3DM: protein superfamily analysis system

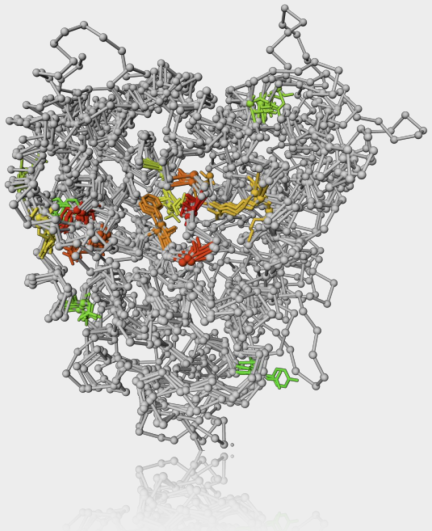
Catalyzing protein R&D

- Protein discovery
- Protein engineering
- Patent analysis

bio-prodict
protein predictions

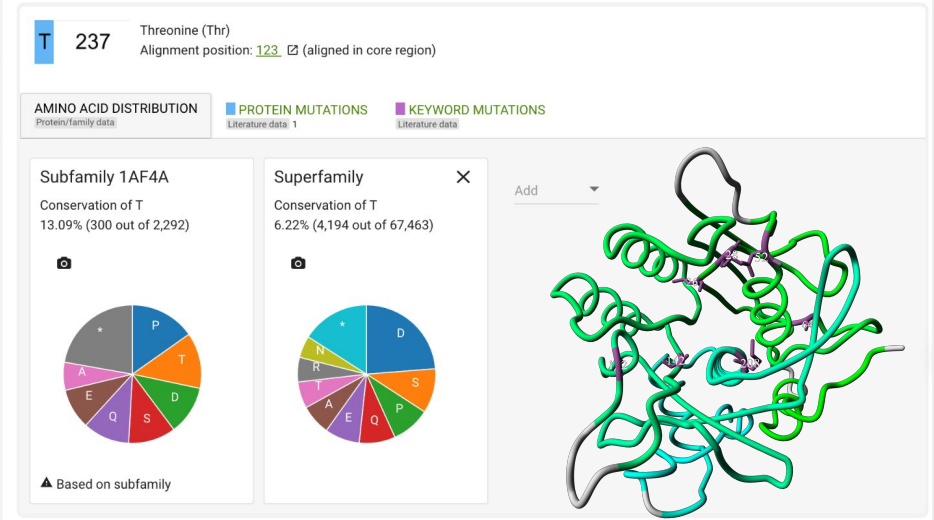
3DM speeds up protein R&D

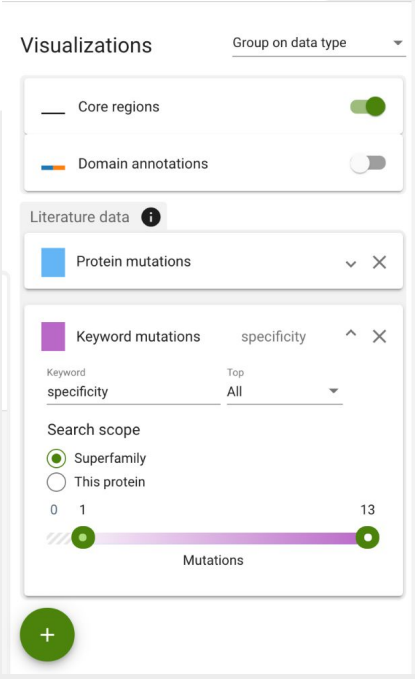
- **Make sense out of the flood of data available for proteins**
  - 3DM integrates data for complete protein superfamilies
- **3DM Tools give insight in your protein**
  - Use superfamily data to analyse your protein
- **Solves the numbering problem**
  - Seamlessly transfer data between homologous proteins
- **High-quality alignments**
  - Structure-based multiple sequence alignment



