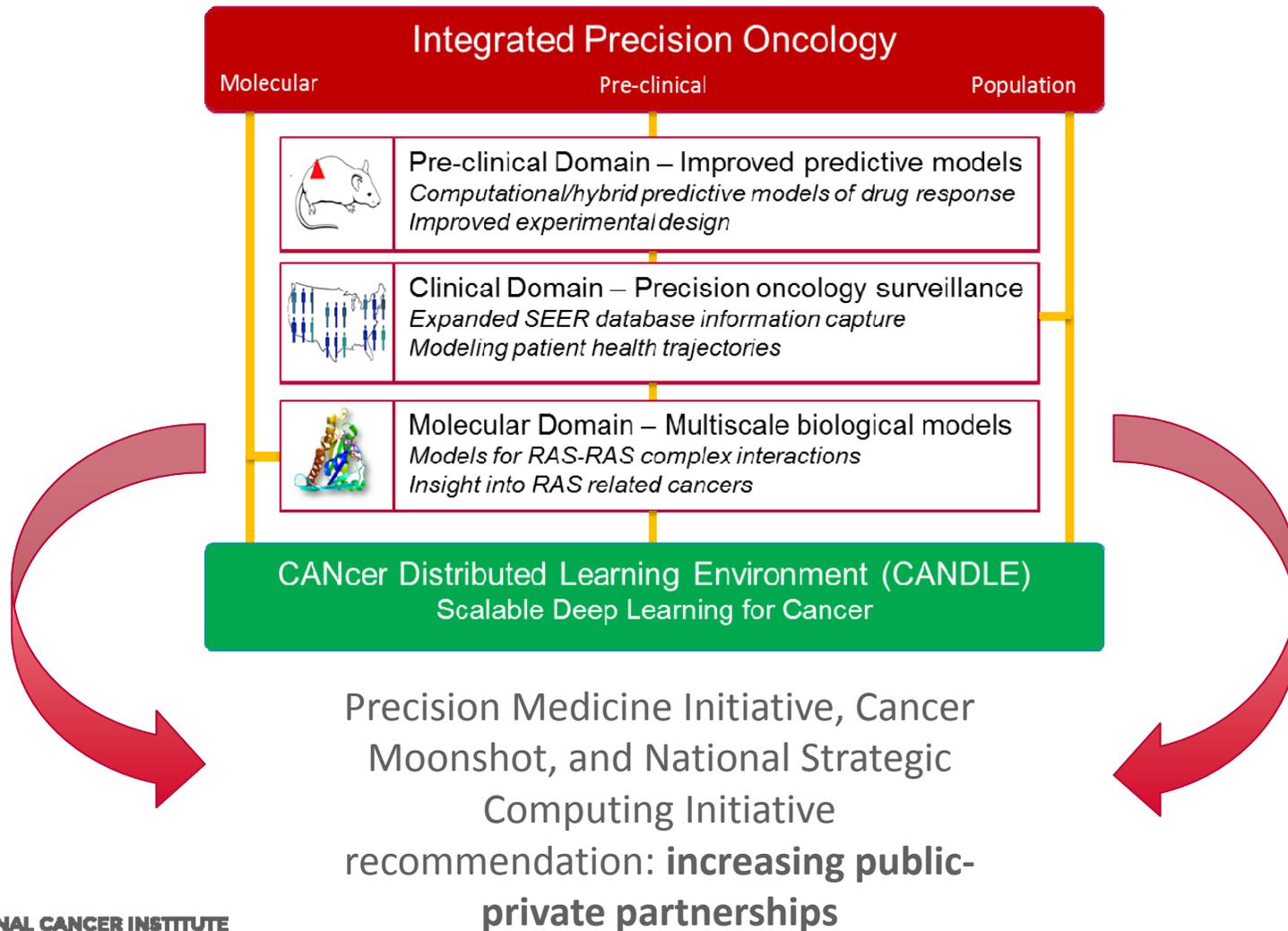


# Accelerating Therapeutics for Opportunities in Medicine (ATOM) Collaboration

*Vision and Status Update*



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# Accelerating Therapeutics for Opportunities in Medicine (ATOM) overview

