

Supporting Information

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Microvawe assisted synthesis of N-(methyl and methoxy) benzylidene-4-fluoroaniline derivatives and their carbonic anhydrase I and II inhibition properties

Hulya Celik^{1*} and Müslüm Kuzu²

¹*Agri Ibrahim Cecen University, Faculty of Pharmacy, Department of Pharmaceutical Technology, Agri, Türkiye*

²*Agri Ibrahim Cecen University, Faculty of Science, Department of Biochemistry, Agri, Türkiye*

³*Karabuk University, Faculty of Health Sciences, Department of Nutrition and Dietetics, Karabuk, Türkiye*

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* Corresponding author: E-Mail: hycelik@agri.edu.tr, Phone: + 05459391196. 17

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S1 : In vitro antibacterial activity

In vitro antibacterial activities of the synthesized compounds were tested using the agar-well diffusion assay (AWDA) as previously described¹ at the Antimikrop R & D and Biocidal Analysis Center (Ankara, Turkey). The microorganisms used were *Escherichia coli* (ATCC 10536), *Pseudomonas aeruginosa* (ATCC 15442), *Staphylococcus aureus* (ATCC 6538), and *Bacillus subtilis* (ATCC 6633). Gentamicin, a clinical antibacterial agent, was used as the standard in the tests. The compounds were used at 20% concentration with 80% DMSO as a diluent, which also served as the compound-free control. The results are presented as zone of inhibition (mm) determined after 24 hours of static incubation at 36 ± 1 °C. A clear zone around the agar well of >6 mm in radius (which is the diameter of the well) was taken as evidence of the susceptibility of the tested bacterial strain to the compounds.

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Table S1. Antibacterial activity of synthesized compounds **6a-f**.

No.	<i>S. aureus</i>	<i>E. coli</i>	<i>P. aeruginosa</i>	<i>B. subtilis</i>
6a	+ (8 mm)	-	+ (8 mm)	-
6b	-	-	-	-
6c	-	-	-	-
6d	+ (9 mm)	-	-	-
6e	+ (7 mm)	-	-	-
6f	-	-	-	-
DMSO	-	-	-	-
Std.	+ (21 mm)	+ (22 mm)	+ (14 mm)	+ (25 mm)

- = No antibacterial activity observed.

+ = Antibacterial activity observed (zone of inhibition in millimeters (mm)).

DMSO = Dimethyl sulfoxide (80%).

Std. = Gentamicin (20 µg).

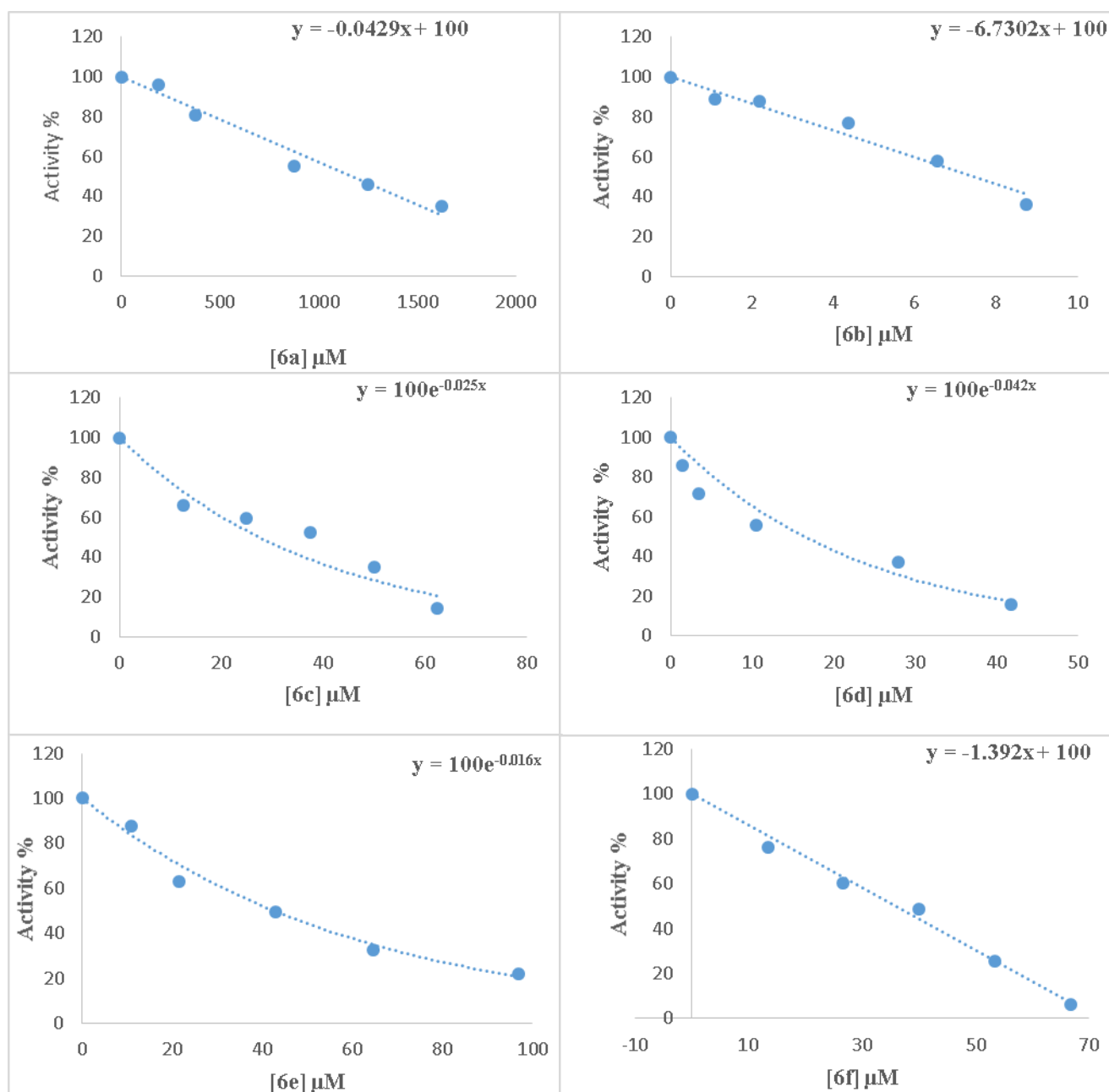


Figure S1 : Activity % versus [compound] graphs of 6a-f for CA-I.

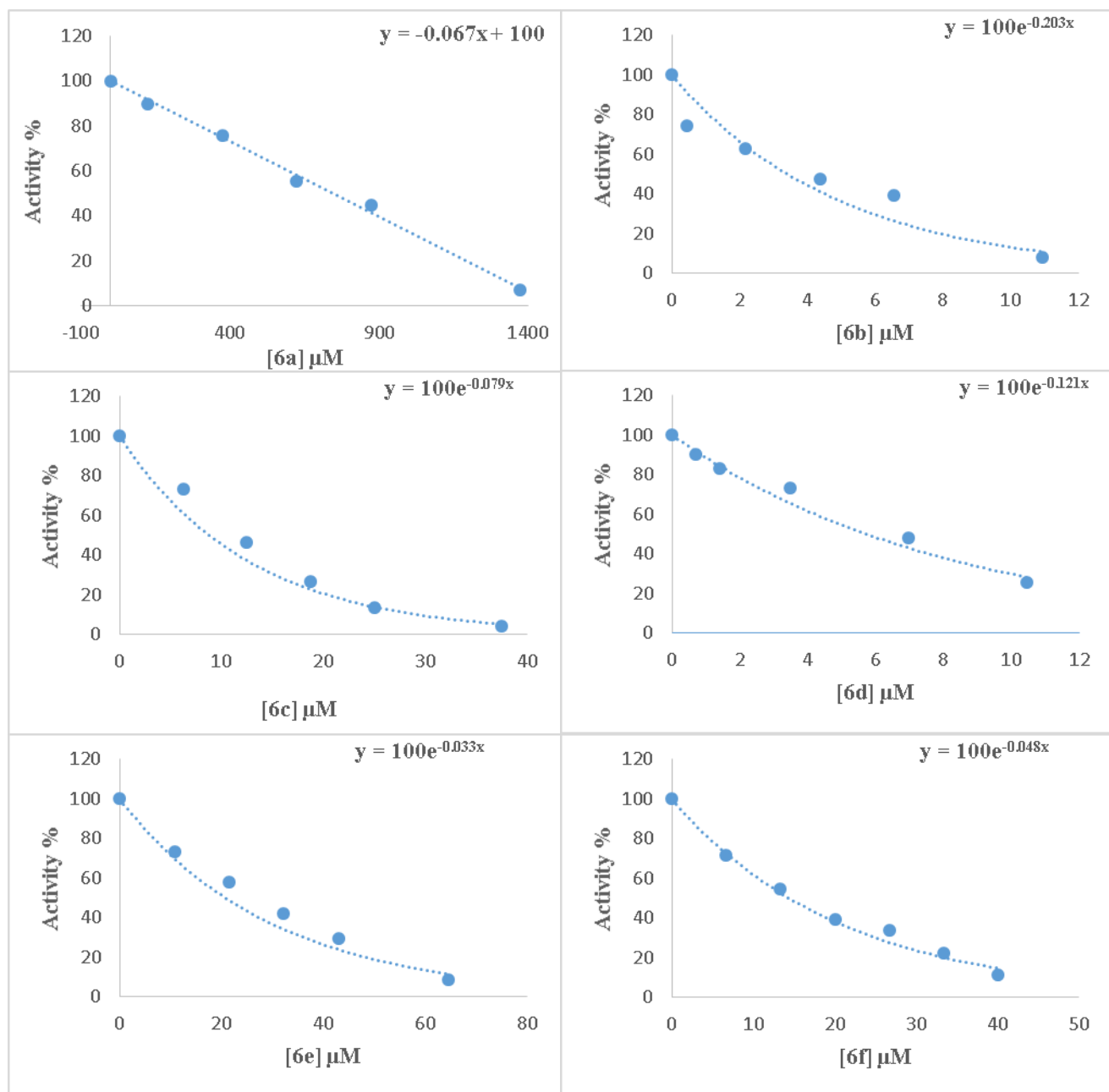


Figure S2. Activity % vs. [compound] graphs of **6a-f** for CA-II.

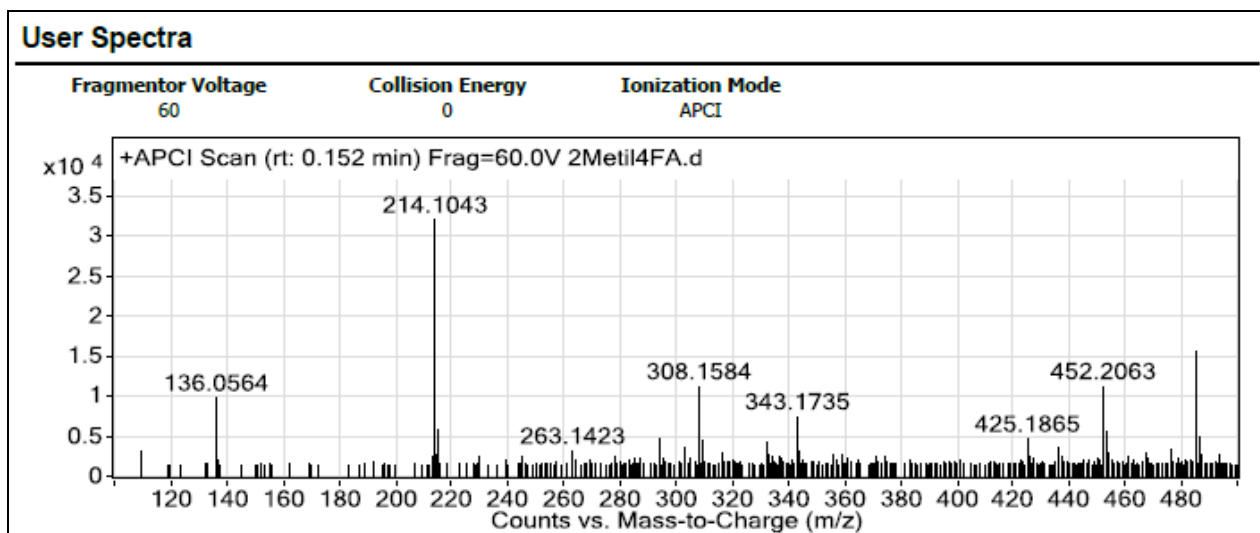
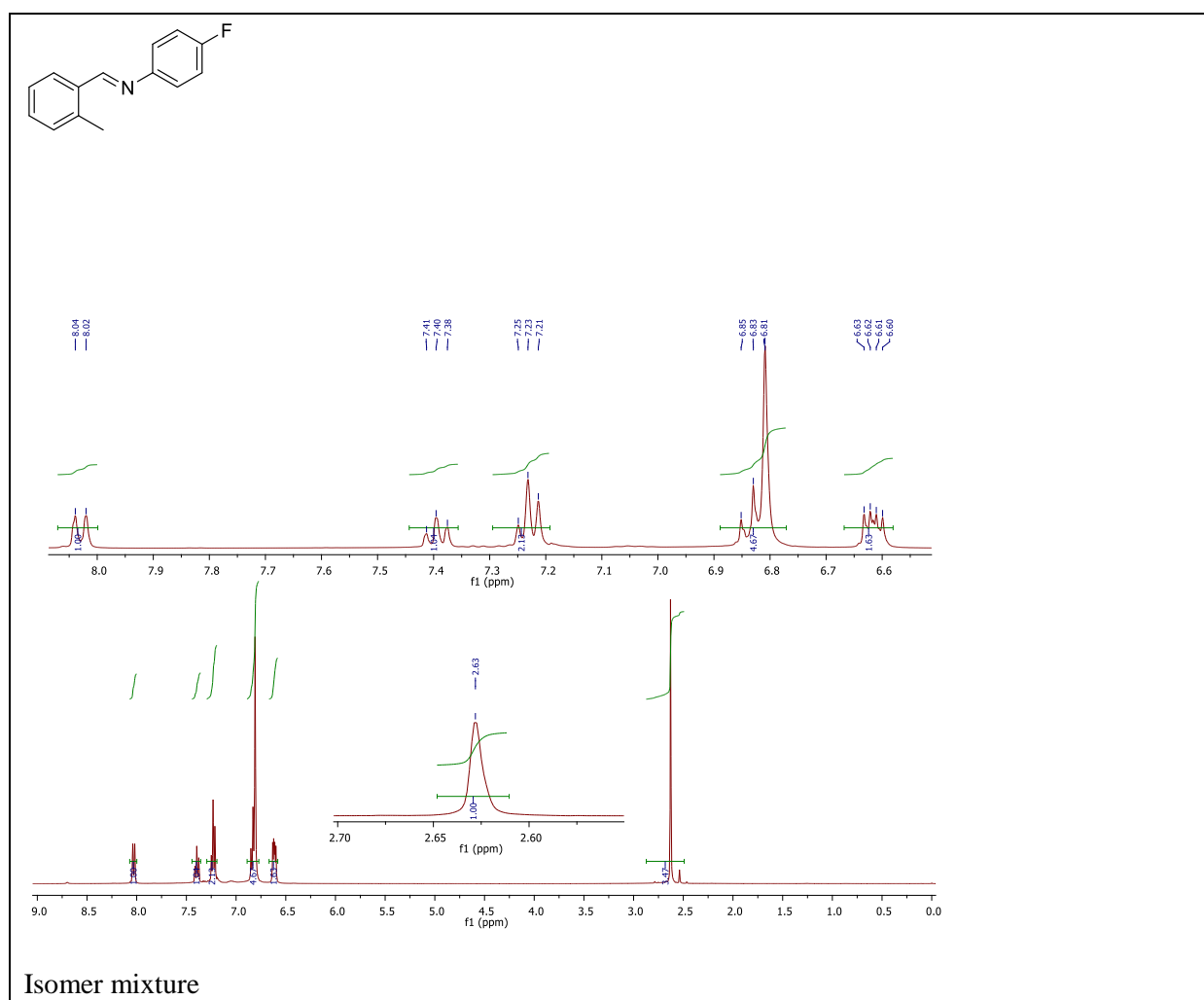


