

Understanding the role of the microbiome in cancer



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Background: Alterations in the composition and function of the gut microbiome can influence the development and progression of neurodegenerative and cancerous diseases.

Post translational modifications are linked to activity and the human microbiome.

EntF* is a metabolite of enterobactin synthase component F (EntF), a sensing peptide produced by intestinal bacteria and plays a role in colorectal cancer metastasis¹.

Rationale: Understanding the structural and dynamic folding mechanisms EntF* will enable the development of novel regulators of host-microbe interactions.

Goal:

- Elucidate the relationship between posttranslational modifications and EntF* activity.

Research questions

1. How sensitive is a metaparticle to internal stimuli?
2. What are the mechanisms of inside-out activation?
3. What are the interaction mechanisms between active metaparticles?

Research approaches

1. Molecular dynamics simulations (enhanced sampling)
2. Molecular design
3. AI

Bibliography

- (1) Wynendaele, E.; Debunne, N.; Janssens, Y.; De Spiegeleer, A.; Verbeke, F.; Tack, L.; Van Welden, S.; Goossens, E.; Knappe, D.; Hoffmann, R.; Van De Wiele, C.; Laukens, D.; Van Eenoo, P.; Vereecke, L.; Van Immerseel, F.; De Wever, O.; De Spiegeleer, B. The Quorum Sensing Peptide EntF* Promotes Colorectal Cancer Metastasis in Mice: A New Factor in the Host-Microbiome Interaction. *BMC Biol.* **2022**, *20* (1), 151. <https://doi.org/10.1186/s12915-022-01317-z>.

