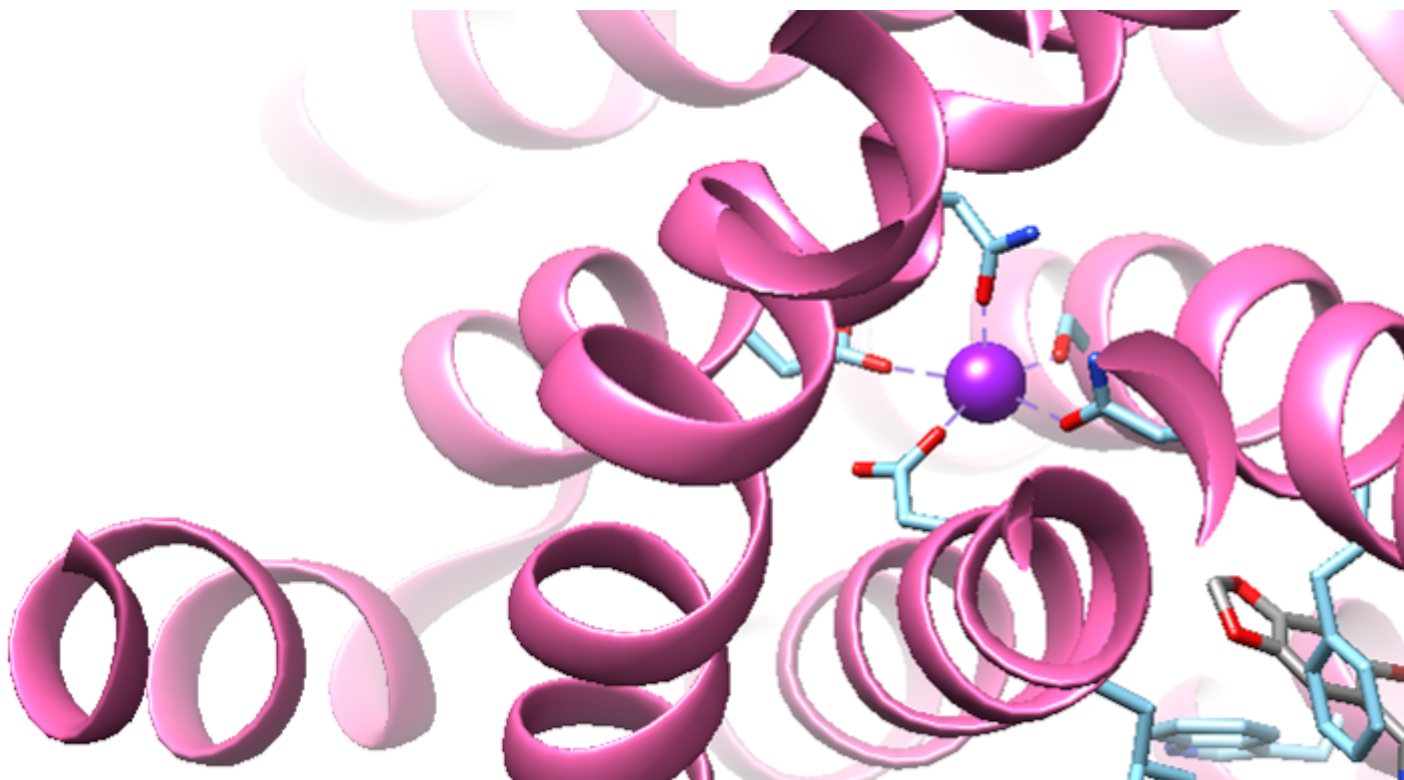


[AstraZeneca accelerates drug discovery thanks to PELE technology](#)

bsc



[AstraZeneca](#) in collaboration with [Heptares Therapeutic](#), has made significant progress with the new target called PAR2, using the [PELE](#) simulation software, as reported in [Nature](#). PAR2 has applications for the generation of new drugs in the inflammatory pain field.

Specifically, this target is considered a highly promising drug target for the treatment of osteoarthritic pain. Until now, the discovery of small molecule antagonists to PAR2 has proven very challenging. Locating multiple allosteric sites within PAR2 offers alternative approaches for structure based drug design. This discovery has a direct impact on the generation of novel and promising new chemical lead series.

PELE is a technology developed at the Barcelona Supercomputing Center (BSC). [Nostrum Biodiscovery \(NBD\)](#) owns exclusive rights for the exploitation of this platform. Due to its latest upgrades and its multiple industrial validations, [PELE](#) is becoming one of the strongest technologies to consolidate relevant predictions in drug discovery.

[English Press Release](#) [Nota de prensa en castellano \(pdf\)](#)

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

Source URL (retrieved on 18 Mar 2025 - 14:37): <https://www.bsc.es/es/astrazeneca-accelerates-drug-discovery-thanks-pele-technology>