



# Using Computational Methods for Accelerating Science-Based Solutions and Solving Emerging Material Issues

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## Impact

Informatics is a powerful technique that connects desired properties with material characteristics, reduces time and cost, and streamlines the development of new materials.

## Approach

Build Database

Molecular Descriptors

Correlation Matrix/Data Transformation

Build Equation

New Material Predictions

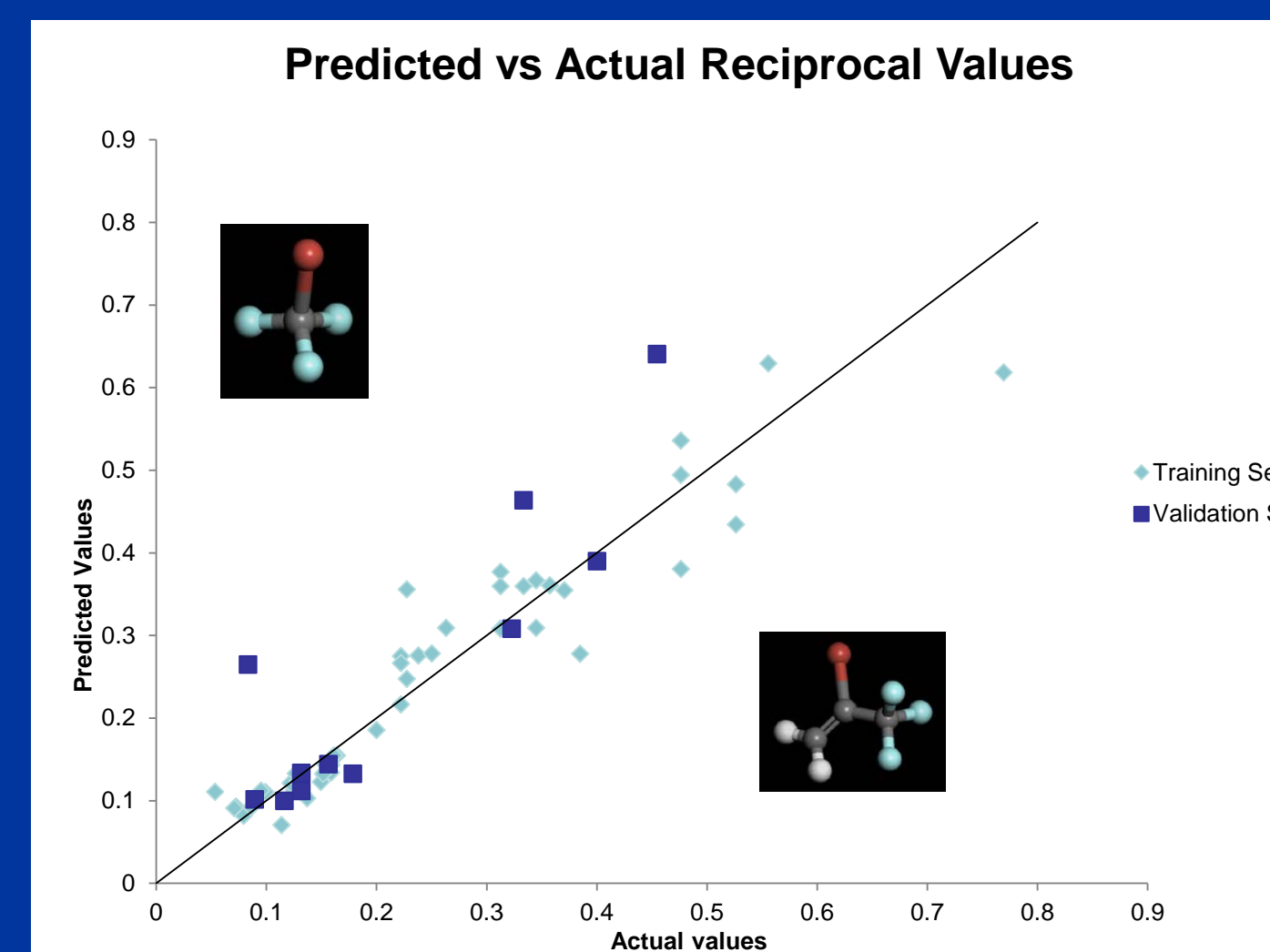


Fire Suppression Testing

## Halon Replacement

**Problem:** Halon 1301 soon to have additional regulations and current stores are slowly being depleted. New fire suppressants needed.