Figure S3: HRMS of compound **3a**



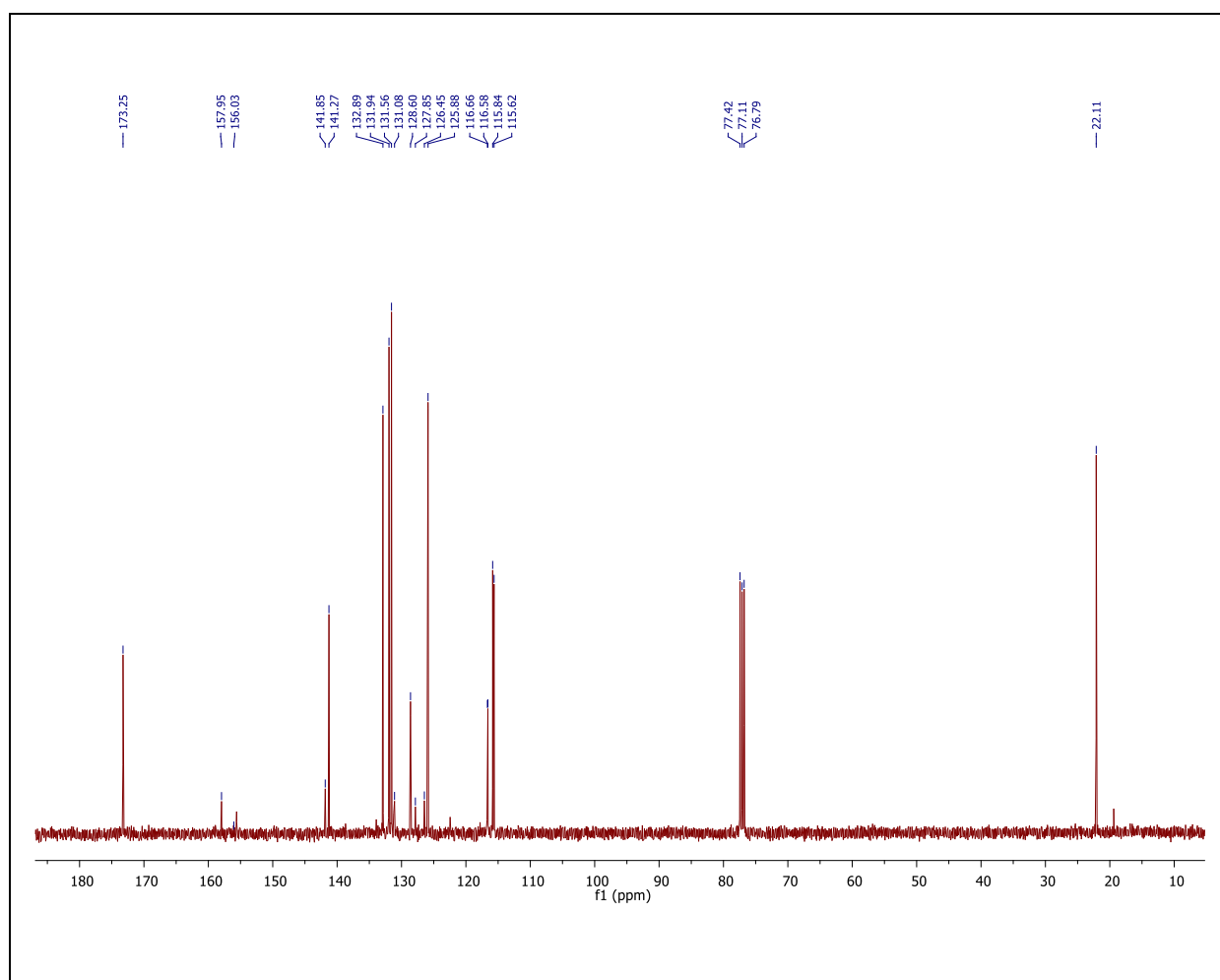


Figure S5: ^{13}C -NMR spectrum (400 MHz) of compound (**3a**) (in CDCl_3)

User Spectra

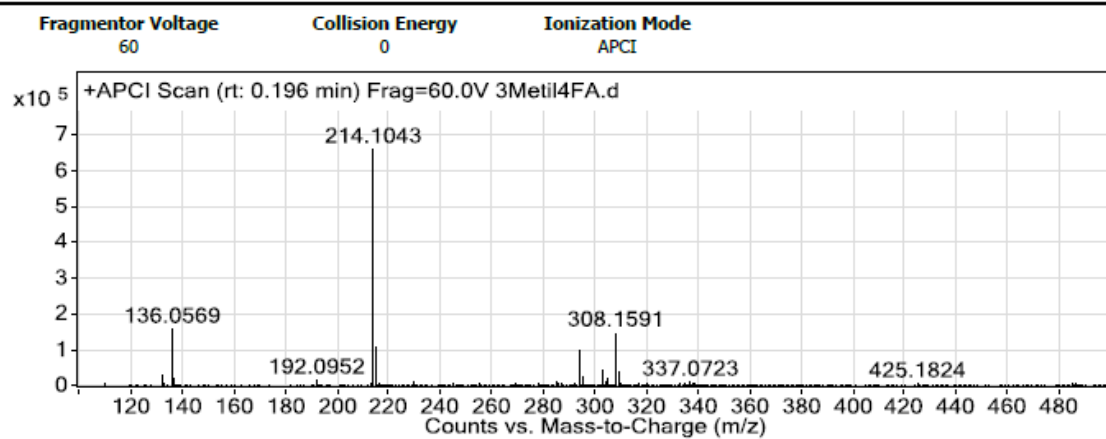


Figure S6: HRMS of compound 3b

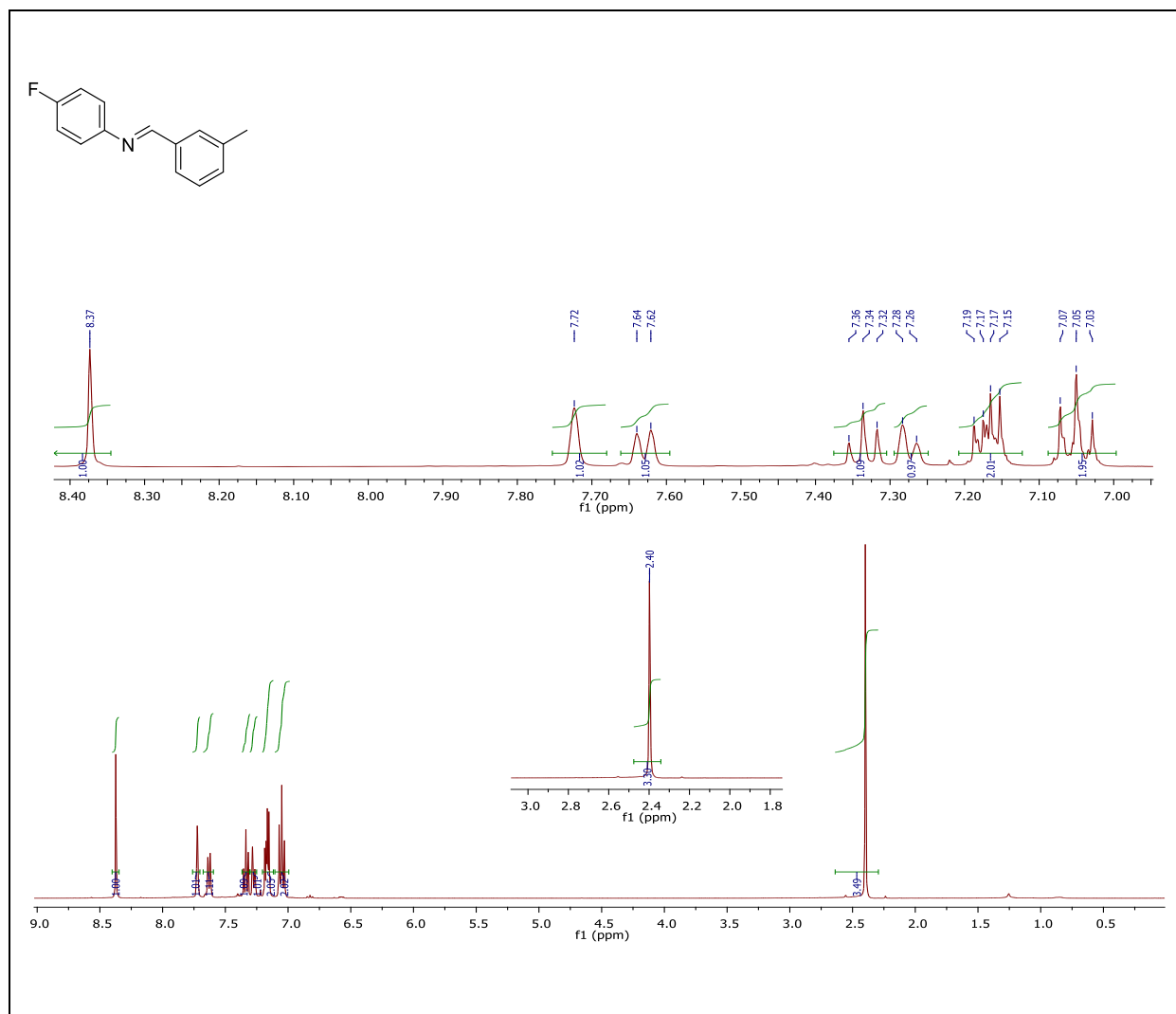


Figure S7: ¹H-NMR spectrum (400 MHz) of compound **3b** (in CDCl₃)

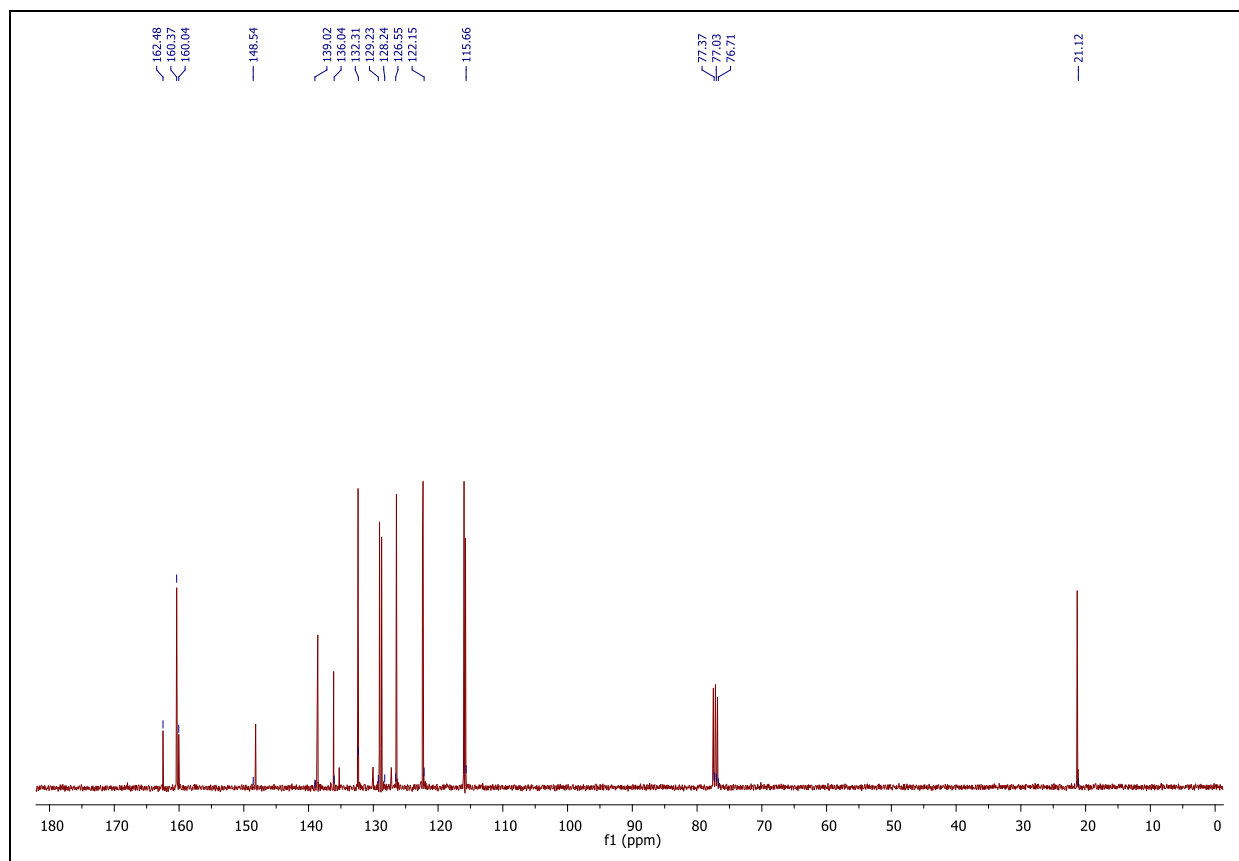


Figure S8: ¹³C-NMR spectrum (400 MHz) of compound **3b** (in CDCl₃)

