

MetaQor™



*Shortening The Drug Discovery Pipeline*

ExQor Technologies, Inc.

Boston MA

# About ExQor

ExQor Technologies, Inc. is a multi-disciplinary company, founded in February 2004 in Boston MA, USA.

ExQor is the only company that has fully embraced the National Science Foundation's **NBIC** principles of "Converging Technologies for Improving Human Performance".

NBIC is integrative product approach that unifies **N**anotechnology, **B**iototechnology, **I**T, and **C**ognitive science.

ExQor has developed a unique new model of human cognition based on the brain's dynamic biological and developmental processes, from infancy to adulthood. It is not AI, nor a neural net. It is something totally new in cognitive science.

The product name is MetaQor <sup>tm</sup> and it uses a cloud computing architecture.

ExQor's breakthrough in cognitive science also led to a major biomedical innovation in understanding the central nervous system and how to treat its diseases and disorders.

In one business role, ExQor is developing innovative new large molecule drugs for treating CNS cancer, and also for enhancing CNS neuroprotection and neuroregeneration for treating neurodegenerative diseases, stroke, and traumatic brain injury.

Some of the biomedical research is being done under non-exclusive license at Harvard Medical School (McLean Hospital), and funded by the NIH, NIDA, NARSAD, private foundations, and other funding sources.

ExQor's bio-nanotechnology is broadly protected under multiple issued patents, with additional patents pending in the US and elsewhere in the world.

# About ExQor

Franco Vitaliano, President and CEO and ExQor co-founder and co-patents holder, was formerly President & CEO of VXM Technologies, a Boston-based firm that specialized in advanced bio-nanomaterials and novel, network parallel and massively parallel computer architectures for extremely high performance systems.

These systems were based on his more than two decades of work in developing advanced models of human neuro-biosystems and modeling proteins in the brain. VXM's clients included General Motors, Ford, Chrysler, GTE, the U.S. Air Force, the U.S. Navy, MITRE, the NSA, General Dynamics, Sandia National Labs, Argonne National Labs, and the DOT, among other major clients.

At ExQor he conceived and developed the company's unique and extensive bio-nanotechnologies and also formulated its global business strategy.

He also has extensive expertise in formulating global IP/patent strategies, and was primarily responsible for the conceptualization, technical drafting, and successful defense and approval for all of ExQor's patents.

He has served as an expert in bio-nanotechnology at the President's Innovation and Technology Advisory Committee (The White House), and on DOD conferences.

Gordana Vitaliano, M.D., Vice President and ExQor co-founder and co-patents holder, was formerly the Director of the Nanomedicine Lab for Neuroscience at Caritas St. Elizabeth's Medical Center in Boston MA.

She is an NIH grant recipient and sits on NIH review panels for bio-behavioral science. She emigrated from Serbia to the U.S. in 1991 (where she received her medical degree at Belgrade University) when she won a highly prestigious NIH Fogarty Fellowship.

She is currently employed at McLean Hospital (Harvard Medical School) in Belmont MA, where she is designing bio-nanotechnology with the potential to become a powerful tool in medicine, and in the future may lead to the development of diagnostic tools, targeted delivery systems and cellular repair platforms for the CNS.

This nanotechnology research work, for which she has received 3<sup>rd</sup> party grant support after extensive scientific panel review, involves utilizing ExQor's patented bio-nanotechnology for advanced CNS applications in medical imaging and drug delivery. The work is being done under a non-exclusive license from ExQor.

She has served as an expert in bio-nanotechnology at the President's Innovation and Technology Advisory Committee (The White House), on NIH review panels and on NIDA and DOD conferences.

# MetaQor

- Pharma's don't waste time on fruitless compound searches.
- MetaQor does all the work.
- The MetaQor cloud automatically keeps the Pharma abreast of continually changing drug data and requirements in real time.



# Current Discovery Systems

- Pharma's run down promising drug leads, only to find they are dead ends.
- What looks like a promising drug emerging from a morass of data is just a phantom reflection of the best compound result.
- The real, meaningful data about the best compound lies buried deep, but current tools are unable to see it.



