

# **Electron microscopy data in PDB and EMDB - deposition and browsing**

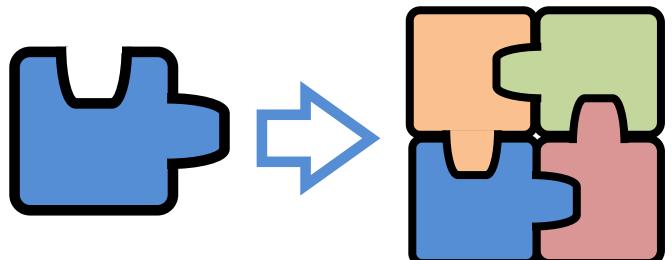
**EMDBとPDBにおける電子顕微鏡データ  
– 登録と閲覧**

**Hirofumi Suzuki**

**BSJ-2016 luncheon seminar  
2016-11-27**

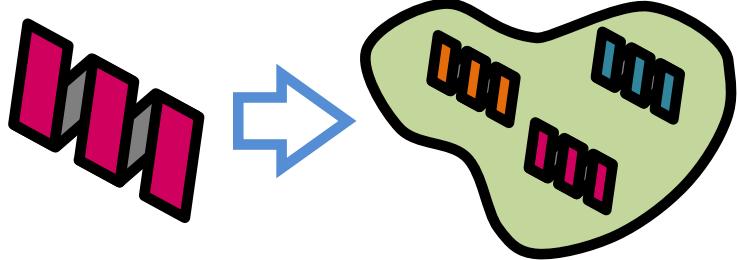
# Multi things going multi

## Methodology



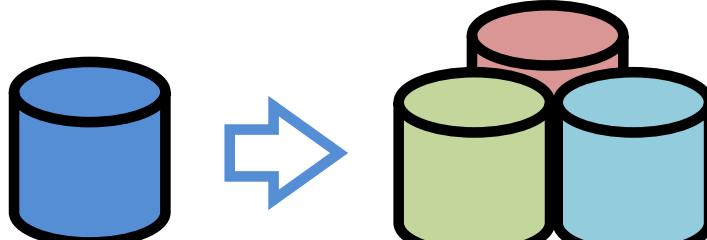
X-ray/NMR,  
alone              + 3DEM, etc.,  
                        hybrid

## Scale



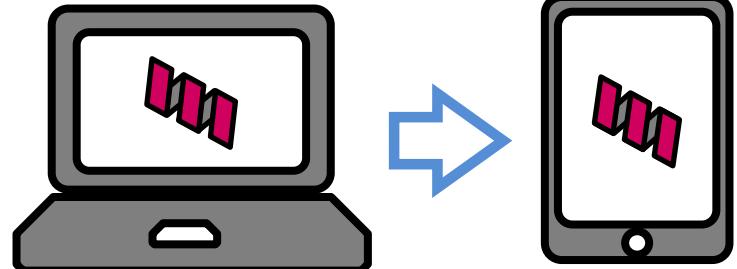
molecule              + complex,  
                        organelle, etc.

## Databank



PDB              + EMDB, BMRB,  
                        SASBDB, etc.

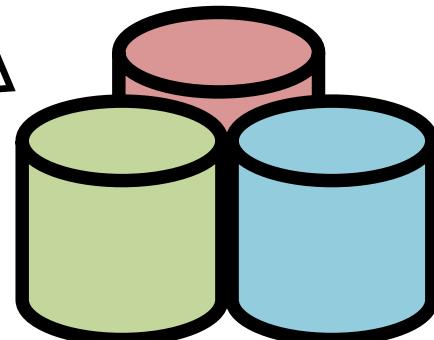
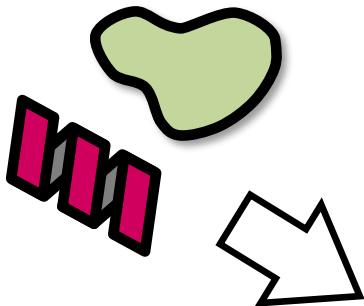
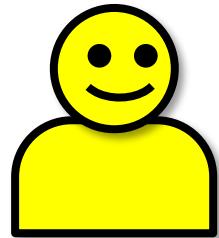
## Browsing device



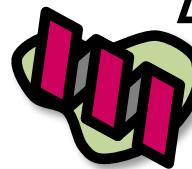
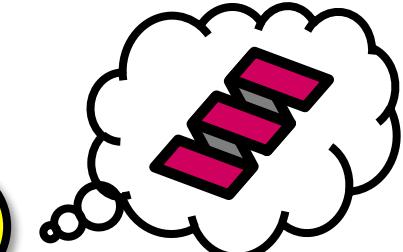
PC              + phone,  
                        tablet

# One for the multi

**Deposition**



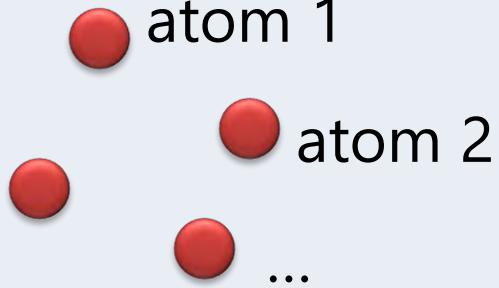
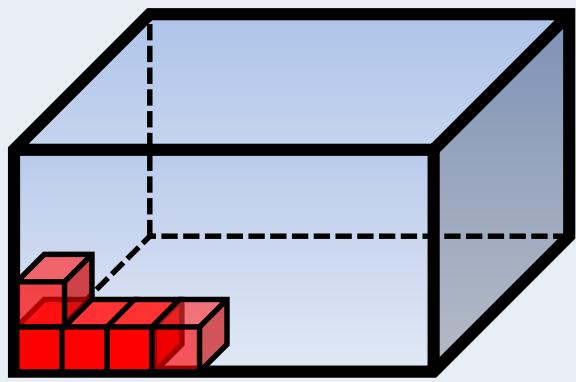
**Search & browse**



