

Supporting Information
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Supporting Information

Accessing *meta*-Enone Substituted Anisoles using ArN_2BF_4 as Precatalyst *via* Rearrangement of Alkyne-Tethered Cyclohexadienones

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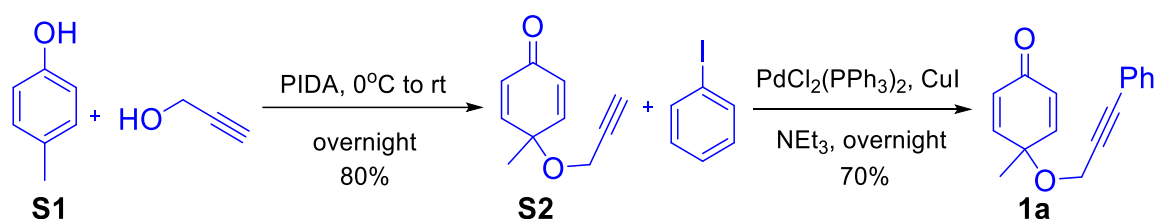
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1. Substrate Preparation:

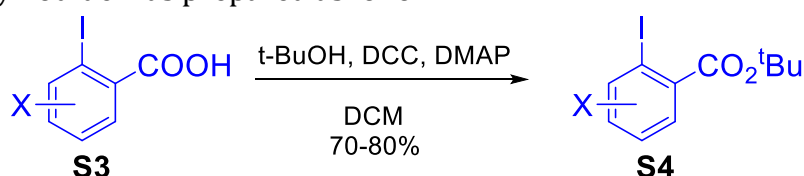
The 1,6-dienyne substrate were prepared as follow¹:



General Procedure for S2: To a well-stirred solution of *p*-cresol **S1** (1.0 mmol) in 1 mL of propargyl alcohol was added PIDA (1.5 mmol) in various portion at 0 °C. The reaction mixture was further stirred at room temperature for overnight. After completion (monitored by TLC), the reaction mixture was diluted with water and extracted with ethyl acetate. The combined organic layer was washed with brine, dried (Na₂SO₄), and concentrated under reduced pressure. The crude reaction mixture was purified by column chromatography using 9:1 petroleum ether/ethyl acetate to give desired product **S2**.

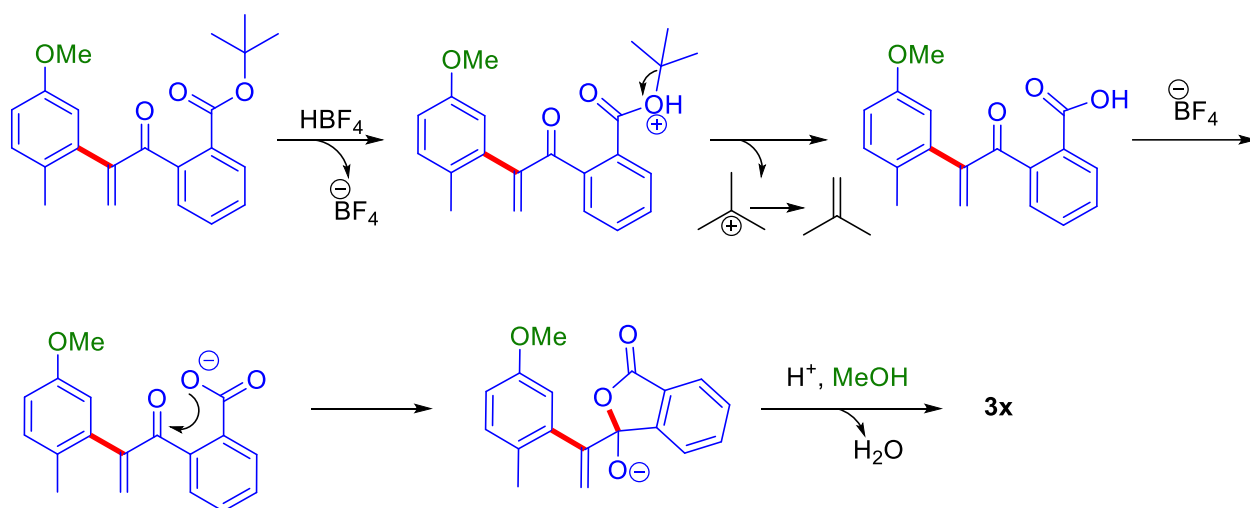
General Procedure for 1a: To PdCl₂(PPh₃)₂ (5 mol%) and CuI (2.5 mol%) in a two-neck round bottom flask under nitrogen atmosphere NEt₃ (1 mL) was added followed by **S2** (1 mmol) and phenyl iodide (1.2 mmol) was added and stirred for overnight. After completion (monitored by TLC), to the reaction mixture 10% of aqueous solution of HCl (2 mL) was added and extracted by ethyl acetate. The organic layer was concentrated in *vacuo* and purified by column chromatography using 9:1 petroleum ether/ethyl acetate to give desired product.

Starting material **1a** to **1z** was prepared by above methods. For compound **1n**, **1x-1z** substituted aryl iodide was prepared as follow²:



To a solution of substituted iodo-benzoic acid **S3** (1 mmol) in DCM (0.2 M) was added DMAP (0.5 mmol) and DCC (1.1 mmol) at 0 °C and stirred for 10 minutes at same temperature and was added tert-butanol. The reaction was stirred at room temperature for overnight. After completion (monitored by TLC), the reaction mixture was filtered through pad of celite and washed with diethyl ether followed by brine, dried and concentrated in *vacuo*. The crude reaction mixture was purified by column chromatography in petroleum ether to give protected aryl iodide **S4**.

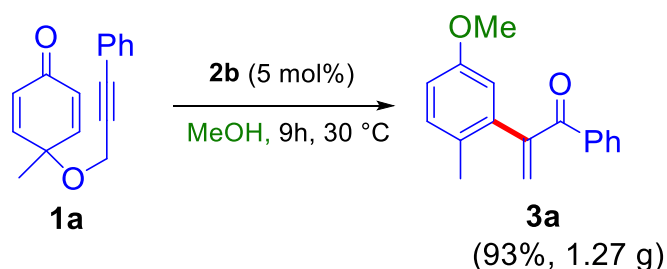
Plausible mechanism for the further cyclisation of *meta*-en-substituted cresol to *meta*-en-lactone substituted cresols:



Based on the literature precedents, in acidic medium tert-butyl benzoate involving the elimination of isobutylene followed by cyclisation and elimination of water gave the *meta*-en-lactone substituted cresol **3x**.

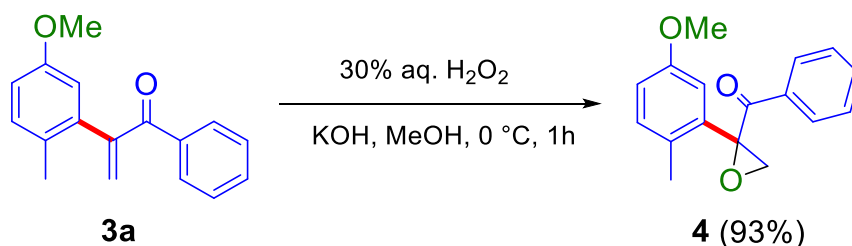
2. Synthetic Utility

Gram Scale Synthesis:



An oven dried round bottom flask was charged with cyclohexadienone-tethered alkynes **1a** (5.4 mmol) and aryl diazonium salts (5 mol %) in anhydrous methanol (27 mL). The reaction mixture was stirred at room temperature for 9h. After completion (monitored by TLC), the mixture was diluted with water and extracted by ethyl acetate, dried (Na_2SO_4) and concentrated under reduced pressure. The crude reaction mixture was purified by column chromatography using 19:1 petroleum ether/ethyl acetate to give desired product **3a** weighing 1.27 g as a light-yellow solid.

(2-(5-methoxy-2-methylphenyl)oxiran-2-yl)(phenyl)methanone (**4**)



3a (0.2 mmol) and KOH (0.1 mmol) were dissolved in 1 mL MeOH in a pressure tube, the reaction was cooled to 0 °C. 30% H_2O_2 solution (0.5 mmol) was then added slowly under stirring and the reaction was continued until the starting material was consumed. The

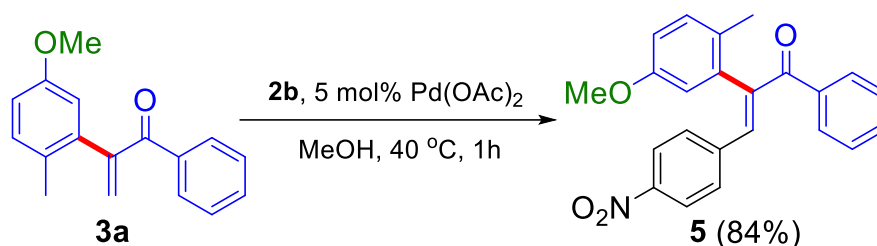
mixture was then evaporated under vacuum and purified by flash chromatography to give **4**³. $R_f = 0.40$ (19:1 hexane/EtOAc); 89% (47 mg) yield; colourless oil.

¹H NMR (400 MHz, CDCl₃) δ 8.02 (dd, $J = 5.2, 3.3$ Hz, 2H), 7.55 – 7.48 (m, 1H), 7.39 (dd, $J = 10.6, 4.8$ Hz, 2H), 7.13 (d, $J = 2.7$ Hz, 1H), 7.04 (d, $J = 8.4$ Hz, 1H), 6.79 (dd, $J = 8.4, 2.7$ Hz, 1H), 3.81 (s, 3H), 3.44 (d, $J = 5.8$ Hz, 1H), 3.14 (d, $J = 5.8$ Hz, 1H), 2.27 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 195.8, 157.9, 135.6, 135.1, 133.3, 131.6, 129.5, 129.5, 128.4, 114.1, 113.3, 63.8, 55.5, 53.1, 18.9.

HRMS (ESI, m/z): calcd for C₁₇H₁₇O₃ ([M + H]⁺): 269.1172; found 269.1171.

2-(5-methoxy-2-methylphenyl)-3-(4-nitrophenyl)-1-phenylprop-2-en-1-one (**5**)



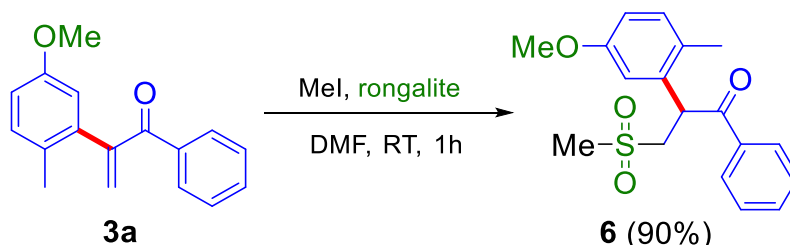
3a (0.2 mmol), **2b** (0.3 mmol) and Pd(OAc)₂ (0.01 mmol) were dissolved in 2 mL MeOH under argon atmosphere. The reaction mixture was heated at 40 °C for 1h. After completion (monitored by TLC), the mixture was then evaporated under vacuum and purified by flash chromatography to give **5**⁴. $R_f = 0.30$ (9:1 hexane/EtOAc); 84% (63 mg) yield; white solid; mp = 136–138 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.07 – 8.00 (m, 2H), 7.91 – 7.84 (m, 2H), 7.63 – 7.55 (m, 1H), 7.53 – 7.45 (m, 2H), 7.32 (s, 1H), 7.22 – 7.15 (m, 3H), 6.87 (dd, $J = 8.4, 2.7$ Hz, 1H), 6.67 (d, $J = 2.7$ Hz, 1H), 3.73 (s, 3H), 2.10 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 196.4, 158.3, 147.5, 143.7, 141.3, 138.2, 137.7, 136.3, 132.6, 132.0, 130.7, 129.7, 128.6, 127.9, 123.6, 115.0, 114.4, 55.4, 19.0.

HRMS (ESI, m/z): calcd for C₂₃H₂₀NO₄ ([M + H]⁺): 374.1387; found 374.1386.

2-(5-methoxy-2-methylphenyl)-3-(methylsulfonyl)-1-phenylpropan-1-one (**6**)



3a (0.2 mmol) and rongalite (0.3 mmol) was added in DMF (2 mL) and stirred at rt for 10 min. Then MeI (0.3 mmol) was added, and reaction mixture was further stirred for 1h. After completion (monitored by TLC), the mixture was then evaporated under vacuum and purified by flash chromatography to give **6**⁵. $R_f = 0.10$ (4:1 hexane/EtOAc); 90% (60 mg) yield; white solid; mp = 132–134 °C.

^1H NMR (400 MHz, CDCl_3) δ 7.89 – 7.81 (m, 2H), 7.50 (dd, $J = 10.6, 4.3$ Hz, 1H), 7.39 (m, 2H), 7.16 (d, $J = 8.4$ Hz, 1H), 6.71 (dd, $J = 8.4, 2.7$ Hz, 1H), 6.54 (d, $J = 2.7$ Hz, 1H), 5.36 (dd, $J = 9.2, 3.3$ Hz, 1H), 4.29 (dd, $J = 14.6, 9.2$ Hz, 1H), 3.67 (s, 3H), 3.14 (dd, $J = 14.6, 3.1$ Hz, 1H), 2.84 (s, 3H), 2.53 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 197.3, 158.5, 135.9, 135.7, 133.7, 132.8, 128.8, 128.8, 127.2, 113.5, 113.1, 57.3, 55.3, 45.2, 42.5, 18.9.

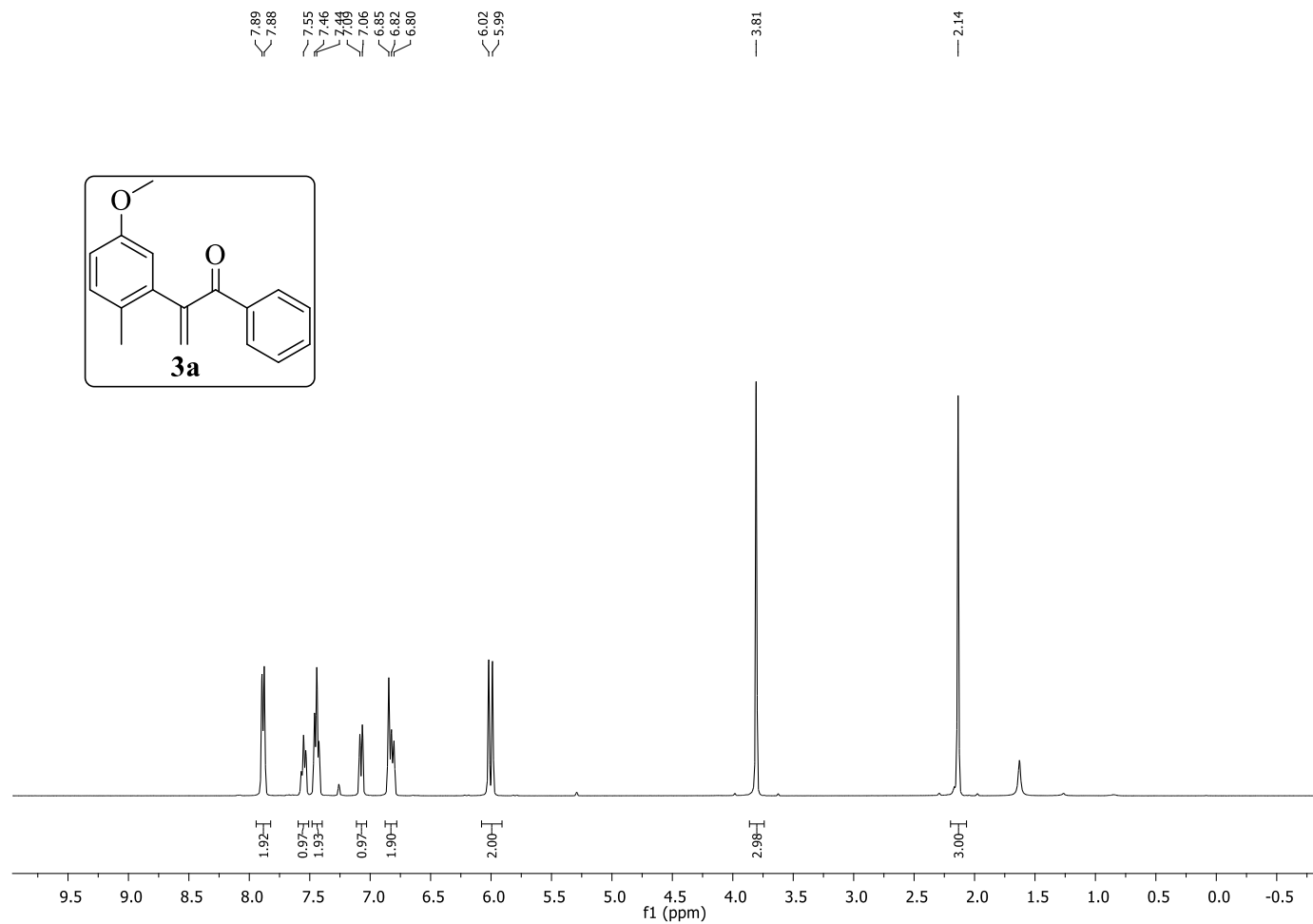
HRMS (ESI, m/z): calcd for $\text{C}_{18}\text{H}_{21}\text{O}_4\text{S}$ ($[\text{M} + \text{H}]^+$): 333.1155; found 333.1147.

3. References

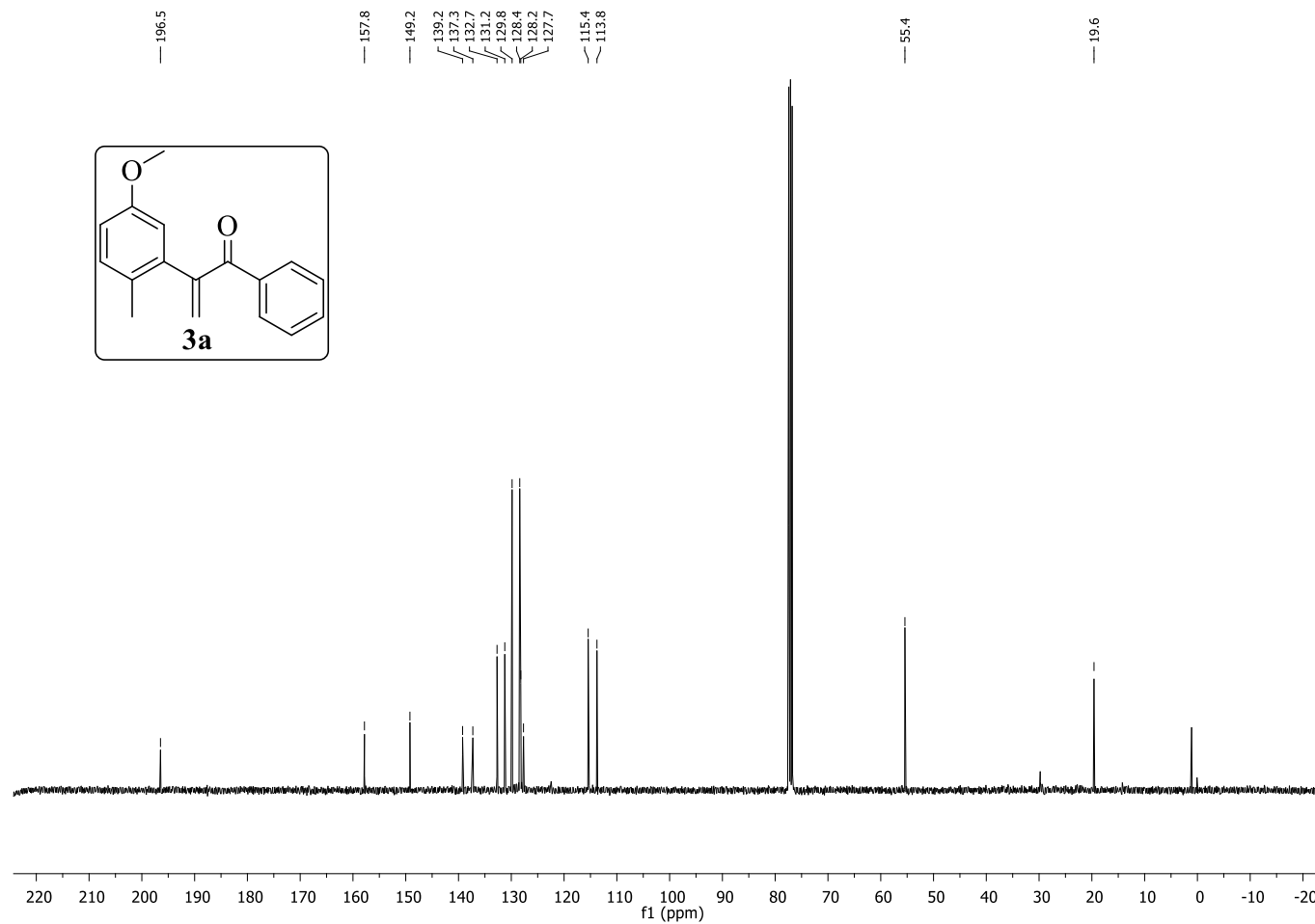
- (1) Munakala, A.; Chegondi, R., *Org. Lett.* **2021**, *23*, 317-323.
- (2) Wang, H.; Niu, Y.; Zhang, G.; Ye, X. S., *Tetrahedron Letters.* **2016**, *57*, 4544-4548.
- (3) Nair, A. M.; Halder, I.; Sharma, R.; Volla, C. M. R., *Org. Lett.* **2021**, *23*, 1840-1845.
- (4) Darses, S.; Pucheault, M.; Gene, J. P., *Eur. J. Org. Chem.* **2001**, 1121.
- (5) Kale, S. B.; Jori, P. K.; Das, U., *Chem Asian J.* **2022**, *17*, e202200408.

4. ^1H NMR, ^{13}C NMR, Mass spectra of compounds

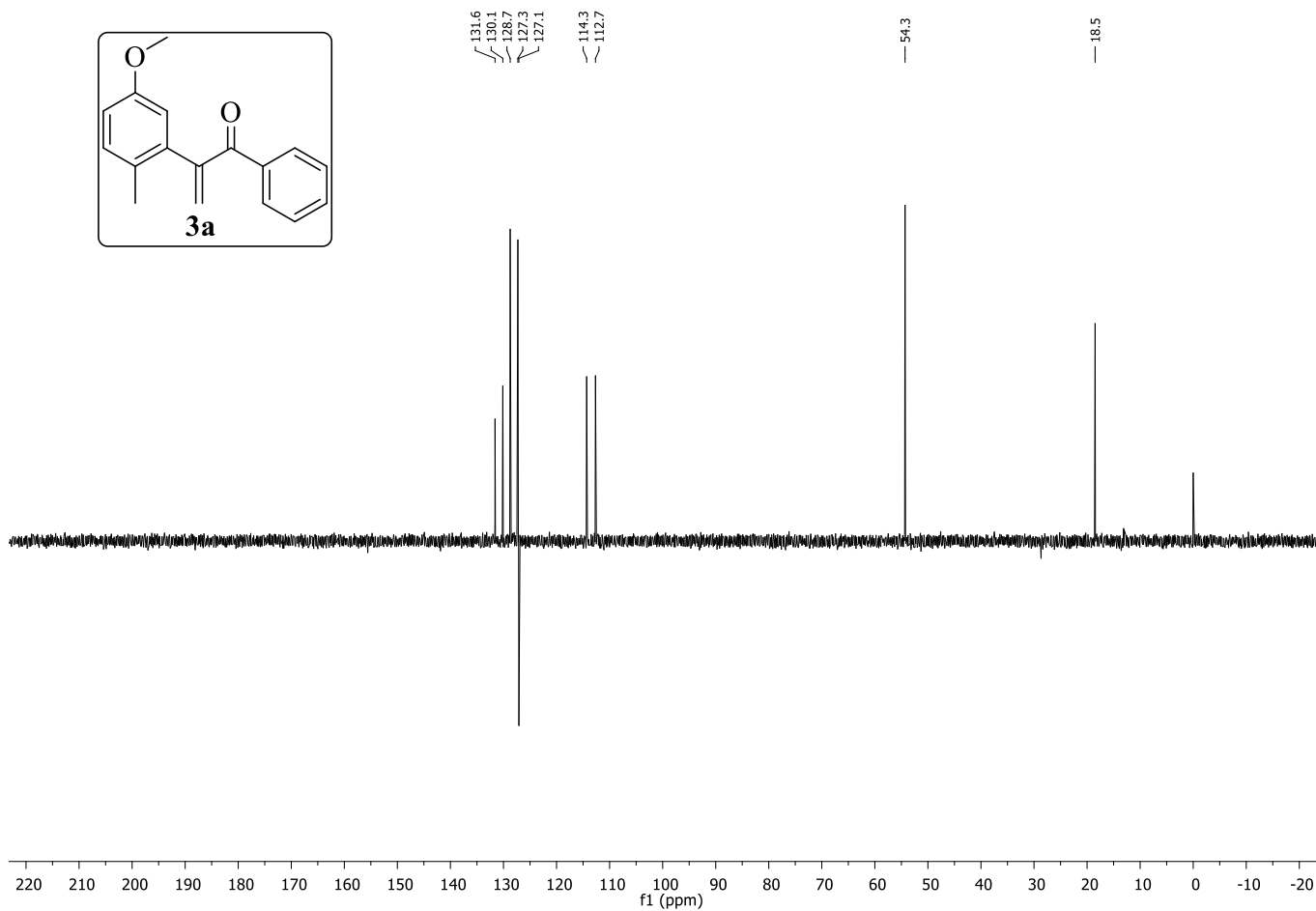
^1H NMR spectrum of compound **3a** (400 MHz, CDCl_3)



^{13}C { ^1H } NMR spectrum of compound **3a** (101 MHz, CDCl_3)

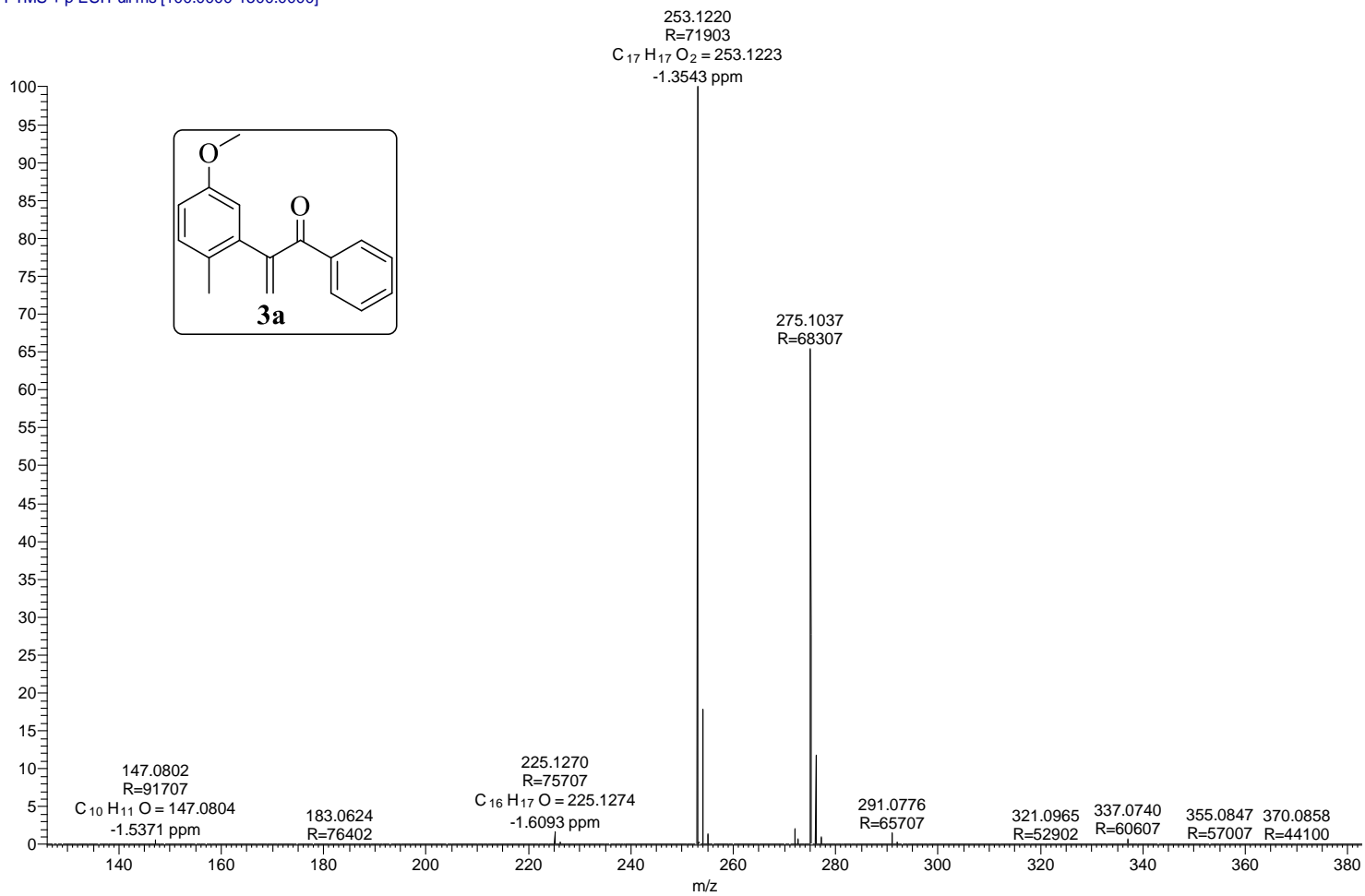


^{13}C $\{^1\text{H}\}$ DEPT NMR spectrum of compound **3a** (101 MHz, CDCl_3)

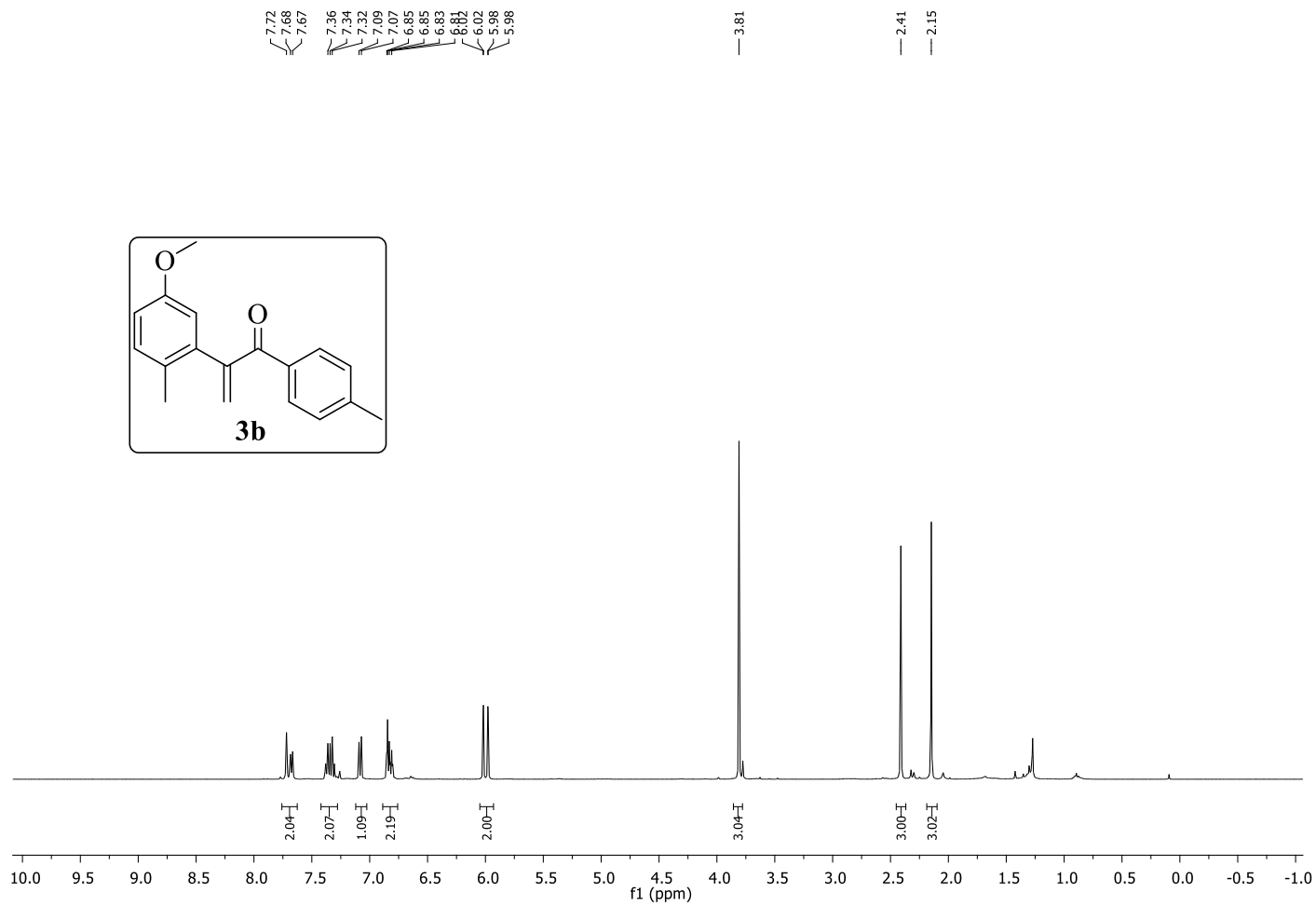


HRMS spectrum of compound 3a

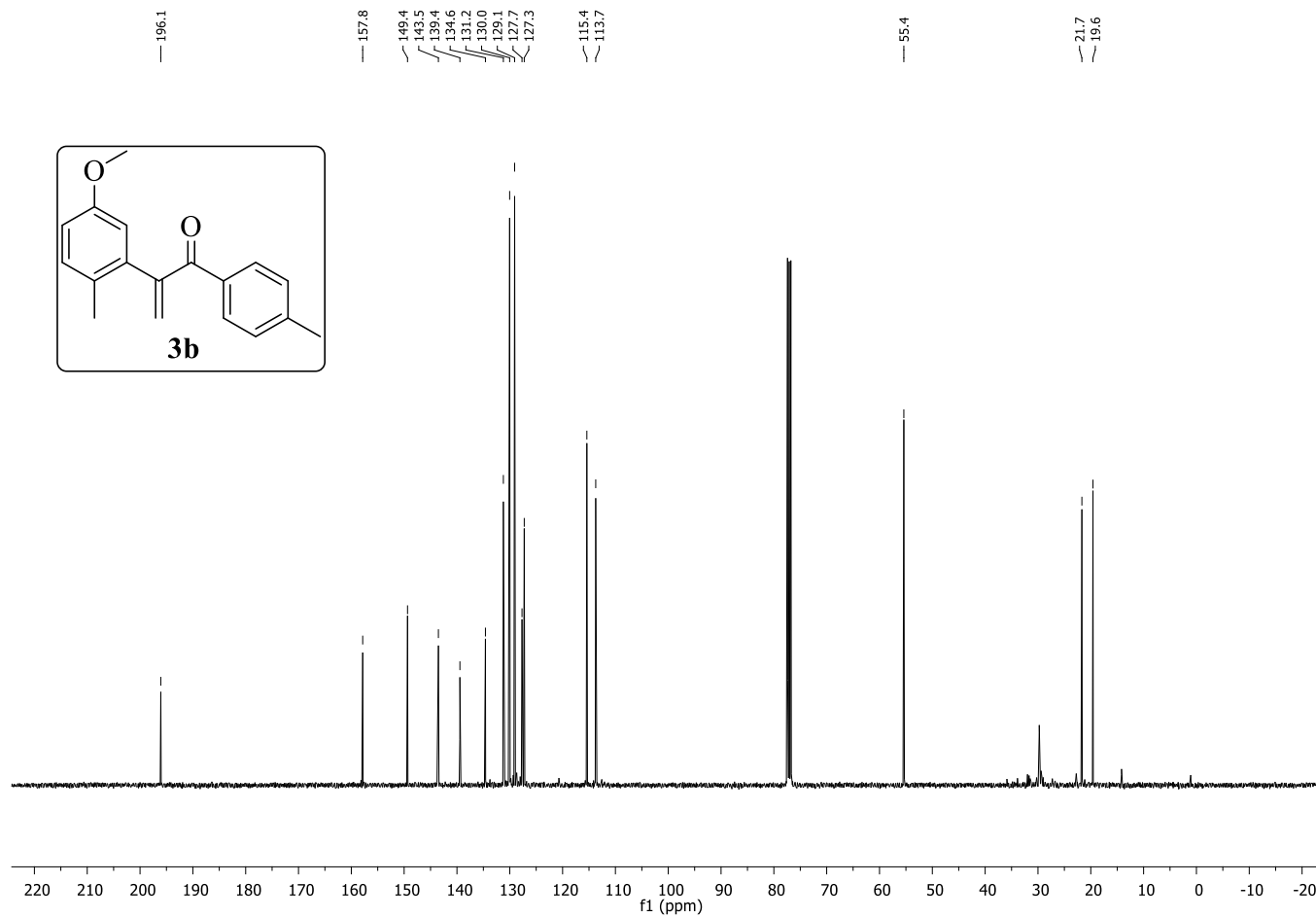
ARC-1 #437 RT: 1.95 AV: 1 NL: 5.30E9
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^1H NMR spectrum of compound **3b** (400 MHz, CDCl_3)

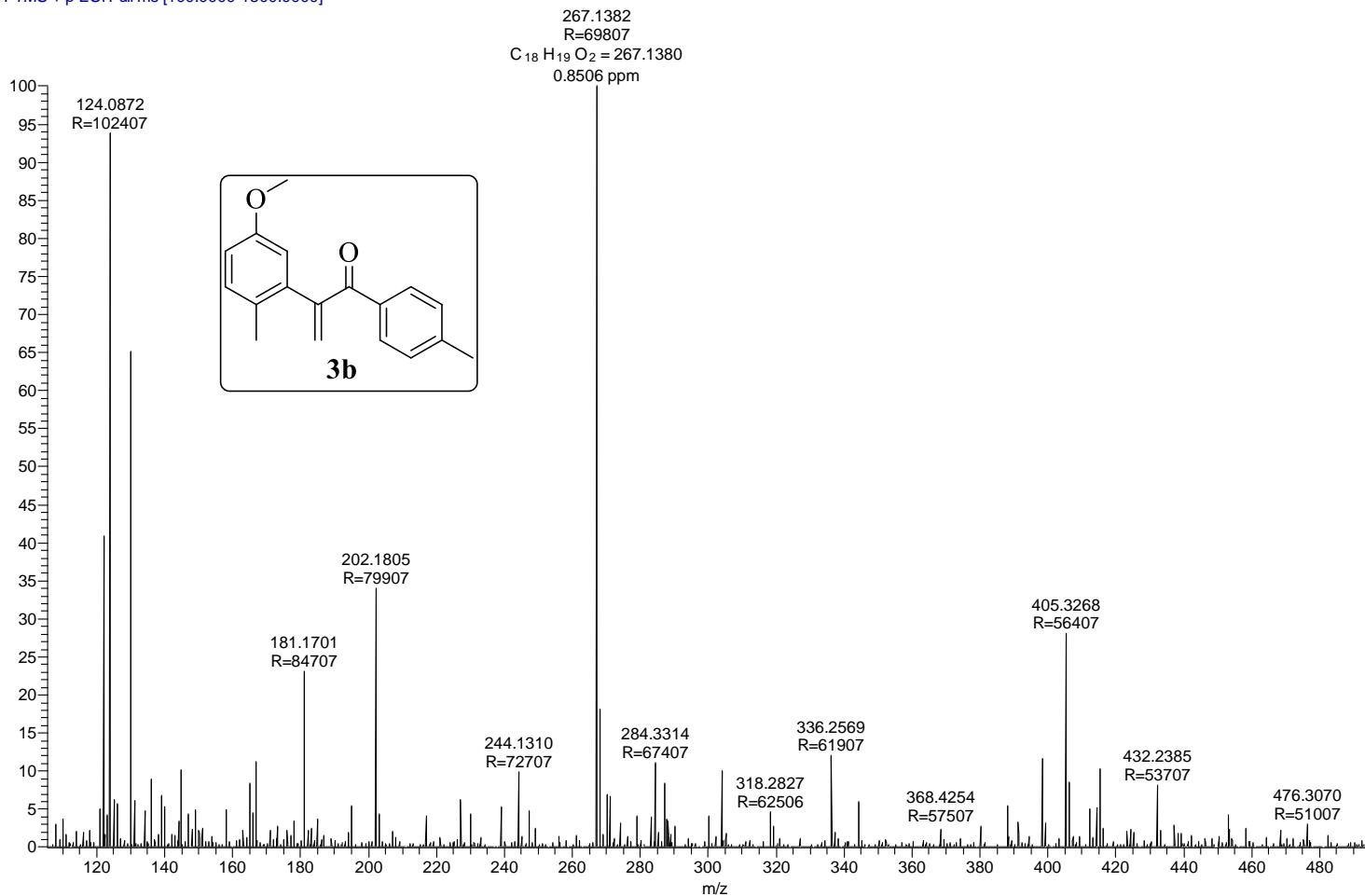


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3b** (101 MHz, CDCl_3)

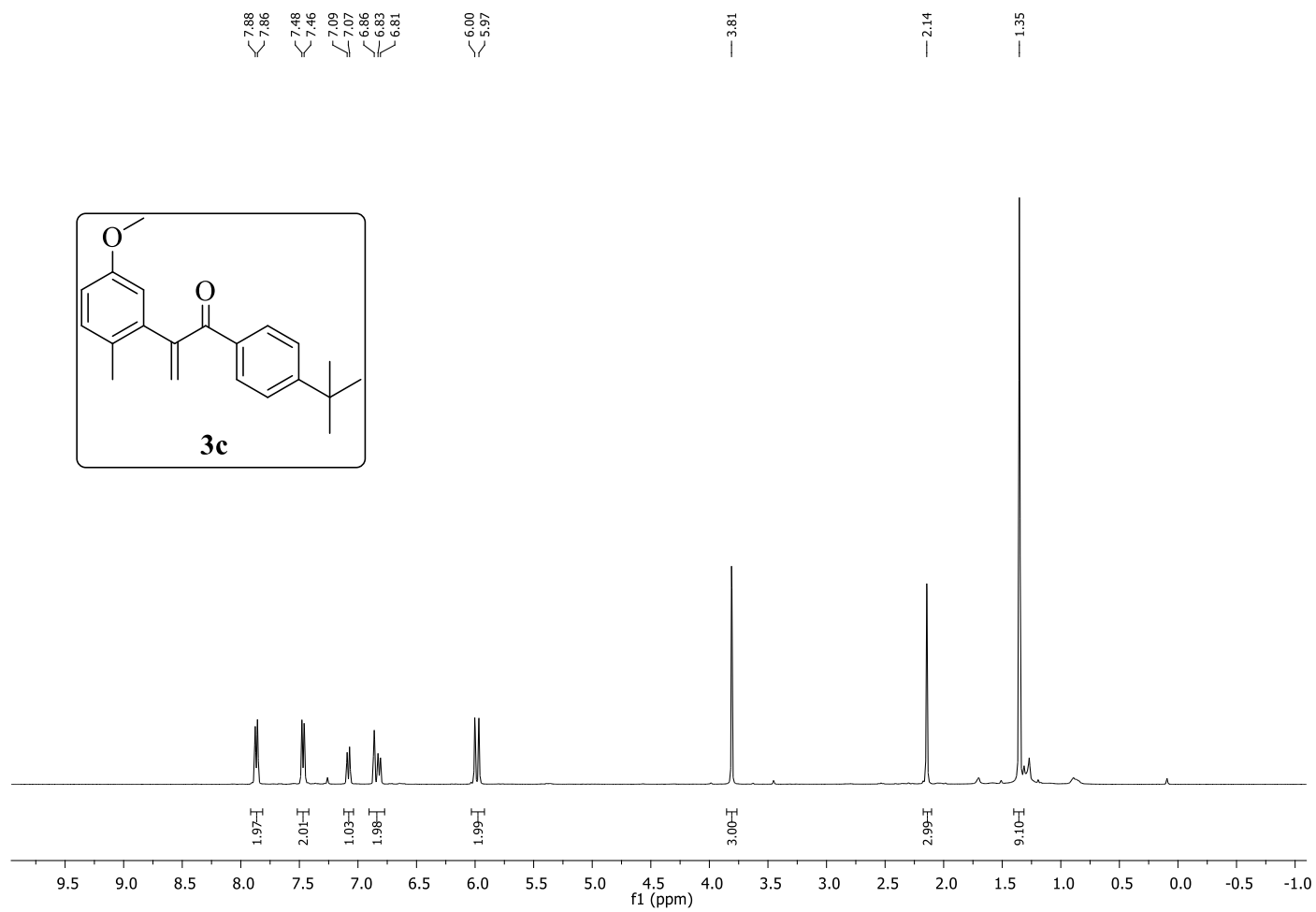


HRMS spectrum of compound **3b**

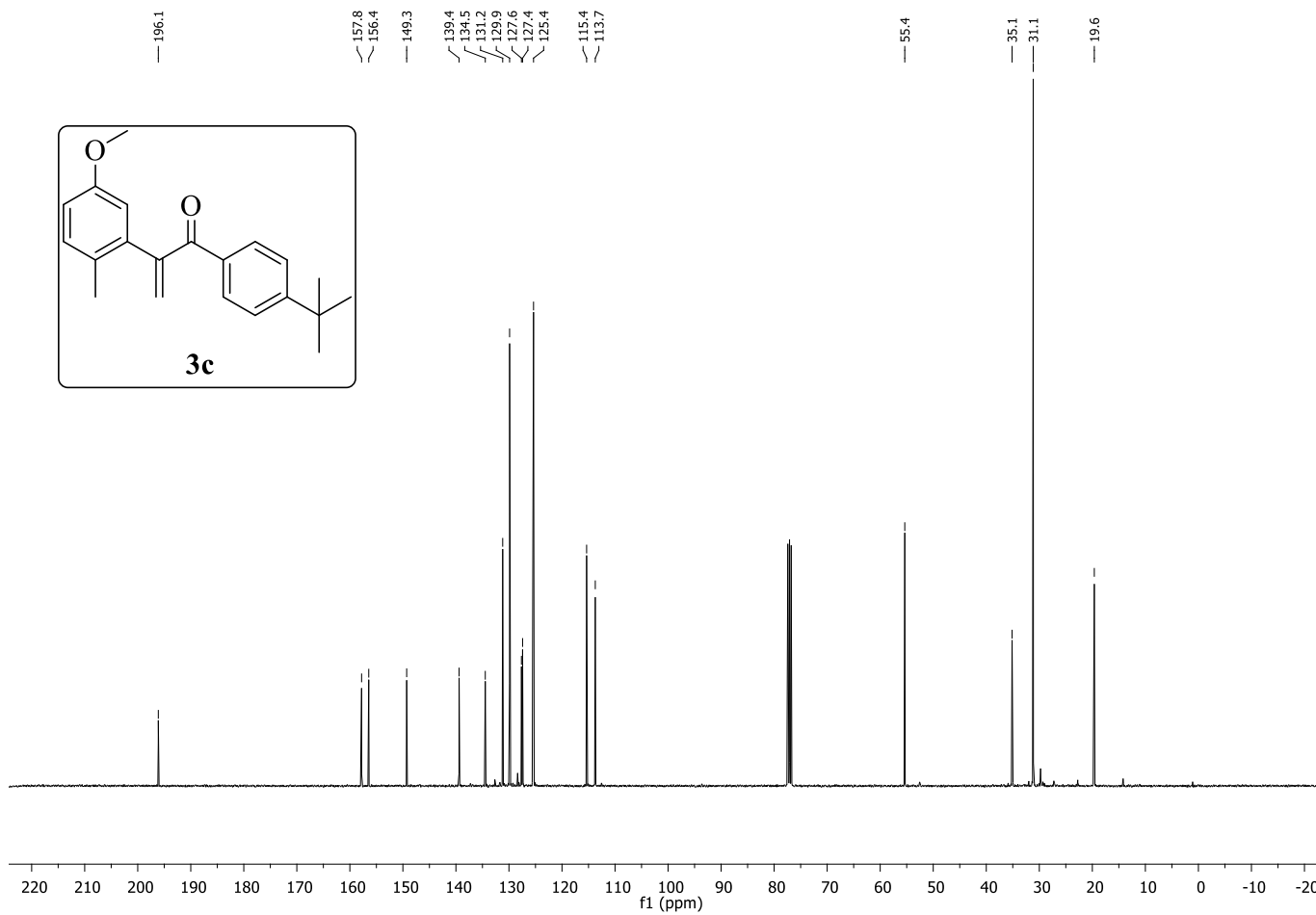
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^1H NMR spectrum of compound **3c** (400 MHz, CDCl_3)

