

## **Supporting Information**

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

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## Elemental Analysis Data

Compd	Formula	Calcd	Found
<b>3b</b>	$C_{10}H_{13}Cl_2N \cdot HCl$	C, 47.18; H, 5.54; N, 5.50	C, 47.17; H, 5.72; N, 5.63
<b>4a</b>	$C_{17}H_{21}Cl_3N_2O_2$	C, 52.12; H, 5.40; N, 7.15	C, 51.99; H, 5.50; N, 6.95
<b>4b</b>	$C_{18}H_{24}Cl_2N_2O_2$	C, 58.23; H, 6.52; N, 7.54	C, 57.97; H, 6.50; N, 7.27
<b>5a</b>	$C_{28}H_{34}Cl_2FN_3O_2S \cdot HCl \cdot 0.5H_2O$	C, 54.95; H, 5.93; N, 6.87	C, 54.81; H, 5.98; N, 7.13
<b>5b</b>	$C_{28}H_{34}Cl_2FN_3O_3S \cdot 0.75H_2O$	C, 56.42; H, 6.00; N, 7.05	C, 56.58; H, 6.18; N, 7.19
<b>5c</b>	$C_{28}H_{34}Cl_2FN_3O_4S \cdot HCl \cdot 0.5H_2O$	C, 52.22; H, 5.63; N, 6.52	C, 52.11; H, 5.83; N, 6.71
<b>5d</b>	$C_{29}H_{36}Cl_2N_4O_3S \cdot 0.5H_2O$	C, 57.99; H, 6.21; N, 9.33	C, 58.07; H, 6.09; N, 9.29
<b>5e</b>	$C_{30}H_{39}Cl_2N_3O_5S \cdot 0.75H_2O$	C, 56.47; H, 6.40; N, 6.58	C, 56.41; H, 6.25; N, 6.66
<b>5f</b>	$C_{29}H_{38}Cl_2N_4O_4S$	C, 57.14; H, 6.28; N, 9.19	C, 57.05; H, 6.38; N, 9.06
<b>5g</b>	$C_{29}H_{38}Cl_2N_4O_4S$	C, 57.14; H, 6.28; N, 9.19	C, 56.89; H, 6.13; N, 9.03
<b>5h</b>	$C_{29}H_{38}Cl_2N_4O_4S \cdot H_2O$	C, 55.50; H, 6.42; N, 8.93	C, 55.67; H, 6.20; N, 9.01
<b>5i</b>	$C_{30}H_{40}Cl_2N_4O_4S \cdot HCl \cdot 2H_2O$	C, 51.76; H, 6.52; N, 8.05	C, 51.76; H, 6.40; N, 7.97
<b>5j</b>	$C_{33}H_{46}Cl_2N_4O_4S \cdot 0.5H_2O$	C, 58.74; H, 7.02; N, 8.30	C, 58.58; H, 7.12; N, 8.08
<b>5k</b>	$C_{31}H_{42}Cl_2N_4O_4S \cdot HCl \cdot 2H_2O$	C, 52.43; H, 6.67; N, 7.89	C, 52.41; H, 6.58; N, 7.75
<b>5l</b>	$C_{30}H_{38}Cl_2N_4O_3 \cdot 0.5H_2O$	C, 61.85; H, 6.75; N, 9.62	C, 61.64; H, 6.84; N, 9.70
<b>5m</b>	$C_{31}H_{41}ClN_4O_3$	C, 67.31; H, 7.47; N, 10.13	C, 67.08; H, 7.67; N, 10.23
<b>6</b>	$C_{29}H_{37}Cl_2N_3O_5S \cdot 2H_2O$	C, 53.87; H, 6.39; N, 6.50	C, 53.75; H, 6.00; N, 6.41
<b>7</b>	$C_{22}H_{29}Cl_2N_3O_3 \cdot H_2O$	C, 55.93; H, 6.61; N, 8.89	C, 55.91; H, 6.43; N, 8.77
<b>8</b>	$C_{28}H_{35}Cl_2FN_4O_2 \cdot 2HCl \cdot 1.5H_2O$	C, 51.78; H, 6.21; N, 8.63	C, 52.00; H, 6.09; N, 8.56
<b>9</b>	$C_{26}H_{40}Cl_2N_4O_5S$	C, 52.79; H, 6.82; N, 9.47	C, 52.54; H, 6.89; N, 9.42
<b>10</b>	$C_{21}H_{32}Cl_2N_4O_3S \cdot 2HCl \cdot 0.5H_2O$	C, 43.99; H, 6.15; N, 9.77	C, 43.94; H, 6.38; N, 9.77
<b>11a</b>	$C_{27}H_{35}Cl_2FN_4O_5S_2 \cdot HCl \cdot 0.5H_2O$	C, 46.65; H, 5.37; N, 8.06	C, 46.78; H, 5.38; N, 8.19
<b>11b</b>	$C_{28}H_{35}Cl_2FN_4O_4S \cdot 0.75H_2O$	C, 53.63; H, 5.87; N, 8.93	C, 53.97; H, 6.26; N, 8.62