# **Supporting Information**

# Defluorinative Functionalization of Perfluoroalkyl Alkenes with Ureas: Synthesis of C4-Perfluoroalkenyl

# 2-Imidazolones

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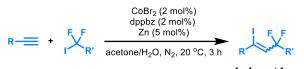
## **General information**

Unless otherwise stated, all reagents were purchased from commercial suppliers and used without further purification. All reactions were carried out under 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), quintet (quint), multiplet (m), doublet of doublets (dd), doublet of triplets (dt), doublet of quartets (dq), triplet of doublets (td), tt (triplet of triplets), quartet of doublets (qd), and quartet of triplets (qt). 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. 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.

<u>Caution: The reaction should be performed under basic conditions; otherwise, attention should</u> <u>be paid to the possible release of HF! After the completion of the defluorination reaction, the</u> <u>etching was observed.</u>

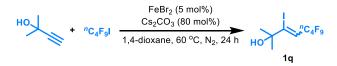
# General procedure for the synthesis of perfluoroalkyl alkenyl iodides 1

General procedure A (GPA)<sup>[1]</sup>



According to Jacobi von Wangelin's reported method, a flask (50 mL), equipped with a magnetic stir bar, was charged with alkyne (5 mmol, 1 equiv.), polyfluoroalkyl iodide (7.5 mmol, 1.5 equiv.), CoBr<sub>2</sub> (21.9 mg, 0.1 mmol, 0.02 equiv.), 1,2-bis(diphenylphosphino)benzene (44.6 mg, 0.1 mmol, 0.02 equiv.), dppbz), Zn (16.3 mg, 0.25 mmol, 0.05 equiv.), and acetone/H<sub>2</sub>O (10 mL, 30/1) under N<sub>2</sub> atmosphere. The reaction mixture was stirred at 20 °C under N<sub>2</sub> atmosphere for 3 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (50 mL) and extracted with EtOAc (50 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 (200/1~20/1) as eluent to afford the pure product **1**.

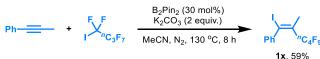
#### General procedure B (GPB)<sup>[2]</sup>



According to Hu's reported method, a flask (50 mL), equipped with a magnetic stir bar, was charged with 2-methylbut-3-yn-2-ol (420.6 mg, 5 mmol, 1 equiv.), perfluorobutyl iodide (2594.4 mg, 7.5 mmol, 1.5 equiv.), FeBr<sub>2</sub> (53.9 mg, 0.25 mmol, 0.05 equiv.), Cs<sub>2</sub>CO<sub>3</sub> (1303.0 mg, 4 mmol, 0.8 equiv.), and anhydrous 1,4-dioxane (20 mL) under N<sub>2</sub> atmosphere. The reaction mixture was stirred at 60  $^{\circ}$ C under N<sub>2</sub> atmosphere for 24 h. The reaction was then quenched by saturated

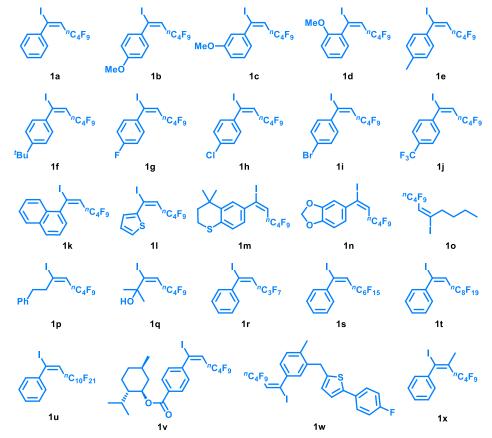
 $NH_4Cl$  solution (50 mL) and extracted with EtOAc (50 mL x 3). The organic layer was washed with saturated brine twice, dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The crude product was purified by flash silica gel column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (100/1~80/1) as eluent to afford the pure product **1q** (1978.2 mg, 46% yield).

#### General procedure C (GPC)<sup>[3]</sup>



According to Yang's reported method, a flask (50 mL) equipped with a magnetic stir bar was charged with 1-phenyl-1-propyne (223 mg, 2 mmol, 1 equiv.), perfluorobutyl iodide (2.075 g, 6 mmol, 3 equiv.),  $B_2Pin_2$  (152.4 mg, 0.6 mmol, 0.3 equiv.),  $K_2CO_3$  (552 mg, 4 mmol, 2 equiv.), and MeCN (4 mL) under N<sub>2</sub> atmosphere. The reaction mixture was stirred at 130 °C under N<sub>2</sub> atmosphere for 8 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (40 mL) and extracted with EtOAc (40 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 as eluent to afford the pure product **1x** (546.7 mg, 59%).

## Perfluoroalkyl alkenyl iodides 1 used in the reaction:



# Representative examples: (*E*)-(3,3,4,4,5,5,6,6,6-Nonafluoro-1-iodohex-1-en-1-yl)benzene (1a)<sup>[1a]</sup>:

Following general procedure GPA.

Yield = 78% (6.99 g, 20 mmol scale). Colorless oil.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.36–7.27 (m, 5H), 6.59 (t, *J* = 13.6 Hz, 1H) ppm.

<sup>19</sup>**F** NMR (376 MHz, CDCl<sub>3</sub>):  $\delta$  = -80.86 - -81.04 (m, 3F), -105.37 (q, *J* = 10.6 Hz, 2F), -123.71 (t, *J* = 9.7 Hz, 2F), -125.78 (q, *J* = 110.0 Hz, 2F) ppm.

### (*E*)-1-Methyl-4-(3,3,4,4,5,5,6,6,6-nonafluoro-1-iodohex-1-en-1-yl)benzene (1e)<sup>[1b]</sup>:

Following general procedure GPA.

Yield = 78% (3.60 g, 10 mmol scale). Colorless oil.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 7.22–7.12 (m, 4H), 6.57 (t, *J* = 13.5 Hz, 1H), 2.36 (s, 3H) ppm. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>):  $\delta$  = -80.92 (t, *J* = 10.3 Hz, 3F), -105.20 (q, *J* = 13.0 Hz, 2F), -123.64 - -123.77 (m, 2F), -125.69 - -125.79 (m, 2F) ppm.

### (*E*)-1-(*tert*-Butyl)-4-(3,3,4,4,5,5,6,6,6-nonafluoro-1-iodohex-1-en-1-yl)benzene (1f)<sup>[1b]</sup>:

Following general procedure GPA.

Yield = 76% (3.83 g, 10 mmol scale). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>**H** NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 7.36–7.31 (m, 2H), 7.25–7.21 (m, 2H), 6.57 (t, *J* = 13.6 Hz, 1H), 1.32 (s, 9H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>):**  $\delta$  = -80.89 (t, *J* = 9.9 Hz, 3F), -105.14 (q, *J* = 12.4 Hz, 2F), -123.70 - -123.80 (m, 2F), -125.67 - -125.79 (m, 2F) ppm.

### (*E*)-1-Fluoro-4-(3,3,4,4,5,5,6,6,6-nonafluoro-1-iodohex-1-en-1-yl)benzene (1g)<sup>[1b]</sup>:

Following general procedure GPA.

Yield = 82% (3.83 g, 10 mmol scale). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.31–7.26 (m, 2H), 7.06–6.99 (m, 2H), 6.59 (t, *J* = 13.5 Hz, 1H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>):**  $\delta$  = -80.92 (t, *J* = 9.7 Hz, 3F), -105.37 (q, *J* = 12.3 Hz, 2F), -110.74 (dq, *J* = 12.0, 6.6 Hz, 1F), -123.73 (q, *J* = 9.8 Hz, 2F), -125.85 (tt, *J* = 11.2, 6.4 Hz, 2F) ppm.

#### (*E*)-1-Chloro-4-(3,3,4,4,5,5,6,6,6-nonafluoro-1-iodohex-1-en-1-yl)benzene (1h)<sup>[1b]</sup>:

Following general procedure GPA.

Yield = 80% (3.86 g, 10 mmol scale). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.35–7.30 (m, 2H), 7.26–7.20 (m, 2H), 6.60 (t, *J* = 13.5 Hz, 1H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>):**  $\delta$  = -80.89 (t, *J* = 9.9 Hz, 3F), -105.41 (q, *J* = 13.0 Hz, 2F), -123.69 (q, *J* = 9.7 Hz, 2F), -125.72 - -125.93 (m, 2F) ppm.

(*E*)-1-(3,3,4,4,5,5,6,6,6-Nonafluoro-1-iodohex-1-en-1-yl)-4-(trifluoromethyl)benzene (1j)<sup>[1b]</sup>: Following general procedure GPA.

Yield = 70% (903 mg, 2.5 mmol scale). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.63–7.60 (m, 2H), 7.40 (d, *J* = 8.1 Hz, 2H), 6.65 (t, *J* = 13.4 Hz, 1H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>):**  $\delta$  = -62.83 (s, 3F), -80.91 (t, *J* = 9.7 Hz, 3F), -105.54 (q, *J* = 12.7 Hz, 2F), -123.66 (q, *J* = 9.4 Hz, 2F), -125.74 (dt, *J* = 13.4, 6.1 Hz, 2F) ppm.

#### (*E*)-1-(3,3,4,4,5,5,6,6,6-Nonafluoro-1-iodohex-1-en-1-yl)naphthalene (1k)<sup>[1b]</sup>:

Following general procedure GPA.

Yield = 20% (298.9 mg, 3 mmol scale). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.94–7.83 (m, 3H), 7.63–7.59 (m, 1H), 7.55–7.49 (m, 1H), 7.45–7.36 (m, 2H), 6.86 (t, *J* = 13.2 Hz, 1H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>):**  $\delta$  = -80.89 (s, 3F), -107.42 (t, *J* = 15.7 Hz, 2F), -123.67 (s, 2F), -125.77 (s, 2F) ppm.

# $(E)-4,4-Dimethyl-6-(3,3,4,4,5,5,6,6,6-nonafluoro-1-iodohex-1-en-1-yl) thiochromane (1m)^{[1b]}:$

Following general procedure GPA.

Yield = 94% (1.65 g, 3.2 mmol scale). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>**H** NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 7.28 (s, 1H), 7.06–6.97 (m, 2H), 6.53 (t, *J* = 13.6 Hz, 1H), 3.06–3.01 (m, 2H), 1.99–1.92 (m, 2H), 1.31 (s, 6H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>):**  $\delta$  = -80.92 (s, 3F), -105.09 (d, *J* = 17.8 Hz, 2F), -123.58 (s, 2F), -125.74 (s, 2F) ppm.

# (*E*)-5-(3,3,4,4,5,5,6,6,6-Nonafluoro-1-iodohex-1-en-1-yl)benzo[*d*][1,3]dioxole (1n)<sup>[1b]</sup>:

Following general procedure GPA.

Yield = 39% (973 mg, 5 mmol scale). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 6.85–6.70 (m, 3H), 6.53 (t, *J* = 13.5 Hz, 1H), 6.00 (s, 2H) ppm. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>):  $\delta$  = -80.86 (s, 3F), -105.21 (d, *J* = 28.2 Hz, 2F), -123.70 (s, 2F), -125.73 (s, 2F) ppm.

#### (*E*)-1,1,1,2,2,3,3,4,4-Nonafluoro-6-iododec-5-ene (10)<sup>[1b]</sup>:

Following general procedure GPA.

Yield = 52% (2.23 g, 10 mmol scale). Colorless oil.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 6.32 (t, *J* = 14.8 Hz, 1H), 2.63 (t, *J* = 7.6 Hz, 2H), 1.59–1.53 (m, 2H), 1.36 (q, *J* = 7.6 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>):**  $\delta$  = -81.04 (dd, *J* = 30.8, 13.8 Hz, 3F), -105.60 (q, *J* = 12.6 Hz, 2F), -124.18 (dq, *J* = 16.8, 8.9 Hz, 2F), -125.66 - -125.94 (m, 2F) ppm.

#### (*E*)-(5,5,6,6,7,7,8,8,8-Nonafluoro-3-iodooct-3-en-1-yl)benzene (1p)<sup>[1b]</sup>:

Following general procedure GPA.

Yield = 38% (721.3 mg, 4 mmol scale). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.34–7.29 (m, 2H), 7.26–7.19 (m, 3H), 6.36 (t, *J* = 14.4 Hz, 1H), 2.99–2.86 (m, 4H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>):**  $\delta$  = -80.91 (t, *J* = 9.7 Hz, 3F), -105.94 (q, *J* = 13.2 Hz, 2F), -124.10 (q, *J* = 9.1 Hz, 2F), -125.70 (q, *J* = 9.9 Hz, 2F) ppm.

#### (*E*)-5,5,6,6,7,7,8,8,8-Nonafluoro-3-iodo-2-methyloct-3-en-2-ol (1q)<sup>[2]</sup>:

Following general procedure GPB.

Yield = 74% (6.36 g, 20 mmol scale). Colorless oil.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 6.91–6.80 (m, 1H), 1.52 (s, 6H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>):**  $\delta$  = -81.08 (t, *J* = 9.8 Hz, 3F), -108.64 (q, *J* = 13.0 Hz, 2F), -123.97 (q, *J* = 9.6 Hz, 2F), -125.82 (tt, *J* = 10.6, 5.3 Hz, 2F) ppm.

# (E)-2-(4-Fluorophenyl)-5-(2-methyl-5-(3,3,4,4,5,5,6,6,6-nonafluoro-1-iodohex-1-en-1-yl)benzy l)thiophene $(1w)^{[1b]}$ :

Following general procedure GPA.

Yield = 69% (905.7 mg, 2 mmol scale). Colorless oil.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 7.50–7.45 (m, 2H), 7.18–7.13 (m, 3H), 7.06–7.01 (m, 3H), 6.62 (dt, *J* = 3.5, 1.1 Hz, 1H), 6.60–6.52 (m, 1H), 4.11 (s, 2H), 2.31 (s, 3H) ppm.

<sup>19</sup>**F** NMR (376 MHz, CDCl<sub>3</sub>):  $\delta$  = -80.87 (t, *J* = 9.7 Hz, 3F), -105.12 (q, *J* = 12.9 Hz, 2F), -114.96 - -115.06 (m, 1F), -123.56 (q, *J* = 9.3 Hz, 2F), -125.71 (dt, *J* = 13.0, 5.1 Hz, 2F) ppm.

#### (*E*)-(3,3,4,4,5,5,6,6,6-Nonafluoro-1-iodo-2-methylhex-1-en-1-yl)benzene (1x)<sup>[3]</sup>:

Following general procedure GPC.

Yield = 59% (546.7 mg, 2 mmol scale). White solid.

Purified by flash column chromatography through silica gel (petroleum ether).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 7.31–7.23 (m, 3H), 7.17 (d, *J* = 8.3 Hz, 2H), 2.28 (s, 3H) ppm. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>):  $\delta$  = -80.86 (t, *J* = 10.0 Hz, 3F), -103.30 (t, *J* = 14.4 Hz, 2F), -120.38 (q, *J* = 10.1 Hz, 2F), -126.09 (dt, *J* = 17.3, 10.2 Hz, 2F) ppm.

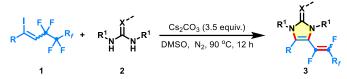
## General procedure for the synthesis of ureas 2

General procedure D (GPD)<sup>[4]</sup>

$$\mathbb{R}^{1}$$
-NH<sub>2</sub> + (Boc)<sub>2</sub>O  $\xrightarrow{\text{DABCO (0.1 equiv.)}}$   $\mathbb{R}^{1}$   $\mathbb{R}^{1}$ 

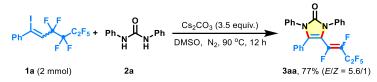
According to Sun's reported method, a flask (50 mL), equipped with a magnetic stir bar, was charged with amine (2 mmol, 2.0 equiv.), DABCO (11.2 mg, 0.1 mmol, 0.1 equiv.), (Boc)<sub>2</sub>O (218 mg, 1.0 mmol, 1.0 equiv.), and CH<sub>2</sub>Cl<sub>2</sub> (10 mL) under air. The reaction mixture was stirred at room temperature under air for 30 min to 6 h. After the completion of the reaction as detected by TLC, the reaction mixture was cooled to 0 °C, *n*-hexane was then added. The resulting solid was collected and further washed with cold water and diethyl ether to afford the corresponding product

# <u>General procedure for the defluorinative synthesis of C4-perfluoroalkenyl</u> <u>2-imidazolones 3</u>



A tube (10 mL), equipped with a magnetic stir bar, was charged with perfluoroalkyl alkenyl iodide (0.3 mmol, 1 equiv., **1**), urea derivative (0.45 mmol, 1.5 equiv., **2**),  $Cs_2CO_3$  (342.1 mg, 1.05 mmol, 3.5 equiv.), and DMSO (2 mL) under N<sub>2</sub> atmosphere. The reaction mixture was stirred at 90 °C (oil bath) under N<sub>2</sub> atmosphere for 12 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 (20/1~2/1) as eluent to afford the pure product **3**.

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



A tube (10 mL), equipped with a magnetic stir bar, was charged with (3,3,4,4,5,5,6,6,6-nonafluoro-1-iodohex-1-en-1-yl)benzene (896.9 mg, 2 mmol, 1 equiv., **1a**), *N*,*N*-diphenylurea (636.8 mg, 3 mmol, 1.5 equiv., **2a**), Cs<sub>2</sub>CO<sub>3</sub> (2280.0 mg, 7 mmol, 3.5 equiv.), and DMSO (10 mL) under N<sub>2</sub> atmosphere. The reaction mixture was stirred at 90 °C (oil bath) under N<sub>2</sub> atmosphere for 12 h. The reaction was then quenched by saturated NH<sub>4</sub>Cl solution (60 mL) and extracted with EtOAc (60 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) as eluent to afford the pure product **3aa** (756.8 mg, 77% yield).

#### **Mechanistic studies**

#### a) Radical trapping experiment

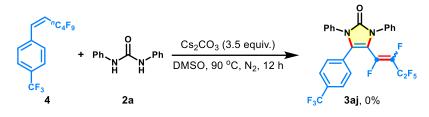


A tube (10 mL), equipped with a magnetic stir bar, was charged with (3,3,4,4,5,5,6,6,6-nonafluoro-1-iodohex-1-en-1-yl)benzene (134.4 mg, 0.3 mmol, 1 equiv., **1a**), *N*,*N*'-diphenylurea (95.5 mg, 0.45 mmol, 1.5 equiv., **2a**), TEMPO (93.7 mg, 0.6 mmol, 2 equiv.), Cs<sub>2</sub>CO<sub>3</sub> (342.1 mg, 1.05 mmol, 3.5 equiv.), and DMSO (2 mL) under N<sub>2</sub> atmosphere. The reaction mixture was stirred at 90 °C (oil bath) under N<sub>2</sub> atmosphere for 12 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) as eluent to afford the pure product **3aa** (102.7 mg, 70% yield).

A reaction pathway involving open shell intermediates is unlikely.

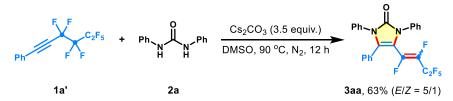
#### b) The reactivity of perfluoroalkylated alkene



A tube (10 mL), equipped with a magnetic stir bar, was charged with (*Z*)-1-(3,3,4,4,5,5,6,6,6-nonafluorohex-1-en-1-yl)-4-(trifluoromethyl)benzene (78.0 mg, 0.2 mmol, 1 equiv., **4**), *N*,*N*'-diphenylurea (63.7 mg, 0.3 mmol, 1.5 equiv., **2a**), Cs<sub>2</sub>CO<sub>3</sub> (228.1 mg, 0.7 mmol, 3.5 equiv.), and DMSO (2 mL) under N<sub>2</sub> atmosphere. The reaction mixture was stirred at 90 °C (oil bath) under N<sub>2</sub> atmosphere for 12 h. No desired product **3aj** was detected.

