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Several 1,2,4-triazines were synthesized. ^{13}C - and ^{15}N -nmr spectroscopy was employed for structure determination.

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Utilizing (1) α -diketones (**a**, **1-7**) and 3-nitrobenzimidic acid hydrazide (**8**), we have synthesized 1,2,4-triazines (**b**, **1-7**) of pharmaceutical interest (2,3).

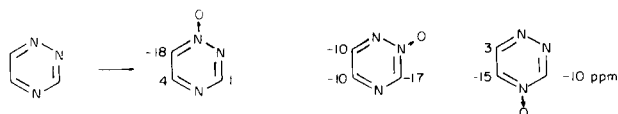
The α -diketones **1a-6a** were purchased from Aldrich, (-)-2,3-dioxocineole (**7a**) was prepared both by a published (4) and by a new procedure (5), and the amidrazone **8** (2) was synthesized by an improved procedure (see Experimental).

The formation of regioisomers is possible, in principle, in all of the above cases except **2b** and **5b**, in which the starting diketones are symmetric. Nevertheless, only one regioisomer was isolated with compounds **1b**, **3b**, and **7b**, due presumably to sufficient steric (**1a**, **7a**) and electronic (**3a**) differentiation between the carbonyls in each of these molecules. On the other hand, both regioisomers were isolated or observed with compounds **4b** and **6b**, respectively.

The regiochemistry for the two triazines **4b** and **4d** (which we will call the major and minor isomers) as well as for triazine **6b**, was assessed utilizing ^1H , ^{13}C and ^{15}N -nmr spectroscopy. Proton nmr at 200 MHz, while dispersing the signal multiplicities well enough for peak assignment, did not reveal significant differences between the major and minor isomer. Oxidation (6) of the major isomer to the *N*-oxide gave rise to downfield shifts for the resonance assigned to the C-7 methyl group *syn* to the triazine ring and for the C-1 methine proton resonance.

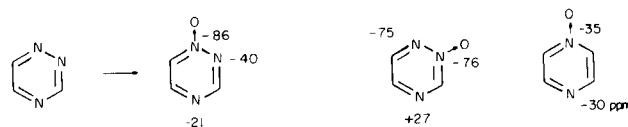
The ^{13}C -nmr proton-decoupled spectra for the major and minor isomers were very similar and again did not allow structural assignment (see Table I). However, the *N*-oxide of the major isomer revealed the regiochemistry of these compounds as follows.

The ^{13}C -nmr assignments were straightforward and were based on model systems (7,8) and single frequency proton decoupling experiments. The position of *N*-oxidation was determined based upon literature substituent shift values shown below (9).

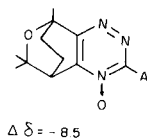


The structural assessment was further confirmed by the ^{15}N -nmr data obtained. The literature substituent shifts in

ppm shown below (10) should be compared with those in Table II.

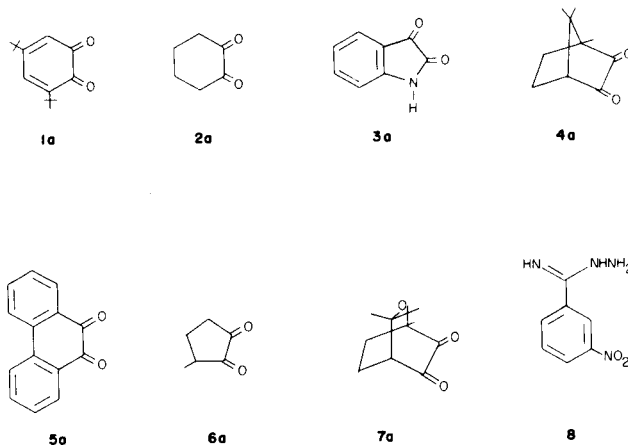


Once the position of oxidation was firmly established, the regiochemistry obtained in the major and minor isomers could be determined from the ^{13}C -nmr data. The *N*-oxidation causes a large upfield substituent shift for the methine carbon resonance reflecting a γ *syn* relationship. This is similar to that observed in an analogous triazine 4-oxide system (7).