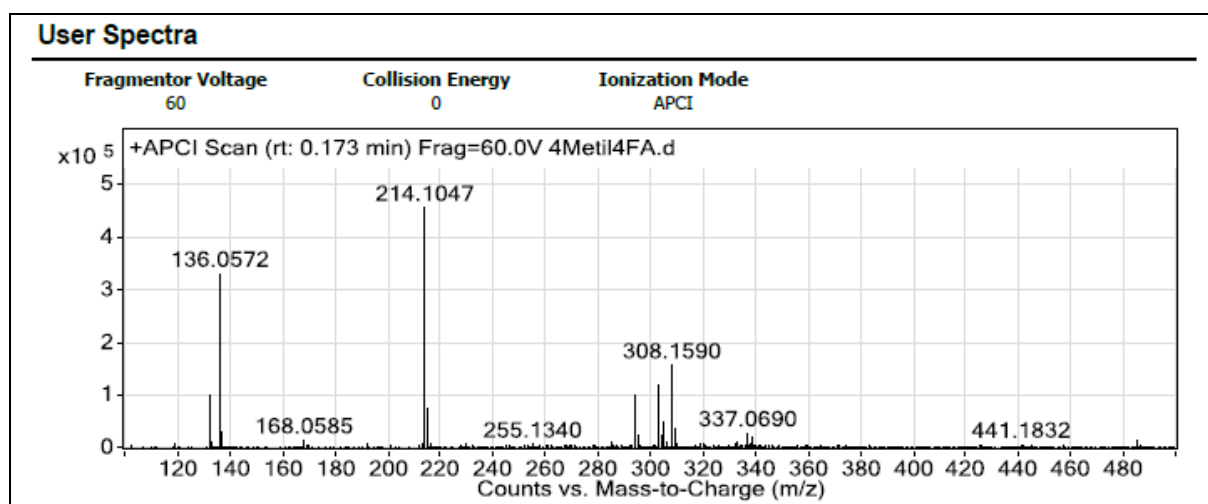


Figure S9: HRMS of compound **3c**

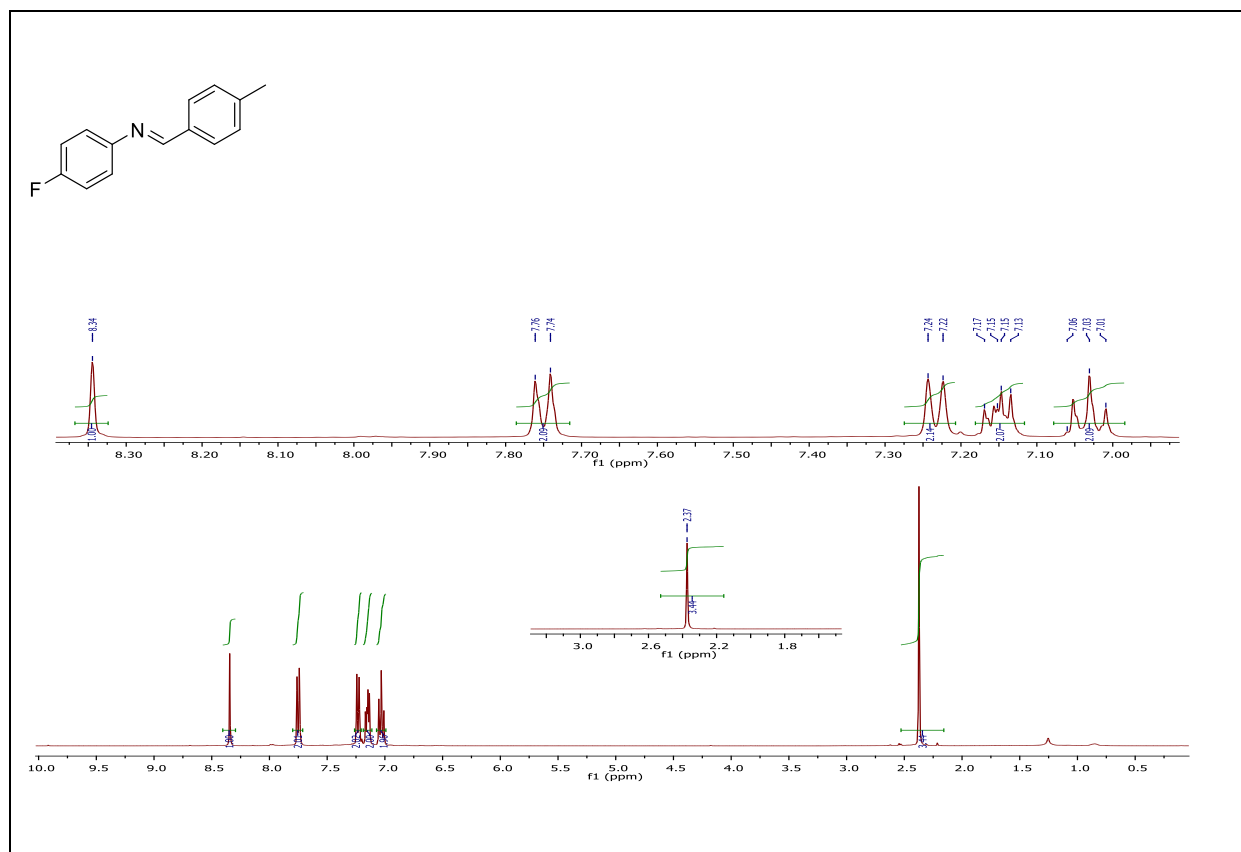


Figure S10: $^1\text{H-NMR}$ spectrum (400 MHz) of Compound **3c** (in CDCl_3)

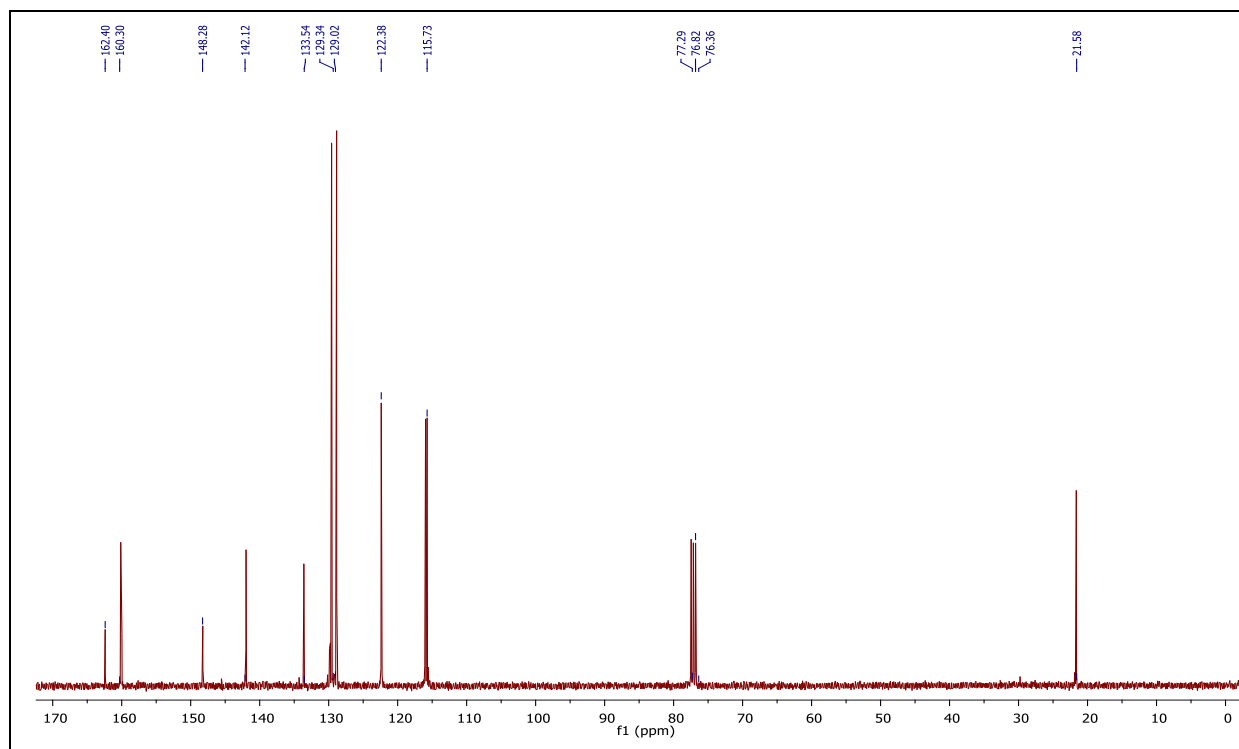
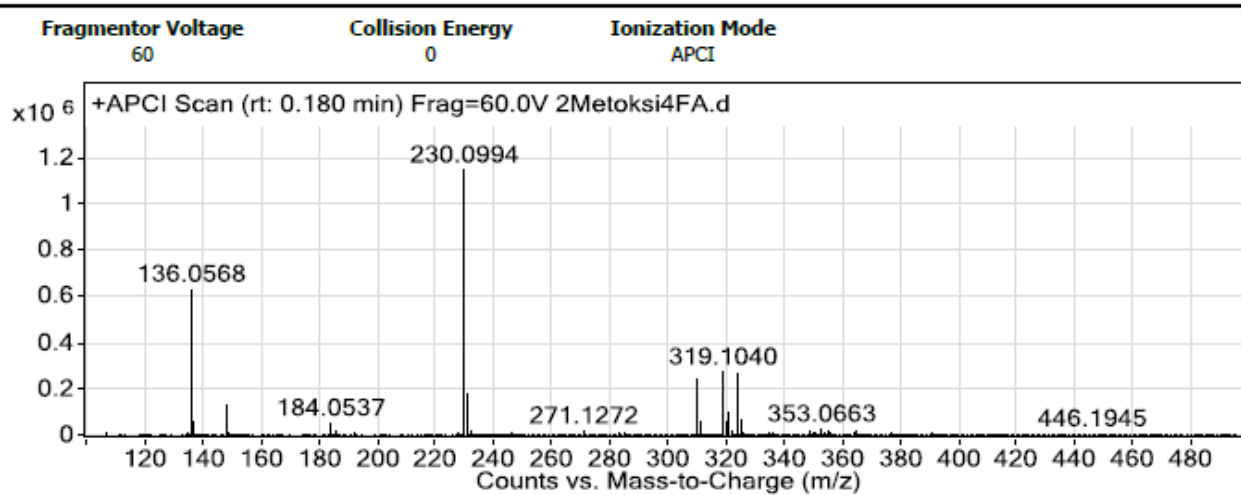


Figure S11: ^{13}C -NMR spectrum (400 MHz) of compound **3c** (in CDCl_3)

User Spectra

Figure S12: HRMS compound **3d**

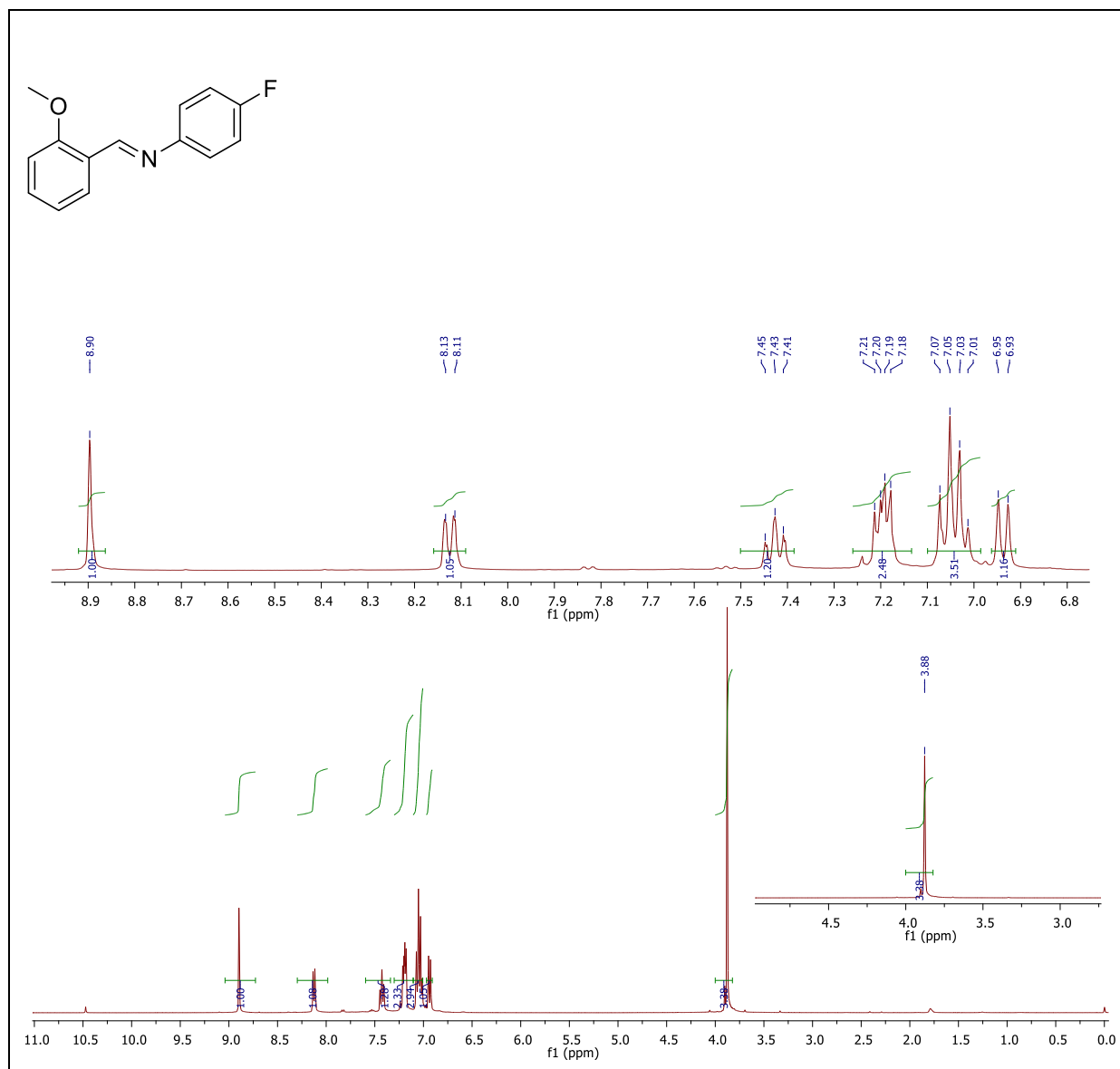


Figure S13: ¹H-NMR spectrum (400 MHz) of compound **3d** (in CDCl₃)

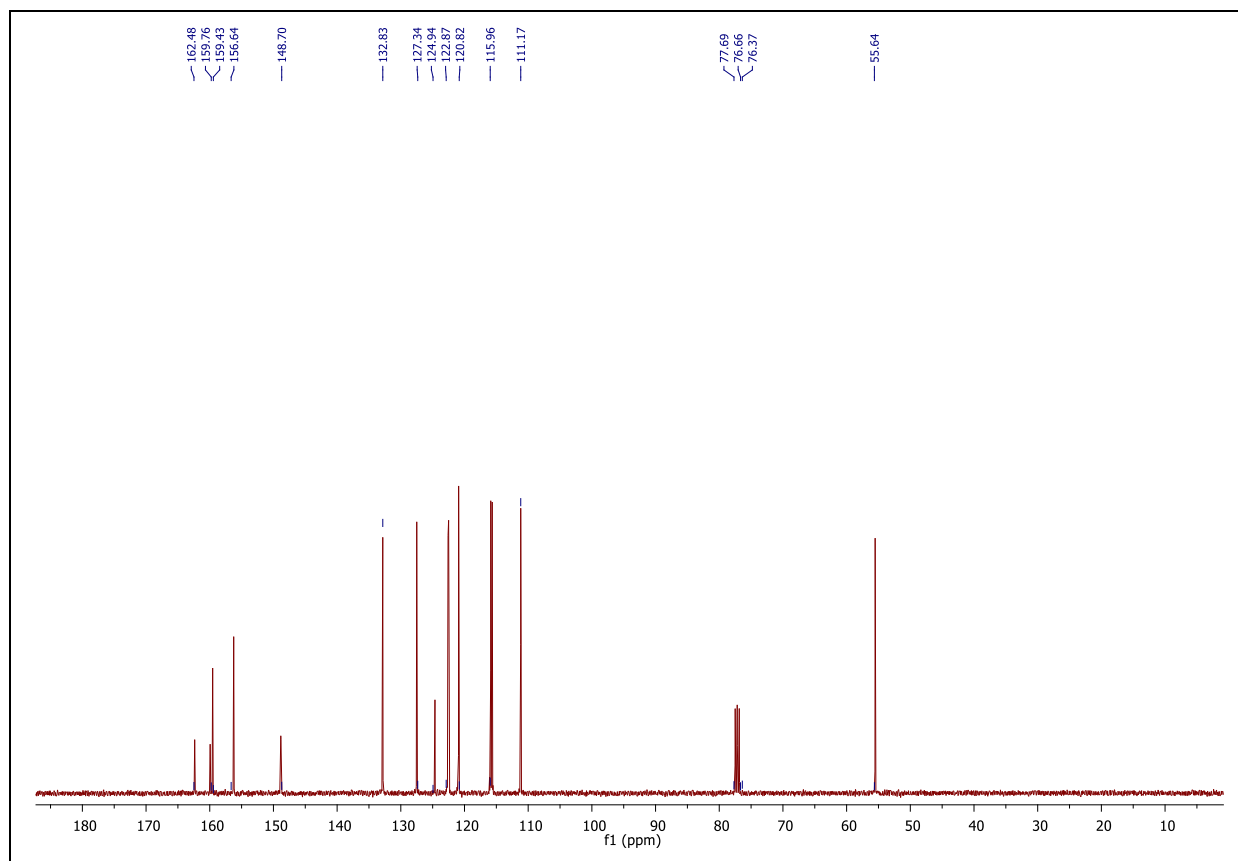


Figure S14: ^{13}C -NMR spectrum (400 MHz) of compound **3d** (in CDCl_3)

