

## Supporting Information

for *Adv. Sci.*, DOI 10.1002/adv.202407931

Ring Transformation of Cyclopropenes to Benzo-Fused Five-Membered Oxa- and Aza-Heterocycles via a Formal [4+1] Cyclization

*Fengyan Gu, Binyan Lin, Zhi-Huan Peng, Shijie Liu, Yuanqing Wu, Mei Luo, Ning Ding, Qichen Zhan, Peng Cao\*, Zhi Zhou\* and Tao Cao\**

## Supporting Information

### **Ring Transformation of Cyclopropenes to Benzo-Fused Five-Membered Oxa- and Aza-Heterocycles via a Formal [4+1] Cyclization**

*Fengyan Gu, Binyan Lin, Zhi-Huan Peng, Shijie Liu, Yuanqing Wu, Mei Luo, Ning Ding, Qichen Zhan, Peng Cao,\* Zhi Zhou,\* and Tao Cao\**

## Table of Contents

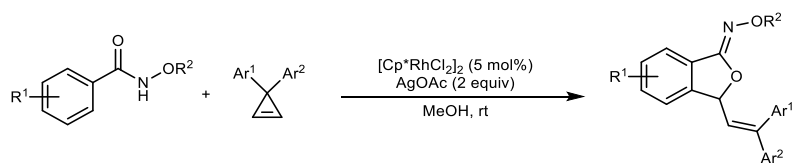
<b>1. Supplementary Notes</b> .....	<b>S3</b>
<b>2. Supplementary Methods</b> .....	<b>S3</b>
2.1 Synthesis of isobenzofuranone <i>O</i> -alkyl oximes.....	S3
2.2 Synthesis of <i>N</i> -alkoxy isoindolinones.....	S27
2.3 Transformation of products to assess the potential for post-modifications. ....	S37
2.4 Synthesis of a potential PD-L1 down-regulator.....	S41
2.5 Biological activity evaluation. ....	S44
2.6 Experimental mechanistic studies.....	S45
2.7 Computational Mechanistic Studies .....	S49
<b>3. Supplementary References</b> .....	<b>S119</b>
<b>4. <sup>1</sup>H NMR, <sup>13</sup>C NMR, and <sup>19</sup>F NMR Spectra</b> .....	<b>S123</b>

## 1. Supplementary Notes

Commercially available reagents and solvents for synthesis of compounds were purchased from Adamas, Sinopharm, Sigma-Aldrich and used without further purification. All the temperatures are referred to the preheated oil baths used.  $^1\text{H}$  NMR spectra were recorded on a Bruker AVANCE III 500 spectrometer and are internally referenced to residual protic  $\text{CDCl}_3$  (7.26 ppm) or  $\text{DMSO-}d_6$  (2.50 ppm). The data are reported as follows: chemical shift ( $\delta$  ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, td = triplet of doublets, tt = triplet of triplets), coupling constant (Hz), and integration.  $^{13}\text{C}$  NMR spectra were recorded on a Bruker AVANCE III 500 spectrometer and data are reported in terms of chemical shift relative to  $\text{CDCl}_3$  (77.10 ppm) or  $\text{DMSO-}d_6$  (39.50).  $^{19}\text{F}$  NMR spectra were recorded on a Bruker AVANCE III 500 spectrometer. The *N*-alkoxy benzamides<sup>[S1-S5]</sup> and cyclopropenes<sup>[S6-S10]</sup> were prepared according to published procedures.

## 2. Supplementary Methods

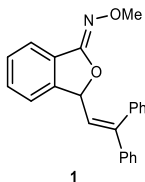
### 2.1 Synthesis of isobenzofuranone *O*-alkyl oximes.



**General procedure I:** To a 25 mL reaction tube equipped with a magnetic stir bar was added *N*-alkoxy benzamide (1.0 equiv), cyclopropene (1.5 equiv),  $[\text{Cp}^*\text{RhCl}_2]_2$  (5 mol%),  $\text{AgOAc}$  (2 equiv), and  $\text{MeOH}$  (0.1 M) successively. After being stirred at room temperature for indicated time, the reaction was complete as monitored by TLC. The mixture was filtered through a short pad of silica gel, washed with ethyl acetate, and

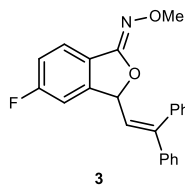
concentrated in vacuo to afford corresponding isobenzofuranone *O*-alkyl oxime via flash chromatography on silica gel.

**(1) (Z)-3-(2,2-Diphenylvinyl)isobenzofuran-1(3H)-one *O*-methyl oxime (1) (GFY-3-19, GFY-3-37).**



Following General Procedure I, after being stirred overnight, **1** was afforded as a white solid (0.2 mmol scale, 58.9 mg, 86%), eluent (0-7% of ethyl acetate in petroleum ether): m.p.= 139.3-140.9 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.68 (d, *J* = 7.6 Hz, 1H), 7.49 - 7.45 (m, 1H), 7.44 - 7.42 (m, 2H), 7.41 - 7.36 (m, 4H), 7.33 - 7.30 (m, 1H), 7.27 (d, *J* = 1.3 Hz, 5H), 6.12 (d, *J* = 9.9 Hz, 1H), 5.99 (d, *J* = 9.9 Hz, 1H), 3.96 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 156.07, 147.82, 144.01, 140.72, 138.16, 130.90, 129.91, 128.91, 128.54, 128.41, 128.29, 128.23, 128.06, 127.73, 123.58, 122.18, 121.70, 84.18, 62.72; HRMS calcd for C<sub>23</sub>H<sub>19</sub>NNaO<sub>2</sub><sup>+</sup> ([M+Na]<sup>+</sup>): 364.1308; found: 364.1315.

**(2) (Z)-3-(2,2-Diphenylvinyl)isobenzofuran-1(3H)-one *O*-methyl oxime (3) (GFY-3-49).**

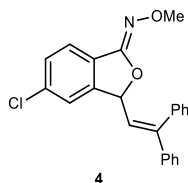


Following General Procedure I, after being stirred overnight, **3** was afforded as a white solid (0.2 mmol scale, 47.9 mg, 67%), eluent (0-6% of ethyl acetate in petroleum ether): m.p.= 140.0-149.9 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.65 (dd, *J* = 8.5, 4.8 Hz, 1H), 7.49 - 7.41 (m, 2H), 7.43 - 7.37 (m, 1H), 7.40 - 7.34 (m, 2H), 7.32 - 7.26 (m, 5H), 7.11 (td, *J* = 8.7, 2.3 Hz, 1H), 6.99 (dd, *J* = 7.8, 2.3 Hz, 1H), 6.08 (d, *J* = 9.9 Hz, 1H), 5.97 (d, *J* = 9.9 Hz, 1H), 3.95 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.59 (d, *J* = 251.9 Hz), 155.09, 148.49, 146.35 (d, *J* = 8.9 Hz), 140.50,

137.97, 129.83, 128.64, 128.46, 128.29, 128.20, 127.74, 124.37, 123.57 (d,  $J = 9.5$  Hz), 122.83, 116.90 (d,  $J = 23.9$  Hz), 109.51 (d,  $J = 24.4$  Hz) 83.64, 62.77.  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -108.21; HRMS calcd for  $\text{C}_{23}\text{H}_{19}\text{FNO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 360.1394; found: 360.1400.

**(3) (Z)-5-Chloro-3-(2,2-diphenylvinyl)isobenzofuran-1(3H)-one O-methyl oxime**

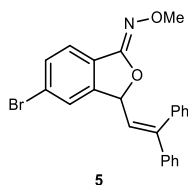
**(4) (GFY-3-50).**



Following General Procedure I, after being stirred overnight, **4** was afforded as a white solid (0.2 mmol scale, 38.2 mg, 51%), eluent (0-7% of ethyl acetate in petroleum ether): m.p.= 43.8-45.5 °C (ethyl acetate/petroleum ether);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60 (d,  $J = 8.3$  Hz, 1H), 7.47 - 7.43 (m, 2H), 7.41 - 7.35 (m, 4H), 7.31 - 7.27 (m, 6H), 6.08 (d,  $J = 9.9$  Hz, 1H), 5.96 (d,  $J = 9.9$  Hz, 1H), 3.95 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.05, 148.63, 145.66, 140.48, 137.93, 137.06, 129.84, 129.54, 128.64, 128.49, 128.29, 128.22, 127.76, 127.06, 122.83, 122.69, 122.57, 83.67, 62.83; HRMS calcd for  $\text{C}_{23}\text{H}_{19}^{35}\text{ClNO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 376.1099; found: 376.1106.

**(4) (Z)-5-Bromo-3-(2,2-diphenylvinyl)isobenzofuran-1(3H)-one O-methyl oxime**

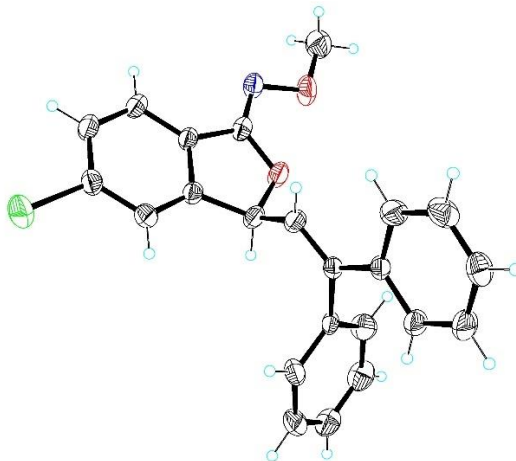
**(5) (GFY-4-4, GFY-10-39).**



Following General Procedure I, after being stirred overnight, **5** was afforded as a white solid (0.2 mmol scale, 58.3 mg, 68%), eluent (0-15% of ethyl acetate in petroleum ether): m.p.= 59.3-61.7 °C (ethyl acetate/petroleum ether);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.53 (s, 2H), 7.46 - 7.43(m, 3H), 7.41 - 7.35 (m, 3H), 7.30 - 7.22 (m, 5H), 6.09 (d,  $J = 10.0$  Hz, 1H), 5.96 (d,  $J = 9.9$  Hz, 1H), 3.95 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.08, 148.67, 145.87, 140.47, 137.92, 132.33, 129.83, 128.62, 128.47, 128.27,

128.20, 127.75, 127.58, 125.52, 125.16, 123.02, 122.67, 83.59, 62.80; HRMS calcd for  $C_{23}H_{18}^{79}BrNNaO_2^+$  ( $[M+Na]^+$ ): 442.0413; found: 442.0409.

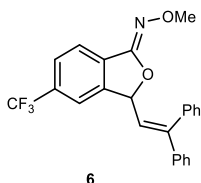
**Crystal data and structure refinement of 5:**



Bond precision:	C-C = 0.0055 Å	Wavelength=1.54178	
Cell:	a=11.6213(7)	b=16.4338(11)	c=11.4359(8)
	alpha=90	beta=115.688(3)	gamma=90
Temperature:	300 K		
	Calculated	Reported	
Volume	1968.2(2)	1968.2(2)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C <sub>23</sub> H <sub>18</sub> Br N O <sub>2</sub>	C <sub>23</sub> H <sub>18</sub> Br N O <sub>2</sub>	
Sum formula	C <sub>23</sub> H <sub>18</sub> Br N O <sub>2</sub>	C <sub>23</sub> H <sub>18</sub> Br N O <sub>2</sub>	
Mr	420.28	420.29	
Dx,g cm <sup>-3</sup>	1.418	1.418	
Z	4	4	
Mu (mm <sup>-1</sup> )	2.979	2.979	
F000	856.0	856.0	
F000'	855.37		
h,k,lmax	14,20,14	14,20,14	
Nref	3880	3829	

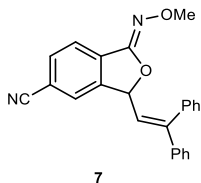
Tmin,Tmax            0.545,0.585            0.864,0.864  
 Tmin'                 0.495  
 Correction method= # Reported T Limits: Tmin=0.864 Tmax=0.864  
 AbsCorr = MULTI-SCAN  
 Data completeness= 0.987            Theta(max)= 72.271  
 R(reflections)= 0.0897( 3292)            wR2(reflections)= 0.2464( 3829)  
 S = 1.054                                Npar= 244

**(5) (Z)-3-(2,2-Diphenylvinyl)-5-(trifluoromethyl)isobenzofuran-1(3H)-one O-methyl oxime (6) (GFY-3-31, GFY-3-44).**



Following General Procedure I, after being stirred overnight, **6** was afforded as a white solid (0.2 mmol scale, 47.2 mg, 58%), eluent (0-7% of ethyl acetate in petroleum ether): m.p.= 49.7-50.5 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.78 (d, *J* = 8.1 Hz, 1H), 7.68 (d, *J* = 8.6 Hz, 1H), 7.52 (s, 1H), 7.46 (t, *J* = 7.1 Hz, 2H), 7.43 - 7.37 (m, 3H), 7.32 - 7.27 (m, 5H), 6.17 (d, *J* = 9.9 Hz, 1H), 5.98 (d, *J* = 9.9 Hz, 1H), 3.98 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 154.65, 149.11, 144.44, 140.39, 137.85, 132.95 (q, *J* = 32.6 Hz), 132.06, 129.83, 128.66, 128.57, 128.30, 128.28, 127.78, 126.26, 123.60 (q, *J* = 273.3 Hz), 122.31, 122.65, 119.45 (q, *J* = 3.9 Hz). 84.10, 62.96; <sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) δ -62.33; HRMS calcd for C<sub>24</sub>H<sub>19</sub>F<sub>3</sub>NO<sub>2</sub><sup>+</sup> ([M+H]<sup>+</sup>): 410.1362; found: 410.1372.

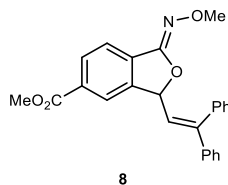
**(6) (Z)-3-(2,2-Diphenylvinyl)-1-(methoxyimino)-1,3-dihydroisobenzofuran-5-carbonitrile (7) (GFY-7-44).**





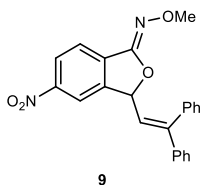
Following General Procedure I, after being stirred overnight, **7** was afforded as a white solid (0.2 mmol scale, 48.6 mg, 67%), eluent (0-17% of ethyl acetate in petroleum ether): m.p.= 175.3-176.1 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.78 (d, *J* = 8.3 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.60 (s, 1H), 7.51 - 7.45 (m, 2H), 7.44 - 7.42 (m, 1H), 7.40 - 7.36 (m, 2H), 7.32 - 7.29 (m, 3H), 7.28 - 7.25 (m, 2H), 6.16 (d, *J* = 9.9 Hz, 1H), 5.96 (d, *J* = 9.9 Hz, 1H), 3.99 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 154.23, 149.36, 144.52, 140.22, 137.73, 132.85, 132.75, 129.72, 128.70, 128.64, 128.34, 128.31, 127.73, 126.30, 122.49, 121.92, 117.98, 114.32, 83.97, 63.04; HRMS calcd for C<sub>24</sub>H<sub>19</sub>N<sub>2</sub>O<sub>2</sub><sup>+</sup> ([M+H]<sup>+</sup>): 367.1441; found: 367.1447.

**(7) Methyl (Z)-3-(2,2-diphenylvinyl)-1-(methoxyimino)-1,3-dihydroisobenzofuran-5-carboxylate (8) (GFY-7-34).**



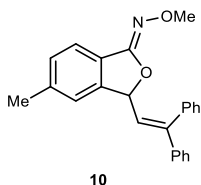
Following General Procedure I, after being stirred overnight, **8** was afforded as a white solid (0.2 mmol scale, 61.5 mg, 76%), eluent (0-15% of ethyl acetate in petroleum ether): m.p.= 62.4-62.7 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.10 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.97 (s, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.49 - 7.43 (m, 2H), 7.43 - 7.37 (m, 3H), 7.28 (s, 5H), 6.16 (d, *J* = 10.0 Hz, 1H), 5.97 (d, *J* = 10.0 Hz, 1H), 3.98 (s, 3H), 3.95 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 166.09, 155.08, 148.76, 144.14, 140.56, 137.96, 132.74, 132.56, 130.40, 129.91, 128.58, 128.44, 128.25, 128.18, 127.78, 123.59, 122.71, 121.62, 84.11, 62.92, 52.49; HRMS calcd for C<sub>25</sub>H<sub>22</sub>NO<sub>4</sub><sup>+</sup> ([M+H]<sup>+</sup>): 400.1543; found: 400.1550.

**(8) (Z)-3-(2,2-Diphenylvinyl)-5-nitroisobenzofuran-1(3H)-one O-methyl oxime (9) (GFY-12-25).**



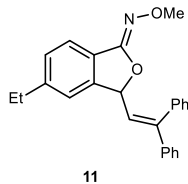
Following General Procedure I, after being stirred 2 h, **9** was afforded as an oil (0.2 mmol scale, 45.9 mg, 59%), eluent (0-7% of ethyl acetate in petroleum ether);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.31 (dd,  $J = 8.5, 2.0$  Hz, 1H), 8.18 - 8.14 (m, 1H), 7.83 (d,  $J = 8.5$  Hz, 1H), 7.53 - 7.47 (m, 2H), 7.46 - 7.42 (m, 3H), 7.34 - 7.27 (m, 5H), 6.22 (d,  $J = 9.9$  Hz, 1H), 6.00 (d,  $J = 9.9$  Hz, 1H), 4.01 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  153.88, 149.71, 149.66, 145.09, 140.24, 137.74, 134.48, 129.79, 128.73, 128.69, 128.39, 128.33, 127.82, 127.78, 124.70, 122.54, 121.75, 118.02, 83.95, 63.14; HRMS calcd for  $\text{C}_{25}\text{H}_{22}\text{NO}_4^+$  ( $[\text{M}+\text{H}]^+$ ): 400.1543; found: 400.1550.

**(9) (Z)-3-(2,2-Diphenylvinyl)-5-methylisobenzofuran-1(3H)-one O-methyl oxime**  
**(10) (GFY-4-5).**



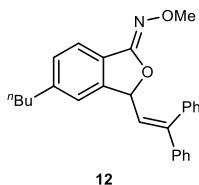
Following General Procedure I, after being stirred overnight, **10** was afforded as a white solid (0.2 mmol scale, 55.9 mg, 78%), eluent (0-6% of ethyl acetate in petroleum ether): m.p. = 44.5-46.5 °C (ethyl acetate/petroleum ether);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57 (d,  $J = 7.9$  Hz, 1H), 7.48 - 7.41 (m, 2H), 7.40 (dt,  $J = 7.8, 2.3$  Hz, 3H), 7.28 (s, 5H), 7.23 - 7.20 (m, 1H), 7.10 (s, 1H), 6.08 (d,  $J = 9.9$  Hz, 1H), 5.98 (d,  $J = 9.9$  Hz, 1H), 3.96 (s, 3H), 2.43 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.18, 147.69, 144.41, 141.51, 140.75, 138.16, 129.98, 129.91, 128.49, 128.23, 128.19, 128.01, 127.71, 125.74, 123.70, 122.47, 121.43, 83.88, 62.60, 21.71; HRMS calcd for  $\text{C}_{24}\text{H}_{22}\text{NO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 356.1645; found: 356.1654.

**(10) (Z)-3-(2,2-Diphenylvinyl)-5-ethylisobenzofuran-1(3H)-one O-methyl oxime**  
**(11) (GFY-4-7).**



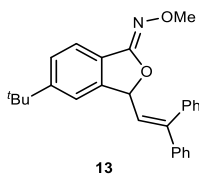
Following General Procedure I, after being stirred overnight, **11** was afforded as an oil (0.2 mmol scale, 65.5 mg, 85%), eluent (0-3% of ethyl acetate in petroleum ether):  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J = 7.9$  Hz, 1H), 7.50 - 7.43 (m, 2H), 7.44 - 7.37 (m, 3H), 7.29 (d,  $J = 10.2$  Hz, 6H), 7.12 (d,  $J = 1.4$  Hz, 1H), 6.11 (d,  $J = 9.9$  Hz, 1H), 6.01 (d,  $J = 9.9$  Hz, 1H), 3.97 (s, 3H), 2.74 (q,  $J = 7.6$  Hz, 2H), 1.28 (t,  $J = 7.6$  Hz, 3H);  $^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.24, 147.94, 147.71, 144.46, 140.79, 138.18, 129.95, 128.91, 128.52, 128.26, 128.22, 128.04, 127.75, 125.94, 123.74, 121.56, 121.29, 83.97, 62.65, 29.08, 15.49; HRMS calcd for  $\text{C}_{25}\text{H}_{24}\text{NO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 370.1802; found: 370.1810.

**(11) (Z)-5-Butyl-3-(2,2-diphenylvinyl)isobenzofuran-1(3H)-one O-methyl oxime**  
**(12) (GFY-4-12).**



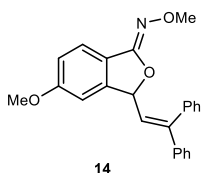
Following General Procedure I, after being stirred overnight, **12** was afforded as an oil (0.2 mmol scale, 62.3 mg, 78%), eluent (0-7% of ethyl acetate in petroleum ether):  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 (d,  $J = 7.9$  Hz, 1H), 7.49 - 7.43 (m, 2H), 7.42 - 7.37 (m, 3H), 7.28 (s, 5H), 7.23 (dd,  $J = 7.9, 1.5$  Hz, 1H), 7.09 (s, 1H), 6.09 (d,  $J = 9.9$  Hz, 1H), 6.00 (d,  $J = 10.0$  Hz, 1H), 3.96 (s, 3H), 2.72 - 2.65 (m, 2H), 1.67 - 1.57 (m, 2H), 1.43 - 1.34 (m, 2H), 0.95 (t,  $J = 7.3$  Hz, 3H);  $^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.21, 147.70, 146.64, 144.38, 140.79, 138.17, 129.94, 129.37, 128.49, 128.23, 128.19, 128.01, 127.74, 125.91, 123.73, 121.76, 121.44, 83.93, 62.61, 35.84, 33.52, 22.34, 13.86; HRMS calcd for  $\text{C}_{27}\text{H}_{28}\text{NO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 398.2115; found: 398.2120.

**(12) (Z)-5-(tert-Butyl)-3-(2,2-diphenylvinyl)isobenzofuran-1(3H)-one O-methyl oxime (13) (GFY-4-14).**



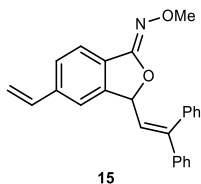
Following General Procedure I, after being stirred overnight, **13** was afforded as a white solid (0.2 mmol scale, 54.5 mg, 68%), eluent (0-15% of ethyl acetate in petroleum ether): m.p.= 46.2-48.2 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.61 (d, *J* = 8.2 Hz, 1H), 7.49 - 7.42 (m, 3H), 7.44 - 7.36 (m, 3H), 7.40 - 7.25 (m, 6H), 6.10 (d, *J* = 9.9 Hz, 1H), 6.02 (d, *J* = 9.9 Hz, 1H), 3.96 (s, 3H), 1.35 (s, 9H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 156.22, 154.93, 147.59, 144.20, 140.76, 138.24, 129.94, 128.54, 128.25, 128.22, 128.03, 126.58, 125.63, 123.88, 121.25, 118.50, 84.16, 62.64, 35.21, 31.30; HRMS calcd for C<sub>27</sub>H<sub>28</sub>NO<sub>2</sub><sup>+</sup> ([M+H]<sup>+</sup>): 398.2115; found: 398.2120.

**(13) (Z)-3-(2,2-Diphenylvinyl)-5-methoxyisobenzofuran-1(3H)-one O-methyl oxime (14) (GFY-4-6, GFY-8-15).**



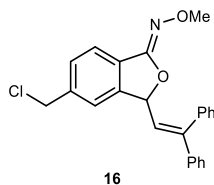
Following General Procedure I, after being stirred for 2 h, **14** was afforded as a white solid (0.2 mmol scale, 50.3 mg, 67%), eluent (0-14% of ethyl acetate in petroleum ether): m.p.= 51.8-62.9 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.59 (d, *J* = 8.5 Hz, 1H), 7.47 - 7.41 (m, 2H), 7.41 - 7.36 (m, 3H), 7.29 - 7.26 (m, 5H), 6.94 (dd, *J* = 8.5, 2.3 Hz, 1H), 6.75 (d, *J* = 2.2 Hz, 1H), 6.06 (d, *J* = 9.9 Hz, 1H), 5.99 (d, *J* = 9.9 Hz, 1H), 3.94 (s, 3H), 3.85 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 162.29, 156.04, 147.85, 146.21, 140.71, 138.15, 129.91, 128.56, 128.31, 128.24, 128.08, 127.74, 123.60, 122.96, 120.64, 115.71, 106.80, 83.67, 62.61, 55.68; HRMS calcd for C<sub>24</sub>H<sub>22</sub>NO<sub>3</sub><sup>+</sup> ([M+H]<sup>+</sup>): 372.1594; found: 372.1604.

**(14) (Z)-3-(2,2-Diphenylvinyl)-5-vinylisobenzofuran-1(3H)-one O-methyl oxime (15) (GFY-3-43, GFY-3-30, GFY-10-42).**



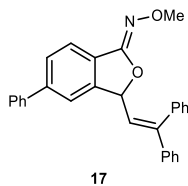
Following General Procedure I, after being stirred overnight, **15** was afforded as a white solid (0.2 mmol scale, 46.2 mg, 63%), eluent (0-6% of ethyl acetate in petroleum ether): m.p.= 59.2-61.9 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.63 (d, *J* = 8.0 Hz, 1H), 7.49 - 7.43 (m, 3H), 7.40 (d, *J* = 7.1 Hz, 3H), 7.29 - 7.25 (m, 6H), 6.75 (dd, *J* = 17.6, 10.9 Hz, 1H), 6.11 (d, *J* = 9.9 Hz, 1H), 5.99 (d, *J* = 9.9 Hz, 1H), 5.83 (d, *J* = 17.5 Hz, 1H), 5.37 (d, *J* = 10.9 Hz, 1H), 3.96 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 155.90, 148.02, 144.63, 140.70, 140.55, 138.12, 135.92, 129.94, 128.56, 128.34, 128.25, 128.21, 128.11, 127.77, 127.12, 123.45, 121.80, 119.71, 116.09, 83.97, 62.75; HRMS calcd for C<sub>25</sub>H<sub>21</sub>NNaO<sub>2</sub><sup>+</sup> ([M+Na]<sup>+</sup>): 390.1465; found: 390.1457.

**(15) (Z)-5-(Chloromethyl)-3-(2,2-diphenylvinyl)isobenzofuran-1(3H)-one O-methyl oxime (16) (GFY-7-35).**



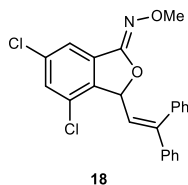
Following General Procedure I, after being stirred overnight, **16** was afforded as a white solid (0.2 mmol scale, 67.8 mg, 87%), eluent (0-10% of ethyl acetate in petroleum ether): m.p.= 55.8-56.3 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.67 (d, *J* = 8.0 Hz, 1H), 7.50 - 7.42 (m, 3H), 7.41 - 7.38 (m, 3H), 7.33 - 7.25 (m, 6H), 6.12 (d, *J* = 9.9 Hz, 1H), 5.98 (d, *J* = 10.0 Hz, 1H), 4.63 (s, 2H), 3.97 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 155.47, 148.32, 144.63, 140.58, 140.55, 138.01, 129.87, 129.51, 128.64, 128.57, 128.38, 128.24, 128.13, 127.74, 123.08, 122.21, 122.04, 83.96, 62.76, 45.50; HRMS calcd for C<sub>24</sub>H<sub>20</sub><sup>35</sup>ClNNaO<sub>2</sub><sup>+</sup> ([M+Na]<sup>+</sup>): 412.1075; found: 412.1082.

**(16) (Z)-3-(2,2-Diphenylvinyl)-5-phenylisobenzofuran-1(3H)-one O-methyl oxime (17) (GFY-4-13, GFY-9-37).**



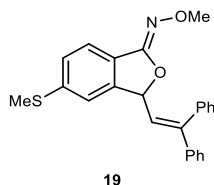
Following General Procedure I, after being stirred for 2 h, **17** was afforded as a white solid (0.2 mmol scale, 51.7 mg, 62%), eluent (0-9% of ethyl acetate in petroleum ether): m.p.= 56.4-59.2 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.74 (d, *J* = 8.0 Hz, 1H), 7.64 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.61 - 7.57 (m, 2H), 7.50 - 7.45 (m, 4H), 7.44 (s, 1H), 7.43 - 7.38 (m, 4H), 7.28 (s, 5H), 6.18 (d, *J* = 10.0 Hz, 1H), 6.05 (d, *J* = 10.0 Hz, 1H), 3.99 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 155.93, 148.11, 144.86, 144.40, 140.71, 140.15, 138.15, 129.96, 128.97, 128.57, 128.34, 128.30, 128.24, 128.11, 128.08, 127.79, 127.37, 127.33, 123.49, 122.02, 120.70, 84.13, 62.77; HRMS calcd for C<sub>29</sub>H<sub>23</sub>NNaO<sub>2</sub><sup>+</sup> ([M+Na]<sup>+</sup>): 440.1621; found: 440.1630.

**(17) (Z)-4,6-Dichloro-3-(2,2-diphenylvinyl)isobenzofuran-1(3H)-one O-methyl oxime (18) (GFY-4-27, GFY-11-46).**



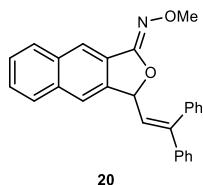
Following General Procedure I, after being stirred overnight, **18** was afforded as a white solid (0.2 mmol scale, 56.0 mg, 68%), eluent (0-4% of ethyl acetate in petroleum ether): m.p.= 143.7-146.3 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.56 (d, *J* = 1.7 Hz, 1H), 7.45 - 7.42 (m, 4H), 7.41 - 7.34 (m, 2H), 7.29 - 7.27 (m, 2H), 7.25 - 7.23 (m, 2H), 6.09 (d, *J* = 10.2 Hz, 1H), 5.84 (d, *J* = 10.4 Hz, 1H), 3.95 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 153.98, 150.30, 141.15, 139.72, 138.20, 136.07, 132.18, 131.10, 129.94, 129.67, 128.48, 128.46, 128.22, 128.14, 127.92, 120.87, 120.27, 84.06, 63.01; HRMS calcd for C<sub>23</sub>H<sub>18</sub><sup>35</sup>Cl<sub>2</sub>NO<sub>2</sub><sup>+</sup> ([M+H]<sup>+</sup>): 410.0709; found: 410.0711.

**(18) (Z)-3-(2,2-Diphenylvinyl)-5-(methylthio)isobenzofuran-1(3H)-one O-methyl oxime (19) (GFY-4-34, GFY-9-1).**



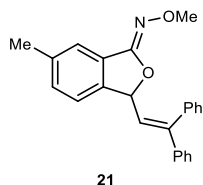
Following General Procedure I, after being stirred for 2 h, **19** was afforded as an oil (0.2 mmol scale, 34.8 mg, 44%), eluent (0-18% of ethyl acetate in petroleum ether):  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 (d,  $J = 8.1$  Hz, 1H), 7.50 - 7.43 (m, 2H), 7.43 - 7.38 (m, 3H), 7.31 - 7.24 (m, 6H), 7.12 (s, 1H), 6.10 (d,  $J = 9.9$  Hz, 1H), 6.01 (d,  $J = 9.9$  Hz, 1H), 3.97 (s, 3H), 2.54 (s, 3H);  $^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.78, 148.03, 144.85, 143.03, 140.61, 138.09, 129.88, 128.57, 128.34, 128.23, 128.10, 127.72, 126.54, 125.12, 123.34, 121.84, 119.02, 83.76, 62.68, 15.46; HRMS calcd for  $\text{C}_{24}\text{H}_{21}\text{NNaO}_2\text{S}^+$  ( $[\text{M}+\text{Na}]^+$ ): 410.1185; found: 410.1194.

