

Supporting Information, Part B

Small-Molecule Inhibitors of Protein Geranylgeranyltransferase Type I

Sabrina Castellano, Hannah D. G. Fiji, Sape S. Kinderman, Masaru Watanabe,¹ Pablo de Leon, Fuyuhiko Tamanoi,¹
Ohyun Kwon*

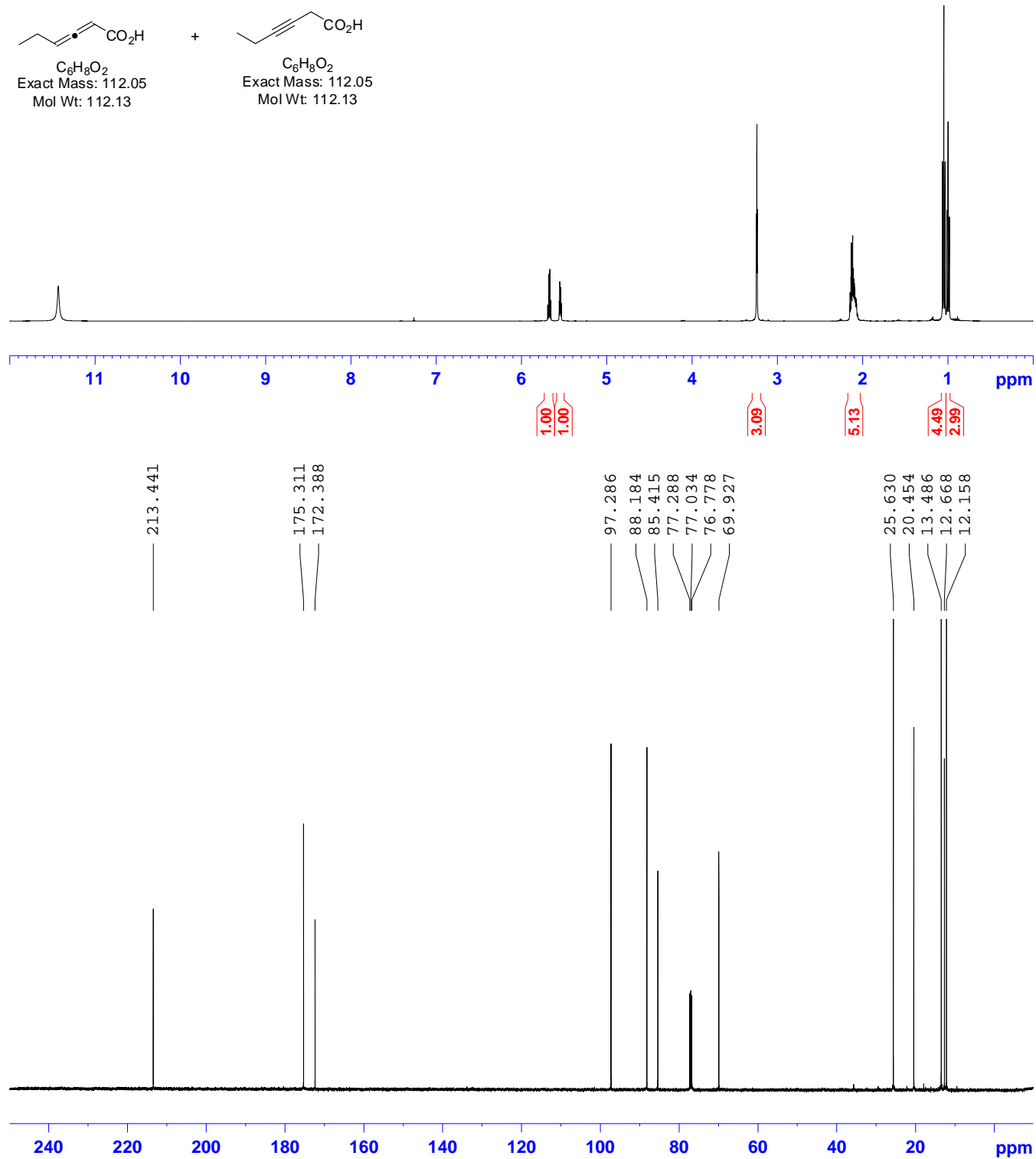
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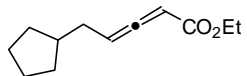
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¹ Department of Microbiology, Immunology and Molecular Genetics

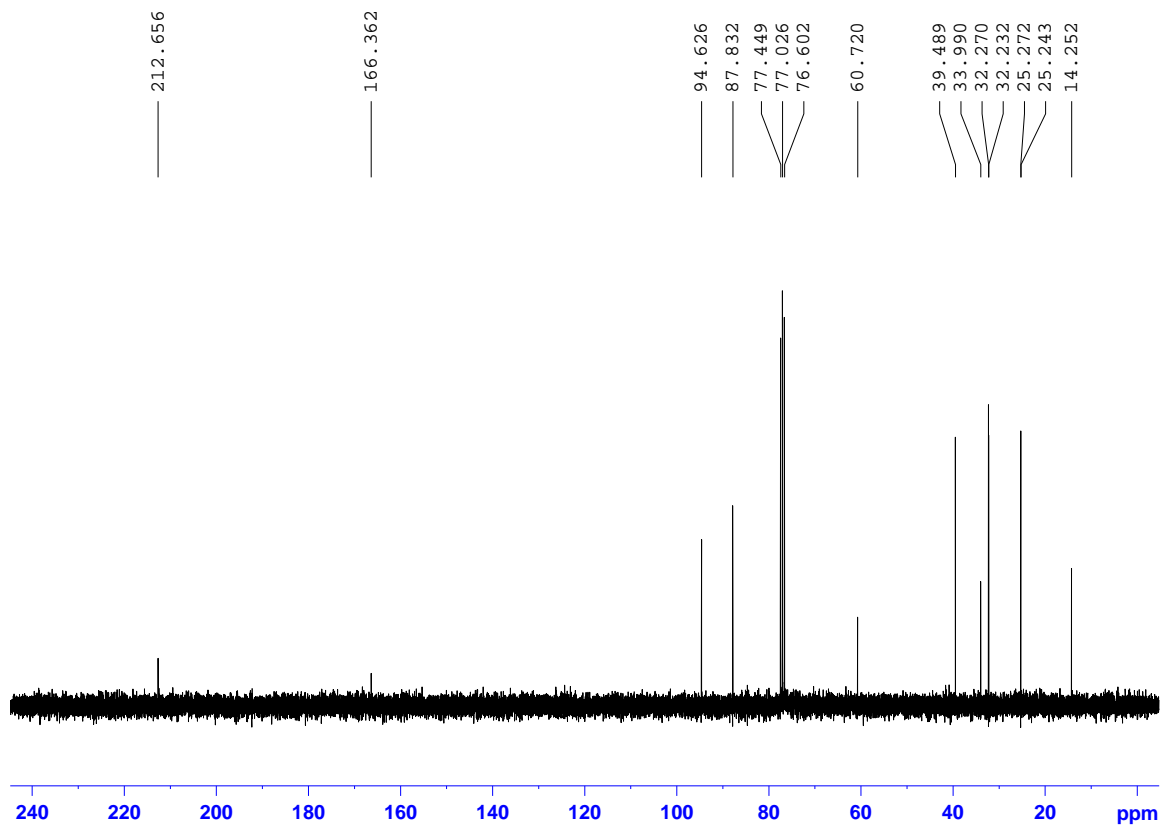
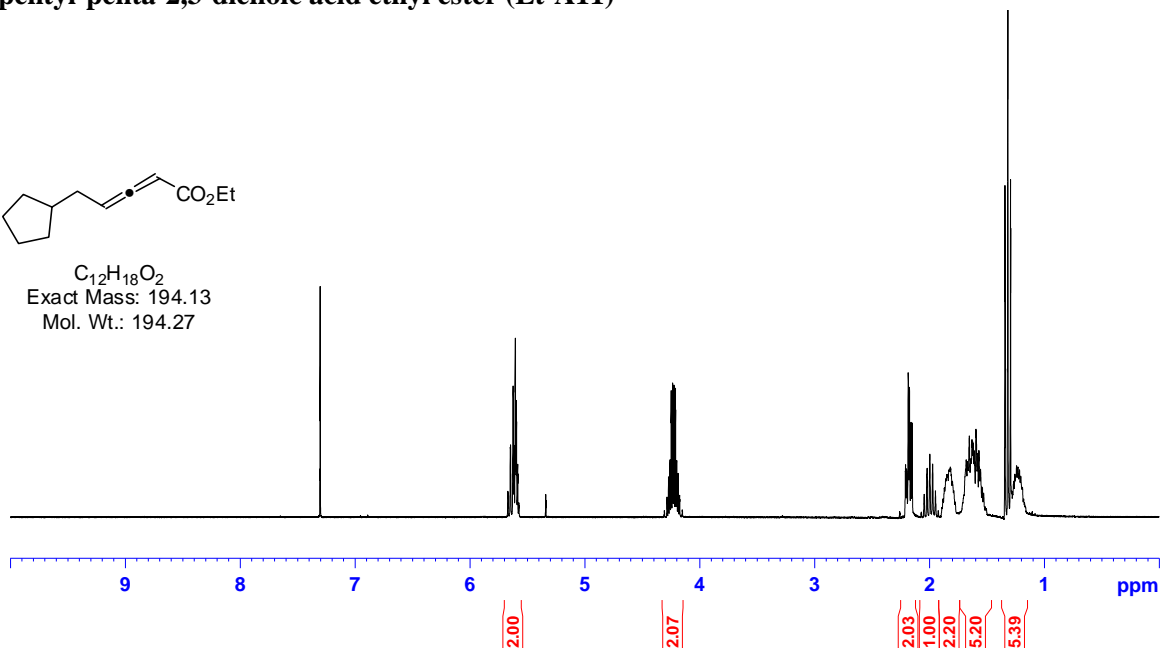
4-Ethyl-but-2,3-dienoic acid and hex-3-ynoic acid (A05)



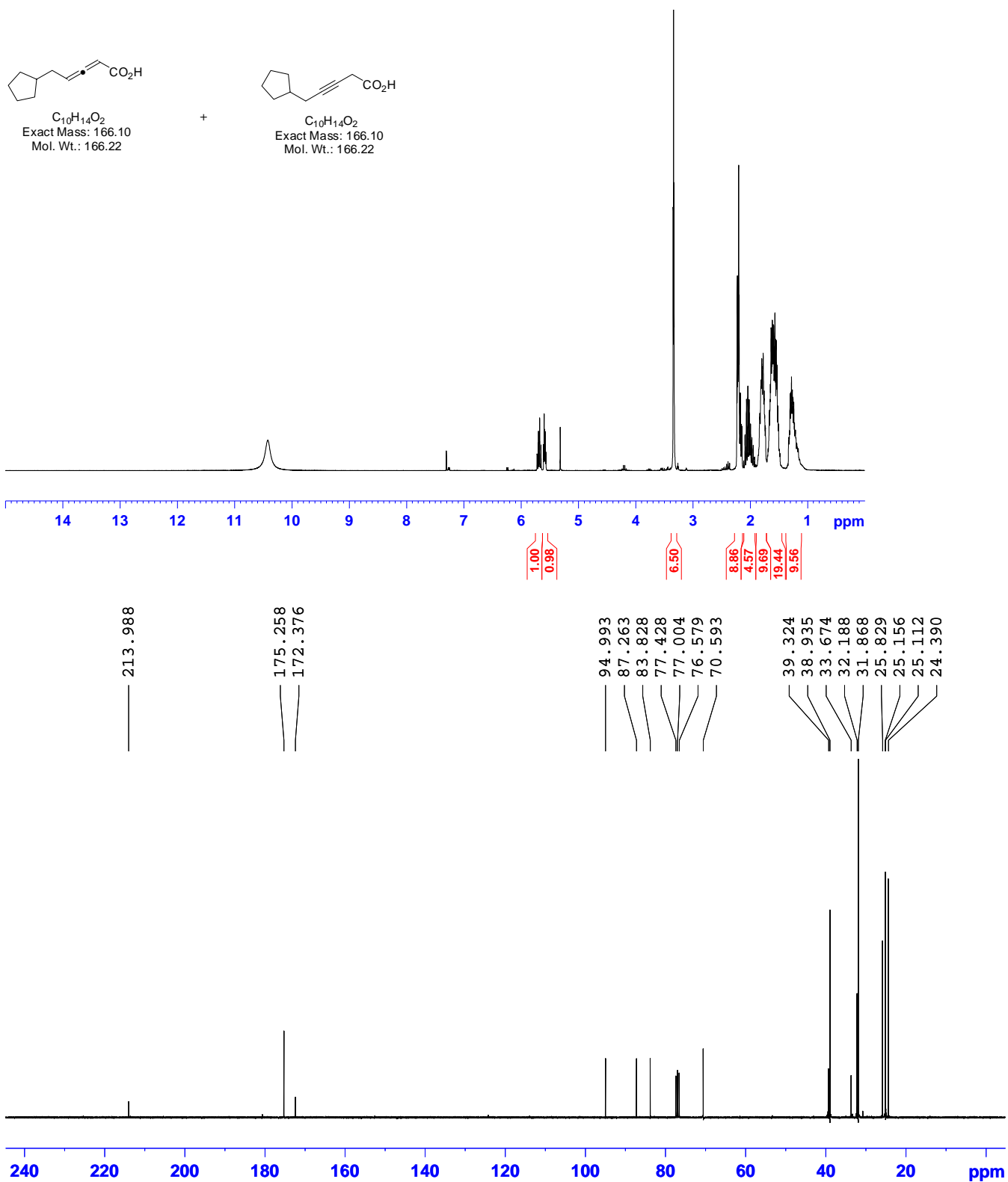
5-Cyclopentyl-penta-2,3-dienoic acid ethyl ester (Et-A11)



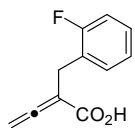
$C_{12}H_{18}O_2$
Exact Mass: 194.13
Mol. Wt.: 194.27