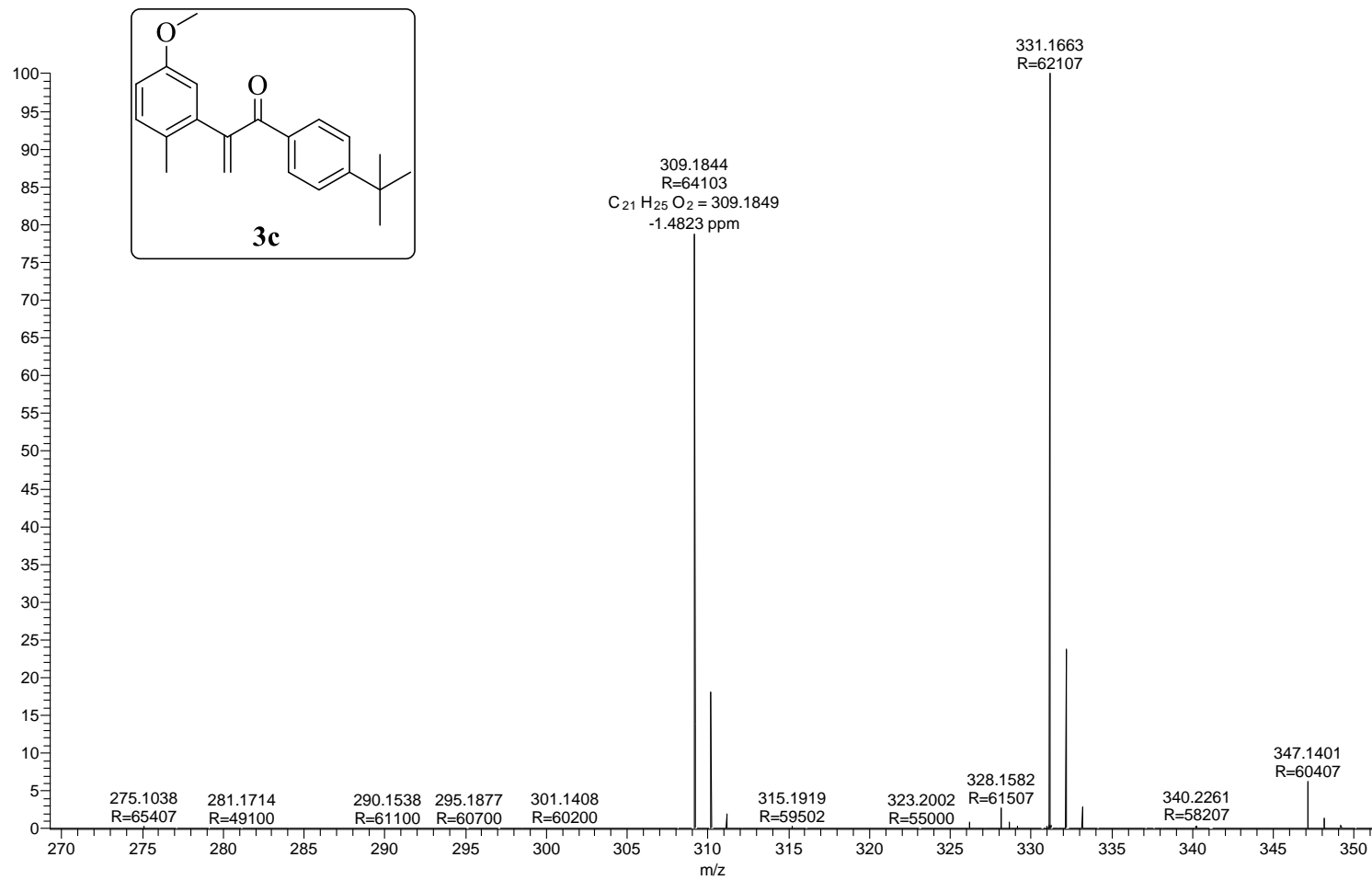


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3c** (101 MHz, CDCl_3)

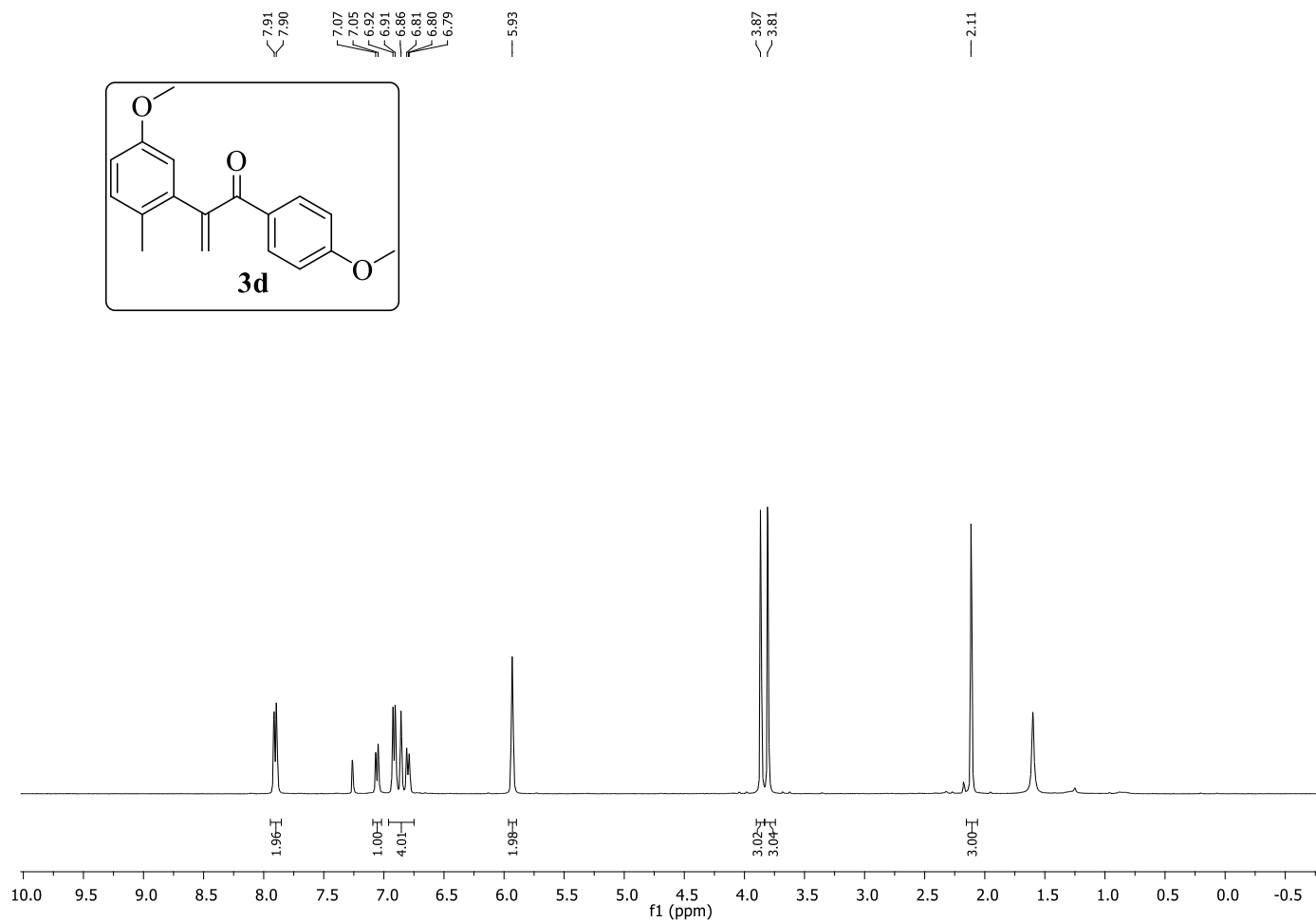


HRMS spectrum of compound 3c

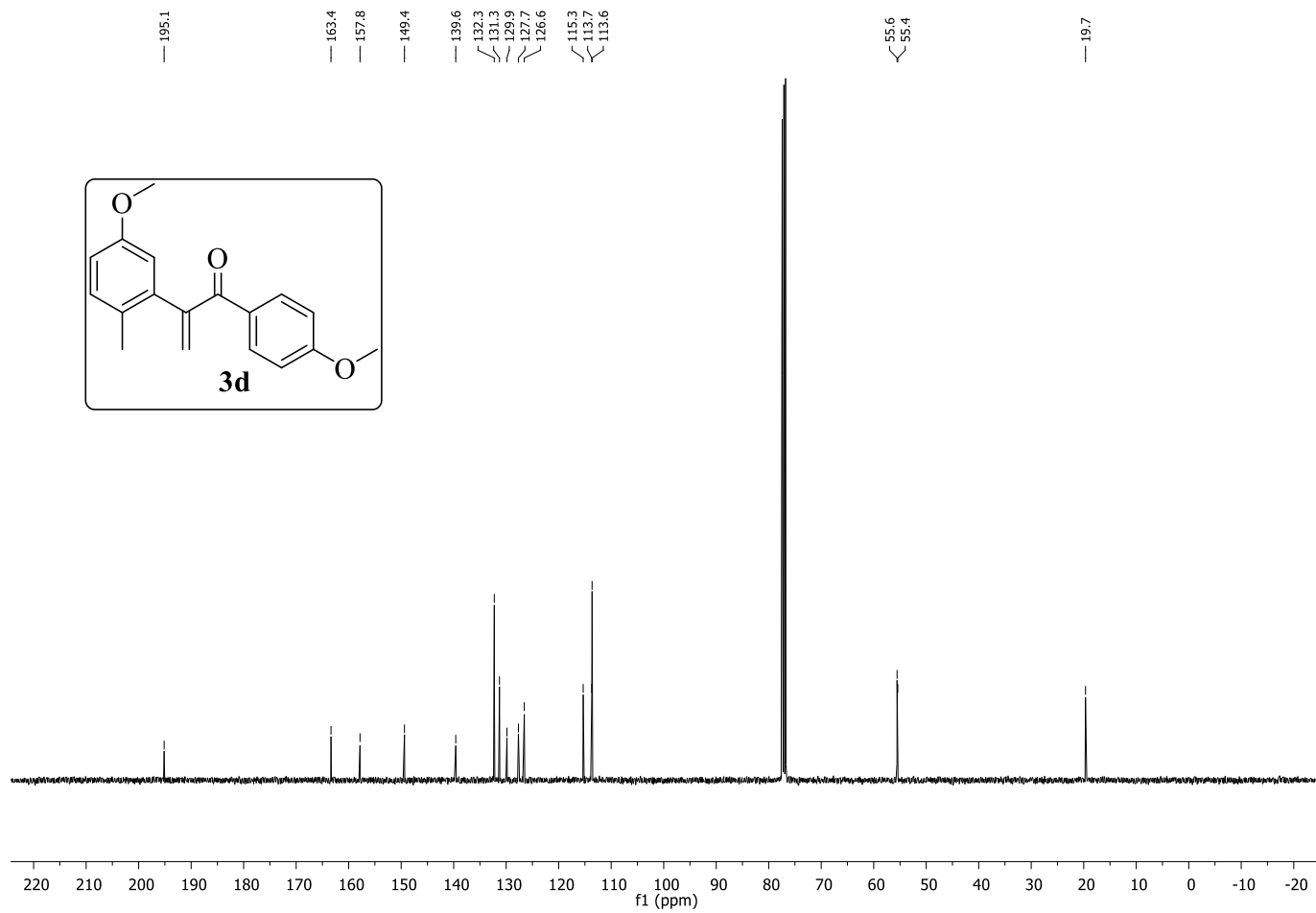
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^1H NMR spectrum of compound **3d** (400 MHz, CDCl_3)

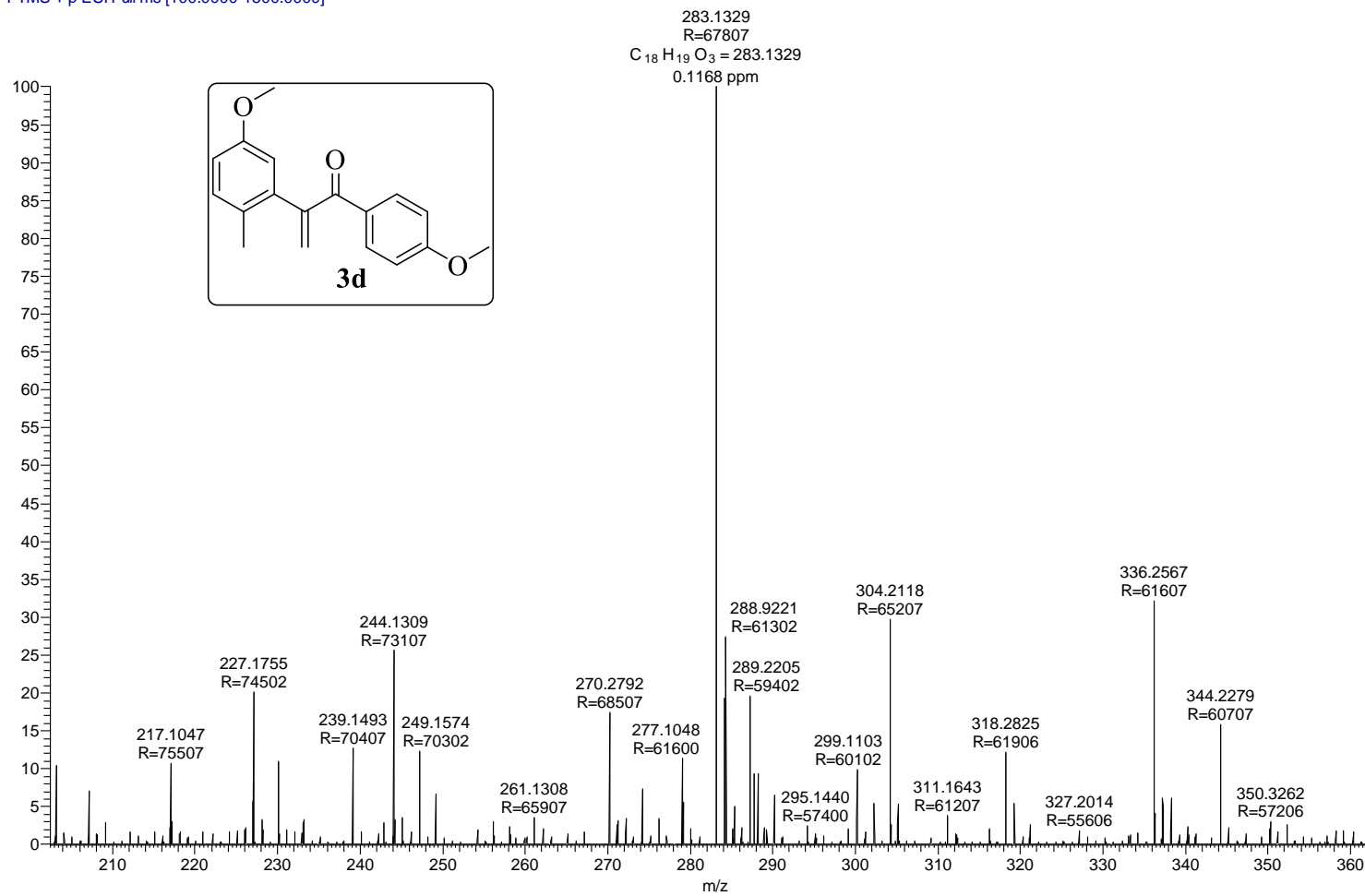


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3d** (101 MHz, CDCl_3)

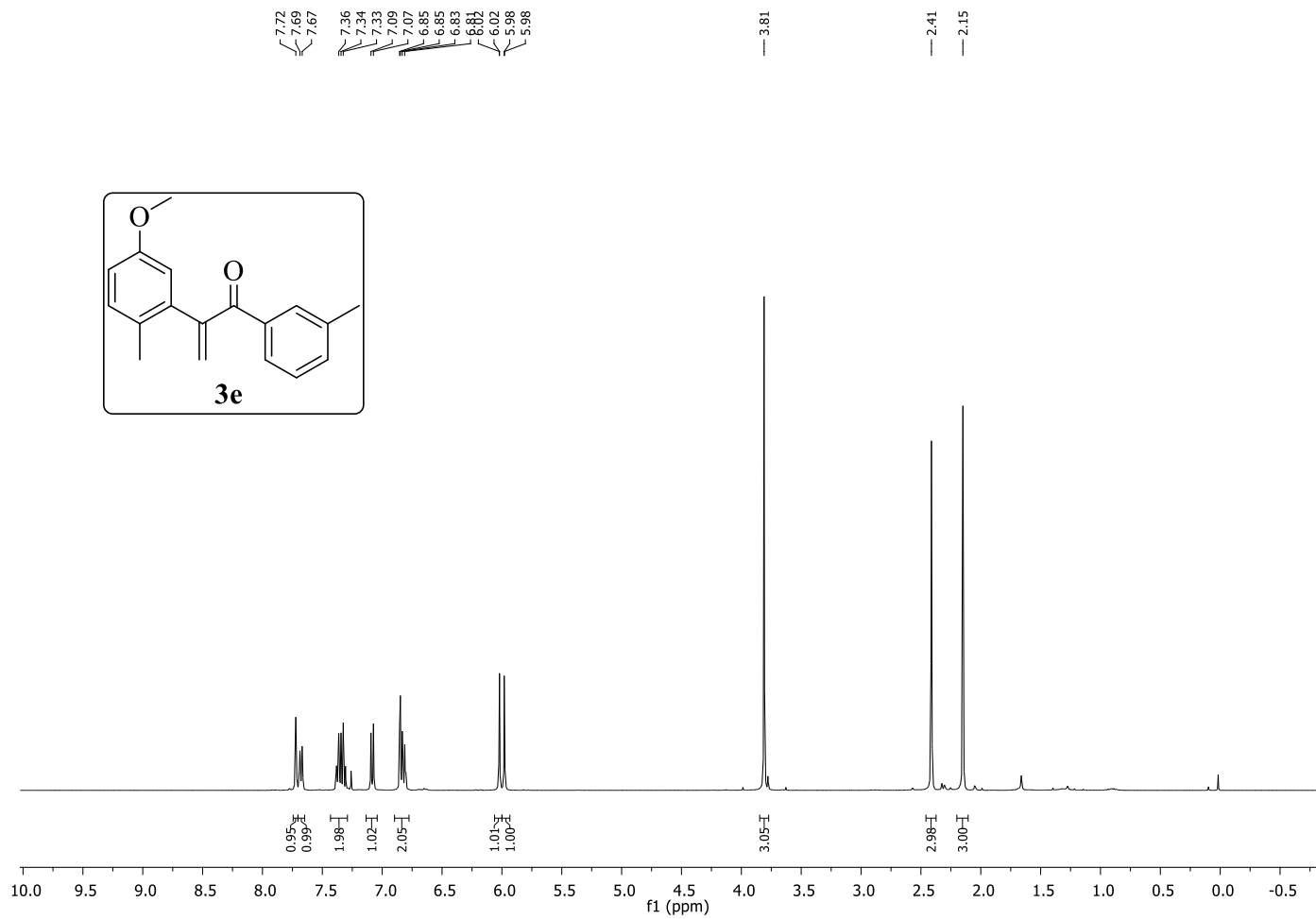


HRMS spectrum of compound **3d**

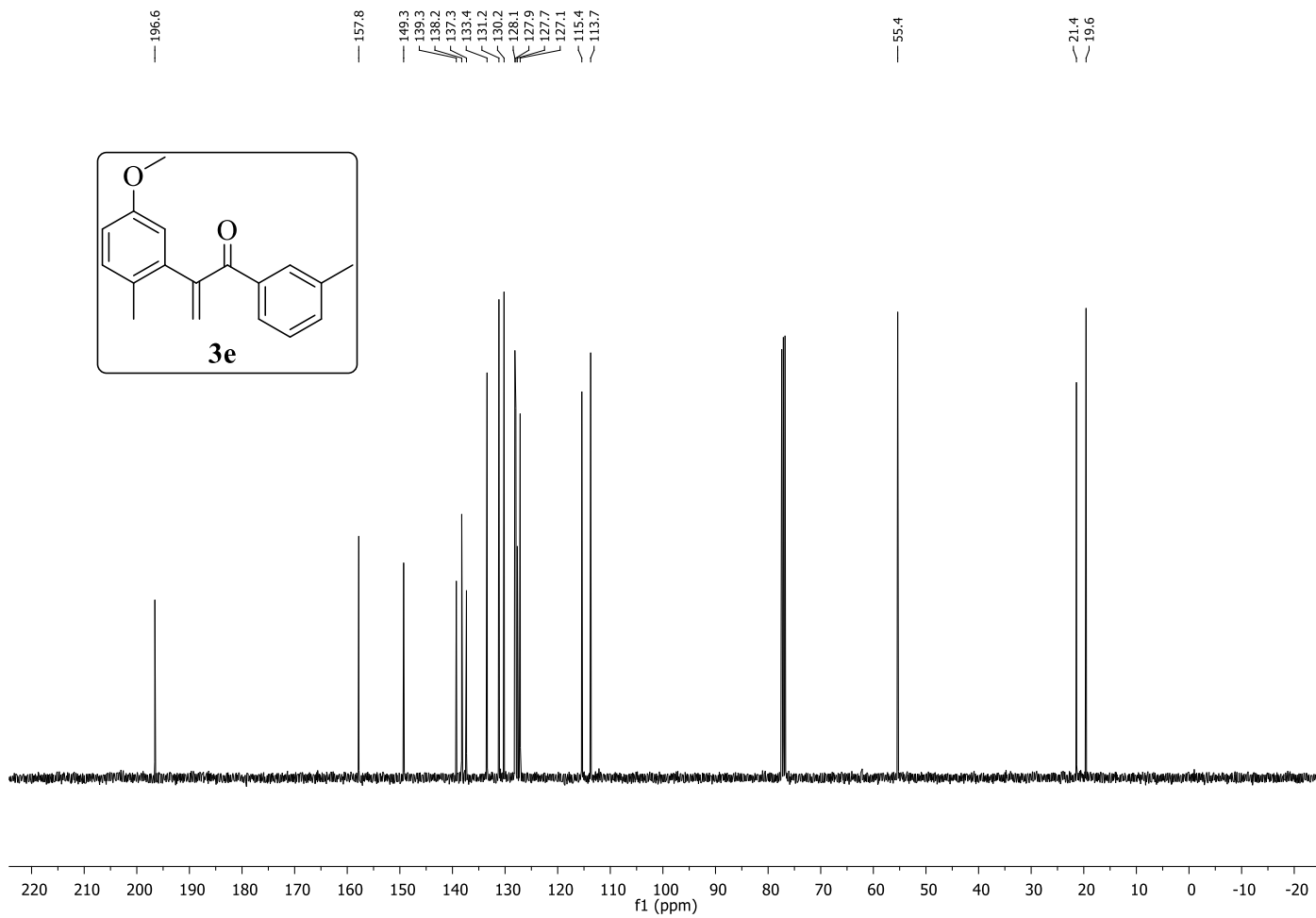
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^1H NMR spectrum of compound **3e** (400 MHz, CDCl_3)

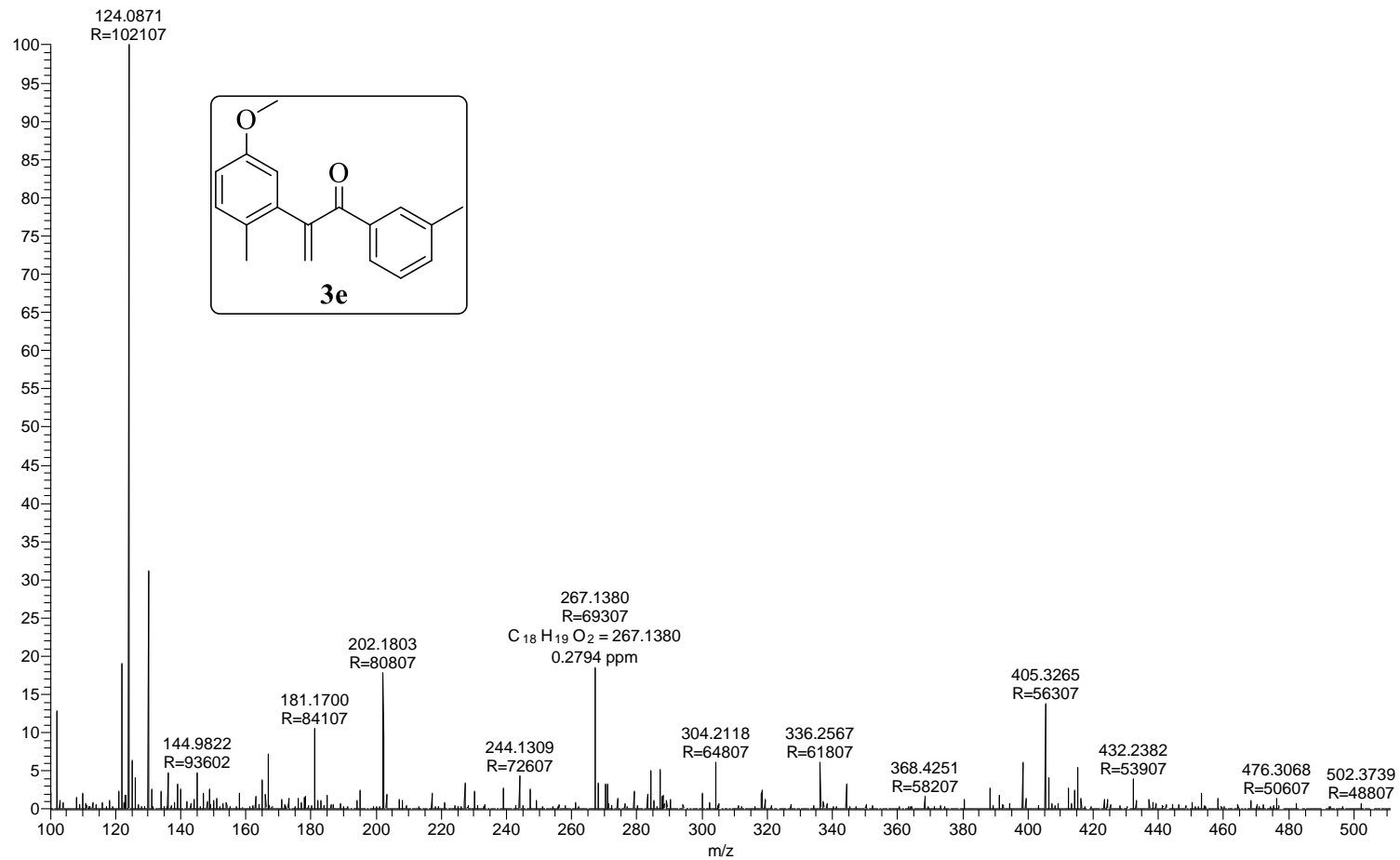


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3e** (101 MHz, CDCl_3)

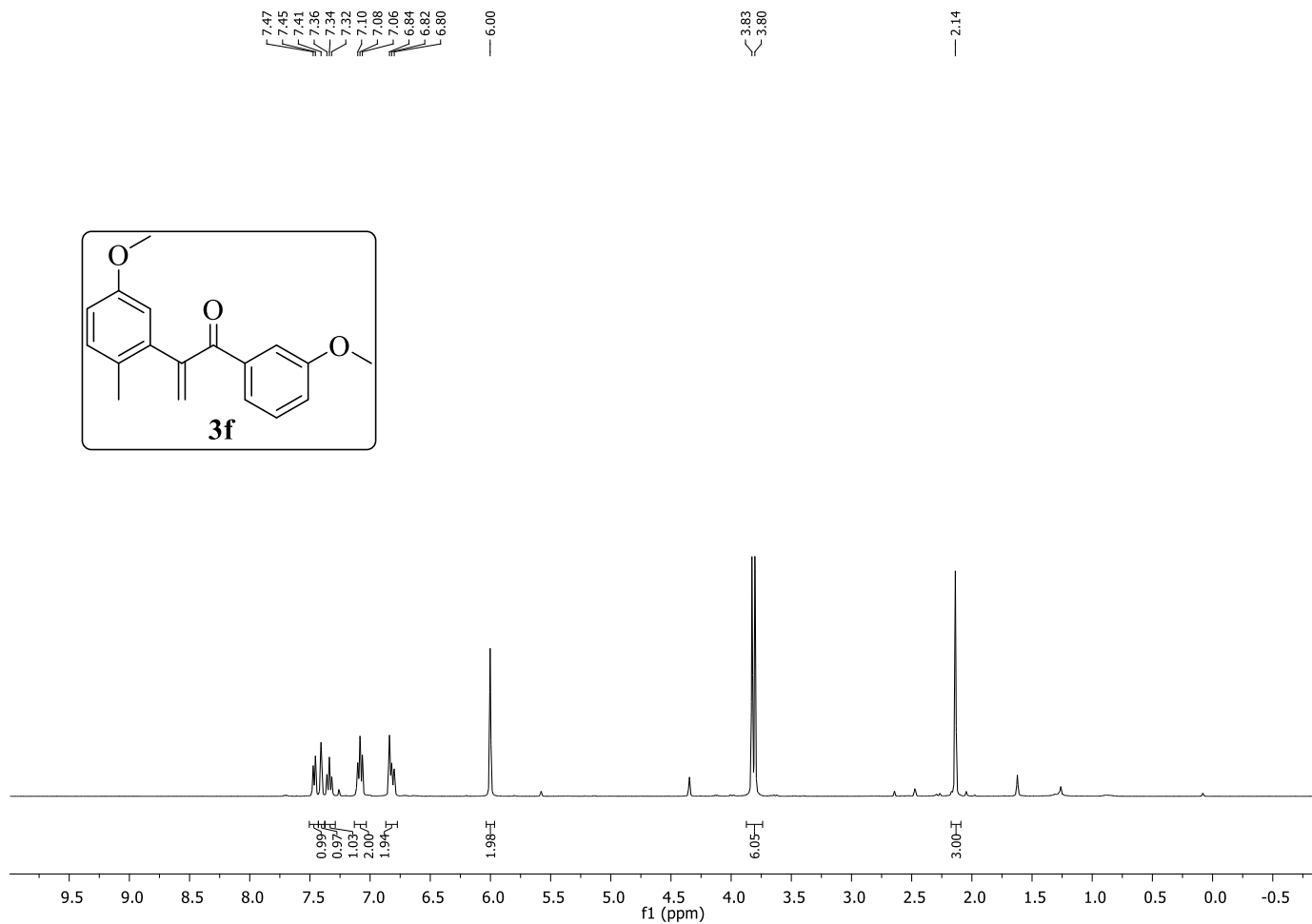


HRMS spectrum of compound 3e

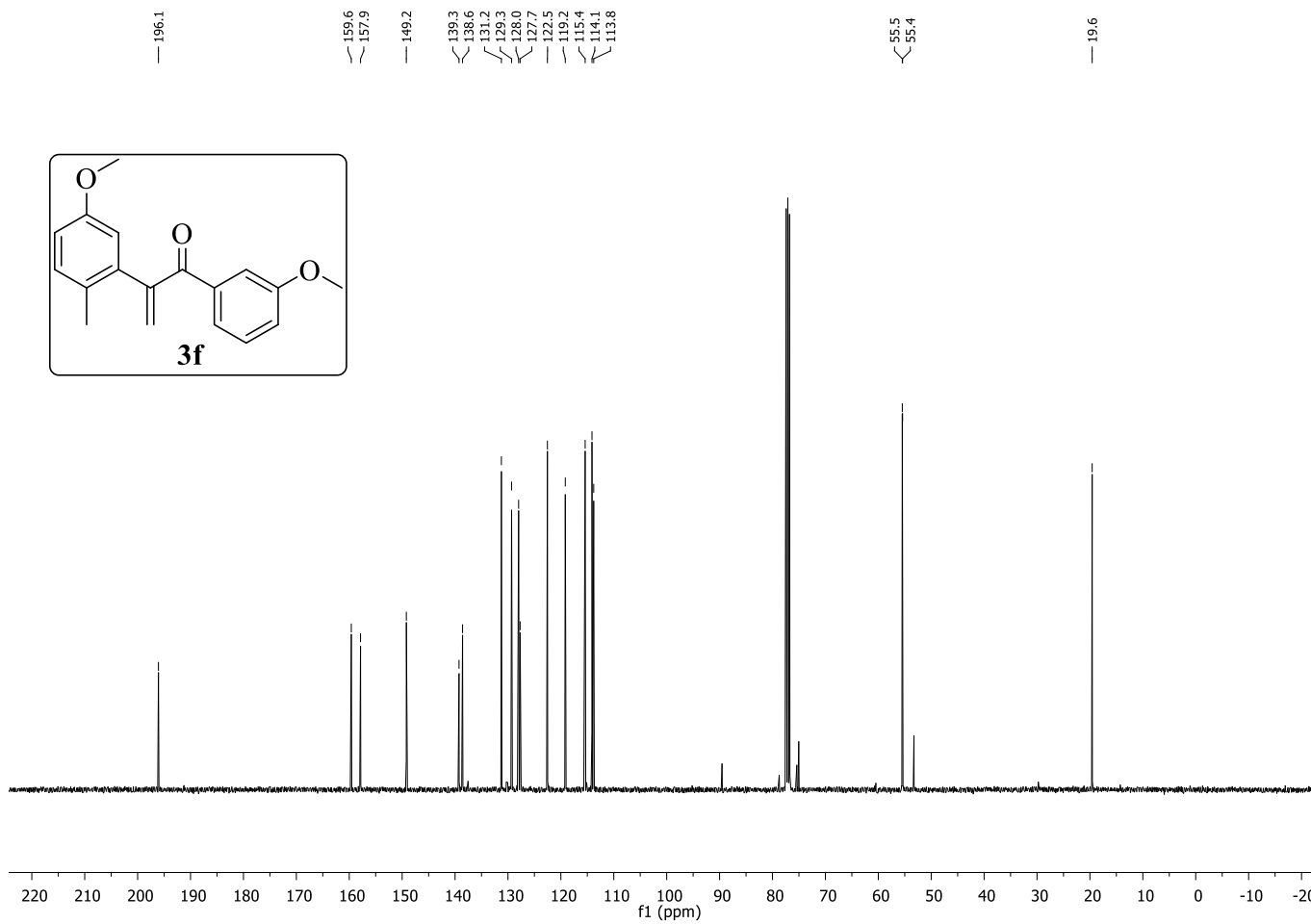
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^1H NMR spectrum of compound **3f** (400 MHz, CDCl_3)

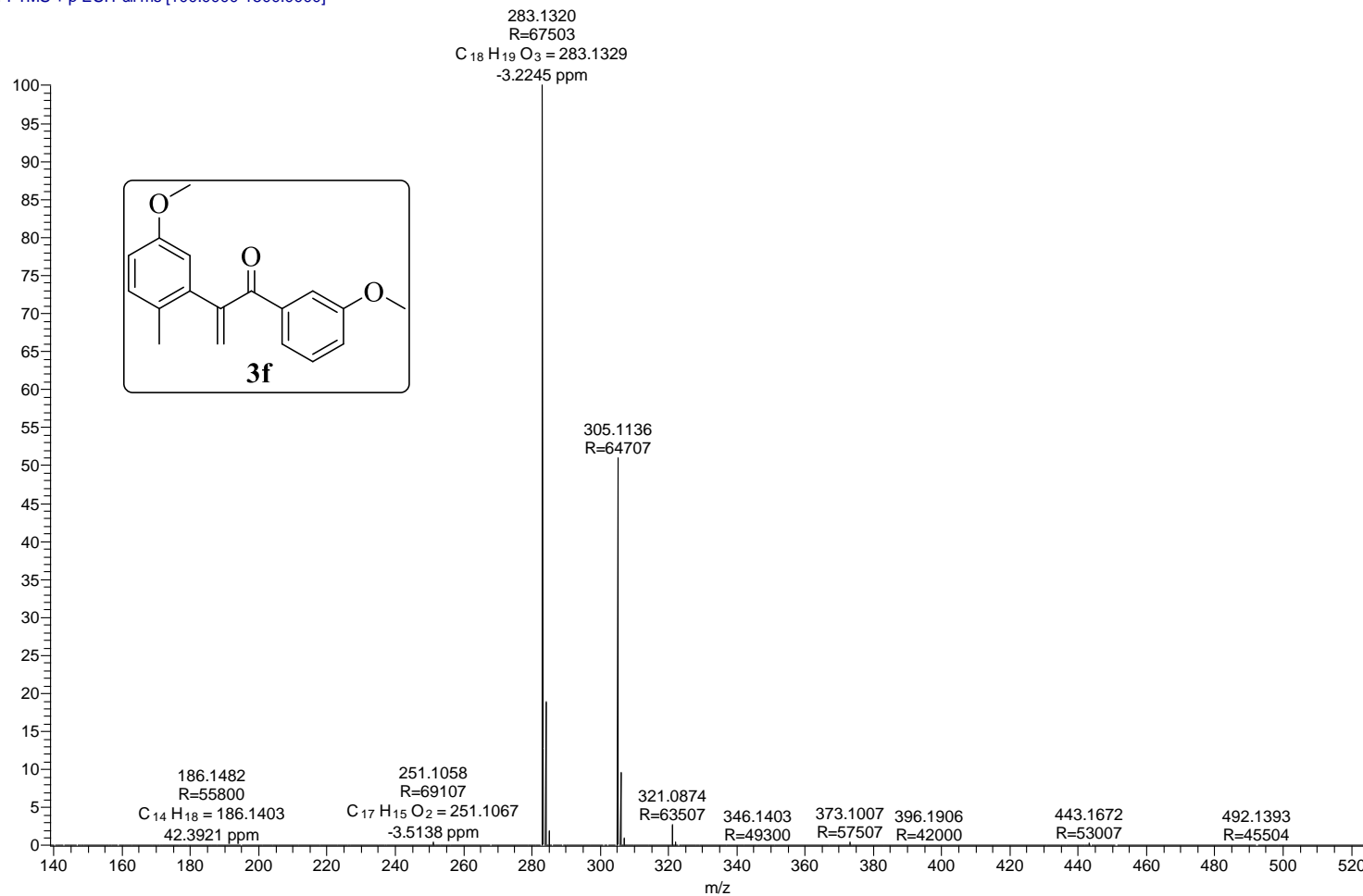


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3f** (101 MHz, CDCl_3)

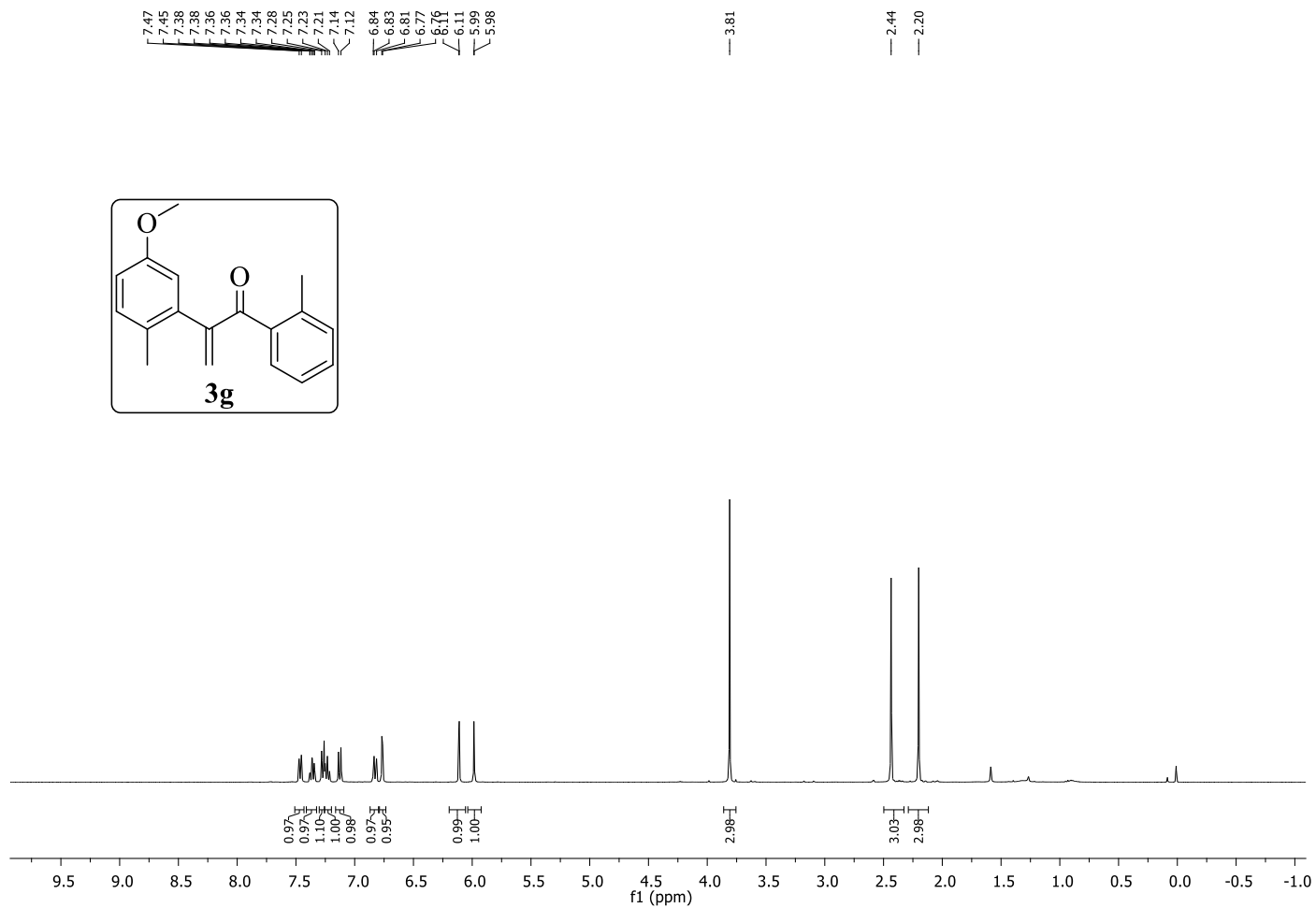


HRMS spectrum of compound 3f

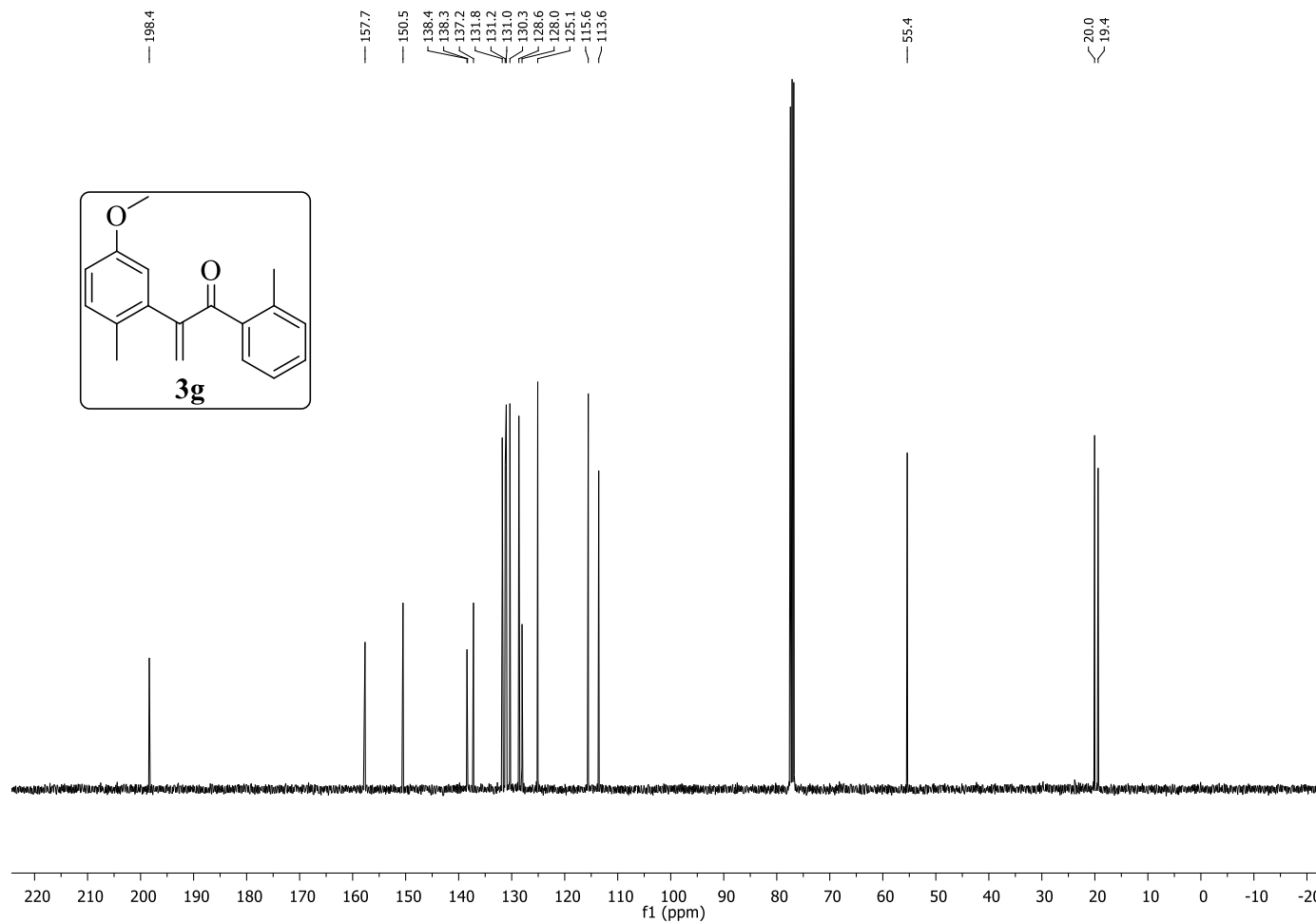
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¹H NMR spectrum of compound **3g** (400 MHz, CDCl₃)