# Current Drug Discovery Systems

- Drug discovery requirements in today's large scale, multi-departmental Pharma environments present highly complex data management challenges.
- High-throughput technologies have created a drug discovery crisis by generating vast amounts of disparate data that must be processed and analyzed.
- A wealth of data are continuously being collected, and in some cases, simulated, including:

- Historical data
- New data
- Lab data
- Sensor data
- Analytical data
- Field data
- Trial data
- Third party data
- Regulatory data



# Current Discovery Systems

Only with intelligent, transformational technologies and tools can Pharma's:

- Accurately identify and qualify high value compound targets
- Accelerate new drug development
- Plan effective business strategies
- Rapidly respond to events
- Bring innovative new products to market at the accelerated pace now required.



# Challenges in Drug Discovery Systems

Several types of discovery systems are currently available, such as those that use Bayesian or probabilistic models, neural networks, etc. Each has their strengths, but they also have notable deficiencies, below.

## Neural Networks

- The performance of a neural network can be sensitive to the quality and type of preprocessing of the input data.
- The most commonly used methods for training neural networks are well-known to have difficulties with local minima (trapping in sub-optimal solutions); these can be demonstrated to occur even for simple problems such as XOR, requiring a network with only a few neurons. Worse, the more efficient the algorithm (moving for example from error backpropagation to conjugate gradient descent) the more likely the algorithm is to be trapped in a local minimum.
- Neural networks cannot explain the results they obtain; their rules of operation are completely unknown.
- Performance is measured by statistical methods giving rise to distrust on the part of potential users.
- Many of the design decisions required in developing an application are not well understood.

## Bayesian Models

- Bayesian results cannot be averaged, added, etc.
- There is the computational difficulty of exploring a previously unknown network. To calculate the probability of any branch of the network, all branches must be calculated. While the resulting ability to describe the network can be performed in linear time, this process of network discovery is an NP-hard task which might either be too costly to perform, or impossible given the number and combination of variables.
- A Bayesian network is only as useful as this prior knowledge is reliable. Either an excessively optimistic or pessimistic expectation of the quality of these prior beliefs will distort the entire network and invalidate the results. Related to this concern is the selection of the statistical distribution induced in modeling the data. Selecting the proper distribution model to describe the data has a notable effect on the quality of the resulting network.



# Discovery Challenges & Solutions

- To overcome current drug discovery limitations and produce a successful method, we leverage ExQor's deep expertise in cognitive development and developing new CNS drugs. We apply this collective knowledge to an innovative, robust discovery method that produces global results faster, better, and more intelligently than any other drug discovery approach currently available.
- To solve the problem of fusing large, multi-attribute data sets, ExQor has undertaken the development and implementation of an algorithm based on human cognitive functioning, which has several unique characteristics that make it ideally suited and superior to other kinds of drug discovery solutions. The end product is called MetaQor™

## *MetaQor*

- ⊙ **Self-knowledge**—Can identify its purpose and understand its internal functions.
- ⊙ **Perception**—Has the ability to recognize, interpret, and understand highly complex sensory inputs.
- ⊙ **Reasoning**—Capable of making intelligent, autonomous decisions based on its perception of the environment and carrying out tasks to successful completion by using its own initiative.
- ⊙ **Cognition**—Its intellectual processes include all aspects of knowing, such as awareness, perception, reasoning, and judgment

# MetaQor Transforms Discovery

The MetaQor cloud best uses the information in *ALL* of the drug data.

- There is no hidden layer problem as in neural networks.
  - ✧ All MetaQor operations are exposed.
- Unlike Bayesian approaches:
  - ✧ MetaQor results can be averaged, added.
  - ✧ NP-hard tasks are avoided that are either too costly to perform, or impossible given the number and combination of variables
  - ✧ Validates prior knowledge with new knowledge

