Supporting Information for

Molecular Switch Controlling the Binding of Anionic Bile Acid Conjugates to Human Apical Sodium-dependent Bile Acid Transporter

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Table S1. NMR and mass spectrometry results for **1**-**35**.

Compound 1. MS: [M+1] 597.4. ^{13}C NMR (DMSO-d6): δ 11.64, 18.35, 20.24, 22.69, 23.14, 26.73, 27.78, 30.54, 31.49, 32.10, 32.26, 32.75, 34.72, 34.82, 34.98, 35.29, 39.09, 39.41, 39.61, 41.40, 41.89, 49.99, 51.42, 55.59, 66.14, 70.32, 119.00, 119.00, 122.92, 128.60, 128.60, 139.24, 170.31, 172.75, 173.55

Compound 2. MS: [M+1] 631.3. ^{13}C NMR (DMSO-d6): δ 11.62, 18.32, 20.22, 22.69, 23.12, 26.74, 27.77, 30.54, 31.49, 32.16, 32.24, 32.78, 34.71, 34.81, 34.97, 35.30, 39.09, 39.41, 39.61, 41.40, 41.89, 49.97, 51.46, 55.59, 66.14, 70.31, 120.48, 120.48, 126.42, 128.51, 128.51, 138.21, 170.55, 172.67, 173.51

Compound 3. MS: [M+1] 665.4. ^{13}C NMR (DMSO-d6): δ 11.62, 18.32, 20.22, 22.68, 23.12, 26.45, 27.77, 30.52, 31.49, 32.12, 32.25, 32.81, 34.71, 34.81, 34.97, 35.28, 39.09, 39.41, 39.61, 41.40, 41.89, 49.99, 51.26, 55.61, 66.14, 70.31, 118.80, 118.93, 123.07, 123.31, 125.97, 125.97, 142.77, 171.00, 172.77, 173.50

Compound 4. MS: [M+1] 615.2. ^{13}C NMR (DMSO-d6): δ 11.64, 18.35, 20.24, 22.69, 23.14, 26.74, 27.78, 30.54, 31.49, 32.09, 32.27, 32.28, 34.72, 34.82, 34.97, 35.29, 39.09, 39.41, 39.61, 41.40, 41.89, 49.99, 51.37, 55.60, 66.14, 70.32, 115.33, 124.21, 125.11, 126.09, 126.18, 154.61, 170.77, 172.76, 173.52

Compound 5. MS: [M+1] 615.3. ^{13}C NMR (DMSO-d6): δ 11.64, 18.35, 20.24, 22.69, 23.14, 26.49, 27.78, 30.54, 31.49, 32.11, 32.27, 32.75, 34.72, 34.82, 34.97, 35.30, 39.09, 39.41, 39.61, 41.40, 41.89, 49.99, 51.29, 55.60, 66.14, 70.32, 109.29, 109.45, 114.68, 130.27**,** 140.99 161.15, 170.77, 172.76, 173.52

Compound 6. MS: [M+1] 615.4. ^{13}C NMR (DMSO-d6): δ 11.63, 18.33, 20.24, 22.69, 23.13, 26.69, 27.78, 30.54, 31.49, 32.11, 32.27, 32.64, 34.71, 34.82, 34.98, 35.30, 39.09, 39.41, 39.61, 41.40, 41.89, 49.99, 51.40, 55.60, 66.14, 70.33, 115.05, 115.23, 120.66, 120.72, 135.64, 158.75, 170.20, 172.79, 173.54

Compound 7. MS: [M+1] 611.4. ^{13}C NMR (DMSO-d6): δ 11.65, 17.82, 18.33, 20.24, 22.70, 23.14, 27.00, 27.78, 30.54, 31.49, 32.08, 32.19, 32.27, 34.72, 34.82, 34.98, 35.30, 39.09, 39.41, 39.61, 41.40, 41.89, 50.01, 51.40, 55.61, 66.15, 70.32, 125.08, 125.08, 125.81, 130.2, 131.70, 136.36, 170.23, 172.78, 173.58

Compound 8. MS: [M+1] 611.3. ^{13}C NMR (DMSO-d6): δ 11.63, 18.33, 20.22, 21.18, 22.70, 23.12, 26.67, 27.76, 30.53, 31.49, 32.09, 32.25, 32.71, 34.72, 34.81, 34.97, 35.30, 39.09, 39.41, 39.61, 41.39, 41.89, 49.98, 51.32, 55.59, 66.13, 70.32,116.21, 119.54, 123.63, 128.42, 137.72, 139.16, 170.22, 172.78, 173.54

Compound 9. MS: [M+1] 611.3. ^{13}C NMR (DMSO-d6): δ 11.63, 18.33, 20.22, 20.41, 22.70, 23.12, 26.69, 27.76, 30.54, 31.48, 32.11, 32.25, 32.68, 34.72, 34.81, 34.97, 35.30, 39.09, 39.41, 39.61, 41.40, 41.89, 49.99, 51.40, 55.59, 66.14, 70.32,119.01, 119.01, 128.97, 128.97, 131.76, 136.75, 170.03, 172.78, 173.54

Compound 10. MS: [M+1] 627.2. ^{13}C NMR (DMSO-d6): δ 11.63, 18.33, 20.24, 22.70, 23.14, 26.94, 27.78, 30.54, 31.48, 32.09, 32.27, 32.67, 34.72, 34.82, 34.98, 35.30, 39.09, 39.41, 39.61, 41.41, 41.89, 49.99, 51.40, 55.61, 55.8, 66.15, 70.33, 111.08, 120.13, 121.99, 124.24, 127.31, 149.55, 170.52, 172.77, 173.56

Compound 11. MS: [M+1] 627.1. ^{13}C NMR (DMSO-d6): δ 11.64, 18.35, 20.25, 22.70, 23.15, 26.59, 27.78, 30.55, 31.49, 32.11, 32.27, 32.78, 34.72, 34.82, 34.99, 35.30, 39.09, 39.41, 39.61, 41.41, 41.89,

49.99, 51.38, 54.92, 55.60, 66.16, 70.32, 104.86, 108.34, 111.32, 129.39, 140.43, 159.44, 170.35, 172.78, 173.53

Compound 12. MS: [M+1] 627.4. ^{13}C NMR (DMSO-d6): δ 11.64, 18.35, 20.25, 22.70, 23.14, 26.75, 27.79, 30.54, 31.50, 32.12, 32.27, 32.59, 34.72, 34.82, 34.99, 35.29, 39.09, 39.41, 39.61, 41.41, 41.89, 50.002, 51.41, 55.11, 55.60, 66.16, 70.32, 113.73, 113.73, 120.54, 120.54, 132.43, 154.99, 169.75, 172.78, 173.54

Compound 13. MS: [M+1] 653.4. ^{13}C NMR (DMSO-d6): δ 11.66, 18.37, 20.25, 22.70, 23.15, 26.85, 27.79, 30.54, 30.76, 30.76, 30.76, 31.53, 32.12, 32.27, 32.72, 34.72, 34.83, 34.99, 35.30, 39.09, 39.41, 39.61, 41.41, 41.91, 50.01, 51.44, 51.47, 55.64, 66.15, 70.32, 126.24, 126.46, 126.76, 131.79, 136.01, 146.42, 171.13, 172.78, 173.57

Compound 14. MS: [M+1] 653.5. ^{13}C NMR (DMSO-d6): δ 11.63, 18.35, 20.25, 22.70, 23.14, 26.74, 27.77, 30.54, 31.09, 31.09, 31.09, 31.53, 32.12, 32.26, 32.75, 34.72, 34.81, 34.97, 35.29, 39.09, 39.41, 39.61, 41.39, 41.90, 49.99, 51.36, 51.43, 55.61, 66.14, 70.32,115.99, 116.28, 119.94, 128.22, 139.01, 151.04, 170.23, 172.72, 173.54

Compound 15. MS: [M+1] 653.5. ^{13}C NMR (DMSO-d6): δ 11.64, 18.35, 20.24, 22.70, 23.14, 26.71, 27.78, 30.54, 31.19, 31.19, 31.19, 31.49, 32.12, 32.26, 32.75, 33.94, 34.72, 34.81, 34.98, 35.29, 39.09, 39.41, 39.61, 41.40, 41.89, 50.00, 51.38, 55.62, 66.14, 70.31, 118.82, 118.82, 125.17, 125.17, 136.4, 145.22, 170.06, 172.77, 173.54

Compound 16. MS: [M+1] 655.3. ^{13}C NMR (DMSO-d6): δ 11.64, 18.35, 20.25, 22.71, 23.15, 26.59, 27.78, 30.56, 31.52, 32.21, 32.27, 32.74, 34.74, 34.81, 34.98, 35.30, 39.09, 39.41, 39.61, 41.42, 41.93, 50.01, 51.22, 51.40, 55.55, 66.18, 70.34, 117.52, 121.01, 123.08, 130.45, 133.93, 139.67, 167.6, 170.47, 172.75, 173.41

Compound 17. MS: [M+1] 655.4. ^{13}C NMR (DMSO-d6): δ 11.63, 18.33, 20.24, 22.70, 23.14, 26.58, 27.77, 30.54, 31.49, 32.13, 32.26, 32.72, 34.72, 34.82, 34.97, 35.30, 39.09, 39.41, 39.61, 41.41, 41.89, 49.99, 51.28, 51.31, 55.60, 66.14, 70.31, 119.49, 123.42, 123.58, 129.12, 130.02, 139.61, 166.11, 170.65, 172.78, 173.51

Compound 18. MS: [M+1] 655.4. ^{13}C NMR (DMSO-d6): δ 11.63, 18.31, 20.23, 22.70, 23.13, 26.48, 27.78, 30.54, 31.49, 32.16, 32.25, 32.72, 34.72, 34.82, 34.97, 35.30, 39.09, 39.41, 39.61, 41.40, 41.89, 49.99, 51.28, 51.79, 55.62, 66.14, 70.31, 118.21, 118.32, 123.64, 130.22, 130.32, 143.63, 165.81, 170.98, 172.77, 173.50

