

III. Röntgenstrukturanalytische Daten und Kreuzpeakprotokolle

1. Allgemeine Anmerkungen

Bei ^1H - ^1H -NOESY-Messungen und ^1H - ^1H -COSY-Messungen sind Kreuzpeaks zwischen Signalen, deren Verschiebungen sich um weniger als $\Delta\delta = 0.10$ ppm unterscheiden, nicht eindeutig bestimmbar. Deshalb wird in den Kreuzpeakprotokollen im allgemeinen auf entsprechende Zuordnungen verzichtet.

2. Röntgenstrukturanalytische Daten

(*IR**, *4aR**, *10aS**)-2,4,4a,9,10,10a-Hexahydro-1-hydroxy-phenanthren-3-on (42)

Summenformel	$\text{C}_{14}\text{H}_{16}\text{O}_2$
Formelgewicht	216.27
Kristallgröße [mm]	ca. 0.66*0.26*0.21
Meßtemperatur [K]	150
Kristallsystem	monoklin
Raumgruppe	$\text{P}2_1/\text{c}$
a [Å]	17.346(2)
b [Å]	5.179(1)
c [Å]	12.404(1)
β [°]	98.22(1)
V [Å ³]	1102.86
Z	4
$\mu(\text{MoK}_\alpha)$ [mm ⁻¹]	0.09
D_x [gcm ⁻³]	1.303
Meßgerät	Siemens P4RA-Vierkreisdiffraktometer, (Drehanodengenerator, Graphitmonochromator, Szintillationszähler, $\lambda = 0.71073$ Å (MoK $_\alpha$))
Meßmethode	ω -Scan
Absorptionskorrektur	nicht erforderlich
Transmissionsbereich	0.984 - 0.961
Meßbereich	$4^\circ < 2\Theta < 54^\circ$ (+h,+k, \pm l)

Meßgeschwindigkeit	intensitätsabhängig (8 bis 29 °min ⁻¹)
Strukturlösung	SHELXTL PLUS (direkte Methoden), H-Atome berechnet
Verfeinerung	Kleinste Quadrate (volle Matrix), alle Schweratome anisotrop, H-Atome berechnet und gruppenweise mit gemeinsamen isotropen Temperaturfaktoren verfeinert, ein Skalierungsfaktor, ein isotroper Extinktionsparameter
Gewichtsschema	$w = [\sigma^2(F_o) + (0.01 * F_o)^2]^{-1}$
Zahl der symmetrie-unabhängigen Reflexe	2412, davon 2025 beobachtet ($I > 2 * \sigma(I)$)
Zahl der Variablen	147
$R = (\sum F_o - F_c) / \sum F_o $	0.0370
$R_w = [\sum w(F_o - F_c)^2 / \sum w F_o^2]^{1/2}$	0.0452

Atomkoordinaten und Koeffizienten der äquivalenten isotropen Temperaturfaktoren (ohne H-Atome)

Atom	x	y	z	U
3-O	1.0146(1)	-0.1424(2)	0.3336(1)	0.023(1)
1-O	1.1274(1)	0.0708(2)	0.5885(1)	0.025(1)
C-4b	1.2929(1)	-0.0402(3)	0.3694(1)	0.019(1)
C-5	1.3031(1)	-0.2217(3)	0.2891(1)	0.023(1)
C-6	1.3751(1)	-0.2611(3)	0.2557(1)	0.027(1)
C-7	1.4387(1)	-0.1165(3)	0.3019(1)	0.029(1)
C-8	1.4296(1)	0.0626(3)	0.3815(1)	0.028(1)
C-8a	1.3576(1)	0.1031(3)	0.4173(1)	0.022(1)
C-9	1.3524(1)	0.3025(3)	0.5052(1)	0.025(1)
C-10	1.2771(1)	0.2835(3)	0.5552(1)	0.026(1)
C-10a	1.2074(1)	0.2519(3)	0.4662(1)	0.019(1)
C-4a	1.2132(1)	-0.0052(2)	0.4067(1)	0.018(1)
C-4	1.1449(1)	-0.0291(3)	0.3125(1)	0.021(1)
C-3	1.0679(1)	0.0132(3)	0.3529(1)	0.018(1)
C-2	1.0611(1)	0.2532(3)	0.4187(1)	0.021(1)
C-1	1.1302(1)	0.2734(3)	0.5107(1)	0.021(1)

Abstände und Winkel

Abstände [Å]		Winkel [°]	
1-O...3-O'	2.796(2)	1-O - H(1-O) - 3-O'	173.2
H(1-O)...3-O'	1.950	C-5 - C-4b - C-8a	118.8(1)
C-4b - C-5	1.399(2)	C-5 - C-4b - C-4a	120.4(1)
C-4b - C-8a	1.404(2)	C-8a - C-4b - C-4a	120.8(1)
C-4b - C-4a	1.531(2)	C-4b - C-5 - C-6	121.5(1)
C-5 - C-6	1.386(2)	C-5 - C-6 - C-7	119.6(1)
C-6 - C-7	1.387(2)	C-6 - C-7 - C-8	119.5(1)
C-7 - C-8	1.380(2)	C-7 - C-8 - C-8a	121.7(1)
C-8 - C-8a	1.401(2)	C-4b - C-8a - C-8	118.8(1)
C-8a - C-9	1.514(2)	C-4b - C-8a - C-9	122.6(1)
C-9 - C-10	1.527(2)	C-8 - C-8a - C-9	118.6(1)
C-10 - C-10	1.525(2)	C-8a - C-9 - C-10	113.0(1)
C-10a - C-4a	1.533(2)	C-9 - C-10 - C-10a	110.4(1)
C-10a - C-1	1.523(2)	C-10 - C-10a - C-4a	110.0(1)
C-4a - C-4	1.545(2)	C-10 - C-10a - C-1	112.2(1)
C-4 - C-3	1.508(2)	C-4a - C-10a - C-1	111.0(1)
C-3 - C-2	1.501(2)	C-4b - C-4a - C-10a	111.8(1)
C-3 - 3-O	1.224(2)	C-4b - C-4a - C-4	112.9(1)
C-2 - C-1	1.535(2)	C-10a - C-4a - C-4	109.8(1)
C-1 - 1-O	1.432(2)		

