JOC The Journal of Organic Chemistry

J. Org. Chem., 1998, 63(20), 6947-6951, DOI:10.1021/jo980732y

Reported Spectral data

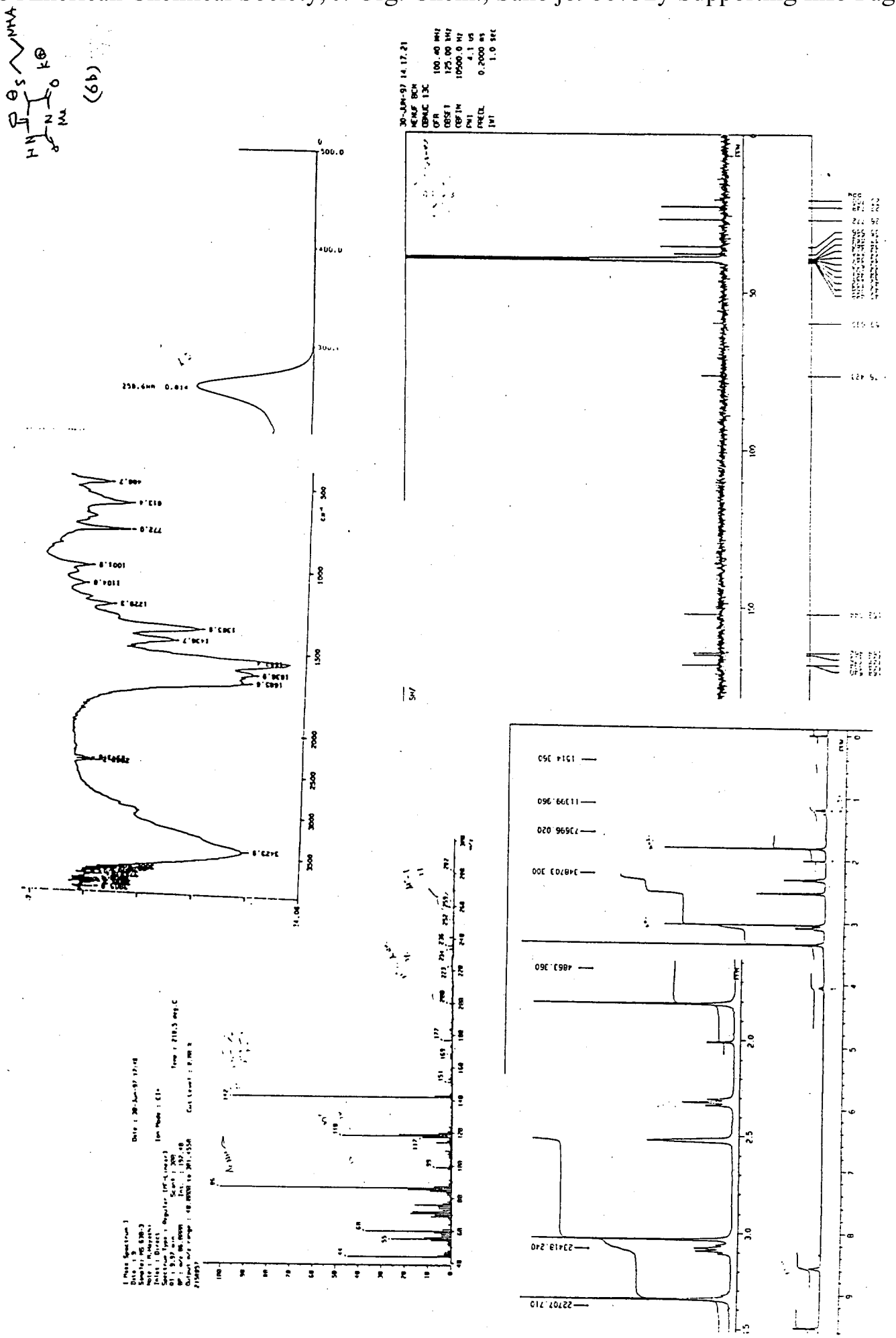
4,6-Dimethyl-4*H*-[1,2,5]oxadiazolo[3,4-*d*]pyrimidine-5,7-dione 1-oxide (2a):
mp 245 ℃ dec (Ref. 15b: Yoneda, F *et al.*, *J. Heterocycl. Chem.*, 1973, 993
mp 245℃ dec (Ref. 14b: Nutiu, R. *et al.*, *J. Chem. Soc., Perkin 1*, 1976, 1327
IR (KBr) 1744, 1684, 1639, 1602 cm^{-1}
UV (EtOH, ε) λ_{max} 317 (1550), 268 (11350) nm
Mass: 198 (M^+, 30%), 183 (20%), 168 (10%), 152 (7%), 111 (10%), 83 (60%), 81 (100%)

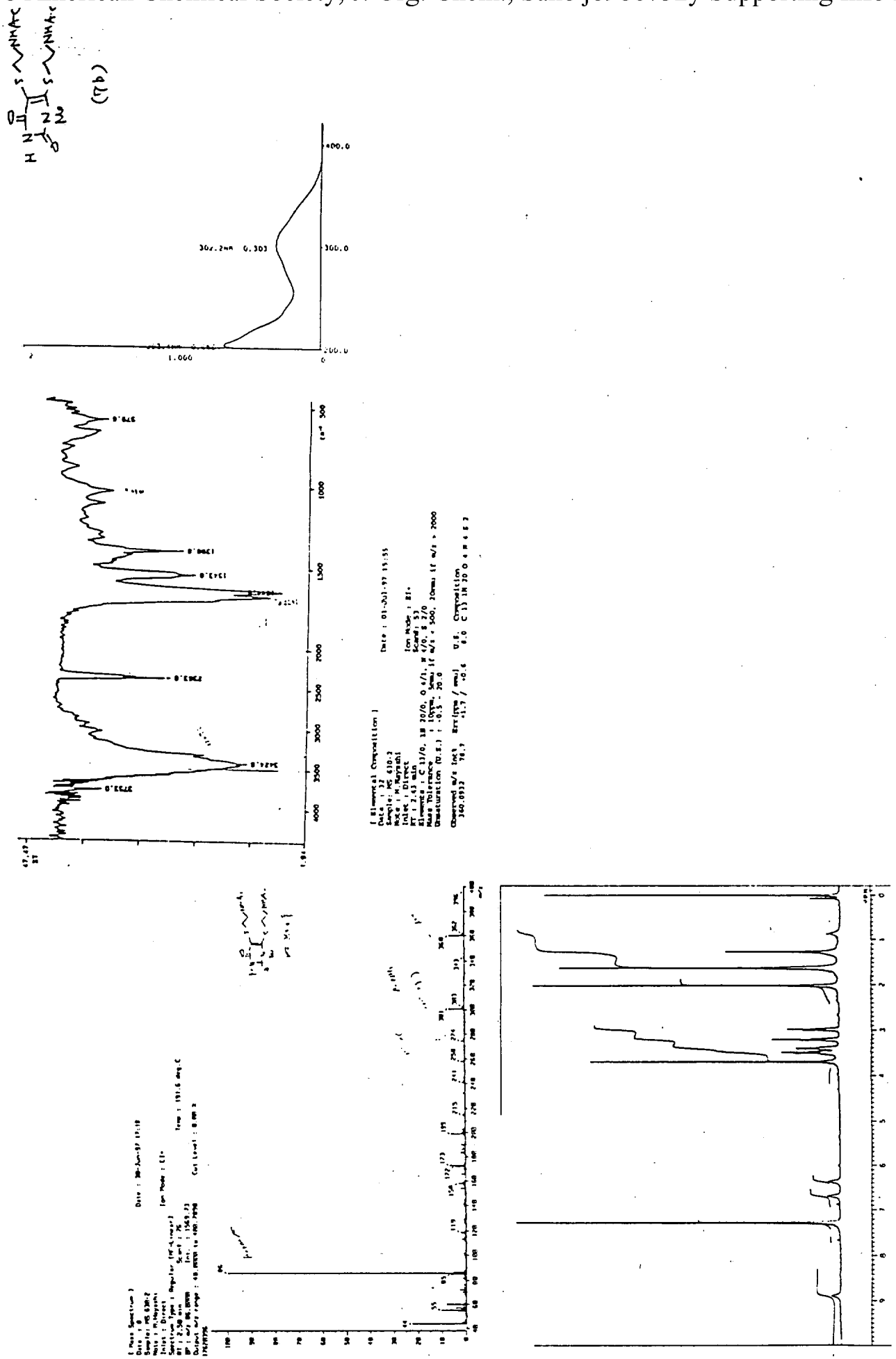
6-Methyl-4*H*-[1,2,5]oxadiazolo[3,4-*d*]pyrimidine-5,7-dione 1-oxide (2c):
mp 211-1℃ dec (Ref. 14b: Nutiu, R. *et al.*, *J. Chem. Soc., Perkin 1*, 1976, 1327
mp 210℃ (Ref. 10: Yoneda F. *et al.*, *Heterocycles* 1981, 15 341
UV (Dioxane, ε) λ_{max} 312 (1700), 267.5 (11400) nm
IR (KBr) 3160w, 3040w, 1730m, 1700s, 1650s, 1600w cm^{-1}