Compound 19. MS: [M+1] 669.3. ^{13}C NMR (DMSO-d6): δ 11.63, 13.98, 18.32, 20.23, 22.70, 23.13, 26.48, 27.73, 30.54, 31.52, 31.77, 32.25, 32.72, 34.72, 34.78, 34.93, 35.30, 39.09, 39.41, 39.61, 41.40, 41.92, 49.99, 51.11, 55.59, 57.91, 66.14, 70.31, 117.51, 120.92, 123.03, 130.46, 133.89, 139.75, 167.12, 170.98, 172.77, 173.50

Compound 20. MS: [M+1] 669.3. ^{13}C NMR (DMSO-d6): δ 11.63, 14.21, 18.32, 20.24, 22.69, 23.13, 26.48, 27.80, 30.54, 31.50, 32.17, 32.25, 32.86, 34.72, 34.81, 34.99, 35.30, 39.09, 39.41, 39.61, 41.41, 41.89, 49.99, 51.21, 55.62, 60.36, 66.15, 70.32, 118.30, 118.30, 123.94, 130.16, 130.16, 143.58, 165.32, 170.96, 172.78, 173.50

Compound 21. MS: [M+1] 712.2. ^{13}C NMR (DMSO-d6): δ 11.64, 18.35, 20.23, 22.70, 23.14, 26.72, 27.78, 28.12, 28.12, 28.12, 30.55, 31.49, 32.11, 32.26, 32.70, 34.72, 34.82, 34.98, 35.30, 39.09, 39.41, 39.61, 41.40, 41.89, 49.99, 51.39, 55.62, 66.14, 70.31, 78.88, 109.11, 113.04, 113.12, 128.58, 139.51, 139.76, 152.68, 170.22, 172.75, 173.55

Compound 22. MS: [M+1] 712.4. ^{13}C NMR (DMSO-d6): δ 11.63, 18.33, 20.23, 22.69, 23.13, 26.75, 27.78, 28.13, 28.13, 28.13, 30.53, 31.49, 32.16, 32.25, 32.61, 34.72, 34.81, 34.97, 35.29, 39.09, 39.41,

39.61, 41.40, 41.89, 49.99, 51.37, 55.61, 66.14, 70.31, 78.75, 118.34, 118.34, 119.48, 119.48, 133.75, 134.74, 152.78, 169.85, 172.74, 173.54

Compound 23. MS: [M+1] 612.5 ^{13}C NMR (DMSO-d6): δ 11.65, 18.37, 20.25, 22.72, 23.16, 26.70, 27.79, 30.55, 31.49, 32.12, 32.28, 32.79, 34.74, 34.84, 34.99, 35.31, 39.09, 39.41, 39.61, 41.42, 41.91, 50.02, 51.34, 55.63, 66.17, 70.33, 115.68, 121.18, 123.26, 125.52, 125.79, 142.09, 170.28, 172.81, 173.51

Compound 24. MS: [M+1] 612.1 ^{13}C NMR (DMSO-d6): δ 11.64, 18.36, 20.24, 22.70, 23.14, 26.63, 27.78, 30.53, 31.48, 32.06, 32.28 32.79, 34.72, 34.82, 34.99, 35.29, 39.09, 39.41, 39.61, 41.40, 41.89, 50.01, 51.38, 55.61, 66.14, 70.29, 112.88, 113.69, 116.79, 117.29, 129.81, 140.34,170.77, 172.81, 173.48

Compound 25. MS: [M+1] 612.5 ^{13}C NMR (DMSO-d6): δ 11.64, 18.35, 20.22, 22.70, 23.14, 26.89, 27.76, 30.54, 31.48, 32.06, 32.54, 34.72, 34.82, 34.99, 35.29, 39.09, 39.41, 39.61, 41.40, 41.89, 49.99, 51.45, 55.60, 66.16, 70.32, 114.18, 114.18, 120.79, 120.79, 129.08, 143.48, 169.31, 172.76, 173.57

Compound 26. MS: [M+1] 633.2.^{13}C NMR (DMSO-d6): δ 11.63, 18.34, 20.24, 22.70, 23.13, 26.70, 27.77, 30.53, 31.48, 32.08, 32.26, 32.78, 34.72, 34.82, 34.97, 35.29, 39.09, 39.41, 39.61, 41.39, 41.89, 49.99, 51.33, 55.60, 66.14, 70.30, 104.02, 110.89, 122.82, 125.87, 152.96, 159.39, 170.74, 172.76, 173.51.

Compound 27. MS: [M+1] 625.4. ^{13}C NMR (DMSO-d6): δ 11.65, 18.07, 18.07, 18.37, 20.24, 22.69, 23.14, 27.21, 27.78, 30.53, 31.52, 32.08, 32.27, 32.78, 34.72, 34.82, 34.98, 35.30, 39.09, 39.41, 39.61, 41.41, 41.90, 50.01, 51.47, 55.63, 66.15, 70.3, 126.25, 127.56, 127.56, 135.13, 135.13, 135.21, 169.88, 172.79, 173.58

Compound 28 MS: [M+1] 625.5. ^{13}C NMR (DMSO-d6): δ 11.64, 13.96, 18.35, 20.12, 20.24, 22.69, 23.14, 27.02, 27.77, 30.52, 31.49, 32.10, 32.26, 32.78 34.71, 34.81, 34.97, 35.28, 39.09, 39.41, 39.61, 41.39, 41.89, 50.00, 51.46, 55.60, 66.15, 70.30, 123.6, 125.05, 126.78, 131.13, 136.12, 136.78, 170.74, 172.76, 173.5

Compound 29. MS: [M+1] 657.3. ^{13}C NMR (DMSO-d6): δ 11.63, 18.33, 20.24, 22.68, 23.13, 26.58, 27.78, 30.54, 31.49, 32.13, 32.26, 32.8, 34.71, 34.82, 34.98, 35.30, 39.09, 39.41, 39.61, 41.40, 41.89, 49.99, 51.35, 54.97, 55.01, 55.61, 66.15, 70.32, 94.98, 97.34, 97.36, 140.48, 160.40, 160.40,170.39, 172.76, 173.53

Compound 30. MS: [M+1] 731.6. ^{13}C NMR (DMSO-d6): δ 11.61, 18.31, 20.23, 22.69, 23.13, 26.23, 27.76, 30.55, 31.49, 32.05, 32.27, 32.48, 34.73, 34.96, 35.30, 39.09, 39.41, 39.61, 41.40, 41.90, 50.0030, 51.58, 55.59, 65.87, 66.17, 70.35, 119.78, 123.05, 123.81, 127.72, 127.72, 127.98, 128.38, 128.38, 128.89, 131.23, 135.98, 139.41, 167.16, 170.42, 171.92, 173.02

Compound 31. MS: [M-1] 639.5. ^{13}C NMR (DMSO-d6): δ 11.63, 18.34, 20.23, 22.70, 23.14, 26.35, 27.77, 30.55, 31.49, 32.13, 32.27, 32.66, 34.74, 34.82, 34.93, 35.31, 39.09, 39.41, 39.61, 41.42, 41.92, 49.99, 51.21, 55.62, 66.17, 70.33, 116.28, 119.90, 122.53, 131.06, 134.05, 140.40, 169.49, 170.37, 172.79, 173.42

Compound 32. MS: [M-1] 639.4. ^{13}C NMR (DMSO-d6): δ 11.64, 18.35, 20.24, 22.71, 23.15, 26.57, 27.78, 30.54, 31.49, 32.12, 32.27, 32.72, 34.73, 34.82, 34.97, 35.31, 39.09, 39.41, 39.61, 41.42, 41.90, 50.003, 51.30, 55.62, 66.17, 70.32, 119.78, 123.11, 123.8, 128.91, 131.19,139.45,167.16, 170.61, 172.81, 173.51

Compound 33. MS: [M-1] 639.5. ^{13}C NMR (DMSO-d6): δ 11.65, 18.37, 20.25, 22.72, 23.16, 26.50, 27.81, 30.57, 31.51, 32.13, 32.28, 32.85, 34.74, 34.83, 34.98, 35.31, 39.09, 39.41, 39.61, 41.43,

41.92, 50.02, 51.30, 55.64, 66.17, 70.32, 118.14, 118.35, 125.84, 130.37, 130.37, 143.29, 166.92, 170.90, 172.82, 173.5

Compound 34. MS: [M-1] 653.6 ^{13}C NMR (DMSO-d6): δ 11.64, 18.35, 20.25, 22.72, 23.15, 27.06, 27.79, 30.55, 31.50, 32.07, 32.29, 32.81, 34.73, 34.82, 35.0003, 35.32, 39.09, 39.41, 39.61, 41.42, 41.79, 41.90, 50.02, 51.55, 55.63, 66.17, 70.34, 128.01, 128.13, 128.52, 130.92, 131.69, 140.13, 167.30, 171.43, 172.75, 173.53

Compound 35. MS: [M-1] 653.4 ^{13}C NMR (DMSO-d6): δ 11.65, 18.37, 20.25, 22.72, 23.15, 26.94, 27.79, 30.55, 31.50, 32.08, 32.29, 32.81, 34.74, 34.81, 34.99, 35.31, 39.09, 39.41, 39.61, 41.42, 41.81, 41.92, 50.02, 51.41, 55.63, 66.14, 70.31, 127.13, 127.13, 129.19, 129.37, 129.41, 144.83, 167.15, 171.43, 172.78, 173.55

Note: Peaks 39.09, 39.41, 39.61 were obscured by DMSO-d6 solvent, obtained from HMQC spectra of **32**.

Table S2. Elemental analysis results for **1**-**35**.

