Interactions of Quantum Dot Nanoparticles with Protein and Membrane

David Bell

Computational Biology Center

IBM Research

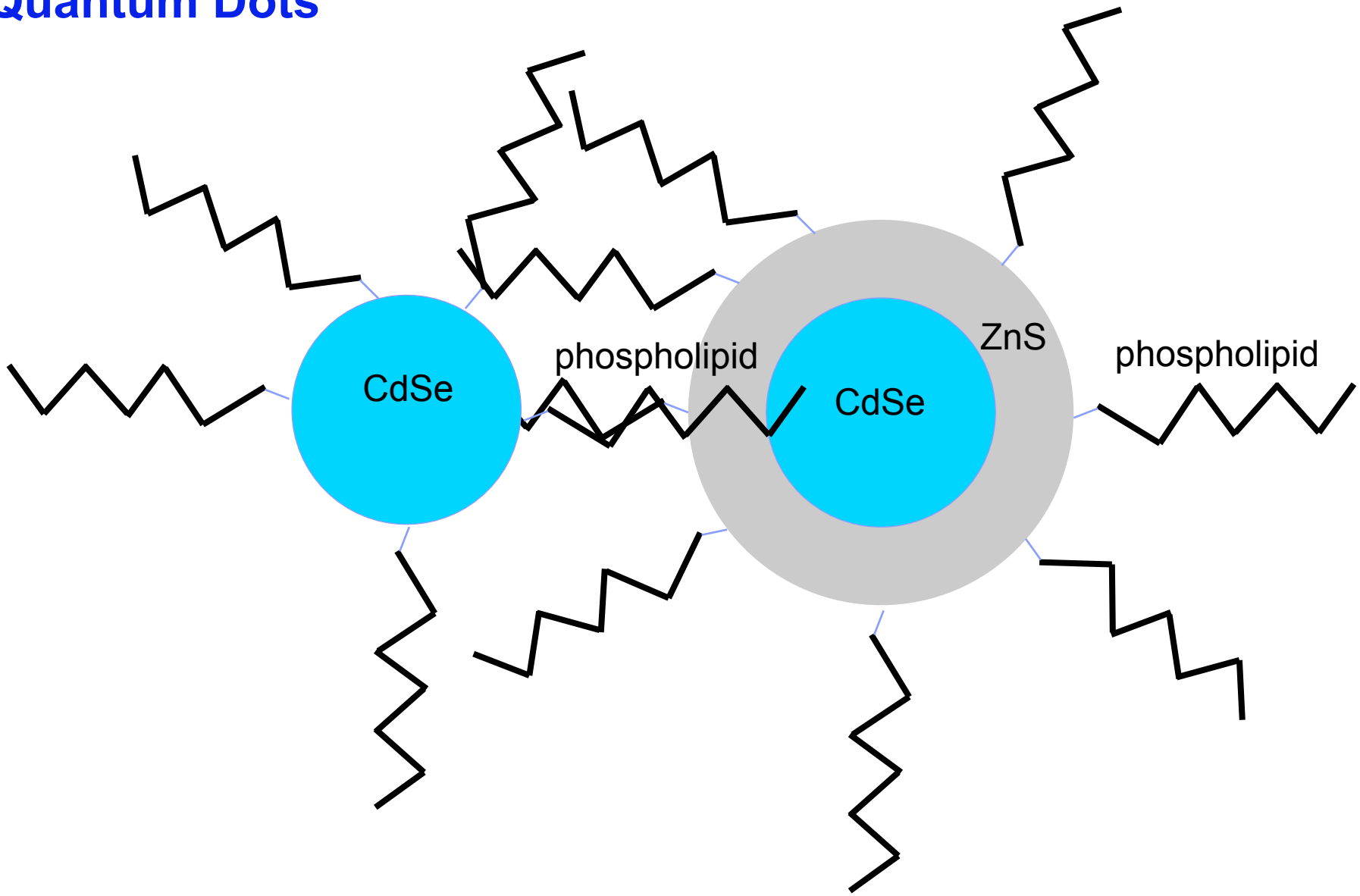
Quantum Dots

SIGMA-ALDRICH®

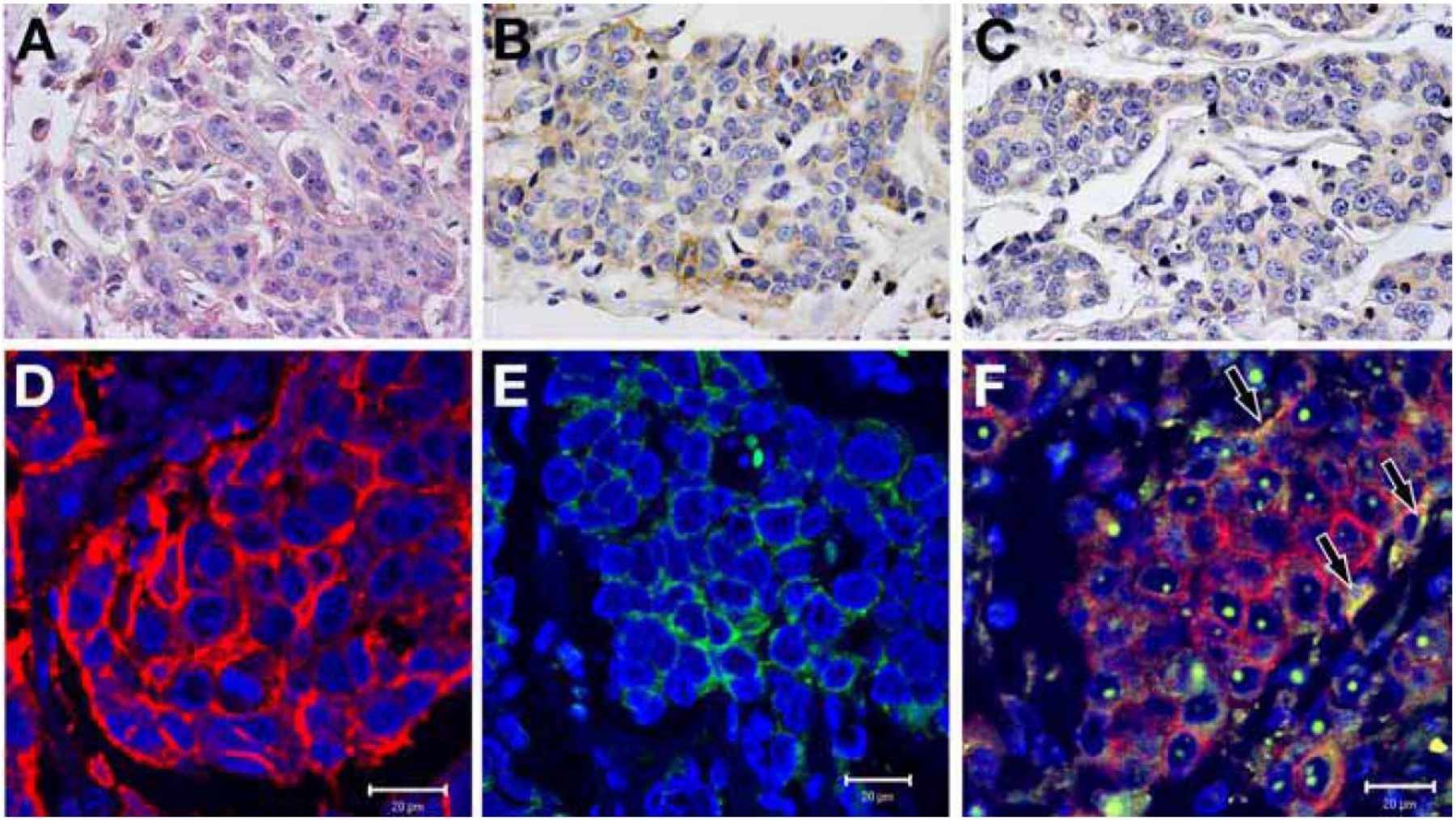
life technologies



Quantum Dots

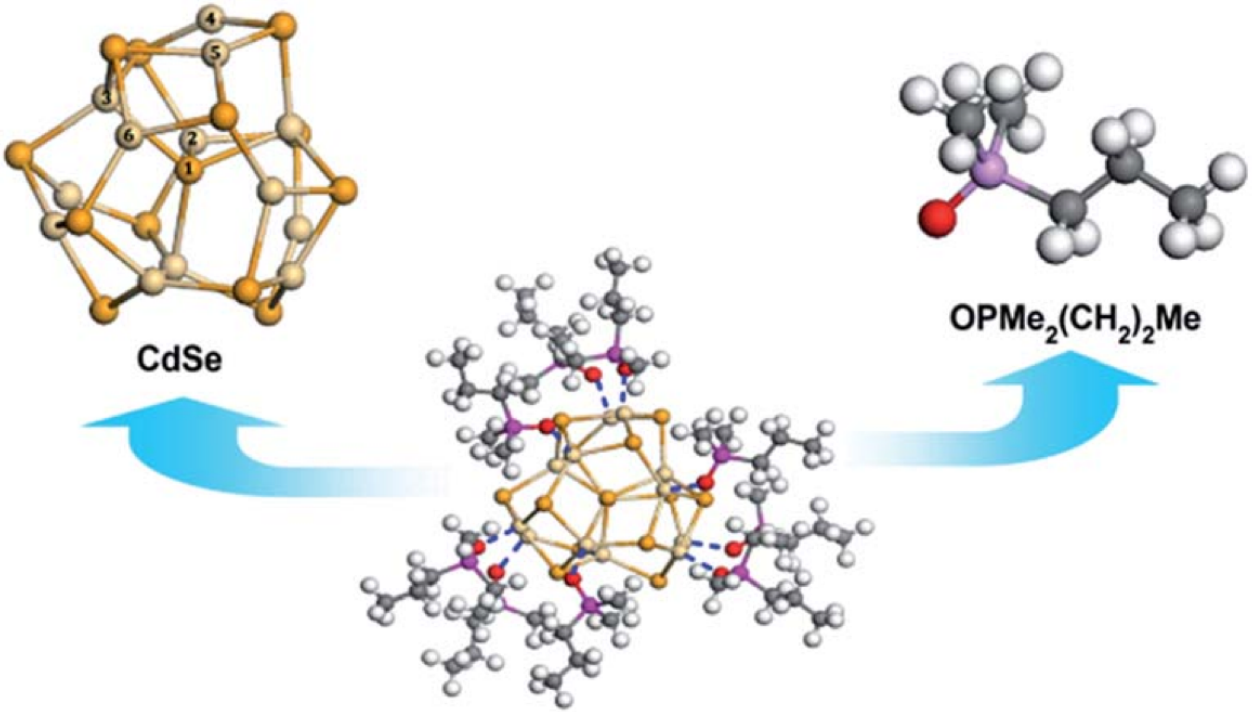


Quantum Dots

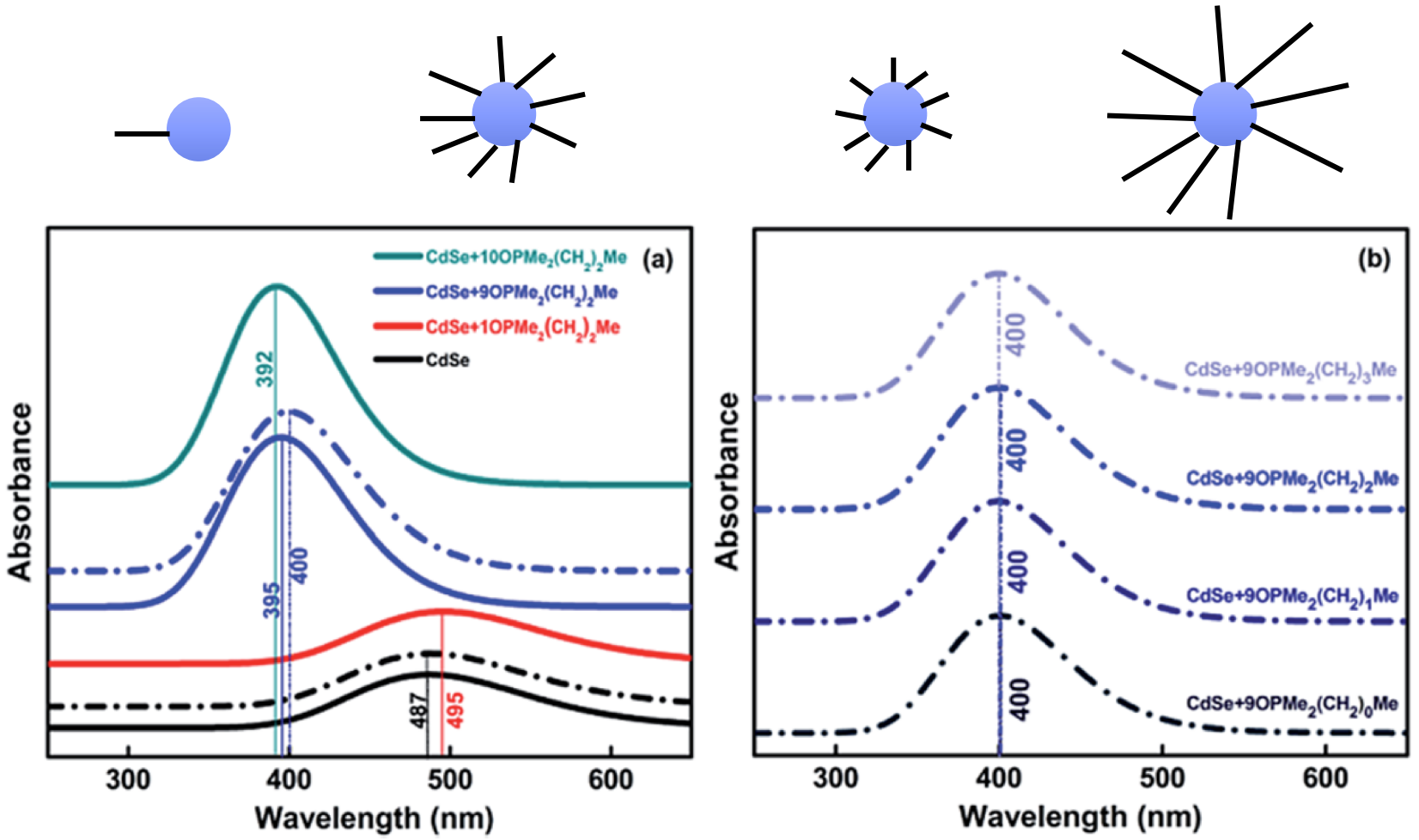


