

## CENTER FOR GREEN CHEMISTRY & GREEN ENGINEERING AT YALE

Using a computer game to introduce green chemistry and safer chemical design concepts into an undergraduate curriculum



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# Education is undergoing transformation

- Conventional teaching is frequently static and fails to develop skills such as critical thinking and problem solving.
- Modern curriculum can retain students at a higher rate.
- Studies have advocated for increasing interdisciplinary content and improving the relevance for high school and undergraduate students.
- Videos, simulations and hands-on activities allow students to make more connections between the scientific topics.





“...digital game-based learning has been recognized as a promising approach for motivating students to learn “



# Education and computer games

## Is this a new trend?

### Where in the world is Carmen Sandiego? '85

Educational mystery game where player uses the knowledge of geography, history and world cultures to track the thief.

As more thieves are arrested, the player rises in the ranks and cases become more difficult.

Where in the USA is Carmen Sandiego? '86

Where in the Europe is Carmen Sandiego? '88

Where in the Time is Carmen Sandiego? '89

Where in the Space is Carmen Sandiego? '93



# Educational games now

- Emerging are *epistemic games* (virtual internships) which allow students to role-play professionals (including architects, journalists, urban planners, and engineers).
  - Exposure to practices, design process, experience, team work, minimal financial resources
- Virtual internships allow solving complex science, technology, engineering and math (STEM) problems.
- However the majority of educational games are intended for K-12

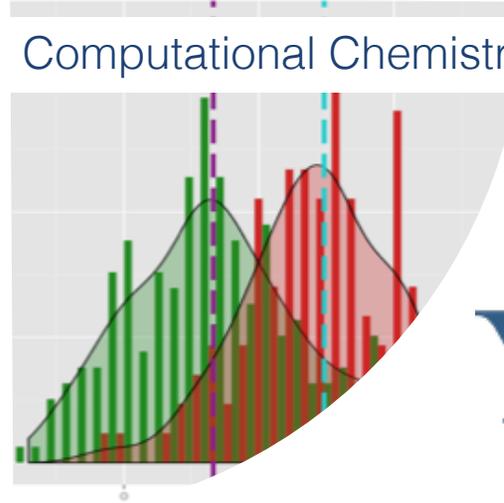


# MoDRN

Molecular Design  
Research Network



**THE GEORGE  
WASHINGTON  
UNIVERSITY**  
WASHINGTON, DC



**W**  
UNIVERSITY of  
WASHINGTON



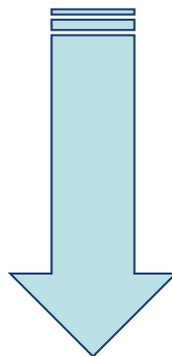
**Yale**

# Molecular Design Research Network (MoDRN)



# Our educational approach

Novel research in chemistry and toxicology  
(scientific literature, MoDRN's research)



Scientifically rigorous, easily accessible educational materials which:

- Engage students in safer chemical design of the next generation molecules
- Allow seamless integration in the chemistry, biology or environmental science curriculum.



