

Supplementary Material

Synthesis of novel pyrroloazepinones by Schmidt expansions of 6-indolones

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

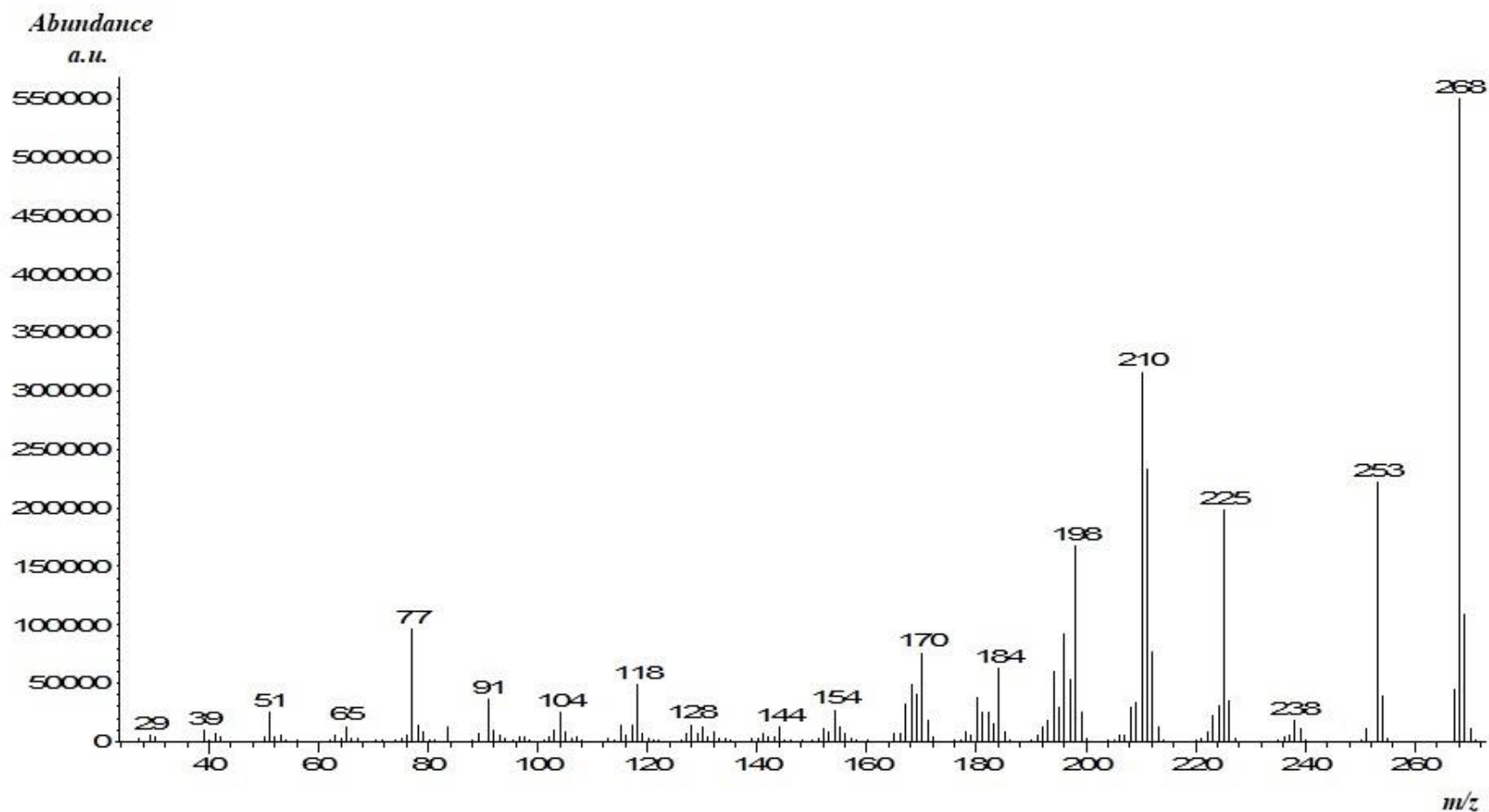
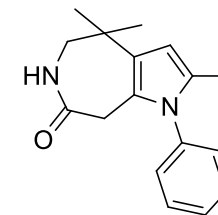
Email: gcomm@uaslp.mx

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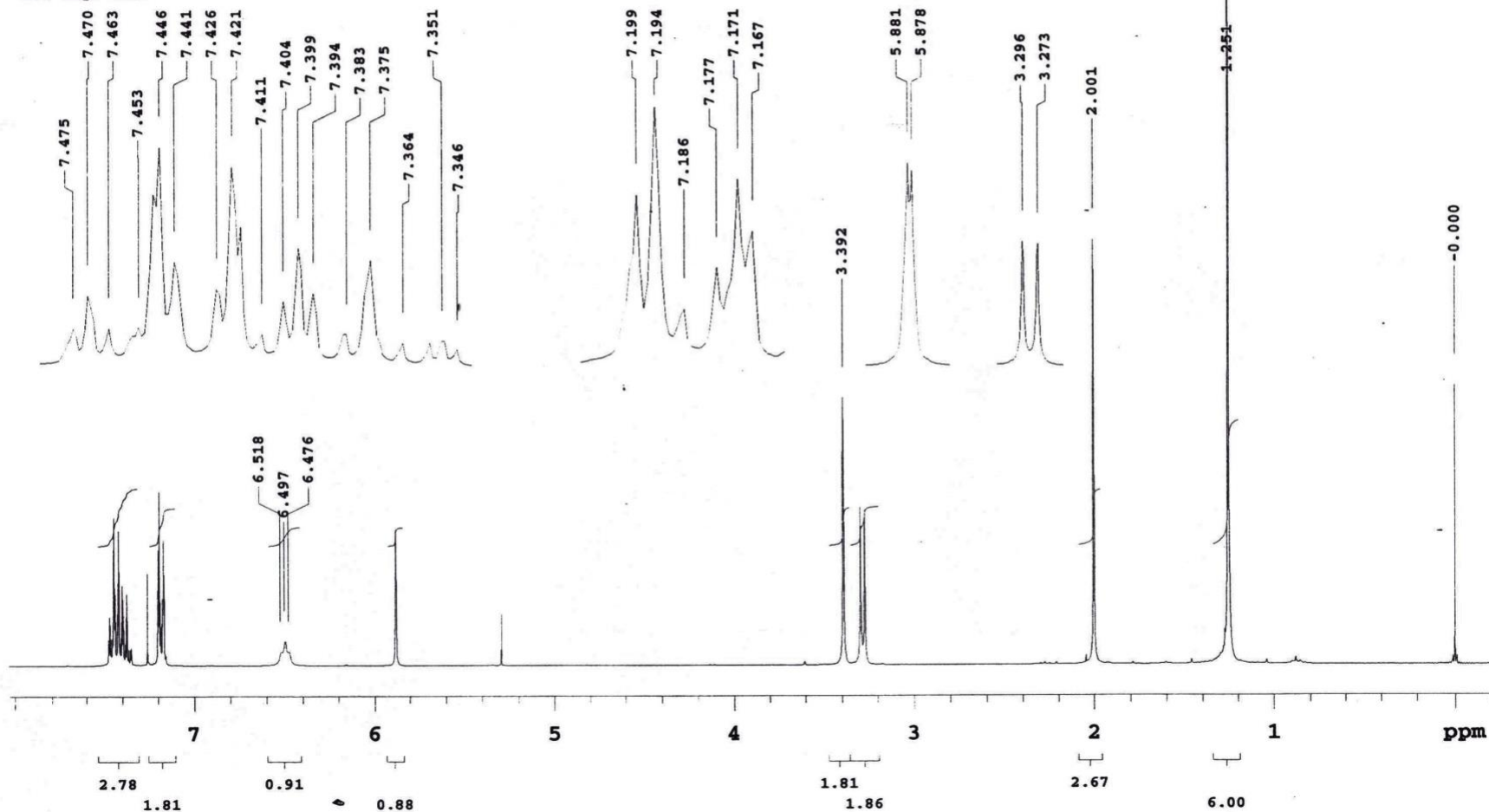
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MS



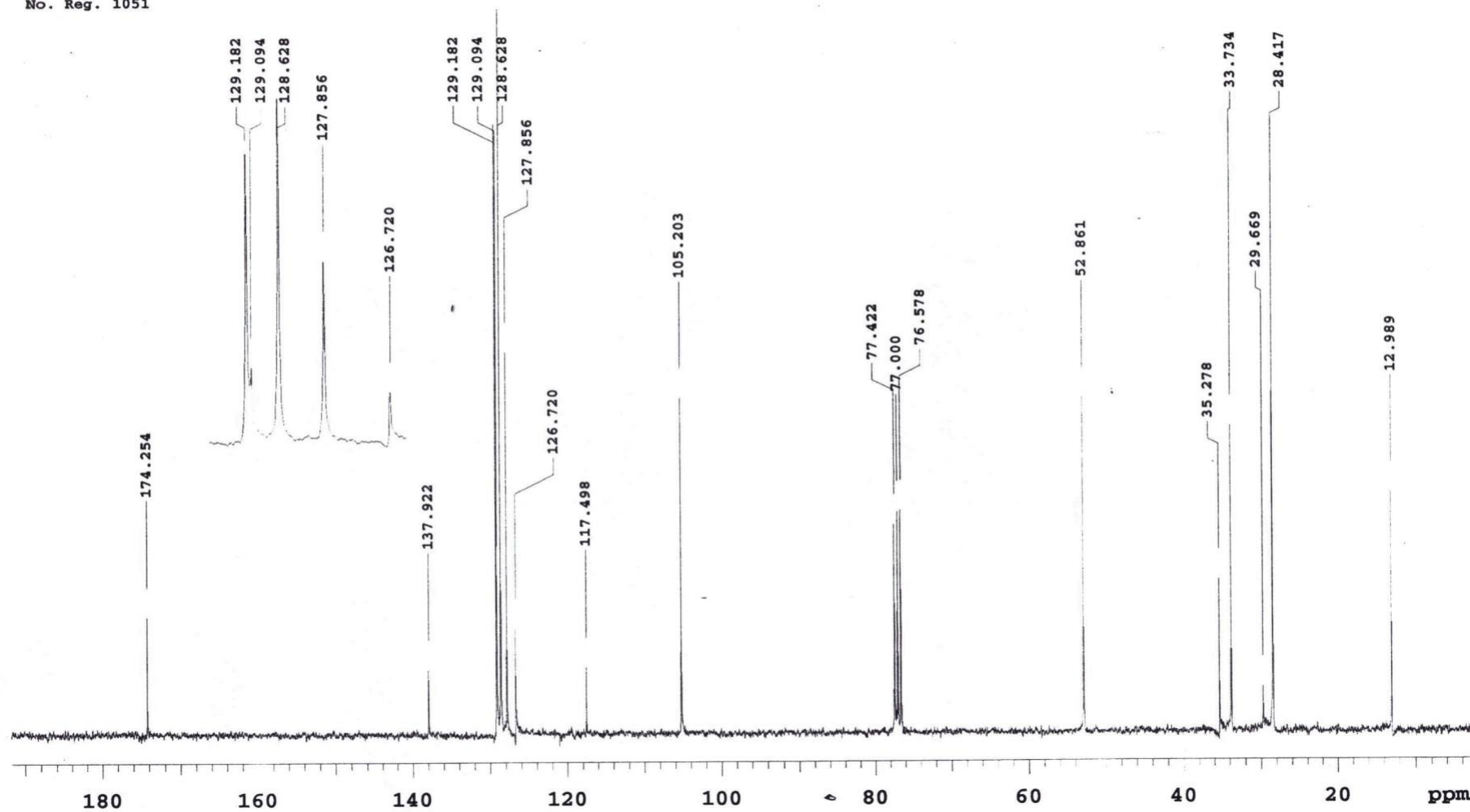
^1H -NMR

UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E. Reyes
Clave: P.A-1
Disolvente: CDCl_3
Hidrogeno-1
Unity-300 MHz Varian (D)
22-04-09
No. Reg. 1051



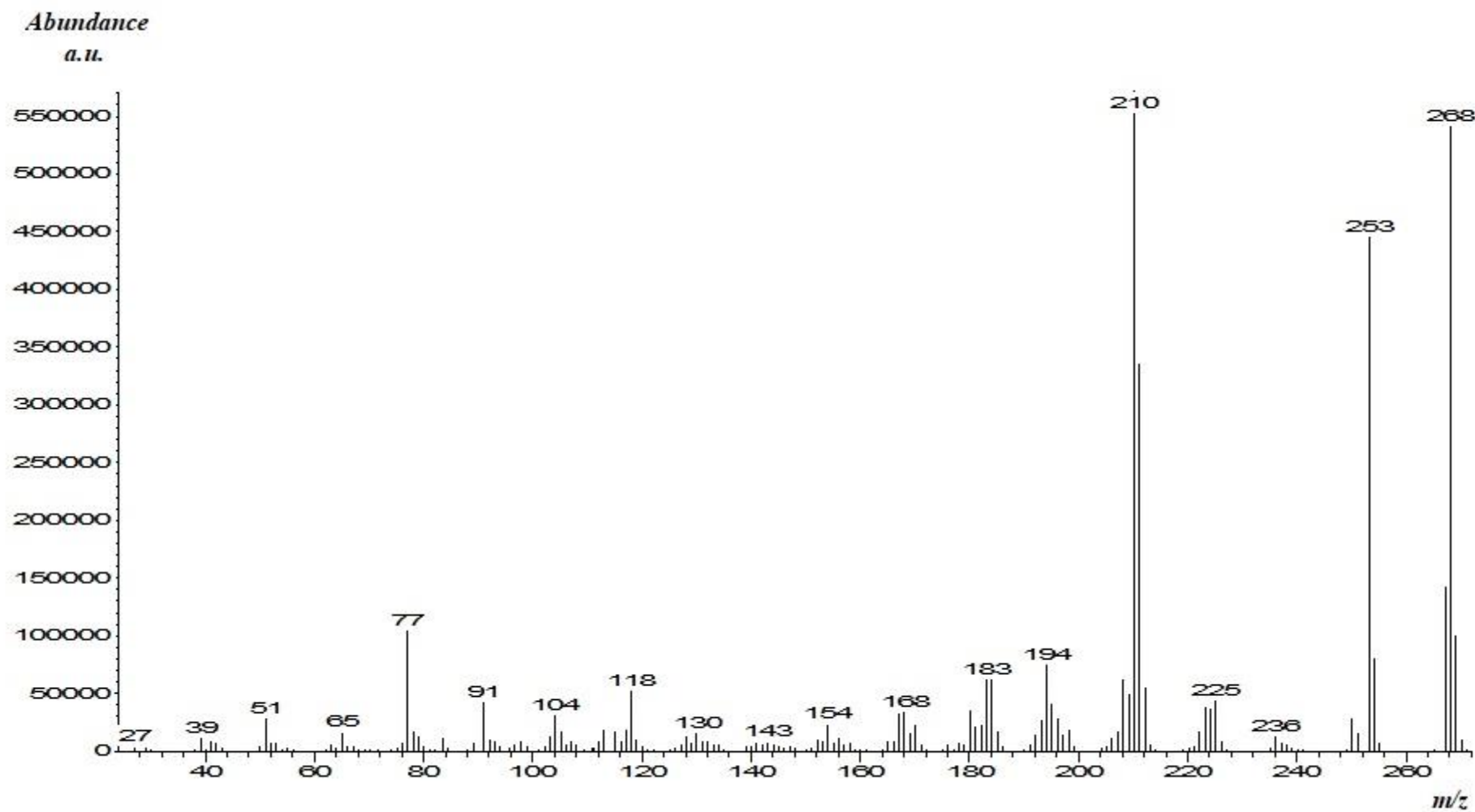
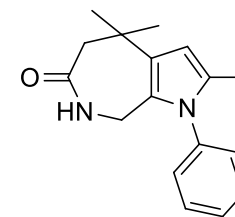
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UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E, Reyes
Clave: P.A-1
Disolvente: CDCl₃
Carbpono-13
Unity 75 MHz, Varian (D)
22-04-09
No. Reg. 1051



