



chemistry
at BOSTON UNIVERSITY



UNIVERSITY of ST. THOMAS



Learn by Doing

Creating an effective undergraduate learning experience through teaching and research

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UNIVERSITY OF MINNESOTA

DEPARTMENT OF
CHEMISTRY

A department of the Institute of Technology

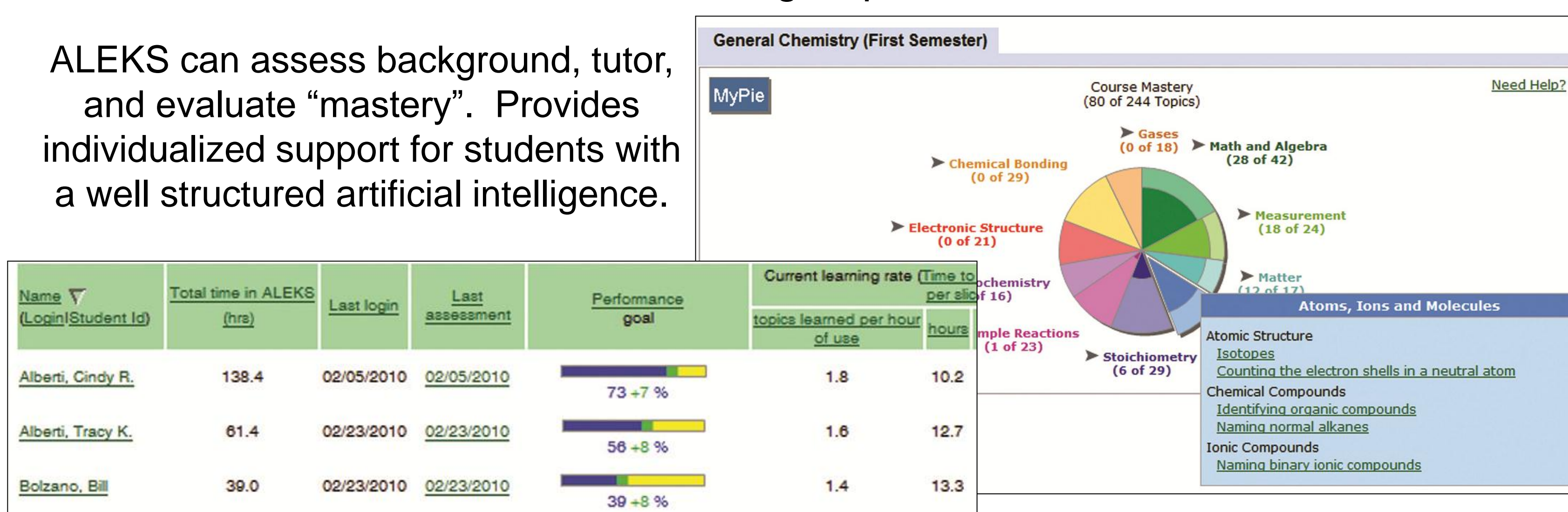
Technology in the Classroom

ALEKS

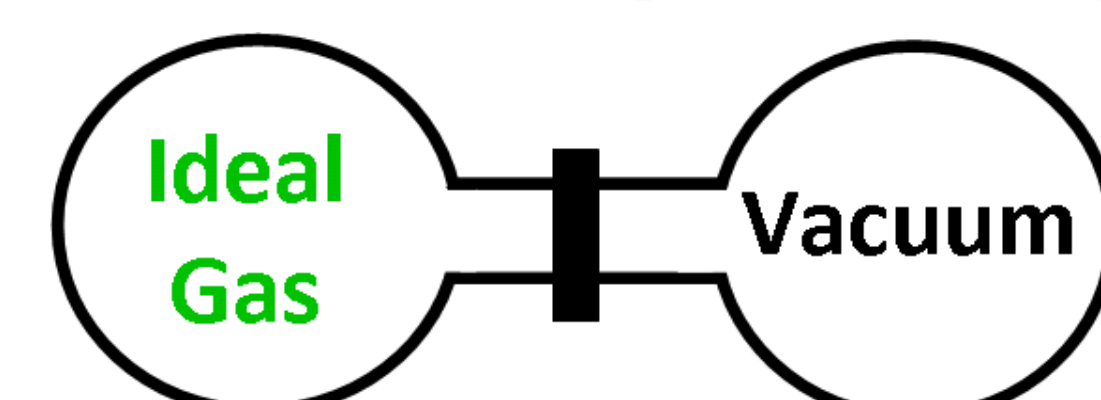
Assessment and LEarning
in Knowledge Spaces

<http://www.aleks.com/>

ALEKS can assess background, tutor, and evaluate "mastery". Provides individualized support for students with a well structured artificial intelligence.



Student Response Systems & Forward Based Assessment



If the wall separating the two bulbs is removed, what the work, heat, ΔE , and ΔH for the gas expansion?



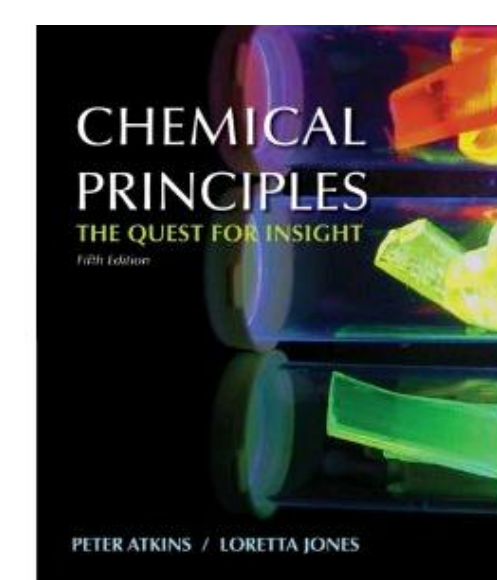
Forward based assessment rewards preparation and provides low stakes assessment. Student response systems allow fast grading and anonymous, instant feedback.

<http://www.einstruction.com> & <http://www.turningtechnologies.com>

Dynamic Books

dynamicbooks.
<http://www.dynamicbooks.com>

Dynamic books allows you to add, remove, edit, and move text, images, or equations within the text book. Customize the text to your course, often at a lower cost to the students.



Thinking point: Before reading further, predict how the effective nuclear charge might affect some atomic properties, such as the size of an atom or the ease with which an outer electron can be removed.

