

## Supporting Information

### Multi-Functionalization of $\beta$ -Trifluoromethyl Enones Enabled 2,3-Dihydrofurans Synthesis

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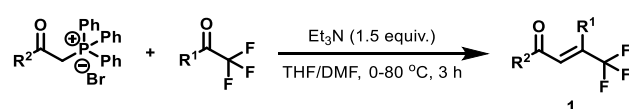
## General information

Unless otherwise stated, all reagents were purchased from commercial suppliers and used without further purification. All reactions were carried out under air or N<sub>2</sub> atmosphere using undistilled solvent. Melting points were recorded on an electrothermal digital melting point apparatus. <sup>1</sup>H, <sup>19</sup>F, and <sup>13</sup>C NMR spectra were recorded in CDCl<sub>3</sub> on Bruker Avance or Joel 400 MHz spectrometers. NMR splitting patterns are designated as singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), broad (br), doublet of doublets (dd), *etc.* The chemical shifts ( $\delta$ ) are reported in ppm and coupling constants ( $J$ ) in Hz. High resolution mass spectrometry (HRMS) data were obtained on a Waters LC-TOF mass spectrometer (Xevo G2-XS QToF) using electrospray ionization (ESI) in positive or negative mode. A suitable crystal was selected and recorded on a XtaLAB AFC12 (RINC): Kappa single diffractometer. Column chromatography was generally performed on silica gel (300-400 mesh) and reactions were monitored by thin layer chromatography (TLC) using UV light to visualize the course of the reactions.

## General procedure for the synthesis of trifluoromethyl enones 1

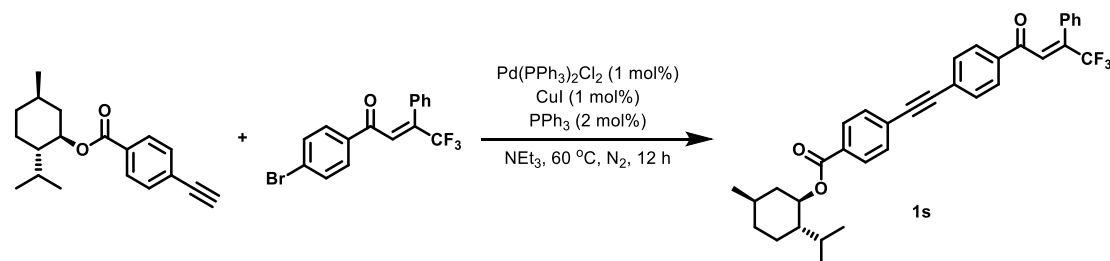
The trifluoromethyl enones **1** utilized in the reaction are known compounds, which were synthesized by following previously reported methods.<sup>[1-2]</sup>

### a) General procedure A (GPA)



To a solution of triphenylphosphonium salt (7.5 mmol, 1.5 equiv.) and triethylamine (758.9 mg, 7.5 mmol, 1.5 equiv.) in THF (20 mL) was added a solution of a trifluoromethyl ketone (5.0 mmol, 1 equiv.) in DMF (1.6 mL) at 0 °C (ice bath) under air. The mixture was stirred for 15 min at this temperature. After warming to room temperature, the solution was heated at 80 °C (oil bath) for 3 h. The solution was quenched with saturated aqueous NH<sub>4</sub>Cl solution (30 mL) and extracted with ethyl acetate (50 mL x 3). The organic extract was dried over MgSO<sub>4</sub> and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate: 100/1) to give the pure trifluoromethylated enones **1a-1r** and **1t-1x**.

### b) General procedure B (GPB)



A solution of (1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl 4-ethynylbenzoate (1.4 g, 5.0 mmol, 1 equiv.), (*E*)-1-(4-bromophenyl)-4,4,4-trifluoro-3-phenylbut-2-en-1-one (2.1 g, 6.0 mmol, 1.2 equiv.), bis(triphenylphosphine)palladium(II) chloride (35.0 mg, 0.05 mmol, 1.0 mol%), copper(I) iodide (9.5 mg, 0.05 mmol, 1.0 mol%), and triphenylphosphine (26.2 mg, 0.1 mmol, 2.0 mol%) in NEt<sub>3</sub> (10 mL) was stirred at 60 °C (oil bath) under N<sub>2</sub> for 12 h. The reaction was then quenched by

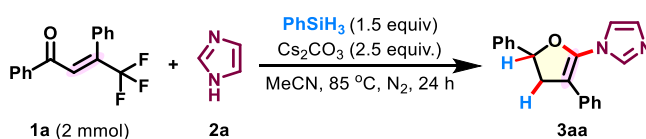
saturated NH<sub>4</sub>Cl solution (10 mL) and extracted with EtOAc (20 mL x 3). The organic layer was washed with saturated brine twice, dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The crude product was purified by flash silica gel column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (100/1~50/1) as eluent to afford the pure product **1s** (1.8 g, 64% yield).

### General procedure for the synthesis of 2,3-dihydrofurans **3**



A solution of trifluoromethyl enone (0.3 mmol, 1 equiv.; **1**), N-nucleophile (0.45 mmol, 1.5 equiv.; **2**), phenylsilane (48.7 mg, 0.45 mmol, 1.5 equiv.), and Cs<sub>2</sub>CO<sub>3</sub> (244.4 mg, 0.75 mmol, 2.5 equiv.) in MeCN (3.5 mL) was stirred at 85 °C (oil bath) under nitrogen atmosphere for 24 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (10 mL) and extracted with EtOAc (10 mL x 3). The organic layer was washed with saturated brine twice, dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The crude product was purified by flash silica gel column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (10/1~4/1) as eluent to afford the pure product **3**.

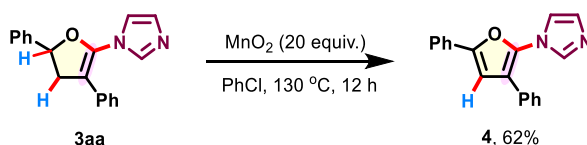
### Scale-up synthesis of product **3aa**



A solution of (*E*)-4,4,4-trifluoro-1,3-diphenylbut-2-en-1-one (552.5 mg, 2 mmol, 1 equiv.; **1a**), imidazole (204.3 mg, 3 mmol, 1.5 equiv.; **2a**), phenylsilane (324.6 mg, 3 mmol, 1.5 equiv.), and Cs<sub>2</sub>CO<sub>3</sub> (1629.2 mg, 5 mmol, 2.5 equiv.) in MeCN (10 mL) was stirred at 85 °C (oil bath) under nitrogen atmosphere for 24 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (20 mL) and extracted with EtOAc (20 mL x 3). The organic layer was washed with saturated brine twice, dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The crude product was purified by flash silica gel column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (10/1~4/1) as eluent to afford the pure product **3aa** (496.0 mg, 86% yield).

### Further transformations of products **3aa** and **3ab**

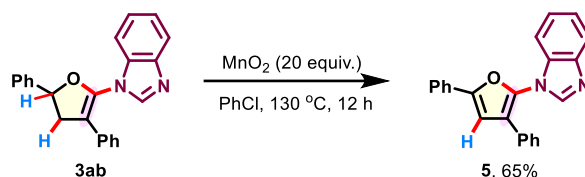
#### a) Oxidation of product **3aa**



A solution of 1-(3,5-diphenyl-4,5-dihydrofuran-2-yl)-1*H*-imidazole (86.5 mg, 0.3 mmol, 1 equiv.; **3aa**) and MnO<sub>2</sub> (521.6 mg, 6.0 mmol, 20 equiv.) in PhCl (3.5 mL) was stirred at 130 °C (oil bath) under air for 12 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (10 mL) and

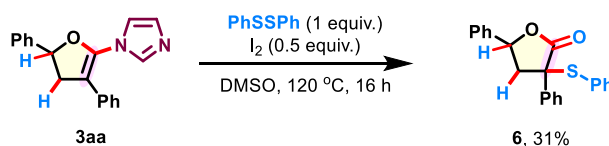
extracted with EtOAc (10 mL x 3). The organic layer was washed with saturated brine twice, dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The crude product was purified by flash silica gel column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (10/1~4/1) as eluent to afford the pure product **4** (53.3 mg, 62% yield).

#### b) Oxidation of product **3ab**



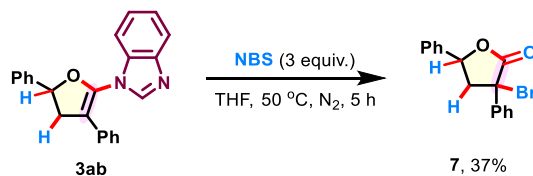
A solution of 1-(3,5-diphenyl-4,5-dihydrofuran-2-yl)-1*H*-benzo[*d*]imidazole (101.5 mg, 0.3 mmol, 1 equiv.; **3ab**) and MnO<sub>2</sub> (521.6 mg, 6.0 mmol, 20 equiv.) in PhCl (3.5 mL) was stirred at 130 °C (oil bath) under air for 12 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (10 mL) and extracted with EtOAc (10 mL x 3). The organic layer was washed with saturated brine twice, dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The crude product was purified by flash silica gel column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (10/1~4/1) as eluent to afford the pure product **5** (65.6 mg, 65% yield).

#### c) The thioetherification of product **3aa**



A solution of 1-(3,5-diphenyl-4,5-dihydrofuran-2-yl)-1*H*-imidazole (86.5 mg, 0.3 mmol, 1 equiv.; **3aa**), diphenyl sulfide (65.5 mg, 0.3 mmol, 1 equiv.), and iodine (19.0 mg, 0.15 mmol, 0.5 equiv.) in DMSO (3.5 mL) was stirred at 120 °C (oil bath) under air for 16 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (10 mL) and extracted with EtOAc (10 mL x 3). The organic layer was washed with saturated brine twice, dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The crude product was purified by flash silica gel column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (10/1~4/1) as eluent to afford the pure product **6** (32.2 mg, 31% yield).

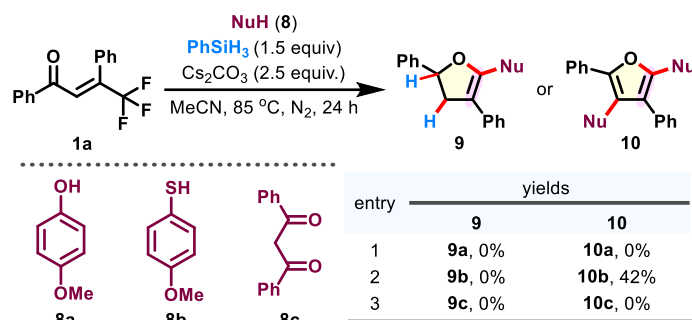
#### d) The bromination of product **3ab**



A solution of 1-(3,5-diphenyl-4,5-dihydrofuran-2-yl)-1*H*-benzo[*d*]imidazole (101.5 mg, 0.3 mmol, 1 equiv.; **3ab**) and NBS (160.2 mg, 0.9 mmol, 3 equiv.) in THF (3.5 mL) was stirred at 50 °C (oil bath) under nitrogen atmosphere for 5 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (10 mL) and extracted with EtOAc (10 mL x 3). The organic layer was washed with saturated brine twice, dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The crude

product was purified by flash silica gel column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (10/1~4/1) as eluent to afford the pure product **7** (35.2 mg, 37% yield).

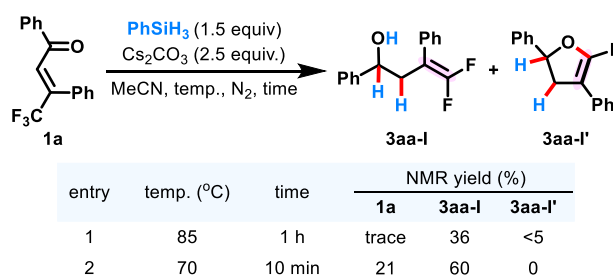
### General procedure for the reactions of trifluoromethyl enone **1a** with O-/S-/C-nucleophiles **8**



A solution of (*E*)-4,4,4-trifluoro-1,3-diphenylbut-2-en-1-one (82.9 mg, 0.3 mmol, 1 equiv.), O-/S-/C-nucleophile (0.45 mmol, 1.5 equiv.; **8**), phenylsilane (48.7 mg, 0.45 mmol, 1.5 equiv.), and Cs<sub>2</sub>CO<sub>3</sub> (244.4 mg, 0.75 mmol, 2.5 equiv.) in MeCN (3.5 mL) was stirred at 85 °C (oil bath) under nitrogen atmosphere for 24 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (10 mL) and extracted with EtOAc (10 mL x 3). The organic layer was washed with saturated brine twice, dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The crude product was purified by flash silica gel column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (50/1~20/1) as eluent to afford the pure product **10b** (62.6 mg, 42% yield).

### Mechanistic studies

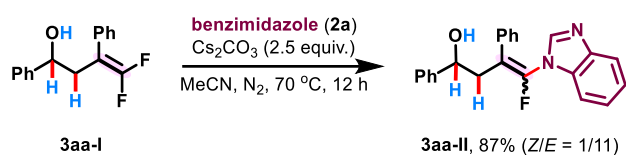
#### a) Hydrodefluorination of trifluoromethylated enone **1a**



A solution of (*E*)-4,4,4-trifluoro-1,3-diphenylbut-2-en-1-one (82.9 mg, 0.3 mmol, 1 equiv.; **1a**), phenylsilane (48.7 mg, 0.45 mmol, 1.5 equiv.), and Cs<sub>2</sub>CO<sub>3</sub> (244.4 mg, 0.75 mmol, 2.5 equiv.) in MeCN (3.5 mL) was stirred at 70 or 85 °C (oil bath) under nitrogen atmosphere for 10 min or 1 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (10 mL) and extracted with EtOAc (10 mL x 3). The organic layer was washed with saturated brine twice, dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. <sup>1</sup>H NMR analysis of the obtained residue by using 4-fluoroanisole (0.1 mmol) as an internal standard indicated the formation of products **3aa-I** and **3aa-I'**, as well as the presence of residual **1a**.

*This result suggested that OH-containing gem-difluoroalkene 3aa-I might be a reaction intermediate.*

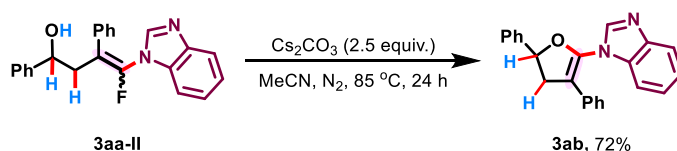
### b) The intermediacy of *gem*-difluoroalkene **3aa-I**



A solution of 4,4-difluoro-1,3-diphenylbut-3-en-1-ol (78.1 mg, 0.3 mmol, 1 equiv.; **3aa-I**), benzimidazole (53.2 mg, 0.45 mmol, 1.5 equiv.; **2a**), and Cs<sub>2</sub>CO<sub>3</sub> (244.4 mg, 0.75 mmol, 2.5 equiv.) in MeCN (3.5 mL) was stirred at 70 °C (oil bath) under nitrogen atmosphere for 12 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (10 mL) and extracted with EtOAc (10 mL x 3). The organic layer was washed with saturated brine twice, dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The crude product was purified by flash silica gel column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (4/1~2/1) as eluent to afford the pure product **3aa-II** (93.5 mg, 87% yield, Z/E = 1/11).

**This result suggested that OH-containing *gem*-difluoroalkene **3aa-I** might be a possible reaction intermediate.**

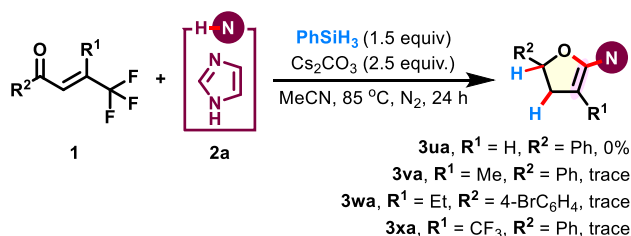
### c) The intermediacy of $\alpha$ -fluoroenamide **3aa-II**



A solution of 4-(1*H*-benzo[*d*]imidazol-1-yl)-4-fluoro-1,3-diphenylbut-3-en-1-ol (107.5 mg, 0.3 mmol, 1 equiv.; **3aa-II**) and Cs<sub>2</sub>CO<sub>3</sub> (244.4 mg, 0.75 mmol, 2.5 equiv.) in MeCN (3.5 mL) was stirred at 85 °C (oil bath) under nitrogen atmosphere for 24 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (10 mL) and extracted with EtOAc (10 mL x 3). The organic layer was washed with saturated brine twice, dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The crude product was purified by flash silica gel column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (10/1~4/1) as eluent to afford the pure product **3ab** (73.1 mg, 72% yield).

**This result suggested that  $\alpha$ -fluoroenamide **3aa-II** might be a reaction intermediate.**

### d) The effect of R<sup>1</sup> substituent on the reactivity of trifluoromethylated enones



A solution of trifluoromethyl enone (0.3 mmol, 1 equiv.; **1**), imidazole (30.6 mg, 0.45 mmol, 1.5 equiv.; **2a**), phenylsilane (48.7 mg, 0.45 mmol, 1.5 equiv.), and Cs<sub>2</sub>CO<sub>3</sub> (244.4 mg, 0.75 mmol, 2.5 equiv.) in MeCN (3.5 mL) was stirred at 85 °C (oil bath) under nitrogen atmosphere for 24 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (10 mL) and extracted with EtOAc (10 mL x 3). The organic layer was washed with saturated brine twice, dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The residue was directly analyzed by NMR analysis. No desired product

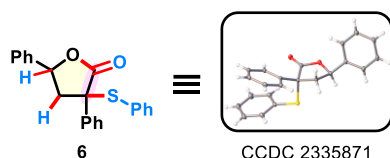
**3ua** was observed, and only trace amounts of the desired products **3va-xa** were formed.

**This result suggested that the presence of an aryl substituent significantly contributes to electron acceptance into the  $\pi$ -system and subsequent fluoride extrusion.**

### **The X-ray crystal structure of product 6**

The single crystal was grown from the mixed solution of EtOAc/DCM by slowly evaporating the above solvents at room temperature.

**3,5-Diphenyl-3-(phenylthio)dihydrofuran-2(3H)-one (6**; displacement ellipsoids are drawn at the 50% probability levels):



**Table S1.** Crystal data and structure refinement for product **6**.

Identification code	product <b>6</b>
Empirical formula	C <sub>22</sub> H <sub>18</sub> O <sub>2</sub> S
Formula weight	346.42
Temperature/K	293.15
Crystal system	monoclinic
Space group	Pn
a/Å	11.5209(2)
b/Å	6.01778(11)
c/Å	12.8734(2)
$\alpha$ /°	90
$\beta$ /°	98.9962(16)
$\gamma$ /°	90
Volume/Å <sup>3</sup>	881.53(3)
Z	2
$\rho_{\text{calc}}/\text{cm}^3$	1.305
$\mu/\text{mm}^{-1}$	1.717
F(000)	364.0
Crystal size/mm <sup>3</sup>	0.14 × 0.13 × 0.12
Radiation	Cu K $\alpha$ ( $\lambda$ = 1.54184)
2 $\theta$ range for data collection/°	15.574 to 152.288
Index ranges	-14 ≤ h ≤ 14, -5 ≤ k ≤ 7, -16 ≤ l ≤ 16
Reflections collected	5356
Independent reflections	2786 [R <sub>int</sub> = 0.0171, R <sub>sigma</sub> = 0.0156]
Data/restraints/parameters	2786/2/226
Goodness-of-fit on F <sup>2</sup>	1.066

Final R indexes [ $I \geq 2\sigma(I)$ ]  $R_1 = 0.0331$ ,  $wR_2 = 0.0910$

Final R indexes [all data]  $R_1 = 0.0332$ ,  $wR_2 = 0.0912$

Largest diff. peak/hole/e  $\text{\AA}^{-3}$  0.21/-0.26

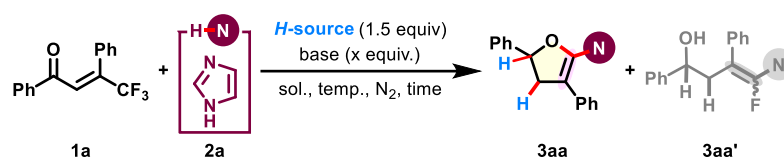
Flack parameter 0.046(11)

### Crystal structure determination of product 6.

**Crystal Data** for  $C_{22}H_{18}O_2S$  ( $M = 346.42$  g/mol): monoclinic, space group Pn (no. 7),  $a = 11.5209(2)$   $\text{\AA}$ ,  $b = 6.01778(11)$   $\text{\AA}$ ,  $c = 12.8734(2)$   $\text{\AA}$ ,  $\beta = 98.9962(16)^\circ$ ,  $V = 881.53(3)$   $\text{\AA}^3$ ,  $Z = 2$ ,  $T = 293.15$  K,  $\mu(\text{Cu K}\alpha) = 1.717$   $\text{mm}^{-1}$ ,  $D_{\text{calc}} = 1.305$   $\text{g/cm}^3$ , 5356 reflections measured ( $15.574^\circ \leq 2\theta \leq 152.288^\circ$ ), 2786 unique ( $R_{\text{int}} = 0.0171$ ,  $R_{\text{sigma}} = 0.0156$ ) which were used in all calculations. The final  $R_1$  was 0.0331 ( $I > 2\sigma(I)$ ) and  $wR_2$  was 0.0912 (all data).

### Optimization of the reaction conditions

**Table S2.** Optimization of reaction conditions<sup>a</sup>

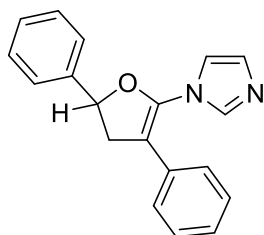


Entry	H-source	Base (x equiv)	Temp. (°C)	Solvent	Time (h)	Yield (%) <sup>b</sup>	
						3aa	3aa' (Z/E) <sup>c</sup>
1	PhSiH <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	70	MeCN	12	12	55 (1/8)
2	PhSiH <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	70	MeCN	24	15	60 (1/11)
3	PhSiH <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	70	MeCN	2	4	83 (1/7)
4	PhSiH <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	70	MeCN	1	5	62 (1/11)
5	PhSiH <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	70/85	MeCN	2/24	61	21 (1/6)
<b>6</b>	<b>PhSiH<sub>3</sub></b>	<b>Cs<sub>2</sub>CO<sub>3</sub> (2.5)</b>	<b>85</b>	<b>MeCN</b>	<b>24</b>	<b>83 (80)<sup>d</sup></b>	<b>6 (1/5)</b>
7	PhSiH <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	85	DMF	24	53	trace
8	PhSiH <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	85	DMSO	24	52	trace
9	PhSiH <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	85	THF	24	22	41 (1/2)
10	PhSiH <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	100	Toluene	24	trace	41 (1/2)
11	PhSiH <sub>3</sub>	CsF (2.5)	85	MeCN	24	78	8 (1/8)
12	PhSiH <sub>3</sub>	K <sub>2</sub> CO <sub>3</sub> (2.5)	85	MeCN	24	trace	38 (1/11)
13	PhSiH <sub>3</sub>	LiOH (2.5)	85	MeCN	24	trace	22 (1/50)
14	PhSiH <sub>3</sub>	DABCO (2.5)	85	MeCN	24	trace	trace
15	PhSiH <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub> (3.5)	85	MeCN	24	58	trace
16	PhSiH <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub> (1.5)	85	MeCN	24	51	33 (1/4)
17	PhMe <sub>2</sub> SiH	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	85	MeCN	24	trace	trace
18	NaBH <sub>4</sub>	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	85	MeCN	24	24	23 (1/3)
19	LiAlH <sub>4</sub>	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	85	MeCN	24	trace	trace
20	HP(O)Ph <sub>2</sub>	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	85	MeCN	24	trace	trace
21	Rongalite	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	85	MeCN	24	trace	trace
22	PhSiH <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	85	MeCN	36	35	30 (1/5)

<sup>a</sup> Reaction conditions: **1a** (0.3 mmol), **2a** (0.45 mmol), H-source (0.45 mmol), and base (0.45-1.05 mmol) in solvent (3.5 mL) at 70-100 °C under N<sub>2</sub> for 1-36 h. <sup>b</sup> Yields were determined by <sup>19</sup>F NMR analysis with 4-fluoroanisole (0.1 mmol) as an internal standard. <sup>c</sup> Z/E ratio was given in parentheses. <sup>d</sup> Isolated yield.



## Characterization data for products



### **1-(3,5-Diphenyl-4,5-dihydrofuran-2-yl)-1H-imidazole (3aa):**

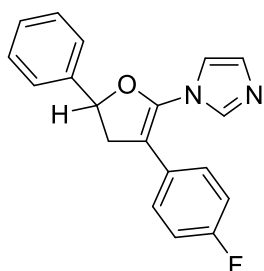
Yield = 80% (69.2 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.65 (s, 1H), 7.39 (dd,  $J$  = 8.2, 1.2 Hz, 2H), 7.37–7.32 (m, 2H), 7.31–7.27 (m, 1H), 7.22–7.16 (m, 2H), 7.13–7.08 (m, 1H), 7.05 (d,  $J$  = 6.1 Hz, 2H), 6.97–6.92 (m, 2H), 5.74–5.65 (m, 1H), 3.53 (dd,  $J$  = 14.6, 10.2 Hz, 1H), 3.24 (dd,  $J$  = 14.6, 8.7 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 141.1, 140.6, 136.6, 132.4, 129.9, 128.9, 128.8, 128.5, 127.0, 126.4, 125.8, 118.1, 100.8, 80.7, 41.8 ppm.

**HRMS (m/z):** calcd for C<sub>19</sub>H<sub>17</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 289.1335, found: 289.1331.



### **1-(3-(4-Fluorophenyl)-5-phenyl-4,5-dihydrofuran-2-yl)-1H-imidazole (3ba):**

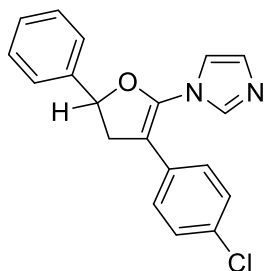
Yield = 81% (74.4 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.71 (s, 1H), 7.49–7.41 (m, 4H), 7.39–7.35 (m, 1H), 7.15–7.12 (m, 1H), 7.10–7.09 (m, 1H), 6.99–6.95 (m, 4H), 5.82–5.75 (m, 1H), 3.59 (dd,  $J$  = 14.6, 10.2 Hz, 1H), 3.29 (dd,  $J$  = 14.6, 8.7 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 161.6 (d,  $J$  = 247.2 Hz), 141.0, 140.5, 136.5, 130.0, 129.0, 128.6, 128.0 (d,  $J$  = 7.9 Hz), 125.8, 118.0, 116.0, 115.7, 99.9, 80.7, 41.9 ppm.

**HRMS (m/z):** calcd for C<sub>19</sub>H<sub>16</sub>FN<sub>2</sub>O [M+H]<sup>+</sup> 307.1241, found: 307.1236.



### **1-(3-(4-Chlorophenyl)-5-phenyl-4,5-dihydrofuran-2-yl)-1H-imidazole (3ca):**

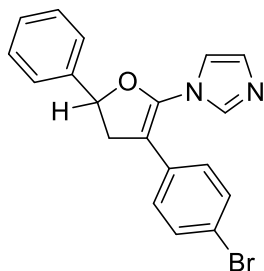
Yield = 90% (87.2 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.71 (s, 1H), 7.49–7.41 (m, 4H), 7.40–7.35 (m, 1H), 7.25–7.21 (m, 2H), 7.14 (s, 1H), 7.09 (s, 1H), 6.97–6.91 (m, 2H), 5.83–5.75 (m, 1H), 3.58 (dd,  $J$  = 14.5, 10.2 Hz, 1H), 3.29 (dd,  $J$  = 14.5, 8.8 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 141.0, 140.8, 136.5, 134.2, 132.5, 130.9, 130.1, 129.0, 128.6, 127.5, 125.8, 118.0, 99.9, 80.8, 41.6 ppm.

**HRMS (m/z):** calcd for C<sub>19</sub>H<sub>16</sub>ClN<sub>2</sub>O [M+H]<sup>+</sup> 323.0946, found: 323.0941.



**1-(3-(4-Bromophenyl)-5-phenyl-4,5-dihydrofuran-2-yl)-1H-imidazole (3da):**

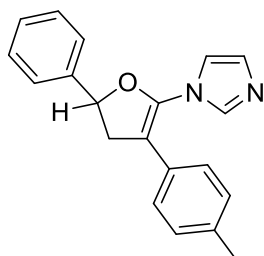
Yield = 89% (98.1 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.71 (s, 1H), 7.50–7.42 (m, 4H), 7.40 (d,  $J$  = 8.9 Hz, 3H), 7.11 (d,  $J$  = 19.2 Hz, 2H), 6.87 (d,  $J$  = 8.5 Hz, 2H), 5.79 (t,  $J$  = 9.5 Hz, 1H), 3.57 (dd,  $J$  = 14.5, 10.2 Hz, 1H), 3.29 (dd,  $J$  = 14.5, 8.8 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 141.1, 140.7, 136.4, 131.9, 131.4, 130.1, 129.0, 128.6, 127.8, 125.8, 120.5, 118.0, 99.9, 80.8, 41.5 ppm.

**HRMS (m/z):** calcd for C<sub>19</sub>H<sub>16</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup> 367.0441, found: 367.0443.



**1-(5-Phenyl-3-(p-tolyl)-4,5-dihydrofuran-2-yl)-1H-imidazole (3ea):**

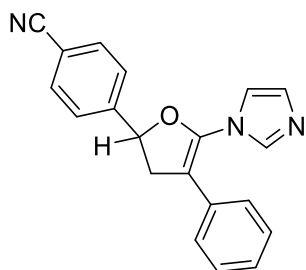
Yield = 56% (50.8 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.72 (s, 1H), 7.49–7.41 (m, 4H), 7.39–7.35 (m, 1H), 7.14–7.07 (m, 4H), 6.92 (d,  $J$  = 8.1 Hz, 2H), 5.77 (t,  $J$  = 9.4 Hz, 1H), 3.59 (dd,  $J$  = 14.6, 10.2 Hz, 1H), 3.30 (dd,  $J$  = 14.6, 8.7 Hz, 1H), 2.32 (s, 3H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 141.2, 140.0, 136.8, 136.6, 129.8, 129.5, 129.4, 128.9, 128.5, 126.3, 125.8, 118.1, 100.8, 80.6, 41.7, 21.2 ppm.

**HRMS (m/z):** calcd for C<sub>20</sub>H<sub>19</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 303.1492, found: 303.1488.



**4-(5-(1*H*-Imidazol-1-yl)-4-phenyl-2,3-dihydrofuran-2-yl)benzonitrile (3fa):**

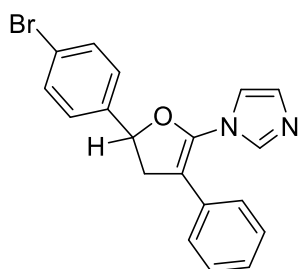
Yield = 91% (85.5 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.82–7.76 (m, 3H), 7.65 (d,  $J$  = 8.2 Hz, 2H), 7.38–7.32 (m, 2H), 7.31–7.27 (m, 1H), 7.24–7.18 (m, 2H), 7.12–7.07 (m, 2H), 5.95–5.88 (m, 1H), 3.76 (dd,  $J$  = 14.6, 10.4 Hz, 1H), 3.33 (dd,  $J$  = 14.6, 8.6 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 146.3, 140.3, 136.4, 132.8, 131.8, 130.0, 128.8, 127.3, 126.34, 126.27, 118.5, 118.0, 112.2, 100.7, 79.4, 41.8 ppm.

**HRMS (m/z):** calcd for C<sub>20</sub>H<sub>16</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 314.1288, found: 314.1283.



**1-(5-(4-Bromophenyl)-3-phenyl-4,5-dihydrofuran-2-yl)-1*H*-imidazole (3ga):**

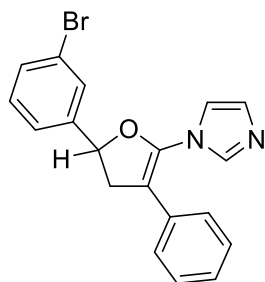
Yield = 88% (97.0 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.80 (s, 1H), 7.66–7.61 (m, 2H), 7.43 (d,  $J$  = 8.4 Hz, 2H), 7.35 (t,  $J$  = 7.4 Hz, 2H), 7.31–7.27 (m, 1H), 7.20 (d,  $J$  = 12.0 Hz, 2H), 7.12–7.08 (m, 2H), 5.82 (t,  $J$  = 9.4 Hz, 1H), 3.69 (dd,  $J$  = 14.6, 10.2 Hz, 1H), 3.35 (dd,  $J$  = 14.6, 8.7 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 140.4, 140.1, 136.5, 132.1, 132.0, 129.9, 128.8, 127.5, 127.1, 126.3, 122.4, 118.0, 100.7, 80.0, 41.7 ppm.

**HRMS (m/z):** calcd for C<sub>19</sub>H<sub>16</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup> 367.0441, found: 367.0439.



**1-(5-(3-Bromophenyl)-3-phenyl-4,5-dihydrofuran-2-yl)-1*H*-imidazole (3ha):**

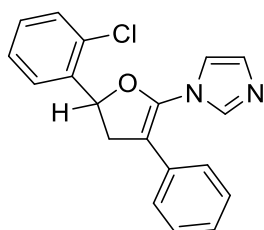
Yield = 83% (91.4 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.74–7.71 (m, 1H), 7.61 (t,  $J$  = 1.7 Hz, 1H), 7.50–7.48 (m, 1H), 7.39 (d,  $J$  = 7.8 Hz, 1H), 7.28 (dd,  $J$  = 8.5, 1.4 Hz, 2H), 7.25 (d,  $J$  = 1.4 Hz, 1H), 7.22–7.18 (m, 1H), 7.15–7.13 (m, 1H), 7.11 (t,  $J$  = 1.3 Hz, 1H), 7.03–7.00 (m, 2H), 5.77–5.71 (m, 1H), 3.60 (dd,  $J$  = 14.6, 10.2 Hz, 1H), 3.28 (dd,  $J$  = 14.6, 8.8 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 143.3, 140.4, 136.6, 136.5, 132.1, 131.5, 130.6, 130.0, 128.9, 127.1, 126.4, 124.4, 123.0, 118.1, 100.8, 79.7, 41.8 ppm.

**HRMS (m/z):** calcd for C<sub>19</sub>H<sub>16</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup> 367.0441, found: 367.0438.



**1-(5-(2-Chlorophenyl)-3-phenyl-4,5-dihydrofuran-2-yl)-1H-imidazole (3ia):**

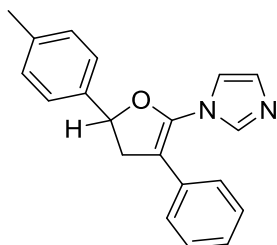
Yield = 89% (86.2 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.75 (s, 1H), 7.61–7.57 (m, 1H), 7.42 (dd,  $J$  = 7.7, 1.4 Hz, 1H), 7.34 (dd,  $J$  = 7.4, 1.3 Hz, 1H), 7.32–7.26 (m, 2H), 7.25 (d,  $J$  = 1.4 Hz, 1H), 7.20–7.15 (m, 3H), 7.03–6.98 (m, 2H), 6.06 (dd,  $J$  = 10.3, 8.3 Hz, 1H), 3.80 (dd,  $J$  = 14.8, 10.4 Hz, 1H), 3.13 (dd,  $J$  = 14.8, 8.3 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 140.3, 139.1, 136.5, 132.1, 131.3, 130.0, 129.9, 129.3, 128.8, 127.3, 127.1, 126.4, 126.2, 118.1, 100.9, 77.7, 41.1 ppm.

