

Future Directions in Catalysis: Structures that Function on the Nanoscale

- NSF Sponsored Workshop
- June 19-20, 2003 - Arlington, VA, USA
- Participants are experts in catalytic science and technology from the US and Europe, working in industry, national laboratories and universities

Future Directions in Catalysis: Structures that Function on the Nanoscale - Background

- NNI - National Nanotechnology Initiative
- Working at the 1-100 nm range in order to create materials, devices and systems with fundamentally new properties and functions because of their small structure
- Initial long-term vision formulated in Jan. 1999
- Revisit the NNI long-term vision in Jan. 2004

Future Directions in Catalysis: Structures that Function on the Nanoscale - Background

- Catalysis is real nanotechnology -- not just nanoscience
- Prof. J. Heath “it is easy to point to industrial processes such as - catalysis - in which nanostructured materials play some key role. On the other hand, most of these applications are not new, and do not utilize the “high technology” that many people envision as the promise of nanoscience.” -- Acc. Chem. Res. 1999.
- “Chemical catalysis, which underlies a significant portion of the country’s gross national product, is an example of “old nanotechnology.” -- NSTC, 1999
- NRC Report reviewing NNI does not even mention catalysis

Future Directions in Catalysis: Structures that Function on the Nanoscale - Background

- What makes the nanoscale different? Properties that can be obtained with control of structure at this length scale that do not manifest themselves at larger length scales.
- Many examples of this in heterogeneous catalysis, e.g., small metal particles.
- Conversion from nanoscience to nanotechnology --- catalysis has made this transition by bridging the length scale gap (critical issue for other areas of nanoscience)
- Synthetic capabilities to produce materials on the large scale that have control of nanoscale uniformity

Future Directions in Catalysis: Structures that Function on the Nanoscale - Objectives

1. Assess the state-of-the-art in synthetic methodologies aimed at specifically creating organization at the nanometer length scale whether the goal is to create catalytic materials or the consequence of exploiting catalytic materials to create other solids.
2. Assess the state-of-the-art analytical methodologies as they apply to the study of reacting materials in order to address the issue of whether or not they are sufficient to provide reliable information sufficient to define structure/function at the nanometer length scale.
3. Assess the state-of-the-art computational methodologies as to their ability to describe structures that have nanometer scale organization.
4. Provide visionary statements as to what future synthetic methodologies might be and the nanometer scale architectures that may arise from these assembly strategies.

