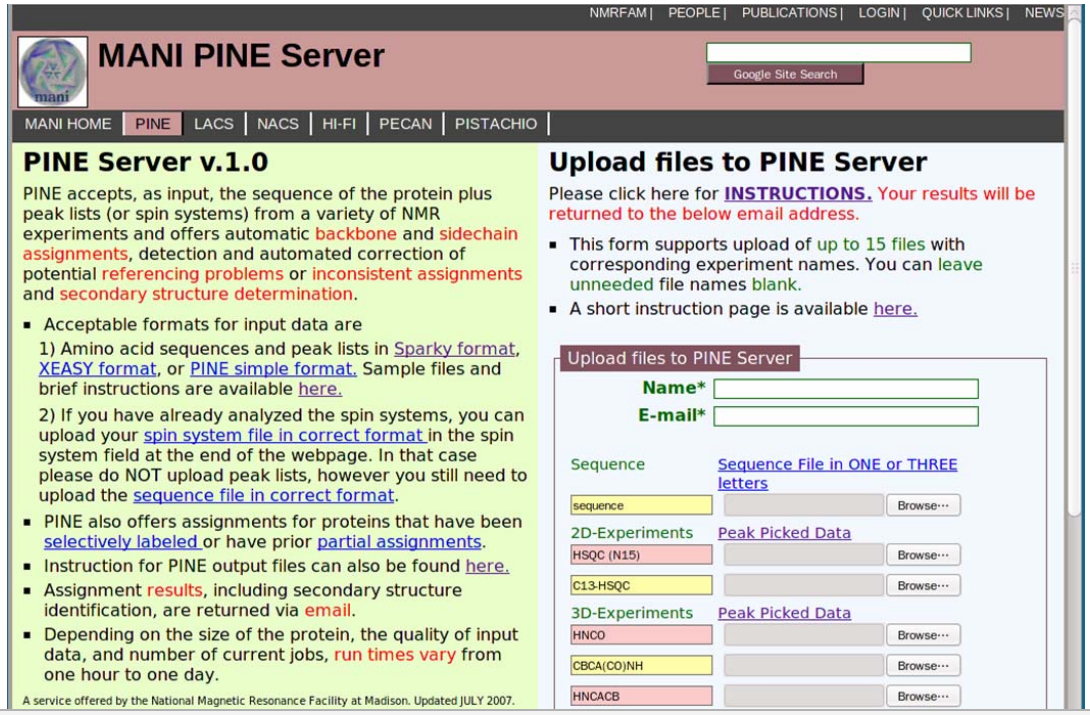
Primary Contact	http://miranda.nmrfam.wisc.edu/PINE/



Summary

PINE, which is available from a webserver at http://miranda.nmrfam.wisc.edu/PINE/, is the implementation of a multiple step probabilistic data analysis platform for protein NMR spectroscopy. As of 12/08 PINE has been used more than 1300 times by external Users. PINE incorporates the capabilities of separate probabilistic tools: PISTACIO [1] (automated backbone and sidechain assignment), PECAN[2] (secondary structure determination), and LACS [3] (referencing offset and outlier detection). The input to PINE is the amino acid sequence and sets of peak lists generated from one or more of the standard types of protein NMR experiments; these can be either probabilistic (e.g., peak lists generated by HIFI-NMR) or traditional peak lists generated by popular NMR data analysis tools. PINE takes into account the interconnectedness of different stages of analysis. PINE begins with a set of local statistical potentials. It then proceeds iteratively until a stationary state for a consistent global similarity measure is achieved. The resulting software enables a seamless and robust integration of multiple steps in the NMR structure determination pipeline. PINE provides as output a probabilistic assignment of backbone and sidechain signals and the secondary structure of the protein. At the same time, it identifies, verifies, and if needed rectifies, problems related to referencing, assignment, or outlying data. PINE can make use of prior information supplied from selective labeling or spin system assignments derived independently by other means. The performance of PINE is much superior to that of the individual tools used sequentially.

Publications:

[1] Eghbalnia, H.R., Bahrami, A., Wang, L., Assadi, A., and Markley, J.L. (2005) *J Biomol NMR* 32(3):219-33.
[2] Eghbalnia, H.R., Wang, L., Bahrami, A., Assadi, A., and Markley, J.L. (2005) *J Biomol NMR* 32(1):71-81.
[3] Wang, L., Eghbalnia, H.R., Bahrami, A., and Markley, J.L. (2005) *J Biomol NMR* 32(1):13-22.

Acquiring the Technology	Available from: http://miranda.nmrfam.wisc.edu/PINE/
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