Table 4. Observed and calculated ^{1}H NMR chemical shifts (δ, ppm) of 3*H*-phenoxazin-3-one derivatives. Apparent $^{3}J_{H,H}$ (Hz) in parentheses.

	1		**2**		**3**	**4**		**5**		**6**			**7**		**8**	**9**
	calc.	lit.*	obs.	calc.	obs.	obs.	calc.	obs.	calc.	obs.	calc.	calc.**	obs.	calc.	obs.	obs.
1	7.30	6.87	7.45 d (10.0)	7.25	7.30 q (1.2)	8.44 s	8.61									
2	6.56	7.50	6.87 dd (10.0; 1.8)	6.60												
4	6.07	6.20	6.33 d (1.8)	6.06	6.34 s	6.47 s	6.26	6.51 s	6.19	6.53 s	6.12	6.18	6.52	6.34	6.51	6.50 s
6	7.19	7.87	7.24 d (8.3)	7.13	7.23 d (8.4)	7.43	7.36	7.51 m	7.38	7.52 m	7.36	7.31	7.52	7.37	7.51	7.49
7	7.36	7.35	7.37 dd (8.3; 1.8)	7.28	7.33 dd (8.4; 2.0)	7.57 t (8.0)	7.40	7.66	7.38	7.67	7.55	7.53	7.58	7.46	7.53	7.20 m
8	7.21	7.35				7.43	7.27	7.66	7.56	7.67	8.56	7.95	7.63	8.01	7.65	7.49
9	7.74	7.60	7.61 bs	7.55	7.59 bs	7.88 d (8.0)	7.92									
R1			2.47 s	2.11	2.47 s											
R2								2.75 s	2.68	2.71 s	2.56	2.53		2.46	[a]	[c]
R3								2.65 s	2.54	2.64 s	2.37	2.32		2.66	[a]	[c]
R4					2.23 s	2.30 s	1.80							1.82	[b]	[d]

Other signals: [a]OC*H*$_3$ (3.71), *CH*NHCOC*H*$_3$ (4.98; 2.02), C*H*$_2$CO (3.95, 3.70), [b]NHCOC*H*$_3$ (2.02), [c]OC*H*$_3$ (3.72), C*H*$_2$C*H*$_2$CO (2.7, 2.8; 3.4, 3.5), [d]NHCOC*H*$_3$ (2.31)

*Ref.9a.

**Values calculated by Boltzmann averaging over a C-9 acetyl dihedral scan (see text).

Table 5. Observed and calculated ^{13}C NMR chemical shifts (δ, ppm) of 3*H*-phenoxazin-3-one derivatives.

	1		**2**		**3**	**4**			**5**			**6**			**7**		**8**	**9**
	calc.	lit.*	obs.	calc.	obs.	obs.	calc.	lit.	obs. DMSO	obs. $CHCl_3$	calc	obs.	calc.	calc.***	obs.	calc.	obs.	obs.
1	135.1	135.2	134.4	135.1	131.3	114.0	112.1	113.9	105.2	105.8	103.5	141.6	142.0	142.0	126.3	124.5	141.7	141.8
2	137.0	134.8	134.8	137.2	144.3	137.2	137.3	149.4	149.8**	150.5**	150.6	135.0	143.2	143.1	131.1	131.7	136.7	136.1
3	184.3	186.4	186.0	184.2	186.0	179.9	177.9	179.7	178.5	178.6	176.6	177.1	175.2	175.2	179.4	178.1	178.1	178.5
4	106.7	107.0	106.7	106.4	106.3	104.2	102.5	104.1	104.5	105.2	103.5	106.4	105.8	106.0	104.7	102.6	105.2	105.1
4a	148.0	149.7	149.6	148.1	149.5	149.6	148.6	149.1	150.1**	149.8**	149.2	146.0**	146.3	146.7	148.1	146.8	151.3	150.6
5a	144.5	148.8	141.7	142.4	141.5	143.4	142.7	147.9	141.4	141.8	141.3	143.1	142.8	142.6	142.7	142.0	147.1	147.1
6	116.2	116.2	115.5	115.8	115.7	116.3	116.1	116.1	117.8	118.0	118.7	119.4	120.4	119.1	118.8	119.3	119.2	117.8
7	131.1	132.8	133.6	134.2	133.1	132.0	131.5	131.8	129.1	129.3	128.9	133.5	133.1	133.7	132.2	131.3	129.4	130.1
8	125.5	125.5	135.2	135.4	135.2	125.9	125.3	125.7	123.2	123.6	127.5	126.0	129.5	128.1	125.1	128.2	125.2	123.8
9	132.8	130.5	129.9	132.6	129.9	130.3	132.9	130.1	139.2	139.9	139.9	139.8	134.9	140.2	140.2	138.0	137.7	139.5
9a	134.4	133.4	132.9	134.0	133.3	134.2	135.2	134.0	129.7	130.3	131.3	130.4	132.1	131.1	130.4	131.3	130.2	131.8
10a	150.2	144.0	148.3	149.6	148.8	149.0	149.2	143.3	147.0**	147.1**	145.8	148.0**	146.6	146.3	147.4	147.4	149.6	149.8
R1			20.5	17.7	20.8													
R2									202.2	34.1	28.7	32.5	31.0	31.0	31.9	30.4	[a]	
										202.2	202.2	200.0	196.0	200.3	200.7	199.4		
R3									200.0	32.0	31.3	31.3	28.8	28.7	29.7	31.7	[a]	
										201.0	201.5	197.8	201.0	201.0	198.3	200.0		
R4					16.5	24.9	20.7	24.9							24.3	20.6	[b]	
						169.4	166.9	169.2							168.1	166.4		

