

Organic Structure Determination

Chemistry 5.46

Spring 2007

"It's amazing who they let teach..."

Goals

- Gain ability to choose experiments wisely
- Process and Interpret data
- Attain instrument experience through setup and acquisition
- Generate easy-to-understand figures

These problems are little puzzles.

Each problem offers a fascinating
glimpse into the inner workings of
nature.

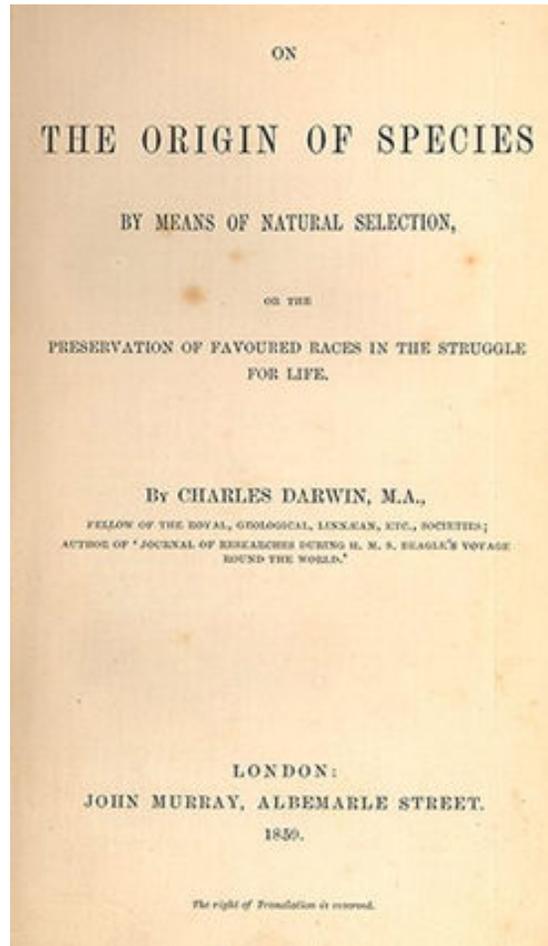
The final goal is to make
doing this easy, which leads
naturally to a corollary of
Murphy's Law

The Law of Unintended Consequences

"This isn't that hard, so now Jeff doesn't look like such a smart guy"