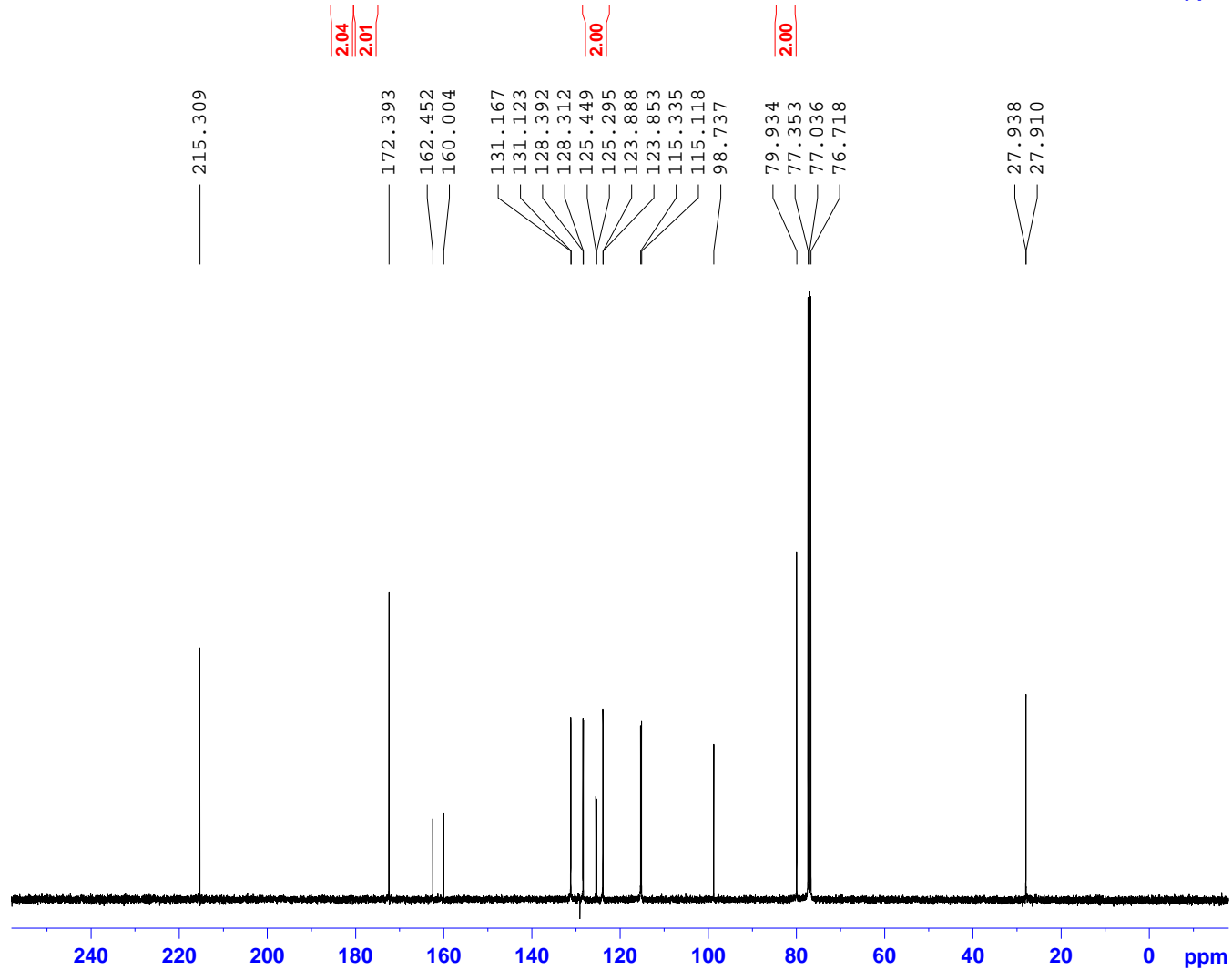
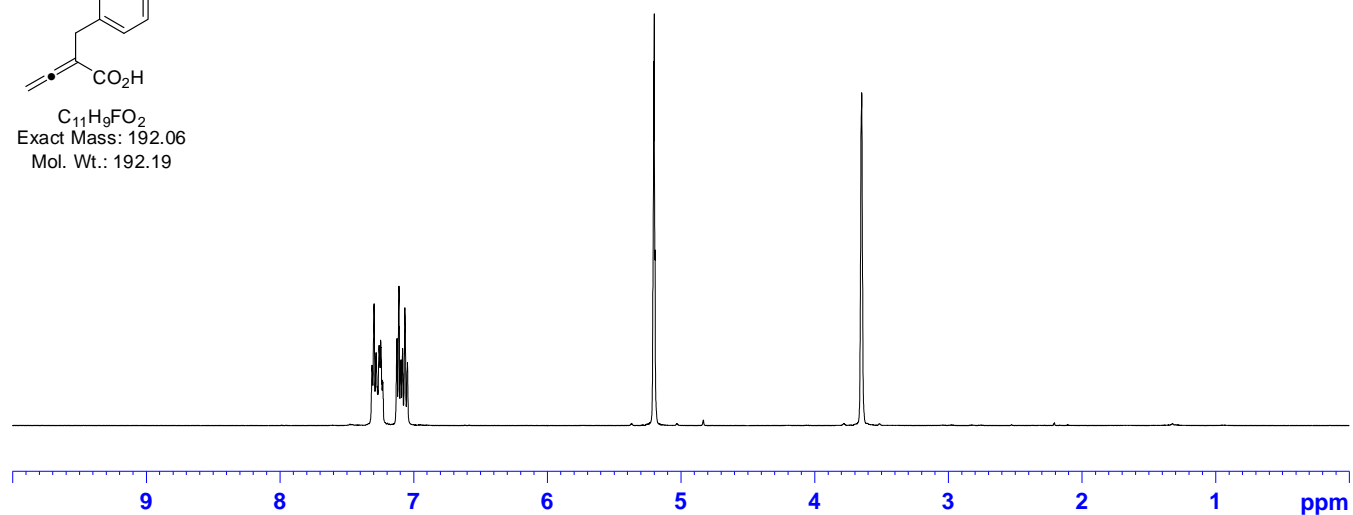
5-Cyclopentyl-penta-2,3-dienoic acid and 5-cyclopentyl-pent-3-ynoic acid (A11)



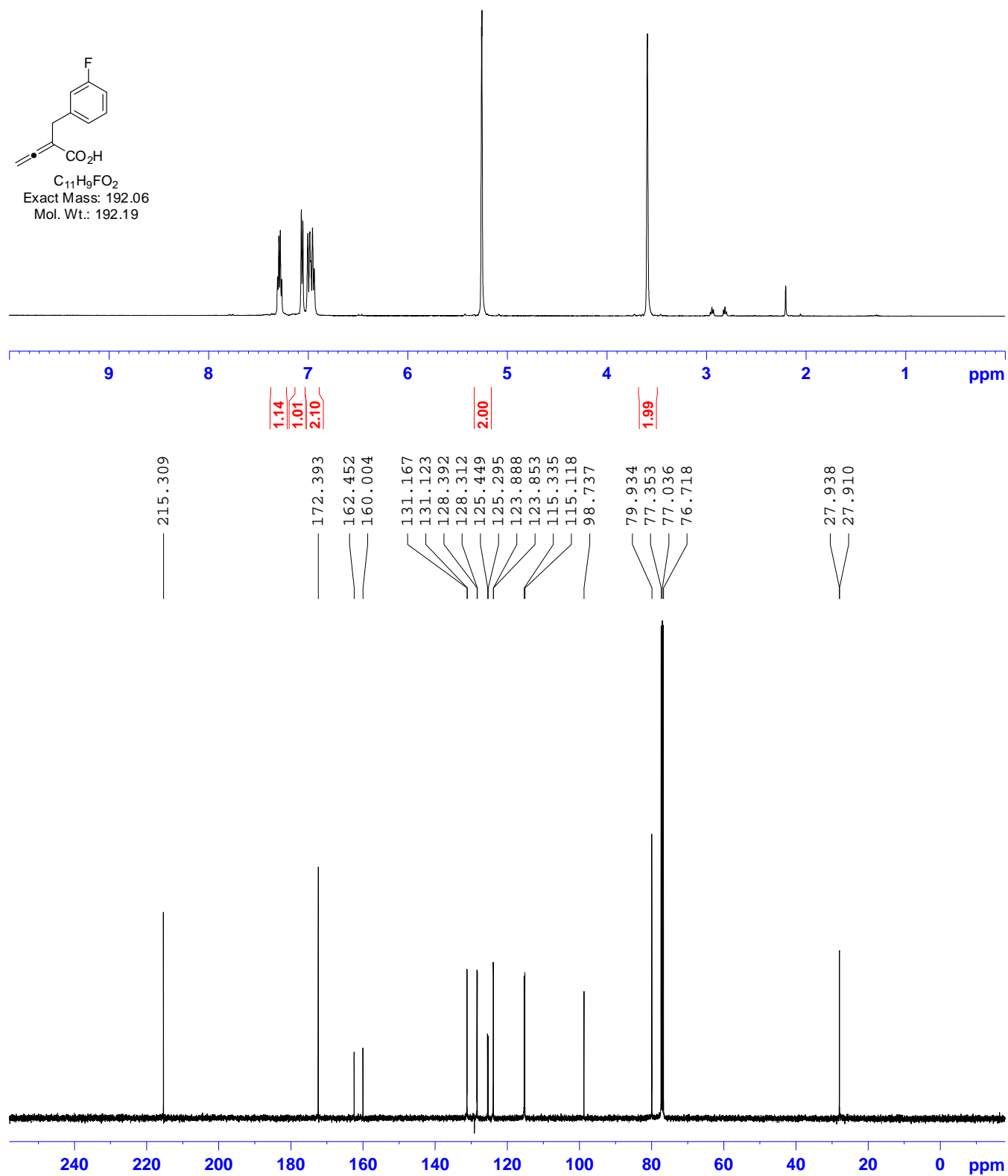
2-(2-Fluorobenzyl)-buta-2,3-dienoic acid (B03)



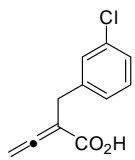
C₁₁H₉FO₂
Exact Mass: 192.06
Mol. Wt.: 192.19



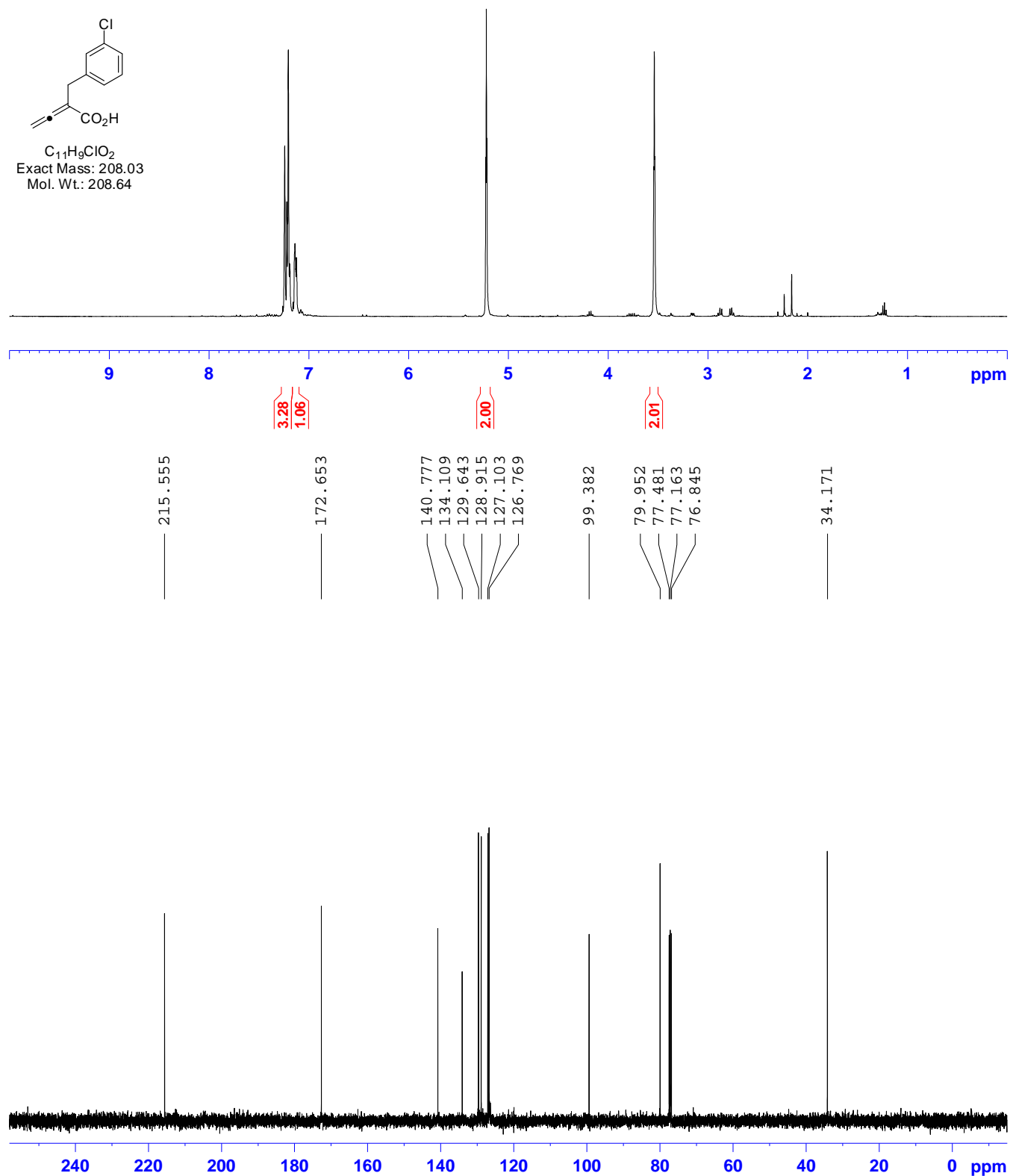
2-(3-Fluorobenzyl)-buta-2,3-dienoic acid (B04)



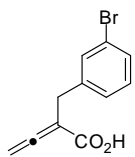
2-(3-Chlorobenzyl)-buta-2,3-dienoic acid (B05)



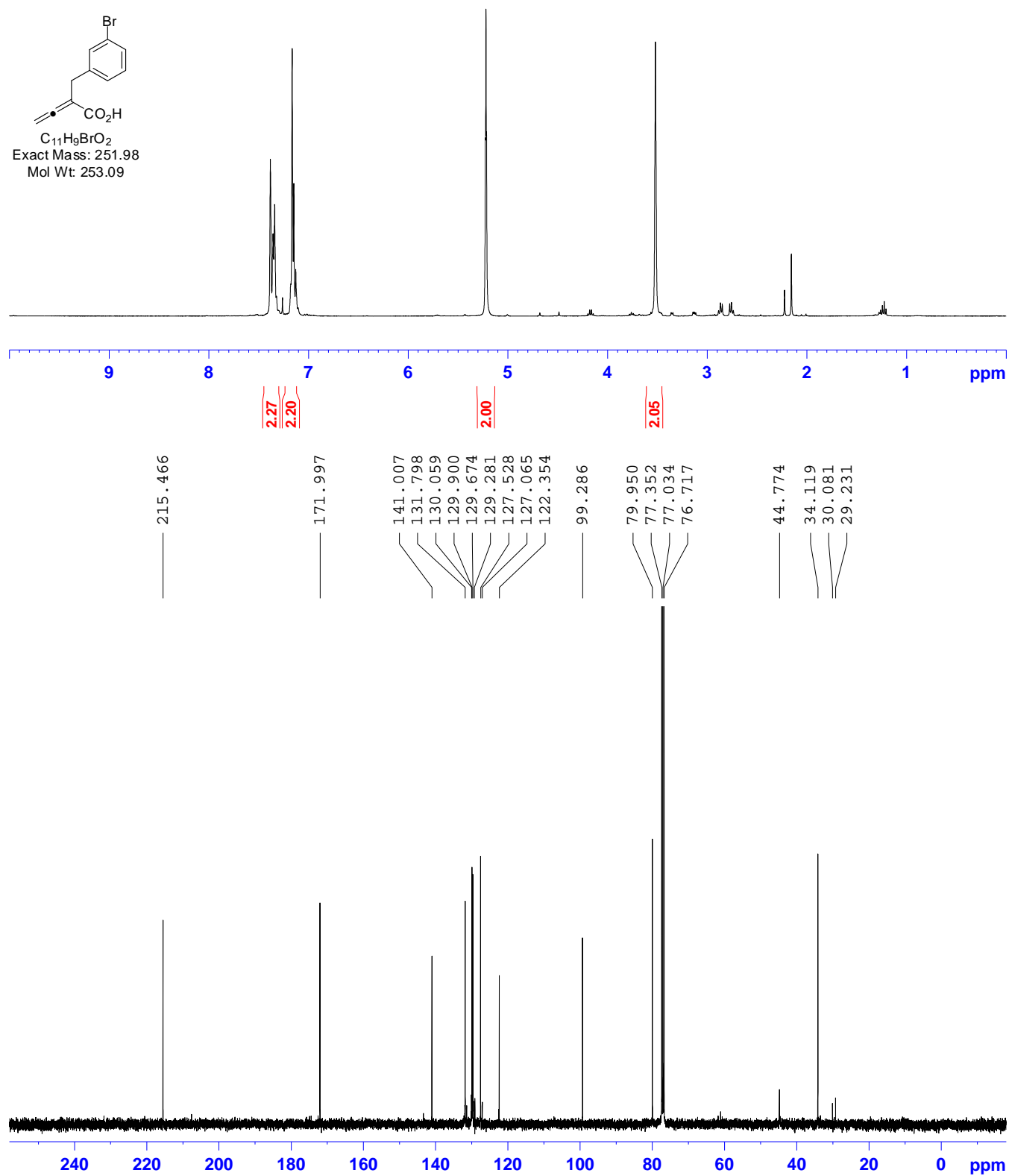
C₁₁H₉ClO₂
Exact Mass: 208.03
Mol. Wt.: 208.64



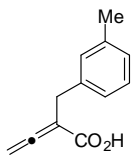
2-(3-Bromobenzyl)-buta-2,3-dienoic acid (B06)



