

α , β - UNSATURATED NITRILES IN
HETEROCYCLIC SYNTHESIS : SYNTHESIS OF
CYCLOHEXENO[b]PYRANS AND CYCLOHEXENO[b]
PYRANO [2,3-b] PYRIDINES.

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ABSTRACT

The reaction of 5, 5'- dimethylcyclohexan-1, 3-dione (1) with cinnamitriles (2) afforded Cyclohexeno [b] pyrans (5). The structure of reaction products was established based on ^1H NMR and ^{13}C NMR. The ^1H NMR revealed heteroring at C - 4 affecting the CH_2CO moiety in space making CH_2 protons magnetically nonequivalent. Replacement of the heteroring by an aryl moiety results in disappearance of this effect.

The reaction of (5) with (2) resulted in formation of cyclohexeno [b]- pyrano [2,3 - b] pyridines whose structure was established based also on spectral data .

α , β -Unsaturated nitriles are versatile reagents that have been extensively employed in heterocyclic synthesis.¹⁻⁴ Recently several new approaches for the synthesis of polyfunctional substituted mono and condensed heteroaromatics utilizing α , β -unsaturated nitriles have been reported.⁵⁻⁷ Elnagdi *et al.*⁸ and Soto *et al.*⁹ have reported that the reaction of β -diketones with cinnamitriles yields enamino-pyran derivatives. This approach has been extensively utilized for the synthesis of substituted pyrans. Although cyclohexenopyrans are interesting as

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potential starting points for the synthesis of certain male fertility regulators, only very few derivatives of this ring system have been reported. Elnagdi *et al.*^{10,11} reported that 5, 5'-dimethyl cyclohexanedione (1) reacts with benzylidenemalononitrile yielding pyrans. This reported synthesis coupled with the interest in the chemistry of these important heterocycles, led the author to report the synthesis of several new cyclohexenopyrans. The conversion of these compounds into the corresponding pyranopyridines is also studied.

RESULTS AND DISCUSSION

Several interesting features of ¹H NMR and ¹³C NMR of the synthesized compounds are discussed. Thus it has been found that 5, 5'-dimethyl cyclohexanedione (1) reacts with (2 a, b) to yield 1 : 1 adducts. These may be formulated as either the Michael adducts 3 or 4 or isomeric cyclic 5 or 6 (cf. Chart 1). ¹H NMR of product of reacting 2a with 1 revealed two singlets for the CH₃ groups at δ 0.99 and δ 1.04 ppm; four doublets at δ 2.3, and 2.5 ppm; a one proton signal at δ 4.33 ppm in addition to the three furan protons at δ 6.05 (H - 3), 6.32 (H - 4) and 7.47 (H - 5). A D₂O exchangeable two proton signal at δ 7.05 ppm also appeared and was then interpreted for NH₂ group. This spectra clearly indicate that the reaction product is neither the acyclic Michael adduct 3 or 4 as for both a multiplet for protons linked to Sp³ carbons should have appeared at δ 2 - 3 ppm. However although the ¹H NMR may be interpreted better for 5 than for form 6 as the methylene protons of the CH₂ flanked by C = O and C = C - O functions in 6 should appear at lower field.

A further proof for this conclusion seems mandatory. Conclusive evidence for this structure was thus obtained through ¹³C NMR spectroscopy (cf. formula

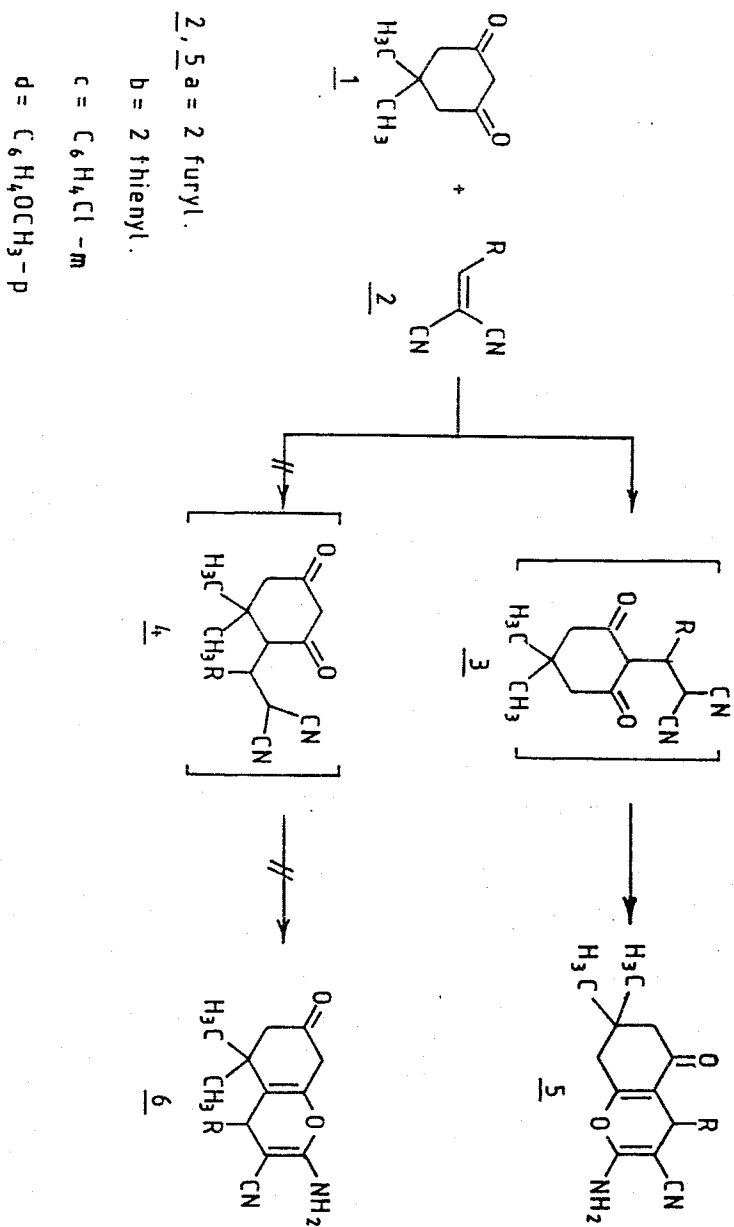
$\alpha\beta$ - Unsaturated nitriles.....

5 a), which showed six signals for sp³. These were interpreted for : (C - 8) δ 26.44; (C - 9) 28.27; (C - 10) 28.88; (C - 6) 31.65; (C - 7) 49.79 and (C - 4) 55.38. If this product was isomeric 6a, one would expect (C - 8) to appear at much lower field. This combined with observation from ¹H NMR that pyran H appeared as singlet - it should appear as multiplet by long range coupling with CH₂ in isomeric 6 a - no doubt is left thus for structure interpretation of reaction products.