Itoh, J. and R. Osamura, *Quantum Dots for Multicolor Tumor Pathology and Multispectral Imaging*, in *Quantum Dots*, M. Bruchez and C. Hotz, Editors. 2007, Humana Press. p. 29-42.

Quantum Mechanics Work



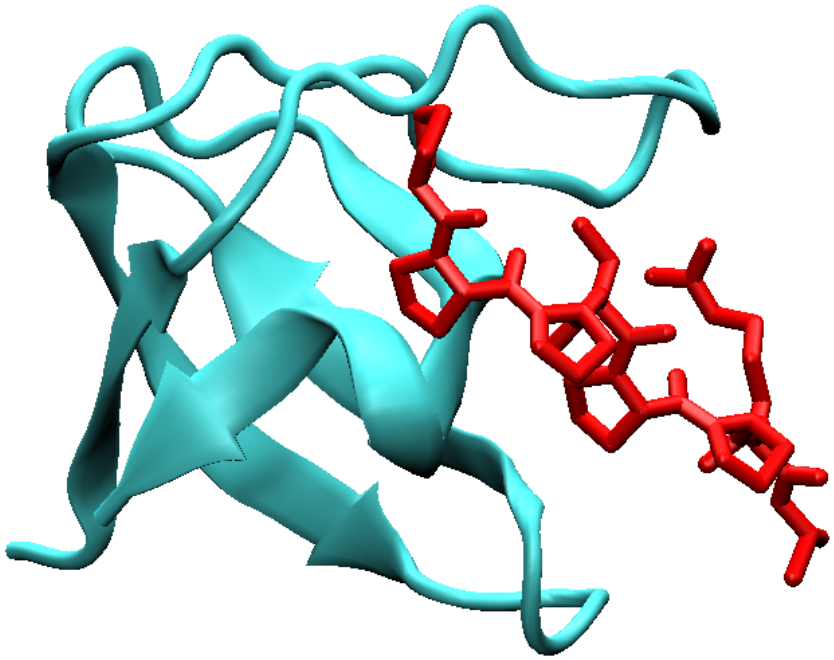
Gao, Y., et al., *Effect of ligands on the characteristics of (CdSe)(13) quantum dots.* Rsc Advances, 2014. **4**(52): p. 27146-27151.



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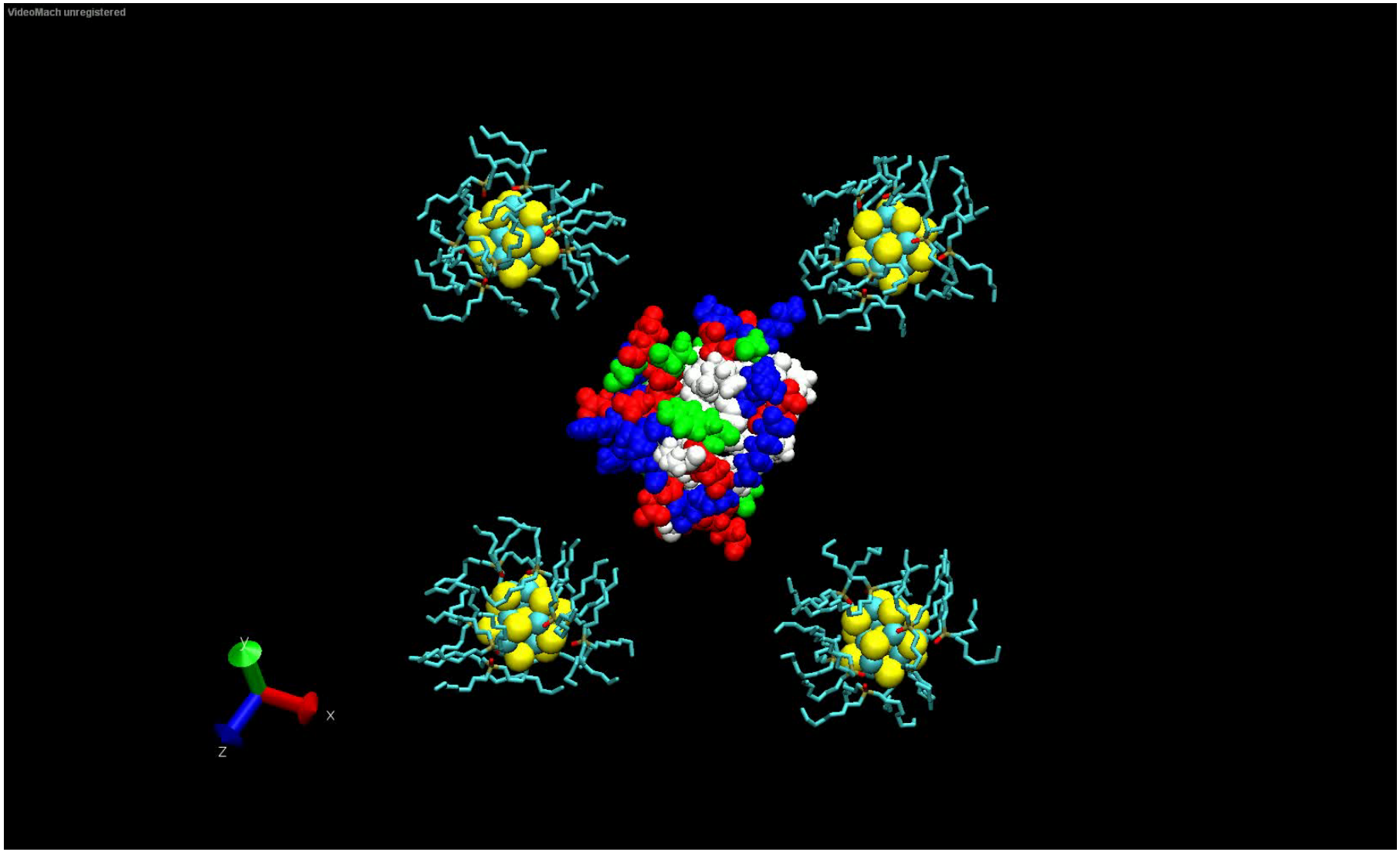
SH3 Protein

