Synthesis and Spectral Properties of 7-(*p*-bromophenyl)-10,10-dimethyl-8-Alkylthio-7,9,10,11-tetrahydro-benz[*c*]acridines and Deprotection-aromatization of 7-[(*o*-; and *p*-Substituted)phenyl]-10,10-dimethyl-7,8,9,10,11,12-hexahydrobenz[*c*]acridin-8-thione.

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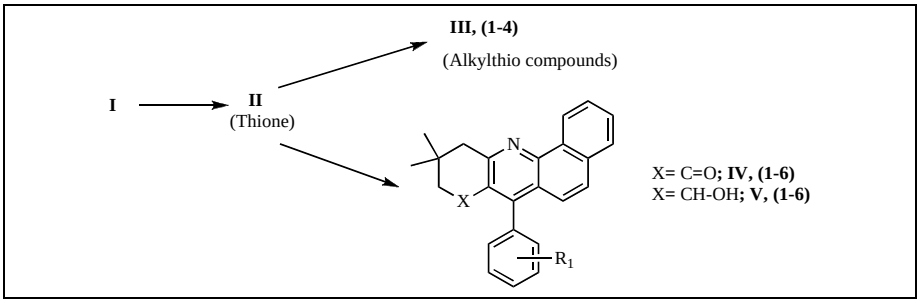

A series of sixteen new derivatives have been obtained and all have potentially useful pharmacological activity. The treatment of 7-[(*o*-chloro and *p*-bromo)phenyl]-7,8,9,10,11,12-hexahydrobenz[*c*]acridin-8-one and Lawesson´s reagent obtains the corresponding 7-[(*o*- and *p*-substituted)phenyl]-10,10-dimethyl-7,8,9,10,11,12-hexahydrobenz[*c*]acridin-8-thione **II** which was alkylated in presence of sodium hydride and the corresponding alkyl iodide under nitrogen atmosphere to obtain 8-alkylthio-7,9,10,11-tetrahydro-benz[*c*]acridines **III, 1-4**. The thione **II** was desprotected and aromatized in presence of sodium hydride in absence of nitrogen atmosphere to produce a mixture of 7-[(*o*- and *p*-substituted)phenyl]-10,10-dimethyl-8,9,10,11-tetrahydrobenz[*c*]-acridin-8-one **IV, 1-6** and 7-[(*o*- and *p*-substituted)phenyl]-10,10-dimethyl-8-hydroxi-8,9,10,11-tetrahydrobenz[*c*]acridine **V, 1-6**. The structure of all products was corroborated by ir, ^{1}H NMR, ^{13}C NMR with bidimensional experiments and ms with CID experiments.

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INTRODUCTION

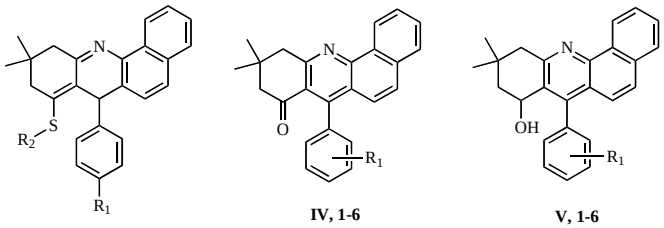
The acridine derivatives are considered to be important chemotherapeutics as they have shown fungicidal, bactericidal and antimalarial effects [3]. Also the acridine derivatives have been applied for the treatment of protozoal infections caused by Plasmodium microorganisms [4]. The importance of those derived of acridines has grown due to recently their antineoplasmic properties [5] as the acridine-4-carboxamides [6], which are in clinical trial [7].

Papers have been published describing the synthesis of benz[*c*]acridine derivatives [8-11]. We have previously reported the synthesis of 7-[(*o*- and *p*-R)phenyl]-10,10-dimethyl-8,9,10,11-tetrahydrobenz[*c*]-acridin-8-ones, and the mass spectra patterns [12-13]. In addition, we have reported the synthesis of derivatives of 12-[(*o*-; and *p*-R)phenyl]-9,9-dimethyl-7,8,9,10,11,12-hexahydro and 8,9,10,11-tetrahydro-benz[a]acridin-11-ones [14].

The oxidation of C=S of the thioketones by air is well known, but neither the mechanism nor the reactive species have been established. The oxidation of the derivatives of benz[*c*]acridin-8-thione is carried out through molecular oxygen, which transforms the thioketones in the corresponding carbonyl compound in this reaction [15-16].

To continue with our research program on the synthesis and the spectral property determination of benz[*c*]acridine derivatives with possible pharmacological activity, we describe in this report the synthesis of the novel compounds 7-(*p*-bromophenyl)-10,10-dimethyl-8-alkylthio-7,9,10,11-tetrahydrobenz[*c*]-acridines **III, 1-4,** and the deprotection and aromatization of 7-[(*o* - and *p*-substituted)phenyl]-10,10-dimethyl-7,8,9,10,11,12-hexahydrobenz[*c*]acridin-8-thione **II** in presence of sodium hydride in the atmosphere to obtain a mixture of 7-[(*o*- and *p*-substituted)phenyl]-10,10-dimethyl-8,9,10,11-tetrahydrobenz[*c*]acridin-8-one **IV, 1-6** and 7-[(*o*- and *p*-substituted)phenyl]-10,10-dimethyl-8-hydroxi-8,9,10,11-tetrahydrobenz[*c*]-acridine **V, 1-6** (Scheme 1). The synthesis of these compounds was carried out in Scheme 2.

Scheme 1



III, 1-4, (R_1= p-Br)

IV, 1-6

V, 1-6

R_2	
1	CH_3
2	CH_2CH_3
3	$CH_2CH_2CH_3$
4	$CH_2CH_2CH_2CH_3$

R_1	
1	o-Cl
2	o-Br
3	o-OMe
4	p-Cl
5	p-Br
6	p-OMe

RESULTS AND DISCUSSION

The compound 7-(*p*-bromophenyl)-10,10-dimethyl-7,8,9,10,11,12-hexahydrobenz[*c*]acridin-8-one **I** and the Lawesson´s reagent in dry toluene was heated at reflux under nitrogen atmosphere for 3 hours. The benz[*c*]-acridin-8-thiones **II**, have been obtained in a 19-25% yield. The treatment of compounds **II**, with sodium hydride and the corresponding alkyl iodide at reflux in anhydrous toluene under nitrogen atmosphere for 4 to 20 hours afforded the compounds 7-(*p*-bromophenyl)-10,10-dimethyl-8-alkylthio-7,9,10,11-tetrahydrobenz[*c*]acridines **III, 1-4**, which have been obtained in a 15-65% yield.

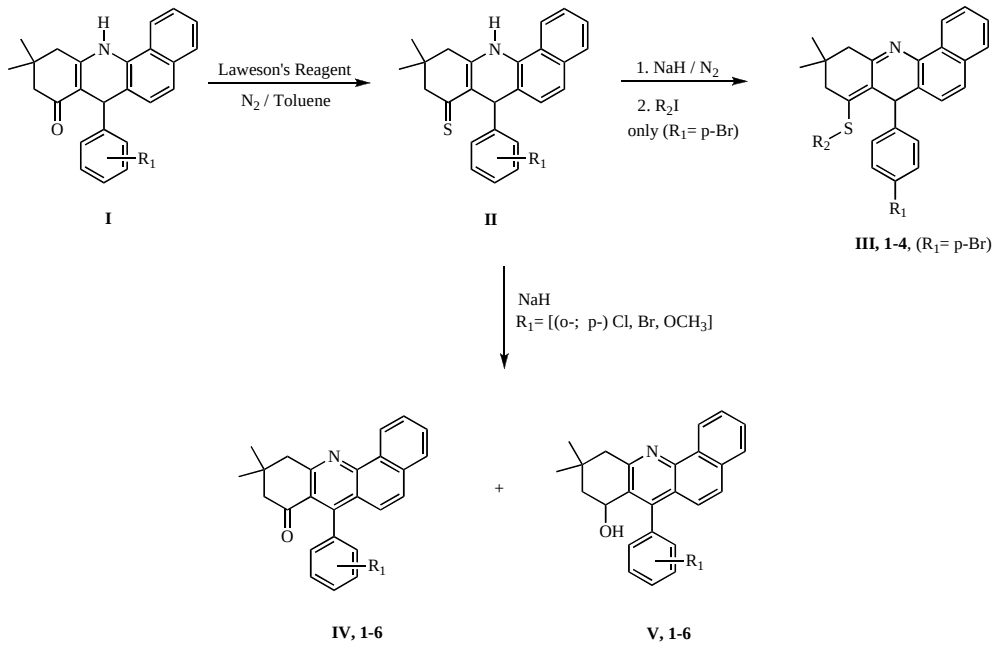
The infrared of compounds **III, 1-4** displayed absorptions at 1585-1590 cm^{-1} for C=N stretching, at 1315 cm^{-1} for C-S stretching, at 1350- 1355 and 1275- 1260 cm^{-1} for C-N stretching.

In the ^{1}H-nmr spectra for the compounds **III, 1-4** displayed the presence of two-three protons signals at δ 1.11-0.99 singlet for the gem-dimethyl; one proton signal at δ 8.90-8.76 doublet for the proton in C-1; this signal is out of the aromatic protons field, because the free electrons of the nitrogen in the acridine compounds shifts this proton-signal at low field; the other aromatic protons appear as multiplet and AA'BB' signals at 8.00-7.04, and with the signal for the R_2-substituents. The ^{13}C-nmr spectra of compounds **III, 1-4**; are given in Table 1.

