Supporting Information

Computational and functional mapping of human and rat α6β4 nicotinic acetylcholine receptors reveals species-specific ligand-binding motifs

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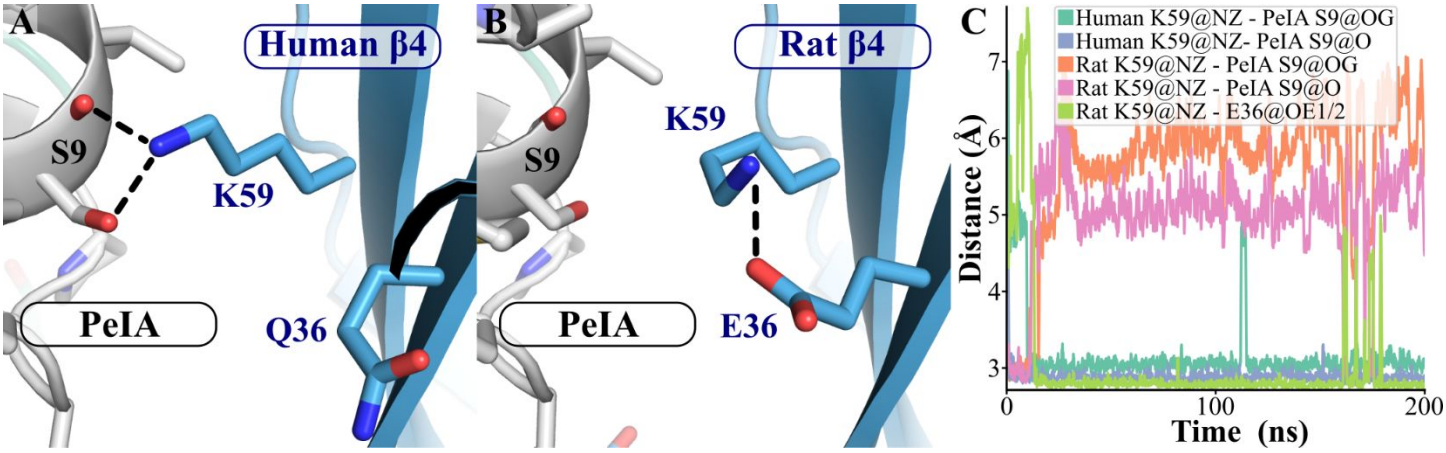

Figure 1. Molecular models of the interactions of PeIA Ser[9] with human or rat α6β4 nAChRs. (A,B) Molecular models of the interactions between Ser[9] and human β4 residues (A) or rat β4 residues (B). (C) Evolution of several distances between atoms potentially forming hydrogen bonds during the 200 ns molecular dynamics simulations of the human and rat receptors. The molecular models shown in (A,B) correspond to those described in Figure 1. The inter atom distances monitored in (C) are considered representative of hydrogen bonding if the they are under 3.2 Å.

