

## Supporting Information

### **Ru(II)-Catalyzed Synthesis of Poly-Substituted Furans via Intramolecular Oxidative Annulation Reaction of Ethyl 3-oxo-3-phenylpropanoates with Diaryl alkynes/ Heteroaryl alkynes**

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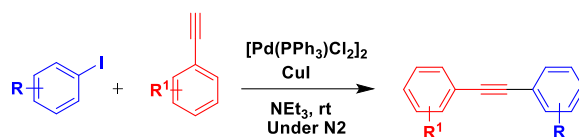
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## 1. General Information

All reagents and solvents were purchased from commercial sources and used as received. The progress of the reaction was monitored by analytical TLC on silica gel G/GF 254 plates. The column chromatography was performed with silica gel 100-200 mesh.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on a 300 MHz or 400 MHz or 100MHz instrument respectively using TMS as an internal standard and chemical shifts are presented in  $\delta$  ppm. Melting points are uncorrected were determined in capillary tubes on a hot stage melting point apparatus containing silicon oil. High resolution mass spectra were taken with a 3000 mass spectrometer and Q-TOF Analyzer. IR spectra were recorded using FTIR spectrophotometer.

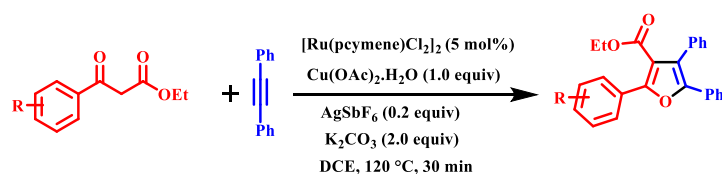
## 2. General Procedure for the Preparation of Alkynes

$[\text{Pd}(\text{PPh}_3)\text{Cl}_2]_2$  (2 mol%), CuI (4 mol%),  $\text{Et}_3\text{N}$  (2 equiv.) and iodobenzene (1.1 equiv.) were dissolved in 10.0 mL  $\text{NEt}_3$  at room temperature. Subsequently, phenylacetylene (1.0 equiv.) was added to the resulting mixture by syringe, and the reaction was stirred under argon atmosphere for 10 h. After the solvent was removed and extracted with  $\text{CH}_2\text{Cl}_2$  (4 $\times$ 50 mL). The combined organic layer was washed with brine, dried over  $\text{Na}_2\text{SO}_4$ , concentrated under reduced pressure to give crude alkyne<sup>1</sup>. The residue was purified by silica gel flash chromatography using petroleum ether to afford the desired product.



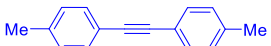
## 3. General Procedure for the Preparation of Substituted Furans

In an oven dried 50 ml R.B. flask charged with stir bar, Ethyl 3-(4-methoxyphenyl)-3-oxopropionate (1.0 equiv.), diarylalkyne (1.0 equiv.),  $[\text{RuCl}_2(\text{pymene})]_2$  (5 mol%),  $\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$  (1.0 equiv.) and  $\text{AgSbF}_6$  (20 mol%) in 2 ml DCE, resulting mixture was stirred at 120 °C with oil bath for 6 h. Completion of reaction was monitored by TLC (1:20 Ethyl acetate and Hexane). Reaction mixture was cooled down to room temperature and diluted with 10 mL of  $\text{H}_2\text{O}$ . The resultant mixture was extracted with DCM (3  $\times$  15 mL). The combined organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ . After removal of the solvent under reduced pressure, the crude product was purified by column chromatography on silica gel (100-200 mesh) by using hexane/ethyl acetate solvent system to give the desired product tetrasubstituted furan compounds.




## 4. Spectral data of Internal Alkynes


### 1,2-di-p-tolyne (2b)

 Yield 88% (181 mg); White solid; (KBr)  $\text{cm}^{-1}$ :  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.40 (d,  $J = 8.0\text{ Hz}$ , 4H), 7.12 (d,  $J = 7.8\text{ Hz}$ , 4H), 2.34 (s, 6H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  138.1, 132.4, 129.1, 120.4, 88.9, 21.5; mass ESI-MS( $m/z$ ) = 207.20 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS (ESI)  $m/z$  [ $\text{M}+\text{H}$ ] $^+$ calcd for  $\text{C}_{16}\text{H}_{15}$  207.1174 Found 207.1179


### 1,2-bis(4-methoxyphenyl)ethyne (2c)

 Yield 89% (212 mg); White solid; (KBr)  $\text{cm}^{-1}$ :  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.46-7.44 (d,  $J = 8.8\text{ Hz}$ , 4H), 6.88-6.86 (d,  $J = 8.8\text{ Hz}$ , 4H), 3.82 (s, 6H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  159.4, 132.8, 115.7, 113.9, 87.9, 55.3; mass ESI-MS( $m/z$ ) = 239.10 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS (ESI)  $m/z$  [ $\text{M}+\text{H}$ ] $^+$ calcd for  $\text{C}_{16}\text{H}_{15}$  239.1072 Found 207.1179.


### 1,2-bis(4-fluorophenyl)ethyne (2d)

 Yield 72% (154 mg); White solid;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.51-7.48 (m, 4H), 7.06-7.02 (m, 4H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  162.8 (d, C-F,  $^1\text{J}_{\text{C-F}} = 253.0\text{ Hz}$ ), 134.4 (d, C-F,  $^3\text{J}_{\text{C-F}} = 8.6\text{ Hz}$ ), 133.4 (d, C-F,  $^3\text{J}_{\text{C-F}} = 8.7\text{ Hz}$ ), 119.2 (d, C-F,  $^4\text{J}_{\text{C-F}} = 3.4\text{ Hz}$ ), 115.5 (d, C-F,  $^2\text{J}_{\text{C-F}} = 22.5\text{ Hz}$ ), 88.0;  $^{19}\text{F NMR}$  (376 MHz,  $\text{CDCl}_3$ ):  $\delta$  112.3 (s), 115.2 (s); mass ESI-MS( $m/z$ ) = 215.03 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS (ESI)  $m/z$  [ $\text{M}+\text{H}$ ] $^+$ calcd for  $\text{C}_{14}\text{H}_9\text{F}_2$  215.0720 Found 215.0687.

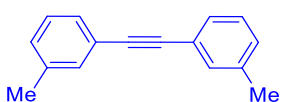
### 1,2-bis(4-(tert-butyl)phenyl)ethyne (2e)

 Yield 89% (258 mg); White solid;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.46-7.43 (m, 4H), 7.36-7.32 (m, 4H), 1.31 (s, 9H), 1.30 (s, 9H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  151.3, 137.1, 132.2, 127.6, 125.5, 120.5, 88.9, 34.9, 34.8, 31.2; mass ESI-MS( $m/z$ ) = 291.2 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS (ESI)  $m/z$  [ $\text{M}+\text{H}$ ] $^+$ calcd for  $\text{C}_{22}\text{H}_{27}$  291.2113; Found 291.2108

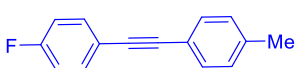
### 1,2-bis(4-bromophenyl)ethyne (2f)

 Yield 81% (270 mg); White solid;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.49-7.47 (d,  $J = 8.5\text{ Hz}$ , 4H), 7.38-7.36 (d,  $J = 8.5\text{ Hz}$ , 4H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  138.1, 132.4, 129.1, 120.4, 88.9, 21.5; mass ESI-MS( $m/z$ ) = 334.90 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS (ESI)  $m/z$  [ $\text{M}+\text{H}$ ] $^+$ calcd for  $\text{C}_{14}\text{H}_9\text{Br}_2$  334.9071 Found 334.1179

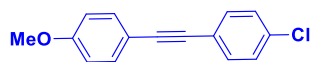
### 1,2-di-m-tolyne (2g)

 Yield 84% (173 mg); White solid; (KBr)  $\text{cm}^{-1}$ :  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.39 (s, 2H), 7.38-7.36 (d,  $J = 8.1\text{ Hz}$ , 2H), 7.28-7.25 (t,  $J = 7.5\text{ Hz}$ , 2H), 7.18-7.16 (d,  $J = 7.5\text{ Hz}$ , 2H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  138.0, 132.2, 129.1, 128.6, 128.2, 123.2, 89.2, 21.2; mass ESI-MS( $m/z$ ) = 207.20 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS (ESI)  $m/z$  [ $\text{M}+\text{H}$ ] $^+$ calcd for  $\text{C}_{16}\text{H}_{15}$  207.1174 Found 207.1179.

### 1-fluoro-4-(p-tolyne)benzene (2h)

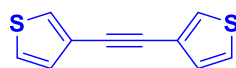
 Yield 79% (166 mg); white solid; mp 123-128°C; (KBr)  $\text{cm}^{-1}$ :  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.48-7.51 (m, 2H), 7.40-7.43 (d,  $J = 8.16\text{ Hz}$ , 2H), 7.15-7.17 (d,  $J = 7.98\text{ Hz}$ , 2H), 7.01-7.06 (t,  $J = 8.84\text{ Hz}$ , 2H), 2.37 (s, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  162.40 (d, C-F  $^1\text{J}_{\text{C-F}} = 248.9\text{ Hz}$ ), 138.49, 133.40 (d, C-F  $^3\text{J}_{\text{C-F}} = 8.21\text{ Hz}$ ), 131.45, 129.15, 120.01, 119.59 (d, C-F  $^4\text{J}_{\text{C-F}} = 3.66\text{ Hz}$ ), 115.59 (d, C-F  $^2\text{J}_{\text{C-F}} = 22.14\text{ Hz}$ ), 89.22, 87.64, 21.50; mass (ES+)  $m/z$  = 211.09.

### 1-chloro-4-((4-methoxyphenyl)ethynyl)benzene (2i)



Yield 83% (200 mg); white solid; mp 123-128 °C; (KBr)  $\text{cm}^{-1}$ :  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.44-7.46 (d,  $J = 8.86$  Hz, 2H), 7.41-7.43 (d,  $J = 8.60$  Hz, 2H), 7.29-7.31 (d,  $J = 8.60$  Hz, 2H), 7.25 (s), 6.86-6.88 (d,  $J = 8.81$  Hz, 2H), 3.82 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  159.80, 133.88, 133.08, 132.64, 128.64, 122.15, 115.04, 114.07, 90.37, 87.00, 55.32; mass (ES+)  $m/z = 243.05$ .

### 1,2-di(thiophen-3-yl)ethyne (2k)



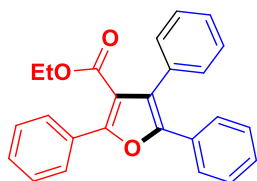
Yield 78% (147 mg); White solid; (KBr)  $\text{cm}^{-1}$ :  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.57-7.56 (m, 2H), 7.35-7.33 (dd,  $J = 3.0$  Hz, 2H), 7.25-7.24 (d,  $J = 5.0$  Hz, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  129.7, 128.4, 125.3, 122.1, 84.0; mass ESI-MS( $m/z$ ) = 190.9 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS (ESI)  $m/z$  [ $\text{M}+\text{H}$ ] $^+$  calcd for  $\text{C}_{10}\text{H}_6\text{S}_2$  190.9989 Found 190.1179.

## 1. References

1. Doucet, H.; Hierso, J. C.; *Angew. Chem., Int. Ed.*, **2007**, 46, 834.
2. Stuart, D.R.; Laperle, M. B.; Burgess, K. M. N.; Fagnou, K. *J. Am. Chem. Soc.*, **2008**, 130, 16474.

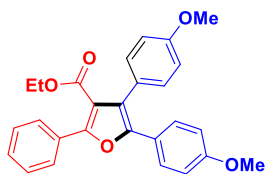
## 4. Spectral data of the Obtained Compound

### Ethyl 2,4,5-triphenylfuran-3-carboxylate (3aa)



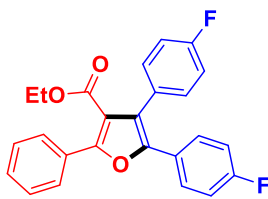
Eluent: Hexane/EA = 95:05,  $R_f$  = 0.63; Yield 67% (246 mg); light yellow oil; (KBr)  $\text{cm}^{-1}$ : 816, 1082, 1222, 1340, 1451, 1498, 1556, 1657, 1702, 2919,  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.85 (dd,  $J$  = 8.5 Hz,  $J$  = 1.5 Hz, 2H), 7.38-7.34 (m, 5H), 7.33-7.29 (m, 5H), 7.19-7.13 (m, 3H), 3.99 (q,  $J$  = 7.2 Hz, 2H), 0.86 (s, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.4, 154.8, 147.9, 139.3, 133.5, 130.3, 130.0, 128.9, 128.4, 127.8, 127.7, 164.2, 154.2, 148.2, 133.2, 130.1, 130.0, 129.8, 129.0, 128.8, 128.3, 128.2, 127.7, 127.6, 123.6, 60.5, 13.05; mass (ES+)  $m/z$  = 369.14 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{25}\text{H}_{21}\text{O}_3$  369.1491 Found 369.1480.

### Ethyl 4,5-bis(4-methoxyphenyl)-2-phenylfuran-3-carboxylate (3ac)



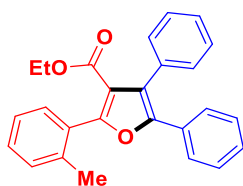
Eluent: Hexane/EA = 80:20,  $R_f$  = 0.61; Yield 74% (316 mg); light yellow oil. (KBr)  $\text{cm}^{-1}$ : 769, 836, 1030, 1113, 1248, 1331, 1462, 1514, 1603, 1717, 2958  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.8 (d,  $J$  = 7.5 Hz, 2H), 7.46-7.37 (m, 5H), 7.28 (d,  $J$  = 8.7 Hz, 2H), 6.94 (d,  $J$  = 8.5 Hz, 2H), 6.79 (d,  $J$  = 8.8 Hz, 2H), 4.11 (q,  $J$  = 7.2 Hz, 2H), 3.86 (s, 3H), 3.78 (s, 3H), 1.0 (t,  $J$  = 1.0 Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.6, 159.2, 159.0, 153.6, 148.6, 135.3, 131.3, 130.0, 128.9, 128.3, 127.7, 125.5, 125.0, 123.0, 121.9, 116.9, 113.9, 60.6, 55.3, 55.3, 13.8; mass (ES+)  $m/z$  = 429.18 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{27}\text{H}_{25}\text{O}_5$  429.1697 Found 429.1693.

### Ethyl 4,5-bis(4-fluorophenyl)-2-phenylfuran-3-carboxylate (3ad)



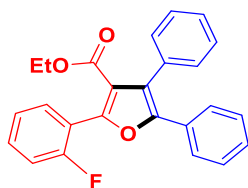
Eluent: Hexane/EA = 80:20,  $R_f$  = 0.51; Yield 63% (254 mg); light yellow oil. (KBr)  $\text{cm}^{-1}$ : 747, 845, 1015, 1160, 1233, 1471, 1585, 1730, 3022  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.48-7.88 (m, 2H), 7.48-7.33 (m, 7H), 7.11 (t,  $J$  = 8.8 Hz, 2H), 6.95 (t,  $J$  = 8.8 Hz, 2H), 4.11-4.06 (q,  $J$  = 7.1 Hz, 2H), 1.01-0.97 (t,  $J$  = 0.9 Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.1, 162.6 (d, C-F  $^1\text{JC-F}$  = 248.1 Hz), 162.4 (d, C-F  $^1\text{JC-F}$  = 249.4 Hz), 154.8, 147.9, 131.9 (d, C-F  $^3\text{JC-F}$  = 8.1 Hz), 129.8, 129.4, 129.1 (d, C-F  $^4\text{JC-F}$  = 3.3 Hz), 128.4, 128.0, 127.8 (d, C-F  $^3\text{JC-F}$  = 8.1 Hz), 127.7, 126.3 (d, C-F  $^4\text{JC-F}$  = 3.5 Hz), 122.4, 115.7 (d, C-F  $^2\text{JC-F}$  = 21.8 Hz), 115.7 (d, C-F  $^2\text{JC-F}$  = 21.8 Hz), 60.7, 13.7; mass (ES+)  $m/z$  = 405.13 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{25}\text{H}_{19}\text{F}_2\text{O}_3$  405.1302 Found 405.1303.

### Ethyl 4,5-diphenyl-2-(o-tolyl)furan-3-carboxylate (3ba)



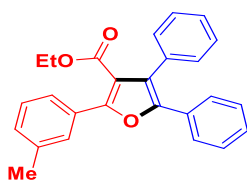
Eluent: Hexane/EA = 95:05,  $R_f$  = 0.53; Yield 70% (267 mg); light yellow solid. mp 125-130  $^{\circ}\text{C}$ ; (KBr)  $\text{cm}^{-1}$ : 698, 732, 1022, 1102, 1263, 1329, 1714, 2925  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.59-7.61 (d,  $J$  = 7.5 Hz, 1H), 7.47-7.51 (m, 6H), 7.28-7.45 (m, 7H), 4.03-4.08 (q,  $J$  = 7.1 Hz, 2H), 2.50 (s, 3H) 0.93-0.97 (t,  $J$  = 7.2 Hz, 2H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  163.4, 156.7, 148.6, 137.8, 133.3, 130.8, 130.2, 130.1, 129.5, 128.3, 127.6, 127.6, 125.6, 125.2, 122.7, 117.6, 60.1, 20.3, 13.4; mass (ES+)  $m/z$  = 383.16 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{26}\text{H}_{23}\text{O}_3$  383.1647 Found 383.1637.

### Ethyl 2-(2-fluorophenyl)-4,5-diphenylfuran-3-carboxylate (3ca)



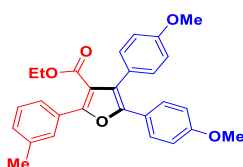
Eluent: Hexane/EA = 90:10,  $R_f$  = 0.51; Yield 61% (235 mg); light yellow solid. mp 130-135  $^{\circ}\text{C}$ ; (KBr)  $\text{cm}^{-1}$ : 759, 843, 949, 1088, 1175, 1227, 1332, 1446, 1598, 1721, 2960  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.76-7.72 (td,  $J$  = 7.4 Hz,  $J$  = 1.7 Hz, 1H), 7.43-7.38 (m, 7H), 7.29-7.14 (m, 6H), 4.09-4.03 (q,  $J$  = 7.1 Hz, 2H), 0.98-0.94 (t,  $J$  = 7.2 Hz, 2H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  163.4, 159.7 (d, C-F  $^1\text{JC-F}$  = 251.3 Hz), 149.3, 132.7, 131.0 (d, C-F  $^3\text{JC-F}$  = 8.2 Hz), 130.5, 130.2, 130.0, 128.3, 127.8, 127.7, 125.8, 123.9 (d, C-F  $^4\text{JC-F}$  = 3.6 Hz), 123.2, 119.1, 118.5, 116.0, 115.9 (d, C-F  $^2\text{JC-F}$  = 21.9), 60.4, 13.5; mass (ES+)  $m/z$  = 387.13 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{25}\text{H}_{20}\text{FO}_3$  387.1396 Found 387.1395.

### Ethyl 4,5-diphenyl-2-(*m*-tolyl)furan-3-carboxylate (3da)



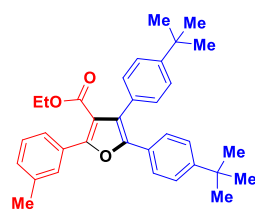
Eluent: Hexane/EA = 95:05,  $R_f$  = 0.61; Yield 69% (263 mg); light yellow solid; (KBr)  $\text{cm}^{-1}$ : 791, 827, 949, 1069, 1161, 1230, 1329, 1498, 1592, 1675, 1715, 2924  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.64-7.66 (d,  $J$  = 7.2 Hz, 2H), 7.28-7.38 (m, 8H), 7.13-7.19 (m, 4H), 3.98-4.03 (q,  $J$  = 7.1 Hz, 2H), 2.36 (s, 3H), 0.87-0.91 (t,  $J$  = 7.2 Hz, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.3, 154.4, 148.1, 137.8, 133.3, 130.1, 130.0, 129.9, 129.7, 128.4, 128.3, 128.3, 128.2, 127.7, 127.6, 125.8, 125.0, 123.7, 116.8, 60.5, 21.5, 13.5; mass (ES+)  $m/z$  = 383.16 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{26}\text{H}_{23}\text{O}_3$  383.1647 Found 383.1643.

### Ethyl 4,5-bis(4-methoxyphenyl)-2-(*m*-tolyl)furan-3-carboxylate (3dc)



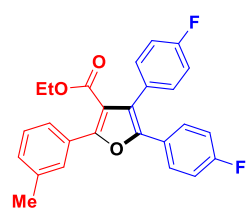
Eluent: Hexane/EA = 90:10,  $R_f$  = 0.42; Yield 75% (331 mg); light orange oil. (KBr)  $\text{cm}^{-1}$ : 701, 1031, 1175, 1262, 1515, 1607, 1712, 3355  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.66-7.68 (m, 2H), 7.25-7.39 (m, 5H), 7.18-7.21 (m, 1H), 6.92-6.94 (d,  $J$  = 8.7 Hz, 2H), 6.77-6.80 (d,  $J$  = 9.0, 2H), 4.07-4.12 (q,  $J$  = 7.1 Hz, 2H), 3.8 (s, 3H), 3.7 (s, 3H), 2.42 (s, 3H), 1.00-1.03 (t,  $J$  = 7.2 Hz, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.5, 159.1, 159.0, 150.7, 148.4, 137.8, 131.2, 130.2, 129.9, 129.6, 128.2, 128.1, 127.2, 125.5, 124.9, 123.1, 121.7, 116.8, 113.8, 60.5, 55.2, 21.5, 13.7; mass (ES+)  $m/z$  = 443.18 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{28}\text{H}_{27}\text{O}_5$  443.1858 Found 443.1848.

### Ethyl 4,5-bis(4-(*tert*-butyl)phenyl)-2-(*m*-tolyl)furan-3-carboxylate (3de)



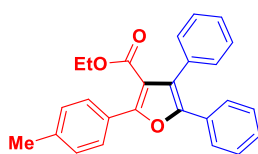
Eluent: Hexane/EA = 95:05,  $R_f$  = 0.56; Yield 71% (350 mg); light yellow solid. mp 102-125  $^{\circ}\text{C}$ ; (KBr)  $\text{cm}^{-1}$ : 737, 835, 1035, 1113, 1230, 1267, 1330, 1405, 1517, 1657, 1718, 2960  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.71-7.73 (d,  $J$  = 7.22 Hz, 2H), 7.74-7.44 (m, 4H), 7.27-7.36 (m, 5H), 7.21-7.23 (d,  $J$  = 7.75 Hz, 1H), 4.04-4.09 (q,  $J$  = 7.1 Hz, 2H), 2.4 (s, 3H), 1.39 (s, 9H), 1.30 (s, 9H), 0.08-0.93 (t,  $J$  = 6.99 Hz, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.5, 153.9, 150.6, 150.4, 148.1, 137.8, 130.3, 129.9, 129.7, 129.5, 128.2, 128.1, 127.5, 125.3, 125.3, 125.2, 124.8, 123.0, 117.1, 60.4, 34.6, 31.4, 31.2, 21.5, 13.4 mass (ES+)  $m/z$  = 495.28 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{34}\text{H}_{39}\text{O}_3$  495.2899 Found 495.2891.

### Ethyl 2-(4-bromophenyl)-4,5-bis(4-methoxyphenyl)furan-3-carboxylate (3dd)



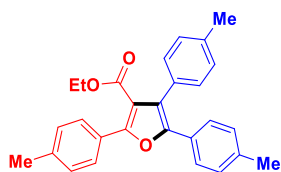
Eluent: Hexane/EA = 90:10,  $R_f$  = 0.51; Yield 64% (267 mg); light yellow solid. (KBr)  $\text{cm}^{-1}$ : 705, 845, 950, 1021, 1130.3, 1232, 1335, 1448, 1600, 1721, 2995  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ): 7.67-7.69 (d,  $J$  = 6.5 Hz, 2H), 7.31-7.39 (m, 5H), 7.22-7.24 (d,  $J$  = 7.5 Hz, 1H), 7.09-7.13 (t,  $J$  = 8.8 Hz, 2H), 6.93-6.97 (t,  $J$  = 8.8 Hz, 2H), 4.06-4.11 (q,  $J$  = 7.2 Hz), 2.43 (s, 3H), 1.55 (s, 3H), 0.99-1.02 (t,  $J$  = 7.16 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.0, 162.4 (d, C-F  $^1J$  C-F = 246.5 Hz), 162.2 (d, C-F  $^1J$  C-F = 248.7 Hz), 154.8, 147.6, 137.9, 131.7 (d, C-F  $^3J$  C-F = 8.1 Hz), 130.1, 129.5, 129.0 (d, C-F  $^4J$  C-F = 3.2 Hz), 128.4, 128.1, 127.6 (d, C-F  $^3J$  C-F = 8.1 Hz), 126.2 (d, C-F  $^4J$  C-F = 3.1 Hz), 125.1, 122.2, 116.6 (d, C-F  $^2J$  C-F = 21.7 Hz), 60.6, 21.5, 13.6; mass (ES+)  $m/z$  = 419.14 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{26}\text{H}_{21}\text{F}_2\text{O}_3$  419.1459 Found 419.1450.

### Ethyl 4,5-diphenyl-2-(*p*-tolyl)furan-3-carboxylate (3ea)



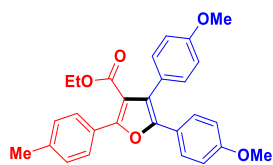
Eluent: Hexane/EA = 95:05,  $R_f$  = 0.39; Yield 69% (263 mg); light yellow oil. (KBr)  $\text{cm}^{-1}$ ; (KBr)  $\text{cm}^{-1}$ : 819, 1085, 1232, 1365, 1460, 1504, 1604, 1715, 2923,  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.82 (d,  $J$  = 8.0 Hz, 2H), 7.43-7.35 (m, 7H), 7.27-7.21 (m, 6H), 4.05 (q,  $J$  = 7.2 Hz, 2H), 2.41 (s, 3H), 0.93 (t,  $J$  = 0.9 Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.4, 154.8, 147.9, 139.3, 133.5, 130.3, 130.0, 128.9, 128.4, 127.8, 127.7, 127.6, 127.0, 125.8, 123.7, 116.5, 60.5, 21.5, 13.6; mass (ES+)  $m/z$  = 383.11 (M+H) $^+$ ; HRMS(ESI-TOF) calcd for  $\text{C}_{26}\text{H}_{23}\text{O}_3$  383.1642 Found 383.1662.

### Ethyl 2,4,5-tri-p-tolylfuran-3-carboxylate (3eb)



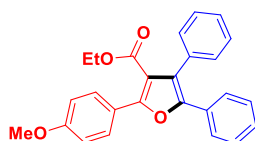
Eluent: Hexane/EA = 95:05,  $R_f$  = 0.27; Yield 72% (295 mg); light yellow oil. (KBr)  $\text{cm}^{-1}$ : 758, 818, 923, 1012, 1114, 1219, 1367, 1460, 1507, 1716, 2924  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.81 (d,  $J$  = 8.4 Hz, 2H), 7.32 (d,  $J$  = 7.8 Hz, 2H), 7.25-7.23 (m, 4H), 7.19 (d,  $J$  = 8.0 Hz, 2H), 7.00 (d,  $J$  = 7.9 Hz, 2H), 4.08 (q,  $J$  = 7.2 Hz, 2H), 2.40 (s, 6H), 2.29 (s, 3H), 0.91 (t,  $J$  = 0.9 Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.2, 154.2, 148.2, 139.0, 137.5, 137.0, 130.3, 129.9, 129.0, 128.9, 127.8, 127.7, 127.3, 125.8, 122.9, 116.5, 115.9, 60.5, 21.4, 21.3, 21.2, 13.7; mass(ES+)  $m/z$  = 411.19 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{28}\text{H}_{27}\text{O}_3$  411.1955 Found 411.1970.

### Ethyl 4,5-bis(4-methoxyphenyl)-2-(p-tolyl)furan-3-carboxylate (3ec)



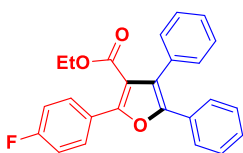
Eluent: Hexane/EA = 80:20,  $R_f$  = 0.46; Yield 73% (322 mg); light red oil. (KBr)  $\text{cm}^{-1}$ : 634, 831, 951, 1031, 1111, 1178, 1247, 1330, 1461, 1507, 1716, 2926  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.78 (d,  $J$  = 8.1 Hz, 2H), 7.36 (d,  $J$  = 9.0 Hz, 2H), 7.27 (d,  $J$  = 8.8 Hz, 2H), 7.24 (d,  $J$  = 7.6 Hz, 2H), 6.93 (d,  $J$  = 9.0 Hz, 2H), 6.78 (d,  $J$  = 9.0 Hz, 2H), 4.09 (q,  $J$  = 7.3 Hz, 2H), 3.86 (s, 3H), 3.77 (s, 3H), 2.40 (s, 3H), 0.91 (t,  $J$  = 0.9 Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.4, 159.0, 159.0, 153.9, 148.2, 138.9, 131.3, 128.9, 127.7, 127.4, 127.2, 125.7, 123.2, 121.8, 116.4, 113.9, 113.9, 60.5, 55.3, 55.3, 21.5, 13.8; mass (ES+)  $m/z$  = 443.19 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{28}\text{H}_{27}\text{O}_5$  443.1853 Found 443.1867.

### Ethyl 2-(4-methoxyphenyl)-4,5-diphenylfuran-3-carboxylate (3fa)



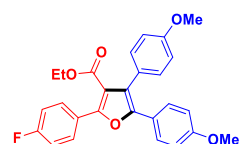
Eluent: Hexane/EA = 90:10,  $R_f$  = 0.43; Yield 69% (274 mg); light green oil. (KBr)  $\text{cm}^{-1}$ : 759, 956, 1101, 1220, 1399, 1469, 1615, 2960, 3020, 3582  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.94 (d,  $J$  = 8.9 Hz, 2H), 7.45-7.39 (m, 7H), 7.26-7.22 (m, 3H), 7.01 (d,  $J$  = 8.9 Hz, 2H), 4.09 (q,  $J$  = 7.0 Hz, 2H), 3.89 (s, 3H), 0.95 (t,  $J$  = 0.9 Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.4, 159.4, 159.2, 152.5, 148.9, 134.8, 131.3, 128.9, 128.6, 127.4, 125.4, 122.9, 121.9, 117.4, 113.9, 113.9, 60.7, 55.3, 13.7; mass (ES+)  $m/z$  = 399.15 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{26}\text{H}_{23}\text{O}_4$  399.1591 Found 399.1598.

### Ethyl 2-(4-fluorophenyl)-4,5-diphenylfuran-3-carboxylate (3ga)



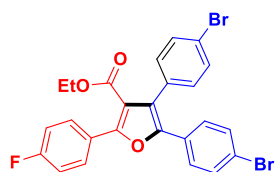
Eluent: Hexane/EA = 90:10,  $R_f$  = 0.62; Yield 63% (243 mg); light yellow solid. mp 118-125  $^{\circ}\text{C}$ ; (KBr)  $\text{cm}^{-1}$ : 841, 1025, 1117, 1218, 1329, 1445, 2925  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.97-7.93 (m, 2H), 7.42-7.34 (m, 7H), 7.25-7.21 (m, 3H), 7.15 (t,  $J$  = 7.1 Hz, 2H), 4.06 (q,  $J$  = 7.0 Hz, 2H), 0.92 (t,  $J$  = 0.9 Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.1, 163.1 (d, C-F  $^1\text{J}_{\text{C-F}}$  = 249.7 Hz), 153.7, 148.2, 133.3, 129.9 (d, C-F  $^3\text{J}_{\text{C-F}}$  = 8.7 Hz), 128.4, 127.8, 127.6, 126.1 (d, C-F  $^4\text{J}_{\text{C-F}}$  = 3.1 Hz), 125.7, 123.6, 116.7, 115.3 (d, C-F  $^2\text{J}_{\text{C-F}}$  = 21.8 Hz), 60.5, 13.5; mass (ES+)  $m/z$  = 386.13 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{25}\text{H}_{20}\text{FO}_3$  387.1391 Found 387.1411.

### Ethyl 2-(4-fluorophenyl)-4,5-bis(4-methoxyphenyl)furan-3-carboxylate (3gc)



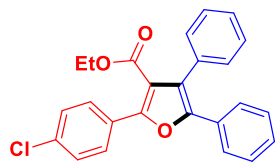
Eluent: Hexane/EA = 90:10,  $R_f$  = 0.29; Yield 65% (289 mg); light yellow oil. (KBr)  $\text{cm}^{-1}$ : 733, 834, 950, 1029, 1081, 1113, 1230, 1331, 1462, 1500, 1712, 2935  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.92-7.89 (m, 2H), 7.37-7.35 (m, 2H), 7.27-7.26 (m, 2H), 7.15-7.10 (m, 2H), 6.95-6.92 (m, 2H), 6.79-6.77 (m, 2H), 4.08 (q,  $J$  = 7.4 Hz, 2H), 3.85 (s, 3H), 3.77 (s, 3H), 1.00 (t,  $J$  = 0.9 Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.3, 163.0 (d, C-F  $^1\text{J}_{\text{C-F}}$  = 249.6 Hz), 159.2, 159.0, 152.9, 148.5, 131.2, 129.8 (d, C-F  $^3\text{J}_{\text{C-F}}$  = 8.2 Hz), 127.2, 126.3 (d, C-F  $^4\text{J}_{\text{C-F}}$  = 3.3 Hz), 125.4, 122.9, 121.7, 116.7, 115.3 (d, C-F  $^2\text{J}_{\text{C-F}}$  = 21.6 Hz), 113.8, 60.5, 55.2, 55.2, 13.6; mass (ES+)  $m/z$  = 447.02 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{27}\text{H}_{24}\text{FO}_5$  447.1602 Found 447.1620.

### Ethyl 4,5-bis(4-bromophenyl)-2-(4-fluorophenyl)furan-3-carboxylate (3gf)



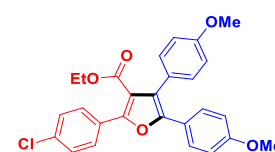
Eluent: Hexane/EA = 90:10,  $R_f$  = 0.62; Yield 59% (319 mg); light yellow oil. (KBr)  $\text{cm}^{-1}$ : 791, 827, 1009, 1115, 1230, 1329, 1498, 1592, 1675, 1715, 2924  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.93 -7.90 (m, 2H), 7.55 (d,  $J$  = 8.4 Hz, 2H), 7.39 (d,  $J$  = 8.7 Hz, 2H), 7.24-7.21 (m, 4H), 7.14 (t,  $J$  = 7.1 Hz, 2H), 4.07 (q,  $J$  = 7.1 Hz, 2H), 0.99 (t,  $J$  = 0.9 Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  163.6, 163.3 (d, C-F  $^1\text{JC-F}$  = 250.4 Hz), 154.5, 147.5, 132.0, 131.7, 131.6, 130.1 (d, C-F  $^3\text{JC-F}$  = 8.4 Hz), 128.5, 127.2, 125.7 (d, C-F  $^4\text{JC-F}$  = 3.3 Hz), 122.9, 122.1 (d, C-F  $^3\text{JC-F}$  = 8.5 Hz), 116.4, 115.4 (d, C-F  $^2\text{JC-F}$  = 21.9 Hz), 60.8, 13.7; mass (ES+)  $m/z$  = 542.17 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{25}\text{H}_{18}\text{Br}_2\text{FO}_3$  542.9601 Found 542.9615.

### Ethyl 2-(4-chlorophenyl)-4,5-diphenylfuran-3-carboxylate (3ha)



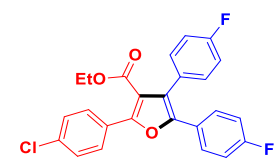
Eluent: Hexane/EA = 90:10,  $R_f$  = 0.51; Yield 59% (237 mg); light green oil. (KBr)  $\text{cm}^{-1}$ : 836, 1021, 1217, 1485, 1602, 1714, 2926  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.80 (d,  $J$  = 8.0 Hz, 2H), 7.44-7.34 (m, 7H), 7.36-7.34 (m, 2H), 7.24-7.23 (m, 3H), 4.05 (q,  $J$  = 6.8 Hz, 2H), 0.93 (t,  $J$  = 0.9 Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.2, 153.2, 148.6, 135.0, 133.2, 129.9, 129.9, 129.0, 128.6, 128.5, 128.4, 127.9, 127.9, 125.9, 123.9, 117.4, 60.7, 13.6; mass (ES+)  $m/z$  = 403.07 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{25}\text{H}_{20}\text{ClO}_3$  403.1095 Found 403.1093.

### Ethyl 2-(4-chlorophenyl)-4,5-bis(4-methoxyphenyl)furan-3-carboxylate (3hc)



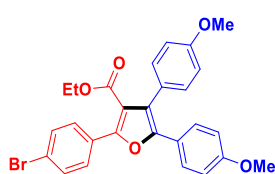
Eluent: Hexane/EA = 90:10,  $R_f$  = 0.23; Yield 68% (314 mg); light green oil; (KBr)  $\text{cm}^{-1}$ : 759, 835, 951, 1030, 1114, 1247, 1329, 1500, 1603, 1713, 2847  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.85 (d,  $J$  = 8.4 Hz, 2H), 7.40 (d,  $J$  = 8.7 Hz, 2H), 7.36 (d,  $J$  = 8.9 Hz, 2H), 7.25 (d,  $J$  = 8.6 Hz, 2H), 6.93 (d,  $J$  = 8.5 Hz, 2H), 6.78 (d,  $J$  = 8.8 Hz, 2H), 4.09 (q,  $J$  = 7.3 Hz, 2H), 3.86 (s, 3H), 3.77 (s, 3H), 0.95 (t,  $J$  = 0.9 Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.3, 152.9, 148.7, 138.0, 137.9, 134.9, 133.0, 130.6, 129.9, 128.9, 128.7, 128.6, 128.5, 128.4, 128.3, 127.4, 126.4, 123.9, 123.0, 117.4, 60.7, 13.6; mass (ES+)  $m/z$  = 463.21 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{27}\text{H}_{24}\text{ClO}_5$  463.1307 Found 463.1308.

### Ethyl 2-(4-chlorophenyl)-4,5-bis(4-fluorophenyl)furan-3-carboxylate (3hd)



Eluent: Hexane/EA = 90:10,  $R_f$  = 0.61; Yield 53% (232 mg); light green oil; (KBr)  $\text{cm}^{-1}$ : 760, 836, 952, 1018, 1160, 1228, 1330, 1369, 1501, 1598, 1715, 2927  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.88-7.86 (m, 2H), 7.44-7.42 (m, 2H), 7.38-7.29 (m, 4H), 7.21 (t,  $J$  = 7.1 Hz, 2H), 6.95 (t,  $J$  = 6.9 Hz, 2H), 4.09 (q,  $J$  = 7.1 Hz, 2H), 1.00 (t,  $J$  = 0.9 Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  163.8, 162.5 (d, C-F  $^1\text{JC-F}$  = 246.6 Hz), 162.3 (d, C-F  $^1\text{JC-F}$  = 248.5 Hz), 153.5, 148.0, 135.2, 131.7 (d, C-F  $^3\text{JC-F}$  = 8.1 Hz), 129.1, 128.9 (d, C-F  $^4\text{JC-F}$  = 3.6 Hz), 128.5, 128.4, 127.7 (d, C-F  $^3\text{JC-F}$  = 8.1 Hz), 126.0 (d, C-F  $^4\text{JC-F}$  = 3.3 Hz), 122.3, 117.0, 115.6 (d, C-F  $^2\text{JC-F}$  = 21.8 Hz), 115.5 (d, C-F  $^2\text{JC-F}$  = 21.6 Hz), 60.8, 13.7; mass (ES+)  $m/z$  = 439.19 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{25}\text{H}_{18}\text{ClF}_2\text{O}_3$  439.0907 Found 439.0901.

### Ethyl 2-(4-bromophenyl)-4,5-bis(4-methoxyphenyl)furan-3-carboxylate (3ic)

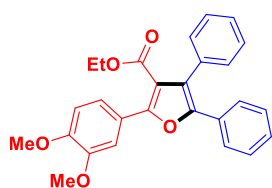


Eluent: Hexane/EA = 80:20,  $R_f$  = 0.46; Yield 58% (293 mg); light green oil; (KBr)  $\text{cm}^{-1}$ : 760, 835, 1031, 1217, 1411, 1507, 1604, 1714, 2926 759, 956, 1101, 1220, 1399, 1469, 1615, 2960, 3020, 3582  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.79 (d,  $J$  = 8.7 Hz, 2H), 7.56 (d,  $J$  = 8.7 Hz, 2H), 7.36 (d,  $J$  = 8.9 Hz, 2H), 7.26 (d,  $J$  = 8.6 Hz, 2H), 6.93 (d,  $J$  = 8.7 Hz, 2H), 6.79 (d,  $J$  = 8.9 Hz, 2H), 4.09 (q,  $J$  = 7.1 Hz, 2H), 3.86 (s, 3H), 3.77 (s, 3H), 1.00 (t,  $J$  = 0.9 Hz, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.4, 159.4, 159.2, 152.5, 148.9, 131.5, 131.3, 129.2, 128.9, 127.4, 125.4, 123.2, 122.9, 121.9, 117.5, 113.9, 113.9,



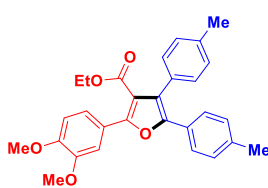
60.7, 55.3, 55.2, 13.8; mass (ES+)  $m/z = 507.20$  (M+H)<sup>+</sup>; HRMS(ESI-TOF) calcd for C<sub>27</sub>H<sub>24</sub>BrO<sub>5</sub> 507.0802 Found 507.0810.

### Ethyl 2-(3,4-dimethoxyphenyl)-4,5-diphenylfuran-3-carboxylate (3ja)



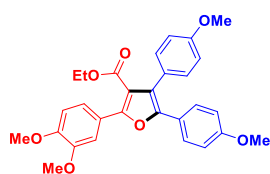
Eluent: Hexane/EA = 80:20, R<sub>f</sub> = 0.53; Yield 71% (303 mg); colourless oil; (KBr) cm<sup>-1</sup>: 758, 1026, 1172, 1227, 1326, 1461, 1507, 1602, 1712, 2927 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.60 (d, *J* = 8.0 Hz, 1H), 7.57 (dd, *J* = 2.1, 2.1 Hz, 1H), 7.43-7.34 (m, 8H), 7.24-7.20 (m, 3H), 6.95 (d, 8.4 Hz, 1H), 4.05 (q, *J* = 7.0 Hz, 2H), 3.97 (s, 3H), 3.94 (s, 3H), 0.91 (t, *J* = 0.9 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 164.6, 154.6, 149.9, 148.7, 147.7, 133.6, 130.2, 129.9, 128.4, 127.7, 127.6, 125.8, 123.8, 122.8, 121.1, 116.1, 11.2, 110.9, 60.5, 55.9, 13.6; mass (ES+)  $m/z = 429.17$  (M+H)<sup>+</sup>; HRMS (ESI-TOF) calcd for C<sub>27</sub>H<sub>25</sub>O<sub>5</sub> 429.1702 Found 429.1737.

### Ethyl 2-(3,4-dimethoxyphenyl)-4,5-di-p-tolylfuran-3-carboxylate (3jb)



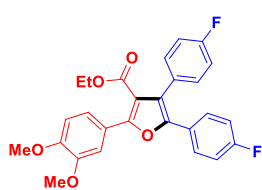
Eluent: Hexane/EA = 80:20, R<sub>f</sub> = 0.48; Yield 74% (337 mg); light green oil; (KBr) cm<sup>-1</sup>: 758, 817, 1025, 1148, 1219, 1265, 1460, 1511, 1716, 2927 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.55 (d, *J* = 1.9 Hz, 1H), 7.53 (dd, *J* = 2.1, 1.9 Hz, 1H), 7.32 (d, *J* = 8.2 Hz, 2H), 7.23-7.18 (m, 4H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.94 (d, *J* = 8.5 Hz, 1H), 4.06 (q, *J* = 6.9 Hz, 2H), 3.96 (s, 3H), 3.94 (s, 3H), 2.40 (s, 3H), 2.29 (s, 3H), 0.91 (t, *J* = 0.9 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 164.7, 154.0, 149.9, 148.7, 147.9, 137.5, 137.0, 130.5, 129.9, 127.6, 125.8, 123.0, 122.9, 120.9, 116.2, 111.1, 110.9, 60.5, 56.0, 55.9, 21.4, 21.3, 13.7; mass (ES+)  $m/z = 457.23$  (M+H)<sup>+</sup>; HRMS (ESI-TOF) calcd for C<sub>29</sub>H<sub>29</sub>O<sub>5</sub> 457.2020 Found 457.2031.

### Ethyl 2-(3,4-dimethoxyphenyl)-4,5-bis(4-methoxyphenyl)furan-3-carboxylate (3jc)



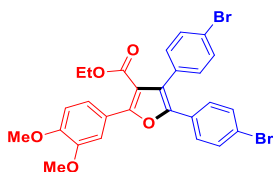
Eluent: Hexane/EA = 80:20, R<sub>f</sub> = 0.48; Yield 75% (366 mg); light green oil; (KBr) cm<sup>-1</sup>: 768, 848, 1050, 1175, 1230, 1475, 1560, 1765, 2930 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.54 (d, *J* = 1.9 Hz, 1H), 7.52 (dd, *J* = 2.0, 2.0 Hz, 1H), 7.36 (d, *J* = 9.1 Hz, 2H), 7.27-7.25 (m, 2H), 6.94 (dd, *J* = 2.4, 2.6 Hz, 3H), 6.79 (d, *J* = 9.1 Hz, 2H), 4.07 (q, *J* = 7.1 Hz, 2H), 3.96 (s, 3H), 3.94 (s, 3H), 3.86 (s, 3H), 3.78 (s, 3H), 1.00 (t, *J* = 0.9 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 164.7, 155.5, 150.3, 148.7, 146.9, 132.4, 131.7, 128.8, 127.2, 123.0, 122.3, 121.9, 115.8, 111.4, 110.9, 60.7, 56.0, 55.9, 55.3, 55.3, 13.9; mass (ES+)  $m/z = 489.14$  (M+H)<sup>+</sup>; HRMS (ESI-TOF) calcd for C<sub>29</sub>H<sub>29</sub>O<sub>7</sub> 489.1908 Found 489.1906.

### Ethyl 2-(3,4-dimethoxyphenyl)-4,5-bis(4-fluorophenyl)furan-3-carboxylate (3jd)



Eluent: Hexane/EA = 80:20, R<sub>f</sub> = 0.39; Yield 69% (320 mg); light green oil; (KBr) cm<sup>-1</sup>: 812, 1023, 1113, 1263, 1327, 1462, 1509, 1713, 2925, cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.55 (d, *J* = 2.0 Hz, 1H), 7.53 (dd, *J* = 2.0, 2.0 Hz, 1H), 7.38-7.30 (m, 4H), 7.12 (t, *J* = 7.1 Hz, 2H), 6.97-6.93 (m, 3H), 4.05 (q, *J* = 7.1 Hz, 2H), 3.96 (s, 3H), 3.95 (s, 3H), 0.93 (t, *J* = 0.9 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 164.1, 162.4 (d, C-F <sup>1</sup>J<sub>C-F</sub> = 246.0 Hz), 162.2 (d, C-F <sup>1</sup>J<sub>C-F</sub> = 248.6 Hz), 154.9, 150.1, 148.6, 147.1, 131.7 (d, C-F <sup>3</sup>J<sub>C-F</sub> = 8.0 Hz), 129.3 (d, C-F <sup>4</sup>J<sub>C-F</sub> = 3.8 Hz), 127.5 (d, C-F <sup>3</sup>J<sub>C-F</sub> = 8.0 Hz), 126.2 (d, C-F <sup>4</sup>J<sub>C-F</sub> = 3.0 Hz), 122.4, 122.2, 121.2, 115.8, 115.5 (d, C-F <sup>2</sup>J<sub>C-F</sub> = 21.7 Hz), 115.5 (d, C-F <sup>2</sup>J<sub>C-F</sub> = 21.4 Hz), 115.5, 115.5, 112.3, 110.9, 60.6, 56.1, 55.9, 13.7; mass (ES+)  $m/z = 465.06$  (M+H)<sup>+</sup>; HRMS (ESI-TOF) calcd for C<sub>27</sub>H<sub>23</sub>F<sub>2</sub>O<sub>5</sub> 465.1505 Found 465.1501.

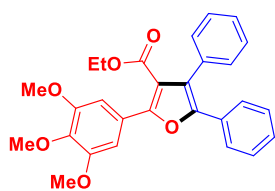
### Ethyl 4,5-bis(4-bromophenyl)-2-(3,4-dimethoxyphenyl)furan-3-carboxylate (3jf)



Eluent: Hexane/EA = 80:20, R<sub>f</sub> = 0.47; Yield 71% (413 mg); light green oil; (KBr) cm<sup>-1</sup>: 735, 827, 1011, 1113, 1227, 1460, 1507, 1713, 2957 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.56-7.51 (m, 4H), 7.39 (d, *J* = 8.8 Hz, 2H), 7.25-7.21 (m, 4H), 6.95 (d, *J* = 8.3 Hz, 1H), 4.06 (q, *J* = 7.1 Hz, 2H), 3.96 (s, 3H), 3.94 (s, 3H), 0.91 (t, *J* = 0.9 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 163.9, 155.5, 150.3, 148.7, 146.9, 132.4,

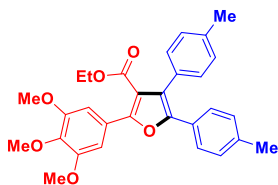
131.7, 128.8, 127.3, 123.0, 122.3, 121.9, 115.8, 111.4, 110.9, 60.7, 56.0, 55.9, 13.9; mass (ES+)  $m/z = 584.19$  (M+H)<sup>+</sup>; HRMS (ESI-TOF) calcd for C<sub>27</sub>H<sub>23</sub>Br<sub>2</sub>O<sub>5</sub> 584.9907 Found 584.9932.

#### Ethyl 4,5-diphenyl-2-(3,4,5-trimethoxyphenyl)furan-3-carboxylate (3ka)



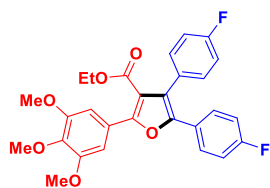
Eluent: Hexane/EA = 80:20, R<sub>f</sub> = 0.47; Yield 73% (334 mg); light yellow oil; (KBr) cm<sup>-1</sup>: 767, 948, 1003, 1178, 1234, 1335, 1415, 1501, 1677, 1717, 2930 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.43 -7.34 (m, 8H), 7.27-7.23 (4H), 4.07 (q, *J* = 7.1 Hz, 2H), 3.95 (s, 6H), 3.91 (s, 3H), 0.91 (t, *J* = 0.9 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 164.5, 153.9, 153.0, 147.9, 139.3, 139.2, 133.4, 130.0, 129.9, 128.5, 127.7, 127.6, 125.8, 125.2, 123.8, 116.9, 114.0, 105.4, 60.9, 60.6, 56.3, 13.6; mass (ES+)  $m/z = 459.13$  (M+H)<sup>+</sup>; HRMS (ESI-TOF) calcd for C<sub>28</sub>H<sub>27</sub>O<sub>6</sub> 459.1802 Found 459.1807.

#### Ethyl 4,5-di-p-tolyl-2-(3,4,5-trimethoxyphenyl)furan-3-carboxylate (3kb)



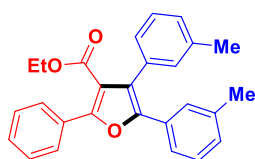
Eluent: Hexane/EA = 80:20, R<sub>f</sub> = 0.41; Yield 81% (393 mg); light yellow oil; (KBr) cm<sup>-1</sup>: 791, 827, 949, 1069, 1161, 1230, 1329, 1498, 1592, 1715, 2924 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.33 (d, *J* = 8.4 Hz, 2H), 7.25-18 (m, 6H), 7.05 (d, *J* = 8.1 Hz, 2H), 4.06 (q, *J* = 7.6 Hz, 2H), 3.97 (s, 6H), 3.91 (s, 3H), 2.40 (s, 3H), 2.30 (s, 3H), 0.91 (t, *J* = 0.9 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 164.5, 153.9, 153.0, 147.9, 139.3, 139.2, 133.4, 130.0, 129.9, 128.5, 127.7, 127.6, 125.8, 125.2, 123.8, 116.9, 114.0, 105.4, 60.9, 60.6, 56.3, 13.6; mass (ES+)  $m/z = 487.21$  (M+H)<sup>+</sup>; HRMS (ESI-TOF) calcd for C<sub>28</sub>H<sub>27</sub>O<sub>6</sub> 487.2121 Found 487.2109.