# MetaQor Transforms Discovery

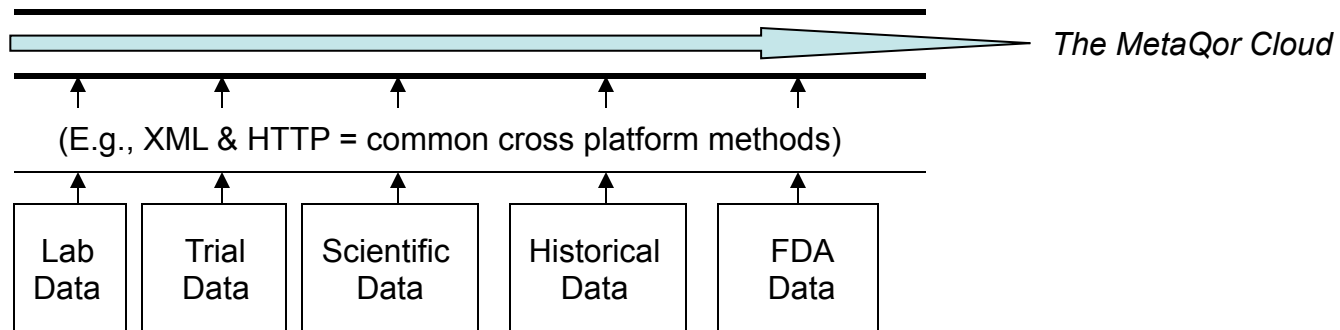
MetaQor capabilities include:

- ✧ Altering searches based on its own "outside" observations or interpretations.
- ✧ Cognitively categorizing new and old drug data based on prior results.
- ✧ Deciphering incomplete or inaccurate data by considering it in conjunction with related information and human judgment.
- ✧ These are human *cognitive functions* replicated in MetaQor.



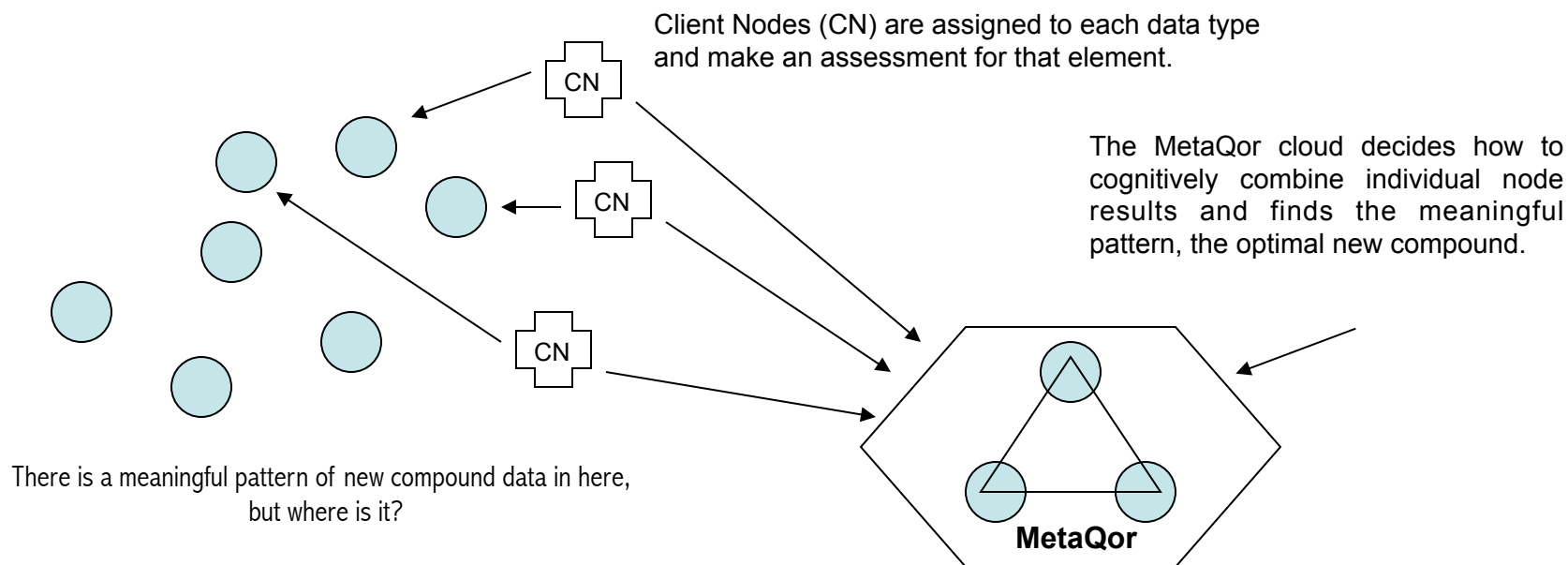
# MetaQor Architecture

- The MetaQor Cloud can handle vast quantities of heterogeneous data in real time, which allows seamless integration of the multitude of point applications that have sprung up and captures multi-workflows for analysis, design, deployment, and compliance reasons.
- The MetaQor Cloud is a computational approach to managing the exchange of information among various data sets in order to maximize both the flexibility for addressing unexpected data types and for introducing both human and machine insight.



