Supporting Information

Structural Determinants for Transport Across the Intestinal Bile Acid Transporter Using C-24 Bile Acid Conjugates

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Table S1a. Multiple reaction monitoring (MRM) transitions for conjugates **1-32.**

Compound #	Q1 Mass (amu)	Q3 Mass (amu)	Starting Gradient (A:B)	Run time (min)
1	597.4	339.05	50:50	6
2	631.3	238.95	50:50	6
3	665.4	290.95	50:50	6
4	615.2	321.16	55:45	6
5	615.4	339.10	55:45	6
6	615.4	339.39	55:45	6
7	611.4	218.7	55:45	8
8	611.4	107.98	55:45	8
9	611.5	219.23	55:45	8
10	627.2	235.50	50:50	6
11	627.1	123.89	50:50	6
12	627.3	123.65	50:50	6
13	653.4	261.14	50:50	8
14	655.3	152.01	50:50	6
15	669.3	119.79	50:50	8
16	669.4	276.81	50:50	8
17	712.8	153.36, 620.29	50:50	8
18	712.2	637.94	50:50	8
19	612.5	219.97	70:30	8
20	612.1	108.95	70:30	8
21	612.5	108.59, 174.69	70:30	8
22	633.2	130.05	50:50	6
23	625.39	121.83	50:50	6
24	625.5	121.85	50:50	6
25	657.3	153.95	50:50	6

26	732.1	90.53, 340.49	55:45	7
27	641.9	339.90	55:45	8
28	641.3	249.96	55:45	8
29	655.51	134.70	55:45	8
30	694.3	90.66	70:30	8.5
31	618.2	581.98	70:30	8.5
32	694.4	173.70	70:30	8.5

The mobile phase for all compounds **1-29** comprised of**:** A;HPLC grade water with 0.1% formic, B; HPLC grade acetonitrile with 0.1% formic acid. For compounds **30-32** 0.1% ammonium hydroxide was used as a modifier. Following gradient was used for most compounds.

Table S1b. Stereochemical SMILES of the compounds used in this study.

Compound #	SMILES
1	[H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@](C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([H])c([H])c4[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]
2	[H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@](C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c(C)c([H])c4[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]
3	[H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@](C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c(c([H])c4[H])[C+](F)(F)F)[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]
4	[H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@](C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([H])c([H])c4F)[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]
5	[H]O[C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])(O[H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@](C([H])([H])[H])C([H])([H])C([H])([H])C(=O)N([H])[C@]([H])(c(:o):o)C([H])([H])C([H])([H])C(=O)N([H])c4c([H])c([H])c([H])c(F)c4[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]
6	[H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@](C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([H])c(F)c([H])c4[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]
7	[H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@](C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([H])c([H])c4C([H])([H])[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]
8	[H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@](C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([H])c([H])c(c4[H])C([H])([H])[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]
9	[H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@](C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([H])c(c([H])c4[H])C([H])([H])[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]
10	[H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@](C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([H])c([H])c4OC([H])([H])[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]
11	[H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@](C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([H])c(OC([H])([H])[H])c4[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

12 [H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c(OC([H])([H])[H])c([H])c4[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

13 [H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c(c([H])c4[H])C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

14 [H]O[C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])(O[H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])C(=O)N([H])[C@]([H])(c(:o):o)C([H])([H])C([H])([H])C(=O)N([H])c4c([H])c([H])c([H])c(c([H])c4[H])C(=O)OC([H])([H])[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

15 [H]O[C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])(O[H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])C(=O)N([H])[C@]([H])(c(:o):o)C([H])([H])C([H])([H])C(=O)N([H])c4c([H])c([H])c([H])c([H])c4C(=O)OC([H])([H])C([H])([H])[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

16 [H]O[C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])(O[H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])C(=O)N([H])[C@]([H])(c(:o):o)C([H])([H])C([H])([H])C(=O)N([H])c4c([H])c([H])c(c([H])c4[H])C(=O)OC([H])([H])C([H])([H])[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

17 [H]O[C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])(O[H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])C(=O)N([H])[C@]([H])(c(:o):o)C([H])([H])C([H])([H])C(=O)N([H])c4c([H])c([H])c([H])c(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])c4[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

18 [H]O[C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])(O[H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])C(=O)N([H])[C@]([H])(c(:o):o)C([H])([H])C([H])([H])C(=O)N([H])c4c([H])c([H])c(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])c([H])c4[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

19 [H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([H])c([H])c4[N-]([H])[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

20 [H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([H])c([N-]([H])[H])c4[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

21 [H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([N-]([H])[H])c([H])c4[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

22 [H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c(F)c([H])c4F)[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

23 [H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c(c([H])c([H])c([H])c4C([H])([H])[H])C([H])([H])[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

24 [H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-]

	][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([H])c(c4C([H])([H])[H])C([H])([H])[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]
	[H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c(OC([H])([H])[H])c([H])c(OC([H])([H])[H])c4[H])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]
	[H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([C+](=[O-])OC([H])([H])c4c([H])c([H])c([H])c([H])c4[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([H])c(c4[H])-[c+](:[o-]):[o-])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]
	[H][O-][C@]1([H])C([H])([H])C([H])([H])[C@@]2(C([H])([H])[H])[C@@]([H])(C1([H])[H])C([H])([H])[C@@]([H])([O-][H])[C@@]1([H])[C@]3([H])C([H])([H])C([H])([H])[C@]([H])([C@]([H])(C([H])([H])[H])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])[C@]([H])([c+](:[o-]):[o-])C([H])([H])C([H])([H])[C+](=[O-])[N-]([H])c4c([H])c([H])c([H])c(c4[H])-[c+](:[o-]):[o-])[C@@]3(C([H])([H])[H])C([H])([H])C([H])([H])[C@]21[H]

Table S2. Correlation matrix between descriptors for aniline conjugates of glu-CDCA. Units of ΔG_w are kcal/mol. Units of molar reflectivity are m^3/mol. Units of area (e.g. $SASA_{side}$) is $Å^2$. Other descriptors are dimensionless.

	ΔG_w	logP	C19-GS-O3	O7-AA-C18	O7-C19-GS	C18-GS-O7	O7-C18-GS	HA	MW	O7-AA-BC	O3-C19-GS	C19-GS_{min}	O7-AA-GS	O3-GS_{min}
ΔG_w	1.00													
logP	0.90	1.00												
C19-GS-O3	0.61	0.46	1.00											
O7-AA-C18	0.43	0.24	0.86	1.00										
O7-C19-GS	0.60	0.47	0.97	0.84	1.00									
C18-GS-O7	0.68	0.54	0.65	0.62	0.61	1.00								
O7-C18-GS	0.61	0.54	0.90	0.74	0.94	0.46	1.00							
HA	-0.40	-0.36	-0.12	0.07	-0.08	-0.13	-0.10	1.00						
MW	-0.08	0.13	-0.04	-0.12	0.02	0.09	0.09	0.57	1.00					
O7-AA-BC	0.35	0.20	0.83	0.95	0.81	0.44	0.79	0.08	-0.12	1.00				
O3-C19-GS	0.40	0.27	0.87	0.75	0.88	0.34	0.91	-0.06	-0.08	0.84	1.00			
C19-GS_{min}	0.51	0.34	0.84	0.86	0.85	0.80	0.73	-0.03	-0.01	0.77	0.70	1.00		
O7-AA-GS	0.57	0.45	0.95	0.83	0.94	0.77	0.85	-0.06	0.10	0.76	0.79	0.92	1.00	
O3-GS_{min}	0.52	0.36	0.91	0.86	0.91	0.77	0.79	-0.04	0.00	0.78	0.78	0.97	0.96	1.00
O3-C18-GS	0.54	0.45	0.96	0.82	0.96	0.59	0.94	-0.08	0.05	0.81	0.89	0.83	0.93	0.91
MR	-0.05	0.15	0.05	-0.03	0.10	0.09	0.20	0.62	0.91	0.00	0.01	0.02	0.15	0.05
C18-GS-O3	0.52	0.40	0.95	0.88	0.93	0.74	0.81	0.00	0.07	0.79	0.77	0.91	0.97	0.96
AA-GS-O7	0.55	0.42	0.83	0.80	0.80	0.88	0.68	-0.02	0.09	0.69	0.63	0.96	0.93	0.95
O7-GS_{min}	0.53	0.39	0.91	0.83	0.90	0.78	0.80	-0.06	0.03	0.75	0.76	0.96	0.97	0.99
O7-AA-C20	0.39	0.31	0.82	0.84	0.83	0.31	0.89	0.06	-0.03	0.94	0.89	0.68	0.74	0.72
brotN	-0.09	0.03	-0.01	-0.03	0.05	0.10	0.07	0.69	0.90	-0.05	-0.06	0.01	0.09	0.02
BC-GS_{min}	0.51	0.36	0.83	0.80	0.85	0.78	0.73	-0.05	0.03	0.71	0.68	0.99	0.92	0.97
O3-AA-GS	0.51	0.39	0.92	0.85	0.91	0.78	0.81	-0.02	0.11	0.77	0.75	0.96	0.98	0.98
O7-GS	0.52	0.40	0.90	0.83	0.90	0.79	0.81	0.00	0.12	0.76	0.76	0.96	0.98	0.97
GS-O7-C18	0.49	0.40	0.93	0.83	0.97	0.53	0.96	0.02	0.11	0.85	0.91	0.85	0.92	0.90
AA-GS-O3	0.51	0.35	0.77	0.78	0.76	0.89	0.61	0.02	0.11	0.65	0.54	0.95	0.89	0.92
O3-GS	0.50	0.37	0.91	0.85	0.91	0.77	0.81	0.03	0.13	0.77	0.77	0.96	0.97	0.98
C18-GS_{min}	0.48	0.31	0.78	0.80	0.80	0.81	0.66	0.01	0.04	0.69	0.63	0.99	0.90	0.95
O7-AA	0.39	0.31	0.83	0.87	0.84	0.38	0.88	0.07	0.01	0.95	0.86	0.72	0.77	0.75

Table S2. Contd.

