

## INFORMATION SUPPLEMENTARY

### Neoflavonoids as Inhibitors of HIV-1 Replication by targeting the Tat and NF- $\kappa$ B Pathways

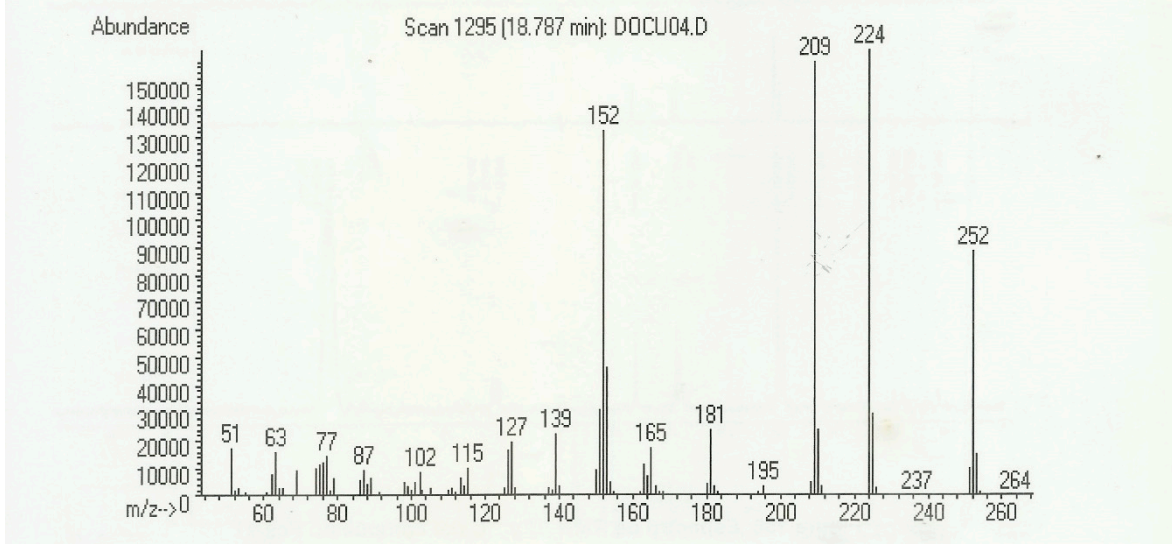
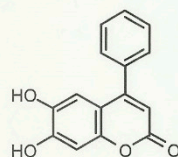
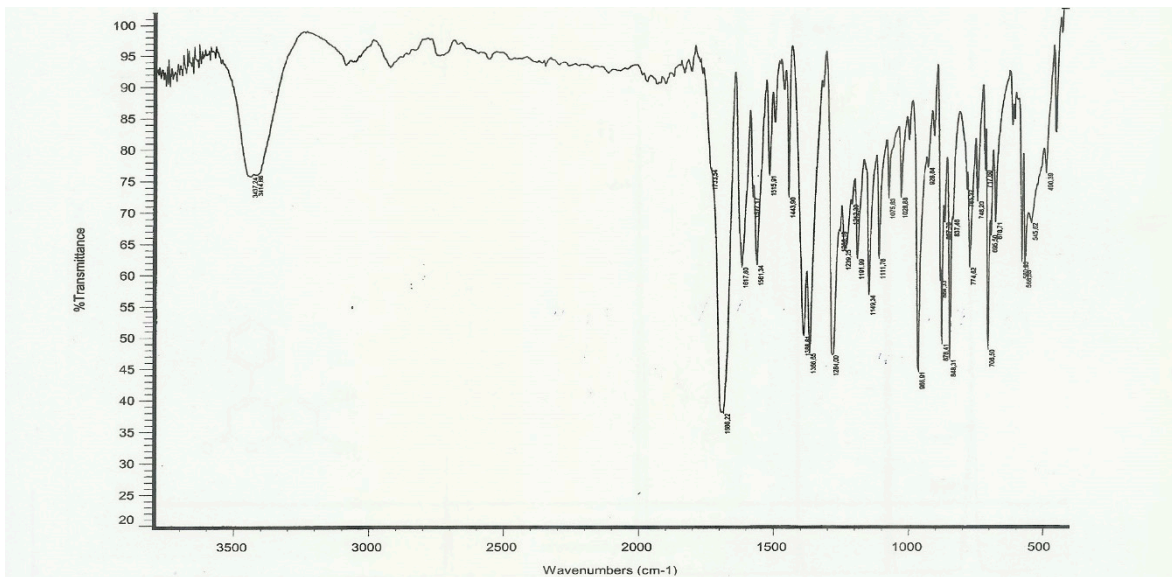
Dionisio A. Olmedo <sup>1\*</sup>, José Luis López-Pérez <sup>1</sup>, Esther del Olmo <sup>1</sup>, Luis M. Bedoya <sup>4,5</sup>, Rocío Sancho <sup>2</sup>, José Alcamí <sup>4</sup>, Eduardo Muñoz <sup>2</sup>, Arturo San Feliciano <sup>1</sup> and Mahabir P. Gupta<sup>3\*</sup>.

### FIGURE S1: SPECTRA OF THE NEOFLAVONOIDS DERIVATIVES 3-10, 12-15, 17-28

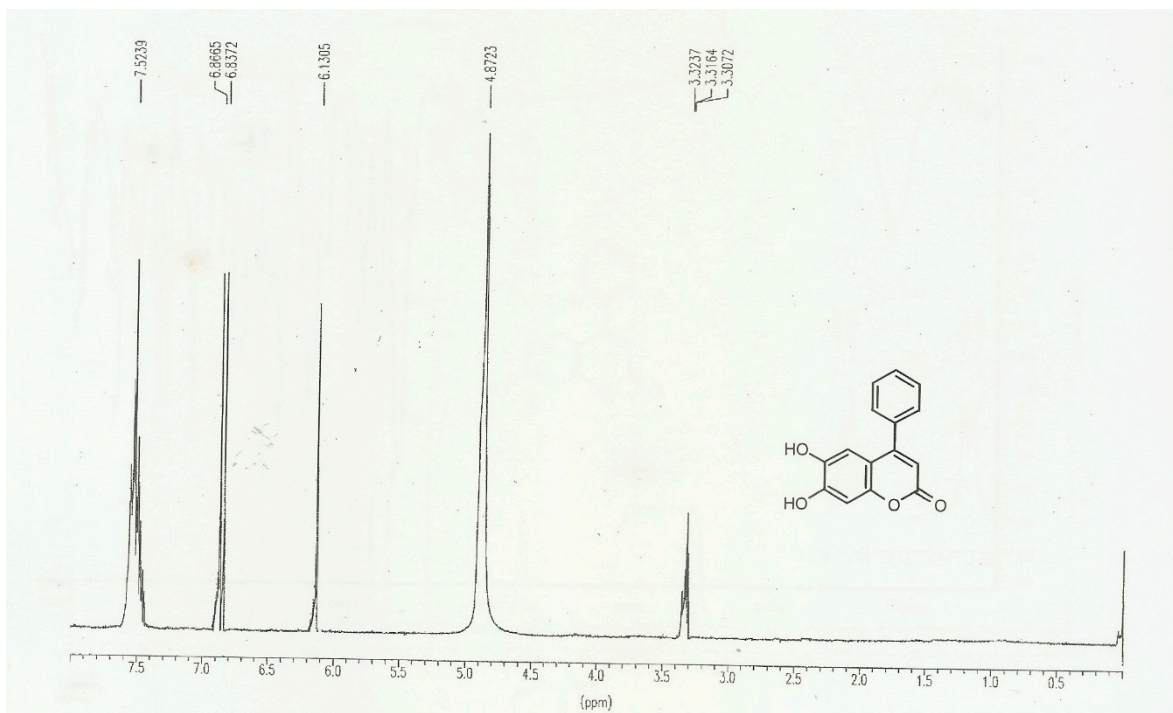
S1: *6,7-dihydroxy-4-phenyl-2H-chromen-2-one* (3)

S2: *8-phenyl-6H-[1,3]dioxolo[4,5-g]chromen-6-one* (4)

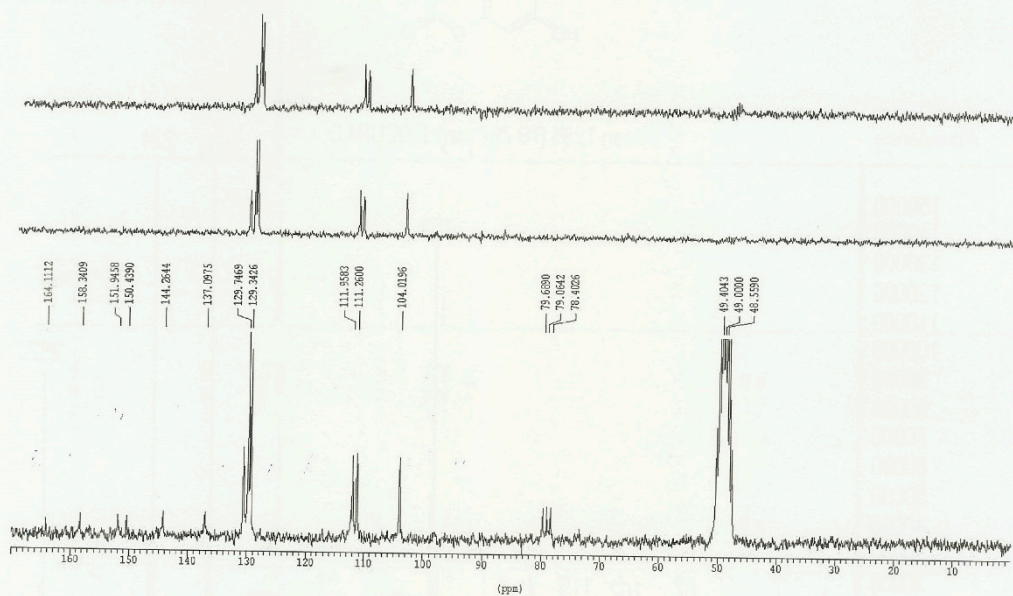
S3: *8-hydroxy-7-methoxy-4-phenyl-2H-chromen-2-one* (5)



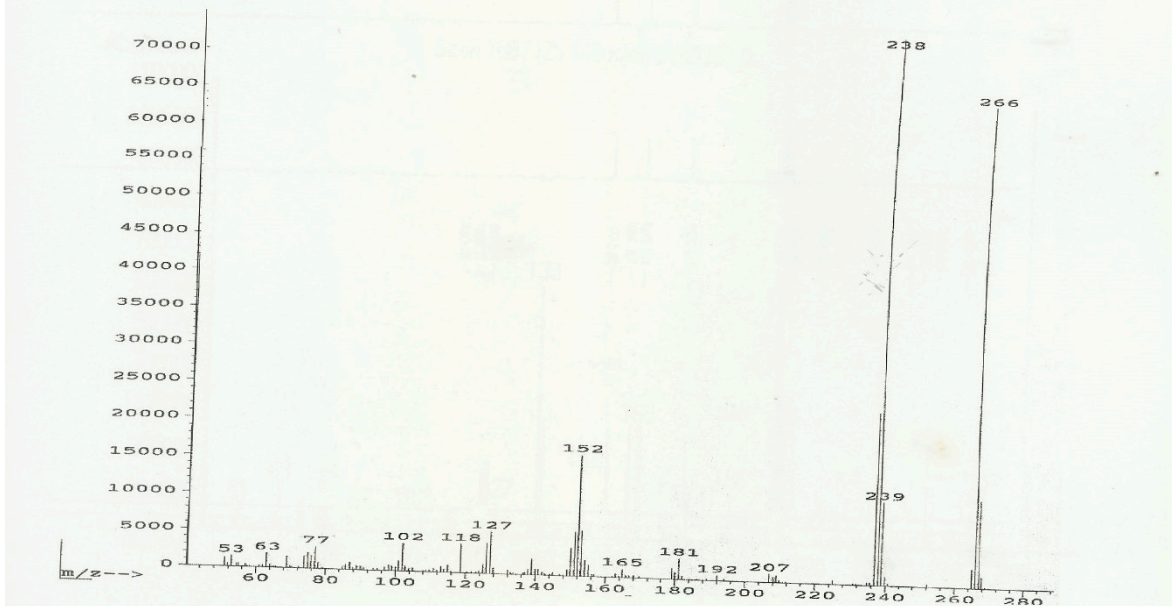
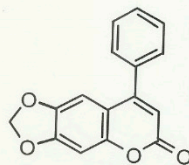
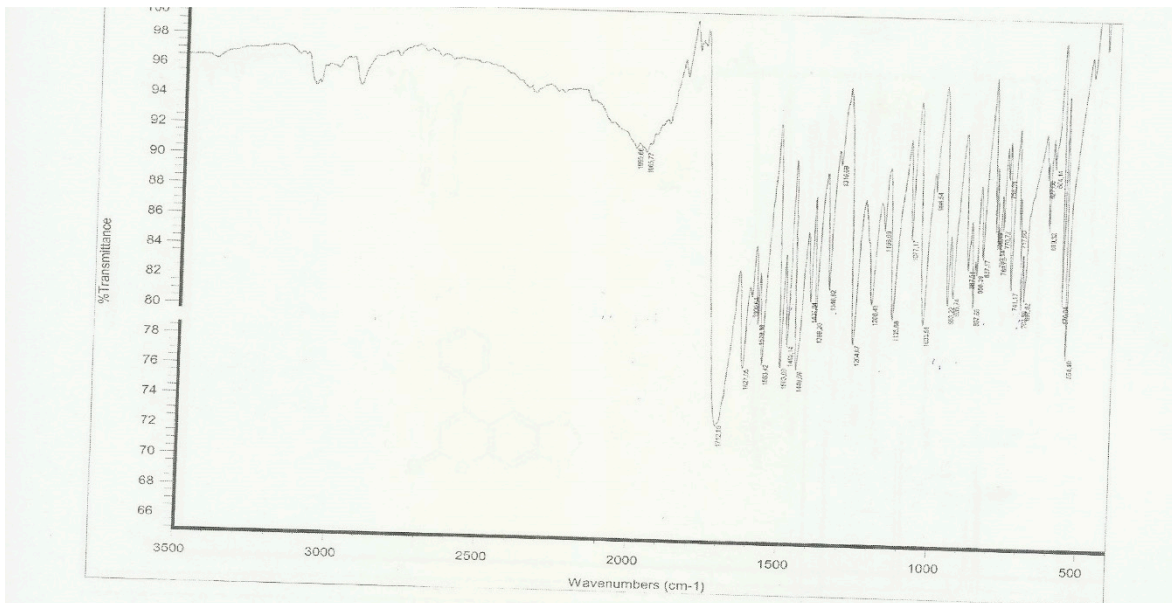
6,7-dihydroxy-4-phenyl-2H-chromen-2-one (3)



docum8 6,7-dihidroxi-4-fenilcumarina

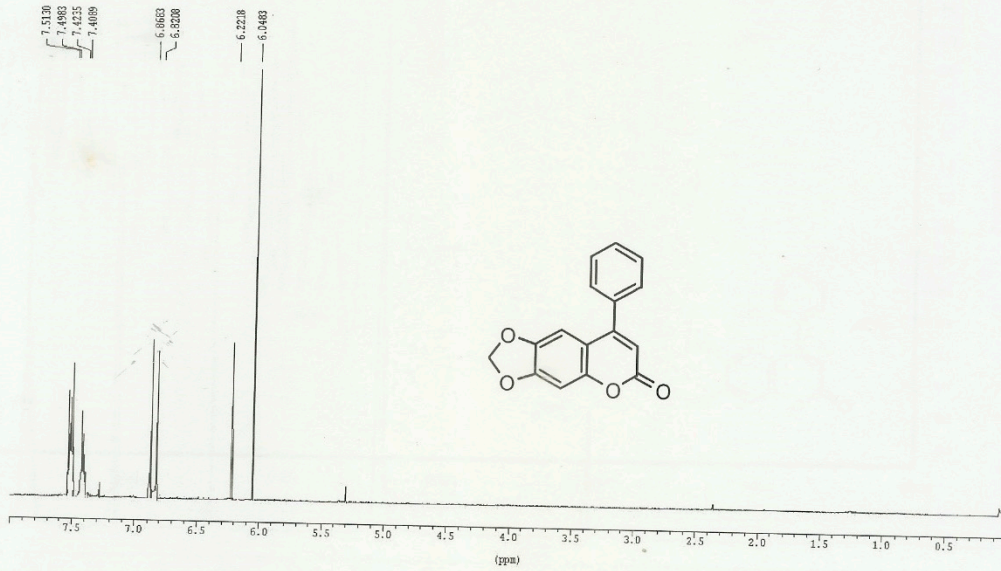


6,7-dihydroxy-4-phenyl-2H-chromen-2-one (3)

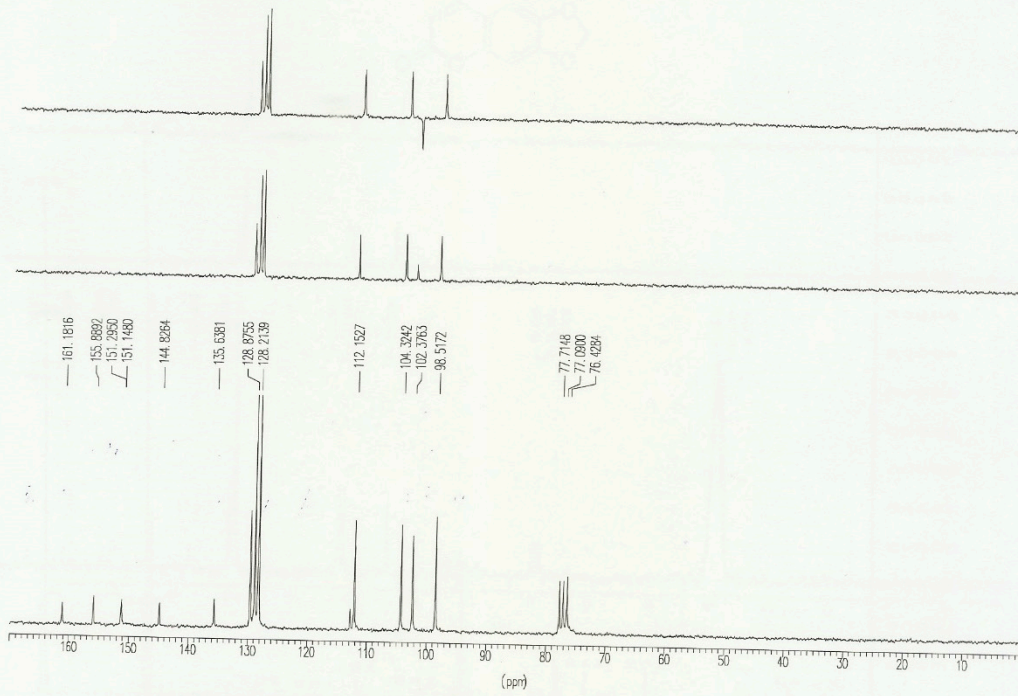


8-phenyl-6H-[1,3]dioxolo[4,5-g]chromen-6-one (4)

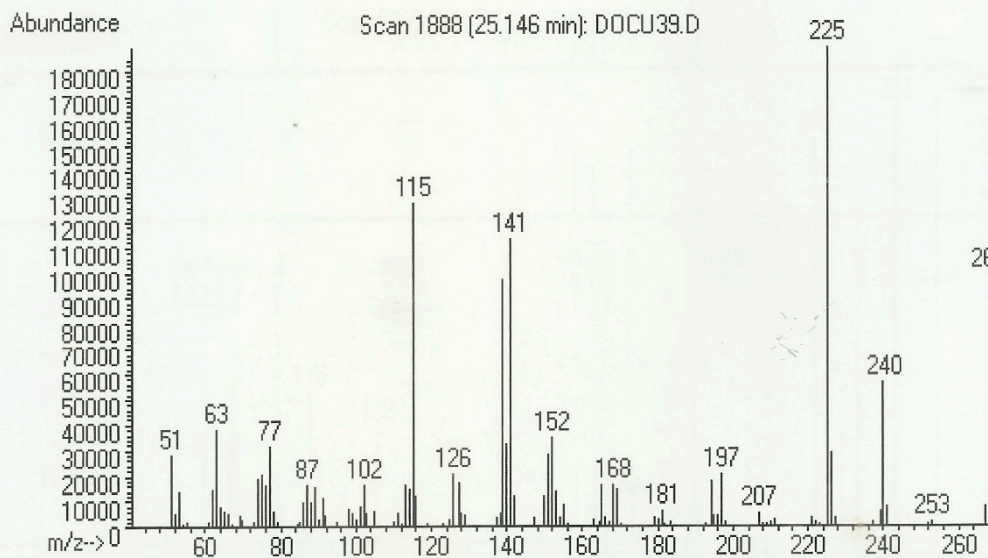
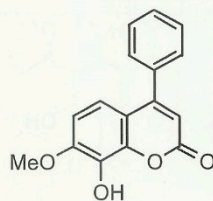
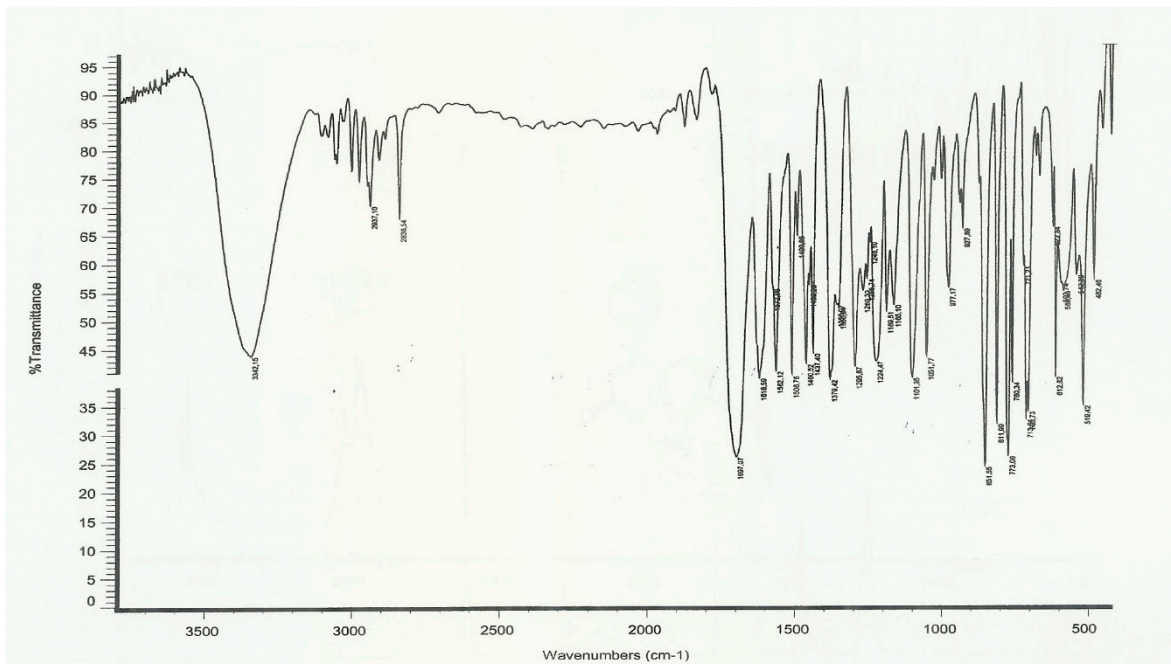
docum9.006 (3,4'-metilendioksi-4-fenilcumarina)



docum9.13 (3',4'-metilendioksi-4-fenilcumarina)

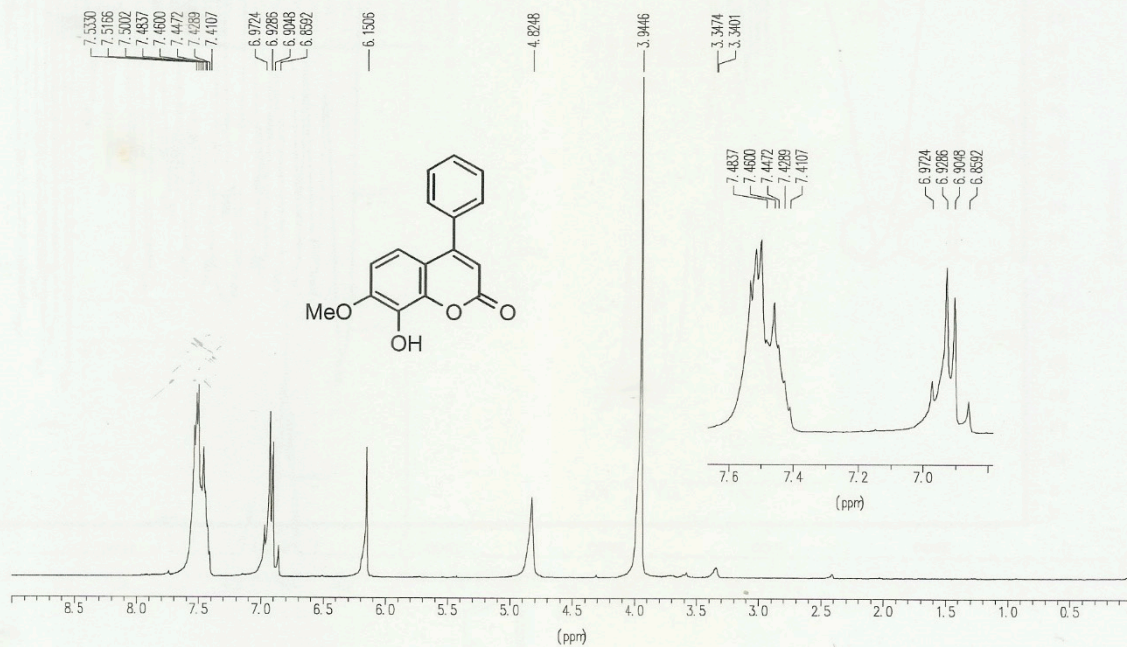


8-phenyl-6H-[1,3]dioxolo[4,5-g]chromen-6-one (4)