The signals were confirmed by using HETCOR, LONG RANGE HETCOR, FLOCK, APT, DEPT, COSY and NOESY nmr experiments operating at 300 and 500 MHz. The mass spectra of compounds **III, 1-4** include the ion molecular $[M]^+$, and m/z ion for $[M-(76-R_1)]^+$ as the base peak, in all the compounds. Other important fragments are: $[M-15]^+$, $[M-17]^+$, $[M-R_2]^+$, $[M-SR_2]^+$, and m/z 366, 350, 258, 244 and 243.

When we try to obtain the derived thioalkylated with substituents *o*-Cl; *o*-Br; *o*-OCH_3; *p*-Cl and *p*-OCH_3 under similar conditions of 7-(*p*-bromophenyl)-10,10-dimethyl-7,8,9,10,11,12-hexahydrobenz[*c*]acrdin-8-thione **II**, the alkylthio derivates were not obtained but two new derivatives were obtained with differences in two units of mass. So we obtained two different compounds to alkyl-thio derivatives, when we carried out the reaction with

Scheme 2



I **II** **III, 1-4**, (R_1= p-Br)

IV, 1-6 **V, 1-6**

R_1= [(o-; p-) Cl, Br, OCH_3]

NaH in absence of nitrogen atmosphere to obtain a mixture of 7-[(*o*- and *p*-substituted)phenyl]-10,10-dimethyl-8,9,10,11-tetrahydrobenz[*c*]acridin-8-one **IV, 1-6** and 7-[(*o*- and *p*-substituted)phenyl]-10,10-dimethyl-8-hydroxi-8,9,10,11-tetrahydrobenz[*c*]acridine **V, 1-6**; which have been obtained in a 8-32% and 6-67% yield respectively.

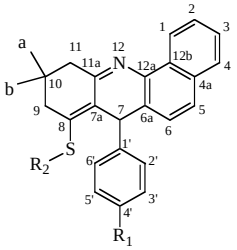
We can explain that the deprotection of thioketone is carried out by means of the molecular oxygen of the atmosphere to give the corresponding carbonyl compound, which can suffer the aromatization in presence of NaH to obtain the compound **IV, 1-6**, and this compound is reduced in presence of NaH to obtain as well the compound **V, 1-6**.

The infrared spectrum of compounds **IV, 1-6** displayed absorptions at 1687-1694 cm^{-1} for C=O stretching, at 1547-1554 cm^{-1} for C=N stretching, at 1255 and 1302 cm^{-1} for C-N stretching, and the corresponding absorptions for the R-substituent.

The infrared spectrum of compounds **V, 1-6** displayed absorptions at 3577-3597 cm^{-1} for OH stretching, at 1552-1573 cm^{-1} for C=N stretching, at 1288 and 1305 cm^{-1} for C-N stretching, 1024-1087 cm^{-1} for C-O stretching, and the corresponding absorptions for the R-substituent. In the ^{1}H-nmr spectra for the compounds **IV, 1-6** displayed the presence of two-three protons or six protons at δ 1.19-1.08 singlet for the gem-dimethyl; one proton signal at δ

Table 1

^{13}C NMR Spectral Data for Compounds **III, 1-4**



III, 1-4

Compounds	**1**	**2**	**3**	**4**
R_1	*p*-Br	*p*-Br	*p*-Br	*p*-Br
R_2	CH_3	CH_2CH_3	$CH_2CH_2CH_3$	$CH_2CH_2CH_2CH_3$
	(C-1")	(C-2"-C-1")	(C-3"-C-2"-C-1")	(C-4"-C-3"-C-2"-C-1")
C-1	123.5	123.4	123.6	123.6
C-2	125.6	125.6	125.3	125.3
C-3	125.6	125.2	125.3	125.3
C-4	127.3	126.8	127.2	127.3
C-4a	132.7	132.6	132.8	132.8
C-5	125.7	125.4	125.8	125.9
C-6	126.6	125.9	125.8	125.9
C-6a	124.2	125.2	124.9	125.0
C-7	44.0	44.6	40.9	40.9
C-7a	130.9	130.1	131.0	131.0
C-8	150.5	147.2	150.6	150.6
C-9	47.0	47.3	47.2	47.3
C-10	31.8	31.7	31.9	31.9
C-11	42.4	43.1	42.8	42.8
C-11a	160.4	160.1	160.6	160.7
C-12a	143.8	142.8	142.9	142.9
C-12b	129.9	130.1	130.1	130.1
C-1'	136.2	136.4	135.9	135.9
C-2'	131.2	130.9	129.2	129.2
C-3'	129.4	128.9	127.9	128.0
C-4'	119.4	119.7	119.0	119.0
C-5'	129.4	128.9	128.2	128.2
C-6'	131.2	130.9	129.5	129.6
C-1"	13.4	14.6	12.9	13.4
C-2"	-	24.7	22.9	21.1
C-3"	-	-	31.8	29.7
C-4"	-	-	-	31.6
CH_{3a}	26.9	26.6	27.0	27.0
CH_{3b}	28.6	28.8	28.6	28.6

Note: The numbering of the phenyl ring and alkylthio chain is only for the assignment of the chemical shifts of the carbon in ^{13}C nmr spectra.

9.38-9.24 doublet for the proton in C-1; as same as by the nitrogen effects in the compounds **III-1-4**; the other aromatic protons appear as multiplet and AA'BB' signals at δ 8.00-7.04.

In the ^{1}H-nmr spectra for the compounds **V, 1-6** displayed the presence of two-three protons signals at δ 1.21-0.87 singlet for the gem-dimethyl; one proton signal resonating at δ 9.23-9.18 doublet for the proton at C-1; as same as by the nitrogen effects in the compounds **III-1-4**; the other aromatic protons appear as multiplet and AA'BB' signals at δ 7.95-7.02; and the new hydroxyl-proton signal at δ 4.63-4.48 doublet, deuterium oxide exchangeable.

The ^{13}C-nmr spectra of compounds **IV, 1-6** and **V, 1-6** are given in Tables 2.

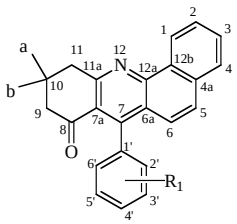
The signals were confirmed by using HETCOR, LONG RANGE HETCOR, FLOCK, APT, DEPT, COSY and NOESY nmr experiments operating at 300 and 500 MHz.

The mass spectra of compounds **IV, 1-6** include ions at m/z ion molecular $[M]^+$ as the base peak when the substituents are *p*-Cl and *p*-OCH_3 and the fragment ion $[M\text{-}R_1]^+$ as the base peak when the substituents are *o*-Br; *o*-Cl and *o*-OCH_3, in the case of *p*-Br the base peak is the fragment at m/z 266. Other important fragments ions are: $[M\text{-}1]^+$, $[M\text{-}15]^+$, $[M\text{-}29]^+$, $[M\text{-}43]^+$, $[M\text{-}56]^+$, $[M\text{-}R_1]^+$, $[M\text{-}(HR_1+56)]^+$, $[M\text{-}84]^+$, when the substituents are *o*-Br; *o*-Cl and *o*-OCH_3 other important fragments are: $[M\text{-}(R_1+16)]^+$, $[M\text{-}R_1]^+$, $[M\text{-}(R_1+30)]^+$, and m/z 266, 264, 239.

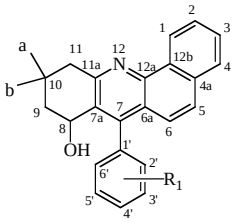
The mass spectra of compound **V, 1-6** includes ions at m/z ion molecular $[M]^+$ as the base peak for all compounds, except when the substituent is *p*-Br the base peak is the fragment ion $[M\text{-}84]^+$. Other important fragments ions are: $[M\text{-}1]^+$, $[M\text{-}15]^+$, $[M\text{-}17]^+$, $[M\text{-}18]^+$, $[M\text{-}33]^+$, $[M\text{-}43]^+$, $[M\text{-}56]^+$, $[M\text{-}57]^+$, $[M\text{-}84]^+$, when the substituents are *o*-Br; *o*-Cl and *o*-OCH_3 other important fragments ions appear at m/z $[M\text{-}(R_1+18)]^+$, $[M\text{-}R_1]^+$, $[M\text{-}(HR_1+33)]^+$, $[M\text{-}(HR_1+47)]^+$, [M-