Example: Subtilisin

Highlight positions described in literature to affect specificity

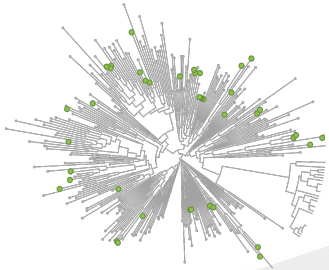


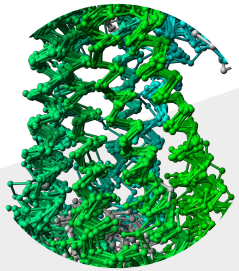


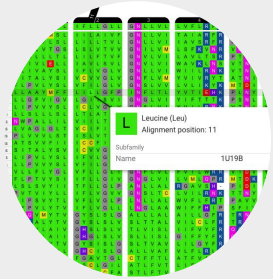
The power of 3DM

Structure-based MSA

1. Select structural templates to represent subfamilies
2. Structural alignment to connect sequentially diverse subfamilies
3. MSAs to include all proteins







Protein data integration

- Literature
- Patents
- Structure data
- Alignment data

Example: **GPCR 3DM System**

43 subfamilies connected:

- >900 integrated protein structures
- >85,000 WT proteins aligned
- >20,000 patented sequences
- >50,000 mutations described in the literature
  - searchable for their effects!

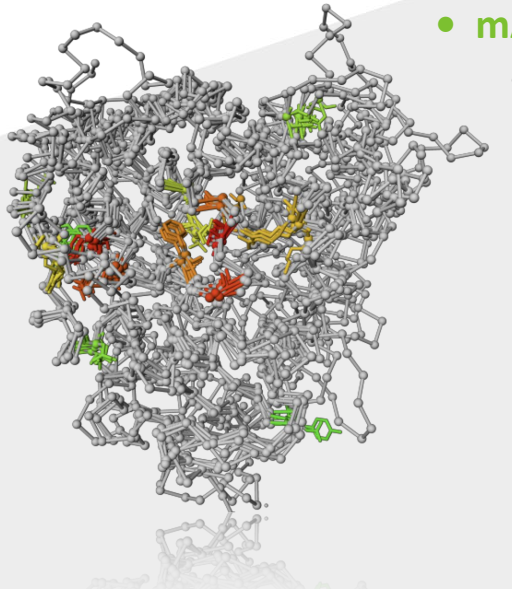
This data can be visualized in any protein or structure!

Powerful information system that **enhances your protein R&D**

Enhance your protein R&D with 3DM

Applications and Capabilities

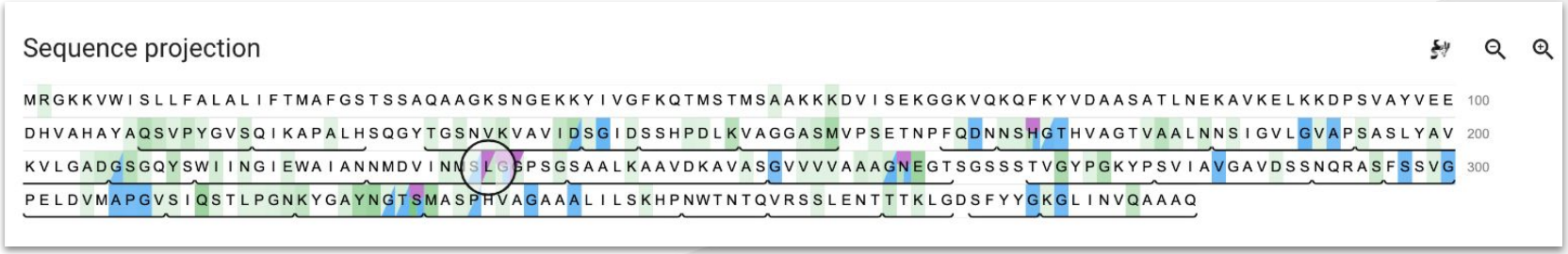
- **Protein Insights**
  - Conservation, contacts and literature
- **Protein discovery**
  - Find new enzymes
- **Protein engineering**
  - Smart mutation libraries
- **Patent analysis**
  - Determine IP & FTO