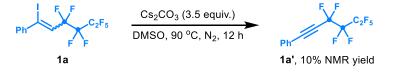
This result suggested that the initial reaction might start with an  $S_NV$ -type (nucleophilic vinylic substitution)  $C(sp^2)$ -I bond displacement.

c) The reaction of perfluorobutyl phenyl alkyne 1a' with urea 2a



А tube (10 mL), equipped with a magnetic stir bar, was charged with (perfluorohex-1-yn-1-yl)benzene (96.1 mg, 0.3 mmol, 1 equiv., 1a'), N,N'-diphenylurea (95.5 mg, 0.45 mmol, 1.5 equiv., 2a), Cs<sub>2</sub>CO<sub>3</sub> (342.1 mg, 1.05 mmol, 3.5 equiv.), and DMSO (2 mL) under N<sub>2</sub> atmosphere. The reaction mixture was stirred at 90 °C (oil bath) under N<sub>2</sub> atmosphere for 12 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  $(10/1 \sim 4/1)$  as eluent to afford the pure product 3aa (93.1 mg, 63% yield).

#### d) Dehydroiodination of perfluoroalkyl alkenyl iodide 1a

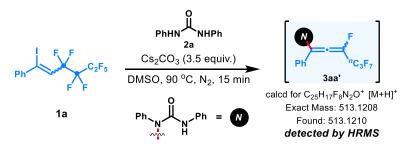


A tube (10 mL), equipped with a magnetic stir bar, was charged with (3,3,4,4,5,5,6,6,6-nonafluoro-1-iodohex-1-en-1-yl)benzene (134.4 mg, 0.3 mmol, 1 equiv., **1a**),

 $Cs_2CO_3$  (342.1 mg, 1.05 mmol, 3.5 equiv.), and DMSO (2 mL) under N<sub>2</sub> atmosphere. The reaction mixture was stirred at 90 °C (oil bath) under N<sub>2</sub> atmosphere for 12 h. The tube was then cooled to room temperature and the reaction mixture was quenched by saturated NH<sub>4</sub>Cl solution (20 mL) followed by extraction 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 residue was directly analyzed by NMR analysis. ~10% NMR yield of (perfluorohex-1-yn-1-yl)benzene (1a') was determined by <sup>19</sup>F NMR analysis of the residue using 1-fluoro-4-methoxybenzene (0.3 mmol) as an internal standard.

<u>Although the condensation of presynthesized 1a' with N,N'-diphenylurea 2a readily occurred,</u> the generation of (perfluorohex-1-yn-1-yl)benzene 1a' (~10% NMR yield) in a low yield in the absence of urea 2a under the standard conditions reflected that 1a' might not be a real reaction intermediate.

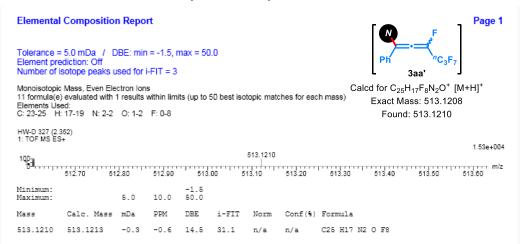
e) Detection of possible intermediate 3aa'



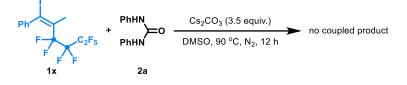
A tube (10 mL), equipped with a magnetic stir bar, was charged with (3,3,4,4,5,5,6,6,6-nonafluoro-1-iodohex-1-en-1-yl)benzene (134.4 mg, 0.3 mmol, 1 equiv., **1a**), *N*,*N*-diphenylurea (95.5 mg, 0.45 mmol, 1.5 equiv.), Cs<sub>2</sub>CO<sub>3</sub> (342.1 mg, 1.05 mmol, 3.5 equiv.), and DMSO (2 mL) under N<sub>2</sub> atmosphere. The reaction mixture was stirred at 90 °C (oil bath) under N<sub>2</sub> atmosphere for 15 min. Upon completion of the reaction, the tube was cooled to room temperature, and the mixture was passed through a short pad of Celite and rinsed with MeOH. A sample was taken from the filtrate and was directly analyzed by HRMS.

HRMS analysis of the reaction mixture suggested the involvement of possible intermediate <u>3aa'</u>.

The intermediate 3aa' was detected by HRMS analysis:

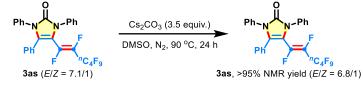


#### f) The use of perfluorobutyl alkenyl iodide 1x



A tube (10 mL) equipped with a magnetic stir bar was charged with (*E*)-(3,3,4,4,5,5,6,6,6-nonafluoro-1-iodo-2-methylhex-1-en-1-yl)benzene (138.6 mg, 0.3 mmol, 1 equiv., **1x**), *N*,*N*'-diphenylurea (95.5 mg, 0.45 mmol, 1.5 equiv., **2a**), Cs<sub>2</sub>CO<sub>3</sub> (342.1 mg, 1.05 mmol, 3.5 equiv.), and DMSO (2 mL) under N<sub>2</sub> atmosphere. The reaction mixture was stirred at 90 °C (oil bath) under N<sub>2</sub> atmosphere for 12 h. No defluorinative coupled product was observed. *This result indicates the involvement of a fluoroallene intermediate.* 

#### g) The effect of reaction conditions on the E/Z ratio of product 3as



A tube (10 mL) equipped with a magnetic stir bar was charged with 4-(perfluorohex-1-en-1-yl)-1,3,5-triphenyl-1,3-dihydro-2*H*-imidazol-2-one (59.2 mg, 0.1 mmol, 1 equiv., 3as), Cs<sub>2</sub>CO<sub>3</sub> (114.0 mg, 0.35 mmol, 3.5 equiv.), and DMSO (2 mL) under N<sub>2</sub> atmosphere. The reaction mixture was stirred at 90 °C (oil bath) under N<sub>2</sub> atmosphere for 24 h. The tube was then cooled to room temperature and the reaction mixture was quenched by saturated NH<sub>4</sub>Cl solution (20 mL) followed by extraction 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 residue was directly analyzed by NMR analysis. >95% NMR yield of 4-(perfluorohex-1-en-1-yl)-1,3,5-triphenyl-1,3-dihydro-2H-imidazol-2-one (**3as**), with a E/Z ratio of 6.8/1, was determined through <sup>19</sup>F NMR analysis of the residue, employing 1-fluoro-4-methoxybenzene (0.1 mmol) as the internal standard.

# **Optimization of reaction conditions**

Table S1. Optimization of reaction conditions<sup>a</sup>

	Ph	$F$ $F$ $C_2F_5$ + Ph	O N Ph − H H	Base (x equiv Sol., Temp., N <sub>2</sub> ,	Time Ph-	N <sup>Ph</sup> F <sup>†</sup> Ph		5
		1a	2a			F C <sub>2</sub> F <sub>5</sub> 3aa	1a'	
Enter	1/2	D ()	C - 1	T (0 <b>C</b> )	Time (b)	Yields	$(\%)^b$	
Entry	1a/2a	Base (x equiv)	Sol.	Temp. (°C)	Time (h)	<b>3aa</b> ( <i>E</i> / <i>Z</i> ) <sup><i>c</i></sup>	1a	<b>1a'</b>
1	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	NMP	90	12	14 (5.9/1)	2	21
2	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	DMSO	90	12	50 (5.7/1)	1	5
3	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	MeCN	80	12	29 (5.6/1)	3	9
4	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	DMF	90	24	40 (5.7/1)	3	21
5	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	DMSO	90	24	44 (5.3/1)	2	5
6	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	DMSO	50	12	27 (6.6/1)	2	31
7	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	DMSO	70	12	36 (6.2/1)	2	22
8	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	DMSO	110	12	51 (3.6/1)	0	1
9	1/2	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	DMSO	90	12	45 (5.4/1)	0	3
10	1/3	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	DMSO	90	12	39 (4.6/1)	2	3
11	1.5/1	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	DMSO	90	12	32 (5.4/1)	9	11
12	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (2)	DMSO	90	12	29 (5.4/1)	3	5
13	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (3)	DMSO	90	12	59 (5.5/1)	0	2
14	1/1.5	$Cs_2CO_3$ (3.5)	DMSO	90	12	74 (70%) <sup>d</sup> (5.6/1)	0	1
15	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (4)	DMSO	90	12	71 (5.5/1)	1	0
16	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (5)	DMSO	90	12	68 (5.5/1)	0	0
17	1/1.5	K <sub>2</sub> CO <sub>3</sub> (3.5)	DMSO	90	12	21 (5/1)	0	3
18	1/1.5	K <sub>3</sub> PO <sub>4</sub> (3.5)	DMSO	90	12	9 (5/1)	0	4
19	1/1.5	LiOH (3.5)	DMSO	90	12	44 (5.8/1)	0	5
20	1/1.5	<sup>t</sup> BuOLi (3.5)	DMSO	90	12	43 (5.6/1)	0	2
21	1/1.5	DABCO (3.5)	DMSO	90	12	trace	trace	trace
22	1/1.5	Et <sub>3</sub> N (3.5)	DMSO	90	12	trace	trace	trace
23	1/1.2	Cs <sub>2</sub> CO <sub>3</sub> (3.5)	DMSO	90	12	60 (5.7/1)	1	1
24	1/1	Cs <sub>2</sub> CO <sub>3</sub> (3.5)	DMSO	90	12	63 (5.6/1)	1	1
$25^{e}$	1/1.5	$Cs_2CO_3$ (3.5)	DMSO	90	12	56 (5.6/1)	1	1
26 <sup>f</sup>	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (3.5)	DMSO	90	12	71 (5/1)	1	1
27	1/1.5	Cs <sub>2</sub> CO <sub>3</sub> (3.5)	DMSO	90	6	68 (5.7/1)	1	2

<sup>*a*</sup> Reaction conditions: **1a** (0.3-0.45 mmol), **2a** (0.3-0.9 mmol), and base (0.6-1.5 mmol) in solvent (2 mL) at 50-110 °C under N<sub>2</sub> for 6-24 h. <sup>*b*</sup> Yields were determined by <sup>19</sup>F NMR analysis with 1-methoxy-4-(trifluoromethyl)benzene (0.3 mmol) as an internal standard. <sup>*c*</sup> The ratio of E/Z isomers was determined through <sup>19</sup>F NMR analysis of the crude products. <sup>*d*</sup> Isolated yield. <sup>*e*</sup> DMSO (1 mL) was used. <sup>*f*</sup> DMSO (3 mL) was used.

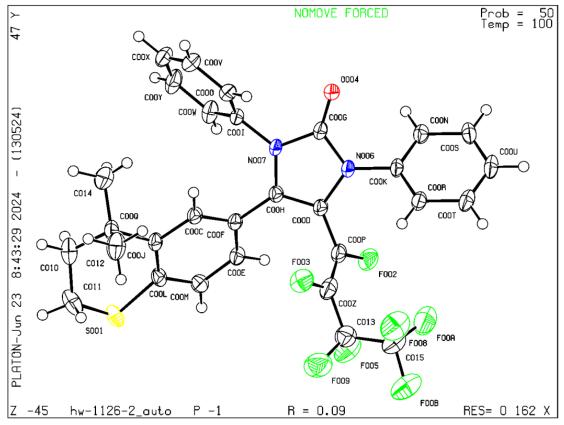
# The X-ray crystal structure of product (E)-3am

The single crystal was grown from the mixed solution of DCM/EtOAc/DMF (v/v/v = 10/3/1) by slowly evaporating the above solvents at room temperature.

# $(E) \hbox{-} 4 \hbox{-} (4, 4 \hbox{-} Dimethyl thiochroman \hbox{-} 6 \hbox{-} yl) \hbox{-} 5 \hbox{-} (perfluorobut \hbox{-} 1 \hbox{-} en \hbox{-} 1 \hbox{-} yl) \hbox{-} 1, 3 \hbox{-} diphenyl \hbox{-} 1, 3 \hbox{-} 1,$

*H*-imidazol-2-one [(*E*)-3am; displacement ellipsoids are drawn at the 50% probability levels]:





\_chemical\_name\_systematic P1 \_chemical\_formula\_moiety 'C30 H23 F7 N2 O S' chemical formula sum 'C30 H23 F7 N2 O S' \_chemical\_formula\_weight 592.56 \_space\_group\_crystal\_system 'triclinic' \_space\_group\_IT\_number 2 \_space\_group\_name\_H-M\_alt 'P -1' '-P 1' \_space\_group\_name\_Hall \_cell\_length\_a 6.9880(2)\_cell\_length\_b 12.2498(4)

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3	$\mathbf{w}$	-114.00 -	-29.00	1.00	1.00	 -41.73 -3	38.00 -6	0.00	85
4	$\mathbf{w}$	25.00	94.00	1.00	1.00	 41.73	-125.00	-90.00	69
5	$\mathbf{w}$	55.00	84.00	1.00	1.00	 41.73	-129.00	80.00	29
6	$\mathbf{w}$	25.00	100.00	1.00	1.75	 106.33	-94.00 1	20.00	75
7	$\mathbf{w}$	116.00	172.00	1.00	1.75	 106.33	30.00	-180.00	56
8	$\mathbf{w}$	107.00	172.00	1.00	1.75	 106.33	125.00-	180.00	65
9	$\mathbf{w}$	45.00	88.00	1.00	1.75	 106.33	-125.00	0.00	43
10	$\mathbf{w}$	111.00	151.00	1.00	1.75	 106.33	125.00	120.00	40
11	$\mathbf{w}$	85.00	178.00	1.00	1.75	 106.33	30.00	-120.00	93
12	$\mathbf{w}$	73.00	112.00	1.00	1.75	 106.33-	125.00	-30.00	39
13	$\mathbf{w}$	52.00	117.00	1.00	1.75	 106.33-	125.00	60.00	65
14	$\mathbf{w}$	26.00	64.00	1.00	1.75	 106.33	-94.00	150.00	38
15	$\mathbf{w}$	84.00	109.00	1.00	1.75	 106.33	-94.00 1	50.00	25
16	$\mathbf{w}$	36.00	131.00	1.00	1.75	 106.33	-61.00 1	50.00	95
17	$\mathbf{w}$	120.00	178.00	1.00	1.75	 106.33	30.00	120.00	58
18	$\mathbf{w}$	142.00	178.00	1.00	1.75	 106.33	45.00	-60.00	36
19	$\mathbf{w}$	84.00	130.00	1.00	1.75	 106.33	45.00	-60.00	46

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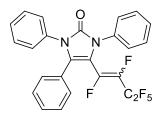
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### **Characterization data for products**

Note: All <sup>19</sup>F NMR analyses of the E/Z isomer ratio were based on two characteristic fluorine peaks within the range of -119 to -121 ppm.



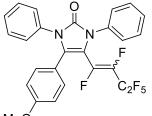
4-(Perfluorobut-1-en-1-yl)-1,3,5-triphenyl-1,3-dihydro-2*H*-imidazol-2-one (3aa):

Yield = 70% (103.5 mg, E/Z = 5.3/1). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.50 (d, *J* = 4.4 Hz, 4H), 7.42–7.38 (m, 1H), 7.35–7.23 (m, 8H), 7.21–7.16 (m, 2H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.36 (t, *J* = 3.4 Hz, 3F), -120.64 – -120.80 (m, 2F), -127.18 – -127.77 (m, 1F), -156.04 – -156.58 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.22 (d, *J* = 9.0 Hz, 3F), -99.96 (d, *J* = 22.6 Hz, 1F), -119.66 (d, *J* = 15.0 Hz, 2F), -140.72 – -140.93 (m, 1F) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 151.4, 145.0 (dd, *J*<sub>C-F</sub> = 257.0, 42.5 Hz), 143.9–137.9 (m, 1C), 129.34, 129.28, 128.9, 128.73, 128.71, 128.6, 128.2, 127.8, 127.3, 126.7, 126.6, 126.3, 125.8, 107.5 (dd, *J*<sub>C-F</sub> = 27.3, 5.1 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

**HRMS** (m/z): calcd for C<sub>25</sub>H<sub>16</sub>F<sub>7</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 493.1145, found: 493.1148.





4-(4-Methoxyphenyl)-5-(perfluorobut-1-en-1-yl)-1,3-diphenyl-1,3-dihydro-2*H*-imidazol-2-one (3ab):

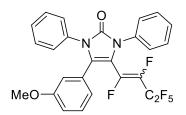
Yield = 55% (86.8 mg, E/Z = 6.9/1). Yellow solid.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.50–7.46 (m, 4H), 7.42–7.36 (m, 1H), 7.34 (dt, *J* = 6.5, 1.4 Hz, 2H), 7.32–7.28 (m, 1H), 7.26–7.22 (m, 2H), 7.12–7.06 (m, 2H), 6.83–6.79 (m, 2H), 3.76 (s, 3H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.35 (t, *J* = 4.4 Hz, 3F), -120.58 (dd, *J* = 24.8, 14.1 Hz, 2F), -126.97 - -127.56 (m, 1F), -156.27 - -156.80 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.88 (s, 3F), -95.53 (d, *J* = 22.3 Hz, 1F), -119.54 (dd, *J* = 31.3, 17.4 Hz, 2F), -141.06 - -141.23(m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 160.3, 151.5, 145.2 (dd,  $J_{C-F}$  = 258.6, 42.4 Hz), 145.8–137.8 (m, 1C), 134.3, 134.2, 130.2, 129.3, 129.0, 128.1, 127.8, 127.4, 126.3, 125.8, 118.8, 114.1, 107.0 (dd,  $J_{C-F}$  = 22.3, 5.1 Hz), 55.1 ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot

be identified due to C-F coupling. **HRMS (m/z):** calcd for  $C_{26}H_{18}F_7N_2O_2$  [M+H]<sup>+</sup> 523.1251, found: 523.1255.



# 4-(3-Methoxyphenyl)-5-(perfluorobut-1-en-1-yl)-1,3-diphenyl-1,3-dihydro-2*H*-imidazol-2-one (3ac):

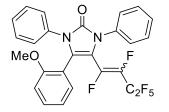
Yield = 56% (87.7 mg, E/Z = 4.7/1). Yellow solid.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.50–7.45 (m, 5H), 7.28–7.25 (m, 2H), 7.23–7.18 (m, 5H), 6.93 (t, *J* = 7.5 Hz, 1H), 6.75 (d, *J* = 8.4 Hz, 1H), 3.42 (s, 3H) ppm.

<sup>19</sup>**F** NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.40 (t, *J* = 4.2 Hz, 3F), -120.60 - -120.77 (m, 2F), -126.73 - -127.36 (m, 1F), -155.76 - -156.27 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.19 - -83.26 (m, 3F), -95.89 (d, *J* = 20.6 Hz, 1F), -119.55 - -119.63 (m, 2F), -140.64 - -140.85 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 159.5, 151.4, 145.0 (dd,  $J_{C-F}$  = 258.6, 42.4 Hz), 140.1–138.1 (m, 1C), 134.2, 134.1, 129.6, 129.3, 129.0, 128.4, 128.2, 127.9, 127.3, 126.3, 125.9, 121.1, 115.6, 113.8, 107.5 (dd,  $J_{C-F}$  = 22.2, 4.1 Hz), 55.0 ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>26</sub>H<sub>18</sub>F<sub>7</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> 523.1251, found: 523.1249.



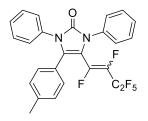
4-(2-Methoxyphenyl)-5-(perfluorobut-1-en-1-yl)-1,3-diphenyl-1,3-dihydro-2*H*-imidazol-2-one (3ad):

Yield = 34% (53.3 mg, E/Z = 4.8/1). Yellow solid.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.50–7.45 (m, 5H), 7.28–7.25 (m, 2H), 7.20 (dddd, *J* = 10.4, 6.1, 2.1, 1.1 Hz, 5H), 6.93 (td, *J* = 7.5, 1.0 Hz, 1H), 6.75 (dd, *J* = 8.4, 1.0 Hz, 1H), 3.42 (s, 3H) ppm.

<sup>19</sup>**F NMR** (**376 MHz**, **CDCl**<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.40 (t, *J* = 4.2 Hz, 3F), -120.60 – -120.77 (m, 2F), -126.73 – -127.36 (m, 1F), -155.76 – -156.27 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.19 – -83.26 (m, 3F), -95.89 (d, 1F), -119.55 – -119.63 (m, 2F), -140.64 – -140.85 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 156.9, 151.4, 145.3 (dd,  $J_{C-F}$  = 256.5, 42.4 Hz), 141.4–137.3 (m, 1C), 134.8, 134.6, 131.6, 131.0, 129.3, 128.5, 128.2, 127.9, 127.5, 126.4, 125.7, 120.7, 115.8, 111.1, 107.8 (dd,  $J_{C-F}$  = 26.3, 5.1Hz), 54.9 ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.