#### Ethyl 4,5-bis(4-fluorophenyl)-2-(3,4,5-trimethoxyphenyl)furan-3-carboxylate (3kd)



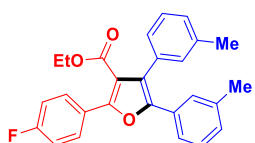
Eluent: Hexane/EA = 80:20, R<sub>f</sub> = 0.31; Yield 69% (340 mg); light yellow oil; (KBr) cm<sup>-1</sup>: 746, 838, 1001, 1126, 1214, 1461, 1585, 1711, 3020 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.38 -7.29 (m, 4H), 7.23 (s, 2H), 7.10 (t, *J* = 7.1 Hz, 2H), 6.95 (t, *J* = 6.9 Hz, 2H), 4.07 (q, *J* = 7.1 Hz, 2H), 3.94 (s, 6H), 3.91 (s, 3H), 0.98 (t, *J* = 0.9 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 164.3, 162.6 (d, C-F <sup>1</sup>J<sub>C-F</sub> = 246.5 Hz), 162.4 (d, C-F <sup>1</sup>J<sub>C-F</sub> = 249.0 Hz), 154.5, 153.2, 147.5, 139.5, 131.8 (d, C-F <sup>3</sup>J<sub>C-F</sub> = 8.0 Hz), 129.2 (d, C-F <sup>4</sup>J<sub>C-F</sub> = 3.8 Hz), 127.8 (d, C-F <sup>3</sup>J<sub>C-F</sub> = 8.1 Hz), 126.2 (d, C-F <sup>4</sup>J<sub>C-F</sub> = 2.8 Hz), 125.1, 122.4, 116.8, 115.7 (d, C-F <sup>2</sup>J<sub>C-F</sub> = 21.8 Hz), 115.7 (d, C-F <sup>2</sup>J<sub>C-F</sub> = 21.6 Hz), 105.7, 61.1, 60.8, 56.4, 13.8; mass (ES+)  $m/z = 495.16$  (M+H)<sup>+</sup>; HRMS (ESI-TOF) calcd for C<sub>28</sub>H<sub>25</sub>F<sub>2</sub>O<sub>6</sub> 495.1619 Found 495.1621.

#### 1-(2-phenyl-4,5-di-m-tolylfuran-3-yl)propan-1-one (3ag)



Eluent: Hexane/EA = 95:05, R<sub>f</sub> = 0.39; Yield 70% (277 mg); light yellow oil; (KBr) cm<sup>-1</sup>: 759, 832, 1033, 1118, 1217, 1331, 1461, 1605, 1710, 2926 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.93-7.91 (m, 2H), 7.47-7.43 (m, 2H), 7.41-7.39 (m, 1H), 7.33 (s, 1H), 7.30-7.26 (m, 1H), 7.18-7.14 (m, 3H), 7.10 (t, *J* = 7.1 Hz, 1H), 7.03 (d, *J* = 7.3 Hz, 1H), 4.07 (q, *J* = 6.1 Hz, 2H), 2.36 (s, 6H), 2.27 (s, 3H), 0.91 (t, *J* = 0.9 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 164.5, 153.9, 148.4, 137.9, 137.9, 133.2, 130.6, 130.2, 129.9, 129.0, 128.5, 128.3, 127.8, 127.1, 126.4, 123.7, 122.9, 117.0, 60.6, 21.6, 21.4, 13.6; mass (ES+)  $m/z = 397.18$  (M+H)<sup>+</sup>; HRMS (ESI-TOF) calcd for C<sub>27</sub>H<sub>25</sub>O<sub>2</sub> 397.1804 Found 397.1807.

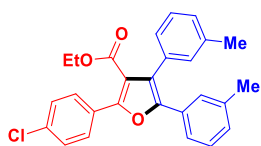
#### Ethyl 2-(4-fluorophenyl)-4,5-di-m-tolylfuran-3-carboxylate (3gg)



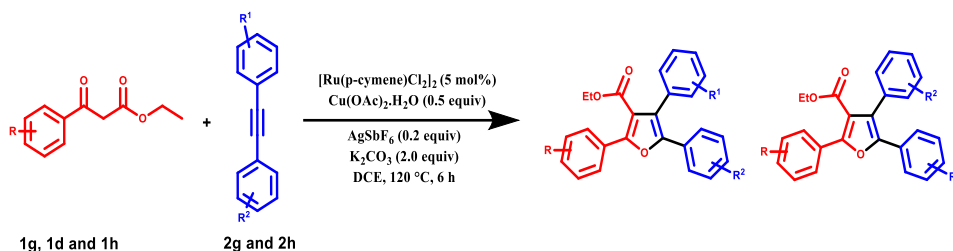
Eluent: Hexane/EA = 90:10, R<sub>f</sub> = 0.53; Yield 63% (260 mg); light yellow oil; (KBr) cm<sup>-1</sup>: 789, 840, 1031, 1114, 1234, 1330, 1500, 1604, 2925 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.96-7.92 (m, 2H), 7.31-7.25 (m, 2H), 7.19-7.08 (m, 7H), 7.03 (d, *J* = 7.1 Hz, 1H), 4.07 (q, *J* = 7.1 Hz, 2H), 2.36 (s, 3H), 2.27 (s, 3H), 0.91 (t, *J* = 0.9 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 164.3, 163.3 (d, C-F <sup>1</sup>J<sub>C-F</sub> = 249.4 Hz), 153.4, 148.3, 137.9, 137.8, 133.1, 130.5, 129.9, 129.8 (d, C-F <sup>3</sup>J<sub>C-F</sub> = 8.5 Hz), 128.5, 128.3, 128.2, 127.0, 126.3, 126.2 (d, C-

$F^4JC-F = 3.5$  Hz), 123.7, 122.9, 116.7, 115.3 (d, C-F  $^2JC-F = 21.8$  Hz), 60.5, 21.4, 21.3, 13.5; mass (ES+)  $m/z = 415.19$  (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $C_{27}H_{24}FO_3$  415.1704 Found 415.1710.

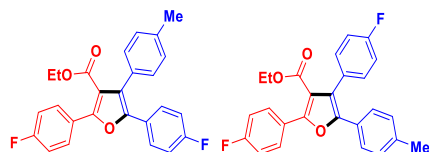
### Ethyl 2-(4-chlorophenyl)-4,5-di-m-tolylfuran-3-carboxylate (3hg)



Eluent: Hexane/EA = 90:10,  $R_f = 0.41$ ; Yield 59% (253 mg); light green oil; (KBr)  $cm^{-1}$ : 759, 835, 1025, 1217, 1329, 1485, 1603, 1712, 2926  $cm^{-1}$ ;  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.89 (d,  $J = 8.8$  Hz, 2H), 7.42 (d,  $J = 8.4$  Hz, 2H), 7.31-7.26 (m, 2H), 7.19-7.08 (m, 5H), 7.02 (d,  $J = 7.3$  Hz, 1H), 4.07 (q,  $J = 7.1$  Hz, 2H), 2.36 (s, 3H), 2.27 (s, 3H), 0.95 (t,  $J = 0.9$  Hz, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  164.3, 152.9, 148.7, 138.0, 137.9, 134.9, 133.0, 130.6, 129.9, 128.9, 128.7, 128.6, 128.5, 128.4, 128.3, 127.4, 126.4, 123.9, 123.0, 117.4, 60.7, 21.5, 21.4, 13.6; mass (ES+)  $m/z = 431.21$  (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $C_{27}H_{24}ClO_3$  431.1408 Found 431.1407.

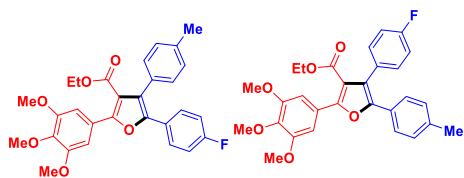


### Ethyl 2,5-bis(4-fluorophenyl)-4-(p-tolyl)furan-3-carboxylate (3gh)



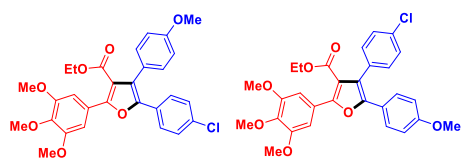
Eluent: Hexane/EA = 90:10,  $R_f = 0.54$ ; Yield 62% (65:35, 259 mg); light yellow oil; (KBr)  $cm^{-1}$ : 745, 835, 956, 1035, 1138, 1216, 1336, 1482, 1670, 1730, 2927, 3018,  $cm^{-1}$ ;  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.95-7.89 (m, 2H), 7.41-7.38 (m, 1H), 7.16-7.05 (m, 4H), 6.96-6.91 (t,  $J = 8.5$  Hz, 1H), 4.09-4.04 (q,  $J = 7.1$  Hz, 2H), 2.41 (s, 2H), 3.91 (s, 3H), 0.98 (t,  $J = 0.9$  Hz, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  164.1, 164.0, 163.2 (d, C-F  $^1JC-F = 250.0$  Hz), 163.1 (d, C-F,  $^1JC-F = 250.0$  Hz), 162.4 (d, C-F  $^1JC-F = 247.3$  Hz), 162.2 (d, C-F  $^1JC-F = 247.3$  Hz), 153.7, 153.4, 148.8, 147.5, 138.0, 137.4, 131.8 (d, C-F  $^3JC-F = 8.1$  Hz), 130.0 (d, C-F  $^3JC-F = 8.1$  Hz), 129.9 (d, C-F  $^3JC-F = 8.1$  Hz), 129.7 (d, C-F  $^4JC-F = 3.4$  Hz), 129.2, 129.1, 128.9, 127.6 (d, C-F  $^3JC-F = 7.7$  Hz), 127.0, 126.3 (d, C-F  $^4JC-F = 3.4$  Hz), 126.1 (d, C-F  $^4JC-F = 3.4$  Hz), 125.7, 123.3, 121.8, 116.8, 116.4, 115.9, 115.4 (d, C-F  $^2JC-F = 21.8$  Hz), 115.3 (d, C-F  $^2JC-F = 21.8$  Hz), 115.3 (d, C-F  $^2JC-F = 21.8$  Hz), 60.6, 60.5, 21.3, 21.2, 13.6, 13.5; mass (ES+)  $m/z = 419.14$  (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $C_{26}H_{21}F_2O_3$  419.1459 Found 419.1448.

### Ethyl 4-(4-fluorophenyl)-5-(p-tolyl)-2-(3,4,5-trimethoxyphenyl)furan-3-carboxylate (3kh)



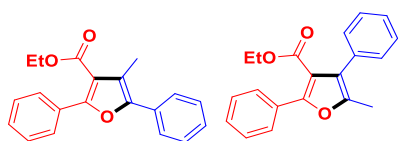
Eluent: Hexane/EA = 80:20,  $R_f = 0.37$ ; Yield 79% (60:40, 387 mg); light yellow oil; (KBr)  $cm^{-1}$ : 766, 838, 959, 1006, 1125, 1229, 1348, 1417, 1663, 1726, 2848, 2936,  $cm^{-1}$ ;  $^1H$  NMR (400 MHz,  $CDCl_3$ ): 7.45-7.41 (m, 1H), 7.36-7.32 (m, 1H), 7.32-7.30 (d,  $J = 8.3$  Hz), 7.28 (s, 0.3H), 7.27 (s, 1H), 7.24 (s, 1H), 7.24 (s, 2H), 7.14-7.09 (m, 2H), 6.99-6.95 (t,  $J = 8.5$  Hz, 1H), 4.08 (q,  $J = 7.1$  Hz, 2H), 3.96 (s, 6H), 3.94 (s, 3H), 2.44 (s, 2H), 2.34 (s, 1H), 0.97 (t,  $J = 0.9$  Hz, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  164.4, 164.3, 162.8 (d, C-F  $^1JC-F = 246.3$  Hz), 162.1 (d, C-F  $^1JC-F = 248.6$  Hz), 154.0, 153.7, 153.0, 153.0, 148.5, 147.1, 139.1, 137.9, 137.4, 131.7 (d, C-F  $^3JC-F = 8.4$  Hz), 129.9, 129.7, 129.4 (d, C-F  $^4JC-F = 3.6$  Hz), 129.2, 129.1, 127.6 (d,  $^3JC-F = 7.9$  Hz), 127.0, 126.4 (d, C-F  $^4JC-F = 3.3$  Hz), 125.8, 125.1, 123.4, 121.9, 116.9, 116.4, 115.4 (d, C-F  $^2JC-F = 21.8$  Hz), 105.4 (d, C-F  $^2JC-F = 21.3$  Hz), 105.3, 60.9, 60.6, 60.6, 56.2, 21.3, 21.2, 13.6, 13.6; mass (ES+)  $m/z = 491.18$  (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $C_{29}H_{28}F_2O_6$  491.1870 Found 491.1875.

### Ethyl 5-(4-chlorophenyl)-4-(4-methoxyphenyl)-2-(3,4,5-trimethoxyphenyl)furan-3-carboxylate (3ki)



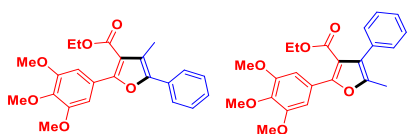
Eluent: Hexane/EA = 80:20,  $R_f$  = 0.47; Yield 73% (63:37, 381 mg); light yellow oil; (KBr)  $\text{cm}^{-1}$ : 747, 850, 962, 1062, 1129, 1214, 1333, 1465, 1664, 1728, 2925, 3020,  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.32-7.14 (m, 9H), 6.89-6.86 (d,  $J$  = 8.8 Hz, 1H), 6.75-6.73 (d,  $J$  = 8.8 Hz, 1H), 4.02-3.96 (q,  $J$  = 7.1 Hz, 2H), 3.86 (s, 6H), 3.84 (s, 3H), 3.79 (s, 2.2H), 3.71 (s, 1.1H), 0.92-0.88 (t,  $J$  = 7.0 Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.4, 159.4, 159.3, 154.0, 153.0, 153.0, 148.4, 147.0, 139.2, 133.4, 132.1, 131.5, 130.9, 129.3, 129.1, 128.6, 127.4, 126.9, 125.1, 125.0, 125.0, 123.8, 122.4, 117.1, 114.0, 105.4, 105.3, 60.9, 60.6, 56.2, 56.2, 55.2, 13.7, 13.6; mass (ES+)  $m/z$  = 523.15 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{29}\text{H}_{28}\text{ClO}_7$  523.1524 Found 523.1526.

### ethyl 4-methyl-2,5-diphenylfuran-3-carboxylate (3aj)



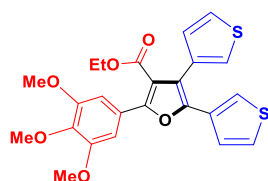
Eluent: Hexane/EA = 95:05,  $R_f$  = 0.63; Yield 47% (86:14, 143 mg); light yellow oil; (KBr)  $\text{cm}^{-1}$ : 759, 843, 949, 1088, 1175, 1227, 1332, 1446, 1598, 1721, 2960  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.82 (dd,  $J$  = 8.2 Hz,  $J$  = 1.6 Hz, 2H), 7.67 (d,  $J$  = 8.4 Hz, 2H), 7.46-7.36 (m, 5H), 7.35-7.31 (m, 1H), 4.32 (q,  $J$  = 7.1 Hz, 2H), 2.44 (s, 3H), 1.31 (t,  $J$  = 7.1 Hz, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.6, 156.0, 135.8, 130.7, 128.9, 128.5, 128.3, 128.0, 127.5, 126.6, 118.1, 116.3, 60.5, 14.1, 11.0; mass (ES+)  $m/z$  = 307.13 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{20}\text{H}_{19}\text{O}_3$  307.1334 Found 307.1334.

### ethyl 4-methyl-5-phenyl-2-(3,4,5-trimethoxyphenyl)furan-3-carboxylate (3kj)



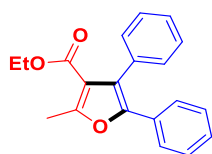
Eluent: Hexane/EA = 80:20,  $R_f$  = 0.56; Yield 54% (90:10, 213 mg); green oil; (KBr)  $\text{cm}^{-1}$ : 758, 845, 943, 1085, 1180, 1230, 1350, 1446, 1632, 1721, 2960  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.66 (d,  $J$  = 7.1 Hz, 2H), 7.46 (t,  $J$  = 7.5 Hz, 3H), 7.41-7.28 (m, 3H), 7.20 (s, 0.4H), 7.16 (s, 2H), 4.34 (q,  $J$  = 7.1 Hz, 2H), 3.92 (s, 6H), 3.91 (s, 3H), 1.35 (t,  $J$  = 7.1 Hz, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  165.4, 155.2, 153.8, 150.8, 149.7, 140.0, 130.4, 127.5, 127.1, 118.0, 114.6, 106.2, 60.9, 60.5, 56.2, 14.2, 11.1; mass (ES+)  $m/z$  = 397.16 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{20}\text{H}_{19}\text{O}_3$  397.1651 Found 397.1653.

### Ethyl 4,5-di(thiophen-3-yl)-2-(3,4,5-trimethoxyphenyl)furan-3-carboxylate (3kk)



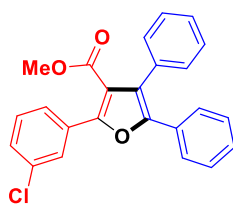
Eluent: Hexane/EA = 90:10,  $R_f$  = 0.51; Yield 56% (263 mg); light green oil; mp 182-185  $^{\circ}\text{C}$ ; (KBr)  $\text{cm}^{-1}$ : 734, 1054, 1125, 1262.3, 1416, 1462, 1501, 1732, 2853, 2923,  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.40-7.42 (dd,  $J$  = 3.0,  $J$  = 2.9 Hz, 1H), 7.30-7.31 (dd,  $J$  = 1.2 Hz,  $J$  = 1.3 Hz, 1H), 7.27-7.28 (dd,  $J$  = 1.2 Hz,  $J$  = 1.1 Hz, 1H), 7.23-7.24 (m, 3H), 7.10-7.11 (dd,  $J$  = 1.3 Hz,  $J$  = 1.1 Hz, 1H), 7.04-7.05 (dd,  $J$  = 1.2 Hz,  $J$  = 1.3 Hz, 1H), 4.07-4.12 (q,  $J$  = 7.1 Hz, 2H), 3.93 (s, 6H), 3.91 (s, 3H), 0.99-1.03 (t,  $J$  = 7.2 Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.2, 153.7, 153.0, 146.2, 139.1, 132.6, 131.0, 130.2, 129.4, 125.7, 125.3, 125.2, 125.1, 124.3, 121.3, 117.4, 116.4, 105.4, 60.9, 60.6, 56.2, 13.6; mass (ES+)  $m/z$  = 471.09 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{24}\text{H}_{23}\text{O}_6\text{S}_2$  471.0936 Found 471.0929.

### ethyl 2-methyl-4,5-diphenylfuran-3-carboxylate (3la)



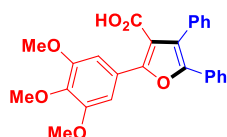
Eluent: Hexane/EA = 95:05,  $R_f$  = 0.62; Yield 58% (177 mg); light yellow solid; mp 130-135  $^{\circ}\text{C}$ ; (KBr)  $\text{cm}^{-1}$ : 759, 843, 949, 1088, 1175, 1227, 1332, 1446, 1598, 1721, 2960  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.27-7.19 (m, 7H), 7.08-7.04 (m, 2H), 3.98 (q,  $J$  = 7.1 Hz, 2H), 2.58 (s, 3H), 0.92 (t,  $J$  = 7.01 Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.0, 158.2, 147.4, 133.8, 130.3, 130.2, 128.3, 128.1, 127.3, 125.4, 122.3, 115.7, 59.8, 14.2, 13.8; mass (ES+)  $m/z$  = 307.13 (M+H) $^+$ ; HRMS (ESI-TOF) calcd for  $\text{C}_{20}\text{H}_{19}\text{O}_3$  307.1334 Found 307.1332.

### methyl 2-(3-chlorophenyl)-4,5-diphenylfuran-3-carboxylate (3ma)



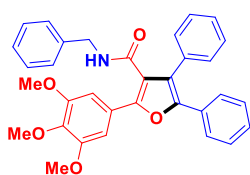
Yield 53% (205 mg); light yellow oil; (KBr)  $\text{cm}^{-1}$ : 696, 750, 832, 1015, 1119, 1259, 1334, 1487, 1602, 1720, 2851, 2922  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.85 (d,  $J = 8.7$  Hz, 2H), 7.44-7.38 (m, 7H), 7.36-7.34 (m, 2H), 7.25-7.23 (m, 3H), 3.58 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.5, 135.1, 132.8, 129.9, 129.0, 128.6, 128.4, 128.3, 127.9, 127.7, 125.9, 57.5.

### 4,5-diphenyl-2-(3,4,5-trimethoxyphenyl)furan-3-carboxylic acid (4)



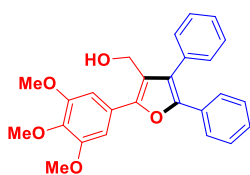
Potassium hydroxide (0.152 g, 2.71 mmol) was added to a stirred solution of the Ethyl 4,5-diphenyl-2-(3,4,5-trimethoxyphenyl)furan-3-carboxylate (**3ka**) (0.500 g, 1.08 mmol) in ethanol (10.0 mL) and water (5.0 mL) under  $\text{N}_2$ . The reaction was heated to reflux for 7 h and monitored via TLC. On completion, the reaction mixture was cooled to room temperature and then concentrated in vacuum. The remaining solid was dissolved in water, and the solution was acidified with 1N HCl until a precipitate formed. The solid was filtered and dried to afford 0.427 g (92%) of the desired product. 4,5-diphenyl-2-(3,4,5-trimethoxyphenyl)furan-3-carboxylic acid, yield 0.427 g (92%); Colourless oil; (KBr)  $\text{cm}^{-1}$ : 663, 748, 823, 998, 1024, 1216, 1354, 1650, 1721, 2129, 2257, 2995  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  7.47 – 7.27 (m, 10H), 7.24 (s, 1H), 3.84 (s, 6H), 3.74 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  165.8, 160.5, 153.3, 147.7, 138.8, 137.0, 133.0, 130.1, 130.0, 129.0, 128.5, 128.2, 126.0, 125.2, 123.8, 105.2, 60.6, 56.4; mass (ES+)  $m/z = 431.14$  (M+H) $^+$ ; ESMS (ESI-TOF) calcd for  $\text{C}_{28}\text{H}_{27}\text{O}_6$  431.1 Found 431.4.

### N-benzyl-4,5-diphenyl-2-(3,4,5-trimethoxyphenyl)furan-3-carboxamide (5)



To a stirred solution of benzylamine (0.074 g, 0.691 mmol, 1.0 equiv.) in DCM (5 mL) was added 4,5-diphenyl-2-(3,4,5-trimethoxyphenyl)furan-3-carboxylic acid (**4**) (0.200 g, 0.581 mmol, 1.0 equiv.), EDC (0.111 g, 0.581 mmol, 1.0 eq), HOBt (0.078 g, 0.577 mmol, 1 equiv.) and 4-DMAP (0.035 g, 0.286 mmol, 0.4 equiv.) at rt for 8 h. The reaction was monitored via TLC (eluent phase = Hexane/EA = 70:30,  $R_f = 0.41$ ). After completion of the reaction, its solvent was evaporated by rotary and concentrated under reduced pressure. Then, the reaction mixture was diluted with EtOAc, quenched with saturated  $\text{NaHCO}_3$  solution, extracted with EtOAc (2x100 mL). The combined organic extracts were dried over anhydrous  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated under reduced pressure. The crude compound was purified by column chromatography over silica gel (20% EA/hexanes) to afford the desired product, Yield 0.274 g (91%); light green oil; (KBr)  $\text{cm}^{-1}$ : 696.6, 742.8, 872.1, 999.3, 1027.6, 1124.0, 1214.7, 1383.6, 1449.4, 1558.0, 1645.3, 2929.2  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.44 (dd,  $J = 1.8$  Hz,  $J = 8.2$  Hz, 2H), 7.39 (s, 5H), 7.34-7.24 (m, 5H), 7.19-7.16 (m, 3H), 6.90-6.88 (m, 2H), 5.6 (t,  $J = 5.2$  Hz, N-H), 4.36 (d,  $J = 5.6$  Hz, 2H), 3.9 (s, 3H), 3.8 (s, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.3, 153.3, 147.7, 138.7, 137.4, 132.3, 130.0, 129.8, 129.1, 128.5, 128.4, 128.2, 127.8, 127.5, 127.3, 125.9, 125.2, 122.5, 120.2, 104.1, 60.9, 56.2, 43.8; mass (ES+)  $m/z = 520.2$  (M+H) $^+$ ; ESMS (ESI-TOF) calcd for  $\text{C}_{28}\text{H}_{27}\text{O}_6$  520.2 Found 521.5.

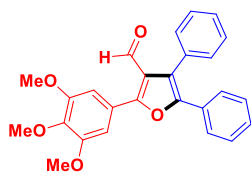
### (4,5-diphenyl-2-(3,4,5-trimethoxyphenyl)furan-3-yl)methanol (6)



To a solution of Ethyl 4,5-diphenyl-2-(3,4,5-trimethoxyphenyl)furan-3-carboxylate (**3ka**) (0.250 g, .543 mmol) in  $\text{Et}_2\text{O}$  (8 mL),  $\text{LiAlH}_4$  (0.042 g, 1.08 mmol) was added in portions wise at 0 °C. After that reaction mixture was stirred at rt for 1h, followed by quenching with  $\text{H}_2\text{O}$  (0.3 mL), NaOH 1 M (0.2 mL) and  $\text{H}_2\text{O}$  (6 mL) at 0 °C. The resulting white precipitate was filtered off and the solvent was removed under reduced pressure affording compound **6** (0.212 g, 94%) as a colourless oil.  $R_f = 0.2$  (eluent phase = Hexane/EA = 60:40,  $R_f = 0.28$ ) Yield 0.212 g (94%); (KBr)  $\text{cm}^{-1}$ : 646.6, 755.5, 895.6, 1067.6, 1168.0, 1210.7, 1370.2, 1410.1, 1532.4, 1655.3, 1785.2, 2905.8, 3352  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  7.51-7.41 (m, 7H), 7.31 (t,  $J = 7.1$  Hz, 2H), 7.27 (s, 2H), 7.26-7.22 (m, 1H), 5.1 (t,  $J = 4.1$  Hz, 1H), 4.26 (d,  $J = 3.9$  Hz),

3.88 (s, 6H), 3.74 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  153.7, 150.8, 146.8, 138.1, 133.0, 130.7, 130.4, 129.3, 129.0, 128.2, 127.9, 126.0, 125.7, 122.9, 104.0, 60.6, 56.4, 53.6.

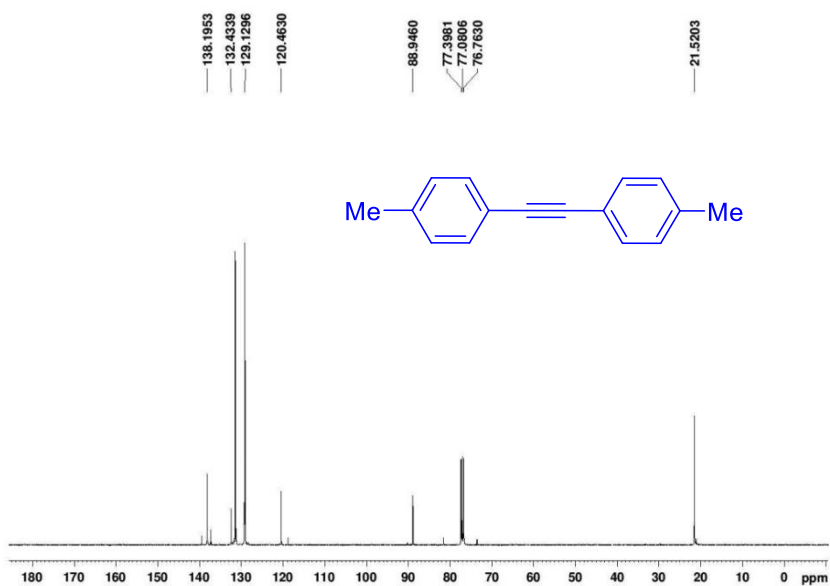
#### 4,5-diphenyl-2-(3,4,5-trimethoxyphenyl)furan-3-carbaldehyde (7)



In a round bottom flask equipped with a condenser the 4,5-diphenyl-2-(3,4,5-trimethoxyphenyl)furan-3-yl)methanol was dissolved in the toluene (8 ml) and  $\text{MnO}_2$  was added. The mixture vigorously stirred under reflux for 12 h until most of the starting material was consumed monitored *via* TLC (eluent phase = Hexane/EA = 80:20,  $R_f$  = 0.41). After cooling to room temperature, the suspension is filtered over celite with a glass frit. The crude compound was purified by column chromatography over silica gel (10% EA/hexanes) to afford the desired product Yield 92% (0.228 g); yellow oil; (KBr)  $\text{cm}^{-1}$ : 642.3, 720.8, 852.7, 965.2, 1024.2, 1253.8, 1358.7, 1485.2, 1507.5, 1640.5, 1725.6, 2980.7,  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  9.83 (s, 1H), 7.49 (s, 2H), 7.48-7.40 (m, 7H), 7.29-7.26 (m, 3H), 3.99 (s, 6H), 3.94 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.4, 157.6, 153.3, 148.2, 140.1, 131.4, 130.3, 129.6, 128.9, 128.5, 128.3, 128.1, 125.5, 124.2, 124.0, 122.2, 105.5, 61.0, 56.4 mass (ES+)  $m/z$  = 415.1 (M+H) $^+$ ; ESMS (ESI-TOF) calcd for  $\text{C}_{28}\text{H}_{27}\text{O}_6$  415.1 Found 415.4.

## 7. Copies of NMR Spectra

<sup>1</sup>H NMR spectrum of compound- 2b (400 MHz, CDCl<sub>3</sub>)

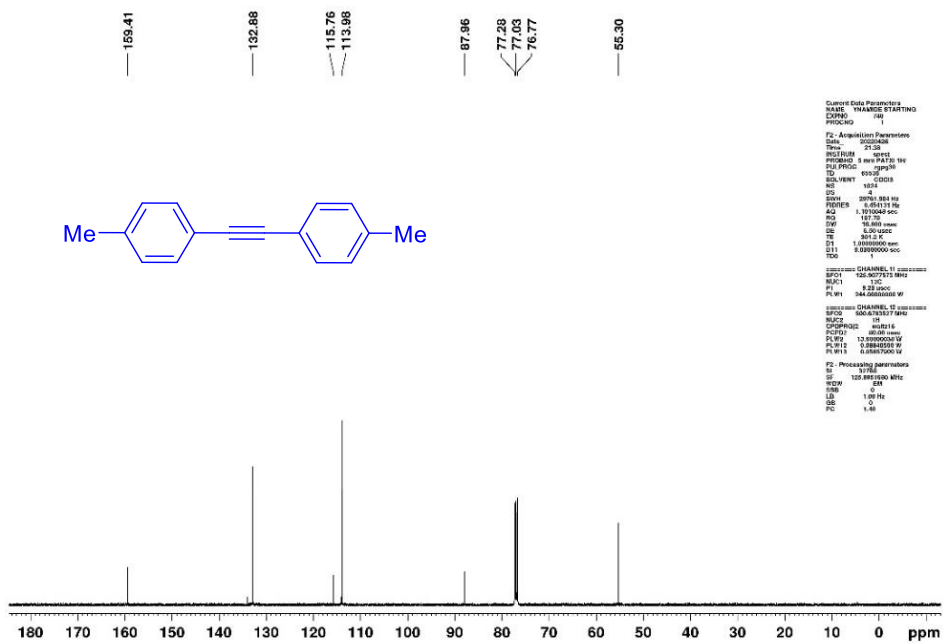


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<sup>13</sup>C NMR spectrum of compound- 2b (100 MHz, CDCl<sub>3</sub>)

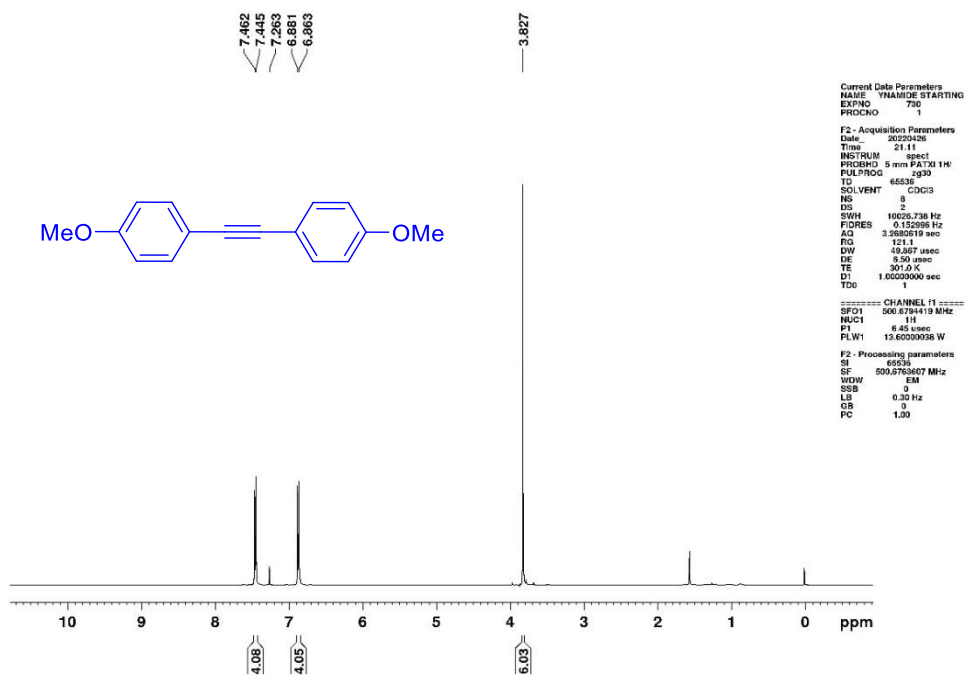


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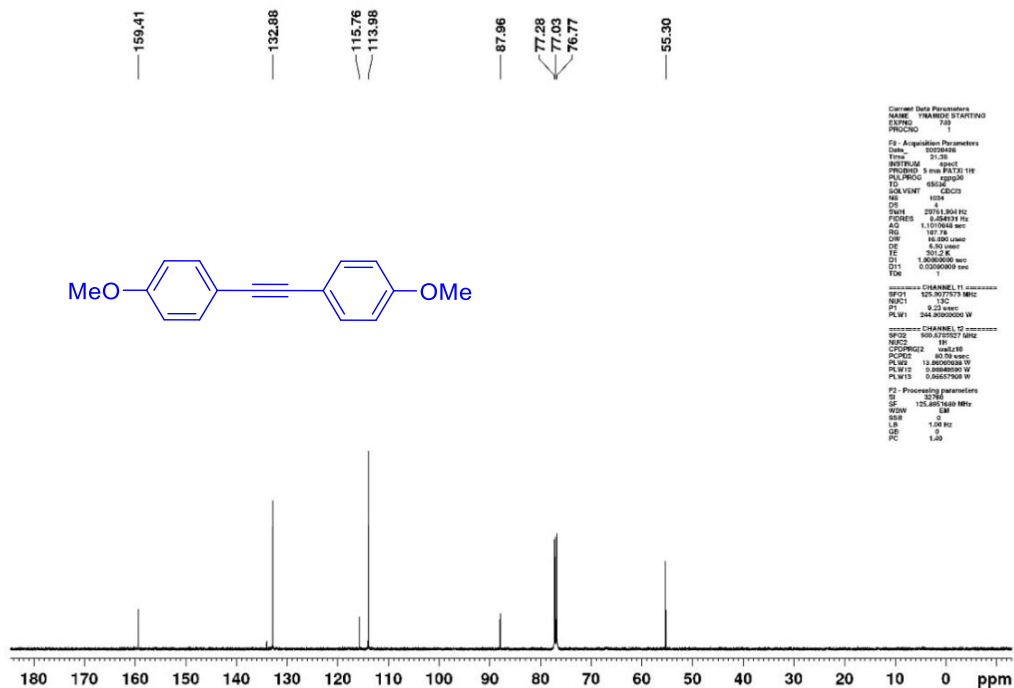
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Current Data Parameters
NAME: 2b
PROCNO: 1
F2 - Acquisition Parameters
Date_: 202308
Time: 10.50
INSTRUM: spect
PROBHD: 5 mm QNP 1H
PULPROG: zgpg30
AQ: 6.0000000
SOLVENT: CDCl3
NS: 1631
DS: 4
SWH: 12000.000 Hz
FIDRES: 0.001111 Hz
AQRES: 0.001111 Hz
RG: 1024
AQ: 1.0000000 sec
DE: 6.20 uV
TE: 300.2 K
=====
===== CHANNEL f1 =====
NUC1: 13C
P1: 0.12000000 sec
PLW1: 0.08000000 W
===== CHANNEL f2 =====
NUC2: 1H
P2: 0.00000000 sec
PLW2: 0.00000000 W
=====
P2 - Processing parameters
SI: 32768
SF: 125.7611800 MHz
RG: 655
LB: 0
LB2: 1.00 Hz
GB: 0
PC: 1.50

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<sup>1</sup>H NMR spectrum of compound- 2c (400 MHz, CDCl<sub>3</sub>)

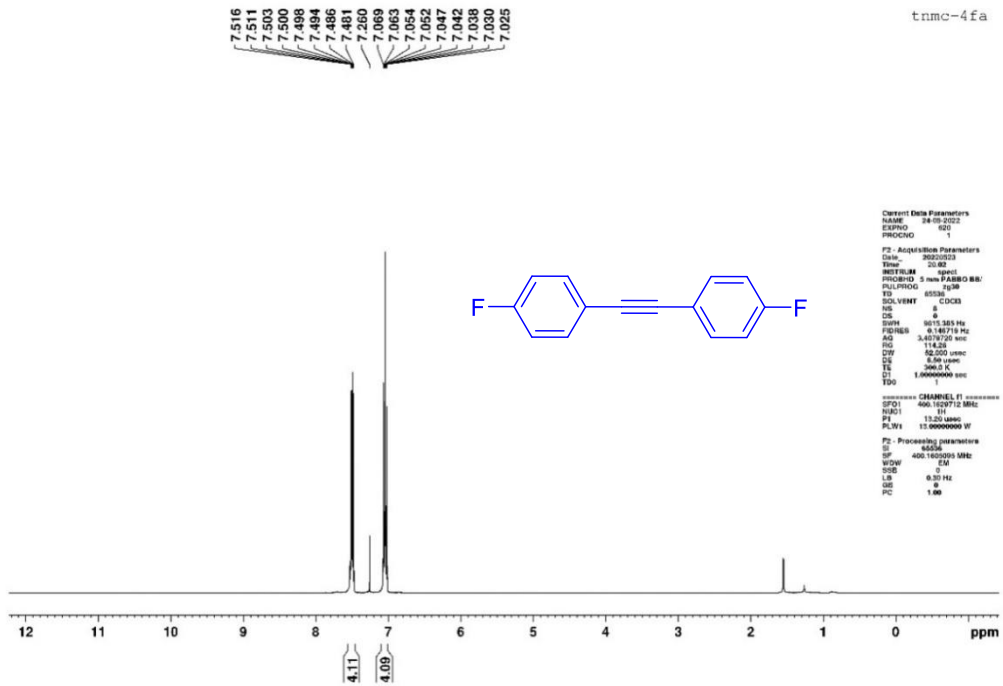


<sup>13</sup>C NMR spectrum of compound- 2c (100 MHz, CDCl<sub>3</sub>)

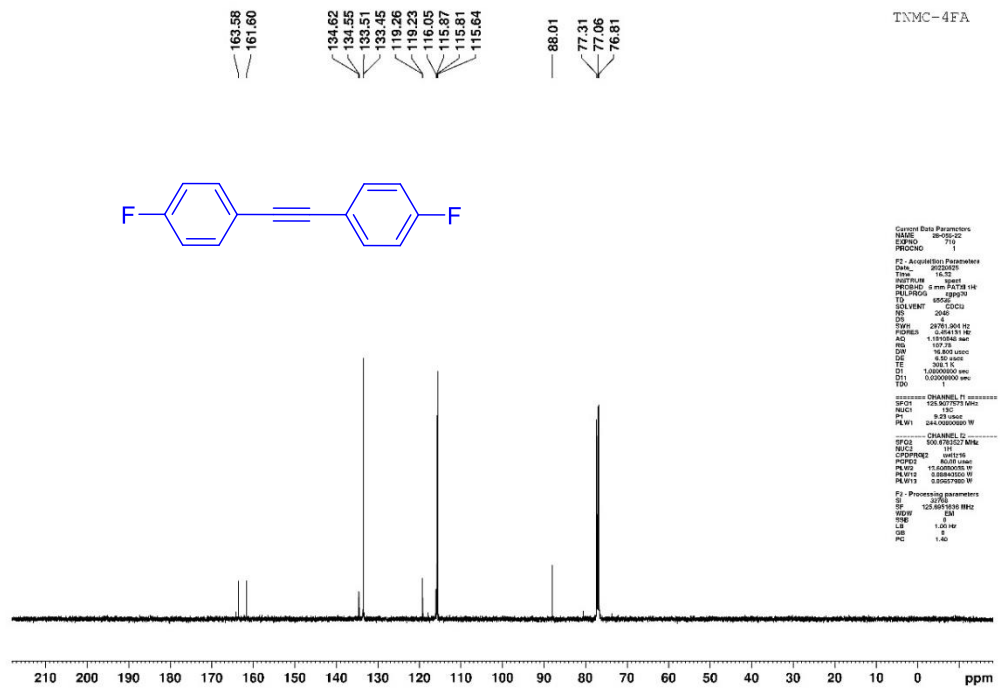




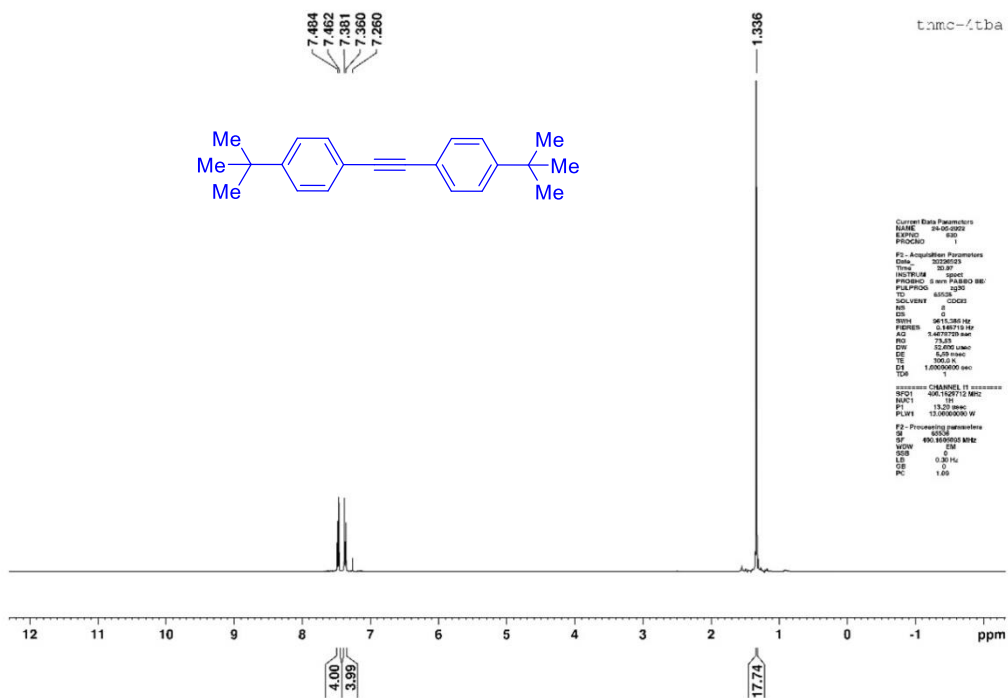
<sup>1</sup>H NMR spectrum of compound- 2d (400 MHz, CDCl<sub>3</sub>)



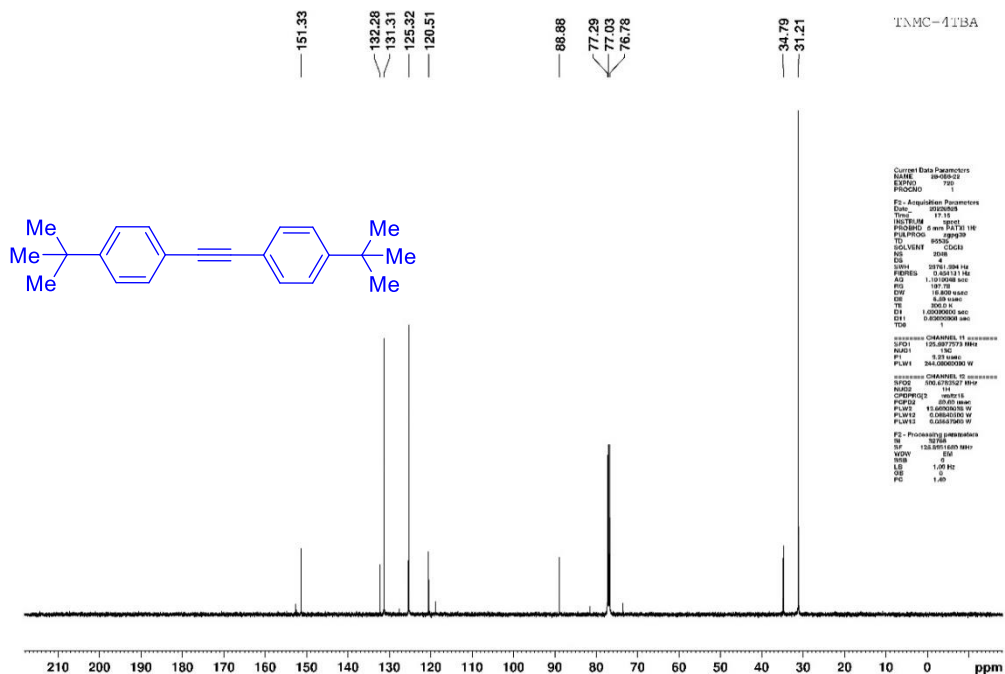
<sup>13</sup>C NMR spectrum of compound- 2d (100 MHz, CDCl<sub>3</sub>)



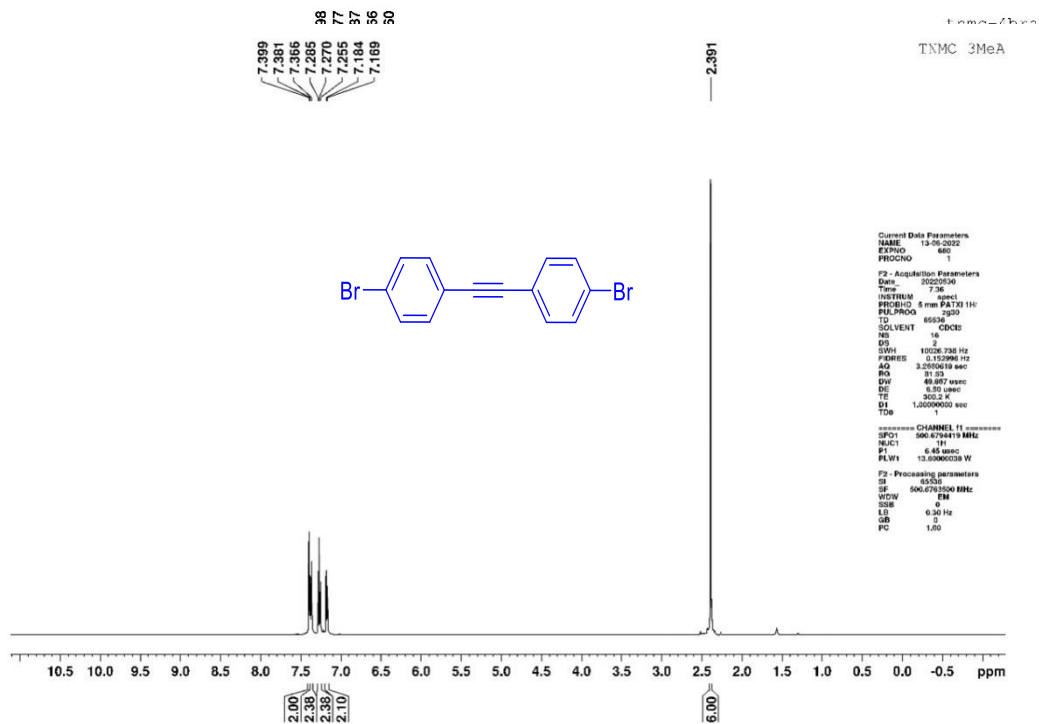
<sup>1</sup>H NMR spectrum of compound- 2e (400 MHz, CDCl<sub>3</sub>)



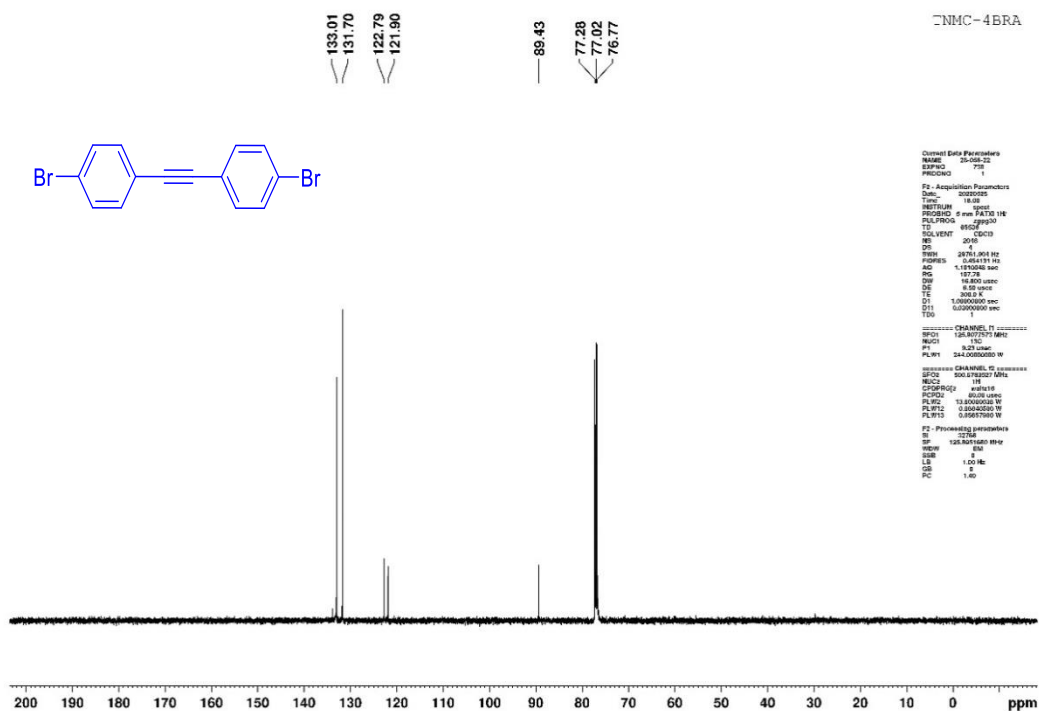
<sup>13</sup>C NMR spectrum of compound- 2e (100 MHz, CDCl<sub>3</sub>)



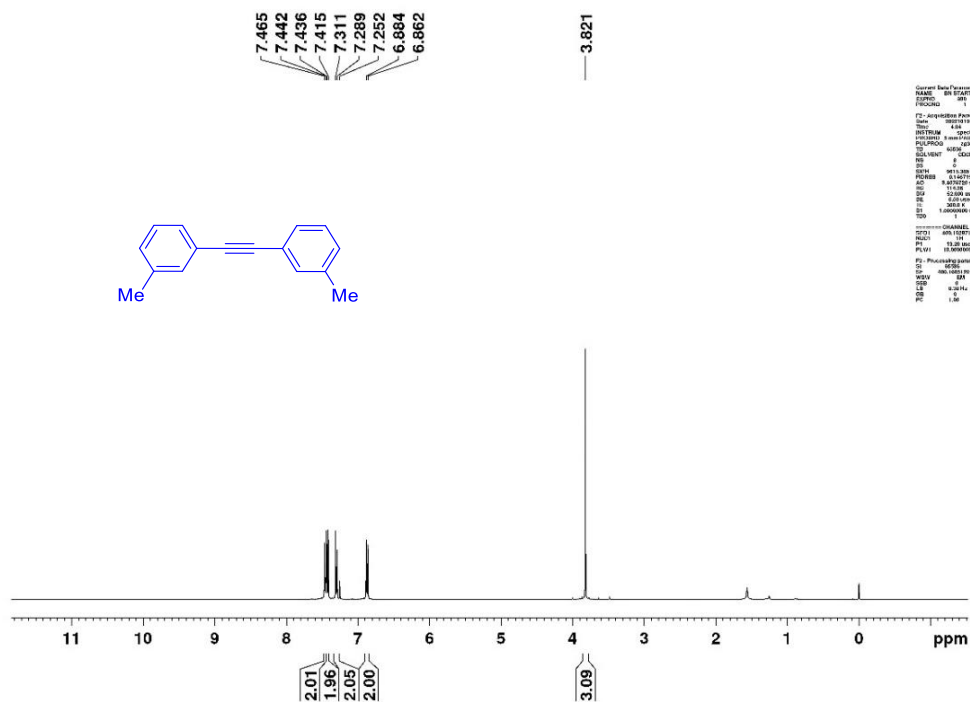
**<sup>1</sup>H NMR spectrum of compound- 2f (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of compound- 2f (100 MHz, CDCl<sub>3</sub>)**