This regiochemistry is also consistent with the ^1H -nmr results, the downfield shift of the methine proton. In conclusion, the major isomer is **4b**, and the *N*-oxide **4c**, as indicated.

The structure of **6b** was analyzed in an analogous manner. See Tables III and IV. Again the position of *N*-oxidation leads to ready analysis of the ^{13}C -nmr substituent shifts and hence determination of structure, as shown in **6b** and **6c**.



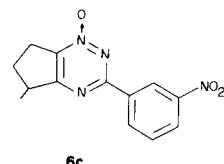
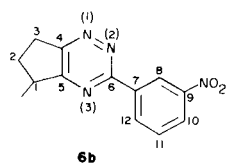
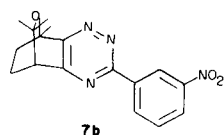
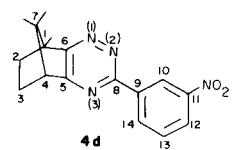
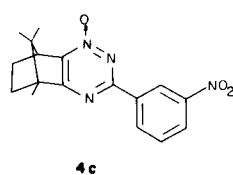
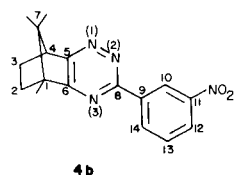
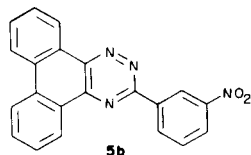
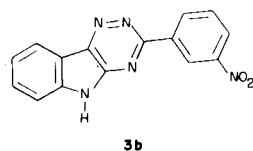
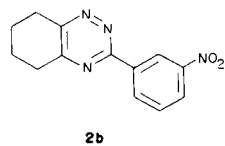
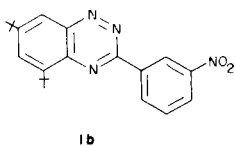


Table I

Carbon-13 Chemical Shift Values in ppm and Assignments for Triazines **4b**, **4c**, **4d**

Carbon (a)	4b	4c	4d
1	54.6	55.1*	54.4
1'	8.3	8.6	8.6
2	30.4	31.3	30.3
3	23.5	22.6	23.0
4	50.4	47.1	52.1
5	159.1	140.0	158.9
6	164.4	162.1	165.4
7	53.5	54.9*	52.1
7' <i>syn</i>	19.2	19.1	19.0
7' <i>anti</i>	17.4	17.4	17.1
8	170.0	177.1	168.1
9	137.0	134.7	136.7
10	121.8	127.2	121.8
11	147.9	147.7	147.8
12	124.4	125.3	124.2
13	128.9	129.0	128.6
14	132.7	133.0	132.5

(a) Atom numbers refer to the diagrams and are different from those employed in naming the compounds.

Table II

Nitrogen-15 Chemical Shifts in ppm and Assignments for Triazines **4b**, **4c**, **4d**

Nitrogen	4b	4c	4d	$\Delta\delta$ 4c-4b (a)
1	373.8	314.4	373.8	-59.4
2	344.2	328.2	344.2	-16.0
3	273.4	257.6	273.5	-15.8
NO ₂	369.3	369.1	369.3	-0.2

(a) Negative sign indicates upfield shift.

Table III

Carbon-13 Chemical Shifts in ppm and Assignments for Triazines **6b** and **6c**

Carbon	6b	6c
1	38.3	39.4
1'	16.9	17.6
2	28.6	28.4
3	29.9	25.5
4	160.0	138.8
5	162.7	163.5
6	169.2	176.0
7	137.2	135.1
8	122.5	122.8
9	148.4	148.3
10	125.2	125.8
11	129.4	129.5
12	133.4	133.6

Table IV

Nitrogen-15 Chemical Shifts in ppm and Assignments for Triazines **6b** and **6c**

Nitrogen	6b	6c	$\Delta\delta$ 6c-6b
1	393.0	312.5	-80.5
2	352.8	326.9	-25.9
3	280.3	263.2	-17.1
NO ₂	367.2	367.9	+0.7