Koeffizienten der anisotropen Temperaturfaktoren

Atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
3-O	0.023(1)	0.022(1)	0.023(1)	-0.002(1)	0.003(1)	-0.001(1)
1-O	0.023(1)	0.033(1)	0.021(1)	0.003(1)	0.006(1)	0.003(1)
C-4b	0.021(1)	0.018(1)	0.018(1)	0.002(1)	0.003(1)	0.005(1)
C-5	0.023(1)	0.023(1)	0.023(1)	0.000(1)	0.004(1)	0.000(1)
C-6	0.028(1)	0.028(1)	0.026(1)	0.004(1)	0.007(1)	-0.001(1)
C-7	0.021(1)	0.036(1)	0.032(1)	0.003(1)	0.009(1)	0.003(1)
C-8	0.021(1)	0.032(1)	0.029(1)	-0.003(1)	0.001(1)	0.003(1)
C-8a	0.023(1)	0.022(1)	0.020(1)	0.001(1)	0.002(1)	0.004(1)

Atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C-9	0.022(1)	0.028(1)	0.024(1)	-0.002(1)	-0.002(1)	-0.001(1)
C-10	0.025(1)	0.031(1)	0.020(1)	-0.001(1)	-0.001(1)	-0.005(1)
C-10a	0.022(1)	0.018(1)	0.018(1)	0.000(1)	0.001(1)	-0.001(1)
C-4a	0.020(1)	0.017(1)	0.017(1)	0.000(1)	0.003(1)	0.001(1)
C-4	0.022(1)	0.022(1)	0.019(1)	0.000(1)	0.003(1)	-0.004(1)
C-3	0.022(1)	0.019(1)	0.013(1)	0.003(1)	-0.001(1)	0.004(1)
C-2	0.022(1)	0.019(1)	0.022(1)	0.003(1)	0.002(1)	0.000(1)
C-1	0.024(1)	0.018(1)	0.019(1)	0.001(1)	0.003(1)	-0.003(1)

Parameter der H-Atome

Atom	x	y	z	U
OH	1.0852	0.0819	0.6157	0.029(1)
5-H	1.2591	-0.3203	0.2560	0.029(1)
6-H	1.3814	-0.3891	0.2017	0.029(1)
7-H	1.4885	-0.1397	0.2782	0.029(1)
8-H	1.4738	0.1616	0.4136	0.029(1)
9-H _A	1.3552	0.4715	0.4742	0.029(1)
9-H _B	1.3963	0.2830	0.5612	0.029(1)
10-H _A	1.2705	0.4356	0.5972	0.029(1)
10-H _B	1.2801	0.1370	0.6030	0.029(1)
10a-H	1.2097	0.3880	0.4142	0.029(1)
4a-H	1.2070	-0.1406	0.4577	0.029(1)
4-H _A	1.1454	-0.1967	0.2796	0.029(1)
4-H _B	1.1512	0.0980	0.2581	0.029(1)
2-H _A	1.0133	0.2486	0.4491	0.029(1)
2-H _B	1.0600	0.4016	0.3722	0.029(1)
1-H	1.1281	0.4369	0.5466	0.029(1)

3. Kreuzpeakprotokolle

(4aR*,10aR*)-4a,9,10,10a-Tetrahydro-phenanthren-3(4H)-on (*trans*-17a)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	199.49	s	-
B	155.23	d	6.94 (e)
C	137.45	s	-
D	135.92	s	-
E	129.65	d	6.10 (f)
F	129.31	d	7.11-7.20 (a, b, c, d)
G	126.56	d	7.11-7.20 (a, b, c, d)
H	126.15	d	7.11-7.20 (a, b, c, d)
I	124.65	d	7.11-7.20 (a, b, c, d)
J	42.52	t	2.37 (l); 3.24 (g)
K	41.28	d	2.99-3.13 (h, i, j)
L	39.29	d	2.46 (k)
M	29.50	t	2.99-3.13 (h, i, j)
N	28.32	t	1.72 (n); 2.19 (m)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY
a, b, c, d	7.11-7.20	
e	6.94	f; k
f	6.10	e; k
g	3.24	h, i, j; l
h, i, j	2.99-3.13	g; k; l; m; n
k	2.46	e; f; h, i, j; m; n
l	2.37	g; h, i, j
m	2.19	h, i, j; k; n
n	1.72	h, i, j; k; m

(4aR*,10aS*)-4a,9,10,10a-Tetrahydro-phenanthren-3(4H)-on (cis-17a)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	199.03	s	-
B	153.24	d	7.02 (e)
C	138.18	s	-
D	135.33	s	-
E	129.22	d	7.12-7.20 (a, b, c, d)
F	128.86	d	6.06 (f)
G	128.64	d	7.12-7.20 (a, b, c, d)
H	126.50	d	7.12-7.20 (a, b, c, d)
I	126.33	d	7.12-7.20 (a, b, c, d)
J	43.29	t	2.63 (k, l)
K	37.18	d	3.46 (g)
L	35.45	d	2.72 (j)
M	29.58	t	2.93 (h, i)
N	23.43	t	1.99 (m); 1.83 (n)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a, b, c, d	7.12-7.20		g; h, i; k, l
e	7.02	f; j	f; j; m
f	6.06	e; j; k, l	e
g	3.46	j; k, l	a, b, c, d; j; k, l
h, i	2.93	m; n	a, b, c, d; j; m; n
j	2.72	e; f; g; m; n	e; g; h, i; m
k, l	2.63	g; f	a, b, c, d; g; n
m	1.99	h, i; j; n	e; h, i; j; n
n	1.83	h, i; j; m	h, i; k, l; m