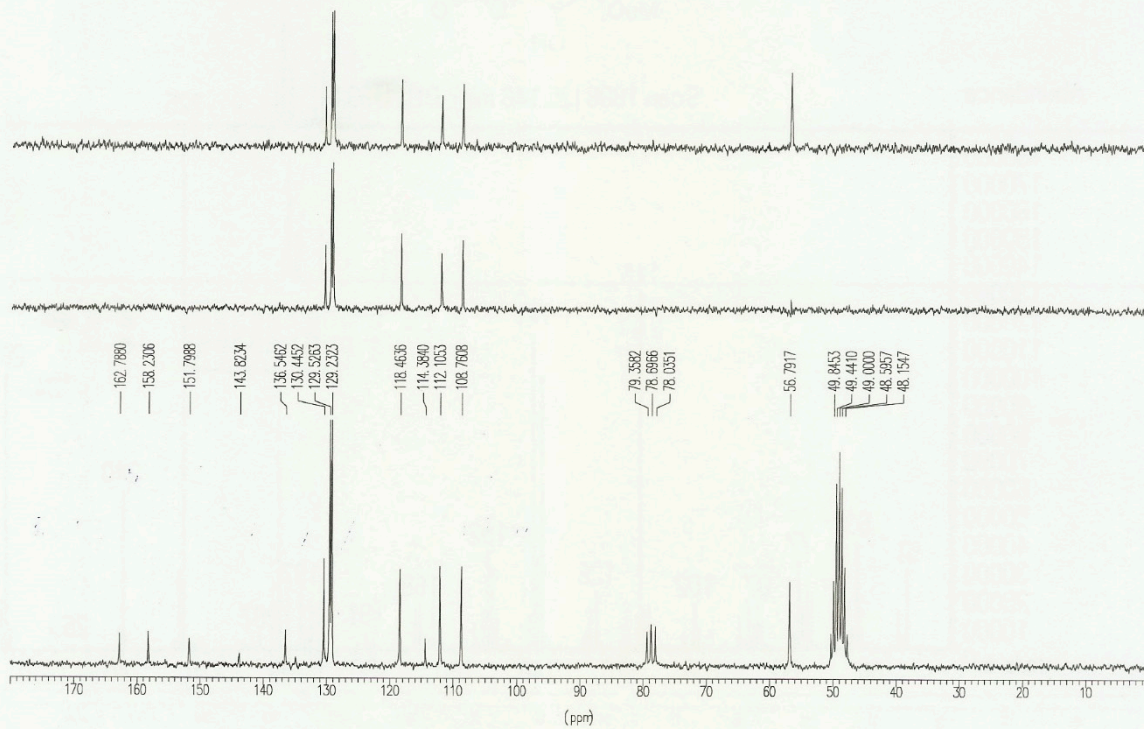


*8-hydroxy-7-methoxy-4-phenyl-2H-chromen-2-one (5)*

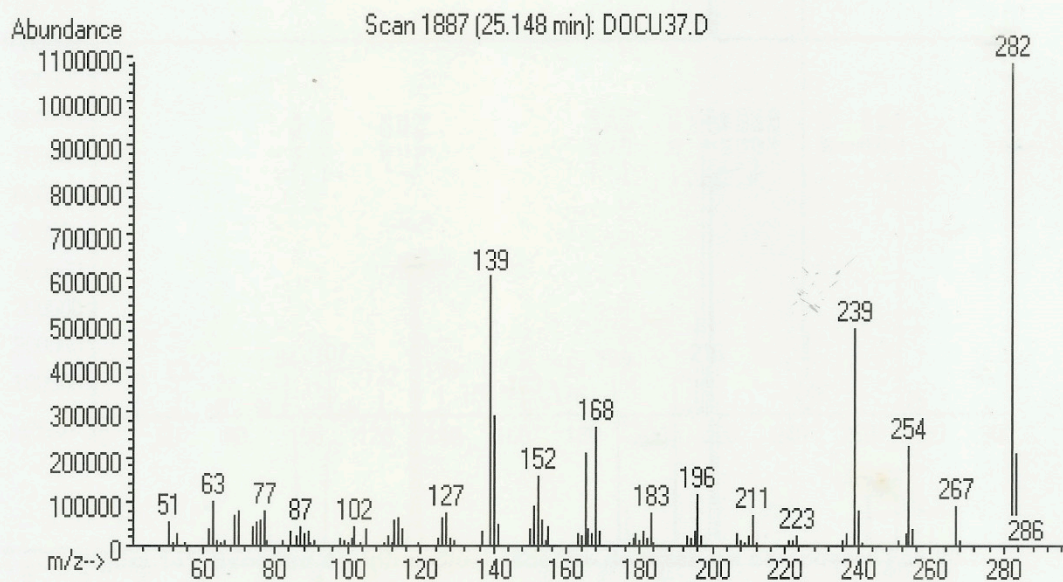
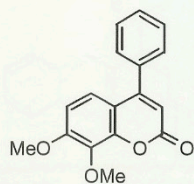
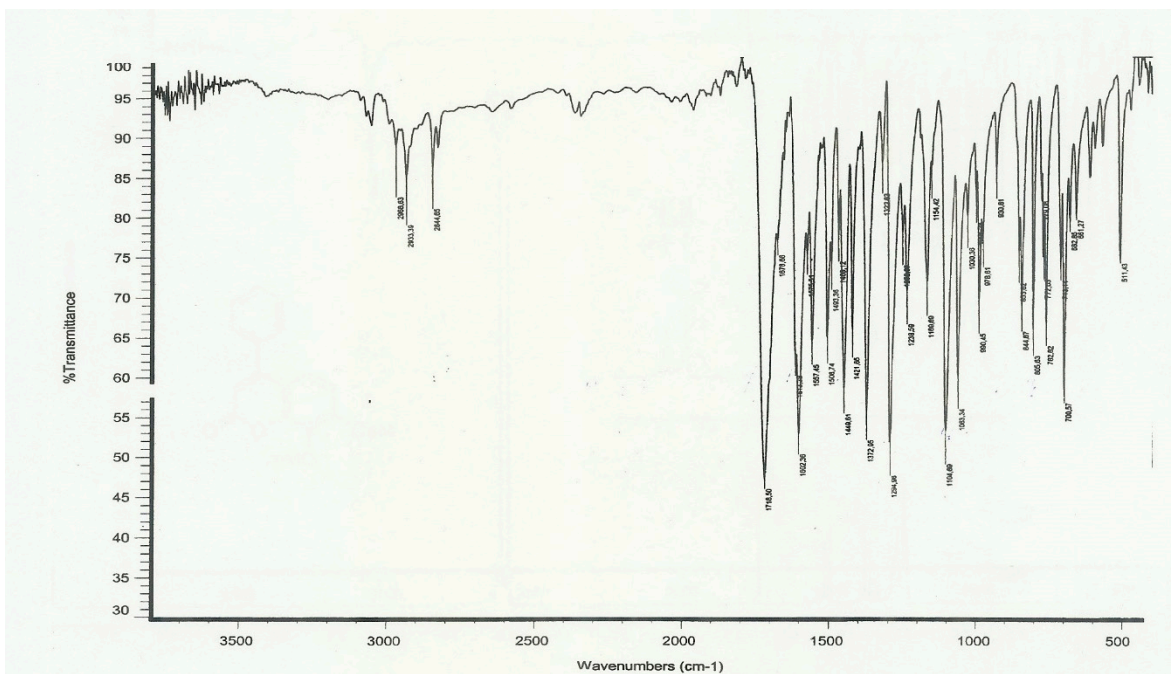
DOCUMA39.001 7-METOXI -8-HI DROXI -4-FENI LOUMARI NA MEOD



documa39.013, 012, 011 cdcl 3/meod

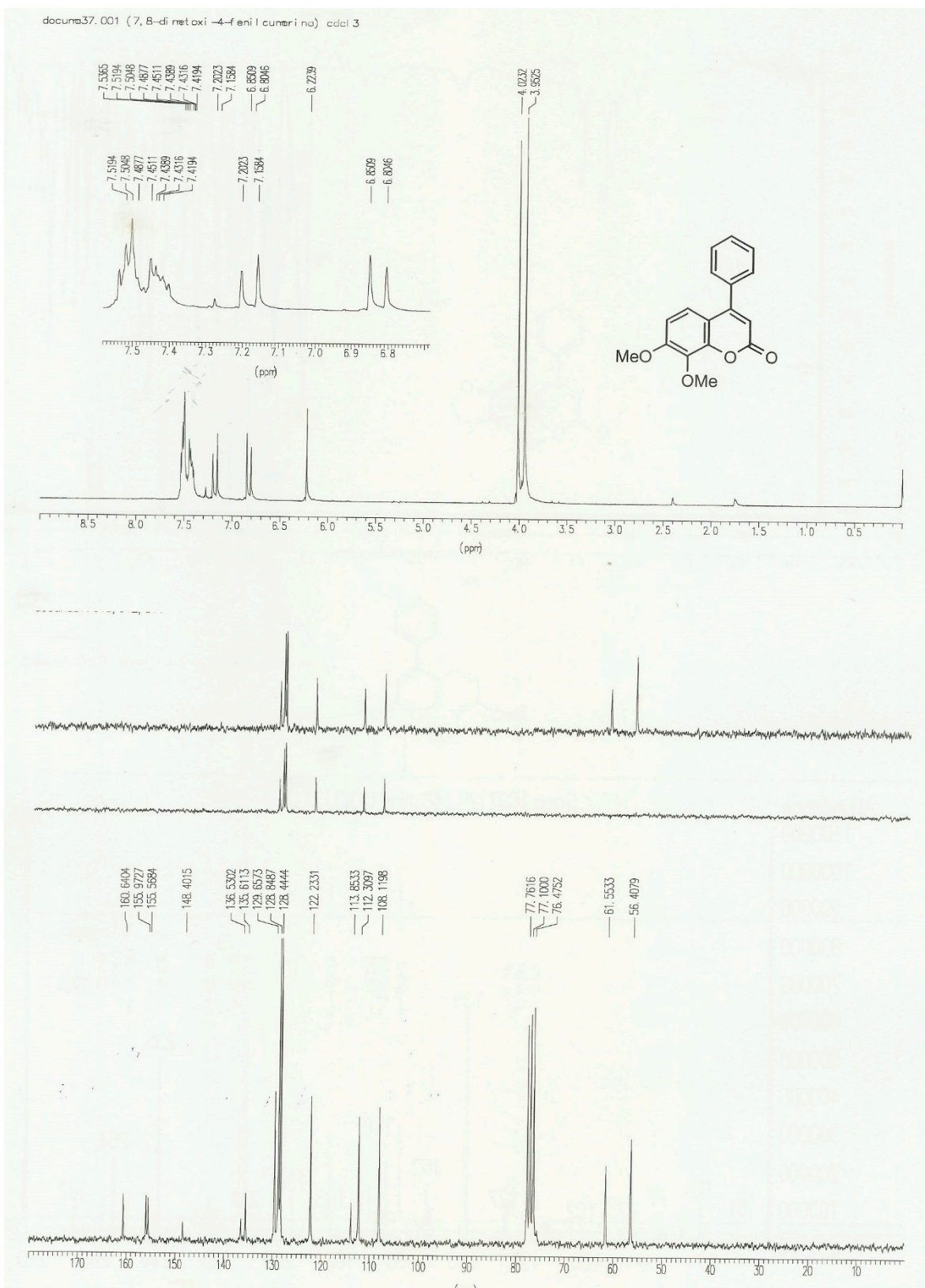


8-hydroxy-7-methoxy-4-phenyl-2H-chromen-2-one (5)

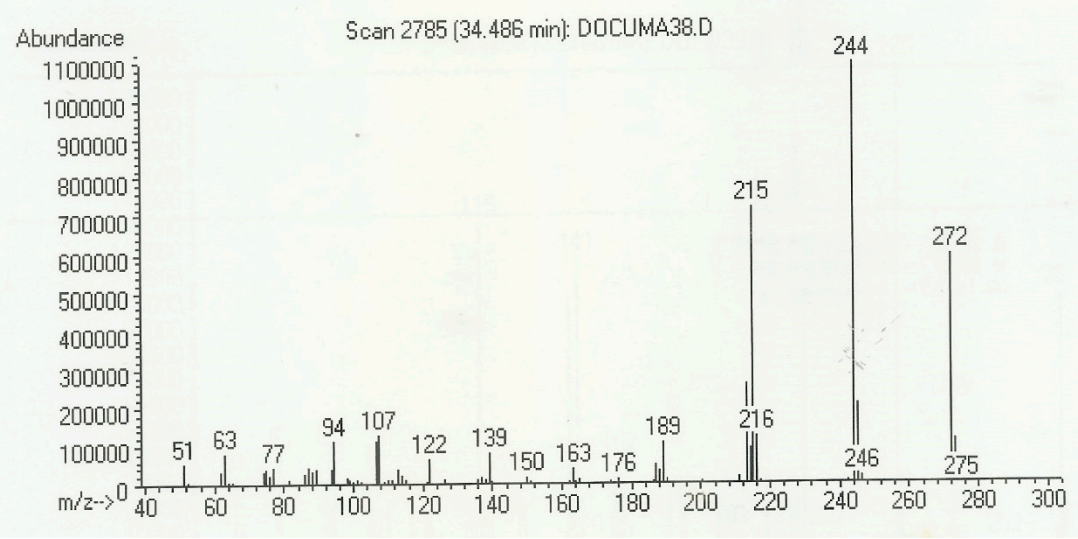
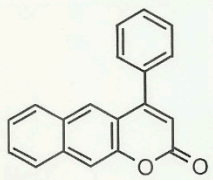
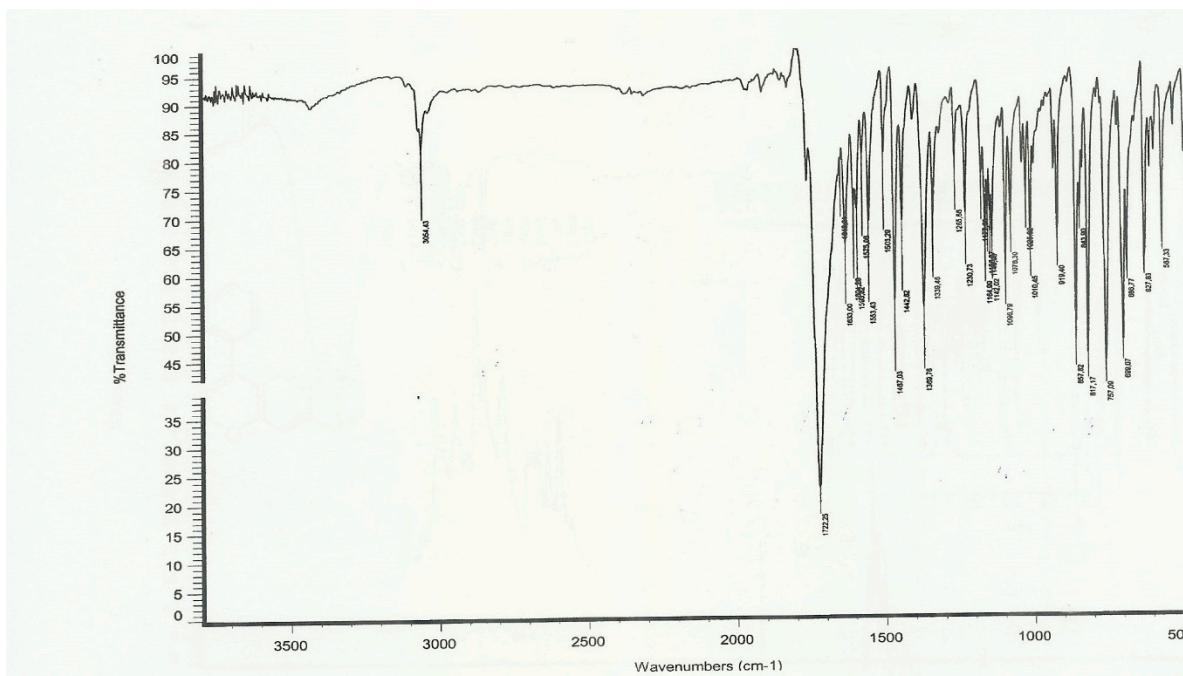


7,8-dimethoxy-4-phenyl-2H-chromen-2-one (6)



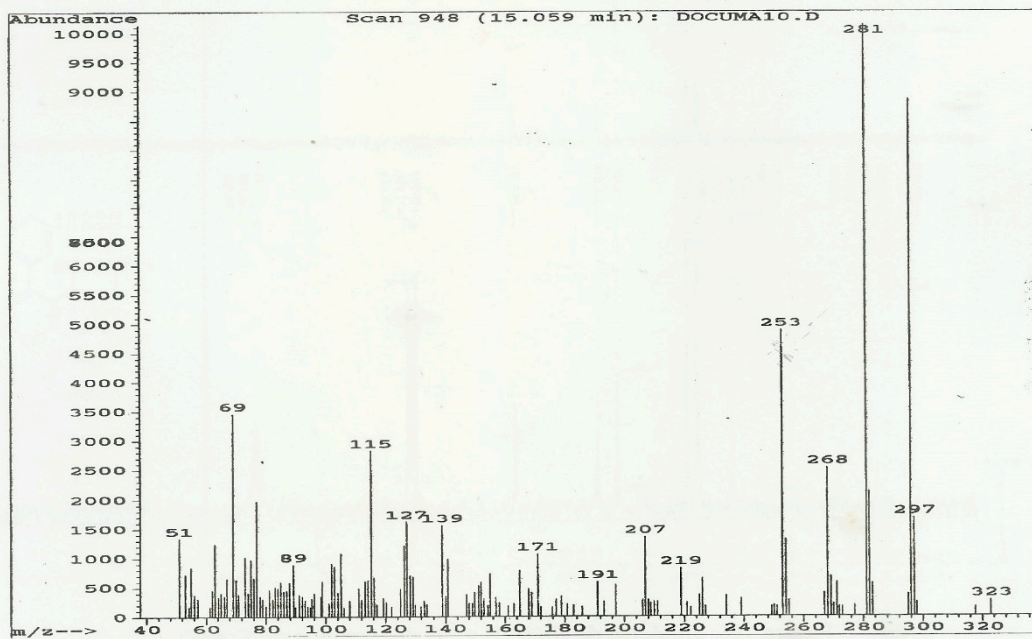
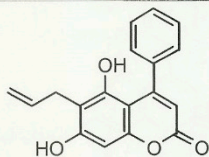
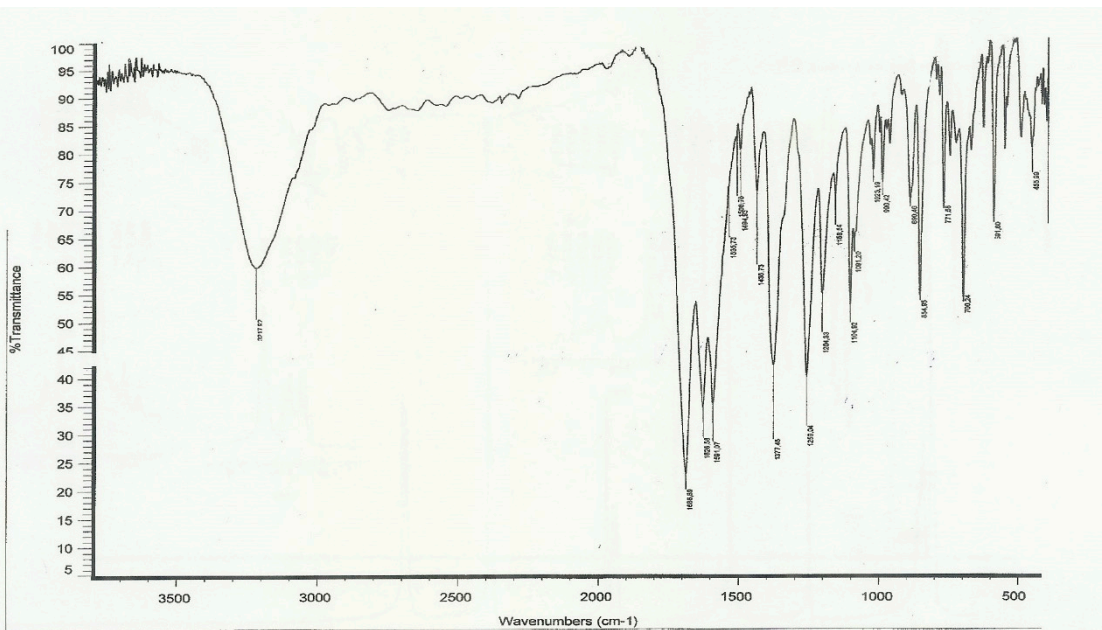


7,8-dimethoxy-4-phenyl-2H-chromen-2-one (6)



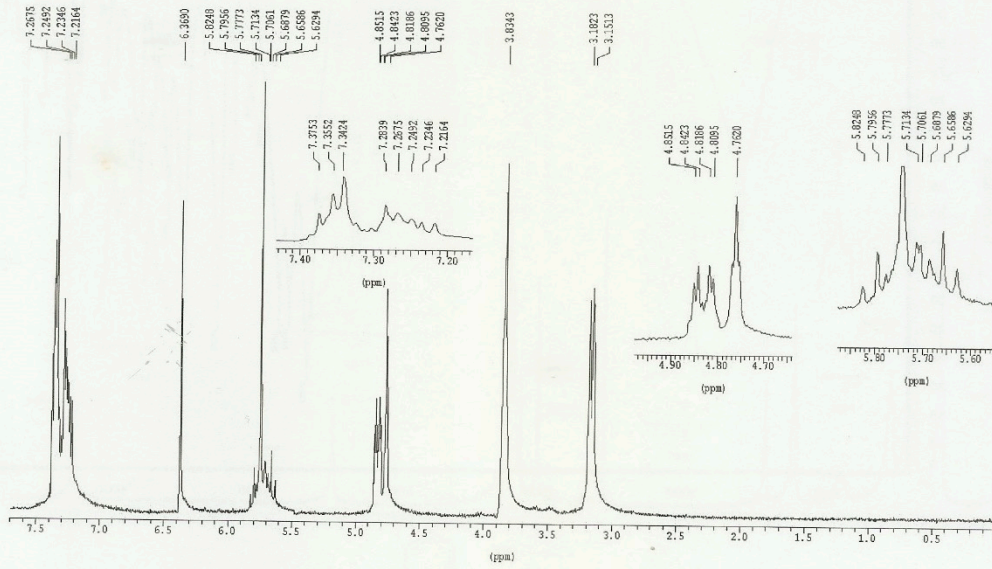
4-phenyl-2H-benzo[g]chromen-2-one (7)



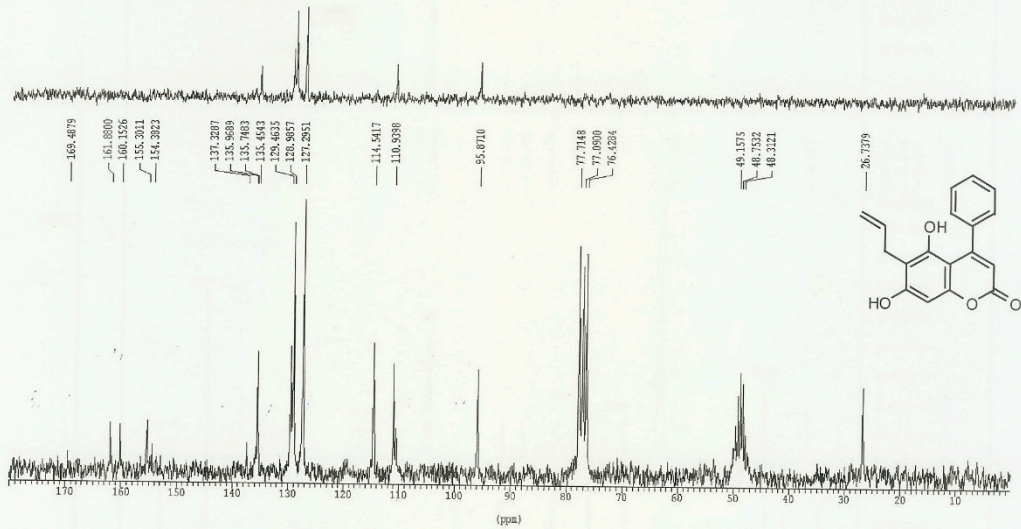


6-allyl-5,7-dihydroxy-4-phenyl-2H-chromen-2-one (8)