EXPERIMENTAL

Melting points were determined on a Thomas Hoover capillary melting point apparatus and were not corrected. Mass spectra were obtained on a LKB 9000 Mass Spectrometer at 70 eV. Infrared spectra were taken on a Perkin-Elmer Model 727 B Infrared Spectrograph. The ¹H-nmr spectra were obtained on a Varian EM-360, JEOL FX-90Q or JEOL FX-200 nmr spectrometer. The ¹³C-nmr spectra were obtained on a JEOL FX-90Q or FX-200 spectrometer in the Fourier transform mode with full proton decoupling. Single frequency proton decoupling was obtained in the gated mode on the FX-200 spectrometer. General spectral and instrumental parameters were: internal deuterium lock to solvent, spectral width of 5000 Hz (FX-90Q), 10,000 Hz (FX-200) with a pulse width of 45°, and a pulse repetition time of 1.8 seconds, utilizing 8K (FX-90Q) or 16K (FX-200) data points. All chemical shifts are referenced to internal TMS. The ¹⁵N-nmr spectra were obtained on approximately 1 M solutions, 10-mm tubes, in chloroform containing Cr(acac)₃ to facilitate relaxation, in the reverse gated mode. Typical conditions were pulse width of 20°, repetition time 6 seconds, spectral width of 20,000 Hz with 16K time do-

main data points; 20K scans were necessary to obtain adequate signal-to-noise. All chemical shifts are referenced to external ammonium nitrate, $^{15}\text{NH}_4^+ = 20.6$ ppm.

5,7-Bis(1,1-dimethylethyl)-3-(3-nitrophenyl)-1,2,4-benzotriazine (**1b**).

A mixture of 3,5-di-*t*-butyl-*o*-benzoquinone, **1a**, (10 g, 45 mmoles) and 3-nitrobenzimidic acid hydrazide, **8**, (8.1 g, 45 mmoles) in 250 ml of absolute ethanol was refluxed under nitrogen with stirring for 20 hours. The solution was cooled to 0° and filtered. The solid was dried to give 9.7 g (59% yield) of **1b**. An analytical sample was obtained by dissolving the product in chloroform, filtering, and concentrating the filtrate. To the residue was added 2-propanol to afford a bright-yellow solid, mp 170-171°; ms: m/e 364 (M⁺); ir (Nujol): (2900 br), 1600 w, 1530 m, (1460 s), 1400 m, (1375 m), 1350 s, 1320 m, 1300 w, 1235 w, 1090 m, 1040 m, 1010 w, 925 w, 885 w, 835 w, 810 w, 725 m cm⁻¹; ¹H-nmr (deuteriochloroform): δ = 1.50 (s, 9, *t*-butyl), 1.75 (s, 9, *t*-butyl), 7.78 (dd, 1) and 8.38 (ddd, 1) and 9.07 (ddd, 1) and 9.56 (dd, 1) (nitrophenyl), 8.08 (d, 1, aromatic), 8.32 (d, 1, aromatic); ¹³C-nmr (deuteriochloroform): δ = 30.63 (3C), 30.95 (3C), 35.63, 36.62, 122.70, 123.02, 125.15, 129.76, 131.31, 133.62, 137.97, 138.64, 147.69, 147.84, 148.86, 154.06, 154.85.

Anal. Calcd. for C₂₁H₂₄N₄O₂: C, 69.2; H, 6.6; N, 15.4. Found: C, 69.1; H, 6.8; N, 15.5.

5,6,7,8-Tetrahydro-3-(3-nitrophenyl)-1,2,4-benzotriazine (**2b**).

A mixture of 1,2-cyclohexanedione, **2a**, (10 g, 89 mmoles) and 3-nitrobenzimidic acid hydrazide, **8**, (16 g, 89 mmoles) in 245 ml of absolute ethanol was refluxed with stirring under nitrogen for 18 hours. The reaction mixture was cooled to 0° to afford 19 g (83% yield) of **2b**. A gold-colored sample was obtained by recrystallization from absolute ethanol, mp 135-136°; ms: m/e 256 (M⁺); ir (Nujol): (2900 br), 1520 s, (1460 s), 1420 w, 1390 m, (1375 m), 1350 s, 1270 w, 1110 w, 1080 m, 920 w, 860 w, 820 w, 790 w, 740 m cm⁻¹; ¹H-nmr (deuteriochloroform): δ = 2.0 (m, 4), 3.1 (m, 4), 7.65 (dd, 1) and 8.32 (ddd, 1) and 8.82 (ddd, 1) and 9.26 (dd, 1) (nitrophenyl); ¹³C-nmr (deuteriochloroform): δ = 21.73, 22.00, 29.43, 31.65, 122.88, 125.42, 129.70, 133.55, 137.18, 148.77, 157.87, 159.66 (2C).

