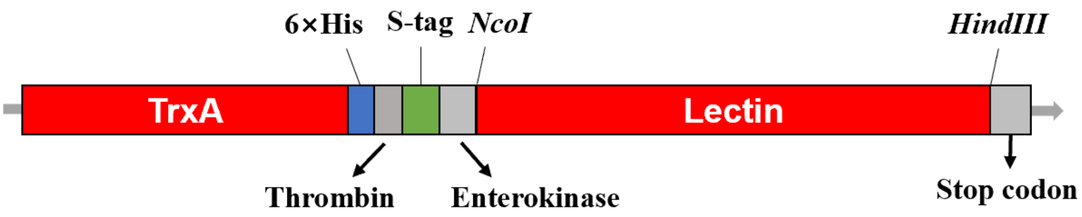
# Supplementary materials



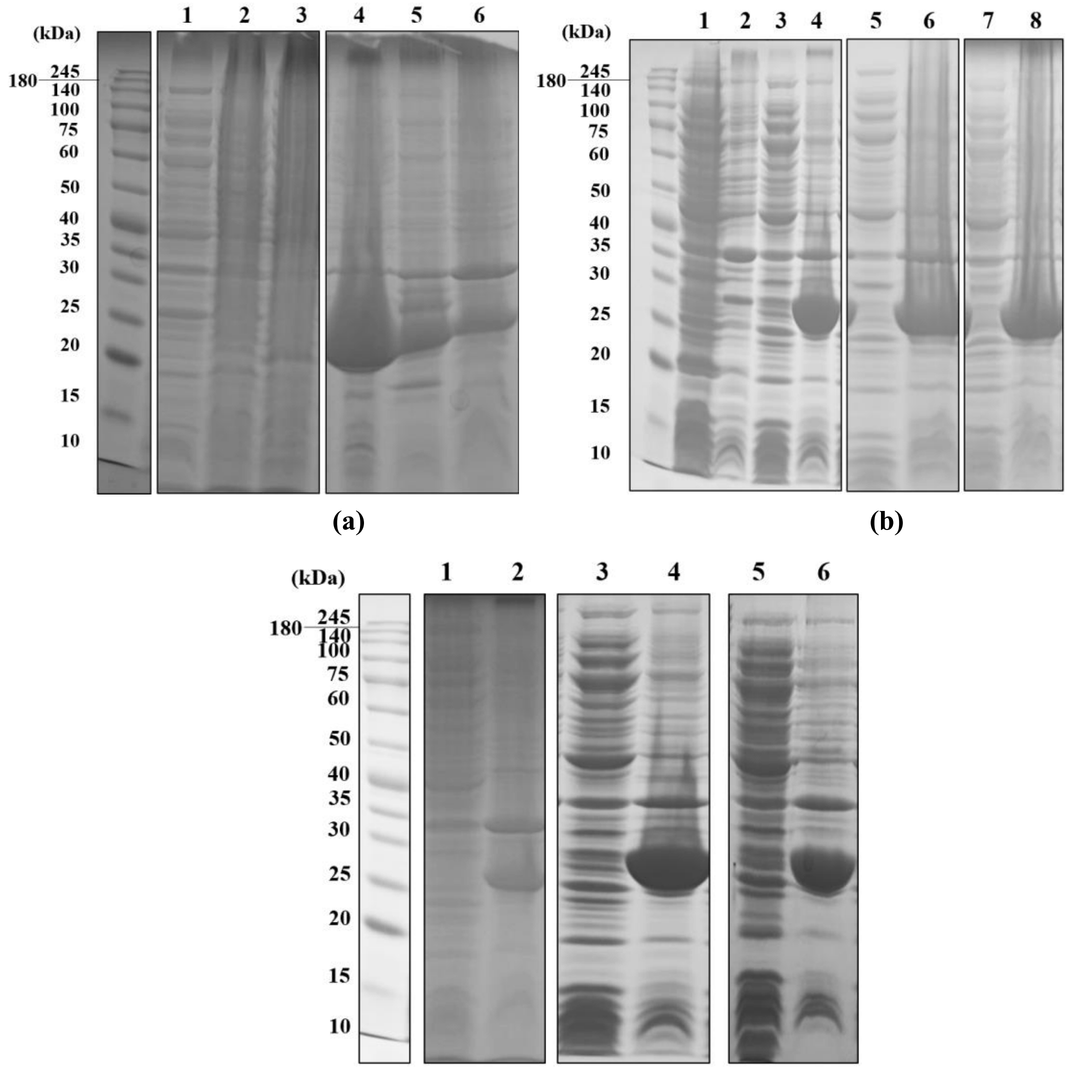
(a)

