Allostery in Drug Discovery

"Allostery is the second secret of life" Jacques Monod (1960)

ALLODD Overview

ALLODD

The ALLODD project is a collaboration between 24 academic and industrial organizations for training 14 Early Stage Researchers.

ALLODD Governing Bodies



Scientist-in-Charge Dr. Zoe Cournia

Why allostery in drug discovery? Most current drugs are designed to bind directly to the primary active sites of their biological targets. Allosteric modulators offer a powerful yet underexploited therapeutic approach. They can elicit a richer variety of biological responses and, since they target less conserved binding sites, higher selectivity and less adverse effects may be obtained (Changeux, Drug Disc Today 2013).



Project Coordinator

ESR1 Supervisor Francho Nerín Fonz



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ALLODD Goals

The ALLODD project aims to train a new generation of scientists in exploiting the concept of allostery in drug design, putting together a whole array of technologies to identify and characterize allosteric modulators of protein function that will be applied to therapeutically relevant systems.

Eyes on the Future

Allosteric targeting need not be achieved solely through the design of synthetic small molecules, but also can also be reached via conformationally specific allosteric antibodies, which represents an important field of future research. There are already clear examples of monoclonal antibodies that allosterically target ion channels (Lee et al., 2014b), GPCRs (Mukund et al., 2013), and RTKs (De Smet et al., 2014), as well as cytokine and integrin receptors (Rizk et al., 2015; Schwarz et al.,





ALLODD Beneficiaries & Partner Organizations

2006).

Events



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D., Kagelmacher, M., Kurzbach, D., Nazaré, M., Rademacher, C., 2022. Identification of the Allosteric Binding Site for Thiazolopyrimidine on the C-Type Lectin Langerin. ACS Chem. Biol.



https://doi.org/10.1021/acschembio.2c00626

Barreto Gomes, D.E., Galentino, K., Sisquellas, M., Monari, L., Bouysset, C., Cecchini, M., 2023. ChemFlow–From 2D Chemical Libraries to Protein–Ligand Binding Free Energies. J. Chem. Inf. Model. https://doi.org/10.1021/acs.jcim.2c00919

Leusmann, S., Ménová, P., Shanin, E., Titz, A., Rademacher, C., 2023. Glycomimetics for the inhibition and modulation of lectins. Chem. Soc. Rev. https://doi.org/10.1039/d2cs00954d



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