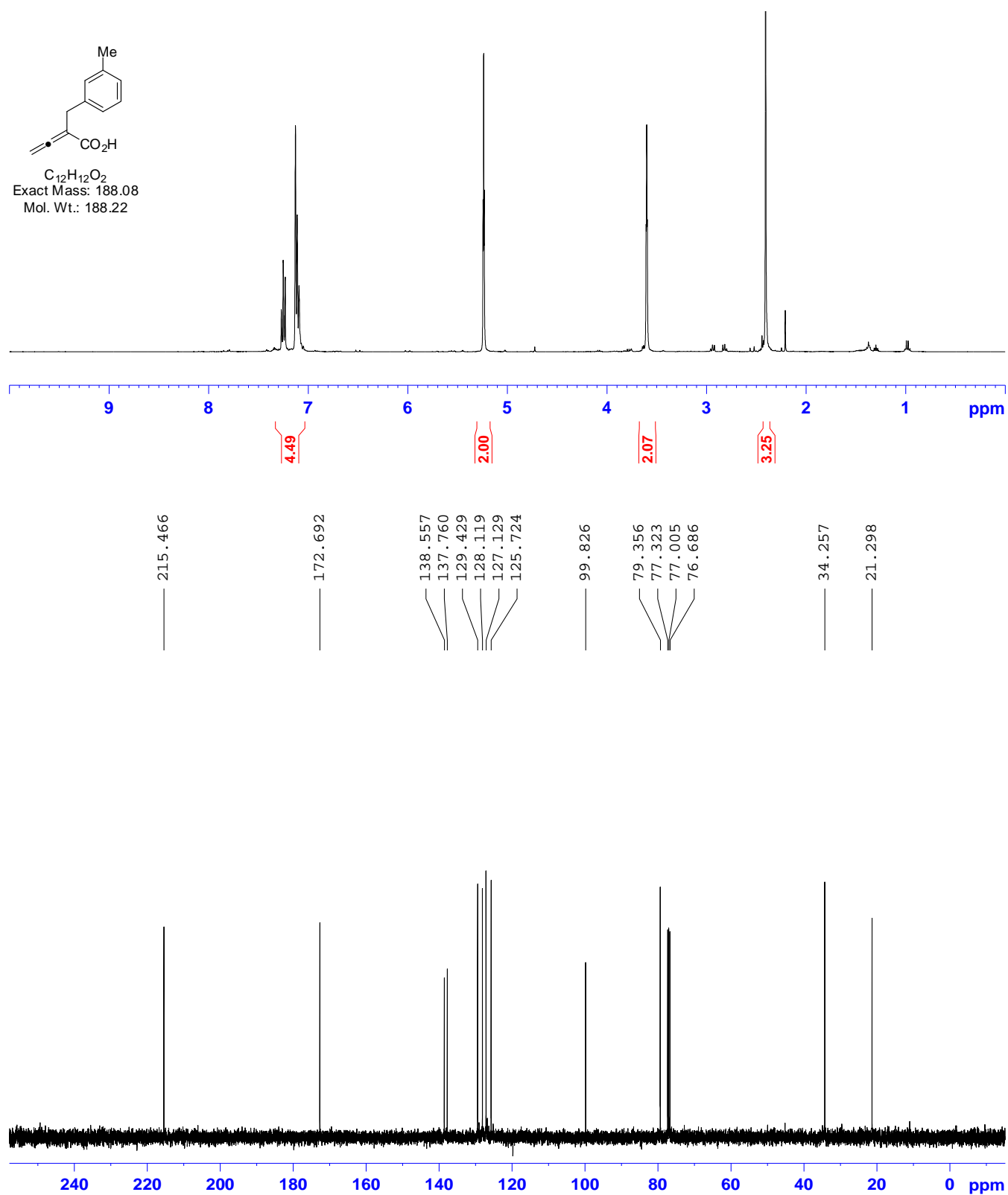
C₁₁H₉BrO₂
Exact Mass: 251.98
Mol Wt: 253.09



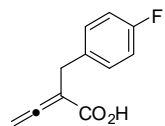
2-(3-Methylbenzyl)-buta-2,3-dienoic acid (B07)



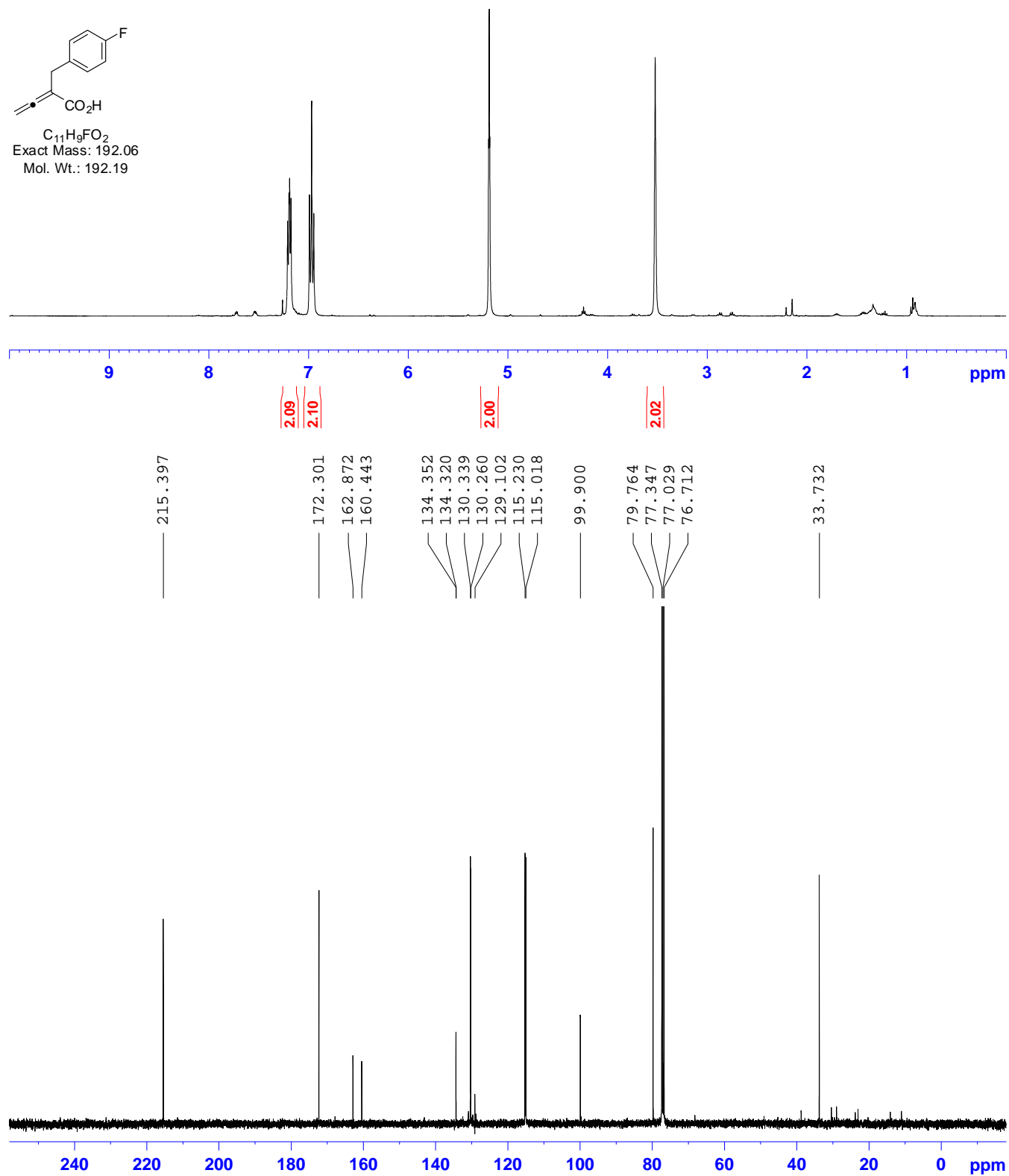
C₁₂H₁₂O₂
Exact Mass: 188.08
Mol. Wt.: 188.22



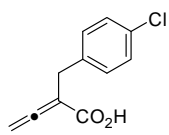
2-(4-Fluorobenzyl)-buta-2,3-dienoic acid (B08)



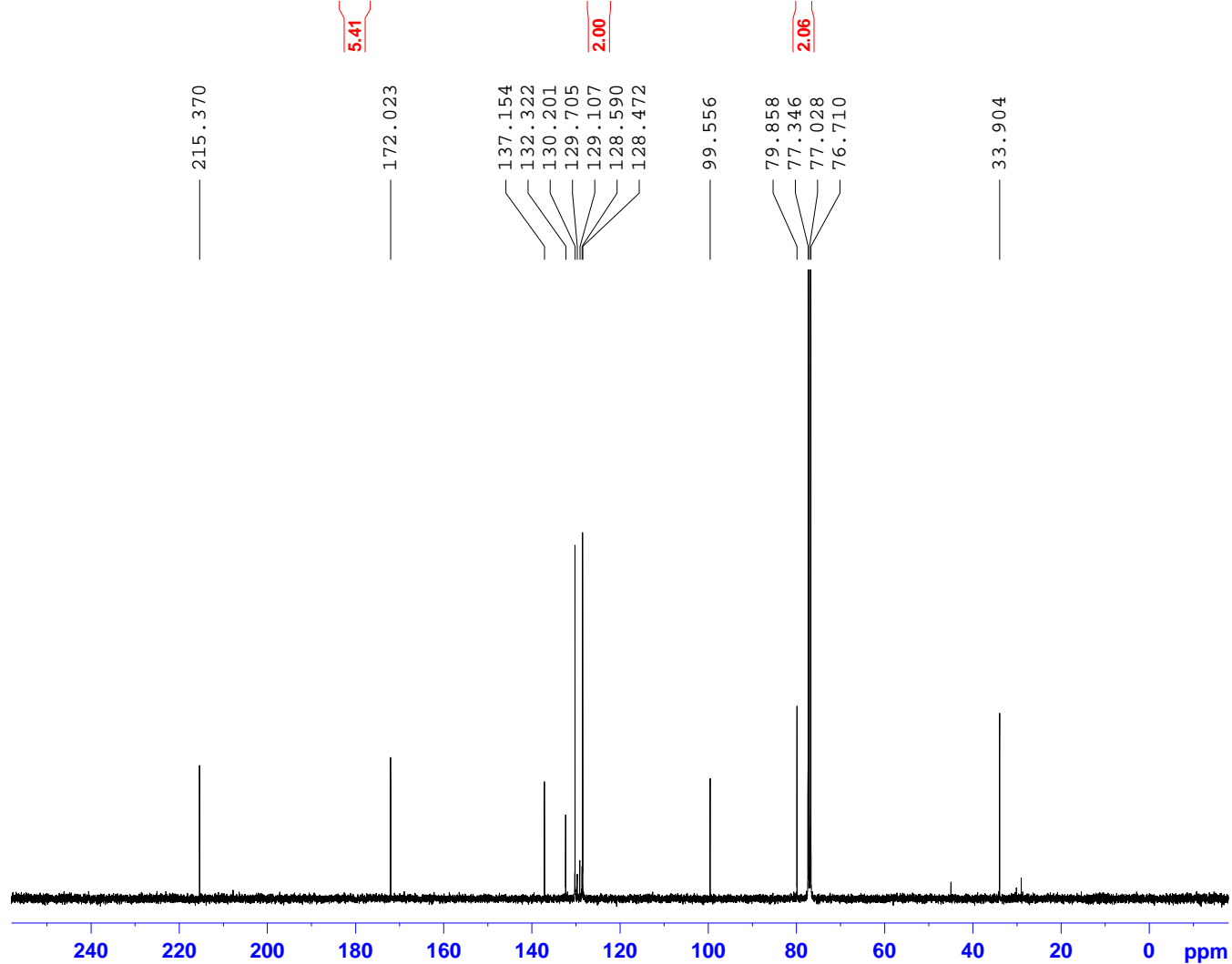
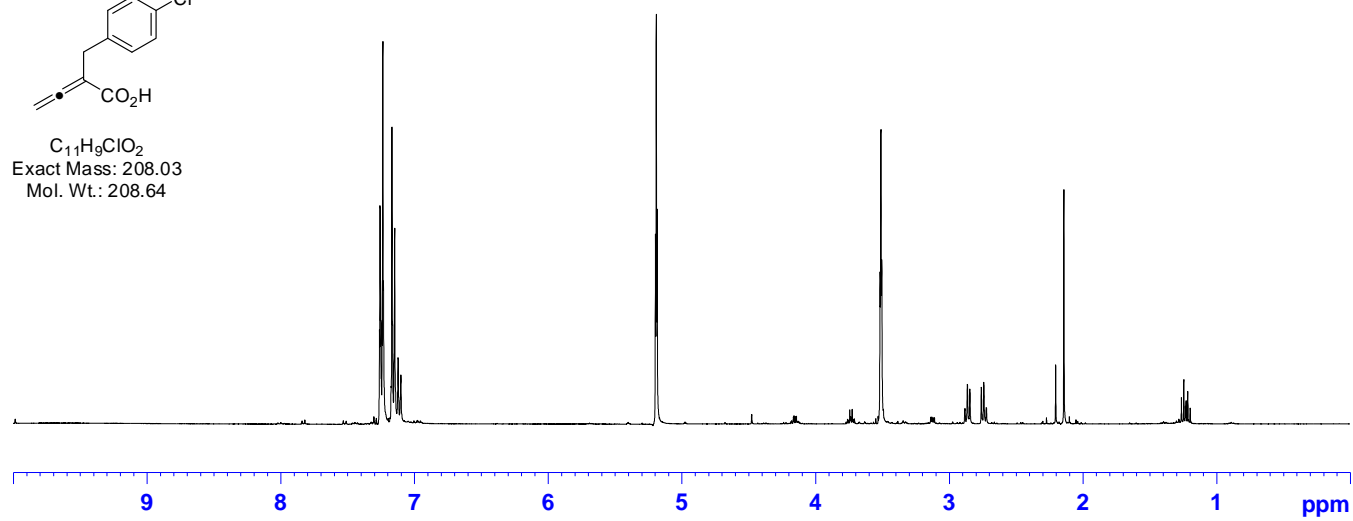
$C_{11}H_9FO_2$
Exact Mass: 192.06
Mol. Wt.: 192.19



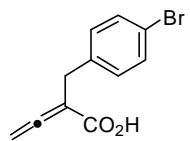
2-(4-Chlorobenzyl)-buta-2,3-dienoic acid (B09)



