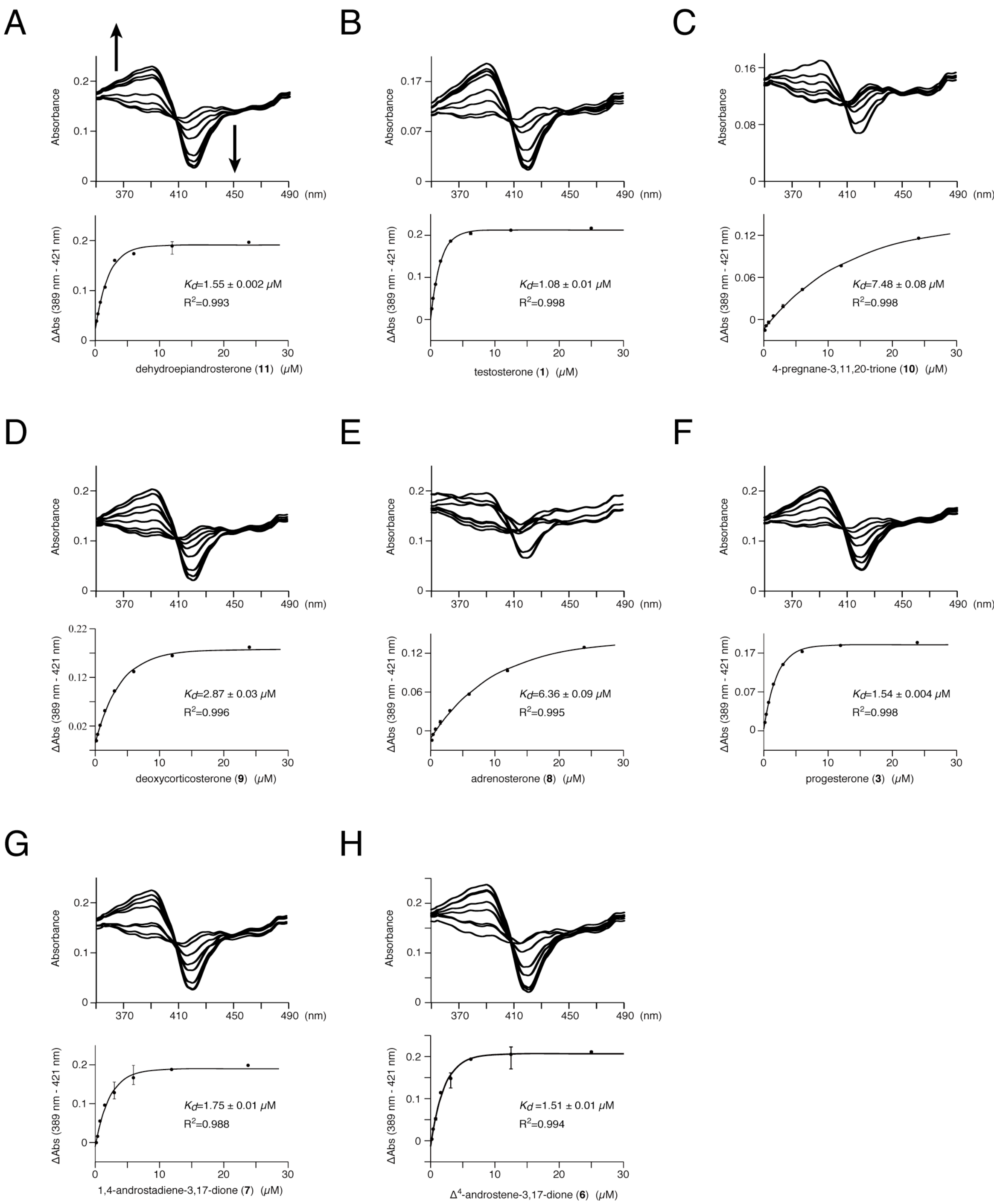

FIGURE S1. Equilibrium dissociation constants between CYP154C3 and the substrates. Each upper panel shows the shift of the spin state of the heme (type I spectral shift) induced by the binding between CYP154C3 and a steroid compound (final concentrations [μM] are 0, 0.195, 0.391, 0.781, 1.56, 3.13, 6.25, 12.5 and 25.0). The shift accompanied by the increasing substrate concentrations is indicated by arrows in panel A as a representative. Each lower panel shows a plot of the peak-to-trough absorbance against the corresponding concentrations of the steroid. The equilibrium dissociation constant (apparent K_d value) was calculated from this plot. Equilibrium dissociation constants between CYP154C3 and dehydroepiandrosterone (**11**) (A), testosterone (**1**) (B), 4-pregnane-3,11,20-trione (**10**) (C), deoxycorticosterone (**9**) (D), adrenosterone (**8**) (E), progesterone (**3**) (F), 1,4-androstadiene-3,17-dione (**7**) (G), and Δ^4-androstene-3,17-dione (**6**) (H) were determined.

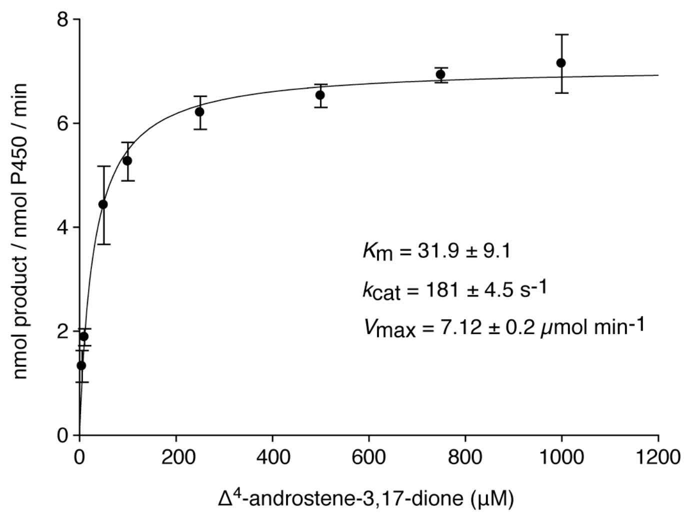

FIGURE S2. Determination of kinetic parameters of the CYP154C3-catalyzed hydroxylation of Δ^4-androstene-3,17-dione (**6**). The vertical and horizontal axes show the initial velocity of the reaction and concentration of the substrate, respectively. Values indicate the mean of four independent experiments with standard deviations.

Table S1. Spectroscopic data of 16α-hydroxytestosterone (in methanol-d_4)[a]. The yield of 16α-hydroxytestosterone was 36.7 mg. HREI-MS: calculated for $C_{19}H_{27}O_3$ $[M-H^+]^-$, 303.19602; found 303.19684.

