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Reported Spectral data

4,6-Dimethyl-4*H*-[1,2,5]oxadiazolo[3,4-*d*]pyrimidine-5,7-dione 1-oxide (2a):

mp 245 °C dec (Ref. 15b: Yoneda, F *et al.*, *J. Heterocycl. Chem.*, 1973, 993

mp 245°C dec (Ref. 14b: Nutiu, R. *et al.*, *J. Chem. Soc., Perkin I*, 1976, 1327

IR (KBr) 1744, 1684, 1639, 1602 cm^{-1}

UV (EtOH, ϵ) λ_{max} 317 (1550), 268 (11350) nm

Mass: 198 (M^+ , 30%), 183 (20%), 168 (10%), 152 (7%), 111 (10%),
83 (60%), 81 (100%)

6-Methyl-4*H*-[1,2,5]oxadiazolo[3,4-*d*]pyrimidine-5,7-dione 1-oxide (2c):

mp 211-1°C dec (Ref. 14b: Nutiu, R. *et al.*, *J. Chem. Soc., Perkin I*, 1976, 1327

mp 210°C (Ref. 10: Yoneda F. *et al.*, *Heterocycles* 1981, 15 341

UV (Dioxane, ϵ) λ_{max} 312 (1700), 267.5 (11400) nm

IR (KBr) 3160w, 3040w, 1730m, 1700s, 1650s, 1600w cm^{-1}

4*H*-[1,2,5]Oxadiazolo[3,4-*d*]pyrimidine-5,7-dione 1-oxide (2d):

mp 260°C dec (Ref. 14a: Temple, C. Jr. *et al.*, *J. Org. Chem.*, 1968, 33, 2086

IR (KBr) 3300, 3190, 3105, 1740, 1715, 1640, 1600 cm^{-1}

UV (pH 7) λ_{max} 346 (3.65×10^3), 272 (9.15×10^3) nm

[1,2,5]Oxadiazolo[3,4-*d*]pyrimidine-5,7-diamine 1-oxide (3):

mp >264°C (Ref. 14a: Tempe, C. Jr. *et al.*, *J. Org. Chem.*, 1968, 33, 2086

IR (KBr) 3425, 3320, 3115, 1645, 1600 cm^{-1}

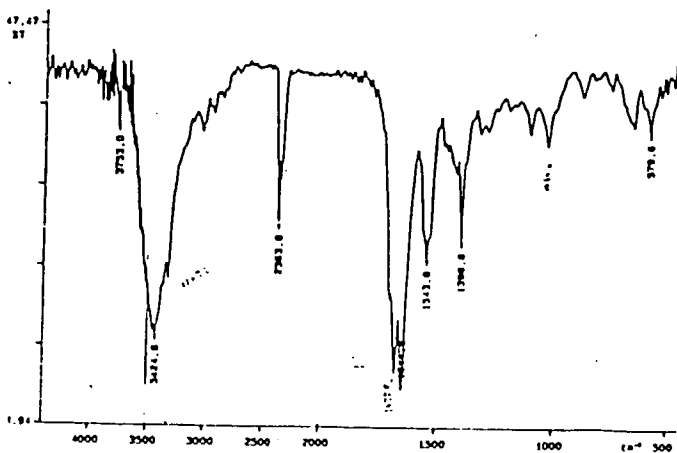
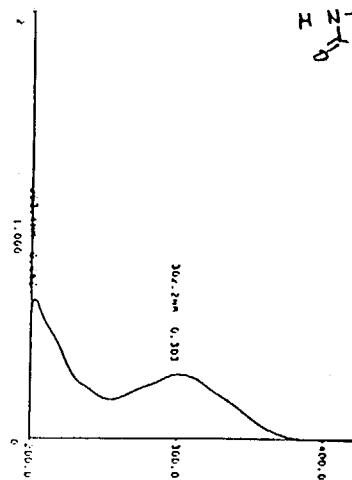
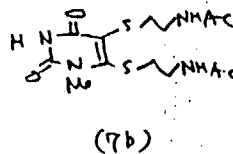
UV (pH 7) λ_{max} 365 (2.64×10^3), 289 (1.2×10^4) nm

$^1\text{H-NMR}$ (2.5% DMSO- d_6) δ 8.13 (br), 7.03 (1, 1, NH_2)

5-Amino-6*H*-[1,2,5]oxadiazolo[3,4-*d*]pyrimidin-7-one 1-oxide (4):

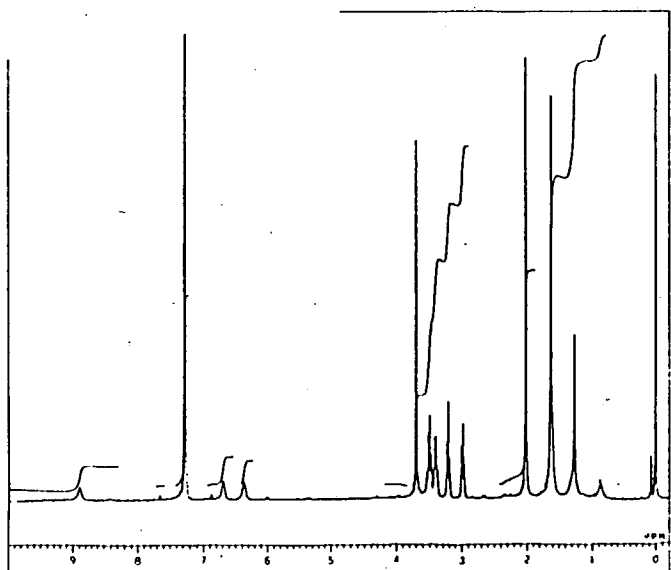
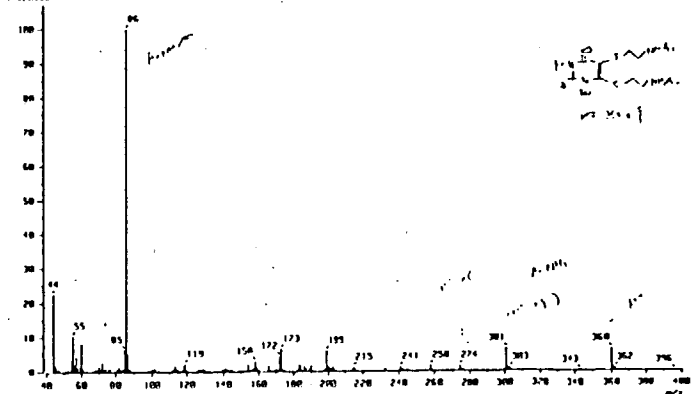
mp >264°C (Ref. 14a: Tempe, C. Jr. *et al.*, *J. Org. Chem.*, 1968, 33, 2086

