Supporting Information
(6 pages of crystal details)

Table 1. Atomic coordinates (Å × 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)		x	y	z	U(eq)
C1(1)	1950(6)	6031(4)	-771(3)	51(2)	O2(4)	6468(5)	9538(3)	2034(3)	80(2)
C2(1)	2825(6)	5587(4)	-603(3)	59(2)	O3(4)	6465(5)	10544(4)	1290(2)	82(2)
C3(1)	3072(6)	5738(5)	-91(3)	58(2)	O4(4)	4504(5)	10896(3)	979(2)	69(2)
C4(1)	2150(6)	5660(4)	220(3)	53(2)	O5(4)	4097(4)	10418(3)	2223(2)	52(1)
C5(1)	1281(6)	6100(4)	14(3)	55(2)	O6(4)	3400(5)	11782(4)	1950(3)	89(2)
C6(1)	358(6)	6015(5)	281(3)	64(2)	C1(5)	4396(9)	11591(5)	786(4)	83(3)
O2(1)	3665(5)	5751(4)	-894(2)	75(2)	C2(5)	5189(10)	11667(6)	391(4)	99(4)
O3(1)	3807(5)	5272(4)	83(2)	76(2)	C3(5)	5006(8)	11156(6)	-7(3)	74(3)
O4(1)	2408(4)	5933(3)	684(2)	55(1)	C4(5)	3959(8)	11226(5)	-183(3)	70(2)
O5(1)	1128(4)	5900(3)	-473(2)	54(1)	C5(5)	3203(8)	11146(6)	224(3)	79(3)
N1(1)	-421(6)	6512(5)	200(3)	78(2)	C6(5)	2157(10)	11263(9)	91(5)	113(4)
C7(1)	-1178(7)	6481(5)	-133(3)	67(2)	O2(5)	6178(7)	11559(5)	588(3)	119(3)
C8(1)	-1211(7)	5965(5)	-474(3)	71(2)	O3(5)	5697(6)	11273(5)	-386(2)	111(3)
C9(1)	-1993(8)	5968(6)	-808(4)	86(3)	O4(5)	3793(4)	10687(3)	-528(2)	59(1)
C10(1)	-2689(9)	6475(7)	-825(4)	100(4)	O5(5)	3442(6)	11666(4)	580(2)	91(2)
C11(1)	-2612(8)	7004(6)	-482(4)	89(3)	O6(5)	2035(13)	11873(10)	-108(5)	176(7)
C12(1)	-1892(7)	7005(5)	-140(3)	67(2)	O6'(5)	1490(20)	11200(20)	435(11)	48(15)
C1(2)	2110(6)	5554(4)	1092(3)	53(2)	C1(6)	3521(6)	10886(5)	-996(3)	54(2)
C2(2)	3050(6)	5361(4)	1364(3)	49(2)	C2(6)	4153(6)	10490(4)	-1332(3)	56(2)
C3(2)	3554(5)	5993(4)	1553(2)	42(2)	C3(6)	3923(6)	9710(4)	-1334(3)	57(2)
C4(2)	2841(6)	6449(4)	1832(3)	48(2)	C4(6)	2813(6)	9579(4)	-1402(3)	53(2)
C5(2)	1916(6)	6621(4)	1523(3)	54(2)	C5(6)	2255(6)	10011(5)	-1024(3)	56(2)
C6(2)	1162(8)	7038(6)	1781(5)	93(3)	C6(6)	1142(6)	9947(5)	-1071(3)	60(2)
O2(2)	3686(4)	4937(3)	1071(2)	59(1)	O2(6)	5193(4)	10596(3)	-1238(2)	68(2)
O3(2)	4361(4)	5784(3)	1852(2)	54(1)	O3(6)	4457(4)	9347(3)	-1711(2)	68(2)
O4(2)	3346(4)	7094(2)	1938(2)	51(1)	O4(6)	2657(4)	8843(3)	-1327(2)	56(1)
O5(2)	1471(4)	5973(3)	1370(2)	58(1)	O5(6)	2507(4)	10737(3)	-1075(2)	60(1)
O6(2)	393(11)	7234(7)	1454(5)	112(6)	O6(6)	823(4)	10146(3)	-1536(2)	67(2)
O6'(2)	865(18)	6714(13)	2177(9)	122(10)	C1(7)	2022(6)	8485(5)	-1642(3)	62(2)
C1(3)	3400(7)	7299(4)	2421(3)	58(2)	C2(7)	2580(7)	7867(4)	-1855(3)	61(2)
C2(3)	4456(7)	7469(4)	2554(3)	62(2)	C3(7)	2820(6)	7358(4)	-1450(3)	57(2)
C3(3)	4809(6)	8093(4)	2288(3)	59(2)	C4(7)	1899(6)	7136(4)	-1181(3)	56(2)
C4(3)	4129(7)	8719(4)	2358(3)	61(2)	C5(7)	1371(6)	7792(5)	-1006(3)	61(2)
C5(3)	3062(6)	8513(4)	2244(3)	61(2)	C6(7)	391(7)	7640(6)	-760(4)	87(3)
C6(3)	2313(9)	9067(5)	2362(5)	104(4)	O2(7)	3443(5)	8096(3)	-2089(2)	81(2)
O2(3)	5014(6)	6844(3)	2463(2)	84(2)	O3(7)	3308(6)	6765(3)	-1654(2)	86(2)
O3(3)	5782(5)	8258(3)	2448(3)	93(2)	O4(7)	2233(4)	6736(3)	-784(2)	50(1)