no.	δ_c, mult.[b]	δ_H (*J* in Hz)	COSY	HMBC[c]	NOESY[d]
1α	36.69, CH_2	1.65, m, 2H	1β, 2α, 2β	2, 9, 10, 19	1β, 2α, 9
1β	36.69, CH_2	2.07, m, 2H	1α, 2β	2, 3, 5	1α, 2α, 2β, 11α, 19
2α	33.82, CH_2	2.34, m, 2H	1α, 2β	10	1α, 1β, 2β
2β	35.82, CH_2	2.47, m, 2H	1α, 1β	1, 3, 4, 10	1β, 2α, 19
3	202.28, C	—	—	—	—
4	124.20, CH	5.69, s, 1H	—	2, 6, 10	6α
5	175.00, C	—	—	—	—
6α	34.69, CH_2	2.34, m, 2H	7α, 6β	8, 10	4, 6β, 9
6β	34.69, CH_2	2.47, m, 2H	6α, 7β	4, 7, 8, 10	6α, 7β, 19
7α	32.82, CH_2	1.00, m, 2H	6α, 6β, 7β, 8β	8	6β, 17α
7β	32.82, CH_2	1.81, m, 2H	6β, 7α,	8	6β, 7α
8	36.38, CH	1.65, m, 1H	9α, 7α, 7β, 14	—	7β, 18, 19
9	55.42, CH	1.00, m, 1H	8, 11β, 11α	8, 10	1α, 14α,
10	40.04, C	—	—	—	—
11α	21.33, CH_2	1.65, m, 2H	11β, 12α	—	1β, 12α, 18, 19
11β	21.33, CH_2	1.48, m, 2H	9α, 11α, 12α, 12β	9, 12, 13	11α, 18, 19
12α	37.72, CH_2	1.17, dt, 2H (13.0, 4.0)	11β, 11α, 12β	13, 14, 17, 18	12β, 17α
12β	37.72, CH_2	1.81, m, 2H	12α	14, 17	11α, 12α, 18
13	44.55, C	—	—	—	—
14	49.51, CH	1.31, ddd, 1H (18.5, 7.5, 3.0)	8β, 15α, 15β	9, 8, 13, 15, 17	9, 15β, 17α
15α	35.08, CH_2	1.79, d, 2H (4)	14α, 15β, 16β	8, 14, 16, 17	15β, 16β
15β	35.08, CH_2	1.81, m, 2H	14α	13, 14, 16, 17	15α
16β	78.60, CH	4.01, dddd, 1H (8.0, 8.0, 5.5, 2.0)	15α, 17α	14, 17	15α, 18
17α	90.36, CH	3.37, d, 1H (6.0)	16β	12, 13, 16, 18,	12α, 14α
18 (CH_3)	12.73, CH_3	0.79, s, 3H	—	12, 13, 14, 17, 18	8, 11β, 12β, 16β, 19
19 (CH_3)	17.69, CH_3	1.22, s, 3H	—	1, 5, 9, 10, 19	1β, 2β, 8, 11β, 18
16-OH	—	—	—	—	—
17-OH	—	—	—	—	—