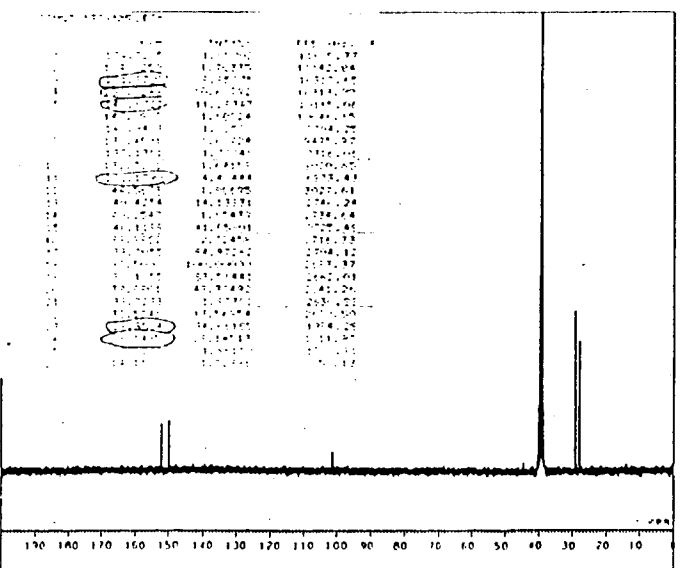
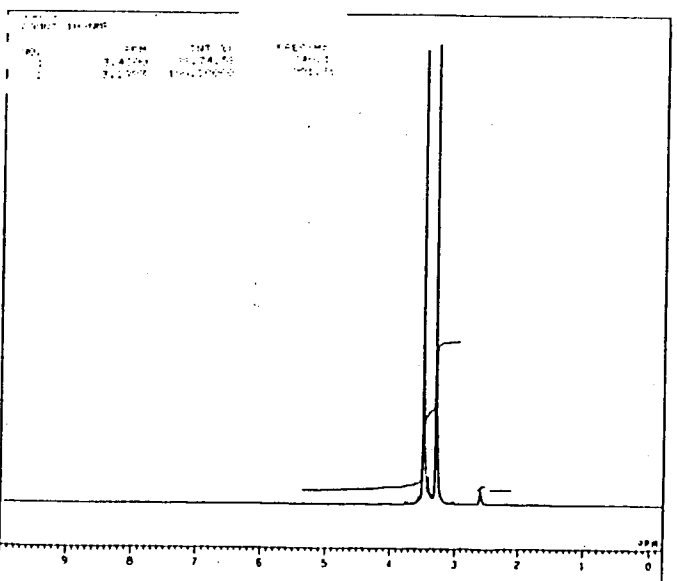
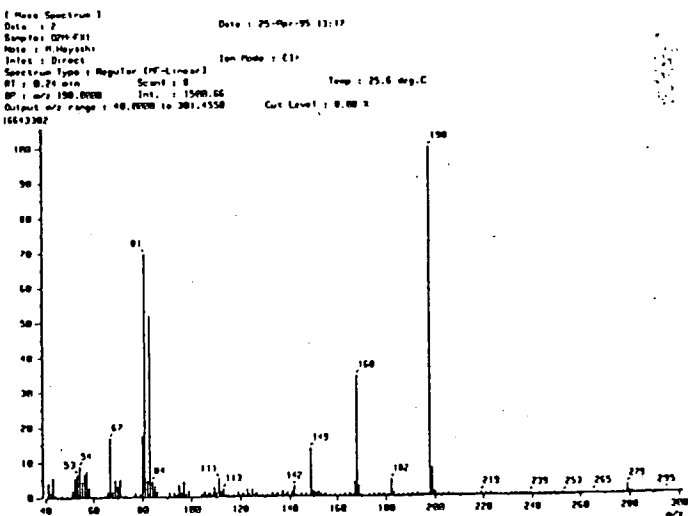
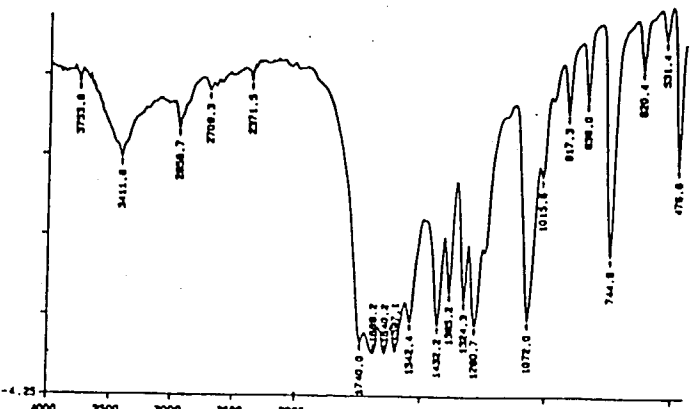
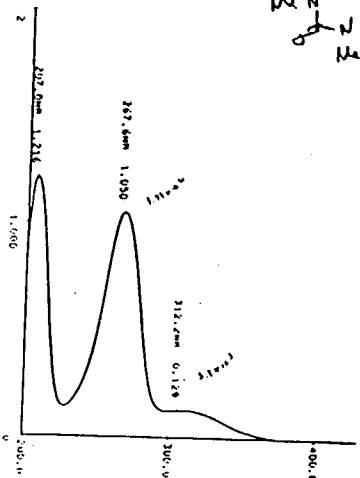
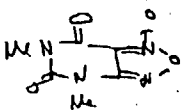
IR (KBr) 3350, 3285, 3170, 1725, 1700, 1630 cm^{-1}