	ΔG_w	logP	C19-GS-O3	O7-AA-C18	O7-C19-GS	C18-GS-O7	O7-C18-GS	HA	MW	O7-AA-BC	O3-C19-GS	C19-GS_{min}	O7-AA-GS	O3-GS_{min}
C19-GS	0.46	0.32	0.80	0.82	0.81	0.79	0.70	0.04	0.12	0.73	0.66	0.97	0.91	0.94
BC-GS	0.49	0.36	0.81	0.78	0.83	0.79	0.73	0.00	0.15	0.69	0.67	0.96	0.92	0.94
GS-O3-C18	0.47	0.35	0.90	0.79	0.92	0.55	0.92	0.01	0.08	0.82	0.91	0.85	0.90	0.91
GS-O3-C19	0.33	0.16	0.86	0.85	0.86	0.55	0.79	0.10	0.04	0.83	0.89	0.87	0.88	0.90
GS-O7-C19	0.41	0.24	0.80	0.79	0.84	0.70	0.64	0.06	0.08	0.63	0.60	0.87	0.86	0.87
C18-GS	0.44	0.32	0.73	0.76	0.75	0.78	0.66	0.02	0.13	0.67	0.61	0.95	0.86	0.90
O7-GS_{max}	0.48	0.37	0.81	0.78	0.82	0.80	0.73	0.10	0.23	0.70	0.67	0.93	0.92	0.92
O3-GS_{max}	0.47	0.37	0.83	0.79	0.84	0.78	0.75	0.12	0.26	0.71	0.69	0.92	0.92	0.92
BC-GS_{max}	0.45	0.34	0.74	0.73	0.76	0.79	0.66	0.07	0.25	0.64	0.60	0.91	0.87	0.88
O3-AA-C20	0.37	0.29	0.86	0.80	0.87	0.35	0.92	0.07	0.05	0.88	0.92	0.71	0.80	0.78
$SASA_{side}$	-0.01	0.12	-0.13	-0.06	-0.10	0.18	0.00	0.53	0.75	-0.05	-0.17	-0.03	0.01	-0.06
C19-GS_{max}	0.40	0.31	0.68	0.70	0.69	0.78	0.59	0.07	0.23	0.61	0.53	0.90	0.81	0.84
KierFlex	0.00	0.09	0.04	0.04	0.10	0.19	0.15	0.61	0.90	0.04	0.00	0.09	0.15	0.08
C18-AA	0.12	-0.07	0.61	0.77	0.57	0.64	0.31	0.12	-0.12	0.61	0.44	0.74	0.67	0.72
C18-GS_{max}	0.38	0.28	0.63	0.67	0.63	0.75	0.55	0.08	0.22	0.58	0.50	0.86	0.77	0.80
GS-O3-AA	-0.14	-0.10	0.26	0.30	0.29	0.20	0.34	0.34	0.42	0.34	0.37	0.45	0.40	0.43
O3-AA-C19	0.25	0.16	0.76	0.81	0.76	0.38	0.76	0.03	-0.15	0.86	0.80	0.75	0.73	0.79
O3-AA-C18	0.21	0.08	0.83	0.89	0.83	0.45	0.76	0.14	-0.04	0.91	0.85	0.81	0.82	0.86
C19-AA	0.11	-0.05	0.71	0.87	0.65	0.55	0.49	0.19	-0.05	0.81	0.61	0.75	0.72	0.75
BC-AA	0.17	0.06	0.79	0.89	0.76	0.50	0.68	0.14	-0.02	0.89	0.75	0.77	0.78	0.80
C19-GS-O7	0.31	0.20	0.57	0.64	0.59	0.70	0.51	0.09	0.19	0.55	0.46	0.88	0.74	0.79
O3-AA	0.21	0.16	0.76	0.77	0.78	0.26	0.83	0.12	0.02	0.88	0.88	0.66	0.71	0.72
GS-O7-AA	-0.06	-0.03	0.29	0.32	0.36	0.17	0.40	0.16	0.30	0.33	0.38	0.45	0.41	0.41
O7-AA-C19	-0.06	-0.21	0.58	0.79	0.54	0.48	0.36	0.22	-0.11	0.73	0.53	0.71	0.63	0.70
HD	0.06	-0.11	-0.06	0.10	-0.11	0.09	-0.14	0.19	-0.19	0.07	-0.10	0.06	-0.07	0.05
O3-AA-BC	0.05	-0.04	0.73	0.79	0.74	0.34	0.68	0.18	-0.02	0.84	0.81	0.75	0.74	0.79
SASA	0.21	0.26	0.42	0.45	0.44	0.52	0.46	0.54	0.66	0.43	0.32	0.50	0.54	0.51
PSA_{side}	-0.10	-0.17	-0.02	0.08	-0.04	0.09	-0.13	-0.01	-0.04	0.01	-0.03	0.20	0.07	0.16
PSA	-0.03	-0.10	0.18	0.25	0.17	0.13	0.10	-0.01	-0.06	0.21	0.21	0.35	0.25	0.33

Table S2. Contd.

	O3-C18-GS	MR	C18-GS-O3	AA-GS-O7	O7-GS_{min}	O7-AA-C20	brotN	BC-GS_{min}	O3-AA-GS	O7-GS	GS-O7-C18	AA-GS-O3	O3-GS	C18-GS_{min}
O3-C18-GS	1.00													
MR	0.15	1.00												
C18-GS-O3	0.94	0.13	1.00											
AA-GS-O7	0.79	0.12	0.90	1.00										
O7-GS_{min}	0.91	0.08	0.96	0.95	1.00									
O7-AA-C20	0.85	0.12	0.74	0.60	0.71	1.00								
brotN	0.06	0.85	0.11	0.07	0.04	0.01	1.00							
BC-GS_{min}	0.83	0.04	0.90	0.95	0.96	0.64	0.02	1.00						
O3-AA-GS	0.91	0.14	0.97	0.95	0.98	0.71	0.09	0.96	1.00					
O7-GS	0.90	0.18	0.95	0.96	0.98	0.72	0.10	0.96	0.98	1.00				
GS-O7-C18	0.97	0.20	0.91	0.79	0.89	0.89	0.11	0.84	0.90	0.91	1.00			
AA-GS-O3	0.73	0.13	0.87	0.97	0.92	0.54	0.12	0.93	0.93	0.92	0.74	1.00		
O3-GS	0.91	0.18	0.96	0.94	0.97	0.73	0.11	0.96	0.99	0.99	0.91	0.91	1.00	
C18-GS_{min}	0.77	0.05	0.87	0.95	0.94	0.60	0.06	0.98	0.94	0.94	0.79	0.95	0.94	1.00
O7-AA	0.87	0.14	0.78	0.64	0.75	0.98	0.04	0.67	0.76	0.76	0.90	0.59	0.76	0.64
C19-GS	0.81	0.13	0.89	0.94	0.92	0.63	0.09	0.97	0.95	0.95	0.82	0.94	0.96	0.97
BC-GS	0.81	0.16	0.88	0.95	0.94	0.62	0.10	0.97	0.95	0.96	0.83	0.92	0.97	0.96
GS-O3-C18	0.96	0.18	0.88	0.80	0.90	0.86	0.09	0.85	0.89	0.91	0.97	0.74	0.91	0.81
GS-O3-C19	0.87	0.08	0.88	0.80	0.87	0.80	0.09	0.84	0.88	0.87	0.89	0.77	0.90	0.83
GS-O7-C19	0.75	0.08	0.88	0.82	0.85	0.54	0.15	0.87	0.89	0.85	0.78	0.86	0.88	0.87
C18-GS	0.74	0.14	0.83	0.92	0.89	0.58	0.08	0.95	0.91	0.93	0.77	0.91	0.93	0.96
O7-GS_{max}	0.80	0.27	0.88	0.96	0.92	0.63	0.18	0.94	0.94	0.97	0.83	0.93	0.96	0.93
O3-GS_{max}	0.82	0.29	0.89	0.93	0.92	0.64	0.22	0.93	0.95	0.95	0.85	0.90	0.97	0.92
BC-GS_{max}	0.74	0.24	0.83	0.92	0.88	0.55	0.19	0.93	0.91	0.92	0.77	0.91	0.93	0.93
O3-AA-C20	0.91	0.17	0.80	0.64	0.78	0.96	0.08	0.68	0.78	0.78	0.93	0.58	0.78	0.64
$SASA_{side}$	-0.04	0.83	-0.03	0.07	-0.04	0.00	0.73	-0.05	0.01	0.07	0.00	0.13	0.05	0.01
C19-GS_{max}	0.68	0.22	0.78	0.88	0.82	0.50	0.17	0.90	0.87	0.87	0.71	0.88	0.89	0.91
KierFlex	0.11	0.89	0.14	0.15	0.08	0.06	0.91	0.10	0.16	0.18	0.17	0.22	0.20	0.13
C18-AA	0.53	-0.13	0.74	0.71	0.69	0.37	0.00	0.68	0.72	0.67	0.51	0.75	0.70	0.72
C18-GS_{max}	0.63	0.21	0.72	0.86	0.79	0.47	0.13	0.88	0.82	0.85	0.67	0.85	0.85	0.88

Table S2. Contd.

	O3-C18-GS	MR	C18-GS-O3	AA-GS-O7	O7-GS_{min}	O7-AA-C20	brotN	BC-GS_{min}	O3-AA-GS	O7-GS	GS-O7-C18	AA-GS-O3	O3-GS	C18-GS_{min}
GS-O3-AA	0.37	0.47	0.33	0.43	0.42	0.37	0.26	0.46	0.44	0.50	0.45	0.38	0.51	0.48
O3-AA-C19	0.80	0.03	0.74	0.68	0.77	0.88	-0.15	0.72	0.75	0.77	0.84	0.62	0.77	0.69
O3-AA-C18	0.84	0.06	0.85	0.75	0.83	0.87	0.02	0.78	0.83	0.83	0.88	0.70	0.85	0.77
C19-AA	0.67	-0.02	0.79	0.70	0.72	0.61	0.07	0.68	0.76	0.70	0.66	0.72	0.74	0.70
BC-AA	0.81	0.05	0.83	0.71	0.78	0.78	0.05	0.72	0.81	0.77	0.81	0.69	0.80	0.71
C19-GS-O7	0.60	0.20	0.70	0.85	0.78	0.47	0.12	0.88	0.81	0.83	0.65	0.87	0.83	0.90
O3-AA	0.83	0.13	0.71	0.58	0.71	0.92	0.02	0.63	0.71	0.71	0.87	0.51	0.72	0.59
GS-O7-AA	0.39	0.31	0.32	0.37	0.41	0.37	0.11	0.47	0.44	0.49	0.49	0.34	0.51	0.47
O7-AA-C19	0.55	-0.08	0.70	0.66	0.67	0.51	-0.02	0.65	0.69	0.65	0.57	0.68	0.68	0.69
HD	-0.10	-0.09	-0.02	0.11	0.02	0.03	-0.17	0.02	-0.04	0.02	-0.10	0.14	-0.01	0.03
O3-AA-BC	0.77	0.08	0.76	0.68	0.77	0.81	0.01	0.72	0.76	0.77	0.82	0.63	0.78	0.71
SASA	0.50	0.79	0.54	0.57	0.52	0.44	0.68	0.48	0.55	0.61	0.53	0.60	0.59	0.51
PSA_{side}	-0.03	-0.29	0.08	0.17	0.16	-0.08	-0.20	0.24	0.13	0.13	-0.02	0.17	0.14	0.24
PSA	0.20	-0.26	0.26	0.30	0.34	0.16	-0.22	0.38	0.30	0.31	0.21	0.27	0.31	0.36

Table S2. Contd.