Compound[a]	Theoretical %			Found %			Consistent Formula
	C	H	N	C	H	N	
1	68.49	8.70	4.56	68.75	8.87	4.53	$C_{35}H_{52}N_2O_6$ + 1.0 H_2O
2	65.71	8.11	4.38	65.46	8.23	4.34	$C_{35}H_{51}ClN_2O_6$ + 0.5 H_2O
3	63.03	7.68	4.08	62.76	7.74	4.16	$C_{36}H_{51}F_3N_2O_6$ + 1.25 H_2O
4	66.54	8.29	4.43	66.30	8.30	4.47	$C_{35}H_{51}FN_2O_6$ + 1.0 H_2O
5	66.54	8.29	4.43	66.53	8.26	4.50	$C_{35}H_{51}FN_2O_6$ + 1.0 H_2O
6	67.44	8.33	4.50	67.11	8.33	4.48	$C_{35}H_{51}FN_2O_6$ + 0.5 H_2O
7	70.27	8.93	4.55	70.26	8.85	4.27	$C_{36}H_{54}N_2O_6$ + 0.5 H_2O
8	68.87	8.83	4.46	68.54	8.70	4.53	$C_{36}H_{54}N_2O_6$ + 1.0 H_2O
9	67.44	8.87	4.25	67.69	8.79	3.88	$C_{36}H_{54}N_2O_6$ + 2.0 CH_3OH
10	66.28	8.58	4.29	66.11	8.42	4.43	$C_{36}H_{54}N_2O_7$ + 1.5 H_2O
11	67.16	8.61	4.35	67.19	8.41	4.66	$C_{36}H_{54}N_2O_7$ + 1.0 H_2O
12	68.05	8.65	4.41	67.98	8.70	4.33	$C_{36}H_{54}N_2O_7$ + 0.5 H_2O
13	69.92	9.18	4.18	69.59	9.27	4.29	$C_{39}H_{60}N_2O_6$ + 1.0 H_2O
14	70.36	9.20	4.20	70.15	9.20	4.17	$C_{39}H_{60}N_2O_6$ + 1.0 H_2O
15	70.82	9.22	4.24	70.73	9.11	4.42	$C_{39}H_{60}N_2O_6$ + 0.75H_2O
16	66.15	8.25	4.17	66.52	8.47	4.18	$C_{37}H_{54}N_2O_8$ + 0.5 H_2O
17	66.99	8.29	4.22	66.75	8.32	4.20	$C_{37}H_{54}N_2O_8$ + 0.5 H_2O
18	66.64	8.16	4.20	66.38	8.32	4.44	$C_{37}H_{54}N_2O_8$ + 0.75 H_2O
19	65.32	8.33	4.01	65.08	8.46	3.79	$C_{38}H_{56}N_2O_8$ + 1.75 H_2O
20	67.81	8.42	4.16	67.45	8.61	3.82	$C_{38}H_{56}N_2O_8$ + 0.25 H_2O
21	65.82	8.70	5.76	65.48	8.66	5.97	$C_{40}H_{61}N_3O_8$ +1.5 H_2O
22	64.26	8.51	5.62	64.01	8.11	6.02	$C_{40}H_{61}N_3O_8$ +2.0 H_2O
23	63.83	8.53	6.38	63.43	8.23	6.30	$C_{35}H_{53}N_3O_6$ + 2.75 H_2O

24	67.77	8.69	6.77	67.68	8.55	6.64	$C_{35}H_{53}N_3O_6$ + 0.5 H_2O
25	67.31	8.67	6.73	67.14	8.74	6.63	$C_{35}H_{53}N_3O_6$ + 0.75 H_2O
26	64.28	7.90	4.28	64.05	7.59	4.60	$C_{35}H_{50}F_2N_2O_6$ + 1.25 H_2O
27	69.24	8.95	4.36	69.49	8.93	4.43	$C_{37}H_{56}N_2O_6$ + 1.0 H_2O
28	68.78	8.93	4.34	68.77	8.97	4.45	$C_{37}H_{56}N_2O_6$ + 1.25 H_2O
29	65.94	8.52	4.16	66.21	8.55	4.38	$C_{37}H_{56}N_2O_8$ + 0.5 H_2O
30	68.28	7.93	3.70	68.25	7.88	3.75	$C_{43}H_{58}N_2O_8$ +1.25 H_2O
31	66.16	8.14	4.29	65.78	8.28	4.32	$C_{36}H_{52}N_2O_8$ + 0.75H_2O
32	65.73	8.12	4.25	65.60	8.22	4.29	$C_{36}H_{52}N_2O_8$ + 1.0 H_2O
33	64.89	8.09	4.20	64.69	8.16	4.09	$C_{36}H_{52}N_2O_8$ + 1.5 H_2O
34	65.32	8.22	4.11	65.25	8.39	3.92	$C_{37}H_{54}N_2O_8$ + 1.5 H_2O
35	65.32	8.22	4.11	64.93	7.91	3.89	$C_{37}H_{54}N_2O_8$ + 1.5 H_2O

Table S3. Correlation matrix of structural descriptors for aniline conjugates of glu-CDCA.

	ΔG_w	$logP_c$	C18-GS-O7	C19-GS-O3	O7-C18-GS	O7-AA	O7-AA-C20	O7-AA-GS	HA	O3-C18-GS	O7-C19-GS	$O7\text{-}GS_{min}$	PSA_{side}	O7-GS
ΔG_w	1.00													
$logP_c$	0.93	1.00												
C18-GS-O7	0.56	0.44	1.00											
C19-GS-O3	0.53	0.44	0.65	1.00										
O7-C18-GS	0.47	0.45	0.43	0.90	1.00									
O7-AA	0.49	0.45	0.37	0.82	0.86	1.00								
O7-AA-C20	0.48	0.43	0.30	0.81	0.87	0.99	1.00							
O7-AA-GS	0.44	0.35	0.77	0.93	0.83	0.73	0.69	1.00						
HA	-0.42	-0.44	-0.10	-0.11	-0.08	0.02	0.02	0.00	1.00					
O3-C18-GS	0.41	0.37	0.53	0.94	0.94	0.84	0.82	0.90	-0.04	1.00				
O7-C19-GS	0.39	0.33	0.54	0.94	0.93	0.80	0.79	0.89	-0.01	0.95	1.00			
$O7\text{-}GS_{min}$	0.43	0.30	0.80	0.87	0.75	0.68	0.64	0.97	0.00	0.84	0.82	1.00		
PSA_{side}	-0.27	-0.35	0.08	-0.08	-0.17	-0.16	-0.19	0.07	0.11	-0.07	-0.06	0.16	1.00	
O7-GS	0.42	0.32	0.80	0.88	0.78	0.70	0.67	0.97	0.03	0.85	0.84	0.98	0.13	1.00
O3-AA-GS	0.40	0.30	0.78	0.90	0.78	0.72	0.67	0.99	0.05	0.88	0.87	0.97	0.12	0.97
C18-GS-O3	0.41	0.32	0.71	0.94	0.81	0.75	0.72	0.96	0.06	0.93	0.92	0.92	0.06	0.92
$O3\text{-}GS_{min}$	0.41	0.28	0.79	0.88	0.75	0.69	0.66	0.96	0.02	0.85	0.84	0.99	0.16	0.97
$BC\text{-}GS_{min}$	0.42	0.30	0.80	0.81	0.69	0.62	0.59	0.92	-0.01	0.77	0.78	0.97	0.22	0.96
AA-GS-O3	0.41	0.27	0.90	0.75	0.57	0.54	0.50	0.89	0.07	0.67	0.70	0.93	0.17	0.93
O3-GS	0.39	0.29	0.78	0.89	0.79	0.71	0.67	0.97	0.06	0.87	0.87	0.97	0.13	0.99
GS-O7-C18	0.34	0.30	0.49	0.92	0.96	0.85	0.85	0.89	0.06	0.96	0.97	0.84	-0.04	0.87
$O3\text{-}GS_{max}$	0.38	0.30	0.79	0.82	0.73	0.64	0.60	0.92	0.11	0.78	0.80	0.91	0.12	0.95
$C19\text{-}GS_{min}$	0.41	0.27	0.81	0.82	0.70	0.66	0.63	0.93	0.02	0.78	0.79	0.96	0.19	0.96
$C18\text{-}GS_{min}$	0.40	0.27	0.82	0.76	0.63	0.60	0.56	0.90	0.05	0.72	0.73	0.94	0.21	0.94
$O7\text{-}GS_{max}$	0.38	0.30	0.81	0.81	0.71	0.63	0.59	0.92	0.10	0.76	0.78	0.92	0.13	0.97
O3-AA-C20	0.32	0.29	0.32	0.85	0.92	0.94	0.94	0.78	0.09	0.91	0.87	0.73	-0.09	0.74
BC-GS	0.39	0.29	0.81	0.80	0.70	0.62	0.58	0.92	0.02	0.77	0.78	0.94	0.20	0.97
AA-GS-O7	0.38	0.27	0.88	0.80	0.64	0.57	0.53	0.92	0.05	0.73	0.74	0.95	0.19	0.96
O7-AA-BC	0.38	0.30	0.40	0.82	0.79	0.94	0.94	0.72	0.07	0.81	0.80	0.67	-0.09	0.70
$BC\text{-}GS_{max}$	0.36	0.28	0.80	0.74	0.65	0.56	0.52	0.87	0.07	0.71	0.72	0.88	0.17	0.93

Table S3. Contd.