O4(3)	4436(4)	9259(2)	2047(2)	55(1)	O5(7)	1160(4)	8266(3)	-1392(2)	62(1)
O5(3)	2784(5)	7895(3)	2496(2)	72(2)	O6(7)	32(7)	8205(5)	-500(4)	126(3)
O6(3)	1391(6)	8952(5)	2155(6)	170(5)	OW1	871(18)	9389(12)	76(8)	151(7)
C1(4)	4793(6)	9889(4)	2253(3)	54(2)	OW2	6608(17)	2779(13)	1027(9)	285(10)
C2(4)	5767(7)	10088(4)	2014(3)	57(2)	OW3	8224(13)	10061(9)	2407(6)	110(5)
C3(4)	5550(7)	10280(5)	1500(3)	63(2)	OW4	5226(18)	3445(14)	1378(9)	298(10)
C4(4)	4743(7)	10818(4)	1470(3)	59(2)	OW5	-254(10)	8209(7)	2397(5)	178(5)
C5(4)	3820(6)	10605(4)	1742(3)	53(2)	OW6	6262(10)	11069(7)	-1971(5)	171(4)
C6(4)	3031(7)	11159(5)	1765(4)	69(2)	OW7	-162(7)	7990(5)	634(3)	120(3)

Table 2. Bond lengths (Å) for mono(6-anilino-6-deoxy)-β-cyclodextrin (**1**)