The ORF of pET32a-MVL

**MSDKIIHLTDDSFDTDVLKADGAILVDFWAEWCGPCKMIAPILDEIADEYQGKLTVAKLNIDQNPGTAPKYGIRGIPTLLLFKNGEVAATKVGALSKGQLKEFLDANLA**GSGSGHMHHHHHHSSGLVPRGSGMKETAAAKFERQHMDSPDLGTDDDDKAMASYKVNIPAGPLWSNAEAQQVGPKIAAAHQGNFTGQWTTVVESAMSVVEVELQVENTGIHEFKTDVLAGPLWSNDEAQKLGPQIAASYGAEFTGQWRTIVEGVMSVIQIKYTF*

(b)

**Supplementary Fig. S1: Schematic diagram of an open reading frame (ORF) composed of lectin and thioredoxin (a) and amino acid sequence of TrxA-MVL fusion protein (b).** The bolded portion represents the TrxA tag, and the underline section denotes the lectin sequence.

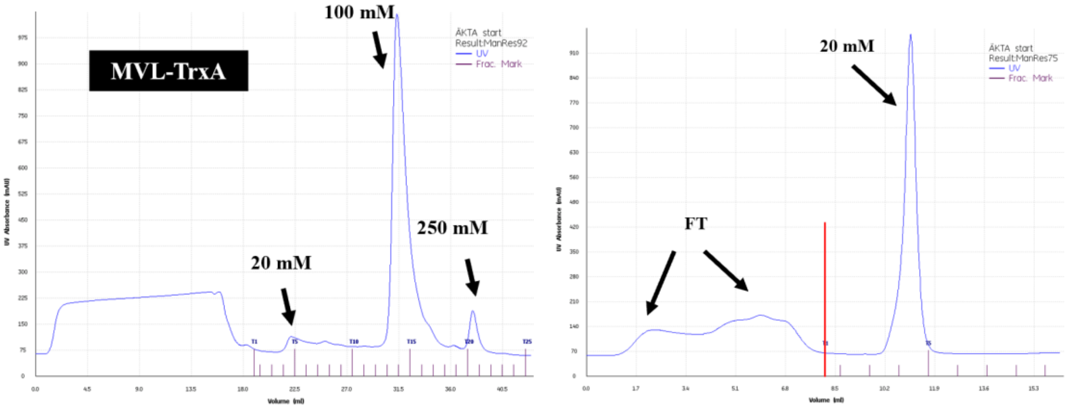


(a) (b)

(c)