	ΔG_w	$logP_c$	C18-GS-O7	C19-GS-O3	O7-C18-GS	O7-AA	O7-AA-C20	O7-AA-GS	HA	O3-C18-GS	O7-C19-GS	$O7\text{-}GS_{min}$	PSA_{side}	O7-GS
PSA	-0.20	-0.28	0.13	0.12	0.05	0.06	0.03	0.24	0.11	0.15	0.14	0.33	0.97	0.29
C19-GS	0.38	0.28	0.80	0.79	0.68	0.64	0.60	0.91	0.05	0.77	0.77	0.93	0.19	0.95
O7-AA-C18	0.37	0.26	0.56	0.85	0.74	0.86	0.84	0.80	0.10	0.82	0.84	0.76	0.00	0.77
GS-O3-C18	0.30	0.23	0.53	0.88	0.91	0.81	0.80	0.89	0.07	0.94	0.91	0.87	0.01	0.89
O3-C19-GS	0.30	0.22	0.32	0.85	0.90	0.83	0.85	0.79	0.02	0.88	0.87	0.73	-0.06	0.74
C18-GS	0.36	0.27	0.79	0.73	0.64	0.58	0.54	0.87	0.03	0.70	0.70	0.89	0.23	0.93
$C19\text{-}GS_{max}$	0.34	0.27	0.78	0.68	0.58	0.52	0.47	0.81	0.06	0.65	0.65	0.82	0.18	0.88
SASA	0.26	0.30	0.52	0.46	0.48	0.52	0.48	0.55	0.43	0.51	0.45	0.52	-0.21	0.61
O3-AA	0.23	0.22	0.24	0.76	0.83	0.93	0.91	0.69	0.11	0.84	0.78	0.66	-0.04	0.68
BC-AA	0.23	0.17	0.45	0.79	0.70	0.85	0.79	0.75	0.11	0.82	0.76	0.72	-0.02	0.72
$C18\text{-}GS_{max}$	0.33	0.25	0.76	0.64	0.54	0.48	0.44	0.78	0.06	0.59	0.60	0.80	0.22	0.86
GS-O7-C19	0.23	0.13	0.63	0.77	0.64	0.55	0.52	0.83	0.15	0.75	0.85	0.79	0.11	0.80
C19-GS-O7	0.27	0.18	0.72	0.57	0.49	0.47	0.43	0.76	0.10	0.55	0.54	0.80	0.26	0.84
GS-O7-AA	0.21	0.21	0.30	0.34	0.38	0.39	0.37	0.42	-0.01	0.33	0.30	0.45	0.10	0.53
O7-AA-C19	-0.15	-0.25	0.41	0.55	0.36	0.50	0.45	0.60	0.30	0.55	0.55	0.62	0.23	0.61
O3-AA-C18	0.15	0.07	0.40	0.81	0.76	0.85	0.84	0.80	0.20	0.84	0.83	0.78	0.07	0.79
O3-AA-C19	0.16	0.12	0.32	0.74	0.76	0.83	0.84	0.70	0.11	0.80	0.77	0.69	-0.04	0.71
GS-O3-C19	0.16	0.05	0.50	0.81	0.77	0.73	0.72	0.86	0.20	0.85	0.84	0.82	0.11	0.83
HD	0.09	-0.05	0.12	-0.06	-0.16	0.00	0.01	-0.06	0.12	-0.12	-0.15	0.03	0.25	0.03
C19-AA	0.13	0.03	0.50	0.71	0.51	0.68	0.63	0.70	0.22	0.68	0.67	0.67	0.07	0.67
$SASAS_{side}$	0.07	0.18	0.18	-0.06	0.04	0.10	0.07	0.02	0.40	0.00	-0.05	-0.03	-0.30	0.09
MR	0.12	0.03	0.22	0.07	0.05	-0.06	-0.05	0.06	-0.20	0.04	0.02	0.03	-0.13	0.06
KierFlex	0.11	0.03	0.18	0.00	0.00	-0.09	-0.07	-0.01	-0.20	-0.02	-0.05	-0.02	-0.18	0.00
O3-AA-BC	0.05	-0.01	0.32	0.72	0.69	0.79	0.78	0.73	0.24	0.77	0.74	0.73	0.07	0.74
GS-O3-AA	0.05	0.07	0.32	0.32	0.33	0.36	0.35	0.42	0.18	0.32	0.26	0.47	0.08	0.54
brotN	0.03	-0.03	0.11	-0.08	-0.09	-0.21	-0.20	-0.08	-0.21	-0.10	-0.16	-0.09	-0.16	-0.09
MW	0.03	-0.04	0.15	-0.04	-0.08	-0.22	-0.20	-0.03	-0.21	-0.08	-0.10	-0.04	-0.09	-0.03
C18-AA	0.02	-0.10	0.56	0.59	0.32	0.41	0.36	0.65	0.21	0.54	0.58	0.63	0.19	0.62

Table S3. Contd.

	O3-AA-GS	C18-GS-O3	O3-GS_{min}	BC-GS_{min}	AA-GS-O3	O3-GS	GS-O7-C18	O3-GS_{max}	C19-GS_{min}	C18-GS_{min}	O7-GS_{max}	O3-AA-C20	BC-GS	AA-GS-O7
O3-AA-GS	1.00													
C18-GS-O3	0.96	1.00												
O3-GS_{min}	0.97	0.93	1.00											
BC-GS_{min}	0.95	0.88	0.97	1.00										
AA-GS-O3	0.92	0.85	0.93	0.94	1.00									
O3-GS	0.98	0.94	0.98	0.96	0.92	1.00								
GS-O7-C18	0.88	0.90	0.85	0.80	0.70	0.89	1.00							
O3-GS_{max}	0.94	0.87	0.92	0.93	0.90	0.97	0.83	1.00						
C19-GS_{min}	0.96	0.89	0.97	0.99	0.95	0.96	0.81	0.92	1.00					
C18-GS_{min}	0.93	0.85	0.95	0.99	0.96	0.94	0.76	0.92	0.99	1.00				
O7-GS_{max}	0.94	0.86	0.92	0.94	0.93	0.96	0.81	0.98	0.93	0.93	1.00			
O3-AA-C20	0.76	0.80	0.74	0.65	0.55	0.75	0.93	0.66	0.68	0.61	0.64	1.00		
BC-GS	0.95	0.86	0.94	0.97	0.93	0.97	0.81	0.97	0.96	0.96	0.98	0.63	1.00	
AA-GS-O7	0.94	0.87	0.95	0.95	0.97	0.94	0.75	0.93	0.96	0.95	0.95	0.60	0.95	1.00
O7-AA-BC	0.72	0.78	0.71	0.64	0.59	0.72	0.83	0.67	0.70	0.63	0.65	0.88	0.64	0.61
BC-GS_{max}	0.90	0.81	0.88	0.93	0.91	0.93	0.75	0.98	0.92	0.93	0.98	0.56	0.98	0.92
PSA	0.28	0.23	0.32	0.36	0.27	0.30	0.18	0.26	0.33	0.33	0.27	0.14	0.34	0.31
C19-GS	0.95	0.87	0.94	0.97	0.94	0.96	0.80	0.96	0.97	0.97	0.96	0.64	0.99	0.94
O7-AA-C18	0.81	0.87	0.79	0.73	0.71	0.80	0.83	0.74	0.79	0.73	0.73	0.81	0.73	0.72
GS-O3-C18	0.88	0.88	0.88	0.82	0.72	0.90	0.96	0.83	0.84	0.79	0.82	0.91	0.82	0.78
O3-C19-GS	0.75	0.77	0.75	0.67	0.53	0.76	0.90	0.68	0.69	0.62	0.65	0.92	0.66	0.61
C18-GS	0.90	0.80	0.90	0.95	0.92	0.93	0.75	0.94	0.95	0.96	0.96	0.58	0.99	0.92
C19-GS_{max}	0.86	0.76	0.84	0.90	0.88	0.89	0.69	0.94	0.90	0.91	0.94	0.50	0.96	0.88
SASA	0.56	0.55	0.51	0.50	0.59	0.60	0.54	0.65	0.52	0.53	0.66	0.51	0.58	0.57
O3-AA	0.69	0.71	0.68	0.59	0.48	0.69	0.87	0.61	0.63	0.56	0.59	0.96	0.58	0.53
BC-AA	0.77	0.81	0.74	0.66	0.63	0.76	0.80	0.69	0.72	0.66	0.67	0.83	0.66	0.64
C18-GS_{max}	0.82	0.71	0.81	0.88	0.85	0.86	0.65	0.93	0.87	0.89	0.93	0.46	0.95	0.87
GS-O7-C19	0.86	0.87	0.82	0.81	0.79	0.84	0.78	0.81	0.82	0.81	0.78	0.61	0.81	0.77
C19-GS-O7	0.81	0.68	0.81	0.89	0.88	0.84	0.62	0.87	0.89	0.91	0.89	0.47	0.92	0.86
GS-O7-AA	0.44	0.30	0.45	0.52	0.40	0.53	0.44	0.59	0.49	0.52	0.57	0.36	0.60	0.42

Table S3. Contd.

	O3-AA-GS	C18-GS-O3	O3-GS_{min}	BC-GS_{min}	AA-GS-O3	O3-GS	GS-O7-C18	O3-GS_{max}	C19-GS_{min}	C18-GS_{min}	O7-GS_{max}	O3-AA-C20	BC-GS	AA-GS-O7
O7-AA-C19	0.67	0.68	0.66	0.61	0.63	0.65	0.57	0.62	0.67	0.63	0.60	0.53	0.60	0.62
O3-AA-C18	0.81	0.84	0.81	0.73	0.66	0.81	0.88	0.74	0.78	0.72	0.72	0.89	0.72	0.70
O3-AA-C19	0.72	0.73	0.72	0.66	0.56	0.73	0.84	0.64	0.69	0.64	0.63	0.87	0.64	0.62
GS-O3-C19	0.86	0.86	0.85	0.79	0.73	0.86	0.87	0.80	0.84	0.79	0.77	0.84	0.79	0.76
HD	-0.04	-0.03	0.06	0.03	0.15	0.00	-0.13	-0.06	0.06	0.04	0.03	-0.03	0.00	0.11
C19-AA	0.74	0.79	0.71	0.64	0.67	0.71	0.67	0.67	0.71	0.66	0.65	0.66	0.63	0.65
$SASA_{side}$	0.02	-0.01	-0.04	-0.02	0.13	0.08	0.04	0.18	0.00	0.04	0.19	0.06	0.09	0.08
MR	0.04	0.00	0.05	0.06	0.05	0.08	0.01	0.14	0.05	0.06	0.11	-0.07	0.14	0.09
KierFlex	-0.05	-0.07	-0.01	-0.01	-0.01	0.01	-0.06	0.07	-0.02	0.01	0.05	-0.11	0.06	0.03
O3-AA-BC	0.75	0.76	0.75	0.69	0.60	0.76	0.83	0.69	0.72	0.68	0.67	0.85	0.67	0.64
GS-O3-AA	0.45	0.31	0.47	0.51	0.44	0.55	0.42	0.62	0.50	0.54	0.59	0.37	0.59	0.49
brotN	-0.11	-0.15	-0.07	-0.07	-0.08	-0.07	-0.15	-0.01	-0.09	-0.08	-0.03	-0.20	-0.02	-0.02
MW	-0.06	-0.09	-0.03	-0.01	-0.03	-0.02	-0.11	0.02	-0.04	-0.01	0.01	-0.19	0.04	0.03
C18-AA	0.70	0.73	0.67	0.63	0.69	0.66	0.53	0.64	0.69	0.67	0.62	0.43	0.63	0.66

Table S3. Contd.