[a]500 MHz for ^1H NMR and 125.65 MHz for ^{13}C NMR. [b]Numbers of attached protons were determined by analysis of 2D spectra. [c]HMBC correlations are from the started protons to the indicated carbons. [d]NOESY correlations are from the started protons to the indicated protons.

Table S2. Spectroscopic data of 16α-hydroxyprogesterone (in methanol-d_4)[a]. The yield of 16α-hydroxyprogesterone was 67.1 mg. HREI-MS: calculated for $C_{21}H_{29}O_3$ $[M-H^+]^-$, 329.21167; found 329.21189.

no.	δ_c, mult.[b]	δ_H (*J* in Hz)	COSY	HMBC[c]	NOESY[d]
1α	36.81, CH_2	1.71, m, 2H	1β, 2β	2, 9, 10, 19	1β, 2α
1β	36.81, CH_2	2.09, m, 2H	1α	2, 3, 5, 10, 19	2α, 2β、19
2α	33.94, CH_2	2.31, m, 2H	1α	1, 3, 10	1α
2β	33.94, CH_2	2.50, m, 2H	1α, 1β	1, 3, 10	19, 2α
3	202.37, C	—	—	—	—
4	124.41, C	5.72, s, 1H	—	2, 4, 10	6α
5	174.87, C	—	—	—	—
6α	34.82, CH_2	2.28, m, 2H	6β	4, 5, 7, 8, 10	4, 7α
6β	34.82, CH_2	2.47, m, 2H	7α, 7β	4, 5, 7, 8	6α, 7β, 19
7α	32.28, CH_2	1.09, m, 2H	6β, 7β, 8	9	6α, 7β
7β	32.28, CH_2	1.87, m, 2H	7α	4, 8, 9, 14, 15	6α, 6β, 7α
8	36.54, CH	1.64, m, 1H	9	9	19
9	55.10, CH	1.09, m, 1H	8, 11β	7, 8, 10, 11, 14, 19	1α, 14
10	40.10, C	—	—	—	—
11α	21.92, CH_2	1.67, m, 2H	9	12	11β
11β	21.92, CH_2	1.49, dq, 2H (13.0, 3.5)	9, 11α	8, 9, 10, 11, 12	12β, 18
12α	39.92, CH_2	1.59, m, 2H	12β	11, 13, 18	12β
12β	39.92, CH_2	2.02, m, 2H	11β	9, 11, 14, 18	18
13	46.26, C	—	—	—	—
14	55.20, CH	1.60, m, 1H	—	8, 12, 13, 18	9, 17α
15α	36.54, CH_2	1.77, m, 2H	15β, 16β	8, 13, 14	14, 15β, 16β, 18
15β	36.54, CH_2	1.60, m, 2H	15α	8, 13	15α, 18
16β	72.94, CH	4.72, dddd, 1H (7.0, 7.0, 4.2, 1.5)	15α, 17α	14, 16, 17, 20	17α, 15α, 18
17α	74.62, CH	2.56, d, 1H (6.5)	16β	12, 13, 14, 17, 18, 20	14, 16β
18 (CH_3)	14.97, CH_3	0.68, s, 3H	—	12, 13, 14, 17, 18	15β
19 (CH_3)	17.78, CH_3	1.23, s, 3H	—	1, 5, 9, 10, 19	6β
20	210.77, C	—	—	—	—
21 (CH_3)	33.22, CH_3	2.17, s, 3H	—	17, 20, 21	12β, 17α, 18
16-OH	—	—	—	—	—