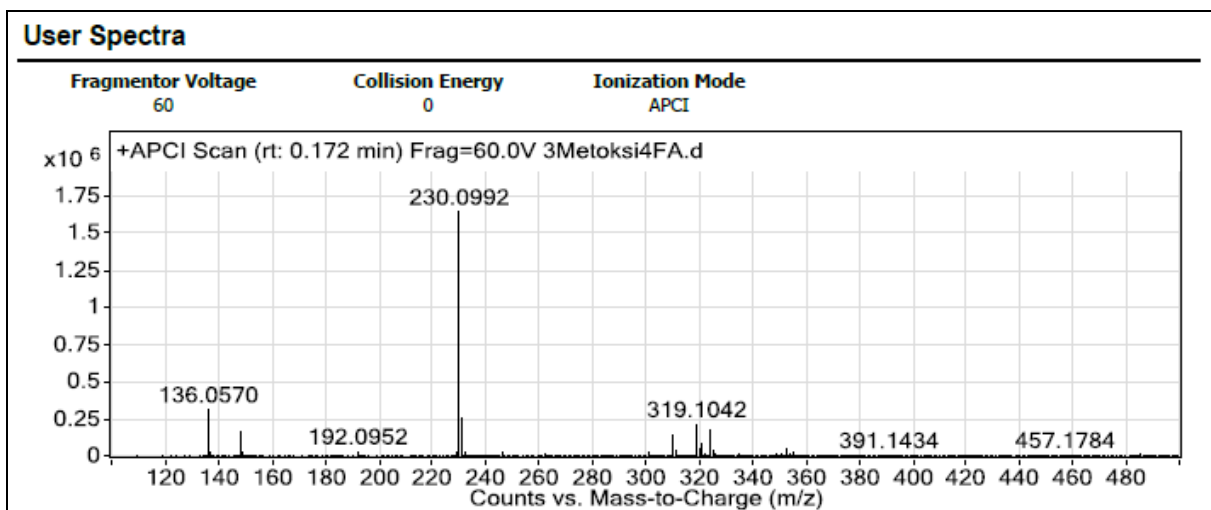


Figure S15: HRMS compound 3e

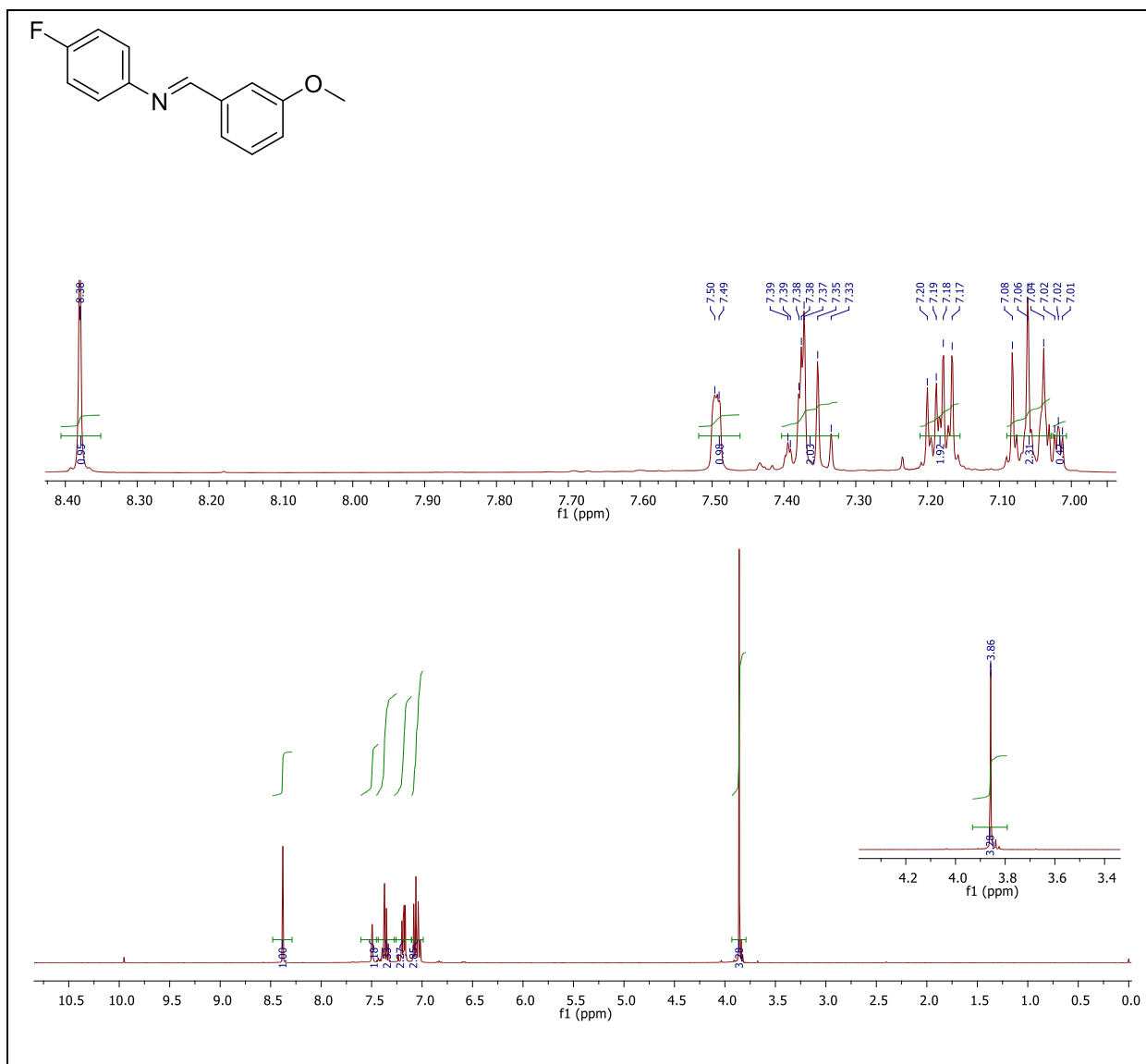


Figure S16: ¹H-NMR spectrum (400 MHz) of compound **3e** (in CDCl₃)

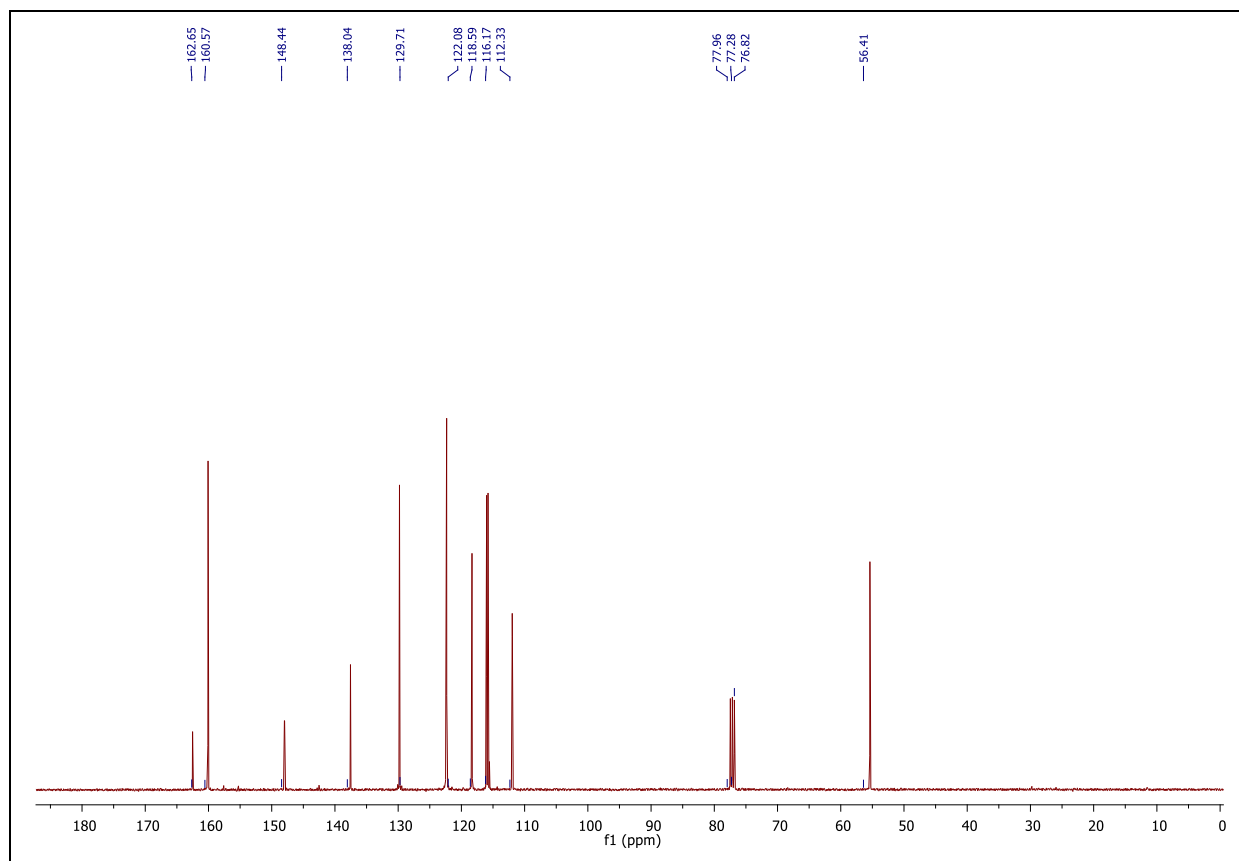


Figure S17: ^{13}C -NMR spectrum (400 MHz) of compound **3e** (in CDCl_3)

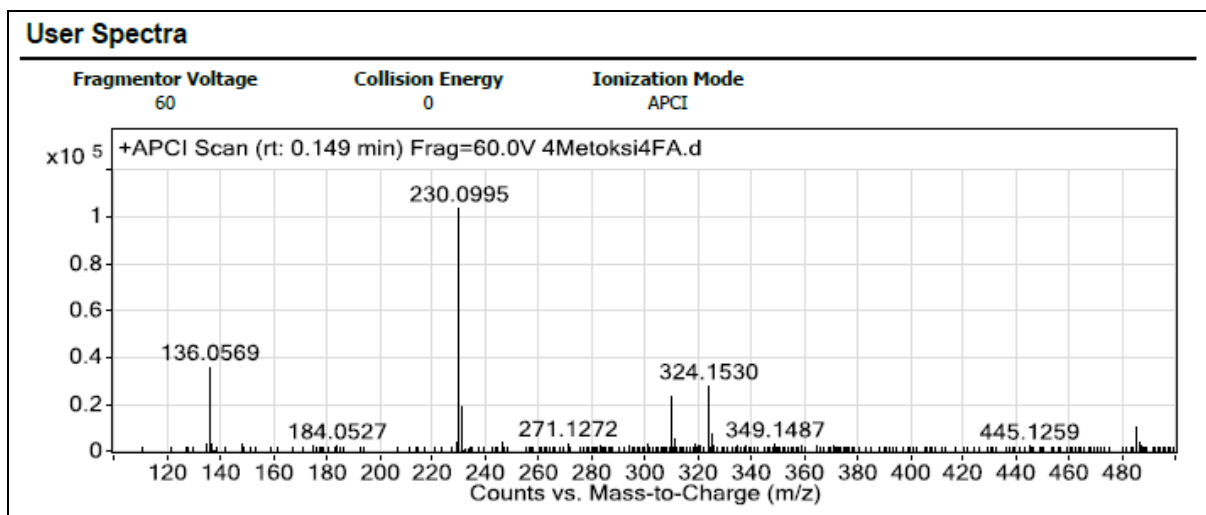


Figure S18: HRMS of compound **3f**

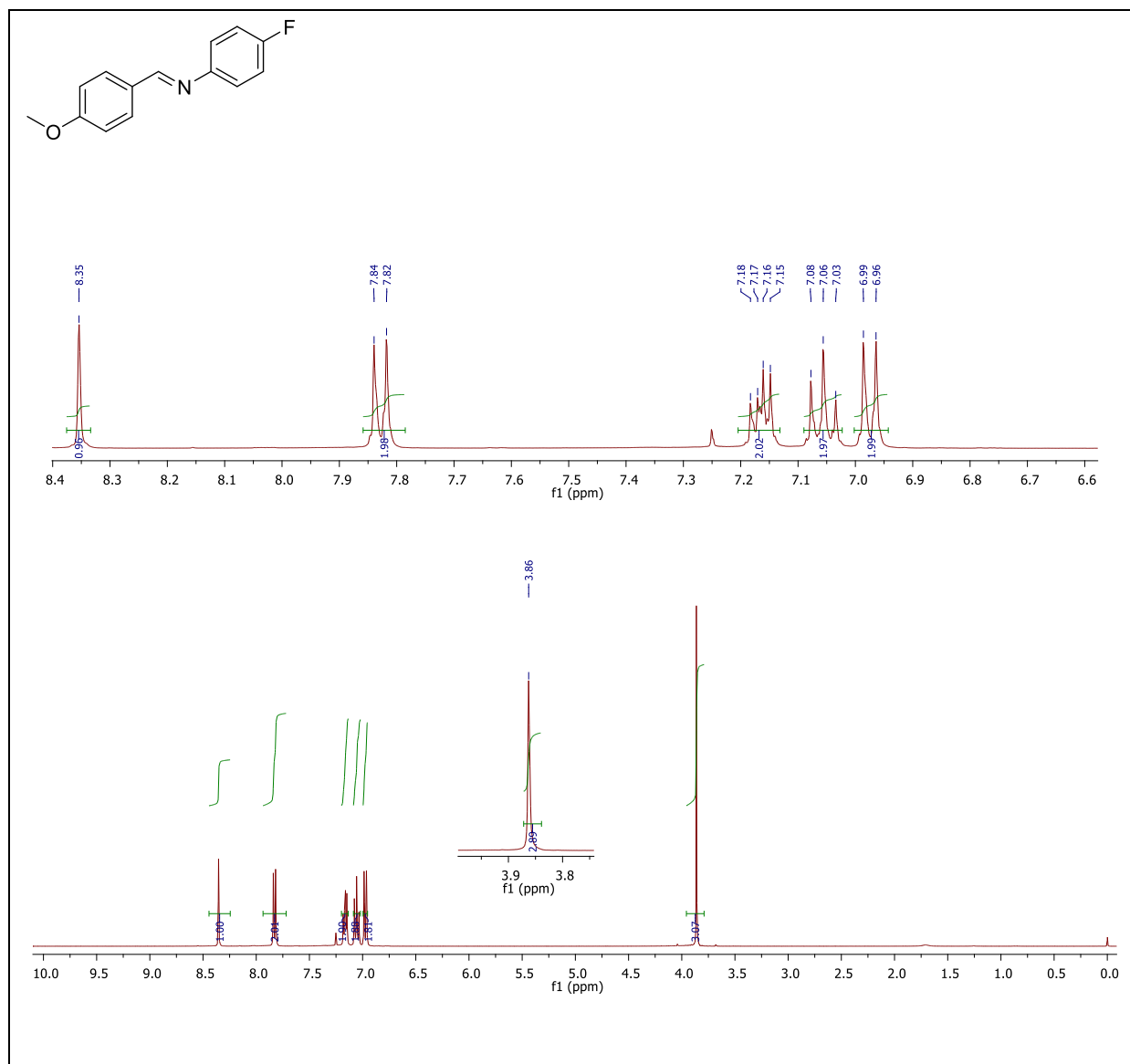


Figure S19: ¹H-NMR spectrum (400 MHz) of compound **3f** (CDCl₃)