	O7-AA-BC	BC-GS_{max}	PSA	C19-GS	O7-AA-C18	GS-O3-C18	O3-C19-GS	C18-GS	C19-GS_{max}	SASA	O3-AA	BC-AA	C18-GS_{max}	GS-O7-C19
O7-AA-BC	1.00													
BC-GS_{max}	0.60	1.00												
PSA	0.11	0.28	1.00											
C19-GS	0.68	0.97	0.32	1.00										
O7-AA-C18	0.95	0.69	0.17	0.77	1.00									
GS-O3-C18	0.78	0.76	0.23	0.81	0.78	1.00								
O3-C19-GS	0.82	0.60	0.17	0.66	0.75	0.91	1.00							
C18-GS	0.62	0.98	0.34	0.99	0.70	0.77	0.60	1.00						
C19-GS_{max}	0.57	0.98	0.27	0.96	0.66	0.70	0.53	0.97	1.00					
SASA	0.46	0.62	-0.12	0.58	0.48	0.57	0.35	0.57	0.60	1.00				
O3-AA	0.88	0.51	0.19	0.60	0.78	0.86	0.87	0.54	0.47	0.49	1.00			
BC-AA	0.90	0.62	0.16	0.71	0.90	0.78	0.75	0.63	0.61	0.52	0.87	1.00		
C18-GS_{max}	0.53	0.97	0.31	0.94	0.62	0.67	0.50	0.97	0.99	0.58	0.43	0.54	1.00	
GS-O7-C19	0.63	0.78	0.22	0.82	0.78	0.72	0.62	0.77	0.74	0.44	0.53	0.69	0.69	1.00
C19-GS-O7	0.50	0.93	0.34	0.93	0.58	0.68	0.47	0.96	0.94	0.60	0.44	0.53	0.95	0.67
GS-O7-AA	0.31	0.60	0.19	0.58	0.28	0.45	0.34	0.63	0.63	0.44	0.41	0.33	0.67	0.32
O7-AA-C19	0.68	0.58	0.33	0.65	0.76	0.59	0.55	0.60	0.58	0.36	0.59	0.82	0.54	0.70
O3-AA-C18	0.89	0.66	0.27	0.74	0.89	0.88	0.86	0.68	0.60	0.49	0.90	0.89	0.57	0.75
O3-AA-C19	0.85	0.56	0.17	0.66	0.81	0.85	0.81	0.61	0.52	0.46	0.89	0.80	0.50	0.61
GS-O3-C19	0.78	0.74	0.29	0.81	0.81	0.91	0.89	0.76	0.70	0.50	0.80	0.82	0.66	0.81
HD	0.03	-0.04	0.23	0.01	0.05	-0.05	-0.13	0.02	-0.06	0.18	-0.04	-0.04	0.00	-0.12
C19-AA	0.81	0.62	0.20	0.69	0.88	0.65	0.63	0.61	0.61	0.45	0.68	0.93	0.54	0.74
$SASA_{side}$	0.02	0.18	-0.33	0.09	-0.01	0.07	-0.12	0.12	0.19	0.81	0.05	0.06	0.19	-0.03
MR	-0.02	0.19	-0.16	0.10	-0.03	0.06	0.07	0.12	0.18	0.05	-0.09	0.00	0.18	0.01
KierFlex	-0.04	0.11	-0.21	0.03	-0.08	0.02	0.05	0.05	0.10	0.02	-0.13	-0.07	0.11	-0.10
O3AABC	0.82	0.61	0.27	0.69	0.80	0.84	0.82	0.64	0.56	0.48	0.89	0.86	0.53	0.67
GSO3AA	0.30	0.61	0.17	0.57	0.26	0.49	0.35	0.62	0.64	0.58	0.43	0.36	0.67	0.27
brotN	-0.18	0.04	-0.20	-0.05	-0.22	-0.06	-0.02	-0.03	0.04	-0.08	-0.23	-0.17	0.05	-0.21
MW	-0.18	0.07	-0.13	0.00	-0.18	-0.04	-0.03	0.02	0.06	-0.08	-0.23	-0.16	0.07	-0.08
C18-AA	0.60	0.62	0.25	0.68	0.76	0.51	0.47	0.62	0.61	0.33	0.43	0.74	0.56	0.82

Table S3. Contd.

	C19-GS-O7	GS-O7-AA	O7-AA-C19	O3-AA-C18	O3-AA-C19	GS-O3-C19	HD	C19-AA	$SASA_{side}$	MR	KierFlex	O3-AA-BC	GS-O3-AA	brotN	MW	C18-AA
C19-GS-O7	1.00															
GS-O7-AA	0.66	1.00														
O7-AA-C19	0.56	0.21	1.00													
O3-AA-C18	0.59	0.37	0.81	1.00												
O3-AA-C19	0.55	0.39	0.67	0.93	1.00											
GS-O3-C19	0.69	0.38	0.76	0.90	0.80	1.00										
HD	0.11	-0.10	0.03	0.00	0.07	-0.04	1.00									
C19-AA	0.53	0.19	0.93	0.84	0.67	0.79	0.00	1.00								
$SASA_{side}$	0.22	0.26	-0.06	-0.01	0.01	0.01	0.18	0.00	1.00							
MR	0.09	0.10	-0.05	-0.04	-0.10	0.09	-0.14	-0.01	0.14	1.00						
KierFlex	0.01	0.02	-0.10	-0.08	-0.14	0.01	-0.14	-0.08	0.12	0.93	1.00					
O3-AA-BC	0.58	0.42	0.80	0.98	0.93	0.87	-0.02	0.78	0.00	-0.06	-0.09	1.00				
GS-O3-AA	0.69	0.91	0.32	0.44	0.45	0.44	-0.04	0.26	0.41	0.13	0.08	0.51	1.00			
brotN	-0.04	-0.05	-0.17	-0.20	-0.25	-0.05	-0.15	-0.16	0.04	0.90	0.94	-0.20	0.04	1.00		
MW	0.00	-0.02	-0.13	-0.14	-0.20	-0.02	-0.16	-0.14	0.01	0.93	0.94	-0.14	0.03	0.93	1.00	
C18-AA	0.55	0.12	0.92	0.70	0.52	0.72	0.00	0.91	-0.10	0.02	-0.06	0.65	0.17	-0.14	-0.05	1.00

Table S4. 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_i potency.[a]

Compound	K_i (μM)	ΔG_w (kcal/mol)	$logP_c$	C18-GS-O7	C19-GS-O3	O7-C18-GS	O7-AA	O7-AA-C20	O7-AA-GS	HA	O3-C18-GS	O7-C19-GS	O7-GS_{min}	PSA_{side} ($Å^2$)	O7-GS
14	0.587	-78.2	2.59	0.761	0.850	0.877	0.912	0.908	0.772	6	0.854	0.837	0.728	168	0.751
8	0.890	-78.1	1.65	0.857	0.825	0.747	0.779	0.771	0.747	6	0.852	0.742	0.732	162	0.675
19	1.15	-76.9	1.71	0.730	0.908	0.885	0.905	0.908	0.809	8	0.846	0.864	0.701	181	0.688
5	1.25	-75.2	1.45	0.909	0.869	0.834	0.930	0.916	0.868	6	0.877	0.853	0.880	251	0.835
2	1.91	-73.8	2.04	0.843	0.808	0.849	0.845	0.831	0.788	6	0.847	0.820	0.794	225	0.782
1	2.00	-79.3	1.10	0.767	0.870	0.858	0.856	0.891	0.819	6	0.881	0.856	0.808	173	0.762
3	2.02	-69.5	2.57	0.926	0.788	0.760	0.808	0.802	0.774	6	0.770	0.753	0.755	236	0.745
30	2.24	-88.1	2.25	0.781	0.745	0.872	0.847	0.836	0.801	8	0.871	0.789	0.794	187	0.796
16	2.31	-78.6	1.15	0.653	0.754	0.875	0.892	0.887	0.686	6	0.820	0.805	0.676	207	0.644
4	2.31	-75.6	1.30	0.672	0.783	0.843	0.923	0.944	0.767	8	0.893	0.843	0.703	184	0.661
7	2.63	-79.4	1.58	0.666	0.815	0.838	0.908	0.900	0.652	6	0.850	0.789	0.637	167	0.603
23	2.64	-75.4	0.748	0.806	0.859	0.814	0.894	0.896	0.756	7	0.801	0.859	0.796	192	0.747
6	3.02	-70.4	2.07	0.791	0.566	0.542	0.601	0.604	0.570	6	0.538	0.647	0.549	199	0.545
26	3.16	-74.2	1.60	0.750	0.851	0.881	0.873	0.883	0.794	6	0.857	0.843	0.757	245	0.735
9	3.20	-79.8	1.43	0.882	0.873	0.878	0.930	0.931	0.870	6	0.880	0.844	0.887	173	0.856
10	3.89	-80.6	0.303	0.669	0.762	0.889	0.892	0.895	0.723	7	0.835	0.832	0.698	177	0.675
13	3.93	-76.7	2.78	0.594	0.799	0.850	0.900	0.910	0.602	6	0.860	0.850	0.510	164	0.550
18	4.03	-75.6	1.22	0.893	0.894	0.882	0.926	0.934	0.852	8	0.883	0.870	0.817	191	0.832
11	4.22	-80.6	0.248	0.907	0.907	0.897	0.928	0.937	0.883	7	0.903	0.905	0.885	186	0.875
28	4.30	-75.7	2.12	0.468	0.612	0.809	0.804	0.863	0.494	6	0.624	0.636	0.451	153	0.468
20	5.16	-74.0	1.99	0.847	0.828	0.889	0.926	0.936	0.777	8	0.906	0.867	0.790	185	0.795
29	5.19	-77.0	-0.0331	0.874	0.790	0.752	0.777	0.786	0.750	6	0.775	0.773	0.712	173	0.688
22	5.26	-73.4	1.72	0.812	0.453	0.449	0.711	0.704	0.449	7	0.444	0.463	0.451	188	0.433
12	6.09	-79.6	0.441	0.922	0.927	0.883	0.886	0.884	0.880	7	0.903	0.885	0.861	186	0.845
21	6.53	-79.6	1.09	0.894	0.856	0.915	0.923	0.923	0.850	7	0.886	0.869	0.799	187	0.868
17	7.65	-77.8	1.06	0.904	0.934	0.903	0.921	0.935	0.852	8	0.892	0.906	0.865	198	0.848
27	8.07	-79.1	2.04	0.748	0.876	0.894	0.933	0.941	0.795	6	0.892	0.857	0.707	164	0.714
25	15.9	-82.5	0.067	0.697	0.848	0.800	0.859	0.894	0.752	7	0.851	0.811	0.782	239	0.737
24	16.3	-84.1	-0.061	0.812	0.823	0.805	0.888	0.894	0.786	7	0.865	0.769	0.815	245	0.791
32	35.9	-165	-5.41	0.308	0.291	0.286	0.642	0.638	0.285	8	0.329	0.359	0.285	215	0.284
31	40.4	-179	-6.40	0.617	0.655	0.747	0.705	0.713	0.667	8	0.768	0.807	0.619	235	0.614

Table S4. Contd.