**(19) (Z)-3-(2,2-Diphenylvinyl)naphtho[2,3-*c*]furan-1(3*H*)-one O-methyl oxime (20) (GFY-4-37).**



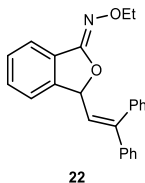
Following General Procedure I, after being stirred overnight, **20** was afforded as a white solid (0.2 mmol scale, 57.2 mg, 73%), eluent (0-18% of ethyl acetate in petroleum ether): m.p. = 142.4-144.1 °C (ethyl acetate/petroleum ether);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 (s, 1H), 7.91 (d,  $J = 7.9$  Hz, 1H), 7.86 (d,  $J = 7.0$  Hz, 1H), 7.72 (s, 1H), 7.57 - 7.49 (m, 2H), 7.47 (d,  $J = 4.4$  Hz, 4H), 7.43 - 7.38 (m, 1H), 7.31 - 7.26 (m, 5H), 6.26 (d,  $J = 10.0$  Hz, 1H), 6.07 (d,  $J = 9.9$  Hz, 1H), 4.01 (s, 3H);  $^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.58, 147.82, 140.78, 140.36, 138.18, 134.69, 133.40, 129.99, 128.92, 128.55, 128.29, 128.23, 128.11, 128.07, 127.78, 127.44, 126.72, 126.50, 123.85, 121.26, 121.03, 83.73, 62.81; HRMS calcd for  $\text{C}_{27}\text{H}_{22}\text{NO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 392.1645; found: 392.1651.

**(20) (Z)-3-(2,2-Diphenylvinyl)-6-methylisobenzofuran-1(3*H*)-one O-methyl oxime (21) (GFY-4-29).**



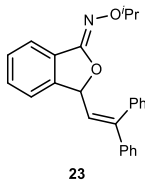
Following General Procedure I, after being stirred overnight, **21** was afforded as a white solid (0.2 mmol scale, 63.2 mg, 88%), eluent (0-15% of ethyl acetate in petroleum ether): m.p.= 123.2-125.6 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.51 (s, 1H), 7.46 - 7.40 (m, 2H), 7.39 (d, *J* = 7.1 Hz, 3H), 7.29 (s, 5H), 7.20 (d, *J* = 7.8 Hz, 1H), 6.09 (d, *J* = 9.9 Hz, 1H), 5.97 (d, *J* = 9.9 Hz, 1H), 3.97 (s, 3H), 2.41 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 156.10, 147.55, 141.35, 140.76, 139.04, 138.18, 131.98, 129.89, 128.53, 128.47, 128.19, 128.18, 127.99, 127.69, 123.83, 121.83, 121.80, 84.07, 62.65, 21.16; HRMS calcd for C<sub>24</sub>H<sub>22</sub>NO<sub>2</sub><sup>+</sup> ([M+H]<sup>+</sup>): 356.1645; found: 356.1655.

**(21) (Z)-3-(2,2-Diphenylvinyl)isobenzofuran-1(3H)-one O-ethyl oxime (22) (GFY-7-40).**



Following General Procedure I, after being stirred overnight, **22** was afforded as an oil (0.2 mmol scale, 48.3 mg, 68%), eluent (0-5% of ethyl acetate in petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.69 (d, *J* = 7.6 Hz, 1H), 7.48 - 7.42 (m, 3H), 7.42 - 7.37 (m, 4H), 7.34 - 7.30 (m, 1H), 7.28 (s, 5H), 6.14 (d, *J* = 9.9 Hz, 1H), 6.00 (d, *J* = 9.9 Hz, 1H), 4.25 - 4.16 (m, 2H), 1.39 (t, *J* = 7.1 Hz, 6H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 155.72, 147.38, 143.89, 140.75, 138.17, 130.72, 129.88, 128.81, 128.66, 128.49, 128.21, 128.19, 128.01, 127.69, 123.85, 122.13, 121.66, 84.02, 70.34, 14.58; HRMS calcd for C<sub>24</sub>H<sub>22</sub>NO<sub>2</sub><sup>+</sup> ([M+H]<sup>+</sup>): 356.1645; found: 356.1655.

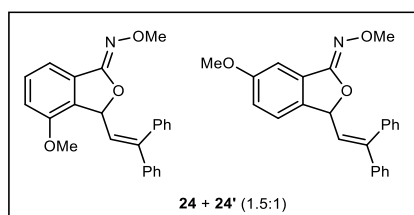
**(22) (Z)-3-(2,2-Diphenylvinyl)isobenzofuran-1(3H)-one O-isopropyl oxime (23) (GFY-11-26).**





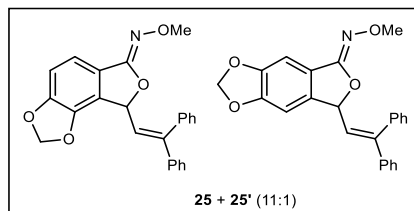
Following General Procedure I, after being stirred for 2h, **23** was afforded as an oil (0.2 mmol scale, 34.3 mg, 45%), eluent (0-7% of ethyl acetate in petroleum ether);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (dd,  $J = 7.6, 1.1$  Hz, 1H), 7.47 - 7.41 (m, 3H), 7.40 - 7.35 (m, 4H), 7.31 (dd,  $J = 7.6, 1.0$  Hz, 1H), 7.27 (s, 5H), 6.13 (d,  $J = 9.9$  Hz, 1H), 6.00 (d,  $J = 9.8$  Hz, 1H), 4.39 - 4.30 (m,  $J = 6.2$  Hz, 1H), 1.37 - 1.34 (m,  $J = 8.7$ , 6H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.22, 146.95, 143.82, 140.86, 138.25, 130.57, 129.92, 129.02, 128.76, 128.50, 128.21, 128.18, 128.00, 127.72, 124.23, 122.13, 121.65, 83.92, 76.17, 21.57, 21.54; HRMS calcd for  $\text{C}_{25}\text{H}_{23}\text{NNaO}_2^+$  ( $[\text{M}+\text{Na}]^+$ ): 392.1621; found: 392.1621.

**(23) (Z)-3-(2,2-Diphenylvinyl)-4-methoxyisobenzofuran-1(3H)-one O-methyl oxime (24) and (Z)-3-(2,2-diphenylvinyl)-6-methoxyisobenzofuran-1(3H)-one O-methyl oxime (24') (GFY-4-50).**



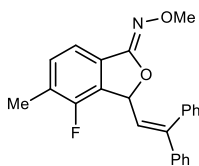
Following General Procedure I, after being stirred overnight, a mixture of **24** and **24'** was afforded as a white solid (0.2 mmol scale, 55.7 mg, 73%; **24:24'** = 1.5: 1), eluent (0-20% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.46 - 7.44 (m, 2H), 7.43 - 7.40 (m, 2H), 7.43 - 7.36 (m, 4.34H), 7.39 - 7.33 (m, 3H), 7.29 - 7.23 (m, 7H), 7.19 (d,  $J = 8.4$  Hz, 1H), 7.13 - 7.11 (m, 0.67H), 7.03 (dd,  $J = 8.4, 2.4$  Hz, 0.67H), 6.90 (d,  $J = 8.0$  Hz, 1H), 6.17 (d,  $J = 10.1$  Hz, 1H), 6.06 (d,  $J = 9.8$  Hz, 0.67H), 5.95 (d,  $J = 9.7$  Hz, 0.67H), 5.89 (d,  $J = 10.0$  Hz, 1H), 3.96 (s, 2H), 3.95 (s, 3H), 3.84 (s, 5H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  160.55, 156.30, 154.60, 147.55, 147.36, 141.43, 140.79, 138.63, 138.21, 136.41, 131.70, 130.83, 130.36, 130.20, 129.91, 129.72, 128.52, 128.24, 128.22, 128.15, 128.11, 128.02, 128.00, 127.86, 127.72, 123.94, 123.04, 122.95, 119.76, 113.61, 112.19, 104.14, 83.98, 83.24, 62.70, 55.72, 55.41; HRMS calcd for  $\text{C}_{24}\text{H}_{22}\text{NO}_3^+$  ( $[\text{M}+\text{H}]^+$ ): 372.1594; found: 372.1591.

**(24) (Z)-8-(2,2-Diphenylvinyl)-[1,3]dioxolo[4,5-*e*]isobenzofuran-6(8*H*)-one *O*-methyl oxime (25) and (Z)-7-(2,2-diphenylvinyl)-[1,3]dioxolo[4,5-*f*]isobenzofuran-5(7*H*)-one *O*-methyl oxime (25') (GFY-4-21).**



Following General Procedure I, after being stirred overnight, a mixture of **25** and **25'** was afforded as a white solid (0.2 mmol scale, 38.8 mg, 50%; **25:25'** = 11: 1), eluent (0-9% of ethyl acetate in petroleum ether): <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.44 - 7.40 (m, 4.36H), 7.39 - 7.36 (m, 1.08H), 7.28 (s, 5.45H), 7.22 (d, *J* = 8.1 Hz, 1.08H), 7.03 (s, 0.08H), 6.88 (d, *J* = 8.1 Hz, 1H), 6.67 (s, 0.08H), 6.12 (d, *J* = 10.2 Hz, 1H), 6.10 (d, *J* = 1.4 Hz, 1H), 6.07 (d, *J* = 1.4 Hz, 1H), 6.05 (d, *J* = 1.2 Hz, 0.09H), 6.04 (d, *J* = 1.3 Hz, 0.09H), 5.96 (d, *J* = 10.1 Hz, 1.18H), 3.93 (s, 3.27H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 155.51, 150.18, 148.11, 141.56, 140.94, 138.21, 130.22, 128.29, 128.26, 128.20, 127.98, 127.94, 124.33, 123.59, 122.12, 115.54, 109.74, 102.25, 81.26, 62.66; HRMS calcd for C<sub>24</sub>H<sub>20</sub>NO<sub>4</sub><sup>+</sup> ([M+H]<sup>+</sup>): 386.1387; found: 386.1394.

**(25) (Z)-3-(2,2-Diphenylvinyl)isobenzofuran-1(3*H*)-one *O*-ethyl oxime (26) and (Z)-3-(2,2-diphenyl vinyl)-4-fluoro-5-methylisobenzofuran-1(3*H*)-one *O*-methyl oxime (26') (GFY-4-35, GFY-7-15).**

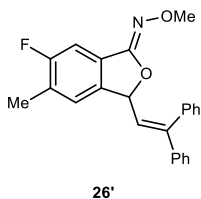


**26**

Following General Procedure I on 0.2 mmol scale, after being stirred overnight, **26** (44.1 mg, 59%) and **26'** (6.4 mg, 9%.) were afforded via flash chromatography on silica gel (0-6% of ethyl acetate in petroleum ether):

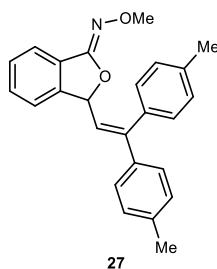
**26:** more polar product; white solid; m.p.= 149.6-150.1 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.43 (d, *J* = 4.4 Hz, 4H), 7.40 - 7.34 (m, 2H), 7.28 (s, 5H), 7.24 (dd, *J* = 12.3, 5.0 Hz, 1H), 6.19 (s, 1H), 5.96 (d, *J* =

10.1 Hz, 1H), 3.95 (s, 3H), 2.33 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.53 (d,  $J = 249.2$  Hz), 155.29, 148.31, 140.92, 138.23, 133.05 (d,  $J = 4.0$  Hz), 130.11 (d,  $J = 18.3$  Hz), 129.99 (d,  $J = 2.0$  Hz), 129.23 (d,  $J = 4.5$  Hz), 128.36, 128.25, 128.18, 127.94, 127.833 (d,  $J = 15.9$  Hz), 127.827, 122.07, 117.01 (d,  $J = 4.4$  Hz), 82.09 (d,  $J = 2.1$  Hz), 62.75, 14.44 (d,  $J = 3.4$  Hz);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -122.71; HRMS calcd for  $\text{C}_{24}\text{H}_{21}\text{FNO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 374.1551; found: 374.1558.



**26'**: less polar product; oil;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.44 (dd,  $J = 7.8, 6.5$  Hz, 2H), 7.39 - 7.35 (m, 3H), 7.31 - 7.25 (m, 6H), 7.08 (d,  $J = 6.4$  Hz, 1H), 6.05 (d,  $J = 9.9$  Hz, 1H), 5.95 (d,  $J = 10.0$  Hz, 1H), 3.94 (s, 3H), 2.33 (d,  $J = 2.2$  Hz, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  161.78 (d,  $J = 247.0$  Hz), 155.37, 148.01, 140.69, 139.43 (d,  $J = 2.6$  Hz), 138.11, 129.90, 129.09 (d,  $J = 19.5$  Hz), 128.57, 128.37, 128.27, 128.13, 127.75, 124.69 (d,  $J = 5.8$  Hz), 123.49, 107.91 (d,  $J = 26.2$  Hz), 83.82, 62.76, 29.69, 15.25 (d,  $J = 4.0$  Hz);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -115.92; HRMS calcd for  $\text{C}_{24}\text{H}_{21}\text{FNO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 374.1551; found: 374.1557.

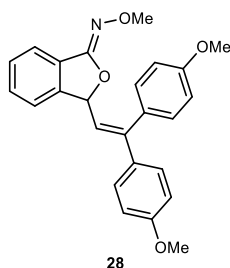
**(26) (Z)-3-(2,2-Di-*p*-tolylvinyl)isobenzofuran-1(3*H*)-one O-methyl oxime (27) (GFY-5-18).**



Following General Procedure I, after being stirred overnight, **27** was afforded as a white solid (0.2 mmol scale, 54.0 mg, 72%), eluent (0-9% of ethyl acetate in petroleum ether): m.p.= 130.1-132.2 °C (ethyl acetate/petroleum ether);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 (d,  $J = 7.7$  Hz, 1H), 7.50 - 7.40 (m, 1H), 7.39 (t,  $J = 7.5$  Hz, 1H), 7.32 -

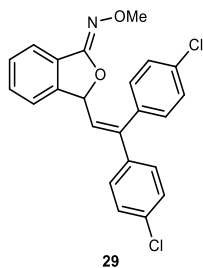
7.26 (m, 3H), 7.24 (d,  $J = 7.9$  Hz, 2H), 7.17 (d,  $J = 8.2$  Hz, 2H), 7.08 (d,  $J = 8.0$  Hz, 2H), 6.14 (d,  $J = 9.9$  Hz, 1H), 5.93 (d,  $J = 9.9$  Hz, 1H), 3.97 (s, 3H), 2.40 (s, 3H), 2.33 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.13, 147.77, 144.20, 138.15, 138.12, 137.74, 135.34, 130.83, 129.80, 129.80, 129.66, 129.35, 129.13, 128.99, 128.87, 128.78, 127.65, 127.34, 122.43, 122.18, 121.62, 84.42, 62.65, 21.20, 21.08; HRMS calcd for  $\text{C}_{25}\text{H}_{24}\text{NO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 370.1802; found: 370.1810.

**(27) (Z)-3-(2,2-Bis(4-methoxyphenyl)vinyl)isobenzofuran-1(3H)-one O-methyl oxime (28) (GFY-10-3, GFY-10-20).**



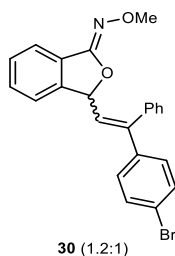
Following General Procedure I, after being stirred for 2 h, **28** was afforded as an oil (0.2 mmol scale, 58.2 mg, 72%), eluent (0-15% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (d,  $J = 7.6$  Hz, 1H), 7.49 - 7.43 (m, 1H), 7.40 (t,  $J = 7.5$  Hz, 1H), 7.34 - 7.28 (m, 3H), 7.28 - 7.17 (m, 2H), 6.96 (dd,  $J = 8.6, 1.7$  Hz, 2H), 6.83 - 6.77 (m, 2H), 6.13 (d,  $J = 9.9$  Hz, 1H), 5.84 (d,  $J = 9.9$  Hz, 1H), 3.96 (s, 3H), 3.84 (s, 3H), 3.79 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.76, 145.66, 143.50, 138.81, 136.08, 134.55, 134.49, 131.22, 130.99, 129.10, 128.98, 128.95, 128.55, 128.42, 124.54, 121.98, 121.84, 83.68, 77.25, 62.75; HRMS calcd for  $\text{C}_{25}\text{H}_{23}\text{NNaO}_4^+$  ( $[\text{M}+\text{Na}]^+$ ): 424.1519; found: 424.1519.

**(28) (Z)-3-(2,2-Bis(4-chlorophenyl)vinyl)isobenzofuran-1(3H)-one O-methyl oxime (29) (GFY-10-11).**



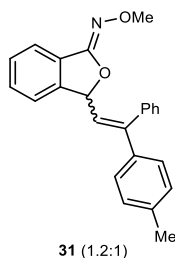
Following General Procedure I, after being stirred for 2 h, **29** was afforded as an oil (0.2 mmol scale, 32.2 mg, 40%), eluent (0-7% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 7.8$  Hz, 1H), 7.50 (td,  $J = 7.5, 1.2$  Hz, 1H), 7.45 (d,  $J = 8.3$  Hz, 3H), 7.40 - 7.31 (m, 2H), 7.31 - 7.25 (m, 3H), 7.22 - 7.15 (m, 2H), 6.07 (d,  $J = 9.9$  Hz, 1H), 5.99 (d,  $J = 9.9$  Hz, 1H), 3.98 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.76, 145.66, 143.50, 138.81, 136.08, 134.55, 134.49, 131.22, 130.99, 129.10, 128.98, 128.95, 128.55, 128.42, 124.54, 121.98, 121.84, 83.68, 77.25, 62.75; HRMS calcd for  $\text{C}_{23}\text{H}_{17}^{35}\text{Cl}_2\text{NNaO}_2^+$  ( $[\text{M}+\text{Na}]^+$ ): 432.0529; found: 432.0526.

**(29) 3-(2-(4-Bromophenyl)-2-phenylvinyl)isobenzofuran-1(3H)-one O-methyl oxime (30) (GFY-5-38).**



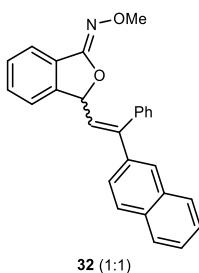
Following General Procedure I, after being stirred overnight, **30** was afforded as an oil (0.2 mmol scale, 62.5 mg, 74%, stereoisomers ratio = 1.2:1), eluent (0-9% of ethyl acetate in petroleum ether):  $\delta$  7.70 - 7.66 (m, 1.11H), 7.58 (d,  $J = 8.1$  Hz, 1.11H), 7.49 - 7.46 (m, 1.11H), 7.44 - 7.41 (m, 2.22H), 7.40 - 7.35 (m, 2.22H), 7.31 - 7.25 (m, 4.44H), 7.24 - 7.22 (m, 1.11H), 7.13 (d,  $J = 8.3$  Hz, 1.11H), 6.11 - 6.02 (m, 1.11H), 6.00 - 5.96 (m, 1.11H), 3.96 (s, 3.33H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.93, 155.89, 146.81, 146.75, 143.75, 143.72, 140.26, 139.69, 137.61, 137.08, 131.81, 131.61, 131.41, 130.96, 129.84, 129.30, 129.03, 129.01, 128.70, 128.55, 128.43, 128.35, 128.33, 127.71, 124.09, 122.55, 122.39, 122.12, 122.04, 121.80, 121.78, 83.89, 62.76, 29.04, 11.41; HRMS calcd for  $\text{C}_{23}\text{H}_{18}^{79}\text{BrNNaO}_2^+$  ( $[\text{M}+\text{Na}]^+$ ): 442.0413; found: 442.0422.

**(30) 3-(2-Phenyl-2-(p-tolyl)vinyl)isobenzofuran-1(3H)-one O-methyl oxime (31) (GFY-9-40).**



Following General Procedure I, after being stirred for 2 h, **31** was afforded as an oil (0.2 mmol scale, 64.2 mg, 91%, stereoisomers ratio = 1.2:1), eluent (0-9% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 7.6$  Hz, 1.84H), 7.52 - 7.43 (m, 5.52H), 7.48 - 7.37 (m, 3.68H), 7.34 (d,  $J = 7.7$  Hz, 2H), 7.30 (d,  $J = 4.6$  Hz, 5.52H), 7.27 (d,  $J = 8.0$  Hz, 2.68H), 7.19 (d,  $J = 8.3$  Hz, 2H), 7.11 (d,  $J = 8.1$  Hz, 2.52H), 6.18 (d,  $J = 9.9$  Hz, 0.84H), 6.13 (d,  $J = 10.0$  Hz, 1H), 5.99 (d,  $J = 2.7$  Hz, 1H), 5.97 (d,  $J = 2.6$  Hz, 0.84H), 4.00 (s, 5.52H), 2.42 (s, 2.52H), 2.35 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.08, 147.87, 147.72, 144.10, 140.96, 138.32, 138.24, 137.87, 137.85, 135.18, 130.85, 129.88, 129.80, 129.18, 128.92, 128.83, 128.47, 128.40, 128.19, 128.16, 127.96, 127.75, 127.60, 123.36, 122.64, 122.16, 121.65, 84.29, 84.27, 62.67, 21.20, 21.08; HRMS calcd for  $\text{C}_{24}\text{H}_{21}\text{NNaO}_2^+$  ( $[\text{M}+\text{Na}]^+$ ): 378.1465; found: 378.1469.

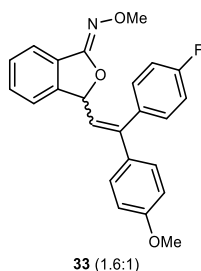
**(31) 3-(2-(Naphthalen-2-yl)-2-phenylvinyl)isobenzofuran-1(3H)-one O-methyl oxime (32) (GFY-10-21).**



Following General Procedure I, after being stirred for 2 h, **32** was afforded as a white solid (0.2 mmol scale, 59.7 mg, 78%, stereoisomers ratio = 1:1), eluent (0-7% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.93 (s, 1H), 7.90 - 7.86 (m, 3H), 7.80 - 7.76 (m, 1H), 7.74 (d,  $J = 8.7$  Hz, 1H), 7.72 - 7.67 (m, 3H), 7.62 (s, 1H), 7.55 - 7.50 (m, 2H), 7.49 - 7.44 (m, 5H), 7.44 - 7.38 (m, 8H), 7.35 (d,  $J = 7.7$  Hz, 2H), 7.31 - 7.24 (m, 5H), 6.19 (d,  $J = 5.5$  Hz, 1H), 6.17 (d,  $J = 5.8$  Hz, 1H), 6.13

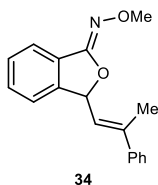
(d,  $J = 9.9$  Hz, 1H), 6.07 (d,  $J = 9.9$  Hz, 1H), 3.98 (s, 3H), 3.97 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.04, 147.74, 147.63, 143.98, 143.93, 140.61, 138.13, 138.00, 135.59, 133.07, 132.83, 130.90, 129.97, 128.90, 128.81, 128.59, 128.42, 128.33, 128.30, 128.28, 128.25, 128.13, 128.11, 127.83, 127.77, 127.70, 127.57, 127.46, 126.49, 126.44, 126.35, 126.24, 125.04, 123.99, 123.97, 122.18, 122.09, 121.71, 84.20, 62.69; HRMS calcd for  $\text{C}_{27}\text{H}_{21}\text{NNaO}_2^+$  ( $[\text{M}+\text{Na}]^+$ ): 414.1465; found: 414.1465.

**(32) 3-(2-(4-Fluorophenyl)-2-(4-methoxyphenyl)vinyl)isobenzofuran-1(3H)-one O-methyl oxime (33) (GFY-10-19, GFY-10-27).**



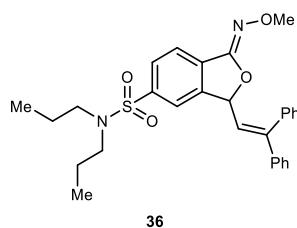
Following General Procedure I, after being stirred for 2 h, **33** was afforded as an oil (0.2 mmol scale, 60.8 mg, 80%, stereoisomers ratio = 1.6:1), eluent (0-6% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (d,  $J = 7.6$  Hz, 1.63H), 7.48 - 7.45 (m, 1.63H), 7.42 - 7.39 (m, 1.63H), 7.38 - 7.35 (m, 1.89H), 7.31 - 7.28 (m, 2.63H), 7.26 (d,  $J = 5.1$  Hz, 0.63H), 7.24 - 7.22 (m, 1H), 7.17 (d,  $J = 8.5$  Hz, 2H), 7.14 - 7.11 (m, 1.89H), 6.97 - 6.94 (m, 2.63H), 6.82 - 6.79 (m, 2H), 6.15 (d,  $J = 9.9$  Hz, 0.63H), 6.05 (d,  $J = 9.9$  Hz, 1H), 5.90 (d,  $J = 10.0$  Hz, 1H), 5.86 (d,  $J = 9.9$  Hz, 0.63H), 3.96 (s, 4.89H), 3.84 (s, 1.89H), 3.79 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  163.71, 163.45, 161.74, 161.48, 159.84, 159.53, 155.99, 155.95, 146.76, 146.52, 144.02, 143.98, 137.35, 137.32, 134.28, 134.25, 133.09, 131.65, 131.58, 131.10, 130.87, 130.15, 129.56, 129.49, 128.93, 128.88, 128.40, 123.05, 122.07, 122.02, 121.68, 115.58, 115.41, 115.14, 114.97, 113.97, 113.62, 84.20, 76.75, 62.65, 55.21;  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -113.61, -113.66; HRMS calcd for  $\text{C}_{24}\text{H}_{20}\text{FNNaO}_3^+$  ( $[\text{M}+\text{Na}]^+$ ): 412.1319; found: 412.1314.

**(33) (Z)-3-((E)-2-Phenylprop-1-en-1-yl)isobenzofuran-1(3H)-one O-methyl oxime (34) (GFY-6-12/GFY-9-9).**



Following General Procedure I, after being stirred for 2 h, **34** was afforded as a white solid (0.2 mmol scale, 22.6 mg, 32%), eluent (0-8% of ethyl acetate in petroleum ether): m.p.= 120.4-120.9 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.70 (d, *J* = 7.6 Hz, 1H), 7.47 (td, *J* = 7.5, 1.2 Hz, 1H), 7.44 - 7.39 (m, 3H), 7.34 - 7.30 (m, 2H), 7.30 - 7.26 (m, 2H), 6.48 (d, *J* = 9.3 Hz, 1H), 5.74 (dd, *J* = 9.3, 1.4 Hz, 1H), 3.97 (s, 3H), 2.35 (d, *J* = 1.5 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 156.19, 144.26, 141.95, 141.76, 130.95, 128.86, 128.37, 128.29, 127.90, 125.98, 123.40, 121.89, 121.67, 83.11, 62.68, 16.66; HRMS calcd for C<sub>18</sub>H<sub>18</sub>NO<sub>2</sub><sup>+</sup> ([M+H]<sup>+</sup>): 280.1332; found: 280.1338.

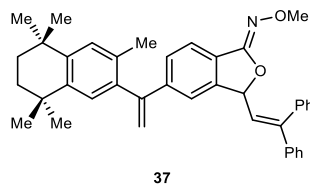
**(34)**                    **(Z)-3-(2,2-Diphenylvinyl)-1-(methoxyimino)-*N,N*-dipropyl-1,3-dihydroisobenzofuran-5-sulfonamide (36) (GFY-6-18).**



Following General Procedure I, after being stirred overnight, **36** was afforded as a white solid (0.2 mmol scale, 72.2 mg, 71%), eluent (0-21% of ethyl acetate in petroleum ether): m.p.= 130.1-132.2 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.84 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.73 (s, 1H), 7.49 - 7.42 (m, 2H), 7.43 - 7.38 (m, 3H), 7.31 - 7.24 (m, 3H), 7.28 - 7.21 (m, 2H), 6.17 (d, *J* = 9.9 Hz, 1H), 5.96 (d, *J* = 9.9 Hz, 1H), 3.97 (s, 3H), 3.11 (q, *J* = 7.3 Hz, 4H), 1.55 (q, *J* = 7.5 Hz, 4H), 0.87 (t, *J* = 7.3 Hz, 6H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 154.47, 149.25, 144.66, 142.97, 140.42, 137.86, 132.20, 129.86, 128.61, 128.54, 128.25, 127.76, 127.67, 122.29, 122.25, 121.15, 84.10, 62.94, 49.78, 21.81, 11.09; HRMS calcd for C<sub>29</sub>H<sub>33</sub>N<sub>2</sub>O<sub>4</sub>S<sup>+</sup> ([M+H]<sup>+</sup>): 505.2156; found: 505.2165.

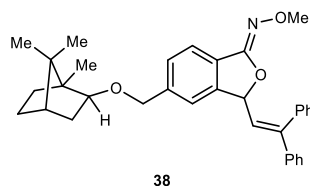


(35) **(Z)-3-(2,2-Diphenylvinyl)-5-(1-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-yl)vinyl)isobenzofuran-1(3H)-one O-methyl oxime (37)** (GFY-6-21).



Following General Procedure I, after being stirred overnight, **37** was afforded as an oil (0.1 mmol scale, 20.8 mg, 36%, dr = 1:1), eluent (0-11% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.58 (d,  $J$  = 8.1 Hz, 1H), 7.41 - 7.32 (m, 4H), 7.27 - 7.25 (m, 3H), 7.23 - 7.20 (m,  $J$  = 7.3, 4.5, 2.9 Hz, 4H), 7.10 (s, 3H), 6.02 (d,  $J$  = 9.7 Hz, 1H), 5.96 (d,  $J$  = 9.7 Hz, 1H), 5.81 (d,  $J$  = 1.3 Hz, 1H), 5.31 (d,  $J$  = 1.3 Hz, 1H), 3.95 (s, 3H), 1.97 (s, 3H), 1.68 (s, 4H), 1.30 (s, 3H), 1.27 (s, 6H), 1.21 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.01, 148.75, 147.35, 144.41, 144.40, 144.06, 142.39, 140.66, 138.22, 138.01, 132.70, 129.79, 128.51, 128.21, 128.06, 128.03, 127.94, 127.61, 127.39, 127.32, 123.90, 121.46, 120.19, 116.18, 84.07, 62.71, 35.19, 35.15, 33.98, 33.86, 31.92, 31.87, 31.85, 19.90; HRMS calcd for  $\text{C}_{40}\text{H}_{42}\text{NO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 568.3210; found: 568.3220.

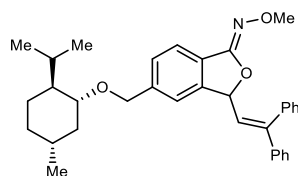
(36) **(Z)-3-(2,2-diphenylvinyl)-5-(((1S,2S,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)methyl)isobenzofuran-1(3H)-one O-methyl oxime (38)** (GFY-12-50, WYQ-6-1).