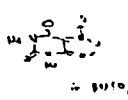
[Elemental Composition]
 Date : 01-Jul-97 15:55
 Sample : MS 610-2
 Name : M. Hayashi
 Inlet : Direct
 Ion Mode : EI+
 Scan: 57
 RT : 2.43 min
 Elements : C 13/0, H 20/0, O 4/1, N 4/0, S 2/0
 Mass Tolerance : 10ppm, Scan if m/z > 500, 20ms if m/z > 2000
 Densitization (U.S.) : -0.5 - 20.0
 Observed m/z Inlet Err(ppm / ms) U.S. Composition
 360.0312 76.3 -1.7 / +0.6 8.0 C 13 H 20 O 4 N 4 S 2

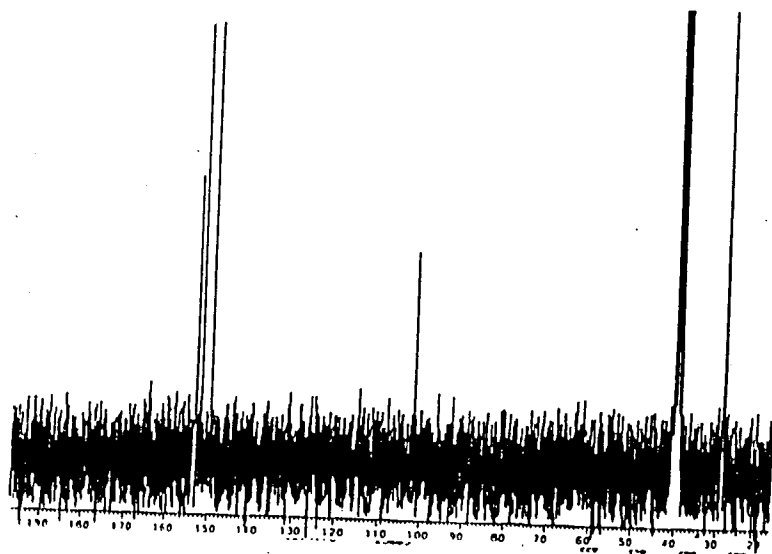
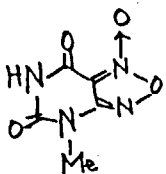
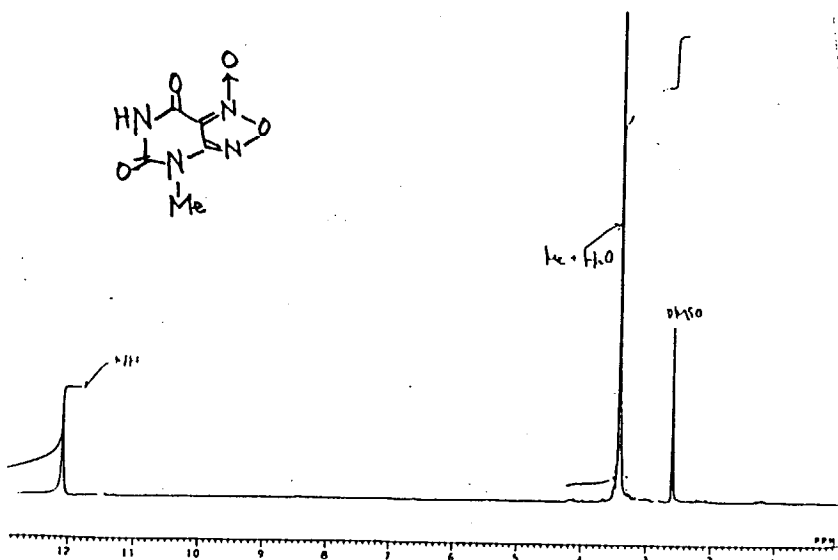
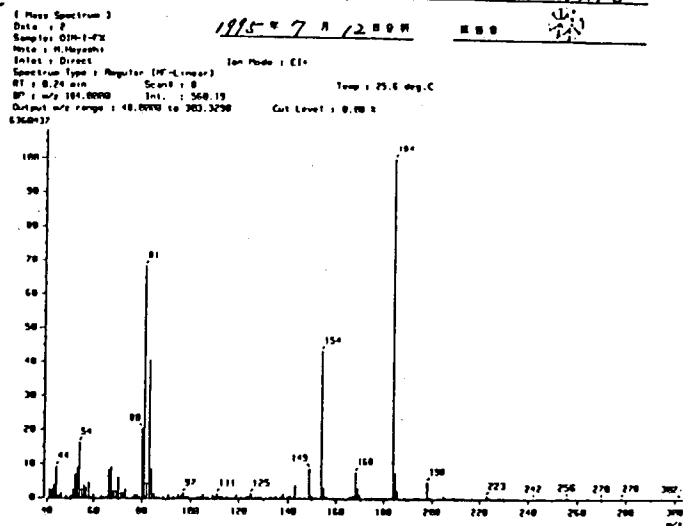
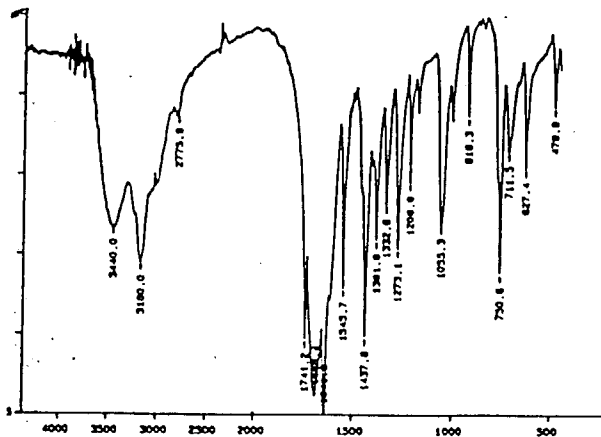
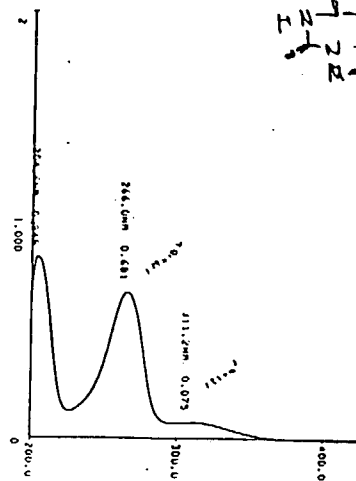
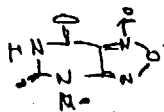
[Mass Spectrum]
 Date : 0
 Sample : MS 610-2
 Name : M. Hayashi
 Inlet : Direct
 Spectrum Type : Regular (PE-4, linear)
 Ion Mode : EI+
 RT : 2.50 min
 Scan: 76
 Temp : 191.6 deg.C
 BP : m/z 96.0000
 Int. : 1569.73
 Output file range : 40.0000 to 400.0000
 Cut Level : 0.000 2
 17678756

