

Supporting Information

Potent Dmt-Tic Pharmacophoric δ - and μ -Opioid Receptor Antagonists

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Table 1. The elemental analyses of Dmt-Tic dimers.

Compound	Calcd.	Found	Formula
8	C, 57.74; H, 6.58; N, 10.99	C, 57.70; H, 6.28; N, 10.90	C ₄₉ H ₅₆ N ₈ O ₇ ·2HCl·4.3H ₂ O
9	C, 58.80; H, 6.77; N, 10.80	C, 58.80; H, 6.34; N, 10.80	C ₅₁ H ₆₀ N ₈ O ₇ ·2HCl·4H ₂ O
10	C, 59.50; H, 6.97; N, 10.50	C, 59.30; H, 6.48; N, 10.50	C ₅₃ H ₆₄ N ₈ O ₇ ·2HCl·4H ₂ O
11	C, 59.67; H, 7.19; N, 10.12	C, 59.77; H, 6.98; N, 10.10	C ₅₅ H ₆₈ N ₈ O ₇ ·2HCl·4.5H ₂ O
12	C, 59.53; H, 7.09; N, 10.28	C, 59.41; H, 6.77; N, 10.20	C ₅₄ H ₆₆ N ₈ O ₇ ·2HCl·4.3H ₂ O
13	C, 59.80; H, 7.07; N, 10.30	C, 59.70; H, 6.74; N, 10.30	C ₅₄ H ₆₆ N ₈ O ₇ ·2HCl·4H ₂ O
14	C, 58.99; H, 7.00; N, 10.38	C, 58.89; H, 6.66; N, 10.35	C ₅₃ H ₆₄ N ₈ O ₇ ·2HCl·4.5H ₂ O
18	C, 60.9; H, 7.00; N, 9.27	C, 60.90; H, 6.71; N, 9.28	C ₄₆ H ₅₆ N ₆ O ₆ ·2HCl·2.5H ₂ O
19	C, 59.50; H, 7.30; N, 8.67	C, 59.50; H, 6.88; N, 8.66	C ₄₈ H ₆₀ N ₆ O ₆ ·2HCl·4.4H ₂ O
20	C, 61.24; H, 7.73; N, 8.24	C, 61.2; H, 7.38; N, 8.09	C ₅₂ H ₆₈ N ₆ O ₆ ·2HCl·4.1H ₂ O
21	C, 61.3; H, 7.66; N, 8.25	C, 61.40; H, 7.25; N, 8.36	C ₅₂ H ₆₈ N ₆ O ₆ ·2HCl·4H ₂ O
22	C, 60.60; H, 7.35; N, 9.92	C, 60.62; H, 6.93; N, 9.84	C ₅₉ H ₈₀ N ₈ O ₇ ·2HCl·4.2H ₂ O

Table 2. The elemental analyses of compounds 1-7.

Compound	Calcd.	Found	Formula
1	C, 63.90; H, 6.89; N, 10.10	C, 63.80; H, 6.90; N, 10.5	$C_{59}H_{72}N_8O_{11} \cdot 2.2H_2O$
2	C, 65.60; H, 6.99; N, 10.00	C, 65.60; H, 6.77; N, 10.10	$C_{61}H_{76}N_8O_{11} \cdot H_2O$
3	C, 65.60; H, 7.20; N, 9.72	C, 65.60; H, 6.84; N, 9.74	$C_{63}H_{80}N_8O_{11} \cdot 1.5H_2O$
4	C, 65.90; H, 7.38; N, 9.46	C, 65.80; H, 7.25; N, 9.44	$C_{63}H_{80}N_8O_{11} \cdot 1.7H_2O$
5	C, 65.3; H, 7.32; N, 9.53	C, 65.30; H, 7.17; N, 9.54	$C_{64}H_{82}N_8O_{11} \cdot 2H_2O$
6	C, 66.40; H, 7.26; N, 9.68	C, 66.50; H, 7.15; N, 9.68	$C_{64}H_{82}N_8O_{11} \cdot 0.87H_2O$
7	C, 65.40; H, 7.21; N, 9.69	65.40; H, 7.08; N, 9.69	$C_{63}H_{80}N_8O_{11} \cdot 1.7H_2O$

Table 3. The elemental analyses of compounds **15-17**.

Compound	Calcd.	Found	Formula
15	C, 67.10; H, 7.34; N, 8.38	C, 66.90; H, 7.29; N, 8.45	$C_{56}H_{72}N_6O_{11} \cdot 0.8H_2O$
16	C, 64.43; H, 7.68; N, 7.77	C, 64.39; H, 7.24; N, 7.80	$C_{58}H_{76}N_6O_{11} \cdot 3.5H_2O$
17	C, 64.95; H, 8.03; N, 7.33	C, 64.63; H, 7.70; N, 7.29	$C_{62}H_{84}N_6O_{10} \cdot 4H_2O$