(4aR*,10aR*)-4a,9,10,10a-Tetrahydro-2-methyl-phenanthren-3(4H)-on (trans-17b)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	199.70	s	-
B	150.51	d	6.69 (e)
C	137.67	s	-
D	136.02	s	-
E	135.76	s	-
F	129.33	d	7.12-7.22 (a, b, c, d)
G	126.49	d	7.12-7.22 (a, b, c, d)
H	126.11	d	7.12-7.22 (a, b, c, d)
I	124.78	d	7.12-7.22 (a, b, c, d)
J	42.65	t	3.37 (f); 2.37 (k)
K	41.63	d	2.95-3.09 (g, h, i)
L	39.48	d	2.45 (j)
M	29.52	t	2.95-3.09 (g, h, i)
N	28.61	t	1.71 (p); 2.15 (l)
O	15.72	q	1.84 (m, n, o)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a, b, c, d	7.12-7.22		f; g, h, i
e	6.69	j; m, n, o	j; l; m, n, o; p
f	3.37	g, h, i; k	a, b, c, d; g, h, i; k
g, h, i	2.95-3.09	f; j; k; l; p	a, b, c, d; f; j; k; l; p
j	2.45	e; g, h, i; l; m, n, o; p	e; g, h, i; l
k	2.37	f; g, h, i	f; g, h, i
l	2.15	g, h, i; j; p	e; g, h, i; j; p
m, n, o	1.84	e; j	e
p	1.71	g, h, i; j; l	e; g, h, i; l

(4aR*,10aR*)-4a,9,10,10a-Tetrahydro-10a-methyl-phenanthren-3(4H)-on (trans-17c)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	199.52	s	-
B	160.98	d	6.91 (e)
C	136.76	s	-
D	135.22	s	-
E	128.98	d	7.11-7.20 (a, b, c, d)
F	127.24	d	5.99 (f)
G	126.40	d	7.11-7.20 (a, b, c, d)
H	126.10	d	7.11-7.20 (a, b, c, d)
I	124.51	d	7.11-7.20 (a, b, c, d)
J	42.97	d	3.29 (g)
K	37.23	t	3.10 (h); 2.52 (k)
L	35.27	s	-
M	34.56	t	1.89 (l, m)
N	25.74	t	3.01 (i, j)
O	17.12	q	n, o, p (0.96)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a, b, c, d	7.11-7.20		g; h; i, j; k
e	6.91	f	f; l, m; n, o, p
f	5.99	e	e
g	3.29	h; k	a, b, c, d; h; k; l, m; n, o, p
h	3.10	g; k	a, b, c, d; g; k
i, j	3.01	l, m	a, b, c, d; l, m; n, o, p
k	2.52	g; h	a, b, c, d; g; h; n, o, p
l, m	1.89	i, j	e; g; i, j; n, o, p
n, o, p	0.96	-	e; g; i, j; k; l, m

(4aR*,10aS*)-4a,9,10,10a-Tetrahydro-10a-methyl-phenanthren-3(4H)-on (cis-17c)

Messungen in CDCl₃*)

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	199.36	s	-
B	159.10	d	6.73 (e)
C	137.85	s	-
D	134.20	s	-
E	129.16	d	[7.10-7.20] (a, b, c, d)
F	129.15	d	[7.10-7.20] (a, b, c, d)
G	127.02	d	5.96 (f)
H	126.37	d	[7.10-7.20] (a, b, c, d)
I	126.10	d	[7.10-7.20] (a, b, c, d)
J	44.10	t	2.66 (j); 2.54 (k)
K	43.78	d	[2.95-3.07] (g)
L	35.04	s	-
M	28.58	t	[1.84-1.96] (l); 1.67 (m)
N	25.79	t	[2.87-2.92] (h, i)
O	24.37	q	1.16 (n, o, p)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY
a, b, c, d	[7.10-7.20]	
e	6.73	f
f	5.96	e
g	[2.95-3.07]	j; k
h, i	[2.87-2.92]	l; m
j	2.66	g; k
k	2.54	g; j
l	[1.84-1.96]	h, i; m
m	1.67	h, i; l
n, o, p	1.16	-

*) Messungen erfolgen im Gemisch mit dem *trans*-Diastereoisomer. Die Verschiebungswerte in eckigen Klammern sind von den Signalen des *trans*-Diastereoisomers überlagert.

(4aR*,10aS*)-4,9,10,10a-Tetrahydro-4a-methyl-phenanthren-3-on (*trans*-17d)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	199.41	s	-
B	153.31	d	6.78 (e)
C	144.52	s	-
D	134.44	s	-
E	129.69	d	7.11-7.21 (a, b, c, d)
F	129.31	d	6.12 (f)
G	126.38	d	7.11-7.21 (a, b, c, d)
H	126.18	d	7.11-7.21 (a, b, c, d)
I	123.97	d	7.11-7.21 (a, b, c, d)
J	51.17	t	3.12 (g); 2.53 (k)
K	42.23	d	2.82 (j)
L	40.39	s	-
M	28.94	t	3.02 (h, i)
N	23.49	t	2.04 (l); 1.95 (m)
O	22.82	q	1.15 (n, o, p)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a, b, c, d	7.11-7.21		g; h, i; k; n, o, p
e	6.78	f; j	f; j; l; m; n, o, p
f	6.12	e; j; g	e; n, o, p
g	3.12	k; f	a, b, c, d; k; n, o, p
h, i	3.02	l; m	a, b, c, d; j; l; m
j	2.82	e; f; l; m	e; h, i; k; l; m
k	2.53	g; n, o, p	a, b, c, d; g; j
l	2.04	h, i; j; m	e; h, i; j; m
m	1.95	h, i; j; l	e; h, i; j; l; n, o, p
n, o, p	1.15	k	a, b, c, d; e; f; g; m