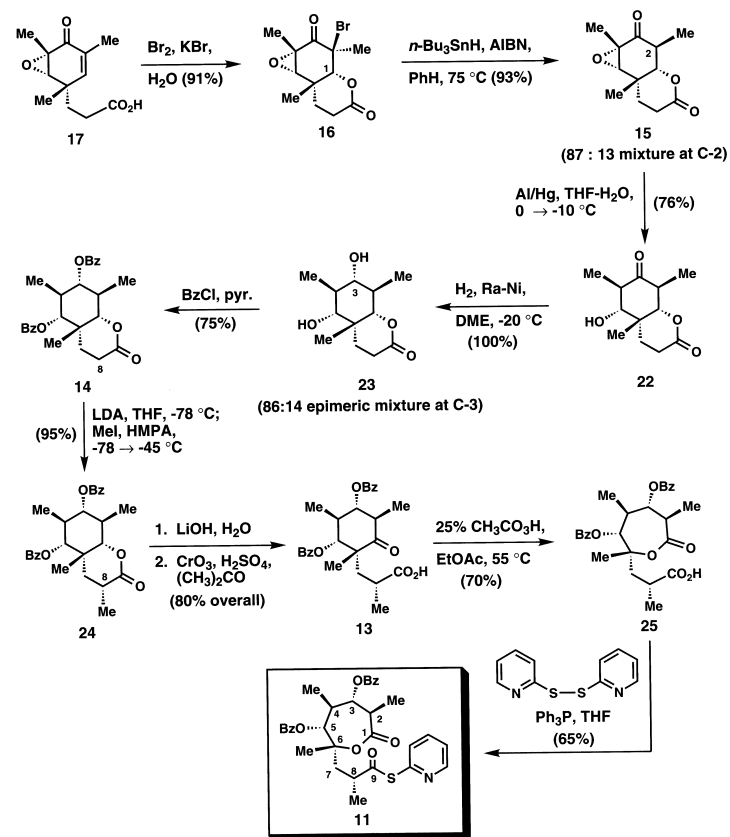
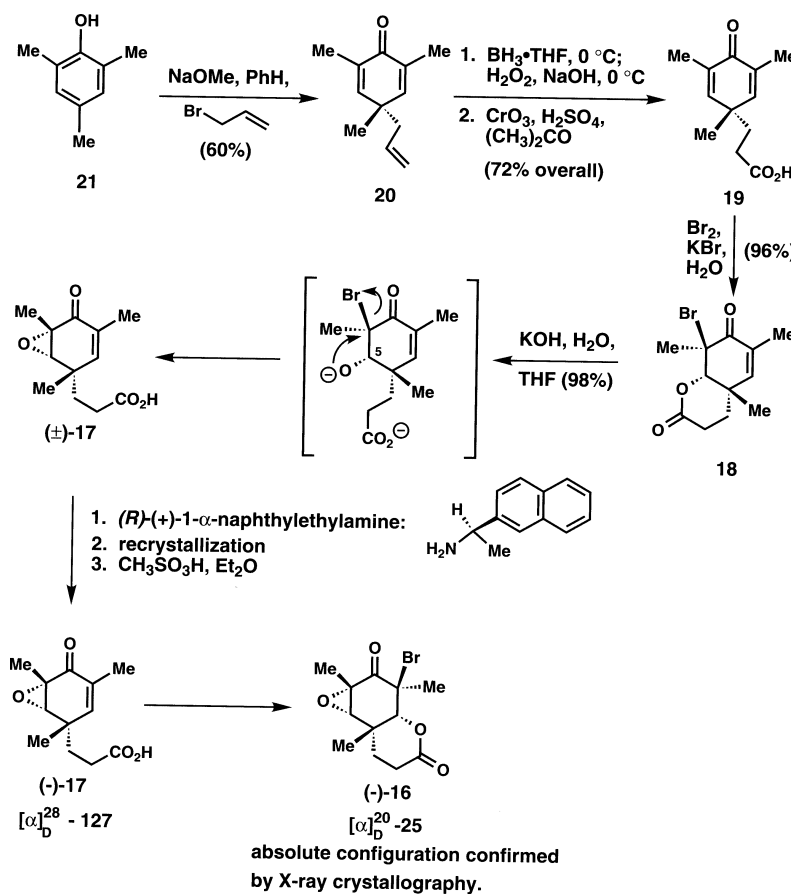
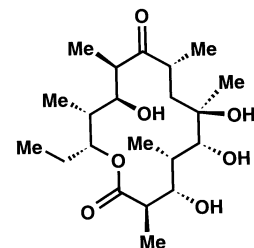
Future Directions in Catalysis: Structures that Function on the Nanoscale - Strategy