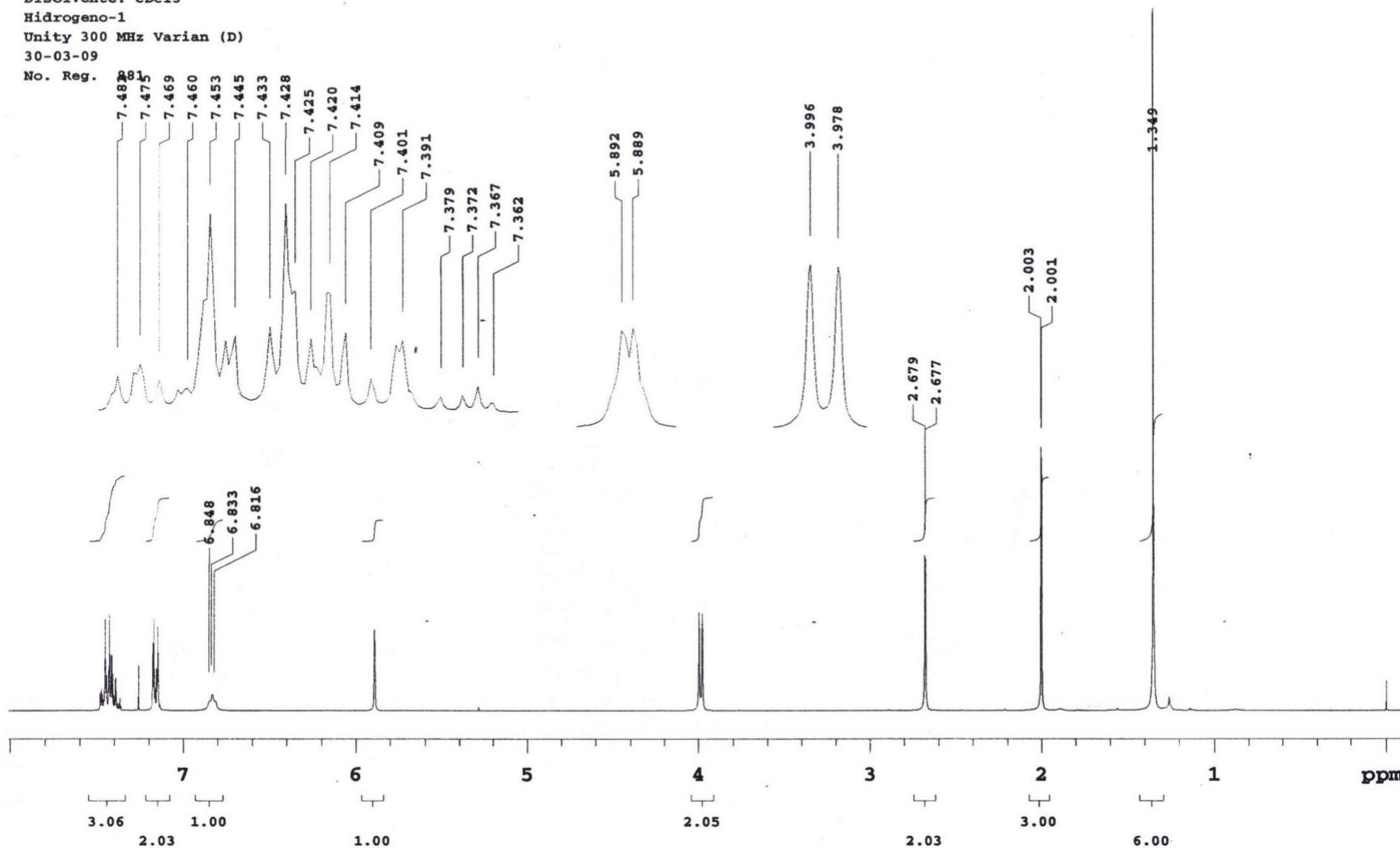
Compound 12a. 2,4,4-Trimethyl-1-phenyl-4,5,7,8-tetrahydropyrrolo[2,3-*c*]-6(1*H*)-one

MS



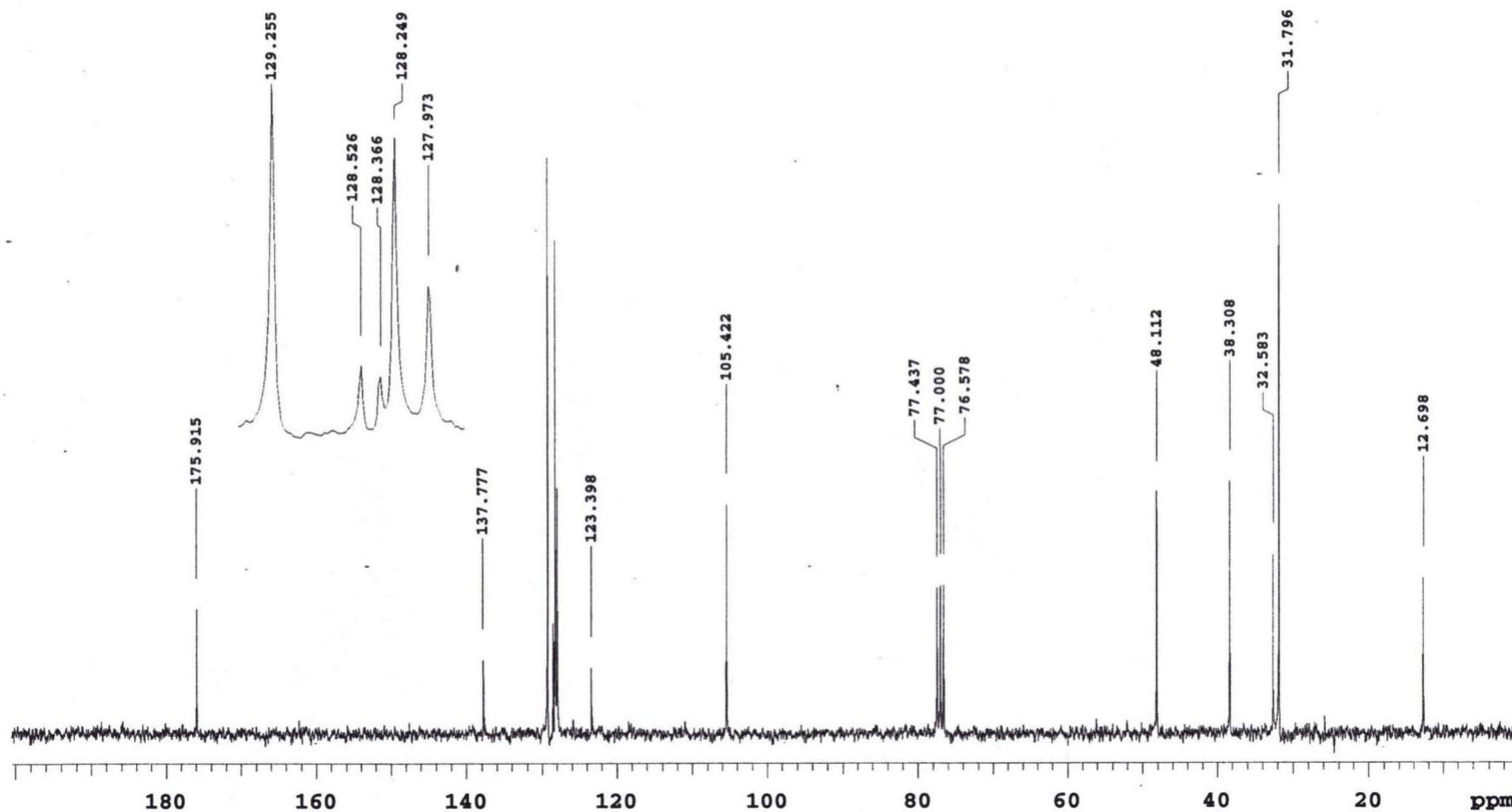
^1H -NMR

UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E. Reyes
Clave: P.A-2
Disolvente: CDCl_3
Hidrogeno-1
Unity 300 MHz Varian (D)
30-03-09
No. Reg.



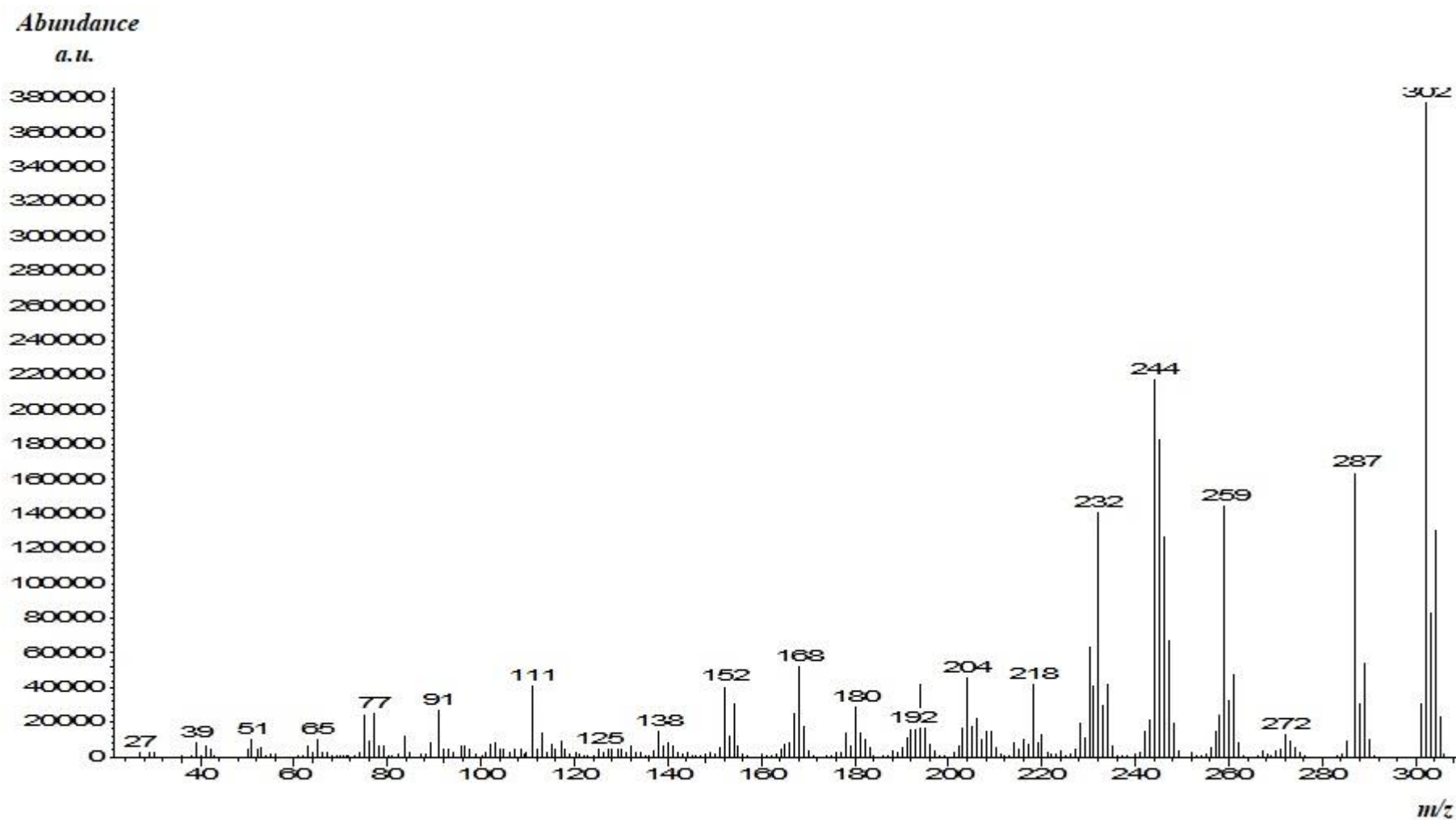
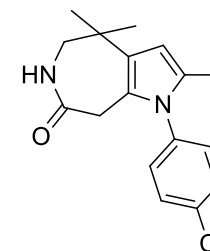
¹³C-NMR

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



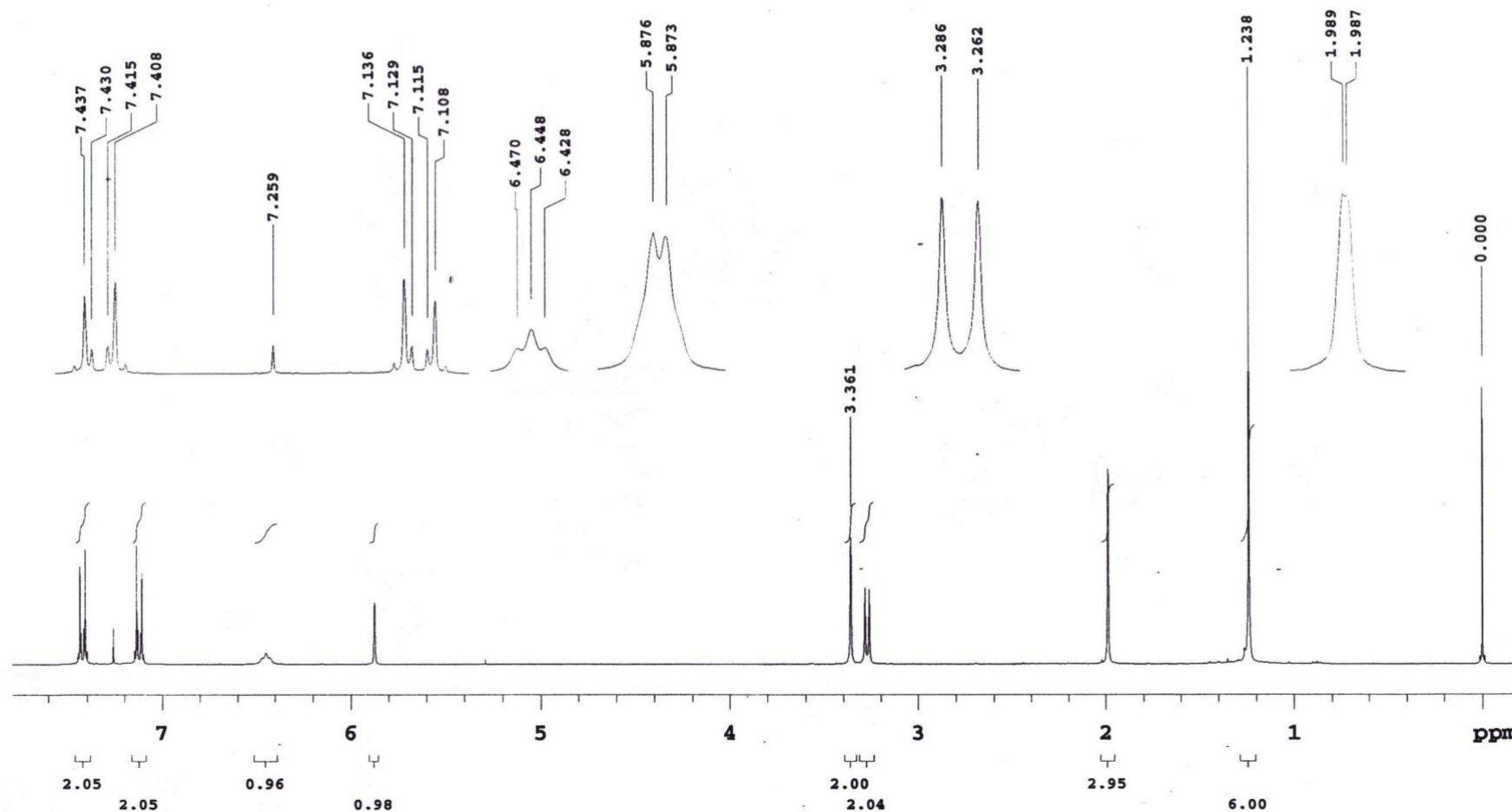
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MS