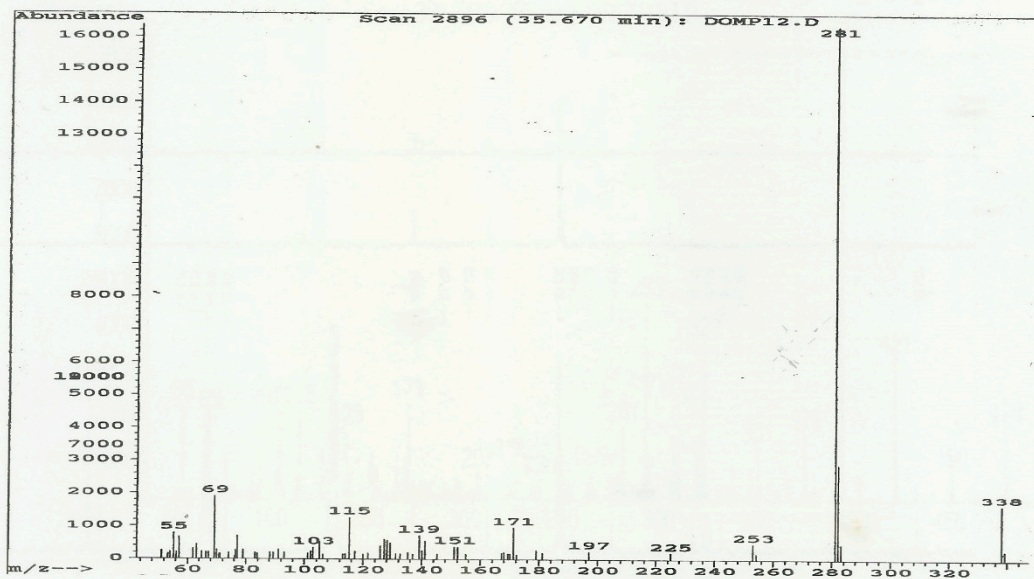
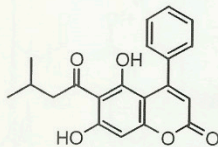
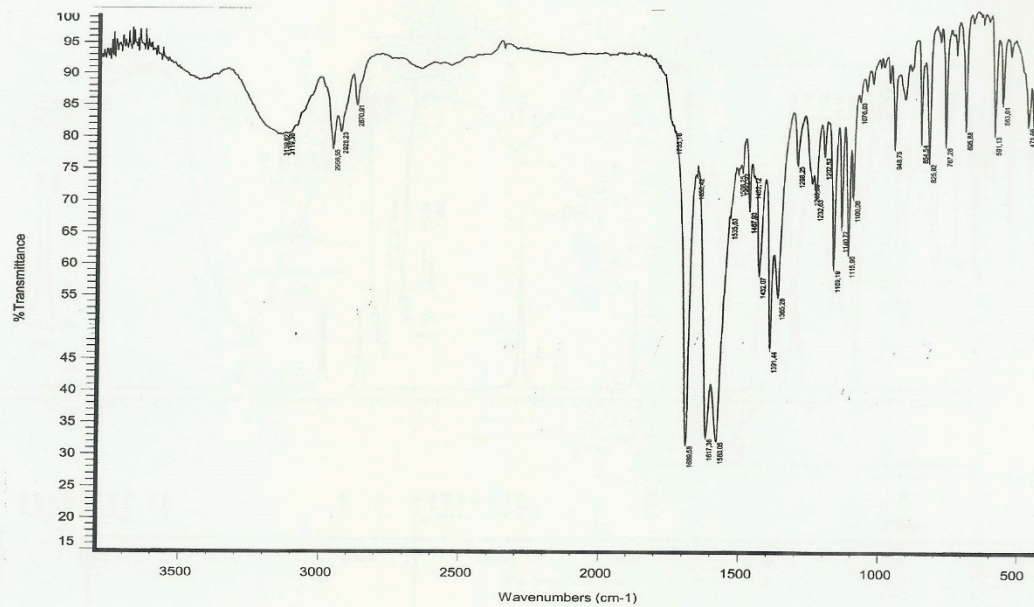
DOCUMA10.005 CDCL3/MEOD



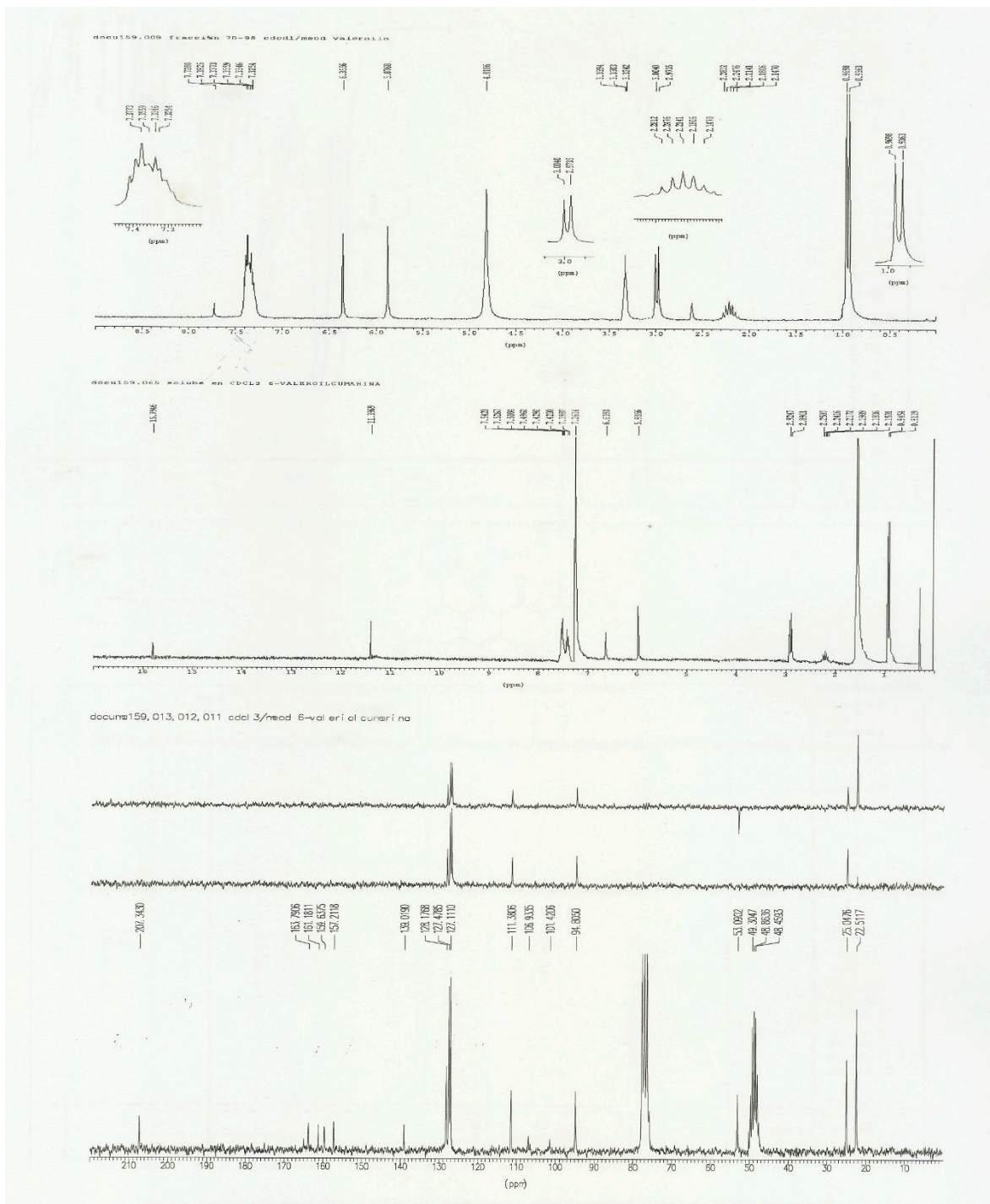
DOCUMA10.019, 012, 011



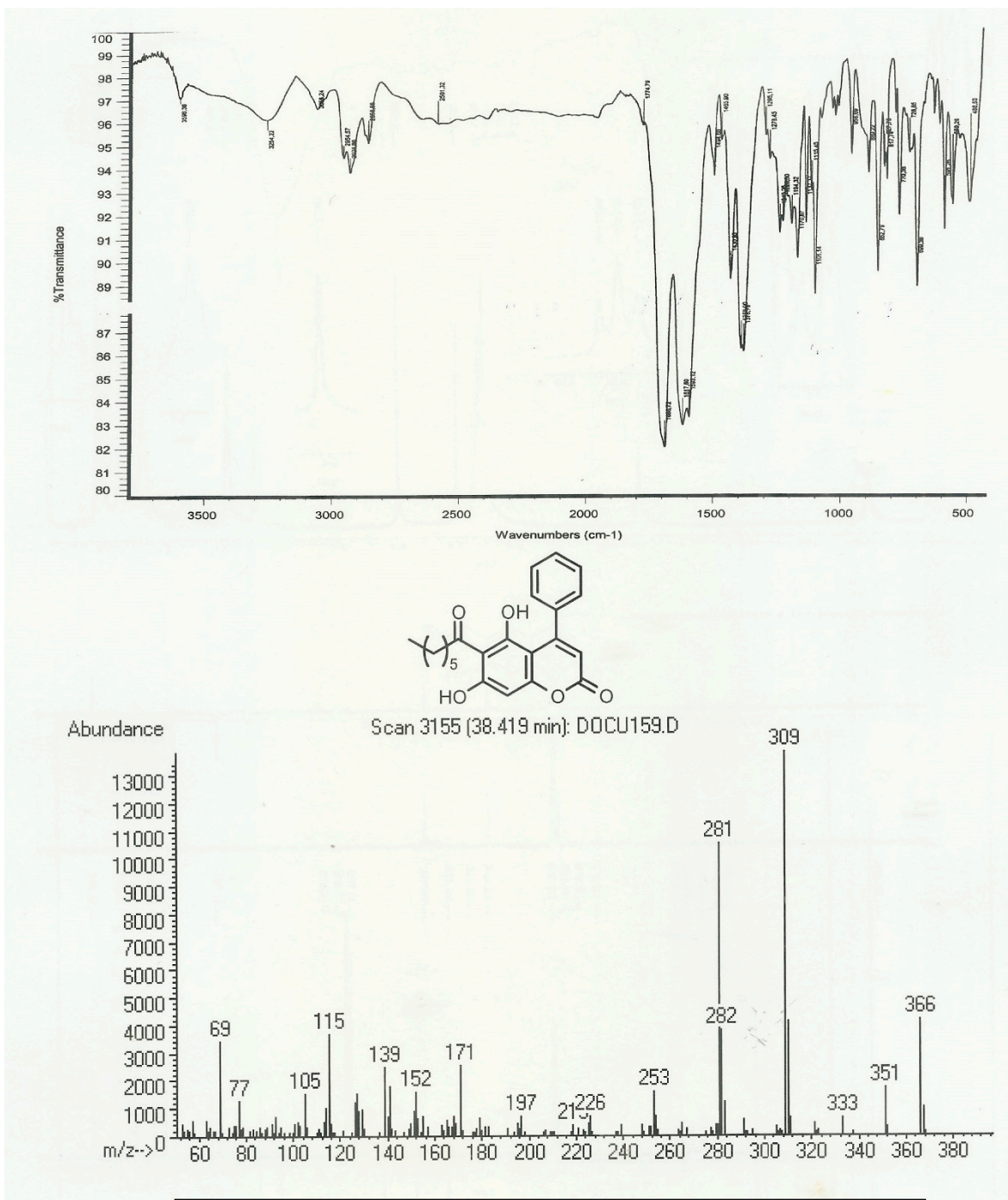
6-allyl-5,7-dihydroxy-4-phenyl-2H-chromen-2-one (8)



5,7-dihydroxy-6-(3-methylbutanoyl)-4-phenyl-2H-chromen-2-one (9)

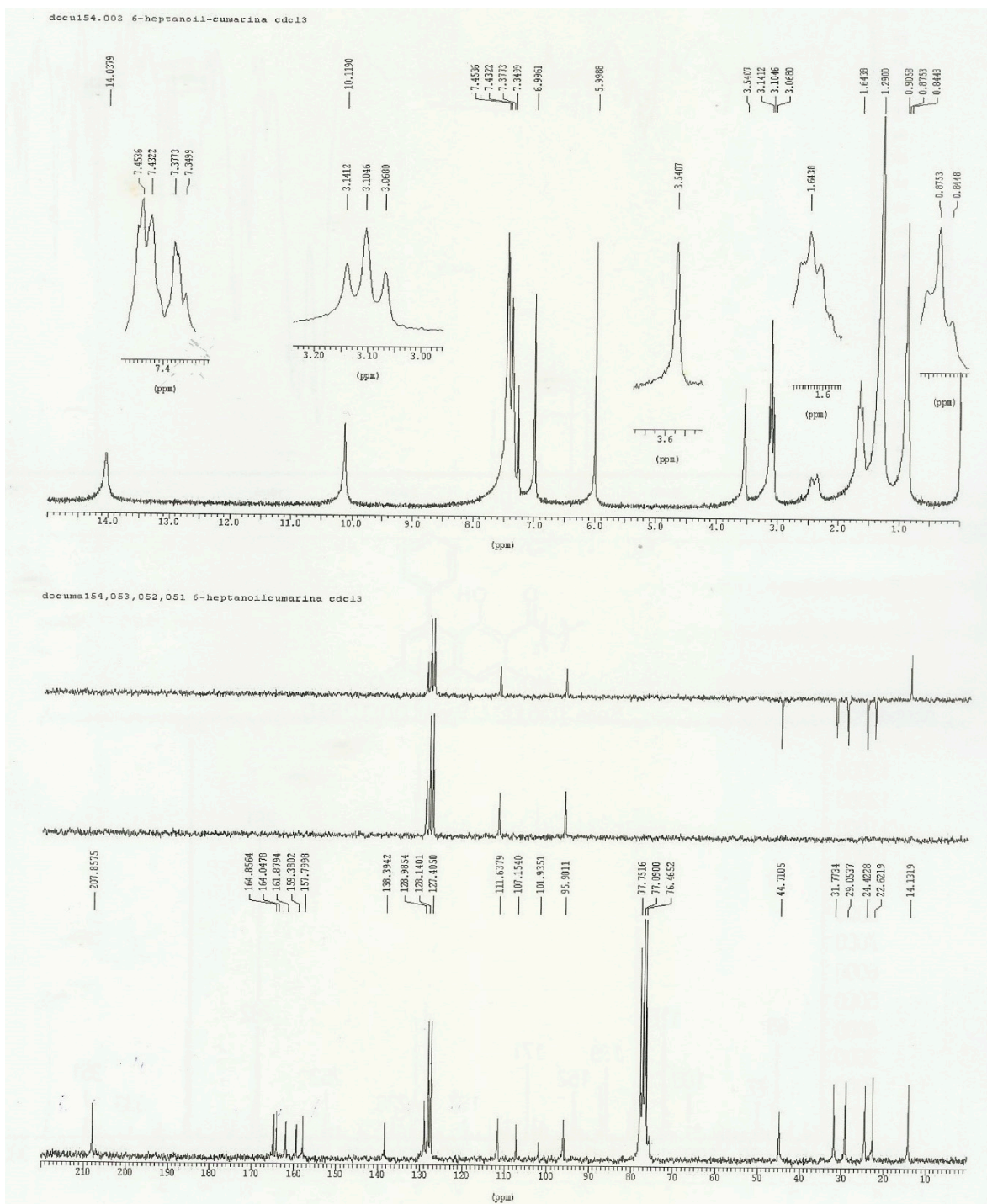


5,7-dihydroxy-6-(3-methylbutanoyl)-4-phenyl-2H-chromen-2-one (9)

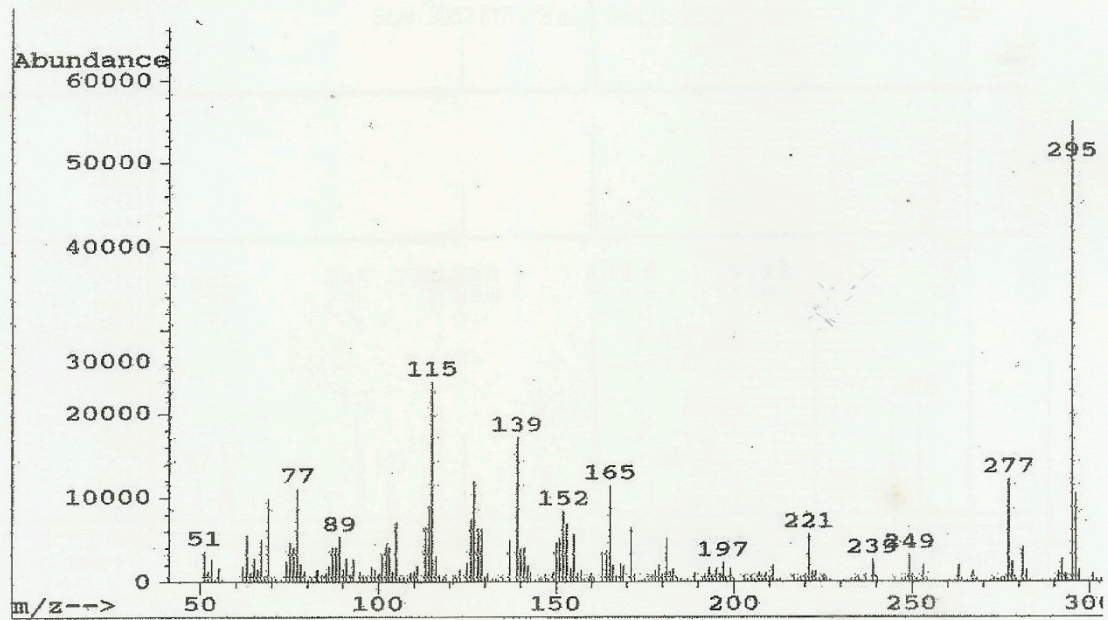
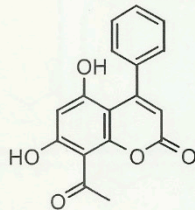
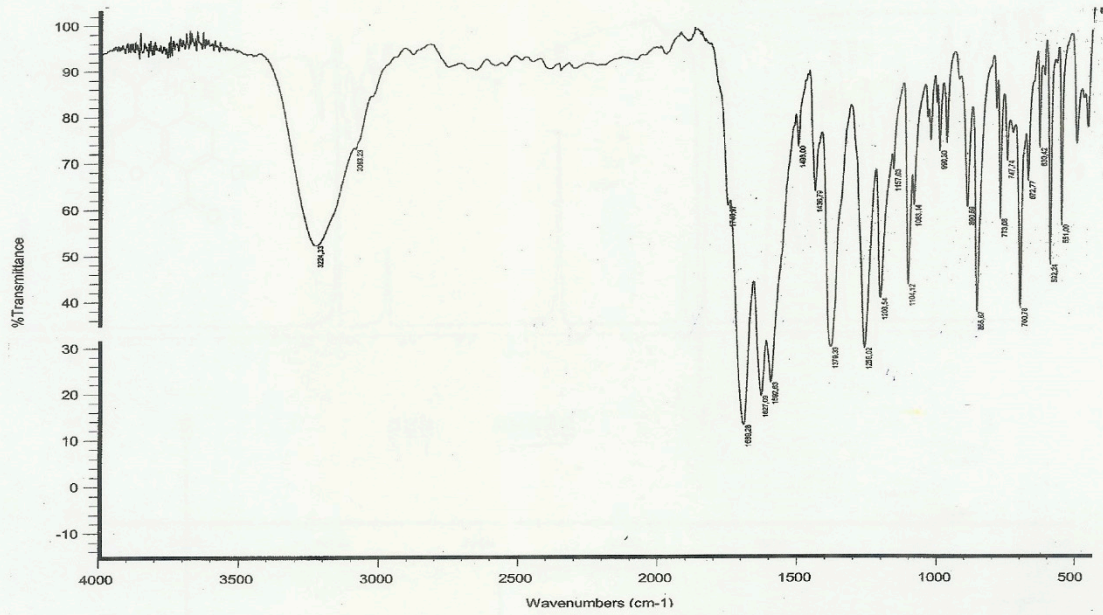


6-heptanoyl-5,7-dihydroxy-4-phenyl-2H-chromen-2-one (10)

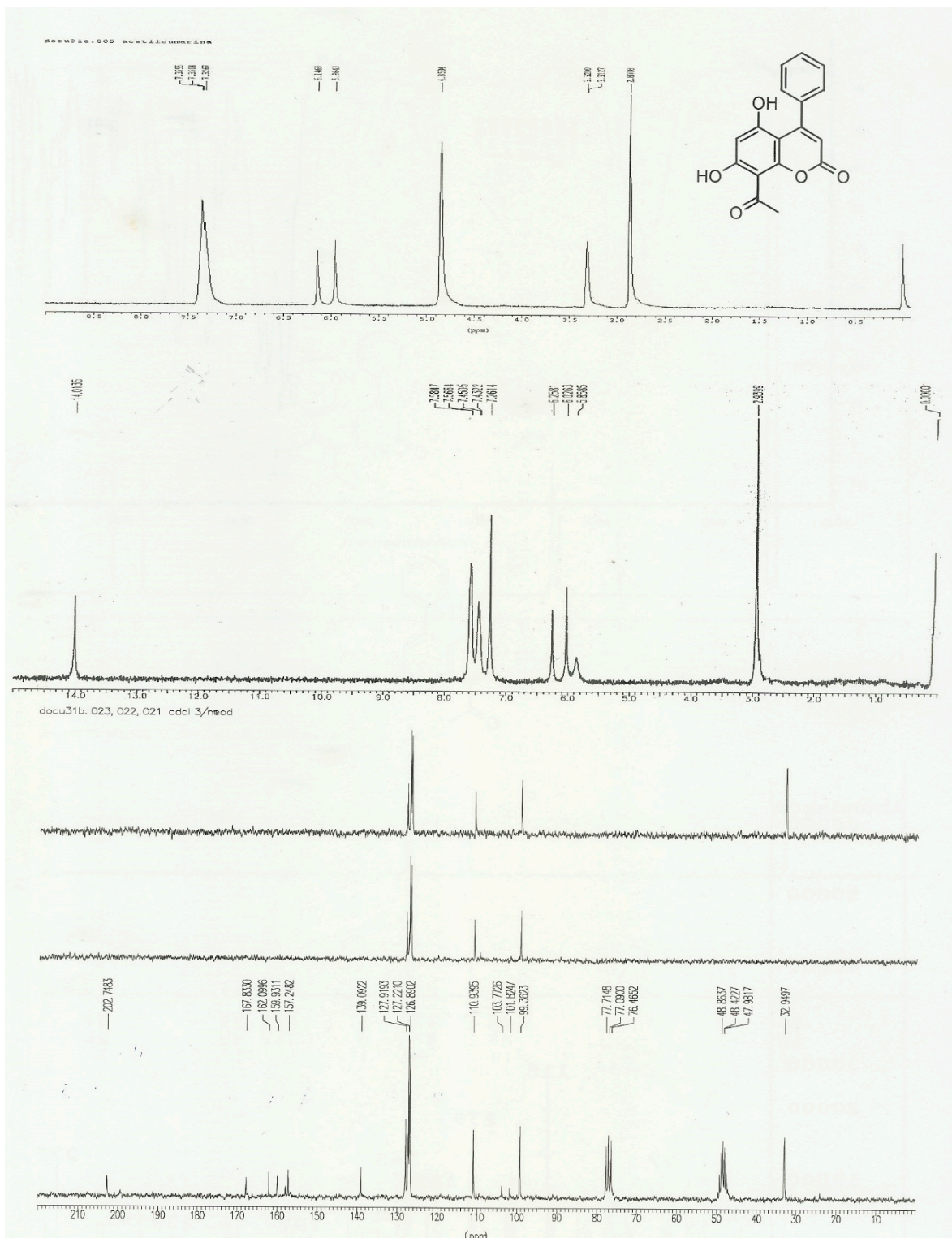




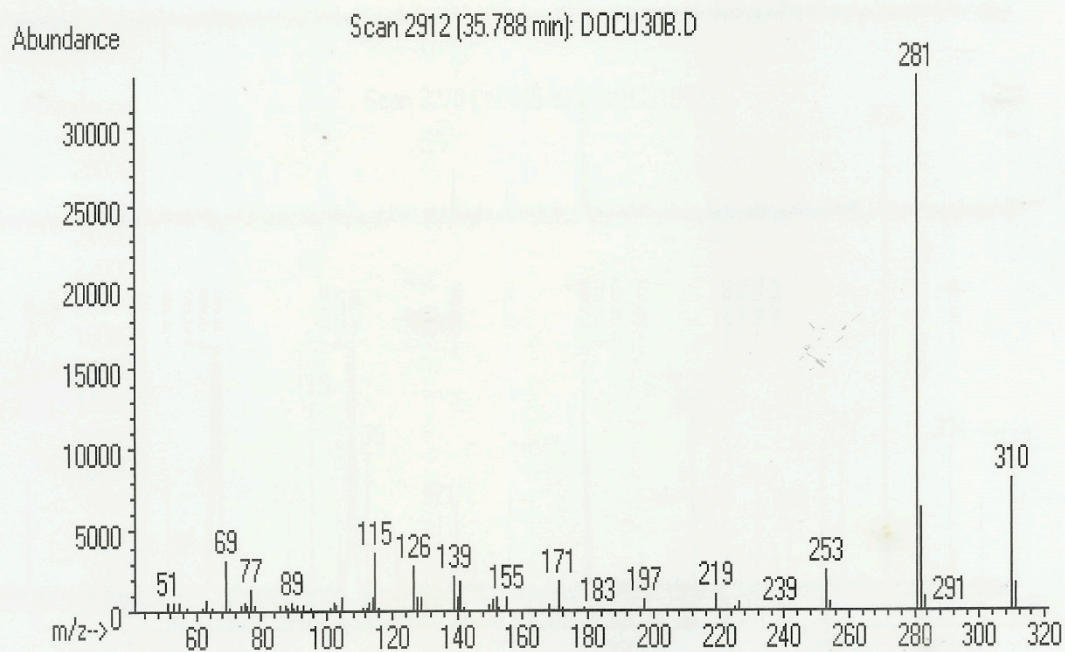
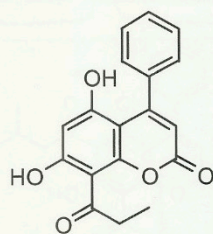
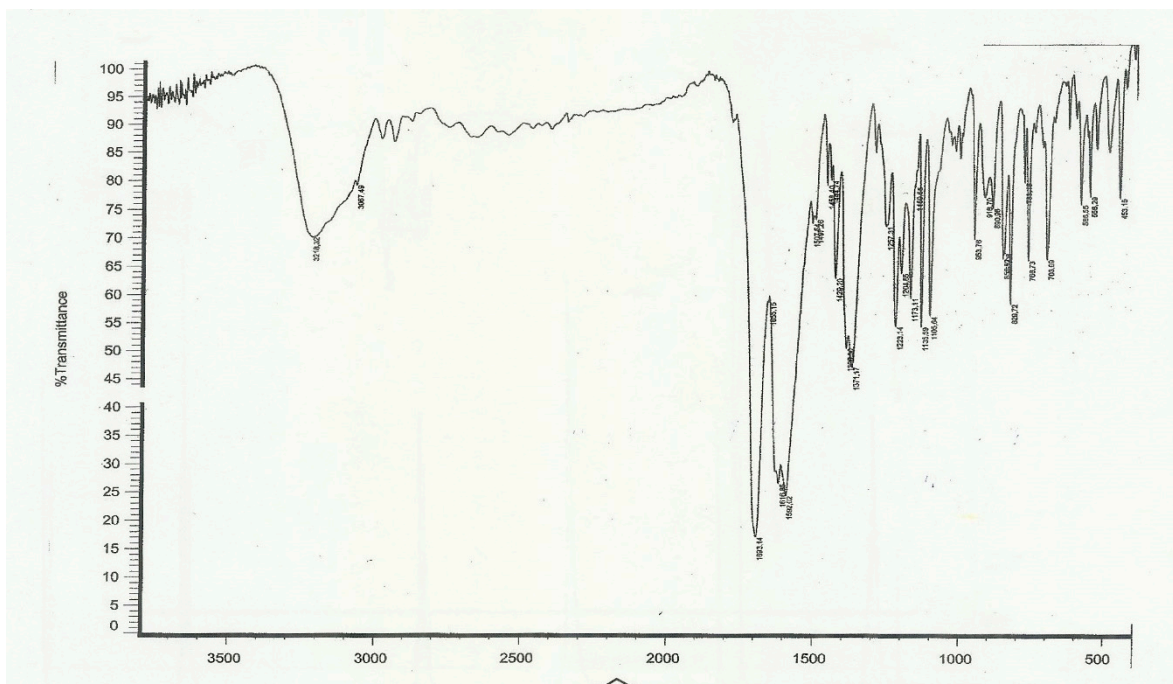
6-heptanoyl-5,7-dihydroxy-4-phenyl-2H-chromen-2-one (10)