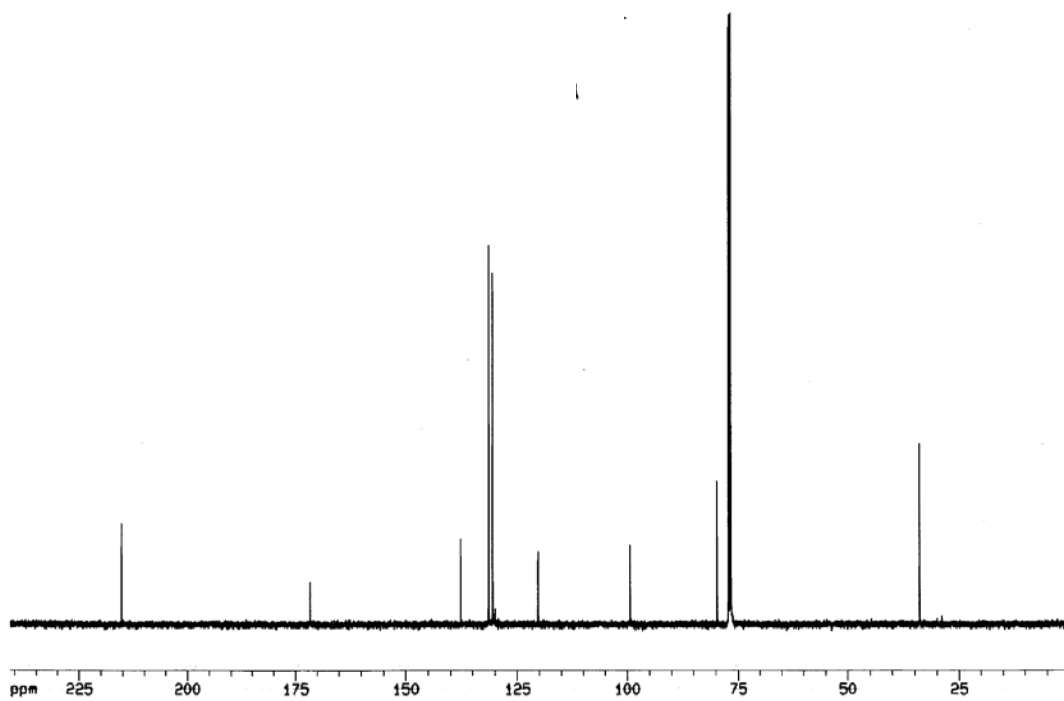
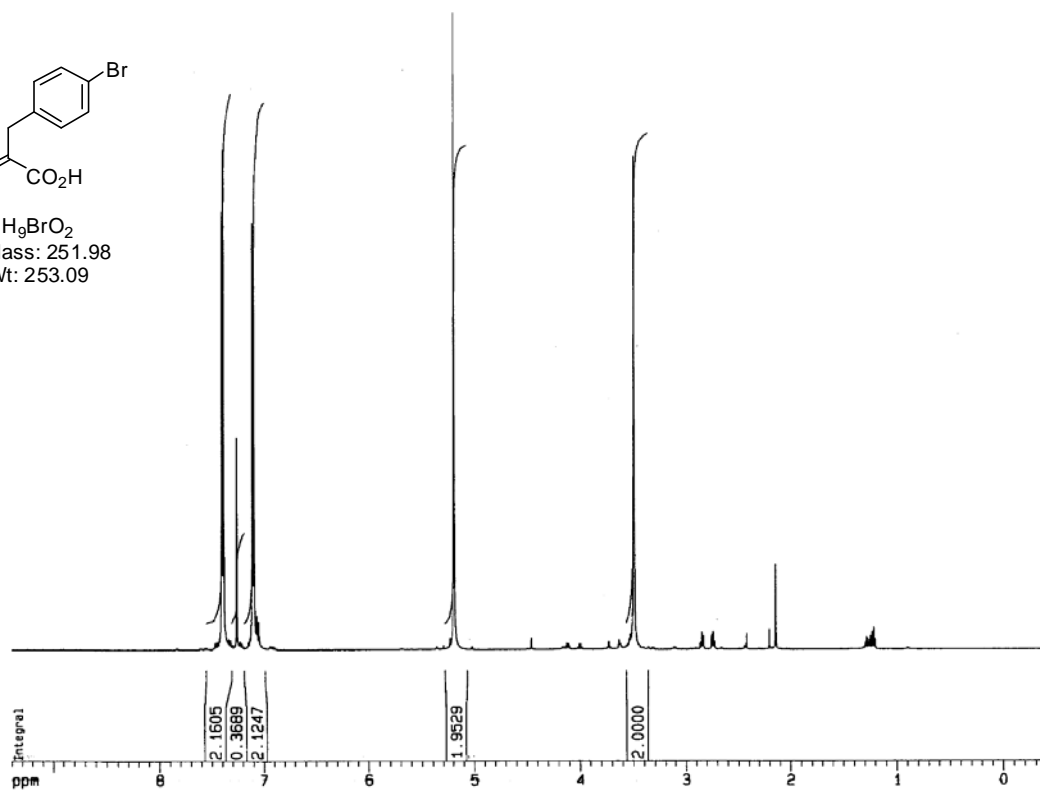
C₁₁H₉ClO₂
Exact Mass: 208.03
Mol. Wt.: 208.64



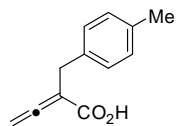
2-(4-bromobenzyl)-buta-2,3-dienoic acid (B10)



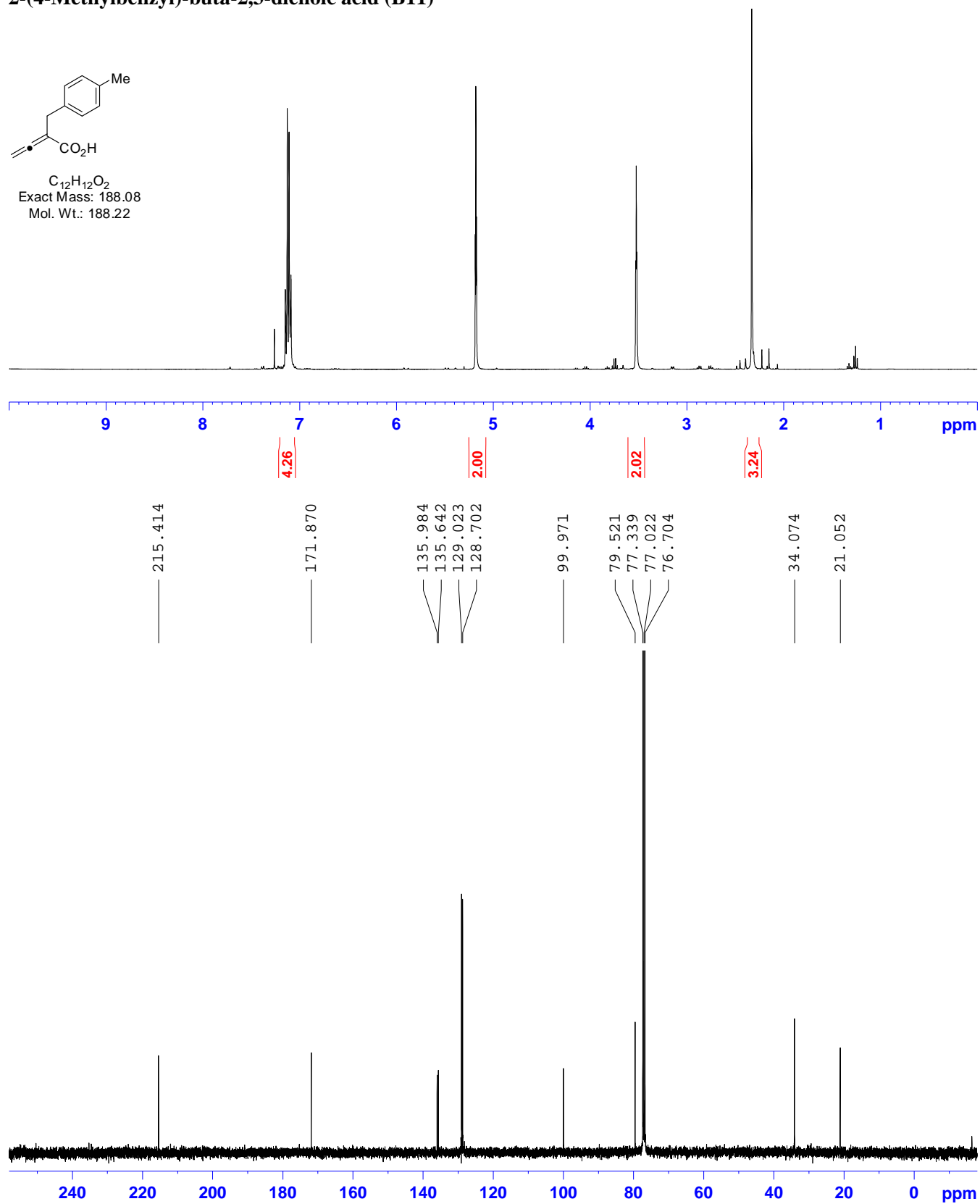
$C_{11}H_9BrO_2$
Exact Mass: 251.98
Mol Wt: 253.09



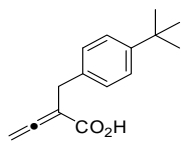
2-(4-Methylbenzyl)-buta-2,3-dienoic acid (B11)



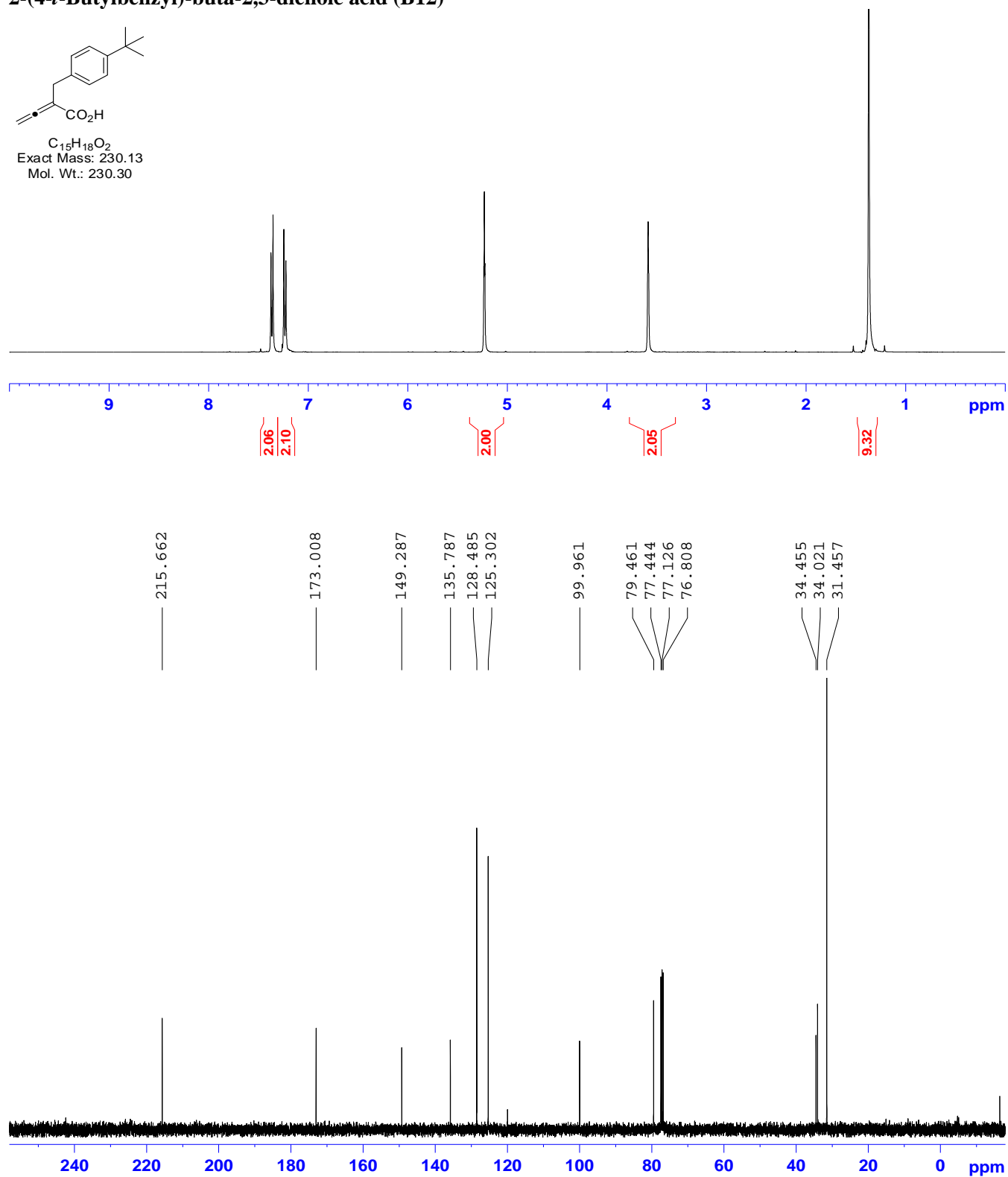
$C_{12}H_{12}O_2$
Exact Mass: 188.08
Mol. Wt.: 188.22



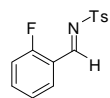
2-(4-*t*-Butylbenzyl)-buta-2,3-dienoic acid (B12)



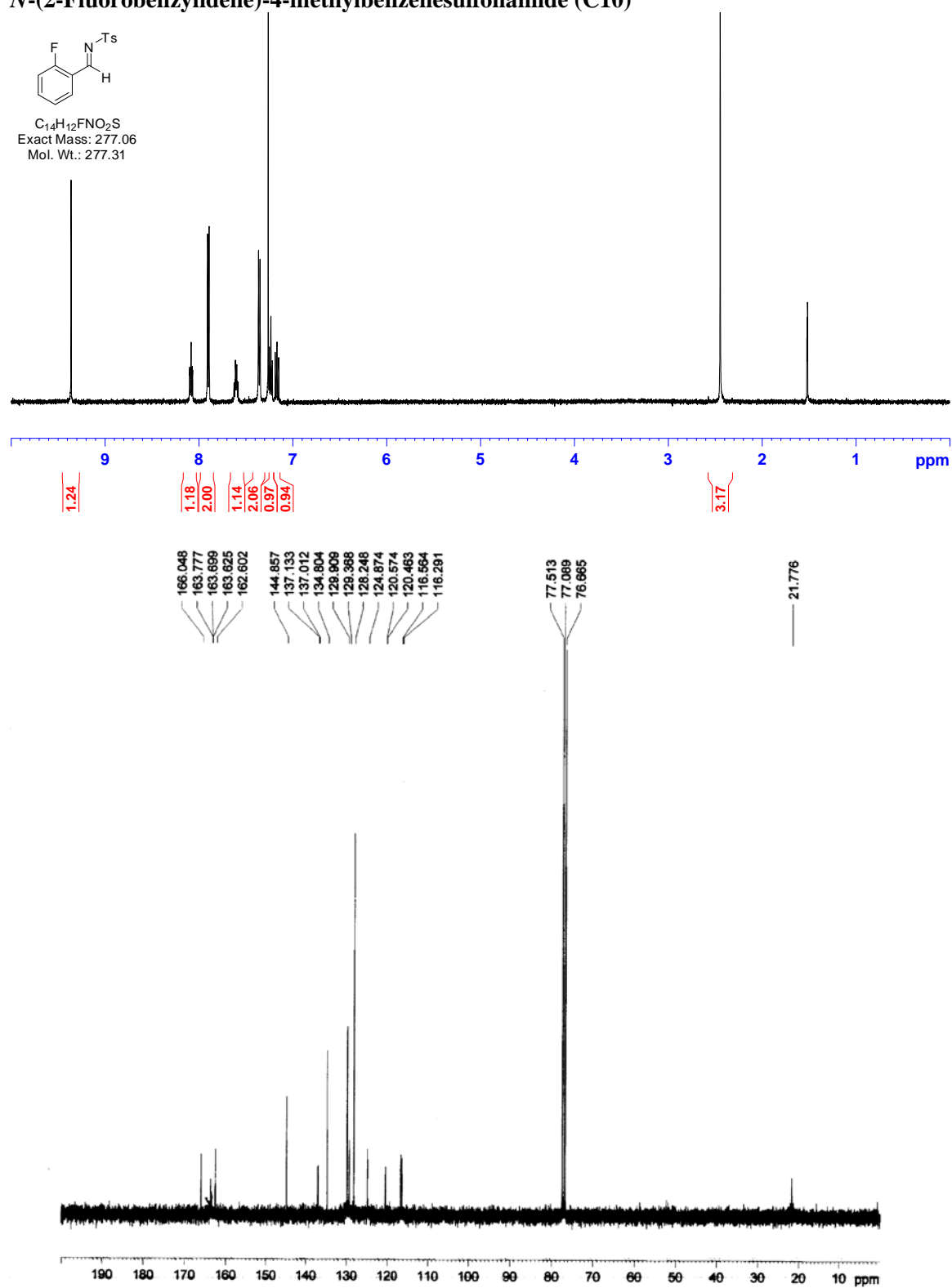
C₁₅H₁₈O₂
Exact Mass: 230.13
Mol. Wt.: 230.30