(4aR*,10aR*)-4,9,10,10a-Tetrahydro-4a-methyl-phenanthren-3-on (cis-17d)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	198.89	s	-
B	152.36	d	6.87 (e)
C	141.87	s	-
D	134.76	s	-
E	129.17	d	7.06 (d)
F	128.99	d	5.99 (f)
G	126.68	d	7.28 (a)
H	126.56	d	7.18 (b)
I	126.13	d	7.11 (c)
J	50.05	t	2.88 (g); 2.57 (k)
K	43.43	d	2.60 (j)
L	39.38	s	-
M	29.45	q	1.42 (n, o, p)
N	28.81	t	2.85 (h, i)
O	24.34	t	2.13 (l); 1.88 (m)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY
a	7.28	b
b	7.18	a, c
c	7.11	c, d
d	7.06	c
e	6.87	f; j
f	5.99	e; j
g	2.88	k
h, i	2.85	l; m
j	2.60	e; f; l; m
k	2.57	g
l	2.13	h, i; j; m
m	1.88	h, i; j; l
n, o, p	1.42	-

(4aR*,10aS*)-4a,9,10,10a-Tetrahydro-phenanthren-1(4H)-on (*trans*-18a)

a) Messungen in CDCl₃^{*)}

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	200.55	s	-
B	148.50	d	7.08 (e)
C	137.80	s	-
D	136.69	s	-
E	129.76	d	6.15 (f)
F	129.35	d	7.11-7.22 (b, c, d)
G	126.40	d	7.11-7.22 (b, c, d)
H	126.09	d	7.11-7.22 (b, c, d)
I	125.62	d	7.27 (a)
J	48.91	d	2.36 (m)
K	39.76	d	3.09-3.18 (g, h)
L	32.47	t	3.09-3.18 (g, h); 2.42 (l)
M	29.18	t	2.90 (i, j)
N	21.54	t	2.54 (k); 1.59 (n)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a	7.27	b, c, d	b, c, d; g, h; l
b, c, d	7.11-7.22	a	a; i, j
e	7.08	f; g, h; l	f; g, h; l
f	6.15	e; g, h; l	e
g, h	3.09-3.18	e; f; l; m	a; e; l; m; n
i, j	2.90	k; n	b, c, d; k; m; n
k	2.54	i, j; m; n	i, j; m; n
l	2.42	e; f; g, h	a; e; g, h
m	2.36	g, h; k; n	g, h; i, j; k; n
n	1.59	i, j; k; m	g, h; i, j; k; m

b) Messungen in C₆D₆

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a	7.05	b; c, d	c, d
b	7.01	a; c, d	c, d
c, d	6.88-6.91	a; b	g; h, i, j; k; m
e	6.28	f; k; m	f; k; m
f	6.00	e; k; m	e
g	2.68	k; l; m	c, d; k; l; m; n
h, i, j	2.48-2.59	l; n	c, d; l; n
k	2.35	e; f; g; m	c, d; e; g; m
l	1.87	g; h, i, j; n	g; h, i, j; m; n
m	1.74	e; f; g; k	c, d; e; g; k; l
n	1.46	h, i, j; l	g; h, i, j; l

(4aR*,10aR*)-4a,9,10,10a-Tetrahydro-phenanthren-1(4H)-on (cis-18a)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	202.04	s	-
B	148.94	d	6.96 (e)
C	138.23	s	-
D	135.35	s	-
E	129.35	d	7.09-7.18 (a, b, c, d)
F	129.10	d	6.10 (f)
G	128.38	d	7.09-7.18 (a, b, c, d)
H	126.60	d	7.09-7.18 (a, b, c, d)
I	126.04	d	7.09-7.18 (a, b, c, d)
J	46.20	d	2.70 (j)
K	37.45	d	3.40 (g)
L	31.82	t	2.43 (l); 2.60 (k)
M	28.83	t	2.93 (h, i)
N	21.28	t	1.94 (m, n)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY
a, b, c, d	7.09-7.18	
e	6.96	f; k; l
f	6.10	e; k; l
g	3.40	j; k; l
h, i	2.93	m, n
j	2.70	g; m, n
k	2.60	e; f; g; l
l	2.43	e; f; g; k
m, n	1.94	h, i; j

(4aR*,10aS*)-4a,9,10,10a-Tetrahydro-2-methyl-phenanthren-1(4H)-on (*trans*-18b)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	200.70	s	-
B	143.27	d	6.83 (e)
C	138.16	s	-
D	136.68	s	-
E	135.62	s	-
F	129.28	d	7.01-7.21 (b, c, d)
G	126.30	d	7.01-7.21 (b, c, d)
H	126.04	d	7.01-7.21 (b, c, d)
I	125.56	d	7.27 (a)
J	48.83	d	2.31 (l)
K	40.02	d	3.05-3.13 (f, g)
L	32.40	t	3.05-3.13 (f, g); 2.45 (k)
M	29.31	t	2.89 (h, i)
N	21.84	t	2.56 (j); 1.57 (p)
O	15.97	q	1.85 (m, n, o)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY
a	7.27	b, c, d
b, c, d	7.01-7.21	a
e	6.83	f, g; k; m, n, o
f, g	3.05-3.13	e; k; l; m, n, o
h, i	2.89	j; p
j	2.56	h, i; l; p
k	2.45	e; f, g; m, n, o
l	2.31	f, g; j; p
m, n, o	1.85	e; f, g; k
p	1.57	h, i; j; l

(4aR*,10aR*)-4a,9,10,10a-Tetrahydro-2-methyl-phenanthren-1(4H)-on (cis-18b)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	201.96	s	-
B	143.91	d	6.72 (e)
C	138.66	s	-
D	135.47	s	-
E	135.01	s	-
F	129.33	d	7.09-7.17 (a, b, c, d)
G	128.38	d	7.09-7.17 (a, b, c, d)
H	126.52	d	7.09-7.17 (a, b, c, d)
I	126.03	d	7.09-7.17 (a, b, c, d)
J	46.27	d	2.71 (i)
K	37.96	d	3.39 (f)
L	32.13	t	2.54 (j); 2.43 (k)
M	29.02	t	2.93 (g, h)
N	21.40	t	1.93 (l, m)
O	16.05	q	1.83 (n, o, p)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a, b, c, d	7.09-7.17		f; g, h; j; k
e	6.72	j; k; n, o, p	j; k; n, o, p
f	3.39	i; j; k	a, b, c, d; i; j; k
g, h	2.93	l, m	a, b, c, d; i; l, m
i	2.71	f; l, m	f; g, h; l, m
j	2.54	e; f; k; n, o, p	a, b, c, d; e; f; k
k	2.43	e; f; j; n, o, p	a, b, c, d; e; f; j; l, m
l, m	1.93	g, h; i	g, h; i; k
n, o, p	1.83	e; j; k	e

