

Zoe Cournia wins inaugural PRACE Ada Lovelace Award for HPC

In 2016, computational chemist **Zoe Cournia** was awarded the first ever PRACE Ada Lovelace Award for HPC for her work in computer-aided drug design. She talks about her work and how she believes more needs to be done to bridge the gap between researchers and the general public.

In May 2016, Dr Zoe Cournia — a computational chemist at the Biomedical Research Foundation, Academy of Athens (BRFAA) — was presented with the inaugural PRACE Ada Lovelace Award for HPC. The award — named after the British mathematician widely thought to have written the first algorithm for a machine — was created to recognise women who have made outstanding contributions to the field of high performance computing in Europe.

Dr Cournia's work involves using simulations to investigate how mutations in proteins can lead to cancer. Using data acquired from these simulations allows researchers to investigate potential mechanisms by which small molecules can bind to mutated proteins and inactivate them. "We look at small cavities on proteins where small molecules can potentially bind," explains Cournia. "We then design candidate drugs specifically for those cavities, which are then tested in the lab by our collaborators.

We have come up with a number of drug candidates, which have so far been shown to be effective in biological assays and mouse models."

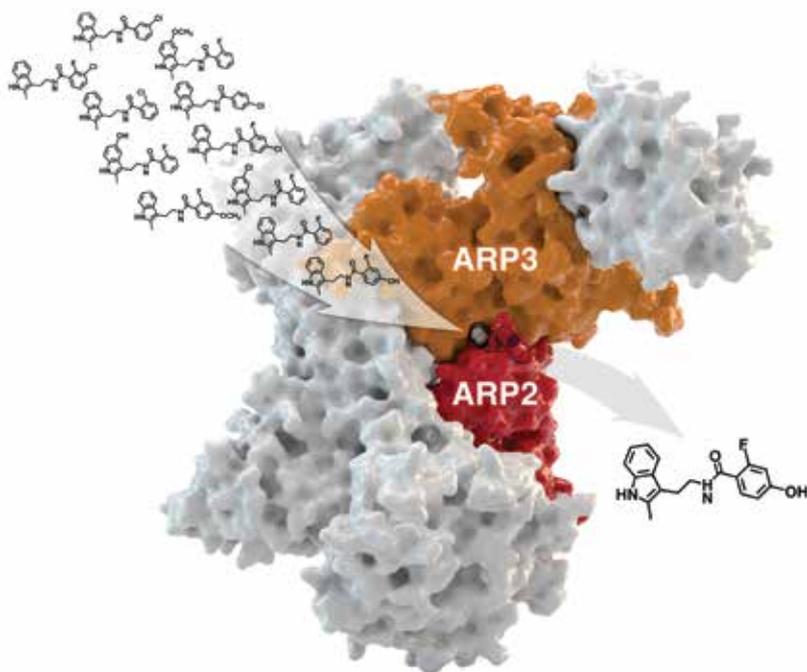


Figure 1: Demonstration of small molecules - candidate drugs binding to a protein implicated in cancer. A simulation approach is employed with which candidate drugs are optimised and the best is selected for experiments.

REF: Structural characterization and computer-aided optimization of a small-molecule inhibitor of the Arp2/3 complex, a key regulator of the actin cytoskeleton. Baggett AW*, Cournia Z*, Han MS, Patargias G, Glass AC, Liu SY, Nolen BJ. *ChemMedChem*. 2012, 7(7):1286-94.

"I believe that our work is a good example of how computers help develop products that have the potential to save millions of lives worldwide. I am honoured to receive this prestigious award and hope that this serves as inspiration to other female researchers in the field."

Cournia and her team are now advancing their projects, and are looking to move their research beyond the state-of-the-art. This will be achieved by mapping the entire landscape of motion of a mutant protein, simulating a system of 400 000 atoms. "We also want to try and recreate the proteins in virtual reality for educational purposes," says Cournia. "This will be useful in helping us to grasp the movement of proteins and how drugs interact with them, and we also hope that students in schools can try it out to see for themselves what we are doing. Hopefully this might push some of them on to following a career in science!"

News of Cournia's success has been well received in her home country, Greece, and she has subsequently been the subject of numerous articles and interviews. Her success has been featured on national TV (NET, STAR channel, SKAI, Alpha), Lifo, politicsonline.gr and news247.gr, and she believes that this kind of publicity is much needed by the HPC community. "The award has helped to increase the visibility of HPC to the public and helped them realise how important a role it plays in our everyday lives," she says. "Every product we use, from cell phones to cars to aeroplanes to clothes, at some point goes through a stage of testing which uses HPC."