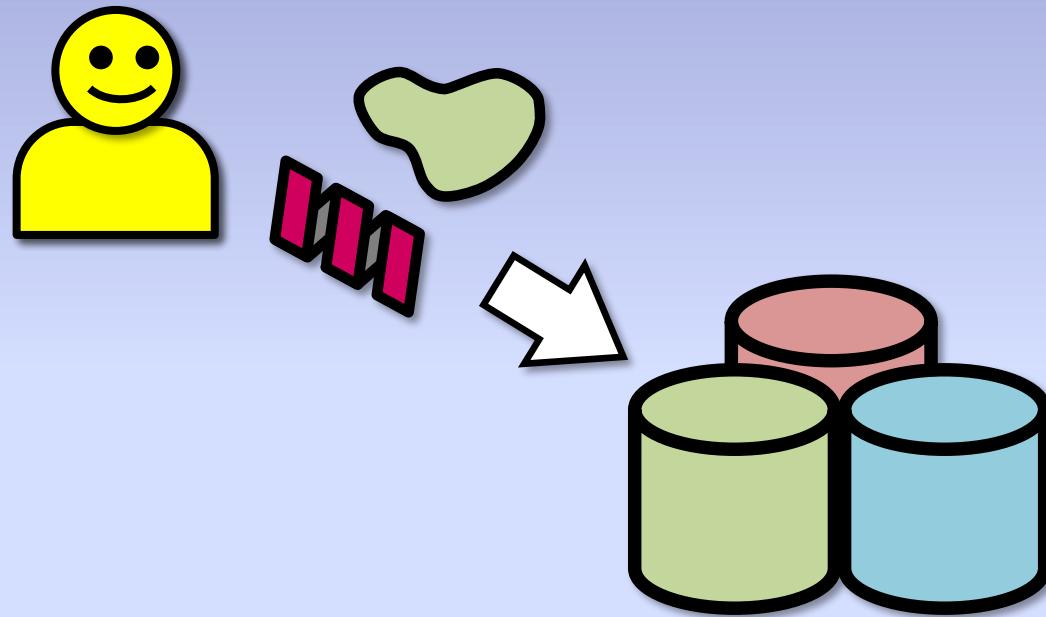
**Comparison**

**Structure viewing**

# PDB vs. EMDB

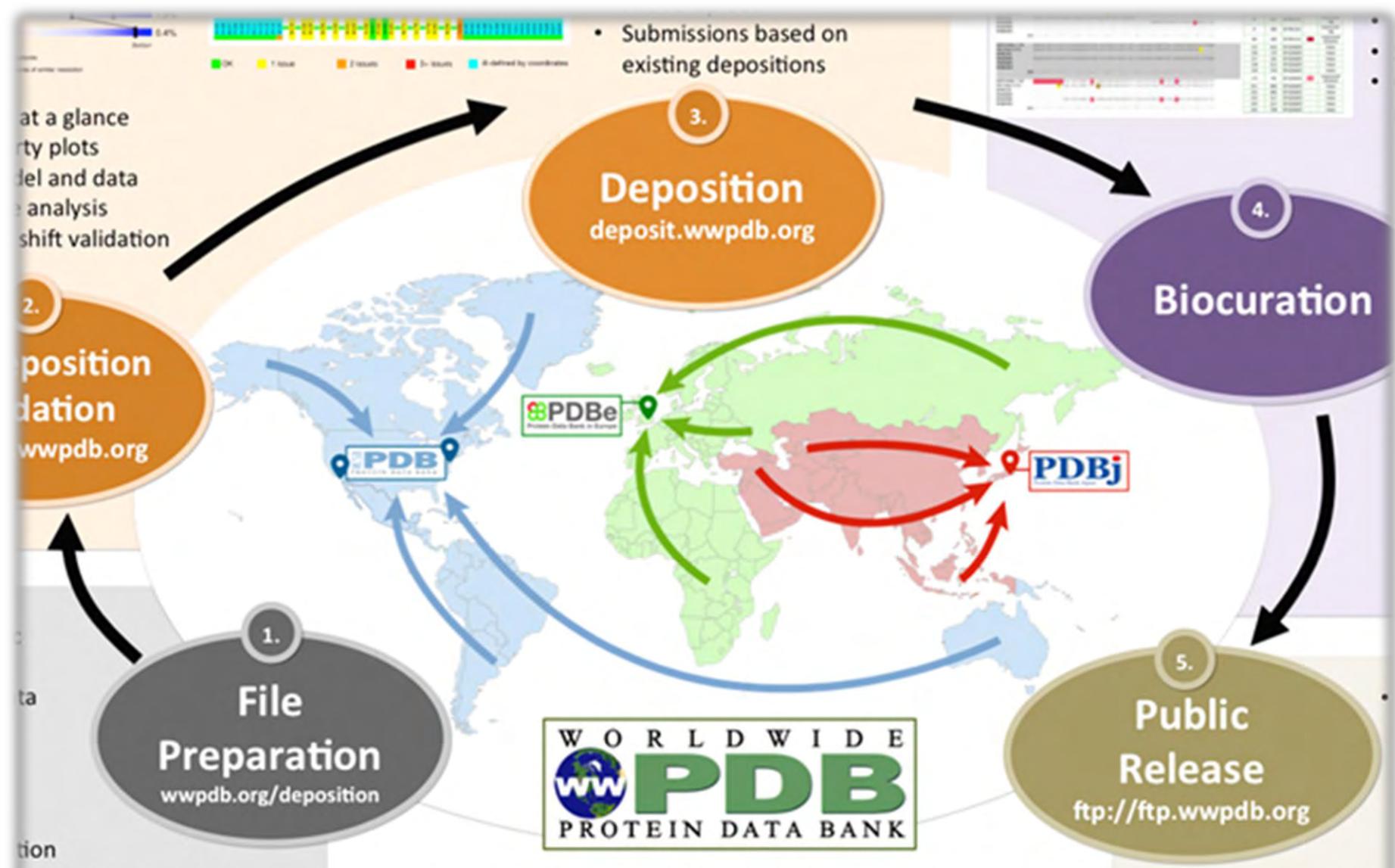
		
method	various	EM
main data	atomic model 	3D map ( $\div$ ED map)  voxels 1,2,3...
num. of entries	$\sim 124,000$	$\sim 4,500$

# Deposition:



*OneDep*

# OneDep: One for ...



# One for 3 databanks

OneDep wwPDB OneDep System FAQ Tutorials

Deposition ID  
Your e-mail address  
Password (optional, or we will provide one)  
This is a shared "group password"  
(6 to 16 alphanumeric characters)

Country: Japan Reset country

Experimental method:

- X-Ray Diffraction
- Electron Microscopy
- Solution NMR
- Neutron Diffraction
- Electron Crystallography
- Solid-state NMR
- Fiber Diffraction

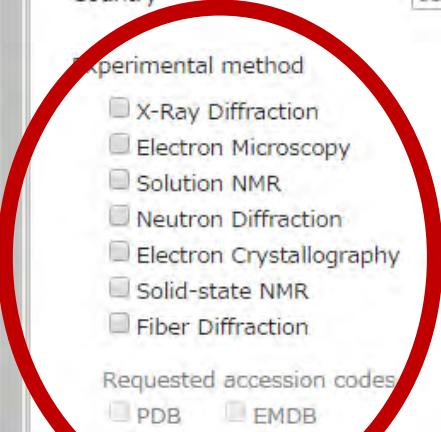
Requested accession codes:

- PDB
- EMDB
- BMRB

Structural genomics: No

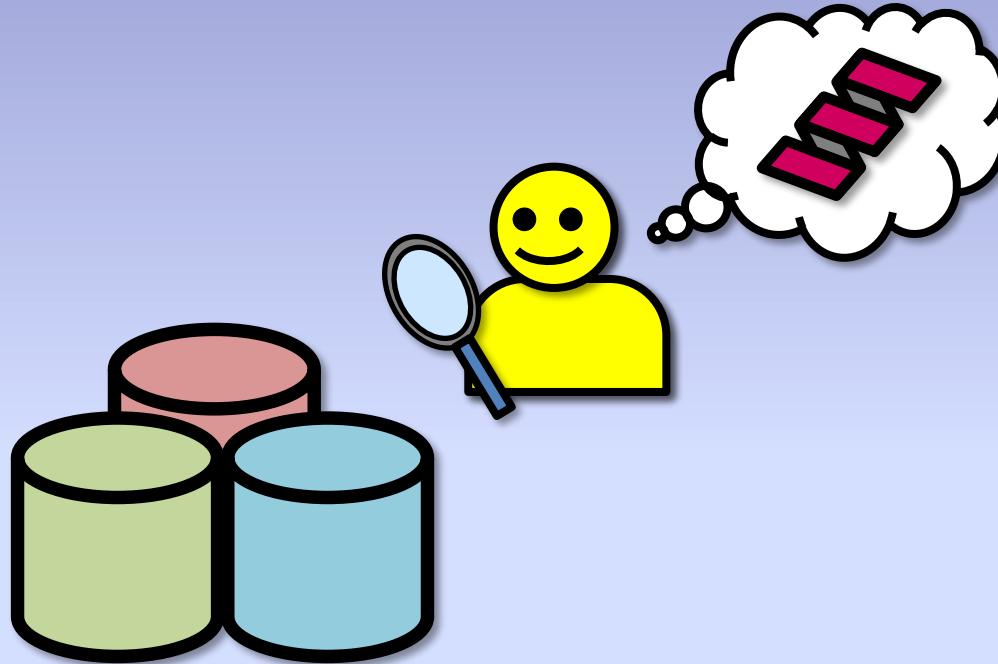
Please copy this code: 19128

Start deposition



Checkboxes for Methods & databanks

# Search & browse:



*EM Navigator,  
& Omokage search*

## EM Navigator

- 3DEMデータを見る -

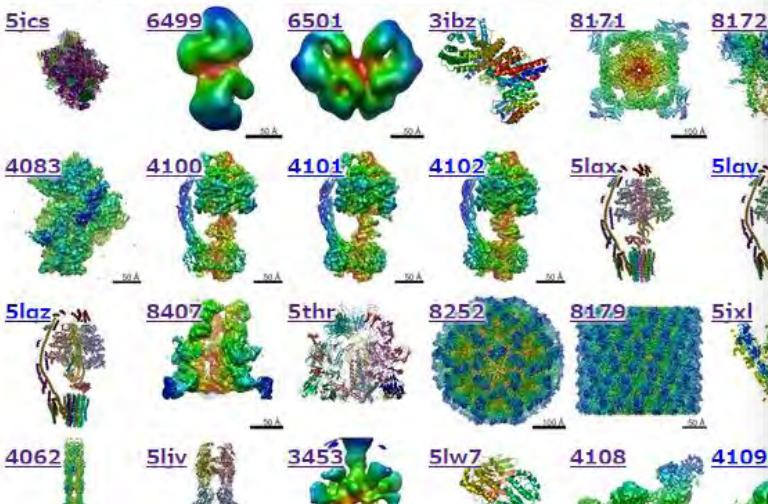
- キーワード / EMDB-ID / PDB-ID

送信

- [EM Navigator旧バージョン](#)
- [詳細な検索、表形式による表示など](#)
- [Omokage検索 - 形状が似ている構造データを探す](#)
- [万観 - EMDB/PDBの付随情報と構造ビュアを統合](#)
- [ギャラリー](#) [統計情報](#) [3DEM文献](#) [生物種](#)

### 最近公開されたデータ

- 2016年11月16日 (EMDB: 18, PDB: 9)



EMN Search

## EM Navigator

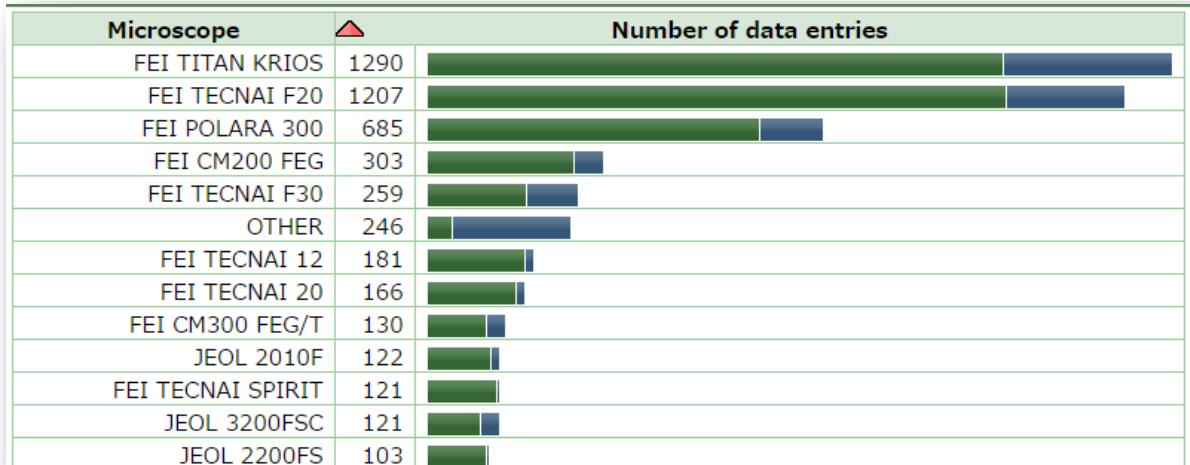
### Search result

Showing 1 - 50 of 257 items for keywords: test

DB-ID	Data Release Date	Aggregation State	Resolution Method
<a href="#">EMDB-1133</a>	2005-06-07	particle	FSC 0.333
<a href="#">EMDB-1134</a>	2006-07-01	particle	3D SSNR = 1
<a href="#">EMDB-1136</a>	2005-07-21	particle	FSC 0.333
<a href="#">EMDB-1137</a>	2005-07-21	particle	FSC 0.333
<a href="#">EMDB-1144</a>	2005-09-02	particle	FSC 0.333
<a href="#">EMDB-1145</a>	2005-09-02	particle	FSC 0.333
<a href="#">EMDB-1165</a>	2006-09-28	particle	FSC 0.5
<a href="#">EMDB-1316</a>	2007-06-25	filament	5.0
<a href="#">EMDB-1317</a>	2007-01-30	particle	FSC 0.5
<a href="#">EMDB-1418</a>	2008-01-02	particle	FSC 0.5
<a href="#">EMDB-1437</a>	2008-04-23	particle	FSC
<a href="#">EMDB-1457</a>	2008-06-24	particle	FSC 0.5
EMDB-1458			

# Statistics

10



Microscope hit-chart

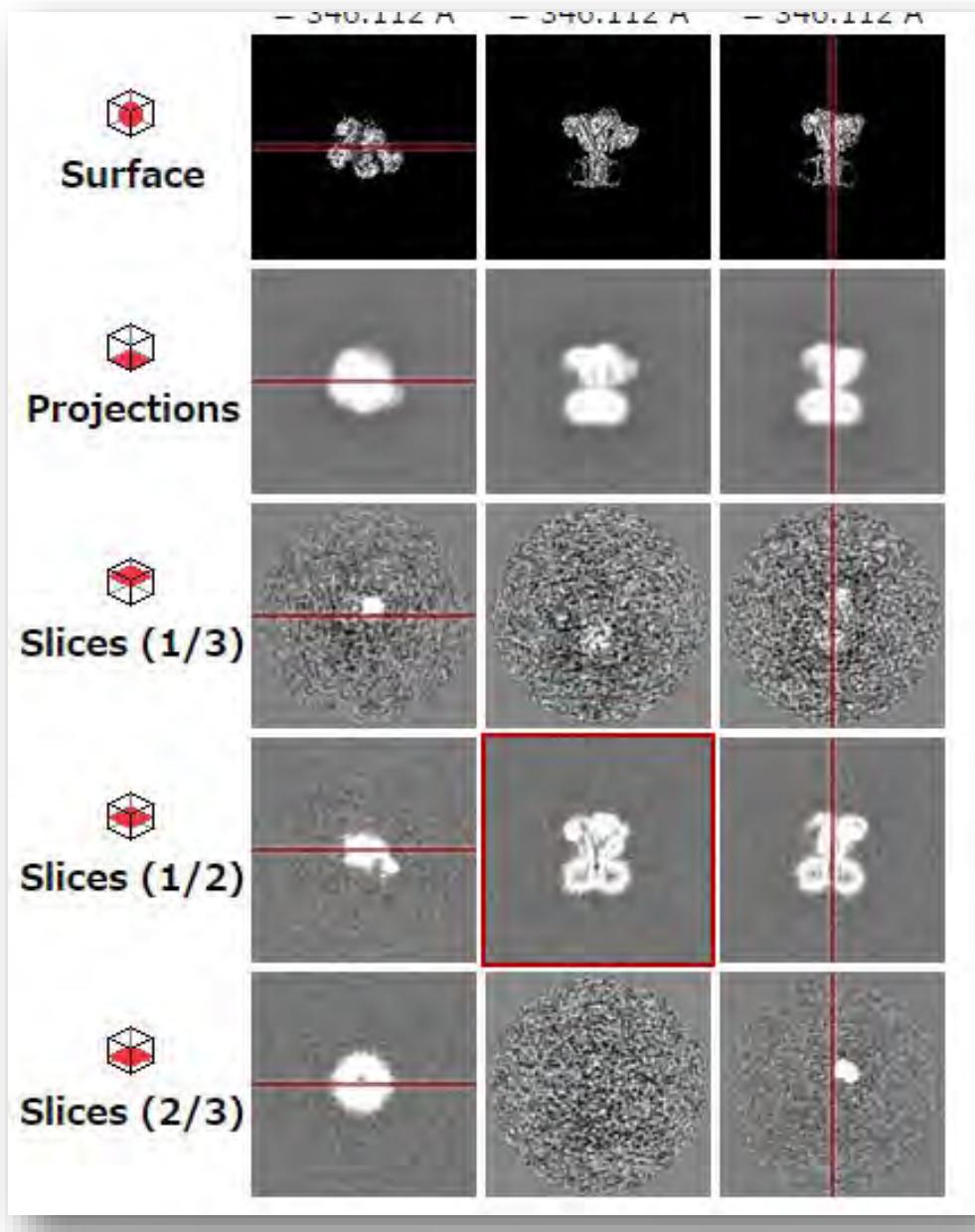
"Resolution revolution"