[a]500 MHz for ^1H NMR and 125.65 MHz for ^{13}C NMR. [b]Numbers of attached protons were determined by analysis of 2D spectra. [c]HMBC correlations are from the started protons to the indicated carbons. [d]NOESY correlations are from the started protons to the indicated protons.

Table S3. Spectroscopic data of 16α-hydroxy-Δ^4-androstene-3,17-dione (in chloroform-d_4)[a]. The yield of 16α-hydroxy-Δ^4-androstene-3,17-dione was 40.2 mg. HREI-MS: calculated for $C_{19}H_{25}O_3$ $[M-H^+]^-$, 301.18037; found 301.18119.

no.	δ_c, mult.[b]	δ_H (*J* in Hz)	gDQCOSY	gHMBC[c]	NOESY[d]
1α	35.80, CH_2	1.71, m, 2H	1β, 2α, 2β	2, 3, 5, 10, 19	1β
1β	35.80, CH_2	2.03, m, 2H	1α, 2α, 2β	1, 2, 3, 5, 10, 19	1α, 2β
2α	34.05, CH_2	2.42, m, 2H	1α, 1β	1, 3,10	—
2β	34.05, CH_2	2.34, m, 2H	1α, 1β	1, 3	1α, 1β
3	199.49, C	—	—	—	—
4	124.42, CH	5.75, s, 1H	—	2, 3, 4, 5, 6, 10	6β
5	170.26, C	—	—	—	—
6α	32.65, CH_2	2.42, m, 2H	7α, 7β	4, 5, 6, 7, 8, 10	6β, 19
6β	32.65, CH_2	2.32, m, 2H	7α, 7β	4, 5, 6, 7, 8, 10	7α
7α	30.56, CH_2	1.92, m, 2H	7β, 6α, 6β	5, 6, 8, 9, 14	9, 14
7β	30.56, CH_2	1.11, dt, 2H (13.0, 4.0)	6α, 6β, 7α, 8	5, 6, 8, 14	7α
8	35.25, CH	1.70, m, 1H	7α, 7β, 9, 14	6, 9, 10, 11, 13	18, 19
9	53.83, CH	1.01, m, 1H	8, 11β	5, 7, 8, 11, 19	14
10	38.78, C	—	—	—	—
11α	31.24, CH_2	1.85, m, 2H	9, 11β, 12α, 12β	9, 12, 13	—
11β	31.24, CH_2	1.37, m, 2H	9, 11α, 12α	9, 11, 12, 13	9, 11α, 12α
12α	20.09, CH_2	1.68, m, 2H	11α, 11β, 12β	11, 14	12β
12β	20.09, CH_2	1.44, m, 2H	11α, 12α	9, 14	12α, 11β, 18
13	47.59, C		—	—	—
14	47.93, CH	1.52, m, 1H	8, 15α, 15β	7, 8, 9, 12, 13, 15, 17, 18	7α, 9
15α	30.71, CH_2	1.89, m, 2H	14, 15β	13, 16, 17	15β
15β	30.71, CH_2	1.99, m, 2H	14, 15α, 16β	8, 13, 14, 15, 16, 17	15α, 16β
16β	71.36, CH	4.38, d, 1H (8.0)	—	14, 15, 17	15β, 18
17	218.92, C	—	—	—	—
18 (CH_3)	14.21, CH_3	1.01, s, 3H	—	10, 12, 14, 17, 18	8
19 (CH_3)	17.55, CH_3	1.21, s, 3H	—	1, 5, 9, 10, 19	—
16-OH	—	—	—	—	—
17-OH	—	—	—	—	—

[a]500 MHz for ^{1}H NMR and 125.65 MHz for ^{13}C NMR. [b]Numbers of attached protons were determined by analysis of 2D spectra. [c]gHMBC correlations are from the started protons to the indicated carbons. [d]NOESY correlations are from the started protons to the indicated protons.