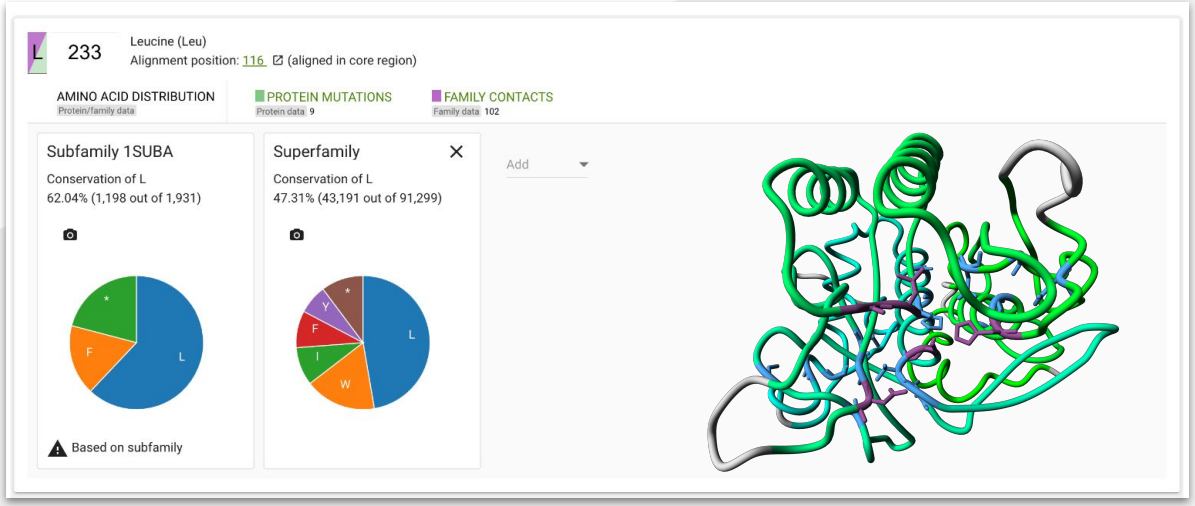


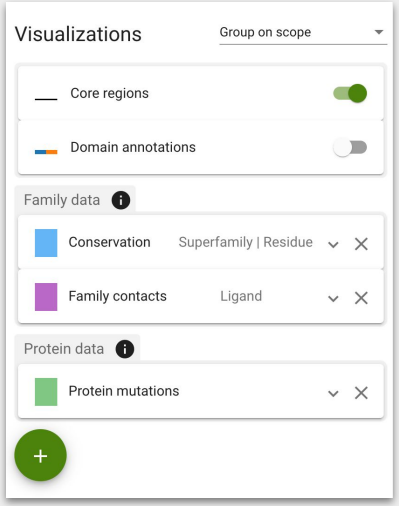
- **Strain engineering**
  - Investigate top variants
- **Small molecule tractability**
  - Compare (human) pockets in the family
- **mAb therapeutics**
  - antibody sequence analysis