- MOA to establish public-private partnership with GSK, DOE, and NCI in January 2017
- Goal is to accelerate pre-clinical drug design/development through use of advanced computational and *in silico* technologies
  - Relevant research tools, models, data, etc. **pre-competitive** and **ultimately made open/shareable**,
  - Create a network of parallel activities, and
  - Ultimately shorten time required to achieve eIND starting from known cancer-relevant target(s)
- Aligns with NCI/FNL interests in delivering open data, open tools, and new capabilities to the broader cancer research community as well as ultimately improving cancer patient treatment and outcomes
- NCI/FNL contributes expertise in cancer, computational chemistry/biology, high performance computing, and supports sharing/distribution of data and models

# ATOM Team (GSK, DOE, NCI, LLNL, and FNLCR): January 2017



# NCI, DOE, GSK partnership is basis for ATOM Consortium

- Intended Consortium Founding Members: GSK, LLNL, FNLCR, and UCSF
  - Member resources and expertise are well positioned to integrate, build multi-disciplinary workflows, and support team science
- Intended Consortium model will allow **expansion** to make **additional partnerships** with qualified pharma, biotech, academic, government, and other organizations



# Proposed timelines for ATOM Consortium

## Year1

Establish place, recruit people, establish workflows, invite other partners to join, identify problems

- Expect establishment of Consortium in Spring 2017
- Plan for Consortium location near UCSF's Mission Bay Campus
- FNL to provide specific research expertise onsite and remote
- NCI to provide subject matter expertise, program management onsite and remote