Interesting features of ¹³C NMR worth mention here. Namely the appearance of C - 3 at δ 104 ppm higher than expected for olefinic carbon. This is in my opinion may be due to both electron donation by NH₂, as well as, shielding by CN function. similarly, the reaction of 2b with 1 affords 5b.

Compounds 5a, b and 11 reacted with the acrylonitriles 2a, b in refluxing pyridine to yield 1:1 adducts. Three isomeric structures seemed possible for these products (cf. structures 7 - 9).

Structure 7 was readily eliminated as ¹H NMR in each case revealed that the methylene groups was not involved in the reaction. Structure 9, rather than 8 could be established based on ¹H NMR which revealed the pyridine H-2 as singlet. if this product was isomeric 8, this proton should appear as a doublet. ¹³C NMR supports further this conclusion (cf. formula 9b). Thus, the two carbons and the two methylene carbons appeared at almost the same field as in the parent compound. Two new Sp³ carbons appeared at δ 31.50 for pyridine C - 3 and at δ 58.05 for pyridine C - 2. Also two new higher field signals appeared at almost the same field as in parents (cf. formula 9b). ¹³C NMR revealed extra carbons for C = O and for CH₂. This is due to existence of stereoisomers whose rate of interconversion is seemingly slower than the rate of relaxation of ¹³C NMR assessment. The formation of pyranopyridines by this way seems to be the first reported example of such addition in condensed pyran systems.



$\underline{2}, \underline{5} a = 2$ furyl.

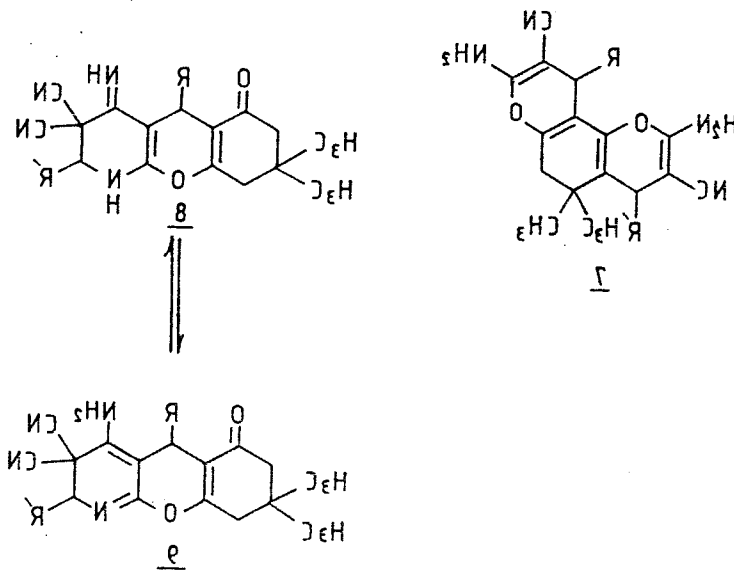
b = 2 thieryl.

c = C₆H₄Cl-m

d = C₆H₄OCH₃-p

Chart (1)

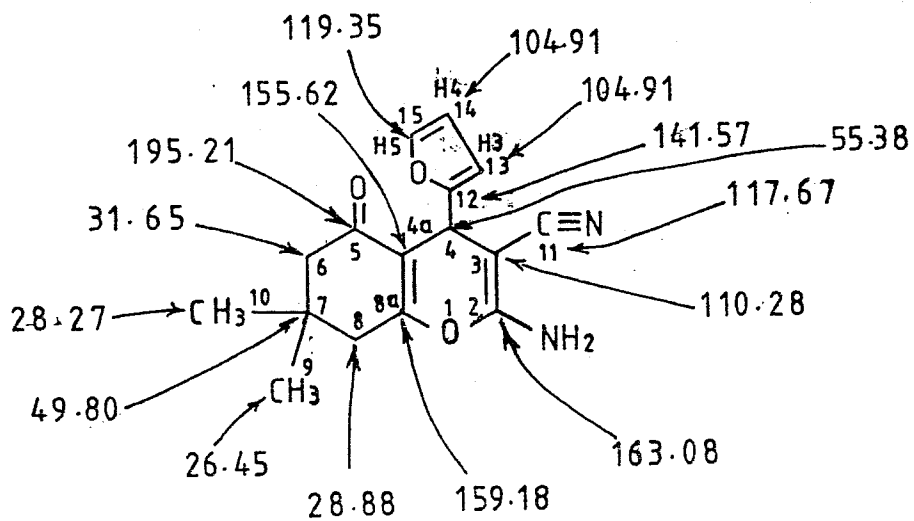
$\alpha\beta$ - Unsaturated nitriles.....



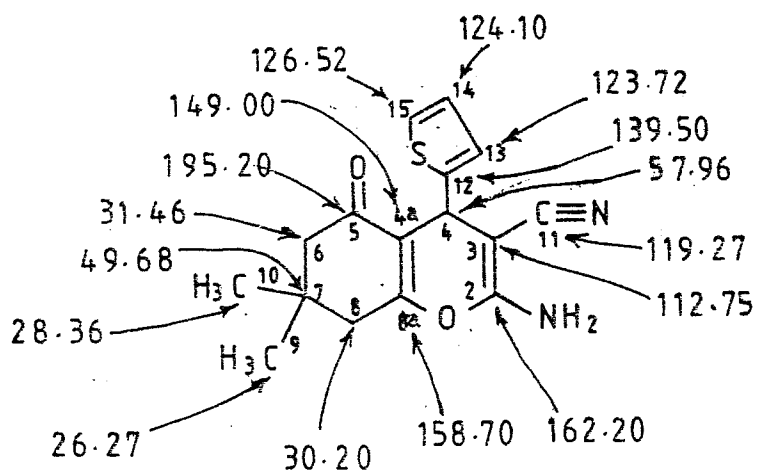
\underline{a} = 2-furyl R
 \underline{b} = 2-furyl R
 \underline{c} = C₆H₄OCH₃-p, 2-furyl

Chart (2)

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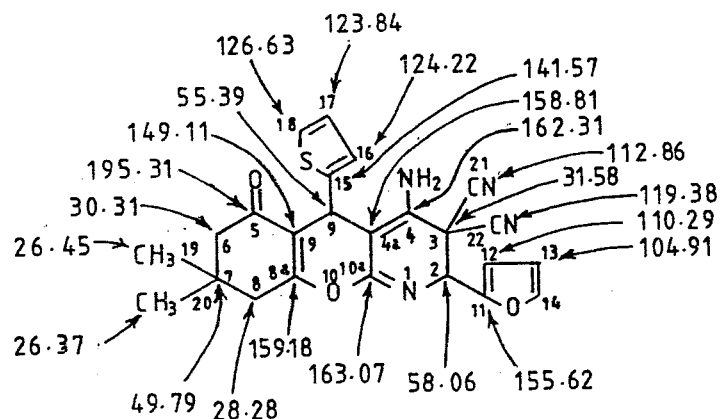