**Supplementary Fig. S2: Optimization of culture conditions for MVL-TrxA expression**

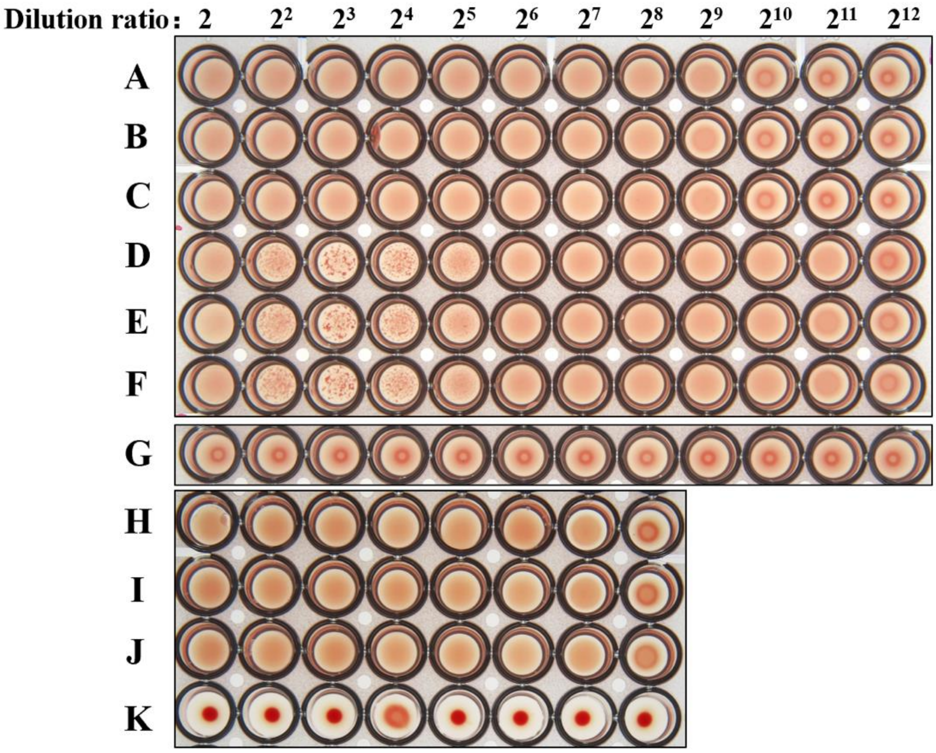
**a**: Host cell screening. Samples 1, 2, 3 correspond to the supernatant of BL21(DE3), Rosetta gami2 (DE3), BL21-CodonPlus (DE3)-RIPL; 4, 5, 6 correspond to the pellet of BL21(DE3), Rosetta gami2 (DE3), BL21-CodonPlus (DE3)-RIPL. **b**: Culture time screening. Samples 1 and 2 correspond to the supernatant and pellet after 4 h of culture of empty vector pET32a, 3 and 4 correspond to the supernatant and pellet after 4 h of cultivation, and 5 and 6 correspond to the supernatant and pellet after 8 h of cultivation, 7 and 8 correspond to the supernatant and pellet after 16 h of cultivation. **c**: Culture temperature screening. Samples 1 and 2 correspond to the supernatant and pellet after 4 h of cultivation at 37°C, 3 and 4 correspond to the supernatant and pellet after 4 h of cultivation at 23°C, and 5 and 6 correspond to the supernatant and pellet after 4 h of cultivation at 16°C.



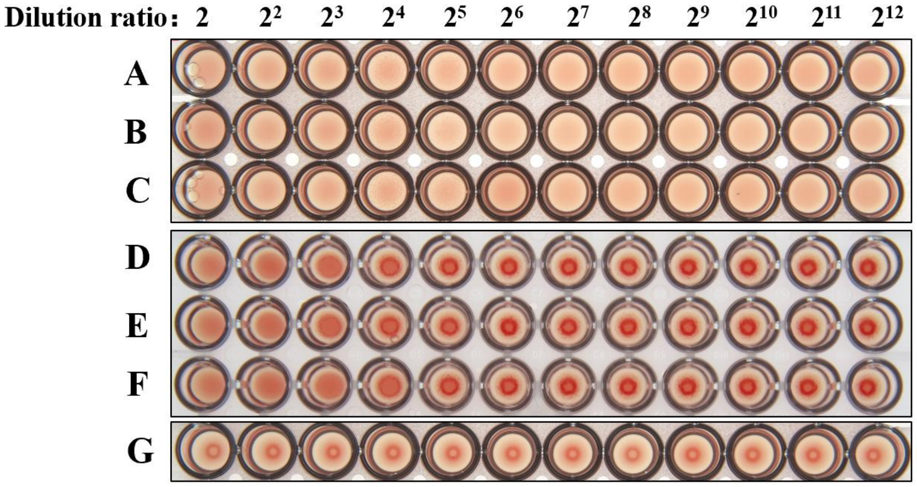
**(a)** **(b)**

**Supplementary Fig. S3: The purification profiles of rMVL-Trx fusion protein (a) and thrombin-digested MVL-TrxA (b) on His-trap HP column.**