Compound	K_i (μM)	O3-AA-GS	C18-GS-O3	O3-GS_{min}	BC-GS_{min}	AA-GS-O3	O3-GS	GS-O7-C18	O3-GS_{max}	C19-GS_{min}	C18-GS_{min}	O7-GS_{max}	O3-AA-C20	BC-GS	AA-GS-O7	O7-AA-BC
14	0.587	0.769	0.785	0.731	0.754	0.757	0.759	0.862	0.727	0.763	0.773	0.732	0.941	0.753	0.745	0.903
8	0.890	0.718	0.802	0.721	0.620	0.670	0.670	0.725	0.597	0.623	0.611	0.592	0.813	0.592	0.702	0.781
19	1.15	0.768	0.901	0.687	0.627	0.721	0.692	0.843	0.667	0.650	0.637	0.672	0.934	0.622	0.699	0.914
5	1.25	0.851	0.924	0.842	0.841	0.848	0.815	0.835	0.739	0.805	0.842	0.755	0.924	0.782	0.835	0.945
2	1.91	0.846	0.859	0.817	0.877	0.868	0.792	0.848	0.779	0.821	0.828	0.807	0.810	0.832	0.825	0.882
1	2.00	0.799	0.907	0.817	0.794	0.807	0.745	0.878	0.639	0.802	0.805	0.660	0.910	0.707	0.781	0.882
3	2.02	0.801	0.792	0.755	0.801	0.799	0.751	0.763	0.738	0.761	0.773	0.744	0.792	0.810	0.839	0.803
30	2.24	0.799	0.815	0.747	0.753	0.787	0.773	0.862	0.733	0.699	0.743	0.751	0.915	0.742	0.766	0.734
16	2.31	0.687	0.704	0.679	0.663	0.640	0.656	0.822	0.569	0.672	0.670	0.550	0.932	0.625	0.598	0.848
4	2.31	0.780	0.859	0.711	0.680	0.723	0.675	0.838	0.603	0.696	0.698	0.603	0.947	0.645	0.652	0.947
7	2.63	0.649	0.762	0.636	0.577	0.590	0.611	0.797	0.521	0.580	0.550	0.505	0.881	0.544	0.566	0.901
23	2.64	0.787	0.829	0.814	0.770	0.848	0.732	0.834	0.648	0.766	0.742	0.690	0.921	0.673	0.833	0.920
6	3.02	0.560	0.576	0.534	0.588	0.636	0.529	0.557	0.513	0.555	0.607	0.528	0.553	0.581	0.579	0.573
26	3.16	0.760	0.793	0.755	0.722	0.736	0.725	0.856	0.665	0.736	0.721	0.658	0.926	0.701	0.726	0.883
9	3.20	0.866	0.882	0.866	0.881	0.885	0.818	0.872	0.774	0.871	0.862	0.829	0.945	0.847	0.893	0.960
10	3.89	0.724	0.730	0.704	0.706	0.668	0.692	0.842	0.628	0.706	0.712	0.613	0.924	0.662	0.621	0.873
13	3.93	0.602	0.749	0.528	0.509	0.541	0.573	0.819	0.551	0.537	0.528	0.533	0.887	0.539	0.522	0.946
18	4.03	0.863	0.897	0.826	0.806	0.868	0.852	0.888	0.861	0.826	0.836	0.862	0.925	0.840	0.853	0.974
11	4.22	0.895	0.928	0.881	0.892	0.913	0.848	0.916	0.784	0.869	0.885	0.815	0.947	0.843	0.873	0.963
28	4.30	0.444	0.433	0.439	0.428	0.417	0.435	0.675	0.432	0.427	0.429	0.441	0.799	0.435	0.453	0.770
20	5.16	0.792	0.908	0.837	0.827	0.812	0.806	0.898	0.770	0.815	0.819	0.767	0.924	0.808	0.788	0.976
29	5.19	0.730	0.781	0.711	0.698	0.825	0.698	0.740	0.667	0.699	0.710	0.667	0.787	0.688	0.721	0.784
22	5.26	0.467	0.455	0.451	0.460	0.647	0.421	0.468	0.407	0.533	0.562	0.409	0.625	0.422	0.551	0.715
12	6.09	0.884	0.909	0.891	0.885	0.883	0.874	0.896	0.835	0.854	0.887	0.839	0.896	0.865	0.893	0.936
21	6.53	0.835	0.881	0.805	0.779	0.865	0.839	0.898	0.793	0.775	0.772	0.859	0.935	0.832	0.844	0.946
17	7.65	0.859	0.920	0.870	0.868	0.882	0.837	0.915	0.806	0.846	0.859	0.814	0.947	0.825	0.903	0.964
27	8.07	0.799	0.854	0.727	0.701	0.751	0.735	0.841	0.639	0.719	0.703	0.632	0.931	0.691	0.711	0.935
25	15.9	0.770	0.860	0.828	0.798	0.745	0.781	0.828	0.703	0.760	0.765	0.672	0.906	0.734	0.736	0.879
24	16.3	0.779	0.848	0.795	0.796	0.824	0.745	0.808	0.640	0.796	0.785	0.733	0.915	0.777	0.812	0.906
32	35.9	0.335	0.304	0.291	0.297	0.371	0.301	0.422	0.314	0.335	0.371	0.286	0.587	0.311	0.296	0.650
31	40.4	0.672	0.722	0.632	0.601	0.648	0.640	0.794	0.583	0.628	0.613	0.585	0.813	0.606	0.679	0.763

Table S4. Contd.

Compound	K_i (μM)	BC-GS_{max}	PSA (Å^2)	C19-GS	O7-AA-C18	GS-O3-C18	O3-C19-GS	C18-GS	C19-GS_{max}	SASA (Å^2)	O3-AA	BC-AA	C18-GS_{max}	GS-O7-C19	C19-GS-O7	GS-O7-AA
14	0.587	0.733	247	0.765	0.859	0.885	0.888	0.764	0.744	1033	0.932	0.918	0.719	0.809	0.844	0.856
8	0.890	0.548	240	0.597	0.745	0.822	0.835	0.551	0.546	960	0.828	0.871	0.488	0.702	0.606	0.626
19	1.15	0.614	256	0.637	0.892	0.790	0.854	0.589	0.583	1006	0.853	0.882	0.537	0.824	0.646	0.607
5	1.25	0.717	328	0.762	0.927	0.869	0.849	0.769	0.684	953	0.920	0.921	0.655	0.823	0.776	0.709
2	1.91	0.834	299	0.823	0.837	0.845	0.788	0.855	0.846	965	0.832	0.872	0.837	0.805	0.918	0.753
1	2.00	0.629	251	0.719	0.860	0.895	0.874	0.712	0.617	956	0.881	0.853	0.571	0.843	0.805	0.718
3	2.02	0.784	303	0.774	0.797	0.780	0.762	0.796	0.764	966	0.785	0.786	0.781	0.791	0.861	0.796
30	2.24	0.708	264	0.713	0.692	0.890	0.737	0.709	0.685	1122	0.893	0.794	0.656	0.773	0.826	0.857
16	2.31	0.546	285	0.642	0.785	0.843	0.875	0.622	0.565	918	0.915	0.860	0.512	0.754	0.685	0.761
4	2.31	0.604	262	0.668	0.928	0.863	0.898	0.629	0.582	986	0.925	0.910	0.539	0.857	0.741	0.614
7	2.63	0.481	245	0.562	0.875	0.783	0.738	0.514	0.498	942	0.886	0.878	0.447	0.725	0.586	0.725
23	2.64	0.610	270	0.676	0.878	0.825	0.836	0.629	0.568	971	0.918	0.884	0.517	0.823	0.687	0.610
6	3.02	0.549	255	0.577	0.619	0.577	0.545	0.581	0.556	877	0.539	0.552	0.543	0.792	0.650	0.698
26	3.16	0.644	322	0.702	0.842	0.868	0.896	0.683	0.647	941	0.940	0.877	0.621	0.809	0.743	0.846
9	3.20	0.814	251	0.839	0.944	0.886	0.869	0.855	0.805	993	0.927	0.934	0.821	0.841	0.916	0.825
10	3.89	0.618	255	0.679	0.818	0.872	0.888	0.665	0.615	959	0.926	0.860	0.562	0.787	0.739	0.776
13	3.93	0.530	241	0.566	0.889	0.776	0.777	0.532	0.548	977	0.892	0.903	0.491	0.791	0.583	0.673
18	4.03	0.839	269	0.839	0.953	0.887	0.875	0.849	0.831	1035	0.919	0.924	0.849	0.853	0.887	0.893
11	4.22	0.782	264	0.830	0.948	0.928	0.882	0.833	0.755	1005	0.922	0.936	0.748	0.876	0.865	0.817
28	4.30	0.422	232	0.427	0.623	0.726	0.808	0.436	0.417	906	0.778	0.588	0.410	0.524	0.551	0.699
20	5.16	0.774	263	0.814	0.936	0.916	0.898	0.806	0.778	1074	0.933	0.921	0.746	0.860	0.815	0.762
29	5.19	0.699	237	0.687	0.782	0.787	0.755	0.671	0.681	993	0.726	0.789	0.638	0.821	0.765	0.698
22	5.26	0.414	241	0.493	0.699	0.564	0.490	0.484	0.487	989	0.654	0.685	0.439	0.600	0.667	0.594
12	6.09	0.835	263	0.848	0.909	0.913	0.884	0.837	0.826	996	0.898	0.942	0.814	0.877	0.865	0.803
21	6.53	0.806	265	0.799	0.912	0.928	0.875	0.836	0.751	1111	0.923	0.923	0.775	0.840	0.898	0.869
17	7.65	0.787	276	0.823	0.947	0.913	0.899	0.822	0.781	1042	0.932	0.928	0.780	0.882	0.870	0.847
27	8.07	0.621	242	0.732	0.875	0.820	0.865	0.695	0.659	973	0.911	0.886	0.591	0.826	0.743	0.751
25	15.9	0.673	317	0.715	0.869	0.873	0.866	0.714	0.654	960	0.869	0.826	0.666	0.822	0.814	0.807
24	16.3	0.692	323	0.791	0.873	0.874	0.833	0.793	0.704	987	0.894	0.874	0.723	0.752	0.856	0.737
32	35.9	0.318	275	0.375	0.574	0.495	0.533	0.358	0.385	891	0.693	0.711	0.341	0.589	0.556	0.743
31	40.4	0.575	304	0.613	0.771	0.833	0.791	0.600	0.578	934	0.799	0.771	0.533	0.817	0.693	0.584

Table S4. Contd.

