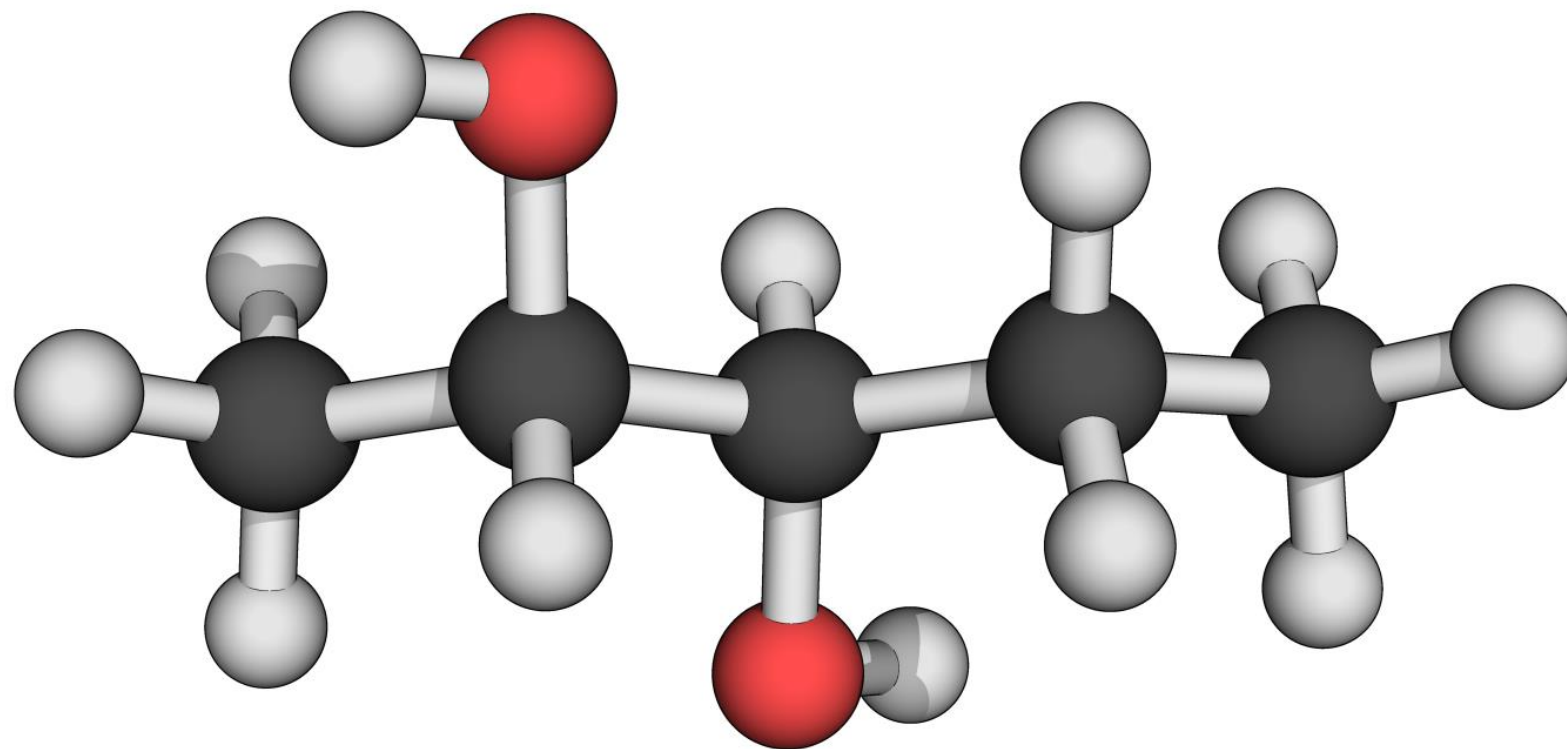