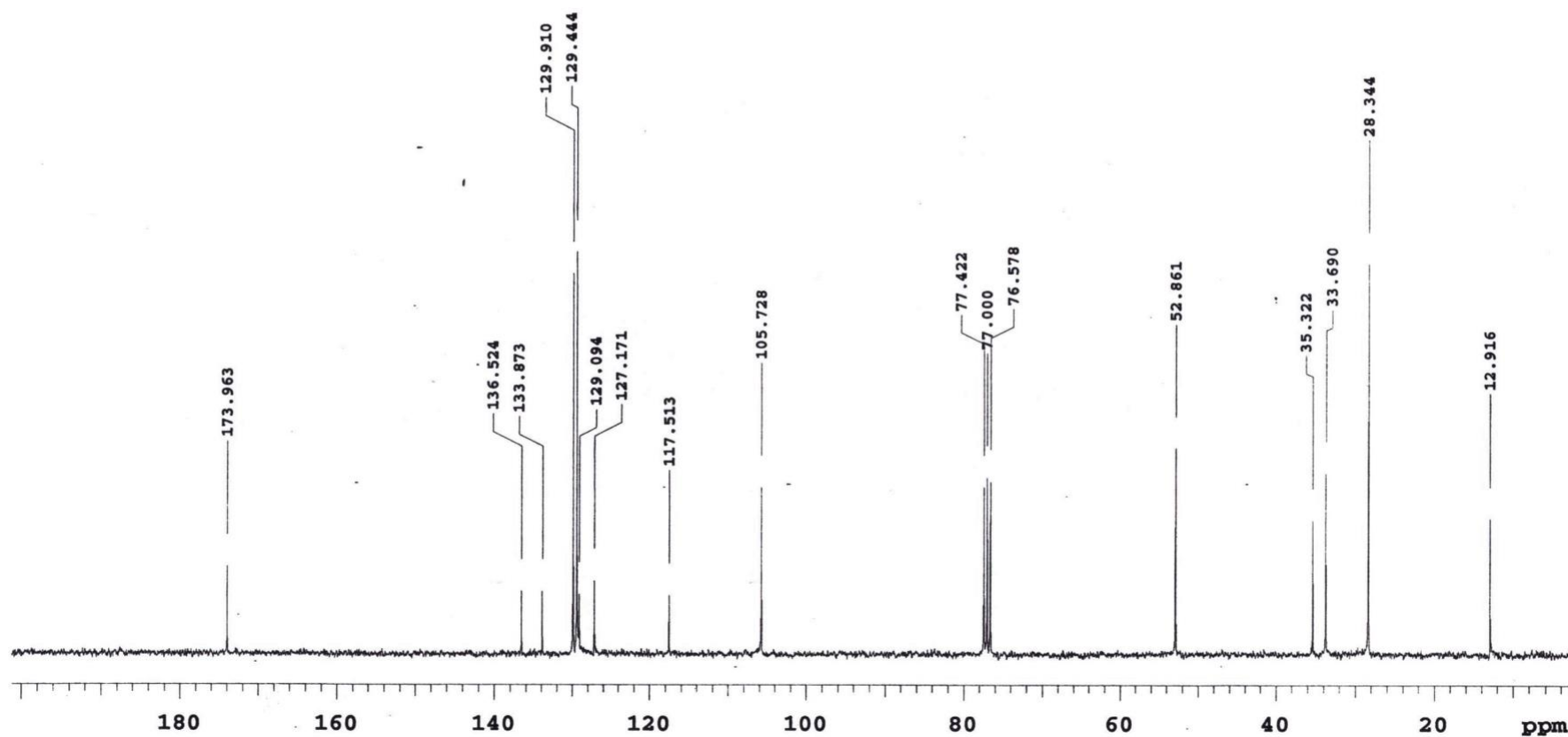
^1H -NMR

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



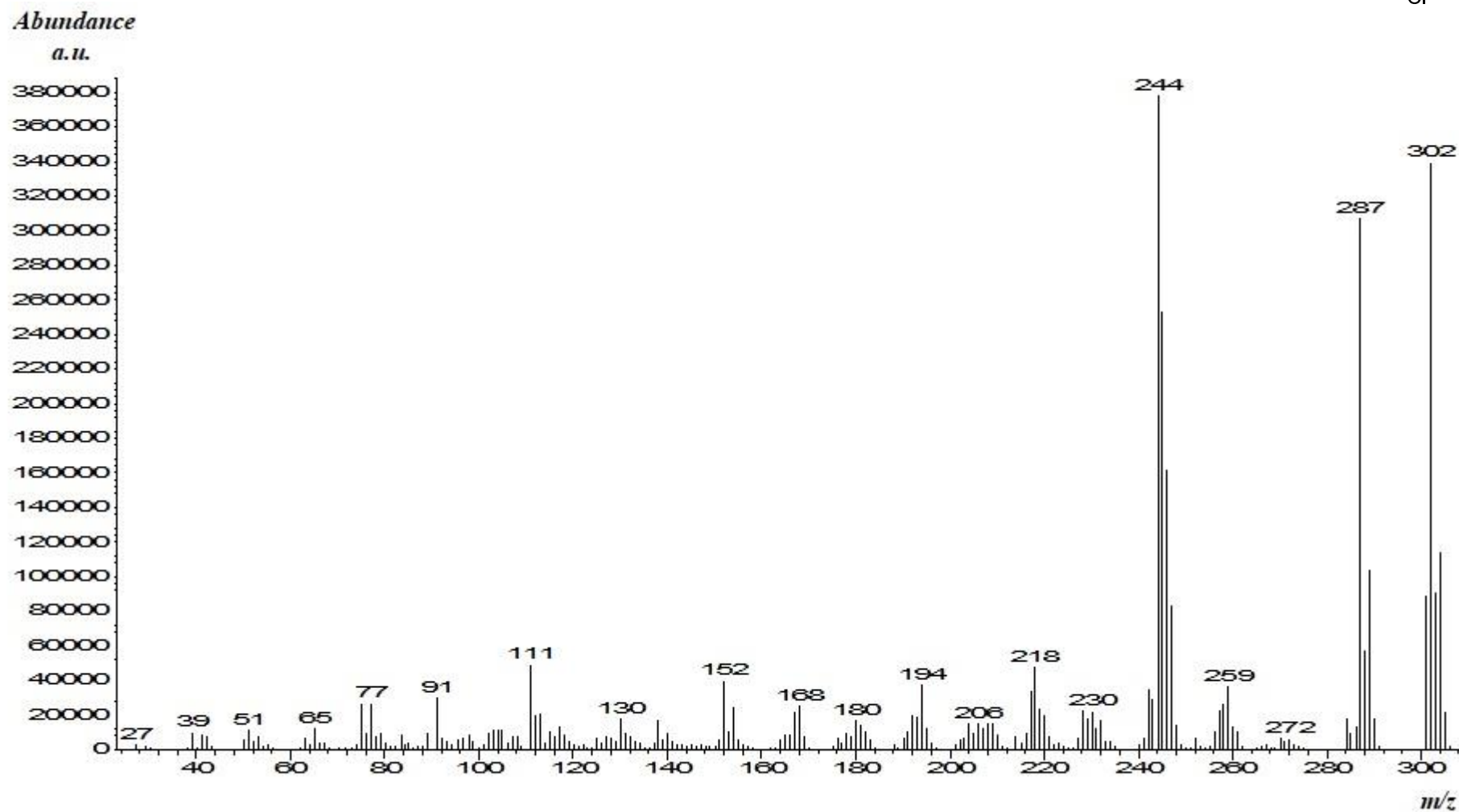
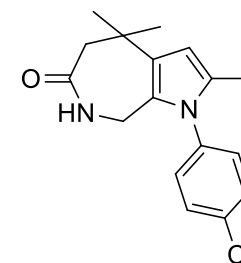
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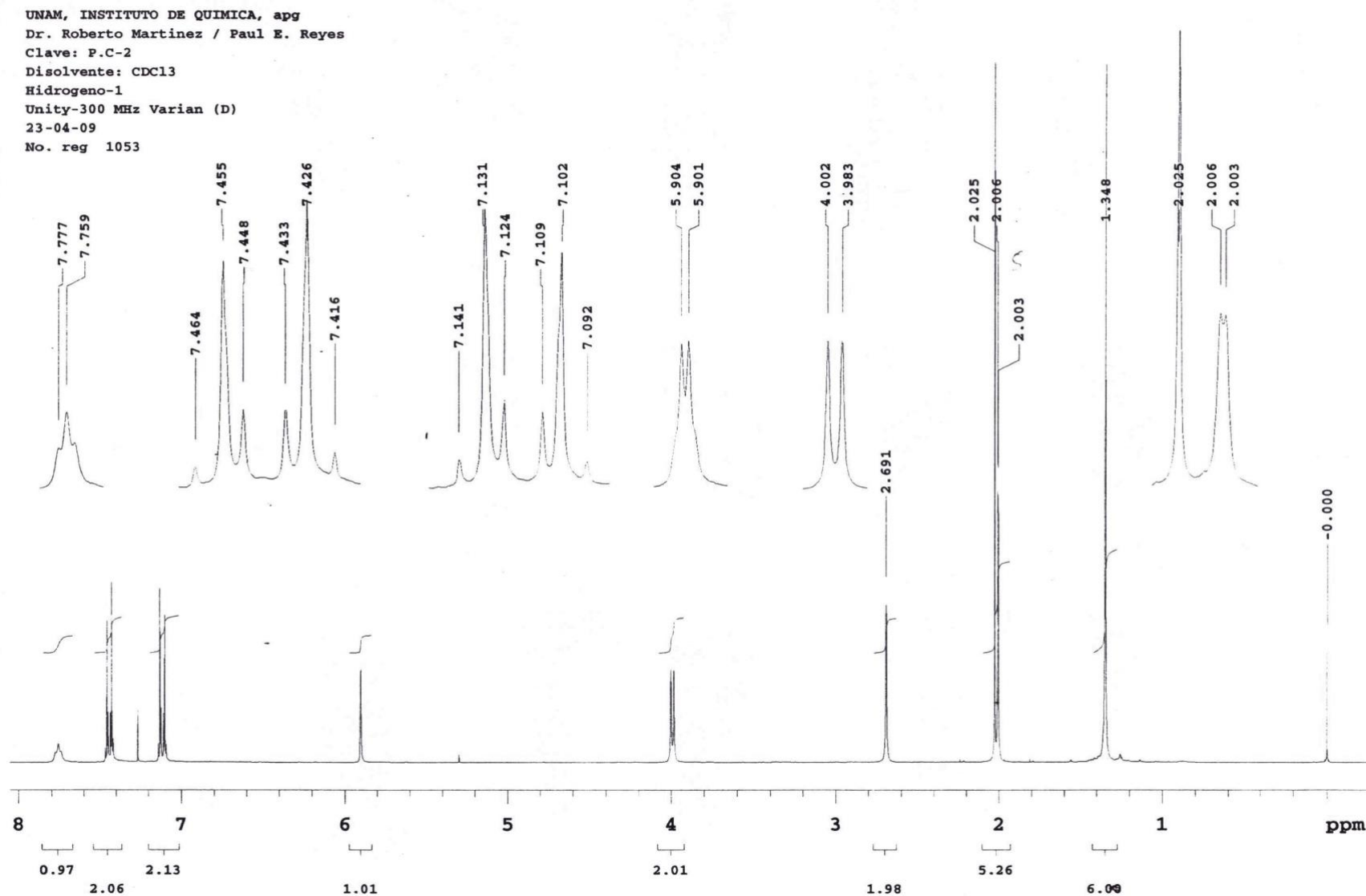
UNAM, INSTITUTO DE QUIMICA, E. Huerta
Dr. Roberto Martinez / Paul E, Reyes
Clave: P.C-1
Disolvente: CDCl_3
Carbbono- 13
Unity 75 MHz, Varian (D)
13-05-09
No. Reg. 1106



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

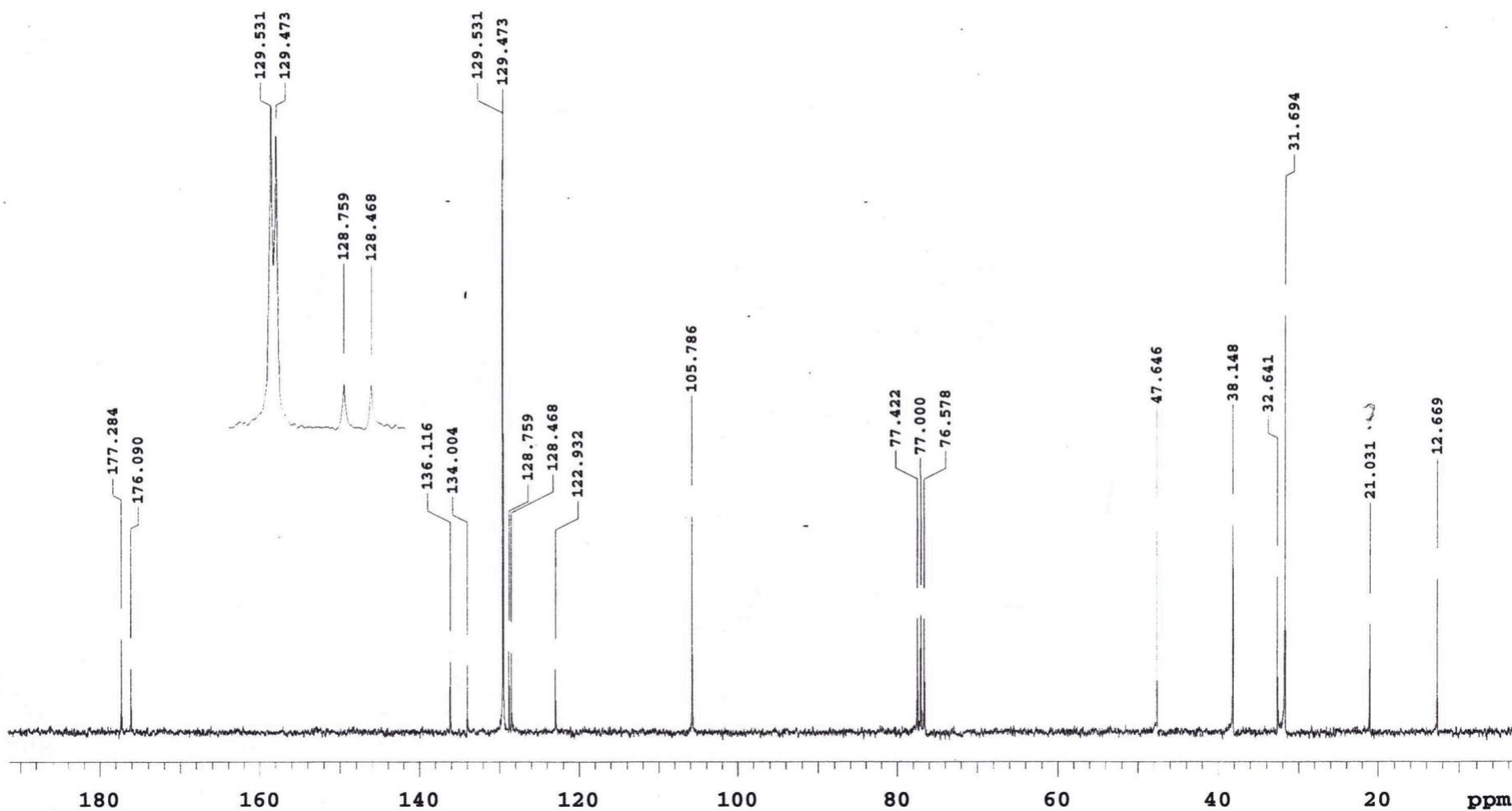
MS



^1H -NMR

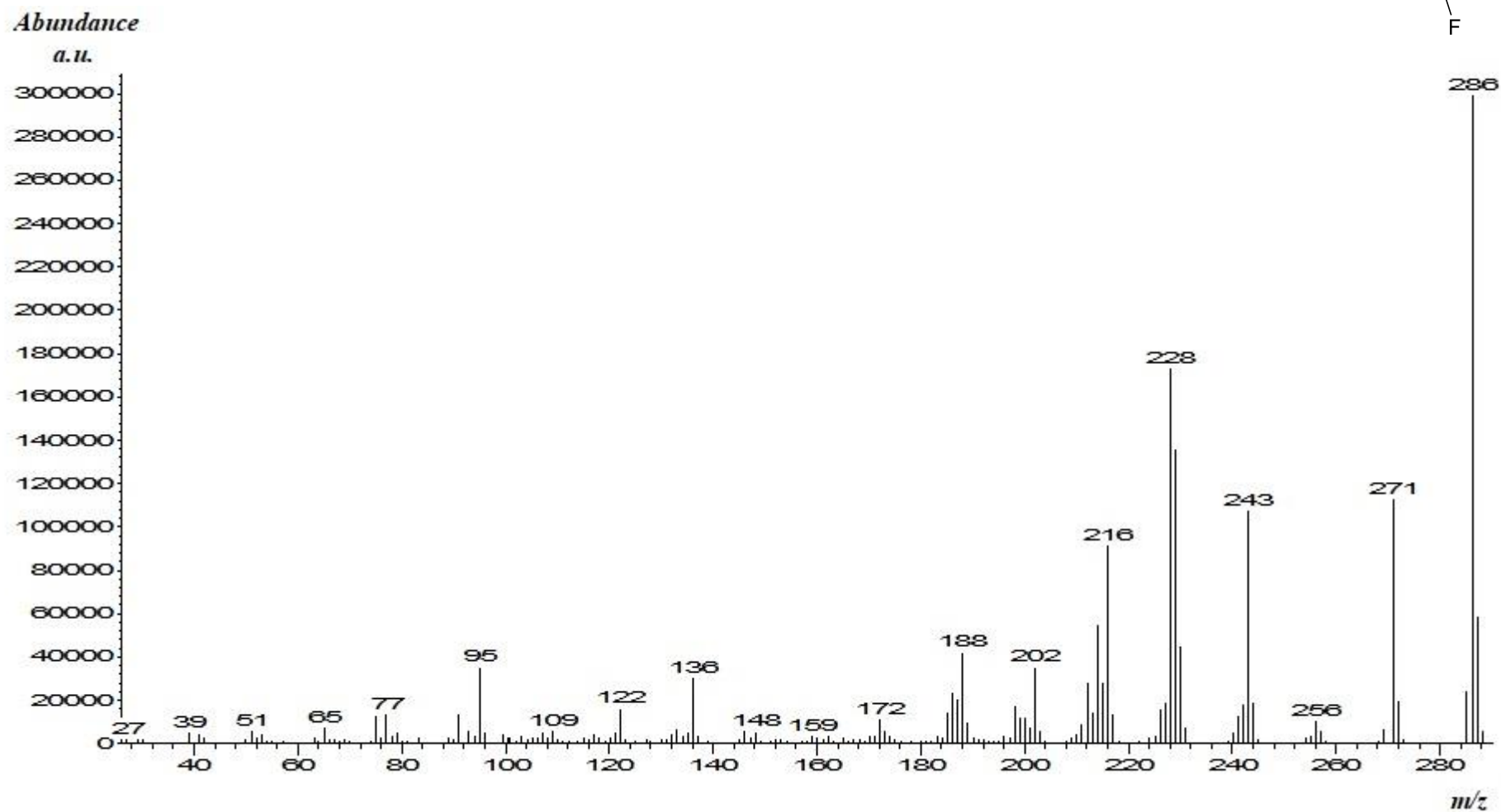
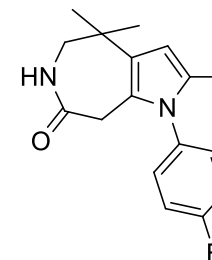
¹³C-NMR