Other signals: [a]O*C*H_3 (52.7, 52.6), *C*HNHCO*C*H_3 (48.7; 22.8), *C*H2*C*O (45.2, 200.0 or 200.5), carboxyl (173.1; 172.5; 172.0; 171.5; 169.7), [b]NHCO*C*H_3 (23.2), [c]O*C*H_3 (51.9, 51.6), *C*H2*C*H2*C*O (28.1, 28.6; 39.0, 40.4; 202.3, 201.1), carboxyl (173.8, 173.0, 171.3), [d]NHCO*C*H_3 (21.2)

*Ref.13.

**Assignments may be interchanged

***Values calculated by Boltzmann averaging over a C-9 acetyl dihedral scan (see text).

Table 6. Observed and calculated ^{1}H-NMR chemical shifts (δ, ppm) of 5*H*-pyrido[2,3-a]phenoxazin-5-one derivatives. Apparent $^{3}J_{H,H}$ (Hz) in parentheses.

	10		**11**		**12**	
	obs.	calc.	obs.	calc.	obs.	calc.
1a						
2	9.16 dd (1.8; 4.6)	8.98	9.19 dd (1.7; 4.5)	9.09	9.15 dd (1.7; 4.5)	9.04
3	7.71 dd (4.6; 8.0)	7.47	7.77 dd (4.5; 7.6)	7.55	7.72 dd (4.5; 8.0)	7.52
4	8.64 dd (1.8; 8.0)	8.78	8.62 dd (1.7; 7.6)	8.60	8.61 dd (1.7; 8.0)	8.70
4a						
5						
6	6.51 s	6.25	6.58 s	6.27	6.49 s	6.21
6a						
7a						
8	7.36 dd (1.3; 8.0)	7.20	7.45 d (9.1)	7.13	7.29 d (8.0)	7.08
9	7.57 dt (1.3-8.0)	7.40	8.41 dd (2.7; 9.1)	8.35	7.50 dd (2.6; 8.0)	7.32
10	7.41 dt (1.5; 8.3)	7.27				
11	8.12 dd (1.8; 8.0)	8.01	8.99 d (2.7)	8.93	8.08 d (2.6)	7.95
11a						
12a						

Table 7. Observed and calculated ^{13}C NMR chemical shifts (δ, ppm) of 5*H*-pyrido[2,3-a]phenoxazin-5-one derivatives.