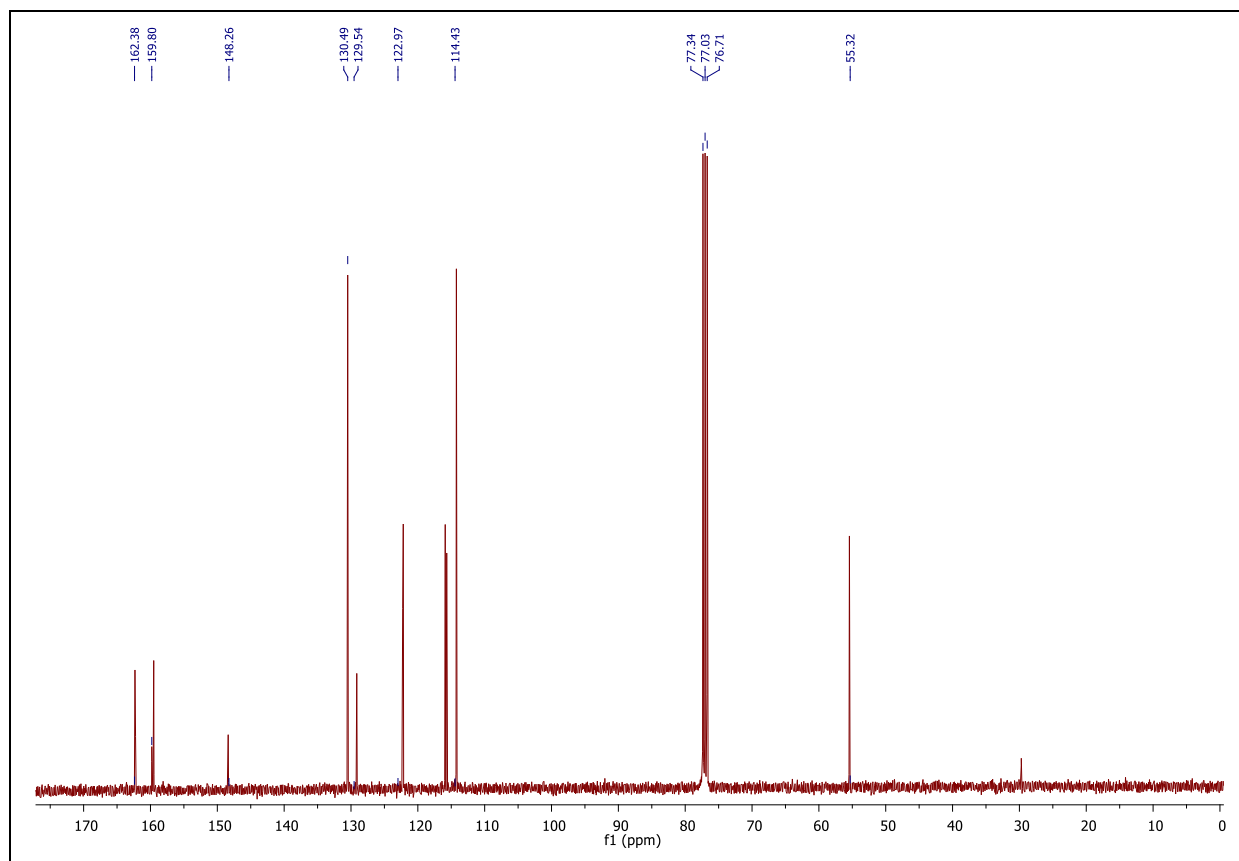


Figure S20: ^{13}C -NMR spectrum (400 MHz) of compound **3f** (in CDCl_3)

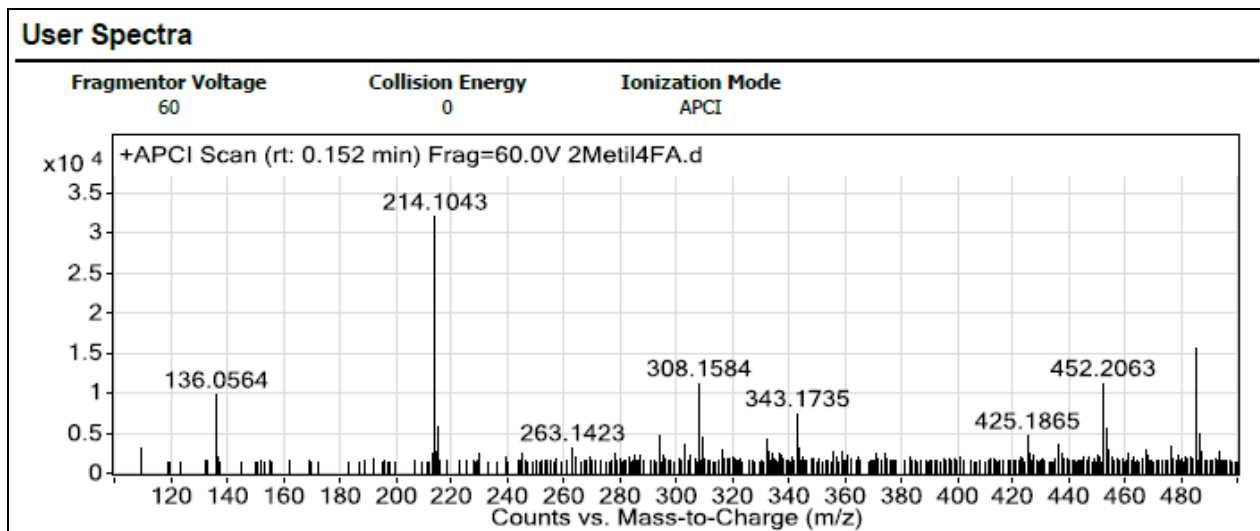


Figure S21: HRMS of compound **6a**

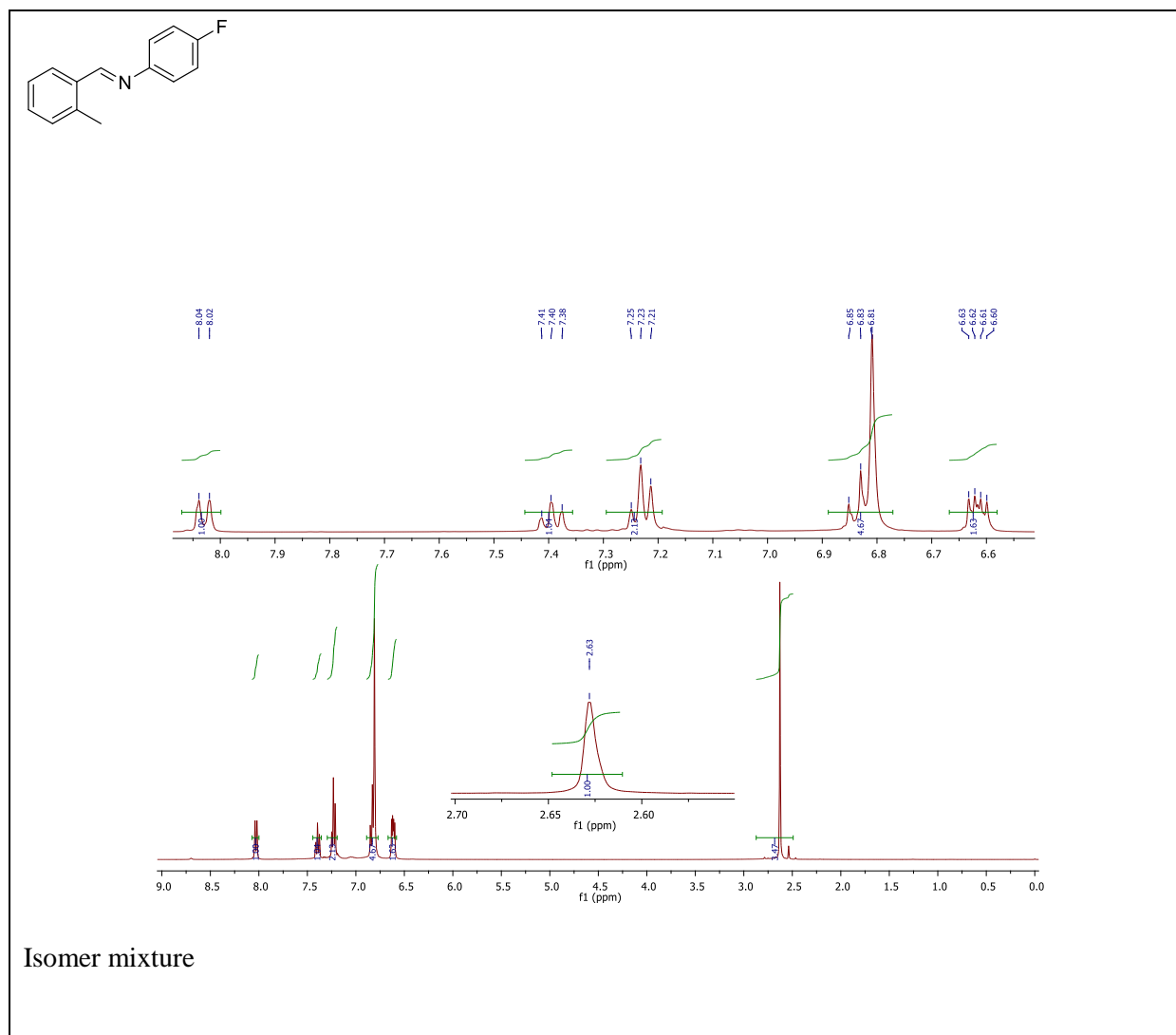


Figure S22: ¹H-NMR spectrum (400 MHz) of compound **6a** (in CDCl₃)

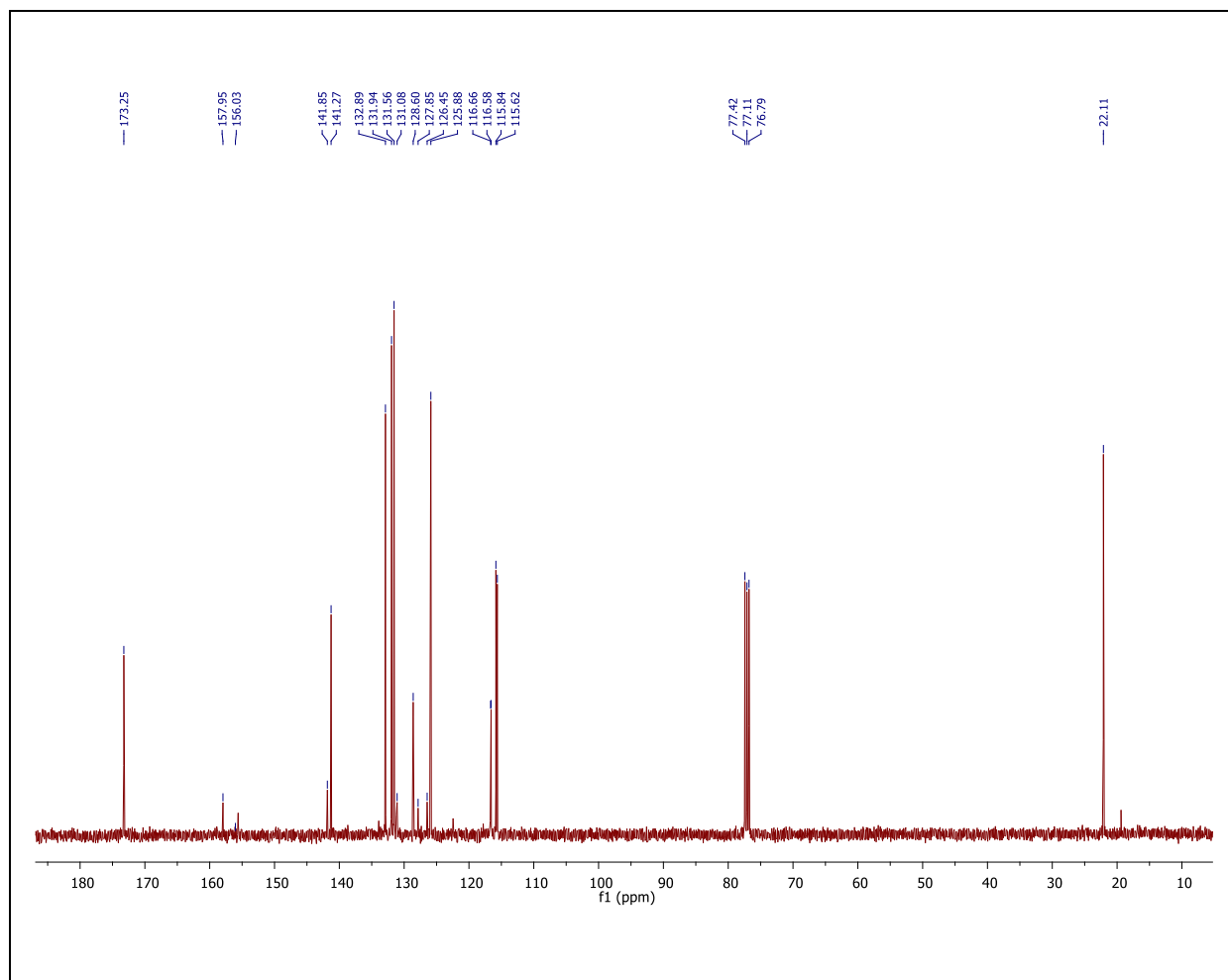


Figure S23: ¹³C-NMR spectrum (400 MHz) of compound **6a** (in CDCl₃)