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



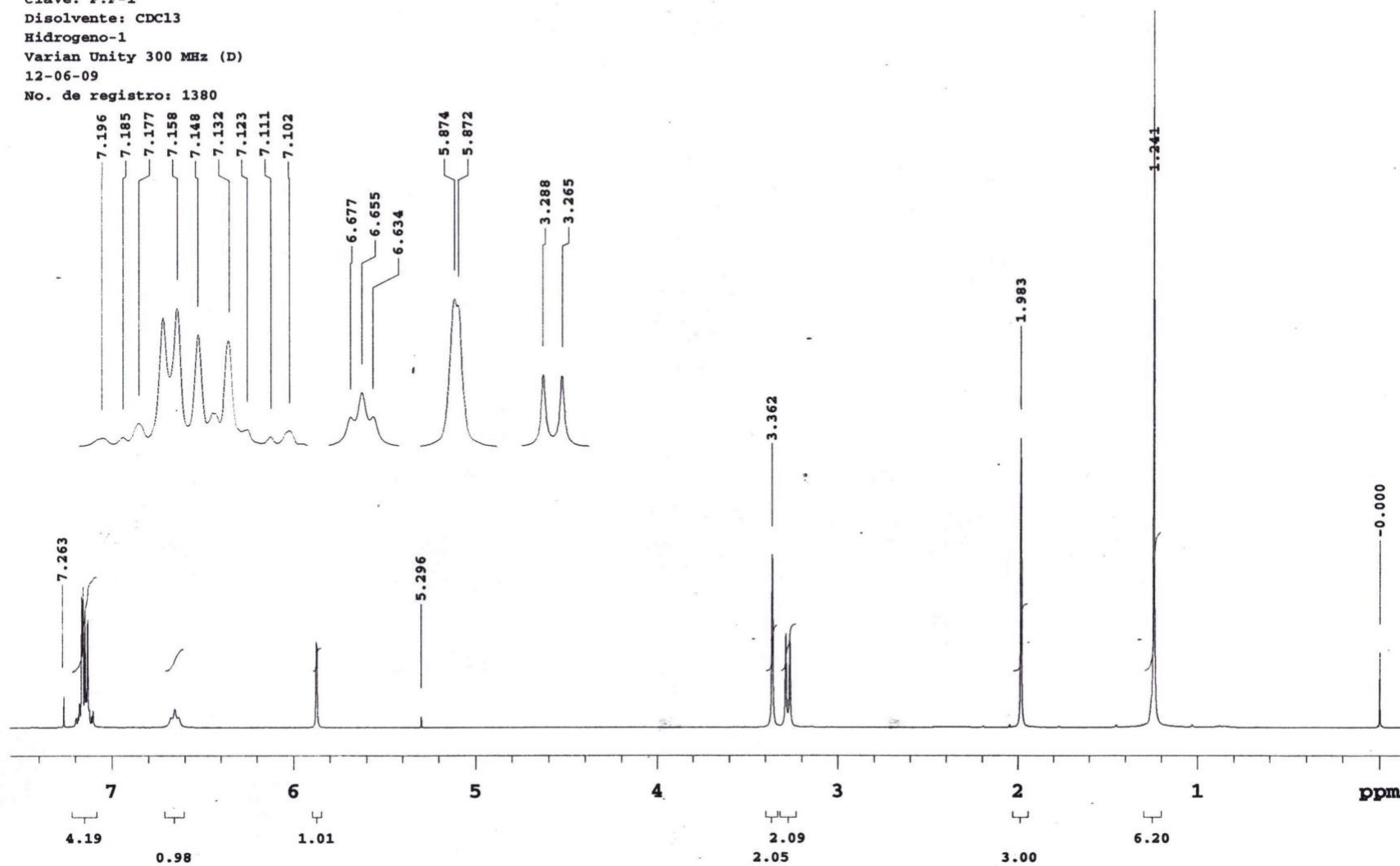
Compound 11c. 1-(4-Fluorophenyl)-2,4,4-trimethyl-4,5,6,8-tetrahydropyrrolo[2,3-d]azepin-7(1H)-one

MS



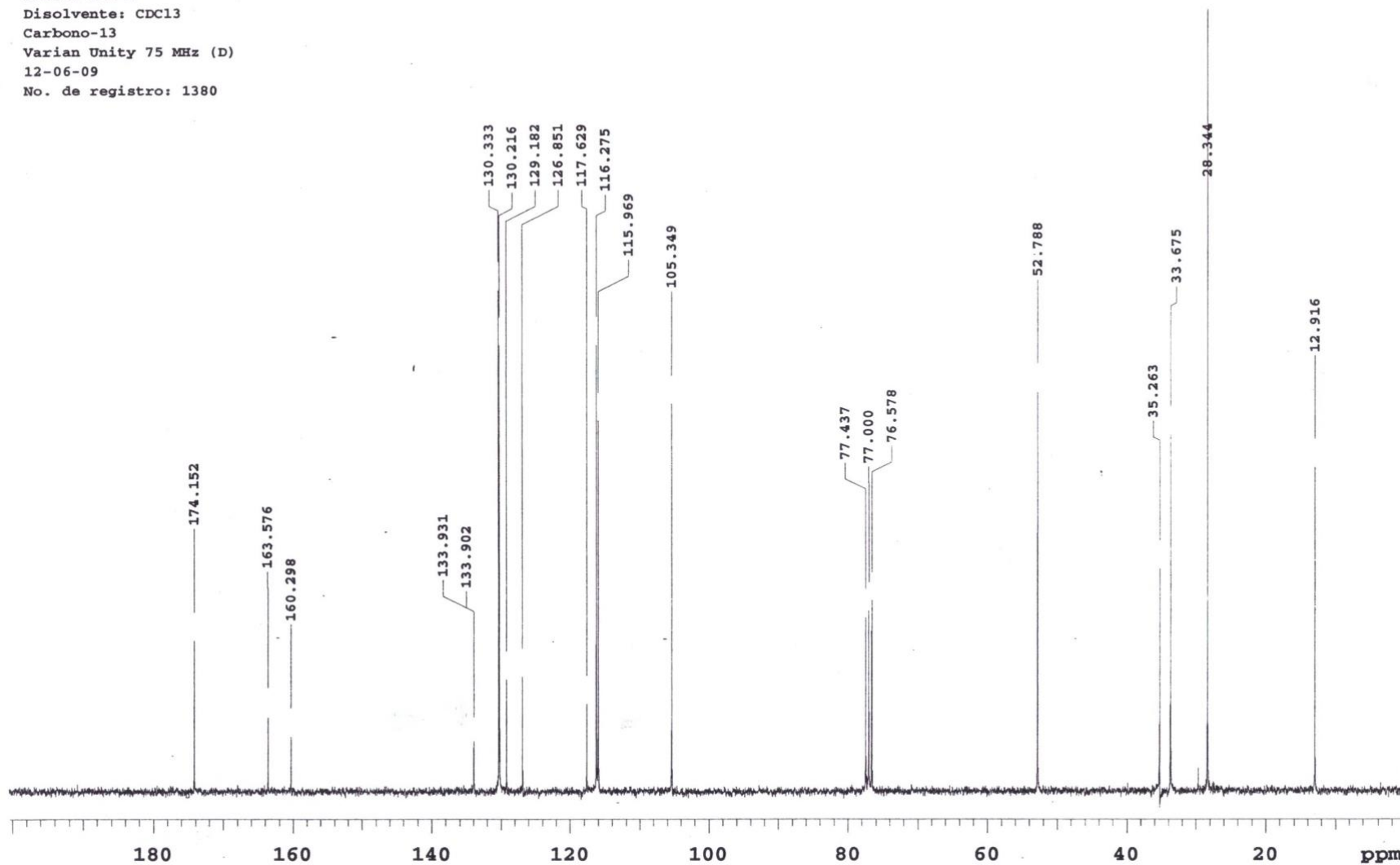
^1H -NMR

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



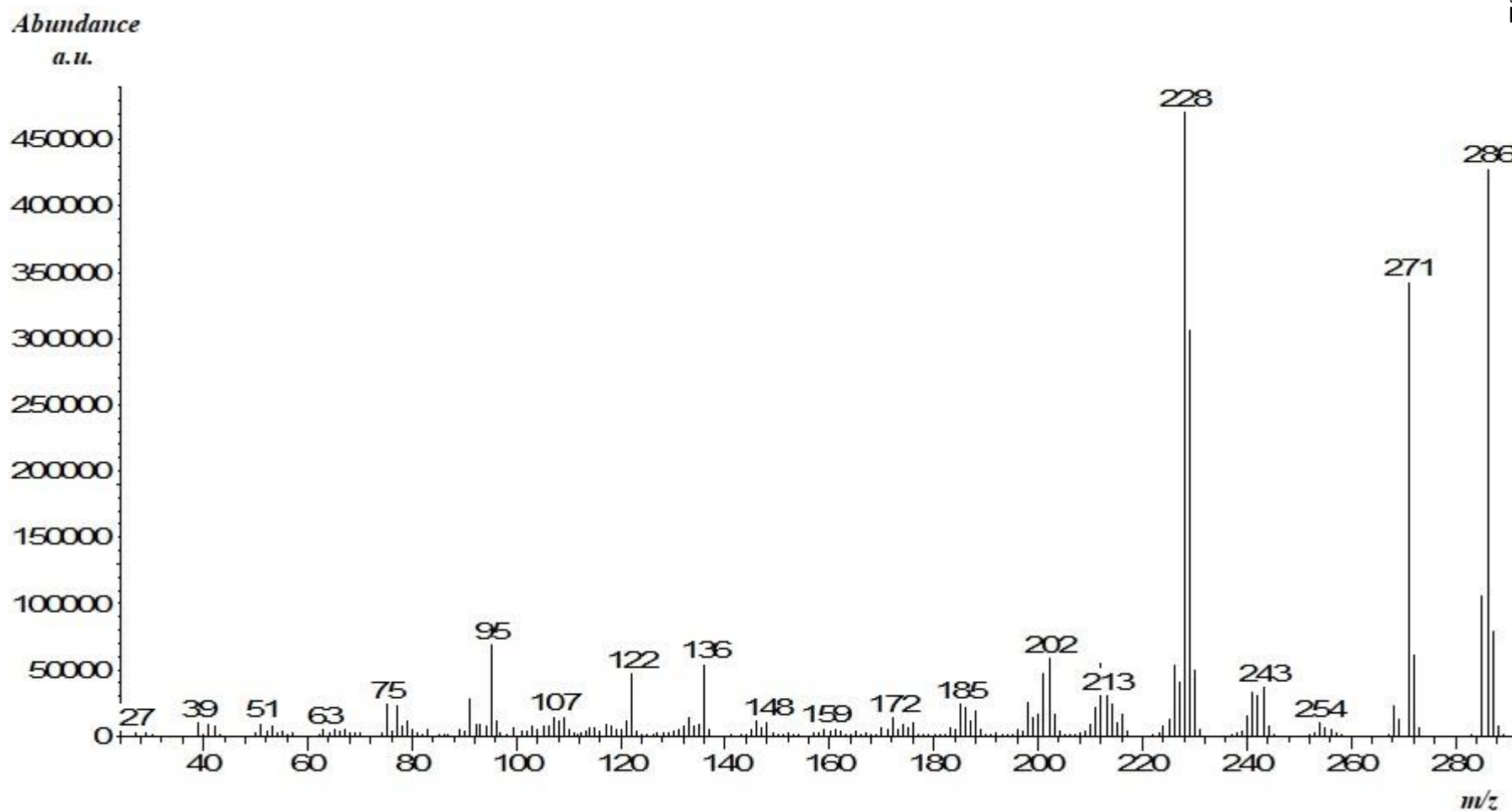
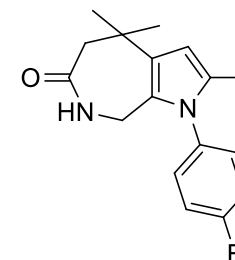
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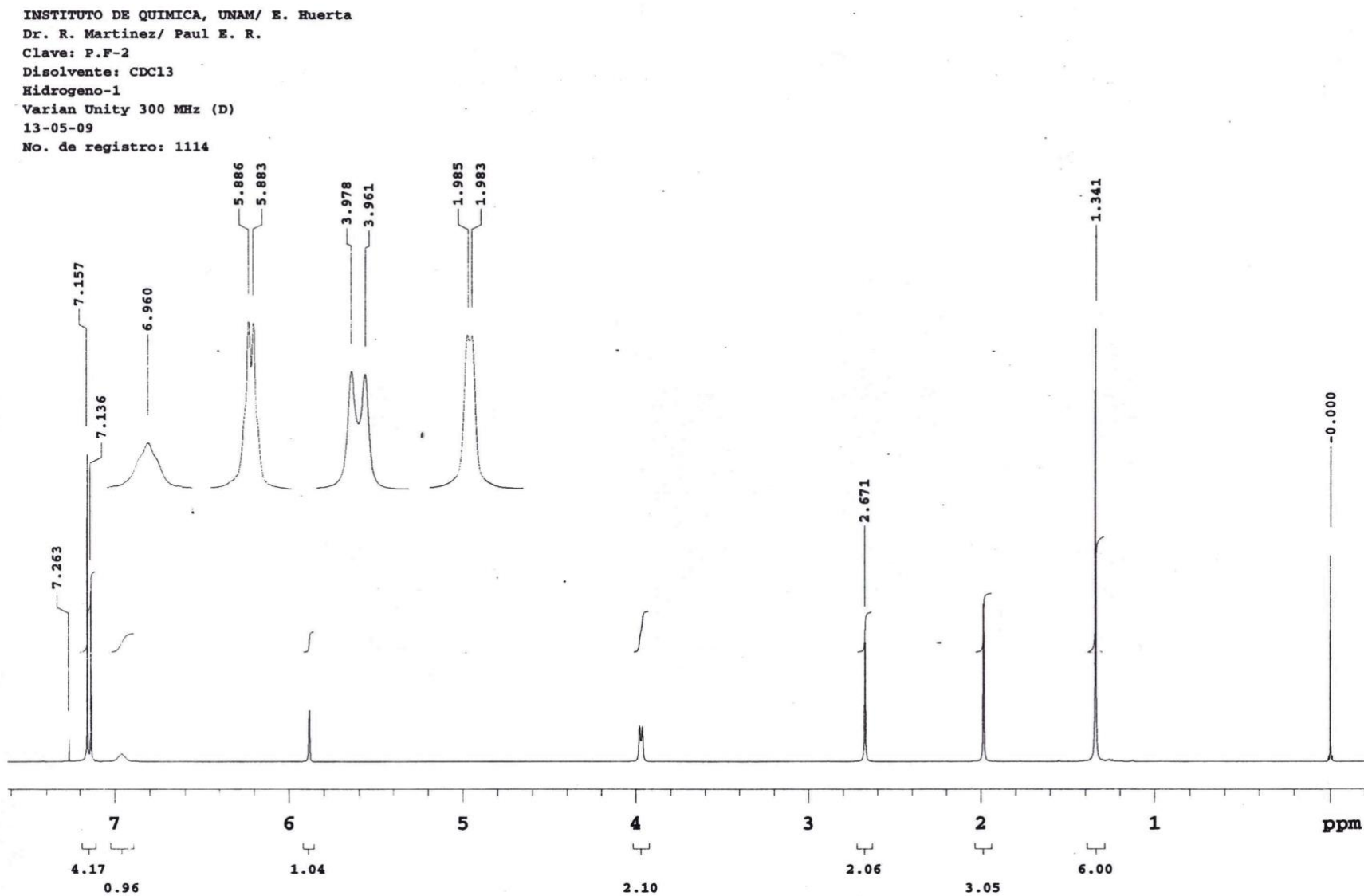
INSTITUTO DE QUIMICA, UNAM/ E. Huerta
Dr. R. Martinez/ Paul E. R.
Clave: P.F-1
Disolvente: CDCl_3
Carbono-13
Varian Unity 75 MHz (D)
12-06-09
No. de registro: 1380



