

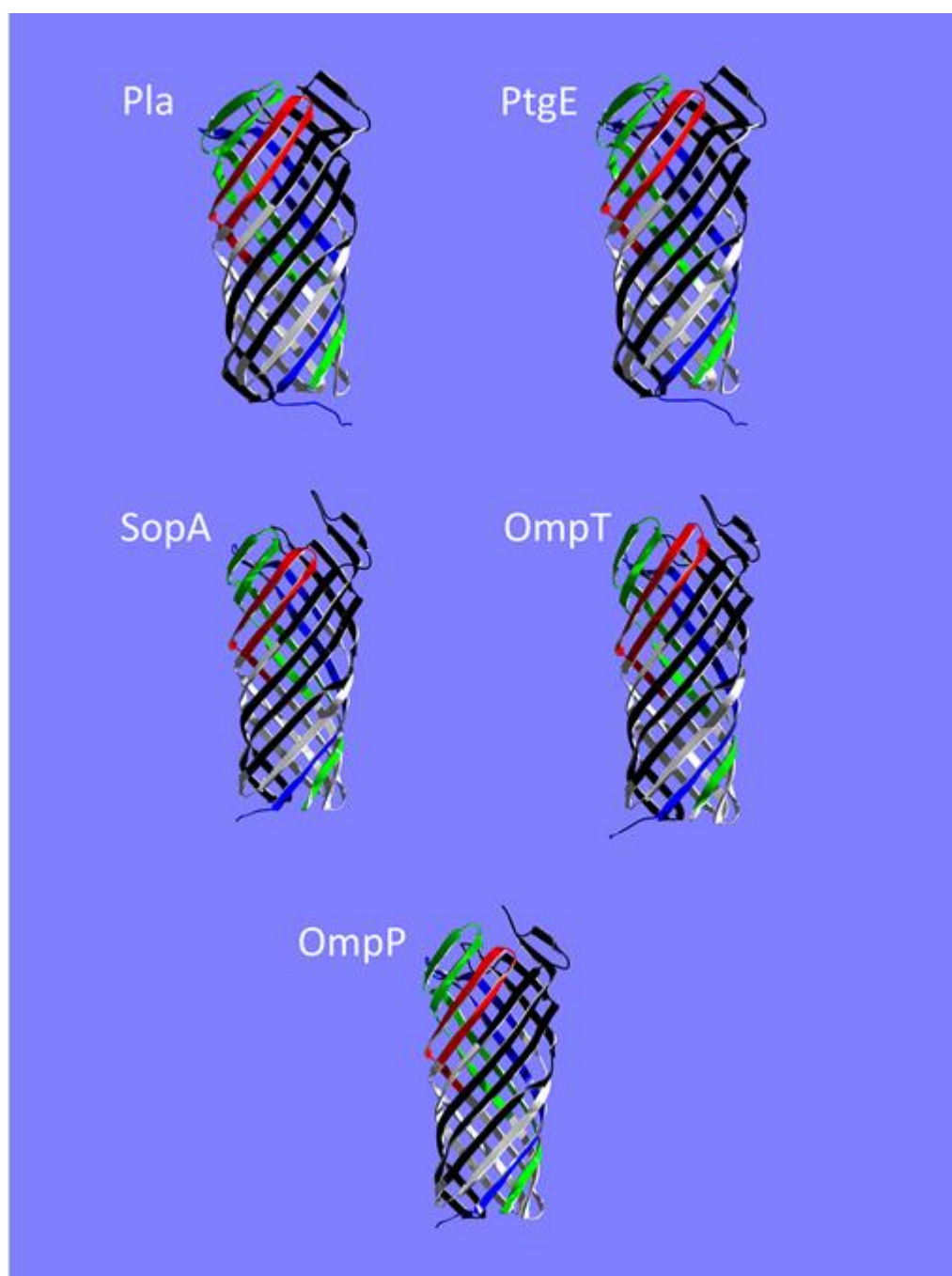
Article

# New Promising Targets for Synthetic Omptin-Based