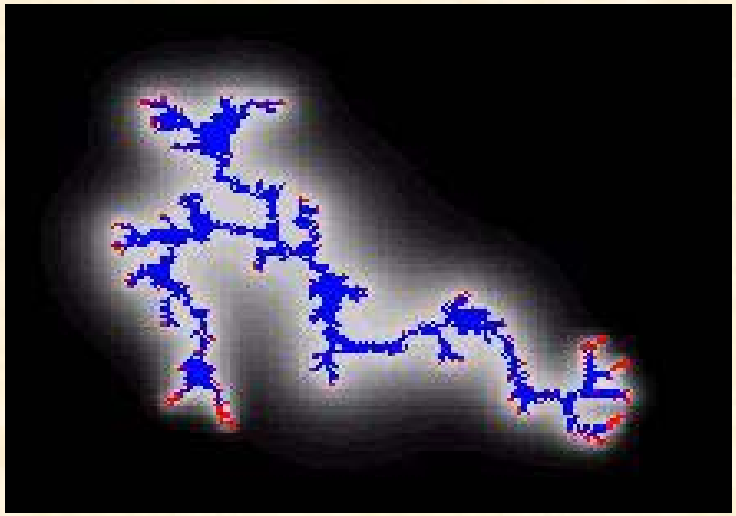
What is Artificial Intelligence?

And why would a chemistry teacher need to know anyway?



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Why use Artificial Intelligence in Science?

Some current uses to follow, but we might ask…

Have all the easy discoveries been made? If so…

We may need new tools to make further progress.

What makes a scientific problem hard to solve?

No known methods of solution

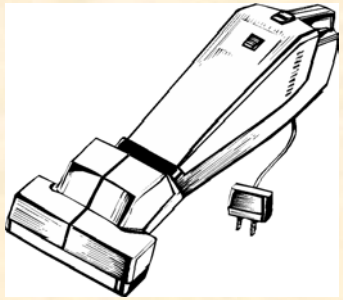
Chaos may intervene

Too much time required to find a solution

Too many solutions to inspect ($C_{30}H_{36}O_4$)

A solution for tough problems: Artificial Intelligence – but what is it?

Clever vacuum cleaners?



Talking PCs?

A working definition:

Programs that can learn - this implies memory.

AI methods used in science

Genetic algorithms

Neural networks

Knowledge-based systems

Intelligent data mining

Self-organizing maps

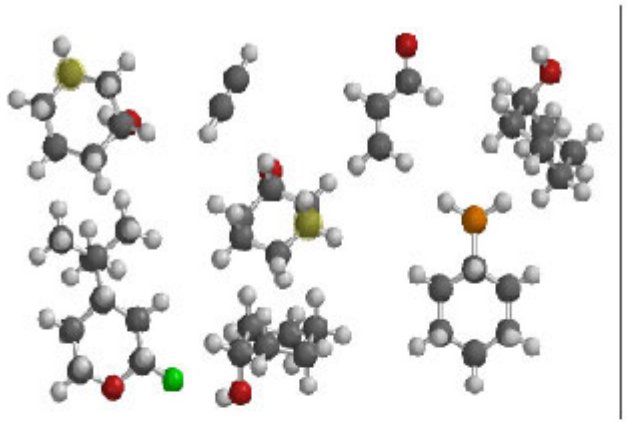
.....

Application of AI to Science

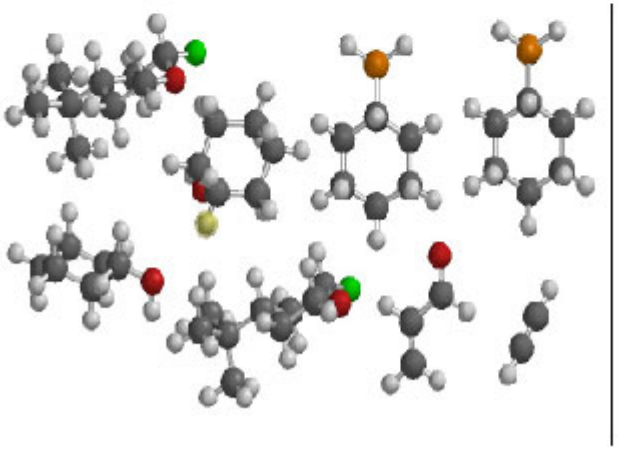
- Solving problems for which conventional methods of solution are inadequate (main current use)
- Tackling "hard" science (potential future use)
- Automatic science (see later…)