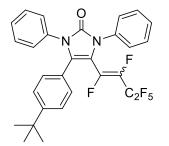
4-(Perfluorobut-1-en-1-yl)-1,3-diphenyl-5-(p-tolyl)-1,3-dihydro-2H-imidazol-2-one (3ae): Yield = 66% (100.7 mg, E/Z = 5.6/1). Yellow solid.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>) of** *E***-isomer:**  $\delta$  = 7.49–7.45 (m, 4H), 7.38 (ddd, *J* = 6.4, 5.4, 2.5 Hz, 1H), 7.34–7.30 (m, 2H), 7.30–7.27 (m, 1H), 7.24–7.20 (m, 2H), 7.06 (q, *J* = 8.2 Hz, 4H), 2.30 (s, 3H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.36 (t, *J* = 4.2 Hz, 3F), -120.58 – -120.73 (m, 2F), -126.93 – -127.51 (m, 1F), -156.17 – -156.67 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.22 (d, *J* = 8.8 Hz, 3F), -95.67 (d, *J* = 20.8 Hz, 1F), -119.47 – -119.66 (m, 2F), -141.07 (ddt, *J* = 30.0, 17.4, 8.7 Hz, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 151.5, 144.7 (dd,  $J_{C-F}$  = 256.5, 42.4 Hz), 139.6, 138.9–137.9 (m, 1C), 134.3, 134.2, 129.4, 129.3, 129.0, 128.6, 128.3, 128.1, 127.8, 127.4, 125.9, 123.7 (d,  $J_{C-F}$  = 2.2Hz), 107.2 (dd,  $J_{C-F}$  = 26.3, 5.1Hz), 21.2 ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>26</sub>H<sub>18</sub>F<sub>7</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 507.1302, found: 507.1302.



4-(4-(*tert*-Butyl)phenyl)-5-(perfluorobut-1-en-1-yl)-1,3-diphenyl-1,3-dihydro-2*H*-imidazol-2-one (3af):

Yield = 62% (101.6 mg, E/Z = 6.1/1). Yellow solid.

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

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.49–7.46 (m, 5H), 7.34–7.28 (m, 5H), 7.24 (dt, *J* = 7.0, 1.5 Hz, 2H), 7.10–7.05 (m, 2H), 1.27 (s, 9H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.36 (t, *J* = 4.3 Hz, 3F), -120.57 – -120.76 (m, 2F), -126.71 – -127.32 (m, 1F), -156.26 (ddtd, *J* = 149.1, 13.4, 8.8, 4.3 Hz, 1F) ppm; *Z*-isomer:  $\delta$  = -83.24 (d, *J* = 8.9 Hz, 3F), -95.82 (d, *J* = 22.2 Hz, 1F), -119.69 (dd, *J* = 76.7, 17.7 Hz, 2F), -141.18 (ddt, *J* = 29.8, 17.7, 8.9 Hz, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 152.7, 151.5, 145.2 (dd,  $J_{C-F}$  = 256.5, 42.4 Hz), 141.1–138.6 (m, 1C), 134.3, 134.2, 129.3, 128.9, 128.4, 128.1, 127.8, 127.4, 126.3, 125.9, 125.6, 123.7 (d,  $J_{C-F}$  = 3.4 Hz), 107.3 ((dd,  $J_{C-F}$  = 28.3, 5.1 Hz), 34.7, 31.0 ppm, carbons corresponding to

the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling. **HRMS (m/z):** calcd for C<sub>29</sub>H<sub>24</sub>F<sub>7</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 549.1771, found: 549.1770.



4-(4-Fluorophenyl)-5-(perfluorobut-1-en-1-yl)-1,3-diphenyl-1,3-dihydro-2*H*-imidazol-2-one (3ag):

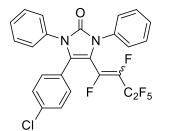
Yield = 35% (53.0 mg, E/Z = 4.3/1). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta = 7.53-7.41$  (m, 5H), 7.37–7.31 (m, 3H), 7.23–7.20 (m, 2H), 7.15 (ddt, J = 8.0, 5.1, 2.5 Hz, 2H), 7.04–6.96 (m, 2H) ppm.

<sup>19</sup>**F** NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.37 (q, *J* = 4.4 Hz, 3F), -110.05 – -110.14 (m, 1F), -120.62 – -120.76 (m, 2F), -127.33 – -127.93 (m, 1F), -155.90 – -156.47 (m, 1F) ppm; *Z*-isomer:  $\delta$  = -83.23 (d, *J* = 8.8 Hz, 3F), -96.20 (d, *J* = 20.8 Hz, 1F), -110.17 (t, *J* = 5.2 Hz, 1F), -119.60 (d, *J* = 17.5 Hz, 2F), -140.26 – -140.53 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta = 163.1$  (d,  $J_{C-F} = 251.5$  Hz), 151.4, 145.7 (dd,  $J_{C-F} = 256.5$ , 42.4 Hz), 141.1–138.6 (m, 1C), 134.2, 133.9, 130.9 (d,  $J_{C-F} = 8.2$  Hz), 129.4, 129.1, 128.3, 128.1, 127.4, 126.3, 125.9, 122.9, 116.1 (d,  $J_{C-F} = 22.2$  Hz), 107.9 (dd,  $J_{C-F} = 22.2$ , 7.2 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for  $C_{25}H_{15}F_8N_2O$  [M+H]<sup>+</sup> 511.1051, found: 511.1050.



4-(4-Chlorophenyl)-5-(perfluorobut-1-en-1-yl)-1,3-diphenyl-1,3-dihydro-2*H*-imidazol-2-one (3ah):

Yield = 52% (82.7 mg, E/Z = 4.6/1). Yellow solid.

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

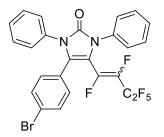
<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>) of** *E***-isomer:**  $\delta$  = 7.51–7.42 (m, 5H), 7.37–7.34 (m, 2H), 7.30–7.26 (m, 3H), 7.24–7.20 (m, 2H), 7.12–7.08 (m, 2H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.33 (d, *J* = 3.7 Hz, 3F), -120.62 – -120.76 (m, 2F), -127.20 – -127.79 (m, 1F), -155.51 – -156.29 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.22 (d, *J* = 9.0 Hz, 3F), -96.20 (d, *J* = 19.4 Hz, 1F), -119.59 (dd, *J* = 17.9, 7.7 Hz, 2F), -140.04 – -140.26 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta = 151.4$ , 144.5 (dd,  $J_{C-F} = 257.6$ , 44.5 Hz),

141.0–137.7 (m, 1C), 135.7, 134.1, 133.8, 130.0, 129.4, 129.2, 129.1, 128.4, 128.1, 127.3, 126.3, 125.9, 125.2 (d,  $J_{C-F} = 3.4$  Hz), 108.0 (dd,  $J_{C-F} = 27.6$ , 5.1 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>25</sub>H<sub>15</sub>ClF<sub>7</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 527.0756, found: 527.0756.



4-(4-Bromophenyl)-5-(perfluorobut-1-en-1-yl)-1,3-diphenyl-1,3-dihydro-2*H*-imidazol-2-one (3ai):

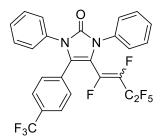
Yield = 40% (68.4 mg, E/Z = 4.6/1). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.51–7.41 (m, 8H), 7.38–7.34 (m, 2H), 7.23–7.19 (m, 2H), 7.05–7.01 (m, 2H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.31 (t, *J* = 3.9 Hz, 3F), -120.62 – -120.77 (m, 2F), -127.19 – -127.78 (m, 1F), -155.58 – -156.08 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.18 – -83.24 (m, 3F), -96.21 (d, *J* = 19.7 Hz, 1F), -119.60 (dd, *J* = 17.3, 10.1 Hz, 2F), -139.94 – -140.16 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 151.4, 144.9 (dd,  $J_{C-F}$  = 256.5, 45.5 Hz), 141.4–137.8 (m, 1C), 134.0, 133.8, 132.0, 130.2, 129.4, 129.2, 128.4, 128.2, 127.3, 126.3, 125.9, 125.7, 123.9, 107.7 (dd,  $J_{C-F}$  = 28.2, 5.1 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>25</sub>H<sub>15</sub>BrF<sub>7</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 571.0250, found: 571.0255.



4-(Perfluorobut-1-en-1-yl)-1,3-diphenyl-5-(4-(trifluoromethyl)phenyl)-1,3-dihydro-2*H*-imidazol-2-one (3aj):

Yield = 44% (73.8 mg, E/Z = 4.6/1). Yellow solid.

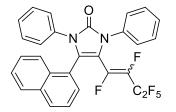
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.56 (d, *J* = 8.3 Hz, 2H), 7.53–7.42 (m, 5H), 7.40–7.27 (m, 5H), 7.25–7.20 (m, 2H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>) of** *E*-isomer:  $\delta$  = -62.91 (s, 3F), -84.37 (t, *J* = 4.4 Hz, 3F), -120.72 - -120.87 (m, 2F), -127.24 - -127.86 (m, 1F), -155.29 - -155.84 (m, 1F) ppm; *Z*-isomer:  $\delta$  = -62.88, (s, 3F), -83.31 (d, *J* = 8.9 Hz, 3F), -96.57 (d, *J* = 19.3 Hz, 1F), -119.71 (s, 2F), -139.65 (ddt,

#### *J* = 26.8, 17.9, 8.9 Hz, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 151.4, 144.5 (dd,  $J_{C-F}$  = 266.7, 41.5 Hz), 141.2–138.1 (m, 1C), 131.3 (q,  $J_{C-F}$  = 33.3 Hz), 130.5, 129.6, 129.5, 129.3, 129.1, 128.5, 128.3, 127.3, 126.4, 126.0, 125.7 (q,  $J_{C-F}$  = 4.5 Hz), 124.9, 122.2, 108.6 (dd,  $J_{C-F}$  = 26.7, 3.3 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for  $C_{26}H_{15}F_{10}N_2O$  [M+H]<sup>+</sup> 561.1019, found: 561.1017.



4-(Naphthalen-1-yl)-5-(perfluorobut-1-en-1-yl)-1,3-diphenyl-1,3-dihydro-2*H*-imidazol-2-one (3ak):

Yield = 43% (70.3 mg, E/Z = 10.6/1). Yellow oil.

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

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>) of** *E***-isomer:**  $\delta$  = 7.90–7.85 (m, 1H), 7.81 (dt, *J* = 7.3, 3.0 Hz, 2H), 7.59–7.39 (m, 9H), 7.20–7.07 (m, 5H) ppm.

<sup>19</sup>**F** NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.78 (t, *J* = 2.9 Hz, 3F), -120.82 (dd, *J* = 25.0, 13.1 Hz, 2F), -130.33 - -131.00 (m, 1F), -156.46 - -157.20 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.18 (d, *J* = 9.0 Hz, 3F), -96.44 (d, *J* = 19.9 Hz, 1F), -118.89 - -119.07 (m, 2F), -141.79 - -142.02 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 151.6, 144.8 (dd,  $J_{C-F}$  = 266.7, 41.5 Hz), 140.6–137.3 (m, 1C), 134.5, 134.1, 133.3, 131.4, 130.6, 129.5, 129.4, 129.3, 128.7, 128.4, 128.2, 127.8, 127.0, 126.6, 126.4, 125.7, 124.9, 124.4, 124.2, 109.2 (dd,  $J_{C-F}$  = 26.7, 5.1 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for  $C_{29}H_{18}F_7N_2O$  [M+H]<sup>+</sup> 543.1302, found: 543.1306.



4-(Perfluorobut-1-en-1-yl)-1,3-diphenyl-5-(thiophen-2-yl)-1,3-dihydro-2*H*-imidazol-2-one (3al):

Yield = 67% (100.3 mg, E/Z = 11.8/1). Yellow solid.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta = 7.53-7.38$  (m, 8H), 7.37–7.30 (m, 3H), 6.98–6.89 (m, 2H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>) of** *E*-isomer:  $\delta$  = -84.29 (t, *J* = 4.7 Hz, 3F), -120.62 - -120.77 (m, 2F), -126.84 - -127.58 (m, 1F), -155.03 (dddt, *J* = 150.1, 13.9, 8.9, 4.3 Hz, 1F) ppm; *Z*-isomer:  $\delta$  = -83.25 (d, *J* = 8.5 Hz, 3F), -96.67 (d, *J* = 20.6 Hz, 1F), -119.62 (dd, *J* = 17.5, 8.5 Hz, 2F),

-139.93 (ddd, *J* = 29.6, 16.9, 8.6 Hz, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 151.3, 144.6 (dd,  $J_{C-F}$  = 246.4, 43.4 Hz), 141.8–138.6 (m, 1C), 134.0, 133.9, 129.4, 129.2, 128.62, 128.58, 128.4, 127.9, 127.2, 126.70, 126.67, 125.9, 123.6, 108.2 (dd,  $J_{C-F}$  = 26.7, 4.2 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

**HRMS** (m/z): calcd for C<sub>23</sub>H<sub>14</sub>F<sub>7</sub>N<sub>2</sub>OS [M+H]<sup>+</sup> 499.0710, found: 499.0712.



4-(4,4-Dimethylthiochroman-6-yl)-5-(perfluorobut-1-en-1-yl)-1,3-diphenyl-1,3-dihydro-2*H*-imidazol-2-one (3am):

Yield = 60% (107.1 mg, E/Z = 4.8/1). Yellow solid.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.52–7.44 (m, 5H), 7.43–7.35 (m, 4H), 7.32 (dd, *J* = 7.1, 1.8 Hz, 1H), 7.04–7.00 (m, 2H), 6.88 (dd, *J* = 8.2, 1.9 Hz, 1H), 3.03–2.97 (m, 2H), 1.92–1.86 (m, 2H), 1.06 (s, 6H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.28 - -84.39 (m, 3F), -120.39 - -120.55 (m, 2F), -125.70 - -126.31 (m, 1F), -155.81 (dddd, *J* = 149.8, 17.9, 9.2, 4.3 Hz, 1F) ppm; *Z*-isomer:  $\delta$  = -83.23 (dd, *J* = 8.5, 2.3 Hz, 3F), -95.48 (dd, *J* = 21.6, 4.0 Hz, 1F), -119.53 - -119.70 (m, 2F), -140.96 (dt, *J* = 23.5, 9.0 Hz, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 151.4, 145.5 (dd,  $J_{C-F}$  = 257.6, 43.4 Hz), 142.1, 141.1–138.5 (m, 1C), 134.3, 134.2, 134.1, 129.4, 129.3, 129.1, 128.1, 127.9, 127.5, 127.2, 126.7, 126.3, 125.9, 125.7, 121.9, 106.8 (dd,  $J_{C-F}$  = 27.8, 4.3 Hz), 36.9, 32.7, 29.7, 23.0 ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

**HRMS** (m/z): calcd for C<sub>30</sub>H<sub>24</sub>F<sub>7</sub>N<sub>2</sub>OS [M+H]<sup>+</sup> 593.1492, found: 593.1496.



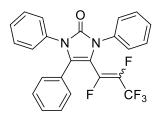
# 4-(Benzo[*d*][1,3]dioxol-5-yl)-5-(perfluorobut-1-en-1-yl)-1,3-diphenyl-1,3-dihydro-2*H*-imidazol-2-one (3an):

Yield = 46% (74.2 mg, E/Z = 8.4/1). Yellow solid.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.51–7.43 (m, 4H), 7.40–7.30 (m, 4H), 7.25–7.22 (m, 2H), 6.75–6.70 (m, 2H), 6.56 (d, *J* = 1.6 Hz, 1H), 5.96 (s, 2H) ppm. <sup>19</sup>**F NMR** (**376 MHz, CDCl**<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.37 (t, *J* = 4.4 Hz, 3F), -120.55 – -120.71 (m, 2F), -127.00 – -127.60 (m, 1F), -155.97 – -156.58 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.14 (d, *J* = 8.7 Hz, 3F), -95.63 (d, *J* = 20.8 Hz, 1F), -119.50 (dd, *J* = 50.6, 17.3 Hz, 2F), -140.66 – -140.93 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 151.4, 148.6, 147.9, 145.0 (dd,  $J_{C-F}$  = 263.6, 43.4 Hz), 140.9–137.7 (m, 1C), 134.2, 134.1, 129.4, 129.1, 128.2, 128.0, 127.3, 126.3, 125.9, 123.3, 120.2, 109.0, 108.6, 107.3 (dd,  $J_{C-F}$  = 26.6, 5.1 Hz), 101.5 ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

**HRMS** (m/z): calcd for C<sub>26</sub>H<sub>16</sub>F<sub>7</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 537.1044, found: 537.1045.



#### 4-(Perfluoroprop-1-en-1-yl)-1,3,5-triphenyl-1,3-dihydro-2*H*-imidazol-2-one (3ar):

Yield = 61% (80.5 mg, E/Z = 2.5/1). Yellow oil.

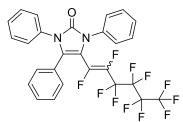
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>) of** *E***-isomer:**  $\delta$  = 7.52–7.47 (m, 4H), 7.44–7.39 (m, 1H), 7.35–7.29 (m, 6H), 7.26–7.22 (m, 2H), 7.19–7.15 (m, 2H) ppm.

<sup>19</sup>**F** NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -68.00 (dd, *J* = 20.8, 11.9 Hz, 3F), -128.54 – -129.14 (m, 1F), -158.22 – -158.74 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -68.67 (dd, *J* = 12.0, 7.4 Hz, 3F), -103.39 – -103.59 (m, 1F), -142.64 (dq, *J* = 20.3, 13.1 Hz, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 151.5, 144.4–141.4 (m, 1C), 140.3–137.9 (m, 1C), 134.3, 134.1, 129.5, 129.43, 129.36, 129.0, 128.8, 128.6, 128.2, 127.9, 127.3, 126.4, 125.9, 107.3 (dd,  $J_{C-F}$  = 26.6, 5.1 Hz) ppm, carbons corresponding to the CF<sub>3</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>24</sub>H<sub>16</sub>F<sub>5</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 443.1177, found: 443.1180.



### 4-(Perfluorohex-1-en-1-yl)-1,3,5-triphenyl-1,3-dihydro-2*H*-imidazol-2-one (3as):

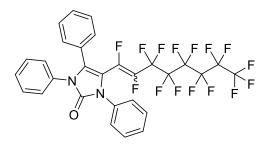
Yield = 60% (106.9 mg, E/Z = 7.5/1). Yellow solid.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.50–7.45 (m, 4H), 7.35–7.21 (m, 9H), 7.18–7.15 (m, 2H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>) of** *E***-isomer:**  $\delta$  = -80.95 (t, *J* = 9.9 Hz, 3F), -117.42 (dq, *J* = 25.3, 13.0 Hz, 2F), -124.31 - -124.60 (m, *J* = 8.9 Hz, 2F), -126.43 (t, *J* = 11.7 Hz, 2F), -126.50 - -127.07 (m, 1F), -154.77 - -155.49 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta = 151.5$ , 144.8 (dd,  $J_{C-F} = 263.6$ , 43.4 Hz), 140.7–137.8 (m, 1C), 134.3, 134.1, 129.4, 129.3, 129.0, 128.8, 128.6, 128.4, 128.2, 127.9, 127.4, 126.7, 126.3, 107.6 (dd,  $J_{C-F} = 27.6$ , 5.1 Hz) ppm, carbons corresponding to the C<sub>4</sub>F<sub>9</sub> group cannot be identified due to C-F coupling.

**HRMS** (m/z): calcd for C<sub>27</sub>H<sub>16</sub>F<sub>11</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 593.1081, found: 593.1089.



#### 4-(Perfluorooct-1-en-1-yl)-1,3,5-triphenyl-1,3-dihydro-2*H*-imidazol-2-one (3at):

Yield = 58% (120.8 mg, E/Z = 7.3/1). Yellow solid.

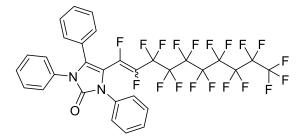
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1).