**HRMS (m/z):** calcd for C<sub>19</sub>H<sub>16</sub>ClN<sub>2</sub>O [M+H]<sup>+</sup> 323.0946, found: 323.0941.



**1-(3-Phenyl-5-(p-tolyl)-4,5-dihydrofuran-2-yl)-1H-imidazole (3ja):**

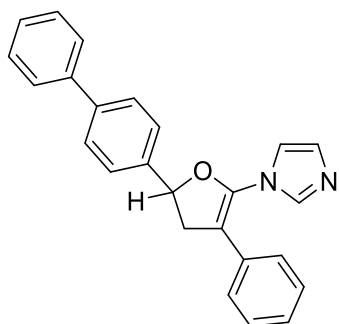
Yield = 78% (70.8 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.72 (s, 1H), 7.38 (d,  $J$  = 8.1 Hz, 2H), 7.29–7.27 (m, 1H), 7.26–7.17 (m, 4H), 7.12 (d,  $J$  = 6.0 Hz, 2H), 7.05–7.01 (m, 2H), 5.75 (t,  $J$  = 9.5 Hz, 1H), 3.58 (dd,  $J$  = 14.6, 10.1 Hz, 1H), 3.32 (dd,  $J$  = 14.6, 8.8 Hz, 1H), 2.39 (s, 3H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 140.6, 138.4, 138.0, 136.6, 132.5, 129.8, 129.6, 128.8, 126.9, 126.3, 125.9, 118.1, 100.8, 80.8, 41.7, 21.3 ppm.

**HRMS (m/z):** calcd for C<sub>20</sub>H<sub>19</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 303.1492, found: 303.1487.



**1-(5-([1,1'-Biphenyl]-4-yl)-3-phenyl-4,5-dihydrofuran-2-yl)-1H-imidazole (3ka):**

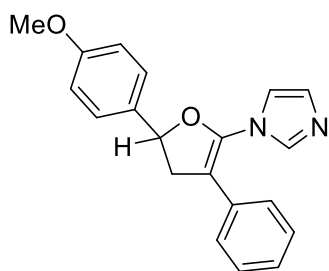
Yield = 94% (102.8 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.76 (s, 1H), 7.70–7.66 (m, 2H), 7.64–7.61 (m, 2H), 7.59–7.55 (m, 2H), 7.50–7.46 (m, 2H), 7.41–7.37 (m, 1H), 7.33–7.27 (m, 2H), 7.24–7.19 (m, 1H), 7.16–7.14 (m, 2H), 7.07–7.05 (m, 2H), 5.88–5.81 (m, 1H), 3.65 (dd,  $J$  = 14.6, 10.2 Hz, 1H), 3.38 (dd,  $J$  = 14.6, 8.8 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 141.5, 140.6, 140.5, 140.0, 136.5, 132.4, 129.9, 128.9, 128.8, 127.7, 127.6, 127.2, 127.0, 126.34, 126.33, 118.1, 100.8, 80.5, 41.7 ppm.

**HRMS (m/z):** calcd for C<sub>25</sub>H<sub>21</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 365.1648, found: 365.1643.



**1-(5-(4-Methoxyphenyl)-3-phenyl-4,5-dihydrofuran-2-yl)-1H-imidazole (3la):**

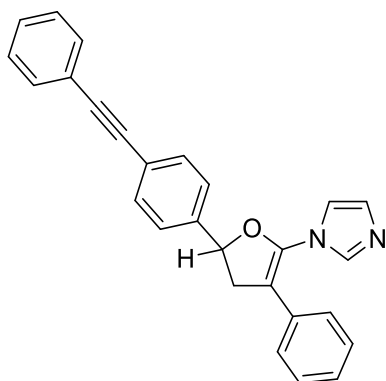
Yield = 58% (55.4 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.79 (s, 1H), 7.51 (d,  $J$  = 8.7 Hz, 2H), 7.36 (dd,  $J$  = 9.2, 5.7 Hz, 2H), 7.29 (d,  $J$  = 7.3 Hz, 1H), 7.19 (d,  $J$  = 6.3 Hz, 2H), 7.14–7.10 (m, 2H), 7.04 (d,  $J$  = 8.7 Hz, 2H), 5.82 (t,  $J$  = 9.5 Hz, 1H), 3.92 (s, 3H), 3.64 (dd,  $J$  = 14.6, 10.1 Hz, 1H), 3.42 (dd,  $J$  = 14.6, 8.9 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 159.9, 140.5, 136.6, 132.9, 132.5, 129.8, 128.8, 127.5, 126.9, 126.3, 118.1, 114.3, 100.8, 80.8, 55.5, 41.6 ppm.

**HRMS (m/z):** calcd for C<sub>20</sub>H<sub>19</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> 319.1441, found: 319.1443.



**1-(3-Phenyl-5-(4-(phenylethynyl)phenyl)-4,5-dihydrofuran-2-yl)-1H-imidazole (3ma):**

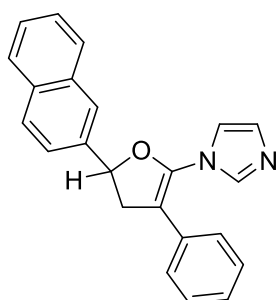
Yield = 87% (101.4 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.70 (s, 1H), 7.58–7.51 (m, 4H), 7.41 (d,  $J$  = 8.2 Hz, 2H), 7.32 (d,  $J$  = 2.0 Hz, 3H), 7.24 (dd,  $J$  = 7.2, 6.0 Hz, 2H), 7.19–7.14 (m, 1H), 7.12–7.08 (m, 2H), 7.02–6.98 (m, 2H), 5.75 (t,  $J$  = 9.5 Hz, 1H), 3.57 (dd,  $J$  = 14.6, 10.2 Hz, 1H), 3.26 (dd,  $J$  = 14.6, 8.8 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 141.0, 140.5, 136.5, 132.2, 132.1, 131.7, 129.9, 128.8, 128.51, 128.47, 127.0, 126.3, 125.9, 123.5, 123.1, 118.1, 100.8, 90.1, 89.0, 80.3, 41.7 ppm.

**HRMS (m/z):** calcd for C<sub>27</sub>H<sub>21</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 389.1648, found: 389.1651.



**1-(5-(Naphthalen-2-yl)-3-phenyl-4,5-dihydrofuran-2-yl)-1H-imidazole (3na):**

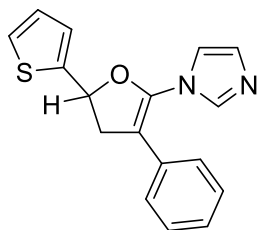
Yield = 82% (83.2 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.95–7.86 (m, 4H), 7.80 (s, 1H), 7.60 (dd,  $J$  = 8.5, 1.7 Hz, 1H), 7.56–7.50 (m, 2H), 7.30 (t,  $J$  = 7.5 Hz, 2H), 7.24–7.16 (m, 3H), 7.09–7.04 (m, 2H), 5.95 (t,  $J$  = 9.5 Hz, 1H), 3.66 (dd,  $J$  = 14.6, 10.2 Hz, 1H), 3.42 (dd,  $J$  = 14.6, 8.9 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 140.6, 138.2, 136.6, 133.24, 133.15, 132.3, 129.9, 129.0, 128.8, 128.1, 127.8, 126.9, 126.6, 126.5, 126.3, 124.9, 123.4, 118.1, 100.8, 80.9, 41.7 ppm.

**HRMS (m/z):** calcd for C<sub>23</sub>H<sub>19</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 339.1492, found: 339.1490.



**1-(3-Phenyl-5-(thiophen-2-yl)-4,5-dihydrofuran-2-yl)-1H-imidazole (3oa):**

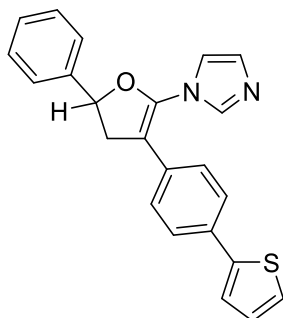
Yield = 84% (74.2 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.75 (s, 1H), 7.41 (dd,  $J$  = 5.1, 1.1 Hz, 1H), 7.37–7.32 (m, 2H), 7.30–7.27 (m, 1H), 7.24 (dd,  $J$  = 5.3, 2.3 Hz, 1H), 7.16 (d,  $J$  = 13.5 Hz, 2H), 7.12–7.08 (m, 3H), 6.04 (dd,  $J$  = 9.4, 8.0 Hz, 1H), 3.72 (dd,  $J$  = 14.7, 9.8 Hz, 1H), 3.47 (dd,  $J$  = 14.7, 7.7 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 143.6, 140.1, 136.5, 132.2, 129.9, 128.8, 127.02, 126.98, 126.3, 126.1, 125.8, 118.1, 101.0, 76.6, 41.8 ppm.

**HRMS (m/z):** calcd for C<sub>17</sub>H<sub>15</sub>N<sub>2</sub>OS [M+H]<sup>+</sup> 295.0900, found: 295.0905.



**1-(5-Phenyl-3-(4-(thiophen-2-yl)phenyl)-4,5-dihydrofuran-2-yl)-1H-imidazole (3pa):**

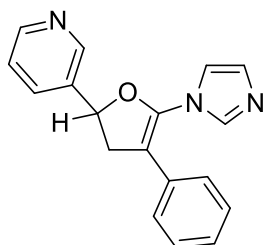
Yield = 84% (93.4 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.71 (s, 1H), 7.51–7.41 (m, 5H), 7.37 (dd,  $J$  = 8.1, 4.4 Hz, 4H), 7.11 (d,  $J$  = 16.6 Hz, 3H), 6.91–6.83 (m, 2H), 5.82–5.76 (m, 1H), 3.58 (dd,  $J$  = 14.5, 10.2 Hz, 1H), 3.30 (dd,  $J$  = 14.5, 8.8 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 141.1, 140.7, 136.5, 134.6, 134.4, 133.9, 133.7, 131.9, 131.4, 130.1, 129.0, 128.6, 127.8, 125.8, 120.6, 118.0, 99.9, 80.8, 41.5 ppm.

**HRMS (m/z):** calcd for C<sub>23</sub>H<sub>19</sub>N<sub>2</sub>OS [M+H]<sup>+</sup> 371.1213, found: 371.1210.



**3-(5-(1H-Imidazol-1-yl)-4-phenyl-2,3-dihydrofuran-2-yl)pyridine (3qa):**

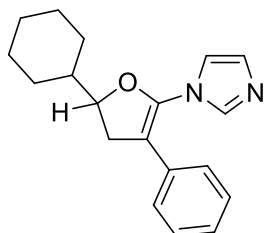
Yield = 61% (52.9 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 8.79 (d,  $J$  = 1.7 Hz, 1H), 8.73–8.69 (m, 1H), 7.90 (d,  $J$  = 7.9 Hz, 1H), 7.80 (s, 1H), 7.44 (dd,  $J$  = 7.8, 4.8 Hz, 1H), 7.35 (t,  $J$  = 7.5 Hz, 2H), 7.29 (d,  $J$  = 7.3 Hz, 1H), 7.20 (d,  $J$  = 11.9 Hz, 2H), 7.10 (d,  $J$  = 7.3 Hz, 2H), 5.89 (t,  $J$  = 9.4 Hz, 1H), 3.74 (dd,  $J$  = 14.6, 10.2 Hz, 1H), 3.38 (dd,  $J$  = 14.6, 8.6 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 150.0, 147.7, 140.4, 139.6, 136.5, 133.4, 131.9, 130.0, 128.9, 127.2, 126.4, 123.8, 118.0, 100.7, 78.4, 41.6 ppm.

**HRMS (m/z):** calcd for C<sub>18</sub>H<sub>16</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 290.1288, found: 290.1283.



**1-(5-Cyclohexyl-3-phenyl-4,5-dihydrofuran-2-yl)-1H-imidazole (3ra):**

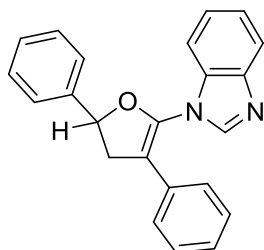
Yield = 42% (37.1 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.75 (s, 1H), 7.38–7.34 (m, 2H), 7.30–7.27 (m, 1H), 7.21 (s, 1H), 7.15 (s, 1H), 7.10–7.07 (m, 2H), 4.66–4.59 (m, 1H), 3.30–3.10 (m, 2H), 2.09 (d,  $J$  = 12.7 Hz, 1H), 1.95–1.79 (m, 5H), 1.45–1.34 (m, 4H), 1.27–1.16 (m, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 140.8, 136.5, 132.9, 129.7, 128.8, 126.6, 126.2, 118.1, 100.9, 84.1, 43.0, 36.7, 28.4, 28.1, 26.5, 25.9, 25.8 ppm.

**HRMS (m/z):** calcd for C<sub>19</sub>H<sub>23</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 295.1805, found: 295.1804.



**1-(3,5-Diphenyl-4,5-dihydrofuran-2-yl)-1H-benzo[d]imidazole (3ab):**

Yield = 71% (72.1 mg). Yellow oil.

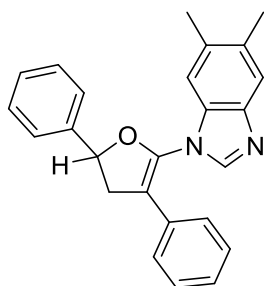
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 2/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 8.06–8.05 (m, 1H), 7.88–7.86 (m, 1H), 7.57–7.52 (m, 2H), 7.48–7.43 (m, 2H), 7.41–7.38 (m, 1H), 7.37–7.32 (m, 2H), 7.30–7.27 (m, 1H), 7.22–7.14 (m, 3H), 6.99–6.93 (m, 2H), 5.92–5.84 (m, 1H), 3.77–3.70 (m, 1H), 3.48–3.42 (m, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 143.5, 142.0, 141.1, 140.2, 132.32, 132.28, 132.2, 129.0, 128.8, 128.6, 126.9, 125.9, 124.3, 123.4, 120.6, 112.2, 103.5, 80.7, 41.2 ppm.

**HRMS (m/z):** calcd for C<sub>23</sub>H<sub>19</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 339.1492, found: 339.1491.





**1-(3,5-Diphenyl-4,5-dihydrofuran-2-yl)-5,6-dimethyl-1H-benzo[d]imidazole (3ac):**

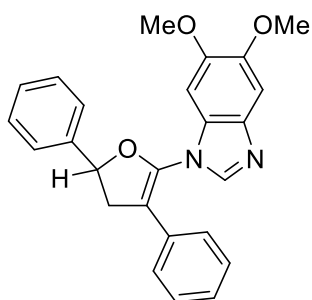
Yield = 68% (74.8 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.90 (s, 1H), 7.62 (s, 1H), 7.57–7.53 (m, 2H), 7.49–7.43 (m, 2H), 7.41–7.36 (m, 1H), 7.22–7.14 (m, 4H), 6.99–6.92 (m, 2H), 5.88 (t,  $J$  = 9.5 Hz, 1H), 3.72 (dd,  $J$  = 14.7, 10.2 Hz, 1H), 3.44 (dd,  $J$  = 14.7, 8.8 Hz, 1H), 2.38 (s, 3H), 2.31 (s, 3H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 142.0, 141.2, 140.5, 134.3, 133.5, 132.32, 132.30, 130.9, 128.9, 128.7, 128.5, 126.7, 125.92, 125.87, 120.5, 112.2, 103.4, 80.6, 41.1, 20.6, 20.4 ppm.

**HRMS (m/z):** calcd for C<sub>25</sub>H<sub>23</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 367.1805, found: 367.1808.



**1-(3,5-Diphenyl-4,5-dihydrofuran-2-yl)-5,6-dimethoxy-1H-benzo[d]imidazole (3ad):**

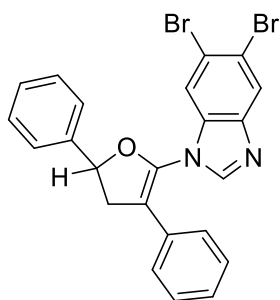
Yield = 59% (70.5 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.93 (s, 1H), 7.56–7.52 (m, 2H), 7.47–7.41 (m, 2H), 7.40–7.35 (m, 1H), 7.28 (s, 1H), 7.21–7.13 (m, 3H), 6.96–6.92 (m, 2H), 6.57 (s, 1H), 5.86 (dd,  $J$  = 10.1, 8.4 Hz, 1H), 3.91 (s, 3H), 3.75 (dd,  $J$  = 14.6, 10.2 Hz, 1H), 3.61 (s, 3H), 3.44 (dd,  $J$  = 14.7, 8.3 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 147.8, 147.2, 141.1, 140.22, 140.18, 136.7, 132.4, 129.0, 128.7, 128.6, 126.8, 126.1, 125.9, 125.6, 102.3, 102.0, 94.9, 80.5, 56.3, 56.0, 41.0 ppm.

**HRMS (m/z):** calcd for C<sub>25</sub>H<sub>23</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 399.1703, found: 399.1701.



**5,6-Dibromo-1-(3,5-diphenyl-4,5-dihydrofuran-2-yl)-1H-benzo[d]imidazole (3ae):**

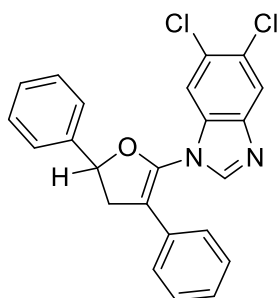
Yield = 56% (83.4 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 8.12 (d,  $J$  = 1.8 Hz, 1H), 7.99 (d,  $J$  = 1.1 Hz, 1H), 7.66–7.62 (m, 1H), 7.53 (d,  $J$  = 7.9 Hz, 2H), 7.47 (t,  $J$  = 7.4 Hz, 2H), 7.42 (d,  $J$  = 7.2 Hz, 1H), 7.25–7.19 (m, 3H), 6.93 (d,  $J$  = 7.5 Hz, 2H), 5.90 (t,  $J$  = 9.6 Hz, 1H), 3.70 (dd,  $J$  = 14.8, 10.2 Hz, 1H), 3.48 (dd,  $J$  = 14.8, 9.1 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 143.6, 140.6, 139.0, 134.1, 132.2, 131.6, 129.0, 128.9, 128.7, 127.8, 127.3, 125.9 (d,  $J$  = 3.0 Hz), 124.9, 119.8, 118.9, 116.8, 104.2, 81.1, 41.0 ppm.

**HRMS (m/z):** calcd for C<sub>23</sub>H<sub>17</sub>Br<sub>2</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 494.9702, found: 494.9701.



**5,6-Dichloro-1-(3,5-diphenyl-4,5-dihydrofuran-2-yl)-1H-benzo[d]imidazole (3af):**

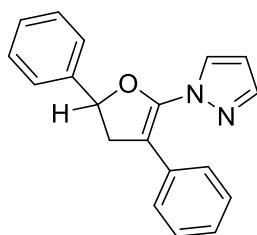
Yield = 40% (48.9 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 8.00 (s, 1H), 7.91 (s, 1H), 7.53–7.50 (m, 2H), 7.47–7.41 (m, 4H), 7.25–7.21 (m, 2H), 7.19 (dd,  $J$  = 3.4, 2.0 Hz, 1H), 6.91 (dd,  $J$  = 8.1, 1.3 Hz, 2H), 5.88 (t,  $J$  = 9.6 Hz, 1H), 3.69 (dd,  $J$  = 14.8, 10.2 Hz, 1H), 3.46 (dd,  $J$  = 14.8, 9.1 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 143.7, 142.7, 140.6, 139.1, 131.7, 131.4, 129.1, 129.0, 128.8, 128.5, 127.7, 127.3, 125.98, 125.96, 121.8, 113.7, 104.2, 81.1, 41.1 ppm.

**HRMS (m/z):** calcd for C<sub>23</sub>H<sub>17</sub>Cl<sub>2</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 407.0712, found: 407.0713.



**1-(3,5-Diphenyl-4,5-dihydrofuran-2-yl)-1H-pyrazole (3ag):**

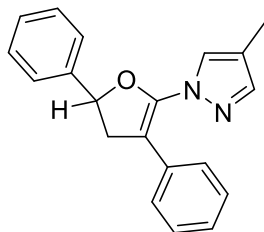
Yield = 51% (44.1 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.71 (d,  $J$  = 1.5 Hz, 1H), 7.56 (d,  $J$  = 2.5 Hz, 1H), 7.46 (d,  $J$  = 7.3 Hz, 2H), 7.35 (t,  $J$  = 7.4 Hz, 2H), 7.28 (dd,  $J$  = 5.9, 3.7 Hz, 1H), 7.17 (t,  $J$  = 7.4 Hz, 2H), 7.09 (dd,  $J$  = 8.3, 6.4 Hz, 1H), 6.91 (s, 2H), 6.35–6.33 (m, 1H), 5.79–5.72 (m, 1H), 3.57 (dd,  $J$  = 14.6, 10.2 Hz, 1H), 3.28 (dd,  $J$  = 14.6, 8.8 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 143.2, 142.0, 141.3, 132.6, 130.8, 128.8, 128.4, 128.3, 126.6, 126.4, 125.9, 107.3, 102.1, 80.5, 41.6 ppm.

**HRMS (m/z):** calcd for C<sub>19</sub>H<sub>17</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 289.1330, found: 289.1332.



**1-(3,5-Diphenyl-4,5-dihydrofuran-2-yl)-4-methyl-1H-pyrazole (3ah):**

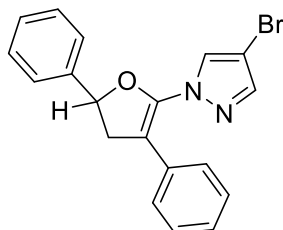
Yield = 55% (49.9 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.51 (s, 1H), 7.47–7.42 (m, 2H), 7.37–7.31 (m, 3H), 7.29–7.27 (m, 1H), 7.19–7.15 (m, 2H), 7.11–7.06 (m, 1H), 6.95 (dd,  $J$  = 8.3, 1.2 Hz, 2H), 5.75–5.68 (m, 1H), 3.55 (dd,  $J$  = 14.5, 10.2 Hz, 1H), 3.26 (dd,  $J$  = 14.5, 8.7 Hz, 1H), 2.04 (s, 3H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 143.3, 142.8, 141.4, 132.8, 128.84, 128.75, 128.3, 128.2, 126.39, 126.35, 125.9, 117.8, 101.2, 80.3, 41.6, 8.9 ppm.

**HRMS (m/z):** calcd for C<sub>20</sub>H<sub>19</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 303.1492, found: 303.1489.



**4-Bromo-1-(3,5-diphenyl-4,5-dihydrofuran-2-yl)-1H-pyrazole (3ai):**

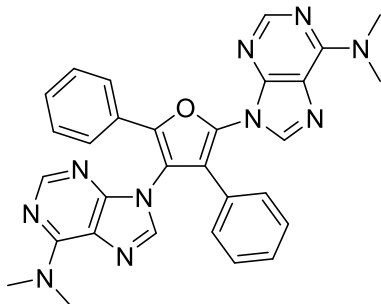
Yield = 48% (52.9 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.61 (dd,  $J$  = 12.2, 1.2 Hz, 2H), 7.45–7.40 (m, 2H), 7.34 (t,  $J$  = 6.6 Hz, 2H), 7.31–7.27 (m, 1H), 7.22–7.17 (m, 2H), 7.14–7.10 (m, 1H), 6.99–6.93 (m, 2H), 5.73 (t,  $J$  = 9.5 Hz, 1H), 3.56 (dd,  $J$  = 14.7, 10.2 Hz, 1H), 3.28 (dd,  $J$  = 14.7, 8.8 Hz, 1H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 150.7, 142.5, 141.0, 132.1, 130.5, 128.9, 128.5, 128.4, 126.9, 126.5, 125.9, 102.5, 95.4, 80.7, 41.6 ppm.

**HRMS (m/z):** calcd for C<sub>19</sub>H<sub>16</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup> 367.0441, found: 367.0440.



**9,9'-(3,5-Diphenylfuran-2,4-diyl)bis(*N,N*-dimethyl-9H-purin-6-amine) (3aj):**

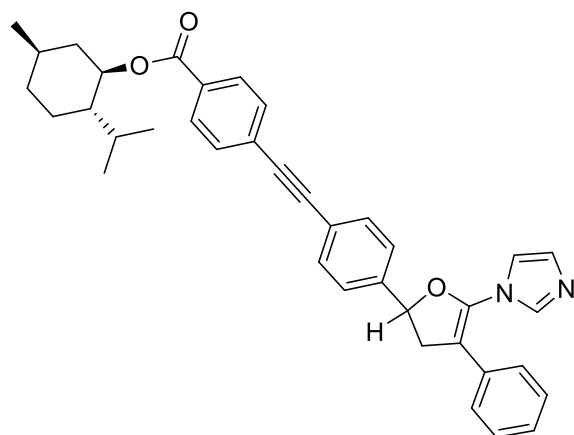
Yield = 30% (48.8 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 1/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 8.45 (s, 1H), 8.40 (s, 1H), 7.74 (s, 1H), 7.66 (s, 1H), 7.23 (s, 5H), 7.16–7.10 (m, 1H), 7.07 (t,  $J$  = 7.5 Hz, 2H), 6.99 (d,  $J$  = 7.8 Hz, 2H), 3.51 (brs, 12H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 155.2, 155.1, 153.9, 153.7, 152.8, 152.0, 149.0, 138.5, 138.3, 134.9, 134.1, 129.4, 128.9, 128.6, 128.1, 127.4, 127.1, 125.3, 122.8, 119.8, 119.3, 115.5, 39.2–38.0 (m, 2C) ppm.

**HRMS (m/z):** calcd for C<sub>30</sub>H<sub>27</sub>N<sub>10</sub>O [M+H]<sup>+</sup> 543.2364, found: 543.2359.



**(1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl 4-((4-(5-(1H-imidazol-1-yl)-4-phenyl-2,3-dihydrofuran-2-yl)phenyl)ethynyl)benzoate (3sa):**

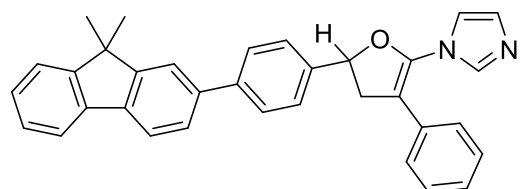
Yield = 84% (143.8 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.96 (d,  $J$  = 8.3 Hz, 2H), 7.64 (d,  $J$  = 8.8 Hz, 1H), 7.52 (dd,  $J$  = 8.2, 3.7 Hz, 4H), 7.38 (d,  $J$  = 8.1 Hz, 2H), 7.18 (dd,  $J$  = 9.4, 5.3 Hz, 2H), 7.11 (t,  $J$  = 6.8 Hz, 1H), 7.07–7.03 (m, 2H), 6.97–6.92 (m, 2H), 5.71 (t,  $J$  = 9.5 Hz, 1H), 4.90–4.84 (m, 1H), 3.57–3.48 (m, 1H), 3.26–3.12 (m, 1H), 2.05 (d,  $J$  = 12.0 Hz, 1H), 1.92–1.85 (m, 1H), 1.65 (d,  $J$  = 11.7 Hz, 2H), 1.55–1.42 (m, 2H), 1.13–0.98 (m, 2H), 0.85 (d,  $J$  = 6.6 Hz, 7H), 0.72 (d,  $J$  = 6.9 Hz, 3H) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 165.6, 141.6, 140.5, 136.5, 132.3, 131.6, 130.4, 129.9, 129.6, 128.8, 127.6, 127.1, 126.3, 125.8, 122.9, 118.1, 100.8, 91.7, 89.4, 80.2, 75.2, 47.3, 41.8, 41.0, 34.3, 31.5, 26.6, 23.7, 22.1, 20.9, 16.6 ppm.

**HRMS (m/z):** calcd for C<sub>38</sub>H<sub>39</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 571.2955, found: 571.2952.



**1-(5-(4-(9,9-Dimethyl-9H-fluoren-2-yl)phenyl)-3-phenyl-4,5-dihydrofuran-2-yl)-1H-imidazole (3ta):**

Yield = 81% (116.8 mg). Yellow oil.

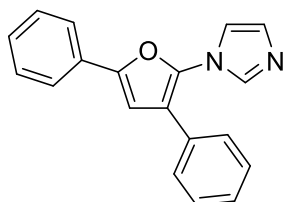
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.84–7.79 (m, 2H), 7.79–7.73 (m, 3H), 7.70 (d,  $J$  = 1.3 Hz, 1H), 7.63–7.58 (m, 3H), 7.51–7.48 (m, 1H), 7.41–7.36 (m, 2H), 7.34–7.29 (m, 2H), 7.25–7.21 (m, 1H),

7.20–7.17 (m, 2H), 7.10–7.06 (m, 2H), 5.85 (t,  $J = 9.4$  Hz, 1H), 3.66 (dd,  $J = 14.6, 10.2$  Hz, 1H), 3.40 (dd,  $J = 14.6, 8.7$  Hz, 1H), 1.58 (s, 6H) ppm.

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 154.4, 153.9, 141.9, 140.6, 139.8, 139.7, 138.81, 138.77, 136.6, 134.3, 134.2, 132.4, 129.9, 128.8, 127.7, 127.5, 127.1, 126.9, 126.34, 126.25, 122.7, 121.4, 120.4, 120.2, 118.1, 100.8, 80.5, 47.0, 41.7, 27.3$  ppm.

HRMS ( $m/z$ ): calcd for  $\text{C}_{34}\text{H}_{29}\text{N}_2\text{O}$   $[\text{M}+\text{H}]^+$  481.2274, found: 481.2273.



**1-(3,5-Diphenylfuran-2-yl)-1H-imidazole (4):**

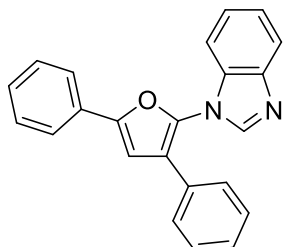
Yield = 62% (53.3 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.72$  (s, 1H), 7.70 (t,  $J = 1.6$  Hz, 1H), 7.69–7.68 (m, 1H), 7.43–7.40 (m, 2H), 7.35–7.28 (m, 4H), 7.21 (d,  $J = 1.7$  Hz, 2H), 7.19 (t,  $J = 1.5$  Hz, 1H), 7.17 (d,  $J = 1.3$  Hz, 1H), 6.95 (s, 1H) ppm.

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 151.0, 137.7, 137.5, 130.4, 130.2, 129.5, 129.1, 129.0, 128.4, 128.0, 127.0, 123.9, 119.8, 118.4, 106.6$  ppm.

HRMS ( $m/z$ ): calcd for  $\text{C}_{19}\text{H}_{15}\text{N}_2\text{O}$   $[\text{M}+\text{H}]^+$  287.1179, found: 287.1179.



**1-(3,5-Diphenylfuran-2-yl)-1H-benzo[d]imidazole (5):**

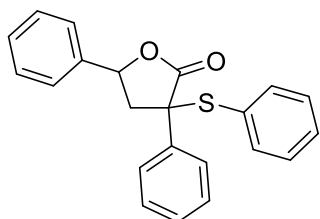
Yield = 65% (65.6 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 4/1).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.97$  (s, 1H), 7.89 (d,  $J = 7.6$  Hz, 1H), 7.72–7.68 (m, 2H), 7.40 (t,  $J = 7.7$  Hz, 2H), 7.35–7.28 (m, 4H), 7.24–7.20 (m, 3H), 7.17–7.14 (m, 2H), 7.06 (s, 1H) ppm.

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 151.9, 143.2, 142.8, 136.3, 133.9, 130.2, 129.5, 129.1, 129.0, 128.5, 128.0, 126.7, 124.5, 123.9, 123.5, 120.6, 120.4, 111.2, 106.3$  ppm.

HRMS ( $m/z$ ): calcd for  $\text{C}_{23}\text{H}_{17}\text{N}_2\text{O}$   $[\text{M}+\text{H}]^+$  337.1335, found: 337.1330.



**3,5-Diphenyl-3-(phenylthio)dihydrofuran-2(3H)-one (6):**

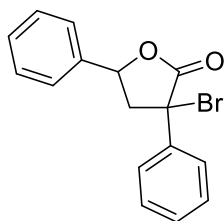
Yield = 31% (32.2 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 7.61–7.52 (m, 3H), 7.39–7.34 (m, 6H), 7.30–7.28 (m, 3H), 7.23 (dd,  $J$  = 7.2, 1.7 Hz, 3H), 5.73 (dd,  $J$  = 10.5, 5.6 Hz, 1H), 3.14 (dd,  $J$  = 13.8, 5.6 Hz, 1H), 2.77 (dd,  $J$  = 13.8, 10.5 Hz, 1H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 172.8, 144.6, 138.3 (d,  $J$  = 6.4 Hz), 137.0, 130.2, 129.5, 128.9, 128.8, 128.3, 128.0, 127.6, 125.8, 122.1, 77.8, 57.3, 46.3 ppm.

**HRMS** ( $m/z$ ): calcd for  $\text{C}_{22}\text{H}_{19}\text{O}_2\text{S}$  [ $\text{M}+\text{H}$ ] $^+$  347.1100, found: 347.1102.



**3-Bromo-3,5-diphenyldihydrofuran-2(3H)-one (7):**

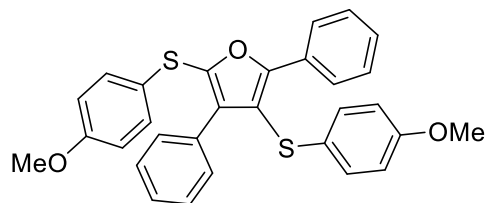
Yield = 37% (35.2 mg). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 7.86–7.83 (m, 2H), 7.45–7.37 (m, 8H), 5.80 (dd,  $J$  = 10.1, 4.7 Hz, 1H), 3.35 (dd,  $J$  = 14.5, 4.7 Hz, 1H), 2.80 (dd,  $J$  = 14.5, 10.1 Hz, 1H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 172.0, 137.3, 136.9, 129.5, 129.2, 129.1, 128.9, 127.8, 126.0, 78.9, 57.2, 49.0 ppm.

**HRMS** ( $m/z$ ): calcd for  $\text{C}_{16}\text{H}_{14}\text{BrO}_2$  [ $\text{M}+\text{H}$ ] $^+$  317.0172, found: 317.0176.