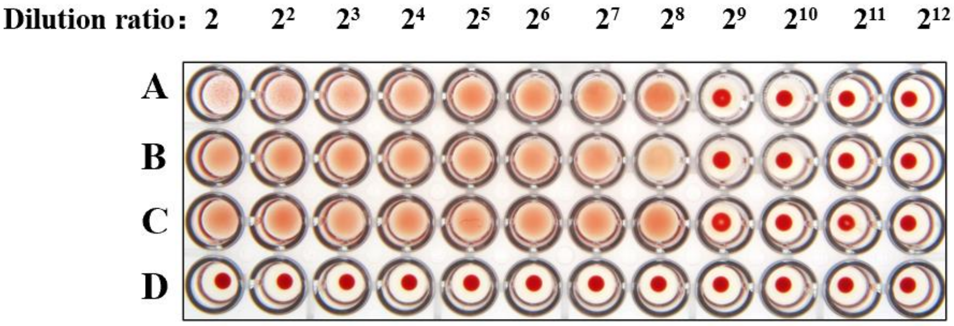
Elution of His-tag protein was conducted by imidazole (20 mM, 100 mM and 250 mM). Flow throw fraction (FT in panel (b)) contained rMVL.



(a)



(b)

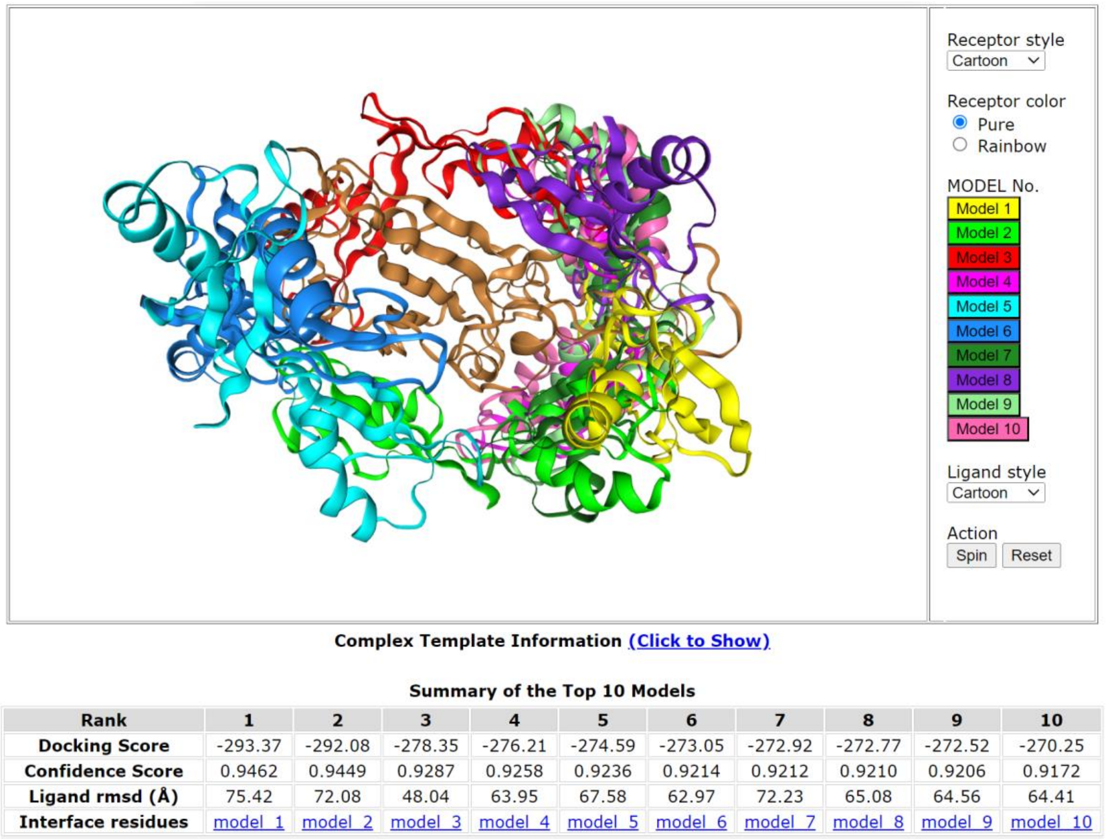


(c)

**Supplementary Fig. S4: Hemagglutination assays of lectins using rabbit**

**erythrocyte.**

(a): Hemagglutination assay results of PHA-M (A-C), Jacalin (D-F) and Con A (H-G) lectins; negative controls (G, K). (b): Hemagglutination assay results of CSL3 (A-C) and DB1 (D-F) lectins; negative control (G). (c): Hemagglutination assay result of recombinant MVL (A-C); negative control (D).