	O7-AA	C19-GS	BC-GS	GS-O3-C18	GS-O3-C19	GS-O7-C19	C18-GS	O7-GS_{max}	O3-GS_{max}	BC-GS_{max}	O3-AA-C20	$SASA_{side}$	C19-GS_{max}	KierFlex
O7-AA	1.00													
C19-GS	0.68	1.00												
BC-GS	0.66	0.99	1.00											
GS-O3-C18	0.87	0.82	0.84	1.00										
GS-O3-C19	0.81	0.85	0.83	0.91	1.00									
GS-O7-C19	0.58	0.87	0.86	0.71	0.81	1.00								
C18-GS	0.62	0.99	0.99	0.78	0.79	0.82	1.00							
O7-GS_{max}	0.67	0.96	0.98	0.83	0.81	0.83	0.96	1.00						
O3-GS_{max}	0.68	0.95	0.97	0.84	0.84	0.86	0.94	0.98	1.00					
BC-GS_{max}	0.59	0.97	0.98	0.77	0.77	0.82	0.98	0.98	0.98	1.00				
O3-AA-C20	0.96	0.66	0.66	0.92	0.86	0.60	0.60	0.67	0.68	0.57	1.00			
$SASA_{side}$	0.04	0.06	0.06	0.05	-0.01	-0.06	0.09	0.16	0.15	0.15	0.01	1.00		
C19-GS_{max}	0.55	0.96	0.96	0.71	0.74	0.79	0.97	0.94	0.94	0.98	0.51	0.15	1.00	
KierFlex	0.09	0.21	0.21	0.15	0.13	0.17	0.21	0.31	0.34	0.34	0.09	0.80	0.34	1.00
C18-AA	0.44	0.72	0.67	0.49	0.71	0.81	0.66	0.66	0.68	0.66	0.41	-0.13	0.65	0.02
C18-GS_{max}	0.51	0.94	0.94	0.68	0.69	0.73	0.97	0.93	0.92	0.97	0.47	0.16	0.99	0.31
GS-O3-AA	0.37	0.53	0.55	0.52	0.51	0.32	0.57	0.55	0.58	0.58	0.40	0.40	0.59	0.36
O3-AA-C19	0.88	0.70	0.69	0.86	0.80	0.58	0.66	0.68	0.67	0.59	0.87	-0.04	0.55	-0.10
O3-AA-C18	0.89	0.77	0.75	0.88	0.91	0.73	0.71	0.75	0.77	0.68	0.89	-0.05	0.63	0.02
C19-AA	0.68	0.72	0.66	0.64	0.80	0.74	0.65	0.68	0.70	0.64	0.64	-0.04	0.64	0.10
BC-AA	0.85	0.74	0.70	0.80	0.86	0.69	0.67	0.71	0.73	0.64	0.82	-0.01	0.63	0.09
C19-GS-O7	0.50	0.92	0.92	0.68	0.70	0.71	0.96	0.89	0.86	0.93	0.48	0.21	0.94	0.27
O3-AA	0.94	0.62	0.60	0.87	0.83	0.52	0.56	0.61	0.62	0.52	0.96	0.00	0.48	0.03
GS-O7-AA	0.37	0.55	0.58	0.50	0.48	0.41	0.60	0.53	0.57	0.58	0.39	0.21	0.60	0.23
O7-AA-C19	0.57	0.69	0.64	0.58	0.75	0.68	0.64	0.64	0.66	0.62	0.53	-0.08	0.62	0.03
HD	0.01	0.00	-0.01	-0.02	0.00	-0.08	0.02	0.02	-0.07	-0.05	0.00	0.22	-0.07	-0.13
O3-AA-BC	0.83	0.71	0.70	0.84	0.87	0.65	0.67	0.69	0.71	0.62	0.85	-0.04	0.57	0.01
SASA	0.49	0.56	0.56	0.56	0.50	0.44	0.56	0.65	0.63	0.60	0.48	0.80	0.57	0.74
PSA_{side}	-0.04	0.22	0.22	0.01	0.11	0.12	0.26	0.15	0.14	0.19	-0.03	-0.26	0.21	-0.21
PSA	0.19	0.35	0.36	0.24	0.30	0.23	0.37	0.29	0.28	0.31	0.21	-0.30	0.31	-0.23

Table S2. Contd.

	C18-AA	C18-GS_{max}	GS-O3-AA	O3-AA-C19	O3-AA-C18	C19-AA	BC-AA	C19-GS-O7	O3-AA	GS-O7-AA	O7-AA-C19	HD	O3-AA-BC	SASA	PSA_{side}	PSA
C18-AA	1.00															
C18-GS_{max}	0.61	1.00														
GS-O3-AA	0.21	0.62	1.00													
O3-AA-C19	0.48	0.53	0.54	1.00												
O3-AA-C18	0.69	0.59	0.50	0.92	1.00											
C19-AA	0.91	0.58	0.29	0.65	0.83	1.00										
BC-AA	0.76	0.57	0.39	0.80	0.90	0.93	1.00									
C19-GS-O7	0.59	0.95	0.66	0.59	0.61	0.57	0.56	1.00								
O3-AA	0.42	0.43	0.47	0.90	0.90	0.67	0.86	0.46	1.00							
GS-O7-AA	0.19	0.64	0.89	0.49	0.45	0.22	0.34	0.65	0.45	1.00						
O7-AA-C19	0.92	0.58	0.39	0.65	0.81	0.95	0.87	0.60	0.61	0.30	1.00					
HD	0.05	-0.01	-0.06	0.14	0.04	0.04	-0.01	0.11	0.00	-0.16	0.07	1.00				
O3-AA-BC	0.63	0.54	0.58	0.92	0.98	0.77	0.86	0.59	0.90	0.50	0.80	0.02	1.00			
SASA	0.32	0.56	0.56	0.44	0.47	0.43	0.49	0.59	0.45	0.39	0.37	0.21	0.46	1.00		
PSA_{side}	0.20	0.26	0.13	0.00	0.11	0.13	0.07	0.29	0.03	0.22	0.22	0.26	0.11	-0.16	1.00	
PSA	0.26	0.35	0.23	0.22	0.32	0.26	0.25	0.37	0.27	0.31	0.33	0.23	0.32	-0.08	0.96	1.00

Table S3. Values of structural and physico-chemical descriptors for the anilinyl conjugate of glu-CDCA in quantitative CSP-SAR analysis. Conjugates are listed in the decreasing order of K_m potency.[a]

CMPD	K_m (μM)	ΔG_w (kcal/mol)	logP	C19-GS-O3	O7-AA-C18	O7-C19-GS	C18-GS-O7	O7-C18-GS	HA	MW
9	0.100	-79.8	1.43	0.873	0.944	0.844	0.882	0.878	6	610
2	0.100	-73.8	2.04	0.808	0.837	0.820	0.843	0.849	6	630
6	0.100	-70.4	2.07	0.566	0.619	0.647	0.791	0.542	6	614
5	0.450	-75.2	1.45	0.869	0.927	0.853	0.909	0.834	6	614
22	0.549	-74.2	1.60	0.851	0.842	0.843	0.750	0.881	6	632
1	0.823	-79.3	1.10	0.870	0.860	0.856	0.767	0.858	6	596
8	0.919	-78.1	1.65	0.825	0.745	0.742	0.857	0.747	6	610
4	1.11	-78.6	1.15	0.754	0.785	0.805	0.653	0.875	6	614
11	1.21	-80.6	0.248	0.907	0.948	0.905	0.907	0.897	7	626
7	1.69	-79.4	1.58	0.815	0.875	0.789	0.666	0.838	6	610
3	2.22	-69.5	2.57	0.788	0.797	0.753	0.926	0.760	6	664
24	2.53	-75.7	2.12	0.612	0.623	0.636	0.468	0.809	6	624
16	2.54	-74.0	1.99	0.828	0.936	0.867	0.847	0.889	8	668
14	3.42	-75.6	1.22	0.894	0.953	0.870	0.893	0.882	8	650
10	3.87	-80.6	0.303	0.762	0.818	0.832	0.669	0.889	7	626
12	6.56	-79.6	0.441	0.927	0.909	0.885	0.922	0.883	7	626
15	7.27	-76.9	1.71	0.908	0.892	0.864	0.730	0.885	8	669
23	7.82	-79.1	2.04	0.876	0.875	0.857	0.748	0.894	6	624
21	7.91	-82.5	0.067	0.848	0.869	0.811	0.697	0.800	7	611
19	9.89	-75.4	0.748	0.859	0.878	0.859	0.806	0.814	7	611
17	10.3	-79.6	1.09	0.856	0.912	0.869	0.894	0.915	7	650
25	11.4	-77.0	-0.033	0.790	0.782	0.773	0.874	0.752	6	656
20	14.9	-84.1	-0.061	0.823	0.873	0.769	0.812	0.805	7	611
18	17.5	-73.4	1.72	0.453	0.699	0.463	0.812	0.449	7	626
26	495	-88.1	2.25	0.745	0.692	0.789	0.781	0.872	8	730
27	607	-165	-5.41	0.291	0.574	0.359	0.308	0.286	8	639

Table S3. Contd.

CMPD	K_m (μM)	AA-GS-O7	O7-GS $_{min}$	O7-AA-C20	brotN	BC-GS $_{min}$	O3-AA-GS	O7-GS	GS-O7-C18
9	0.100	0.893	0.887	0.931	12	0.881	0.866	0.856	0.872
2	0.100	0.825	0.794	0.831	12	0.877	0.846	0.782	0.848
6	0.100	0.579	0.549	0.604	12	0.588	0.560	0.545	0.557
5	0.450	0.835	0.880	0.916	12	0.841	0.851	0.835	0.835
22	0.549	0.726	0.757	0.883	12	0.722	0.760	0.735	0.856
1	0.823	0.781	0.808	0.891	12	0.794	0.799	0.762	0.878
8	0.919	0.702	0.732	0.771	12	0.620	0.718	0.675	0.725
4	1.11	0.598	0.676	0.887	12	0.663	0.687	0.644	0.822
11	1.21	0.873	0.885	0.937	13	0.892	0.895	0.875	0.916
7	1.69	0.566	0.637	0.900	12	0.577	0.649	0.603	0.797
3	2.22	0.839	0.755	0.802	13	0.801	0.801	0.745	0.763
24	2.53	0.453	0.451	0.863	12	0.428	0.444	0.468	0.675
16	2.54	0.788	0.790	0.936	15	0.827	0.792	0.795	0.898
14	3.42	0.853	0.817	0.934	13	0.806	0.863	0.832	0.888
10	3.87	0.621	0.698	0.895	13	0.706	0.724	0.675	0.842
12	6.56	0.893	0.861	0.884	13	0.885	0.884	0.845	0.896
15	7.27	0.699	0.701	0.908	15	0.627	0.768	0.688	0.843
23	7.82	0.711	0.707	0.941	12	0.701	0.799	0.714	0.841
21	7.91	0.736	0.782	0.894	12	0.798	0.770	0.737	0.828
19	9.89	0.833	0.796	0.896	12	0.770	0.787	0.747	0.834
17	10.3	0.844	0.799	0.923	13	0.779	0.835	0.868	0.898
25	11.4	0.721	0.712	0.786	14	0.698	0.730	0.688	0.740
20	14.9	0.812	0.815	0.894	12	0.796	0.779	0.791	0.808
18	17.5	0.551	0.451	0.704	13	0.460	0.467	0.433	0.468
26	495	0.766	0.794	0.836	16	0.753	0.799	0.796	0.862
27	607	0.296	0.285	0.638	13	0.297	0.335	0.284	0.422

Table S3. Contd.