Anal. Calcd. for C₁₃H₁₂N₄O₂: C, 60.9; H, 4.7; N, 21.9. Found: C, 60.6; H, 4.5; N, 22.0.

3-(3-Nitrophenyl)-5*H*-1,2,4-triazino[5,6-*b*]indole (**3b**).

A mixture of 2,3-indolinedione, **3a**, (6.1 g, 41 mmoles) and 3-nitrobenzimidic acid hydrazide, **8**, (7.4 g, 41 mmoles) in 200 ml of glacial acetic acid was refluxed with stirring under nitrogen for 20 hours. The reaction mixture was cooled to 20° and filtered. Drying *in vacuo* afforded 10.5 g (87% yield) of **3b**. Crystallization from dimethyl sulfoxide gave a yellow solid, mp > 300°; ms: m/e 291 (M⁺); ir (Nujol): (2900 br), 1600 m, 1520 m, (1460 s), 1420 m, (1380 m), 1350 s, 1320 w, 1280 w, 1250 w, 1160 w, 1140 w, 880 m, 750 m cm⁻¹; ¹H-nmr (trifluoroacetic acid-*d* and acetone-*d*₆): δ = 7.7-9.4 (m, aromatic); ¹³C-nmr (trifluoroacetic acid-*d* and acetone-*d*₆): δ = 115.72, 117.73, 124.82, 125.47, 127.75, 129.97, 131.32, 132.62, 135.71, 137.17, 142.97, 144.92, 149.36, 150.18, 157.11.

Anal. Calcd. for C₁₅H₈N₅O₂: C, 61.9; H, 3.1; N, 24.0. Found: C, 61.6; H, 2.9; N, 24.2.

5,6,7,8-Tetrahydro-5,9,9-trimethyl-3-(3-nitrophenyl)-5,8-methano-1,2,4-benzotriazine (**4b**); 5,6,7,8-Tetrahydro-8,9,9-trimethyl-3-(3-nitrophenyl)-5,8-methano-1,2,4-benzotriazine (**4d**).

A mixture of *d*,1-camphoroquinone, **4a**, (19.8 g, 119 mmoles) and 3-nitrobenzimidic acid hydrazide, **8**, (21.2 g, 118 mmoles) in 440 ml of 2-propanol was refluxed with stirring under nitrogen for 8 hours. The reaction mixture was cooled to 0° and filtered to obtain 27.6 g (75% yield) of a mixture of isomers (about 5:1, as judged by ¹³C-nmr). The crude product was dissolved in 250 ml of hot methanol and slowly cooled to 28°. On filtration, 4.4 g (12% yield) of the minor isomer was obtained.

The filtrate was stirred at 0° to afford 14.9 g (40% yield) of the major isomer.

The major isomer was recrystallized from 145 ml of methanol to obtain 5.4 g (14.7% yield) of **4b** as an off-white solid, mp 110-112°; ms: m/e

310 (M⁺); ir (Nujol): (2900 br), 1595 m, 1530 s, (1460 s), (1375 s), 1365 s, 1350 s, 1285 m, 1270 m, 1175 w, 1165 w, 1125 m, 1090 w, 1070 w, 1000 w, 925 w, 860 w, 815 w, 730 m, 695 m, 670 w cm⁻¹; ¹H-nmr (deuteriochloroform): δ = 0.68 (s, 3, methyl), 1.15 (s, 3, methyl), 1.42 (s, 3, methyl), 1.3-1.6 (m, 2, methylene), 1.9-2.5 (m, 2, methylene), 3.28 (dd, 1, methine), 7.69 (dd, 1) and 8.35 (ddd, 1) and 8.88 (ddd, 1) and 9.33 (dd, 1) (nitrophenyl). For ¹³C- and ¹⁵N-nmr see Tables.