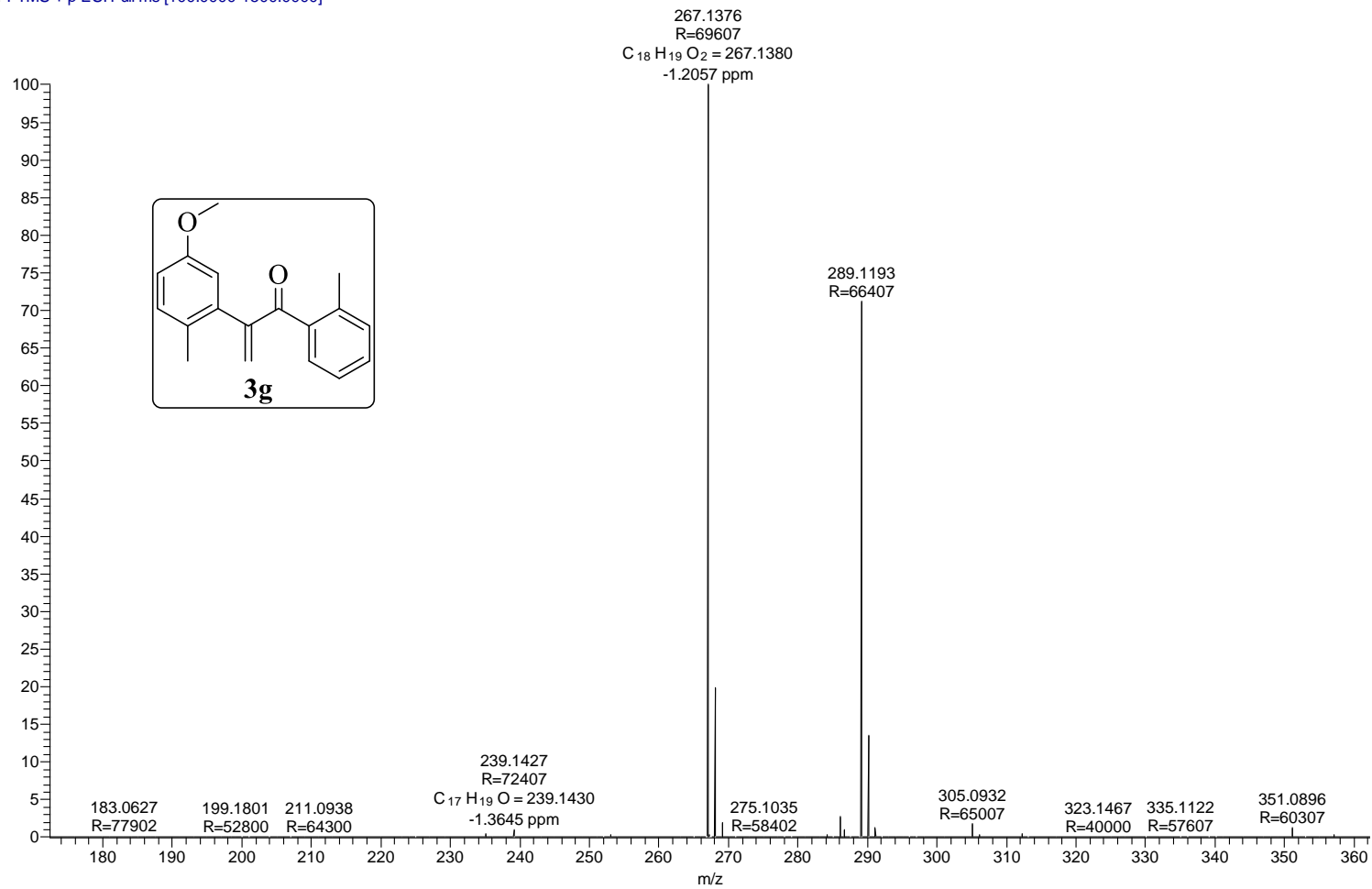


^{13}C { ^1H } NMR spectrum of compound **3g** (101 MHz, CDCl_3)

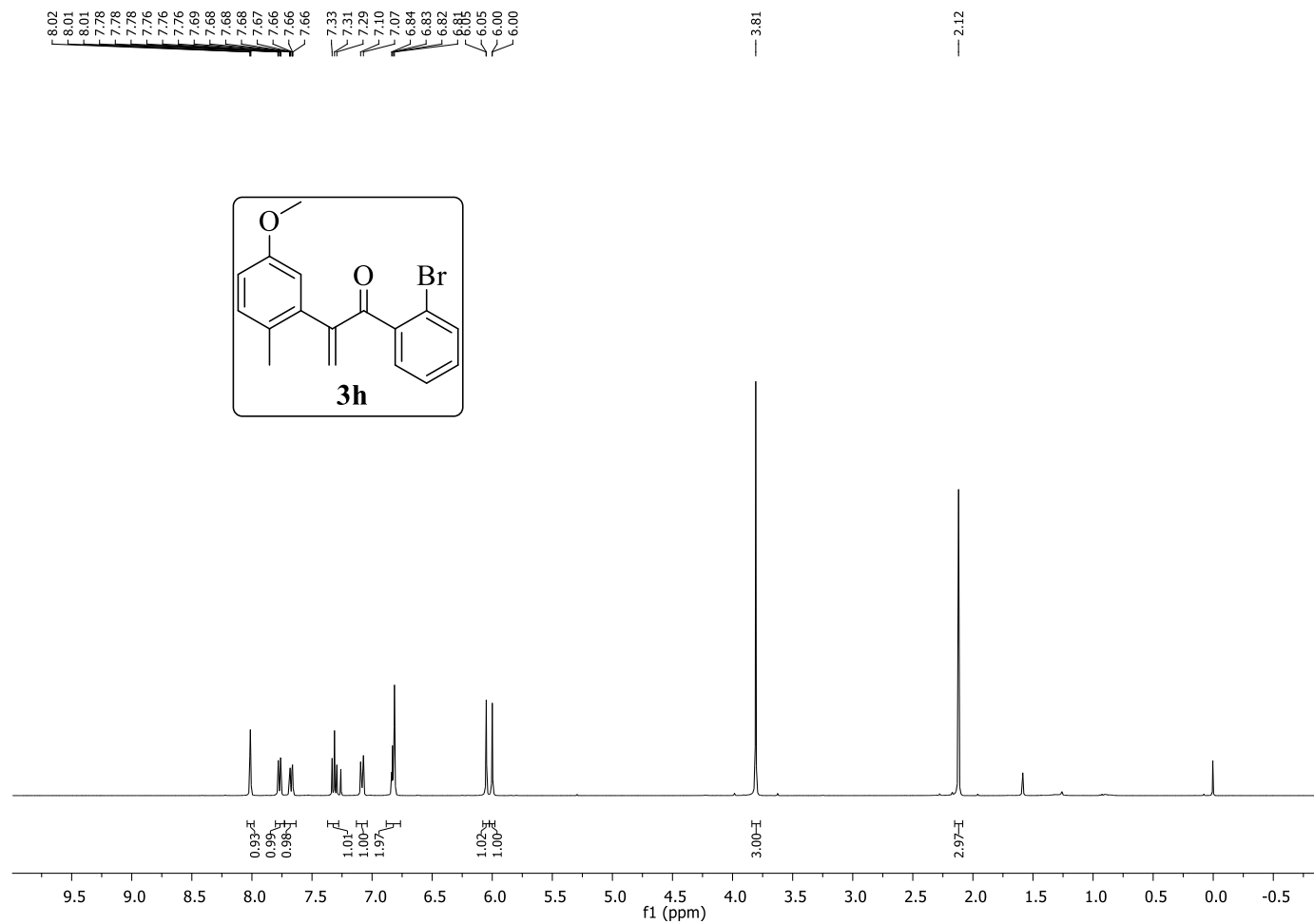


HRMS spectrum of compound **3g**

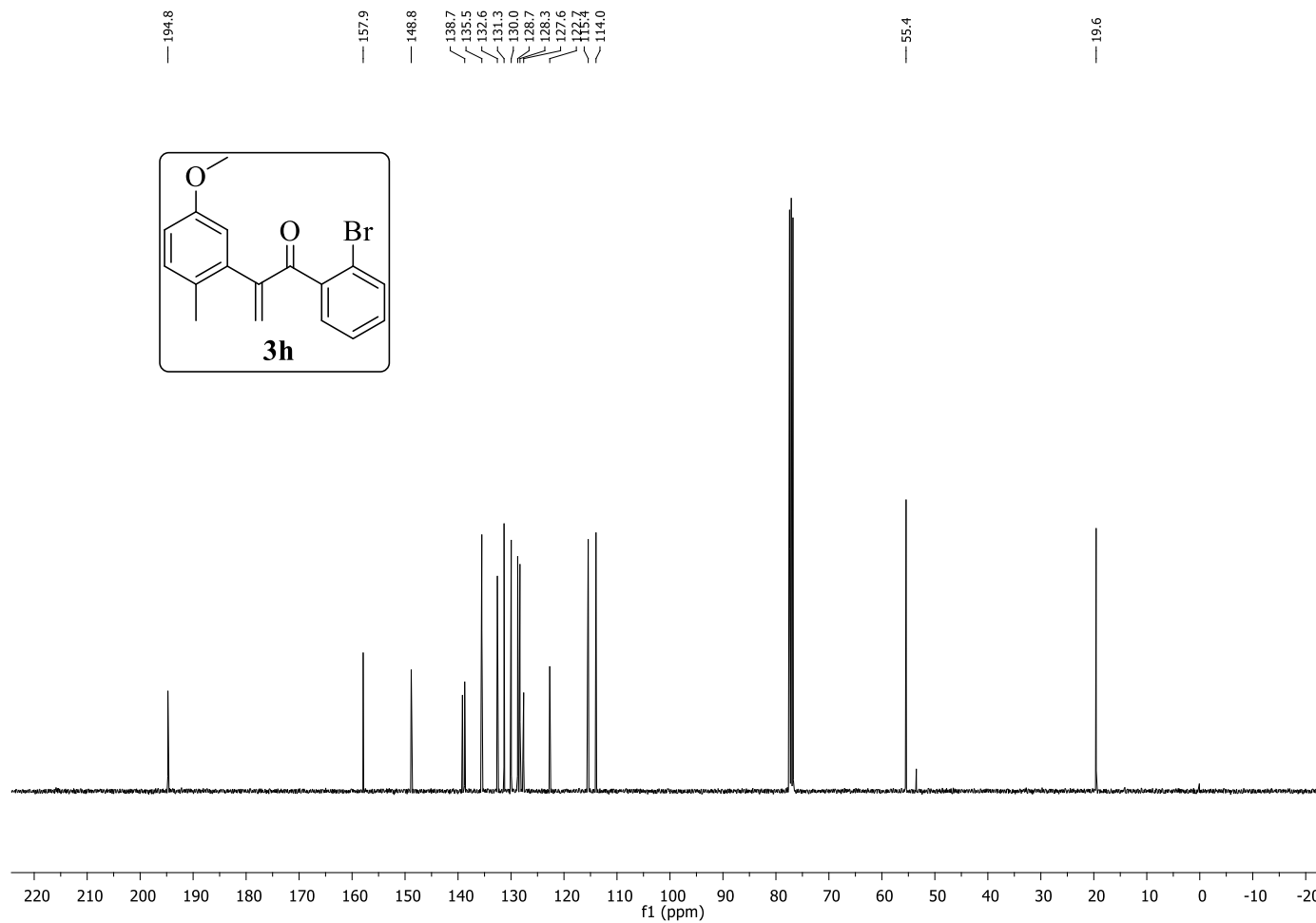
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^1H NMR spectrum of compound **3h** (400 MHz, CDCl_3)

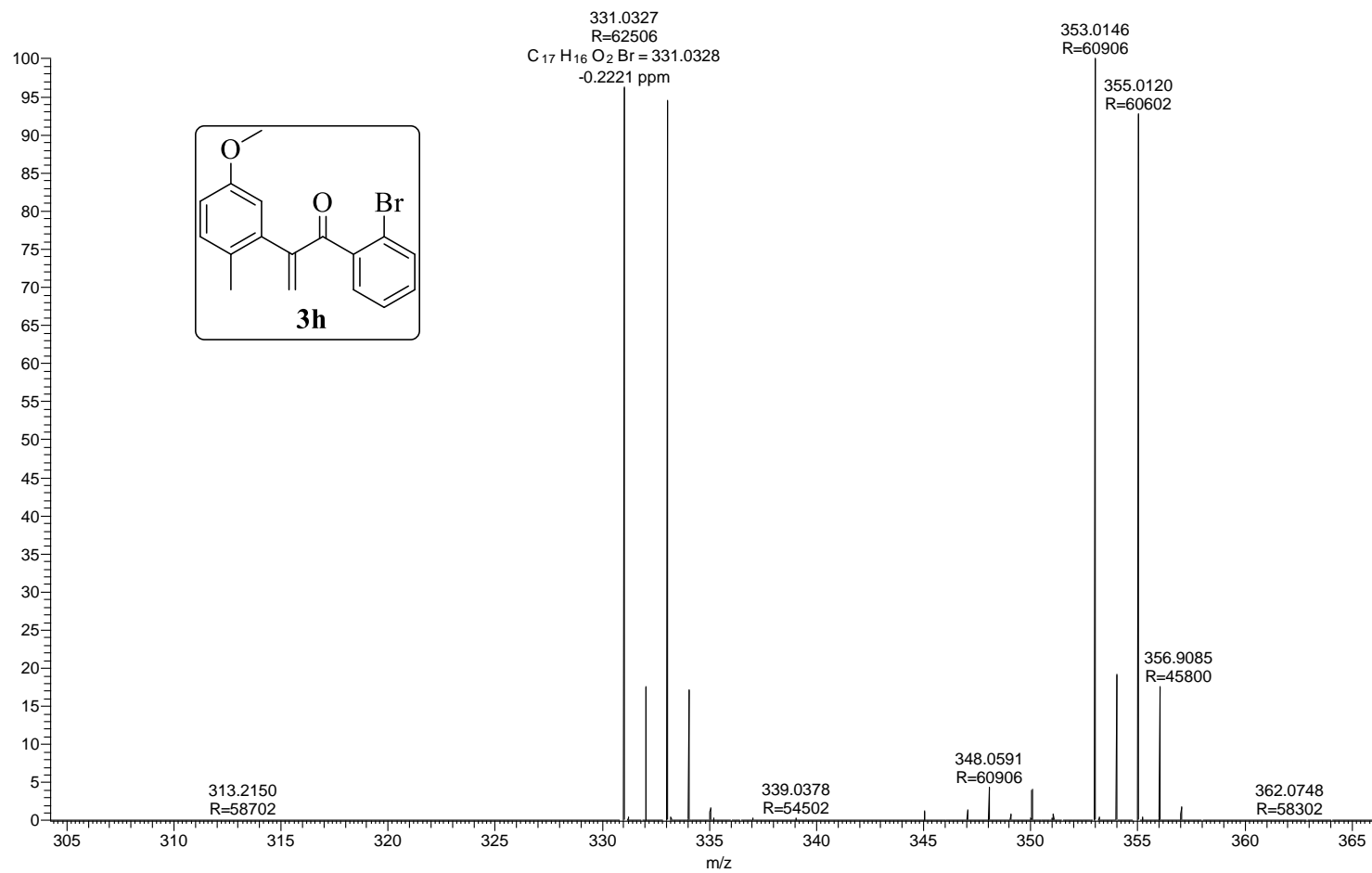


$^{13}\text{C} \{^1\text{H}\}$ NMR spectrum of compound **3h** (101 MHz, CDCl_3)

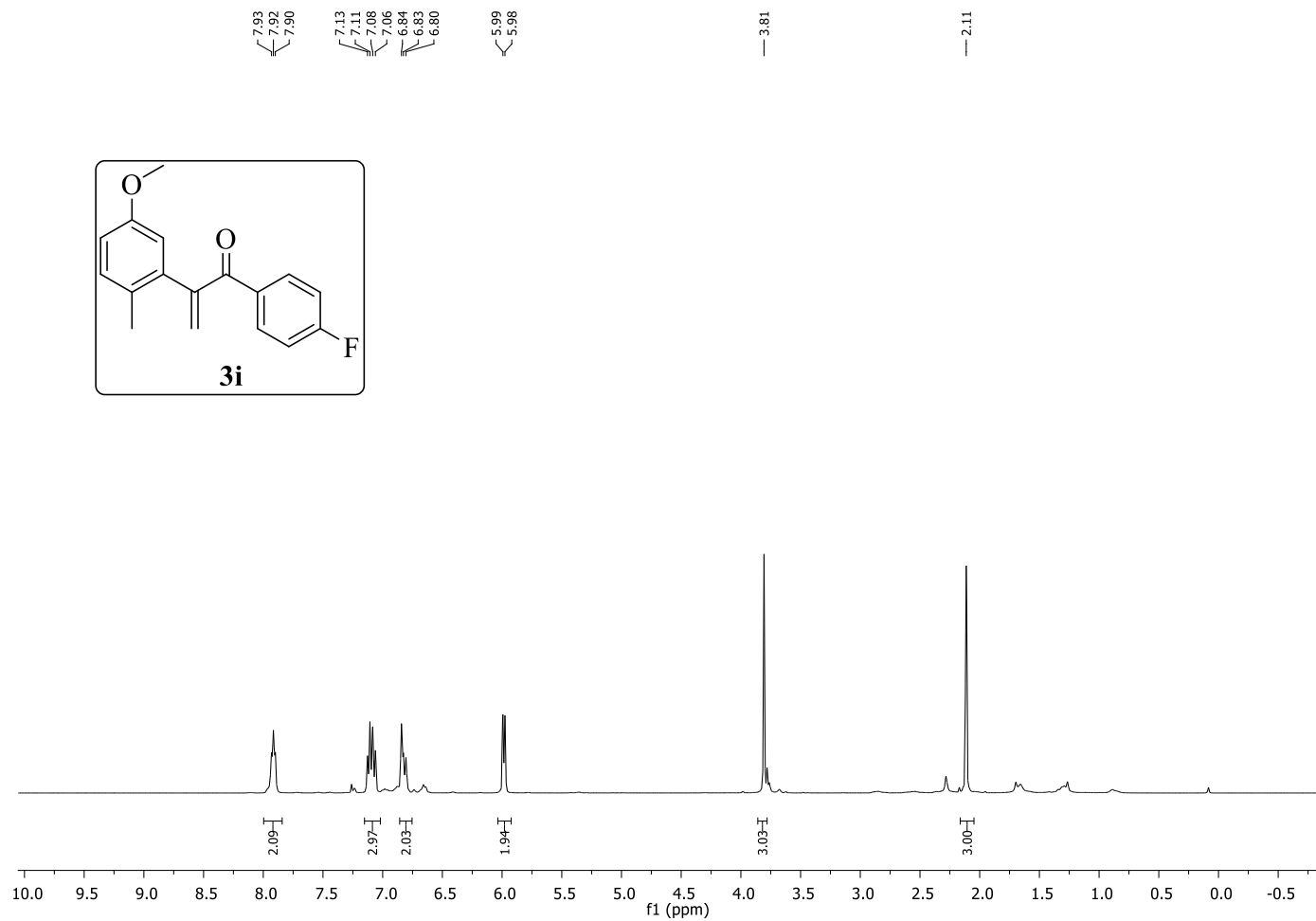


HRMS spectrum of compound **3h**

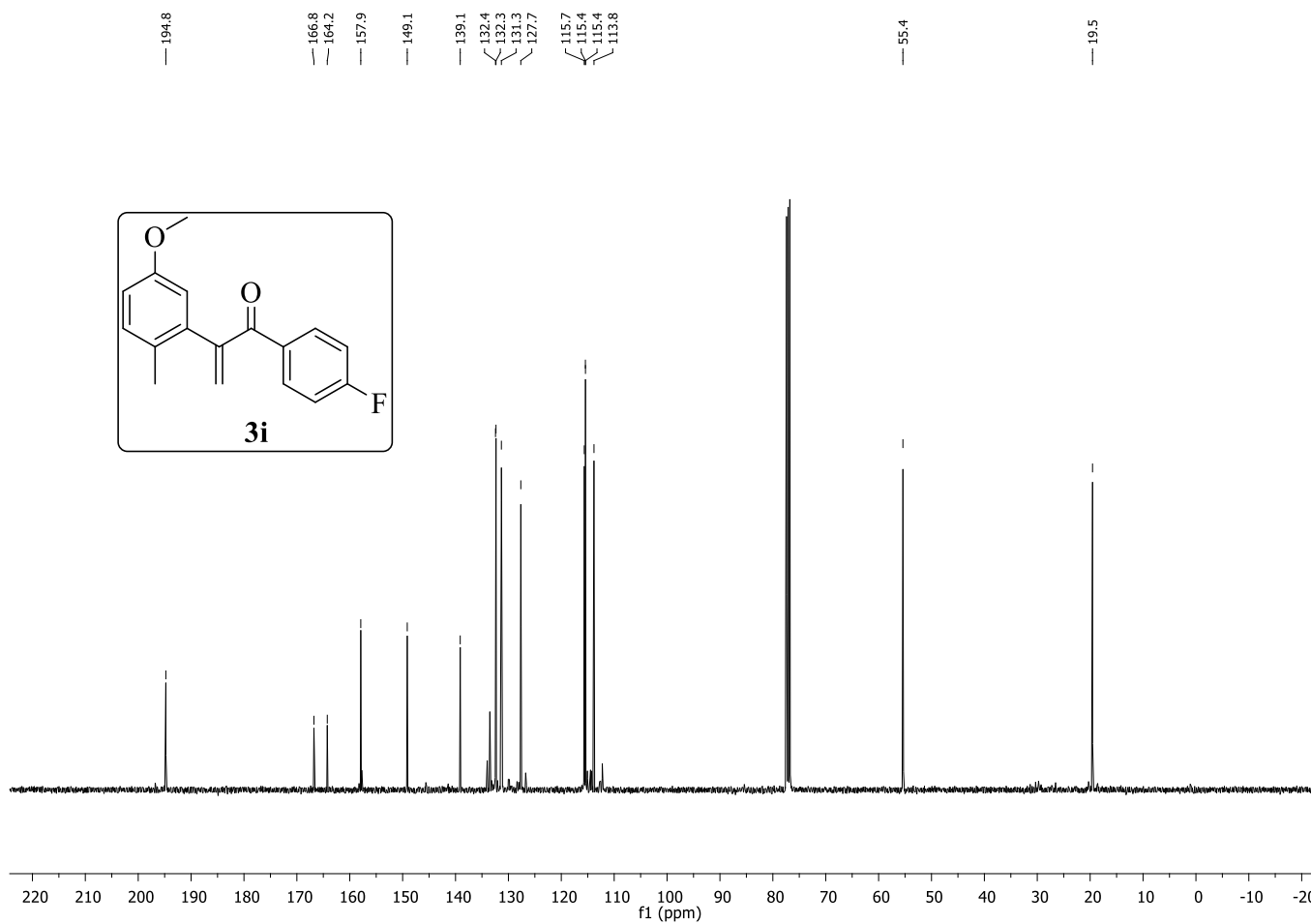
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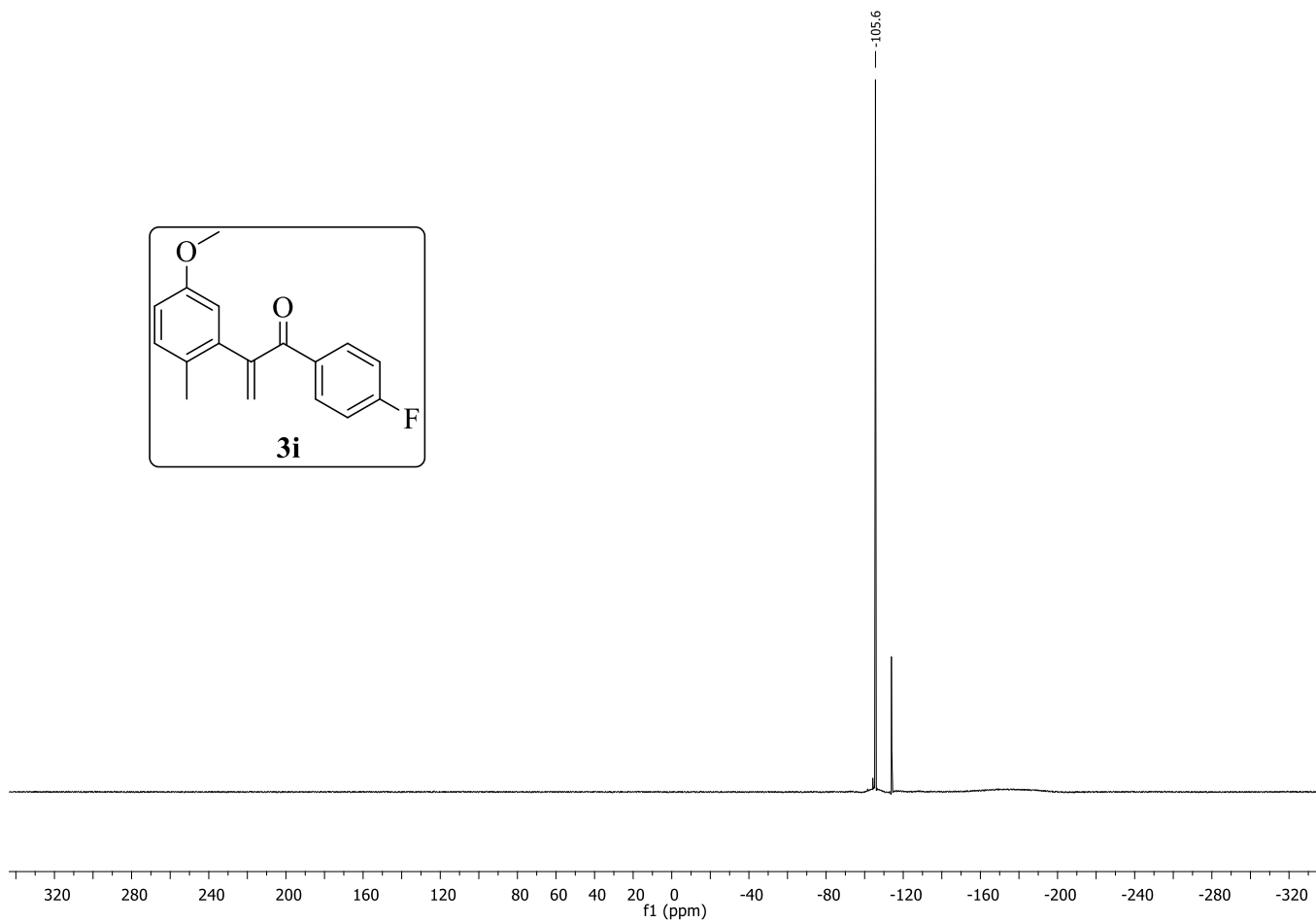
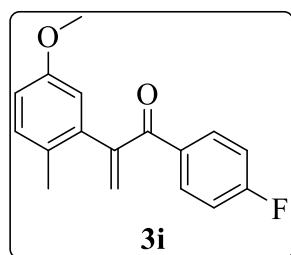
^1H NMR spectrum of compound **3i** (400 MHz, CDCl_3)



^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3i** (101 MHz, CDCl_3)

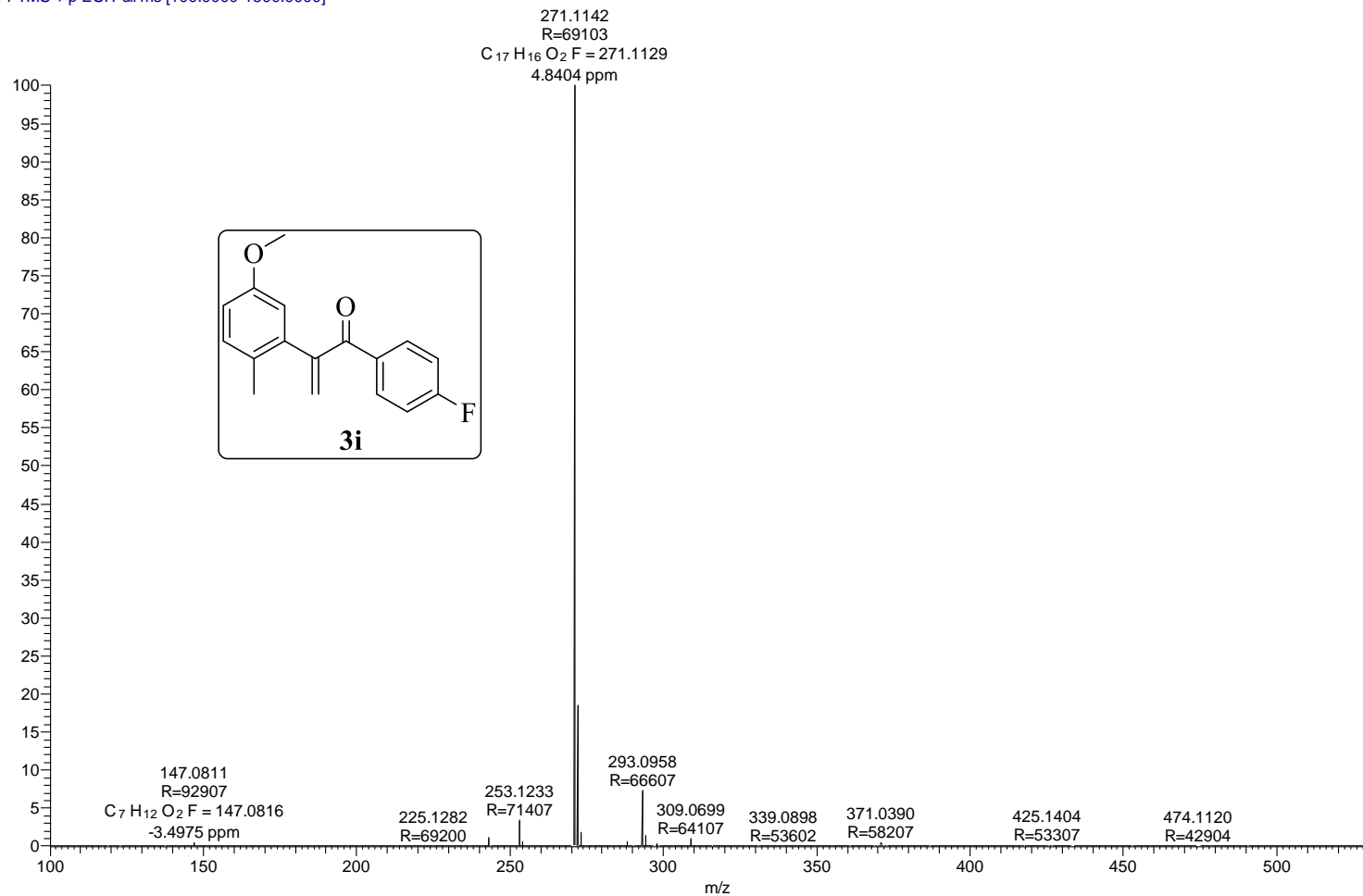


^{19}F NMR spectrum of compound **3i** (400 MHz, CDCl_3)

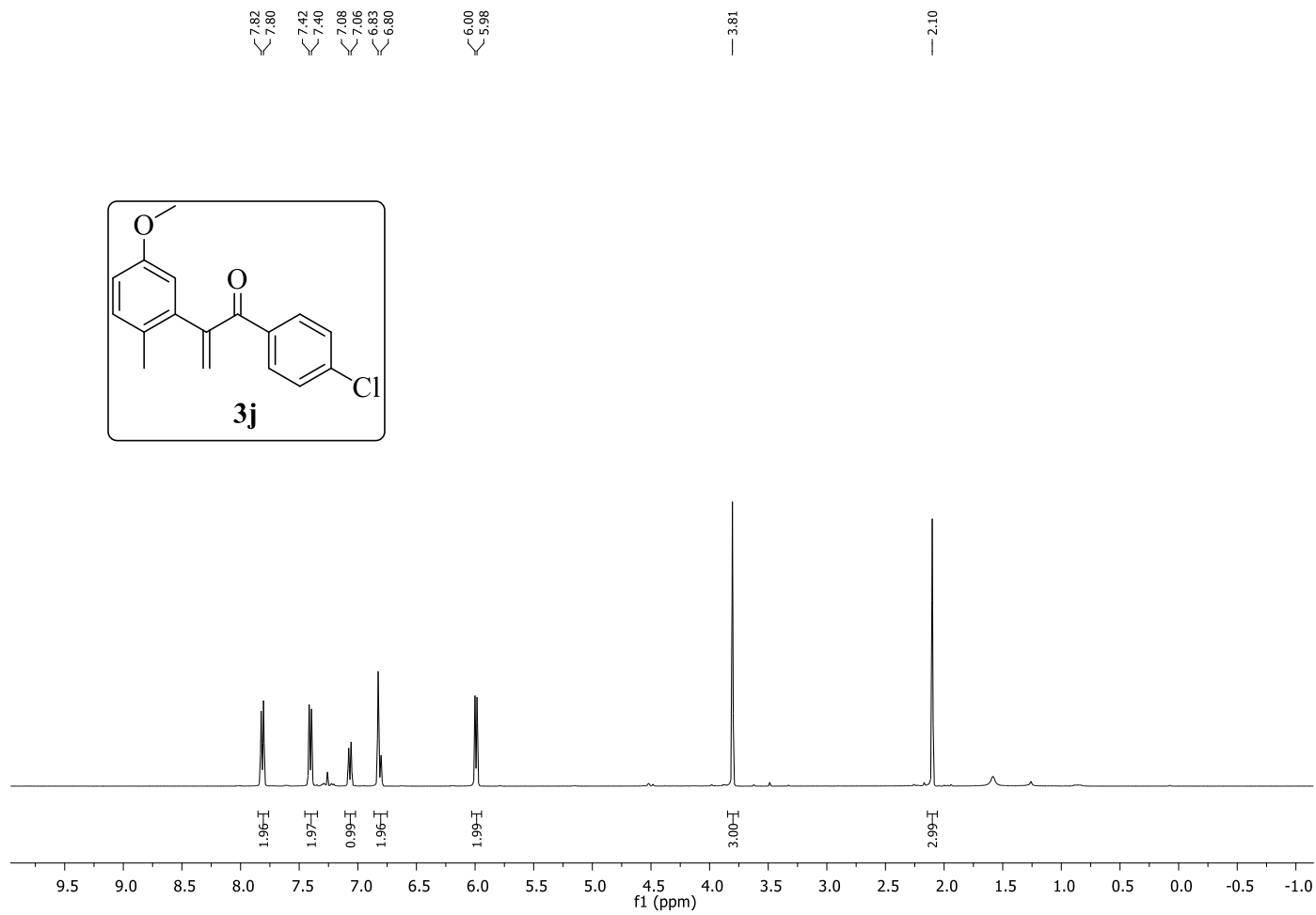


HRMS spectrum of compound **3i**

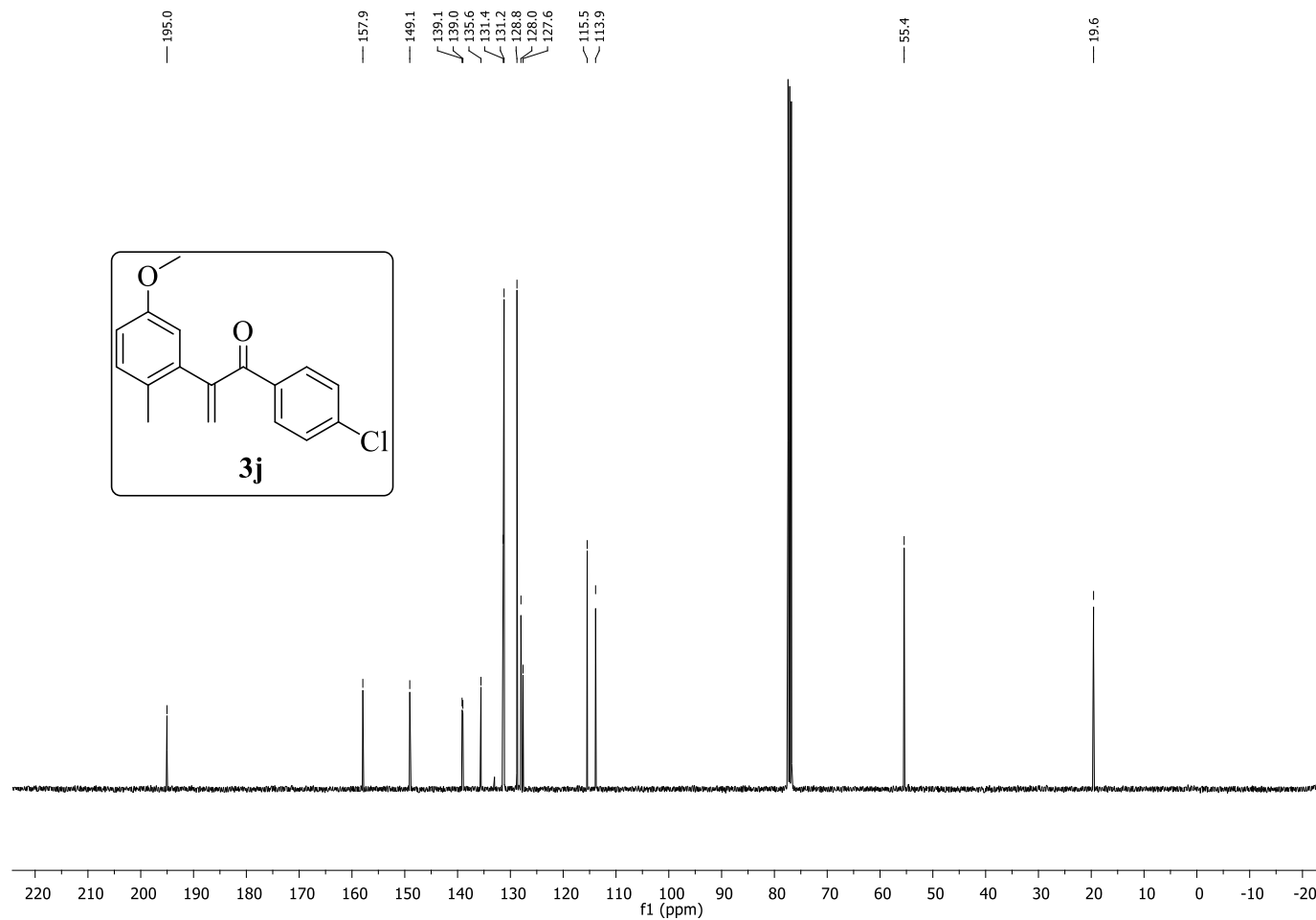
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^1H NMR spectrum of compound **3j** (400 MHz, CDCl_3)

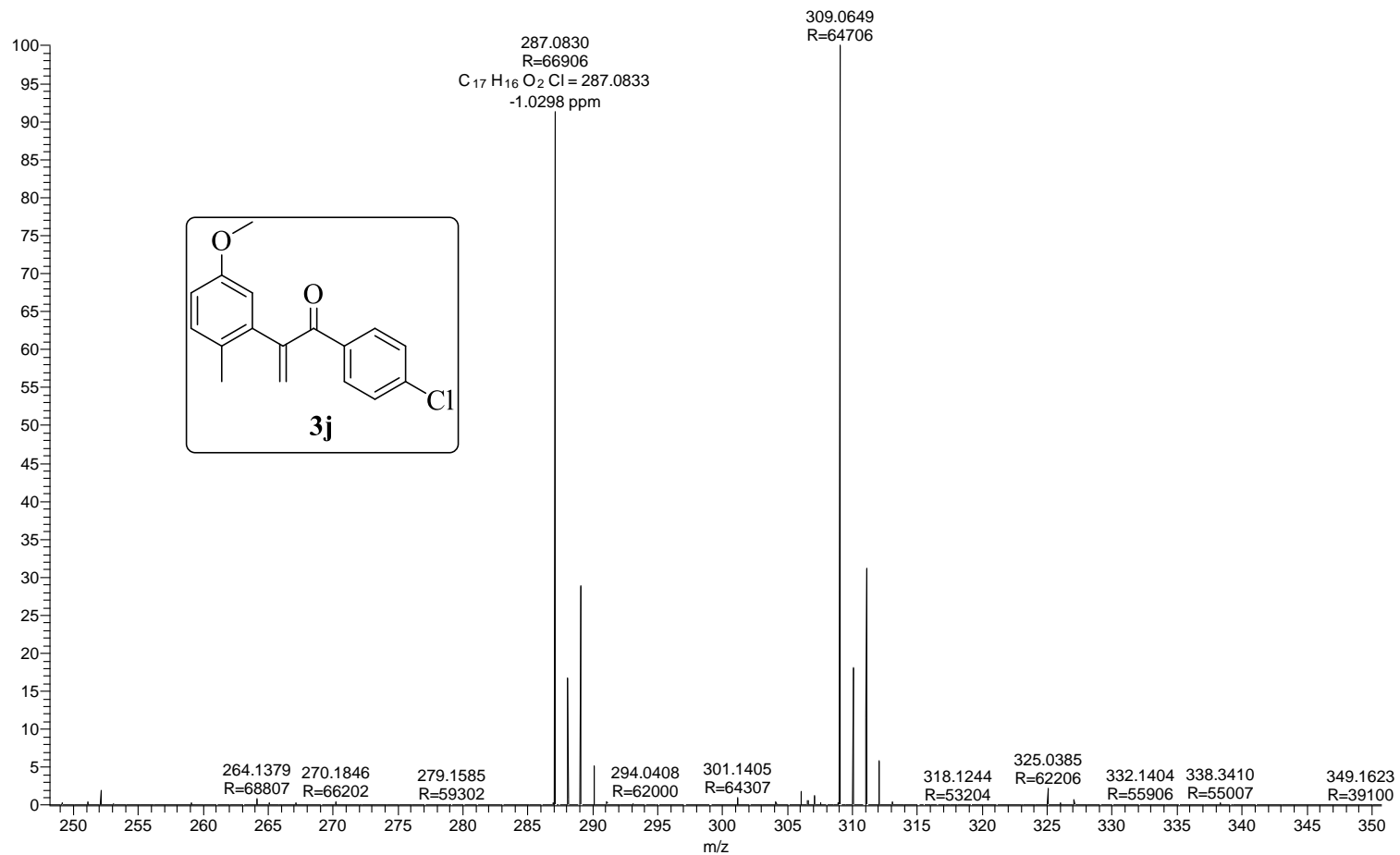


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3j** (101 MHz, CDCl_3)

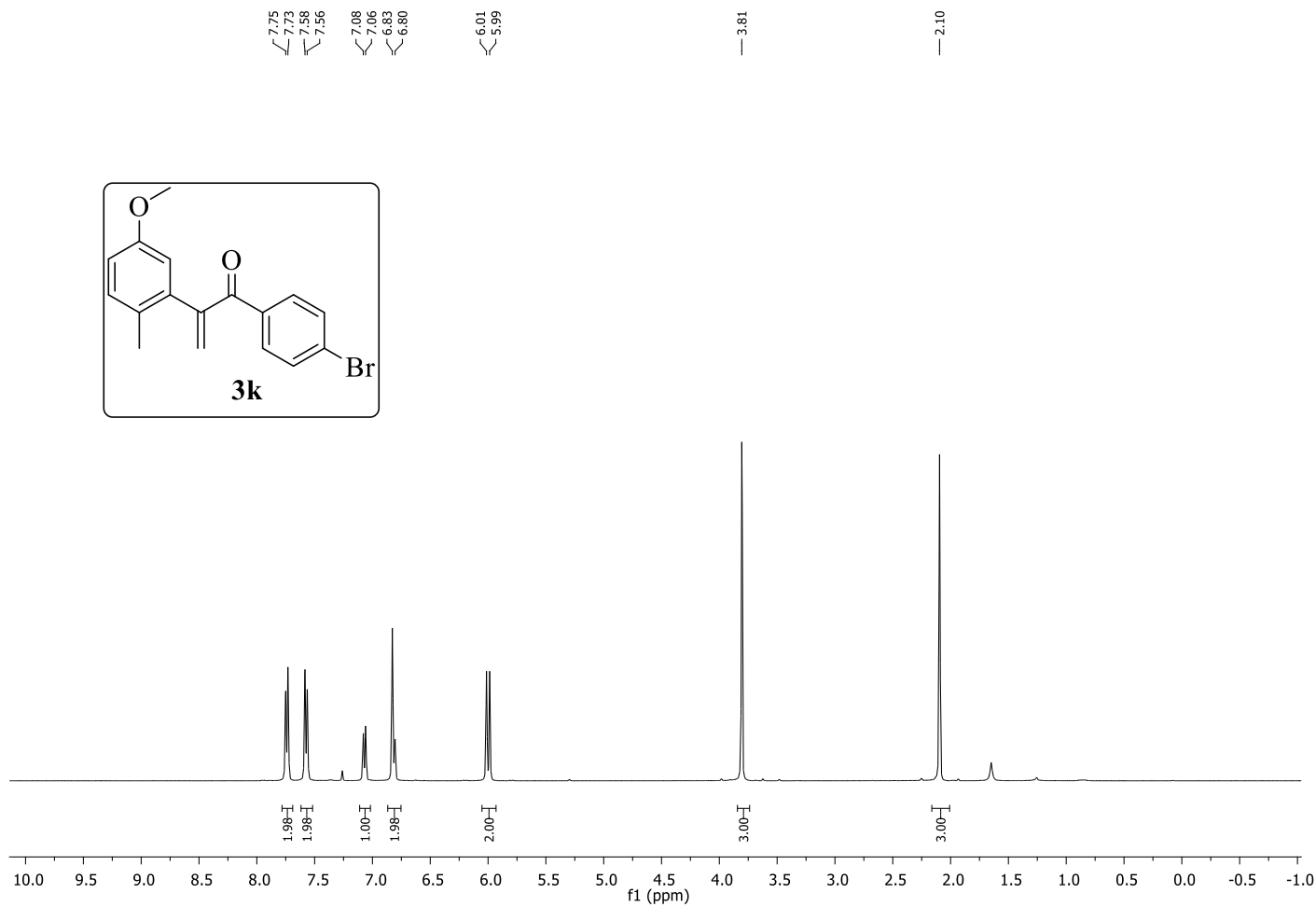


HRMS spectrum of compound 3j

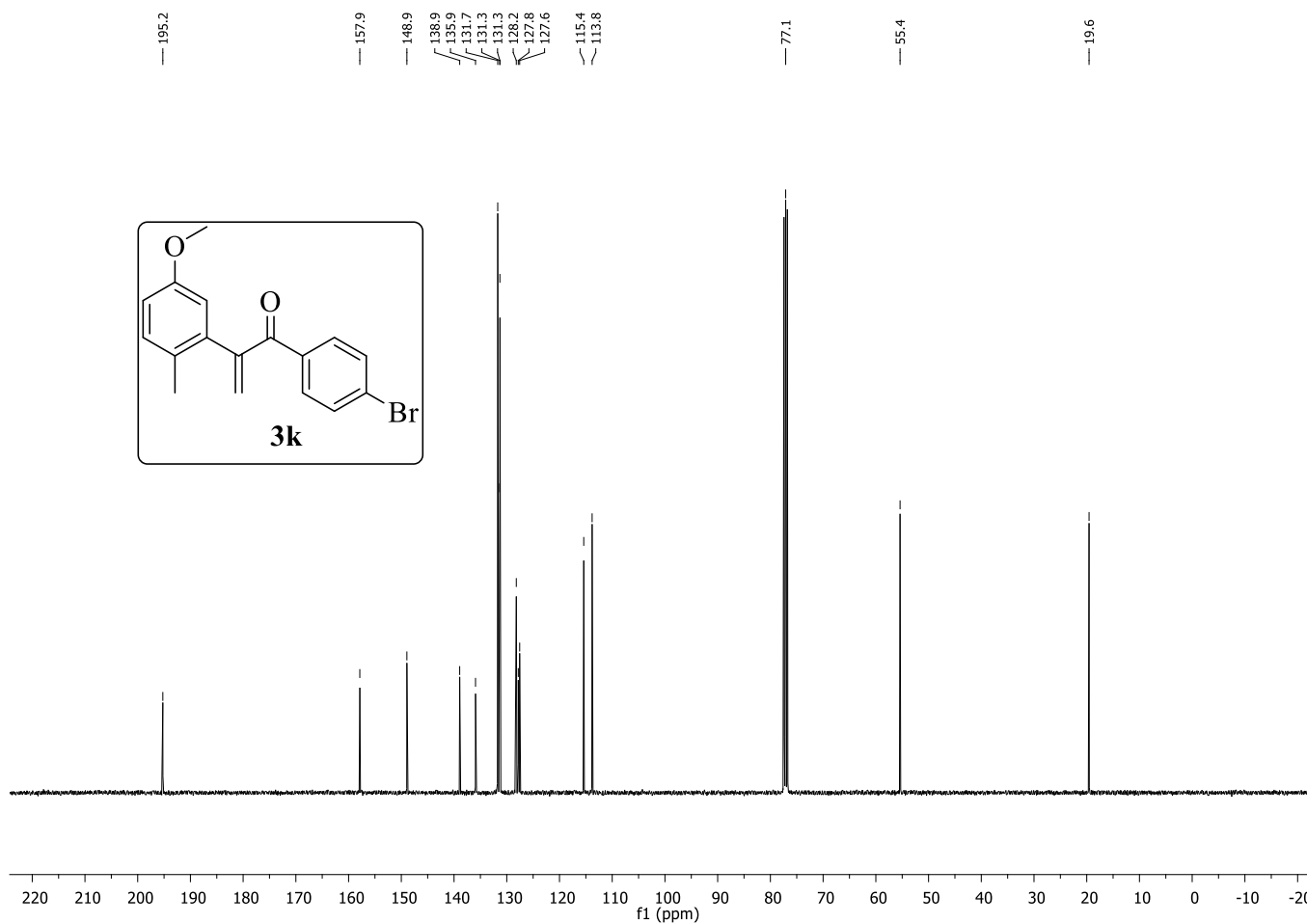
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^1H NMR spectrum of compound **3k** (400 MHz, CDCl_3)

