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MDPI

*SUPPLEMENTARY MATERIAL*

# Peimine, an Anti-Inflammatory Compound from Chinese Herbal Extracts, Modulates Muscle-Type Nicotinic Receptors

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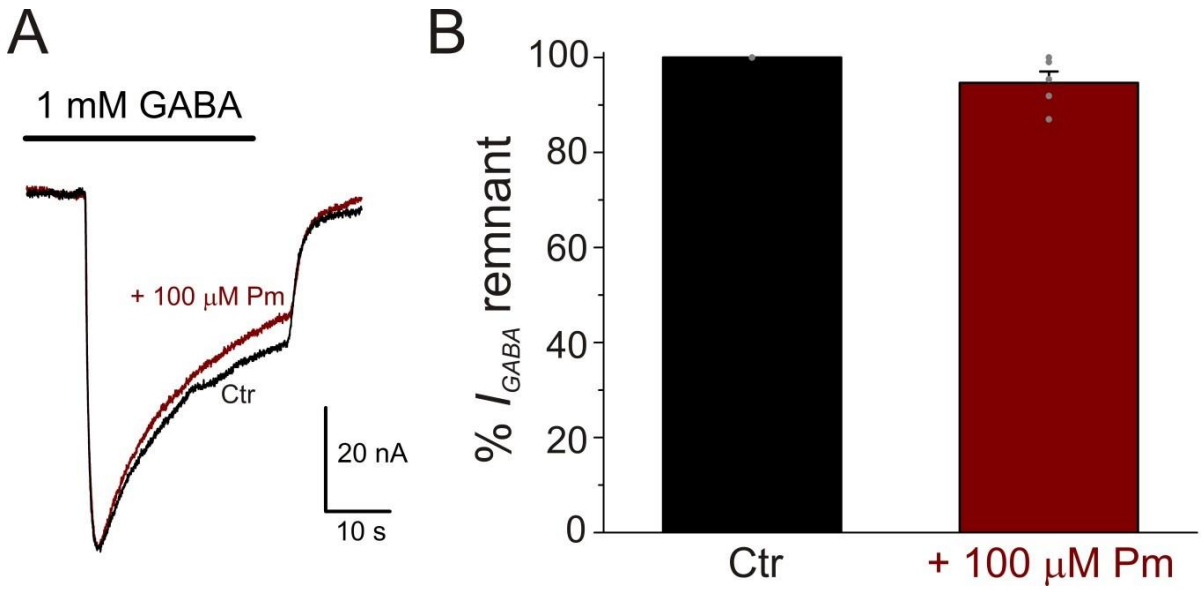


**Supplementary Figure S1.** Lack of effect of Pm on GABA-elicited currents ($I_{GABA}$). **A**. Superimposed $I_{GABA}$s elicited by 1 mM GABA alone (black recording) or together with 100 μM Pm (red trace) in an oocyte previously injected with synaptosomal-enriched rat-brain membranes. Notice that Pm, even at concentrations as high as 100 μM, 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.

**Scheme 1.** Putative nAChR residues interacting with Pm in the open and theclosed conformation, as predicted from molecular docking simulations.

| nAChR State | Dmain | Pm Cluter | Binding energy (Kcal/mo) | 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) |