BIOL 555

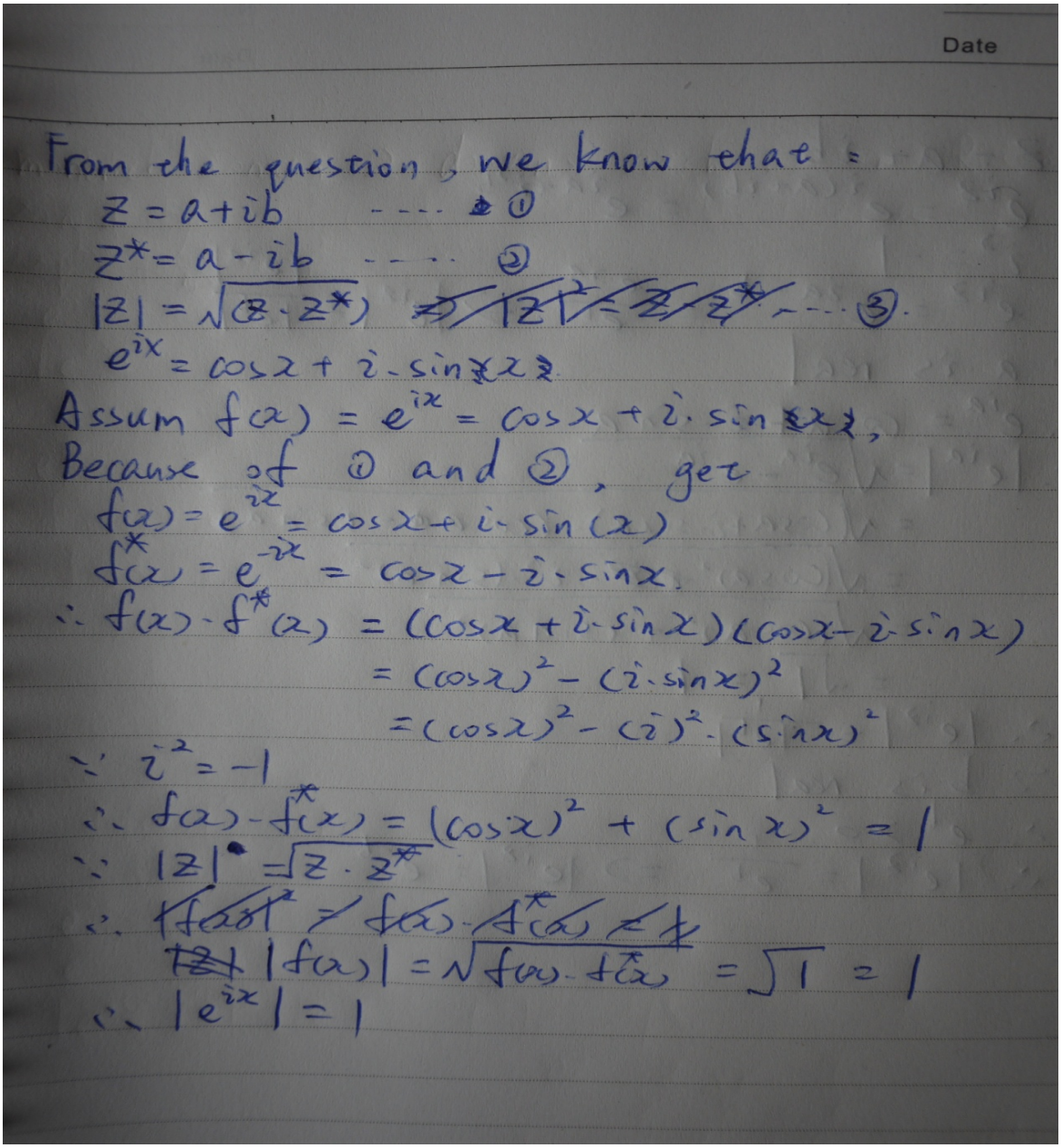
Final

Chunlei Chen

A20272196

1.

1)



2)

Date

$\because z = a + ib$

$\therefore e^{iz} = e^{i(a+ib)} = e^{ia+i^2b}$

$\because i^2 = -1$

$\therefore e^{iz} = e^{ia-b} = \frac{e^{ia}}{e^b} \Rightarrow |e^{iz}| = \frac{|e^{ia}|}{|e^b|}$

$\because a$ is real

$\therefore e^{ia} = \cos a + i \cdot \sin a$

$\therefore |e^{ia}| = \sqrt{e^{ia} \cdot e^{-ia}}$

$= \sqrt{(\cos a + i \cdot \sin a) \cdot (\cos a - i \sin a)}$

$= \sqrt{(\cos a)^2 - i^2 \cdot (\sin a)^2}$

$= \sqrt{(\cos a)^2 + (\sin a)^2}$

$= \sqrt{1} = 1$

$\therefore |e^{iz}| = \frac{1}{|e^b|}$

$\because b$ is real

$\therefore e^b > 0$

$\therefore |e^{iz}| = \frac{1}{e^b} \Rightarrow |e^{ia}| = e^{-b}$

2.