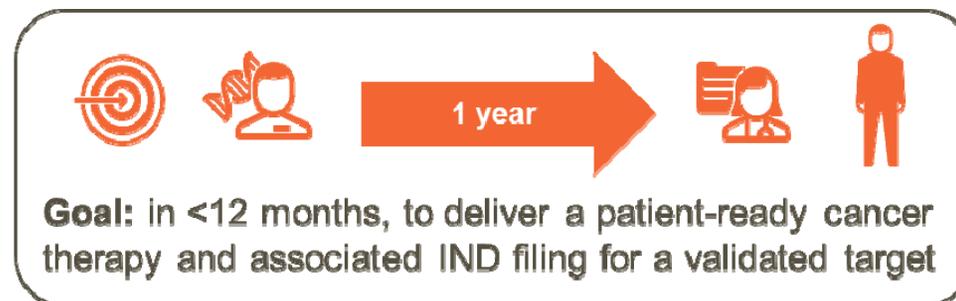
## Year2

Refine processes, solve problems, gain expertise, build and test models

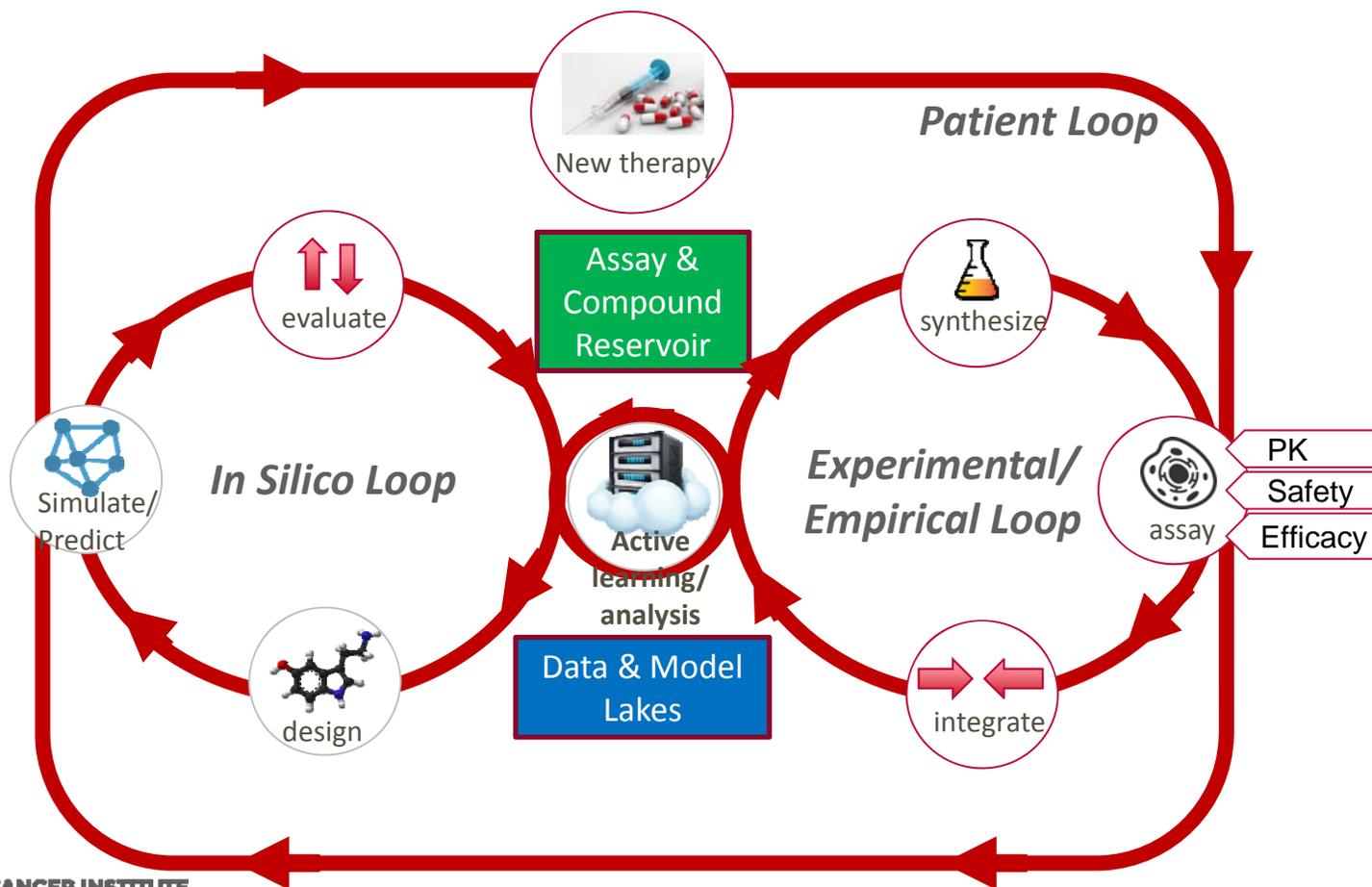
## Year3

Start: Patient presents indication where there is an identified target on a pathway that is druggable

End: File Investigational New Drug (IND) application with FDA



# ATOM workflow: hybrid computational/experimental process



## FNL specific technical/research contributions

- Data management and computing infrastructure
  - Developing and deploying methods for representing ATOM-developed computational models
  - Proposing and establishing the infrastructure, policies, and procedures for the public release of models and data.
- Computational models R&D
  - Gap analysis and plan to fill gaps for multi-scale, mechanistic, and data-driven models
  - Building initial models and assessing the predictivity and uncertainty thereof. Identifying missing parameters and/or experimental data needed to optimize models.
- Active Learning R&D
  - Developing initial framework for integrating mechanistic predictions, data-driven models, translational assays, and design and synthesis processes

## Ideas for increased engagement across broader research communities

- NCI/FNL have focus on expanding involvement and impact to broader cancer research community
- ATOM has the potential to integrate and draw capabilities from across the NCI-DOE pilots (JDACS4C) and CANDLE
- Specific modes of engagement and impact include:
  - Open/shareable models, tools, data, other capabilities
  - Fellowship/training exchange program
  - SBIR contract topic
  - SMEs/consultants and compound libraries/data from NCI DCTD and CCR (intramural)
  - Supplements to existing grants in related areas
  - Outreach to establish additional partnerships

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### NCI/FNLCR

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Betsy Hsu  
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### DOE/LLNL

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