Bond	Length (Å)	Bond	Length (Å)
C11-O47	1.394(9)	C24-O24	1.407(10)
C11-O51	1.408(9)	C24-C34	1.515(12)
C11-C21	1.523(12)	C34-O34	1.452(11)
C21-O21	1.427(10)	C34-C44	1.493(13)
C21-C31	1.500(11)	C44-O44	1.423(9)
C31-O31	1.414(10)	C44-C54	1.511(12)
C31-C41	1.522(11)	C54-O54	1.441(9)
C41-O41	1.443(9)	C54-C64	1.497(12)
C41-C51	1.548(11)	C64-O64	1.385(11)
C51-O51	1.433(9)	O44-C15	1.437(11)
C51-C61	1.456(11)	C15-O55	1.412(13)
C61-N11	1.428(12)	C15-C25	1.543(16)
O41-C12	1.411(9)	C25-O25	1.453(15)
N11-C71	1.382(11)	C25-C35	1.501(13)
C71-C81	1.371(13)	C35-O35	1.428(11)
C71-C121	1.383(13)	C35-C45	1.495(14)
C81-C91	1.407(13)	C45-O45	1.428(10)
C91-C101	1.345(15)	C45-C55	1.535(14)
C101-C111	1.397(16)	C55-O55	1.442(11)
C111-C121	1.362(14)	C55-C65	1.470(17)
C12-O52	1.407(10)	C65-O65	1.30(2)
C12-C22	1.520(11)	C65-O6'5	1.32(3)
C22-O22	1.435(9)	O45-C16	1.412(9)
C22-C32	1.478(10)	C16-O56	1.408(9)
C32-O32	1.426(8)	C16-C26	1.476(11)
C32-C42	1.511(10)	C26-O26	1.436(10)
C42-O42	1.432(9)	C26-C36	1.515(11)
C42-C52	1.550(11)	C36-O36	1.453(10)
C52-O52	1.435(9)	C36-C46	1.524(11)
C52-C62	1.476(13)	C46-O46	1.431(9)
C62-O6'2	1.33(3)	C46-C56	1.538(11)
C62-O62	1.430(17)	C56-O56	1.428(10)

O42-C13	1.413(9)	C56-C66	1.506(12)
C13-O53	1.421(10)	C66-O66	1.424(10)
C13-C23	1.501(12)	O46-C17	1.405(10)
C23-O23	1.430(11)	C17-O57	1.417(10)
C23-C33	1.479(12)	C17-C27	1.516(13)
C33-O33	1.418(11)	C27-O27	1.401(11)
C33-C43	1.515(12)	C27-C37	1.527(12)
C43-O43	1.409(10)	C37-O37	1.424(10)
C43-C53	1.520(13)	C37-C47	1.509(11)
C53-O53	1.422(10)	C47-O47	1.422(9)
C53-C63	1.494(13)	C47-C57	1.517(12)
C63-O63	1.385(16)	C57-O57	1.439(10)
O43-C14	1.414(9)	C57-C67	1.513(12)
C14-O54	1.377(9)	C67-O67	1.386(14)
C14-C24	1.517(12)		

Table 3 Bond angles (°) for mono(6-anilino-6-deoxy)-β-cyclodextrin (**1**)

Bond	Angle (°)	Bond	Angle (°)
O47-C11-O51	113.5(6)	C34-C24-C14	108.3(7)
O47-C11-C21	109.3(6)	O34-C34-C44	110.8(7)
O51-C11-C21	108.8(6)	O34-C34-C24	107.9(7)
O21-C21-C31	109.3(7)	C44-C34-C24	111.0(7)
O21-C21-C11	108.1(6)	O44-C44-C34	106.8(6)
C31-C21-C11	111.2(6)	O44-C44-C54	109.4(7)
O31-C31-C21	111.3(7)	C34-C44-C54	112.6(7)
O31-C31-C41	108.0(6)	O54-C54-C64	108.4(7)
C21-C31-C41	110.5(7)	O54-C54-C44	109.0(6)
O41-C41-C31	106.6(6)	C64-C54-C44	114.4(7)
O41-C41-C51	108.8(6)	O64-C64-C54	111.4(7)
C31-C41-C51	110.3(6)	C44-O44-C15	118.9(6)
O51-C51-C61	109.7(7)	C14-O54-C54	114.4(6)
O51-C51-C41	108.7(6)	O55-C15-O44	109.7(8)
C61-C51-C41	113.0(7)	O55-C15-C25	108.9(8)
N11-C61-C51	118.0(7)	O44-C15-C25	106.7(9)
C12-O41-C41	118.6(5)	O25-C25-C35	109.9(11)
C11-O51-C51	114.0(6)	O25-C25-C15	110.2(8)
C71-N11-C61	128.1(8)	C35-C25-C15	111.1(8)
C81-C71-C121	118.9(9)	O35-C35-C45	110.6(7)
C81-C71-N11	121.8(9)	O35-C35-C25	110.2(8)
C121-C71-N11	119.2(8)	C45-C35-C25	110.0(9)
C71-C81-C91	119.0(9)	O45-C45-C35	107.9(8)
C101-C91-C81	123.1(10)	O45-C45-C55	109.2(8)
C91-C101-C111	116.1(10)	C35-C45-C55	111.6(7)
C121-C111-C101	122.6(10)	O55-C55-C65	106.5(9)