1) Orthorhombic

2) 2-fold axis: along the Z direction

2-fold screw axes: along with X and Y directions.

3)

(u,v,w)=(x,y,z)-(-x,-y,z)=(2x,2y,0)

(u,v,w)= (x, y, z)- (-x+1/2, y+1/2, -z) = (2x-1/2, -1/2, 2z)

(u,v,w)= (x, y, z)- (x+1/2, -y+1/2, -z).= (-1/2, 2y-1/2, 2z)

3.

In this part, MM domain is as object. It is the MM domain of PIN1. This domain has 39 amino acids. The similarity of NMR and x-ray is the structure is an antiparallel beta-sheet is composed by three beta-strands.

In the method of X-ray with resolution is 1.90Å, the structure shows difference in different resolution. And Loop 1 of the domain has an unusual conformation.

In the method of NMR, it use distance geometry simulated annealing to refinement. Through NMR, the binding element can be acquired. And it can show the loop 1 is intrinsically flexible. In addition, NMR can provide the data of chemical shift which produce of aromatic ring and 20 favorable WW conformers.

Reference

[1] Wintjens, R., Wieruszeski, J.M., Drobecq, H., Rousselot-Pailley, P., Buee, L., Lippens, G., Landrieu, I..^{1}H NMR study on the binding of Pin1 Trp-Trp domain with phosphothreonine peptides. (2001) J.Biol.Chem. **276:** 25150-25156.

[2] Verdecia, M.A., Bowman, M.E., Lu, K.P., Hunter, T., Noel, J.P.Structural basis for phosphoserine-proline recognition by group IV WW domains. (2000) Nat.Struct.Biol. 7: 639-643

[3] Mark A. Verdecia, Marianne E. Bowman, Kun Ping Lu3, Tony Hunter4 and Joseph P. Noel. Structural basis for phosphoserine-proline recognition by group IV WW domains.(2000) Nat.Struct.Biol. 7: 639-643

4.

1)

No affect. Although it will affect the original structure amplitudes, this error do not affect refinement structure amplitudes. Only small part is error, most of it is correct is can be refinement by refinement tools. Structure is made to better fit the electron density after refining it.

2)

Through careful check by Fo-Fc can help find new atom and delete “error” atom. Atom can be refining after find all un- hydrogen atoms. The position of hydrogen can be confirmed or can be calculated. We also can refine the rest part again and again after extract 5% of structure until no error can be found.

5.

Molecular replacement is straightforward. It does not need to prepare heavy atom derivatives and does not need to collect their data. Model building is simplified. The disadvantage is that the model must sit in the correct orientation and absolute position with the unit cell. This method also can makes irreparable mistake.

MIR or MAR needs a heavy-atom and use tools to collect data. The process is so complex. However, the error is so small. It is only us one sample.

6.

1) Helical twist
2) Roll
3) Rise
4) Slide
5) Tilt
6) Propeller twist
7) Stagger
8) Stretch
9) Shear
10) Buckle
11) Propeller twist
12) Opening

7.

1) The long-spacing repeat distance is 232 nm

2) Come from Troponin Bridges.

3) The intensity will change. It will cause diffraction pattern change. The distance between the two layer lines will change.

8.

1)

Quantum Models (picoseconds)

Atomistic models (microseconds)

Coarse-grained/Mean-field Models (milliseconds)

Mechanical Models (seconds)

Kinetic Models (hours)

2)

For various time scales, the computational tools being able to use are mechanical models, kinetic models and so on because they are modeled based on Hamiltonian mechanics which can be used in various coordinates and therefore in various time scales.

First, we can get structure simulation from the pico-second models (quantum models) combined with the experimental data. Then by calibrating the the previous models and the experimental data, we can replace

this combination with atomistic models (microseconds). Again, by combining this atomistic models with experimental models and calibrate to get another Coarse-grained/Mean-field models (milliseconds). Next, by calibrating atomistic models with mean-field models, we get kinetic models which is a longer time scales.

Thus, by replacing the structure simulation and the experimental data and calibrate them to a relatively longer time scale models such as atomistic models and so on and by repeating this process until we get to the kinetic models, the results derivable at the longer time scales can be informed from the results at the faster time scales.