(4aR*,10aS*)-4a,9,10,10a-Tetrahydro-10a-methyl-phenanthren-1(4H)-on (*trans*-18c)

Messungen in CDCl₃*)

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	204.41	s	-
B	147.27	d	7.02 (e)
C	136.65	s	-
D	135.62	s	-
E	129.11	d	[7.08-7.21] (b, c, d)
F	127.99	d	[6.03-6.07] (f)
G	126.27	d	[7.08-7.21] (b, c, d)
H	126.06	d	[7.08-7.21] (b, c, d)
I	125.53	d	7.24 (a)
J	43.52	s	-
K	41.73	d	3.21 (g)
L	28.62	t	2.25 (l); 1.76 (m)
M	27.59	t	[3.01-3.08] (h); [2.39-2.48] (k)
N	25.63	t	[2.89-2.93] (i, j)
O	15.00	q	0.98 (n, o, p)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a	7.24	b, c, d	b, c, d; h; k
b, c, d	[7.08-7.21]	a	a; i, j
e	7.02	f; h; k	f; h
f	[6.03-6.07]	e; k	e
g	3.21	h; k	h; k; m
h	[3.01-3.08]	e; g; k	a; e; g; k
i, j	[2.89-2.93]	l; m	b, c, d; l; m; n, o, p
k	[2.39-2.48]	e; f; g; h	a; g; h; n, o, p
l	2.25	i, j; m	i, j; m; n, o, p
m	1.76	i, j; l	g; i, j; l
n, o, p	0.98	-	i, j; k; l

*) Messungen erfolgen im Gemisch mit *cis*-Diastereoisomer. Die Verschiebungswerte in eckigen Klammern sind von den Signalen des *cis*-Diastereoisomers überlagert.

(4aR*,10aR*)-4a,9,10,10a-Tetrahydro-10a-methyl-phenanthren-1(4H)-on (*cis*-18c)

Messungen in CDCl₃*)

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	204.95	s	-
B	147.30	d	6.87 (e)
C	138.41	s	-
D	134.51	s	-
E	129.31	d	7.08-7.16 (a, b, c, d)
F	128.81	d	6.04 (f)
G	128.59	d	7.08-7.16 (a, b, c, d)
H	126.41	d	7.08-7.16 (a, b, c, d)
I	126.01	d	7.08-7.16 (a, b, c, d)
J	44.12	d	3.05 (g)
K	44.03	s	-
L	33.10	t	2.62 (j); 2.44 (k)
M	26.50	t	2.09 (l); 1.56 (m)
N	25.07	t	2.90 (h, i)
O	20.01	q	1.15 (n, o, p)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a, b, c, d	7.08-7.16		g; h, i; k
e	6.87	f; j; k	f; j; k
f	6.04	e; k	e
g	3.05	j; k	a, b, c, d; j; k; n, o, p
h, i	2.90	l; m	a, b, c, d; l; m; n, o, p
j	2.62	e; g; k	e; g; k; n, o, p
k	2.44	e; f; j; g	a, b, c, d; e; g; j; l
l	2.09	h, i; m; n, o, p	h, i; k; m; n, o, p
m	1.56	h, i; l	h, i; l; n, o, p
n, o, p	1.15	l	g; h, i; j; l; m

*) Messungen erfolgen im Gemisch mit *trans*-Diastereoisomer.

(9*R,10*S**)-6,7,8,9,11,15,16,17-Octahydro-cyclopenta[a]phenanthren-12-on (*trans*-20)**

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	196.87	s	-
B	168.35	s	-
C	138.15	s	-
D	137.76	s	-
E	135.85	s	-
F	129.23	d	7.11-7.19 (b, c,d)
G	126.42	d	7.11-7.19 (b, c, d)
H	126.11	d	7.11-7.19 (b, c,d)
I	125.02	d	7.24 (a)
J	42.82	t	3.23 (e); 2.39 (n)
K	42.12	d	3.12 (f)
L	40.07	d	2.48 (m)
M	34.76	t	2.77 (i); 2.56-2.64 (j, k, l)
N	29.45	t	3.01 (g, h)

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
O	29.33	t	2.56-2.64 (j, k, l)
P	26.14	t	2.30 (o); 1.66 (r)
Q	21.79	t	1.96 (p, q)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a	7.24	b, c, d	b, c, d; e; f
b, c, d	7.11-7.19	a	a; g, h
e	3.23	f; n	a; f; n
f	3.12	e; m; n	a; e; m; n; r
g, h	3.01	o; r	b, c, d; m; o; r
i	2.77	j, k, l; p, q	j, k, l; o; p, q
j, k, l	2.56-2.64	i; p, q	i; m; o; p, q
m	2.48	f; o; r	f; g, h; j, k, l; n; o
n	2.39	e; f	e; f; m
o	2.30	g, h; m; r	g, h; i; j, k, l; m; r
p, q	1.96	i; j, k, l	i; j, k, l
r	1.66	g, h; m; o	f; g, h; o

(9R*,10R*)-6,7,8,9,11,15,16,17-Octahydro-cyclopenta[a]phenanthren-12-on (cis-20)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	196.61	s	-
B	168.13	s	-
C	138.53	s	-
D	137.16	s	-
E	135.50	s	-
F	129.13	d	7.11-7.19 (a, b, c, d)
G	128.86	d	7.11-7.19 (a, b, c, d)
H	126.33	d	7.11-7.19 (a, b, c, d)
I	126.15	d	7.11-7.19 (a, b, c, d)
J	43.39	t	2.51-2.61 (j, k, l, m, n)
K	38.88	d	3.46 (e)
L	36.62	d	2.65 (i)
M	35.93	t	2.78 (h); 2.51-2.61 (j, k, l, m, n)
N	29.72	t	2.93 (f, g)
O	29.09	t	2.51-2.61 (j, k, l, m, n)