Table S4. Spectroscopic data of 16α-hydroxyadrenosterone (in methanol-d_4)[a]. The yield of 16α- hydroxyadrenosterone was 21.4 mg. HREI-MS: calculated for $C_{19}H_{24}O_3$ $[M-H^+]^-$, 315.15963; found 315.16045.

no.	δc, mult.[b]	δH (*J* in Hz)	COSY	HMBC[c]	NOESY[d]
1α	34.59, CH_2	2.52, m, 2H	1β	3	1β
1β	34.59, CH_2	2.24, m, 2H	1α, 2β	—	—
2α	33.51, CH_2	2.31, m, 2H	2β	—	—
2β	33.51, CH_2	2.49, m, 2H	1β, 2α	3	1β, 2α
3	202.53, C	—	—	—	—
4	125.05, CH	5.73, s, 1H	—	4, 6	6β
5	172.52, C	—	—	—	—
6α	33.31, CH_2	2.37, m, 2H	6β, 7α, 7β	—	6β, 7α
6β	33.31, CH_2	2.53, m, 2H	6α, 7α, 7β	4, 5, 7, 8	6α, 19
7α	31.95, CH_2	2.10, m, 2H	6α, 6α, 7β	5, 6, 9, 14	7β
7β	31.95, CH_2	1.32, m, 2H	6α, 6β, 7α	—	1, 7α, 15β
8	35.62, CH	2.72, m, 1H	9, 14	13	19
9	64.22, CH	2.19, m, 1H	8	11, 14, 19	—
10	35.69, C	—	—	—	—
11	209.89, C	—	—	—	—
12α	51.47, CH_2	2.50, m, 2H	—	11, 12, 18	12β
12β	51.47, CH_2	2.31, m, 2H	—	9, 11, 17, 18	12α, 18
13	39.82, C	—	—	—	—
14	37.69, CH	2.18, m, 1H	8	13, 15, 18	—
15α	32.47, CH_2	1.94, m, 2H	15β, 16β	16, 17	15β
15β	32.47, CH_2	2.19, m, 2H	15α, 16β	—	7β, 15α, 18
16β	72.57, CH	4.40, d, 1H (8.0)	15α, 15β	15, 17	15β, 18
17	217.59, C	—	—	—	—
18 (CH_3)	15.53, CH_3	0.91, s, 3H	—	12, 17, 18	15β
19 (CH_3)	17.79, CH_3	1.45, s, 3H	—	5, 9, 10, 19	—
16-OH	72.57, CH	—	—	—	—

[a]500 MHz for ^1H NMR and 125.65 MHz for ^{13}C NMR. [b]Numbers of attached protons were determined by analysis of 2D spectra. [c]HMBC correlations are from the started protons to the indicated carbons. [d]NOESY correlations are from the started protons to the indicated protons.

Table S5. Spectroscopic data of 16α-hydroxy-1,4-androstadione-3,17-dione (in chloroform-d_4)[a]. The yield of 16α-hydroxy-1,4-androstadione-3,17-dione was 38.0 mg. HREI-MS: calculated for $C_{19}H_{23}O_3$ $[M\text{-}H^+]^-$, 229.16472; found 229.16450.