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

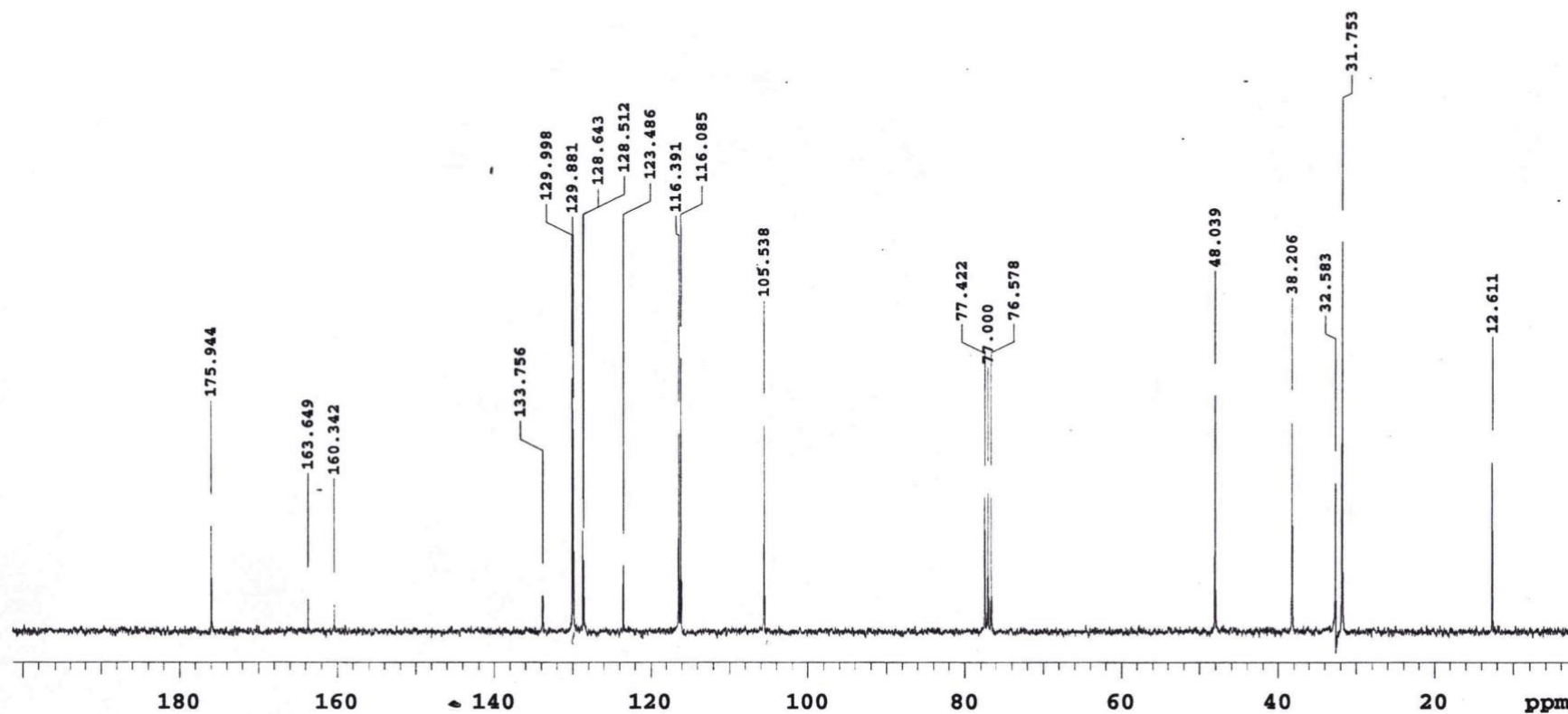
MS



^1H -NMR

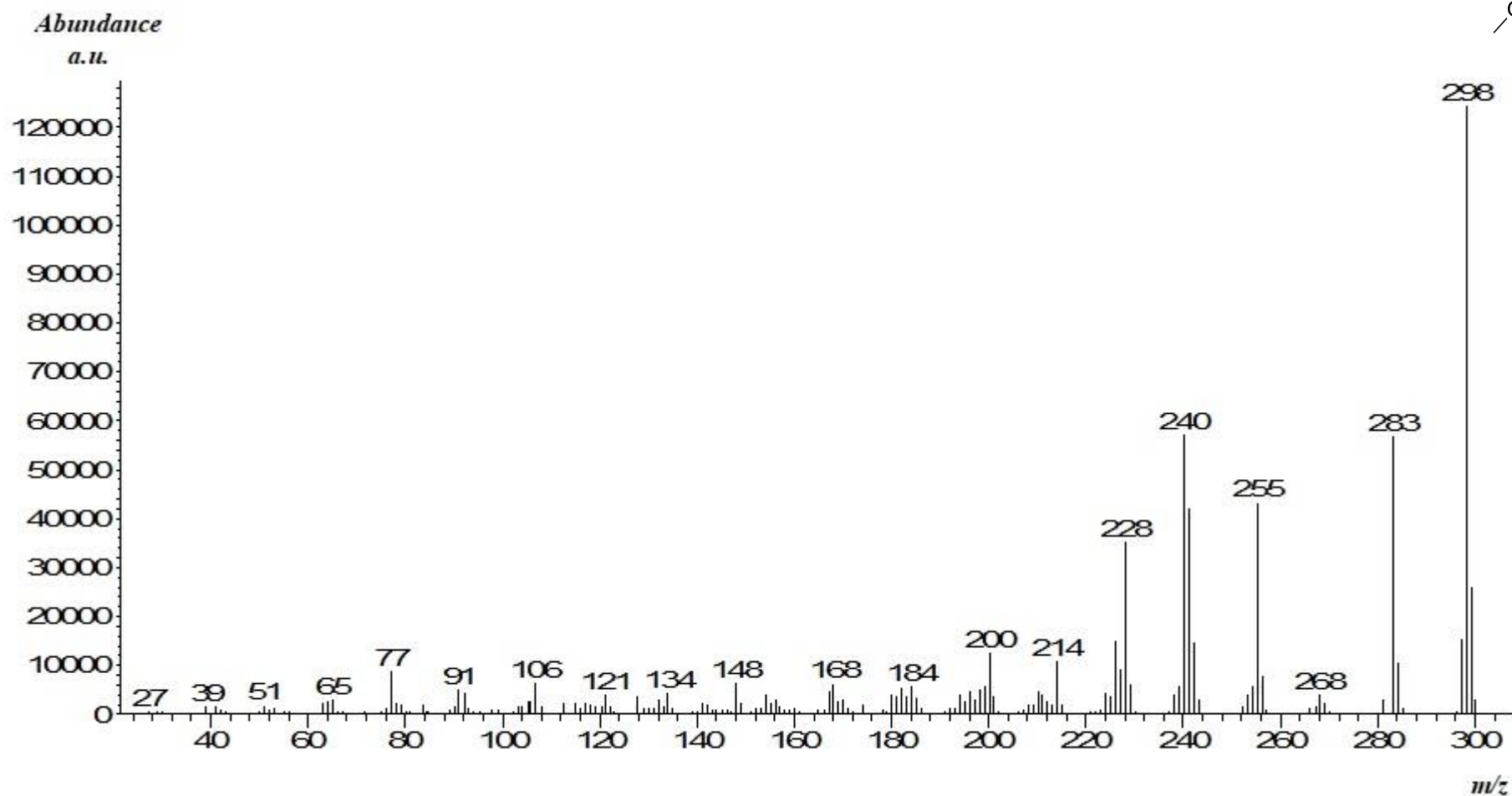
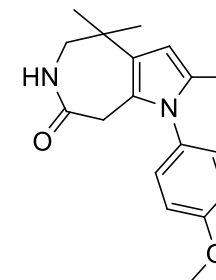
¹³C-NMR

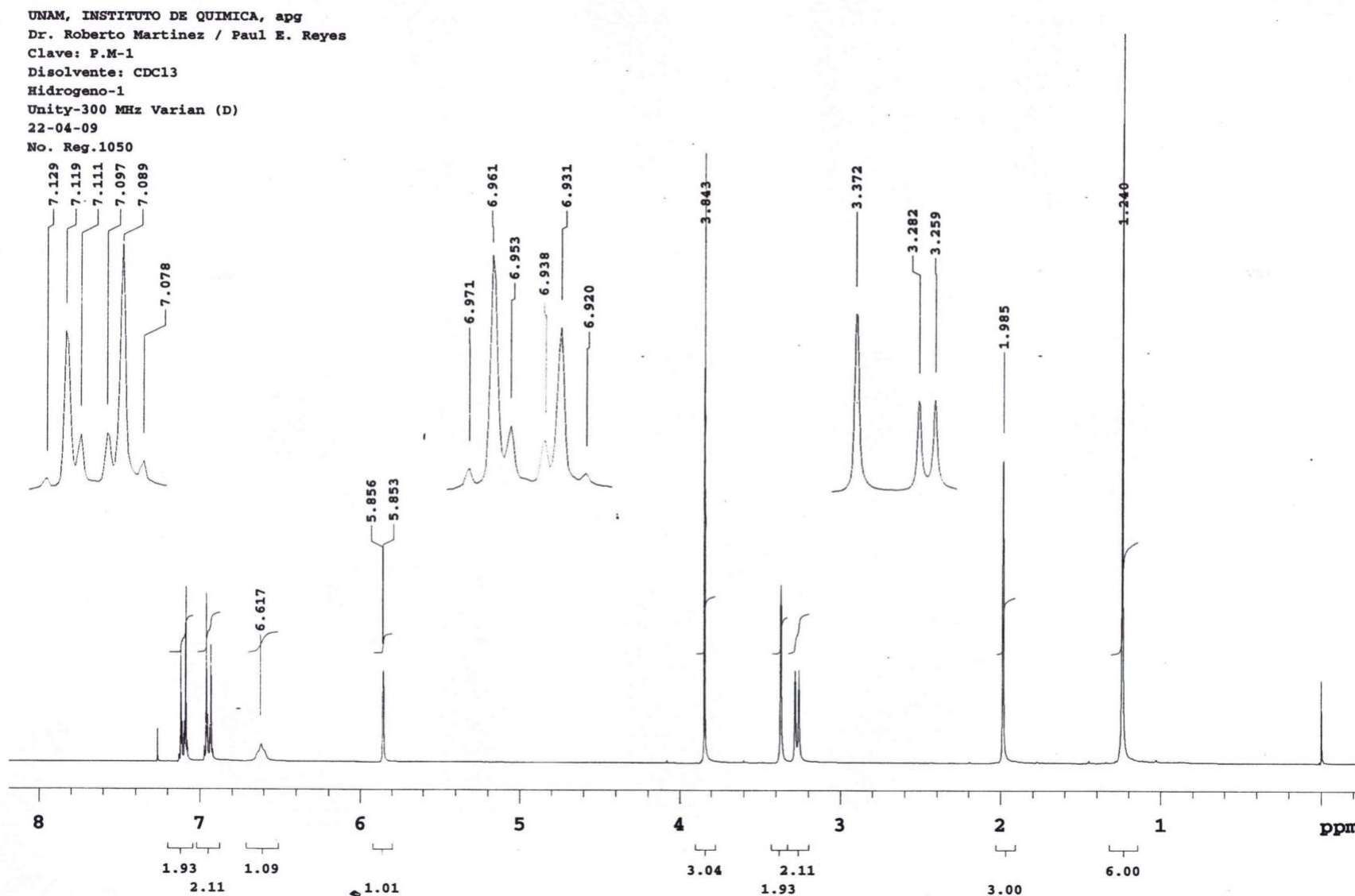
UNAM, INSTITUTO DE QUIMICA, E. Huerta
Dr. Roberto Martinez / Paul E. Reyes
Clave: P-E-2 44
Disolvente: CDCl₃
Carbpono-13
Unity 75 MHz, Varian (D)
13-05-09
No. Reg. 1114