<sup>1</sup>H NMR spectrum of compound- 2i (400 MHz, CDCl<sub>3</sub>)

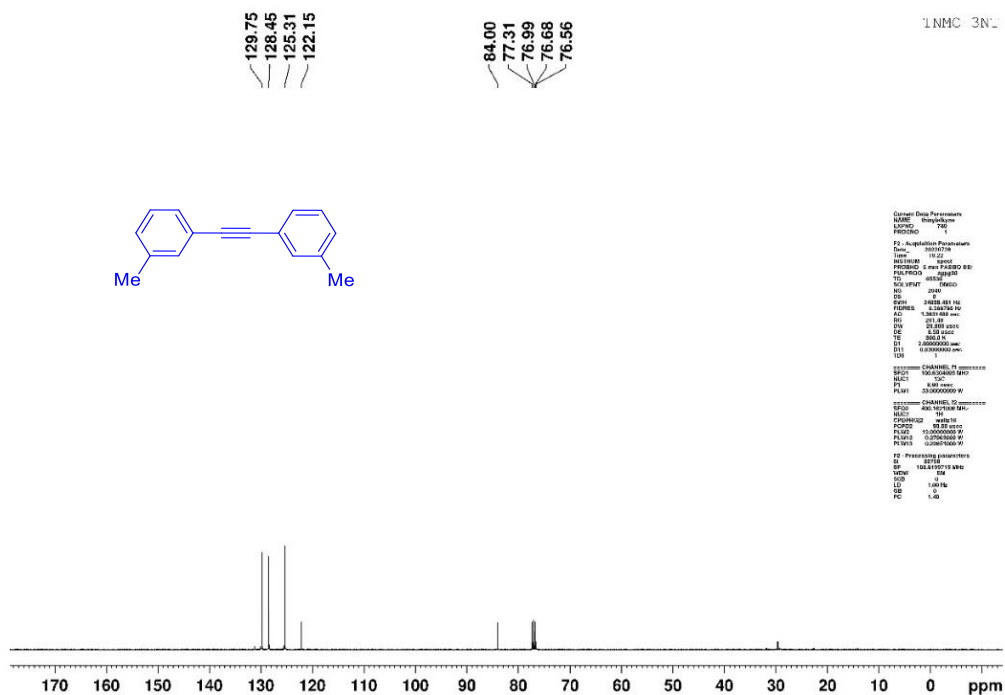


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General Parameters
NAME: 4i-20210629
EXPNO: 1
PROCNO: 1
F2-Processing Parameters
Date_ 20210629
Time 14.51
INSTRUM: spect
PROBHD: zgpg30
PULPROG: zgpg30
SOLVENT: ccdcl3
NS: 2048
DS: 4
SWH: 400.138 MHz
FIDRES: 0.132779 Hz
AQ: 0.453250 sec
RG: 655.36
DE: 3.250000 mm
TE: 300.2 K
D1: 0.050000 sec
DELTA: 1.000000 sec
TD: 65536
===== CHANNEL f1 =====
NUC1: 13C
P1: 12.000000 sec
PL1: 0.000000 dB
===== CHANNEL f2 =====
NUC2: 1H
P2: 4.000000 sec
PL2: 0.000000 dB
===== CHANNEL f3 =====
NUC3: 1H
P3: 1.500000 sec
PL3: 0.000000 dB
===== CHANNEL f4 =====
NUC4: 1H
P4: 1.500000 sec
PL4: 0.000000 dB
===== CHANNEL f5 =====
NUC5: 1H
P5: 1.500000 sec
PL5: 0.000000 dB

```

<sup>13</sup>C NMR spectrum of compound- 2g (100 MHz, CDCl<sub>3</sub>)

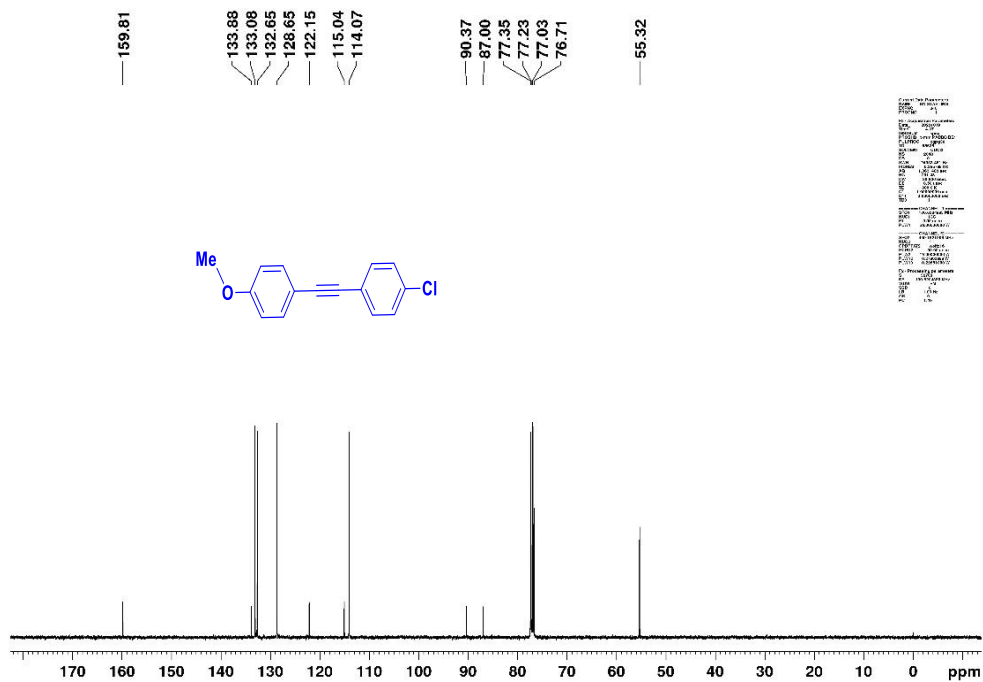


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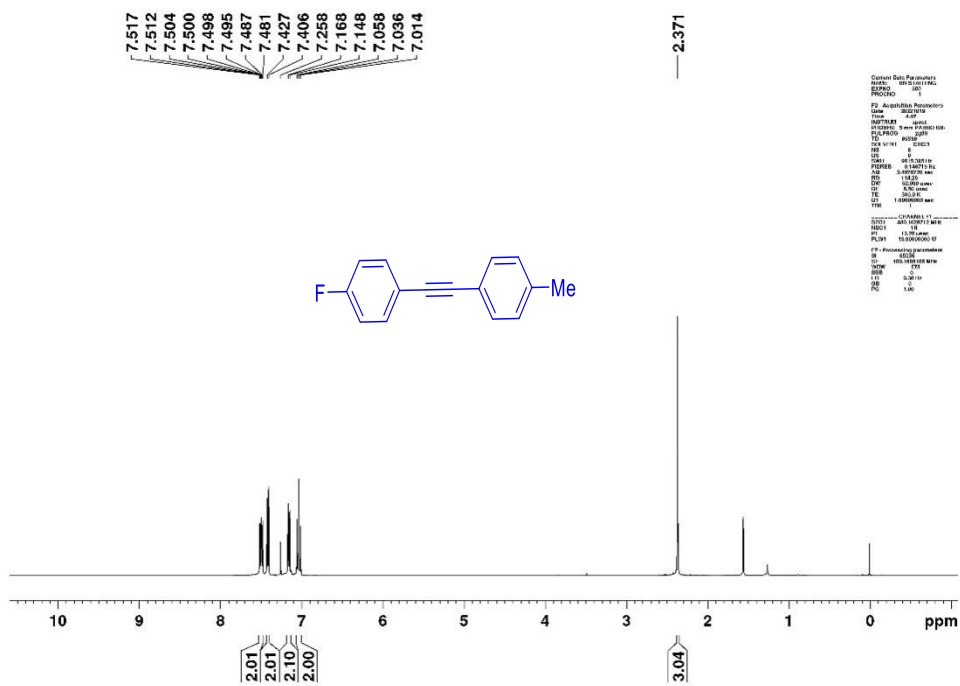
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PROCNO: 1
F2-Processing Parameters
Date_ 20210629
Time 14.51
INSTRUM: spect
PROBHD: zgpg30
PULPROG: zgpg30
SOLVENT: ccdcl3
NS: 2048
DS: 4
SWH: 100.626 MHz
FIDRES: 0.132779 Hz
AQ: 0.453250 sec
RG: 655.36
DE: 3.250000 mm
TE: 300.2 K
D1: 0.050000 sec
DELTA: 1.000000 sec
TD: 65536
===== CHANNEL f1 =====
NUC1: 13C
P1: 12.000000 sec
PL1: 0.000000 dB
===== CHANNEL f2 =====
NUC2: 1H
P2: 4.000000 sec
PL2: 0.000000 dB
===== CHANNEL f3 =====
NUC3: 1H
P3: 1.500000 sec
PL3: 0.000000 dB
===== CHANNEL f4 =====
NUC4: 1H
P4: 1.500000 sec
PL4: 0.000000 dB
===== CHANNEL f5 =====
NUC5: 1H
P5: 1.500000 sec
PL5: 0.000000 dB

```

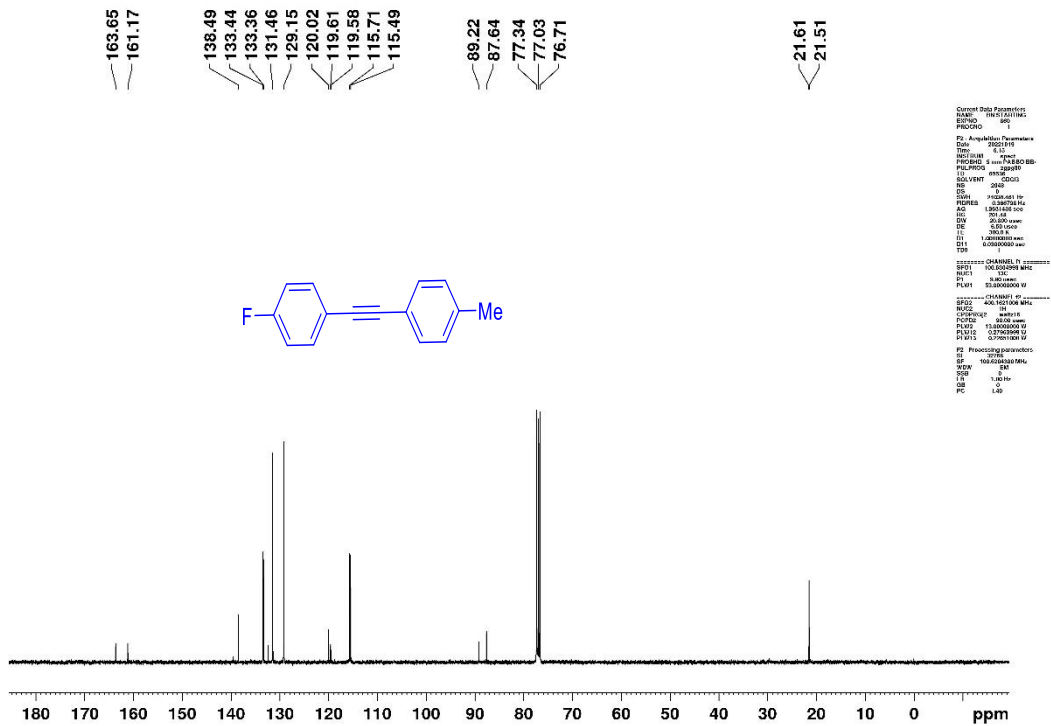
<sup>13</sup>C NMR spectrum of compound- 2i (100 MHz, CDCl<sub>3</sub>)



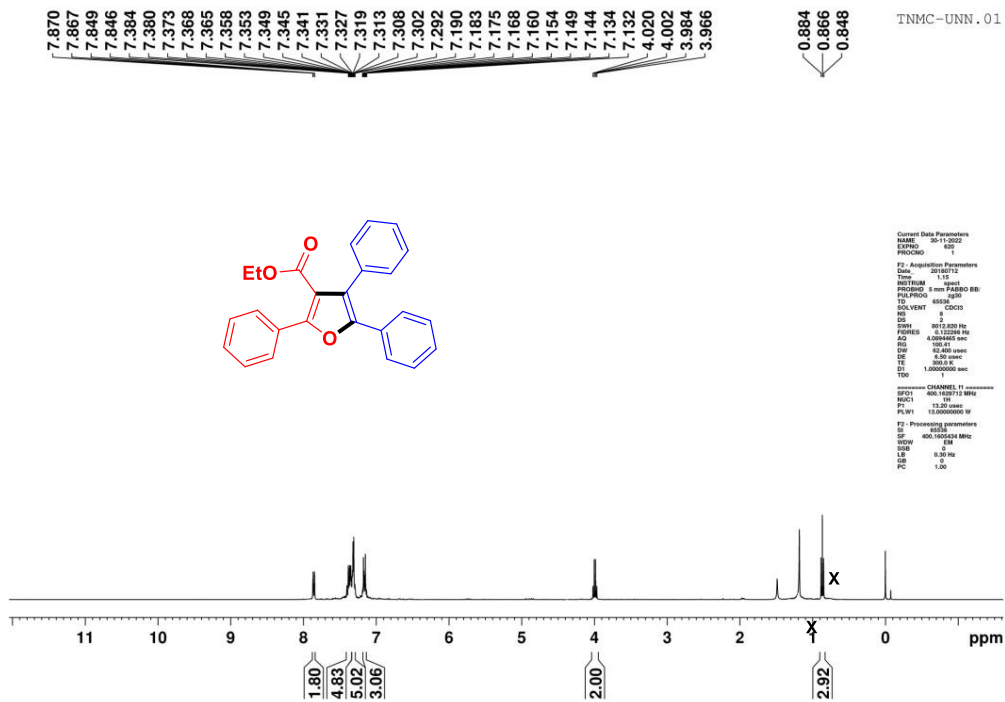
<sup>1</sup>H NMR spectrum of compound- 2j (400 MHz, CDCl<sub>3</sub>)



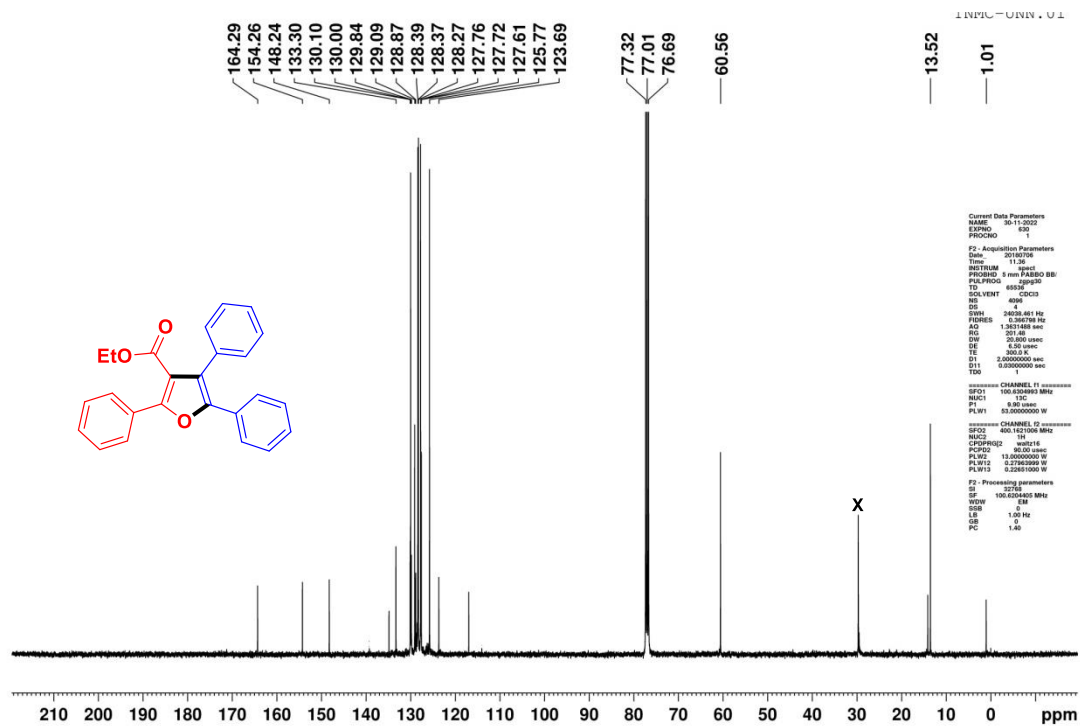
<sup>13</sup>C NMR Spectrum of compound- 2j (100 MHz, CDCl<sub>3</sub>)



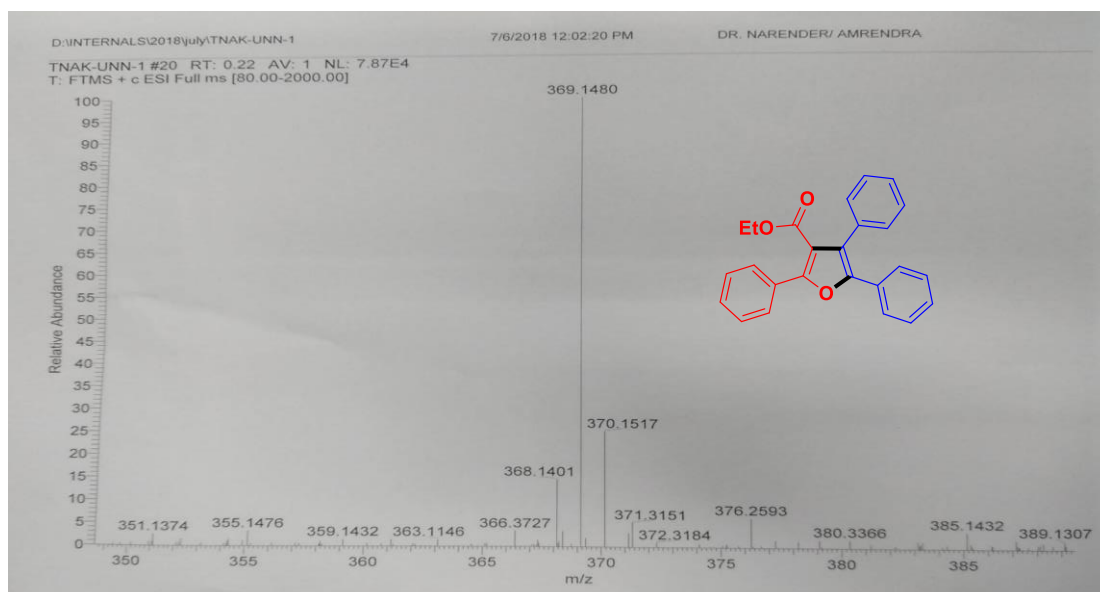
<sup>1</sup>H NMR Spectrum of compound- 3aa (400 MHz, CDCl<sub>3</sub>); X= wax impurity



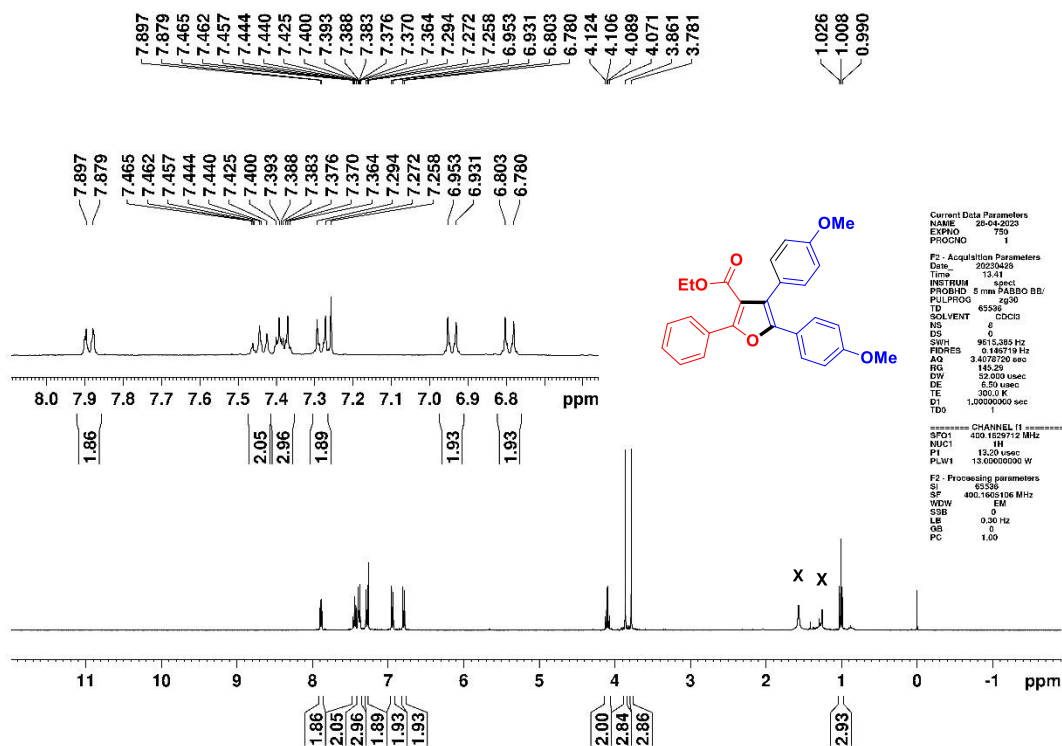
<sup>13</sup>C NMR Spectrum of compound- 3aa (100 MHz, CDCl<sub>3</sub>); X= wax impurity



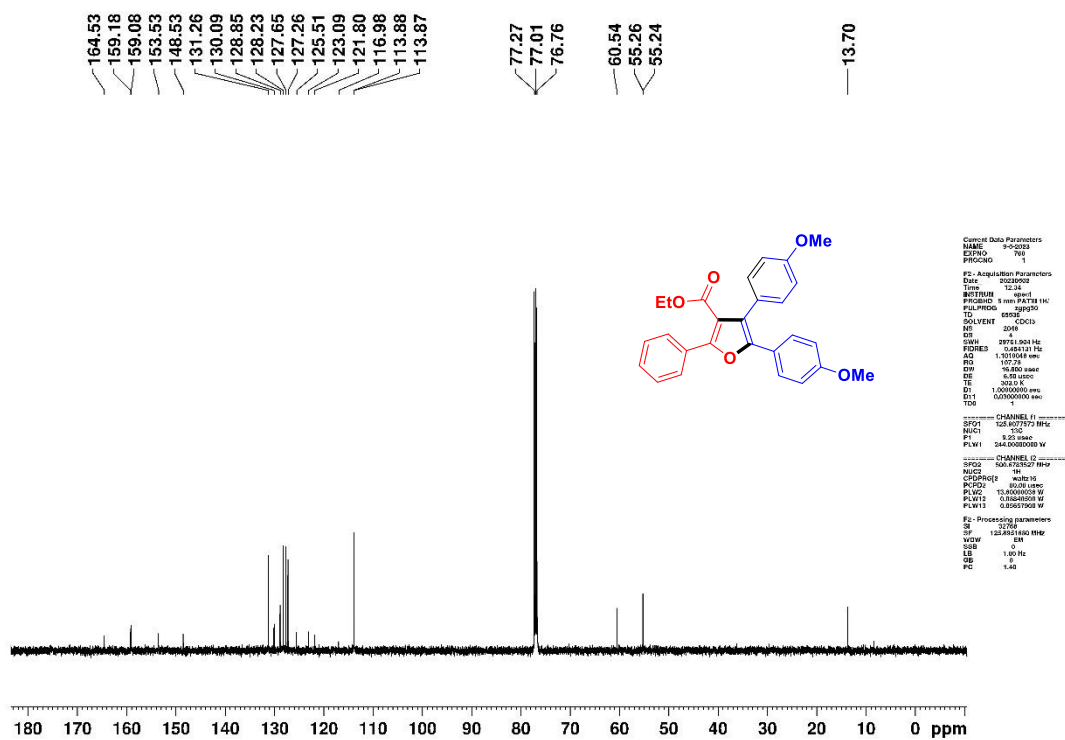
HRMS spectrum of compound-3aa



<sup>1</sup>H NMR Spectrum of compound- 3ac (400 MHz, CDCl<sub>3</sub>); X= wax impurity

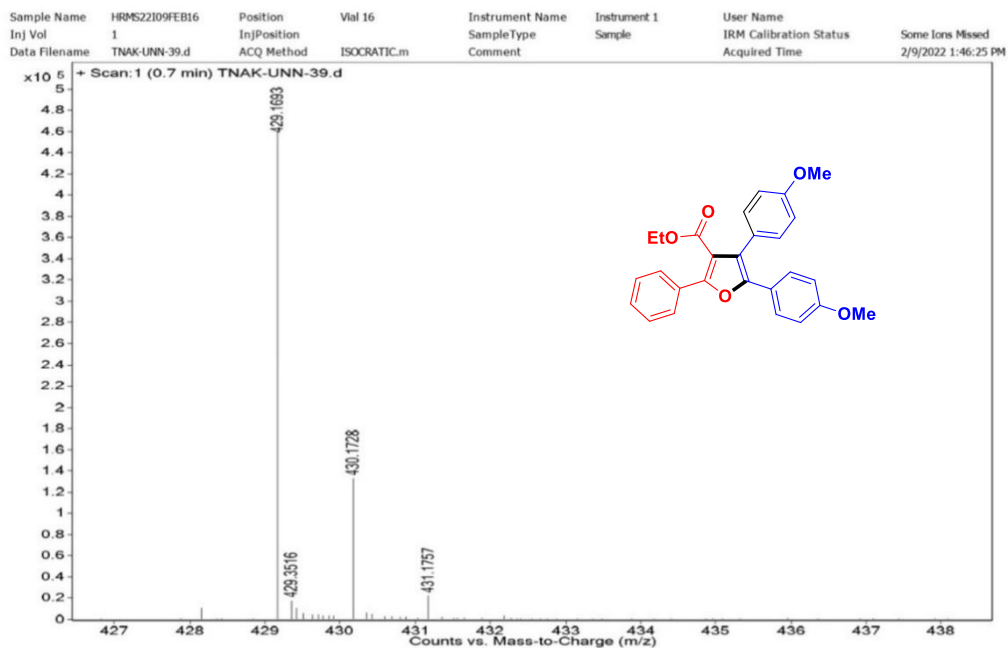


<sup>13</sup>C NMR Spectrum of compound- 3ac (100 MHz, CDCl<sub>3</sub>);

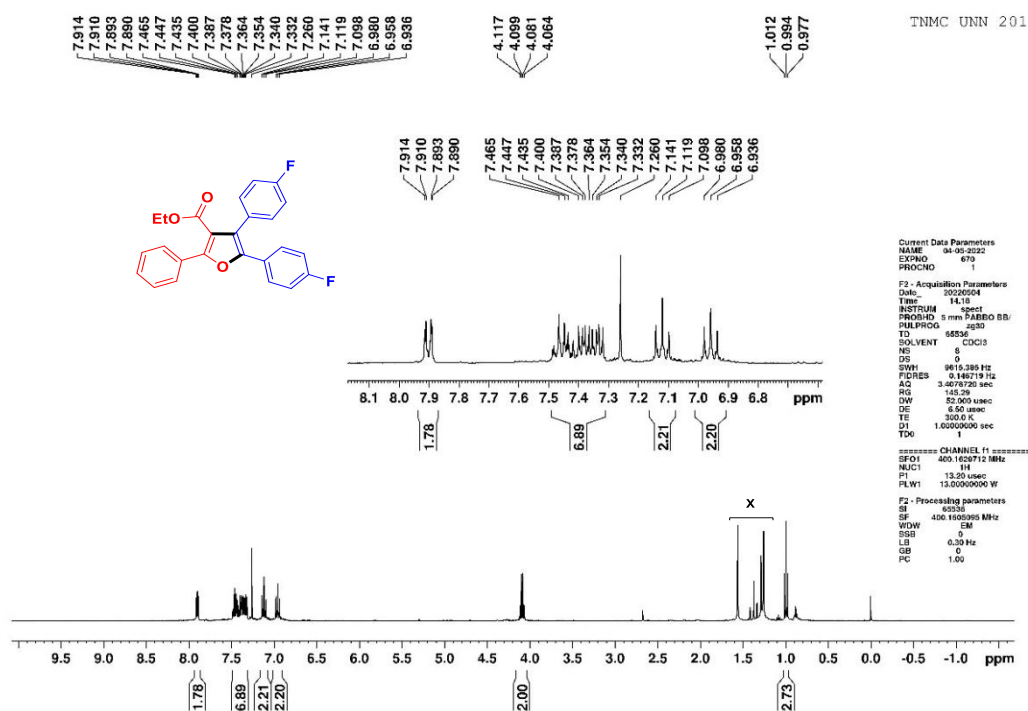




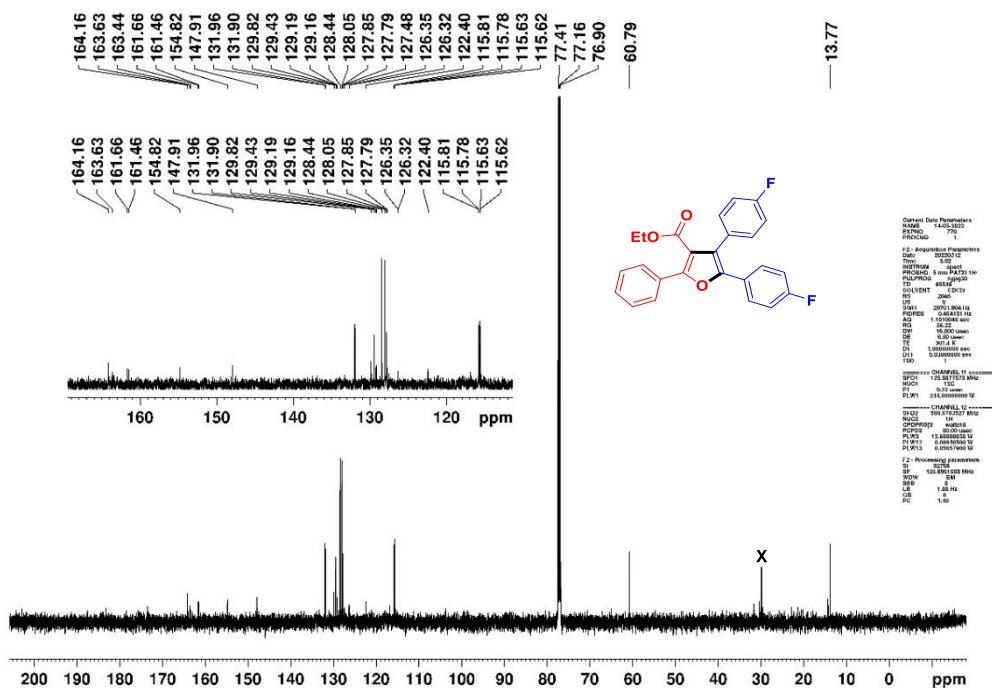
## HRMS spectrum of compound-3ac



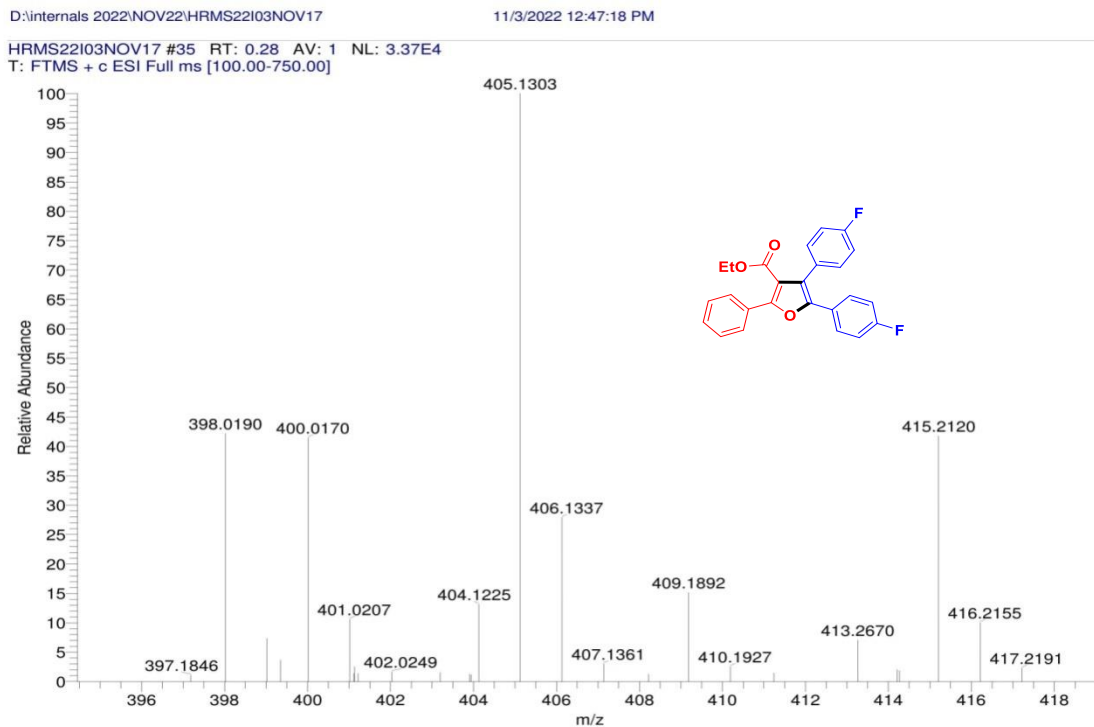
## <sup>1</sup>H NMR spectrum of compound- 3ad (400 MHz, CDCl<sub>3</sub>); X= wax impurity



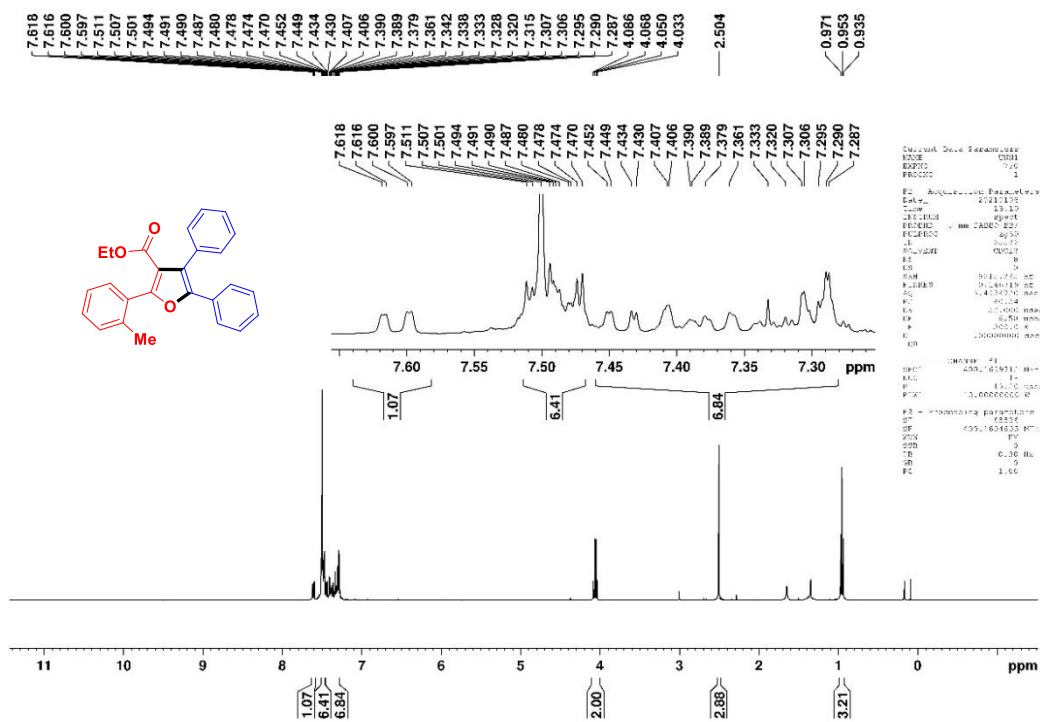
<sup>13</sup>C NMR spectrum of compound- 3ad (100 MHz, CDCl<sub>3</sub>); X= wax impurity



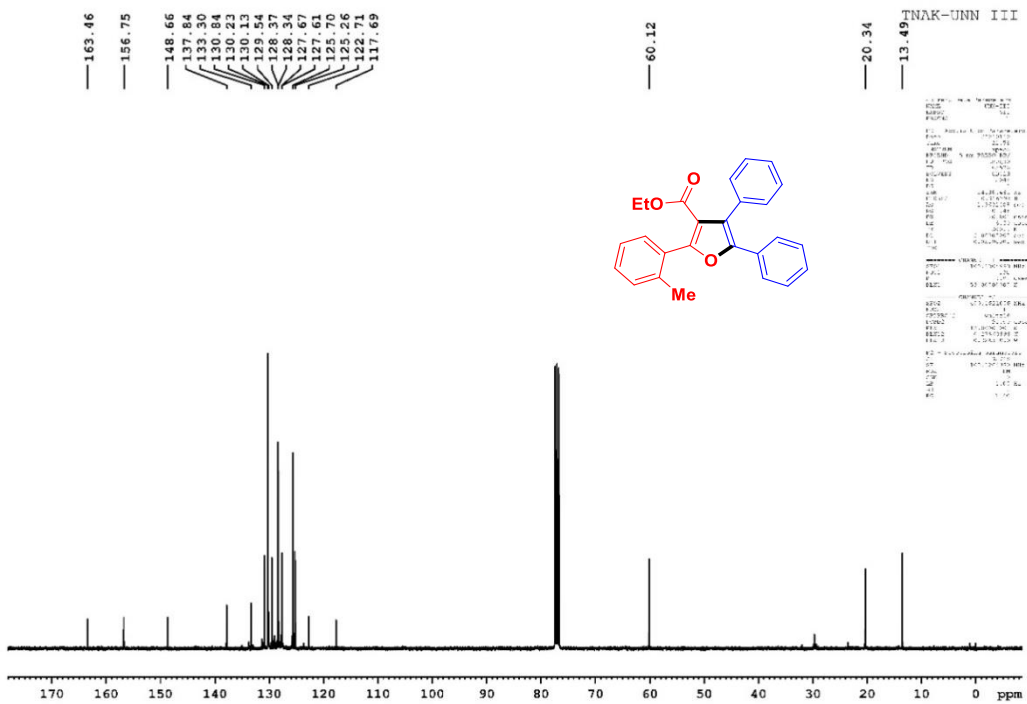
HRMS spectrum of compound-3ad



<sup>1</sup>H NMR spectrum of compound- 3ba (400 MHz, CDCl<sub>3</sub>)



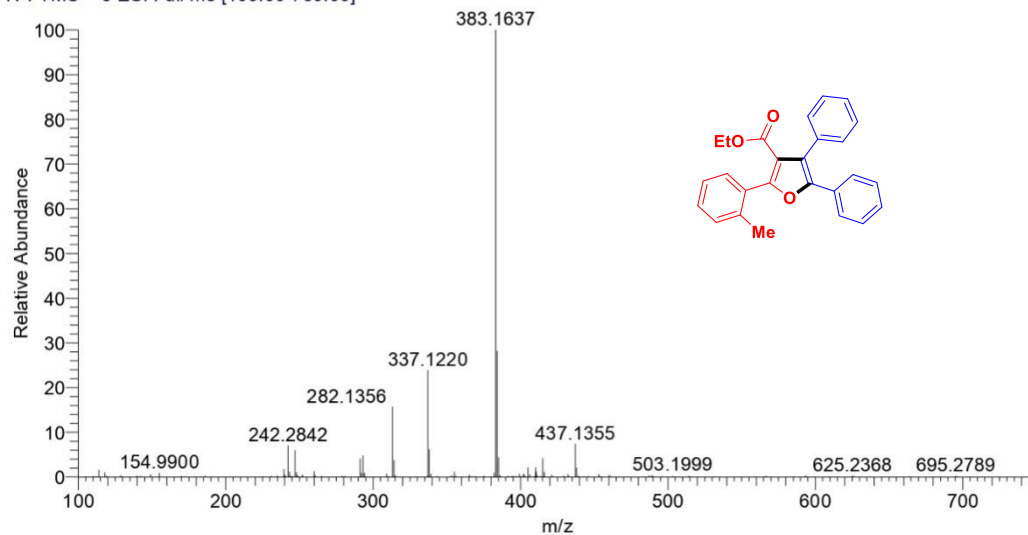
<sup>13</sup>C NMR spectrum of compound- 3ba (100 MHz, CDCl<sub>3</sub>)



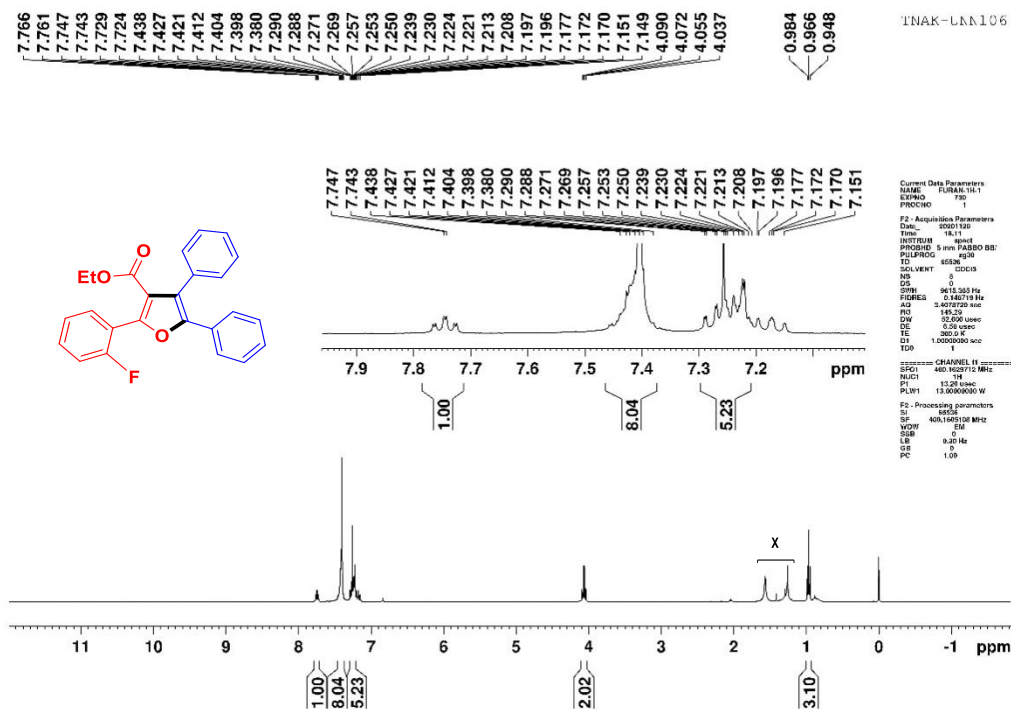
## HRMS spectrum of compound-3ba

Data File: HRMS21I23FEB32	Original Data Path: D:\INTERNAL NEW\2021\Feb	
		2021
Sample ID: TNAK-UNN11	Sample Name:	
Acquisition Date: 02/23/21 11:33:35 AM	Run Time(min):	0.00
Vial: CStk1-01:32	Injection Volume(μl):	1.00

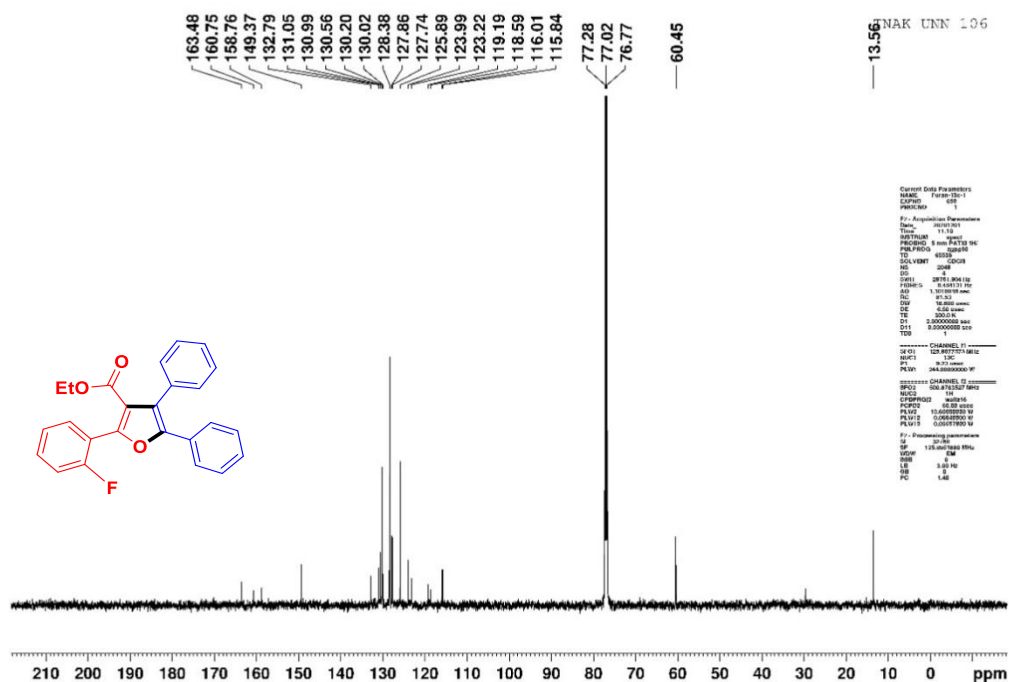
HRMS21I23FEB32 #30-64 RT: 0.25-0.50 AV: 35 SB: 1 0.01 NL: 2.68E7  
T: FTMS + c ESI Full ms [100.00-750.00]



## <sup>1</sup>H NMR spectrum of compound- 3ca (400 MHz, CDCl<sub>3</sub>); X= wax impurity



<sup>13</sup>C NMR spectrum of compound- 3ca (100 MHz, CDCl<sub>3</sub>)

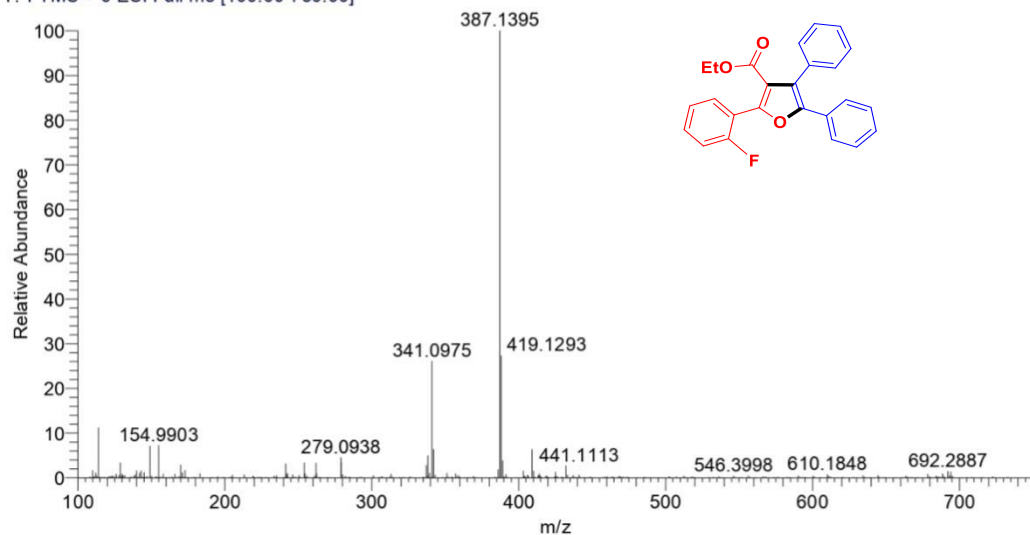


HRMS spectrum of compound-3ca

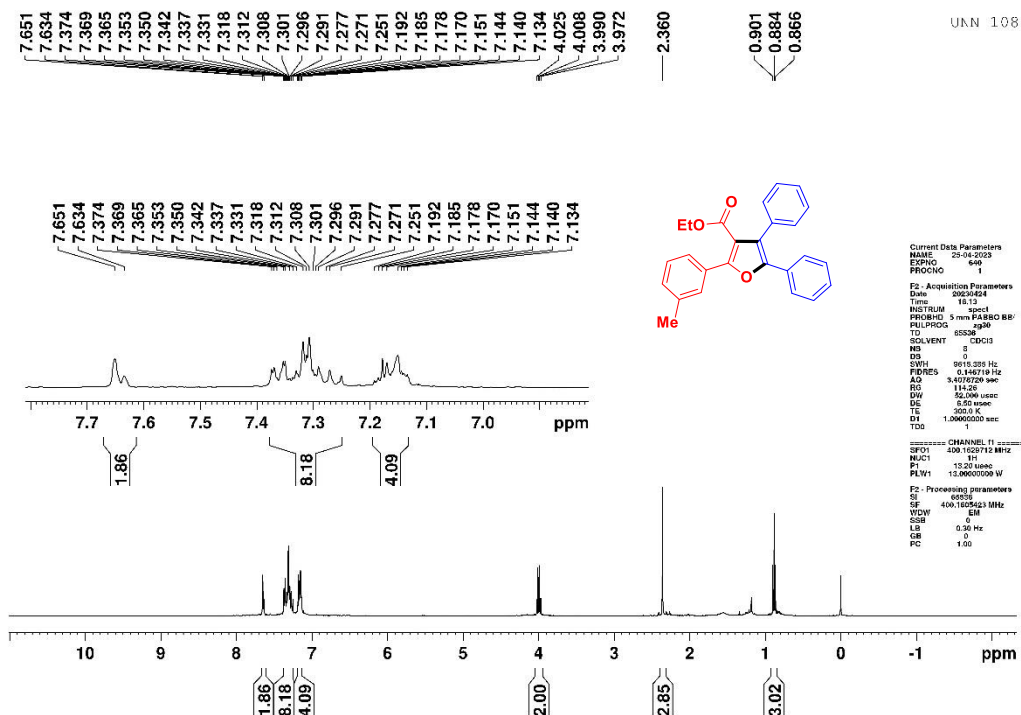
SAIF [HRMS Report]

Data File:	HRMS20I07DEC06	Original Data Path:	D:\INTERNAL NEW\2020\DEC 2020
Sample ID:	TNAKUNN106	Sample Name:	
Acquisition Date:	12/07/20 12:46:18 PM	Run Time(min):	0.00
Vial:	CS1k1-01:6	Injection Volume(μl):	1.00

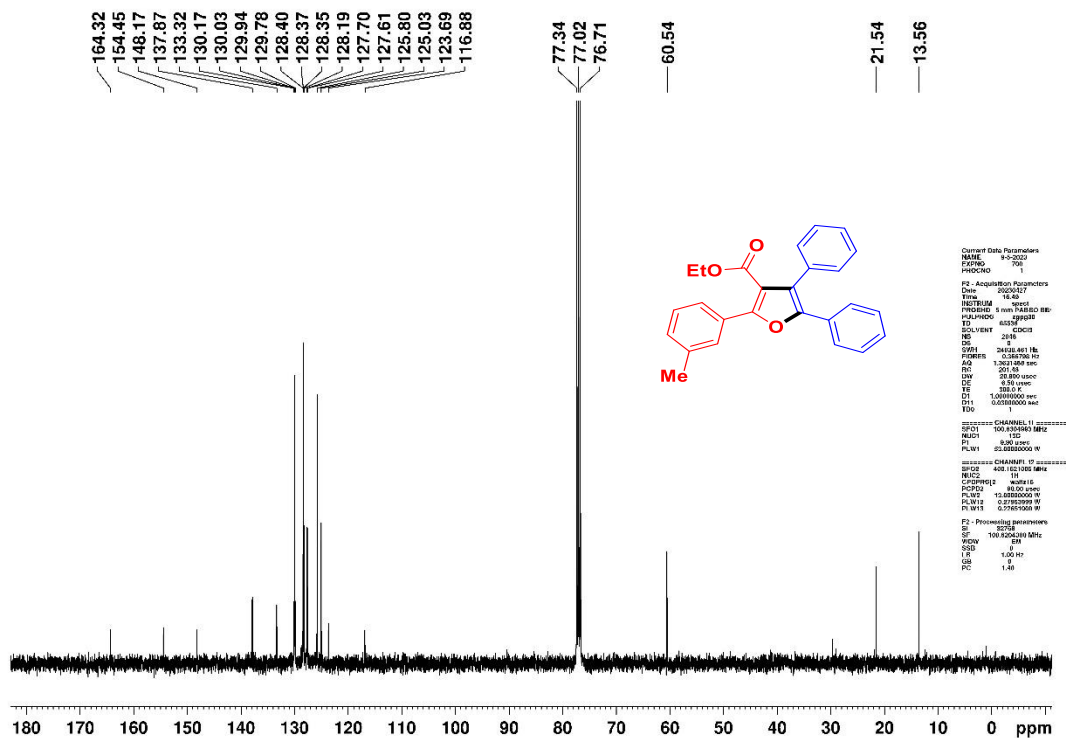
HRMS20I07DEC06 #30-62 RT: 0.25-0.50 AV: 33 SB: 1 0.01 NL: 2.41E6  
T: FTMS + c ESI Full ms [100.00-750.00]



