

表1 leave-category-out cross-validationによる評価結果：ROC-AUC

		SVM_ linear	SVM_ non-linear	logistic- regression	lightGBM	LSTM	proteinBERT
1	apple	0.998	0.851	0.998	0.999	1.000	1.000
2	bovine	0.927	0.909	0.932	0.940	0.837	0.945
3	buckwheat	0.874	0.532	0.872	0.827	0.842	0.985
4	carrot	0.947	0.794	0.942	0.898	0.968	0.976
5	chicken	0.797	0.492	0.795	0.829	0.927	0.963
6	corn	0.972	0.866	0.971	0.975	0.966	0.984
7	crab	1.000	1.000	1.000	1.000	1.000	1.000
8	kiwi	0.866	0.758	0.874	0.926	0.883	0.896
9	mustard	0.835	0.451	0.844	0.844	0.842	0.918
10	olive	0.980	0.107	0.988	0.996	0.863	1.000
11	oyster	1.000	1.000	1.000	1.000	0.988	0.992
12	peach	0.998	0.848	0.998	1.000	0.998	0.998
13	peanut	0.699	0.672	0.678	0.401	0.524	0.856
14	potato	0.674	0.685	0.680	0.749	0.711	0.960
15	rice	0.840	0.444	0.837	0.831	0.815	0.934
16	salmon	0.924	0.755	0.927	0.866	0.810	0.978
17	shrimp	1.000	0.778	1.000	0.833	1.000	1.000
18	soybean	0.766	0.836	0.762	0.780	0.757	0.961
19	tomato	0.871	0.669	0.861	0.825	0.885	0.841
20	wheat	0.855	0.567	0.852	0.839	0.809	0.927
21	AVERAGE	0.891	0.701	0.891	0.868	0.871	0.956

