

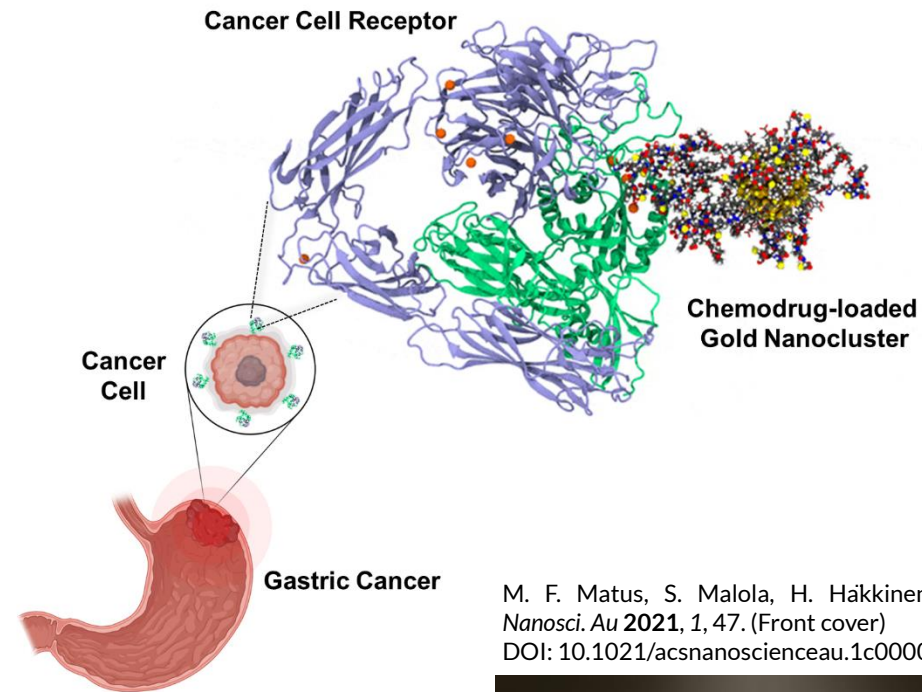
NanoGaC – Chimeric Gold Nanoclusters as Novel Drug Carriers against Gastric Cancer

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Abstract:

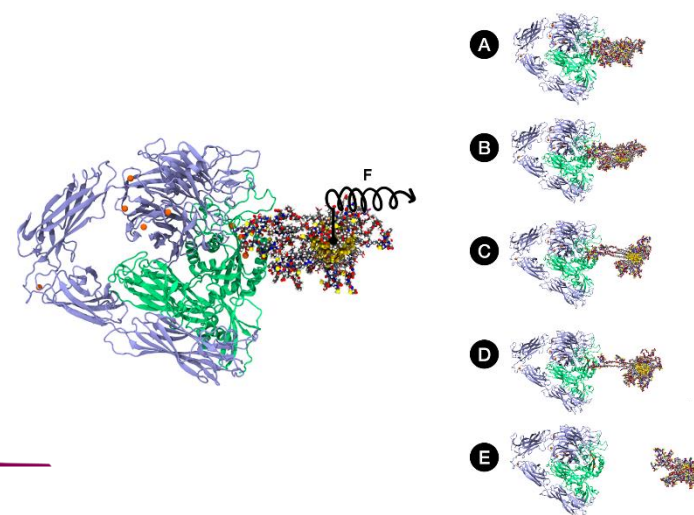
NanoGaC focuses on investigating novel treatment modalities for gastric cancer using functionalized gold nanoclusters (AuNCs) containing both cancer cell-recognizing molecules and drugs on their surface to improve the efficacy of current chemotherapy by directly killing cancer cells as well as inhibiting signaling pathways associated with cell survival.

The interaction modes and binding affinities between AuNCs and cancer cell receptor are studied via large-scale atomistic molecular dynamics (MD) simulations for prediction and guidance of the experimental stage.



M. F. Matus, S. Malola, H. Häkkinen, *ACS Nanosci. Au* 2021, 1, 47. (Front cover)
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Estimation of binding free energy of the AuNC-cancer cell receptor complex:



CSC Grand Challenge Project 2021