Table 2

^{13}C NMR Spectral Data for Compounds **IV, 1-6** and **V, 1-6**



IV, 1-6



V, 1-6

Compounds	**IV, 1**	**IV, 2**	**IV, 3**	**IV, 4**	**IV, 5**	**IV, 6**	**V, 1**	**V, 2**	**V, 3**	**V, 4**	**V, 5**	**V, 6**
R_1	*o*-Cl	*o*-Br	*o*-OCH_3	*p*-Cl	*p*-Br	*p*-OCH_3	*o*-Cl	*o*-Br	*o*-OCH_3	*p*-Cl	*p*-Br	*p*-OCH_3
C-1	124.8	124.8	124.8	125.6	125.6	125.4	124.0	124.0	124.0	124.0	124.1	124.1
C-2	127.9	127.8	127.3	127.3	127.3	127.6	127.0	127.1	129.5	126.9	126.5	128.0
C-3	127.5	127.5	127.2	127.7	129.5	129.9	128.2	128.2	126.0	128.1	127.8	126.0
C-4	127.9	127.9	127.8	127.7	127.7	128.3	127.7	127.7	127.6	127.7	127.4	127.6
C-4a	133.7	133.7	133.6	134.2	134.2	134.1	131.4	130.4	131.1	132.7	132.9	132.7
C-5	129.6	129.7	129.4	129.4	127.6	127.8	126.7	126.7	126.7	126.4	126.1	126.7
C-6	122.5	122.5	123.2	123.5	123.5	123.9	122.3	122.4	123.1	122.9	122.8	123.4
C-6a	123.5	123.4	124.1	124.6	124.6	124.9	123.4	123.3	123.4	123.5	123.4	124.1
C-7	145.6	147.2	146.0	148.5	148.5	149.5	144.2	145.9	145.5	146.1	145.9	146.9
C-7a	122.9	122.6	123.9	123.1	123.0	124.1	130.4	130.3	129.0	130.0	129.7	130.3
C-8	198.9	196.8	196.9	198.2	198.2	197.9	64.5	64.5	64.7	63.9	64.0	64.2
C-9	52.8	52.8	53.0	54.2	54.2	54.0	45.4	45.4	45.1	45.0	45.0	44.9
C-10	32.0	31.9	31.9	32.5	32.5	32.5	30.7	30.8	30.4	30.2	30.1	30.2
C-11	47.4	47.4	47.5	48.4	48.4	48.2	47.5	47.4	47.4	47.6	47.5	47.4
C-11a	160.6	160.6	160.3	160.5	160.5	161.0	157.3	157.5	157.1	157.1	157.0	157.3
C-12a	147.1	147.2	146.9	148.1	148.2	147.2	144.2	144.2	143.7	144.1	144.2	144.0
C-12b	129.8	129.8	129.9	130.6	130.0	130.1	130.6	130.3	130.5	130.4	130.4	130.5
C-1'	136.6	138.7	133.6	136.5	137.1	134.1	135.1	137.1	132.7	135.4	135.7	135.5
C-2'	131.2	121.5	155.9	129.6	129.9	130.1	117.9	122.0	157.3	130.2	130.3	129.8
C-3'	129.2	132.0	111.1	128.4	131.4	113.9	128.9	132.0	111.2	127.9	130.8	113.5
C-4'	128.9	129.3	129.0	133.5	121.6	159.0	129.8	129.9	127.9	123.5	121.0	158.7
C-5'	127.0	127.5	120.3	128.4	131.4	113.9	126.6	127.0	120.1	127.9	130.6	113.4
C-6'	129.7	129.7	129.2	129.6	129.9	130.1	132.8	132.8	131.8	132.4	132.6	131.6
CH_{3a}	27.1	27.0	27.4	27.7	28.3	28.3	28.3	28.3	30.6	29.4	29.4	30.1
CH_{3b}	28.2	28.3	28.0	27.7	28.3	28.3	30.7	30.8	31.0	30.3	30.3	30.3
OCH_3	-	-	55.3	-	-	55.5	-	-	55.4	-	-	55.0

Note: The numbering of the phenyl ring is only for the assignment of the chemical shifts of the carbon in ^{13}C nmr spectra

$(HR_1+56)]^+$, m/z 276, 267 and 239. The mass spectra of the compounds exhibit a stable molecular ion and the main fragmentation was consistent with the assigned structures. The proposed fragmentation pathways that lead to the formation of number of important daughter ions have been confirmed for the corresponding parent ion spectra by collision-induced dissociation (CID) experiments. The elemental composition of the molecular ion and the principal fragment ion was determined by exact mass measurements.

In order to confirm the structure of the compounds (**IV, 1-6**) and (**V, 1-6**) X-ray crystal structure determination was carried out for the compounds 7-(*o*-methoxyphenyl)-10,10-dimethyl-8,9,10,11-tetrahydrobenz[*c*]acridin-8-one (**IV, 3**) and 7-(*p*-chlorophenyl)-10,10-dimethyl-8-hydroxi-8,9,10,11-tetrahydrobenz[*c*]acridine (**V, 4**). The Figures 1 and 2 respectively show the molecular structure together with the atom numbering Scheme. The bond distances (Å) and the angles (deg) are given in Tables 3 and 4. The X-ray crystallographic data for the compounds (**IV, 3**) and (**V, 4**) show that the tetrahydro ring on the acridine moiety adopts a half-chair conformation while the rest of this group is planar and the substituent R_1-phenyl of the position C_7 is outside of the plane of acridine unit.

Crystal data collection parameters and structure refinement parameters for the compounds (**IV, 3**) and (**V, 4**), are given in Table 5.

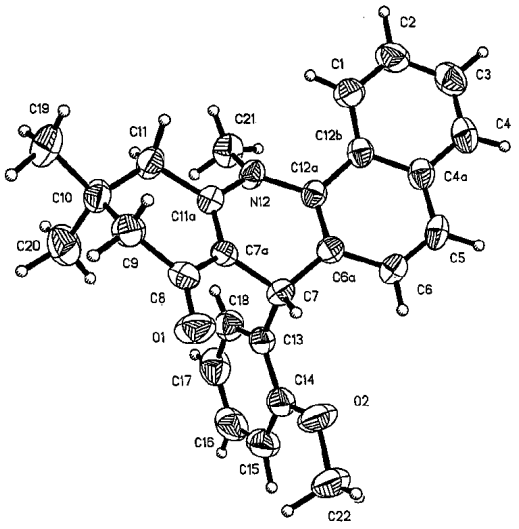


Figure 1. Crystal structure of compound **IV**, 3 with the atom numbering scheme.

EXPERIMENTAL

The ir spectra were recorded on a Nicolet Magna TR-750 spectrophotometer. The ^{1}H-nmr spectra were recorded on a Varian Unity 300 spectrometer operating at 300 MHz and the ^{13}C-nmr

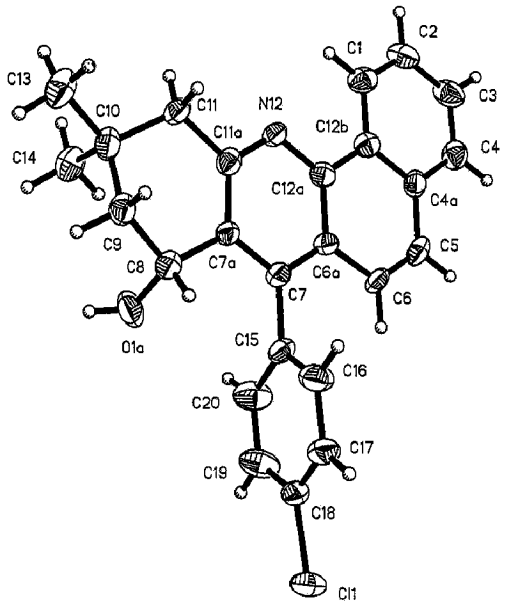


Figure 2. Crystal structure of compound **V**, 4 with the atom numbering scheme.

spectra were recorded on a Varian Unity 500 spectrometer operating at 125 MHz in deuteriochloroform solution containing tetramethylsilane as the internal standard with chemical shifts δ (ppm) expressed downfield from tetramethylsilane. The mass spectra were measured on a JEOL JMS-AX505 and JEOL MS-SX 102A high-resolution mass spectrometer with accurate mass determination of the molecular ion and the principal fragments ions, using the direct inlet system. The spectra were recorded by electron impact at an ionization chamber temperature of 190° and ionizing electron energy of 70 eV.

The compounds **I** were prepared following literature methods with modifications [12].

General Procedure for the Synthesis of 7-[(*o*-, and *p*-substituted)phenyl]-10,10-dimethyl-7,8,9,10,11,12-hexahydrobenz[*c*]acridin-8-thiones II. A mixture of 2.58 x 10^{-3} mole of 7-[(*o*-; and *p*-substituted)phenyl]-10,10-dimethyl-7,8,9,10,11,12-hexahydrobenz[*c*]acridin-8-ones **I**, 1.29 x 10^{-3} mole of Lawesson's reagent, in 150 ml of dry toluene was heated at reflux for three hours, under nitrogen atmosphere. After reaction mixture was evaporated *in vacuo* to yield a solid or semisolid, which were purified by crystallization (acetone-hexane), the crystals were collected and washed with hexane afforded the benz[*c*]acridin-8-thiones **II**, with 19-25% yield.

General Procedure for the Synthesis of the 7-(*p*-Bromophenyl)-10,10-dimethyl-8-alkylthio-7,9,10,11-tetrahydrobenz[*c*]acridines III, 1-4. A mixture of 0.33 x 10^{-3} mole of 7-(*p*-bromophenyl)-10,10-dimethyl-7,8,9,10,11,12-hexahydrobenz[*c*]acridin-8-thiones **II**, 0.33 x 10^{-3} mole of sodium hydride in 30 ml of dry toluene was heated at reflux for one hour under nitrogen atmosphere. After the reaction mixture was cooled at room temperature, subsequently was added dropwise over a few minutes 0.33 x 10^{-3} mole of alkyl iodide and the reflux continued for 4 to 20 hours. After reaction mixture was evaporated *in vacuo* to yield a solid, which was purified by crystallization (acetone-hexane), the crystals was collected and washed with hexane afforded the 8-alkylthio-7,9,10,11-tetrahydrobenz[*c*]acridines **III, 1-4**, in a 15-65% yield.

Table 3

Bond Distances (Å) an the Angles (deg) for the 7-(*o*-methoxyphenyl)-10,10-dimethyl-8,9,10,11-tetrahydrobenz[*c*]acridin-8-one (**IV, 3**) with standard deviations in parentheses.

