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Title	Crystals of Mn-carbonyl/RNaseA adduct as a template to track metal complex reaction
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Abstract

The investigation of metal complex reactions through the determination of intermediate structures in three dimensions holds great appeal as it unravels intricate details of the reaction mechanisms. While there are various spectral and analytical methods available to identify reaction intermediates, the utilization of X-ray structure determination is particularly advantageous. This approach offers intricate coordination structures and changes that cannot be obtained through other methods.

In this study, we selected RNaseA as a suitable protein template due to its ability to form a porous crystal upon crystallization. This property proves beneficial as it allows small molecules to easily diffuse into the crystal, reaching the appropriate binding sites. By soaking the RNaseA crystal, we successfully prepared the Mn-carbonyl adduct. Notably, the X-ray crystal structure analysis of the Mn-carbonyl/RNaseA adduct revealed the presence of multiple metal binding sites with diverse Mn coordination structures. The occurrence of multiple metal binding sites within a single crystal is intriguing as it enables the examination and comparison of the effects arising from variable coordination structures in the metal complex reaction.

Through a series of X-ray crystal structure analyses, we investigated the changes in Mn coordination structure during the CO release reaction, as well as the role played by protein side-chains. This presentation will encompass the preparation of the Mn-carbonyl/RNaseA adduct, the determination of its X-ray crystal structure, and the structural examination of the CO release reaction under light irradiation.

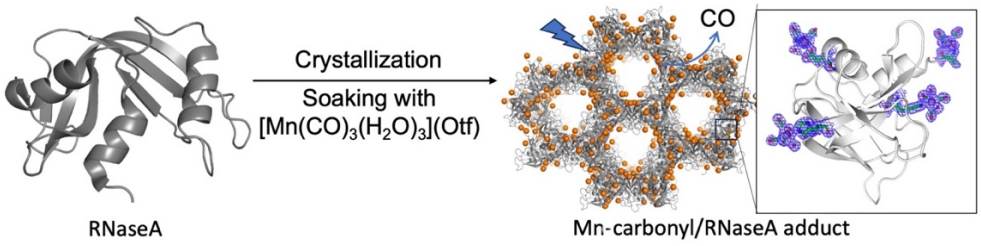

Figure 1: Preparation and structure of Mn-carbonyl/RNaseA-adduct.