**Solution:** Use QSAR techniques to predict heptane cup burner values and probe a large design space to search for a suitable Halon Replacement



**Conclusions:** Can successfully predict heptane cup burner values for alkanes and alkenes. Several new promising candidates identified.

**Next Steps:** Extend method to other classes of molecules, (e.g. ethers), run experimental validation, and down select for further testing (materials compatibility, GWP, ODP, etc...)

## Pros

- Fast Calculations
- Easy to Process Large Test Matrices
- Low Cost
- Reduced Testing
- Leverage existing data
- Reduce Development Cycle

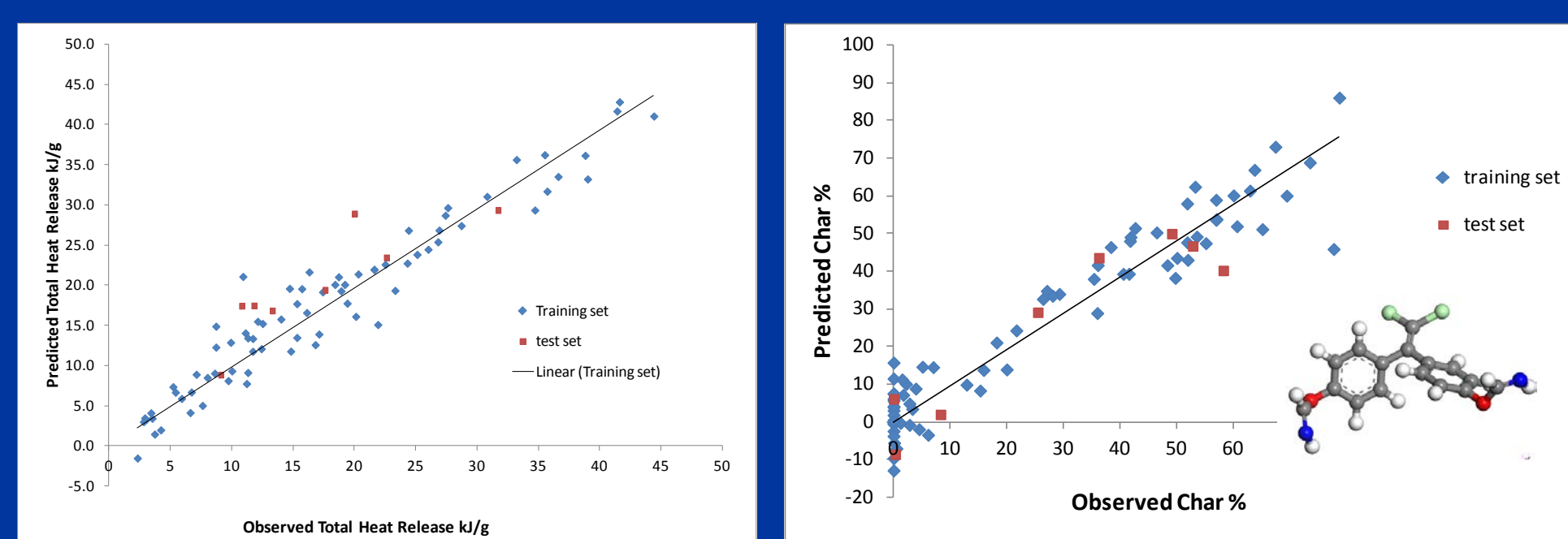
## Cons

- Requires Large Dataset
- Correlation not Causation

## Polymer Flammability

**Problem:** Improvements in fire safety necessary to reduce risk during fire event, however many flame retardants have been found to have serious health and environmental effects leading to increased regulations.