C111-C121-C71	120.1(9)	O55-C55-C45	107.4(8)
O52-C12-O41	109.4(6)	C65-C55-C45	115.4(9)
O52-C12-C22	111.4(6)	O65-C65-O6'5	108(2)
O41-C12-C22	107.2(6)	O65-C65-C55	111.4(15)
O22-C22-C32	112.9(6)	O6'5-C65-C55	116.4(18)
O22-C22-C12	110.0(6)	C16-O45-C45	118.5(6)
C32-C22-C12	111.4(6)	C15-O55-C55	114.6(8)
O32-C32-C22	109.4(6)	O56-C16-O45	110.0(6)
O32-C32-C42	109.7(5)	O56-C16-C26	110.7(6)
C22-C32-C42	111.2(6)	O45-C16-C26	107.9(6)
O42-C42-C32	107.3(6)	O26-C26-C16	111.7(6)
O42-C42-C52	108.4(6)	O26-C26-C36	109.7(6)
C32-C42-C52	109.9(6)	C16-C26-C36	112.6(7)
O52-C52-C62	108.8(7)	O36-C36-C26	111.6(7)
O52-C52-C42	108.7(6)	O36-C36-C46	108.3(6)
C62-C52-C42	112.9(7)	C26-C36-C46	111.1(6)
O6'2-C62-O62	116.0(15)	O46-C46-C36	106.5(6)
O6'2-C62-C52	111.4(14)	O46-C46-C56	110.5(6)
O62-C62-C52	108.8(11)	C36-C46-C56	107.6(7)
C13-O42-C42	117.3(5)	O56-C56-C66	107.8(7)
C12-O52-C52	113.5(6)	O56-C56-C46	109.4(6)
O42-C13-O53	109.3(7)	C66-C56-C46	112.3(7)
O42-C13-C23	110.2(7)	O66-C66-C56	110.9(7)
O53-C13-C23	109.9(6)	C17-O46-C46	118.1(6)
O23-C23-C33	114.1(7)	C16-O56-C56	114.1(6)
O23-C23-C13	105.7(6)	O46-C17-O57	109.1(7)
C33-C23-C13	110.6(7)	O46-C17-C27	108.9(7)
O33-C33-C23	108.3(7)	O57-C17-C27	111.8(7)
O33-C33-C43	109.9(6)	O27-C27-C17	110.6(7)
C23-C33-C43	111.9(7)	O27-C27-C37	111.7(7)
O43-C43-C33	108.5(7)	C17-C27-C37	107.7(7)
O43-C43-C53	109.6(7)	O37-C37-C47	110.9(7)
C33-C43-C53	109.8(6)	O37-C37-C27	107.5(7)
O53-C53-C63	107.3(7)	C47-C37-C27	112.1(7)
O53-C53-C43	110.9(8)	O47-C47-C37	106.4(6)
C63-C53-C43	114.0(8)	O47-C47-C57	109.4(6)
O63-C63-C53	113.4(10)	C37-C47-C57	108.4(7)
C14-O43-C43	117.7(6)	O57-C57-C47	111.3(7)
C13-O53-C53	115.8(6)	O57-C57-C67	106.9(7)
O54-C14-O43	111.4(6)	C47-C57-C67	113.4(8)
O54-C14-C24	112.1(6)	O67-C67-C57	113.2(9)
O43-C14-C24	108.9(6)	C11-O47-C47	116.7(6)
O24-C24-C34	110.2(7)	C17-O57-C57	113.3(6)
O24-C24-C14	112.0(7)		