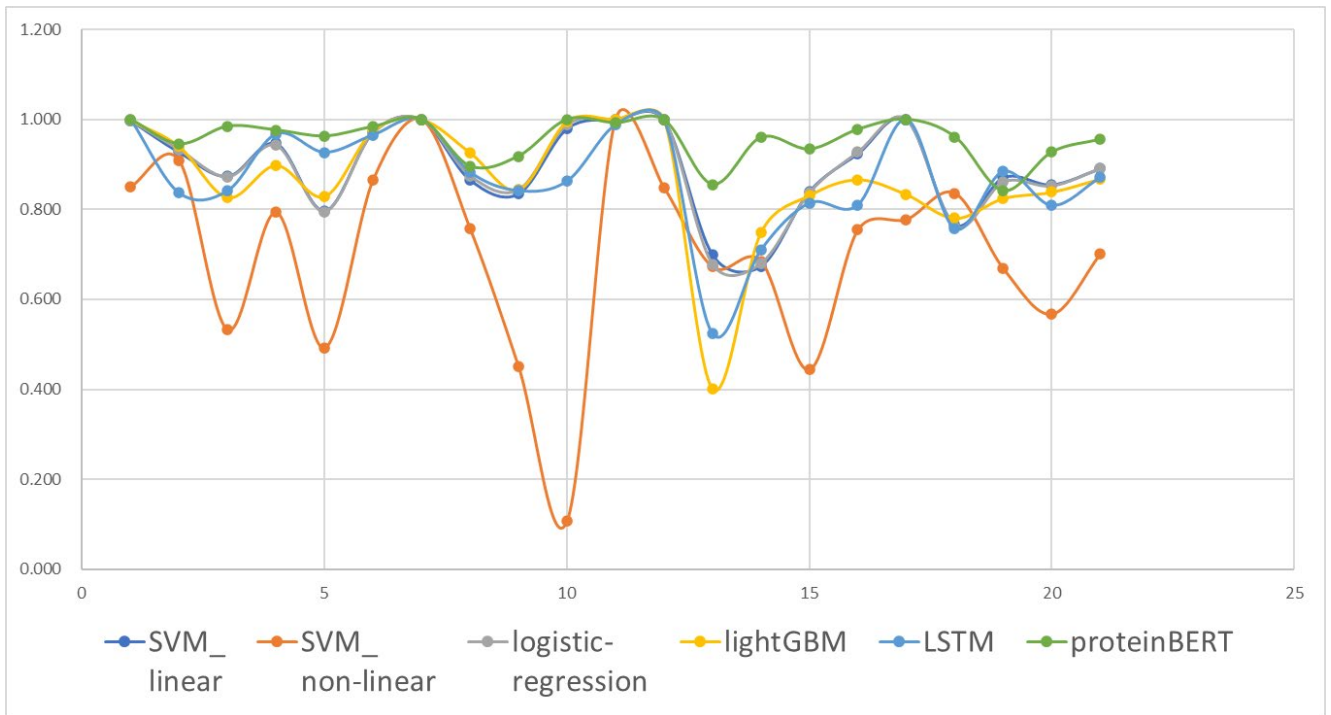


図1 leave-category-out cross-validationによる評価結果：ROC-AUC  
 ※横軸の数字は表1の番号に対応

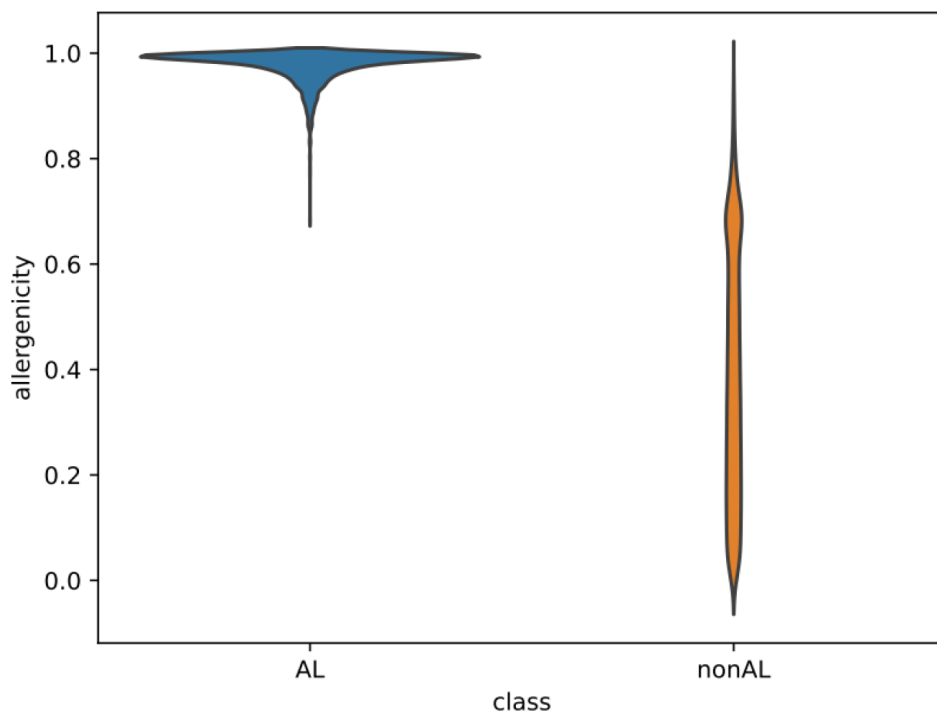
表2 令和4年度にエピトープ情報収集のためピアレビューした論文

1.	Múnera M, Martínez D, Wortmann J, Zakzuk J, Keller W, Caraballo L, Puerta L. Structural and allergenic properties of the fatty acid binding protein from shrimp <i>Litopenaeus vannamei</i> <b>Allergy.</b> 2022 May;77(5):1534-1544. PMID : 34695231
2.	He XR, Yang Y, Kang S, Chen YX, Zheng PY, Chen GX, Chen XM, Cao MJ, Jin T, Liu GM. Crystal Structure Analysis and IgE Epitope Mapping of Allergic Predominant Region in <i>Scylla paramamosain</i> Filamin C. <i>Scy p 9</i> <b>J Agric Food Chem.</b> 2022 Feb 2;70(4):1282-1292. PMID : 35040643
3.	Schmalz S, Mayr V, Shosherova A, Gepp B, Ackerbauer D, Sturm G, Bohlé B, Breiteneder H, Radauer C. Isotype-specific binding patterns of serum antibodies to multiple conformational epitopes of Bet v 1 <b>J Allergy Clin Immunol.</b> 2022 May;149(5):1786-1794. PMID : 34740603
4.	Han TJ, Huan F, Liu M, Li MS, Yang Y, Chen GX, Lai D, Cao MJ, Liu GM. IgE epitope analysis of sarcoplasmic calcium-binding protein, a heat-resistant allergen in <i>Crassostrea angulata</i> <b>Food Funct.</b> 2021 Sep 20;12(18):8570-8582. PMID : 34338271
5.	Moten D, Kolchakova D, Todorov K, Mladenova T, Dzhambazov B. Design of an Epitope-Based Peptide Vaccine Against the Major Allergen Amb a 11 Using Immunoinformatic Approaches <b>Protein J.</b> 2022 Apr;41(2):315-326. PMID : 35362839
6.	Li M, Xia F, Chen Y, Liu M, Liu Q, Yang Y, Chen G, Wang L, Cao M, Liu G. Two hypo-allergenic derivatives lacking the dominant linear epitope of Scy p 1 and Scy p 3 <b>Food Chem.</b> 2022 Mar 30;373(Pt B):131588. PMID : 34801289
7.	Curin M, Huang HJ, Garmatuk T, Gutfreund S, Resch-Marat Y, Chen KW, Fauland K, Keller W, Ziegelmayer P, Ziegelmayer R, Lemell P, Horak F, Hemmer W, Focke-Tejkl M, Flicker S, Vrtala S, Valenta R. IgE Epitopes of the House Dust Mite Allergen Der p 7 Are Mainly Discontinuous and Conformational <b>Front Immunol.</b> 2021 Jun 15;12:687294. PMID : 34220841
8.	Li WY, Cai ZL, Zhang BP, Chen JJ, Ji K. Identification of an immunodominant IgE epitope of Der p 39, a novel allergen of <i>Dermatophagoides pteronyssinus</i> <b>World Allergy Organ J.</b> 2022 May 6;15(5):100651. PMID : 35600837
