

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 %			Experimental in %			Formula
	C	H	N	C	H	N	
1	47.17	5.61	10.0	46.95	5.34	10.23	C ₁₁ H ₁₅ ClN ₂ O ₄ ·0.3H ₂ O
2	59.54	5.93	8.68	59.31	5.82	8.41	C ₁₆ H ₁₉ ClN ₂ O ₃
3	56.72	5.65	8.27	56.65	5.75	7.99	C ₁₆ H ₁₉ ClN ₂ O ₄
4	62.92	5.28	6.99	62.72	5.27	6.98	C ₂₁ H ₂₁ ClN ₂ O ₄
5	50.93	4.56	11.88	50.81	4.62	11.71	C ₁₅ H ₁₆ ClN ₃ O ₅
6	51.01	4.28	7.44	50.86	4.31	7.44	C ₁₆ H ₁₆ ClF ₃ N ₂ O ₃
7	52.24	5.85	10.15	52.45	5.62	10.05	C ₁₈ H ₁₈ ClN ₃ O ₃ ·3H ₂ O
8	43.75	5.51	12.75	43.45	5.02	13.04	C ₁₆ H ₂₀ Cl ₂ N ₄ O ₄ ·2H ₂ O
9	47.36	5.92	12.27	47.59	5.83	12.07	C ₁₈ H ₂₄ Cl ₂ N ₄ O ₄ ·1.4H ₂ O
10	48.95	4.93	12.68	48.96	4.79	12.59	C ₁₈ H ₂₀ Cl ₂ N ₄ O ₄ ·0.8H ₂ O
11	52.29	6.14	12.20	52.07	5.93	12.50	C ₂₀ H ₂₈ Cl ₂ N ₄ O ₄
12	54.61	5.96	9.55	54.88	5.30	9.51	C ₂₀ H ₂₀ ClN ₃ O ₃ ·3H ₂ O
13	63.06	5.46	5.88	63.23	5.64	5.53	C ₂₅ H ₂₃ ClN ₂ O ₄ ·1.4H ₂ O
14	59.36	5.46	9.89	59.45	5.32	9.55	C ₂₁ H ₂₂ ClN ₃ O ₄ ·0.5H ₂ O

Table 2. Data Collection and Refinement Statistics.

CD38-Compound 4	
Data collection	
Space group	P1
Cell dimensions	
<i>a</i> , <i>b</i> , <i>c</i> (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
$R_{\text{work}} / R_{\text{free}}$ (%)	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