Compound	K_i (μM)	O7-AA-C19	O3-AA-C18	O3-AA-C19	GS-O3-C19	HD	C19-AA	$SASA_{side}$ ($Å^2$)	MR (m^3/mol)	KierFlex	O3-AA-BC	GS-O3-AA	brotN	MW	C18-AA
14	0.587	0.889	0.883	0.916	0.856	4	0.870	606	17.0	8.79	0.902	0.864	12	610	0.872
8	0.890	0.883	0.780	0.793	0.790	4	0.850	525	18.3	9.87	0.804	0.651	15	669	0.878
19	1.15	0.855	0.830	0.737	0.817	4	0.925	568	16.7	8.71	0.801	0.569	12	614	0.894
5	1.25	0.954	0.945	0.915	0.819	4	0.915	508	17.1	9.39	0.951	0.686	12	630	0.917
2	1.91	0.910	0.787	0.806	0.778	4	0.875	518	16.6	8.55	0.796	0.712	12	596	0.864
1	2.00	0.920	0.915	0.928	0.849	4	0.870	497	17.2	9.28	0.946	0.721	13	664	0.907
3	2.02	0.816	0.790	0.796	0.789	4	0.791	547	20.3	10.4	0.795	0.784	16	730	0.851
30	2.24	0.718	0.800	0.844	0.767	4	0.703	698	16.7	8.71	0.858	0.919	12	614	0.699
16	2.31	0.798	0.818	0.858	0.811	4	0.782	501	17.8	9.61	0.848	0.690	14	654	0.781
4	2.31	0.920	0.918	0.954	0.883	4	0.925	547	17.0	8.79	0.939	0.574	12	610	0.923
7	2.63	0.785	0.805	0.867	0.688	4	0.817	522	16.9	8.79	0.795	0.628	12	611	0.774
23	2.64	0.911	0.898	0.917	0.802	5	0.878	507	16.7	8.71	0.914	0.601	12	614	0.894
6	3.02	0.626	0.563	0.579	0.602	4	0.582	491	16.8	8.87	0.570	0.545	12	632	0.779
26	3.16	0.845	0.849	0.808	0.858	4	0.842	516	17.0	8.79	0.858	0.781	12	610	0.847
9	3.20	0.944	0.909	0.944	0.862	4	0.916	533	17.2	9.27	0.931	0.817	13	626	0.930
10	3.89	0.806	0.828	0.855	0.846	4	0.792	544	18.4	9.50	0.846	0.708	13	652	0.796
13	3.93	0.836	0.835	0.876	0.738	4	0.855	577	18.4	9.66	0.833	0.615	13	650	0.853
18	4.03	0.973	0.915	0.933	0.860	4	0.931	579	17.2	9.27	0.923	0.918	13	626	0.935
11	4.22	0.969	0.939	0.963	0.876	4	0.920	548	17.5	9.03	0.955	0.815	12	624	0.935
28	4.30	0.532	0.674	0.761	0.638	4	0.511	546	18.2	10.1	0.704	0.688	15	668	0.514
20	5.16	0.940	0.922	0.875	0.877	4	0.909	612	17.9	10.0	0.920	0.758	14	656	0.918
29	5.19	0.820	0.748	0.701	0.791	4	0.824	591	20.0	10.6	0.739	0.681	16	707	0.867
22	5.26	0.717	0.605	0.659	0.617	5	0.712	657	17.2	9.27	0.608	0.613	13	626	0.744
12	6.09	0.926	0.905	0.893	0.885	4	0.931	547	20.0	10.6	0.924	0.821	16	707	0.924
21	6.53	0.942	0.919	0.950	0.864	5	0.899	680	18.4	9.66	0.938	0.848	13	650	0.909
17	7.65	0.955	0.935	0.962	0.881	4	0.919	586	17.5	9.03	0.949	0.864	12	624	0.935
27	8.07	0.850	0.866	0.926	0.835	4	0.846	544	16.9	8.79	0.873	0.708	12	611	0.844
25	15.9	0.889	0.898	0.923	0.861	5	0.839	513	16.9	8.79	0.900	0.826	12	611	0.862
24	16.3	0.861	0.847	0.874	0.824	5	0.837	522	17.2	9.12	0.859	0.694	13	639	0.849
32	35.9	0.863	0.675	0.651	0.613	4	0.750	540	17.2	9.12	0.762	0.751	13	639	0.789
31	40.4	0.947	0.831	0.864	0.837	4	0.800	529	17.2	9.12	0.845	0.618	13	639	0.894

[a] Entries for structural descriptors are the overlap coefficients of the conjugate with respect to **15**.

Table S5. Results from multivariable regression analysis and modified Akaike Information Criterion (AIC_C) for the best CSP-SAR model for anilinyl conjugates **1**-**33** of glu-CDCA.[a]

CSP-SAR Model	r^2	Q^2	F	W_i	***K*** **(μM)**	***A*** **(μM/kcal /mol)**	***B*** **(μM/Å^2)**	***C*** **(μM)**	***D*** **(μM)**	**Standa-rdized *A* (μM)**	**Standa-rdized *B* (μM/Å^2)**	**Standa-rdized *C* (μM)**	**Standa-rdized *D* (μM)**
ΔGw, O7-AA-C20, C18-GS-O7, GS-O3-C19	0.837	0.347	34.6	0.207	-93.0 ± 18	-0.765 ± 0.068	95.7 ± 29	51.5 ± 16	-106 ± 32	-1.092	0.441	0.461	-0.611

[a] *A* and *B* represent the coefficient of the independent variables (molecular descriptors); *K* represents the coefficient of the intercept.

Table S6. Results from single variable regression of molecular descriptors used for multivariable analysis.[a]

Molecular Descriptor	Linear r^2	Coeff. independent variable[b]	SEM of coeff. of independent variable[b]	Coeff. of intercept (μM)	SEM of coeff. of intercept (μM)
ΔG_w (kcal/mol)	0.868	-0.358	0.026	-23.4	2.3
$logP_c$	0.862	-4.30	0.32	10.5	0.69
C18-GS-O7	0.259	-33.3	10	32.1	8.1
C19-GS-O3	0.253	-32.8	10	32.4	8.4
O7-C18-GS	0.238	-32.2	11	32.5	8.8
O7-AA	0.225	-49.5	17	49.0	15
O7-AA-C20	0.202	-45.9	17	46.1	15
O7-AA-GS	0.189	-29.3	11	28.2	8.5
HA	0.186	4.69	1.8	-25.2	12
O3-C18-GS	0.172	-27.6	11	28.9	9.2
O7-C19-GS	0.162	-30.7	13	30.9	10
$O7\text{-}GS_{min}$	0.158	-25.7	11	25.0	8.0
PSA_{side} (Å^2)	0.156	0.130	0.056	-18.7	11
O7-GS	0.152	-25.9	11	24.8	8.1
O3-AA-GS	0.150	-26.5	12	26.2	8.8
C18-GS-O3	0.149	-23.2	10	24.8	8.3
$O3\text{-}GS_{min}$	0.133	-23.3	11	23.4	8.1
$BC\text{-}GS_{min}$	0.132	-22.8	11	22.8	7.9
AA-GS-O3	0.129	-24.5	12	24.7	8.9
O3-GS	0.126	-24.0	12	23.5	8.4
GS-O7-C18	0.125	-27.0	13	28.2	11
$O3\text{-}GS_{max}$	0.123	-25.0	12	23.0	8.3
$C19\text{-}GS_{min}$	0.121	-24.5	12	23.9	8.8
$C18\text{-}GS_{min}$	0.121	-24.5	12	24.1	8.9
$O7\text{-}GS_{max}$	0.119	-22.5	11	21.5	7.7
O3-AA-C20	0.114	-29.2	15	31.9	13
BC-GS	0.110	-22.0	12	21.7	8.1
AA-GS-O7	0.109	-21.2	11	21.8	8.2
O7-AA-BC	0.108	-29.8	16	32.4	14
$BC\text{-}GS_{max}$	0.101	-21.6	12	20.6	8.0
PSA (Å^2)	0.0997	0.105	0.058	-21.6	16
C19-GS	0.0991	-23.5	13	22.9	9.3
O7-AA-C18	0.0973	-27.6	16	29.6	13
GS-O3-C18	0.0902	-26.1	15	28.1	13
O3-C19-GS	0.0840	-24.6	15	26.6	12
C18-GS	0.0824	-19.6	12	20.0	8.5
$C19\text{-}GS_{max}$	0.0753	-20.7	14	20.1	8.9
SASA (Å^2)	0.0702	-0.0436	0.029	49.3	29
O3-AA	0.0690	-25.3	17	28.3	15
BC-AA	0.0653	-24.0	17	26.9	14
$C18\text{-}GS_{max}$	0.0584	-15.9	12	16.5	7.6
GS-O7-C19	0.0468	-23.5	20	25.1	16

C19-GS-O7	0.0348	-15.3	15	18.1	11
GS-O7-AA	0.0272	-17.1	19	19.3	14
O7-AA-C19	0.0219	13.4	17	-4.9	14
O3-AA-C18	0.0203	-13.5	17	17.8	15
O3-AA-C19	0.0197	-12.9	17	17.6	14
GS-O3-C19	0.0186	-14.8	20	18.5	16
HD	0.0177	3.27	4.5	-7.03	19
C19-AA	0.0172	-12.1	17	16.7	14
$SASA_{side}$ ($Å^2$)	0.00957	-0.0174	0.033	16.2	18
MR (m^3/mol)	0.00742	-0.798	1.7	20.6	30
KierFlex	0.00628	-1.24	2.9	18.2	27
O3-AA-BC	0.00438	-6.29	18	11.9	15
GS-O3-AA	8.59E-04	-2.58	16	8.46	12
brotN	2.41E-04	-0.110	1.3	8.01	17
MW	1.78E-04	-0.00384	0.053	9.04	34
C18-AA	1.35E-05	-0.384	19	6.91	17

[a] Regression analysis of structural descriptors (e.g. C18-GS-O7) employed the overlap coefficients with respect to **15**.