Protein analysis

Visualise data from the family on top of any protein





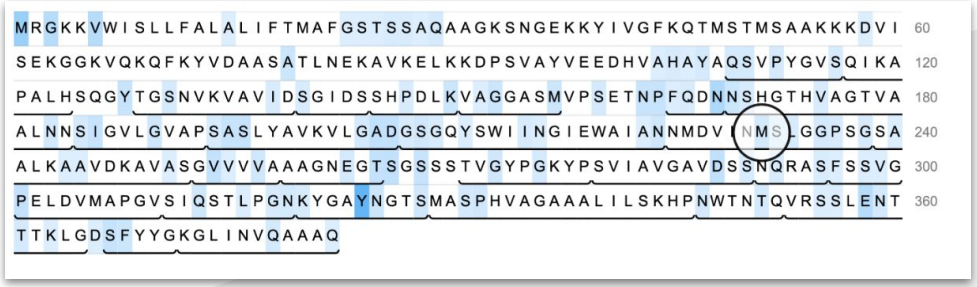


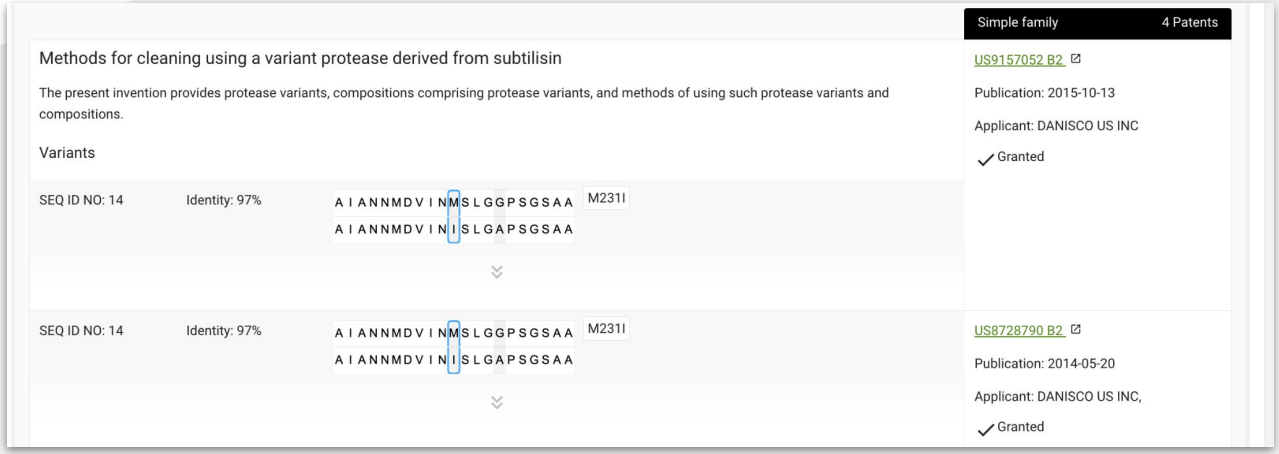
Patent analysis

Determine FTO

Quickly assess IP, including:

- Patented mutations
- Patent sequence variations





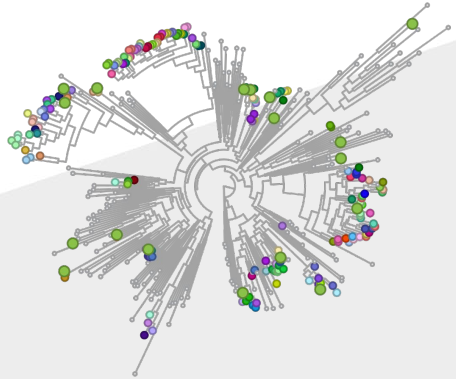
Intelligent in-silico panel design with 3DM

Use the alignment to determine diversity

A single active-site residue can change specificity

- Smart diversity: focus on diversity at key positions
- Select likely to express proteins
- Evaluate FTO