- Ubiquitous from yeast to humans
- Intracellular signaling
- Ligand is PRM
- PDB ID: 1CKB

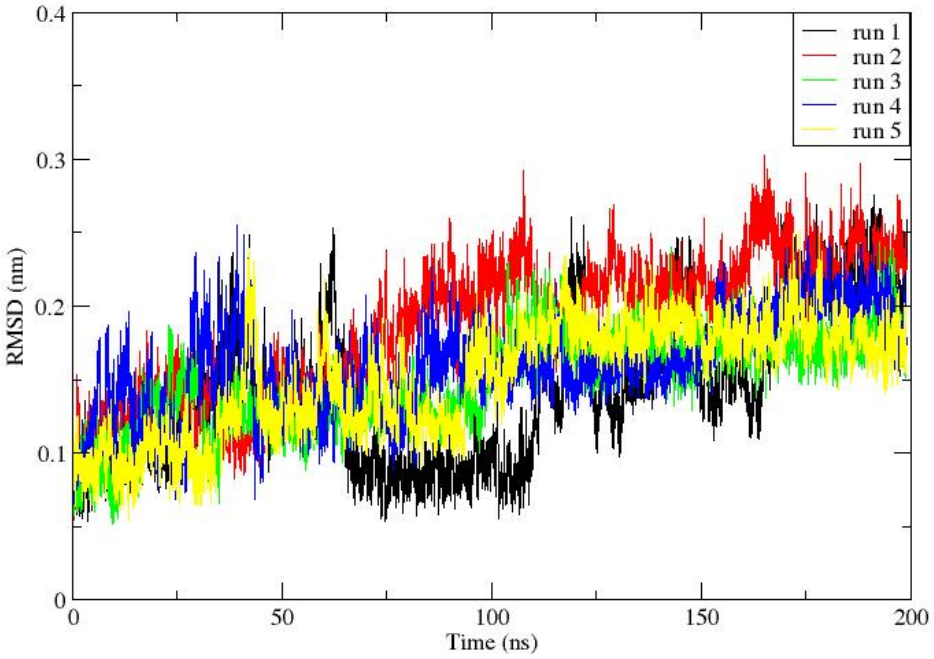


Wu, X.D., et al., *STRUCTURAL BASIS FOR THE SPECIFIC INTERACTION OF LYSINE-CONTAINING PROLINE-RICH PEPTIDES WITH THE N-TERMINAL SH3 DOMAIN OF C-CRK.* Structure, 1995. **3**(2): p. 215-226.