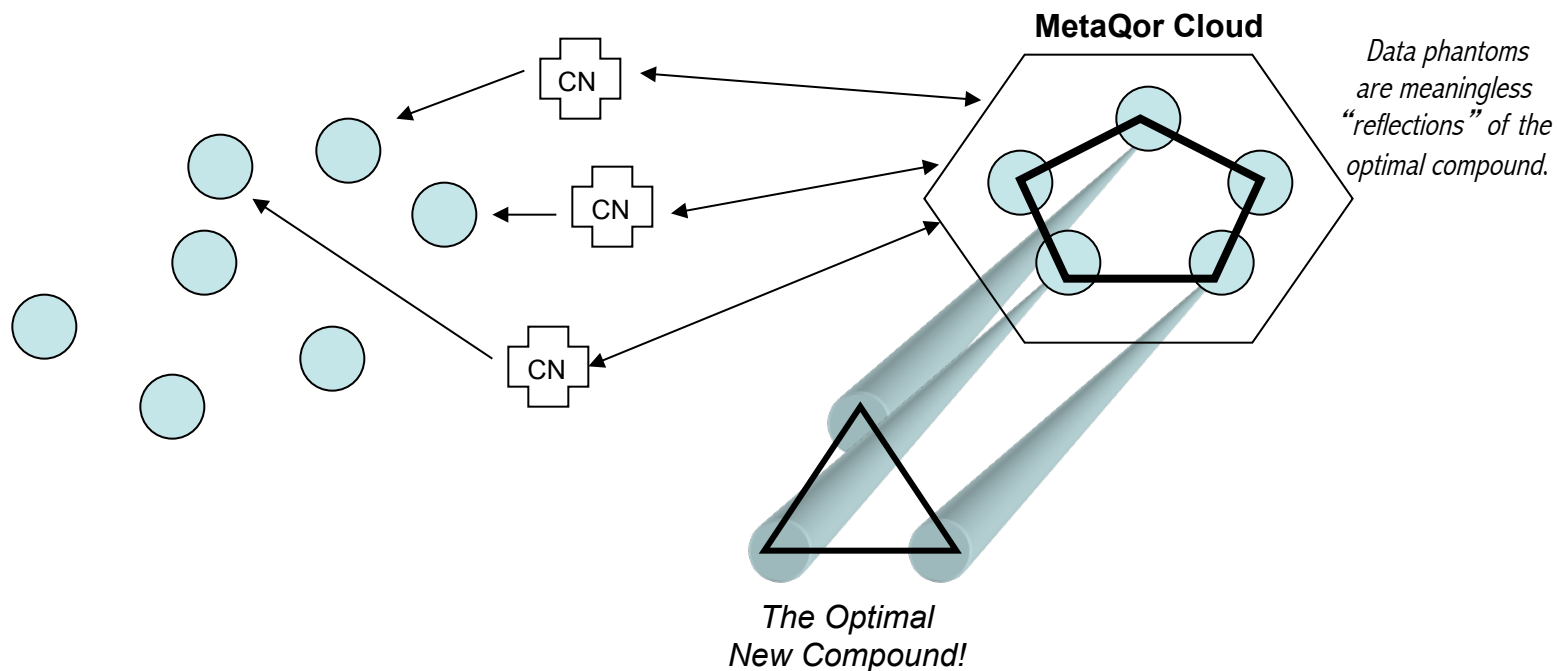
# MetaQor At Work

- The advantages of MetaQor derive from a unique architecture that globally coordinates and optimizes the states determined by its client nodes, which can run on local systems or operate anywhere worldwide via the Internet.
- Each MetaQor client has only partial access to new and old data that may be remotely distributed, be intermittently or newly available, or represent interactive human interpretation.
- The MetaQor cloud combines individual client findings into one global, cognitive discovery of a new compound that best uses the information in ALL of the data.