Receptor style
Cartoon

Receptor color
● Pure
○ Rainbow

MODEL No.

Ligand style
Cartoon

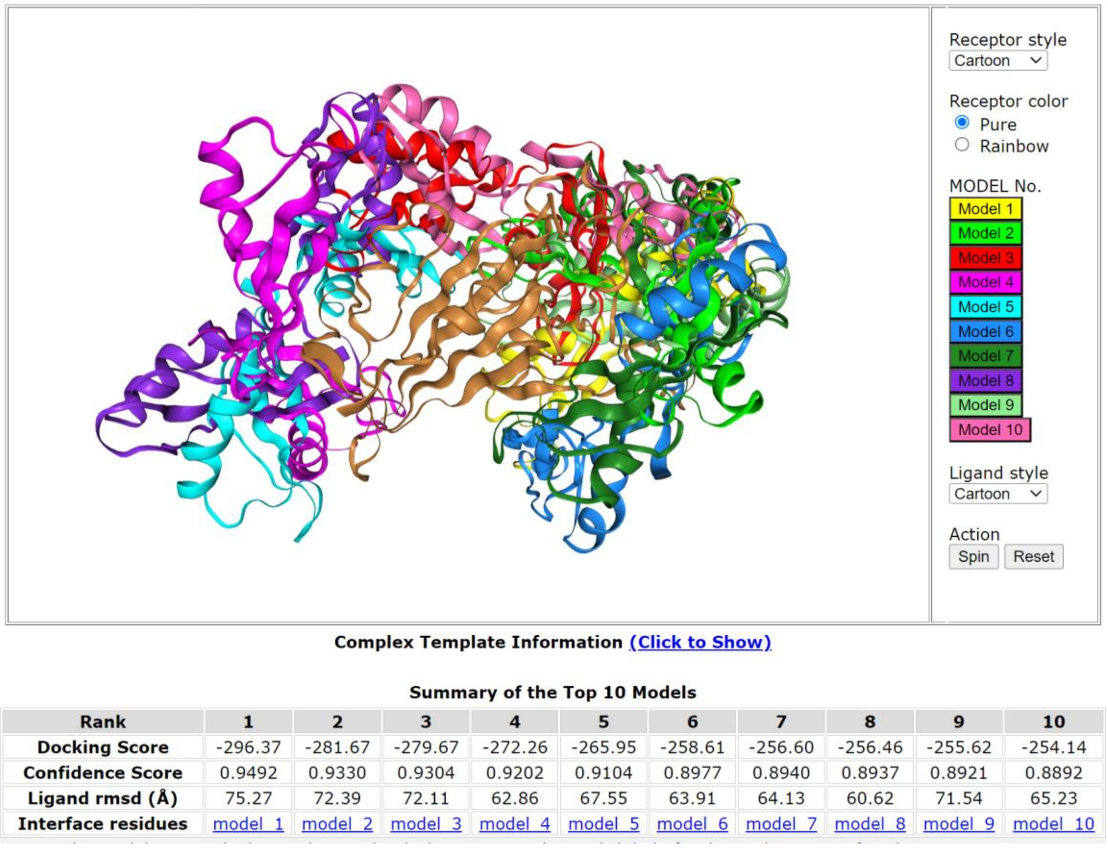
Action

**Complex Template Information** (Click to Show)

**Summary of the Top 10 Models**

| Rank | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| **Docking Score** | -293.37 | -292.08 | -278.35 | -276.21 | -274.59 | -273.05 | -272.92 | -272.77 | -272.52 | -270.25 |
| **Confidence Score** | 0.9462 | 0.9449 | 0.9287 | 0.9258 | 0.9236 | 0.9214 | 0.9212 | 0.9210 | 0.9206 | 0.9172 |
| **Ligand rmsd (Å)** | 75.42 | 72.08 | 48.04 | 63.95 | 67.58 | 62.97 | 72.23 | 65.08 | 64.56 | 64.41 |
| **Interface residues** | model_1 | model_2 | model_3 | model_4 | model_5 | model_6 | model_7 | model_8 | model_9 | model_10 |

**(a)**



Receptor style
Cartoon

Receptor color
● Pure
○ Rainbow

MODEL No.