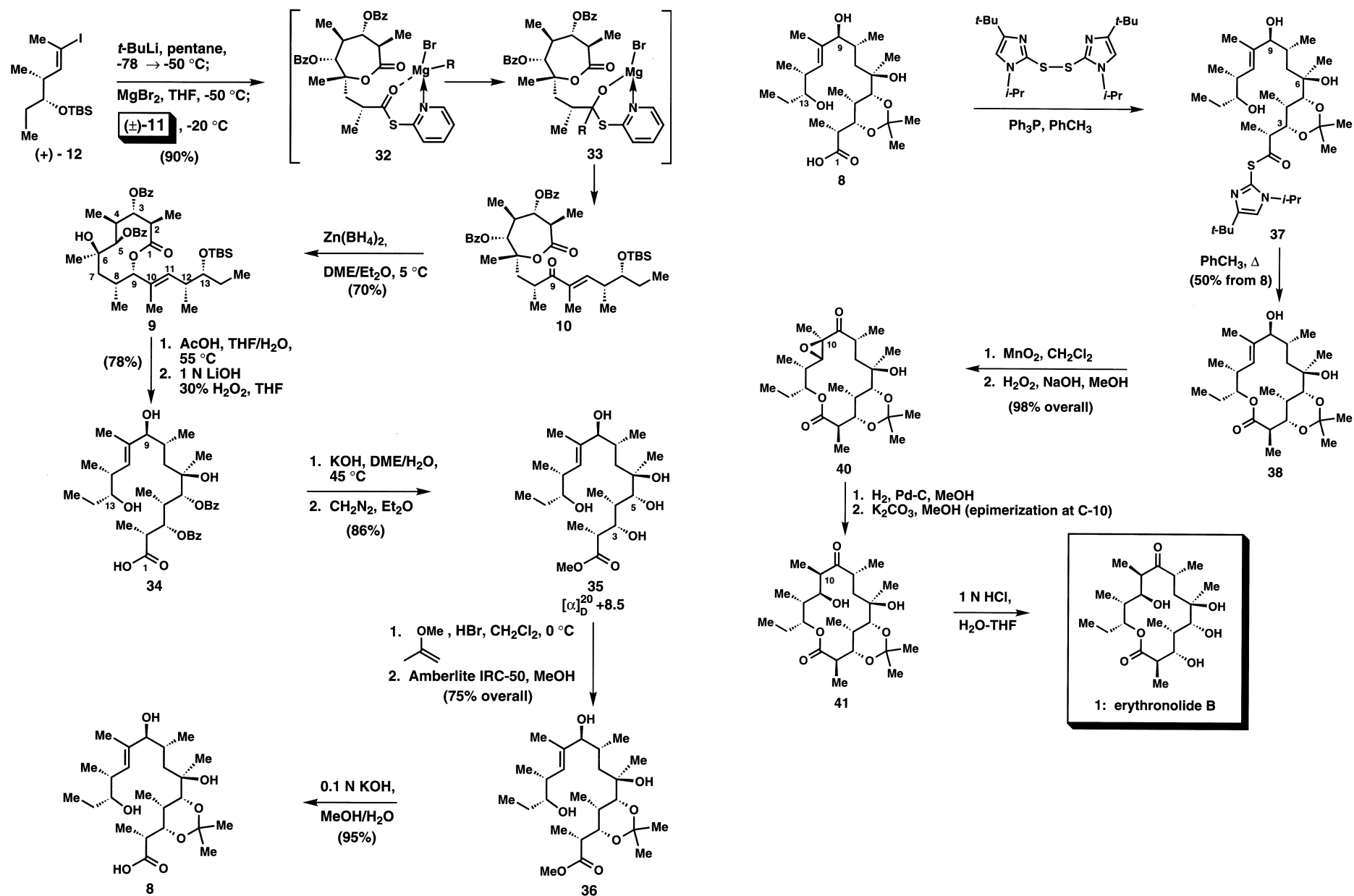
- Provide thoughts for future directions on:
 - Synthetic methodologies
 - Characterization methodologies
 - Computational methodologies
- Provide input for the next NNI research directions meeting -- get catalysis on the map!
- Provide thoughts on how catalysis and its concepts could integrate into other areas like sensors, materials fabrication, etc.

Future Directions in Catalysis: Structures that Function on the Nanoscale - Strategy

- Think big!
- Think about what NSF could do to create initiatives that would provide the basis for launching new technologies.
- What could be some of the future grand challenges?
- Has catalysis missed anything new in other fields and have other fields missed anything new from catalysis?

