

SEI Bioanalytics & Bioinformatics Core

Bioanalytics & Bioinformatics



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Key functional capabilities of this core are:

- (1) small molecule analysis (pharmaceuticals, metabolites, etc.);
- (2) proteomic analysis of tissues from both normal and pathological specimens; and
- (3) bioinformatics and computational modeling applications for creation, management, and correlative analysis of large data sets, *e.g.*, those derived from genomics, lipidomics and proteomics analyses, as well as other *in silico* applications (*e.g.*, small molecule therapeutics design, ribozyme design and accessibility predictions, etc.).

Instrumentation in Core:

Bioanalytics

- This facility is housed at the New York State Center of Excellence in Bioinformatics and Life Sciences (CEBLS) in Buffalo. It contains several mass spectrometers, including a high-resolution ThermoFinnigan LTQ/Orbitrap XL/ETD instrument with conventional- and nano-flow (New Objective) ionization sources, as well as two highly sensitive ThermoFinnigan Quantum Ultra EMR triple quadrupole MS for small molecule and peptide quantification. Six chromatography systems provide conventional-flow LC (two Shimadzu SIL 20A systems), ultra-high pressure LC (Waters UPLC), nano-flow capillary/nano gradient LC (two Eksigent systems and one GE Healthcare MDLC 2D-nano system), and off-line pre-fractionation using reverse-phase and ion chromatography (Waters Biosep LC system). The LTQ/Orbitrap XL/ETD provides high mass resolution (>100,000) and mass accuracy (<5 ppm), which will provide highly confident identification of peptides from FADS proteins.

Bioinformatics

- The functions of this Core are carried out in the **Center for Computational Research (CCR)** (<http://www.ccr.buffalo.edu/>), located within the CEBLS. The CCR is a leading academic supercomputing facility, and maintains a high-performance computing environment, high-end visualization laboratories, and multiple support staff with expertise in scientific computing, software engineering, parallel computing, grid computing, visualization, advanced database design, and networking. The CCR's extensive computing facilities include a 2112 processor Dell P4 (64-bit) Linux cluster, and a 64 processor shared memory SGI Altix. The Center also maintains a 25 Tbyte EMC SAN. In 2010-11, the CCR did undergo substantial upgrades—funded through grants from the [NSF](#), the [NIH](#), and the New York State Energy Research & Development Authority ([NYSERDA](#))—that will significantly increase the Center's computing and storage capacity (about 70 Tflops of computational capacity and over 600 TBytes of storage capacity) as well as introduced several advanced, novel computing architectures, which will be leveraged to support the University's research activities. The **Computer Visualization Laboratory** features a tiled display wall, a VisDuo passive stereo system, and an Access Grid Node. Based on aggregate computer capacity, the CCR is one of the most powerful university based supercomputing sites in the U.S., with more than 13 Tflops of peak performance. The CCR provides several layers of support for the life sciences/bioinformatics initiatives, including access to state-of-the-art hardware and software to facilitate research, the development of customized software and databases to support data analysis, workshops/training on software packages supported by the CCR, and collaboration with CCR scientists and programmers for proposal development and data analysis.