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U.S. DEPARTMENT OF ENERGY

Developing a *National Virtual Biosecurity of Bioenergy Crops Center* (NVBBCC)

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NVBBCC: Historical Context

DOE established the *National Virtual Biotechnology Lab* (NVBL) to facilitate research on COVID 19

NVBL leveraged DOE facilities and expertise:

- Structural biology
- Omics
- Nanomaterials
- Dispersion modeling
- Computing infrastructure

NVBL identified barriers to implementation

- Intellectual property
- Safety concerns
- Sharing of data and materials

NVBL was highly productive

www.nature.com/scientificreports

scientific reports

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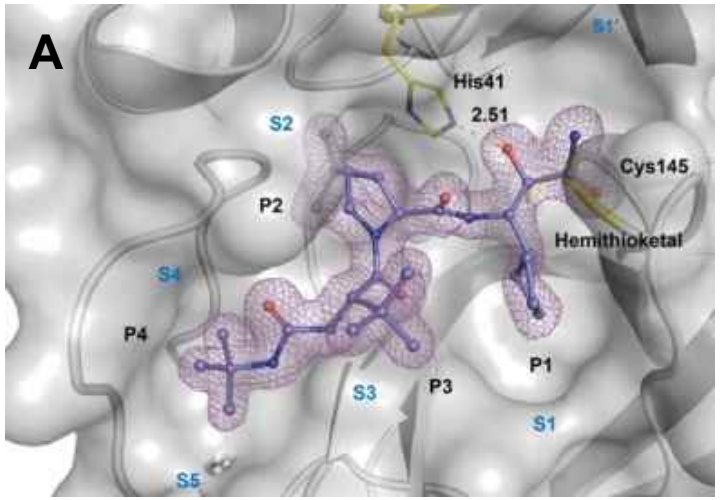
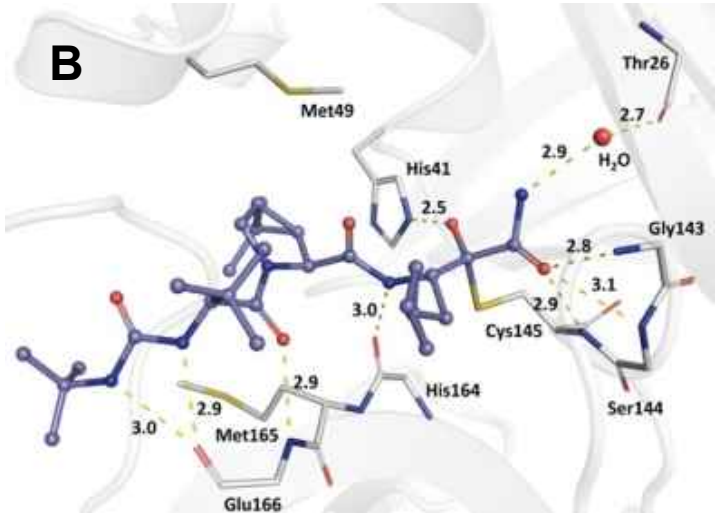
OPEN

Hepatitis C virus NS3/4A inhibitors and other drug-like compounds as covalent binders of SARS-CoV-2 main protease

Babak Andi[1,7], Desigan Kumaran[2,7], Dale F. Kreitler[1], Alexei S. Soares[1], Jantana Keereetaweep[2], Jean Jakoncic[1], Edwin O. Lazo[1], Wuxian Shi[1], Martin R. Fuchs[1], Robert M. Sweet[1], John Shanklin[2], Paul D. Adams[3,4,7], Jurgen G. Schmidt[5,7], Martha S. Head[6,7] & Sean McSweeney[1,2,7]

Scientific Reports | (2022) 12:12197 | https://doi.org/10.1038/s41598-022-15930-z nature portfolio





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BRaVE: a new initiative spawned by NVBL

Biopreparedness Research Virtual Environment

More global in scope: host-pathogen interactions in world's ecosystem

- Basic research on mechanisms of disease and resistance
- Establish pipelines for rapid response to emerging biothreats
- Computational platforms to integrate various data and advance modeling/prediction
- Develop new protective materials and biothreat detection/characterization techniques