<sup>1</sup>H NMR spectrum of compound- 3da (400 MHz, CDCl<sub>3</sub>);



<sup>13</sup>C NMR spectrum of compound- 3da (100 MHz, CDCl<sub>3</sub>)

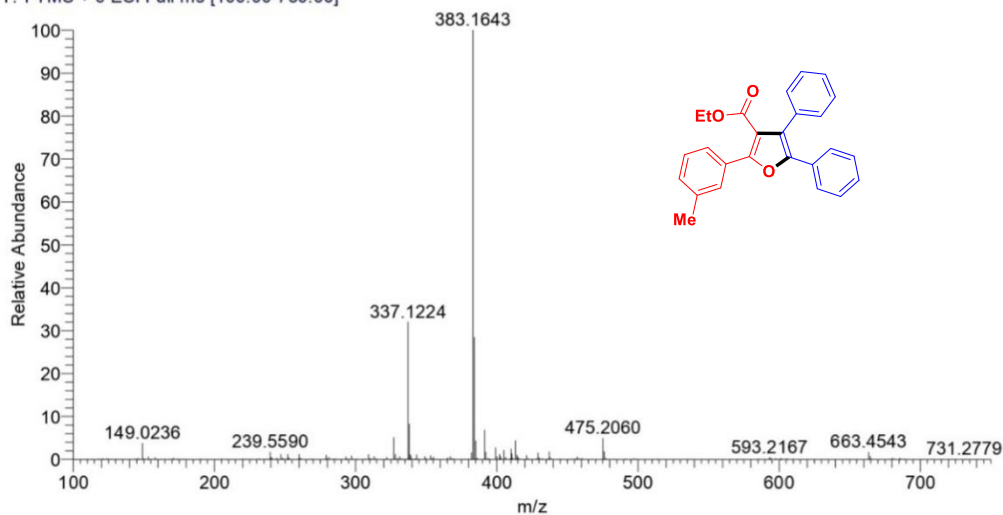


# HRMS spectrum of compound -3da

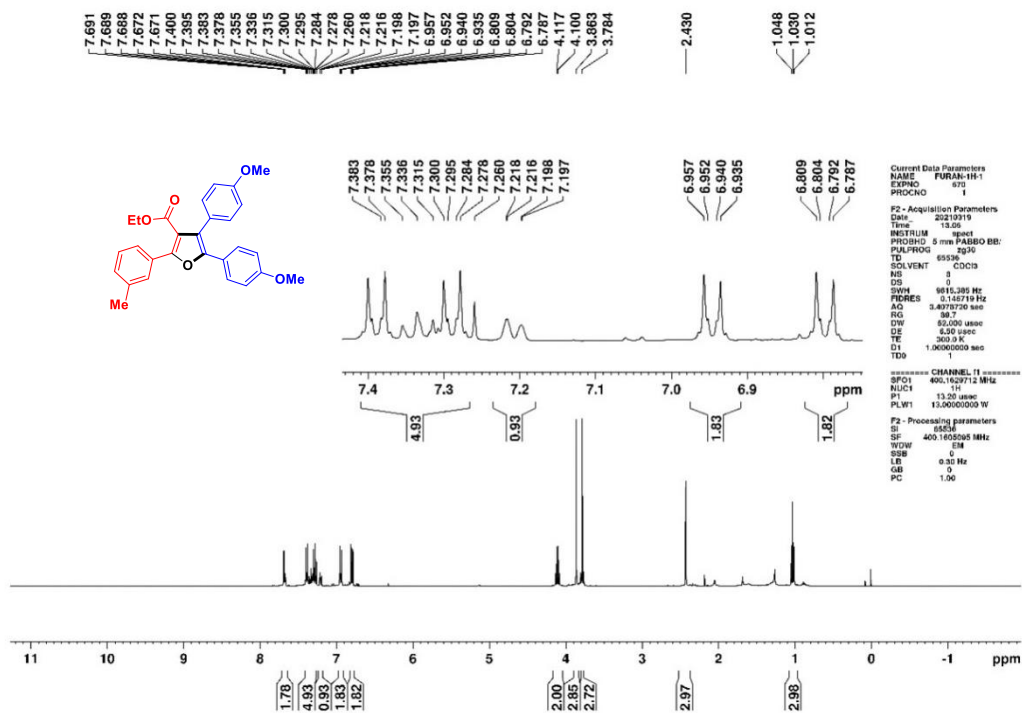
## SAIF [HRMS Report]

Data File: HRMS20I07DEC07 Original Data Path: D:\INTERNAL NEW\2020\DEC  
 Sample ID: TNAKUNN108 Sample Name: 2020  
 Acquisition Date: 12/07/20 12:48:17 PM Run Time(min): 0.00  
 Vial: CStk1-01:7 Injection Volume(μl): 1.00

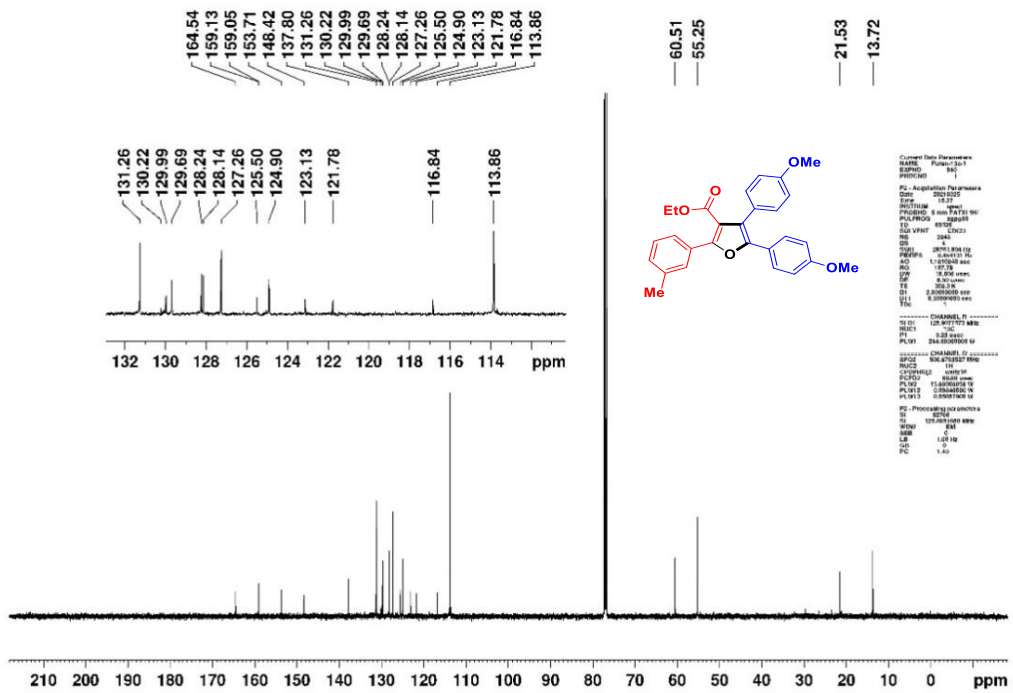
HRMS20I07DEC07 #31-64 RT: 0.25-0.50 AV: 34 SB: 1 0.01 NL: 1.54E7  
 T: FTMS + c ESI Full ms [100.00-750.00]



## <sup>1</sup>H NMR spectrum of compound- 3dc (400 MHz, CDCl<sub>3</sub>)



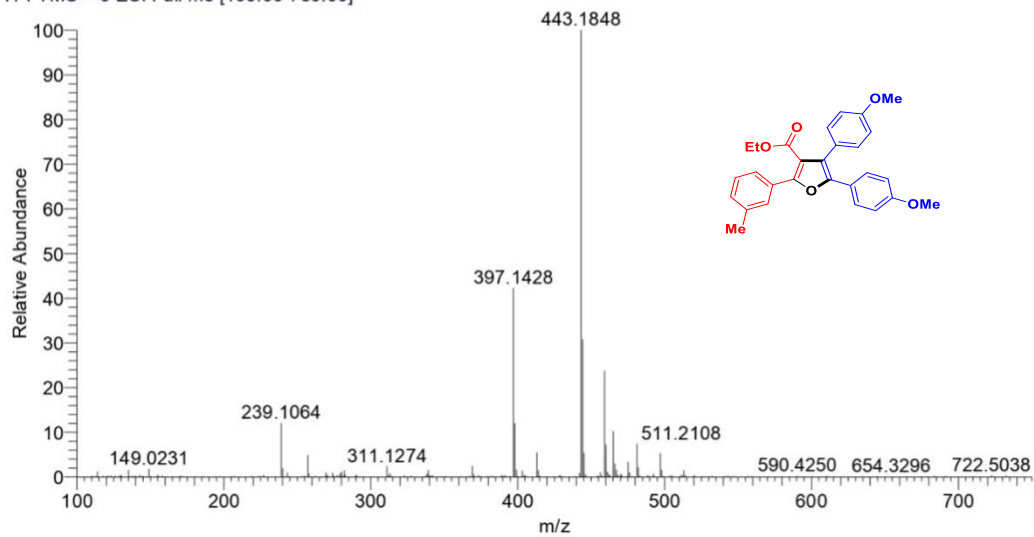
<sup>13</sup>C NMR spectrum of compound- dc (100 MHz, CDCl<sub>3</sub>)



HRMS spectrum of compound-3dc

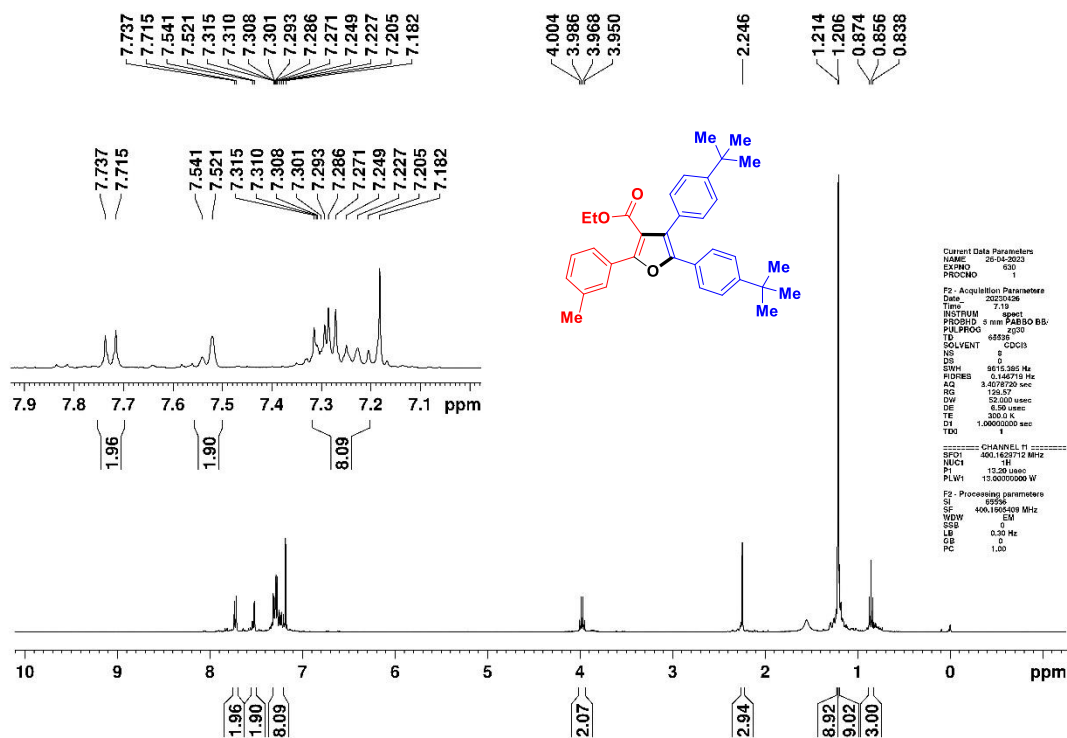
Data File:	HRMS21I06APR22	Original Data Path:	D:\INTERNAL NEW\2021\April 2021
Sample ID:	TNAKUNN127	Sample Name:	
Acquisition Date:	04/06/21 11:30:07 AM	Run Time(min):	0.00
Vial:	CStk1-01:22	Injection Volume(µl):	1.00

HRMS21I06APR22 #33-67 RT: 0.25-0.50 AV: 35 SB: 1 0.01 NL: 9.00E6  
T: FTMS + c ESI Full ms [100.00-750.00]

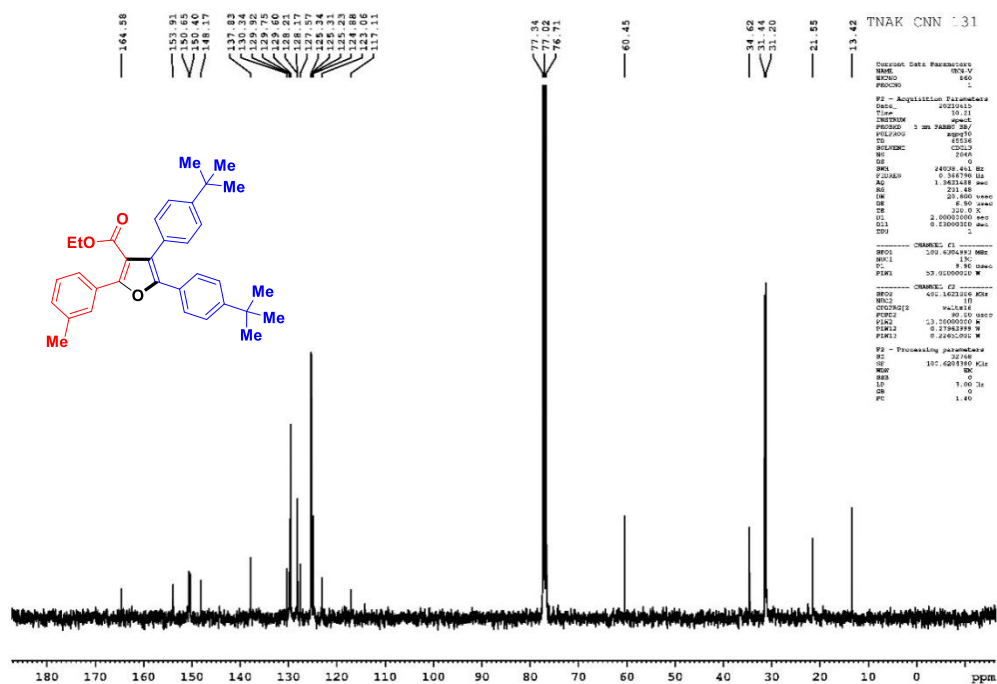




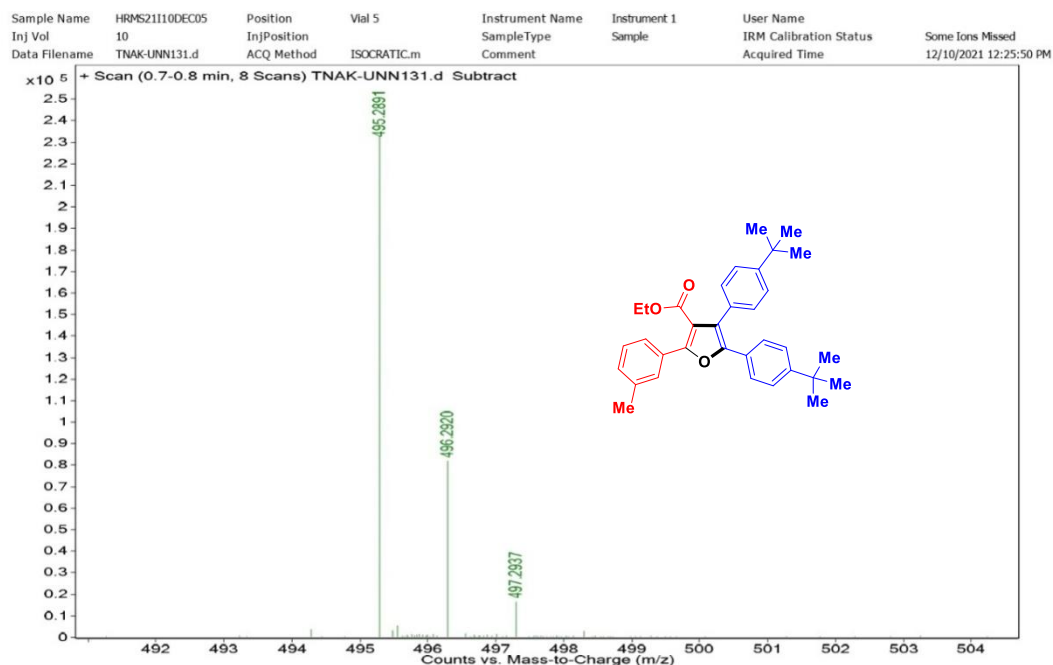
<sup>1</sup>H NMR spectrum of compound- 3de (400 MHz, CDCl<sub>3</sub>)



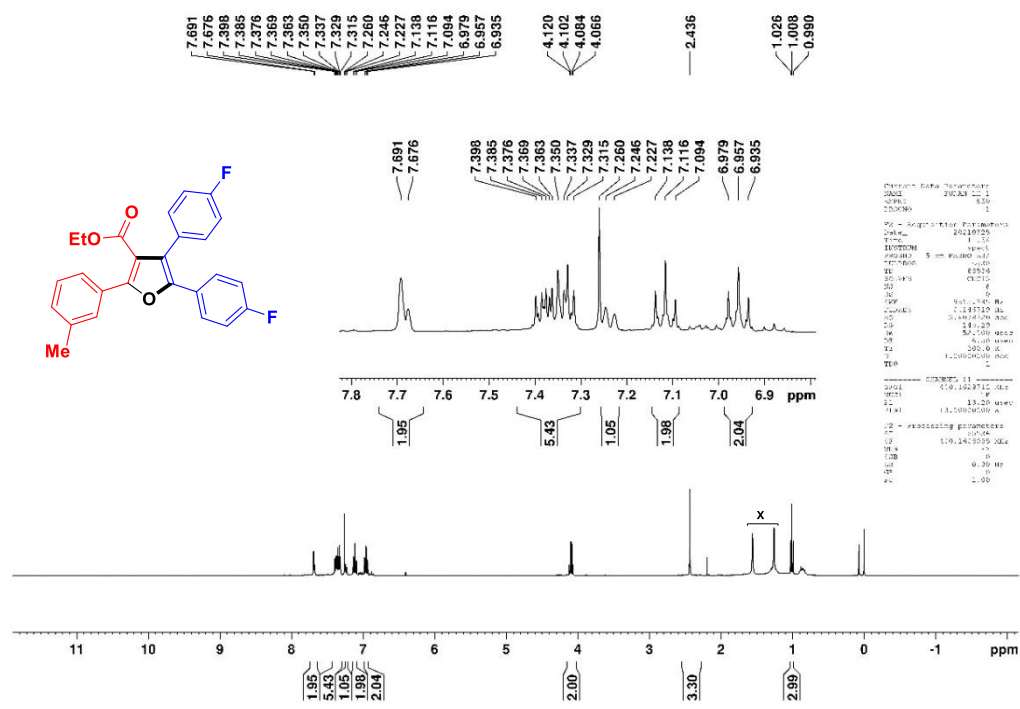
<sup>13</sup>C NMR spectrum of compound- 3de (100 MHz, CDCl<sub>3</sub>)



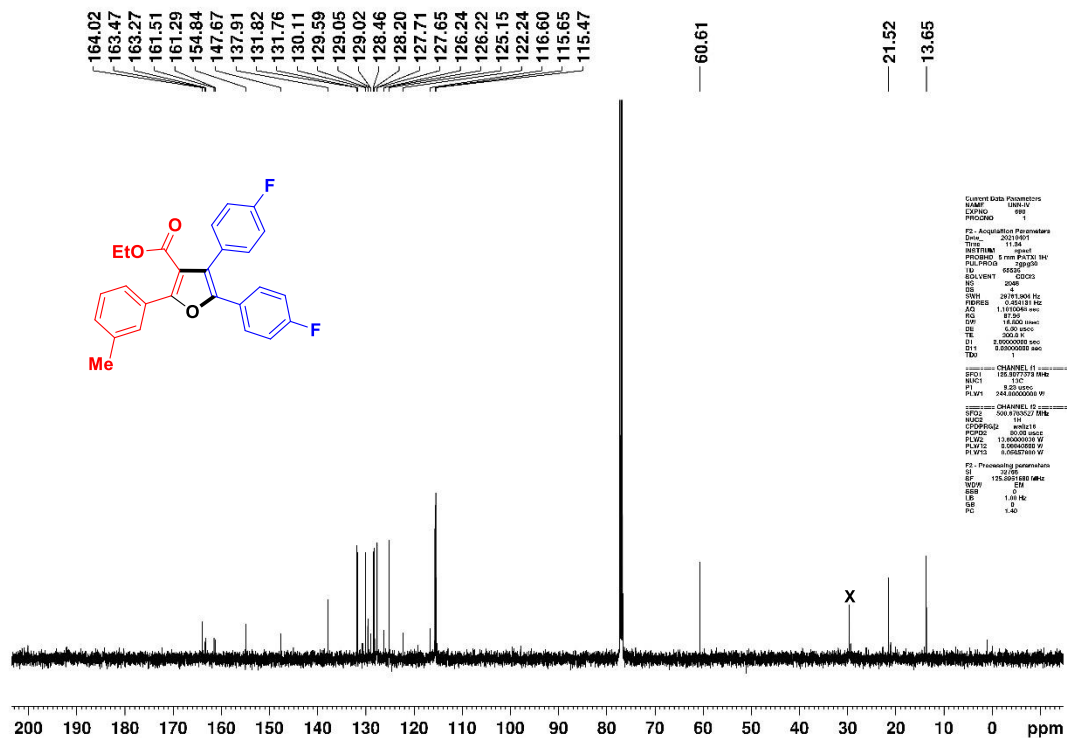
### HRMS spectrum of compound-3de



### <sup>1</sup>H NMR spectrum of compound- 3dd (400 MHz, CDCl<sub>3</sub>); X= wax impurity



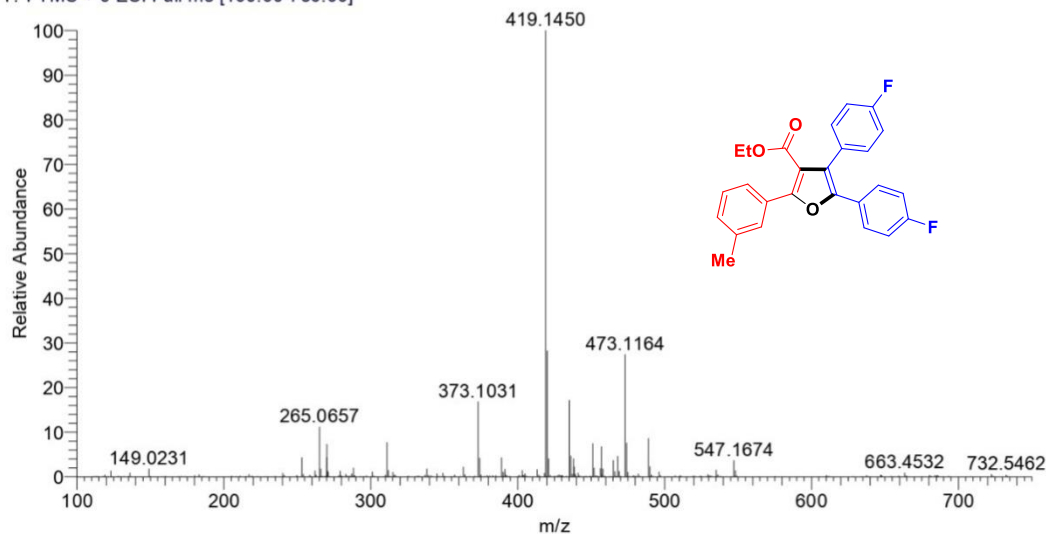
<sup>13</sup>C NMR spectrum of compound- 3dd (100 MHz, CDCl<sub>3</sub>)



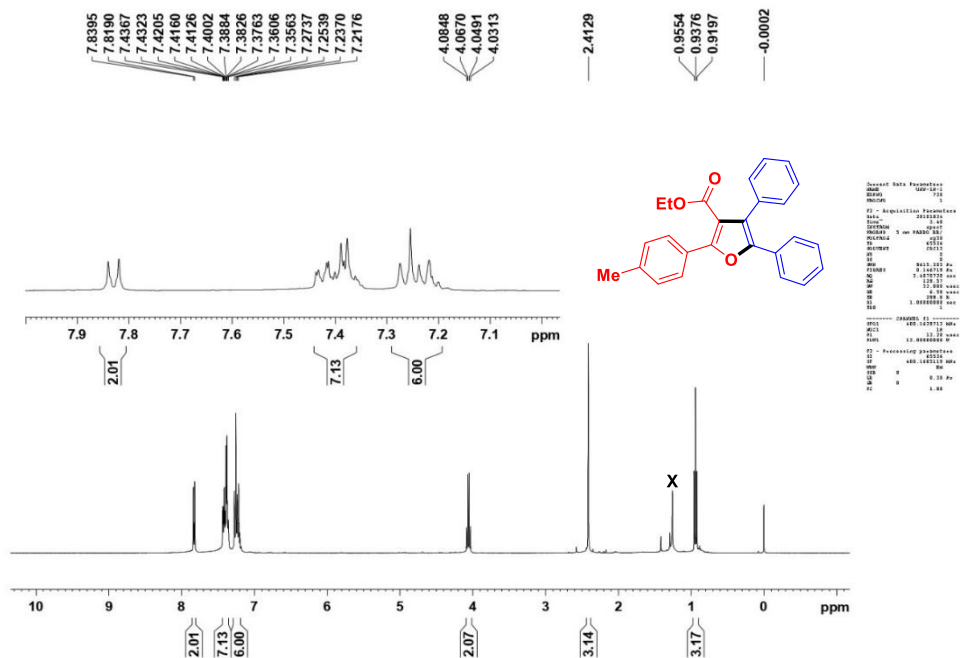
HRMS spectrum of compound-3dd

Data File:	HRMS21I06APR23	Original Data Path:	D:\INTERNAL NEW\2021\April 2021
Sample ID:	TNAKUNN128	Sample Name:	
Acquisition Date:	04/06/21 11:32:08 AM	Run Time(min):	0.00
Vial:	CStk1-01:23	Injection Volume(μl):	1.00

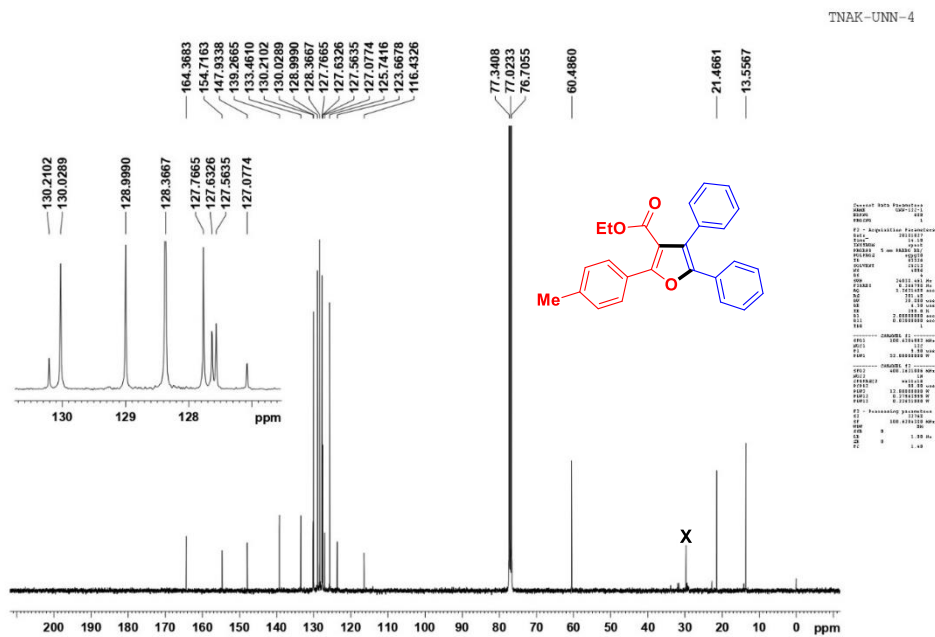
HRMS21I06APR23 #33-66 RT: 0.25-0.50 AV: 34 SB: 1 0.01 NL: 3.90E6  
 T: FTMS + c ESI Full ms [100.00-750.00]



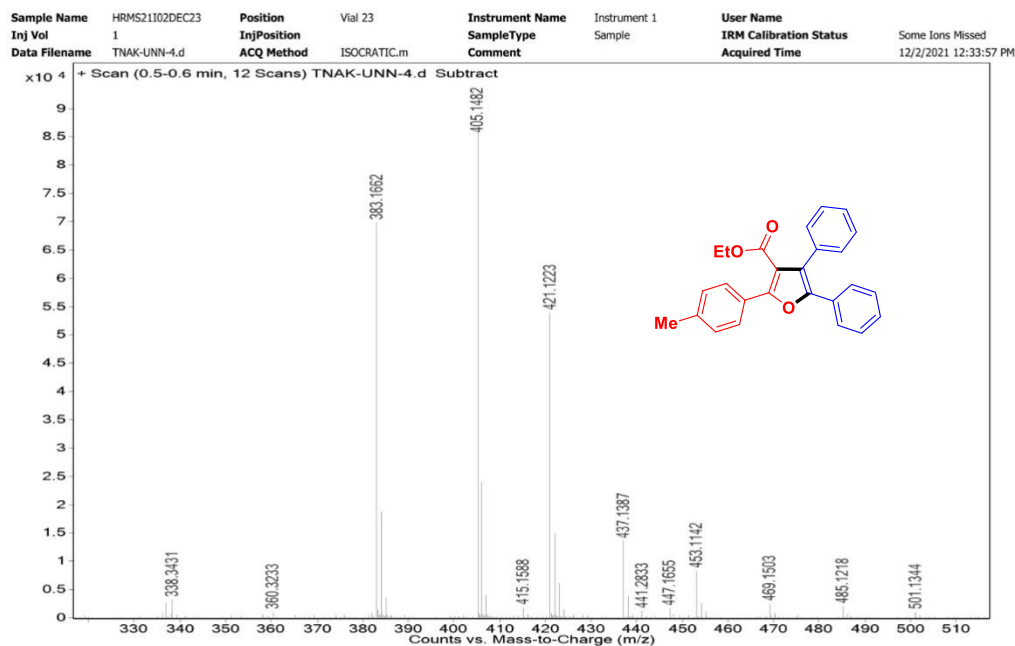
<sup>1</sup>H NMR spectrum of compound- 3ea (400 MHz, CDCl<sub>3</sub>); X= wax impurity



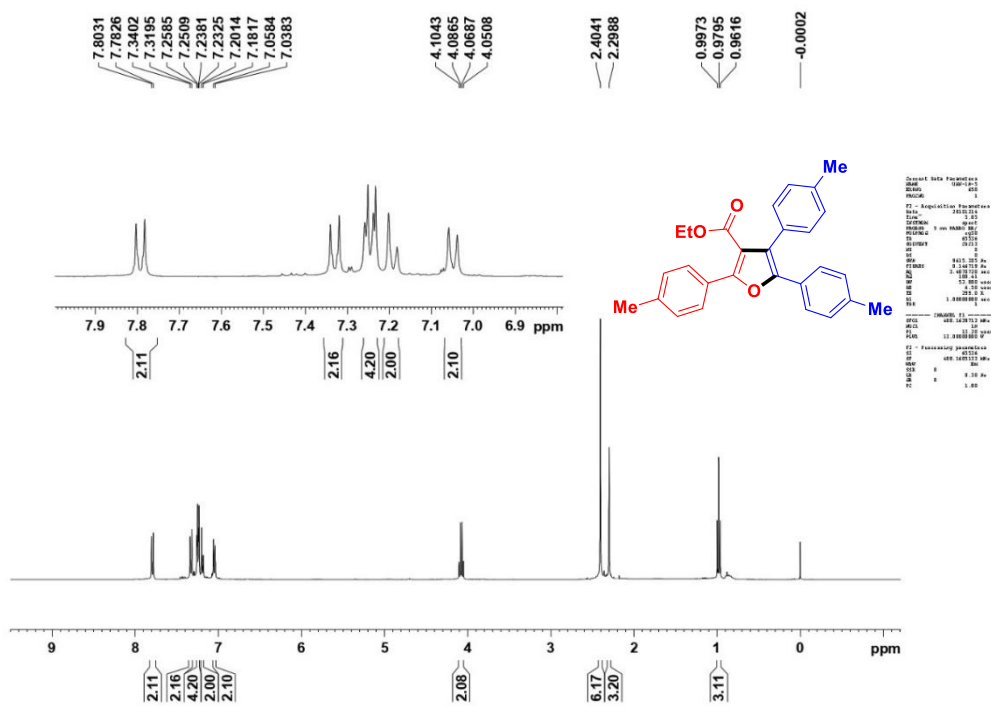
<sup>13</sup>C NMR spectrum of compound- 3ea (100 MHz, CDCl<sub>3</sub>); X= wax impurity



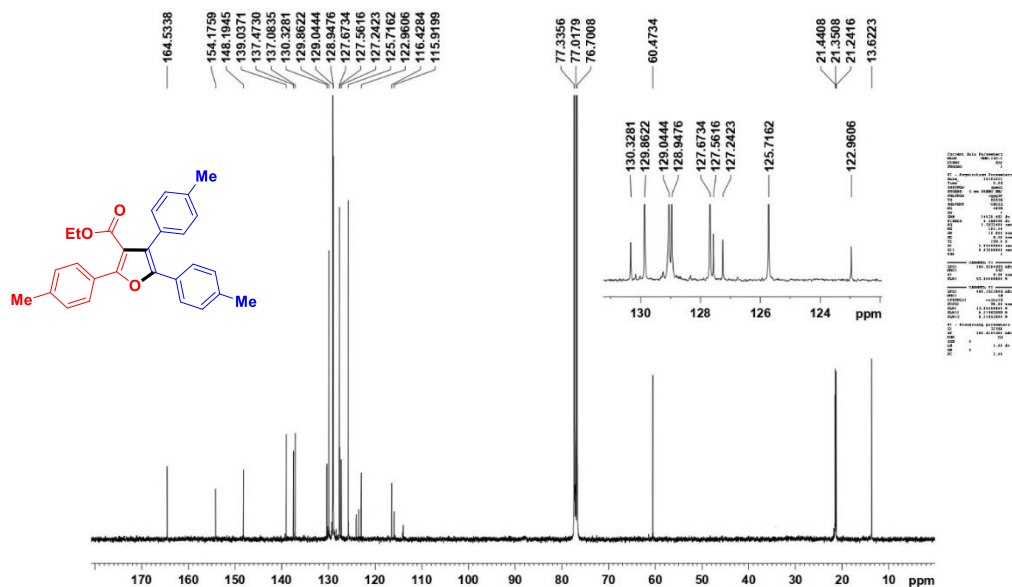
### HRMS spectrum of compound-3ea



### <sup>1</sup>H NMR spectrum of compound- 3eb (400 MHz, CDCl<sub>3</sub>)

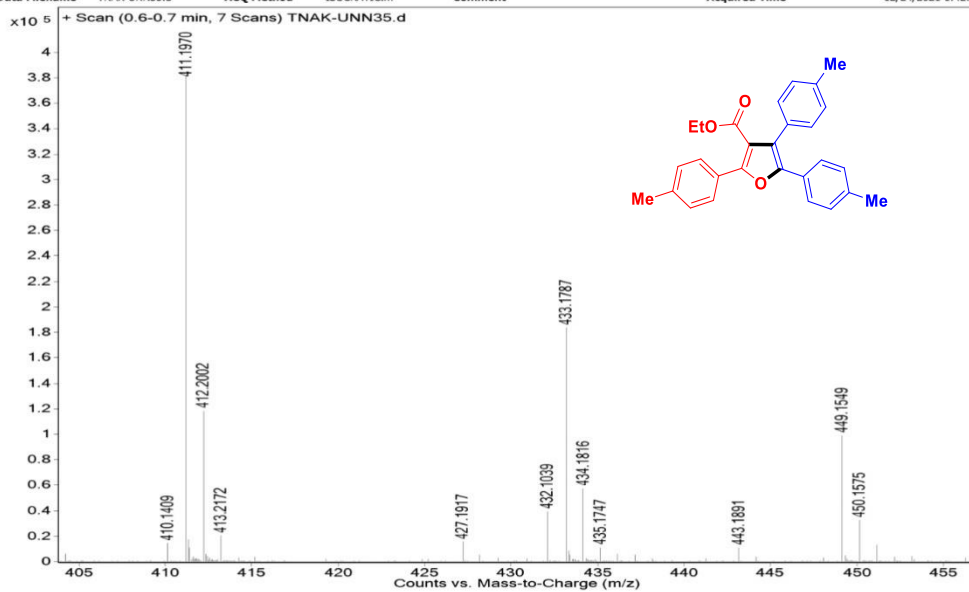


<sup>13</sup>C NMR spectrum of compound- 3eb (100 MHz, CDCl<sub>3</sub>)

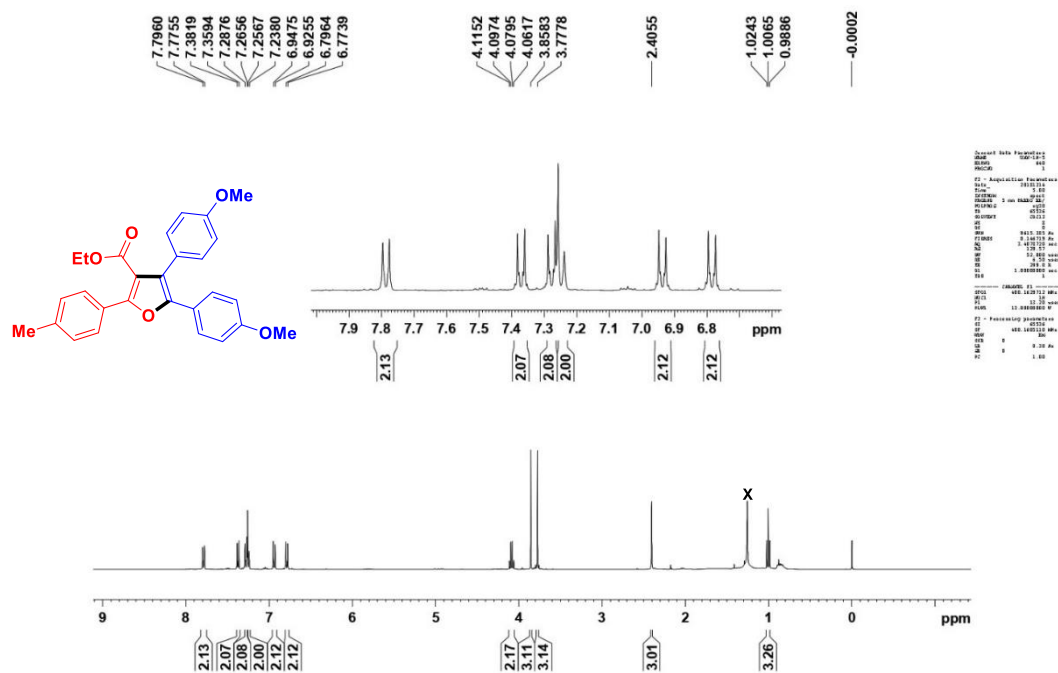


HRMS spectrum of compound-3eb

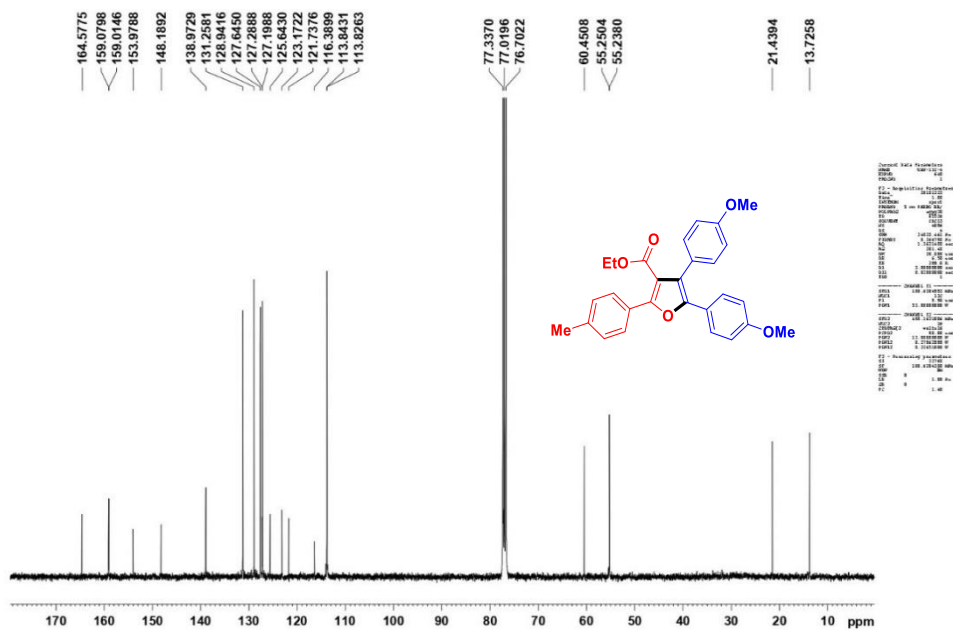
Sample Name	HRMS21124DEC20	Position	Vial 20	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	TNAK-UNN35.d	ACQ Method	ISOCRATIC.m	Comment		Acquired Time	12/24/2021 1:42:34 PM



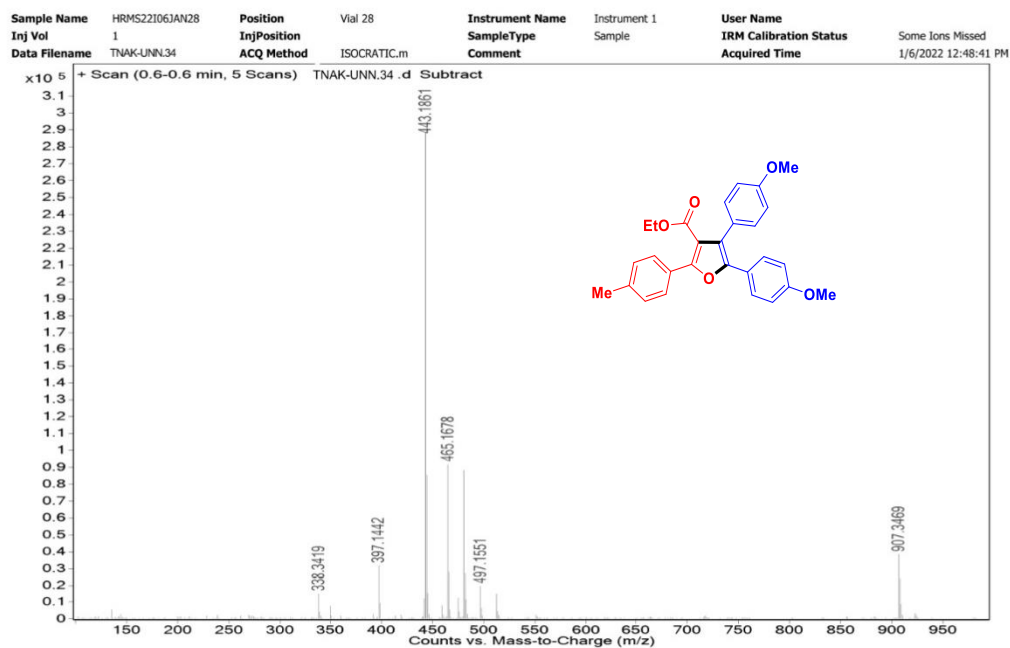
<sup>1</sup>H NMR spectrum of compound- 3ec (400 MHz, CDCl<sub>3</sub>); X= wax impurity



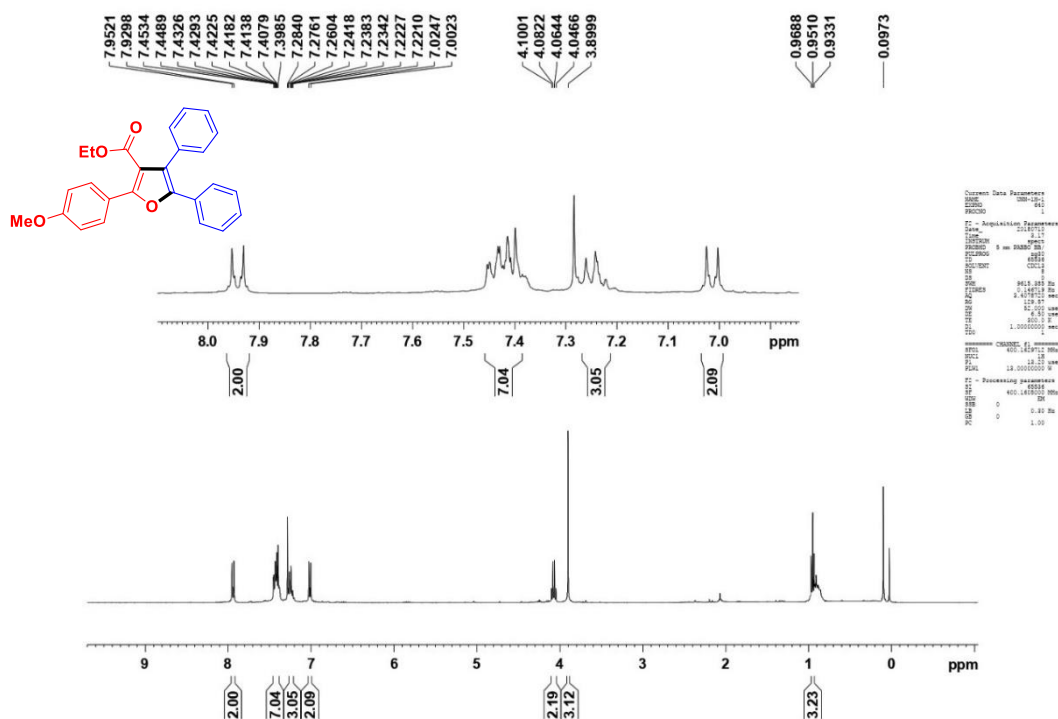
<sup>13</sup>C NMR spectrum of compound- 3ec (100 MHz, CDCl<sub>3</sub>)



### HRMS spectrum of compound-3ec

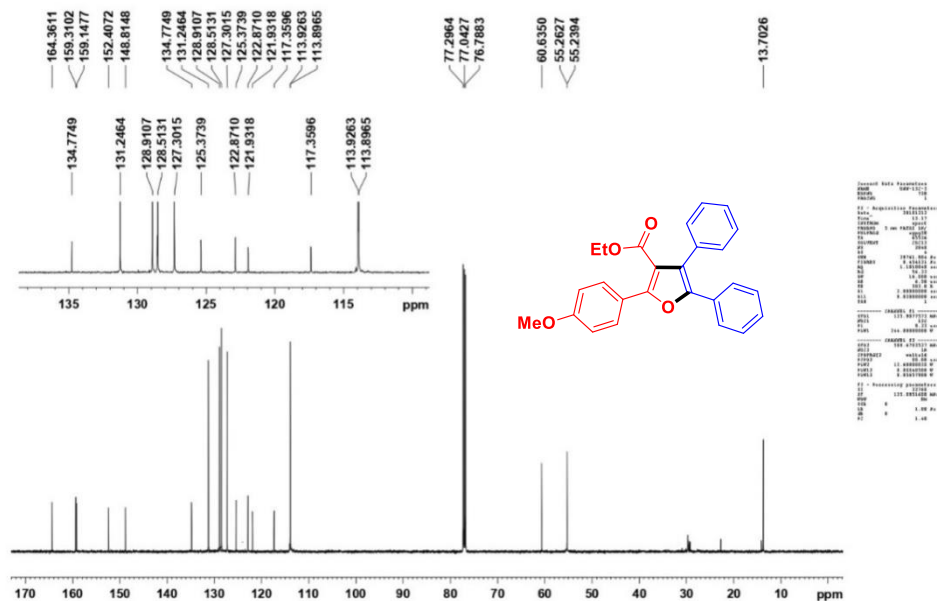


### <sup>1</sup>H NMR spectrum of compound- 3fa (400 MHz, CDCl<sub>3</sub>)

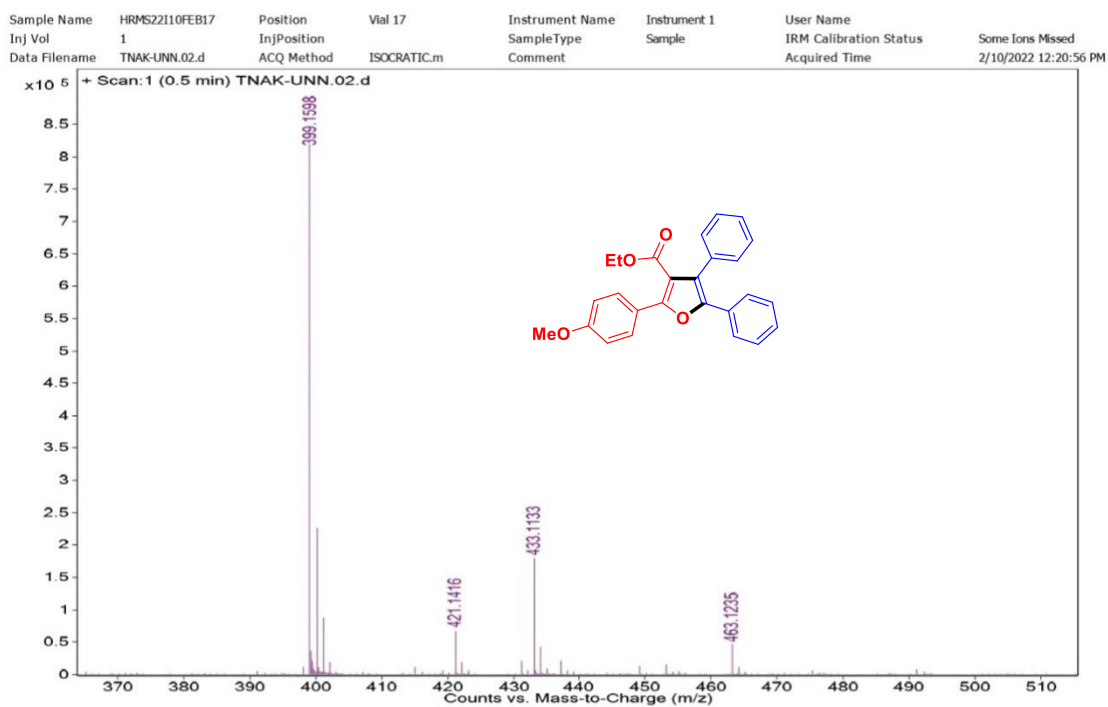




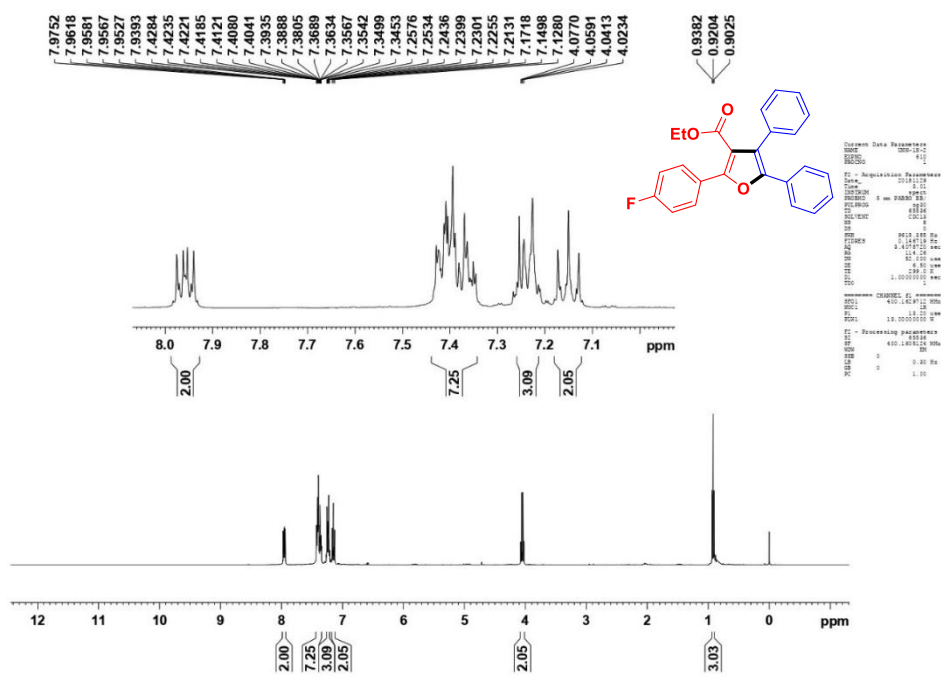
<sup>13</sup>C NMR spectrum of compound- 3fa (100 MHz, CDCl<sub>3</sub>)