CMPD	K_m (μM)	AA-GS-O3	O3-GS	C18-GS_{min}	O7-AA	C19-GS	BC-GS	GS-O3-C18	GS-O3-C19	GS-O7-C19
9	0.100	0.885	0.818	0.862	0.930	0.839	0.847	0.886	0.862	0.841
2	0.100	0.868	0.792	0.828	0.845	0.823	0.832	0.845	0.778	0.805
6	0.100	0.636	0.529	0.607	0.601	0.577	0.581	0.577	0.602	0.792
5	0.450	0.848	0.815	0.842	0.930	0.762	0.782	0.869	0.819	0.823
22	0.549	0.736	0.725	0.721	0.873	0.702	0.701	0.868	0.858	0.809
1	0.823	0.807	0.745	0.805	0.856	0.719	0.707	0.895	0.849	0.843
8	0.919	0.670	0.670	0.611	0.779	0.597	0.592	0.822	0.790	0.702
4	1.11	0.640	0.656	0.670	0.892	0.642	0.625	0.843	0.811	0.754
11	1.21	0.913	0.848	0.885	0.928	0.830	0.843	0.928	0.876	0.876
7	1.69	0.590	0.611	0.550	0.908	0.562	0.544	0.783	0.688	0.725
3	2.22	0.799	0.751	0.773	0.808	0.774	0.810	0.780	0.789	0.791
24	2.53	0.417	0.435	0.429	0.804	0.427	0.435	0.726	0.638	0.524
16	2.54	0.812	0.806	0.819	0.926	0.814	0.808	0.916	0.877	0.860
14	3.42	0.868	0.852	0.836	0.926	0.839	0.840	0.887	0.860	0.853
10	3.87	0.668	0.692	0.712	0.892	0.679	0.662	0.872	0.846	0.787
12	6.56	0.883	0.874	0.887	0.886	0.848	0.865	0.913	0.885	0.877
15	7.27	0.721	0.692	0.637	0.905	0.637	0.622	0.790	0.817	0.824
23	7.82	0.751	0.735	0.703	0.933	0.732	0.691	0.820	0.835	0.826
21	7.91	0.745	0.781	0.765	0.859	0.715	0.734	0.873	0.861	0.822
19	9.89	0.848	0.732	0.742	0.894	0.676	0.673	0.825	0.802	0.823
17	10.3	0.865	0.839	0.772	0.923	0.799	0.832	0.928	0.864	0.840
25	11.4	0.825	0.698	0.710	0.777	0.687	0.688	0.787	0.791	0.821
20	14.9	0.824	0.745	0.785	0.888	0.791	0.777	0.874	0.824	0.752
18	17.5	0.647	0.421	0.562	0.711	0.493	0.422	0.564	0.617	0.600
26	495	0.787	0.773	0.743	0.847	0.713	0.742	0.890	0.767	0.773
27	607	0.371	0.301	0.371	0.642	0.375	0.311	0.495	0.613	0.589

Table S3. Contd.

CMPD	K_m (μM)	C18-GS	O7-GS $_{max}$	O3-GS$_{max}$	BC-GS$_{max}$	O3-AA-C20	SASA $_{side}$ (Å^2)	C19-GS$_{max}$	KierFlex	C18-AA
9	0.100	0.855	0.829	0.774	0.814	0.945	533	0.805	8.79	0.930
2	0.100	0.855	0.807	0.779	0.834	0.810	518	0.846	9.39	0.864
6	0.100	0.581	0.528	0.513	0.549	0.553	491	0.556	8.71	0.779
5	0.450	0.769	0.755	0.739	0.717	0.924	508	0.684	8.71	0.917
22	0.549	0.683	0.658	0.665	0.644	0.926	516	0.647	8.87	0.847
1	0.823	0.712	0.660	0.639	0.629	0.910	497	0.617	8.55	0.907
8	0.919	0.551	0.592	0.597	0.548	0.813	525	0.546	8.79	0.878
4	1.11	0.622	0.550	0.569	0.546	0.932	501	0.565	8.71	0.781
11	1.21	0.833	0.815	0.784	0.782	0.947	548	0.755	9.27	0.935
7	1.69	0.514	0.505	0.521	0.481	0.881	522	0.498	8.79	0.774
3	2.22	0.796	0.744	0.738	0.784	0.792	547	0.764	9.28	0.851
24	2.53	0.436	0.441	0.432	0.422	0.799	546	0.417	9.03	0.514
16	2.54	0.806	0.767	0.770	0.774	0.924	612	0.778	10.10	0.918
14	3.42	0.849	0.862	0.861	0.839	0.925	579	0.831	9.66	0.935
10	3.87	0.665	0.613	0.628	0.618	0.924	544	0.615	9.27	0.796
12	6.56	0.837	0.839	0.835	0.835	0.896	547	0.826	9.27	0.924
15	7.27	0.589	0.672	0.667	0.614	0.934	568	0.583	9.87	0.894
23	7.82	0.695	0.632	0.639	0.621	0.931	544	0.659	9.03	0.844
21	7.91	0.714	0.672	0.703	0.673	0.906	513	0.654	8.79	0.862
19	9.89	0.629	0.690	0.648	0.610	0.921	507	0.568	8.79	0.894
17	10.3	0.836	0.859	0.793	0.806	0.935	680	0.751	9.66	0.909
25	11.4	0.671	0.667	0.667	0.699	0.787	591	0.681	10.01	0.867
20	14.9	0.793	0.733	0.640	0.692	0.915	522	0.704	8.79	0.849
18	17.5	0.484	0.409	0.407	0.414	0.625	657	0.487	9.27	0.744
26	495	0.709	0.751	0.733	0.708	0.915	698	0.685	10.39	0.699
27	607	0.358	0.286	0.314	0.318	0.587	540	0.385	9.12	0.789

Table S3. Contd.

CMPD	K_m (μM)	C18-GS_{max}	GS-O3-AA	O3-AA-C19	O3-AA-C18	C19-AA	BC-AA	C19-GS-O7	O3-AA	GS-O7-AA
9	0.100	0.821	0.817	0.944	0.909	0.916	0.934	0.916	0.927	0.825
2	0.100	0.837	0.712	0.806	0.787	0.875	0.872	0.918	0.832	0.753
6	0.100	0.543	0.545	0.579	0.563	0.582	0.552	0.650	0.539	0.698
5	0.450	0.655	0.686	0.915	0.945	0.915	0.921	0.776	0.920	0.709
22	0.549	0.621	0.781	0.808	0.849	0.842	0.877	0.743	0.940	0.846
1	0.823	0.571	0.721	0.928	0.915	0.870	0.853	0.805	0.881	0.718
8	0.919	0.488	0.651	0.793	0.780	0.850	0.871	0.606	0.828	0.626
4	1.11	0.512	0.690	0.858	0.818	0.782	0.860	0.685	0.915	0.761
11	1.21	0.748	0.815	0.963	0.939	0.920	0.936	0.865	0.922	0.817
7	1.69	0.447	0.628	0.867	0.805	0.817	0.878	0.586	0.886	0.725
3	2.22	0.781	0.784	0.796	0.790	0.791	0.786	0.861	0.785	0.796
24	2.53	0.410	0.688	0.761	0.674	0.511	0.588	0.551	0.778	0.699
16	2.54	0.746	0.758	0.875	0.922	0.909	0.921	0.815	0.933	0.762
14	3.42	0.849	0.918	0.933	0.915	0.931	0.924	0.887	0.919	0.893
10	3.87	0.562	0.708	0.855	0.828	0.792	0.860	0.739	0.926	0.776
12	6.56	0.814	0.821	0.893	0.905	0.931	0.942	0.865	0.898	0.803
15	7.27	0.537	0.569	0.737	0.830	0.925	0.882	0.646	0.853	0.607
23	7.82	0.591	0.708	0.926	0.866	0.846	0.886	0.743	0.911	0.751
21	7.91	0.666	0.826	0.923	0.898	0.839	0.826	0.814	0.869	0.807
19	9.89	0.517	0.601	0.917	0.898	0.878	0.884	0.687	0.918	0.610
17	10.3	0.775	0.848	0.950	0.919	0.899	0.923	0.898	0.923	0.869
25	11.4	0.638	0.681	0.701	0.748	0.824	0.789	0.765	0.726	0.698
20	14.9	0.723	0.694	0.874	0.847	0.837	0.874	0.856	0.894	0.737
18	17.5	0.439	0.613	0.659	0.605	0.712	0.685	0.667	0.654	0.594
26	495	0.656	0.919	0.844	0.800	0.703	0.794	0.826	0.893	0.857
27	607	0.341	0.751	0.651	0.675	0.750	0.711	0.556	0.693	0.743

Table S3. Contd.

CMPD	K_m (μM)	O7-AA-C19	HD	O3-AA-BC	SASA (Å^2)	PSA_{side} (Å^2)	PSA (Å^2)
9	0.100	0.944	4	0.931	993	173	251
2	0.100	0.910	4	0.796	965	225	299
6	0.100	0.626	4	0.570	877	199	255
5	0.450	0.954	4	0.951	953	251	328
22	0.549	0.845	4	0.858	941	245	322
1	0.823	0.920	4	0.946	956	173	251
8	0.919	0.883	4	0.804	960	162	240
4	1.11	0.798	4	0.848	918	207	285
11	1.21	0.969	4	0.955	1005	186	264
7	1.69	0.785	4	0.795	942	167	245
3	2.22	0.816	4	0.795	966	236	303
24	2.53	0.532	4	0.704	906	153	232
16	2.54	0.940	4	0.920	1074	185	263
14	3.42	0.973	4	0.923	1035	191	269
10	3.87	0.806	4	0.846	959	177	255
12	6.56	0.926	4	0.924	996	186	263
15	7.27	0.855	4	0.801	1006	181	256
23	7.82	0.850	4	0.873	973	164	242
21	7.91	0.889	5	0.900	960	239	317
19	9.89	0.911	5	0.914	971	192	270
17	10.3	0.942	5	0.938	1111	187	265
25	11.4	0.820	4	0.739	993	173	237
20	14.9	0.861	5	0.859	987	245	323
18	17.5	0.717	5	0.608	989	188	241
26	495	0.718	4	0.858	1122	187	264
27	607	0.863	4	0.762	891	215	275

[a] Entries for structural descriptors are the overlap coefficients of the conjugate with respect to **13**, the most potent compound in terms of Km and Vmax**.**