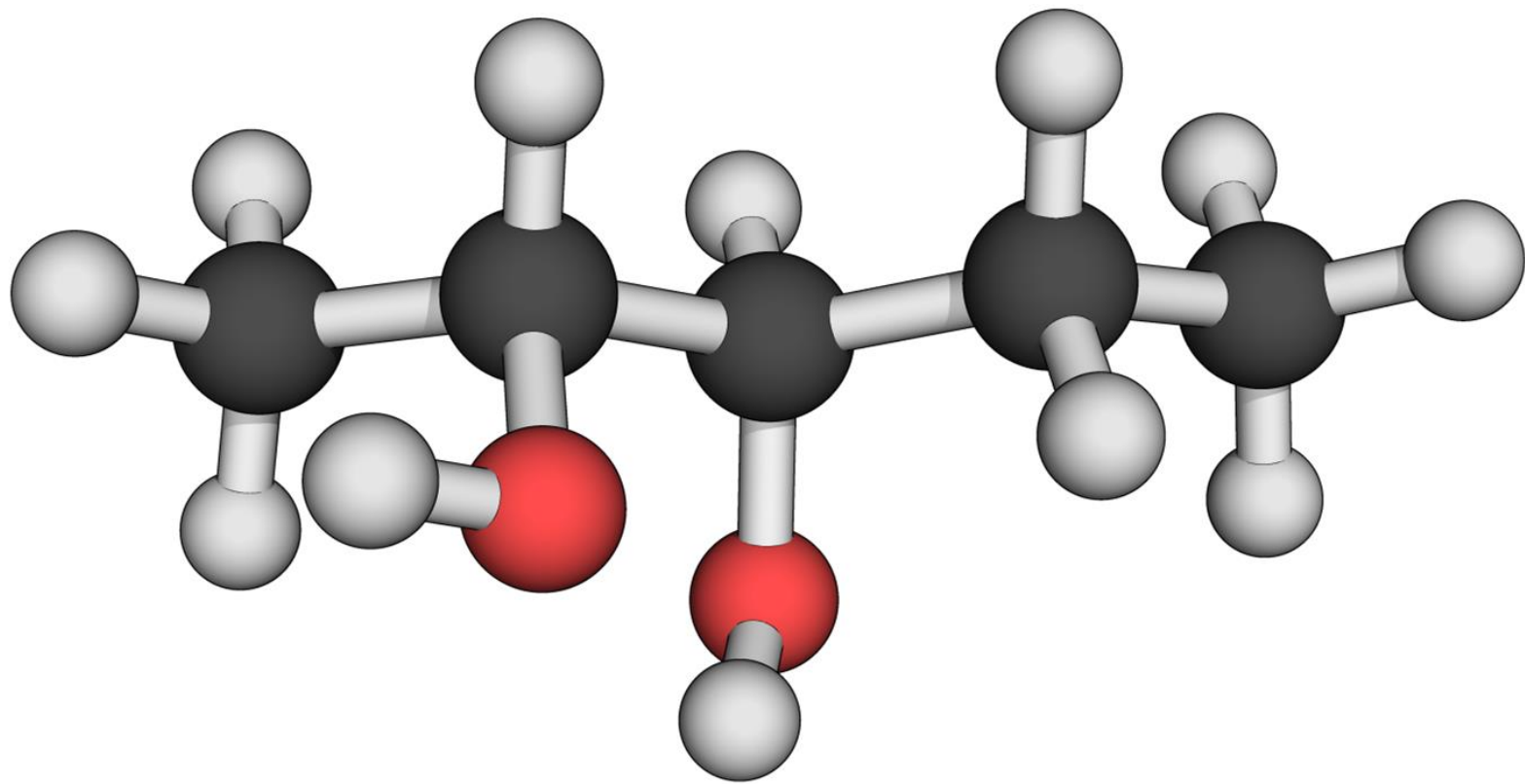