no.	δ_c, mult.[b]	δ_H (J in Hz)	gDQCOSY	gHMBC[c]	NOESY[d]
1	155.24, CH	7.04, d, 1H (10.0)	2	1, 2, 3, 5, 9, 10, 19	2, 11α 19
2	128.01, CH	6.25, dd, 1H (10.5, 2.5)	1	2, 4, 10	1
3	186.36, C	—	—	—	—
4	124.43, CH	6.09, s, 1H	—	2, 6, 10	6α
5	168.20, C	—	—	—	—
6α	32.65, CH_2	2.42, m, 2H	7α, 7β	4, 5, 7, 8, 10	4, 6β, 7α
6β	32.65, CH_2	2.50, dt, 2H (13.5, 5.0)	7α, 7β	4, 5, 7, 8, 10	6α, 19
7α	32.14, CH_2	2.03, m, 2H	6α, 6β, 7β, 8	5, 6, 8, 9	6α, 7β
7β	32.14, CH_2	1.13, m, 2H	6α, 6β, 7α	5, 8, 9, 14	7α, 18
8	35.22, CH	1.80, dt, 1H (11.5, 4.0)	7α, 9, 14	6, 9, 14	18, 19
9	52.24, CH	1.13, m, 1H	8, 11α, 11β	1, 8, 10, 11, 14, 19	14
10	43.53, C	—	—	—	—
11α	21.89, CH_2	1.86, m, 2H	9, 11β, 12α	8, 9, 10	1, 11β
11β	21.89, CH_2	1.69, m, 2H	12α, 12β, 11α	8, 9, 10, 13	11α, 18, 19
12α	31.18, CH_2	1.39, dt, 2H (13.0, 2.0)	11α, 11β, 12β	9, 11, 13, 17, 18	12β
12β	31.18, CH_2	1.86, m, 2H	11β, 12α	11, 14, 18	12α, 18
13	47.77, C	—	—	—	—
14	47.56, CH	1.52, ddd, 1H (13.0, 11.5, 7.0)	8, 15α, 15β	8, 9, 12, 13, 17, 18	7α, 9, 15α
15α	30.87, CH_2	1.88, m, 2H	14, 15β	13, 14, 16, 17	14, 18
15β	30.87, CH_2	2.01, m, 2H	14, 15α	14, 16, 17	15α, 16β
16β	71.25, CH	4.39, d, 1H	15α, 15β	14, 15, 16, 17, 18	15β, 18
17	218.49, C	—	—	—	—
18 (CH_3)	14.31, CH_3	1.04, s, 3H	—	12, 13, 14, 17	8, 11β, 15β, 16β
19 (CH_3)	18.94, CH_3	1.25, s, 3H	—	1, 5, 9, 10	1, 6β, 8, 11β
16-OH	—	—	—	—	—

[a]500 MHz for ^{1}H NMR and 125.65 MHz for ^{13}C NMR. [b]Numbers of attached protons were determined by analysis of 2D spectra. [c]gHMBC correlations are from the started protons to the indicated carbons. [d]NOESY correlations are from the started protons to the indicated protons.

Table S6. Spectroscopic data of 16α-hydroxydehydroepiandrosterone (in chloroform-d_4)[a]. The yield of 16α-hydroxydehydroepiandrosterone was 38.0 mg. HREI-MS: calculated for $C_{19}H_{27}O_3$ $[M-H^+]^-$, 303.19602; found 303.19484.

no.	δc, mult.[b]	δH (*J* in Hz)	COSY	HMBC[c]	NOESY[d]
1α	37.28, CH_2	1.10, m, 2H	2α, 2β	2, 3, 9, 10, 19	2α
1β	37.28, CH_2	1.86, m, 2H	2β	2, 3, 5, 9	1α, 2β
2α	31.40, CH_2	1.83, m, 2H	1β	3, 10	—
2β	31.40, CH_2	1.50, m, 2H	1α	1	19
3β	71.78, CH	3.54, ddt, 1H (11.5, 4.5, 4.5)	2α, 2β, 4α, 4β	—	1β, 4β
4α	42.34, CH_2	2.25, m, 2H	4β	2, 3, 5, 6	4β, 19
4β	42.34, CH_2	2.33, m, 2H	4α	2, 3, 5, 6	4α, 6
5	141.07, C	—	—	—	—
6	121.07, C	5.38, m, 1H	7α, 7β	6, 7, 8, 10, 14	4β, 7α, 7β
7α	30.78, CH_2	1.65, m, 2H	—	4, 5, 6, 9	6, 14
7β	30.78, CH_2	2.08, m, 2H	8	5, 6, 9	6, 8
8	31.69, CH	1.65, m, 1H	7β, 9, 11α	6, 7	7β, 18, 19
9	50.30, CH	1.02, m, 1H	1α, 8, 11β	—	—
10	36.80, C	—	—	—	—
11α	20.16, CH_2	1.49, m, 2H	9, 11β, 12α, 12β	12, 13	9, 18, 11β, 12β
11β	20.16, CH_2	1.67, m, 2H	9, 11α, 12α, 12β	9, 11	11β, 12α, 12β, 19
12α	31.40, CH_2	1.39, dt, 2H (13.0, 4.0)	11α, 11β, 12β	11, 12, 13, 18	12β
12β	31.40, CH_2	1.85, m, 2H	11α, 11β, 12α	9, 12, 13, 14	11β, 12α, 18
13	47.65, C	—	—	—	—
14	48.78, CH	1.51, m, 1H	8, 15α, 15β	9, 16, 18	—
15α	30.58, CH_2	1.89, m, 2H	14, 15β	13, 14, 16, 17	15β
15β	30.58, CH_2	1.97, m, 2H	14, 15α	13, 14, 16,	14, 15α, 16β, 18
16β	71.50, CH	4.39, dd, 1H (8.0, 1.0)	15α, 15β	14, 15, 16, 17	15β, 18
17	129.60, C	—	—	—	—
18 (CH_3)	19.65, C	0.99, s, 3H	—	12, 13, 14, 17	8
19 (CH_3)	14.09, C	1.04, s, 3H	—	1, 5, 9, 10, 19	2β, 4α, 8, 11β
3 (OH)	—	—	—	—	—
16 (OH)	—	—	—	—	—

