Article

Rational Design of Peptides Derived from Odorant-Binding Proteins for SARS-CoV-2-Related Volatile Organic Compounds Recognition

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Aaegobp39 sequence was obtained from https://www.uniprot.org/uniprot/Q176B6:

MYVVNLVLVLLSLEILSTSDAAMTMKQLKNSLEMMRKACAPKFNVVEASLDELKAGRFAN
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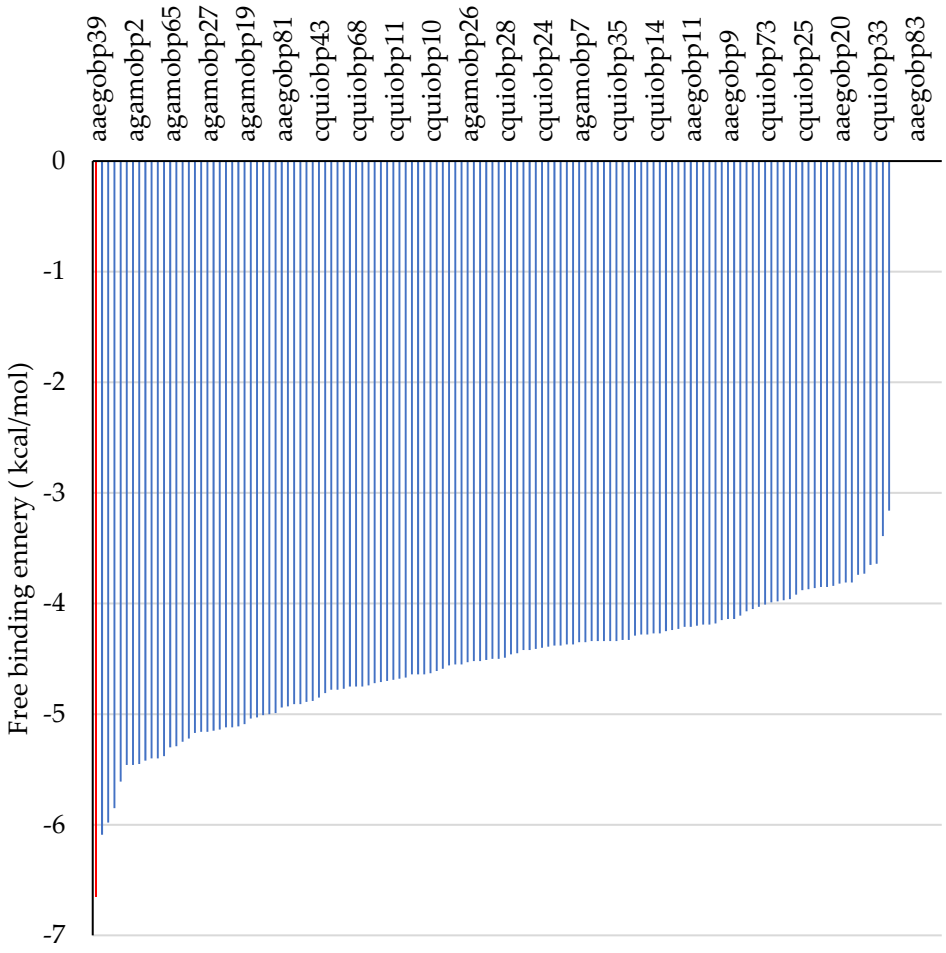

Figure S1. The free binding energy of mosquito classic and Plus-C OBPs corresponding to ligand nonanal (data was obtained from mOBP Database: http://www.bo-protscience.fr/mobpdb/)

Table S1. The prediction reports of binding pocket for ligand ethanol and the amino acids composition.