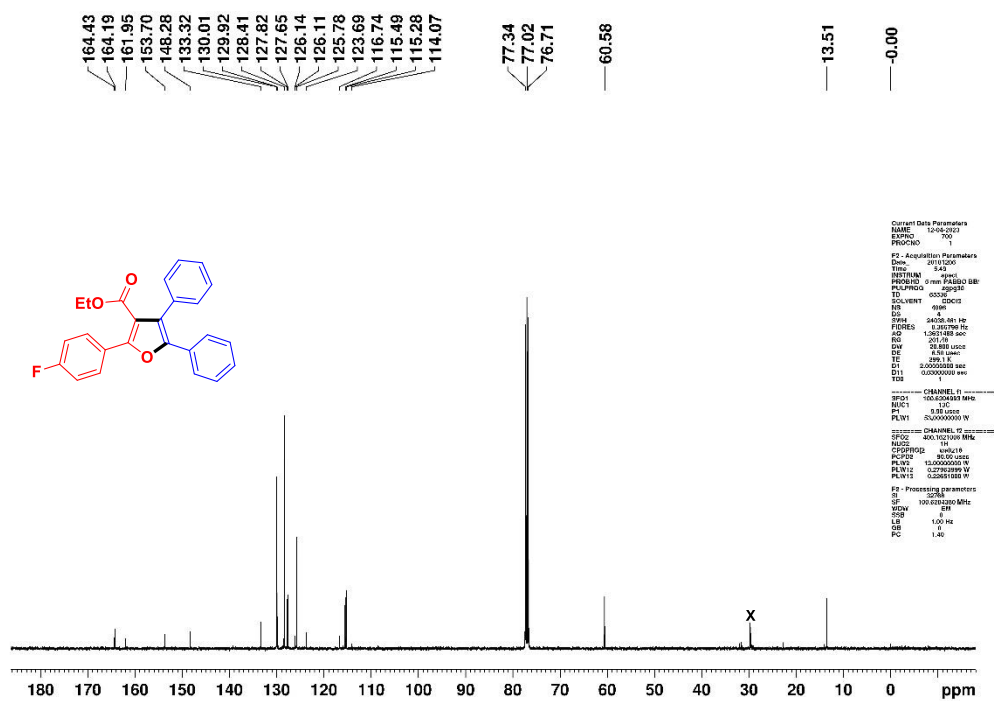
HRMS spectrum of compound-3fa



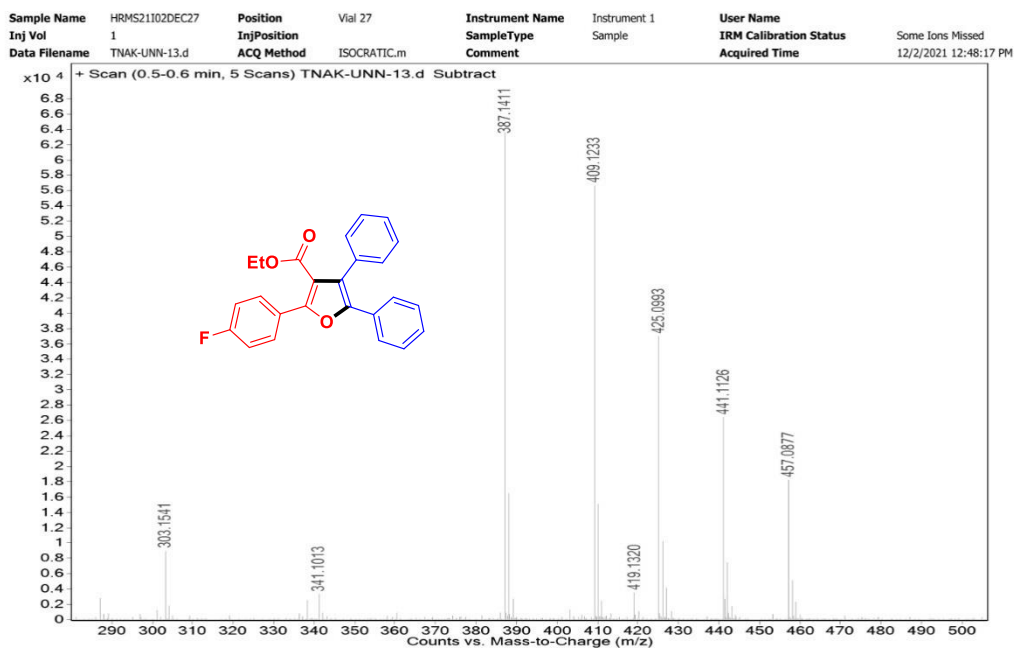
<sup>1</sup>H NMR spectrum of compound- 3ga (400 MHz, CDCl<sub>3</sub>)



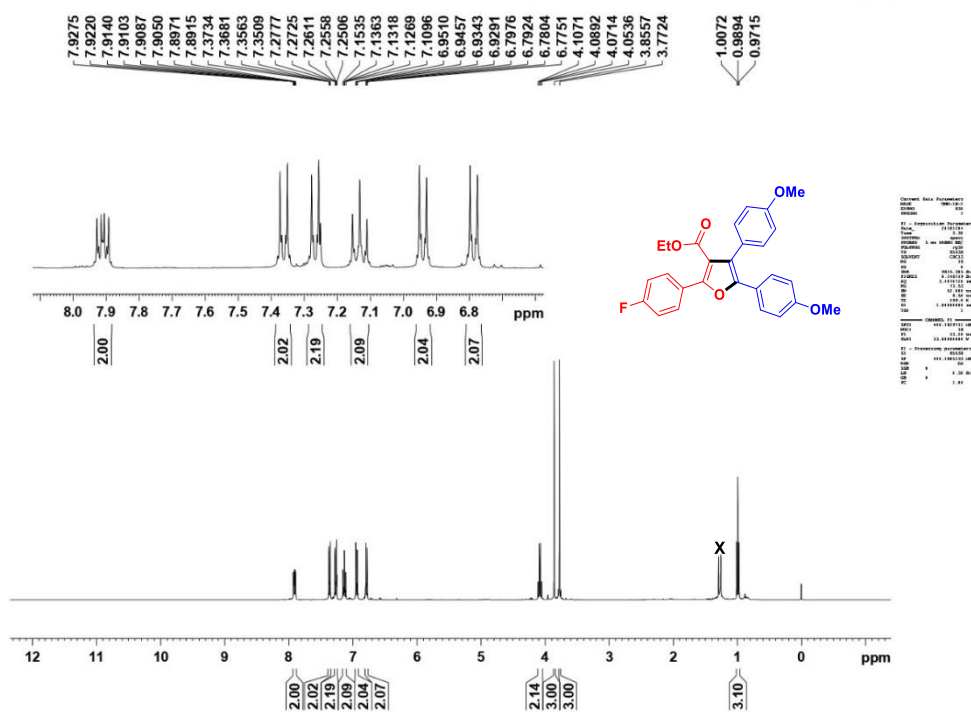
<sup>13</sup>C NMR spectrum of compound- 3ga (100 MHz, CDCl<sub>3</sub>); X= wax impurity



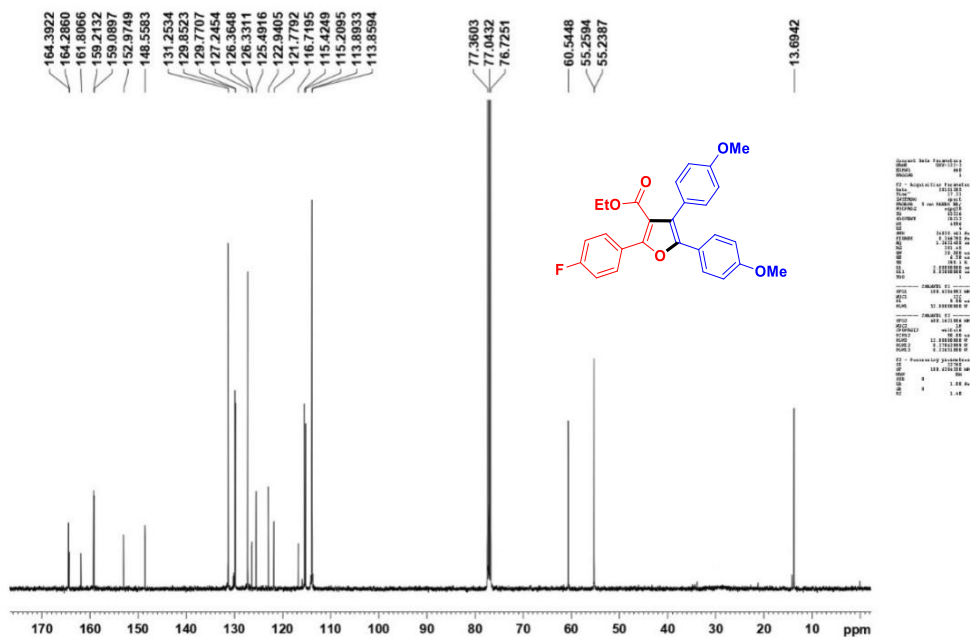
### HRMS spectrum of compound-3ga



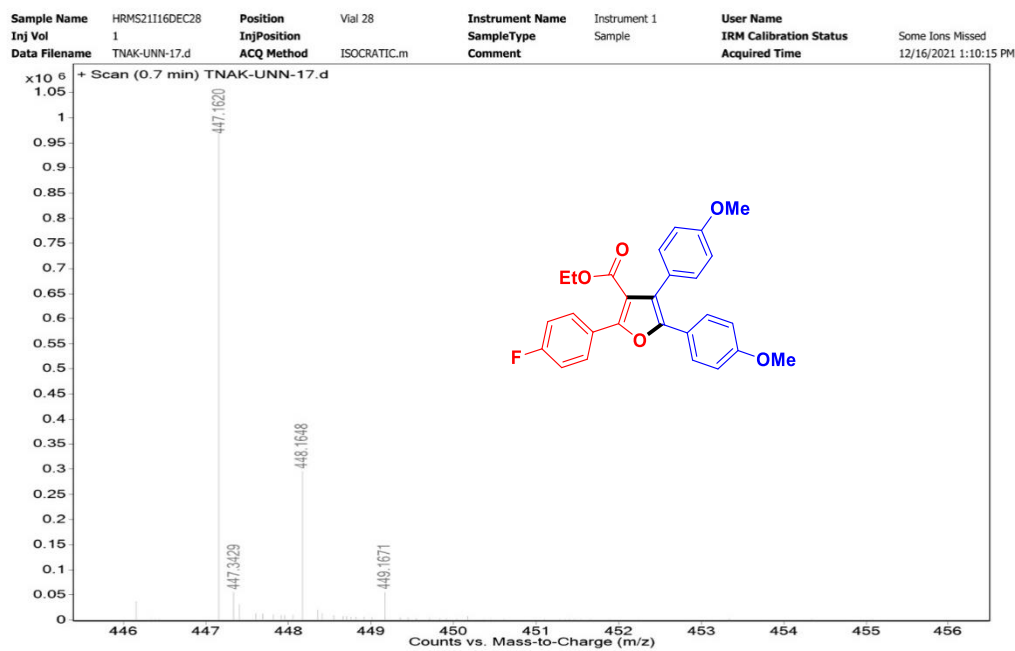
### <sup>1</sup>H NMR spectrum of compound- 3gc (400 MHz, CDCl<sub>3</sub>); X= wax impurity



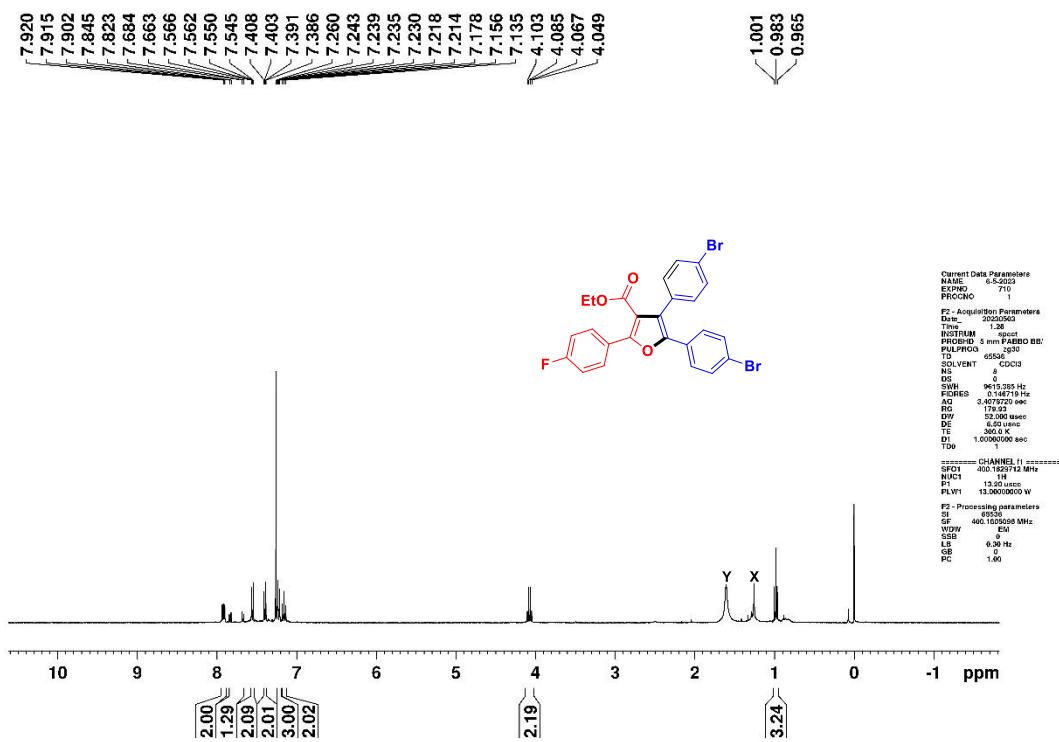
**<sup>13</sup>C NMR spectrum of compound- 3gc (100 MHz, CDCl<sub>3</sub>)**



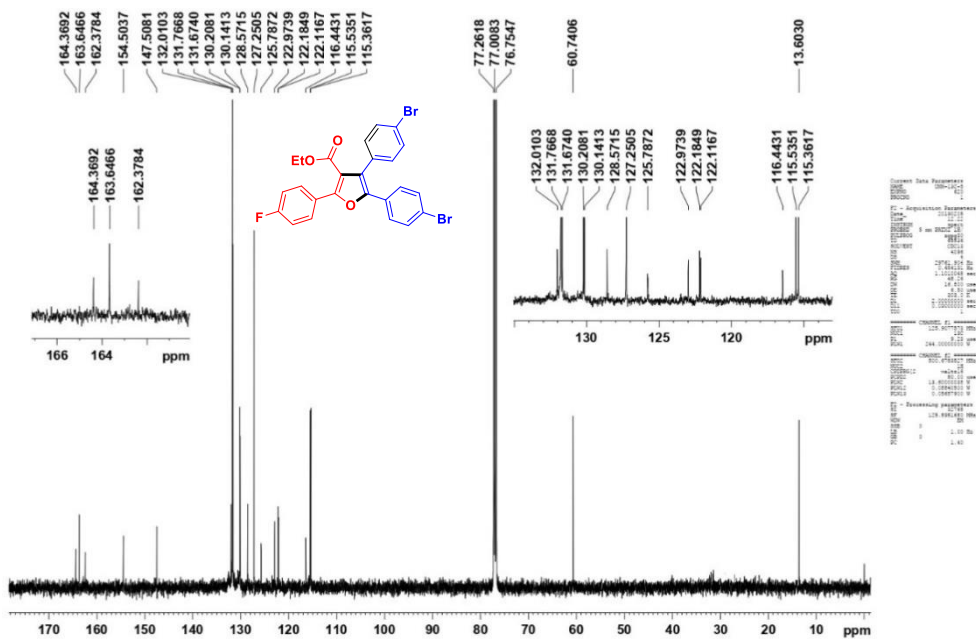
**HRMS spectrum of compound-3gc**



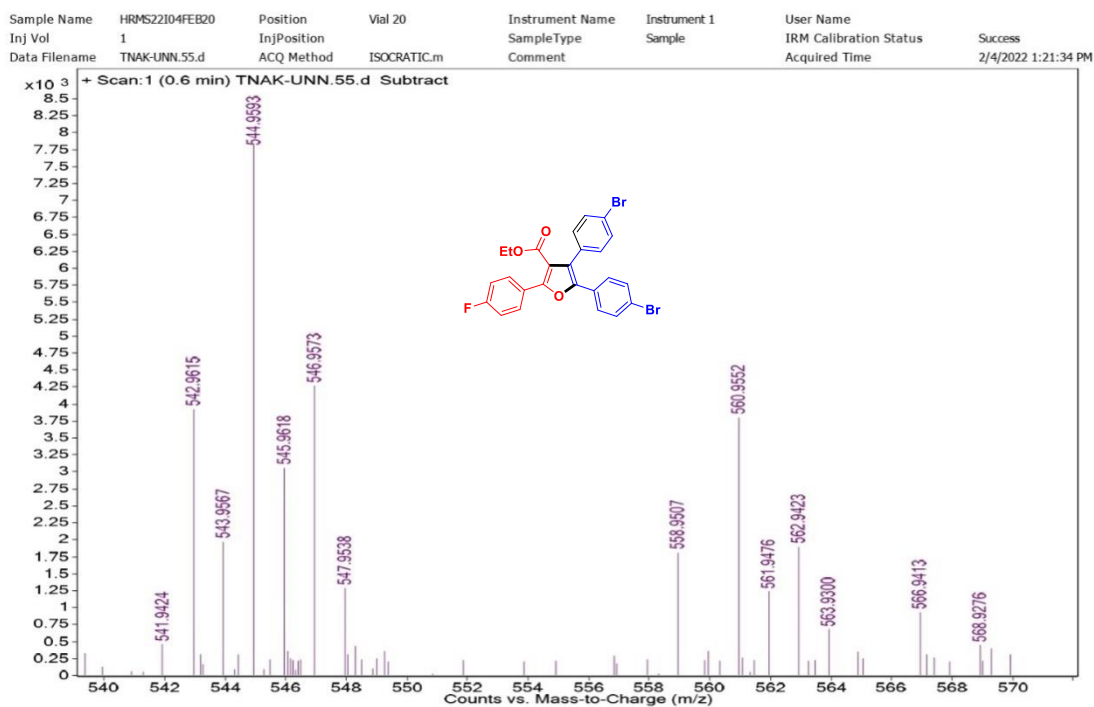
<sup>1</sup>H NMR spectrum of compound- 3gf (400 MHz, CDCl<sub>3</sub>); X= wax impurity, Y = H<sub>2</sub>O



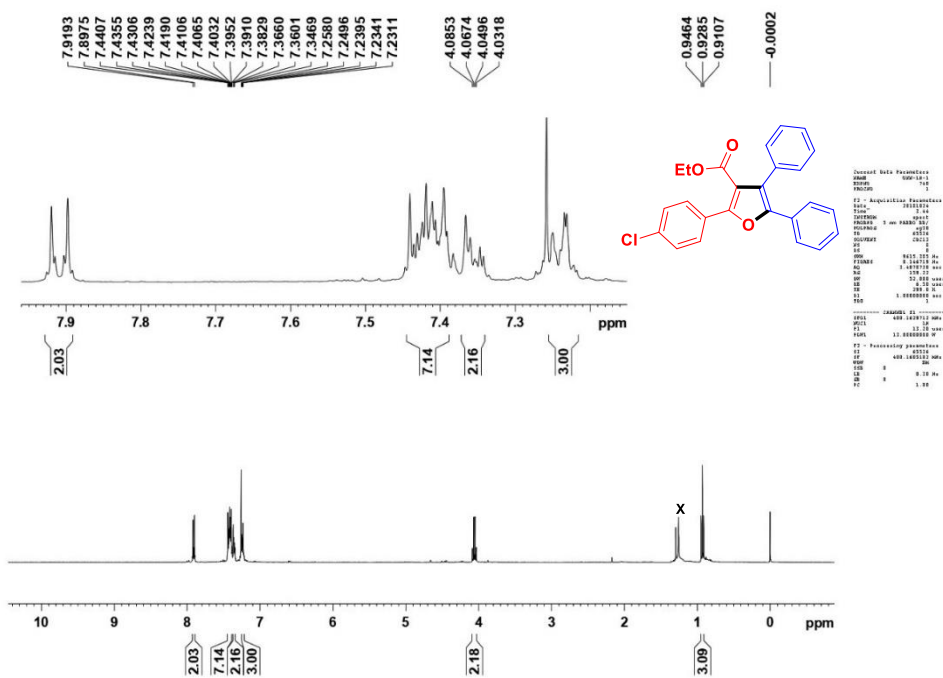
<sup>13</sup>C NMR spectrum of compound- 3gf (100 MHz, CDCl<sub>3</sub>)



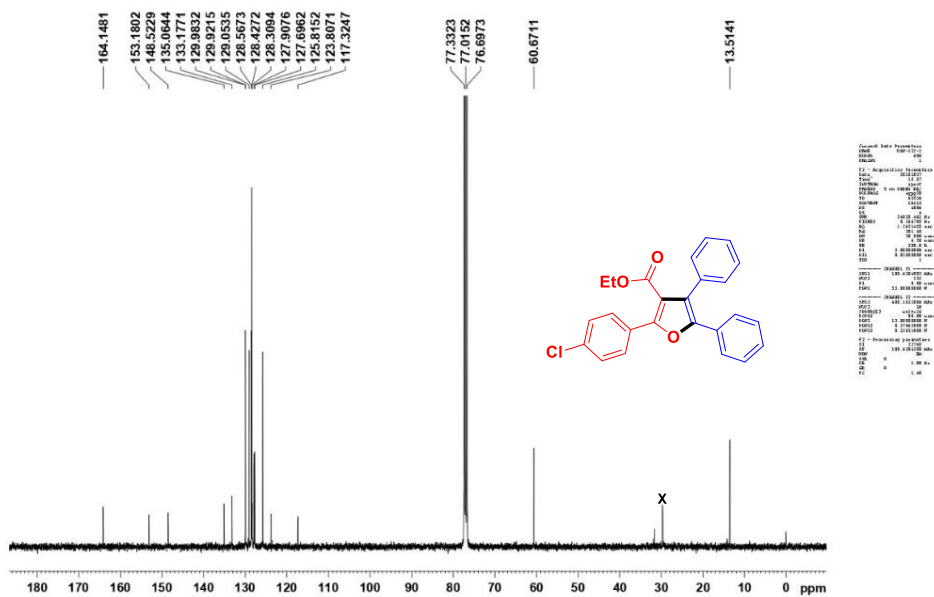
## HRMS spectrum of compound-3gf



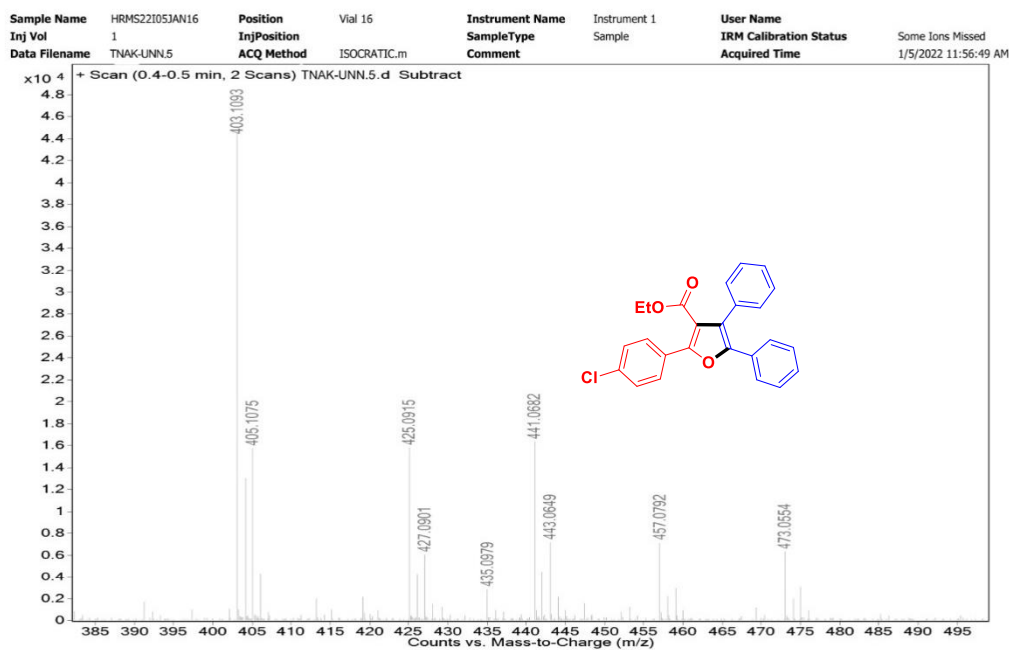
## <sup>1</sup>H NMR spectrum of compound- 3ha (400 MHz, CDCl<sub>3</sub>); X= wax impurity



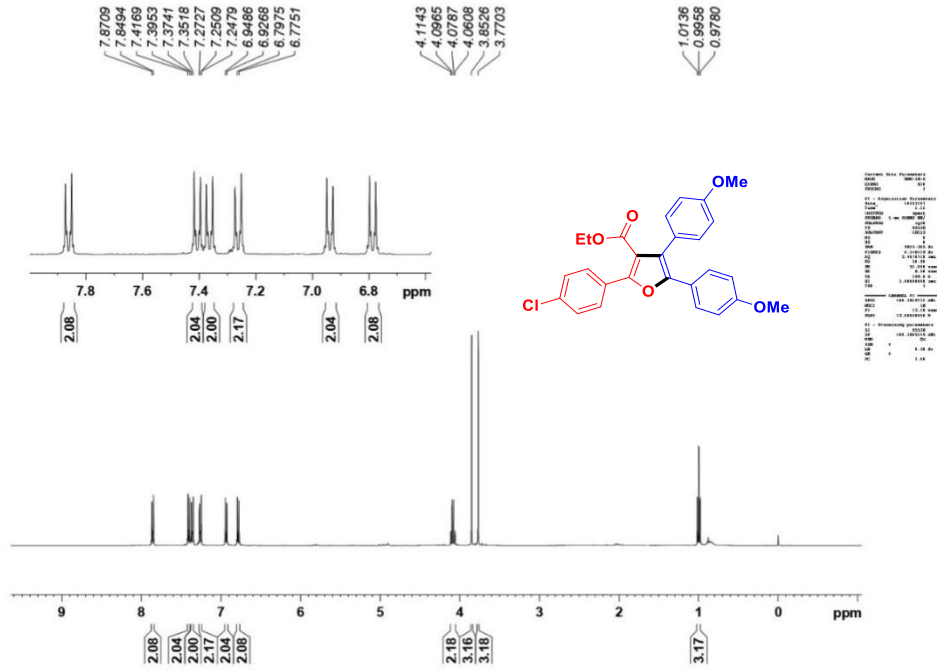
<sup>13</sup>C NMR spectrum of compound- 3ha (100 MHz, CDCl<sub>3</sub>); X= wax impurity



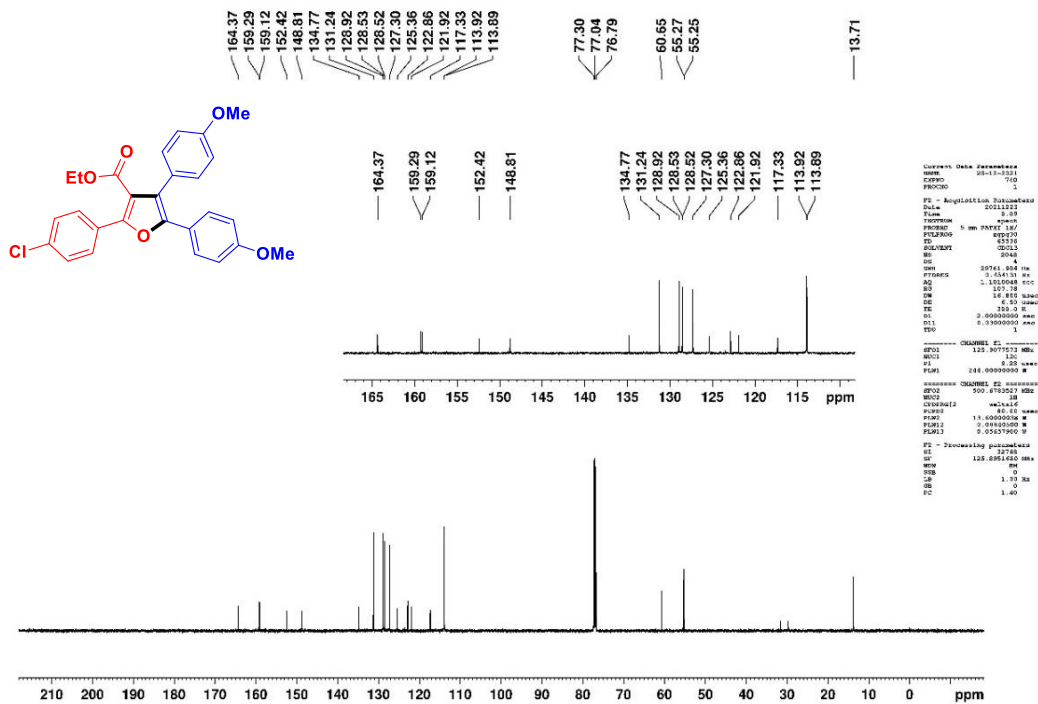
HRMS spectrum of compound-3ha



<sup>1</sup>H NMR spectrum of compound- 3hc (400 MHz, CDCl<sub>3</sub>)

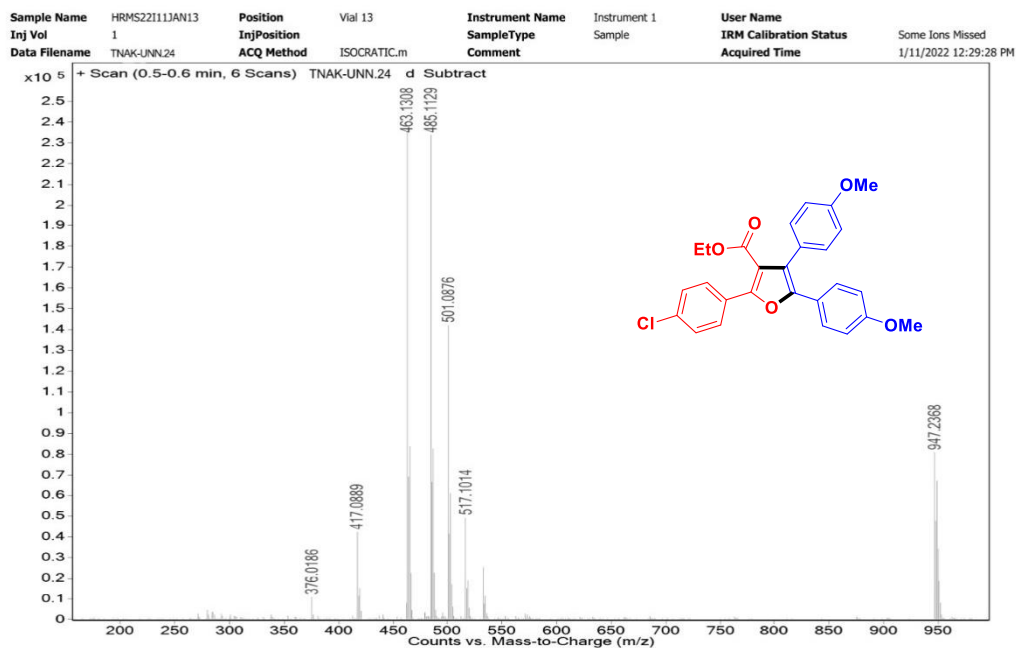


<sup>13</sup>C NMR spectrum of compound- 3hc (100 MHz, CDCl<sub>3</sub>)

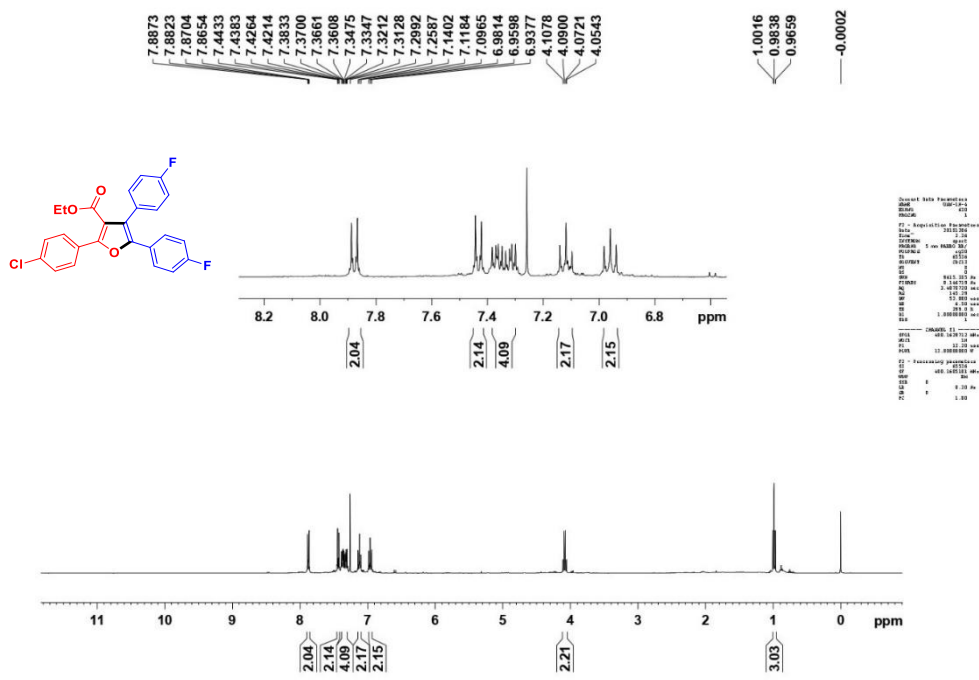




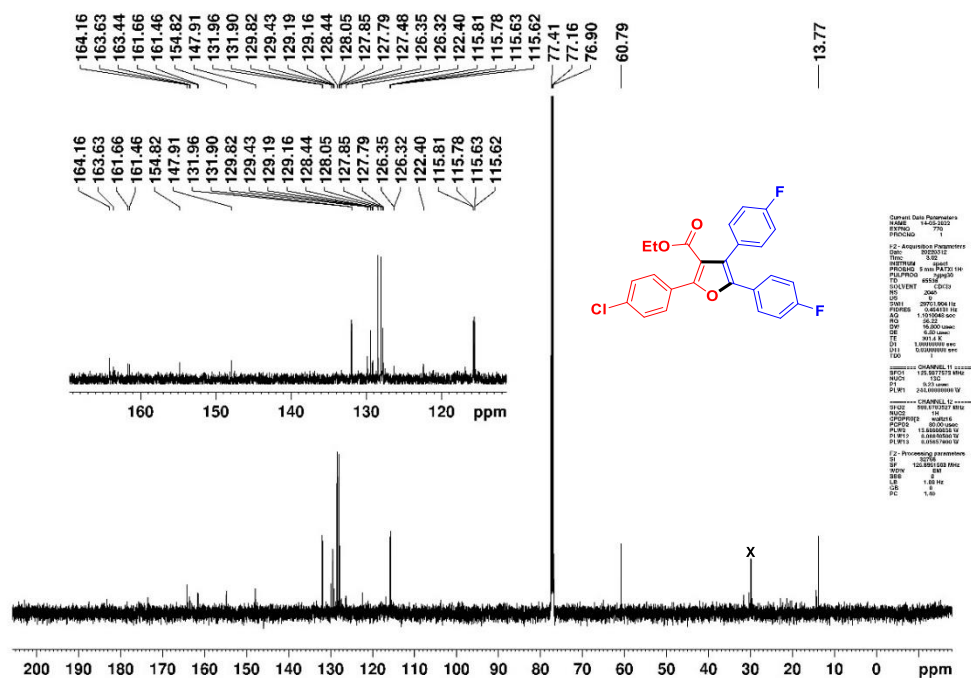
### HRMS spectrum of compound-3hc



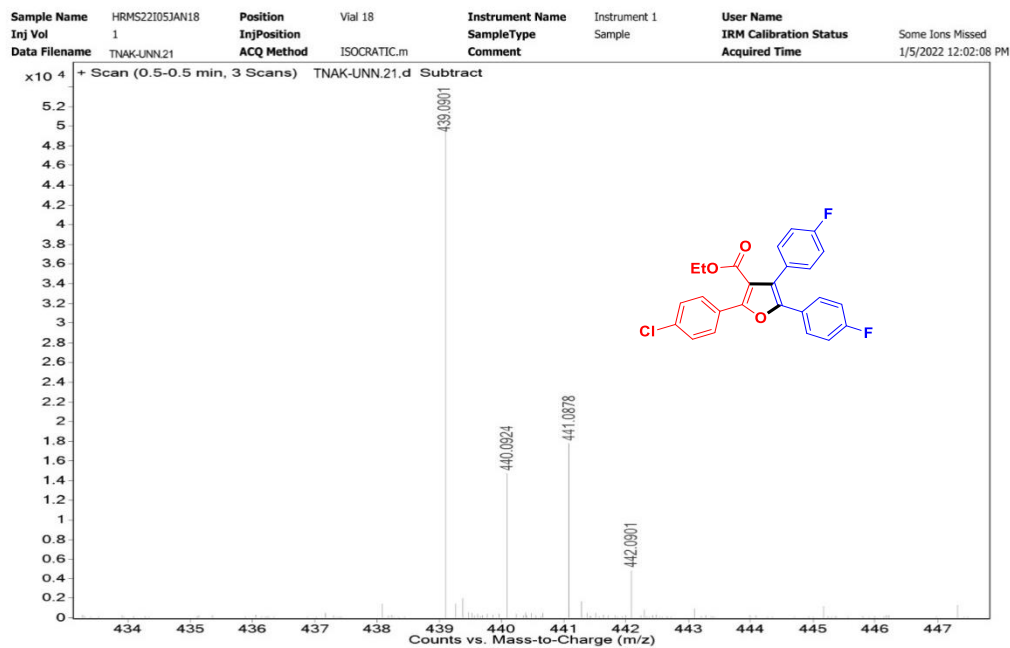
### <sup>1</sup>H NMR spectrum of compound- 3hd (400 MHz, CDCl<sub>3</sub>)



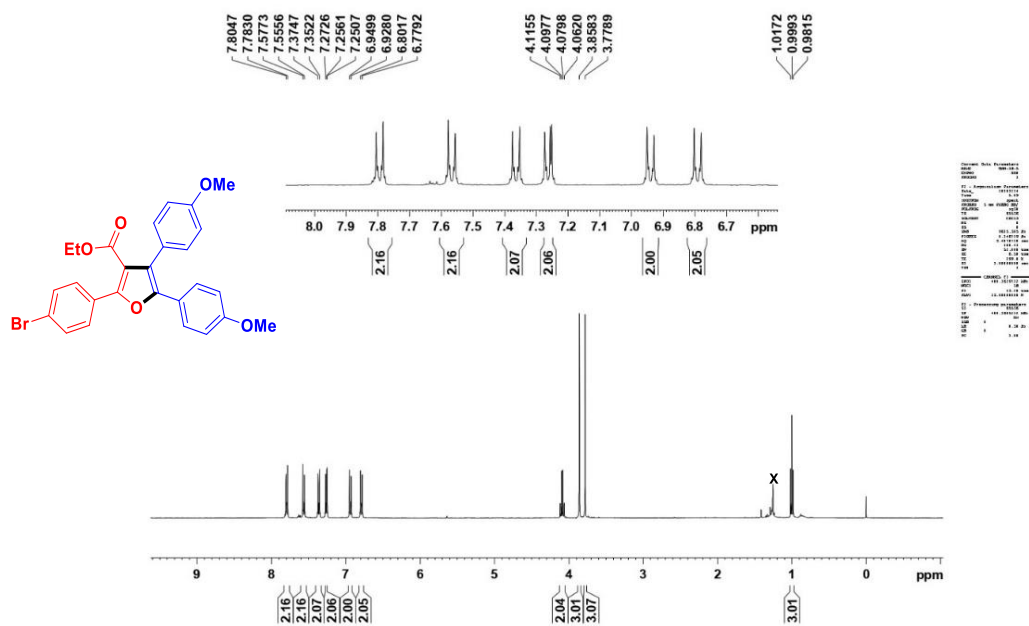
<sup>13</sup>C NMR spectrum of compound- 3hd (100 MHz, CDCl<sub>3</sub>); X= wax impurity



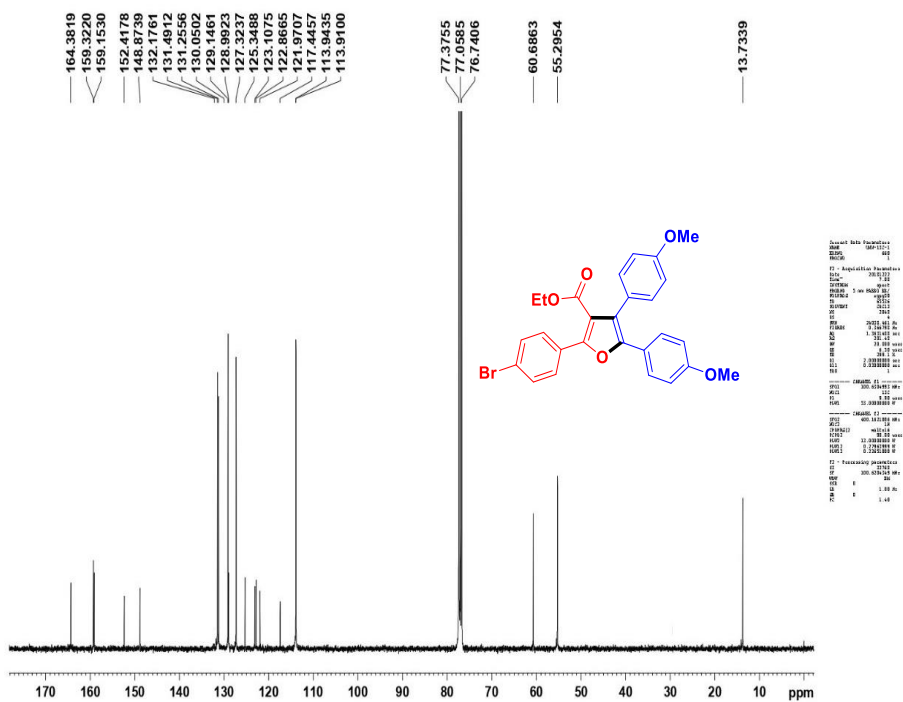
HRMS spectrum of compound-3hd



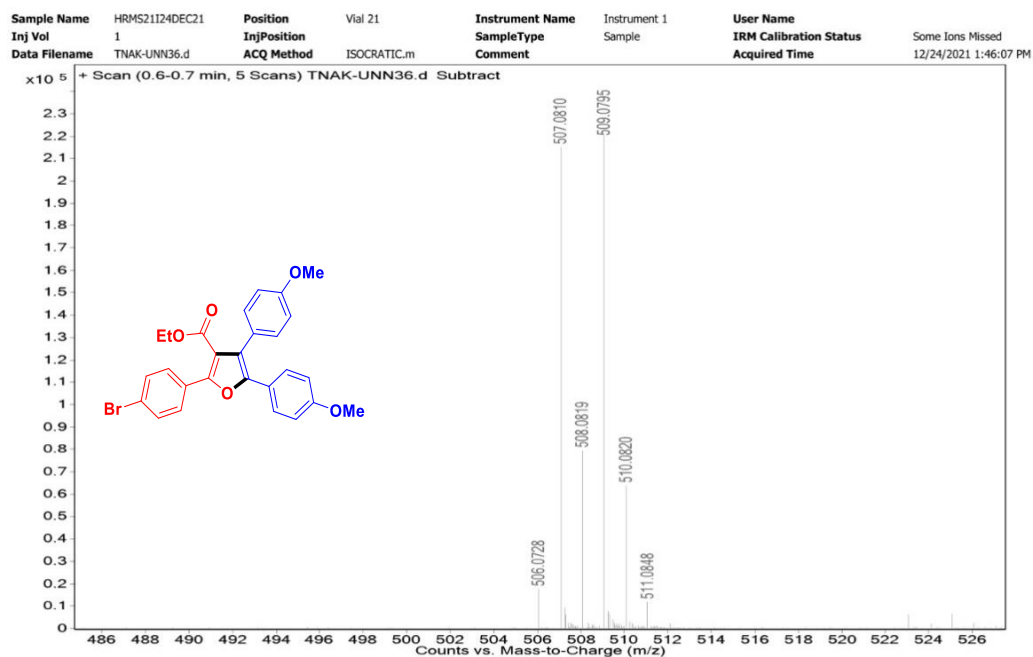
<sup>1</sup>H NMR spectrum of compound- 3ic (400 MHz, CDCl<sub>3</sub>); X= wax impurity



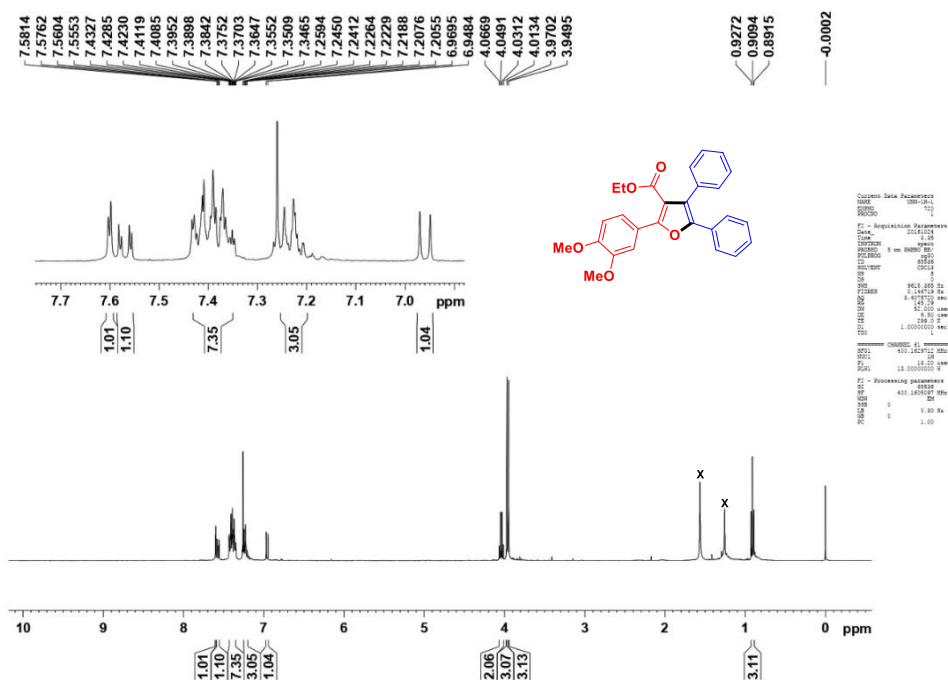
<sup>13</sup>C NMR spectrum of compound- 3ic (100 MHz, CDCl<sub>3</sub>)



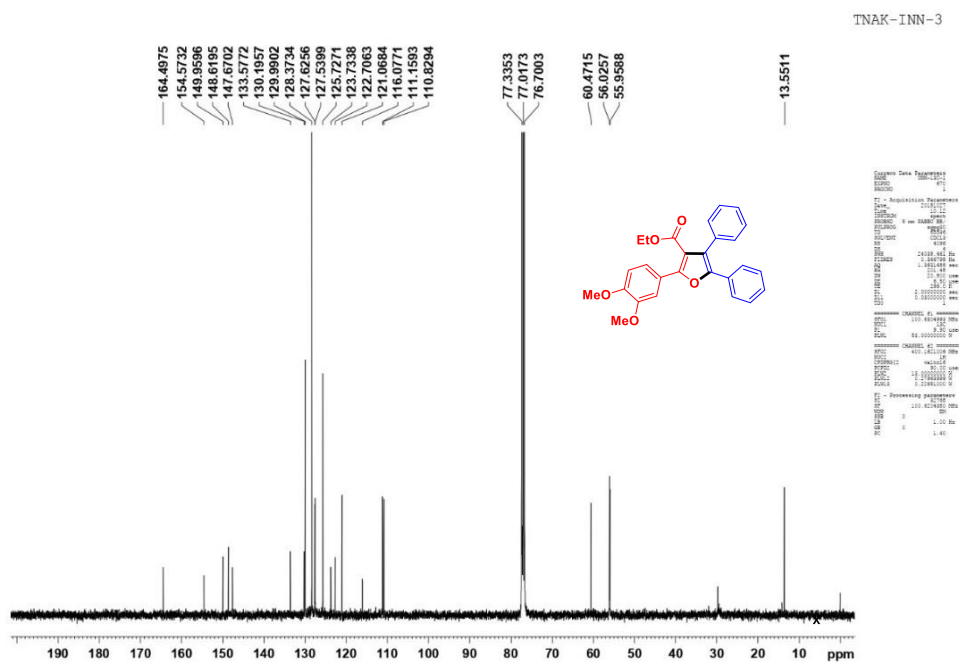
### HRMS spectrum of compound-3ic



### <sup>1</sup>H NMR spectrum of compound- 3ja (400 MHz, CDCl<sub>3</sub>); X= wax impurity

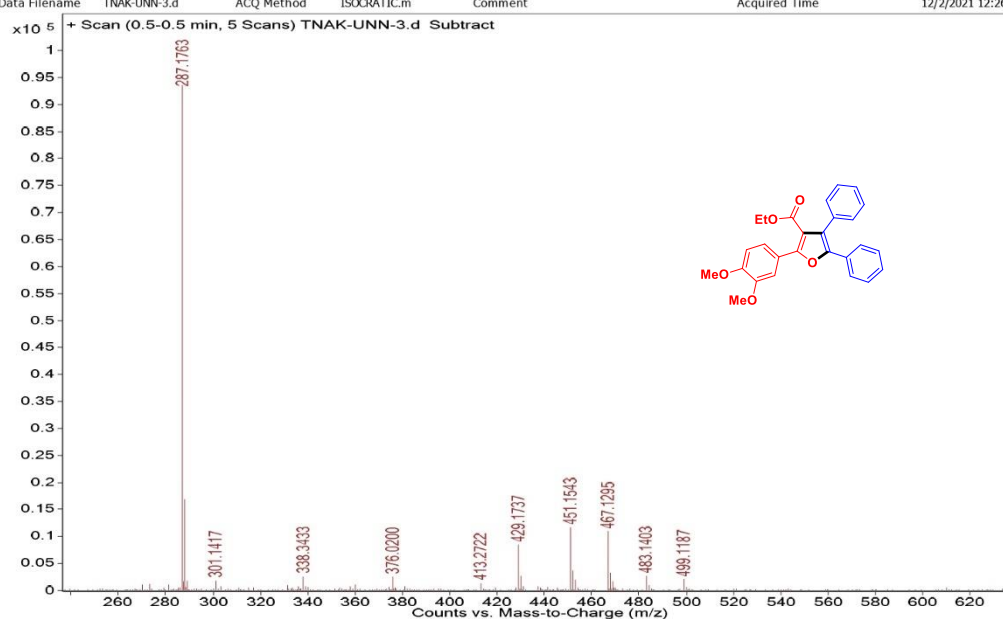


### <sup>13</sup>C NMR spectrum of compound- 3ja (100 MHz, CDCl<sub>3</sub>); X= wax impurity

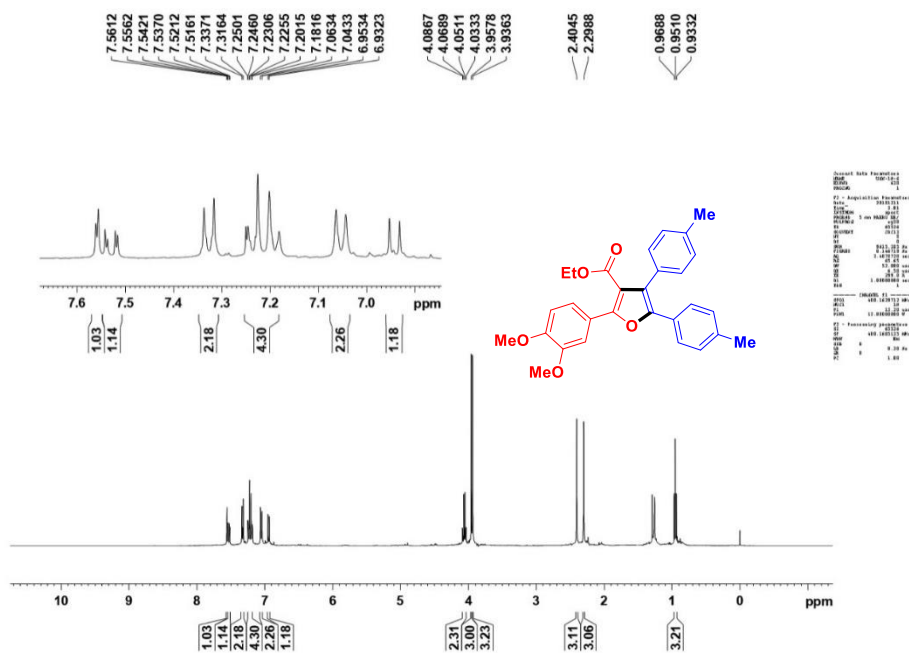


### HRMS spectrum of compound-3ja

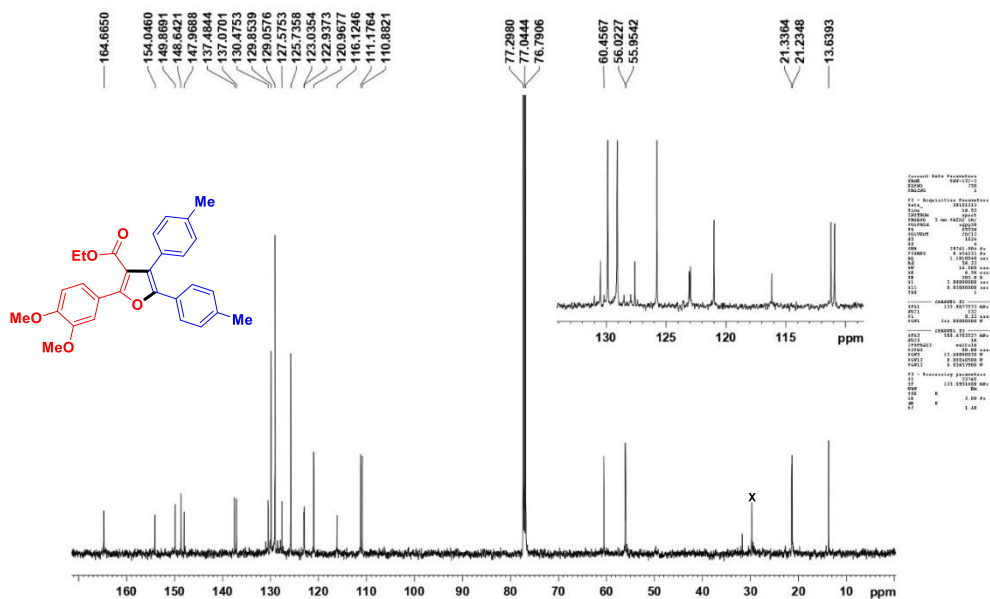
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Inj Vol	1	InjPosition		SampleType	Sample			
Data Filename	TNAK-UNN-3.d	ACQ Method	ISOCRATIC.m	Comment		Acquired Time		12/2/2021 12:26:49 PM