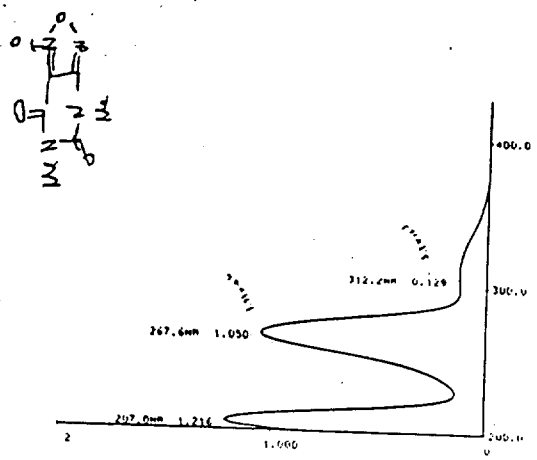
4*H*-[1,2,5]Oxadiazolo[3,4-*d*]pyrimidine-5,7-dione 1-oxide (2d):
mp 260℃ dec (Ref. 14a: Temple, C. Jr.*et al.*, *J. Org. Chem.*, 1968, 33, 2086
IR (KBr) 3300, 3190, 3105, 1740, 1715, 1640, 1600 cm^{-1}
UV (pH 7) λ_{max} 346 (3.65×10^3), 272 (9.15×10^3) nm

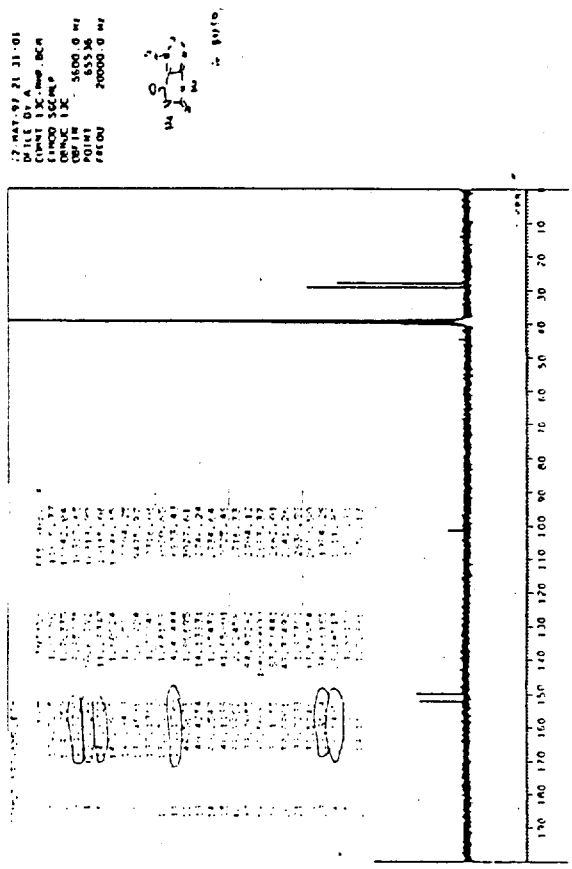
[1,2,5]Oxadiazolo[3,4-*d*]pyrimidine-5,7-diamine 1-oxide (3):
mp >264℃ (Ref. 14a: Tempe, C. Jr. *et al.*, *J. Org. Chem.*, 1968, 33, 2086
IR (KBr) 3425, 3320, 3115, 1645, 1600 cm^{-1}
UV (pH 7) λ_{max} 365 (2.64×10^3), 289 (1.2×10^4) nm
^{1}H-NMR (2.5% DMSO-d_6) δ 8.13 (br), 7.03 (1, 1, NH_2)

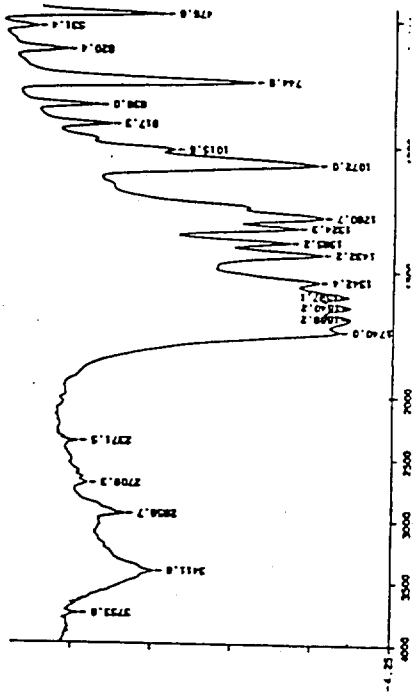
5-Amino-6*H*-[1,2,5]oxadiazolo[3,4-*d*]pyrimidin-7-one 1-oxide (4):
mp >264℃ (Ref. 14a: Tempe, C. Jr. *et al.*, *J. Org. Chem.*, 1968, 33, 2086
IR (KBr) 3350, 3285, 3170, 1725, 1700, 1630 cm^{-1}