# Green Chemistry & Safer Chemical Design Game

## Main objectives

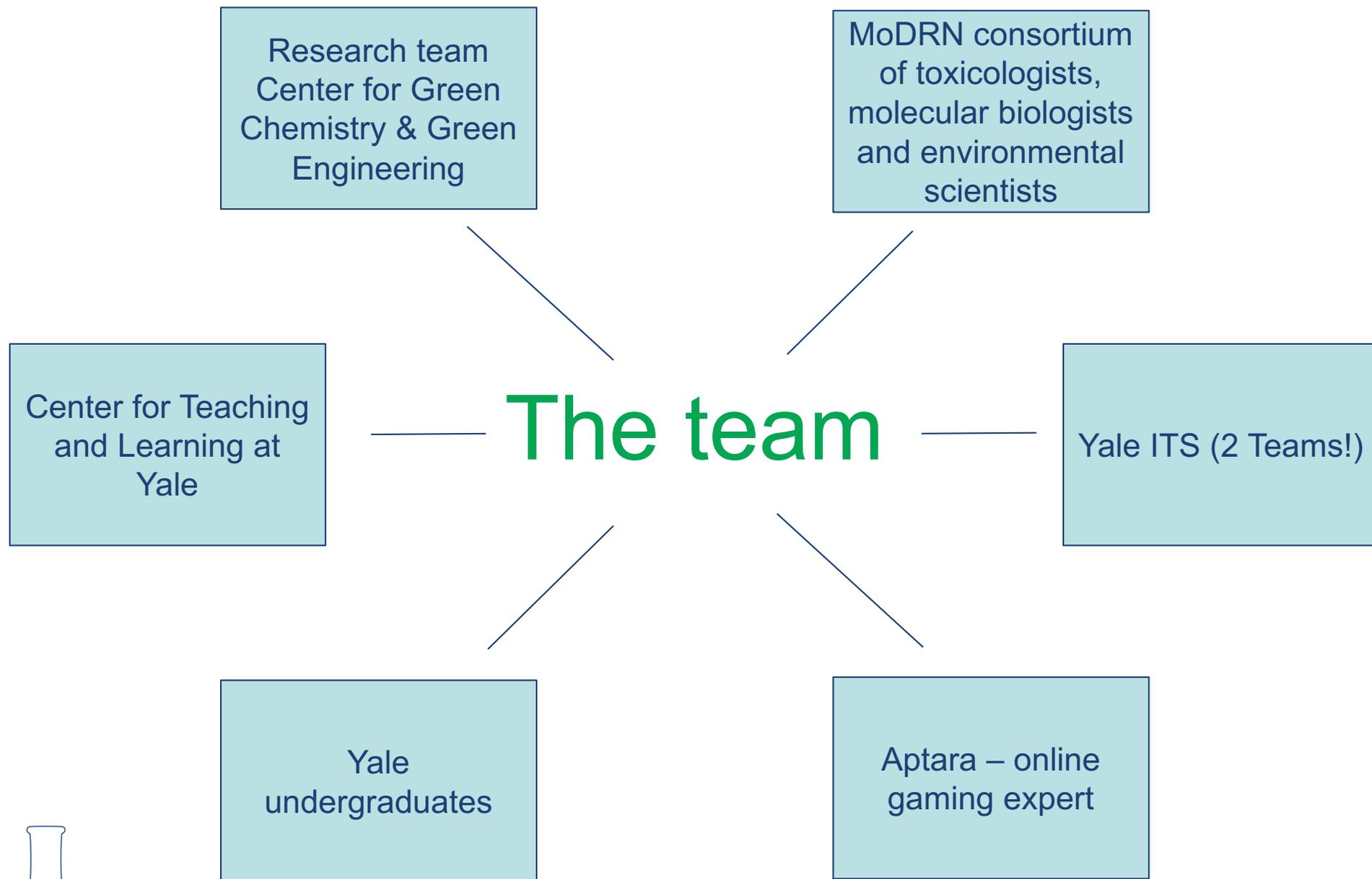
- Develop an educational game which can be used by non-major undergraduate students to make connection between physiochemical properties and health.
- Disseminate 4<sup>th</sup> Principle of Green Chemistry



# Green Chemistry & Safer Chemical Design Game

- Unique activity which incorporates systems thinking into the product design.
- It simulates scenarios to model decision making process used by professionals to develop a new chemical product.
- Players complete multiple stages of product design with respect to environmental and human impacts, and performance.





# Steps in building the game

1. Define which chemistry and toxicology concepts do we want to highlight in the game.
2. Decide what other life-cycle concepts should be included.
3. Define metrics, boundaries, data sources, IT requirements.
4. Develop a framework which includes scientific and educational components and links them together.
5. Build a 'wireframe' (storyline, avatars, graphics).
6. Develop scientifically accurate language which supports a wireframe (tasks, tips, feedback).
7. Test the game logic.
8. Engage the group and receive feedback.



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Define which chemistry and toxicology concepts we want to highlight in the game.

- ADME - Absorption, Distribution, Metabolism and Elimination.
- Differences/similarities between human and aquatic toxicity.
- Physicochemical parameters like molecular weight, log P and physical state and their role in ADME. Limiting bioavailability and enhancing DME.
- The role and the structure of product, in this case a surfactant.



## Decide what other life-cycle concepts should be included

- Chemical performance: what is detergent's cleaning ability?



