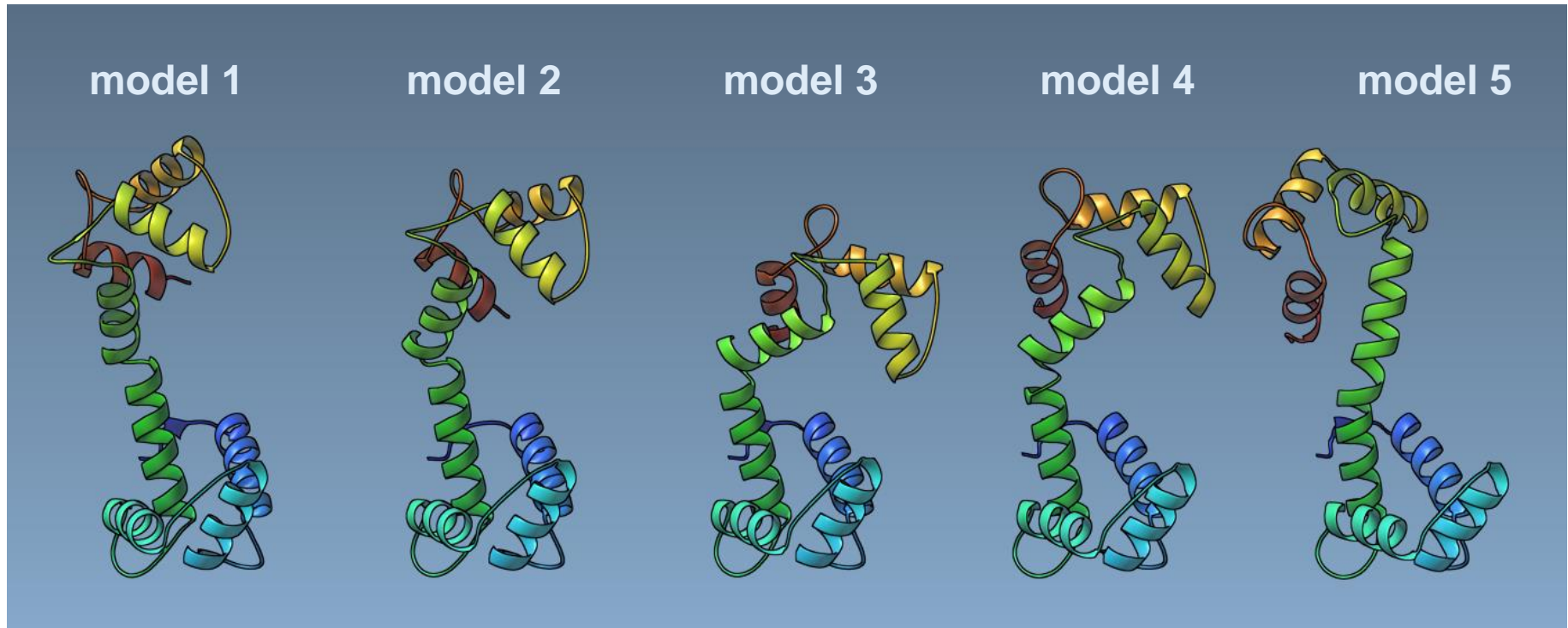


# **Pepsi-SAXSを使用したタンパク質予測構造の評価 (SAMSON connectを使用)**

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AlphaFoldにより、ヒトCalmodulin-1の構造について5つのモデルを得ました。

# Pepsi-SAXSツールの起動

test.sam - SAMSON 2022 R2

Workspace Complete Home Edit Select Visualization Animation Biology Apps Editors Interface Help Professional Edition Send feedback Find everything (Shift+E)

1Å Add apps All (21) Assembly (1) Biology (11) Chemistry (3) General (12) Materials (3) Medicine (1) Visualization (1)

Extend All apps

test.sam Filter nodes... (Shift+F) Look in All nodes

Selection filter Atoms and bonds Quick access

PEPSI SAXS

Experimental curve C:/Users/Public/Downloads/SASDNX3 (1).dat Browse...

Curve

Save Fit the figure

Output scattering curve path Enter the path to output file Browse...

Expansion order Units  Number of points Max. angle  Number of CPU's

20 1/Å, 4πsin(θ)/λ 51 0.50 1

Run program Run  Auto-update  $\chi^2$ :

Info

```
-----Authors: XXX-----^
-----References: XXX-----^
^-----Copyright (c): NANO-D team, Inria/CNRS Grenoble, France &-----^
^-----Laboratory of Advanced Studies of Membrane Proteins,-----^
^-----MIFT Moscow, Russia,-----^
^-----2012 - 2014,-----^
^-----e-mail: sergei.grudinin@inria.fr-----^
^-----^
```

SASDNX3 (SASBDB)