Following General Procedure I, after being stirred for 2 h, **38** was afforded as an oil (0.1 mmol scale, 32.0 mg, 46%, dr = 1:1), eluent (0-7% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J$  = 8.2 Hz, 1H),  $\delta$  7.45 - 7.41 (m, 2H), 7.40 - 7.35 (m, 4H), 7.31 (d,  $J$  = 7.0 Hz, 2H), 7.27 (s, 5H), 6.08 (d,  $J$  = 9.9 Hz, 1H), 5.97 (d,  $J$  = 9.9 Hz, 1H), 4.60 (dd,  $J$  = 13.2, 5.8 Hz, 1H), 4.43 (dd,  $J$  = 13.2, 6.3 Hz, 1H), 3.95

(s, 3H), 3.33 (dd,  $J = 7.6, 3.6$  Hz, 1H), 1.87 - 1.82 (m, 1H), 1.74 - 1.67 (m, 2H), 1.67 - 1.58 (m, 2H), 1.56 (s, 3H), 1.53 - 1.48 (m, 1H), 1.06 (d,  $J = 2.4$  Hz, 3H), 0.97 (d,  $J = 2.3$  Hz, 3H), 0.83 (d,  $J = 2.1$  Hz, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.14, 147.60, 144.30, 143.45, 140.82, 138.27, 129.89, 128.54, 128.23, 128.02, 127.73, 127.47, 127.17, 123.84, 121.42, 120.31, 87.08, 84.17, 84.14, 70.16, 62.67, 49.43, 46.53, 45.11, 38.45, 34.40, 27.26, 20.29, 20.23, 11.98; HRMS calcd for  $\text{C}_{34}\text{H}_{38}\text{NO}_3^+$  ( $[\text{M}+\text{H}]^+$ ): 508.2846; found: 508.2856.

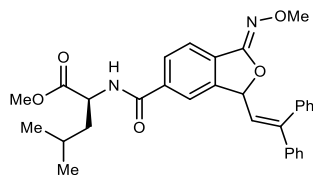
**(37)** (Z)-3-(2,2-Diphenylvinyl)-5-((((1R,2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)methyl)isobenzofuran-1(3H)-one O-methyl oxime (**39**) (GFY-7-50).



39

Following General Procedure I, after being stirred overnight, **39** was afforded as an oil (0.1 mmol scale, 31.8 mg, 61%, dr = 1:1), eluent (0-6% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.64 (d,  $J = 7.9$  Hz, 1H), 7.43 (d,  $J = 7.0$  Hz, 2H), 7.41 - 7.35 (m, 3H), 7.34 (d,  $J = 9.6$  Hz, 2H), 7.27 (s, 5H), 6.10 (dd,  $J = 9.9, 2.7$  Hz, 1H), 5.97 (dd,  $J = 10.0, 3.1$  Hz, 1H), 4.73 (dd,  $J = 12.1, 6.9$  Hz, 1H), 4.45 (dd,  $J = 12.1, 5.3$  Hz, 1H), 3.96 (s, 3H), 3.22 - 3.17 (m, 1H), 2.33 - 2.25 (m, 1H), 2.21 - 2.17 (m, 1H), 1.68 - 1.62 (m, 3H), 1.44 - 1.24 (m, 3H), 0.98 - 0.92 (m, 3H), 0.91 (d,  $J = 2.6$  Hz, 2H), 0.89 (d,  $J = 2.7$  Hz, 1H), 0.86 (t,  $J = 2.5$  Hz, 1H), 0.72 (t,  $J = 6.8$  Hz, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.03, 147.77, 144.35, 142.80, 140.74, 138.16, 129.87, 128.51, 128.29, 128.24, 128.20, 128.03, 127.71, 123.59, 121.54, 121.16, 121.07, 84.06, 79.39, 69.79, 62.67, 48.25, 40.26, 34.45, 31.50, 25.69, 25.66, 23.24, 22.31, 20.94; HRMS calcd for  $\text{C}_{34}\text{H}_{40}\text{NO}_3^+$  ( $[\text{M}+\text{H}]^+$ ): 510.3003; found: 510.3013.

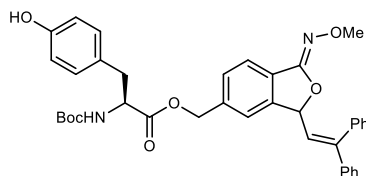
**(38)** Methyl ((Z)-3-(2,2-diphenylvinyl)-1-(methoxyimino)-1,3-dihydroisobenzofuran-5-carbonyl)-L-leucinate (**40**) (GFY-8-18).



40

Following General Procedure I, after being stirred for 2 h, **40** was afforded as a white solid (0.1 mmol scale, 36.7 mg, 71%, dr = 1:1), eluent (0-25% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  7.82 - 7.75 (m, 1H), 7.74 - 7.69 (m, 1H), 7.45 - 7.42 (m, 2H), 7.40 - 7.38 (m, 3H), 7.28 - 7.72 (s, 4H), 6.67 (s, 1H), 6.15 - 6.12 (m, 1H), 5.96 - 5.92 (m, 1H), 4.88 - 4.83 (m, 1H), 3.97 (s, 3H), 3.77 (s, 3H), 1.81 - 1.66 (m, 1H), 1.00 - 0.97 (m, 5H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  173.48, 166.13, 155.10, 148.79, 148.73, 144.54, 140.51, 137.92, 136.44, 131.65, 129.87, 128.57, 128.41, 128.21, 128.15, 127.75, 127.36, 122.62, 121.81, 121.75, 84.14, 62.85, 52.45, 51.29, 41.72, 24.95, 22.75, 21.98; HRMS calcd for  $\text{C}_{31}\text{H}_{33}\text{N}_2\text{O}_5^+$  ( $[\text{M}+\text{H}]^+$ ): 513.2384; found: 513.2392.

**(39) ((Z)-3-(2,2-Diphenylvinyl)-1-(methoxyimino)-1,3-dihydroisobenzofuran-5-yl)methyl (tert-butoxycarbonyl)-L-tyrosinate (41) (GFY-8-37).**

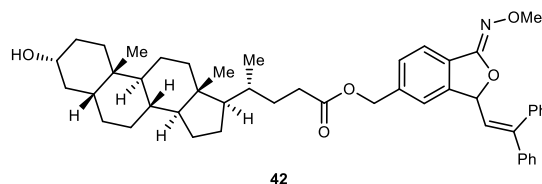


41

Following General Procedure I, after being stirred for 2 h, **41** was afforded as a white solid (0.1 mmol scale, 41.2 mg, 67%, dr = 1:1), eluent (0-40% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 (d,  $J$  = 7.9 Hz, 1H), 7.46 - 7.43 (m, 2H), 7.42 - 7.39 (m, 3H), 7.30 - 7.27 (m, 6H), 7.22 (d,  $J$  = 5.9 Hz, 1H), 6.87 (d,  $J$  = 8.0 Hz, 2H), 6.62 (dd,  $J$  = 8.7, 6.9 Hz, 2H), 6.13 (dd,  $J$  = 9.9, 2.1 Hz, 1H), 5.97 (dd,  $J$  = 9.9, 3.9 Hz, 1H), 5.21 (d,  $J$  = 12.6 Hz, 1H), 5.11 (dd,  $J$  = 12.6, 4.3 Hz, 1H), 5.00 (dd,  $J$  = 8.3, 4.3 Hz, 1H), 4.57 (q,  $J$  = 6.9 Hz, 1H), 3.98 (s, 3H), 3.01 - 2.96 (m, 1H), 1.80 (s, 1H), 1.41 (s, 9H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  171.86, 155.86, 155.13, 148.42, 144.51, 140.63, 138.04, 130.32, 129.93, 129.31, 128.62, 128.42, 128.28, 128.18, 127.81, 127.79, 127.31, 123.08, 122.07, 121.97, 115.42, 84.13, 80.15, 77.20, 66.31,

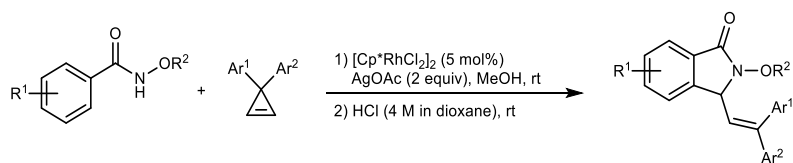
66.27, 62.74, 54.65, 37.49, 28.26; HRMS calcd for  $C_{38}H_{38}N_2NaO_7^+$  ( $[M+Na]^+$ ):657.2571; found: 657.2577.

**(40)** ((*Z*)-3-(2,2-Diphenylvinyl)-1-(methoxyimino)-1,3-dihydroisobenzofuran-5-yl)methyl **(4R)**-4-((*3R,5R,8R,9S,10S,13R,14S,17R*)-3-hydroxy-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)pentanoate **(42)** (GFY-8-5, GFY-8-17, GFY-10-43).



Following General Procedure I, after being stirred for 2 h, **42** was afforded as an oil (0.1 mmol scale, 32.3 mg, 45%, dr = 1:1), eluent (0-37% of ethyl acetate in petroleum ether):  $^1H$  NMR (500 MHz,  $CDCl_3$ ) (d,  $J = 7.9$  Hz, 1H), 7.47 - 7.41 (m, 2H), 7.42 - 7.34 (m, 5H), 7.30 - 7.25 (m, 5H), 6.11 (d,  $J = 9.9$  Hz, 1H), 5.97 (d,  $J = 9.9$  Hz, 1H), 5.15 (t,  $J = 4.0$  Hz, 2H), 3.96 (s, 3H), 3.63 (td,  $J = 10.8, 5.3$  Hz, 1H), 2.41 (td,  $J = 10.0, 4.7$  Hz, 1H), 2.34 - 2.24 (m, 1H), 1.95 - 1.89 (m, 2H), 1.88 - 1.77 (m, 6H), 1.76 - 1.66 (m, 2H), 1.56 - 1.46 (m, 3H), 1.44 - 1.30 (m, 10H), 1.28 - 1.18 (m, 6H), 1.12 - 1.04 (m, 4H), 1.03 - 0.95 (m, 4H), 0.93 - 0.87 (m, 6H), 0.59 (s, 3H);  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  173.91, 155.70, 148.18, 144.48, 140.65, 139.46, 138.07, 129.91, 128.90, 128.66, 128.57, 128.37, 128.25, 128.13, 127.75, 123.25, 121.90, 121.70, 84.05, 71.83, 65.40, 62.75, 56.43, 55.84, 42.69, 42.04, 40.38, 40.10, 36.41, 35.79, 35.30, 35.27, 34.53, 31.17, 30.93, 30.50, 28.15, 27.15, 26.37, 24.14, 23.34, 20.77, 18.23, 11.98; HRMS calcd for  $C_{48}H_{59}NNaO_5^+$  ( $[M+Na]^+$ ): 752.4285; found: 752.4290.

## 2.2 Synthesis of *N*-alkoxy isoindolinones.

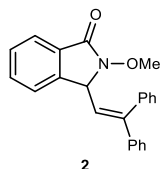


**General Procedure II:** To a 25 mL reaction tube equipped with a magnetic stir bar was added *N*-alkoxy benzamide (1.0 equiv), cyclopropene (1.5 equiv),  $[Cp^*RhCl_2]_2$

(5 mol%), AgOAc (2 equiv), and MeOH (0.1 M) successively. After being stirred at room temperature for 2 h, the reaction was complete as monitored by TLC. The mixture was filtered through a short pad of silica gel, washed with ethyl acetate, and concentrated in vacuo to afford a crude mixture.

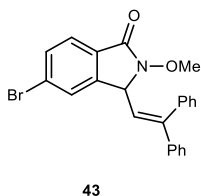
To the above mixture was added HCl (4 M in dioxane) with a syringe to make a 0.05 M solution (concentration corresponding to *N*-alkoxy benzamide). After being stirred overnight at room temperature, the isomerization was complete as monitored by TLC. The resulting mixture was quenched with saturated NaHCO<sub>3</sub> solution (5 mL), extracted with ethyl acetate (5 mL × 3), washed with brine (5 mL), dried over anhydrous MgSO<sub>4</sub>, filtered, and concentrated. The residue was purified by column chromatography on silica gel to afford corresponding *N*-alkoxy isoindolinone.

**(1) 3-(2,2-Diphenylvinyl)-2-methoxyisoindolin-1-one (2) (GFY-8-7).**



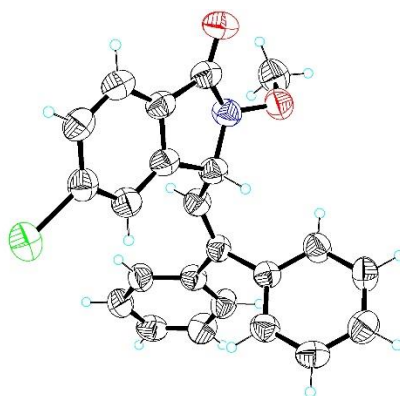
Following General Procedure II, **2** was afforded as an oil (0.2 mmol scale, 64.5 mg, 94%), eluent (0-15% of ethyl acetate in petroleum ether): <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.85 (d, *J* = 7.6 Hz, 1H), 7.57 (td, *J* = 7.5, 1.2 Hz, 1H), 7.51 - 7.46 (m, 3H), 7.44 - 7.39 (m, 3H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.29 - 7.26 (m, 5H), 5.89 (d, *J* = 10.1 Hz, 1H), 5.33 (d, *J* = 10.0 Hz, 1H), 3.95 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.83, 148.60, 141.84, 140.63, 138.32, 132.27, 129.73, 129.59, 128.70, 128.67, 128.30, 128.21, 127.95, 127.38, 123.77, 123.08, 64.33, 60.01; HRMS calcd for C<sub>23</sub>H<sub>20</sub>NO<sub>2</sub><sup>+</sup> ([M+H]<sup>+</sup>): 342.1489; found: 342.1498.

**(2) 5-Bromo-3-(2,2-diphenylvinyl)-2-methoxyisoindolin-1-one (43) (GFY-7-49, GFY-6-39-3).**



Following General Procedure II, **43** was afforded as a white solid (0.2 mmol scale, 65.9 mg, 78%), eluent (0-16% of ethyl acetate in petroleum ether): m.p.= 72.8-73.0 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.70 (d, *J* = 8.1 Hz, 1H), 7.62 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.50 - 7.47 (m, 3H), 7.43 - 7.39 (m, 3H), 7.33 - 7.30 (m, 4H), 7.29 (d, *J* = 3.8 Hz, 1H), 5.86 (d, *J* = 10.0 Hz, 1H), 5.30 (d, *J* = 10.0 Hz, 1H), 3.94 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 163.97, 149.44, 143.59, 140.36, 138.07, 132.19, 129.67, 128.80, 128.54, 128.42, 128.36, 128.11, 127.42, 126.96, 126.43, 125.31, 122.00, 64.45, 59.70; HRMS calcd for C<sub>23</sub>H<sub>18</sub><sup>79</sup>BrNNaO<sub>2</sub><sup>+</sup> ([M+Na]<sup>+</sup>): 442.0414; found: 442.0418.

### Crystal data and structure refinement of **43**:



Bond precision:	C-C = 0.0084 Å	Wavelength=1.54178	
Cell:	a=11.00000	b=13.97200	c=15.42300
	alpha=73.4700	beta=72.0400	gamma=84.3400
Temperature:	300 K		
	Calculated	Reported	
Volume	2161.541	2162	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C <sub>23</sub> H <sub>18</sub> Br N O <sub>2</sub> [+ solvent]	C <sub>23</sub> H <sub>18</sub> Br N O <sub>2</sub>	
Sum formula	C <sub>23</sub> H <sub>18</sub> Br N O <sub>2</sub> [+ solvent]	C <sub>23</sub> H <sub>18</sub> Br N O <sub>2</sub>	
Mr	420.28	420.29	
Dx,g cm <sup>-3</sup>	1.291	1.291	

Z	4	4
Mu (mm-1)	2.713	2.713
F000	856.0	856.0
F000'	855.37	
h,k,lmax	13,16,18	0,0,0
Nref	7609	7504
Tmin,Tmax	0.758,0.805	0.864,0.864
Tmin'	0.688	

Correction method= # Reported T Limits: Tmin=0.864 Tmax=0.864

AbsCorr = MULTI-SCAN

Data completeness= 0.986

Theta(max)= 66.453

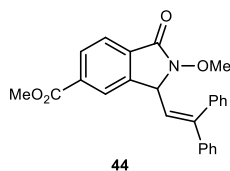
R(reflections)= 0.0898( 4846)

wR2(reflections)= 0.2935( 7504)

S = 1.065

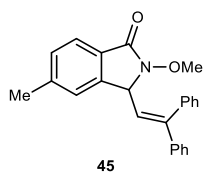
Npar= 488

**(3) Methyl 3-(2,2-diphenylvinyl)-2-methoxy-1-oxoisindoline-5-carboxylate (44) (GFY-8-20).**



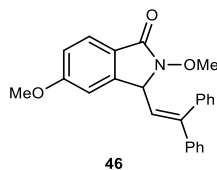
Following General Procedure II, **44** was afforded as a white solid (0.2 mmol scale, 70.4 mg, 89%), eluent (0-20% of ethyl acetate in petroleum ether): m.p.= 64.2-64.5 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.16 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.01 (s, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.53 - 7.46 (m, 2H), 7.48 - 7.40 (m, 3H), 7.33 - 7.25 (m, 5H), 5.86 (d, *J* = 10.0 Hz, 1H), 5.38 (d, *J* = 10.0 Hz, 1H), 3.96 (s, 3H), 3.95 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 166.12, 163.44, 149.56, 141.85, 140.43, 138.13, 133.73, 133.72, 130.09, 129.76, 128.79, 128.41, 128.37, 128.10, 127.44, 124.41, 123.83, 121.95, 77.26, 64.44, 60.00, 52.56; HRMS calcd for C<sub>25</sub>H<sub>22</sub>NO<sub>4</sub><sup>+</sup> ([M+H]<sup>+</sup>): 400.1543; found: 400.1552.

**(4) 3-(2,2-Diphenylvinyl)-2-methoxy-5-methylisindolin-1-one (45) (GFY-8-3).**



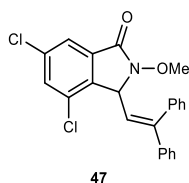
Following General Procedure II, **45** was afforded as a white solid (0.2 mmol scale, 56.7 mg, 80%), eluent (0-7% of ethyl acetate in petroleum ether): m.p.= 136.3-136.7 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.73 (d, *J* = 7.7 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.45 - 7.39 (m, 3H), 7.32 - 7.24 (m, 6H), 7.14 (s, 1H), 5.89 (d, *J* = 10.0 Hz, 1H), 5.28 (d, *J* = 10.0 Hz, 1H), 3.93 (s, 3H), 2.45 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 165.27, 148.40, 143.14, 142.23, 140.72, 138.36, 129.79, 129.68, 128.70, 128.32, 128.20, 127.94, 127.42, 126.90, 123.69, 123.52, 123.35, 64.36, 59.98, 22.00; HRMS calcd for C<sub>24</sub>H<sub>22</sub>NO<sub>2</sub><sup>+</sup> ([M+H]<sup>+</sup>): 356.1645; found: 356.1654.

**(5) 3-(2,2-Diphenylvinyl)-2,5-dimethoxyisoindolin-1-one (46) (GFY-8-8).**



Following General Procedure II, **46** was afforded as a white solid (0.2 mmol scale, 62.3 mg, 85%), eluent (0-30% of ethyl acetate in petroleum ether): m.p.= 148.0-148.4 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.76 (d, *J* = 8.4 Hz, 1H), 7.50 - 7.44 (m, 2H), 7.44 - 7.37 (m, 3H), 7.32 - 7.27 (m, 5H), 6.98 (dd, *J* = 8.5, 2.3 Hz, 1H), 6.81 (d, *J* = 2.2 Hz, 1H), 5.92 (d, *J* = 10.0 Hz, 1H), 3.93 (s, 3H), 3.86 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 165.56, 163.38, 148.44, 144.24, 140.70, 138.34, 129.75, 128.72, 128.33, 128.23, 127.97, 127.42, 125.47, 123.37, 121.83, 114.76, 108.41, 64.42, 60.14, 55.64; HRMS calcd for C<sub>24</sub>H<sub>22</sub>NO<sub>3</sub> ([M+H]<sup>+</sup>): 372.1594; found: 372.1603.

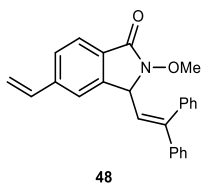
**(6) 4,6-Dichloro-3-(2,2-diphenylvinyl)-2-methoxyisoindolin-1-one (47) (GFY-8-12).**





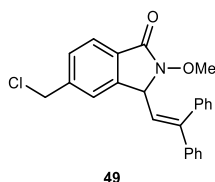
Following General Procedure II, **47** was afforded as an oil (0.2 mmol scale, 50.8 mg, 61%), eluent (0-11% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,  $J = 1.9$  Hz, 1H), 7.52 (d,  $J = 1.9$  Hz, 1H), 7.49 - 7.40 (m, 5H), 7.34 - 7.28 (m, 3H), 7.28 - 7.23 (m, 2H), 5.68 (d,  $J = 10.1$  Hz, 1H), 5.36 (d,  $J = 10.1$  Hz, 1H), 3.94 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  161.64, 150.56, 140.87, 138.46, 137.25, 135.81, 133.27, 132.57, 130.63, 129.72, 128.54, 128.39, 128.33, 128.03, 127.55, 122.56, 119.62, 64.52, 59.17; HRMS calcd for  $\text{C}_{23}\text{H}_{17}^{35}\text{Cl}_2\text{NNaO}_2^+$  ( $[\text{M}+\text{Na}]^+$ ): 432.0529; found: 432.0536.

**(7) 3-(2,2-Diphenylvinyl)-2-methoxy-5-vinylisindolin-1-one (48) (GFY-8-11).**



Following General Procedure II, **48** was afforded as a white solid (0.2 mmol scale, 59.6 mg, 84%), eluent (0-20% of ethyl acetate in petroleum ether): m.p.= 90.2-91.1 °C (ethyl acetate/petroleum ether);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 (d,  $J = 7.8$  Hz, 1H), 7.54 - 7.46 (m, 3H), 7.45 - 7.40 (m, 3H), 7.34 - 7.32 (m, 1H), 7.30 (s, 4H), 6.77 (dd,  $J = 17.6, 10.9$  Hz, 1H), 5.91 (d,  $J = 10.0$  Hz, 1H), 5.85 (d,  $J = 17.5$  Hz, 1H), 5.39 (d,  $J = 10.9$  Hz, 1H), 5.33 (d,  $J = 10.0$  Hz, 1H), 3.94 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.76, 148.71, 142.40, 141.82, 140.61, 138.30, 136.02, 129.76, 128.86, 128.73, 128.33, 128.27, 128.00, 127.41, 126.78, 124.02, 122.95, 120.64, 116.56, 64.37, 60.03; HRMS calcd for  $\text{C}_{25}\text{H}_{22}\text{NO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 368.1645; found: 368.1644.

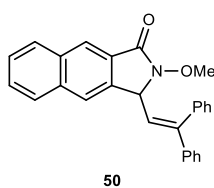
**(8) 5-(Chloromethyl)-3-(2,2-diphenylvinyl)-2-methoxyisindolin-1-one (49) (GFY-8-23).**



Following General Procedure II, **49** was afforded as a white solid (0.2 mmol scale, 61.8 mg, 79%), eluent (0-18% of ethyl acetate in petroleum ether): m.p.= 120.3-120.7

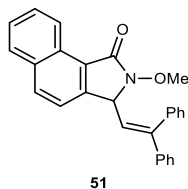
°C (ethyl acetate/petroleum ether);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.83 (d,  $J = 7.8$  Hz, 1H), 7.51 - 7.48 (m, 3H), 7.45 - 7.40 (m, 3H), 7.37 (s, 1H), 7.32 - 7.27 (m, 5H), 5.89 (d,  $J = 10.0$  Hz, 1H), 5.34 (d,  $J = 10.0$  Hz, 1H), 4.64 (s, 2H), 3.94 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.16, 149.06, 142.42, 141.95, 140.49, 138.18, 129.71, 129.16, 128.75, 128.32, 128.03, 127.40, 124.19, 123.14, 122.49, 64.37, 59.92, 45.51; HRMS calcd for  $\text{C}_{24}\text{H}_{20}^{35}\text{ClNNaO}_2^+$  ( $[\text{M}+\text{Na}]^+$ ): 412.1075; found: 412.1083.

**(9) 3-(2,2-Diphenylvinyl)-2-methoxy-2,3-dihydro-1H-benzo[f]isoindol-1-one (50)**  
**(GFY-8-26, W-5-46).**



Following General Procedure II, **50** was afforded as an oil (0.2 mmol scale, 57.6 mg, 74%), eluent (0-31% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.38 (s, 1H), 7.99 (d,  $J = 8.0$  Hz, 1H), 7.90 (d,  $J = 8.0$  Hz, 1H), 7.76 (s, 1H), 7.62 - 7.53 (m, 2H), 7.51 - 7.49 (m, 4H), 7.47 - 7.39 (m, 1H), 7.30 (s, 5H), 5.98 (d,  $J = 10.0$  Hz, 1H), 5.48 (d,  $J = 9.9$  Hz, 1H), 3.99 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.45, 148.55, 140.72, 138.39, 137.01, 135.37, 133.06, 129.86, 129.50, 128.75, 128.35, 128.26, 128.04, 128.02, 127.85, 127.46, 127.29, 126.66, 124.33, 123.59, 122.28, 64.34, 59.88; HRMS calcd for  $\text{C}_{27}\text{H}_{21}\text{NNaO}_2^+$  ( $[\text{M}+\text{Na}]^+$ ): 414.1465; found: 414.1474.

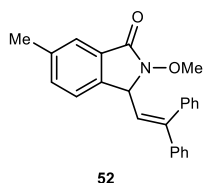
**(10) 3-(2,2-Diphenylvinyl)-2-methoxy-2,3-dihydro-1H-benzo[e]isoindol-1-one (51)**  
**(GFY-4-36, GFY-10-5, GFY-11-39).**



Following General Procedure II, **51** was afforded as a white solid (0.2 mmol scale, 31.2 mg, 40%), eluent (0-18% of ethyl acetate in petroleum ether): m.p.= 141.1-143.5 °C (ethyl acetate/petroleum ether);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.13 (d,  $J = 8.4$  Hz,

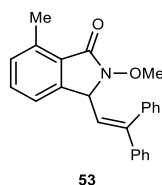
1H), 8.03 (d,  $J = 8.4$  Hz, 1H), 7.90 (d,  $J = 8.2$  Hz, 1H), 7.67 (t,  $J = 7.6$  Hz, 1H), 7.57 (t,  $J = 7.6$  Hz, 1H), 7.53 - 7.45 (m, 4H), 7.43 - 7.39 (m, 2H), 7.29 (s, 5H), 5.91 (d,  $J = 10.1$  Hz, 1H), 5.39 (d,  $J = 10.1$  Hz, 1H), 4.01 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.84, 148.79, 142.24, 140.81, 138.49, 133.24, 129.84, 129.23, 128.80, 128.37, 128.26, 128.21, 128.02, 127.47, 126.87, 124.00, 123.66, 123.19, 120.00, 64.58, 60.22; HRMS calcd for  $\text{C}_{27}\text{H}_{22}\text{NO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 392.1645; found: 392.1653.

**(11) 3-(2,2-Diphenylvinyl)-2-methoxy-6-methylisoindolin-1-one (52) (GFY-8-27).**



Following General Procedure II, **52** was afforded as an oil (0.2 mmol scale, 75.3 mg, 99%), eluent (0-25% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (s, 1H), 7.50 (t,  $J = 7.5$  Hz, 2H), 7.48 - 7.41 (m, 3H), 7.40 (d,  $J = 7.5$  Hz, 1H), 7.36 - 7.24 (m, 5H), 5.90 (d,  $J = 10.0$  Hz, 1H), 5.31 (d,  $J = 10.1$  Hz, 1H), 3.97 (s, 3H), 2.45 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  165.09, 148.31, 140.73, 139.06, 138.84, 138.38, 133.22, 129.76, 129.59, 128.68, 128.29, 128.16, 127.91, 127.39, 124.02, 123.43, 122.85, 64.31, 59.91, 21.35; HRMS calcd for  $\text{C}_{24}\text{H}_{22}\text{NO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 356.1645; found: 356.1654.

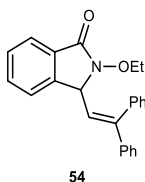
**(12) 3-(2,2-Diphenylvinyl)-2-methoxy-7-methylisoindolin-1-one (53) (GFY-4-22, GFY-10-4).**



Following General Procedure II, **53** was afforded as an oil (0.2 mmol scale, 26.9 mg, 38%), eluent (0-15% of ethyl acetate in petroleum ether):  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.50 - 7.45 (m, 2H), 7.44 - 7.39 (m, 4H), 7.30 - 7.27 (m, 5H), 7.20 (d,  $J = 7.4$  Hz, 1H), 7.15 (d,  $J = 7.2$  Hz, 1H), 5.89 (d,  $J = 10.0$  Hz, 1H), 5.24 (d,  $J = 10.0$  Hz, 1H), 3.94 (s, 3H), 2.70 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  150.29, 149.63, 144.42,

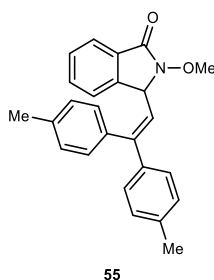
140.15, 137.67, 132.57, 129.73, 128.78, 128.75, 128.46, 128.39, 127.76, 125.88, 124.67, 121.81, 121.58, 83.71, 77.20, 63.43; HRMS calcd for  $C_{24}H_{22}NO_2^+$  ( $[M+H]^+$ ): 356.1645; found: 356.1651.

**(13) 3-(2,2-Diphenylvinyl)-2-ethoxyisoindolin-1-one (54) (GFY-8-24).**



Following General Procedure II, **54** was afforded as a white solid (0.2 mmol scale, 62.0 mg, 87%), eluent (0-15% of ethyl acetate in petroleum ether): m.p.= 166.0-166.5 °C (ethyl acetate/petroleum ether);  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.84 (d,  $J = 7.6$  Hz, 1H), 7.56 (td,  $J = 7.5, 1.2$  Hz, 1H), 7.51 - 7.44 (m, 1H), 7.43 - 7.38 (m, 3H), 7.36 (d,  $J = 7.6$  Hz, 1H), 7.32 - 7.26 (m, 5H), 5.88 (d,  $J = 10.1$  Hz, 1H), 5.32 (d,  $J = 10.1$  Hz, 1H), 4.19 - 4.13 (m, 2H), 1.36 (t,  $J = 7.1$  Hz, 3H);  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  165.23, 148.40, 141.98, 140.71, 138.39, 132.19, 129.75, 129.73, 128.68, 128.64, 128.31, 128.19, 127.95, 127.40, 123.79, 123.38, 123.07, 72.29, 60.49, 13.78; HRMS calcd for  $C_{24}H_{21}NNaO_2^+$  ( $[M+Na]^+$ ): 378.1465; found: 378.1474.