User Spectra

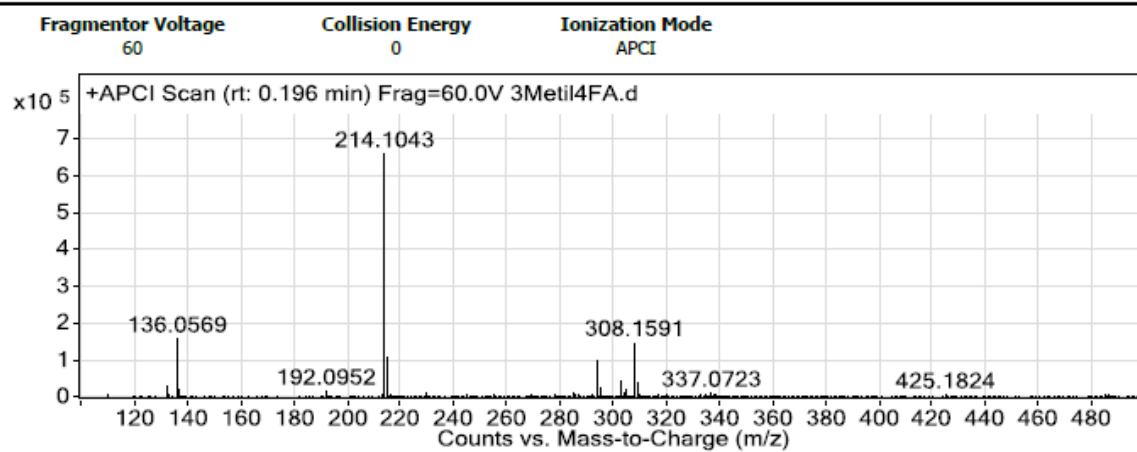


Figure S24: HRMS of compound **6b**

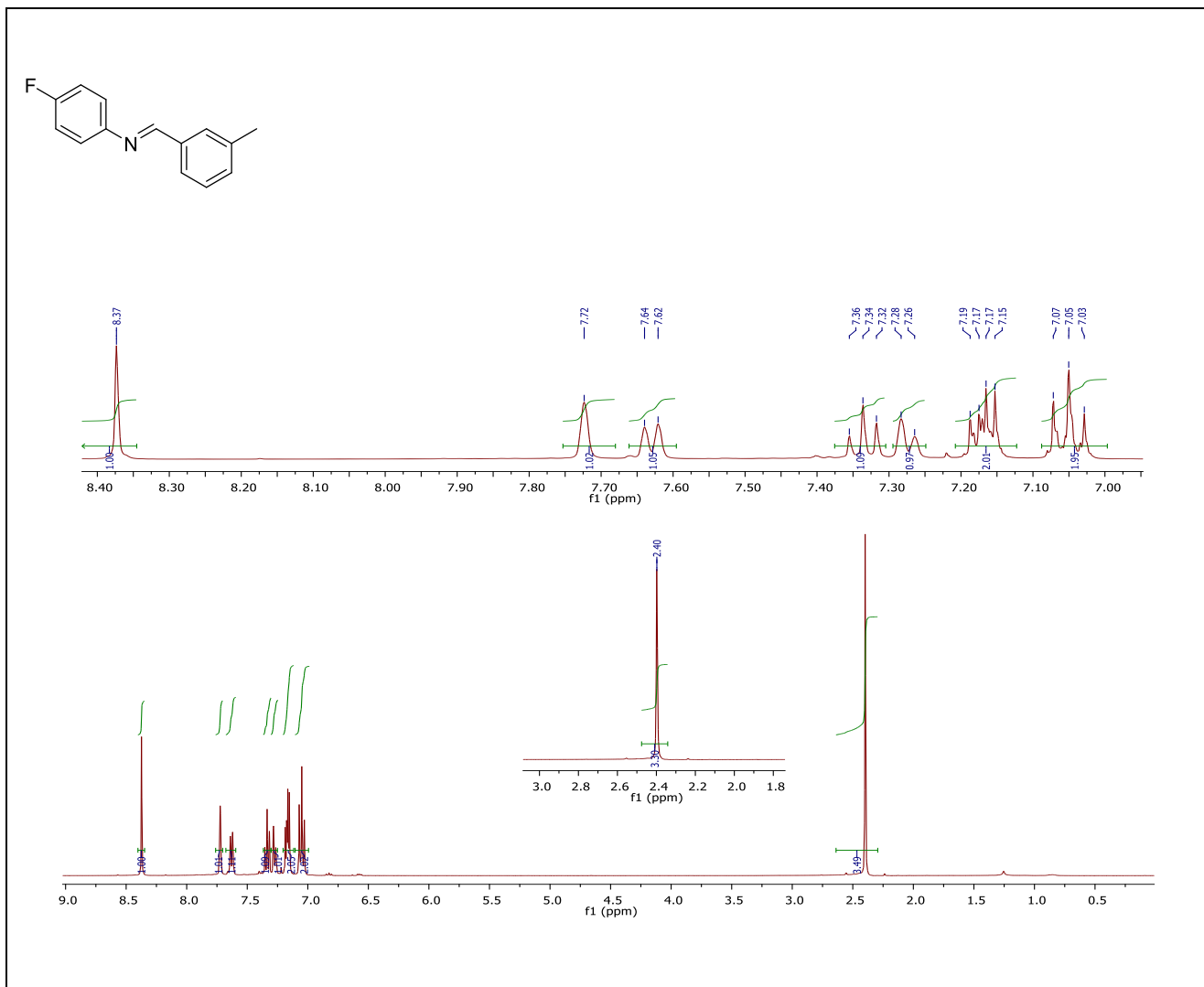


Figure S25: ¹H-NMR spectrum (400 MHz) of compound **6b** (in CDCl₃)

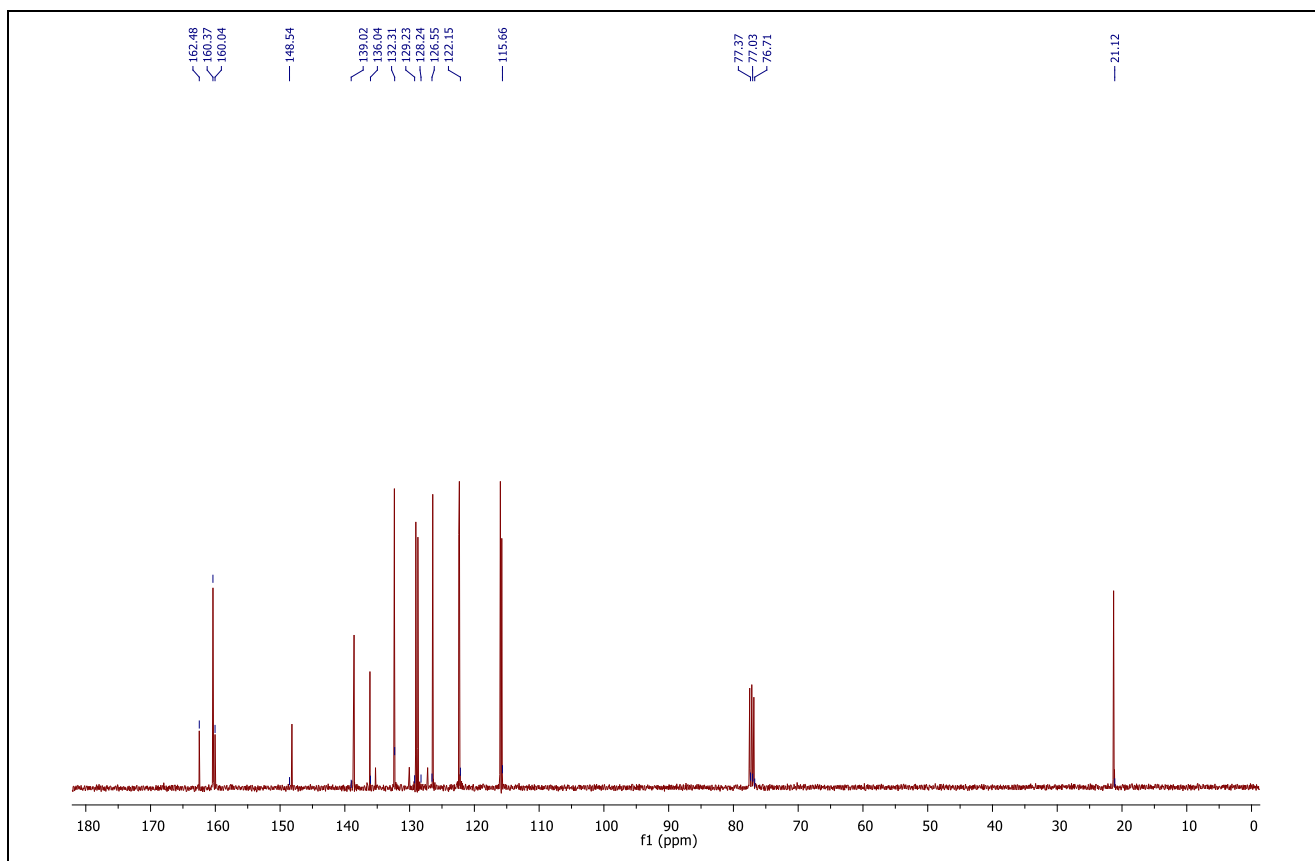


Figure S26: ^{13}C -NMR spectrum (400 MHz) of compound **6b** (in CDCl_3)

User Spectra

Fragmentor Voltage
60

Collision Energy
0

Ionization Mode
APCI

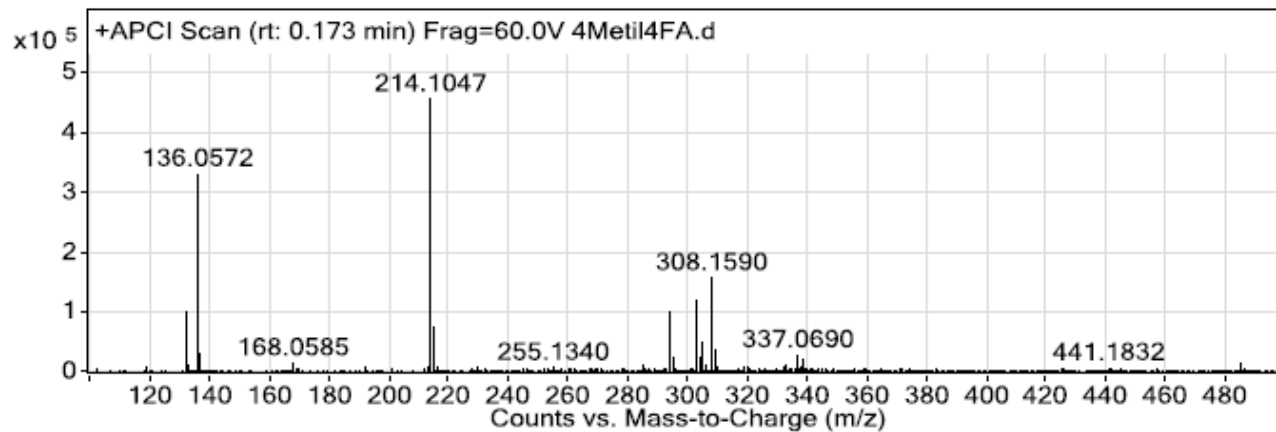


Figure S27: HRMS of compound **6c**

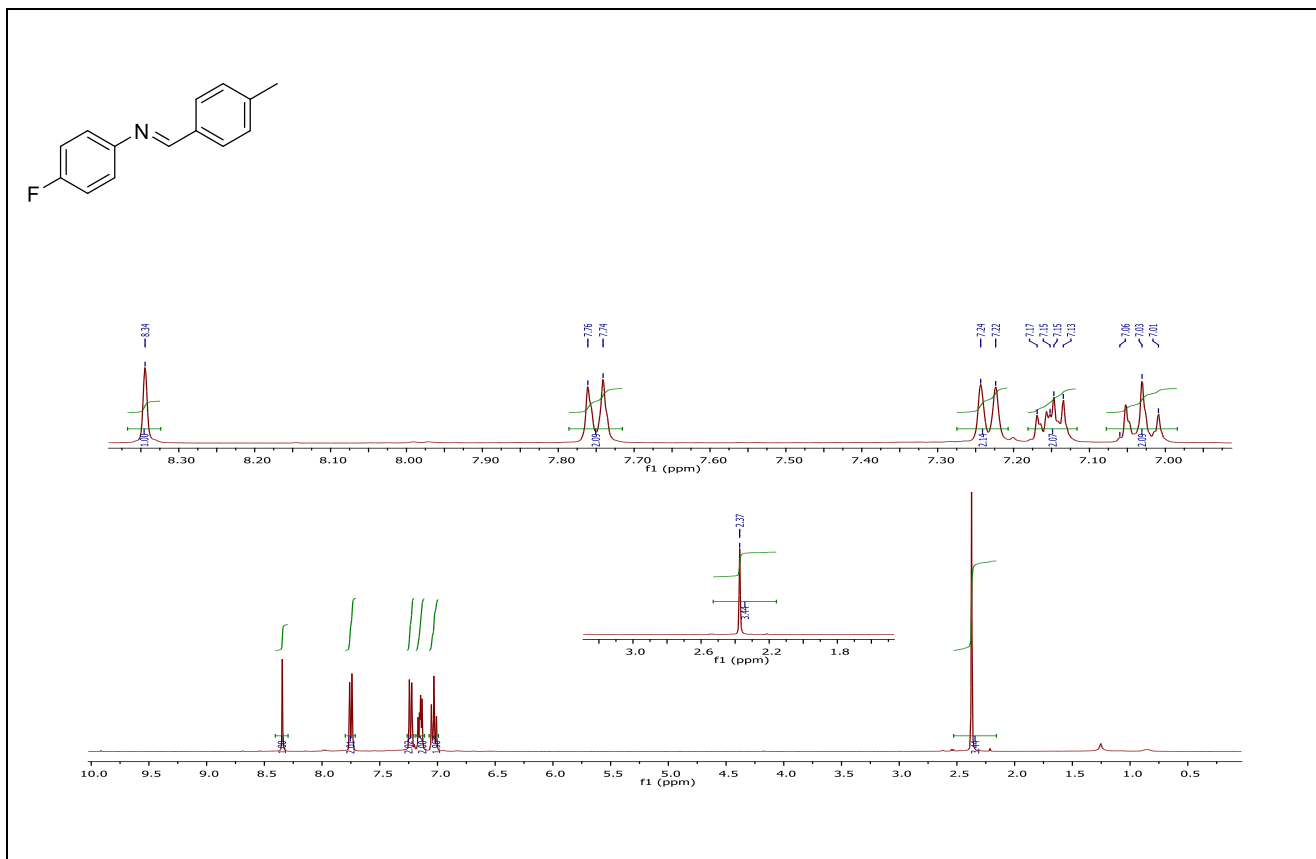


Figure S28: ¹H-NMR spectrum (400 MHz) of compound **6c** (in CDCl₃)

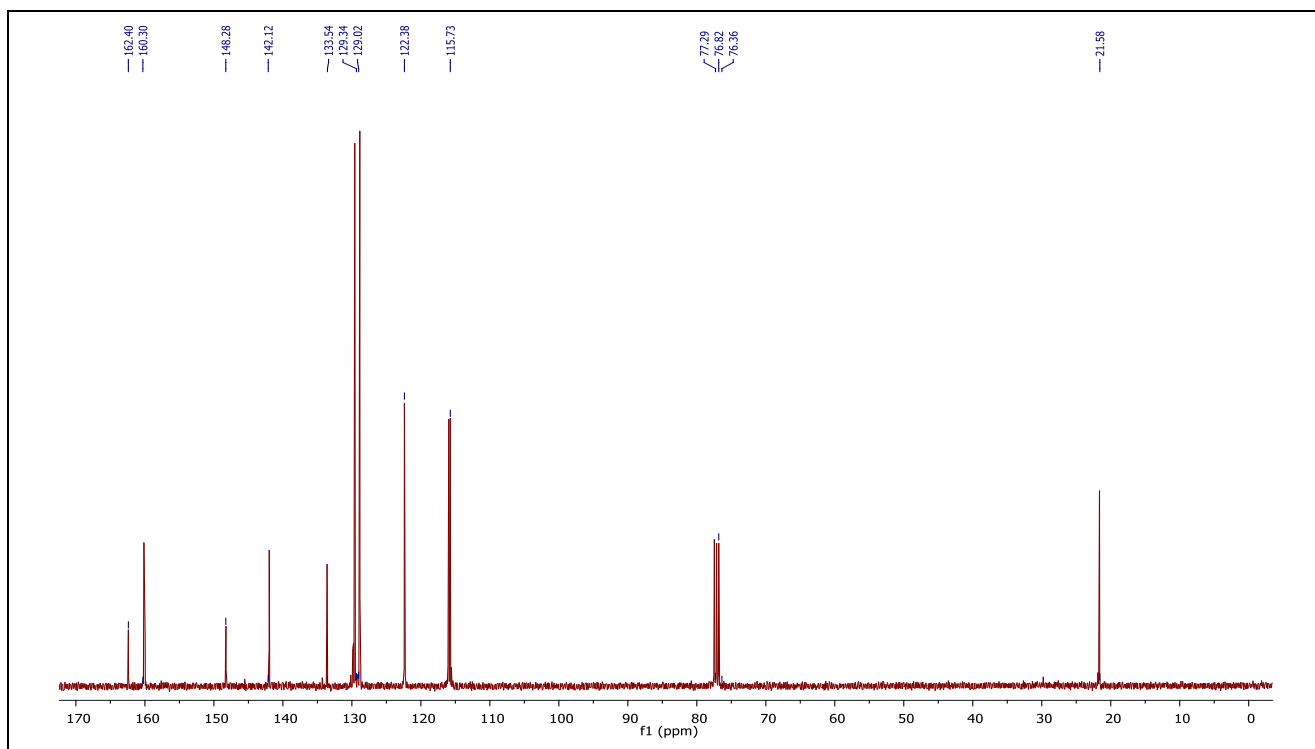


Figure S29: ^{13}C -NMR spectrum (400 MHz) of compound **6c** (in CDCl_3)