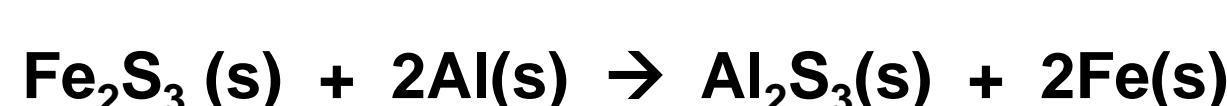
1.15: Atomic Radius

Electron clouds do not have sharp boundaries, and so we cannot measure the exact radius of an atom. However, when atoms pack together in solids and bond together to form molecules, their centers are found at definite distances from one another. The **atomic radius** of an element is defined as half the distance between the centers of neighboring atoms (11). If the element is a metal, its atomic radius is taken to be half the distance between the centers of neighboring atoms in a solid sample. For instance, because the distance between neighboring nuclei in solid copper is 256 pm, the atomic radius of copper is 128 pm. If the element is a nonmetal or a metalloid, we use half the distance between the nuclei of atoms joined by a chemical bond; this radius is also called the **covalent radius** of the element, for reasons that will become clear in **Chapter 2**. For instance, the distance between the nuclei in a Cl_2 molecule is 198 pm, and so the covalent radius of chlorine is 99 pm. If the element is a noble gas, we use the **van der Waals radius**, which is half the distance between the centers of neighboring atoms in a sample of the solidified gas. The atomic radii of the

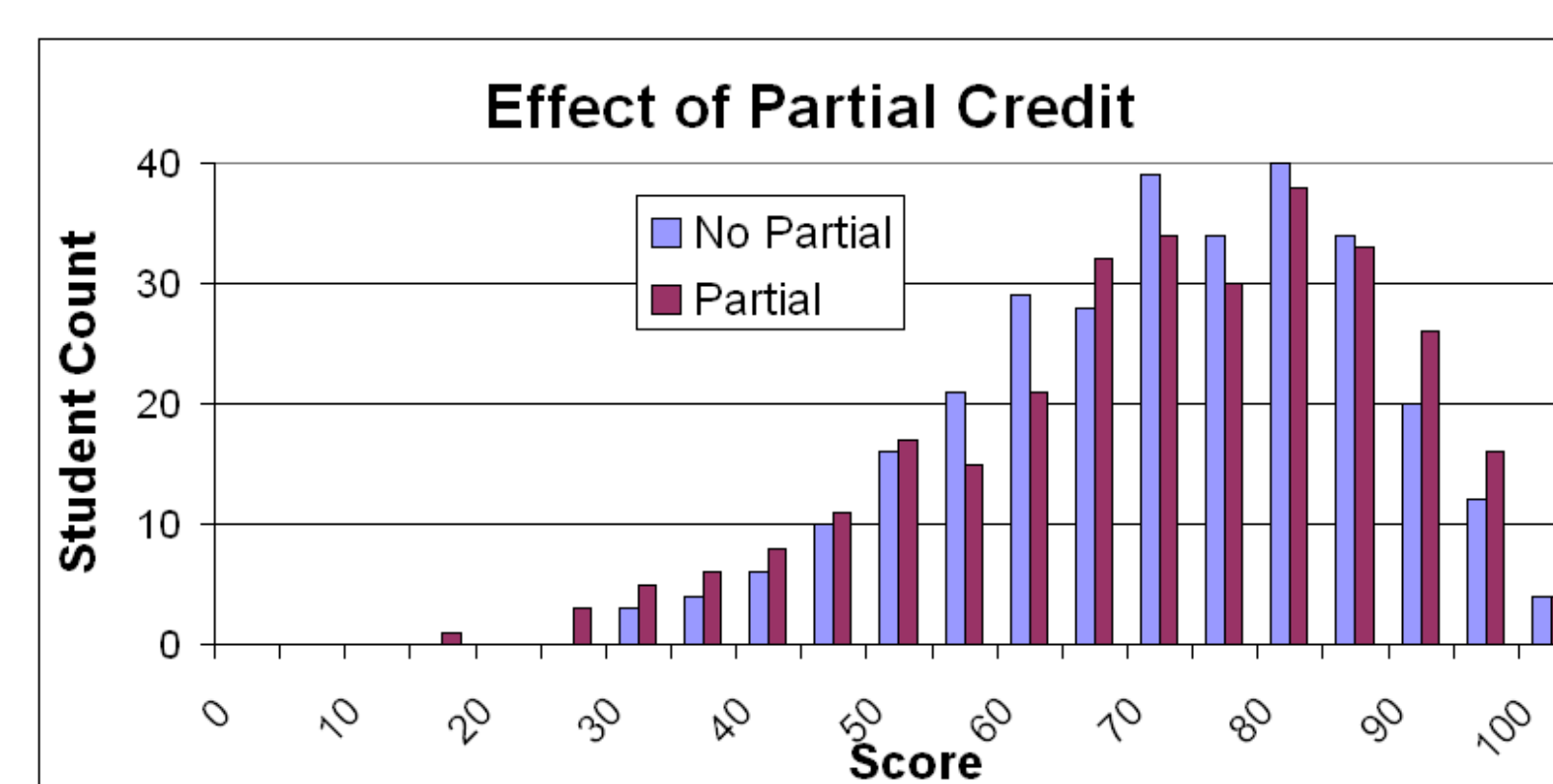
Partial Credit Multiple Choice

Michelle Driessen, University of Minnesota
"Grading Multiple Choice Questions: Rewarding Understanding and Preventing Plagiarism"
Garth Denyer and Dale Hancock. J. Chem. Ed., 79(8), 961 (2002)

How many moles of Al_2S_3 are formed from the reaction of 20.0 g of Fe_2S_3 and 10.0 g of Al?



- a. 0.1850 moles Al_2S_3
 - b. 0.1440 moles Al_2S_3
 - c. 0.0962 moles Al_2S_3
 - d. 0.2000 moles Al_2S_3
 - e. 0.2780 moles Al_2S_3
- Close (+2)
Wrong limiting reagent
Correct (+5)
Incorrect (-3)
Nonsense answer

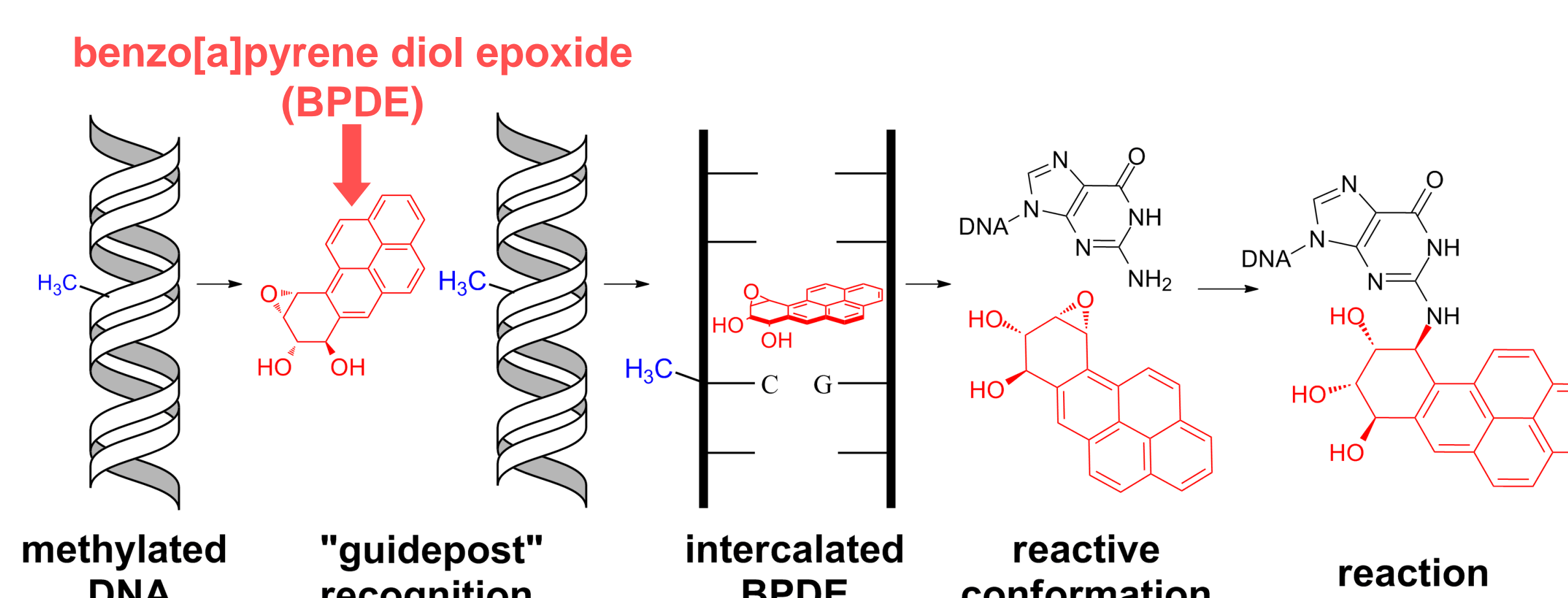
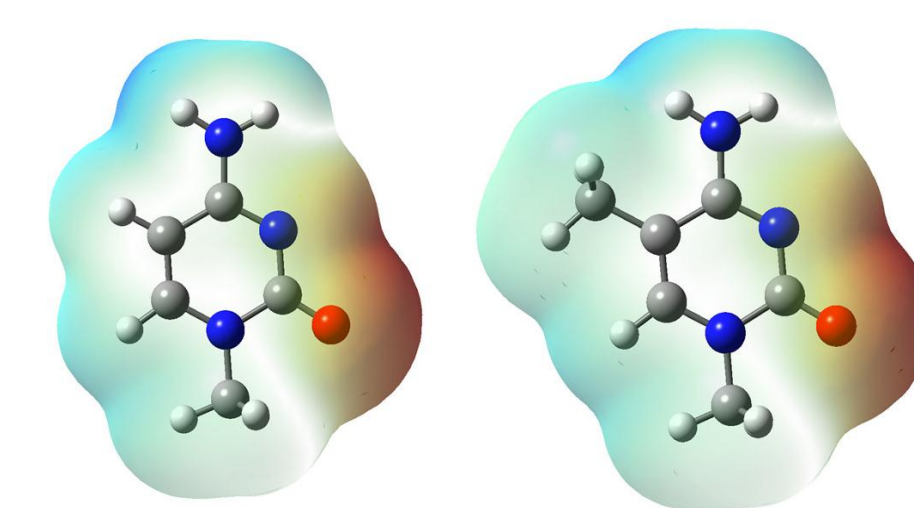


Computational Chemistry for Biochemical Questions

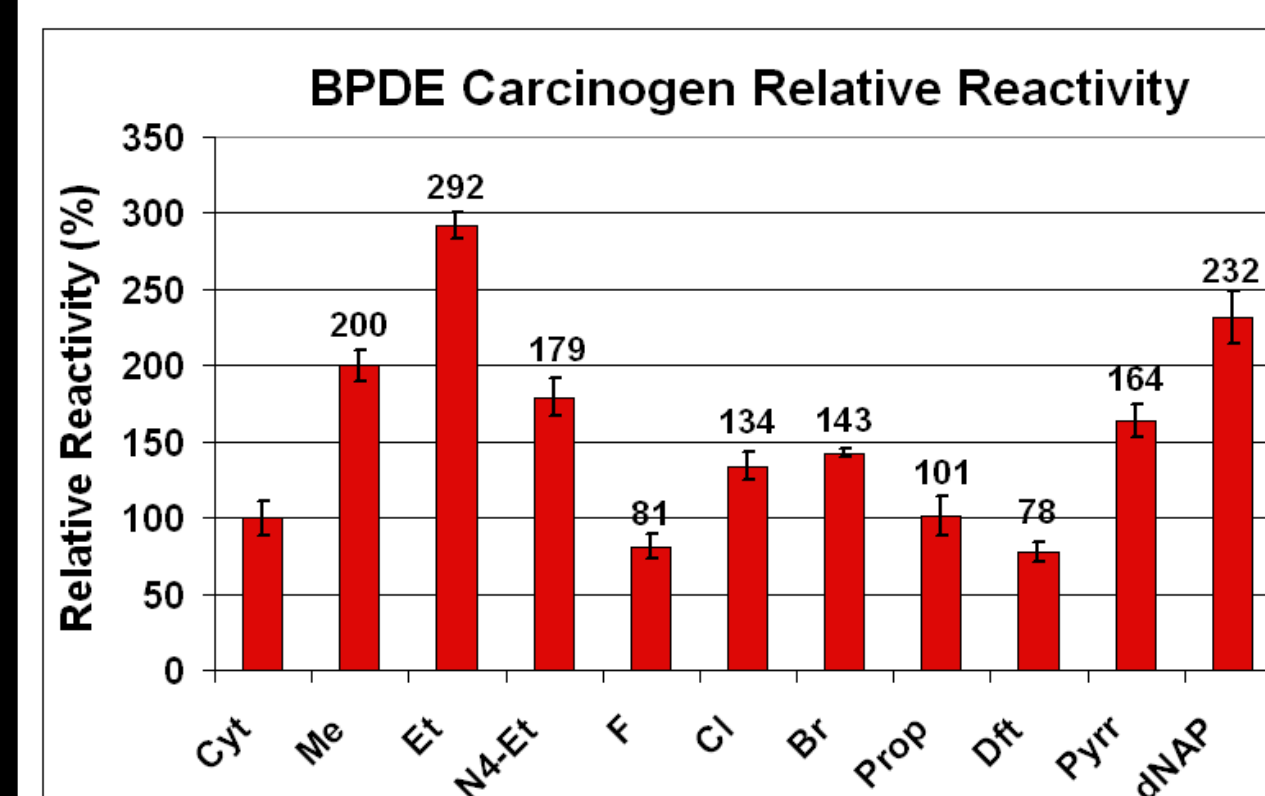
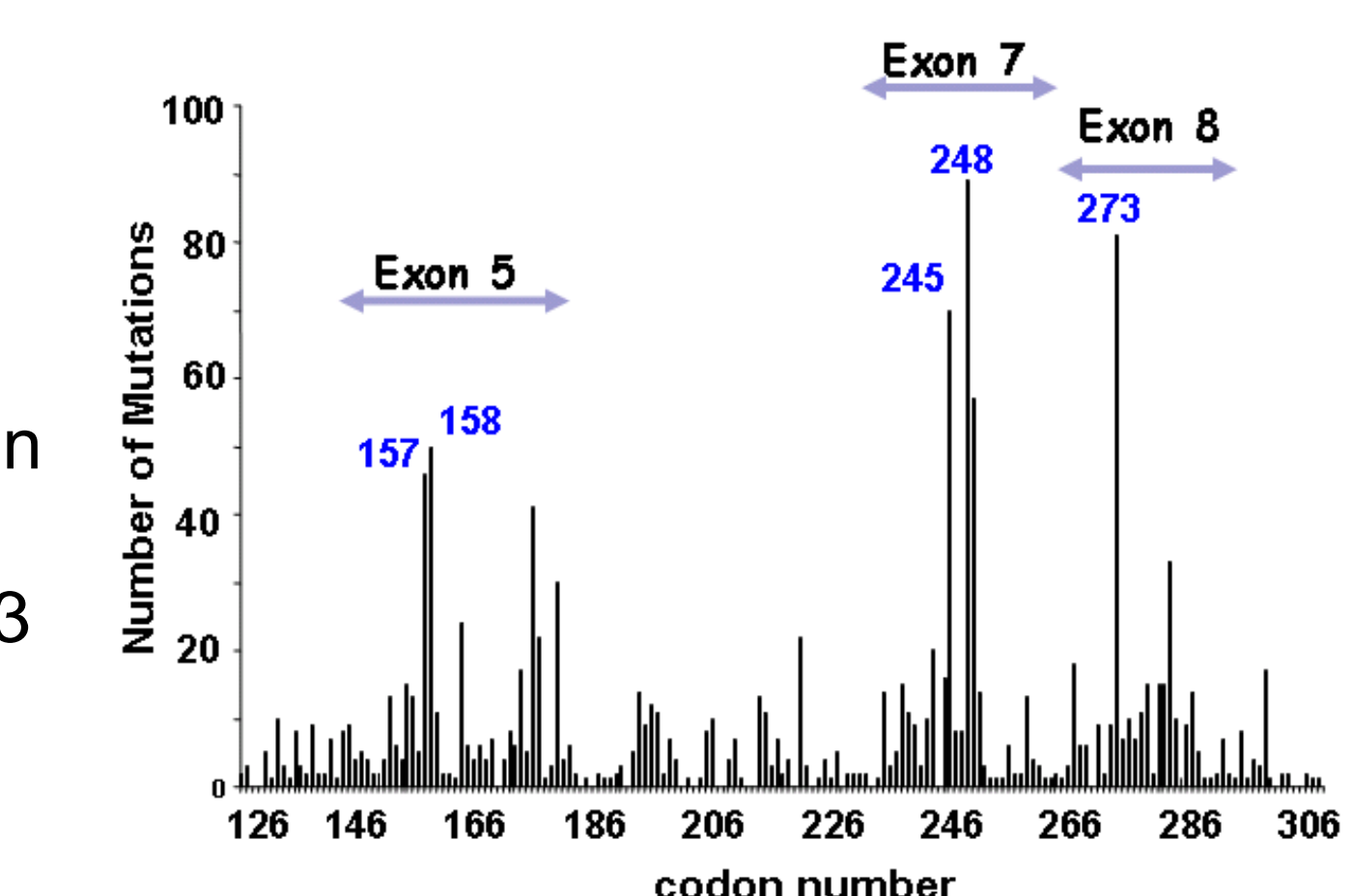
Density Functional Study of the Influence of C5 Cytosine Substitution in Base Pairs with Guanine

Adam Moser, Becky Guza, Natalia Tretyakova, Darrin York. Theor. Chem. Acc., 122, 179-188 (2009).

Understanding the role of C5 methylated cytosine in susceptibility of DNA CG base pairs to tobacco smoke carcinogen attack using C5 substituted cytosine analogs

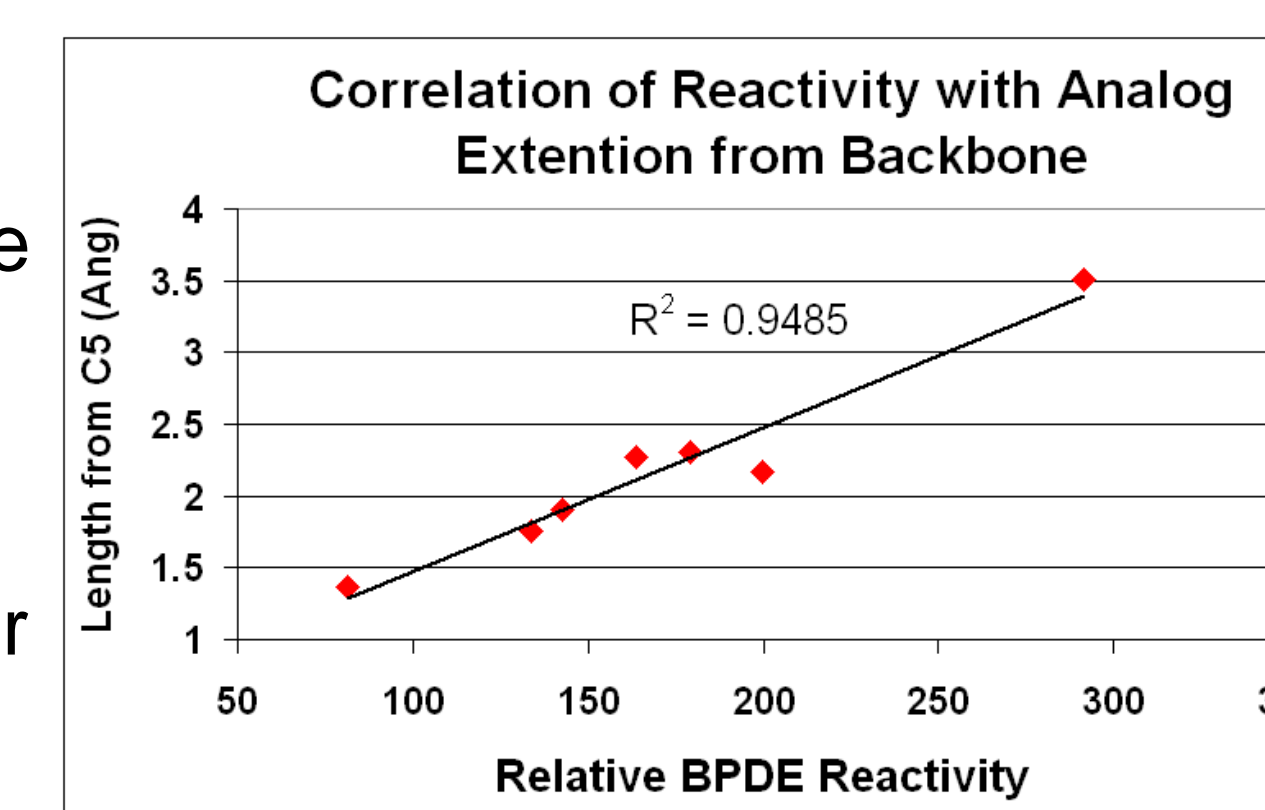


Guanines within MeCG dinucleotides within the $p53$ gene are mutational "hotspots" in smoking-induced lung cancer. The $p53$ gene codes for the P53 protein, an integral protein in natural cancer defense.



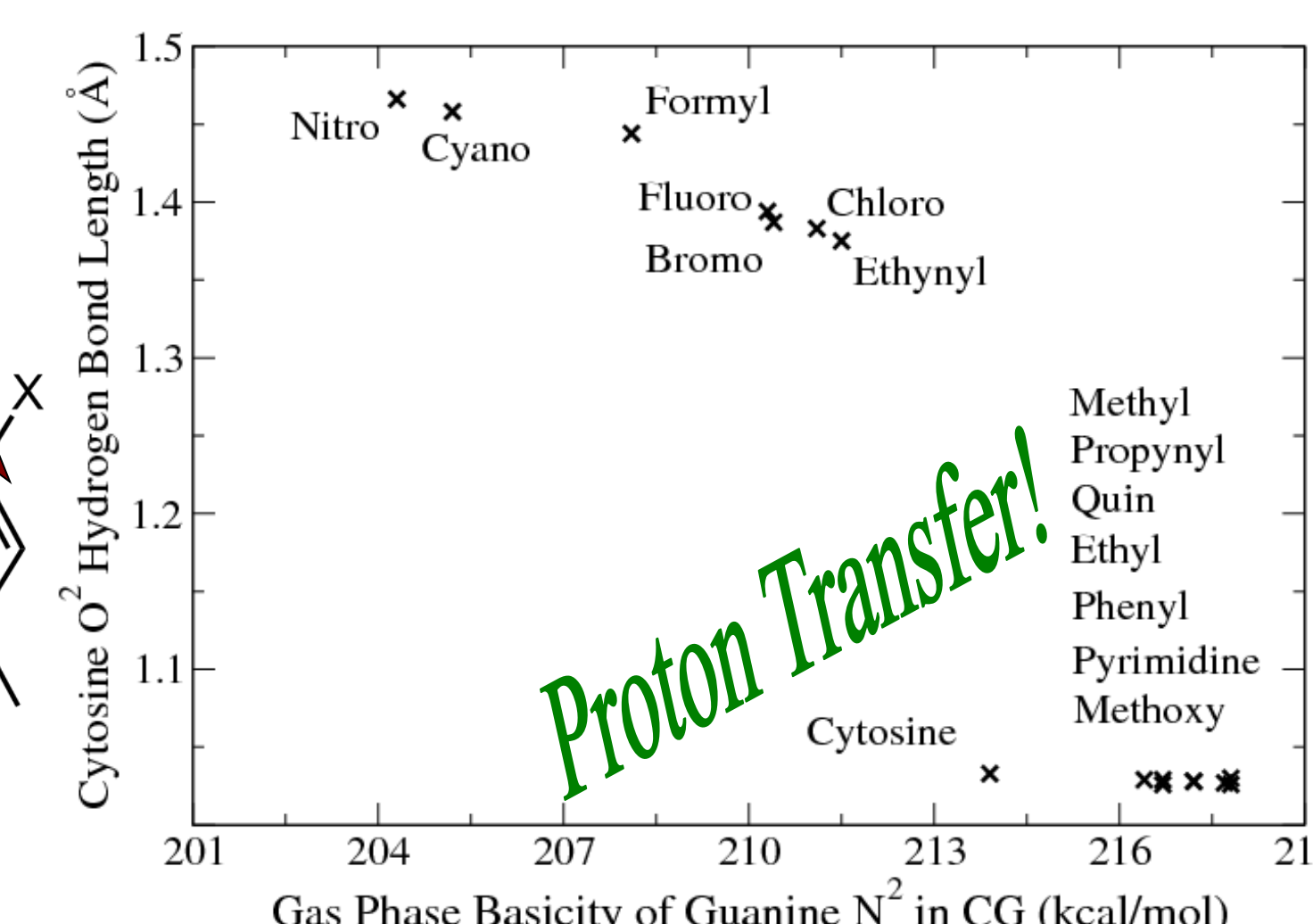
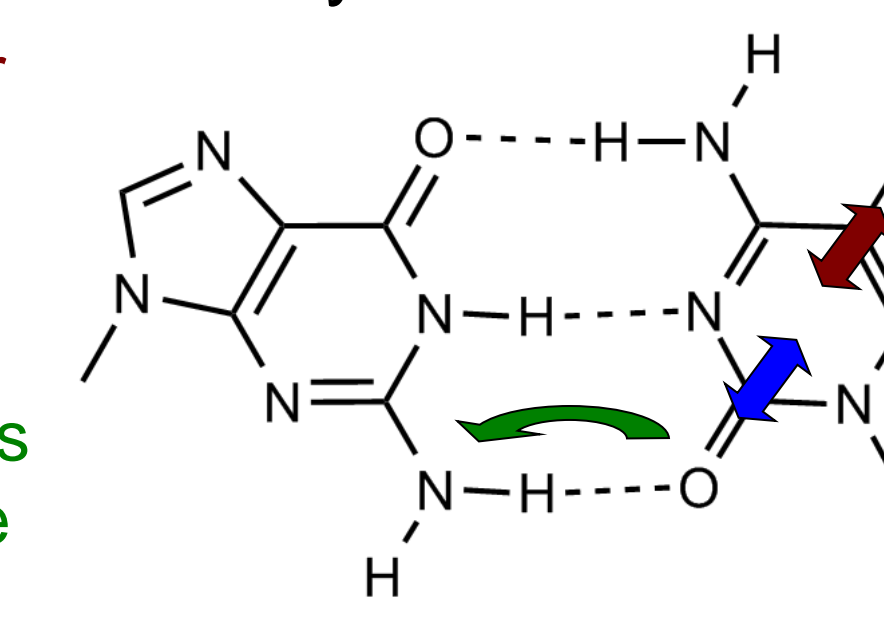
Reactivity of BPDE with DNA CG base pair analogs compared relative to native cytosine (left)

Correlation of analog extension from DNA major groove with relative reactivity (right)



Donated nucleophilicity measured by gas phase basicity

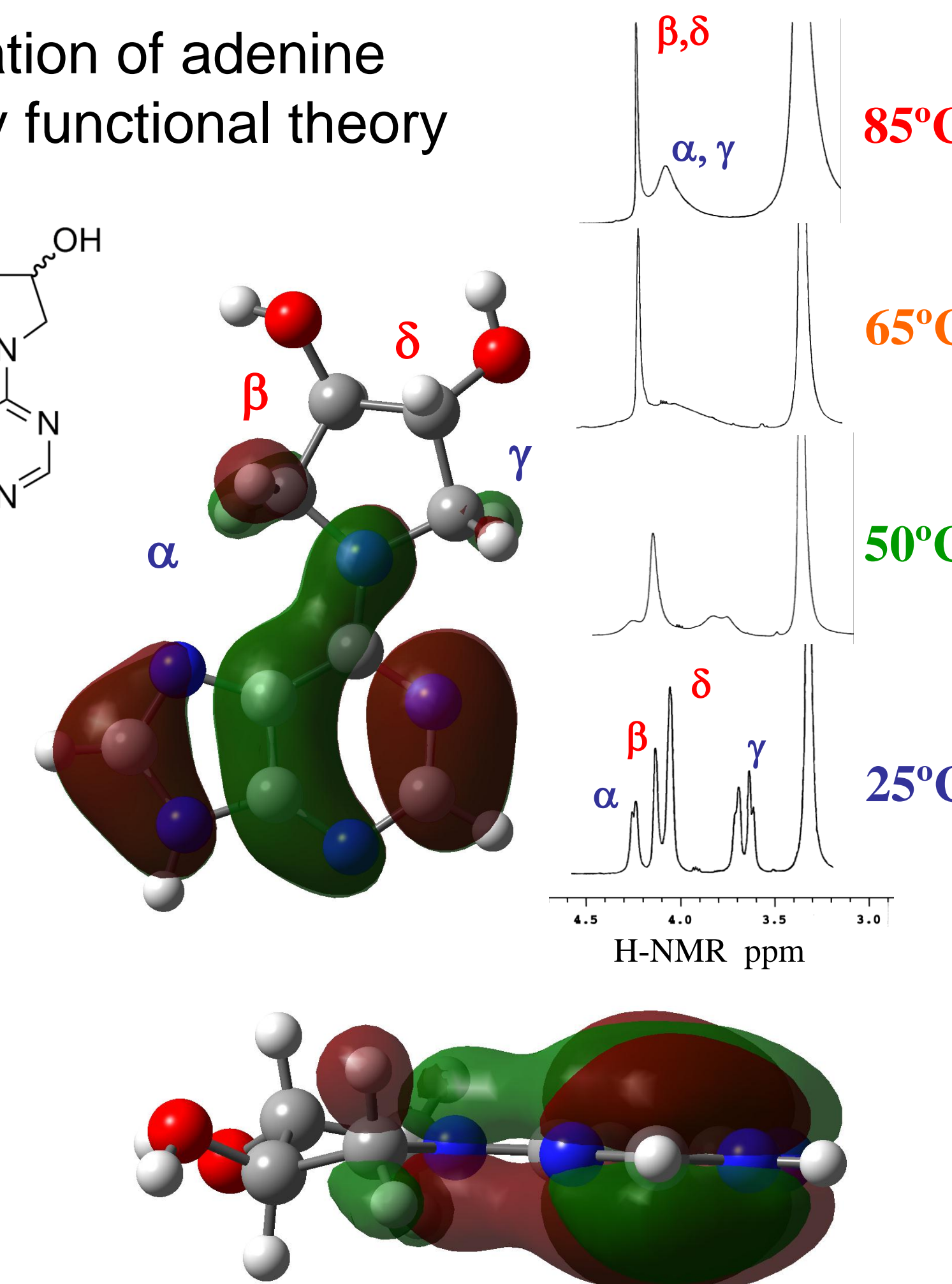
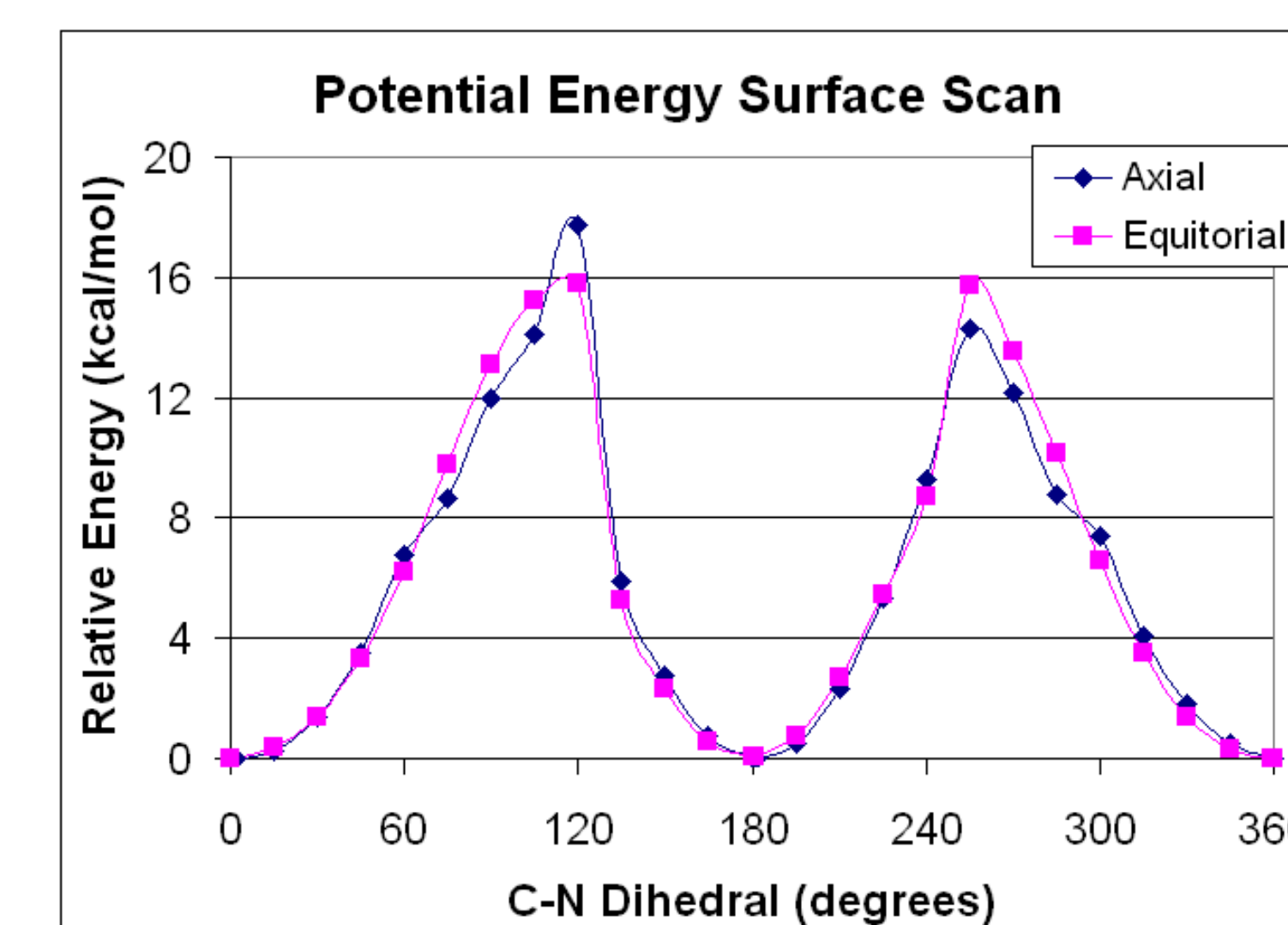
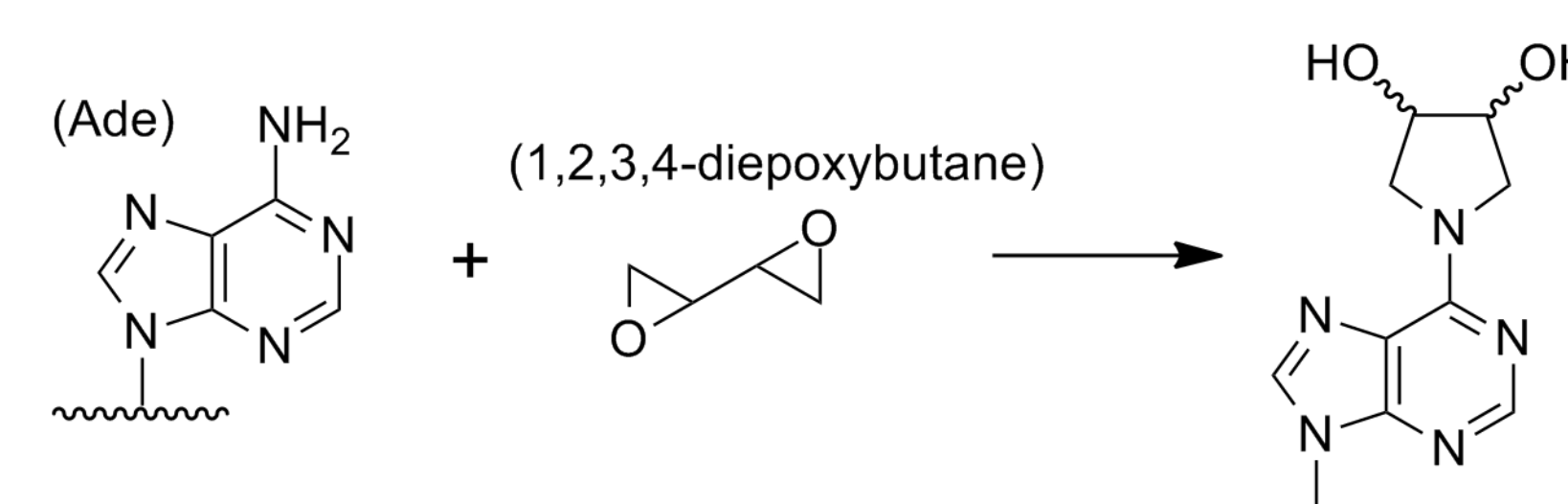
1. Substitution (X) donates or withdraws electron density
2. Cytosine oxygen becomes more or less nucleophilic
3. Cytosine oxygen influences guanine amine through the hydrogen bond