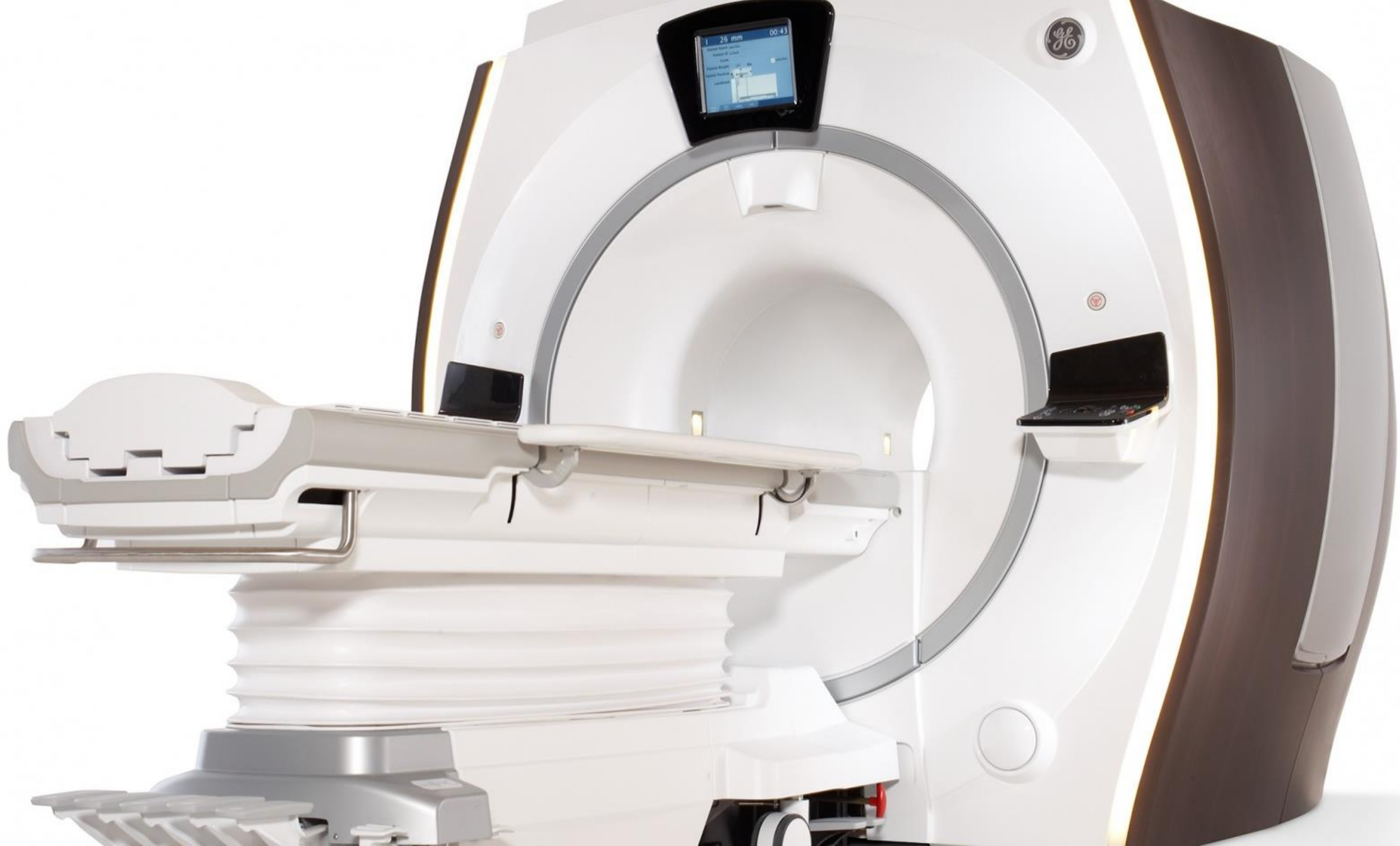


