

# SYNTHESIS OF SOME PYRIDINE AND PYRIMIDINE DERIVATIVES VIA MICHAEL-ADDITION

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(Received 21<sup>st</sup> Oct. 2005; Accepted 15<sup>th</sup> Dec. 2005))

تم تشييد بعض مشتقات البيريدين والبيريدين 4 & 9-6 وذلك عبر إضافة مايكل لمركبات محتوية على مجموعات ميثيلين نشطة مثل المألونونيتريل وخلات إثيل سيانو و 1-تترالون وكذلك مركبات محتوية على ذرات هيدروجين نشطة مثل الجوانيديين في وجود عامل مؤكسد وثيوريا إلى 2-أريل ميثيلدين-1-تترالون و 2-أريل ميثيلدين-6-ميثوكسي-1-تترالون (2).

إضافة المألونونيتريل إلى 2 في وجود البيريدين أدى إلى تكوين مشتقات 2-أمينو-3-سيانو-نفثو[1,2-b]بيران (3) و التي عوملت بميثوكسيد الصوديوم لتعطى 4. و تم تحضير المركب 4 من إضافة المألونونيتريل في وجود ألكوكسيد الصوديوم أو هيدروكسيد الصوديوم إلى 2. تخلق المشتق 3a بواسطة بلا ماء حمض الخل في وجود حمض الكبريت المركز إلى نفثوبيرانو[2,3-d]بيريميدين-8-أون (5). وقد أدى تكاثف مشتقات البيريدين ثيون 9 مع كلور حمض الخل الى تكون مشتقات 3-أكسوبيزو[h]ثيازوليدينو[2,3-b]كينازولين 10 والتي تفاعلت بدورها من خلال مجموعات الميثيلين النشطة مع ألدهيدات عطرية لتعطى مشتقات الأريلدين 11. حضرت هذه المشتقات أيضا بخطوة واحدة وذلك بتفاعل المركبات 9 مع كلور حمض الخل والألدهيدات العطرية. تكاثف 9 مع 3-بروموحمض البروبانويك أعطى مشتقات 4-أكسوبيزو[h] 3،1 ثيازينو[2,3-b]كينازولين (12). وقد تم التأكد من التركيب البنائي للمركبات المشيدة بواسطة الطرق الطيفية.

Synthesis of pyridine and pyrimidine analogues 4 & 6-9 were achieved by Michael-addition of compounds containing either active methylene groups like, malononitrile, ethyl cyanoacetate and 1-tetralone or compounds containing active hydrogen atoms like, guanidine in the presence of an oxidizing agent and thiourea to 2-arylmethylidene-1-tetralone and 2-arylmethylidene-6-methoxy-1-tetralone (2) (enones). Addition of malononitrile in piperidine at room temperature to 2 gave 2-amino-3-cyano-naphtho[1,2-b]pyran derivatives 3 which were converted to 4 upon treatment with sodium methoxide. Addition of malononitrile in sodium alkoxide or sodium hydroxide to 2 gave 4. Cyclization of 3a with acetic anhydride in the presence of conc. H<sub>2</sub>SO<sub>4</sub> gave the naphtho-pyrano[2,3-d]pyrimidin-8-one (5). Condensation of the pyrimidine thione derivatives 9 with chloroacetic acid gave the 3-oxo-benzo[h]thiazolidino[2,3-b]quinazoline derivatives (10), which were reacted through their active methylene groups with aromatic aldehydes to give the arylidine derivatives 11. These compounds were also prepared in one step by reacting 9 with chloroacetic acid and aromatic aldehydes. Condensation of 9 with 3-bromopropanoic acid gave 4-oxo-benzo[h]1,3-thiazino[2,3-b]quinazoline derivatives (12). The structures of the prepared compounds were mainly confirmed on the basis of spectroscopic methods.

## INTRODUCTION

Chalcones have been very attractive starting materials in combinatorial chemistry, they are easy to prepare with large variability at the two aromatic rings and the enone provides a

bifunctional site for 1,3-dinucleophiles affording several heterocyclic ring-systems [1].

It was found that chalcones have different biological activities including anti-malarial [2-4], anticancer [5-8], antimicrobial [9] and anti-inflammatory [10-13] activities. In addition

several pyridine and pyrimidine derivatives were reported to possess significant activities, e.g. antibacterial [14,15], antiviral [16-18], analgesic, antitussive [19], anti-inflammatory [20], antifungal [21], anticoagulant [22] and anticancer [23] activities. This prompted our interest to synthesize some novel pyridine and pyrimidine analogues fused with naphthalene nucleus, a combination which is expected to show high biological activities.

## EXPERIMENTAL

Melting points were determined on a Tottoli capillary melting point apparatus and are uncorrected. IR spectra were run for KBr discs on Perkin Elmer FT spectrophotometer 1000.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on a JEOL ECP 400 NMR spectrometer operating at 400 MHz in  $\text{CDCl}_3$  (or  $\text{DMSO-d}_6$ ) with TMS as internal standard. Chemical shifts are given in  $\delta$  ppm and coupling constants ( $J$ ) are given in Hz. Electron impact (EI) MS spectra were carried on Shimadzu GCMSQP5050A spectrometer, DB-1 glass column 30 m, 0.25 mm, ionization energy 70 eV, at Chemistry Department, College of Science, King Saud University.

All prepared compounds were identified by physical properties, IR, MS (Table 1),  $^1\text{H}$  NMR (Table 2) and  $^{13}\text{C}$  NMR (Table 3).

### 2-Arylmethylidene-1-tetralones (2a-h)

### 2-Arylmethylidene-6-methoxy-1-tetralones (2i-l):

#### Method A:

A mixture of NaOH (2.2 g, 0.055 mol), water (20 ml), ethanol (12.25 ml), 1-tetralone or 6-methoxy-1-tetralone (**1**) (0.043 mol) and the appropriate aromatic aldehyde (0.043 mol) was stirred at 15–30°C for 48 h and left in the refrigerator overnight. It was then filtered, washed with water, then washed with the least amount of ethanol, dried, refluxed with glacial acetic acid (15 ml) for 3 h. The crystals separated after cooling were filtered and washed with water. It did not need re-crystallization since it was found pure.

#### Method B: (for the preparation of 2a-d)

A mixture of 1-tetralone or 6-methoxy-1-tetralone (**1**) (0.01 mol) and the appropriate aromatic aldehyde (0.01 mol) in 10% NaOH (10 ml) was placed in a conical flask covered with an inverted funnel, then irradiated with microwaves (600 W) for 30 sec, cooled to room temperature, treated with ethanol and filtered. The solid obtained was pure and did not need re-crystallization.

### 2-Amino-4-aryl-3-cyano-5,6-dihydro-4H-naphtho[1,2-b]pyran (3a-c)

### 2-Amino-4-aryl-3-cyano-8-methoxy-5,6-dihydro-4H-naphtho[1,2-b]pyran (3d, e):

These compounds were prepared following the same procedure as in ref. [24].

### 2-Alkoxy-4-aryl-3-cyano-5,6-dihydrobenzo[h]-quinolines (4a-g)

### 4-Aryl-3-cyano-2,8-dimethoxy-5,6-dihydrobenzo[h]quinolines (4h, i):

#### Method A & B:

These compounds were prepared following the same procedures as in ref. [24].

#### Method C:

To a freshly prepared sodium methoxide solution (0.005 mol of sodium metal in 50 ml of methanol), **3a-d** (0.005 mol) was added with stirring. The mixture was heated under reflux for 1 h, the solid product obtained after cooling was collected by filtration, washed with alcohol and re-crystallized.

#### Method D:

A mixture of **3a-d** (0.005 mol), NaOH (20%, 25 ml) and methanol (25 ml) was stirred at room temperature for 6 h; the solid formed was filtered, washed with water and re-crystallized.

### 7-(4'-Bromophenyl)-10-methyl-5,6,8,9-tetrahydro-7H-naphtho[1',2':5,6]pyrano[2,3-d]pyrimidin-8-one (**5**):

This compound was prepared following the same procedure as in ref. [24].



**2-Amino-4-aryl-5,6-dihydrobenzo[h]quinazoline (6a)****2-Amino-4-aryl-8-methoxy-5,6-dihydrobenzo[h]quinazoline (6b-d):**

A mixture of **2a**, **i**, **j**, **l** (0.1 mol), guanidine.HCl (0.14 mol), ethanol (200 ml) and 50% KOH (40 ml) was heated under reflux for 1 h. Under the same conditions, 30% H<sub>2</sub>O<sub>2</sub> (31 ml) was added to the above mixture in small portions over a period of 1 h. The ethanol was removed under reduced pressure and water (200 ml) was added to the residue. The precipitate was filtered, washed thoroughly on the funnel with water. The slightly still wet crude solid was re-crystallized and the crystalline product was dried in a vacuum desiccator over P<sub>2</sub>O<sub>5</sub>/KOH.

**4-(4'-Bromophenyl)-3-cyano-1,2,5,6-tetrahydrobenzo[h]quinolin-2-one (7):**

This compound was prepared following the same procedure as in ref. [24].

**9-(4'-Bromophenyl)-3:4,5:6-dibenzo-1,2,7,8-tetrahydroacridine (8a)****9-(4'-Bromophenyl)-3:4(3''-methoxybenzo),5:6-benzo-1,2,7,8-tetrahydro acridine (8b):****Method A:**

A mixture of **2a**, **i** (0.2 mol) 1-tetralone (29.2 g, 0.2 mol), ammonium acetate (38.5 g, 0.5 mol) and piperidine (0.1 ml) was fused at 160-170 °C for 10 h, cooled, then diluted with ice-cold water and stirred for 10 min. 2 M HCl (1 ml) was added and the mixture was extracted with dichloromethane (50 ml×3). The organic layer was separated, washed with water, dried (Na<sub>2</sub>SO<sub>4</sub>) and evaporated. The residue was treated with the least amount of ethanol, filtered and re-crystallized.

**Method B:**

The same mixture was placed in a conical flask covered with an inverted funnel and irradiated with microwaves (600 W) for 4 min., then treated as mentioned in method A.

**4-Aryl-1,2,3,4,5,6-hexahydronaphtho[1,2-d]-pyrimidine-2-thione (9a-c):**

These compounds were prepared following the same procedure as in ref. [24].

**5-Aryl-3-oxo-6,7-dihydro-5H-benzo[h]thiazolidino[2,3-b]quinazoline (10a-c)****5-Aryl-3-oxo-9-methoxy-6,7-dihydro-5H-benzo[h]thiazolidino[2,3-b]quinazoline (10d, e):**

These compounds were prepared following the same procedure as in ref. [24].

**5-Aryl-3-oxo-2-arylmethylidene-6,7-dihydro-5H-benzo[h]thiazolo[2,3-b]quinazoline (11a, d)****5-Aryl-3-oxo-9-methoxy-2-arylmethylidene-6,7-dihydro-5H-benzo[h]thiazolo[2,3-b]quinazoline (11b,c):****Method A:**

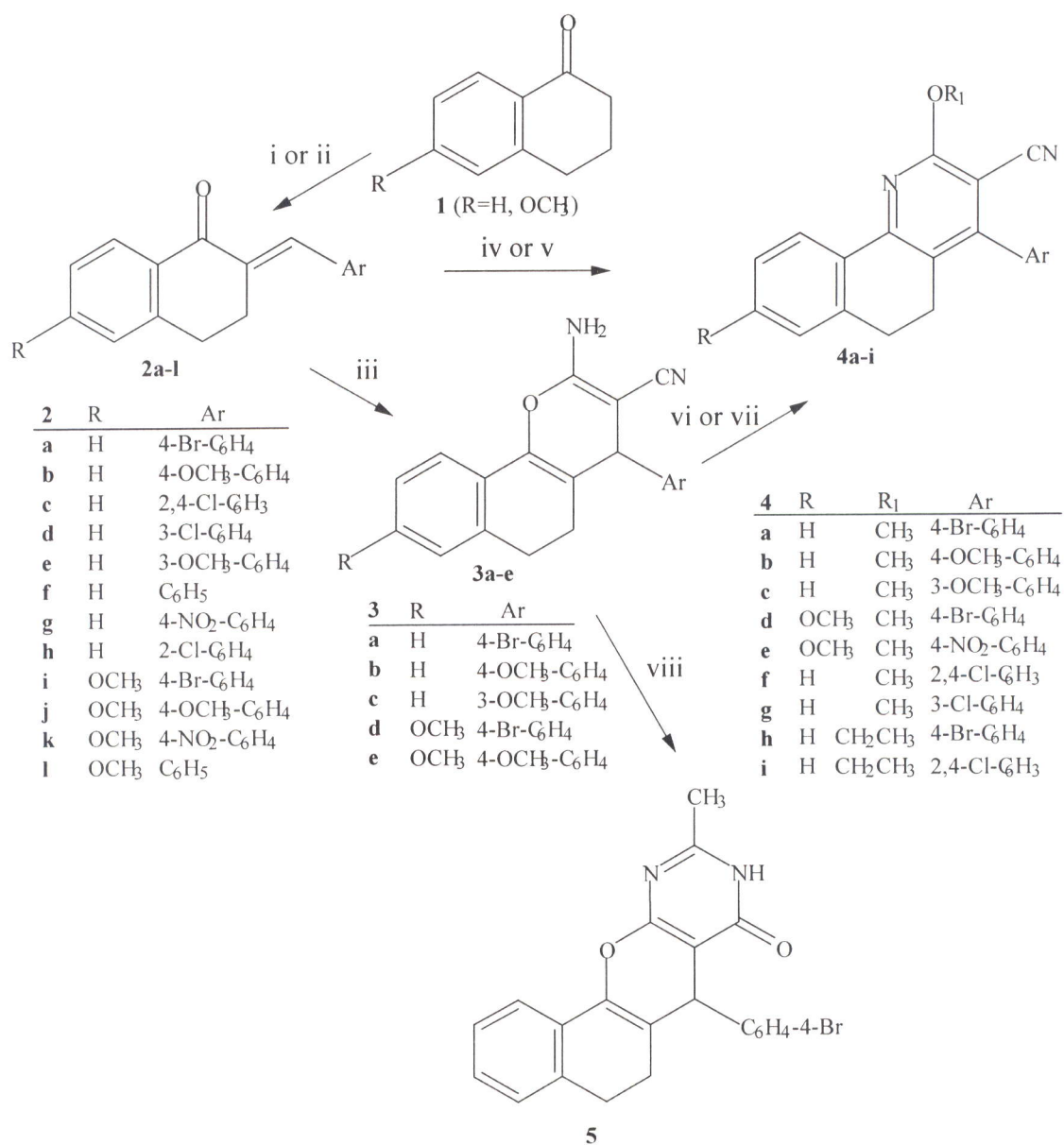
A mixture of **10a**, **c-e** (0.01 mol), the appropriate aromatic aldehyde (0.01 mol), fused sodium acetate (2 g), glacial acetic acid (15 ml) and acetic anhydride (10 ml) was heated under reflux for 4 h. The mixture was cooled and poured onto ice-cold water, then filtered. The separated solid was washed with water and re-crystallized.

