

Supplementary Material

Synthesis of novel pyrroloazepinones by Schmidt expansions of 6-indolones

Carmen Gámez-Gómez^a, Roberto Martínez^b, Perla Niño-Moreno^a, José G. Ávila-Zárraga^c, Manuel García-Gamboa^a, Ana Cristina Miranda-Torres^a, Ángel J. Alonso-Castro^d, Marco M. González-Chávez^{*a}

^a*Facultad de Ciencias Químicas. Universidad Autónoma de San Luis Potosí; Av. Dr. Manuel Nava No.6 Zona Universitaria, San Luis Potosí, S.L.P. 78210, México.*

^b*Instituto de Química, ^cFacultad de Química; Universidad Nacional Autónoma de México, Circuito Exterior, Ciudad Universitaria, Coyoacán, Ciudad de México 04510 México.*

^d*Departamento de Farmacia, División de Ciencias Naturales y Exactas, Universidad de Guanajuato, Noria Alta S/N, Guanajuato, Guanajuato 36050, México.*

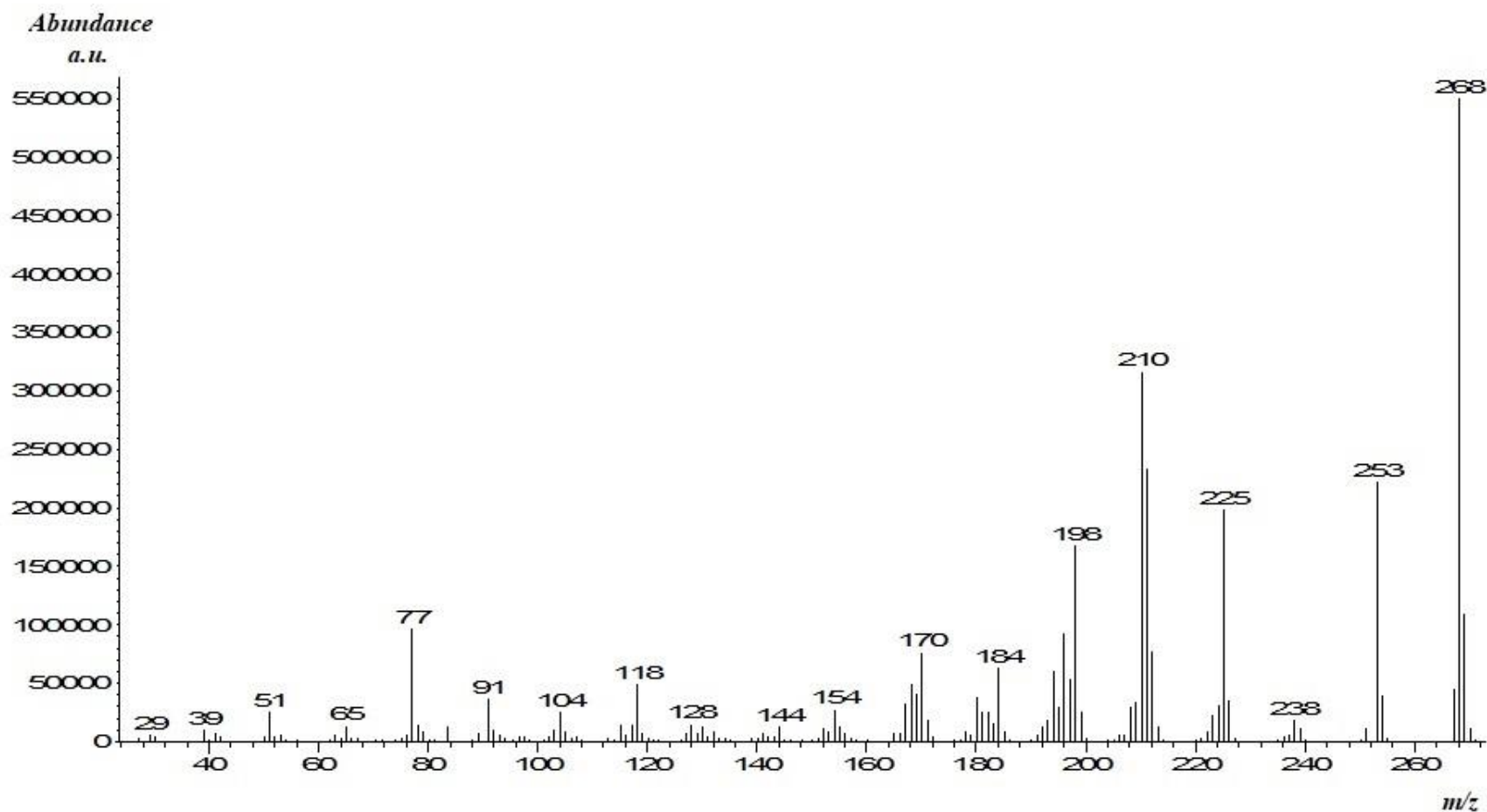
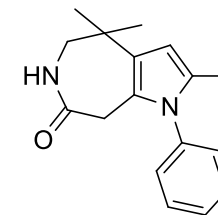
Email: gcomm@uaslp.mx

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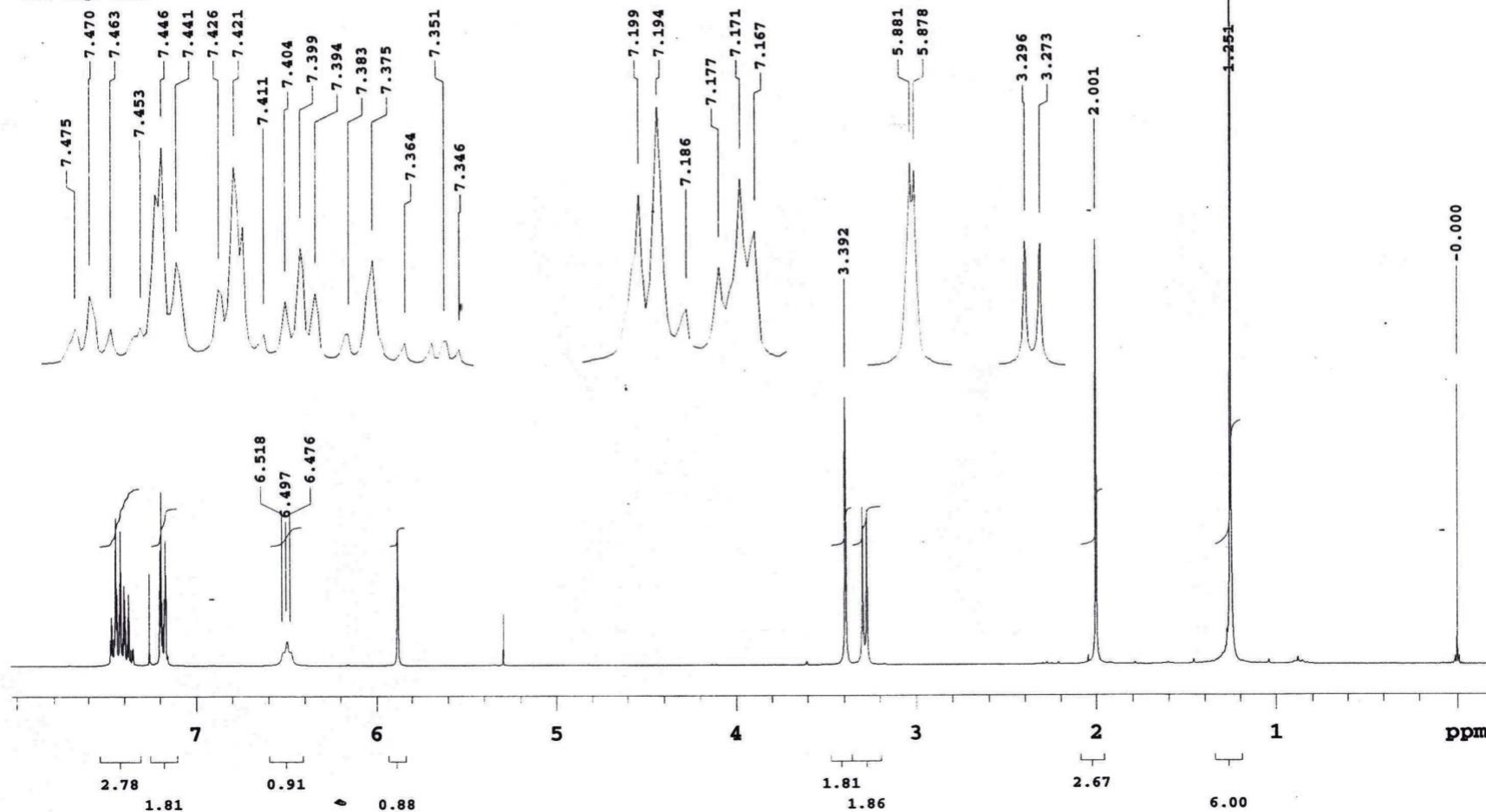
Compound 11a. 2,4,4-Trimethyl-1-phenyl-4,5,6,8-tetrahydropyrrolo[2,3-d]azepin-7(1H)-one

MS



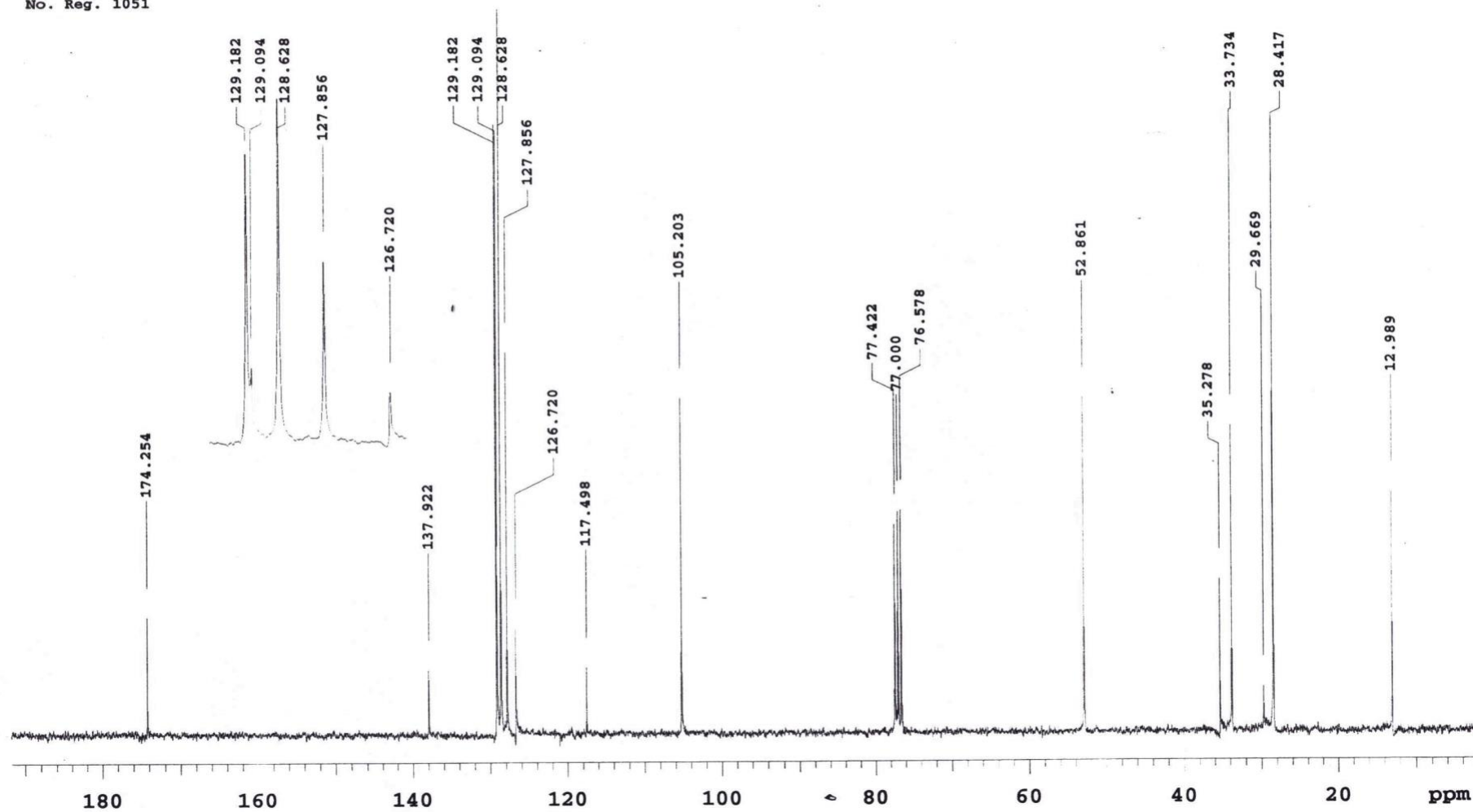
¹H-NMR

UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E. Reyes
Clave: P.A-1
Disolvente: CDC13
Hidrogeno-1
Unity-300 MHz Varian (D)
22-04-09
No. Reg. 1051



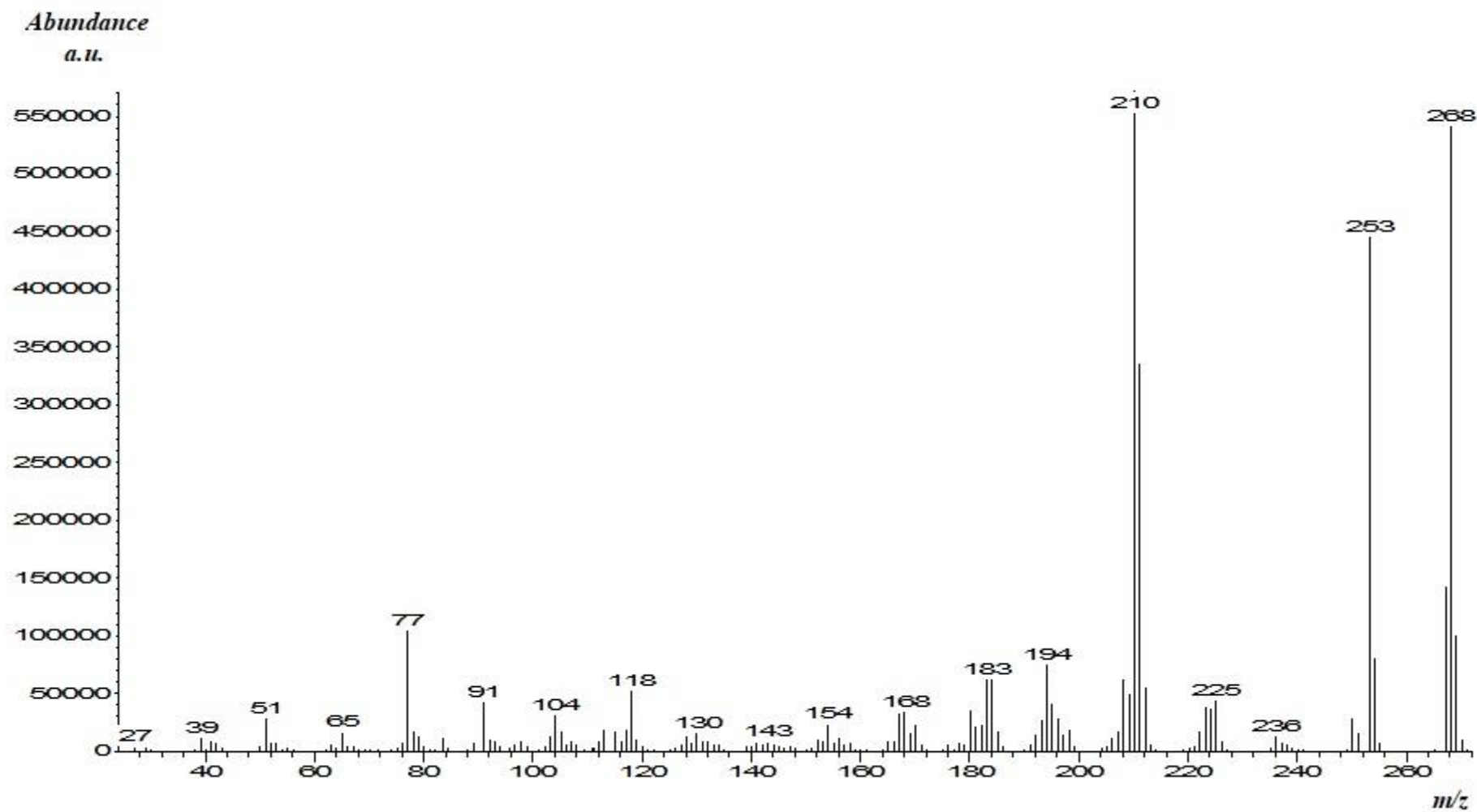
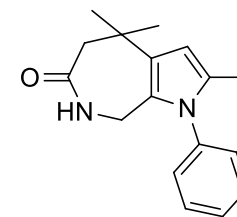
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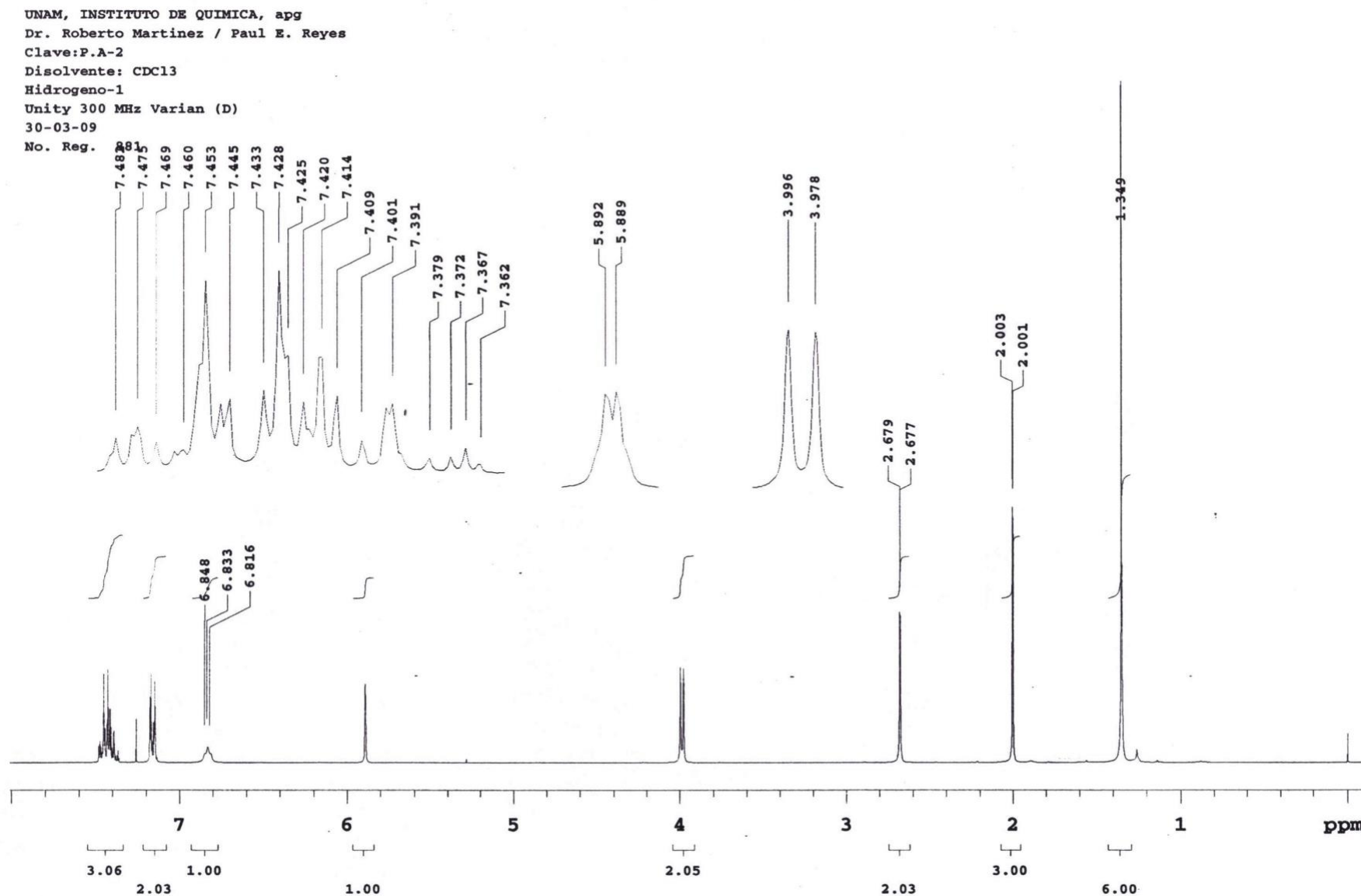
UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E, Reyes
Clave: P.A-1
Disolvente: CDCl₃
Carbpono-13
Unity 75 MHz, Varian (D)
22-04-09
No. Reg. 1051