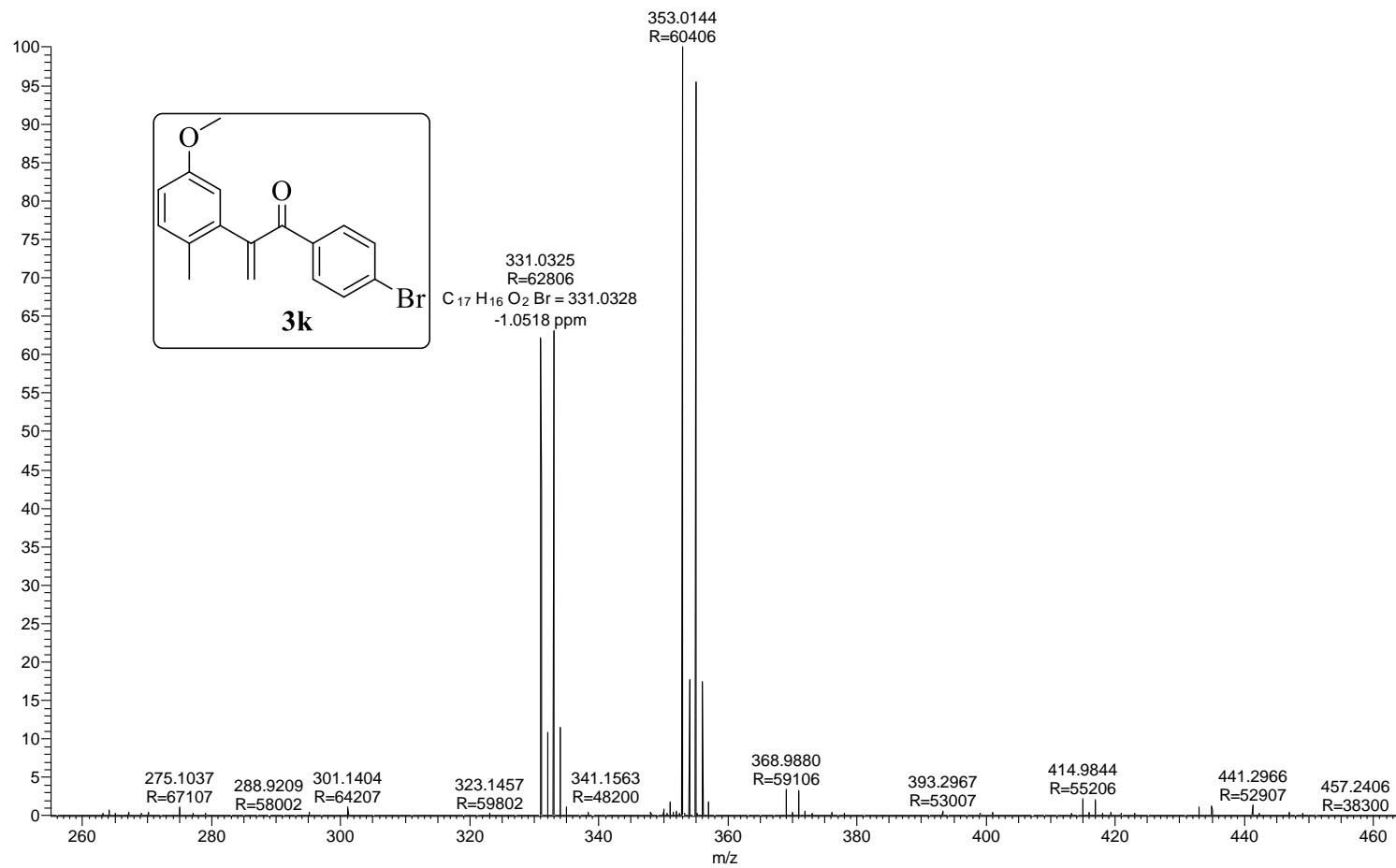


$^{13}\text{C} \{^1\text{H}\}$ NMR spectrum of compound **3k** (101 MHz, CDCl_3)

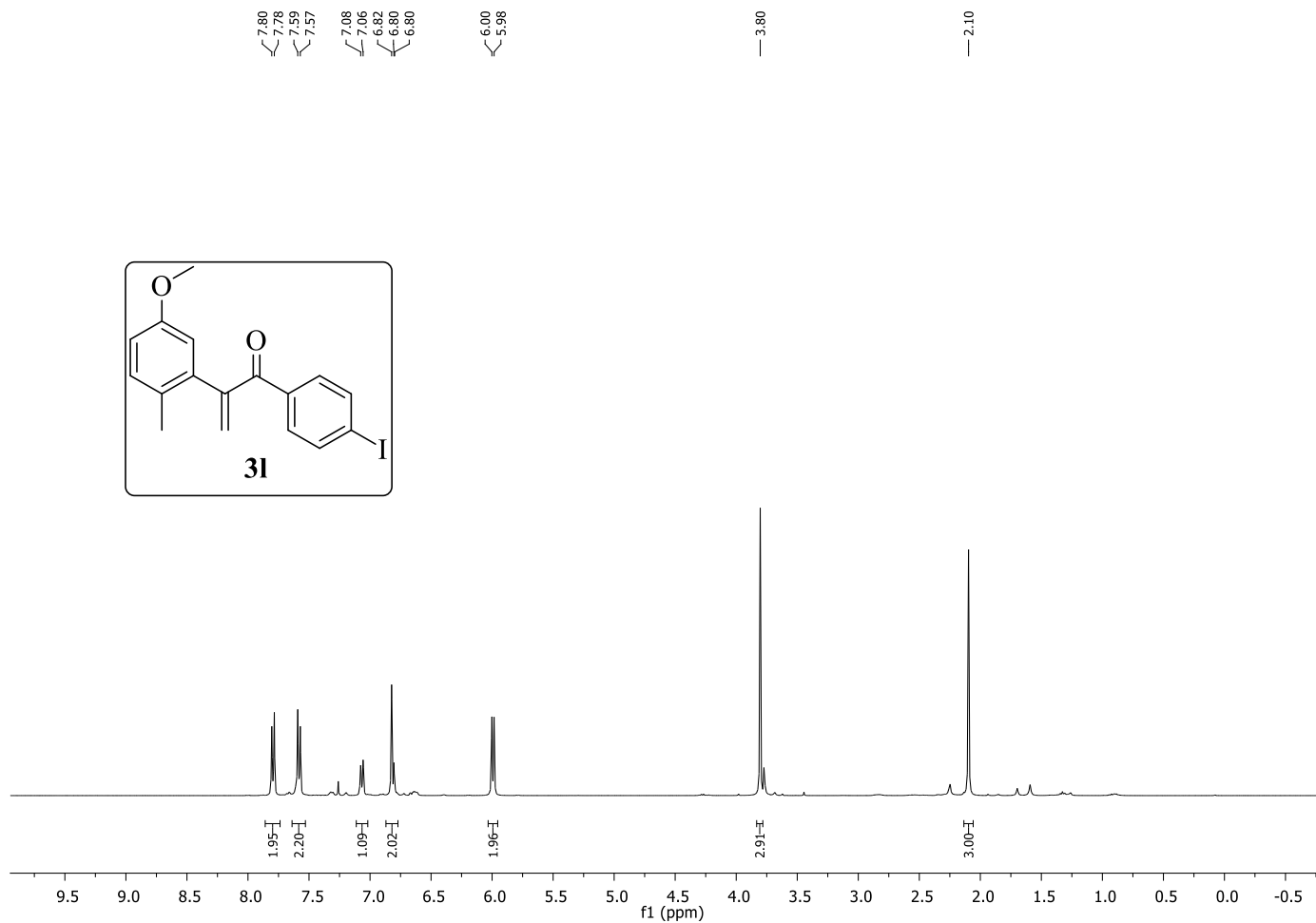


HRMS spectrum of compound 3k

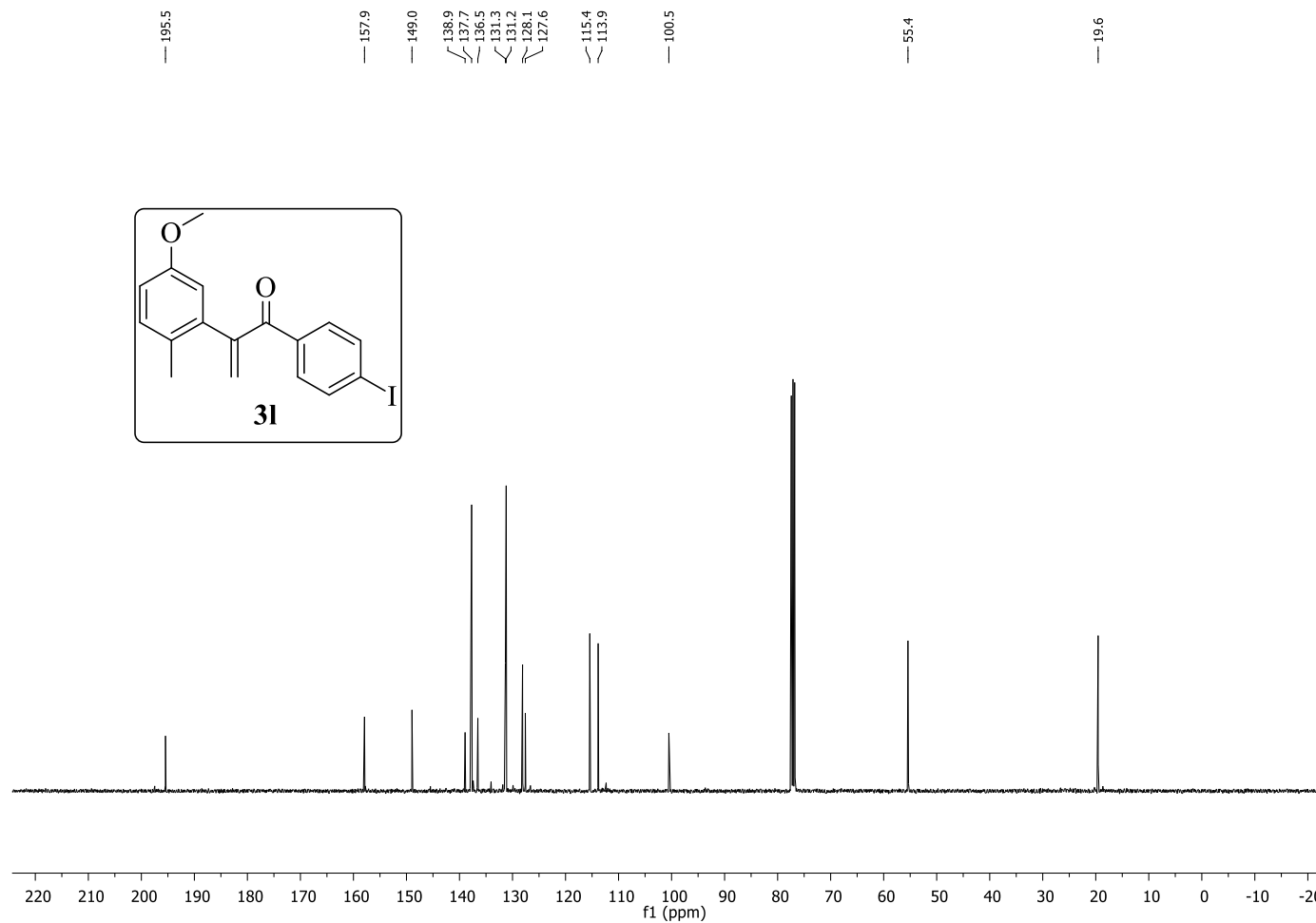
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^1H NMR spectrum of compound **31** (400 MHz, CDCl_3)

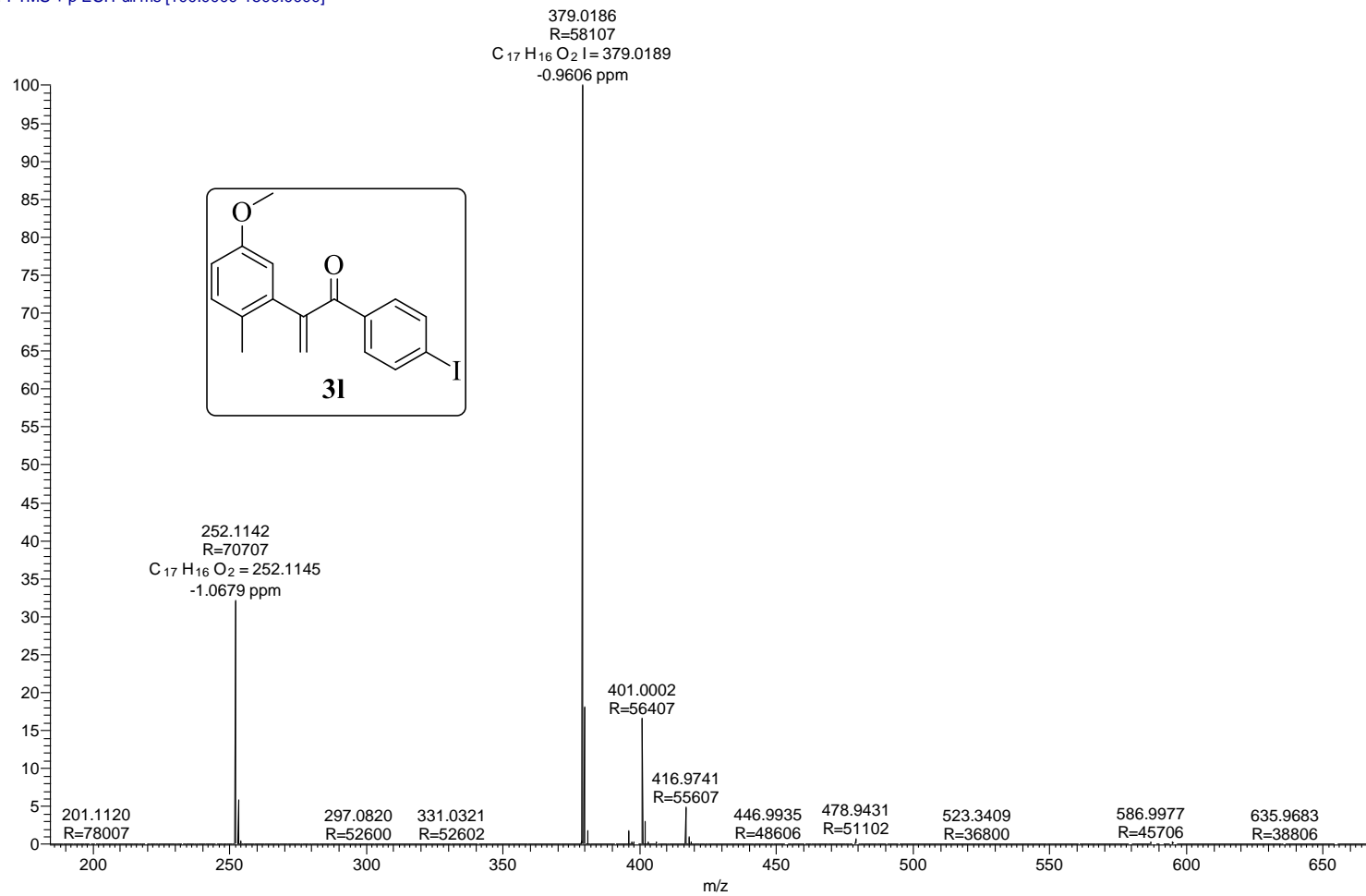


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3I** (101 MHz, CDCl_3)

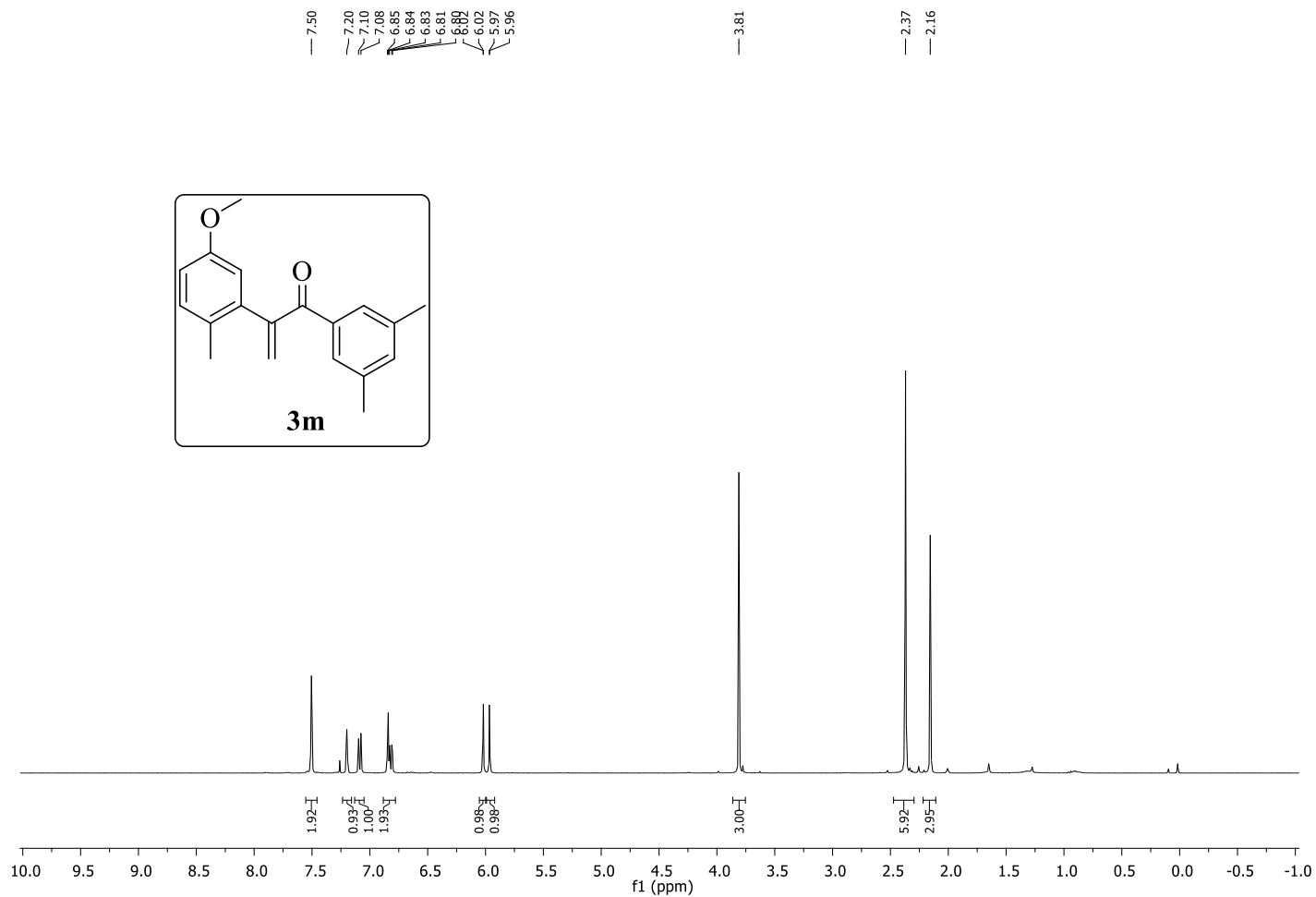


HRMS spectrum of compound 31

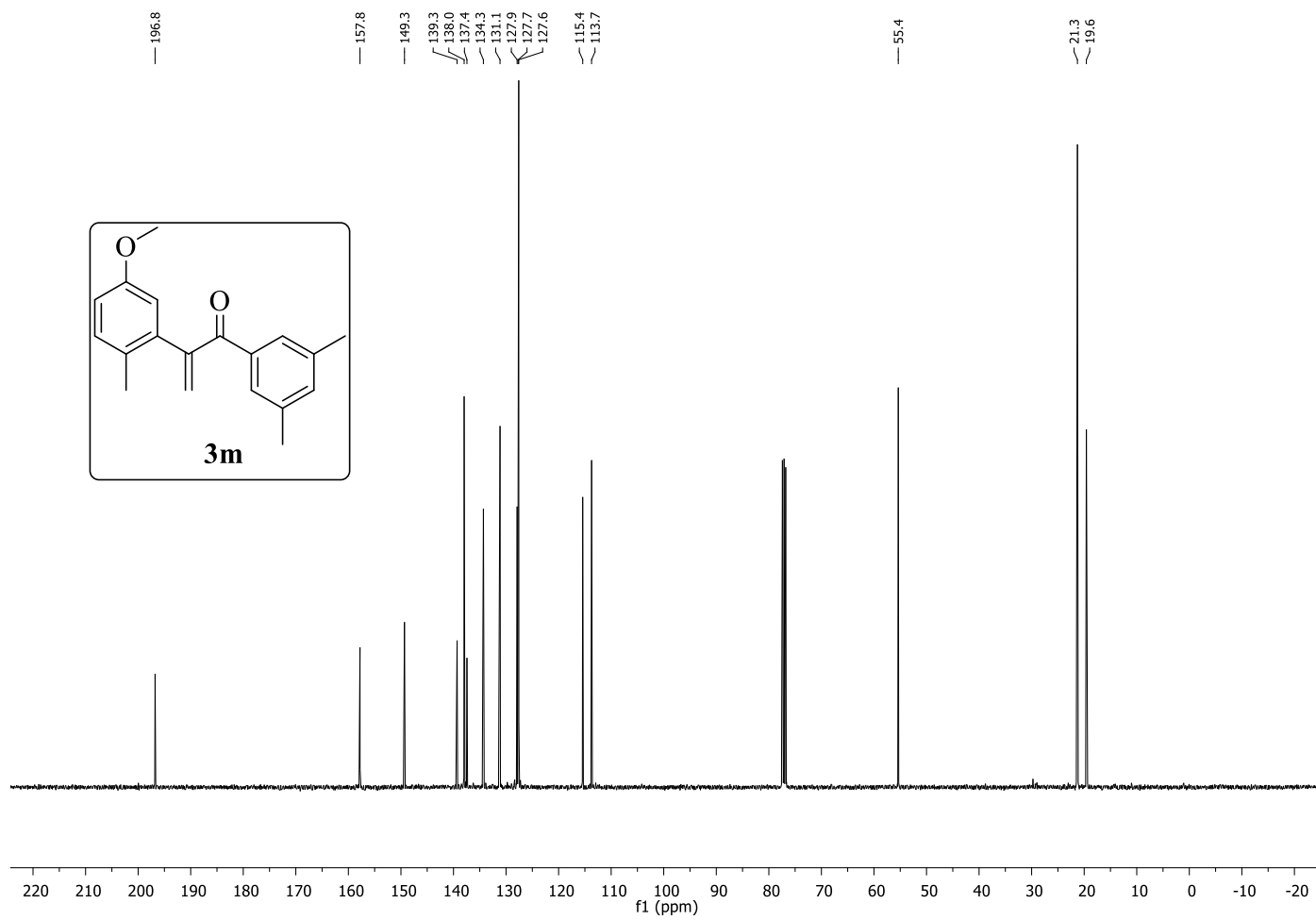
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T: FTMS + p ESI Full ms [100.0000-1500.0000]



¹H NMR spectrum of compound **3m** (400 MHz, CDCl₃)

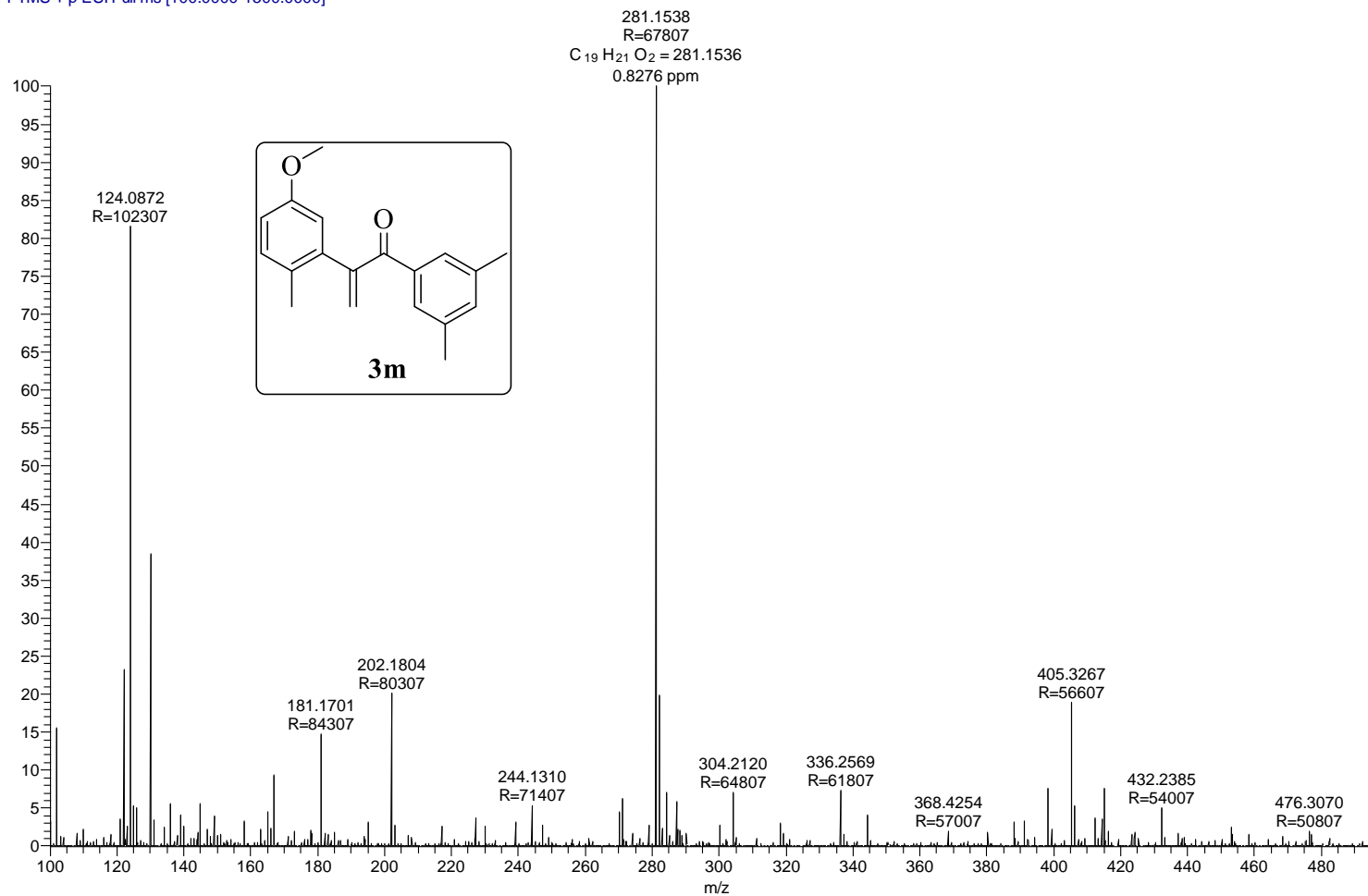


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3m** (101 MHz, CDCl_3)

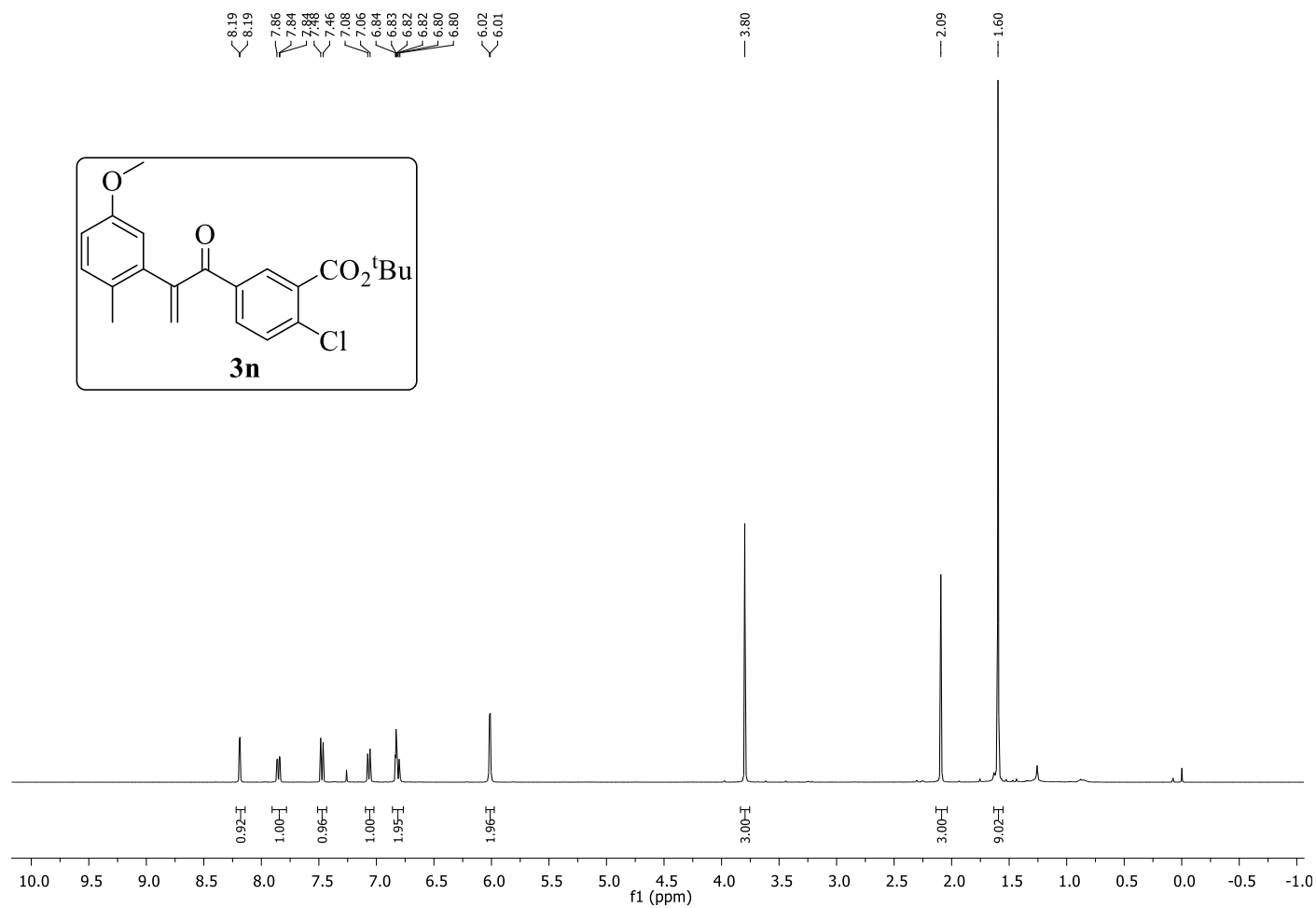


HRMS spectrum of compound **3m**

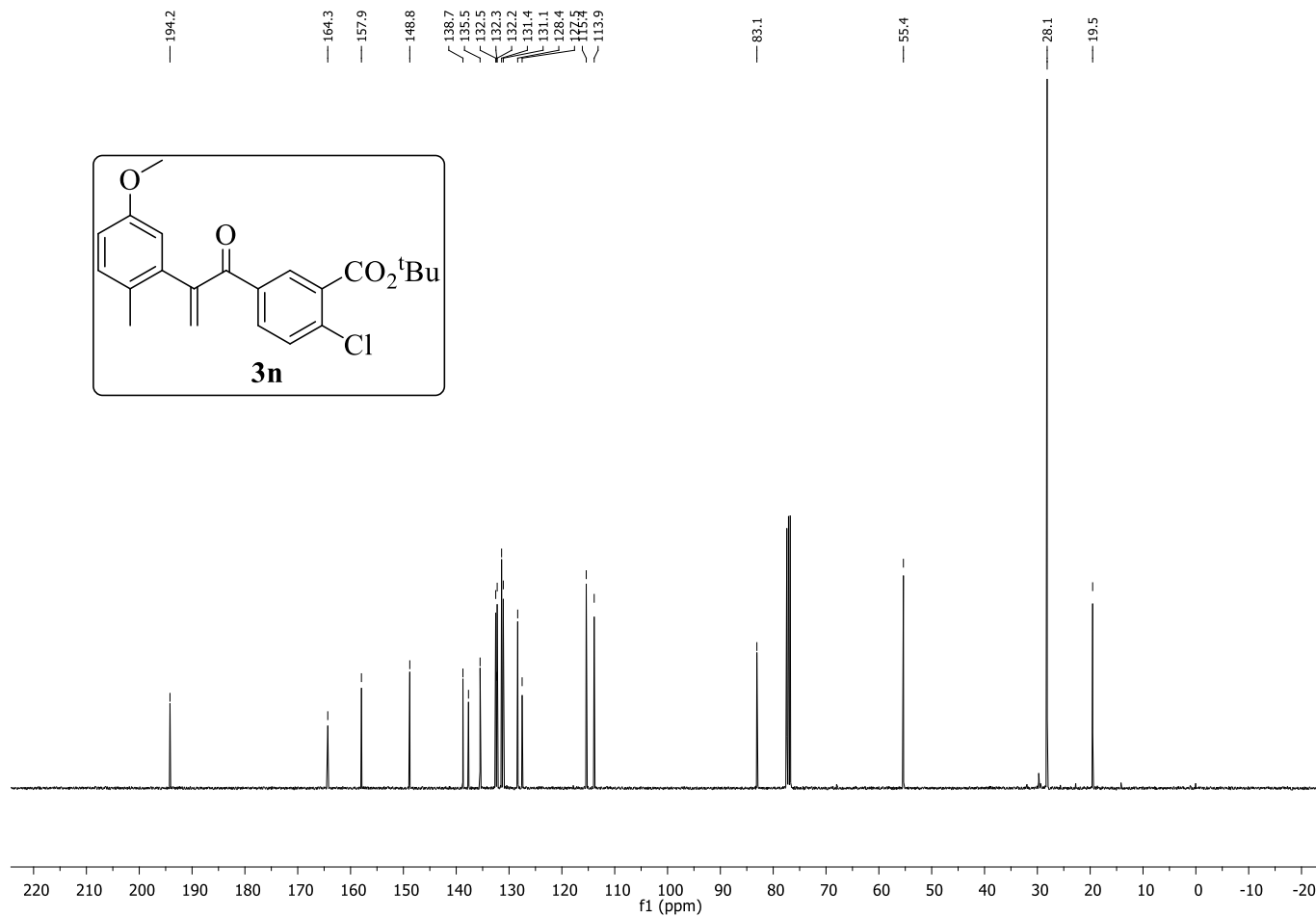
AR-7 #412 RT: 1.84 AV: 1 NL: 3.56E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3n** (400 MHz, CDCl_3)

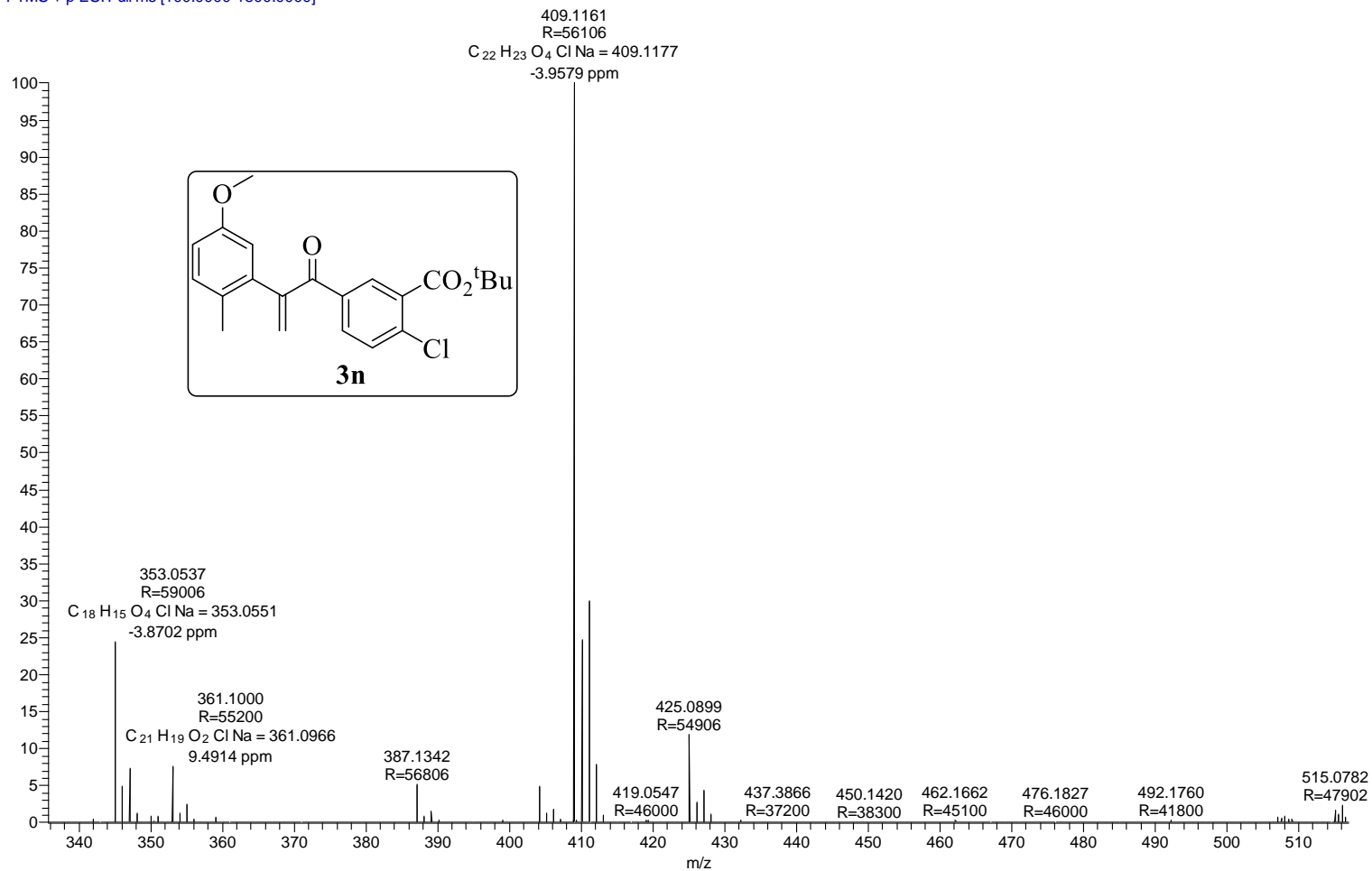


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3n** (101 MHz, CDCl_3)

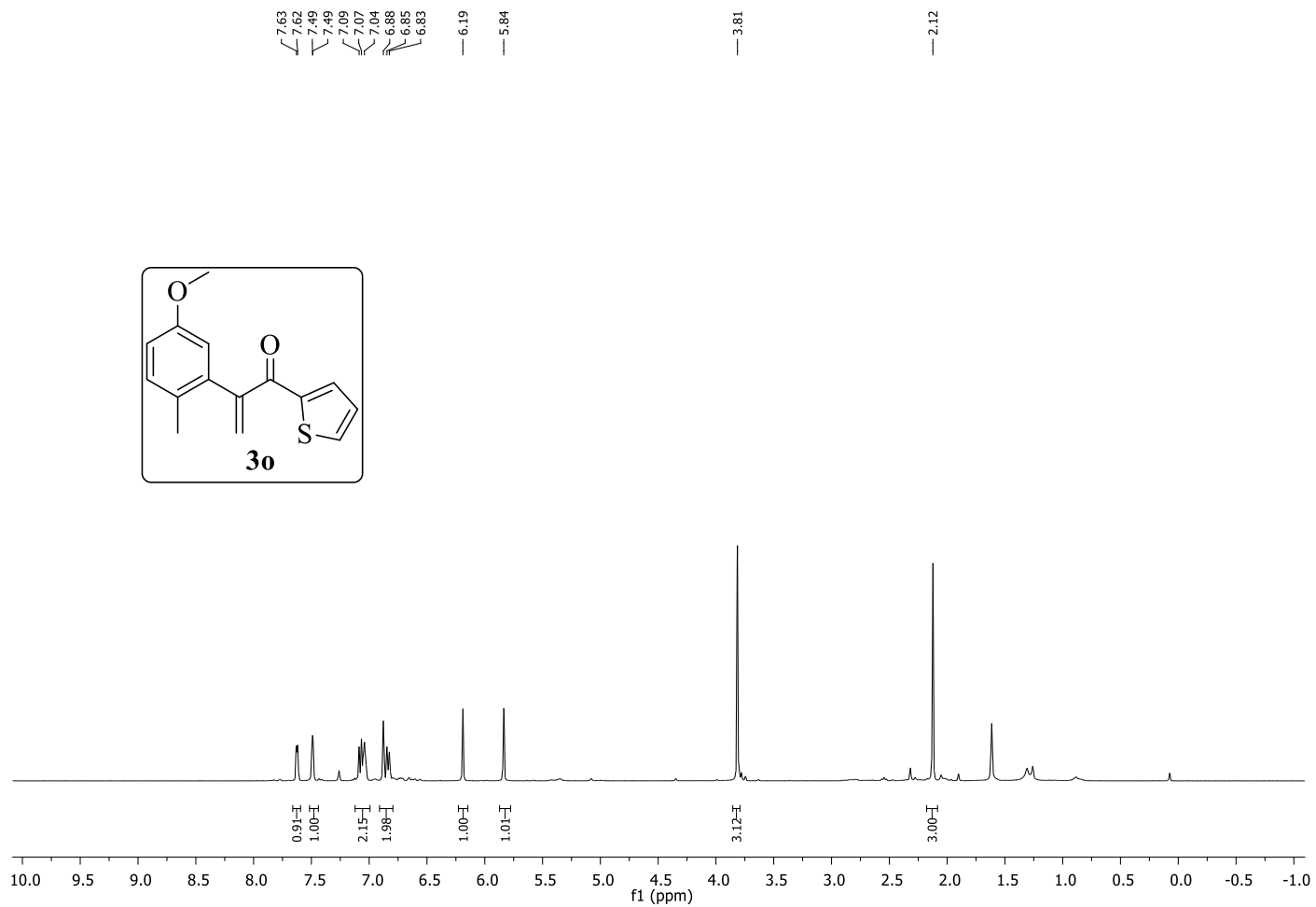


HRMS spectrum of compound **3n**

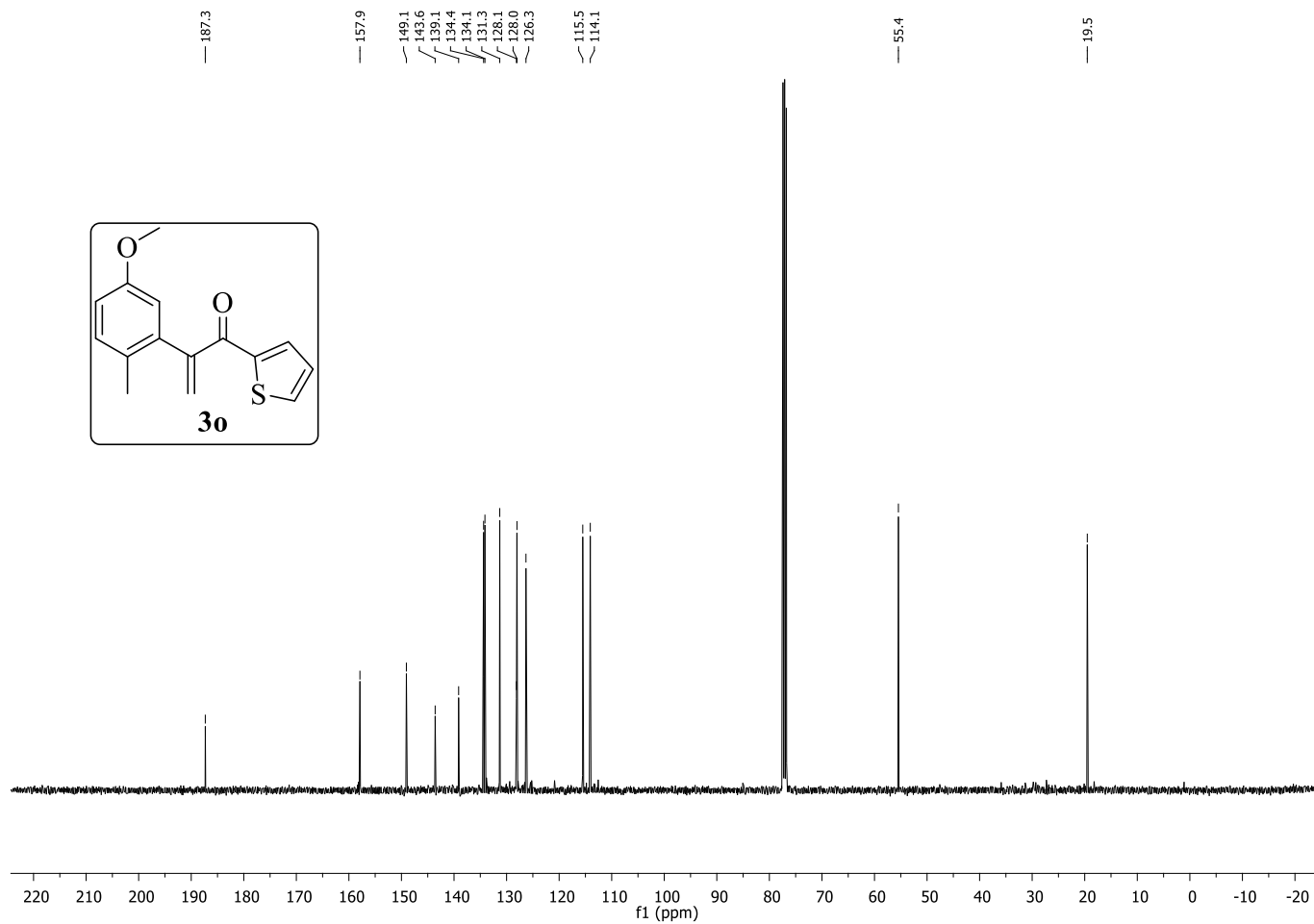
ARC-464 #626 RT: 2.79 AV: 1 NL: 9.93E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3o** (400 MHz, CDCl_3)