9.	Chen G, Shrock EL, Li MZ, Spergel JM, Nadeau KC, Pongracic JA, Umetsu DT, Rachid R, MacGinnitie AJ, Phipatanakul W, Schneider L, Oettgen HC, Elledge SJ. High-resolution epitope mapping by AllerScan reveals relationships between IgE and IgG repertoires during peanut oral immunotherapy <b>Cell Rep Med.</b> 2021 Oct 19;2(10):100410. PMID : 34755130
10.	Sharma S, Vashisht S, Gaur SN, Lavasa S, Arora N. Effects of the Maillard reaction on the epitopes and immunoreactivity of tropomyosin, a major allergen in <i>Chlamys nobiles</i> . <b>Immunobiology.</b> 2021 Nov;226(6):152146. PMID : 34717182
11.	Huan F, Han TJ, Liu M, Li MS, Yang Y, Liu QM, Lai D, Cao MJ, Liu GM. Identification and characterization of <i>Crassostrea angulata</i> arginine kinase, a novel allergen that causes cross-reactivity among shellfish <b>Food Funct.</b> 2021 Oct 19;12(20):9866-9879. PMID : 34664604
12.	Cheng Q, Feng X, Zhao X, Gu R, Lu J, Liu W, Li G. Physicochemical characterization and identification of major linear epitopes of sarcoplasmic calcium-binding protein (SCP) allergen from Pacific oyster ( <i>Crassostrea gigas</i> ) <b>J Sci Food Agric.</b> 2021 Dec 1. PMID : 34854091
13.	Calzada D, Aranda T, M Gallego G, Escutia MR, Balsa D, Álvarez J, Mayorga C, Salas M, Odena MA, Oliveira E, Pascal M, Carnés J. Immunological mechanisms involved in the human response to a dog dander allergoid <b>Mol Immunol.</b> 2022 May;145:88-96. PMID : 35306358
14.	Xu LL, Gasset M, Lin H, Yu C, Zhao JL, Dang XW, Li ZX. Identification of the Dominant T-Cell Epitopes of Lit v 1 Shrimp Major Allergen and Their Functional Overlap with Known B-Cell Epitopes <b>J Agric Food Chem.</b> 2021 Jul 7;69(26):7420-7428. PMID : 34170668
15.	Brassee-Estandante HA, Martínez-Cruz O, Cárdenas-López JL, García-Orozco KD, Ochoa-Leyva A, López-Zavala AA. Identification of arginine kinase as an allergen of brown crab, <i>Callinectes bellicosus</i> , and in silico analysis of IgE-binding epitopes <b>Mol Immunol.</b> 2022 Mar;143:147-156. PMID : 35131595
16.	Kumagai A, Nara T, Uematsu M, Kakinuma Y, Saito T, Masuda K. Development and characterization of a unique anti-IgE mouse monoclonal antibody cross-reactive between human and canine IgE <b>Immun Inflamm Dis.</b> 2021 Dec;9(4):1740-1748. PMID : 34533288
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表3 令和4年度に新たにADFSに追加したエピトープ情報