Relevance to ICR23

Impact of climate change

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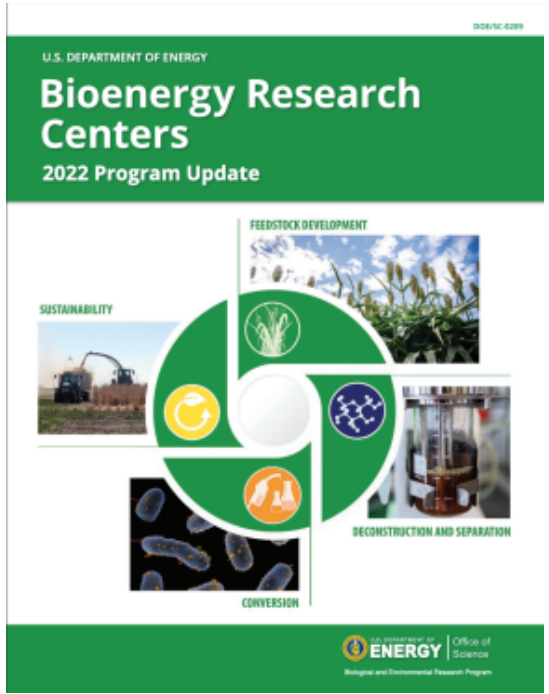
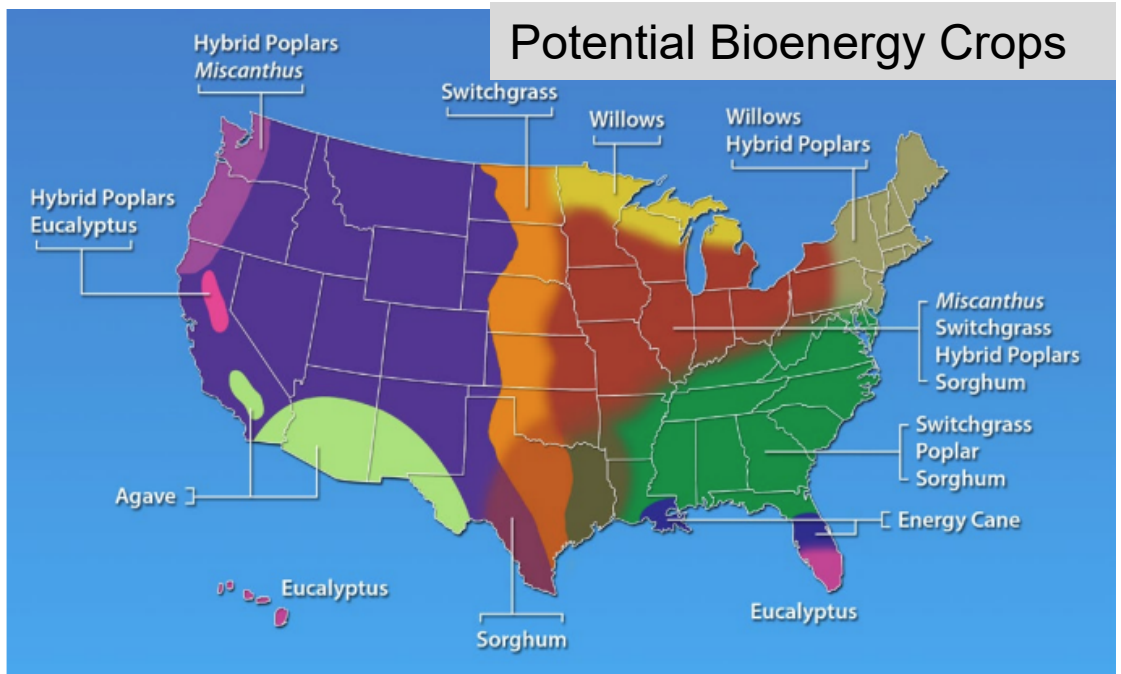
NVBBCC: Rationale