<sup>1</sup>**H** NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.47 (d, *J* = 3.8 Hz, 4H), 7.33–7.21 (m, 9H), 7.18–7.15 (m, 2H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>) of** *E*-isomer:  $\delta$  = -80.75 (t, *J* = 9.8 Hz, 3F), -117.26 (dq, *J* = 25.7, 13.1 Hz, 2F), -122.32 (s, 2F), -122.83 (s, 2F), -123.64 (s, 2F), -126.06 - -126.24 (m, 2F), -126.68 (dtt, *J* = 149.3, 25.0, 6.3 Hz, 1F), -154.72 - -155.31 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 151.5, 145.2 (dd,  $J_{C-F}$  = 258.3, 42.6 Hz), 141.2–138.2 (m, 1C), 134.3, 134.1, 129.4, 129.3, 129.0, 128.9, 128.6, 128.2, 127.9, 127.4, 126.8, 126.3, 126.0, 107.6 (dd,  $J_{C-F}$  = 27.3, 5.1 Hz) ppm, carbons corresponding to the C<sub>6</sub>F<sub>13</sub> group cannot be identified due to C-F coupling.

**HRMS** (m/z): calcd for C<sub>29</sub>H<sub>16</sub>F<sub>15</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 693.1018, found: 693.1018.



4-(Perfluorodec-1-en-1-yl)-1,3,5-triphenyl-1,3-dihydro-2*H*-imidazol-2-one (3au):

Yield = 38% (91.1 mg, E/Z = 6.8/1). Yellow solid.

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

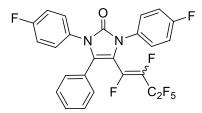
<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>) of** *E***-isomer:**  $\delta$  = 7.49–7.46 (m, 4H), 7.34–7.20 (m, 9H), 7.18–7.15 (m, 2H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -80.69 (t, *J* = 9.7 Hz, 3F), -117.24 (dq, *J* = 25.2, 12.0 Hz, 2F), -121.56 - -122.24 (m, 6F), -122.67 (dq, *J* = 19.3, 8.9 Hz, 2F), -123.45 - -123.72 (m, 2F), -126.06 (q, *J* = 8.1 Hz, 2F), -126.36 - -126.98 (m, 1F), -154.97 (dt, *J* = 150.4, 14.6 Hz, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta = 151.5$ , 145.1 (dd,  $J_{C-F} = 258.3$ , 42.6 Hz),

141.2–138.1 (m, 1C), 134.3, 134.1, 129.4, 129.3, 129.0, 128.9, 128.6, 128.3, 127.9, 127.4, 126.8, 126.3, 126.0, 107.6 (dd,  $J_{C-F} = 26.5$ , 5.2 Hz) ppm, carbons corresponding to the C<sub>8</sub>F<sub>17</sub> group cannot be identified due to C-F coupling.

**HRMS** (m/z): calcd for  $C_{31}H_{16}F_{19}N_2O$  [M+H]<sup>+</sup> 793.0954, found: 793.0954.



1,3-Bis(4-fluorophenyl)-4-(perfluorobut-1-en-1-yl)-5-phenyl-1,3-dihydro-2*H*-imidazol-2-one (3ba):

Yield = 67% (105.9 mg, E/Z = 5.9/1). Yellow oil.

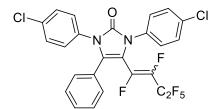
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>) of** *E***-isomer:**  $\delta$  = 7.46–7.41 (m, 2H), 7.36–7.29 (m, 3H), 7.23–7.13 (m, 6H), 7.06–7.00 (m, 2H) ppm.

<sup>19</sup>**F NMR** (**376 MHz**, **CDCl**<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.41 (t, *J* = 3.8 Hz, 3F), -112.31 (dt, *J* = 8.9, 4.4 Hz, 1F), -112.62 (d, *J* = 8.9 Hz, 1F), -120.75 (dd, *J* = 25.0, 12.3 Hz, 2F), -127.64 - -128.24 (m, 1F), -155.56 - -156.22 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.28 (d, *J* = 8.9 Hz, 3F), -96.57 (d, *J* = 19.4 Hz, 1F), -112.02 (dd, *J* = 10.7, 6.7 Hz, 1F), -112.65 - -112.74 (m, 1F), -119.58 (d, *J* = 17.1 Hz, 2F), -140.17 (ddt, *J* = 26.7, 17.8, 9.0 Hz, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta = 163.2$  (d,  $J_{C-F} = 36.4$  Hz), 160.7 (d,  $J_{C-F} = 36.4$  Hz), 151.5, 144.5 (dd,  $J_{C-F} = 257.5$ , 42.7 Hz), 141.2–137.9 (m, 1C), 130.0 (d,  $J_{C-F} = 3.0$  Hz), 129.6, 129.1 (d,  $J_{C-F} = 9.2$  Hz), 128.82, 128.78, 128.44, 128.35, 128.0 (d,  $J_{C-F} = 8.1$  Hz), 126.4, 116.5 (d,  $J_{C-F} = 23.2$  Hz), 116.2 (d,  $J_{C-F} = 23.2$  Hz), 107.6 (dd,  $J_{C-F} = 27.3$ , 5.1 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

**HRMS** (m/z): calcd for C<sub>25</sub>H<sub>14</sub>F<sub>9</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 529.0957, found: 529.0959.



1,3-Bis(4-chlorophenyl)-4-(perfluorobut-1-en-1-yl)-5-phenyl-1,3-dihydro-2*H*-imidazol-2-one (3ca):

Yield = 66% (111.2 mg, E/Z = 5/1). Yellow solid.

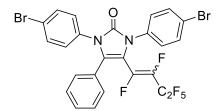
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.48 (dq, *J* = 9.4, 2.7 Hz, 2H), 7.43–7.38 (m, 2H), 7.38–7.28 (m, 5H), 7.18–7.13 (m, 4H) ppm.

<sup>19</sup>**F** NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.32 (d, *J* = 5.5 Hz, 3F), -120.60 – -120.79 (m, 2F), -127.66 – -128.28 (m, 1F), -155.35 – -155.90 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.26 (d, *J* = 9.0 Hz, 3F), -96.34 (d, *J* = 19.3 Hz, 1F), -119.63 (dd, *J* = 18.0, 7.6 Hz, 2F), -139.76 (dq, *J* = 17.9, 8.9

Hz, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 151.1, 144.6 (dd,  $J_{C-F}$  = 257.5, 42.7 Hz), 140.1–138.4 (m, 1C), 134.2, 133.8, 132.6, 132.4, 129.8, 129.6, 129.3, 128.9, 128.8, 128.4, 127.5, 127.1, 126.2, 107.5 (dd,  $J_{C-F}$  = 27.2, 4.1 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

**HRMS** (m/z): calcd for C<sub>25</sub>H<sub>14</sub>Cl<sub>2</sub>F<sub>7</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 561.0366, found: 561.0369.



1,3-Bis(4-bromophenyl)-4-(perfluorobut-1-en-1-yl)-5-phenyl-1,3-dihydro-2*H*-imidazol-2-one (3da):

Yield = 73% (141.5 mg, E/Z = 5.1/1). Yellow oil.

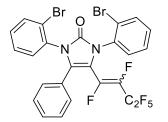
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>) of** *E***-isomer:**  $\delta$  = 7.66–7.60 (m, 2H), 7.47 (dd, *J* = 9.0, 2.6 Hz, 2H), 7.38–7.30 (m, 5H), 7.17–7.07 (m, 4H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.24 - -84.34 (m, 3F), -120.68 (dd, *J* = 26.0, 12.7 Hz, 2F), -127.99 (dtd, *J* = 149.1, 24.7, 5.7 Hz, 1F), -155.15 - -155.88 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.24 (d, *J* = 8.8 Hz, 3F), -96.32 (d, *J* = 19.4 Hz, 1F), -119.63 (dd, *J* = 17.4, 9.7 Hz, 2F), -139.56 - -139.77(m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 151.0, 144.6 (dd,  $J_{C-F}$  = 258.1, 43.2 Hz), 141.2–137.9 (m, 1C), 133.1, 132.9, 132.8, 132.6, 132.2, 129.8, 128.9, 128.8, 128.7, 127.3, 126.2, 122.2, 121.8, 107.5 (dd,  $J_{C-F}$  = 26.2, 5.1 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>25</sub>H<sub>14</sub>Br<sub>2</sub>F<sub>7</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 648.9356, found: 648.9354.



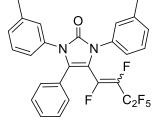
1,3-Bis(2-bromophenyl)-4-(perfluorobut-1-en-1-yl)-5-phenyl-1,3-dihydro-2*H*-imidazol-2-one (3ea):

Yield = 56% (109.9 mg, E/Z = 14.1/1). Yellow oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.67–7.64 (m, 1H), 7.57–7.53 (m, 1H), 7.37 (ddd, *J* = 7.5, 3.8, 1.7 Hz, 1H), 7.27 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.24–7.12 (m, 9H) ppm.

<sup>19</sup>**F** NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.49 (t, *J* = 4.0 Hz, 3F), -120.77 - -120.96 (m, 2F), -131.50 - -132.20 (m, 1F), -155.63 - -156.30 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -82.94 (dd, *J* = 24.6, 9.2 Hz, 3F), -100.03 (s, 1F), -118.82 (d, *J* = 18.4 Hz, 2F), -140.19 - -141.53 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 150.3, 144.6 (dd,  $J_{C-F}$  = 258.1, 43.2 Hz), 140.6–137.8 (m, 1C), 133.73, 133.69, 133.5, 133.4, 131.5, 131.1, 131.0, 130.7, 130.5, 129.6, 128.7, 128.6, 128.4, 128.3, 126.5, 124.1, 123.5, 108.0 (dd,  $J_{C-F}$  = 27.1, 7.1 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling. HRMS (m/z): calcd for C<sub>25</sub>H<sub>14</sub>Br<sub>2</sub>F<sub>7</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 648.9356, found: 648.9355.



**4-(Perfluorobut-1-en-1-yl)-5-phenyl-1,3-di***m***-tolyl-1,3-di***h***ydro-2***H***-imidazol-2-one (3fa):** Yield = 44% (69.5 mg, *E*/*Z* = 9.6/1). Yellow solid.

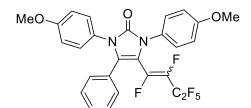
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>) of** *E***-isomer:**  $\delta$  = 7.40–7.26 (m, 6H), 7.24–7.14 (m, 5H), 7.10 (d, *J* = 7.9 Hz, 1H), 6.94 (d, *J* = 8.0 Hz, 1H), 2.41 (s, 3H), 2.30 (s, 3H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.42 (d, *J* = 4.3 Hz, 3F), -120.65 – -120.83 (m, 2F), -126.90 – -127.52 (m, 1F), -156.02 – -156.80 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.20 (d, *J* = 9.0 Hz, 3F), -96.19 (d, *J* = 20.9 Hz, 1F), -119.59 (dd, *J* = 17.2, 8.0 Hz, 2F), -141.24 (dd, *J* = 19.6, 9.2 Hz, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 151.6, 147.4–143.4 (m, 1C), 141.8–140.5 (m, 1C), 139.4, 139.0, 134.1, 134.0, 129.3, 129.2, 129.1, 129.0, 128.8, 128.72, 128.66, 128.6, 128.0, 126.9, 126.5, 124.4, 122.8, 107.5 (dd,  $J_{C-F}$  = 27.1, 6.1 Hz), 21.2 (2C) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>27</sub>H<sub>20</sub>F<sub>7</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 521.1458, found: 521.1460.



1,3-Bis(4-methoxyphenyl)-4-(perfluorobut-1-en-1-yl)-5-phenyl-1,3-dihydro-2*H*-imidazol-2-one (3ga):

Yield = 61% (100.6 mg, E/Z = 5.4/1). Yellow oil.

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

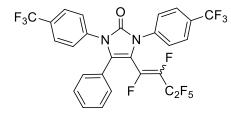
<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>) of** *E***-isomer:**  $\delta$  = 7.39–7.35 (m, 2H), 7.33–7.27 (m, 3H), 7.18–7.11 (m, 4H), 7.01–6.98 (m, 2H), 6.87–6.82 (m, 2H), 3.83 (s, 3H), 3.76 (s, 3H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.37 (d, *J* = 5.0 Hz, 3F), -120.68 (dd, *J* = 23.1, 15.6 Hz, 2F), -127.22 - -127.82 (m, 1F), -156.39 - -156.94 (m, 1F) ppm; *Z*-isomer:  $\delta$  = -83.24 (d, *J* = 9.0 Hz, 3F), -96.21 (d, *J* = 21.5 Hz, 1F), -119.39 - -119.59 (m, 2F), -141.06 - -141.26 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 159.3, 158.9, 151.9, 145.2 (dd,  $J_{C-F}$  = 256.9, 43.0

Hz), 140.9–137.4 (m, 1C), 129.6, 129.3, 128.9, 128.8, 128.6, 128.0, 127.5, 127.0, 126.9, 114.6, 114.2, 107.4 (dd,  $J_{C-F} = 26.3$ , 5.1 Hz), 55.4, 55.3 ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>27</sub>H<sub>20</sub>F<sub>7</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 553.1357, found: 553.1349.



4-(Perfluorobut-1-en-1-yl)-5-phenyl-1,3-bis(4-(trifluoromethyl)phenyl)-1,3-dihydro-2*H*-imidazol-2-one (3ha):

Yield = 55% (102.9 mg, E/Z = 4.8/1). Yellow solid.

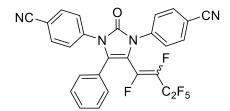
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1).

<sup>1</sup>**H** NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta = 7.79$  (dd, J = 8.8, 2.8 Hz, 2H), 7.62 (dd, J = 8.7, 2.4 Hz, 4H), 7.42–7.32 (m, 5H), 7.18 (tt, J = 6.8, 1.5 Hz, 2H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -62.59 (s, 3F), -62.62 (s, 3F), -84.39 (q, *J* = 4.1 Hz, 3F), -120.81 (ddd, *J* = 25.8, 13.0, 3.2 Hz, 2F), -127.85 - -128.46 (m, 1F), -155.04 (dtt, *J* = 149.4, 13.9, 4.2 Hz, 1F) ppm; *Z*-isomer:  $\delta$  = -62.54 (s, 3F), -62.56 (s, 3F), -83.33 (d, *J* = 8.2 Hz, 3F), -96.48 (d, *J* = 18.6 Hz, 1F), -119.75 - -119.90 (m, 2F), -139.07 (dq, *J* = 17.4, 8.8 Hz, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 150.9, 145.9, 145.4 (dd,  $J_{C-F}$  = 257.7, 43.4 Hz), 141.8–138.7 (m, 1C), 137.1, 136.9, 130.5, 130.1 (q,  $J_{C-F}$  = 43.0 Hz), 129.8, 129.1, 128.8, 127.3, 126.7 (q,  $J_{C-F}$  = 3.7 Hz), 126.3, 126.2 (q,  $J_{C-F}$  = 7.2 Hz), 125.9, 124.9 (d,  $J_{C-F}$  = 4.7 Hz), 122.2 (d,  $J_{C-F}$  = 4.7 Hz), 107.7 (dd,  $J_{C-F}$  = 27.4, 5.1 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>27</sub>H<sub>14</sub>F<sub>13</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 629.0893, found: 629.0896.



# 4,4'-(2-Oxo-4-(perfluorobut-1-en-1-yl)-5-phenyl-1*H*-imidazole-1,3(2*H*)-diyl)dibenzonitrile (3ia):

Yield = 72% (117.9 mg, E/Z = 3.9/1). Yellow oil.

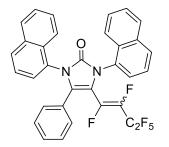
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.84–7.78 (m, 2H), 7.65–7.58 (m, 4H), 7.44–7.31 (m, 5H), 7.17–7.10 (m, 2H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.24 (d, *J* = 4.2 Hz, 3F), -120.69 (dd, *J* = 24.1, 13.6 Hz, 2F), -127.92 - -128.58 (m, 1F), -154.15 - -154.71 (m, 1F) ppm; *Z*-isomer:  $\delta$  = -83.28 (d, *J* = 8.6 Hz, 3F), -96.21 (d, *J* = 19.1 Hz, 1F), -119.83 (d, *J* = 16.6 Hz, 2F), -138.28 (dt, *J* = 17.5, 8.8 Hz, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta = 150.4$ , 143.2 (dd,  $J_{C-F} = 259.6$ , 43.5 Hz), 141.3–138.9 (m, 1C), 137.8, 137.5, 133.4, 132.9, 130.4, 129.2, 128.7, 127.5, 126.1, 125.9, 125.6, 117.8, 112.0, 111.79, 111.76, 107.6 (dd,  $J_{C-F} = 27.2$ , 5.2 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>27</sub>H<sub>14</sub>F<sub>7</sub>N<sub>4</sub>O [M+H]<sup>+</sup> 543.1050, found: 543.1054.



1,3-Di(naphthalen-1-yl)-4-(perfluorobut-1-en-1-yl)-5-phenyl-1,3-dihydro-2*H*-imidazol-2-one (3ja):

Yield = 72% (128.4 mg, E/Z = 8.6/1). Yellow oil.

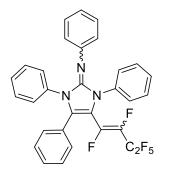
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1).

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>) of** *E***-isomer:** δ = 8.02–7.94 (m, 4H), 7.93–7.86 (m, 3H), 7.73 (dd, *J* = 7.3, 1.3 Hz, 1H), 7.68–7.58 (m, 4H), 7.55–7.46 (m, 2H), 7.24–7.12 (m, 5H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.57 - -84.78 (m, 3F), -120.97 (td, *J* = 23.5, 22.5, 11.6 Hz, 2F), -129.05 - -130.04 (m, 1F), -155.76 - -156.57 (m, 1F) ppm; *Z*-isomer:  $\delta$  = -82.83 (t, *J* = 9.7 Hz, 3F), -97.16 (dd, *J* = 27.1, 19.8 Hz, 1F), -119.15 (d, *J* = 19.8 Hz, 2F), -140.73 - -141.63 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta = 152.1$ , 145.2 (dd,  $J_{C-F} = 259.6$ , 47.5 Hz), 140.7–137.9 (m, 1C), 134.4, 134.3, 134.2, 130.7, 130.4, 130.0, 129.7, 129.4, 128.5, 128.3, 127.5, 127.3, 127.2, 126.8, 126.61, 126.56, 126.5, 126.3, 125.3, 125.20, 125.15, 122.6, 122.5, 122.4, 122.0, 109.0 (dd,  $J_{C-F} = 26.4$ , 5.2 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>33</sub>H<sub>20</sub>F<sub>7</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 593.1458, found: 593.1459.



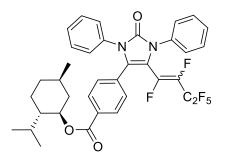
3-(3,5-Dimethyl-4-nitro-1*H*-pyrazol-1-yl)-5,5,6,6,7,7,8,8,8-nonafluoro-2-methyloct-3-en-2-ol (3ma):

Yield = 78% (133.3 mg, E/Z = 4.2/1). Yellow solid.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 7.26–7.10 (m, 15H), 6.78–6.71 (m, 2H), 6.55–6.49 (m, 3H) ppm. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.51 (q, *J* = 4.0 Hz, 3F), -120.68 – -120.83 (m, 2F), -125.72 – -126.31 (m, 1F), -156.01 (dtt, *J* = 153.2, 14.0, 4.5 Hz, 1F) ppm; *Z*-isomer:  $\delta$  = -83.12 – -83.22 (m, 3F), -96.57 (d, *J* = 24.4 Hz, 1F), -119.21 (dd, *J* = 30.4, 18.3 Hz, 2F), -141.34 – -141.57 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 147.8, 145.2 (dd,  $J_{C-F}$  = 259.6, 47.5 Hz), 144.0, 141.6–138.3 (m, 1C), 135.9, 135.6, 132.2, 129.1, 128.9, 128.7, 128.6, 128.5, 128.4, 127.8, 127.7, 127.5, 127.2, 127.0, 122.2, 120.0, 110.3 (dd,  $J_{C-F}$  = 26.4, 4.5 Hz) ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>31</sub>H<sub>21</sub>F<sub>7</sub>N<sub>3</sub> [M+H]<sup>+</sup> 568.1618, found:568.1620.