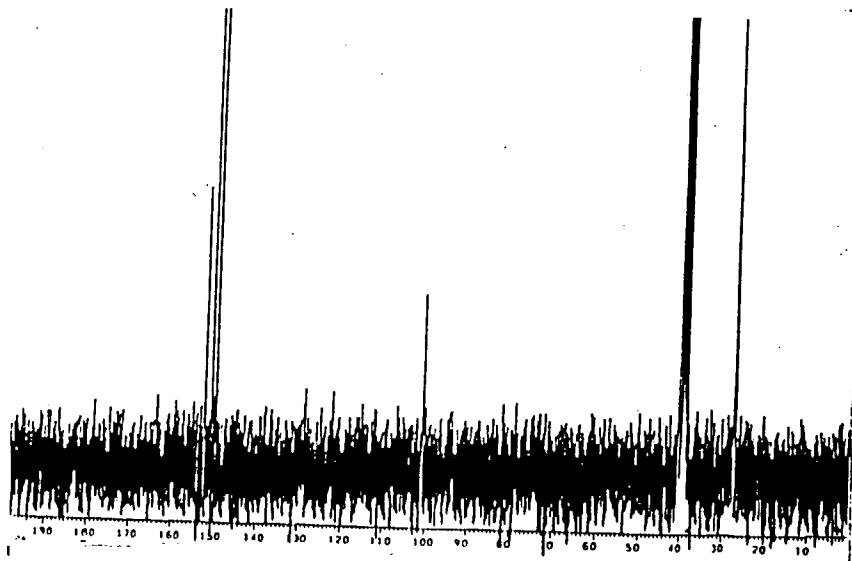
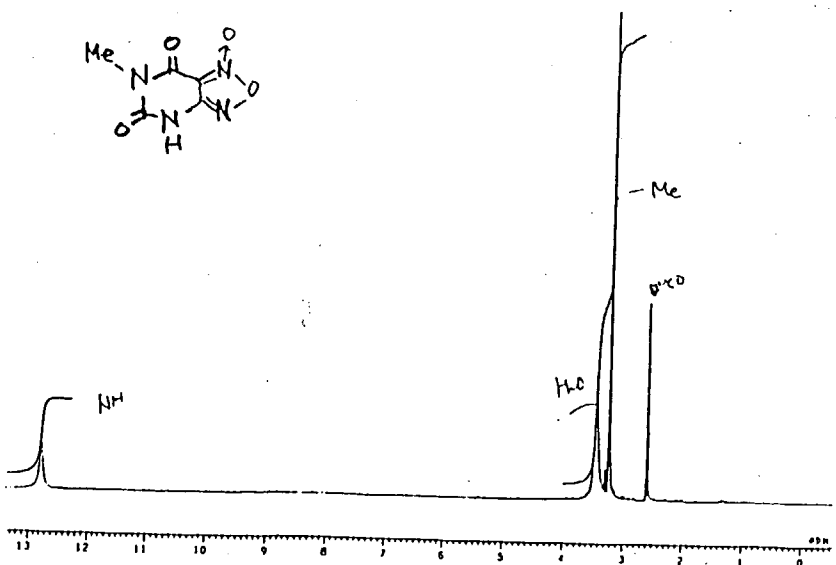
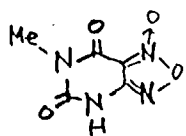
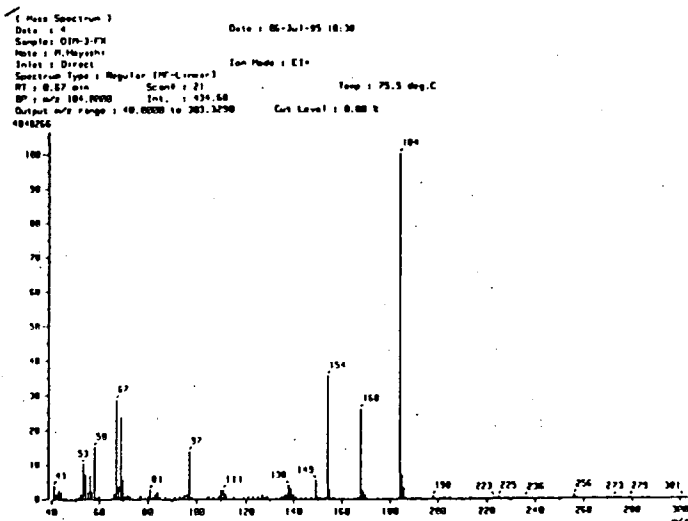
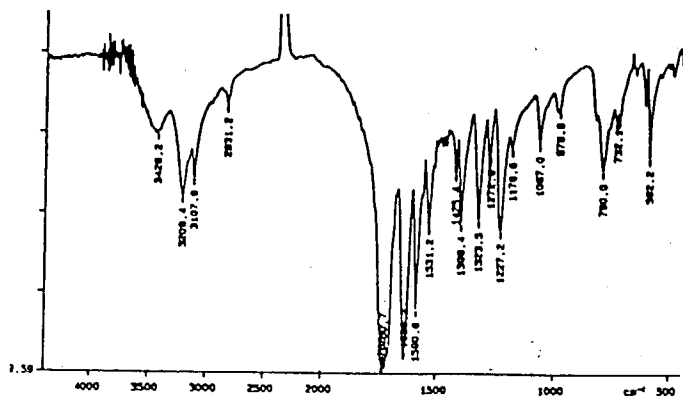
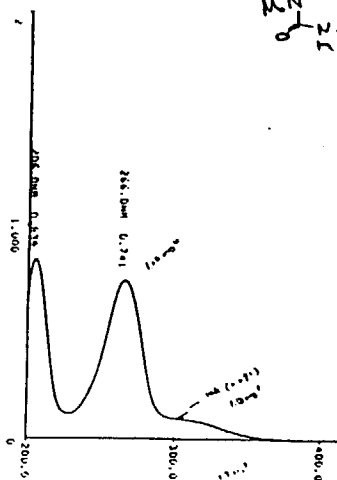
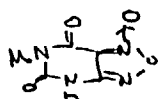