Popular promotion of science is sometimes to the public is sometimes successful; television programmes on astronomy and the natural world are some of the most popular in existence. However, there still remains a huge disconnect between the research community and the general public. "Many people think that research is impossible to understand," says Cournia. "That is why it's important to set an example showing that research and science are not difficult and are accessible to everyone. Awards like this help to demonstrate this, and

I hope that I can be a role model to young people, showing them that they can make a difference by improving people's quality of life through a career in science."

"I also want the public to see that taxes invested in research do not go to waste!" she continues. "I think the perception is often that this money goes into esoteric research which does not really benefit society, but the reality is that it often feeds into products which people use every day and even help to save lives."

A recent survey in the UK revealed how one third of teenage girls do not think they are clever enough to consider science-based careers. Women remain underrepresented in the STEM fields, which was one of the main reasons behind the launch of PRACE's Ada Lovelace Award for HPC. "It's certainly a good idea to have female role models in this field," says Cournia. "I think perceptions are starting to change now, and setting good examples can convince women and girls that it's not a matter of gender, but a matter of preference of what you want to do in life."



Zoe Cournia

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Cournia is now working on a Horizon 2020 project called VI-SEEM that is aiming to encourage scientists in life sciences to get involved with their local e-infrastructures. "When I first arrived back from studying in the US to start my lab, I had no computational resources at all," says Cournia. "I applied for a few PRACE projects, but was unsuccessful at the time. Although eventually I was successful, in the meantime I applied for access to an eastern Mediterranean e-infrastructure (LinkSCEEM), where I was able to produce preliminary results for my work that helped show PRACE that my project was worth investing in. This was hugely important for me and I now want to help encourage more scientists to use local HPC resources."

VI-SEEM is aiming to facilitate interdisciplinary collaboration in the life sciences, digital cultural heritage, and climate research by spreading the word about e-infrastructures in southeast Europe and the eastern Mediterranean. "Apart from providing the



Zoe Cournia presented with the PRACE Ada Lovelace Award

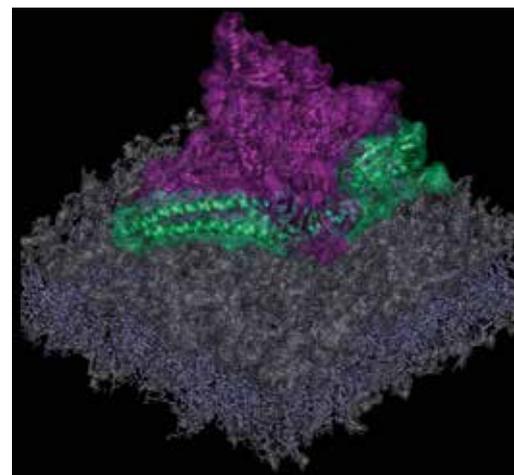


Figure 2: A simulation model of the mutant $PI3K\alpha$ protein binding to a model cell membrane.

REF: Exploring a non-ATP pocket for potential allosteric modulation of $PI3K\alpha$.

Gkeka P, Papafotika A, Christoforidis S, Cournia Z. *J Phys Chem B*. 2015 Jan 22;119(3):1002-16. doi: 10.1021/jp506423e.

REF: Investigating the structure and dynamics of the $PIK3CA$ wild-type and H1047R oncogenic mutant. Gkeka P, Evangelidis T, Pavlaki M, Lazani V, Christoforidis S, Agianian B, Cournia Z.

PLoS Comput Biol. 2014 Oct 23;10(10):e1003895. doi: 10.1371/journal.pcbi.1003895.

e-infrastructure services and facilities, we are also coordinating workshops on performing HPC calculations, carrying out training sessions and workshops, and generally encouraging scientists in local communities to get involved with the regional and local e-infrastructures to advance their own projects", says Cournia. "Hopefully our activities can help introduce them to the benefits of working with computer resources and lead them on to even greater scientific discoveries in the future."

For more information

VI SEEM Project

<https://vi-seem.eu>

LinkSCEEM Project

<http://linksceem.cyi.ac.cy/ls2/index.php>

Women in HPC (WHPC)

www.womeninhpc.org

PRACEdays conference series

www.prace-ri.eu/pracedays

Resources awarded by PRACE

Cournia was awarded 5 247 000 core hours under the 6th PRACE Call for Proposals for Project Access, and 11 200 000 core hours under the 9th Call, both on Curie hosted by GENCI at CEA, France.