>90% expression rates achieved by our partners

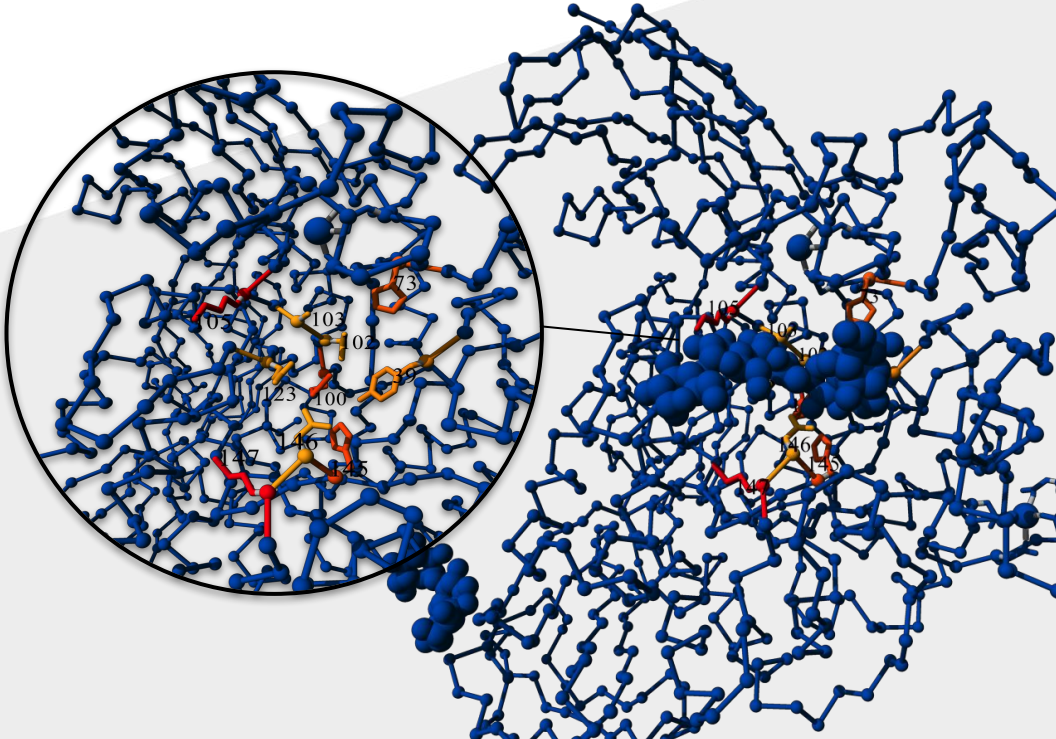


Number	50	54	58	113	207	Proteins
1.	D	H	V	N	S	28,639
2.	D	H	T	S	S	7,999
3.	P	H	C	S	S	4,471
4.	D	H	V	S	S	4,173
5.	D	H	C	S	S	3,492
6.	D	H	T	N	S	2,843

Pocket analysis

- Compare pocket residues between human proteins of the same fold
- Compare pockets with model organisms
- Analyse compounds present in pockets

	39	40	73	100	102	103	105	123	145	146
P19961	Y	Q	H	R	D	A	K	E	H	D
P04746	Y	Q	H	R	D	A	K	E	H	D
P04745	Y	Q	H	R	D	A	K	E	H	D
Q04446	Y	Q	H	R	D	G	T	E	H	D
Q07837	Y	G	H	S	D	A	K	-	P	D
P17050	-	-	N	K	D	G	F	S	I	G
P06280	D	S	N	K	D	G	Y	E	I	G
P08195	V	A	Y	Q	R	D	E	G	-	-

