

Navdeep Jaitly

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Work Experience

Senior Research Scientist IV (Jan '08 – July'08) & Senior Research Scientist III (Sept '04 – Dec '07), Pacific Northwest National Laboratory

- Developed a Multivariate Mixture Model to statistically characterize noise and signal in high throughput scientific data and used the model to develop a search engine using Expectation Maximization which allowed optimal selection of results at different levels of confidence.
- Developed algorithms for discovering common features in hundreds of mass spectrometry datasets using dynamic programming algorithms to align time series data and hierarchical clustering algorithms to group features.
- Developed improved signal processing and peak detection algorithms for mining of mass spectra where each dataset is of an average size of 8 Gb and sped up previous algorithms by 80%.
- Developed two analytical software tools: Decon2LS (open source) and MultiAlign in C++ and C# for manual and automated analysis of spectral data.
- Performed statistical analysis (using Matlab and R) and communicated results in various interdisciplinary settings related to different biological projects (burn patients, Malaria, Rat Mouse brain study, etc) to guide the interpretation of biological data.

Bioinformatics Lead, Collaborative Project with Université De Montréal, Apr '04 – Sept '04

- Developed Peptide Miner software for feature detection in mass spectrometry data, in collaboration with Dr. Pierre Thibault, University of Montreal.
- Software developed is now used to perform LC-MS data analysis at the Institute of Cancerology and Immunovirology, University of Montreal.

Group Leader, Senior Bioinformatics Scientist(Mar'01-'02), Caprion Pharmaceuticals Inc., Mar '01 – Apr '04

- Investigated and implemented several Data Mining, and AI approaches to discover, classify and predict trends in Biochemical data sets from Mass Spectrometry.
- Developed indexing method for searching for tags in the human genome
- Developed *Deep Search*, an algorithm to identify genetic differences, mutations and Biochemical Modifications using peptide mass spectra.
- Developed clustering algorithm to organize and assess the certainty of Protein Identification. Used it for comparing results of experiments from different conditions as a first pass at detecting biomarkers.

Software Developer, SMART Research Group, IBM Toronto Labs, Aug '00 – Mar '01

- Modernized existing tool (Smart Guide) for automatic database configuration of DB2, IBM's Universal Database.
- Laid a framework for learning of optimal database configurations in DB2.

Education:

- Master's in Computer Science (MMath). University of Waterloo, Waterloo, ON. August 200
- B.S., Computer Science & Mathematics. Hanover College, Hanover, IN. May 1998.
- B.Tech (one year) Indian Institute of Technology, I.I.T. Delhi.

Publications & Patents:

- Sorensen, C.M., Ding, J., Jaitly, N., et. al. *Journal of Chromatography B Analytical Technologies in the Biomedical and Life Sciences*. 2008 May 7. Application of the accurate mass and time tag approach in studies of the human blood lipidome.
- Polpitiya A.D., Qian, W.J., Jaitly N., et. al. *Bioinformatics*. 2008 Jul 1;24(13):1556-8. DAnTE: A statistical tool for quantitative analysis of -omics data.
- Ham B.M., et. al. *Journal of Proteome Research*. 2008 Jun; 7(6):2215-21. The influence of sample preparation and replicate analyses on HeLa Cell phosphoproteome coverage.
- Mayampurath A.M., Jaitly N., Purvine S.O., Monroe M.M., Auberry K.A., Adkins J.N., Smith R.D. *Bioinformatics*. 2008 Apr 1;24(7):1021-3. DeconMSn: A software tool for accurate parent ion monoisotopic mass determination for tandem mass spectra.
- Petyuk, V.A., Jaitly, et. Al. *Analytical Chemistry* 2008 Feb 1;80(3):693-706. Elimination of systematic mass measurement errors in liquid chromatography-mass spectrometry based proteomics using regression models and a priori partial knowledge of the sample content.
- Yang, F., Jaitly, N., Jayachandran, H., et. Al. *Journal of Proteome Research* 2007 Nov;6(11):4489-97. Epub 2007 Oct 12. Applying a Targeted Label-Free Approach Using LC-MS AMT Tags to Evaluate Changes in Protein Phosphorylation Following Phosphatase Inhibition.
- Gupta, N., Tanner, S., Jaitly, N., Adkins, J.N., Liptono, M., Edwards, R., Romine, M., Osterman, A., Bafna, V., Smith, R.D., Pevzner, P.A. *Genome Research*. 2007 Sep; 17(9): 1362-77. Whole proteome analysis of post-translational modifications: Applications of mass-spectrometry for proteogenomic annotation.
- Liu, T., Belov, M.E., Jaitly, N., Qian, W.J., Smith, R.D. *Chemical Reviews* 2007 Aug; 107(8): 3621-53. Accurate Mass Measurements in Proteomics.
- Ding, J., Sorensen, C.M., Zhang, Q., Jiang, H., Jaitly, N., Livesay, E.A., Shen, Y., Smith, R.D., Metz, T.O. *Analytical Chemistry* 2007 Aug 15; 79(16): 6081-93. Capillary LC coupled with high-mass measurement accuracy mass spectrometry for metabolic profiling.
- Monroe, M.E., Tolic, N., Jaitly, N., Shaw, J.L., Adkins, J.N., Smith, R.D. *Bioinformatics* Aug 1;23(15):2021-3. VIPER: an advanced software package to support high-throughput LC-MS peptide identification.
- Jaitly, N., Monroe, M.E., Petyuk, V.A., Clauss, T.R.W, Adkins, J.N., Smith, R.D. *Analytical Chemistry* 2006 Nov 1;78(21):7397-409. Robust Algorithm for Alignment of Liquid Chromatography-Mass Spectrometry Analyses in an Accurate Mass and Time Tag Data Analysis Pipeline.

