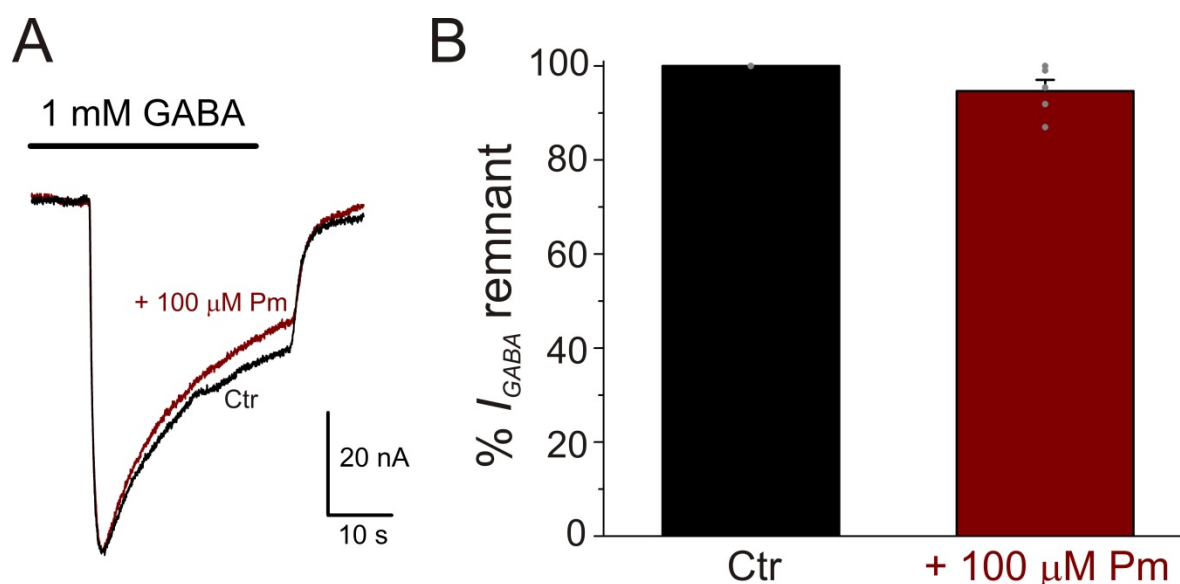


SUPPLEMENTARY MATERIAL

Peimine, an anti-inflammatory compound from Chinese herbal extracts, modulates muscle-type nicotinic receptors.

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Supplementary Figure 1. Lack of effect of Pm on GABA-elicited currents (I_{GABA}). **A.** Superimposed I_{GABA} s elicited by 1 mM GABA alone (black recording) or together with 100 μ M Pm (red trace) in an oocyte previously injected with synaptosomal-enriched rat-brain membranes. Notice that Pm, even at concentrations as high as 100 μ M, did not attenuate I_{GABA} . **B.** Column graph showing the percentage of I_{GABA} in the control (black) and Pm (red) groups. There was not significant differences between both groups ($p < 0.05$, t -test). Data are from 5 oocytes of 3 donor frogs.

Supp. Table 1. Putative nAChR residues interacting with Pm in the open and the closed conformation, as predicted from molecular docking simulations.

