Temperature-dependent Radiolysis Reveals Dynamics of Bound Protein Waters

Scientific Achievement

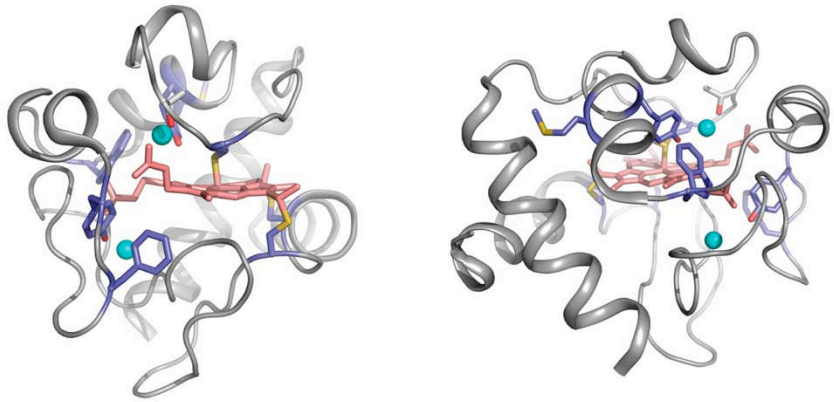
Devised temperature-dependent radiolysis and mass spectrometry X-ray footprinting technique to identify position of bound water vs. free water within proteins, and to measure dynamics of bound water interactions on timescales relevant to catalysis and macromolecular assembly.

Significance and Impact

This method could be a tool to investigate protein therapies as it allows researchers to see where water binds tightly or loosely to the surface of proteins, giving insight into how the structure of water manipulates the timescale of enzyme reactions or how bound water influences movement through ion channels.

Research Details

- Researchers targeted millisecond processes because method detects slow exchange rates of water within proteins; most tightly bound water takes longest time to exchange.
- Use of water (^{16}O) and heavy water (^{18}O) allowed researchers to see how fast mass of the protein changed, evidence that heavy water had been exchanged for lighter water.



Cyt c 18O-labeling map. The sites of 18O-modifications are visualized from the crystal structure 1HRC (27) using PyMOL. The 18O-labeled residues (light blue) in and around the heme (light pink) crevices, and the position of residue T78 (gray) and conserved waters (cyan spheres) HOH112, HOH139 are shown in two orientations of the cyt c molecule.

Sayan Gupta, Rhijuta D'Mello, and Mark R. Chance , *PNAS* v. 109, no.37 (2012)
Work was performed at Brookhaven National Laboratory