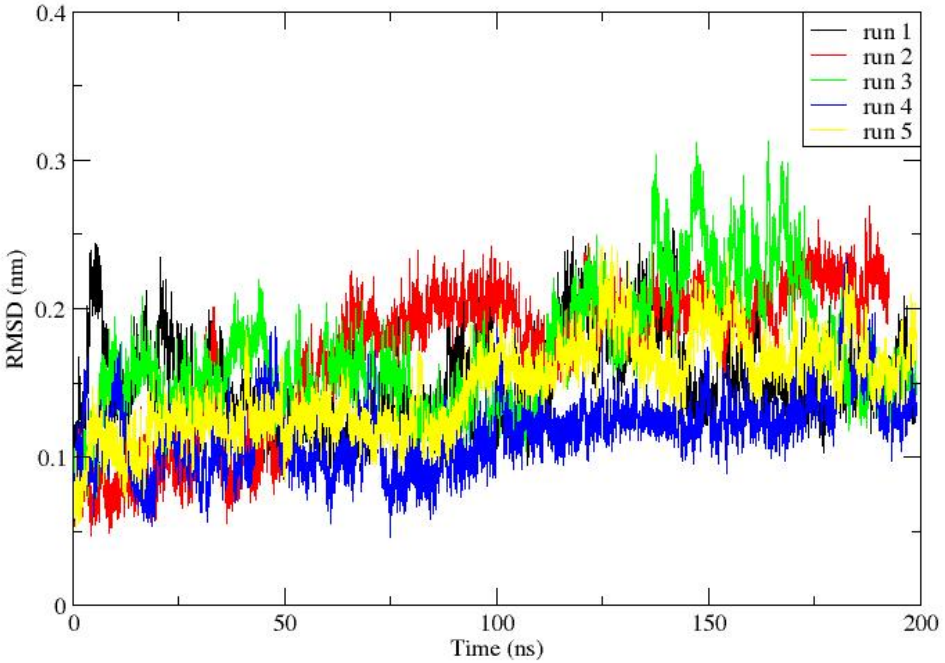
QD and SH3 Protein



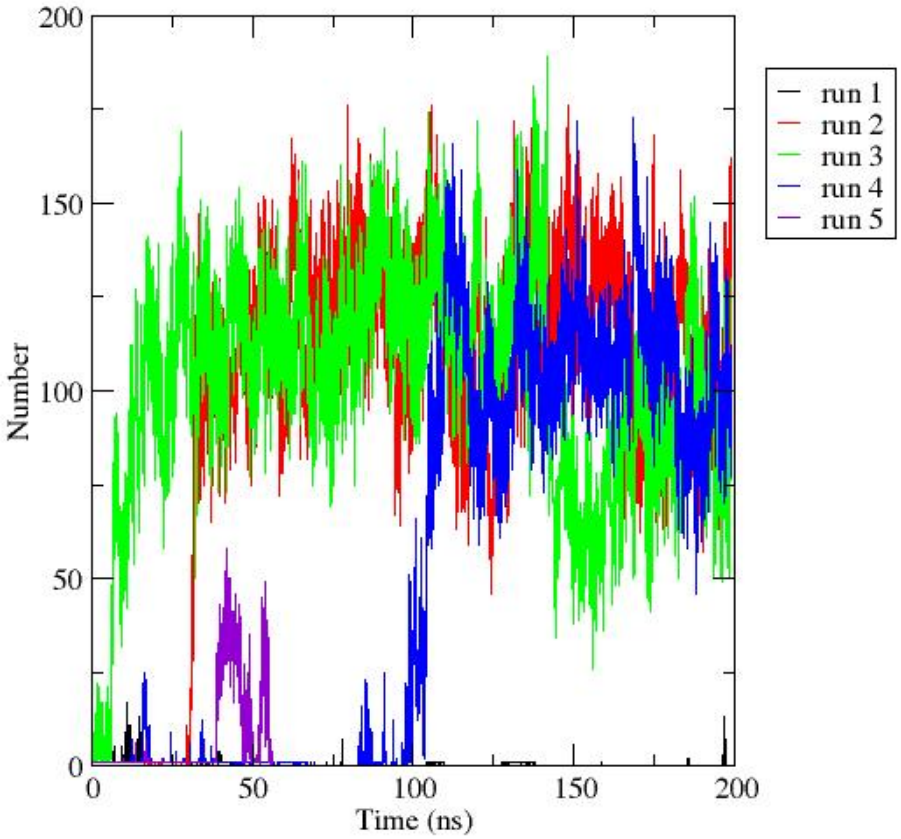
RMSD SH3-QD



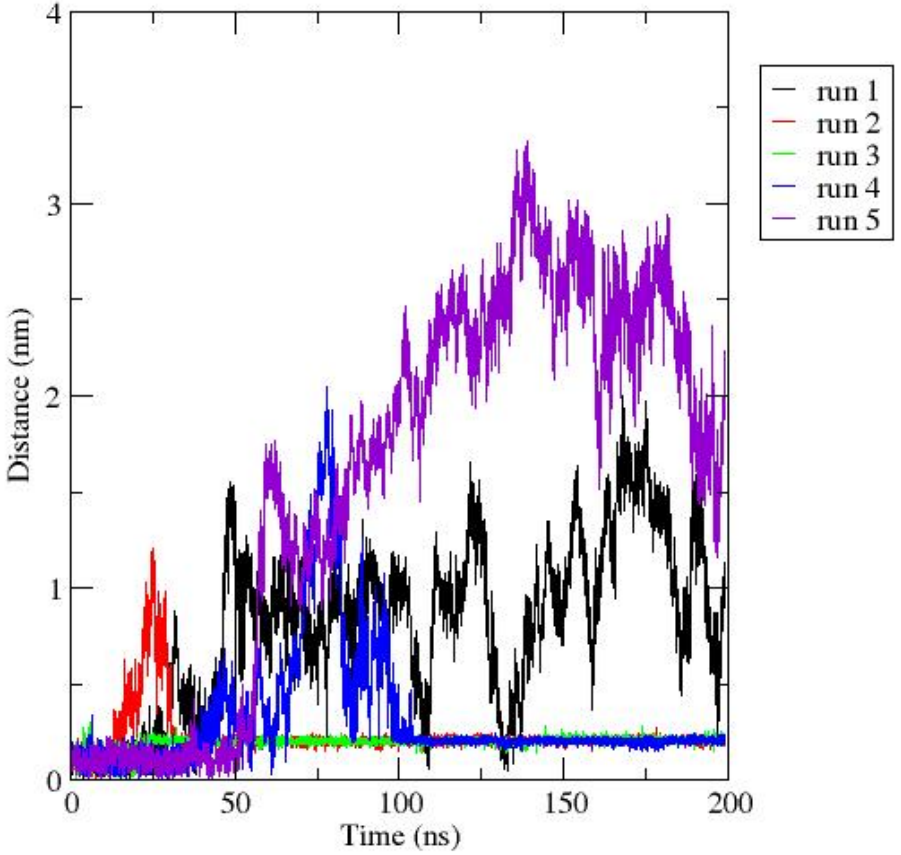
RMSD SH3-4QD



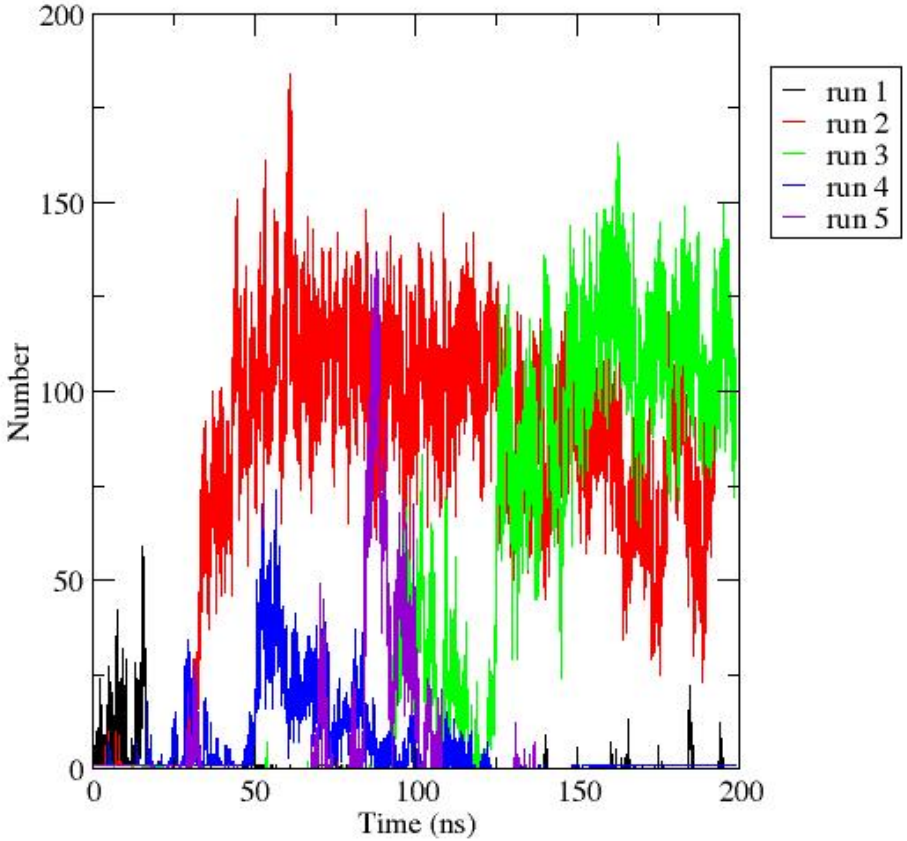
Number of Contacts < 0.5 nm, SH3-QD



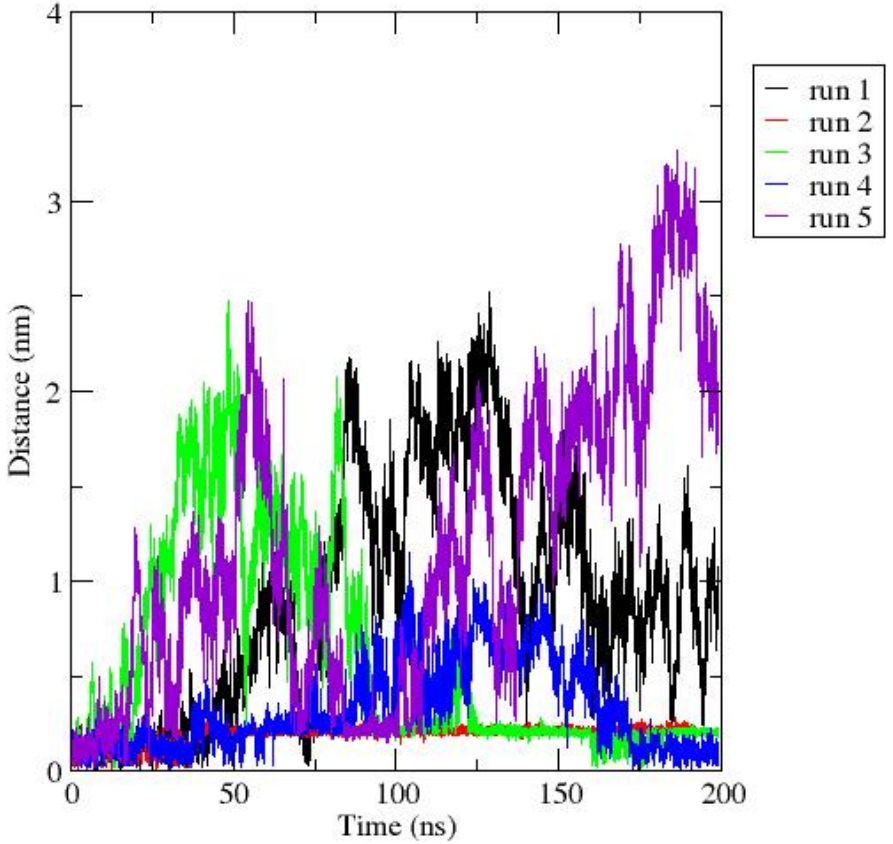
Minimum Separation Distance, SH3-QD

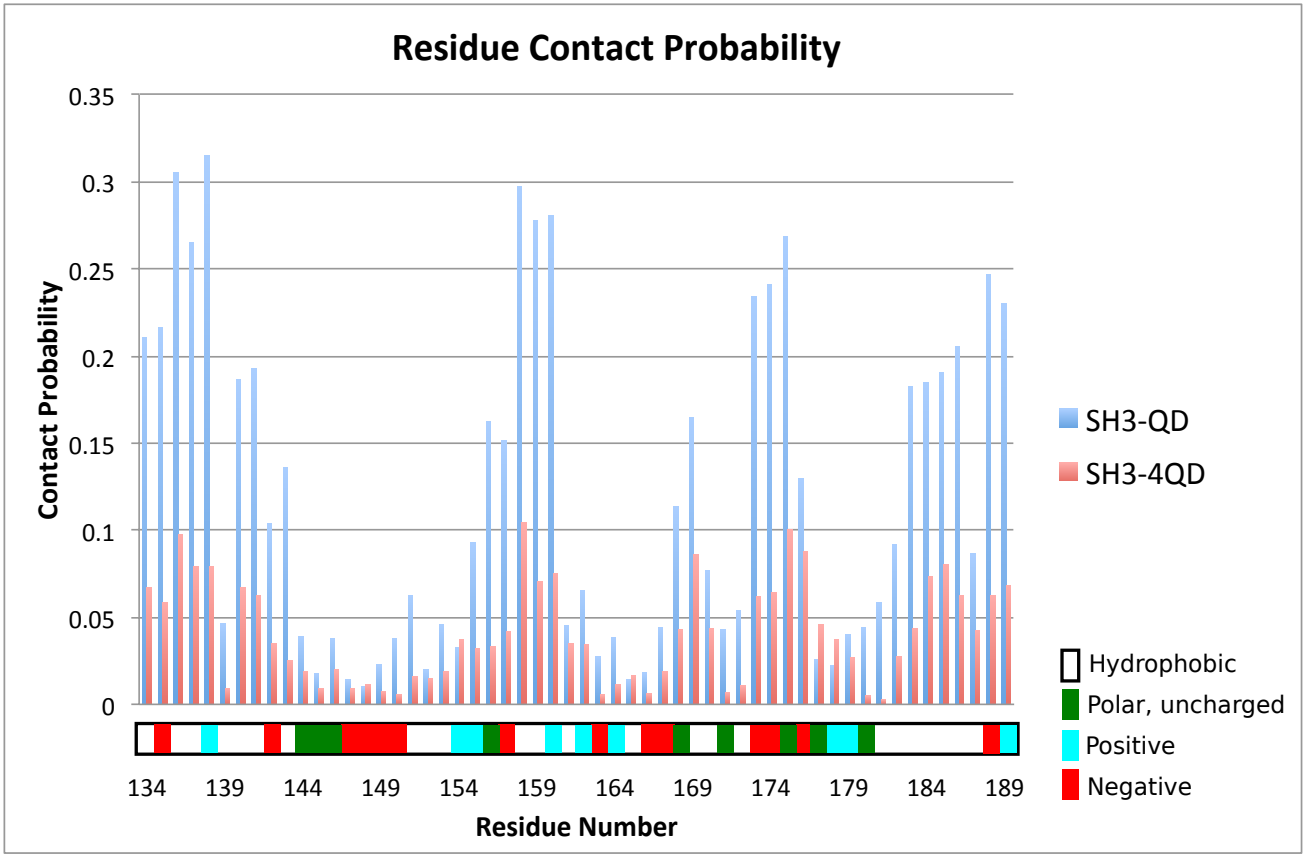


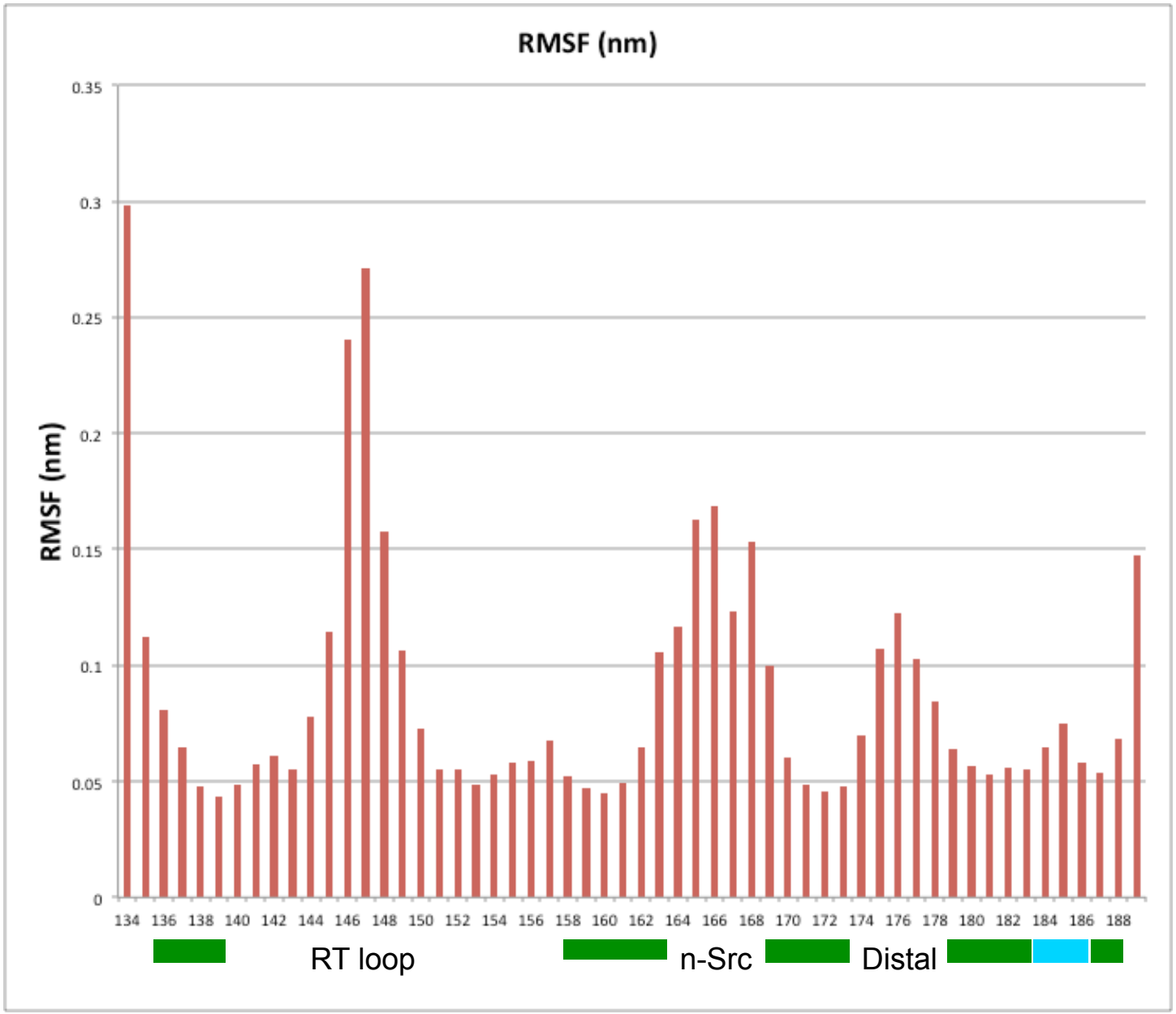
Number of Contacts < 0.5 nm, SH3-4QD