O(1)-C(8)	1.234 (6)	C(15)-C(16)	1.359 (9)	C(7A)-C(11A)	1.351 (6)
O(2)-C(22)	1.406 (7)	C(16)-C(17)	1.376 (9)	C(8)-C(9)	1.504 (7)
C(1)-C(12B)	1.402 (7)	C(17)-C(18)	1.388 (8)	C(9)-H(9A)	0.980 (5)
C(2)-C(3)	1.400 (8)	C(18)-H(18)	0.850 (6)	C(10)-C(19)	1.518 (8)
C(3)-C(4)	1.364 (8)	C(19)-H(19B)	1.120 (6)	C(10)-C(20)	1.537 (8)
C(4)-C(4A)	1.418 (7)	C(20)-H(20A)	0.950 (7)	C(11)-H(11A)	1.060 (5)
C(4A)-C(5)	1.412 (7)	C(20)-H(20C)	0.960 (7)	C(11A)-N(12)	1.387 (6)
C(5)-C(6)	1.373 (7)	C(21)-H(21B)	0.970 (6)	N(12)-C(21)	1. 468 (6)
C(6)-C(6A)	1.416 (6)	C(22)-H(22A)	1.070 (7)	C(13)-C(18)	1.377 (7)
C(6A)-C(12A)	1.366 (6)	C(22)-H(22C)	1.000 (7)	C(14)-C(15)	1.389 (7)
C(7)-C(7A)	1.511 (6)	O(2)-C(14)	1.363 (6)	C(15)-H(15)	1.000 (6)
C(7)-H(7)	0.920 (5)	C(1)-C(2)	1.359 (7)	C(16)-H(16)	0.940 (6)
C(7A)-C(8)	1.452 (6)	C(1)-H(1)	0.950 (5)	C(17)-H(17)	0.890 (6)
C(9)-C(10)	1.528 (7)	C(2)-H(2)	1.050 (6)	C(19)-H(19A)	0.910 (6)
C(9)-H(9B)	0.980 (6)	C(3)-H(3)	1.040 (6)	C(19)-H(19C)	0.950 (6)
C(10)-C(11)	1.521 (7)	C(4)-H(4)	0.930 (6)	C(20)-H(20B)	1.150 (7)
C(11)-C(11A)	1.505 (7)	C(4A)-C(12A)	1.428 (6)	C(21)-H(21A)	0.990 (6)
C(11)-H(11B)	0.920 (5)	C(5)-H(5)	0.970 (6)	C(21)-H(21C)	1.080 (6)
N(12)-C(12A)	1.419 (5)	C(6)-H(6)	0.960 (5)	C(22)-H(22B)	0.970 (7)
C(12A)-C(12B)	1.451 (6)	C(6A)-C(7)	1.520 (6)		
C(13)-C(14)	1.402 (6)	C(7)-C(13)	1.528 (6)		
C(14)-O(2)-C(22)	118.5 (5)	C(16)-C(15)-H(15)	121.0 (4)	C(10)-C(9)-H(9A)	109.0 (3)
C(2)-C(1)-H(1)	117.0 (3)	C(15)-C(16)-C(17)	120.8 (5)	C(10)-C(9)-H(9B)	114.0 (3)
C(1)-C(2)-C(3)	120.7 (5)	C(17)-C(16)-H(16)	124.0 (4)	C(19)-C(10)-C(11)	109.2 (5)
C(3)-C(2)-H(2)	118.0 (3)	C(16)-C(17)-H(17)	123.0 (4)	C(11)-C(10)-C(9)	108.3 (4)
C(4)-C(3)-H(3)	120.0 (3)	C(13)-C(18)-C(17)	121.5 (5)	C(11)-C(10)-C(20)	110.8 (5)
C(3)-C(4)-C(4A)	121.6 (5)	C(17)-C(18)-H(18)	118.0 (4)	C(11A)-C(11)-C(10)	115.1 (4)
C(4A)-C(4)-H(4)	121.0 (4)	C(10)-C(19)-H(19B)	102.0 (3)	C(10)-C(11)-H(11A)	110.0 (3)
C(5)-C(4A)-C(12B)	119.7 (4)	C(10)-C(19)-H(19C)	114.0 (4)	C(10)-C(11)-H(11B)	110.0 (3)
C(6)-C(5)-C(4A)	120.3 (4)	H(19B)-C(19)-H(19C)	106.0 (5)	C(7A)-C(11A)-N(12)	121.3 (4)
C(4A)-C(5)-H(5)	116.0 (3)	C(10)-C(20)-H(20B)	111.0 (3)	N(12)-C(11A)-C(11)	115.6 (4)
C(5)-C(6)-H(6)	123.0 (3)	C(10)-C(20)-H(20C)	117.0 (4)	C(11A)-N(12)-C(21)	119.1 (4)
C(12A)-C(6A)-C(6)	119.9 (4)	H(20B)-C(20)-H(20C)	103.0 (5)	C(6A)-C(12A)-N(12)	121.3 (4)
C(6)-C(6A)-C(7)	120.3 (4)	N(12)-C(21)-H(21B)	112.0 (3)	N(12)-C(12A)-C(12B)	118.1 (4)
C(7A)-C(7)-C(13)	112.8 (4)	N(12)-C(21)-H(21C)	116.0 (3)	C(1)-C(12B)-C(12A)	124.0 (4)
C(7A)-C(7)-H(7)	105.0 (3)	H(21B)-C(21)-H(21C)	104.0 (4)	C(18)-C(13)-C(14)	117.9 (5)
C(13)-C(7)-H(7)	108.0 (3)	O(2)-C(22)-H(22B)	114.0 (4)	C(14)-C(13)-C(7)	119.9 (4)
C(11A)-C(7A)-C(7)	120.9 (4)	O(2)-C(22)-H(22C)	109.0 (4)	O(2)-C(14)-C(13)	116.3 (4)
O(1)-C(8)-C(7A)	122.0 (4)	H(22B)-C(22)-H(22C)	105.0 (6)	C(16)-C(15)-C(14)	120.1 (5)
C(7A)-C(8)-C(9)	117.1 (4)	C(2)-C(1)-C(12B)	121.8 (5)	C(14)-C(15)-H(15)	119.0 (4)
C(8)-C(9)-H(9A)	110.0 (3)	C(12B)-C(1)-H(1)	121.0 (3)	C(15)-C(16)-H(16)	115.0 (4)
C(8)-C(9)-H(9B)	107.0 (3)	C(1)-C(2)-H(2)	121.0 (3)	C(16)-C(17)-C(18)	119.3 (6)
H(9A)-C(9)-H(9B)	103.0 (4)	C(4)-C(3)-C(2)	119.4 (5)	C(18)-C(17)-H(17)	118.0 (4)
C(19)-C(10)-C(9)	109.9 (5)	C(2)-C(3)-H(3)	120.0 (3)	C(13)-C(18)-H(18)	121.0 (4)
C(19)-C(10)-C(20)	109.6 (5)	C(3)-C(4)-H(4)	117.0 (3)	C(10)-C(19)-H(19A)	110.0 (4)
C(9)-C(10)-C(20)	109.1 (5)	C(5)-C(4A)-C(4)	122.0 (5)	H(19A)-C(19)-H(19B)	111.0 (5)
C(11A)-C(11)-H(11A)	105.0 (3)	C(4)-C(4A)-C(12B)	118.3 (5)	H(19A)-C(19)-H(19C)	114.0 (5)
C(11A)-C(11)-H(11B)	109.0 (3)	C(6)-C(5)-H(5)	124.0 (3)	C(10)-C(20)-H(20A)	113.0 (4)
H(11A)-C(11)-H(11B)	108.0 (4)	C(5)-C(6)-C(6A)	121.2 (5)	H(20A)-C(20)-H(20B)	105.0 (5)
C(7A)-C(11A)-C(11)	123.1 (4)	C(6A)-C(6)-H(6)	116.0 (3)	H(20A)-C(20)-H(20C)	107.0 (6)
C(11A)-N(12)-C(12A)	117.1 (4)	C(12A)-C(6A)-C(7)	119.8 (4)	N(12)-C(21)-H(21A)	111.0 (3)
C(12A)-N(12)-C(21)	119.5 (4)	C(7A)-C(7)-C(6A)	109.3 (4)	H(21A)-C(21)-H(21B)	107.0 (4)
C(6A)-C(12A)-C(12B)	120.5 (4)	C(6A)-C(7)-C(13)	111.6 (4)	H(21A)-C(21)-H(21C)	106.0 (4)
C(1)-C(12B)-C(4A)	118.0 (4)	C(6A)-C(7)-H(7)	110.0 (3)	O(2)-C(22)-H(22A)	111.0 (4)
C(4A)-C(12B)-C(12A)	117.9 (4)	C(11A)-C(7A)-C(8)	120.2 (4)	H(22A)-C(22)-H(22B)	112.0 (5)
C(18)-C(13)-C(7)	122.1 (4)	C(8)-C(7A)-C(7)	118.9 (4)	H(22A)-C(22)-H(22C)	107.0 (5)
O(2)-C(14)-C(15)	123.3 (5)	O(1)-C(8)-C(9)	120.8 (4)		
C(15)-C(14)-C(13)	120.4 (5)	C(8)-C(9)-C(10)	113.4 (4)		

7-(*p*-Bromophenyl)-10,10-dimethyl-8-methylthio-7,9,10,11-tetrahydrobenz[*c*]acridine (III, 1). This compound was obtained as a yellow solid in a 15% yield, mp 150°; ir (chloroform): υ C=N 1591, R_2-S 1315, C-N 1262 and 1254 cm^{-1}; ^1H nmr (deuteriochloroform): δ 0.99 (s, 3H, C_{10}-CH_{3a}), 1.06 (s, 3H, C_{10}-CH_{3b}), 2.37 (s, 3H, S-CH_3), 2.49 (s, 1H, 11-Ha), 2.53 (s, 1H, 11-Hb), 2.66 (s, 1H, 9-Ha), 2.71 (s, 1H, 9-Hb), 5.12 (s, 1H, 7-H), 7.15 and 7.38 (AA'BB', 4H, J = 8.4 Hz, phenyl protons of "E" ring), 7.30 (d, 1H, J = 8.7 Hz, 6-H), 7.45 (dt, 1H, J = 1.2, 8.1 Hz, 3-H), 7.52 (dt, 1H, J = 1.2, 6.9 Hz, 2-H), 7.58 (d, 1H, J = 8.4 Hz, 5-H), 7.7 (d, 1H, J = 8.1 Hz, 4-H), 8.76 (d, 1H, J = 7.8 Hz, 1-H); ms: m/z 461 $(M)^+$, 463 $[M+2]^+$, 465 $[M+4]^+$. *Anal.* Calcd. for: $C_{26}H_{24}BrNS$: C, 67.53; H, 5.23; N, 3.03. Found: C, 67.45; H, 5.16; N, 3.10.