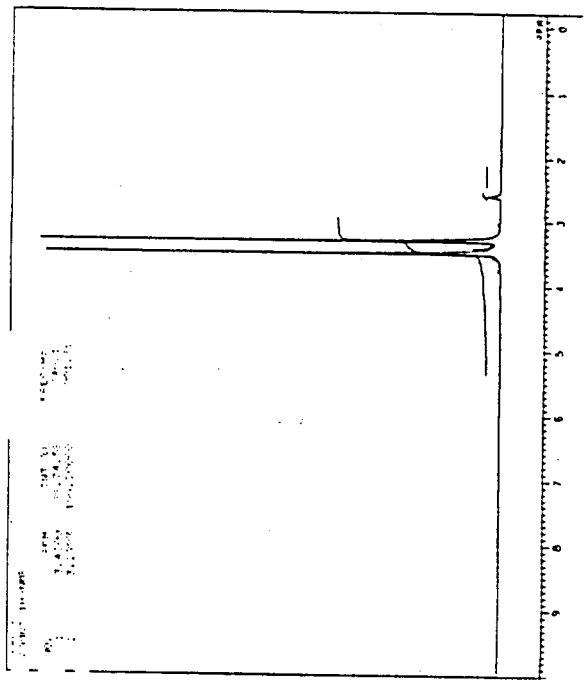


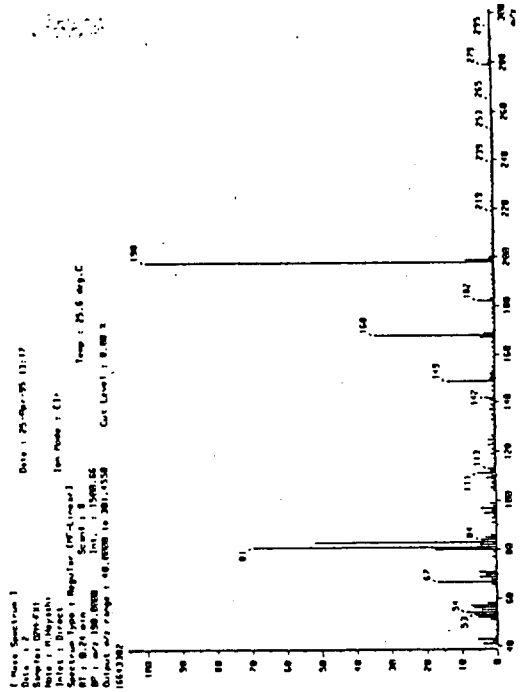












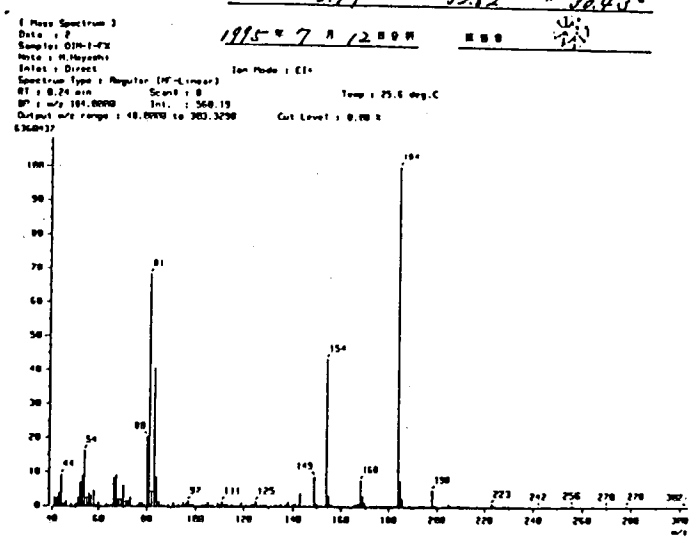
物質名 01H-1-FX 融点 mp °C

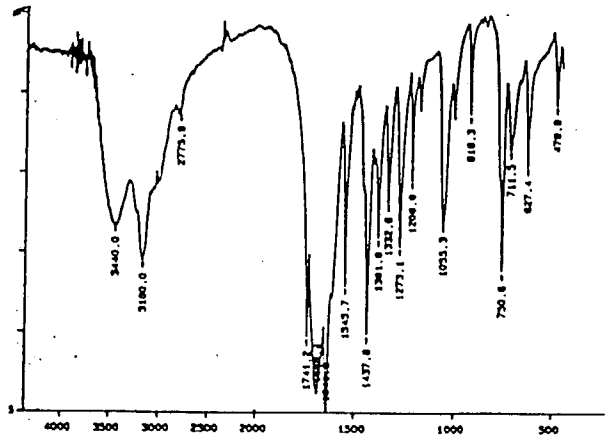
元素	%	N	%	C	%	H	%
		2.030		32.60		30.35	
		2.37					