Anal. Calcd. for C₁₇H₁₈N₄O₂: C, 65.8; H, 5.8; N, 18.1. Found: C, 65.8; H, 5.7; N, 18.0.

The minor isomer was recrystallized from 125 ml of methanol to obtain 1.5 g (4% yield) of **4d** as a white solid, mp 174-175°; ms: m/e 310 (M⁺); ir (Nujol): (2900 br), 1580 w, 1525 s, 1480 m, (1465 s), 1390 m, (1375 m), 1370 s, 1350 m, 1275 m, 1215 w, 1180 w, 1135 w, 1080 w, 1000 w, 925 w, 860 w, 820 w, 725 m cm⁻¹; ¹H-nmr (deuteriochloroform): δ = 0.68 (s, 3, methyl), 1.15 (s, 3, methyl), 1.50 (s, 3, methyl), 1.3-1.6 (m, 2, methylene), 1.9-2.5 (m, 2, methylene), 3.09 (dd, 1, methine), 7.69 (dd, 1) and 8.35 (ddd, 1) and 8.87 (ddd, 1) and 9.35 (dd, 1) (nitrophenyl). For ¹³C- and ¹⁵N-nmr see Tables.

Anal. Calcd. for C₁₇H₁₈N₄O₂: C, 65.8; H, 5.8; N, 18.1. Found: C, 65.8; H, 5.6; N, 18.1.

5,6,7,8-Tetrahydro-5,9,9-trimethyl-3-(3-nitrophenyl)-5,8-methano-1,2,4-benzotriazine 1-Oxide (**4c**).

A solution of **4b** (3.55 g, 12 mmoles) and *m*-chloroperoxybenzoic acid (3.21 g, 80%, 15 mmoles) in 91 ml of dichloromethane was refluxed for 24 hours and stirred at room temperature for 48 hours. The reaction mixture was washed with 10% aqueous sodium bicarbonate three times (20 + 10 + 10 ml). The organic layer was dried over magnesium sulfate, filtered, and concentrated to obtain a yellow oil. On addition of 100 ml of methanol, two crops of **4c**, a pale-yellow solid (2.9 g, 78% yield), were obtained, mp 149.5-150.5°, solidifies at 160° and melts again at 167°; ms: m/e 326 (M⁺); ir (Nujol): (2950 br), 1590 m, 1550 s, 1535 s, (1465 s), 1420 m, 1395 s, (1380 s), 1355 s, 1335 s, 1300 m, 1180 w, 1165 w, 1120 m, 1090 m, 1055 w, 1010 w, 1000 m, 940 w, 920 w, 910 w, 860 m, 850 w, 820 w, 815 m, 730 m, 715 m cm⁻¹; ¹H-nmr (deuteriochloroform): δ = 0.85 (s, 3, methyl), 1.15 (s, 3, methyl), 1.45 (s, 3, methyl), 1.3-1.7 (m, 2, methylene), 2.0-2.5 (m, 2, methylene), 3.45 (dd, 1, methine), 7.72 (dd, 1) and 8.38 (ddd, 1), and 8.77 (ddd, 1) and 9.20 (dd, 1) (nitrophenyl). For ¹³C- and ¹⁵N-nmr see Tables.

Anal. Calcd. for C₁₇H₁₈N₄O₃: C, 62.6; H, 5.6; N, 17.2. Found: C, 62.2; H, 5.5; N, 17.1.

3-(3-Nitrophenyl)phenanthro[9,10-*e*]-1,2,4-triazine (**5b**).