User Spectra

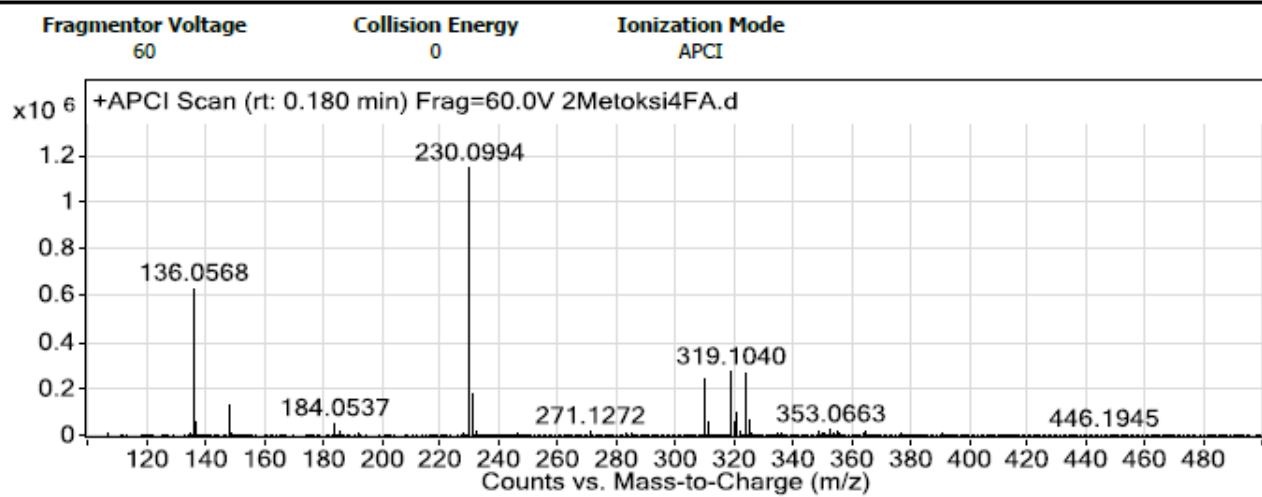


Figure S30: HRMS of compound **6d**

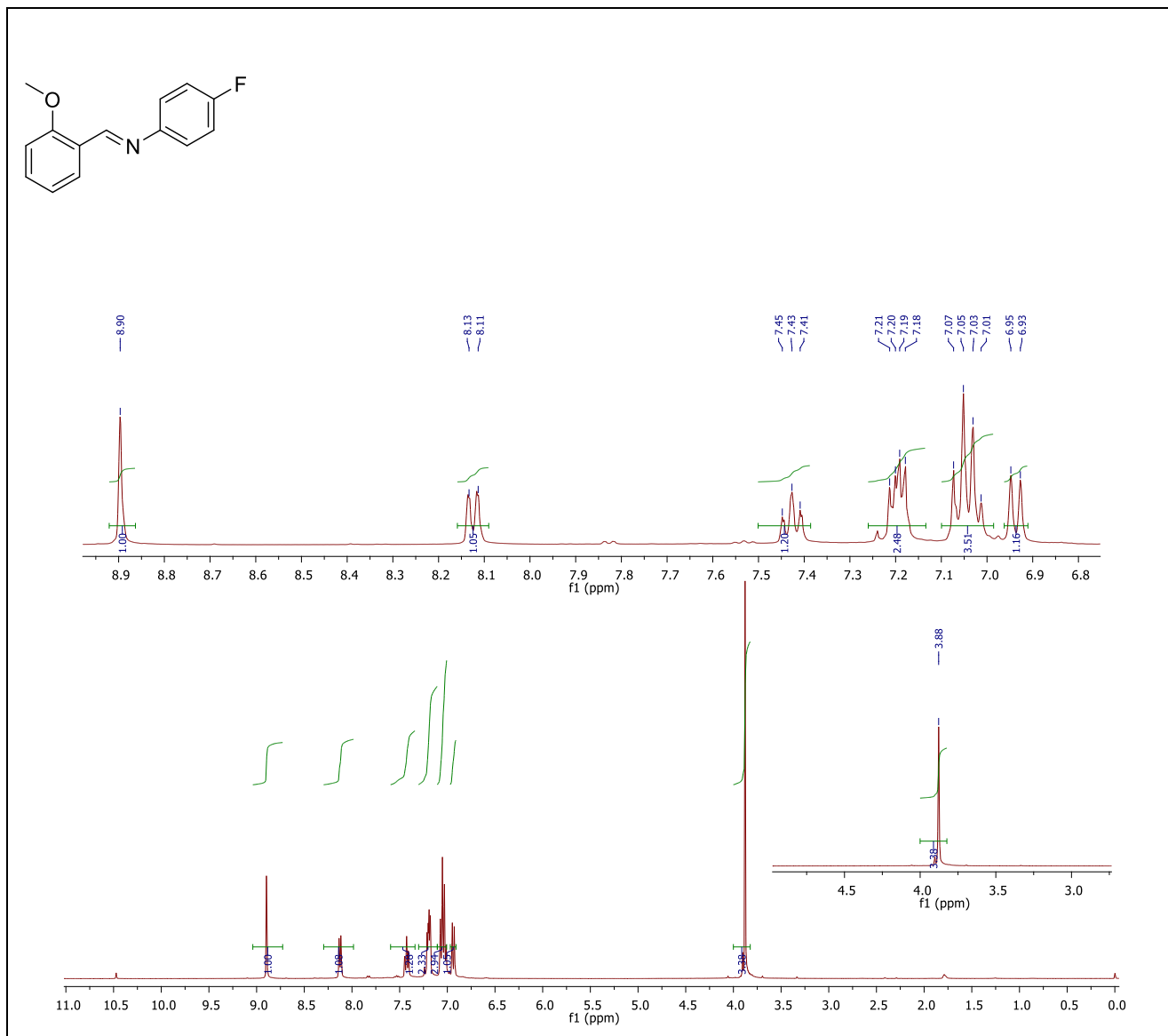


Figure S31: ¹H-NMR spectrum (400 MHz) of compound **6d** (in CDCl₃)

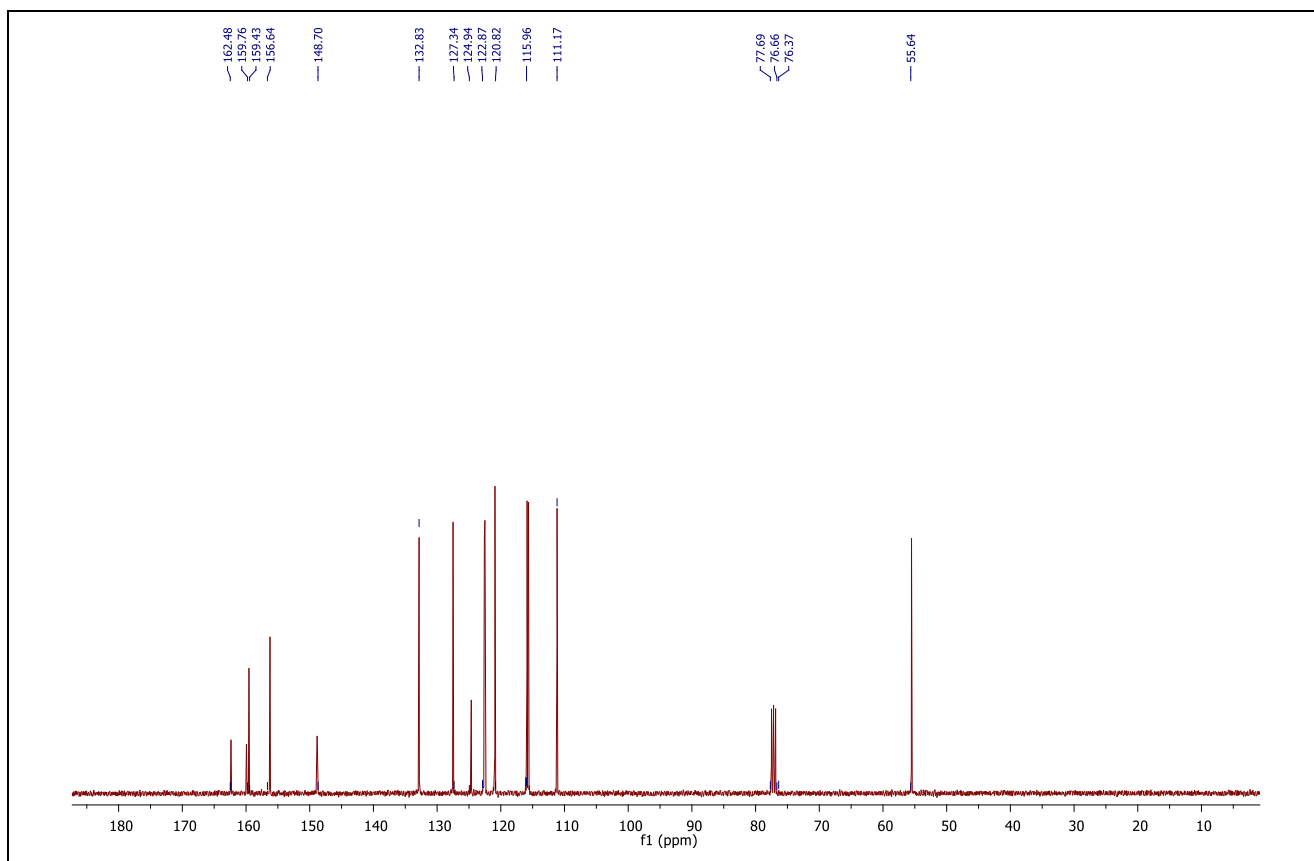


Figure S32 ^{13}C -NMR spectrum (400 MHz) of compound **6d** (in CDCl_3)

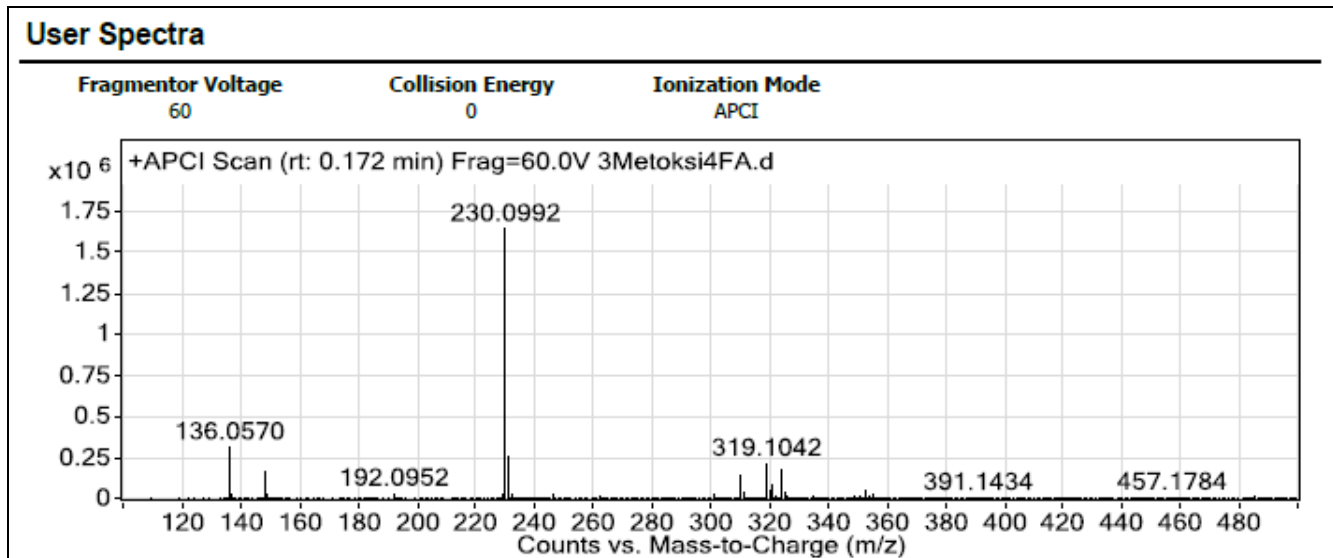


Figure S33: HRMS of compound **6e**

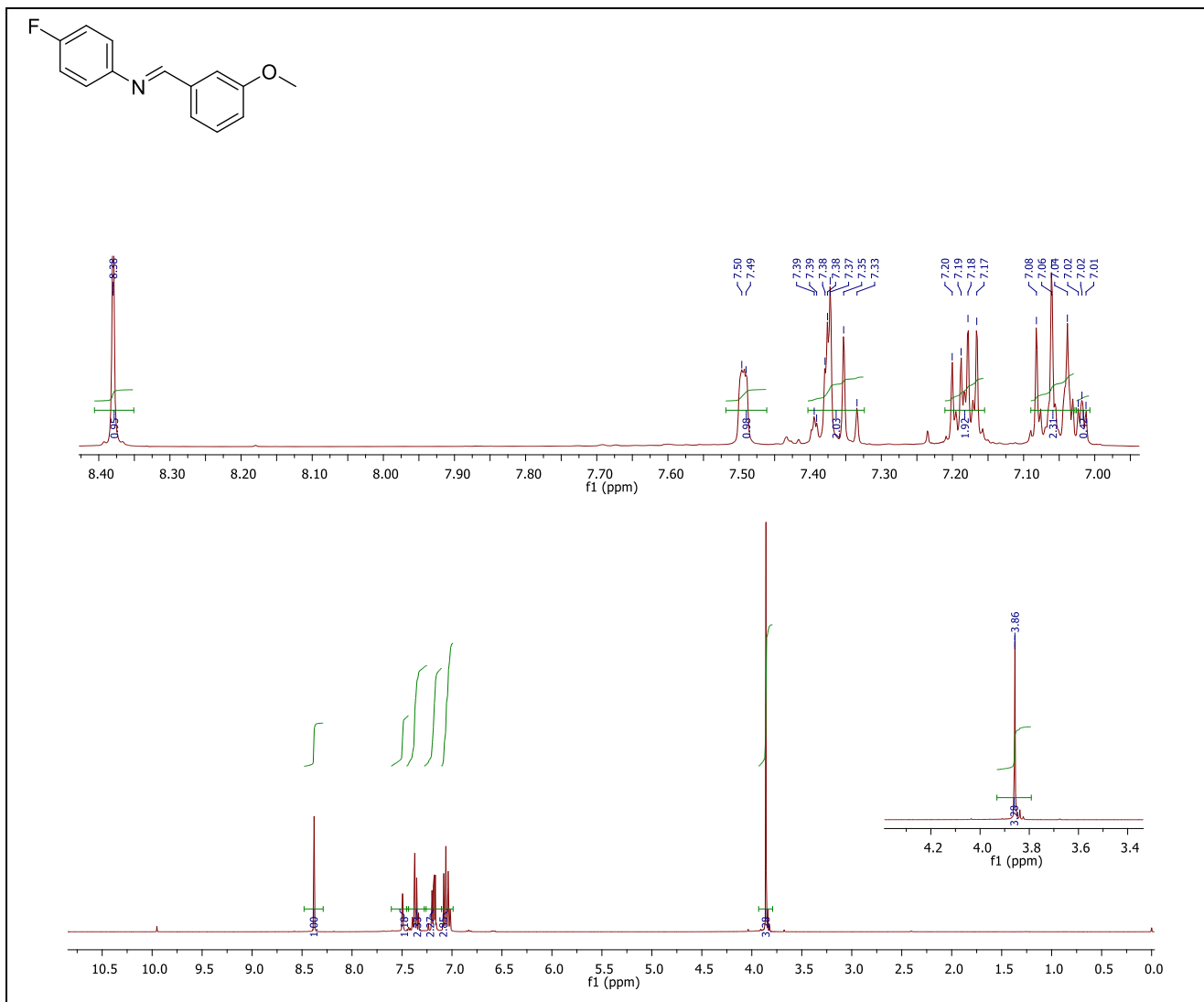


Figure S34: ¹H-NMR spectrum (400 MHz) of compound **6e** (in CDCl₃)