7-(*p*-Bromophenyl)-10,10-dimethyl-8-ethylthio-7,9,10,11-tetrahydrobenz[*c*]acridine (III, 2). This compound was obtained as a yellow solid in a 65% yield, mp 191°; ir (chloroform): υ C=N 1590, CH_3-S 1315, C-N 1263 and 1260 cm^{-1}; ^1H nmr (deuteriochloroform): δ 1.05 (s, 3H, C_{10}-CH_{3a}), 1.11 (s, 3H, C_{10}-CH_{3b}), 1.27 (t, 3H, J= 8.4 Hz, S-CH_2CH_3), 2.47 (s, 1H, 11-Ha), 2.47 (s, 1H, 11-Hb), 2.76 (s, 1H, 9-Ha), 2.81 (s, 1H, 9-Hb), 2.91 (q, 2H, J= 8.0 Hz, S-CH_2CH_3), 5.17 (s, 1H, 7-H), 7.10 and 7.28 (AA'BB', 4H, J = 8.4 Hz, phenyl protons of "E" ring), 7.17 (d, 1H, J = 8.4 Hz, 6-H), 7.44 (dt, 1H, J = 1.2, 7.8 Hz, 3-H), 7.53 (dt, 1H, J = 1.5, 8.4 Hz, 2-H), 7.54 (d, 1H, J = 8.4 Hz, 5-H), 7.72 (d, 1H, J = 7.8 Hz, 4-H), 8.90 (d, 1H, J = 8.7 Hz 1-H); ms: m/z 475 $(M)^+$, 477 $[M+2]^+$, 479 $[M+4]^+$. *Anal.* Calcd. for: $C_{27}H_{26}BrNS$: C, 68.06; H, 5.50; N, 2.94. Found: C, 68.14; H, 5.43; N, 2.85.

7-(*p*-Bromophenyl)-10,10-dimethyl-8-propylthio-7,9,10,11-tetrahydrobenz[c]acridine (III, 3). This compound was obtained as a yellow solid in a 37% yield, mp 229°; ir (chloroform): υ C=N 1597, CH_3-S 1317, C-N 1258 and 1250 cm^{-1}; ^1H nmr (deuteriochloroform): δ 0.91 (t, 3H, J= 8.2 Hz, S-$CH_2CH_2CH_3$), 1.03 (s, 3H, C_{10}-CH_{3a}), 1.11 (s, 3H, C_{10}-CH_{3b}), 1.50 (m, 2H, S-$CH_2CH_2CH_3$), 1.91 (t, 2H, J= 8.4 Hz, S-$CH_2CH_2CH_3$), 2.56 (s, 1H, 11-Ha), 2.60 (s, 1H, 11-Hb), 2.78 (d, 1H, 9-Ha), 2.82 (d, 1H, 9-Hb), 5.69 (s, 1H, 7-H), 7.13 and 7.40 (AA'BB', 4H, J = 8.7 Hz, phenyl protons of "E" ring), 7.14 (d, 1H, J = 8.7 Hz, 6-H), 7.47 (dt, 1H, J = 1.5, 7.8 Hz, 3-H), 7.54 (dt, 1H, J = 1.2, 8.4 Hz, 2-H), 7.60 (d, 1H, J = 8.4 Hz, 5-H), 7.77 (d, 1H, J = 7.8 Hz, 4-H), 8.77 (d, 1H, J = 7.5 Hz, 1-H); ms: m/z 489 $(M)^+$, 491 $[M+2]^+$,493 $[M+4]^+$. *Anal.* Calcd. for: $C_{28}H_{28}BrNS$: C, 68.56; H, 5.75; N, 2.85. Found: C, 68.65; H, 5.84; N, 2.80.

7-(*p*-Bromophenyl)-10,10-dimethyl-8-butylthio-7,9,10,11-tetrahydrobenz[*c*]acridine (III, 4). This compound was obtained as a yellow solid in a 19% yield, mp 173°; ir (chloroform): υ C=N 1590, CH_3-S 1316, C-N 1254 and 1250 cm^{-1}; ^1H nmr (deuteriochloroform): δ 0.83 (t, 3H, J= 8.3 Hz, S-$CH_2CH_2CH_2CH_3$), 1.02 (s, 3H, C_{10}-CH_{3a}), 1.10 (s, 3H, C_{10}-CH_{3b}), 1.32 (m, 2H, S-$CH_2CH_2CH_2CH_3$), 1.44 (m, 2H, S-$CH_2CH_2CH_2CH_3$), 2.51 (s, 1H, 11-Ha), 2.53 (s, 1H, 11-Hb), 2.72 (s, 1H, 9-Ha), 2.77 (s, 1H, 9-Hb), 2.82 (t, 2H, J= 8.4 Hz, S-$CH_2CH_2CH_2CH_3$), 5.67 (s, 1H, 7-H), 7.12 and 7.38 (AA'BB', 4H, J = 8.7 Hz, phenyl protons of "E" ring), 7.13 (d, 1H, J = 8.7 Hz, 6-H),7.45 (dt, 1H, J = 1.2, 8.4 Hz, 3-H), 7.52 (dt, 1H, J Hz, 6-H), 7.45 (dt, 1H, J = 1.2, 8.4 Hz, 3-H), 7.52 (dt, 1H, J = 1.2, 8.4 Hz, 2-H), 7.58 (d, 1H, J = 8.7 Hz, 5-H), 7.75 (d, 1H, J = 7.5

Table 4

Bond Distances (Å) an the Angles (deg) for the 7-(*p*-Chlorophenyl)-10,10-dimethyl-8-hydroxi-8,9,10,11-tetrahydro-benz[*c*]acridine (**V, 4**) with standard deviations in parentheses

O(1)-C(18)	1.738 (9)	C(11A)-N(12)	1.328 (11)	C(7A)-C(8)	1.522 (12)
C(1)-C(12B)	1.403 (13)	C(12A)-C(12B)	1.431 (12)	C(8)-O(1A)	1.428 (12)
C(3)-C(4)	1.372 (14)	C(15)-C(20)	1.395 (13)	C(9)-C(10)	1.529 (13)
C(4A)-C(12B)	1.427 (12)	C(17)-C(18)	1.374 (14)	C(10)-C(14)	1.538 (13)
C(5)-C(6)	1.356 (12)	C(19)-C(20)	1.346 (14)	C(11)-C(11A)	1.514 (12)
C(6A)-C(7)	1.411 (12)	C(1)-C(2)	1.378 (13)	N(12)-C(12A)	1. 359 (10)
C(7)-C(7[a])	1.386 (11)	C(2)-C(3)	1.391 (14)	C(15)-C(16)	1.373 (13)
C(7A)-C(11A)	1.418 (12)	C(4)-C(4A)	1.409 (13)	C(16)-C(17)	1.391 (13)
C(8)-O(1B)	1.390 (4)	C(4A)-C(5)	1.437 (13)	C(18)-C(19)	1.348 (15)
C(8)-C(9)	1.521 (12)	C(6)-C(6A)	1.431 (12)		
C(10)-C(11)	1.509 (12)	C(6A)-C(12A)	1.414 (12)		
C(10)-C(13)	1.544 (13)	C(7)-C(15)	1.500 (12)		
C(2)-C(1)-C(12B)	121.3 (10)	N(12)-C(12A)-C(6A)	121.0 (8)	O(1B)-C(8)-C(9)	111.9 (16)
C(4)-C(3)-C(2)	119.1 (10)	C(6A)-C(12A)-C(12B)	121.2 (8)	C(7A)-C(8)-C(9)	113.8 (8)
C(4)-C(4A)-C(12B)	118.9 (9)	C(1)-C(12B)-C(12A)	122.9 (9)	C(11)-C(10)-C(9)	106.4 (7)
C(12B)-C(4A)-C(5)	118.3 (8)	C(16)-C(15)-C(20)	117.8 (9)	C(9)-C(10)-C(14)	112.6 (8)
C(5)-C(6)-C(6A)	121.5 (8)	C(20)-C(15)-C(7)	122.3 (9)	C(9)-C(10)-C(13)	108.3 (9)
C(7)-C(6A)-C(6)	122.1 (8)	C(18)-C(17)-C(16)	119.0 (11)	C(10)-C(11)-C(11A)	115.2 (8)
C(7A)-C(7)-C(6A)	118.1 (8)	C(19)-C(18)-Cl(1)	121.5 (9)	N(12)-C(11A)-C(11)	116.2 (8)
C(6A)-C(7)-C(15)	120.0 (8)	C(20)-C(19)-C(18)	120.5 (10)	C(11A)-N(12)-C(12A)	119.1 (8)
C(7)-C(7A)-C(8)	120.9 (8)	C(1)-C(2)-C(3)	120.9 (10)	N(12)-C(12A)-C(12B)	117.9 (8)
O(1B)-C(8)-O(1A)	100.0 (16)	C(3)-C(4)-C(4A)	121.8 (9)	C(1)-C(12B)-C(4A)	117.9 (8)
O(1A)-C(8)-C(7A)	107.0 (8)	C(4)-C(4A)-C(5)	122.7 (9)	C(4A)-C(12B)-C(12A)	119.2 (8)
O(1A)-C(8)-C(9)	112.8 (8)	C(6)-C(5)-C(4A)	121.7 (8)	C(16)-C(15)-C(7)	119.9 (8)
C(8)-C(9)-C(10)	115.3 (8)	C(7)-C(6A)-C(12A)	119.8 (8)	C(15)-C(16)-C(17)	120.6 (10)
C(11)-C(10)-C(14)	110.2 (9)	C(12A)-C(6A)-C(6)	118.1 (8)	C(19)-C(18)-C(17)	120.7 (9)
C(11)-C(10)-C(13)	110.1 (8)	C(7A)-C(7)-C(15)	121.9 (8)	C(17)-C(18)-Cl(1)	117.8 (9)
C(14)-C(10)-C(13)	109.1 (8)	C(7)-C(7A)-C(11A)	118.8 (8)	C(19)-C(20)-C(15)	121.4 (11)
N(12)-C(11A)-C(7A)	123.2 (8)	C(11A)-C(7A)-C(8)	120.3 (7)		
C(7A)-C(11A)-C(11)	120.5 (8)	O(1B)-C(8)-C(7A)	110.5 (16)		