**2,4-Bis((4-methoxyphenyl)thio)-3,5-diphenylfuran (10b):**

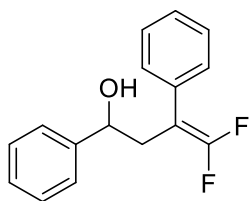
Yield = 42% (62.6 mg). Colorless oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 20/1).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 8.02 (d,  $J$  = 7.2 Hz, 2H), 7.30 (t,  $J$  = 7.4 Hz, 2H), 7.23 (d,  $J$  = 9.5 Hz, 6H), 7.17–7.14 (m, 2H), 6.87 (d,  $J$  = 8.8 Hz, 2H), 6.72 (d,  $J$  = 8.8 Hz, 2H), 6.59 (d,  $J$  = 8.8 Hz, 2H), 3.67 (s, 3H), 3.62 (s, 3H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 159.3, 158.2, 141.8, 137.2, 131.5, 131.3, 130.2, 129.8, 129.2, 129.0, 128.6, 127.99–127.94 (3C), 127.5, 126.7, 125.8, 115.0, 114.8, 112.2, 55.5, 55.4 ppm.

**HRMS** ( $m/z$ ): calcd for  $\text{C}_{30}\text{H}_{25}\text{O}_3\text{S}_2$  [ $\text{M}+\text{H}$ ] $^+$  497.1240, found: 497.1242.



**4,4-Difluoro-1,3-diphenylbut-3-en-1-ol (3aa-I):**

Yield = 36% (28.1 mg). Colorless oil.

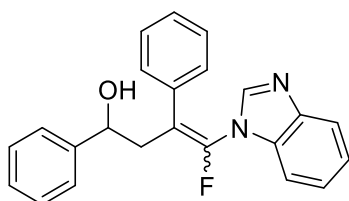
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 100/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.43–7.38 (m, 2H), 7.37–7.33 (m, 5H), 7.32–7.28 (m, 3H), 4.62 (dd,  $J$  = 8.1, 5.7 Hz, 1H), 2.99–2.88 (m, 1H), 2.81–2.75 (m, 1H), 2.13 (brs, 1H) ppm.

**<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>):**  $\delta$  = -89.9 – -90.0 (m, 2F) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 163.5–149.5 (m, 1C), 143.6, 133.3, 128.7, 128.6, 128.5, 128.0, 127.6, 126.0, 89.6 (dd,  $J$  = 19.3, 16.9 Hz), 72.3 (t,  $J$  = 2.9 Hz), 37.7 ppm.

**HRMS (m/z):** calcd for C<sub>16</sub>H<sub>15</sub>F<sub>2</sub>O [M+H]<sup>+</sup> 261.1085, found: 261.1080.



**4-(1H-Benzo[d]imidazol-1-yl)-4-fluoro-1,3-diphenylbut-3-en-1-ol (3aa-II):**

Yield = 87% (93.5 mg,  $Z/E$  = 1/11). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 2/1).

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:**  $\delta$  = 7.60–7.56 (m, 1H), 7.34–7.31 (m, 5H), 7.29–7.27 (m, 1H), 7.25–7.21 (m, 2H), 7.11–7.07 (m, 4H), 6.90–6.87 (m, 2H), 4.66 (t,  $J$  = 7.1 Hz, 1H), 3.74 (brs, 1H), 3.25–3.10 (m, 2H) ppm.

**<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:**  $\delta$  = -92.68 (s, 1F) ppm; ***Z*-isomer:**  $\delta$  = -91.31 (s, 1F) ppm.

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:**  $\delta$  = 144.0, 143.7, 142.3, 141.4, 134.6 (d,  $J$  = 3.8 Hz), 133.1 (d,  $J$  = 3.9 Hz), 128.8, 128.4, 128.1, 127.9, 127.74, 127.71, 126.3, 120.2, 115.7, 115.4, 111.0, 72.0 (d,  $J$  = 2.9 Hz), 39.6 ppm.

**HRMS (m/z):** calcd for C<sub>23</sub>H<sub>20</sub>FN<sub>2</sub>O [M+H]<sup>+</sup> 359.1554, found: 359.1553.

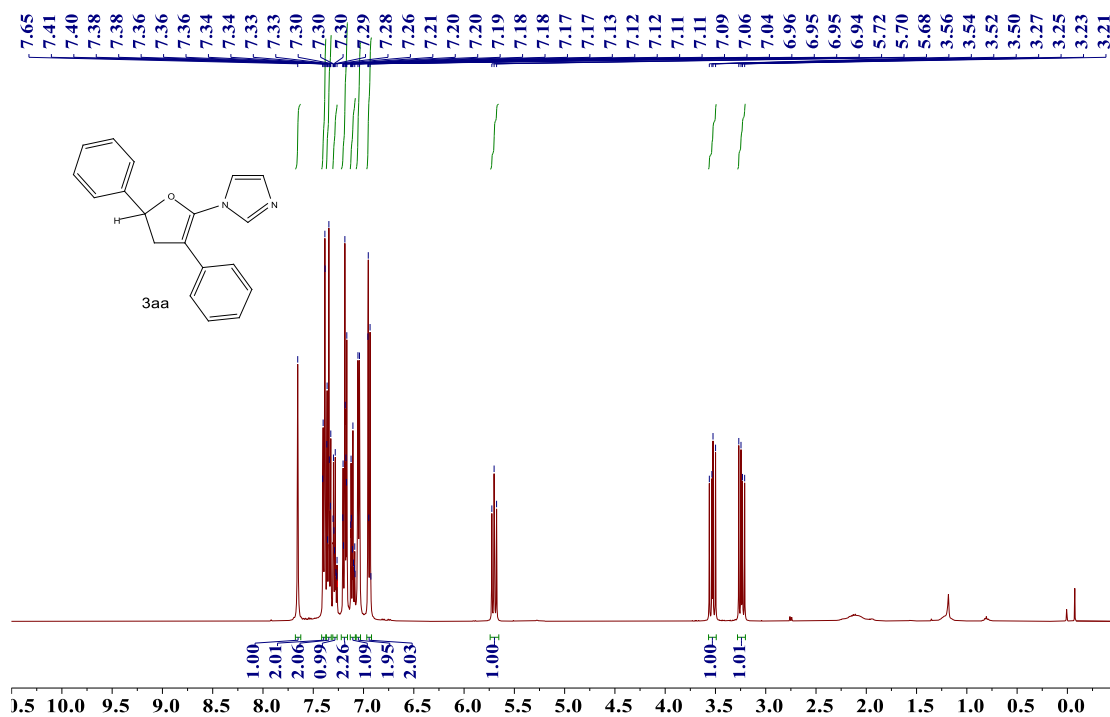
**References**

[1] Chu, X.-Q.; Sun, L.-W.; Chen, Y.-L.; Chen, J.-W.; Yu, Z.-L.; Ma, M.; Shen, Z.-L. HP(O)Ph<sub>2</sub>/H<sub>2</sub>O-Promoted Hydrodefluorination of Trifluoromethyl Alkenes, *Green Chem.* **2022**, *24*, 2777–2782.

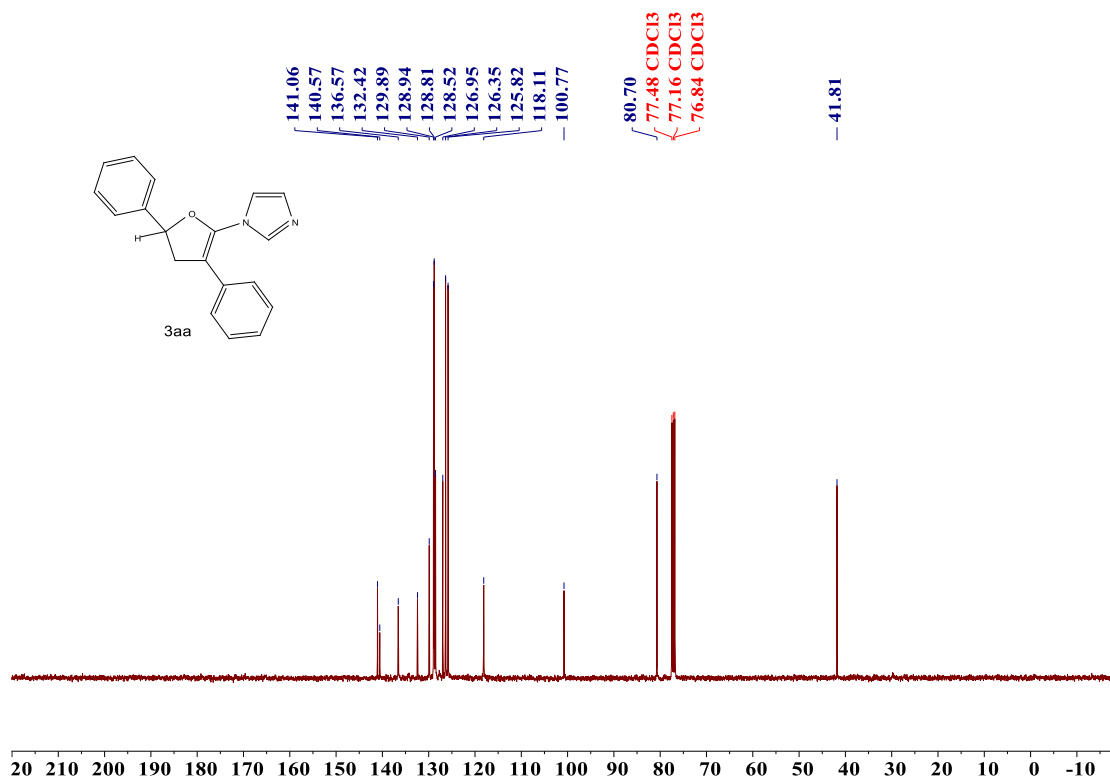
[2] Hu, Y.-F.; Feng, M.-H.; Zhang, P.-Y.; Xu, H.; Ma, M.; Shen, Z.-L.; Chu, X.-Q. Combining Hydrodefluorination and Defluorophosphorylation for Chemo- and Stereoselective Synthesis of *gem*-Fluorophosphine Alkenes, *Org. Lett.* **2023**, *25*, 6368–6373.

# $^1\text{H}$ , $^{19}\text{F}$ , and $^{13}\text{C}$ NMR spectra of products

$^1\text{H}$  NMR spectra of the product **3aa** (400 MHz,  $\text{CDCl}_3$ )

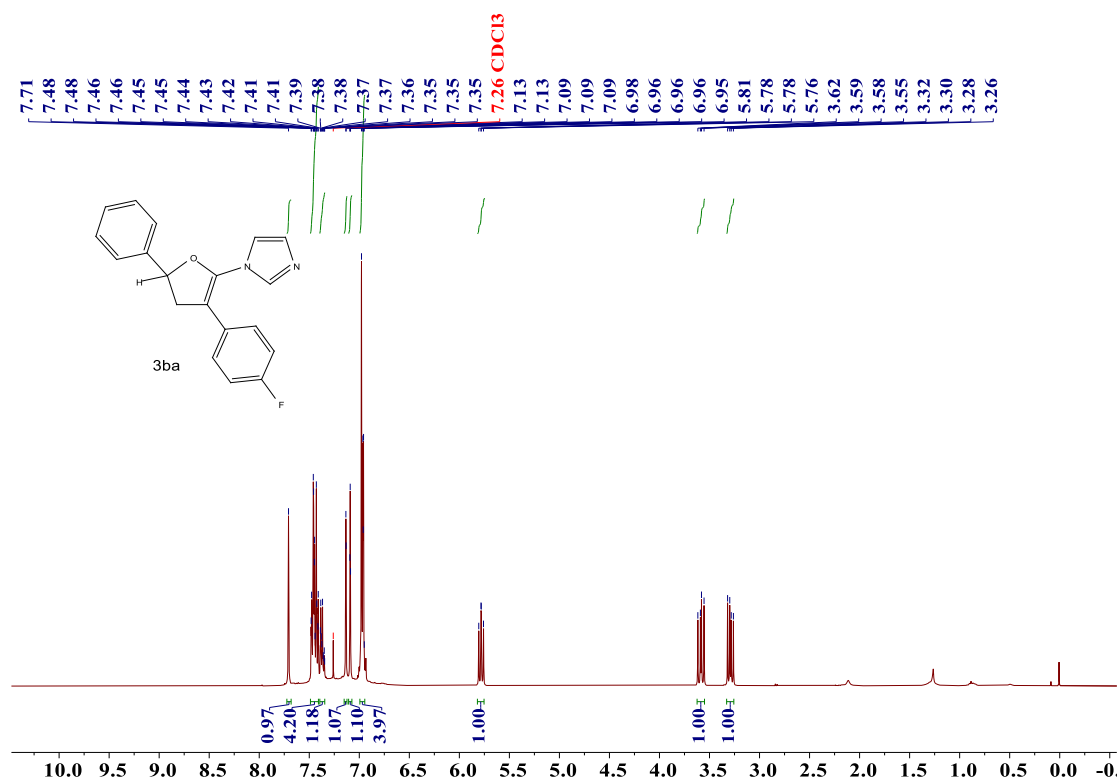


$^{13}\text{C}$  NMR spectra of the product **3aa** (100 MHz,  $\text{CDCl}_3$ )

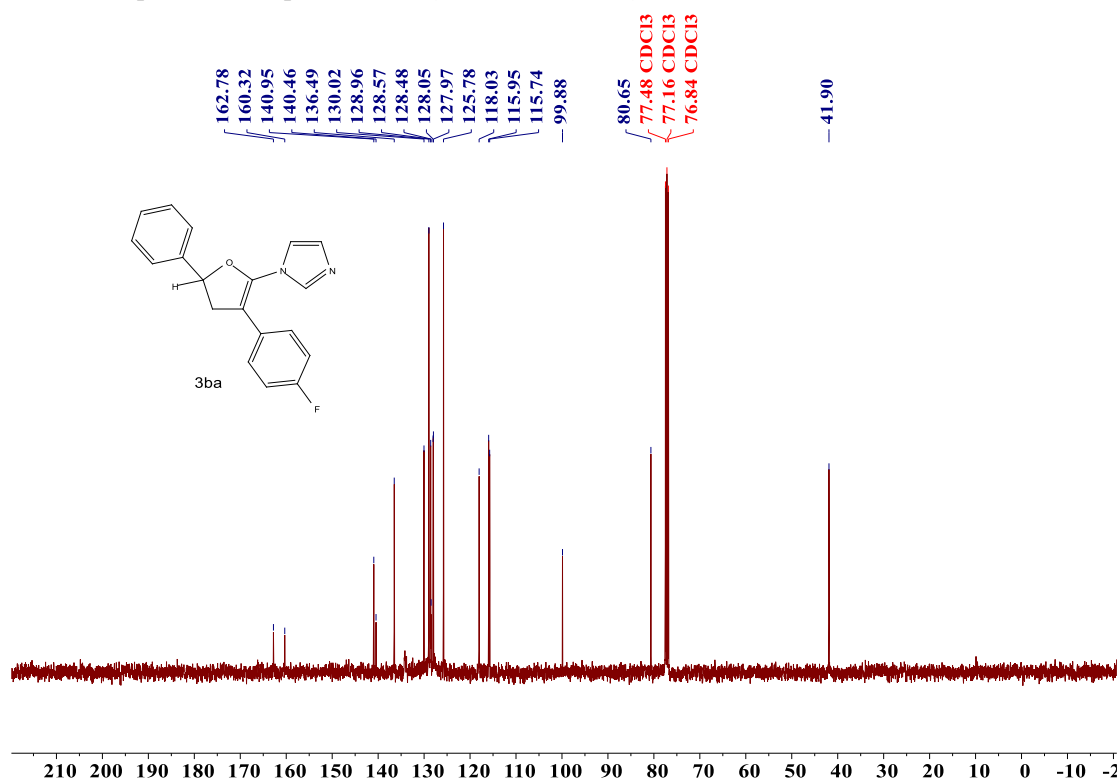




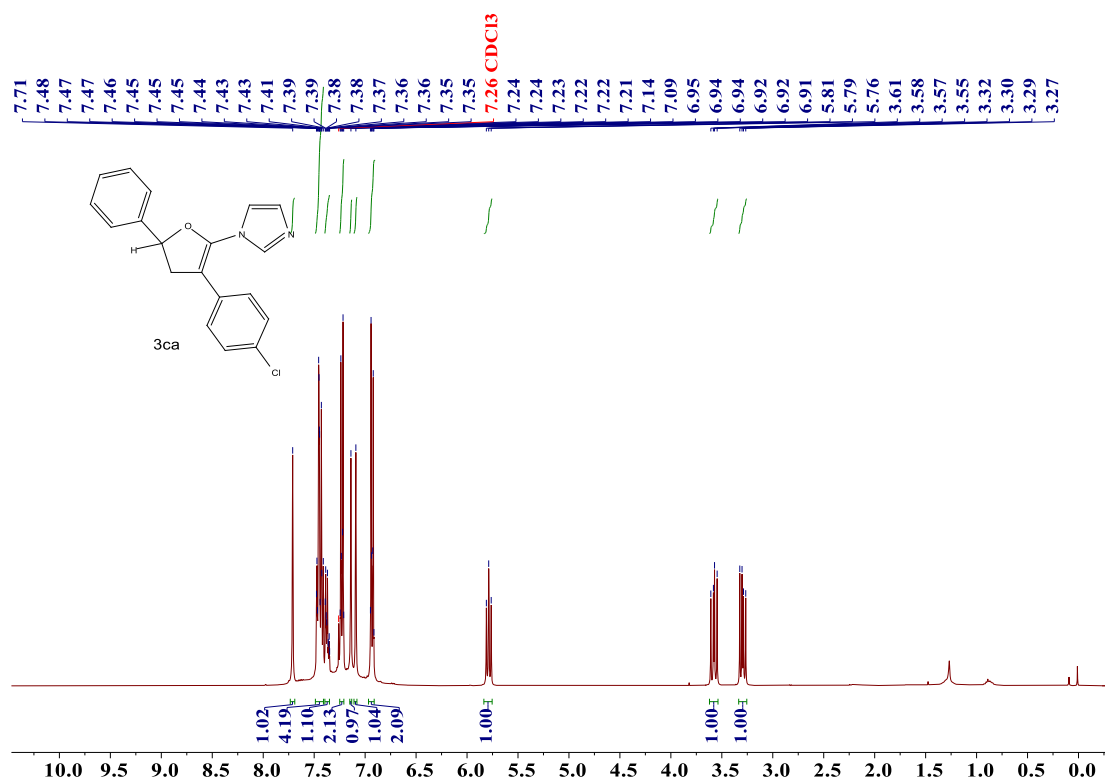
$^1\text{H}$  NMR spectra of the product **3ba** (400 MHz,  $\text{CDCl}_3$ )



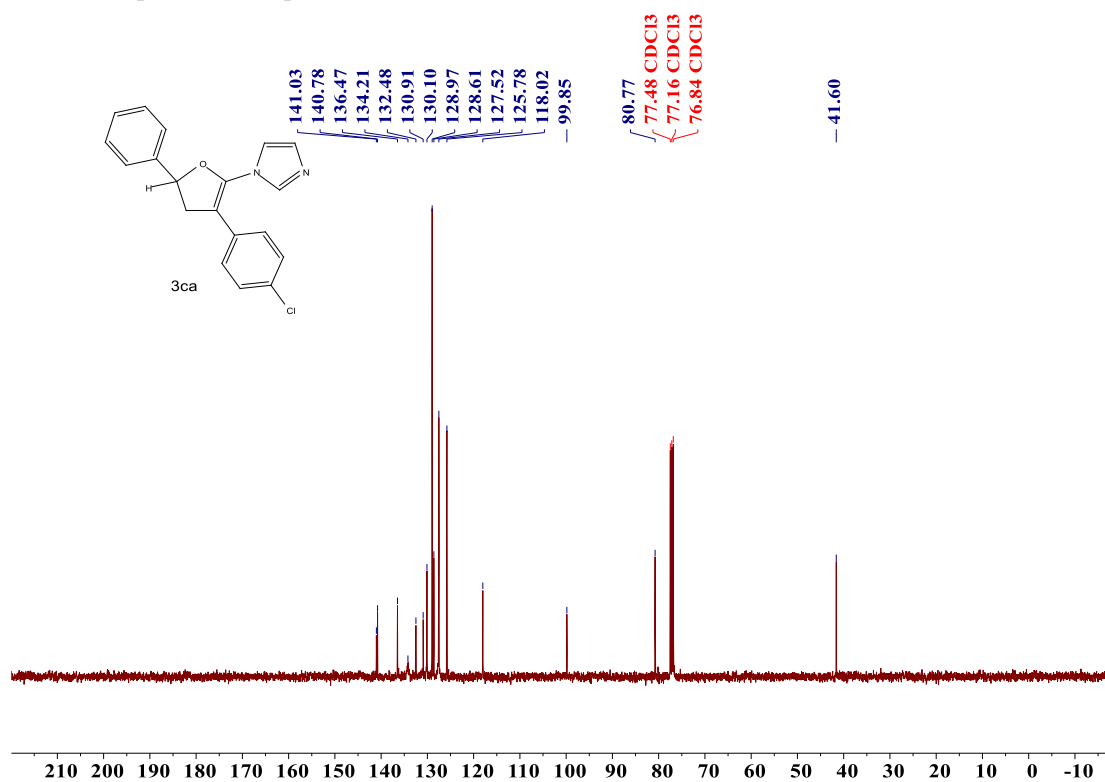
$^{13}\text{C}$  NMR spectra of the product **3ba** (100 MHz,  $\text{CDCl}_3$ )



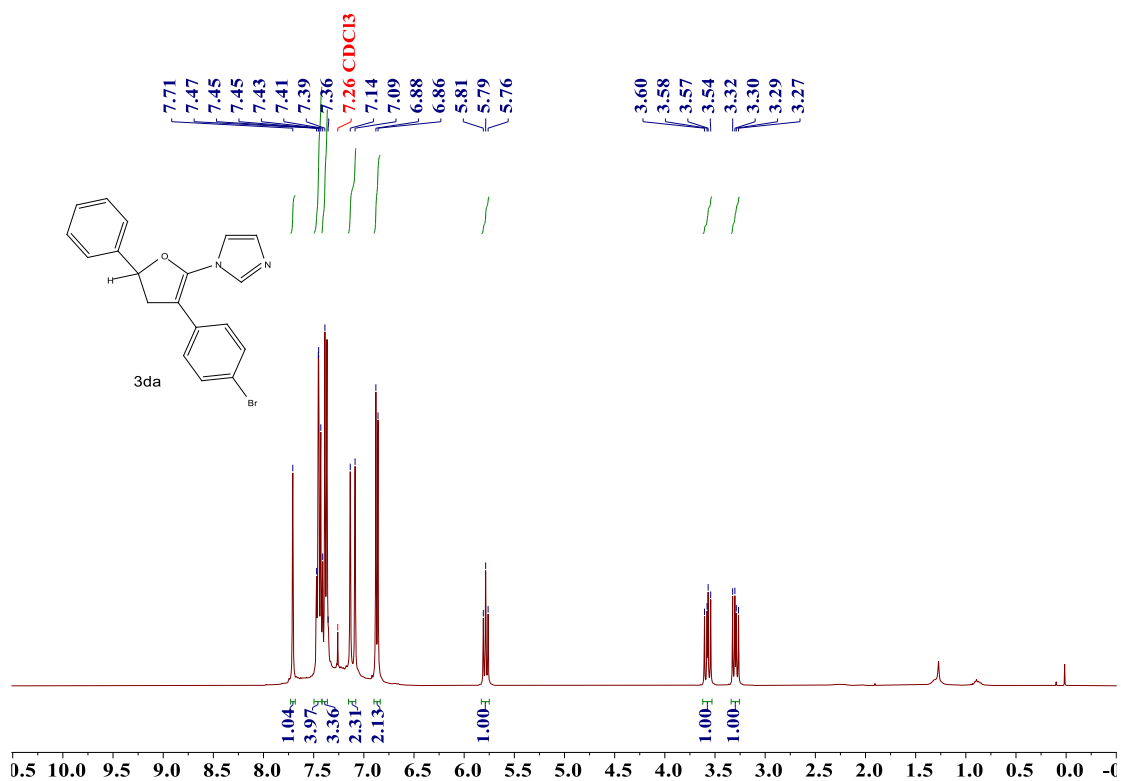
<sup>1</sup>H NMR spectra of the product **3ca** (400 MHz, CDCl<sub>3</sub>)



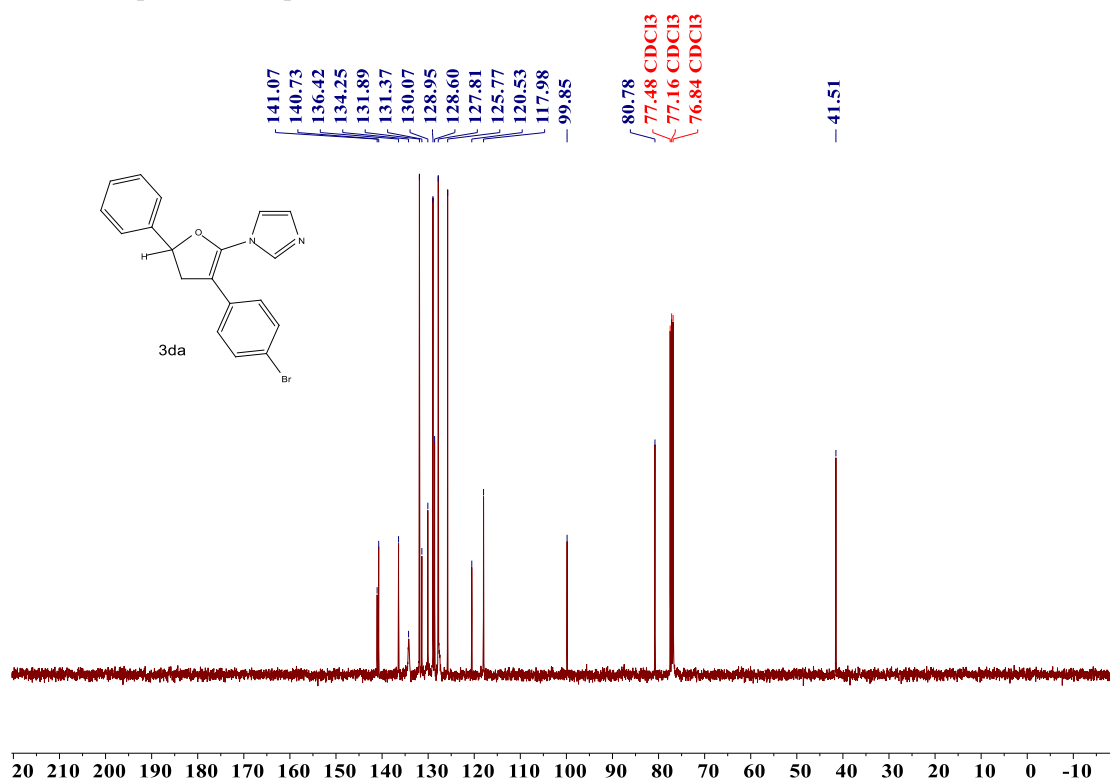
<sup>13</sup>C NMR spectra of the product **3ca** (100 MHz, CDCl<sub>3</sub>)



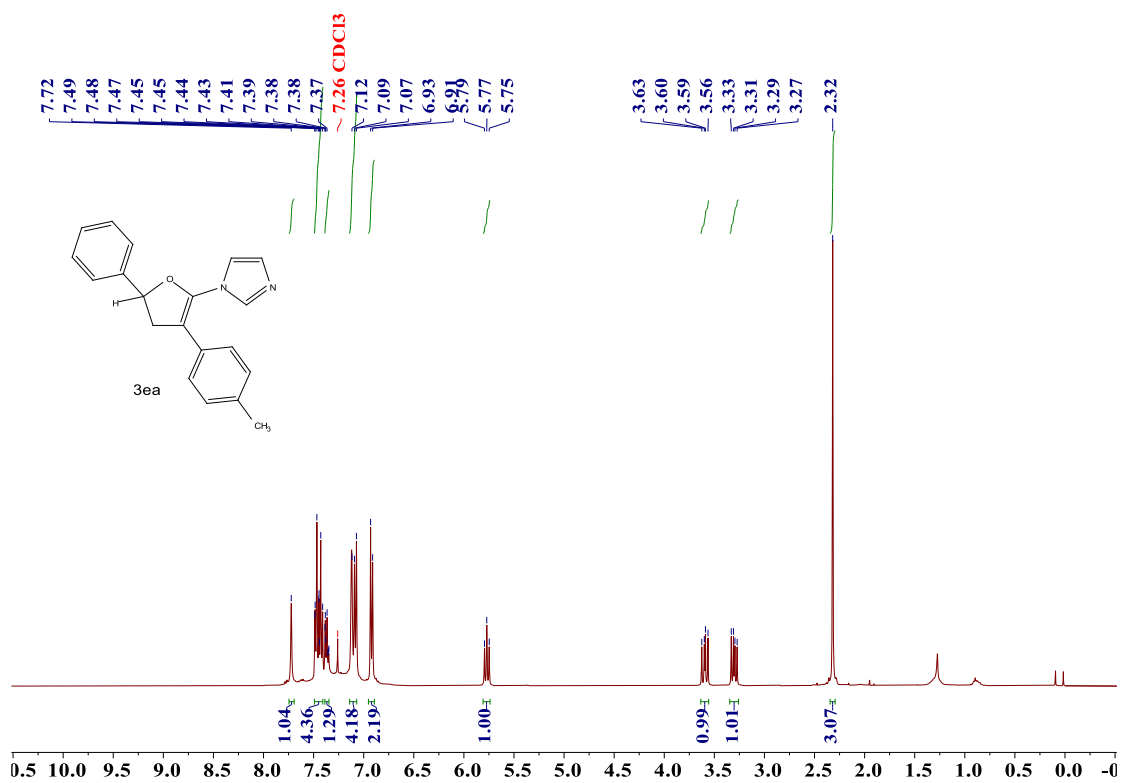
<sup>1</sup>H NMR spectra of the product **3da** (400 MHz, CDCl<sub>3</sub>)



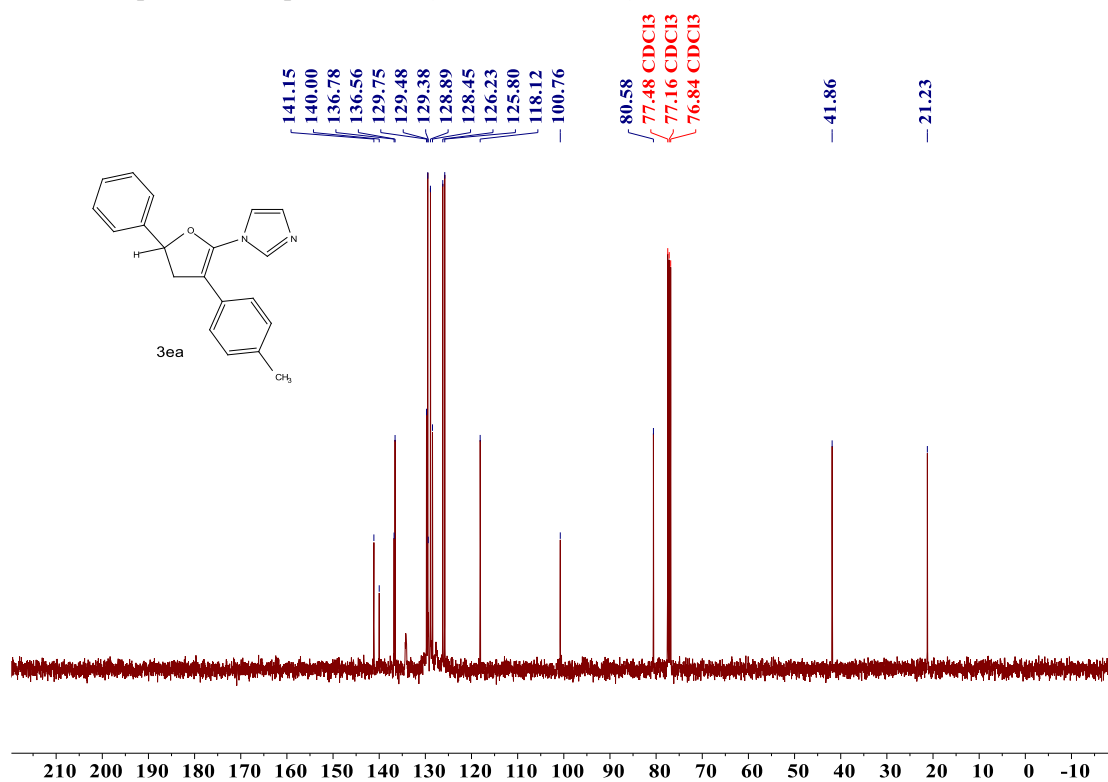
<sup>13</sup>C NMR spectra of the product **3da** (100 MHz, CDCl<sub>3</sub>)



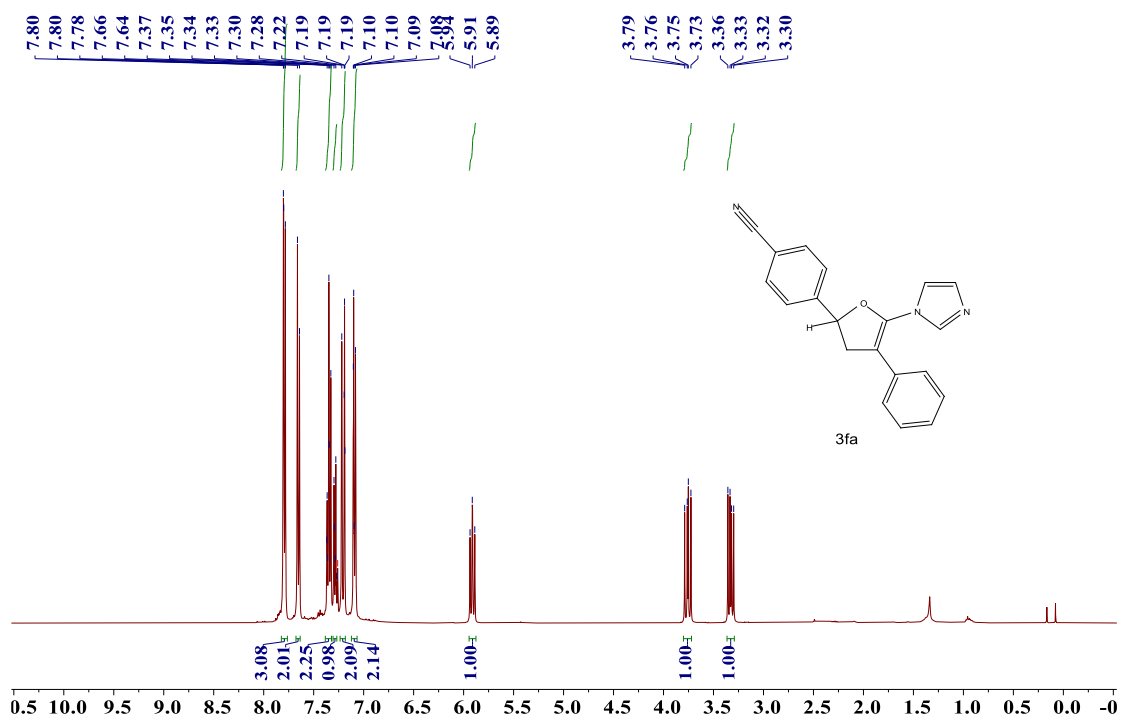
<sup>1</sup>H NMR spectra of the product **3ea** (400 MHz, CDCl<sub>3</sub>)