Ligand style
Cartoon

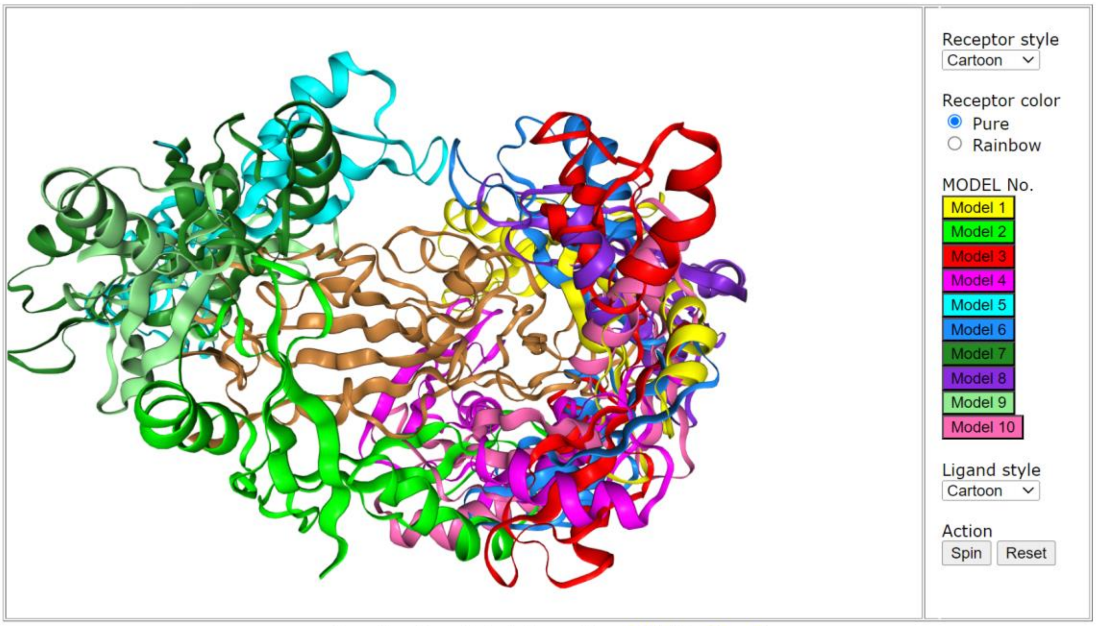
Action

**Complex Template Information** (Click to Show)

**Summary of the Top 10 Models**

| Rank | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| **Docking Score** | -296.37 | -281.67 | -279.67 | -272.26 | -265.95 | -258.61 | -256.60 | -256.46 | -255.62 | -254.14 |
| **Confidence Score** | 0.9492 | 0.9330 | 0.9304 | 0.9202 | 0.9104 | 0.8977 | 0.8940 | 0.8937 | 0.8921 | 0.8892 |
| **Ligand rmsd (Å)** | 75.27 | 72.39 | 72.11 | 62.86 | 67.55 | 63.91 | 64.13 | 60.62 | 71.54 | 65.23 |
| **Interface residues** | model_1 | model_2 | model_3 | model_4 | model_5 | model_6 | model_7 | model_8 | model_9 | model_10 |