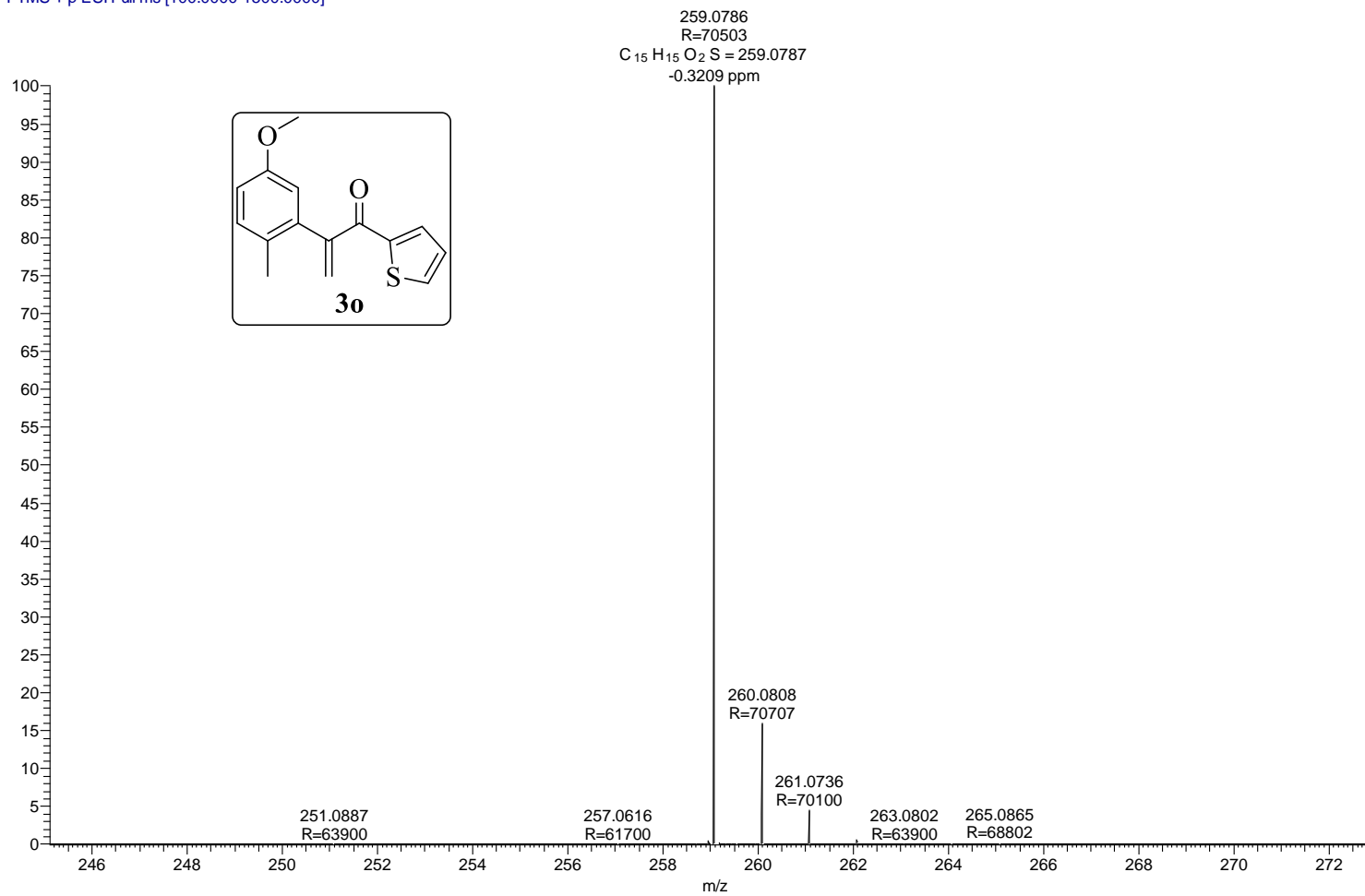


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3o** (101 MHz, CDCl_3)

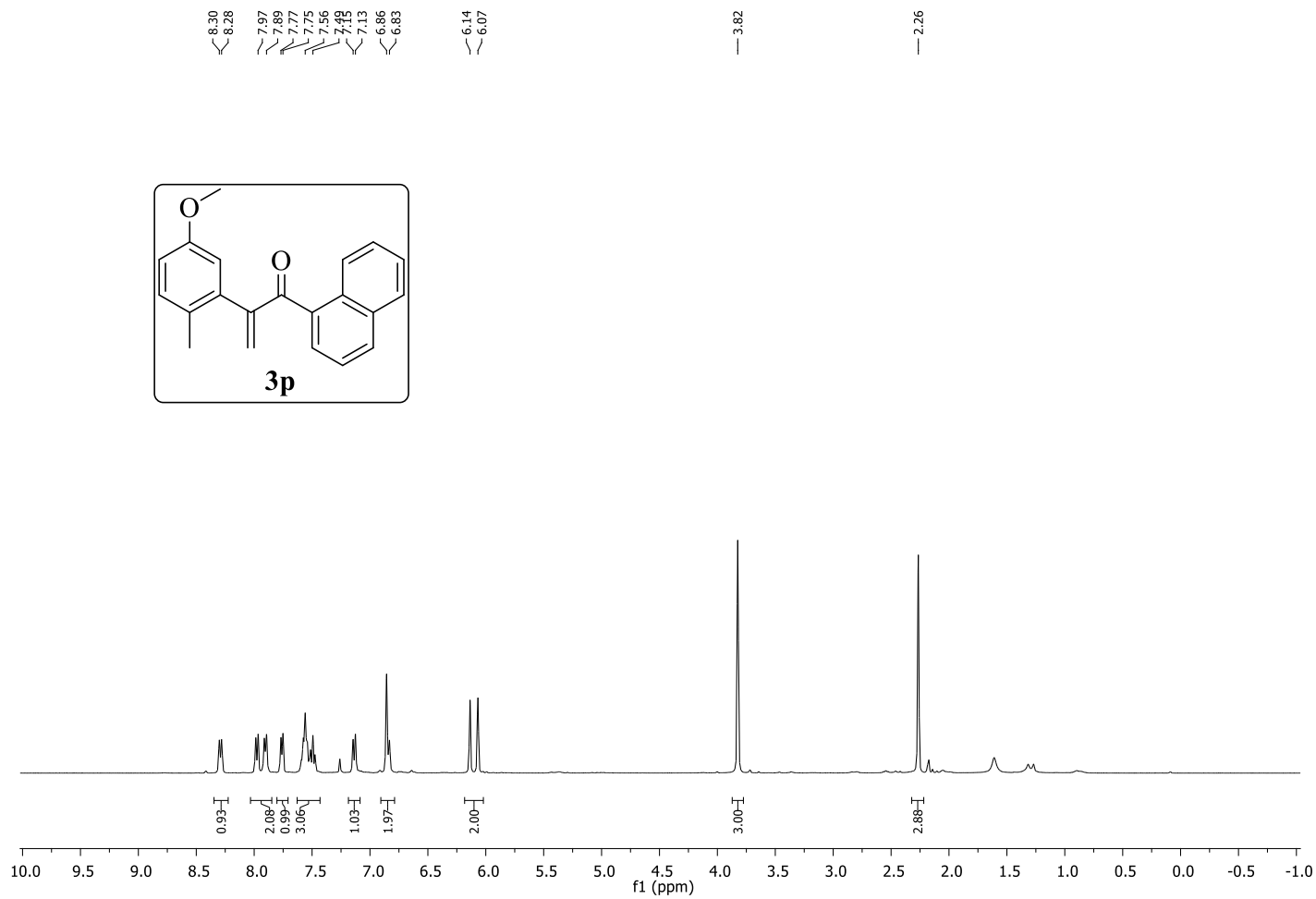


HRMS spectrum of compound **3o**

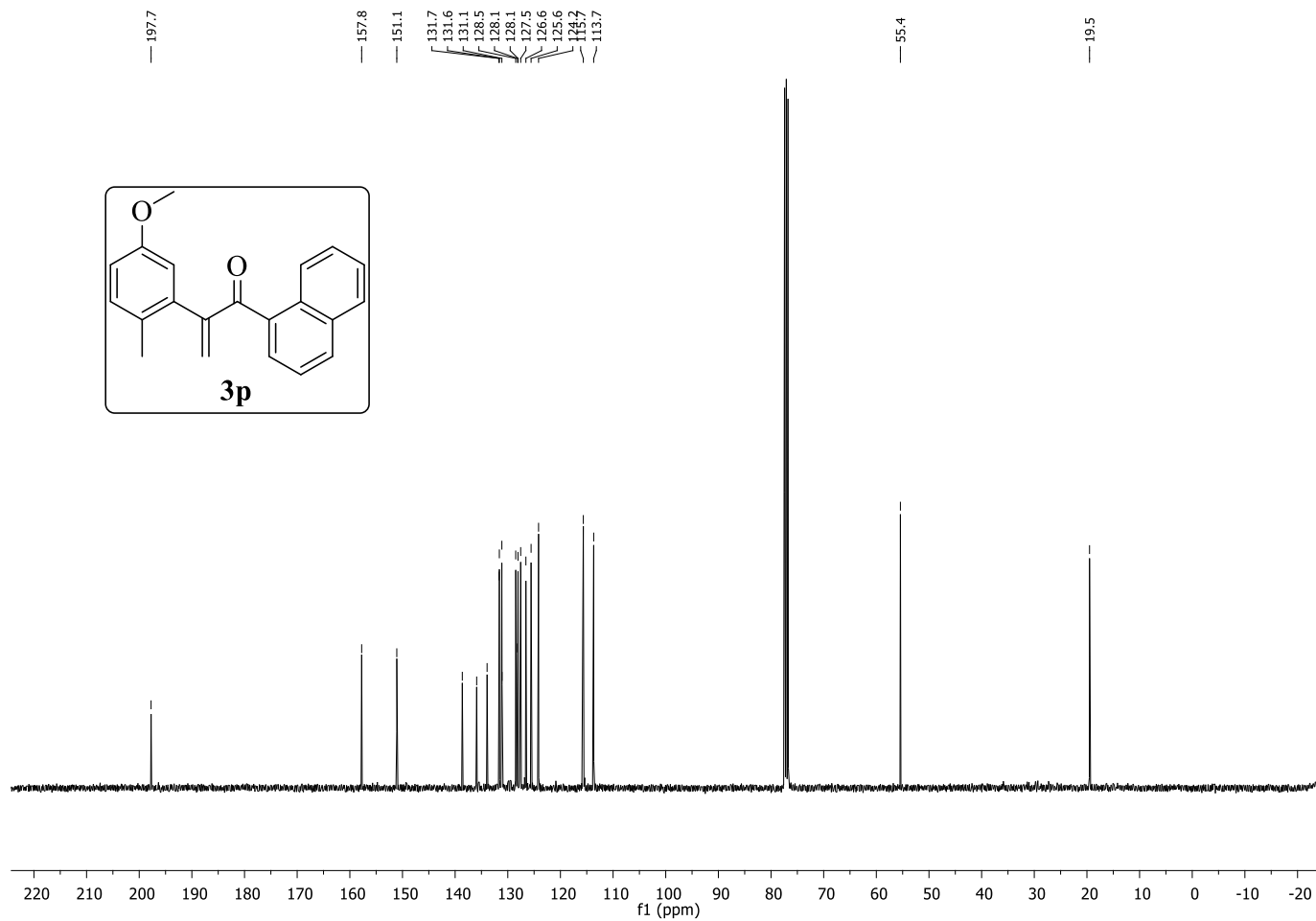
ARC-24A #453 RT: 2.02 AV: 1 NL: 6.39E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3p** (400 MHz, CDCl_3)

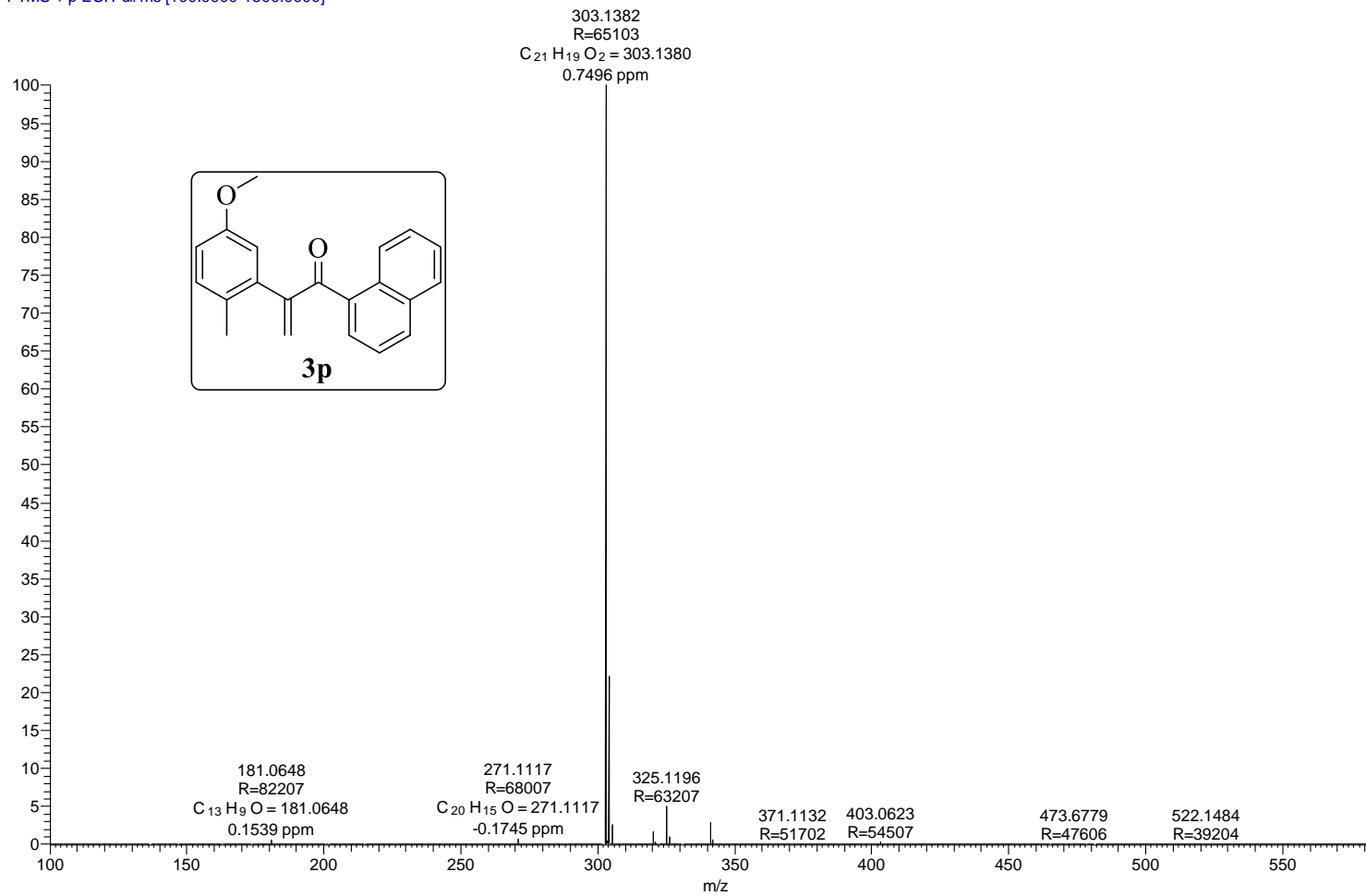


$^{13}\text{C} \{^1\text{H}\}$ NMR spectrum of compound **3p** (101 MHz, CDCl_3)

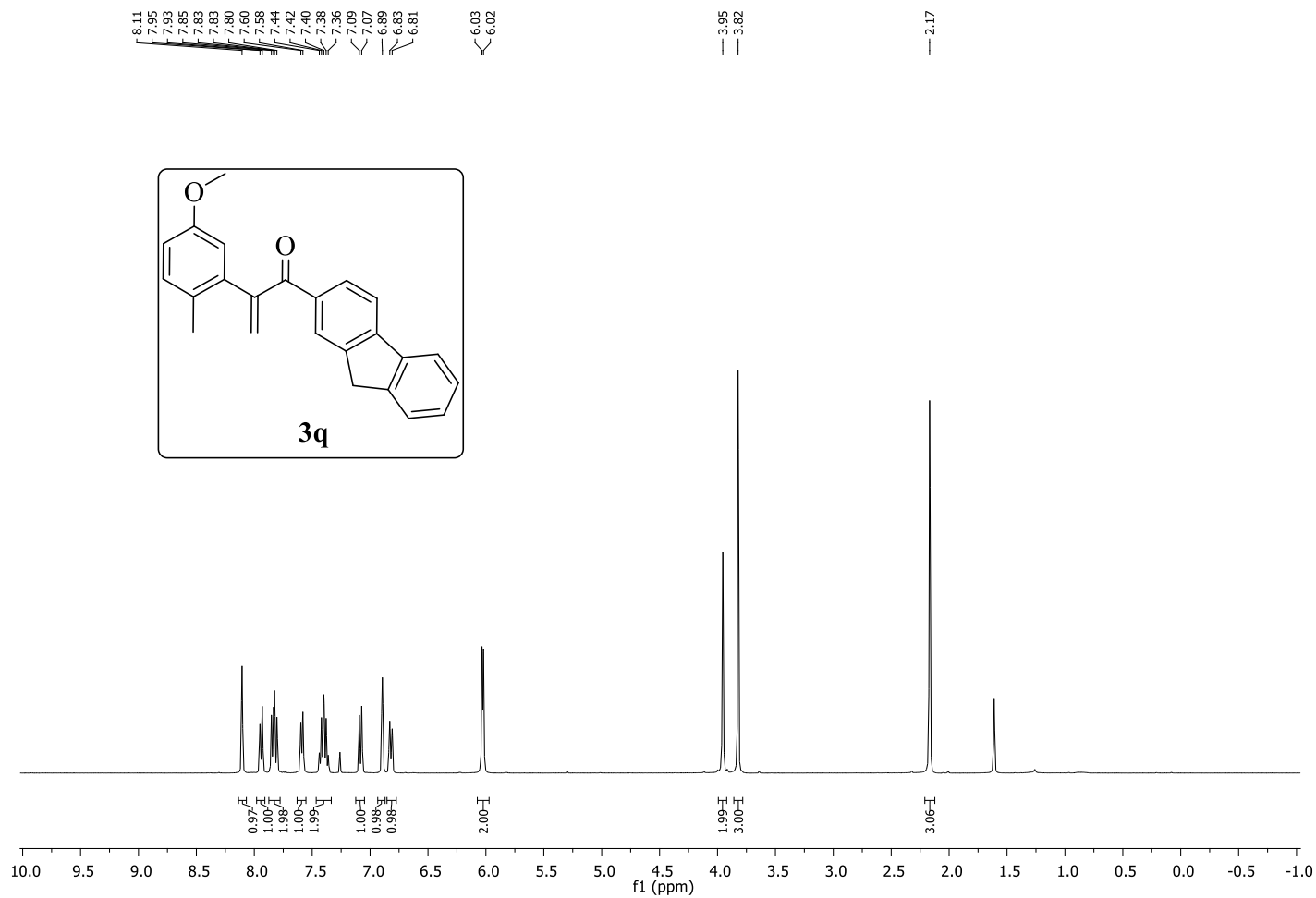


HRMS spectrum of compound 3p

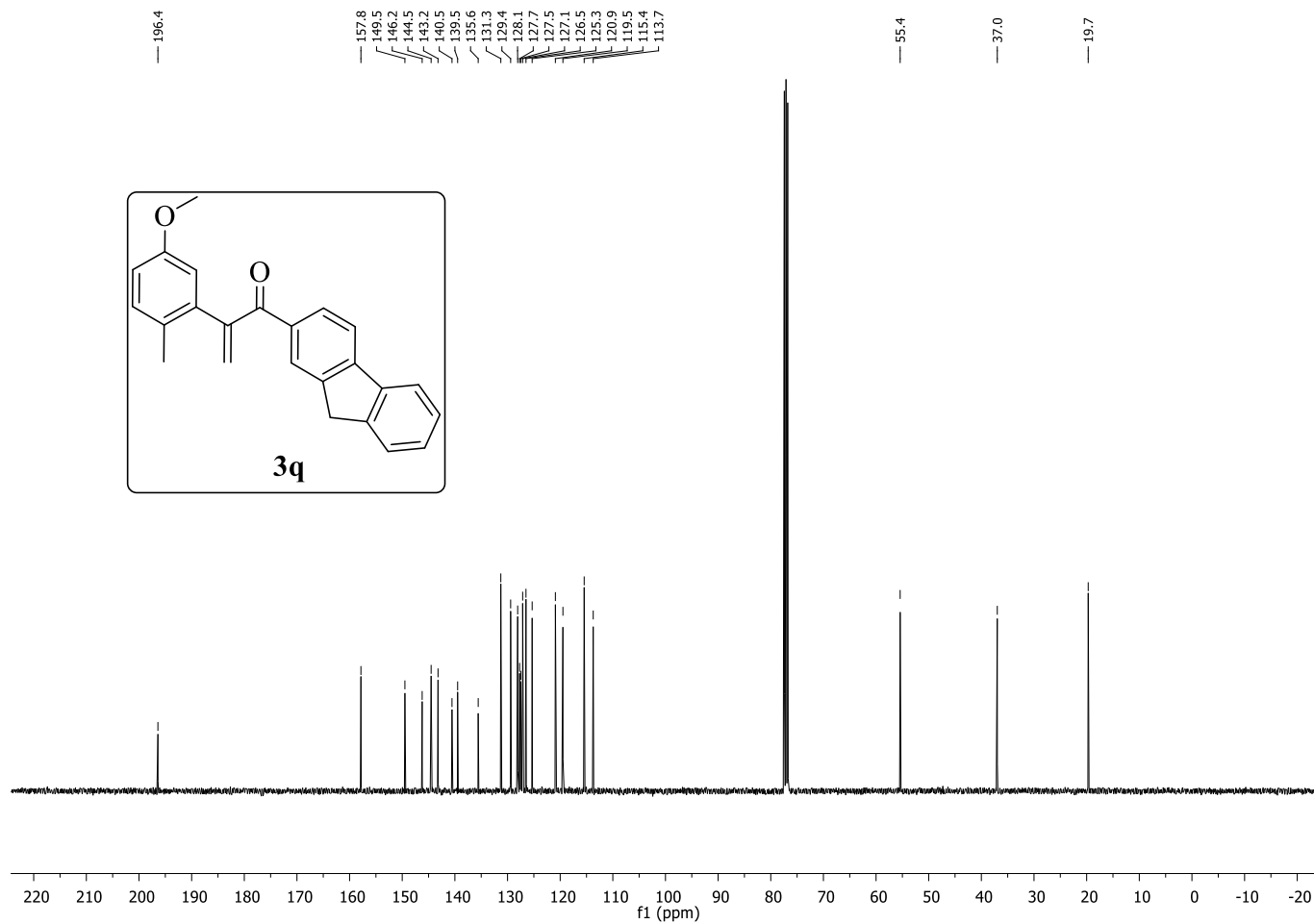
ARC-17C #507 RT: 2.26 AV: 1 NL: 7.63E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3q** (400 MHz, CDCl_3)

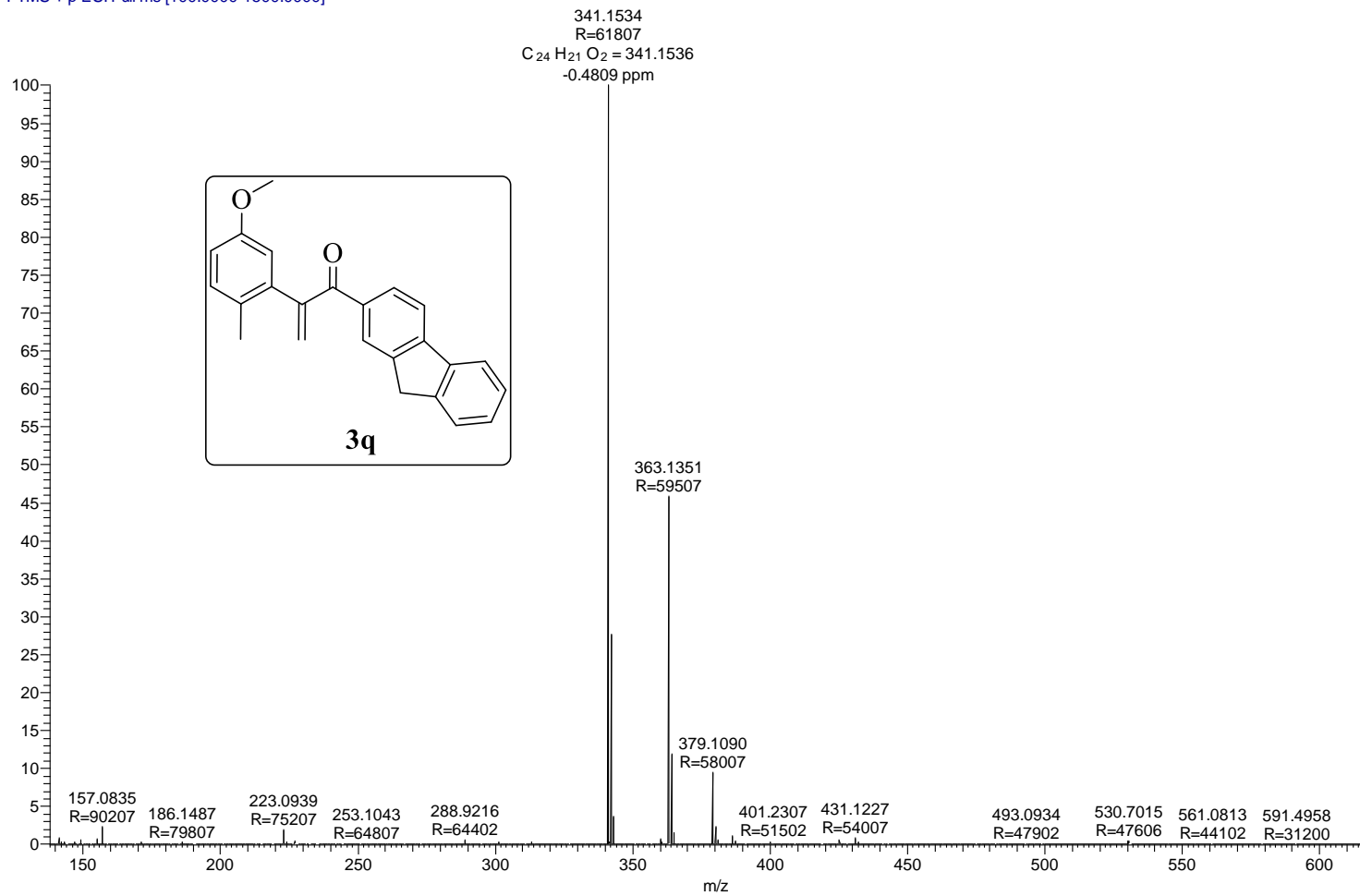


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3q** (101 MHz, CDCl_3)

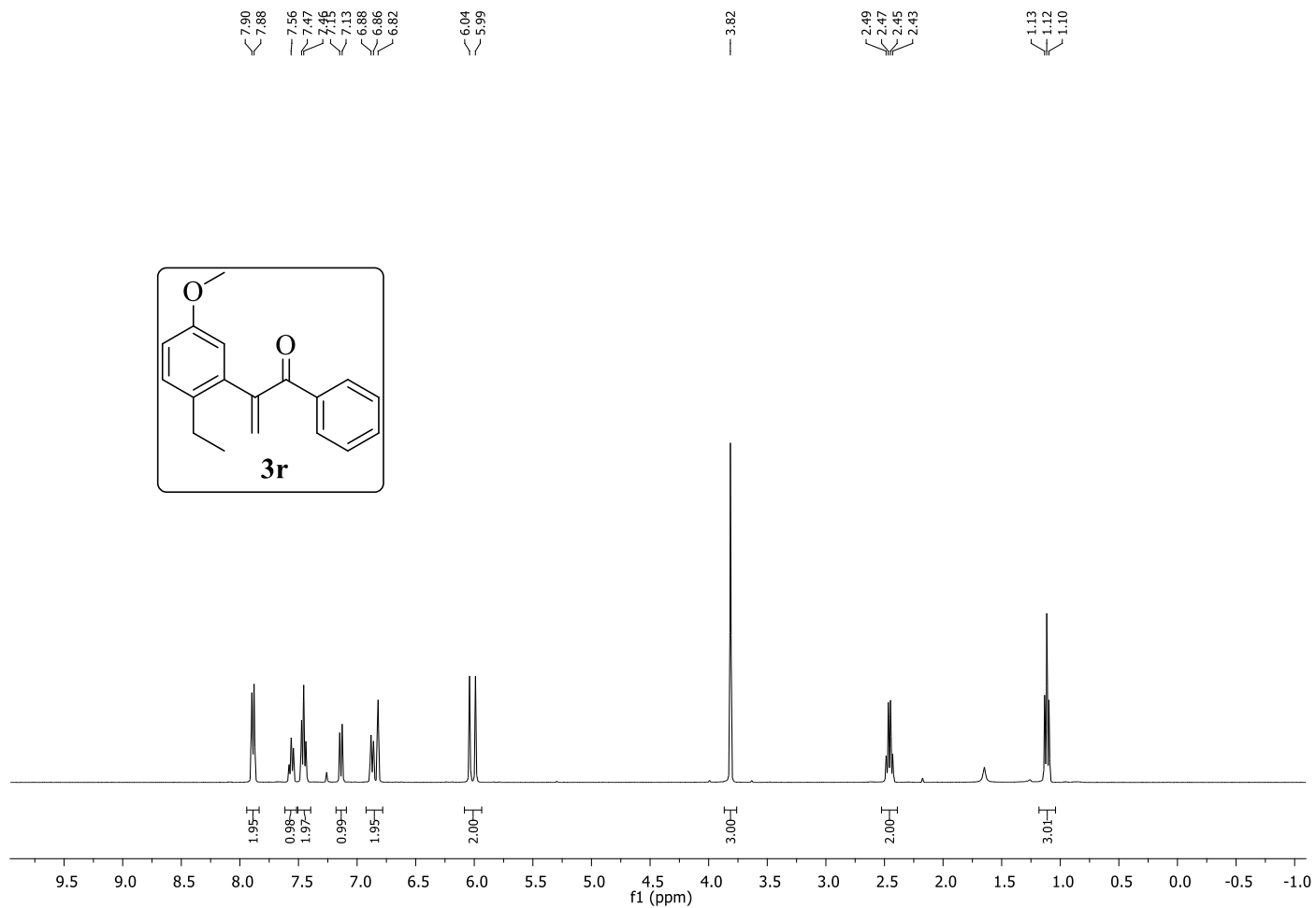


HRMS spectrum of compound **3q**

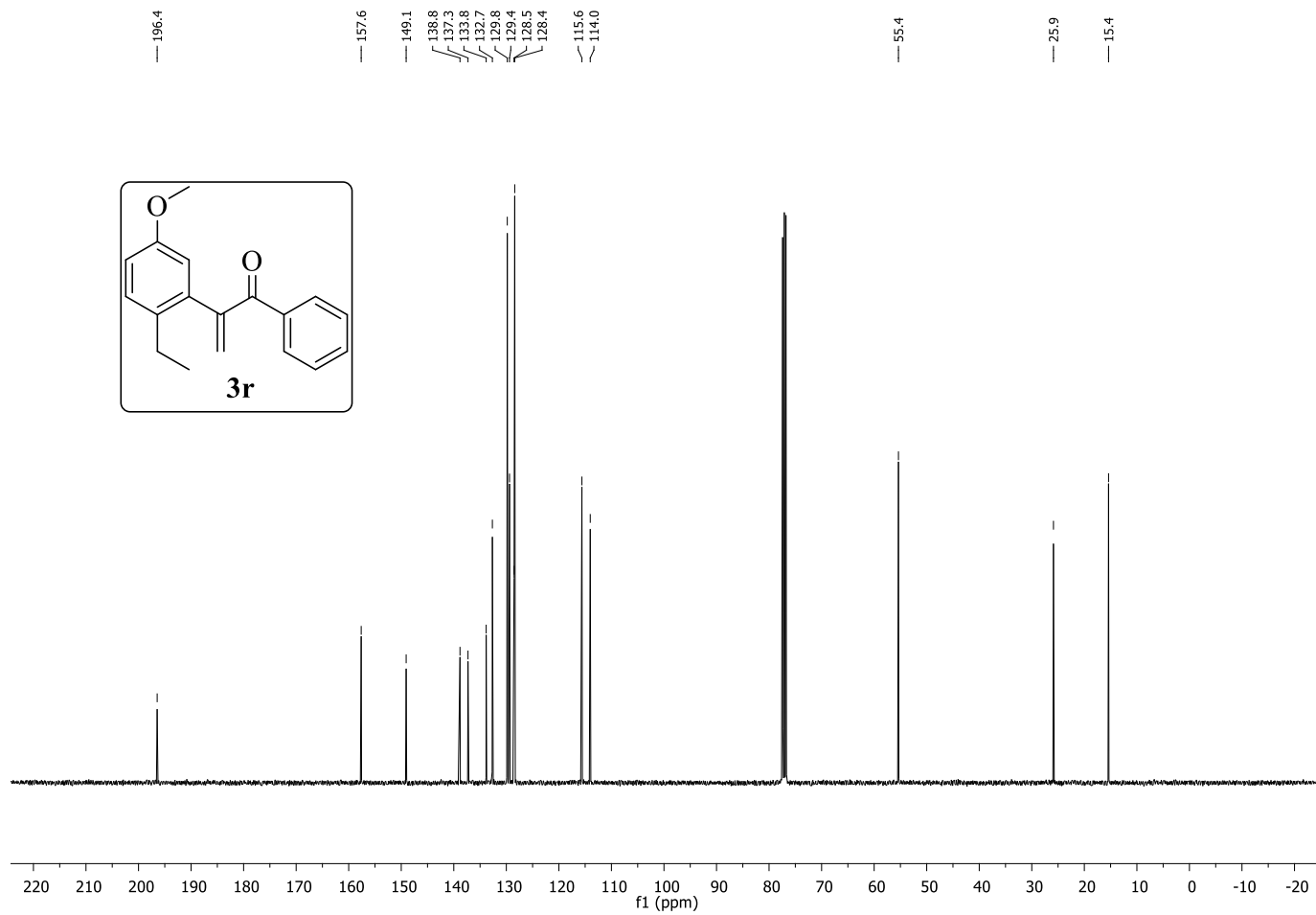
ARC-25-A #633 RT: 2.82 AV: 1 NL: 1.27E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3r** (400 MHz, CDCl_3)

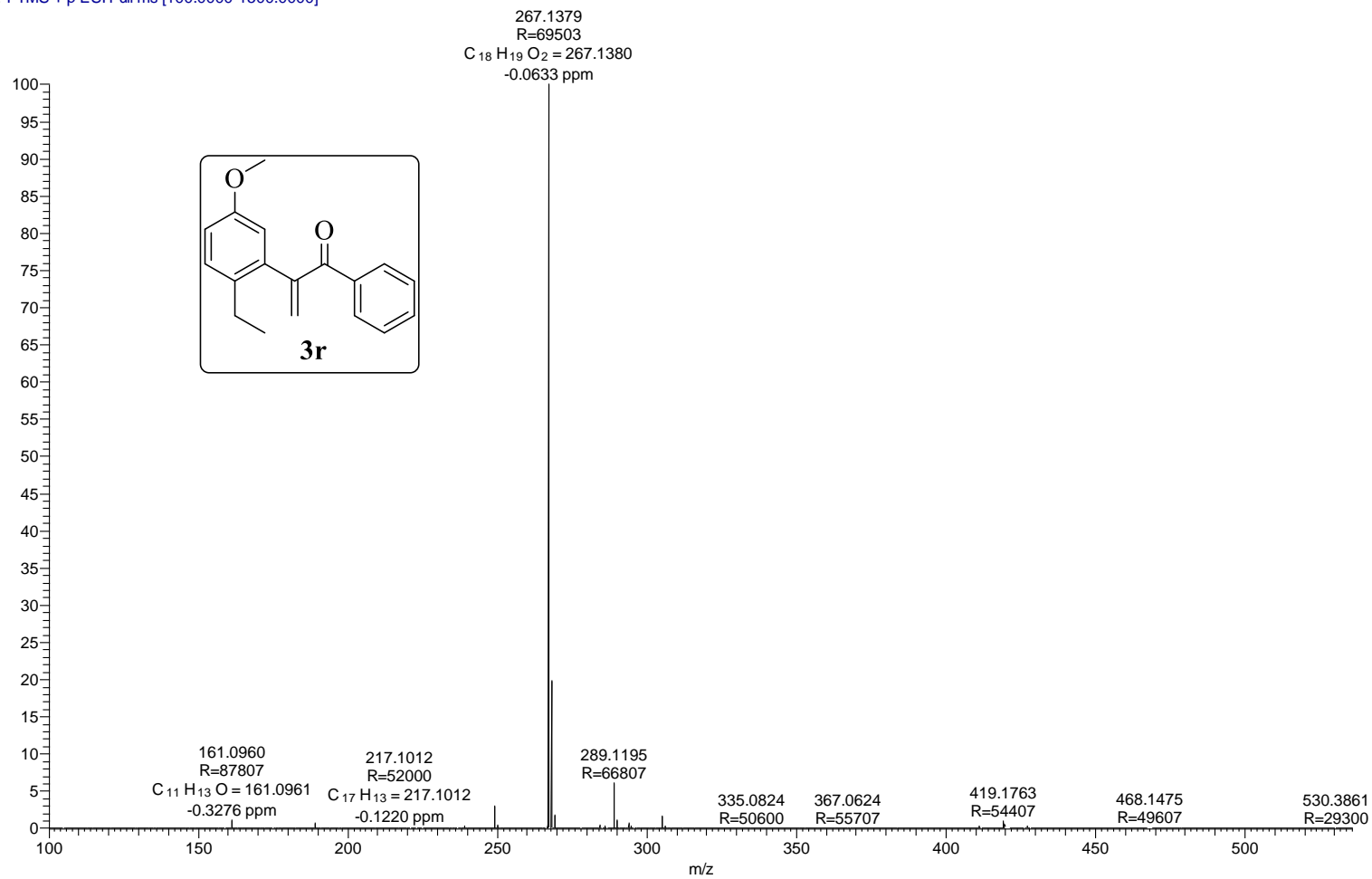


^{13}C { ^1H } NMR spectrum of compound **3r** (101 MHz, CDCl_3)

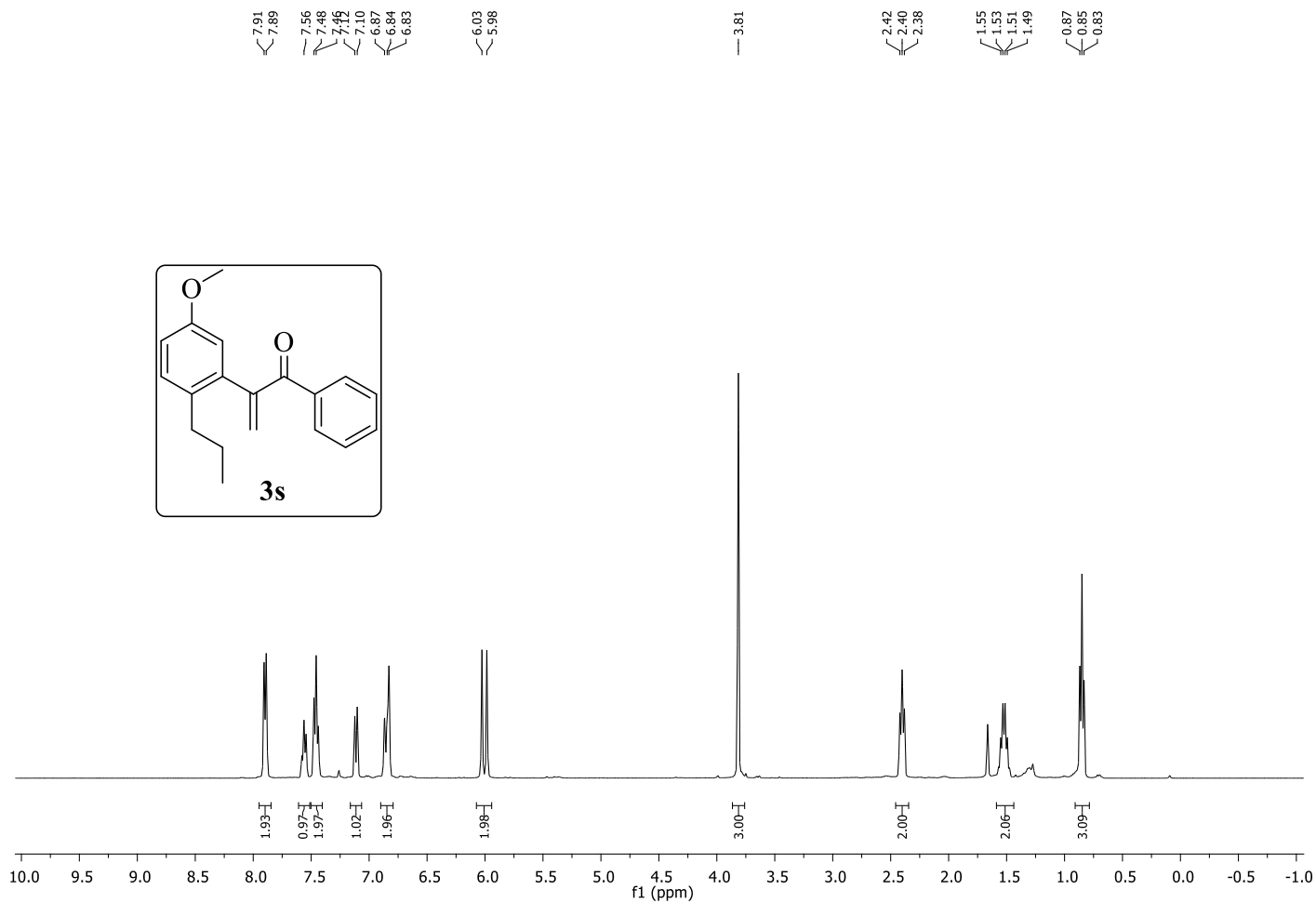


HRMS spectrum of compound 3r

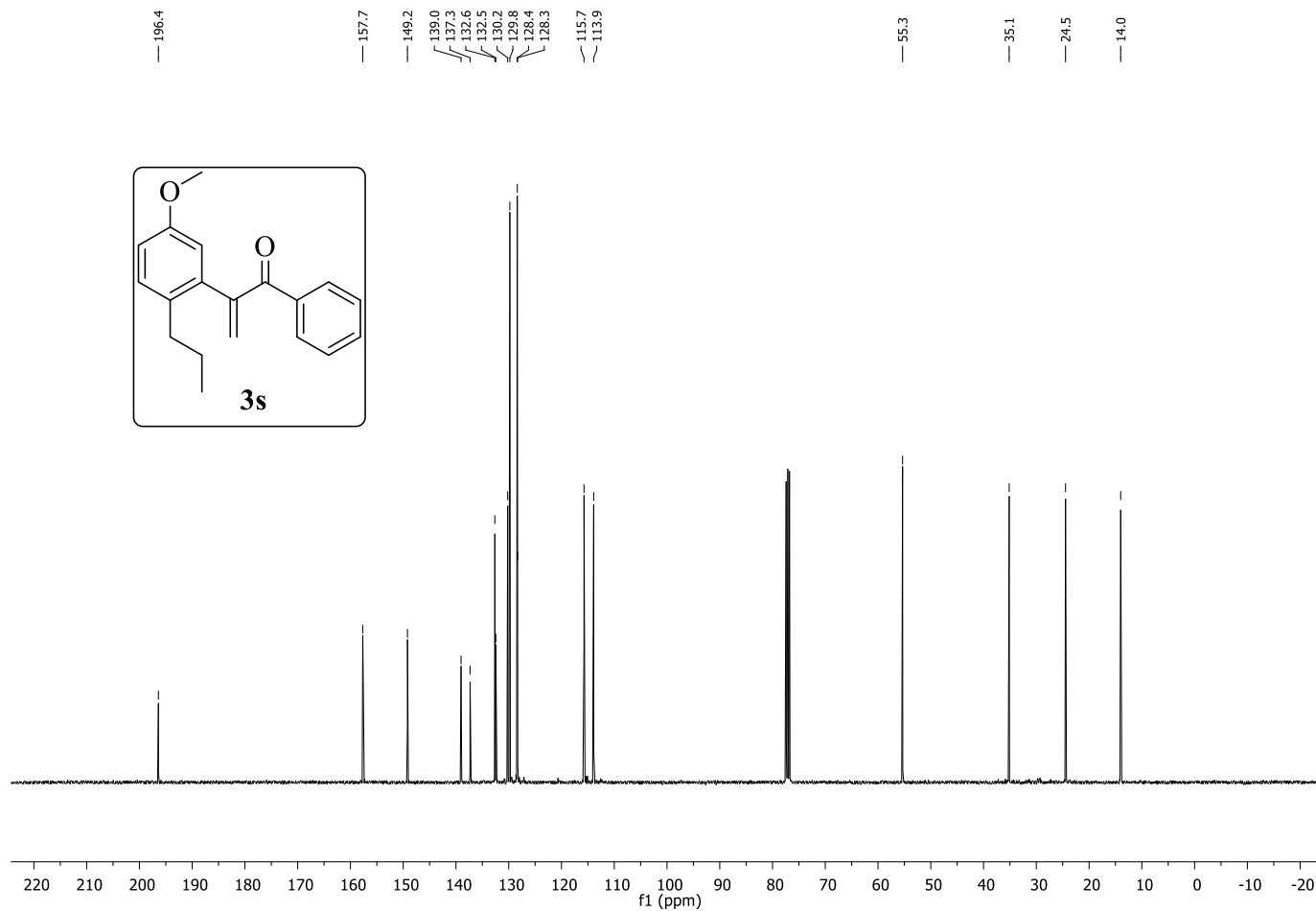
ARC-22C #477 RT: 2.13 AV: 1 NL: 1.16E10
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3s** (400 MHz, CDCl_3)