Table S4. Results from single-variable regression of molecular descriptors against K_m for **Set 1**.[a]

Molecular Descriptor	r^2	Coeff. indep. variable[b]	SEM of coeff. Indep. Variable[b]	Coeff. of intercept (μM)	SEM of coeff. of intercept (μM)
ΔG_w (kcal/mol)	0.679	-6.97	0.98	-517	81
logP	0.344	-57.7	16	107	30
C19-GS-O3	0.331	-578	168	500	134
O7-AA-C18	0.290	-744	238	661	198
O7-C19-GS	0.286	-621	200	533	159
C18-GS-O7	0.276	-550	182	474	143
O7-C18-GS	0.247	-496	177	443	144
HA	0.246	93.9	34	-582	226
MW	0.246	2.62	0.94	-1610	593
O7-AA-BC	0.232	-689	256	638	222
O3-C19-GS	0.218	-609	235	537	191
C19-GS_{min}	0.215	-514	201	411	145
O7-AA-GS	0.209	-474	188	397	141
O3-GS_{min}	0.209	-460	183	380	135
O3C18GS	0.208	-459	183	413	149
MR (m^3/mol)	0.205	84	34	-1415	588
C18-GS-O3	0.201	-409	166	367	133
AA-GS-O7	0.187	-442	188	366	138
O7-GS_{min}	0.183	-437	189	363	139
O7AAC20	0.179	-699	305	645	263
brotN	0.179	57.1	25	-682	320
BC-GS_{min}	0.178	-419	184	346	134
O3-AA-GS	0.168	-432	196	366	148
O7-GS	0.160	-415	194	341	140
GS-O7-C18	0.160	-463	217	414	174
AA-GS-O3	0.160	-434	203	371	154
O3-GS	0.160	-418	196	342	141
C18-GS_{min}	0.158	-448	211	367	154
O7-AA	0.155	-664	316	613	271
C19-GS	0.149	-450	219	359	155
BC-GS	0.146	-395	195	319	137
GS-O3-C18	0.146	-505	249	460	206
GS-O3-C19	0.139	-636	323	551	257
GS-O7-C19	0.135	-615	317	528	250
C18-GS	0.131	-389	204	314	143
O7-GS_{max}	0.120	-352	195	281	133
O3-GS_{max}	0.116	-376	213	294	142
BC-GS_{max}	0.112	-353	203	277	135
O3-AA-C20	0.109	-439	256	424	222
$SASA_{side}$ (Å^2)	0.107	0.890	0.52	-445	291
C19-GS_{max}	0.0940	-363	230	283	152
KierFlex	0.0919	91.2	58	-791	538
C18-AA	0.0882	-478	314	450	266
C18-GS_{max}	0.0878	-307	202	239	130

GS-O3-AA	0.0836	439	297	-273	218
O3-AA-C19	0.0815	-413	283	393	239
O3-AA-C18	0.0727	-393	286	370	238
C19-AA	0.0717	-381	280	361	233
BC-AA	0.0688	-382	287	367	242
C19-GS-O7	0.0440	-276	262	256	201
O3-AA	0.0429	-307	296	309	254
GS-O7-AA	0.0232	280	370	-163	279
O7-AA-C19	0.0196	-196	283	213	242
HD	0.0134	-43.0	75	227	317
O3-AA-BC	0.0109	-154	299	176	253
SASA ($Å^2$)	7.75E-03	0.225	0.52	-174	510
PSA_{side} ($Å^2$)	5.26E-03	0.382	1.1	-27.8	212
PSA ($Å^2$)	2.44E-09	0.000258	1.1	46.7	289

[a] Regression analysis of structural descriptors (e.g. C18-GS-O7) employed the overlap coefficients with respect to **13**.

[b] Coefficient of independent variable has units of μM divided by units of the molecular descriptor (e.g. $μM/Å^2$ for SASA).

Table S5. Results from single-variable regression of molecular descriptors against K_m for **Set 2**.[a]

Molecular Descriptor	r^2	Coeff of indep variable[b]	SEM of coeff of indep variable[b]	coeff of intercept (μM)	SEM of coeff of intercept (μM)
HD	0.579	9.23	1.7	-34.0	7.1
$SASA_{side}$ (Å^2)	0.294	0.0568	0.019	-26.2	10
logP	0.162	-2.64	1.3	8.13	1.9
HA	0.143	2.66	1.4	-12.7	9.2
SASA (Å^2)	0.132	0.0367	0.020	-31.1	20
O7-C18-GS	0.114	-15.3	9.1	17.3	7.5
O7-C19-GS	0.106	-16.5	10	18.0	8.3
GS-O7-AA	0.0876	-18.2	13	18.4	9.4
GS-O7-C18	0.0857	-13.6	9.5	15.7	7.7
O3-C19-GS	0.0835	-14.1	9.9	16.3	8.2
O3-C18-GS	0.0786	-12.0	8.8	14.6	7.2
KierFlex	0.0707	2.97	2.3	-22.4	21
MR (m^3/mol)	0.0686	2.33	1.8	-35.5	32
ΔG_w (kcal/mol)	0.0593	-0.341	0.29	-21.6	22
brotN	0.0562	1.29	1.1	-11.5	14
GS-O3-C18	0.0507	-11.9	11	14.7	9.2
C19-GS-O3	0.0488	-9.79	9.2	12.7	7.5
O7-AA-GS	0.0455	-9.35	9.1	11.9	7.0
$O7\text{-}GS_{min}$	0.0422	-8.63	8.8	11.2	6.6
$BC\text{-}GS_{min}$	0.0413	-7.94	8.2	10.6	6.0
$O3\text{-}GS_{max}$	0.0358	-7.96	8.8	10.1	6.0
O3-AA-GS	0.0348	-7.83	8.8	10.7	6.7
BC-GS	0.0323	-7.10	8.3	9.80	5.9
GS-O7-C19	0.0322	-10.8	13	13.4	10
O3-AA-BC	0.0318	-8.59	10	12.0	8.6
$O3\text{-}GS_{min}$	0.0317	-7.20	8.5	10.1	6.4
O3-GS	0.0310	-7.31	8.7	10.1	6.4
O7-GS	0.0297	-7.28	8.9	10.1	6.5
O3-AA	0.0295	-8.72	11	12.3	9.2
C18-GS-O3	0.0278	-6.11	7.7	9.69	6.3
$BC\text{-}GS_{max}$	0.0227	-5.87	8.2	8.70	5.6
O3-AA-C18	0.0216	-7.25	10	10.8	8.7
MW	0.0211	0.0353	0.051	-17.3	32
GS-O3-AA	0.0193	-7.45	11	10.2	8.2
O3-AA-C19	0.0169	-6.54	11	10.3	9.0
C18-GS	0.0166	-5.10	8.4	8.36	5.9
O3-AA-C20	0.0163	-6.33	10	10.3	9.2
$C18\text{-}GS_{min}$	0.0152	-5.29	9.1	8.66	6.7
$C19\text{-}GS_{max}$	0.0148	-5.15	9.0	8.20	6.0
C19-GS	0.0138	-5.13	9.3	8.43	6.6
$O7\text{-}GS_{max}$	0.0135	-4.52	8.2	7.87	5.7
$C19\text{-}GS_{min}$	0.0131	-4.99	9.2	8.42	6.8
$C18\text{-}GS_{max}$	0.0114	-3.91	7.8	7.29	5.1
GS-O3-C19	0.00919	-5.84	13	9.48	10

O7-AA	0.00840	-5.71	13	9.72	11
O7-AA-C20	0.00834	-5.62	13	9.67	11
BC-AA	0.00671	-4.01	10	8.19	8.9
AA-GS-O3	0.00521	3.05	9.0	2.48	6.9
PSA ($Å^2$)	0.00471	-0.0116	0.036	7.92	9.7
C18-GS-O7	0.00463	3.10	9.7	2.33	7.8
O7-AA-C19	0.00369	-2.84	10	7.22	8.6
O7-AA-BC	0.00263	-2.71	11	7.17	9.9
AA-GS-O7	0.00182	-1.75	8.7	6.09	6.5
C18-AA	0.00179	-2.34	12	6.79	10
O7-AA-C18	0.00126	-1.89	11	6.39	9.6
PSA_{side} ($Å^2$)	4.93E-05	0.00121	0.037	4.56	7.2
C19-GS-O7	1.14E-05	0.155	9.8	4.68	7.5
C19-AA	7.47E-06	-0.131	10	4.91	8.6

[a] Regression analysis of structural descriptors (e.g. C18-GS-O7) employed the overlap coefficients with respect to **13**.

[b] Coefficient of independent variable has units of μM divided by units of the molecular descriptor (e.g. $μM/Å^2$ for SASA).

Table S6. Results from single-variable regression of molecular descriptors against K_m/normV_{max} for **Set 1**.[a]

Molecular Descriptor	r^2	Coeff of indep variable[b]	SEM of coeff of indep variable[b]	Coeff of intercept (μM)	SEM of coeff of intercept (μM)
ΔG_w (kcal/mol)	0.902	-10.5	0.71	-788	58
logP	0.590	-98.5	17	164	30
C19-GS-O3	0.466	-894	195	762	156
O7-C19-GS	0.438	-1003	232	846	184
O7-C18-GS	0.424	-848	202	739	164
C18-GS-O7	0.387	-850	218	721	172
O3-C18-GS	0.362	-790	214	692	174
O7-AA-GS	0.354	-804	222	655	167
O3-GS_{min}	0.324	-747	220	603	163
C18-GS-O3	0.320	-673	200	587	160
O7-GS_{min}	0.316	-750	225	604	166
C19-GS_{min}	0.306	-801	246	629	178
O7-AA-C18	0.298	-984	308	873	257
AA-GS-O7	0.298	-727	228	586	168
GS-O7-C18	0.292	-816	260	708	208
O7-GS	0.288	-727	233	575	168
O3-AA-GS	0.287	-738	237	606	178
BC-GS_{min}	0.286	-694	224	557	163
O3-C19-GS	0.281	-902	295	786	239
O3-GS	0.277	-718	237	567	170
GS-O3-C18	0.273	-901	301	797	248
AA-GS-O3	0.251	-709	250	591	190
O7-AA-C20	0.247	-1071	382	979	329
C18-GS_{min}	0.247	-731	260	584	190
BC-GS	0.244	-665	239	520	169
O7-AA-BC	0.234	-904	334	837	289
C19-GS	0.230	-729	273	567	192
O7-AA	0.227	-1047	395	953	338
O7-GS_{max}	0.218	-619	240	474	163
HA	0.213	114	45	-703	302
O3-GS_{max}	0.213	-667	262	498	175
O3-AA-C20	0.203	-781	316	732	274
C18-GS	0.202	-630	255	493	179
GS-O7-C19	0.197	-968	399	818	314
BC-GS_{max}	0.191	-602	253	454	169
GS-O3-C19	0.187	-961	409	823	326
C19-GS_{max}	0.154	-606	290	455	192
C18-GS_{max}	0.138	-504	257	376	165
O3-AA-C19	0.124	-667	361	619	304
O3-AA-C18	0.0989	-598	368	553	306
O3-AA	0.0871	-571	378	548	324
C19-GS-O7	0.0861	-503	335	443	257
BC-AA	0.0816	-543	372	517	314
C18-AA	0.0528	-483	418	468	354
C19-AA	0.0522	-425	369	411	307

$SASA_{side}$ ($Å^2$)	0.0421	0.729	0.71	-342	394
GS-O3-AA	0.0356	374	397	-211	292
O3-AA-BC	0.0232	-293	388	307	328
KierFlex	0.0199	-44.6	64	478	599
MR (m^3/mol)	0.0170	-24.0	37	483	656
PSA_{side} ($Å^2$)	0.0127	0.773	1.4	-90	275
brotN	0.00691	-11.8	29	216	381
SASA ($Å^2$)	0.00637	-0.267	0.68	322	667
MW	0.00604	-0.449	1.2	349	756
GS-O7-AA	0.00508	171	488	-67.0	367
O7-AA-C19	0.00480	-127	373	168	318
HD	0.00371	-29.5	99	185	416
PSA ($Å^2$)	1.07E-04	0.0703	1.4	41.9	377

[a] Regression analysis of structural descriptors (e.g. C18-GS-O7) employed the overlap coefficients with respect to **13**.

