

Supporting Information

**Discovery of a Piperidine-4-carboxamide CCR5 Antagonist (TAK-220)
with Highly Potent Anti-HIV-1 Activity**

Shinichi Imamura, Takashi Ichikawa, Youichi Nishikawa, Naoyuki Kanzaki, Katsunori Takashima,

Shinichi Niwa, Yuji Iizawa, Masanori Baba, and Yoshihiro Sugihara

Elemental Analysis Data

Compd	Formula	Calcd	Found
3b	C ₁₀ H ₁₃ Cl ₂ N·HCl	C, 47.18; H, 5.54; N, 5.50	C, 47.17; H, 5.72; N, 5.63
4a	C ₁₇ H ₂₁ Cl ₃ N ₂ O ₂	C, 52.12; H, 5.40; N, 7.15	C, 51.99; H, 5.50; N, 6.95
4b	C ₁₈ H ₂₄ Cl ₂ N ₂ O ₂	C, 58.23; H, 6.52; N, 7.54	C, 57.97; H, 6.50; N, 7.27
5a	C ₂₈ H ₃₄ Cl ₂ FN ₃ O ₂ S·HCl·0.5H ₂ O	C, 54.95; H, 5.93; N, 6.87	C, 54.81; H, 5.98; N, 7.13
5b	C ₂₈ H ₃₄ Cl ₂ FN ₃ O ₃ S·0.75H ₂ O	C, 56.42; H, 6.00; N, 7.05	C, 56.58; H, 6.18; N, 7.19
5c	C ₂₈ H ₃₄ Cl ₂ FN ₃ O ₄ S·HCl·0.5H ₂ O	C, 52.22; H, 5.63; N, 6.52	C, 52.11; H, 5.83; N, 6.71
5d	C ₂₉ H ₃₆ Cl ₂ N ₄ O ₃ S·0.5H ₂ O	C, 57.99; H, 6.21; N, 9.33	C, 58.07; H, 6.09; N, 9.29
5e	C ₃₀ H ₃₉ Cl ₂ N ₃ O ₅ S·0.75H ₂ O	C, 56.47; H, 6.40; N, 6.58	C, 56.41; H, 6.25; N, 6.66
5f	C ₂₉ H ₃₈ Cl ₂ N ₄ O ₄ S	C, 57.14; H, 6.28; N, 9.19	C, 57.05; H, 6.38; N, 9.06
5g	C ₂₉ H ₃₈ Cl ₂ N ₄ O ₄ S	C, 57.14; H, 6.28; N, 9.19	C, 56.89; H, 6.13; N, 9.03
5h	C ₂₉ H ₃₈ Cl ₂ N ₄ O ₄ S·H ₂ O	C, 55.50; H, 6.42; N, 8.93	C, 55.67; H, 6.20; N, 9.01
5i	C ₃₀ H ₄₀ Cl ₂ N ₄ O ₄ S·HCl·2H ₂ O	C, 51.76; H, 6.52; N, 8.05	C, 51.76; H, 6.40; N, 7.97
5j	C ₃₃ H ₄₆ Cl ₂ N ₄ O ₄ S·0.5H ₂ O	C, 58.74; H, 7.02; N, 8.30	C, 58.58; H, 7.12; N, 8.08
5k	C ₃₁ H ₄₂ Cl ₂ N ₄ O ₄ S·HCl·2H ₂ O	C, 52.43; H, 6.67; N, 7.89	C, 52.41; H, 6.58; N, 7.75
5l	C ₃₀ H ₃₈ Cl ₂ N ₄ O ₃ ·0.5H ₂ O	C, 61.85; H, 6.75; N, 9.62	C, 61.64; H, 6.84; N, 9.70
5m	C ₃₁ H ₄₁ ClN ₄ O ₃	C, 67.31; H, 7.47; N, 10.13	C, 67.08; H, 7.67; N, 10.23
6	C ₂₉ H ₃₇ Cl ₂ N ₃ O ₅ S·2H ₂ O	C, 53.87; H, 6.39; N, 6.50	C, 53.75; H, 6.00; N, 6.41
7	C ₂₂ H ₂₉ Cl ₂ N ₃ O ₃ ·H ₂ O	C, 55.93; H, 6.61; N, 8.89	C, 55.91; H, 6.43; N, 8.77
8	C ₂₈ H ₃₅ Cl ₂ FN ₄ O ₂ ·2HCl·1.5H ₂ O	C, 51.78; H, 6.21; N, 8.63	C, 52.00; H, 6.09; N, 8.56
9	C ₂₆ H ₄₀ Cl ₂ N ₄ O ₅ S	C, 52.79; H, 6.82; N, 9.47	C, 52.54; H, 6.89; N, 9.42
10	C ₂₁ H ₃₂ Cl ₂ N ₄ O ₃ S·2HCl·0.5H ₂ O	C, 43.99; H, 6.15; N, 9.77	C, 43.94; H, 6.38; N, 9.77
11a	C ₂₇ H ₃₅ Cl ₂ FN ₄ O ₅ S ₂ ·HCl·0.5H ₂ O	C, 46.65; H, 5.37; N, 8.06	C, 46.78; H, 5.38; N, 8.19
11b	C ₂₈ H ₃₅ Cl ₂ FN ₄ O ₄ S·0.75H ₂ O	C, 53.63; H, 5.87; N, 8.93	C, 53.97; H, 6.26; N, 8.62