**Method B:**

A mixture of **9c-e** (0.01 mol), chloroacetic acid (0.94 g, 0.01 mol), the appropriate aromatic aldehyde (0.01 mol), fused sodium acetate (2 g), glacial acetic acid (20 ml) and acetic anhydride (14 ml) was heated under reflux for 3 h and treated as in method A.

**6-Aryl-4-oxo-2,3,7,8-tetrahydro-6H-benzo[h]-1,3-thiazino[2,3-b]quinazoline (12a-c):****10-Methoxy-6-Aryl-4-oxo-2,3,7,8-tetrahydro-6H-benzo[h]1,3-thiazino[2,3-b]quinazoline (12d):**

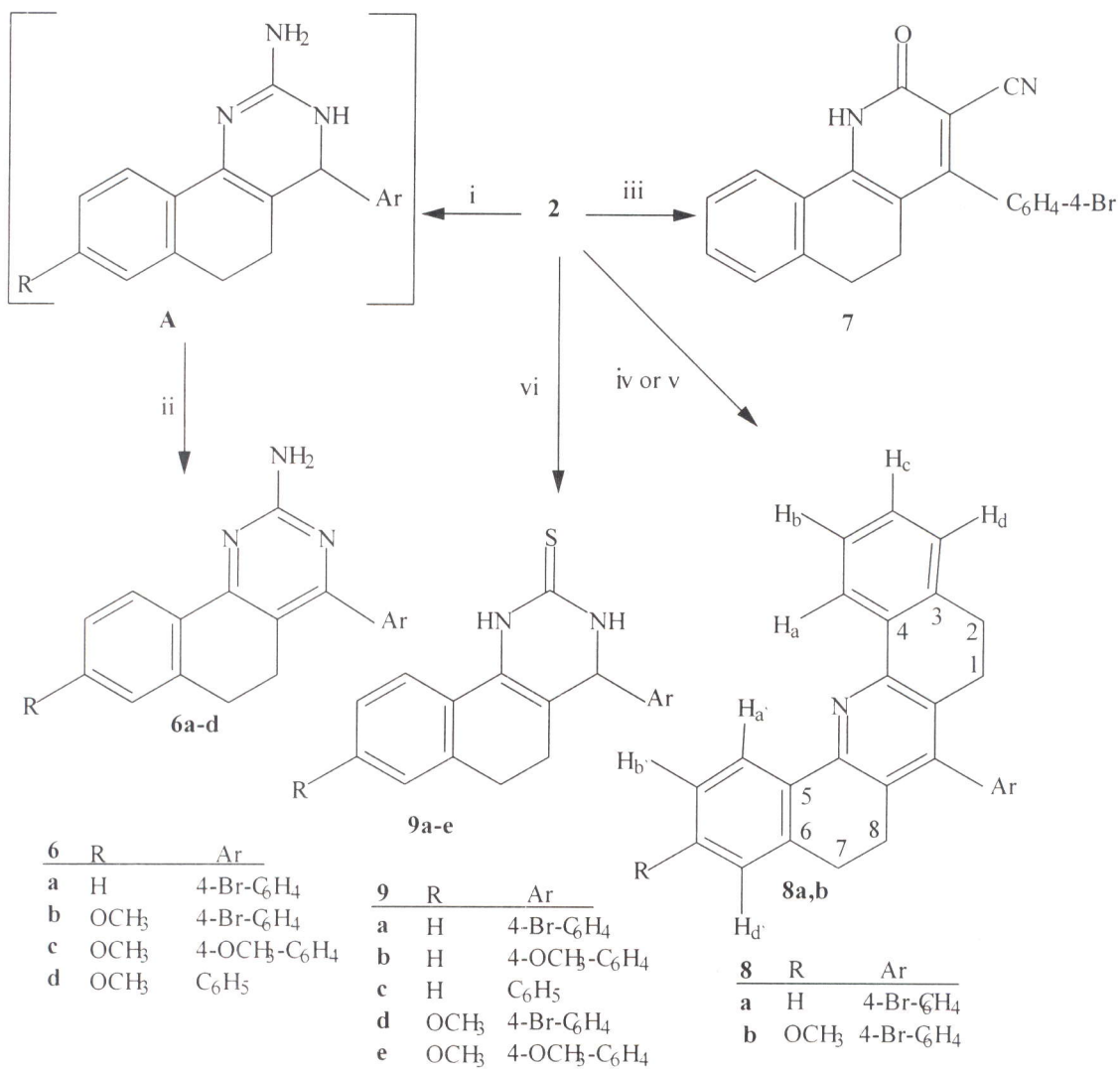
A mixture of **9a-c,e** (0.01 mol), 3-bromopropanoic acid (0.01 mol), fused sodium acetate (2 g), glacial acetic acid (20 ml) and acetic anhydride (7 ml) was heated under reflux for 3 h. The mixture was cooled and poured onto ice-cold water, then filtered. The separated solid was washed with water and re-crystallized.



i = a: ArCHO; b: gla. AcOH, reflux. ii = ArCHO, microwave. iii = CNCH<sub>2</sub>CN, DMF, piperidine. iv = CNCH<sub>2</sub>CN, ROH, R<sub>1</sub>ONa. v = CNCH<sub>2</sub>CN, ROH, NaOH. vi = CH<sub>3</sub>OH, CH<sub>3</sub>ONa. vii = CH<sub>3</sub>OH, NaOH. viii = Ac<sub>2</sub>O, H<sub>2</sub>SO<sub>4</sub>.

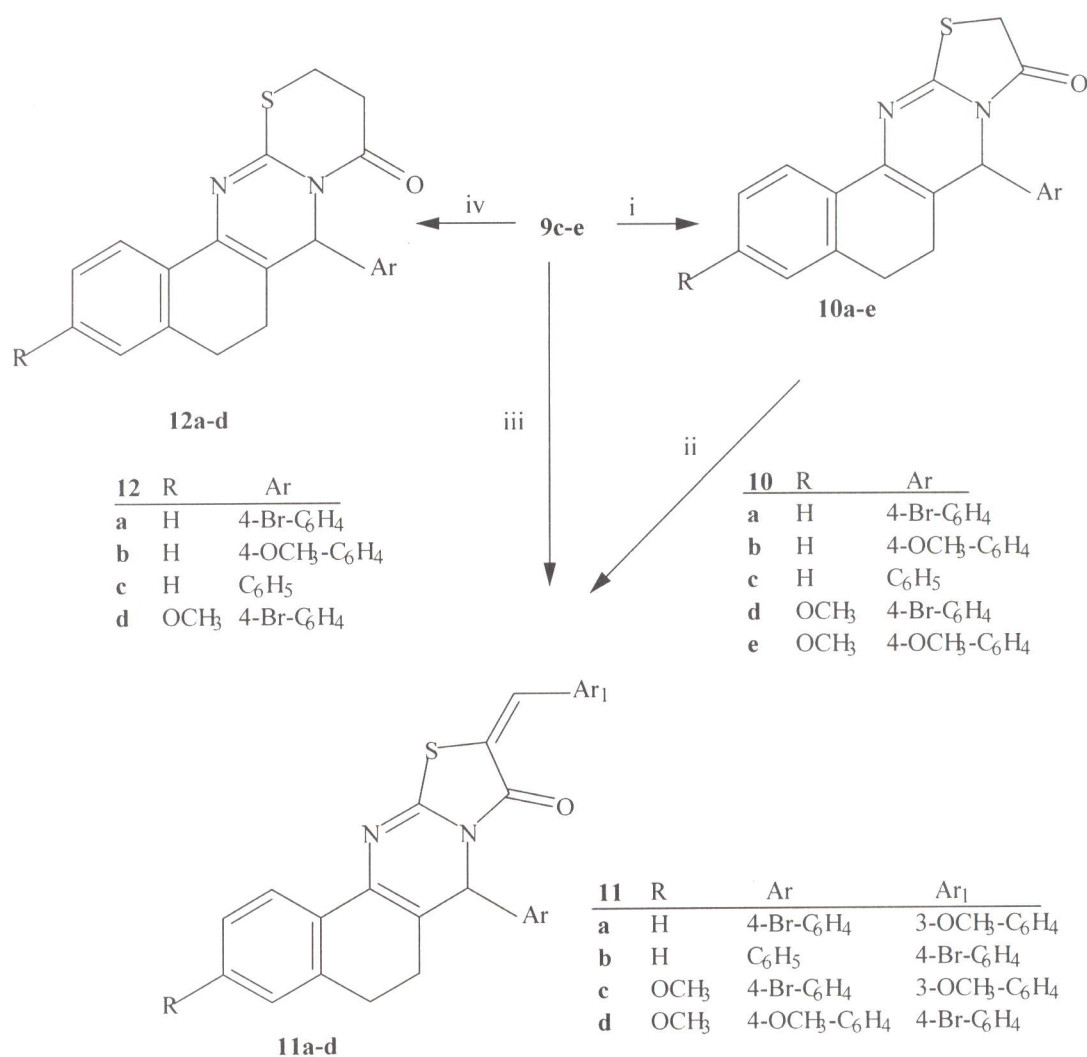
(Scheme 1)





i = NH<sub>2</sub>CNHNH<sub>2</sub>·HCl, ii = H<sub>2</sub>O<sub>2</sub>, iii = CNCH<sub>2</sub>COOC<sub>2</sub>H<sub>5</sub>, CH<sub>3</sub>COONH<sub>4</sub>, iv = i-tetralone, CH<sub>3</sub>COONH<sub>4</sub>, piperidine, fusion, v = i-tetralone, CH<sub>3</sub>COONH<sub>4</sub>, piperidine, microwave, vi = H<sub>2</sub>NCSNH<sub>2</sub>.

(Scheme 2)



i = ClCH<sub>2</sub>COOH, Ac<sub>2</sub>O, CH<sub>3</sub>COONa. ii = Ar<sub>1</sub>CHO, Ac<sub>2</sub>O, CH<sub>3</sub>COOH, CH<sub>3</sub>COONa. iii = ClCH<sub>2</sub>COOH, Ar<sub>1</sub>CHO, Ac<sub>2</sub>O, CH<sub>3</sub>COOH, CH<sub>3</sub>COONa. iv = BrCH<sub>2</sub>CH<sub>2</sub>COOH, Ac<sub>2</sub>O, CH<sub>3</sub>COOH, CH<sub>3</sub>COONa.

(Scheme 3)

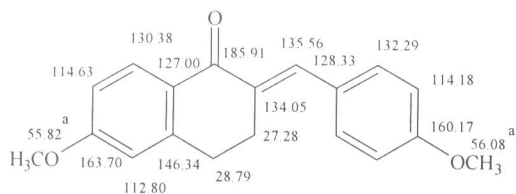
## RESULTS AND DISCUSSION

As a continuation of our previous work [24], the starting chalcones (enones) derived from 1-tetralone and 6-methoxy-1-tetralone were prepared by the conventional methods, but a mixture of the  $\alpha,\beta$ -unsaturated ketones as well as the corresponding  $\beta$ -hydroxy-ketones was obtained as indicated by <sup>1</sup>H and <sup>13</sup>C NMR.

Refluxing this mixture with glacial acetic acid for 3h led to dehydration of the  $\beta$ -hydroxy-ketones and gave the desired ketones in a pure form.

Compounds **2a-d**, **i-k** (Scheme 1) were also prepared by irradiating the reaction mixture by microwaves (600 W) for 30 sec. the products were pure and the yields were higher. The identity of compounds **2a-l** is established by spectroscopic

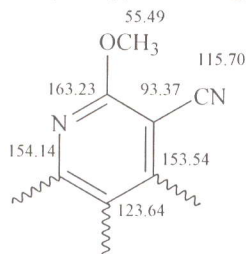
methods. Fig. 1 illustrates the chemical shifts of  $^{13}\text{C}$  NMR of **2j**.



a = interchangeable assignment

**Figure 1** ( $^{13}\text{C}$  Chemical shifts of **2j**)

Michael addition of malononitrile to 2-arylmethylidene-1-tetralone or 2-arylmethylidene-6-methoxy-1-tetralone (**2a**, **b**, **e**, **i**, **j**) in the presence of piperidine and DMF at room temperature gave the amino-cyanopyran derivatives **3a-e**. Carrying the same addition in the presence of sodium alkoxide or sodium hydroxide led to the formation of the alkoxy-cyanobenzo[h]quinoline derivatives **4a-I**, through the intermediate **3** (Scheme 1). This was proved by the conversion of **3a-d** to **4a-d** upon treatment with sodium methoxide in methanol and refluxing for 1 h. Fig. 2 illustrates the  $^{13}\text{C}$  NMR chemical shifts of the heterocyclic pyridine ring in **4d**.