Peptide Vaccine against Gram-Negative Pathogens

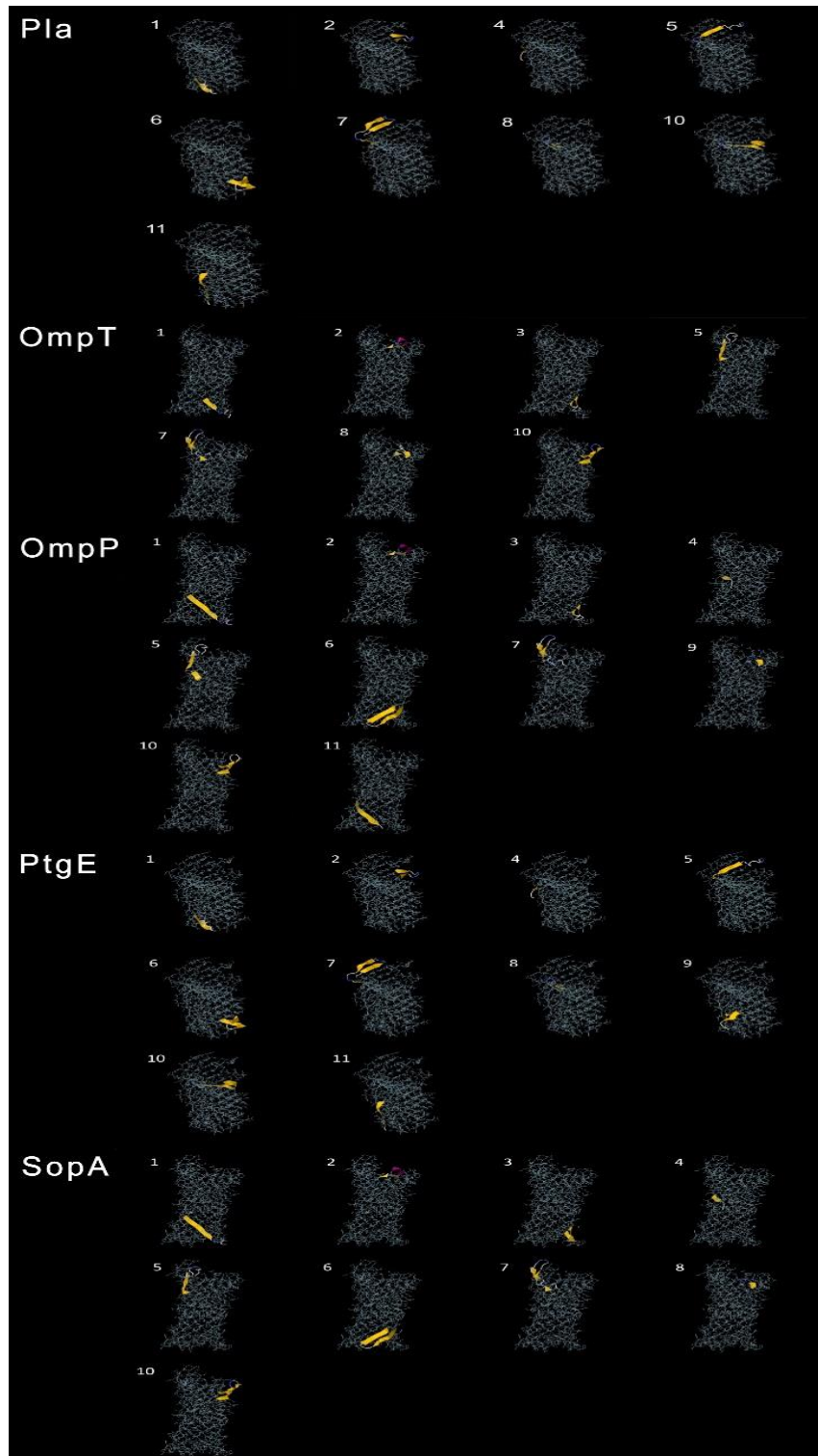