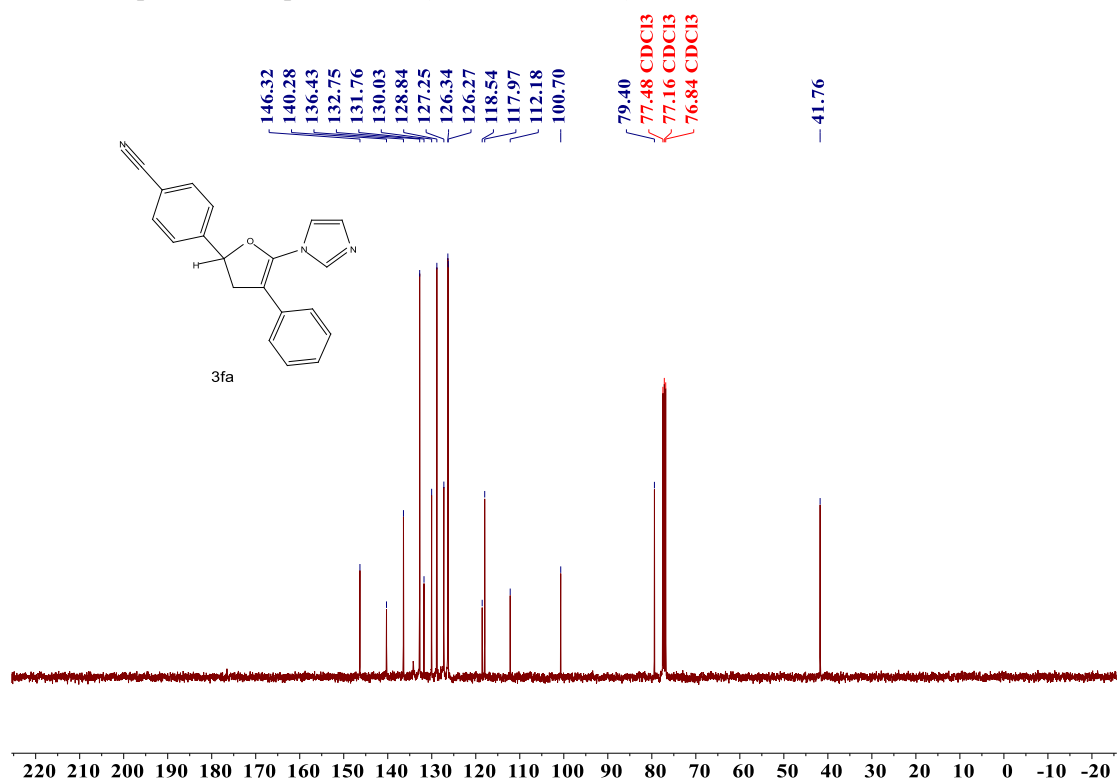
<sup>13</sup>C NMR spectra of the product **3ea** (100 MHz, CDCl<sub>3</sub>)



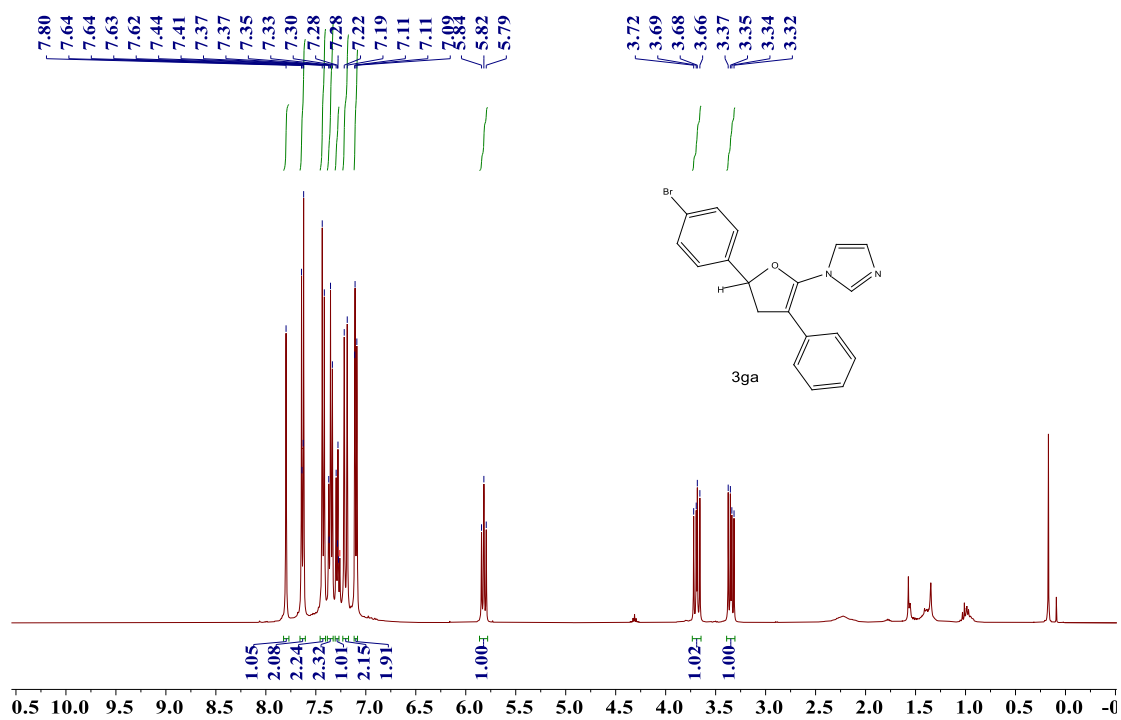
$^1\text{H}$  NMR spectra of the product **3fa** (400 MHz,  $\text{CDCl}_3$ )



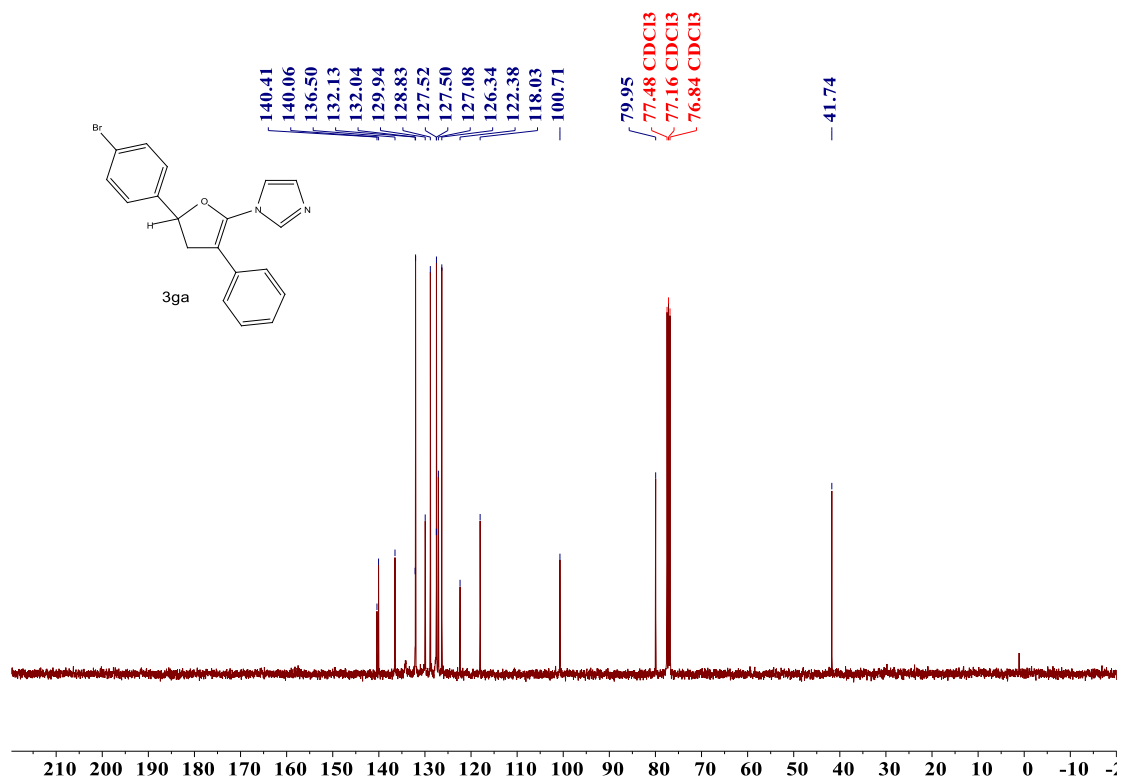
$^{13}\text{C}$  NMR spectra of the product **3fa** (100 MHz,  $\text{CDCl}_3$ )



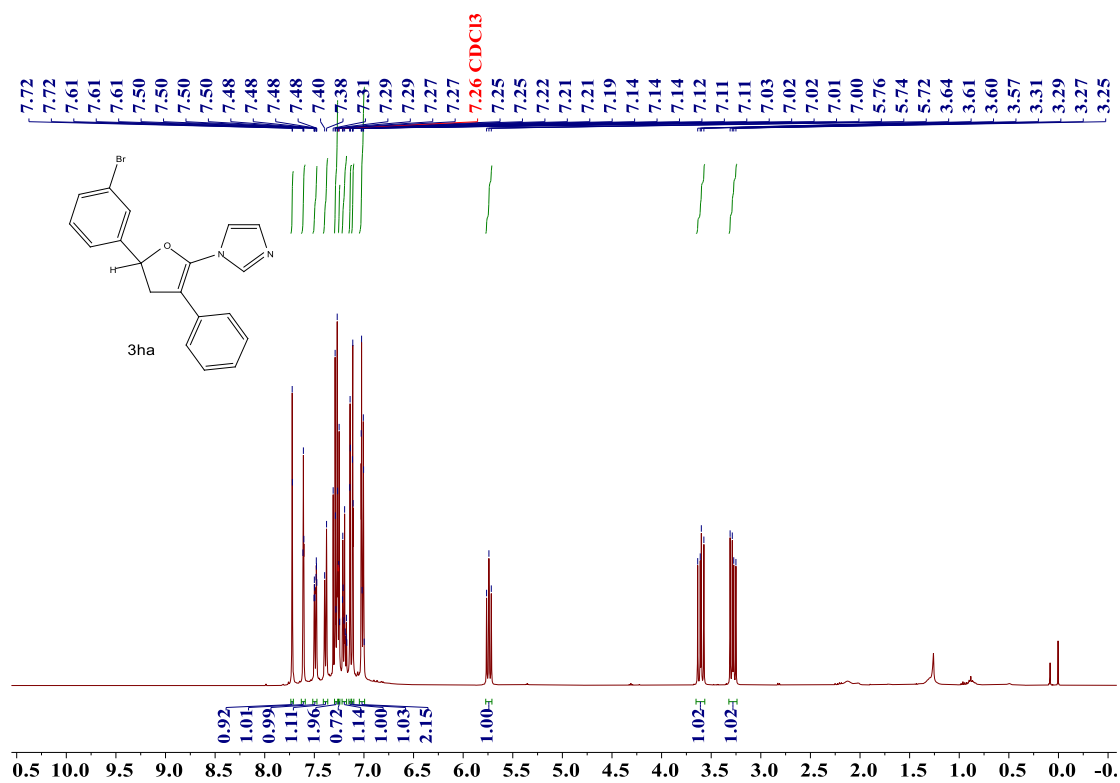
$^1\text{H}$  NMR spectra of the product **3ga** (400 MHz,  $\text{CDCl}_3$ )



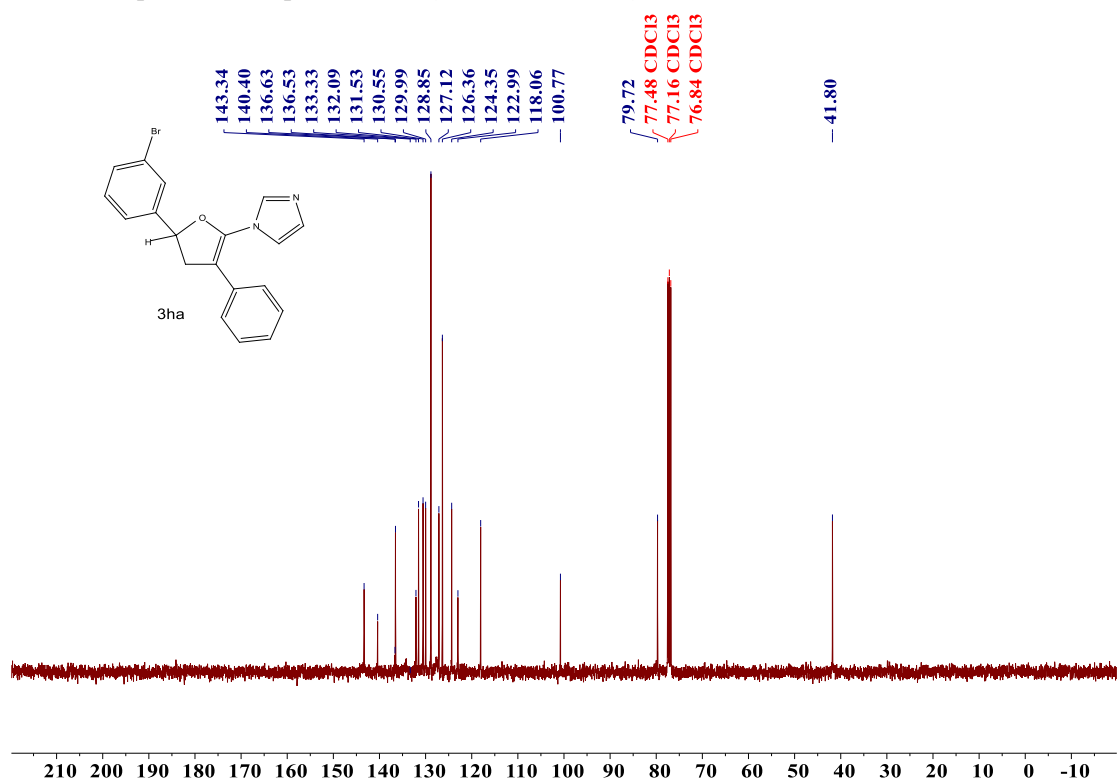
$^{13}\text{C}$  NMR spectra of the product **3ga** (100 MHz,  $\text{CDCl}_3$ )



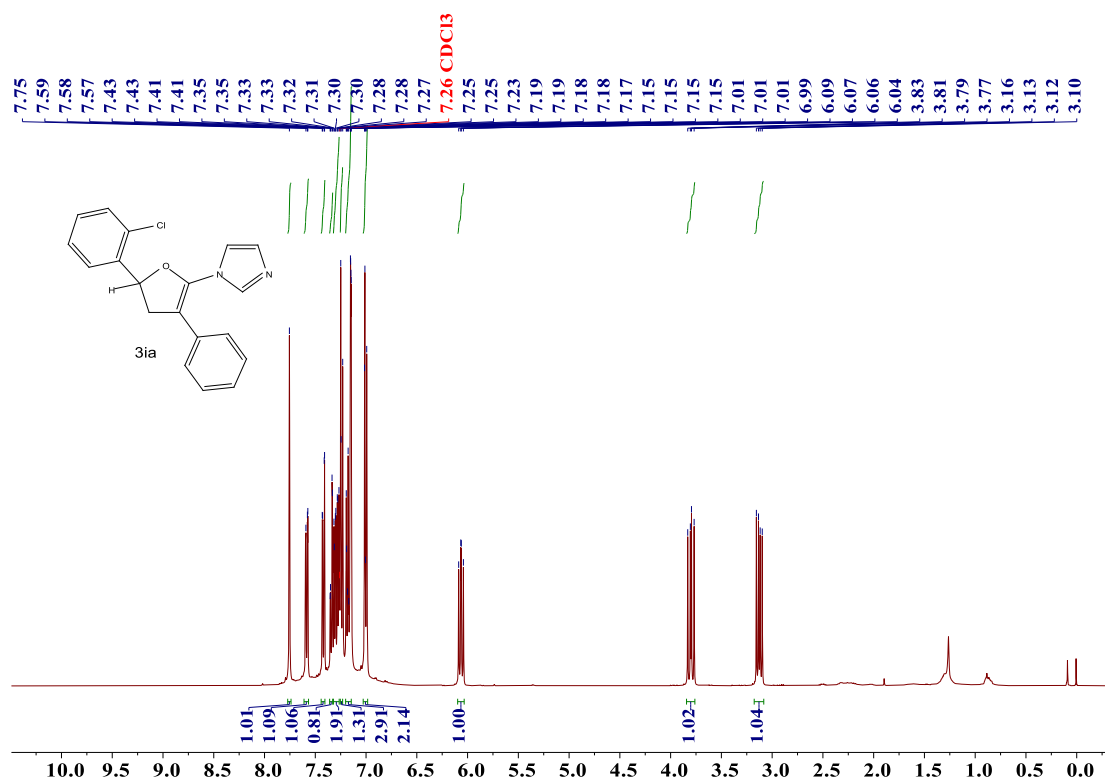
<sup>1</sup>H NMR spectra of the product **3ha** (400 MHz, CDCl<sub>3</sub>)



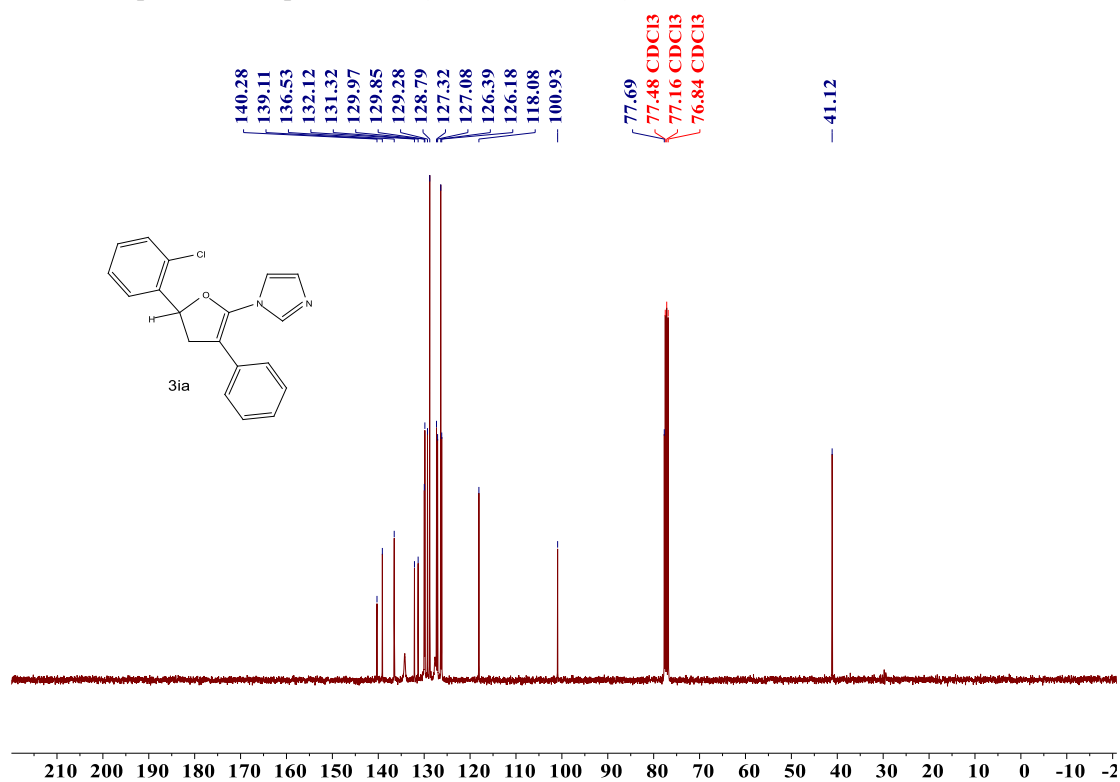
<sup>13</sup>C NMR spectra of the product **3ha** (100 MHz, CDCl<sub>3</sub>)



<sup>1</sup>H NMR spectra of the product **3ia** (400 MHz, CDCl<sub>3</sub>)

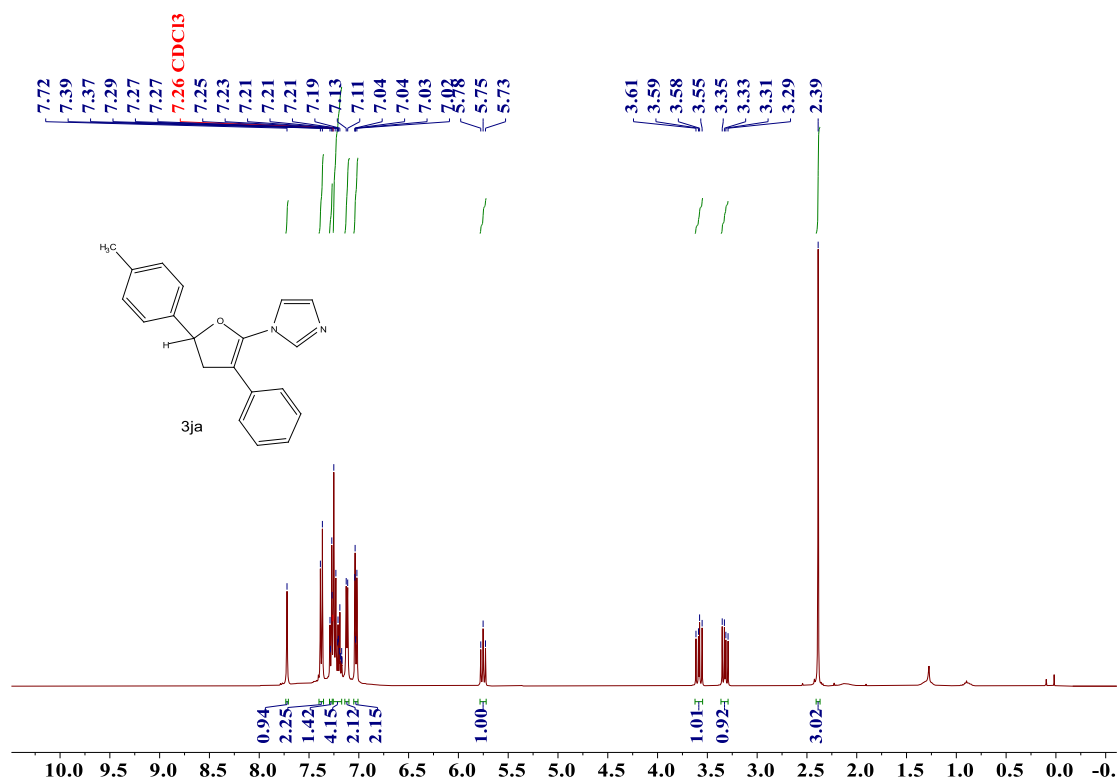


<sup>13</sup>C NMR spectra of the product **3ia** (100 MHz, CDCl<sub>3</sub>)

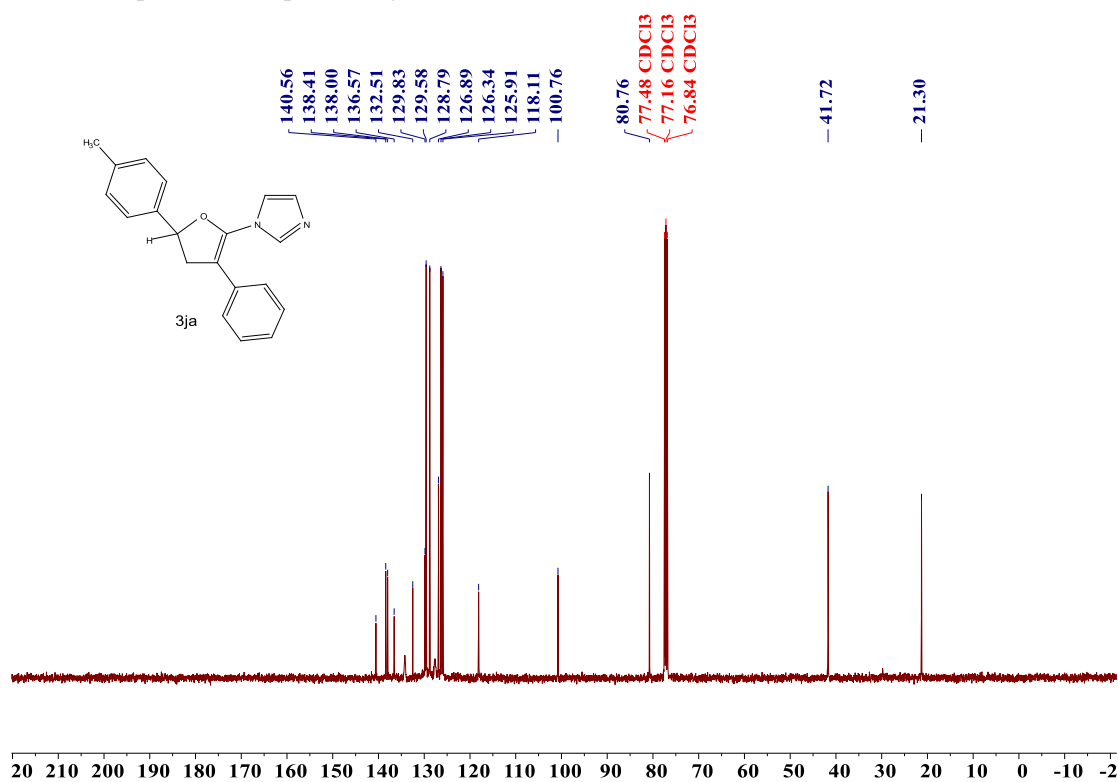




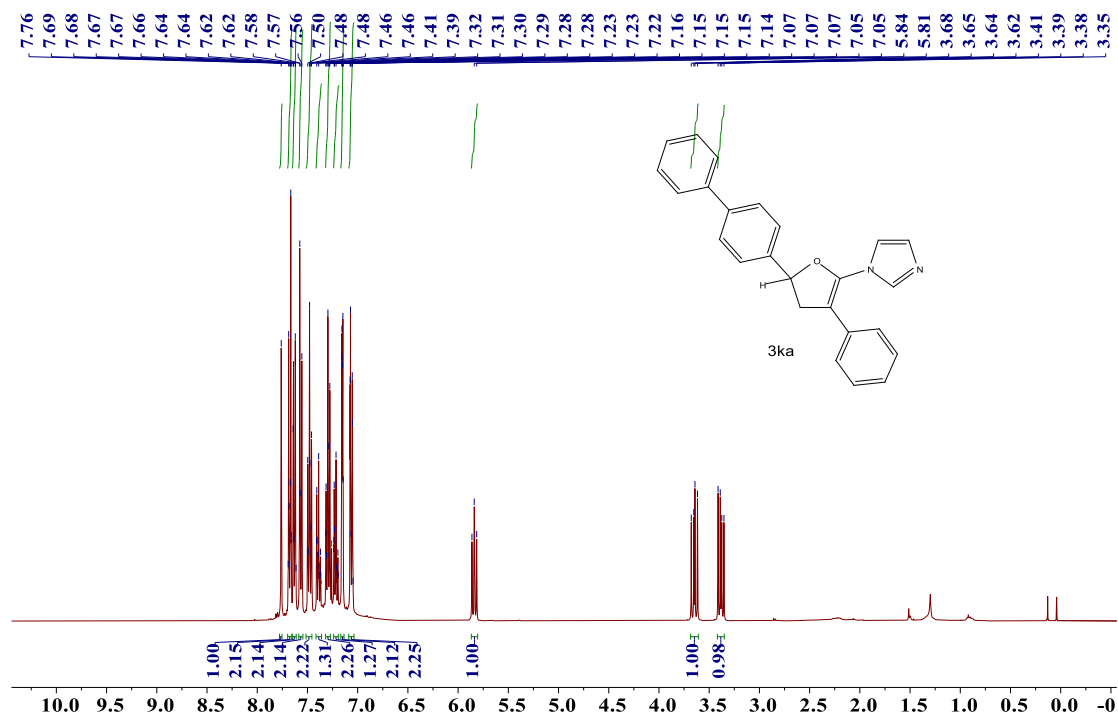
$^1\text{H}$  NMR spectra of the product **3ja** (400 MHz,  $\text{CDCl}_3$ )



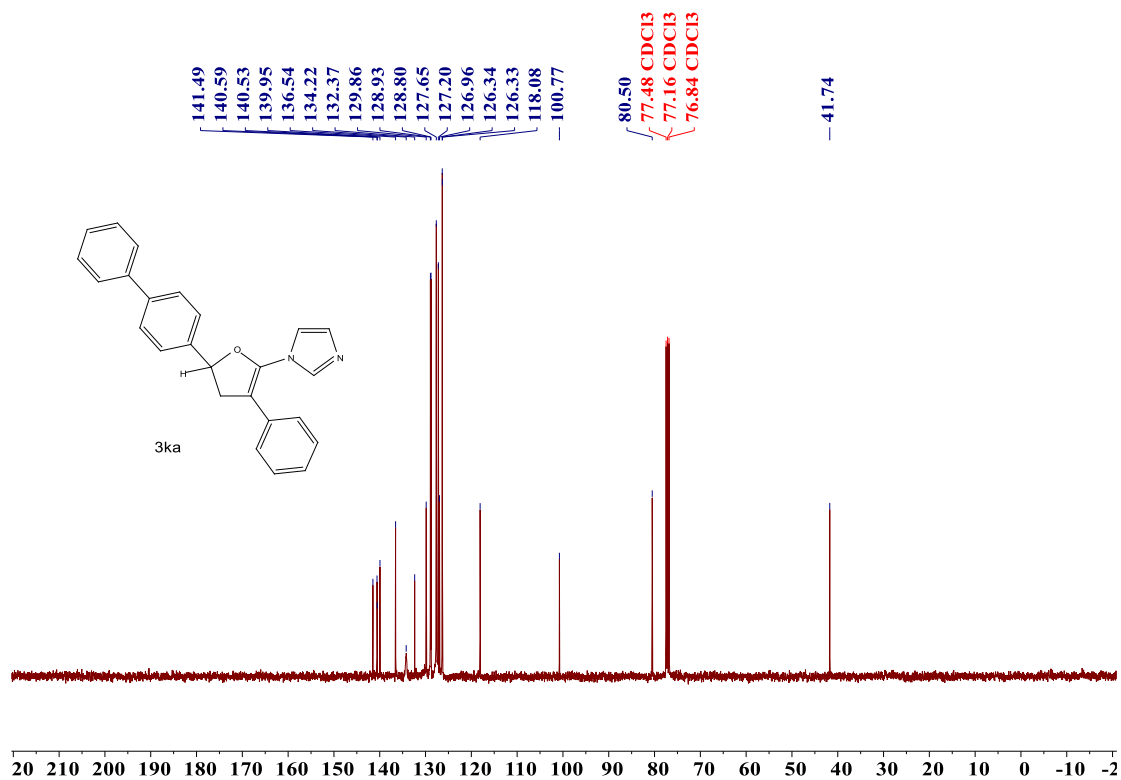
$^{13}\text{C}$  NMR spectra of the product **3ja** (100 MHz,  $\text{CDCl}_3$ )



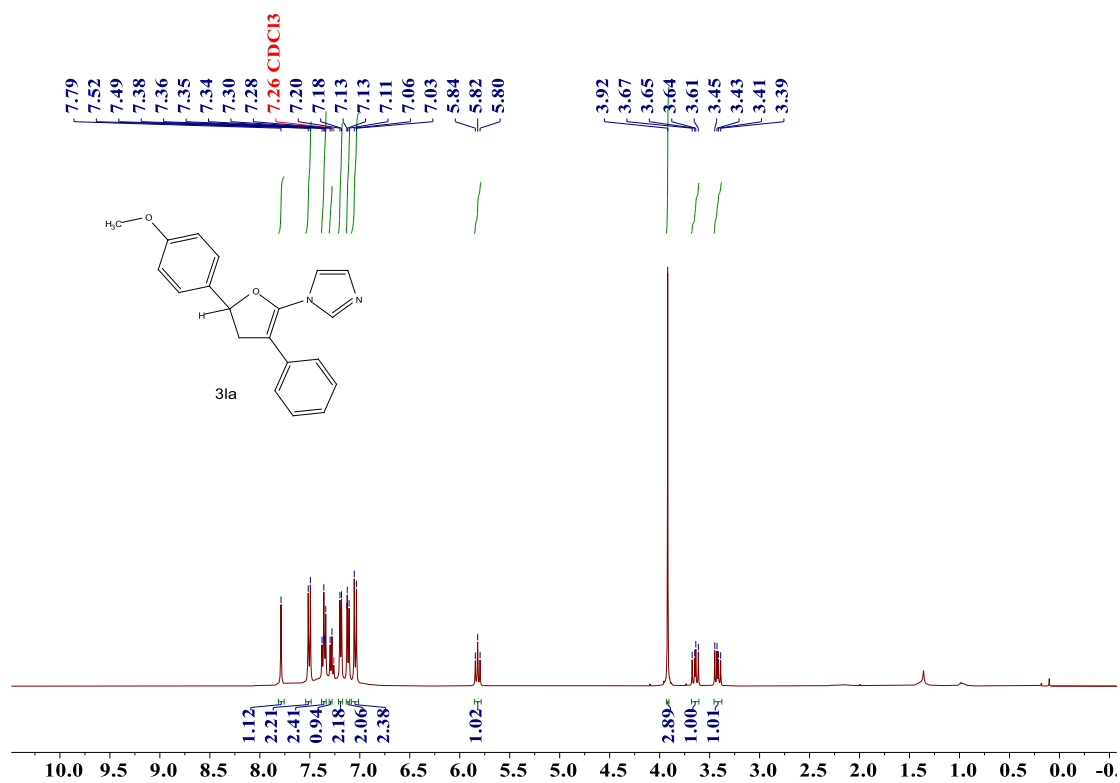
<sup>1</sup>H NMR spectra of the product **3ka** (400 MHz, CDCl<sub>3</sub>)