5a

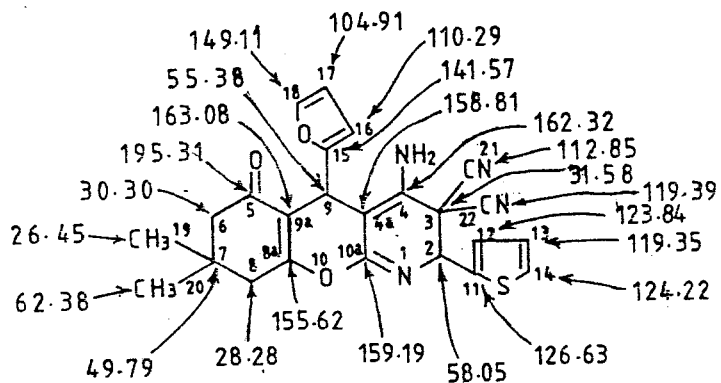


5b

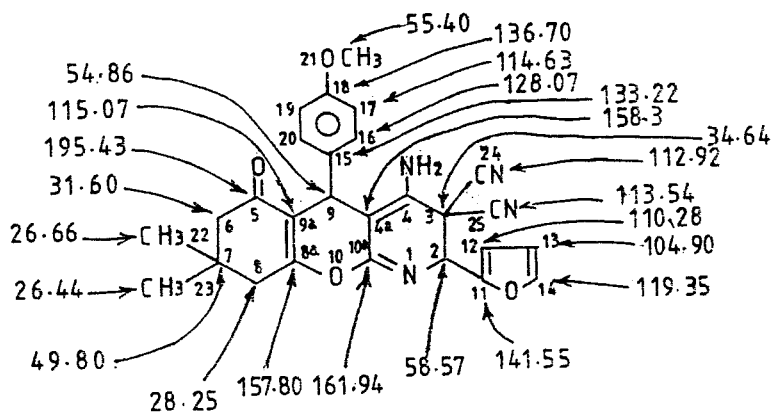
$\alpha\beta$ - Unsaturated nitriles.....



9a

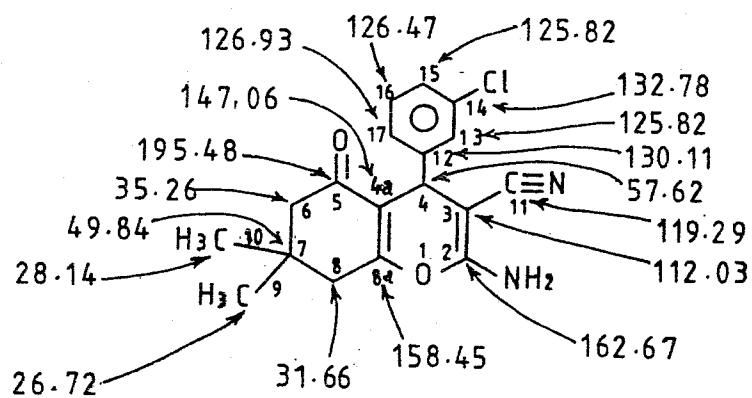


9b

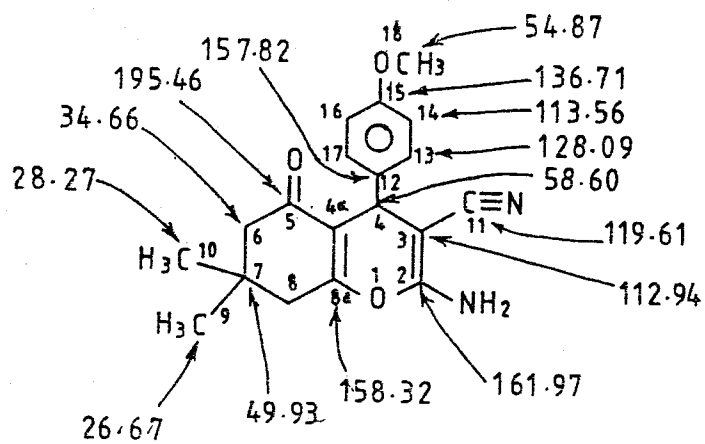


9c

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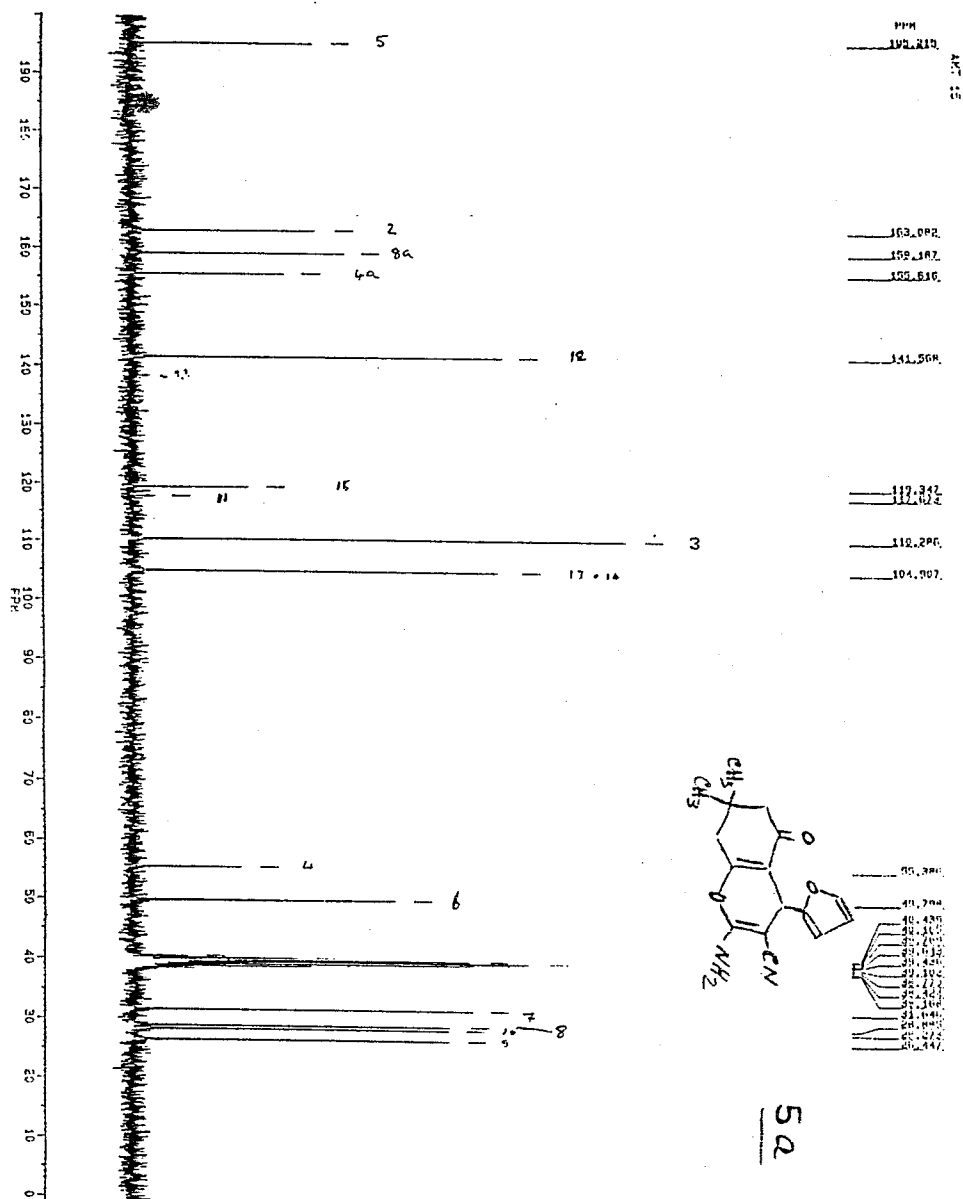


