Supporting Information

Further studies at neuropeptide S position 5: discovery of novel neuropeptide S receptor antagonists

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Table 1. analytical properties of the [X^5]NPS analogues

		[a]t_r		[b]MH^+	
no	Abbreviated names	I	II	calculated	found
	hNPS	9.59	13.06	2188.5	2188.2
	[D-Val^5]hNPS	9.92	13.92	2230.6	2230.8
1	[D-Ile^5]hNPS	8.44	13.84	2244.6	2245.6
2	[D-allo-Ile^5]hNPS	8.60	13.92	2244.6	2244.8
3	[D-Thr^5]hNPS	8.03	13.15	2232.6	2233.4
4	[D-allo-Thr^5]hNPS	7.88	13.30	2232.6	2233.4
5	[D-Nva^5]hNPS	8.44	13.27	2230.6	2231.6
6	[cyclohexyl-D-Gly^5]hNPS	8.87	14.61	2270.7	2271.2
7	[D-Cha^5]hNPS	9.62	15.85	2284.7	2285.2
8	[D-Phg^5]hNPS	8.36	13.91	2264.6	2265.2
9	[tBu-D-Gly^5]hNPS	8.66	13.16	2244.7	2245.2
10	[D-Pen^5]hNPS	8.41	13.41	2260.2	2262.6
11	[tBu-D-Ala^5]hNPS	8.44	13.62	2258.7	2259.6

[a]t_r is the retention time determined by analytical HPLC. Retention time I was obtained using a Nucleodur C_{18} column (4.6 x 100 mm, 2 μm particle size) with the solvent system A (10%, v/v, acetonitrile in 0.1% TFA) and solvent system B (60%, v/v, acetonitrile in 0.1% TFA). The column was perfused at a flow rate of 0.6 mL / min using a linear gradient from 0% to 70% B over 25 min. Retention time II was obtained using a Hypersil BDS C_{18} column (4.6 x 150 mm, 5 μm particle size) with solvent system A (35 mM NaH_2PO_4 (pH 2.1)) and solvent system B (59 mM NaH_2PO_4 (pH 2.1)-acetonitrile (60:40 v/v)). The column was perfused at a flow rate of 1 mL/min with a linear gradient from 5% to 65% B over 25 min

[b]The mass ion (MH^+) was obtained by electro spray mass spectrometry.