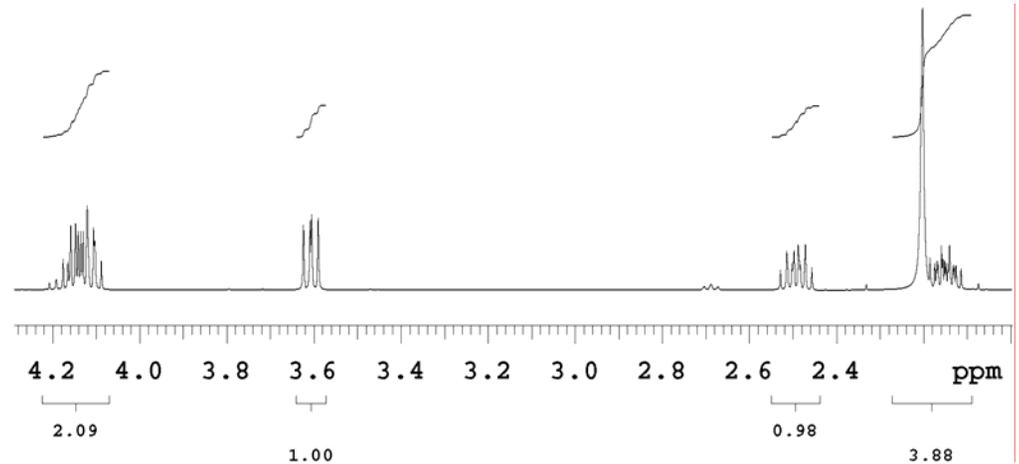


We will follow the evolution of NMR as a problem-solving discipline

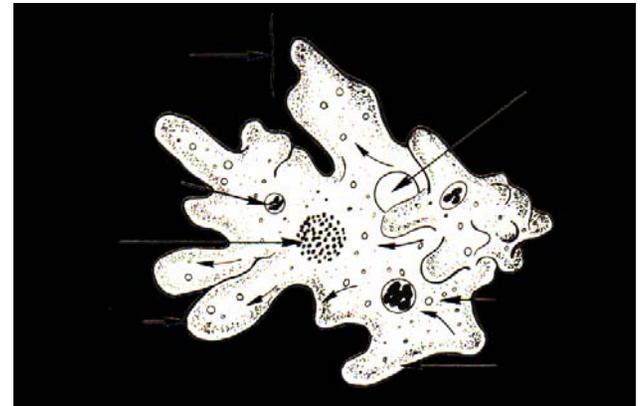


First, there was primitive NMR

1-D NMR with chemical shifts, J-couplings, and integrals



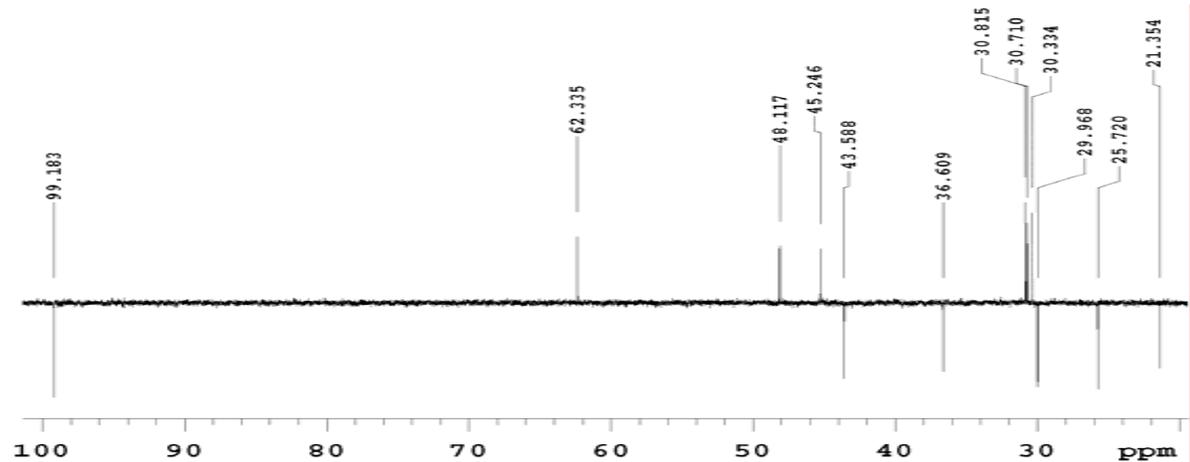
Like the one-celled amoeba



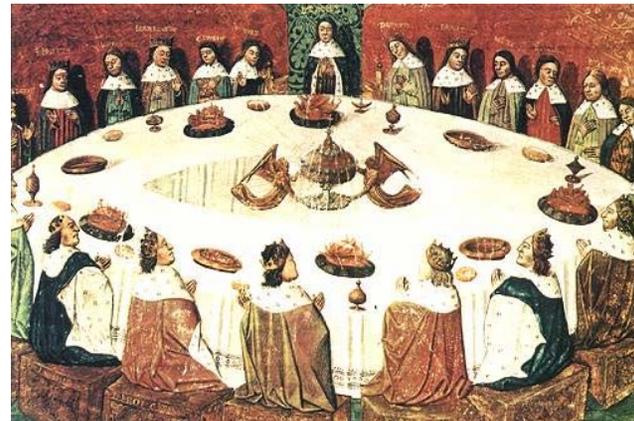
(Image by Pearson Scott Foresman)

