How do we shape the future?

What are the critical issues to be addressed?
What should IUPAC be doing now?

Digital IUPAC Theme at the GA

Chemical Space

Augmented Intelligence

Applications
- devices
- materials
- crystals
- Drug targets
- Personalized medicine
- People and animals
- Rare diseases
- Genomics
- Environment
- Precision agriculture
- Machines
- Complex formulations
- Engineering
Vastness of chemical Space

• How have we coped so far?
• Inspired by nature!
• Imagination and creativity?

Characterization Techniques

The more of chemical space we plan to explore the more molecules we need to make to provide the data and the less of each molecules we can afford to make.

AI needed to interpret complex measurements
Measurements in context needed – in the cell or device and on the field


Laws of Geography

• The First Law
  “Everything is related to everything else, but near things are more related than distant things”.
• The Second Law
  "The phenomenon external to an area of interest affects what goes on inside".

Learning
The more data we have the more we need to throw away

Machine Learning, Statistical Mechanics & Simulations

Molecular Dynamics

- Develop Force Fields
- Faster Integrations
- Identify patterns
- Enhanced sampling

Machine Learning

- Generative Models
  - ML network learns the essential features for molecules with selected properties (e.g., a suitable drug candidate)
  - Can be used to select suitable molecules from a library
  - But a generative network "creates" possible molecules
  - Then check if there is a synthetic pathway to make them!
Proteins

DATA Driven

- quantity
- quality
- uncertainty
- provenance
- availability

Data revival

Graphs

- Molecular Graphs
- Knowledge Graphs
- Graph Neural Networks

Standards – as much time converting as extracting....
How do we communicate models and process?

- Surprisingly difficult to explain what a process involves
- Much of the detail is assumed to be understood and not explicitly discussed
- This is where the misunderstandings usually arise.

If you can't describe what you are doing as a process, you don't know what you're doing.

W. Edwards Deming
IUPAC must drive this work otherwise non-chemists will do this first – they can see the need even if we have not!

Not a good idea!
The Logic of Scientific Discovery

Abduction

Outliers

Finding the Underlying System

Small Data Learning
Include chemical knowledge
Deal with non-linearity
Ethical AI – The Problems of Bias

Explainable
Accountable
Reproducible

All needed for scientific discovery

When chemistry becomes a discipline, mathematical chemists will design new materials, predict their properties, and tell engineers how to make them — without ever entering a laboratory. We've got a long way to go on that one!

Robert A. Heinlein, "Where to?" 1950

The Future (is ours to see)

Can Scientific Discovery Be Automated?

The twin challenges of too much quantity and too little quality are rooted in the finite neurological capacity of the human mind. Scientists are deriving hypotheses from a smaller and smaller fraction of our collective knowledge and consequently, more and more, asking the wrong questions, or asking ones that have already been answered. Also, human creativity seems to depend increasingly on the stochasticity of previous experiences—particular life events that allow a researcher to notice something others do not. Although chance has always been a factor in scientific discovery, it is currently playing a much larger role than it should.
The Laboratory

AI in the Lab

Talk2Lab

AI enabled ELNs

Quality annotated record
Telling the story
Machine readable

Intelligent Automation

Limits of Chemical Computation

There are computationally undecidable problems in quantum chemistry!
Culture

We are still in a Liminal period
A Key worry

Overreliance on artificial intelligence may put us in intellectual debt.

All I am saying is that now is the time to develop the technology to deflect an asteroid.

Trust me Mort - no electronic communications superhighway, no matter how vast and sophisticated, will ever replace the art of the schmooze.

Thank you for listening.