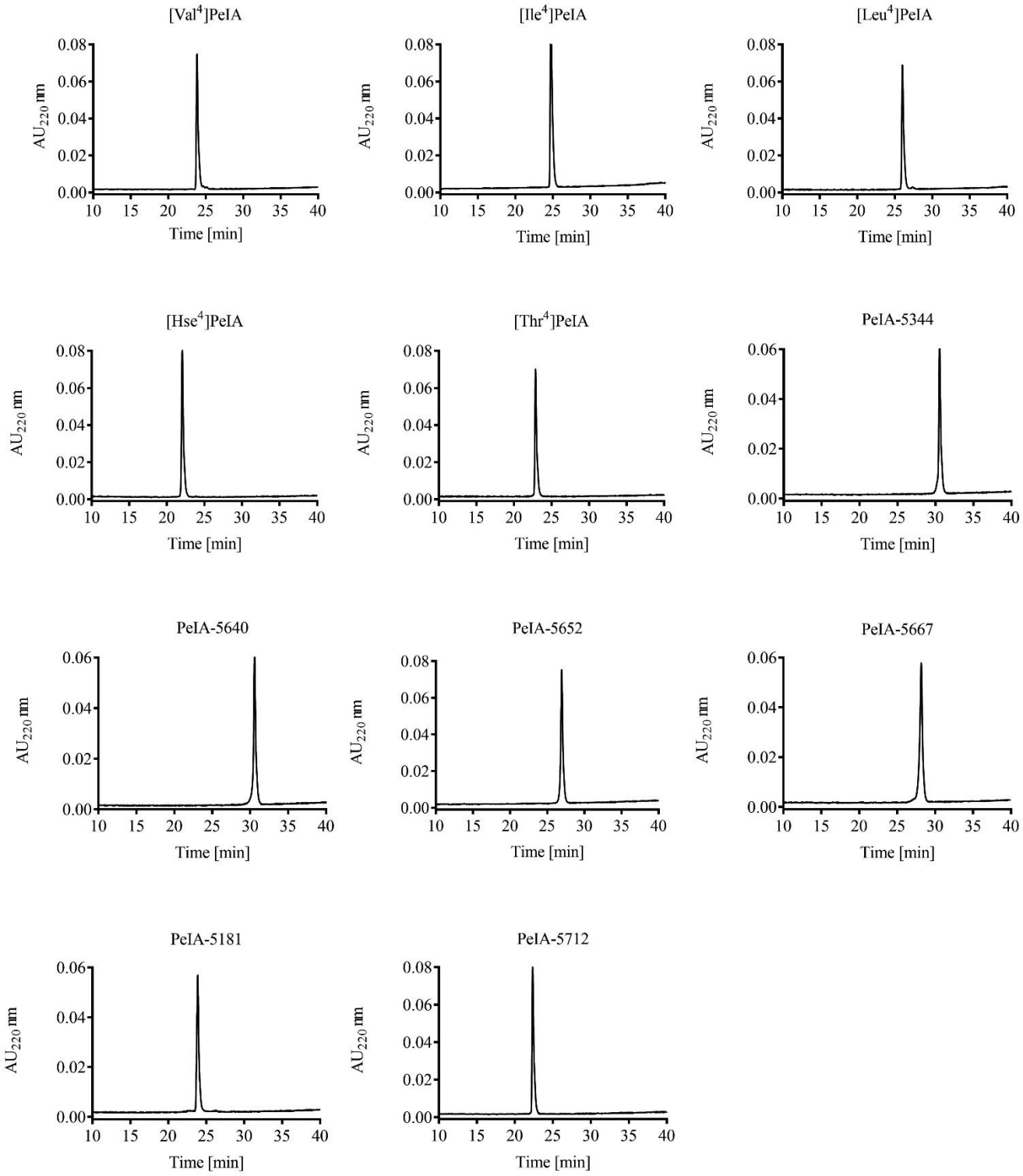

Figure 2. RP-HPLC chromatograms showing the purity of synthesized peptides. The solvent gradient used for all peptides was 10% to 50% B60 in 40 min and resolved on an analytical C18-column (Vydac, 5 µM, 250x4.6 mm) (solvent A: 0.1% trifluoroaceitic acid in water; solvent B60: 60% acetonitrile 0.092% trifluoroaceitic acid, 40% water). Retention times and purity values are provided in Table 1.

Table 1. Retention Time, Yield, Purity, and Mass Spectrometry for Synthetic Peptides[a]

peptide	retention time (min)	% yield	% purity	calculated M^+ (Da)	observed M^+ (Da)
[Hse^4]PeIA	22.0	77	99	1665.67	1665.71
[Thr^4]PeIA	22.9	16	99	1665.67	1665.75
[Val^4]PeIA	23.8	25	99	1663.69	1663.68
[Ile^4]PeIA	25.1	67	99	1677.71	1677.75
[Leu^4]PeIA	26.0	93	99	1677.71	1677.76
PeIA-5344	30.5	77	99	1771.74	1771.70
PeIA-5640	30.6	87	99	1771.74	1771.73
PeIA-5652	28.4	79	99	1748.72	1748.71
PeIA-5667	28.2	67	99	1748.72	1748.71
PeIA-5181	23.9	64	97	1704.74	1704.73
PeIA-5712	22.4	19	99	1763.79	1763.78

[a]MALDI-TOF mass spectrometry was used to determine the masses of all peptides.