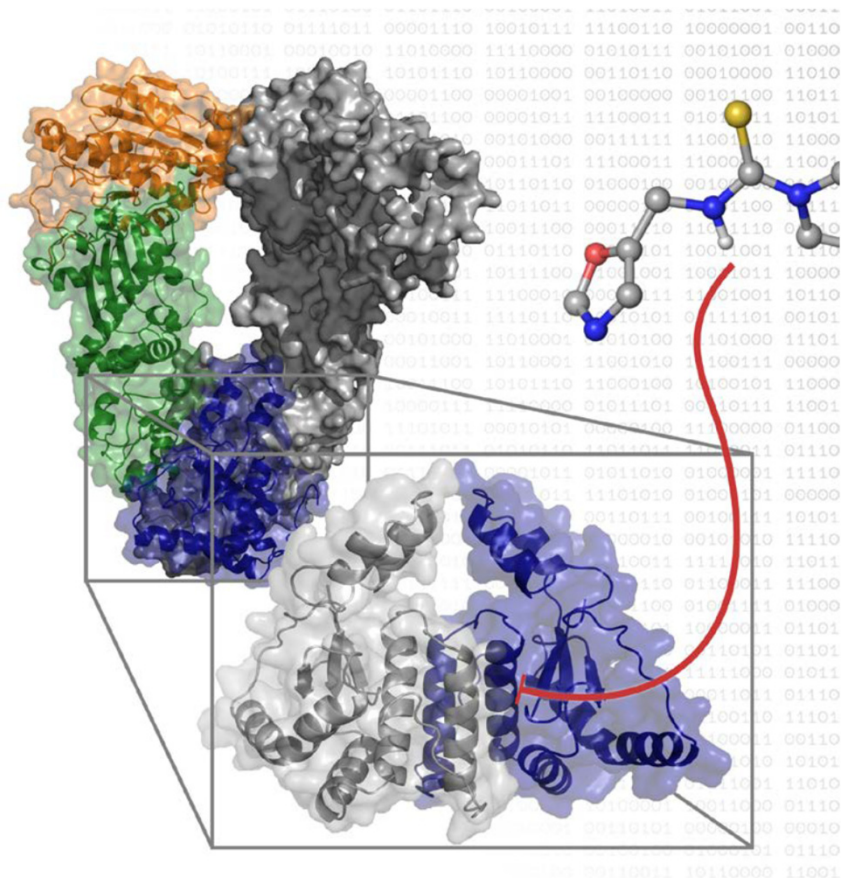


## Lead structure generation for HSP90 dimerization inhibitors and classification of protein-protein interfaces



Regulation of many physiological and pathophysiological processes is transmitted by multiprotein complexes. HSP90 is a chaperone protein that promotes cell survival under stress conditions. Especially tumor cells are under constant stress due to malnutrition and hypoxia, but also due to cytostatic therapies. Thus, they highly depend on the function of this chaperone. Inhibiting the function of HSP90 therefore might prove an innovative approach to overcome therapy resistances in tumor cells.

Based on previous work in the group and with experimental collaborators, it was shown that the C-terminal dimerization of HSP90 is essential for its function and can be inhibited by rationally designed peptides, peptidomimetics, and small-molecule compounds. In collaboration with experimental groups (organic synthesis, biophysical and cell biological characterization), this thesis aims to generate lead structures from the currently know inhibitors with better physico-chemical and biopharmaceutical properties. Furthermore, the thesis aims to develop a method to identify protein-protein interfaces based on image recognition and machine learning.

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