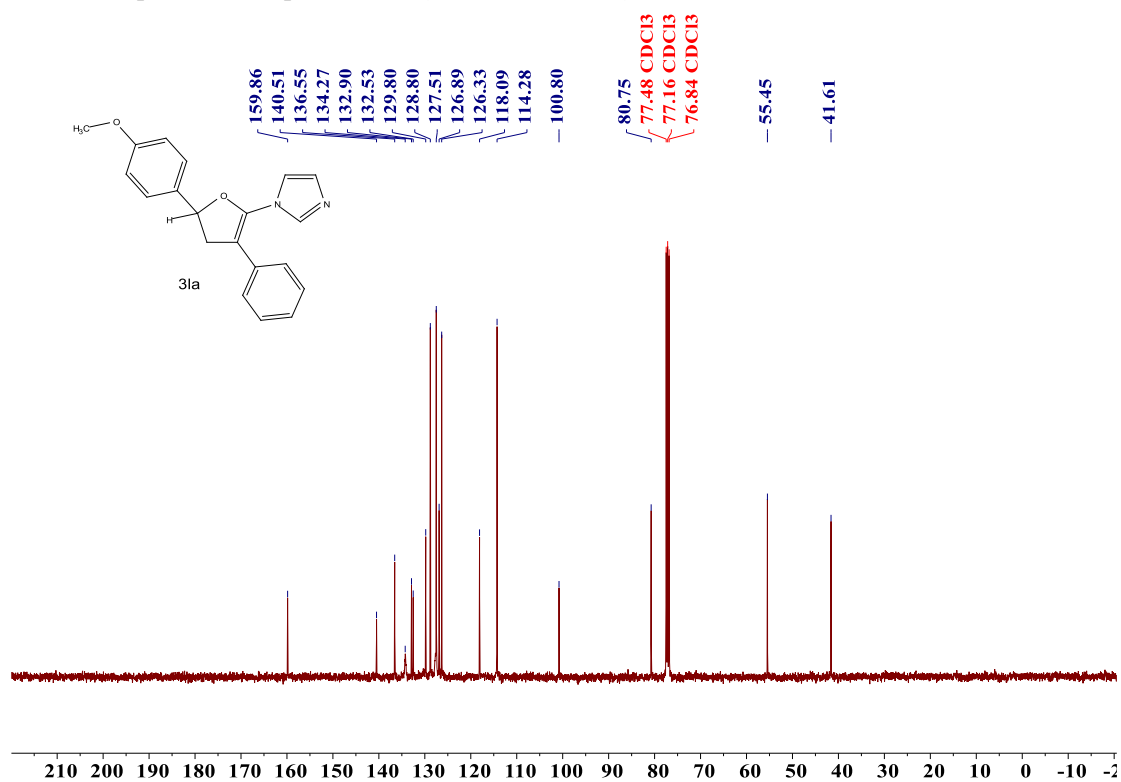
<sup>13</sup>C NMR spectra of the product **3ka** (100 MHz, CDCl<sub>3</sub>)



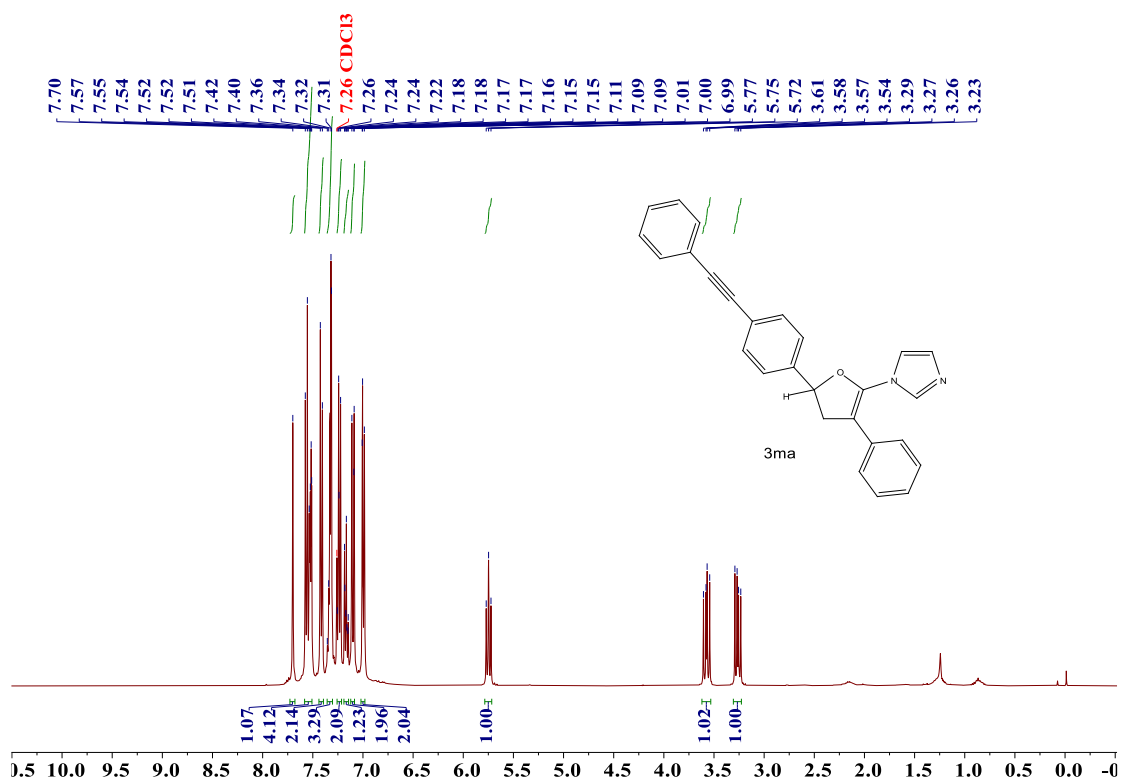
$^1\text{H}$  NMR spectra of the product **3a** (400 MHz,  $\text{CDCl}_3$ )



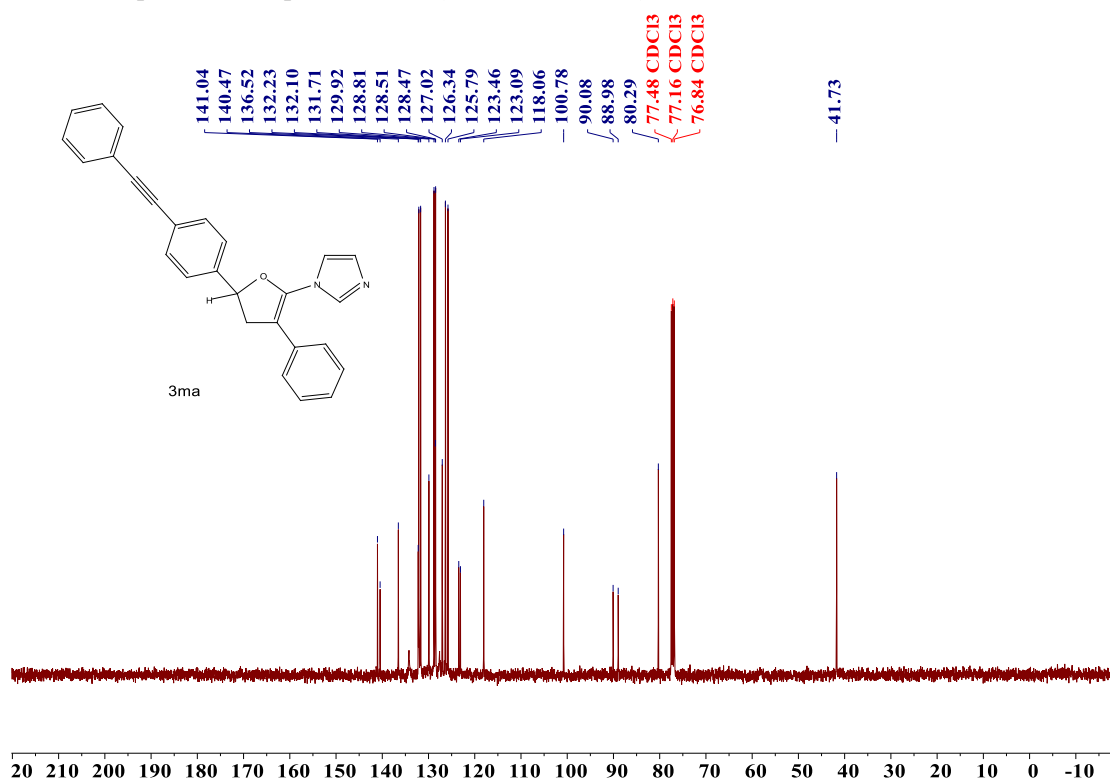
$^{13}\text{C}$  NMR spectra of the product **3a** (100 MHz,  $\text{CDCl}_3$ )



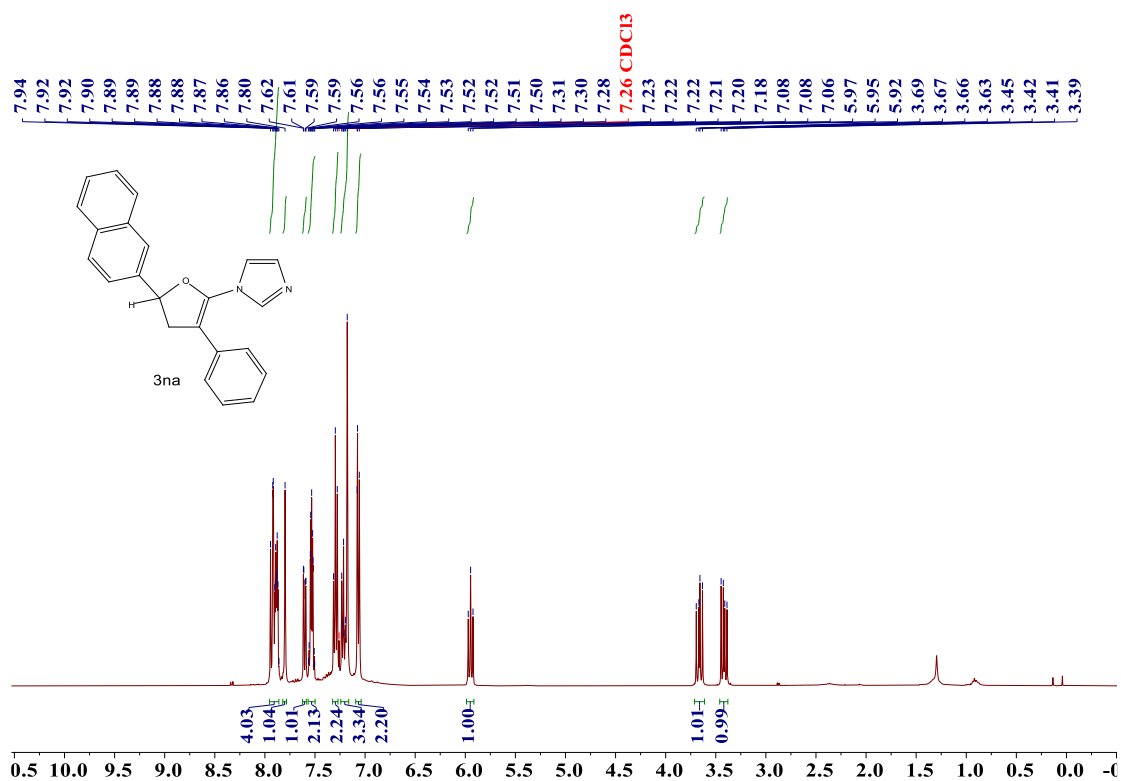
$^1\text{H}$  NMR spectra of the product **3ma** (400 MHz,  $\text{CDCl}_3$ )



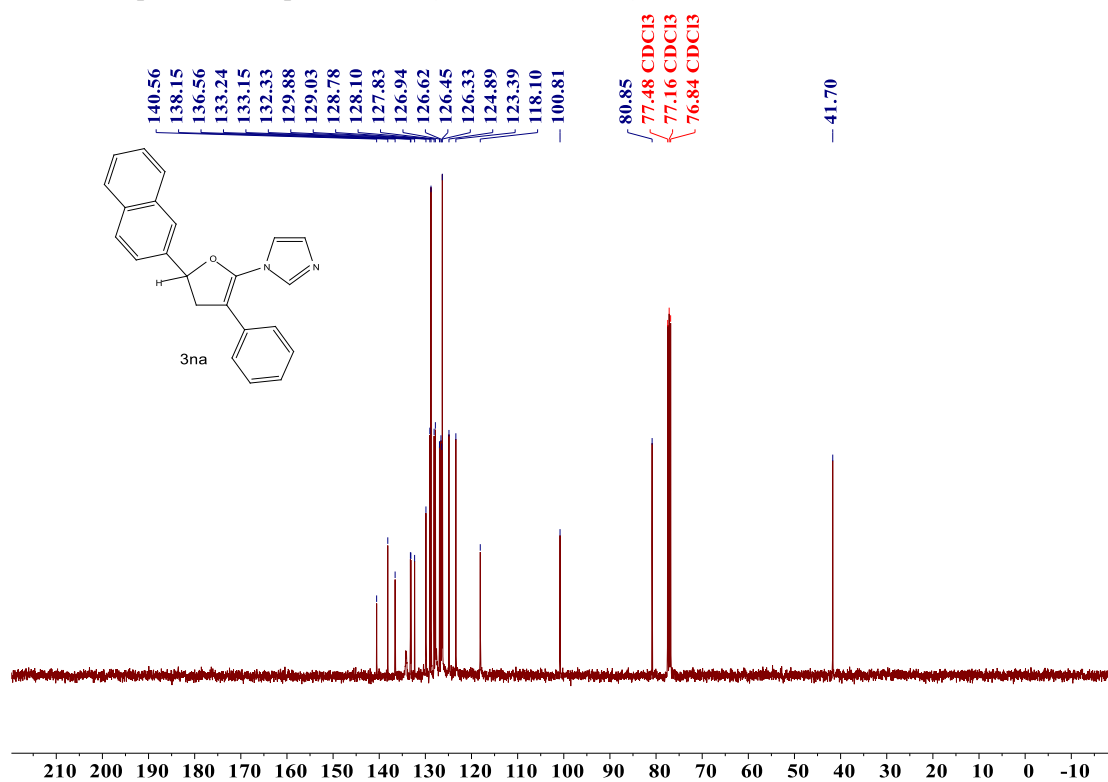
$^{13}\text{C}$  NMR spectra of the product **3ma** (100 MHz,  $\text{CDCl}_3$ )



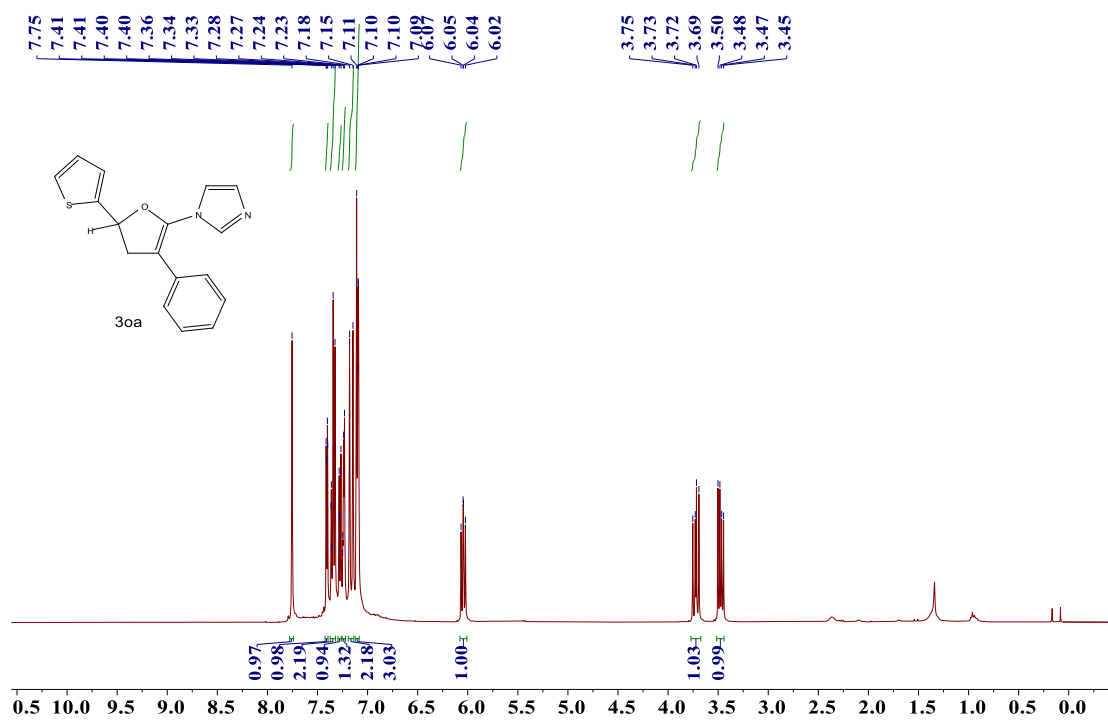
<sup>1</sup>H NMR spectra of the product **3na** (400 MHz, CDCl<sub>3</sub>)



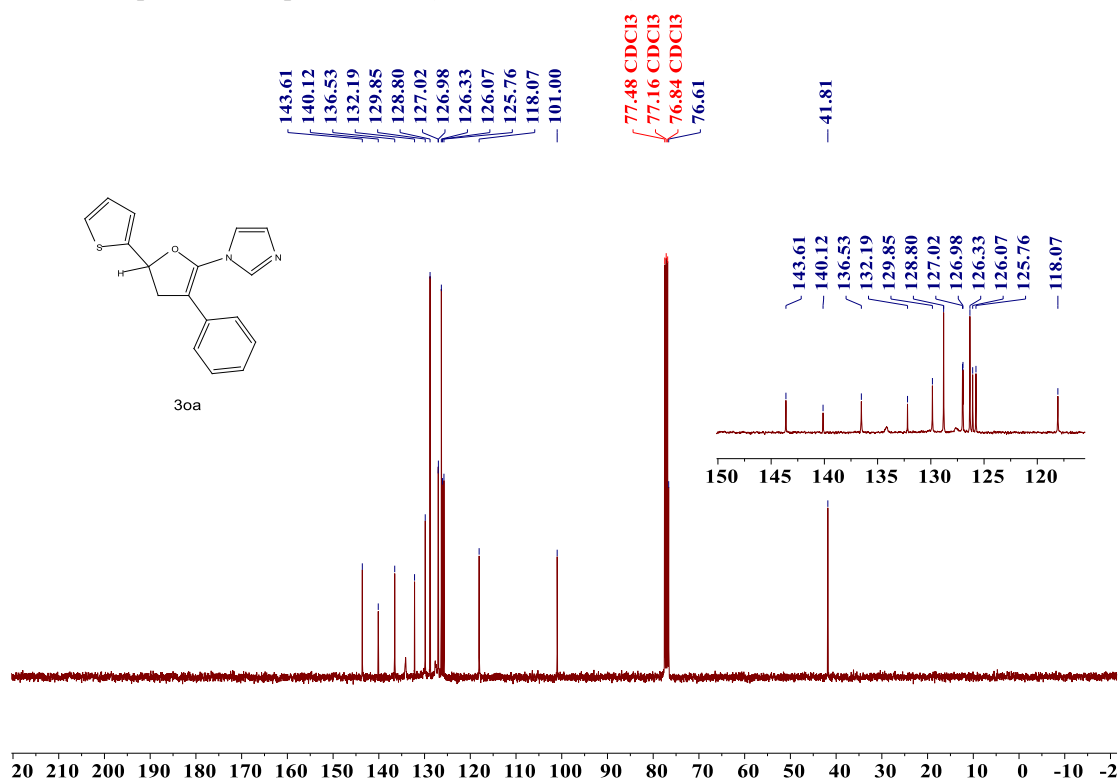
<sup>13</sup>C NMR spectra of the product **3na** (100 MHz, CDCl<sub>3</sub>)



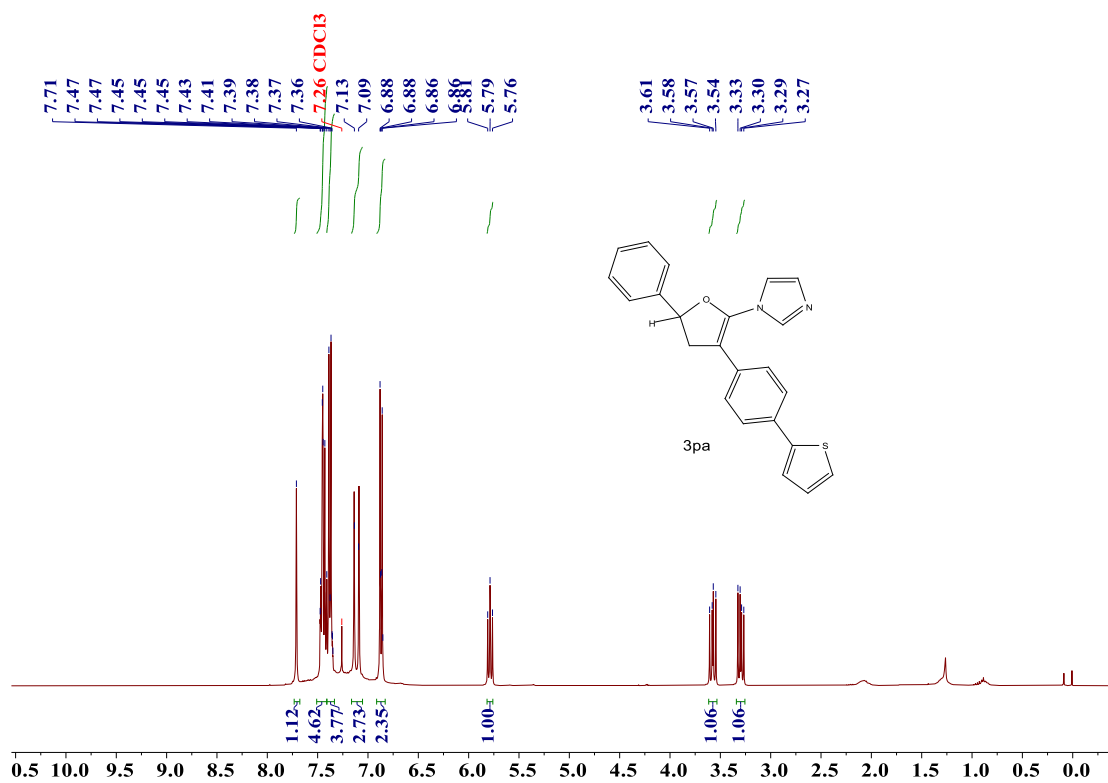
$^1\text{H}$  NMR spectra of the product **3oa** (400 MHz,  $\text{CDCl}_3$ )



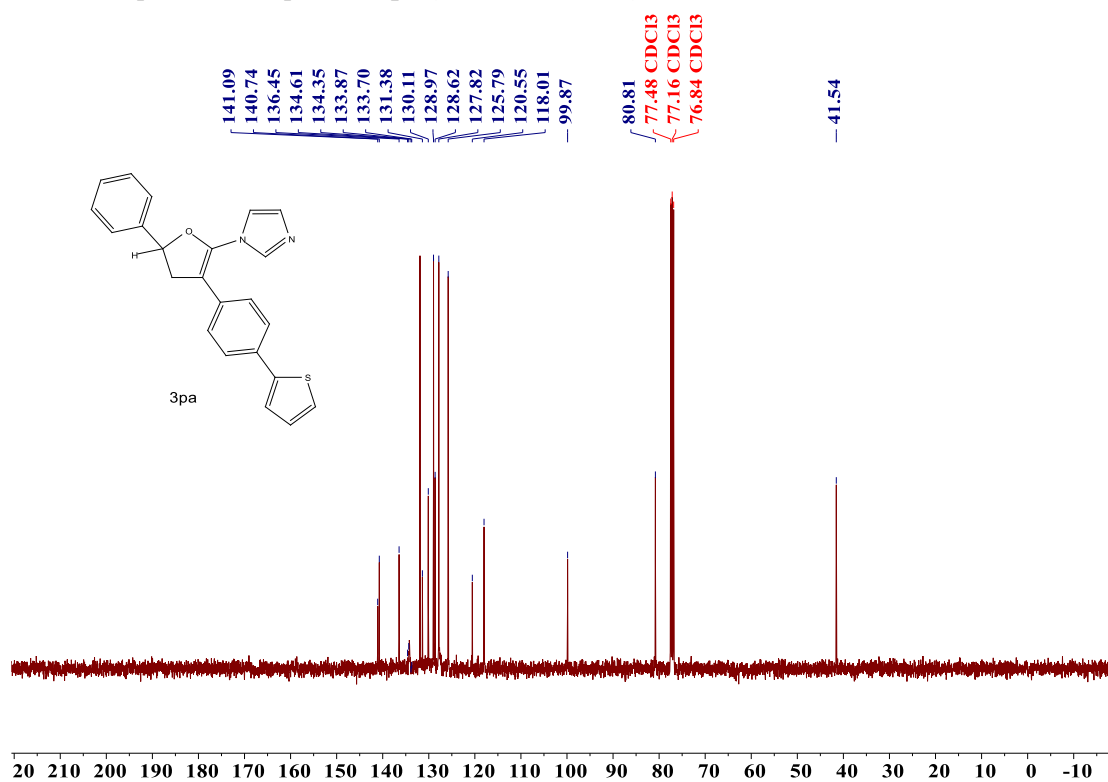
$^{13}\text{C}$  NMR spectra of the product **3oa** (100 MHz,  $\text{CDCl}_3$ )



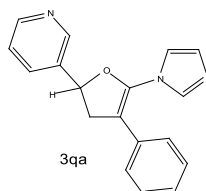
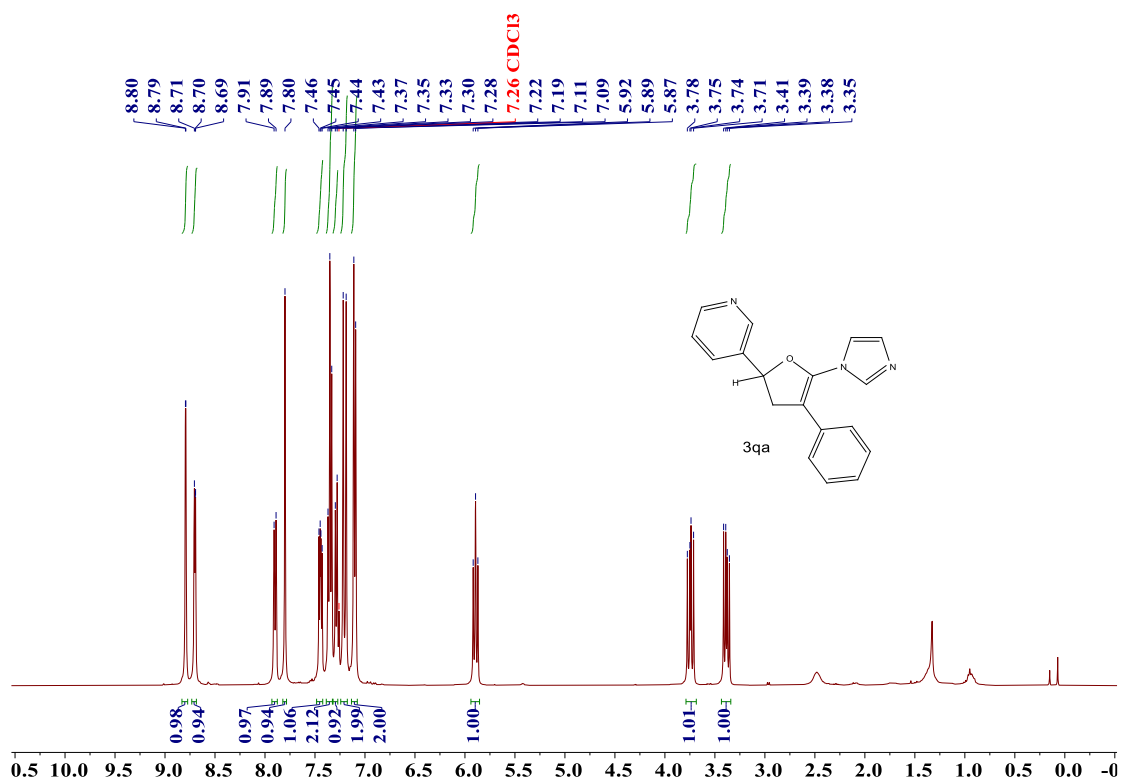
$^1\text{H}$  NMR spectra of the product **3pa** (400 MHz,  $\text{CDCl}_3$ )



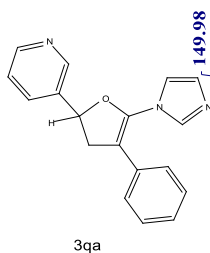
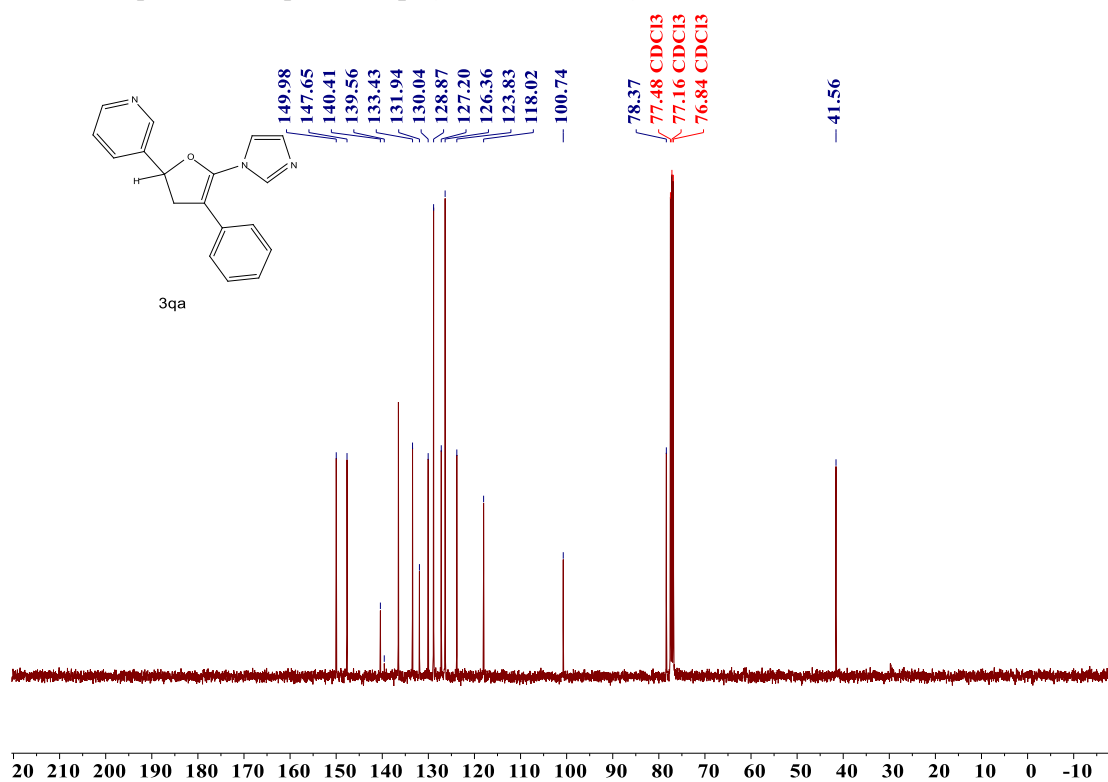
$^{13}\text{C}$  NMR spectra of the product **3pa** (100 MHz,  $\text{CDCl}_3$ )



$^1\text{H}$  NMR spectra of the product **3qa** (400 MHz,  $\text{CDCl}_3$ )

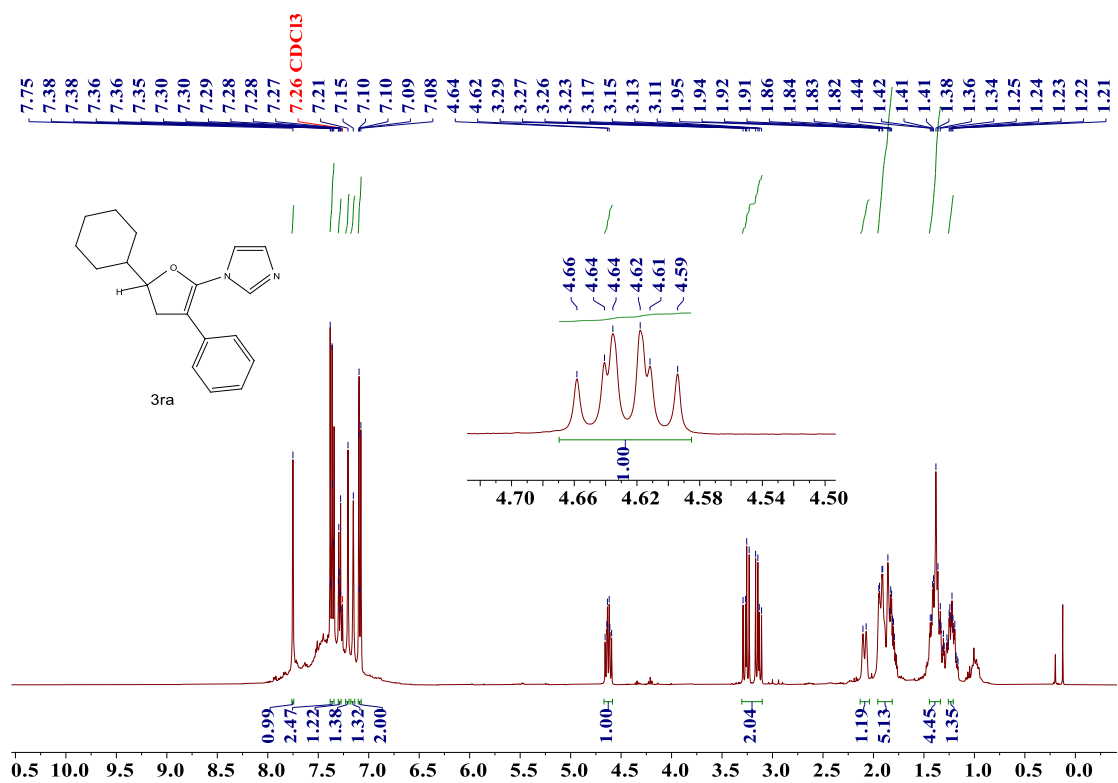


$^{13}\text{C}$  NMR spectra of the product **3qa** (100 MHz,  $\text{CDCl}_3$ )