A mixture of phenanthrenequinone, **5a**, (9.2 g, 44 mmoles) and 3-nitrobenzimidic acid hydrazide, **8**, (8.0 g, 44 mmoles) in 200 ml of dioxane was refluxed under nitrogen with stirring for 5 hours. The reaction mixture was cooled to 0° and filtered. The solid was dried at 50°/20 mm to obtain 12.6 g (80% yield) of **5b**. Recrystallization from *N,N*-dimethylformamide afforded a yellow solid, mp 279-280°; ms: m/e 352 (M⁺); ir (Nujol): (2900 br), 1600 m, 1520 s, (1465 s), 1390 w, (1370 s), 1340 s, 1290 w, 1270 w, 1160 w, 1085 m, 1060 w, 920 w, 850 w, 810 w, 750 m, 720 m cm⁻¹; ¹H-nmr (deuteriochloroform + trifluoroacetic acid-*d*): δ = 7.8-9.5 (m, aromatic); ¹³C-nmr (trifluoroacetic acid-*d* + acetone-*d*₆): δ = 124.68 (2C), 124.87, 126.04, 126.82, 130.14, 130.46 (2C), 130.72, 131.18, 132.55, 134.04, 135.41, 135.73, 138.79, 139.50, 145.10, 149.91, 152.05, 153.09, 156.54.

Anal. Calcd. for C₂₁H₁₂N₄O₂: C, 71.6; H, 3.4; N, 15.9. Found: C, 71.4; H, 3.3; N, 16.0.

6,7-Dihydro-5-methyl-3-(3-nitrophenyl)-5*H*-cyclopenta[*e*]-1,2,4-triazine (**6b**).

A mixture of 3-methyl-1,2-cyclopentanedione, **6a**, (12.4 g, 111 mmoles) and 3-nitrobenzimidic acid hydrazide, **8**, (20 g, 111 mmoles) in 205 ml of 2-propanol was refluxed with stirring under nitrogen for 8 hours. The solution was cooled to 0° and filtered. After drying at 50°/20 mm, there was obtained 13.2 g (46% yield) of a mixture of isomers. The sample was dissolved in chloroform, and the solution was filtered. The filtrate was washed with 2 *M* aqueous hydrochloric acid and with water. The organic layer was dried over magnesium sulfate, filtered, and concentrated. Cryst-

tallization of the residue from 2-propanol gave 10.9 g (38%) of **6b**, peach-colored solid, mp 105-107°; ms: m/e 256 (M⁺); ir (Nujol): (2900 br), 1615 w, 1565 m, 1530 s, 1480 m, (1460 s), 1430 w, (1375 s), 1350 s, 1290 m, 1270 w, 1200 w, 1170 w, 1140 w, 1080 m, 1020 w, 920 m, 870 m, 840 w, 830 w, 790 m, 740 m, 695 m cm⁻¹; ¹H-nmr (deuteriochloroform): δ = 1.50 (d, 3, methyl), 1.85 (m, 1) and 2.58 (m, 1) (methylene), 3.2-3.5 (m, 3, α-methylene and methine), 7.70 (dd, 1) and 8.35 (ddd, 1) and 8.88 (ddd, 1) and 9.32 (dd, 1) (nitrophenyl). For ¹³C- and ¹⁵N-nmr see Tables.

Anal. Calcd. for C₁₃H₁₂N₄O₂: C, 60.9; H, 4.7; N, 21.9. Found: C, 60.9; H, 4.7; N, 21.8.

6,7-Dihydro-5-methyl-3-(3-nitrophenyl)-5H-cyclopenta[e]-1,2,4-triazine 1-Oxide (**6c**).

A solution of **6b** (5 g, 19.5 mmoles) and *m*-chloroperoxybenzoic acid (4.9 g, 80%, 22.7 mmoles) in 30 ml of chloroform was stirred at 25° for 70 hours. The reaction mixture was washed with 10% aqueous sodium bicarbonate and with water. The organic layer was dried over magnesium sulfate. The filtrate was concentrated to give 6.5 g of light-brown oil. Crystallization from methanol afforded 3.9 g (73%) of white solid which sublimed at 130°/0.3 mm, mp 151-152°; ms: m/e 272 (M⁺); ir (Nujol): (2900 br), 1610 w, 1585 w, 1560 m, 1520 s, (1460 s), 1425 m, 1385 m, (1375 m), 1350 s, 1265 w, 1095 w, 1000 w, 925 w, 865 w, 825 w, 775 w, 740 w, 705 w cm⁻¹; ¹H-nmr (deuteriochloroform): δ = 1.50 (d, 3, methyl), 1.85 (m, 1) and 2.58 (m, 1) (methylene), 3.0-3.7 (m, 3, α-methylene and methine), 7.68 (dd, 1) and 8.35 (ddd, 1) and 8.71 (ddd, 1) and 9.19 (dd, 1) (nitrophenyl). For ¹³C- and ¹⁵N-nmr see Tables.