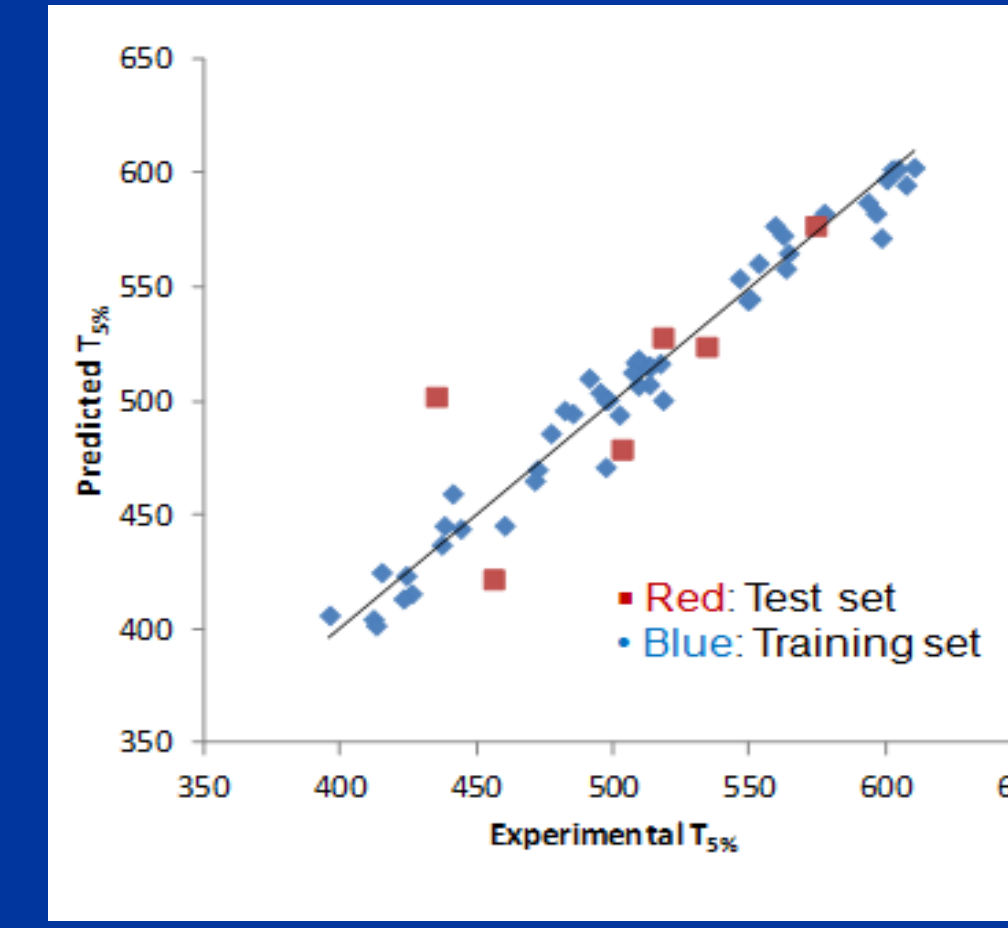
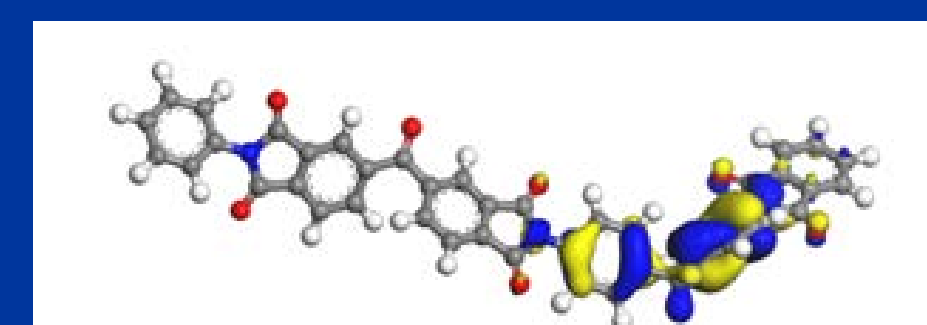
**Solution:** Select materials that are inherently flame safe while providing other necessary properties such as stiffness and ease of processing. QSAR techniques were used to predict heat release and char formation for polymeric materials. The model can be used to screen new materials for fire properties



## Polyimide Decomposition Temperatures

**Problem:** Polymeric material that can survive at high temperatures for an extended period of time desired for areas of aircraft exposed to high heat

**Solution:** Use QSAR techniques to predict decomposition temperatures for polyimide polymers. New candidate polyimides developed based on QSAR model.



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## References

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2. NFPA 2001 Standard on Clean Agent Fire Extinguishing Systems 1994 Edition
3. <http://www.fire.tc.faa.gov/research/research.stm>

## More Examples

- Sealants
  - Tg
  - Crystallinity
- Vapor Degreasers
  - Cleaning Efficiency
  - GWP
  - HAPs/VOCs
- Hydraulic Fluids\*
  - flashpoint
- Corrosion\*
- Thermoset Tg
- Fluid Sensitivity

