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Salle des séminaires IBS

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par **Alexis Courbet**

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Towards the computational design of genetically encodable nanomachines

Biomolecular machines have so far remained inaccessible to synthetic approaches. In this talk, I will discuss our recent efforts to leverage advances in computational protein design for the fabrication of genetically encodable nanoscale machinery. I will present novel computational methods powered by the deep learning revolution, and show how to use them for the systematic design and experimental realization of functional de novo protein folds and mechanical systems approaching natural complexity.

Selected recent work

1. Watson, J. L., Juergens, D., Bennett, N. R., Trippe, B. L., Yim, J., Eisenach, H. E., Ahern, W., Borst, A. J., Ragotte, R. J., Milles, L. F., Wicky, B. I. M., Hanikel, N., Pellock, S. J., Courbet, A., Sheffler, W., Wang, J., Venkatesh, P., Sappington, I., Torres, S. V., Lauko, A., De Bortoli, V., Mathieu, E., Barzilay, R., Jaakkola, T. S., DiMaio, F., Baek, M., and Baker, D. (2022) Broadly applicable and accurate protein design by integrating structure prediction networks and diffusion generative models. In *bioRxiv* p. 2022.12.09.519842,

2. Sahtoe, D. D., Praetorius, F., Courbet, A., Hsia, Y., Wicky, B. I. M., Edman, N. I., Miller, L. M., Timmermans, B. J. R., Decarreau, J., Morris, H. M., Kang, A., Bera, A. K., and Baker, D. (2022) Reconfigurable asymmetric protein assemblies through implicit negative design. *Science* 375, eabj7662

3. Wicky, B. I. M., Milles, L. F., Courbet, A., Ragotte, R. J., Dauparas, J., Kinfu, E., Tipps, S., Kibler, R. D., Baek, M., DiMaio, F., Li, X., Carter, L., Kang, A., Nguyen, H., Bera, A. K., and Baker, D. (2022) Hallucinating symmetric protein assemblies. *Science* eadd1964

4. Dauparas, J., Anishchenko, I., Bennett, N., Bai, H., Ragotte, R. J., Milles, L. F., Wicky, B. I. M., Courbet, A., de Haas, R. J., Bethel, N., Leung, P. J. Y., Huddy, T. F., Pellock, S., Tischer, D., Chan, F., Koepnick, B., Nguyen, H., Kang, A., Sankaran, B., Bera, A. K., King, N. P., and Baker, D. (2022) Robust deep learning based protein sequence design using ProteinMPNN. In *bioRxiv* p. 2022.06.03.494563

Hôte : Hugues Nury (IBS/Groupe Transport Membranaire)