# MetaQor At Work

MetaQor saves Pharma's wasted years chasing after phantom leads.



# MetaQor Workflow

This workflow in the MetaQor cloud can be explained in more detail as follows:

- Each piece of drug data anywhere on the network is processed according to its data type.
- Client information is sent back to the MetaQor cloud that employs a cognitive algorithm.
- It is the job of the MetaQor cloud to cognitively determine the optimal overall results in order to make the best global assessment of all the data in the entire system.
- The MetaQor cloud will iterate back to its distributed clients and share relevant information about the states of the other data types until optimal discriminate variables are achieved, and a global, cognitive discovery of the optimal drug compound is made.
- The MetaQor cloud allows the exchange of information between data types without requiring them to be translated into the same format. Moreover, data classification and drug discovery can be improved by using previous results or by introducing additional related information.

# MetaQor

## Key Characteristics

- Cognitive mastery of logical operations is not obtained all at once, but by degrees of comprehension determined by the complexity of the structure of the logical operation.
- Also, computational ability, defined as the number of terms and relations that may be computed simultaneously, increases with maturation and development.
- However, cognitive mastery of logical operations is not only a matter of mere computational power.
- It also involves strategies and rules for the cognitive organization of information.



# MetaQor

## Key Characteristics

- MetaQor is an all-software tool.
- MetaQor breaks down the barriers to writing powerful parallel processing applications, heretofore a huge hurdle. In addition, you also get powerful cognitive capabilities.
- Thus, a unique new capability for drug discovery:
  - Executes in parallel.
  - Employs and integrates multiple types of search strategies.
  - Performs very complex searches across disparate, distributed old and new data.
  - Continually refines its queries, scores and ranks hits based on its growing self-knowledge, perception, reasoning and cognitive faculties.
- ⊙ There can be multiple types of cognitively cooperating MetaQor clouds in a global Pharma network, forming a new type of Internet Cloud, a Cognitive Meta-Cloud.

# Multiple MetaQor Clouds = Internet Meta-Cloud = Global Pharma Productivity



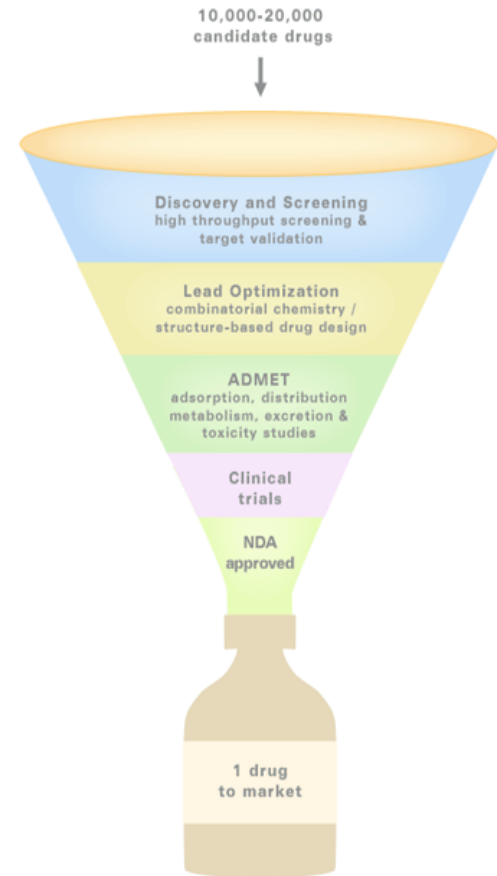
# MetaQor

## SUMMARY

MetaQor enables an easy, fast and reliable way to find meaningful real-time drug discovery results from distributed, disparate data.

- ❖ No more fruitless drug discovery searches.
- ❖ No more chasing after drug compound phantoms.
- ❖ MetaQor does all the work.
- ❖ MetaQor thrives in an environment of continually changing data and requirements.
- ❖ All these MetaQor benefits go straight to the Pharma's bottom line.

## The Drug Discovery Process



## *MetaQor™ for Drug Discovery*



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