Then there was medieval NMR

DEPT, APT,
and other
multi-pulse 1-D
experiments

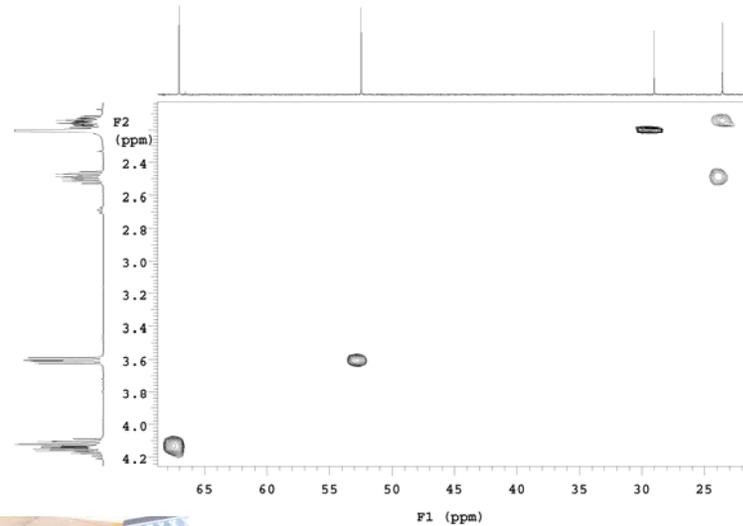


The knights of the round
table used shields and
swords



But then came the modern age

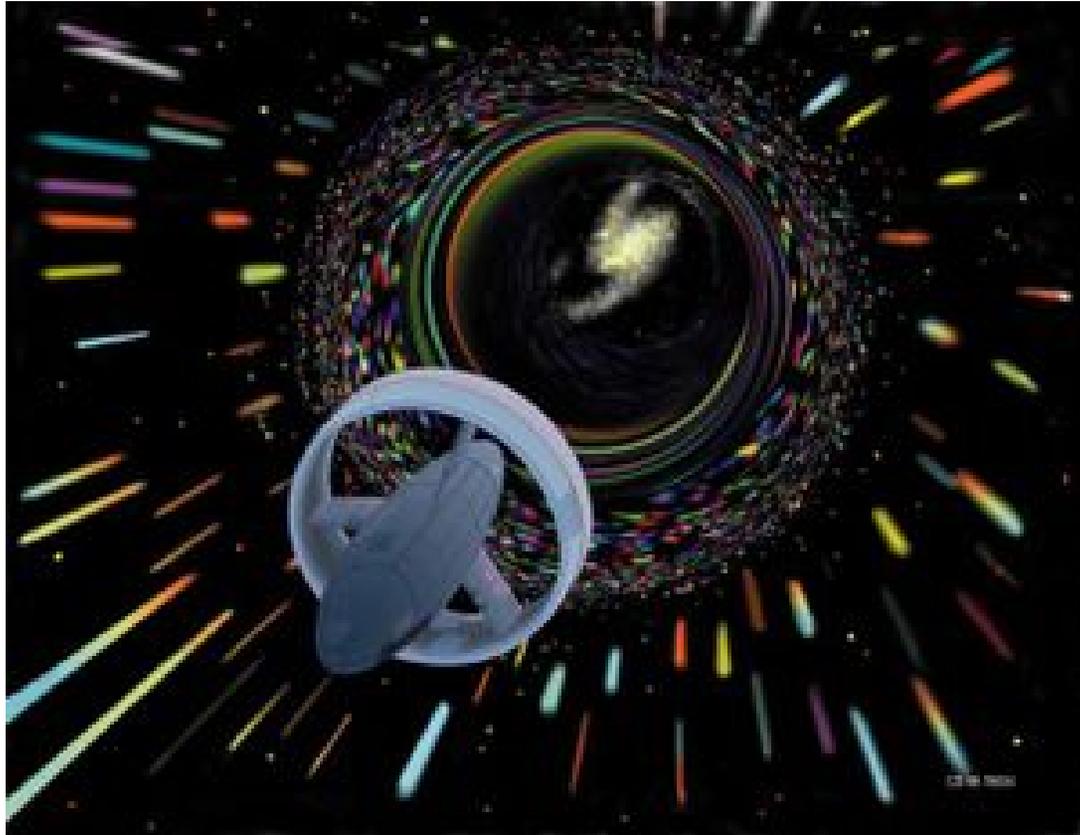
2-D NMR



Like the VTOL

(Photo courtesy of Department of Defense)