10



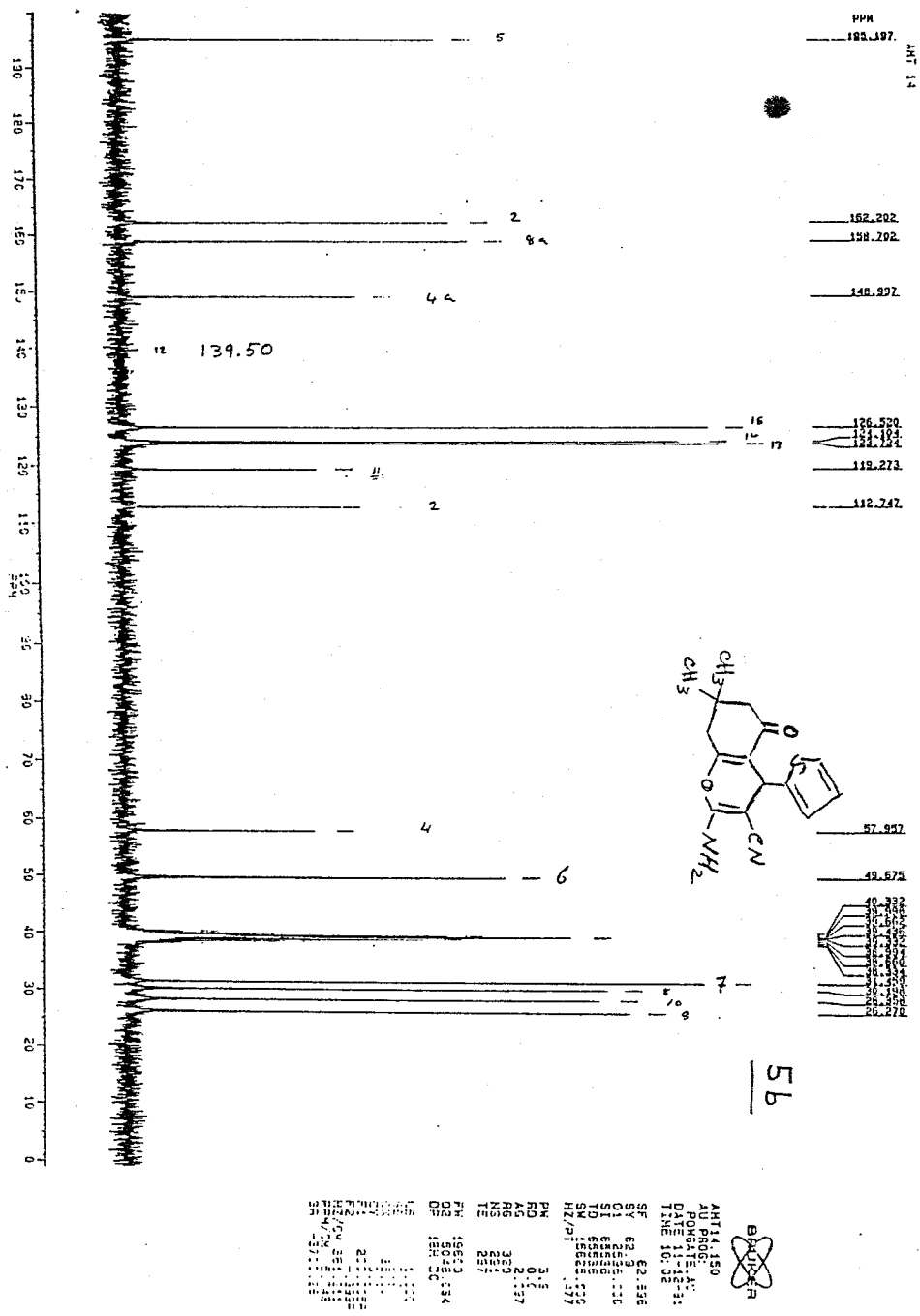
11

$\alpha\beta$ - Unsaturated nitriles.....