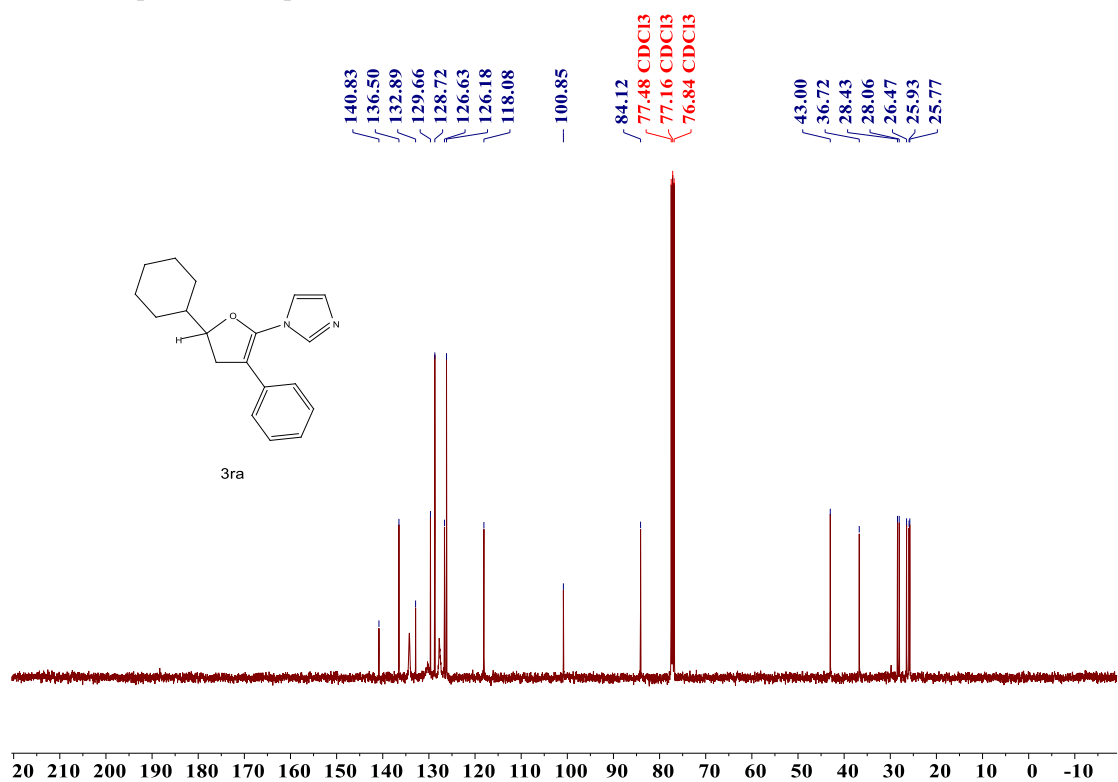




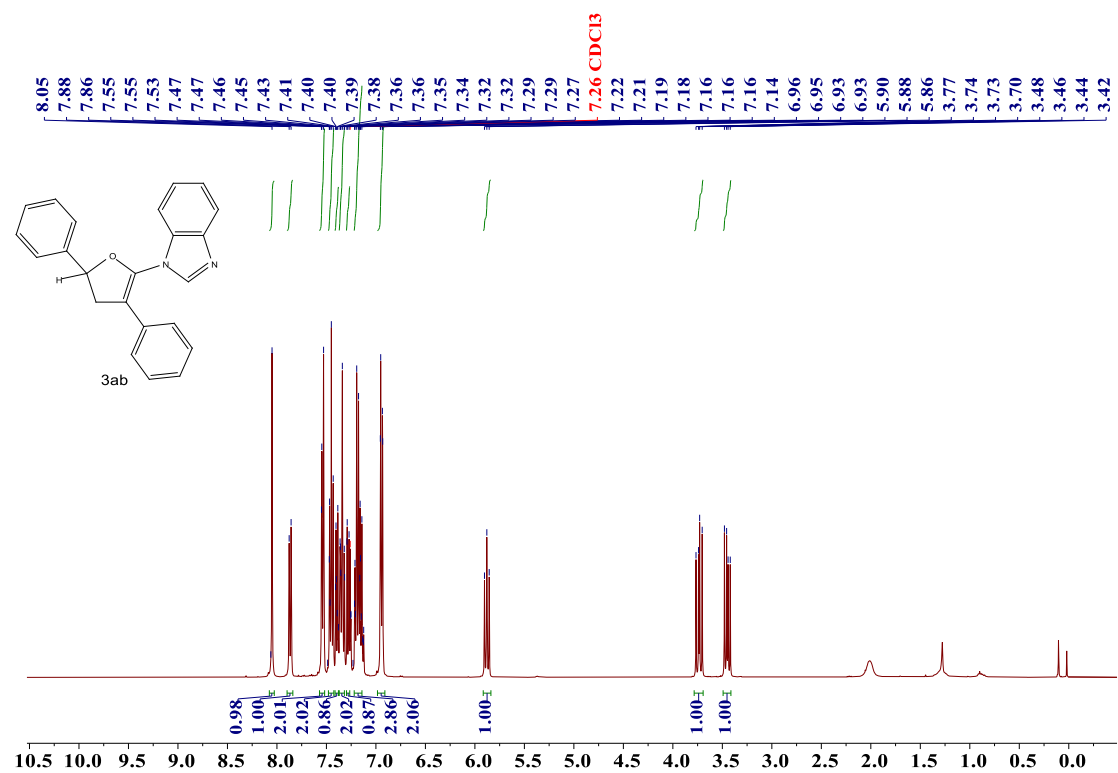
$^1\text{H}$  NMR spectra of the product **3ra** (400 MHz,  $\text{CDCl}_3$ )



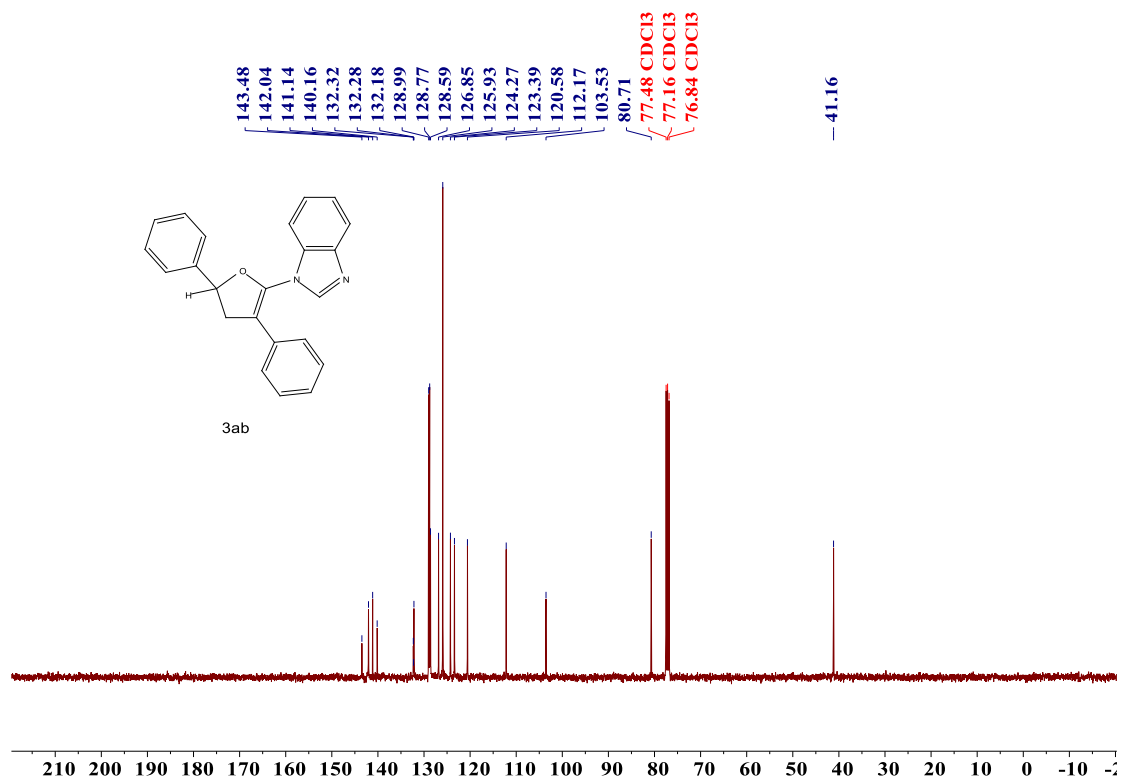
$^{13}\text{C}$  NMR spectra of the product **3ra** (100 MHz,  $\text{CDCl}_3$ )



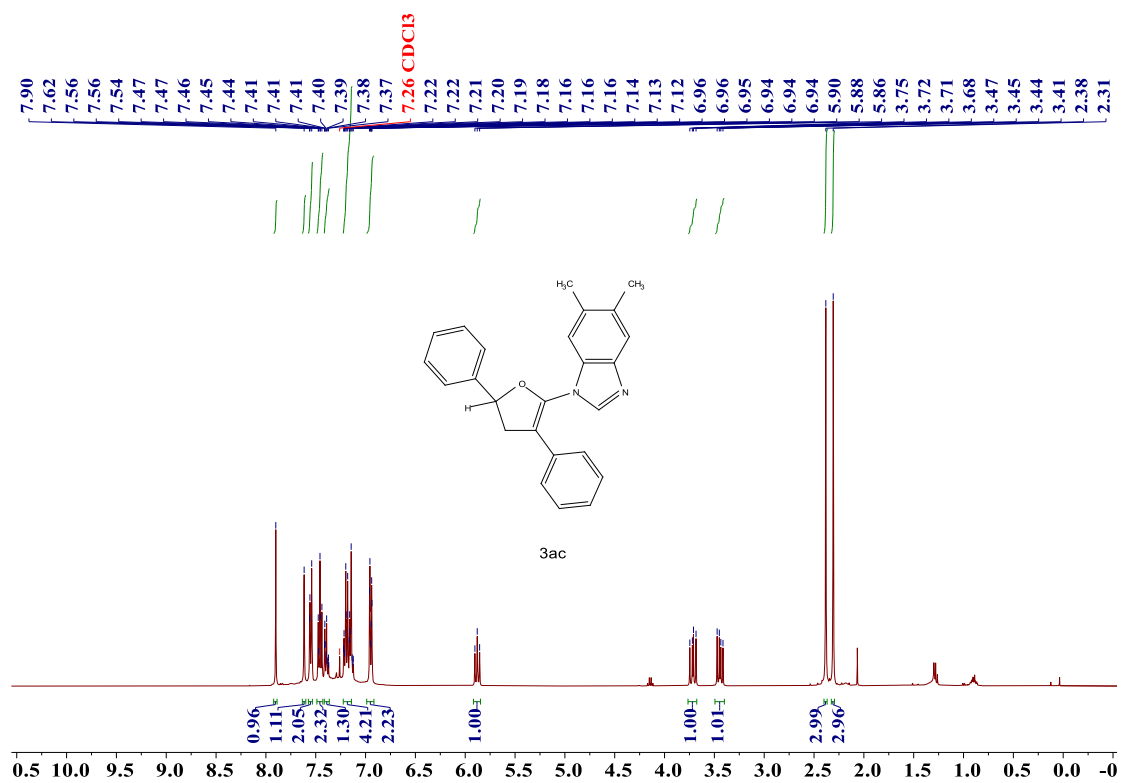
<sup>1</sup>H NMR spectra of the product **3ab** (400 MHz, CDCl<sub>3</sub>)



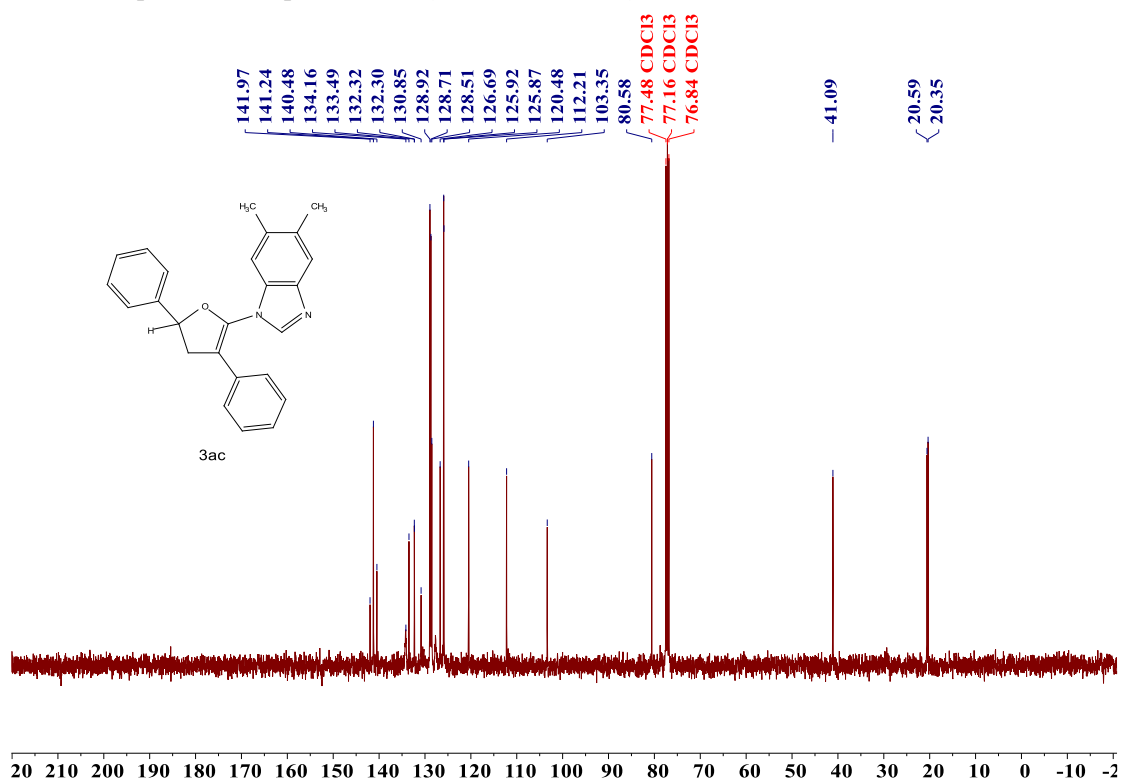
<sup>13</sup>C NMR spectra of the product **3ab** (100 MHz, CDCl<sub>3</sub>)



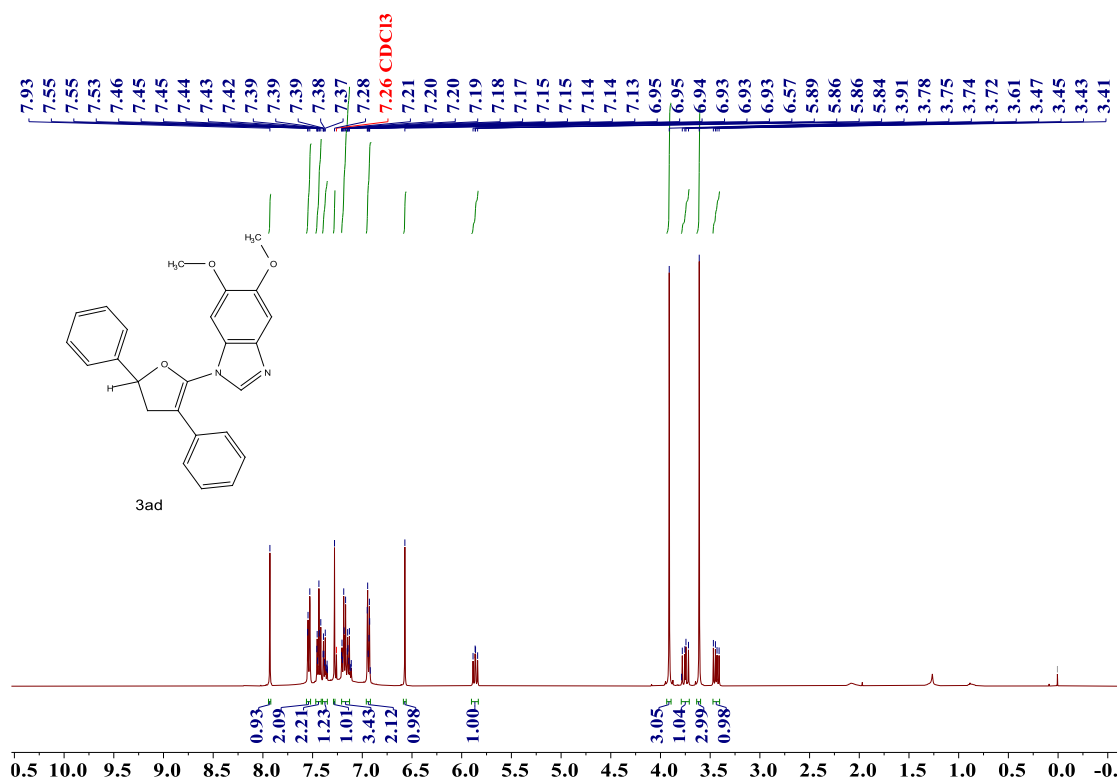
$^1\text{H}$  NMR spectra of the product **3ac** (400 MHz,  $\text{CDCl}_3$ )



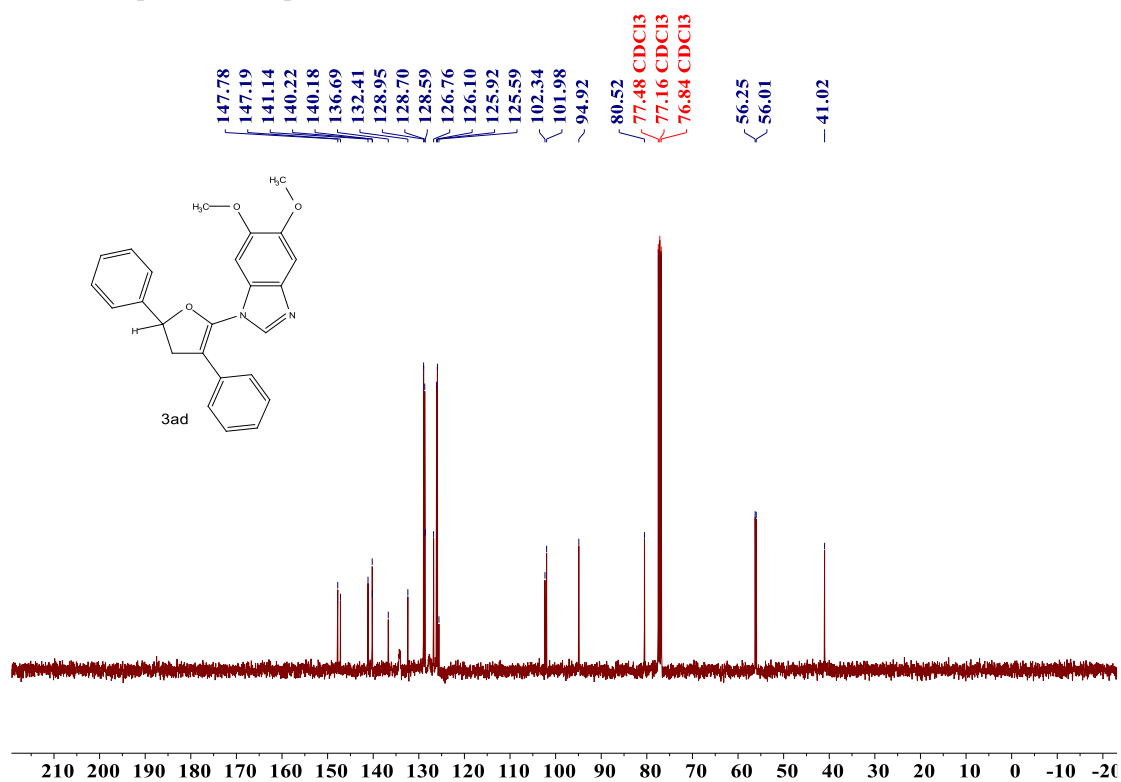
$^{13}\text{C}$  NMR spectra of the product **3ac** (100 MHz,  $\text{CDCl}_3$ )



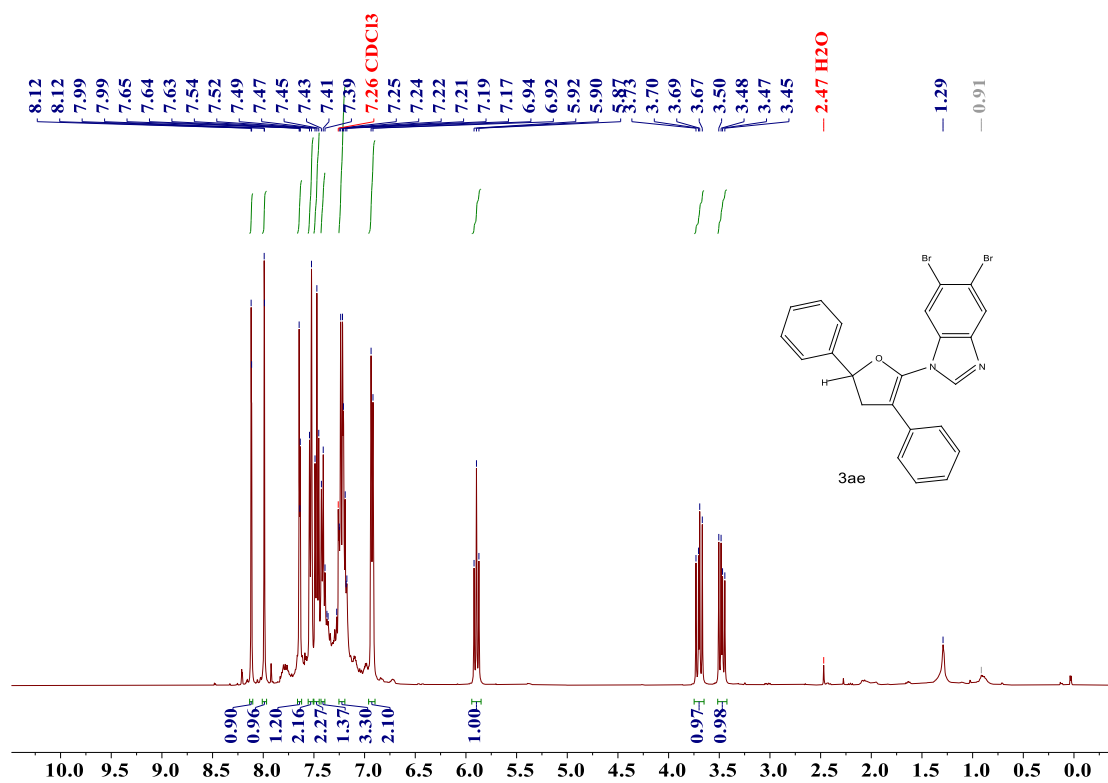
$^1\text{H}$  NMR spectra of the product **3ad** (400 MHz,  $\text{CDCl}_3$ )



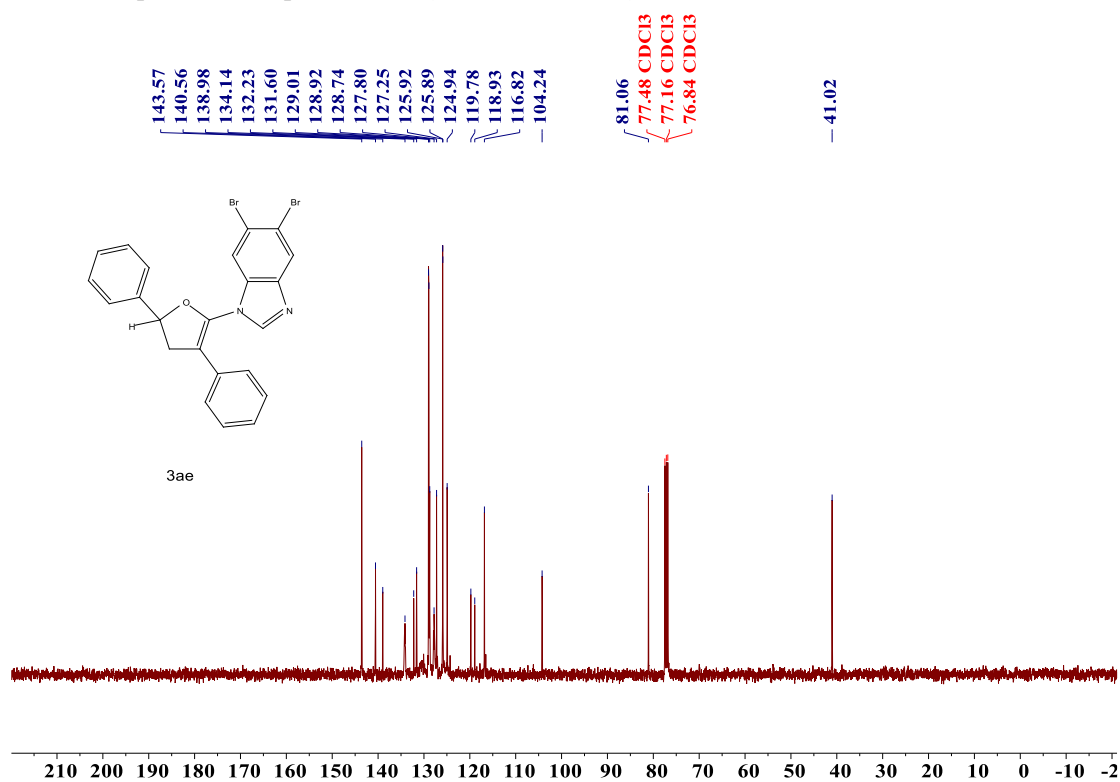
$^{13}\text{C}$  NMR spectra of the product **3ad** (100 MHz,  $\text{CDCl}_3$ )



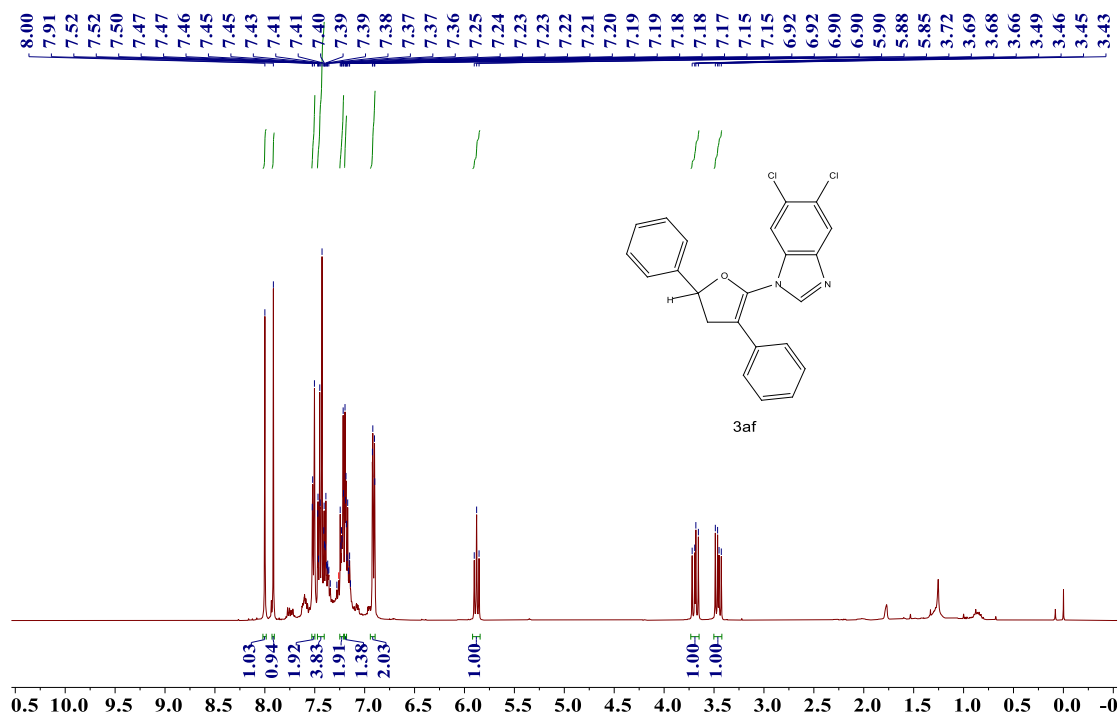
$^1\text{H}$  NMR spectra of the product **3ae** (400 MHz,  $\text{CDCl}_3$ )



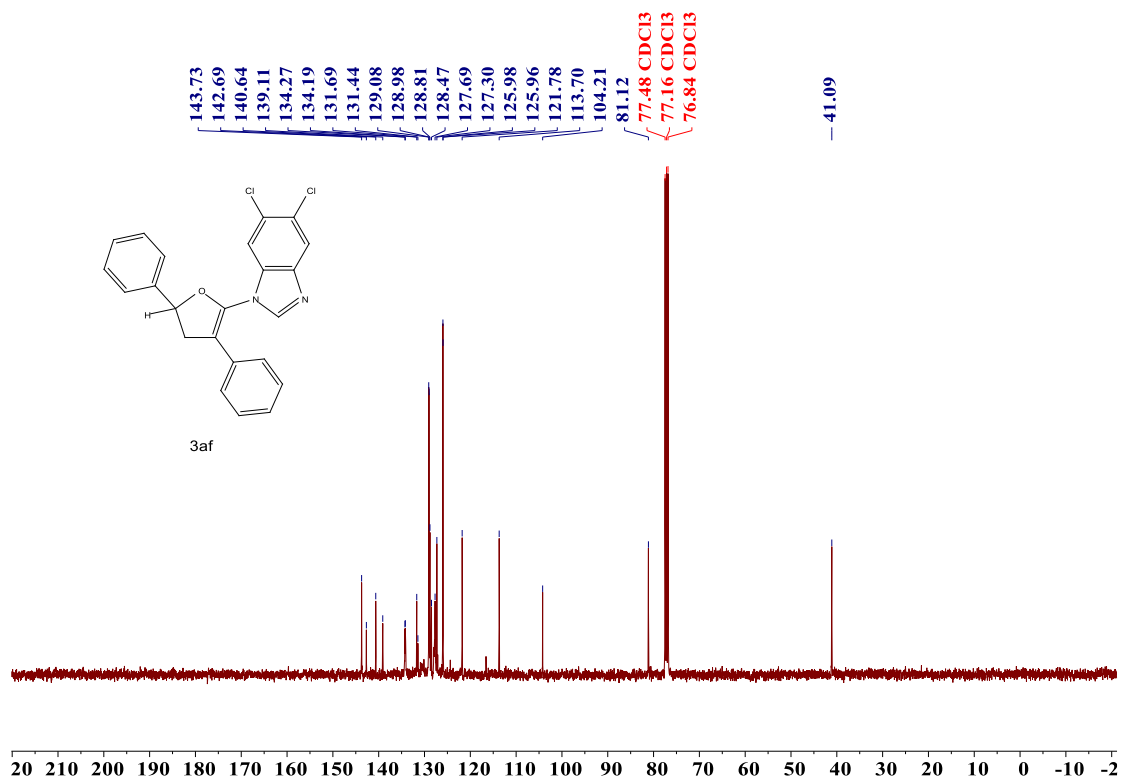
$^{13}\text{C}$  NMR spectra of the product **3ae** (100 MHz,  $\text{CDCl}_3$ )



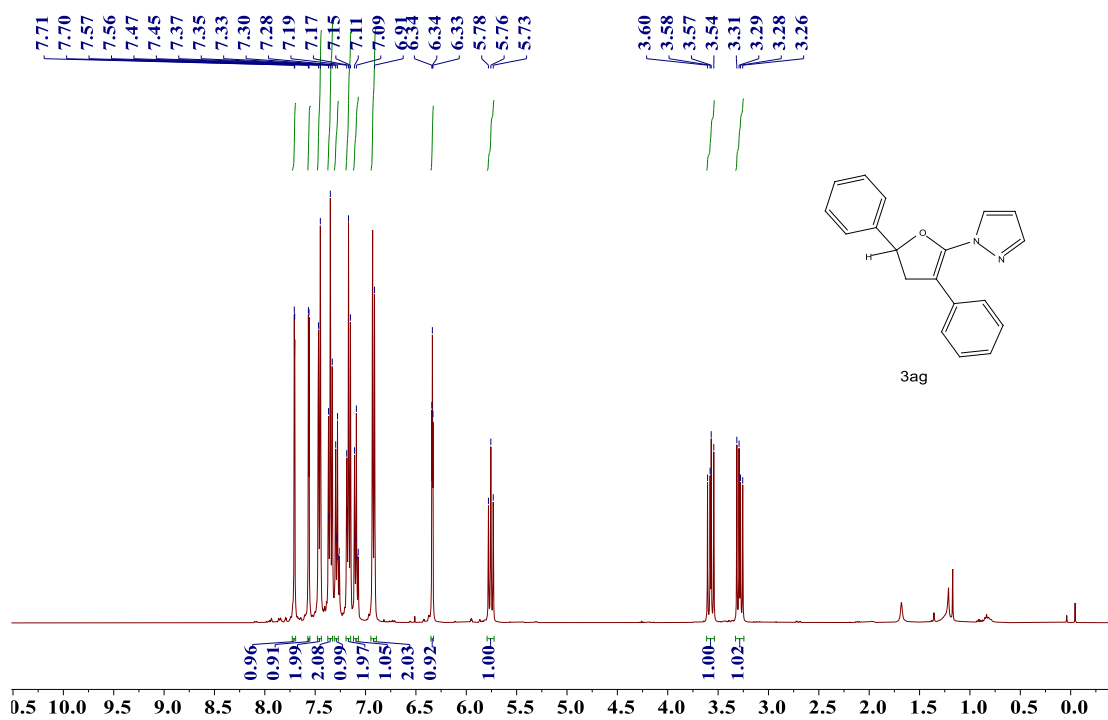
$^1\text{H}$  NMR spectra of the product **3af** (400 MHz,  $\text{CDCl}_3$ )



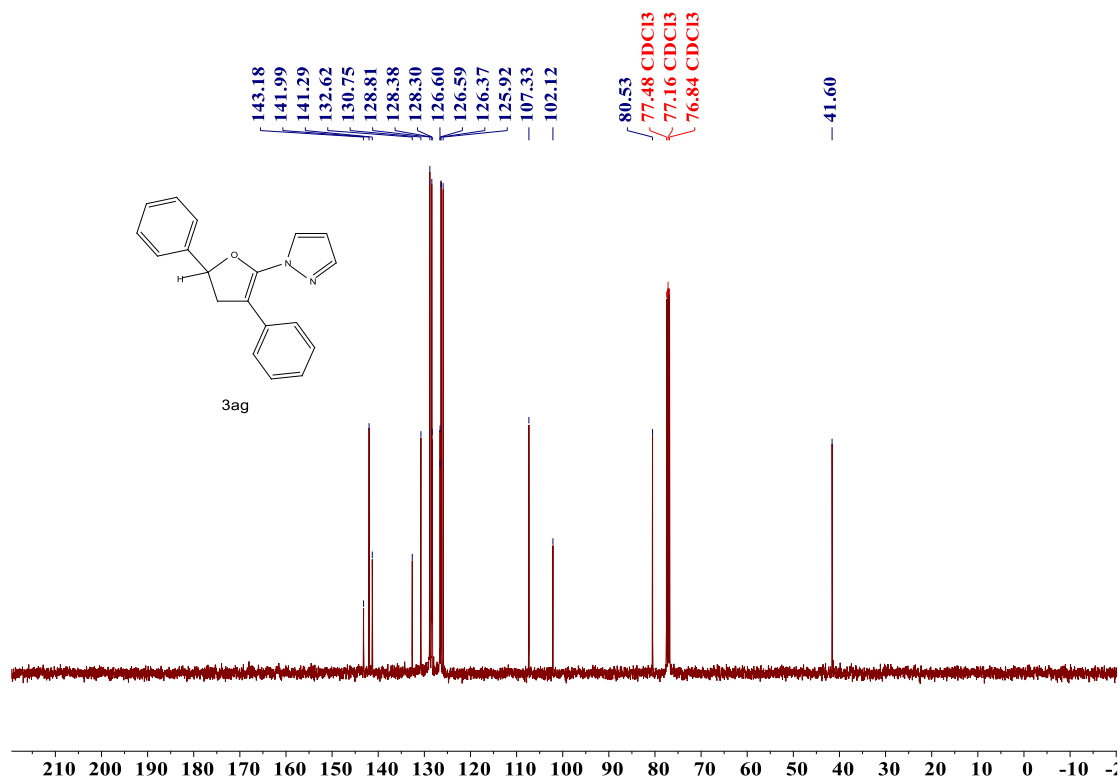
$^{13}\text{C}$  NMR spectra of the product **3af** (100 MHz,  $\text{CDCl}_3$ )