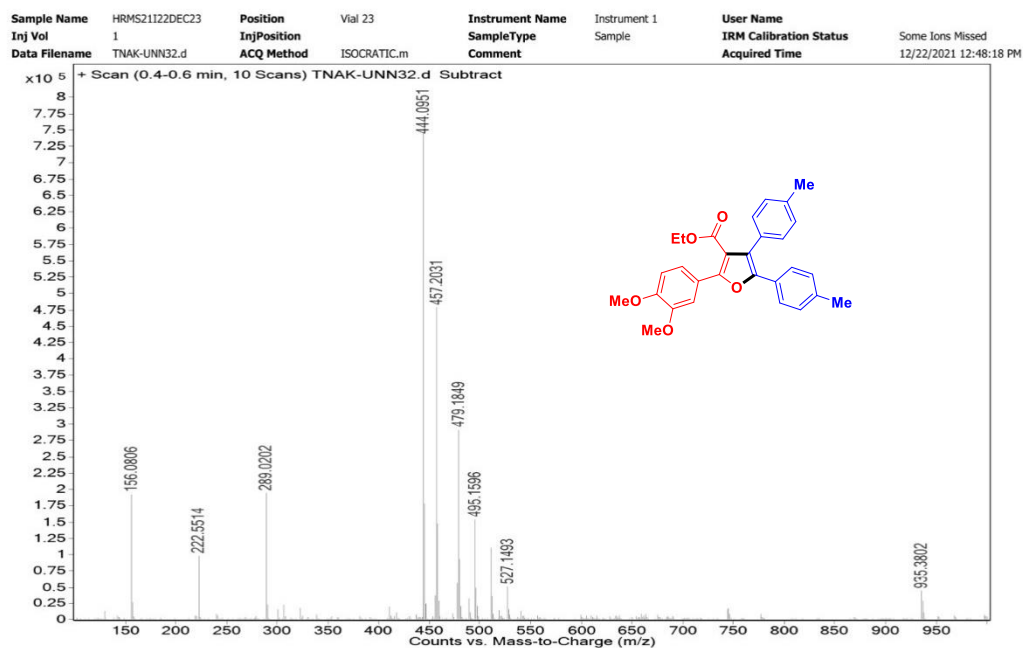
<sup>1</sup>H NMR spectrum of compound- 3jb (400 MHz, CDCl<sub>3</sub>);



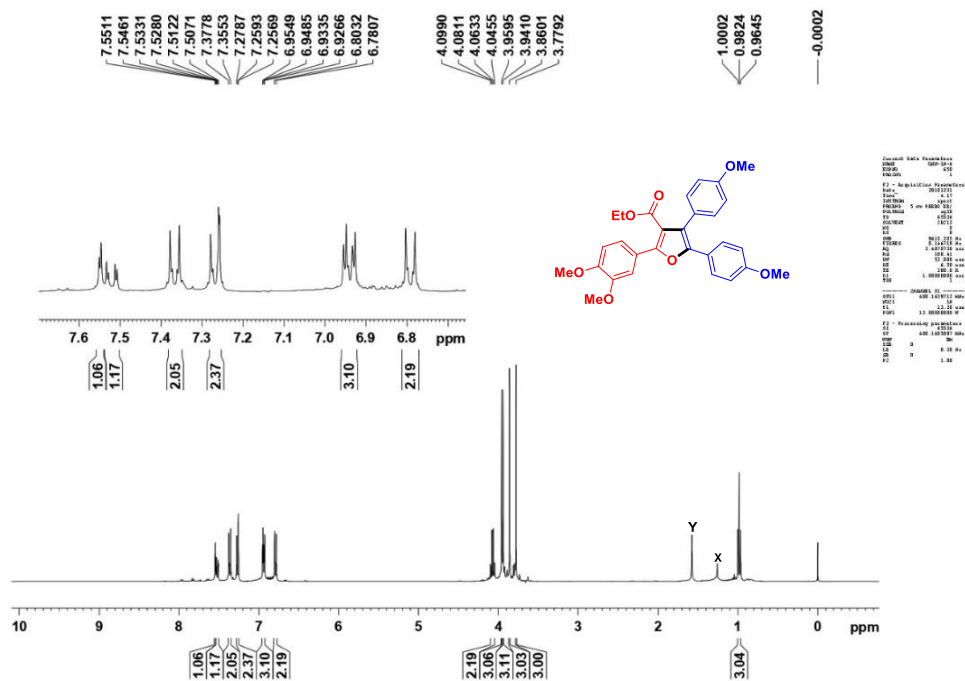
<sup>13</sup>C NMR spectrum of compound- 3jb (100 MHz, CDCl<sub>3</sub>); X= wax impurity



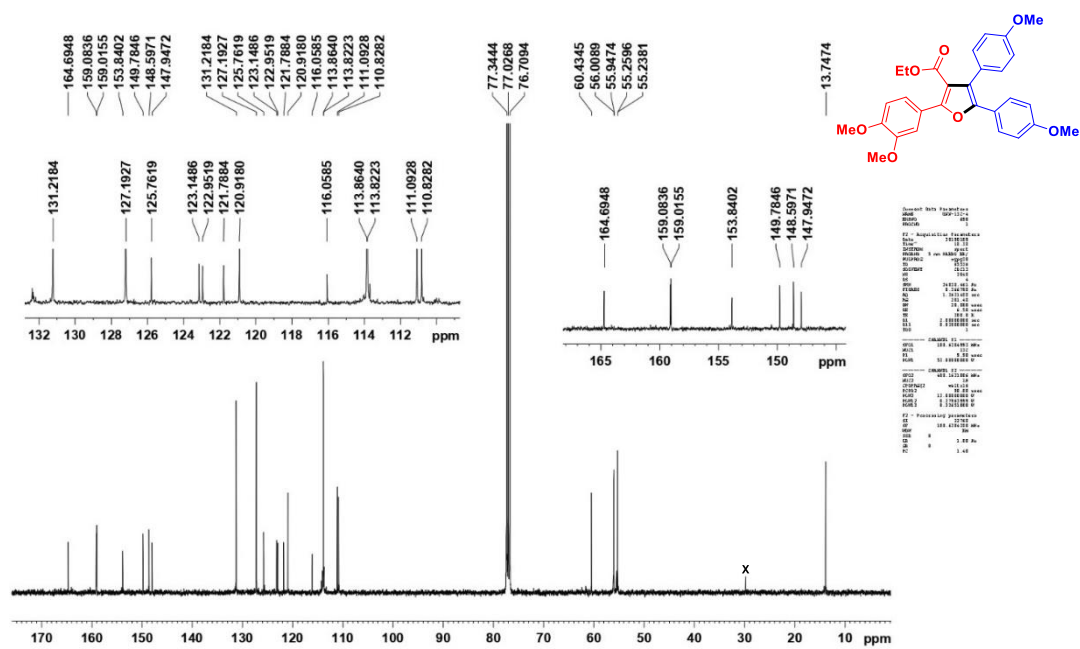
### HRMS spectrum of compound-3jb



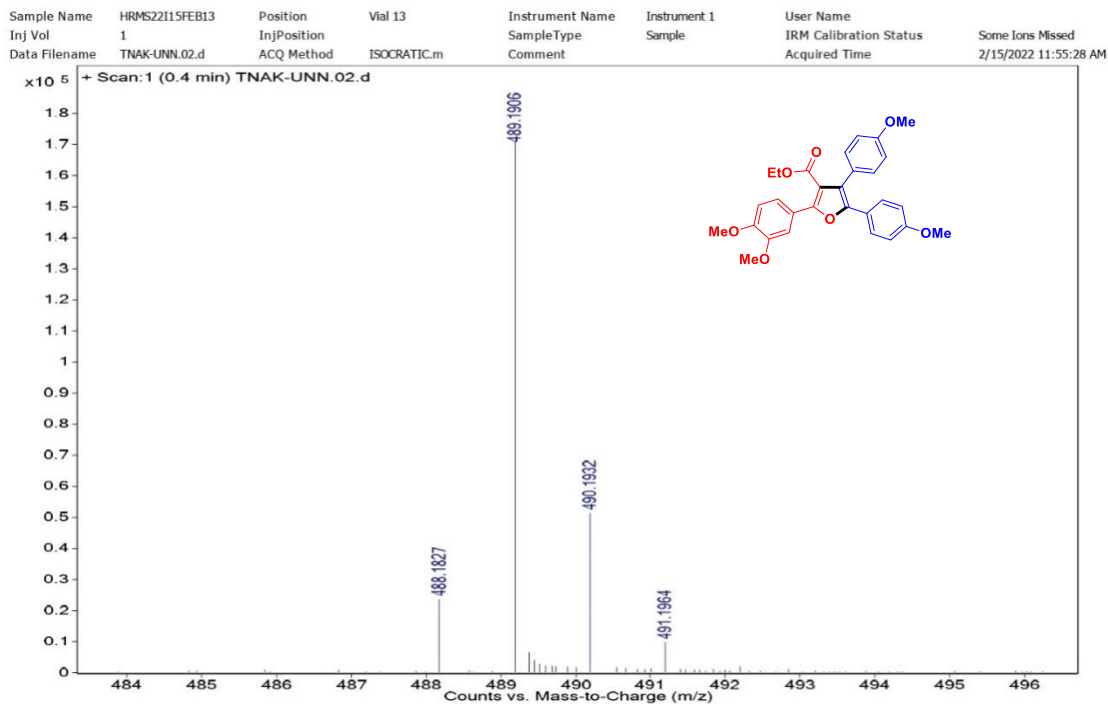
### <sup>1</sup>H NMR spectrum of compound- 3jc (400 MHz, CDCl<sub>3</sub>); X= wax impurity, Y = H<sub>2</sub>O



<sup>13</sup>C NMR spectrum of compound- 3jc (100 MHz, CDCl<sub>3</sub>); X= wax impurity

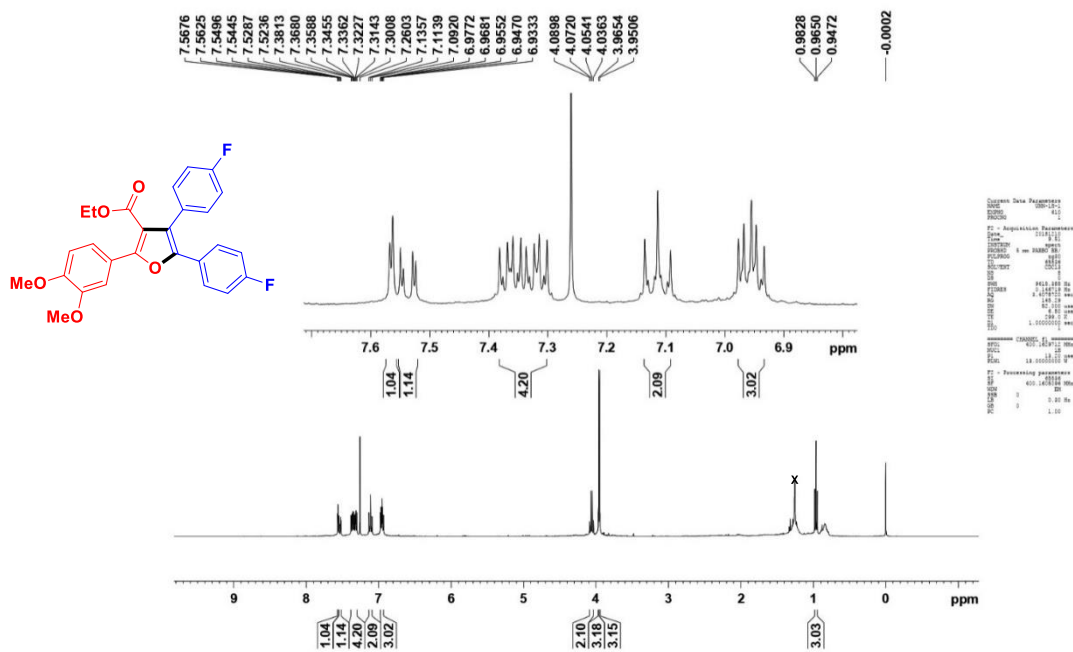


HRMS spectrum of compound-3jc

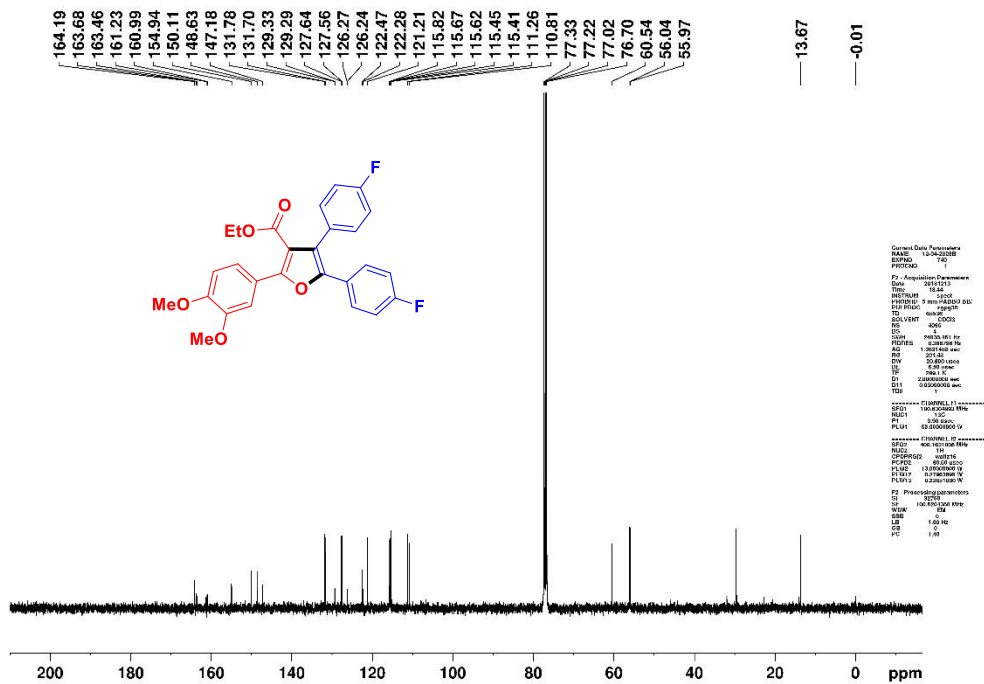




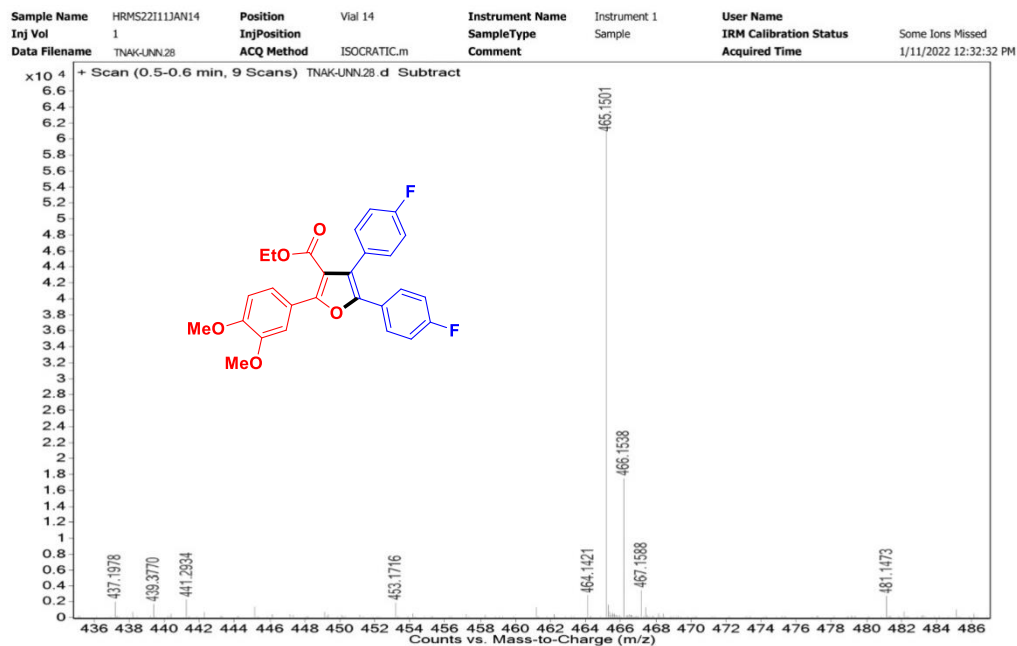
<sup>1</sup>H NMR spectrum of compound- 3jd (400 MHz, CDCl<sub>3</sub>); X= wax impurity



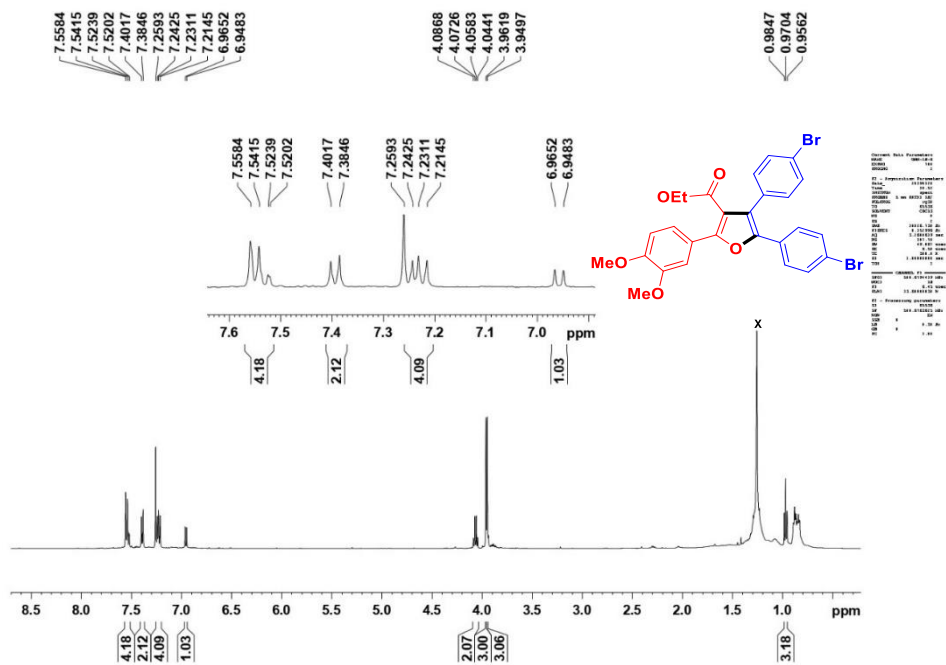
<sup>13</sup>C NMR spectrum of compound- 3jd (100 MHz, CDCl<sub>3</sub>)



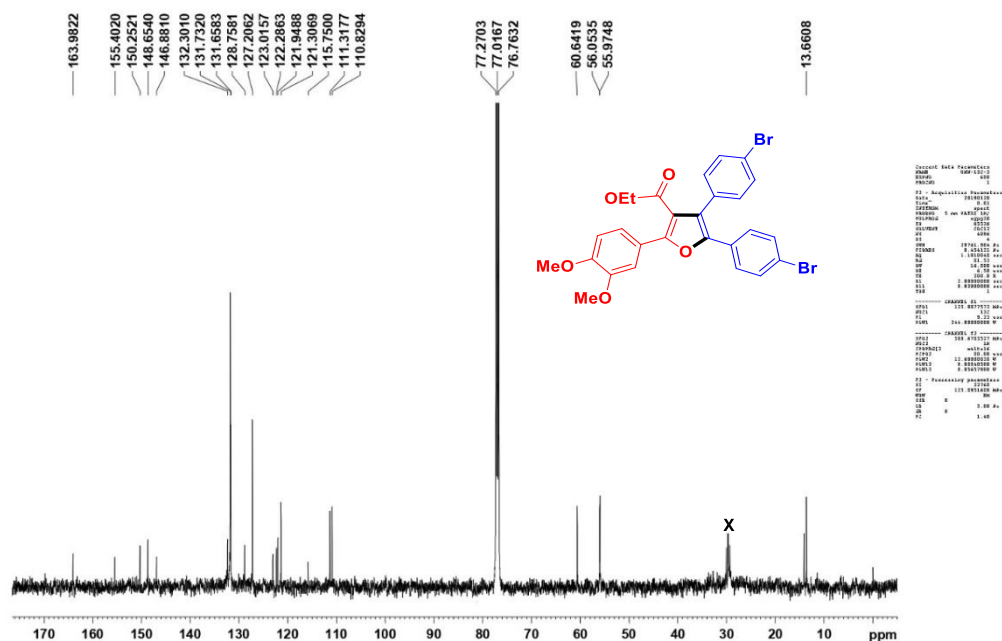
## HRMS spectrum of compound-3jd



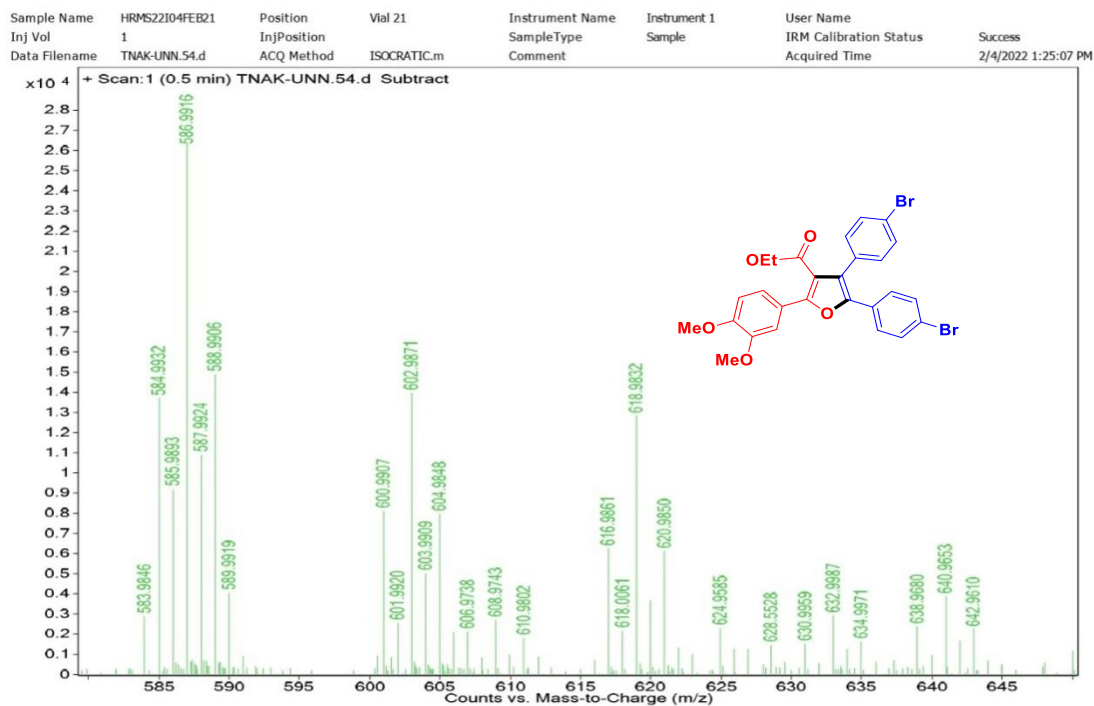
## <sup>1</sup>H NMR spectrum of compound- 3jf (400 MHz, CDCl<sub>3</sub>); X= wax impurity



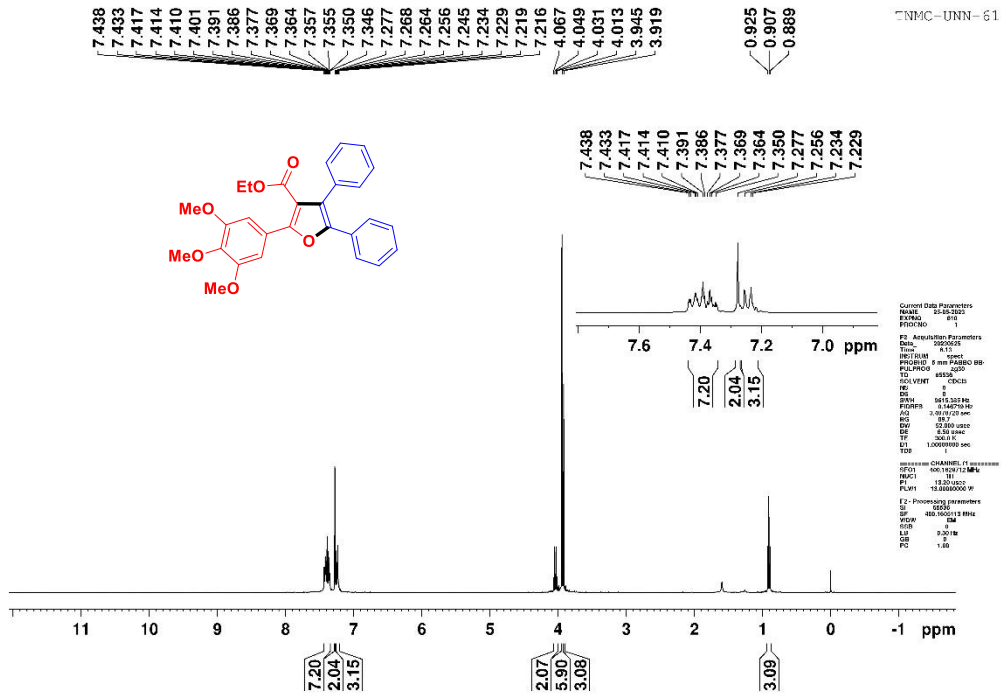
<sup>13</sup>C NMR spectrum of compound- 3jf (100 MHz, CDCl<sub>3</sub>); X= wax impurity



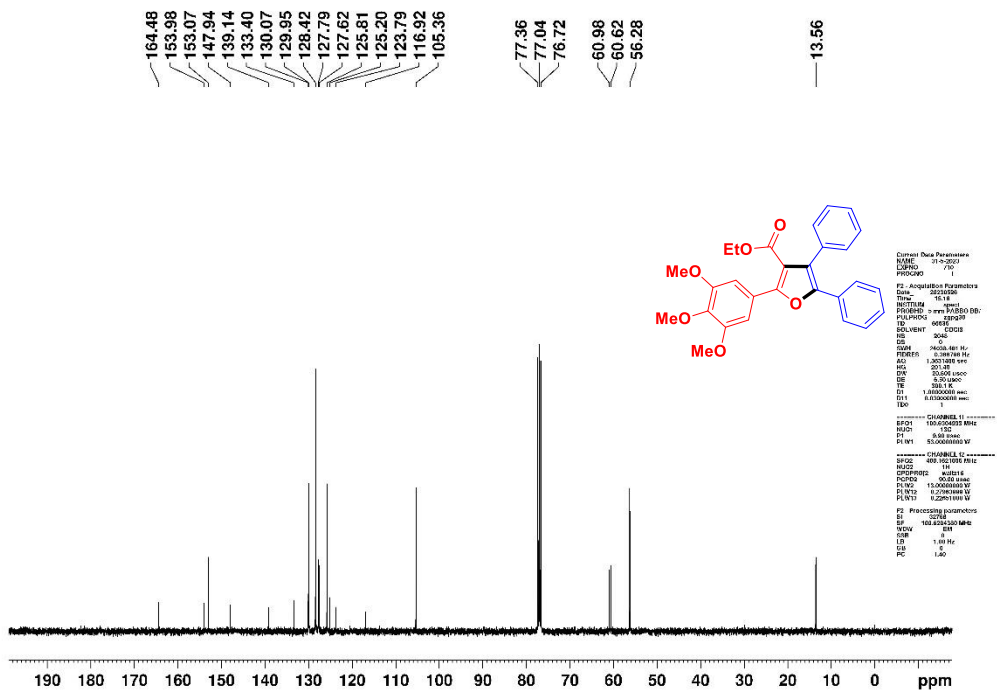
HRMS spectrum of compound-3jf



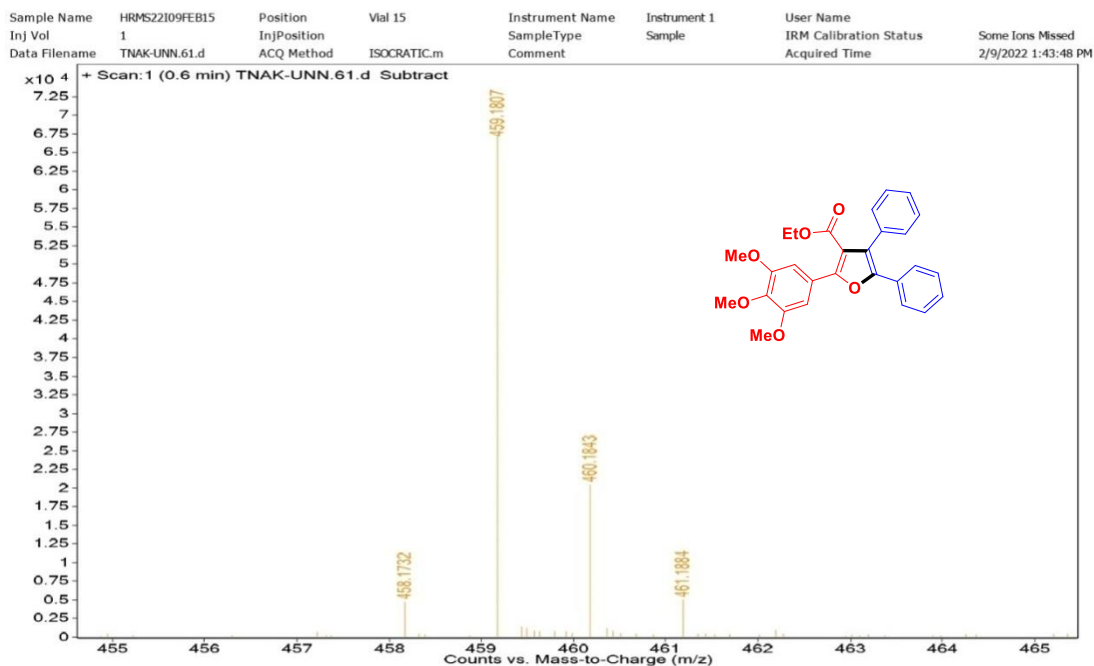
<sup>1</sup>H NMR spectrum of compound- 3ka (400 MHz, CDCl<sub>3</sub>)



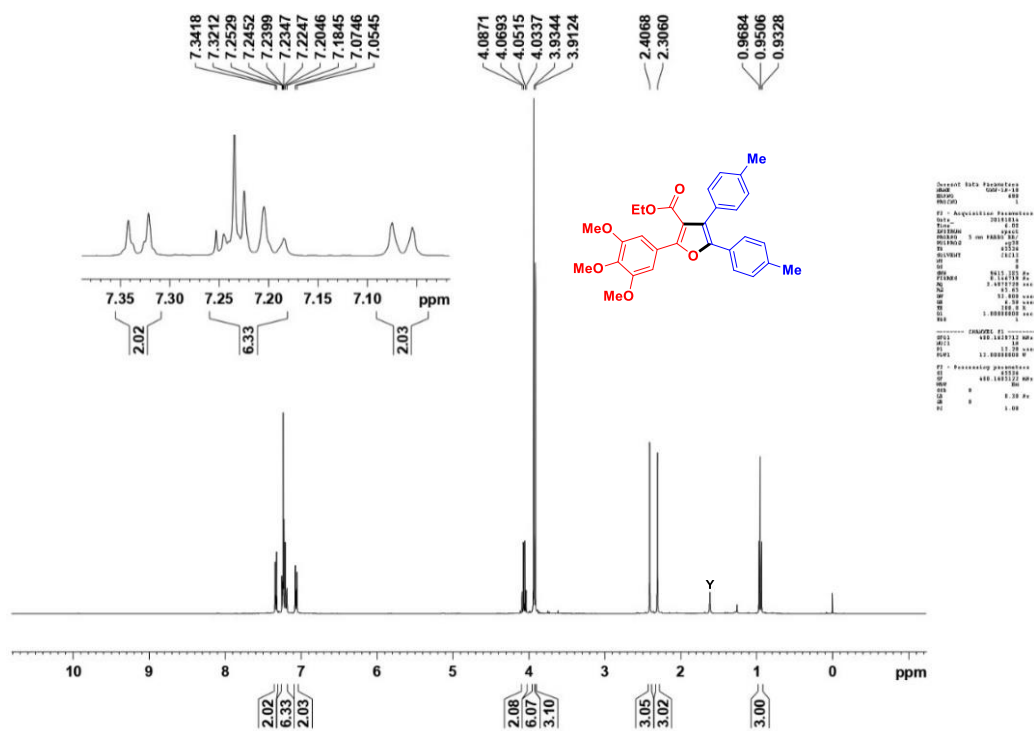
<sup>13</sup>C NMR spectrum of compound- 3ka (100 MHz, CDCl<sub>3</sub>);



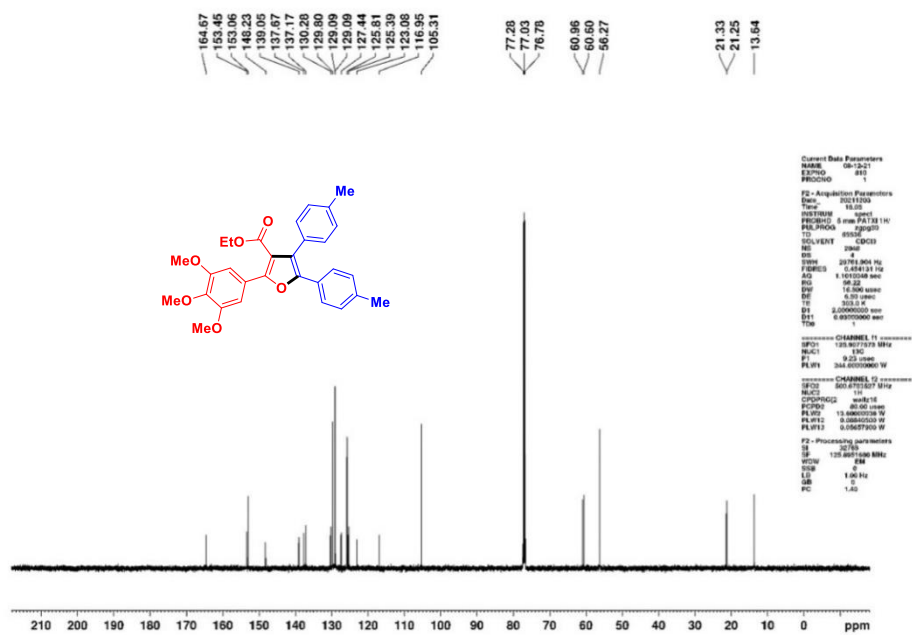
### HRMS spectrum of compound-3ka



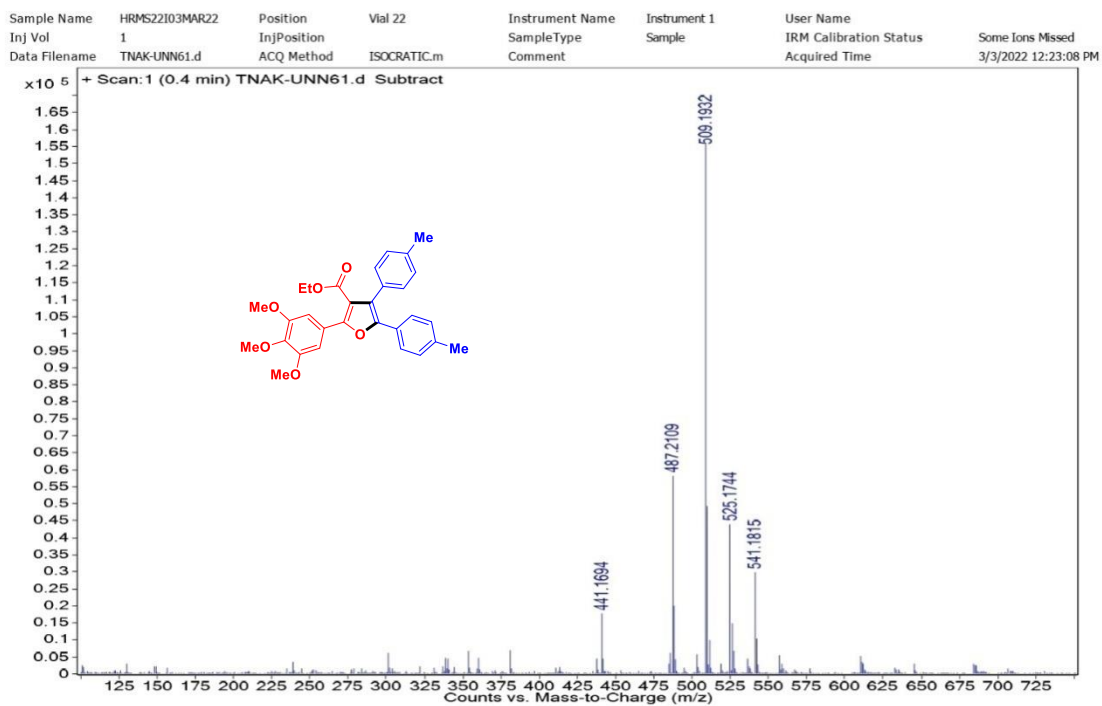
### <sup>1</sup>H NMR spectrum of compound- 3kb (400 MHz, CDCl<sub>3</sub>); Y=H<sub>2</sub>O impurity



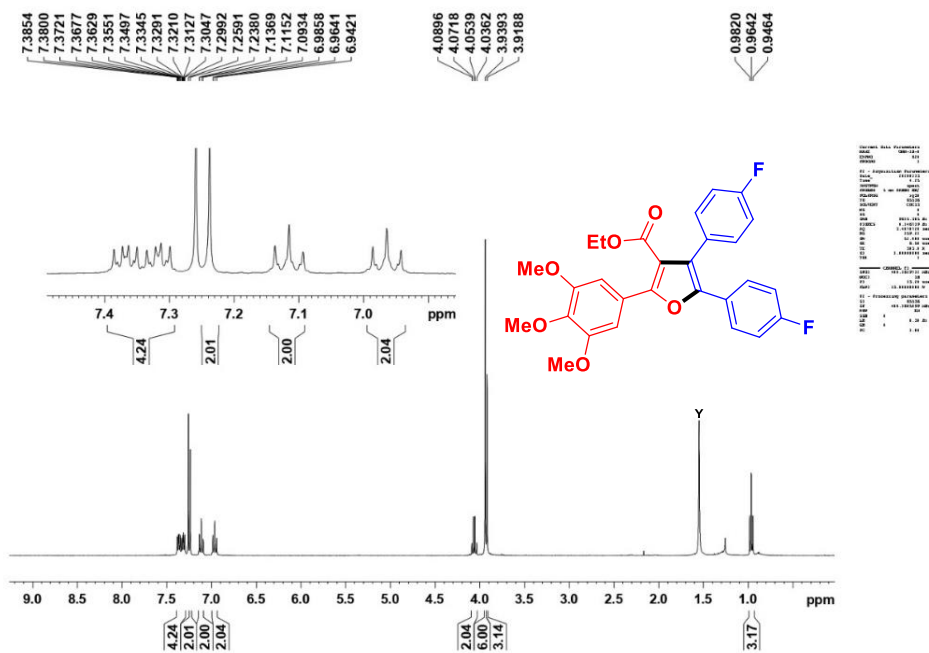
### <sup>13</sup>C NMR spectrum of compound- 3kb (100 MHz, CDCl<sub>3</sub>)



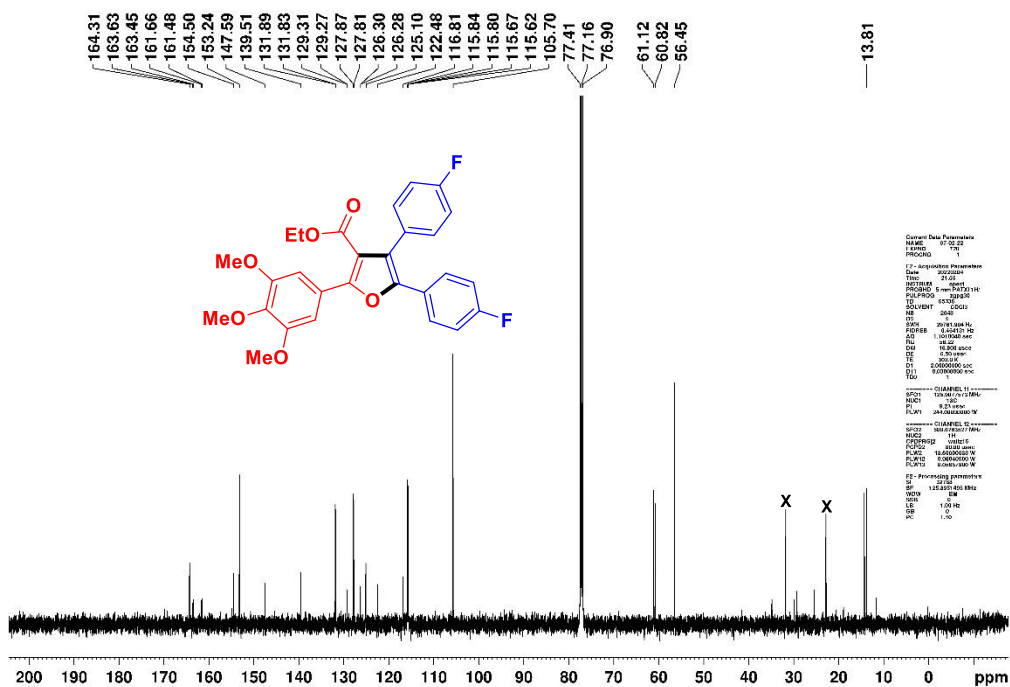
### HRMS spectrum of compound-3kb



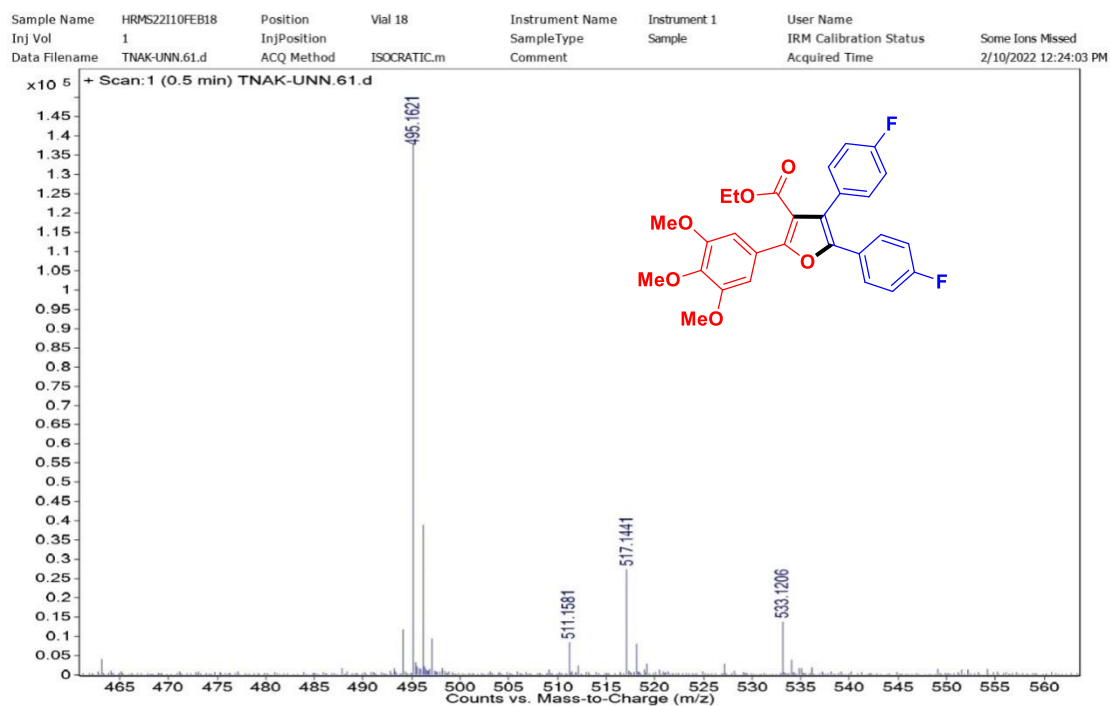
<sup>1</sup>H NMR spectrum of compound- 3kd (400 MHz, CDCl<sub>3</sub>); Y=H<sub>2</sub>O impurity



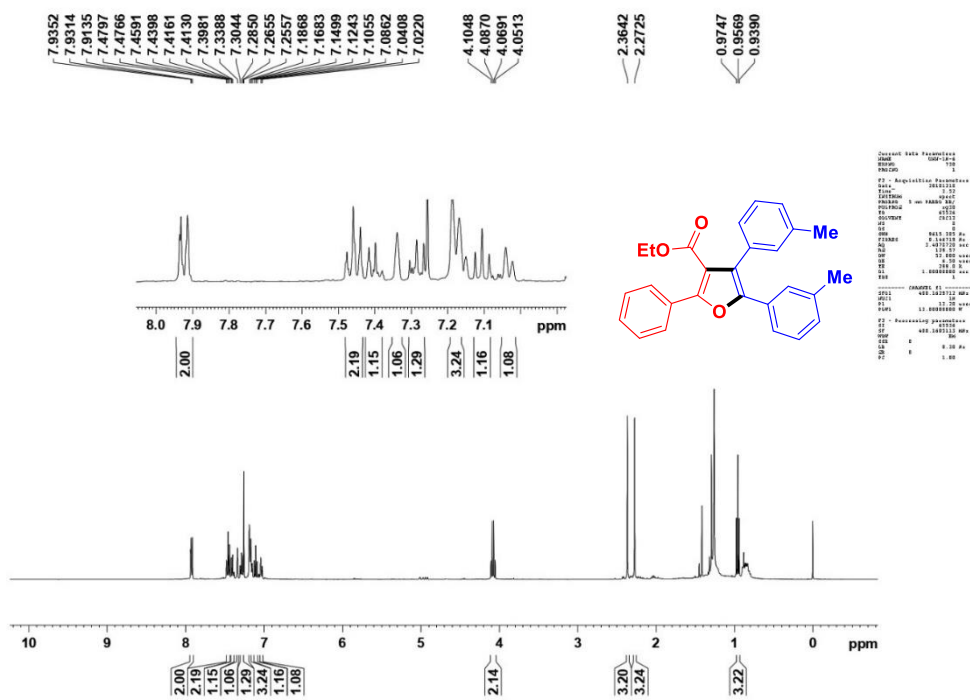
<sup>13</sup>C NMR spectrum of compound- 3kd (100 MHz, CDCl<sub>3</sub>)



