


Program – Day 1

“Allosteric Drug Design: where Academia meets Pharma”

Day 1  22.05.2023	14:00 – 14:15	Welcome
	14:15 – 15:00	Towards a new allosteric pharmacology of receptors: Historical development of a concept Jean-Pierre CHANGEUX, Institut Pasteur
	15:00 – 15:30	LMW inhibitors of IL-1b, from a fragment hit to cellular PoC Anna VULPETTI, Novartis
	15:30 – 16:00	Coffee Break
	16:00 – 16:30	Binding of drugs and neurotransmitters to the transmembrane part of cell membrane receptors. Targeting GPCR and RTK receptors with biomolecular simulations Ilpo VATTULAINEN, University of Helsinki
	16:30 – 17:00	Detection of β2 adrenergic receptor agonists using single-ligand dynamic interaction data Esther KELLENBERGER, University of Strasbourg
	17:00 – 17:30	Structure-based design of orthosteric and allosteric GPCR ligands Jens Gustaf CARLSSON, Uppsala University
	17:30 – 17:45	Coffee Break
	17:45 – 18:15	Chemical Cartography and the uncharted land of allosteric modulators Dragos HORVATH, University of Strasbourg
	18:15 – 18:45	Allostery in nuclear receptor proteins Roland STOTE, University of Strasbourg
	18:45 –	Wine & bretzels

 **Salle des Conférences, Institut de Science et d'Ingénierie Supramoléculaires - ISIS**



This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 956314.

Program – Day 2

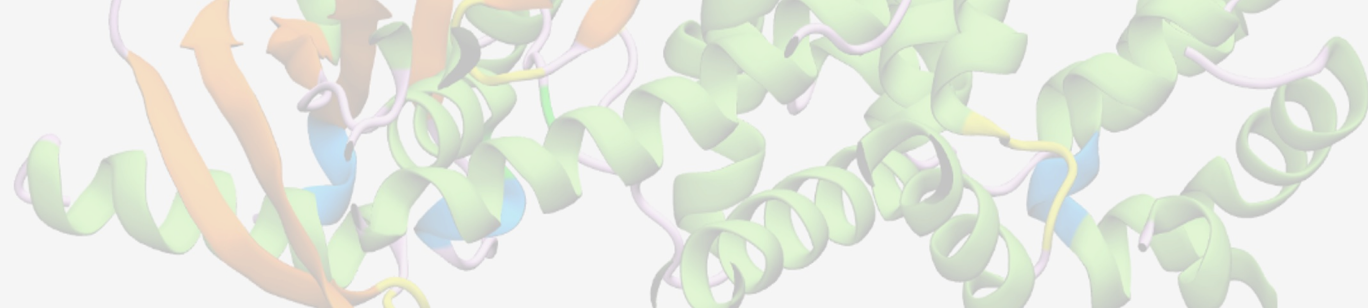
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Day 2 23.05.2023	09:00 – 09:45	Molecular mechanisms of allosteric modulation & agonist selectivity in ligand-gated ion channels through integrative structural biology Erik LINDAHL, Stockholm University
	09:45 – 10:15	Discovery of novel allosteric EGFR L858R inhibitors for the treatment of non-small-cell lung cancer Antonio RICCI, Hoffmann-La Roche
	10:15 – 10:45	NMDA receptors: allosteric machines in neurotransmission Pierre PAOLETTI, ENS PSL
	10:45 – 11:00	Coffee Break
	11:00 – 11:30	Generation and mechanistic study of nanobodies positively modulating the brain alpha7 nicotinic receptor Pierre-Jean CORRINGER, Institut Pasteur
	11:30 – 12:00	Small molecules modulating force production: A new perspective against myosin-associated diseases Anne HOUDUSSE, Institut Curie
	12:00 – 12:30	Molecular design against modeled conformational ensembles Huafeng XU, Atommap
	12:30 – 14:00	Lunch
	14:00 – 14:30	The organization of pharmaceutical discovery research: from highly integrated to highly coordinated Stephan JENN, Novalix
	14:30 – 15:00	FLT3 negative allosteric modulators: From screening hits to a clinical candidate for the treatment of neuropathic pain Didier ROGNAN, University of Strasbourg
	15:00 – 15:30	Mapping and sculpting the allosteric GPCRome for SBDD - From binding site druggability to medicinal chemistry tractability Ijen CHEN, Sosei Heptares
	15:30 – 15:45	Coffee Break
	15:45 – 16:15	Function and inhibition of cation-coupled chloride cotransporters Marco DE VIVO, IIT
	16:15 – 16:45	Conformation locking for drug discovery: From muteins to antibodies as allosteric modulators Harald KOLMAR, TU Darmstadt
	16:45 – 17:00	Concluding Remarks