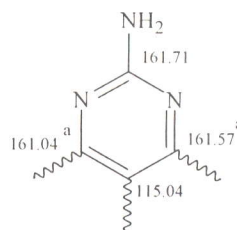


**Figure 2** ( $^{13}\text{C}$  Chemical shifts of heterocyclic pyridine ring in **4d**)

The amino-cyanopyran derivative **3a** was cyclized to the methyl-pyrimidinone derivative **5** by treatment with acetic anhydride and a catalytic amount of conc.  $\text{H}_2\text{SO}_4$  (Scheme 1). The structure of **5** was confirmed by IR spectral data which indicated the disappearance of CN and  $\text{NH}_2$  stretching bonds and the appearance of NH stretching at  $3151\text{ cm}^{-1}$  and C=O stretching at  $1684\text{ cm}^{-1}$ . The  $^1\text{H}$  NMR illustrated a singlet for the methyl protons at  $\delta$  2.32 ppm, a singlet for H-7 at  $\delta$  4.47 ppm and a broad singlet at  $\delta$  12.97 ppm for NH, beside other protons of the compound (Table 2). The  $^{13}\text{C}$  NMR spectrum showed a line at  $\delta$  21.18 ppm for the methyl carbon while C-7

appeared at  $\delta$  40.39 ppm and lactam carbonyl carbon at  $\delta$  165.32 ppm as well as the other lines of  $\text{sp}^3$  and  $\text{sp}^2$  carbons of the molecule (Table 3). The MS spectrum showed the molecular radical cation  $[\text{M}^+]$  at  $m/z=420$  (18%) ( $\text{C}_{22}\text{H}_{17}^{79}\text{BrN}_2\text{O}_2$ ), 422 (19%)  $[\text{M}+2]$  ( $\text{C}_{22}\text{H}_{17}^{81}\text{BrN}_2\text{O}_2$ ). Loss of the bromine radical offered the cation at  $m/z=341$  (1%), while loss of the aryl group ( $\text{C}_6\text{H}_4\text{Br}$ ) gave the cation at  $m/z=265$  (100%).

The desired target compounds, 2-amino-benzo[h]quinazoline derivatives (**6**), were prepared from the enones **2a**, **i**, **j**, **l** and guanidine.HCl by refluxing them together in basic alcoholic media, by which time the dihydropyrimidine (compound A) had been formed (Scheme 2). At this point, hydrogen peroxide (30% aqueous solution) was added to the hot solution. By portion-wise addition of the oxidizing agent in large excess, not only was the aromatization completed, but also all the undesired tarry side-products were oxidatively degraded, resulting in a clean solution in each case [25]. This procedure allowed easy product isolation of the required amino-pyrimidine, mainly aminobenzoquinazoline products, in good yield, with no difficulty in the purification process. The IR spectra of **6c** showed the disappearance of the carbonyl stretching in the starting material and the appearance of  $\text{NH}_2$  stretching bonds at  $3371$  and  $3210\text{ cm}^{-1}$ . The  $^1\text{H}$  NMR spectrum revealed the disappearance of the olefinic proton of the starting material and the appearance of a broad singlet at  $\delta$  5.21 ppm for the  $\text{NH}_2$  group as well as the other protons of the molecule. Fig. 3 illustrates the  $^{13}\text{C}$  NMR chemical shifts of heterocyclic pyrimidine ring in **6c**.



**Figure 3** ( $^{13}\text{C}$  Chemical shifts of heterocyclic pyrimidine ring in **6c**)

The MS spectrum showed the molecular radical cation  $[\text{M}^+]$  at  $m/z=333$  (88%) ( $\text{C}_{20}\text{H}_{19}\text{N}_3\text{O}_2$ ). Loss of hydrogen radical gave the cation at  $m/z=332$



(100%) and subsequently loss of ammonia gave the cation at 315 (2%).

Fusion of **2a** with ethyl cyanoacetate and ammonium acetate at 140°C gave 3-cyano-1,2,5,6-tetrahydrobenzo[h]quinoline-2-one derivative **7**. The structure of **7** was confirmed by IR spectral data which showed NH stretching peak at 3437 cm<sup>-1</sup>, C≡N stretching peak at 2222 cm<sup>-1</sup> and CO stretching peak at 1638 cm<sup>-1</sup>. The <sup>1</sup>H NMR spectrum showed a broad peak at δ 7.26 ppm attributed to NH, beside the other aliphatic and aromatic protons (Table 2). We were unable to perform the <sup>13</sup>C NMR spectrum as the compound was sparingly soluble in CDCl<sub>3</sub> and DMSO. The MS spectrum of **7** showed the molecular radical cation [M<sup>+</sup>] at *m/z*=376 (5%) (C<sub>20</sub>H<sub>13</sub><sup>79</sup>BrN<sub>2</sub>O) and 378 (8%) [M+2] (C<sub>20</sub>H<sub>13</sub><sup>81</sup>BrN<sub>2</sub>O<sub>2</sub>). Loss of the bromine radical gave a peak at *m/z*=297 (3%).

Treatment of **2a**, **i** with a mixture of 1-tetralone and ammonium acetate in the presence of piperidine as a catalyst at a high temperature yielded 9-(4'-Bromophenyl)-3:4,5:6-dibenzo-1,2,7,8-tetrahydroacridine (**8a**) and 9-(4'-Bromophenyl)-3:4(3"-methoxybenzo),5:6-benzo-1,2,7,8-tetrahydroacridine (**8b**). The reaction may proceed through the formation of the corresponding α,β-unsaturated imines (formed by the reaction of **2a**, **i** with ammonium acetate) which behave like α,β-unsaturated ketones in the Michael addition to form **8a**, **b** [26]. The IR spectrum of **8a** revealed the disappearance of both CO and C=C stretching peaks of the parent compound **2a**. The structure of **8a** seemed to be symmetrical but the <sup>1</sup>H NMR spectrum showed that it is unsymmetrical. This may be attributed to the ease of rotation of the aryl group (*p*-bromophenyl group) around the single bond leading to the shielding effect by anisotropy to one half of the dibenzoacridine nucleus than the other. The <sup>1</sup>H NMR of **8a** showed a multiplet at δ 2.70-2.73 for the methylene group at position 1, multiplet at δ 2.83-2.88 ppm for the two methylene groups at positions 2 and 7 and a multiplet at δ 3.29-3.32 ppm for the methylene group at position 8, besides the other aromatic protons (Table 2). The <sup>13</sup>C NMR spectrum also reveals the asymmetry of **8a**, as indicated by the appearance of four lines at δ 27.46, 27.62, 28.69 and 29.71 ppm for C-1, C-2, C-7 and C-8

respectively, besides 21 lines in the range δ 122.31-153.64 ppm for the aromatic carbons. The MS spectrum of **8a** showed the molecular radical cation [M<sup>+</sup>] at *m/z*=437 (100%) (C<sub>27</sub>H<sub>20</sub><sup>79</sup>BrN) and 439 (97%) [M+2] (C<sub>27</sub>H<sub>20</sub><sup>81</sup>BrN). Loss of the hydrogen radical gave a peak at *m/z*=436 (59%) while the loss of a bromine radical gave a peak at *m/z*=358 (7%). Compounds **8a**, **b** were also prepared by irradiating the reaction mixture with microwaves (600 W) for 4 min and the yield was relatively higher than that of the first method.

Condensation of **2a**, **b**, **f**, **i**, **j** with thiourea was successful in boiling ethanolic potassium hydroxide solution, yielding the corresponding naphtho[1,2-d]pyrimidine-2-thione derivative **9a-e** [27, 28] (Scheme 2). The IR spectrum of **9e** displayed bands for NH stretching at 3198 cm<sup>-1</sup> and C=S stretching at 1204 cm<sup>-1</sup>. The <sup>1</sup>H NMR spectrum displayed a singlet at δ 4.86 ppm for H-4, two broad singlets for the two NH at δ 9.01 and 9.76 ppm respectively, beside the absorption of aliphatic and aromatic protons (Table 2). The <sup>13</sup>C NMR spectrum of **9e** showed absorption at δ 58.42 for C-4 and at δ 174.43 for C=S beside the other lines of sp<sup>3</sup> and sp<sup>2</sup> carbons of the molecule (Table 3). Fig. 4 illustrates the chemical shifts of <sup>13</sup>C NMR of the heterocyclic pyrimidine ring in **9e**.

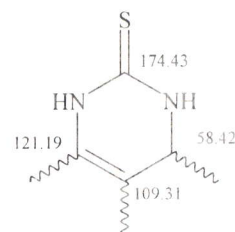


Figure 4 (<sup>13</sup>C Chemical shifts of heterocyclic pyrimidine ring in **9e**)

The MS spectrum of the latter showed the molecular radical cation [M<sup>+</sup>] at *m/z*=352 (100%) (C<sub>20</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub>S). Loss of the hydrogen radical gave a peak at *m/z*=351 (62%). Loss of methyl radical gave a peak at *m/z*=337 (3%), while the loss of ethylene molecule gave a peak at *m/z*=324 (1%), loss of OCH<sub>3</sub> radical gave a peak at *m/z*=321 (2%) and loss of methoxyphenyl radical gave a peak at *m/z*=245 (91%).

Compounds **9a-e** were reacted with chloroacetic acid in acetic acid-acetic anhydride

mixture in the presence of fused sodium acetate to give **10a-e**. The chemical structures were proved by IR, MS,  $^1\text{H}$  and  $^{13}\text{C}$  NMR (Tables 1-3) thus, the IR spectrum of **10b** showed the disappearance of NH and C=S stretching bands and the appearance of C=O stretching band at  $1720\text{ cm}^{-1}$ . The  $^1\text{H}$  NMR of **10b** displayed two doublets forming an AB system at  $\delta$  4.03 and 4.09 ppm ( $J=17.6\text{ Hz}$ ) for the  $\text{CH}_2$  group at position 2 ( $\text{CH}_2$  was close to a chiral carbon) and a singlet at  $\delta$  5.59 ppm for H-5 beside the other aliphatic and aromatic protons of the molecule (Table 2). The  $^{13}\text{C}$  NMR spectrum of **10b** showed a line at  $\delta$  32.14 ppm for C-2, and at  $\delta$  58.79 ppm for C-5 as well as the absorption of other  $\text{sp}^3$  and  $\text{sp}^2$  carbons of the molecule (Table 3). Fig. 5 illustrates the chemical shifts of  $^{13}\text{C}$  NMR of the heterocyclic thiazolidinopyrimidine ring in **10b**.

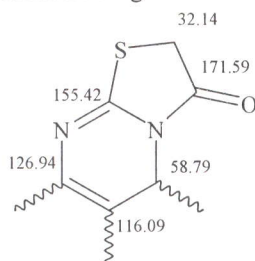


Figure 5 ( $^{13}\text{C}$  Chemical shifts of heterocyclic thiazolidinopyrimidine ring in **10b**)

The MS spectrum of **10b** confirmed the structure as it showed the molecular radical cation  $[\text{M}^\cdot]^+$  at  $m/z=362$  (57%) ( $\text{C}_{21}\text{H}_{18}\text{N}_2\text{O}_2\text{S}$ ). Loss of methoxyphenyl radical gave a fragment at  $m/z=255$  (100%) which loses CO to give a fragment at  $m/z=227$  (39%).

Condensation of **10a, c-e** via their active methylene groups at position 2 with aromatic aldehydes in presence of acetic anhydride, acetic acid and sodium acetate yielded the corresponding arylmethylidene derivatives **11a-d**. However, the arylmethylidene derivatives **11b-d** were prepared directly from **9** by the action of chloroacetic acid, aromatic aldehydes and at the same conditions (Scheme 3). Compounds **11a-d** were characterized by IR, MS,  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR (Tables 1-3). The IR spectrum of **11b** exhibited a shift of C=O stretching peak to lower wave number ( $1703\text{ cm}^{-1}$ ) due to conjugation with the exocyclic double bond. The  $^1\text{H}$  NMR spectrum of

**11b** was characterized by the disappearance of the AB pattern and the appearance of a singlet at  $\delta$  7.57 ppm attributed to the olefinic proton. The MS spectrum of **11b** showed the molecular radical cation  $[\text{M}^\cdot]^+$  at  $m/z=498$  (31%) ( $\text{C}_{27}\text{H}_{19}^{79}\text{BrN}_2\text{OS}$ ), 500 (33%)  $[\text{M}+2]$  ( $\text{C}_{27}\text{H}_{19}^{81}\text{BrN}_2\text{OS}$ ). Loss of the phenyl radical offered the cation at  $m/z=421$  (100%) which in turn lost a molecule of CO to give the cation at  $m/z=393$  (23%). Loss of the bromine radical from the molecular ion gave the cation at  $m/z=419$  (3%).

Compounds **9a-c, e** were also reacted with 3-bromopropanoic acid to give the thiazino[2,3-b]quinoline derivatives **12a-d** for which their structures were confirmed by spectral data (Tables 1-3). Where the IR spectrum of **12d** showed a C=O stretching peak at  $1689\text{ cm}^{-1}$ . The  $^1\text{H}$  NMR spectrum of **12d** was characterized by a multiplet at  $\delta$  2.92-3.10 ppm for the two methylene groups at positions 2 and 3 beside the other aliphatic and aromatic protons of the molecule (Table 2). The  $^{13}\text{C}$  NMR spectrum of **12d** showed a line at  $\delta$  35.80 ppm for C-2, at  $\delta$  21.66 ppm for C-3 and at  $\delta$  169.30 ppm for C=O in addition to absorption of the other  $\text{sp}^3$  and  $\text{sp}^2$  carbons of the molecule (Table 3). Fig. 6 illustrates the chemical shifts of  $^{13}\text{C}$  NMR of the heterocyclic pyrimidothiazine ring in **12d**.