#### (1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl

# 4-(2-oxo-5-(perfluorobut-1-en-1-yl)-1,3-diphenyl-2,3-dihydro-1*H*-imidazol-4-yl)benzoate (3av):

Yield = 37% (49.3 mg, 0.2 mmol scale, E/Z = 5.4/1). Yellow oil.

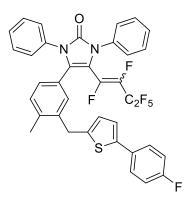
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1).

<sup>1</sup>**H** NMR (400 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta = 7.98-7.94$  (m, 2H), 7.52–7.42 (m, 5H), 7.37–7.33 (m, 2H), 7.25–7.21 (m, 4H), 4.92 (td, J = 10.9, 4.4 Hz, 1H), 2.14–2.07 (m, 1H), 1.97–1.89 (m, 1H), 1.73 (dt, J = 11.6, 3.0 Hz, 2H), 1.57–1.51 (m, 2H), 1.15–1.05 (m, 2H), 0.91 (dd, J = 6.8, 3.4 Hz, 8H), 0.78 (d, J = 6.9 Hz, 3H) ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = -84.31 (t, *J* = 4.2 Hz, 3F), -120.66 – -120.84 (m, 2F), -126.99 – -127.61 (m, 1F), -155.29 – -155.85 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.22 (tt, *J* = 5.5, 2.7 Hz, 3F), -96.01 – -96.44 (m, 1F), -119.54 – -119.76 (m, 2F), -139.75 (dq, *J* = 18.3, 8.9 Hz, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta = 165.3$ , 151.6, 147.5–143.6 (m, 1C), 142.3–138.9 (m, 1C), 134.1, 134.0, 131.6, 131.0, 130.0, 129.6, 129.4, 128.8, 128.6, 128.3, 127.4, 126.1, 109.0–108.3 (m, 1C), 75.5, 47.3, 41.0, 34.3, 31.5, 26.5, 23.6, 22.1, 20.8, 16.5 ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>36</sub>H<sub>34</sub>F<sub>7</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 675.2452, found: 675.2458.



# 4-(3-((5-(4-Fluorophenyl)thiophen-2-yl)methyl)-4-methylphenyl)-5-(perfluorobut-1-en-1-yl)-1,3-diphenyl-1,3-dihydro-2*H*-imidazol-2-one (3aw):

Yield =33% (68.6 mg, E/Z = 4.9/1). Yellow oil.

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

<sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>) of** *E***-isomer:**  $\delta$  = 7.51–7.38 (m, 7H), 7.33–7.20 (m, 5H), 7.15–6.94 (m, 6H), 6.40 (d, *J* = 3.7 Hz, 1H), 3.98 (s, 2H), 2.29 (s, 3H) ppm.

<sup>19</sup>**F NMR (376 MHz, CDCl<sub>3</sub>) of** *E*-isomer:  $\delta$  = -84.32 (q, *J* = 3.8, 3.1 Hz, 3F), -114.72 - -114.88 (m, 1F), -120.54 (dd, *J* = 24.1, 13.8 Hz, 2F), -126.72 - -127.35 (m, 1F), -156.02 - -156.64 (m, 1F) ppm; **Z**-isomer:  $\delta$  = -83.11 (d, *J* = 8.9 Hz, 3F), -95.45 (d, *J* = 20.9 Hz, 1F), -114.83 - -114.93 (m, 1F), -119.44 (dd, *J* = 97.0, 17.5 Hz, 2F), -140.61 - -140.96 (m, 1F) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of *E*-isomer:  $\delta$  = 161.5 (d,  $J_{C-F}$  = 246.5 Hz), 151.5, 146.4 (d,  $J_{C-F}$  = 42.5 Hz), 143.9 (d,  $J_{C-F}$  = 42.3 Hz), 141.9, 141.6, 138.7, 138.1, 134.3, 134.2, 130.8, 129.8, 129.3, 129.0, 128.1, 127.8, 127.4, 127.2, 127.0 (d,  $J_{C-F}$  = 8.2 Hz), 126.3, 126.1, 125.9, 124.6, 122.6, 122.57, 115.7 (d,  $J_{C-F}$  = 21.7 Hz), 107.2 (dd,  $J_{C-F}$  = 27.1, 5.1 Hz), 33.6, 19.3 ppm, carbons corresponding to the C<sub>2</sub>F<sub>5</sub> group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for C<sub>37</sub>H<sub>25</sub>F<sub>8</sub>N<sub>2</sub>OS [M+H]<sup>+</sup> 697.1554, found: 697.1560.

## **References**

[1] a) G. Wu, A. Jacobi von Wangelin, *Chem. Sci.* **2018**, *9*, 1795-1802; b) W. Han, Y.-L. Chen, X. Tang, J. Zhou, M. Ma, Z.-L. Shen, X.-Q. Chu, *Green Chem.* **2023**, *25*, 9672–9679.

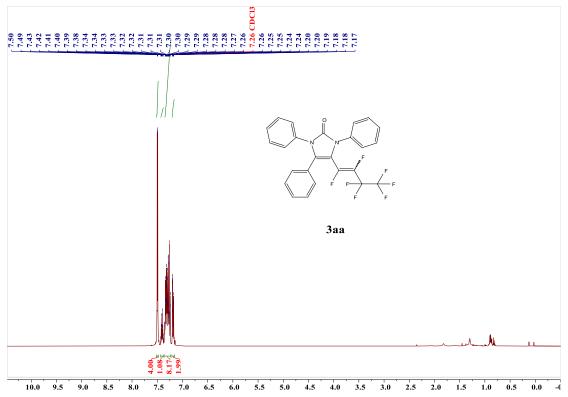
[2] T. Xu, C. W. Cheung, X. Hu, Angew. Chem. Int. Ed. 2014, 53, 4910-4914.

[3] J. Wu, C. Wang, Z. Wang, H. Li, R. Liu, Y. Wang, P. Zhou, D. Li, J. Yang, *Synthesis* **2022**, *54*, 3055–3068.

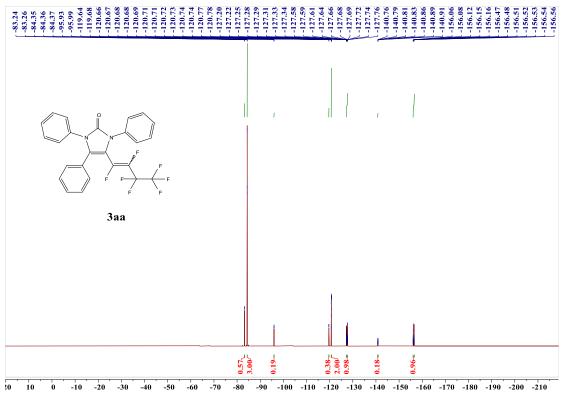
[4] M. Wang, J. Han, X. Si, Y. Hu, J. Zhu, X. Sun, Tetrahedron Lett. 2018, 59, 1614–1618.

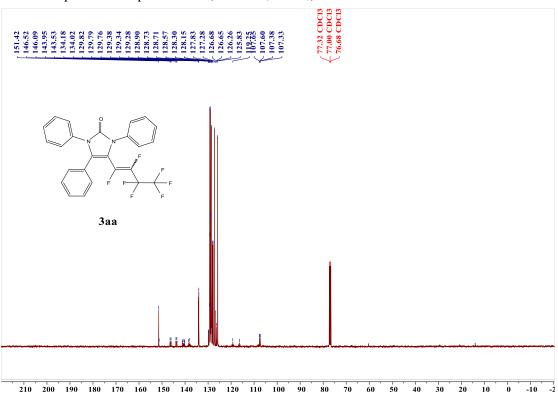
# <sup>1</sup>H, <sup>19</sup>F, and <sup>13</sup>C NMR spectra of products

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



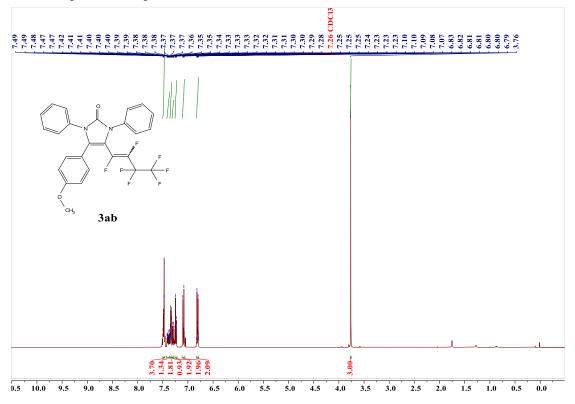
 $^{19}F$  NMR spectra of the product **3aa** (376 MHz, CDCl<sub>3</sub>)

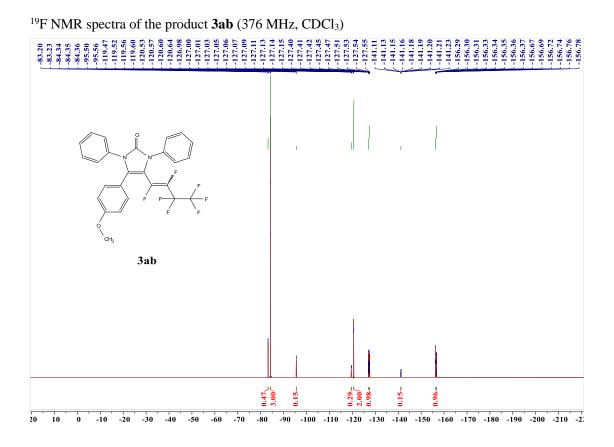




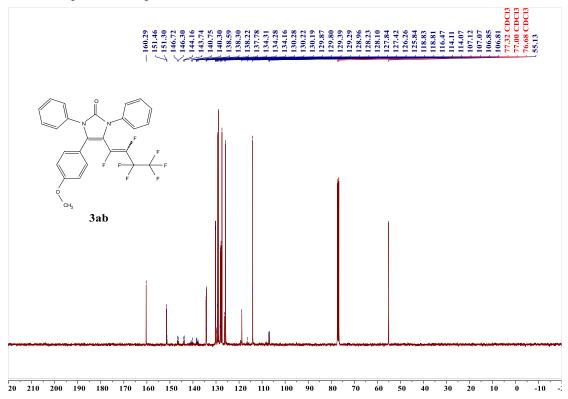
<sup>13</sup>C NMR spectra of the product **3aa** (100 MHz, CDCl<sub>3</sub>)

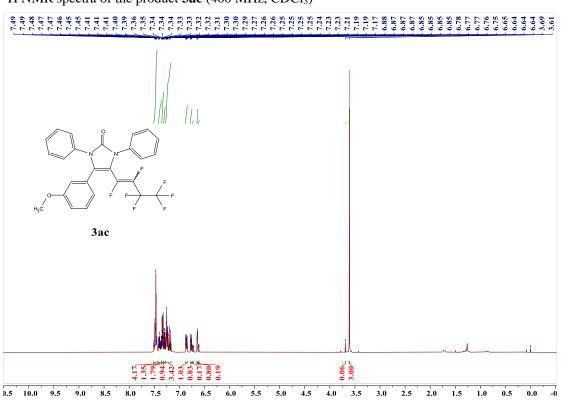
<sup>1</sup>H NMR spectra of the product **3ab** (400 MHz, CDCl<sub>3</sub>)



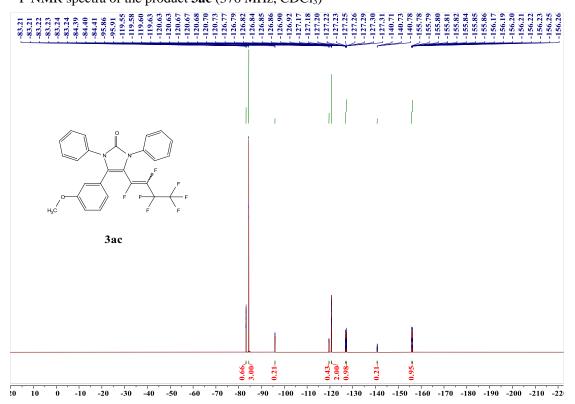


<sup>13</sup>C NMR spectra of the product **3ab** (100 MHz, CDCl<sub>3</sub>)

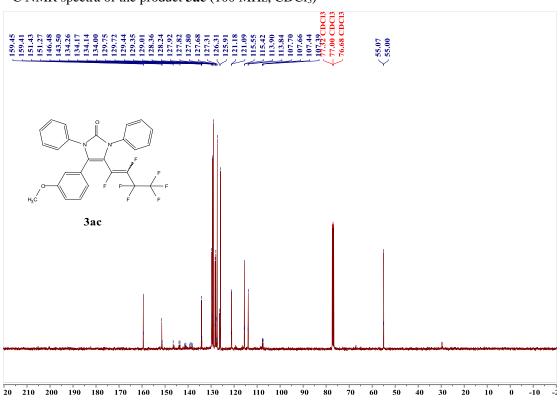




<sup>19</sup>F NMR spectra of the product **3ac** (376 MHz, CDCl<sub>3</sub>)

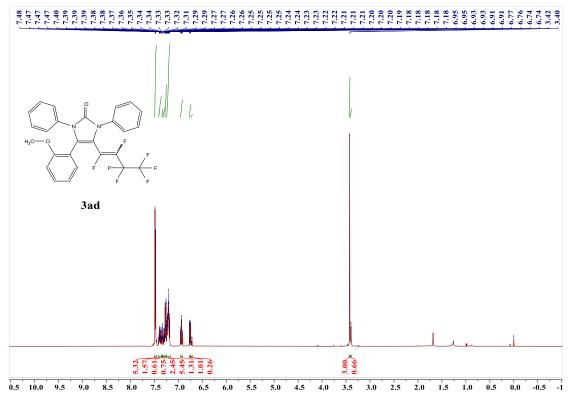


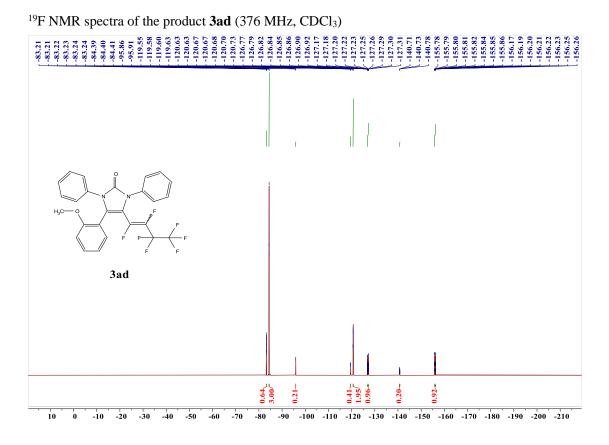
<sup>1</sup>H NMR spectra of the product **3ac** (400 MHz, CDCl<sub>3</sub>)



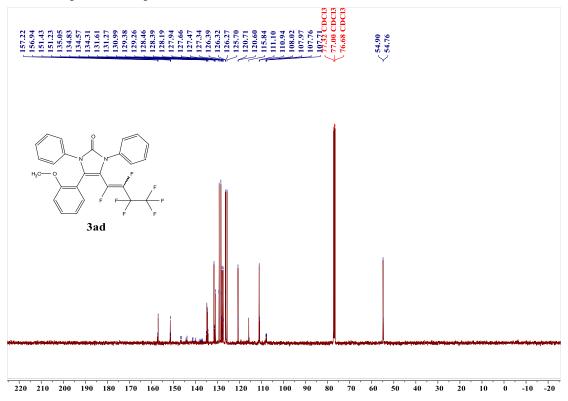
<sup>13</sup>C NMR spectra of the product **3ac** (100 MHz, CDCl<sub>3</sub>)

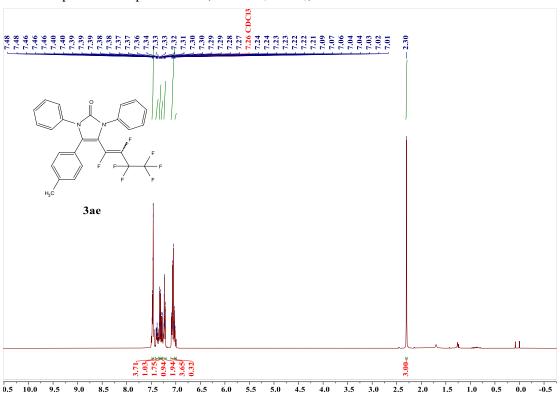
<sup>1</sup>H NMR spectra of the product **3ad** (400 MHz, CDCl<sub>3</sub>)





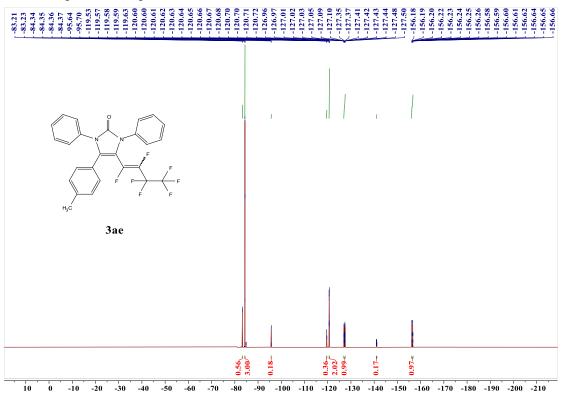
<sup>13</sup>C NMR spectra of the product **3ad** (100 MHz, CDCl<sub>3</sub>)

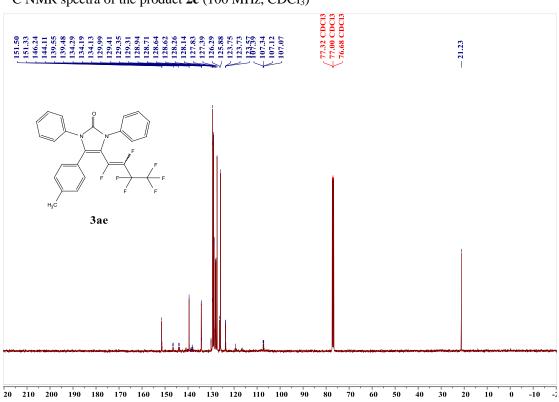




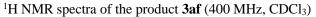
<sup>1</sup>H NMR spectra of the product **3ae** (400 MHz, CDCl<sub>3</sub>)

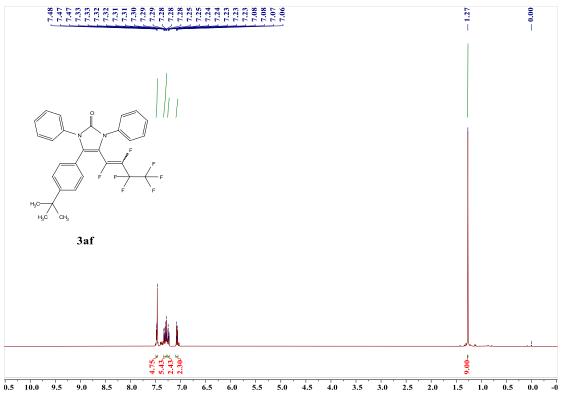
<sup>19</sup>F NMR spectra of the product **3ae** (376 MHz, CDCl<sub>3</sub>)

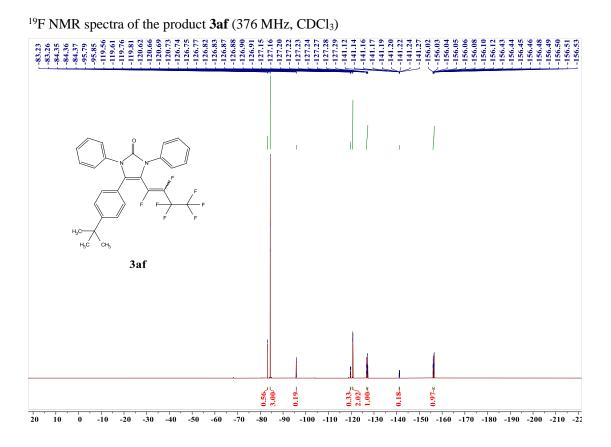




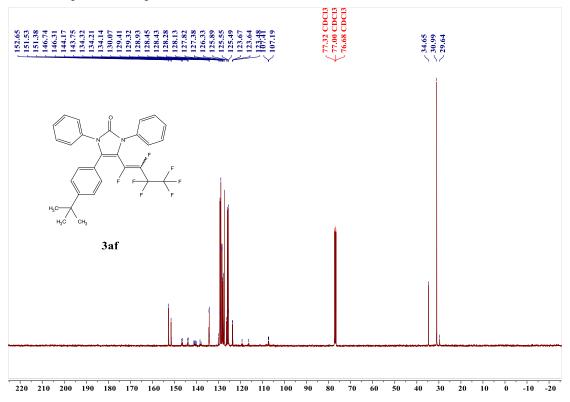
<sup>13</sup>C NMR spectra of the product **2e** (100 MHz, CDCl<sub>3</sub>)