Constructing a Genetic Algorithm to optimize molecular structure

Create a population of molecules

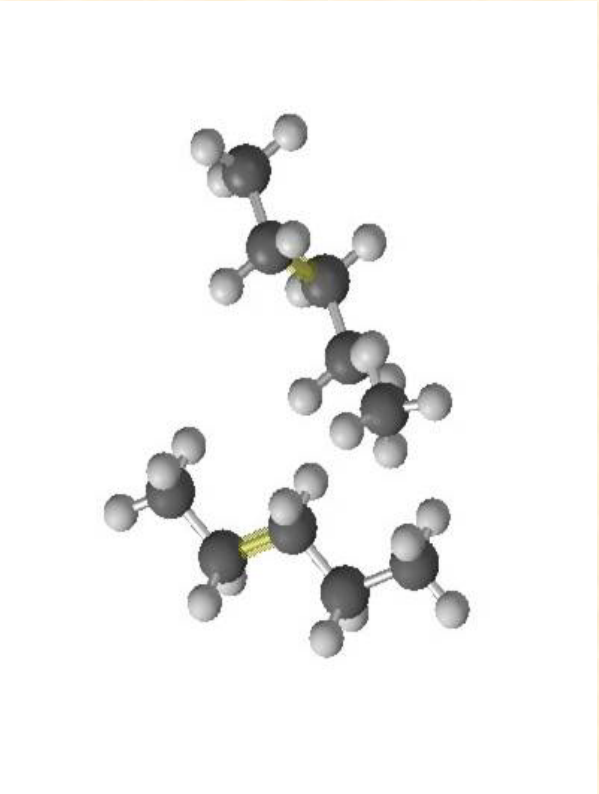


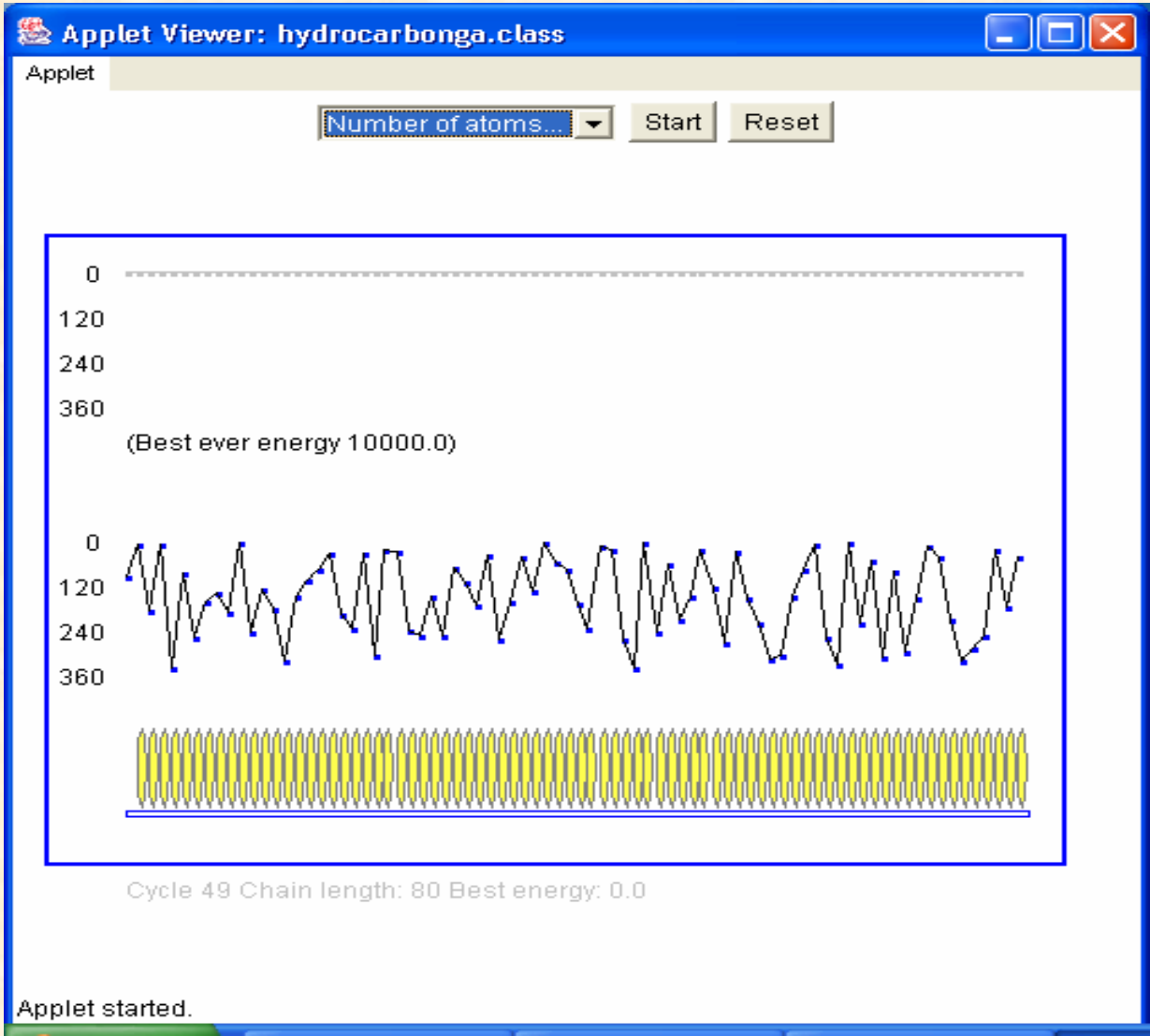
Assess the fitness of each molecule, then create a new population picking the best (stochastically)