### HRMS spectrum of compound-3kd

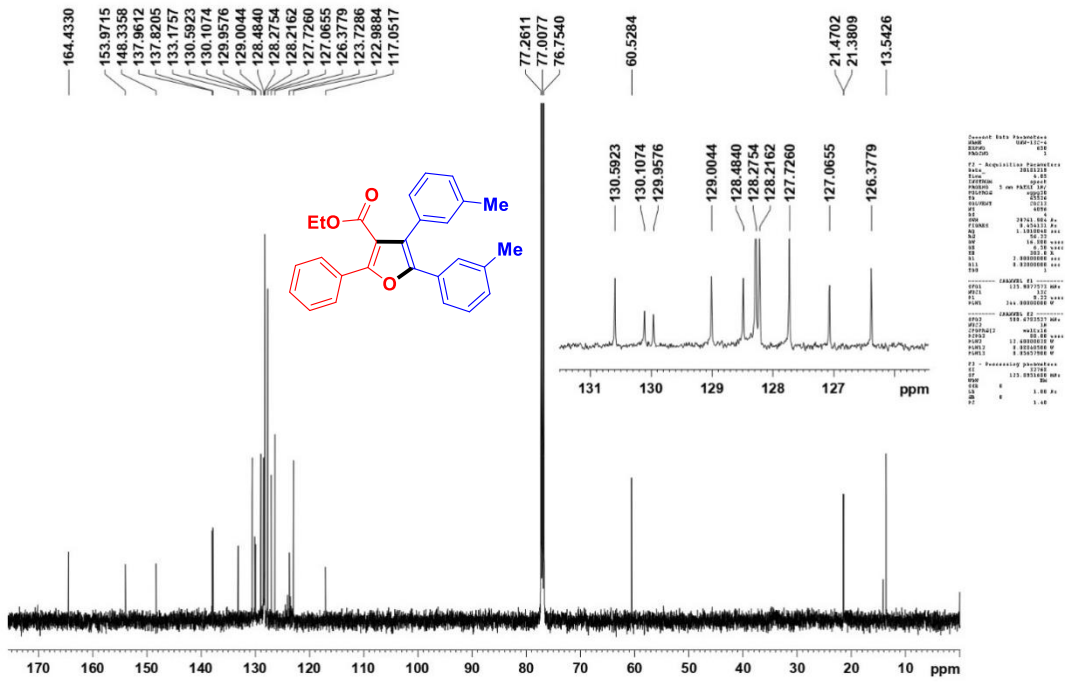


### <sup>1</sup>H NMR spectrum of compound- 3ag (400 MHz, CDCl<sub>3</sub>);

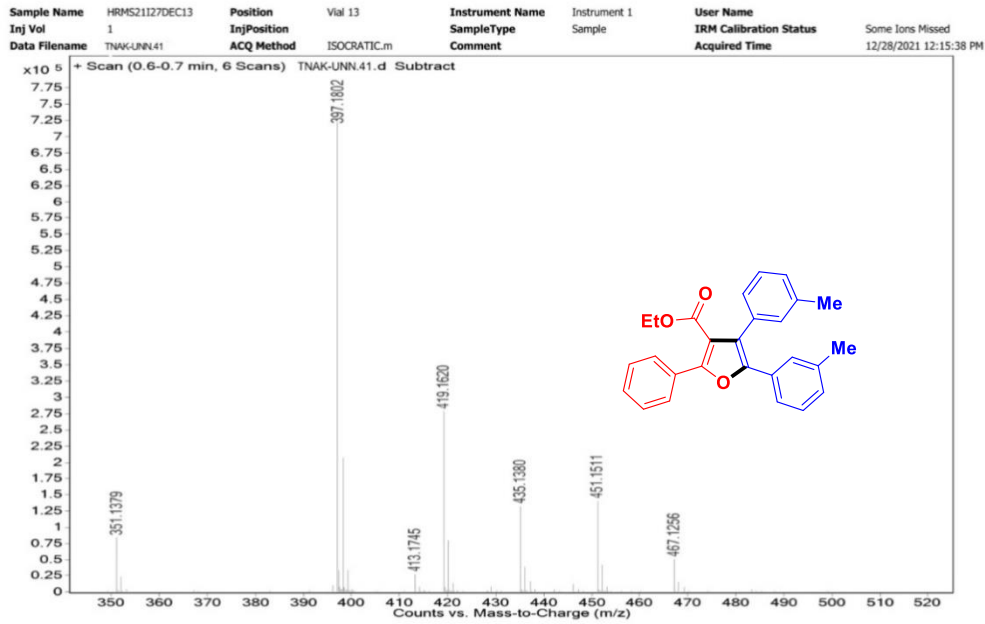




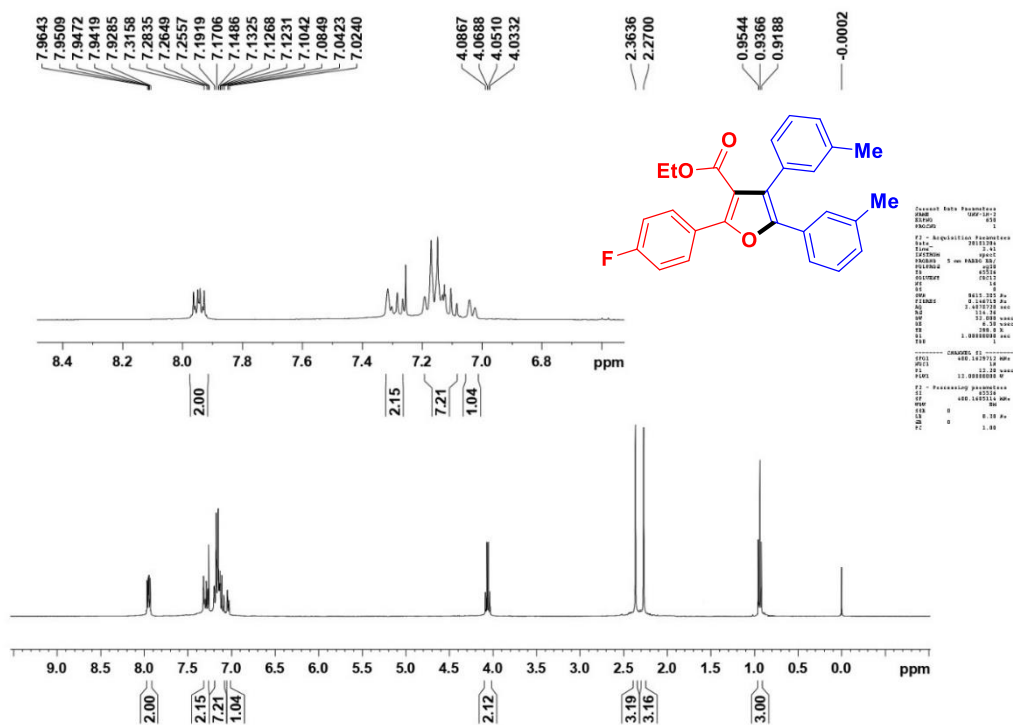
**<sup>13</sup>C NMR spectrum of compound- 3ag (100 MHz, CDCl<sub>3</sub>)**



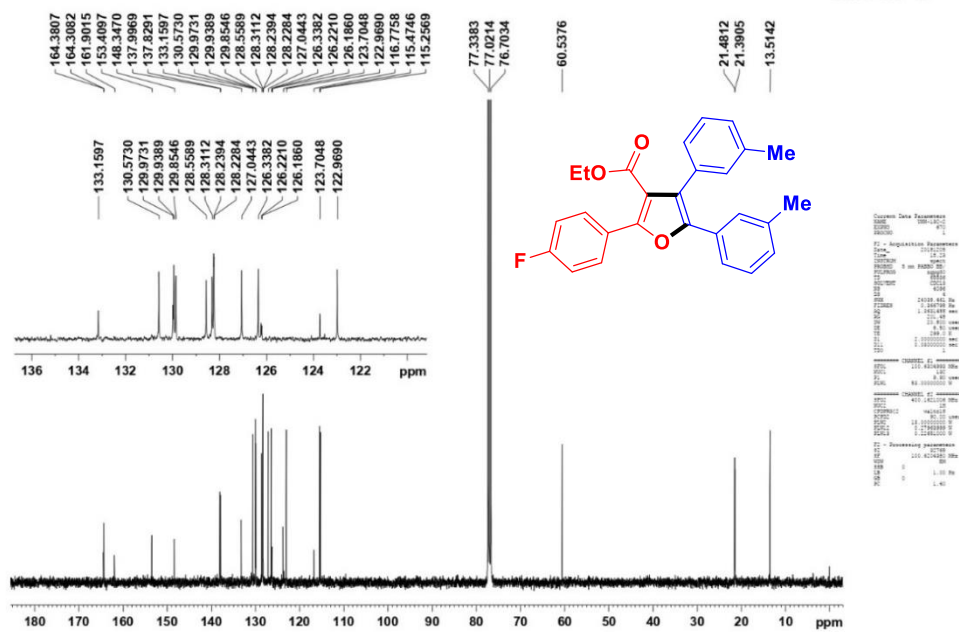
**HRMS spectrum of compound-3ag**



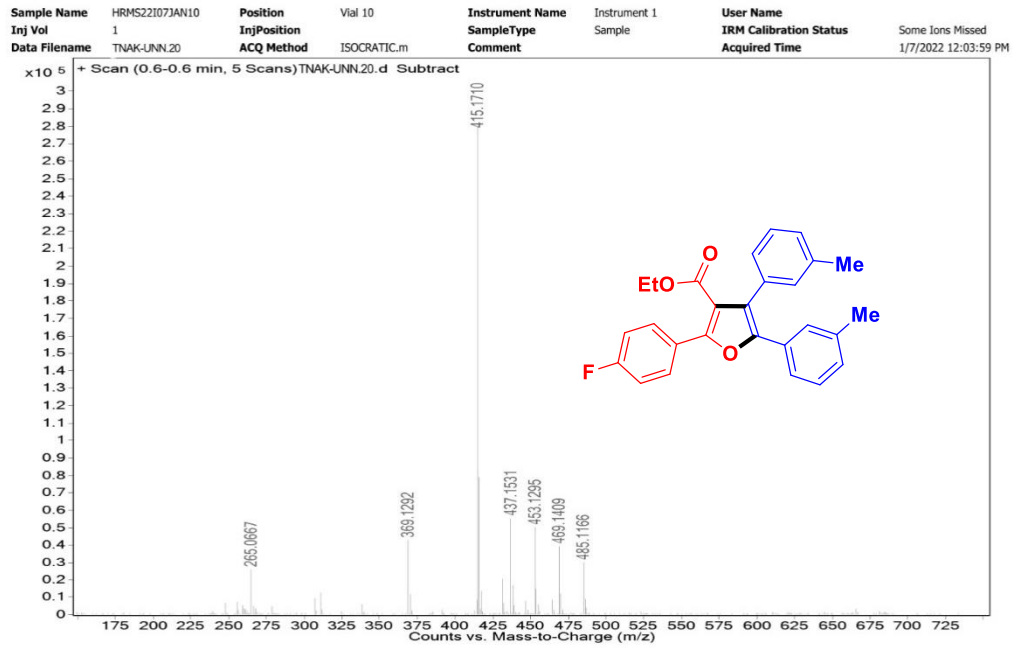
**$^1\text{H}$  NMR spectrum of compound- 3gg (400 MHz,  $\text{CDCl}_3$ )**



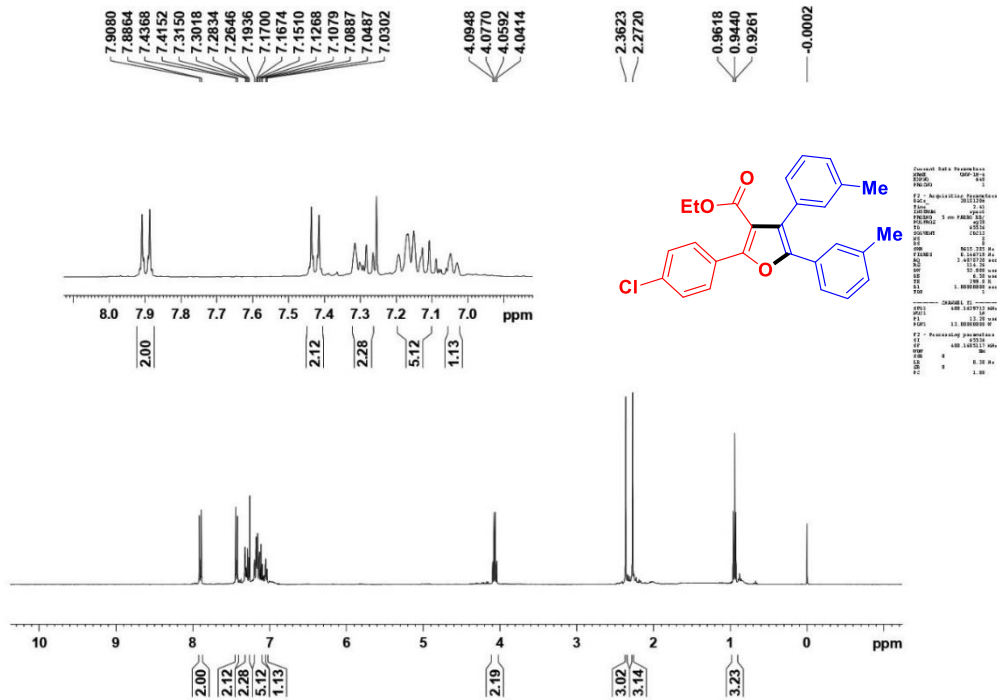
**$^{13}\text{C}$  NMR spectrum of compound- 3gg (100 MHz,  $\text{CDCl}_3$ )**



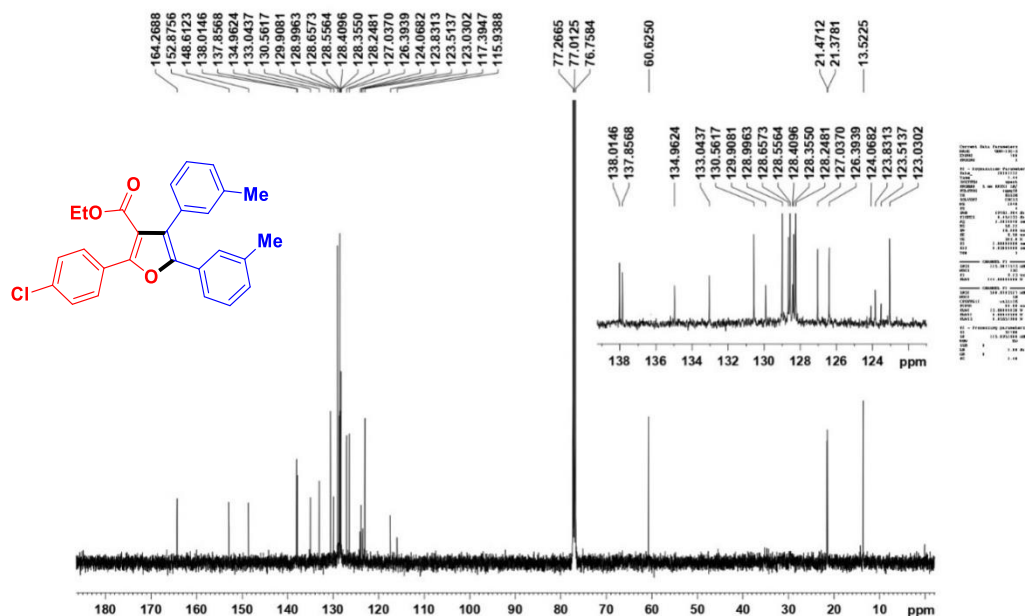
### HRMS spectrum of compound-3gg



### <sup>1</sup>H NMR spectrum of compound- 3hg (400 MHz, CDCl<sub>3</sub>)

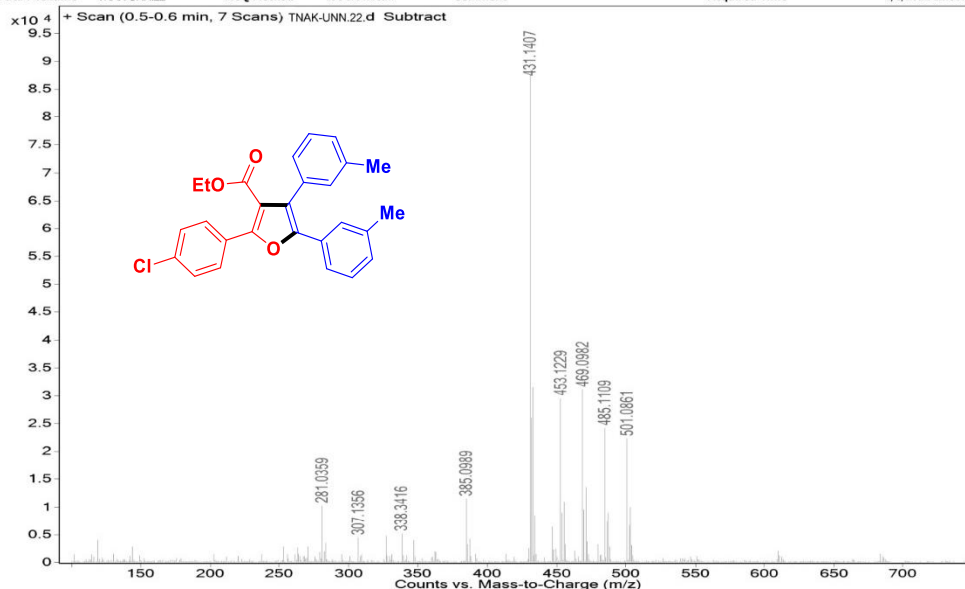


<sup>13</sup>C NMR spectrum of compound- 3hg (100 MHz, CDCl<sub>3</sub>)

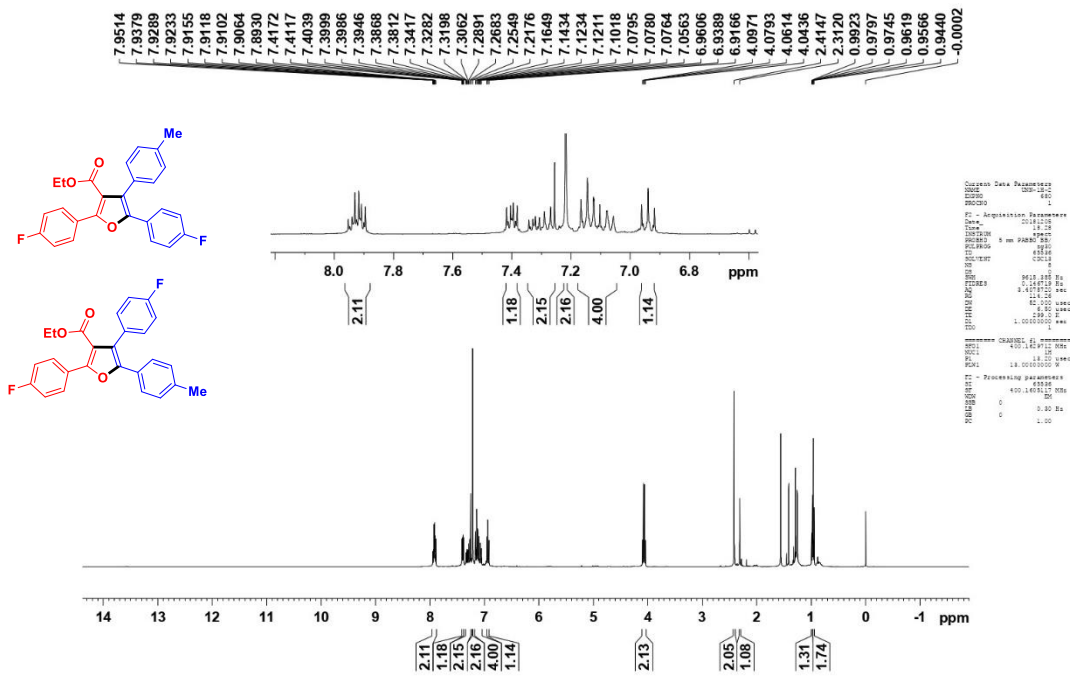


HRMS spectrum of compound-3hg

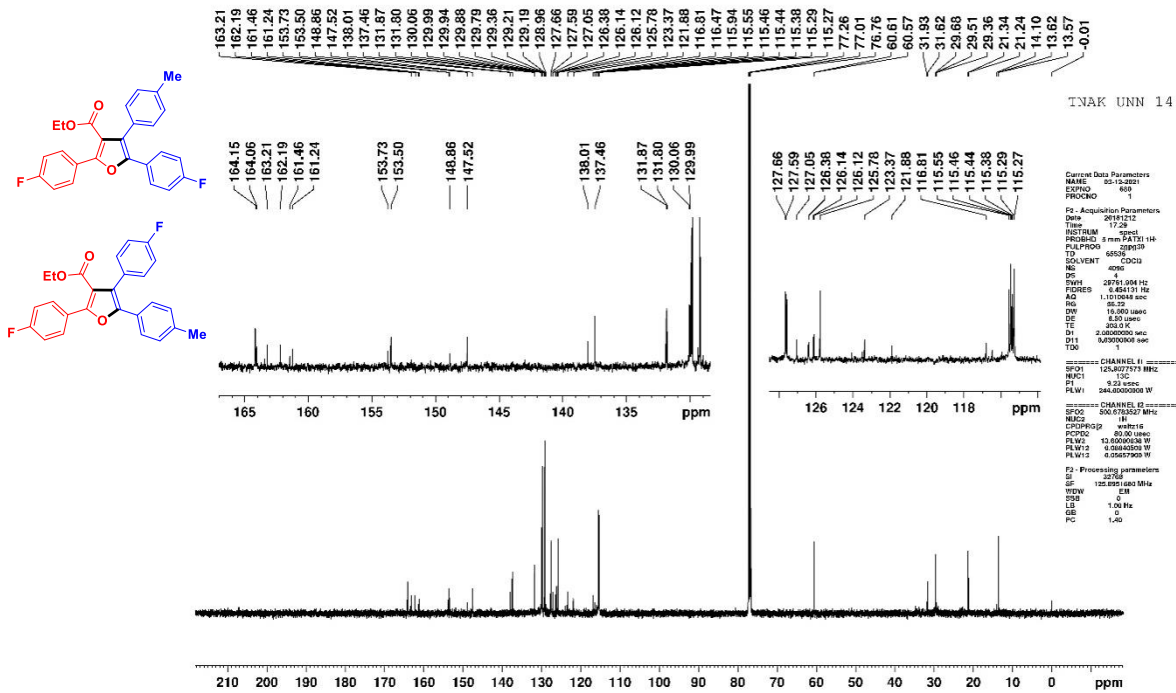
Sample Name	HRMS22106JAN21	Position	Vial 21	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
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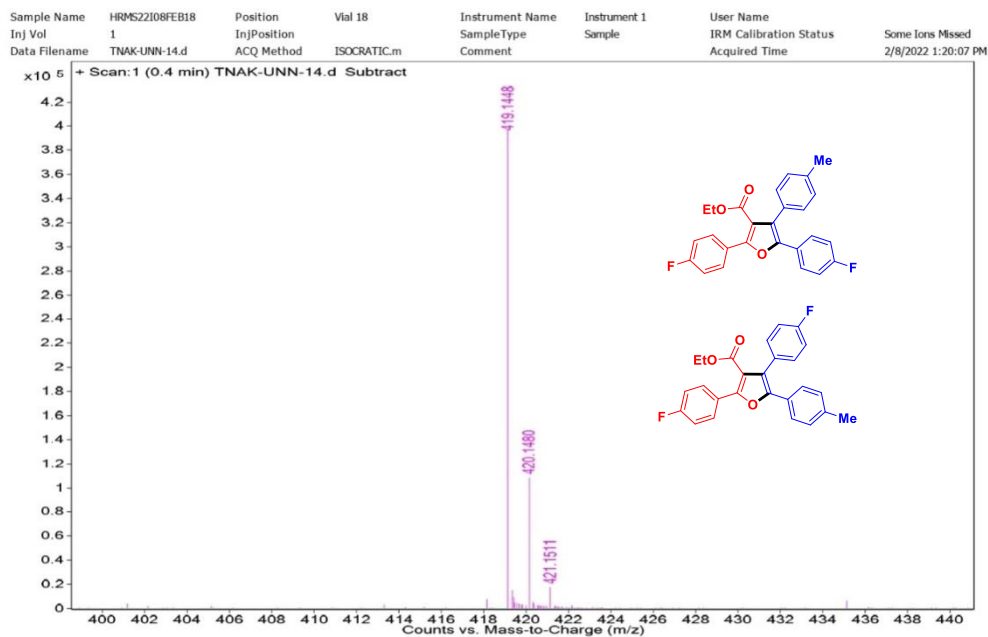
<sup>1</sup>H NMR spectrum of compound- 3gh (400 MHz, CDCl<sub>3</sub>)



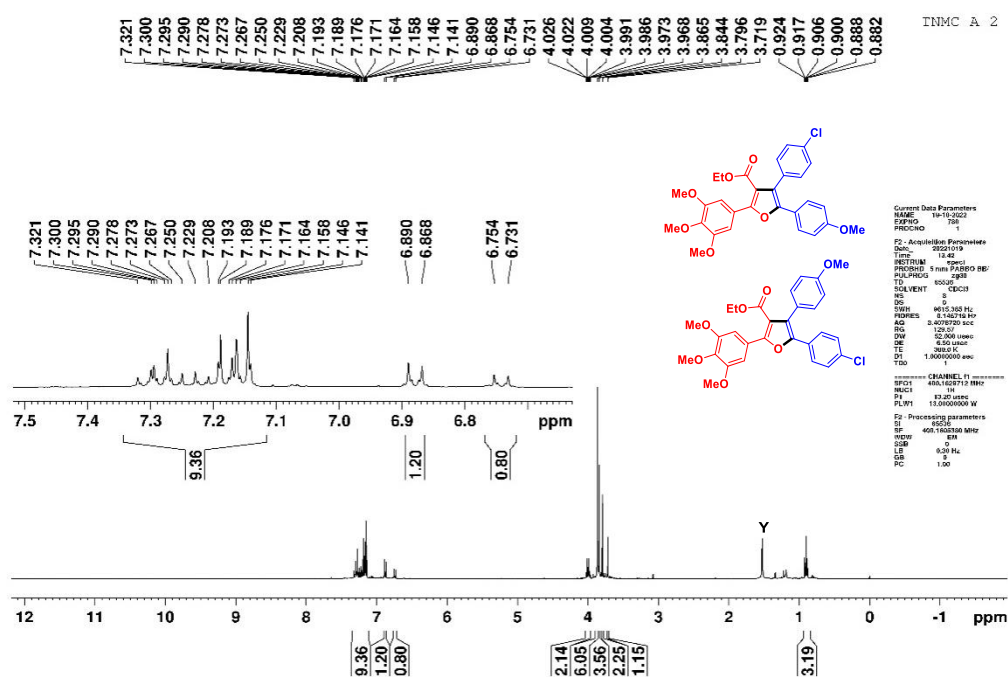
<sup>13</sup>C NMR spectrum of compound- 3gh (100 MHz, CDCl<sub>3</sub>)



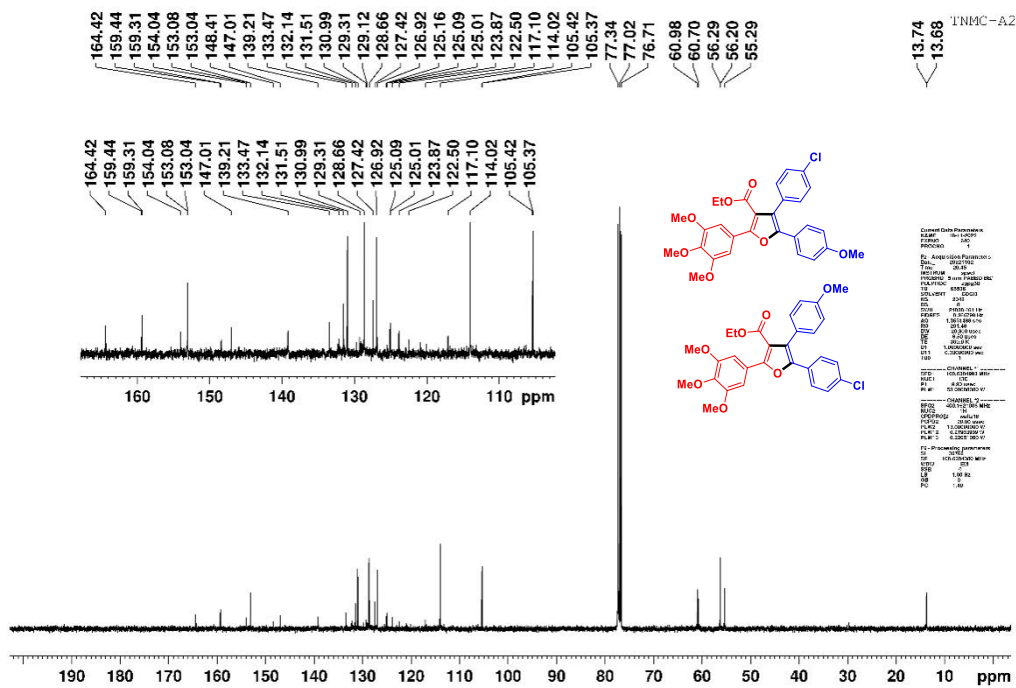
## HRMS spectrum of compound-3gh



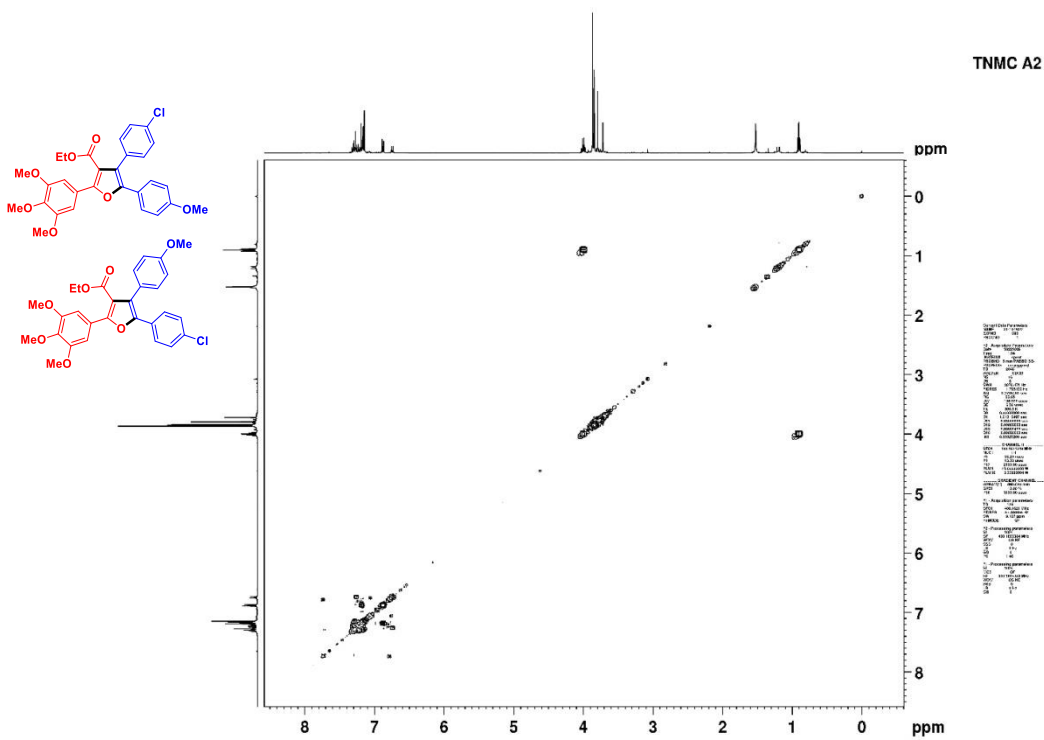
## <sup>1</sup>H NMR spectrum of compound- 3ki (400 MHz, CDCl<sub>3</sub>); Y=H<sub>2</sub>O impurity



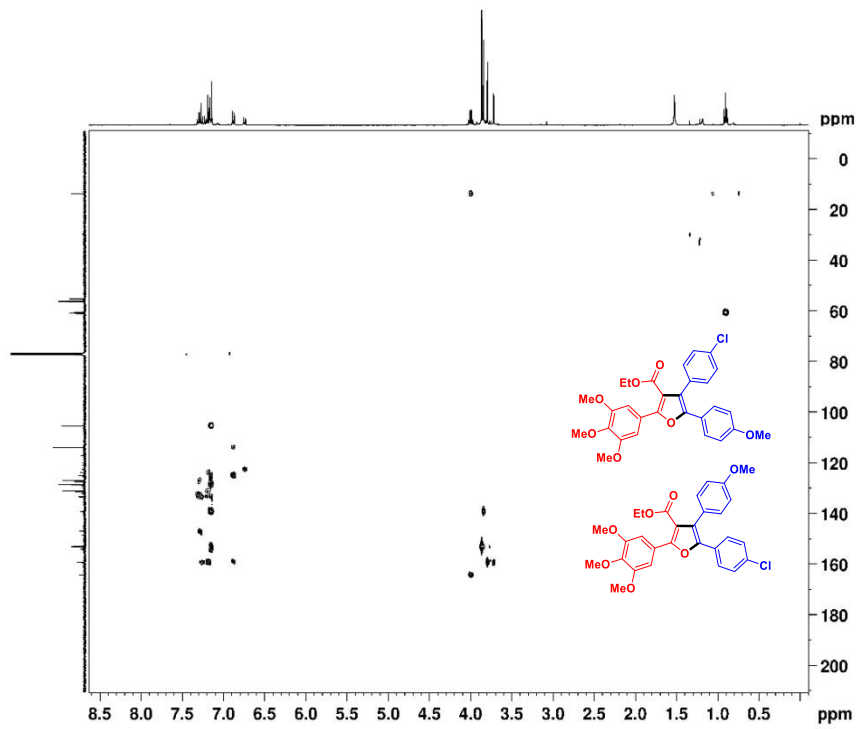
<sup>13</sup>C NMR spectrum of compound- 3ki (100 MHz, CDCl<sub>3</sub>)



Cosy spectrum of compound – 3ki



### HMBC SPECTRUM OF COMPOUND – 3ki

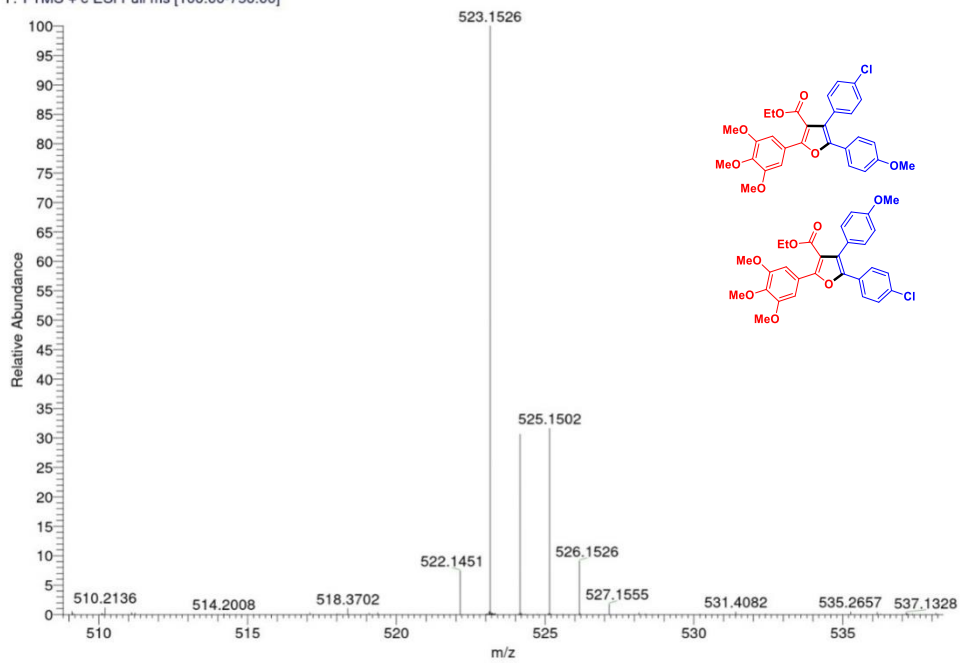


### HRMS SPECTRUM OF COMPOUND-3ki

D:\internals 2022\...\HRMS22121OCT19

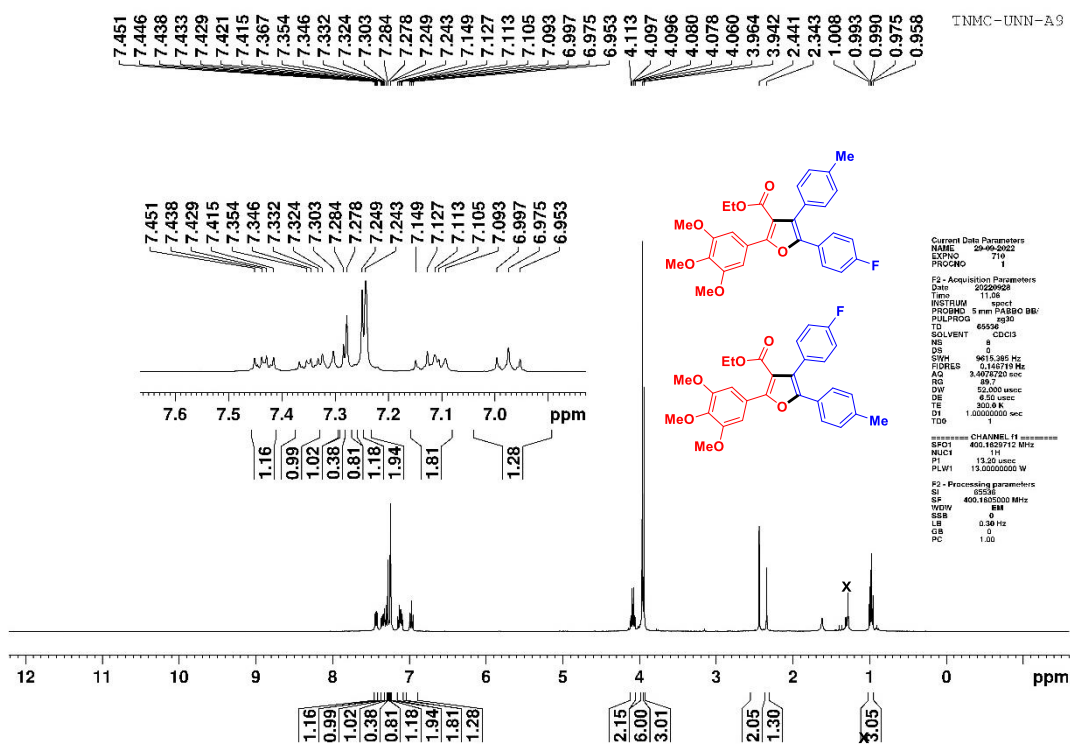
10/21/2022 1:15:00 PM

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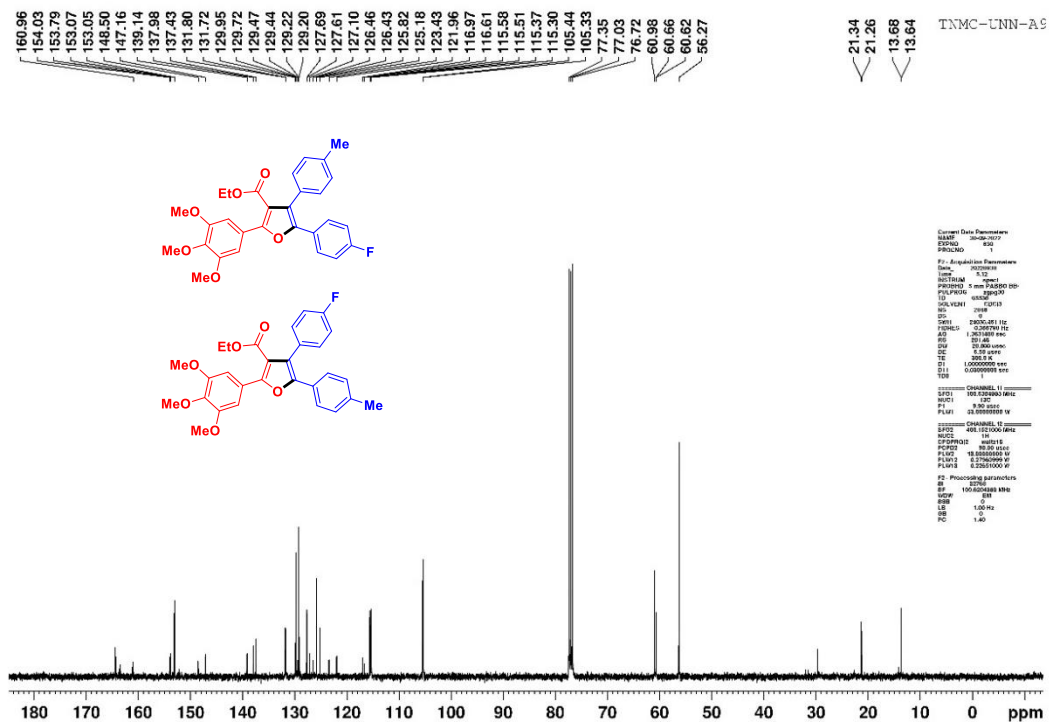




<sup>1</sup>H NMR spectrum of compound- 3kh (400 MHz, CDCl<sub>3</sub>); X= wax impurity



<sup>13</sup>C NMR spectrum of compound- 3kh (400 MHz, CDCl<sub>3</sub>); X= wax impurity

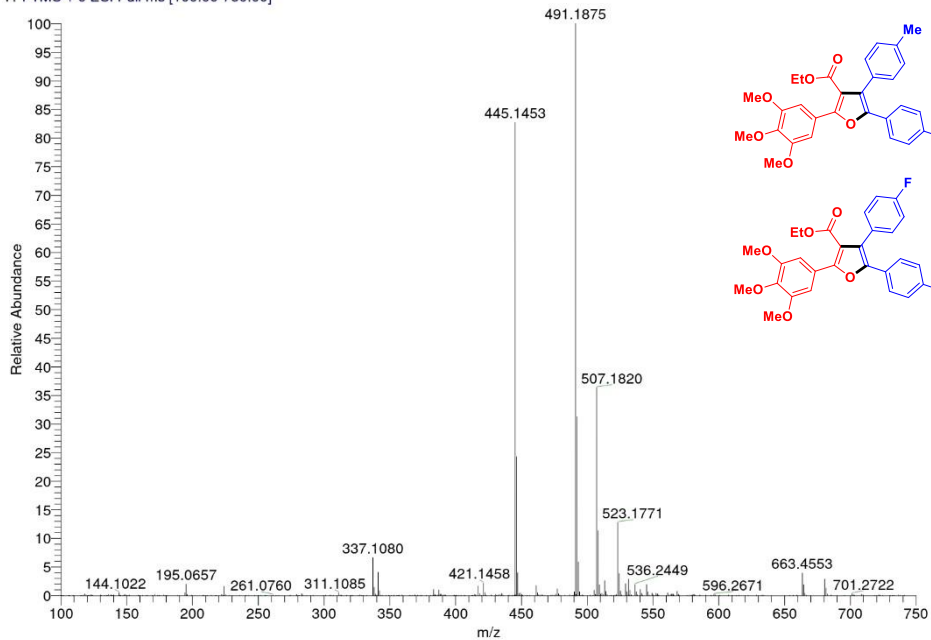


# HRMS SPECTRUM OF COMPOUND-3kh

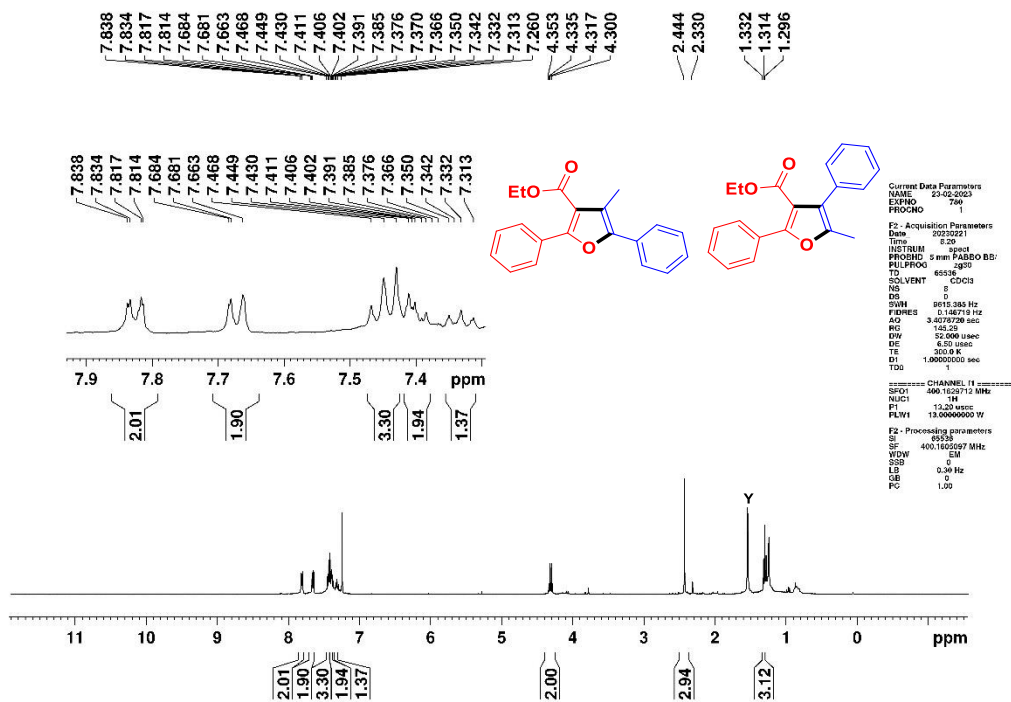
D:\Internals 2022\...HRMS22121OCT20

10/21/2022 1:16:56 PM

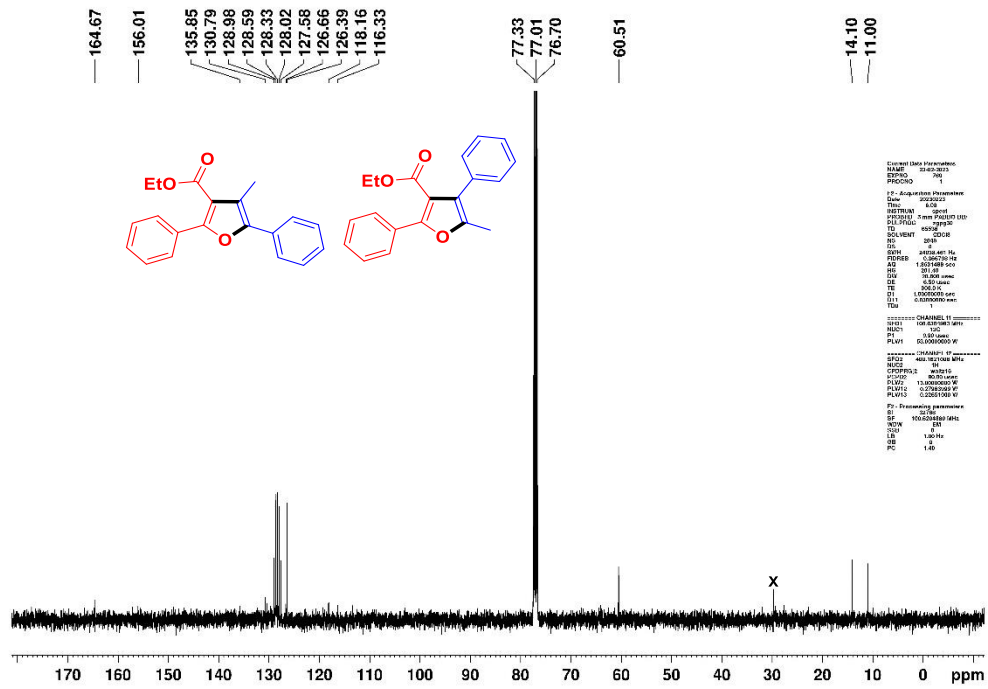
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T: FTMS + c ESI Full ms [100.00-750.00]



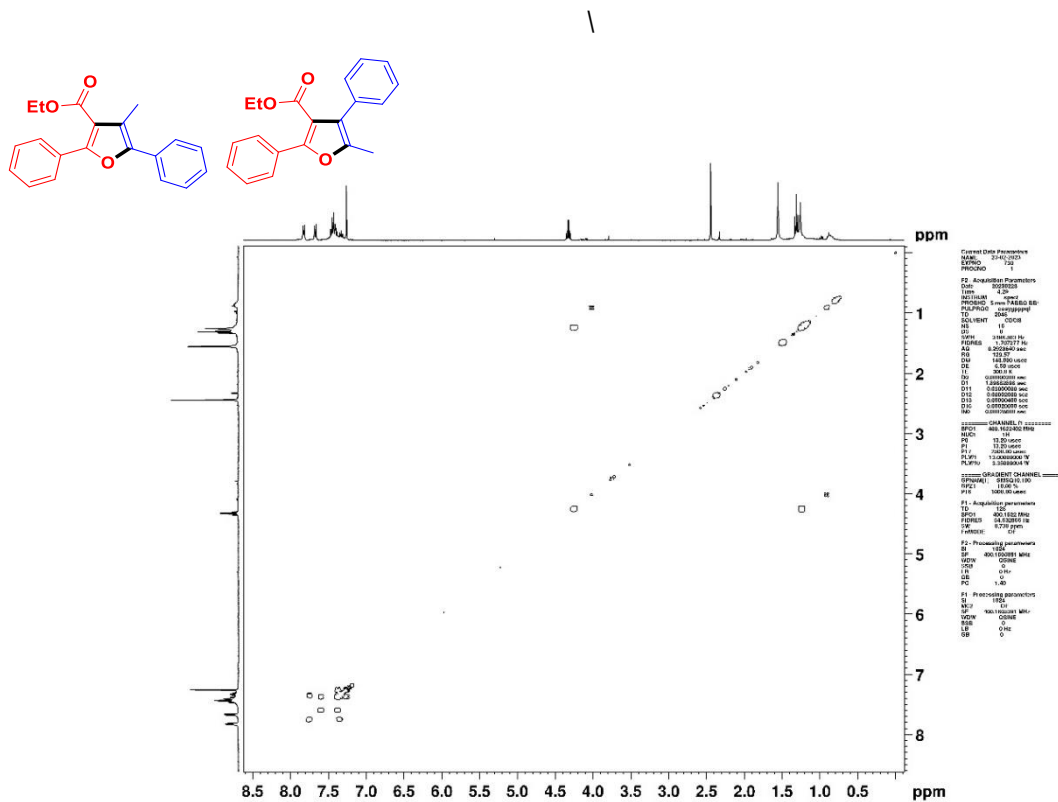
## <sup>1</sup>H NMR spectrum of compound- 3aj (400 MHz, CDCl<sub>3</sub>); Y=H<sub>2</sub>O impurity



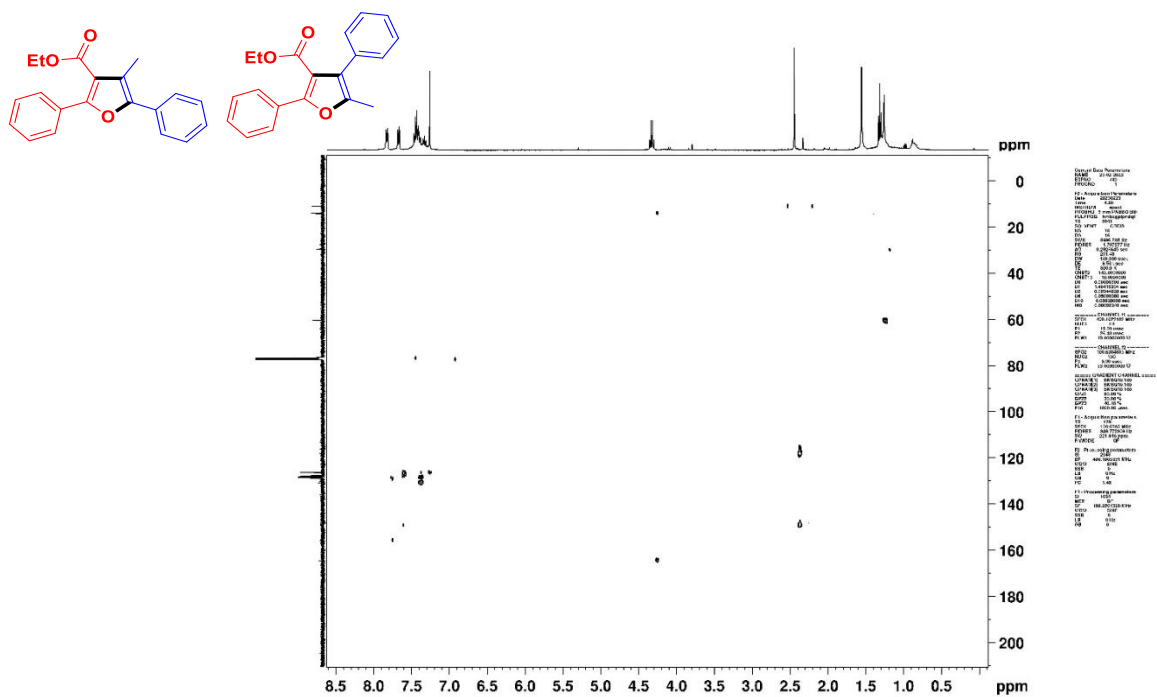
<sup>13</sup>C NMR spectrum of compound- 3aj (100 MHz, CDCl<sub>3</sub>); X= wax impurity