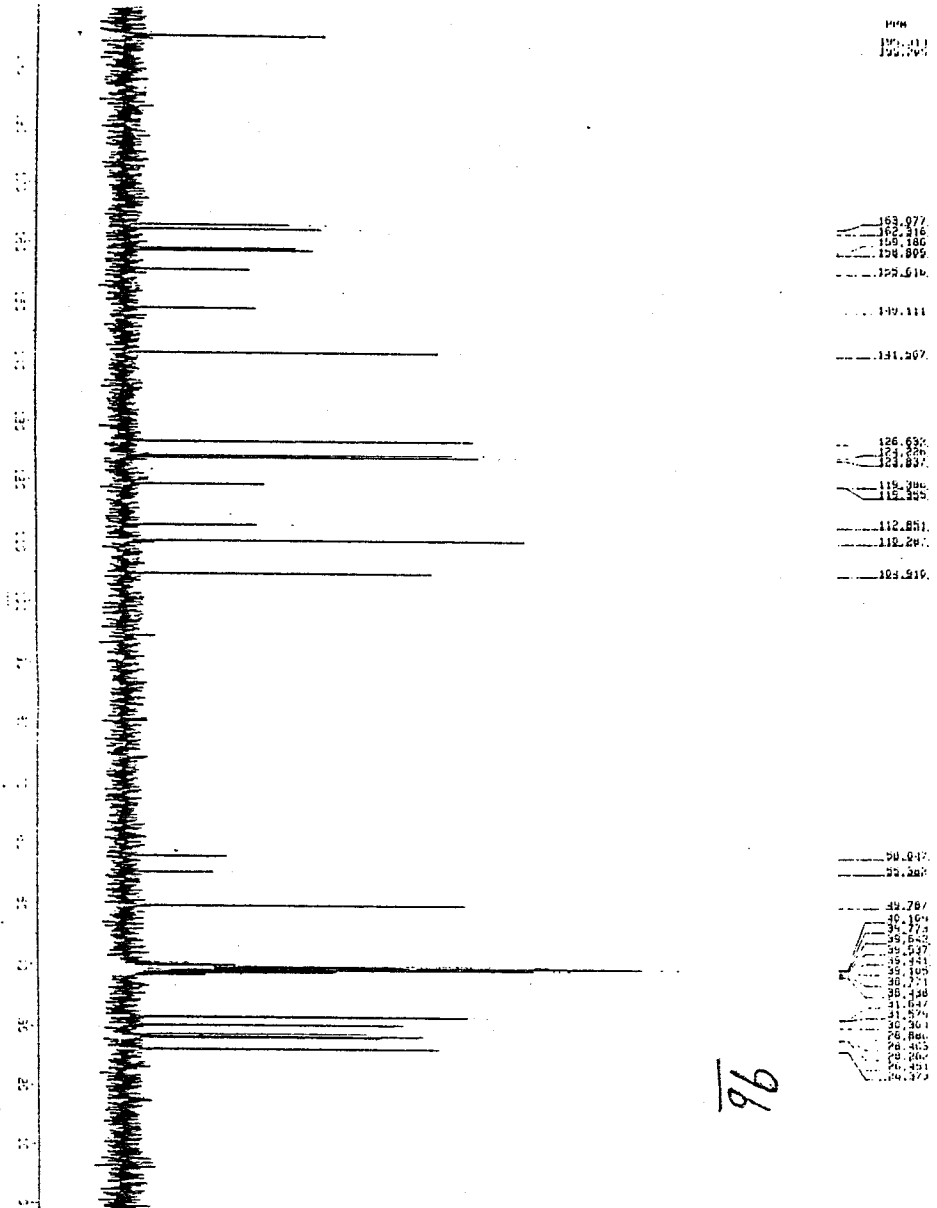


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 39.316
 39.116
 39.016
 38.916
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 38.116
 38.016

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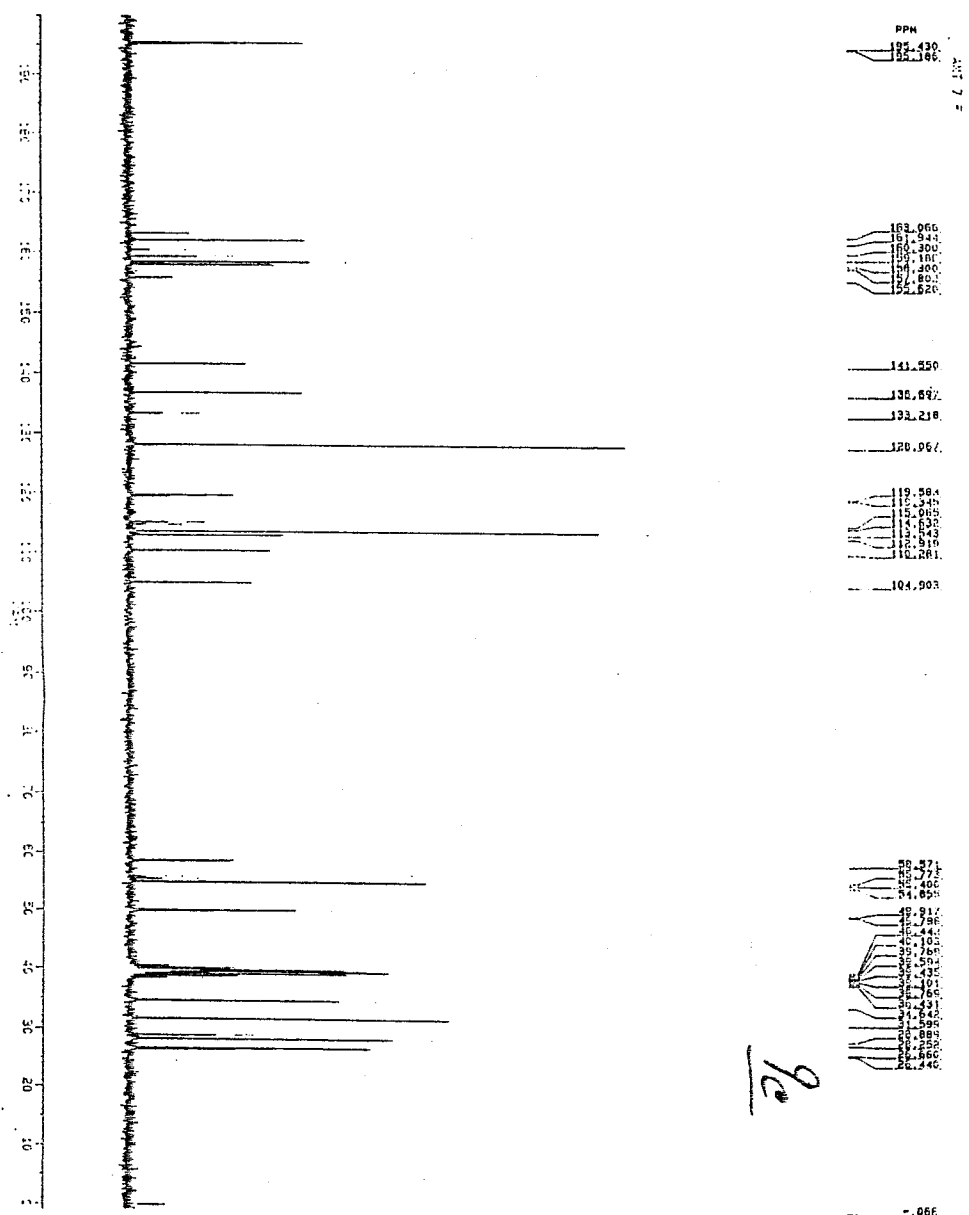