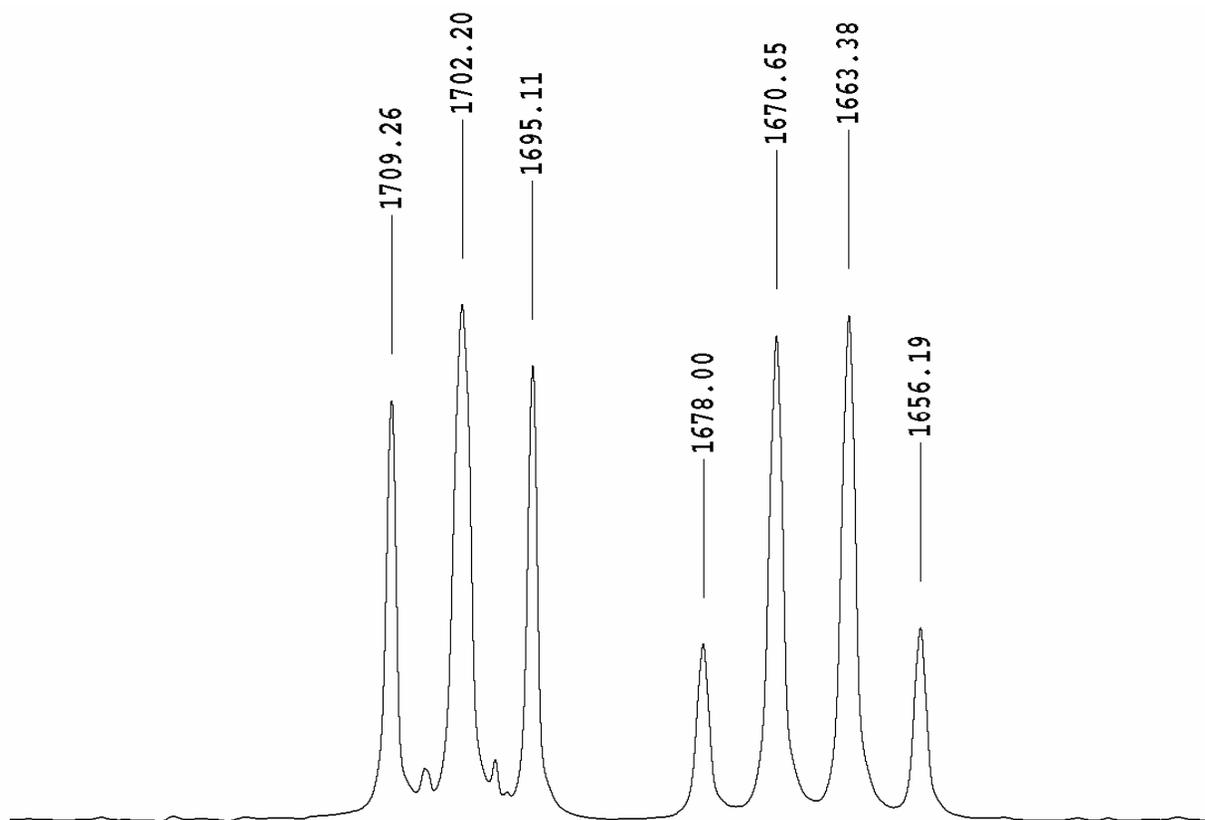
In the future, there will be more developments