Compound 12a. 2,4,4-Trimethyl-1-phenyl-4,5,7,8-tetrahydropyrrolo[2,3-*c*]-6(1*H*)-one

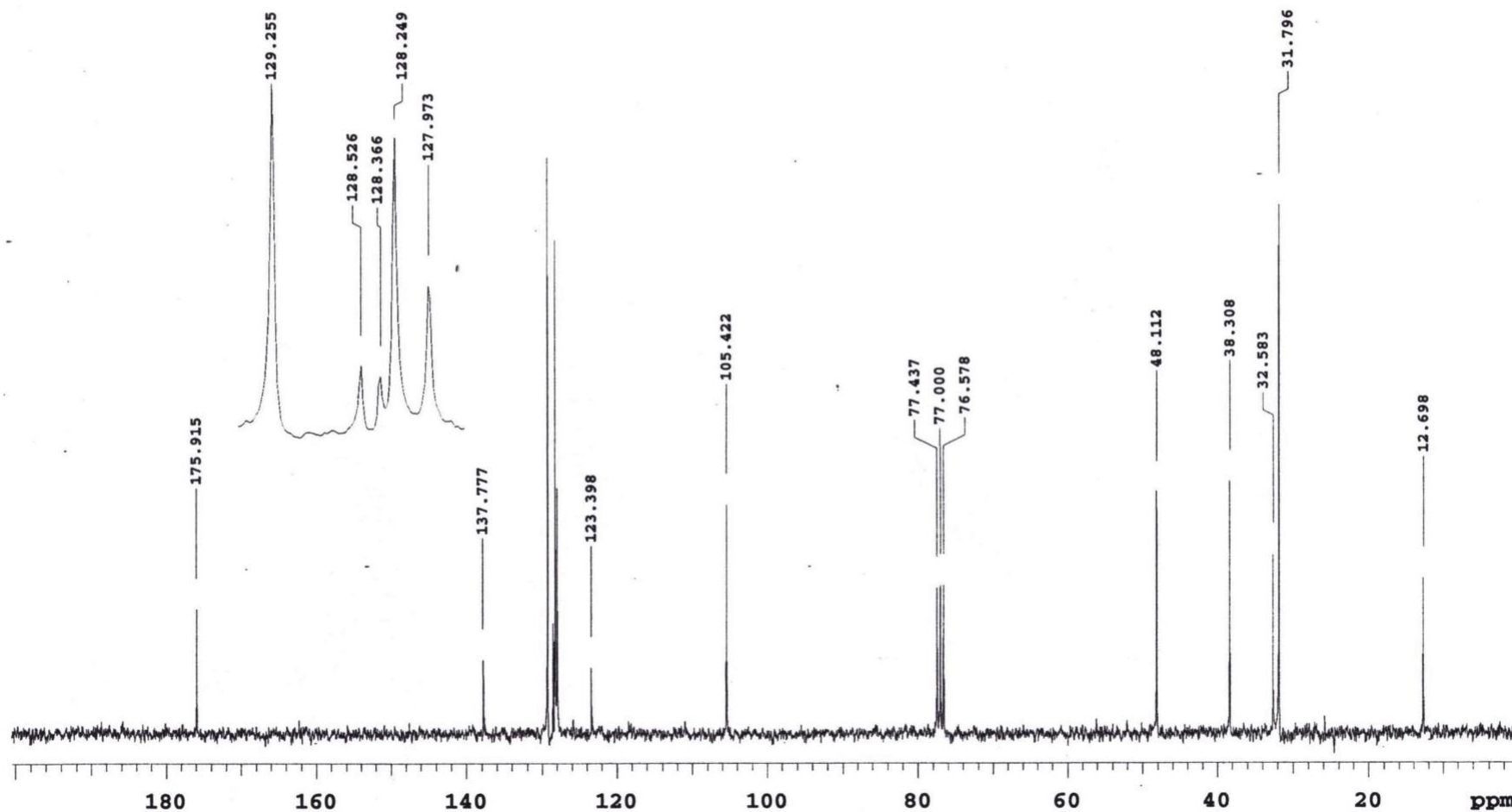
MS



^1H -NMR

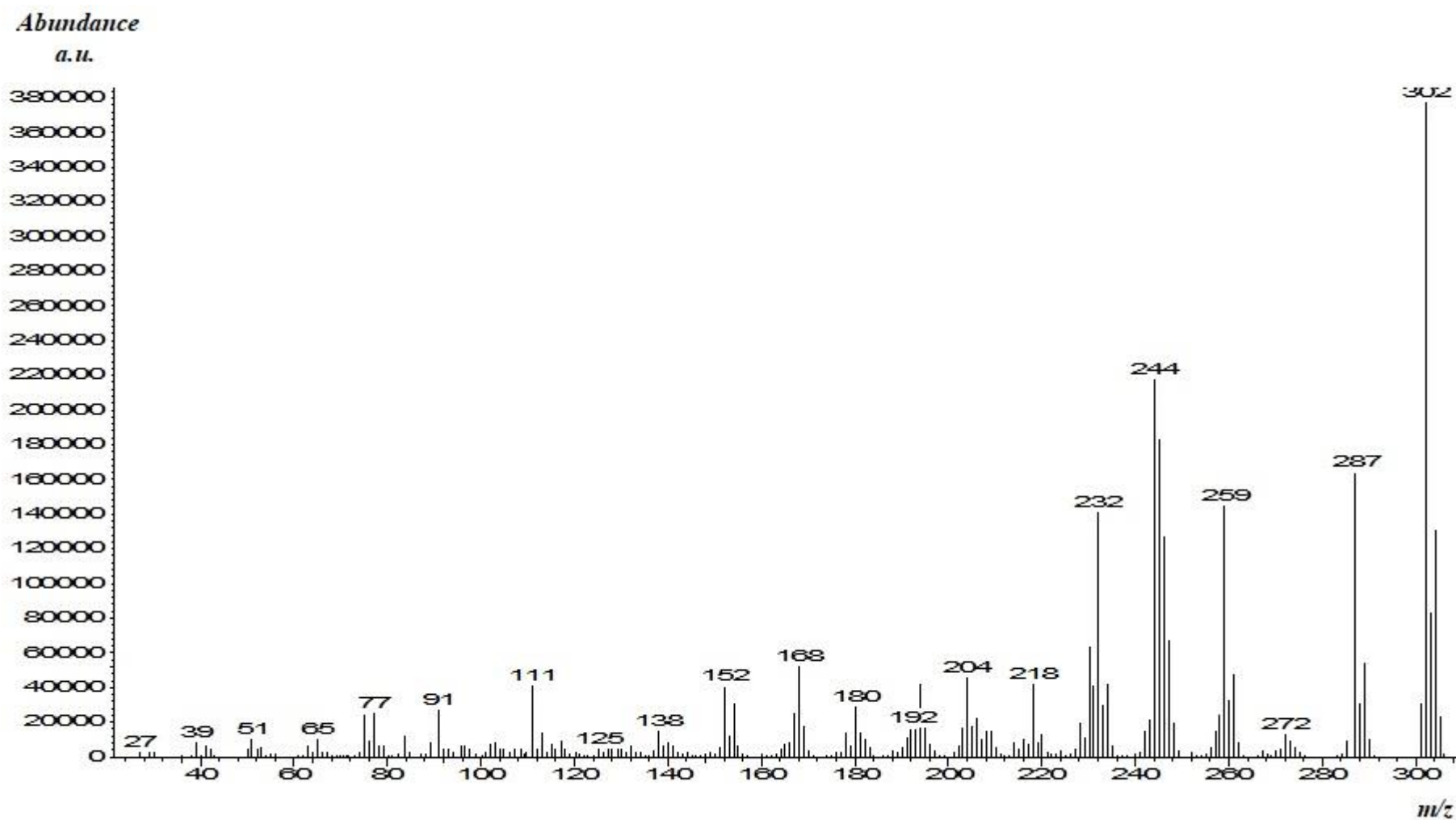
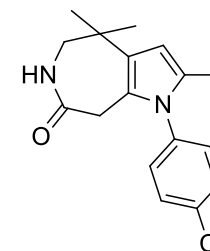
¹³C-NMR

UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E. Reyes
Clave: P.A-2
Disolvente: CDC13
Carbono-13
Unity 75 MHz Varian (D)
30-03-09
No. Reg. 881



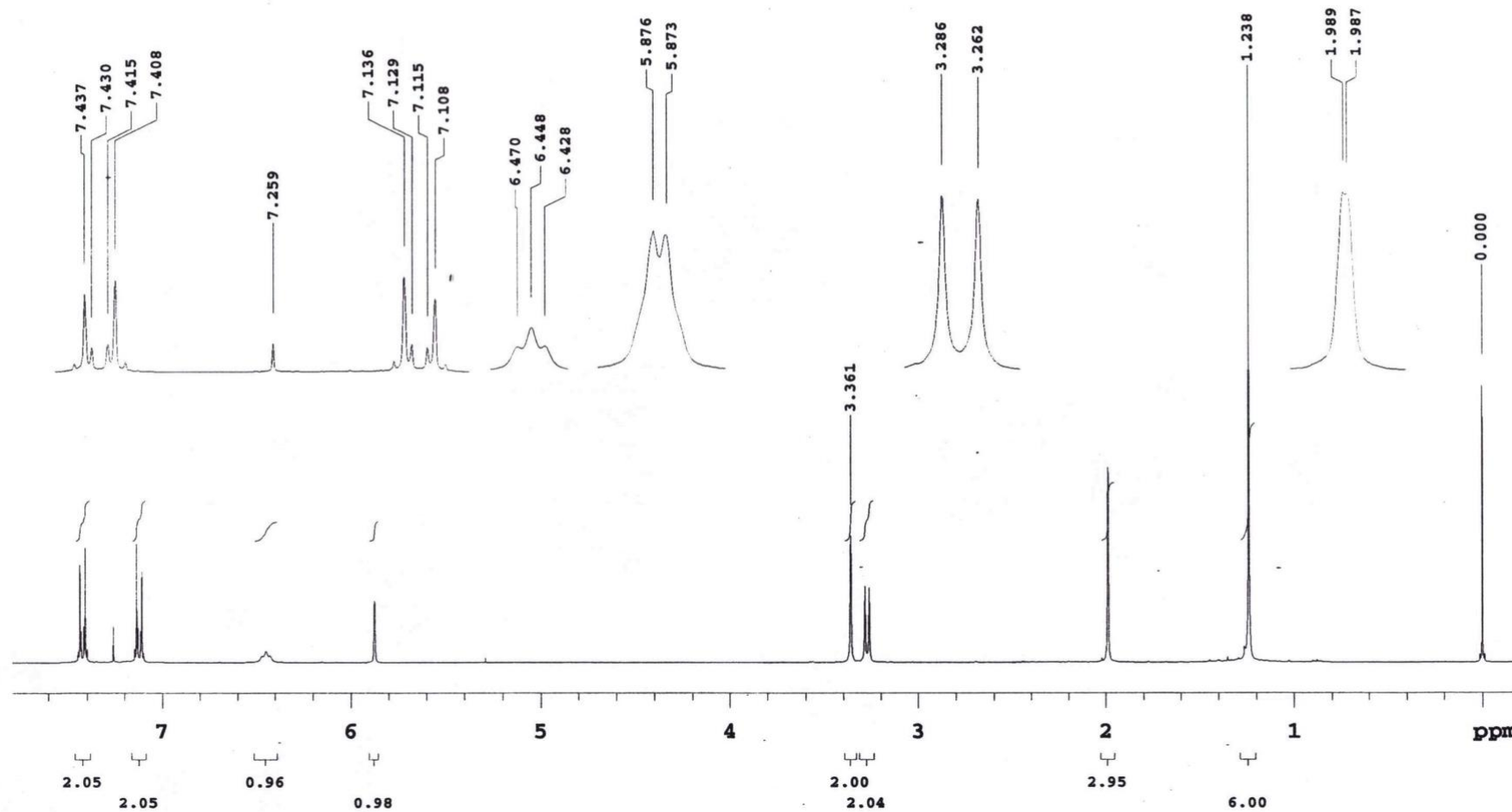
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MS



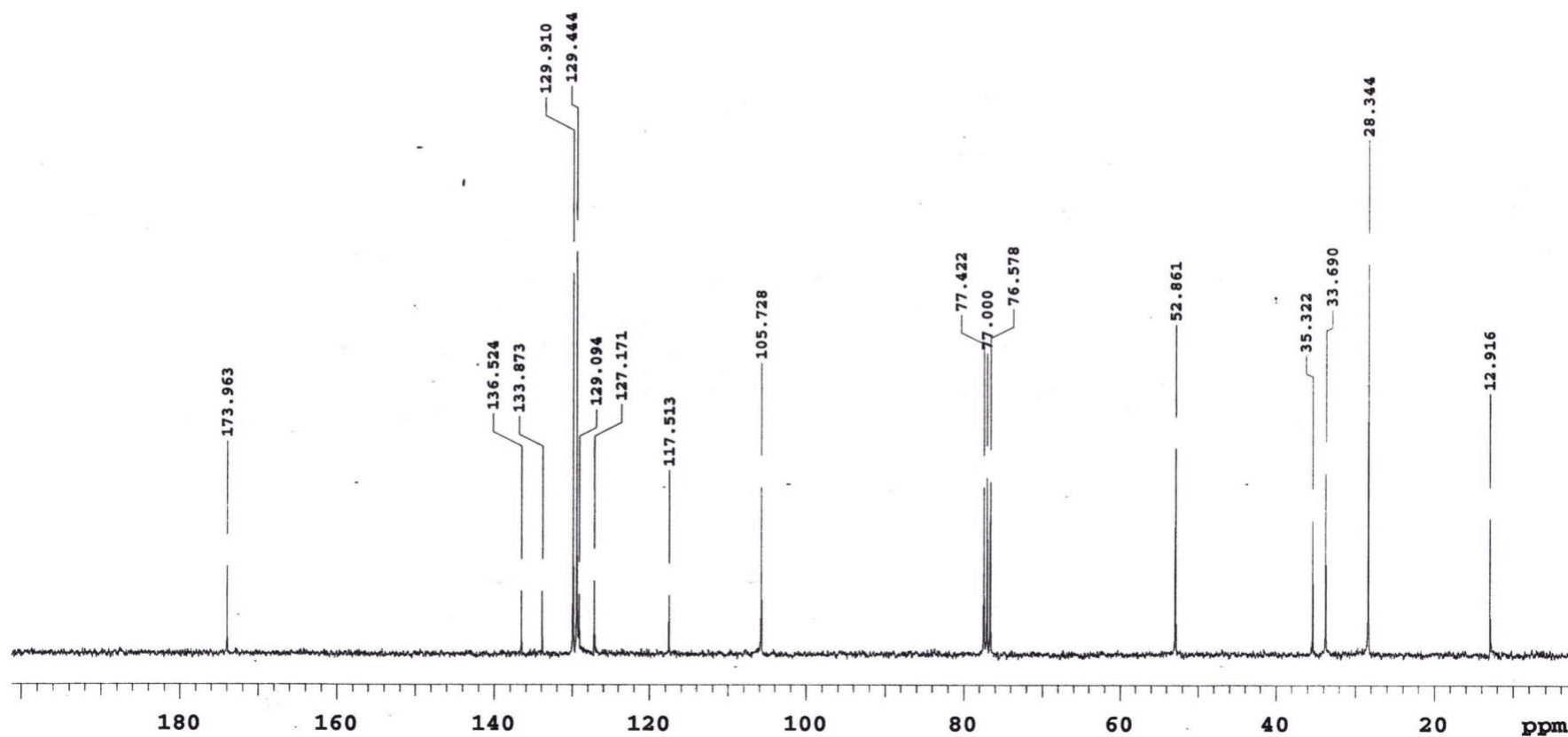
^1H -NMR

INSTITUTO DE QUIMICA, UNAM/ E. Huerta
Dr. R. Martinez/ Paul E. R.
Clave: P.C-1
Disolvente: CDCl_3
Hidrogeno-1
Varian Unity 300 MHz (D)
13-05-09
No. de registro: 1106

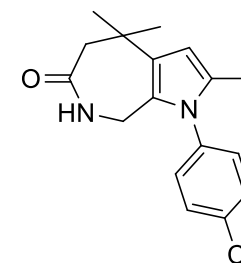


^{13}C -NMR

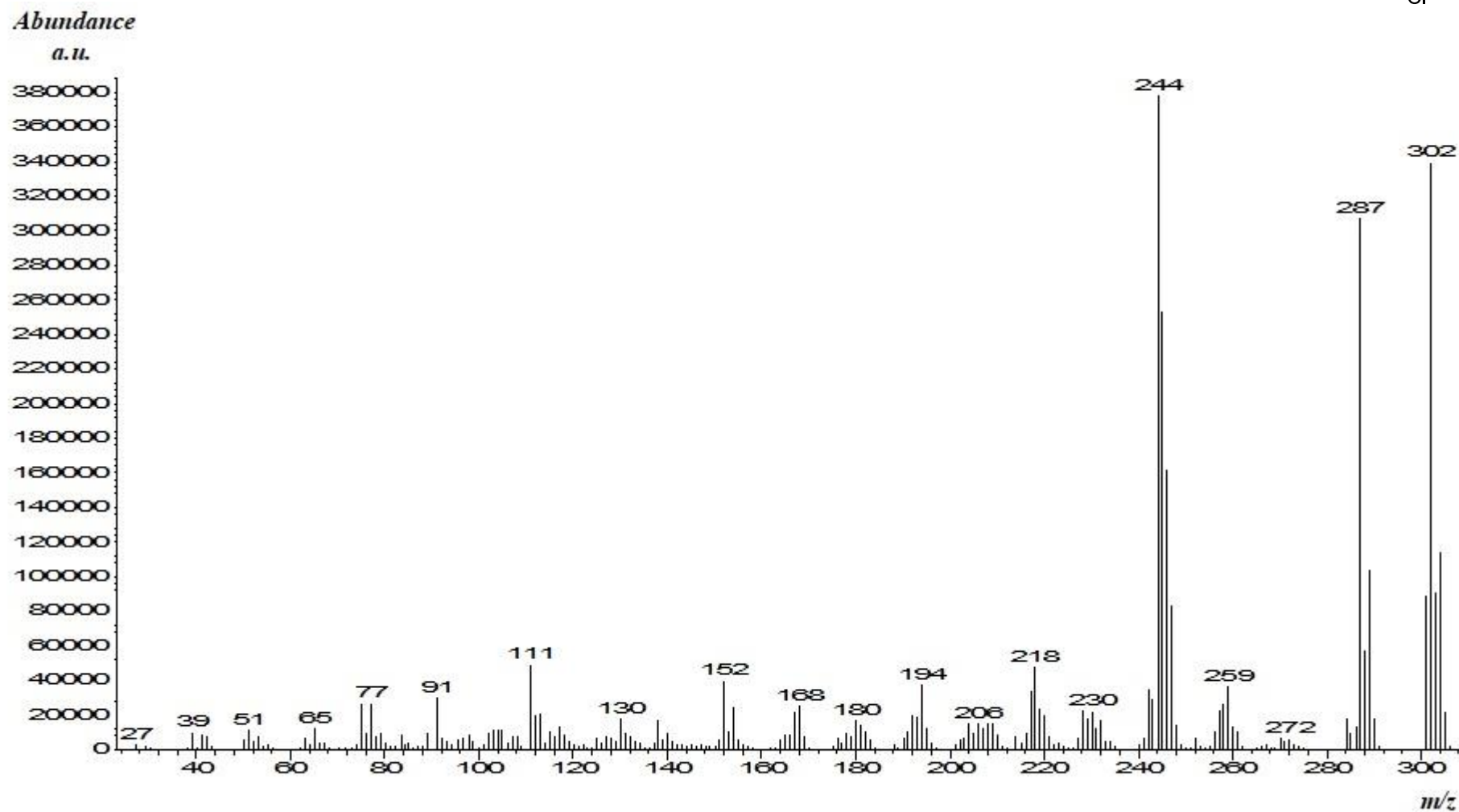
UNAM, INSTITUTO DE QUIMICA, E. Huerta
Dr. Roberto Martinez / Paul E, Reyes
Clave: P.C-1
Disolvente: CDCl_3
Carbbono- 13
Unity 75 MHz, Varian (D)
13-05-09
No. Reg. 1106

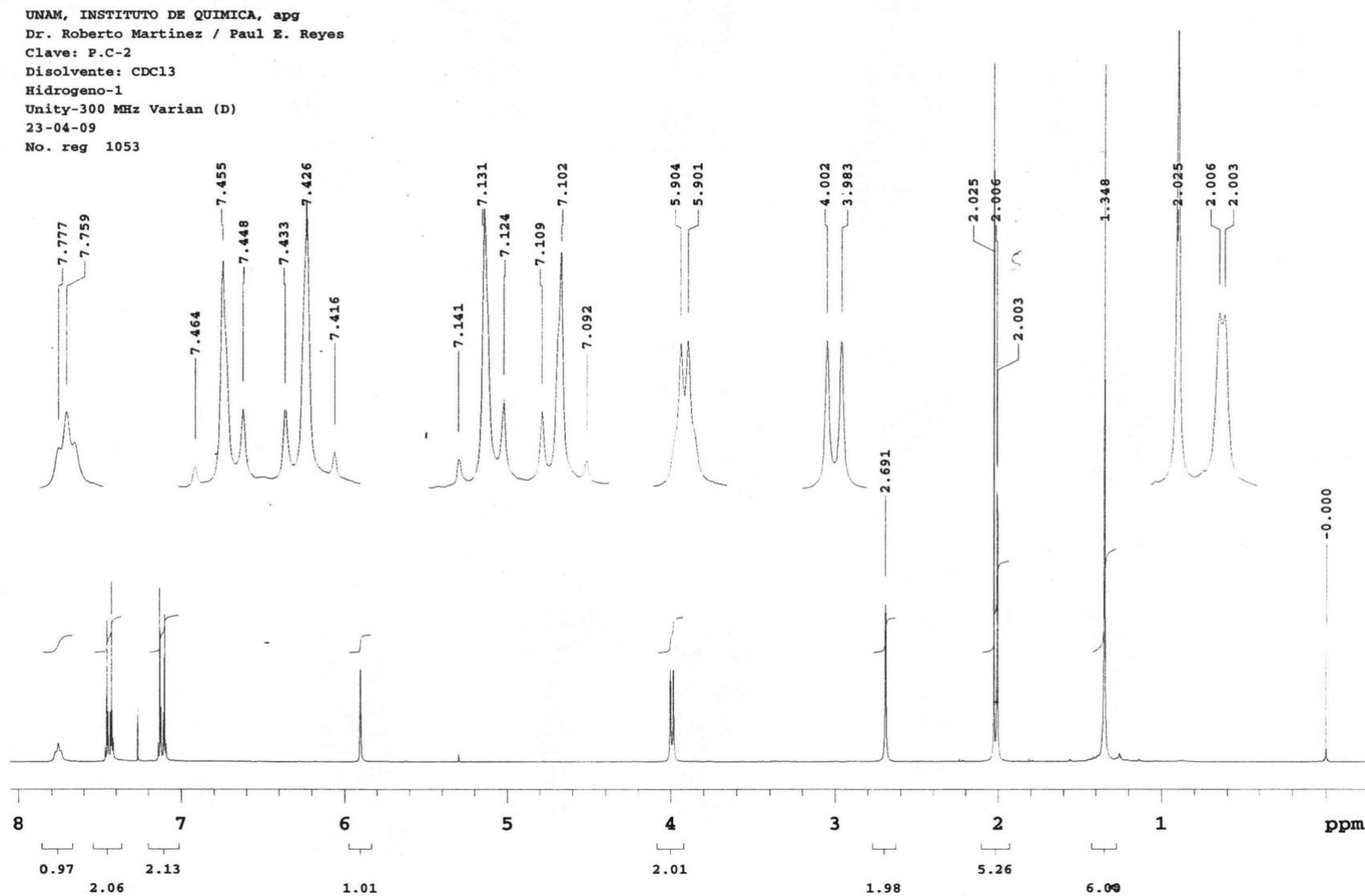


Compound 12b. 1-(4-Chlorophenyl)-2,4,4-trimethyl-4,5,7,8-tetrahydropyrrolo[2,3-c]azepin-6(1H)-one



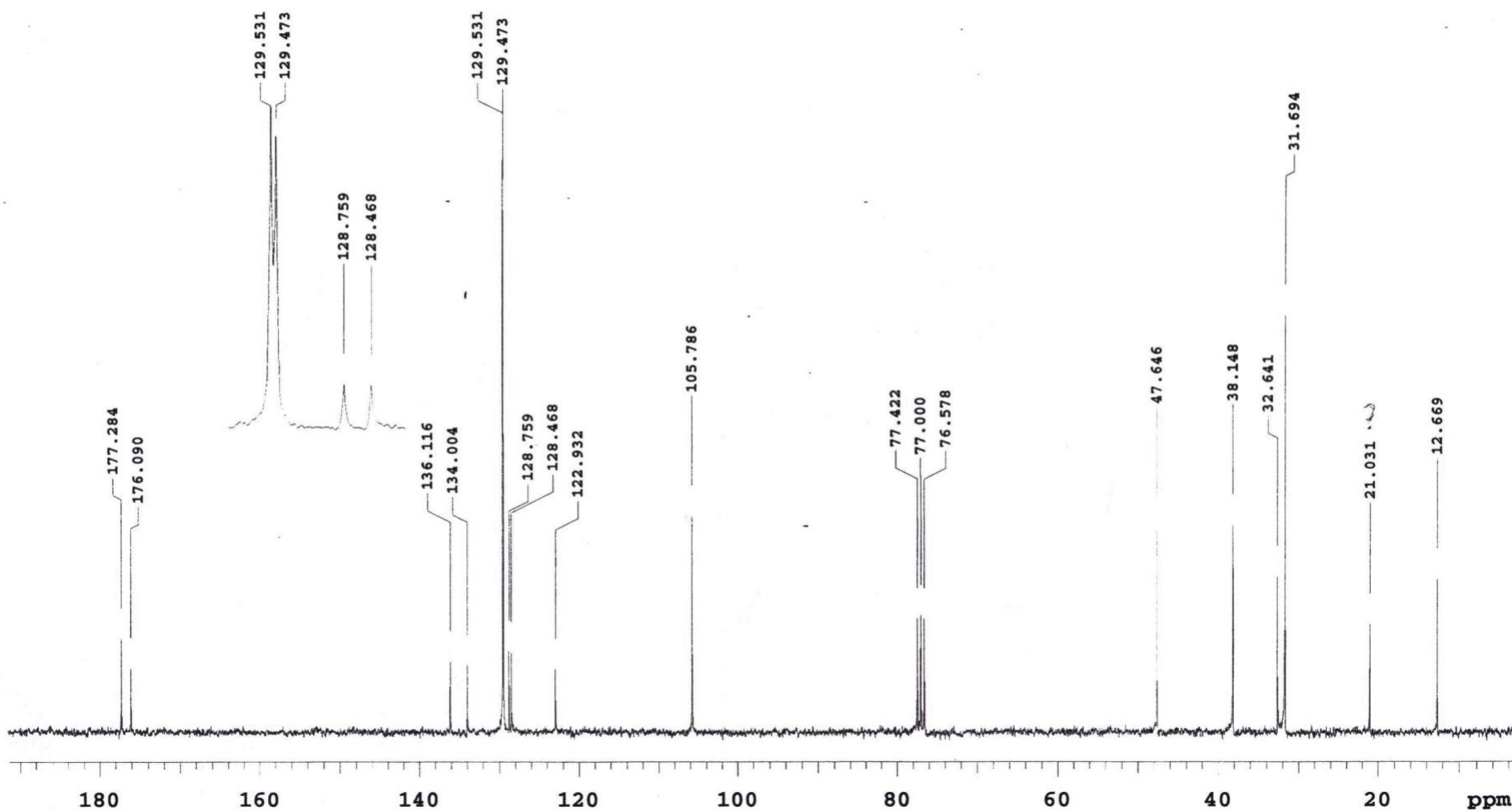
MS



^1H -NMR

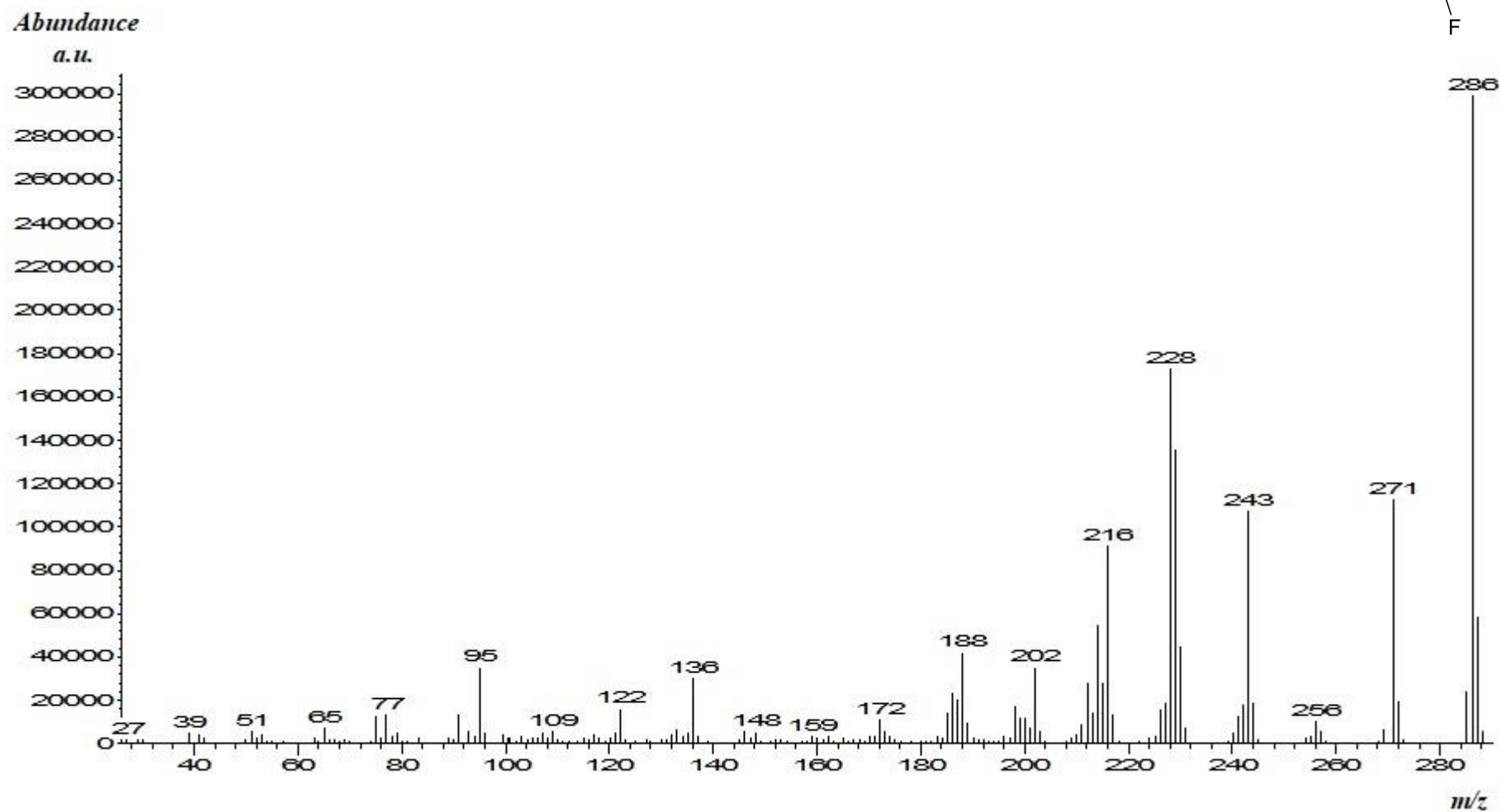
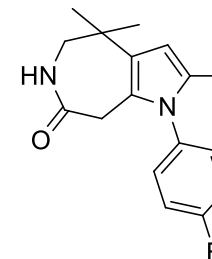
¹³C-NMR

UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E. Reyes
Clave: P.C-2
Disolvente: CDC13
Carbpono-13
Unity 75 MHz, Varian (D)
23-04-09
No. Reg. 1053



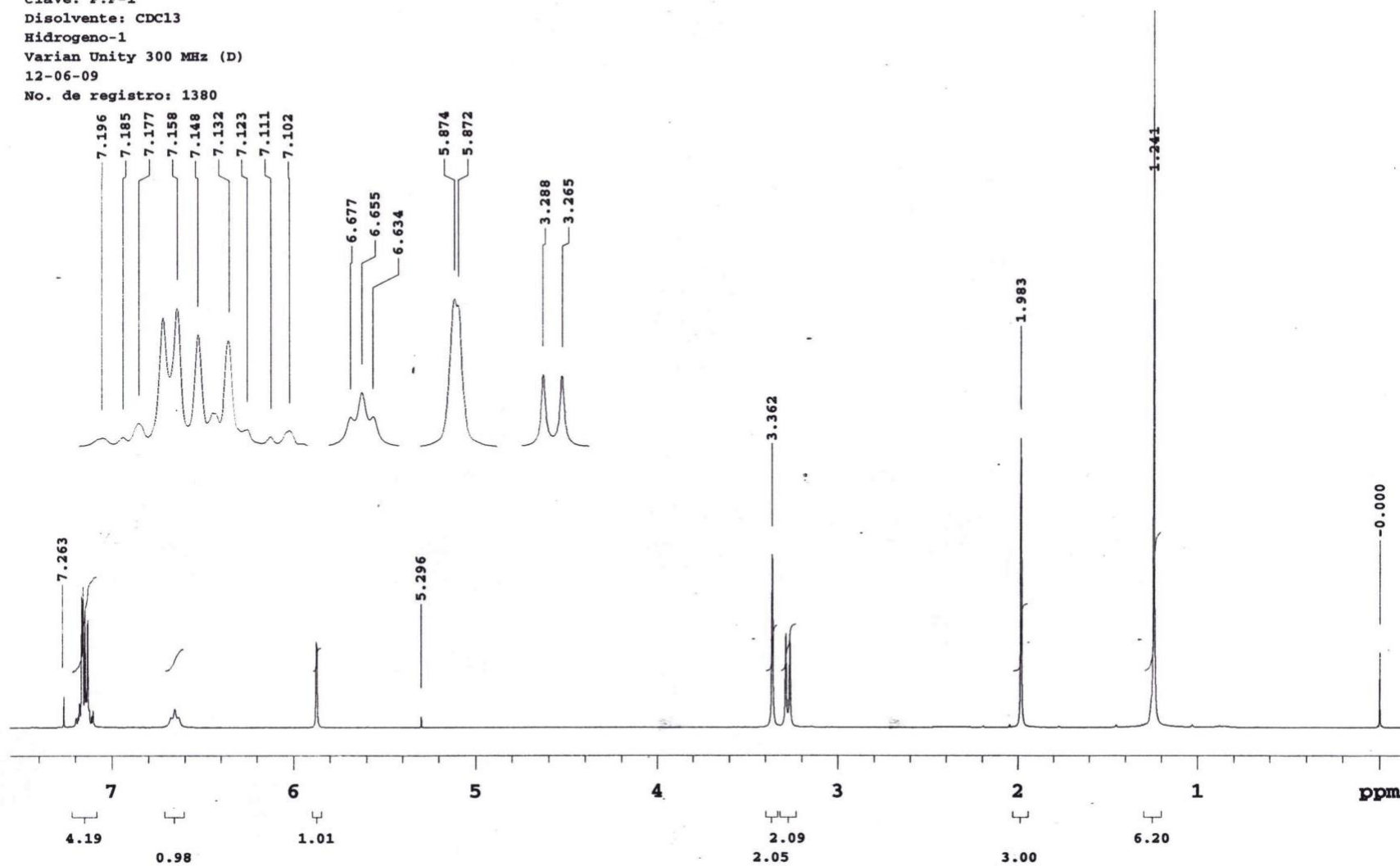
Compound 11c. 1-(4-Fluorophenyl)-2,4,4-trimethyl-4,5,6,8-tetrahydropyrrolo[2,3-d]azepin-7(1H)-one

MS



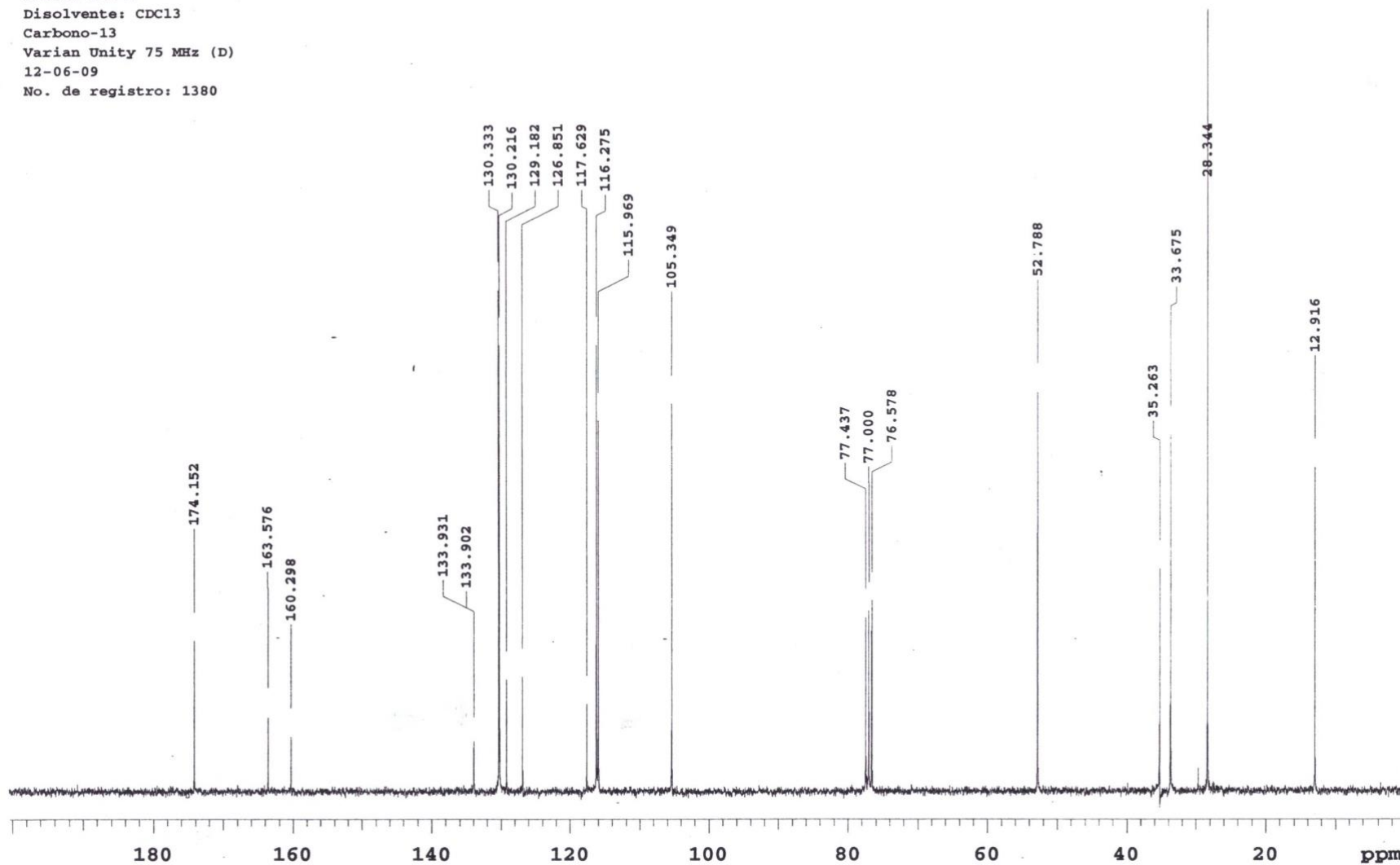
^1H -NMR

INSTITUTO DE QUIMICA, UNAM/ E. Huerta
Dr. R. Martínez/ Paul E. R.
Clave: P.F-1
Disolvente: CDCl_3
Hidrogeno-1
Varian Unity 300 MHz (D)
12-06-09
No. de registro: 1380



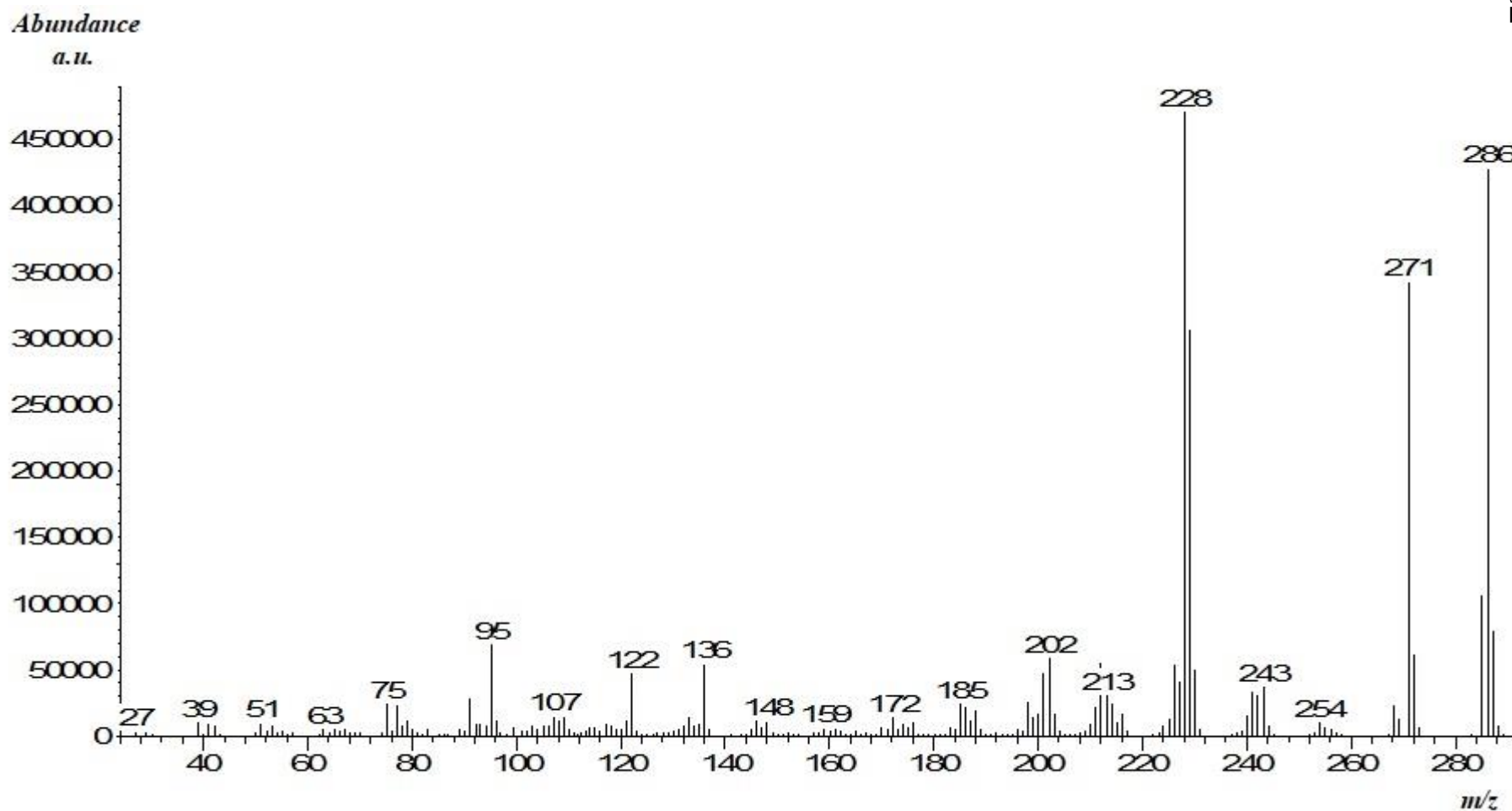
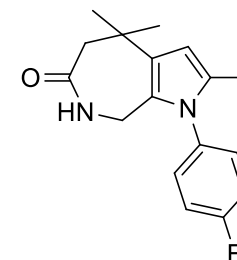
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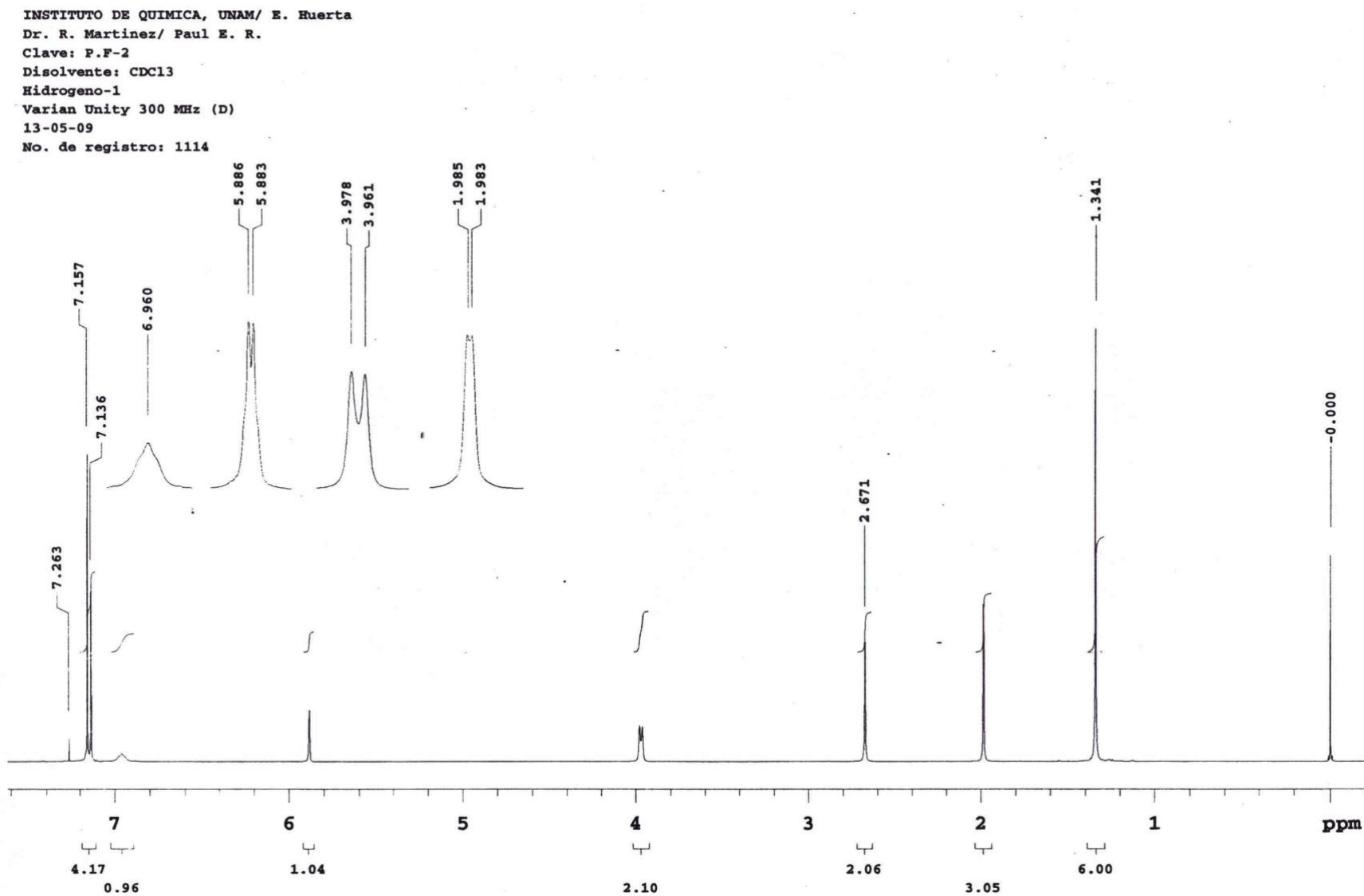
INSTITUTO DE QUIMICA, UNAM/ E. Huerta
Dr. R. Martinez/ Paul E. R.
Clave: P.F-1
Disolvente: CDCl₃
Carbono-13
Varian Unity 75 MHz (D)
12-06-09
No. de registro: 1380



Compound 12c. 1-(4-Fluorophenyl)-2,4,4-trimethyl-4,5,7,8-tetrahydropyrrolo[2,3-c]azepin-6(1H)-one

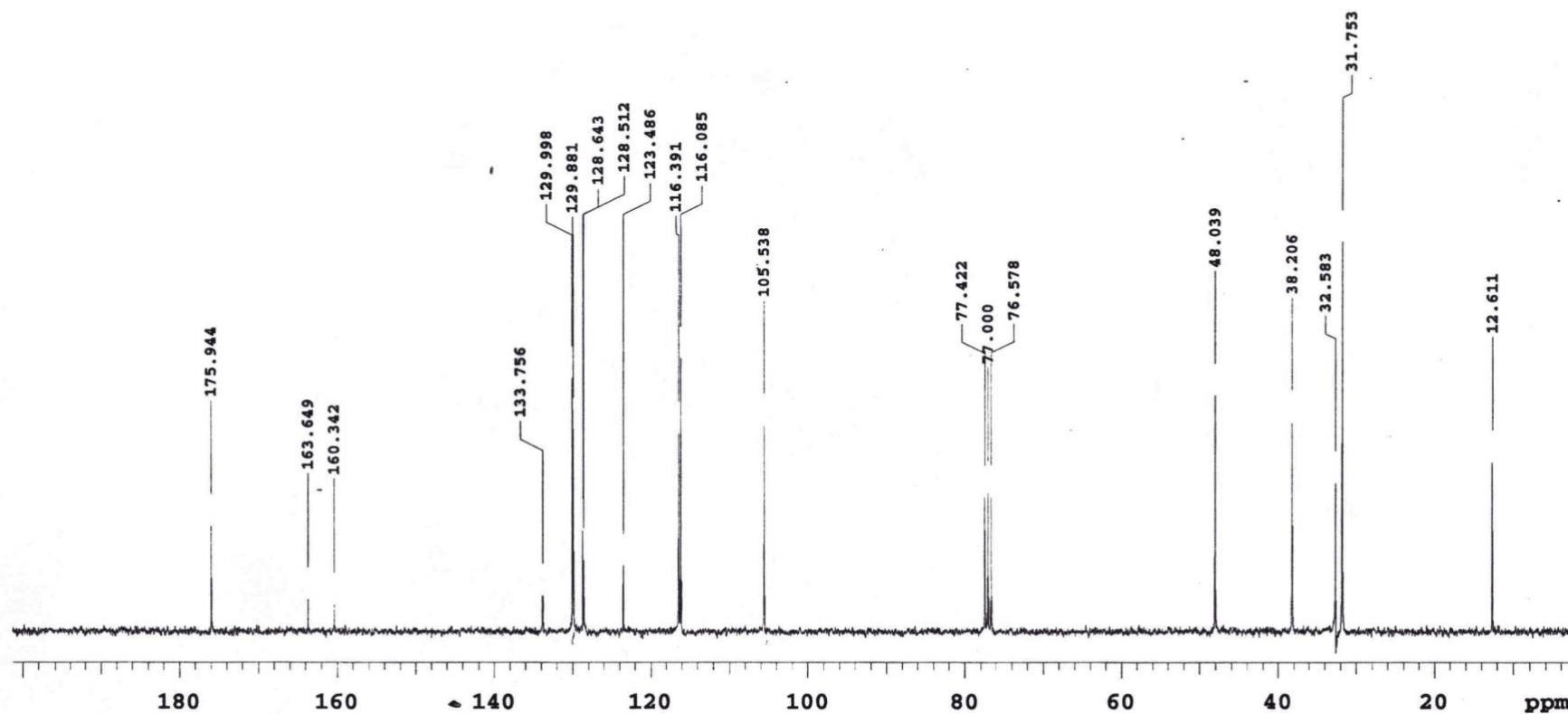
MS



^1H -NMR

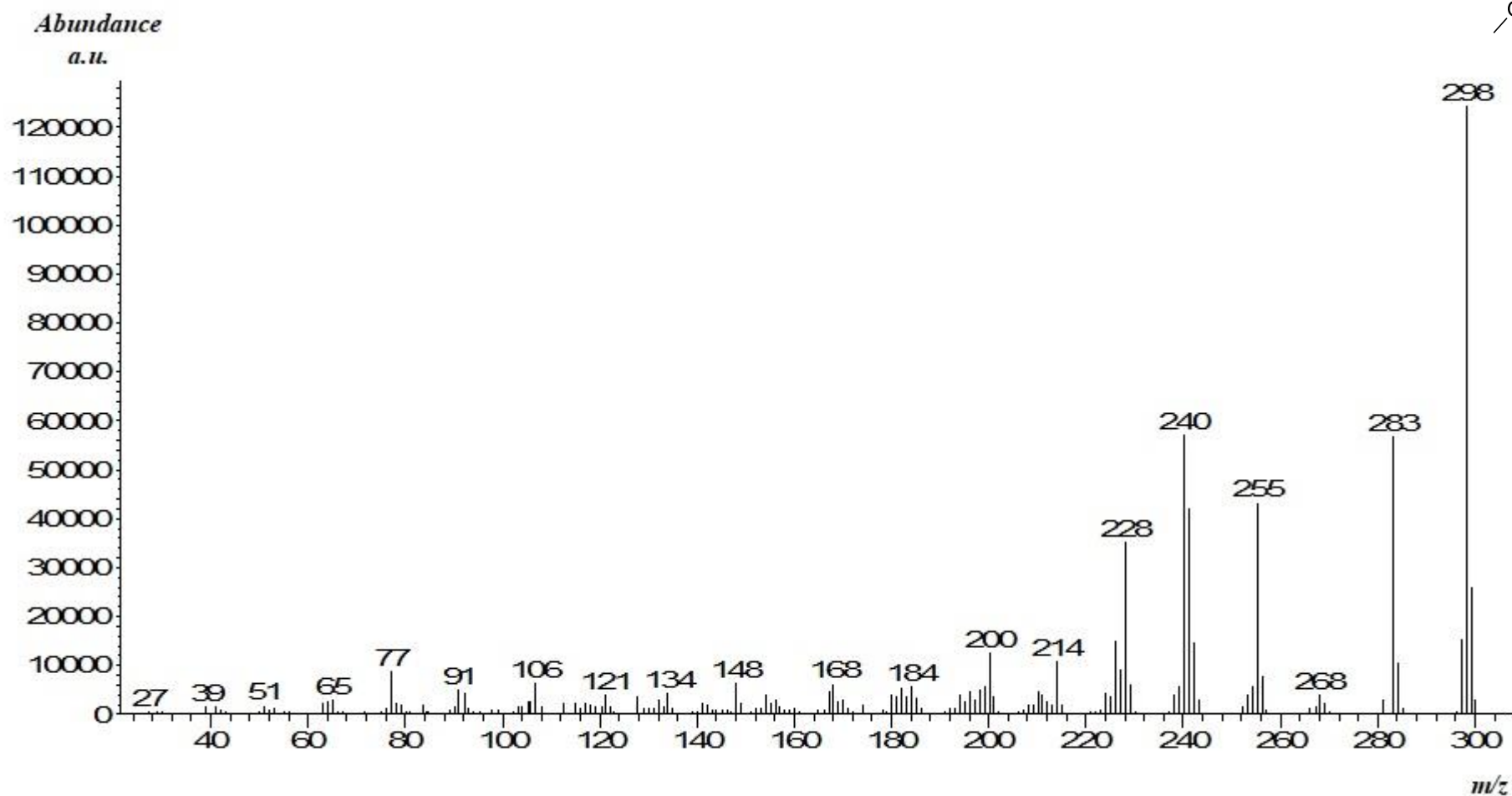
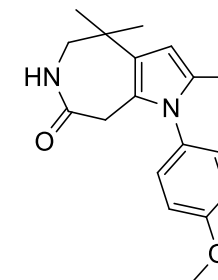
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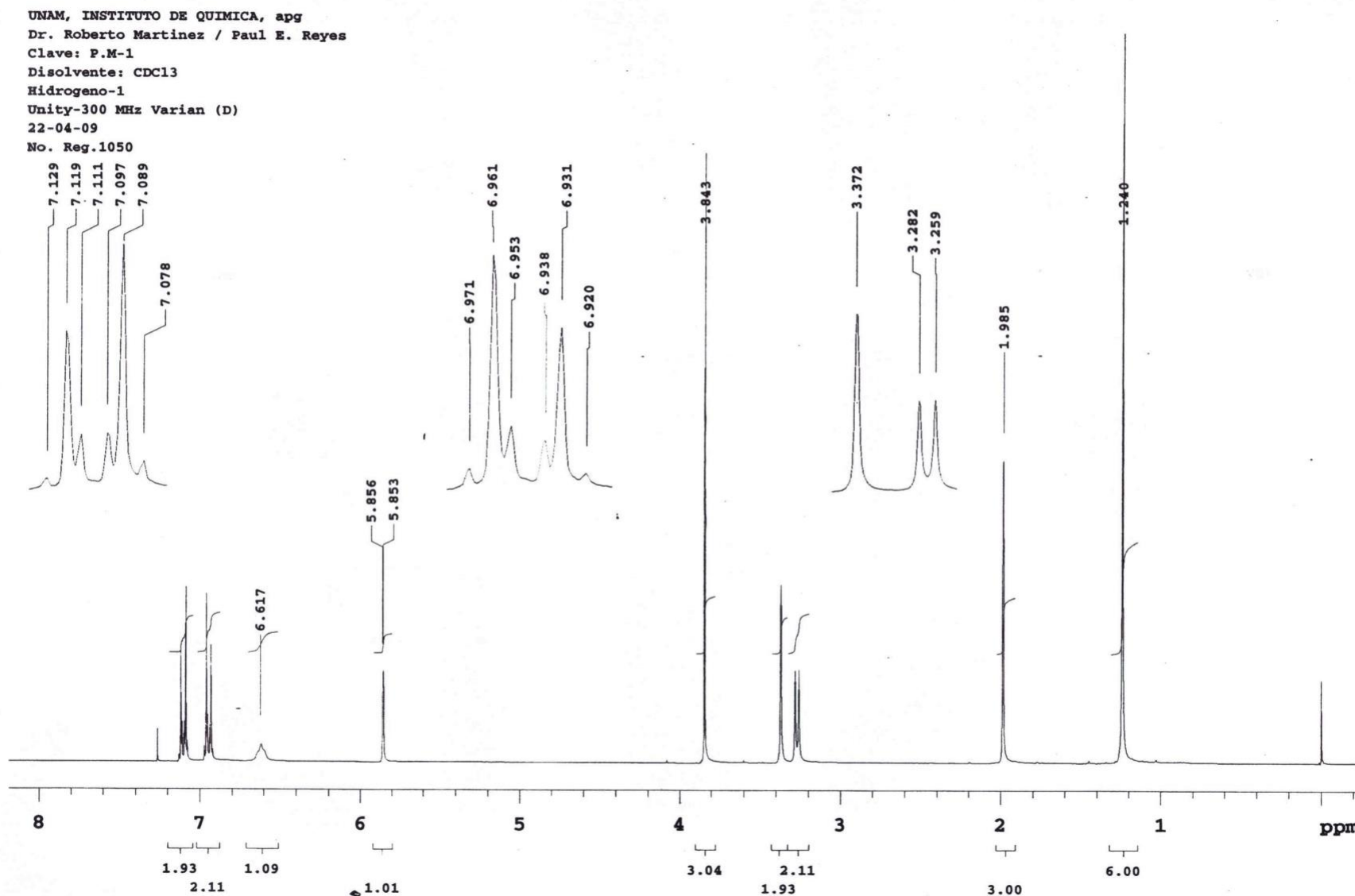
UNAM, INSTITUTO DE QUIMICA, E. Huerta
Dr. Roberto Martinez / Paul E. Reyes
Clave: P-E-2 44
Disolvente: CDCl₃
Carbpono-13
Unity 75 MHz, Varian (D)
13-05-09
No. Reg. 1114



Compound 11d. 1-(4-Methoxyphenyl)-2,4,4-trimethyl-4,5,6,8-tetrahydropyrrolo[2,3-d]azepin-7(1H)-one

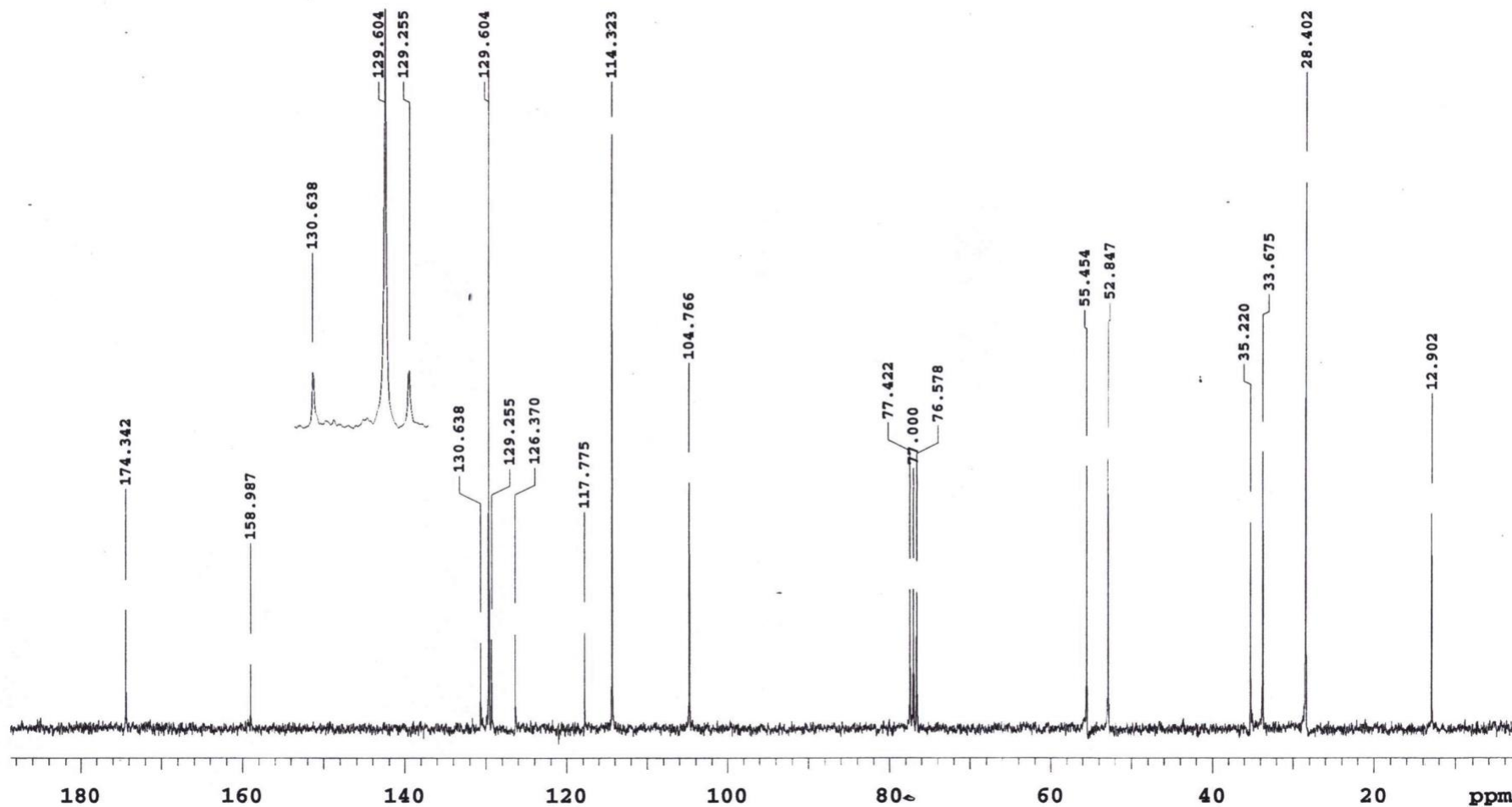
MS



^1H -NMR

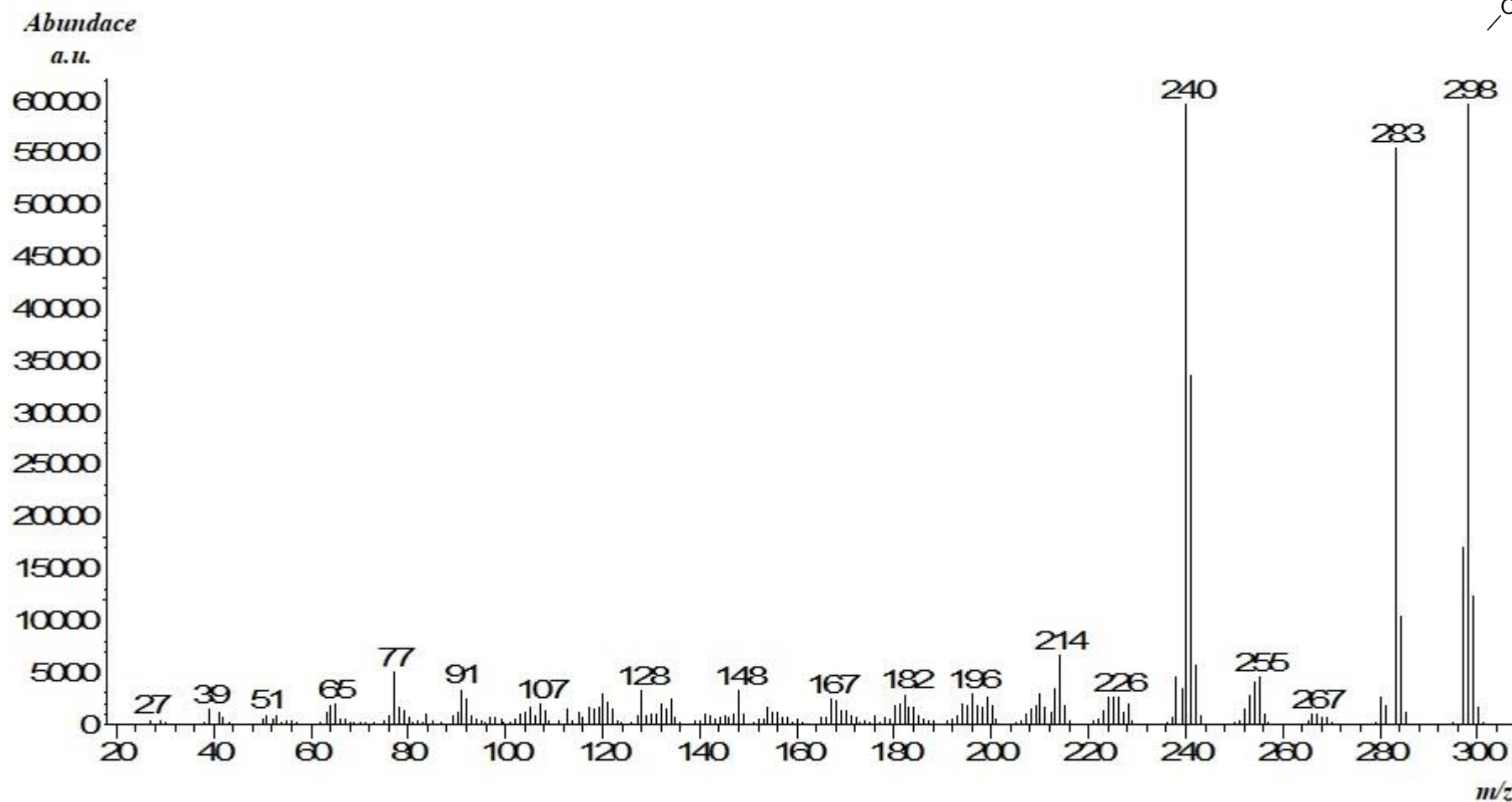
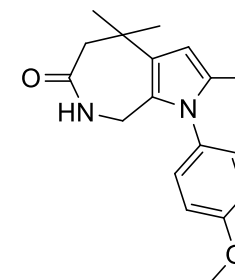
^{13}C -NMR

UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E. Reyes
Clave: P.M-1
Disolvente: CDCl_3
Carbpono-13
Unity 75 MHz, Varian (D)
22-04-09
No. Reg. 1050



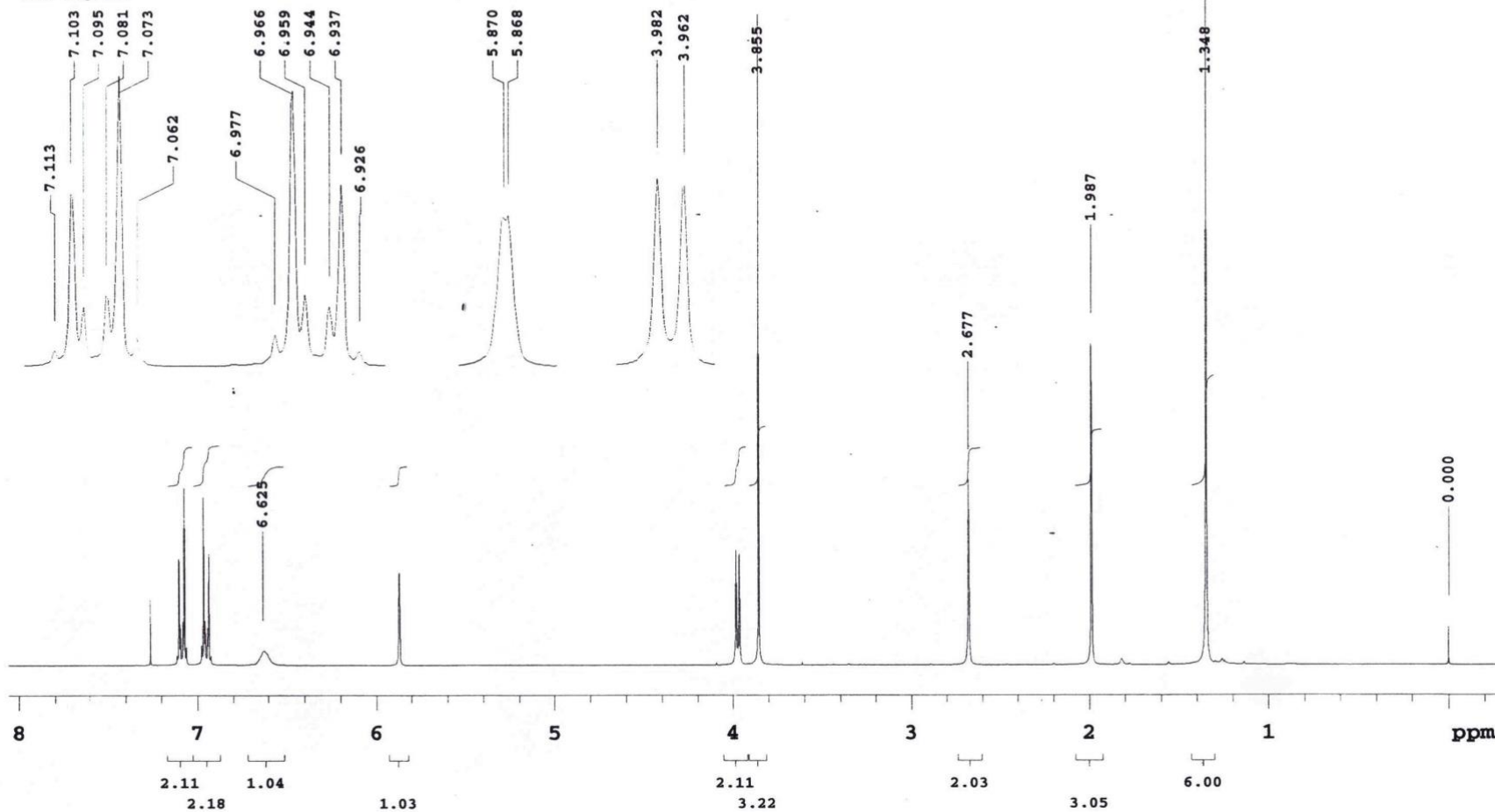
Compound 12d. 1-(4-Methoxyphenyl)-2,4,4-trimethyl-4,5,7,8-tetrahydropyrrolo[2,3-c]azepin-6(1H)-one

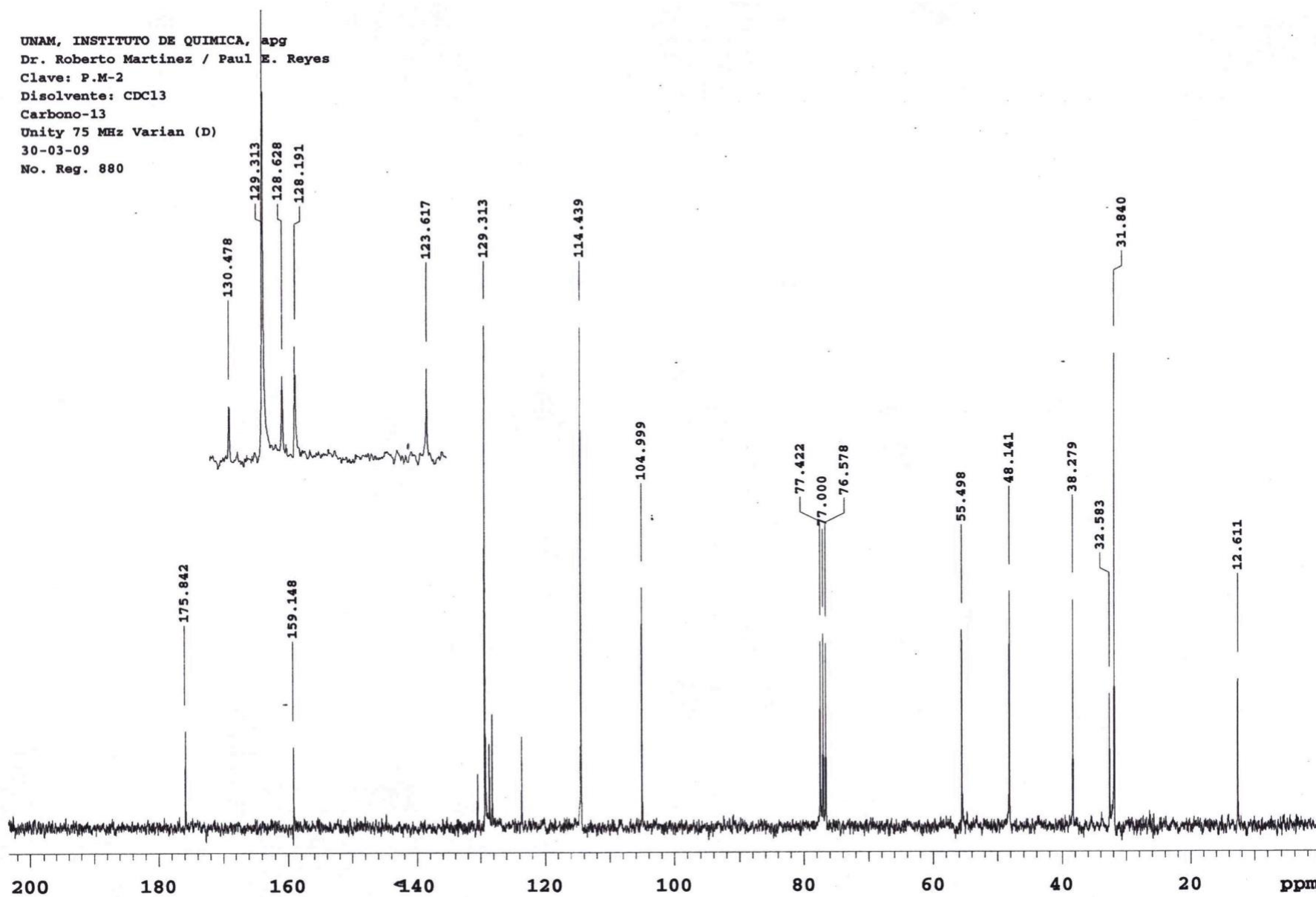
MS



¹H-NMR

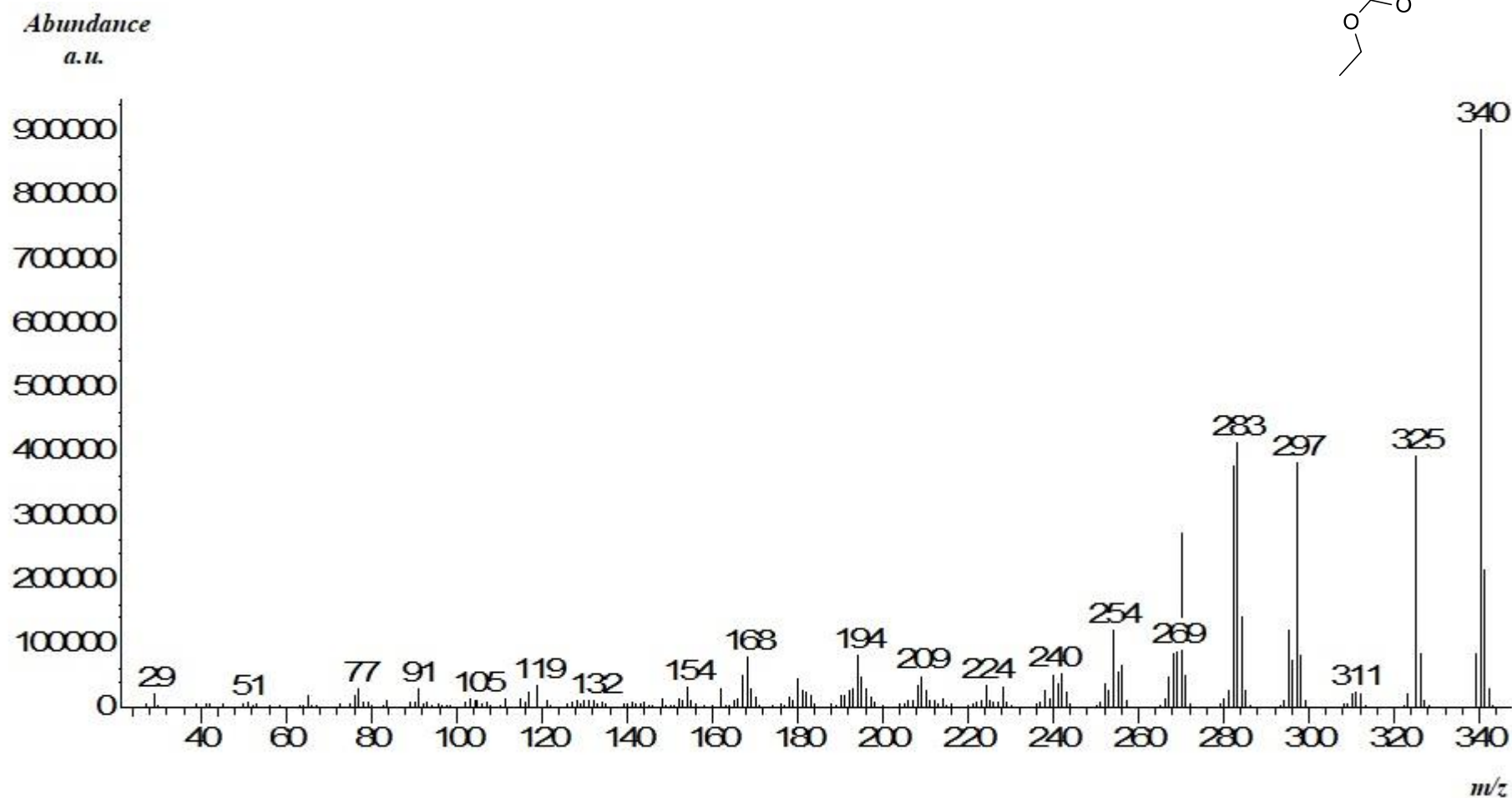
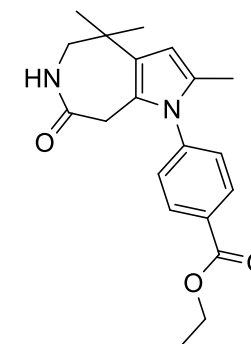
UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E. Reyes
Clave: P.M-2
Disolvente: CDCl₃
Hidrogeno-1
Unity 300 MHz Varian (D)
30-03-09
No. Reg. 880

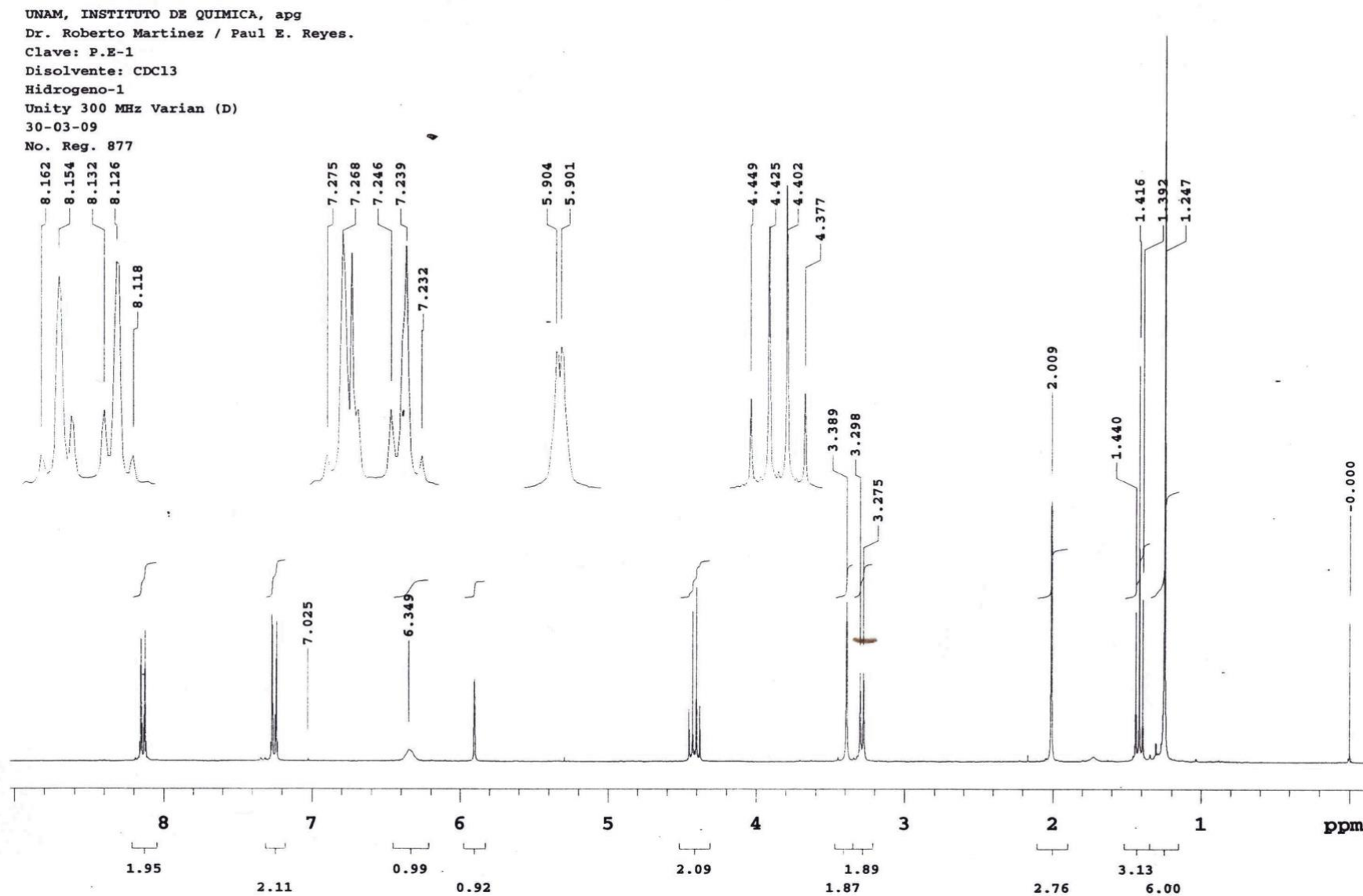


^{13}C -NMR

Compound 11e. Ethyl 4-(2,4,4-trimethyl-7-oxo-5,6,7,8-tetrahydropyrrolo[2,3-d]azepin-1(4H)-yl)benzoate

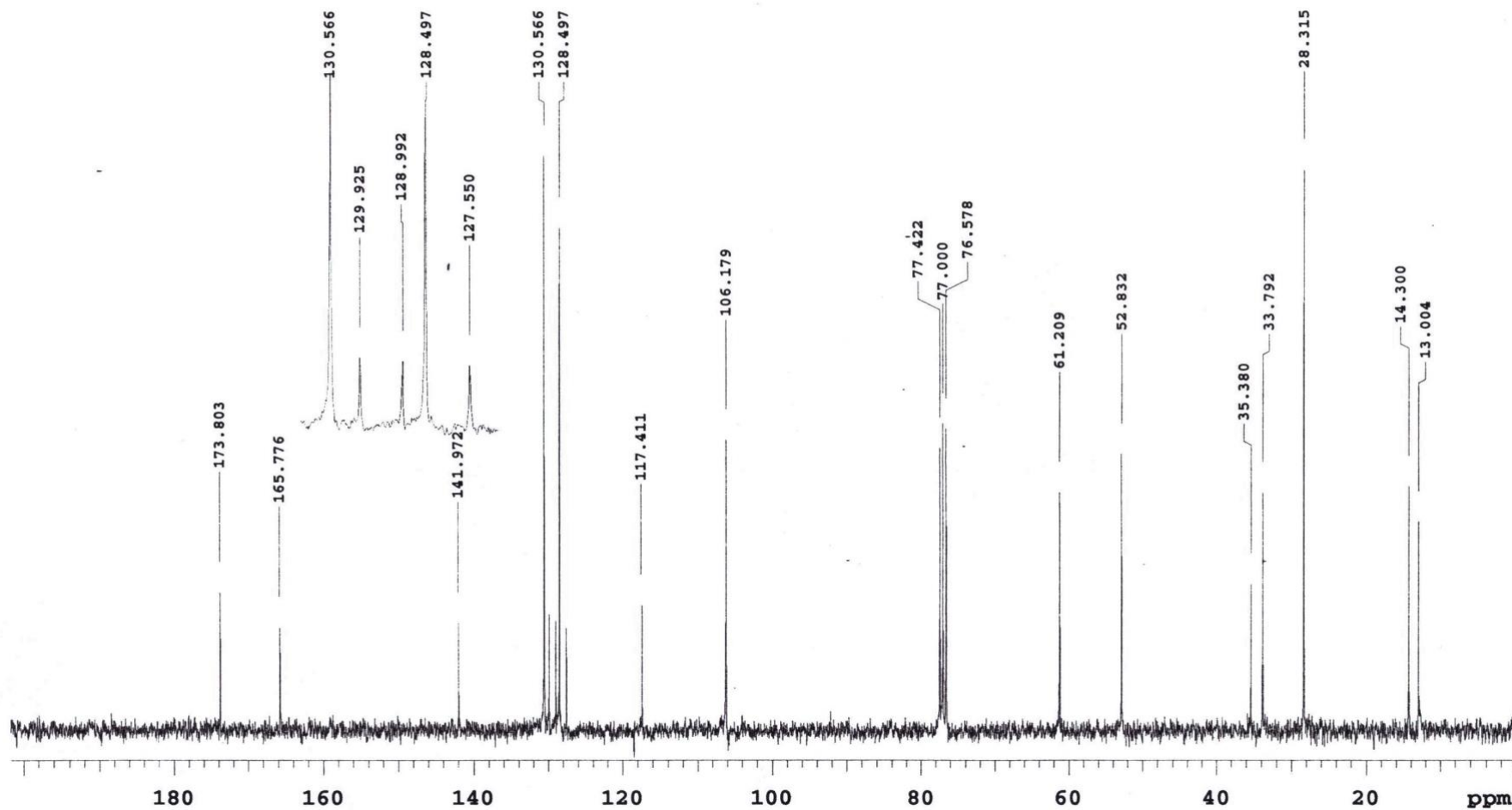
MS



^1H -NMR

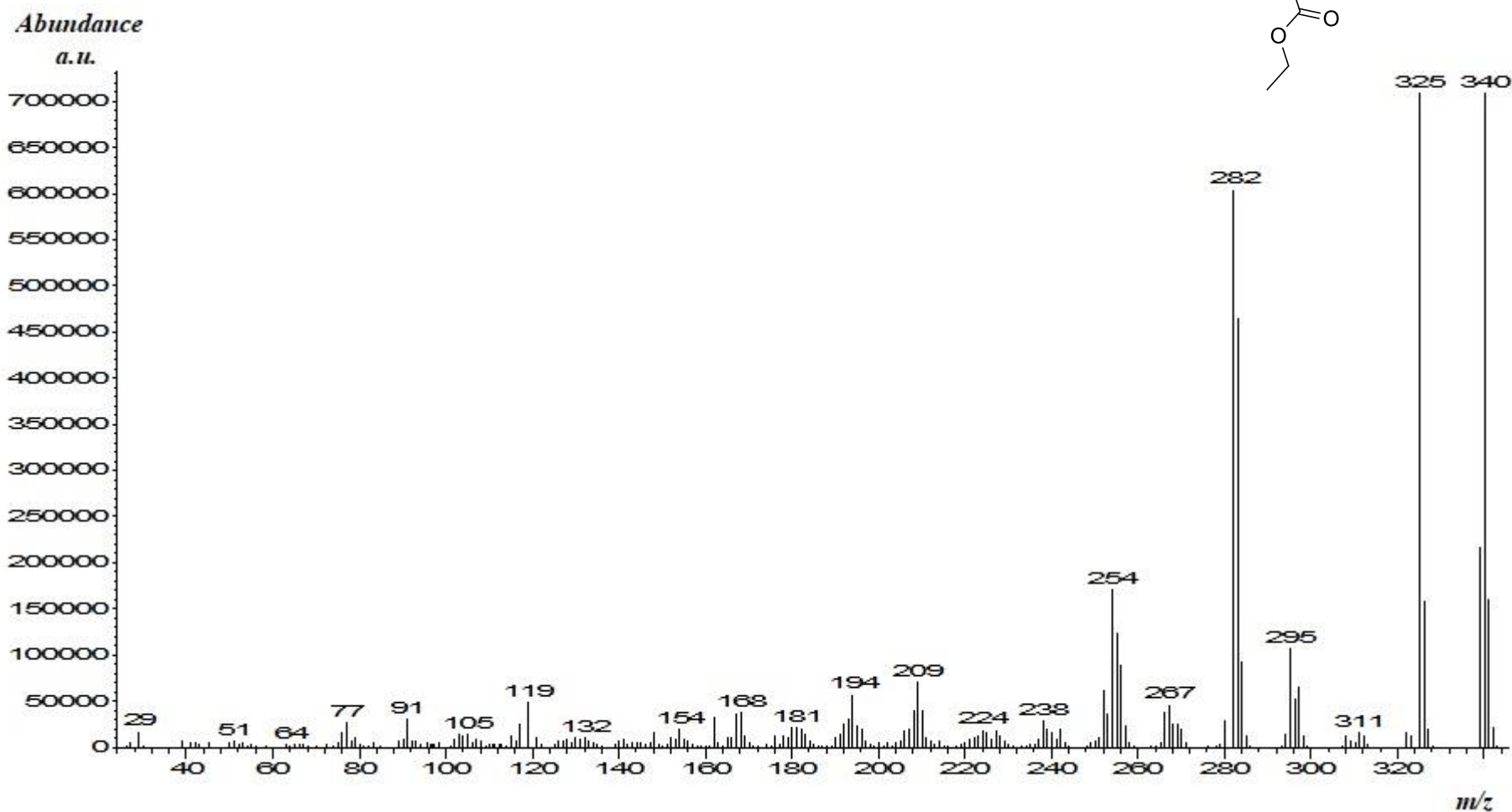
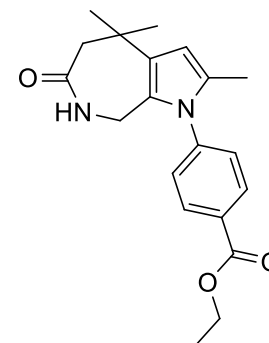
^{13}C -NMR

UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E. Reyes
Clave: P.E-1
Disolvente: CDCl_3
Carbono-13
Unity 75 MHz Varian (D)
30-03-09
No. Reg. 877



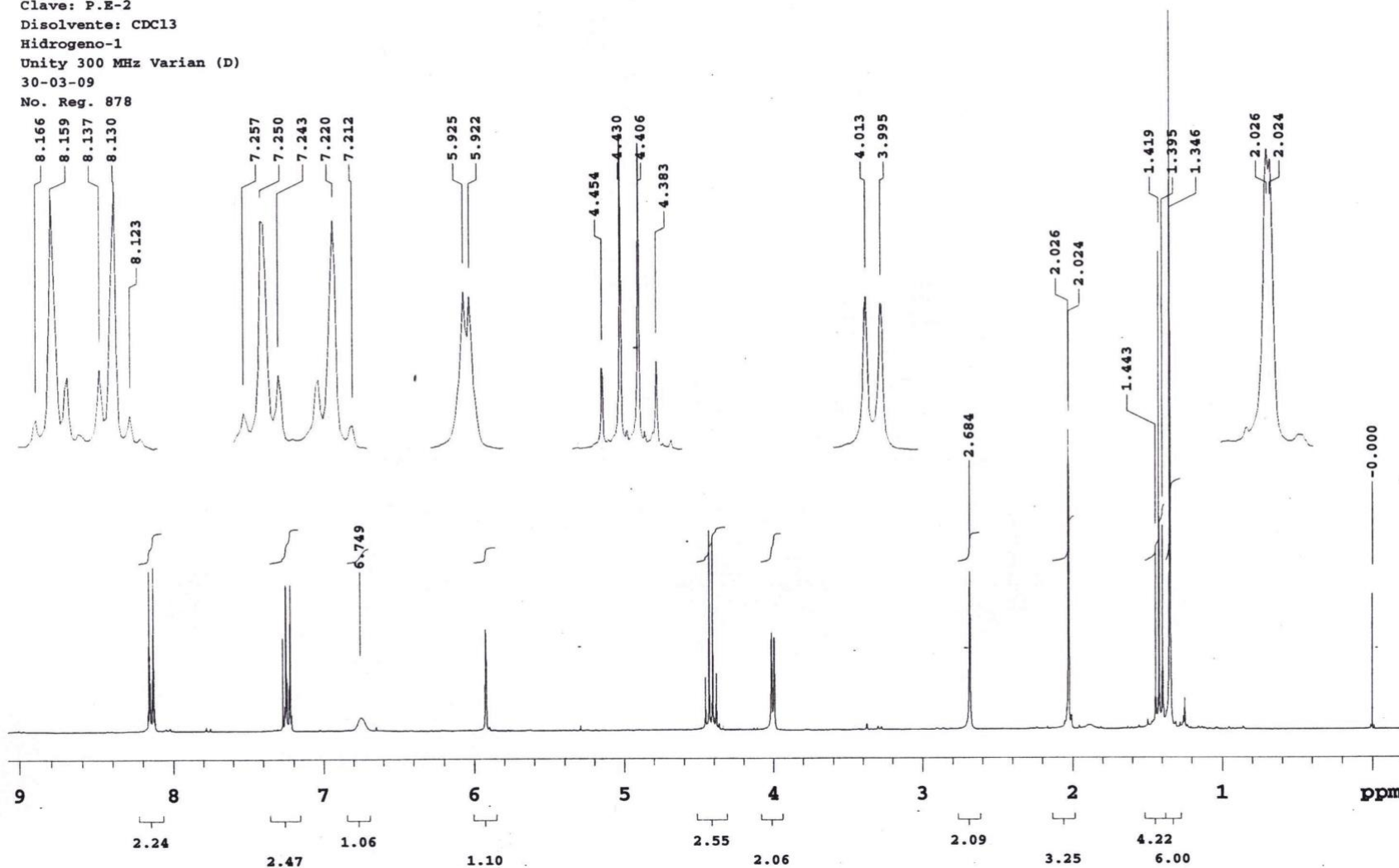
Compound 12e. *Ethyl 4-(2,4,4-trimethyl-6-oxo-5,6,7,8-tetrahydropyrrolo[2,3-c]azepin-1(4H)-yl)benzoate*

MS



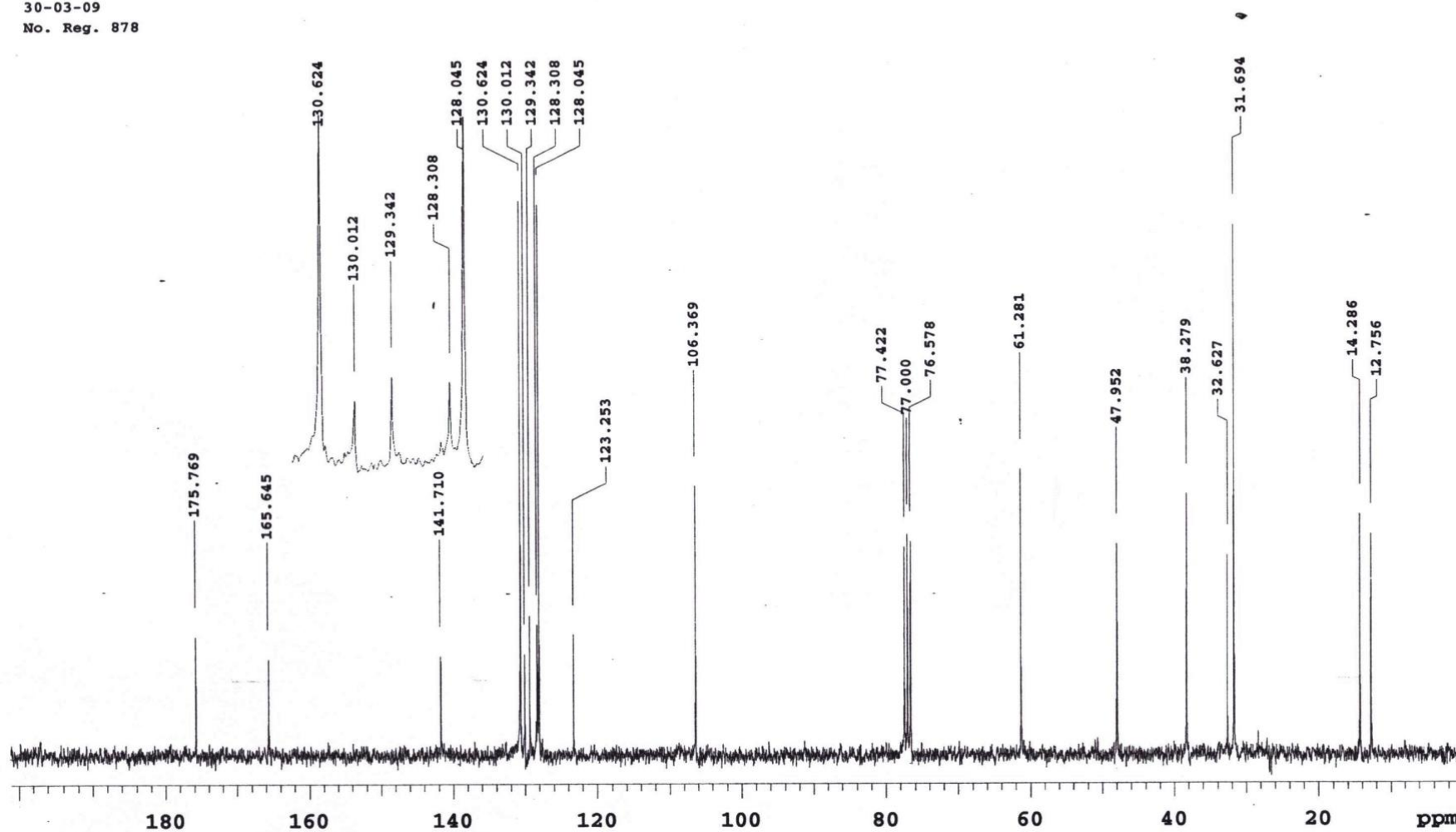
^1H -NMR

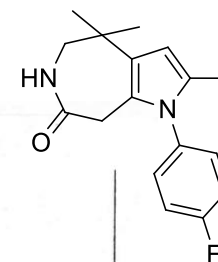
UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E. Reyes.
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Disolvente: CDCl_3
Hidrogeno-1
Unity 300 MHz Varian (D)
30-03-09
No. Reg. 878



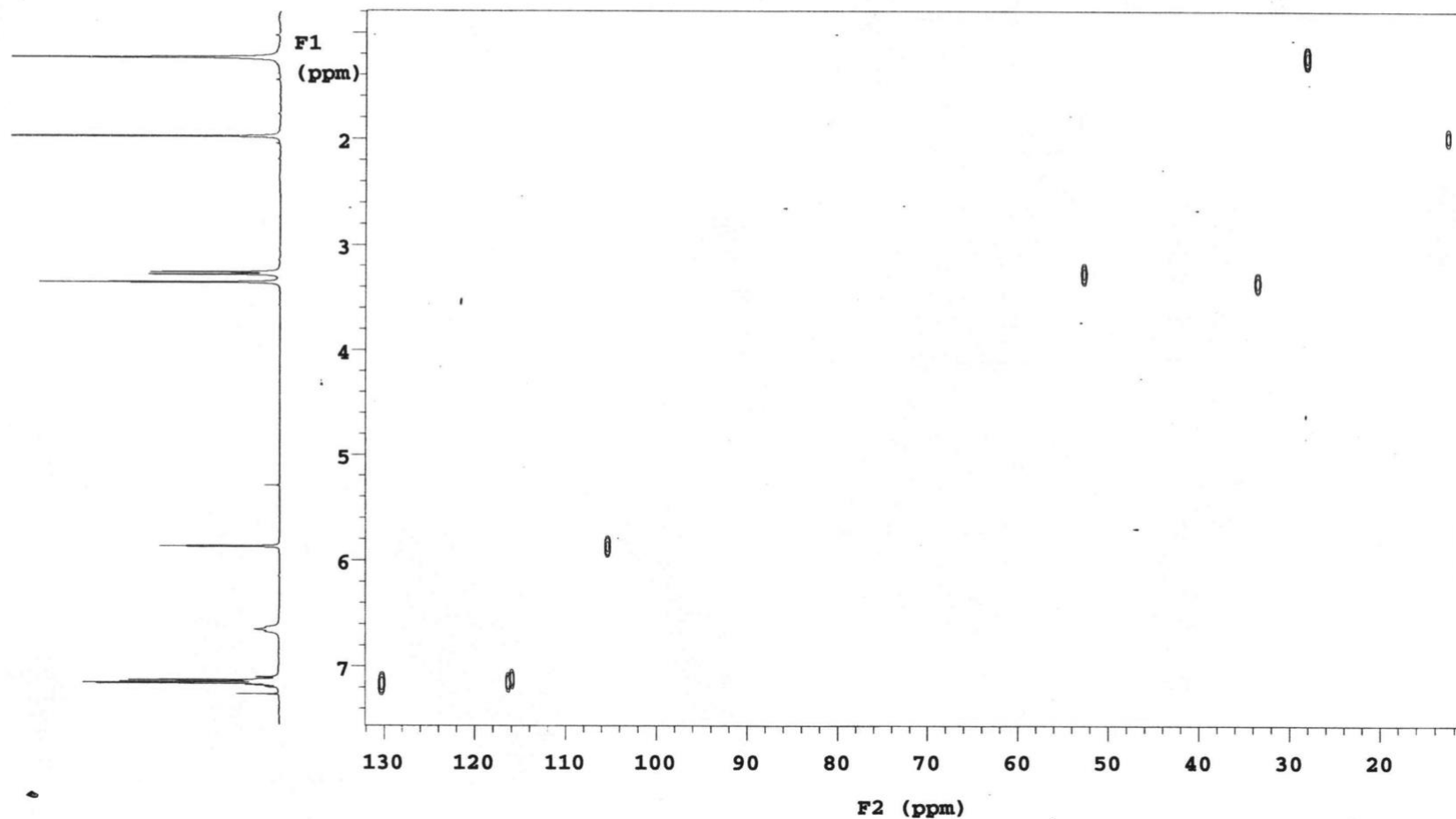
¹³C-NMR

UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E. Reyes
Clave: P.E-2
Disolvente: CDCl₃
Carbono-13
Unity 75 MHz Varian (D)
30-03-09
No. Reg. 878



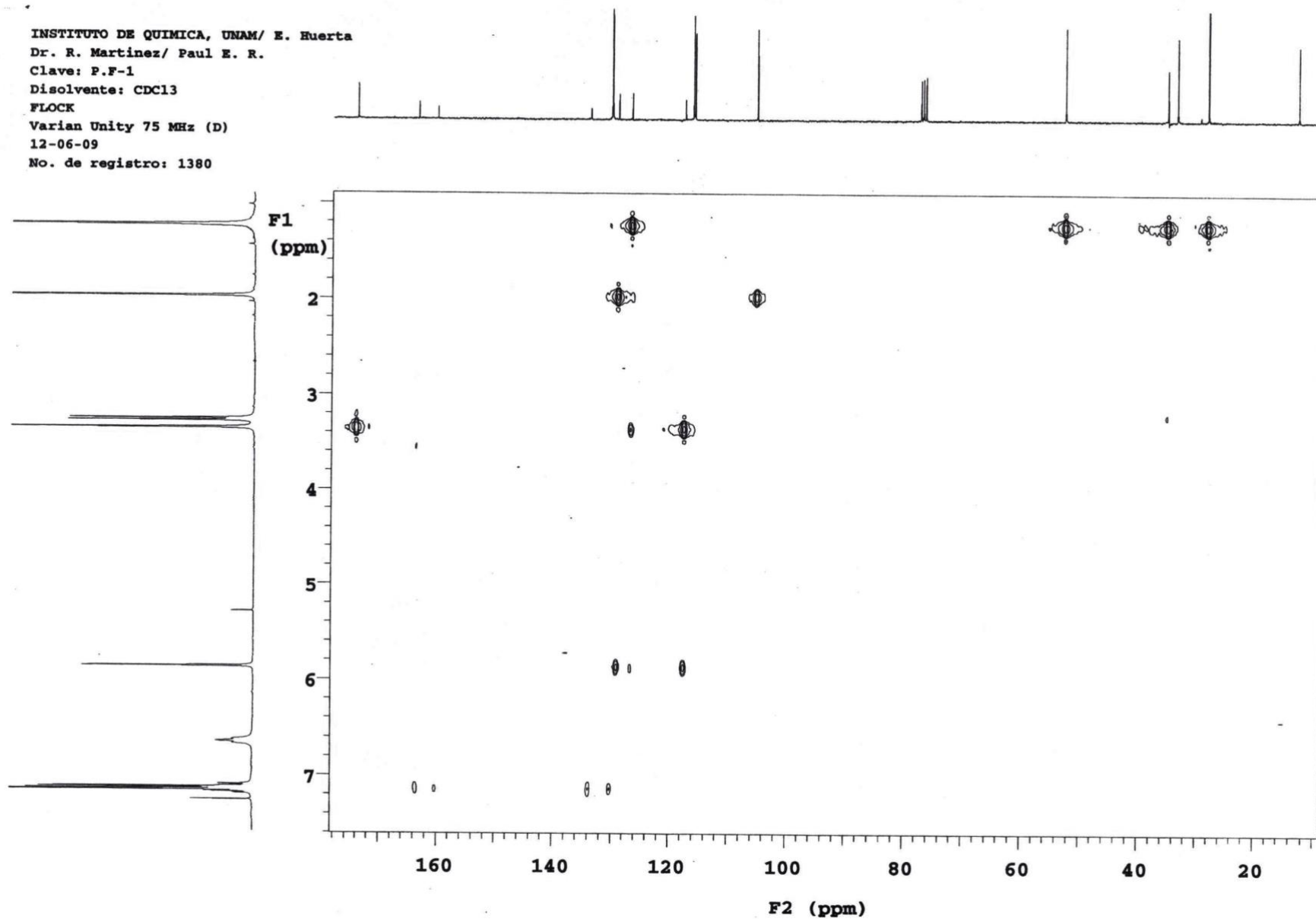
Compound 11c. 1-(4-Fluorophenyl)-2,4,4-trimethyl-4,5,6,8-tetrahydropyrrolo[2,3-d]azepin-7(1H)-one**HETCOR**

INSTITUTO DE QUIMICA, UNAM/ E. Huerta
Dr. R. Martinez/ Paul E. R.
Clave: P.F-1
Disolvente: CDC13
HETCOR
Varian Unity 75 MHz (D)
12-06-09
No. de registro: 1380

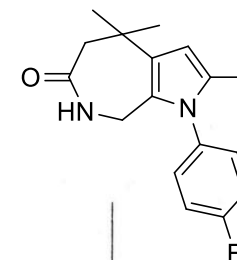


FLOCK

INSTITUTO DE QUIMICA, UNAM/ E. Huerta
Dr. R. Martinez/ Paul E. R.
Clave: P.F-1
Disolvente: CDCl₃
FLOCK
Varian Unity 75 MHz (D)
12-06-09
No. de registro: 1380

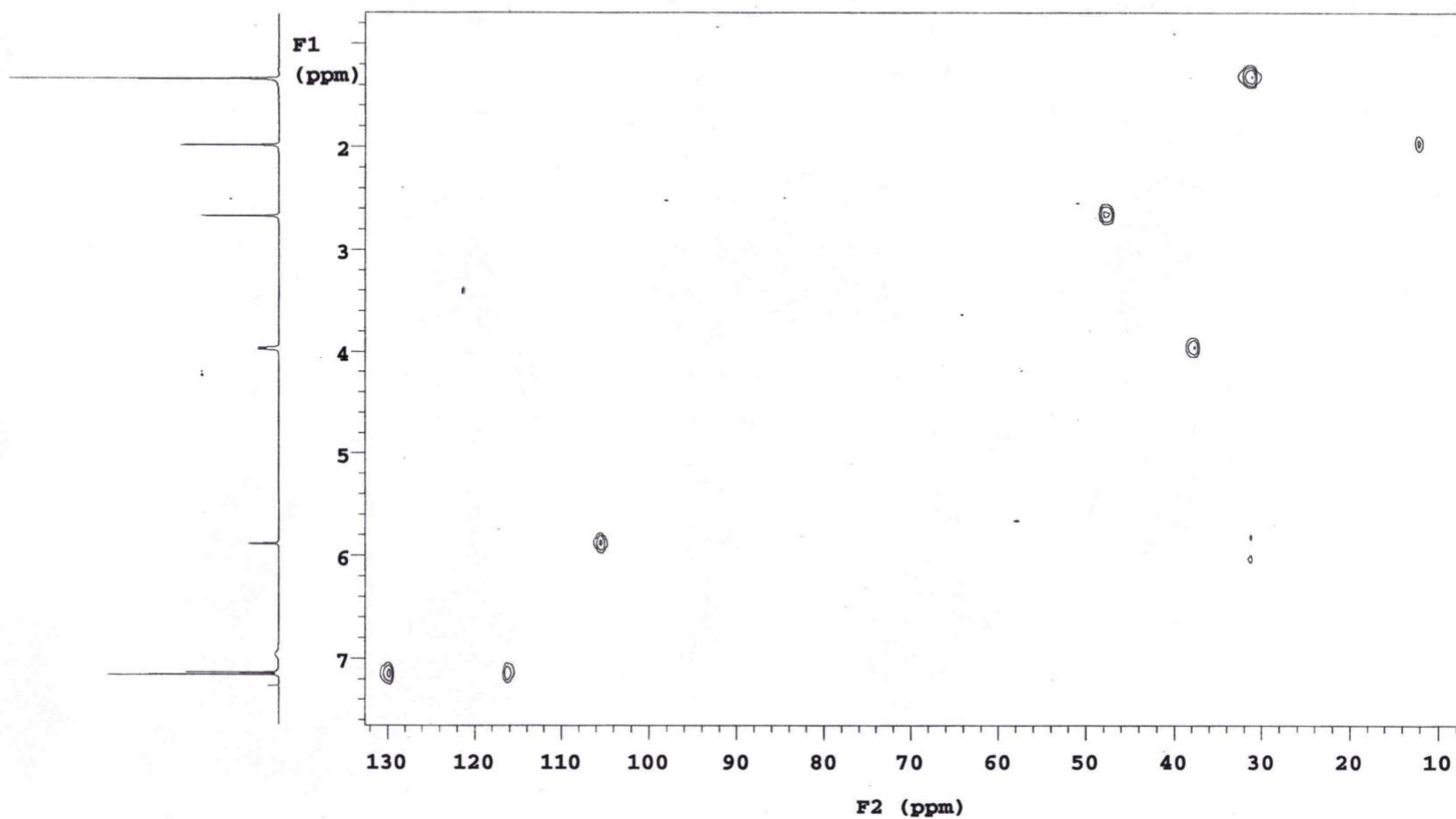
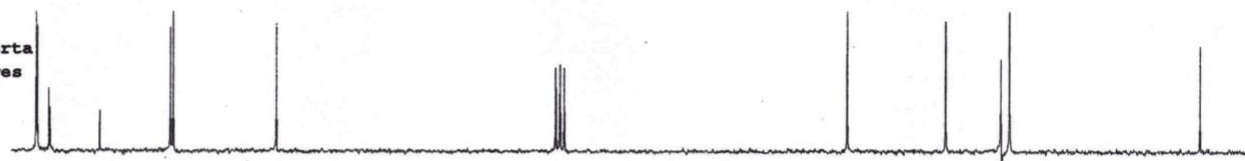


Compound 12c. 1-(4-fluorophenyl)-2,4,4-trimethyl-4,5,7,8-tetrahydropyrrolo[2,3-c]azepin-6(1H)-one



HETCOR

UNAM, INSTITUTO DE QUIMICA, E. Huerta
Dr. Roberto Martinez / Paul E. Reyes
Clave: P.F-2
Disolvente: CDCl₃
Hetcor
Unity 75 MHz, Varian (D)
13-05-09
No. Reg. 1114



FLOCK

UNAM, INSTITUTO DE QUIMICA, E. Huerta
Dr. Roberto Martinez / Paul E. Reyes
Clave: P.F-2
Disolvente: CDCl₃
Flock
Unity 75 MHz, Varian (D)
2-06-09
No. Reg. 1114