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

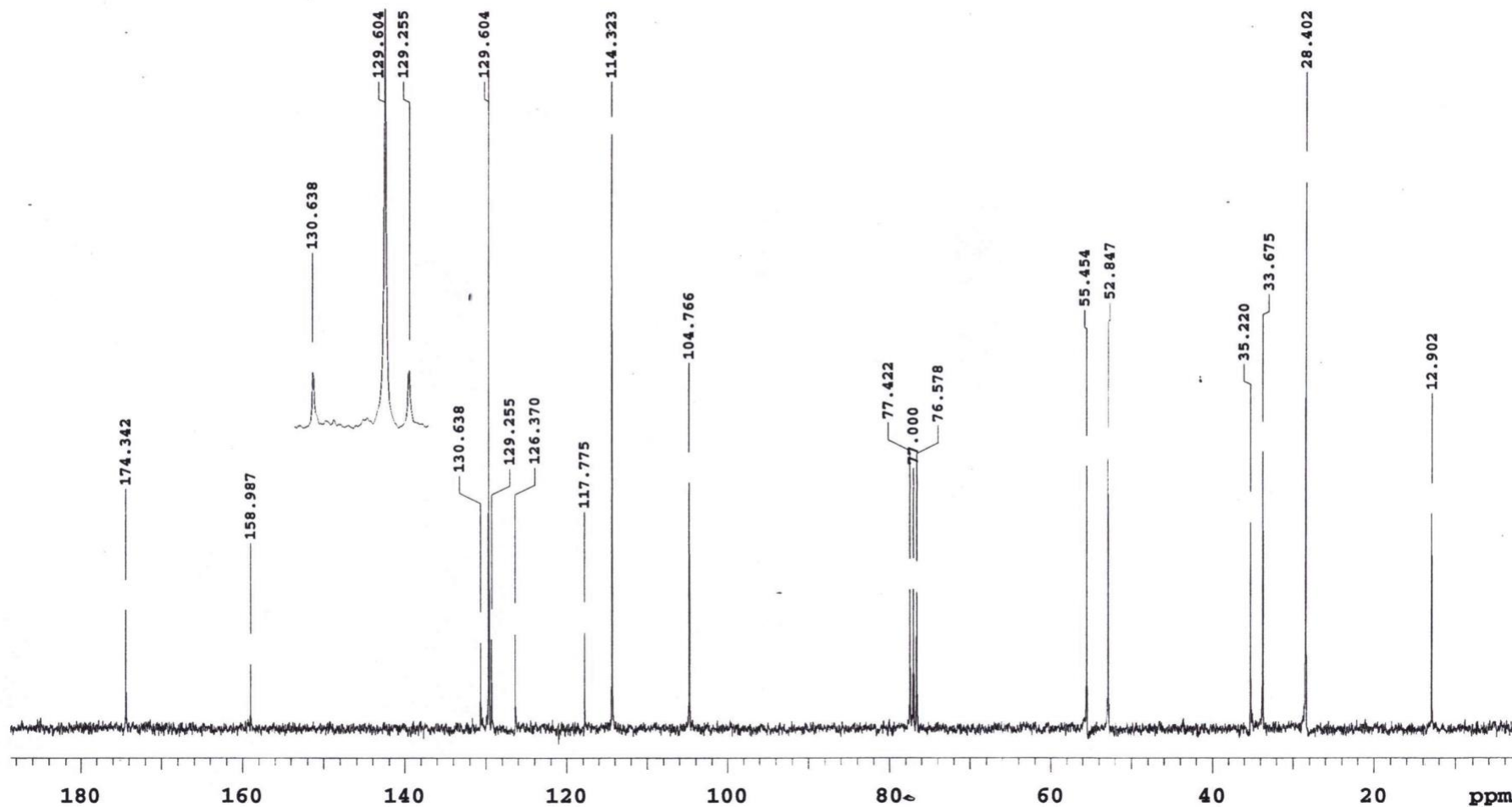
MS



^1H -NMR

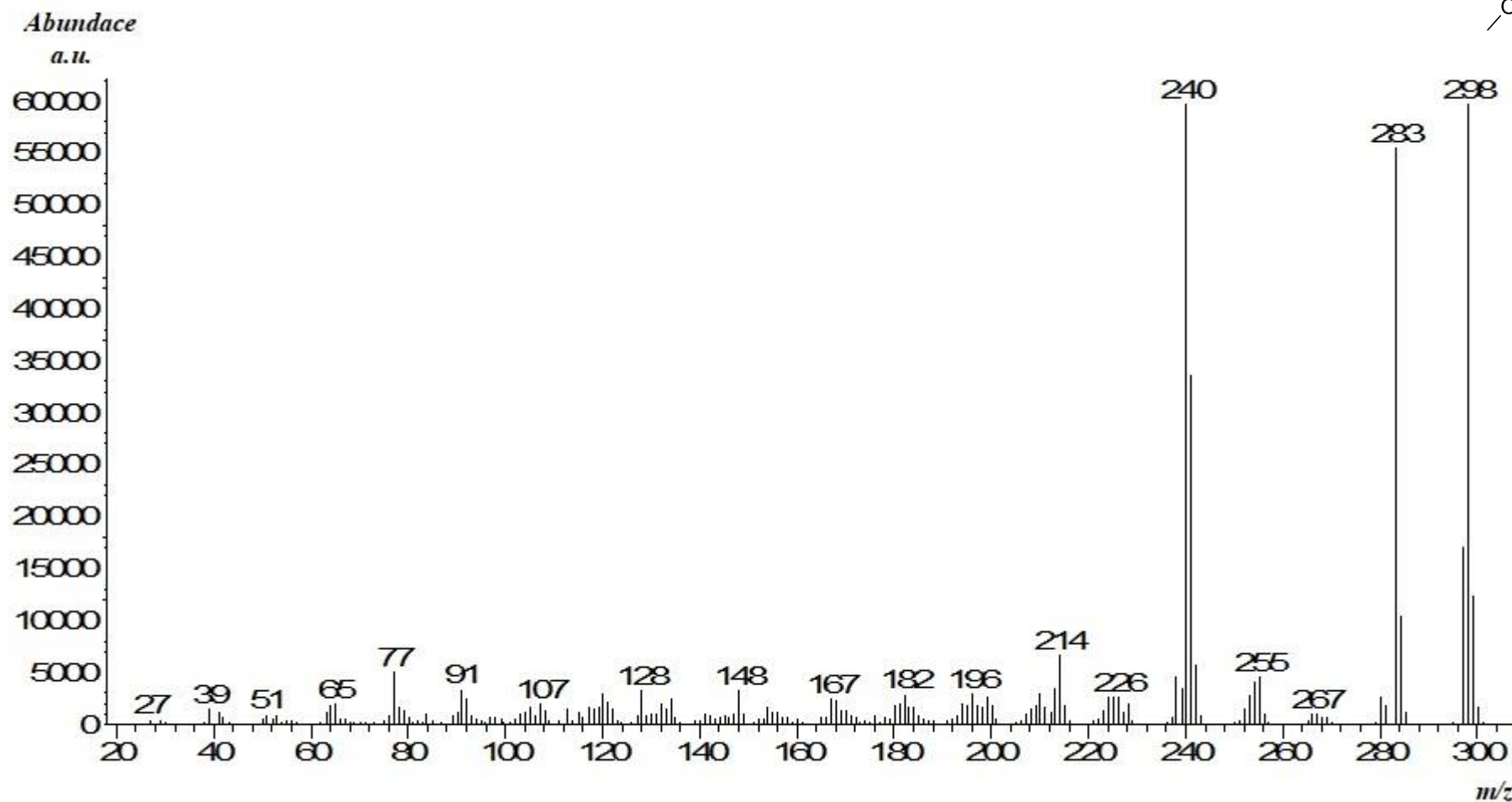
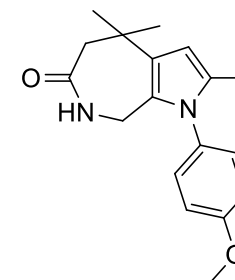
^{13}C -NMR

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



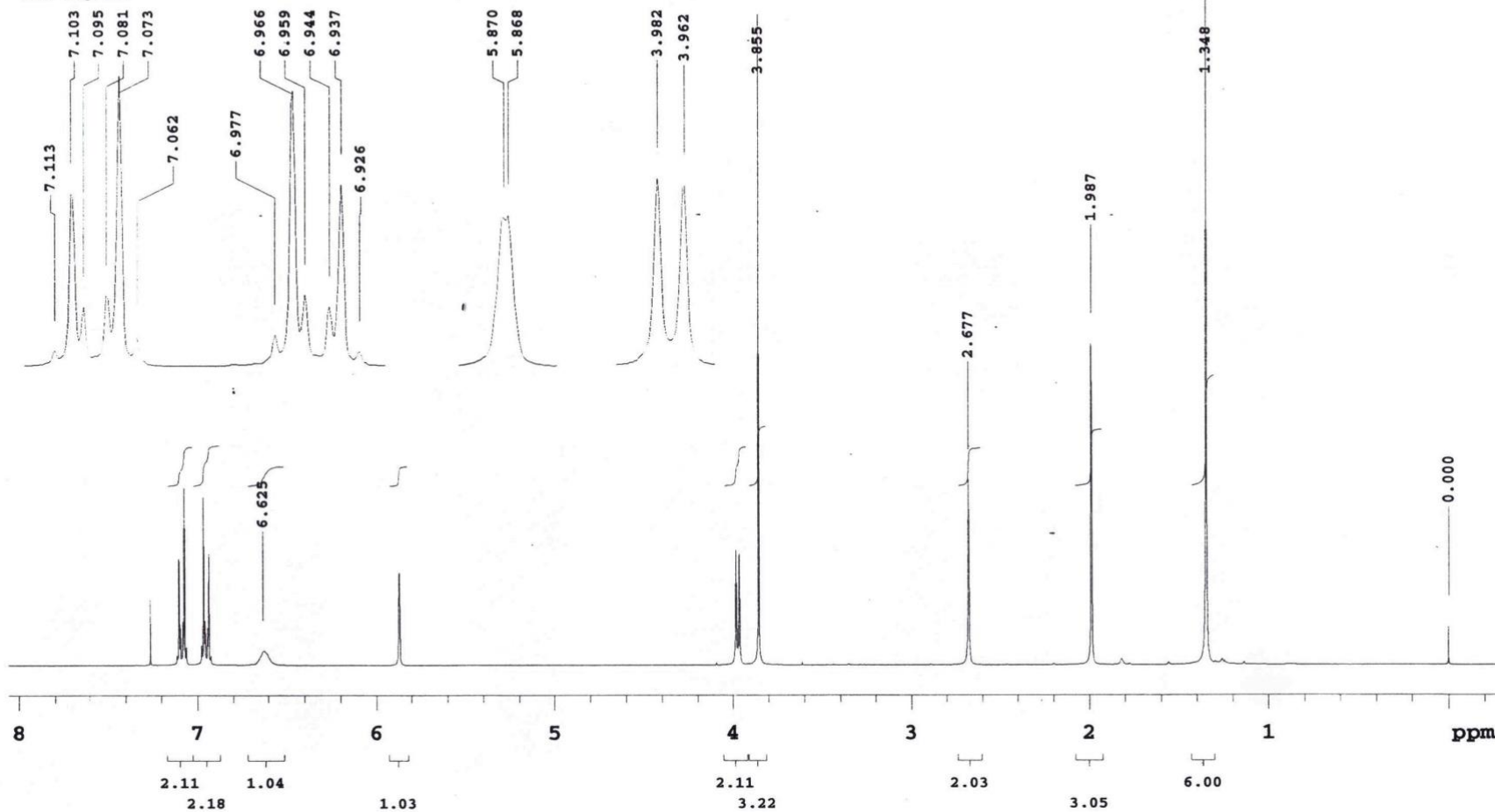
Compound 12d. 1-(4-Methoxyphenyl)-2,4,4-trimethyl-4,5,7,8-tetrahydropyrrolo[2,3-c]azepin-6(1H)-one

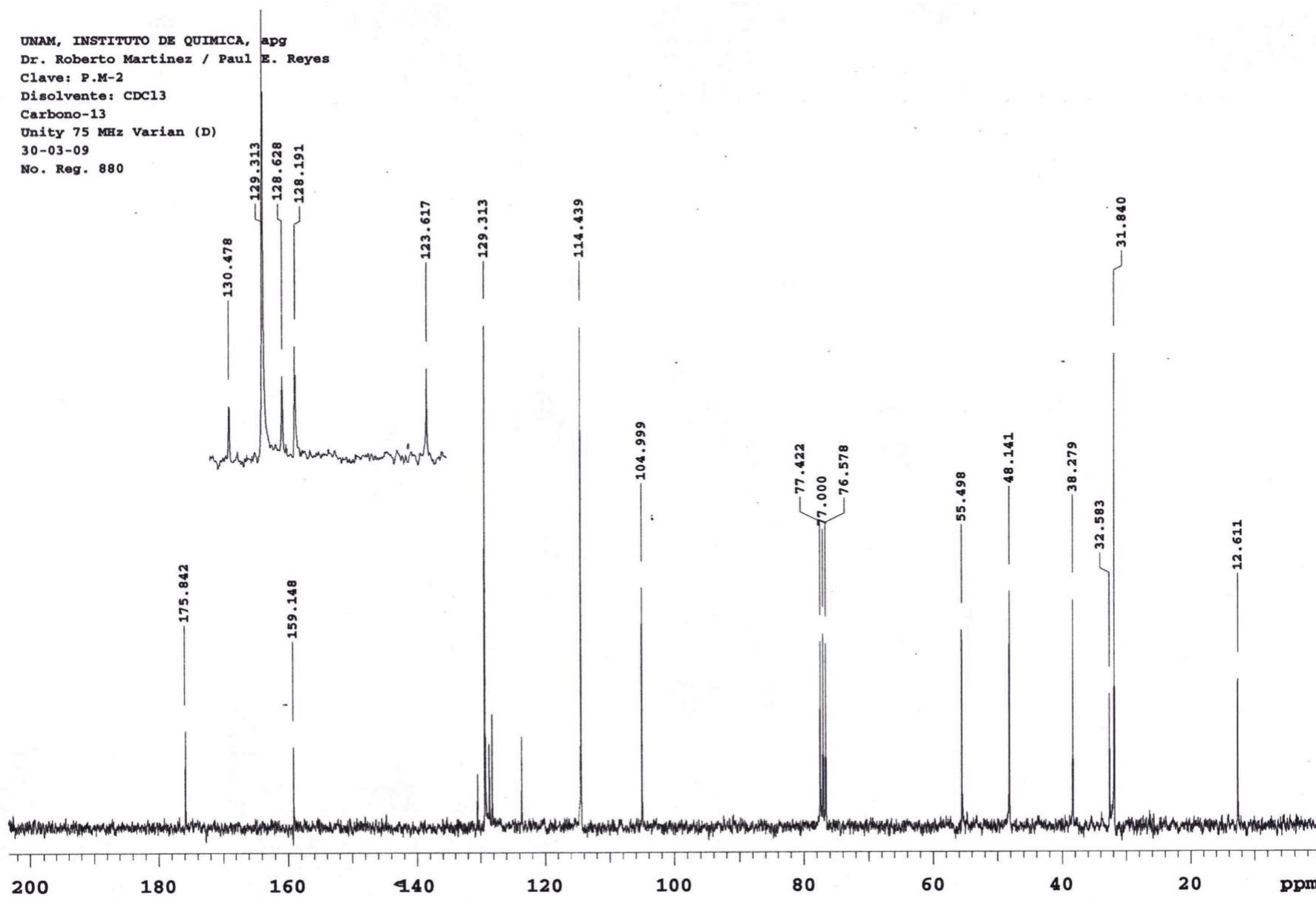
MS



^1H -NMR

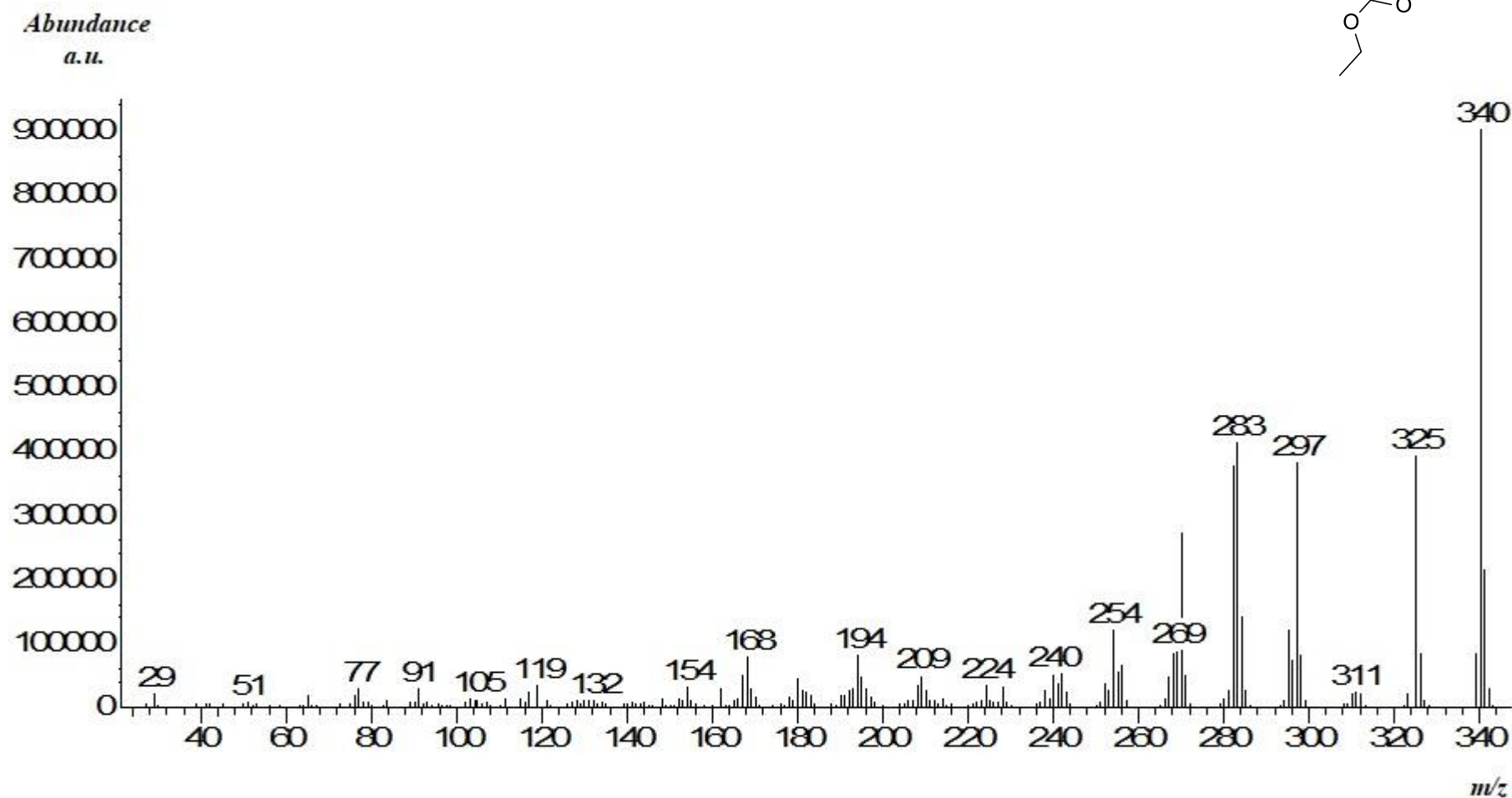
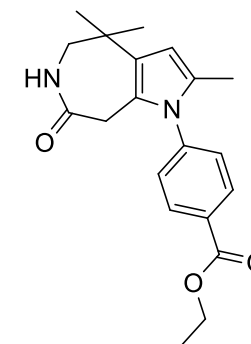
UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E. Reyes
Clave: P.M-2
Disolvente: CDCl_3
Hidrogeno-1
Unity 300 MHz Varian (D)
30-03-09
No. Reg. 880