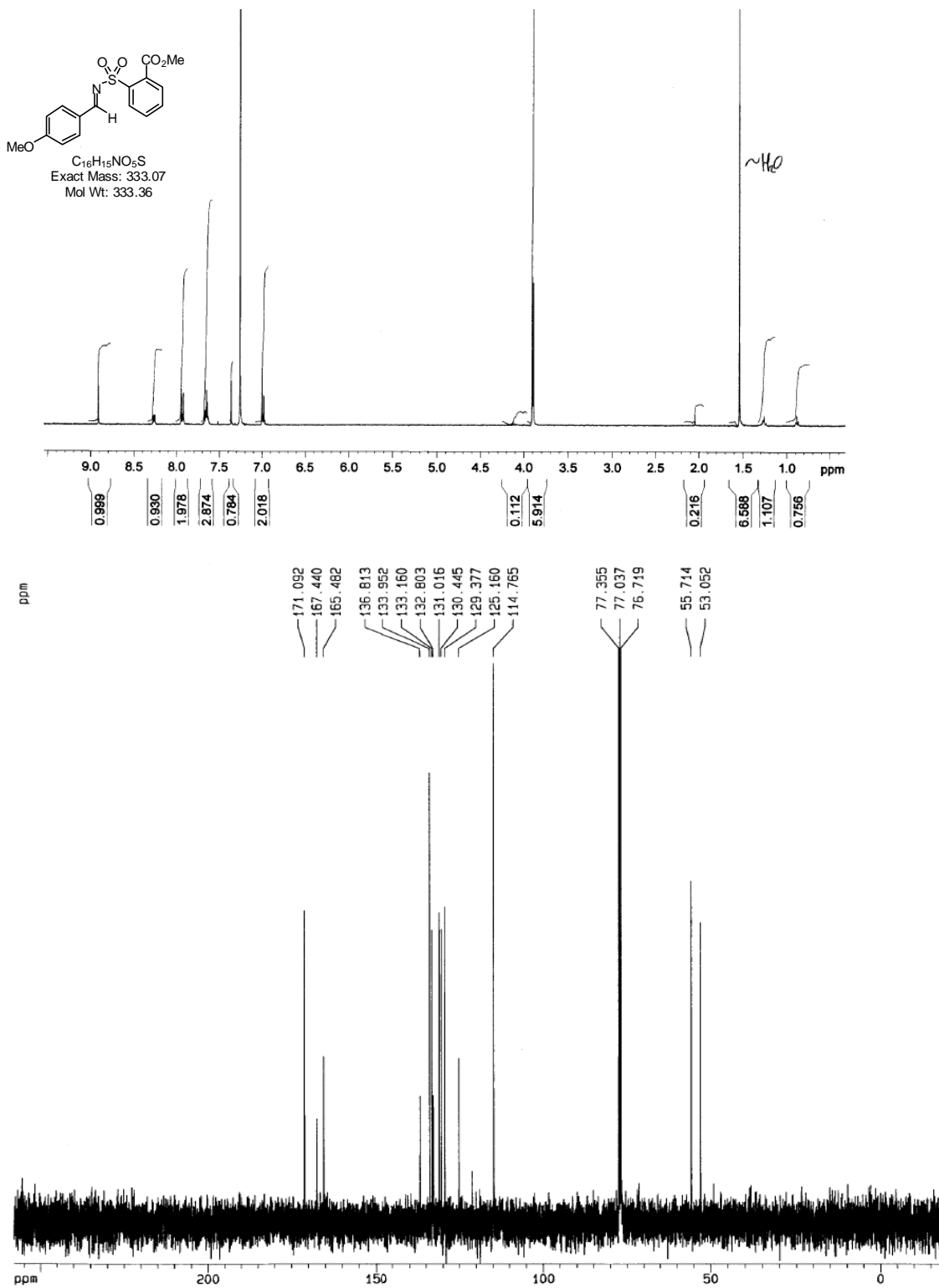
N-(2-Fluorobenzylidene)-4-methylbenzenesulfonamide (C10)



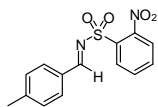
C₁₄H₁₂FNO₂S
Exact Mass: 277.06
Mol. Wt.: 277.31



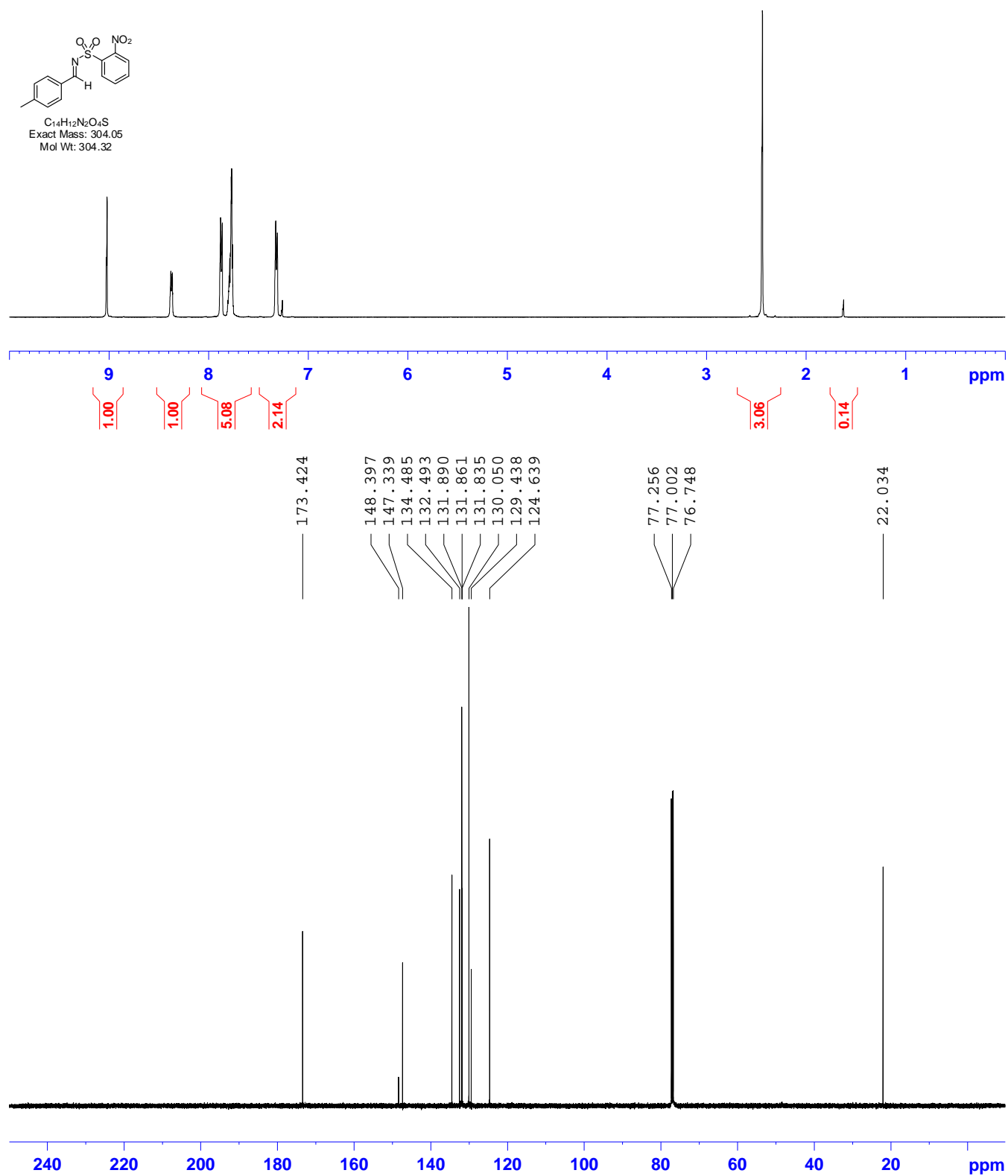
2-[(4-Methoxybenzylidene)-sulfamoyl]-benzoic acid methyl ester (C34)



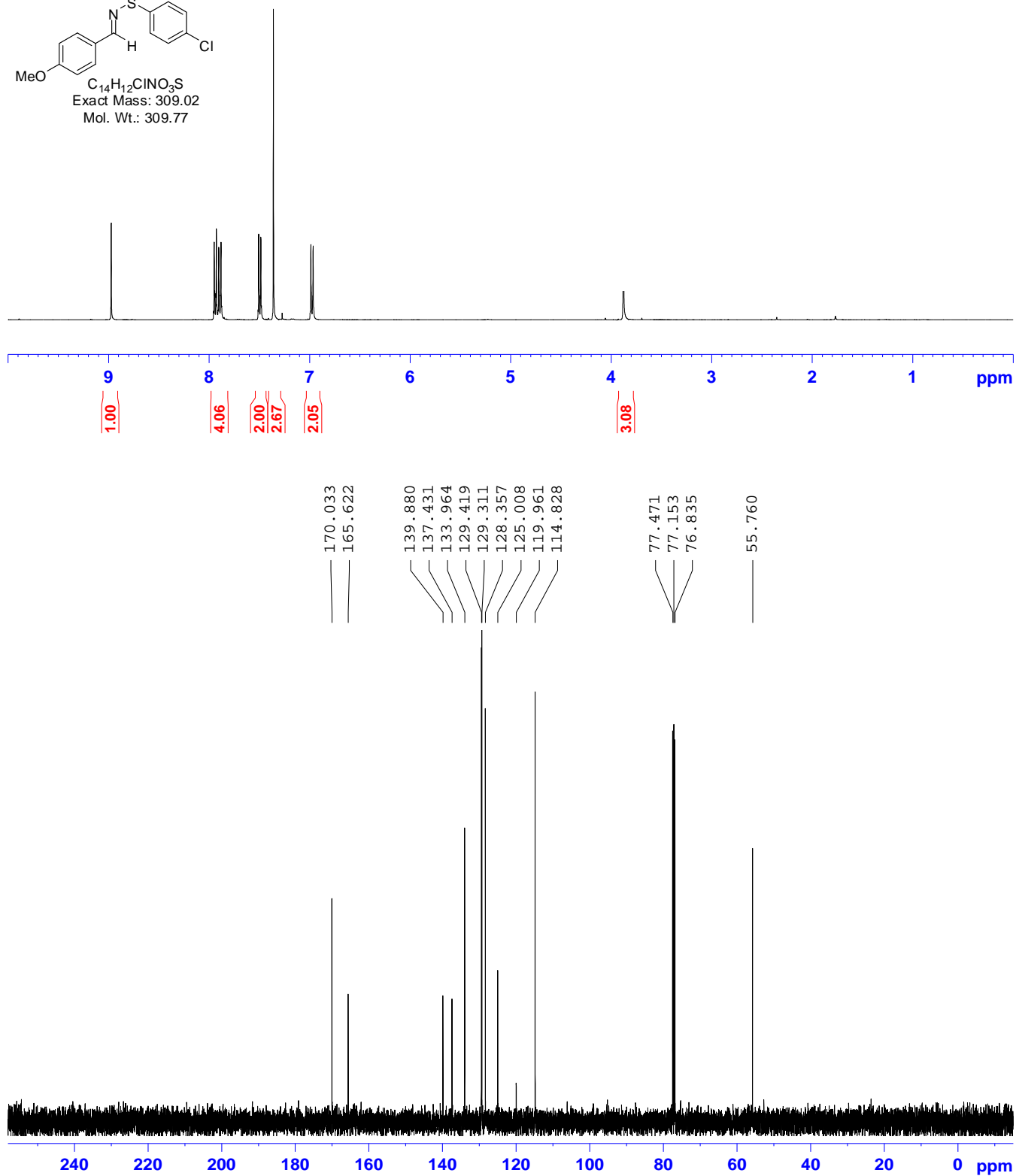
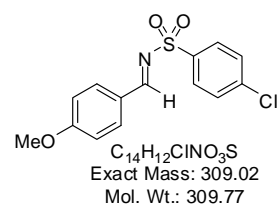
N-(4-Methylbenzylidene)-2-nitrobenzenesulfonamide (C36)



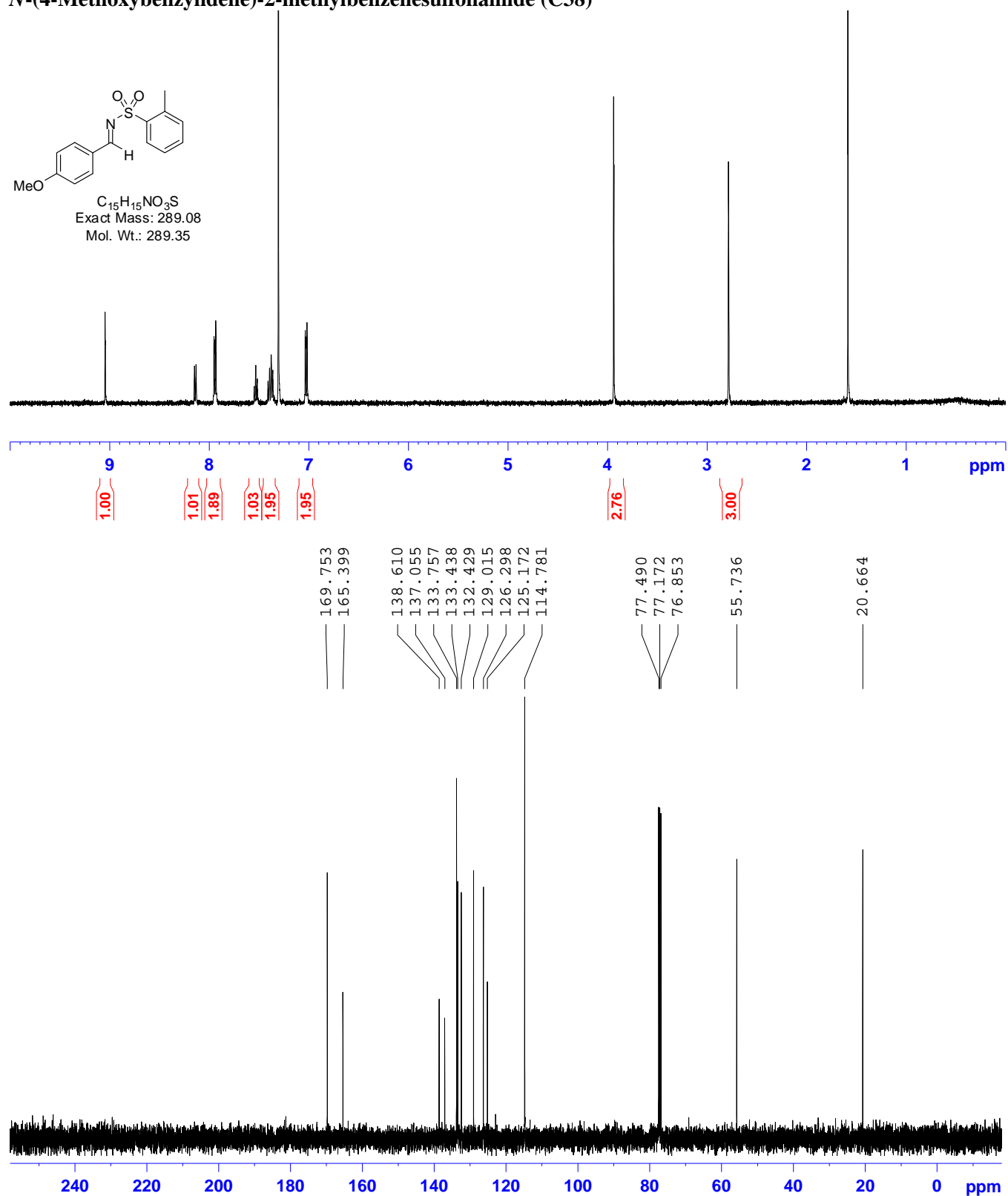
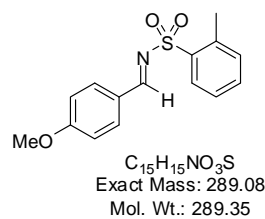
C₁₄H₁₂N₂O₄S
Exact Mass: 304.05
Mol Wt: 304.32