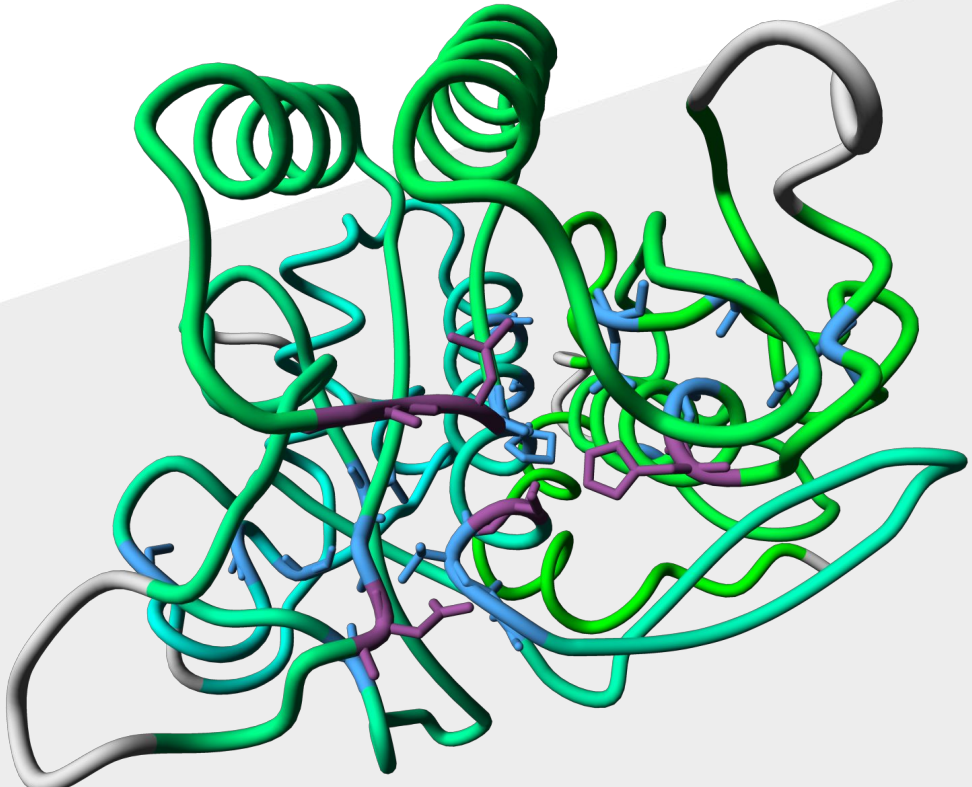


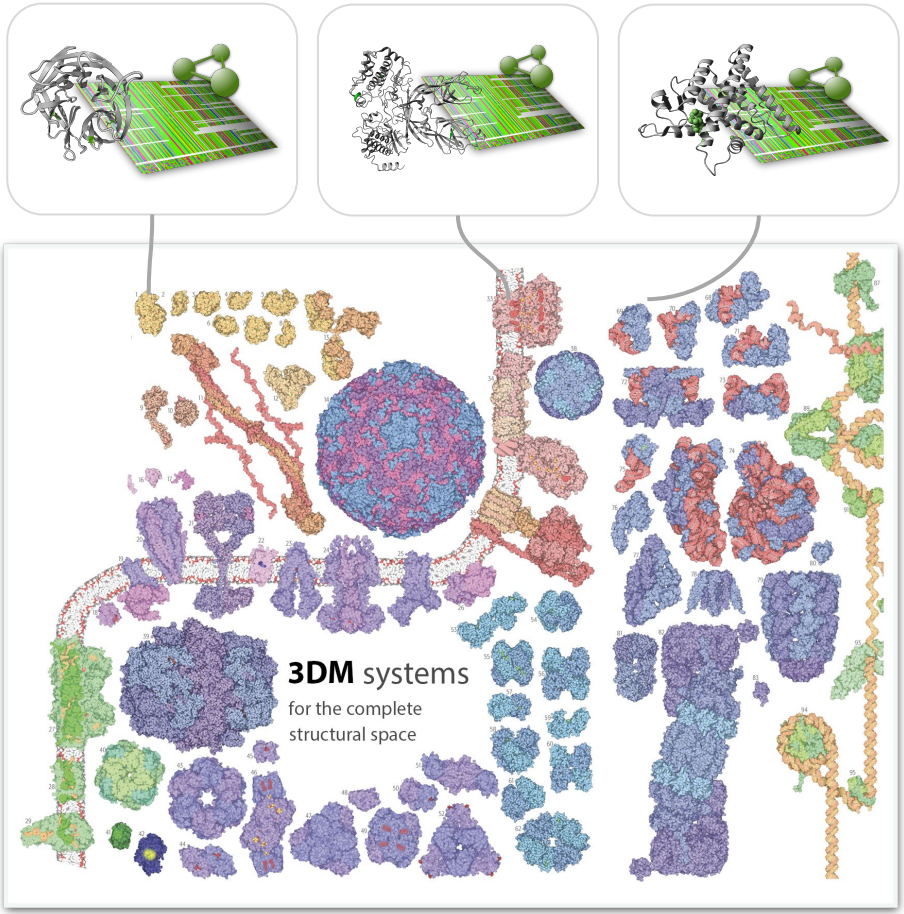
Structure visualisations

Show 3DM data directly in any protein structure

PyMol/Yasara integration:

- Generate scenes from 3DM
- Yasara/PyMol plugin
- Visualise data directly in any structure





With over 50,000 families available, 3DM covers the complete structural space. providing access to the full power of 3DM instantly, including panel design, literature analysis, engineering hotspots, etc.

How we work

Custom 3DM systems (license)

- Custom build 3DM system
- We can include your own structures/sequences
- Alignments fine tuned for your use case

PDB-Wide system access (license)

- 3DM systems ready to go for any protein target
- Includes tickets for custom 3DM systems or custom development

Custom development (tickets or project based)

- Order bespoke features to get the most out of 3DM
- API access: Integrate 3DM data into inhouse computational biology pipelines
- Whole exome 3DM systems for your production strain

Q&A

More information:
www.bio-prodict.com

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protein predictions