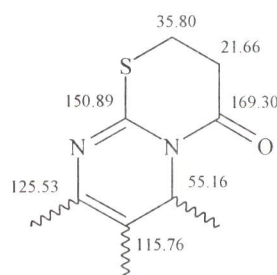


Figure 6 ( $^{13}\text{C}$  Chemical shifts of heterocyclic pyrimidothiazine ring in **12d**)

The MS spectrum of the latter showed the molecular radical cation  $[\text{M}^\cdot]^+$  at  $m/z=406$  (100%) ( $\text{C}_{23}\text{H}_{22}\text{N}_2\text{O}_3\text{S}$ ). Loss of the hydrogen radical gave a peak at  $m/z=405$  (83%) while loss of the methoxyphenyl radical offered cation at  $m/z=299$  (89%) which lost CO to give a cation at  $m/z=271$  (2%). The last fragment loses ethylene molecule and gains two hydrogen to give a cation at  $m/z=245$  (62%).



Table 1: Physical properties, Mass and IR spectral data of Compounds (2-12)

Comp. No.	Molecular Formula	Solvent	m.p. (°C)	Yield (%)	MS m/z (%)	IR (cm <sup>-1</sup> )						
						C=O	C=C	C≡N	C-O	NH	NH <sub>2</sub>	C=S
2a	C <sub>17</sub> H <sub>13</sub> BrO	-	149-150	72 <sup>a</sup> , 88 <sup>b</sup>	312 [M <sup>+</sup> ] (58), 314 [M+2] (57)	1667	1603	-	-	-	-	-
2b	C <sub>18</sub> H <sub>16</sub> O <sub>2</sub>	-	89-90	70 <sup>a</sup> , 75 <sup>b</sup>	264 [M <sup>+</sup> ] (79)	1666	1599	-	-	-	-	-
2c	C <sub>17</sub> H <sub>12</sub> Cl <sub>2</sub> O	-	99-100	73 <sup>a</sup> , 87 <sup>b</sup>	302 [M <sup>+</sup> ] (1), 304 [M+2] (1), 306 [M+4] (0.2)	1664	1605	-	-	-	-	-
2d	C <sub>17</sub> H <sub>13</sub> ClO	-	98-99	68 <sup>a</sup> , 82 <sup>b</sup>	268 [M <sup>+</sup> ] (73), 270 [M+2] (24)	1665	1604	-	-	-	-	-
2e	C <sub>18</sub> H <sub>16</sub> O <sub>2</sub>	-	126-127	67 <sup>a</sup>	264 [M <sup>+</sup> ] (63)	1666	1602	-	-	-	-	-
2f	C <sub>17</sub> H <sub>14</sub> O	-	86-87	80 <sup>a</sup>	234 [M <sup>+</sup> ] (57)	1668	1603	-	-	-	-	-
2g	C <sub>17</sub> H <sub>13</sub> NO <sub>3</sub>	-	132-133	65 <sup>a</sup>	279 [M <sup>+</sup> ] (41)	1667	1597	-	-	-	-	-
2h	C <sub>17</sub> H <sub>13</sub> ClO	-	62-63	66 <sup>a</sup>	268 [M <sup>+</sup> ] (3), 270 [M+2] (1)	1663	1605	-	-	-	-	-
2i	C <sub>18</sub> H <sub>15</sub> BrO <sub>2</sub>	-	123-124	64 <sup>b</sup>	342 [M <sup>+</sup> ] (45), 344 [M+2] (50)	1664	1603	-	-	-	-	-
2j	C <sub>19</sub> H <sub>18</sub> O <sub>3</sub>	-	133-134	64 <sup>b</sup>	294 [M <sup>+</sup> ] (67)	1663	1602	-	-	-	-	-
2k	C <sub>18</sub> H <sub>15</sub> NO <sub>4</sub>	-	169-170	64 <sup>b</sup>	309 [M <sup>+</sup> ] (100)	1660	1592	-	-	-	-	-
2l	C <sub>18</sub> H <sub>16</sub> O <sub>2</sub>	-	84-85	61 <sup>a</sup>	264 [M <sup>+</sup> ] (53)	1660	1605	-	-	-	-	-
3a	C <sub>20</sub> H <sub>15</sub> BrN <sub>2</sub> O	Ethanol	170-172	75	378 [M <sup>+</sup> ] (22), 380 [M+2] (22)	-	-	2194	-	-	3456 3311	-
3b	C <sub>21</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	Ethanol	168-170	73	330 [M <sup>+</sup> ] (100)	-	-	2191	-	-	3408 3313	-
3c	C <sub>21</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	Ethanol	195-196	72	330 [M <sup>+</sup> ] (60)	-	-	2188	-	-	3401 3325	-
3d	C <sub>21</sub> H <sub>17</sub> BrN <sub>2</sub> O <sub>2</sub>	Benzene	183-184	70	408 [M <sup>+</sup> ] (28), 410 [M+2] (29)	-	-	2191	-	-	3462 3328	-
3e	C <sub>22</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>	Benzene	68-70	69	360 [M <sup>+</sup> ] (100)	-	-	2192	-	-	3450 3337	-
4a	C <sub>21</sub> H <sub>15</sub> BrN <sub>2</sub> O	Methanol	208-209	67 <sup>a</sup> , 63 <sup>b</sup>	390 [M <sup>+</sup> ] (100), 392 [M+2] (98)	-	-	2222	1007	-	-	-



Table 1: Cont'd.

<b>4c</b>	C <sub>22</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	Methanol	153-154	47 <sup>a</sup>	342 [M <sup>+</sup> ] (100)	-	-	2216	1020	-	-	-
<b>4d</b>	C <sub>22</sub> H <sub>17</sub> BrN <sub>2</sub> O <sub>2</sub>	Methanol	250-251	52 <sup>a</sup>	420 [M <sup>+</sup> ] (99), 422 [M+2] (100)	-	-	2224	1008	-	-	-
<b>4e</b>	C <sub>22</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub>	Methanol	212-213	45 <sup>a</sup>	387 [M <sup>+</sup> ] (100)	-	-	2222	1036	-	-	-
<b>4f</b>	C <sub>21</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub> O	Methanol	160-161	60 <sup>a</sup> , 57 <sup>b</sup>	380 [M <sup>+</sup> ] (100), 382 [M+2] (68), 384 [M+4] (12)	-	-	2222	1016	-	-	-
<b>4g</b>	C <sub>21</sub> H <sub>15</sub> ClN <sub>2</sub> O	Methanol	142-143	48 <sup>a</sup>	346 [M <sup>+</sup> ] (100) 348 [M+2] (34)	-	-	2222	1024	-	-	-
<b>4h</b>	C <sub>22</sub> H <sub>17</sub> BrN <sub>2</sub> O	Ethanol	199-200	57 <sup>a</sup>	404 [M <sup>+</sup> ] (100), 406 [M+2] (95)	-	-	2218	1011	-	-	-
<b>4i</b>	C <sub>22</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub> O	Ethanol	149-150	51 <sup>a</sup> , 49 <sup>b</sup>	394 [M <sup>+</sup> ] (100), 396 [M+2] (62), 398 [M+4] (12)	-	-	2226	1029	-	-	-
<b>5</b>	C <sub>22</sub> H <sub>17</sub> BrN <sub>2</sub> O <sub>2</sub>	Ethanol	221-223	72	420 [M <sup>+</sup> ] (18), 422 [M+2] (19)	1683	-	-	-	3151	-	-
<b>6a</b>	C <sub>18</sub> H <sub>14</sub> BrN <sub>3</sub>	Ethanol	230-232	57	351 [M <sup>+</sup> ] (83), 353 [M+2] (81)	-	-	-	-	-	3316 3216	-
<b>6b</b>	C <sub>19</sub> H <sub>16</sub> BrN <sub>3</sub> O	Ethanol	172-173	45	381 [M <sup>+</sup> ] (93), 383 [M+2] (91)	-	-	-	-	-	3307 3197	-
<b>6c</b>	C <sub>20</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub>	Ethanol	169-170	44	333 [M <sup>+</sup> ] (88)	-	-	-	-	-	3371 3210	-
<b>6d</b>	C <sub>19</sub> H <sub>17</sub> N <sub>3</sub> O	Ethanol	152-153	48	303 [M <sup>+</sup> ] (93)	-	-	-	-	-	3309 3196	-
<b>7</b>	C <sub>20</sub> H <sub>13</sub> BrN <sub>2</sub> O	Acetic acid	335-337	42	376 [M <sup>+</sup> ] (5), 378 [M+2] (8)	1638	-	2222	-	3437	-	-
<b>8a</b>	C <sub>27</sub> H <sub>20</sub> BrN	Benzene- Pet. ether (60-80)	274-276	43 <sup>a</sup> , 53 <sup>b</sup>	437 [M <sup>+</sup> ] (100), 439 [M+2] (97)	-	-	-	-	-	-	-

Table 1: Cont'd.

8b	C <sub>28</sub> H <sub>22</sub> BrNO	Benzene- Pet. ether (60-80)	260-261	41 <sup>a</sup> , 49 <sup>b</sup>	467 [M <sup>+</sup> ] (90), 469 [M+2] (85)	-	-	-	-	-	-
9a	C <sub>18</sub> H <sub>15</sub> BrN <sub>2</sub> S	Ethanol	230-232	77	370 [M <sup>+</sup> ] (51), 372 [M+2] (47)	-	-	-	3192	-	1196
9b	C <sub>19</sub> H <sub>18</sub> N <sub>2</sub> OS	Ethanol	209-210	62	322 [M <sup>+</sup> ] (100)	-	-	-	3199	-	1194
9c*	C <sub>18</sub> H <sub>16</sub> N <sub>2</sub> S	Ethanol	259-260	71	-	-	-	-	-	-	-
9d	C <sub>19</sub> H <sub>17</sub> BrN <sub>2</sub> OS	Ethanol	254-256	67	400 [M <sup>+</sup> ] (35), 402 [M+2] (36)	-	-	-	3203	-	1207
9e	C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> S	Ethanol	236-237	62	352 [M <sup>+</sup> ] (100)	-	-	-	3198	-	1204
10a	C <sub>20</sub> H <sub>15</sub> BrN <sub>2</sub> OS	Ethanol	198-200	86	410 [M <sup>+</sup> ] (19), 412 [M+2] (20)	1722	-	-	-	-	-
10b	C <sub>21</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub> S	Ethanol	163-165	85	362 [M <sup>+</sup> ] (57)	1720	-	-	-	-	-
10c	C <sub>20</sub> H <sub>16</sub> N <sub>2</sub> OS	Ethanol	239-240	87	332 [M <sup>+</sup> ] (44)	1730	-	-	-	-	-
10d	C <sub>21</sub> H <sub>17</sub> BrN <sub>2</sub> O <sub>2</sub> S	Ethanol	207-209	95	440 [M <sup>+</sup> ] (28), 442 [M+2] (28)	1726	-	-	-	-	-
10e	C <sub>22</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S	Ethanol	148-150	89	392 [M <sup>+</sup> ] (1)	1732	-	-	-	-	-
11a	C <sub>28</sub> H <sub>21</sub> BrN <sub>2</sub> O <sub>2</sub> S	Ethanol	248-250	50 <sup>a</sup> , 82 <sup>b</sup>	528 [M <sup>+</sup> ] (18), 530 [M+2] (14)	1705	1607	-	-	-	-
11b	C <sub>27</sub> H <sub>19</sub> BrN <sub>2</sub> OS	Ethanol	115-117	66 <sup>a</sup> , 95 <sup>b</sup>	498 [M <sup>+</sup> ] (31), 500 [M+2] (33)	1703	1595	-	-	-	-
11c	C <sub>29</sub> H <sub>23</sub> BrN <sub>2</sub> O <sub>3</sub> S	Ethanol	178-180	69 <sup>a</sup> , 98 <sup>b</sup>	558 [M <sup>+</sup> ] (17), 560 [M+2] (19)	1713	1599	-	-	-	-
11d	C <sub>28</sub> H <sub>21</sub> BrN <sub>2</sub> O <sub>2</sub> S	Ethanol	183-184	93 <sup>a</sup>	558 [M <sup>+</sup> ] (35), 560 [M+2] (36)	1708	1597	-	-	-	-
12a	C <sub>21</sub> H <sub>17</sub> BrN <sub>2</sub> OS	Ethanol	138-140	91	424 [M <sup>+</sup> ] (49), 426 [M+2] (49)	1678	-	-	-	-	-
12b	C <sub>22</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> S	Ethanol	90-92	97	376 [M <sup>+</sup> ] (59)	1692	-	-	-	-	-
12c	C <sub>21</sub> H <sub>18</sub> N <sub>2</sub> OS	Ethanol	285-287	85	346 [M <sup>+</sup> ] (51)	1683	-	-	-	-	-
12d	C <sub>23</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub> S	Ethanol	150-151	87	406 [M <sup>+</sup> ] (100)	1689	-	-	-	-	-

a = Method A, b = Method B, \* = prepared in ref.[27]

Table 2:  $^1\text{H}$  NMR data of Compounds (2-12) in  $\text{CDCl}_3$  (\*  $\text{DMSO-d}_6$ ), ( $\delta$  in ppm,  $J$  in Hz)