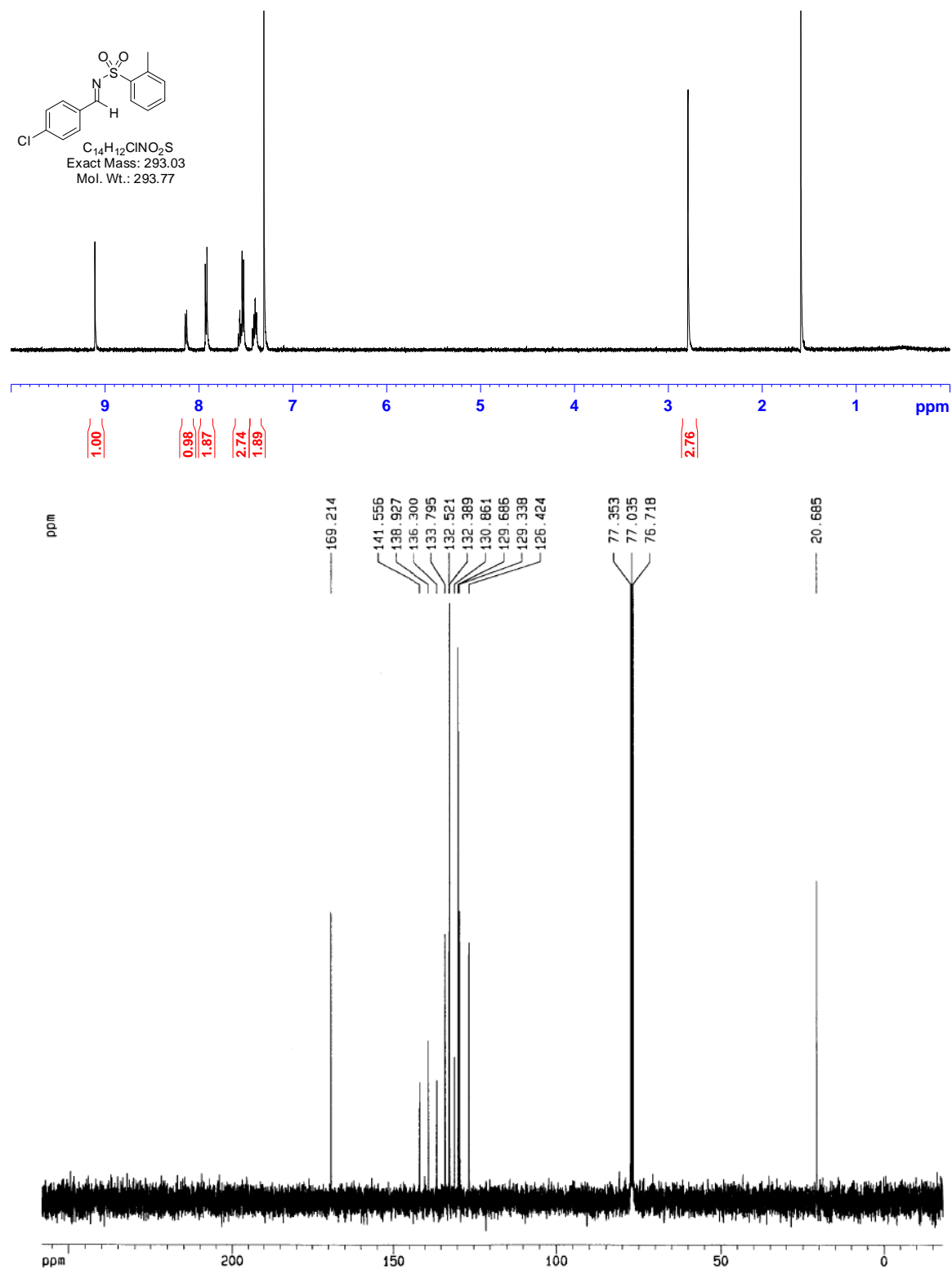
4-Chloro-N-(4-methoxybenzylidene)-benzenesulfonamide (C37)



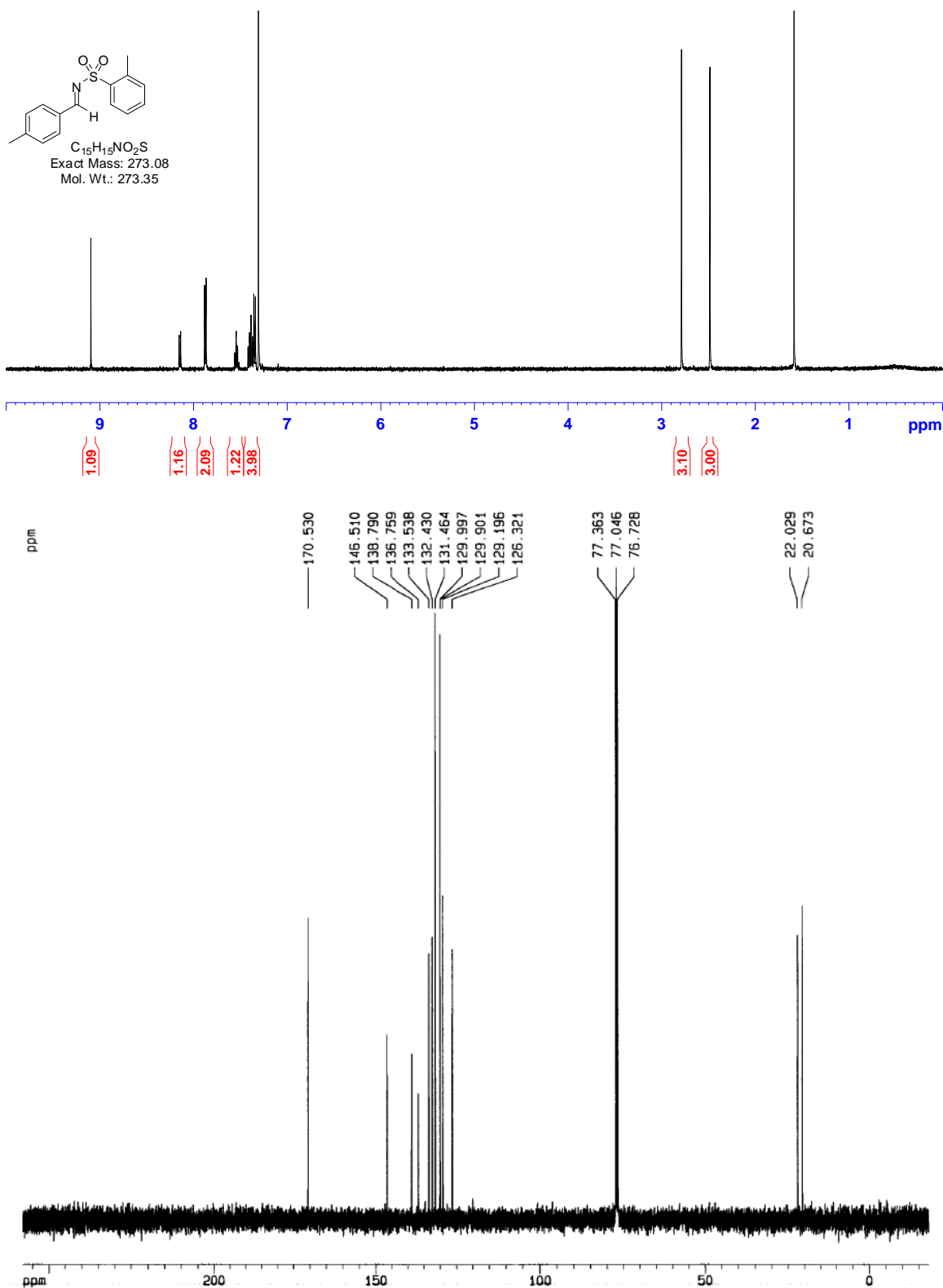
N-(4-Methoxybenzylidene)-2-methylbenzenesulfonamide (C38)



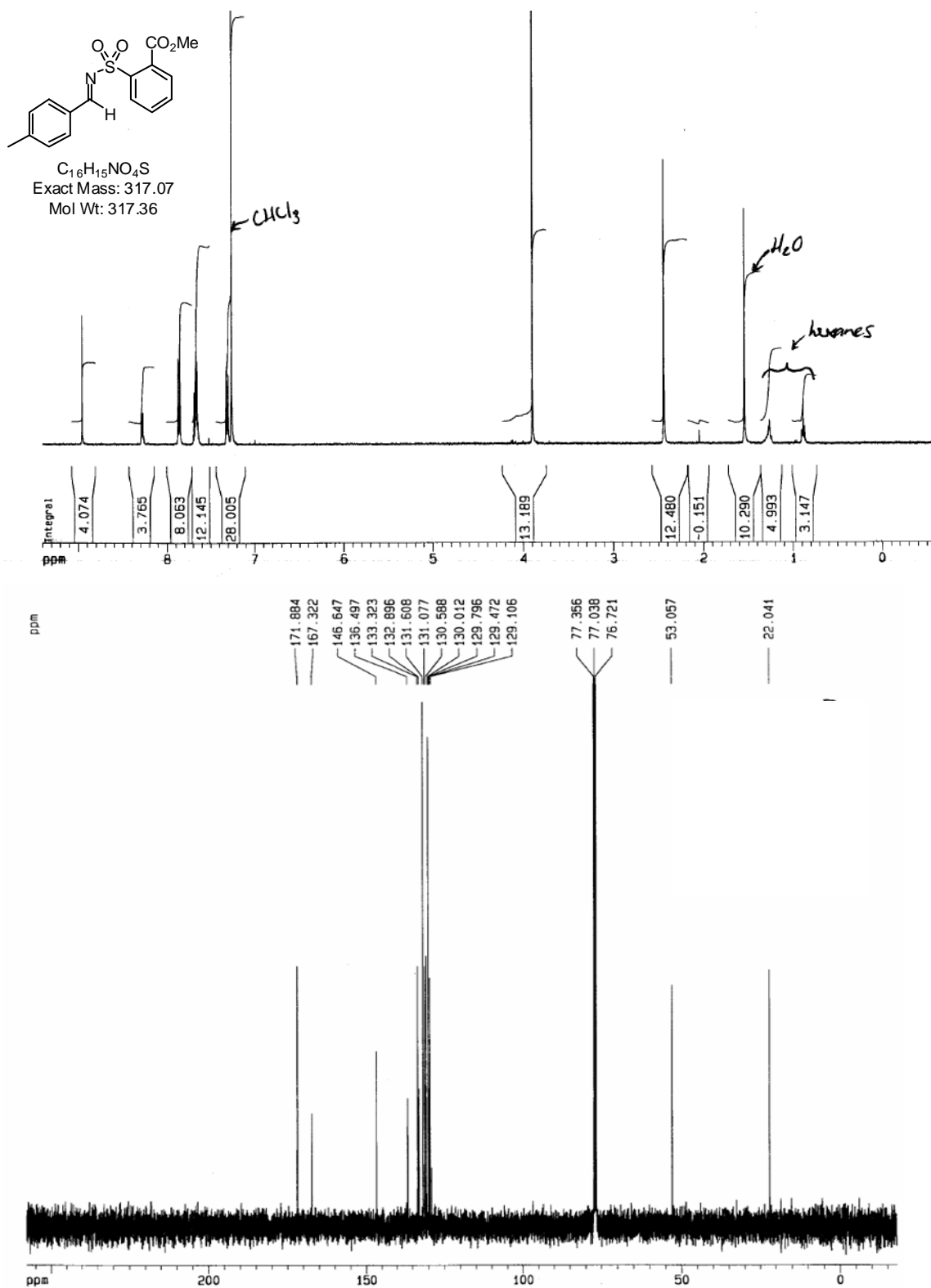
N-(4-Chlorobenzylidene)-2-methylbenzenesulfonamide (C40)



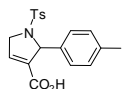
2-Methyl-N-(4-methylbenzylidene)-benzenesulfonamide (C41)



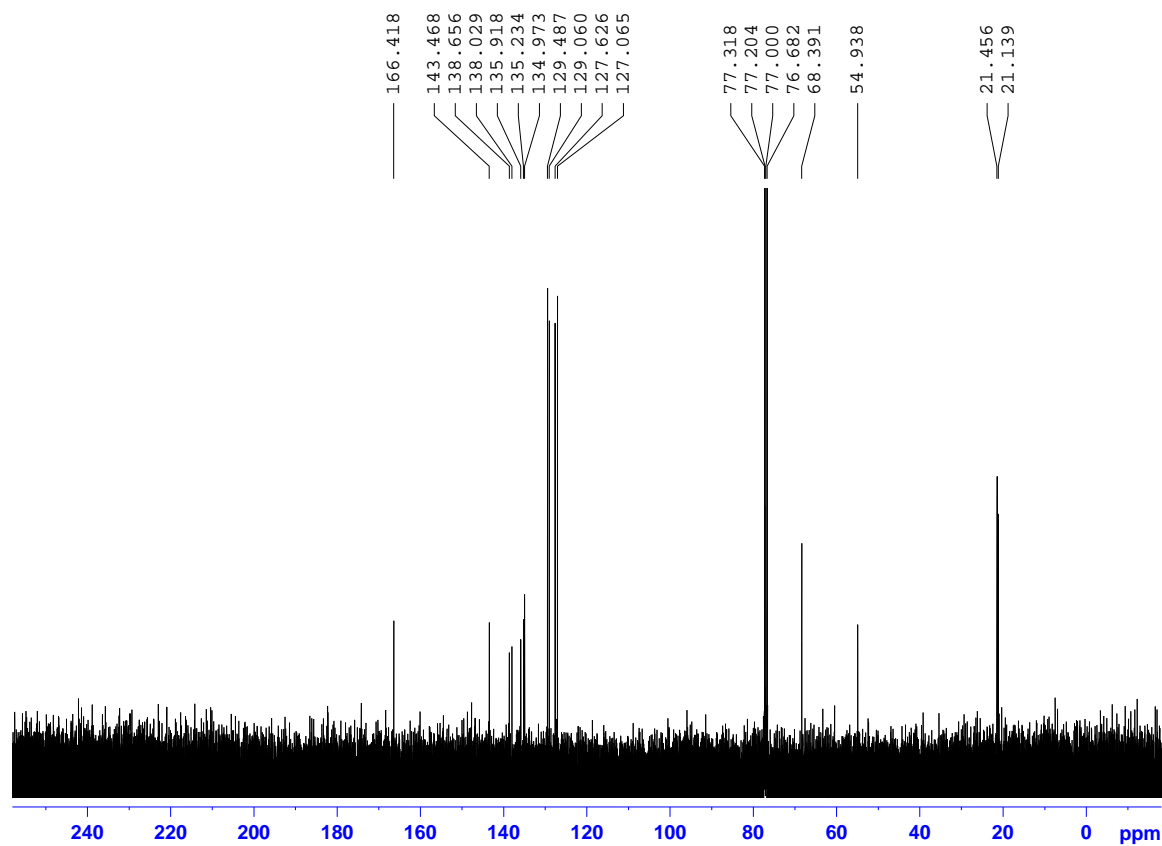
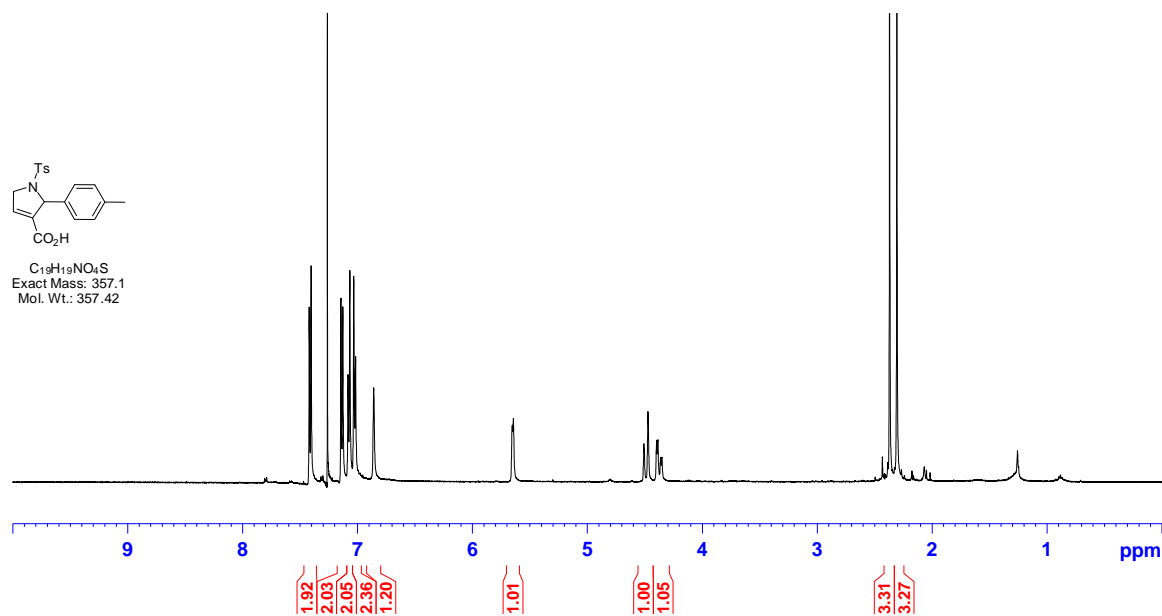
2-[4-Methylbenzylidene)-sulfamoyl]-benzoic acid methyl ester (C42)