**Pepsi-SAXSツールを起動し、  
SAXS実験で得られた散乱曲線のデータを指定します。**

# 各モデルから計算される曲線と実験曲線の比較

The screenshot displays the SAMSON 2022 R2 software interface. The main window shows a protein structure (CALM\_b5361\_unrelaxed\_rank\_005\_alpha) rendered as a ribbon model. The left sidebar contains a tree view of nodes, with the current selection highlighted. The right sidebar shows the SAXS analysis panel, including the experimental curve plot, output scattering curve path, and run parameters. The  $\chi^2$  value is displayed as 3.91152.

test.sam - SAMSON 2022 R2

Workspace: Complete | Home | Edit | Select | Visualization | Animation | Biology | Apps | Editors | Interface | Help

Professional Edition | Send feedback | Find everything (Shift+E)

Selection filter: Atoms and bonds

PEPSI SAXS

Experimental curve: C:/Users/Public/Downloads/SASDNX3 (1).dat

Curve: [Plot showing experimental curve and fit]

Output scattering curve path: [Input field]

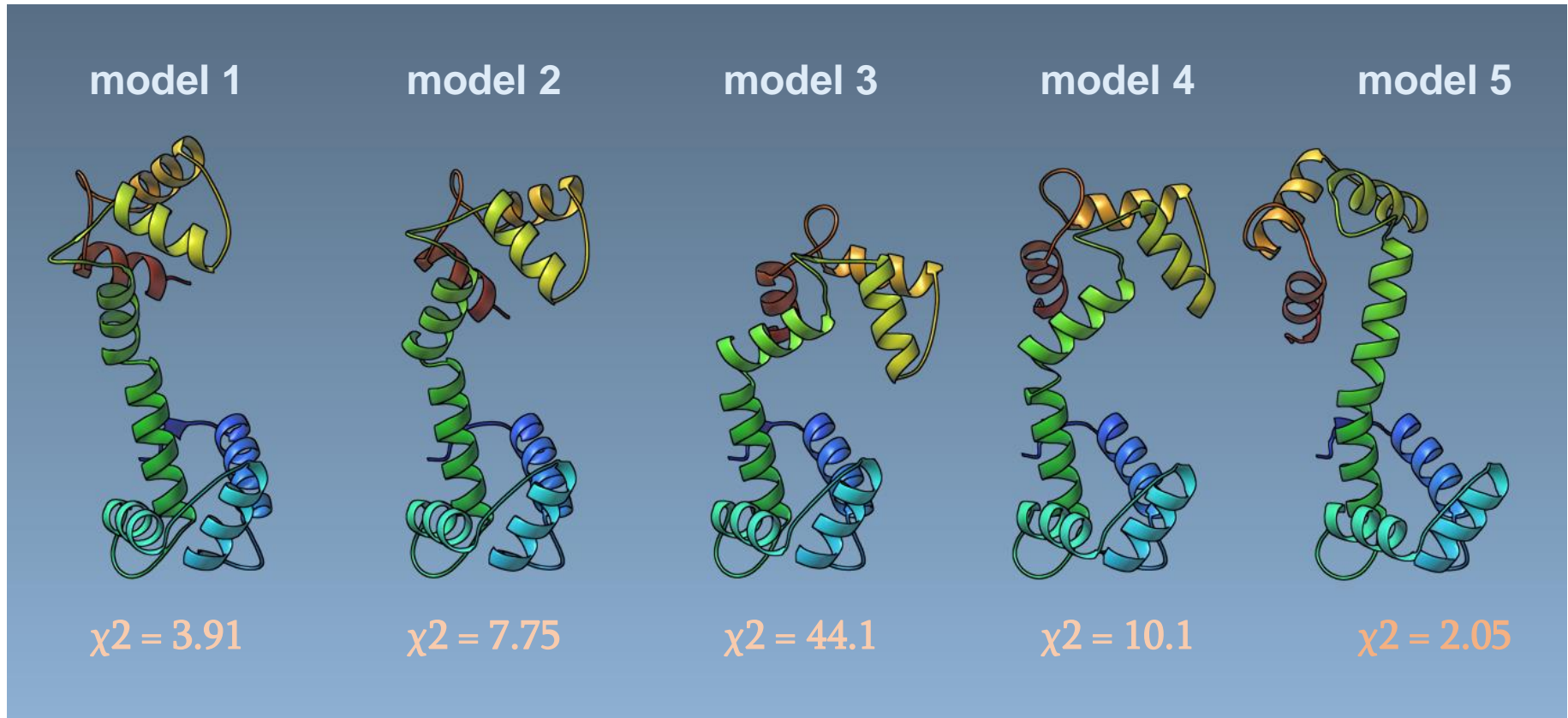
Expansion order: 20 | Units: 1/Å, 4πsin(θ)/λ | Number of points: 51 | Max. angle: 0.50 | Number of CPUs: 1