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
P	22.42	t	2.01 (o); 1.79 (r)
Q	21.75	t	1.96 (p, q)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a, b, c, d	7.11-7.19		e; f, g; j, k, l, m, n
e	3.46	i; j, k, l, m, n	a, b, c, d; i; j, k, l, m, n
f, g	2.93	o; r	a, b, c, d; i; o; r
h	2.78	j, k, l, m, n; p, q	i; j, k, l, m, n; o; p, q
i	2.65	e; o; r	e; f, g; h; j, k, l, m, n; o; r
j, k, l, m, n	2.51-2.61	e; h; p, q	a, b, c, d; e; h; i; p, q; r
o	2.01	f, g; i; r	f, g; h; i; r
p, q	1.96	h; j, k, l, m, n	h; j, k, l, m, n
r	1.79	f, g; i; o	f, g; i; j, k, l, m, n; o

(1R*, 4aR*, 10aS*)-2,4,4a,9,10,10a-Hexahydro-1-hydroxy-phenanthren-3-on (42)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	209.58	s	-
B	138.70	s	-
C	136.18	s	-
D	129.13	d	7.12-7.21 (a, b, c, d)
E	126.20	d	7.12-7.21 (a, b, c, d)
F	126.17	d	7.12-7.21 (a, b, c, d)
G	125.79	d	7.12-7.21 (a, b, c, d)
H	72.49	d	4.40 (e)
I	49.68	t	2.66 (j, k)
J	46.39	t	2.31 (l); 3.16 (g)
K	43.29	d	1.84-1.98 (n, o, p)
L	35.51	d	3.40 (f)
M	30.04	t	2.99 (h, i)
N	26.03	t	1.84-1.98 (n, o, p)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY
a, b, c, d	7.12-7.21	
e	4.40	j, k; n, o, p
f	3.40	g; l; n, o, p
g	3.16	f; j, k; l
h, i	2.99	n, o, p
j, k	2.66	e; g
l	2.31	f; g
m	2.01	-
n, o, p	1.84-1.98	e; f; h, i

2,4,9,10-Tetrahydro-4a-methyl-phenanthren-3-on (43)

Messungen in C₆D₆

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	207.07	s	-
B	143.93	s	-
C	143.66	s	-
D	135.88	s	-
E	129.03	d	6.90-6.92 (c, d)
F	126.99	d	7.02 (a)
G	126.66	d	6.90-6.92 (c, d)
H	126.09	d	6.98 (b)
I	116.80	d	5.04 (e)
J	53.82	t	2.78 (f); 2.22 (k)
K	41.76	s	-
L	39.63	t	2.56-2.65 (g, h, i); 2.52 (j)
M	32.00	t	2.56-2.65 (g, h, i)
N	30.04	t	2.16 (l); 2.07 (m)
O	29.36	q	1.17 (n, o, p)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a	7.02	b; c, d	b; c, d
b	6.98	a; c, d	a; c, d
c, d	6.90-6.92	a; b	a; b; f; g, h, i; n, o, p
e	5.04	g, h, i; j; l	g, h, i; j; m
f	2.78	k	c, d; k; n, o, p
g, h, i	2.56-2.65	e; j; l; m	c, d; e; j; l; m
j	2.52	e; g, h, i; m; l	e; g, h, i
k	2.22	f; n, o, p	f
l	2.16	e; g, h, i; j; m	g, h, i; m; n, o, p
m	2.07	g, h, i; j; l	e; g, h, i; l
n, o, p	1.17	k	c, d; f; l

(4aR*,10aS*)-4a,9,10,10a-Tetrahydro-3-isopropyl-2-methyl-phenanthren-1(4H)-on (trans-45)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	200.58	s	-
B	161.10	s	-
C	138.33	s	-
D	136.89	s	-
E	129.36	s	-
F	129.35	d	7.13 (d)
G	126.29	d	7.16 (c)
H	125.96	d	7.20 (b)
I	125.50	d	7.34 (a)
J	48.20	d	2.19-2.26 (k, l)
K	39.05	d	2.83-2.93 (g, h, i)
L	31.49	d	3.09-3.13 (e, f)
M	31.12	t	2.19-2.26 (k, l); 3.09-3.13 (e, f)
N	29.36	t	2.83-2.93 (g, h, i)
O	22.15	t	2.53 (j); 1.55 (p)
P	20.27	q	1.17 (q, r, s)
Q	19.66	q	1.10 (t, u, v)
R	10.48	q	1.83 (m, n, o)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY
a	7.34	b
b	7.20	a; c
c	7.16	b; d
d	7.13	c
e, f	3.09-3.13	g, h, i; k, l; m, n, o; q, r, s; t, u, v
g, h, i	2.83-2.93	e, f; j; k, l; p
j	2.53	g, h, i; k, l; p
k, l	2.19-2.26	e, f; g, h, i; j; m, n, o; p
m, n, o	1.83	e, f; k, l
p	1.55	g, h, i; j; k, l
q, r, s	1.17	e, f
t, u, v	1.10	e, f

