

Supplemental Table 1. β -lg calyx-binding residues from the XRD structures.

	octanoic acid	decanoic acid	lauric acid	myristic acid	palmitic acid	Bromo-decanoic	linoleic acid	oleic acid	stearic acid	retinol	retinoic acid	Vitamin D3	Decyl Maltoside
I12									Green				
P38				Red	Red		Red	Red	Red			Red	Red
L39		Blue								Blue	Blue	Blue	
V41			Blue	Blue			Blue	Blue			Blue	Blue	
V43												Green	
L46		Red	Red		Red	Red	Red	Red	Red				
L54		Red	Red	Red	Red		Red	Red	Red				
I56	Red	Red	Red			Red	Red	Red			Red	Red	Red
L58				Green									
K60					Red	Red	Red	Red	Red			Red	Red
E62					Blue		Blue	Blue		Blue		Blue	
K69	Red			Red	Red	Red	Red			Red	Red		
I71	Red	Red		Red	Red	Red	Red	Red	Red	Red	Red	Red	
I84		Red	Red	Red	Red	Red		Red	Red			Red	Red
A86												Green	Green
L87													Green
N88													Green
V92	Red		Red			Red	Red	Red	Red	Red	Red		
V94		Blue		Blue	Blue		Blue	Blue	Blue				
L103			Blue	Blue				Blue					Blue
F105		Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
M107	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
Q120										Green	Green		
PDB	3NQ9	3NQ3	3UEU	3UEV	3UEW	1BSO	4DQ4	4DQ3	3UEX	1GX8	1GX9	2GJ5	2R56

Color code is red for residues with at least 7 contacts with the ligand, blue for residues with 3 to 6 contacts and green for residues with 2 or less.