## Resolution

Year

Year	~ 2 Å	~ 3 Å	~ 5 Å	~ 7 Å	~ 10 Å	~ 15 Å	~ 23 Å	~ 34 Å	~ 51 Å	~ 77 Å	~ 115 Å	Total
2016	14	24	425	145	146	77	115	88	25	8	1092	
2015	4	21	332	70	127	81	130	85	44	7	3	978
2014	1	4	105	56	144	69	142	139	57	76	2	818
2013		1	45	41	106	94	144	96	70	19		653
2012			18	31	87	60	121	75	58	9		493
2011		1	10	11	79	78	88	46	13	9	3	355
2010		1	23	23	59	69	53	54	16		3	327
2009		1	16	13	43	46	43	21	5			198
2008			8	8	39	36	52	36	15	1		214
2007			3	3	45	37	40	26	12	1		175
2006			1		23	37	44	38	7	2		156
2005	1		1		19	26	35	20	1	2		106
2004		1	2	3	11	23	16	3			1	60
2003			3	1	9	21	10	26	3			75

# Projections & sections



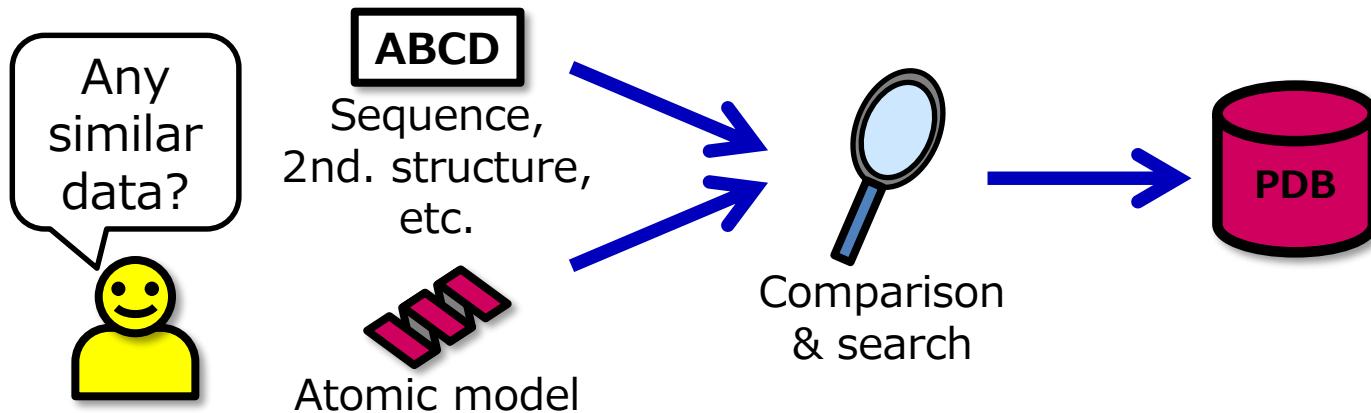
**For each the data**  
 (except for some huge raw tomogram)

**can see background noise in sections**

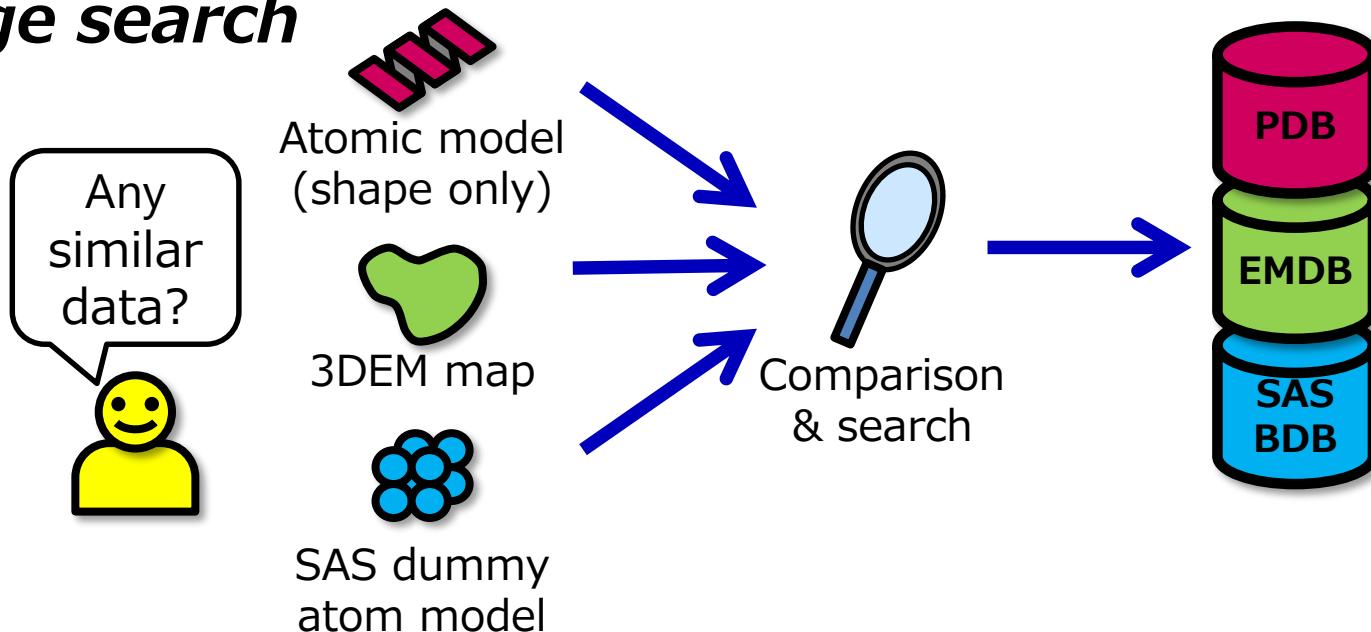
**can peep (盗み見)...**

- type of real-space mask
- CTF amplitude correction
- etc.

## Typical structure search (e.g. Structure Navigator of PDBj)



## *Omokage search*



# Omokage search

★ Omokage search - Shape similarity search of macromolecules -

- Search query

Query structure data: [Registered data structure in databanks](#) [Upload your original/modified data](#) **file upload**

ID of EMDB, PDB or SASBDB:  **ID input box** [Search](#) [?](#)

Samples: [Recommended](#) [EMDB](#) [PDB](#) [SASBDB](#)

Structure data giving symbolic results [Show details](#)

50 Å 100 Å

**Sample data**

# Search results

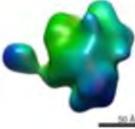
RNAP II  
@25A res.