(4aR*,10aR*)-4a,9,10,10a-Tetrahydro-3-isopropyl-2-methyl-phenanthren-1(4H)-on (cis-45)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	200.96	s	-
B	161.81	s	-
C	138.97	s	-
D	135.76	s	-
E	129.33	d	7.10-7.19 (a, b, c, d)
F	128.78	s	-
G	128.54	d	7.10-7.19 (a, b, c, d)
H	126.50	d	7.10-7.19 (a, b, c, d)
I	126.00	d	7.10-7.19 (a, b, c, d)
J	45.30	d	2.68 (i)
K	37.18	d	3.24 (e)
L	31.42	d	3.03 (f)
M	30.70	t	2.32 (k); 2.51 (j)
N	29.00	t	2.92 (g, h)
O	21.32	t	1.93 (l, m)
P	20.05	q	1.13 (q, r, s)
Q	19.49	q	0.99 (t, u, v)
R	10.29	q	1.84 (n, o, p)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a, b, c, d	7.10-7.19		e; g, h; j; k
e	3.24	i; j; k	a, b, c, d; i; j; k
f	3.03	q, r, s; t, u, v	n, o, p; q, r, s; t, u, v
g, h	2.92	l, m	a, b, c, d; i; l, m
i	2.68	e; l, m	e; g, h; l, m
j	2.51	e; k; n, o, p	a, b, c, d; e; k; q, r, s; t, u, v
k	2.32	e; j; n, o, p	a, b, c, d; e; j; l, m; t, u, v
l, m	1.93	g, h; i	g, h; i; k
n, o, p	1.84	j; k	f; q, r, s; t, u, v
q, r, s	1.13	f	f; j; t, u, v; n, o, p
t, u, v	0.99	f	f; j; k; q, r, s; n, o, p

(4aR*,10aR*)-2-Acetyl-1-ethyl-4a,9,10,10a-tetrahydro-phenanthren-3(4H)-on (48)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	204.46	s	-
B	196.49	s	-
C	167.02	s	-
D	138.89	s	-
E	138.18	s	-
F	134.96	s	-
G	129.27	d	7.14-7.19 (a, b, c)
H	128.65	d	7.08 (d)
I	126.75	d	7.14-7.19 (a, b, c)
J	126.38	d	7.14-7.19 (a, b, c)
K	42.55	t	2.62 (i, j)
L	38.24	d	2.68 (h)
M	37.65	d	3.40 (e)
N	31.98	q	2.37 (l, m, n)
O	29.89	t	2.99 (f, g)
P	26.29	t	2.40 (k); 2.25 (o)
Q	22.68	t	2.06 (p); 1.86 (q)
R	13.30	q	1.16 (r, s, t)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a, b, c	7.14-7.19	d	d; f, g
d	7.08	a, b, c	a, b, c; e; i, j
e	3.40	h; i, j	d; h; i, j
f, g	2.99	p; q	a, b, c; h; p; q
h	2.68	e; p; q	e; f, g; o; p; r, s, t
i, j	2.62	e	d; e; q
k	2.40	o; r, s, t	o; r, s, t
l, m, n	2.37	-	-
o	2.25	k; r, s, t	h; k; p; r, s, t
p	2.06	f, g; h; q	f, g; h; o; q
q	1.86	f, g; h; p	f, g; i, j; p
r, s, t	1.16	k; o	h; k; o

(4aR*,10aS*)-4a,9,10,10a-Tetrahydro-phenanthren-1,3(4H)-dion (trans-54)

a) Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	203.59	s	-
B	203.31	s	-
C	136.82	s	-
D	136.00	s	-
E	129.48	d	7.16-7.25 (a, b, c, d)
F	127.02	d	7.16-7.25 (a, b, c, d)
G	126.52	d	7.16-7.25 (a, b, c, d)
H	126.13	d	7.16-7.25 (a, b, c, d)
I	57.59	t	3.58 (e); 3.52 (f)
J	51.74	d	2.60 (l)
K	46.43	t	3.44 (g); 2.67 (k)
L	35.80	d	3.07 (h)
M	28.87	t	2.93 (i, j)
N	21.82	t	2.43 (m); 1.76 (n)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY
a, b, c, d	7.16-7.25	
e	3.58	f
f	3.52	e; g
g	3.44	f; h; k
h	3.07	g; k; l
i, j	2.93	m; n
k	2.67	g; h
l	2.60	h; m; n
m	2.43	i, j; l; n
n	1.76	i, j; l; m

b) Messungen in DMSO-d₆:

¹H-Atom	¹H-NMR δ	¹H-¹H-COSY	¹H-¹H-NOESY
a	11.16	-	-
b	7.30	c, d, e	c, d, e; g; h
c, d, e	7.09-7.17	b	b; i, j
f	5.32	-	-
g	3.07	h; k, l	b; k, l
h	3.00	g; k, l; m	b; k, l; m; n
i, j	2.82	k, l; n	c, d, e; k, l; m; n
k, l	2.34-2.43	g; h; i, j; m; n	g; h; i, j; m; n
m	2.19	h; k, l; n	h; i, j; k, l; n
n	1.37	i, j; k, l; m	h; i, j; k, l; m

(4aR*,10aS*)-4a,9,10,10a-Tetrahydro-4a-methyl-phenanthren-1,3(4H)-dion (trans-55)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	203.84	s	-
B	203.57	s	-
C	142.01	s	-
D	135.15	s	-
E	129.72	d	7.13-7.25 (a, b, c, d)
F	126.77	d	7.13-7.25 (a, b, c, d)
G	126.60	d	7.13-7.25 (a, b, c, d)
H	125.54	d	7.13-7.25 (a, b, c, d)
I	57.62	t	3.54 (e); 3.42 (f)
J	55.09	d	2.87-3.02 (h, i, j)
K	54.48	t	3.32 (g); 2.83 (k)
L	36.91	s	-
M	28.84	t	2.87-3.02 (h, i, j)
N	25.02	q	1.05 (n, o, p)
O	17.80	t	2.27 (l); 1.87 (m)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a, b, c, d	7.13-7.25		g; h, i, j; n, o, p
e	3.54	f	f; h, i, j; k
f	3.42	e; g	e
g	3.32	f; k	a, b, c, d; k; n, o, p
h, i, j	2.87-3.02	l; m	a, b, c, d; e; k; l; m
k	2.83	g; n, o, p	e; g; h, i, j
l	2.27	h, i, j; m	h, i, j; m
m	1.87	h, i, j; l	h, i, j; l; n, o, p
n, o, p	1.05	k	a, b, c, d; g; m

