**INTRODUCTION**

The M2 Protein from influenza A virus is a pH-regulated proton channel that can be blocked by amantadine. The transmembrane domain of the M2 protein, called M2TMD, also exhibits amantadine-sensitivity. Using PISEMA (Polarization Inversion Spin Exchange at Magic Angle) data collected at the NHMFL, an atomic structure for the blocked M2TMD-amantadine structure has been determined.

PISEMA experiments generate two-dimensional data which describe orientation constraints for the target protein. An initial model was built which satisfied the PISEMA data constraints and was then refined using stereo-chemical, solid-state, and H-bond energy terms to achieve a minimal energy conformation.

**RESULTS AND DISCUSSION**

The M2TMP-Amantadine complex is believed to naturally form a tetramer in the membrane bilayer. The data from the PISEMA gives information detailing the monomer. Below is the atomic structure of the monomer (Fig. 1) and a proposed tetramer complex (Fig. 2). The amantadine is shown in orange.

![Fig. 1](image1.png) ![Fig. 2](image2.png)

**CONCLUSIONS**

PISEMA data was used to build a high resolution atomic model of the M2TMD-Amantadine complex. It is the first known atomic resolution model of the M2TMD-Amantadine complex and provides a good baseline for follow-up binding studies.

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**REFERENCES**