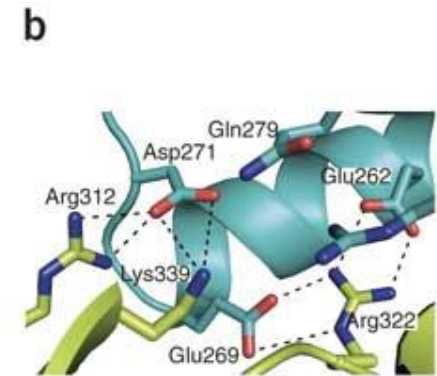
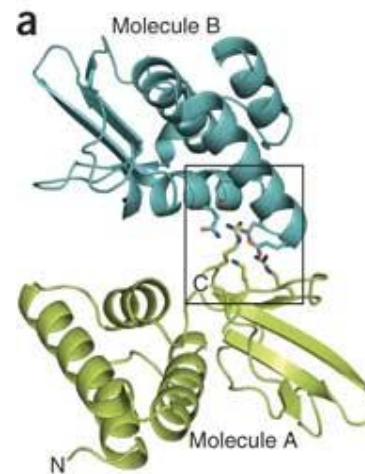
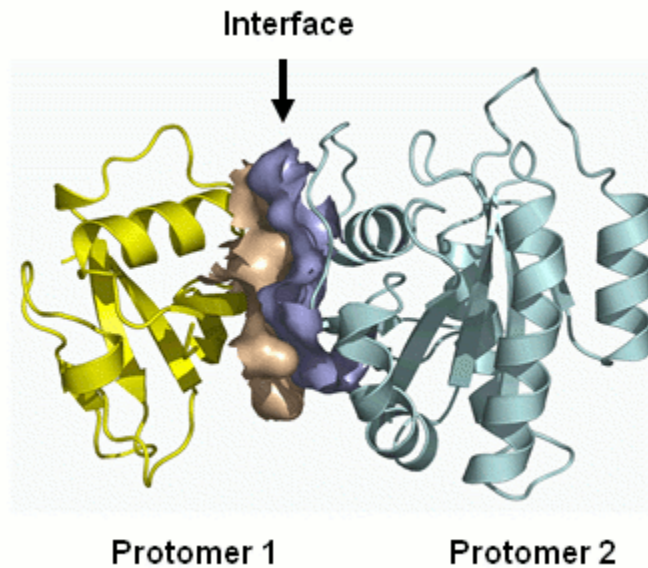


# EXPERIMENT 9: INTERACTION ANALYSIS

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**Dr. Zhiyi Wei**  
SUSTC

# Protein-protein interaction



# Methods

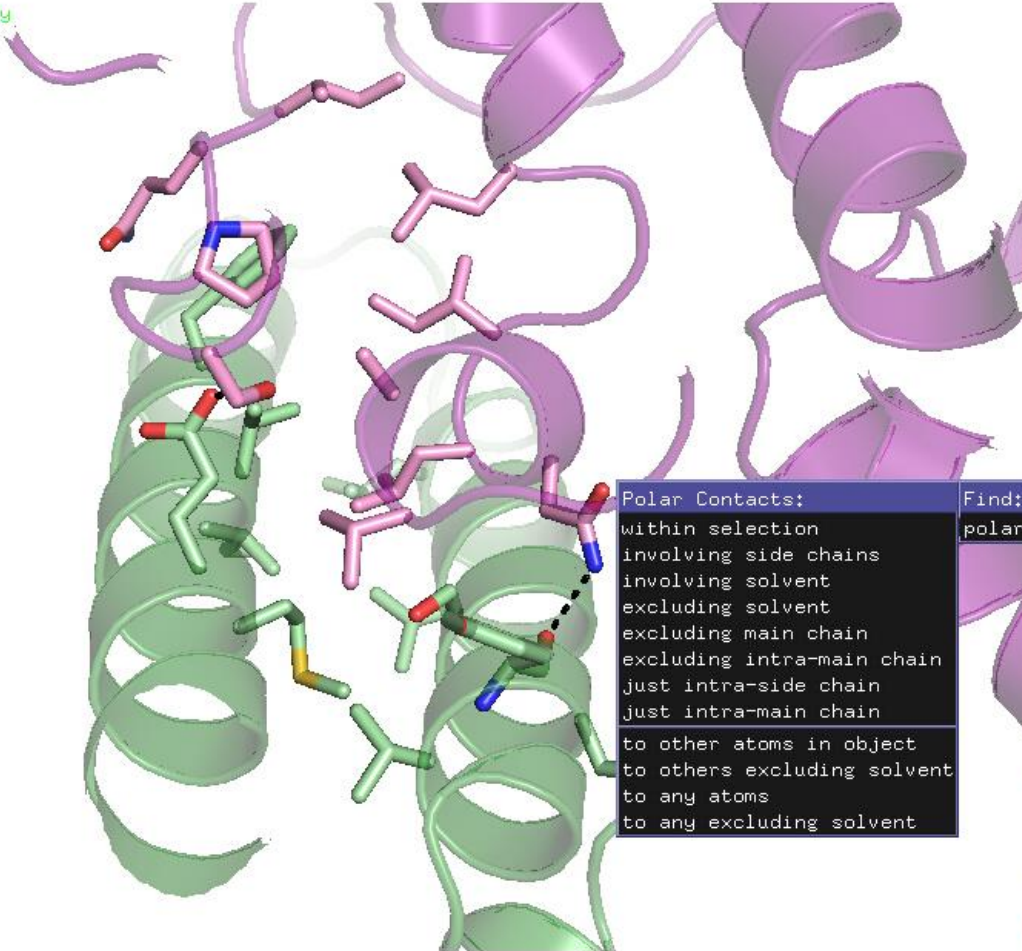
- Quaternary structure analysis
  - Assembly prediction
- Interface analysis
  - Identification of interfaces
  - Calculation of buried area
  - Interface residues

