

Development of 3-Phenyltropane Analogs with High Affinity for the Dopamine and Serotonin Transporter and Low Affinity for the Norepinephrine Transporter

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Supporting Information

Analysis Appendix

Compd	Formula	Calculated			Found		
		C	H	N	C	H	N
7a	C ₁₇ H ₂₄ ClNO ₃ ·H ₂ O	59.38	7.62	4.07	59.08	7.59	3.88
7b	C ₁₈ H ₂₆ ClNO ₃ ·1.75H ₂ O	58.21	8.01	3.77	58.03	8.00	3.76
7c	C ₁₇ H ₂₃ ClFNO ₃ ·1.25H ₂ O	55.74	7.02	3.82	55.80	7.02	3.66
7d	C ₁₇ H ₂₃ BrClNO ₃ ·0.75H ₂ O	48.82	5.90	3.35	48.76	5.91	3.07
7e	C ₁₇ H ₂₂ Br ₂ ClNO ₃	42.22	4.59	2.90	41.87	4.60	2.75
7f	C ₁₇ H ₂₃ ClINO ₃ ·H ₂ O	43.47	5.36	2.98	43.74	5.45	2.90
7g	C ₁₇ H ₂₂ ClI ₂ NO ₃ ·0.5H ₂ O	34.81	3.95	2.39	34.76	3.93	2.29
8a	C ₁₉ H ₂₈ ClNO ₃	64.49	7.98	3.96	64.75	8.05	3.92
8b	C ₁₉ H ₂₆ ClNO ₃ ·1.25H ₂ O	60.95	7.67	3.74	61.19	7.72	3.63
8c	C ₂₀ H ₂₈ ClNO ₃	65.65	7.71	3.83	65.93	7.87	3.70
8d	C ₂₄ H ₂₉ ClN ₂ O ₅ ·0.75H ₂ O	60.76	6.48	5.90	60.57	6.51	5.95
8e	C ₂₄ H ₃₂ Cl ₂ N ₂ O ₃ ·H ₂ O	59.38	7.06	5.77	59.51	6.97	5.73
8f	C ₂₆ H ₃₃ ClN ₂ O ₄ ·1.5H ₂ O	62.45	7.26	5.60	62.30	7.08	5.50
8g	C ₂₄ H ₃₀ BrClN ₂ O ₃ ·1.25H ₂ O	54.15	6.15	5.26	54.07	5.93	5.15
8h	C ₂₄ H ₂₉ Br ₂ ClN ₂ O ₃ ·H ₂ O	47.51	5.15	4.62	47.29	5.18	4.53
8i	C ₂₄ H ₃₀ ClIN ₂ O ₃ ·1.5H ₂ O	49.37	5.70	4.80	49.09	5.62	4.52
8j	C ₂₄ H ₂₉ ClI ₂ N ₂ O ₃ ·H ₂ O	41.13	4.46	4.00	41.28	4.41	3.84
9	C ₂₅ H ₂₉ ClN ₂ O ₂ ·0.25H ₂ O	69.92	6.92	6.52	69.78	6.89	6.41