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Glass-Like Behavior of Magnesium Ions Inside RNA APTamers

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RNA is known to be strongly dependent on Magnesium for stability. In this computational study, we explore the effects of Magnesium concentration on the SAM I riboswitch with several microsecond-plus simulations at varying concentrations. Individual Magnesium binding events are shown to influence the RNA conformation through tertiary bridging interactions. We characterize the behavior of Magnesium near RNA for use in structure-based models, and note that it is glassy.