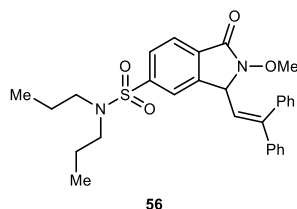
**(14) 3-(2,2-Di-*p*-tolylvinyl)-2-methoxyisoindolin-1-one (55) (GFY-8-13).**



Following General Procedure II, **55** was afforded as an oil (0.2 mmol scale, 30.4 mg, 41%), eluent (0-20% of ethyl acetate in petroleum ether):  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.84 (dt,  $J = 7.5, 1.0$  Hz, 1H), 7.56 (td,  $J = 7.6, 1.2$  Hz, 1H), 7.50 - 7.43 (m, 1H), 7.35 (dd,  $J = 7.4, 1.0$  Hz, 1H), 7.29 (t,  $J = 8.8$  Hz, 4H), 7.17 (d,  $J = 8.2$  Hz, 2H), 7.10 (d,  $J = 8.1$  Hz, 2H), 5.83 (d,  $J = 10.0$  Hz, 1H), 5.34 (d,  $J = 10.0$  Hz, 1H), 3.94 (s, 3H), 2.41 (s, 3H), 2.34 (s, 3H);  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  164.89, 148.51, 142.10, 138.18, 138.13, 137.68, 135.53, 132.25, 129.67, 129.64, 129.37, 129.00, 128.62,

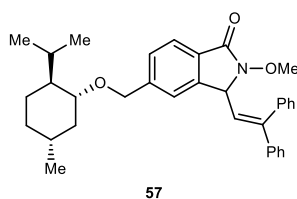
127.36, 123.78, 123.13, 122.01, 64.39, 60.23, 21.22, 21.09; HRMS calcd for  $C_{25}H_{24}NO_2^+$  ( $[M+H]^+$ ): 370.1802; found: 370.1812.

**(15) 3-(2,2-Diphenylvinyl)-2-methoxy-1-oxo-*N,N*-dipropylisoindoline-5-sulfonamide (56) (GFY-8-28).**



Following General Procedure II, **56** was afforded an oil (0.2 mmol scale, 95.8 mg, 93%), eluent (0-24% of ethyl acetate in petroleum ether):  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.97 (d,  $J = 8.0$  Hz, 1H), 7.91 (dd,  $J = 7.9, 1.5$  Hz, 1H), 7.80 (s, 1H), 7.53 - 7.47 (m, 2H), 7.44 (dt,  $J = 8.0, 1.9$  Hz, 3H), 7.34 - 7.29 (m, 3H), 7.29 - 7.26 (m, 2H), 5.86 (d,  $J = 10.0$  Hz, 1H), 5.41 (d,  $J = 10.0$  Hz, 1H), 3.97 (s, 3H), 3.13 - 3.10 (m, 4H), 1.56 (q,  $J = 7.5$  Hz, 4H), 0.87 (t,  $J = 7.4$  Hz, 6H);  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  162.89, 150.06, 144.24, 142.49, 140.29, 138.00, 133.12, 129.68, 128.82, 128.53, 128.37, 128.19, 127.43, 127.32, 124.53, 121.96, 121.35, 64.51, 60.09, 49.79, 21.81, 11.08; HRMS calcd for  $C_{29}H_{33}N_2O_4S^+$  ( $[M+H]^+$ ): 505.2156; found: 505.2164.

**(16) 3-(2,2-Diphenylvinyl)-5-((((1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl)oxy)methyl)-2-methoxyisoindolin-1-one (57) (GFY-8-30).**

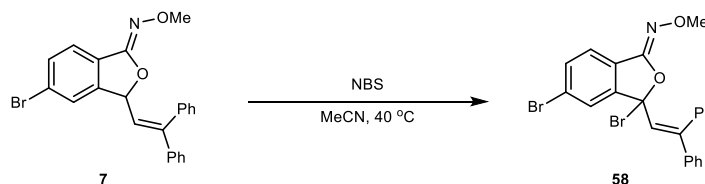


Following General Procedure II, **57** was afforded as an oil (0.1 mmol scale, 47.1 mg, 98%, dr = 1:1), eluent (0-21% of ethyl acetate in petroleum ether):  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.80 (d,  $J = 7.8$  Hz, 1H), 7.50 - 7.45 (m, 2H), 7.42 (d,  $J = 7.5$  Hz, 4H), 7.38 (s, 1H), 7.33 - 7.24 (m, 5H), 5.88 (dd,  $J = 10.1, 3.7$  Hz, 1H), 5.31 (dd,  $J = 10.1, 3.2$  Hz, 1H), 4.75 (dd,  $J = 12.2, 5.5$  Hz, 1H), 4.46 (dd,  $J = 12.3, 4.7$  Hz, 1H), 3.94 (s, 3H), 3.23 - 3.17 (m, 1H), 2.35 - 2.25 (m, 1H), 2.19 (dd,  $J = 12.1, 1.9$  Hz, 1H), 1.69 - 1.61 (m, 2H), 1.45 - 1.24 (m, 3H), 0.94 (dd,  $J = 6.6, 3.6$  Hz, 4H), 0.89 (d,  $J = 7.2$  Hz,

4H), 0.72 (dd,  $J = 7.0, 3.4$  Hz, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.97, 144.30, 142.16, 140.74, 138.37, 129.76, 128.71, 128.32, 128.21, 127.97, 127.89, 127.86, 127.43, 123.74, 123.25, 122.08, 122.02, 79.48, 69.91, 64.41, 60.14, 48.25, 40.25, 34.44, 31.49, 23.19, 22.30, 20.92, 16.13; HRMS calcd for  $\text{C}_{34}\text{H}_{40}\text{NO}_3^+$  ( $[\text{M}+\text{H}]^+$ ): 510.3003; found: 510.3010.

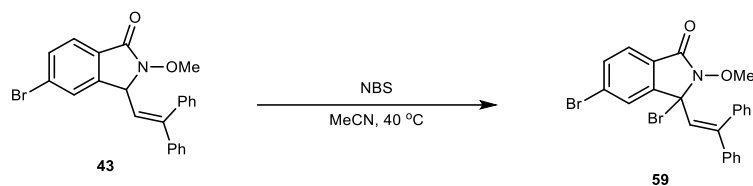
### 2.3 Transformation of products to assess the potential for post-modifications.

#### (1) Synthesis of (*Z*)-3,5-dibromo-3-(2,2-diphenylvinyl)isobenzofuran-1(3*H*)-one *O*-methyl oxime (**58**) (GFY-7-28, GFY-10-25).



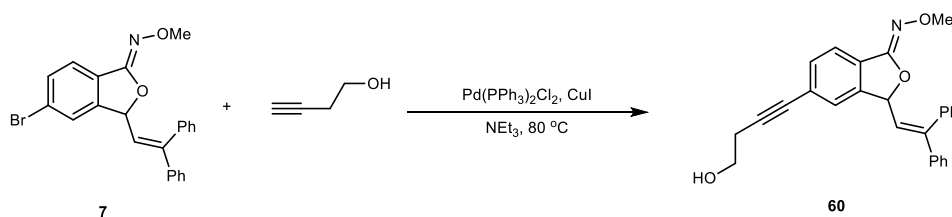
To a 10 mL of Schlenk tube was added *N*-bromosuccinimide (53.2 mg, 0.3 mmol), **7** (86.0 mg, 0.2 mmol), and acetonitrile (1 mL). The mixture was stirred at 40 °C overnight as monitored by TLC. The solution was cooled to room temperature and concentrated under vacuum to afford **58** (84.0 mg, 82%) via flash chromatography on silica gel (eluent: 8% of ethyl acetate in petroleum ether) as a white solid: m.p.= 150.0-150.4 °C (ethyl acetate/petroleum ether);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.67 - 7.54 (m, 2H), 7.51 - 7.43 (m, 1H), 7.41 - 7.37 (m, 4H), 7.36 - 7.34 (m, 2H), 7.33 (dd,  $J = 4.0, 2.9$  Hz, 3H), 7.31 - 7.29 (m, 1H), 6.40 (s, 1H), 3.97 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  154.61, 149.45, 144.38, 141.19, 139.30, 132.77, 128.98, 128.94, 128.87, 128.61, 128.51, 128.17, 125.21, 124.91, 122.94, 121.21, 115.13, 84.79, 62.94; HRMS calcd for  $\text{C}_{23}\text{H}_{18}^{79}\text{Br}_2\text{NO}_2^+$  ( $[\text{M}+\text{H}]^+$ ): 497.9699; found: 497.9707.

#### (2) Synthesis of 3,5-dibromo-3-(2,2-diphenylvinyl)-2-methoxyisindolin-1-one (**59**) (GFY-9-19, GFY-10-34, W-2-25).



To a 10 mL of Schlenk tube was added *N*-bromosuccinimide (47.5 mg, 0.27 mmol), **43** (74.2 mg, 0.18 mmol), and acetonitrile (1 mL). The mixture was stirred at 40 °C overnight as monitored by TLC. The solution was cooled to room temperature and concentrated under vacuum to afford **59** (65.1 mg, 74%) via flash chromatography on silica gel (eluent: 20% of ethyl acetate in petroleum ether) as a white solid: m.p.= 60.5-60.7 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.70 (d, *J* = 8.2 Hz, 1H), 7.66 - 7.61 (m, 1H), 7.55 - 7.51 (m, 1H), 7.44 - 7.40 (m, 4H), 7.37 - 7.34 (m, 5H), 7.33 - 7.30 (m, 1H), 5.65 (s, 1H), 4.08 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.51, 150.66, 142.26, 141.33, 139.48, 132.64, 129.15, 129.06, 128.79, 128.76, 128.45, 128.25, 128.17, 127.22, 125.65, 125.35, 120.62, 64.40, 63.66; HRMS calcd for C<sub>23</sub>H<sub>17</sub><sup>79</sup>Br<sup>81</sup>BrNNaO<sub>2</sub><sup>+</sup> ([M+Na]<sup>+</sup>): 521.9498; found: 521.9494.

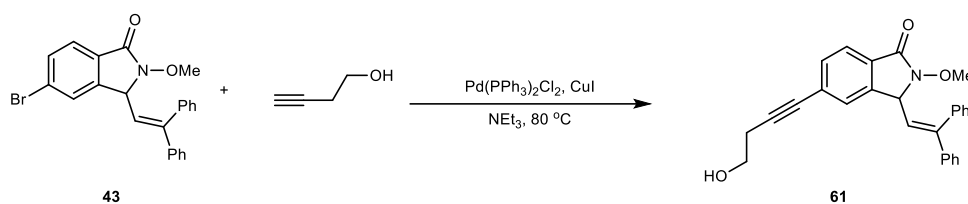
### (3) Synthesis of (Z)-3-(2,2-diphenylvinyl)-5-(4-hydroxybut-1-yn-1-yl)isobenzofuran-1(3*H*)-one *O*-methyl oxime (**60**) (GFY-7-37).



Under a nitrogen atmosphere, to a solution of **7** (42.3 mg, 0.1 mmol) in triethylamine (0.2 mL) was added Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> (0.7 mg, 0.001 mmol), 3-butyn-1-ol (9.1 μL, 0.12 mmol), and CuI (0.3 mg, 1 mol%). The mixture was stirred overnight at 80 °C as monitored by TLC. After cooling to room temperature, the mixture was filtered through a short pad of silica gel and concentrated in vacuo. Flash chromatography on silica gel (eluent: 0-29% of ethyl acetate in petroleum ether) afforded **60** (21.1 mg, 52%) as a white solid: m.p.= 69.9-70.3 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.60 (d, *J* = 8.0 Hz, 1H), 7.47 - 7.41 (m, 3H), 7.40 - 7.36 (m, 3H), 7.33 (d, *J*

= 1.2 Hz, 1H), 7.29 - 7.26 (m, 5H), 6.07 (d,  $J = 10.0$  Hz, 1H), 5.95 (d,  $J = 10.0$  Hz, 1H), 3.95 (s, 3H), 3.83 (t,  $J = 6.2$  Hz, 2H), 2.71 (t,  $J = 6.3$  Hz, 2H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.57, 148.34, 144.13, 140.62, 138.03, 132.52, 129.90, 128.57, 128.38, 128.25, 128.14, 127.83, 127.77, 126.17, 125.28, 123.06, 121.57, 89.19, 83.89, 81.70, 62.79, 60.99, 23.83; HRMS calcd for  $\text{C}_{27}\text{H}_{24}\text{NO}_3^+$  ( $[\text{M}+\text{H}]^+$ ): 410.1751; found: 410.1744.

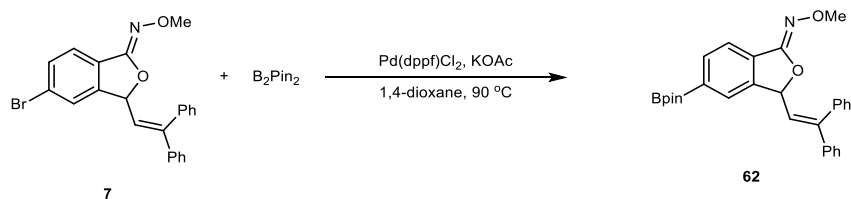
**(4) Synthesis of 3-(2,2-diphenylvinyl)-5-(4-hydroxybut-1-yn-1-yl)-2-methoxyisoindolin-1-one (61) (GFY-9-32, W-2-27).**



Under a nitrogen atmosphere, to a solution of **43** (42.4 mg, 0.1 mmol) in triethylamine (0.2 mL) was added  $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$  (0.8 mg, 0.001 mmol), 3-butyn-1-ol (9.1  $\mu\text{L}$ , 0.12 mmol), and  $\text{CuI}$  (0.3 mg, 0.001). The mixture was stirred overnight at 80  $^\circ\text{C}$  as monitored by TLC. After cooling to room temperature, the mixture was filtered through a short pad of silica gel and concentrated in vacuo. Flash chromatography on silica gel (eluent: 0-40% of ethyl acetate in petroleum ether) afforded **61** (40.3 mg, 98%) as a white solid: m.p.= 159.2-160.0  $^\circ\text{C}$  (ethyl acetate/petroleum ether);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 7.9$  Hz, 1H), 7.50 - 7.47 (m, 3H), 7.44 - 7.39 (m, 3H), 7.36 (s, 1H), 7.31 - 7.26 (m,  $J = 10.3, 4.4$  Hz, 5H), 5.85 (d,  $J = 10.1$  Hz, 1H), 5.28 (d,  $J = 10.2$  Hz, 1H), 3.93 (s, 3H), 3.84 (t,  $J = 6.3$  Hz, 2H), 2.72 (t,  $J = 6.3$  Hz, 2H), 2.10 (s, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.33, 149.08, 141.86, 140.49, 138.18, 132.25, 129.73, 128.75, 128.33, 128.03, 127.70, 127.41, 126.15, 123.68, 122.41, 90.00, 81.53, 64.43, 60.88, 59.88, 23.80; HRMS calcd for  $\text{C}_{27}\text{H}_{24}\text{NO}_3^+$  ( $[\text{M}+\text{H}]^+$ ): 410.1751; found: 410.1751.

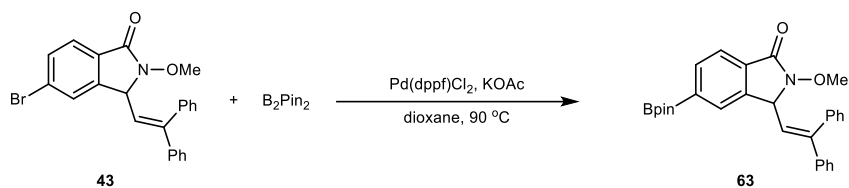
**(5) Synthesis of (Z)-3-(2,2-diphenylvinyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)isobenzofuran-1(3H)-one O-methyl oxime (62) (GFY-8-4).**





Under a nitrogen atmosphere, to a 10 mL of Schlenk tube was added **7** (42.4 mg, 0.1 mmol),  $B_2pin_2$  (38.8 mg, 0.15 mmol),  $Pd(dppf)Cl_2$  (3.7 mg, 0.005 mmol), KOAc (29.9 mg, 0.3 mmol), and 1,4-dioxane (1 mL). The mixture was stirred overnight at 90 °C as monitored by TLC. After cooling to room temperature, the mixture was filtered through a short pad of silica gel and concentrated in vacuo. Flash chromatography on silica gel (eluent: 0-17% of ethyl acetate in petroleum ether) afforded **62** (29.0 mg, 51%) as a white solid: m.p.= 198.4-199.1 °C (ethyl acetate/petroleum ether);  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.86 (d,  $J = 7.7$  Hz, 1H), 7.72 (s, 1H), 7.68 (d,  $J = 7.7$  Hz, 1H), 7.46 - 7.41 (m, 4H), 7.40 - 7.36 (m, 1H), 7.28 (s, 5H), 6.13 (d,  $J = 10.0$  Hz, 1H), 5.97 (d,  $J = 10.1$  Hz, 1H), 3.96 (s, 3H), 1.36 (s, 12H);  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  164.55, 148.90, 141.06, 140.68, 138.27, 135.15, 132.11, 129.93, 129.00, 128.67, 128.33, 128.25, 127.96, 127.45, 122.93, 122.70, 84.31, 75.01, 64.33, 59.91, 24.84, 24.82; HRMS calcd for  $C_{29}H_{31}BNO_4^+$  ( $[M+H]^+$ ): 468.2341; found: 468.2340.

**(6) Synthesis of 3-(2,2-diphenylvinyl)-2-methoxy-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)isoindolin-1-one (63) (GFY-9-36).**

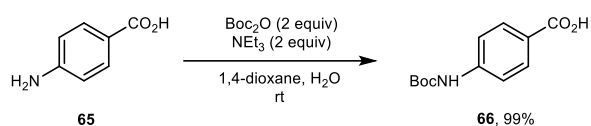


Under a nitrogen atmosphere, to a 10 mL of Schlenk tube was added **43** (42.0 mg, 0.1 mmol),  $B_2pin_2$  (38.1 mg, 0.15 mmol),  $Pd(dppf)Cl_2$  (3.7 mg, 0.005 mmol), KOAc (29.4 mg, 0.3 mmol), and 1,4-dioxane (1 mL). The mixture was stirred overnight at 90 °C as monitored by TLC. After cooling to room temperature, the mixture was filtered through a short pad of silica gel and concentrated in vacuo. Flash chromatography on silica gel (eluent: 0-30% of ethyl acetate in petroleum ether) afforded **63** (46.4 mg, 81%) as an oil:  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.93 (d,  $J = 7.5$  Hz, 1H), 7.84 (d,  $J = 7.5$  Hz,

1H), 7.76 (s, 1H), 7.51 - 7.43 (m, 4H), 7.44 - 7.37 (m, 1H), 7.30 (s, 5H), 5.87 (d,  $J = 10.1$  Hz, 1H), 5.33 (d,  $J = 10.1$  Hz, 1H), 3.91 (s, 3H), 1.36 (s, 12H), 1.24 (s, 8.5H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.55, 148.90, 141.06, 140.68, 138.27, 135.15, 132.11, 129.93, 129.00, 128.67, 128.33, 128.25, 127.96, 127.45, 122.93, 122.70, 84.31, 75.01, 64.33, 59.91, 24.84, 24.82; HRMS calcd for  $\text{C}_{29}\text{H}_{31}\text{BNO}_4^+$  ( $[\text{M}+\text{H}]^+$ ): 468.2341; found: 468.2345.

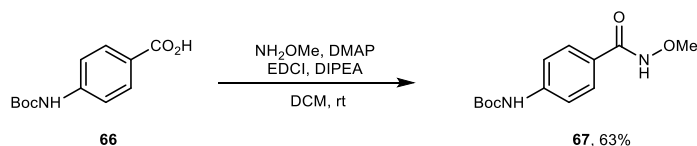
## 2.4 Synthesis of a potential PD-L1 down-regulator.

### (1) 4-((*tert*-Butoxycarbonyl)amino)benzoic acid (**66**) (GFY-8-40).



To a solution of **65** (1.3716 g, 10 mmol) in the mixture of dioxane (20 mL) and water (10 mL) was added triethylamine (2.8 mL, 20 mmol) and  $\text{Boc}_2\text{O}$  (4.6 mL, 20 mmol). The reaction mixture was stirred at room temperature for 24 h as monitored by TLC. After being concentrated in vacuo, to the residue was dropwisely added HCl (3 M, 30 mL). A precipitate formed, which was filtered, washed with water, and dried to provide **66** (2.8725 g, 99%). The characterization data was in agreement with literature.<sup>[S11]</sup>

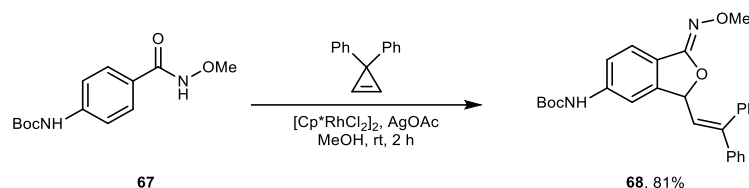
### (2) Methyl 4-((*tert*-butoxycarbonyl)amino)benzoic acid (**67**) (GFY-8-43, GFY-9-29).



To a 250 mL of round bottom flask was added **66** (0.7322 g, 3.1 mmol),  $\text{NH}_2\text{OMe}\cdot\text{HCl}$  (0.3324 g, 4 mmol), DMAP (0.3784 g, 3.1 mmol), EDC-HCl (1.1885 g, 6.2 mmol), DIPEA (2.0 mL, 11.2 mmol), and dichloromethane (40 mL). The mixture was stirred at room temperature overnight as monitored by TLC. After being

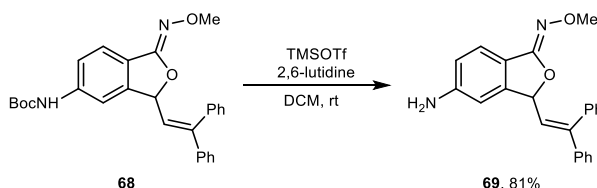
concentrated in vacuo, **67** (0.5177 g, 63%) was obtained via flash chromatography on silica gel (0-44% of ethyl acetate in petroleum ether). The characterization data was in agreement with literature.

**(3) tert-Butyl (Z)-(3-(2,2-Diphenylvinyl)-1-(methoxyimino)-1,3-dihydroisobenzofuran-5-yl)carbamate (68) (GFY-9-3, GFY-8-48).**



Following General Procedure I, after being reacted for 2 h, **68** (74.2 mg, 81%) was obtained via flash chromatography on silica gel (eluent: 11% of ethyl acetate in petroleum ether) as an oil:  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.58 (d,  $J = 8.4$  Hz, 1H), 7.54 (s, 1H), 7.45 - 7.41 (m, 2H), 7.41 - 7.37 (m, 3H), 7.32 - 7.29 (m, 1H), 7.28 - 7.24 (m, 5H), 6.99 (s, 1H), 6.08 - 6.02 (m, 1H), 5.98 - 5.92 (m, 1H), 3.96 (s, 3H), 1.53 (s, 9H);  $^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.98, 148.10, 145.53, 141.34, 140.64, 138.01, 129.93, 128.46, 128.21, 128.13, 127.99, 127.72, 123.27, 122.47, 122.32, 119.12, 111.14, 83.85, 81.09, 62.53, 28.21; HRMS calcd for  $\text{C}_{28}\text{H}_{29}\text{N}_2\text{O}_4^+$  ( $[\text{M}+\text{H}]^+$ ): 457.2122; found: 457.2122.

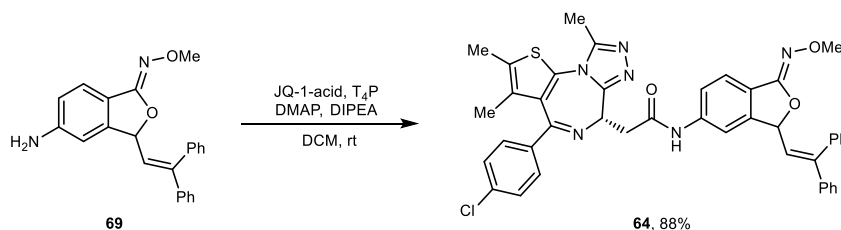
**(4) (Z)-5-Amino-3-(2,2-diphenylvinyl)isobenzofuran-1(3H)-one O-methyl oxime (69) (GFY-9-4/GFY-9-12).**



At 0 °C, to a solution of **68** (70.9 mg, 0.15 mmol) in dichloromethane (5 mL) was added 2,6-lutidine (109  $\mu\text{L}$ , 0.93 mmol) and TMSOTf (112  $\mu\text{L}$ , 0.62 mmol) dropwisely. The reaction mixture was stirred at 0 °C for 30 min, and then at room temperature for 2 hours as monitored by TLC. After being concentrated in vacuo, **69** (44.7 mg, 81%) was obtained via flash chromatography on silica gel (eluent: 0-18% of ethyl acetate in

petroleum ether) as a white solid: m.p.= 86.0-86.2 °C (ethyl acetate/petroleum ether); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.51 - 7.46 (m, 1H), 7.44 (d, *J* = 7.6 Hz, 2H), 7.41 - 7.36 (m, 3H), 7.29 (d, *J* = 1.4 Hz, 5H), 6.69 (dd, *J* = 8.4, 2.1 Hz, 1H), 6.53 (d, *J* = 2.1 Hz, 1H), 6.00 (d, *J* = 2.3 Hz, 2H), 4.04 (s, 2H), 3.94 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 156.63, 149.41, 147.42, 146.35, 140.80, 138.20, 129.92, 128.49, 128.20, 128.00, 127.71, 123.94, 122.95, 118.02, 116.02, 106.90, 83.52, 62.48; HRMS calcd for C<sub>23</sub>H<sub>21</sub>N<sub>2</sub>O<sub>2</sub><sup>+</sup> ([M+H]<sup>+</sup>): 357.1598; found: 357.1595.

**(5) 2-((*S*)-4-(4-Chlorophenyl)-2,3,9-trimethyl-6*H*-thieno[3,2-*f*][1,2,4]triazolo[4,3-*a*][1,4]diazepin-6-yl)-*N*-((*Z*)-3-(2,2-diphenylvinyl)-1-(methoxyimino)-1,3-dihydroisobenzofuran-5-yl)acetamide (**64**) (GFY-10-2).**



Under a nitrogen atmosphere, to a 50 mL of round bottom flask were added **69** (44.2 mg, 0.125 mmol), JQ-1-acid (39.7 mg, 0.1 mmol), DMAP (25.0 mg, 0.2 mmol), T<sub>4</sub>P (50 % in ethyl acetate, 209.4 mg, 0.262 mmol), DIPEA (45 μL, 0.26 mmol), and dichloromethane (10 mL). The mixture was stirred at room temperature overnight as monitored by TLC. After being concentrated in vacuo, **64** (64.4 mg, 88%, dr = 1:1) was obtained via flash chromatography on silica gel (100% of ethyl acetate) as a white solid: m.p.= 215.8-216.1 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.09 (d, *J* = 93.1 Hz, 1H), 7.88 (dd, *J* = 14.9, 1.7 Hz, 1H), 7.54 - 7.36 (m, 7H), 7.34 - 7.30 (m, 3H), 7.29 - 7.24 (m, 6H), 6.54 - 5.62 (m, 2H), 4.79 - 4.72 (m, 1H), 3.96 - 3.84 (m, 4H), 3.65 (ddd, *J* = 16.2, 14.8, 5.5 Hz, 1H), 2.63 (s, 3H), 2.40 (d, *J* = 2.1 Hz, 3H), 1.67 (d, *J* = 2.5 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 169.34, 169.31, 164.13, 155.90, 155.74, 150.05, 147.98, 147.45, 145.17, 145.01, 141.38, 141.23, 140.78, 140.58, 138.09, 138.07, 136.89, 136.88, 136.30, 131.89, 131.10, 130.94, 130.89, 130.49, 129.95, 129.92, 129.83, 128.65, 128.45, 128.16, 128.12, 128.10, 127.93, 127.88, 127.77, 127.71, 123.52, 123.48, 123.36, 123.19, 122.03, 121.93, 120.61, 120.41, 112.99, 112.77, 83.90, 83.87, 62.56,

62.53, 54.41, 54.39, 40.27, 40.19, 14.35, 14.32, 13.03, 11.71; HRMS calcd for  $C_{42}H_{36}^{35}ClN_6O_3S^+$  ( $[M+H]^+$ ): 739.2253; found: 739.2250.

## **2.5 Biological activity evaluation.**

### **(1) Cell culture.**

SUM159PT cells were maintained in RPMI-1640 medium (KeyGen BioTECH) supplemented with 10% (v/v) fetal bovine serum (FBS; VivaCell Bioscience). U-87 MG cells were cultured with Dulbecco's modified Eagle's medium media (DMEM; KeyGen BioTECH) with 10% FBS.

### **(2) Cell preparation.**

Cells were cultured in 6-well plates. After confluence reached 70%, cells were treated with DMSO, JQ-1 (5  $\mu$ M) or compound **64** (5  $\mu$ M) for 12 h. After that, cells were washed by PBS and harvested for the following analysis.

### **(3) RNA extraction and qPCR analysis.**

Total RNA was isolated with RNA isolater total RNA extraction reagent (Vazyme) and 1  $\mu$ g of total RNA was used for cDNA synthesis using the HiScript II Q RT SuperMix (Vazyme). Quantitative PCRs were carried out using AceQ qPCR SYBR green master mix (Vazyme). Samples were obtained and analyzed on the LightCycler 480 System (Roche). The gene expression levels were normalized to  $\beta$ -Actin. The primer sequences were as follows:

$\beta$ -Actin forward: 5'-GATCATTGCTCCTCCTGAGC-3'

$\beta$ -Actin reverse: 5'-ACTCCTGCTTGCTGATCCAC-3'

PD-L1 forward: 5'-TGGCATTGCTGAACGCATTT-3'

PD-L1 reverse: 5'-TGCAGCCAGGTCTAATTGTTTT-3'

### **(4) Statistical analysis.**

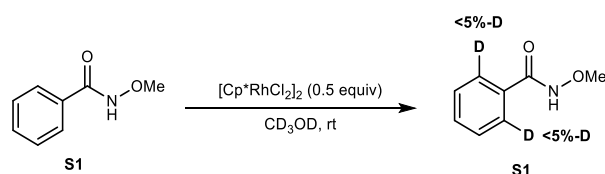
The experiments were carried out in three independent experiments and the results are expressed as mean  $\pm$  SD. One-way analysis of variance (ANOVA) was used for assessment of the statistical significance, and data were considered significant at  $p \leq 0.05$ . GraphPad Prism 8.0 software was used to perform all the statistical analyses and generating the graphics corresponding to these statistics.

### (5) Immunoblotting.

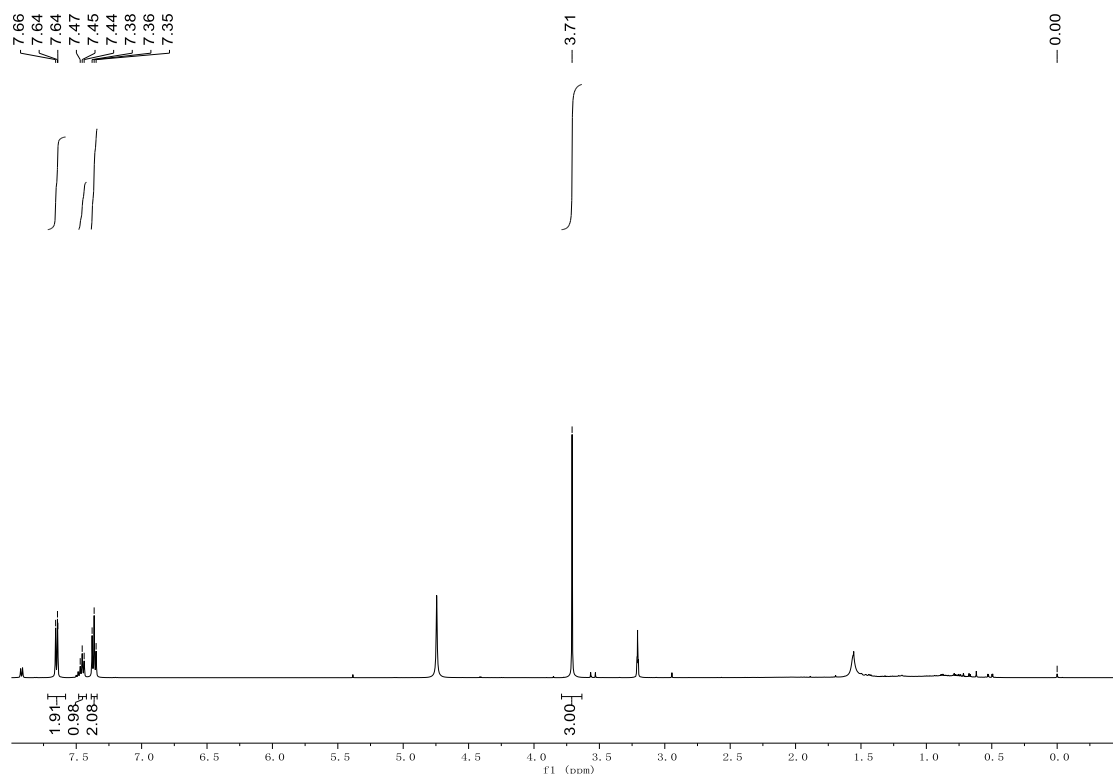
Cells were washed twice with ice-cold PBS, lysed and denatured with SDS-PAGE loading buffer (NCM Biotech). The proteins were separated with SDS-PAGE, transferred to PVDF membranes, and blocked with 5% skim milk and incubated with indicated antibodies ( $\beta$ -Actin (Abclonal, AC026), BRD4 (Proteintech, 28486-1-AP)). Immunoreactive bands were visualized with HRP-conjugated secondary antibodies (HRP Goat Anti-Rabbit IgG (H+L) (Abclonal AS014)).