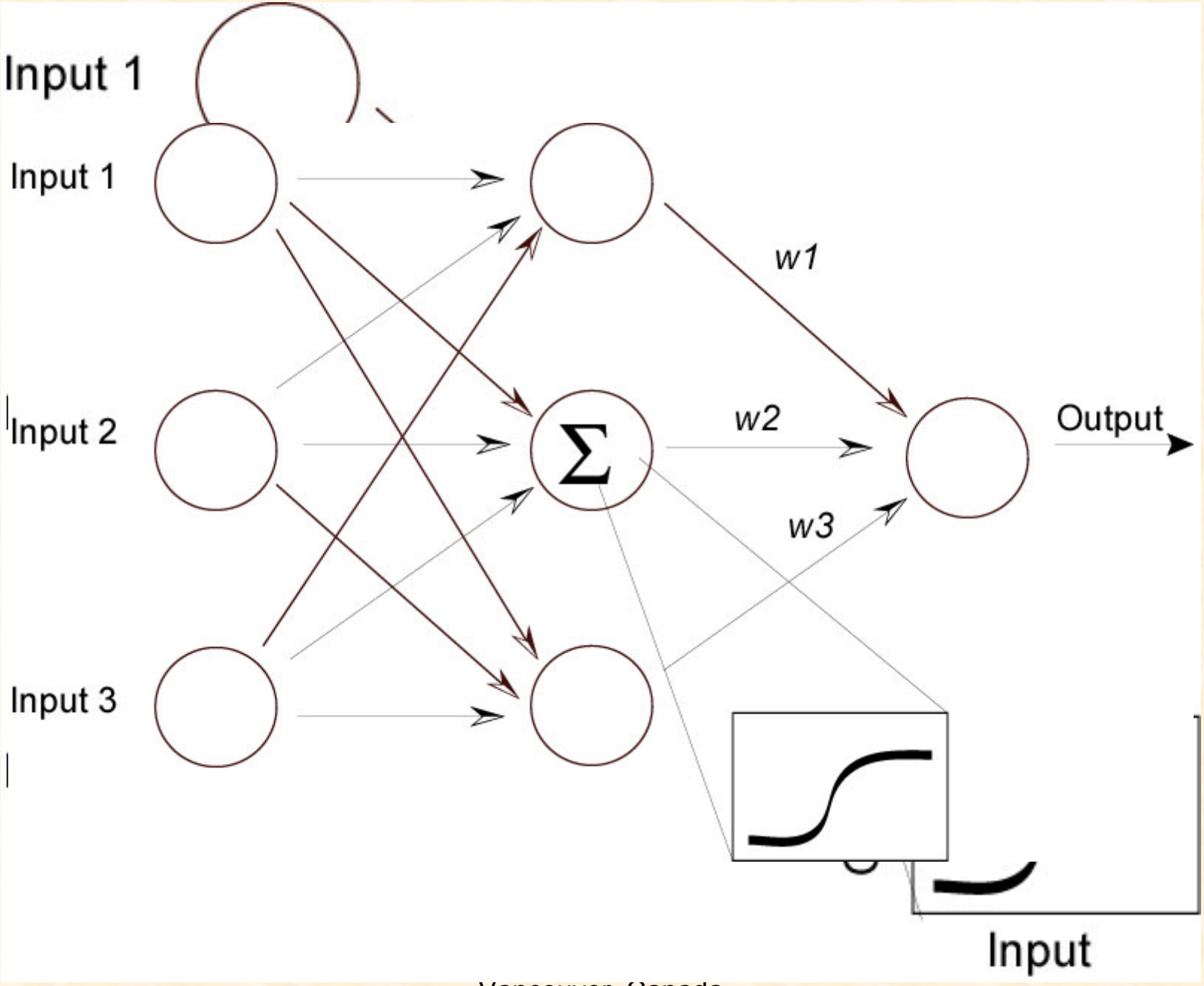


Mate, mutate and continue until tired or bored

GA Geometry Optimization






Input 1
Input 1
Input 2
Input 3
w1
w2
w3
Σ
Output
Input

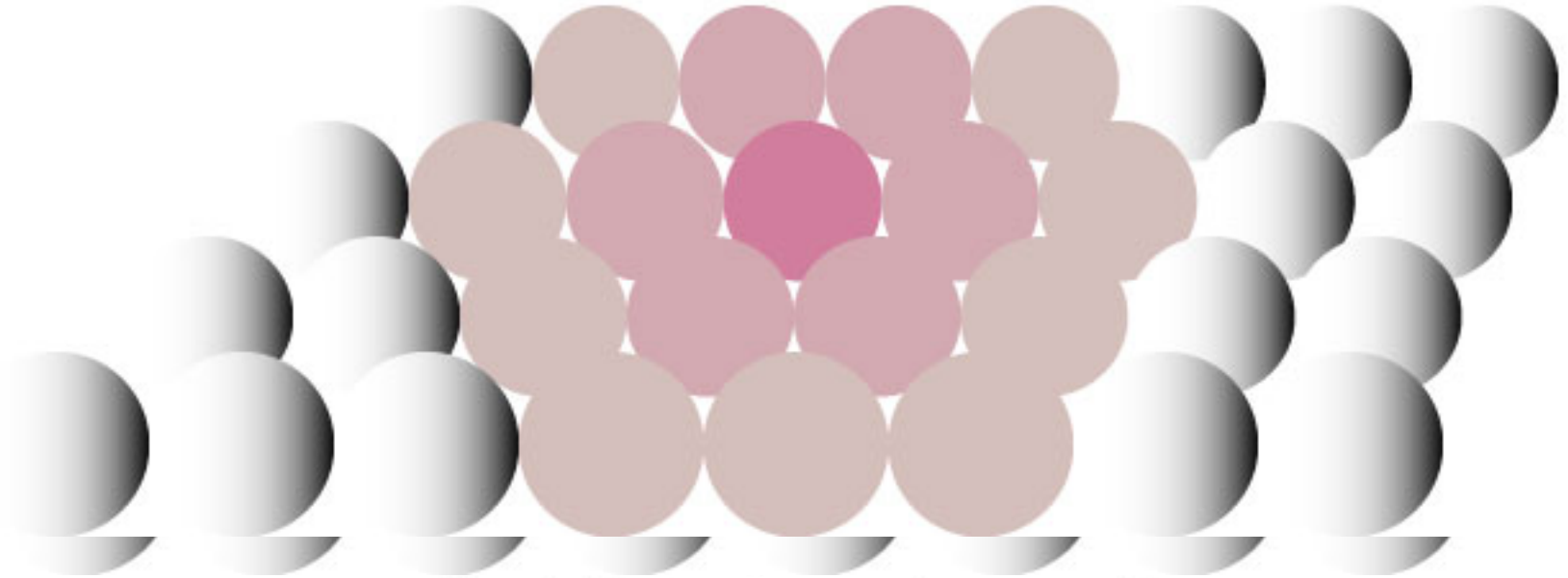
Optimization of polymer recipes using Neural Networks

- **Input:**
  - Physical properties such as flexibility, glass transition temperature, reflectivity, strength…
- **Output:**
  - Predicted composition of ideal polymer

How can random numbers generate useful solutions?