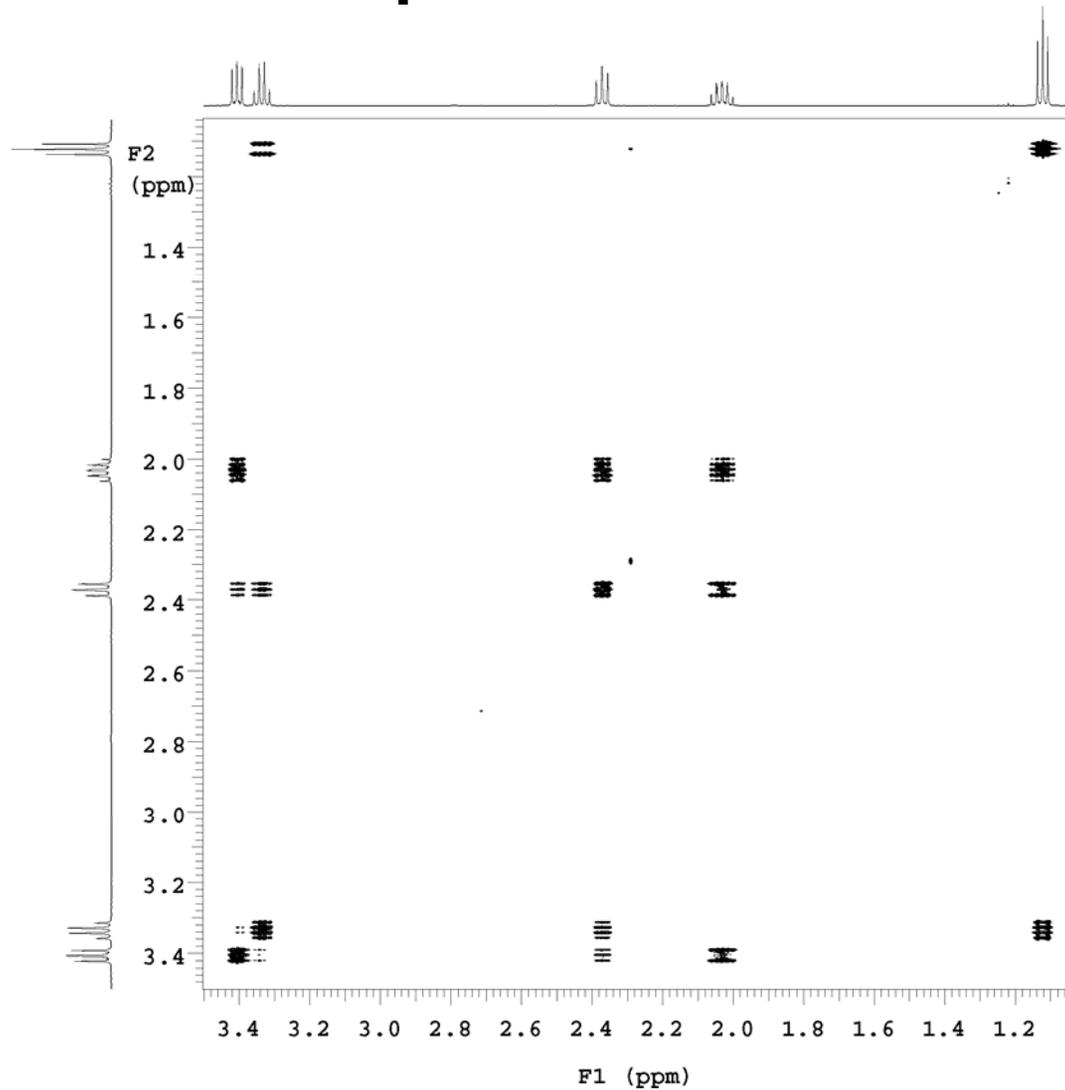
(Image is taken from NASA's Web site: <http://www.nasa.gov>.)

We usually don't need to analyze multiplets in detail

We rarely have to manually calculate the J-couplings



Instead we can use 2-D cross peaks



Many experiments are available