## 2.6 Experimental mechanistic studies.

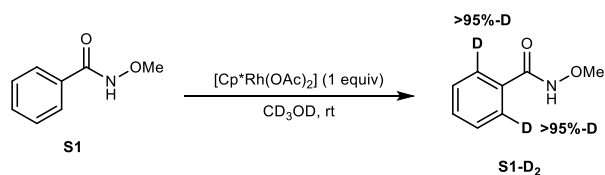
### (1) H/D Exchange with $[\text{RhCp}^*\text{Cl}_2]_2$ (GFY-12-20-1)



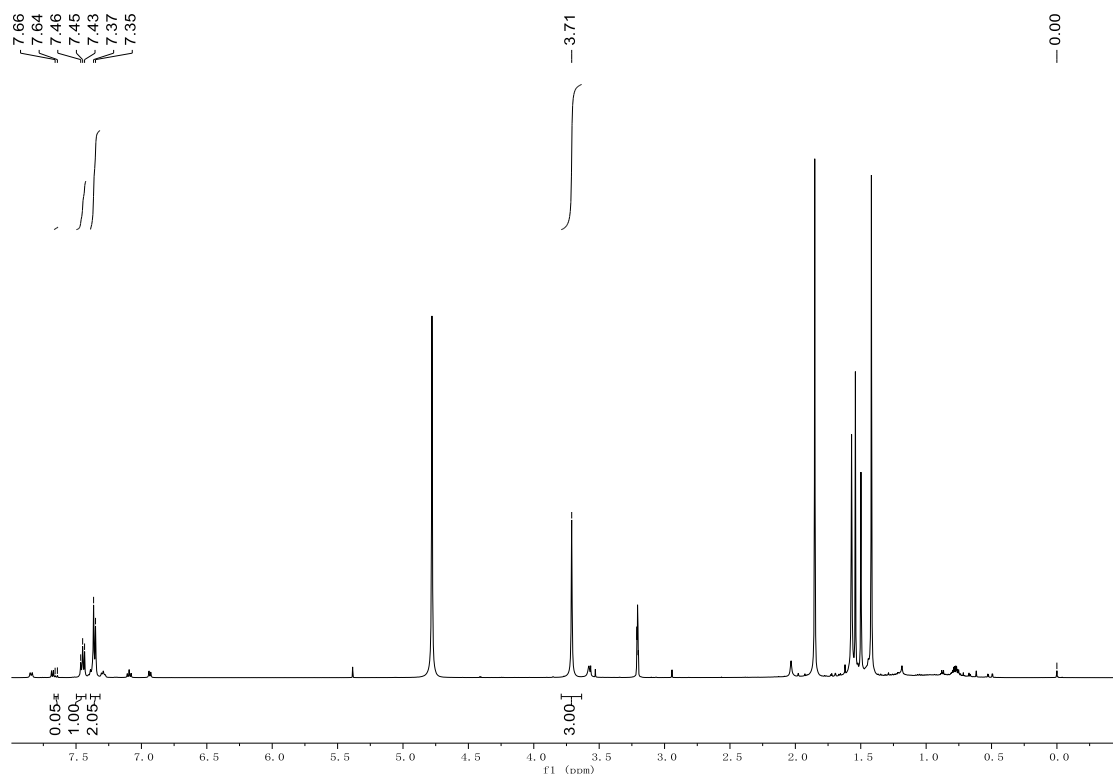
To a 10 mL of Schlenk tube was charged with **S1** (7.8 mg, 0.05 mmol),  $[\text{Cp}^*\text{RhCl}_2]_2$  (15.4 mg, 0.025 mmol) and  $\text{CD}_3\text{OD}$  (0.5 mL). After being stirred at room temperature for 2 hours, the reaction mixture was directly analyzed by  $^1\text{H}$  NMR, and less than 5%-D incorporation was observed at ortho positions.



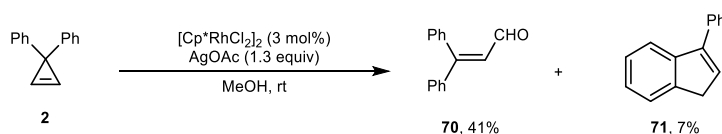
## (2) H/D Exchange with $\text{RhCp}^*(\text{OAc})_2$ (GFY-12-19-1)



To a 10 mL of Schlenk tube was charged with **S1** (7.6 mg, 0.05 mmol),  $\text{Cp}^*\text{Rh}(\text{OAc})_2$  (18.5 mg, 0.05 mmol) and  $\text{CD}_3\text{OD}$  (0.5 mL). After being stirred at room temperature for 2 hours, the reaction mixture was directly analyzed by  $^1\text{H}$  NMR, and an average of more than 95%-D incorporation was observed at ortho positions.



### (3) Reaction of **2** in the absence of **S1**. (GFY-10-40)



To a 10 mL of Schlenk tube equipped with a magnetic stir bar was added **2** (57.7 mg, 0.3 mmol),  $[\text{Cp}^*\text{RhCl}_2]_2$  (6.2 mg, 0.01 mmol), AgOAc (66.8 mg, 0.4 mmol), and MeOH (2 ml) successively. After being stirred at room temperature for 2 h, the crude product was filtered through a short pad of silica gel. After being concentrated in vacuo, the residue was purified by silica gel chromatography on silica gel (eluent: 0-8% of ethyl acetate in petroleum ether) to afford **70** (24.9 mg, 41%) and **71** (4.0 mg, 7%).

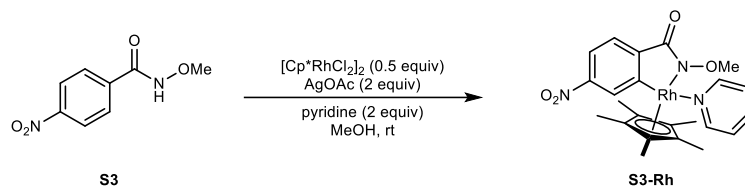
**70**:<sup>[S12]</sup> oil;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.53 (d,  $J = 8.0$  Hz, 1H), 7.51 - 7.41 (m, 3H), 7.39 - 7.34 (m, 4H), 7.32 - 7.27 (m, 3H), 6.60 (d,  $J = 8.0$  Hz, 1H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  193.51, 162.25, 139.70, 136.67, 130.71, 130.47, 129.43, 128.65, 128.60, 128.33, 127.27.

**71**:<sup>[S13]</sup> oil;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.63 - 7.56 (m, 3H), 7.57 - 7.51 (m, 1H), 7.47 - 7.43 (m, 2H), 7.41 - 7.34 (m, 1H), 7.34 - 7.31 (m, 1H), 7.28 - 7.25 (m, 2H), 3.51 (d,  $J = 2.1$  Hz, 2H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  145.16, 144.75, 143.88, 136.12,



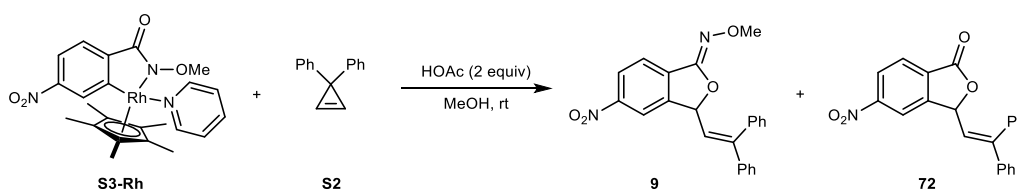
130.95, 128.55, 127.69, 127.55, 126.13, 124.83, 124.10, 120.29, 77.25, 77.00, 76.74, 38.17.

#### (4) Preparation of S3-Rh. (GFY-12-33)



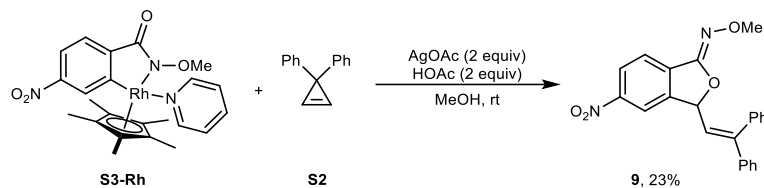
To a 25 mL of Schlenk tube equipped with a magnetic stir bar was added  $[\text{Cp}^*\text{RhCl}_2]_2$  (61.8 mg, 0.1 mmol), pyridine (16  $\mu\text{L}$ , 0.2 mmol) and MeOH (8 mL), after being stirred at room temperature for 2 h, AgOAc (81.0 mg, 0.48 mmol) and **S3** (57.7 mg, 0.3 mmol) was added successively. After being stirred at room temperature overnight, the crude product was purified by silica gel chromatography on silica gel (eluent: 0-5% of methanol in dichloromethane) to afford **S3-Rh**<sup>[S14]</sup> (80.8 mg, 95%) as a red solid;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.49 (d,  $J = 2.2$  Hz, 1H), 8.44 (d,  $J = 4.5$  Hz, 2H), 7.88 (dd,  $J = 8.2, 2.2$  Hz, 1H), 7.68 - 7.60 (m, 2H), 7.23 - 7.16 (m, 2H), 4.04 (s, 3H), 1.64 (s, 15H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  173.96, 173.92, 168.85, 168.60, 153.43, 147.95, 147.53, 137.52, 127.59, 125.90, 125.55, 119.00, 96.09, 96.04, 62.98, 9.20.

#### (5) Stoichiometric reaction of S3-Rh with S2 in the absence of AgOAc (GFY-12-30)



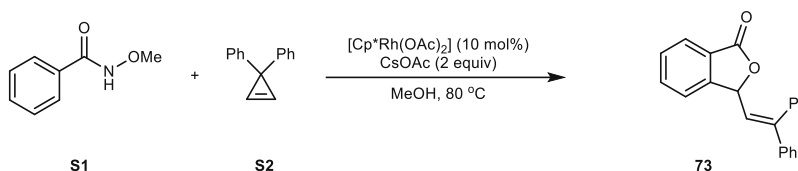
To a 10 mL of Schlenk tube equipped with a magnetic stir bar was added **S3-Rh** (51.7 mg, 0.1 mmol), **S2** (39.8 mg, 0.2 mmol), HOAc (12  $\mu\text{L}$ , 0.2 mmol), and MeOH (1 ml). After being stirred at room temperature overnight, the crude product was purified by silica gel chromatography on silica gel (eluent: 0-7% of methanol in dichloromethane) to afford a mixture of **9** and **70** (29.4 mg, **9:70** = 1:2.5, yield of **9**: 6%, yield of **70**: 15%).

**(6) Stoichiometric reaction of S3-Rh with S2 in the presence of AgOAc (GFY-12-37)**



To a 10 mL of Schlenk tube equipped with a magnetic stir bar was added **S3-Rh** (51.7 mg, 0.1 mmol), **S2** (38.8 mg, 0.2 mmol), HOAc (12  $\mu$ L, 0.2 mmol), AgOAc (33.8 mg, 0.2 mmol), and MeOH (1 ml). After being stirred at room temperature overnight, the crude product was purified by silica gel chromatography on silica gel (eluent: 0-7% of methanol in dichloromethane) to afford **9** (31.3 mg, 23%).

**(7) Reaction of S1 with S2 leading to the formation of 73. (LSJ-3-43-2)**

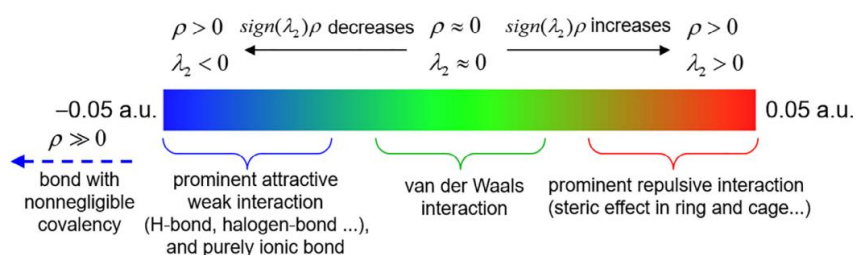


To a 25 mL of Schlenk tube equipped with a magnetic stir bar was added Cp<sup>\*</sup>Rh(OAc)<sub>2</sub> (7.6 mg, 0.02 mmol), CsOAc (76.8 mg, 0.4 mmol), **S1** (31.4 mg, 0.2 mmol), **S2** (58.6 mg, 0.3 mmol) and MeOH (2 ml). After being stirred at 80 °C overnight, the crude product was purified by silica gel chromatography on silica gel (eluent: 0-7% of methanol in dichloromethane) to afford **73**<sup>[15]</sup> (13.3 mg, 20%, containing about 10% of **1**) as a white solid: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.91 (dd,  $J = 7.6, 2.2$  Hz, 1H), 7.70 - 7.66 (m, 1H), 7.56 - 7.52 (m, 1H), 7.51 - 7.35 (m, 5H), 7.34 - 7.23 (m, 6H), 5.97 (dd,  $J = 9.8, 2.2$  Hz, 1H), 5.89 (dd,  $J = 9.3, 1.9$  Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>)  $\delta$  170.50, 149.51, 149.46, 140.63, 138.11, 134.13, 129.94, 129.28, 128.65, 128.51, 128.32, 128.28, 127.78, 126.00, 125.67, 122.62, 122.45, 79.41.

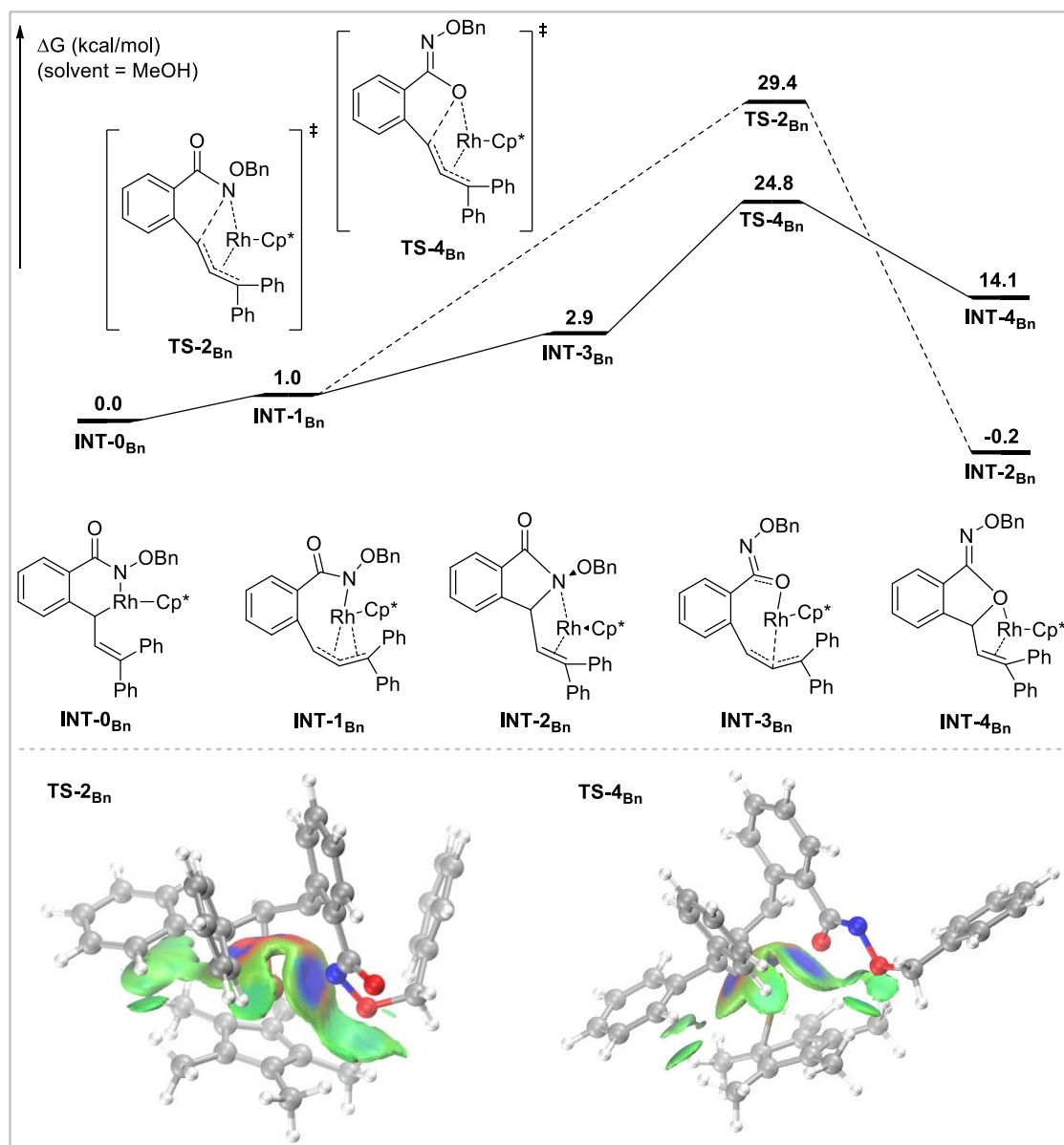
## 2.7 Computational Mechanistic Studies

### (1) Computational details:

Density functional theory (DFT) calculations were performed by using Gaussian 09 quantum chemical package.<sup>[S16]</sup> Unless otherwise specified, geometry optimizations were performed using B3LYP functional<sup>[S17]</sup> with the Stuttgart/Dresden effective core potential (SDD)<sup>[S18]</sup> was used for Rh in conjunction with a standard 6-31G(d,p) basis set for all other atoms. This level of theory is denoted as B3LYP/6-31G(d,p) SDD or B3LYP/BS1. Frequency analysis was conducted at the same level of theory to verify the stationary points to be real minima or saddle points and to obtain the thermodynamic energy corrections. Intrinsic reaction coordinate (IRC) calculation<sup>[S19]</sup> were carried out to confirm that all transition state structures connect the corresponding reactants and products. Solvent effects in Methanol were estimated by using the SMD<sup>[S20]</sup> solvation method at the M06 level of theory.<sup>[S21]</sup> Herein, SDD was used for Rh and 6-31G(d,p) basis set was used for hydrogen atoms meanwhile the 6-311++G(d,p) basis set was used for all other atoms. This level of theory is denoted as M06 SMD/6-311++G(d,p) SDD or M06 SMD/BS2. If not noted, the energies presented in this paper are the (M06 SMD/BS2)-calculated single point energies with (B3LYP/BS1)-calculated thermodynamic corrections which were calculated under standard conditions (1 atm and 298.15 K) (denoted as  $\Delta G_{\text{sol}}(\text{M06 SMD}/6\text{-}311\text{++G}(\text{d,p})\text{ SDD}/\text{B3LYP}/6\text{-}31\text{G}(\text{d,p})\text{ SDD})$  or  $\Delta G$  for clarity). The 3D diagrams of optimized structures are illustrated using CYLView.<sup>[S22]</sup>



**Figure S1.** Common interpretation of coloring method of mapped function  $\text{sign}(\lambda_2)\rho$  in IGMH maps



**Figure S2.** Computed Gibbs free energy changes from -OBn substituted substrate and weak interaction (IGMH) analysis using Multiwfn (version 3.7), isovalue = 0.005.

**Table S1.** Comparison of the key structures and the reaction barriers using different basis-sets.

OPT: <b>B3LYP</b> /6-31G(d)+ SDD for Rh	$\Delta G^1(\text{INT1})$ (kcal/mol)	$\Delta G^2(\text{TS-4})$ (kcal/mol)	$ \Delta G^1  +  \Delta G^2 $ (kcal/mol)
SP: SMD(MeOH) <b>M06</b> /6-311++G(d,p)+SDD for Rh	-3.4	24.5	27.9
SP: SMD(MeOH) <b>TPSS</b> TPSS /6-311++G(d,p)+SDD for Rh	-0.8	26.8	27.6

SP: SMD(MeOH) <b>M11L</b> /6-311++G(d,p)+SDD for Rh	-2.1	22.6	24.7
SP: SMD(MeOH) <b>M06L</b> /6-311++G(d,p)+SDD for Rh	-3.2	23.3	26.5
SP: SMD(MeOH) <b>M062X</b> /6- 311++G(d,p)+SDD for Rh	-2.2	26.8	29.0
SP: SMD(MeOH) <b>wb97xd</b> /6- 311++G(d,p)+SDD for Rh	-4.5	27.0	31.5

**Table S2.** Energy, enthalpy and free energy corrections of the structures calculated at B3LYP/BS1, single point energies at the M06 SMD/BS2//B3LYP/BS1 level (in Hartree) and imaginary frequencies of the transition states.

Structures	corr. to <i>ZPE</i>	corr. to <i>E</i>	corr. to <i>H</i>	corr. to <i>G</i>	SP <sub>SMD</sub>	Imaginary frequency
<b>INT-0</b>	0.585362	0.622003	0.622948	0.515015	-	-
					1593.01863818	
<b>TS-1</b>	0.585142	0.620954	0.621898	0.517323	-	-9.11
					1593.01942684	
<b>INT-1</b>	0.585870	0.622226	0.623170	0.518043	-	-
					1593.02712446	
<b>INT-1'</b>	0.650630	0.692924	0.693868	0.576204	-	-
					1822.07153555	
<b>TS-2</b>	0.583711	0.619585	0.620529	0.517637	-	-174.07
					1592.97207636	
<b>TS-2'</b>	0.648013	0.689414	0.690358	0.574713	-	-263.68
					1822.01444335	
<b>INT-2</b>	0.585598	0.621659	0.622603	0.518216	-	-
					1593.00959719	

<b>INT-2'</b>	0.650298	0.691629	0.692573	0.576446	-	-
					1822.06518743	
<b>TS-3</b>	0.583764	0.620031	0.620975	0.514932	-	-118.81
					1592.98563087	
<b>INT-3</b>	0.585558	0.621898	0.622842	0.517390	-	-
					1593.02042012	
<b>INT-3'</b>	0.650017	0.692104	0.693048	0.575391	-	-
					1822.07046070	
<b>TS-4</b>	0.583157	0.619464	0.620408	0.515468	-	-198.01
					1592.98011872	
<b>TS-4'</b>	0.647995	0.689728	0.690672	0.572221	-	-219.84
					1822.01436648	
<b>INT-4</b>	0.585176	0.621689	0.622633	0.516480	-	-
					1592.99887038	
<b>INT-4'</b>	0.648855	0.691482	0.692427	0.570278	-	-
					1822.04577289	
<b>PC-1</b>	0.362111	0.383758	0.384702	0.308552	-	-
					1092.50703612	
<b>PC-2</b>	0.362496	0.384095	0.385039	0.309632	-	-
					1092.53169836	
<b>HOAc</b>	0.062071	0.066602	0.067547	0.034989	-	-
					229.041981773	
<b>AgOAc</b>	0.050630	0.056762	0.057706	0.018490	-	-
					375.459440779	
<b>Cp*Rh(OAc)<sub>2</sub></b>					-	-
<b>+ 2Ag</b>	0.326508	0.355834	0.356778	0.261855	1251.43067945	-
<b>INT-0<sub>Bn</sub></b>	0.666709	0.707776	0.708720	0.589387	-1823.95171115	-
					-	-
<b>INT-1<sub>Bn</sub></b>	0.667674	0.708328	0.709273	0.593619	1823.95432126	-

---

<b>INT-3<sub>Bn</sub></b>	0.667631	0.707994	0.708938	0.593225	-	-
					1823.95085975	
<b>TS-4<sub>Bn</sub></b>	0.664678	0.705284	0.706228	0.589374	-	-199.05
					1823.91215871	
<b>TS-2<sub>Bn</sub></b>	0.665271	0.705525	0.706469	0.592215	-	-143.68
					1823.90771590	
<b>INT-4<sub>Bn</sub></b>	0.666767	0.707521	0.708466	0.590289	-	-
					1823.93015799	
<b>INT-2<sub>Bn</sub></b>	0.668002	0.708490	0.709434	0.593507	-	-
					1823.95619738	

---

### Cartesian coordinates of the optimized structures

#### INT-0

C	-2.24198300	1.85060900	1.65316300
C	-1.83445400	0.73117600	0.88372300
C	-0.80682300	1.17612600	-0.06191300
C	-1.37364400	2.95949700	1.28987800
C	-0.56066500	2.54002000	0.14858700
C	-2.47061700	-0.62799600	0.85968000
H	-3.02484200	-0.83380800	1.78005500
H	-3.18316700	-0.70507400	0.02612500
H	-1.73040300	-1.42393300	0.73081200
C	-0.15851600	0.29460000	-1.08582000
H	0.10345400	-0.68218900	-0.66586100
H	-0.83876500	0.11314600	-1.93006800
H	0.75409600	0.74618300	-1.48328200
C	0.37450500	3.40290900	-0.64624600
H	1.34993500	2.92438600	-0.77154200
H	-0.03787000	3.60581100	-1.64366600

H	0.54287200	4.36625800	-0.16008000
C	-1.52544600	4.36821600	1.78251200
H	-2.28281200	4.90106200	1.18914000
H	-1.84245300	4.39425400	2.82847800
H	-0.58912400	4.92616600	1.70562000
C	-3.38686800	1.91719400	2.62030200
H	-3.18321600	2.60851300	3.44349100
H	-4.29823600	2.26526500	2.11467800
H	-3.61037600	0.93862100	3.05593000
Rh	-0.11830900	1.45025900	2.20678100
C	0.24565200	1.63664300	7.73392800
C	-0.33334000	1.14964300	6.56639700
C	0.29501400	1.27580000	5.31269400
C	1.53304900	1.94576500	5.25558700
C	2.11608700	2.42247600	6.44174100
C	1.48685200	2.27444200	7.67184200
H	-0.26707500	1.51693900	8.68523300
H	-1.29393500	0.64080900	6.61703000
H	3.07981300	2.91215500	6.35853900
H	1.95588300	2.65792500	8.57417400
C	2.32747600	2.23194900	4.01100100
O	3.50680700	2.59256400	4.10273200
N	1.67128700	2.12648200	2.80949500
O	2.47506200	2.49108100	1.69930800
C	2.82930800	3.87820300	1.69199900
H	3.56420600	4.09707800	2.46767500
H	3.25246300	4.05799500	0.69915200
H	1.93916200	4.50673100	1.83014600
C	-0.42876200	0.68921200	4.14103000



H	-1.50388700	0.79674000	4.30961900
C	-0.18584700	-0.69679300	3.66899400
H	-1.05217100	-1.09000600	3.14376800
C	0.85653100	-1.57894400	3.76339300
C	2.15867800	-1.31104400	4.45126900
C	2.33655500	-1.74545000	5.77516900
C	3.24266200	-0.72555100	3.78287000
C	3.56086000	-1.57764200	6.42011000
H	1.50579600	-2.21157000	6.29817400
C	4.46963000	-0.55890500	4.42954800
H	3.12040500	-0.37720200	2.76175800
C	4.63228800	-0.98487800	5.74723700
H	3.67795800	-1.90933000	7.44872000
H	5.28859100	-0.07757100	3.90404300
H	5.58587300	-0.84972800	6.25084700
C	0.69596600	-2.94798900	3.19640600
C	1.80996700	-3.65733800	2.70403200
C	-0.55814000	-3.59233300	3.14104400
C	1.66988500	-4.92657000	2.14500800
H	2.79286200	-3.20078800	2.75423500
C	-0.69666700	-4.86328000	2.58706100
H	-1.42919700	-3.10818300	3.57249600
C	0.41604400	-5.53713100	2.07813400
H	2.54766700	-5.44174400	1.76318000
H	-1.67534400	-5.33663400	2.57047900
H	0.30905800	-6.53029700	1.65031200

**TS-1**

C	-2.23346200	1.87348900	1.68841500
---	-------------	------------	------------

C	-1.88542500	0.70524200	0.96083300
C	-0.83777900	1.05988300	0.00124300
C	-1.31142700	2.92219200	1.28419400
C	-0.51957200	2.41621000	0.16370600
C	-2.58999200	-0.61994900	0.99136500
H	-3.14212400	-0.76529800	1.92483000
H	-3.31639100	-0.69016300	0.16932400
H	-1.89214800	-1.45635400	0.88210000
C	-0.23694800	0.11069800	-0.99122800
H	-0.03370800	-0.86637100	-0.54046000
H	-0.92187000	-0.05674100	-1.83466900
H	0.70246700	0.49649400	-1.39601800
C	0.45431100	3.20011900	-0.66555000
H	1.40884800	2.67550300	-0.76438900
H	0.05318100	3.37327500	-1.67311700
H	0.66170900	4.17684200	-0.22360700
C	-1.39280500	4.35589900	1.71853700
H	-2.11147500	4.90539600	1.09307900
H	-1.72196400	4.44115800	2.75770500
H	-0.42619700	4.85895800	1.63543400
C	-3.36988700	2.03412700	2.65450100
H	-3.12828600	2.74783900	3.44770000
H	-4.26605500	2.40461700	2.13765500
H	-3.63813100	1.08602300	3.13065100
Rh	-0.13306400	1.38060700	2.25812300
C	0.19037100	1.73321900	7.78304600
C	-0.38374000	1.21867500	6.62506400
C	0.25450900	1.30585900	5.37256100
C	1.49696200	1.96741000	5.30486200

C	2.07344800	2.47318900	6.48190400
C	1.43555300	2.36217000	7.71152100
H	-0.32952400	1.64249600	8.73365100
H	-1.34855500	0.71860400	6.68268200
H	3.04049100	2.95483600	6.39101300
H	1.90085300	2.76789200	8.60607100
C	2.30713100	2.21043300	4.05973600
O	3.48706200	2.57159100	4.15739700
N	1.66600600	2.06286400	2.85891100
O	2.48991200	2.35264500	1.74110800
C	2.88441100	3.72700200	1.67003200
H	3.62243000	3.95988200	2.43844700
H	3.31425700	3.84804000	0.67103200
H	2.01325600	4.38744800	1.77625100
C	-0.47084500	0.69716900	4.21557800
H	-1.54608700	0.80299600	4.38130100
C	-0.21701800	-0.66939900	3.70685500
H	-1.09440500	-1.07192300	3.20885200
C	0.85900700	-1.52199900	3.71947400
C	2.15924000	-1.25089300	4.40919400
C	2.30166300	-1.62441700	5.75568400
C	3.26947700	-0.72442800	3.73401800
C	3.52026900	-1.46352600	6.41325200
H	1.44856500	-2.03929500	6.28558900
C	4.48890900	-0.56149500	4.39507300
H	3.17204600	-0.41143000	2.69887400
C	4.61874700	-0.93308600	5.73284500
H	3.61058300	-1.75058400	7.45779300
H	5.32933100	-0.12479500	3.86438700