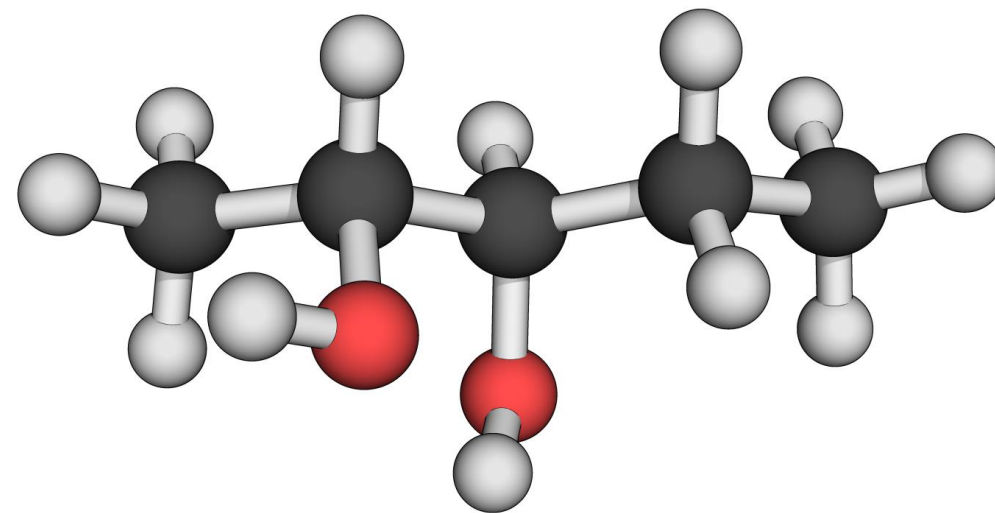
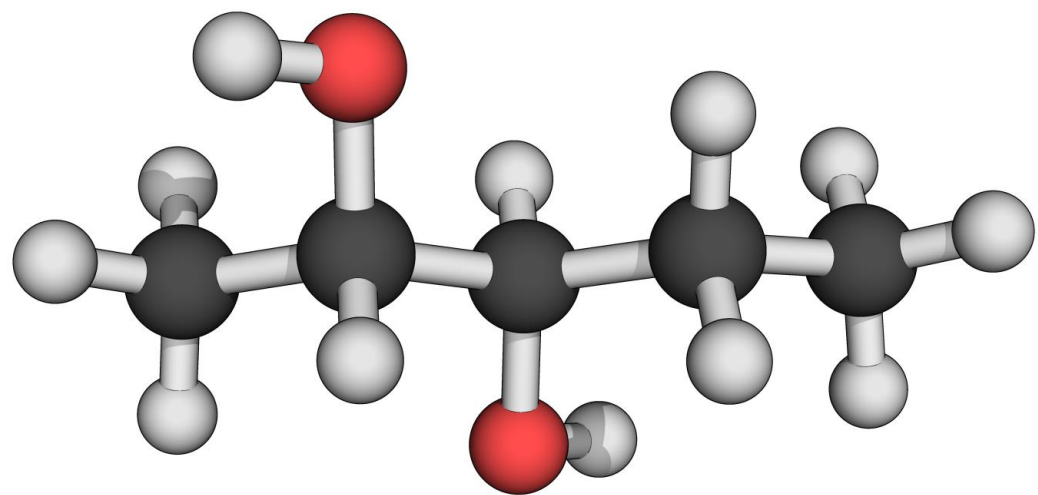
# Competition-based Research in Chemistry