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Allostery in Drug Discovery



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Getting to Strasbourg



Arriving by airplane



Daily domestic and international flights to Strasbourg airport [allow connections](#) to major cities in Europe. A shuttle connects Strasbourg airport and Strasbourg central train station (9 minute ride, 4 times per hour). Noteworthy, [a special fare](#) includes the shuttle and the tram/bus tickets.



There are many alternative travel options: you may take plane to Paris, Stuttgart, Base, Frankfurt airports, and then take a train to Strasbourg – it may be more convenient in some cases, considering that Strasbourg Airport is a relatively small one.



From the Strasbourg Airport entrance you can also take a **taxi**, which should not cost more than 30 euros to the centre of Strasbourg or your place of accomodation, depending on the traffic.

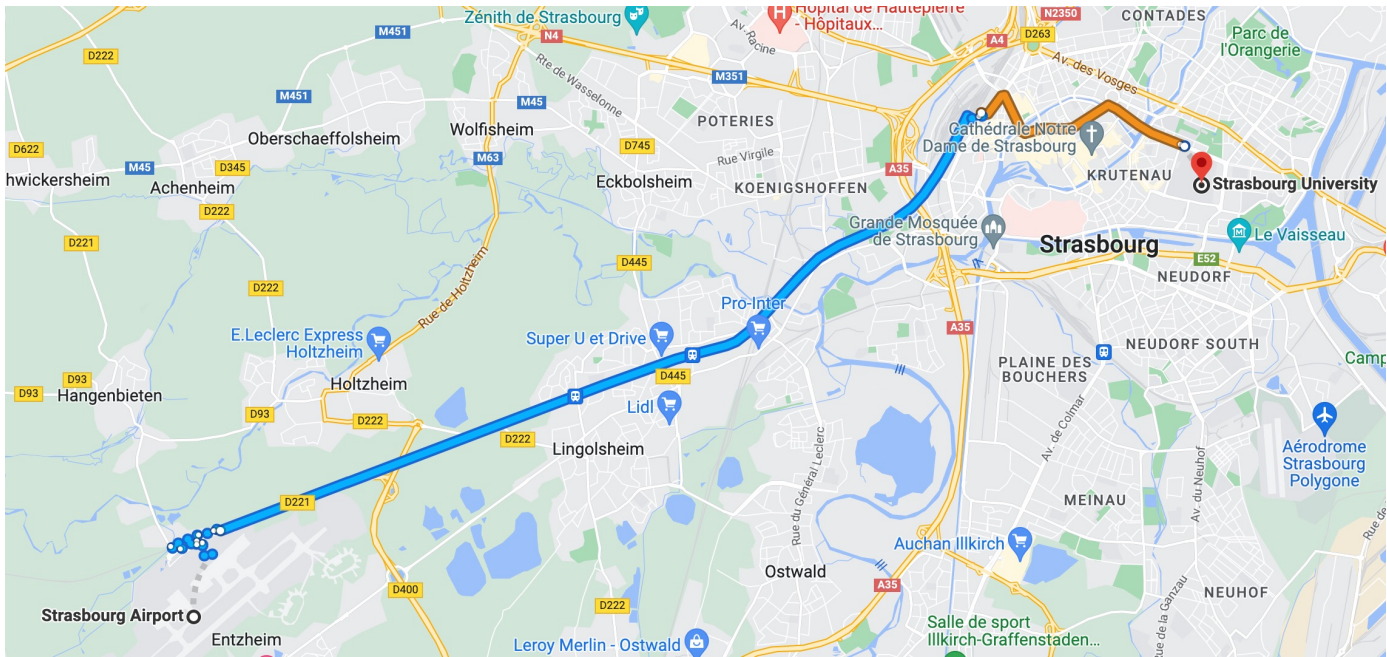
Strasbourg has an extended public transportation system (tram, bus). Maps, timetables, and fares are available on the following website: <https://www.cts-strasbourg.eu/en/>