H	5.56749800	-0.80109000	6.24622000
C	0.72292000	-2.86400600	3.08627400
C	1.84724100	-3.52726200	2.55387000
C	-0.51859900	-3.53162900	3.00505400
C	1.72852300	-4.76910100	1.93202800
H	2.82225500	-3.05759500	2.62378700
C	-0.63515200	-4.77600500	2.38967900
H	-1.39761400	-3.09088000	3.46529400
C	0.48702600	-5.40086300	1.84047600
H	2.61438800	-5.24667400	1.52121200
H	-1.60427400	-5.26765600	2.35618100
H	0.39697200	-6.37308200	1.36359300

**INT-1**

C	-2.16318400	1.74143000	1.78754500
C	-1.93903300	0.44936100	1.20719900
C	-0.83969000	0.56037200	0.26602000
C	-1.12876700	2.61638500	1.31430600
C	-0.33898300	1.87774600	0.33292300
C	-2.82314600	-0.75680300	1.34745500
H	-3.35695100	-0.76421600	2.30336700
H	-3.58263400	-0.77576200	0.55326900
H	-2.25001500	-1.68617400	1.27480200
C	-0.37486600	-0.52477800	-0.65742700
H	-0.27014800	-1.48676300	-0.14599000
H	-1.09255500	-0.66636600	-1.47828300
H	0.59257600	-0.27828600	-1.10336300
C	0.72973000	2.44668100	-0.55272800
H	1.62546400	1.82021500	-0.55621000

H	0.36330300	2.52700600	-1.58514400
H	1.02856800	3.44553300	-0.23102500
C	-1.02327300	4.08724400	1.59263100
H	-1.56767100	4.66930000	0.83535300
H	-1.44108700	4.33948300	2.57113100
H	0.01714100	4.42073200	1.58821200
C	-3.30191600	2.12462200	2.68729200
H	-3.01955800	2.91955700	3.38346200
H	-4.15291000	2.49020500	2.09580900
H	-3.66102100	1.27516900	3.27684200
Rh	-0.13127300	0.99539900	2.50320000
C	-0.01053800	2.19934000	7.97016200
C	-0.56195500	1.54962700	6.87117300
C	0.11364700	1.46145700	5.63642800
C	1.36583300	2.09629900	5.51348600
C	1.91416700	2.74243800	6.63370500
C	1.24521900	2.79814800	7.85055700
H	-0.55709700	2.23764700	8.90907800
H	-1.53744900	1.07676300	6.96563200
H	2.88997900	3.19706500	6.50593000
H	1.69436900	3.31177200	8.69663500
C	2.22896400	2.16840900	4.27524500
O	3.42042700	2.49341900	4.39616700
N	1.61394100	1.96205100	3.08173100
O	2.51939100	1.96758500	1.97896300
C	3.06752800	3.26108900	1.71720900
H	3.79277100	3.53617300	2.48439100
H	3.54928700	3.17549300	0.73763100
H	2.27592600	4.02072500	1.66926300

C	-0.62095300	0.71613500	4.57554800
H	-1.69352300	0.85987500	4.71071400
C	-0.37503100	-0.57647600	3.97291300
H	-1.28234600	-1.08962800	3.66511500
C	0.83437500	-1.13071700	3.50896900
C	2.13290400	-0.98379300	4.24409400
C	2.14078600	-1.36152500	5.59933700
C	3.35065100	-0.63134400	3.64396400
C	3.32918000	-1.39968000	6.32732400
H	1.20639300	-1.63964300	6.07879800
C	4.53645500	-0.66295500	4.37576000
H	3.36455300	-0.25377000	2.62833900
C	4.53455600	-1.05608000	5.71440100
H	3.30931300	-1.69520100	7.37309100
H	5.46252400	-0.35340400	3.90015400
H	5.46224200	-1.07705400	6.28006400
C	0.74287300	-2.34014600	2.62300100
C	1.69223000	-2.58110000	1.61249700
C	-0.26792500	-3.30373600	2.80645000
C	1.62243800	-3.71979100	0.81101200
H	2.48877100	-1.86511200	1.44782800
C	-0.33669500	-4.44549500	2.00611600
H	-0.98880400	-3.18354800	3.60982400
C	0.60619600	-4.65913800	1.00010000
H	2.36849000	-3.87258900	0.03542800
H	-1.12146100	-5.17641300	2.18387400
H	0.55660300	-5.54946100	0.37933400

**INT-1'**

C	-3.64102200	0.70630800	1.40111100
C	-2.84806100	0.75883100	2.59179800
C	-2.05505700	-0.44869100	2.68566400
C	-3.28167500	-0.50503000	0.70672300
C	-2.31287200	-1.21267400	1.50746700
C	-2.92932800	1.82161400	3.64590500
H	-3.09083500	2.81044500	3.20782800
H	-3.76738100	1.61467600	4.32590000
H	-2.01470700	1.85990300	4.24092900
C	-1.28964700	-0.88802400	3.89641900
H	-0.76697700	-0.04975900	4.35983800
H	-1.98033300	-1.31996300	4.63572400
H	-0.53929300	-1.64618400	3.66283400
C	-1.76481400	-2.57427800	1.20160200
H	-0.76142600	-2.70008700	1.61469500
H	-2.40431100	-3.35565700	1.63564400
H	-1.71439300	-2.75876300	0.12401500
C	-3.97821800	-1.06353400	-0.49793400
H	-4.78479200	-1.73868900	-0.17798400
H	-4.42350900	-0.28080800	-1.11424100
H	-3.30352600	-1.64182000	-1.13518100
C	-4.73375900	1.66163400	1.02373200
H	-4.85450300	1.73218800	-0.06020200
H	-5.69655600	1.33359600	1.44158800
H	-4.53735400	2.66707600	1.40826700
Rh	-1.42281600	0.82236600	0.83664800
C	3.27225200	3.15301400	-0.11211300
C	2.08361000	2.45199600	-0.28746500
C	1.88165800	1.16278000	0.24007300

C	2.95590000	0.60167900	0.99006800
C	4.16081400	1.30447100	1.13008400
C	4.32825500	2.57641400	0.59358200
H	3.37123500	4.14544500	-0.54403600
H	1.29660900	2.91090700	-0.86050800
H	4.96386100	0.82362700	1.67798800
H	5.26772000	3.10649300	0.72373800
C	2.97209300	-0.72354400	1.71092600
O	3.97581300	-1.42421700	1.75616100
N	1.78193900	-1.06882500	2.32442900
O	1.87361600	-2.04359200	3.34122400
C	1.97986700	-3.36053700	2.79942400
H	2.93321100	-3.49399000	2.28356000
H	1.92376100	-4.02267100	3.66783100
H	1.14886500	-3.57826400	2.11596100
C	0.68412500	0.35674900	-0.08782700
H	0.84653300	-0.69566300	0.12124900
C	-0.37023200	0.52322900	-1.03903000
H	-0.73861600	-0.43491100	-1.39588700
C	-1.22077800	1.61841800	-1.39443800
C	-0.84865800	3.07428800	-1.56394100
C	-0.13786400	3.42620300	-2.72741400
C	-1.30325900	4.10124300	-0.72776800
C	0.14580900	4.75869000	-3.02197500
H	0.19909000	2.64213800	-3.40086100
C	-1.02602500	5.43778000	-1.02780700
H	-1.84207800	3.84756600	0.17551800
C	-0.29849400	5.77276100	-2.16963100
H	0.70683400	5.00394200	-3.92003500



H	-1.38005900	6.21898000	-0.35988900
H	-0.08257700	6.81326700	-2.39728900
C	-2.35871000	1.28663400	-2.33089200
C	-3.50422200	2.10588300	-2.37440300
C	-2.29149700	0.22609100	-3.25366200
C	-4.54999000	1.84820600	-3.25843100
H	-3.56710300	2.96180000	-1.71038000
C	-3.33479900	-0.02882000	-4.14654900
H	-1.40140000	-0.39330200	-3.30791800
C	-4.47553200	0.77289100	-4.14865200
H	-5.42199400	2.49730400	-3.25933400
H	-3.24360400	-0.85062900	-4.85222600
H	-5.28584600	0.57698300	-4.84530900
H	1.20804500	-0.28427300	2.66344100
C	0.82694700	3.84746600	3.07309100
H	0.92113500	3.86111300	4.16235300
H	1.82806800	3.97743600	2.64614300
H	0.19705300	4.67254900	2.73264000
C	0.28462600	2.49683700	2.61584700
O	0.62576200	1.46498300	3.21610400
O	-0.49533300	2.56791800	1.58363700

**TS-2**

C	-3.07508100	-1.82179200	-1.24777300
C	-3.21307900	-0.37269600	-1.19087600
C	-2.92977900	0.05098000	0.16550800
C	-2.59971900	-2.26164700	-0.00656500
C	-2.44441600	-1.09225200	0.86123800
C	-3.94543700	0.43328300	-2.22374700

H	-3.65948700	0.15264800	-3.24159800
H	-5.02843400	0.26504700	-2.12878300
H	-3.76494700	1.50391500	-2.11584900
C	-3.21286700	1.40423700	0.74827600
H	-3.10592400	2.19751500	0.00418300
H	-4.24341400	1.44981700	1.13002900
H	-2.54464900	1.63476800	1.58341400
C	-2.02584900	-1.15704900	2.30177900
H	-1.80561200	-0.16266800	2.69993500
H	-2.82460700	-1.59129600	2.92050200
H	-1.13100400	-1.77310500	2.42218800
C	-2.40538700	-3.68364700	0.42482900
H	-2.06774600	-4.32028000	-0.39949700
H	-1.67071300	-3.75624700	1.22757400
H	-3.35203700	-4.10245700	0.79658900
C	-3.42376200	-2.67223100	-2.43313300
H	-3.16749700	-2.17787800	-3.37606900
H	-2.90686600	-3.63638900	-2.40570900
H	-4.50329900	-2.88023700	-2.46526600
Rh	-1.01737800	-0.58885300	-0.84081200
C	4.72408600	0.49921200	-2.45057100
C	3.45141600	0.04554700	-2.79598300
C	2.60538700	-0.47400800	-1.80676300
C	3.03958000	-0.51632100	-0.48008800
C	4.30918000	-0.04650700	-0.13303400
C	5.15108200	0.46196900	-1.11789700
H	5.38539700	0.88265800	-3.22322600
H	3.11868300	0.08389100	-3.83013300
H	4.61511800	-0.11108500	0.90631700

H	6.14202100	0.82251100	-0.85538400
C	2.16702400	-1.20483100	0.50844900
O	2.58236400	-1.57255100	1.60915400
N	0.94002900	-1.53191800	-0.03819700
O	0.39591100	-2.69787300	0.55436300
C	1.19329800	-3.85560400	0.30893800
H	2.16657600	-3.78319800	0.80273500
H	0.62750500	-4.69027900	0.73231600
H	1.32520000	-4.01318200	-0.77047000
C	1.25511300	-0.97856300	-2.19280200
H	1.21688600	-1.97622400	-2.62578500
C	0.20630600	-0.10243100	-2.55328000
H	-0.43095400	-0.43747800	-3.36672200
C	-0.11651400	1.15086600	-1.88451400
C	0.87199300	1.93342300	-1.03667600
C	1.77793200	2.80241100	-1.67062700
C	0.83861200	1.92858200	0.36381800
C	2.63754700	3.61210200	-0.93149600
H	1.80530900	2.84103200	-2.75633700
C	1.69327500	2.74600000	1.10934400
H	0.14246700	1.26529500	0.86700900
C	2.59733700	3.58903900	0.46548600
H	3.33684700	4.26606900	-1.44649800
H	1.65040200	2.71641500	2.19503300
H	3.26404400	4.22394000	1.04325700
C	-1.05539700	2.08345900	-2.60363700
C	-1.56720100	3.21823200	-1.94060400
C	-1.40314400	1.92642000	-3.95893100
C	-2.41332100	4.12024300	-2.58247600

H	-1.28120800	3.39751700	-0.90959700
C	-2.24625800	2.83196600	-4.60594000
H	-0.99157400	1.10446400	-4.53569800
C	-2.76564000	3.93058300	-3.92158900
H	-2.79037000	4.98114700	-2.03595400
H	-2.48509800	2.68101200	-5.65590500
H	-3.41878900	4.63712500	-4.42632100

**TS-2'**

C	-4.15044300	0.34983700	1.19146800
C	-3.66567300	0.76505000	2.46045600
C	-2.70952700	-0.23243800	2.94742300
C	-3.38229500	-0.80622300	0.80334300
C	-2.56756500	-1.21189700	1.94544000
C	-4.12563300	1.94503600	3.26132200
H	-4.84187200	2.55549600	2.70470100
H	-4.60923300	1.62373100	4.19363200
H	-3.27330100	2.58226100	3.51960000
C	-2.06953400	-0.22098500	4.30506400
H	-1.94059000	0.80210000	4.66900600
H	-2.68729600	-0.75528300	5.04168900
H	-1.08129900	-0.68962400	4.28853600
C	-1.78467900	-2.48680300	2.04397200
H	-0.99081500	-2.40619500	2.78933700
H	-2.43953000	-3.32084600	2.33628100
H	-1.32613900	-2.76026100	1.08805400
C	-3.64308800	-1.65064300	-0.41136900
H	-4.47120600	-2.35090200	-0.22905000
H	-3.90679600	-1.04134600	-1.27974600

H	-2.76875000	-2.25146600	-0.68309900
C	-5.30015300	0.93806200	0.43258900
H	-5.15639100	0.86197900	-0.64747400
H	-6.23227700	0.40794700	0.67853500
H	-5.45157300	1.99426100	0.67492300
Rh	-1.83044400	0.80761500	1.09124200
C	3.53736900	2.11903200	-2.23366500
C	2.34016000	1.49599000	-1.88611200
C	2.23062000	0.85528000	-0.64603700
C	3.33616500	0.86016700	0.22317000
C	4.53815800	1.48629700	-0.12556200
C	4.63392200	2.12063000	-1.35863000
H	3.61878100	2.61279500	-3.19792200
H	1.49739300	1.50859400	-2.56830300
H	5.36860000	1.46538100	0.57333200
H	5.55596900	2.61711000	-1.64668000
C	3.14626000	0.12696000	1.48255500
O	4.00071900	-0.32139900	2.21995200
N	1.72330800	-0.08220500	1.65544000
O	1.37348200	-1.13311300	2.51436600
C	1.86438400	-2.40788600	2.08958200
H	2.95640800	-2.43551800	2.08414300
H	1.48234000	-3.10676200	2.83589700
H	1.46518700	-2.67965200	1.10447700
C	1.04431900	0.04020500	-0.24565100
H	1.24273100	-1.02406000	-0.35609200
C	-0.34032700	0.33244000	-0.47839300
H	-0.84738600	-0.57750500	-0.79117700
C	-1.08537400	1.55146500	-0.85089600

C	-0.44682500	2.91719100	-0.88713500
C	-0.75535500	3.84580000	-1.90574500
C	0.52937700	3.32182600	0.04461300
C	-0.15156200	5.10293000	-1.96675500
H	-1.46897800	3.58694400	-2.67726300
C	1.13635400	4.57337000	-0.01507000
H	0.82885200	2.65185600	0.83376700
C	0.79654100	5.48260300	-1.01855300
H	-0.42499300	5.78260200	-2.77046900
H	1.88426000	4.83314500	0.73023300
H	1.26637800	6.46171100	-1.06353000
C	-2.10430300	1.32525300	-1.94231400
C	-3.28513000	2.09058700	-1.99666400
C	-1.88913700	0.40280600	-2.98146400
C	-4.20655500	1.93584000	-3.03057900
H	-3.47057700	2.81536500	-1.20925600
C	-2.81822300	0.23242100	-4.01247900
H	-0.97263300	-0.18044100	-2.99648900
C	-3.98268400	0.99794300	-4.04440200
H	-5.10674300	2.54573200	-3.04226300
H	-2.61900700	-0.49145400	-4.79911200
H	-4.70324200	0.87359000	-4.84828200
H	1.25393900	0.78979500	2.13087600
C	-0.15456300	3.85336100	3.97374900
H	0.59687800	3.74839300	4.75937400
H	0.06639700	4.75760200	3.39367300
H	-1.14890600	3.97956800	4.41105000
C	-0.12147900	2.65494800	3.03130200
O	0.93482900	1.96491800	3.01182100

O	-1.14672100	2.49569800	2.30088800
---	-------------	------------	------------

**INT-2**

C	-3.15987300	-1.76588700	-1.12370100
C	-3.34526600	-0.32053900	-1.08306000
C	-3.12192600	0.12864400	0.28683100
C	-2.66045700	-2.15476900	0.12922600
C	-2.61594400	-0.97308100	1.00186800
C	-4.06427900	0.46899800	-2.13783200
H	-3.79118800	0.14300200	-3.14545300
H	-5.15232900	0.34253300	-2.03252800
H	-3.84521300	1.53671900	-2.06911700
C	-3.42031200	1.50384100	0.80986200
H	-3.19039400	2.27686100	0.07010300
H	-4.48548400	1.60592000	1.06531600
H	-2.84606900	1.72769600	1.71459500
C	-2.20320500	-1.01454500	2.44645900
H	-2.08539300	-0.00832200	2.85976200
H	-2.95178700	-1.53680200	3.05976500
H	-1.25074000	-1.53936600	2.57840800
C	-2.33390700	-3.54571900	0.58715600
H	-2.17893800	-4.22202000	-0.25865300
H	-1.42483500	-3.56349000	1.19465400
H	-3.15092700	-3.95778100	1.19766700
C	-3.48097500	-2.64790100	-2.29542200
H	-3.24261600	-2.15839400	-3.24555000
H	-2.92254100	-3.58861000	-2.25799100
H	-4.55114000	-2.90242800	-2.32390200
Rh	-1.17043200	-0.54000100	-0.78895600

C	4.79741100	0.38834700	-2.39321400
C	3.54354200	-0.09579800	-2.77570800
C	2.67723800	-0.54461300	-1.78216800
C	3.06318900	-0.49455100	-0.44007500
C	4.30688400	0.00433200	-0.04781300
C	5.17693900	0.44446700	-1.04263000
H	5.49400600	0.72703100	-3.15575800
H	3.25847000	-0.12455600	-3.82409200
H	4.57608100	0.03369200	1.00353300
H	6.15608800	0.83188800	-0.77618200
C	2.02744900	-1.10909100	0.40814300
O	2.03860800	-1.35052700	1.59431000
N	0.93877000	-1.50296500	-0.48525300
O	0.58273200	-2.87566400	-0.31591100
C	1.68859900	-3.78371500	-0.40947000
H	2.39278100	-3.65223300	0.41824800
H	1.22683300	-4.77120600	-0.34182600
H	2.21180500	-3.69594000	-1.37026400
C	1.28189600	-1.12362600	-1.90710800
H	1.28235700	-2.03961900	-2.50586300
C	0.14018100	-0.23365700	-2.38942200
H	-0.20599700	-0.47326000	-3.39031500
C	-0.14363800	1.07581600	-1.82885700
C	0.83013000	1.86227800	-0.96579600
C	1.80203400	2.66795100	-1.58782500
C	0.74761600	1.90510900	0.43290800
C	2.67686800	3.45407600	-0.84065200
H	1.86562000	2.67675100	-2.67276600
C	1.61863900	2.69766900	1.18766700



H	-0.01128200	1.30401300	0.92537100
C	2.58990300	3.47174800	0.55491200
H	3.42516600	4.05853600	-1.34771100
H	1.53199900	2.70710300	2.27133300
H	3.26859500	4.08840300	1.13875800
C	-1.03373200	2.00400100	-2.61763500
C	-1.51919300	3.18515600	-2.01756600
C	-1.38865000	1.78558300	-3.96246500
C	-2.33113100	4.08096600	-2.71084300
H	-1.24509400	3.40346100	-0.99041800
C	-2.19791000	2.68357200	-4.66074800
H	-1.01952000	0.91230800	-4.48975800
C	-2.68078000	3.83629000	-4.04119400
H	-2.68605200	4.97823800	-2.20939800
H	-2.44257900	2.48117400	-5.70097300
H	-3.30823300	4.53606700	-4.58656700

**INT-2'**

C	-4.17112200	0.30517500	1.19934900
C	-3.76014000	0.59373700	2.50423300
C	-2.73338900	-0.38363000	2.90390400
C	-3.30733100	-0.76615600	0.70586600
C	-2.52375000	-1.26843000	1.82946100
C	-4.30209000	1.65339200	3.41833400
H	-4.93854600	2.36206800	2.88116600
H	-4.90097500	1.21538800	4.22950100
H	-3.49467400	2.22765900	3.88658600
C	-2.18902700	-0.50975600	4.29836400
H	-2.00489200	0.46603800	4.75880500

H	-2.89716000	-1.04151500	4.95127400
H	-1.24650500	-1.06535500	4.31940700
C	-1.70942200	-2.52955000	1.83166900
H	-0.94670000	-2.51484600	2.61556800
H	-2.34434800	-3.41082700	2.00676000
H	-1.19908300	-2.68533800	0.87549200
C	-3.54650900	-1.51909800	-0.57234000
H	-4.36386100	-2.24396100	-0.44313300
H	-3.82002900	-0.85201900	-1.39327700
H	-2.66174300	-2.08297700	-0.88480700
C	-5.30769200	0.91915500	0.44014300
H	-5.05748100	1.07455900	-0.61285500
H	-6.19398900	0.26778400	0.46965600
H	-5.60104600	1.88680800	0.85951200
Rh	-1.78428300	0.76883300	1.10675200
C	3.31497800	1.24471600	-3.03412100
C	2.18267300	0.70413700	-2.41665500
C	2.19244800	0.55401600	-1.03308700
C	3.31123500	0.95512400	-0.29575200
C	4.44317300	1.49574700	-0.90102600
C	4.43677300	1.63543800	-2.28847400
H	3.32384800	1.36706800	-4.11393800
H	1.31741500	0.42147000	-3.00801700
H	5.29447500	1.79607100	-0.29734900
H	5.30061100	2.05417900	-2.79703300
C	3.07238300	0.70394200	1.14248800
O	3.82894100	0.81035300	2.09594700
N	1.74079100	0.28959700	1.19965900
O	1.26546600	-0.35380600	2.33745900

C	1.99994700	-1.55116700	2.67041800
H	3.03666900	-1.30658600	2.90773400
H	1.48999400	-1.95495000	3.54723800
H	1.94317900	-2.26964500	1.84556200
C	1.13558800	-0.03956900	-0.10973800
H	1.18612600	-1.13547000	-0.20759500
C	-0.34305400	0.30871000	-0.36131600
H	-0.78023800	-0.55823000	-0.85468900
C	-0.96293800	1.54621900	-0.81846600
C	-0.27031800	2.88176200	-0.77136900
C	-0.52501600	3.88117500	-1.73602500
C	0.71191900	3.18788500	0.19205000
C	0.13550500	5.11009900	-1.71802500
H	-1.23968500	3.69844400	-2.52844800
C	1.37757100	4.41091900	0.20935500
H	0.95665200	2.45350900	0.94362700
C	1.09078700	5.39068600	-0.74255200
H	-0.09682800	5.84660800	-2.48376400
H	2.13137700	4.59448700	0.97188400
H	1.60806400	6.34651800	-0.72928800
C	-1.98604200	1.41253400	-1.91869900
C	-3.13041200	2.23357500	-1.95328600
C	-1.81523100	0.51068600	-2.98341800
C	-4.05409900	2.15453100	-2.99424600
H	-3.28773500	2.94055700	-1.14352100
C	-2.74516800	0.41697000	-4.02303000
H	-0.93741700	-0.12876400	-3.00563700
C	-3.87025900	1.23986800	-4.03679700
H	-4.92511200	2.80560600	-2.98881000

H	-2.57872400	-0.29386300	-4.82900800
H	-4.59186700	1.17560800	-4.84679900
H	0.56206200	0.96960000	3.30150800
C	-0.42728600	3.89766500	4.27836100
H	-0.55506900	3.63743100	5.33355600
H	0.52295100	4.43568200	4.18613800
H	-1.24064000	4.53974400	3.93982800
C	-0.37092700	2.65165900	3.43244300
O	0.46794600	1.74334700	3.91400000
O	-1.02441500	2.52258300	2.40152300

**TS-3**

C	-1.82646600	-2.86942200	-0.29805000
C	-2.45662000	-1.58903900	-0.56749100
C	-2.58618200	-0.91993500	0.67550600
C	-1.83014500	-3.06994300	1.15568600
C	-2.23495500	-1.87193000	1.74703300
C	-2.97142100	-1.15795900	-1.90853300
H	-2.21541100	-1.24115200	-2.69672900
H	-3.81176200	-1.80296900	-2.20010600
H	-3.33924100	-0.12938600	-1.89513800
C	-3.17964100	0.43582400	0.91864600
H	-2.68345500	0.94183600	1.75235300
H	-3.09324800	1.08467100	0.04398100
H	-4.24544000	0.35037900	1.17482300
C	-2.30793400	-1.55340400	3.20901200
H	-3.35112900	-1.52126800	3.55294100
H	-1.77564000	-2.29628300	3.80726900
H	-1.86247500	-0.57641900	3.42433600

C	-1.44406000	-4.34473900	1.83509000
H	-2.29158400	-5.04483300	1.83022200
H	-0.60996000	-4.83145200	1.32420300
H	-1.14624000	-4.17818900	2.87177900
C	-1.56982300	-3.94069600	-1.31532700
H	-0.74106300	-4.58591700	-1.01210400
H	-2.46016900	-4.57365000	-1.44445900
H	-1.32059700	-3.51388200	-2.29089900
Rh	-0.38980000	-1.37798500	0.30760700
C	4.02627900	0.11758500	-2.59436100
C	2.63272100	0.07836800	-2.59728000
C	1.92770600	-0.29405900	-1.44411000
C	2.64835300	-0.64407800	-0.30095400
C	4.04580800	-0.60529600	-0.28997000
C	4.73578800	-0.21882600	-1.43743300
H	4.56089200	0.41391700	-3.49320200
H	2.08233900	0.35342800	-3.49406500
H	4.58717800	-0.88214100	0.61108100
H	5.82205300	-0.18691200	-1.43369500
C	1.87779300	-1.08105100	0.91715500
O	1.57864900	-0.29924900	1.84701100
N	1.51337600	-2.40931500	0.82987300
O	1.17537600	-2.90247700	2.14848700
C	1.97703900	-4.04912100	2.37716700
H	3.04509600	-3.79505200	2.41150800
H	1.66666200	-4.43895600	3.35212000
H	1.82262900	-4.81416300	1.60392700
C	0.41999400	-0.33649100	-1.41396200
H	0.05276800	-0.98167100	-2.22211600

C	-0.32850600	0.93923400	-1.47172800
H	-1.36631300	0.77290800	-1.74063600
C	-0.02526800	2.26092600	-1.31104500
C	1.28215600	2.86042900	-0.91613200
C	1.84077800	3.86849300	-1.72621700
C	1.94745100	2.51429200	0.26951200
C	3.03770900	4.48923800	-1.37783300
H	1.32860900	4.16047400	-2.63923000
C	3.14287600	3.14564600	0.62200300
H	1.54270400	1.74559000	0.91882700
C	3.69396500	4.13110300	-0.19676700
H	3.45612700	5.25606900	-2.02518300
H	3.64084800	2.85829700	1.54439300
H	4.62433600	4.61961700	0.08195200
C	-1.12117500	3.24669000	-1.57016400
C	-1.28001200	4.37208800	-0.73862700
C	-2.03083600	3.08628200	-2.63309400
C	-2.32167000	5.27612100	-0.94032200
H	-0.58208700	4.52729500	0.07844900
C	-3.07110300	3.99326700	-2.83833400
H	-1.89866600	2.25730600	-3.32306000
C	-3.22545800	5.09100800	-1.98962200
H	-2.42766600	6.12925700	-0.27489400
H	-3.75127700	3.85053100	-3.67457000
H	-4.03243100	5.80074500	-2.15134400

**INT-3**

C	0.80114700	-3.05470800	0.12395800
C	1.44719800	-2.93779900	1.39208200

C	2.67881400	-2.21729800	1.18843200
C	1.69330500	-2.48548400	-0.88947200
C	2.85718300	-2.01054500	-0.23925900
C	0.95458200	-3.48705900	2.69883200
H	-0.13365100	-3.59355700	2.70571000
H	1.38572200	-4.47997200	2.88786100
H	1.23470000	-2.84708600	3.54183000
C	3.72971000	-1.95963900	2.22971000
H	4.29953500	-1.05196400	2.01140400
H	3.29468100	-1.85403300	3.22883400
H	4.44305600	-2.79471200	2.27349000
C	4.07215100	-1.39940900	-0.86896200
H	4.92824900	-2.08506300	-0.80284900
H	3.90511800	-1.17738600	-1.92600200
H	4.35877300	-0.46490900	-0.37651700
C	1.36481500	-2.44339800	-2.35020000
H	1.29862500	-3.45888800	-2.76274600
H	0.39676400	-1.95133800	-2.50024400
H	2.12353500	-1.89879700	-2.91921400
C	-0.48395700	-3.76368900	-0.18410500
H	-1.04125700	-3.23981700	-0.96604500
H	-0.28245400	-4.78634700	-0.53465500
H	-1.12650100	-3.83718600	0.69824100
Rh	0.96881100	-0.87203800	0.55829000
C	-3.39439300	1.88338400	2.82752300
C	-2.11480100	1.34445000	2.90552400
C	-1.54021900	0.62957100	1.83705000
C	-2.30506900	0.43292000	0.67038900
C	-3.59986000	0.98128200	0.60462200

C	-4.14293700	1.69923600	1.66255000
H	-3.80252000	2.44002300	3.66731100
H	-1.53173500	1.47901600	3.81430000
H	-4.16816000	0.82347200	-0.30448700
H	-5.14377300	2.11491100	1.57903200
C	-1.79183900	-0.33002200	-0.51044100
O	-0.51812500	-0.35156700	-0.79400100
N	-2.71960200	-0.88608800	-1.24127900
O	-2.15247500	-1.57960400	-2.34285200
C	-3.21934000	-2.09672400	-3.11648400
H	-3.85785500	-1.29200400	-3.50412500
H	-2.75356900	-2.62964900	-3.95134100
H	-3.84082300	-2.79124300	-2.53507900
C	-0.17744500	0.06139600	2.12226600
H	-0.20434000	-0.57769400	3.00734500
C	1.09398600	0.72550700	1.99112600
H	1.84071300	0.43786300	2.72560200
C	1.52799100	1.47039700	0.86353900
C	0.59897200	2.38449800	0.11063600
C	-0.00597500	3.43043400	0.82686400
C	0.38724300	2.31847000	-1.27508100
C	-0.79934300	4.37981800	0.18264300
H	0.15020400	3.49910400	1.89972000
C	-0.40234400	3.27034100	-1.92047100
H	0.80287300	1.49358300	-1.84079100
C	-0.99787000	4.30469200	-1.19629600
H	-1.26060100	5.17625500	0.76064000
H	-0.56372100	3.19184500	-2.99239000
H	-1.61655000	5.04143300	-1.70198700



C	2.98582700	1.81190800	0.74781300
C	3.53303300	2.23109600	-0.48143700
C	3.85995700	1.77307400	1.85415000
C	4.88070800	2.56552300	-0.60488900
H	2.89254800	2.30178900	-1.35229200
C	5.20772800	2.11333500	1.73293300
H	3.48573300	1.51103700	2.83817500
C	5.73110300	2.50675000	0.50057300
H	5.26416600	2.87987200	-1.57217200
H	5.84524600	2.08465200	2.61304100
H	6.77963400	2.77527900	0.40665500

