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13. ABSTRACT (Maximum 200 words)

This Center is made up of an integrated set of research projects in five areas. The overall mission of the center is to utilize stat-of-the-art systems biology approaches to the generation of novel therapies and diagnostics for human diseases. Drug Discovery & Delivery: Biologically relevant compounds that can be linked to effects on specific gene expression patterns, creating new drug targets. Included in this program are two new start-up companies. Cancer: Identify targets to inhibit tumor growth and cell proliferation. Neurodegenerative Disease: Investigating the disease mechanisms of several neurological disorders, including Alzheimer's, MS, Krabbe's and Parkinson's disease. Major themes include demyelination, amyloid plaque formation, and loss of cellular function. Cardio-Vascular disease; Mechanisms by which inflammatory processes associated with clinical aspiration events progress to pneumonitis and ventilator-associated pneumonias; sudden cardiac failure due to arrhythmias. Pathogenesis & Biodefense: Investigation of virulence factors for bacteria and viruses important in human disease and in bio-warfare. Novel vaccines and anti-microbial agents will be developed based on structure-function understanding of these factors. Data Intensive Core; Analysis of genomic, proteomic, epidemiological and clinical data, imaging, and modeling.

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Enclosure 1

The **New York State Center of Excellence in Bioinformatics and Life Sciences** has been established in Buffalo, NY and is in the process of further developing its infrastructure and hiring faculty members in necessary areas. The **Center of Excellence** has designed several inter-related specialty laboratories that can function alone and in sequence to facilitate the process of disease mechanism, diagnosis, and therapy discovery. The high-throughput analysis begins with the gene, but those genes must be associated with a systematic process for the development and curation of clinically relevant databases. In the **Interventional Population Health Observatory**, Public Health specialists utilize techniques in molecular epidemiology, biostatistics, and telehealth to merge medical informatics with traditional bioinformatics to create a linkage between clinical samples, longitudinal medical information, and functional genomics. Public Health, with a high technology component, therefore becomes the "front end" of the Buffalo bioinformatics initiative, and thereby gives the Center a unique element with both short-term and long-term tangible benefits at local, state, national, and international levels. The **Health Observatory** also serves as the responsible unit within the Center of Excellence for the development of syndromic surveillance and emergency response programs that are related to biodefense and disaster management.

In the **Molecular Targeting Laboratory**, a large number of agents (combinatorially synthesized compounds, drugs, or toxicants) are screened efficiently in live cells for effects on specific gene expression pathways. This Laboratory is also developing a parallel approach for applications to microbial pathogens that should dramatically speed the process of target identification relative to biodefense applications. The strategy of the Molecular Targeting Lab is broadly extensible, and not limited to predetermined target pathways. The initial screen in the Molecular Targeting Laboratory does not seek the specific target; the pharmacophore and a family of responsive cell mutants are delivered to the **Gene Expression Laboratory** for high throughput microaarray dissection of the target gene product and ancillary gene expression pathway. Subsequently, the **Proteomics and Structural Biology Laboratory** has been established to identify the gene product targets of the pharmacophore and determine tertiary structures.

The **Disease Modeling Laboratory** has been established to work out *in vivo* proof of concept studies. The **Clinical Pharmacology Laboratory** has been established for Phase I studies, frequently utilizing the Clinical Research Center (CRC) within the Buffalo VA hsopital**.** All aspects of the discovery process utilize the data storage, data mining and analysis, and virtual reality visualization expertise and infrastructure of the **Biomedical Informatics Laboratory.** In addition, this latter group is also engaged in independent research in areas of computational infrastructure, data mining, data fusion, and data visualization research.

Each individual specialty laboratory within the Center is led by an internationally recognized leader in his or her field. Each of the specialty teams has already been highly successful at securing other additional extramural funding for scientific operations. All aspects of the discovery process utilize the data storage, data mining and analysis, and virtual reality visualization expertise and infrastructure of the **Biomedical Informatics Laboratory.** The Center for Computational Research (CCR), which is part of the New York State Center of Excellence in Bioinformatics and Life Sciences and recently named as one of the top 10 academic supercomputing facilities in the country, provides high performance supercomputing and data storage infrastructure. It is one of only three sites in the world selected to beta-test Intel's next generation chip-the 64-bit Itanium processor. A key test for much of the new IT

technology is how it performs with *SnB*, the protein-structure software developed by UB scientists Dr. Russ Miller and Dr. Herbert Hauptman, based on Dr. Hauptman's Nobel Prize winning algorithm. This bioinformatics program is currently the software of choice for more than 500 drug design and research labs.

The CCR's current computer systems are capable of carrying out more than 9.6 trillion operations per second (teraflops). One advantage of the UB CCR design strategy relative to other supercomputing sites is that it maintains computers designed around all three of today's most popular parallel computing architectures; *shared memory* (SGI Origin 2000), *distributed memory* (IBM SP, SUN cluster, SGI cluster, Dell cluster), and *distributed shared memory* (IBM SP, SGI cluster, Dell cluster). This diversity allows our researchers to design, test, and distribute software that is optimized for the various parallel computers available in the marketplace. The CCR also supports all major parallel programming languages. The current technology infrastructure includes:

- 128 processor SGI Origin 2000 supercomputer
- 78 processor IBM RS/6000 SP supercomputer
- Solaris/Linux cluster of 64 Sun Ultra5 workstations
- 150 processor SGI cluster of 1GHz Pentium III chips
- Pyramid Systems ImmersaDesk Visualization system
- SGI Onyx2 Infinite Reality2 graphics computer
- MechDyne 9'x10' Immersive Wall powered by an SGI Onyx2
- Infinite Reality2 graphics computer
- Fakespace RAVE passive stereo module powered by an SGI
- Onyx 3400 computer with Infinite Reality 3 graphics
- Cluster of SGI Octanes, SGI O2s, SUN Ultra 80s, & SUN Ultra 60s
- Web-based geographically distributed communication capabilities
- 2000 Dell dual processor systems consisting of:
    - 2 1.0GHz Pentium3 Processors with 1 GB RAM
    - 236GB local disks
    - 50 42U racks
    - 4 cisco 6513 switches, 11*48p 10/100, 1*16p 1000

Compaq Storage Area Network-10 terabytes of archived data with $\geq$ 23 dual-attached SAN I/O nodes (one per 64 compute hosts), using NFS server over gigabit connection.

Section a

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Section b

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