EMDB  
entries

PDB  
entries

**Subject structure**

Database: EMDB / ID: 2190  
human RNA polymerase II in complex with AluRA RNA  
[Quick](#), [Yorodumi](#), [EM Navigator](#)



5 Å

**Search result**

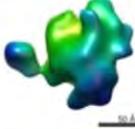
Showing 1 - 100 of 2,000 structures found from all (198,117 structures)

Pages: 1 2 3 4 10 20 Previous Next

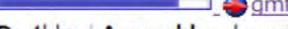
Display: images only as list

#1 Score: 0.8984  gmfit

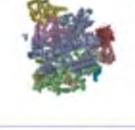
Database: EMDB / ID: 2191  
human RNA polymerase II in complex with B2 RNA  
[Quick](#), [Yorodumi](#), [EM Navigator](#), [Omokage search](#)



5 Å

#2 Score: 0.8598  gmfit

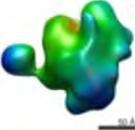
Database: PDB / ID: 4bbf / Assembly: deposited form  
Structure of RNA polymerase II-TFIIB complex  
[Quick](#), [Yorodumi](#), [Omokage search](#)



5 Å

#3 Score: 0.8597  gmfit

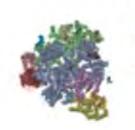
Database: EMDB / ID: 2192  
human RNA polymerase II in complex with B2 81-131 RNA  
[Quick](#), [Yorodumi](#), [EM Navigator](#), [Omokage search](#)



5 Å

#4 Score: 0.8554  gmfit

Database: PDB / ID: 3k1f / Assembly: deposited form  
Crystal structure of RNA Polymerase II in complex with TFIIB  
[Quick](#), [Yorodumi](#), [Omokage search](#)



5 Å

#5 Score: 0.8535  gmfit

Database: PDB / ID: 2r92 / Assembly: deposited form  
Elongation complex of RNA polymerase II with artificial RdRP scaffold  
[Quick](#), [Yorodumi](#), [Omokage search](#)



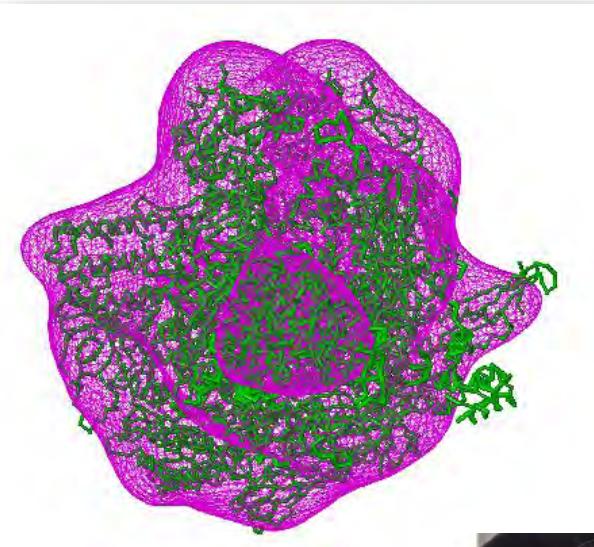
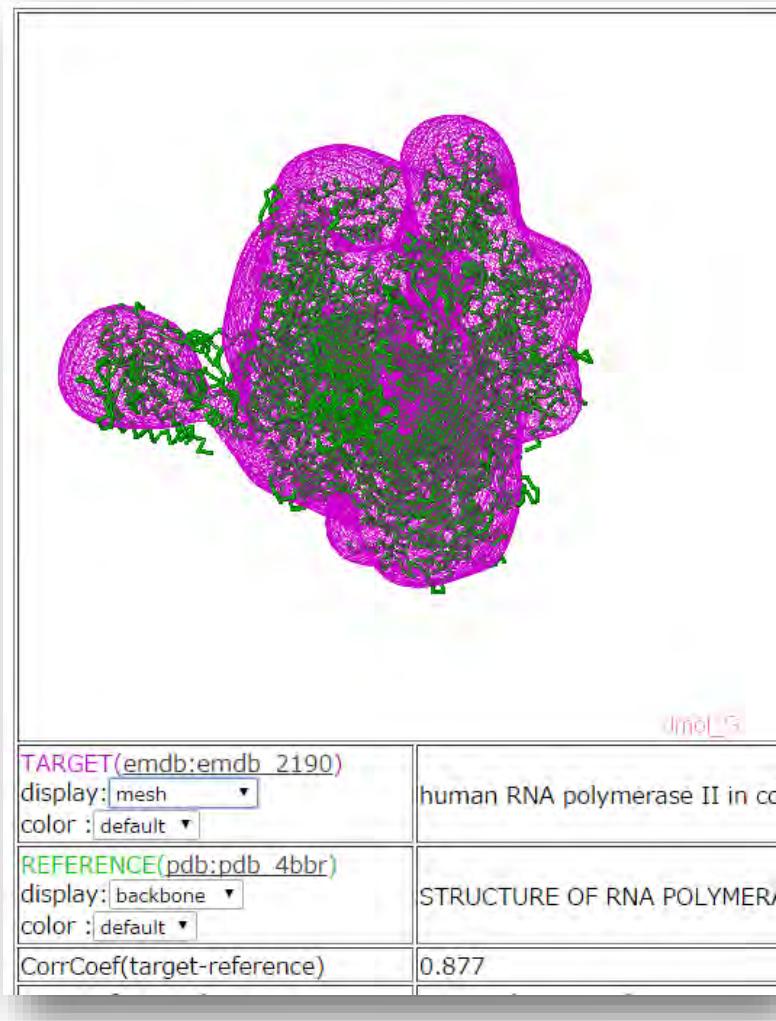
5 Å