[b] Coefficient of independent variable has units of μM divided by units of the molecular descriptor (e.g. μM/$Å^2$ for SASA).

Table S7. Results from single-variable regression of molecular descriptors against K_m/normV_{max} for **Set 2**.[a]

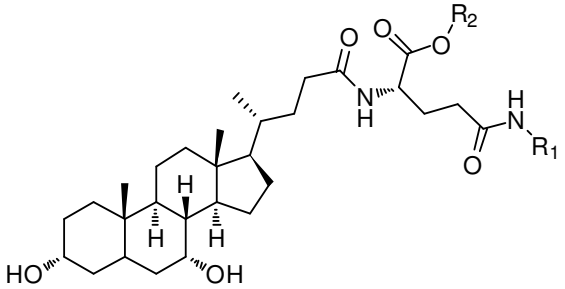
Molecular Descriptor	r^2	Coeff of indep variable[b]	SEM of coeff of indep variable[b]	Coeff of intercept (μM)	SEM of coeff of intercept (μM)
HD	0.598	32.8	5.7	-127	24
$SASA_{side}$ (Å^2)	0.525	0.265	0.054	-134	30
O7-C19-GS	0.209	-81.3	34	76.1	27
O7-C18-GS	0.203	-71.5	30	69.5	25
SASA (Å^2)	0.184	0.152	0.068	-138	67
O3-C19-GS	0.176	-71.6	33	69.7	27
O3-C18-GS	0.160	-59.9	29	59.9	24
GS-O7-C18	0.155	-63.9	32	62.5	26
C19-GS-O3	0.151	-60.2	30	59.6	25
O7-AA-GS	0.0890	-45.8	31	45.6	24
GS-O3-C18	0.0814	-53.0	38	54.9	32
O7-GS_{min}	0.0775	-40.9	30	41.3	23
C18-GS-O3	0.0754	-35.2	26	39.3	21
HA	0.0727	6.62	5.0	-32.5	33
O3-AA-GS	0.0691	-38.7	30	40.2	23
O3-AA-C20	0.0685	-45.4	36	50.5	31
O3-AA	0.0647	-45.2	37	49.8	32
O3-GS_{min}	0.0635	-35.7	29	37.6	22
GS-O7-C19	0.0629	-52.9	44	52.9	35
BC-GS_{min}	0.0612	-33.8	28	35.8	21
logP	0.0550	-5.39	4.8	17.8	7.0
O3-AA-BC	0.0520	-38.5	35	43.4	30
O3-GS	0.0506	-32.7	30	34.6	22
O3-AA-C18	0.0467	-37.3	36	42.1	30
O7-GS	0.0432	-30.7	31	33.3	23
O3-GS_{max}	0.0407	-29.7	31	30.9	21
O7-AA-C20	0.0396	-42.8	45	48.2	39
BC-GS	0.0383	-27.1	29	30.1	21
O7-AA	0.0360	-41.3	46	46.7	39
GS-O3-C19	0.0353	-40.0	45	43.1	36
C19-GS_{min}	0.0251	-24.2	32	28.6	24
BC-AA	0.0229	-25.9	36	33.0	31
BC-GS_{max}	0.0216	-20.1	29	24.4	19
C19-GS	0.0214	-22.4	32	26.9	23
O3-AA-C19	0.0200	-24.9	37	32.1	32
C18-GS_{min}	0.0199	-21.2	32	26.5	23
O7-AA-BC	0.0198	-26.0	39	33.8	34
GS-O7-AA	0.0196	-30.2	45	33.5	34
O7-GS_{max}	0.0182	-18.4	29	23.5	20
C18-GS-O7	0.0181	21.5	34	-6.07	27
ΔG_w (kcal/mol)	0.0142	-0.585	1.0	-34.1	80
C19-GS_{max}	0.0111	-15.6	31	21.4	21
C18-GS	0.0110	-14.5	29	21.2	21
O7-AA-C18	0.0109	-19.5	40	27.5	33
PSA (Å^2)	0.00917	-0.0566	0.13	26.3	34

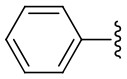
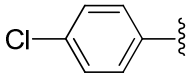
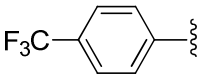
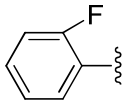
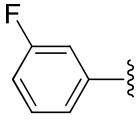
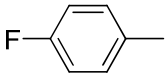
AA-GS-O7	0.00791	-12.8	31	20.5	23
C18-AA	0.00498	-13.7	41	22.7	35
C19-GS-O7	0.00495	11.3	34	2.42	26
C19-AA	0.00477	-11.6	36	20.7	30
C18-GS_{max}	0.00476	-8.85	27	16.7	18
O7-AA-C19	0.00474	-11.3	35	20.7	30
MR (m^3/mol)	0.00264	0.835	3.5	-3.71	61
KierFlex	0.00205	1.27	6.0	-0.880	56
AA-GS-O3	0.00161	5.92	31	6.55	24
MW	9.27E-04	-0.0155	0.11	21.0	70
PSA_{side} ($Å^2$)	1.20E-04	0.00660	0.13	9.77	25
GS-O3-AA	1.67E-05	0.765	40	10.5	29
brotN	1.85E-08	0.00170	2.7	11.0	35

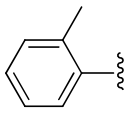
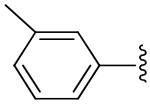
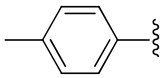
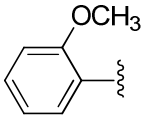
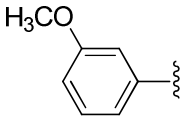
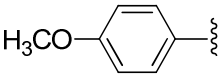
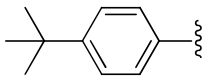
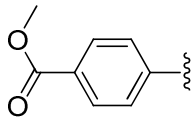
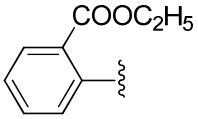
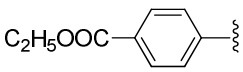
[a] Regression analysis of structural descriptors (e.g. C18-GS-O7) employed the overlap coefficients with respect to **13**.

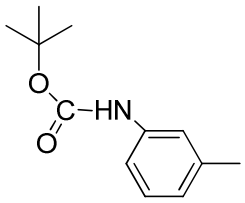
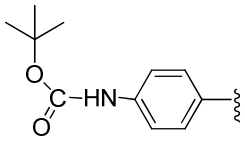
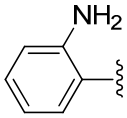
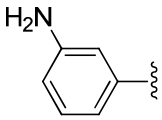
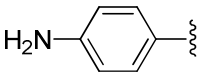
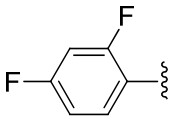
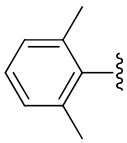
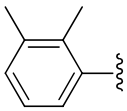
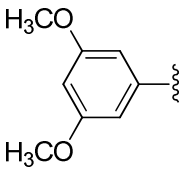
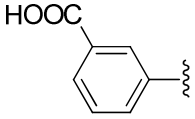
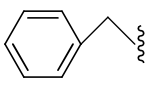
[b] Coefficient of independent variable has units of μM divided by units of the molecular descriptor (e.g. μM/$Å^2$ for SASA).

Table S8. Observed and predicted K_m values of anilinyl conjugated in **Set 1** and **Set 2** (using the best model in respective set).



Compound	R_1	R_2	Observed K_m (µM)[a]	Predicted K_m by Model 1 for Set 1 (µM)	Predicted K_m by Model 1 for Set 2 (µM)
1		**H**	**0.823 ± 0.320**	**-17.6**	**-0.241**
2		**H**	**0.100[a] ± 0.773**	**25.5**	**2.13**
3		**H**	**2.22 ± 1.71**	**6.55**	**0.638**
4		**H**	**1.11 ± 0.35**	**-11.3**	**1.34**
5		**H**	**0.450 ± 0.611**	**-64.8**	**-1.12**
6		**H**	**0.100[a] ± 0.330**	**15.0**	**3.00**

7		**H**	**1.69 ± 0.71**	**-65.7**	**3.58**
8		**H**	**0.919 ± 0.622**	**22.0**	**1.97**
9		**H**	**0.100[a] ± 0.500**	**-7.50**	**1.43**
10		**H**	**3.87 ± 0.55**	**34.9**	**4.68**
11		**H**	**1.21 ± 0.58**	**12.9**	**3.36**
12		**H**	**6.56 ± 0.98**	**28.7**	**3.16**
13		**H**	**0.100[a] ± 5.302**	**78.6**	**0.965**
14		**H**	**3.42 ± 1.23**	**32.5**	**3.51**
15		**H**	**7.27 ± 2.80**	**15.5**	**7.61**
16		**H**	**2.54 ± 0.69**	**30.3**	**4.19**

17		**H**	**10.3 ± 3.1**	**75.8**	**12.8**
18		**H**	**17.5 ± 4.7**	**-18.5**	**15.9**
19		**H**	**9.89 ± 1.15**	**-42.0**	**8.45**
20		**H**	**14.9 ± 1.2**	**26.9**	**12.2**
21		**H**	**7.91 ± 1.94**	**18.6**	**11.3**
22		**H**	**0.549 ± 0.240**	**-51.9**	**-0.826**
23		**H**	**7.82 ± 2.06**	**5.85**	**3.78**
24		**H**	**2.53 ± 0.48**	**52.9**	**4.09**
25		**H**	**11.4 ± 1.5**	**76.8**	**8.40**
26			**495 ± 222**	**401**	**N/A**