	Name	start	end	Sequence	Method	CTYPE	Reference	UniProt acc.No
001	Lit v 13	40	85	VEITKDGDTYTMKTTTTFKTTEIKFKLGEFEETTADGRVVKSTIT	Peptide array/ELISA	L	PMID 34695231	E2IH93
	Lit v 13	107	136	ELLREFTDDKMLMECKVDDVVKRVYSRLR	Peptide array/ELISA	L	PMID 34695231	E2IH93
002	Scy p 9	336	353	GTNRQTERIKRQREAVPL	Dot blot/bioinformatics/ELISA	L	PMID 35040643	A0A5J6X3F8
	Scy p 9	363	377	TFKLPGISPFDLGAT	Dot blot/bioinformatics/ELISA	L	PMID 35040643	A0A5J6X3F8
	Scy p 9	418	433	EMHIPGSPFQFTVGPL	Dot blot/bioinformatics/ELISA	L	PMID 35040643	A0A5J6X3F8
	Scy p 9	446	462	PGLERGEQGMNPEFNWV	Dot blot/bioinformatics/ELISA	L	PMID 35040643	A0A5J6X3F8
	Scy p 9	490	505	DGSCYVSYVAEPGEY	Dot blot/bioinformatics/ELISA	L	PMID 35040643	A0A5J6X3F8
	Scy p 9	512	528	NDKHIPDSPYKYYITPS	Dot blot/bioinformatics/ELISA	L	PMID 35040643	A0A5J6X3F8
	Scy p 9			338 - 343,449 - 456,476 - 482,498 - 504,506,522,524 - 528	Dot blot/bioinformatics/ELISA	C	PMID 35040643	A0A5J6X3F8
	Scy p 9			345,347,349 - 359,379 - 389,403 - 408,430 - 434,467 - 470,512 - 514	Dot blot/bioinformatics/ELISA	C	PMID 35040643	A0A5J6X3F8
	Scy p 9			366 - 375,390 - 397,415 - 420	Dot blot/bioinformatics/ELISA	C	PMID 35040643	A0A5J6X3F8
003	Bet v 1				ELISA	C	PMID 34740603	O23746
004	Cra a 4	22	33	KISIEDVEESRN	ELISA	L	PMID 34338271	A0A6G7MAZ4
	Cra a 4	64	75	TGAGKEISESEF	ELISA	L	PMID 34338271	A0A6G7MAZ4
	Cra a 4	80	90	TEAYKKDKVGF	ELISA	L	PMID 34338271	A0A6G7MAZ4
	Cra a 4	107	116	TNKDRITDED	ELISA	L	PMID 34338271	A0A6G7MAZ4
	Cra a 4	144	159	NKHVPLKDIVSEWVKF	ELISA	L	PMID 34338271	A0A6G7MAZ4
	Cra a 4	131	150	G48, D99, I101, D103, I105, D110, R111, D114, D116, A124, A136, W156	ELISA	C	PMID 34338271	A0A6G7MAZ4
	Cra a 4	170	188	D114, R134, A136, S138, L139, N141, N144, L149, D151, V153, S154, V157, F159	ELISA	C	PMID 34338271	A0A6G7MAZ4
005	Amb a 11	173	186	GKLVKFEQQLVDC	bioinformatics/ELISA	L	PMID 35362839	V5LU01
006	Scy p 1	39	48	TEEEIRATQK	ELISA	L	PMID 34801289	A7L5V2
	Scy p 1	153	162	FLAEEADRKY	ELISA	L	PMID 34801289	A7L5V2
007	Scy p 3	35	47	DCLRALNLNPTLA	ELISA	L	PMID 34801289	A0A514C9K9
	Scy p 3	66	80	DDFLPIFAQVKKDKD	ELISA	L	PMID 34801289	A0A514C9K9
	Scy p 3	109	120	HILLSLGERLEK	ELISA	L	PMID 34801289	A0A514C9K9