name	lig_name	volume	enclosure	surface	depth	surf/vol	hydrophobic interactions	hydrophobicity	Score
P_0	EOH_A_500	695.04	0.03	600.44	20.38	0.86389273	35	0.49	0.840611
P_1	EOH_A_500	106.69	0.15	310.6	10.04	2.91123817	9	0.25	0.278733

name	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE
P_0	4	1	1	0	0	0	1	1	2	1
P_1	1	0	1	1	0	1	1	2	0	0

name	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
P_0	3	0	5	4	1	4	3	1	0	5
P_1	0	1	0	2	0	1	0	0	0	1

Table S2. The prediction reports of binding pocket for ligand benzaldehyde and the amino acids composition.

name	lig_name	volume	enclosure	surface	depth	surf/vol	hydrophobic interactions	hydrophobicity	Score
P_0	HBX_A_200	552.38	0.1	540.53	20.28	0.97854738	18	0.36	0.82617
P_1	HBX_A_200	182.21	0.21	324.39	8.06	1.78030844	17	0.61	0.270989
P_2	HBX_A_200	182.08	0.09	407.51	11.39	2.23808216	16	0.37	0.365149

name	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE
P_0	2	2	4	0	0	1	2	2	0	2
P_1	0	0	1	2	0	0	1	0	1	0
P_2	1	1	1	2	0	0	2	1	1	0

name	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
P_0	5	0	0	3	0	0	0	0	4	3
P_1	1	1	1	1	0	0	0	1	1	0
P_2	2	1	0	0	0	0	1	0	2	0

Table S3. The prediction reports of binding pocket for ligand acetone and the amino acids composition.

name	lig_name	volume	enclosure	surface	depth	surf/vol	hydrophobic interactions	hydrophobicity	Score
P_0	Acetone	1485.44	0.13	1508.9	27.57	1.0157933	75	0.4	0.814444
P_1		279.23	0.15	418.17	11.09	1.49758264	21	0.51	0.489561
P_2		256.45	0.17	554.04	14.71	2.16042113	26	0.49	0.599924

name	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE
P_0	5	1	2	0	6	3	4	6	3	5
P_1	1	0	0	1	0	0	1	1	1	4
P_2	2	0	2	0	2	0	1	1	1	0

name	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
P_0	6	2	4	4	7	0	3	0	2	4
P_1	0	2	0	1	0	0	0	0	0	0
P_2	1	1	1	3	1	1	1	0	0	1

Table S4. The prediction reports of binding pocket for ligand nonanal and the amino acids composition.

name	lig_name	volume	enclosure	surface	depth	surf/vol	hydrophobic interactions	hydrophobicity	Score
P_0	Nonanal	1027.78	0.03	1033.37	23.61	1.00543891	61	0.49	0.821954
P_1	Nonanal	242.69	0.14	453.37	14.27	1.86810334	21	0.46	0.585585
P_2	Nonanal	112.06	0.26	318.06	6.11	2.83830091	15	0.47	0.183907

name	LEU	LYS	MET	PHE	PRO	SER	THR	GLY	HIS	ILE
P_0	6	2	5	3	1	3	3	0	0	4
P_1	1	2	0	3	2	0	0	1	0	0
P_2	1	1	0	1	1	0	0	0	0	0

name	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
P_0	6	2	5	3	1	3	3	0	2	2
P_1	1	2	0	3	2	0	0	0	0	0
P_2	1	1	0	1	1	0	0	0	0	2