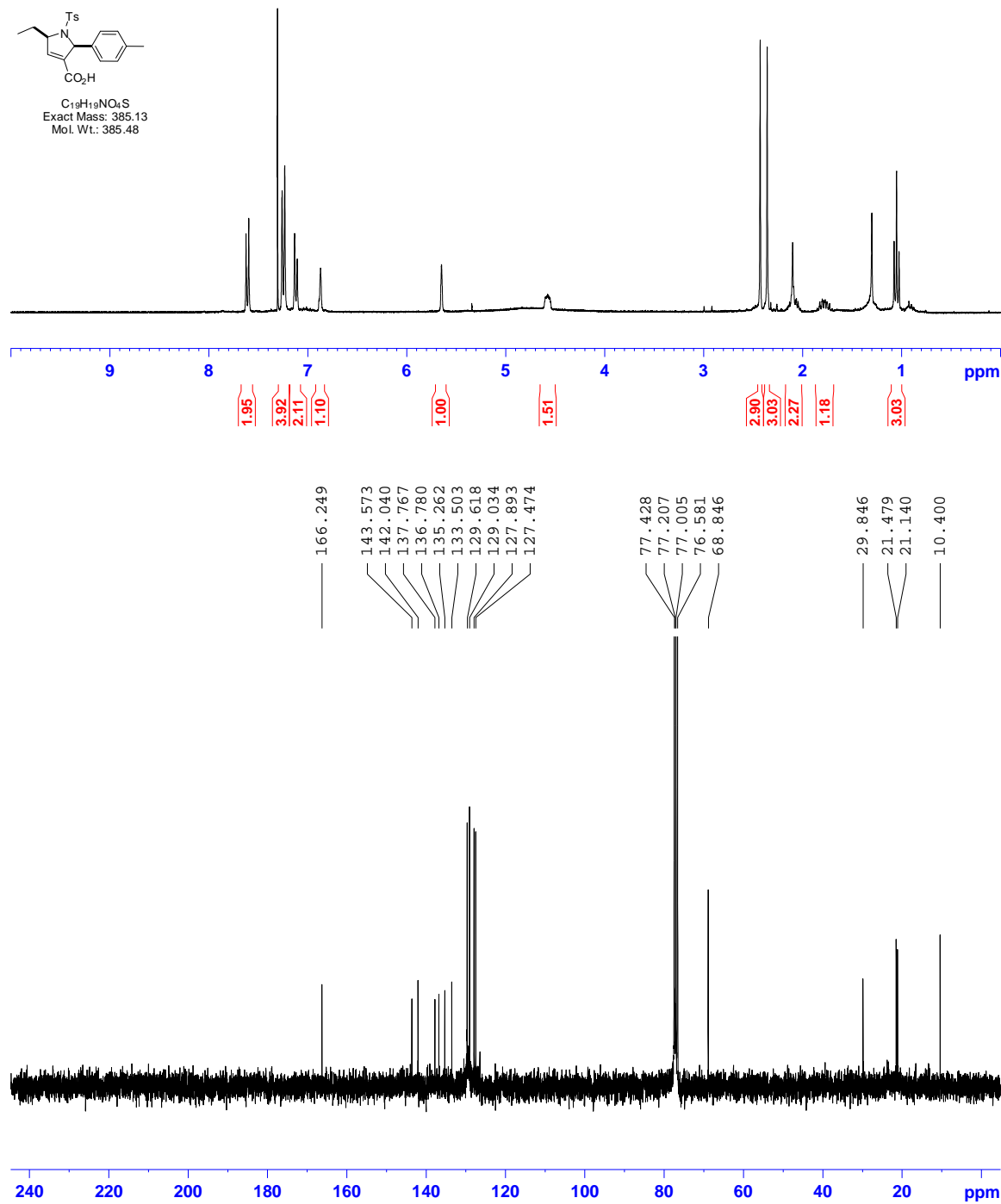
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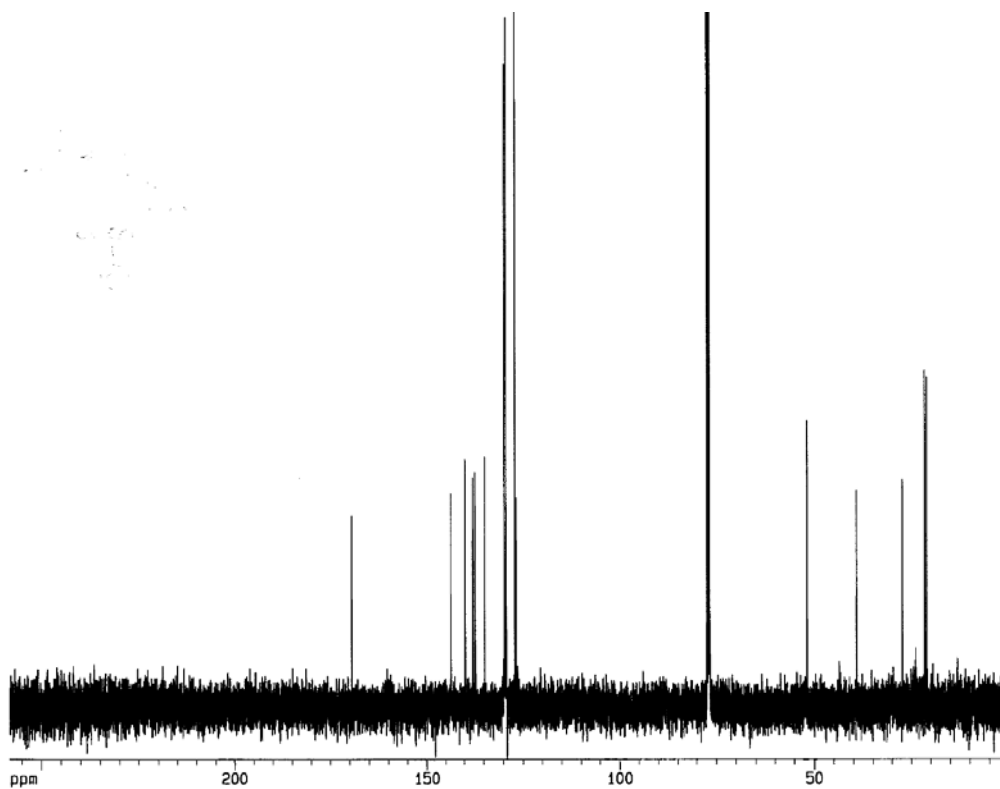
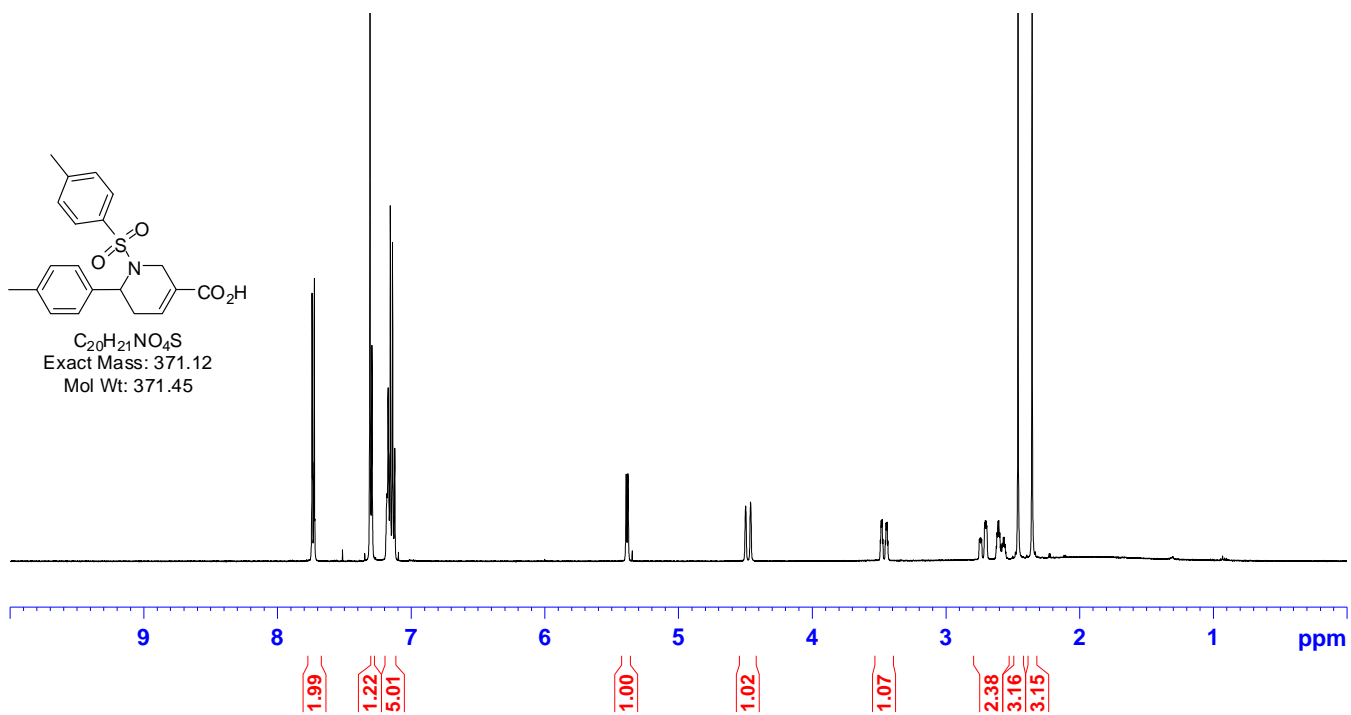
C₁₉H₁₉NO₄S
Exact Mass: 357.1
Mol. Wt.: 357.42



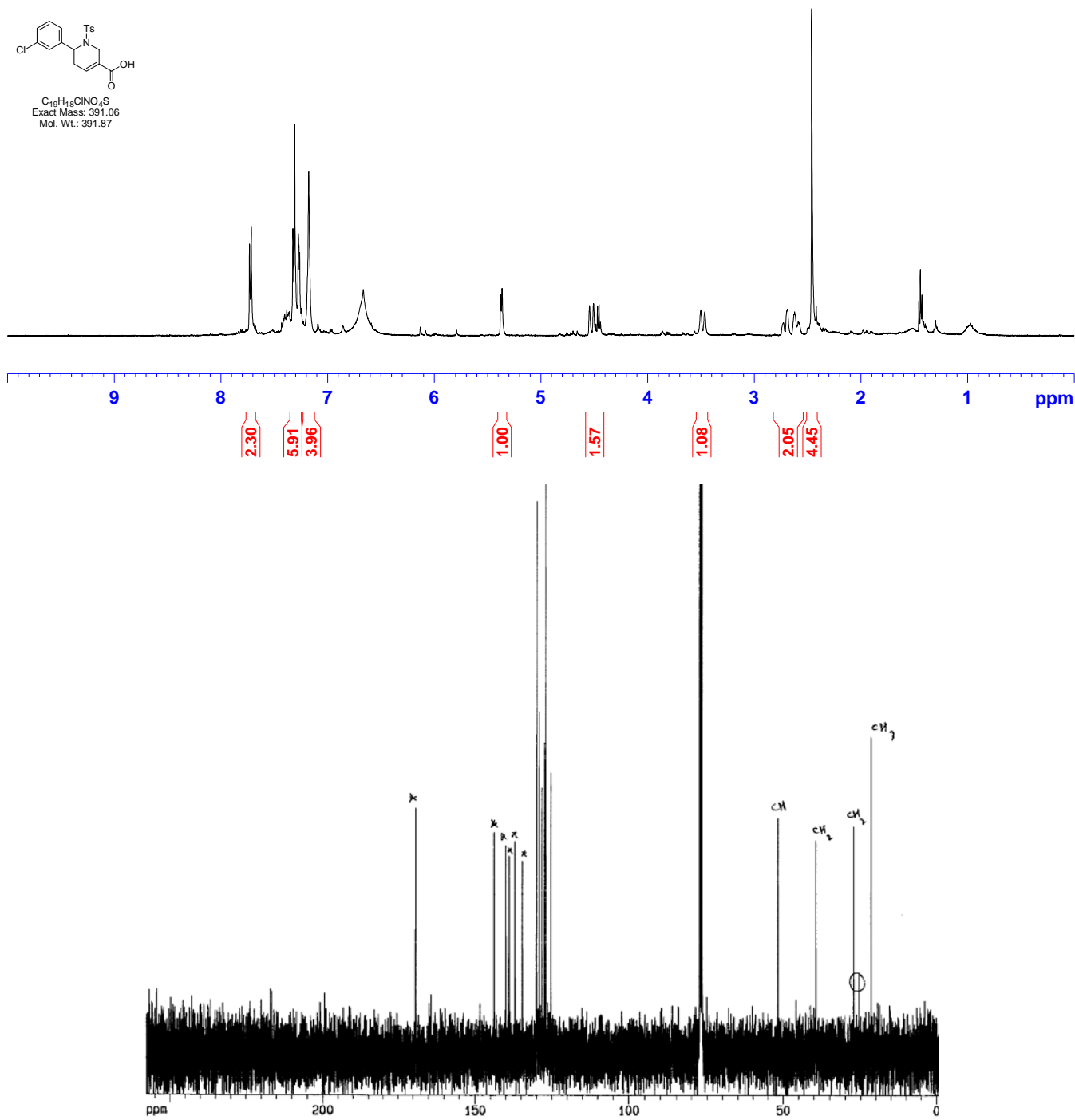
5-Ethyl-1-(4-toluenefonyl)-2-(*p*-tolyl)-2,5-dihydro-1-pyrrole-3-carboxylic acid (A05C02)