	10		**11**		**12**	
	obs.	calc.	obs.	calc.	obs.	calc.
1a	147.2	147.5	147.0	147.1	147.2	147.1
2	153.4	153.5	154.2	154.1	153.8	153.7
3	125.9	125.0	127.0	125.9	126.5	125.3
4	134.1	135.6	134.6	135.2	134.5	135.1
4a	128.6	128.5	129.0	128.1	129.0	128.2
5	182.2	180.8	182.4	181.2	182.4	181.1
6	106.8	105.4	108.8	107.0	107.6	105.5
6a	152.0	151.4	151.9	150.3	151.9	151.5
7a	143.9	144.0	148.1	148.4	142.8	142.2
8	115.7	116.0	116.7	115.6	117.1	116.2
9	132.5	132.9	127.2	129.0	132.5	132.9
10	125.5	125.1	145.0	144.1	133.6	137.2
11	131.0	133.9	126.6	129.3	130.5	132.6
11a	132.8	134.4	132.4	133.6	130.8	134.6
12a	146.4	147.5	149.0	149.2	147.9	148.5

Table 8. Observed and calculated ^{1}H chemical shifts (δ, ppm) of 5*H*-pyrido[3,2-a]phenoxazin-5-one derivatives. Apparent $^{3}J_{H,H}$ (Hz) in parentheses.

	13		**14**	**15**	**16**	**17***	
	obs.	calc.	obs.	obs.	obs.	obs.	calc.
1	9.10 dd (1.8; 8.0)	9.12	9.00 dd (1.5; 7.9)	9.05 dd (1.8; 8.0)	9.05 d (8.0)		
2	7.74 dd (4.5; 8.0)	7.37	7.68 dd (4.4; 7.9)	7.72 dd (4.5; 8.0)	7.72 dd (4.4; 8.0)	6.61 s	6.39
3	9.12 dd (1.8; 4.5)	9.02	9.07 dd (1.3; 4.4)	9.10 dd (1.8; 4.5)	9.09 d (4.4)		
6	6.66 s	6.28	6.66 s	6.63 s	6.61 s	6.40 s	5.82
8	7.39 d (8.0)	7.22	7.10 s	7.29 d (8.4)	7.19 d (8.0)	6.50 dd	6.08
9	7.56 dt (1.8; 8.0)	7.34		7.39 dd (2.2; 8.4)	7.42 t (8.0)	6.47 t	6.10
10	7.40 t (8.0)	7.21		a	7.24 d (8.0)	7.13 d	6.70
11	7.88 dd (1.8; 8.0)	7.79	7.56 s	7.68 d (2.2)			
R1			2.04 s				
R2			2.34 s	[a]			
R3					2.78 s		

*Calculated values refer to model compund **18**

[a]Other signals C*H*$_3$C*H*$_2$(C*H*$_3$)C*H* (0.86 t, 171 m, 1.31 d, 2.75 m)

Table 9. Observed and calculated ^{13}C chemical shifts (δ, ppm) of 5*H*-pyrido[3,2-a]phenoxazin-5-one derivatives.

	13		**14**	**15**	**16**	**17***	
	obs.	calc.	obs.	obs.	obs.	obs.	calc.
1	133.1	133.3	133.0	133.1	133.1	181.7	178.7
1a	127.9	126.9	128.0	128.0	128.0	113.9	113.4
2	126.1	124.0	125.9	126.1	126.0	111.0	111.4
3	153.4	154.6	153.0	153.4	153.2	135.5	132.3
4a	147.2	147.8	147.1	147.2	147.2	126.7	123.8
5	182.3	179.5	182.2	182.4	182.3	141.8	139.4
6	108.6	108.6	108.1	108.4	108.1	103.5	98.7
6a	151.0	149.3	151.2	151.2	150.9	138.6	139.1
7a	144.1	144.6	142.2	142.7	144.2	144.9	146.2
8	116.2	116.4	116.6	115.9	113.7	118.6	117.5
9	132.4	132.3	143.1	131.7	131.9	119.2	117.3
10	125.6	124.8	134.7	145.5	126.8	125.3	126.1
11	130.1	131.7	130.1	128.1	139.4	118.1	116.1
11a	132.6	133.3	130.9	132.4	132.2	135.9	134.9
12a	146.3	148.7	145.2	146.2	145.5	123.5	124.4
R1			20.4				
R2			19.6	§			
R3					16.8	#	196.7
							24.1
R4				2.78 s		162.9	166.2
						53.8	49.1

*Calculated values refer to model compund **18**

§ [a]41.0; [b]31.1; [c]12.1; [d]21.7

[a]192.2; [b]41.2; [c]48.3; [d]170.2; [e]23.2; [f]171.8; [g]52.8; [h]56.3