Compd. No.	$^1\text{H}$ NMR
2a	2.91-2.94 (2H, m, $\text{CH}_2$ at C-3), 3.04-3.08 (2H, m, $\text{CH}_2$ at C-4), 7.23 (1H, d, $J=7.3$ , H-5), 7.28 (2H, d, $J=8.1$ , H-2' & H-6', AA' part of AA'XX' system), 7.35 (1H, t, $J=7.4$ , H-7), 7.47 (1H, td, $J^3=7.3$ , $J^4=1.4$ , H-6), 7.53 (2H, d, $J=8.1$ , H-3' & H-5', XX' part of AA'XX' system), 7.76 (1H, s, C=CH), 8.12 (1H, d, $J=8.1$ , H-8)
2b	2.92-2.96 (2H, m, $\text{CH}_2$ at C-3), 3.12-3.16 (2H, m, $\text{CH}_2$ at C-4), 3.85 (3H, s, $\text{OCH}_3$ ), 6.95 (2H, d, $J=8.8$ , H-3' & H-5', AA' part of AA'XX' system), 7.24 (1H, d, $J=8.1$ , H-5), 7.43 (2H, d, $J=8.1$ , H-2' & H-6', XX' part of AA'XX' system), 7.48 (1H, t, $J=7.3$ , H-6), 7.84 (1H, s, C=CH), 8.11 (1H, d, $J=8.1$ , H-8)
2c	2.93 (4H, s, $2\text{CH}_2$ at C-3 & C-4), 7.22-7.28 (3H, m, H-5, H-5' & H-6'), 7.35 (1H, t, $J=7.3$ , H-7), 7.45 (1H, d, $J=2.2$ , H-3'), 7.48 (1H, td, $J^3=7.3$ , $J^4=1.5$ , H-6), 7.80 (1H, s, C=CH), 8.13 (1H, dd, $J^3=8.0$ , $J^4=1.5$ , H-8)
2d	2.95 (2H, t, $J=6.2$ , $\text{CH}_2$ at C-3), 3.09 (2H, td, $J=6.2$ , 1.5, $\text{CH}_2$ at C-4), 7.24-7.39 (5H, m, H-5, H-7, H-4', H-5' & H-6'), 7.40 (1H, s, H-2'), 7.77 (1H, s, C=CH), 8.12 (1H, d, $J=8.8$ , H-8)
2e	2.94 (2H, t, $J=6.2$ , $\text{CH}_2$ at C-3), 3.13 (2H, td, $J=6.4$ , 1.7, $\text{CH}_2$ at C-4), 3.85 (3H, s, $\text{OCH}_3$ ), 6.90 (1H, dd, $J^3=8.1$ , $J^4=2.2$ , H-4'), 6.97 (1H, s, H-2'), 7.24 (1H, d, $J=7.3$ , H-6'), 7.31-7.38 (2H, m, H-7 & H-5'), 7.48 (1H, td, $J^3=7.3$ , $J^4=1.5$ , H-6), 7.83 (1H, s, C=CH), 8.12 (1H, dd, $J^3=7.3$ , $J^4=1.5$ , H-8)
2f	2.91-2.98 (2H, m, $\text{CH}_2$ at C-3), 3.12-3.18 (2H, m, $\text{CH}_2$ at C-4), 7.23-7.28 (1H, m, H-5), 7.32-7.58 (7H, m, H-6, H-7, H-2', H-3', H-4', H-5' & H-6'), 7.88 (1H, s, C=CH), 8.13 (1H, dd, $J^3=7.5$ , $J^4=1.4$ , H-8)
2g	2.96-2.99 (2H, m, $\text{CH}_2$ at C-3), 3.08-3.11 (2H, m, $\text{CH}_2$ at C-4), 7.26 (1H, d, $J=9.5$ , H-5), 7.38 (1H, t, $J=7.3$ , H-7), 7.51 (1H, t, $J=7.3$ , H-6), 7.56 (2H, d, $J=8.8$ , H-2' & H-6', AA' part of AA'XX' system), 7.83 (1H, s, C=CH), 8.13 (1H, d, $J=7.3$ , H-8), 8.26 (2H, d, $J=8.1$ , H-3' & H-5', XX' part of AA'XX' system)
2h	2.92-2.94 (4H, m, $2\text{CH}_2$ at C-3 & C-4), 7.22 (1H, d, $J=8.1$ , H-6'), 7.26-7.31 (3H, m, H-3', H-4' & H-5'), 7.34 (1H, t, $J=8.0$ , H-7), 7.41-7.44 (1H, m, H-5), 7.47 (1H, td, $J^3=7.3$ , $J^4=1.5$ , H-6), 7.90 (1H, s, C=CH), 8.15 (1H, d, $J=8.1$ , H-8)
2i	2.91 (2H, t, $J=5.8$ , $\text{CH}_2$ at C-3), 3.05 (2H, t, $J=5.8$ , $\text{CH}_2$ at C-4), 3.86 (3H, s, $\text{OCH}_3$ ), 6.70 (1H, d, $J=2.2$ , H-5), 6.87 (1H, dd, $J^3=8.8$ , $J^4=3.0$ , H-7), 7.27 (2H, d, $J=8.1$ , H-2' & H-6', AA' part of AA'XX' system), 7.52 (2H, d, $J=8.1$ , H-3' & H-5', XX' part of AA'XX' system), 7.73 (1H, s, C=CH), 8.10 (1H, d, $J=8.8$ , H-8)
2j	2.90 (2H, t, $J=6.6$ , $\text{CH}_2$ at C-3), 3.06 (2H, t, $J=5.5$ , $\text{CH}_2$ at C-4), 3.80 (3H, s, $\text{OCH}_3$ ), 3.84 (3H, s, $\text{OCH}_3$ ), 6.89 (1H, d, $J=2.2$ , H-5), 6.94 (1H, dd, $J^3=8.8$ , $J^4=3.0$ , H-7), 7.01 (2H, d, $J=8.8$ , H-3' & H-5', AA' part of AA'XX' system), 7.50 (2H, d, $J=8.8$ , H-2' & H-6', XX' part of AA'XX' system), 7.64 (1H, s, C=CH), 7.91 (1H, d, $J=8.8$ , H-8)
2k	2.92-2.96 (2H, m, $\text{CH}_2$ at C-3), 3.05-3.10 (2H, m, $\text{CH}_2$ at C-4), 3.88 (3H, s, $\text{OCH}_3$ ), 6.72 (1H, d, $J=2.5$ , H-5), 6.89 (1H, dd, $J^3=8.8$ , $J^4=2.5$ , H-7), 7.55 (2H, d, $J=8.5$ , H-2' & H-6', AA' part of AA'XX' system), 7.80 (1H, s, C=CH), 8.12 (1H, d, $J=8.8$ , H-8), 8.26 (2H, d, $J=8.5$ , H-3' & H-5', XX' part of AA'XX' system)
2l	2.87 (2H, t, $J=5.9$ , $\text{CH}_2$ at C-3), 3.02 (2H, t, $J=5.9$ , $\text{CH}_2$ at C-4), 3.81 (3H, s, $\text{OCH}_3$ ), 6.87 (1H, d, $J=3.0$ , H-5), 6.93 (1H, dd, $J^3=8.8$ , $J^4=2.2$ , H-7), 7.35-7.49 (5H, m, H-2', H-3', H-4', H-5' & H-6'), 7.63 (1H, s, C=CH), 7.91 (1H, d, $J=8.8$ , H-8)



Table 2: Cont'd.

<b>3a</b>	2.02-2.06 (1H, m, H <sub>ax</sub> -5), 2.12-2.18 (1H, m, H <sub>eq</sub> -5), 2.69-2.71 (1H, m, H <sub>ax</sub> -6), 2.73-2.81 (1H, m, H <sub>eq</sub> -6), 4.06 (1H, s, H-4), 4.62 (2H, br.s, NH <sub>2</sub> ), 7.14 (1H, d, <i>J</i> =9.5, H-7), 7.16 (2H, d, <i>J</i> =8.8, H-2' & H-6', AA' part of AA'XX' system), 7.22-7.25 (2H, m, H-8 & H-9), 7.44-7.47 (3H, m, H-10, H-3' & H-5')
<b>3b</b>	2.01-2.09 (1H, m, H <sub>ax</sub> -5), 2.11-2.19 (1H, m, H <sub>eq</sub> -5), 2.65-2.72 (1H, m, H <sub>ax</sub> -6), 2.74-2.82 (1H, m, H <sub>eq</sub> -6), 3.78 (3H, s, OCH <sub>3</sub> ), 4.03 (1H, s, H-4), 4.62 (2H, br.s, NH <sub>2</sub> ), 6.85 (2H, d, <i>J</i> =8.8, H-3' & H-5', AA' part of AA'XX' system), 7.12 (1H, d, <i>J</i> =8.4, H-7), 7.19 (2H, d, <i>J</i> =8.8, H-2' & H-6', XX' part of AA'XX' system), 7.20-7.26 (2H, m, H-8 & H-9), 7.46 (1H, d, <i>J</i> =7.3, H-10)
<b>3c<sup>*</sup></b>	1.84-1.92 (1H, m, H <sub>ax</sub> -5), 2.14-2.22 (1H, m, H <sub>eq</sub> -5), 2.57-2.65 (1H, m, H <sub>ax</sub> -6), 2.70-2.78 (1H, m, H <sub>eq</sub> -6), 3.73 (3H, s, OCH <sub>3</sub> ), 4.05 (1H, s, H-4), 6.79 (1H, d, <i>J</i> =2.2, H-2'), 6.80-6.84 (2H, m, H-4' & H-6'), 6.88 (2H, br.s, NH <sub>2</sub> ), 7.15 (1H, d, <i>J</i> =7.3, H-7), 7.20-7.30 (3H, m, H-8, H-9 & H-5'), 7.51 (1H, d, <i>J</i> =7.3, H-10)
<b>3d</b>	1.96-2.04 (1H, m, H <sub>ax</sub> -5), 2.08-2.17 (1H, m, H <sub>eq</sub> -5), 2.61-2.82 (2H, m, CH <sub>2</sub> at C-6), 3.81 (3H, s, OCH <sub>3</sub> ), 4.04 (1H, s, H-4), 4.57 (2H, br.s, NH <sub>2</sub> ), 6.68 (1H, d, <i>J</i> =2.5, H-7), 6.76 (1H, dd, <i>J</i> <sup>3</sup> =8.5, <i>J</i> <sup>4</sup> =2.5, H-9), 7.16 (2H, d, <i>J</i> =8.3, H-2' & H-6', AA' part of AA'XX' system), 7.45 (2H, d, <i>J</i> =8.3, H-3' & H-5', XX' part of AA'XX' system), 7.38 (1H, d, <i>J</i> =8.2, H-10)
<b>3e</b>	2.00-2.21 (2H, m, CH <sub>2</sub> at C-5), 2.61-2.82 (2H, m, CH <sub>2</sub> at C-6), 3.80 (3H, s, OCH <sub>3</sub> ), 3.81 (3H, s, OCH <sub>3</sub> ), 4.03 (1H, s, H-4), 4.51 (2H, br.s, NH <sub>2</sub> ), 6.69 (1H, d, <i>J</i> =2.5, H-7), 6.77 (1H, dd, <i>J</i> <sup>3</sup> =8.8, <i>J</i> <sup>4</sup> =2.5, H-9), 6.87 (2H, d, <i>J</i> =8.5, H-3' & H-5', AA' part of AA'XX' system), 7.20 (2H, d, <i>J</i> =8.8, H-2' & H-6', XX' part of AA'XX' system), 7.39 (1H, d, <i>J</i> =8.0, H-10)
<b>4a</b>	2.64-2.68 (2H, m, CH <sub>2</sub> at C-6), 2.80-2.84 (2H, m, CH <sub>2</sub> at C-5), 4.17 (3H, s, OCH <sub>3</sub> ), 7.20 (2H, d, <i>J</i> =8.0, H-2' & H-6', AA' part of AA'XX' system), 7.22-7.24 (1H, m, H-7), 7.38-7.40 (2H, m, H-8 & H-9), 7.56 (2H, d, <i>J</i> =8.8, H-3' & H-5', XX' part of AA'XX' system), 8.33-8.34 (1H, m, H-10)
<b>4b</b>	2.70-2.73 (2H, m, CH <sub>2</sub> at C-6), 2.80-2.83 (2H, m, CH <sub>2</sub> at C-5), 3.87 (3H, s, OCH <sub>3</sub> ), 4.17 (3H, s, OCH <sub>3</sub> ), 7.02 (2H, d, <i>J</i> =8.8, H-3' & H-5', AA' part of AA'XX' system), 7.21-7.23 (1H, m, H-7), 7.27 (2H, d, <i>J</i> =8.8, H-2' & H-6', XX' part of AA'XX' system), 7.35-7.39 (2H, m, H-8 & H-9), 8.33 (1H, d, <i>J</i> =8.8, H-10)
<b>4c</b>	2.67-2.71 (2H, m, CH <sub>2</sub> at C-6), 2.80-2.84 (2H, m, CH <sub>2</sub> at C-5), 3.84 (3H, s, OCH <sub>3</sub> ), 4.18 (3H, s, OCH <sub>3</sub> ), 6.84 (1H, d, <i>J</i> =2.2, H-2'), 6.89 (1H, d, <i>J</i> =7.3, H-4'), 7.00 (1H, dd, <i>J</i> <sup>3</sup> =8.1, <i>J</i> <sup>4</sup> =2.2, H-6'), 7.21-7.23 (1H, m, H-5'), 7.35-7.40 (3H, m, H-7, H-8 & H-9), 8.32-8.35 (1H, m, H-10)
<b>4d</b>	2.62-2.65 (2H, m, CH <sub>2</sub> at C-6), 2.77-2.80 (2H, m, CH <sub>2</sub> at C-5), 3.86 (3H, s, OCH <sub>3</sub> ), 4.15 (3H, s, OCH <sub>3</sub> ), 6.73 (1H, d, <i>J</i> =2.2, H-7), 6.91 (1H, dd, <i>J</i> <sup>3</sup> =8.8, <i>J</i> <sup>4</sup> =2.2, H-9), 7.19 (2H, d, <i>J</i> =8.0, H-2' & H-6', AA' part of AA'XX' system), 7.64 (2H, d, <i>J</i> =8.1, H-3' & H-5', XX' part of AA'XX' system), 8.27 (1H, d, <i>J</i> =8.8, H-10)
<b>4e<sup>*</sup></b>	2.55 (2H, t, <i>J</i> =7.3, CH <sub>2</sub> at C-6), 2.81 (2H, t, <i>J</i> =7.3, CH <sub>2</sub> at C-5), 3.85 (3H, s, OCH <sub>3</sub> ), 4.12 (3H, s, OCH <sub>3</sub> ), 6.91 (1H, s, H-7), 6.99 (1H, dd, <i>J</i> <sup>3</sup> =8.8, <i>J</i> <sup>4</sup> =2.6, H-9), 7.76 (2H, d, <i>J</i> =8.8, H-2' & H-6', AA' part of AA'XX' system), 8.23 (1H, d, <i>J</i> =8.8, H-10), 8.41 (2H, d, <i>J</i> =8.8, H-3' & H-5', XX' part of AA'XX' system)
<b>4f</b>	2.46-2.67 (2H, m, CH <sub>2</sub> at C-6), 2.79-2.92 (2H, m, CH <sub>2</sub> at C-5), 4.12 (3H, s, OCH <sub>3</sub> ), 7.21-7.27 (2H, m, H-7 & H-9), 7.35-7.40 (2H, m, H-8 & H-6'), 7.43 (1H, d, <i>J</i> =8.8, H-5'), 7.57 (1H, s, H-3'), 8.33-8.37 (1H, m, H-10)
<b>4g</b>	2.63-2.68 (2H, m, CH <sub>2</sub> at C-6), 2.81-2.85 (2H, m, CH <sub>2</sub> at C-5), 4.18 (3H, s, OCH <sub>3</sub> ), 7.22-7.25 (2H, m, H-5' & H-6'), 7.30 (1H, s, H-2'), 7.38-7.40 (2H, m, H-7 & H-4'), 7.45-7.47 (2H, m, H-8 & H-9), 8.32-8.34 (1H, m, H-10)

Table 2: Cont'd.