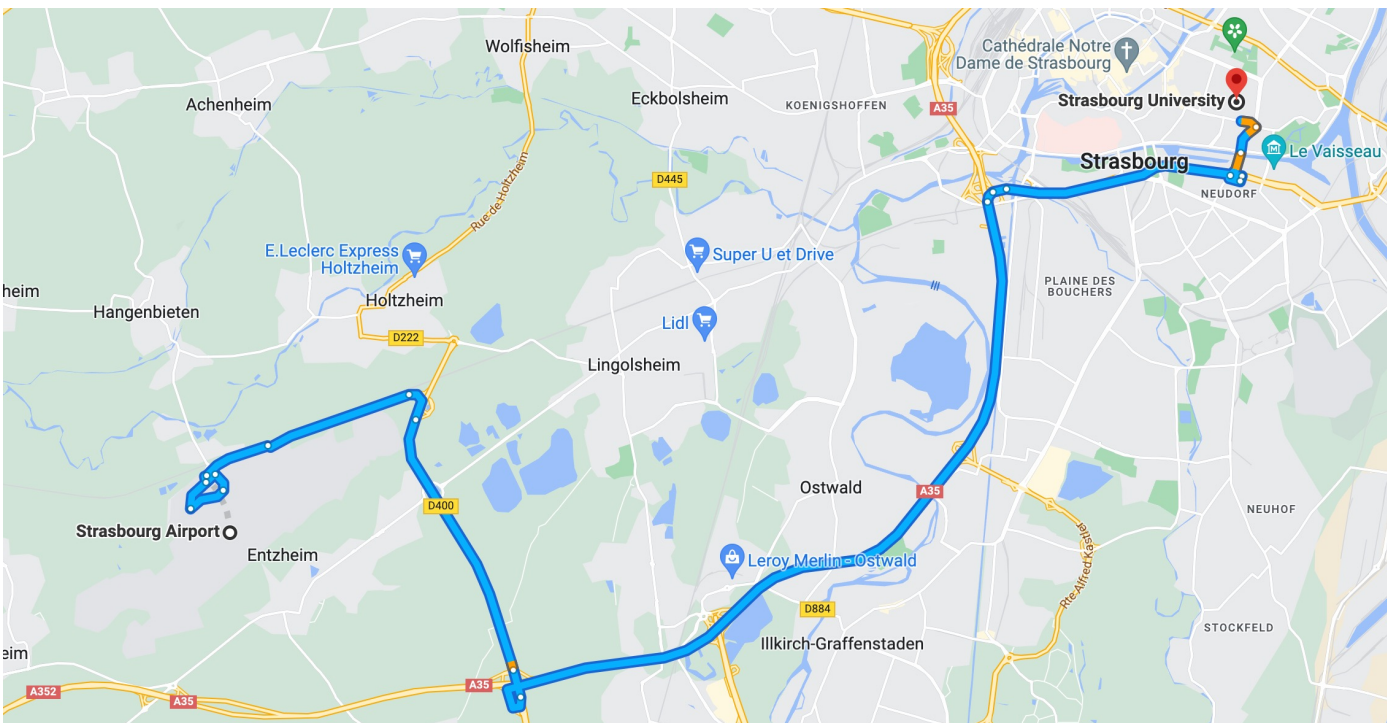
Getting to the University

Possible routes from the Strasbourg Airport:

- by train + tram:



- by car:



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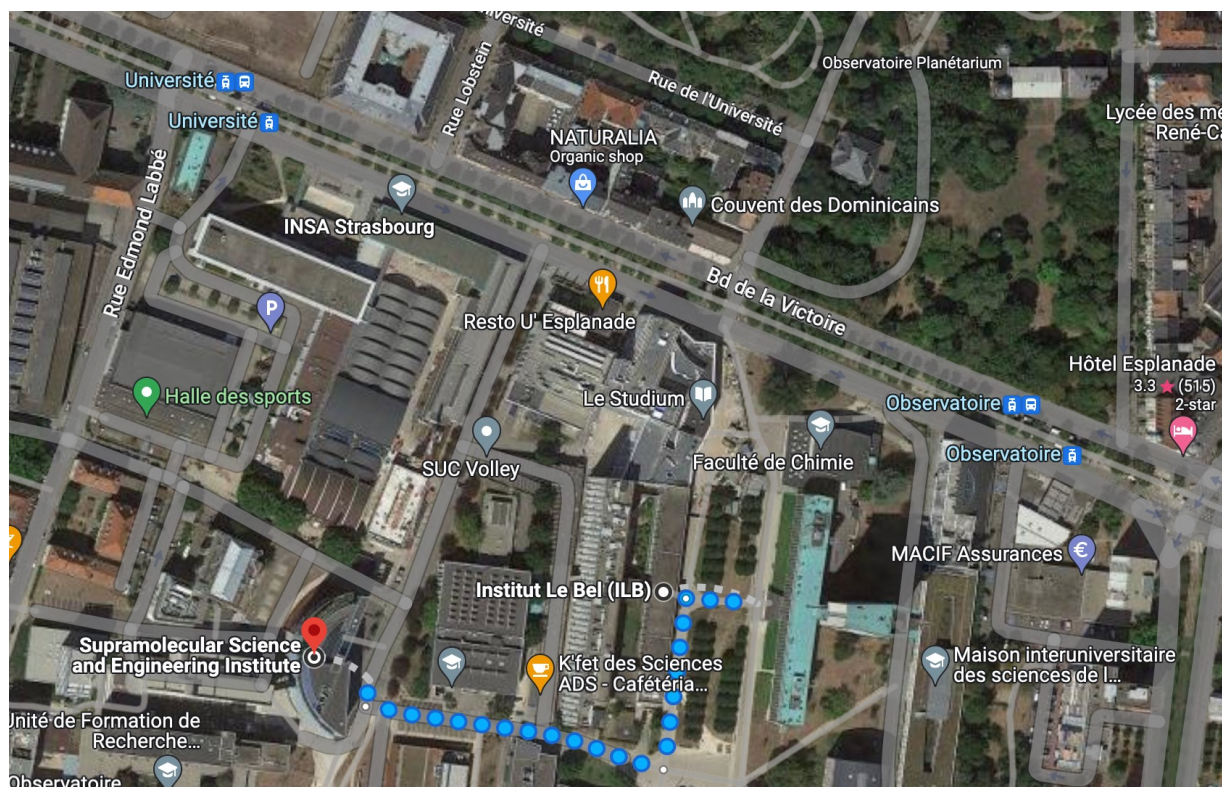
Getting to the University & Symposium

Possible route from the Strasbourg Central Train Station:

- by tram:



Route from the Institut le Bel to ISIS (Institut de Science et d'Ingénierie Supramoléculaires):



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