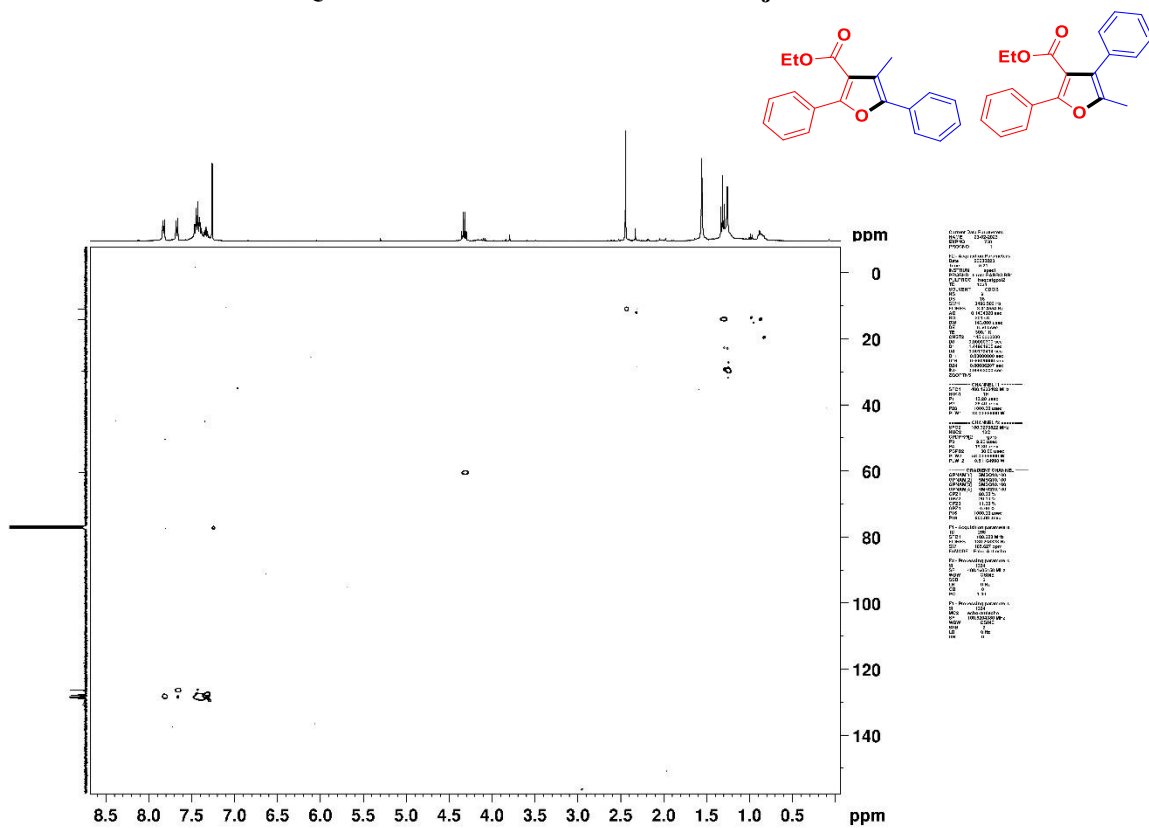
Cosy spectrum of compound – 3aj



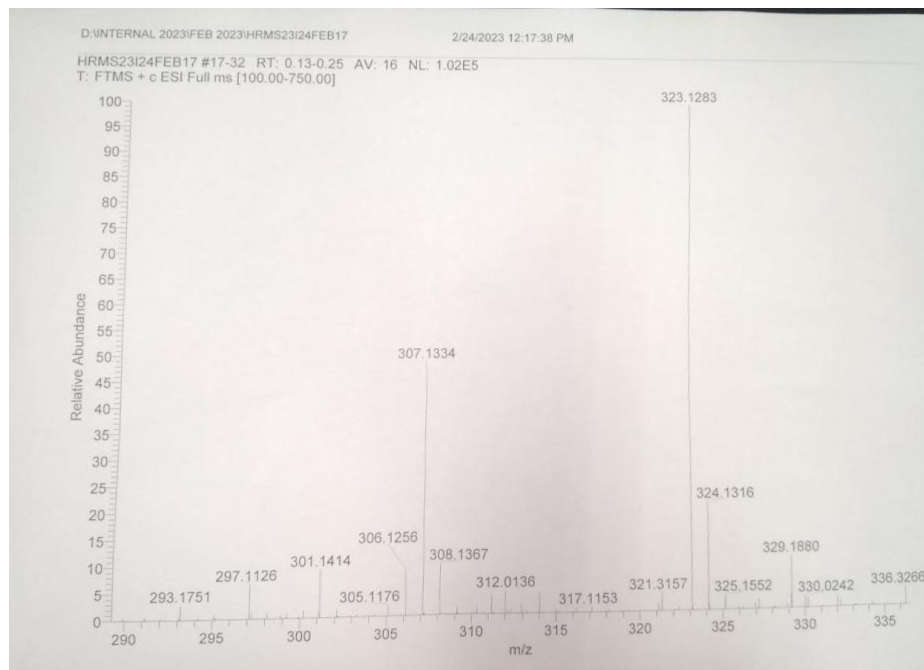
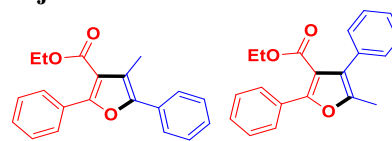
### HMBC spectrum of compound-3aj



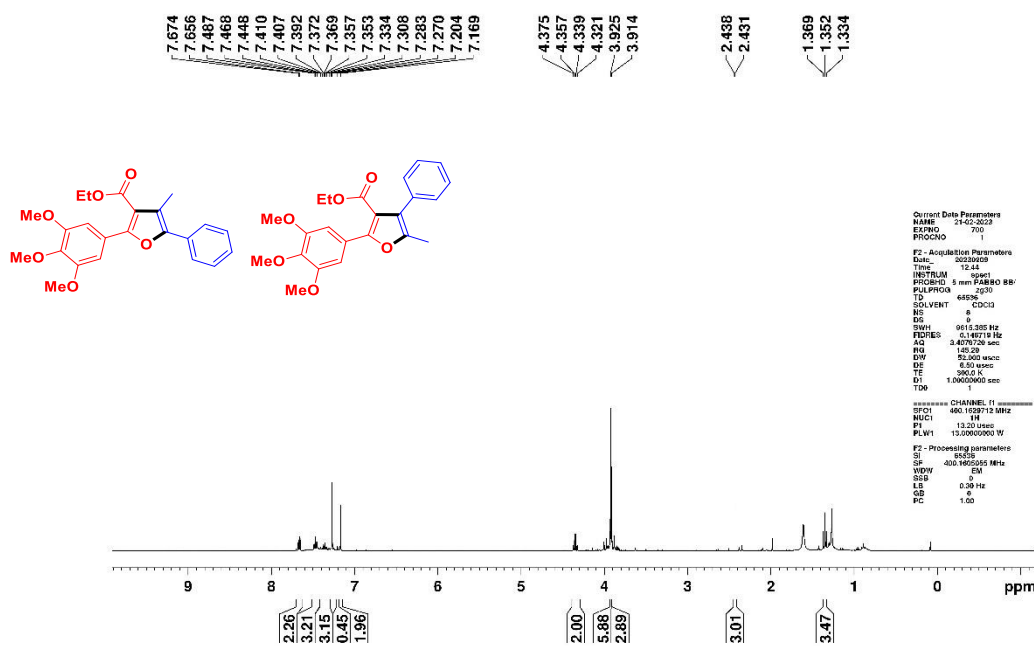
### HSQC SPECTRUM OF COMPOUND – 3aj



### HRMS SPECTRUM OF COMPOUND-3aj

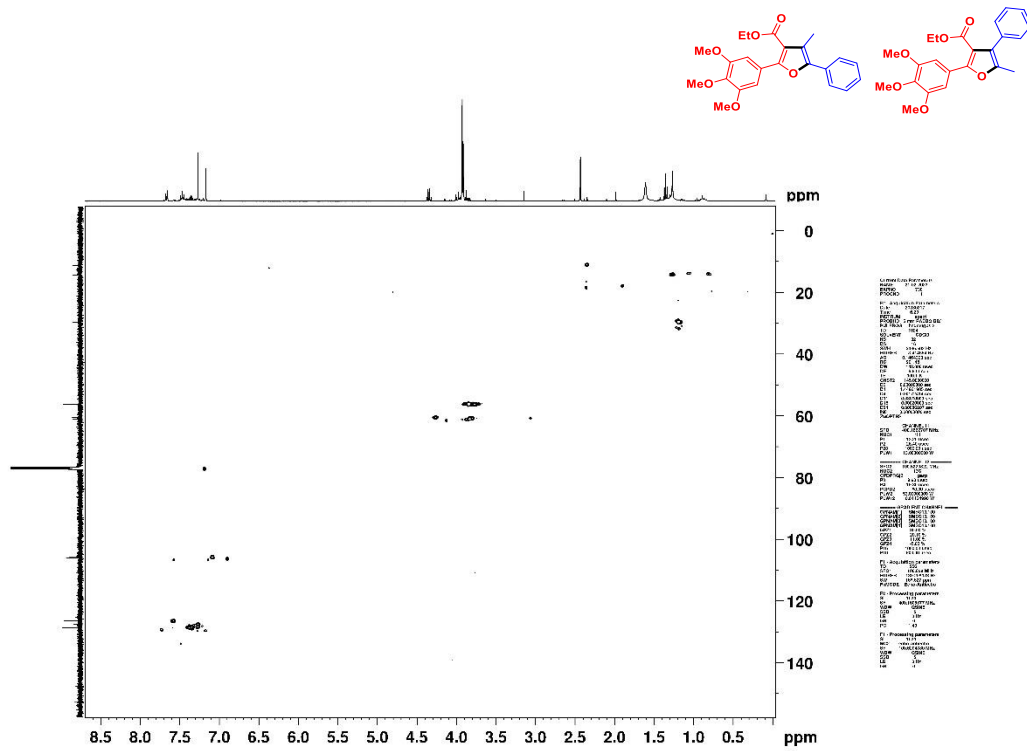


### <sup>1</sup>H NMR spectrum of compound- 3kj (400 MHz, CDCl<sub>3</sub>);

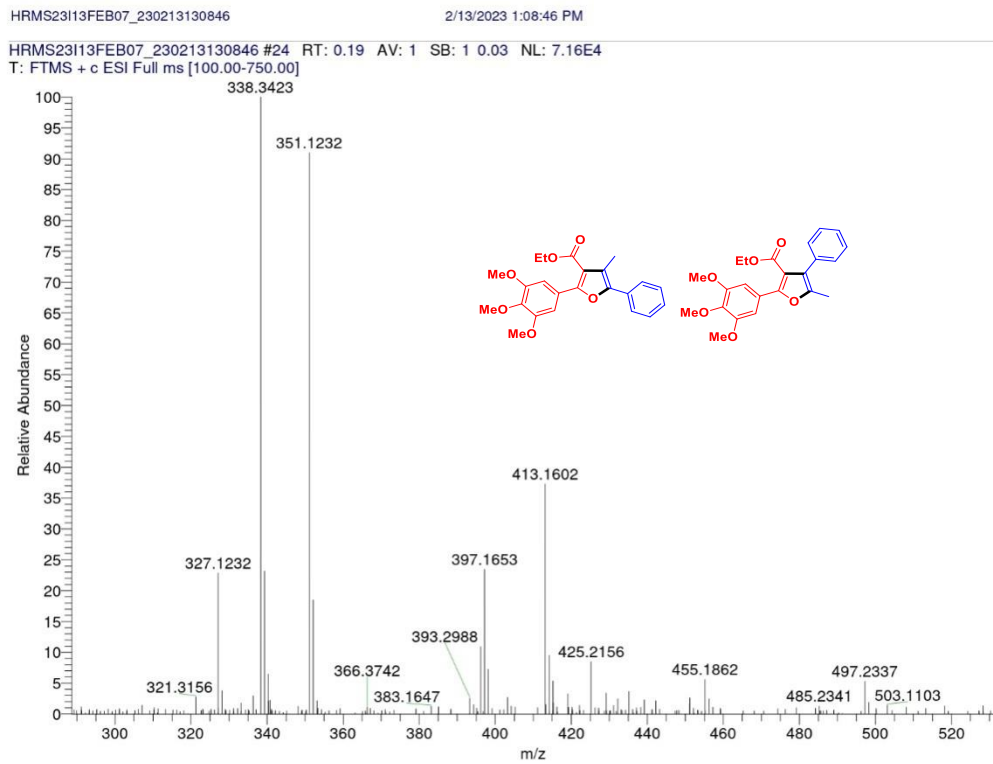




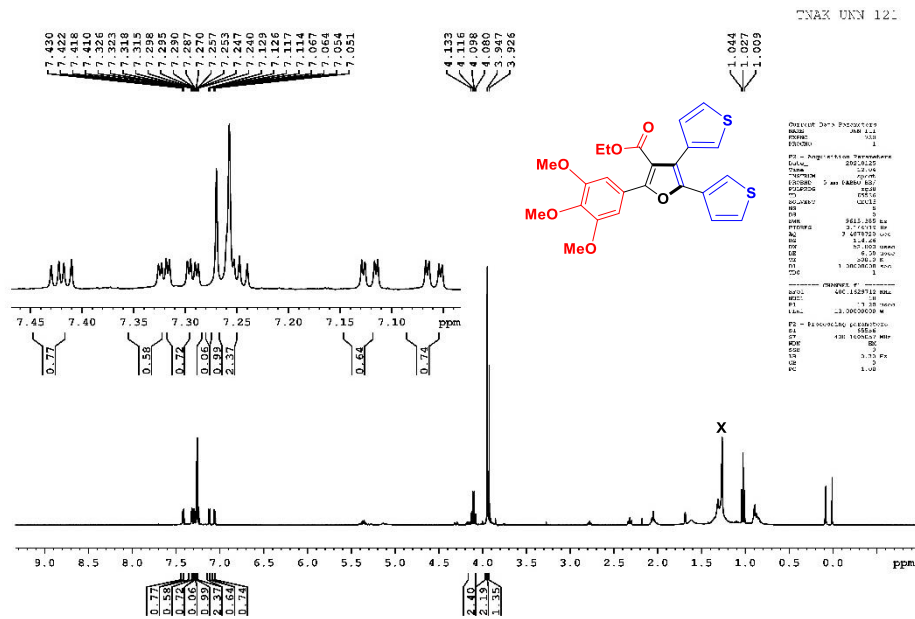
## HSQC SPECTRUM OF COMPOUND – 3kj



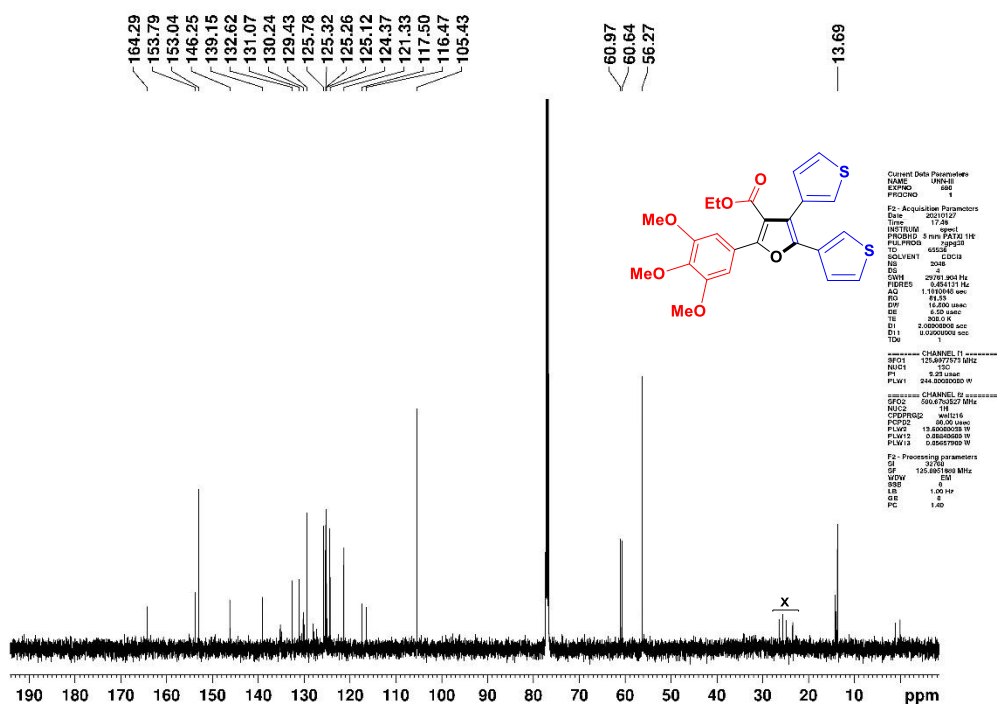
## HRMS spectrum of compound-3kj



<sup>1</sup>H NMR spectrum of compound- 3kj (400 MHz, CDCl<sub>3</sub>); X = Wax impurity



<sup>13</sup>C NMR spectrum of compound- 3kj (100 MHz, CDCl<sub>3</sub>); X=wax impurity

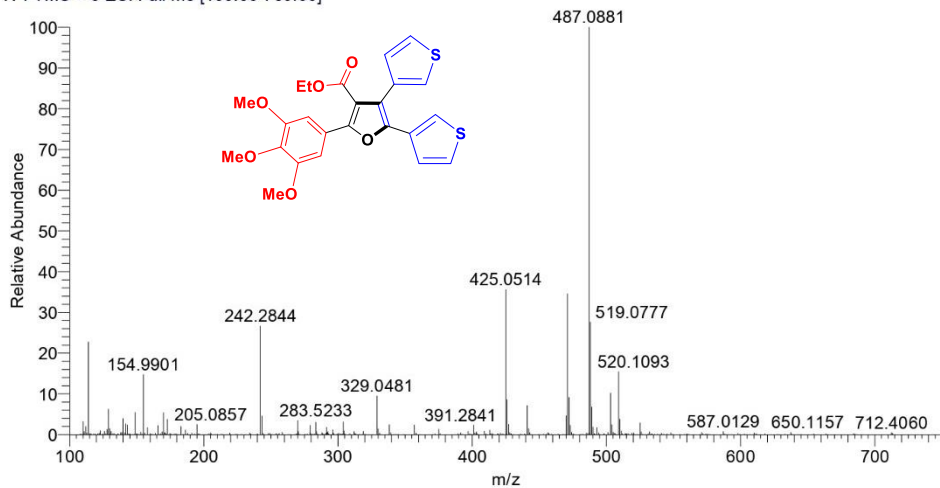




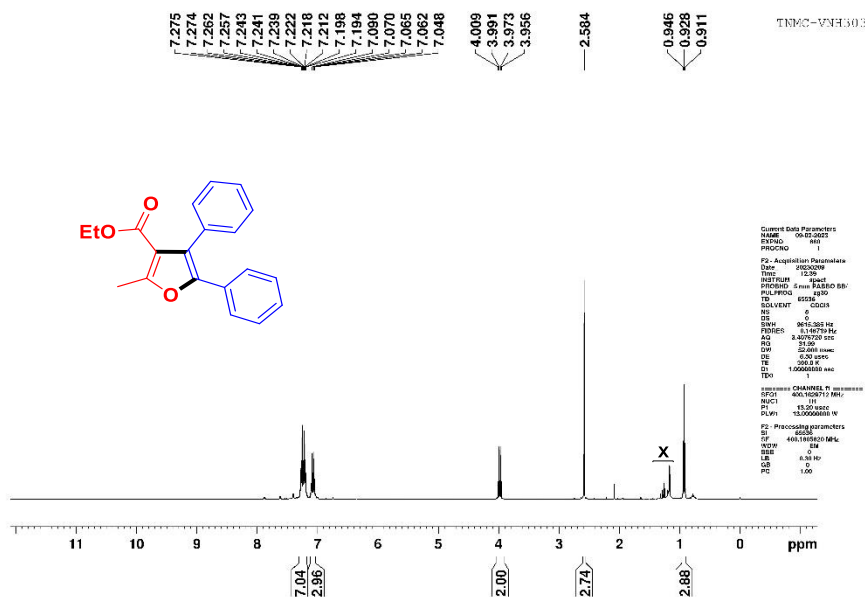
## HRMS spectrum of compound-3kj

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Vial:	CStk1-01:31	Injection Volume(μl):	1.00

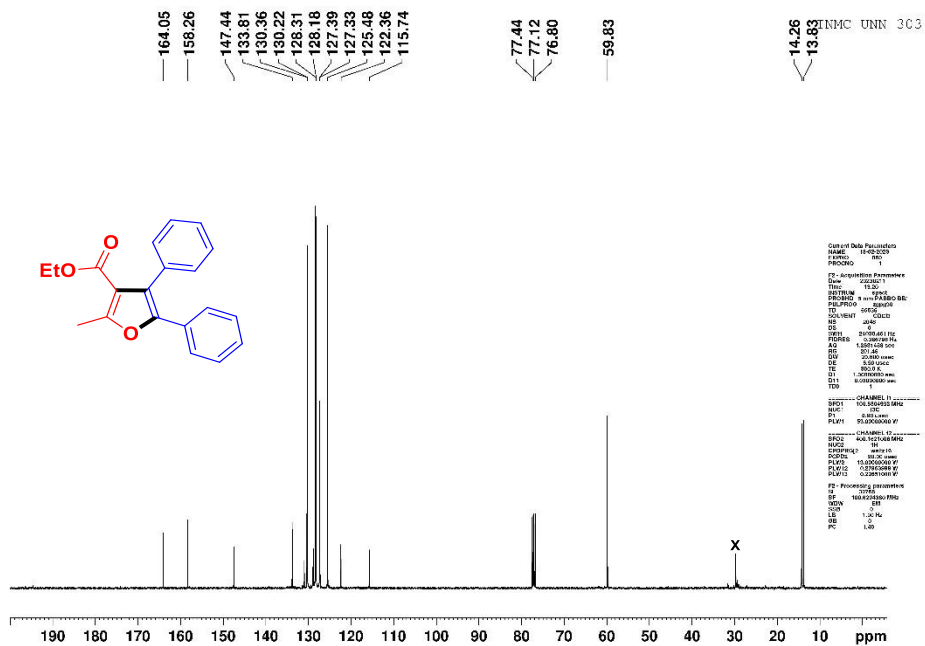
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T: FTMS + c ESI Full ms [100.00-750.00]



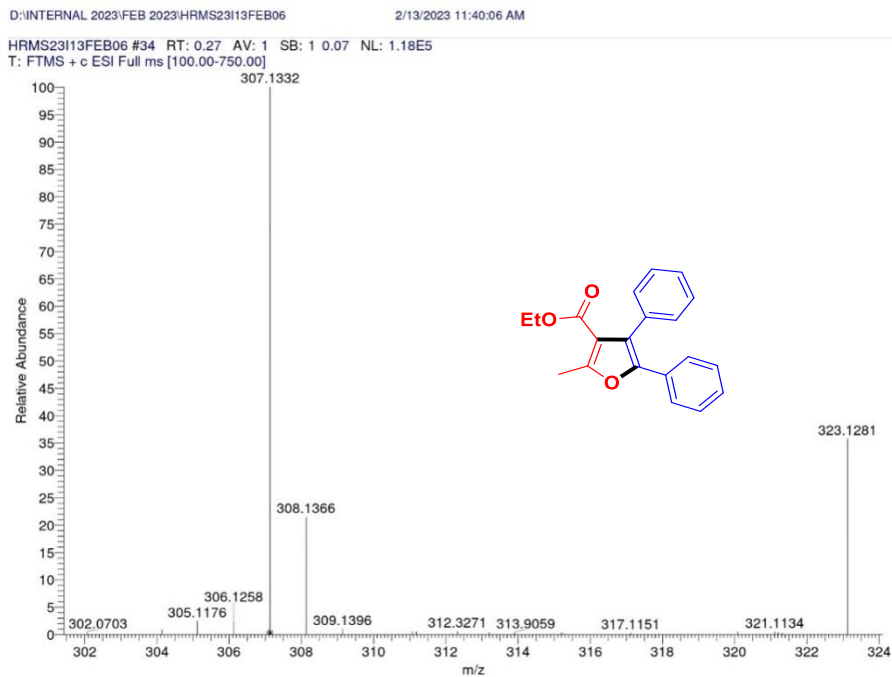
## <sup>1</sup>H NMR spectrum of compound- 3la (400 MHz, CDCl<sub>3</sub>); X= wax impurity



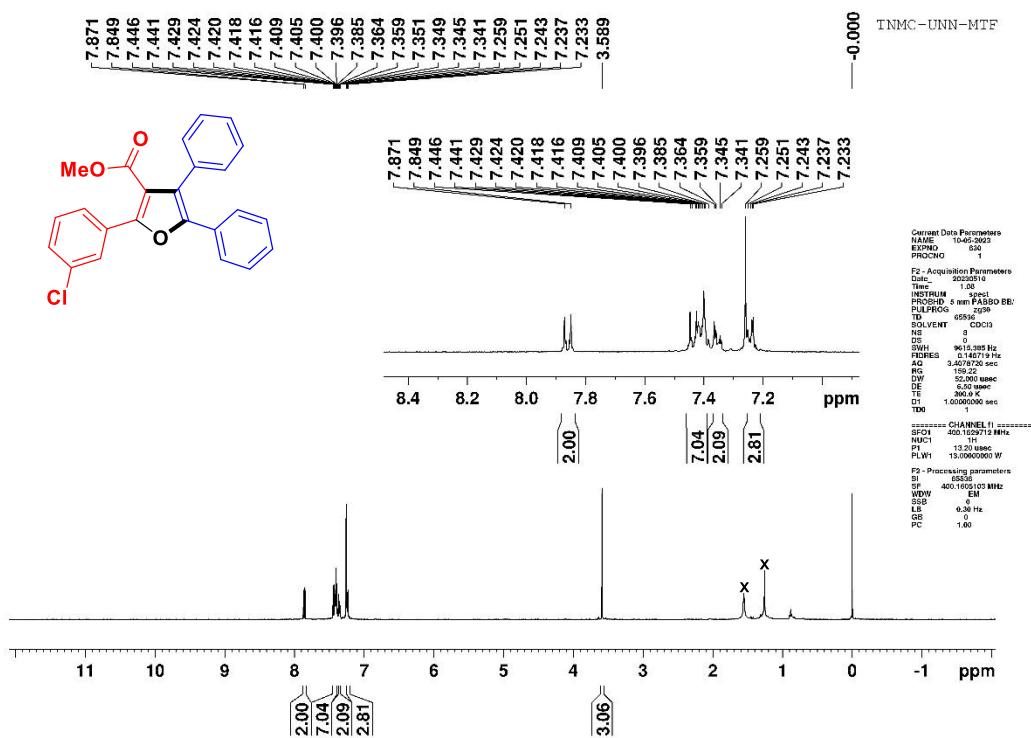
<sup>13</sup>C NMR spectrum of compound- 3la (100 MHz, CDCl<sub>3</sub>); X= wax impurity



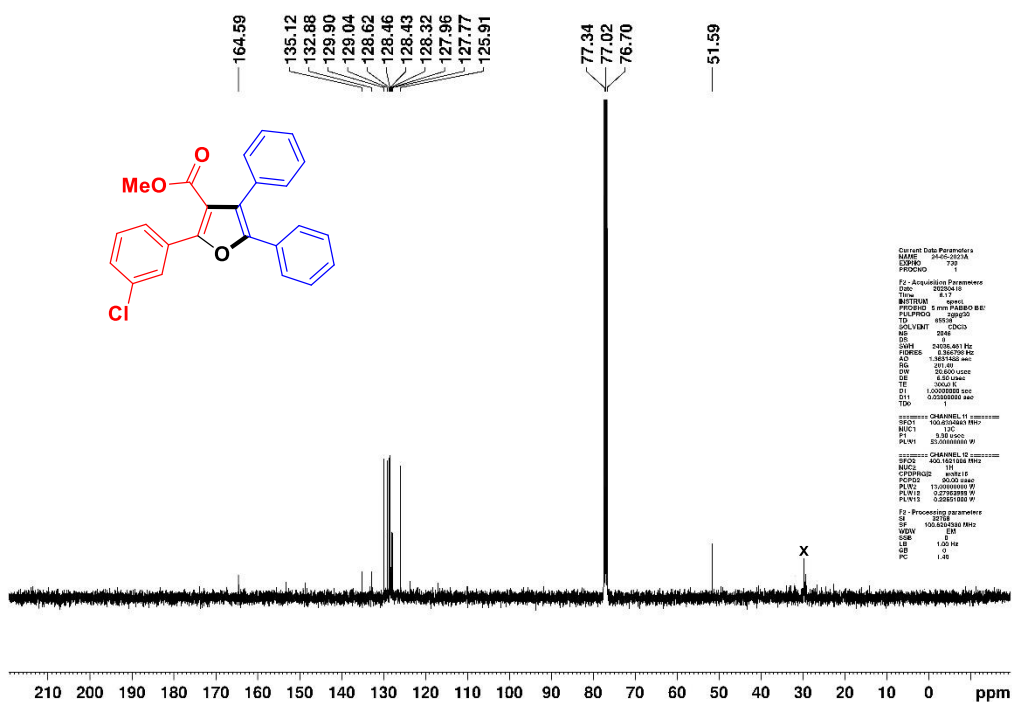
HRMS spectrum of compound-3la



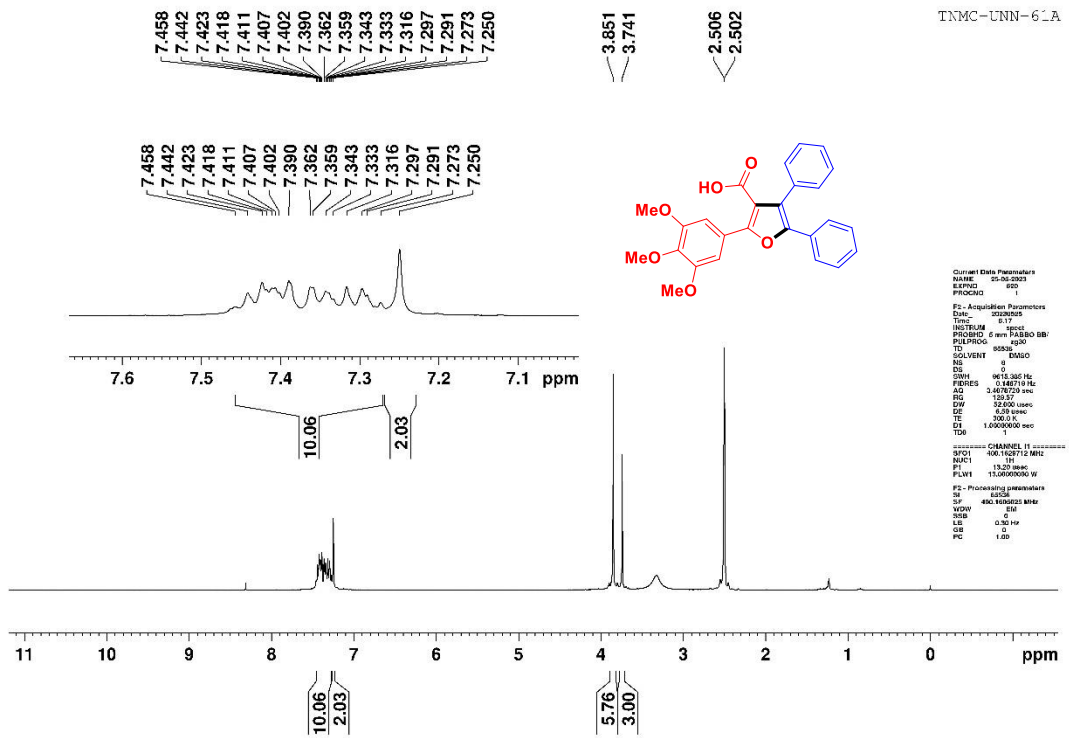
<sup>1</sup>H NMR spectrum of compound- 3ma (400 MHz, CDCl<sub>3</sub>); X= wax impurity



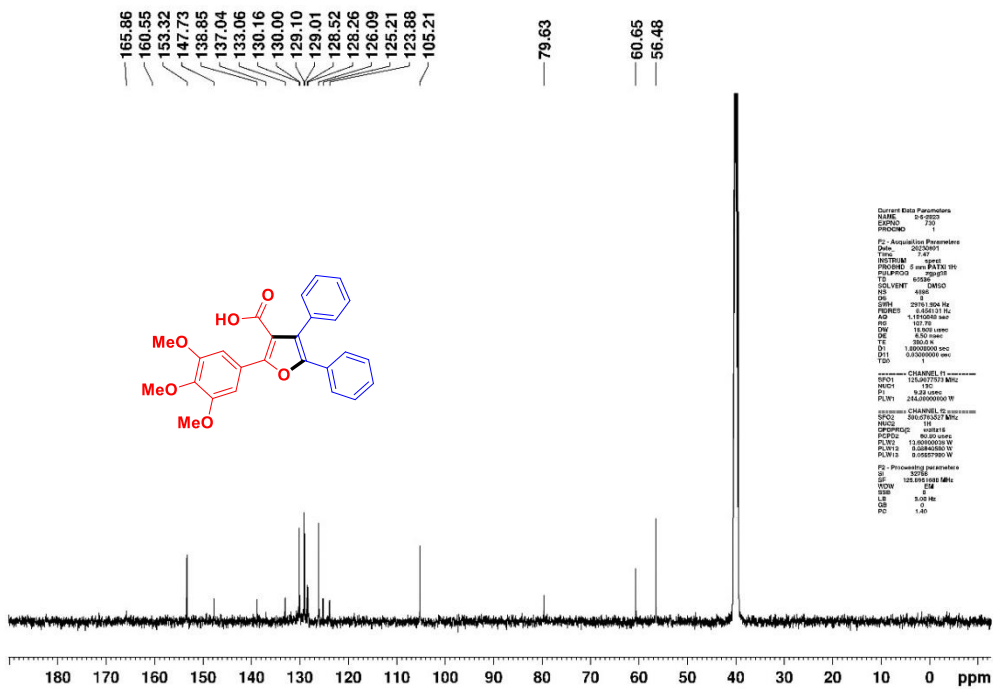
<sup>13</sup>C NMR spectrum of compound- 3ma (100 MHz, CDCl<sub>3</sub>); X= wax impurity



<sup>1</sup>H NMR spectrum of compound- 4 (400 MHz, DMSO-d<sub>6</sub>);



<sup>13</sup>C NMR spectrum of compound- 4 (100 MHz, DMSO-d<sub>6</sub>);



## ESMS spectrum of compound-4

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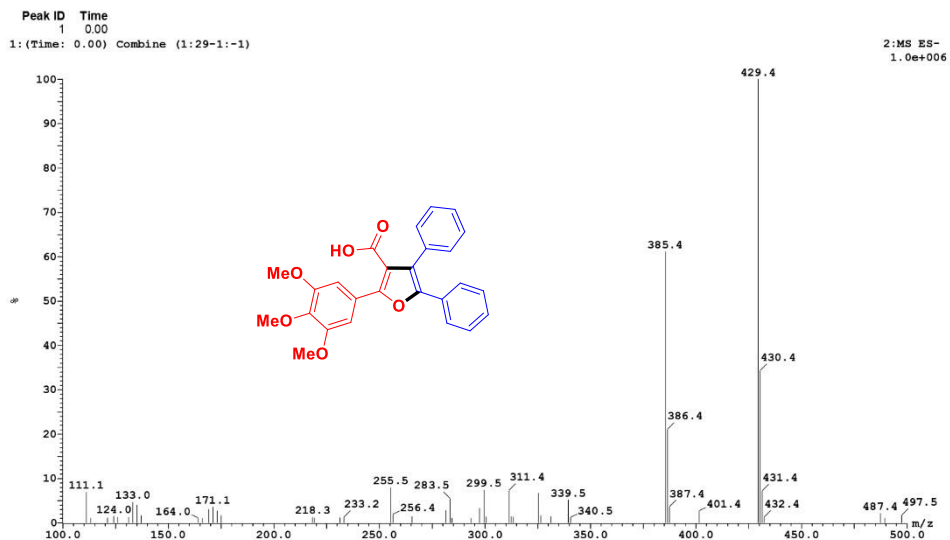
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Date:31-May-2023

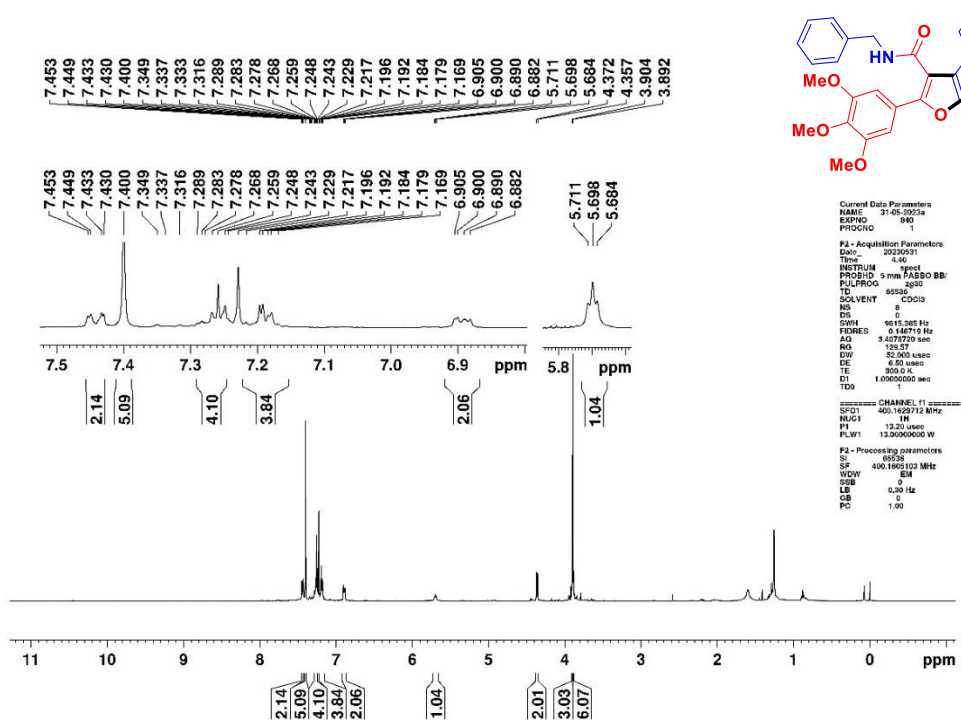
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Page 2

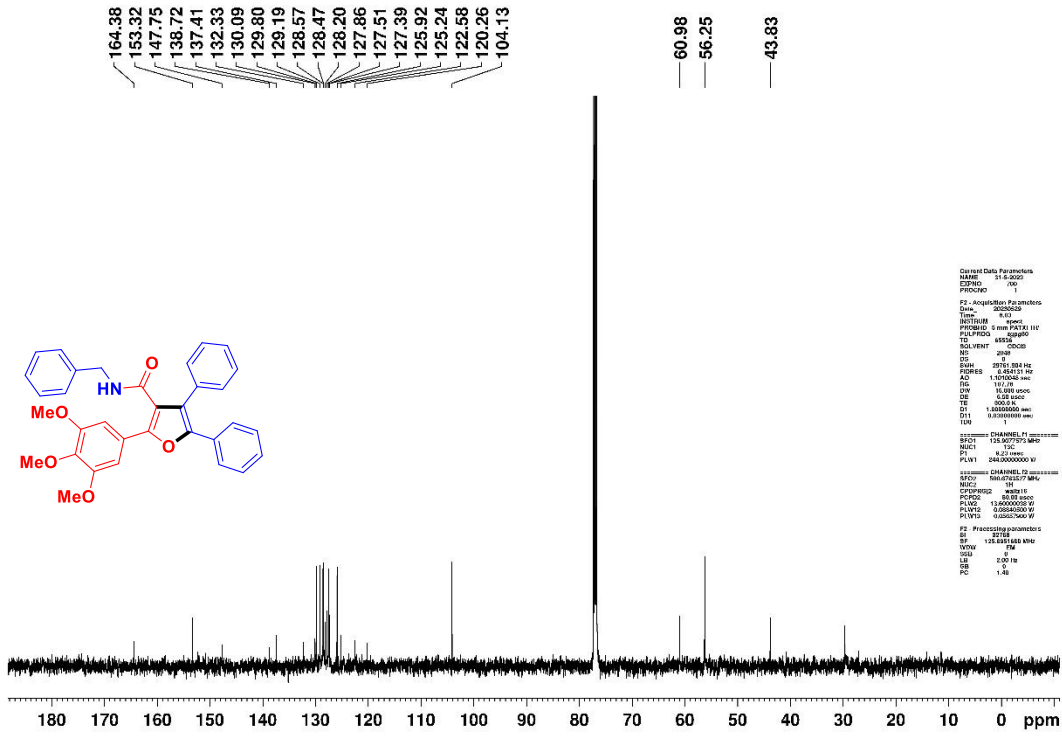
Printed: Wed May 31 14:28:29 2023



## <sup>1</sup>H NMR spectrum of compound- 5 (400 MHz, CDCl<sub>3</sub>)



**$^{13}\text{C}$  NMR spectrum of compound- 5 (100 MHz,  $\text{CDCl}_3$ )**



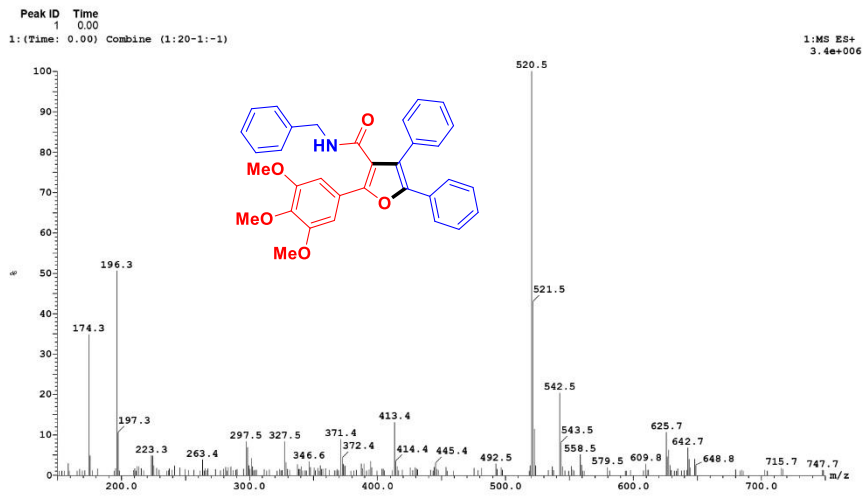
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PUL1 258.00000000 V
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NUC2 13C
PUL2 129.00000000 V
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SFO3 125.807374 MHz
MUL3 4
NUC3 13C
PUL3 258.00000000 V
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PUL4 129.00000000 V
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NUC5 13C
PUL5 258.00000000 V
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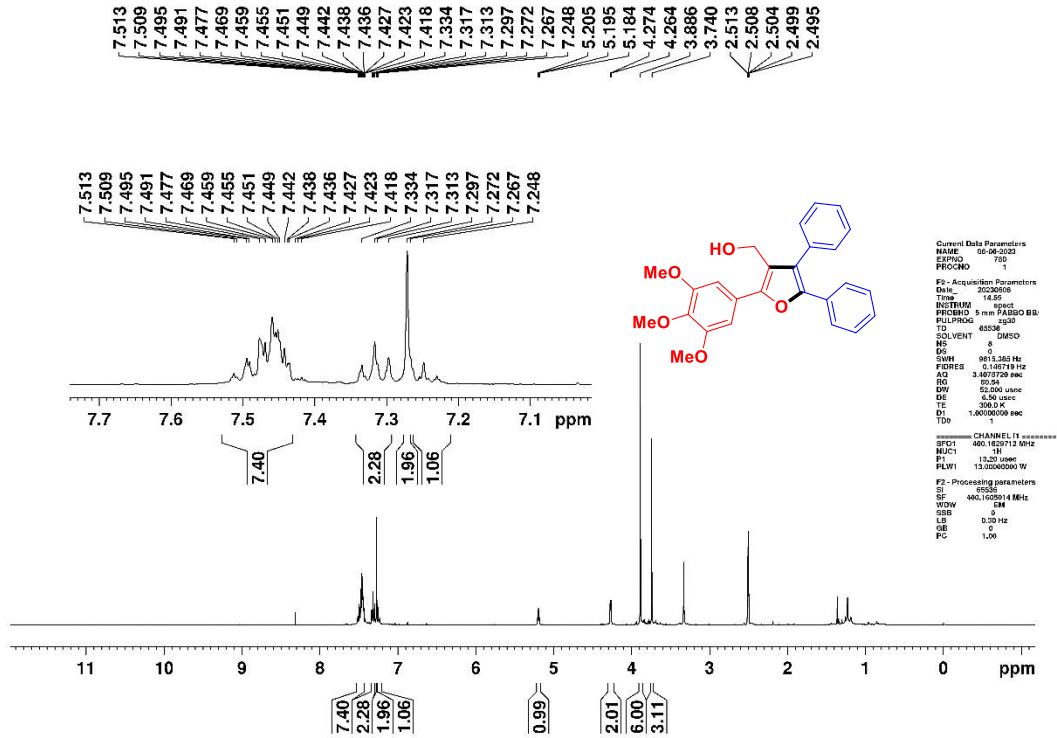
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**ESMS spectrum of compound-5**

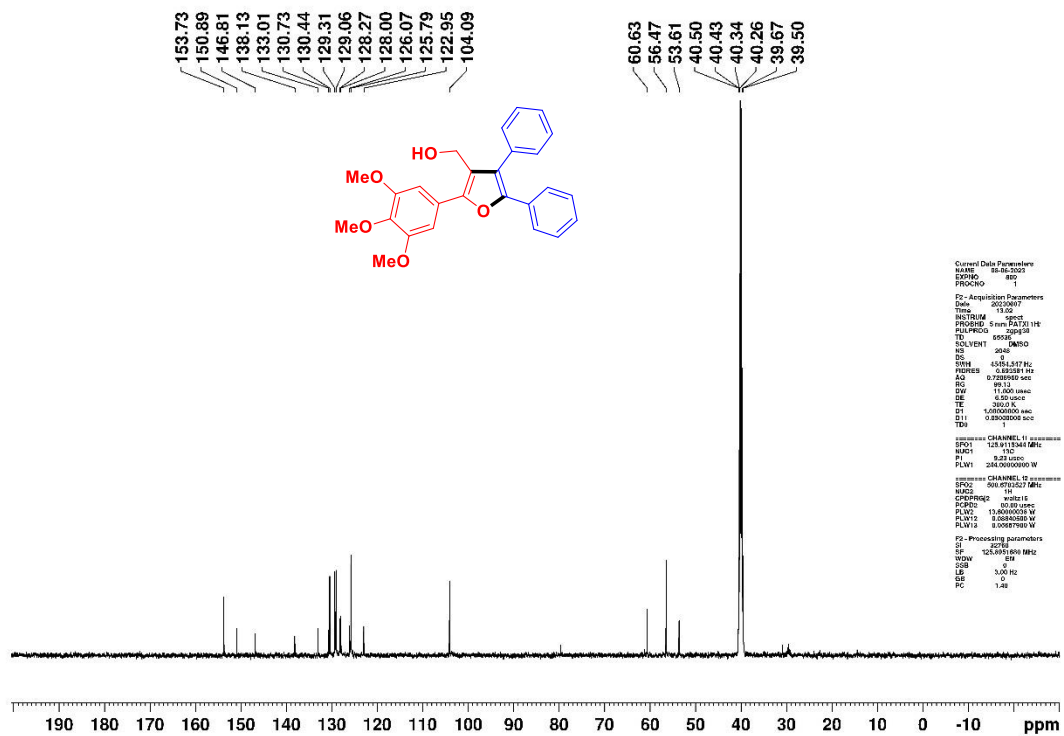
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 Date: 31-May-2023  
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 Page 1



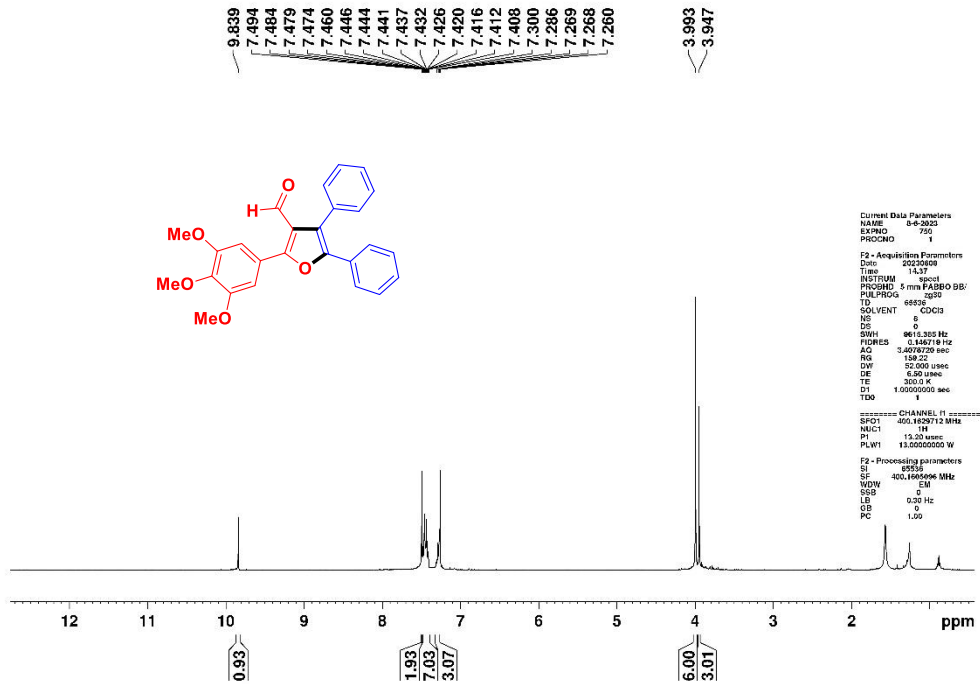
<sup>1</sup>H NMR spectrum of compound- 6 (400 MHz, DMSO-d<sub>6</sub>)



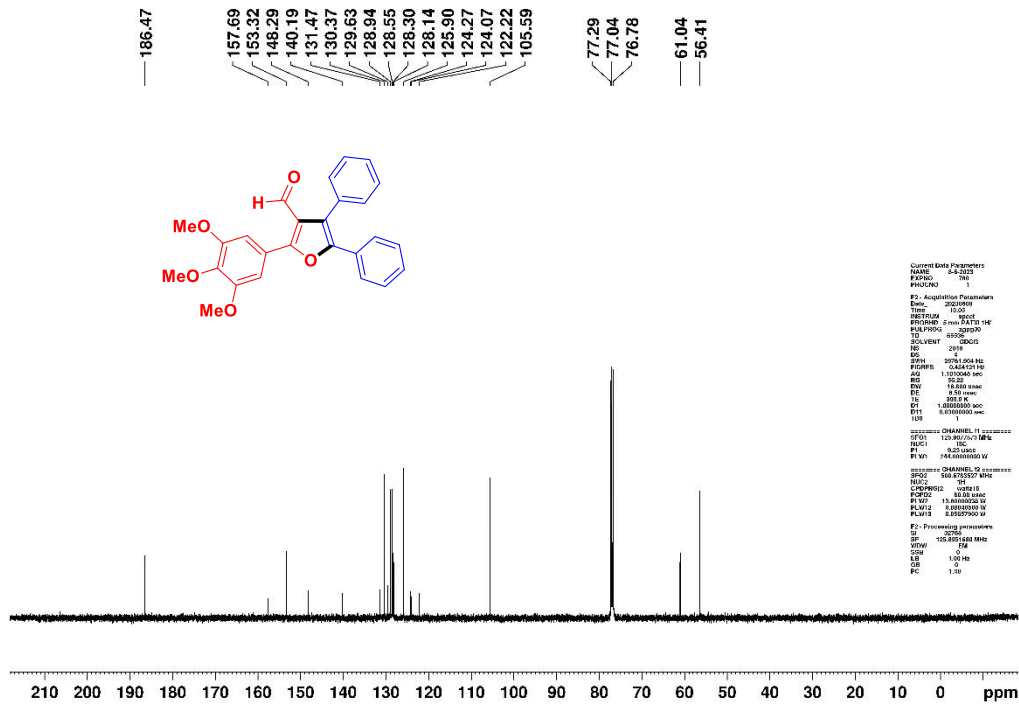
<sup>13</sup>C NMR spectrum of compound- 6 (100 MHz, DMSO-d<sub>6</sub>)



<sup>1</sup>H NMR spectrum of compound- 7 (400 MHz, CDCl<sub>3</sub>)



<sup>13</sup>C NMR spectrum of compound- 7 (100 MHz, CDCl<sub>3</sub>)





## ESMS spectrum of compound-7

Openlynx Report SAIF, CSIR-CDRI, LUCKNOW

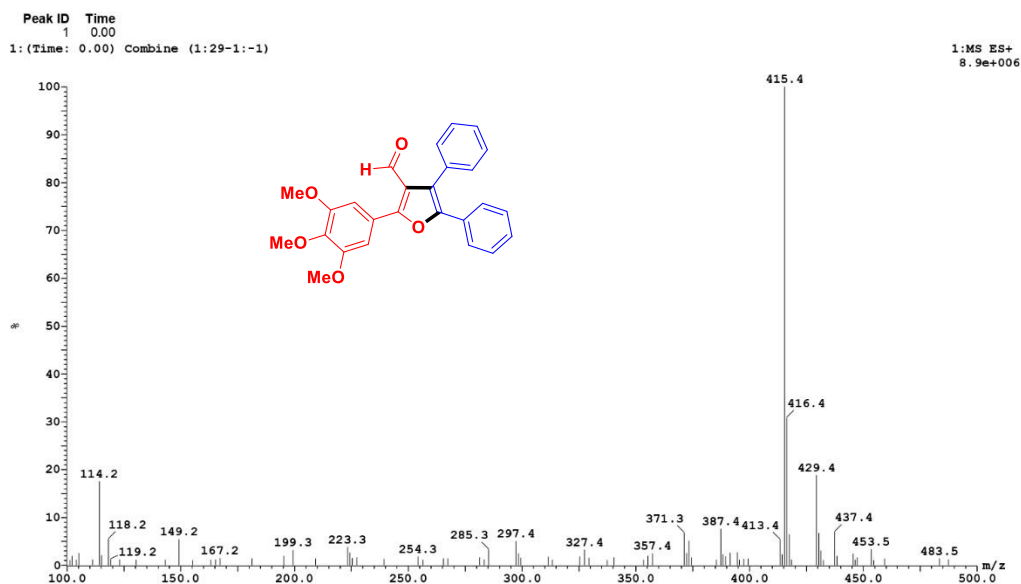
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Description: TNMC-UNN61AD

Vial: 1:B,6  
Date: 08-Jun-2023

ID: ESMS23108JUN18  
Time: 11:55:21

Page 1

Printed: Thu Jun 08 14:38:07 2023



### Control experiments:

