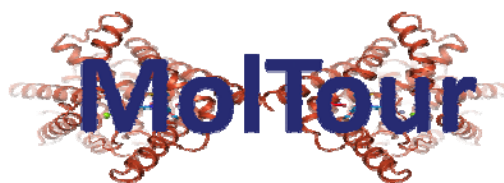




Improving spatial reasoning with virtual reality



Ton Blaazer

AIMMS workshop

Active learning

Amsterdam, May 2, 2019

Improving spatial reasoning

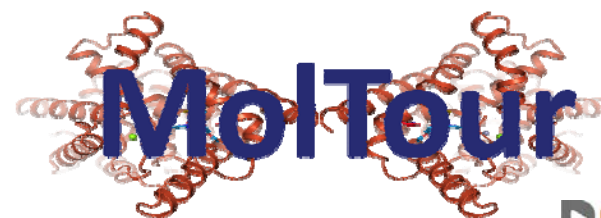
"Live in Life Sciences: een didactiek voor 3D redeneren met een virtual reality tool in het beta- en life science onderwijs"

- Comenius Senior Fellow-beurs

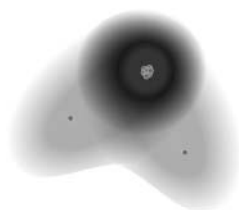
Jacqueline van Muijlwijk (S&F, AIMMS, iH2LS)

Hanna Westbroek (Learn!Academy)

Ton Blaazer (iH2LS, MolTour)

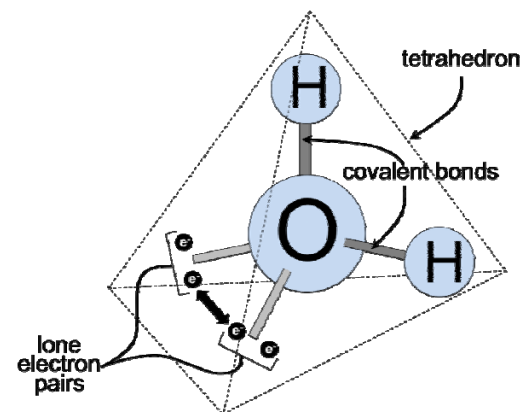


macroscale



sub-microscale

chemistry



H₂O

representation



Improving spatial reasoning

- 3D reasoning
 - An essential competency
 - Chemical misconceptions

“Why some students don’t learn chemistry: Chemical misconceptions” by Mary B. Nakhleh^[1]

“Many students at all levels struggle to learn chemistry, but are often unsuccessful. [...] many *students are not constructing appropriate understandings of fundamental chemical concepts* from the very beginning of their studies. Therefore, **they cannot fully understand the more advanced concepts that build upon the fundamentals.**”



Improving spatial reasoning

- 3D reasoning
 - An essential competency
 - Chemical misconceptions

“Why some students don’t learn chemistry: Chemical misconceptions” by Mary B. Nakhleh^[1]

University students:

“They found that students were generally **quite successful** in naming the parts of an atom or a nucleus. However, the *students were much less successful when they attempted to describe the interactions of these particles*. The students tended to invoke a simplistic Bohr model of the atom in their explanations.”



Improving spatial reasoning

- 3D reasoning
 - An essential competency
 - Chemical misconceptions

“What Makes a Great Medicinal Chemist? A Personal Perspective” by Mark A. Murcko^[1]

Discipline-specific characteristics:

“They think in three dimensions. Of course they are quick to take advantage of protein structural information. But even when that is not available, notable drug discoverers are *constantly imagining what their molecules look like in 3D*, both in water and in lipid, outside of cells and inside, when bound to their receptors or free. Great medicinal chemists welcome any information that helps them *visualize their molecules and understand their conformational preferences.*”



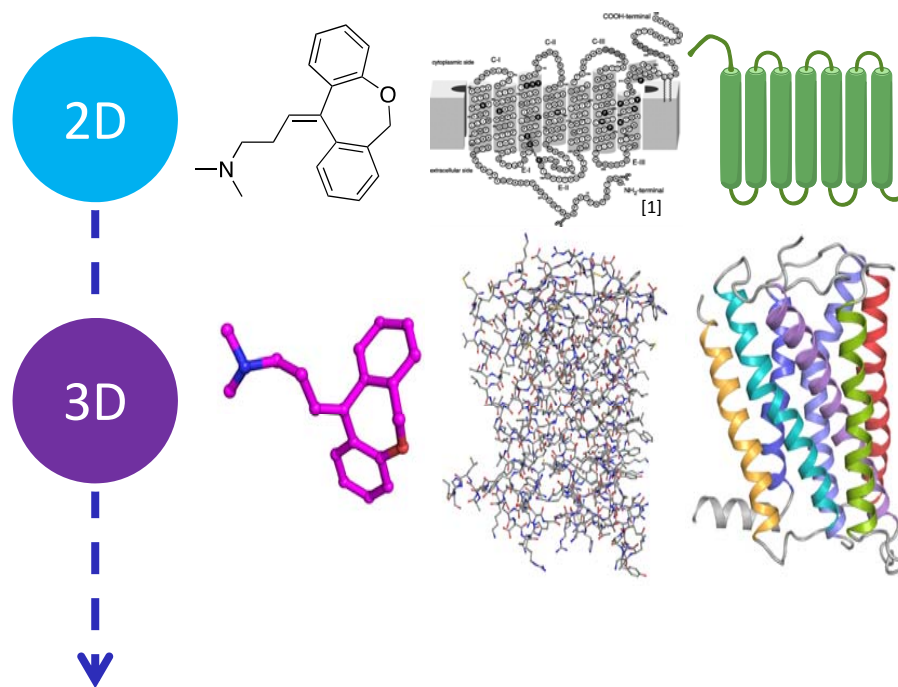
Improving spatial reasoning

- **3D reasoning**
 - **An essential competency**
 - Chemical misconceptions
 - **Future in research**
 - From industry to academia
 - From synthesis to biochemistry
- **Classroom-activating approach**
 - Tool development
 - Development of 3D/VR didactics





Classroom-activating approach

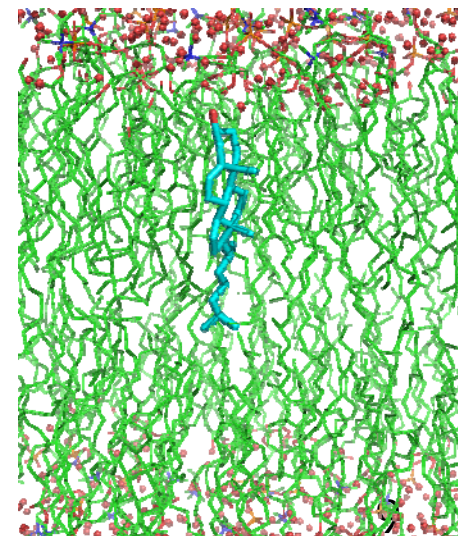
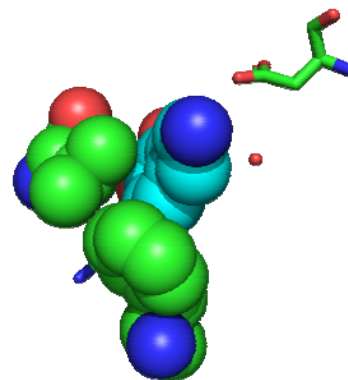
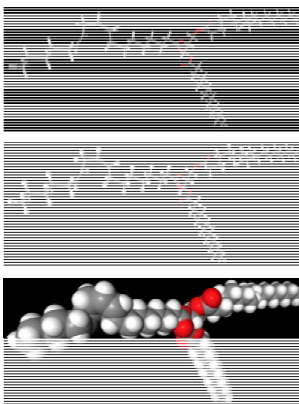
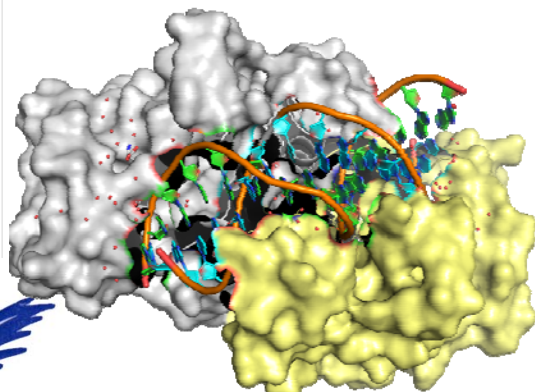
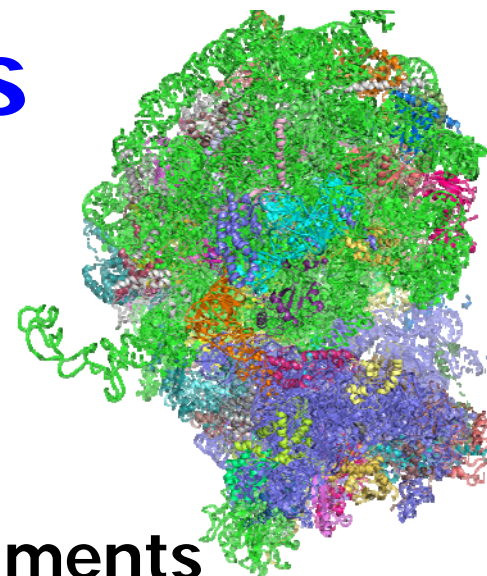


3D is already stimulating

The diagram illustrates the progression from 2D to 3D to VR in protein structure analysis. The 2D section includes a chemical structure of a ligand, a schematic of a protein membrane domain with labels (C-1, C-4, C-8, E-8, COOH-terminal, hydrophobic side, intracellular side, N-terminal), and a green helix bundle. The 3D section shows a pink ribbon structure, a blue wireframe model, and a multi-colored ribbon model. The VR section shows two views of a protein structure in a 3D environment.

Active sessions

- **Development of assignments**
 - Matching to Biochemistry course materials
 - Stryer's Biochemistry, Alberts MBC / ECB, etc.
- **Select 3D models and devise assignments**
 - Examples:
 - Organic chemistry: dopamine, isolated AAs, isolated phospholipid
 - DNA replisome: DNA helicase, RNA polymerase
 - Ribosome: human 80S ribosome
 - Transporters: dopamine transporter (DAT)
 - Membrane: computational model



The MolTour Experience

MolTour 3D demo (*laptop or phone*)

– <http://bit.ly/moltour-3d>

Model: DNA polymerase IV (*E. coli*)

Typical questions:

- Describe the different structural components visible in [View 1]
- Of the two DNA strands, which one is the template strand?
- What is the nucleobase that's being inserted?
- Locate the green spheres, what are they and describe their function.

MolTour VR demo (*phone*)

– <http://bit.ly/moltour-vr>

– Follow the instructions on your screen

– Place your phone into the Cardboard viewer

Model: Abl1 kinase with bosutinib

Typical questions:

- This compound has a direct hydrogen bond with the kinase. Locate it, and describe its features.
- A water molecule is trapped in a sub-pocket. Locate it, and describe its interactions.

MolTour 3D controls

	Touchpad	Mouse	Phone
Rotation	Click & drag	Left button & drag	Touch & move
Zoom	Scroll up/down	Scroll wheel	Two-finger zoom in/out
Translation	Ctrl + click & drag	Right button & drag	Two-finger drag

Link to the answers

<http://bit.ly/moltour-answers>

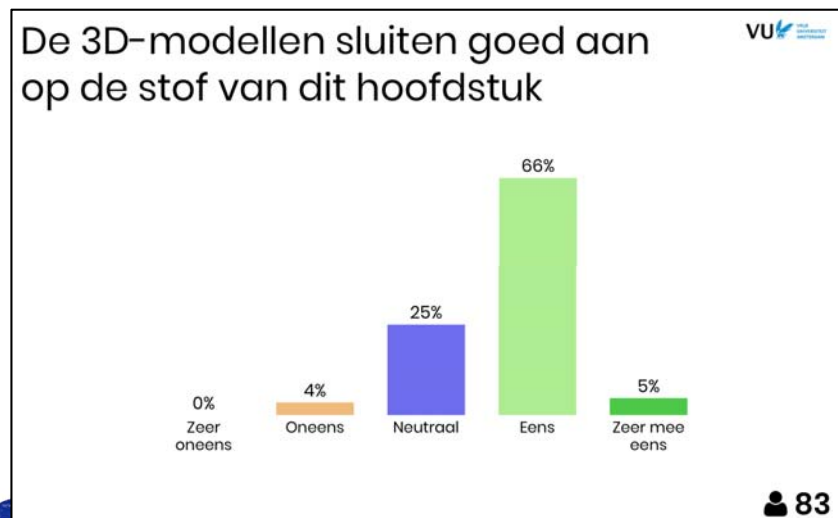
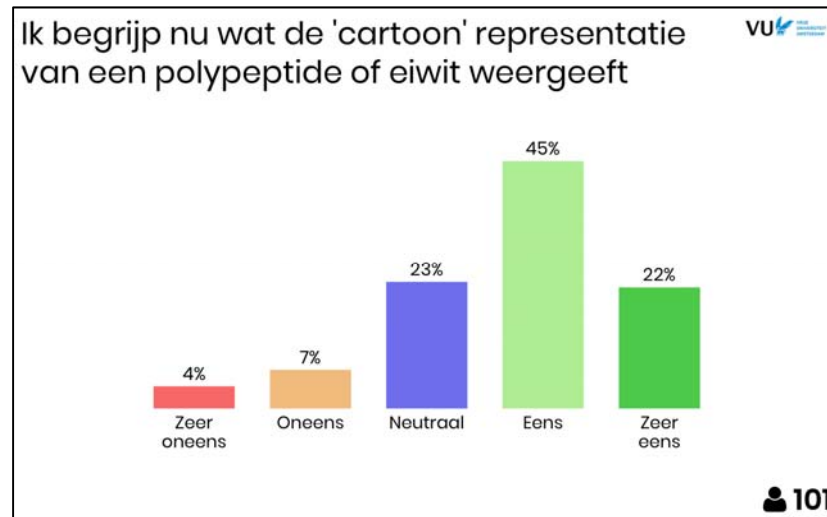
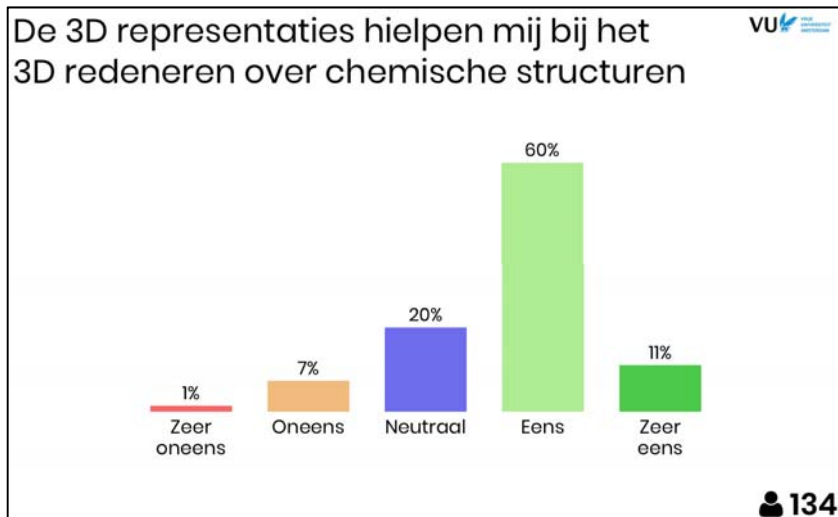
MolTour VR controls

	Cardboard
Rotation	Turn your head
Zoom in	Tap once (tap again to stop)
Zoom out	Tap twice (tap again to stop)
Menu	Tap and hold (look at option)