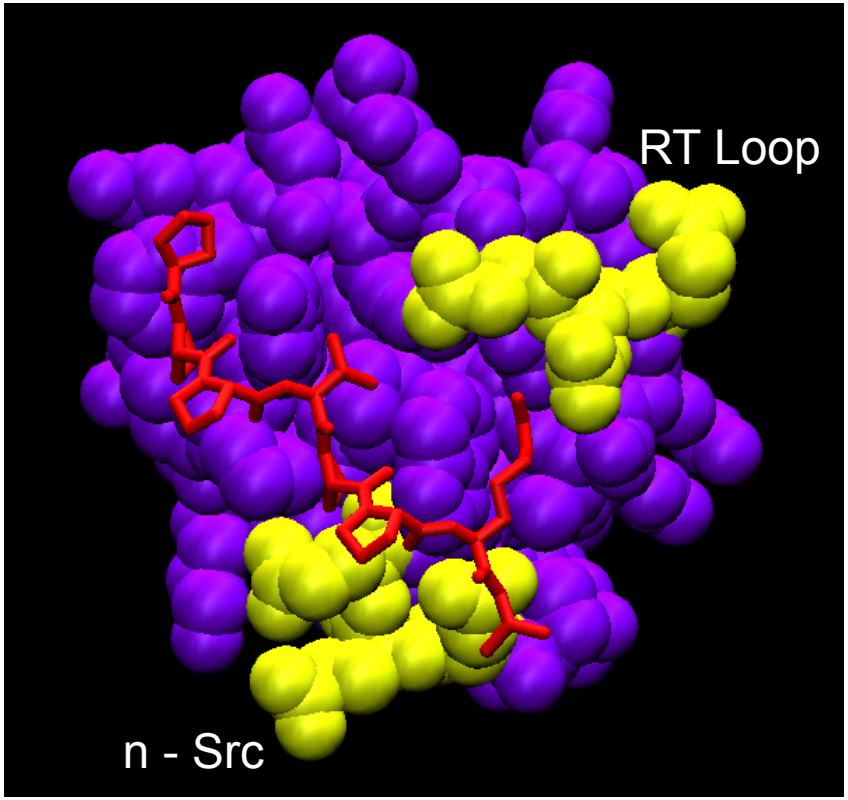
Minimum Separation Distance, SH3-4QD

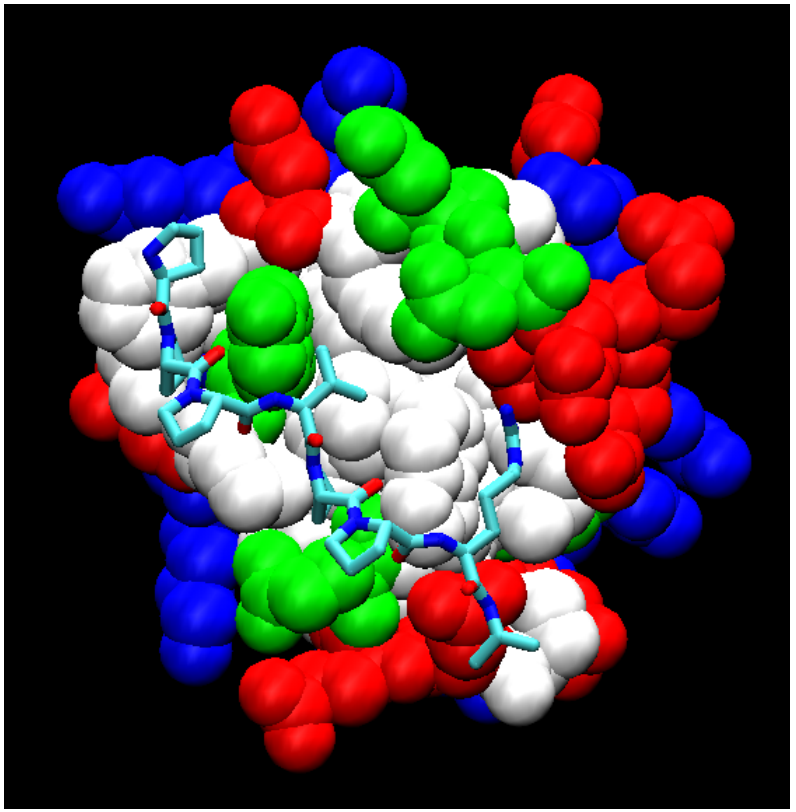


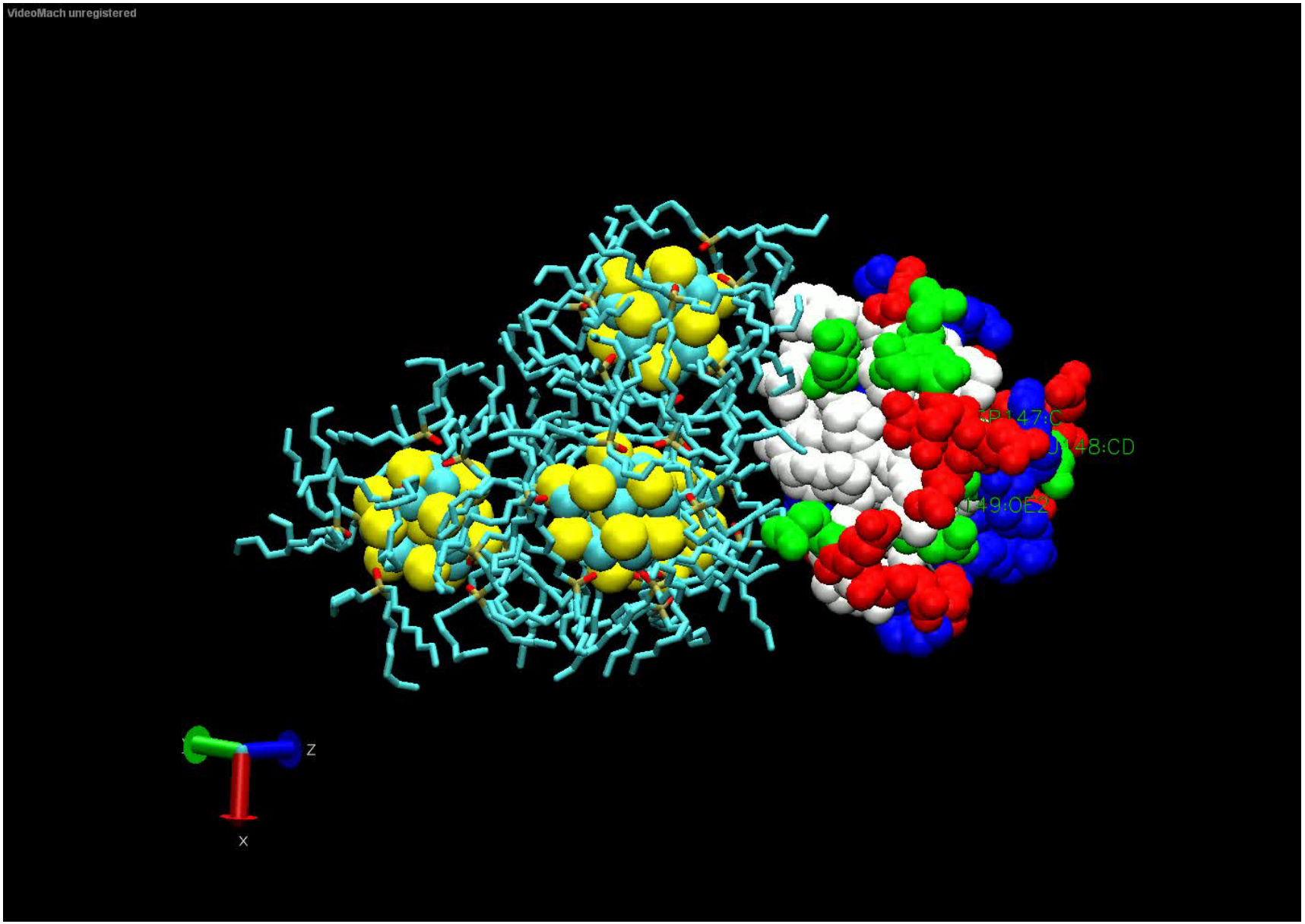

Residue Contact Probability
Contact Probability
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
134
139
144
149
154
159
164
169
174
179
184
189
Residue Number
SH3-QD
SH3-4QD
Hydrophobic
Polar, uncharged
Positive
Negative


RMSF (nm)
RMSF (nm)