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for mono(6-anilino-6-deoxy)-β-cyclodextrin (**1**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C11	48(4)	64(5)	41(4)	-1(4)	-1(4)	-1(4)
C21	68(5)	56(5)	53(5)	-13(4)	12(4)	3(4)
C31	60(5)	72(5)	43(4)	10(4)	-3(4)	17(4)
C41	61(5)	46(4)	50(4)	10(4)	-13(4)	-10(4)
C51	59(5)	54(5)	52(4)	-4(4)	-5(4)	0(4)
C61	49(5)	89(6)	54(5)	13(4)	4(4)	3(5)
O21	76(4)	93(4)	58(3)	14(3)	13(3)	13(4)
O31	74(4)	98(5)	57(3)	13(3)	9(3)	25(4)
O41	59(3)	60(3)	46(3)	4(3)	-5(2)	-12(3)
O51	60(3)	61(3)	41(3)	4(2)	-5(2)	-12(3)
N11	66(5)	96(6)	73(5)	-24(4)	-9(4)	10(5)
C71	70(6)	82(6)	50(5)	-6(5)	2(4)	7(5)
C81	66(6)	70(6)	78(6)	-4(5)	-5(5)	16(5)
C91	78(6)	99(7)	80(6)	-27(6)	-23(5)	28(6)
C101	84(7)	124(9)	90(7)	-13(7)	-16(6)	49(7)
C111	77(7)	103(8)	87(7)	3(7)	11(6)	35(6)
C121	57(5)	72(6)	71(6)	-10(5)	6(5)	19(5)
C12	58(5)	62(5)	38(4)	1(4)	1(4)	-16(4)
C22	53(4)	50(4)	45(4)	3(4)	1(4)	-6(4)
C32	45(4)	43(4)	38(4)	13(3)	-8(3)	10(3)
C42	52(4)	47(4)	45(4)	6(3)	6(4)	-4(4)
C52	49(4)	55(5)	60(5)	1(4)	-3(4)	0(4)
C62	62(6)	88(7)	127(9)	-33(7)	-8(6)	14(6)
O22	63(3)	56(3)	57(3)	-12(3)	-3(3)	9(3)
O32	53(3)	53(3)	57(3)	-5(3)	-14(2)	11(3)
O42	64(3)	45(3)	46(3)	-1(2)	5(2)	-7(2)
O52	48(3)	72(4)	56(3)	-2(3)	0(3)	-10(3)
C13	89(6)	46(4)	39(4)	-11(3)	9(4)	-12(4)
C23	97(7)	46(5)	42(4)	-13(4)	0(4)	8(5)
C33	76(6)	43(4)	58(5)	-11(4)	-12(4)	4(4)
C43	90(6)	48(5)	46(4)	-14(4)	4(4)	-3(4)
C53	68(5)	45(4)	71(5)	-5(4)	28(4)	-4(4)
C63	90(8)	57(6)	165(11)	-13(7)	62(8)	-3(6)
O23	113(5)	58(4)	80(4)	4(3)	-49(4)	-5(4)
O33	99(5)	64(4)	116(5)	-5(4)	-56(5)	-4(4)
O43	79(4)	37(3)	48(3)	-4(2)	-1(3)	-3(3)
O53	84(4)	61(4)	72(4)	-11(3)	27(3)	-6(3)
O63	63(5)	112(7)	334(17)	-31(9)	10(7)	15(5)
C14	71(5)	44(4)	47(4)	-11(4)	-11(4)	-7(4)
C24	73(6)	45(4)	52(4)	-4(4)	-10(4)	3(4)