similarity  
score

"view fitting"  
link to gmfit

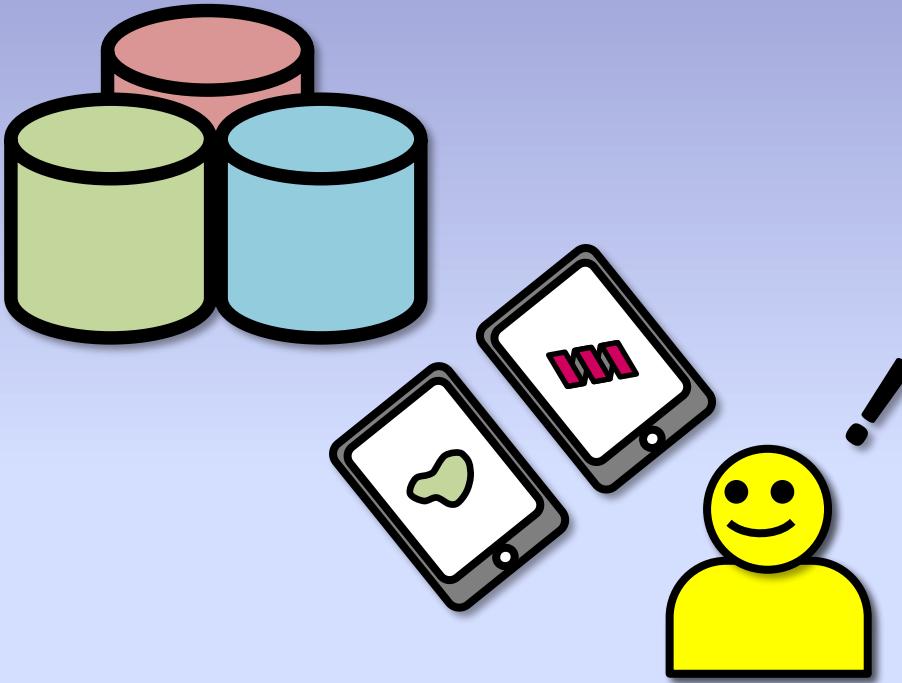
## Fitting by *gmfit*

Side view



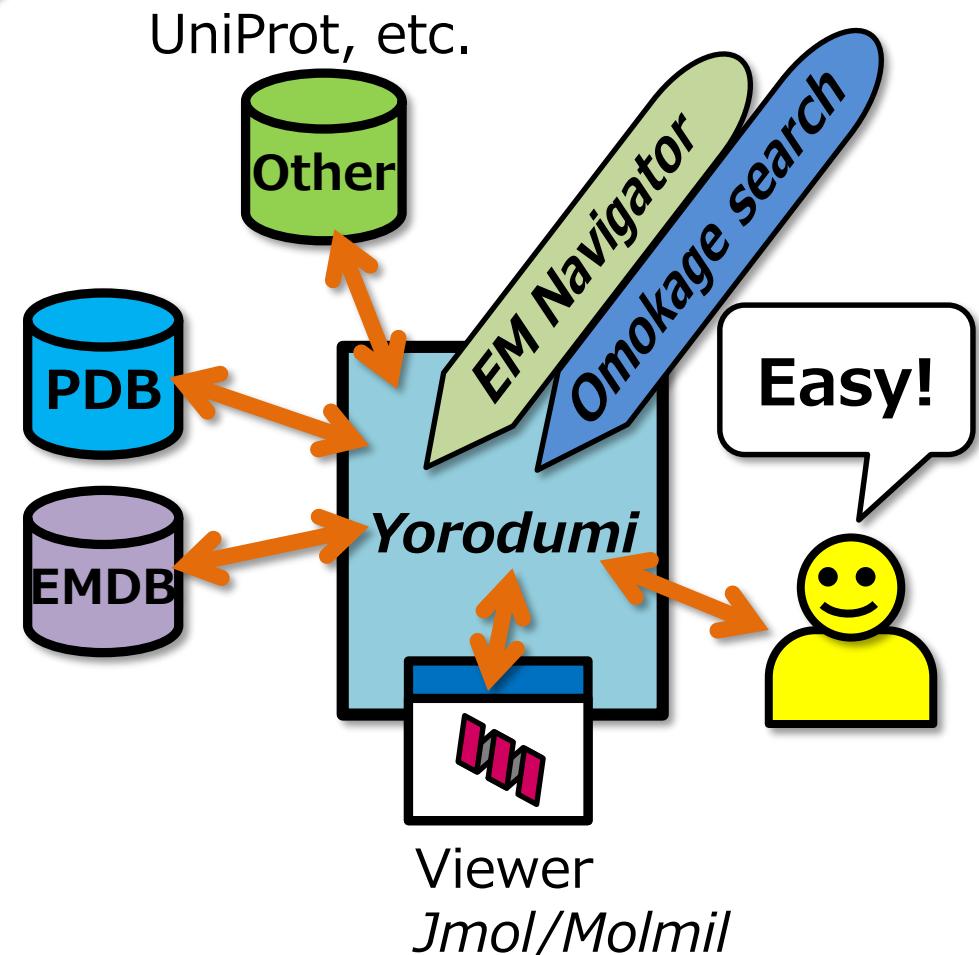
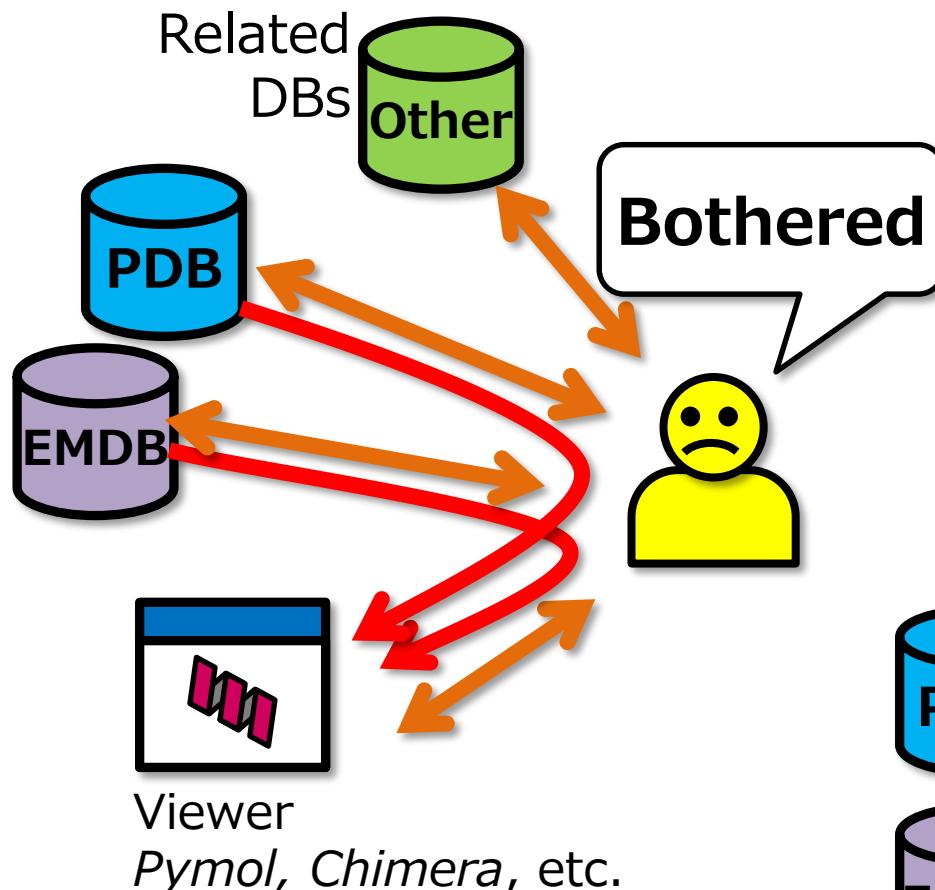
Dr. T. Kawabata

# Structure viewing



*Yorodumi* (万見)  
+ *Molmil*, etc.