Hz, 4-H), 8.76 (d, 1H, J = 8.1 Hz, 1-H);); ms: m/z 503 $(M)^+$, 505 $[M+2]^+$, 507 $[M+4]^+$. *Anal*. Calcd. for: $C_{29}H_{30}BrNS$: C, 69.03; H, 5.99; N, 2.78. Found: C, 69.11; H, 5.90; N, 2.86.

General procedure of the reaction of deprotection and aromatization of 7-[(*o*-; and *p*-substituted)phenyl]-10,10-dimethyl-7,8,9,10,11,12-hexahydrobenz[*c*]acridin-8-thione II, to obtain the compounds IV (1-6) and **V (1-6)**. A mixture of 0.25 x 10^{-3} mole of 7-[(*o*- and *p*-substituted)phenyl]-10,10-dimethyl-7,8,9,10,11,12-hexahydro-benz[*c*]acrdin-8-thione **II**, 0.25 x 10^{-3} mole of sodium hydride in 30 ml of dry toluene was heated at reflux for 24 hours in absence of nitrogen atmosphere. The course of the reaction was monitored by thin layer chromatography. After reaction mixture was evaporated *in vacuo* to yield a semisolid. The residual semisolid was purified on a silica gel chromatography column and elution with hexane-ethyl acetate (85:15) afforded 7-[(*o*- and *p*-substituted)phenyl]-10,10-dimethyl-8,9,10,11-tetrahydro-benz[*c*]acridin-8-one **IV, 1-6** with a 6-67% yield and 7-[(*o*- and *p*-substituted)phenyl]-10,10-dimethyl-8-hydroxi-8,9,10,11-tetrahydrobenz[*c*]acridine **V, 1-6**, with a 8-30% yield.

7-(*o*-Chlorophenyl)-10,10-dimethyl-8,9,10,11-tetrahydrobenz[*c*]acridin-8-one (IV, 1). This compound was obtained as a red solid in a 45% yield, mp 174°; ir (chloroform): υ C=O 1687, C=N 1550, C-N 1255, cm^{-1}; ^1H nmr (deuteriochloroform): δ 1.10 (s, 3H, C_{10}-CH_{3a}), 1.15 (s, 3H, C_{10}-CH_{3b}), 2.55 (d, 1H, J= 16.5 Hz, 9-Ha), 2.63 (d, J= 16.0 Hz, 9-Hb), 3.35 (s, 2H, 11-Ha, 11-Hb), 7.08 (d, 1H, J= 9.3 Hz, 6-H), 7.26 (dd, 1H, J= 2.1, 6.9 Hz, 6'-H), 7.48 (dt, 1H, J= 1.5, 7.2 Hz, 4'-H), 7.53 (dt, 1H, J= 1.8, 7.2 Hz, 5'-H), 7.62 (dd, 1H, J= 1.8, 7.2 Hz, 3'-H), 7.82 (d, 1H, J = 9.3 Hz, 5-H), 7.83 (dt, 1H, J = 2.4, 6.3 Hz, 3-H), 7.84 (dt, 1H, J = 2.4, 6.3 Hz, 2-H), 8.01 (dd, 1H, J = 3.3, 5.7 Hz, 4-H), 9.28 (dd, 1H, J = 3.3, 6.3 Hz, 1-H); ms: m/z 385 $(M)^+$, 387 $[M+2]^+$. *Anal*. Calcd. for: $C_{25}H_{20}ClNO$: C, 77.80; H, 5.22; N, 3.63. Found: C, 77.73; H, 5.30; N, 3.57.

7-(*o*-Bromophenyl)-10,10-dimethyl-8,9,10,11-tetrahydrobenz[*c*]acridin-8-one (IV, 2). This compound was obtained as a red solid in a 67% yield, mp 101°; ir (chloroform): υ C=O 1696, C=N 1554, C-N 1250, cm^{-1}; ^1H nmr (deuteriochloroform): δ 1.08 (s, 3H, C_{10}-CH_{3a}), 1.14 (s, 3H, C_{10}-CH_{3b}), 2.52 (d, 1H, J= 15.6 Hz, 9-Ha), 2.63 (d, J= 16.2 Hz, 9-Hb), 3.36 (s, 1H, 11-Ha), 3.37 (s, 1H, 11-Hb), 7.04 (d, 1H, J= 9.3 Hz, 6-H), 7.24 (dd, 1H, J= 1.5, 7.2 Hz, 6'-H), 7.42 (dt, 1H, J= 2.1, 7.2 Hz, 4'-H), 7.52 (dt, 1H, J= 1.5, 7.5 Hz, 5'-H), 7.76 (dd, 1H, J= 1.5, 7.8 Hz, 3'-H), 7.81 (d, 1H, J = 9.3 Hz, 5-H), 7.81 (dt, 1H, J = 3.3, 7.0 Hz, 3-H), 7.83 (dt, 1H, J = 3.3, 6.9 Hz, 2-H), 8.00 (dd, 1H, J = 3.3, 6.3 Hz, 4-H), 9.25 (dd, 1H, J = 3.6, 6.0 Hz, 1-H); ms: m/z 429 $(M)^+$, 431 $[M+2]^+$. *Anal*. Calcd. for: $C_{25}H_{20}BrNO$: C, 69.77; H, 4.68; N, 3.26. Found: C, 69.70; H, 4.62; N, 3.34.

7-(*o*-Methoxyphenyl)-10,10-dimethyl-8,9,10,11-tetrahydrobenz[*c*]acridin-8-one (IV, 3). This compound was obtained as a red solid in a 19% yield, mp 111°; ir (chloroform): υ C=O 1695, C=N 1550, C-N 1243, cm^{-1}; ^1H nmr (deuteriochloroform): δ 1.09 (s, 3H, C_{10}-CH_{3a}), 1.11 (s, 3H, C_{10}-CH_{3b}), 2.55 (d, 2H, J= 15.6 Hz, 9-Ha, 9-Hb), 3.57 (s, 2H, 11-Ha, 11-Hb), 3.57 (s, 3H, OCH_3), 7.05 (dt, 1H, J= 2.7, 7.8 Hz, 4'-H), 7.07 (dd, 1H, J= 2.0, 7.8 Hz, 3'-H), 7.13 (dd, 1H, J= 2.0, 8.1 Hz, 6'-H), 7.21 (d, 1H, J= 9.3 Hz, 6-H), 7.45 (dt, 1H, J= 2.1, 8.4 Hz, 5'-H), 7.78 (dt, 1H, J = 3.0, 6.0 Hz, 3-H), 7.79 (d, 1H, J = 9.6 Hz, 5-H), 7.80 (dt, 1H, J = 3.0, 6.0 Hz, 2-H), 7.98 (dd, 1H, J = 3.0, 6.3 Hz, 4-H), 9.24 (dd, 1H, J = 3.6, 6.3 Hz, 1-H); ms: m/z 381 $(M)^+$. *Anal*. Calcd. for: $C_{26}H_{23}NO_2$: C, 81.86; H, 6.08; N, 3.67. Found: C, 81.81; H, 6.17; N, 3.76.

7-(*p*-Chlorophenyl)-10,10-dimethyl-8,9,10,11-tetrahydrobenz[*c*]acridin-8-one (IV, 4). This compound was obtained as a red solid in a 6% yield, mp 213°; ir (chloroform): υ C=O 1691, C=N 1547, C-N 1255, cm^{-1}; ^1H nmr (deuteriochloroform): δ 1.19 (s, 6H, C_{10}-CH_{3a}, C_{10}-CH_{3b}), 2.58 (s, 2H, 9-Ha, 9-Hb), 3.32 (s, 2H, 11-Ha, 11-Hb), 7.14 (AA'BB', 2H, J= 8.4 Hz, 2'-H, 6'-H), 7.27 (d, 1H, J= 9.3 Hz, H-6), 7.49 (AA'BB', 2H, J= 8.4 Hz, 3'-H, 5'-H), 7.64 (d, 1H, J = 9.3 Hz, 5-H), 7.73 (dt, 1H, J = 1.5, 6.0 Hz, 3-H), 7.76 (dt, 1H, J = 1.8, 6.0 Hz, 2-H), 7.86 (dd, 1H, J = 2.4, 6.9 Hz, 4-H), 9.38 (dd, 1H, J = 3.3, 6.4 Hz, 1-H); ms: m/z 385 $(M)^+$, 387 $[M+2]^+$. *Anal*. Calcd. for: $C_{25}H_{20}ClNO$: C, 77.80; H, 5.22; N, 3.63. Found: C, 77.73; H, 5.16; N, 3.71.