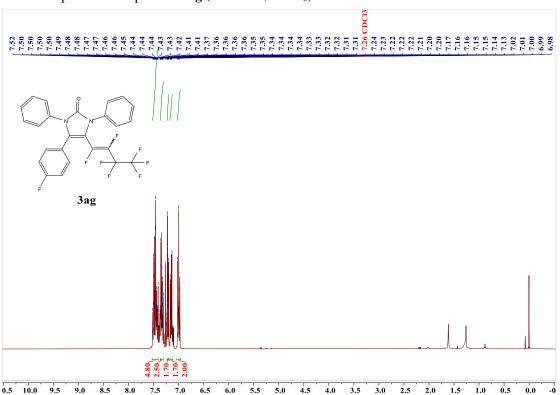






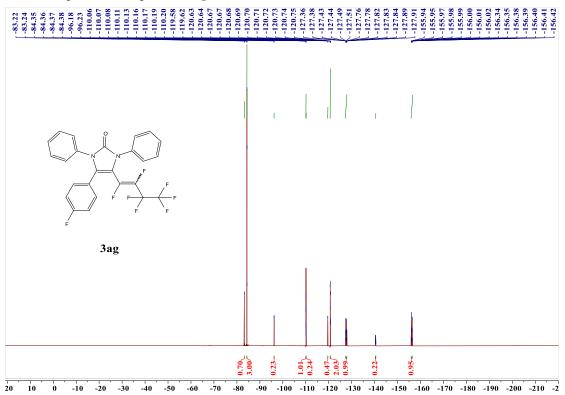
<sup>13</sup>C NMR spectra of the product **3af** (100 MHz, CDCl<sub>3</sub>)

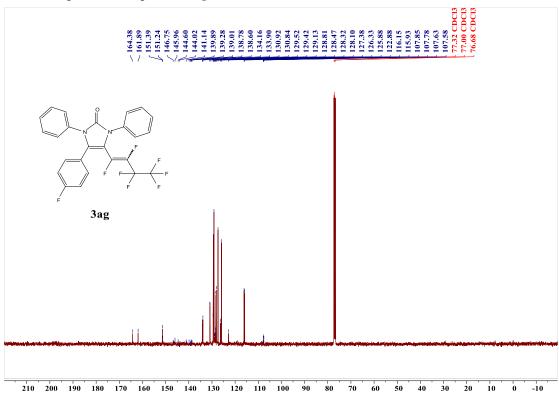




<sup>1</sup>H NMR spectra of the product **3ag** (400 MHz, CDCl<sub>3</sub>)

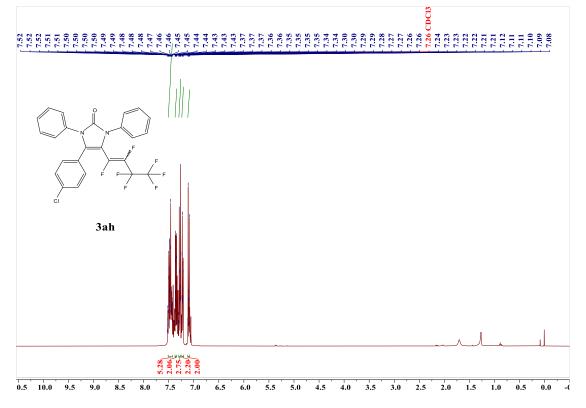
<sup>19</sup>F NMR spectra of the product **3ag** (376 MHz, CDCl<sub>3</sub>)

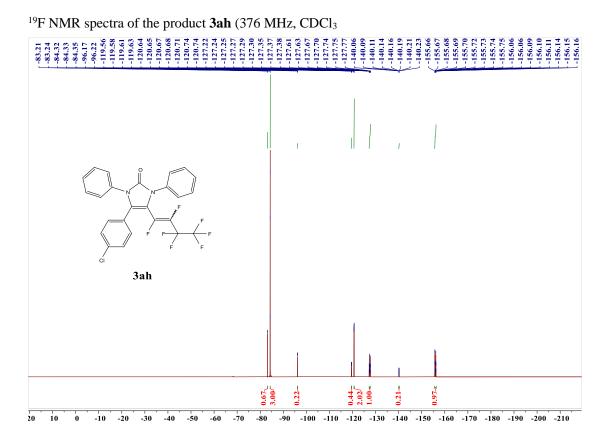




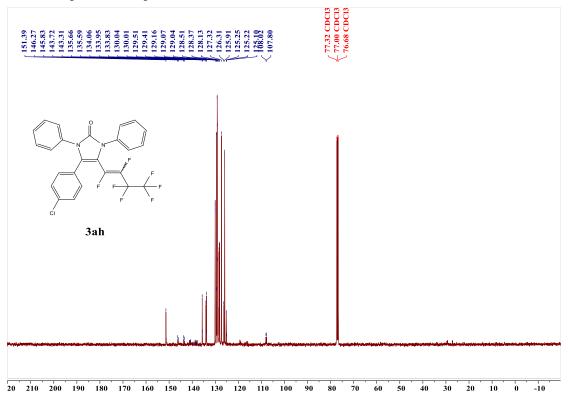
<sup>13</sup>C NMR spectra of the product **3ag** (100 MHz, CDCl<sub>3</sub>)

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

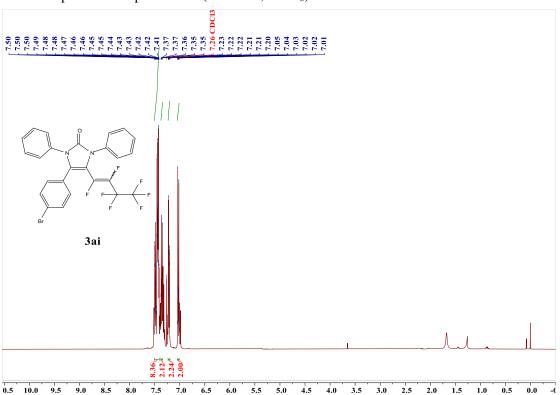




<sup>13</sup>C NMR spectra of the product **3ah** (100 MHz, CDCl<sub>3</sub>)

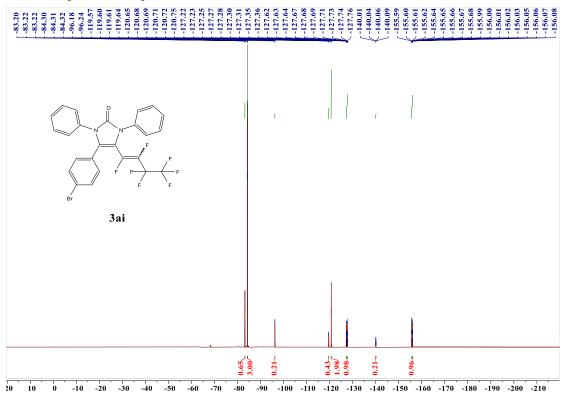


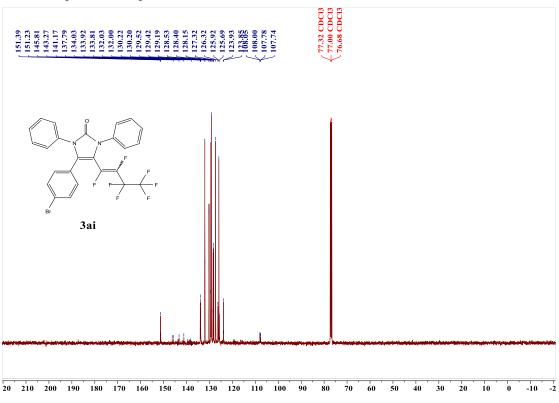
S43



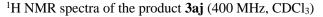
<sup>1</sup>H NMR spectra of the product **3ai** (400 MHz, CDCl<sub>3</sub>)

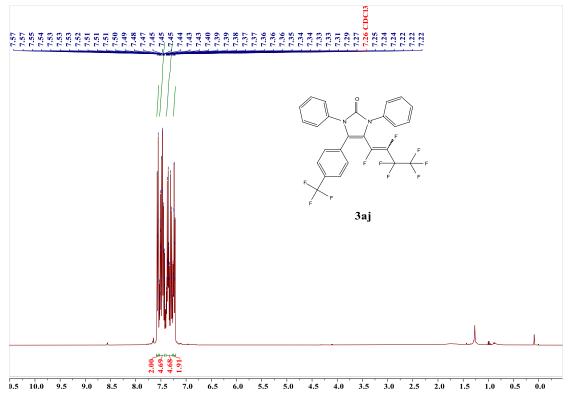
<sup>19</sup>F NMR spectra of the product **3ai** (376 MHz, CDCl<sub>3</sub>)

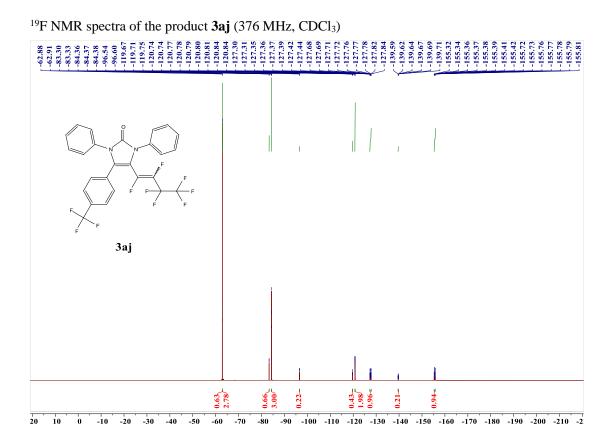




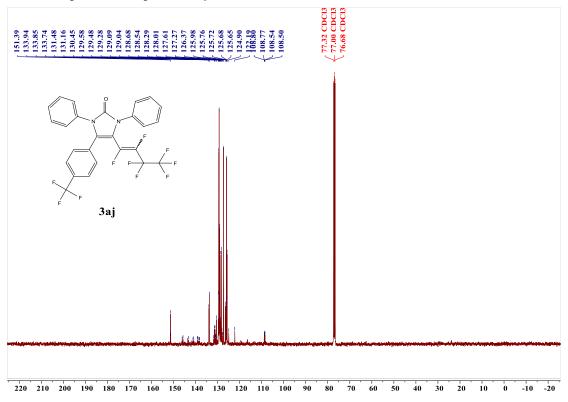
<sup>13</sup>C NMR spectra of the product **3ai** (100 MHz, CDCl<sub>3</sub>)

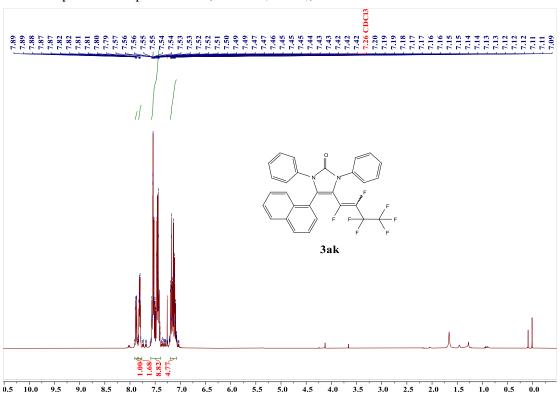




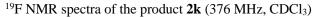


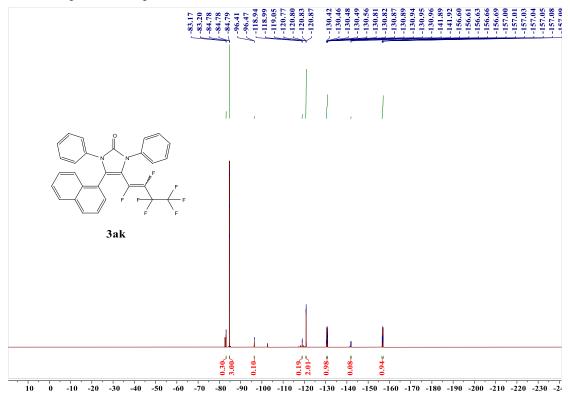
<sup>13</sup>C NMR spectra of the product **3aj** (100 MHz, CDCl<sub>3</sub>)

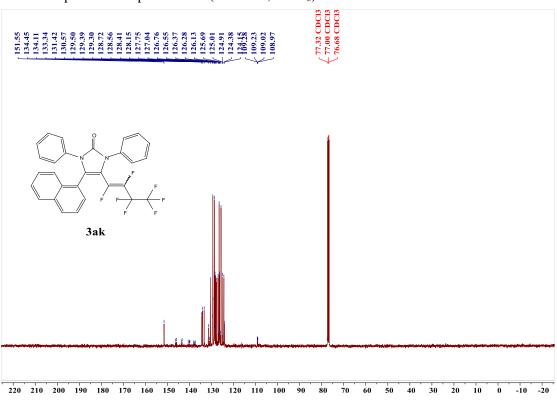




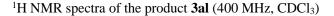
<sup>1</sup>H NMR spectra of the product **3ak** (400 MHz, CDCl<sub>3</sub>)

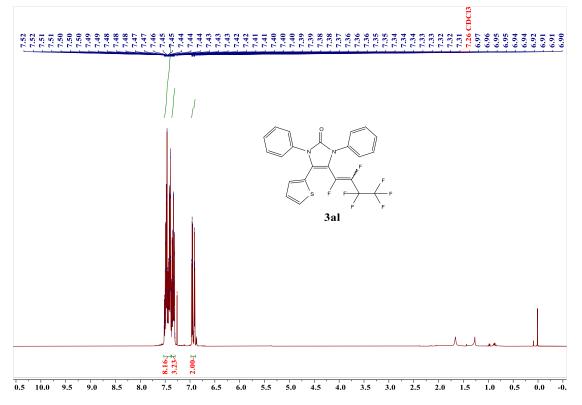


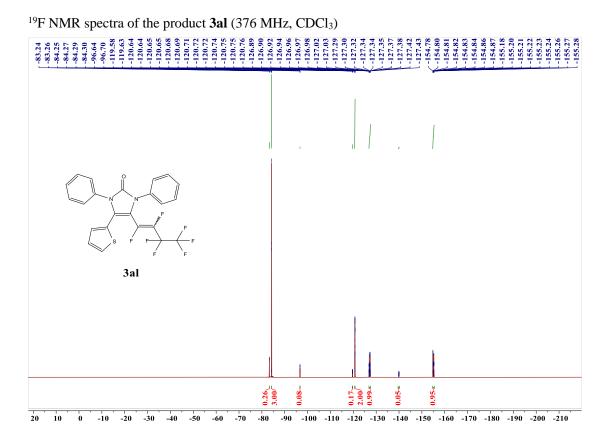




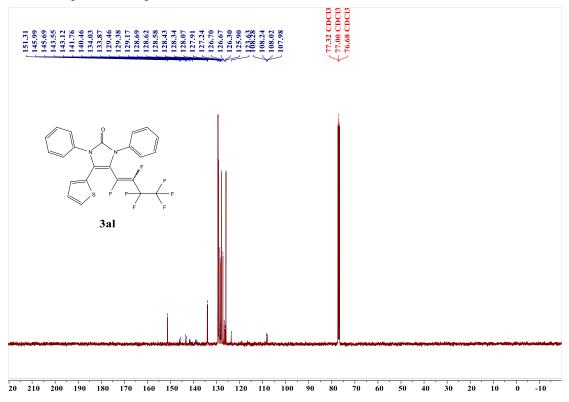
<sup>13</sup>C NMR spectra of the product **3ak** (100 MHz, CDCl<sub>3</sub>)

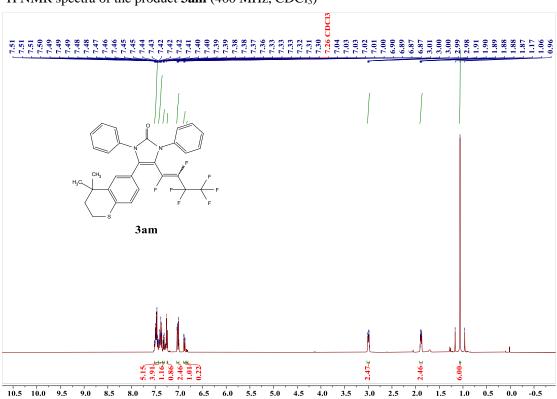




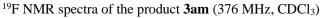


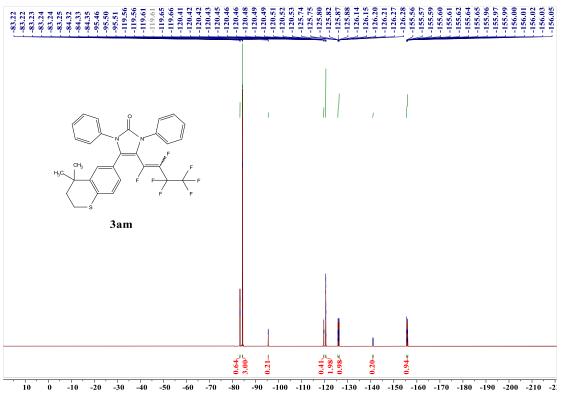
<sup>13</sup>C NMR spectra of the product **3al** (100 MHz, CDCl<sub>3</sub>)

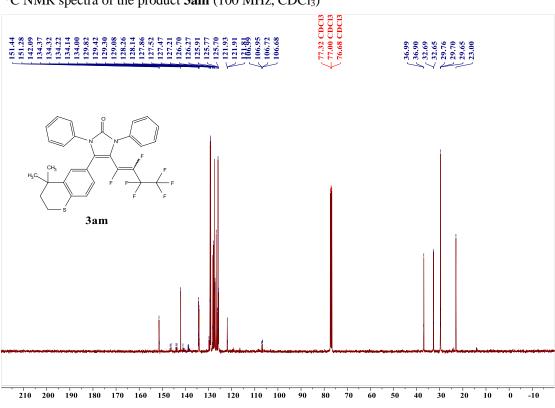




<sup>1</sup>H NMR spectra of the product **3am** (400 MHz, CDCl<sub>3</sub>)

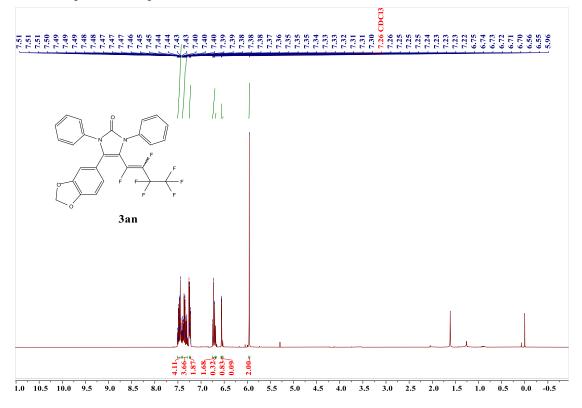


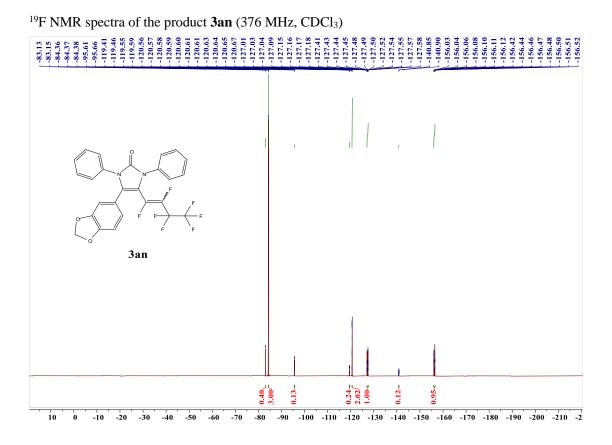




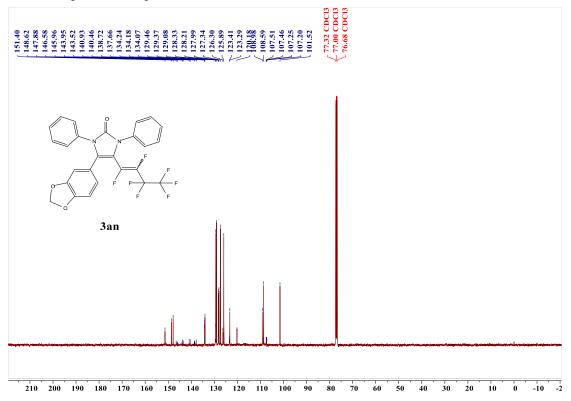
<sup>13</sup>C NMR spectra of the product **3am** (100 MHz, CDCl<sub>3</sub>)