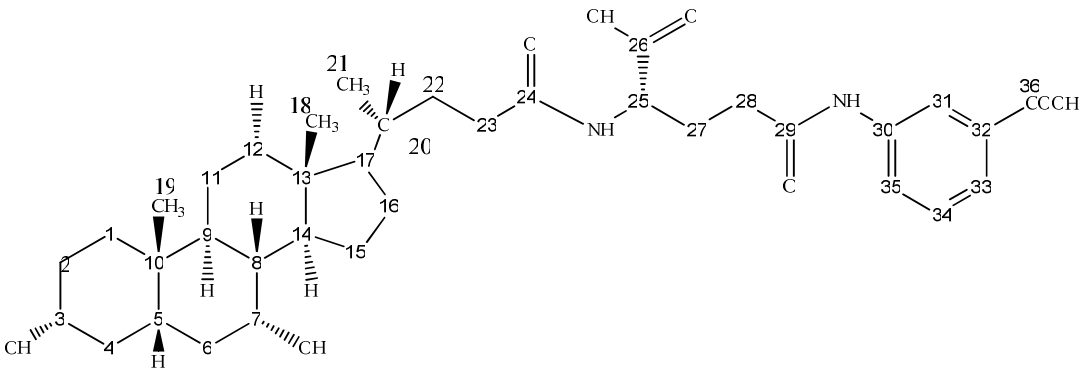
[b] Coefficient of independent variable has units of μM divided by units of the molecular descriptor (e.g. μM/$Å^2$ for SASA).

Table S7. Results from multivariable regression analysis and modified Akaike Information Criterion (AIC_C) for the two best CSP-SAR models for anilinyl conjugates of glu-CDCA using pK_i (i.e. -logK_i) as biological activity.[a]

CSP-SAR Model	r^2	Q^2	F	W_i	K (μM)	A	B (μM)	C (μM)	D (μM)	**Standardized A**	**Standardized B (μM/Å^2)**	**Standardized C (μM)**	**Standardized D (μM)**
1) logP, O7-AA-BC, C18-GS_{max}, O7-AA-C19	0.683	0.532	14.0	0.992	-1.02 ± 0.43	0.237 ± 0.034 (μM)	-1.89 ± 0.80	-0.961 ± 0.44	2.84 ± 0.91	1.14 (μM)	-0.463	-0.325	0.690
2) ΔG_w, HD	0.567	0.495	18.4	0.00785	2.08 ± 0.62	0.0120 ± 0.0022 (μM/kcal/mol)	- 0.401 ± 0.14	N/A	N/A	0.692 (μM/kcal/mol)	- 0.362	N/A	N/A

[a] A and B represent the coefficient of the independent variables (molecular descriptors); K represents the coefficient of the intercept.

Table S8. ^{13}C and ^{1}H chemical shifts of **32** in D_2O-phosphate (pH 7.4).



Carbon No.	Type	^{13}C	^{1}H		
			H	H_α	H_β
C1	CH_2	35.30	-	1.79	0.93
C2	CH_2	29.95	-	1.58	1.27
C3	CH	72.36	3.45	-	-
C4	CH_2	38.96	-	1.97	1.63
C5	CH	41.43	1.34	-	-
C6	CH_2	34.37	-	1.87	1.43
C7	CH	69.07	3.65	-	-
C8	CH	39.38	1.28	-	-
C9	CH	32.82	1.66	-	-
C10	C	39.28	-	-	-
C11	CH_2	20.78	-	1.39	1.16
C12	CH_2	39.66	-	1.86	1.07
C13	C	42.72	-	-	-
C14	CH	50.36	1.20	-	-
C15	CH_2	23.75	-	1.49	0.88
C16	CH_2	28.37	-	1.74	1.08
C17	CH	55.71	0.97	-	-
C18	CH_3	11.64	0.50	-	-
C19	CH_3	22.71	0.80	-	-
C20	CH	35.30	1.28	-	-
C21	CH_3	18.19	0.84	-	-
C22	CH_2	32.41	-	1.67	1.20
C23	CH_2	33.82	-	2.33	2.13
C24	C	177.7	-	-	-
C25	CH	55	4.29	-	-
C26	C	178.9	-	-	-
C27	CH_2	27.87	-	2.19	2.07
C28	CH_2	33.65	-	2.54	2.48
C29	C	174.4	-	-	-
C30	C	137.8	-	-	-
C31	CH	121.7	7.84	-	-
C32	C	126.33	-	-	-
C33	CH	126.1	7.66	-	-
C34	CH	129.5	7.73	-	-
C35	CH	123.8	7.72	-	-
C36	C	175	-	-	-

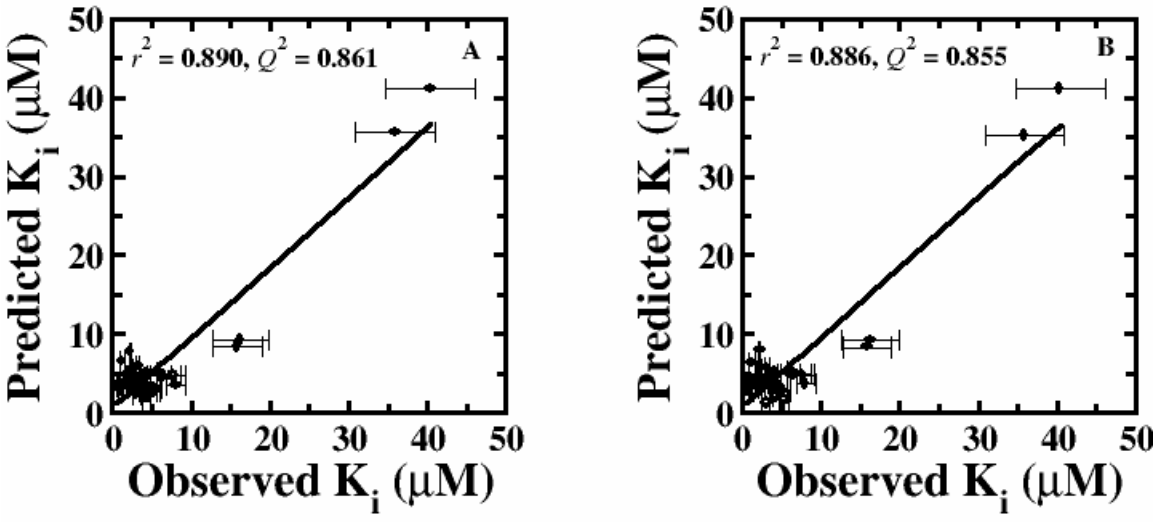


Figure S1. Regression plot for predicted vs. observed K_i values for anilinyl conjugates of glu-CDCA using CSP-SAR (A) Model 2 and (B) Model 3, which are the models in Table 2.

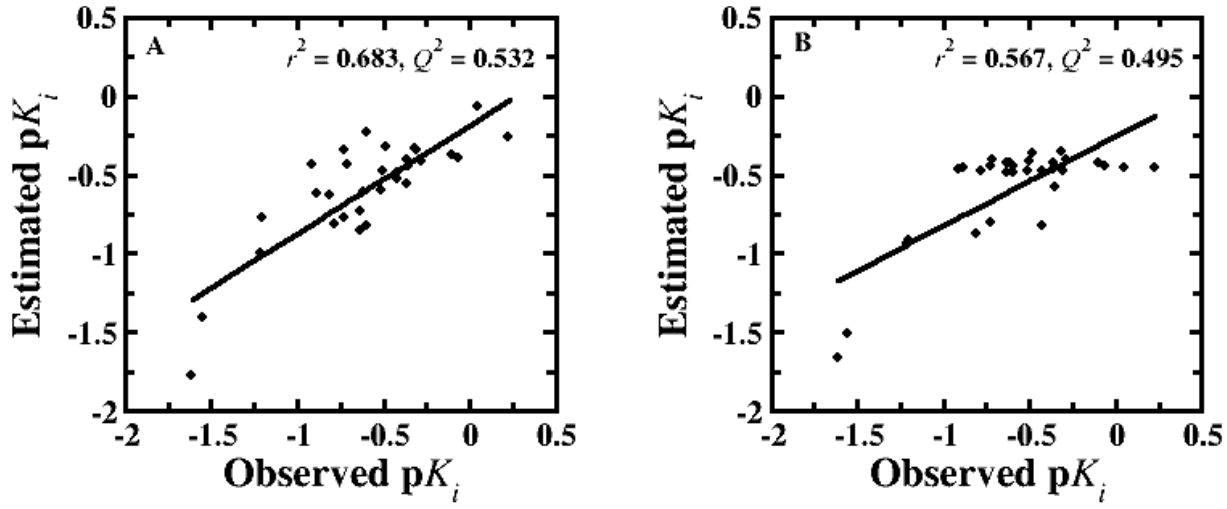


Figure S2. Regression plot for predicted vs. observed pK_i values for anilinyl conjugates of glu-CDCA using CSP-SAR (A) Model 1 and (B) Model 2, which are the models in Table S7.