- Different routes to the same solution
- Different solutions of equivalent value

...with those nodes furthest from the winning node being changed the least



fed into each node

Self-Organizing maps: Linking polymer structure to IR spectra

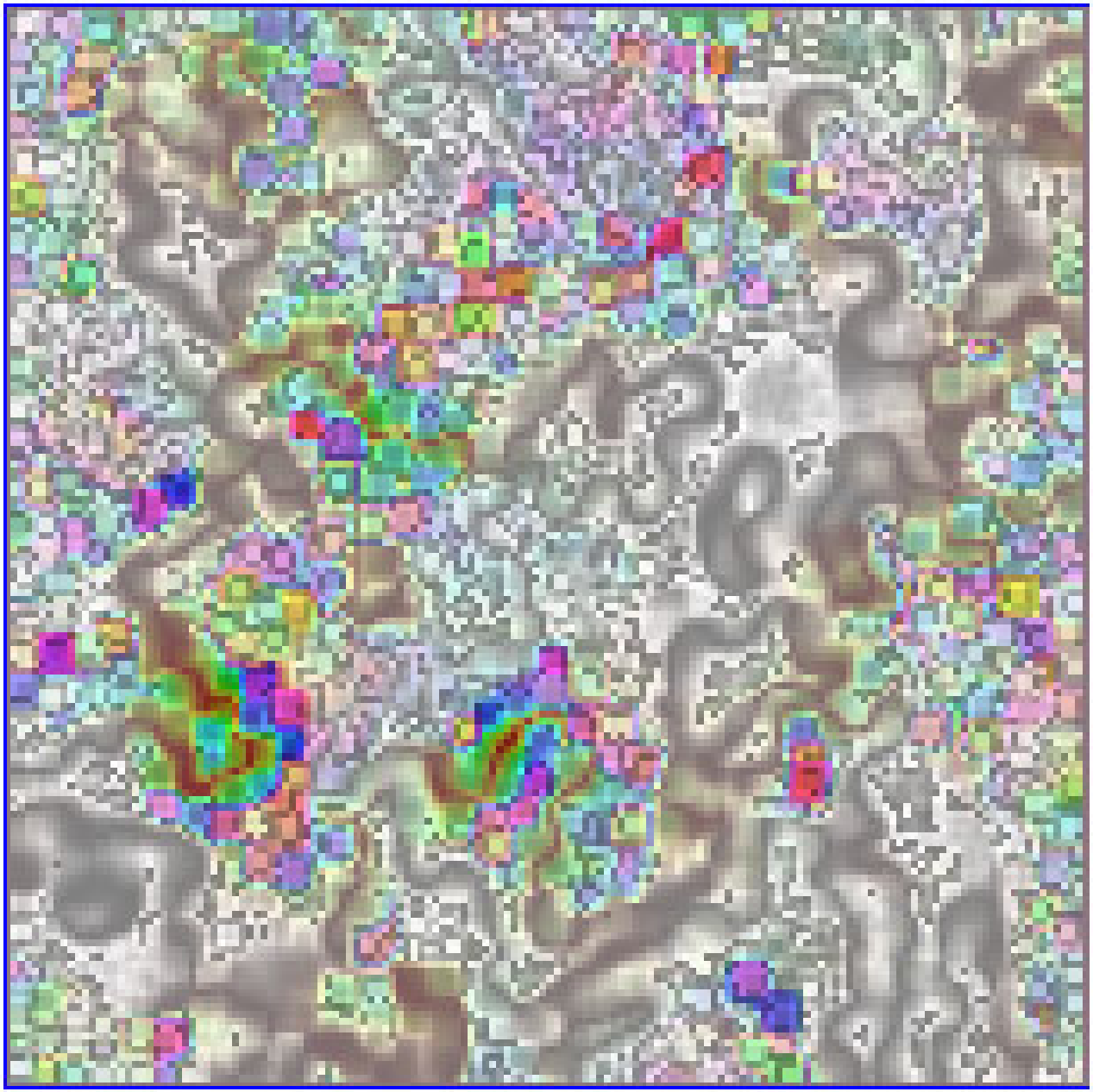
Input:

Digitised Infrared spectra

Data not made available to the map:

Structure of the polymer

Cycle 201030



Coimbra, July 2002

Present and future use of AI in science

- Molecular optimization, synthesis design, spectral analysis, etc. (Good news)
- "Incomprehensible" theories. (Bad news for theoreticians)
- Automatic Science: (Bad news for experimentalists)

  Data mining +

  Intelligent web agents +

  Rule-discovery neural nets +

  "Lights-out" Laboratories =

No longer any need for scientists…

- Hugh.Cartwright@chem.ox.ac.uk