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
134 136 138 140 142 144 146 148 150 152 154 156 158 160 162 164 166 168 170 172 174 176 178 180 182 184 186 188
RT loop
n-Src
Distal

SH3 Binding Site

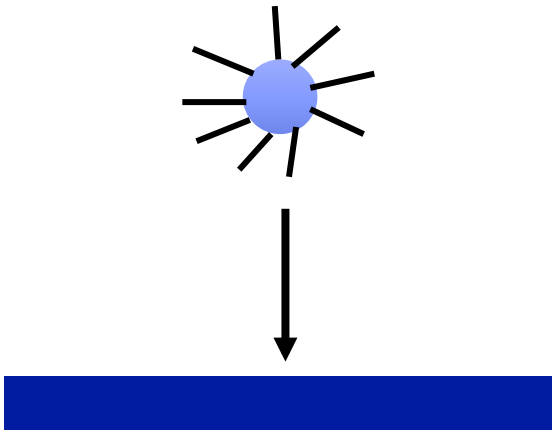





VideoMach unregistered
Z
X

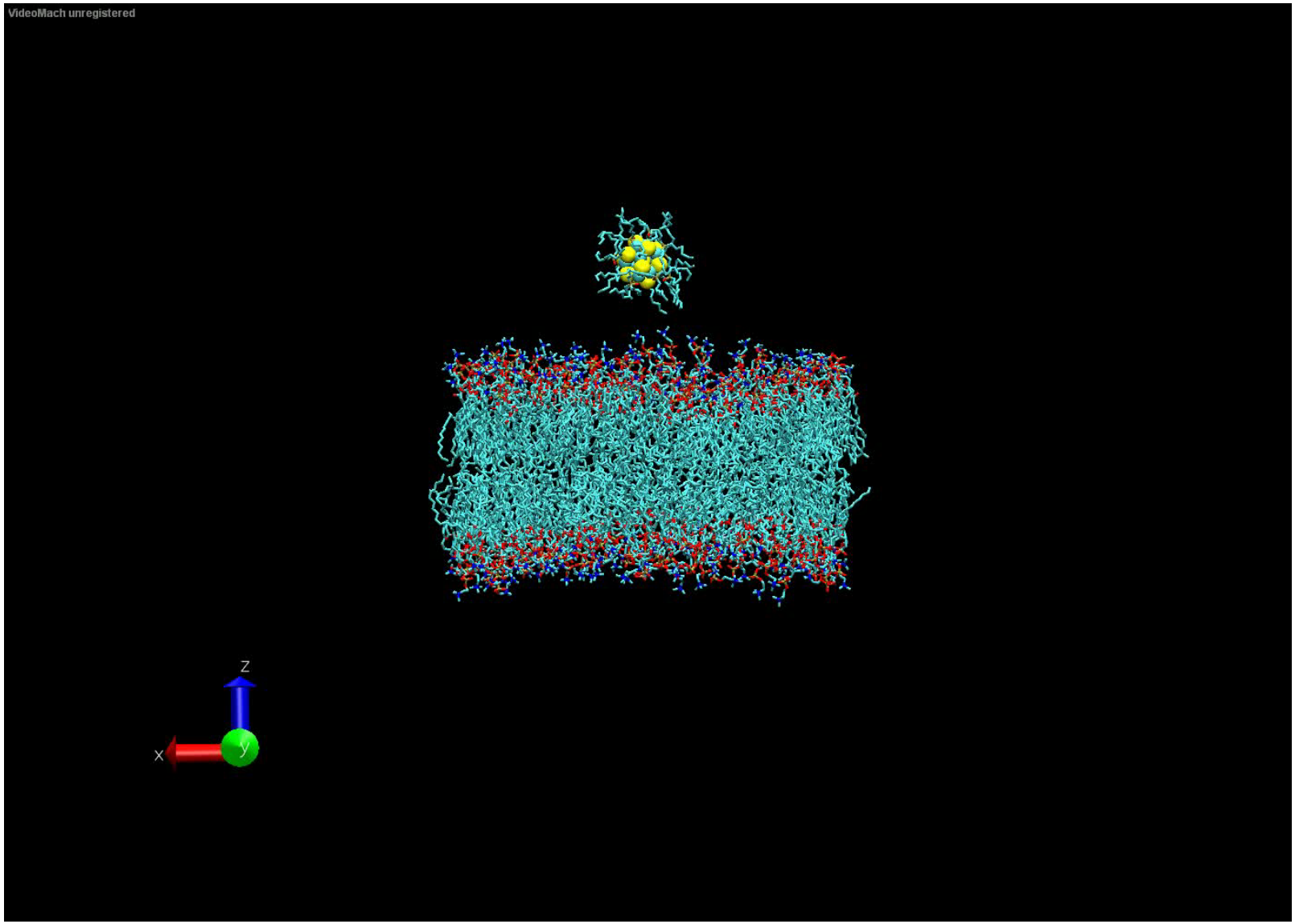
Membrane Study

- Free Energy
- Steered Molecular Dynamics
  - Velocity of 1 Å/ns
  - Spring constant of 5.0 kcal/mol/Å^2
- 100 ns