初步的

# Preliminary interaction analysis in PyMOL

PyMOL Viewer

For Educational Use Only



Polar Contacts:

within selection

involving side chains

involving solvent

excluding solvent

excluding main chain

excluding intra-main chain

just intra-side chain

just intra-main chain

to other atoms in object

to others excluding solvent

to any atoms

to any excluding solvent

Find:

polar contacts

all	A	S	H	L	C
refine 1/2	A	S	H	L	C
(RILPL2-interact	A	S	H	L	C
(RILPL2-dimer1)	A	S	H	L	C
(RILP2-dimer2)	A	S	H	L	C
(M5a-R-interact)	A	S	H	L	C
(M5a-M-interact)	A	S	H	L	C
(MELPH-interact)	A	S	H	L	C
final-pi	Action:				
final-pi	zoom				
obj01	orient				
measure0	center				
measure0	origin				
measure0	drag matrix				
(sele)	reset matrix				
	drag coordinates				
	clean				
	preset				
	find				
	align				
	generate				
	assign sec. struc.				
	rename object				
	duplicate object				
	delete object				
	hydrogens				
	remove waters				
Mouse Mo	state				
Buttons	masking				
& Keys	sequence				
Shft	movement				
Ctrl	compute				
CtSh					
SnglClk					
DbClk					
Selecting	Residues				
State	1/ 1				