## Define metrics, boundaries, data sources, IT requirements

- Use parameters and their preferred/not preferred ranges that limit or enhance toxicity described in peer reviewed literature and MoDRN's work.
- Provide simple explanations of the complex toxicology/biochemistry terms

e.g.: Log P definition = Log P is a measure of lipid solubility (how well the chemical dissolves in fat and passes through cell membranes).

Rather than LogP = **partition-coefficient** is the ratio of concentrations of a compound in a mixture of two immiscible phases (water and octanol) at equilibrium.

$$\log P_{\text{oct/wat}} = \log \left( \frac{[\text{solute}]_{\text{octanol}}^{\text{un-ionized}}}{[\text{solute}]_{\text{water}}^{\text{un-ionized}}} \right)$$



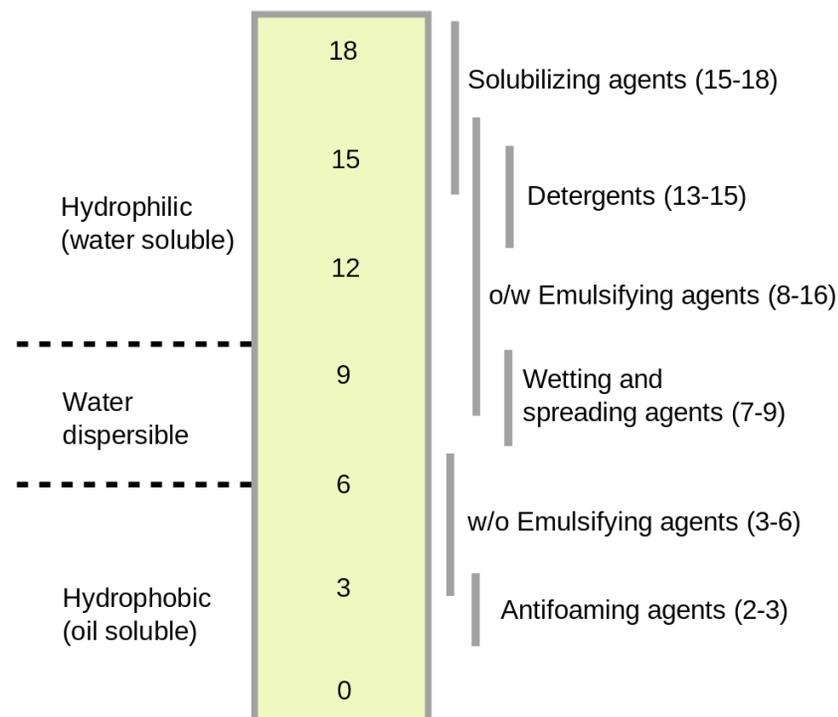
Define metrics, boundaries, data sources, IT requirements

# Performance of the detergent metrics = HLB value

HLB hydrophilic-lipophilic balance is a measure of the degree to which surfactant is hydrophilic or lipophilic.

It's value depends on Log P and the presence of the functional groups (esters, aldehydes, alcohols)

Is expressed on the scale 0-18



# Goal & Gameplay

Player has to come up with the optimal detergent which:

- Is benign by design (does not cause human/aquatic toxicity)
  - LEVEL 1: Has a limited absorption through membranes (limited bioavailability)
  - LEVEL 2: If absorbed, it has a reduced movement through the body (distribution), increased deactivation rate (metabolism) and accelerated removal (elimination)
  - Biodegrades in the environment
- Has an optimal cleaning performance

Notes:

One detergent is optimized throughout the Level – property selection carries from one challenge to another