**INT-3'**

C	-1.49794600	-1.66194100	1.49533400
C	-1.98612100	-1.85401200	0.17066700
C	-2.84954700	-0.74033300	-0.14620800
C	-2.09859600	-0.43593600	2.01573600
C	-2.98137700	0.08843000	1.03794100
C	-1.70380200	-3.03097800	-0.71558000
H	-0.69171400	-3.41700200	-0.56993000
H	-2.41273800	-3.84347300	-0.50185300
H	-1.82047000	-2.77416700	-1.77328900
C	-3.70211400	-0.61981200	-1.37542500
H	-3.90558400	0.42215700	-1.63311400
H	-3.23484000	-1.09574400	-2.24274700
H	-4.66831000	-1.11845400	-1.21415900
C	-3.93422100	1.23167200	1.20585800
H	-4.93928400	0.85570500	1.44554500
H	-3.62948000	1.89356400	2.02191700

H	-4.01872100	1.83483300	0.29789000
C	-1.89213100	0.07558400	3.40990900
H	-2.55461300	-0.44807400	4.11301600
H	-0.86354500	-0.09086500	3.73957000
H	-2.10266500	1.14595200	3.48647100
C	-0.74857800	-2.65810100	2.32783500
H	0.01039700	-2.17764800	2.94800800
H	-1.45504100	-3.18155700	2.98879800
H	-0.24564300	-3.40147100	1.70809000
Rh	-0.80556100	0.12748200	0.23060500
C	4.28852000	1.21533500	-1.08226400
C	2.89755500	1.18024200	-1.17189500
C	2.18976100	-0.03193100	-1.14436500
C	2.94565400	-1.22702200	-0.99932700
C	4.34000300	-1.18406500	-0.93228300
C	5.01983600	0.03271800	-0.97437100
H	4.79801700	2.17502200	-1.11483600
H	2.35959300	2.10848500	-1.28670800
H	4.88365500	-2.11883800	-0.83904300
H	6.10481300	0.05507800	-0.92060200
C	2.27154600	-2.55015800	-0.86129300
O	1.52325700	-2.76802600	0.22803500
N	2.44087700	-3.41545200	-1.79861100
O	1.74749500	-4.61482900	-1.50677300
C	1.98940300	-5.52478200	-2.56441500
H	3.05884300	-5.75351900	-2.66054900
H	1.44169500	-6.43481100	-2.30223000
H	1.62255400	-5.13622300	-3.52401700
C	0.73676400	-0.15749200	-1.40009200

H	0.51387200	-1.13687800	-1.81831100
C	-0.27953900	0.78146000	-1.78087400
H	-1.02996700	0.32433000	-2.42018700
C	-0.66499500	2.05673300	-1.28353500
C	0.22912600	3.18338000	-0.82425500
C	0.91286500	3.90507300	-1.82081200
C	0.27411100	3.66354800	0.49042000
C	1.65073800	5.04590300	-1.50639900
H	0.86146000	3.56539400	-2.85237300
C	1.00669900	4.81109400	0.80423200
H	-0.23968300	3.11682100	1.26987200
C	1.70077800	5.50389600	-0.18796200
H	2.17692600	5.58014700	-2.29323000
H	1.03477100	5.16147800	1.83290300
H	2.27079700	6.39497500	0.06123800
C	-1.95996900	2.61484400	-1.81948300
C	-2.69067600	3.56526800	-1.07964500
C	-2.44113800	2.29049100	-3.10315200
C	-3.86193100	4.13217300	-1.57966500
H	-2.32837700	3.86836500	-0.10288800
C	-3.61057100	2.86210400	-3.60769500
H	-1.88149700	1.60990700	-3.73740100
C	-4.33379700	3.78063900	-2.84659700
H	-4.40328500	4.85775600	-0.97802100
H	-3.94548100	2.59691900	-4.60721500
H	-5.24149000	4.22915600	-3.24060500
H	1.58720800	-1.99661200	0.86843700
C	2.59646000	1.23806800	2.83756200
H	2.96552500	0.69728100	3.71256100

H	3.45389600	1.47789500	2.19764200
H	2.12165900	2.17578200	3.13591500
C	1.64378700	0.35527100	2.03846200
O	1.82288800	-0.87882000	2.04733900
O	0.73754400	1.00235700	1.39449200

**TS-4**

C	1.14697400	-3.28506800	-0.01624600
C	2.01872200	-3.12975400	1.07636400
C	3.01358100	-2.12289600	0.70589300
C	1.62803400	-2.43568800	-1.11294600
C	2.82687400	-1.79683100	-0.69377900
C	1.96195400	-3.83924300	2.39673700
H	0.96278400	-4.23483300	2.59926700
H	2.66424300	-4.68514300	2.41886000
H	2.23367400	-3.17642100	3.22500300
C	4.21921700	-1.76832600	1.52547900
H	4.63912100	-0.80360900	1.23266900
H	3.98130800	-1.71463100	2.59241700
H	5.00360800	-2.52925200	1.40172500
C	3.76233100	-0.98578700	-1.53792000
H	4.60419100	-1.60374900	-1.88184600
H	3.26074500	-0.58902700	-2.42542600
H	4.17845700	-0.13957500	-0.98450900
C	0.99428200	-2.38538400	-2.47101400
H	1.13457500	-3.33847300	-3.00103200
H	-0.08154300	-2.20026500	-2.38779600
H	1.43167700	-1.59629000	-3.08961900
C	-0.07680900	-4.14533300	-0.10924700

H	-0.93599600	-3.55883000	-0.45178600
H	0.07967200	-4.96745800	-0.82175600
H	-0.33312200	-4.58765800	0.85755000
Rh	1.10216900	-1.04150200	0.56651300
C	-3.30225200	2.90994400	2.46725400
C	-2.19420800	2.11380500	2.75674500
C	-1.86110600	1.04876200	1.91052500
C	-2.64723700	0.78654500	0.78303000
C	-3.75410100	1.58911600	0.49028000
C	-4.07967400	2.64857600	1.33324900
H	-3.55869700	3.73533300	3.12600300
H	-1.58807500	2.31842500	3.63563000
H	-4.34319600	1.36860500	-0.39371500
H	-4.94072400	3.27296400	1.11019000
C	-2.19061700	-0.38575900	-0.00076700
O	-1.19194400	-1.03091400	0.55578400
N	-2.84315000	-0.68558200	-1.08160600
O	-2.30486000	-1.83756600	-1.70747300
C	-3.14873800	-2.16822600	-2.79751700
H	-3.20574600	-1.34569800	-3.52219600
H	-2.69836400	-3.04648200	-3.26965200
H	-4.16288300	-2.41208500	-2.45592400
C	-0.72280000	0.14587800	2.25601600
H	-0.96159400	-0.61156700	3.00221400
C	0.65424700	0.42214300	2.13203300
H	1.27316800	0.00841700	2.92393600
C	1.30607700	1.10814500	1.02361200
C	0.52645600	2.02856800	0.10439800
C	0.24302300	3.33873400	0.52946800

C	0.15005200	1.66236200	-1.19387000
C	-0.41400900	4.24007900	-0.30488600
H	0.54207000	3.64847800	1.52752000
C	-0.50591700	2.56512400	-2.03604600
H	0.36665500	0.65552800	-1.53863000
C	-0.79155600	3.85592900	-1.59501400
H	-0.63130300	5.24405700	0.05104600
H	-0.79682500	2.25137300	-3.03511600
H	-1.30393700	4.55825700	-2.24739500
C	2.72123500	1.57260500	1.22586100
C	3.45415000	2.09556200	0.14002900
C	3.36162300	1.56024200	2.48055100
C	4.76308000	2.54946600	0.29298100
H	2.98010600	2.15349400	-0.83461500
C	4.67139200	2.01684400	2.63615300
H	2.82758000	1.21795800	3.36100700
C	5.38594400	2.50846300	1.54320100
H	5.29550800	2.94465500	-0.56871600
H	5.12808600	1.99966900	3.62285100
H	6.40387500	2.86829600	1.66554700

**TS-4'**

C	-2.03186600	-1.82934800	1.19208000
C	-2.55122000	-1.69539900	-0.10491300
C	-3.25272100	-0.40992000	-0.18422600
C	-2.40427200	-0.62689800	1.94243200
C	-3.24759400	0.18500500	1.13227500
C	-2.43197300	-2.69463600	-1.21812600
H	-1.47624200	-3.22475100	-1.17786900

H	-3.23725800	-3.44098700	-1.16057700
H	-2.50724700	-2.21432100	-2.19827300
C	-4.15609200	-0.00091900	-1.31044500
H	-4.33618900	1.07560600	-1.31772900
H	-3.74602900	-0.27241800	-2.28757100
H	-5.12805800	-0.50610500	-1.21332700
C	-4.04607700	1.37410200	1.57362600
H	-5.06895600	1.07494300	1.84629000
H	-3.60182200	1.85446600	2.45092200
H	-4.12314400	2.12595100	0.78388000
C	-2.10345200	-0.40206900	3.39494500
H	-2.85277700	-0.89952500	4.02678700
H	-1.12663900	-0.80743700	3.67330600
H	-2.10841700	0.66225300	3.64667700
C	-1.30629100	-3.02322000	1.74145600
H	-0.59699700	-2.75185700	2.52680200
H	-2.01803000	-3.73976700	2.17716400
H	-0.74122900	-3.54539400	0.96404800
Rh	-1.14887800	0.13018700	0.19931500
C	4.03816000	1.54851200	-3.16348600
C	2.67952700	1.35518200	-2.90902600
C	2.25303200	0.21553300	-2.21895600
C	3.20455800	-0.73905000	-1.81999900
C	4.56341700	-0.55030100	-2.07908700
C	4.97854200	0.60074500	-2.74663800
H	4.36190900	2.44066000	-3.69241300
H	1.95508300	2.07613000	-3.26383200
H	5.27226700	-1.30256000	-1.74907400
H	6.03528900	0.76158400	-2.94314500

C	2.60788400	-1.88925900	-1.11381400
O	1.31565700	-1.73777000	-0.86198200
N	3.36152100	-2.89396300	-0.79465800
O	2.60441700	-3.87928300	-0.11798300
C	3.49029700	-4.89889600	0.30285300
H	4.23699900	-4.51747100	1.01235300
H	2.86645000	-5.65025000	0.79629700
H	4.01099300	-5.35387500	-0.55025600
C	0.82632000	-0.18226000	-2.08836200
H	0.58079100	-1.00487200	-2.75494500
C	-0.34410800	0.58096000	-1.79177200
H	-1.18494900	0.20537500	-2.37025000
C	-0.65308800	1.83040200	-1.08449400
C	0.39192600	2.86411300	-0.67852300
C	0.84803900	3.75262300	-1.67286000
C	0.80375000	3.10673200	0.63729900
C	1.72527100	4.79325800	-1.37966400
H	0.48208800	3.63943100	-2.69017300
C	1.68225400	4.15392400	0.93779500
H	0.44136900	2.47001500	1.43057400
C	2.15559300	4.99573500	-0.06581400
H	2.06104800	5.45503000	-2.17436000
H	1.98759200	4.31233900	1.96950800
H	2.83661300	5.80912500	0.17097300
C	-1.87103100	2.57020100	-1.59551600
C	-2.51451400	3.51005500	-0.76582600
C	-2.34844100	2.44197800	-2.91203600
C	-3.60513200	4.25099900	-1.21451400
H	-2.14084400	3.65890300	0.24307000



C	-3.44169900	3.18593400	-3.36612000
H	-1.84833100	1.77171600	-3.60468300
C	-4.08294900	4.08853600	-2.51963700
H	-4.08019800	4.96467000	-0.54567000
H	-3.78115200	3.06415000	-4.39196800
H	-4.93032900	4.67000700	-2.87257200
H	1.33509800	-1.76141600	0.74916900
C	2.12475600	-0.07869500	3.41638300
H	2.03380400	-0.89157400	4.14341000
H	3.19136500	0.04257900	3.19638600
H	1.73150300	0.84987700	3.83159000
C	1.39736300	-0.43632800	2.14295900
O	1.65351500	-1.64641700	1.71398000
O	0.64148700	0.36742400	1.58506900

**INT-4**

C	1.26691500	-3.36724400	-0.08228200
C	2.07253900	-3.12376500	1.04225500
C	3.05704300	-2.11690700	0.64313100
C	1.82059300	-2.62676100	-1.23008200
C	2.96517000	-1.93388200	-0.80719100
C	1.97319600	-3.75226400	2.40173500
H	0.97117700	-4.14925600	2.59133600
H	2.68338600	-4.58555100	2.50864400
H	2.19887100	-3.03299400	3.19574200
C	4.22149600	-1.67799100	1.48185700
H	4.60409700	-0.70467500	1.16568600
H	3.95193400	-1.59997800	2.53934100
H	5.04395200	-2.40462300	1.40270100

C	3.94057200	-1.15798000	-1.64135800
H	4.85944100	-1.73784600	-1.81209000
H	3.52437700	-0.90829900	-2.62218100
H	4.23301400	-0.22214600	-1.15455200
C	1.25423900	-2.70511200	-2.61857200
H	1.43723800	-3.69179300	-3.06787700
H	0.17043300	-2.54429800	-2.61310600
H	1.69918300	-1.95433200	-3.27831400
C	0.05809000	-4.25269400	-0.17326800
H	-0.79206500	-3.71536100	-0.60888600
H	0.25513000	-5.13052600	-0.80503500
H	-0.24885200	-4.61612500	0.81171000
Rh	1.17067200	-1.09496000	0.40435500
C	-3.16606500	2.99758600	2.84063800
C	-2.11303500	2.09003500	2.98686000
C	-1.94009000	1.11517200	2.00929900
C	-2.81093100	1.04053600	0.91966800
C	-3.86423300	1.94207500	0.76494300
C	-4.03233600	2.92490600	1.73998800
H	-3.31607500	3.77001700	3.59012400
H	-1.44357400	2.15234700	3.84078100
H	-4.52555700	1.87262500	-0.09266800
H	-4.84307800	3.64210800	1.64721400
C	-2.38827000	-0.08116100	0.08139800
O	-1.29027200	-0.67431900	0.64463200
N	-2.96658600	-0.45812700	-0.99726700
O	-2.32760800	-1.56578100	-1.58212500
C	-3.06971500	-1.93978600	-2.73594600
H	-3.10923300	-1.11997000	-3.46321100

H	-2.53590600	-2.79186700	-3.16464300
H	-4.09144800	-2.23681500	-2.47008300
C	-0.94025900	-0.01702300	1.93141800
H	-1.15716300	-0.76002500	2.70931000
C	0.55323600	0.21588700	1.91403700
H	1.01832800	0.05841000	2.88314800
C	1.23393400	1.01773200	0.91474900
C	0.47104500	1.92058200	-0.03836100
C	0.15907900	3.22988700	0.37316600
C	0.10723600	1.54092100	-1.33736500
C	-0.50772700	4.11454900	-0.47152600
H	0.44793100	3.55257500	1.36998900
C	-0.56159100	2.42548300	-2.18934500
H	0.34949300	0.53777500	-1.67835800
C	-0.87288100	3.71465100	-1.76047600
H	-0.74192400	5.11802300	-0.12464900
H	-0.83727600	2.10105000	-3.18960400
H	-1.39240500	4.40335900	-2.42180600
C	2.60819200	1.54616300	1.22097400
C	3.40920400	2.05355000	0.17660500
C	3.14832300	1.59193800	2.51952000
C	4.68894600	2.55160100	0.41303800
H	3.01150000	2.05839500	-0.83380600
C	4.42990000	2.09201500	2.75927700
H	2.55870600	1.25216200	3.36508000
C	5.21327500	2.57028700	1.70881300
H	5.27714200	2.93229100	-0.41861100
H	4.81067400	2.11675500	3.77771600
H	6.20929100	2.96228000	1.89629200

**INT-4'**

C	-2.80493500	-1.78093200	1.23864700
C	-3.03233200	-1.65901500	-0.14326700
C	-3.43427000	-0.27533800	-0.38229400
C	-3.21114700	-0.52670400	1.89534400
C	-3.66842200	0.36075300	0.91695000
C	-2.92662600	-2.73080100	-1.18984100
H	-2.30795200	-3.56784300	-0.85086100
H	-3.91639200	-3.13806100	-1.44441700
H	-2.48780400	-2.35048300	-2.11881500
C	-3.98581700	0.23720200	-1.68225100
H	-3.88438100	1.32142400	-1.76871300
H	-3.48014200	-0.21253500	-2.54319000
H	-5.05472100	-0.00833200	-1.76879000
C	-4.31151500	1.70104100	1.11057700
H	-5.39049600	1.65007100	0.90268000
H	-4.19345200	2.06152100	2.13713000
H	-3.88938300	2.45812500	0.44196300
C	-3.16143000	-0.31403700	3.38027900
H	-3.82598400	-1.01106900	3.90967500
H	-2.14722000	-0.47183000	3.76608200
H	-3.46259800	0.70172800	3.65173900
C	-2.37122000	-3.01088300	1.98190500
H	-1.69695900	-2.76133100	2.80739700
H	-3.23254800	-3.53704500	2.41894900
H	-1.85120800	-3.71820300	1.32833900
Rh	-1.38603300	-0.13892000	0.35005800
C	1.93045700	0.09320700	-5.40258900

C	1.05752300	-0.22784900	-4.35847300
C	1.58270800	-0.37652700	-3.07748200
C	2.95072300	-0.21843600	-2.85331700
C	3.83115800	0.10314400	-3.88750500
C	3.30357500	0.25872700	-5.16893600
H	1.53973400	0.21528600	-6.40904300
H	-0.00409000	-0.35949100	-4.54980100
H	4.89129400	0.22454800	-3.68954200
H	3.96198400	0.50936100	-5.99586400
C	3.19362200	-0.44729200	-1.43405500
O	2.00088000	-0.72241500	-0.80850400
N	4.33732000	-0.40687400	-0.86209200
O	4.23428600	-0.67692000	0.50659300
C	5.52235400	-0.57020000	1.09424900
H	5.91664000	0.44832600	0.99750600
H	5.37865200	-0.81487300	2.14945100
H	6.22516200	-1.27863300	0.63902400
C	0.89694200	-0.73247700	-1.77217600
H	0.54293500	-1.77188700	-1.80751800
C	-0.28761500	0.14447300	-1.40044300
H	-1.00789400	0.03598200	-2.21509800
C	-0.33075600	1.42990600	-0.73017300
C	0.87885300	2.03699200	-0.04101300
C	1.92178500	2.55720200	-0.82822000
C	0.95066400	2.22914900	1.34586400
C	3.01109400	3.20867500	-0.25098900
H	1.86977900	2.45949100	-1.90940400
C	2.03651300	2.88915000	1.92776900
H	0.14979500	1.85108700	1.97153500

C	3.07453700	3.37688300	1.13418400
H	3.80693600	3.59157700	-0.88513100
H	2.06604700	3.02370400	3.00671700
H	3.91940900	3.88974100	1.58703000
C	-1.20465300	2.51677300	-1.30688100
C	-1.68653200	3.55747900	-0.48803300
C	-1.50680000	2.58799300	-2.67850800
C	-2.45600500	4.59621900	-1.00804100
H	-1.44582700	3.54691100	0.57091700
C	-2.28192900	3.62589600	-3.20280800
H	-1.10758700	1.83688000	-3.35333000
C	-2.76676200	4.63453200	-2.37105400
H	-2.81343100	5.38150900	-0.34610500
H	-2.49212100	3.65065800	-4.26964000
H	-3.36488800	5.44576600	-2.77746000
H	1.91695800	-1.47220600	0.79911000
C	1.10591900	-1.87610200	3.89463700
H	1.15005800	-2.96957800	3.92311600
H	2.04209200	-1.50203200	4.32349100
H	0.26391800	-1.51697700	4.48692300
C	0.98430100	-1.39991100	2.46692000
O	1.91226000	-1.92189200	1.68267700
O	0.11932400	-0.60942100	2.09924400

**PC-1**

C	-1.22025700	1.86471700	0.21071300
C	-0.17442400	1.03932600	0.62864300
C	-0.07375600	0.64523500	1.95976100

C	-1.03542300	1.10666200	2.86412700
C	-2.07989800	1.94128000	2.44063700
C	-2.18601000	2.32816600	1.10477400
C	-1.06496600	2.07747800	-1.22795400
C	0.70217900	0.72042100	-0.56642500
H	0.72336500	-0.01349000	2.29341800
H	-0.97500600	0.81102800	3.90794500
H	-2.81640400	2.28575500	3.16126000
H	-2.99135000	2.96825600	0.75900800
O	0.03194500	1.40265000	-1.67684600
N	-1.85015200	2.79244800	-1.94597700
O	-1.45436900	2.80744400	-3.29127000
C	-2.35957600	3.62771700	-4.01304400
H	-3.38408300	3.23854300	-3.95590000
H	-2.01164100	3.60306300	-5.04914100
H	-2.34620900	4.66028200	-3.64162600
C	0.80435600	-0.73846500	-0.90299000
H	-0.15585700	-1.22106900	-1.07194200
C	1.93327200	-1.46305000	-1.05762000
C	3.29684600	-0.91440700	-0.79136400
C	3.63561100	-0.34151300	0.44495600
C	4.28467300	-0.97545500	-1.79053100
C	4.91334500	0.17551900	0.67059300
H	2.89759900	-0.31964000	1.24181100
C	5.55710700	-0.45272100	-1.56908500
H	4.04268700	-1.42622300	-2.74870400
C	5.87645300	0.12558900	-0.33718800
H	5.15480900	0.61126900	1.63645200
H	6.30198100	-0.49712200	-2.35914400

H	6.87073700	0.52811900	-0.16374700
C	1.85128600	-2.87816200	-1.52265300
C	2.72266200	-3.85328900	-1.00608000
C	0.89945300	-3.27561000	-2.47828500
C	2.62720000	-5.18420900	-1.41033000
H	3.47159500	-3.56443700	-0.27461200
C	0.80751000	-4.60573300	-2.88580900
H	0.24632600	-2.52931200	-2.92107500
C	1.66823600	-5.56669500	-2.35071000
H	3.30380000	-5.92361200	-0.98986200
H	0.06983000	-4.88921000	-3.63192000
H	1.59842400	-6.60274200	-2.67104700
H	1.69456400	1.17286200	-0.47628400

**PC-2**

C	-1.10845900	2.38905000	0.25200800
C	-0.11917400	1.44664000	0.54551000
C	-0.02282300	0.90591700	1.82415500
C	-0.91401600	1.35805900	2.80381000
C	-1.89064900	2.32004800	2.50863200
C	-2.00012400	2.84444300	1.21975900
C	-1.00589300	2.78144200	-1.17698100
C	0.71521500	1.16775300	-0.69647500
H	0.71904800	0.14794100	2.06043800
H	-0.84926700	0.95471300	3.81088700
H	-2.56972500	2.65154700	3.28923100
H	-2.75389700	3.58273000	0.96261100
C	0.86304100	-0.29243100	-1.02997700
H	-0.08280400	-0.81309300	-1.16541200



C	2.01261600	-0.98017200	-1.20190400
C	3.36299700	-0.37965000	-0.98029400
C	3.71319400	0.22550800	0.23744500
C	4.32726300	-0.42512800	-2.00282700
C	4.97810600	0.78840100	0.42141400
H	2.99447900	0.24092900	1.05194000
C	5.58709400	0.14222100	-1.82259800
H	4.07739900	-0.90090000	-2.94688500
C	5.91742600	0.75217900	-0.60918500
H	5.22847300	1.24946000	1.37313400
H	6.31330400	0.10805600	-2.63037600
H	6.90168600	1.19025400	-0.46768400
C	1.96956400	-2.40745100	-1.63605700
C	2.89881600	-3.33541100	-1.13307200
C	0.99874400	-2.86782600	-2.54315200
C	2.84224300	-4.67859700	-1.50267100
H	3.66334000	-2.99982100	-0.43886300
C	0.94421000	-4.21016700	-2.91574700
H	0.29623600	-2.16134400	-2.97594300
C	1.86374200	-5.12286500	-2.39432200
H	3.56470500	-5.37942000	-1.09256500
H	0.18921600	-4.54102100	-3.62415900
H	1.82359700	-6.16843600	-2.68751000
H	1.69771500	1.64918700	-0.62160700
O	-1.59791200	3.65129400	-1.78951500
N	-0.07773400	1.88235800	-1.71681700
O	0.63342100	2.28407100	-2.84885800
C	-0.01521900	1.82137300	-4.03637300
H	-0.08935100	0.72711200	-4.04482000

H	-1.00861800	2.26942100	-4.13398400
H	0.62647000	2.15724700	-4.85509100

**HOAc**

C	-0.09234800	0.12567600	-0.00017000
O	-0.64606900	1.20160200	0.00006000
O	-0.77752000	-1.04692700	0.00005800
C	1.39689700	-0.10922500	-0.00002600
H	1.68352300	-0.69397400	-0.88019800
H	1.91626800	0.84909000	-0.00331500
H	1.68408200	-0.68801400	0.88394300
H	-1.72245400	-0.80320700	-0.00020300

**AgOAc**

C	-0.17280800	0.17262400	-0.00051100
O	0.79702800	-0.57351900	0.33267300
O	-0.10503500	1.43974800	-0.06178800
C	-1.51089600	-0.47689700	-0.32979800
H	-2.23070300	-0.22437400	0.45658800
H	-1.89749100	-0.07099100	-1.26894500
H	-1.41341700	-1.56127900	-0.39661500
Ag	2.10624200	1.32917200	0.61423300

**Cp\*Rh(OAc)<sub>2</sub> + 2Ag**

C	1.99232600	-0.57850800	-1.10358200
C	2.19947000	0.55453800	-0.18397400
C	2.04851300	0.08625100	1.16793100
C	1.47635400	-1.23091300	1.06807300

C	1.54421900	-1.66005600	-0.33922000
C	2.55469700	0.76676100	2.40945000
H	3.61984500	0.52810000	2.55944900
H	2.46651900	1.85380100	2.34376200
H	2.01417500	0.44140500	3.30155300
C	1.17986000	-2.16165700	2.20959900
H	0.96423400	-1.61032800	3.12854100
H	0.31235700	-2.79241400	1.99212100
H	2.03294300	-2.82750100	2.40728500
C	1.13506800	-3.02401300	-0.81049500
H	1.81909800	-3.79570100	-0.43188100
H	0.13106200	-3.27957800	-0.45120300
H	1.13039100	-3.09320400	-1.90223300
C	2.21370600	-0.51600400	-2.58649400
H	1.84235600	-1.41388400	-3.08913000
H	1.70751900	0.34551300	-3.03547100
H	3.28299700	-0.42327900	-2.82278000
C	2.76752400	1.87966800	-0.60064300
H	2.61034500	2.63930500	0.16955000
H	3.84864000	1.80249000	-0.78658000
H	2.29499700	2.24031300	-1.51896700
Rh	0.08668000	0.16388100	0.13354800
C	-0.97130500	2.14847900	-2.30059600
O	-1.48206200	1.30498100	-3.11334500
O	-0.63099100	1.93618200	-1.10315700
C	-2.89787600	-1.04331000	1.06533800
O	-3.01885900	-0.31670300	2.06118000
O	-1.89917400	-1.02273300	0.22616200
C	-3.98885100	-2.06239400	0.75137600

H	-4.68161100	-1.63394900	0.01585400
H	-3.56254300	-2.97359500	0.32250600
H	-4.55610000	-2.29710100	1.65417900
C	-0.76623100	3.55250200	-2.85676200
H	-0.07049000	3.51045400	-3.70225600
H	-1.71613800	3.93737000	-3.24131900
H	-0.37486100	4.22431200	-2.09128500
Ag	-1.16707000	1.26070500	2.21466500
Ag	-1.94463800	-0.45958300	-1.92571400

**INT-0<sub>Bn</sub>**

C	-1.63253800	1.36363100	1.24361200
C	-0.46444300	0.81764200	0.63517300
C	0.43264600	1.92653400	0.27065400
C	-1.39106900	2.76964700	1.42209800
C	-0.14582400	3.11696500	0.72684600
C	-0.24461600	-0.60937100	0.23291700
H	-0.86170300	-1.30060600	0.81051700
H	-0.48887200	-0.74393200	-0.83041900
H	0.79805700	-0.91038600	0.37045000
C	1.74791200	1.79055200	-0.43608700
H	2.13746100	0.77166000	-0.36195800
H	1.64865400	2.02837100	-1.50406000
H	2.49417800	2.46380300	-0.00379900
C	0.39236200	4.50228300	0.54331800
H	1.48366300	4.50244300	0.48668800
H	0.00773500	4.94414900	-0.38669600
H	0.09542700	5.16205000	1.36380100
C	-2.36811200	3.75532400	1.98746100

H	-3.01465400	4.15192300	1.19101800
H	-3.01312600	3.29261900	2.73931100
H	-1.86060800	4.60414400	2.45425100
C	-2.90578000	0.65046600	1.59739400
H	-3.22832600	0.86095600	2.62324900
H	-3.71801600	0.96811500	0.93000000
H	-2.80557400	-0.43267700	1.49387200
Rh	0.15744800	1.73974300	2.58150300
C	-0.27640700	0.75367700	8.06479300
C	-0.70792000	0.56365500	6.75620300
C	0.06722800	0.95636500	5.64912900
C	1.30640800	1.57347100	5.89964700
C	1.74571000	1.74568300	7.22496000
C	0.96663900	1.34612500	8.30252600
H	-0.90378500	0.43704800	8.89447300
H	-1.66620100	0.08274100	6.57220600
H	2.71666000	2.20429800	7.37518000
H	1.32154300	1.49692600	9.31853800
C	2.24250900	2.11047700	4.85953700
O	3.41639300	2.36428100	5.14129900
N	1.70637800	2.39704700	3.61195700
O	2.64258300	3.05780200	2.77378800
C	2.87160200	4.42523300	3.17963800
H	1.97189100	5.02429000	2.98728200
H	3.09375300	4.44335300	4.24957500
C	-0.51127700	0.66743500	4.28668700
H	-1.56152700	0.98652100	4.30793600
C	-0.50858700	-0.75000900	3.82799700
H	-1.35079700	-0.95961600	3.17272100

C	0.29696500	-1.82027300	4.06918700
C	1.57784000	-1.77656400	4.83716700
C	1.71379100	-2.50641700	6.03034200
C	2.69180000	-1.07526100	4.35386100
C	2.91754900	-2.50772000	6.73277600
H	0.86337800	-3.06736600	6.40871400
C	3.90041900	-1.07860900	5.05390100
H	2.60702600	-0.51677100	3.42621200
C	4.01584200	-1.79317900	6.24620300
H	2.99896800	-3.06658100	7.66177200
H	4.74230500	-0.50876600	4.67222200
H	4.95397100	-1.79238800	6.79499800
C	-0.08567500	-3.15000000	3.51208400
C	0.90009500	-4.06301900	3.08826500
C	-1.43314400	-3.54409800	3.38695000
C	0.55398400	-5.29438000	2.53383400
H	1.94720300	-3.79483400	3.18899000
C	-1.77954400	-4.77518300	2.83127300
H	-2.21513200	-2.88996300	3.76237500
C	-0.78777400	-5.65730200	2.39702500
H	1.33755900	-5.97362500	2.20715800
H	-2.82784600	-5.05434500	2.75677200
H	-1.05666300	-6.62048700	1.97157600
C	4.05170100	4.92760300	2.38976900
C	3.95567800	6.04858800	1.55879000
C	5.28222000	4.26223300	2.50020500
C	5.07054700	6.50687800	0.85078000
H	3.00619900	6.57262600	1.47080500
C	6.39198100	4.71345700	1.78823300