1-(5,6-Dihydro-10-methyl-benzocycloocten-7-yl)-ethanon (58)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	201.13	s	-
B	140.09	s	-
C	140.05	s	-
D	139.23	s	-
E	136.76	d	6.78 (e)
F	128.94	d	7.18-7.25 (a, b, c, d)
G	127.92	d	7.18-7.25 (a, b, c, d)
H	126.68	d	7.18-7.25 (a, b, c, d)
I	125.77	d	7.18-7.25 (a, b, c, d)
J	122.98	d	6.07 (f)
K	31.39	t	2.73 (i, j)
L	30.14	t	3.00 (g, h)
M	26.11	q	2.18 (n, o, p)
N	25.93	q	2.20 (k, l, m)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY
a, b, c, d	7.18-7.25	
e	6.78	f; i, j; n, o, p
f	6.07	e; i, j; n, o, p
g, h	3.00	i, j
i, j	2.73	e; f; g, h; n, o, p
k, l, m	2.20	-
n, o, p	2.18	e; f; i, j

1-((1*R**,3*aR**,8*R**,8*aR**)-3,3*a*,8,8*a*-Tetrahydro-1-hydroxy-1*H*-2-oxa-cyclopenta[*a*]inden-8-yl)-propan-2-on (63a)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	207.70	s	
B	144.99	s	
C	144.73	s	
D	127.66	d	7.17-7.23 (a, b, c)
E	127.38	d	7.17-7.23 (a, b, c)
F	124.41	d	7.17-7.23 (a, b, c)
G	123.60	d	7.09 (d)
H	104.68	d	5.60 (e)
I	72.59	t	4.37 (f); 3.91 (h)
J	58.01	d	2.62 (m)
K	51.14	t	2.91 (k); 2.71 (l)
L	48.64	d	3.95 (g)
M	44.04	d	3.62 (i)
N	30.39	q	2.17 (n, o, p)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a, b, c	7.17-7.23	d	g, h
d	7.09	a, b, c	i, k
e	5.60	j, m	i, j, m
f	4.37	g, h	g, h
g, h	3.87-3.98	f, m	a, b, c; f, m
i	3.62	k, l, m	d; e; k; l, m; n, o, p
j	3.33	e	e
k	2.91	i, l, n, o, p	d; i, l, n, o, p
l	2.71	i, k	i, k, m, n, o, p
m	2.62	e, g, h, i	e, g, h, i, l
n, o, p	2.17	k	k, l

(6aR*,11aS*)-5,6,6a,8,9,10,11,11a-Octahydro-cyclopenta[b]phenanthren-7-on (trans-70)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	198.16	s	-
B	163.20	s	-
C	138.40	s	-
D	137.76	s	-
E	136.88	s	-
F	129.29	d	7.13-7.22 (b, c, d)
G	126.30	d	7.13-7.22 (b, c, d)
H	126.01	d	7.13-7.22 (b, c, d)
I	125.57	d	7.29 (a)
J	48.53	d	2.29 (o)
K	40.96	d	3.08-3.20 (e, f)
L	37.72	t	2.65 (i, j)
M	32.95	t	3.08-3.20 (e, f); 2.37 (n)
N	29.57	t	2.91 (g, h)

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
O	29.22	t	2.51-2.63 (k, l, m)
P, Q	21.93, 21.92	beide t	2.51-2.63 (k, l, m); 1.96 (p, q); 1.58 (r)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a	7.29	b, c, d	b, c, d; e, f
b, c, d	7.13-7.22	a	a; g, h
e, f	3.08-3.20	n; o	a; i, j; n; o; r
g, h	2.91	k, l, m; r	b, c,d; k, l, m; o; r
i, j	2.65	n; p, q	e, f; p, q
k, l, m	2.51-2.63	g, h; o; p, q; r	g, h; o; p, q; r
n	2.37	e, f; i, j	e, f
o	2.29	e, f; k, l, m; r	e, f; g, h; k, l, m; r
p, q	1.96	i, j; k, l, m	i, j; k, l, m
r	1.58	g, h; k, l, m; o	e, f; g, h; k, l, m; o

(6aR*,11aR*)-5,6,6a,8,9,10,11,11a-Octahydro-cyclopenta[b]phenanthren-7-on (cis-70)

Messungen in CDCl₃

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
A	199.96	s	-
B	164.02	s	-
C	138.90	s	-
D	136.00	s	-
E	135.53	s	-
F	129.35	d	7.10-7.18 (a, b, c, d)
G	128.45	d	7.10-7.18 (a, b, c, d)
H	126.50	d	7.10-7.18 (a, b, c, d)
I	126.02	d	7.10-7.18 (a, b, c, d)
J	46.17	d	2.56-2.64 (h, i, j, k, l, m)
K	38.55	d	3.42 (e)
L	37.66	t	2.56-2.64 (h, i, j, k, l, m)
M	33.18	t	2.56-2.64 (h, i, j, k, l, m); 2.43 (n)
N	29.33	t	2.94 (f, g)

¹³ C-Atom	¹³ C-NMR δ	DEPT	¹³ C- ¹ H-COSY δ
O	29.16	t	2.56-2.64 (h, i, j, k, l, m)
P	21.78	t	1.84-1.99 (o, p, q, r)
Q	21.62	t	1.84-1.99 (o, p, q, r)

¹ H-Atom	¹ H-NMR δ	¹ H- ¹ H-COSY	¹ H- ¹ H-NOESY
a, b, c, d	7.10-7.18		e; f, g; h, i, j, k, l, m
e	3.42	h, i, j, k, l, m; n	a, b, c, d; h, i, j, k, l, m; n
f, g	2.94	o, p, q, r	a, b, c, d; h, i, j, k, l, m; o, p, q, r
h, i, j, k, l, m	2.56-2.64	e; n; o, p, q, r	a, b, c, d; e; f, g; n; o, p, q, r
n	2.43	e; h, i, j, k, l, m	e; h, i, j, k, l, m; o, p, q, r
o, p, q, r	1.84-1.99	f, g; h, i, j, k, l, m	f, g; h, i, j, k, l, m; n