Detergent design is based on properties not a molecular structure



## LEVEL 1

GOAL

HUMAN TOXICITY

AQUATIC TOXICITY

PERFORMANCE

Skin absorption

Avoiding toxicity

Lung absorption

Intestine absorption

## LEVEL 2

GOAL

HUMAN TOXICITY

AQUATIC TOXICITY

PERFORMANCE

Distribution

Biodegradation

Metabolism

Elimination

# Other features that enhance learning experience: Tips for parameter selection

The screenshot displays a simulation interface for parameter selection. At the top left, a circular icon shows '1 Level'. The top navigation bar includes buttons for 'Goal', 'Human Toxicity' (highlighted), 'Aquatic Toxicity', and 'Performance'. Below this, a sub-menu shows 'Skin Absorption' (highlighted), 'Respiratory Absorption', and 'GI Absorption'. The main interface features three sliders: 'Molecular Weight' (range 50-1000, value 300), 'Log P' (range -3 to 7.5, value 6), and 'Physical State' (range Solid to Liquid, value SOLID). A central cylindrical chamber contains a yellow granular substance. A 'Task Description' box is on the right. At the bottom, a laptop screen shows an illustration of hands being washed and the text 'Avoiding Skin Absorption'. Navigation buttons for 'Back', 'Help', and 'Next' are at the bottom.



# Other features that enhance learning experience: Instant feedback & suggestions for improvements

The screenshot displays a simulation interface for designing a detergent. At the top left, a circular icon shows '1 Level'. The top navigation bar includes buttons for 'Goal', 'Human Toxicity' (highlighted in blue), 'Aquatic Toxicity', 'Performance', 'Skin Absorption' (highlighted in green), 'Respiratory Absorption', and 'GI Absorption'. The main area features an illustration of a hand being washed with a sponge. To the right of the illustration, a text box provides feedback: 'Uh-oh! The detergent that you designed may be absorbed through the skin since the values that you selected are not within the preferred range. The compound may be absorbed through skin and be circulated within the body where it may have harmful effects. Below you will find the result of your parameter selection. You really should to go back and adjust the parameters. To redesign your detergent, please select the Back button. To go to the next phase of your chemical design, please select the Next button.'

Below the text, three parameters are shown with sliders and their current values:

- Molecular weight:** A slider ranging from 50 to 950 with a white triangle marker at 300. The value '300' is displayed in a red box on the right.
- Log P:** A slider ranging from -3 to 7 with a white triangle marker at 6. The value '6' is displayed in a green box on the right.
- Physical state:** A slider ranging from 'Solid' to 'Liquid' with a white triangle marker at 'Solid'. The value 'SOLID' is displayed in a green box on the right.

At the bottom left, there is a 'Back' button with a left-pointing arrow, and at the bottom right, there is a 'Next' button with a right-pointing arrow.



# At the end: “stars” and feedback for a successful design

The screenshot shows a simulation interface for designing a detergent. At the top, there are four tabs: Goal, Human Toxicity, Aquatic Toxicity, and Performance. The Performance tab is selected, showing a slider for HLB Value ranging from -4 to 22, with a current value of 14.4844. Below this are two panels for Human Toxicity and Aquatic Toxicity, each with four parameters: Physical state, Log P, Molecular Weight, and Vapour Pressure. The Human Toxicity panel shows values: Physical state (SOLID), Log P (0.1), Molecular Weight (700), and Vapour Pressure (0). The Aquatic Toxicity panel shows values: Physical state (SOLID), Log P (0.1), Molecular Weight (700), and Vapour Pressure (0). A feedback message at the bottom states: "This is a good attempt! You designed the detergent which has an optimal cleaning performance, but may cause aquatic or human toxicity. Your chemical works well, but its safety needs to be improved before global production and distribution. Give it another try." The interface also includes a star rating system (5 stars, with the 5th star empty), a Help button, a Redesign button, and a Level 2 button.

**1**  
Level

Goal Human Toxicity Aquatic Toxicity **Performance**

**Performance**

**HLB Value** 14.4844

**Task Description**

**Human Toxicity**

Physical state	SOLID
Log P	0.1
Molecular Weight	700
Vapour Pressure	0

**Aquatic Toxicity**

Physical state	SOLID
Log P	0.1
Molecular Weight	700
Vapour Pressure	0

This is a good attempt! You designed the detergent which has an optimal cleaning performance, but may cause aquatic or human toxicity. Your chemical works well, but its safety needs to be improved before global production and distribution. Give it another try.

★ ★ ★ ★ ★ Help Redesign Level 2



# Next steps

- Work with a pilot group of students and faculty to conduct a beta testing
- Release the game to the public
- Interested? Please reach out!



# Acknowledgements

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*Yale Center for Teaching and Learning*



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