- Kearney, P. et. al. (*US Patent Application being filed 2006*). TAT-001 and Methods of Assessing and Treating Cancer.
- Sharma, S., Simpson, D.C., Jaitly, N., Mayampurath, A.M., Smith, R.D., Pasa-Tolic, L. *Journal of Proteome Research*. 2007 Feb; 6(2):602-10. Proteomic Profiling of Intact Proteins Using WAX-RPLC 2-D Separations and FTICR Mass Spectrometry
- Petyuk, V.A. et.al. *Genome Research*. 2007 Mar;17(3):328-36. Spatial mapping of protein abundances in the mouse brain by voxelation integrated with high-throughput liquid chromatography-mass spectrometry.
- Tolmachev A.V., Monroe M.E., Jaitly N., Petyuk V.A., Adkins J.N., Smith R.D. *Analytical Chemistry*. 2006 Dec 15;78(24):8374-85. Mass measurement accuracy in analyses of highly complex mixtures based upon multidimensional recalibration
- Norbeck, A.D., Callister, S.J., Monroe, M.E., Jaitly, N., Elias, D.A., Lipton, M.S., Smith, R.D. *Journal of Microbiological Methods*. 2006 Dec;67(3):473-86. Proteomic approaches to bacterial differentiation.
- Kiebel GR, Auberry KJ, Jaitly N, Clark DA, Monroe ME, Peterson ES, Tolic N, Anderson GA, Smith RD. *Proteomics*. 2006 Mar;6(6):1783-90. PRISM: A Data Management System for High-Throughput Proteomics.
- McIntire, T.M., Lea, A.S., Gaspar, D.J., Jaitly, N., Dubowski, Y., Li, Q., Finlayson-Pitts, B.J. *Phys Chem Chem Phys*. 2005 Oct 21;7(20):3605-9. Unusual Aggregates from the Oxidation of Alkene Self-Assembled Monolayers: A Previously Unrecognized Mechanism for SAM Ozonolysis?
- Kearney, P, Jaitly, D., Eng, K. (*US Patent Application# 20060122785*). Constellation Mapping: Software and Methods to match complex peptide maps using nonlinear alignment methods.
- Jaitly, D, Page-Belanger, R., Faubert, D, Thibault, P, Kearney, P. MSMS Peak Identification through Maximum Likelihood Methods And its Application to Analysis of Tandem Mass Spectrometry data. *ISMB 2004*.
- Swamy, S, Furtos-Matei, A, Jaitly, N, Kearney, P, Thibault, P. GlycoTrack: Tool for Automated N-Linked Glycopeptide Identification and Analysis. Poster, *PSB 2003 (Also, US Patent Application# 20040248317)*.
- Jaitly, D, Kearney, P, Lin, G and Ma, B. Methods for Reconstructing the History of Tandem Repeats and Their Application to the Human Genome. *Journal of Computer and System Sciences* 65(3): 494-507. 2002.

Selected Projects & Talks:

- Principal Investigator, Lab Directed Research and Development (LDRD) at PNNL. *High Performance Data Analysis Pipeline for Intelligent Mass Spectrometry*. \$500,000 over 3 years, starting 2007.
- Invited talk at the Training Program in Bioinformatics in Texas A&M University. *Challenges in Interpretation of Proteomics Data from Mass Spectrometry Experiments*. October 2007
- Taught Tutorial at US Human Proteomics Organization (HUPO) with Matthew E. Monroe of PNNL and Jake Jaffe of the Broad Institute, M.I.T. “*Data Extraction and Analysis for LC-MS Based Proteomics*”. March 2007.
- Short Presentation at Intelligent Systems for Molecular Biology. “*MSMS Peak Identification through Maximum Likelihood Methods And its Application to Analysis of Tandem Mass*

Spectrometry data". 2004

Awards and honors:

- Nominated for Environmental and Molecular Sciences Laboratory (EMSL) **Director's Award**, Pacific Northwest National Laboratory, November 2006.
- **Outstanding Performance Award**, Pacific Northwest National Laboratory, 2006 for Development and Implementation of Advanced Algorithms for Mass and Time Alignment of Proteomics Data
- Outstanding Performance Award, Pacific Northwest National Laboratory, 2005.
- Ranked 63rd in **William Lowell Putnam Mathematics Competition**, Dec 1996.
- Ranked in the top 31 in the **Indian National Mathematics Olympiads**, 1993.
- Dean's List
- Horner Scholarship (full tuition), Hanover College, 1995-98.