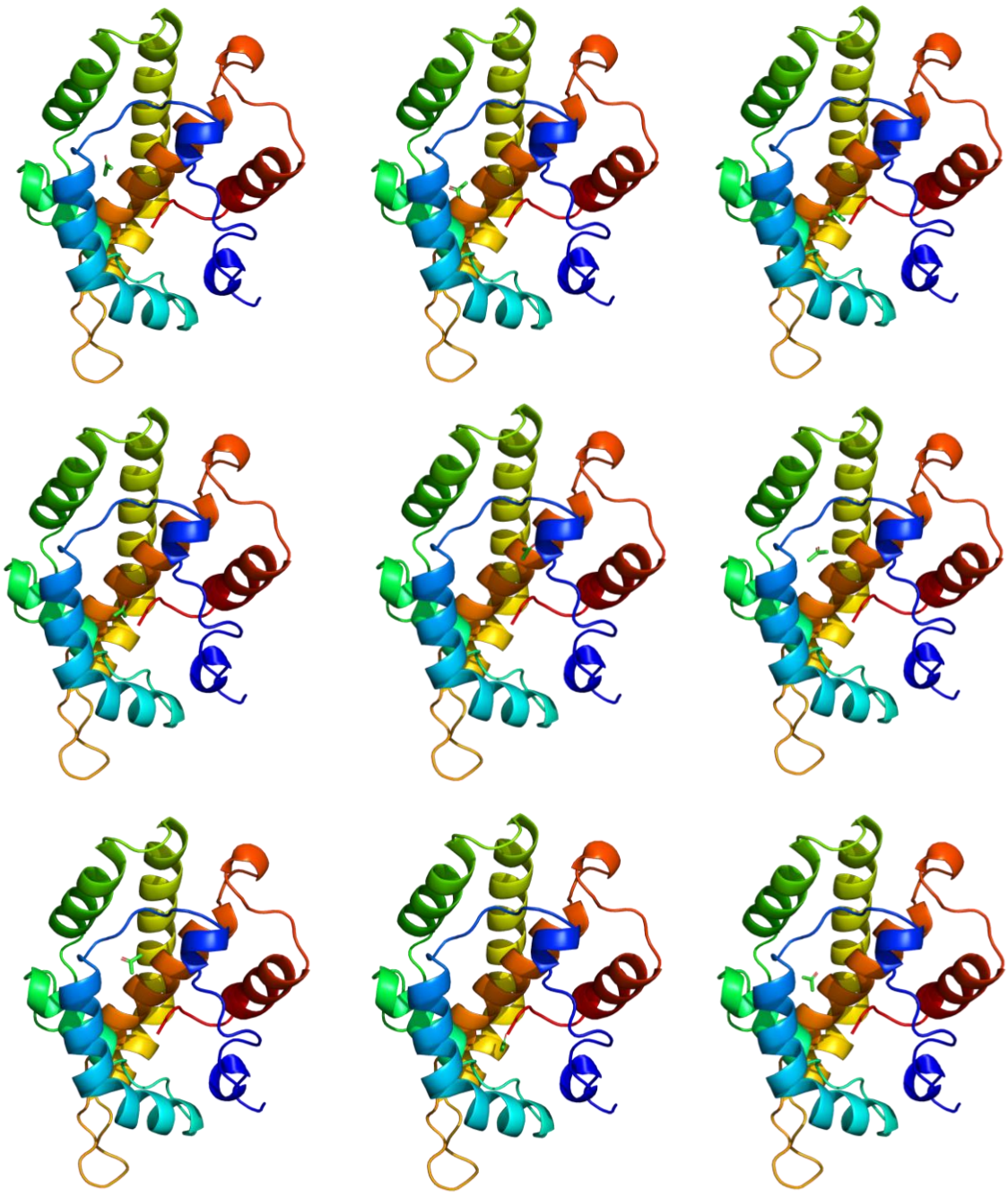

Figure S2. Nine docking modes of AgamOBP47 and ligand acetone complex.