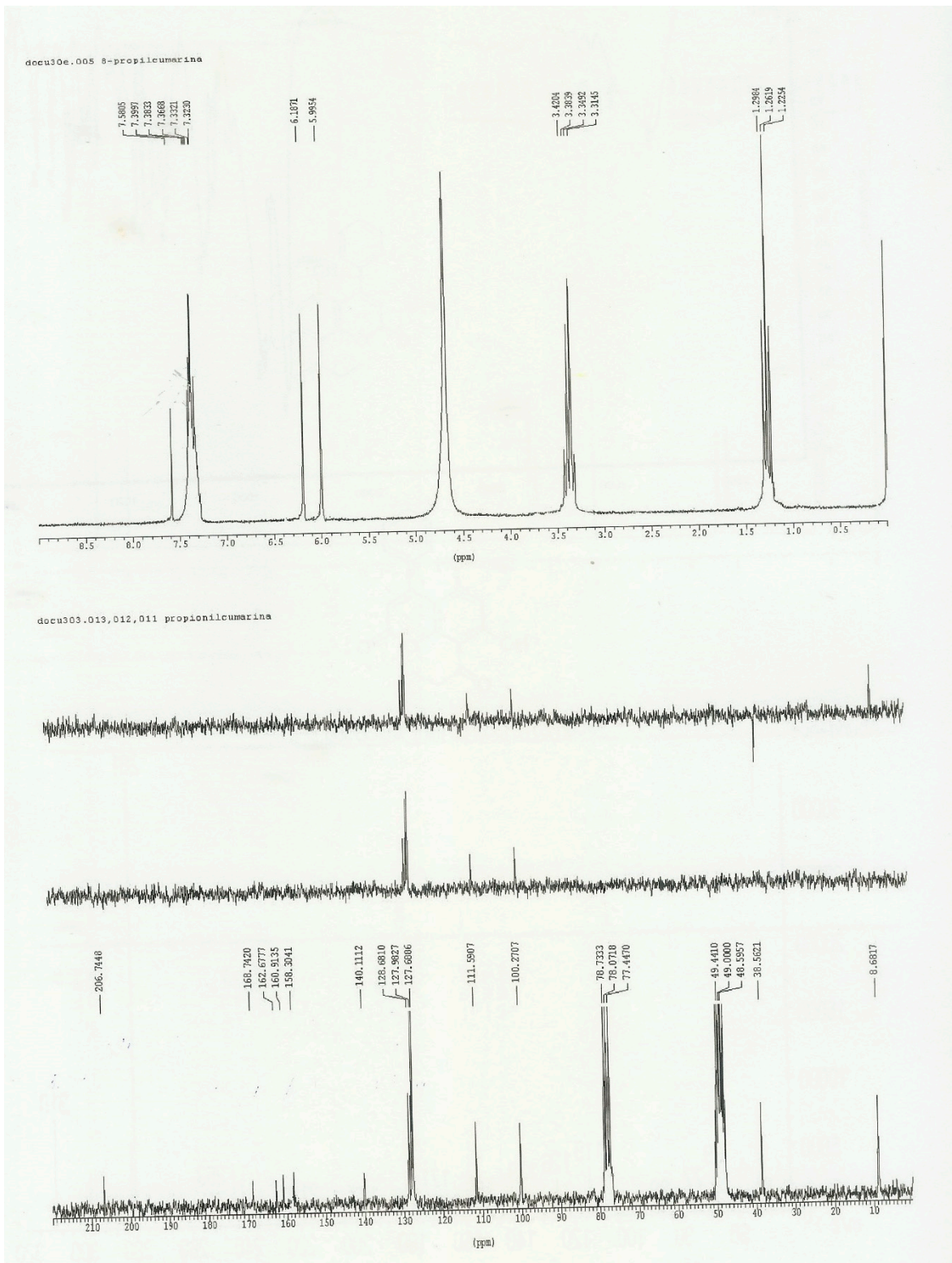
8-acetyl-5,7-dihydroxy-4-phenyl-2H-chromen-2-one (12)



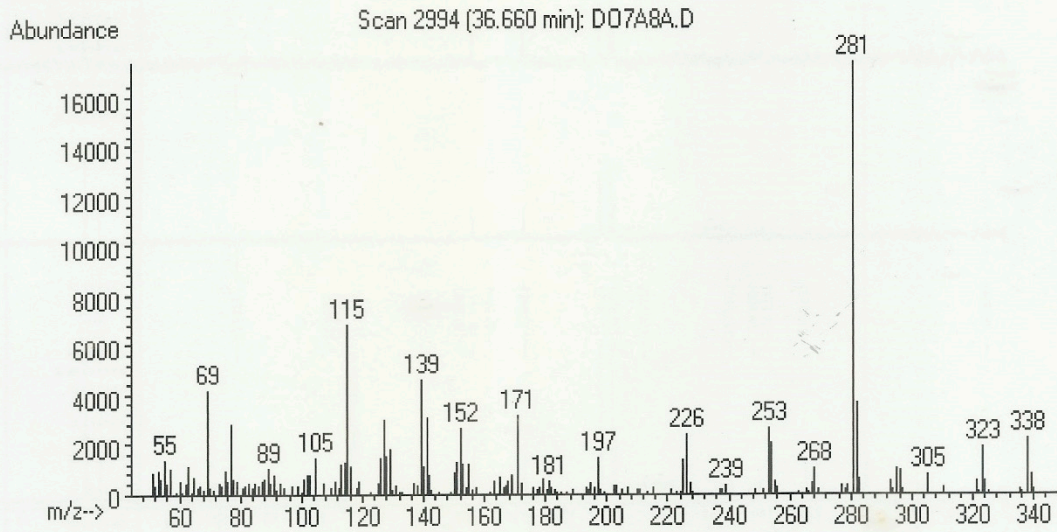
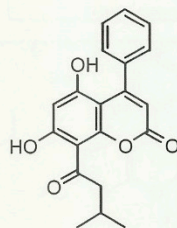
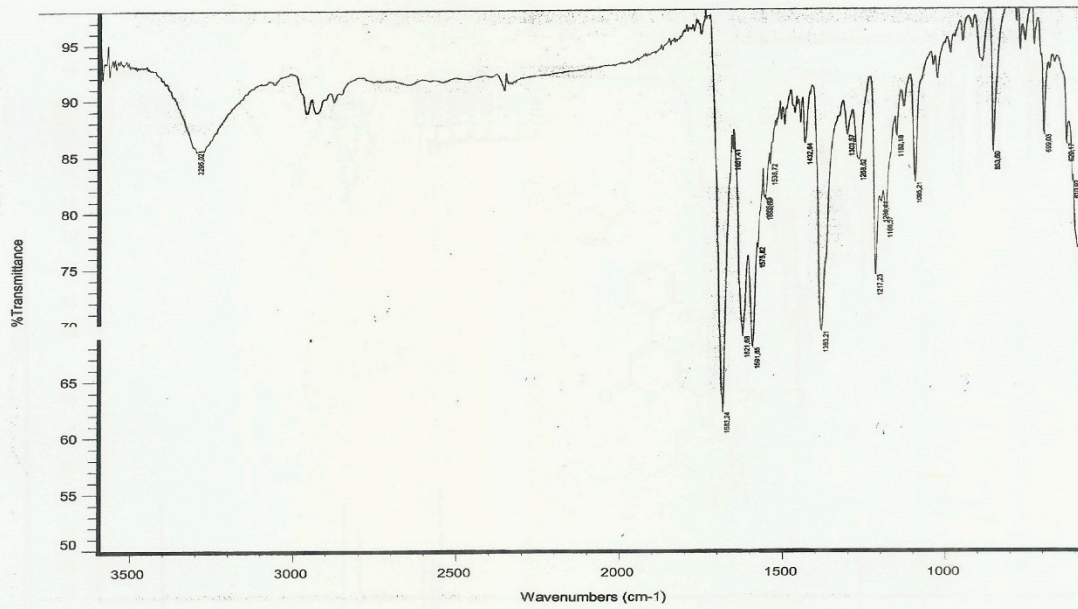
8-acetyl-5,7-dihydroxy-4-phenyl-2H-chromen-2-one (**12**)



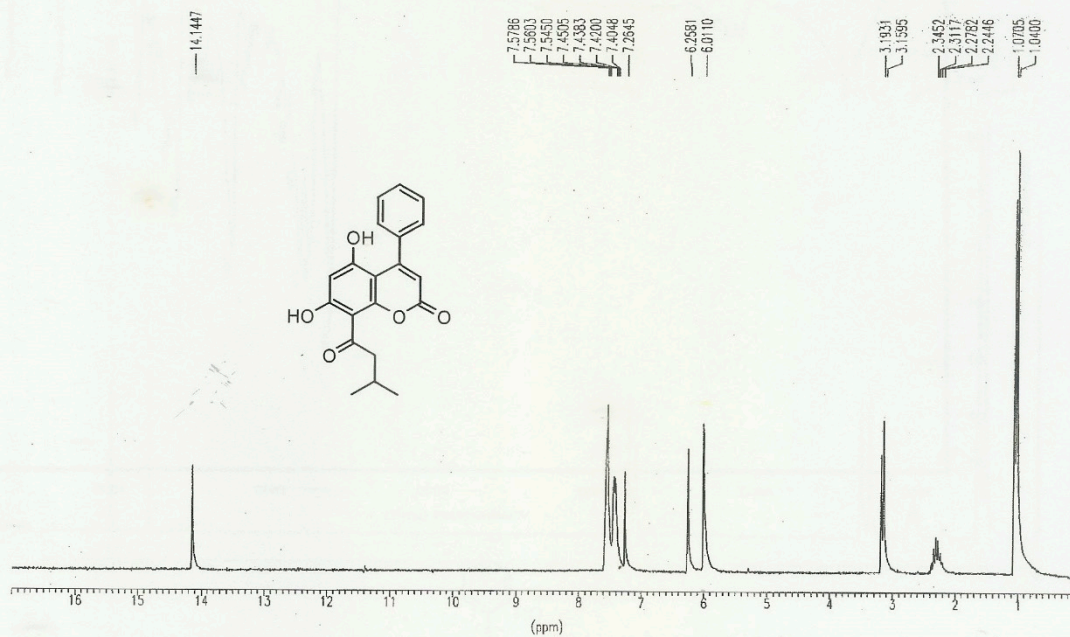
5,7-dihydroxy-4-phenyl-8-propionyl-2H-chromen-2-one (13)



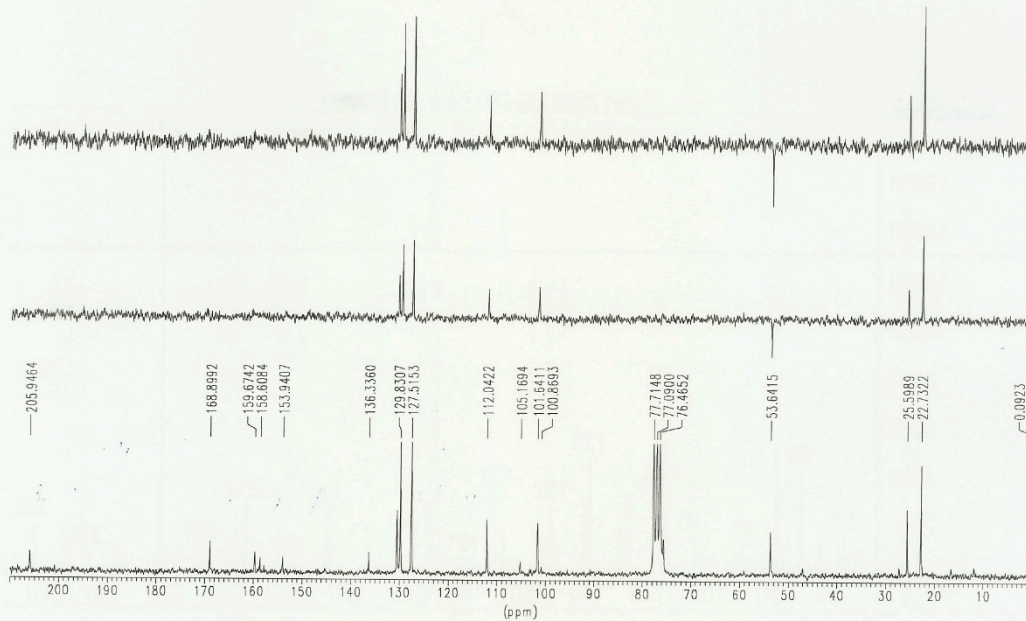
*5,7-dihydroxy-4-phenyl-8-propionyl-2H-chromen-2-one (13)*



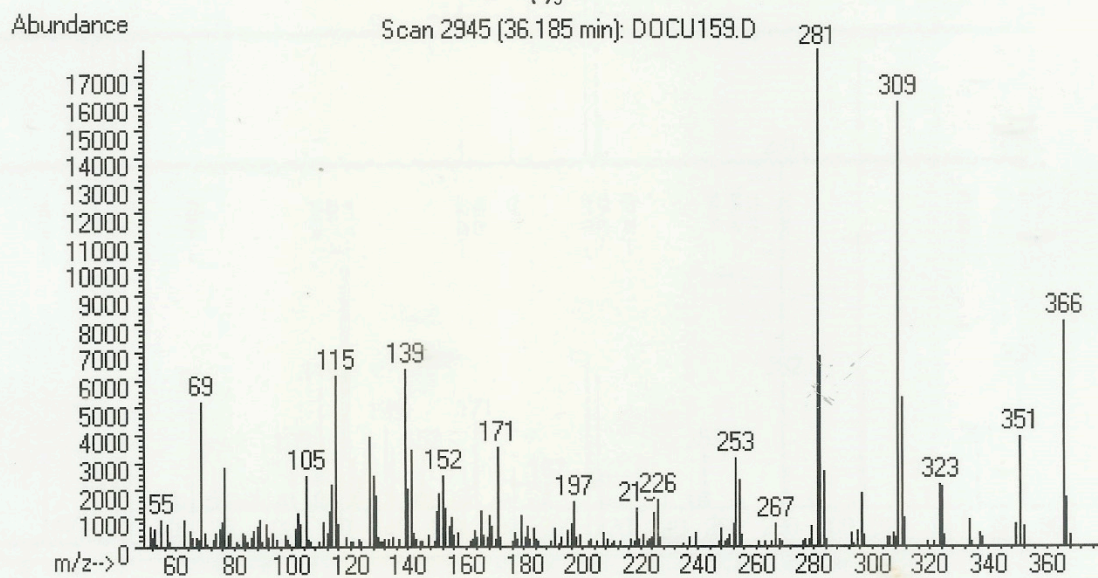
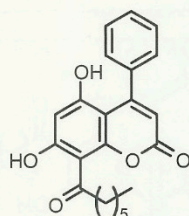
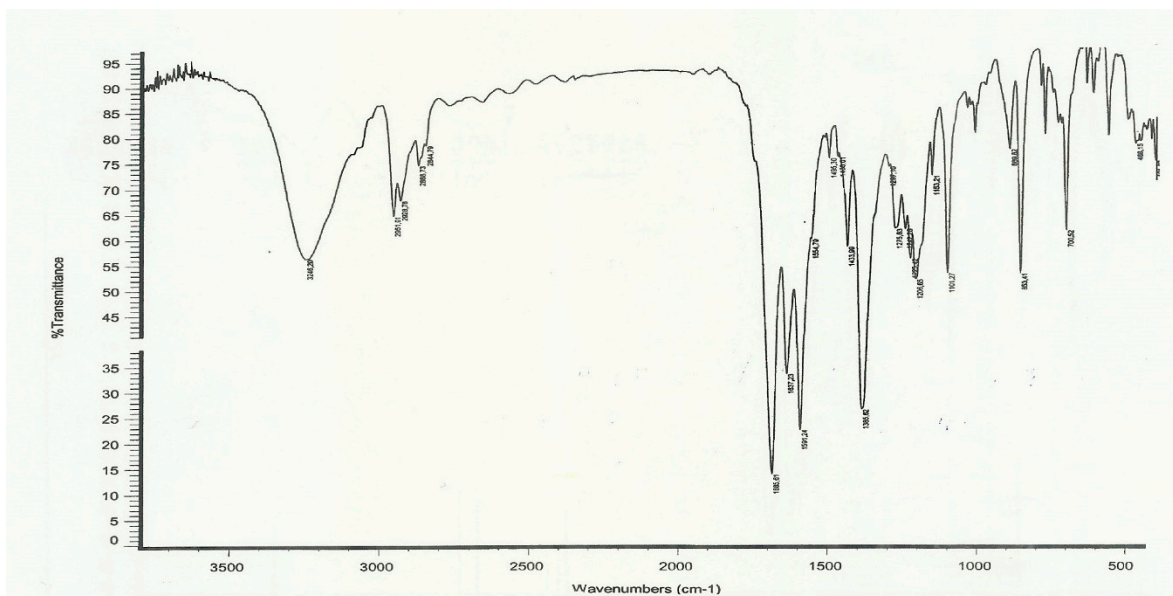
*5,7-dihydroxy-8-(3-methylbutanoyl)-4-phenyl-2H-chromen-2-one (14)*



compuesto damp7a8

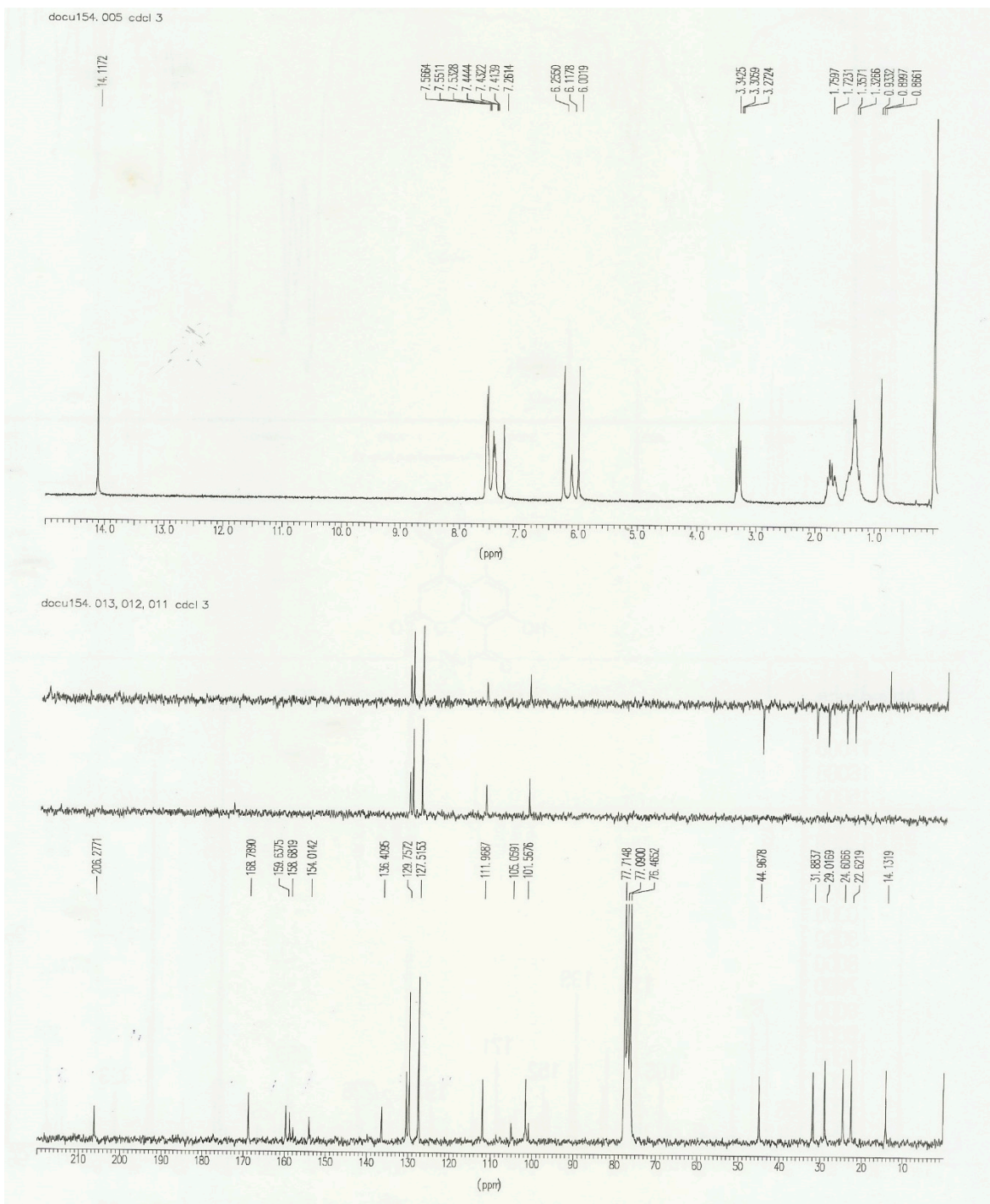


5,7-dihydroxy-8-(3-methylbutanoyl)-4-phenyl-2H-chromen-2-one (14)

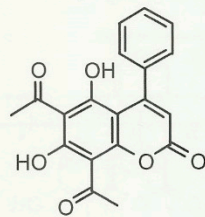
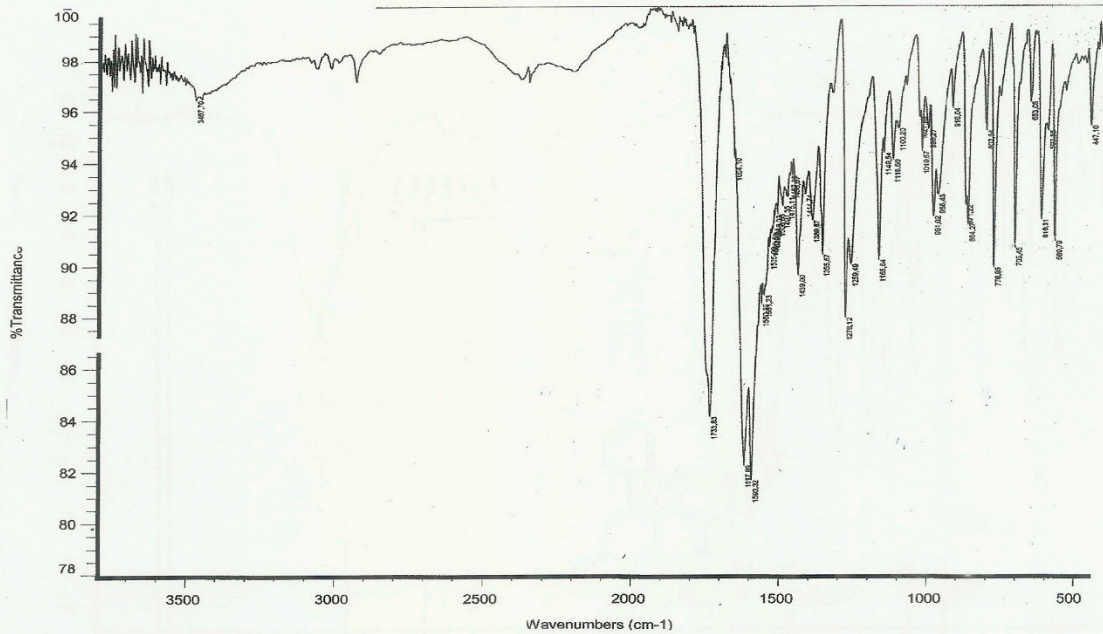