Structural Determination of Exocyclic Deoxyadenosine Lesions by Industrial Carcinogen

Uthpala Seneviratne, Sergey Antsyovich, Melissa Goggin, Danae Quirk Dorr, Rebecca Guza, Adam Moser, Carrie Thompson, Darrin M. York and Natalia Tretyakova. Chem. Res. Toxicol., 23(1), 118-133 (2010)

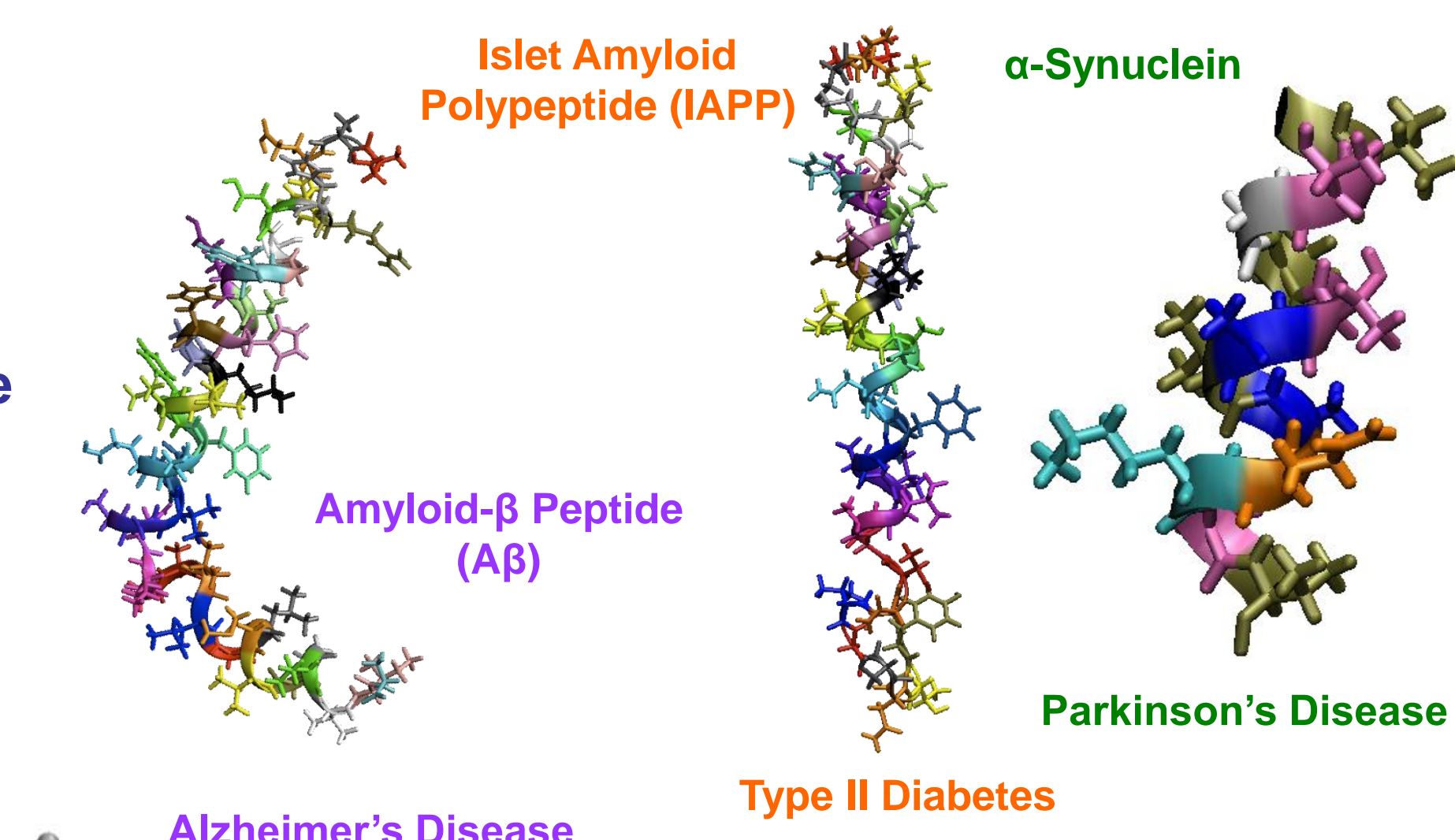
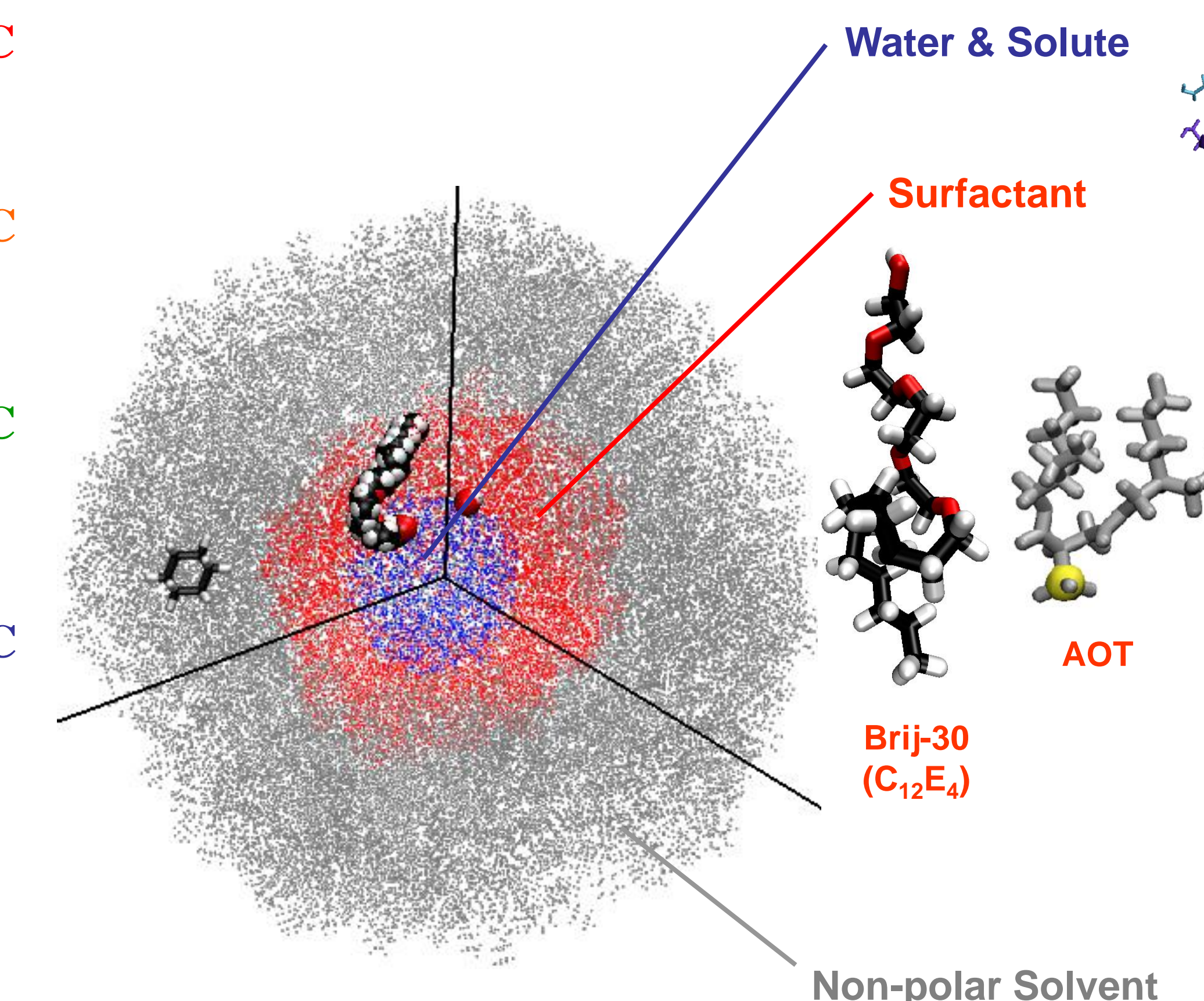
Elucidation of NMR determination of adenine carcinogen lesions using density functional theory



Molecular Dynamic of Amyloidogenic Peptides in Reverse Micelles

Anna Victoria Martinez, Adam Moser, Lani Rush, Dr. John Straub. In Progress

Investigating the role of crowding and dehydration on amyloidogenic proteins aggregation using reverse micelles



Next Projects!!

Amyloidogenic Proteins in Nonionic Reverse Micelles, Synthetic Foldymers, RNA enzymes & Synthetic Catalysts, Departmental collaborations!

Funding and Support

University of Minnesota, NIH, Minnesota Supercomputing Institute, Boston University SCV, Teragrid, DoE