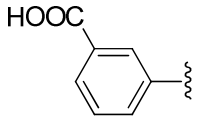
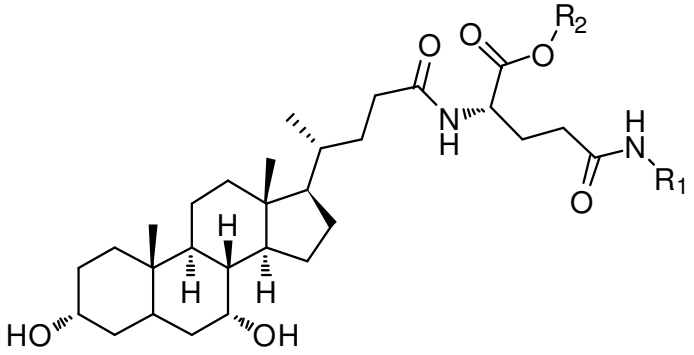
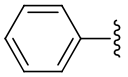
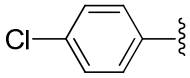
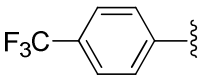
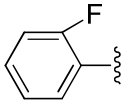
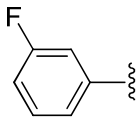
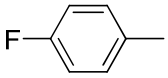
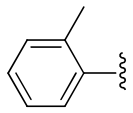
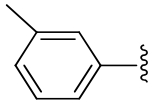
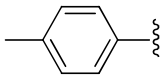
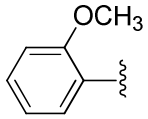
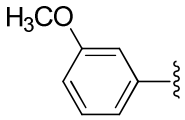
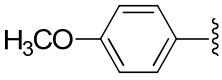
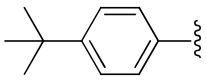
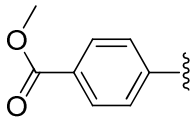
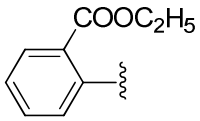
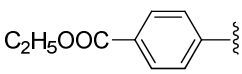
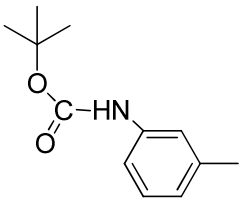
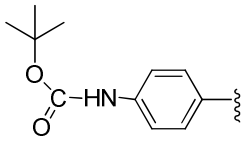
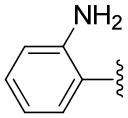
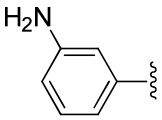
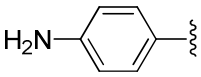
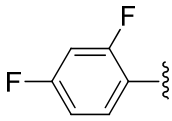
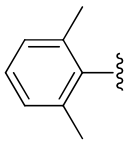
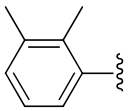
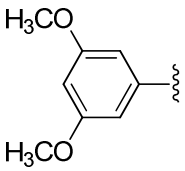
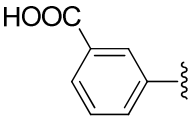
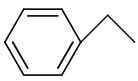
27		**H**	**607 ± 476**	**614**	**N/A**

Table S9. Observed and predicted K_m/normV_{max} values of anilinyl conjugated in **Set 1** and **Set 2** (using the best model in respective set).



Compound	R_1	R_2	Observed K_m/normV_{max} (μM)[a]	Predicted K_m/normV_{max} by Model 1 for Set 1 (μM)	Predicted K_m/normV_{max} by Model 1 for Set 2 (μM)
1		**H**	**0.690**	**-6.42**	**-5.02**
2		**H**	**0.0662**	**-16.3**	**0.212**
3		**H**	**1.71**	**-20.9**	**6.57**
4		**H**	**1.10**	**15.5**	**1.30**
5		**H**	**0.658**	**-36.7**	**3.09**
6		**H**	**0.0917**	**-12.77**	**-1.64**

7		**H**	**0.980**	**-29.1**	**1.47**
8		**H**	**0.885**	**41.5**	**3.33**
9		**H**	**0.0676**	**-7.92**	**0.431**
10		**H**	**3.95**	**33.6**	**7.02**
11		**H**	**2.19**	**7.16**	**4.70**
12		**H**	**7.25**	**10.4**	**4.47**
13		**H**	**0.0431**	**98.1**	**14.7**
14		**H**	**9.09**	**-14.4**	**8.14**
15		**H**	**4.95**	**0.450**	**5.20**
16		**H**	**3.18**	**8.15**	**7.36**

17		**H**	**50.8**	**106**	**52.8**
18		**H**	**69.9**	**60.0**	**68.5**
19		**H**	**13.0**	**-29.4**	**20.3**
20		**H**	**27.9**	**102**	**18.1**
21		**H**	**23.6**	**61.8**	**25.5**
22		**H**	**0.513**	**-15.3**	**3.38**
23		**H**	**14.3**	**-7.02**	**5.50**
24		**H**	**2.56**	**33.1**	**6.93**
25		**H**	**25.8**	**43.7**	**17.7**
26			**369**	**315**	**N/A**

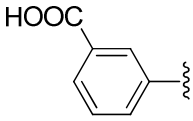
27		**H**	**952**	**944**	**N/A**

Table S10. Results from multivariable regression and AIC_C analysis for the selected CSP-SAR models for $log(K_m)$ for **Set 1**.[a]

CSP-SAR Models	r^2	Q^2	F	W_i	K	A (m^{-3}. mol)	B	C	D	Standardized A (m^{-3}. mol)	Standardized B	Standardized C	Standardized D
MR, logP, HD, C18-GS_{max}	0.837	0.749	26.9	18.3	- 15.4 ± 2.0	0.835 ± 0.10	- 0.310 ± 0.057	0.701 ± 0.21	- 1.91 ± 0.60	0.724	-0.508	0.303	-0.296
MR, logP, HD, BC-GS_{max}	0.832	0.733	26.1	12.9	- 15.4 ± 2.1	0.842 ± 0.11	- 0.302 ± 0.058	0.674 ± 0.21	- 1.94 ± 0.64	0.730	-0.496	0.292	-0.294

[a] *A*, *B, C* and *D* represent the coefficient of the independent variables (molecular descriptors); *K* represents the coefficient of the intercept. **Set 1** includes all compounds that were substrates.

Table S11. Results from multivariable regression and AIC_C analysis for the selected CSP-SAR models for $log(K_m)$ for **Set 2**.[a]

CSP-SAR Models	r^2	Q^2	F	W_i	K	A	B	C	D	Standardized A	Standardized B	Standardized C	Standardized D
HD, ΔG_w, MW, C18-GS_{max}	0.730	0.489	10.2	4.61	- 24.2 ± 4.6	0.811 ± 0.23	- 0.0999 ± 0.030 ($kcal^{-1}$. mol)	0.023 ± 0.0053	- 1.98 ± 0.86	0.490	-0.522 ($kcal^{-1}$. mol)	0.707	-0.344
HD, KierFlex, O7-GS_{max}, C19-GS-O3	0.729	0.578	12.8	4.44	- 14.0 ± 2.2	1.19 ± 0.21	0.970 ± 0.20	- 4.26 ± 1.1	4.14 ± 1.2	0.721	0.635	-0.805	0.688

[a] *A*, *B, C* and *D* represent the coefficient of the independent variables (molecular descriptors); *K* represents the coefficient of the intercept. Set 2 includes all compounds that were substrates excluding 26 and 27.

Table S12. Results from multivariable regression and AIC_C analysis for the selected CSP-SAR models for $\log(K_m/normV_{max})$ for **Set 1**.[a]

CSP-SAR Models	r^2	Q^2	*F*	W_i	*K*	*A*	*B*	*C*	*D*	Standardized *A*	Standardized *B*	Standardized *C*	Standardized *D*
logP, SASA, O7-GS_{max}	0.757	0.631	22.8	7.12	- 12.1 ± 2.1	- 0.361 ± 0.078	0.0164 ± 0.0025 ($Å^{-2}$)	- 4.54 ± 1.0	N/A	-0.525	0.918 ($Å^{-2}$)	-0.638	N/A
logP, HD, SASA, C18-AA	0.781	0.665	18.7	5.78	- 8.34 ± 2.0	- 0.481 ± 0.075	0.584 ± 0.28	0.0116 ± 0.0021 ($Å^{-2}$)	- 5.14 ± 1.2	-0.699	0.225	0.646 ($Å^{-2}$)	-0.460

[a] *A*, *B, C* and *D* represent the coefficient of the independent variables (molecular descriptors); *K* represents the coefficient of the intercept. **Set 1** includes all compounds that were substrates.

Table S13. Results from multivariable regression and AIC_C analysis for the selected CSP-SAR models for $\log(K_m/normV_{max})$ for **Set 2**.[a]

CSP-SAR Models	r^2	Q^2	*F*	W_i	*K*	*A*	*B*	*C*	*D*	Standardized *A*	Standardized *B*	Standardized *C*	Standardized *D*
HD, MR, BC-GS_{min}, O7-AA-C18	0.745	0.611	13.9	8.66	- 15.1 ± 2.5	1.45 ± 0.25	0.420 ± 0.099 (m^{-3}. mol)	- 4.92 ± 1.3	6.69 ± 1.8	0.693	0.527 (m^{-3}. mol)	-0.732	0.730
HD, SASA, logP, BC-GS_{min}	0.720	0.577	12.2	2.78	- 8.47 ± 2.3	0.645 ± 0.30	0.00950 ± 0.0025 ($Å^{-2}$)	- 0.463 ± 0.16	- 3.42 ± 1.0	0.310	0.545 ($Å^{-2}$)	-0.410	-0.509

[a] *A*, *B, C* and *D* represent the coefficient of the independent variables (molecular descriptors); *K* represents the coefficient of the intercept. Set 2 includes all compounds that were substrates excluding 26 and 27.

Table S14. Results from multivariable regression and AIC_C analysis for the selected CSP-SAR models for $log(normV_{max}/K_m)$ for **Set 1**.[a]

CSP-SAR Models	r^2	Q^2	*F*	W_i	*K* (μM)	*A* (μM)	*B*	*C*	*D*	Standardized *A* (μM)	Standardized *B*	Standardized *C*	Standardized *D*
logP, SASA, O7-GS_{max}	0.757	0.632	22.9	7.10	12.1 ± 2.1	0.361 ± 0.078	- 0.0164 ± 0.0025 (μM/Å^2)	4.54 ± 1.0 (μM)	N/A	0.525	-0.918 (μM/Å^2)	0.638 (μM)	N/A
logP, HD, SASA, C18-AA	0.781	0.666	18.7	5.77	8.34 ± 2.0	0.482 ± 0.075	- 0.584 ± 0.28 (μM)	- 0.0116 ± 0.0021 (μM/Å^2)	5.14 ± 1.2 (μM)	0.699	-0.224 (μM)	-0.646 (μM/Å^2)	0.459 (μM)

[a] *A*, *B, C* and *D* represent the coefficient of the independent variables (molecular descriptors); *K* represents the coefficient of the intercept. Set 1 includes all compounds that were substrates.

