

Supplementary Information for

Discovery of potent small-molecule inhibitors of lipoprotein(a) formation

Supplementary Table S1

Crystallography data collection and refinement statistics

	3353871 8TCE	3441732 8V9B	3473329 8V8Z
Data collection			
Space group	P2 ₁	P3 ₁	P2 ₁ 2 ₁ 2 ₁
Cell dimensions			
<i>a</i> , <i>b</i> , <i>c</i> (Å)	37.6, 57.57, 38.31	49.27, 49.27, 63.82	37.76, 75.18, 93.31
α , β , γ (°)	90, 94.7, 90	90, 90, 120	90, 90, 90
Resolution (Å)	1.07 (1.07-1.1)	1.19 (1.19-1.25)	2.01 (2.01-2.12)
<i>R</i> _{merge}	0.068 (0.61)	0.112 (0.638)	0.102 (0.499)
<i>I</i> / σI	7.9 (1.8)	5.7 (1.2)	6.7 (1.5)
Completeness (%)	91.1 (70.7)	94.3 (94.3)	99.3 (98.7)
Redundancy	3.5 (2.9)	5.8 (5.3)	7.3 (7.5)
Refinement			
Resolution (Å)	1.07	1.19	2.01
Number of reflections	61,502	55,431	18,167
<i>R</i> _{work} / <i>R</i> _{free}	0.168/0.187	0.141/0.175	0.217/0.260
Number of atoms			
Protein	1,505	1,385	1,993
Ligand	32	70	107
Water	200	215	91
<i>B</i> -factors			
K _{IV} 7	-	9.54	-
K _{IV} 8	9.45	-	29.10
3353871	16.76	-	-
3441732	-	13.92	-
3473329	-	-	31.38
Water	18.62	21.39	28.50
R.m.s deviations			
Bond lengths (Å)	0.007	0.011	0.008
Bond angles (°)	1.303	1.450	1.199

K_{IV}, kringle type IV domain.