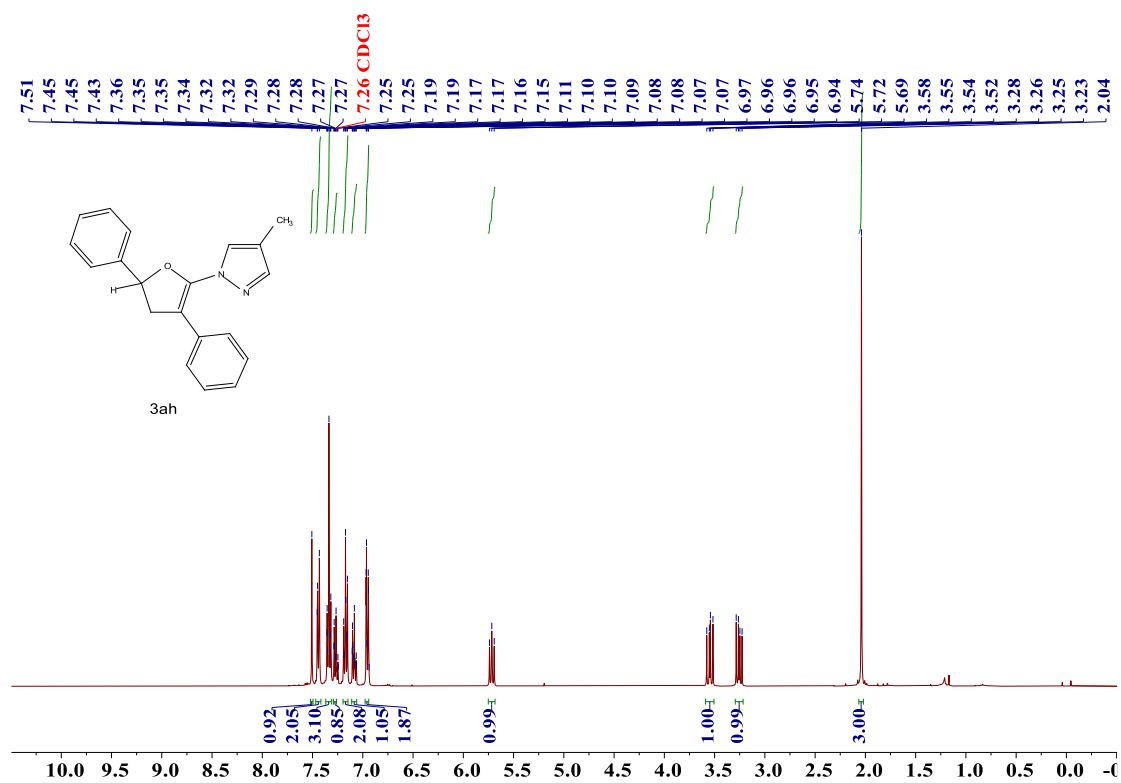
$^1\text{H}$  NMR spectra of the product **3ag** (400 MHz,  $\text{CDCl}_3$ )



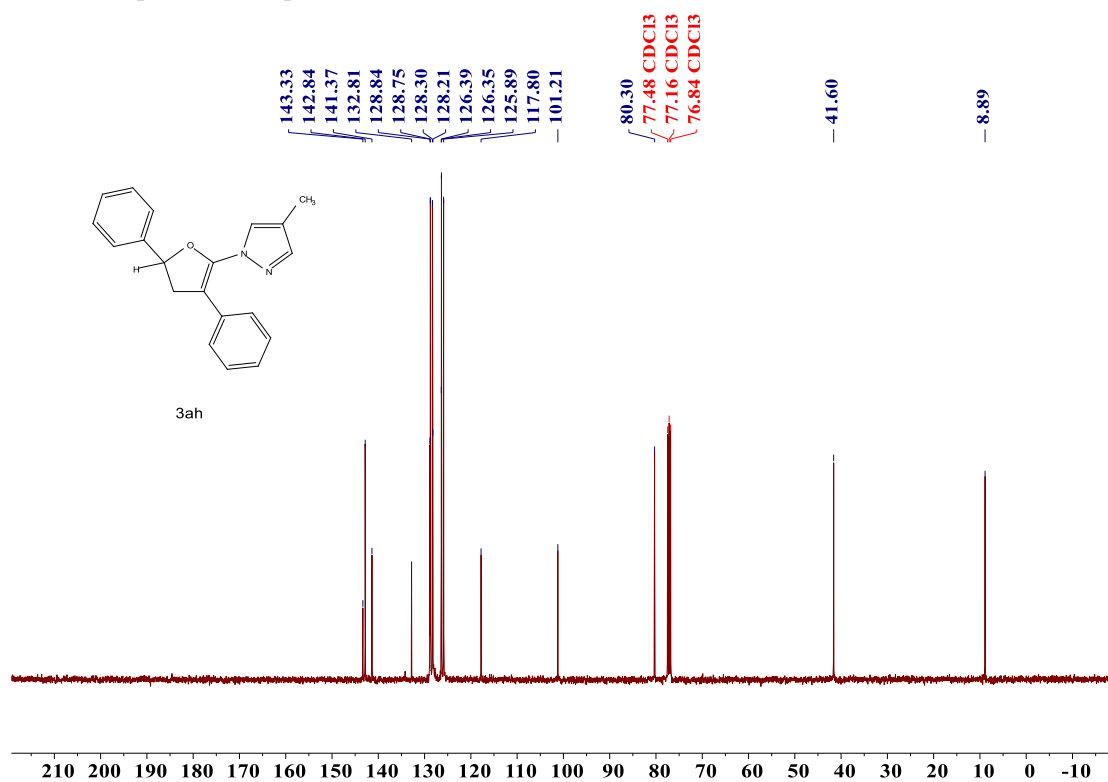
$^{13}\text{C}$  NMR spectra of the product **3ag** (100 MHz,  $\text{CDCl}_3$ )



<sup>1</sup>H NMR spectra of the product **3ah** (400 MHz, CDCl<sub>3</sub>)

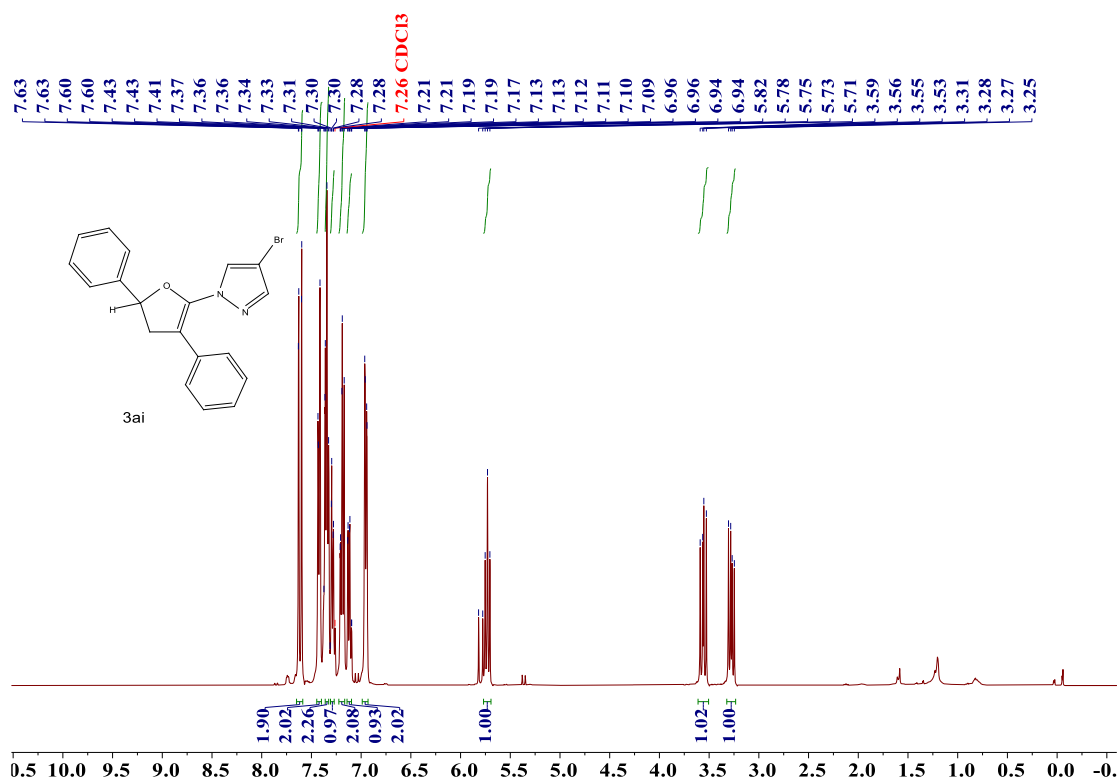


<sup>13</sup>C NMR spectra of the product **3ah** (100 MHz, CDCl<sub>3</sub>)

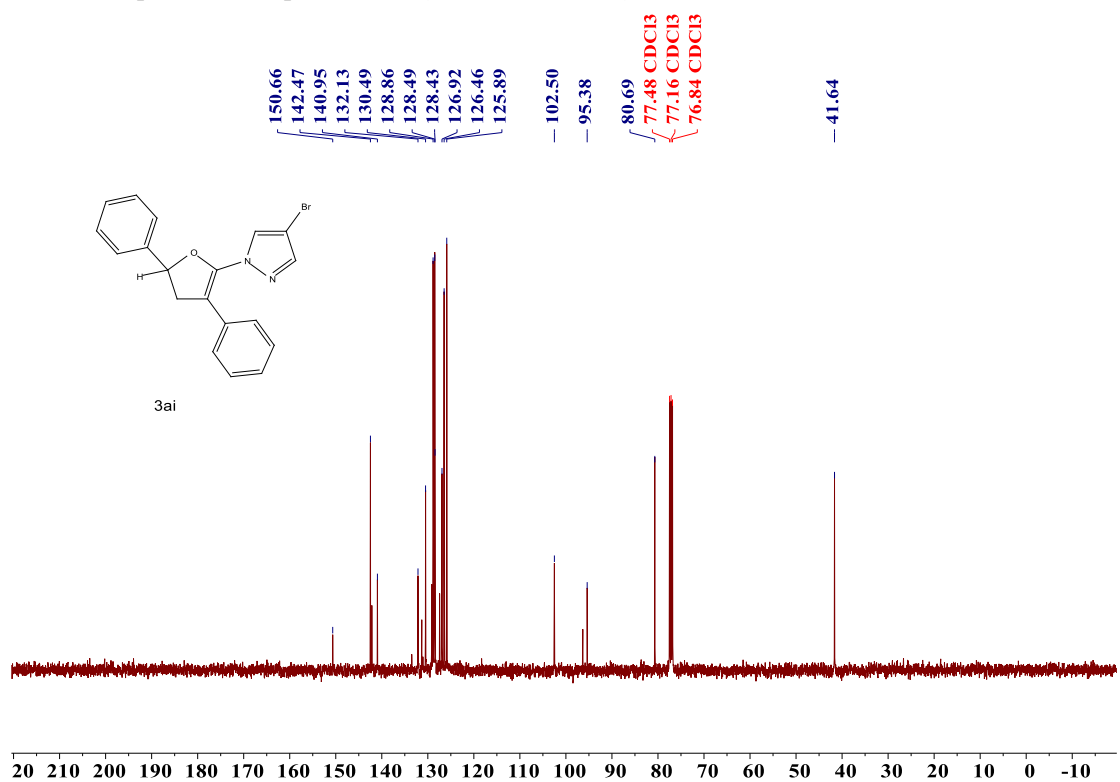




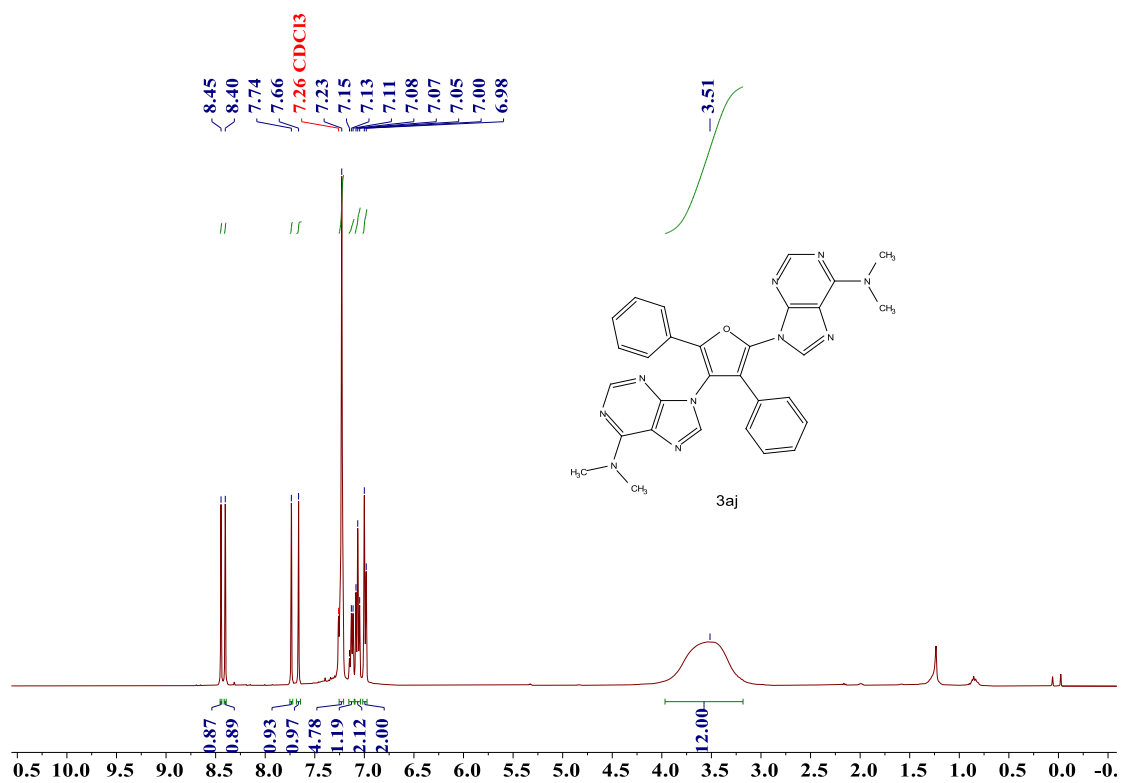
$^1\text{H}$  NMR spectra of the product **3ai** (400 MHz,  $\text{CDCl}_3$ )



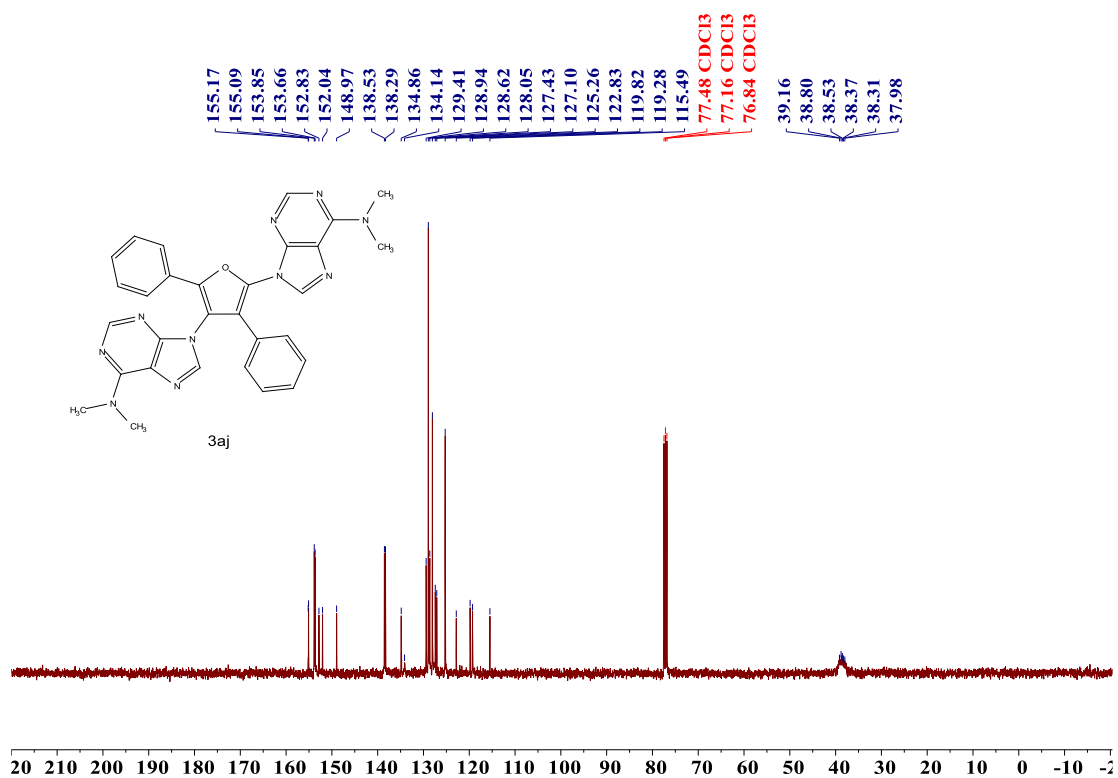
$^{13}\text{C}$  NMR spectra of the product **3ai** (100 MHz,  $\text{CDCl}_3$ )



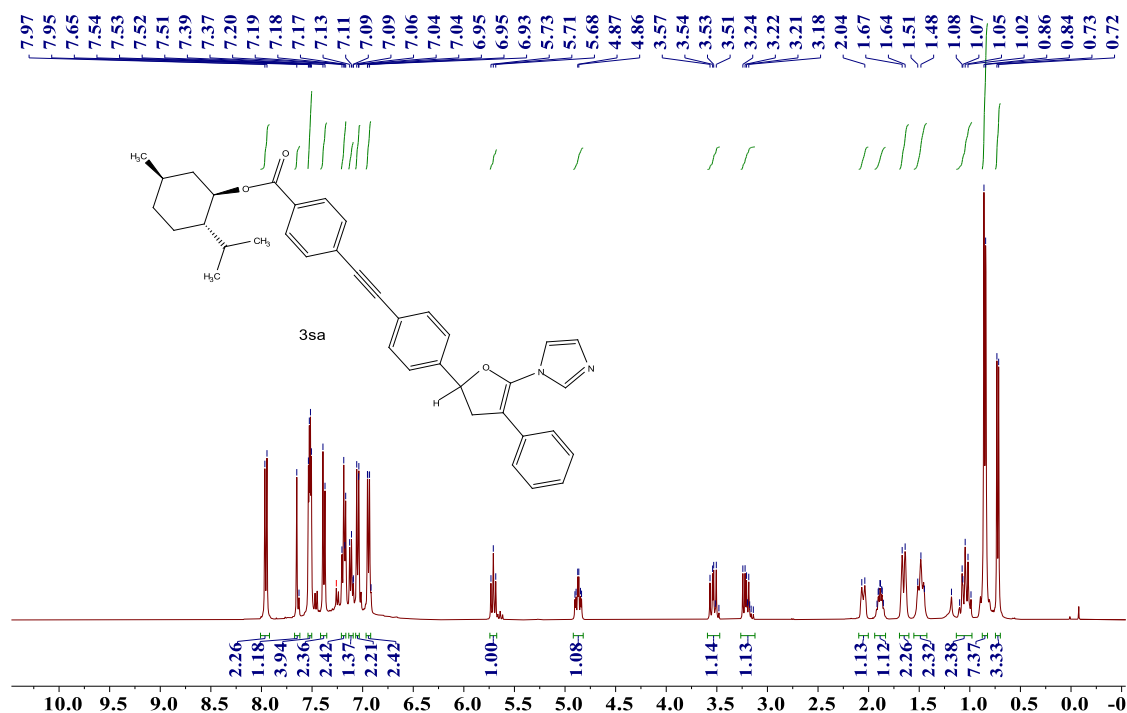
<sup>1</sup>H NMR spectra of the product **3aj** (400 MHz, CDCl<sub>3</sub>)



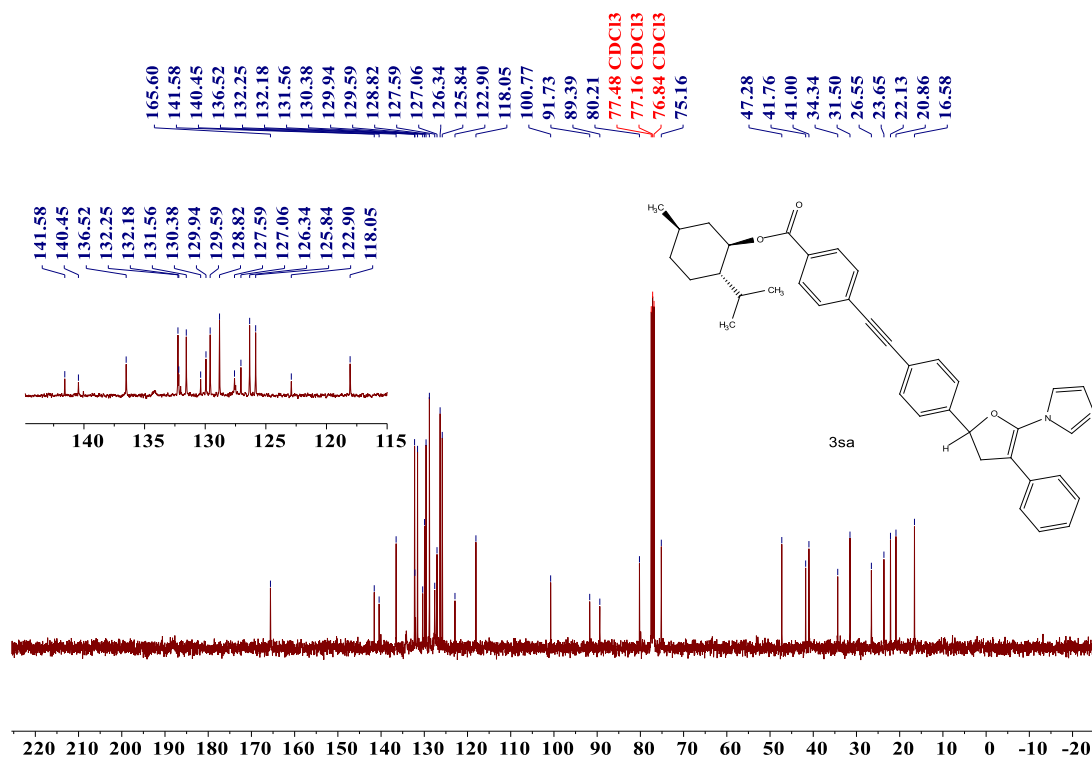
<sup>13</sup>C NMR spectra of the product **3aj** (100 MHz, CDCl<sub>3</sub>)



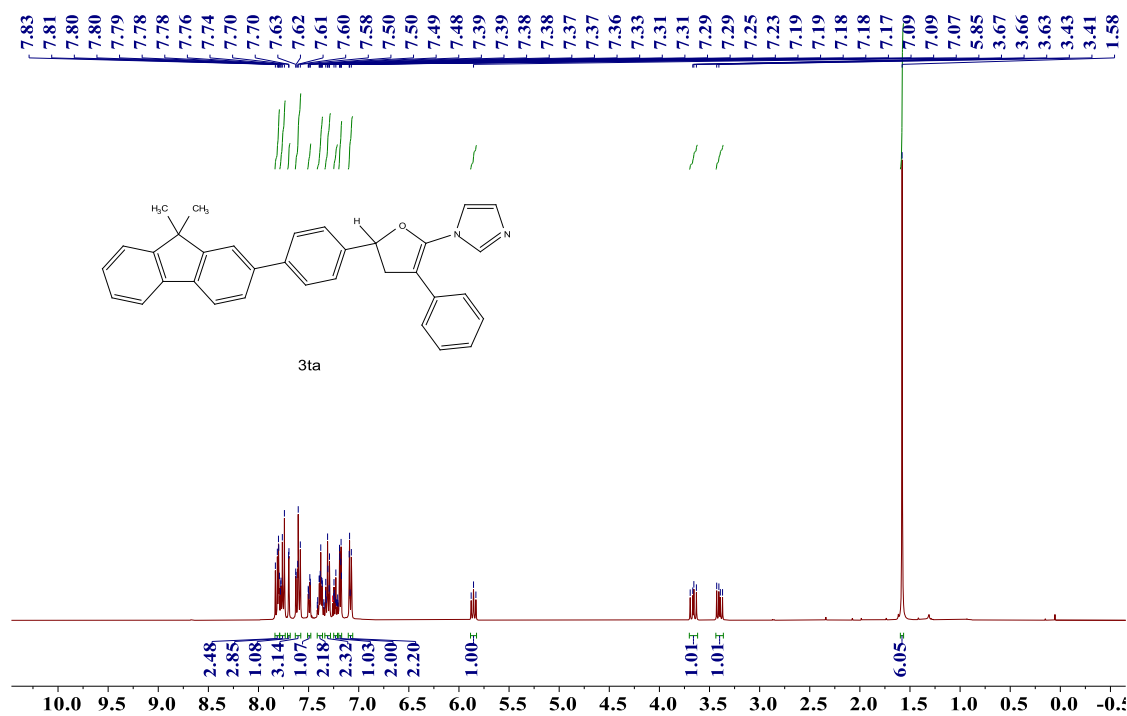
$^1\text{H}$  NMR spectra of the product **3sa** (400 MHz,  $\text{CDCl}_3$ )



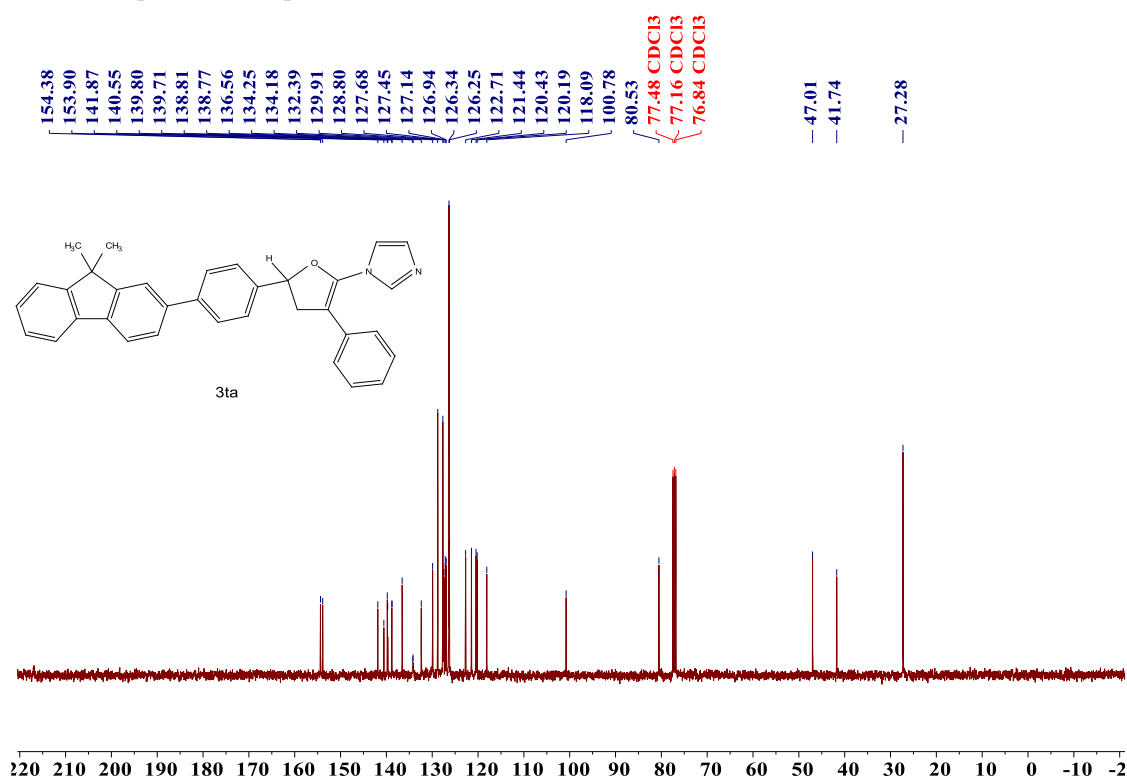
$^{13}\text{C}$  NMR spectra of the product **3sa** (100 MHz,  $\text{CDCl}_3$ )



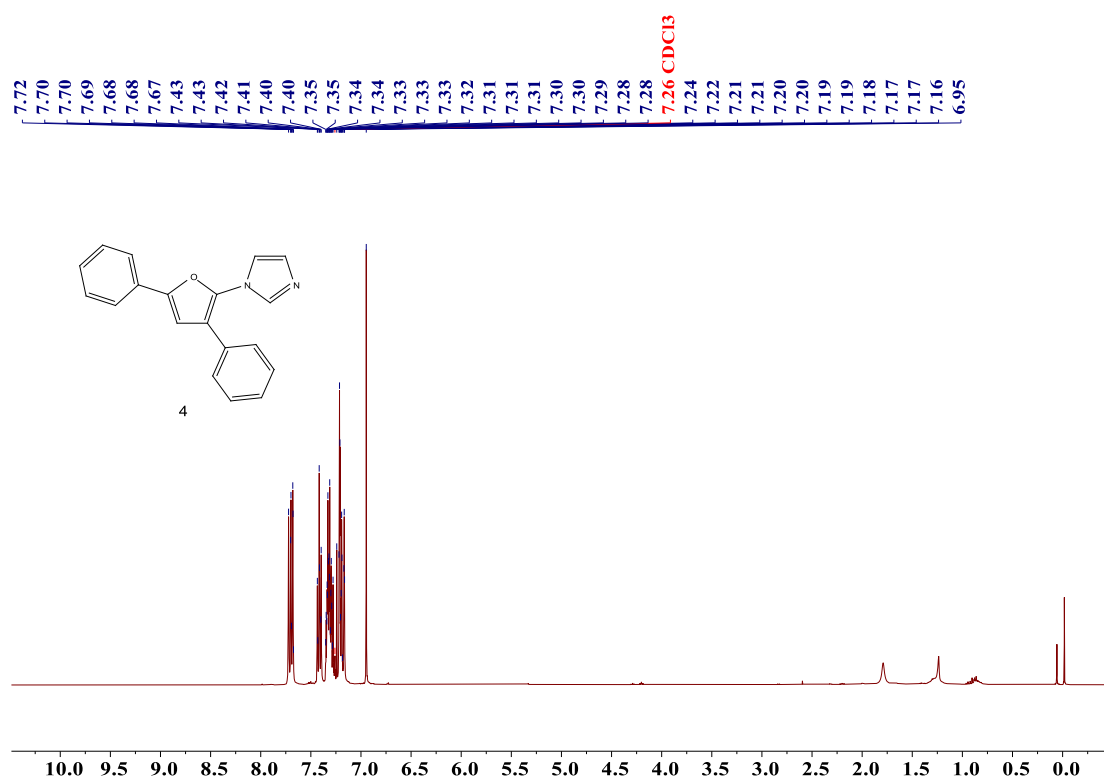
$^1\text{H}$  NMR spectra of the product **3ta** (400 MHz,  $\text{CDCl}_3$ )



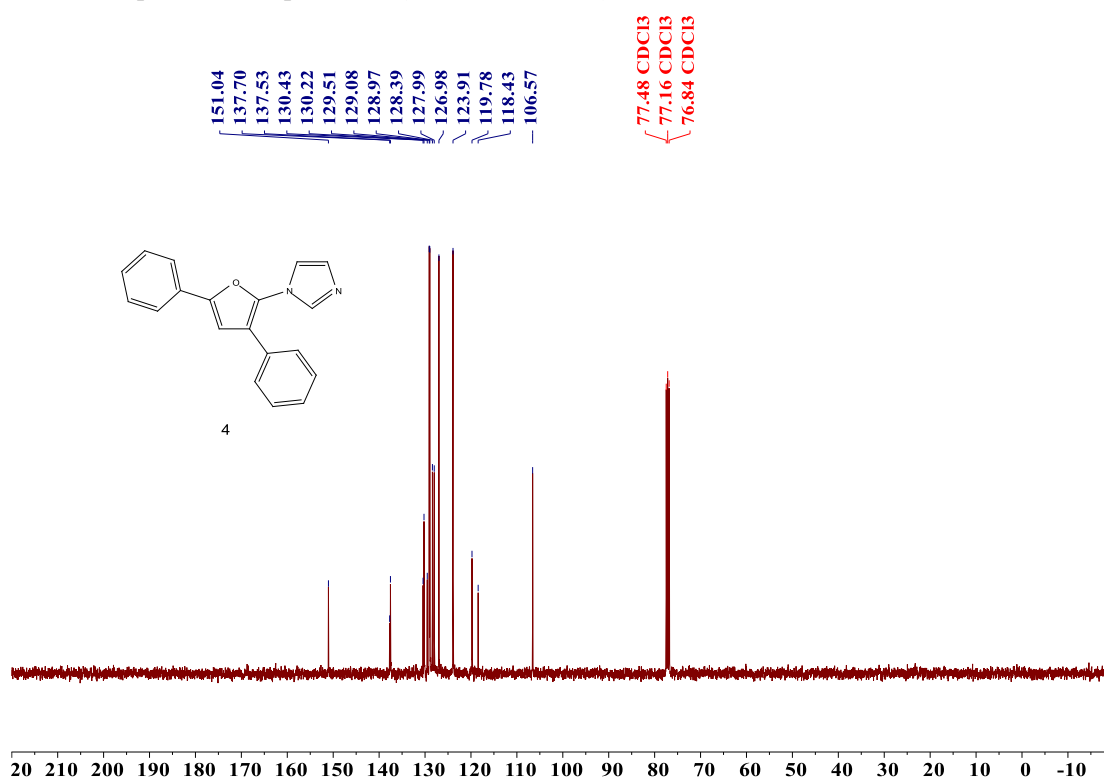
$^{13}\text{C}$  NMR spectra of the product **3ta** (100 MHz,  $\text{CDCl}_3$ )



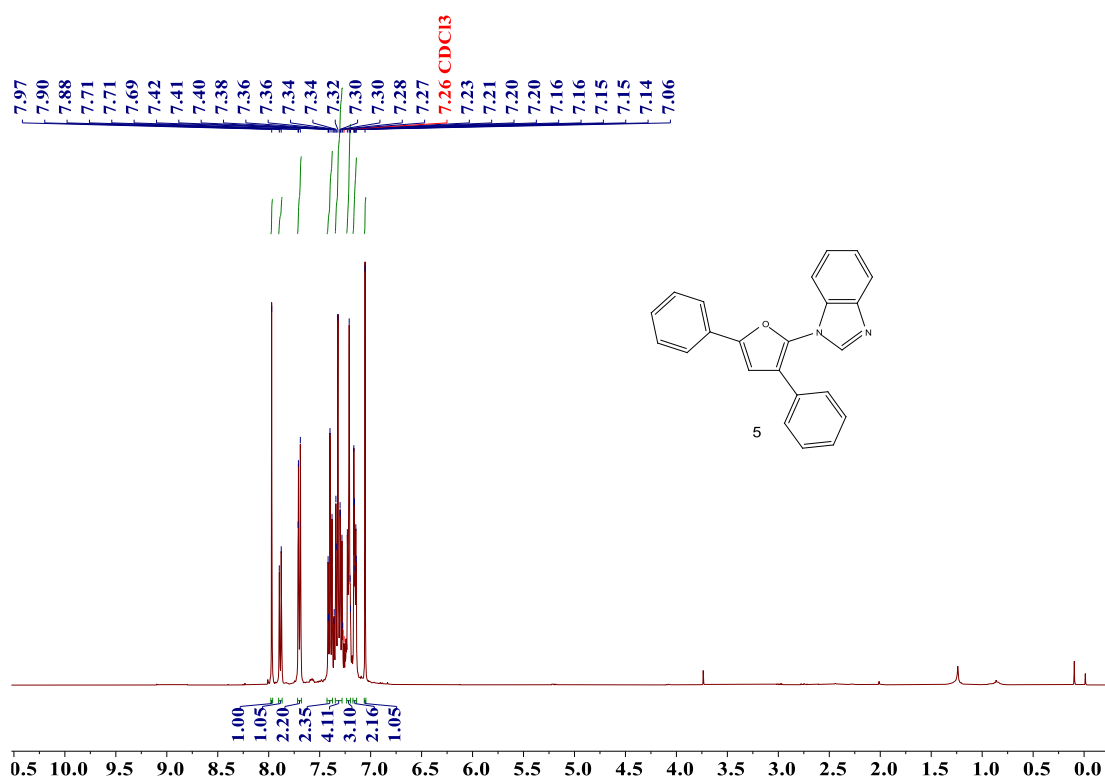
<sup>1</sup>H NMR spectra of the product **4** (400 MHz, CDCl<sub>3</sub>)