Anal. Calcd. for C₁₃H₁₂N₄O₃: C, 57.3; H, 4.4; N, 20.6. Found: C, 57.5; H, 4.2; N, 20.4.

(+)-5,8-Dihydro-6,6,8-trimethyl-3-(3-nitrophenyl)-5,8-ethano-6H-pyrano[4,3-*e*]-1,2,4-triazine (**7b**).

A mixture of 3-nitrobenzimidic acid hydrazide, **8**, (1.8 g, 10 mmoles) and (-)-1,3,3-trimethyl-2-oxabicyclo[2,2,2]octane-5,6-dione, **7a**, (2 g, 11 mmoles) in 70 ml of 2-propanol was stirred at room temperature for 30 minutes. The mixture was cooled to 0° and filtered to give **7b**, a white solid, 2.1 g (64% yield), mp 186-186.5°; ms: m/e 326 (M⁺); [α]_D²⁵ + 67.9 (c = 1.5, toluene); ir (Nujol): (2900 br), 1565 m, 1525 s, (1460 s), (1380 s), 1355 s, 1310 m, 1280 m, 1240 m, 1190 w, 1160 w, 1135 w, 1100 m, 1075 m, 1010 w, 980 m, 950 w, 920 w, 860 w, 840 m, 810 w, 715 m cm⁻¹; ¹H-nmr (deuteriochloroform): δ = 0.9 (s, 3, methyl), 1.59 (s, 3, methyl), 1.88 (s, 3, methyl), 1.55-1.85 (m, 2, methylene), 2.0-2.7 (m, 2, methylene), 3.20 (dd, 1, methine), 7.73 (dd, 1) and 8.37 (ddd, 1) and 8.89 (ddd, 1) and 9.33 (dd, 1) (nitrophenyl); ¹³C-nmr (deuteriochloroform): δ = 19.30, 19.58, 26.89, 29.44, 29.92, 44.66, 72.83, 74.18, 122.56, 125.27, 129.44, 133.23, 136.81, 148.35, 158.10, 160.97, 162.76.

Anal. Calcd. for C₁₇H₁₈N₄O₃: C, 62.6; H, 5.6; N, 17.2. Found: C, 62.2; H, 5.6; N, 17.2.

3-Nitrobenzimidic Acid Hydrazide (**8**).

A thoroughly stirred solution of ethyl 3-nitrobenzenecarboximidate (11) (209 g, 1.07 moles) and hydrazine hydrate (57 g, 97%, 1.1 moles) in 1.24 l of 2-propanol was heated at 45° for 7 hours. The mixture was cooled at 0°, and the solid was filtered and dried to obtain 182 g (93% yield) of **8**. Recrystallization from ethanol gave a copper-colored solid, mp 152-154° dec; ms: m/e 180 (M⁺); ir (Nujol): 3430 m, 3340 m, 3170 m, 3060 m, (2900 br), 1900 w and 1850 w and 1720 br w (*m*-disubstituted benzene), 1640 m, 1620 m, 1580 m, 1535 m, (1460 s), 1440 m, (1380 s), 1350 s, 1320 m, 1280 m, 1145 m, 1080 w, 1040 m, 940 w, 930 m, 895 m, 805 m, 740 m, 690 m cm⁻¹; ¹H-nmr (deuteriochloroform + dimethyl sulfoxide-d₆): δ = 5.15 (br s, 2, NH₂), 5.85 (s, 2, NH), 7.58 (dd, 1) and 8.09 (m, 1) and 8.18 (m, 1) and 8.59 (dd, 1) (nitrophenyl); ¹³C-nmr (deuteriochloroform + dimethyl sulfoxide-d₆): δ = 119.73, 122.17, 128.94, 131.05, 137.01, 143.95, 147.69.

Anal. Calcd. for C₇H₈N₄O₂: C, 46.7; H, 4.5; N, 31.1. Found: C, 46.5; H, 4.4; N, 31.4.

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