4h	1.51 (3H, t, $J=7.1$ OCH <sub>2</sub> CH <sub>3</sub> ), 2.63-2.67 (2H, m, CH <sub>2</sub> at C-6), 2.80-2.84 (2H, m, CH <sub>2</sub> at C-5), 4.65 (2H, q, $J=7.1$ , OCH <sub>2</sub> CH <sub>3</sub> ), 7.19-7.25 (3H, m, H-7, H-2' & H-6'), 7.37-7.39 (2H, m, H-8 & H-9), 7.65 (2H, d, $J=8.1$ , H-3' & H-5', XX' part of AA'XX' system) 8.28-8.30 (1H, m, H-10)
4i	1.52 (3H, t, $J=7.1$ OCH <sub>2</sub> CH <sub>3</sub> ), 2.44-2.76 (2H, m, CH <sub>2</sub> at C-6), 2.77-2.94 (2H, m, CH <sub>2</sub> at C-5), 4.66 (2H, q, $J=7.1$ , OCH <sub>2</sub> CH <sub>3</sub> ), 7.21-7.26 (2H, m, H-5' & H-6'), 7.36-7.44 (2H, m, H-7, H-8 & H-9), 8.30-8.33 (1H, m, H-10)
5	2.07-2.15 (1H, m, H <sub>ax</sub> -6), 2.20-2.28 (1H, m, H <sub>eq</sub> -6), 2.32 (3H, s, CH <sub>3</sub> ), 2.66-2.76 (1H, m, H <sub>ax</sub> -5), 2.77-2.86 (1H, m, H <sub>eq</sub> -5), 4.47 (1H, s, H-7), 7.11 (1H, d, $J=7.3$ , H-4), 7.20-7.28 (4H, m, H-2, H-3, H-2' & H-6'), 7.37 (2H, d, $J=8.8$ , H-3' & H-5', XX' part of AA'XX' system), 7.74 (1H, d, $J=7.3$ , H-1), 13.00 (1H, br.s, NH)
6a*	2.76 (4H, s, 2CH <sub>2</sub> at C-5 & C-6), 6.58 (2H, br.s, NH <sub>2</sub> ), 7.28-7.31 (1H, m, H-7), 7.34-7.44 (2H, m, H-8 & H-9), 7.54 (2H, d, $J=8.2$ , H-2' & H-6', AA' part of AA'XX' system), 7.69 (2H, d, $J=8.3$ , H-3' & H-5', XX' part of AA'XX' system), 8.18 (1H, dd, $J^3=7.1$ , $J^4=1.9$ , H-10)
6b	2.79 (4H, s, 2CH <sub>2</sub> at C-5 & C-6), 3.85 (3H, s, OCH <sub>3</sub> ), 5.15 (2H, br.s, NH <sub>2</sub> ), 6.73 (1H, d, $J=2.5$ , H-7), 6.88 (1H, dd, $J^3=8.8$ , $J^4=2.5$ , H-9), 7.42 (2H, d, $J=8.5$ , H-2' & H-6', AA' part of AA'XX' system), 7.59 (2H, d, $J=8.5$ , H-3' & H-5', XX' part of AA'XX' system), 8.21 (1H, d, $J=8.8$ , H-10)
6c	2.75-2.79 (2H, m, CH <sub>2</sub> at C-6), 2.84-2.89 (2H, m, CH <sub>2</sub> at C-5), 3.84 (3H, s, OCH <sub>3</sub> ), 3.85 (3H, s, OCH <sub>3</sub> ), 5.21 (2H, br.s, NH <sub>2</sub> ), 6.73 (1H, d, $J=2.5$ , H-7), 6.88 (1H, dd, $J^3=8.8$ , $J^4=2.5$ , H-9), 6.98 (2H, d, $J=8.5$ , H-3' & H-5', AA' part of AA'XX' system), 7.52 (2H, d, $J=8.8$ , H-2' & H-6', XX' part of AA'XX' system), 8.20 (1H, d, $J=8.8$ , H-10)
6d	2.75-2.80 (2H, m, CH <sub>2</sub> at C-6), 2.82-2.87 (2H, m, CH <sub>2</sub> at C-5), 3.85 (3H, s, OCH <sub>3</sub> ), 5.10 (2H, br.s, NH <sub>2</sub> ), 6.74 (1H, d, $J=2.2$ , H-7), 6.88 (1H, dd, $J^3=8.8$ , $J^4=2.5$ , H-9), 7.42-7.56 (5H, m, H-2', H-3', H-4', H-5' & H-6'), 8.22 (1H, d, $J=8.5$ , H-10)
7	1.76 (2H, t, $J=7.3$ , CH <sub>2</sub> at C-6), 2.11 (2H, t, $J=7.3$ , CH <sub>2</sub> at C-5), 6.62-6.63 (3H, m, H-7, H-2', H-6'), 6.69-6.77 (2H, m, H-8 & H-9), 7.02 (2H, dd, $J^3=7.3$ , $J^4=1.5$ , H-3' & H-5'), 7.26 (1H, br.s, NH), 7.40 (1H, d, $J=8.5$ , H-10)
8a	2.70-2.73 (2H, m, CH <sub>2</sub> at C-1), 2.83-2.88 (4H, m, 2CH <sub>2</sub> at C-2 & C-7), 3.29-3.32 (2H, m, CH <sub>2</sub> at C-8), 7.31 (1H, dd, $J^3=7.4$ , $J^4=1.5$ , H-d'), 7.33-7.37 (5H, m, H-a', H-b', H-c', H-2' & H-6'), 7.54-7.61 (5H, m, H-b, H-c, H-d, H-3' & H-5'), 8.38 (1H, dd, $J^3=8.1$ , $J^4=1.4$ , H-a)
8b	2.68-2.73 (2H, m, CH <sub>2</sub> at C-1), 2.81-2.88 (4H, m, 2CH <sub>2</sub> at C-2 & C-7), 3.25-3.31 (2H, m, CH <sub>2</sub> at C-8), 3.88 (3H, s, OCH <sub>3</sub> ), 6.88-6.90 (2H, m, H-b' & H-d'), 7.30-7.36 (3H, m, H-b, H-d & H-a'), 7.48-7.56 (3H, m, H-c, H-2' & H-6'), 7.60 (2H, d, $J=8.0$ , H-3' & H-5', XX' part of AA'XX' system), 8.36 (1H, dd, $J^3=8.8$ , $J^4=2.9$ , H-a)
9a	1.86-1.88 (1H, m, H <sub>ax</sub> -5), 2.06-2.08 (1H, m, H <sub>eq</sub> -5), 2.51-2.63 (1H, m, H <sub>ax</sub> -6), 2.65-2.75 (1H, m, H <sub>eq</sub> -6), 4.90 (1H, s, H-4), 7.06 (1H, d, $J=6.6$ , H-7), 7.11-7.18 (2H, m, H-8 & H-9), 7.21 (2H, d, $J=8.0$ , H-2' & H-6', AA' part of AA'XX' system), 7.41 (2H, d, $J=8.0$ , H-3' & H-5', XX' part of AA'XX' system) 8.88 (1H, br.s, NH), 9.26 (1H, br.s, NH)
9b*	1.88-1.97 (1H, m, H <sub>ax</sub> -5), 2.03-2.11 (1H, m, H <sub>eq</sub> -5), 2.63-2.71 (1H, m, H <sub>ax</sub> -6), 2.73-2.81 (1H, m, H <sub>eq</sub> -6), 3.77 (3H, s, OCH <sub>3</sub> ), 5.04 (1H, s, H-4), 6.86 (2H, d, $J=8.1$ , H-3' & H-5', AA' part of AA'XX' system) 7.01 (1H, br.s, NH), 7.15 (1H, d, $J=6.6$ , H-7), 7.20-7.29 (5H, m, H-8, H-9, H-10, H-2' & H-6'), 7.80 (1H, br.s, NH)



Table 2: Cont'd.

<b>9d</b>	1.78-1.82 (1H, m, H <sub>ax</sub> -5), 2.12-2.16 (1H, m, H <sub>eq</sub> -5), 2.53-2.59 (1H, m, H <sub>ax</sub> -6), 2.68-2.71 (1H, m, H <sub>eq</sub> -6), 3.74 (3H, s, OCH <sub>3</sub> ), 4.94 (1H, s, H-4), 6.76 (2H, s, H-7 & H-9), 7.26 (2H, d, <i>J</i> =7.3, H-2' & H-6', AA' part of AA'XX' system), 7.58 (2H, d, <i>J</i> =8.0, H-3' & H-5', XX' part of AA'XX' system), 7.65 (1H, d, <i>J</i> =8.8, H-10), 9.09 (1H, br.s, NH), 9.77 (1H, br.s, NH)
<b>9e</b>	1.76-1.84 (1H, m, H <sub>ax</sub> -5), 2.08-2.16 (1H, m, H <sub>eq</sub> -5), 2.52-2.60 (1H, m, H <sub>ax</sub> -6), 2.65-2.73 (1H, m, H <sub>eq</sub> -6), 3.73 (3H, s, OCH <sub>3</sub> ), 3.74 (3H, s, OCH <sub>3</sub> ), 4.86 (1H, s, H-4), 6.76-6.78 (2H, m, H-7 & H-9), 6.93 (2H, d, <i>J</i> =8.8, H-3' & H-5', AA' part of AA'XX' system), 7.22 (2H, d, <i>J</i> =8.1, H-2' & H-6', XX' part of AA'XX' system), 7.64 (1H, d, <i>J</i> =9.5, H-10), 9.00 (1H, br.s, NH), 9.67 (1H, br.s, NH)
<b>10a</b>	2.01-2.07 (1H, m, H <sub>ax</sub> -6), 2.15-2.23 (1H, m, H <sub>eq</sub> -6), 2.67-2.73 (1H, m, H <sub>ax</sub> -7), 2.76-2.82 (1H, m, H <sub>eq</sub> -7), 3.74 (1H, d, <i>J</i> =17.6), 3.86 (1H, d, <i>J</i> =17.6) (CH <sub>2</sub> at C-2, AB system), 5.56 (1H, s, H-5), 7.10-7.11 (1H, m, H-8), 7.22 (1H, t, <i>J</i> =7.0, H-10), 7.28-7.32 (3H, m, H-9, H-2' & H-6'), 7.47 (2H, d, <i>J</i> =8.0, H-3' & H-5' XX' part of AA'XX' system), 7.99-8.01 (1H, m, H-11)
<b>10b</b>	1.83-1.91 (1H, m, H <sub>ax</sub> -6), 2.18-2.26 (1H, m, H <sub>eq</sub> -6), 2.54-2.64 (1H, m, H <sub>ax</sub> -7), 2.69-2.77 (1H, m, H <sub>eq</sub> -7), [3.72 (3H, s, OCH <sub>3</sub> ), [4.03 (1H, d, <i>J</i> =17.6), 4.09 (1H, d, <i>J</i> =17.6) (CH <sub>2</sub> at C-2, AB system)], 5.59 (1H, s, H-5), 6.91 (2H, d, <i>J</i> =8.1, H-3' & H-5' AA' part of AA'XX' system), 7.11 (1H, d, <i>J</i> =7.3, H-8), 7.18 (1H, t, <i>J</i> =7.3, H-10), 7.22-7.26 (3H, m, H-9, H-2' & H-6'), 7.78 (1H, d, <i>J</i> =7.4, H-11)
<b>10c</b>	1.82-1.88 (1H, m, H <sub>ax</sub> -6), 2.15-2.25 (1H, m, H <sub>eq</sub> -6), 2.54-2.62 (1H, m, H <sub>ax</sub> -7), 2.70-2.76 (1H, m, H <sub>eq</sub> -7), [4.03 (1H, d, <i>J</i> =17.6), 4.10 (1H, d, <i>J</i> =17.6) (CH <sub>2</sub> at C-2, AB system)], 5.65 (1H, s, H-5), 7.10-7.24 (3H, m, H-2', H-4' & H-6'), 7.28-7.40 (5H, m, H-8, H-9, H-10, H-3' & H-5'), 7.70 (1H, dd, <i>J</i> <sup>3</sup> =7.7, <i>J</i> <sup>4</sup> =2.2, H-11)
<b>10d</b>	1.81-1.87 (1H, m, H <sub>ax</sub> -6), 2.18-2.26 (1H, m, H <sub>eq</sub> -6), 2.54-2.62 (1H, m, H <sub>ax</sub> -7), 2.67-2.73 (1H, m, H <sub>eq</sub> -7), 3.73 (3H, s, OCH <sub>3</sub> ), [4.02 (1H, d, <i>J</i> =16.9), 4.09 (1H, d, <i>J</i> =17.6) (CH <sub>2</sub> at C-2, AB system)], 5.64 (1H, s, H-5), 6.73 (1H, d, <i>J</i> =2.2 H-8), 6.79 (1H, dd, <i>J</i> <sup>3</sup> =8.4, <i>J</i> <sup>4</sup> =2.5, H-10), 7.29 (2H, d, <i>J</i> =8.1, H-2' & H-6' AA' part of AA'XX' system), 7.57 (2H, d, <i>J</i> =8.0, H-3' & H-5' XX' part of AA'XX' system), 7.69 (1H, d, <i>J</i> =8.1, H-11)
<b>10e</b>	1.83-1.89 (1H, m, H <sub>ax</sub> -6), 2.15-2.23 (1H, m, H <sub>eq</sub> -6), 2.54-2.61 (1H, m, H <sub>ax</sub> -7), 2.67-2.75 (1H, m, H <sub>eq</sub> -7), 3.81 (3H, s, OCH <sub>3</sub> ), 3.85 (3H, s, OCH <sub>3</sub> ), [4.00 (1H, d, <i>J</i> =15.9), 4.08 (1H, d, <i>J</i> =15.9) (CH <sub>2</sub> at C-2, AB system)], 5.56 (1H, s, H-5), 6.72 (1H, d, <i>J</i> =2.2 H-8), 6.79 (1H, dd, <i>J</i> <sup>3</sup> =8.4, <i>J</i> <sup>4</sup> =2.5, H-10), 6.90 (2H, d, <i>J</i> =8.8, H-3' & H-5' AA' part of AA'XX' system), 7.24 (2H, d, <i>J</i> =8.8, H-2' & H-6' XX' part of AA'XX' system), 7.69 (1H, d, <i>J</i> =8.8, H-11)
<b>11a</b>	2.04-2.12 (1H, m, H <sub>ax</sub> -6), 2.21-2.29 (1H, m, H <sub>eq</sub> -6), 2.70-2.76 (1H, m, H <sub>ax</sub> -7), 2.79-2.87 (1H, m, H <sub>eq</sub> -7), 3.85 (3H, s, OCH <sub>3</sub> ), 5.68 (1H, s, H-5), 6.95 (1H, dd, <i>J</i> <sup>3</sup> =6.0, <i>J</i> <sup>4</sup> =2.2, H-4''), 7.00 (1H, s, H-2''), 7.07-7.12 (2H, m, H-5'' & H-6''), 7.20-7.38 (5H, m, H-8, H-9, H-10, H-2' & H-6'), 7.47 (2H, d, <i>J</i> =8.0, H-3' & H-5' XX' part of AA'XX' system), 7.64 (1H, s, C=CH), 7.98 (1H, d, <i>J</i> =7.3, H-11)
<b>11b</b>	2.06-2.14 (1H, m, H <sub>ax</sub> -6), 2.22-2.30 (1H, m, H <sub>eq</sub> -6), 2.68-2.75 (1H, m, H <sub>ax</sub> -7), 2.79-2.87 (1H, m, H <sub>eq</sub> -7), 5.70 (1H, s, H-5), 7.11 (1H, d, <i>J</i> =6.6, H-8), 7.22 (1H, td, <i>J</i> <sup>3</sup> =7.7, <i>J</i> <sup>4</sup> =1.4, H-10), 7.28-7.36 (7H, m, H-2', H-3', H-4', H-5', H-6', H-2'' & H-6''), 7.43-7.46 (1H, m, H-9), 7.57 (1H, s, C=CH), 7.58 (2H, d, <i>J</i> =8.8, H-3'' & H-5'' XX' part of AA'XX' system), 7.97 (1H, d, <i>J</i> =7.3, H-11)