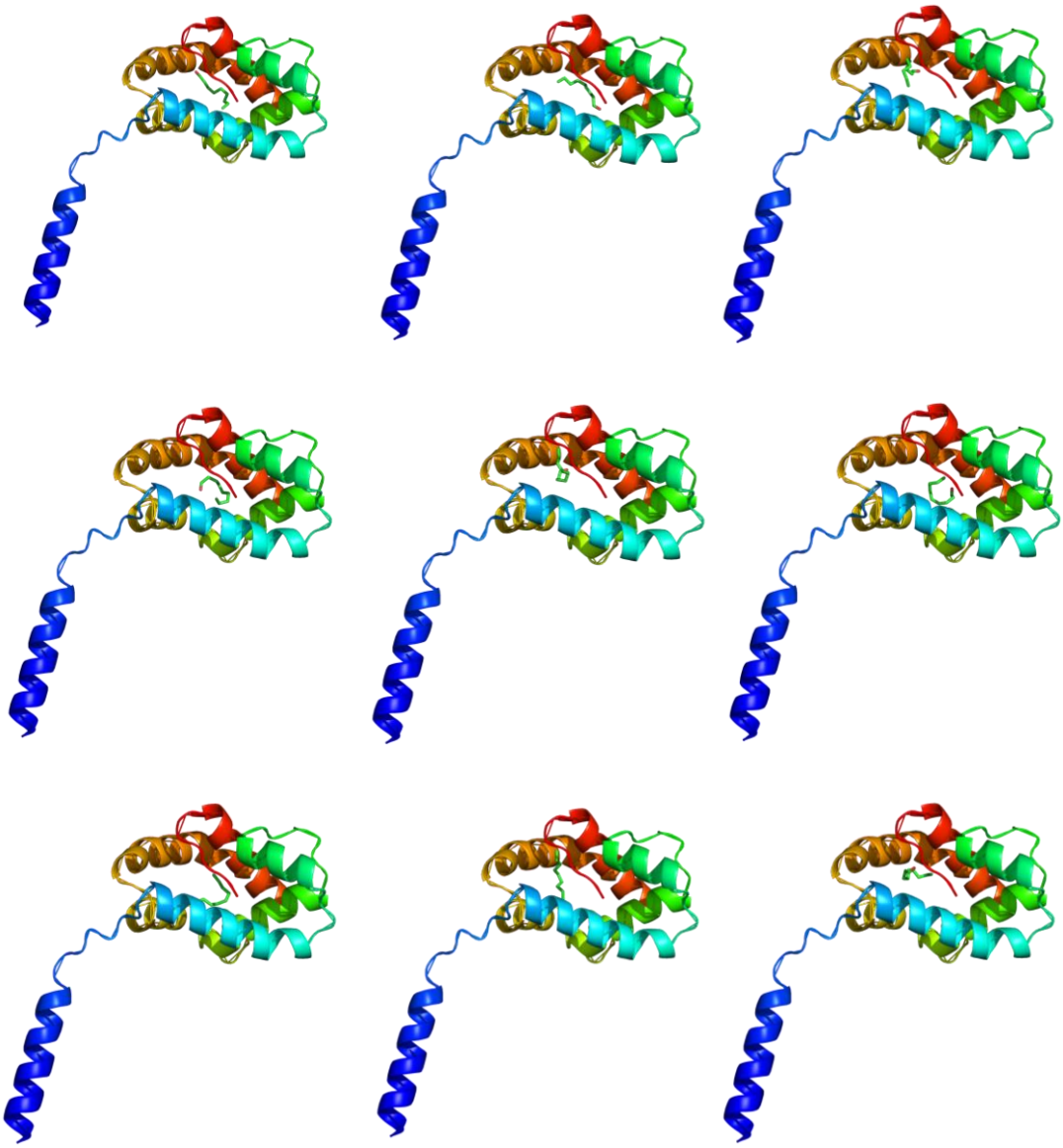

Figure S3. Nine docking modes of Aaegobp39 and ligand nonanal complex.

Table S5. PEPFOLD clustering reports (peptide sequence: TIAATLTILAALVSAANVFFF)

Model	sOPEP	avg	gdt	max	q	tm
PEPFOLD-model1	−44.9829	0.769	0.89	0.825	0.718	0.645
PEPFOLD-model2	−44.7545	0.728	0.874	0.793	0.685	0.56
PEPFOLD-model3	−44.4068	0.767	0.887	0.816	0.716	0.649
PEPFOLD-model4	−43.1849	0.739	0.832	0.798	0.682	0.642
PEPFOLD-model5	−43.1494	0.794	0.919	0.878	0.777	0.602