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

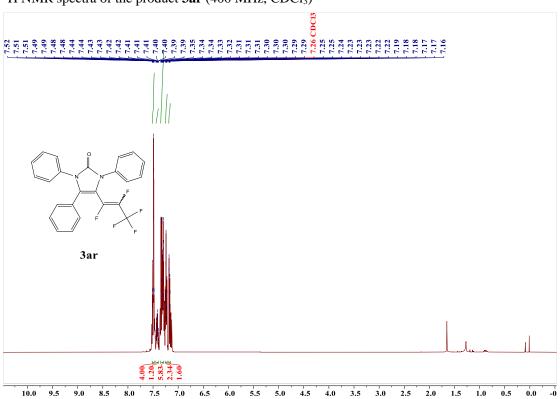




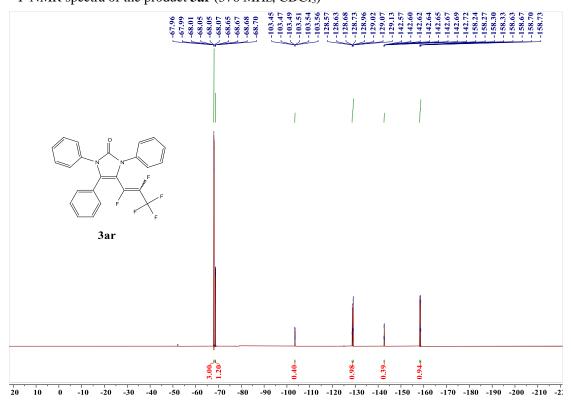
<sup>13</sup>C NMR spectra of the product **3an** (100 MHz, CDCl<sub>3</sub>)

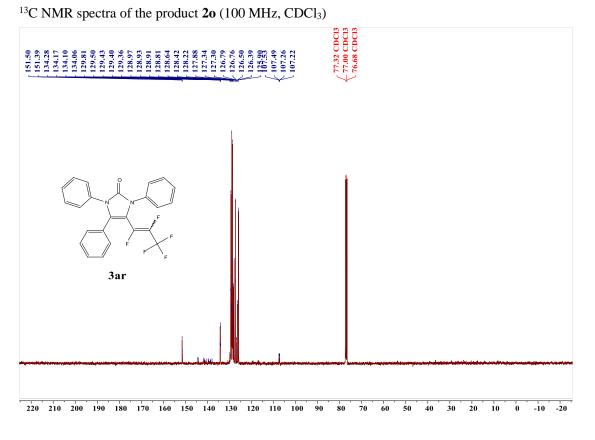


S52

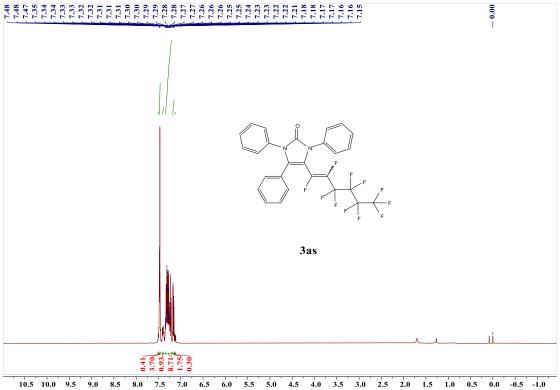


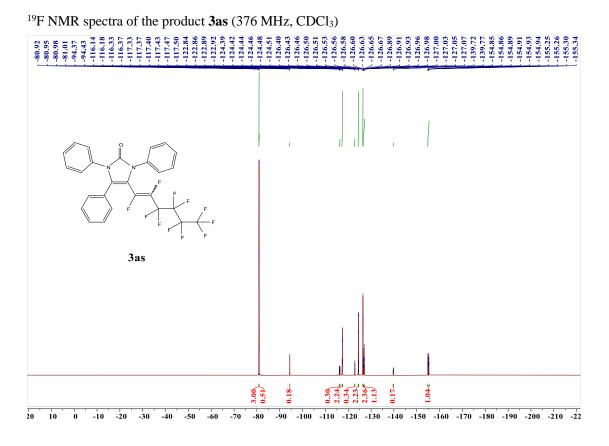
<sup>19</sup>F NMR spectra of the product **3ar** (376 MHz, CDCl<sub>3</sub>)



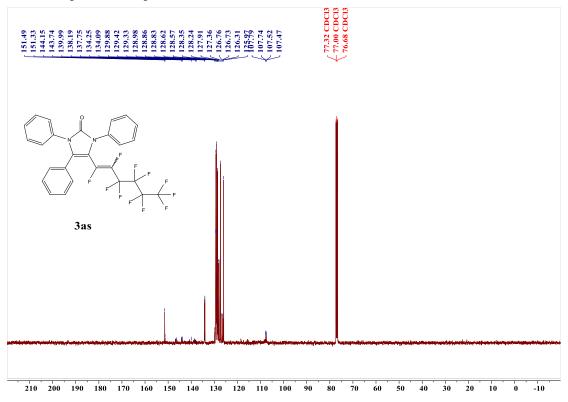


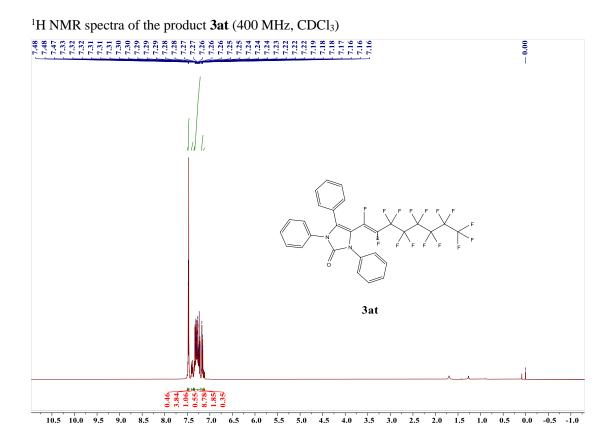
<sup>1</sup>H NMR spectra of the product **3as** (400 MHz, CDCl<sub>3</sub>)



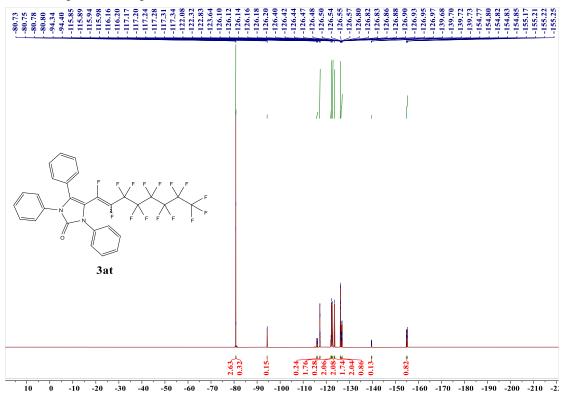


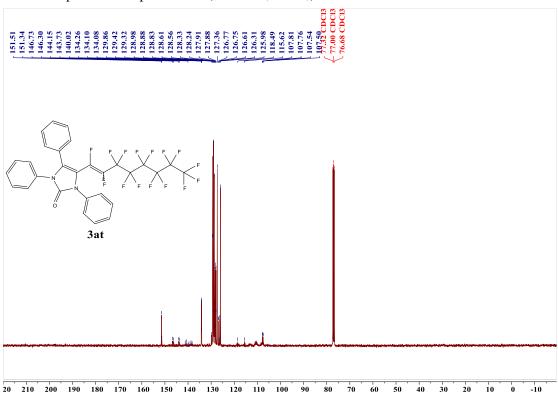
<sup>13</sup>C NMR spectra of the product **3as** (100 MHz, CDCl<sub>3</sub>)



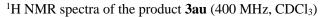


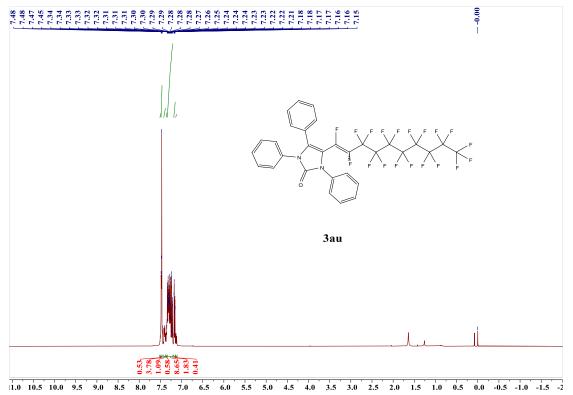
 $^{19}F$  NMR spectra of the product **3at** (376 MHz, CDCl<sub>3</sub>)

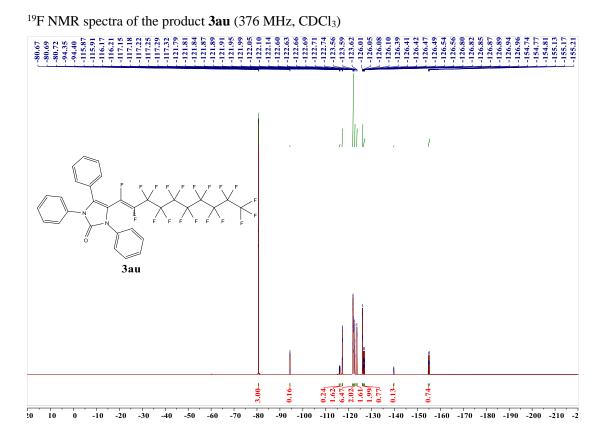




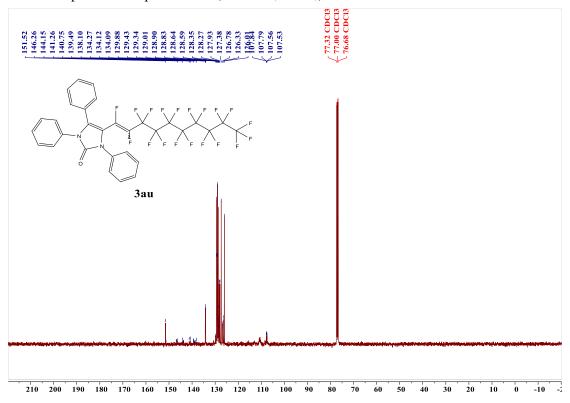
<sup>13</sup>C NMR spectra of the product **3at** (100 MHz, CDCl<sub>3</sub>)



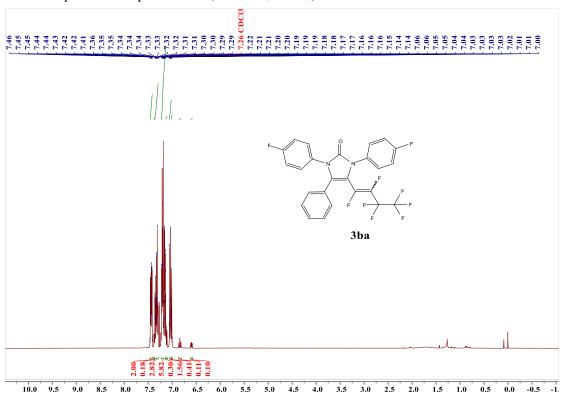




<sup>13</sup>C NMR spectra of the product **3au** (100 MHz, CDCl<sub>3</sub>)

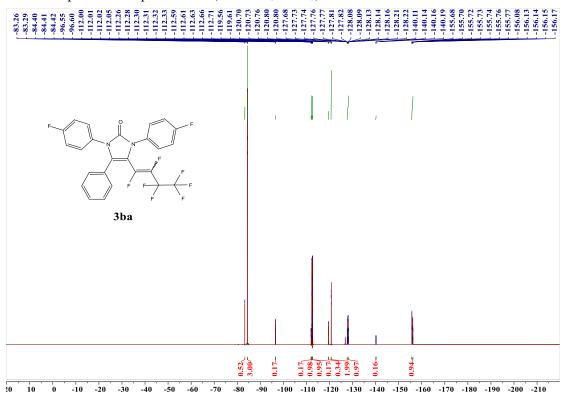


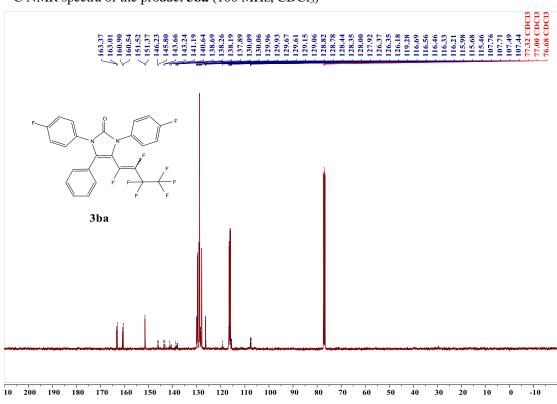
S58



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

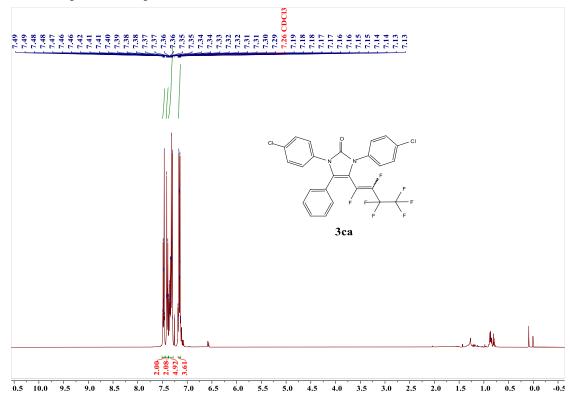
<sup>19</sup>F NMR spectra of the product **3ba** (376 MHz, CDCl<sub>3</sub>)

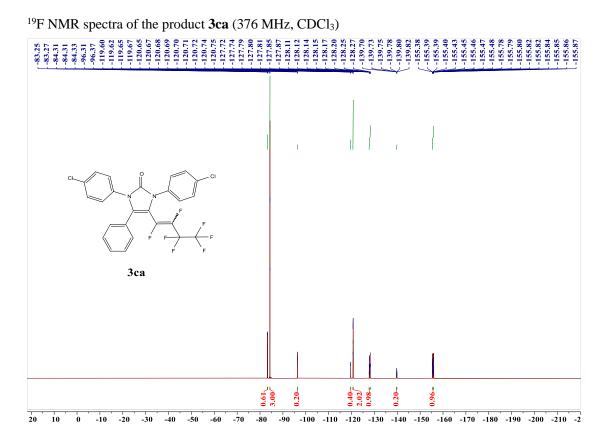




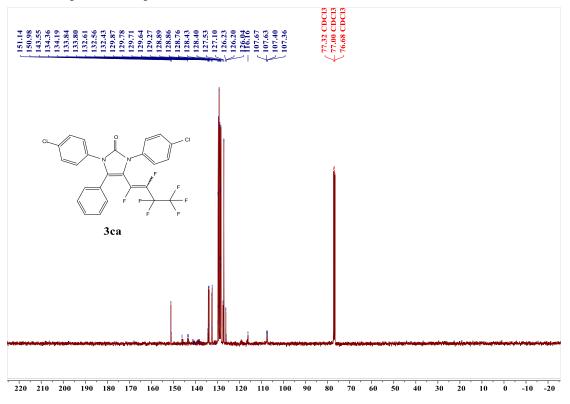
<sup>13</sup>C NMR spectra of the product **3ba** (100 MHz, CDCl<sub>3</sub>)

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

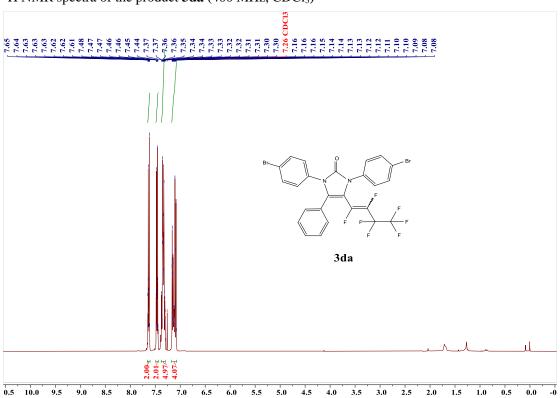




<sup>13</sup>C NMR spectra of the product **3ca** (100 MHz, CDCl<sub>3</sub>)

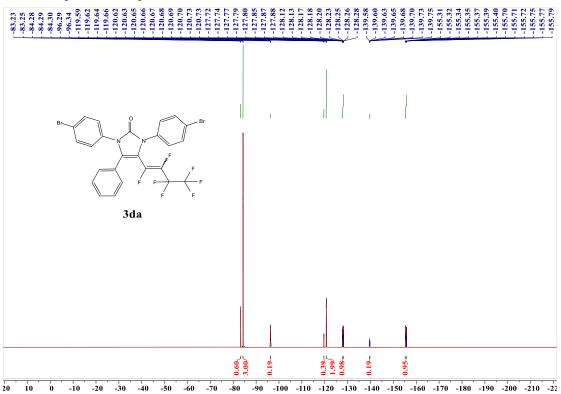


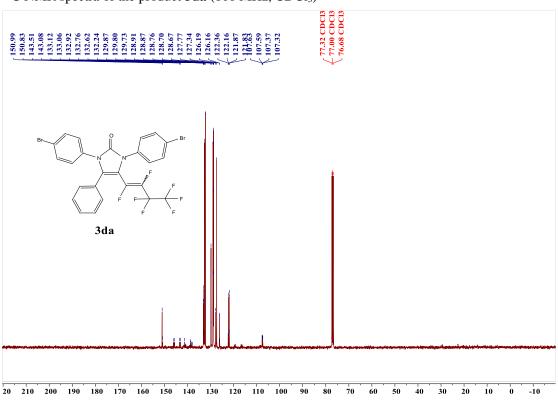
S61



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

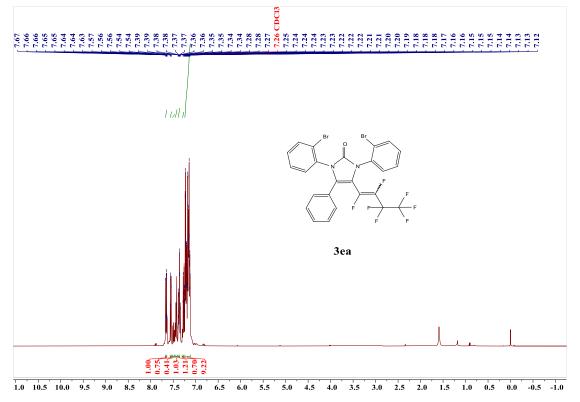
<sup>19</sup>F NMR spectra of the product **3da** (376 MHz, CDCl<sub>3</sub>)

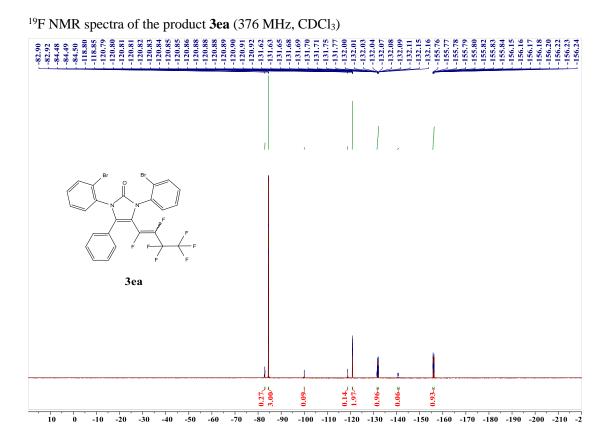




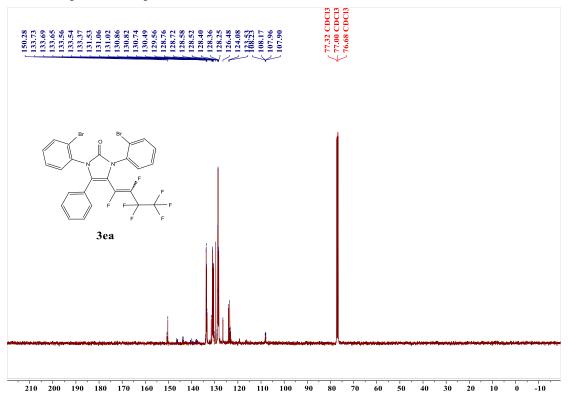
<sup>13</sup>C NMR spectra of the product **3da** (100 MHz, CDCl<sub>3</sub>)