# Make viewing easy



# Future of viewers

18

Java Applet  
1995-2016



**Jmol:**  
ex de-facto-standard  
as molecular viewer on WEB



**"Web-based Molecular Graphics"**  
NII SHONAN MEETING, September 2016

# Viewers in Yorodumi

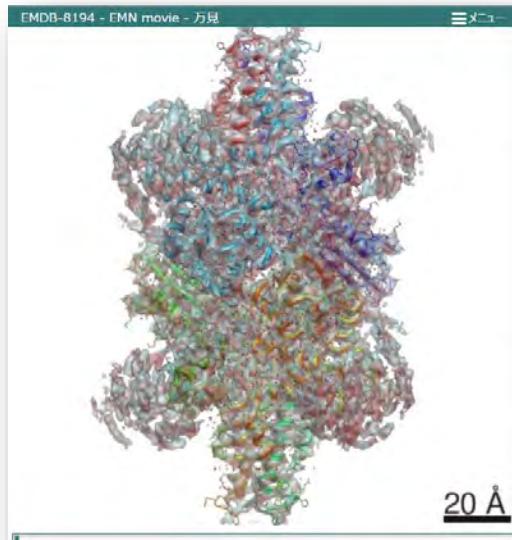
19



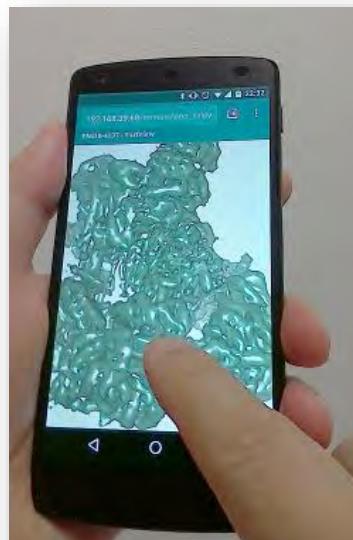
**Molmil** WebGL molecular viewer



G. Bekker



**movie**



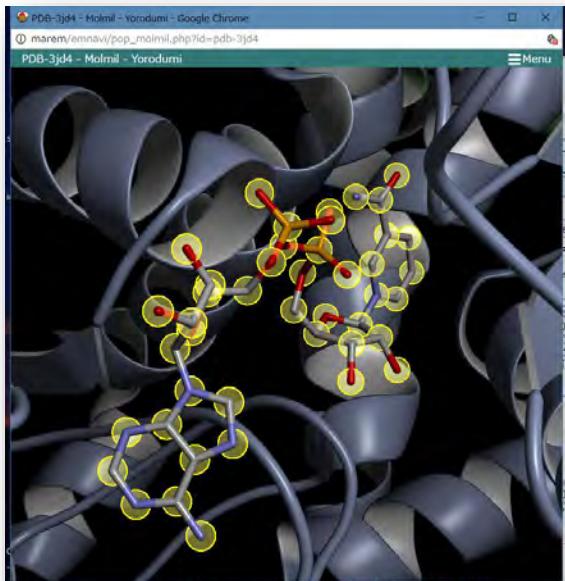
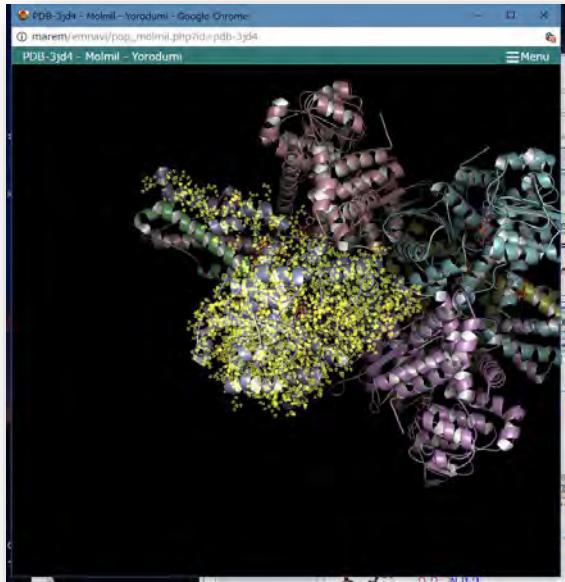
**SurfView**



**JSmol**

# Yorodumi-Molmil integration

Focusing on specific chain



**Components**

#1: Polypeptide(L)

Glutamate dehydrogenase 1, mitochondrial / GDH 1

Details Functions (10) Sequence Sites (72)

Mass: 55802.867 Da / Num. of mol.: 6 / Fragment: UNP residues 58-558 / Source: (natural) Bovine taurine / mammal / ウシ / References: UniProt: P00366, EC: 1.4.1.3

JSON: struct\_site, struct\_site\_gen, plus:struct\_site, plus:struct\_site\_gen

#2: Chemical

ChemComp-NAI / 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE / NADH

Details Sites

Mass: 665.446 Da / Num. of mol.: 12 / Formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>

#3: Chemical

ChemComp-GTP / GUANOSINE-5'-TRIPHOSPHATE / GTP \*YM

Details Sites

Mass: 523.183 Da / Num. of mol.: 6 / Formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>

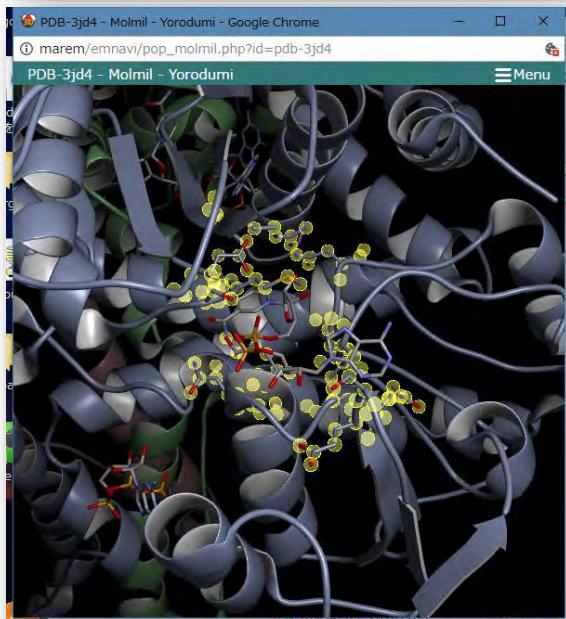
Red arrows point from the text "Focusing on specific chain" to the "Components" section and the "Chemical" sections #2 and #3.

Ligand

<http://pdbj.org/yorodumi/>

# Yorodumi-Molmil integration

sequence



Glutamate dehydrogenase 1, mitochondrial / GDH 1

Details Functions (10) Sequence Sites (72)

Chains: A B C D E F

ABREDDPN<sup>FF</sup> KNEGGFFDRG ASIVEDKLV<sup>E</sup> DLKTRETEEQ KRNRVR<sup>S</sup>ILR I<sup>I</sup>KPCN<sup>H</sup>VLS LSFPIRRDG SWEVIEGYRA QHSQHRT<sup>P</sup>C<sup>K</sup> GGIRYSTDVS VDEV<sup>K</sup>ALASL ITYKCAV<sup>V</sup>D PFGGAKAGVK INPKNYT<sup>O</sup>NE LEKITR<sup>R</sup>FTM ELAKKGFIGP GVDVPAPDMS TGEREMSWIA DTYASTIGHY DINAHACVTG K<sup>T</sup> HG RISATGRGVF HGFINEA SYMSILGNT<sup>P</sup> GFGDKTFV<sup>Q</sup> GFGNVGLHSM RYLHR<sup>F</sup>GAKC ITVGESDGS<sup>I</sup> WNPDGIDPKE LEDFLQHGT T<sup>N</sup> A<sup>W</sup> K<sup>I</sup>Y EGSI<sup>L</sup>EV<sup>V</sup>CD<sup>D</sup> ILIPAA<sup>E</sup>SEKQ LT<sup>K</sup>SNAPR<sup>V</sup>K AK<sup>I</sup>IAEGANG PTTPEADKIF LERNIM<sup>M</sup>VI<sup>P</sup>D LYLNAGGV<sup>T</sup>V SYFEWLN<sup>N</sup>LN HVSYGR<sup>L</sup>TFK D<sup>R</sup> D<sup>A</sup> Y<sup>H</sup>LL MSQESLERK FGKHGGTIPI VPTAEFQDRI SG<sup>A</sup>SEKD<sup>D</sup>IV<sup>H</sup> SGLAYTMERS ARQIMRTAMK YNLGLDLRTA AVVNAIEKFV RVYNEAGVTF T<sup>Q</sup>