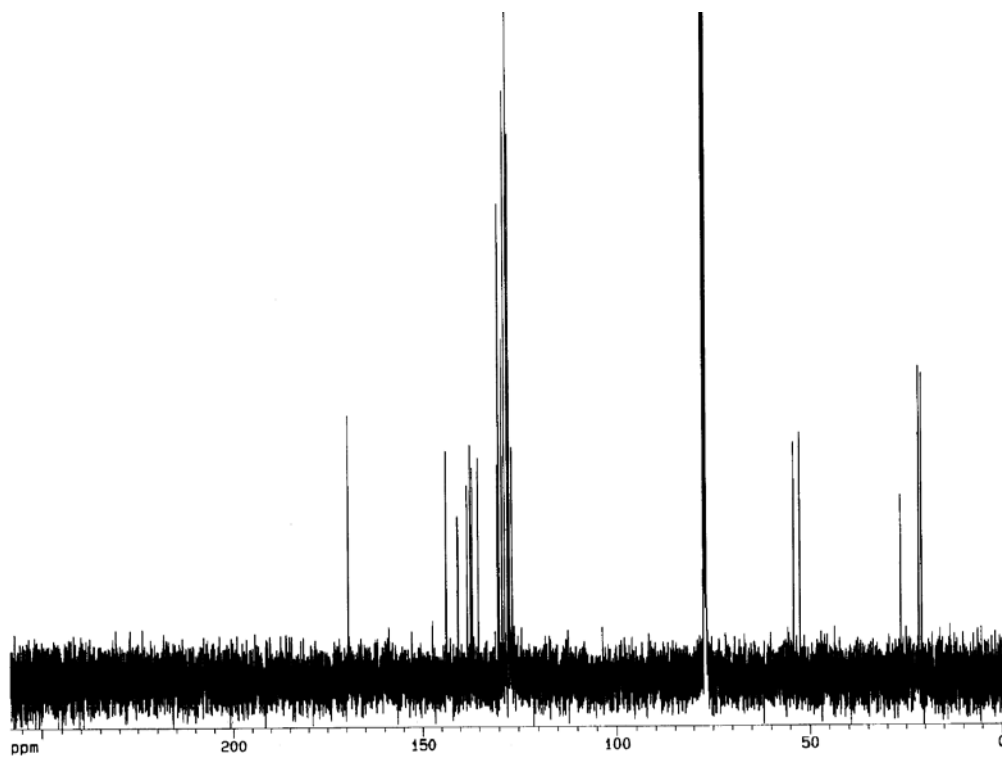
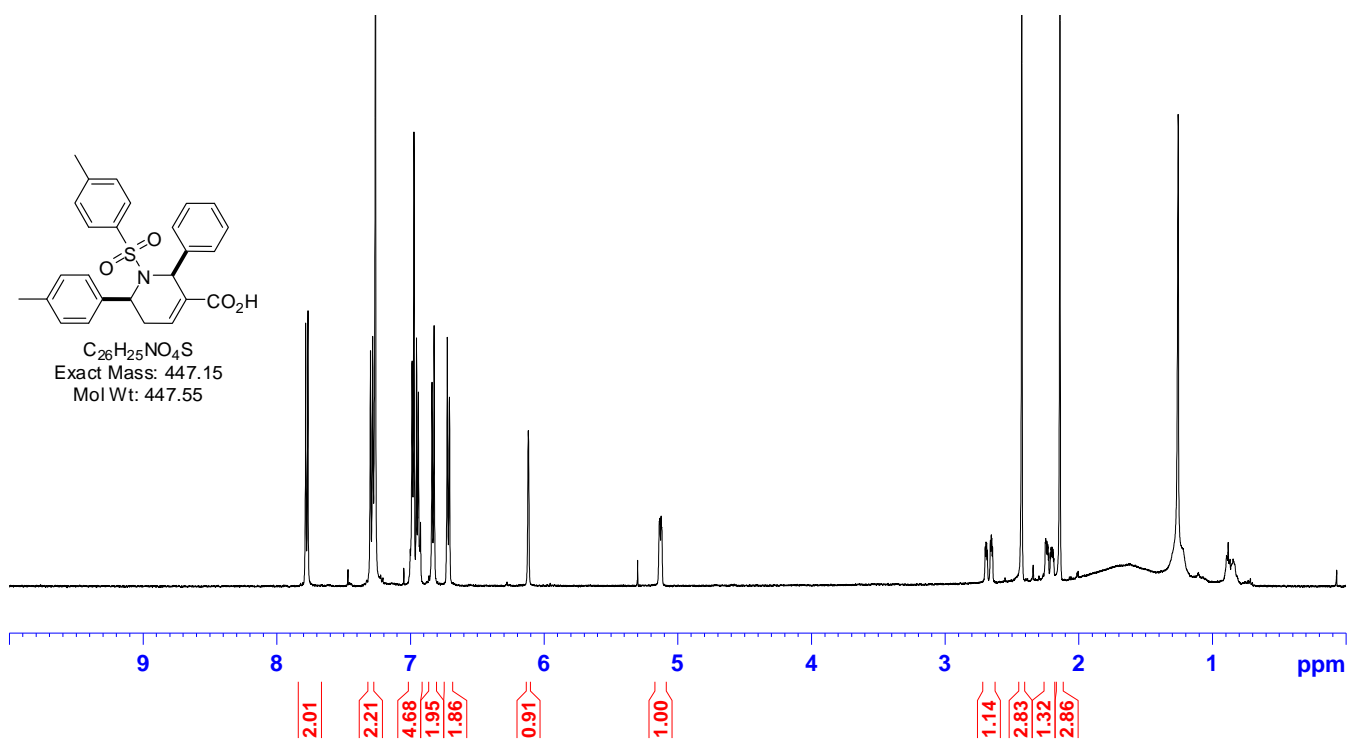
1-(4-Toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C02)



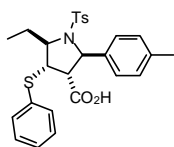
6-(3-Chlorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C12)



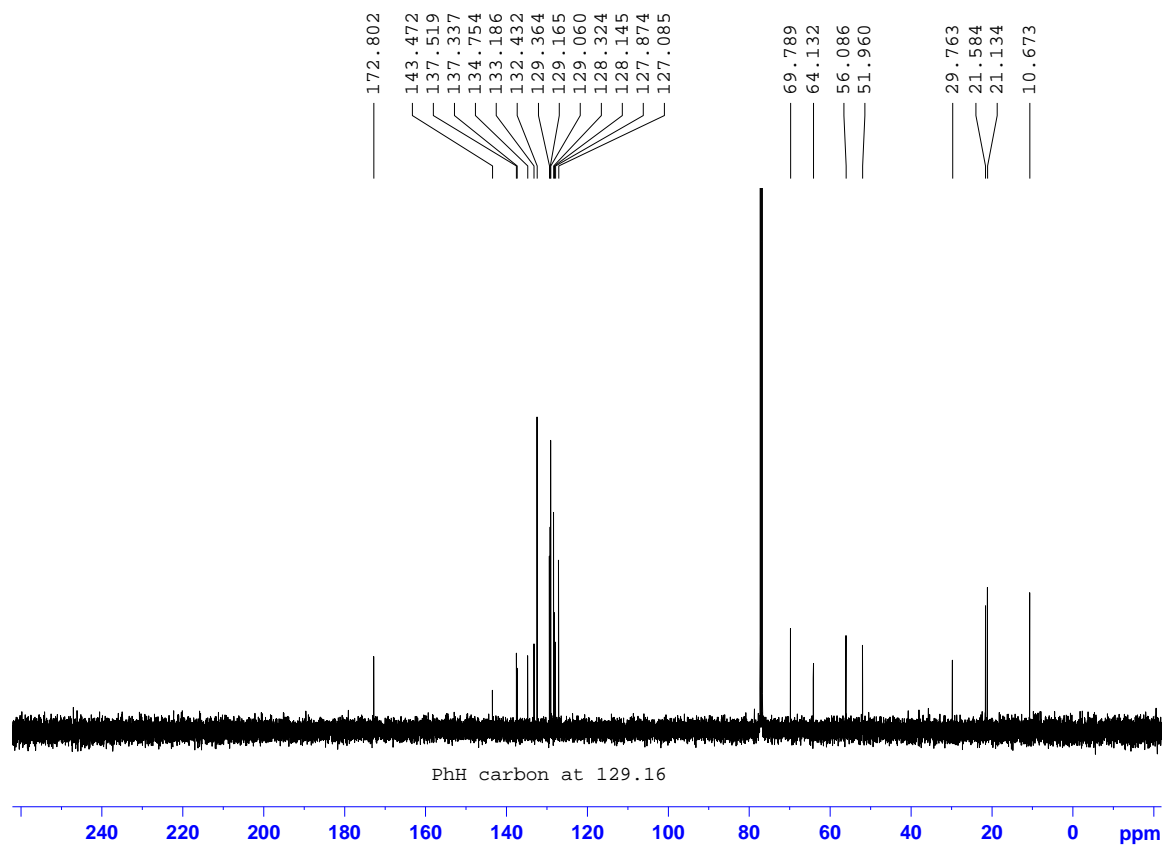
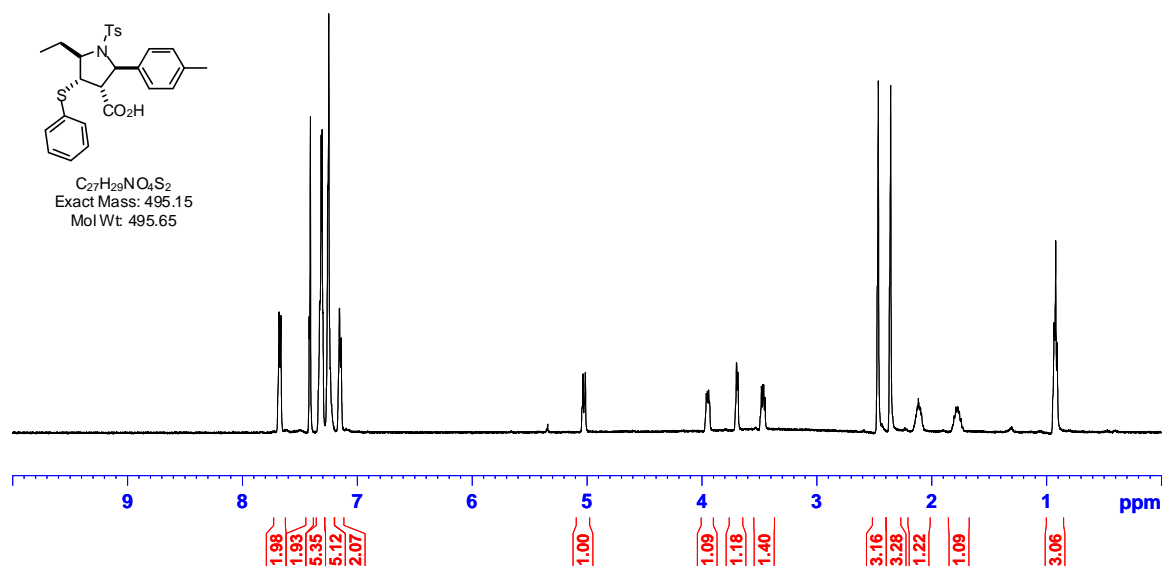
2-Phenyl-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B02C02)



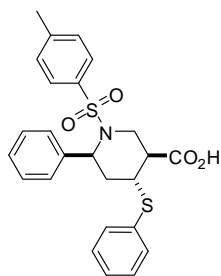
5-Ethyl-4-phenylsulfanyl-1-(4-toluenesulfonyl)-2-(*p*-tolyl)-pyrrolidine-3-carboxylic acid (A05C02E01)



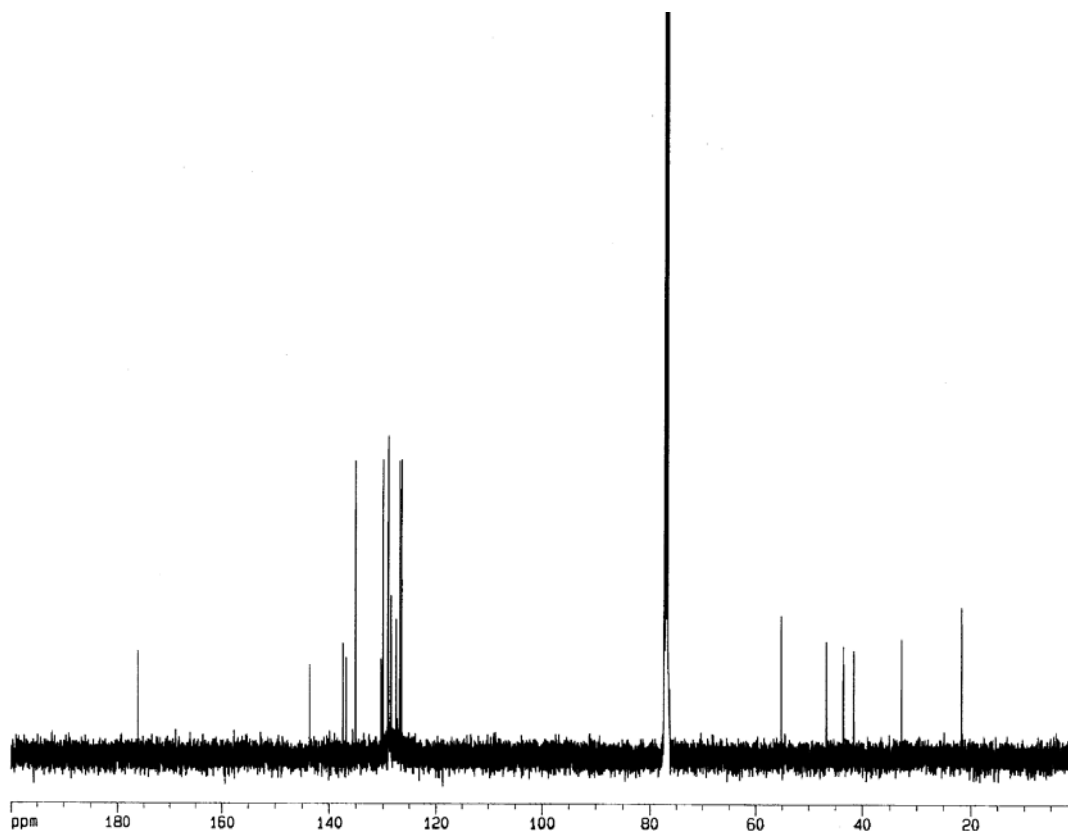
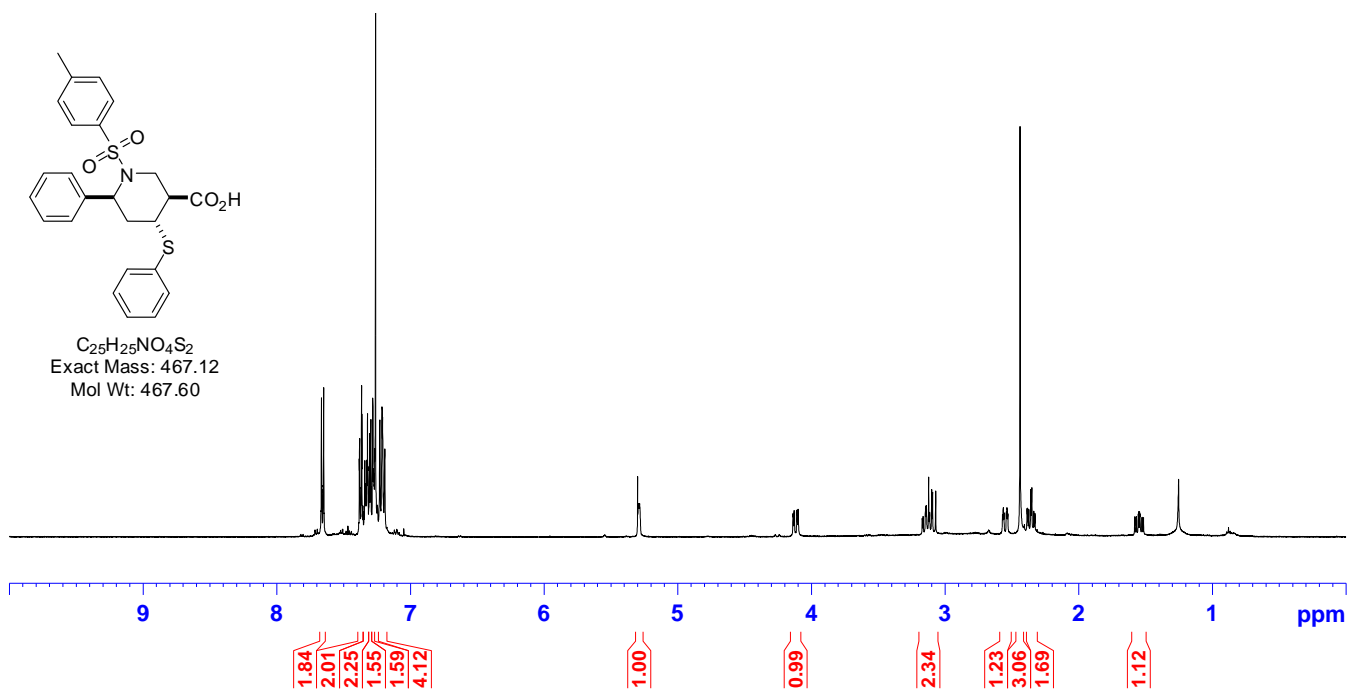
$C_{27}H_{29}NO_4S_2$
Exact Mass: 495.15
Mol Wt: 495.65



6-Phenyl-4-phenylsulfanyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C01E01)



C₂₅H₂₅NO₄S₂
Exact Mass: 467.12
Mol Wt: 467.60



4-(4-*t*-Butylbenzylsulfanyl)-6-phenyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C01E07)