008	Der p 7	18	47	DPIHYDKITEINKAVDEAVAIEKSETFD	immunoblot/inhibition ELISA	L	PMID 34220841	P49273
	Der p 7	37	67	VAAIEKSETFDPMPKVPDHSKFERHIGIIDL	immunoblot/inhibition ELISA	L	PMID 34220841	P49273
	Der p 7	67	97	LKGELDMRNIQVRGLKQMKRVGDANVKSSEDG	immunoblot/inhibition ELISA	L	PMID 34220841	P49273
	Der p 7	107	142	VHDDVVSMEYDLAYKGLDHPNTHVISDIQDFVEL	immunoblot/inhibition ELISA	L	PMID 34220841	P49273
	Der p 7	140	165	VELSLEVSEEGNMTLTSFEVRQFANV	immunoblot/inhibition ELISA	L	PMID 34220841	P49273
	Der p 7	166	193	VNHIGGLSILDPIFAVLSVLTAFQDT	immunoblot/inhibition ELISA	L	PMID 34220841	P49273
	Der p 7	187	215	TAIFQDTRAEEMTKVLAPAFKKELERNNQ	immunoblot/inhibition ELISA	L	PMID 34220841	P49273
	Der p 7				immunoblot/inhibition ELISA	C	PMID 34220841	P49273
	Der p 7				immunoblot/inhibition ELISA	C	PMID 34220841	P49273
009	Der p 39	87	97	QEELREAFRMY	Western Blot/dot blot/ELISA	L	PMID 35600837	A0A6P6YD30
	Der p 39	107	117	TSALREILRAL	Western Blot/dot blot/ELISA	L	PMID 35600837	A0A6P6YD30
	Der p 39	123	133	NDELDEMAIEI	Western Blot/dot blot/ELISA	L	PMID 35600837	A0A6P6YD30
010	Ara h 2.02	21	40	ARQQWELQDGRRCQQLERA	AllerScan	L	PMID 34755130	Q6PSU2
011	Ara h 3.01	301	320	ERDPYSPSQDPYSPSPYDRR	AllerScan	L	PMID 34755130	O82580
012	Ara h 7.01	71	90	QEQDEYPYRRGRSRGRQPGE	AllerScan	L	PMID 34755130	Q9SQH1
013	Per a 5	32	47	VTNLMAGEHLTPEFLK	bioinformatics/ELISA	L	PMID 34717182	A0A2K9YV03
	Per a 5	77	92	QYGKDDSLYPKDAKKR	bioinformatics/ELISA	L	PMID 34717182	A0A2K9YV03
	Per a 5	114	135	YYPIYFAKQAADPEKMKLEEA	bioinformatics/ELISA	L	PMID 34717182	A0A2K9YV03
014	Cra a 2	56	73	SGAGVYACDPGEYEVFKE	dot blot/inhibition ELISA	L	PMID 34664604	
	Cra a 2	77	92	PVIMDYHKVKVEHPP	dot blot/inhibition ELISA	L	PMID 34664604	
	Cra a 2	93	107	CDFGPQDKLGFDPD	dot blot/inhibition ELISA	L	PMID 34664604	
	Cra a 2	121	133	GRSHEGYPPFVVS	dot blot/inhibition ELISA	L	PMID 34664604	
	Cra a 2	134	146	TDEQRKEMENKTI	dot blot/inhibition ELISA	L	PMID 34664604	
	Cra a 2	165	176	TMTPEENQQLID	dot blot/inhibition ELISA	L	PMID 34664604	
	Cra a 2	185	200	DKMLGDAGGYNGWPKA	dot blot/inhibition ELISA	L	PMID 34664604	
	Cra a 2	227	238	QKGGDVEVYKR	dot blot/inhibition ELISA	L	PMID 34664604	
	Cra a 2	306	323	GEHTESVGGYDISNKR	dot blot/inhibition ELISA	L	PMID 34664604	