*8-heptanoyl-5,7-dihydroxy-4-phenyl-2H-chromen-2-one (15)*

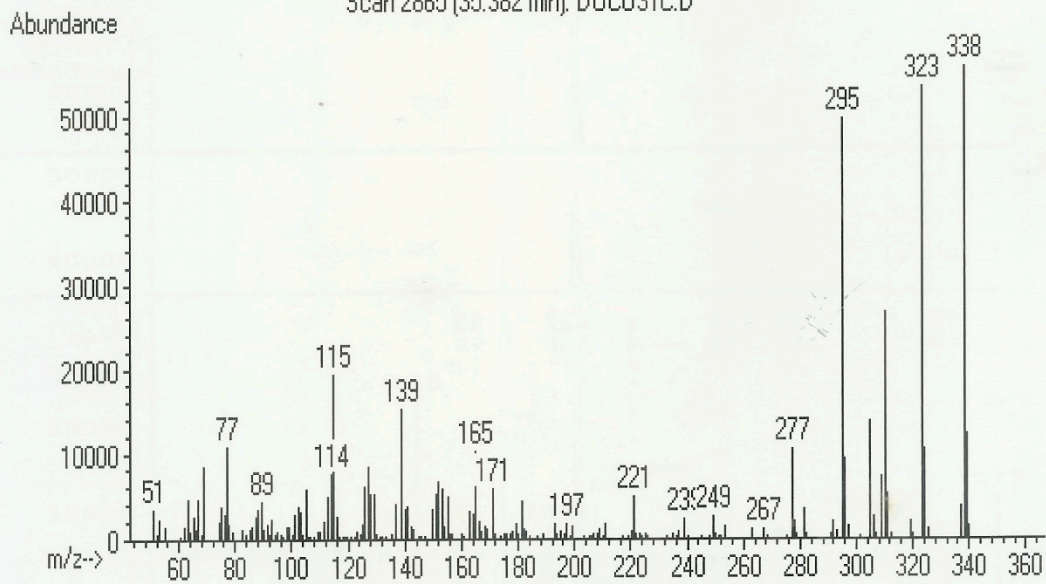




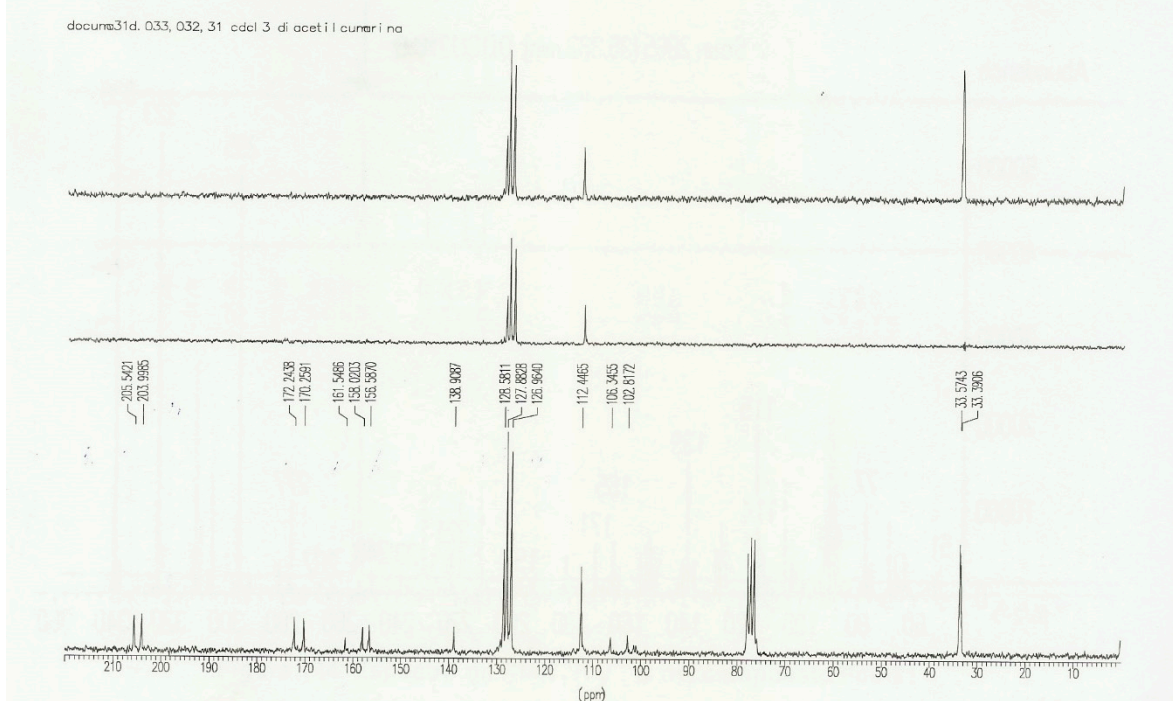
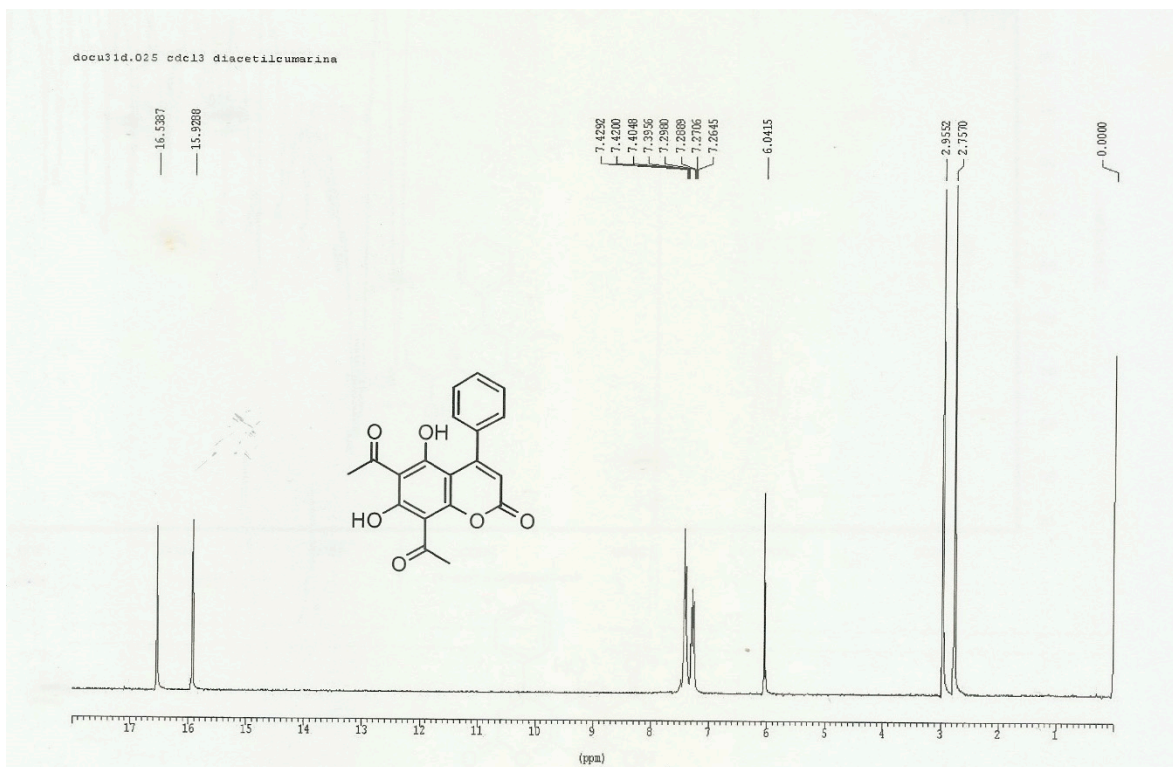
*8*-heptanoyl-5,7-dihydroxy-4-phenyl-2H-chromen-2-one (15)



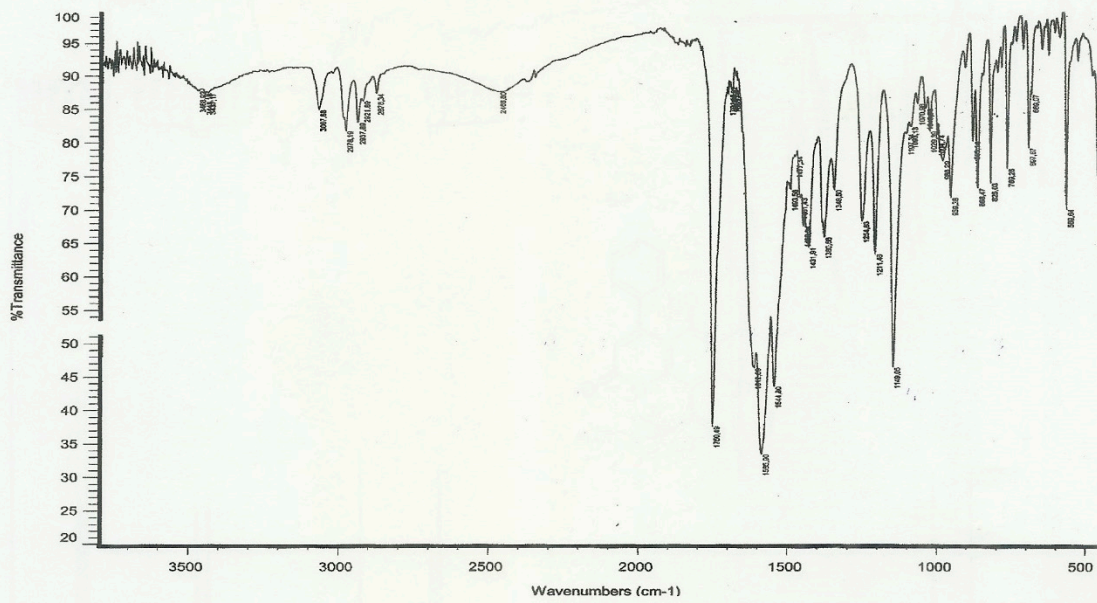
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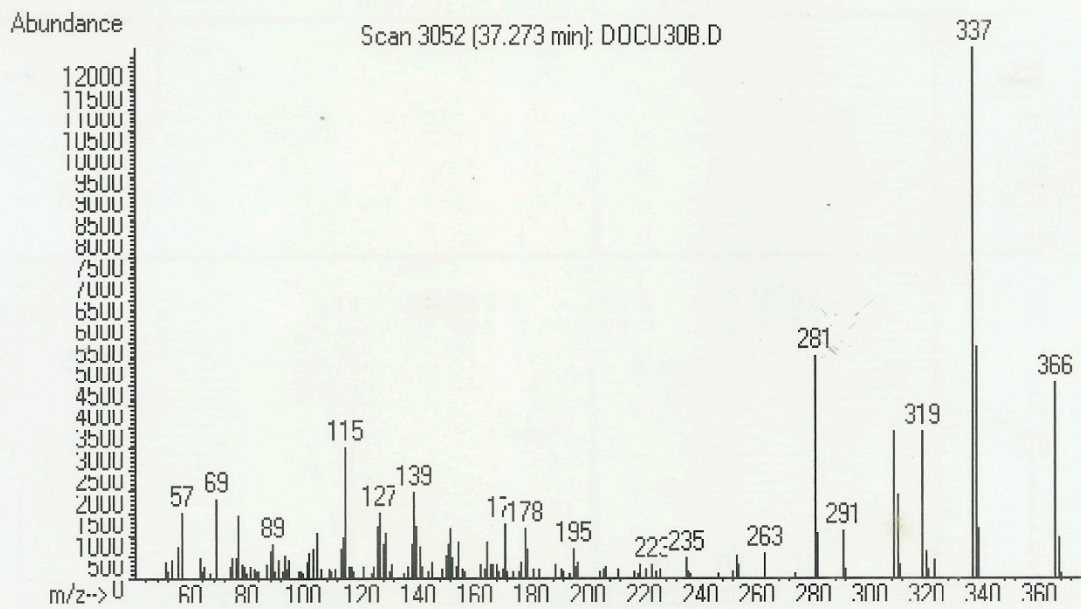
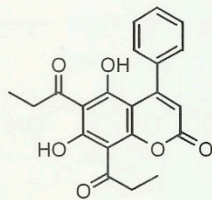
*6,8-diacetyl-5,7-dihydroxy-4-phenyl-2H-chromen-2-one (17)*



6,8-diacetyl-5,7-dihydroxy-4-phenyl-2H-chromen-2-one (17)

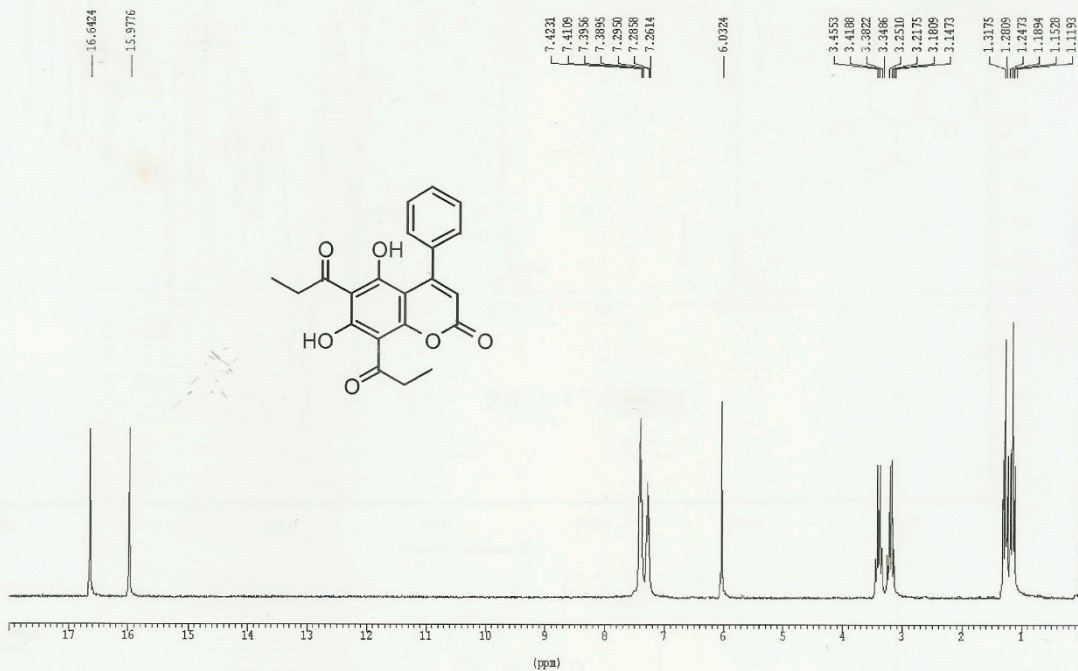


*apropo*

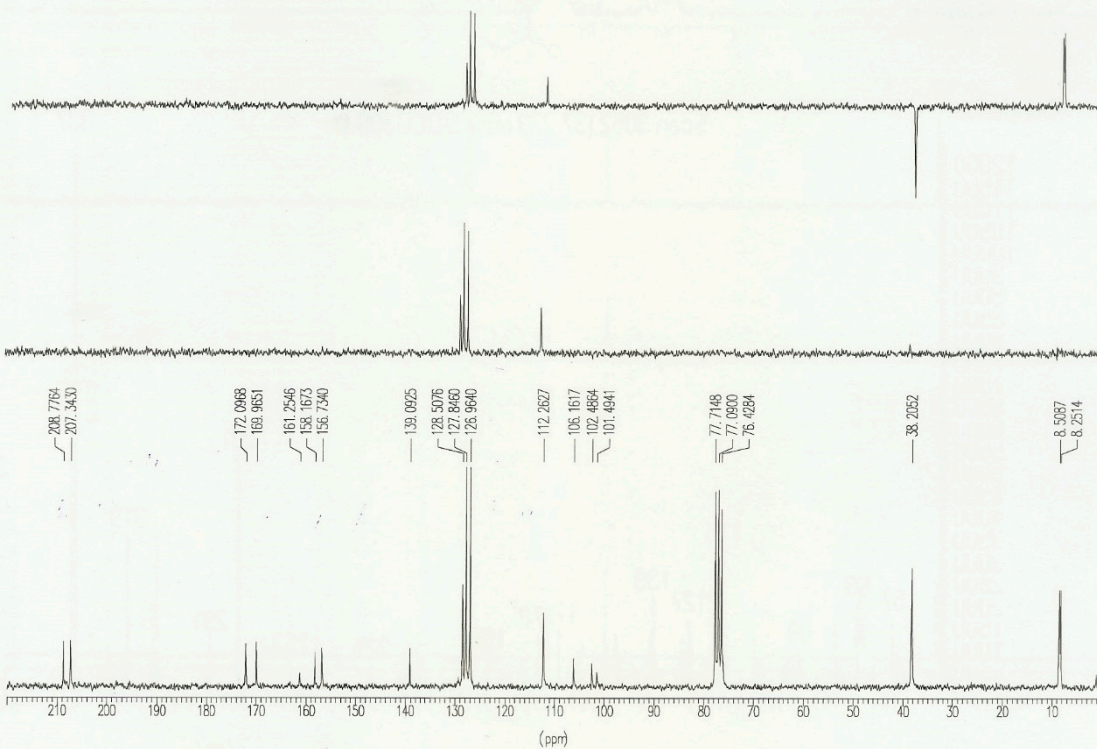


5,7-dihydroxy-4-phenyl-6,8-dipropionyl-2H-chromen-2-one (18)

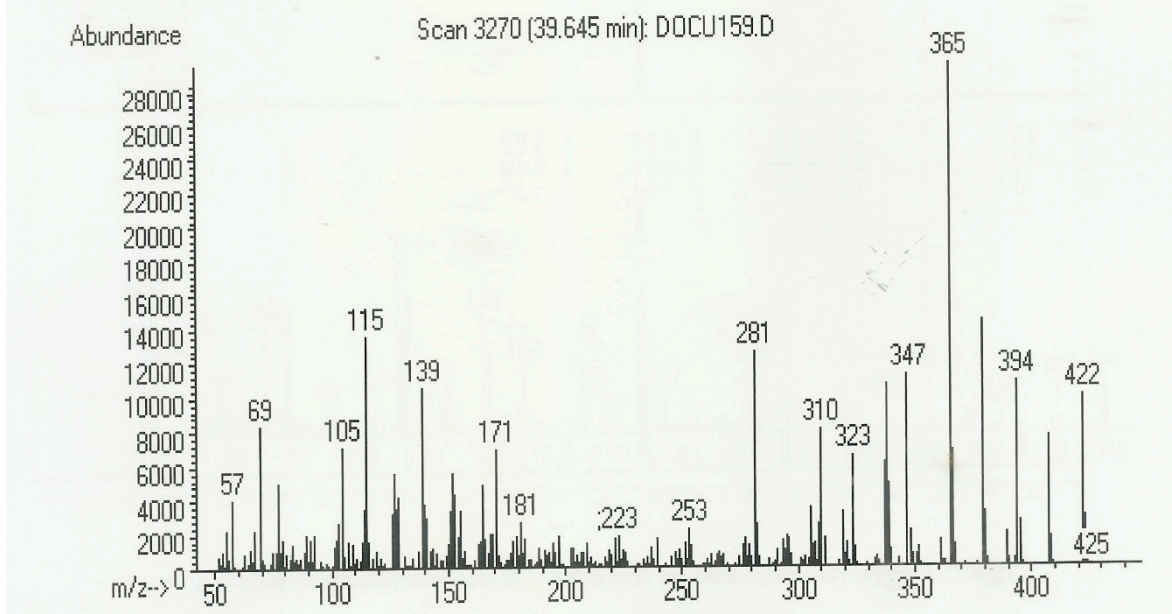
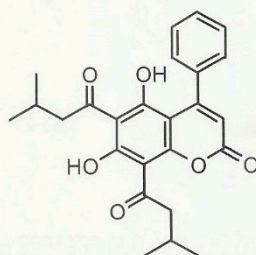
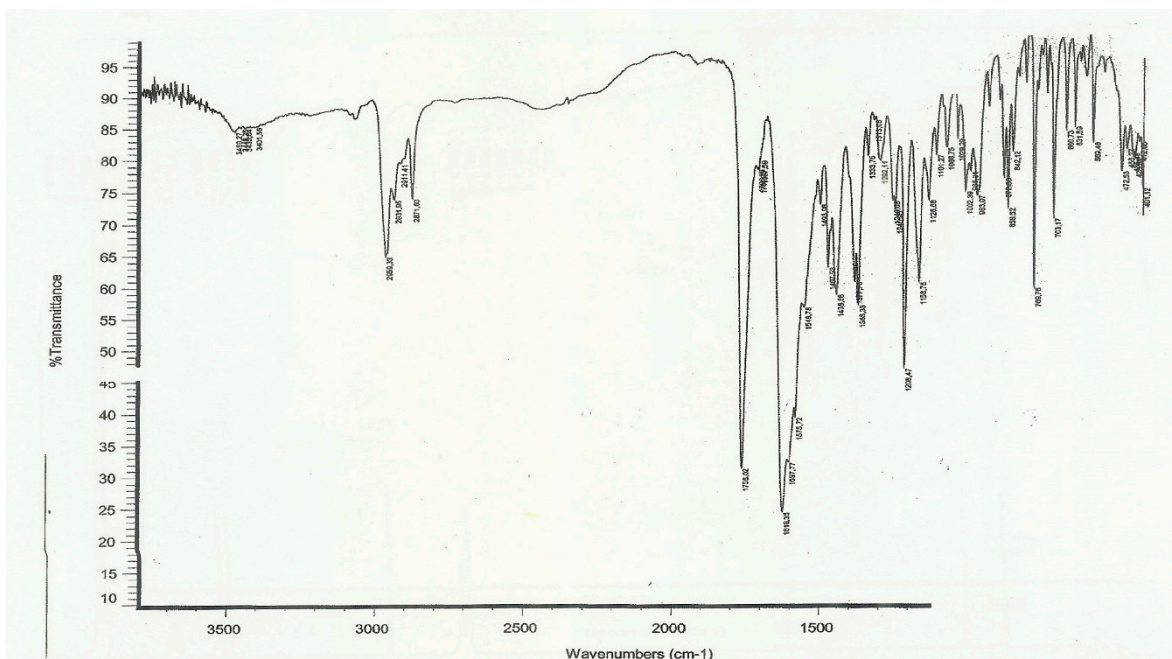
docu30c.005 6,8-dipropyl-4-phenylchromone, cdc13



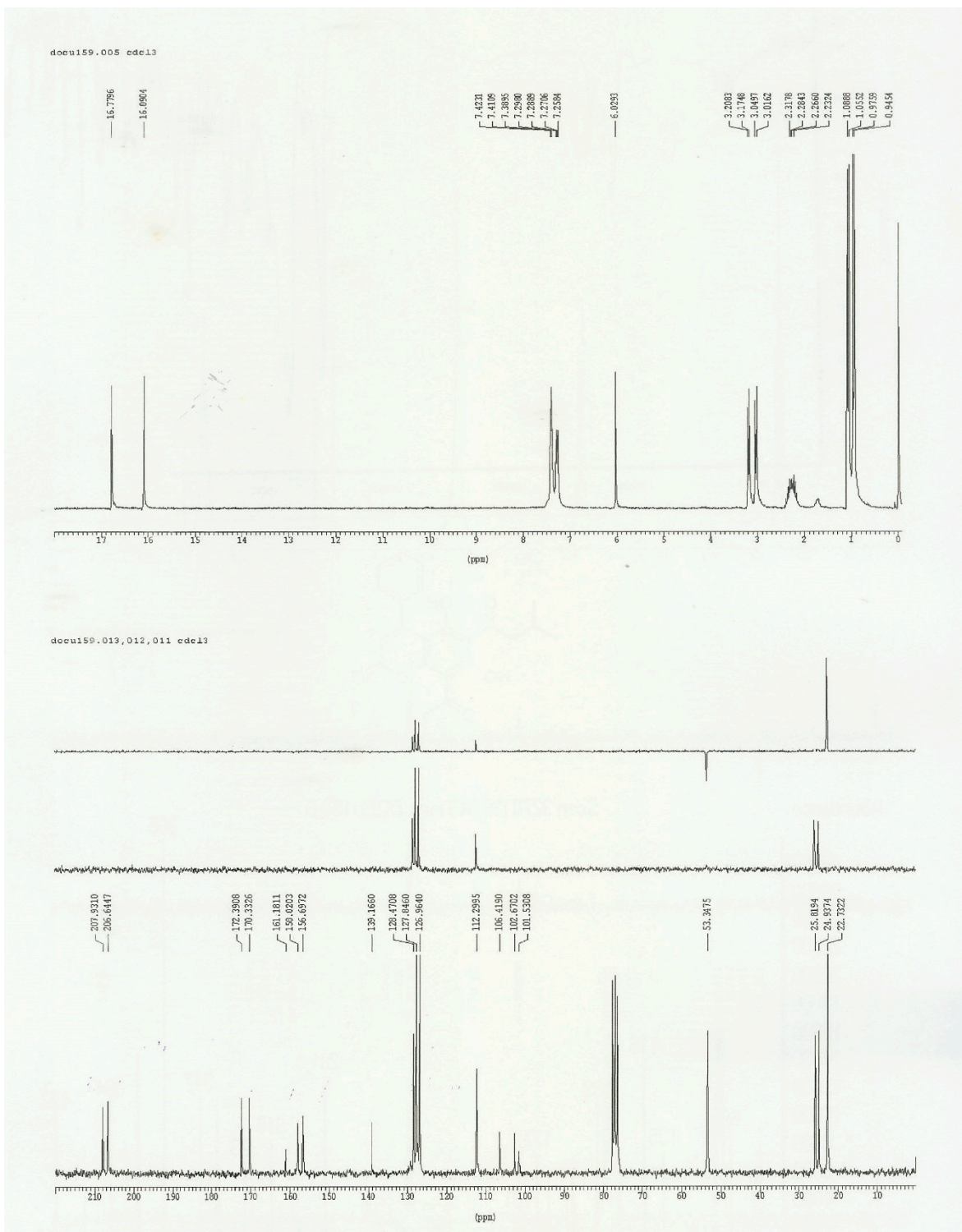
docu30c.013,012,011 cdcl3 di propil-4-fenil cromoni na