Table S6. PEPFOLD clustering reports (peptide sequence: VRGLLYVNAYAFLY)

Model	sOPEP	avg	gdt	max	q	tm
PEPFOLD-model1	−19.4774	0.728	0.865	0.803	0.685	0.561
PEPFOLD-model2	−19.464	0.649	0.766	0.643	0.613	0.573
PEPFOLD-model3	−19.3332	0.642	0.812	0.713	0.585	0.457
PEPFOLD-model4	−19.1929	0.643	0.775	0.646	0.611	0.539
PEPFOLD-model5	−18.9826	0.685	0.8	0.722	0.632	0.584

Table S7. PEPFOLD clustering reports (peptide sequence: TPFLVFVVYLFL)

Model	sOPEP	avg	gdt	max	q	tm
PEPFOLD-model1	−19.1114	0.442	0.629	0.489	0.375	0.275
PEPFOLD-model2	−18.3455	0.48	0.659	0.521	0.404	0.335
PEPFOLD-model3	−17.1037	0.487	0.675	0.56	0.42	0.295
PEPFOLD-model4	−15.848	0.541	0.698	0.62	0.493	0.353
PEPFOLD-model5	−15.5831	0.542	0.707	0.626	0.499	0.337

Table S8. The PEPFOLD clustering reports (peptide sequence: SATVFVTFW)

Model	sOPEP	avg	gdt	max	q	tm
PEPFOLD-model1	−6.28941	0.645	0.817	0.728	0.597	0.439
PEPFOLD-model2	−6.26337	0.626	0.809	0.715	0.592	0.389
PEPFOLD-model3	−6.24768	0.631	0.829	0.738	0.572	0.386
PEPFOLD-model4	−5.46783	0.633	0.822	0.733	0.587	0.392
PEPFOLD-model5	−5.44114	0.673	0.841	0.792	0.662	0.399

sOPEP: the coarse grained energy of PEP-FOLD; gdt: the predicted GDT_TS; q: the predicted Qmean score; tm: the predicted TMscore.