C34	76(6)	60(5)	53(5)	-10(4)	5(4)	-9(5)
C44	76(5)	58(5)	42(4)	-15(4)	-9(4)	-15(4)
C54	59(5)	45(4)	56(5)	-11(4)	-7(4)	-5(4)
C64	60(5)	67(6)	81(6)	6(5)	-17(5)	4(5)
O24	74(4)	71(4)	95(5)	2(4)	-12(4)	13(3)
O34	70(4)	95(5)	81(4)	3(4)	11(3)	-4(4)
O44	109(5)	56(3)	42(3)	-1(3)	-18(3)	-5(3)
O54	68(3)	42(3)	46(3)	-5(2)	-2(2)	5(3)
O64	100(5)	70(4)	97(5)	-9(4)	-31(4)	16(4)
C15	120(8)	63(6)	64(6)	0(5)	-25(6)	-4(6)
C25	139(10)	87(7)	71(6)	6(6)	-28(7)	-55(7)
C35	90(6)	91(6)	42(4)	-11(4)	-12(5)	-18(5)
C45	92(7)	75(6)	43(4)	-8(4)	-9(5)	-1(5)
C55	104(7)	83(6)	50(5)	-9(5)	-9(5)	9(6)
C65	97(9)	141(12)	101(9)	-8(9)	-12(8)	28(9)
O25	143(7)	134(6)	79(5)	25(5)	-47(5)	-69(6)
O35	103(6)	165(8)	65(4)	2(4)	-10(4)	-67(6)
O45	71(4)	59(3)	45(3)	7(3)	-12(3)	-10(3)
O55	139(6)	79(4)	55(4)	-11(3)	-18(4)	18(4)
O65	193(14)	192(15)	142(11)	-16(11)	-38(10)	55(12)
O6'5	21(19)	100(30)	30(20)	-23(18)	-6(14)	-29(17)
C16	50(4)	66(5)	45(4)	3(4)	-6(4)	-3(4)
C26	48(4)	74(5)	46(4)	7(4)	-10(4)	-6(4)
C36	48(4)	67(5)	57(5)	6(4)	-11(4)	0(4)
C46	55(4)	50(4)	52(4)	9(4)	-13(4)	10(4)
C56	54(5)	70(5)	43(4)	9(4)	2(4)	1(4)
C66	49(5)	78(6)	54(5)	-3(4)	-2(4)	-3(4)
O26	63(4)	74(4)	66(4)	-3(3)	-13(3)	-14(3)
O36	56(3)	74(4)	73(4)	-16(3)	0(3)	4(3)
O46	61(3)	57(3)	50(3)	2(3)	-16(3)	-5(3)
O56	58(3)	65(4)	57(3)	-4(3)	-15(3)	6(3)
O66	61(3)	80(4)	60(3)	10(3)	-16(3)	-11(3)
C17	56(5)	71(5)	60(5)	25(4)	-9(4)	-13(4)
C27	71(6)	59(5)	52(5)	5(4)	-4(4)	-12(4)
C37	54(5)	64(5)	53(4)	-2(4)	1(4)	0(4)
C47	65(5)	63(5)	39(4)	5(4)	-13(4)	-17(4)
C57	55(5)	69(5)	58(5)	8(4)	-1(4)	5(4)
C67	62(6)	101(8)	99(7)	40(7)	14(6)	9(6)
O27	98(5)	79(4)	66(4)	-1(3)	24(4)	-16(4)
O37	122(6)	64(4)	71(4)	5(3)	39(4)	17(4)
O47	64(3)	41(3)	46(3)	0(2)	-8(3)	1(2)
O57	56(3)	62(3)	67(3)	17(3)	-2(3)	2(3)
O67	110(6)	110(6)	158(8)	16(6)	56(6)	40(5)

Figure 4. Crystal structure of **1** in a unit cell; only part of the water molecules shown.