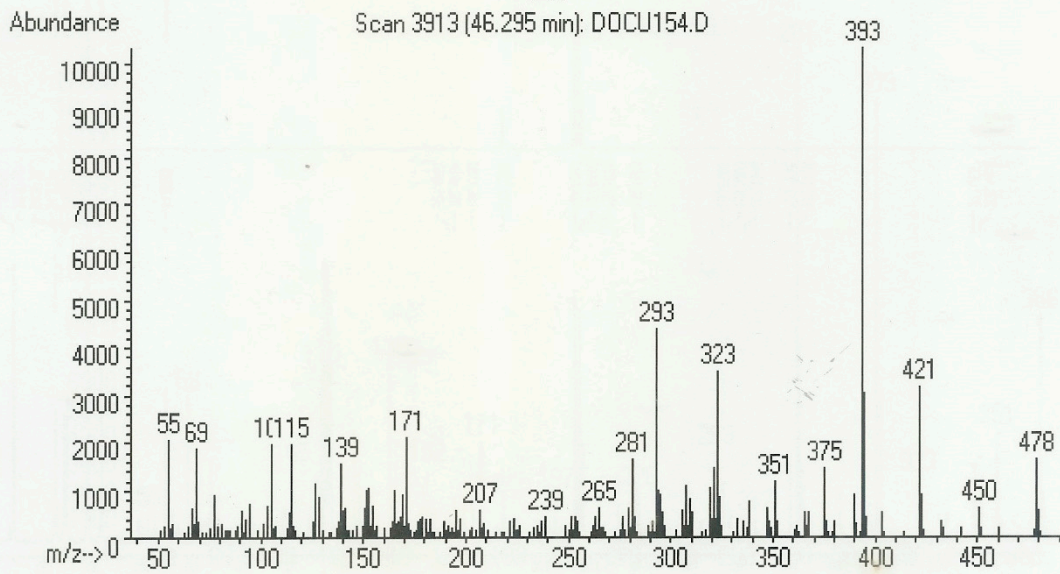
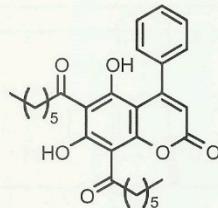
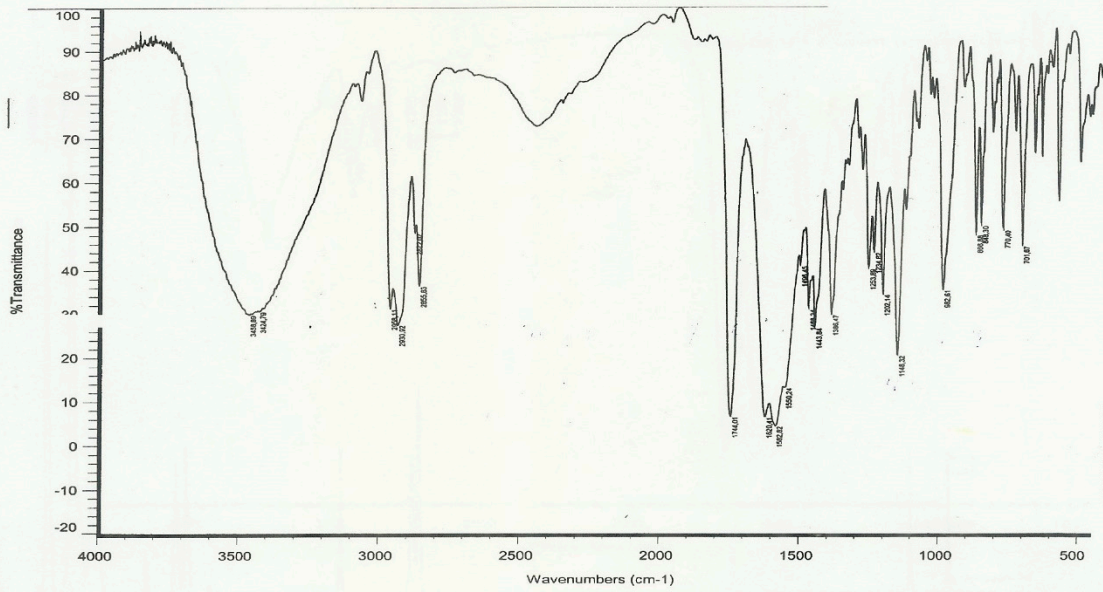
5,7-dihydroxy-4-phenyl-6,8-dipropionyl-2H-chromen-2-one (18)



5,7-dihydroxy-6,8-bis(3-methylbutanoyl)-4-phenyl-2H-chromen-2-one (19)

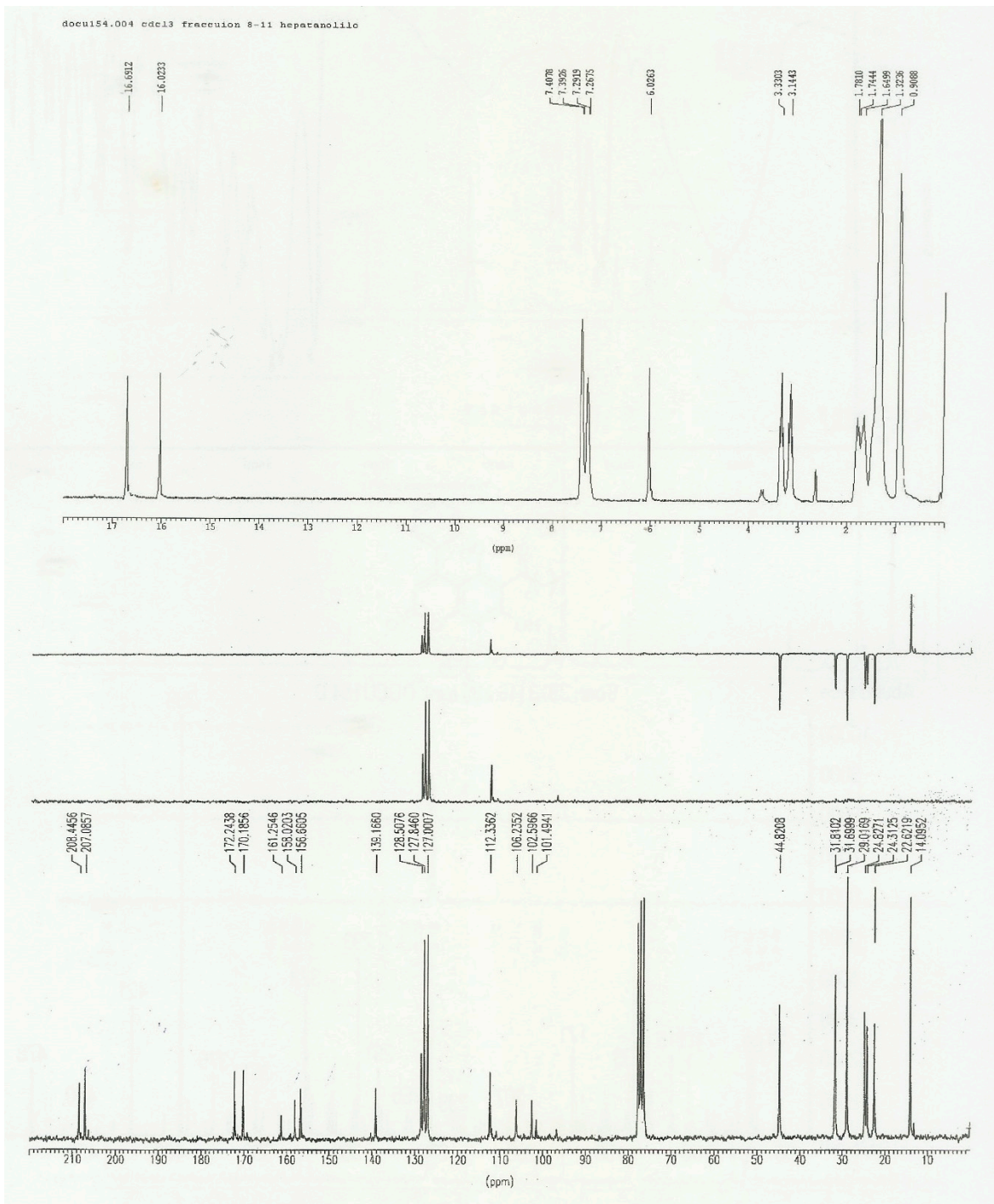


*5,7-dihydroxy-6,8-bis(3-methylbutanoyl)-4-phenyl-2H-chromen-2-one (19)*

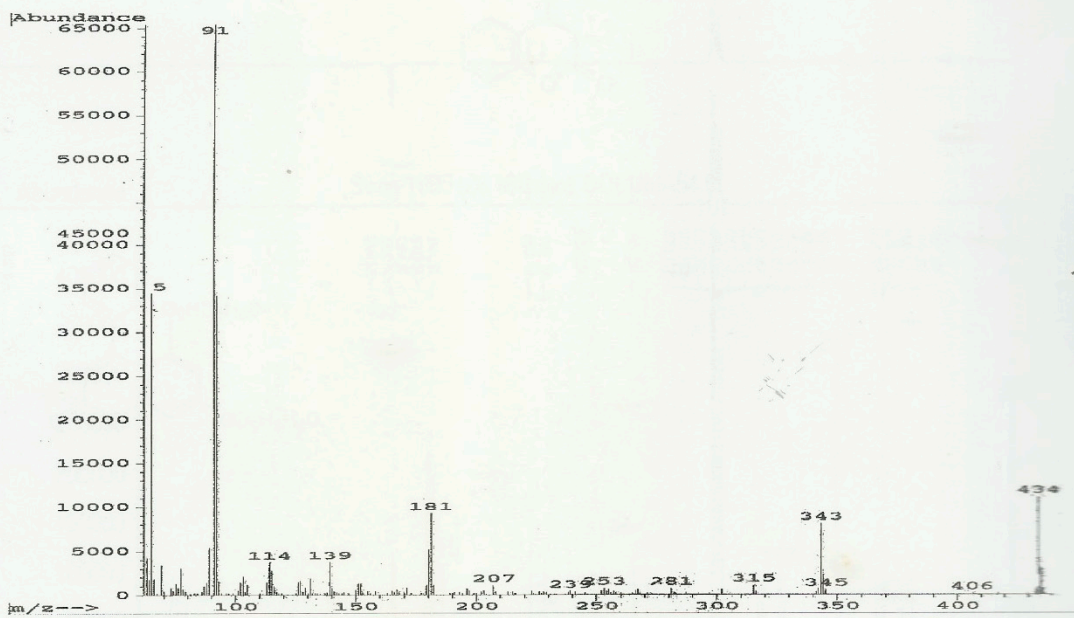
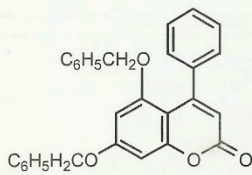
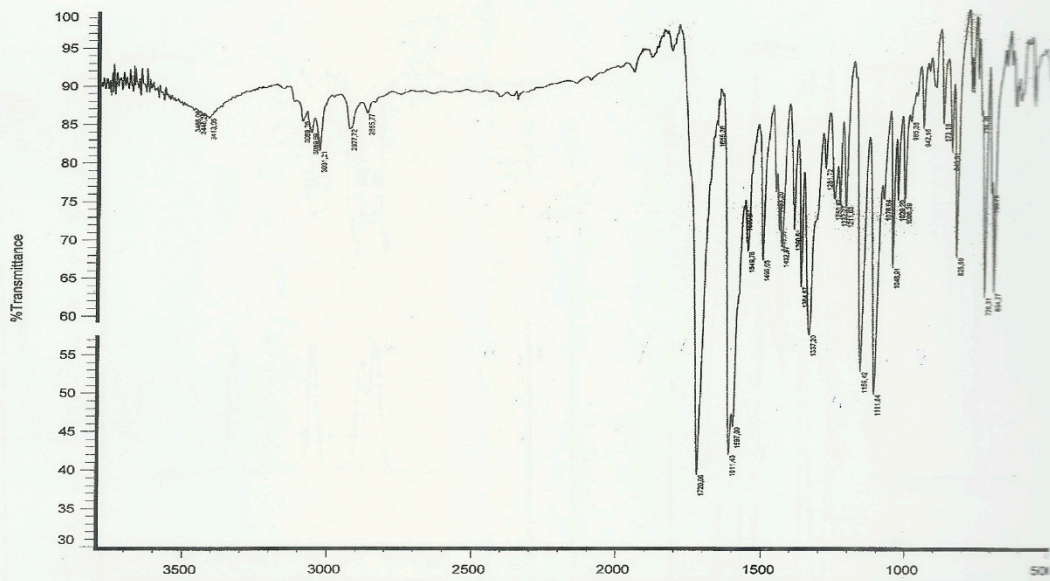


*6,8-diheptanoyl-5,7-dihydroxy-4-phenyl-2H-chromen-2-one (20)*



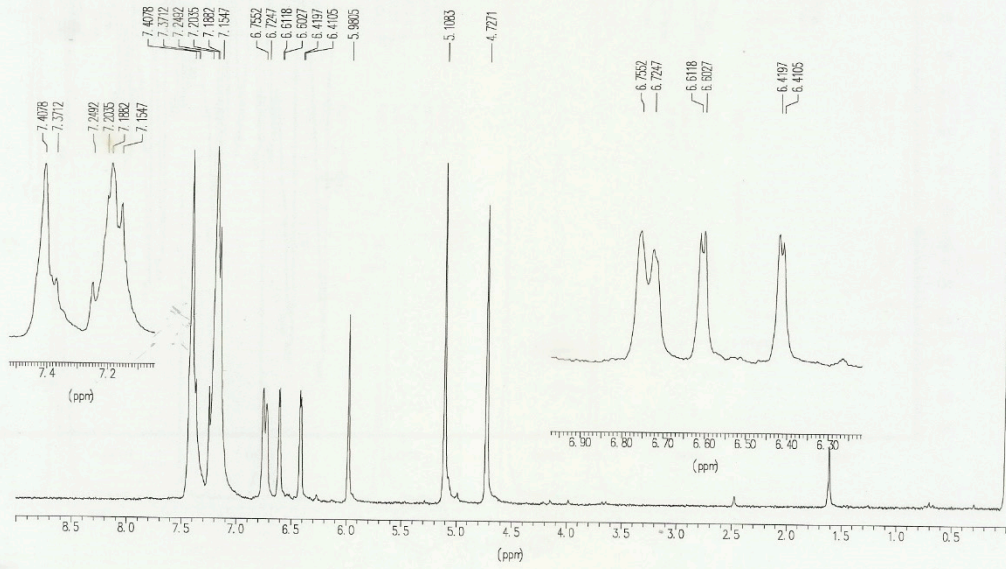


*6,8-diheptanoyl-5,7-dihydroxy-4-phenyl-2H-chromen-2-one (20)*

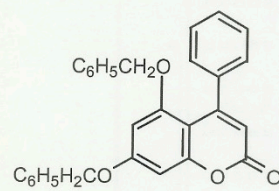
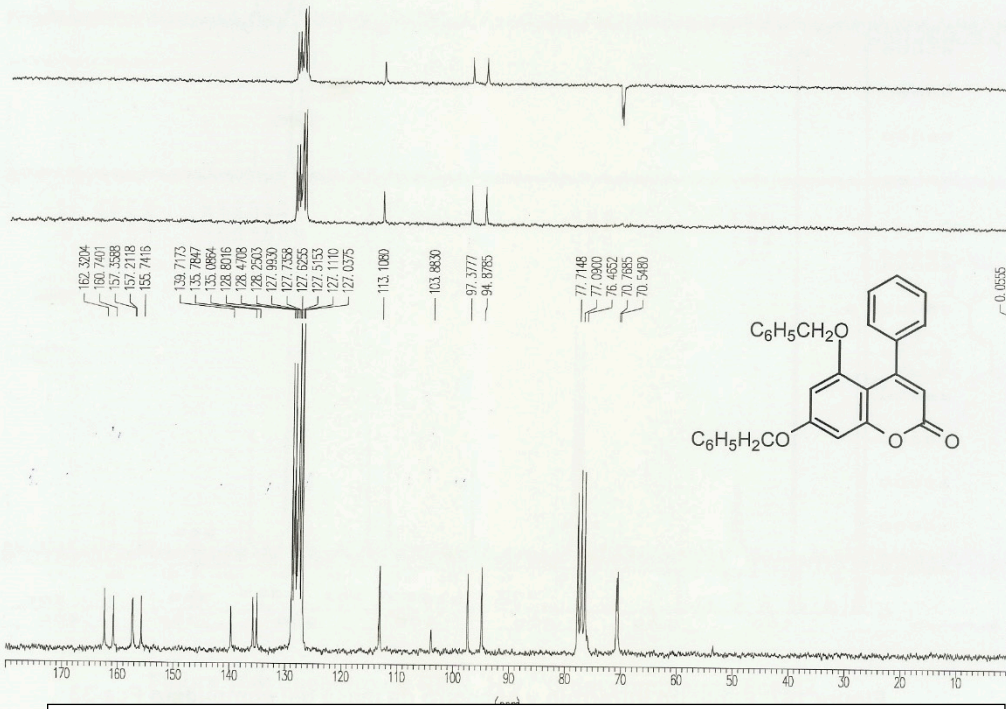


5,7-dibenzyloxy-4-phenyl-2H-chromen-2-one (21)

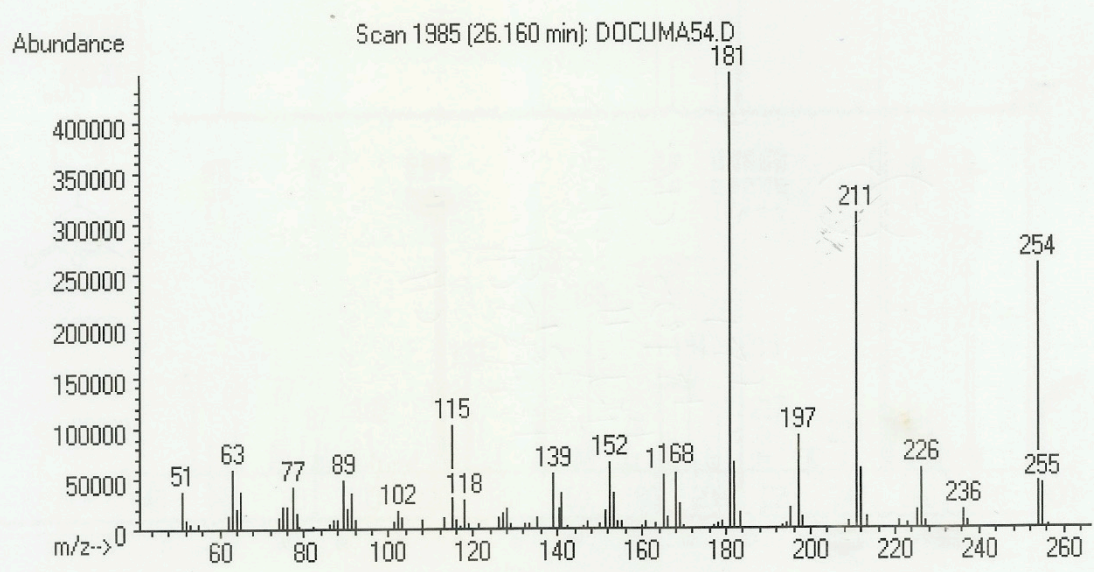
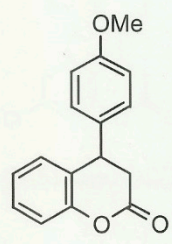
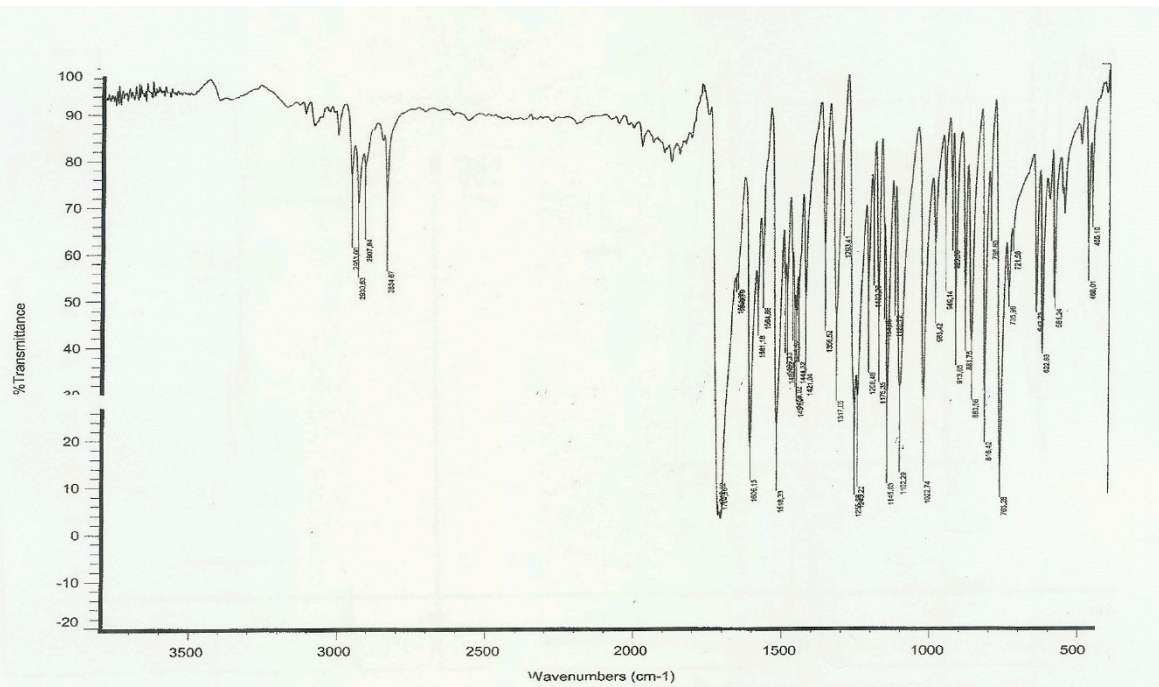
docu177.006 o-di benzi I



docu1770.13.012.011 o-di benzi I cumari na cdcl 3



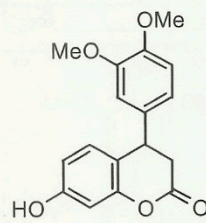
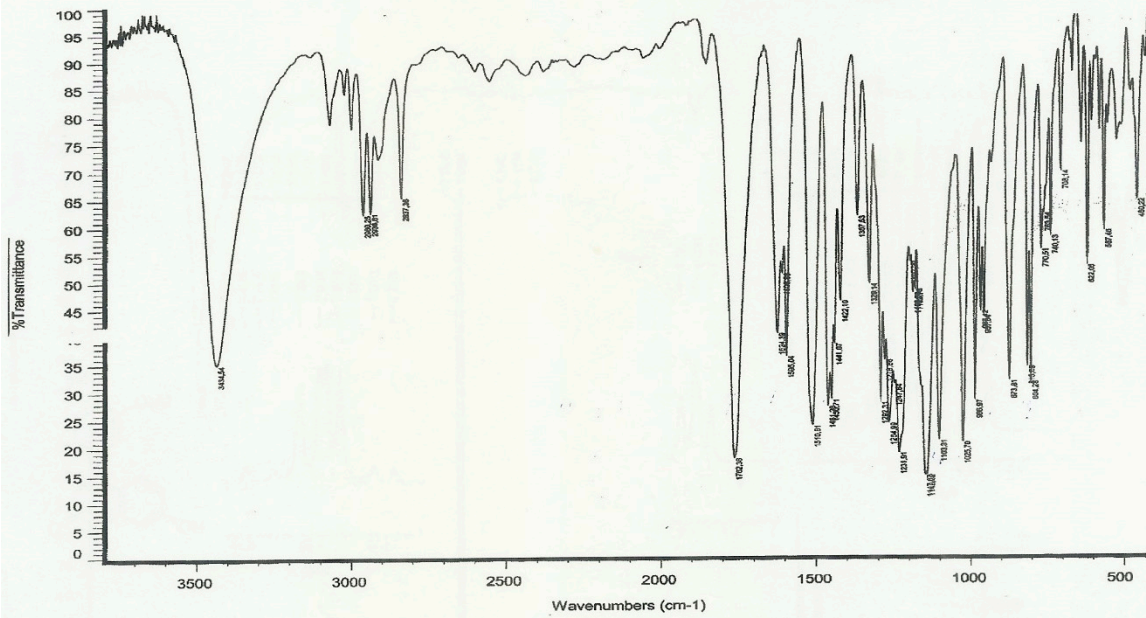
5,7-dibenzoyloxy-4-phenyl-2H-chromen-2-one (21)



4-(4-methoxyphenyl)chroman-2-one (22)