Run program: Run | Auto-update |  $\chi^2$ : 3.91152

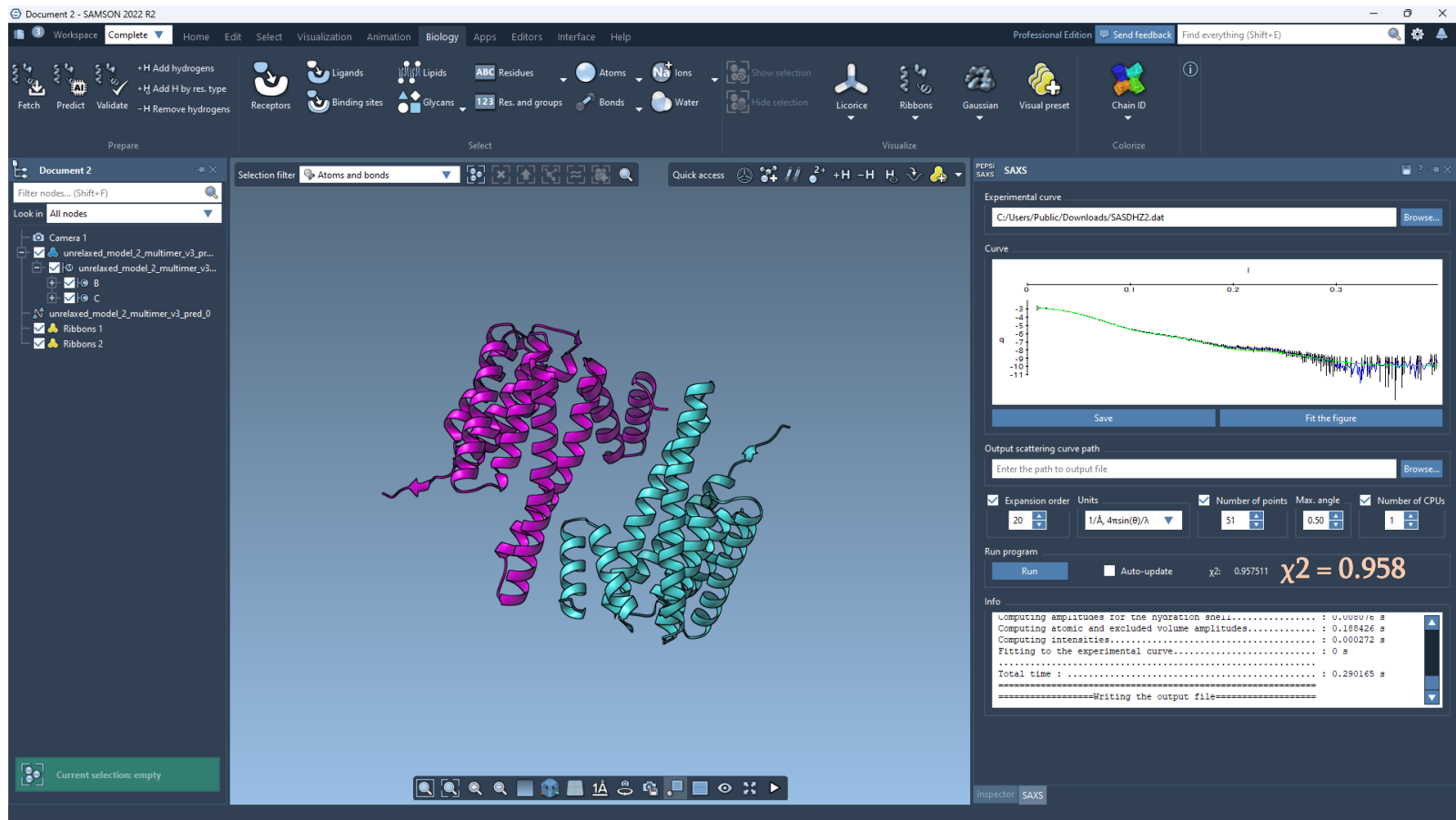
Info:

```
Computing amplitudes for the hydration shell..... : 0.044209 s
Computing atomic and excluded volume amplitudes..... : 0.048916 s
Computing intensities..... : 0.000231 s
Fitting to the experimental curve..... : 1e-06 s
Total time : : 0.205809 s
=====Writing the output file=====
```

model 1を選択した状態で“Run”をクリックすると、  
model 1の構造から計算した散乱曲線、  
および実験で得た散乱曲線との一致度 ( $\chi^2$ ) が表示されます。



他のモデルについても同様に計算を行うと、今回得られたモデルの中では、**model5が溶液中（2mM Ca<sup>2+</sup>）での構造に近いことが分かります。**



SASDHZ2 (SASBDB)

また、AlphaFold-Multimerで予測した複合体構造の妥当性を、実験で得られた散乱曲線に基づいて評価することなども可能です。

## SAMSON connectについて

- **HP**

<https://filgen.jp/Product/BioScience21-software/OneAngstrom/index.html>

- **YouTube**

<https://www.youtube.com/watch?v=reRD38RTI6E>

<https://www.youtube.com/watch?v=GZzJy4cS7o4>

<https://www.youtube.com/watch?v=YG4JXf6v75o>

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