Dr. Lars Andersen Bratholm

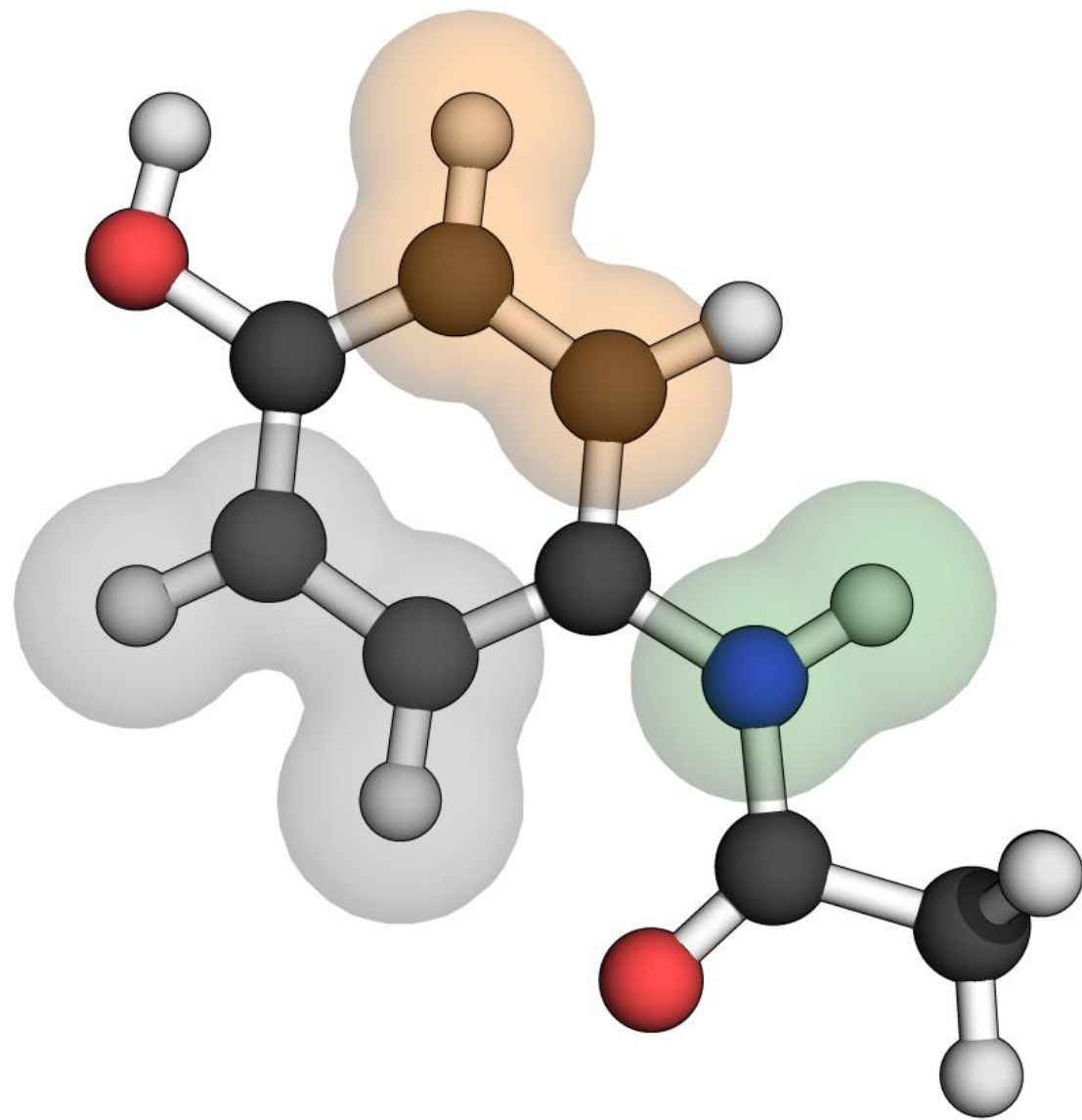








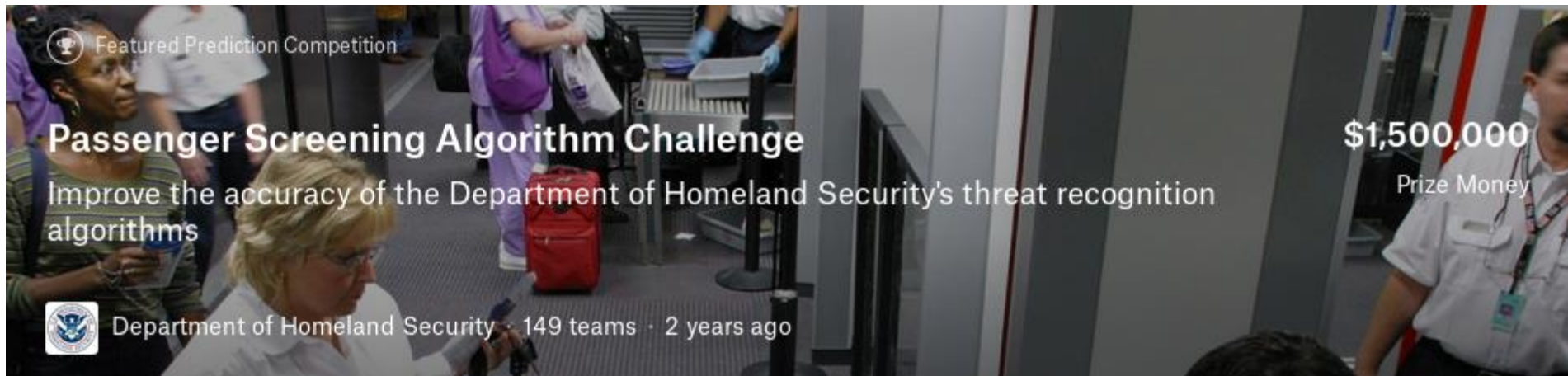
$$\frac{1}{\sqrt{2}} | \text{cat sitting} \rangle + \frac{1}{\sqrt{2}} | \text{cat lying} \rangle$$



kaggle™



# kaggle™




Featured Prediction Competition

## Passenger Screening Algorithm Challenge

Improve the accuracy of the Department of Homeland Security's threat recognition algorithms

**\$1,500,000**  
Prize Money

 Department of Homeland Security · 149 teams · 2 years ago

The banner features a background image of an airport security checkpoint with passengers and staff. The text is overlaid in white and blue, providing details about the competition's title, goal, prize, and organizer.

# kaggle™

 Featured Prediction Competition

## Zillow Prize: Zillow's Home Value Prediction (Zestimate)

Can you improve the algorithm that changed the world of real estate?