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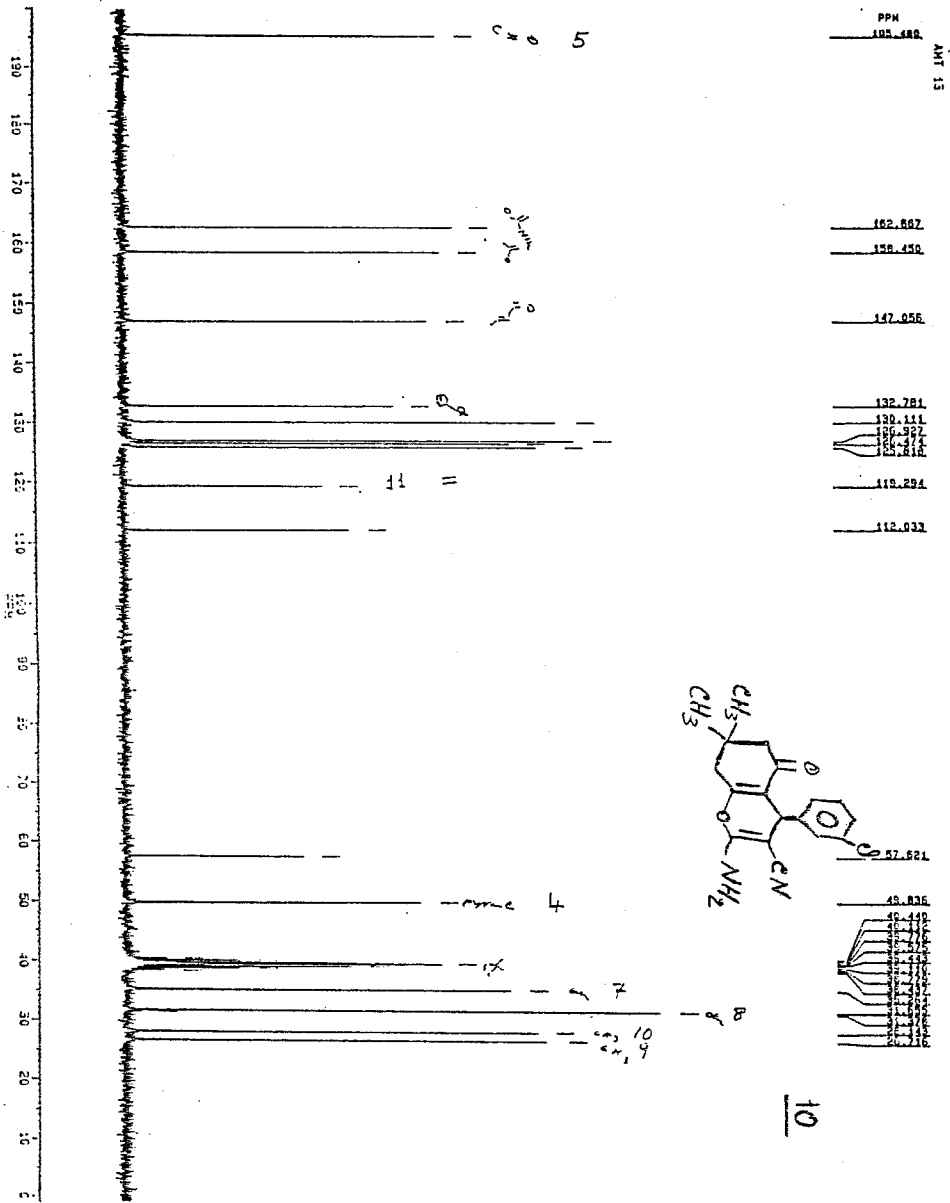
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 103.519
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 39.787
 39.164
 39.173
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 39.141
 39.109
 39.771
 39.158
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 31.874
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 28.888
 28.403
 29.066
 28.491
 28.372

$\alpha\beta$ - Unsaturated nitriles.....



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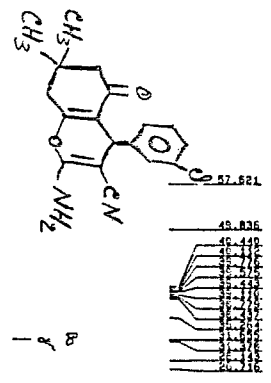
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PPM

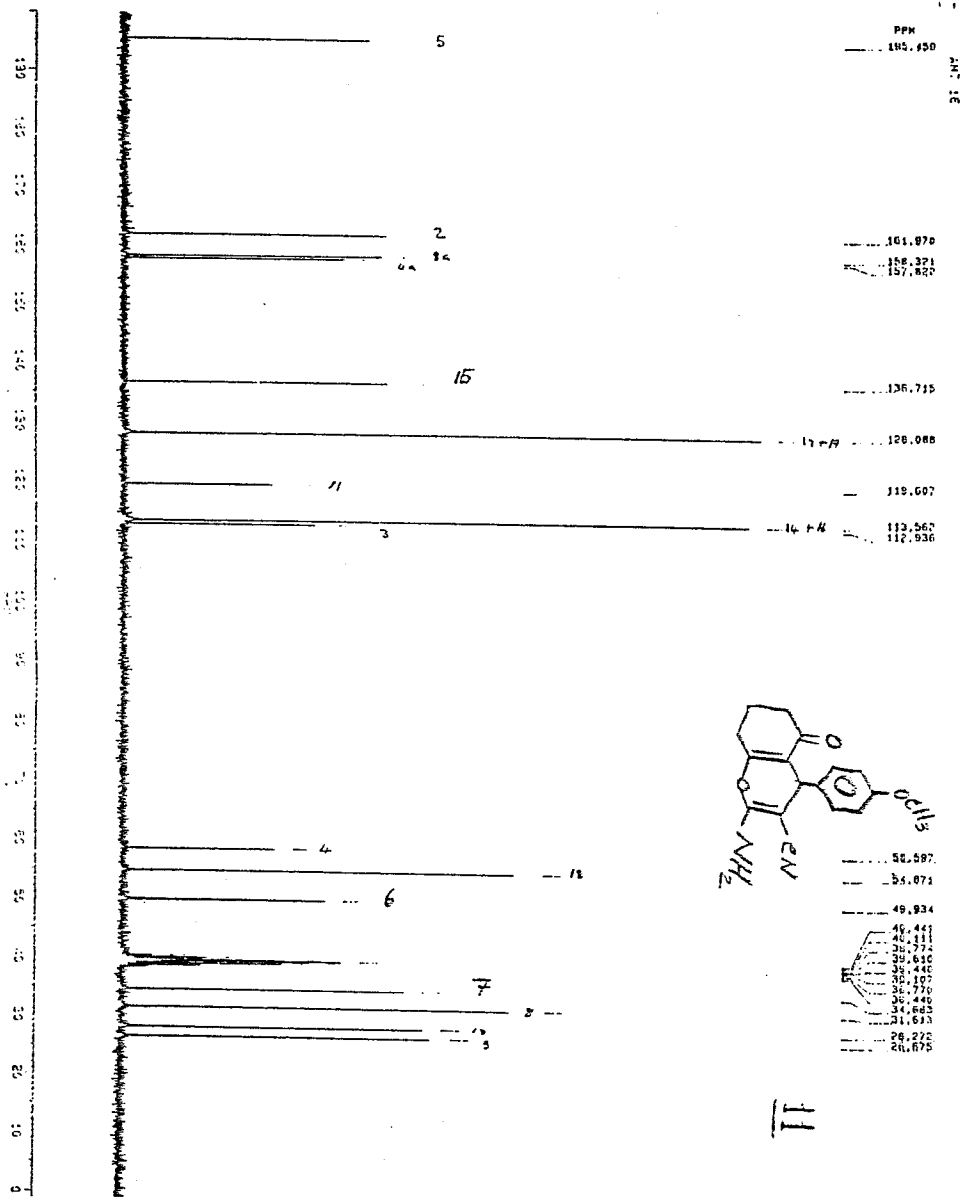
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INT 15



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 S95: 62.596
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 S99: 62.596
 S100: 62.596

$\alpha\beta$ - Unsaturated nitriles.....