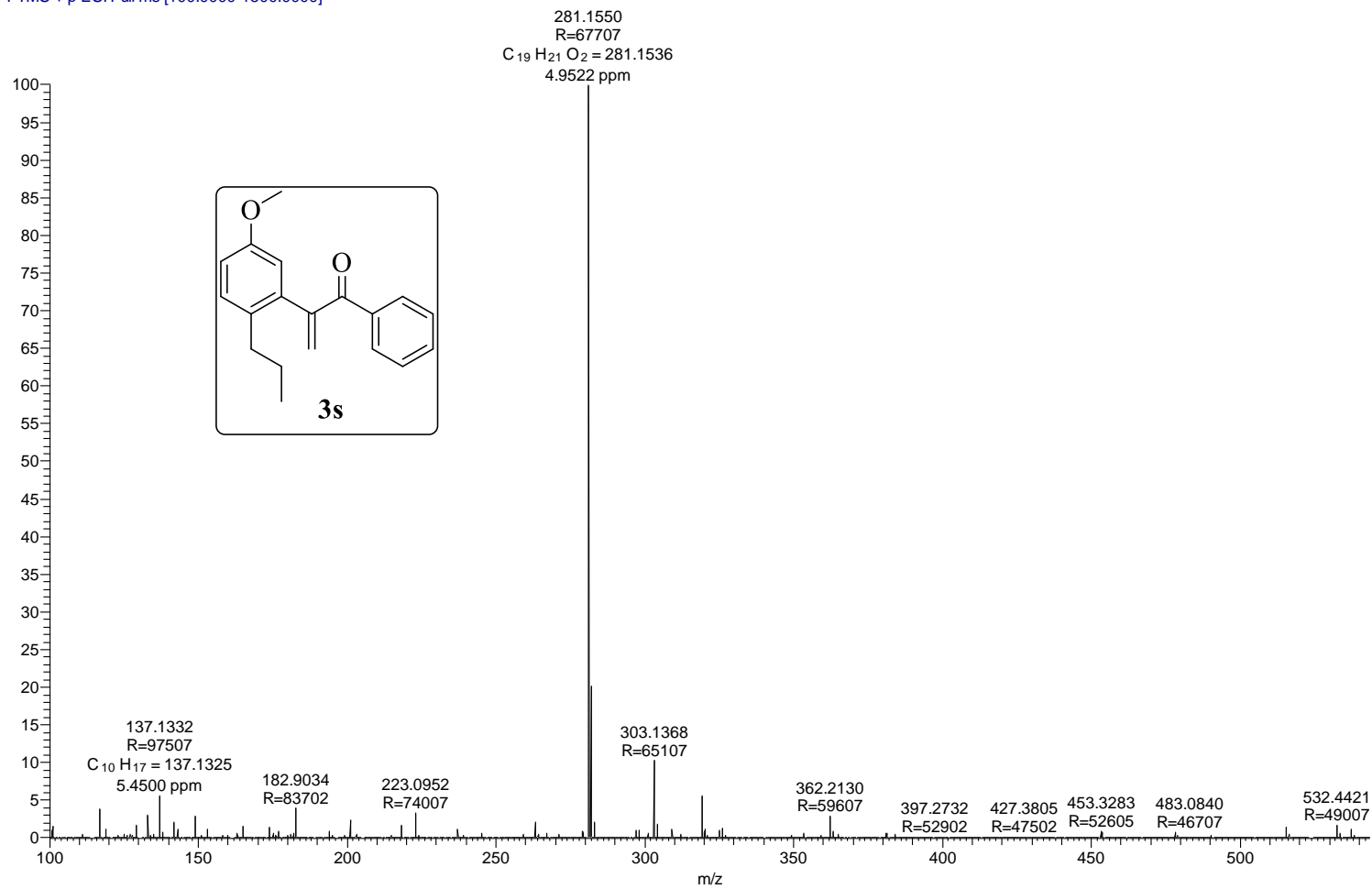


$^{13}\text{C} \{^1\text{H}\}$ NMR spectrum of compound **3s** (101 MHz, CDCl_3)

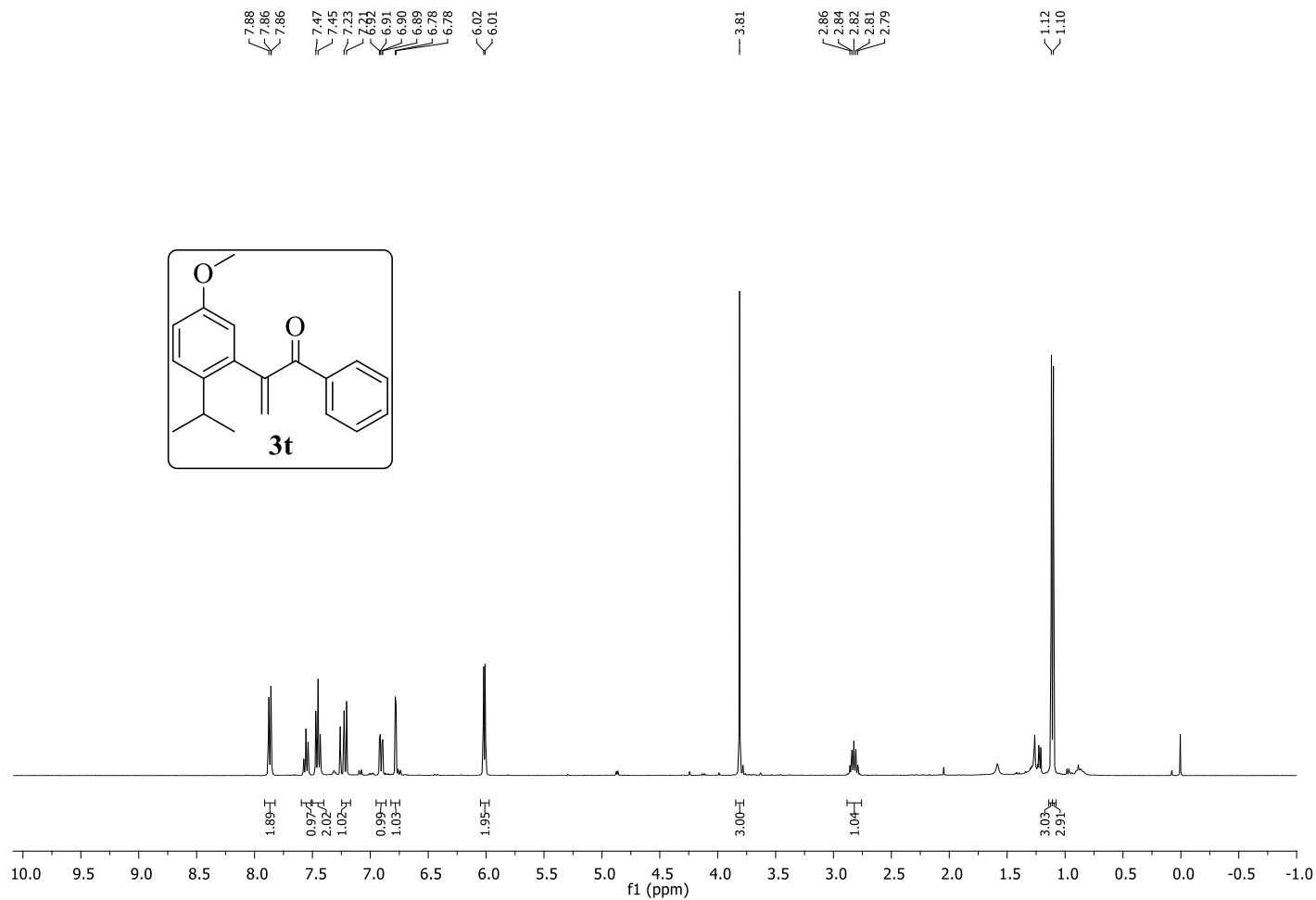


HRMS spectrum of compound 3s

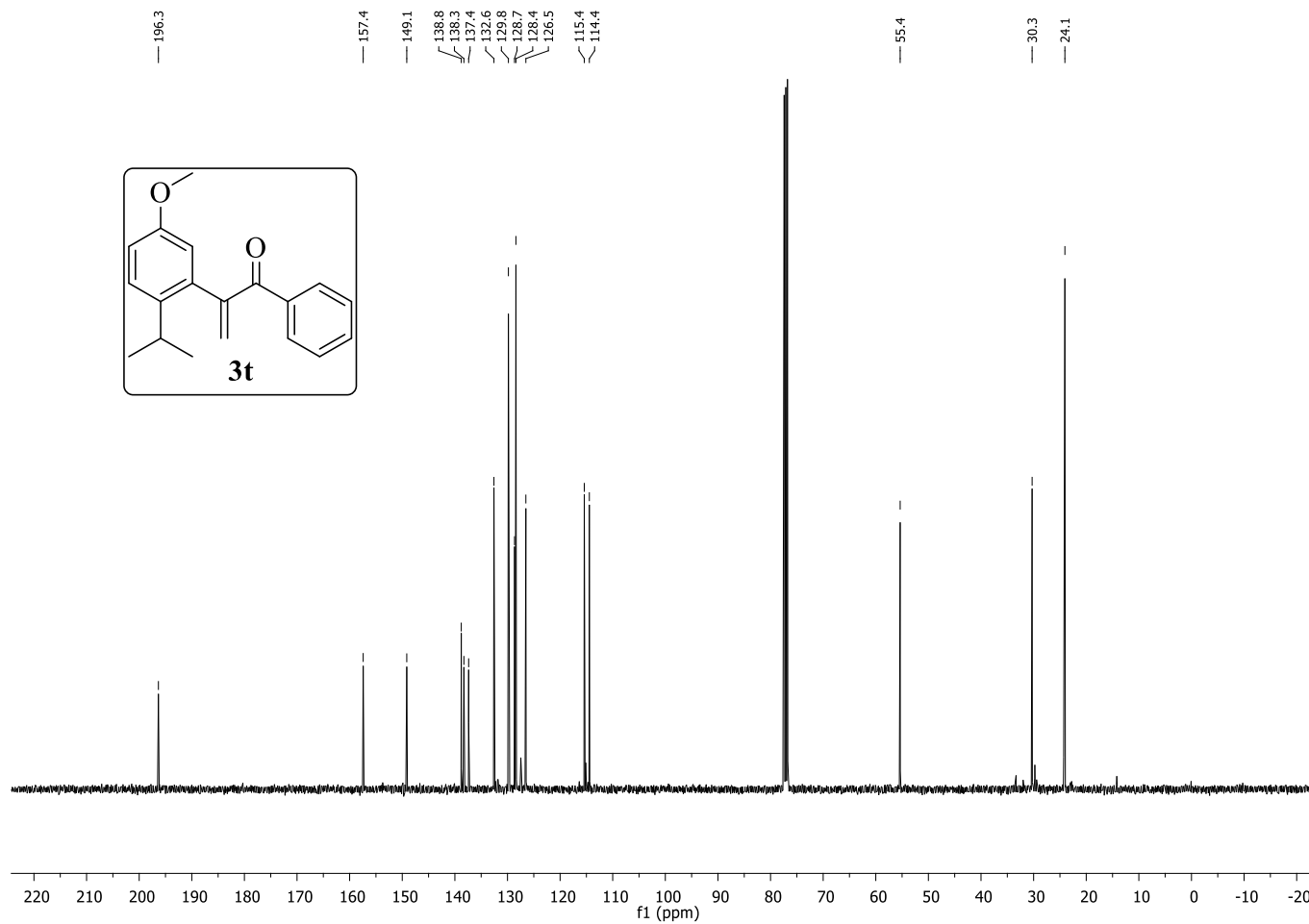
ARC-23C #583 RT: 2.62 AV: 1 NL: 3.31E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3t** (400 MHz, CDCl_3)

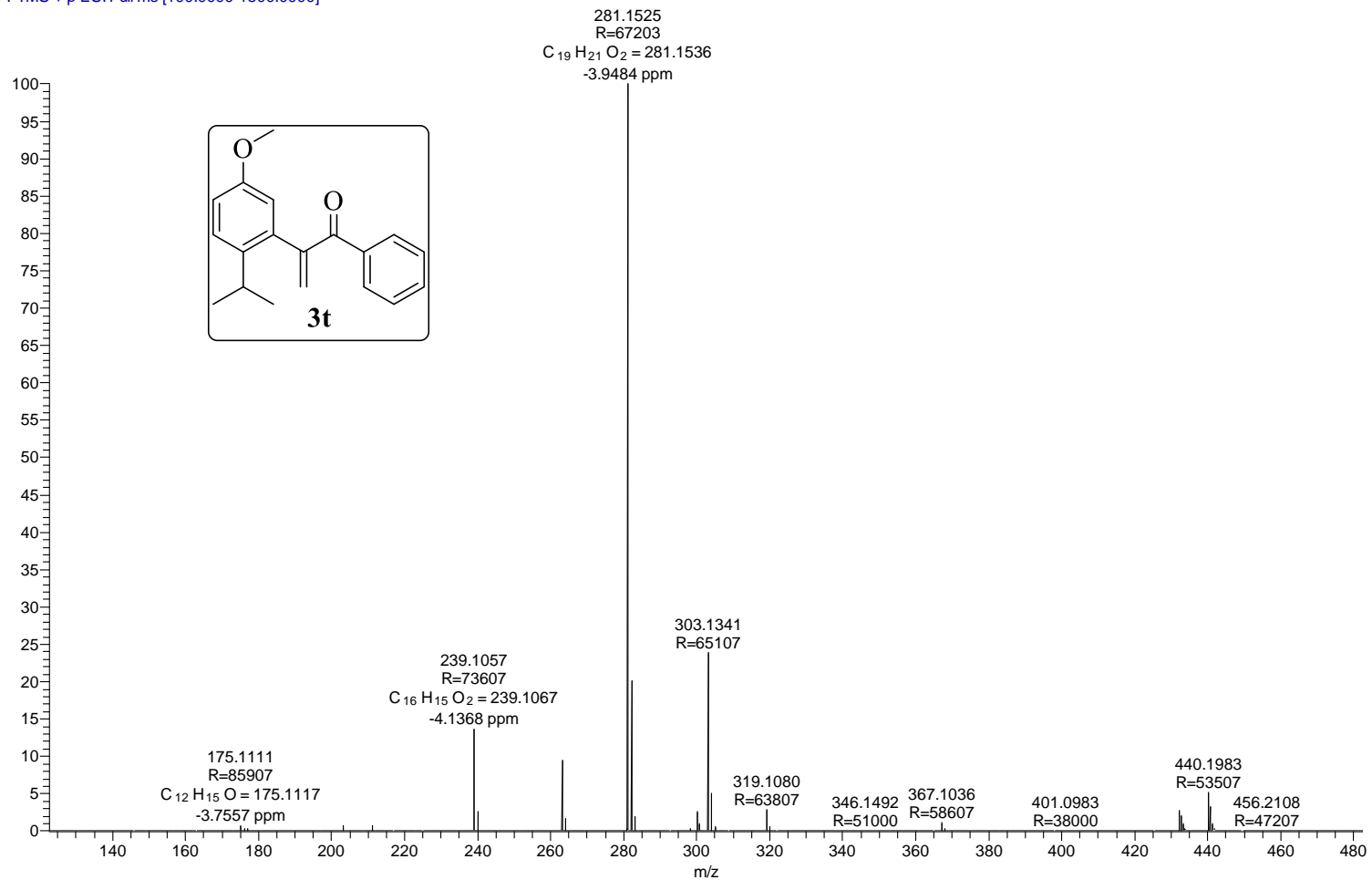


$^{13}\text{C} \{^1\text{H}\}$ NMR spectrum of compound **3t** (101 MHz, CDCl_3)

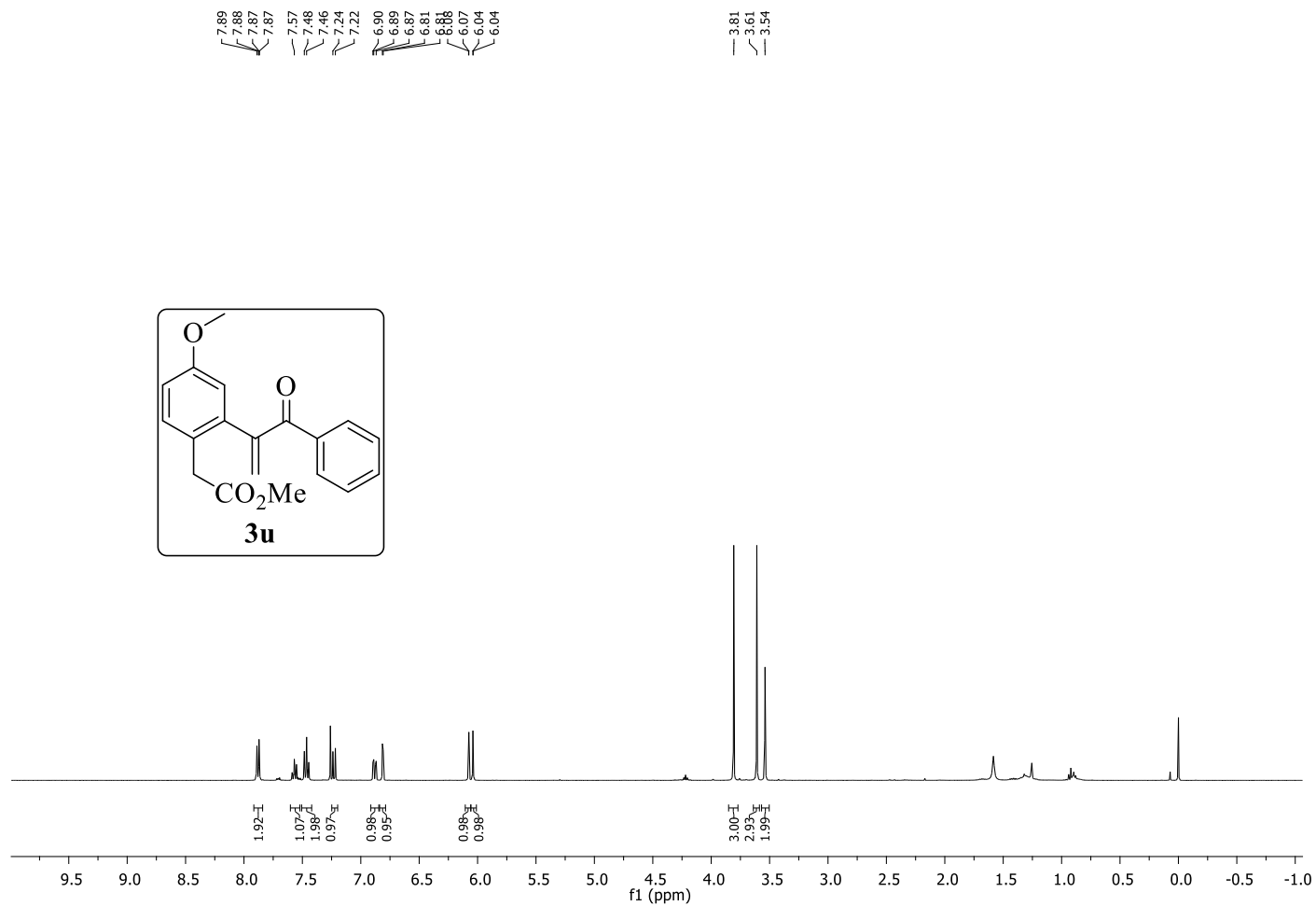


HRMS spectrum of compound 3t

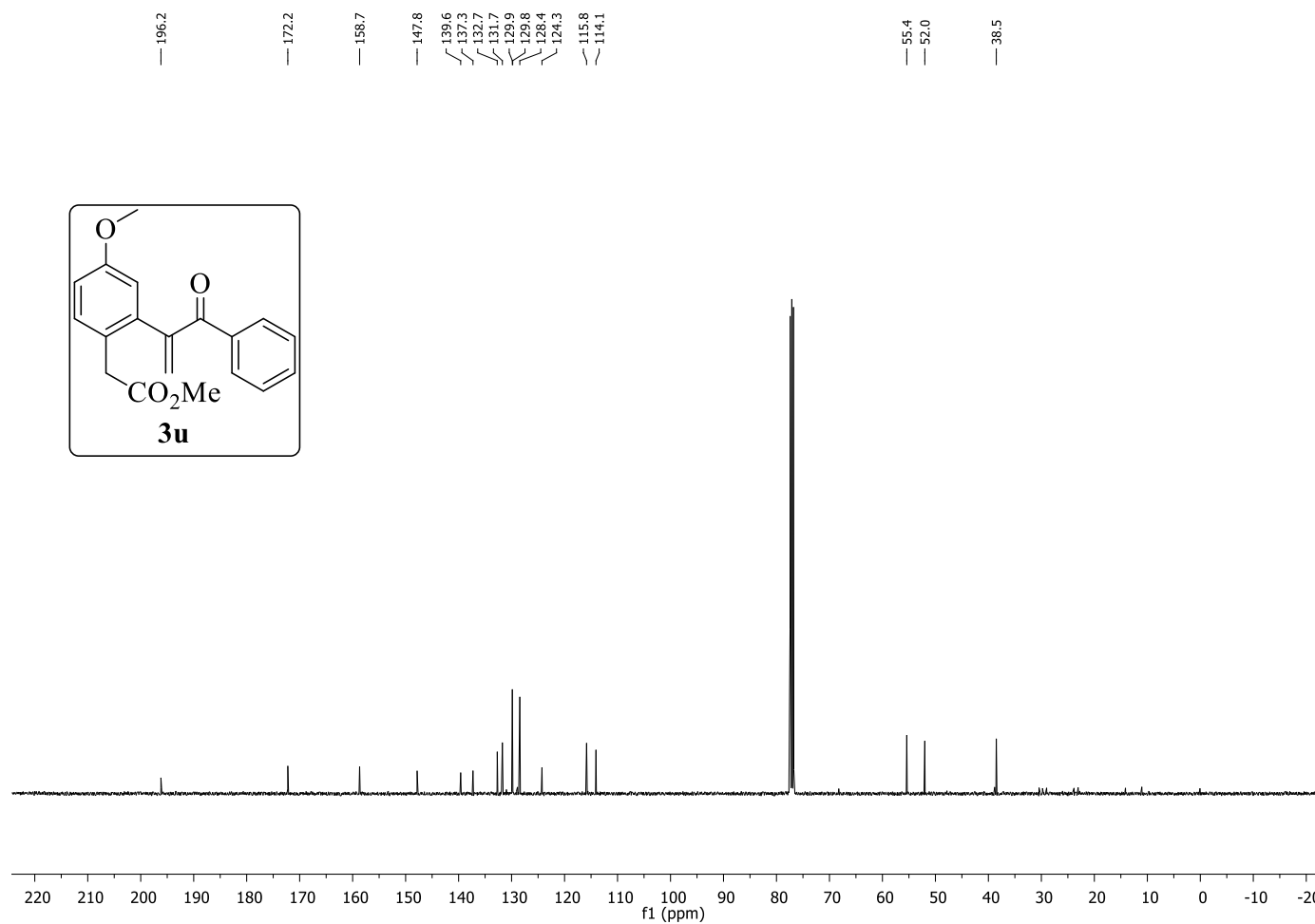
ARC-467 #528 RT: 2.35 AV: 1 NL: 8.02E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3u** (400 MHz, CDCl_3)

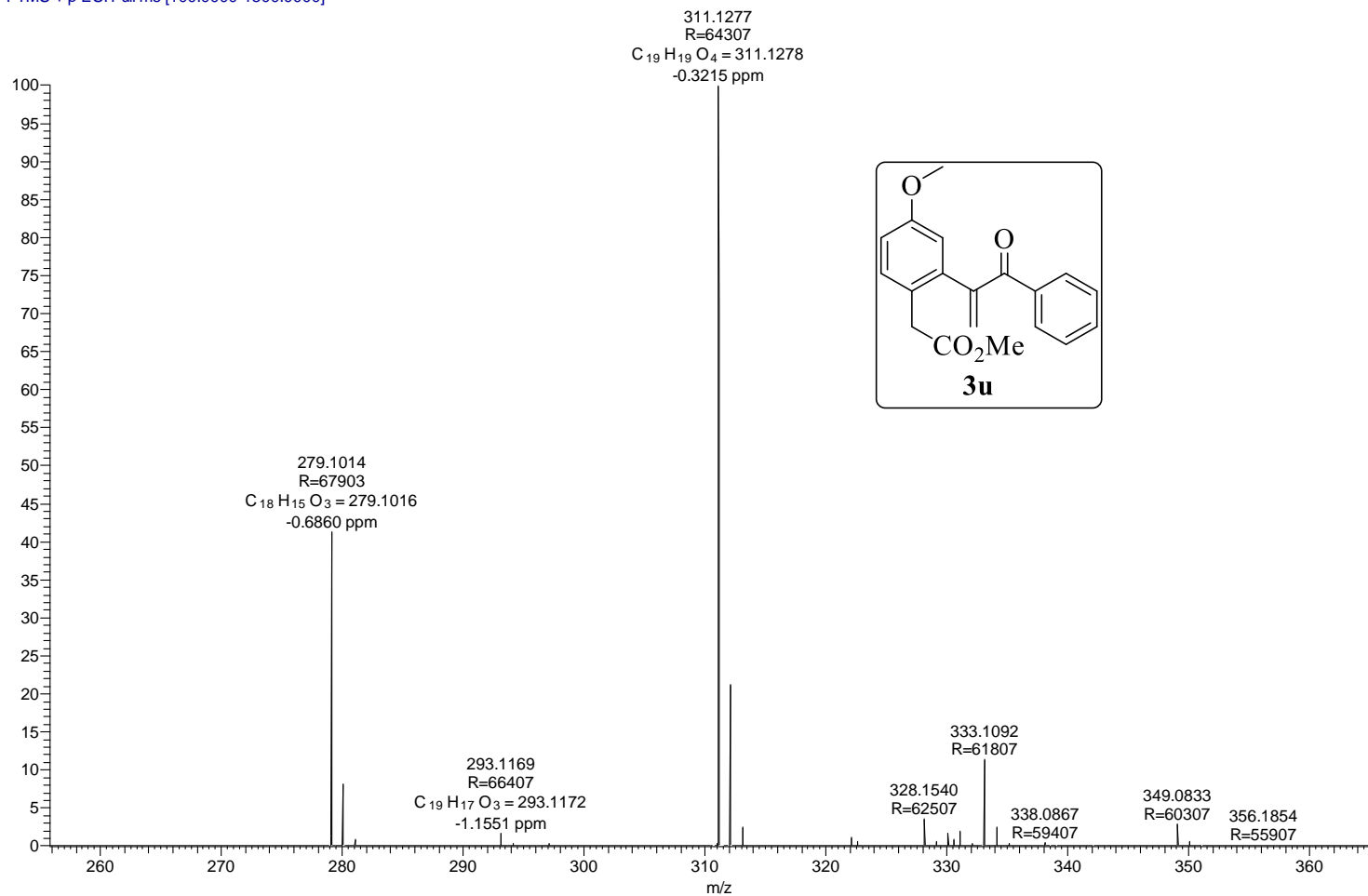


^{13}C { ^1H } NMR spectrum of compound **3u** (101 MHz, CDCl_3)

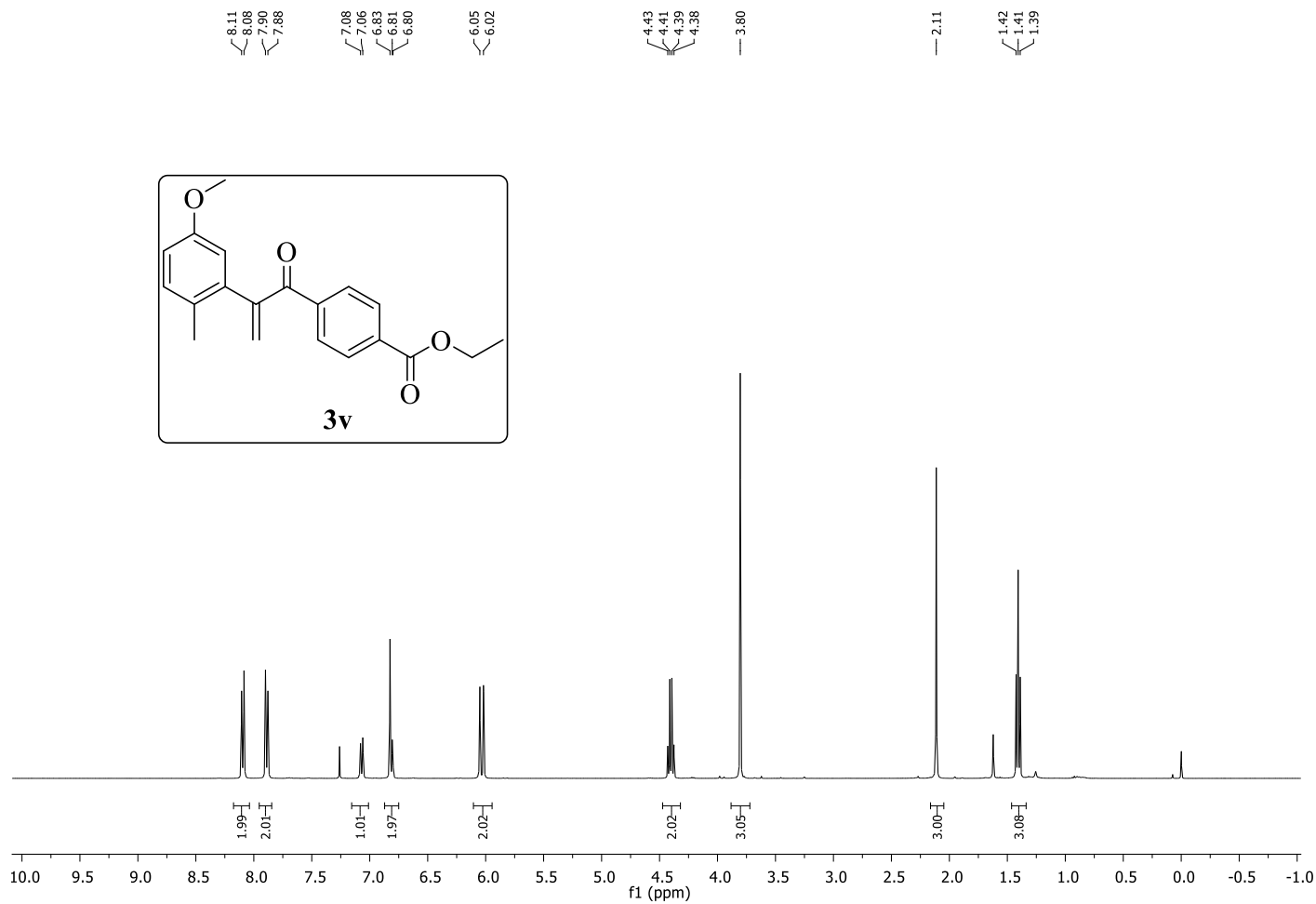


HRMS spectrum of compound **3u**

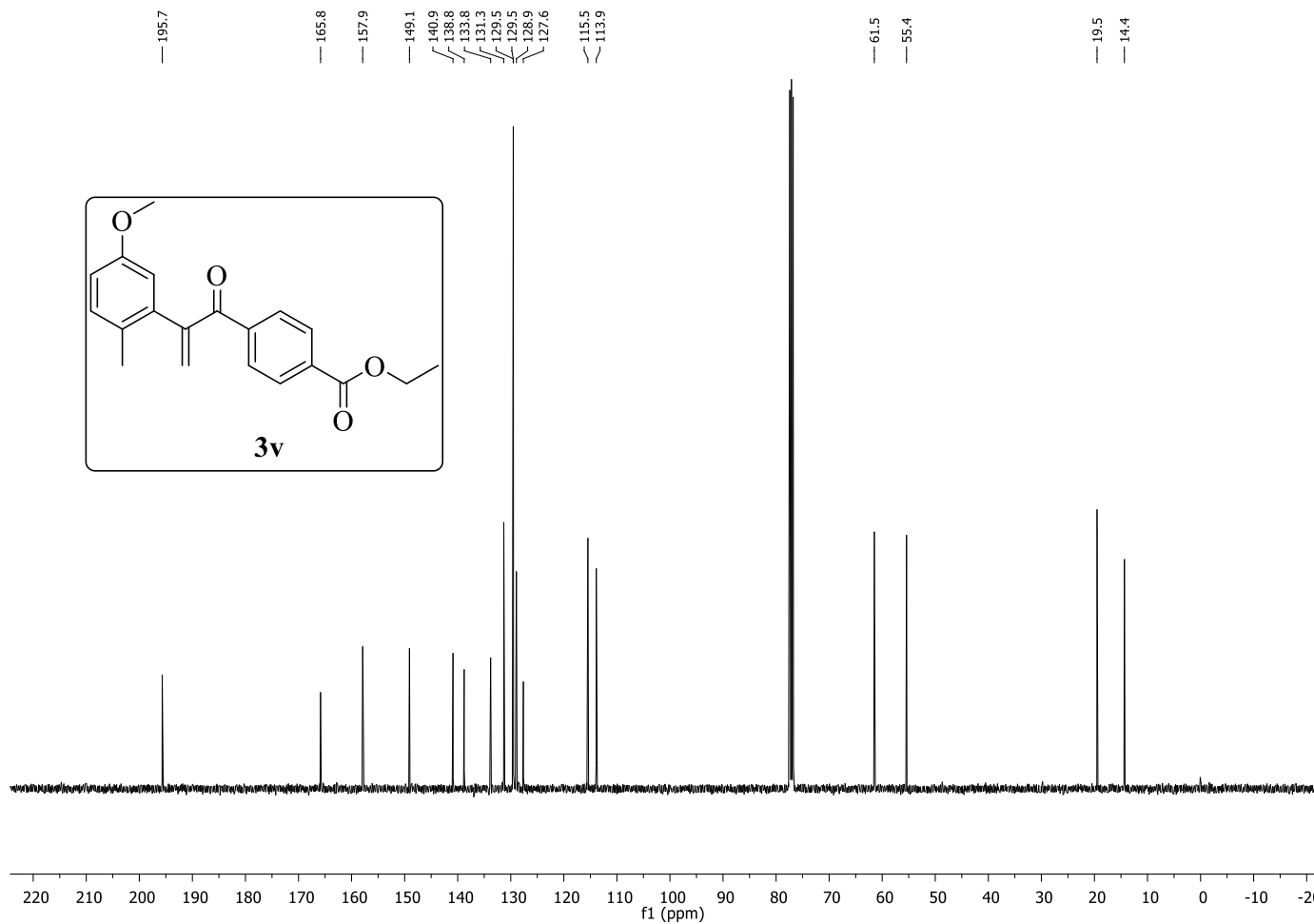
AR-571 #433 RT: 1.93 AV: 1 NL: 5.87E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3v** (400 MHz, CDCl_3)

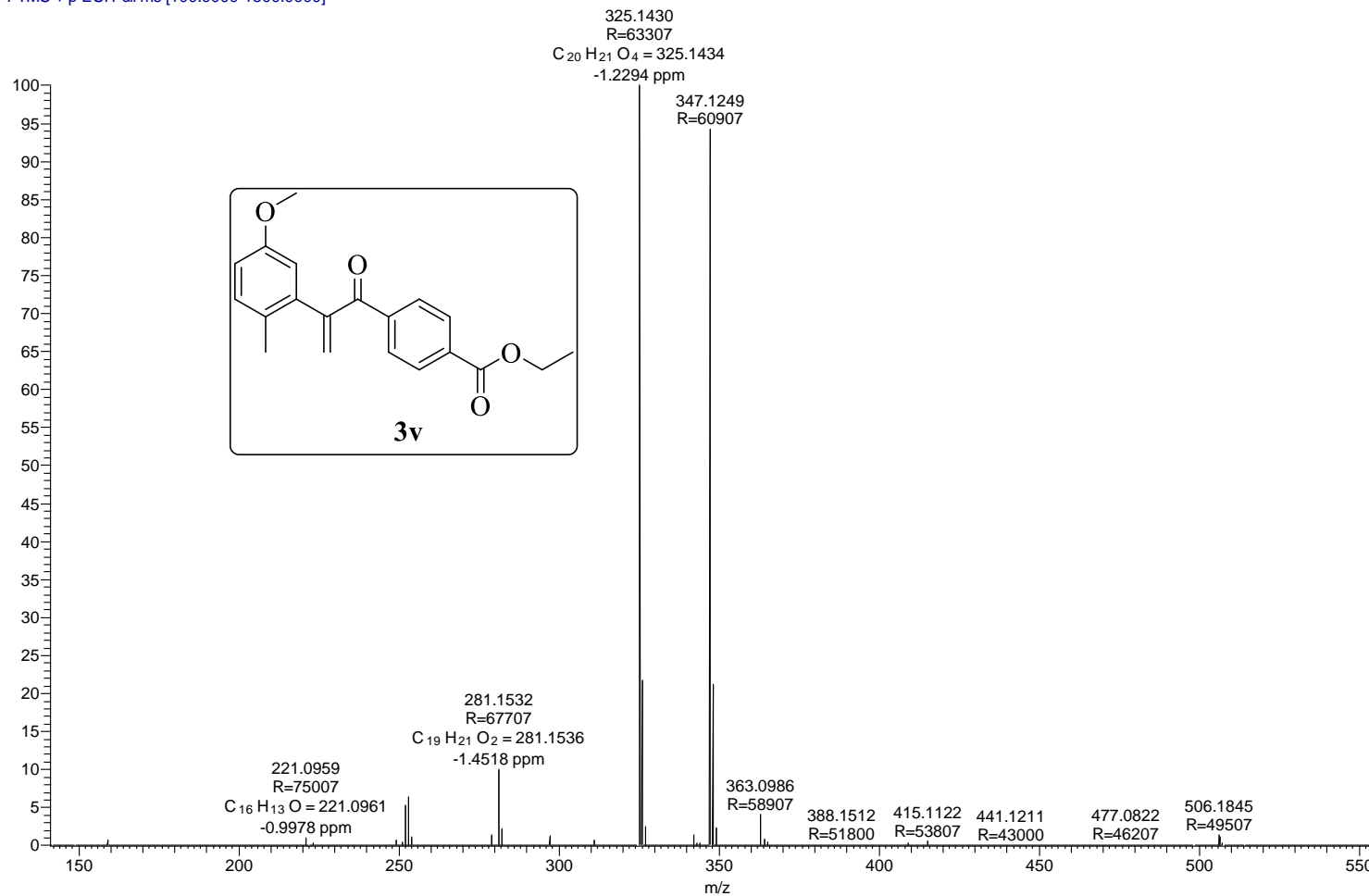


^{13}C { ^1H } NMR spectrum of compound **3v** (101 MHz, CDCl_3)

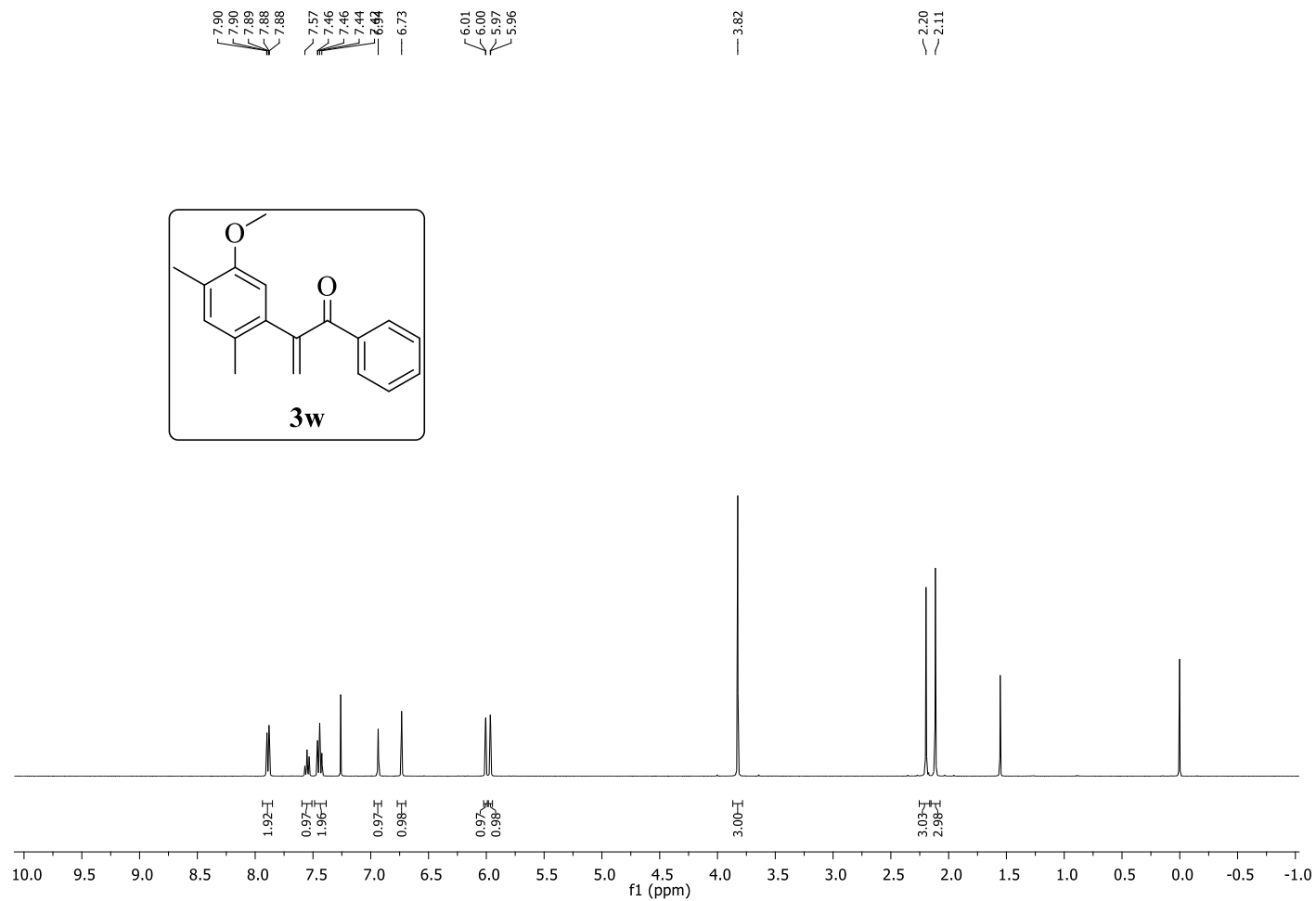


HRMS spectrum of compound **3v**

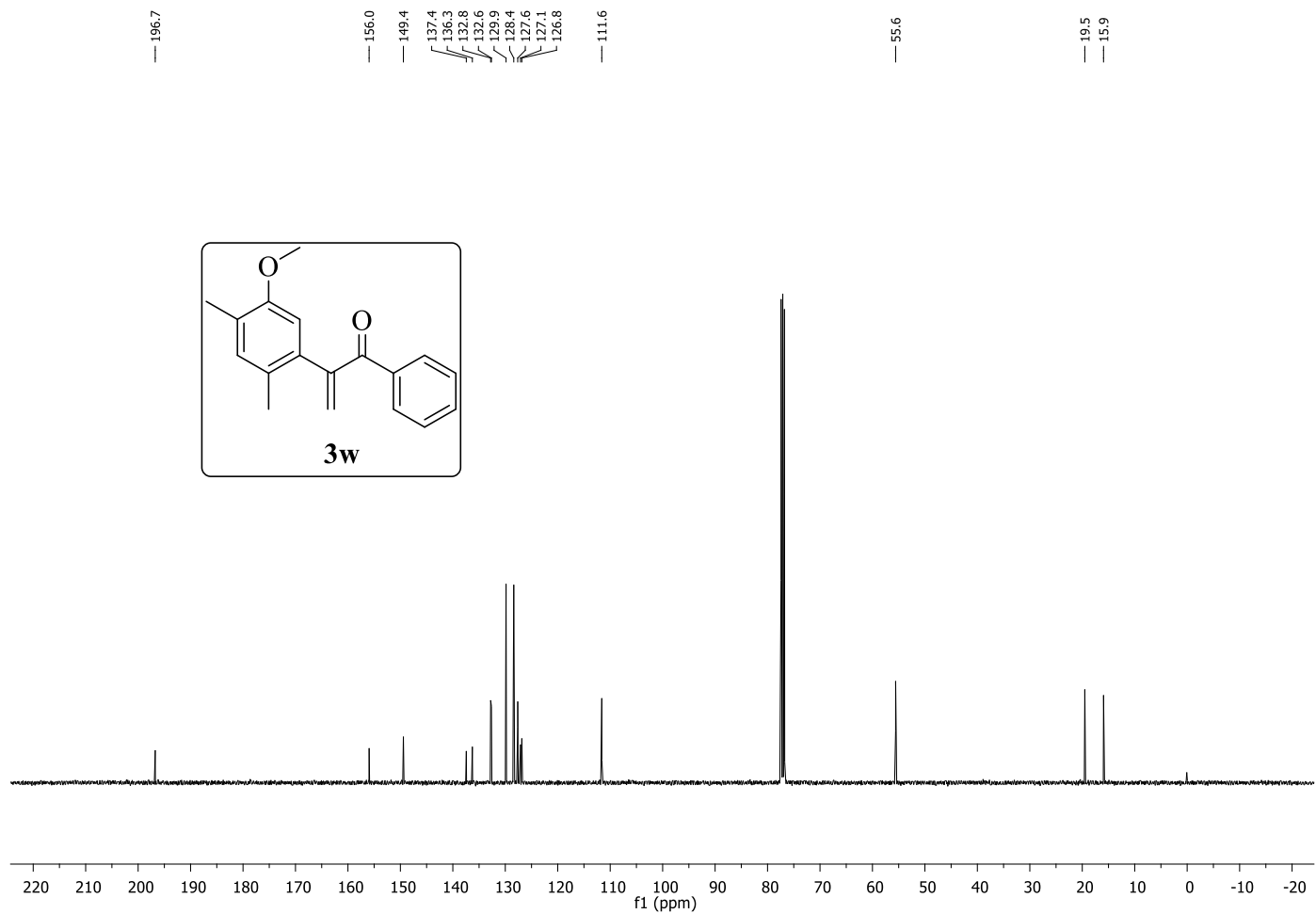
ARC-5 #512 RT: 2.28 AV: 1 NL: 4.25E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3w** (400 MHz, CDCl_3)