Table 2: Cont'd.

<b>11c</b>	1.86-1.91 (1H, m, H <sub>ax</sub> -6), 2.24-2.31 (1H, m, H <sub>eq</sub> -6), 2.57-2.64 (1H, m, H <sub>ax</sub> -7), 2.71-2.79 (1H, m, H <sub>eq</sub> -7), 3.75 (3H, s, OCH <sub>3</sub> ), 3.81 (3H, s, OCH <sub>3</sub> ), 5.83 (1H, s, H-5), 6.74 (1H, d, <i>J</i> =2.2, H-8), 6.82 (1H, dd, <i>J</i> <sup>3</sup> =8.8, <i>J</i> <sup>4</sup> =2.2, H-10), 7.05 (1H, dd, <i>J</i> <sup>3</sup> =8.0, <i>J</i> <sup>4</sup> =2.2, H-4''), 7.14-7.18 (2H, m, H-2'' & H-6''), 7.35 (2H, d, <i>J</i> =8.8, H-2' & H-6' AA' part of AA'XX' system), 7.45 (1H, t, <i>J</i> =8.1, H-5''), 7.57 (2H, d, <i>J</i> =8.8, H-3' & H-5' XX' part of AA'XX' system), 7.65 (1H, s, C=CH), 7.72 (1H, d, <i>J</i> =8.8, H-11)
<b>11d</b>	2.04-2.12 (1H, m, H <sub>ax</sub> -6), 2.17-2.26 (1H, m, H <sub>eq</sub> -6), 2.65-2.73 (1H, m, H <sub>ax</sub> -7), 2.75-2.83 (1H, m, H <sub>eq</sub> -7), 3.67 (3H, s, OCH <sub>3</sub> ), 3.81 (3H, s, OCH <sub>3</sub> ), 5.64 (1H, s, H-5), 6.67 (1H, d, <i>J</i> =2.2, H-8), 6.81 (1H, dd, <i>J</i> <sup>3</sup> =8.4, <i>J</i> <sup>4</sup> =2.5, H-10), 6.84 (2H, d, <i>J</i> =8.8, H-3' & H-5' AA' part of AA'XX' system), 7.31 (2H, d, <i>J</i> =8.8, H-2' & H-6' XX' part of AA'XX' system), 7.36 (2H, d, <i>J</i> =8.8, H-2'' & H-6'' AA' part of AA'XX' system), 7.55 (2H, d, <i>J</i> =8.8, H-3'' & H-5'' XX' part of AA'XX' system), 7.56 (1H, s, C=CH), 7.89 (1H, d, <i>J</i> =8.8, H-11)
<b>12a</b>	2.11-2.20 (1H, m, H <sub>ax</sub> -7), 2.24-2.33 (1H, m, H <sub>eq</sub> -7), 2.73-2.86 (3H, m, H <sub>ax</sub> -3 & CH <sub>2</sub> at C-8), 2.98-3.12 (3H, m, CH <sub>2</sub> at C-2 & H <sub>eq</sub> -3), 6.11 (1H, s, H-6), 7.09 (1H, d, <i>J</i> =7.3, H-9), 7.19 (1H, td, <i>J</i> <sup>3</sup> =7.3, <i>J</i> <sup>4</sup> =1.5, H-11), 7.26 (2H, td, <i>J</i> <sup>3</sup> =7.3, <i>J</i> <sup>4</sup> =2.9, H-10 & H-12), 7.31 (2H, d, <i>J</i> =8.1, H-2' & H-6' AA' part of AA'XX' system), 7.45 (2H, d, <i>J</i> =8.8, H-3' & H-5' XX' part of AA'XX' system)
<b>12b*</b>	2.04-2.13 (1H, m, H <sub>ax</sub> -7), 2.28-2.36 (1H, m, H <sub>eq</sub> -7), 2.63-2.71 (1H, m, H <sub>ax</sub> -8), 2.73-2.82 (1H, m, H <sub>eq</sub> -8), 2.94-3.09 (4H, m, 2CH <sub>2</sub> at C-2 & C-3), 3.72 (3H, s, OCH <sub>3</sub> ), 6.08 (1H, s, H-6), 6.91 (2H, d, <i>J</i> =8.1, H-3' & H-5' AA' part of AA'XX' system), 7.12 (1H, d, <i>J</i> =7.3, H-9), 7.17 (1H, t, <i>J</i> =7.0, H-11), 7.20-7.26 (3H, m, H-10, H-2' & H-6''), 7.69 (1H, d, <i>J</i> =7.4, H-12)
<b>12c</b>	2.18-2.24 (1H, m, H <sub>ax</sub> -7), 2.29-2.37 (1H, m, H <sub>eq</sub> -7), 2.73-2.86 (3H, m, H <sub>ax</sub> -3 & CH <sub>2</sub> at C-8), 3.04-3.15 (3H, m, CH <sub>2</sub> at C-2 & H <sub>eq</sub> -3), 6.21 (1H, s, H-6), 7.10 (1H, d, <i>J</i> =7.3, H-9), 7.18-7.44 (7H, m, H-10, H-11, H-2', H-3', H-4', H-5' & H-6''), 8.02 (1H, d, <i>J</i> =7.3, H-12)
<b>12d</b>	2.02-2.12 (1H, m, H <sub>ax</sub> -7), 2.25-2.33 (1H, m, H <sub>eq</sub> -7), 2.62-2.70 (1H, m, H <sub>ax</sub> -8), 2.72-2.80 (1H, m, H <sub>eq</sub> -8), 2.92-3.10 (4H, m, 2CH <sub>2</sub> at C-2 & C-3), 3.72 (6H, s, 2OCH <sub>3</sub> ), 6.05 (1H, s, H-6), 6.73 (1H, d, <i>J</i> =2.2, H-9), 6.78 (1H, td, <i>J</i> <sup>3</sup> =8.4, <i>J</i> <sup>4</sup> =2.6, H-11), 6.91 (2H, d, <i>J</i> =8.8, H-3' & H-5' AA' part of AA'XX' system), 7.23 (2H, d, <i>J</i> =8.0, H-2' & H-6' XX' part of AA'XX' system), 7.59 (1H, d, <i>J</i> =8.8, H-12)

Table 3: <sup>13</sup>C NMR data of Compounds (2-6, 8-12) in CDCl<sub>3</sub> (\* DMSO-d<sub>6</sub>) (δ in ppm)

Compd. No.	<sup>13</sup> C NMR
<b>2a</b>	27.28 (C-3), 28.85(C-4), 122.81, 127.20, 128.30, 128.35, 131.45, 131.76, 133.40, 133.52, 134.78, 135.38, 136.14, 143.22 (Olefinic and Aromatic Carbons), 187.74 (C=O)
<b>2b</b>	27.32 (C-3), 28.88 (C-4), 55.44 (OCH <sub>3</sub> ), 114.02, 127.06, 128.17, 128.23, 128.47, 131.84, 133.19, 133.60, 133.72, 136.78, 143.14, 160.03 (Olefinic and Aromatic Carbons), 187.96 (C=O)
<b>2c</b>	27.50 (C-3), 29.00 (C-4), 126.90, 127.22, 128.39, 128.43, 129.76, 131.20, 132.25, 133.04, 133.20, 133.66, 134.83, 135.67, 137.78, 143.40 (Olefinic and Aromatic Carbons), 187.36 (C=O)
<b>2d</b>	27.26 (C-3), 28.87 (C-4), 127.20, 128.07, 128.33, 128.36, 128.58, 129.59, 129.82, 133.35, 133.56, 134.45, 135.00, 136.71, 137.72, 143.27 (Olefinic and Aromatic Carbons), 187.67 (C=O)

Table 3: Cont'd.

<b>2e</b>	27.36 (C-3), 28.95 (C-4), 55.39 (OCH <sub>3</sub> ), 114.16, 115.43, 122.38, 127.11, 128.10, 128.31, 129.55, 133.40, 133.53, 135.80, 136.61, 137.26, 143.36, 159.58 (Olefinic and Aromatic Carbons), 187.97 (C=O)
<b>2f</b>	28.96 (C-3), 29.05 (C-4), 126.05, 127.11, 127.34, 128.30, 128.56, 128.66, 129.99, 133.39, 133.57, 135.57, 135.93, 136.73 (Olefinic and Aromatic Carbons), 187.94 (C=O)
<b>2g</b>	27.38 (C-3), 28.77 (C-4), 123.81, 127.38, 128.43, 128.48, 130.50, 133.10, 133.77, 133.87, 138.63, 142.56, 143.21, 147.35 (Olefinic and Aromatic Carbons), 187.35 (C=O)
<b>2h</b>	27.47 (C-3), 29.08 (C-4), 126.54, 127.15, 128.33, 128.46, 129.74, 129.85, 130.52, 133.33, 133.45, 133.58, 134.47, 134.89, 137.27, 143.52 (Olefinic and Aromatic Carbons), 187.61 (C=O)
<b>2i</b>	27.30 (C-3), 29.27 (C-4), 55.56 (OCH <sub>3</sub> ), 112.38, 113.51, 122.58, 126.96, 130.90, 131.38, 131.70, 134.68, 134.97, 136.30, 145.72, 163.76 (Olefinic and Aromatic Carbons), 187.55 (C=O)
<b>2j*</b>	27.28 (C-3), 28.79 (C-4), 55.82 (OCH <sub>3</sub> ), 56.08 (OCH <sub>3</sub> ), 112.80, 114.18, 114.63, 127.00, 128.33, 130.38, 132.29, 134.05, 135.56, 146.34, 160.17, 163.70 (Olefinic and Aromatic Carbons), 185.91 (C=O)
<b>2k</b>	27.40 (C-3), 29.19 (C-4), 55.61 (OCH <sub>3</sub> ), 112.46, 113.75, 123.77, 126.68, 130.43, 131.07, 113.11, 138.84, 142.82, 145.74, 147.40, 164.03 (Olefinic and Aromatic Carbons), 186.12 (C=O)
<b>2l*</b>	27.23 (C-3), 28.80 (C-4), 56.08 (OCH <sub>3</sub> ), 112.83, 114.31, 126.70, 129.16, 129.25, 130.34, 130.54, 135.58, 135.77, 136.16, 146.68, 163.90 (Olefinic and Aromatic Carbons), 186.31 (C=O)
<b>3a</b>	25.03 (C-5), 27.51 (C-6), 42.44 (C-4), 60.54 (C-3), 111.13 (CN), 119.75, 120.94, 121.51, 126.63, 127.62, 128.28, 128.48, 129.86, 132.01, 135.59, 141.14, 141.88, 159.18 (Other Olefinic and Aromatic Carbons)
<b>3b</b>	25.07 (C-5), 27.59 (C-6), 42.08 (C-4), 55.35 (OCH <sub>3</sub> ), 61.37 (C-3), 112.09 (CN), 114.22, 120.05, 120.83, 126.54, 127.55, 128.22, 128.57, 129.15, 134.99, 135.63, 140.73, 158.97, 159.01 (Other Olefinic and Aromatic Carbons)
<b>3c*</b>	24.90 (C-5), 27.29 (C-6), 42.60 (C-4), 55.53 (OCH <sub>3</sub> ), 56.74 (C-3), 112.21 (CN), 112.55, 114.33, 120.52, 121.15, 126.93, 128.03, 128.65, 128.82, 130.31, 133.40, 135.73, 140.35, 146.10, 159.94, 160.49 (Other Olefinic and Aromatic Carbons)
<b>3d</b>	25.00 (C-5), 27.96 (C-6), 42.32 (C-4), 55.42 (OCH <sub>3</sub> ), 60.51 (C-3), 108.43 (CN), 111.29, 113.79, 119.79, 121.24, 121.42, 122.29, 129.85, 131.97, 137.63, 141.11, 142.05, 159.13, 159.82 (Other Olefinic and Aromatic Carbons)
<b>3e</b>	25.05 (C-5), 28.05 (C-6), 41.93 (C-4), 55.41 (2OCH <sub>3</sub> ), 61.59 (C-3), 109.40 (CN), 111.21, 113.76, 114.18, 120.16, 122.17, 125.75, 127.74, 129.16, 135.16, 137.68, 145.36, 158.95, 159.64 (Other Olefinic and Aromatic Carbons)
<b>4a</b>	24.64 (C-6), 27.82 (C-5), 54.45 (OCH <sub>3</sub> ), 115.44 (CN), 94.59, 122.69, 123.77, 126.37, 127.32, 127.89, 130.28, 130.80, 132.16, 133.49, 134.21, 138.91, 153.96, 154.01, 163.19 (Aromatic Carbons)
<b>4b</b>	24.71 (C-6), 27.97 (C-5), 54.33 (OCH <sub>3</sub> ), 55.44 (OCH <sub>3</sub> ), 115.94 (CN), 94.98, 114.23, 123.10, 126.29, 127.23, 127.44, 127.82, 130.12, 130.55, 133.77, 138.97, 153.62, 155.13, 160.30, 163.23 (Aromatic Carbons)
<b>4c</b>	24.63 (C-6), 27.91 (C-5), 54.37 (OCH <sub>3</sub> ), 54.46 (OCH <sub>3</sub> ), 115.54 (CN), 94.82, 114.29, 114.66, 120.81, 122.90, 126.30, 127.24, 127.86, 130.02, 130.63, 133.65, 136.65, 139.01, 153.70, 155.14, 159.72, 163.12 (Aromatic Carbons)



