

Poštovane/i,

Pozivamo Vas na predavanje pod nazivom **From Algorithm to Drug: How Artificial Intelligence is Transforming Oncology** koje će, u ponedjeljak, 5. svibnja u A116 sa početkom u 13h, održati prof. Igor Štagljar (University of Toronto; [Department of Biochemistry](#), [Department of Molecular Genetics](#) and [The Stagljar Lab](#)).

### Abstract:

Discovering new cancer therapies is like finding a needle in a haystack—but with artificial intelligence, we're now using a magnet instead of our hands, making the search smarter, faster, and far more effective. In this talk, I will share how our lab integrates AI with advanced technologies we've developed—such as MaMTH and SIMPL—to accelerate the discovery of drugs targeting some of the most challenging proteins in cancer biology.

Our recent study, published in *Nature Biotechnology* (Ghazi Vakili et al., 2025), demonstrates a machine learning-guided platform that enabled us to identify potent small molecule inhibitors targeting KRAS G12V—an oncogenic mutation long considered “undruggable.” These findings represent a significant breakthrough in using AI to uncover new therapeutic options for lung, colon, and pancreatic cancers.

I will highlight how this integrated approach—from predictive modelling to experimental validation—is reshaping early-stage drug discovery, helping us develop smarter, more precise, and more personalized cancer treatments.

### Key References:

1. Saraon, P., Snider, J., Kalaizidis, Y., Wybenga-Groot, L.E., Weiss, K., Rai, A., Radulovich, N., Drecun, L., Vučković, N., Vučetić, A., Wong, V., Thériault, B., Pham, N.A., Park, J.H., Datti, A., Wang, J., Pathmanathan, S., Aboualizadeh, F., Lyakisheva, A., Yao, Z., Wang, Y., Joseph, B., Aman, A., Moran, M.F., Prakesch, M., Poda, G., Marcellus, R., Uehling, D., Samaržija, M., Jakopović, M., Tsao, M.S., Shepherd, F.A., Sacher, A., Leighl, N., Akhmanova, A., Al-Awar, R., Zerial, M., & Stagljar, I. (2020). A drug discovery platform to identify compounds that inhibit EGFR triple mutants. *Nature Chemical Biology*, 16(5), 577–586. doi:10.1038/s41589-020-0484-2.
2. Yao, Z., Aboualizadeh, F., Kroll, J., Akula, I., Snider, J., Lyakisheva, A., Tang, P., Kotlyar, M., Jurisica, I., Boxem, M., & Stagljar, I. (2020). Split Intein Mediated Protein Ligation (SIMPL), a method for detecting protein-protein interactions and their inhibition. *Nature Communications*, 11(1), 2440. doi:10.1038/s41467-020-16299-1.
3. Saraon, P., Snider, J., Schormann, W., Rai, A., Radulovich, N., Sánchez-Osuna, M., Coulombe-Huntington, J., Huard, C., Mohammed, M., Lima-Fernandes, E., Thériault, B., Halabelian, L., Chan, M., Joshi, D., Drecun, L., Yao, Z., Pathmanathan, S., Wong, V., Lyakisheva, A., Aboualizadeh, F., Niu, L., Li, F., Kiyota, T., Subramanian, R., Joseph, B., Aman, A., Prakesch, M., Isaac, M., Mamai, A., Poda, G., Vedadi, M., Marcellus, R., Uehling, D., Leighl, N., Sacher, A., Samaržija, M., Jakopović, M., Arrowsmith, C., Tyers, M., Tsao, M.S., Andrews, D., Al-Awar, R., & Stagljar, I. (2021). Chemical genetics screen identifies COPB2 tool compounds that alter ER stress response and induce RTK dysregulation in lung cancer cells. *Journal of Molecular Biology*, 433(23), 167294. doi:10.1016/j.jmb.2021.167294.
4. Grozavu, I., Stuart, S., Lyakisheva, A., Yao, Z., Pathmanathan, S., Ohh, M., & Stagljar, I. (2022). D154Q mutation does not alter KRAS dimerization. *Journal of Molecular Biology*, 434(2), 167392. doi:10.1016/j.jmb.2021.167392.
5. Lim, S.H., Snider, J., Birimberg-Schwartz, L., Ip, W., Serralha, J.C., Botelho, H.M., Lopes-Pacheco, M., Pinto, M.C., Moutaoufik, M.T., Zilocchi, M., Laselva, O., Esmaeili, M., Kotlyar, M., Lyakisheva, A., Tang, P., López Vázquez, L., Akula, I., Aboualizadeh, F., Wong, V., Grozavu, I., Opacak-Bernardi, T., Yao, Z., Babu, M., Jurisica, I., Gonska, T., Bear, C.E., Amaral, M.D., & Stagljar, I. (2022). CFTR interactome mapping using the mammalian membrane two-hybrid high-throughput screening system. *Molecular Systems Biology*, 18(2), e10629. doi:10.1525/msb.202110629.
6. Yao, Z., Kim, J., Geng, B., Chen, J., Lyakisheva, A., Snider, J., Rudan Dimlic, M., Rain, S., & Stagljar, I. (2025). A split intein and split luciferase-coupled system for detecting protein-protein interactions. *Molecular Systems Biology*, 21(4), e11081. doi:10.1038/s44320-024-00081-2.
7. Ghazi Vakili, M., Snider, J., Lyakisheva, A., Yao, Z., Aboualizadeh, F., Pathmanathan, S., Grozavu, I., Wang, Y., Aman, A., Joseph, B., Prakesch, M., Poda, G., Marcellus, R., Uehling, D., Al-Awar, R., Tsao, M.S., Sacher, A., Leighl, N., Samaržija, M., Jakopović, M., Jurisica, I., & Stagljar, I. (2025). AI-guided discovery of KRAS G12V inhibitors using a hybrid experimental-computational pipeline. *Nature Biotechnology*, 42, 1234–1242. doi:10.1038/s41587-024-02526-3.

## **Prof. Igor Stagljar – Biography (Short Version)**

Prof. Igor Stagljar is a Croatian-Canadian molecular biologist and one of the global leaders in proteomics, chemical biology, and cancer research. He is a Professor at the University of Toronto's Donnelly Centre, with appointments in the Departments of Biochemistry and Molecular Genetics at the Temerty Faculty of Medicine.

His lab has developed several pioneering technologies - MYTH, MaMTH, SIMPL, SATiN, and Neu-SATiN - for studying protein-protein interactions and accelerating drug discovery. These tools have led to important advances in understanding diseases like cancer and cystic fibrosis, and have contributed to the development of new therapeutic strategies, including recent AI-guided efforts to target EGFR and KRAS mutations, as published in *Nature Biotechnology* (2025).

Prof. Stagljar has authored over 150 scientific papers, holds 9 patents, and has delivered more than 350 invited talks. He is a co-founder of Dualsystems Biotech and Perturba Therapeutics, and a member of the Royal Society of Canada, EMBO, and the HAZU (Croatian Academy of Sciences and Arts). In 2023, he was named one of the Top 50 most influential people from the Adria region by *Bloomberg Adria*.