alpha:	ABC	282
beta:	ABC	54
unobserved:	ABC	4
	all	501

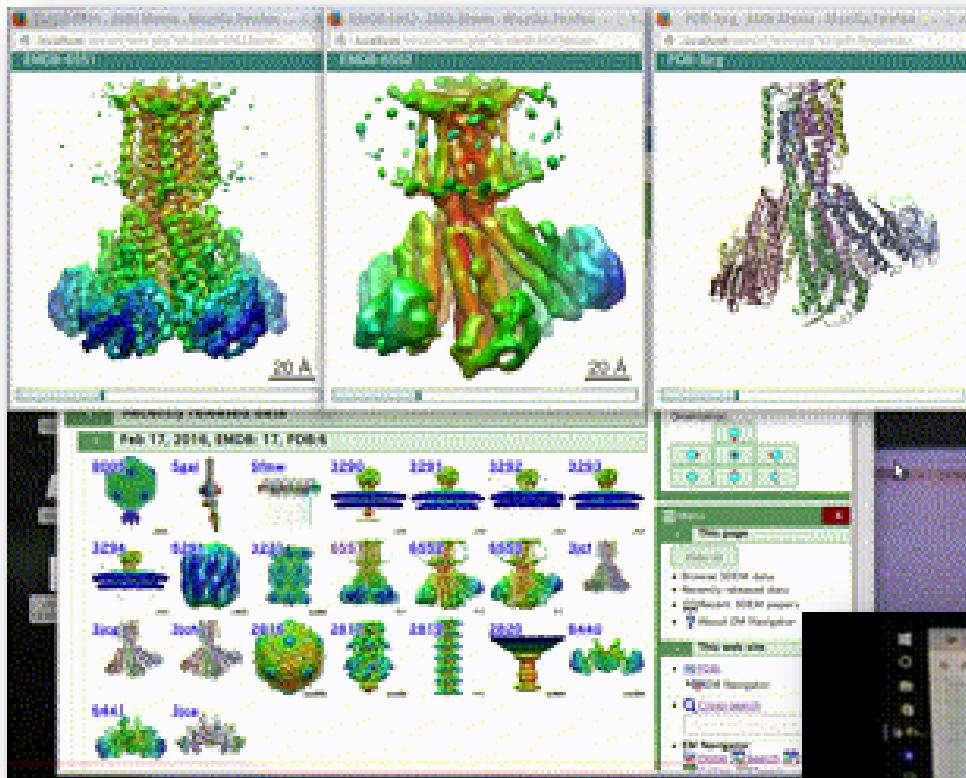
Details Functions (10) Sequence Sites (72)

Chains: A B C D E F

- NAD+
- GTP
- NAD+
- NAD+
- Active site: \*PLUS
- Binding site: ADP. {ECO:0000269|PubMed:12653548}, \*PLUS
- Binding site: GTP. {ECO:0000269|PubMed:11254391}, \*PLUS
- Binding site: NAD+. {ECO:0000269|PubMed:11254391}, \*PLUS

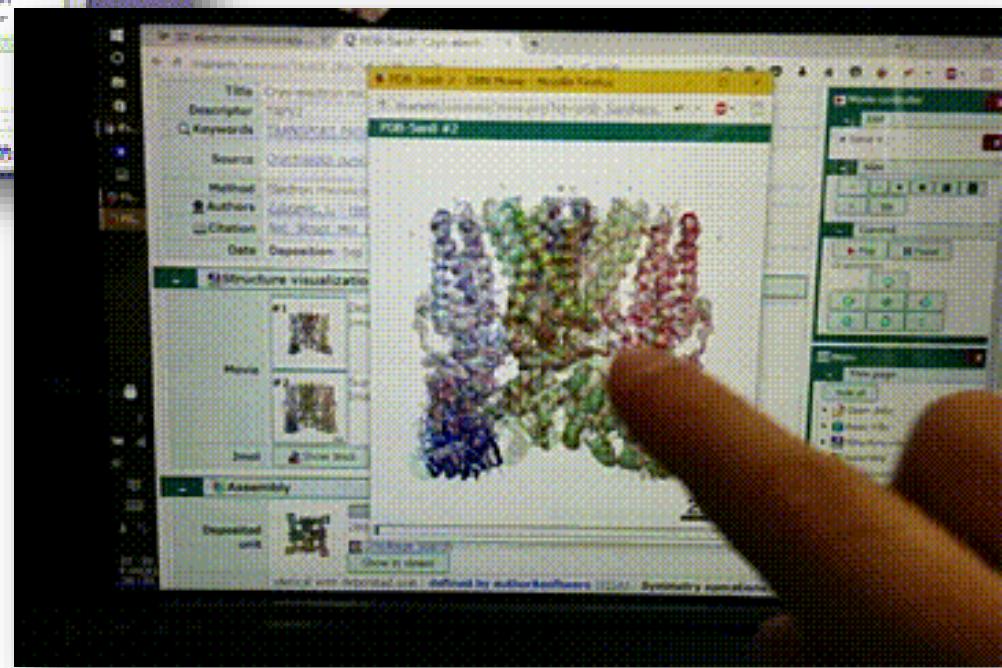
sites  
binding sites  
active sites  
etc.

# New movie interface



Rotation by mouse

Tiled & synchronized  
multiple movies



Rotation by finger  
on a touch device

# For education

**Data** **Explanation** **Open** **Help**

- 光るタンパク質 - GFP
- 表示:  Black BG  Fog effect  Stereo 右目が青、左目が赤のメガネを利  
用します **近くへ** **遠くへ**
- スタイル: 原子をボールで表示 原子のつながりを棒で表示 もどにもどす
- 構造データ: PDB-1ema - GREEN FLUORESCENT PROTEIN FROM AEQUOREA VICTORIA

**光る生き物**

夏、自然の残っている山里に行くと、美しく光る虫、ホタルを見つけることがあります。ホタルは光で会話をします。ホタルの光はルシフェラーゼというタンパク質が出しています。海ホタルや、ホタルイカなど、海にも光る生き物がたくさんいます。ほかの生き物の光  
けいこう  
も、タンパク質がかかわっています。このような光を出すタンパク質が蛍 光タンパク質です。

**これはなにを見ているの？**

海の中で緑色に光るオワンクラゲは、緑色に光る蛍光タンパク質を持っています。緑色  
蛍光タンパク質、英語で略してGFPとよばれます。今見ているのがそのGFPです。  
1960年、当時アメリカにいた下村脩さんたちがこのタンパク質を発見し、2008年にノーベル化学賞を受賞しました。ています。

**これからなにがわかったの？**

GFPが光を出すしくみがわかりました。外側の黄色い部分が丸いつつのような、カゴのよ  
はっしょくだん  
うな形をしていますが、その中にも構造があるのがわかりますか？これが発 色 団とい  
う光を出す部分で、GFPのもつアミノ酸の一部が変化してきたものです。下村さんたち  
が予想していたとおりのしくみでした。

**発色団はこれ！** **もどにもどす**

光を出すタンパク質は、生物学や医学にとってとても便利なタンパク質です。光ると目立

## Yorodumi Prime

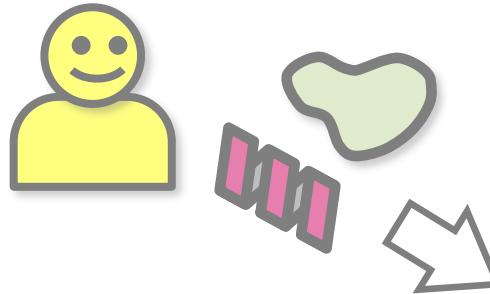
- Molmil + Yorodumi + educational contents
- for outreach activities of PDBj
- supporting mobile devices
- <http://pdbj.org/prime/>



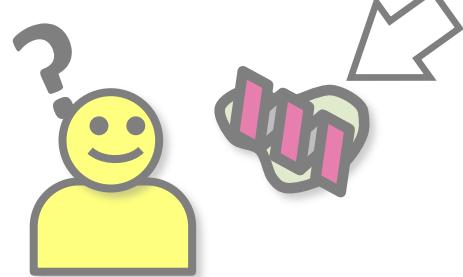
## PDBj, IPR *et al.* in *Science agora 2016*

- Odaiba Tokyo, November 2016
- show protein structures with 3D glass & iPad
- >1000 people, from children to the elderly

## Deposition



## Search & browse



## Comparison



## Structure viewing

<http://wwpdbj.org>

<http://pdbj.org/emnavi>

Poster: 3Pos019