7-(*p*-Bromophenyl)-10,10-dimethyl-8,9,10,11-tetrahydrobenz[*c*]acridin-8-one (IV, 5). This compound was obtained as a red solid in a 12% yield, mp 210°; ir (chloroform): υ C=O 1694, C=N 1547, C-N 1244, cm^{-1}; ^1H nmr (deuteriochloroform): δ 1.19 (s, 6H, C_{10}-CH_{3a}, C_{10}-CH_{3b}), 2.58 (s, 2H, 9-Ha, 9-Hb), 3.39 (s, 2H, 11-Ha, 11-Hb), 7.08 (AA'BB', 2H, J= 8.5 Hz, 2'-H, 6'-H), 7.27 (d, 1H, J= 9.0 Hz, H-6), 7.64 (AA'BB', 2H, J= 8.5 Hz, 3'-H, 5'-H), 7.64 (d, 1H, J = 8.5 Hz, 5-H), 7.73 (dt, 1H, J = 2.5, 6.5 Hz, 3-H), 7.75 (dt, 1H, J = 2.0, 6.0 Hz, 2-H), 7.86 (dd, 1H, J = 2.5, 7.0 Hz, 4-H), 9.38 (dd, 1H, J = 2.8, 7.5 Hz, 1-H); ms: m/z 429 $(M)^+$, 431 $[M+2]^+$. *Anal*. Calcd. for: $C_{25}H_{20}BrNO$: C, 69.77; H, 4.68; N, 3.26. Found: C, 69.87; H, 4.60; N, 3.20.

7-(*p*-Methoxyphenyl)-10,10-dimethyl-8,9,10,11-tetrahydrobenz[c]acridin-8-one (IV, 6). This compound was obtained as a red solid in a 8% yield, mp 220°; ir (chloroform): υ C=O 1693, C=N 1547, C-N 1244, cm^{-1}; ^1H nmr (deuteriochloroform): δ 1.11 (s, 6H, C_{10}-CH_{3a}, C_{10}-CH_{3b}), 2.57 (s, 2H, 11-Ha, 11-Hb), 3.34 (s, 2H, 9-Ha, 9-Hb), 3.85 (s, 3H, OCH_3), 7.04 (AA'BB', 2H, J= 8.5 Hz, 3'-H, 5'-H), 7.12 (AA'BB', 2H, J= 8.5 Hz, 2'-H, 6'-H), 7.29 (d, 1H, J= 9.0 Hz, H-6), 7.78 (d, 1H, J = 9.6 Hz, 5-H), 7.78 (dt, 1H, J = 2.4, 6.3 Hz, 3-H), 7.80 (dt, 1H, J = 2.5, 6.6 Hz, 2-H), 7.98 (dd, 1H, J = 3.3, 6.0 Hz, 4-H), 9.25 (dd, 1H, J = 3.0, 6.3 Hz, 1-H); ms: m/z 381 $(M)^+$. *Anal*. Calcd. for: $C_{26}H_{23}NO_2$: C, 81.86; H, 6.08; N, 3.67. Found: C, 81.93; H, 6.01; N, 3.61.

7-(*o*-Chlorophenyl)-10,10-dimethyl-8-hydroxy-8,9,10,11-tetrahydrobenz[c]acridine (V, 1). This compound was obtained as a red solid in a 8% yield, mp 104°; ir (chloroform): υ OH 3591, C=N 1553, C-N 1302, C-O 1057 cm^{-1}; ^1H nmr (deuteriochloroform): δ 0.90 (s, 3H, C_{10}-CH_{3a}), 1.20 (s, 3H, C_{10}-CH_{3b}), 1.81 (dd, 2H, J= 4.5, 15.0 Hz, 9-Ha, 9-Hb), 2.93 (dd, 1H, J= 1,5, 16.0 Hz, 11-Ha), 3.30 (dd, 1H, J= 1.5, 16.0 Hz, 11-Hb), 4.60 (d, 1H, J= 5.0 Hz, OH, deuterium oxide exchangeable), 4.70 (dd, 1H, J= 5.0, 10.0 Hz, 8-H), 7.02 (d, 1H, J= 9.9 Hz, 6-H), 7.49 (dt, 1H, J= 3.3, 7.2 Hz, 4'-H), 7.51 (dd, 1H, J= 2.4, 6.9 Hz, 3'-H), 7.54 (dd, 1H, J= 3.3, 7.2 Hz, 6'-H), 7.64 (dt, 1H, J= 2.7, 7.2 Hz, 5'-H), 7.72 (dt, 1H, J = 3.3, 6.9 Hz, 3-H), 7.74 (d, 1H, J = 9.9 Hz, 5-H), 7.76 (dt, 1H, J = 3.0, 6.9 Hz, 2-H), 7.95 (dd, 1H, J = 2.1, 6.0 Hz, 4-H), 9.23 (dd, 1H, J = 2.0, 7.0 Hz, 1-H); ms: m/z 387 $(M)^+$, 389 $[M+2]^+$. *Anal*. Calcd. for: $C_{25}H_{22}ClNO$: C, 77.41; H, 5.72; N, 3.60. Found: C, 77.49; H, 5.65; N, 3.66.

7-(*o*-Bromophenyl)-10,10-dimethyl-8-hydroxy-8,9,10,11-tetrahydrobenz[*c*]acridine (V, 2). This compound was obtained as a red solid in a 30% yield, mp 98°; ir (chloroform): υ OH 3597, C=N 1573, C-N 1305, C-O 1024 cm^{-1}; ^1H nmr (deuteriochloroform): δ 0.87 (s, 3H, C_{10}-CH_{3a}), 1.16 (s, 3H, C_{10}-CH_{3b}), 1.73 (dd, 1H, J= 5.5, 13.5 Hz, 9-Ha) , 1.81 (dd, 1H, J= 6.0, 14.0 Hz, 9-Hb), 2.97 (dd, 1H, J= 1.5, 16.0 Hz, 11-Ha), 3.20 (dd, 1H, J= 1.4, 15.5 Hz, 11-Hb), 4.56 (dd, 1H, J= 5.5, 11.0 Hz,

8-H), 4.68 (d, 1H, J= 5.4 Hz, OH, deuterium oxide exchangeable), 6.94 (d, 1H, J= 9.0 Hz, 6-H), 7.41 (dt, 1H, J= 2.0, 7.5 Hz, 4'-H), 7.45 (dd, 1H, J= 1.5, 7.5 Hz, 6'-H), 7.53 (dt, 1H, J= 1.0, 7.5 Hz, 5'-H), 7.68 (dt, 1H, J = 2.0, 7.5 Hz, 3-H), 7.70 (d, 1H, J = 9.5 Hz, 5-H), 7.71 (dt, 1H, J = 2.0, 8.0 Hz, 2-H), 7.76 (dd, 1H, J= 1.0, 8.5 Hz, 3'-H), 7.92 (dd, 1H, J = 1.5, 8.0 Hz, 4-H), 9.18 (dd, 1H, J = 1.5, 7.5 Hz, 1-H); ms: m/z 431 $(M)^+$, 433 $[M+2]^+$. *Anal.* Calcd. for: $C_{25}H_{22}BrNO$: C, 69.45; H, 5.13; N, 3.24. Found: C, 69.40; H, 5.20; N, 3.30.

7-(*o*-Methoxyphenyl)-10,10-dimethyl-8-hydroxy-8,9,10,11-tetrahydrobenz[*c*]acridine (V, 3). This compound was obtained as a red solid in a 21% yield, mp 100°; ir (chloroform): υ OH 3579, C=N 1570, C-OCH_3 1250, C-N 1290, C-O 1025 cm^{-1}; ^1H nmr (deuteriochloroform): δ 0.92 (s, 3H, C_{10}-CH_{3a}), 1.19 (s, 3H, C_{10}-CH_{3b}), 1.78 (dd, 2H, J= 6.0, 13.8 Hz, 9-Ha, 9-Hb) , 2.89 (dd, 1H, J= 6.6, 16.0 Hz, 11-Ha), 3.20 (dd, 1H, J= 6.0, 16.0 Hz, 11-Hb), 3.61 (s, 3H, OCH_3), 4.73 (dd, 1H, J= 5.1, 10.0 Hz, 8-H), 4.48 (d, 1H, J= 4.8 Hz, OH, deuterium oxide exchangeable), 7.10 (dd, 1H, J= 2.0, 8.0 Hz, 3'-H), 7.16 (d, 1H, J= 9.0 Hz, 6-H), 7.20 (dt, 1H, J= 2.4, 8.1 Hz, 5'-H), 7.33 (dd, 1H, J= 2.0, 8.0 Hz, 6'-H), 7.49 (dt, 1H, J= 2.4, 8.1 Hz, 4'-H), 7.70 (d, 1H, J = 9.0 Hz, 5-H), 7.72 (dt, 1H, J = 2.5, 6.8 Hz, 3-H), 7.73 (dt, 1H, J = 2.5, 6.8 Hz, 2-H), 7.93 (dd, 1H, J = 3.0, 6.3 Hz, 4-H), 9.22 (dd, 1H, J = 2.7, 6.6 Hz, 1-H); ms: m/z 383 $(M)^+$. *Anal.* Calcd. for: $C_{26}H_{23}NO_2$: C, 81.43; H, 6.57; N, 3.65. Found: C, 81.51; H, 6.50; N, 3.60.