[a]500 MHz for ^1H NMR and 125.65 MHz for ^{13}C NMR. [b]Numbers of attached protons were determined by analysis of 2D spectra. [c]HMBC correlations are from the started protons to the indicated carbons. [d]NOESY correlations are from the started protons to the indicated protons.

Table S7. Spectroscopic data of 16α-hydroxy-4-pregnane-3,11,20-trione. (in chloroform-d_4)[a]. Yield of 16α-hydroxy-4-pregnane-3,11,20-trione was 32.0 mg. HREI-MS: calculated for $C_{21}H_{27}O_4$ $[M-H^+]^-$, 343.19093; found 343.19125.

no.	δ_c, mult.[b]	δ_H (*J* in Hz)	COSY	HMBC[c]	NOESY[d]
1α	34.90, CH_2	1.66, dt, 2H (14.5, 4.5)	1β, 2α, 2β	2, 9, 10, 19	1β
1β	34.90, CH_2	2.78, m, 2H	1α, 2α, 2β	3, 5	1α, 19
2α	33.83, CH_2	2.33, m, 2H	1α, 1β, 2β	4	2β
2β	33.83, CH_2	2.49, m, 2H	1α, 1β, 2α	1, 3	2α, 19
3	200.24, C	—	—	—	—
4	124.89, CH	5.76, s, 1H	—	2, 4, 6, 10	6β
5	168.83, C	—	—	—	—
6α	32.34, CH_2	2.43, m, 2H	6β, 7α, 7β	4, 5, 7	6β
6β	32.34, CH_2	2.33, m, 2H	6α, 7β	—	6α
7α	32.17, CH_2	1.96, m, 2H	6α, 6β, 7β	—	—
7β	32.17, CH_2	1.31, m, 2H	6α, 6β, 7α, 8	—	9
8	36.90, CH	1.89, m, 1H	9	—	19
9	63.20, CH	1.96, m, 1H	8	1, 7, 8, 9, 10, 11, 19	7β
10	38.43, C	—	—	—	—
11	207.58, C	—	—	—	—
12α	56.81, CH_2	2.63, s, 2H	—	9, 11, 13, 14, 17, 18	17α, 19
12β	56.81, CH_2	2.63, s, 2H	—	11	21
13	47.33, C	—	—	—	—
14	52.99, CH	2.18, m, 1H	15α, 15β	13, 17, 18	12α, 17α
15α	34.90, CH_2	1.80, m, 2H	14	13, 16	—
15β	34.90, CH_2	1.87, m, 2H	14, 16β	—	16β, 18
16β	71.98, CH	4.90, dddd, 1H (9.0, 9.0, 7.0, 2.5)	15β, 17α	14, 20	15β, 18, 21
17α	72.18, CH	2.74, d, 1H (6.5)	16β,	12, 13, 16, 17, 18, 20	12α, 21
18 (CH_3)	15.58, CH_3	0.63, s, 3H	—	12, 13, 14, 17, 18	12, 15β, 16β, 20
19 (CH_3)	17.34, CH_3	1.41, s, 3H	—	1, 5, 9, 10, 19	—
20	207.17, C	—	—	—	—
21 (CH_3)	31.71, CH_3	2.18, s, 3H	—	11, 21	12β, 17α, 18
16 (OH)	—	—	—	—	—