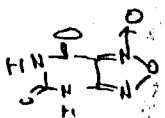


17-MAY-97 21:31:01
 FILE: D:\A
 C:\MSD\13C\MSD.BCH
 C:\MSD\13C
 5600.0 Hz
 65536
 20000.0 Hz

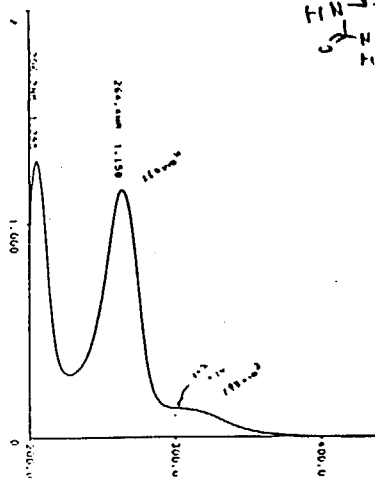
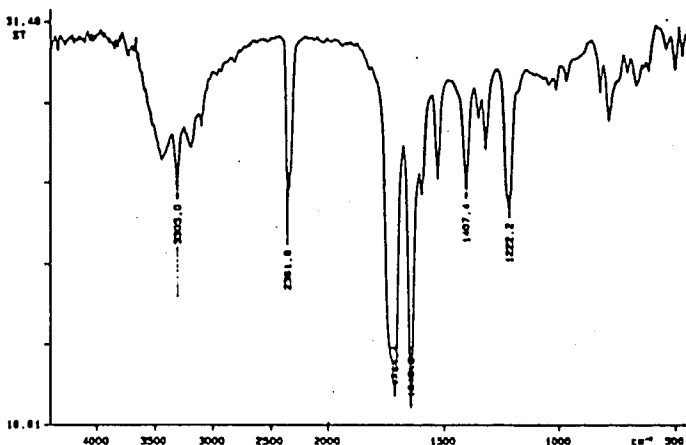
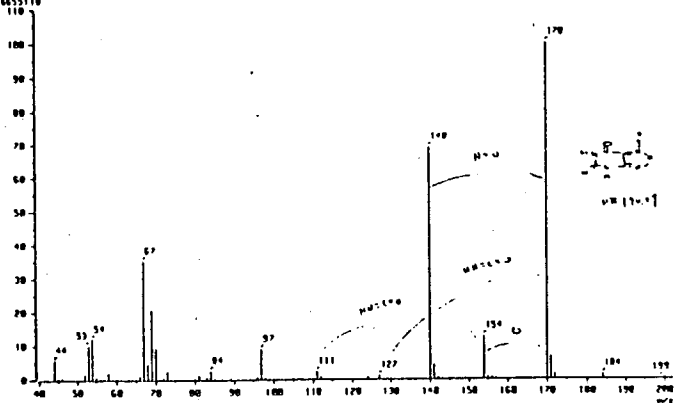