**\$1,200,000**

Prize Money



Zillow · 3,779 teams · 2 years ago

# kaggle™



## Shelter Animal Outcomes

Help improve outcomes for shelter animals

1,604 teams · 3 years ago

# kaggle™



Research Prediction Competition

## LANL Earthquake Prediction

Can you predict upcoming laboratory earthquakes?

**\$50,000**  
Prize Money

 Los Alamos National Laboratory · 4,540 teams · a month ago

# kaggle™



## Data Science Bowl 2017

Can you improve lung cancer detection?  
\$1,000,000 · 394 teams · 2 years ago



## Cervical Cancer Screening

Help prevent cervical cancer by identifying at-risk populations  
\$100,000 · 40 teams · 3 years ago

Playground Prediction Competition

### Histopathologic Cancer Detection

Identify metastatic tissue in histopathologic scans of lymph node sections

Kaggle · 1,157 teams · 3 months ago

A banner for the Histopathologic Cancer Detection competition. It features a grid of various histopathologic scans of lymph node sections, showing different cellular structures and colors. The text is overlaid on the grid.

Featured Prediction Competition

### Intel & MobileODT Cervical Cancer Screening

Which cancer treatment will be most effective?

\$100,000  
Prize Money

Intel · 261 teams · 2 years ago

A banner for the Intel & MobileODT Cervical Cancer Screening competition. It features a dark background with a bokeh effect of light spots. The text is overlaid on the background.



# Predicting Molecular Properties

Can you measure the magnetic interactions between a pair of atoms?



CHAMPS (CHemistry And Mathematics in Phase Space) · 1,895 teams · a month to go (a month to go until merger deadline)

[Overview](#)

[Data](#)

[Kernels](#)

[Discussion](#)

[Leaderboard](#)

[Rules](#)

[Team](#)

[Host](#)

[My Submissions](#)

[Submit Predictions](#)

Overview

Edit

Description

Evaluation

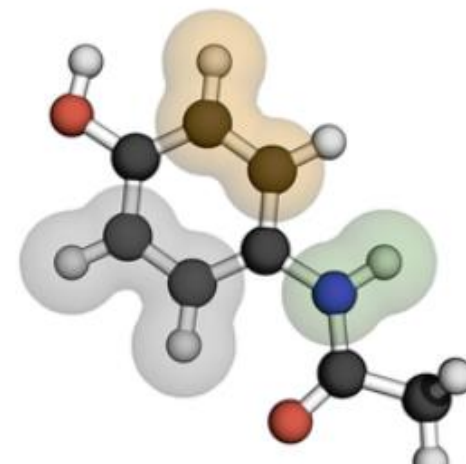
Timeline

Prizes





















+ Add Page

Think you can use your data science smarts to make big predictions at a molecular level?

This challenge aims to predict interactions between atoms. Imaging technologies like MRI enable us to see and understand the molecular composition of tissues. Nuclear Magnetic Resonance (NMR) is a closely related technology which uses the same principles to understand the structure and dynamics of proteins and molecules.



■ In the money
 ■ Gold
 ■ Silver
 ■ Bronze

| #  | Team Name   | Kernel | Team Members  | Score <span>?</span> | Entries | Last |
|----|---|--------|---|----------------------|---------|------|
| 1  | Jaechang Lim  |        |    | -2.686               | 14      | 3d   |
| 2  | outrunner   |        |    | -2.669               | 22      | 4d   |
| 3  | Lam Dang  |        |    | -2.588               | 20      | 5d   |
| 4  | Squid   |        |    | -2.535               | 16      | 2d   |
| 5  |  Quantum Uncertainty  |        |     | -2.461               | 74      | 1h   |
| 6  | Hyperspatial Engineers  |        |      | -2.413               | 22      | 2h   |
| 7  | Mike  |        |    | -2.123               | 48      | 3d   |
| 8  | Time to sleep   |        |    | -2.095               | 16      | 9d   |
| 9  | fmand   |        |    | -2.070               | 43      | 2d   |
| 10 | wowwow  |        |    | -2.045               | 7       | 3d   |
| 11 | 4 GM and the brain  |        |      | -2.027               | 172     | 3d   |

# Thank you

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[kaggle.com/c/champs-scalar-coupling](https://kaggle.com/c/champs-scalar-coupling)