**(b)**

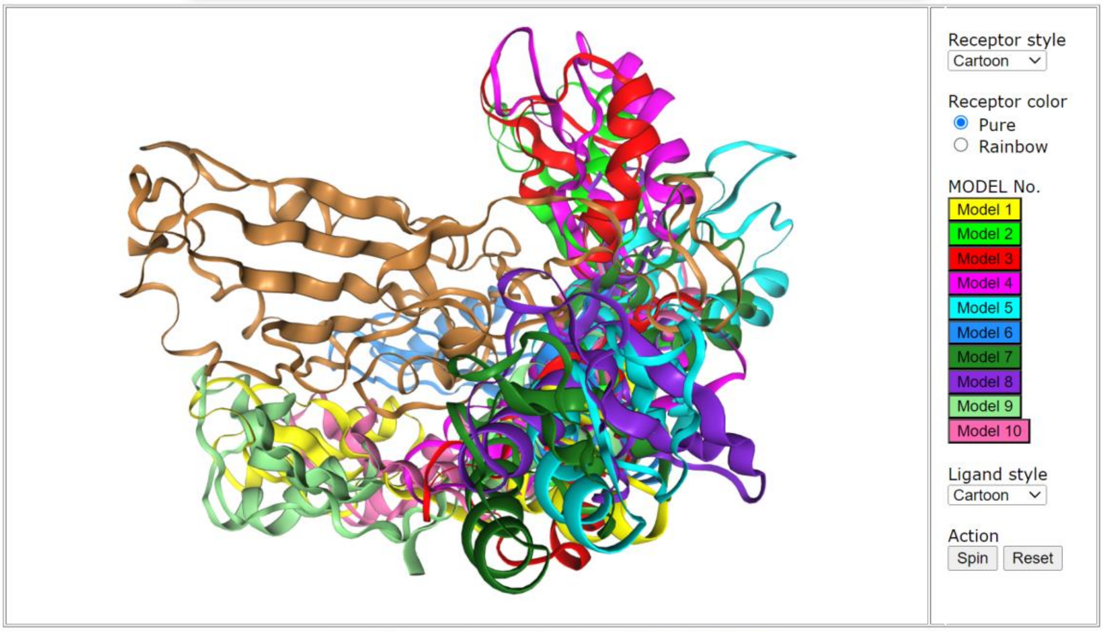


**Complex Template Information** (Click to Show)

**Summary of the Top 10 Models**

| **Rank** | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** |
|---|---|---|---|---|---|---|---|---|---|---|
| **Docking Score** | -294.01 | -281.03 | -278.36 | -276.93 | -273.31 | -272.82 | -269.07 | -267.41 | -265.60 | -264.52 |
| **Confidence Score** | 0.9469 | 0.9322 | 0.9287 | 0.9268 | 0.9217 | 0.9210 | 0.9154 | 0.9128 | 0.9099 | 0.9081 |
| **Ligand rmsd (Å)** | 75.34 | 48.07 | 64.27 | 64.16 | 67.48 | 72.22 | 60.49 | 86.00 | 62.84 | 65.01 |
| **Interface residues** | model_1 | model_2 | model_3 | model_4 | model_5 | model_6 | model_7 | model_8 | model_9 | model_10 |

**(c)**



**Complex Template Information** (Click to Show)

**Summary of the Top 10 Models**

| **Rank** | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** |
|---|---|---|---|---|---|---|---|---|---|---|
| **Docking Score** | -307.74 | -297.35 | -289.80 | -283.11 | -282.17 | -280.75 | -279.02 | -278.64 | -277.12 | -273.65 |
| **Confidence Score** | 0.9591 | 0.9501 | 0.9425 | 0.9348 | 0.9336 | 0.9318 | 0.9296 | 0.9291 | 0.9271 | 0.9222 |
| **Ligand rmsd (Å)** | 71.96 | 65.07 | 73.19 | 66.56 | 83.07 | 64.93 | 82.19 | 75.16 | 69.49 | 66.97 |
| **Interface residues** | model_1 | model_2 | model_3 | model_4 | model_5 | model_6 | model_7 | model_8 | model_9 | model_10 |

**(d)**

**Supplementary Fig. S5: Docking simulation of MVL and spike protein RBDs variants.**

The top 10 models of the complex interaction between MVL and spike protein RBDs variants, alpha (a), delta (b), omcrion (c), and original (d), were estimated by protein-protein docking simulation using the HDOCK server that based on hybrid docking strategies, template-based modeling and *ab initio* docking.