Table S15. Results from multivariable regression and AIC_C analysis for the selected CSP-SAR models for $log(normV_{max}/K_m)$ for **Set 2**.[a]

CSP-SAR Models	r^2	Q^2	*F*	W_i	*K* (μM)	*A* (μM)	*B*	*C* (μM)	*D* (μM)	Standardized *A* (μM)	Standardized *B*	Standardized *C* (μM)	Standardized *D* (μM)
HD, MR, BC-GS_{min}, O7-AA-C18	0.745	0.611	13.9	8.66	15.1 ± 2.5	- 1.45 ± 0.25	- 0.420 ± 0.099 (μM/m^3/mol)	4.92 ± 1.3	- 6.69 ± 1.8	-0.693	-0.527	0.732	-0.730
HD, SASA, logP, BC-GS_{min}	0.720	0.577	12.2	2.78	8.47 ± 2.3	- 0.645 ± 0.30	- 0.00950 ± 0.0025 (μM/Å^2)	0.463 ± 0.16	3.42 ± 1.0	-0.310	-0.545	0.410	0.509

[a] *A*, *B, C* and *D* represent the coefficient of the independent variables (molecular descriptors); *K* represents the coefficient of the intercept. Set 2 includes all compounds that were substrates excluding 26 and 27.

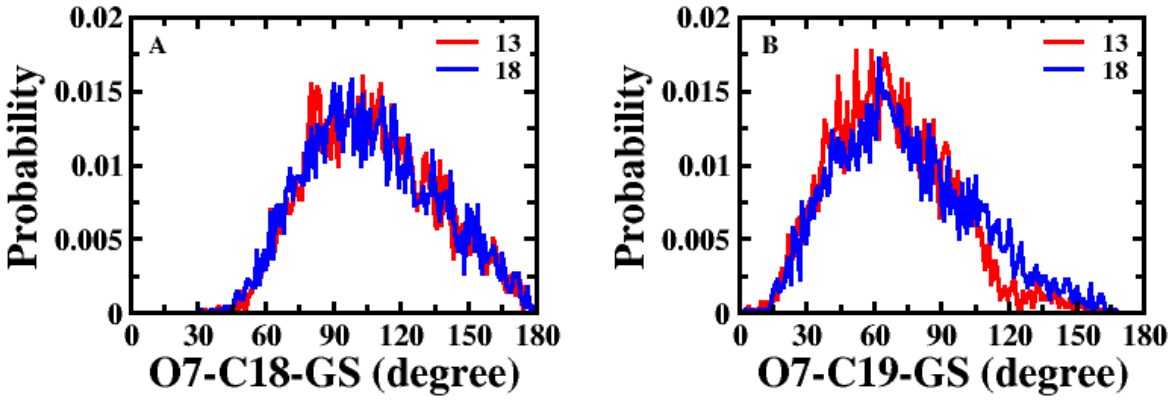


Figure S1. Probability distributions of structural descriptors. (A) Angle O7-C18-GS and (B) angle O7-C19-GS displayed the highest and second highest correlations with K_m for **Set 2** amongst the structural descriptors. Compounds **13** and **18** were the most and least potent substrates in **Set 2**, respectively.

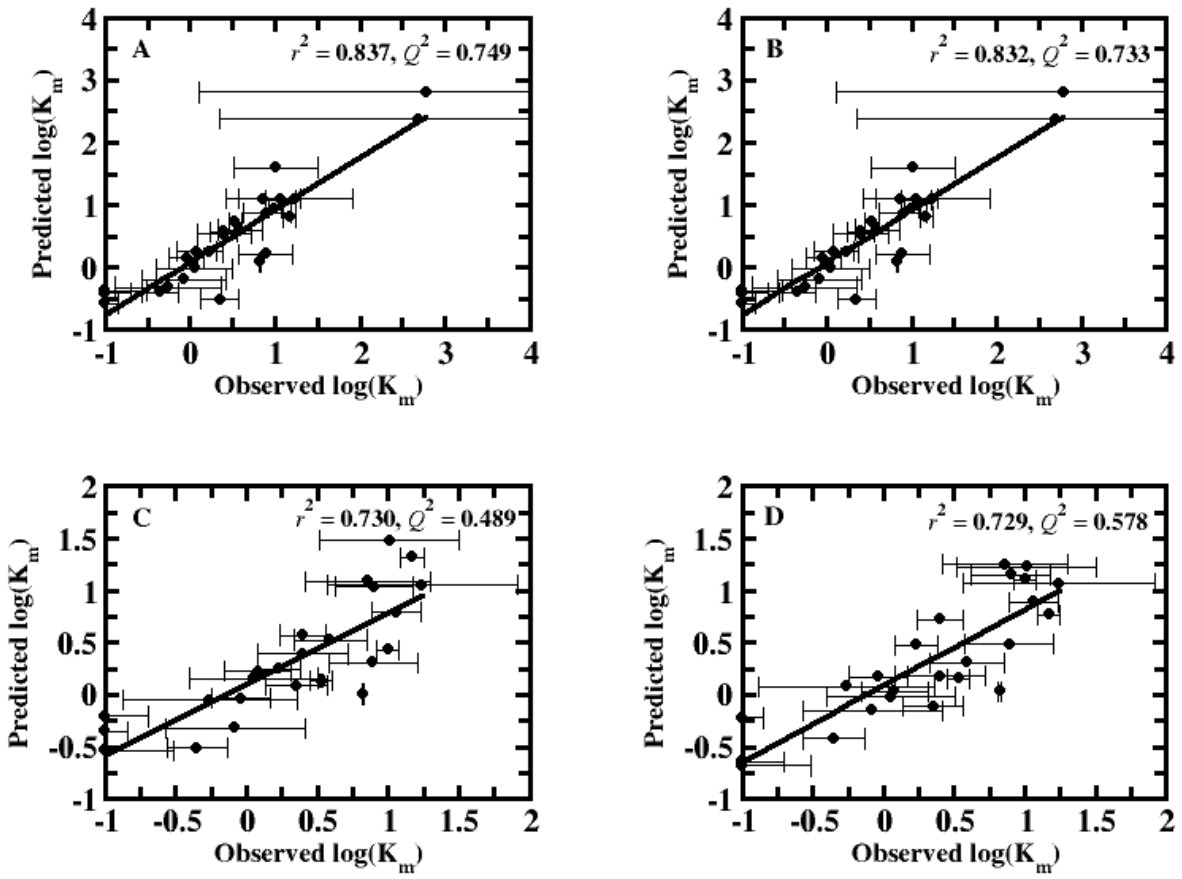


Figure S2. Regression plots of predicted vs. observed log(K_m) values for anilinyl conjugates of glu-CDCA using CSP-SAR models. (A) and (B) represent the best and the second best models for **Set 1**, while (C) and (D) represent the best and the second best models for **Set 2**.

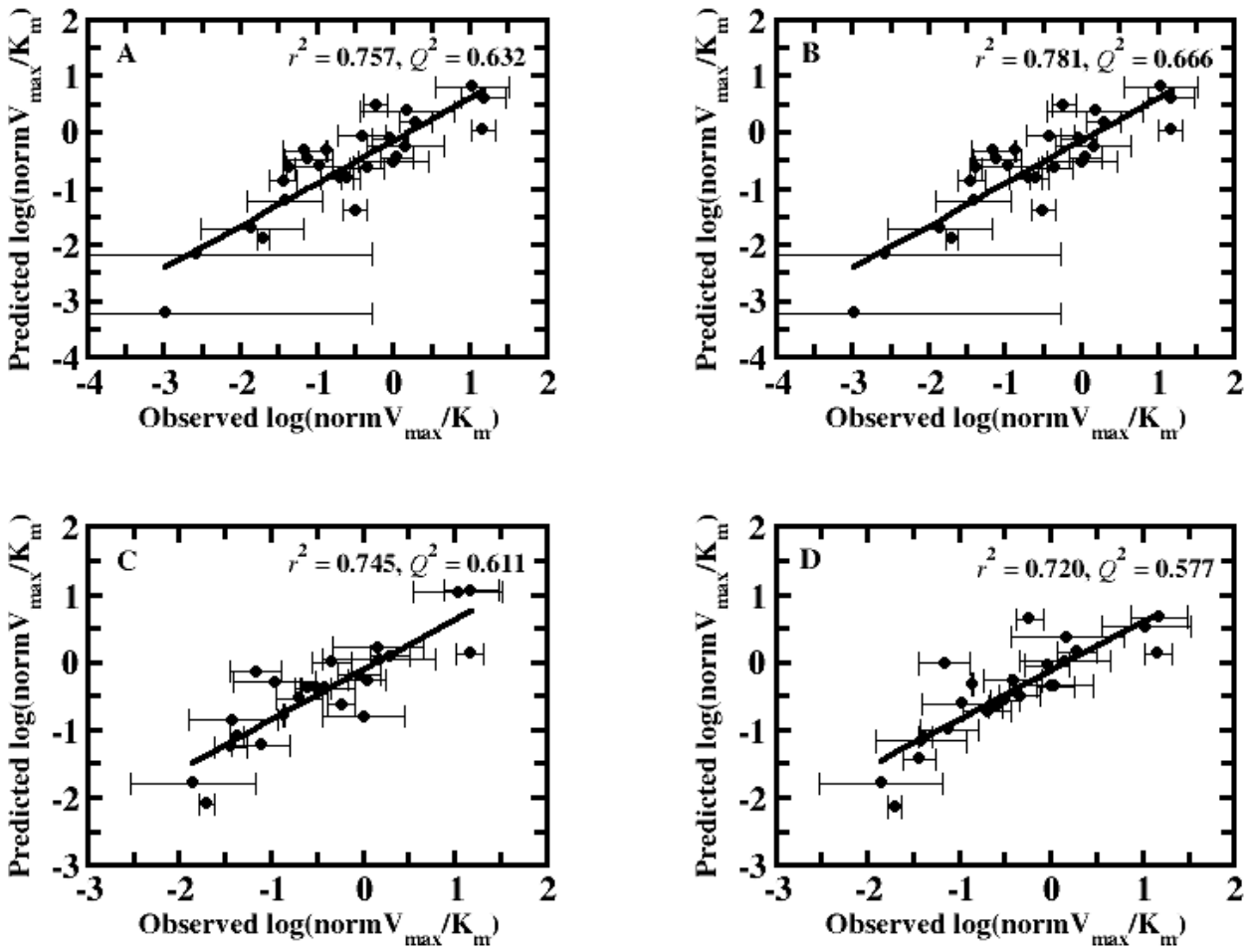


Figure S3. Regression plots of predicted vs. observed log(normV$_{max}$/K$_m$) values for anilinyl conjugates of glu-CDCA using CSP-SAR models. (A) and (B) represent the best and the second best models for **Set 1**, while (C) and (D) represent the best and the second best models for **Set 2**.