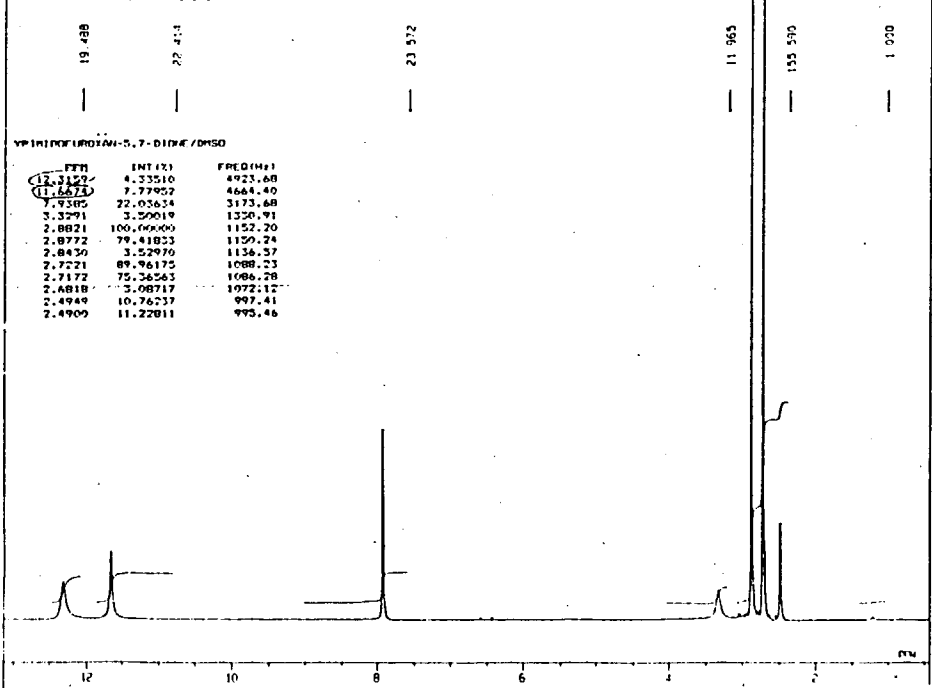




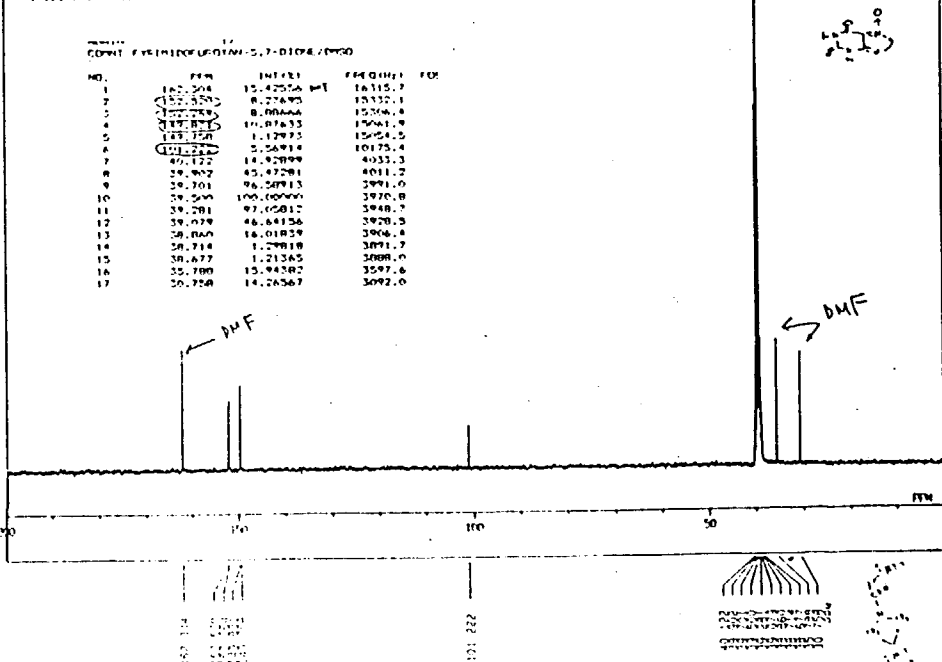
[Mass Spectrum]
Date: 02-Feb-96 14:06
Sample: MS-284
Note: N-Hydroxy
Inlet: Direct
Spectrum Type: Regular (HT-Linear)
RT: 2.18 min Scan: 25
Temp: 114.4 deg.C
SP: 170,000 Int: 1441.46
Output File Range: 40,000 to 200,1210
Cut Level: 0.00 e
16055110