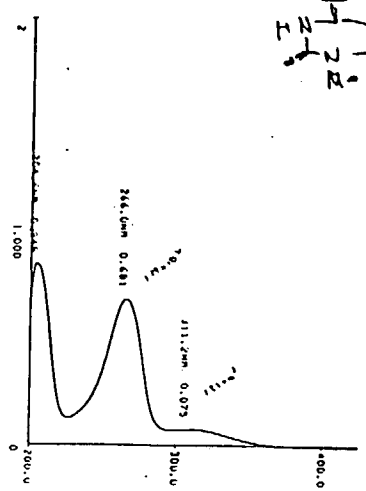
元素	%	

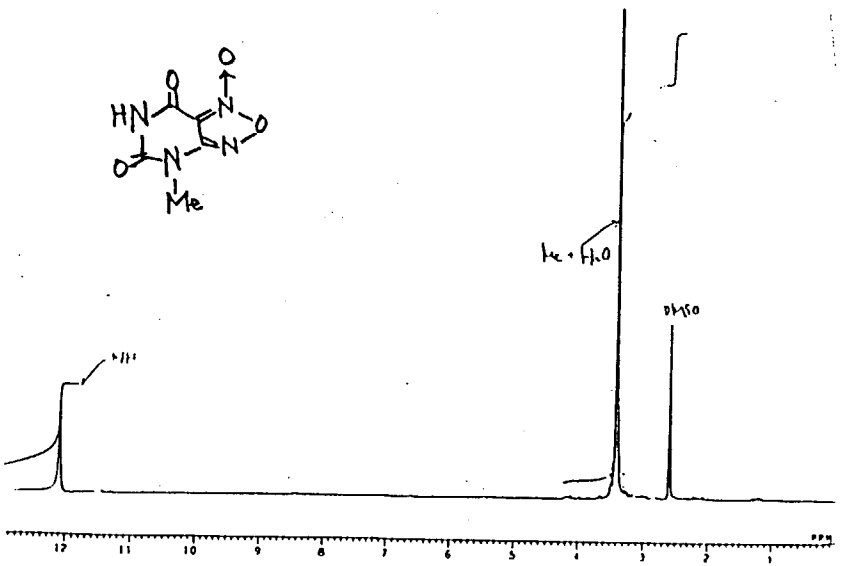
理論値 H-2.19 % C-32.62 % N-30.43 %

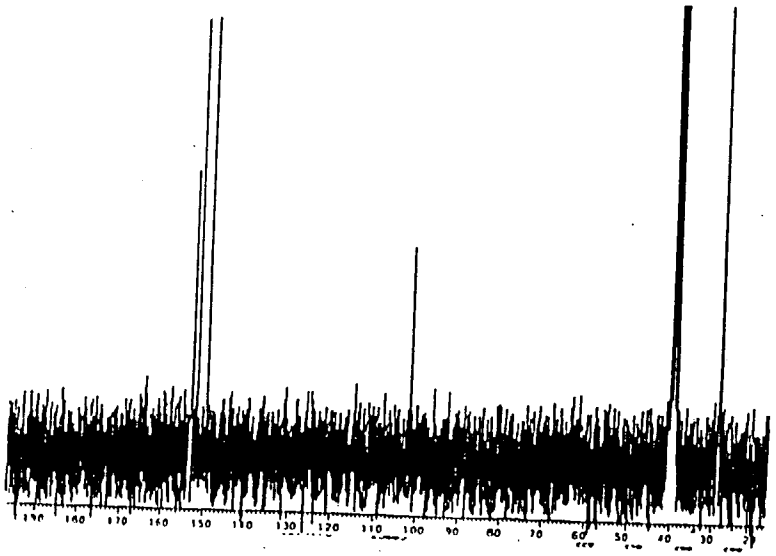
1995年7月12日分析 担当者

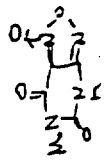


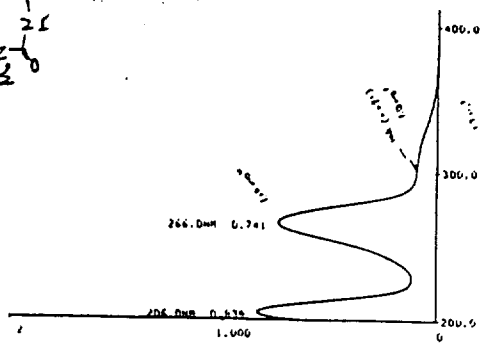


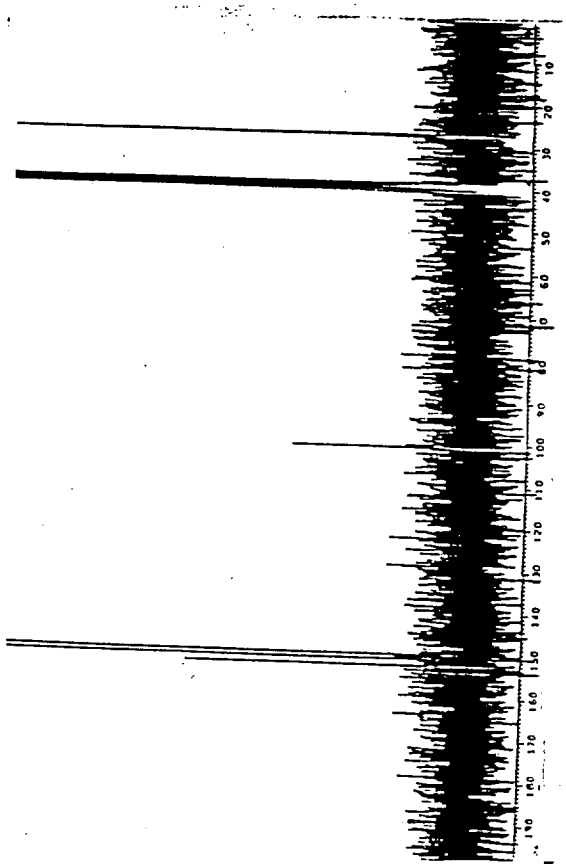


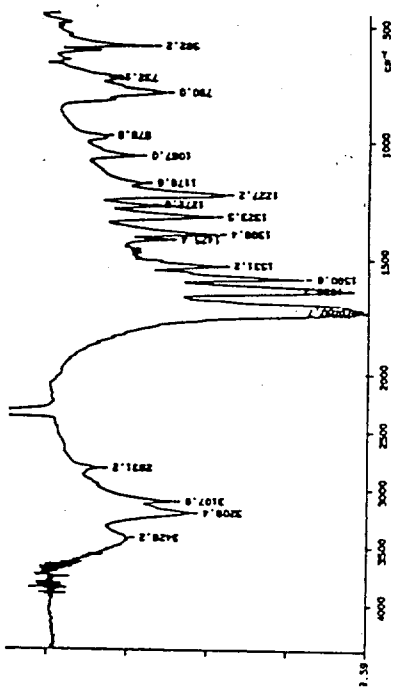


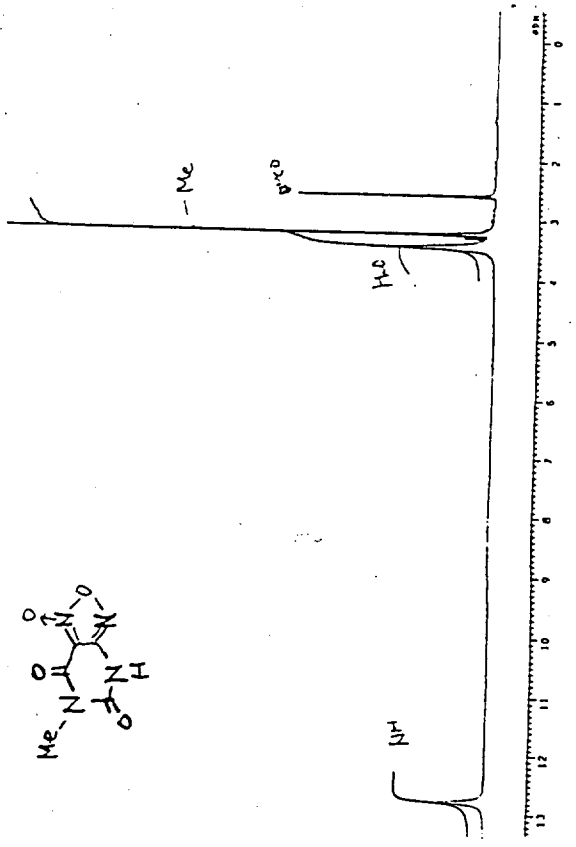


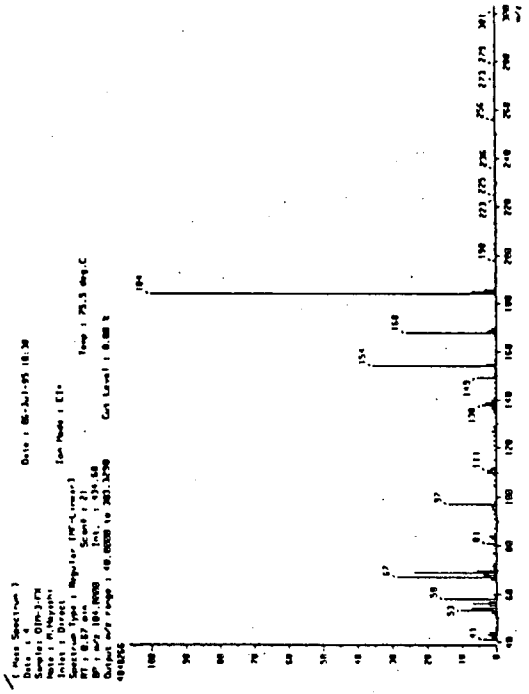


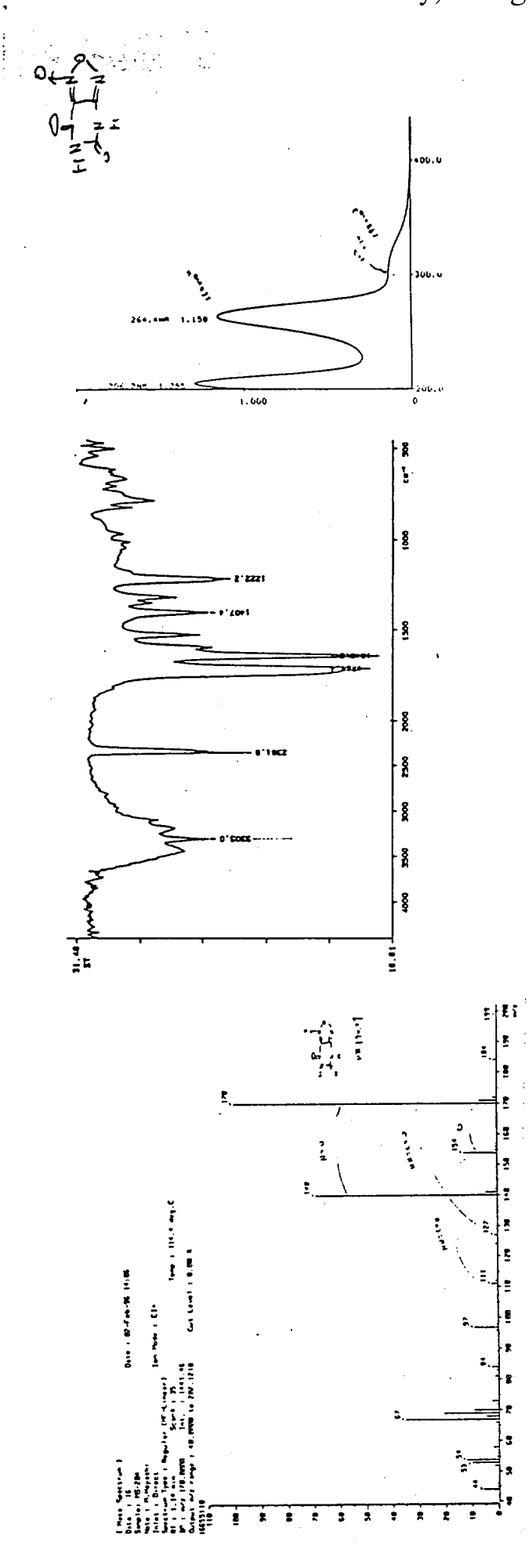


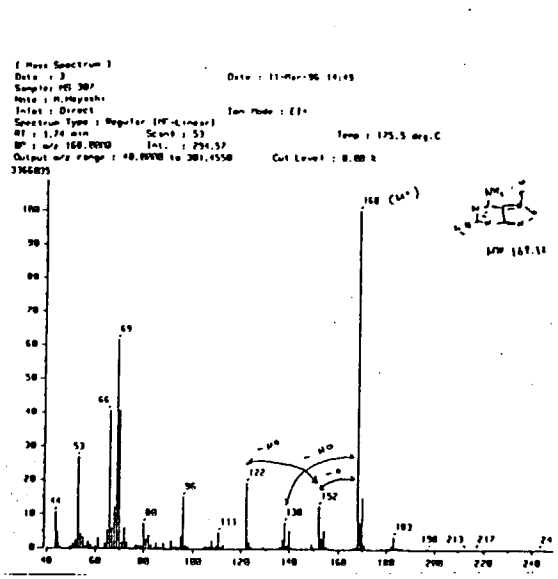


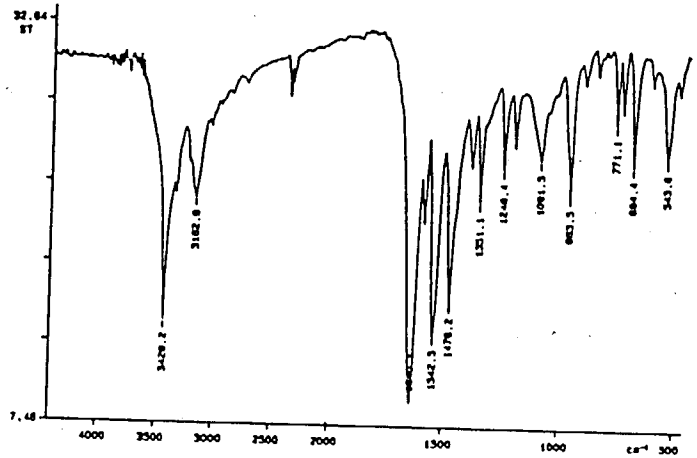


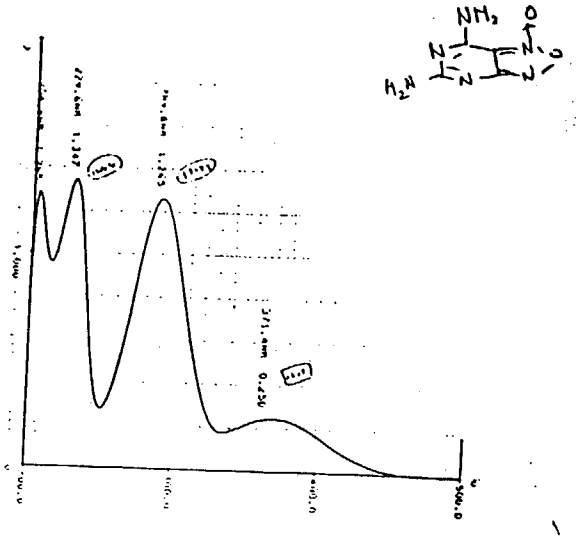


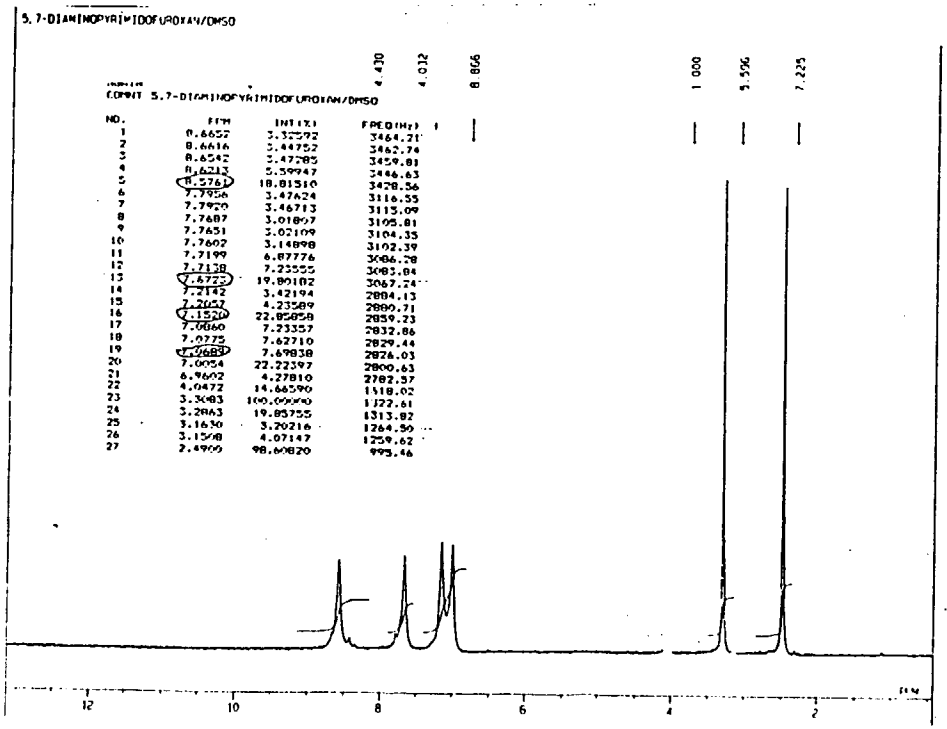


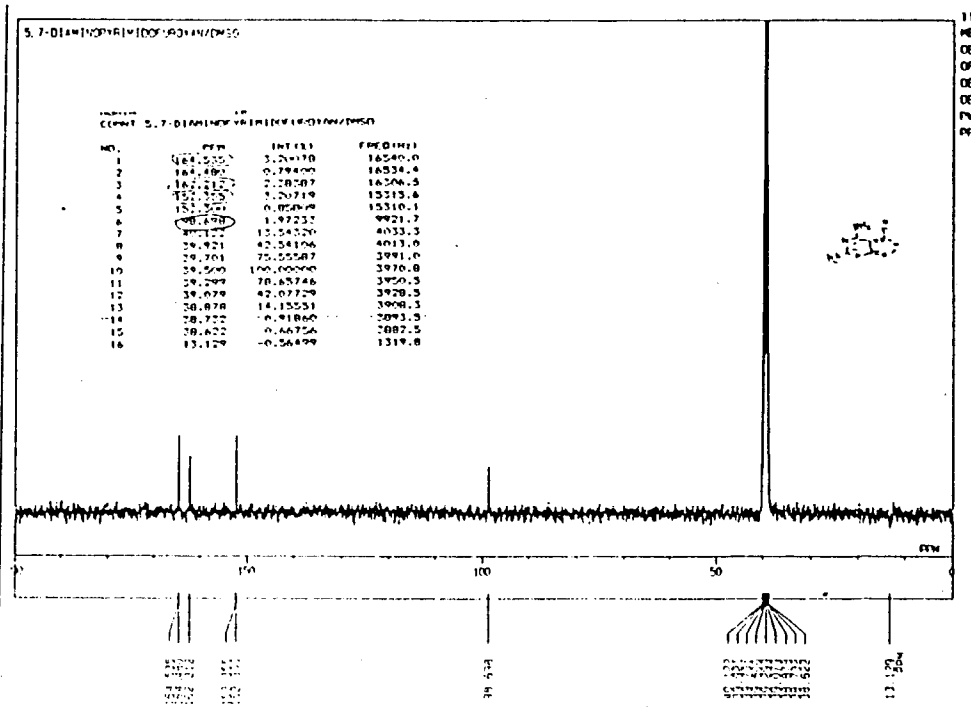


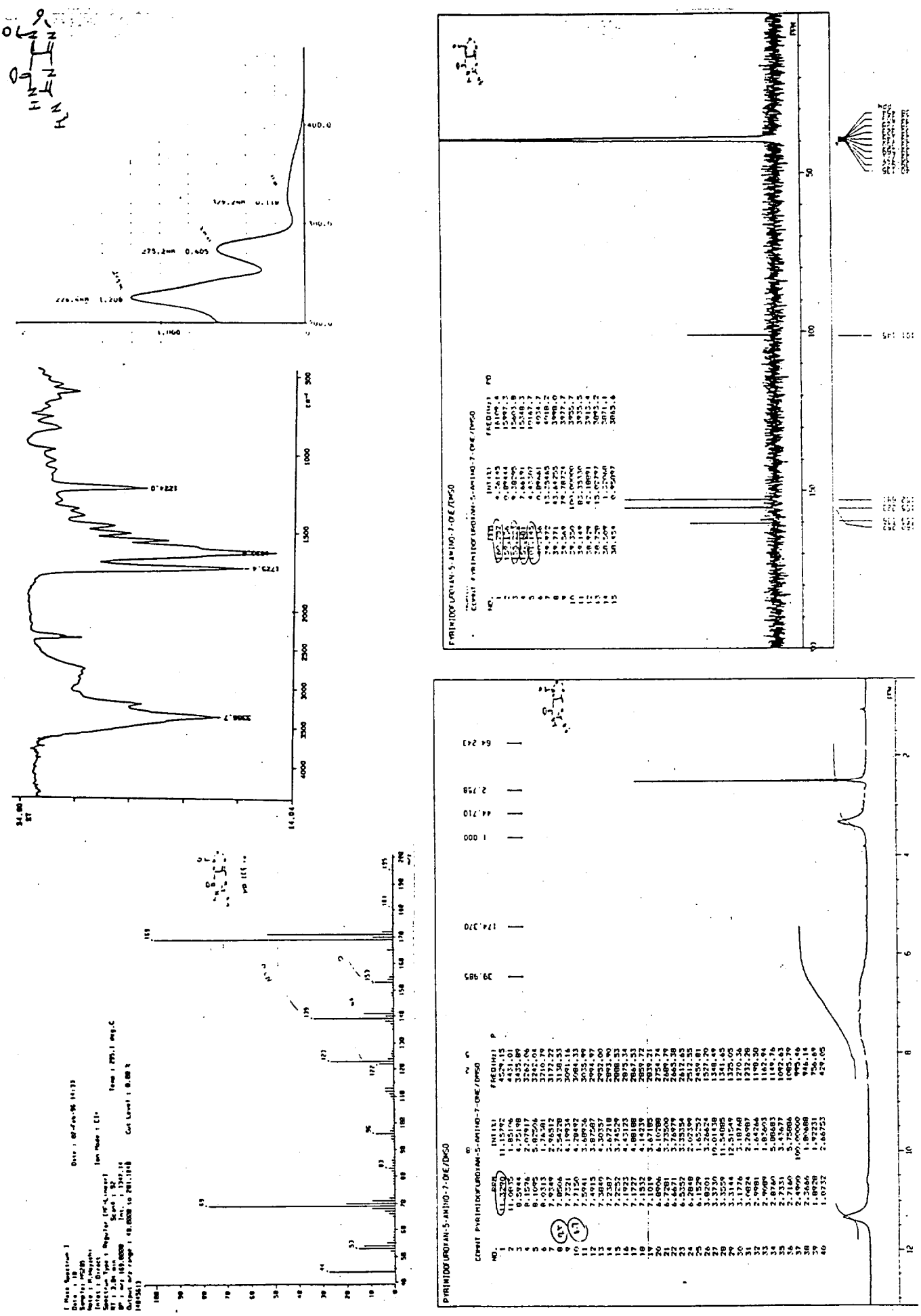


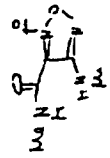


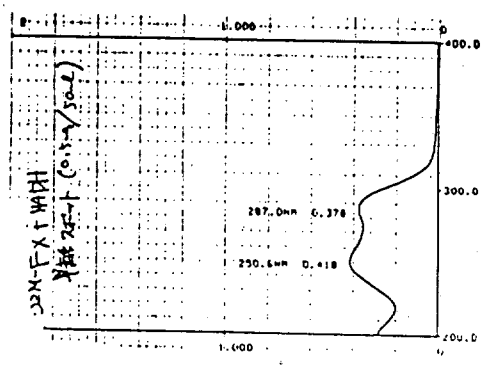


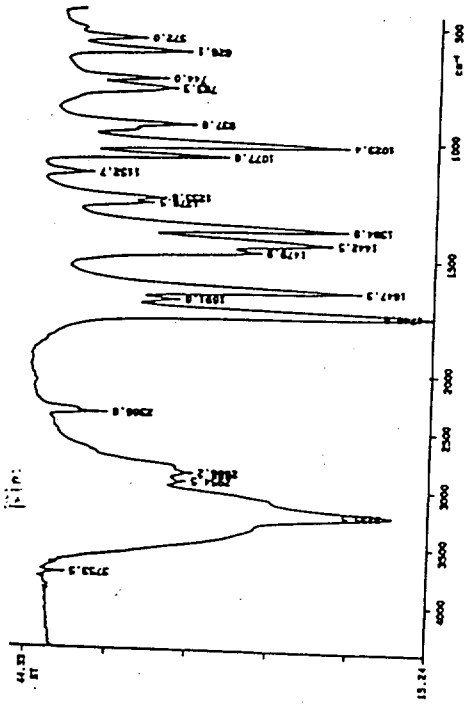


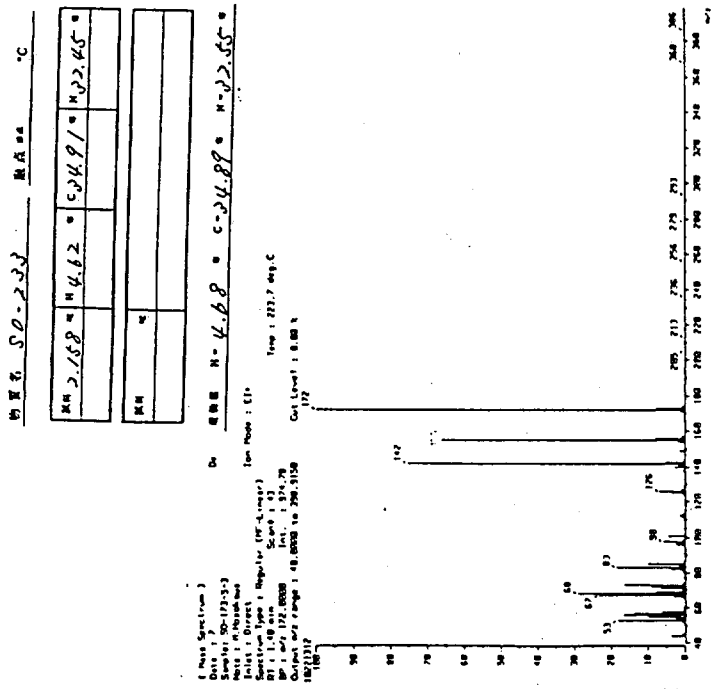


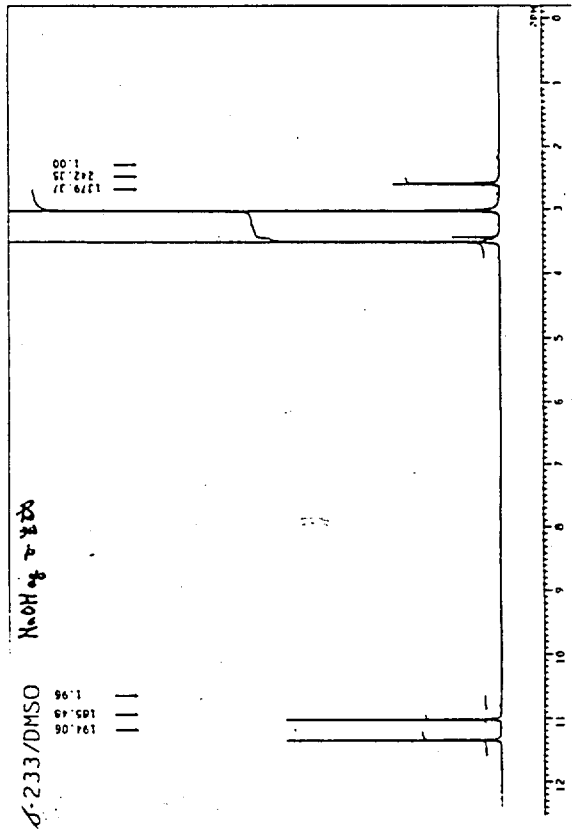








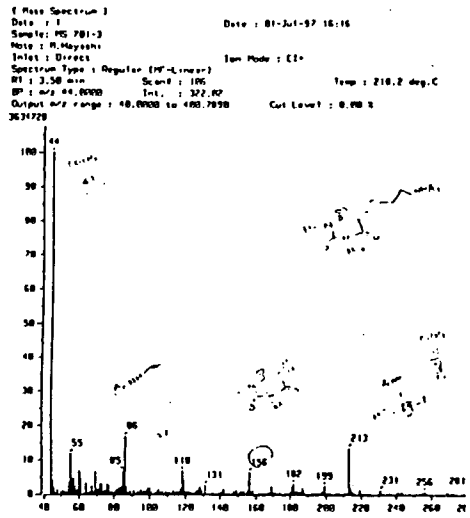


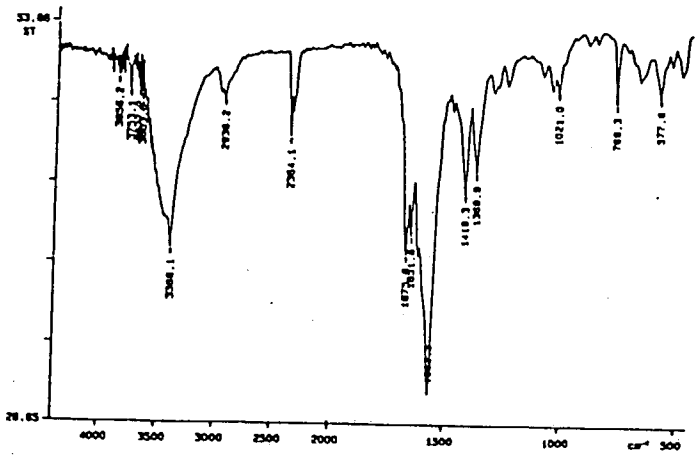


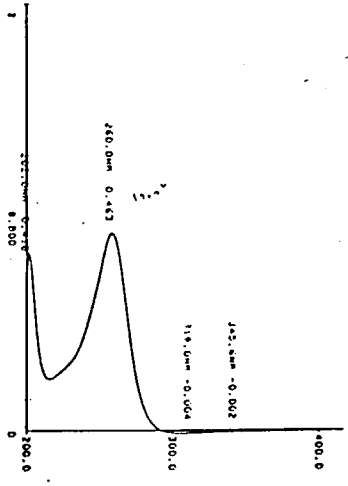
物質名 MS425-3-1 融点 °C

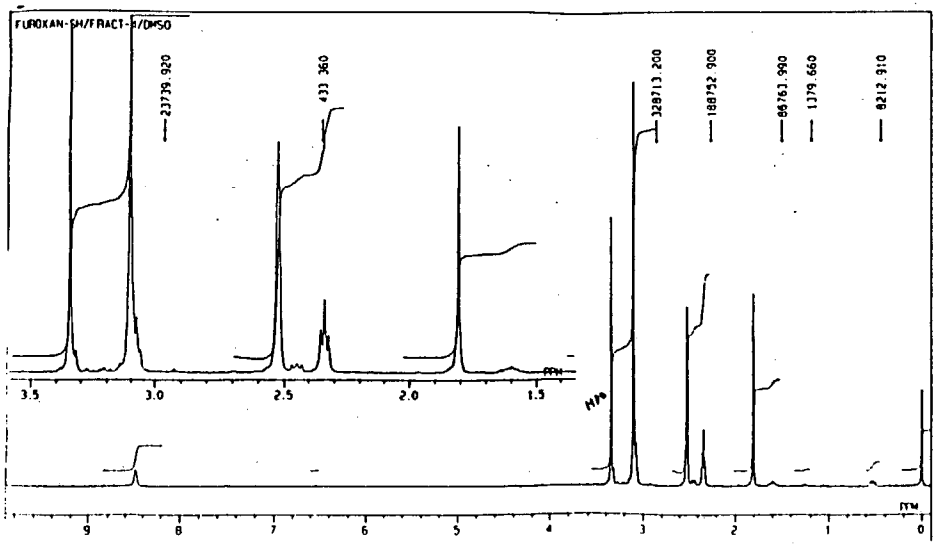
計算 C2H4N4O4S	H 4.49 %	C 32.44 %	N 12.65 %
実測	H 4.49 %	C 32.45 %	N 12.65 %

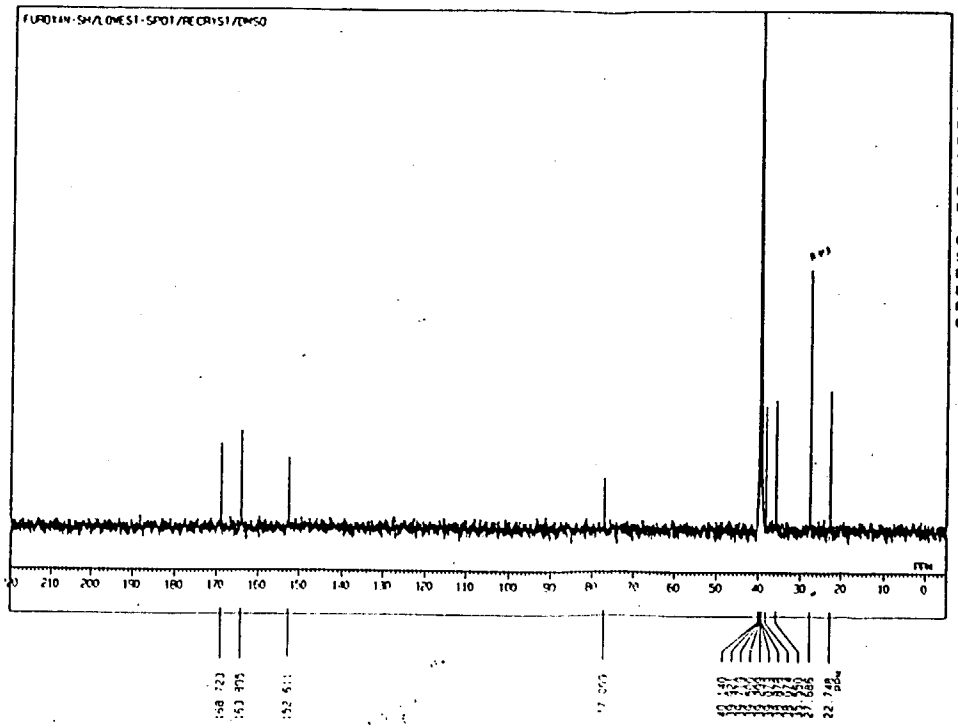
(6a)





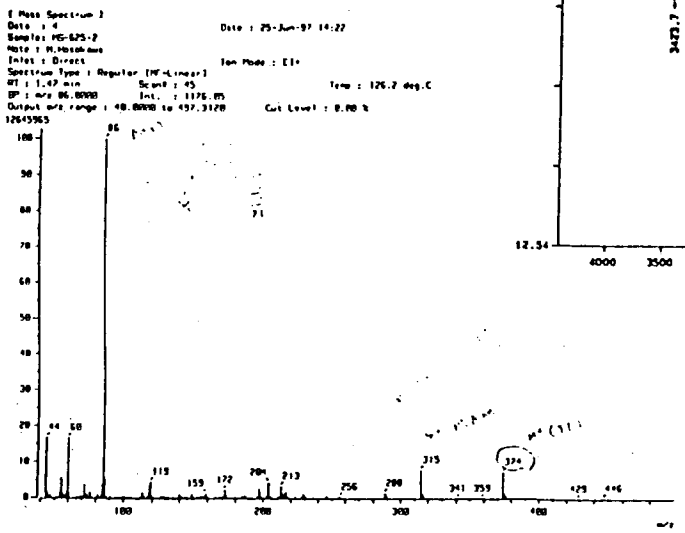


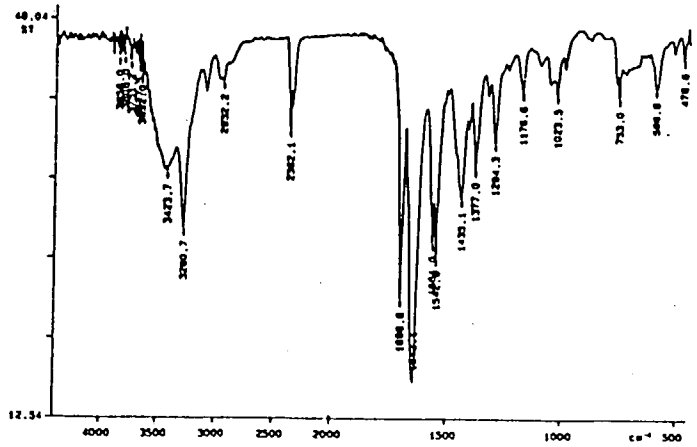




物質名 MS625-2 融点 mp °C

MW 374.36	H 5.92 %	C 44.74 %	N 14.97 %





[Elemental Composition]
Data : 1
Date : 25-Jun-97 17:05
Sample: MS-625-2
Note : M.Hasegawa
Inlet : Direct
Ion Mode : EI+
RT : 7.10 min
Scan# : 46
Elements : C 14/0, H 22/0, O 4/1, N 4/1, S 2/0
Mass Tolerance : 10ppm, 5mmu if m/z < 500, 20mmu if m/z > 2000
Unsaturation (U.S.) : -0.5 - 20.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
374.1079	27.9	-0.9 / -0.3	8.0	C 14 H 22 O 4 N 4 S 2