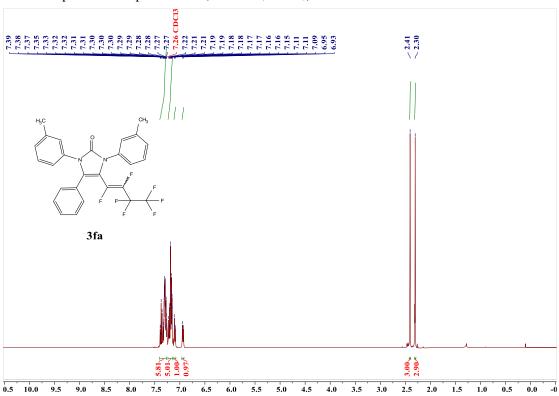
<sup>1</sup>H NMR spectra of the product **3ea** (400 MHz, CDCl<sub>3</sub>)



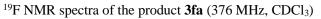


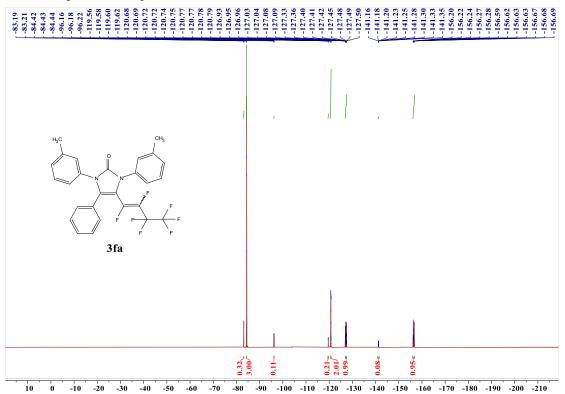
<sup>13</sup>C NMR spectra of the product **3ea** (100 MHz, CDCl<sub>3</sub>)

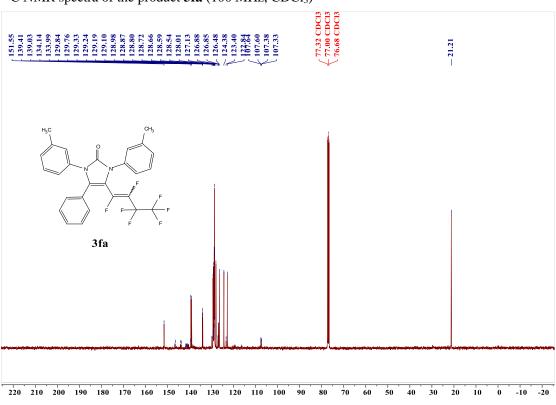




<sup>1</sup>H NMR spectra of the product **3fa** (400 MHz, CDCl<sub>3</sub>)

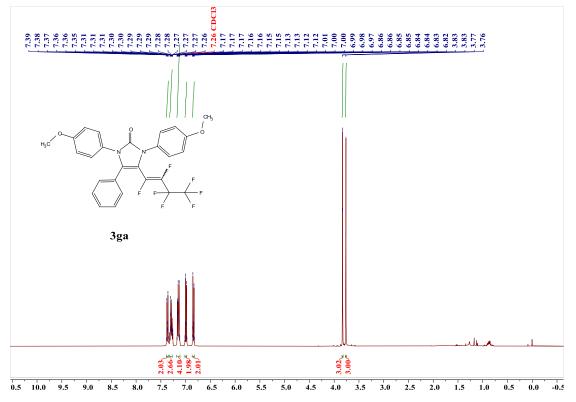


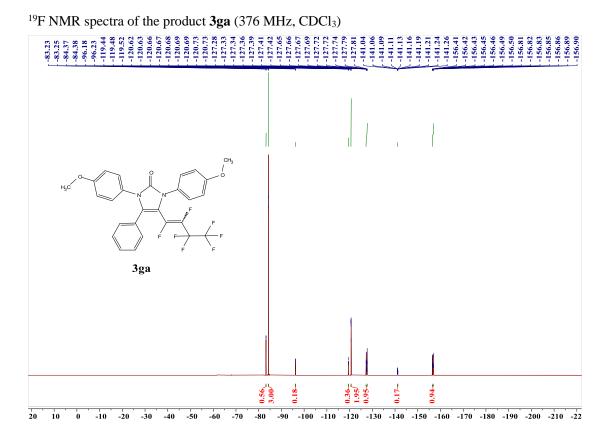




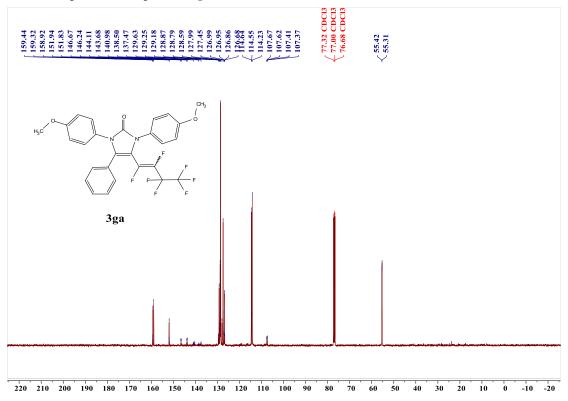
<sup>13</sup>C NMR spectra of the product **3fa** (100 MHz, CDCl<sub>3</sub>)

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

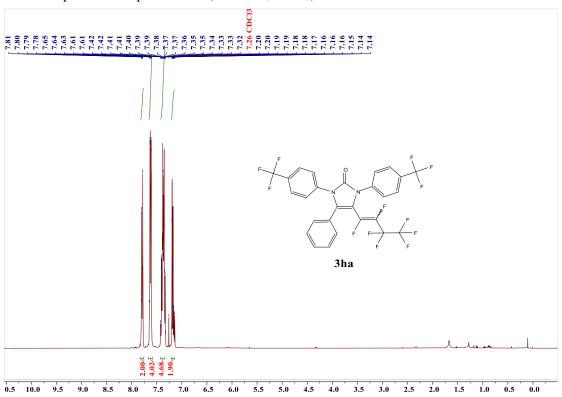




<sup>13</sup>C NMR spectra of the product **3ga** (100 MHz, CDCl<sub>3</sub>)

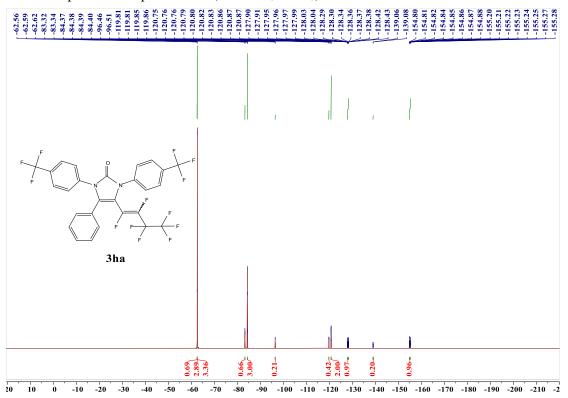


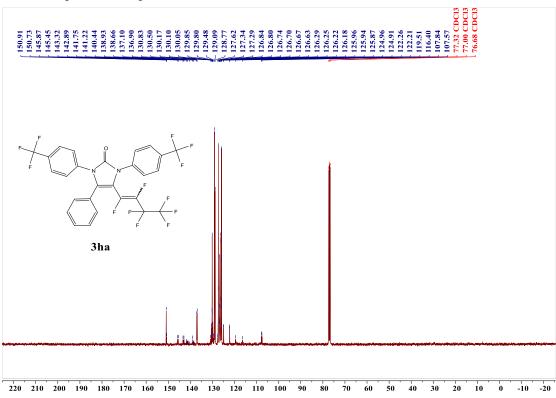
S67



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

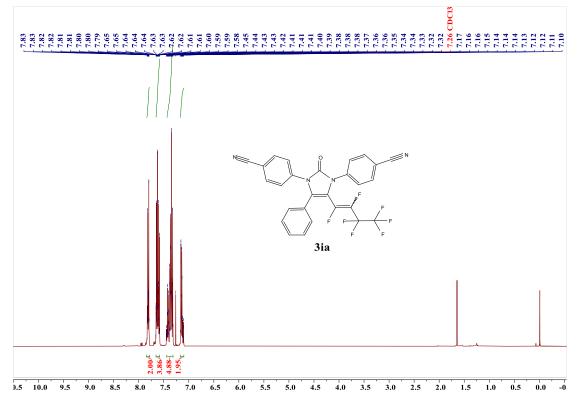
<sup>19</sup>F NMR spectra of the product **3ha** (376 MHz, CDCl<sub>3</sub>)

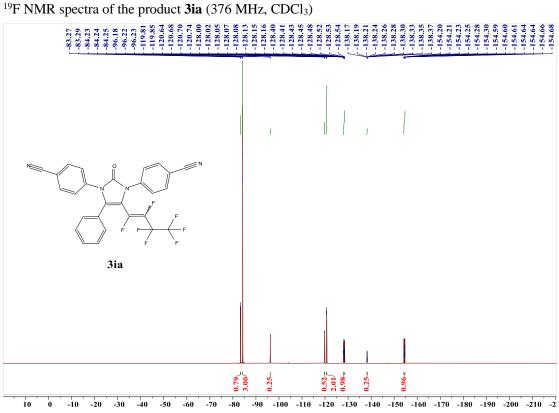




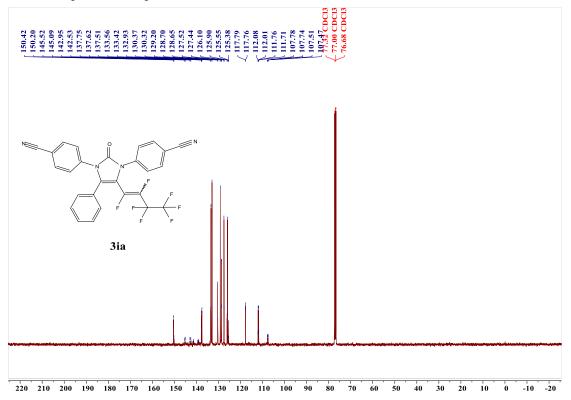
<sup>13</sup>C NMR spectra of the product **3ha** (100 MHz, CDCl<sub>3</sub>)

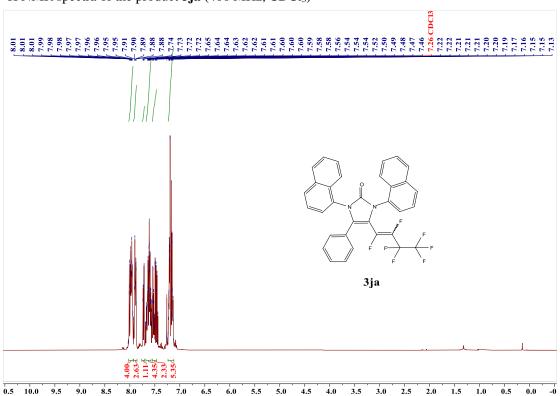
<sup>1</sup>H NMR spectra of the product **3ia** (400 MHz, CDCl<sub>3</sub>)

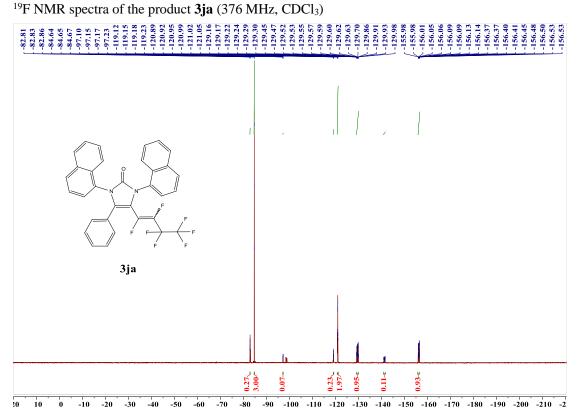




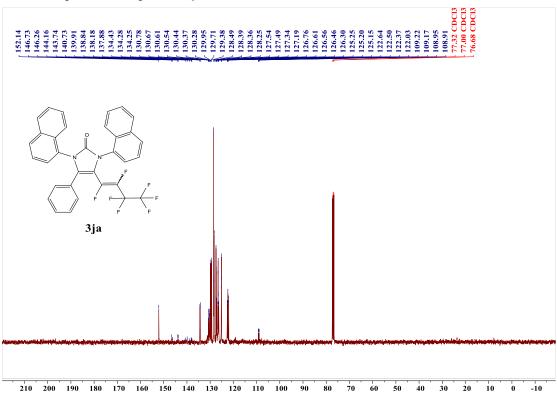
<sup>13</sup>C NMR spectra of the product **3ia** (100 MHz, CDCl<sub>3</sub>)





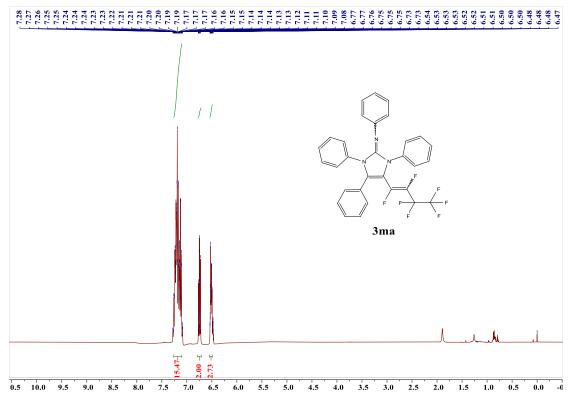


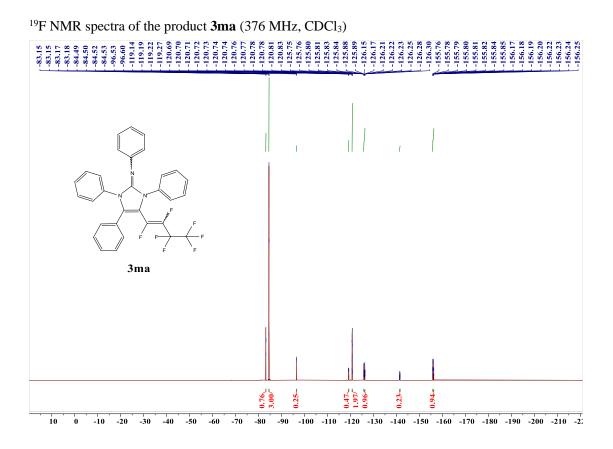
<sup>1</sup>H NMR spectra of the product **3ja** (400 MHz, CDCl<sub>3</sub>)



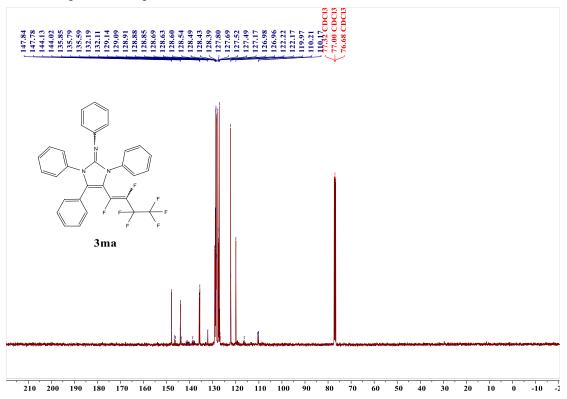
<sup>13</sup>C NMR spectra of the product **3ja** (100 MHz, CDCl<sub>3</sub>)

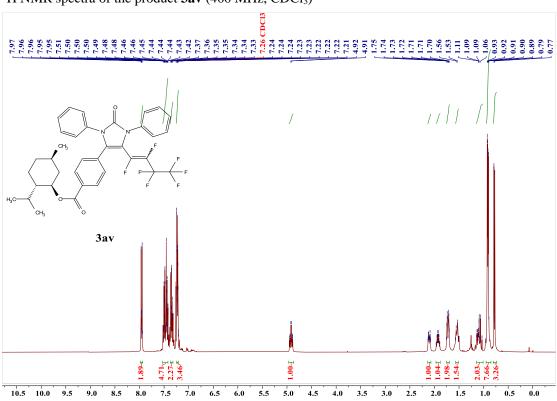
<sup>1</sup>H NMR spectra of the product **3ma** (400 MHz, CDCl<sub>3</sub>)





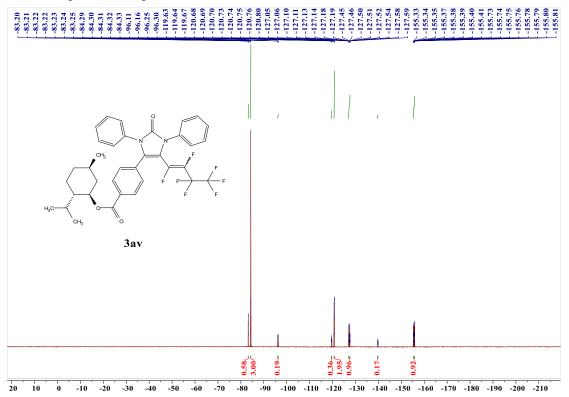
<sup>13</sup>C NMR spectra of the product **3ma** (100 MHz, CDCl<sub>3</sub>)

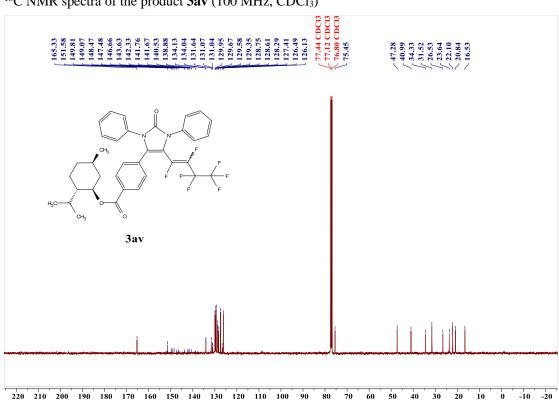




<sup>1</sup>H NMR spectra of the product **3av** (400 MHz, CDCl<sub>3</sub>)

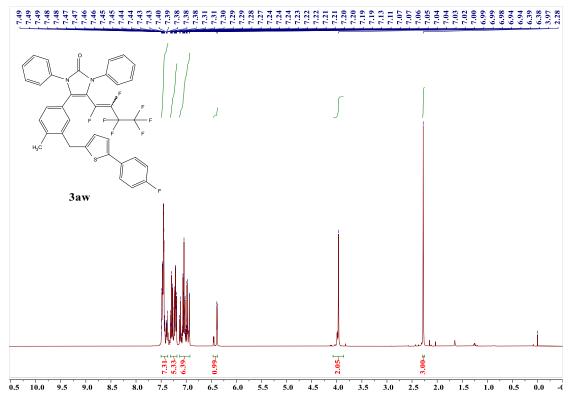
<sup>19</sup>F NMR spectra of the product **3av** (376 MHz, CDCl<sub>3</sub>)

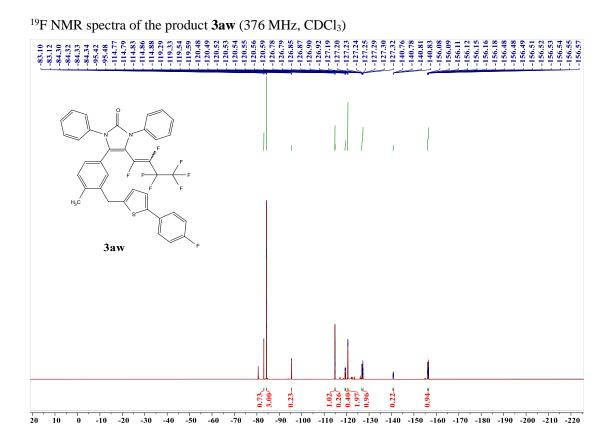




<sup>13</sup>C NMR spectra of the product **3av** (100 MHz, CDCl<sub>3</sub>)

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





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