PYRIMIDOPURAN-5, 7-DIOL/DMSO

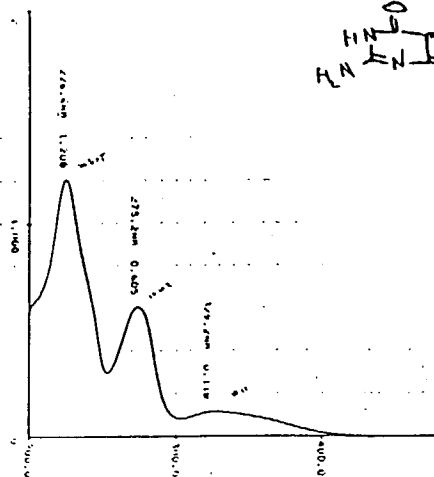
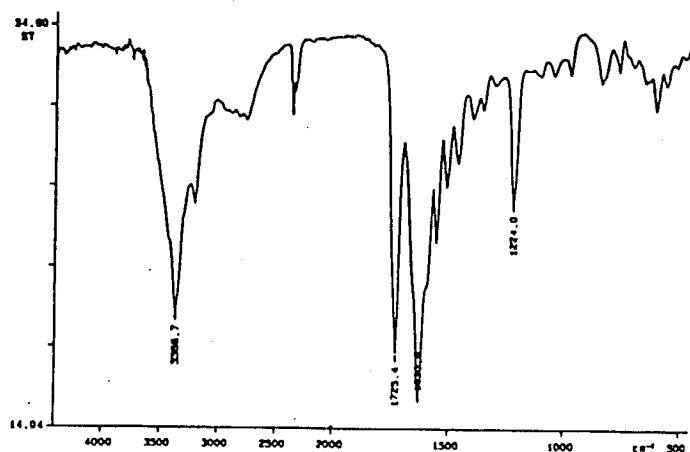
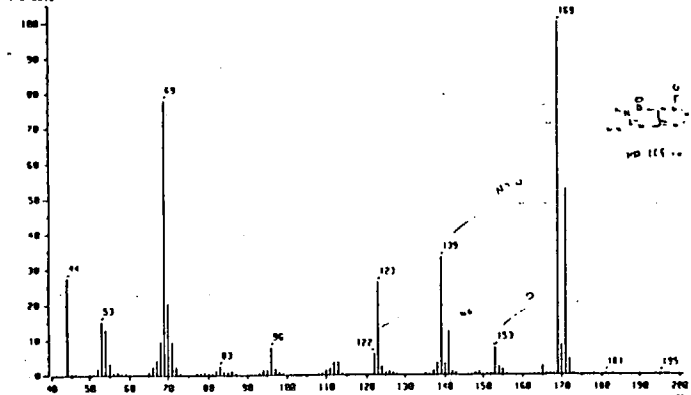


PYRIMIDOPURAN-5, 7-DIOL/DMSO

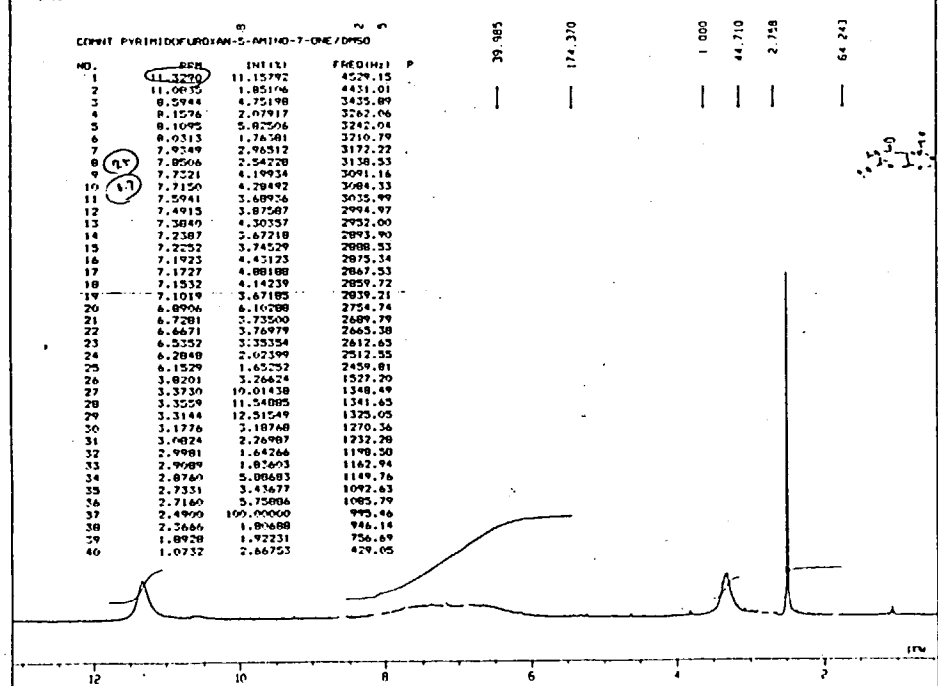


11-MAR-96 09
NAME: BCK
ORAC: IX
O/A
OBS: I
OBS: IN
PUL
PRED
INT

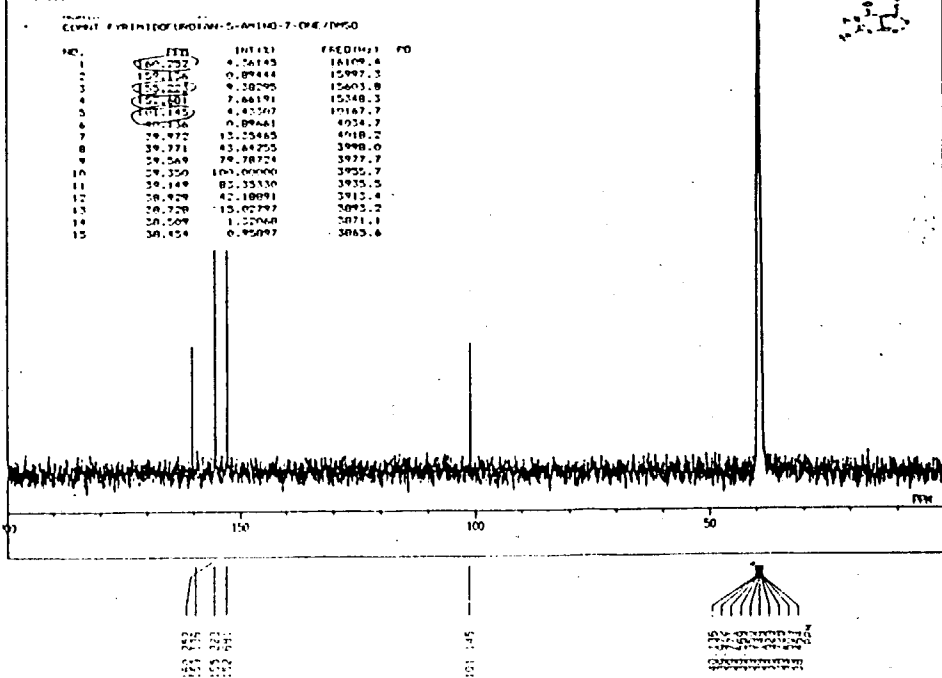
[Mass Spectrum]
Date: 07-Feb-96 14:33
Sample: MS285
Note: R. Mayhew
Inlet: Direct Ion Mode: CI+
Spectrum Type: Regular (M+Linear)
RT: 3.84 min Scan: 52 Temp: 295.1 deg.C
BP: max 100,000 Int: 1347.14
Output range: 40,000 to 201,100 Cut Level: 0.00 %
1483561)