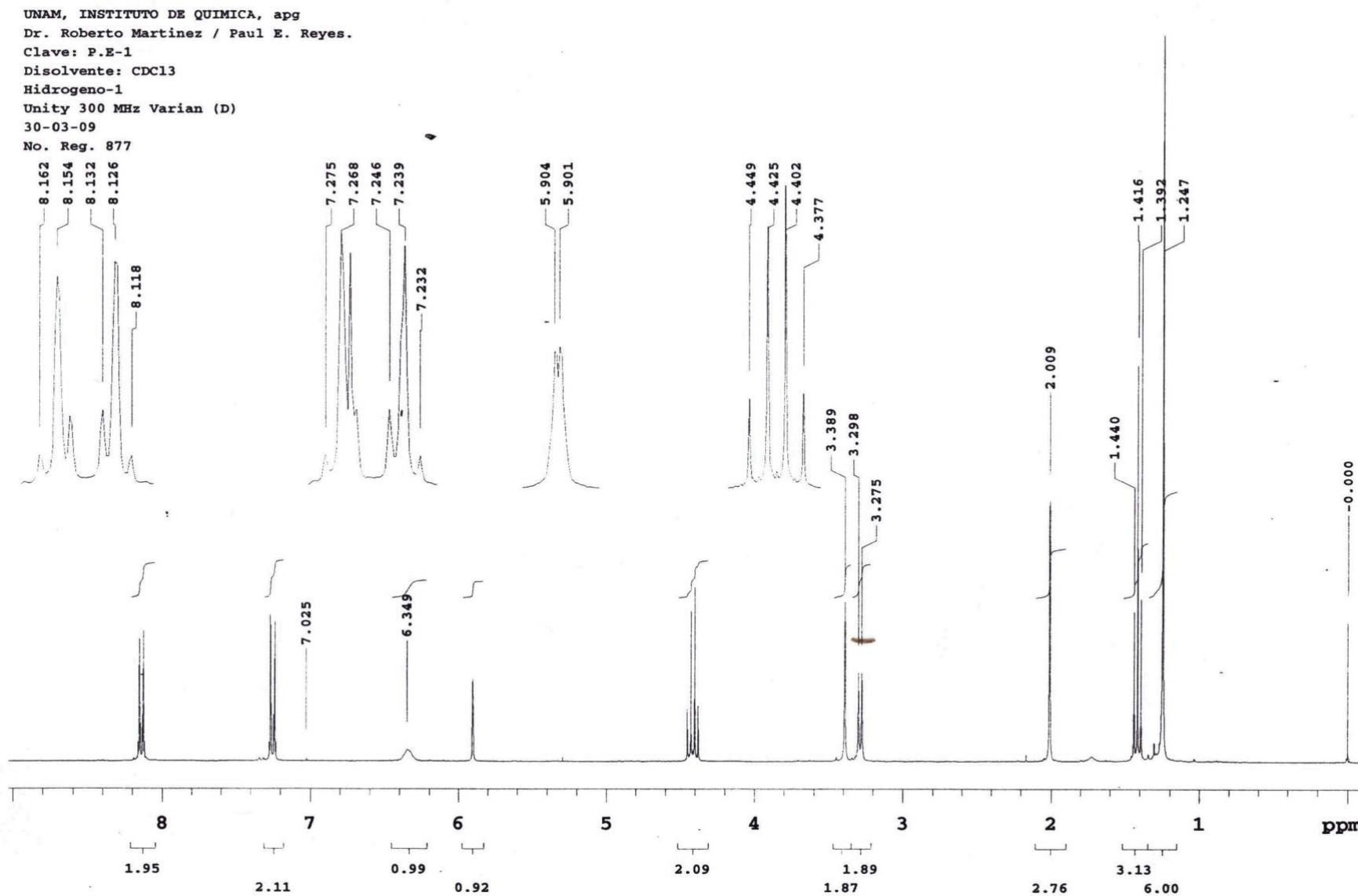


^{13}C -NMR

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

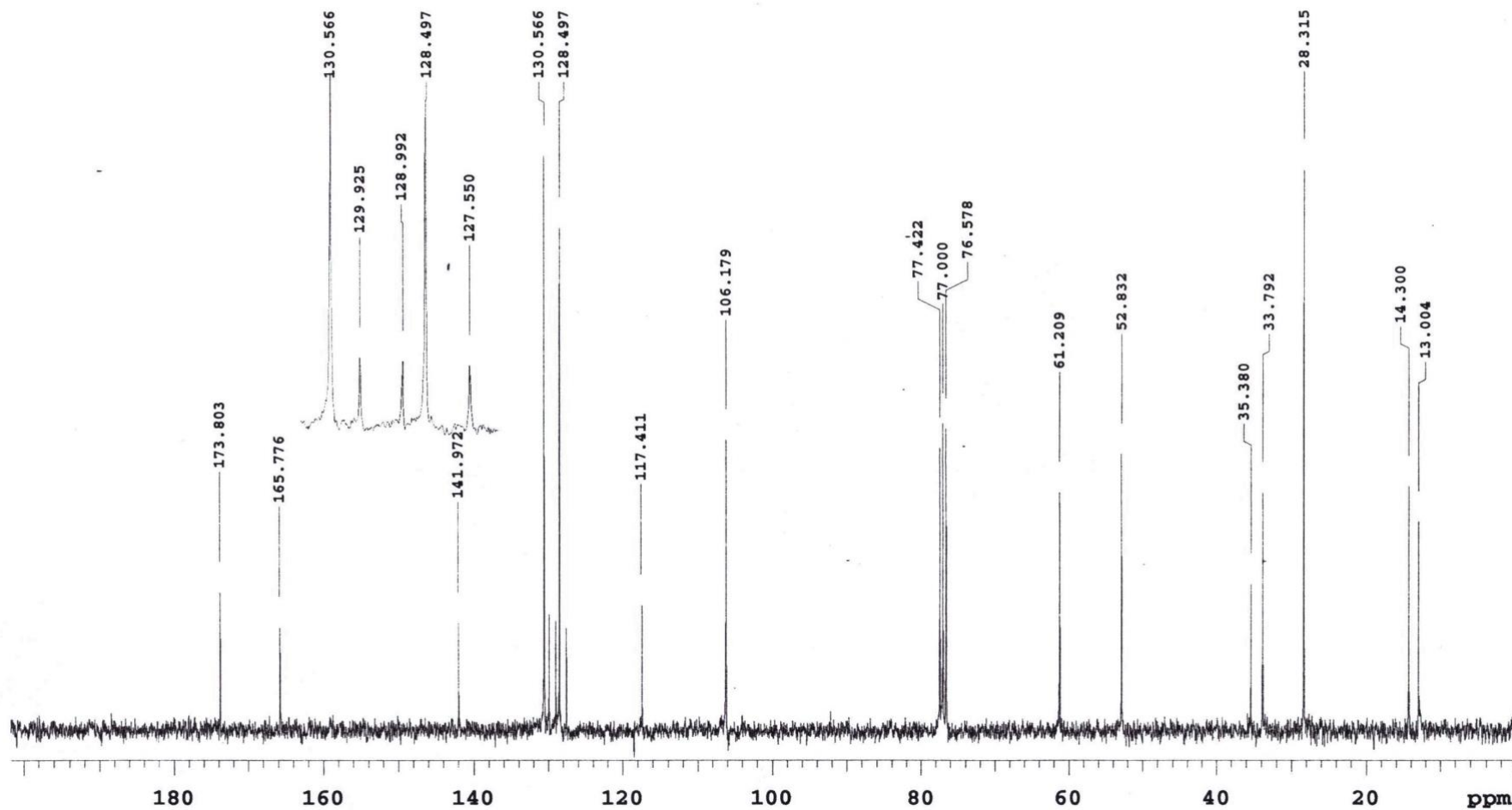
MS



^1H -NMR

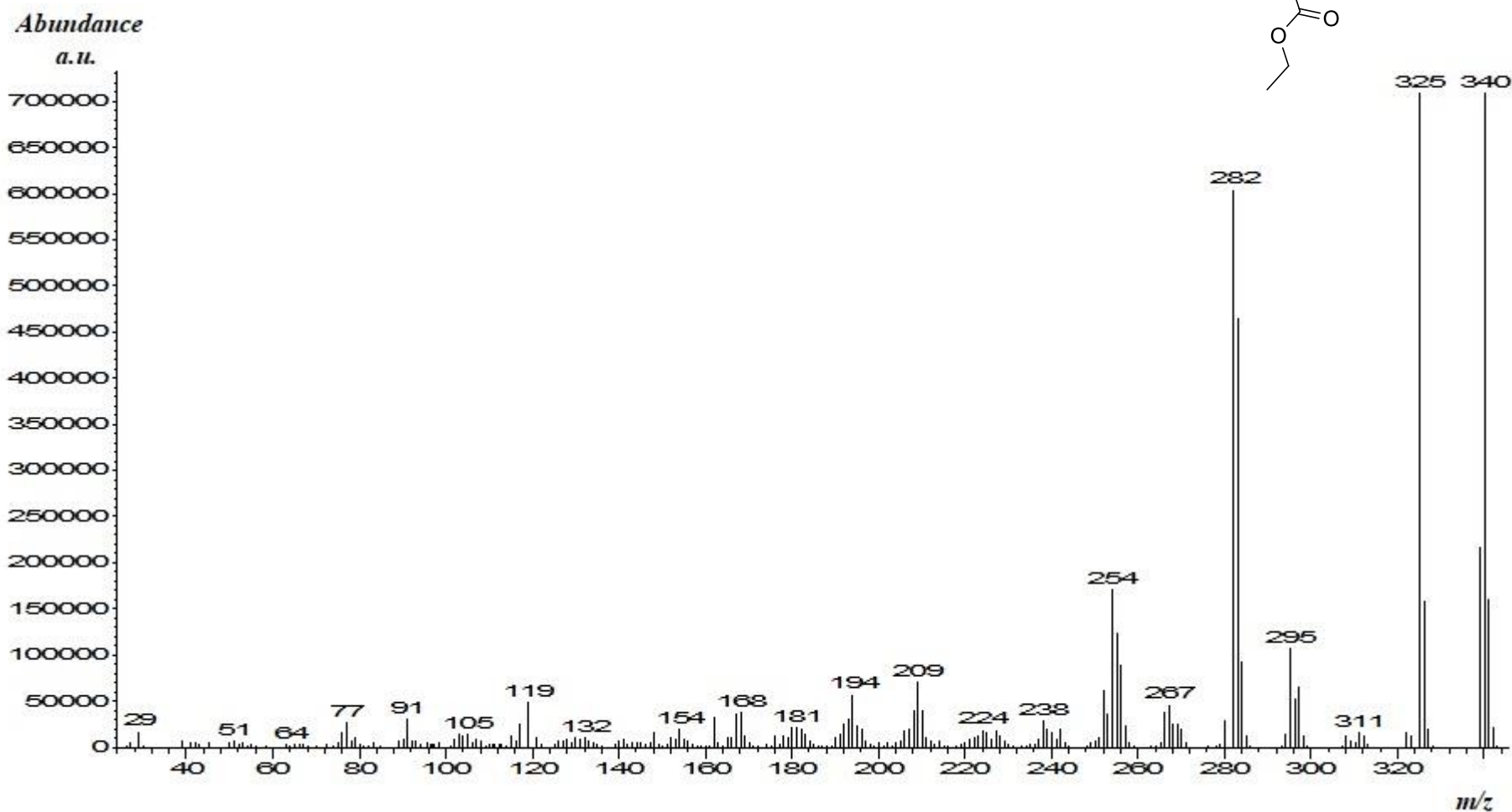
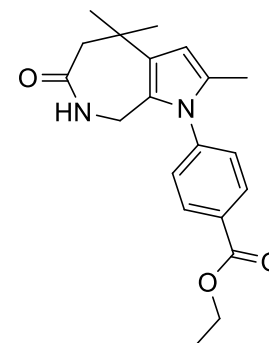
^{13}C -NMR

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



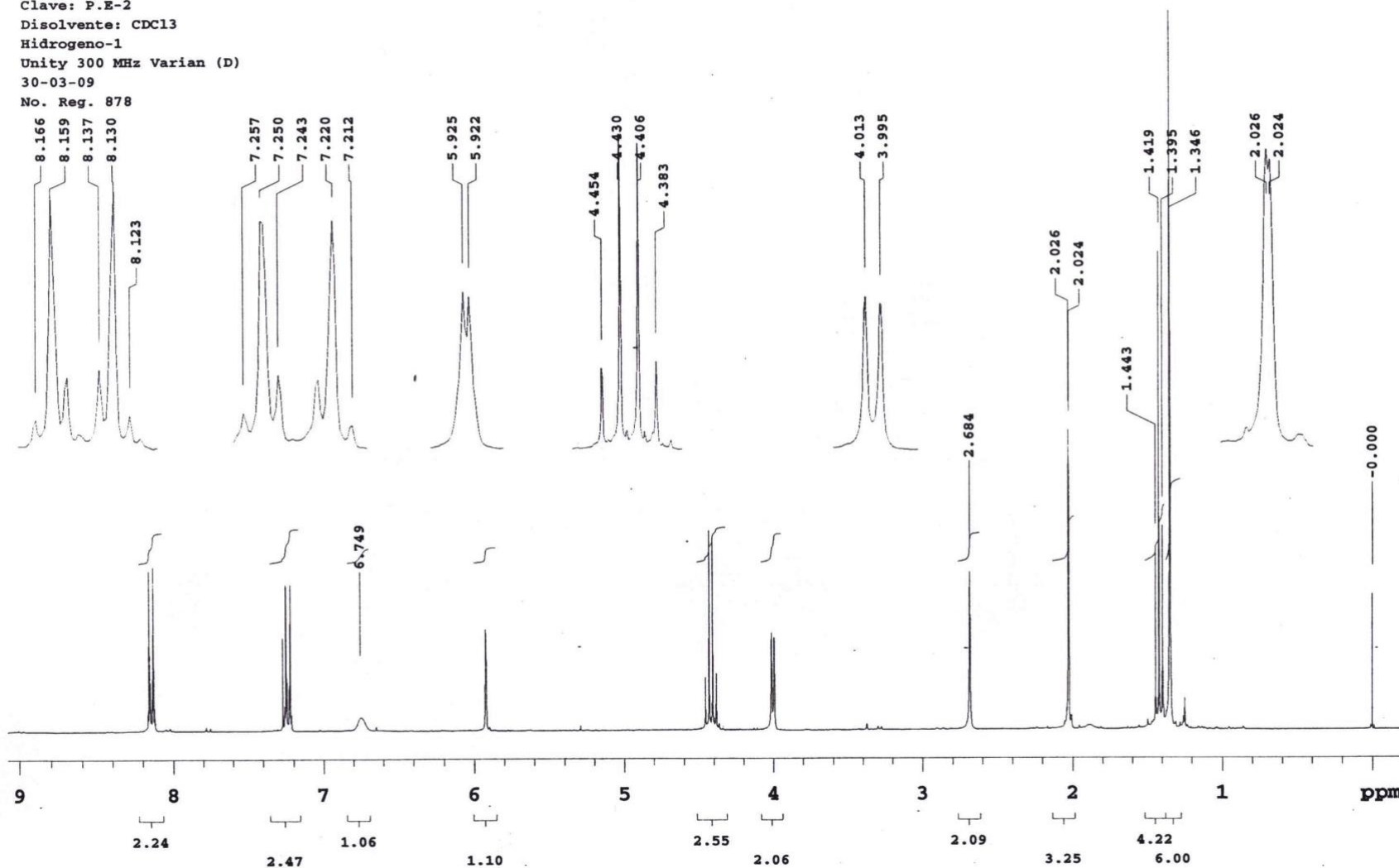
Compound 12e. *Ethyl 4-(2,4,4-trimethyl-6-oxo-5,6,7,8-tetrahydropyrrolo[2,3-c]azepin-1(4H)-yl)benzoate*