BRUKER
 100 MHz
 CDCl₃
 TMS
 300 K

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Although Elnagdi *et al.*¹⁰ have previously reported addition of aryldine malononitrile to dimedone, the reaction of **2c** has not been reported and no ¹³C NMR data have ever been reported for these systems. I have found that **2c** also adds to **1** to yield the cyclohexenopyran **10**. Structure of **10** was inferred from ¹³C NMR spectroscopy. Unexpectedly ¹H NMR revealed one of the two methylenes as doublet of doublet while the other one appeared as clear singlet in contrast to observed multiplicity of both CH₂ signals in **5a, b**. It's believed that this can be rationalised by assuming that the CH₂ protons adjacent to C=O are in this derivative equivalent while the lone pair anisotropy of the hetero ring in **5a,b** renders these two protons different as it affects one of the two protons in the conformation that places the heteroatom over this proton.

In order to confirm this, cyclohexenopyrane **11**, was prepared readily following the procedure of Elnagdi *et al.*¹⁰, and its spectra was recorded and inspected. ¹³C NMR is in accordance with the structure proposed by Elnagdi *et al.*¹⁰ (cf. formula 11). ¹H NMR again revealed one of the CH₂ as singlet and the other as doublet of doublet giving further support for proposed effect of the heteroatom lone pair.

EXPERIMENTAL

Melting points were determined on a Buchi apparatus and uncorrected. Elemental analysis were carried out at Microanalytical Unit, Cairo University. ¹³C NMR and ¹H NMR were determined on a Bruker AC 250 FT - NMR spectrometer using tetramethylsilane as the internal standard; chemical shifts are recorded in parts per million., at chemistry Department, Odense University, Odense M, Danmark.

αβ- Unsaturated nitriles.....

4H-Cyclohexeno [1, 2-b] pyran[5a]:

To a solution of 1.4 g. (10 mmol) of 5, 5'-dimethyl cyclohexanedione (1) in 40 ml ethanol was added 1.44 g (10 mmol) of furfurylidene malononitrile (2a) and 3 drops of triethylamine. The reaction mixture was then heated under reflux for three hr. The solid product (5a) on standing precipitated, collected by filtration and recrystallized from ethanol as pale yellow crystals, M. P. 218-219 °C.

Using this procedure, compound. 5b was obtained via the reaction of equimolar amounts (10 mmol) of (1) and (2b).

4-H cyclohexeno [b] pyran [2,3-b] byridine [9a]:

To a solution of 3.0 g (10 mmol) of (5b) in 50 ml pyridine, 1.44 g (10 mmol) of (2a) was added. The reaction mixture was then heated under reflux for six hrs. The solvent was evaporated under vacuo and the solid product formed was dissolved in 50 ml water, acidified with HCl, filtered washed with water several times and finally recrystallized from ethanol as grey crystals, M.p. 205 °C.

Using this procedure, (9b) was obtained via the reaction of equimolar amounts (10 mmol) of (5a) and (2b) while (9c) was obtained from (11) and (2a).

ACKNOWLEDGEMENT

Thanks for prof. Erik B. Pedersen, Odense University for the ¹H NMR and ¹³C NMR spectra and laboratory facilities provided.

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Table (1) : Physical data of the newly synthesized products

comp. No	Yield (%)	M.P (°C)	Molecular formula (M.Wt.)	Analysis %			
				Calcd./	Found		
				C	H	N	S
5a	85	218 -219	C ₁₆ H ₁₆ N ₂ O ₃ (284.317)	67.50	5.67	9.85	-
				67.3	5.5	9.7	-
5b	95	231 -232	C ₁₆ H ₁₆ N ₂ O ₂ S (300.382)	63.98	5.37	9.33	10.67
				63.8	5.1	9.2	10.4
9a	54	205	C ₂₄ H ₂₀ N ₄ O ₃ S (444.517)	64.85	4.53	12.60	7.21
				65.0	4.7	12.5	7.3
9b	51	200	C ₂₄ H ₂₀ N ₄ O ₃ S (444.517)	64.85	4.53	12.60	7.21
				65.1	4.7	12.8	7.4
9c	62	175	C ₂₇ H ₂₄ N ₄ O ₄ (468.518)	69.22	5.16	11.96	-
				69.0	5.3	12.1	-

All compounds was crystallized from ethanol.