7-(*p*-Chlorophenyl)-10,10-dimethyl-8-hydroxy-8,9,10,11-tetrahydrobenz[*c*]acridine (V, 4). This compound was obtained as a red solid in a 32% yield, mp 206°; ir (chloroform): υ OH 3592, C=N 1571, C-N 1305, C-O 1087 cm^{-1}; ^1H nmr (deuteriochloroform): δ 0.95 (s, 3H, C_{10}-CH_{3a}), 1.19 (s, 3H, C_{10}-CH_{3b}), 1.78 (d, 2H, J= 4.8 Hz, 9-Ha, 9-Hb), 2.90 (d, 1H, J= 15.9 Hz, 11-Ha), 3.21 (d, 1H, J= 15.9 Hz, 11-Hb), 4.63 (d, 1H, J= 4.8 Hz, OH, deuterium oxide exchangeable), 4.59 (dd, 1H, J= 4.8, 9.6 Hz, 8-H), 7.17 (d, 1H, J= 9.3 Hz, 6-H), 7.30 (dd, 1H, J = 2.1, 8.1 Hz, 2'-H), 7.50 (dd, 1H, J = 2.4, 8.1 Hz, 6'-H), 7.57 (dd, 1H, J = 2.4, 8.4 Hz, 3'-H), 7.61 (dd, 1H, J = 2.4, 8.1 Hz, 5'-H), 7.71 (dt, 1H, J = 2.4, 6.0 Hz, 3-H), 7.72 (d, 1H, J = 9.6 Hz, 5-H), 7.74 (dt, 1H, J = 2.4, 6.6 Hz, 2-H), 7.95 (dd, 1H, J = 3.3, 6.3 Hz, 4-H), 9.22 (dd, 1H, J = 2.4, 7.0, 1-H); ms: m/z 387 $(M)^+$, 389 $[M+2]^+$. *Anal.* Calcd. for: $C_{25}H_{22}ClNO$: C, 77.41; H, 5.72; N, 3.61. Found: C, 77.49; H, 5.61; N, 3.67.

7-(*p*-Bromophenyl)-10,10-dimethyl-8-hydroxy-8,9,10,11-tetrahydrobenz[*c*]acridine (V, 5). This compound was obtained as a red solid in a 14% yield, mp 207°; ir (chloroform): υ OH 3580, C=N 1570, C-N 1305, C-O 1069 cm^{-1}; ^1H nmr (deuteriochloroform): δ 0.94 (s, 3H, C_{10}-CH_{3a}), 1.19 (s, 3H, C_{10}-CH_{3b}), 1.77 (d, 1H, J= 5.5 Hz, 9-Ha), 1.78 (d, 1H, J= 5.5 Hz, 9-Hb), 2.88 (d, 1H, J= 16.0 Hz, 11-Ha), 3.21 (d, 1H, J= 16.0 Hz, 11-Hb), 4.55 (d, 1H, J= 5.0 Hz, OH, deuterium oxide exchangeable), 4.74 (dd, 1H, J= 5.0, 10.0 Hz, 8-H), 7.16 (dd, 1H, J = 2.1, 8.1 Hz, 2'-H), 7.17 (d, 1H, J= 9.0 Hz, 6-H), 7.43 (dd, 1H, J = 2.0, 8.5 Hz, 6'-H), 7.63 (dd, 1H, J = 2.0, 7.0 Hz, 3'-H), 7.64 (d, 1H, J = 7.5 Hz, 5-H), 7.65 (dd, 1H, J = 2.0, 7.0 Hz, 5'-H), 7.66 (dt, 1H, J = 2.0, 8.0 Hz, 3-H), 7.68 (dt, 1H, J = 2.0, 8.0 Hz, 2-H), 7.87 (dd, 1H, J = 1.5, 7.5 Hz, 4-H), 9.23 (dd, 1H, J = 2.0, 8.0, 1-H); ms: m/z 431 $(M)^+$, 433 $[M+2]^+$. *Anal.* Calcd. for: $C_{25}H_{22}BrNO$: C, 69.45; H, 5.13; N, 3.24. Found: C, 69.40; H, 5.03; N, 3.32.

Table 5

Crystal Data Collection Parameters and Structure Refinement Parameters of 7-(*o*-methoxyphenyl)-10,10-dimethyl-8,9,10,11-tetrahydro-benz[*c*]acridin-8-one (**IV, 3**) and 7-(*p*-chlorophenyl)-10,10-dimethyl-8-hydroxi-8,9,10,11-tetrahydrobenz[*c*]acridine (**V, 4**).

	Compound **IV, 3**	Compound **V, 4**
Empirical formula	$C_{26}H_{23}NO_2$	$C_{25}H_{22}ClNO$
Crystal dimensions (mm^3)	0.52 x 0.52 x 0.30	0.84 x 0.24 x 0.08
M	381.45	387.89
Temperature (K)	293 (2)	293 (2)
Wavelength (Å)	0.71073	0.71073
Crystal system / Space group	Orthorhombic / Pbca	Monoclinic / $P2_1/c$
Unit cell dimensions		
a (Å)	16.949 (1)	13.388 (3)
b (Å)	11.118 (1)	14.009 (3)
c (Å)	22.527 (3)	10.739 (5)
α (°)	90	90
β (°)	90	98.08 (2)
γ (°)	90	90
Volume ($Å^3$)	4245.0 (7)	1994.1 (11)
Z	8	4
Density (calculated) Mg/m^3	1.244	1.292
Absorption coefficient (mm^{-1})	0.078	0.207
F (000)	1696	816
θ Range (°)	1.50 to 24.99	1.50 to 25.00
Index range	$0 \le h \le 20, 0 \le k \le 13, -26 \le \ell \le 0$	$-15 \le h \le 15, -16 \le k \le 0, 0 \le \ell \le 12$
Reflections measured	3729	3720
Independent reflections/R_{int}	3729/0.0000	3516/0.0642
Absorption correction	None	None
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	3729 / 0 / 353	3516 / 1 / 262
Goodness-of-fit on F^2	1.052	0.980
Final R indices [$I > 2\sigma(I)$]	R1= 0.0659, wR2= 0.1483	R1= 0.0919, wR2= 0.1994
R indices (all data)	R1= 0.1565, wR2= 0.2134	R1= 0.2742, wR2= 0.3100
Extinction coefficient	0.0015 (5)	0.0018 (15)
Largest diff. peak and hole $eÅ^{-3}$	0.254 and -0.234	0.244 and -0.217
System solution	SHELXS 97	SHELXS 97

7-(*p*-Methoxyphenyl)-10,10-dimethyl-8-hydroxy-8,9,10,11-tetrahydrobenz[*c*]acridine (V, 6). This compound was obtained as a red solid in a 13% yield, mp 209°; ir (chloroform): υ OH 3577, C=N 1572, C-N 1288, C-OCH_3 1244, C-O 1028 cm^{-1}; ^1H nmr (deuteriochloroform): δ 0.92 (s, 3H, C_{10}-CH_{3a}), 1.21 (s, 3H, C_{10}-CH_{3b}), 1.71 (dd, 1H, J= 5.1, 14.1 Hz, 9-Ha), 1.81 (d, 1H, J= 5.1, 14.1 Hz, 9-Hb), 2.88 (d, 1H, J= 15.9 Hz, 11-Ha), 3.26 (d, 1H, J= 15.6 Hz, 11-Hb), 3.85 (s, 3H, OCH_3), 4.56 (d, 1H, J= 4.2 Hz, OH, deuterium oxide exchangeable), 4.77 (dd, 1H, J= 2.4, 7.0 Hz, 8-H), 7.07 (dd, 1H, J = 2.4, 8.1 Hz, 3'-H), 7.11 (dd, 1H, J = 2.4, 8.1 Hz, 5'-H), 7.17 (dd, 1H, J = 2.1, 8.1 Hz, 2'-H), 7.25 (d, 1H, J= 9.0 Hz, 6-H), 7.44 (dd, 1H, J = 2.1, 8.4 Hz, 6'-H), 7.70 (d, 1H, J = 9.3 Hz, 5-H), 7.72 (dt, 2H, J = 3.0, 7.0 Hz, 2-H and 3-H), 7.94 (dd, 1H, J = 2.4, 7.5 Hz, 4-H), 9.23 (dd, 1H, J = 2.4, 7.0, 1-H); ms: m/z 383 $(M)^+$. *Anal*. Calcd. for: $C_{26}H_{23}NO_2$: C, 81.43; H, 6.57; N, 3.65. Found: C, 81.35; H, 6.50; N, 3.71.

X-Ray Structure Determinations for the Compounds 7-(*o*-methoxyphenyl)-10,10-dimethyl-8,9,10,11-tetrahydrobenz[*c*]-acridin-8-one (IV, 3) and 7-(*p*-Chlorophenyl)-10,10-dimethyl-8-hydroxi-8,9,10,11-tetrahydrobenz[*c*]acridine (V, 4). Appropriate crystals of (**IV, 3**) and (**V, 4**) were obtained by cooling of chloroform. The X-ray experiments were carried out on a single crystal diffractometer Siemens P4/PC with graphite monochromated MoKa radiation (λ = 0.71073Å).

The structures were solved by direct methods followed by different Fourier techniques and refined by a full-matrix least squares procedure on F^2 [17]. Anisotropic displacement parameters have been applied for all non-hydrogen atoms. More details on data collections and structure determinations are summarized in Table 5.

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