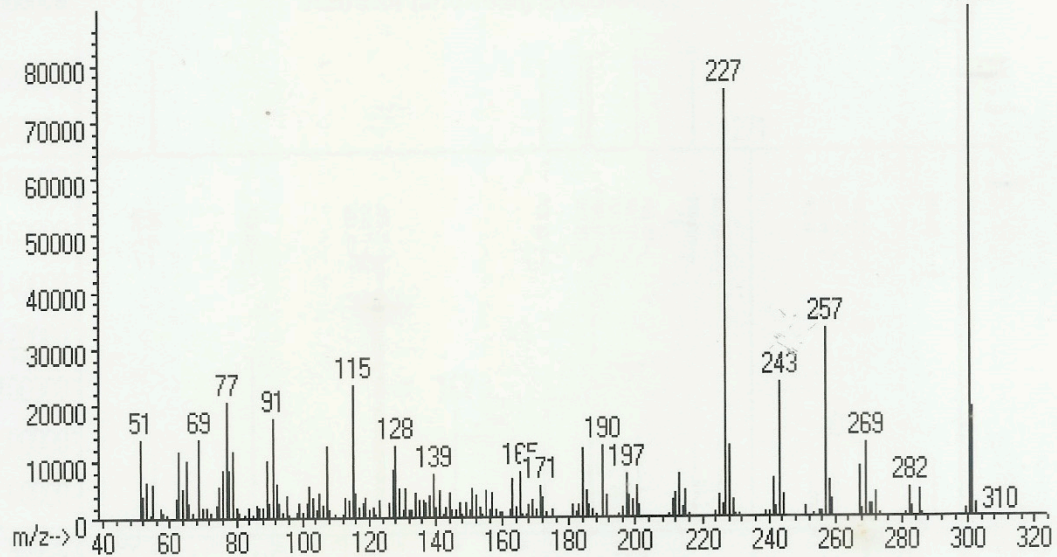


2. Espectros

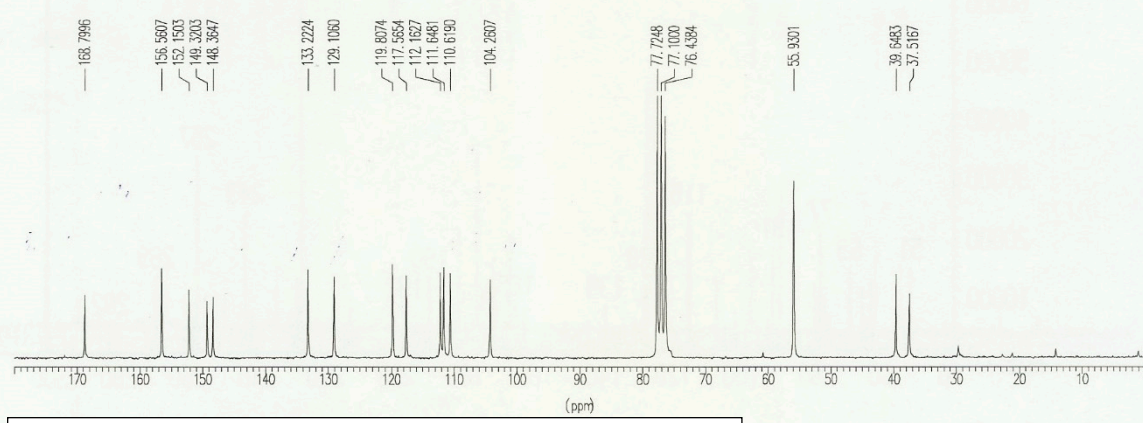
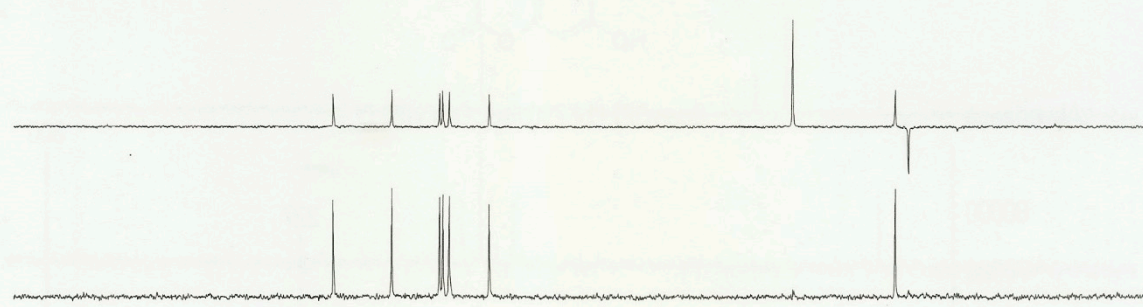
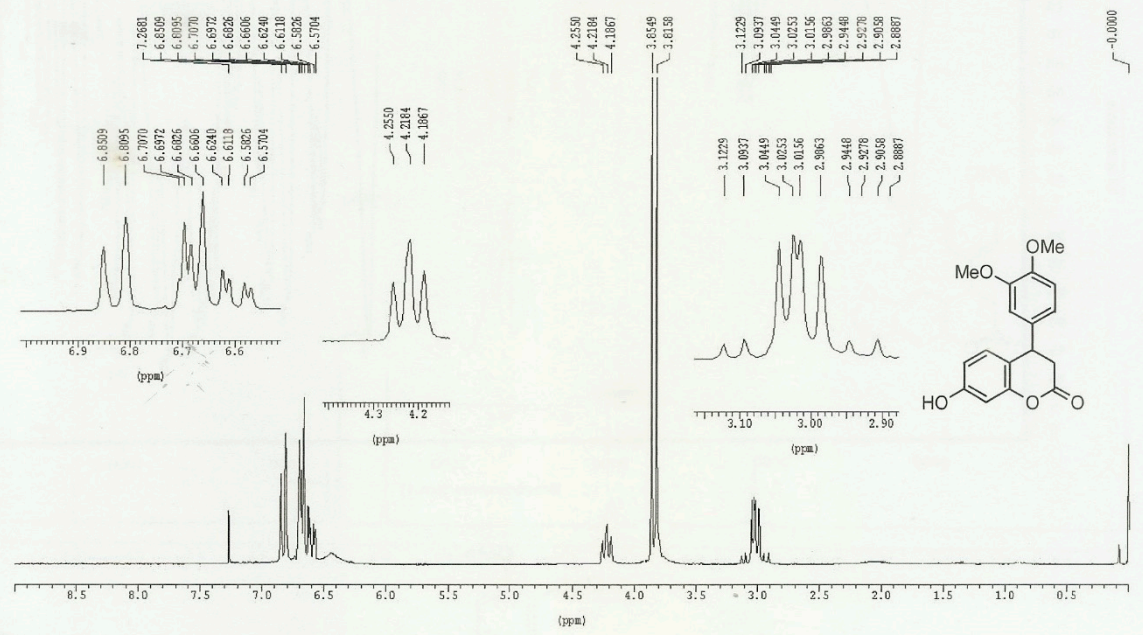


Abundance

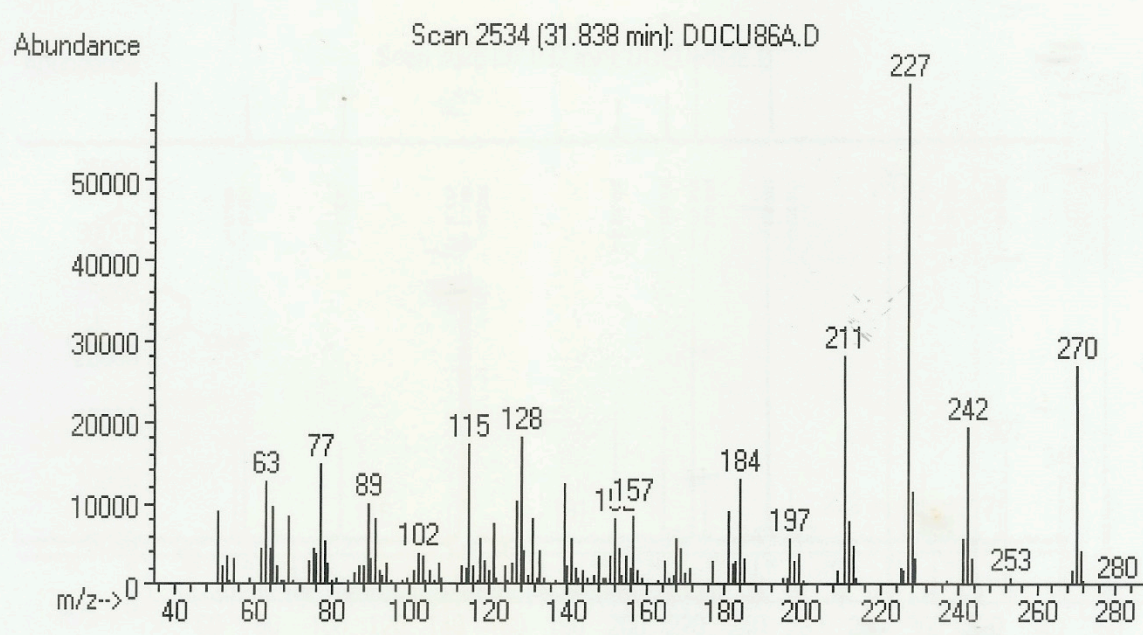
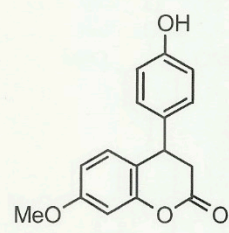
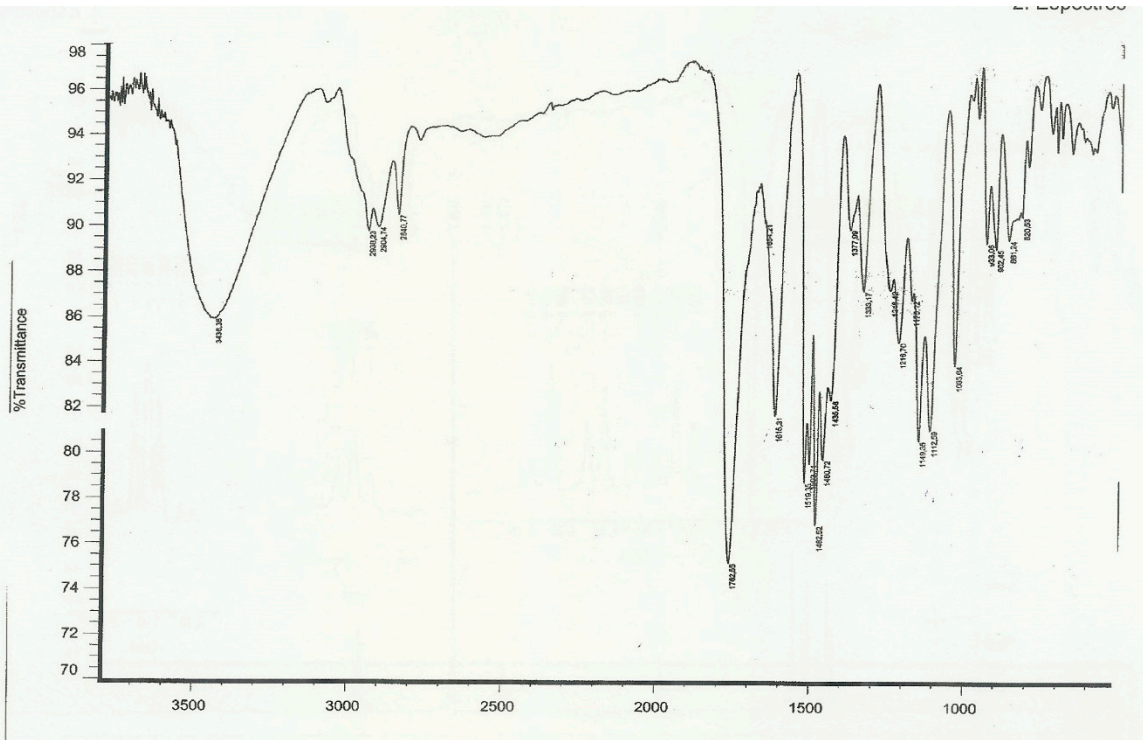
Scan 921 (14.790 min): DOCU82.D



4-(3,4-dimethoxyphenyl)-7-hydroxychroman-2-one (23)



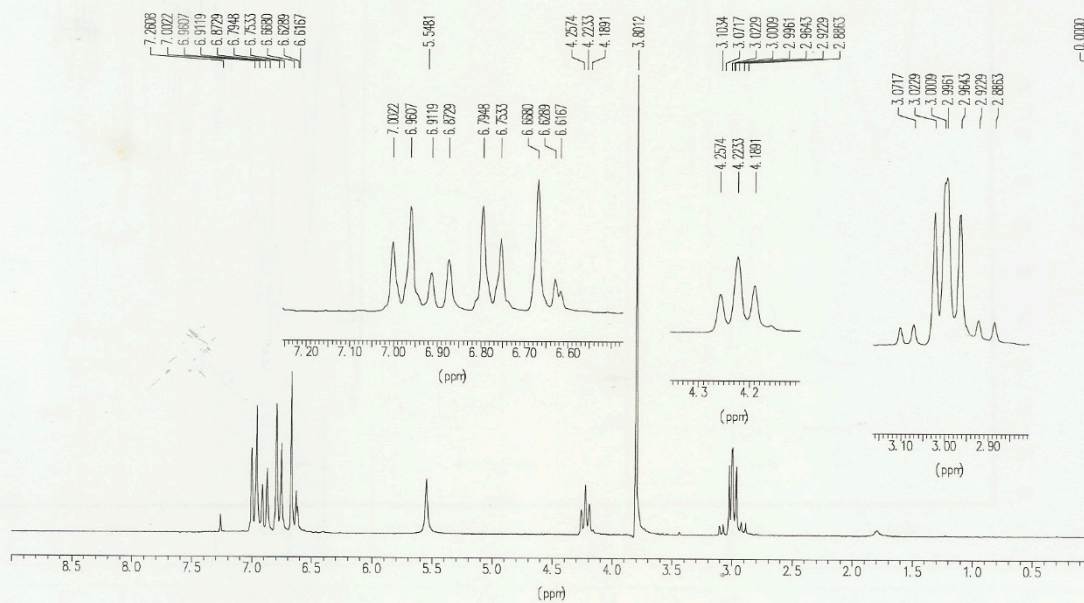
4-(3,4-dimethoxyphenyl)-7-hydroxychroman-2-one (23)



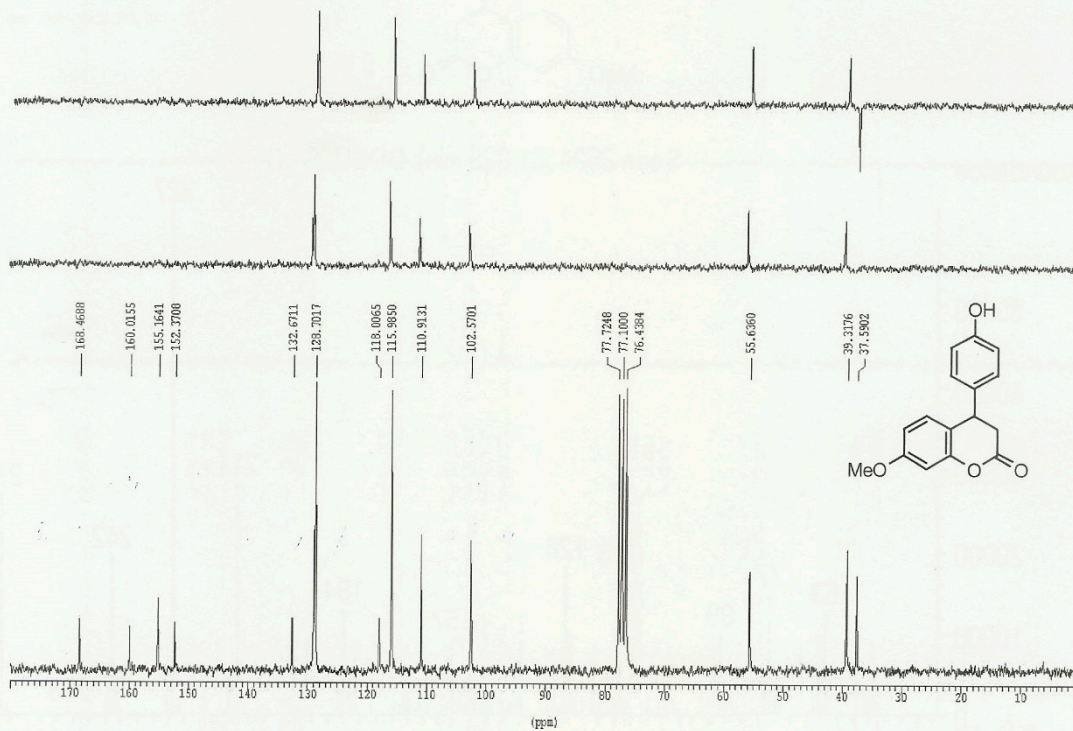
4-(4-hydroxyphenyl)-7-methoxychroman-2-one (24)



docum86.005 pptado en ETER

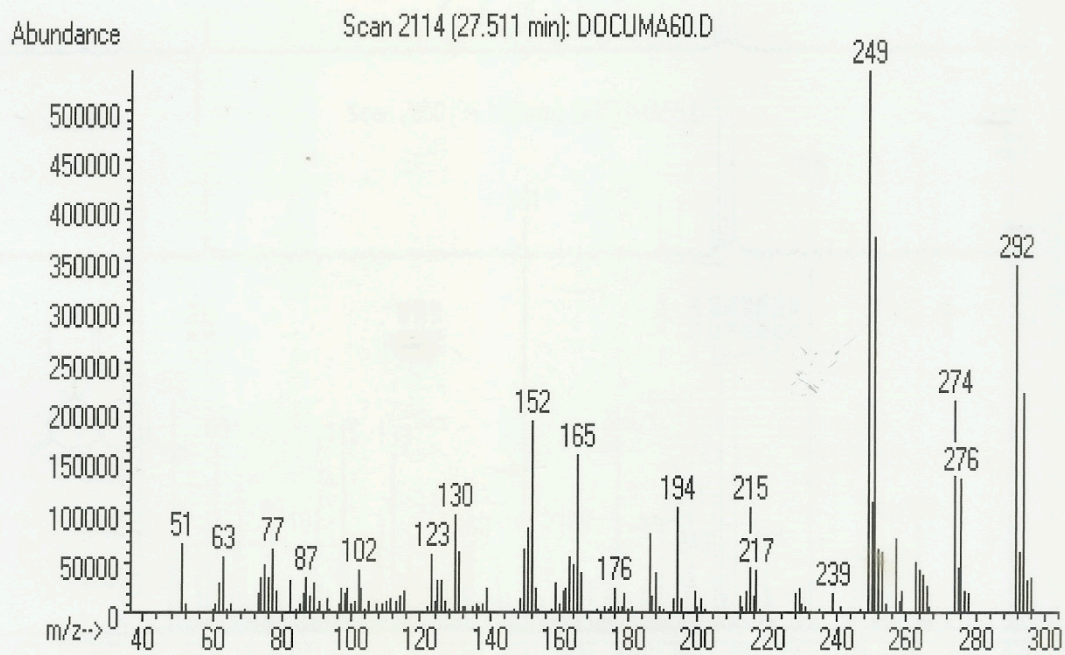
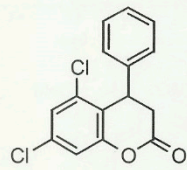
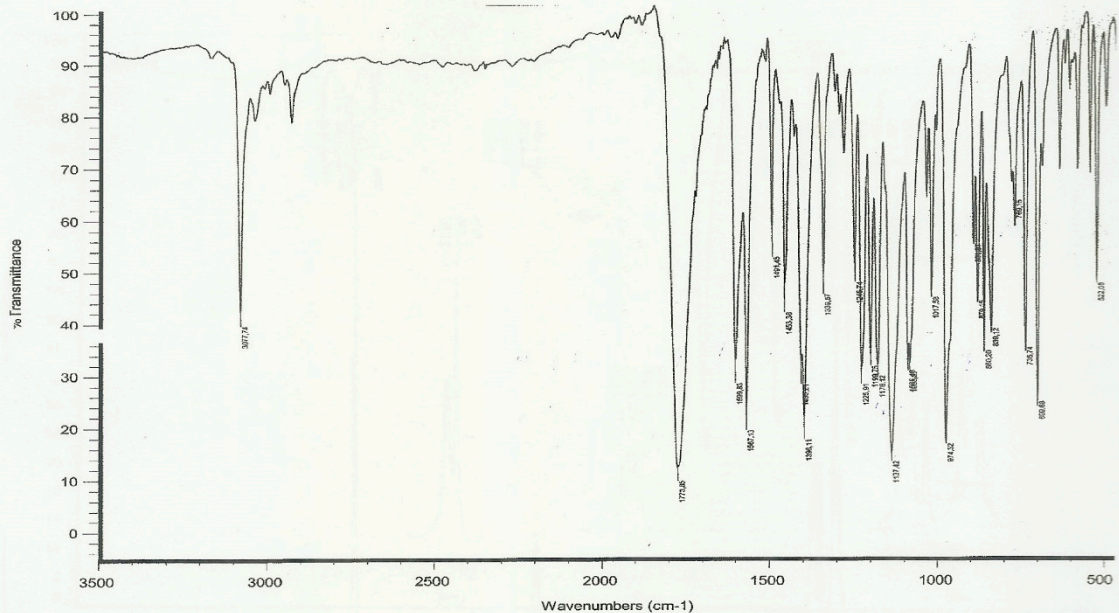


docum86.001

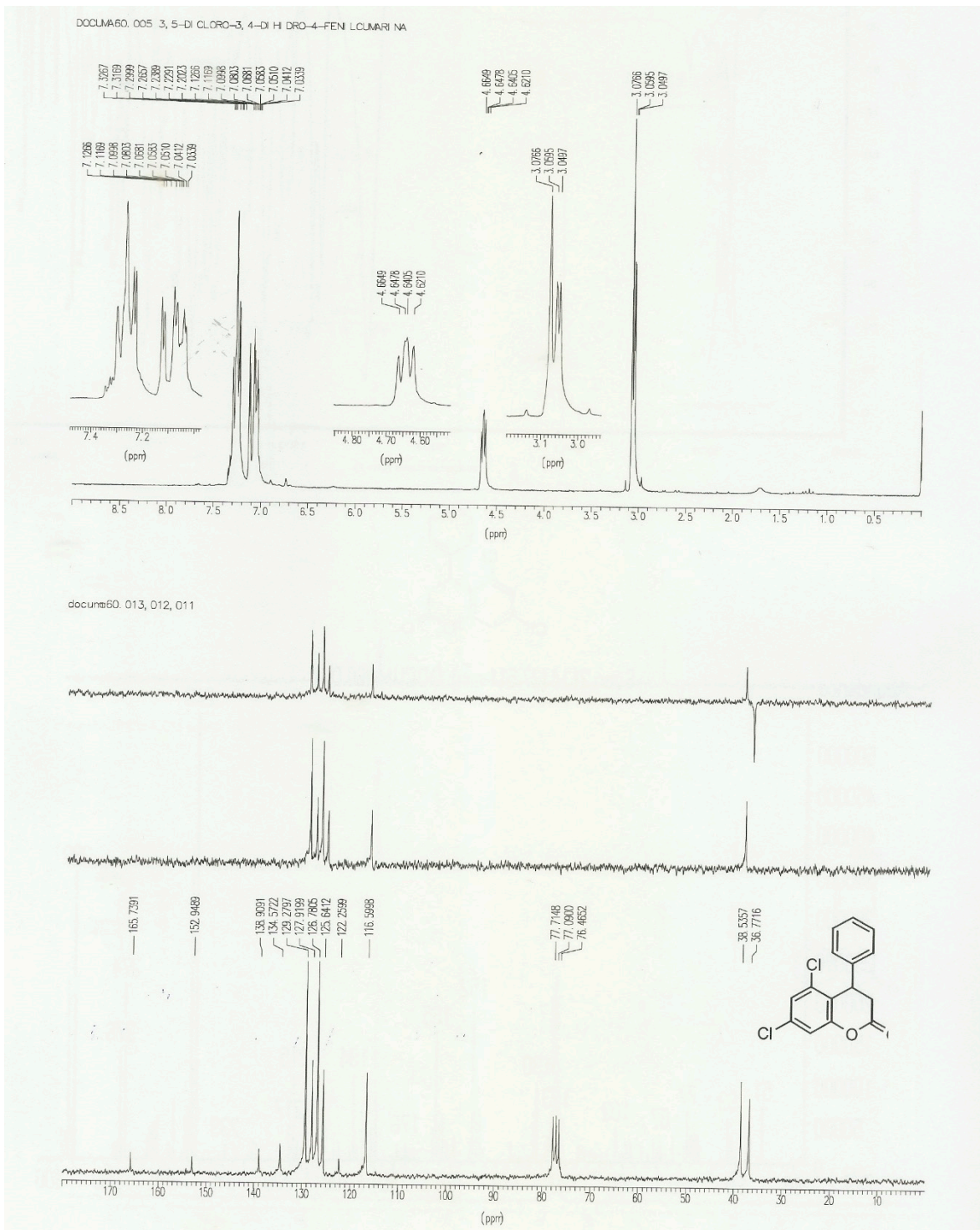


4-(4-hydroxyphenyl)-7-methoxychroman-2-one (24)

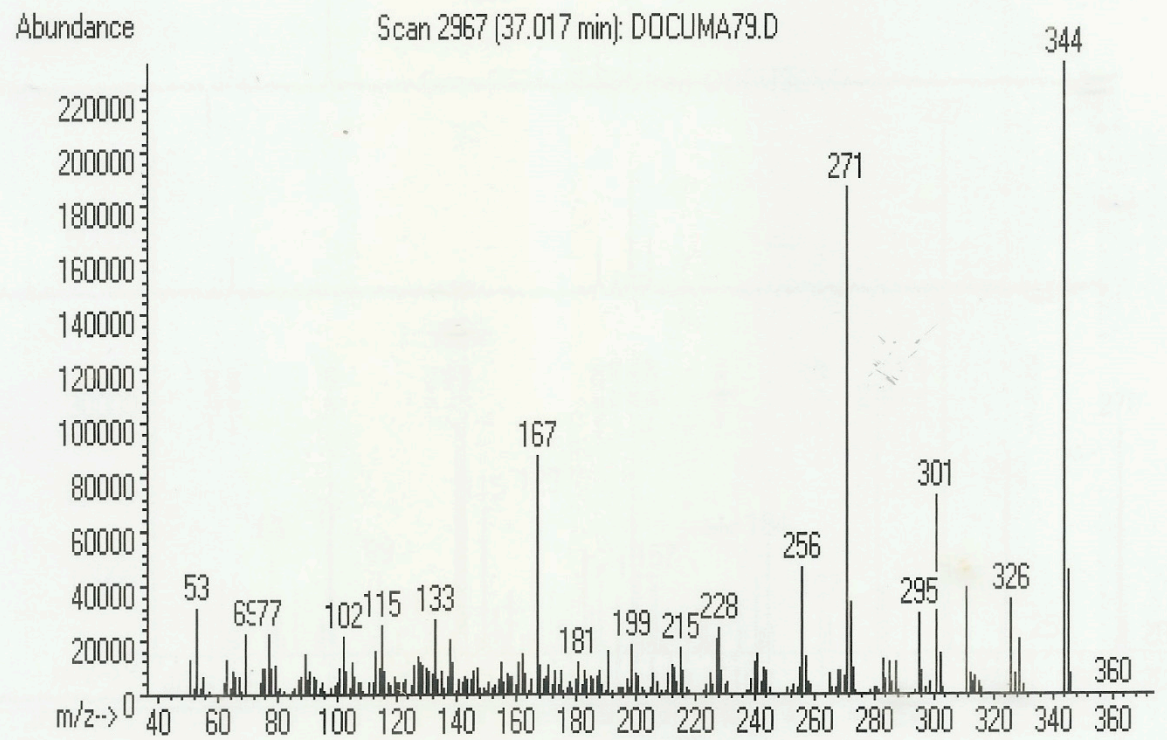
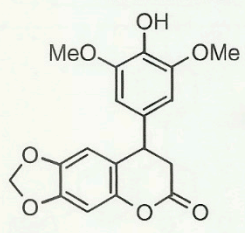
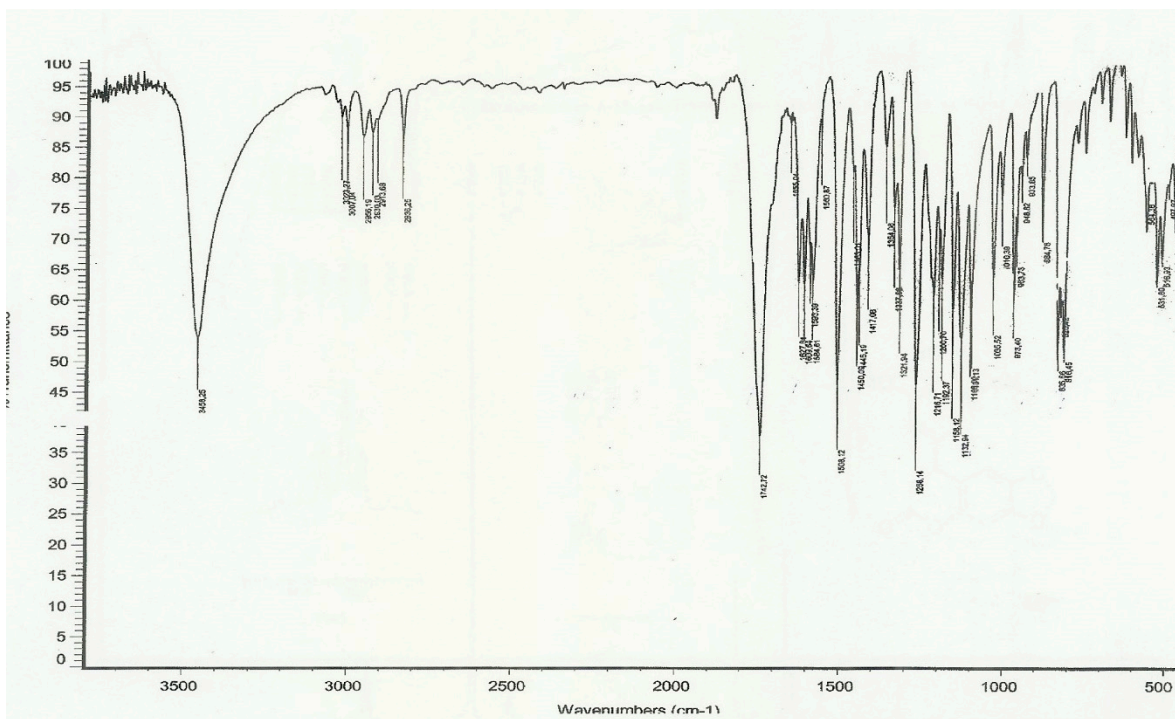
2. Espectros