9.

1)

Through these data, I can get Guinier plot (Figure 1) through the formula:

$$\ln I_{l\text{-}b}=(-R_g^2/3)*q^2+\ln I.$$

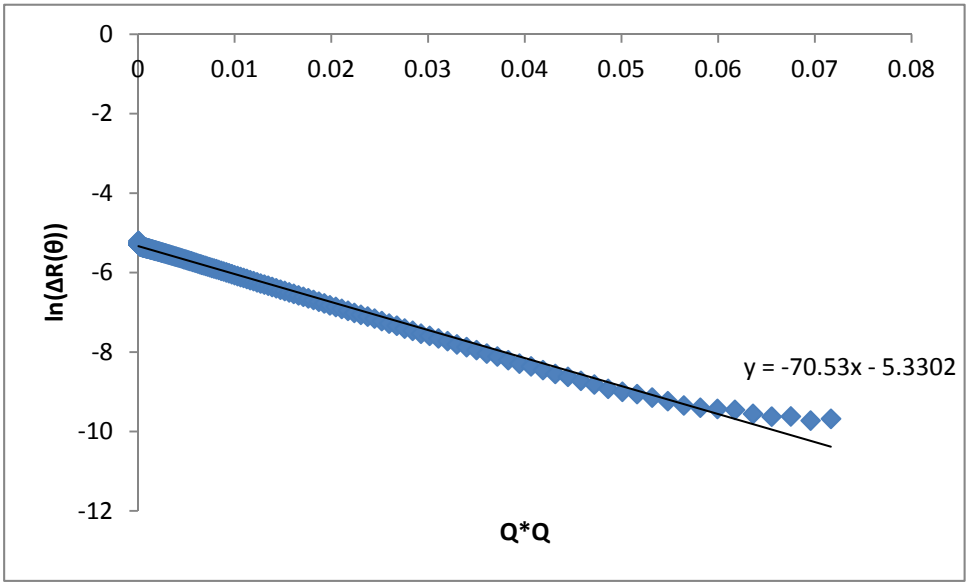


Figure 1(Q value from 0.00689 to 0.267701)

Then slop is $R_g^2/3$, so $R_g^2/3=70.53$.

The R_g estimated value is 14.5461 Å.

Because $Rg*Q_{max}< 1.3$, $Q_{max}<1.3/(R_g)=0.0893$.

Then through the new data I get another Guinier plot(Figure 2)

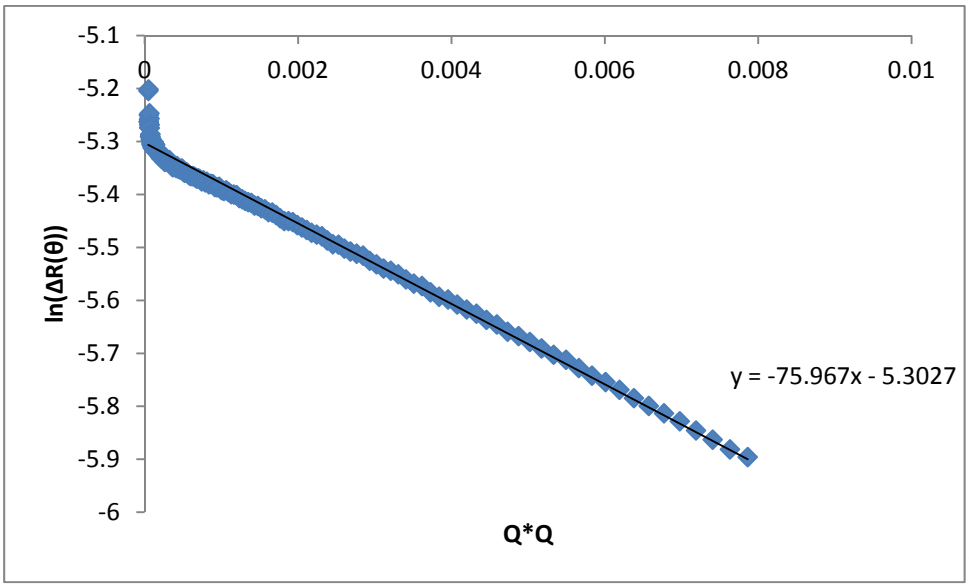


Figure 2

Then slop is $R_g^2/3$, so $R_g^2/3=75.967$.

The more accurate value of R_g is 15.0964 Å at $0.00689<Q_{max}<0.0893$

2)

Because $R_g^2=3/5*r^2$, $R_g=15.0964$,

r=15.0964 Å

3)