## SVM



## proteinBERT

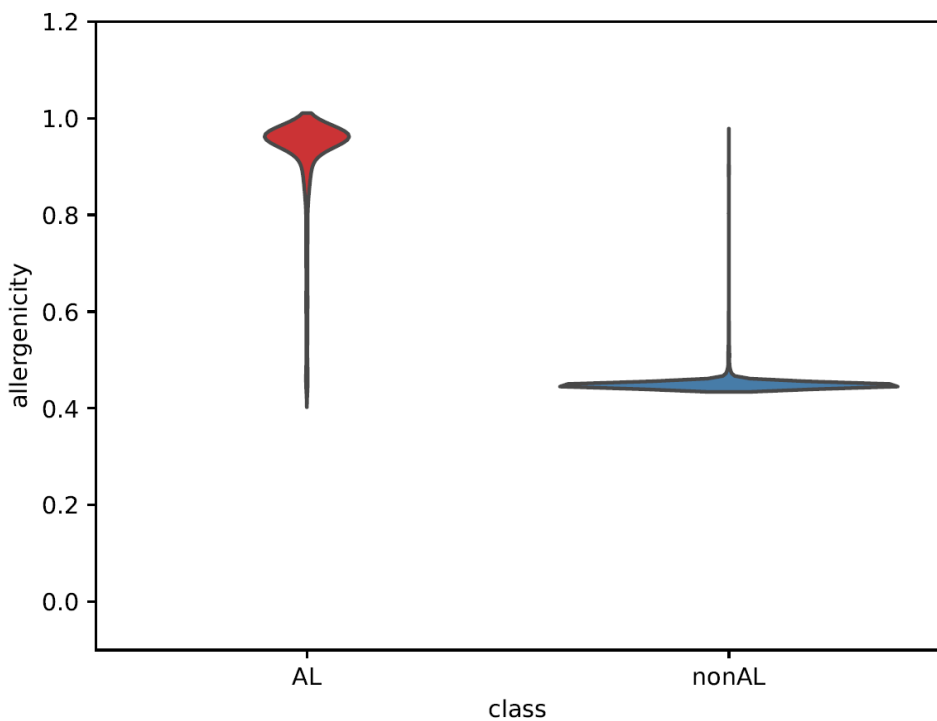


図2 アレルゲン及び非アレルゲンデータの分布  
AL: allergen data, nonAL: non-allergen data