[a]500 MHz for ^1H NMR and 125.65 MHz for ^{13}C NMR. [b]Numbers of attached protons were determined by analysis of 2D spectra. [c]HMBC correlations are from the started protons to the indicated carbons. [d]NOESY correlations are from the started protons to the indicated protons.

Table S8. Spectroscopic data of 16α-hydroxydeoxycorcosterone (in mMethanol-d_4)[a]. The yield of 16α-hydroxydeoxycorticosterone was 51.9 mg. HREI-MS: calculated for $C_{21}H_{29}O_4$ $[M-H^+]^-$, 345.20658; found 345.20544.

no.	δ_c, mult.[b]	δ_H (*J* in Hz)	COSY	HMBC[c]	NOESY[d]
1α	36.28, CH_2	1.62, m, 2H	2α	2, 10	2α, 11β
1β	36.28, CH_2	1.71, dt, 2H (14.5, 4.5)	2β	3, 9, 10, 19	2β
2α	36.02, CH_2	1.81, m, 2H	1α	1, 2	1α
2β	36.02, CH_2	2.07, m, 2H	1β	3, 10, 19	1β, 19
3	201.95, C	—	—	—	—
4	123.98, CH	5.71, s, 1H	—	4, 6, 7, 10, 19	6β
5	174.41, C	—	—	—	—
6α	34.39, CH_2	2.46, m, 2H	6β, 9	4, 8, 10	—
6β	34.39, CH_2	2.29, m, 2H	6α	4, 10	7α
7α	33.49, CH_2	2.47, m, 2H	7β	5, 7, 8, 9	6β
7β	33.49, CH_2	2.29, m, 2H	7α, 15β	5, 8	—
8	36.28, CH_2	1.57, m, 1H	—	13	15β
9	54.83, CH	1.06, m, 2H	11α, 11β	10, 11	—
10	39.67, C	—	—	—	—
11α	21.42, CH_2	1.63, m, 2H	9, 11β, 12α	9, 11, 12	9
11β	21.42, CH_2	1.48, m, 2H	9, 11α, 18	8, 9, 11, 12	1α, 18, 19
12α	39.25, CH_2	1.50, m, 2H	11α, 12β	11, 13, 14, 17, 18	12β, 17α
12β	39.25, CH_2	1.85, m, 2H	11α, 12α	9, 11, 12, 13, 14, 18	12α, 18
13	46.22, C	—	—	—	—
14	54.75, CH	1.58, m, 1H	—	8, 12,13, 17, 18	17α
15α	32.84, CH_2	1.85, m, 2H	15β	13, 14, 16	—
15β	32.84, CH_2	1.06, m, 2H	15α, 7β	14	—
16β	72.98, CH	4.74, dddd, 1H (7.0, 7.0, 3.5, 1.5)	15α, 17α	14, 16, 17, 20	18, 15β
17α	69.53, CH	2.48, m, 2H	—	12, 13, 15, 16, 17, 18, 21	14, 12α
18 (CH_3)	14.68, CH_3	0.71, s, 3H	11β	12, 13, 14, 17, 18	11β, 12β
19 (CH_3)	17.33, CH_3	1.21, s, 3H	—	1, 5, 9, 10, 19	2β, 11β
20	210.54, CH	—	—	—	
21(CH_2)	70.34, CH_2	4.20, dd, 2H (20.5, 19.0)	—	20	12β, 18, 17α
16 (OH)	—	—	—	—	—
21 (OH)	—	—	—	—	—

[a]500 MHz for ^{1}H NMR and 125.65 MHz for ^{13}C NMR. [b]Numbers of attached protons were determined by analysis of 2D spectra. [c]HMBC correlations are from the started protons to the indicated carbons. [d]NOESY correlations are from the started protons to the indicated protons.