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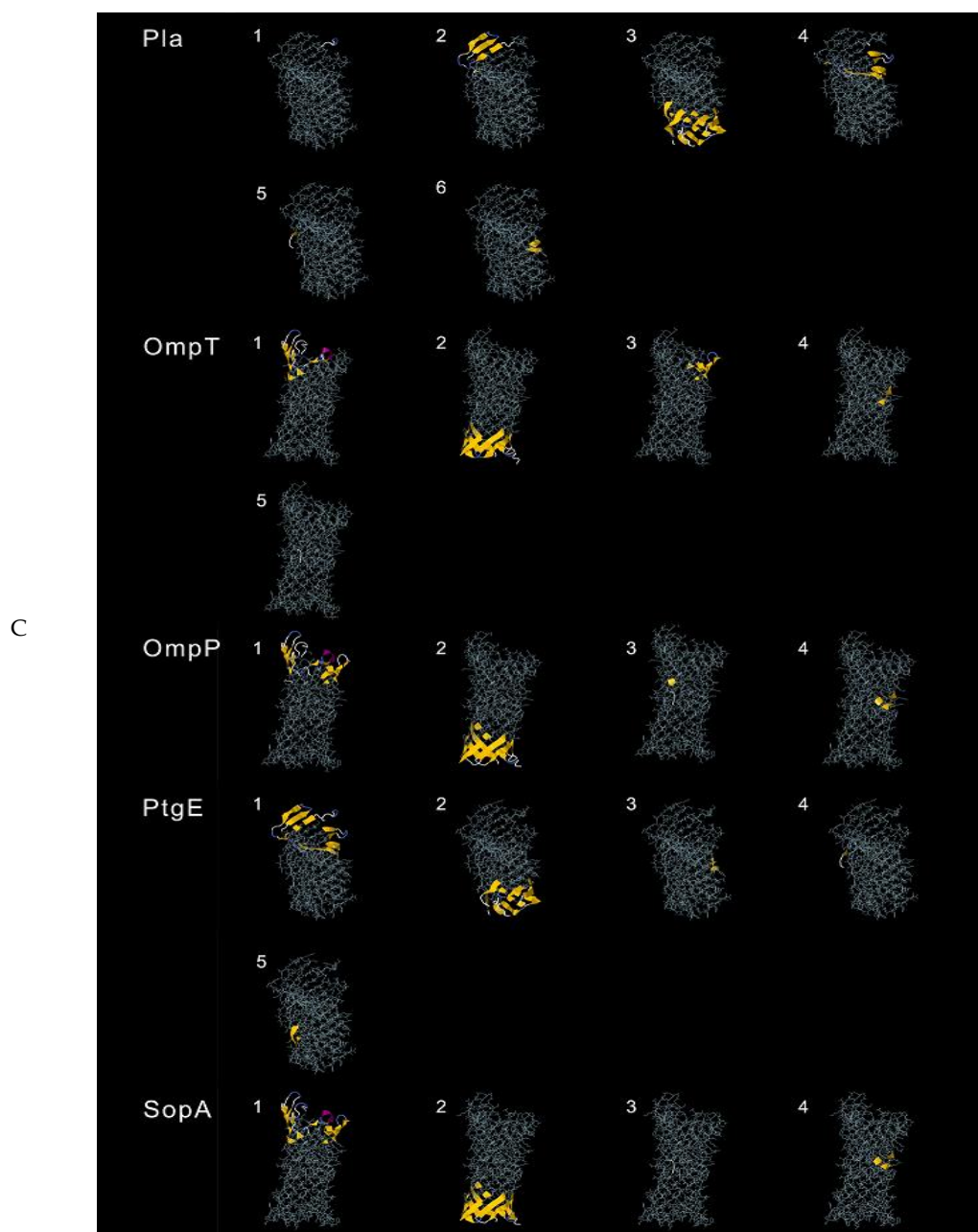
Supplementary Materials:

A



B





**Figure S1.** Structural 3D ribbon diagrams modeling of omptin protein family based on the: (A) original amino acid sequence of Pla, OmpT, OmpP, PgtE, and SopA. The four immune-reactive clusters colored in blue (epitope no. 1), black (epitope no. 2), red (epitope no. 3), and green (epitope no. 4). All models were generated with Swiss-PdbViewer/DeepView v. 4.1. (B) B-cell linear epitope residues of the Pla, OmpT, OmpP, PgtE, and SopA. (C) B-cell conformational epitope residues of Pla, OmpT, OmpP, PgtE, and SopA.

**Table 1S.** Predicted antigenic and allergenic results of the B-cell linear omptins.

Epitope No.	Omptin	Epitope Sequence <sup>2</sup>	Allergenicity of the B-Cell Epitope
1	Pla	<u>SSQLIPNISPDSFTV</u>	Non-Allergenic
	PgtE	<u>SALFIPDVSPDSVTT</u>	Non-Allergenic
	SopA	<u>FIPDNISTDISL</u>	Non-Allergenic
	OmpT	<u>LSFTPEKIST</u>	<b>Probable Allergen</b>
	OmpP	<u>FGPEKISTEINL</u>	Non-Allergenic
2	Pla	<u>YDAETGRKI</u>	Non-Allergenic
	PgtE	<u>YDTDTRKLL</u>	Non-Allergenic

	SopA	<u>HPKEGGR</u>	Non-Allergenic
	OmpT	<u>LPEEKGR</u>	Non-Allergenic
	OmpP	<u>EPEEGGR</u>	Non-Allergenic
	Pla	-	-
	PgtE	-	-
3	SopA	<u>WKLIPKVSF</u>	Probable Allergen
	OmpT	<u>WDLLPRVSV</u>	Probable Allergen
	OmpP	<u>WELNPWLSV</u>	Non-Allergenic
	Pla	<u>LASG</u>	Non-Allergenic
	PgtE	<u>LASG</u>	Non-Allergenic
4	SopA	<u>LGNOK</u>	Non-Allergenic
	OmpT	-	-
	OmpP	<u>LNSR</u>	Non-Allergenic
	Pla	<u>WMNENOSEWTDHSSHPAT</u>	Non-Allergenic
	PgtE	<u>WMSSEOPGWTDRSIHPD</u>	Non-Allergenic
5	SopA	<u>WNSNTPOVWTDQSWHPN</u>	Non-Allergenic
	OmpT	<u>WLDTSNPGTWTDESKHPN</u>	Non-Allergenic
	OmpP	<u>WMDSGTPGTWTDESRHPDTR</u>	Non-Allergenic
	Pla	<u>VKGWLLQDENYKAGI</u>	Non-Allergenic
	PgtE	<u>VKGWLLQGDNYKAGV</u>	Non-Allergenic
6	SopA	<u>LKGWLLNNLDYRLGL</u>	Non-Allergenic
	OmpT	-	-
	OmpP	<u>VKGWFLKESDYRLAI</u>	Non-Allergenic
	Pla	<u>ATGGSYSYNNGAYTGNFPGKVR</u>	Non-Allergenic
	PgtE	<u>RGGSYIYDNGRYIGNFPHGVR</u>	Non-Allergenic
7	SopA	<u>MGGSYIYSENGGSRNKKGAHPSGERT</u>	Non-Allergenic
	OmpT	<u>KGGSYIYSSEGGFRDETGSFPDGER</u>	Non-Allergenic
	OmpP	<u>TGGTYIYSENGGFRNETGALPDKIKV</u>	Non-Allergenic
	Pla	<u>EHYMRDLT</u>	Non-Allergenic
	PgtE	<u>EHYMRKLT</u>	Non-Allergenic
8	SopA	<u>YQETETI</u>	Non-Allergenic
	OmpT	<u>YNPEKRIT</u>	Non-Allergenic
	OmpP	<u>YVROTT</u>	Non-Allergenic
	Pla	-	-
	PgtE	<u>GYIITSNAKI</u>	Probable Allergen
9	SopA	-	-
	OmpT	-	-
	OmpP	<u>AGYYITPEAKVYI</u>	Probable Allergen
	Pla	<u>KGGTQOTIDKNSGDSVSIKGDAA</u>	Non-Allergenic
	PgtE	<u>KGGTQIIDKTSKTDAYFGGDA</u>	Non-Allergenic
10	SopA	<u>KGDTSLYEQSTNISGTIKNS</u>	Non-Allergenic
	OmpT	<u>KGDTSLYSRNLNIDHTKNG</u>	Non-Allergenic
	OmpP	<u>KGDTSLYDRSDNTSEHNNNG</u>	Non-Allergenic
	Pla	<u>AGLQYRF</u>	Non-Allergenic
	PgtE	<u>AGLQYRF</u>	Probable Allergen
11	SopA	-	-
	OmpT	-	-
	OmpP	<u>GTALKYTF</u>	Non-allergenic

<sup>1</sup> AlgPred<sup>31</sup> (<http://crdd.osdd.net/raghava/algpred/index.html>) and AllerTOP<sup>32</sup> v. 2.0 (<http://www.ddg-pharmfac.net/AllerTOP>) services were used for prediction of allergenicity. <sup>2</sup> B-cell epitopes were predicted by ElliPro (<http://tools.immuneepitope.org/toolsElliPro/>).



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