Table (2) : ^1H NMR data of the synthesized compounds

Compound Number	^1H NMR, ppm (DMSO)
5a	δ 0.99 (s, 3H, CH_3), 1.04 (s, 3H CH_3), 2.3 (dd, 2H, CH_2), 2.50 (dd, 2H, CH_2 - CO), 4.33 (s, 1H, pyran H), 6.05 (d, 1H furan H-3), 6.32 (d, 1H, furan furan H -4), 7.05 (br, 2H, NH_2) and 7.47 (d, 1H, furan H -5).
5b	δ 0.97 (s, 3H, CH_3), 1.04 (s, 3H, CH_3), 2.25 (dd, 2H, CH_2), 2.55 (dd, 2H, CH_2 - CO), 4.54 (s, 1H, pyran H), 6.86 (d, 1H, thiophene H - 3), 6.90 (d, 1H, thiophene H - 4), 7.07 (br, 2H, NH_2) and 7.30 (d, 1H, thiophene H - 5).
10	δ 0.96 (s, 3H, CH_3), 1.04 (s, 3H, CH_3), 2.20 (dd, 2H, CH_2), 2.52 (s, 2H, CH_2 - CO), 4.23 (s, 1H, pyran H), 7.07 (br, 2H, NH_2) and 7.11 - 7.36 (m, 4H, arom. H).
11	δ 0.94 (s, 3H, CH_3), 1.03 (s, 3H CH_3), 2.15 (dd, 2H, CH_2), 2.49 (s, 2H, CH_2 - CO), 3.70 (s, 3H, OCH_3), 4.14 (s, 1H, pyran H), 6.85 (d, 2H, ortho protons), 7.05 (br, 2H, NH_2) and 7.08 (d, 2H, m. protons).
9a	δ 0.97 (s, 3H, CH_3), 1.04 (s, 3H, CH_3), 2.20 (dd, 2H, CH_2); 2.47 (dd, 2H, CH_2 - CO), 4.33 (s, 1H, pyran 4H), 4.54 (s, 1H, pyridine 2H), 6.05 (d, 1H, furan H - 3), 6.32 (d, 1H, furan H - 4), 6.87 (d, 1H, thiophene H - 3), 6.91 (d, 1H, thiophene H - 4), 7.07 (br, 2H, NH_2), 7.31 (d, 1H, thiophene H - 2) and 7.47 (d, 1H, furan H - 5).
9b	δ 0.98 (s, 3H, CH_3), 1.05 (s, 3H, CH_3), 2.25 (dd, 2H CH_2), 2.47 (dd, 2H, CH_2 - CO), 4.34 (s, 1H, pyran 4 - H), 4.54 (s, 1H, pyridine 2 -H), 6.05 (d, 1H, furan H - 3), 6.30 (d, 1H, furan H - 4), 6.80 (d, 1H, thiophene H - 3), 6.86 (d, 1H, thiophene H - 4), 7.07 (br, 2H, NH_2), 7.28 (d, 1H, thiophene H -2) and 7.47 (d, 1H, furan - 5).
9c	δ 0.94 (s, 3H, CH_3), 1.03 (s, 3H, CH_3), 2.20 (dd, 2H, CH_2), 2.48 (dd, 2H, CH_2 - CO), 3.33 (s, 1H, pyran 4 - H), 3.71 (s, 3H, OCH_3), 4.13 (s, 1H, pyridine 2-H), 6.06 (d, 1H, furan H - 3), 6.32 (d, 1H, furan H - 4), 6.84 (d, arom. O. protons), 6.93 (br, 2H, NH_2) and 7.05 (d, arom. p-protons).

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Table (3) : ^{13}C NMR data of the synthesized compounds

Compound Number	^{13}C NMR, ppm (DMSO)
5a	δ 26.45 (C - 9), 28.27 (C - 10), 28.88 (C - 8), 31.65 (C - 6), 49.80 (C - 7), 55.38 (C - 4), 104.91 (C - 13), 104.91 (C - 14), 110.28 (C - 3), 117.67 (C - 11), 119.35 (C - 15), 141.57 (C - 12), 155.62 (C - 4a), 159.18 (C - 8a), 163.08 (C - 2) and 195.21 (C - 5).
5b	δ 26.27 (C - 9), 28.36 (C - 10), 30.20 (C - 8), 31.46 (C - 6), 49.68 (C - 7), 57.96 (C - 4), 112.75 (C - 3), 119.27 (C - 11), 123.72 (C - 13), 124.10 (C - 14), 126.52 (C - 15), 139.50 (C - 12), 149.00 (C - 4a), 158.70 (C - 8a), 162.20 (C - 2) and 195.20 (C - 5).
10	δ 26.72 (C - 9), 28.14 (C - 10), 31.66 (C - 8), 35.26 (C - 6), 49.84 (C - 7), 57.62 (C - 4), 112.03 (C - 3), 119.29 (C - 11), 125.82 (C - 15), 126.47 (C - 16), 126.93 (C - 17), 130.11 (C - 12), 132.78 (C - 14), 147.06 (C - 4a), 158.45 (C - 8a), 162.67 (C - 2) and 195.48 (C - 5).
11	δ 26.67 (C - 9), 28.27 (C - 10), 31.61 (C - 8), 34.66 (C - 6), 49.93 (C - 7), 54.87 (C - 18), 58.60 (C - 4), 112.94 (C - 3), 113.56 (C - 14), 119.61 (C - 11), 128.09 (C - 13), 136.71 (C - 15), 157.82 (C - 12), 158.32 (C - 8a), 161.97 (C - 2), 195.46 (C - 5).
9a	δ 26.37 (C - 20), 26.45 (C - 19), 28.28 (C - 8), 30.31 (C - 6), 31.58 (C - 3), 49.79 (C - 7), 55.39 (C - 9), 58.06 (C - 2), 104.91 (C - 13), 110.29 (C - 12), 112.86 (C - 21), 119.38 (C - 22), 123.84 (C - 17), 124.22 (C - 16), 126.63 (C - 18), 141.57 (C - 15), 149.11 (C - 9a), 155.62 (C - 11), 158.81 (C - 4a), 159.18 (C - 8a), 162.31 (C - 4), 163.07 (C - 10a) and 195.31 (C - 5).
9b	δ 26.38 (C - 20), 26.45 (C - 19), 28.28 (C - 8), 30.30 (C - 6), 31.58 (C - 3), 49.79 (C - 7), 55.38 (C - 9), 58.05 (C - 2), 104.91 (C - 17), 110.29 (C - 16), 112.85 (C - 21), 119.35 (C - 13), 119.39 (C - 22), 123.84 (C - 12), 124.63 (C - 14), 126.63 (C - 11), 141.57 (C - 15), 149.11 (C - 18), 155.62 (C - 8a), 158.81 (C - 4a), 159.19 (C - 10a), 162.32 (C - 4), 163.08 (C - 9a), and 195.31 (C - 5).
9c	δ 26.44 (C - 23), 26.66 (C - 22), 28.25 (C - 8), 31.60 (C - 6), 34.64 (C - 3), 49.80 (C - 7), 54.86 (C - 9), 55.40 (C - 21), 85.57 (C - 2), 104.90 (C - 13), 110.28 (C - 12), 112.92 (C - 24), 113.54 (C - 25), 114.63 (C - 17), 115.07 (C - 9a), 119.35 (C - 14), 128.07 (C - 16), 133.22 (C - 15), 136.70 (C - 18), 141.55 (C - 11), 157.80 (C - 8a), 158.30 (C - 4a), and 161.94 (C - 10a) and 195.43 (C - 5).

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النيتريلاز غير المشبعة α, β في مجال تخليق المركبات غير متجانسة الحلقة

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قد تم تحضير مركبات الهكسين الحلقي (ب) بيران (٥) من تفاعل
٥، ٥ ثنائي المثيل ١، ٣ دايون (١) مع السينامونيتريلز (٢). قد تم
إثبات التركيب الجزيئي للمركبات الناتجة إستنادا الى أطيف الرنين النووي
المغناطيسي لها.

كذلك قد تم تحضير مركبات الهكسين الحلقي (ب) - بيرانو
(٢؛ ٣-ب) بيريدينز من تفاعل المركبات (٥) مع (٢) وتم إثبات التركيب
الجزيئي لها إستنادا الى دراسة أطيف الرنين النووي المغناطيسي لها.