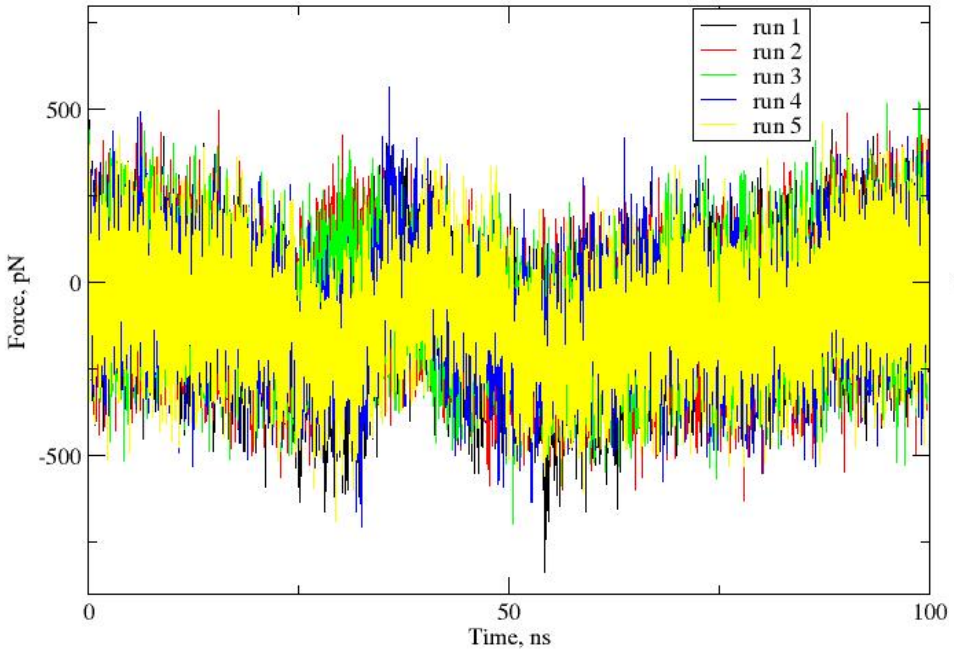




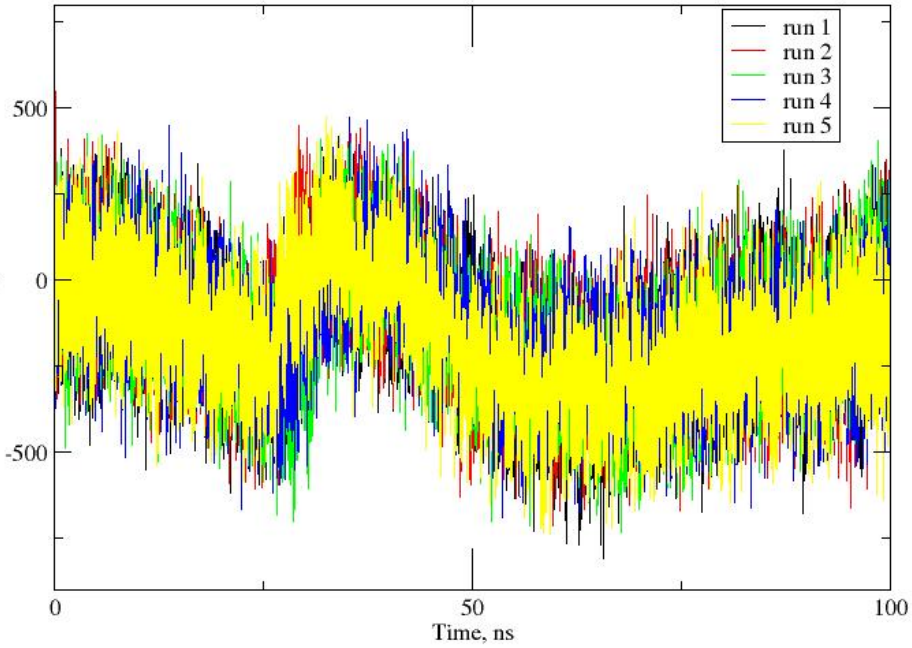
QD and membrane



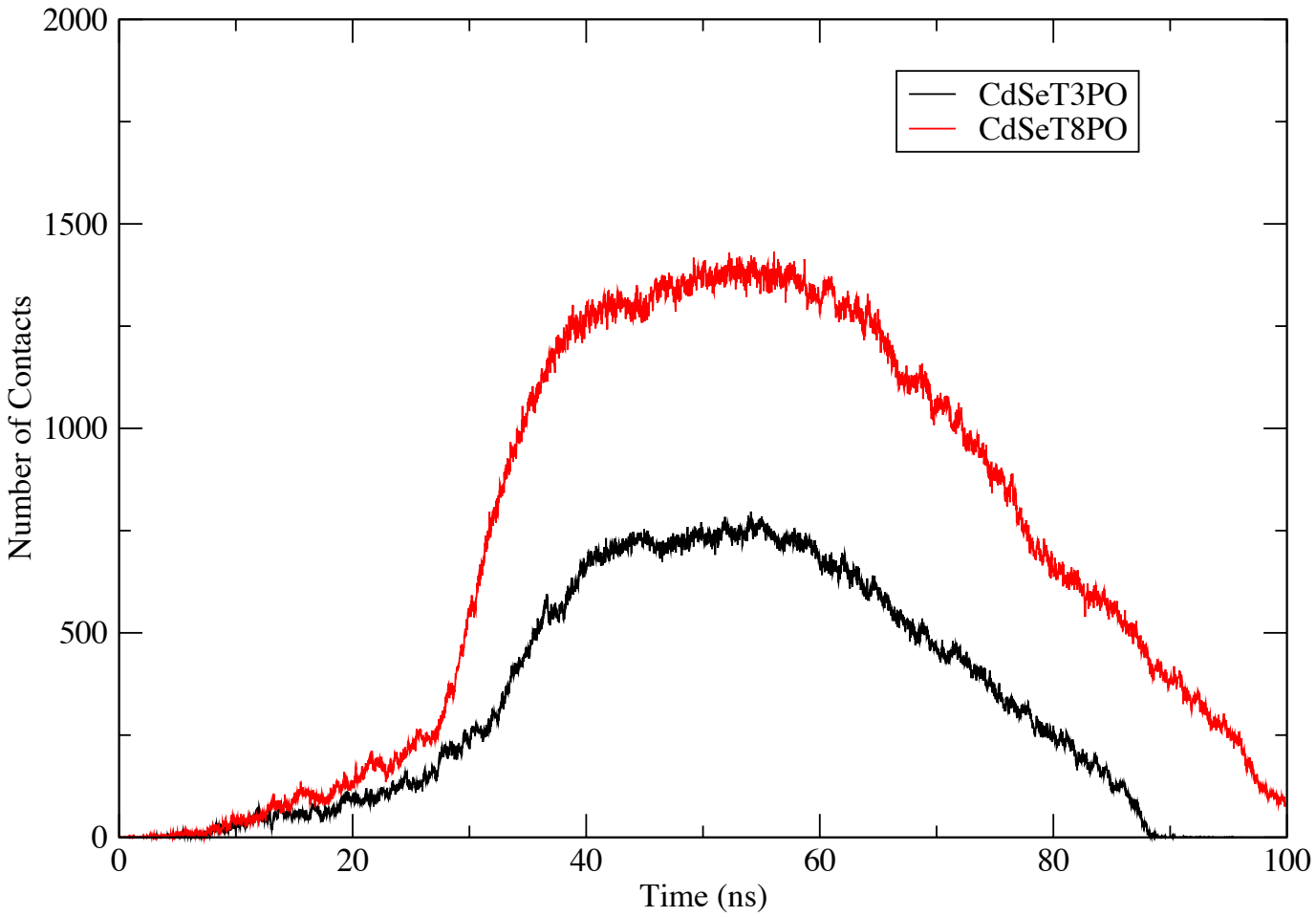
Pulling Force CdSeT3PO



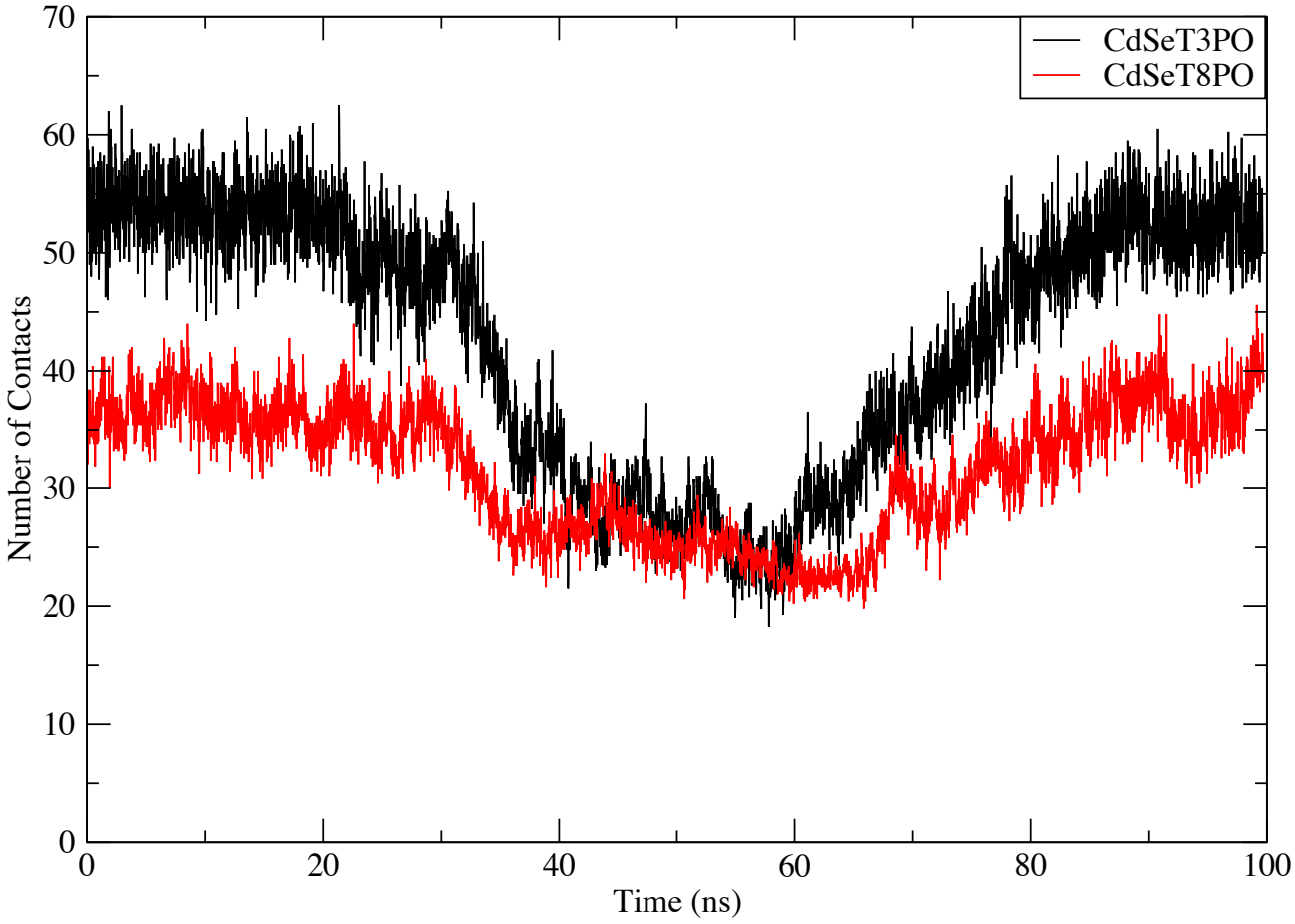
Pulling Force CdSeT8PO

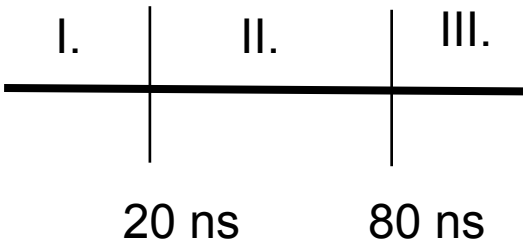


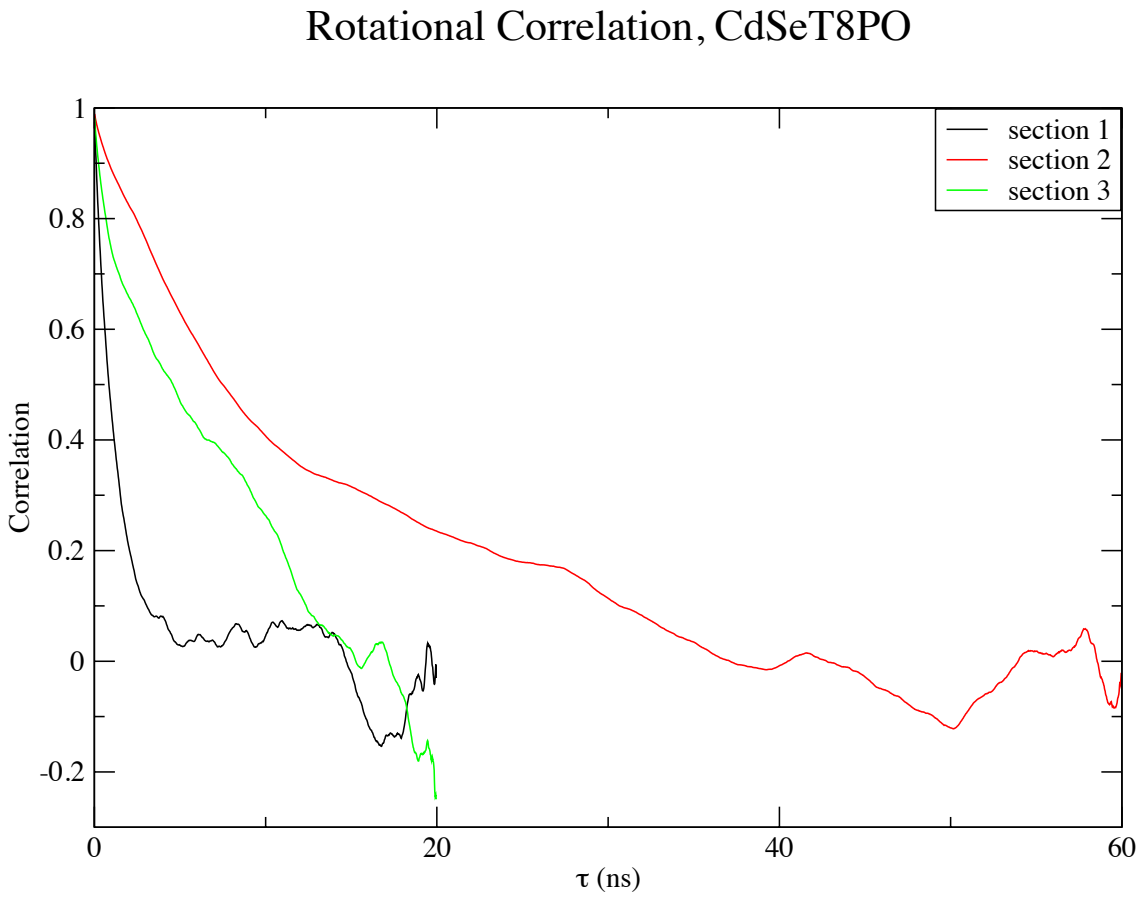
QD-Membrane Average Contact Number



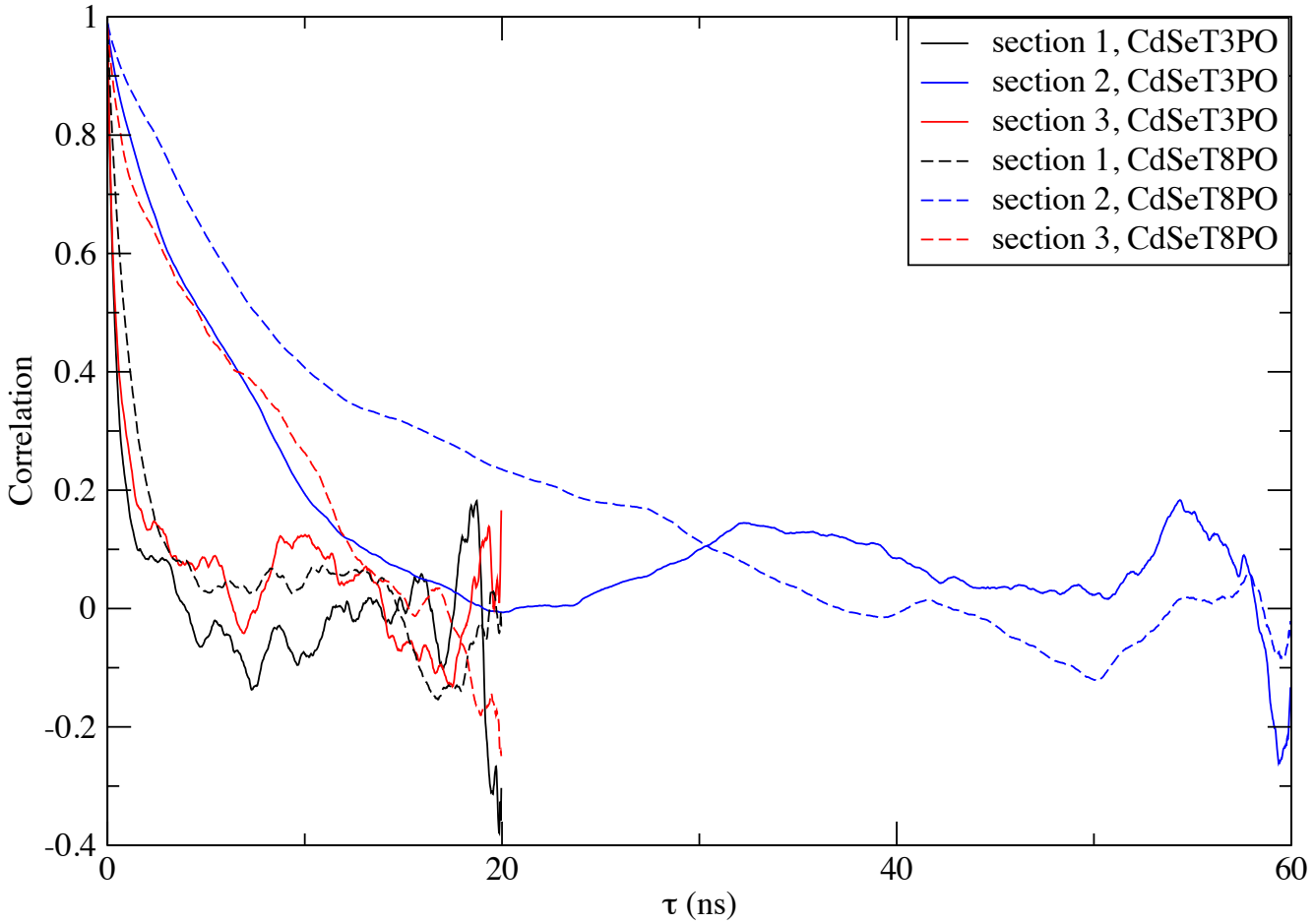
QD Core-Water Average Contact Number




I.
II.
III.
20 ns
80 ns


Rotational Correlation, CdSeT8PO
Correlation
τ (ns)
section 1
section 2
section 3
1
0.8
0.6
0.4
0.2
0
-0.2
0
20
40
60

Rotational Correlation, Combined



Acknowledgements

- Ruhong Zhou, Seung-gu Kang, Tien Huynh, and Jerry Yang
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- Audience

Thanks!

Questions?