PyMOL>\_

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▶

S

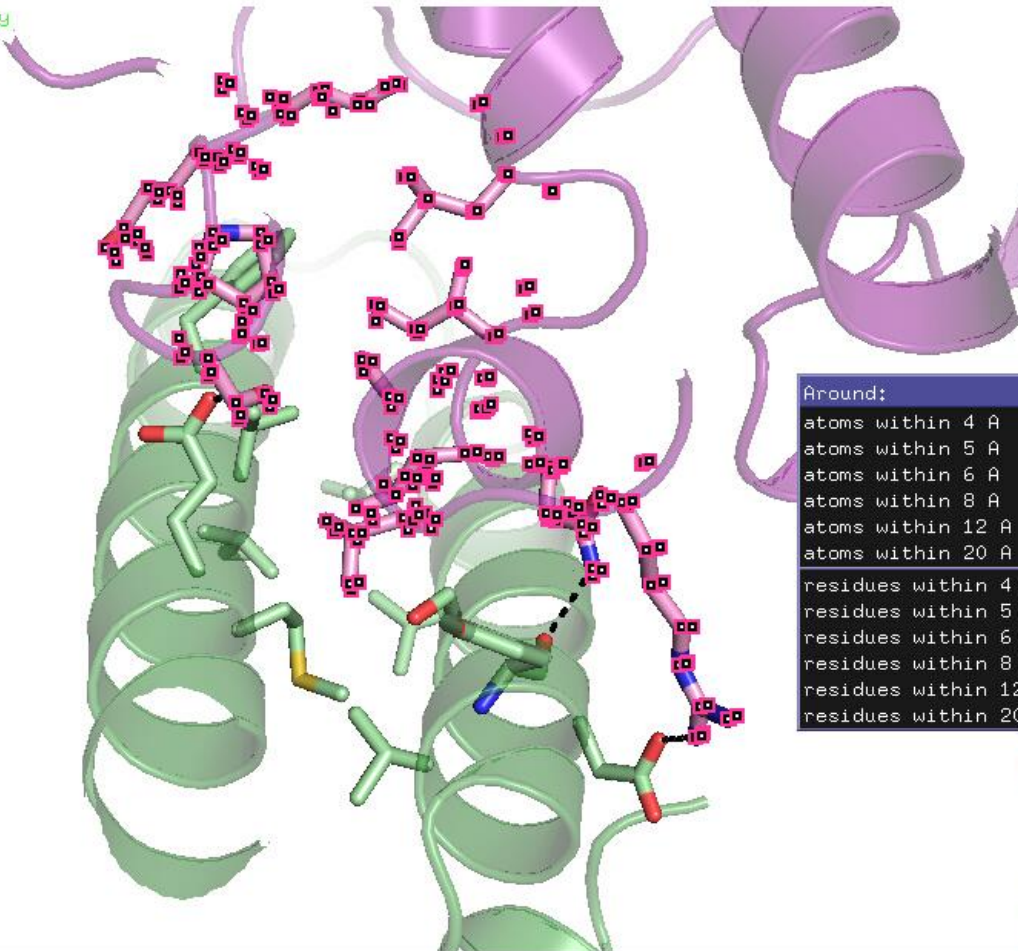
▼

F

# Preliminary interaction analysis in PyMOL

PyMOL Viewer

For Educational Use Only



Around:

atoms within 4 Å

atoms within 5 Å

atoms within 6 Å

atoms within 8 Å

atoms within 12 Å

atoms within 20 Å

residues within 4 Å

residues within 5 Å

residues within 6 Å

residues within 8 Å

residues within 12 Å

residues within 20 Å

Modify:

around

expand

extend

invert

complete

restrict

include

exclude

delete selection

rename selection

zoom

orient

center

origin

drag coordinates

clean

modify

preset

find

align

remove atoms

hydrogens

duplicate

copy to object

extract object

masking

movement

compute

all

refine 1/2

(RILPL2-interact)

(RILPL2-dimer1)

(RILP2-dimer2)

(M5a-R-int)

(M5a-M-int)

(MELPH-int)

final-pi2-

final-pi2-

obj01 1/1

measure01

measure02

Mouse Mode 3-Button Viewing

Buttons L M R Wheel

& Keys Rota Move MovZ Slab

Shft +Box -Box Clip MovS

Ctrl +/- PKAt PK1 MvS2

CtSh Sele Orig Clip MovZ

SnglClk +/- Cent Menu

Db1Clk Menu - PKAt

Selecting Residues

State 1/ 1

PyMOL>

# Automatic interface identification

- The “InterfaceResidues” script in PyMOL
- <http://www.pymolwiki.org/index.php/InterfaceResidues>

# PISA (Proteins, Interfaces, Structures and Assemblies)

- [http://www.ebi.ac.uk/msd-srv/prot\\_int/pistart.html](http://www.ebi.ac.uk/msd-srv/prot_int/pistart.html)
- Structural and chemical properties of macromolecular surfaces and interfaces
- Probable quaternary structures (assemblies), their structural and chemical properties and probable dissociation pattern
- CCP4 PISA
  - [http://www.pymolwiki.org/index.php/Ccp4\\_pisa](http://www.pymolwiki.org/index.php/Ccp4_pisa)
  - Incorporating PISA results into PyMOL



# Tasks

1. Open human hemoglobin structure (PDB id: 2HHB) in PyMOL
2. Analyze the interfaces between alpha- and beta-subunit manually in PyMOL
  - Polar interaction
  - Hydrophobic interaction
3. Use “InterfaceResidues” in PyMOL to calculate the interfaces
  - Compare with your own analysis, which one gives better result?
4. Use PISA server to calculate the assembly and interfaces in human hemoglobin
  - Compare the results with those in previous two steps
5. Present the PISA results in PyMOL



# Lab report format

- Title
- Your name and student No.
- Introduction
- Methods
- Results
- Conclusions