Organic Synthesis: How it's done

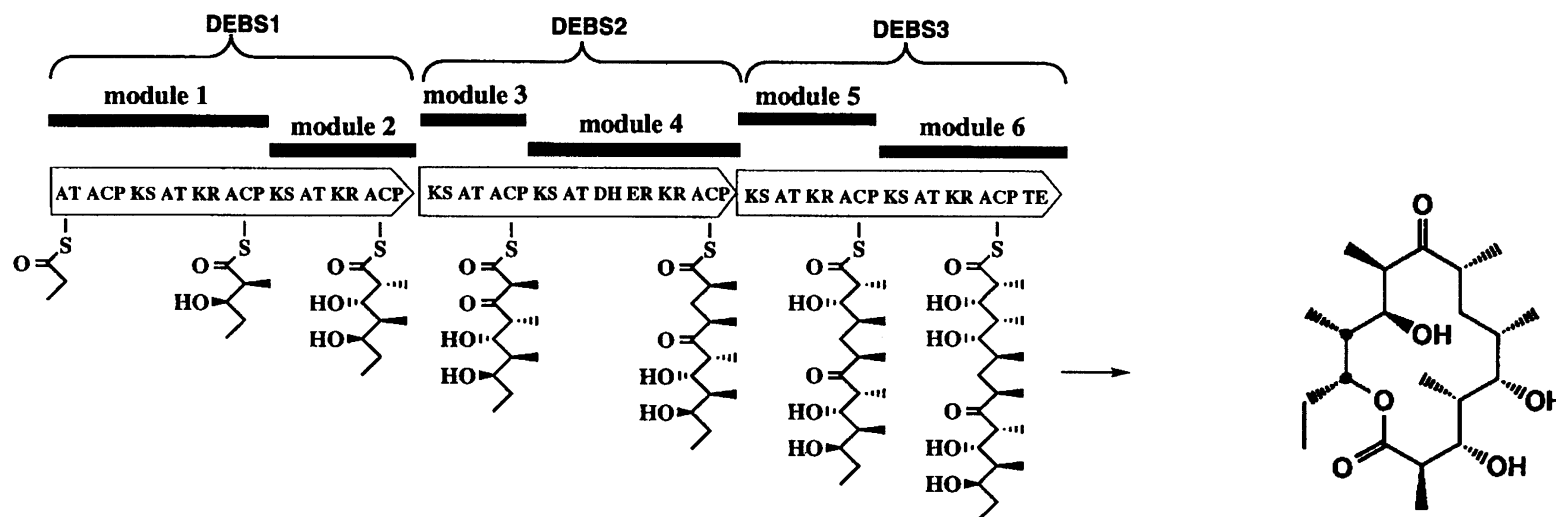




E.J. Corey et al, *J. Am. Chem. Soc.* 100, 4618 (1978)

How Might It Be Done?

Consider the polyketide synthases:



- *New selective chemical transformations*
- *Spatial and temporal control*
- *Harnessing biocatalysis*

IMPLICATIONS

- Abandon synthetic catalysts and move to biocatalysts -- not the correct approach
 - Biocatalysts limited in reactor productivities and reaction conditions for effective operation
 - Types of reactions and substrates limited by biocatalysts
- Use as proof of concept that assemblies of active centers positioning correctly in three dimensional space can efficiently accomplish complex reaction networks

Workshop Schedule

Thursday – June 19, 2003

- 8:00 AM Registration/Reception
- 8:45 AM Welcome – Glenn Schrader/Esin
Gulari/Art Ellis, NSF and NNI overview by Mihail Roco
NSF and Chair of US Nat. Sci. and Tech. Council's
Subcom. On Nanoscale Science, Eng and Tech.
- 9:15 AM Workshop Overview and Objectives – M.E.Davis,
Caltech
- 9:30 AM Molecular Precursors to Catalytic Materials -
D.Tilley, Univ. California, Berkeley
- 10:00 AM Perspective on Assembly from Other Nanoscience
and Engineering Initiatives – C. Mirkin,
Northwestern Univ.
- 10:30 AM *Break*

Workshop Schedule

- 10:45 AM Perspective on Catalysis and Assembly at the Nanoscale by Industry – S.M. Davis, ExxonMobil
- 11:15 AM Perspective on Heterogeneous Catalysis at the Nanoscale from from Europe – R. Schlogl, Fritz Haber Institute, Berlin
- 11:45 AM Perspective on the Use of Catalysis for the Assembly of Other Materials – H. Foley, Penn. State Univ.
- 12:15 PM *Lunch*

Workshop Schedule

- 1:15 PM Perspective on Characterization Methods – R. Lobo, Univ. Delaware
- 1:45 PM Perspective on Computation and Modeling – M. Neurock, Univ. Virginia
- 2:15 PM Open Session for participants to provide 10 minute presentations
- 3:30 PM *Break*
- 3:45 PM Open Session Continued
- 5:30 PM *Adjourn*

Workshop Schedule

Friday – June 20, 2003

- 9:00 AM Discussion on Workshop Report Structure and Content/Major Topics
- 10:15 AM *Break*
- 10:45 AM Discussions on preparation of initial summaries, draft outlines for research needs in each topical area for final report -- may break into sections
- 12:15 PM *Lunch*
- 1:15 PM Assignments for completion of report and time for assigned groups to plan their schedule for submission of report documents - may break into sections
- 3:00pm *Adjourn*

Think About

- What is the vision that should be presented?
- What are the future goals?
- What are the barriers to those goals and how can they be eliminated?
- What should the strategies be to reach the proposed goals in a timely (10-15 years) manner?