

Identification of 1-([1-(4-Fluorophenyl)-5-(2-methoxyphenyl)-1H-pyrazol-3-yl]carbonyl) amino) cyclohexane Carboxylic Acid as a Selective Non-peptide Neurotensin Receptor Type 2 Compound

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SUPPORTING INFORMATION

Analysis Appendix S2

Analysis Appendix

Compd	formula	Calculated			Found		
		C	H	N	C	H	N
7b	C ₂₄ H ₂₄ FN ₃ O ₄	65.89	5.53	9.61	65.67	5.62	9.90
13	C ₃₂ H ₃₃ N ₃ O ₃ •Et ₂ O	74.33	7.45	7.22	74.61	7.26	6.93
14b	C ₂₉ H ₂₉ ClN ₄ O ₅ •H ₂ O	61.43	5.51	9.88	61.73	5.42	9.83
15b	C ₂₉ H ₂₉ ClN ₄ O ₅ •H ₂ O	61.43	5.51	9.88	61.71	5.74	9.51
16b	C ₂₉ H ₂₉ ClN ₄ O ₅ •Et ₂ O	63.61	6.31	8.99	63.87	6.22	9.31
17b	C ₂₈ H ₂₇ ClN ₄ O ₄	64.80	5.24	10.80	64.94	5.55	11.17
18b	C ₂₇ H ₂₃ ClF ₂ N ₄ O ₃	61.78	4.42	10.67	61.85	4.68	10.33
19b	C ₃₁ H ₃₃ ClN ₄ O ₆ •1.5H ₂ O	60.93	5.77	9.17	60.62	6.01	9.12
20b	C ₂₉ H ₂₉ ClN ₄ O ₅	63.44	5.32	10.20	63.52	5.39	10.15
21b	C ₂₈ H ₂₇ ClN ₄ O ₅ •H ₂ O	60.81	5.29	10.13	60.52	5.36	9.94
22b	C ₂₇ H ₂₅ ClN ₄ O ₅	62.25	4.84	10.75	61.89	4.98	10.73
23b	C ₂₇ H ₂₅ ClN ₄ O ₄	64.22	4.99	11.10	64.44	5.03	10.81
24b	C ₃₀ H ₃₁ N ₃ O ₅	70.16	6.08	8.18	70.09	6.36	7.94
25b	C ₂₉ H ₂₉ N ₃ O ₄	72.03	6.04	8.69	71.74	6.22	8.67
26b	C ₂₉ H ₂₉ N ₃ O ₅ •H ₂ O	67.30	6.04	8.12	67.43	6.27	8.41
27b	C ₂₈ H ₂₇ N ₃ O ₄	71.62	5.80	8.95	71.38	6.02	8.59
28b	C ₂₆ H ₂₈ FN ₃ O ₅	64.85	5.86	8.73	64.64	5.79	8.68
29b	C ₂₅ H ₂₆ FN ₃ O ₅ •Et ₂ O	64.31	6.70	7.76	64.13	6.76	8.02
30	C ₂₉ H ₃₀ FN ₃ O ₅	67.04	5.82	8.09	67.35	5.87	7.85