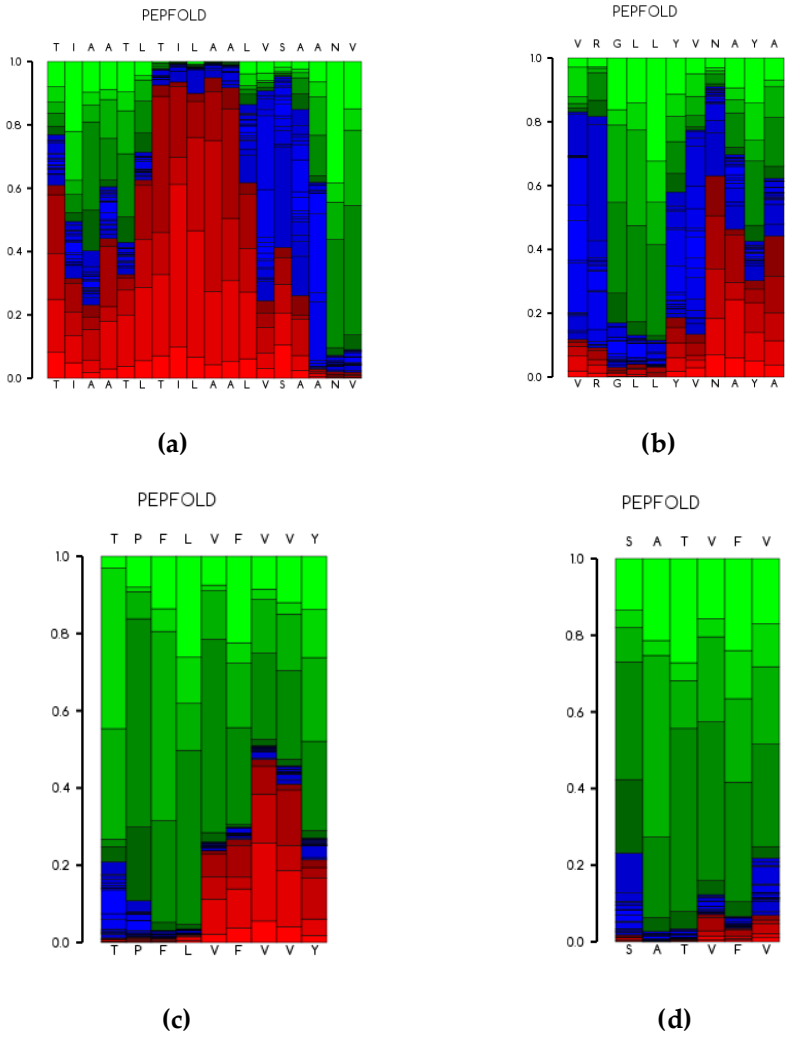

Figure S4. Local structure prediction profile for TIAATLTILAALVSAANVFFF(a); VRGLLYVNAYAFLY (b); TPFLVFVVYLFL (c); SATVFVTFW (d). (The profile is presented using the following color code: red: helical, green: extended, blue: coil)

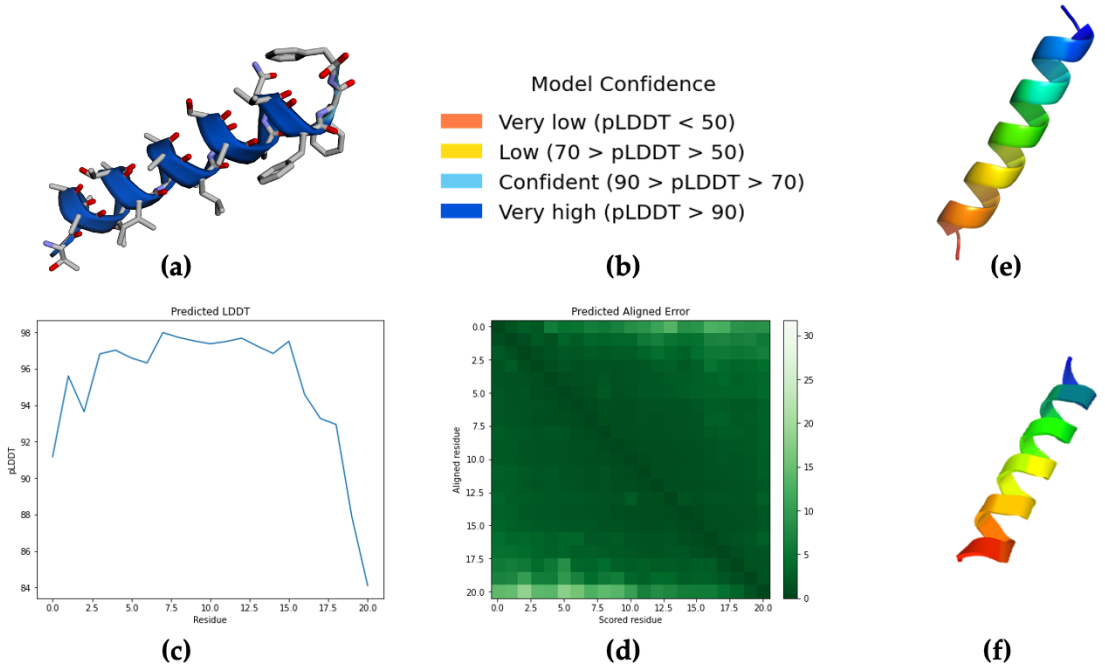

Figure S5. (a) Prediction results of nonanal binding peptide by AlphaFold Colab; (b) Model confidence; (c) In general the predicted local-distance difference test (pLDDT) for intra-domain confidence; (d) Predicted Aligned Error (PAE) for determining between domain or between chain confidence; (e) Peptide helix predicated by AlphaFold; (f) Peptide helix predicated by PEPFOLD3.