Table 3: Cont'd.

4d	24.65 (C-6), 28.24 (C-5), 55.32 (OCH <sub>3</sub> ), 55.49 (OCH <sub>3</sub> ), 115.70 (CN), 93.37, 112.88, 113.07, 121.47, 123.64, 126.54, 128.26, 130.28, 132.10, 134.39, 141.02, 153.54, 154.14, 161.82, 163.23 (Aromatic Carbons)
4e*	24.49 (C-6), 27.60 (C-5), 54.82 (OCH <sub>3</sub> ), 55.95 (OCH <sub>3</sub> ), 115.65 (CN), 92.80, 113.33, 113.89, 122.12, 124.40, 126.08, 128.45, 130.87, 141.83, 142.32, 148.49, 152.97, 154.14, 162.17, 162.92 (Aromatic Carbons)
4f	24.21 (C-6), 27.51 (C-5), 54.49 (OCH <sub>3</sub> ), 114.88 (CN), 94.90, 123.45, 126.35, 127.35, 127.95, 127.98, 128.42, 130.09, 130.89, 133.35, 133.55, 133.66, 136.17, 139.05, 151.44, 154.06, 163.07 (Aromatic Carbons)
4g	24.60 (C-6), 27.80 (C-5), 54.49 (OCH <sub>3</sub> ), 115.30 (CN), 94.64, 122.75, 126.36, 126.85, 127.32, 127.92, 128.57, 129.50, 130.31, 130.84, 133.45, 134.82, 137.10, 138.93, 153.60, 154.03, 163.15 (Aromatic Carbons)
4h	14.62 (CH <sub>3</sub> ), 24.63 (C-6), 27.85 (C-5), 63.19 (OCH <sub>2</sub> ), 115.05 (CN), 94.67, 122.42, 123.72, 126.31, 127.29, 127.87, 130.25, 130.50, 130.71, 132.14, 133.59, 134.31, 138.90, 153.94, 162.92 (Aromatic Carbons)
4i	14.62 (CH <sub>3</sub> ), 24.20 (C-6), 27.66 (C-5), 63.31 (OCH <sub>2</sub> ), 114.97 (CN), 94.92, 123.18, 126.31, 127.33, 127.93, 127.97, 130.09, 130.83, 130.90, 133.10, 133.44, 133.55, 136.13, 139.06, 151.43, 154.00, 162.82 (Aromatic Carbons)
5	21.18 (CH <sub>3</sub> ), 25.15 (C-6), 27.46 (C-5), 40.39 (C-7), 100.10, 112.28, 120.99, 121.75, 126.65, 127.42, 128.33, 128.69, 130.59, 131.38, 135.45, 142.16, 142.25, 158.12, 162.30 (Olefinic and Aromatic Carbons), 165.32 (C=O)
6a*	24.03 (C-6), 28.13 (C-5), 114.64, 122.87, 125.57, 127.29, 128.41, 131.00, 131.43, 131.58, 133.47, 138.00, 139.95, 160.58, 162.72, 164.14 (Aromatic Carbons)
6b	24.19 (C-6), 28.70 (C-5), 55.44 (OCH <sub>3</sub> ), 112.74, 112.97, 115.14, 123.30, 126.03, 127.61, 130.42, 131.54, 137.46, 141.62, 161.43, 161.70, 161.78, 163.86 (Aromatic Carbons)
6c	24.42 (C-6), 28.84 (C-5), 55.42, 55.46 (OCH <sub>3</sub> ), 112.61, 112.93, 113.71, 115.07, 126.34, 127.50, 130.25, 131.00, 141.61, 160.23, 161.04, 161.57, 161.71, 164.71 (Aromatic Carbons)
6d	24.22 (C-6), 28.78 (C-5), 55.42 (OCH <sub>3</sub> ), 112.68, 112.95, 115.29, 126.22, 127.55, 128.35, 128.66, 128.92, 138.61, 141.68, 161.18, 161.67, 161.68, 165.16 (Aromatic Carbons)
8a	27.46 (C-1), 27.62 (C-2), 28.69 (C-7), 29.71 (C-8), 122.31, 125.64, 126.11, 126.93, 127.12, 127.25, 127.71, 128.59, 128.79, 128.84, 130.27, 131.26, 131.40, 132.70, 135.35, 137.86, 139.77, 140.52, 142.33, 151.40, 153.64 (Aromatic Carbons)
8b	27.39 (C-1), 27.66 (C-2), 28.73 (C-7), 30.17 (C-8), 55.45 (OCH <sub>3</sub> ), 111.35, 113.21, 122.21, 125.40, 125.64, 126.42, 127.09, 127.21, 128.70, 129.64, 130.22, 131.23, 131.39, 135.49, 137.81, 139.92, 142.22, 142.44, 151.29, 153.52, 159.68 (Aromatic Carbons)
9a	23.98 (C-5), 27.97 (C-6), 59.07 (C-4), 110.27, 121.49, 121.94, 126.70, 127.33, 127.87, 127.94, 128.12, 129.45, 131.89, 135.77, 141.97 (Olefinic and Aromatic Carbons), 174.55 (C=S)
9b*	23.62 (C-5), 27.84 (C-6), 55.41 (OCH <sub>3</sub> ), 60.17 (C-4), 110.78, 114.47, 119.46, 125.94, 126.93, 127.36, 128.32, 128.52, 128.84, 133.40, 135.83, 160.02 (Olefinic and Aromatic Carbons), 174.50 (C=S)
9d	24.02 (C-5), 28.27 (C-6), 55.69 (OCH <sub>3</sub> ), 58.30 (C-4), 108.49, 111.36, 114.46, 121.02, 121.56, 123.72, 127.30, 129.75, 132.16, 138.07, 142.89, 159.47 (Olefinic and Aromatic Carbons), 174.77 (C=S)



Table 3: Cont'd.

9e	24.13 (C-5), 28.32 (C-6), 55.67 (2OCH <sub>3</sub> ), 58.42 (C-4), 109.31, 111.33, 114.46, 114.55, 121.19, 123.59, 126.91, 128.79, 135.70, 138.01, 159.36, 159.47 (Olefinic and Aromatic Carbons), 174.43 (C=O)
10a*	24.94 (C-6), 27.53 (C-7), 31.97 (C-2), 59.49 (C-5), 114.20, 123.16, 123.50, 126.86, 127.39, 127.80, 127.91, 128.10, 130.07, 132.10, 134.01, 135.29, 138.11 (Olefinic and Aromatic Carbons), 170.71 (C=O)
10b	24.83 (C-6), 27.36 (C-7), 32.14 (C-2), 55.65 (OCH <sub>3</sub> ), 58.79 (C-5), 114.58, 116.09, 123.22, 126.94, 127.84, 128.02, 129.40, 132.62, 133.04, 133.10, 135.60, 155.42, 159.76 (Olefinic and Aromatic Carbons), 171.59 (C=O)
10c	24.18 (C-6), 27.89 (C-7), 32.15 (C-2), 59.06 (C-5), 111.73, 122.24, 126.88, 127.22, 127.53, 127.87, 128.14, 128.30, 128.47, 128.92, 129.25, 135.97, 143.44 (Olefinic and Aromatic Carbons), 174.86 (C=O)
10d	24.57 (C-6), 27.66 (C-7), 32.10 (C-2), 55.63 (OCH <sub>3</sub> ), 58.71 (C-5), 111.78, 112.44, 113.87, 122.08, 124.72, 125.76, 130.21, 132.21, 133.07, 137.48, 140.11, 155.43, 159.46 (Olefinic and Aromatic Carbons), 171.64 (C=O)
10e	24.79 (C-6), 27.75 (C-7), 32.10 (C-2), 55.62 (OCH <sub>3</sub> ), 55.64 (OCH <sub>3</sub> ), 58.76 (C-5), 111.73, 113.30, 113.87, 114.54, 124.62, 125.93, 129.37, 132.78, 132.90, 137.44, 155.23, 159.35, 159.71 (Olefinic and Aromatic Carbons), 171.58 (C=O)
11a	25.07 (C-6), 27.51 (C-7), 55.45 (OCH <sub>3</sub> ), 59.45 (C-5), 114.55, 115.55, 116.29, 121.03, 122.69, 123.13, 123.44, 126.86, 127.43, 128.11, 130.06, 130.23, 131.48, 132.10, 132.45, 134.71, 134.95, 135.30, 138.10, 150.99, 160.04 (Olefinic and Aromatic Carbons), 165.73 (C=O)
11b	25.10 (C-6), 27.52 (C-7), 60.17 (C-5), 116.51, 121.68, 123.39, 124.40, 126.86, 127.41, 128.02, 128.29, 128.94, 129.02, 129.88, 131.25, 132.41, 132.44, 132.47, 132.56, 132.61, 135.31, 138.98 (Olefinic and Aromatic Carbons), 165.53 (C=O)
11c	24.62 (C-6), 27.52 (C-7), 55.64 (OCH <sub>3</sub> ), 55.83 (OCH <sub>3</sub> ), 58.95 (C-5), 111.89, 113.94, 114.31, 115.47, 116.80, 121.05, 122.25, 122.37, 124.72, 125.49, 130.28, 130.99, 131.16, 132.29, 133.31, 135.10, 137.44, 139.64, 150.82, 159.60, 160.18 (Olefinic and Aromatic Carbons), 165.06 (C=O)
11d	25.05 (C-6), 27.98 (C-7), 55.35 (OCH <sub>3</sub> ), 55.39 (OCH <sub>3</sub> ), 59.54 (C-5), 111.30, 113.78, 114.01, 114.19, 121.64, 124.44, 124.76, 125.00, 129.76, 130.10, 131.09, 131.27, 132.47, 132.56, 133.60, 136.02, 137.18, 159.55, 160.02 (Olefinic and Aromatic Carbons), 165.55 (C=O)
12a	21.85 (C-3), 25.18 (C-7), 27.58 (C-8), 36.10 (C-2), 55.59 (C-6), 117.09, 112.82, 123.21, 126.78, 127.43, 127.50, 127.85, 129.95, 131.94, 132.18, 134.08, 135.18, 138.65 (Olefinic and Aromatic Carbons), 168.77 (C=O)
12b*	21.80 (C-3), 25.63 (C-7), 27.39 (C-8), 36.00 (C-2), 55.23 (C-6), 55.62 (OCH <sub>3</sub> ), 114.76, 118.52, 122.90, 126.93, 127.90, 127.95, 129.01, 132.55, 132.73, 133.18, 135.50, 151.13, 159.68 (Olefinic and Aromatic Carbons), 169.30 (C=O)
12c	21.93 (C-3), 25.16 (C-7), 27.58 (C-8), 35.94 (C-2), 56.34 (C-6), 118.27, 123.41, 126.90, 127.46, 127.99, 128.09, 128.93, 129.14, 131.10, 135.15, 138.70, 139.11, 139.28 (Olefinic and Aromatic Carbons), 168.48 (C=O)
12d	21.66 (C-3), 25.21 (C-7), 27.78 (C-8), 35.80 (C-2), 55.16 (C-6), 55.62 (2OCH <sub>3</sub> ), 111.76, 113.97, 114.74, 115.76, 124.26, 125.53, 128.96, 132.90, 133.07, 137.35, 150.89, 159.27, 159.64 (Olefinic and Aromatic Carbons), 169.30 (C=O)

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