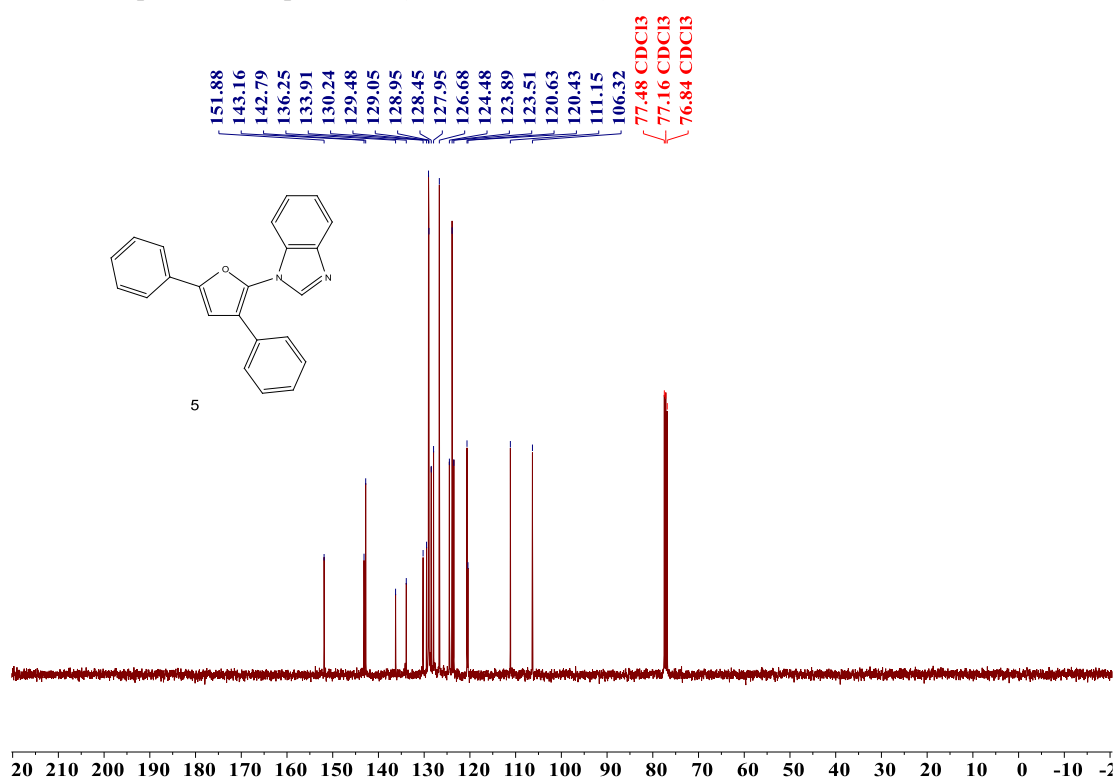
<sup>13</sup>C NMR spectra of the product **4** (100 MHz, CDCl<sub>3</sub>)



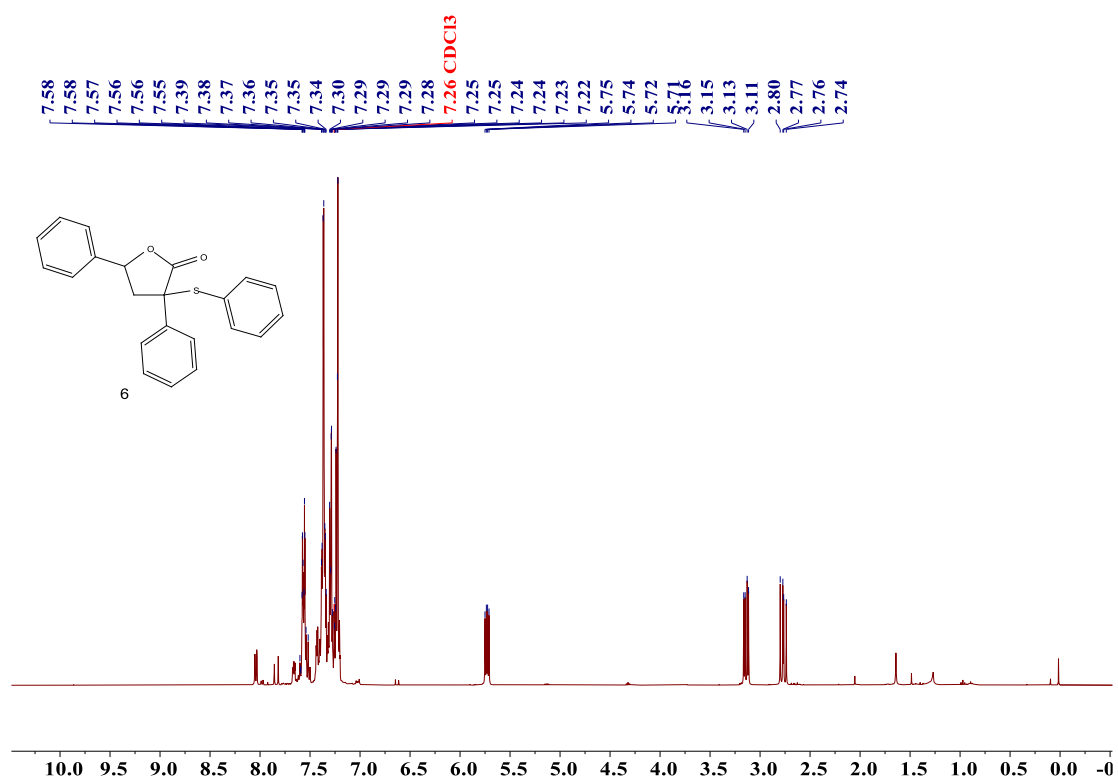
$^1\text{H}$  NMR spectra of the product **5** (400 MHz,  $\text{CDCl}_3$ )



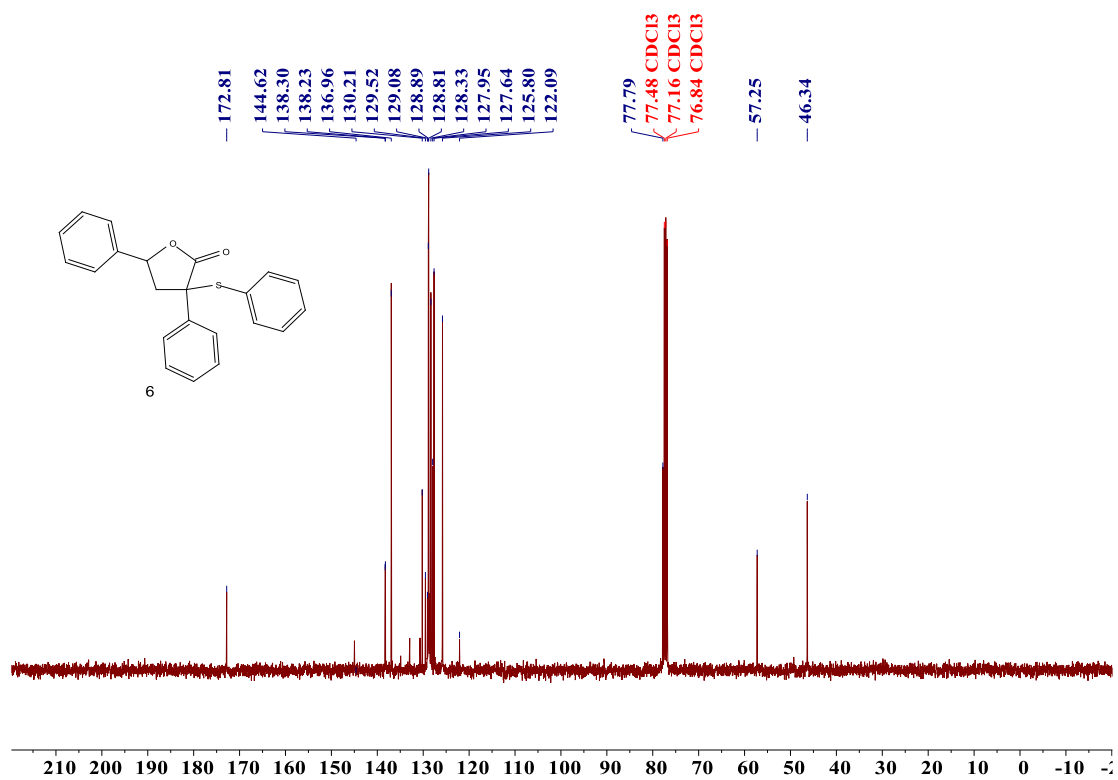
$^{13}\text{C}$  NMR spectra of the product **5** (100 MHz,  $\text{CDCl}_3$ )



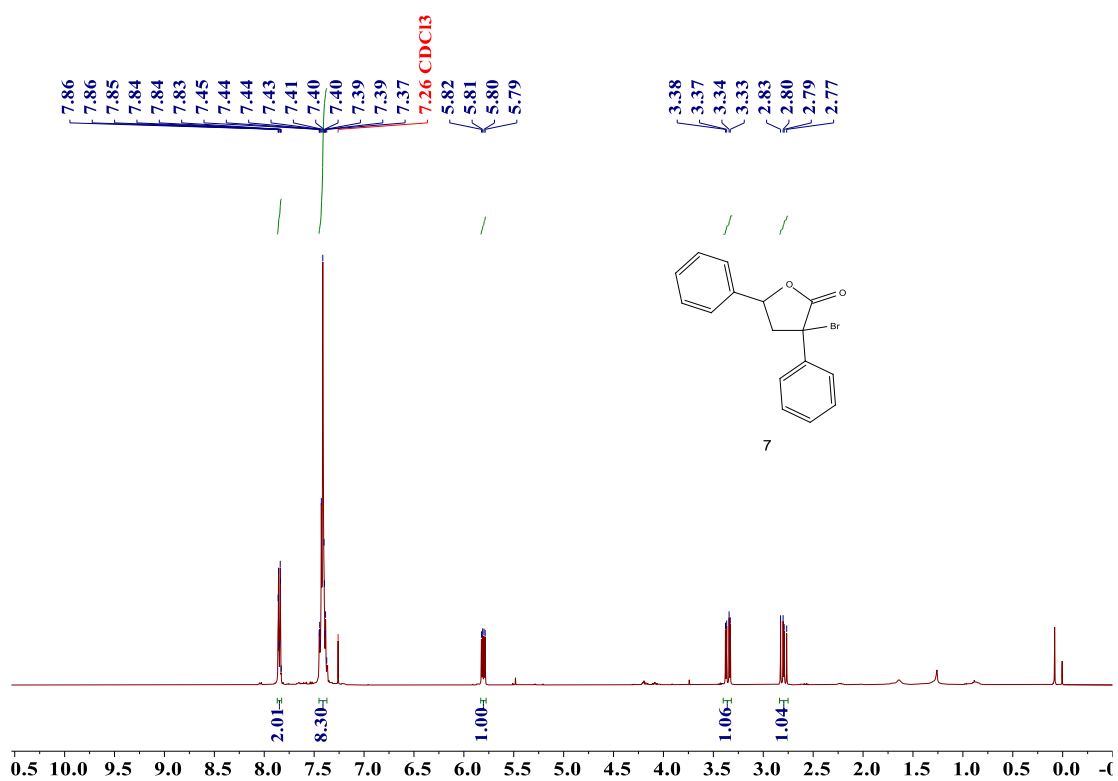
$^1\text{H}$  NMR spectra of the product **6** (400 MHz,  $\text{CDCl}_3$ )



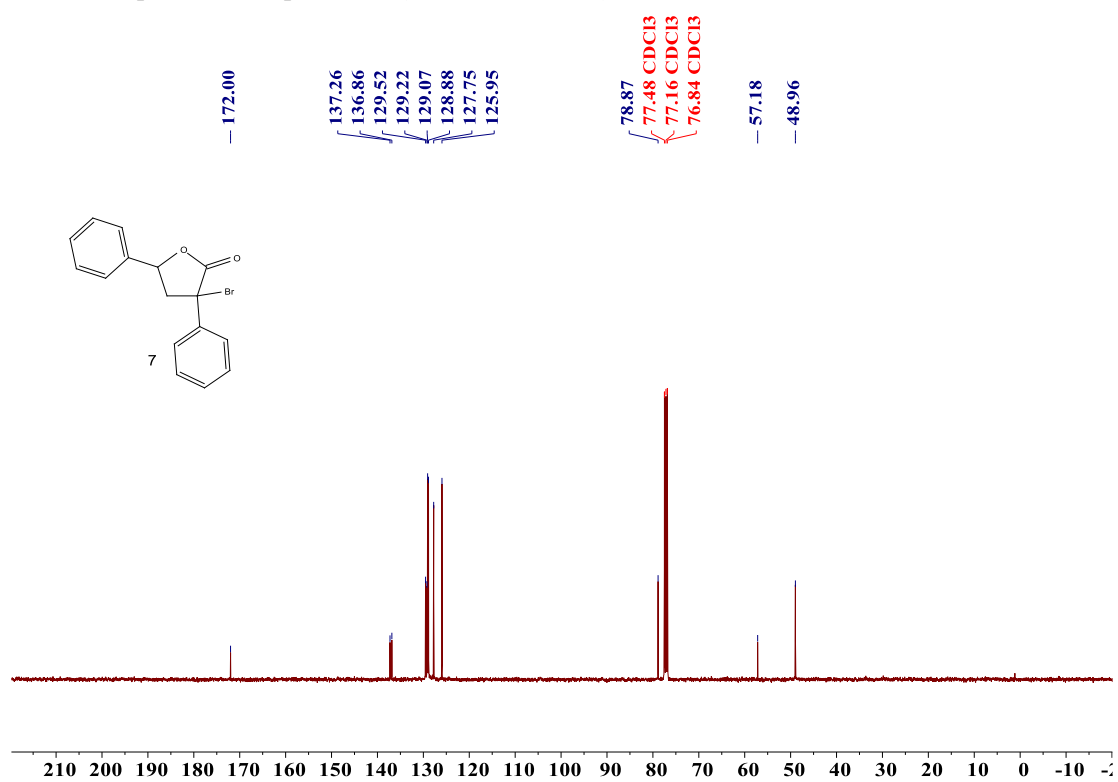
$^{13}\text{C}$  NMR spectra of the product **6** (100 MHz,  $\text{CDCl}_3$ )



$^1\text{H}$  NMR spectra of the product 7 (400 MHz,  $\text{CDCl}_3$ )

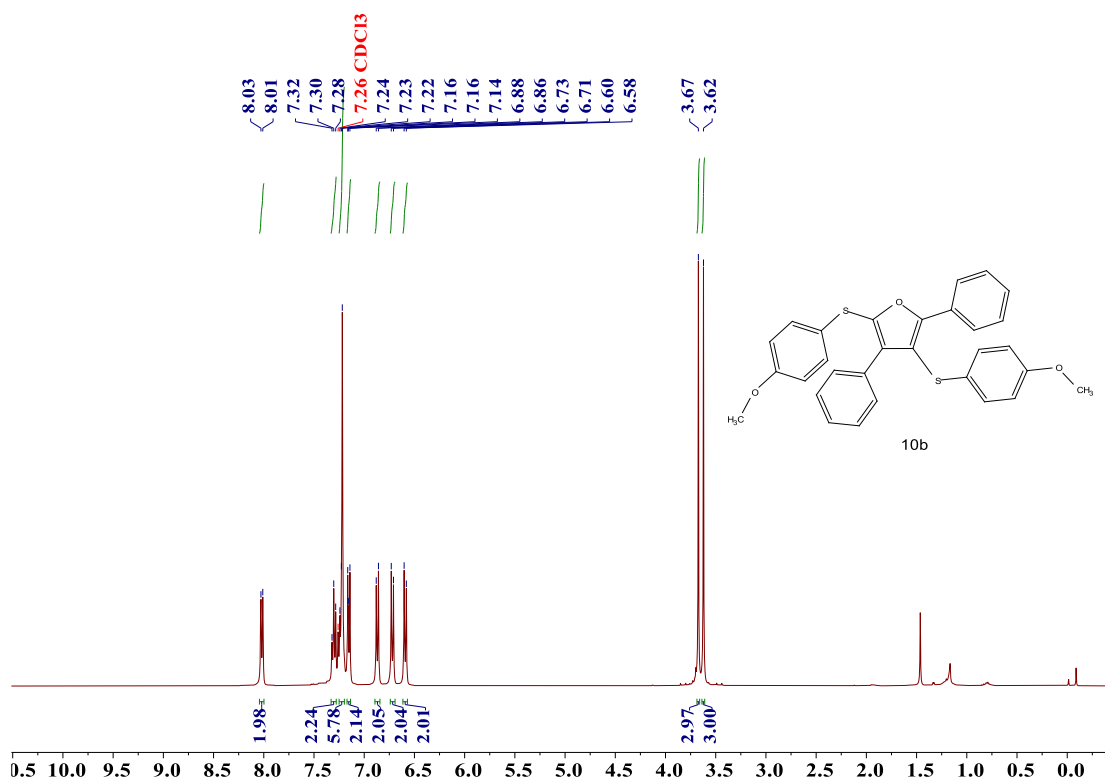


$^{13}\text{C}$  NMR spectra of the product 7 (100 MHz,  $\text{CDCl}_3$ )

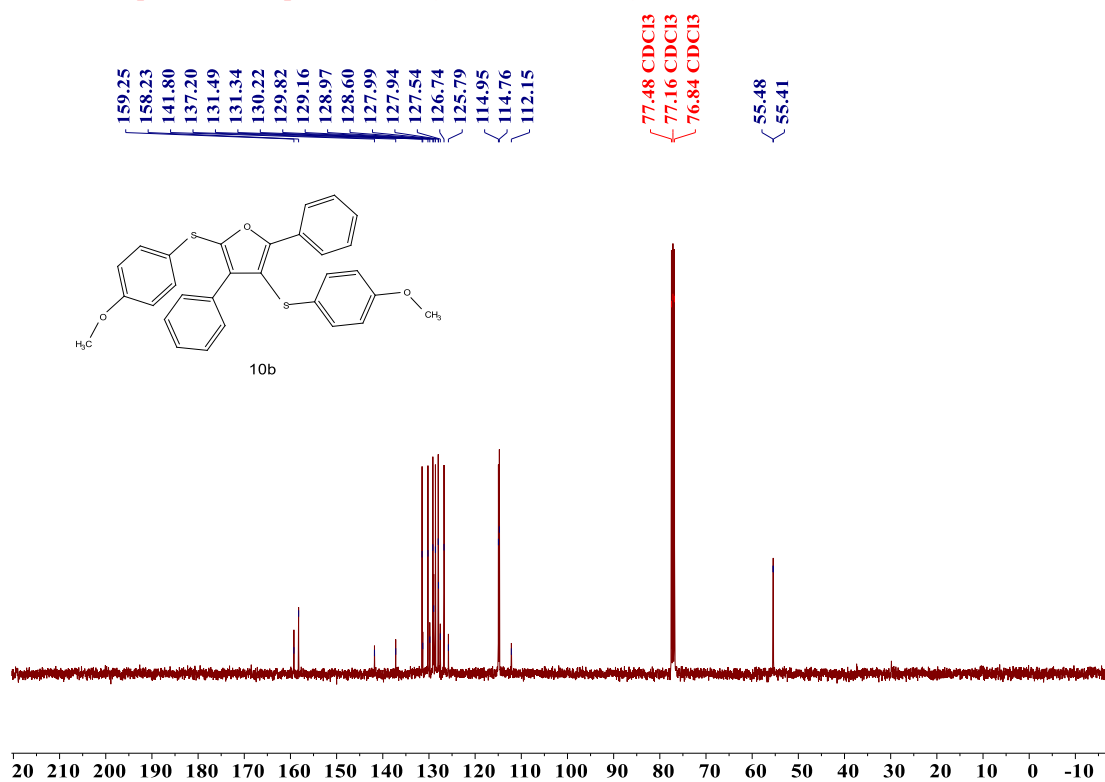




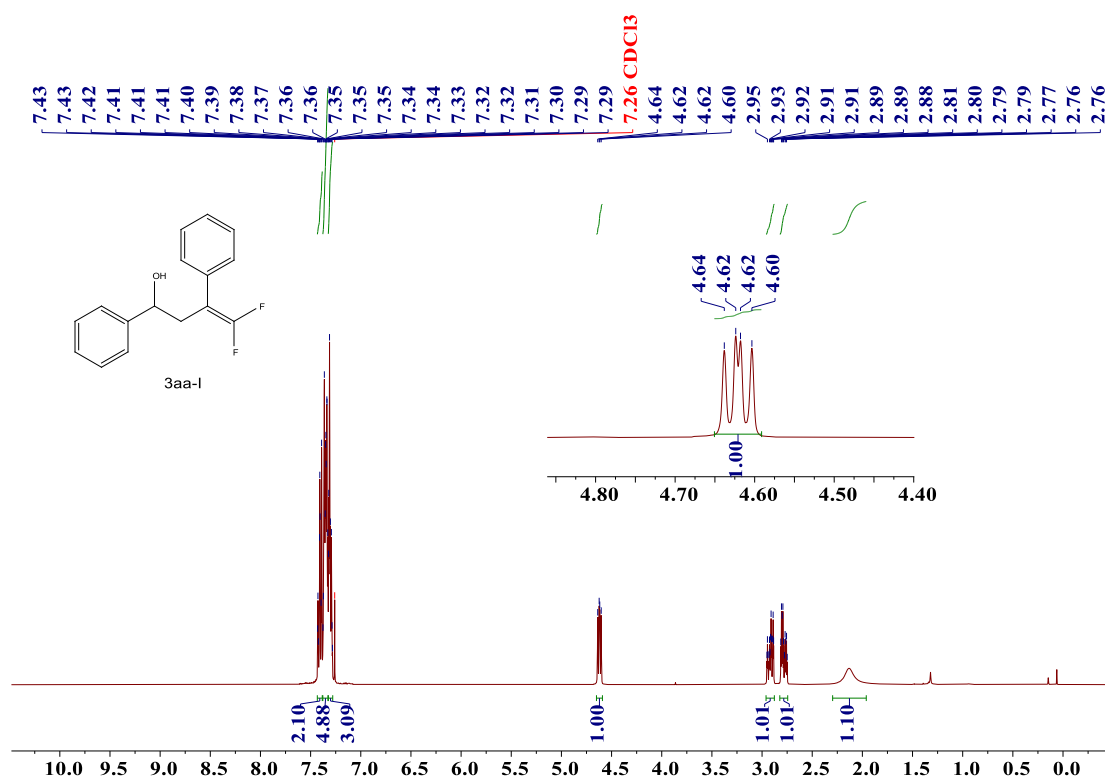
<sup>1</sup>H NMR spectra of the product **10b** (400 MHz, CDCl<sub>3</sub>)



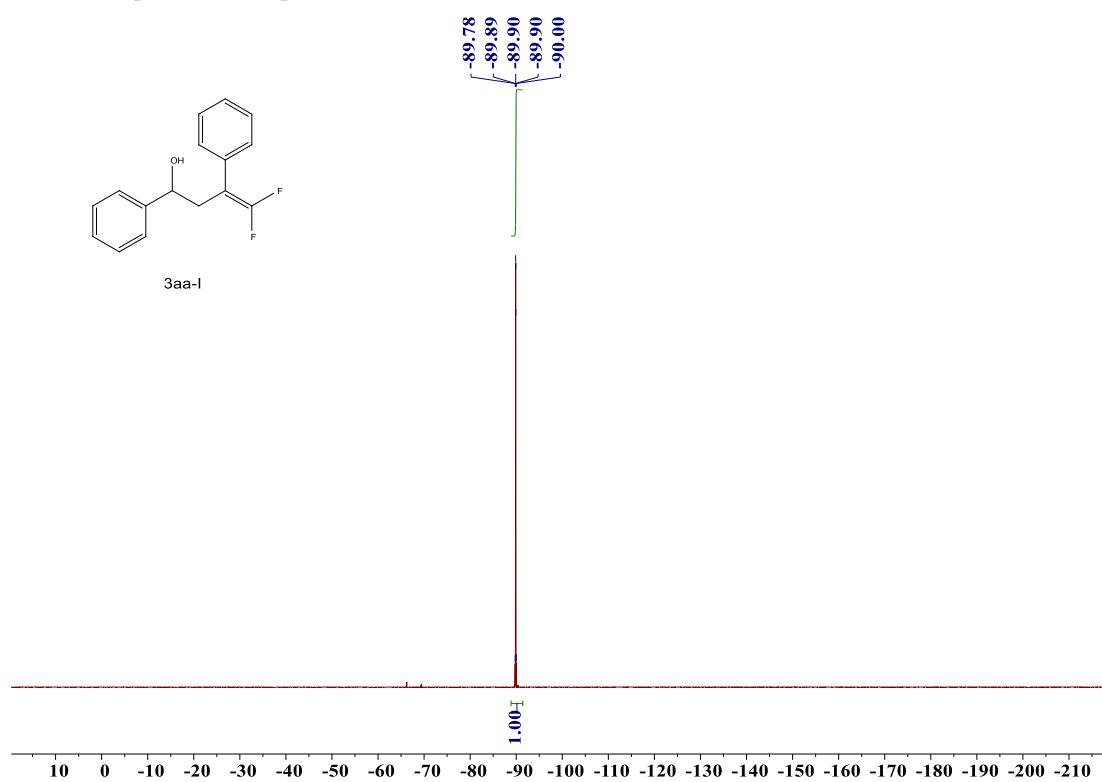
<sup>13</sup>C NMR spectra of the product **10b** (100 MHz, CDCl<sub>3</sub>)



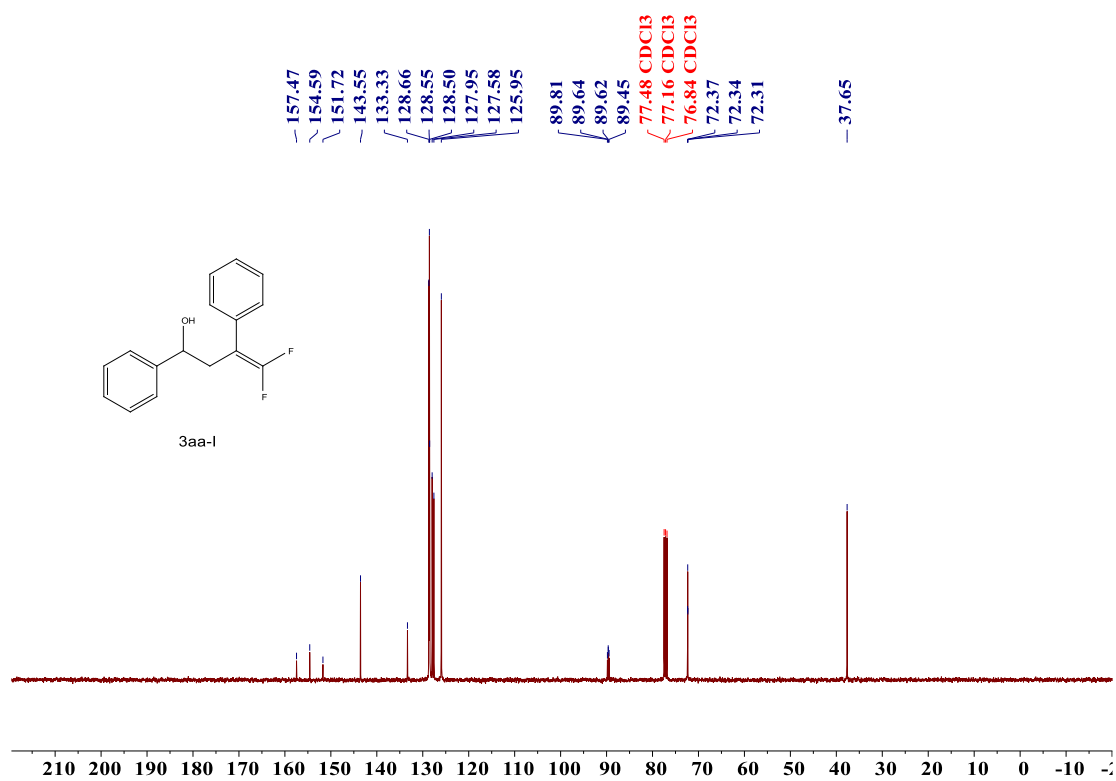
$^1\text{H}$  NMR spectra of the product **3aa-I** (400 MHz,  $\text{CDCl}_3$ )



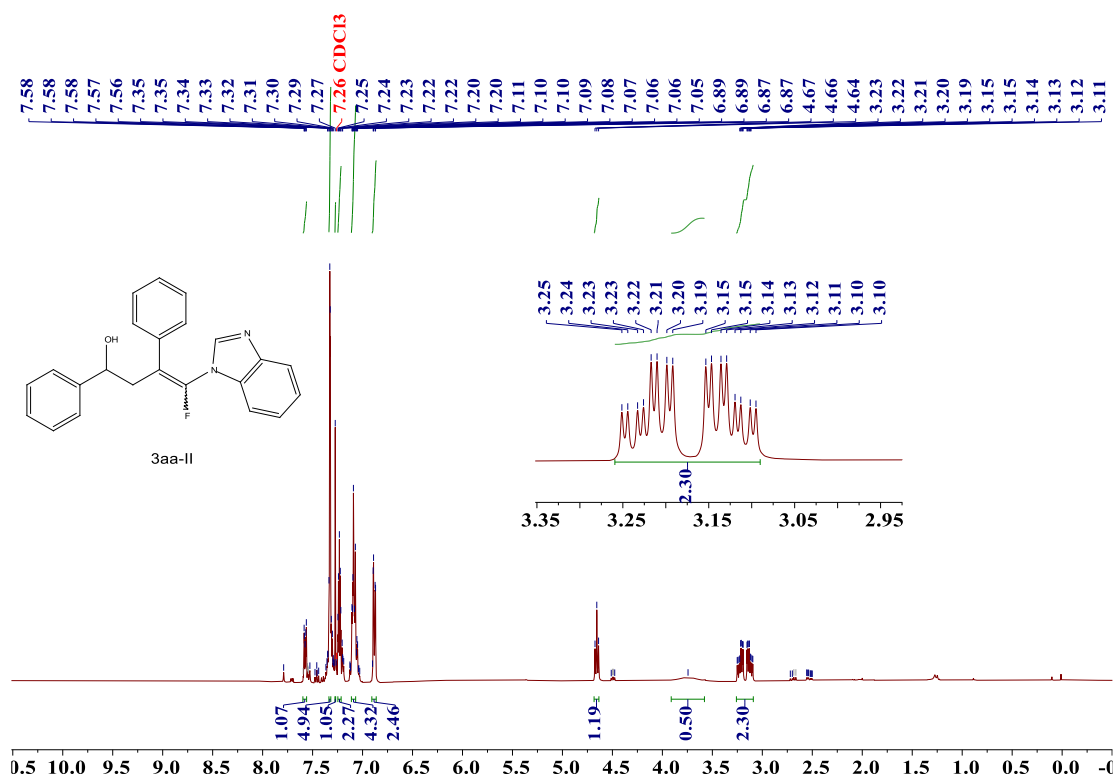
$^{19}\text{F}$  NMR spectra of the product **3aa-I** (376 MHz,  $\text{CDCl}_3$ )



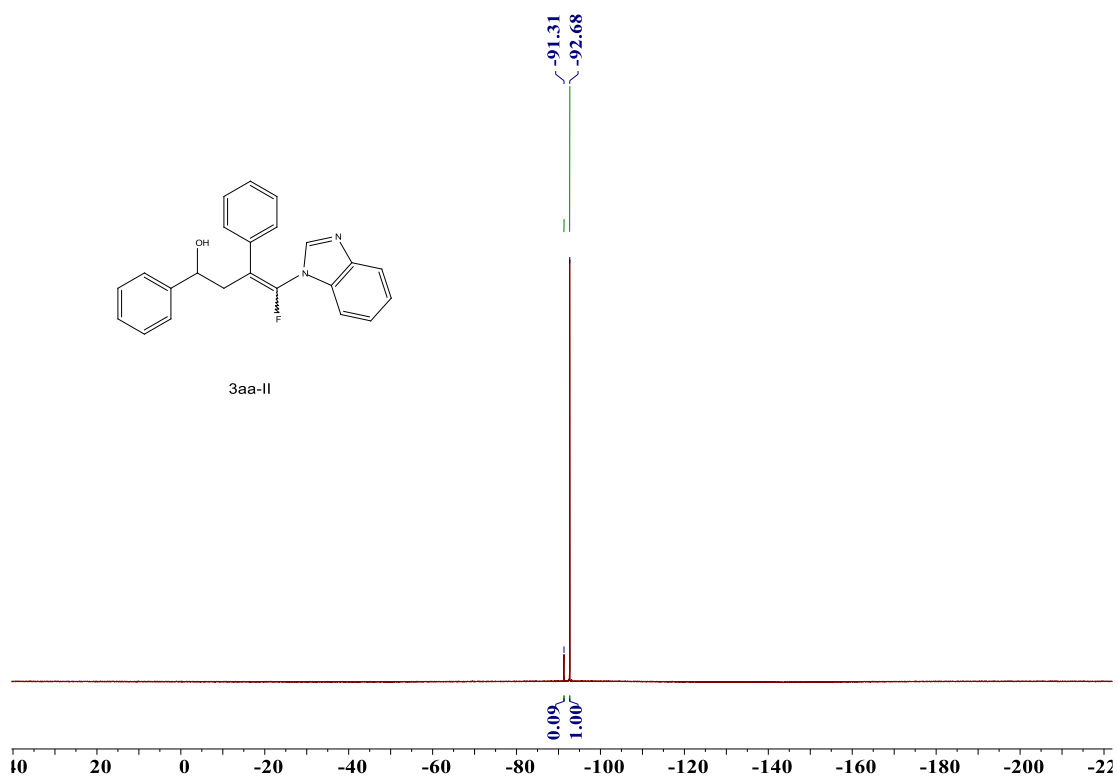
<sup>13</sup>C NMR spectra of the product **3aa-I** (100 MHz, CDCl<sub>3</sub>)



<sup>1</sup>H NMR spectra of the product **3aa-II** (400 MHz, CDCl<sub>3</sub>)



$^{19}\text{F}$  NMR spectra of the product **3aa-II** (376 MHz,  $\text{CDCl}_3$ )



$^{13}\text{C}$  NMR spectra of the product **3aa-II** (100 MHz,  $\text{CDCl}_3$ )