MS



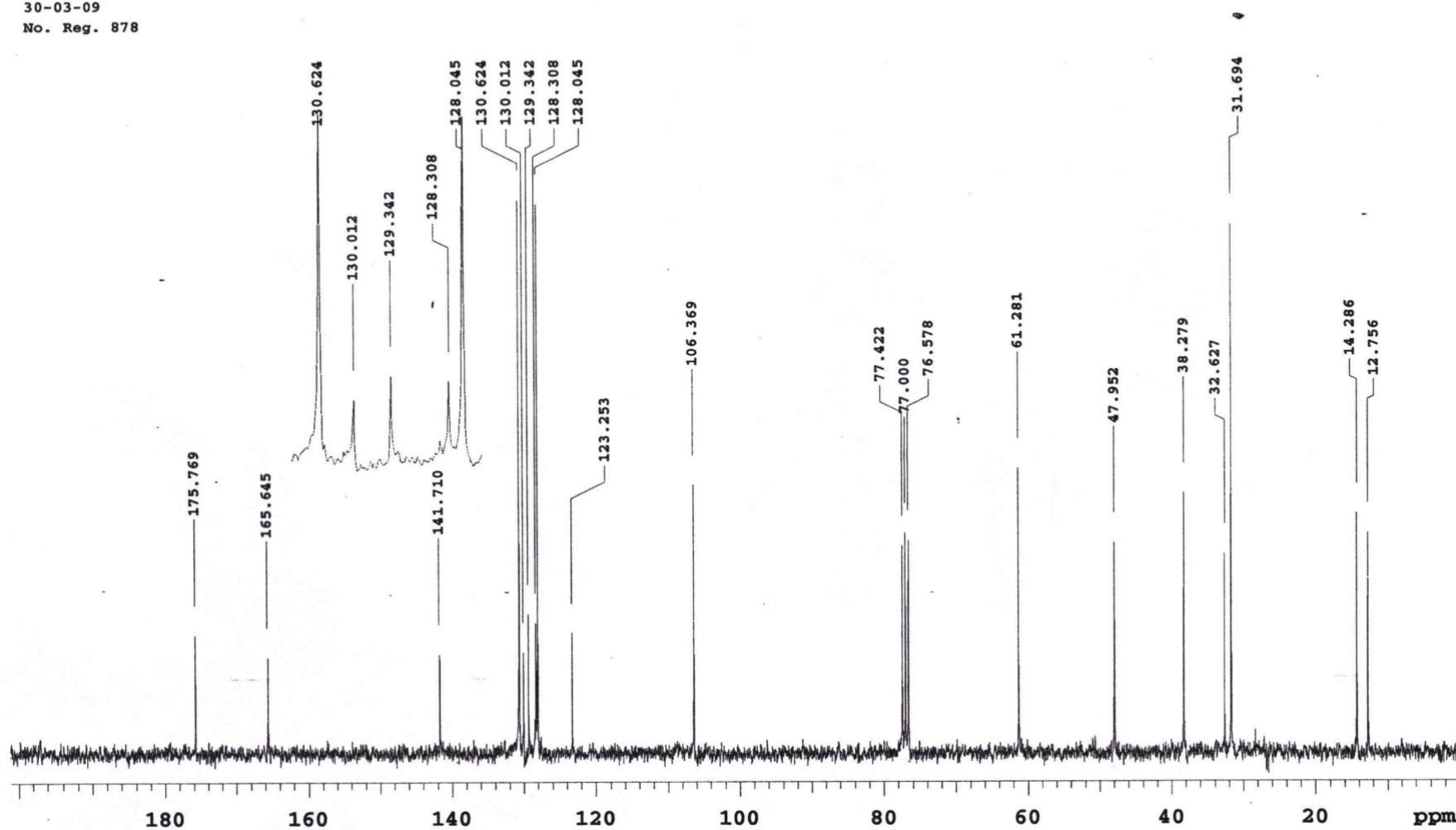
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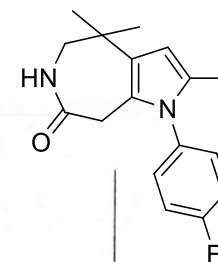
UNAM, INSTITUTO DE QUIMICA, apg
Dr. Roberto Martinez / Paul E. Reyes.
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Disolvente: CDCl_3
Hidrogeno-1
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30-03-09
No. Reg. 878



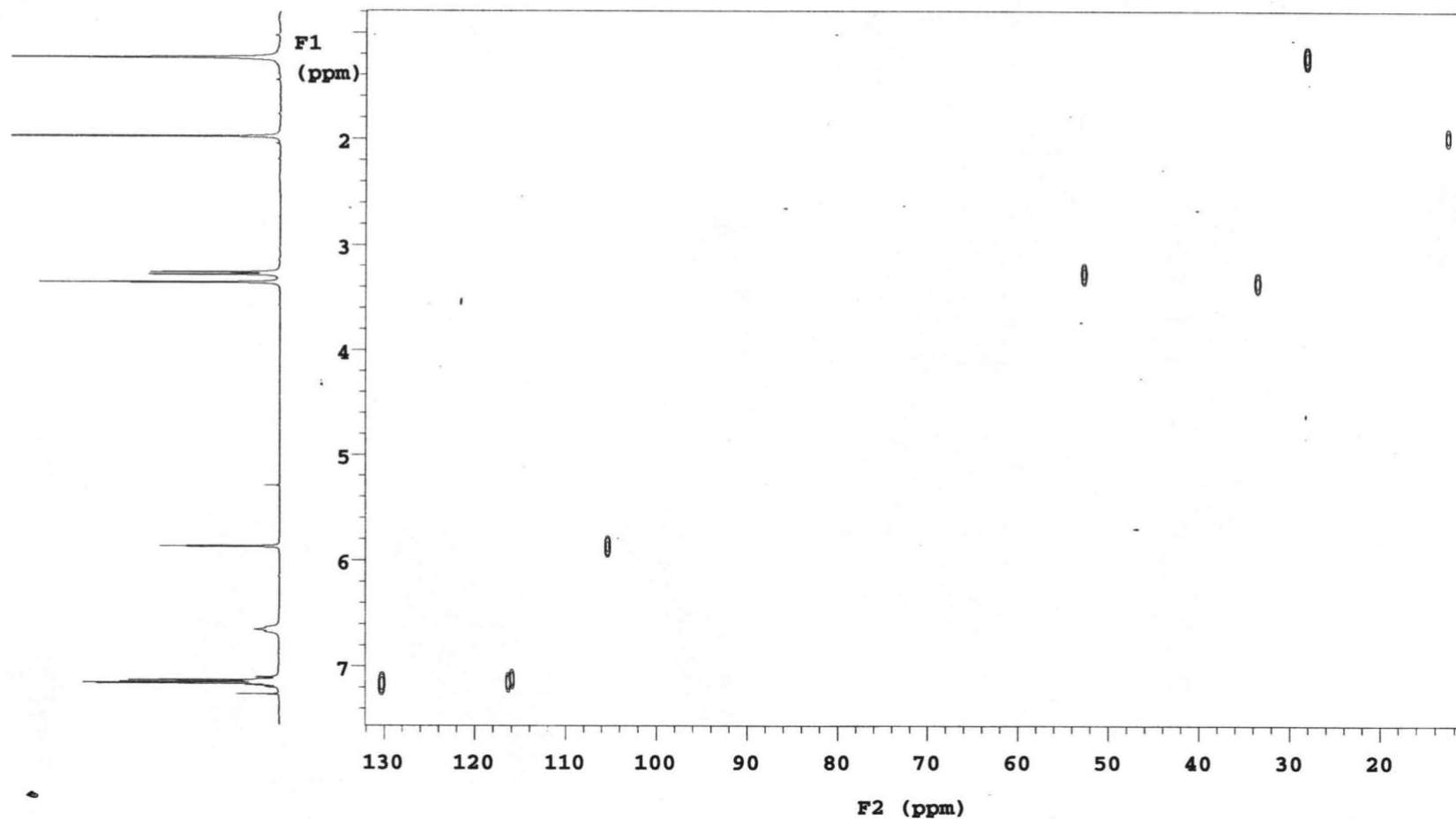
¹³C-NMR

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

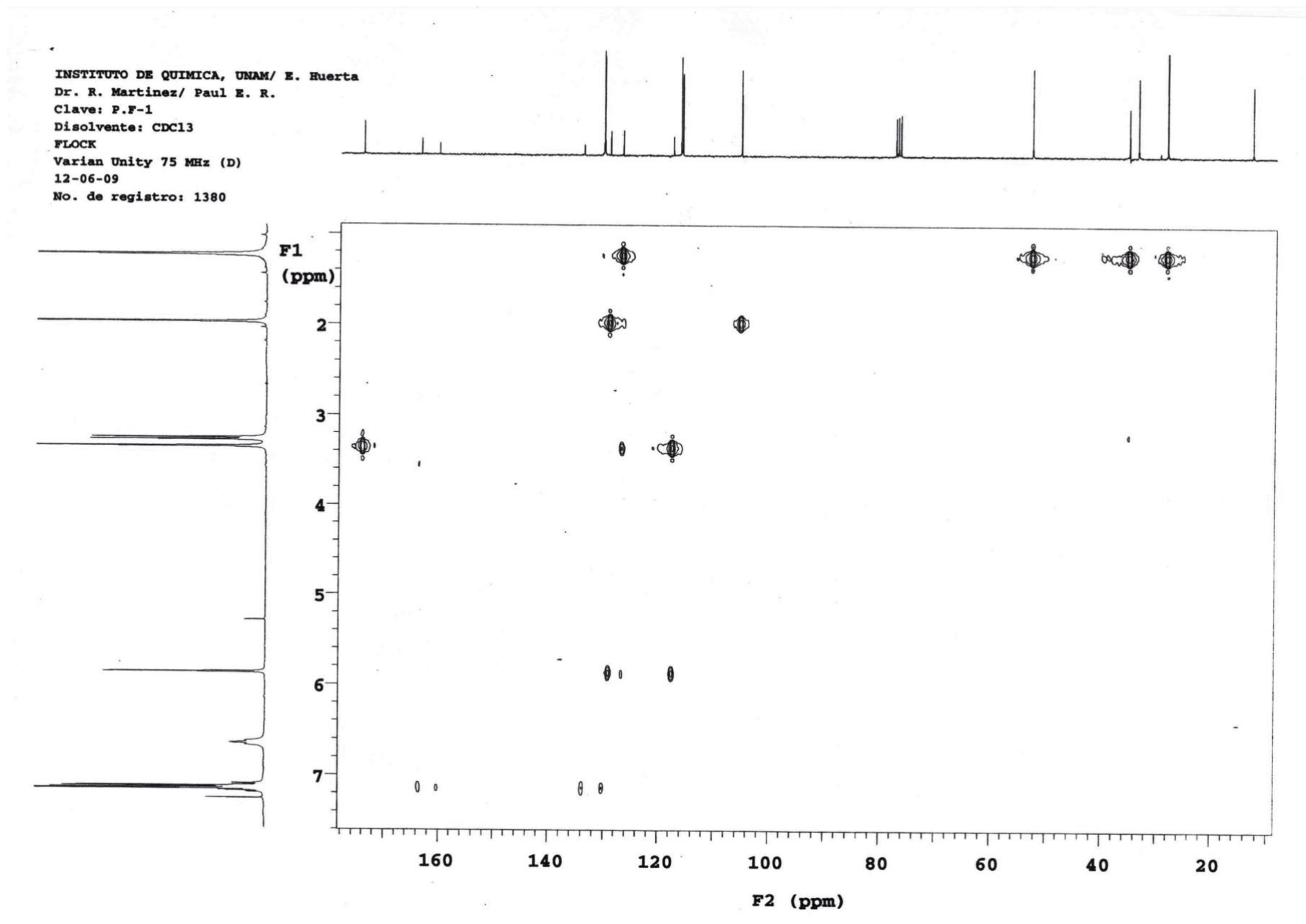


Compound 11c. 1-(4-Fluorophenyl)-2,4,4-trimethyl-4,5,6,8-tetrahydropyrrolo[2,3-d]azepin-7(1H)-one**HETCOR**

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



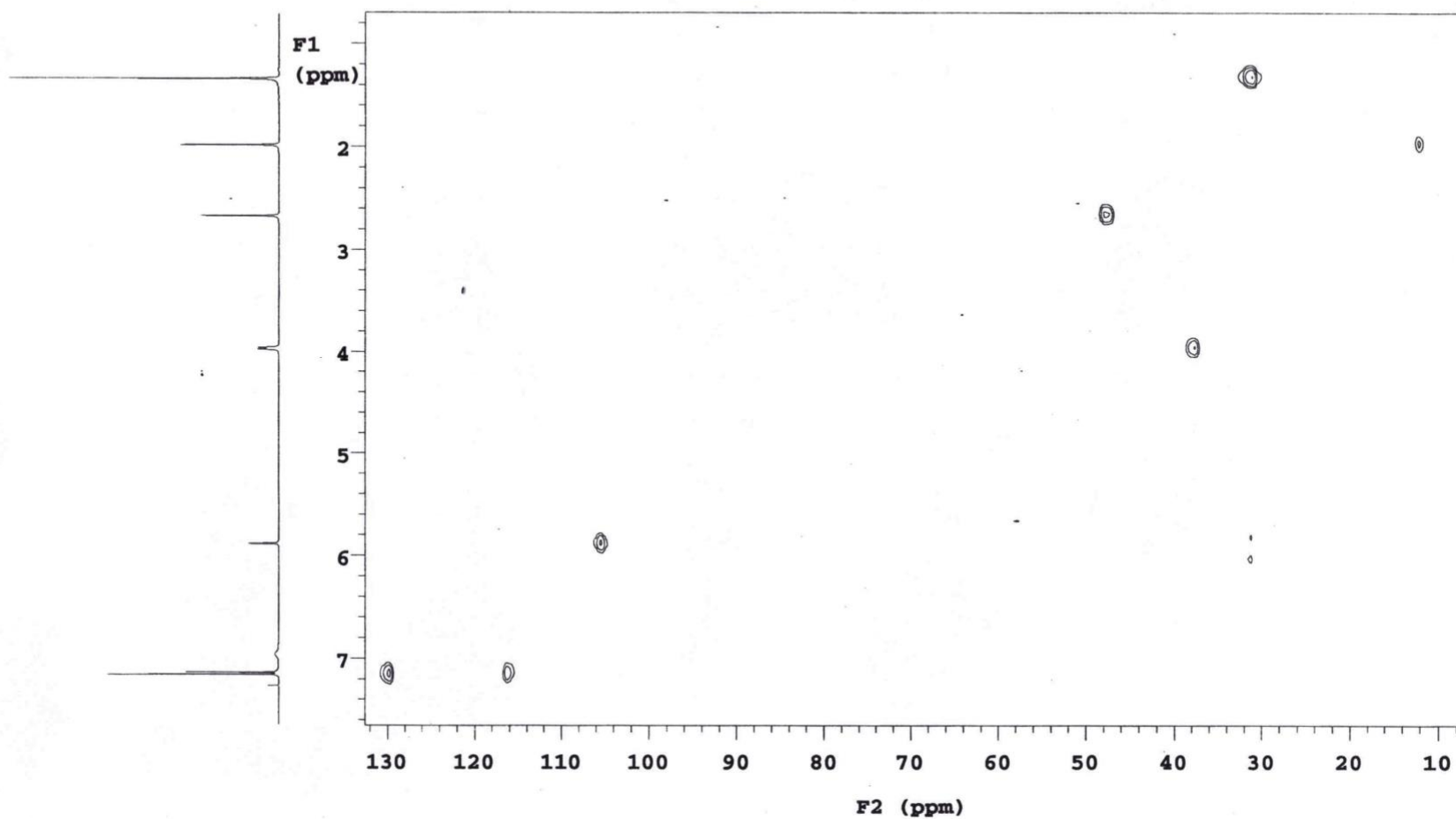
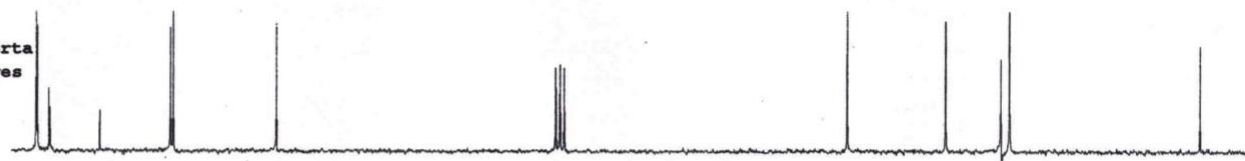
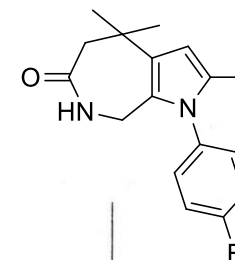
FLOCK



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