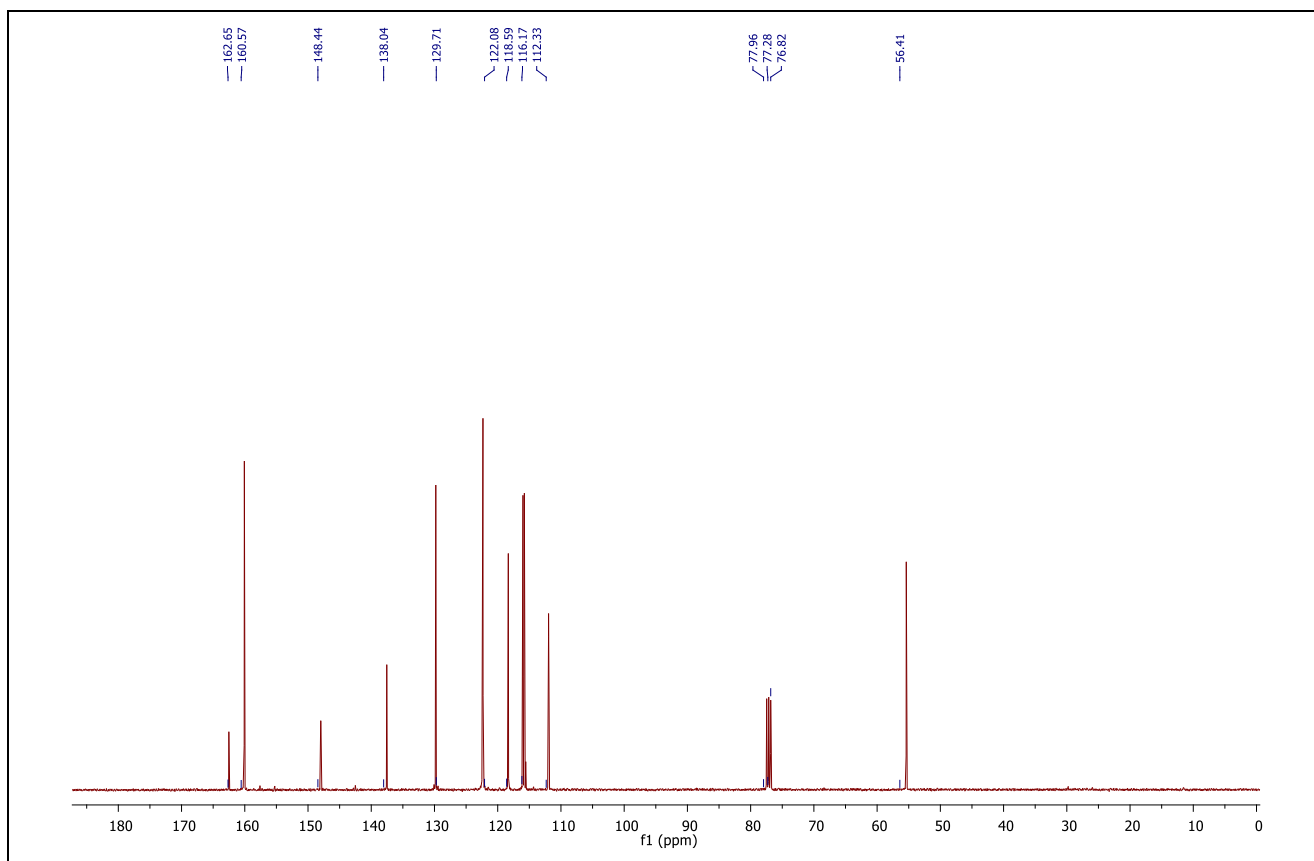


Figure S35: ^{13}C -NMR spectrum (400 MHz) of compound **6e** (in CDCl_3)

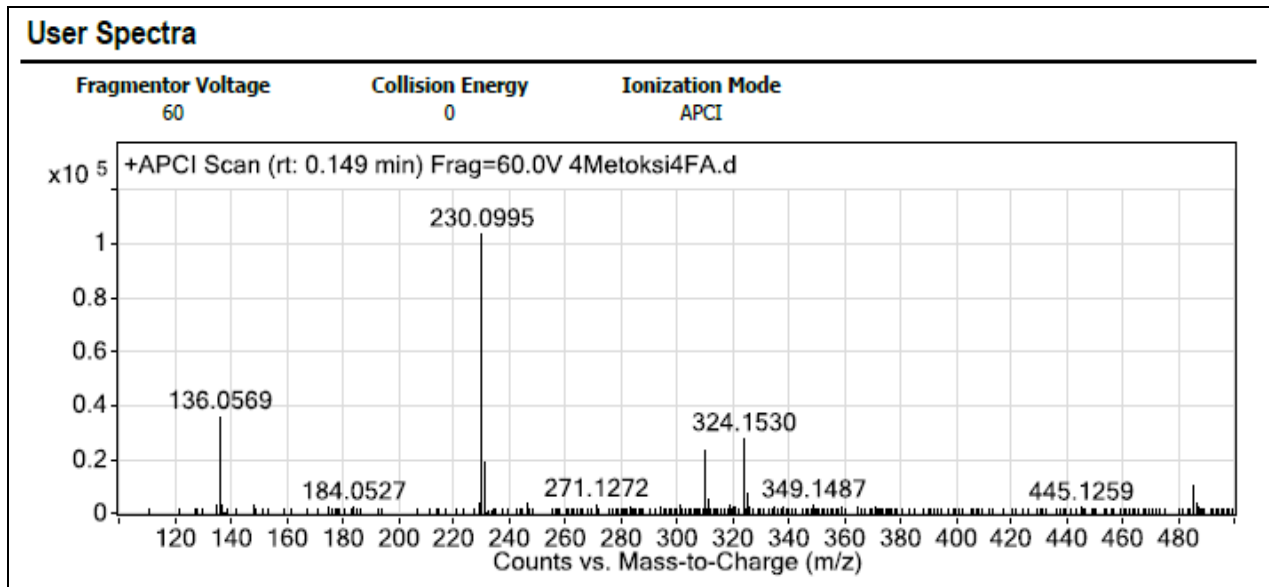


Figure S36: HRMS of compound **6f**

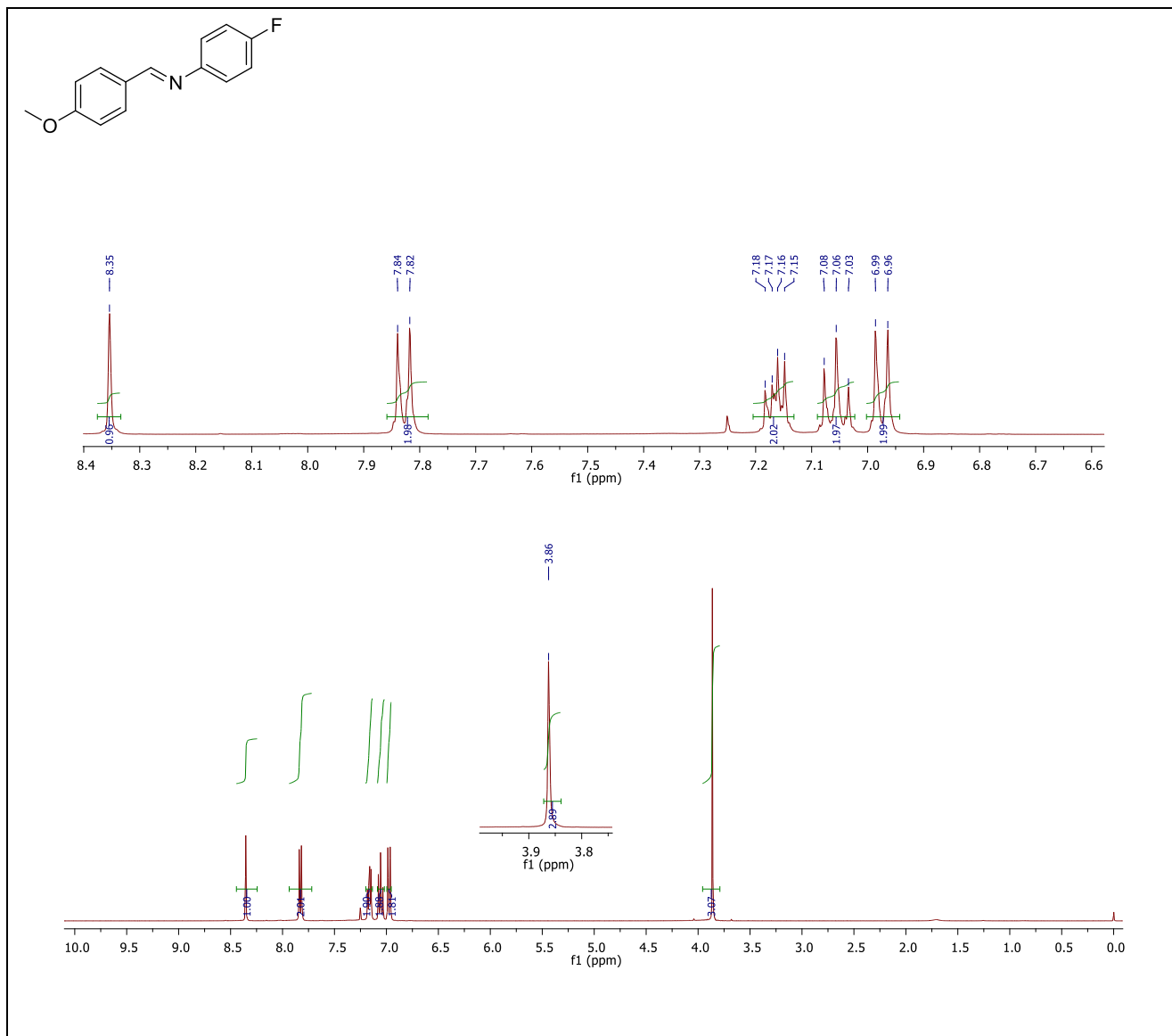


Figure S37: ¹H-NMR spectrum (400 MHz) of compound **6f** (in CDCl₃)

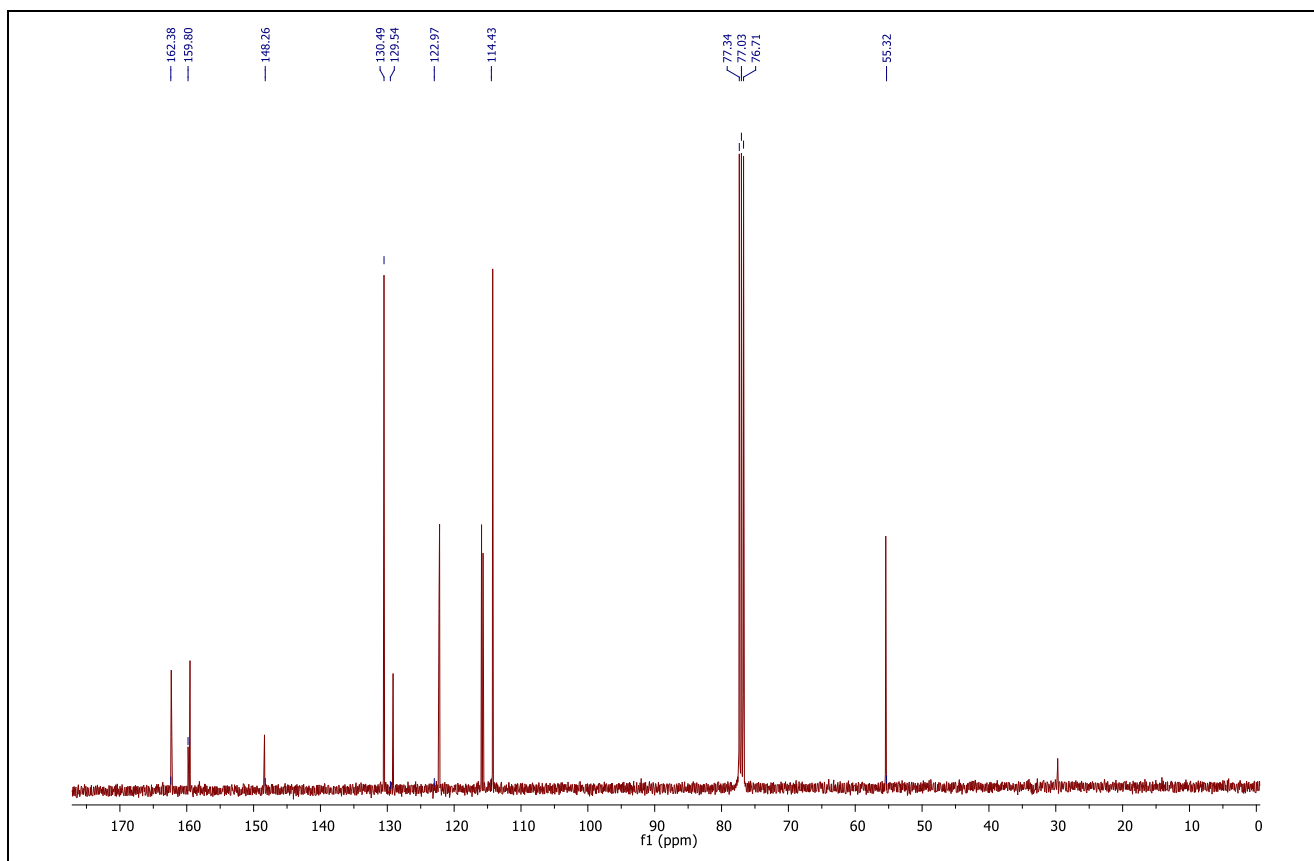


Figure S38: ^{13}C -NMR spectrum (400 MHz) of compound **6f** (in CDCl_3)

References

- [1] Holder, I. A.; Boyce, S.T. Agar well diffusion assay testing of bacterial susceptibility to various antimicrobials in concentrations non-toxic for human cells in culture. *Burns* **1994**, *20*, 426-429.