5,7-dichloro-4-phenylchroman-2-one (25)

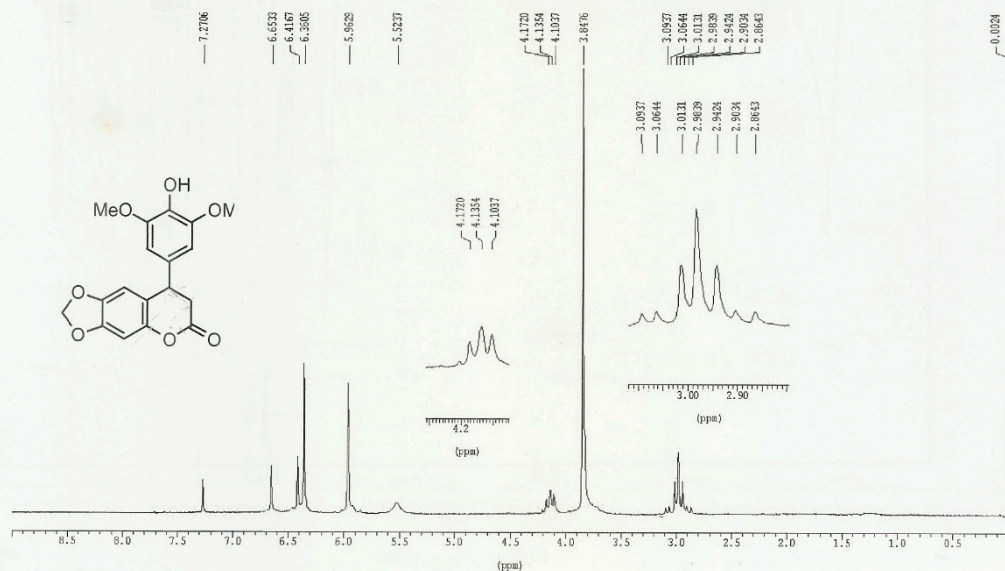


5,7-dichloro-4-phenylchroman-2-one (25)

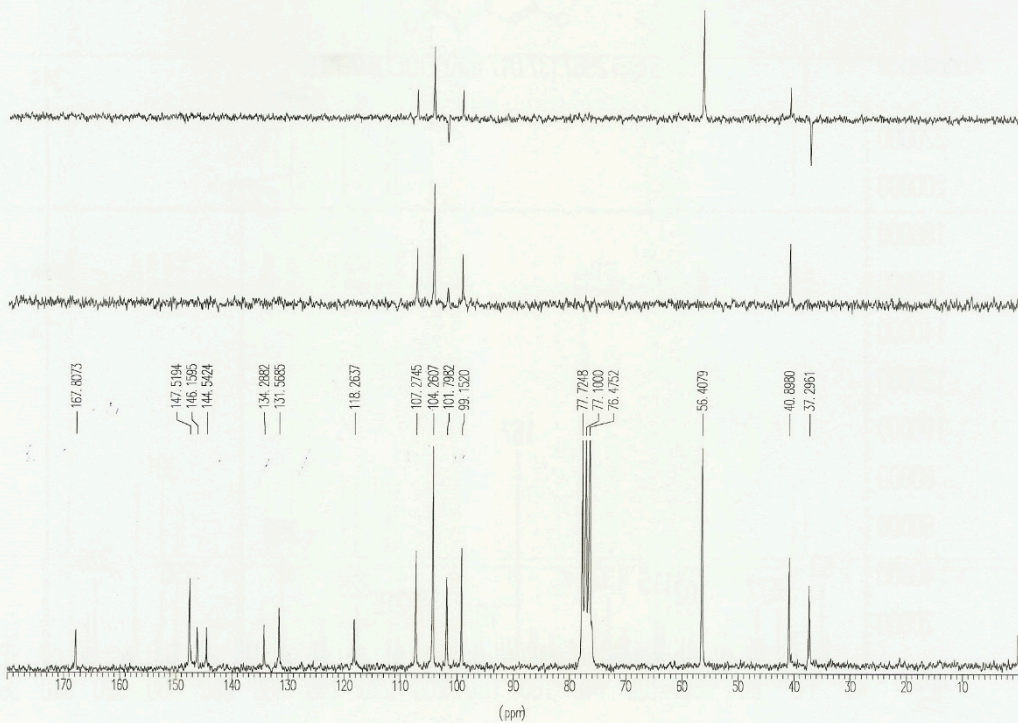


8-(4-hydroxy-3,5-dimethoxyphenyl)-7,8-dihydro-[1,3]dioxolo[4,5-g]chromen-6-one (26)

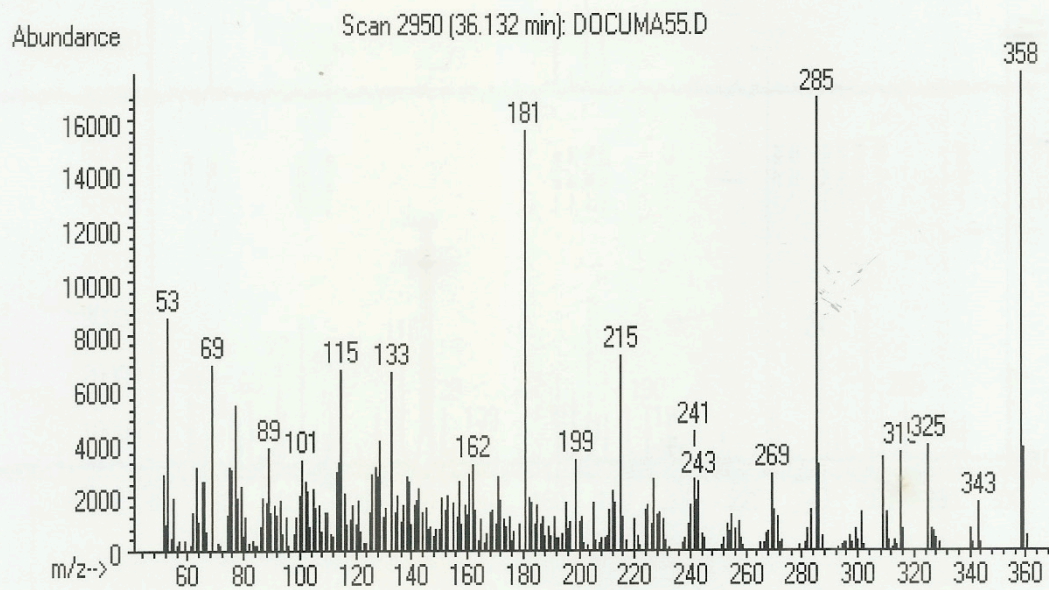
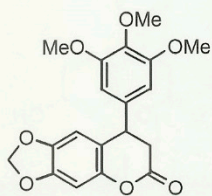
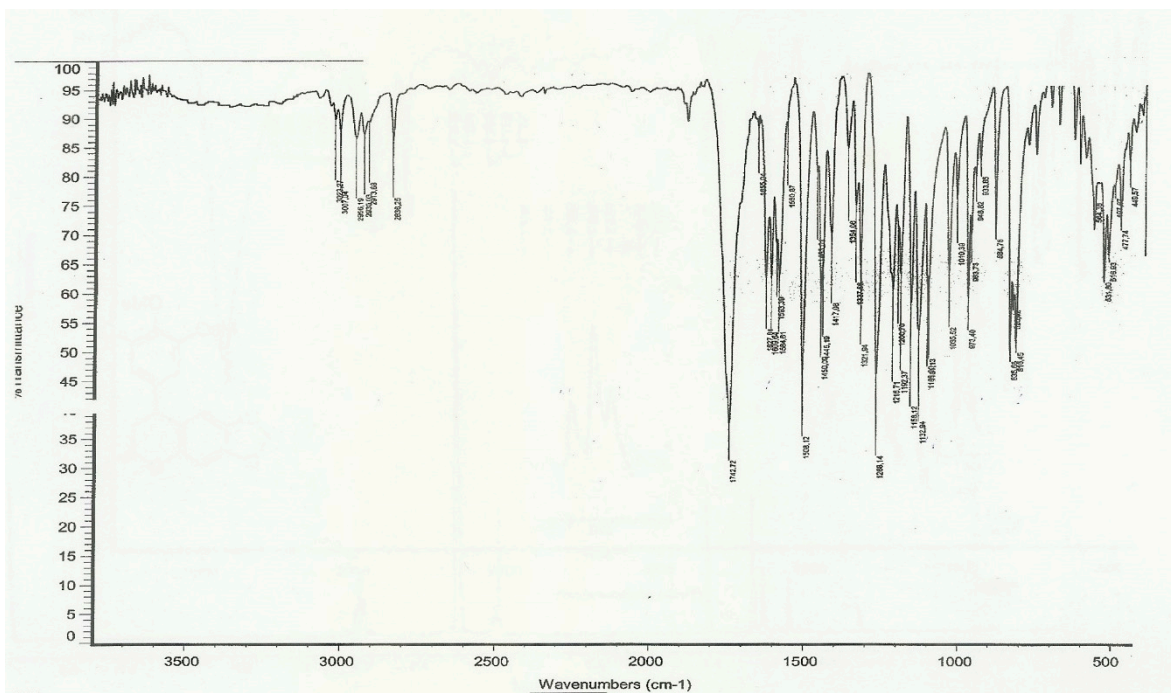
DOCUMENTO 001 CRUDO DE REACCION 3,5-OCH3-4-OH-6,7METILENODIOXI-4-FENILCUMARINA



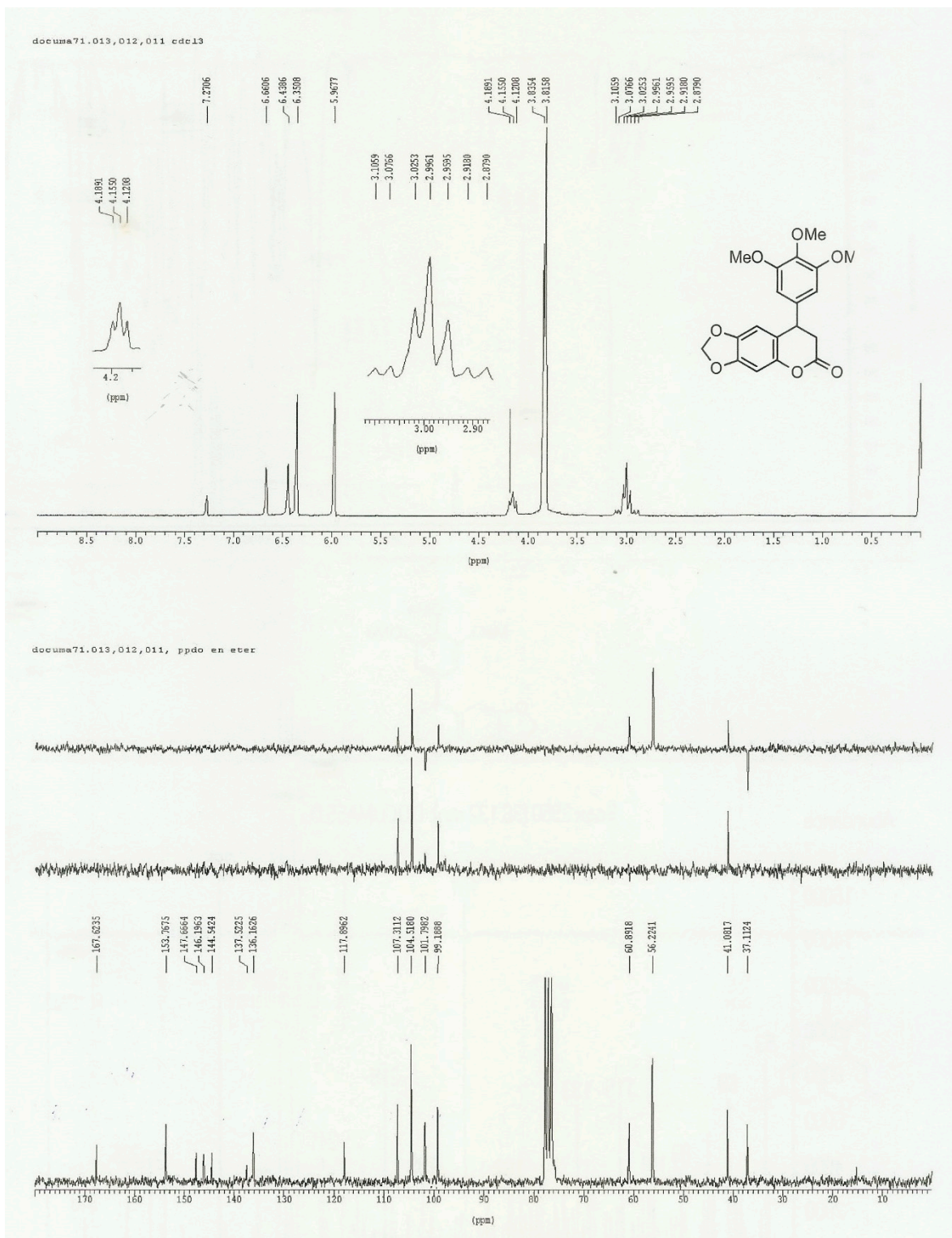
docum84. 013, 012, 011



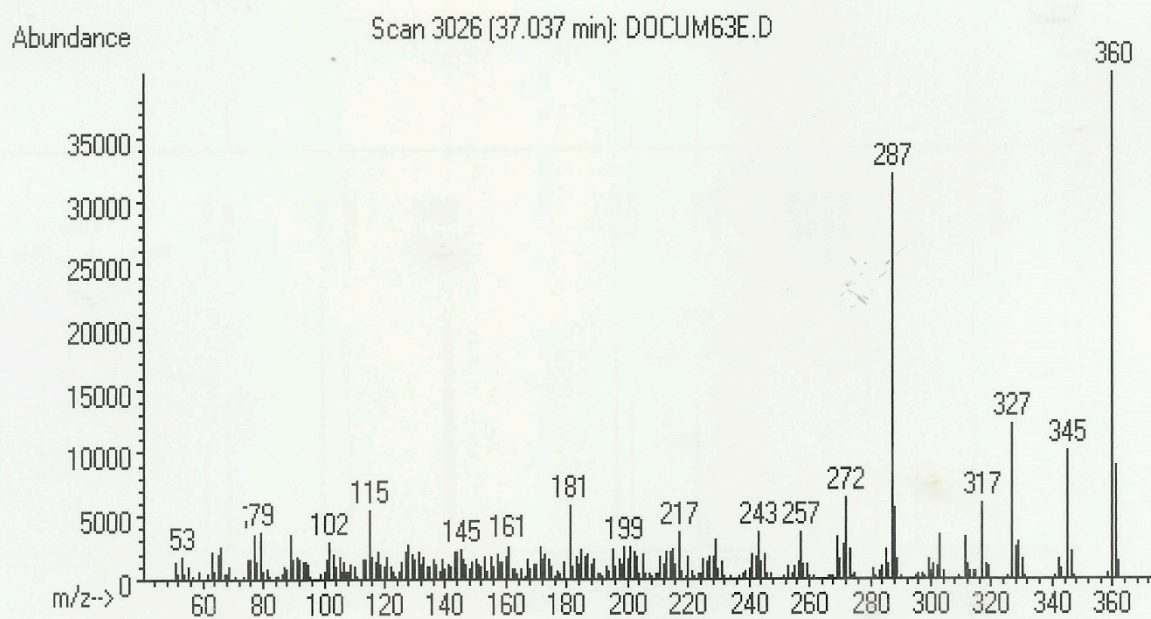
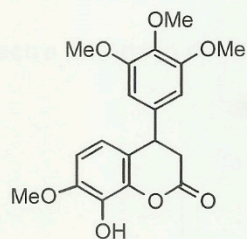
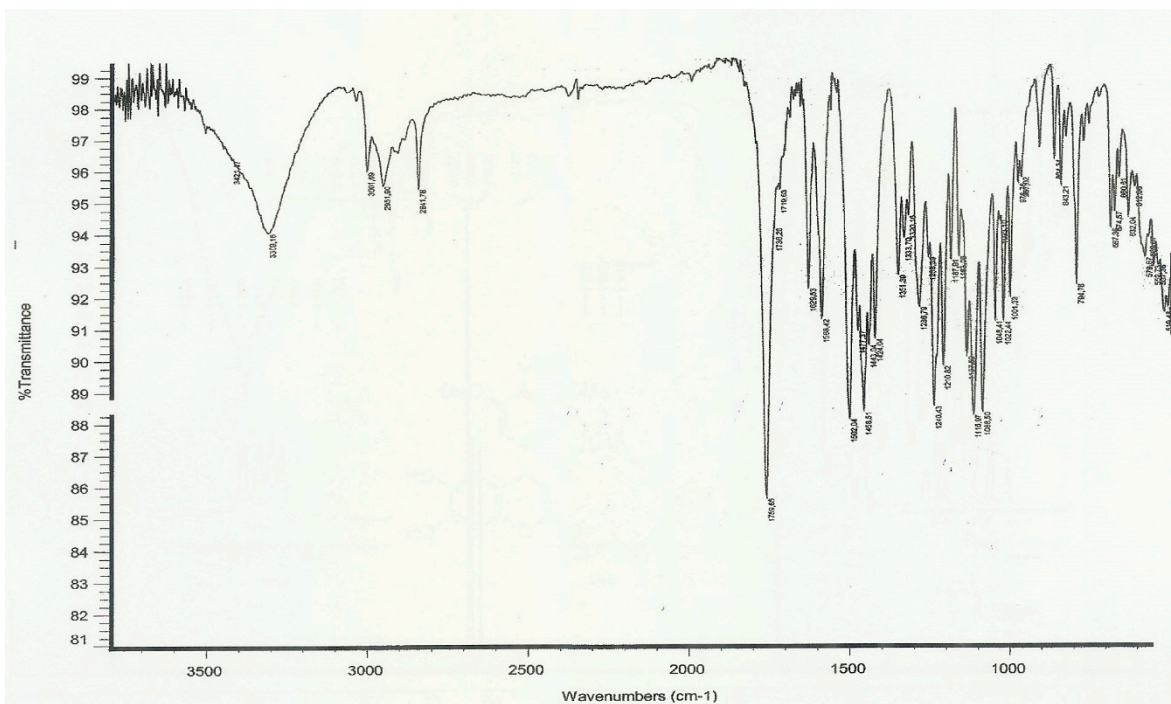
8-(4-hydroxy-3,5-dimethoxyphenyl)-7,8-dihydro-1,3-dioxolo[4,5-g]chromen-6-one (26)



*8-(3,4,5-trimethoxyphenyl)-7,8-dihydro-[1,3]dioxolo[4,5-g]chromen-6-one (27)*

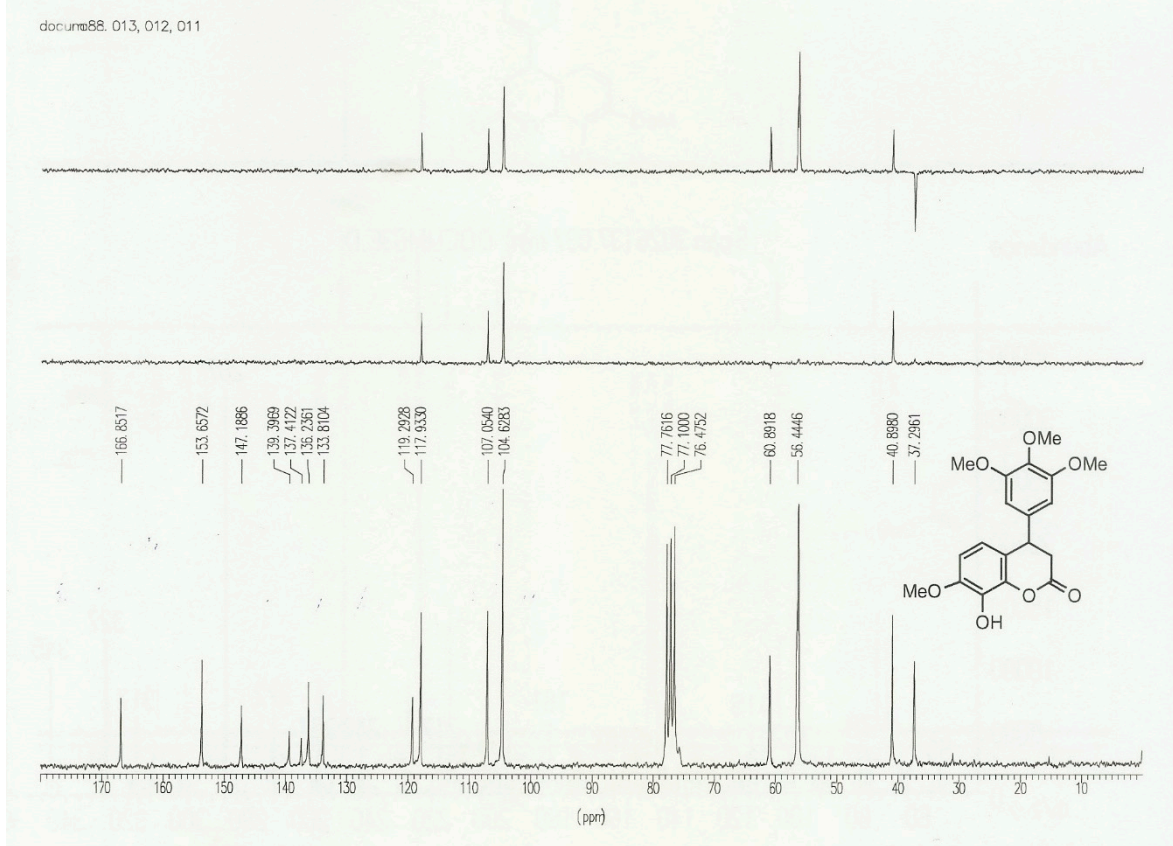
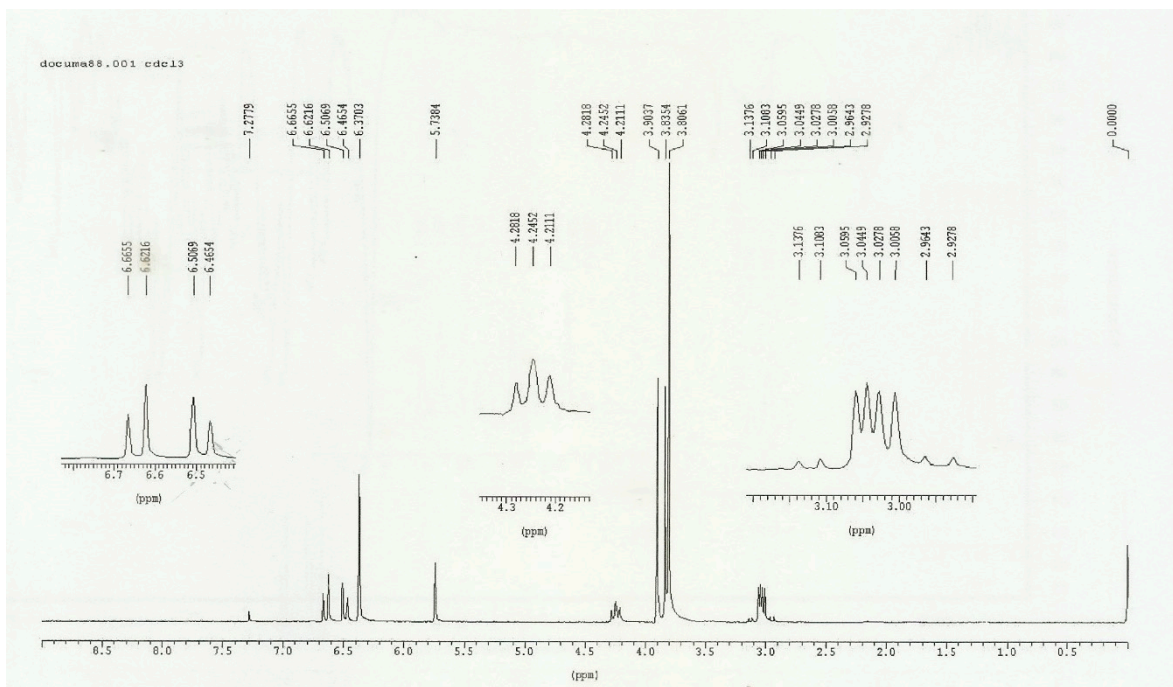


8-(3,4,5-trimethoxyphenyl)-7,8-dihydro-[1,3]dioxolo[4,5-g]chromen-6-one (27)



8-hydroxy-7-methoxy-4-(3,4,5-trimethoxyphenyl)chroman-2-one (28)





8-hydroxy-7-methoxy-4-(3,4,5-trimethoxyphenyl)chroman-2-one (28)