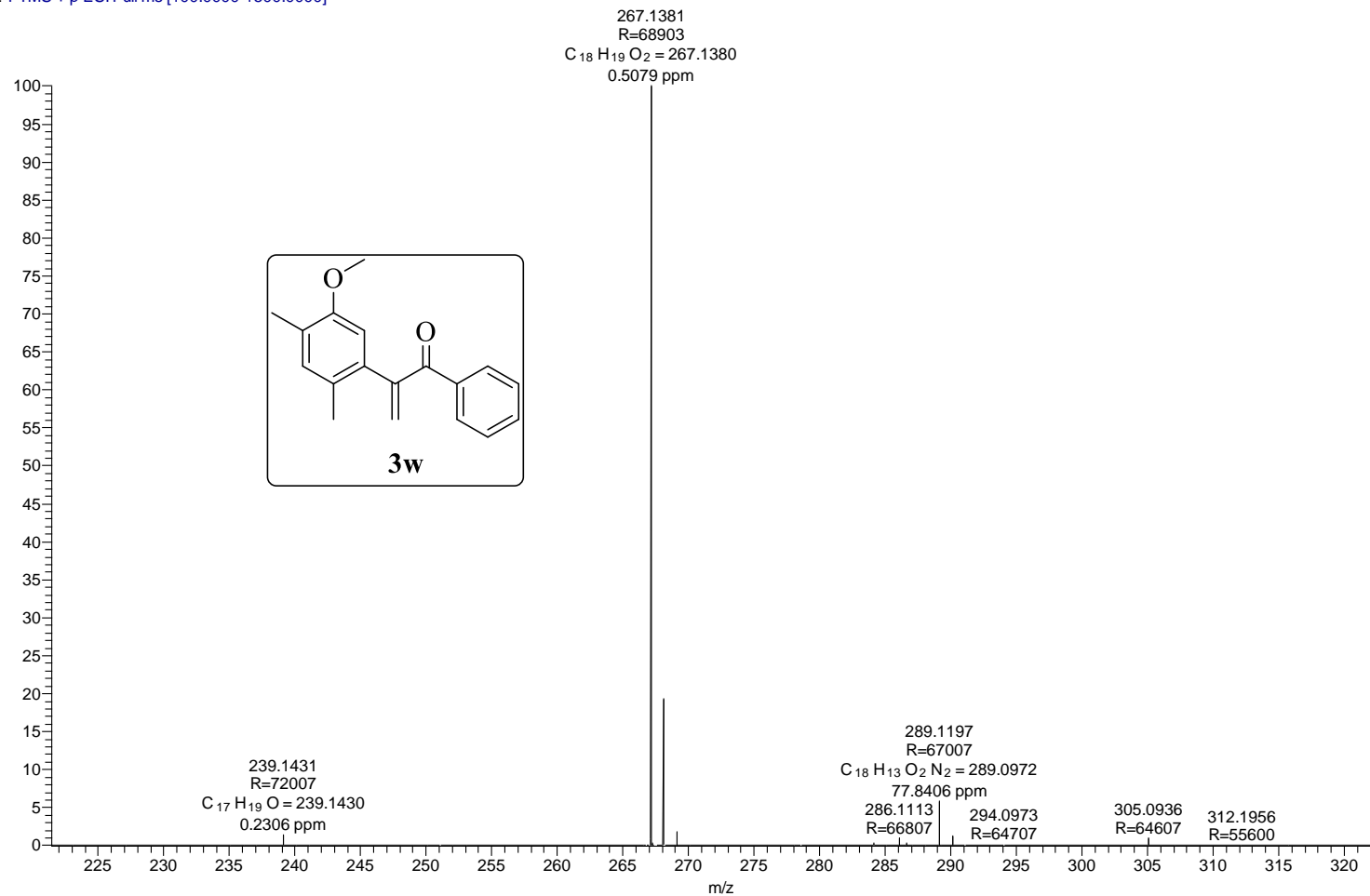


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3w** (101 MHz, CDCl_3)

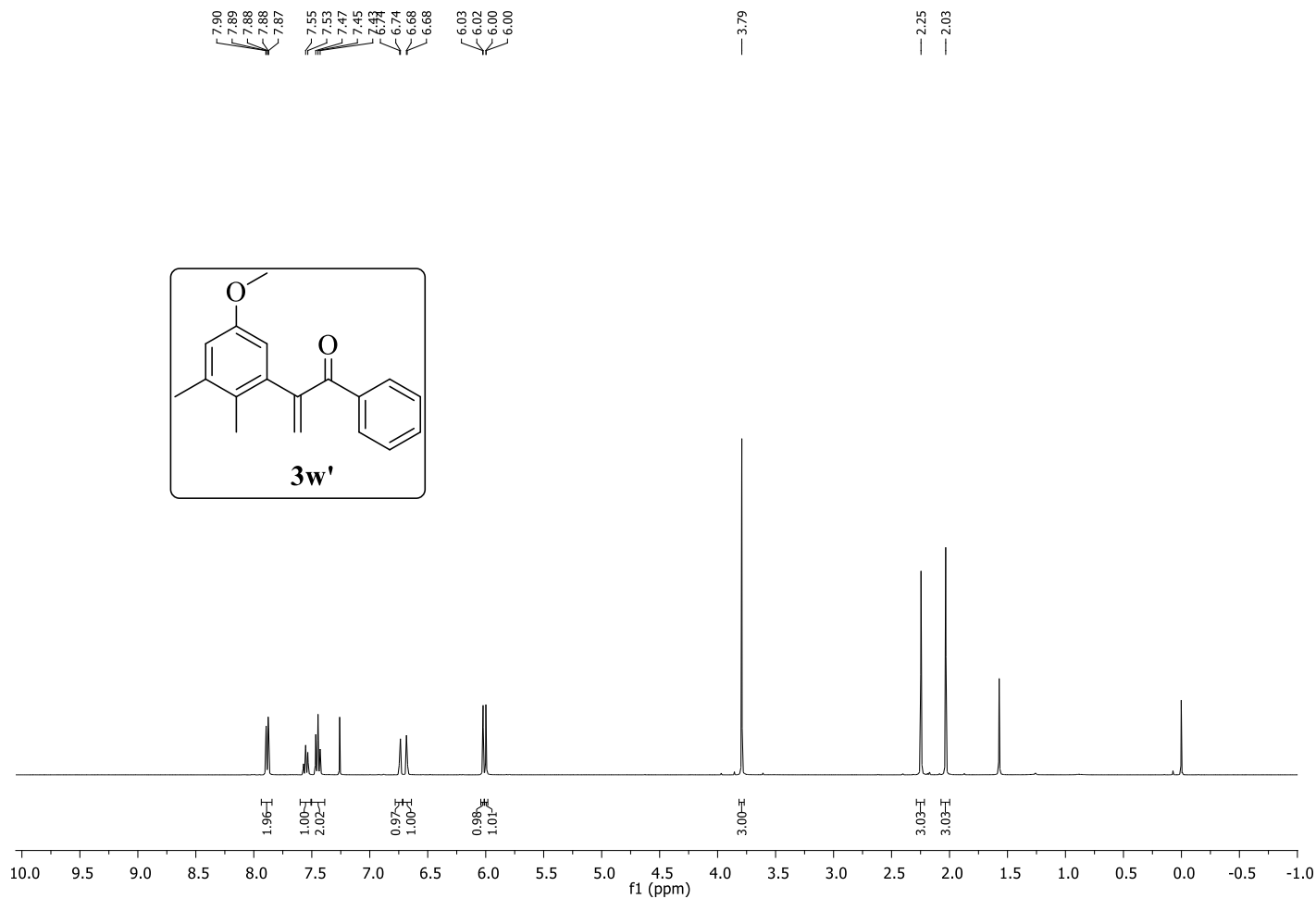


HRMS spectrum of compound **3w**

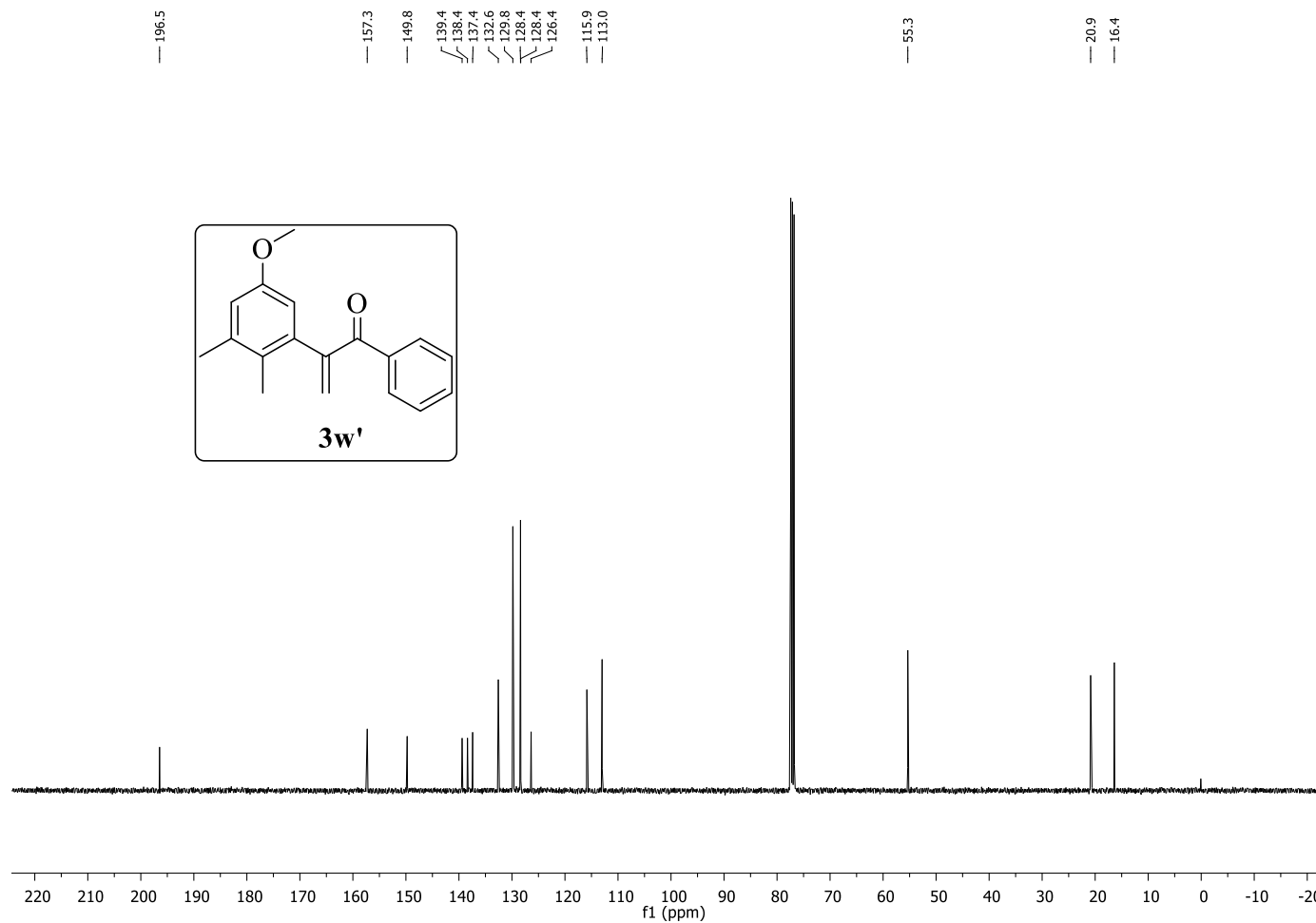
AR-569 #538 RT: 2.40 AV: 1 NL: 8.55E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3w'** (400 MHz, CDCl_3)

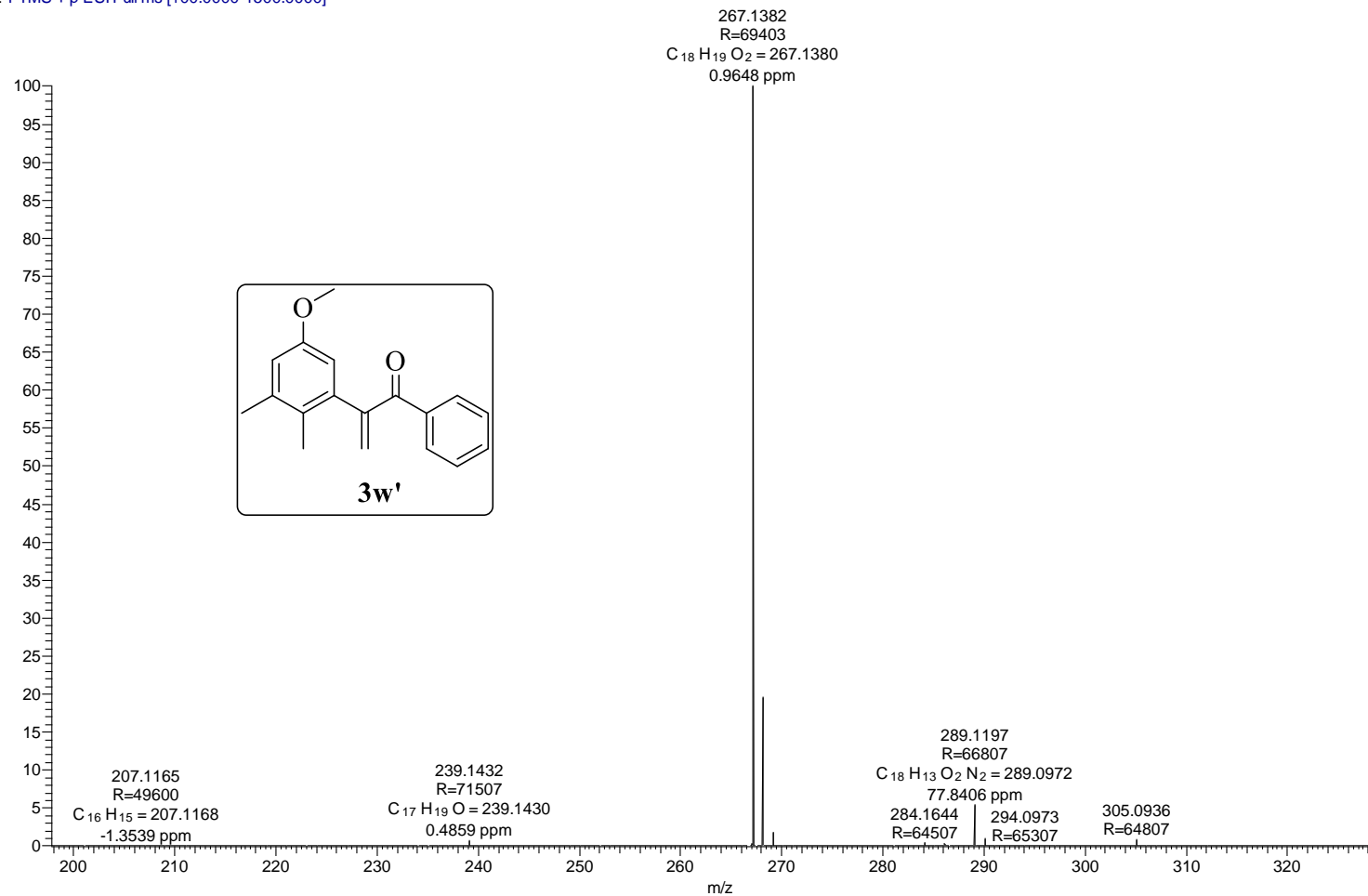


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3w'** (101 MHz, CDCl_3)

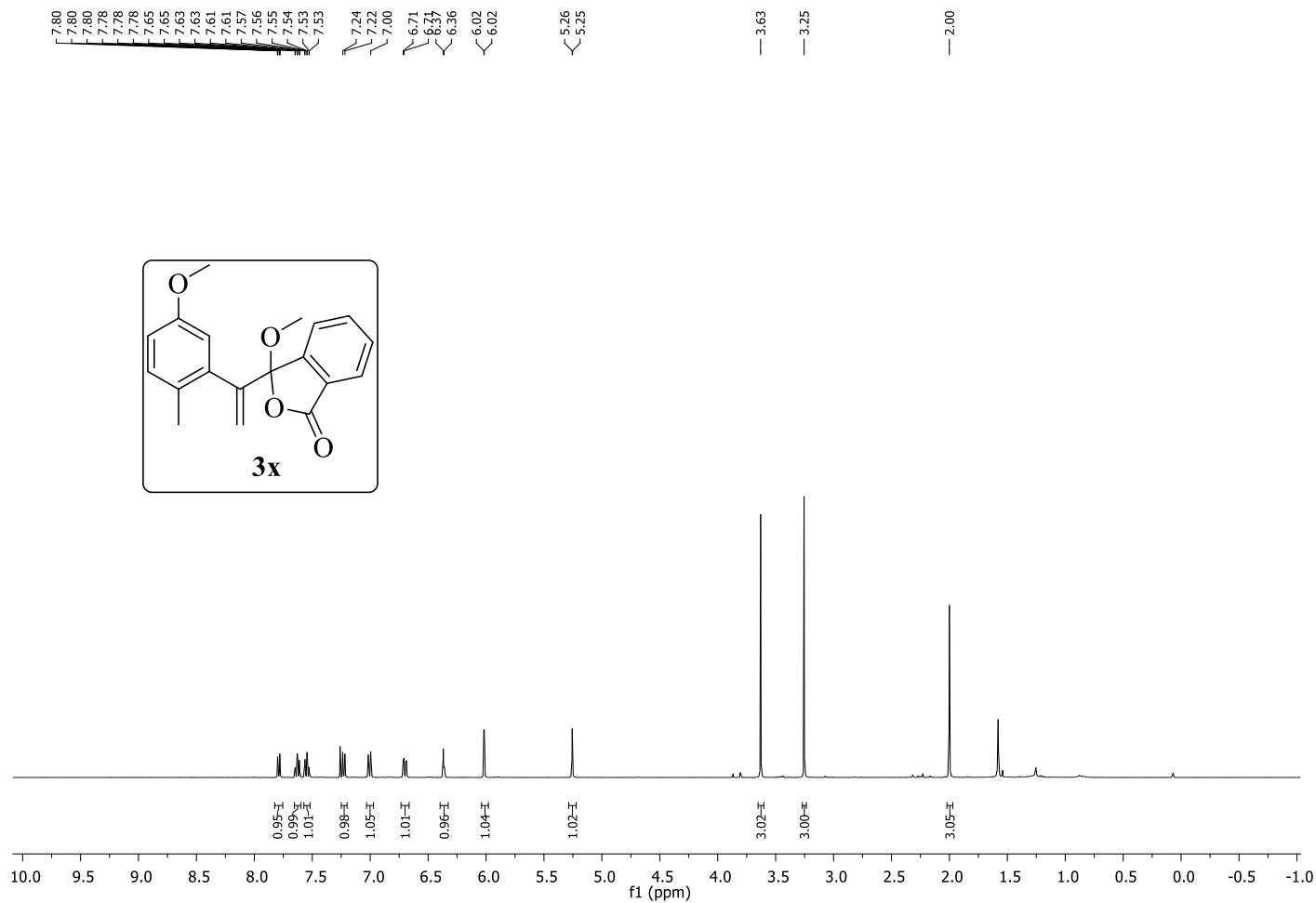


HRMS spectrum of compound **3w'**

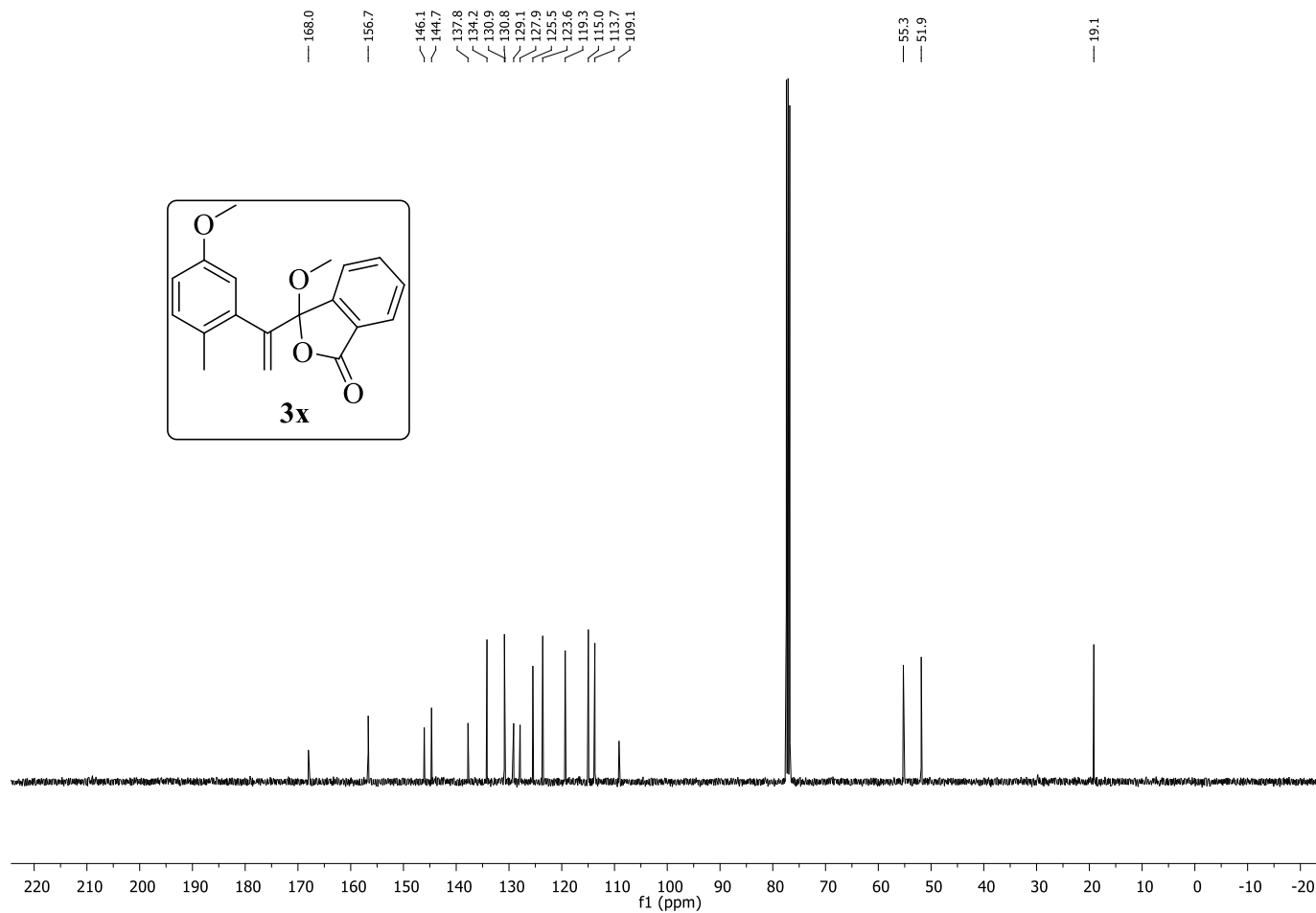
AR-568 #518 RT: 2.31 AV: 1 NL: 1.27E10
T: FTMS + p ESI Full ms [100.0000-1500.0000]



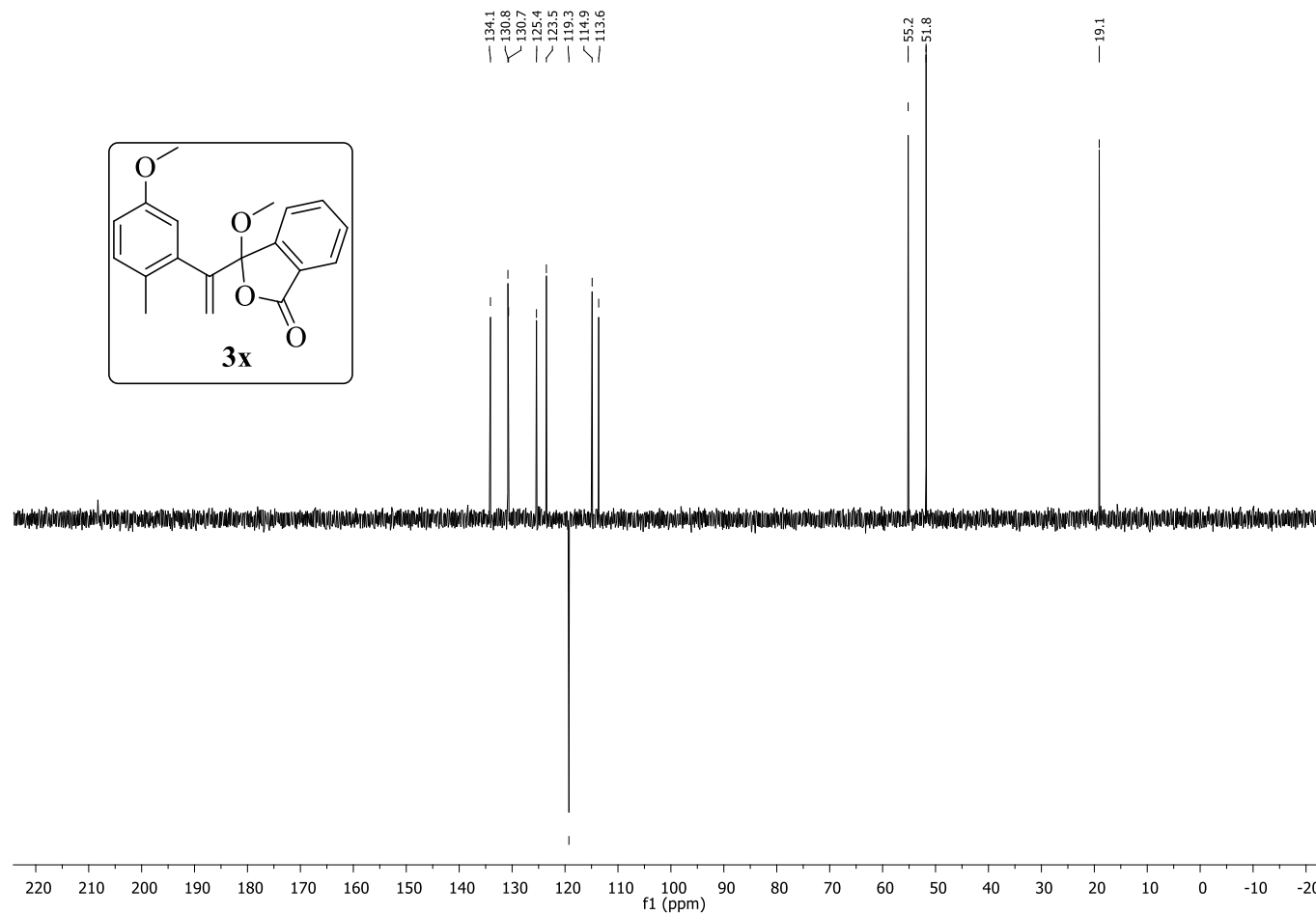
¹H NMR spectrum of compound **3x** (400 MHz, CDCl₃)



$^{13}\text{C} \{^1\text{H}\}$ NMR spectrum of compound **3x** (101 MHz, CDCl_3)

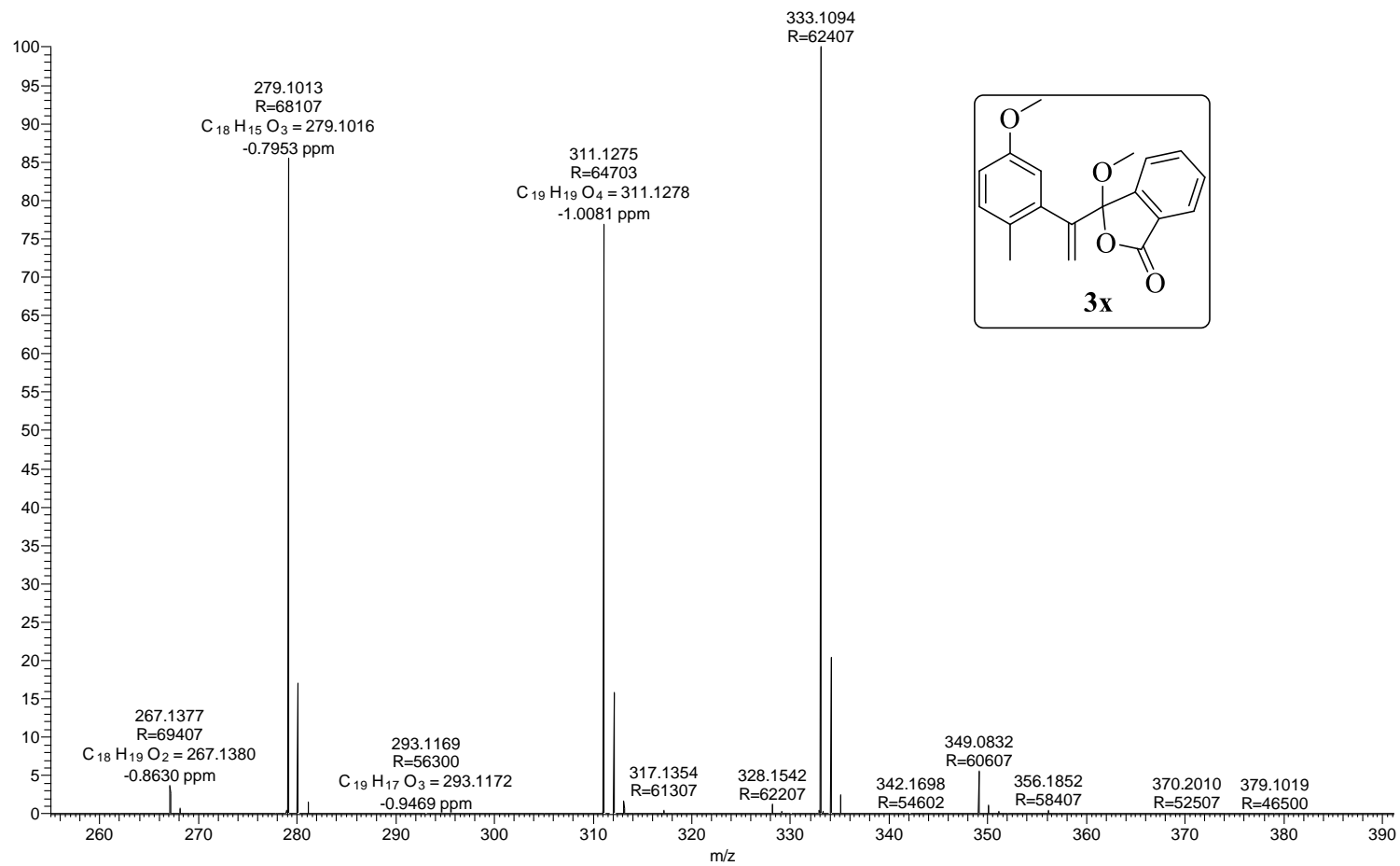


^{13}C $\{^1\text{H}\}$ DEPT NMR spectrum of compound **3x** (101 MHz, CDCl_3)

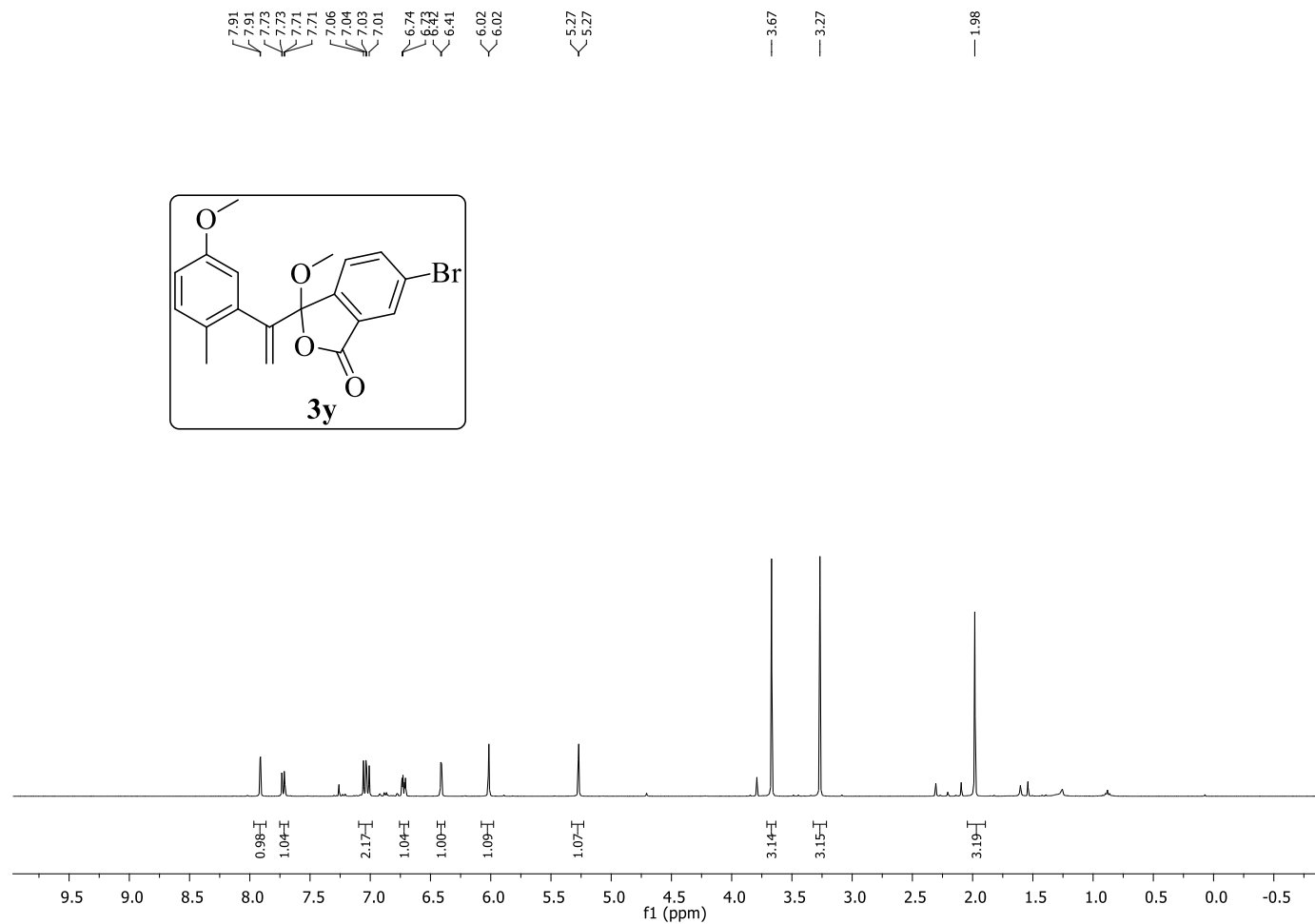


HRMS spectrum of compound 3x

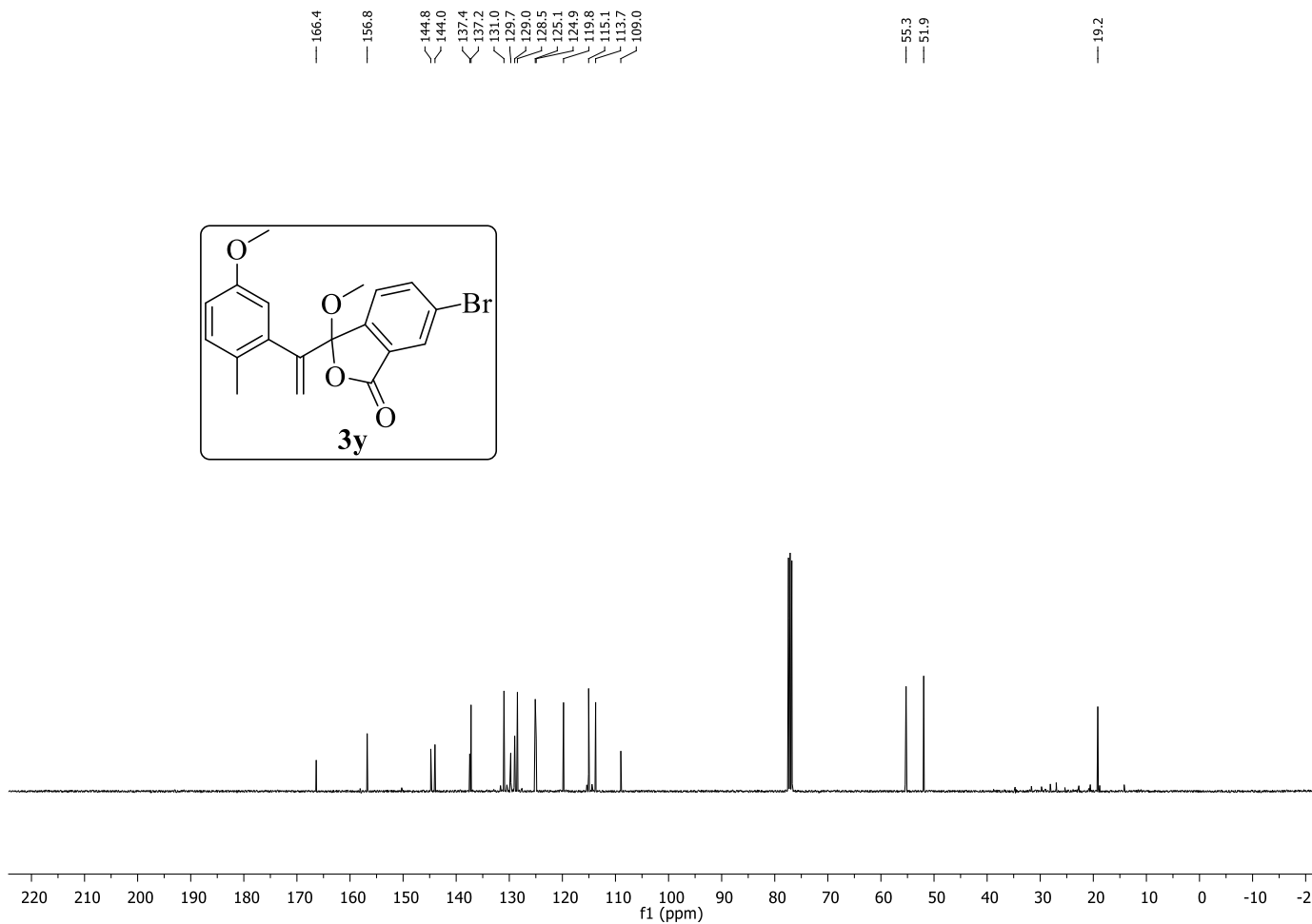
ARC-26 #457 RT: 2.03 AV: 1 NL: 4.08E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3y** (400 MHz, CDCl_3)

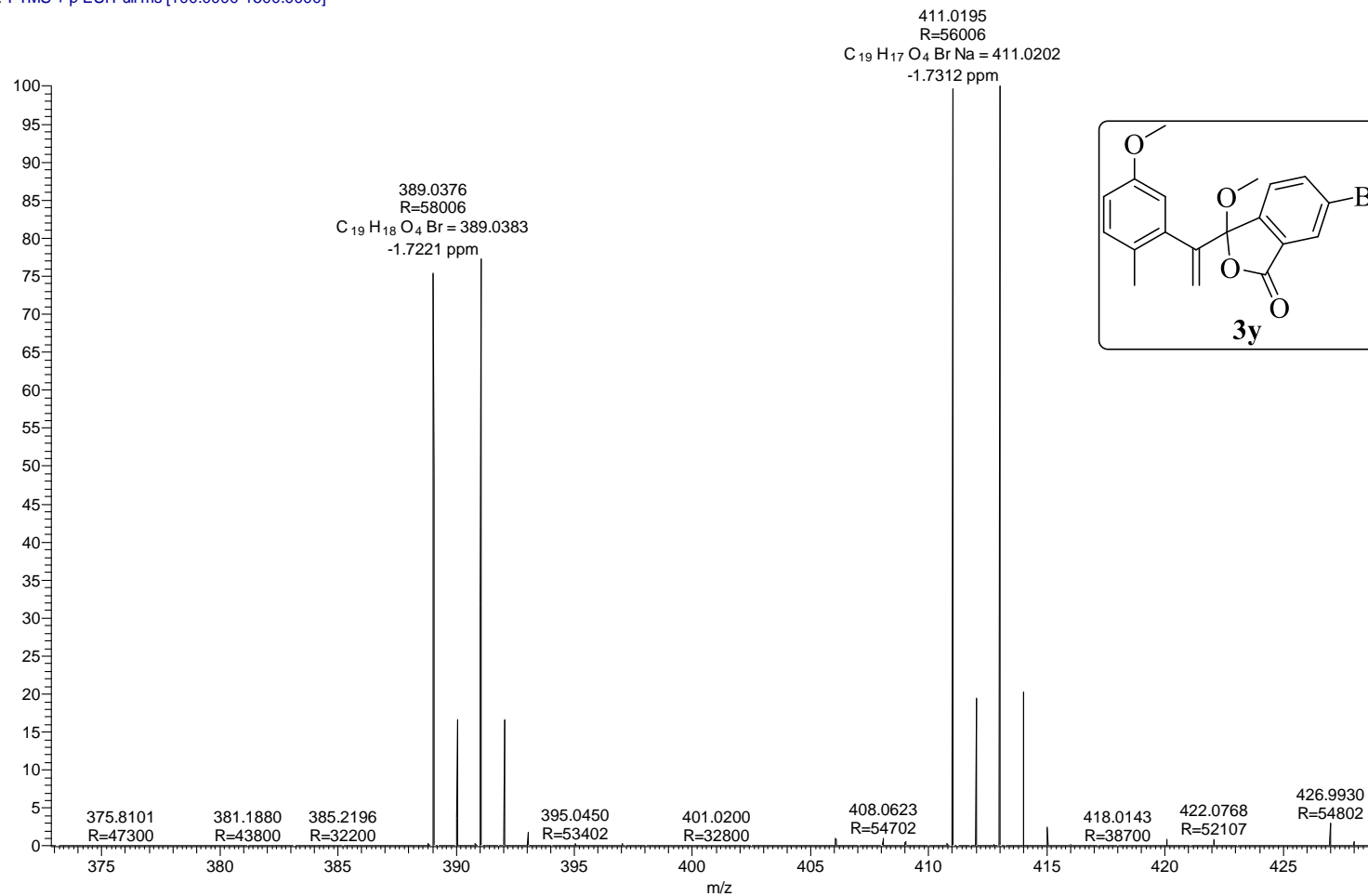


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3y** (101 MHz, CDCl_3)

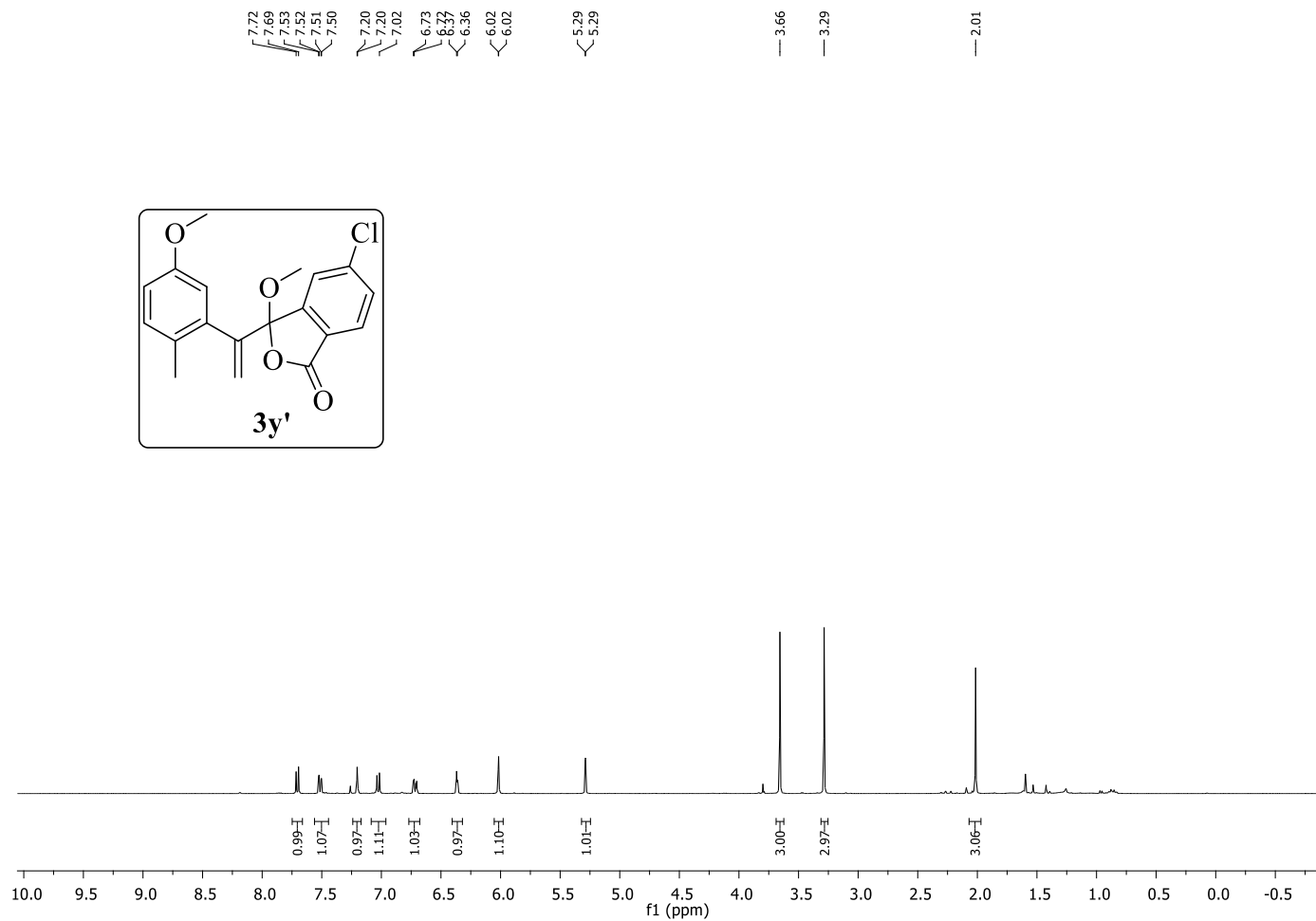


HRMS spectrum of compound **3y**

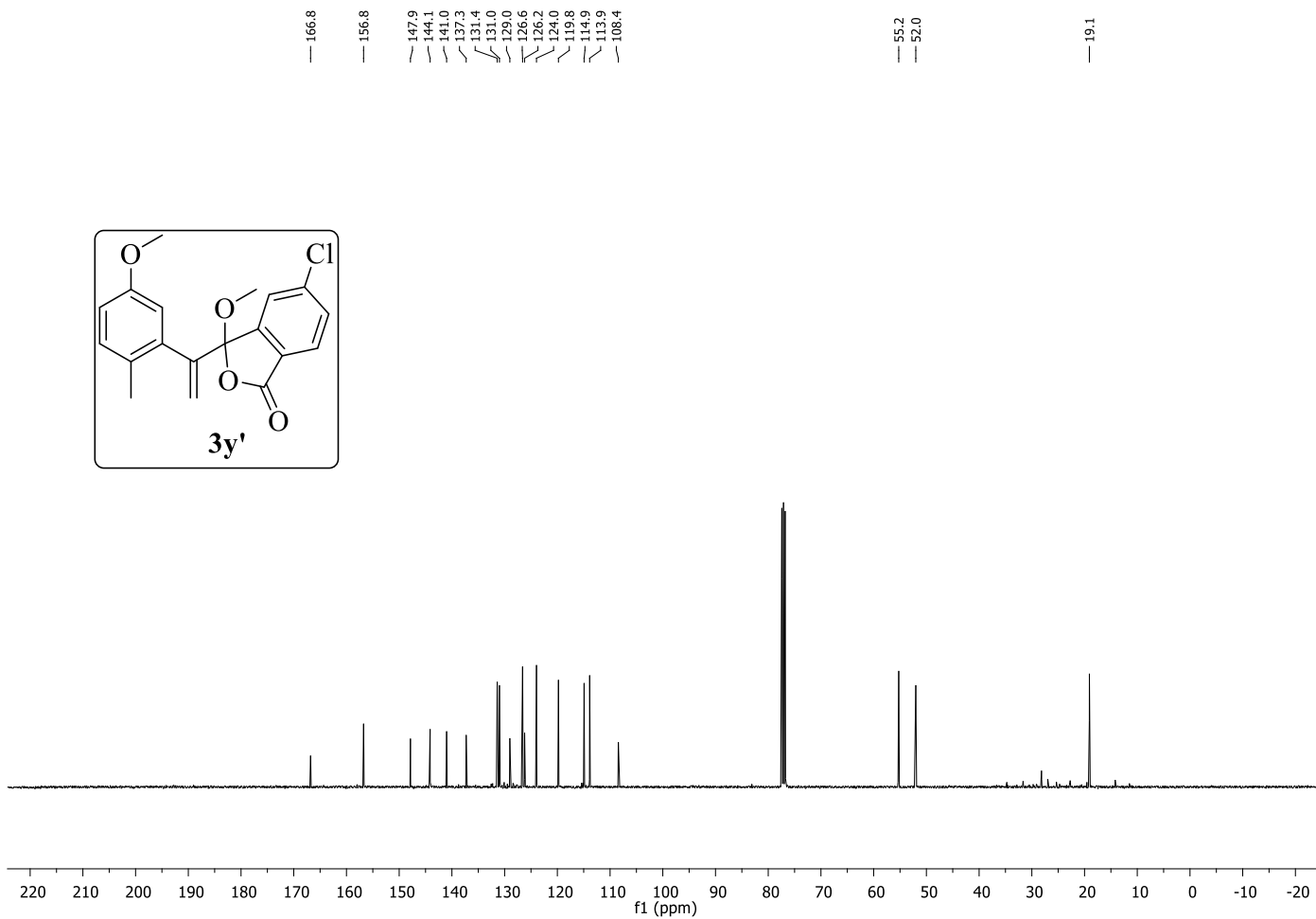
AR-460 #528 RT: 2.35 AV: 1 NL: 1.27E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3y'** (400 MHz, CDCl_3)

