Supporting Information:

Table 1 Elementary analysis data of compounds 1-14

Table 2. Data Collection and Refinement Statistics.

Table 3. AlogP of compounds 1-14

Table 1 Elementary analysis data of compounds 1-14

NO.	Theoretical in % C H N	Experimental in % C H N	Formula
1	47.17, 5.61 10.0	46.95, 5.34, 10.23	$C_{11}H_{15}ClN_2O_4 \cdot 0.3H_2O$
2	59.54, 5.93, 8.68	59.31, 5.82, 8.41	$C_{16}H_{19}ClN_2O_3$
3	56.72, 5.65, 8.27	56.65, 5.75, 7.99	$C_{16}H_{19}ClN_2O_4$
4	62.92, 5.28, 6.99	62.72, 5.27, 6.98	$C_{21}H_{21}ClN_2O_4$
5	50.93, 4.56, 11.88	50.81, 4.62, 11.71	$C_{15}H_{16}ClN_3O_5$
6	51.01, 4.28, 7.44	50.86, 4.31, 7.44	$C_{16}H_{16}ClF_3N_2O_3$
7	52.24, 5.85, 10.15	52.45, 5.62, 10.05	$C_{18}H_{18}ClN_3O_3 \cdot 3H_2O$
8	43.75, 5.51, 12.75	43.45, 5.02, 13.04	$C_{16}H_{20}Cl_2N_4O_4 \cdot 2H_2O$
9	47.36, 5.92, 12.27	47.59, 5.83, 12.07	$C_{18}H_{24}Cl_2N_4O_4 \cdot 1.4H_2O$
10	48.95, 4.93, 12.68	48.96, 4.79, 12.59	$C_{18}H_{20}Cl_2N_4O_4 \cdot 0.8H_2O$
11	52.29, 6.14, 12.20	52.07, 5.93, 12.50	$C_{20}H_{28}Cl_2N_4O_4$
12	54.61, 5.96, 9.55	54.88, 5.30, 9.51	$C_{20}H_{20}ClN_3O_3 \cdot 3H_2O$
13	63.06, 5.46, 5.88	63.23, 5.64, 5.53	$C_{25}H_{23}ClN_2O_4 \cdot 1.4H_2O$
14	59.36, 5.46, 9.89	59.45, 5.32, 9.55	$C_{21}H_{22}ClN_3O_4 \cdot 0.5H_2O$

Table 2. Data Collection and Refinement Statistics.

	CD38-Compound 4
Data collection	
Space group	P1
Cell dimensions	
a, *b*, *c* (Å)	41.98, 96.84, 104.37
α, β, γ (°)	79.84, 83.12, 86.59
Resolution (Å)	30-1.9
R_{sym} or R_{merge} (%)	14.1 (52.3)
$I / \sigma I$	11.17 (1.69)
Completeness (%)	96.2 (91.0)
Redundancy	2.6 (1.8)
Refinement	
Resolution (Å)	30-2.0
No. reflections	119025
R_{work} / R_{free} (%)	20.64/27.15
No. of protein atoms	12192
No. of Compound 4 molecules	6
No. of water	645
R.m.s deviations	
Bond lengths (Å)	0.0256
Bond angles (°)	1.774

Values in parentheses are from the highest resolution shell.

Table 3. AlogP of compounds 1-14

Comp.	1	2	3	4	5	6	7
AlogP	0.13	1.74	1.90	3.48	1.81	2.86	2.11
Comp.	8	9	10	11	12	13	14
AlogP	0.40	1.04	0.99	1.95	2.57	4.68	2.73

AlogP was calculated using Pipeline Pilot V7.5