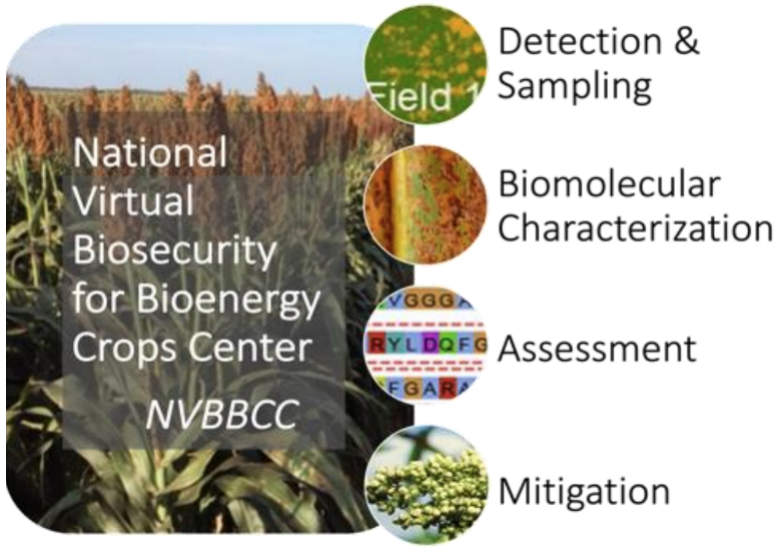
Large-scale deployment of bioenergy crops is a cornerstone of future US bioeconomy

DOE invests $100M/yr in foundational research to develop potential bioenergy crops through its Bioenergy Research Centers