nAChR State	Domain	Pm Cluster	Binding energy (Kcal/mol)	Residues (subunit name-residue name-number)
OPEN	TMD	1	-10.12	β (A258, V261, F262, L265), γ (L265, A266, V269, F270, L273), αγ (V255, F256, V259, E262, I263), δ (F266, L267, Q270)
		2	-10.57	αδ (T244, L245, I247, S248), β (S250, I253, S254, L257, A258, V261, F262), γ (C262, L265, A266, V269, F270), αγ (S248, L251, S252, V255), δ (T252, S256, L259)
		3	-11.24	αγ (Y213, F214, N217, V218, I220, P221, I260, L263, I264, T267), δ (F266, A269, Q270, P273, L277, L281, L286, M290)
		4	-11.06	αδ (F135, F137, I210, F214, V215, V218, I219, C222, I260, I264, Y277, F280, T281, F284, V285, A427, G428, I431, E432)
		5	-10.82	δ (F134, L219, Y221, I222, I225, I226, C229, V230, V272, S276, Y285, L286, F288, V289, V292, A464, I465, T468)
		6	-10.71	β (E45, F135, Q185, W186, R215, P217, F219, Y220, I221, T224, V270, T273, S274, V277, P278, I279, I280, I281, Y283, L284), γ (L283)
		7	-10.68	γ (E47, F137, F139, W141, R223, K224, P225, Y228, V229, F232, I233, L278, T281, V285, L287, Y291, F294, I295, F471, F478)
		8	-10.56	αδ (I219, C222, L223, F225, S226, T229, V230, F233, F284, V285, S287, S288, V291, I417, I420, G421, S424, V425, G428)
		9	-10.42	γ (F137, R223, P225, Y228, V229, F232, I233, C236, L278, T281, V285, L287, Y291, L292, F294, I295, F471)
		10	-10.29	αγ (F135, F137, F214, V218, I219, C222, I264, L273, Y277, M278, F280, T281, F284, S424, V425, G428, R429, I431)
		11	-10	β (Y220, I221, Y223, T224, P227, L266, K269, V270, E272, T273), γ (L273, Q276, P279, E280, L283)
		12	-9.87	αγ (E175, P211, Y213, F214, N217, L263, S266, T267), δ (F266, A269, Q270, K271, P273, E274, L277, L281, M290)
		13	-9.3	γ (E186, N187, G188, E189, W190, P225, L226, F227), αγ (V46, N47, Q48, Y127, I130, V132, S269, P272)
	ECD	14	-11.97	γ (S40, N55, W57, P123), αγ (V91, Y93, N94, A96, W149, T150, Y151, D152, P197, Y198)
		15	-10.89	αδ (V91, L92, Y93, A96, I148, W149, T150, Y190, C192, C193, Y198), δ (T35, T37, N52, W54, E56, Y116, L118, P120)
		16	-10.72	αδ (I148, W149, T150, Y151, D152, Y190, P197, Y198), δ (T35, W54, R78, L108, Y116, L118, E175)
		17	-10.49	αδ (L87, P88, D89, L90, V91, A96, G98, D99, F100, V103, H104, M105, W118, W149), δ (V101, Y104, P120)
CLOSED	TMD	1	-11.2	αδ (T244, L245, I247, S248, L251), β (I253, S254, L257, A258, V261, F262), γ (C262, L265, A266, V269, F270), αγ (S248, L251, S252, V255), δ (T252, S256, L259, I263)
		2	-12.87	β (Q185, L218, F219, Y220, V222, Y223), γ (T48, V134, A282, L283, A284, V285, P286, L287, I288, G289, L292, M293, M296)
		3	-11.49	β (F135, Q185, P217, F219, Y220, I221, T224, K269, V270, T273, S274, V277, P278, I279, I280, I281, Y283, L284, I287), γ (L283)
		4	-10.87	δ (F134, F136, K217, L219, Y221, I222, I225, I226, V272, P273, S276, L281, I282, Y285, L286, V289, I465, T468)
		5	-10.84	αγ (F135, F137, I210, F214, V215, V218, I219, C222, I264, L273, Y277, M278, F280, T281, F284, S424, V425, G428, R429)
		6	10.75	αγ (F135, F137, I210, F214, V215, V218, I219, L273, Y277, M278, F280, T281, F284, G421, S424, V425, G428, R429)
		7	-10.18	β (P242, P243, D244, A245, G246, E247, M249, L304, H305, H306, R307, S308, T311, H312, Y430, V431, A432, A435, D436), γ (P317, S318)
		8	-10.17	αδ (F137, I210, F214, V215, V218, I219, C222, L223, F225, S226, F280, F284, G421, T422, S424, V425, G428)
		9	-10.11	αδ (F137, I210, F214, V215, V218, I219, C222, L223, F225, Y277, F280, T281, F284, G421, T422, S424, V425)
		10	-9.61	αγ (E172, S173, G174, E175, P211, Y213, V271), δ (K45, E46, A130, V131, S276, L277, N278, V279, P280, L281)
	ECD	11	-11.52	αδ (L87, P88, D89, L90, V91, L92, A96, D97, G98, D99, F100, V103, H104, W118, F124, W149), δ (V101, P120)
		12	-10.98	γ (S40, N55, W57, V104, P123), αγ (V91, Y93, I148, W149, T150, Y151, D152, P197, Y198)
		13	-10.6	αδ (V91, L92, Y93, N94, I148, W149, T150, Y190, Y198), δ (T35, T37, W54, E56, Y116, L118, P120)
		14	-10.39	γ (W57, V104, P123, I125), αγ (D89, L90, V91, L92, Y93, N94, N95, A96, D99, F100, I148, W149, Y198)
		15	-10.34	γ (S40, N41, N55, W57, P123), αγ (V91, L92, Y93, N94, N95, A96, G147, I148, W149, T150, Y190, P197, Y198)
		16	-9.59	αγ (E2, E4, L7, V8, L11, A70, D71, G74, I75, I78, R79, L80, P81), δ (R17, L24, Y150)