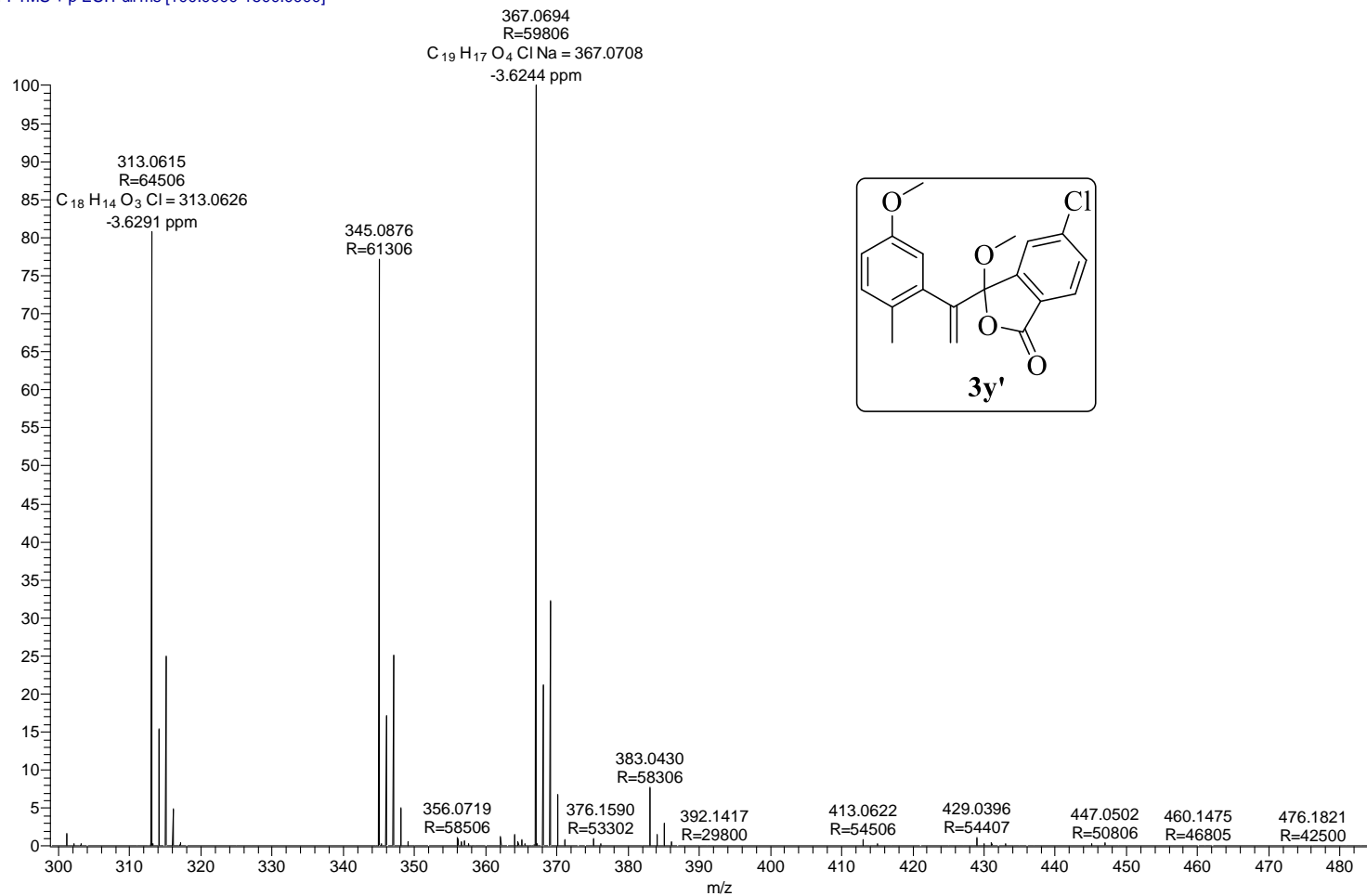


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **3y'** (101 MHz, CDCl_3)

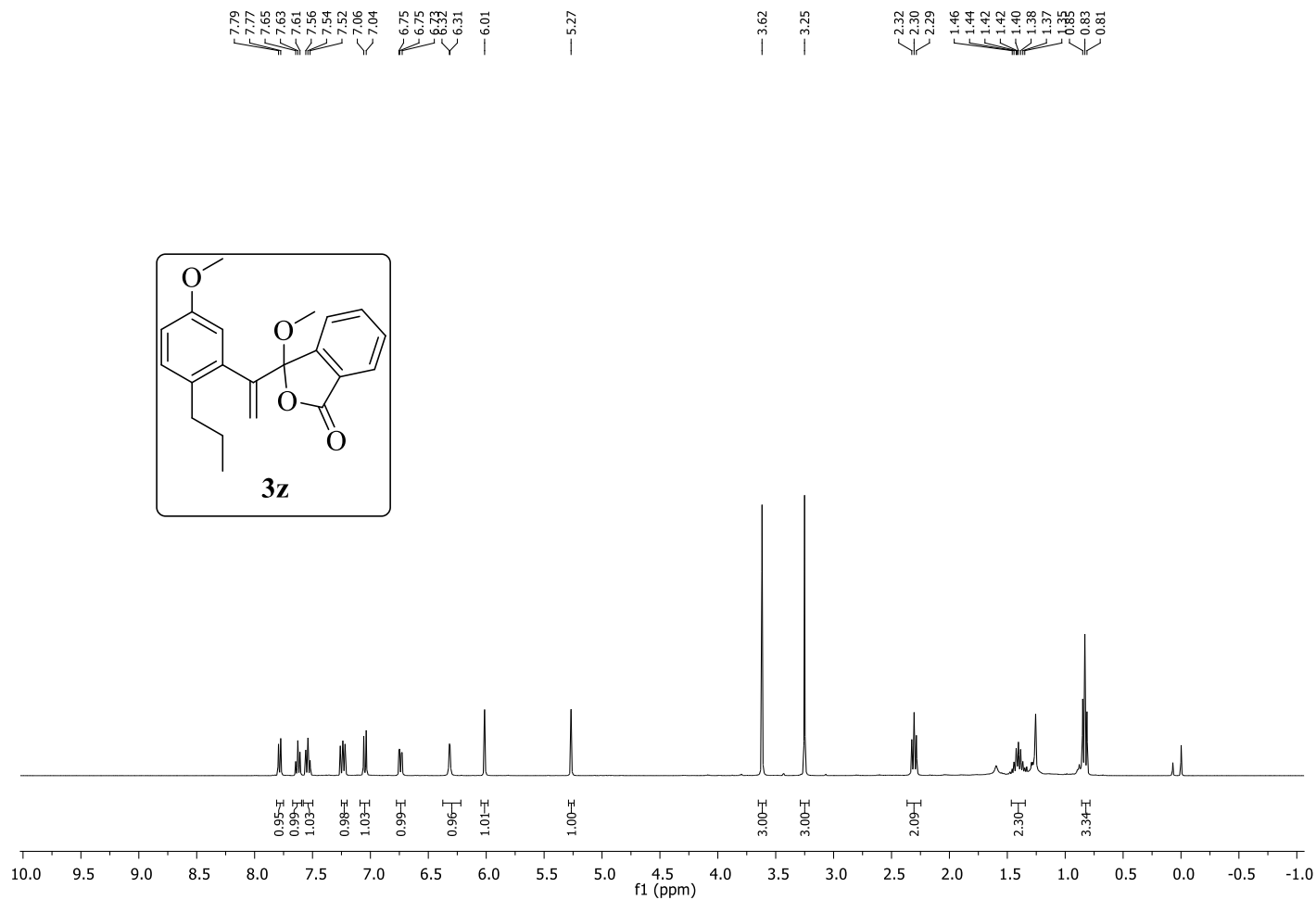


HRMS spectrum of compound **3y'**

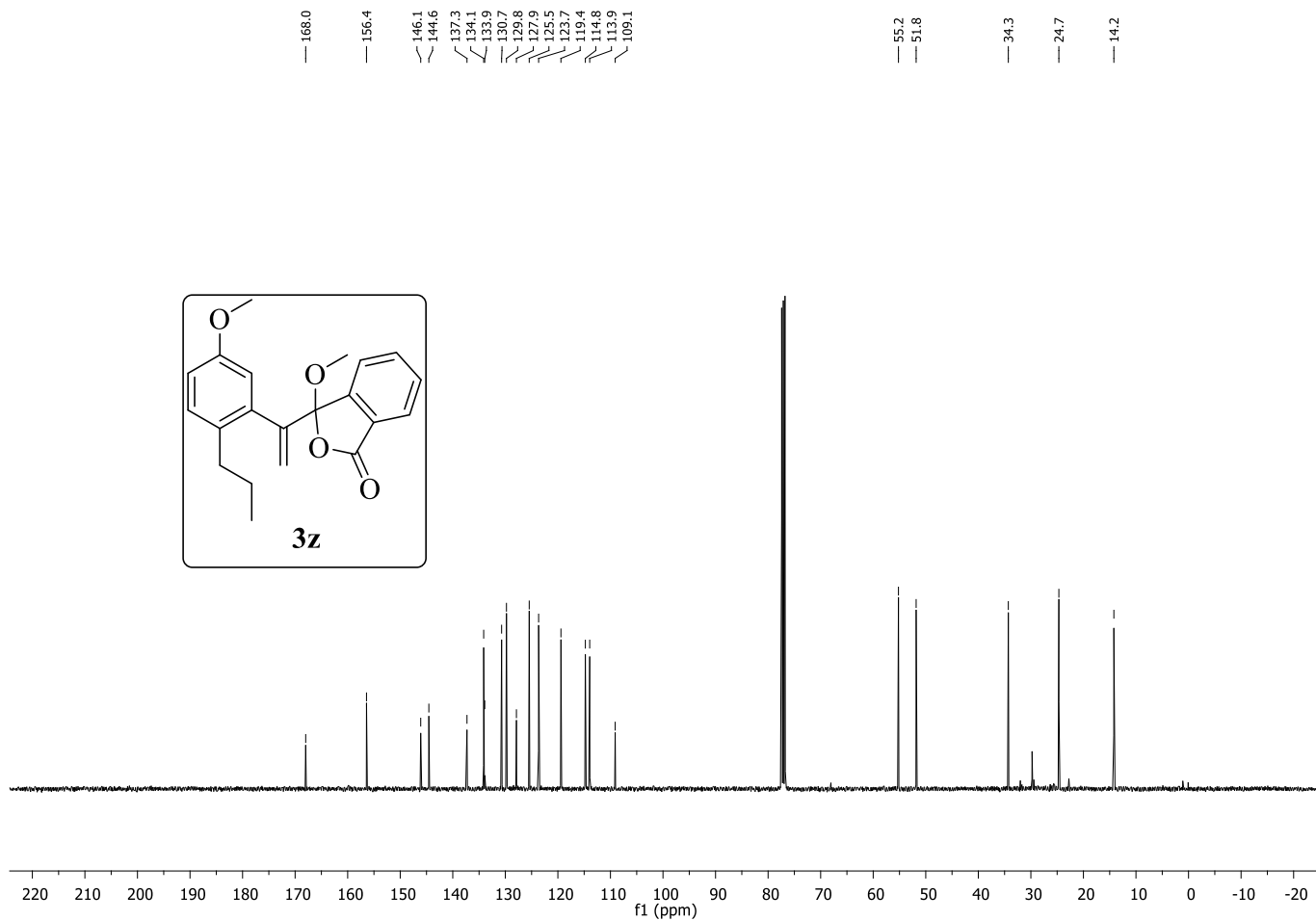
ARC-483 #512 RT: 2.28 AV: 1 NL: 1.83E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **3z** (400 MHz, CDCl_3)

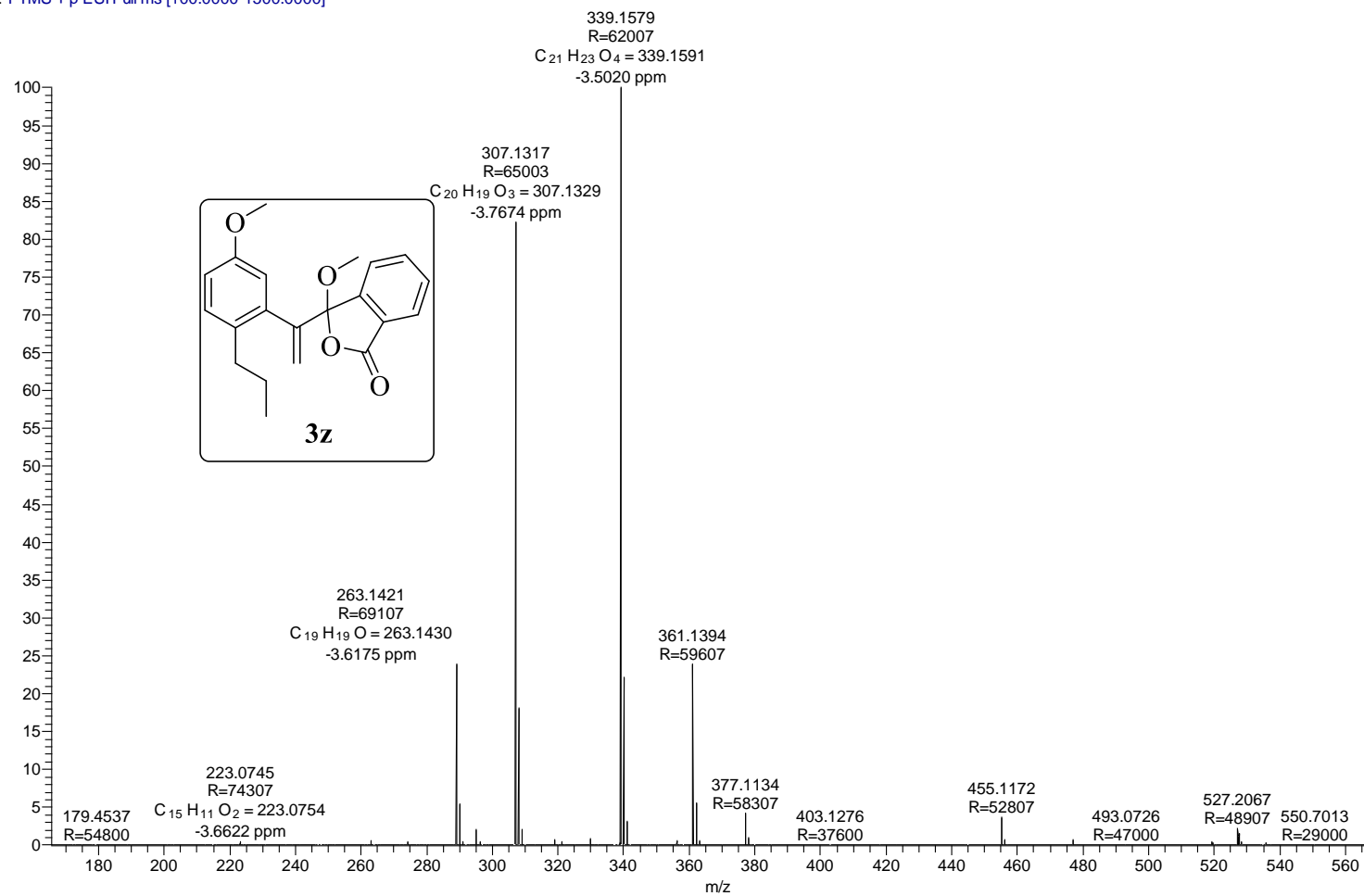


$^{13}\text{C} \{^1\text{H}\}$ NMR spectrum of compound **3z** (101 MHz, CDCl_3)

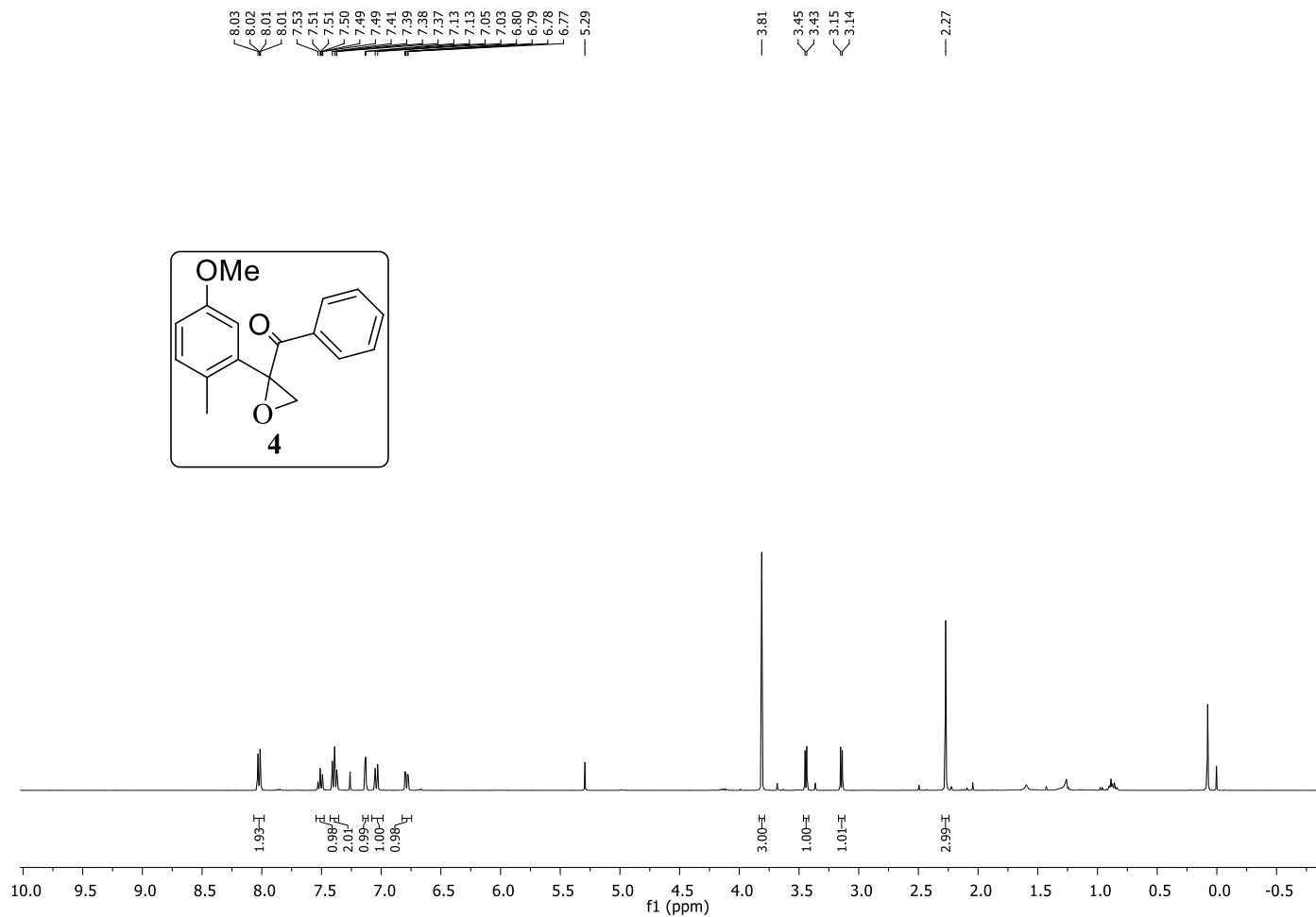


HRMS spectrum of compound **3z**

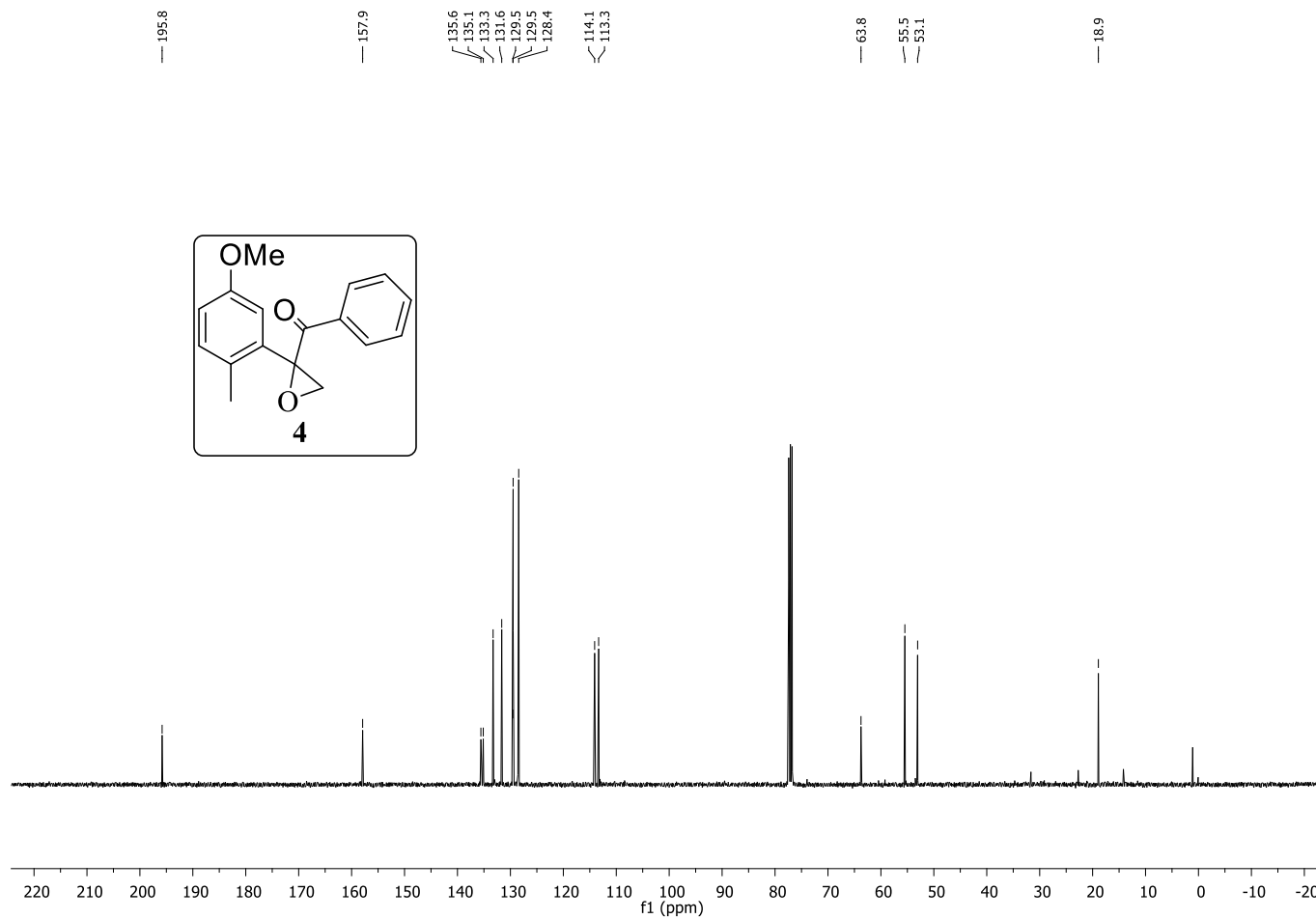
AR-459 #493 RT: 2.20 AV: 1 NL: 5.02E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **4** (400 MHz, CDCl_3)

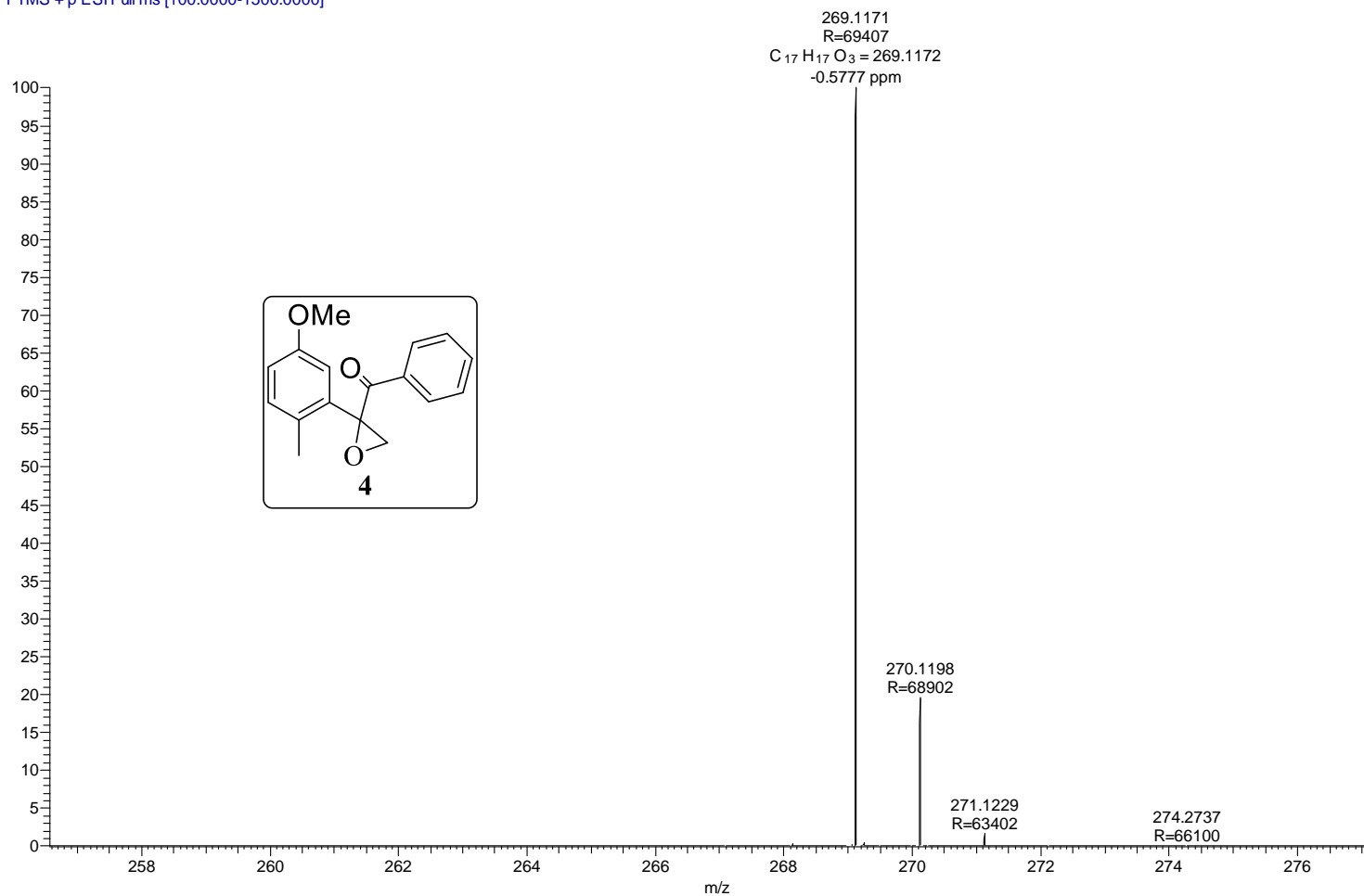


^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **4** (101 MHz, CDCl_3)

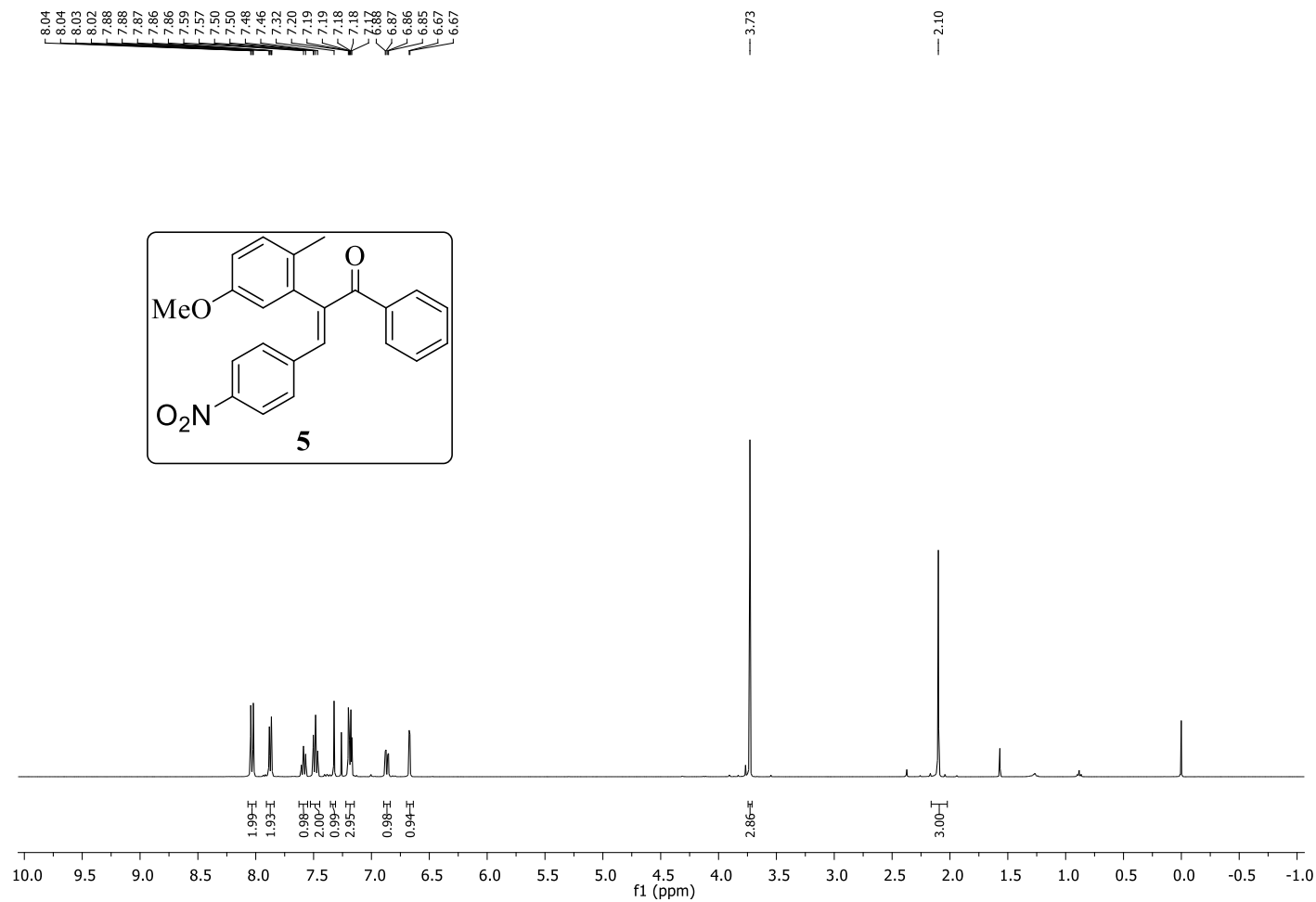


HRMS spectrum of compound 4

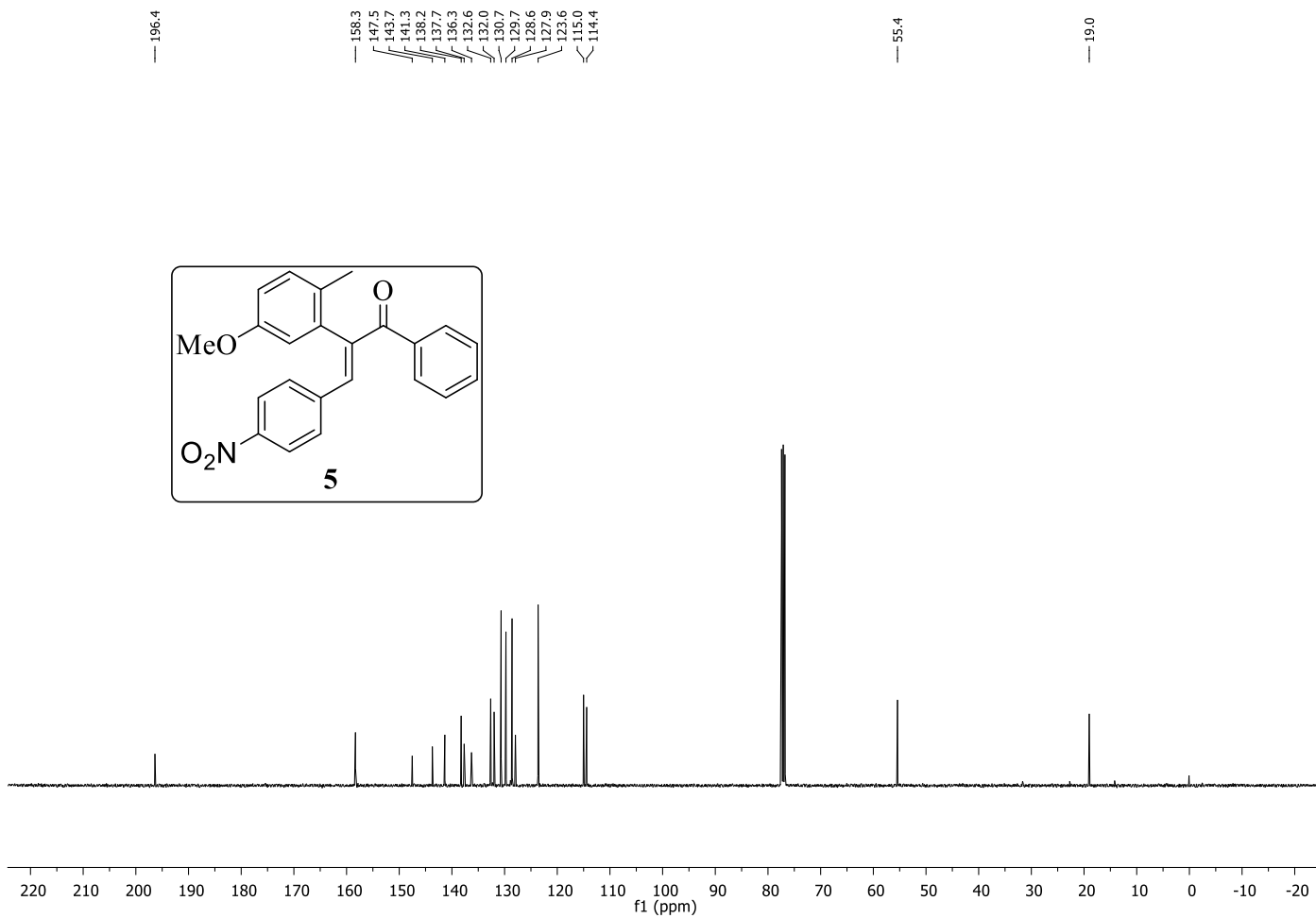
AR-506 #474 RT: 2.11 AV: 1 NL: 1.29E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



^1H NMR spectrum of compound **5** (400 MHz, CDCl_3)

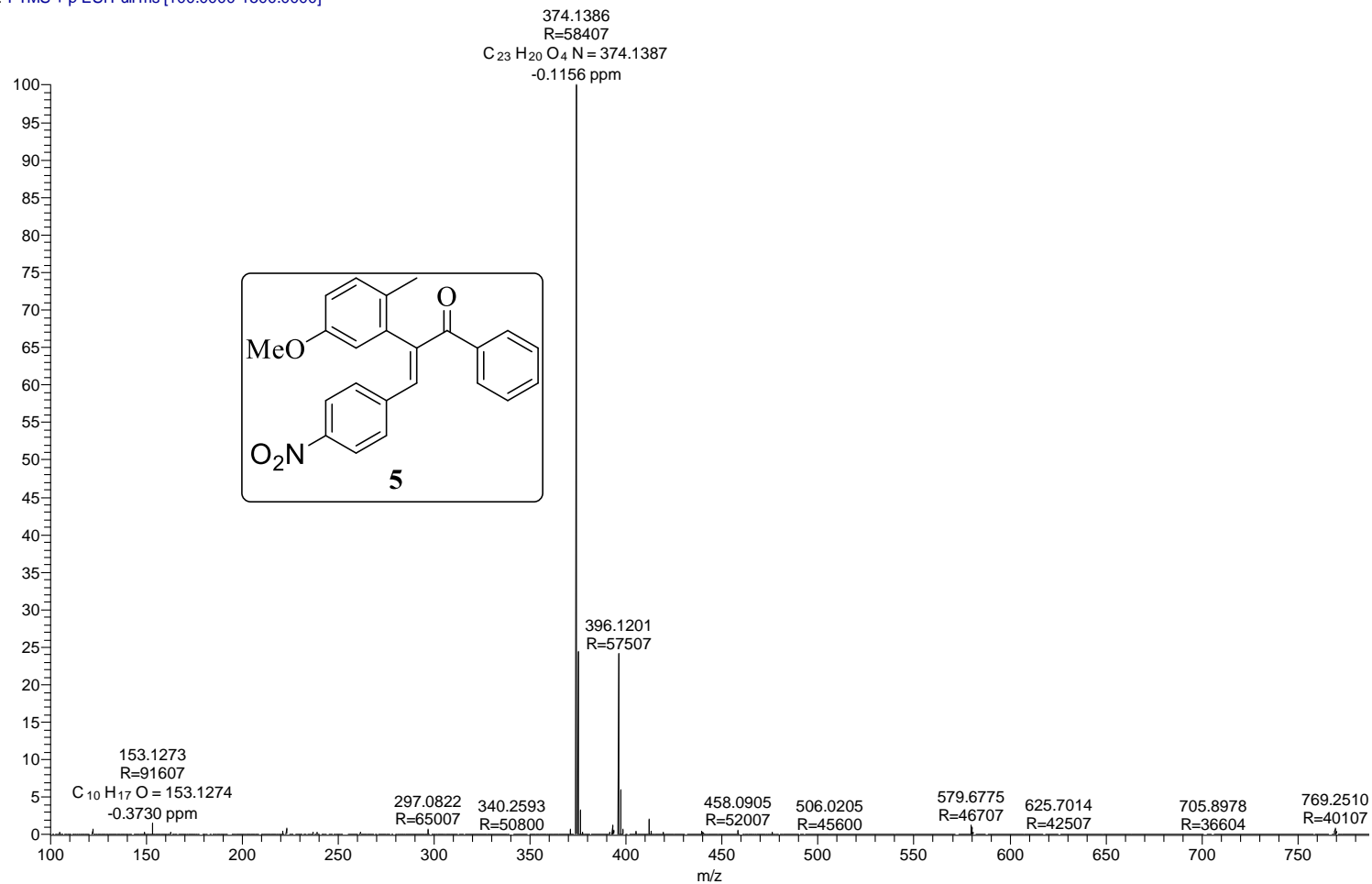


$^{13}\text{C} \{^1\text{H}\}$ NMR spectrum of compound **5** (101 MHz, CDCl_3)

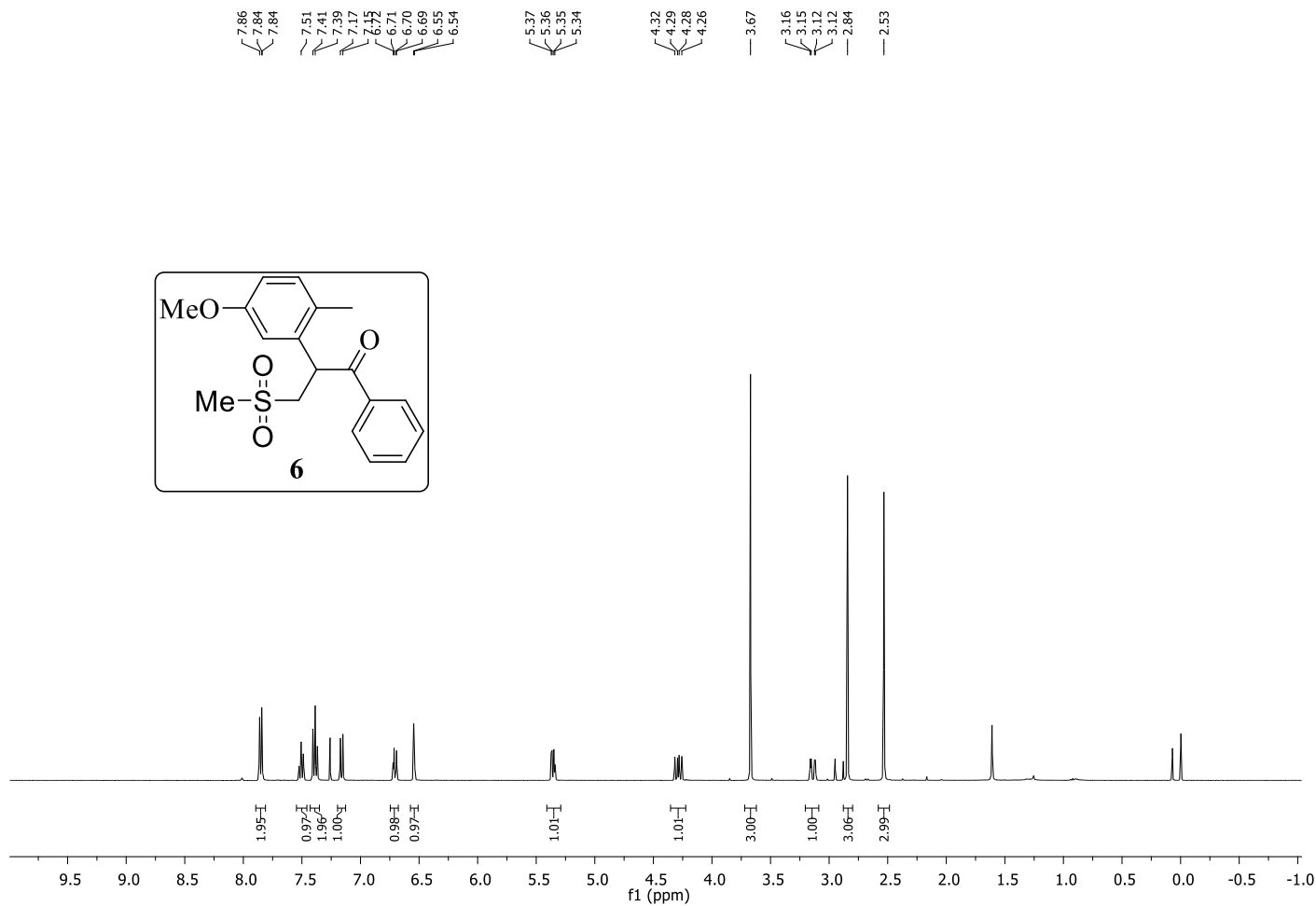


HRMS spectrum of compound 5

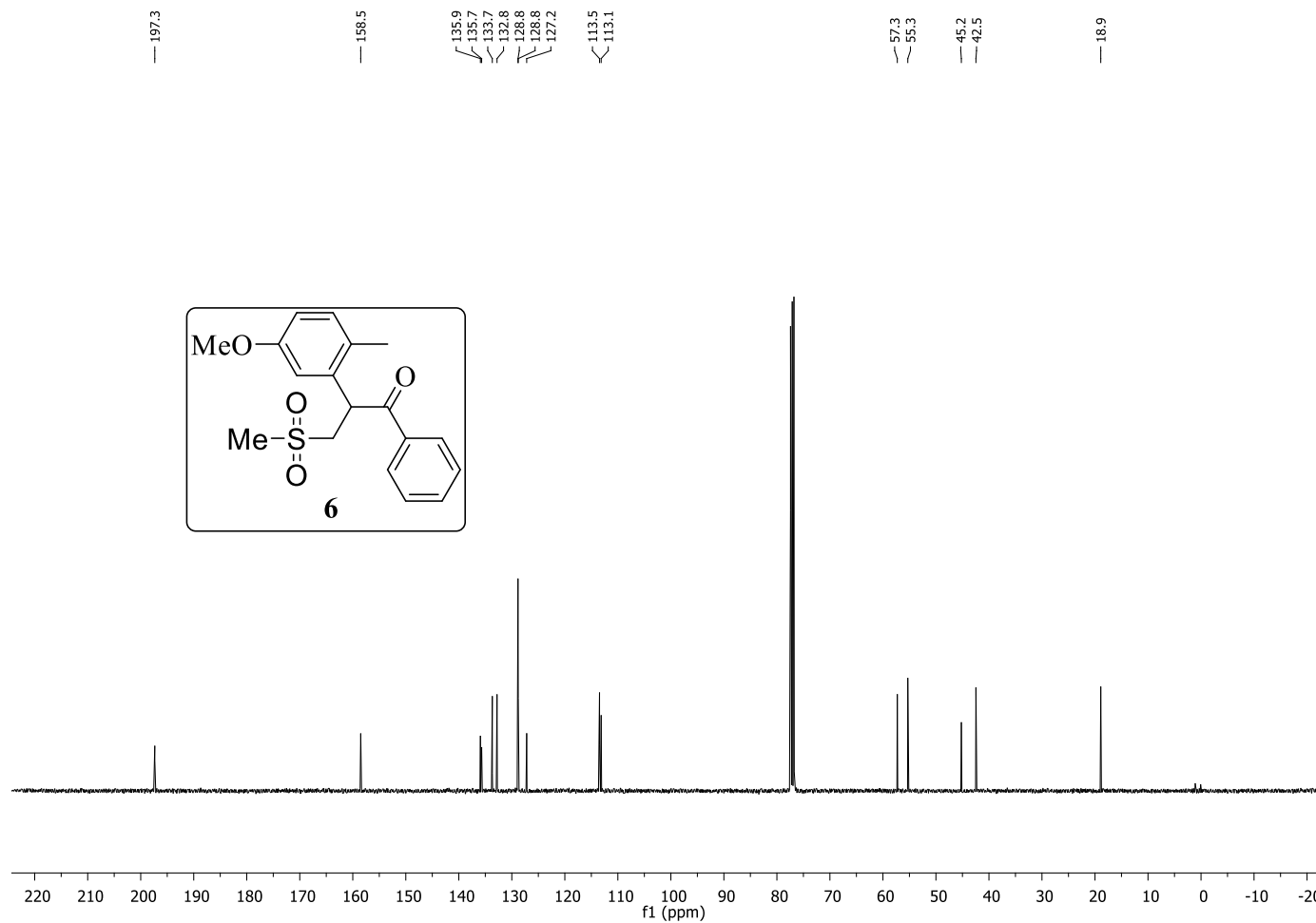
AR-599_231031141606 #571 RT: 2.54 AV: 1 NL: 1.59E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



¹H NMR spectrum of compound **6** (400 MHz, CDCl₃)



^{13}C $\{^1\text{H}\}$ NMR spectrum of compound **6** (101 MHz, CDCl_3)



HRMS spectrum of compound 6

AR-597 #417 RT: 1.86 AV: 1 NL: 1.21E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]