The new center focusses on the biosecurity of bioenergy crops



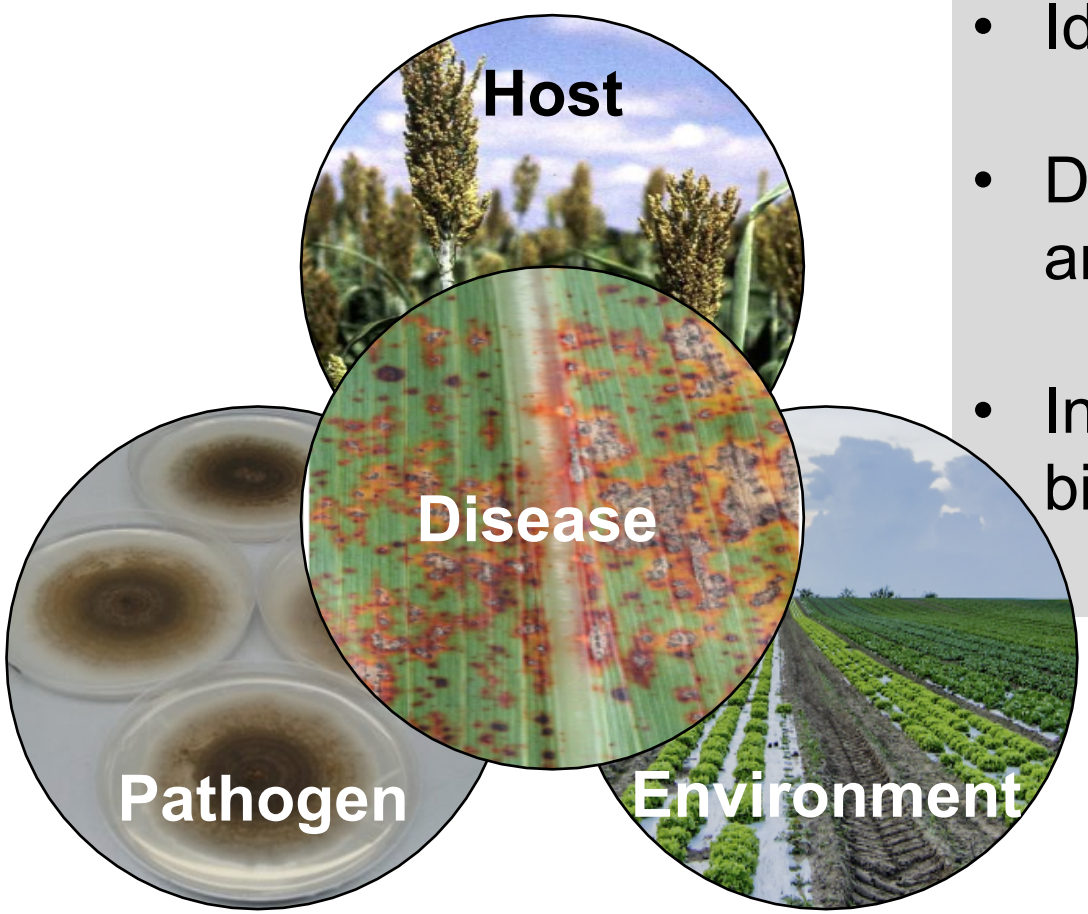




NVBBCC Vision

- A distributed Virtual Center that leverages unique facilities and expertise across the DOE complex
- An efficient pipeline for characterization of emerging threats
  - State-of-the-art resources for biomolecular characterization
  - Scalable computing platform to support collaborative research
  - Detection and modeling of airborne diseases
- Long-term plant pathology research agenda in collaboration with USDA, DHS, Academia and Industry partners
- A resource for sharing protocols, materials, and data with stakeholders

NVBBCC Science Drivers



- Identify pathogens in the environment
- Determine molecular mechanisms of infection and plant resistance
- Integrate data for precision modeling of bioenergy crop ecosystems

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Development Phase of NVBBCC—Community Input

Assemble thought leaders from DOE, USDA, DHS, Academia and Industry in series of topical planning meetings

- Identify knowledge gaps
- Define research agenda to close gaps, leverging expertise and facilities within and outside DOE
- Identify DOE investment needs to advance this research
- Identify barriers to sharing of data, materials, and information

Virtual Planning Meetings

- Biomolecular Characterization (held in February)
- Atmospheric Dispersion and Climate-Driven Dispersion (March 30/31)
- Remote Detection of Disease (May 2nd & 3rd)
- Computing and Cross-Cutting Topics (May 17th & 18th)

Development Phase of NVBBCC—Pilot Study

Focus on Anthracnose impacting Sorghum, a major potential bioenergy crop

Representative of many fungal diseases of important crops, including switchgrass and corn

Transmitted by spores (*Colletotrichum sublineola*)

- Spore germination dependent on moisture and temperature
- Commonly found in Southeastern USA
- Outbreaks can reduce crop yields >50%
- Sorghum strains vary in resistance/susceptibility to infection

Collaboration with Texas A&M and USDA

USDA Collaborator Dr. Louis Prom

NVBBCC studies of Anthracnose of Sorghum

- Molecular interactions of sorghum resistant factors with fungal effectors
- Tomographic imaging plant cells infected by *C. sublineola*
- Field studies of infected vs uninfected crops, using drones
- Establish pipeline for sharing materials with TAMU
  - USDA permits for shipping/receiving spores
  - Local approvals (IBC)
  - Containment protocols and infrastructure

Pilot study will inform the design of an effective NVBBCC

Image from Louis Prom, USDA

NVBBCC Development Phase—Initial Investments

Extend relevant resources and capabilities at BNL

- Bioimaging
  - Purchase cryo-FIB for cryo-ET analysis of disease mechanisms
  - Operated as part of user facility—pathway for supporting other users studying plant diseases
- Atmospheric sampling and remote detection of Sorghum
  - Purchased drones
    - Collaborative project with TAMU and UIUC
- Data science
  - Purchased computing infrastructure and software to manage data via SciServer
    - Establish computing platform to support BRaVE efforts across the DOE NL complex

Conclusion

- Community input and lessons learned from anthracnose pilot study will be captured in a Roadmap for design of the NVBBCC
  - Delivered to DOE by FY24Q1

- NVBBCC integral to DOE-BRaVE effort
  - capabilities and expertise can be pivoted to broader spectrum of biothreats.

Acknowledgments

University collaborators

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} (TAMU)

BNL Leads

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Qun Liu (Biomolecular characterization)
Alistair Rogers (Detection/sampling)
Robert McGraw (Assessment)
John Shanklin
Kerstin Kleese van Dam (Computing platform)
Shantenu Jha
Frances Alexander

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