

# Water in cavity-ligand recognition

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## Supporting Information

### Movie S1

Video clip showing changes in water density distribution along the (N,N) cavity-ligand binding coordinate. See Fig. 2 legend for color coding and the corresponding thermodynamic analysis.

### Movie S2

Video clip showing changes in water density distribution along the (+,N) cavity-ligand binding coordinate. See Fig. 2 legend for color coding, Fig. 3 for the corresponding thermodynamic analysis.

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### **Movie S3**

Video clip showing changes in water density distribution along the  $(-,N)$  cavity-ligand binding coordinate. See Fig. 2 legend for color coding, Fig. 3 for the corresponding thermodynamic analysis.

### **Movie S4**

Video clip showing changes in water density distribution along the  $(-,+)$  cavity-ligand binding coordinate. See Fig. 2 legend for color coding, Fig. 4 for the corresponding thermodynamic analysis.

### **Movie S5**

Video clip showing changes in water density distribution along the  $(+,-)$  cavity-ligand binding coordinate. See Fig. 2 legend for color coding, Fig. 4 for the corresponding thermodynamic analysis.

### **Movie S6**

Video clip showing changes in water density distribution along the  $(N,+)$  cavity-ligand rejection coordinate. See Fig. 2 legend for color coding, Fig. 5 for the corresponding thermodynamic analysis.

### **Movie S7**

Video clip showing changes in water density distribution along the  $(N,-)$  cavity-ligand rejection coordinate. See Fig. 2 legend for color coding, Fig. 5 for the corresponding thermodynamic analysis.