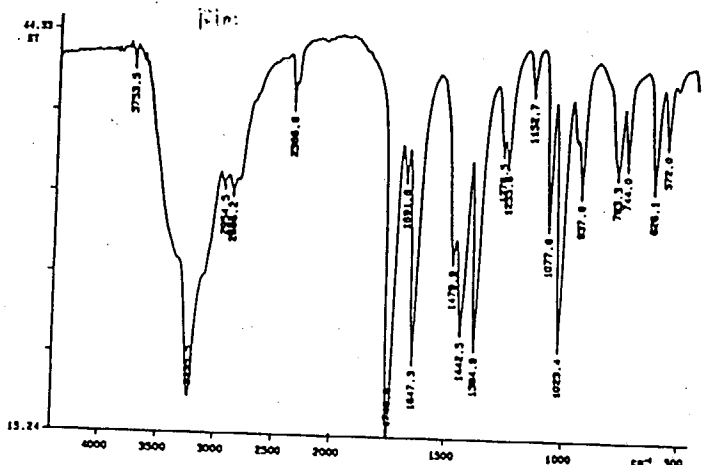
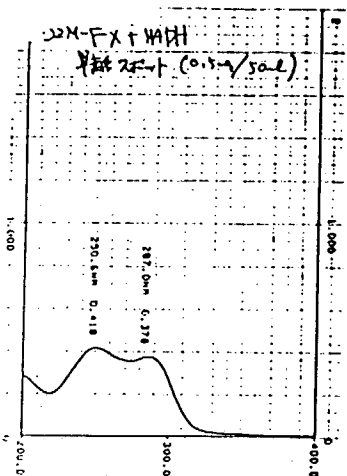
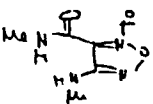


Pyrimidofuran-5-amin-7-OE/DMO



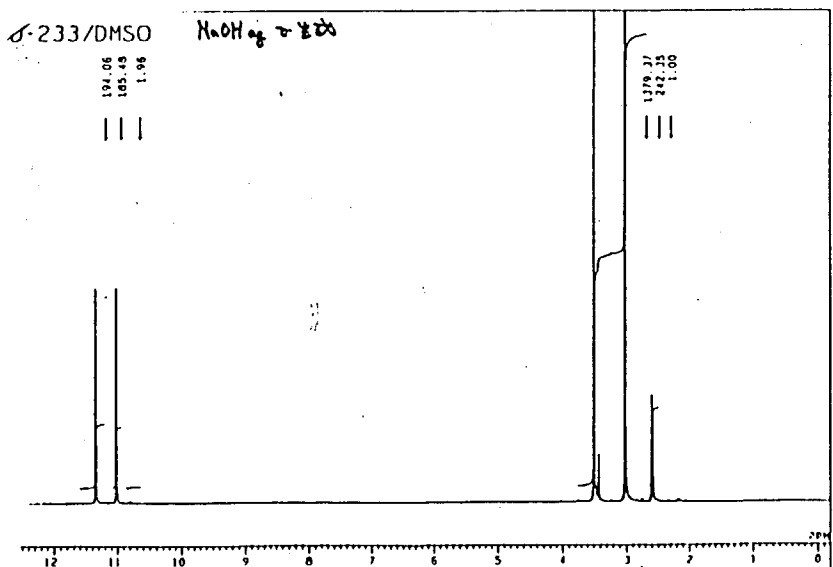
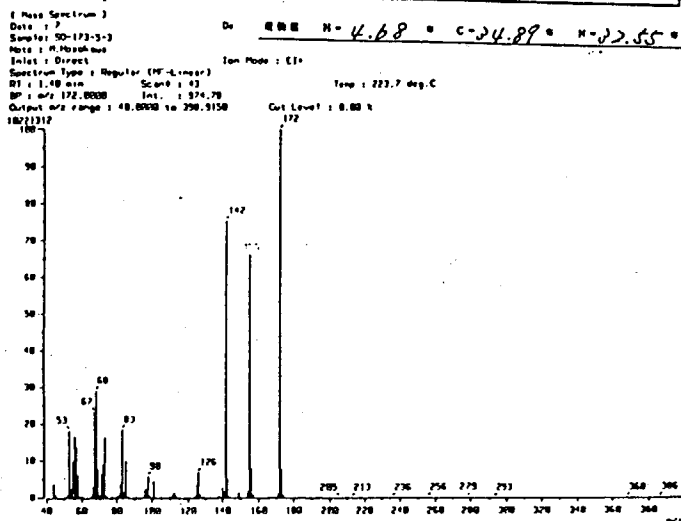
Pyrimidofuran-5-amin-7-OE/DMO





物質名 SD-233 融点 44 °C

HN	2.158	H	4.62	C	24.91	N	22.45
HN		H		C		N	



FURFURAL

^1H NMR Spectrum (Top):
 Peaks (ppm): 7.8641, 7.500, 7.2618, 7.0890, 2.0, 1.9
 Integration curve shown above the peaks.

^{13}C NMR Spectrum (Bottom):
 Peaks (ppm): 152.31, 131.800, 126.203, 120.670, 111.430
 Integration curve shown below the peaks.