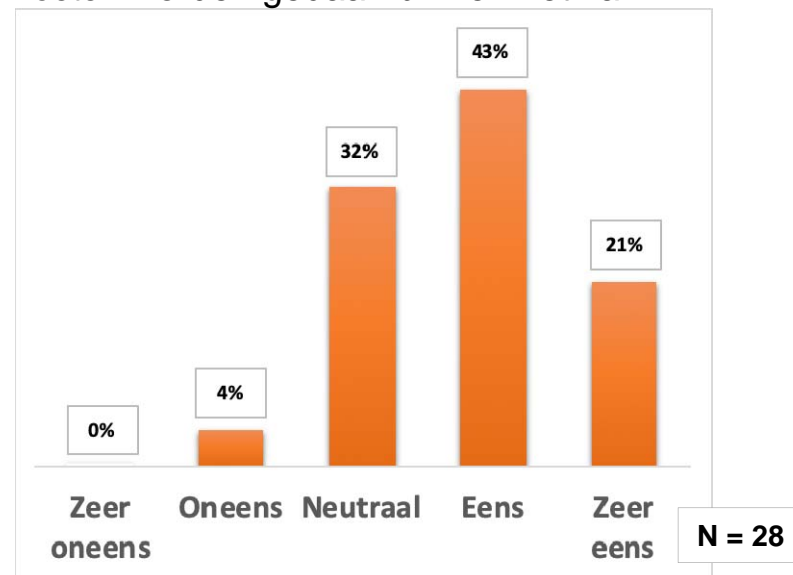
Use this link in case VR fails:

<http://bit.ly/moltour-ab>

Impact & reception



De 3D opdrachten zouden volgend jaar weer moeten worden gedaan binnen het vak



Looking back & forward

- Development of 3D/VR heuristics

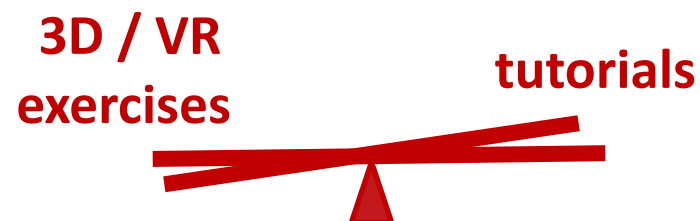
- New 3D model-based questions
- Integration with conventional lectures

- Tool development

- Separate 3D and VR viewers
- Teacher-control of sessions

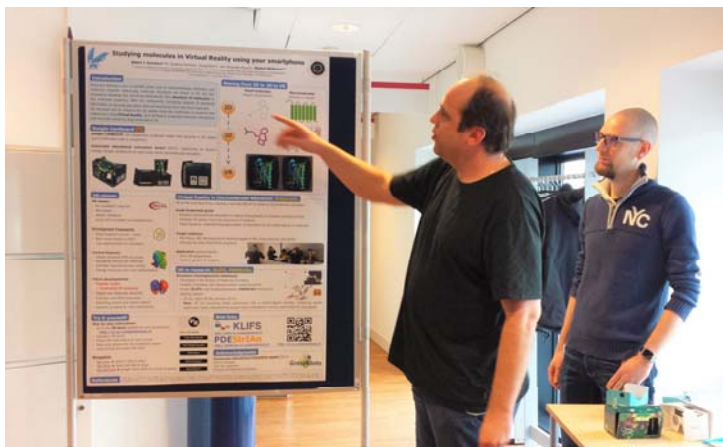
- Other courses?

- Organic chemistry
- Biomedical sciences





Acknowledgements



Concept & early development

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Matthias Debernardini

Daniel Yu

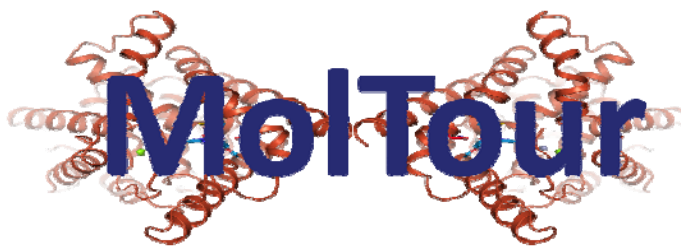
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Marco Siderius

Chris Vos

Stefan Dekker

Anneke Vuuregge

& assistants

iH2LS colleagues



Want to start using MolTour?

Contact us to discuss the possibilities

- **Jacqueline van Muijlwijk-Koezen**

- @: j.e.van.muijlwijk-koezen@vu.nl

- **Ton Blaazer**

- @: a.r.blaazer@vu.nl