H	5.34891400	3.39549900	3.15143500
C	6.28953900	5.83787300	0.96224800
H	4.98411100	7.38247000	0.21238100
H	7.34148000	4.19235500	1.88061500
H	7.15737000	6.19037300	0.41074300

**INT-1<sub>Bn</sub>**

C	-2.01348700	-2.38195500	-2.42274900
C	-2.73196400	-1.14487500	-2.30411300
C	-3.00522400	-0.91294800	-0.89631600
C	-1.72705700	-2.84614900	-1.09742200
C	-2.38444900	-1.94177100	-0.15616200
C	-3.32366300	-0.35292400	-3.43517600
H	-2.74501900	-0.46402300	-4.35805600
H	-4.34571800	-0.69310600	-3.65279900
H	-3.37793200	0.71377600	-3.19732200
C	-3.85034600	0.19693500	-0.34929400
H	-3.72750500	1.12485400	-0.91470800
H	-4.91491300	-0.07571600	-0.39063600
H	-3.60473300	0.40972000	0.69463700
C	-2.49500700	-2.15168300	1.32203300
H	-2.48614100	-1.20258000	1.86504000
H	-3.43300800	-2.67220600	1.56329000
H	-1.66974400	-2.75602600	1.69595400
C	-1.06926100	-4.14468600	-0.74010200
H	-0.41452400	-4.49371900	-1.54317700
H	-0.46494800	-4.05510000	0.16423600
H	-1.82575500	-4.92269200	-0.56328200
C	-1.66633100	-3.08514900	-3.70252000

H	-1.54046000	-2.38336500	-4.53317800
H	-0.74190000	-3.66200600	-3.61002500
H	-2.46606800	-3.78320700	-3.98684200
Rh	-0.67746200	-0.87590900	-1.35398600
C	4.25094700	-1.25247300	-3.98337900
C	2.88598100	-0.98782100	-3.97073500
C	2.16523300	-0.82541500	-2.76949700
C	2.85043300	-0.99058600	-1.54984100
C	4.23289200	-1.24228900	-1.57796300
C	4.93320700	-1.37304700	-2.77125300
H	4.77499900	-1.36055400	-4.92961600
H	2.35482800	-0.88131800	-4.91444800
H	4.73494900	-1.32668200	-0.62111700
H	6.00092100	-1.57592400	-2.75663100
C	2.26254100	-0.92147700	-0.15840200
O	3.04792900	-0.77818500	0.80011800
N	0.93513200	-1.14493300	-0.03383700
C	0.72078300	-0.51502400	-2.94572100
H	0.35447200	-0.99455800	-3.85408400
C	-0.02751700	0.69789000	-2.69719000
H	-0.86602500	0.82886700	-3.37476000
C	0.00628200	1.56619700	-1.58838300
C	1.27478600	1.96452400	-0.89561000
C	2.28726400	2.52337800	-1.69680300
C	1.45603900	1.95013300	0.49486200
C	3.43735100	3.06485300	-1.12441600
H	2.16081200	2.54432100	-2.77574400
C	2.60901800	2.48790300	1.06457300
H	0.73375600	1.44451300	1.12567800



C	3.59825300	3.05628300	0.26162500
H	4.20604600	3.49138800	-1.76358900
H	2.74355600	2.43841400	2.14123500
H	4.49578200	3.47272400	0.71111000
C	-1.11987300	2.55110900	-1.44801900
C	-1.53903400	3.00769100	-0.18438200
C	-1.76336900	3.09394300	-2.57764700
C	-2.56777300	3.93927500	-0.05533700
H	-1.05693600	2.62492600	0.70707800
C	-2.79146600	4.02978800	-2.44946400
H	-1.43292400	2.81619000	-3.57401200
C	-3.20454500	4.45499000	-1.18643900
H	-2.87069500	4.26485400	0.93647400
H	-3.25628900	4.43861200	-3.34306200
H	-4.00169100	5.18624700	-1.08493800
C	1.03597600	-1.73167100	2.39183600
H	0.35417000	-1.48678900	3.21358900
H	2.01728800	-1.29948200	2.57848200
C	1.14697700	-3.23371000	2.25751000
C	2.18954400	-3.81580200	1.51879600
C	0.25216900	-4.08069400	2.92847800
C	2.30457200	-5.20309500	1.42327400
H	2.92003800	-3.16805000	1.04551800
C	0.37036900	-5.47018400	2.84293900
H	-0.53663300	-3.64716100	3.54007600
C	1.39329900	-6.03527200	2.07980400
H	3.11659200	-5.63669600	0.84483100
H	-0.33007200	-6.10766200	3.37679800
H	1.48966100	-7.11577600	2.00920200

O	0.41248800	-1.00195800	1.29274100
---	------------	-------------	------------

**INT-3<sub>Bn</sub>**

C	0.23349300	-2.87530200	0.14366400
C	0.92161700	-2.84171500	1.39496600
C	2.23102500	-2.28688100	1.15672700
C	1.16771500	-2.43013200	-0.89395300
C	2.39979500	-2.11143900	-0.27605800
C	0.39628400	-3.32408000	2.71510800
H	-0.69652800	-3.30437800	2.74394800
H	0.71329600	-4.35964500	2.90098900
H	0.76634000	-2.71837500	3.54883000
C	3.33227000	-2.15027100	2.16839300
H	3.97462700	-1.29212600	1.94910800
H	2.93820200	-2.02725100	3.18217700
H	3.96789500	-3.04700200	2.17340000
C	3.67719700	-1.69425100	-0.94027100
H	4.43666000	-2.48167600	-0.83701100
H	3.53298900	-1.51397200	-2.00871900
H	4.09221700	-0.78024500	-0.50296100
C	0.80947400	-2.34671100	-2.34586600
H	0.56815200	-3.34113300	-2.74366700
H	-0.07145600	-1.70663000	-2.47564400
H	1.62902000	-1.93550700	-2.94179000
C	-1.13744100	-3.41486600	-0.13386600
H	-1.63835300	-2.83432200	-0.91282000
H	-1.07874400	-4.45747900	-0.47780700
H	-1.77022000	-3.39704600	0.75792600
Rh	0.69064900	-0.73313800	0.56821900

C	-3.26360900	2.51242200	2.93385900
C	-2.06776200	1.80527600	2.98825000
C	-1.59410500	1.05399300	1.89528000
C	-2.38080100	0.99401300	0.72794300
C	-3.58968300	1.71483000	0.68561700
C	-4.03018400	2.46722200	1.76693600
H	-3.59290100	3.09209900	3.79242800
H	-1.47098100	1.83294800	3.89763800
H	-4.17409600	1.66572200	-0.22545400
H	-4.96534100	3.01714400	1.70013400
C	-1.98201700	0.19646100	-0.47458300
O	-0.72760200	-0.01077600	-0.76427400
N	-2.98232600	-0.19246100	-1.21864200
O	-2.52455600	-0.91708000	-2.35168000
C	-3.65943500	-1.34358100	-3.10737300
H	-4.38052400	-0.51839400	-3.15101900
H	-3.26844800	-1.51950000	-4.11553400
C	-0.31365500	0.31061700	2.15685900
H	-0.41525800	-0.33330100	3.03282700
C	1.03138900	0.80840600	2.02129000
H	1.74505300	0.41003900	2.73666300
C	1.54616600	1.50270200	0.89555600
C	0.74146100	2.54315200	0.16356700
C	0.27742200	3.64473300	0.90160700
C	0.52152000	2.53163800	-1.22227400
C	-0.38708700	4.70080600	0.27822300
H	0.44225600	3.67173200	1.97501100
C	-0.13877200	3.58982200	-1.84685300
H	0.82289600	1.66941900	-1.80450200

C	-0.59480700	4.67848300	-1.10123400
H	-0.74110700	5.53894500	0.87270100
H	-0.31043800	3.55330100	-2.91940900
H	-1.11351400	5.49862500	-1.59070800
C	3.03594400	1.65856900	0.77732700
C	3.63571300	1.95496000	-0.46255300
C	3.89058000	1.56449000	1.89478200
C	5.01462000	2.12099200	-0.58431400
H	3.01302800	2.06074600	-1.34279500
C	5.27047800	1.73489000	1.77475100
H	3.47825600	1.39500400	2.88414000
C	5.84447800	2.00860900	0.53279100
H	5.43965700	2.34465900	-1.55941000
H	5.89464900	1.66880100	2.66235100
H	6.91823000	2.14534600	0.43935500
C	-4.31442700	-2.60551200	-2.58195500
C	-4.18606600	-3.81416200	-3.27717700
C	-5.05772100	-2.58984600	-1.39129500
C	-4.78473700	-4.98371300	-2.80210700
H	-3.61478300	-3.83922000	-4.20318700
C	-5.65042700	-3.75747200	-0.91053100
H	-5.15221000	-1.65738600	-0.84408100
C	-5.51798800	-4.95773500	-1.61518500
H	-4.67852600	-5.91166000	-3.35866000
H	-6.22308500	-3.73040100	0.01334900
H	-5.98644000	-5.86513000	-1.24224900

**TS-4<sub>Bn</sub>**

C	1.03164300	-3.24844700	-0.05330100
---	------------	-------------	-------------

C	1.92164000	-3.13255600	1.02929200
C	2.93974700	-2.14907300	0.65752300
C	1.52274700	-2.40014700	-1.14624900
C	2.74435800	-1.80106000	-0.73614900
C	1.85981400	-3.85742700	2.34109300
H	0.84720400	-4.20743200	2.56059900
H	2.52031200	-4.73660000	2.33649600
H	2.18086300	-3.22001700	3.17155300
C	4.16886300	-1.84135700	1.46087500
H	4.59756800	-0.87375000	1.19123100
H	3.95704000	-1.82130100	2.53438900
H	4.93743700	-2.60974600	1.29231200
C	3.69058100	-1.00457200	-1.58182700
H	4.51294800	-1.63936000	-1.94184400
H	3.18954600	-0.58515600	-2.45920400
H	4.13336300	-0.17565200	-1.02300700
C	0.87177100	-2.31446000	-2.49425200
H	0.97610000	-3.26449900	-3.03765600
H	-0.19672000	-2.09860100	-2.39325700
H	1.32285600	-1.53058800	-3.10954000
C	-0.21553100	-4.07487900	-0.14209800
H	-1.05713100	-3.46615600	-0.48870100
H	-0.08302500	-4.90472000	-0.85041600
H	-0.48521100	-4.50466700	0.82673000
Rh	1.06062700	-1.01384300	0.56202000
C	-3.16232100	3.06185700	2.61878800
C	-2.08403000	2.21506500	2.87494200
C	-1.80426800	1.15998100	1.99767900
C	-2.61318400	0.95806200	0.87457800

C	-3.69071700	1.81033300	0.61543100
C	-3.96283600	2.86057800	1.48856500
H	-3.37809000	3.87966200	3.30115100
H	-1.46023100	2.37272700	3.75111900
H	-4.30035900	1.63386200	-0.26441200
H	-4.80125000	3.52358900	1.29268500
C	-2.21560200	-0.21595000	0.06130000
O	-1.24143200	-0.91733300	0.59391200
N	-2.89203500	-0.45988900	-1.01828600
O	-2.40897500	-1.62405400	-1.67909900
C	-3.28608800	-1.91451400	-2.75799500
H	-3.45160200	-1.00791100	-3.35447700
H	-2.72297900	-2.62787600	-3.37443300
C	-0.69744000	0.20530400	2.30230100
H	-0.95036500	-0.55490200	3.04101000
C	0.68709500	0.43409300	2.15710200
H	1.30471400	-0.01059400	2.93326700
C	1.34219800	1.11948400	1.05048300
C	0.57839700	2.07701600	0.15593100
C	0.33715600	3.38721300	0.60650700
C	0.18125300	1.74521700	-1.14550500
C	-0.29983100	4.32214900	-0.20605700
H	0.65377500	3.67020200	1.60700800
C	-0.45498700	2.68170900	-1.96574700
H	0.36706900	0.73937800	-1.51074500
C	-0.69909500	3.97207400	-1.49937400
H	-0.48448400	5.32560400	0.16916300
H	-0.76287500	2.39491900	-2.96781000
H	-1.19601900	4.70053500	-2.13481700

C	2.77315300	1.53975000	1.23852000
C	3.50562600	2.05590600	0.14923200
C	3.43033800	1.49126000	2.48354200
C	4.82945800	2.46897000	0.28906500
H	3.01947600	2.14147800	-0.81736800
C	4.75514800	1.90705700	2.62612100
H	2.89874700	1.15235700	3.36679000
C	5.46839200	2.39229100	1.52944800
H	5.36115400	2.86013100	-0.57490200
H	5.22512900	1.86297600	3.60570300
H	6.49820900	2.72013000	1.64173300
C	-4.61476000	-2.52054600	-2.34470200
C	-4.76698800	-3.17228000	-1.11643500
C	-5.70164400	-2.47373200	-3.22577900
C	-5.98331700	-3.76793500	-0.77811100
H	-3.93125300	-3.19683900	-0.42420400
C	-6.91601500	-3.07580900	-2.89327800
H	-5.59866900	-1.95820600	-4.17907600
C	-7.06067500	-3.72553400	-1.66555600
H	-6.09030200	-4.26494300	0.18298800
H	-7.75088800	-3.02922600	-3.58812300
H	-8.00723900	-4.18956500	-1.40067100

**TS-2<sub>Bn</sub>**

C	-3.05085900	-2.00748800	-1.00190000
C	-3.11412200	-0.56123000	-1.17886300
C	-2.96351600	0.05644500	0.12232100
C	-2.74022800	-2.26610400	0.33554700
C	-2.60846200	-0.98127900	1.02974000

C	-3.69475700	0.09381000	-2.39832400
H	-3.30034500	-0.33798100	-3.32291400
H	-4.78612100	-0.04452300	-2.41113500
H	-3.49541200	1.16599700	-2.42657900
C	-3.25313500	1.48829600	0.46340300
H	-3.02103000	2.15836600	-0.36787200
H	-4.31962000	1.61681600	0.70009000
H	-2.68244900	1.82289700	1.33482500
C	-2.35757700	-0.84117200	2.50343300
H	-2.10931600	0.18954200	2.77173600
H	-3.24916600	-1.12775500	3.08017700
H	-1.52893600	-1.47905300	2.82196400
C	-2.68802800	-3.60234000	1.00937400
H	-2.42989800	-4.40503900	0.31162600
H	-1.95750900	-3.60820300	1.81951200
H	-3.66905600	-3.84938300	1.44136200
C	-3.31775000	-3.01045300	-2.08480500
H	-2.89334000	-2.69220200	-3.04298000
H	-2.89993300	-3.99198700	-1.84209100
H	-4.39803500	-3.14304100	-2.24321900
Rh	-0.97809700	-0.76331900	-0.54354300
C	4.91741800	0.11737800	-1.51571700
C	3.69383000	-0.37203900	-1.97162400
C	2.71940400	-0.78086200	-1.05100200
C	2.97626900	-0.67577700	0.31807300
C	4.19678400	-0.16873000	0.77324700
C	5.16697900	0.22784100	-0.14286800
H	5.67854500	0.41325600	-2.23304400
H	3.49828200	-0.45043600	-3.03796400



H	4.36478200	-0.11695300	1.84434100
H	6.12015300	0.61590800	0.20624000
C	1.97659800	-1.25009700	1.25979100
O	2.25241500	-1.48499600	2.44169700
N	0.83143400	-1.64354200	0.60546900
C	1.43270800	-1.34056800	-1.55490800
H	1.43745500	-2.39175700	-1.83338300
C	0.44969900	-0.52579300	-2.15501800
H	-0.09900300	-0.97513400	-2.97767100
C	0.07058100	0.81091000	-1.71559500
C	0.95868300	1.70594800	-0.86780600
C	1.93760800	2.49387400	-1.49939100
C	0.76114000	1.88352600	0.50755100
C	2.70842600	3.40188800	-0.77688100
H	2.09272700	2.39062400	-2.57003700
C	1.52701200	2.79924300	1.23505700
H	0.00530700	1.28519600	1.00632900
C	2.50457100	3.56054100	0.59680600
H	3.46679100	3.99020600	-1.28747800
H	1.35689400	2.91098000	2.30279600
H	3.10221800	4.27214300	1.16060300
C	-0.75238400	1.63254300	-2.67299300
C	-1.29860400	2.86495700	-2.25730500
C	-0.94802900	1.27170700	-4.02008800
C	-2.03668700	3.66765900	-3.12484300
H	-1.12500900	3.20089500	-1.24057900
C	-1.68078500	2.07778500	-4.89316800
H	-0.50161500	0.36374100	-4.41198400
C	-2.23961300	3.27677200	-4.45105200

H	-2.44513000	4.60875700	-2.76496000
H	-1.80217200	1.76871100	-5.92851300
H	-2.80739400	3.90545900	-5.13146600
C	0.99038800	-3.89343400	1.46549500
H	0.27939600	-4.58919900	1.92396400
H	1.77321100	-3.66113500	2.19137600
C	1.57706700	-4.48279800	0.20293700
C	2.95803500	-4.44290600	-0.02335400
C	0.75419500	-5.08102700	-0.76281800
C	3.50792900	-4.98263200	-1.18931200
H	3.60391100	-3.97884600	0.71781300
C	1.29757600	-5.62038800	-1.92873500
H	-0.31887400	-5.12485300	-0.59439900
C	2.67867800	-5.57067100	-2.14552300
H	4.58197100	-4.94084300	-1.34979500
H	0.64777200	-6.08720700	-2.66485300
H	3.10374700	-5.99375100	-3.05200500
O	0.17028100	-2.72247700	1.24829900

**INT-4<sub>Bn</sub>**

C	1.10746600	-3.32729300	-0.12317900
C	1.93870500	-3.13350700	0.99211800
C	2.95273500	-2.15615200	0.59412100
C	1.66912400	-2.58728500	-1.26725700
C	2.84472700	-1.94406000	-0.85145100
C	1.84001700	-3.78501500	2.34064500
H	0.82549800	-4.14102000	2.54464300
H	2.51405600	-4.65122600	2.41527700
H	2.11503000	-3.09313800	3.14336200

C	4.14246700	-1.77275900	1.42415800
H	4.57223500	-0.82173300	1.10120500
H	3.88071700	-1.67496300	2.48192200
H	4.92655800	-2.54066800	1.34593900
C	3.83277900	-1.18542400	-1.68629100
H	4.73223700	-1.78915200	-1.87605100
H	3.41297600	-0.90894600	-2.65828100
H	4.15715700	-0.26593300	-1.18890500
C	1.07092100	-2.61223100	-2.64421600
H	1.17643000	-3.60354200	-3.10757000
H	0.00084300	-2.37794800	-2.61179800
H	1.55133900	-1.88535200	-3.30567900
C	-0.13069900	-4.17108800	-0.21208300
H	-0.96215600	-3.60393400	-0.64573700
H	0.03393400	-5.05341800	-0.84680100
H	-0.44789800	-4.52636400	0.77268500
Rh	1.10081600	-1.06126200	0.40576700
C	-3.02321100	3.18279400	2.94935600
C	-2.00913900	2.22875200	3.07325100
C	-1.89085200	1.25777300	2.08350300
C	-2.77736300	1.23411400	1.00451000
C	-3.79231000	2.18171000	0.87192300
C	-3.90536400	3.16016300	1.85913100
H	-3.13022700	3.95266500	3.70879300
H	-1.32759000	2.25255100	3.91950300
H	-4.46729700	2.14892100	0.02286800
H	-4.68530700	3.91272600	1.78457100
C	-2.41764700	0.10214300	0.15068100
O	-1.34093900	-0.54641900	0.69393500

N	-3.02870100	-0.23632000	-0.92222600
O	-2.43944800	-1.36422600	-1.53246000
C	-3.24018400	-1.74131900	-2.65126700
H	-3.43445800	-0.86154900	-3.27667100
H	-2.58964100	-2.42328000	-3.21307400
C	-0.94225000	0.08419300	1.98101800
H	-1.17888800	-0.65589700	2.75581800
C	0.55967800	0.25342900	1.94227500
H	1.03246900	0.06348300	2.90191500
C	1.25851600	1.04009100	0.94359900
C	0.52052500	1.98467000	0.01140400
C	0.25824100	3.29753900	0.44568100
C	0.13700400	1.63941400	-1.29157300
C	-0.38063000	4.21904800	-0.38101200
H	0.56349600	3.59356400	1.44584300
C	-0.50376400	2.56106900	-2.12559200
H	0.34345100	0.63453700	-1.65035600
C	-0.76641300	3.85330900	-1.67413800
H	-0.57677100	5.22459800	-0.01703000
H	-0.79550500	2.26334300	-3.12959500
H	-1.26422400	4.57083800	-2.32136700
C	2.65722900	1.50846900	1.23628300
C	3.46293800	1.99867000	0.18744000
C	3.21630800	1.51565500	2.52760800
C	4.76415900	2.44380600	0.41227300
H	3.05167000	2.03353500	-0.81690000
C	4.51932600	1.96269700	2.75576900
H	2.62520600	1.18819700	3.37694500
C	5.30630600	2.42465000	1.70064600

H	5.35522500	2.81293800	-0.42252500
H	4.91445700	1.95930700	3.76902000
H	6.31910800	2.77558100	1.87927600
C	-4.53884500	-2.43101600	-2.28396200
C	-4.65355600	-3.17792300	-1.10592800
C	-5.63096000	-2.36922600	-3.15679000
C	-5.83873000	-3.85207100	-0.80913000
H	-3.81340500	-3.21728700	-0.41898700
C	-6.81419900	-3.05062200	-2.86646000
H	-5.55713700	-1.78037500	-4.06909000
C	-6.92150100	-3.79413800	-1.68960200
H	-5.91717200	-4.42396100	0.11207100
H	-7.65430100	-2.99198500	-3.55376200
H	-7.84384400	-4.32020000	-1.45774100

**INT-2<sub>Bn</sub>**

C	-2.92106600	-2.13046000	-1.43248200
C	-3.14775300	-0.68572300	-1.48198100
C	-3.38675100	-0.21734200	-0.11733800
C	-2.82915400	-2.48526300	-0.07980900
C	-3.08994300	-1.28937700	0.73738200
C	-3.55400300	0.05842400	-2.72125300
H	-2.96750800	-0.24906400	-3.59219700
H	-4.61233800	-0.13775200	-2.94956000
H	-3.43144900	1.13717400	-2.60765900
C	-3.90245100	1.13886100	0.26194400
H	-3.48751400	1.92331400	-0.37693300
H	-4.99717300	1.18210500	0.16207700
H	-3.65993800	1.38914000	1.29970500

C	-3.17266000	-1.30321300	2.23765800
H	-3.12904100	-0.29280300	2.65450400
H	-4.11172100	-1.76141500	2.58090200
H	-2.35651700	-1.88123700	2.68632300
C	-2.67736500	-3.86504600	0.49339500
H	-2.35720300	-4.59030800	-0.25943500
H	-1.95262600	-3.90107900	1.31457700
H	-3.63438600	-4.22017000	0.90256600
C	-2.86452600	-3.03769400	-2.62774600
H	-2.35561500	-2.56183000	-3.47232800
H	-2.33615900	-3.97055200	-2.40641500
H	-3.87431500	-3.30713000	-2.97125200
Rh	-1.17252100	-0.80828900	-0.59152300
C	4.66810400	0.08688300	-3.65060300
C	3.36514000	-0.39372900	-3.47374100
C	2.94385200	-0.69878100	-2.18374800
C	3.81584200	-0.53988100	-1.10186700
C	5.11335900	-0.06623900	-1.26760700
C	5.53513300	0.24908300	-2.56093300
H	5.01308700	0.33871000	-4.65000800
H	2.70237200	-0.51552100	-4.32671300
H	5.76483000	0.05340900	-0.40704100
H	6.54169200	0.62282500	-2.72744900
C	3.11625000	-0.90703100	0.15889300
O	3.49539800	-0.83923000	1.31706600
N	1.90913700	-1.42649400	-0.28337300
C	1.60621900	-1.24642800	-1.70276700
H	1.43345700	-2.23453800	-2.15289500
C	0.35416300	-0.41158600	-1.96778000

H	0.01356900	-0.56278900	-2.99027400
C	0.02869400	0.85081100	-1.33588900
C	0.91744300	1.50946500	-0.29367500
C	2.02525600	2.26236100	-0.72400600
C	0.62464400	1.50105000	1.07738100
C	2.82276400	2.95706700	0.18419600
H	2.25749600	2.30504700	-1.78463700
C	1.41960100	2.19922900	1.99007200
H	-0.23724600	0.93802400	1.42361700
C	2.52322900	2.92756300	1.54821100
H	3.67796900	3.52414600	-0.17503400
H	1.17408100	2.16968800	3.04875700
H	3.14441100	3.46758100	2.25796700
C	-0.71101500	1.89000100	-2.13915400
C	-1.34121200	2.96920100	-1.48623700
C	-0.75015200	1.88470000	-3.54534400
C	-2.00848000	3.96458700	-2.19726800
H	-1.29230400	3.02704800	-0.40327400
C	-1.41610800	2.88201800	-4.26142300
H	-0.23452200	1.10529600	-4.09731100
C	-2.05745000	3.92510700	-3.59394200
H	-2.48516000	4.77969300	-1.65796300
H	-1.41984900	2.84667800	-5.34836800
H	-2.57200500	4.70372900	-4.15059400
C	0.99373700	-2.65889500	1.51515900
H	-0.00275900	-2.74656100	1.95818200
H	1.69993500	-2.31928000	2.27553700
C	1.45984900	-3.95058200	0.89082000
C	2.56131700	-4.61814200	1.43776100

C	0.80323200	-4.51347100	-0.21305500
C	2.99086000	-5.83644300	0.90662900
H	3.09100400	-4.17590700	2.27784000
C	1.23930200	-5.72293300	-0.75294800
H	-0.04022900	-3.99025100	-0.65382200
C	2.33100100	-6.39098000	-0.19032400
H	3.84697200	-6.34391900	1.34294500
H	0.72589700	-6.14795000	-1.61172900
H	2.66705000	-7.33559200	-0.60965400
O	0.81671500	-1.56090600	0.57193400

### 3. Supplementary References

[S1] Rakshit, S.; Grohmann, C.; Besset, T.; Glorius, F., Rh(III)-Catalyzed Directed C–H Olefination Using an Oxidizing Directing Group: Mild, Efficient, and Versatile. *J. Am. Chem. Soc.* **2011**, *133*, 2350-2353.

[S2] Chowdhury, D.; Koner, M.; Ghosh, S.; Baidya, M., Regioselective Annulation of Allenylphosphine Oxides with Aromatic Amides under Ruthenium(II) Catalysis. *Org. Lett.* **2022**, *24*, 3604-3608.

[S3] Xu, Y.; Zheng, G.; Yang, X.; Li, X., Rhodium(iii)-catalyzed chemodivergent annulations between N-methoxybenzamides and sulfoxonium ylides via C-H activation. *Chem. Commun.* **2018**, *54*, 670-673.

[S4] Xue, J.-W.; Zeng, M.; Jiang, H.; Li, K.; Chen, Z.; Yin, G., Palladium(II)/Lewis Acid-Catalyzed Oxidative Olefination/Annulation of N-Methoxybenzamides: Identifying the Active Intermediates through NMR Characterizations. *J. Org. Chem.* **2020**, *85*, 8760-8772.

[S5] Wang, C.-Q.; Ye, L.; Feng, C.; Loh, T.-P., C-F Bond Cleavage Enabled Redox-Neutral [4+1] Annulation via C-H Bond Activation. *J. Am. Chem. Soc.* **2017**, *139*, 1762-



1765.

[S6] Huang, Q.; Chen, Y.; Zhou, X.; Dai, L.; Lu, Y., Nickel-Hydride-Catalyzed Diastereo- and Enantioselective Hydroalkylation of Cyclopropenes. *Angew. Chem. Int. Ed.* **2022**, *61*, e202210560.

[S7] Ramachandran, K.; Anbarasan, P., Cobalt-catalyzed multisubstituted allylation of the chelation-assisted C-H bond of (hetero)arenes with cyclopropenes. *Chem. Sci.* **2021**, *12*, 13442-13449.

[S8] Meyer, S.; Göbel, L.; Livingstone, K.; Roblick, C.; Daniliuc, C. G.; Gilmour, R., Cyclopropene activation via I(I)/I(III) catalysis: Proof of principle and application in direct tetrafluorination. *Tetrahedron.* **2022**, *126*, 132925.

[S9] Smyrnov, V.; Muriel, B.; Waser, J., Synthesis of Quinolines via the Metal-free Visible-Light-Mediated Radical Azidation of Cyclopropenes. *Org. Lett.* **2021**, *23*, 5435-5439.

[S10] Zhang, Y.; Li, Y.; Zhou, W.; Zhang, M.; Zhang, Q.; Jia, R.; Zhao, J., Assembly of polysubstituted chiral cyclopropylamines via highly enantioselective Cu-catalyzed three-component cyclopropene alkenylation. *Chem. Commun.* **2020**, *56*, 12250-12253.

[S11] Qin, W.-W.; Sang, C.-Y.; Zhang, L.-L.; Wei, W.; Tian, H.-Z.; Liu, H.-X.; Chen, S.-W.; Hui, L., Synthesis and biological evaluation of 2,4-diaminopyrimidines as selective Aurora A kinase inhibitors. *Eur. J. Med. Chem.* **2015**, *95*, 174-184.

[S12] Matthew R. Smith, J. Y. K., Marco A. Ciufolini Pd-arylurea complexes for the Heck arylation of crotonic and cinnamic substrates. *Tetrahedron Lett.* **2013**, *54*, 2042-2045.

[S13] Wu, X.; Zhou, J., Selective arylation at the vinylic site of cyclic olefins. *Chem. Commun.* **2013**, *49*, 4794-4796.

[S14] Zhou, T.; Li, L.; Li, B.; Song, H.; Wang, B. Syntheses, Structures, and Reactions of Cyclometalated Rhodium, Iridium, and Ruthenium Complexes of N-Methoxy-4-nitrobenzamide. *Organometallics* **2018**, *37*, 476-481.

[S15] Zhu, H.-T.; Fan, M.-J.; Yang, D.-S.; Wang, X.-L.; Ke, S.; Zhang, C.-Y.; Guan, Z.-

H. An iodine-promoted Meyer–Schuster rearrangement for the synthesis of  $\alpha$ -iodo unsaturated ketones. *Org. Chem. Front.* **2015**, *2*, 506-509.

[S16] Frisch, M. J. T.; G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, Jr., J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski J.; Fox, D. J. Gaussian 09, revision D. 01, Gaussian, Inc., Wallingford CT, 2013.

[S17] (a) Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron-Density. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1988**, *37*, 785-789. (b) Becke, A. D. Density-Functional Thermochemistry. III. The Role of Exact Exchange. *J. Chem. Phys.* **1993**, *98*, 5648-5652.

[S18] Andrae, D.; Häußermann, U.; Dolg, M.; Stoll, H.; Preuß, H., Energy-Adjusted ab Initio Pseudo Potentials for the Second and Third Row Transition Elements. *Theor. Chim. Acta.* **1990**, *77*, 123-141.

[S19] (a) Gonzalez, C.; Schlegel, H. B., An Improved Algorithm for Reaction Path Following. *J. Chem. Phys.* **1989**, *90*, 2154-2161. (b) Gonzalez, C.; Schlegel, H. B., Reaction Path Following in Massweighted Internal Coordinates. *J. Phys. Chem.* **1990**, *94*, 5523-5527.

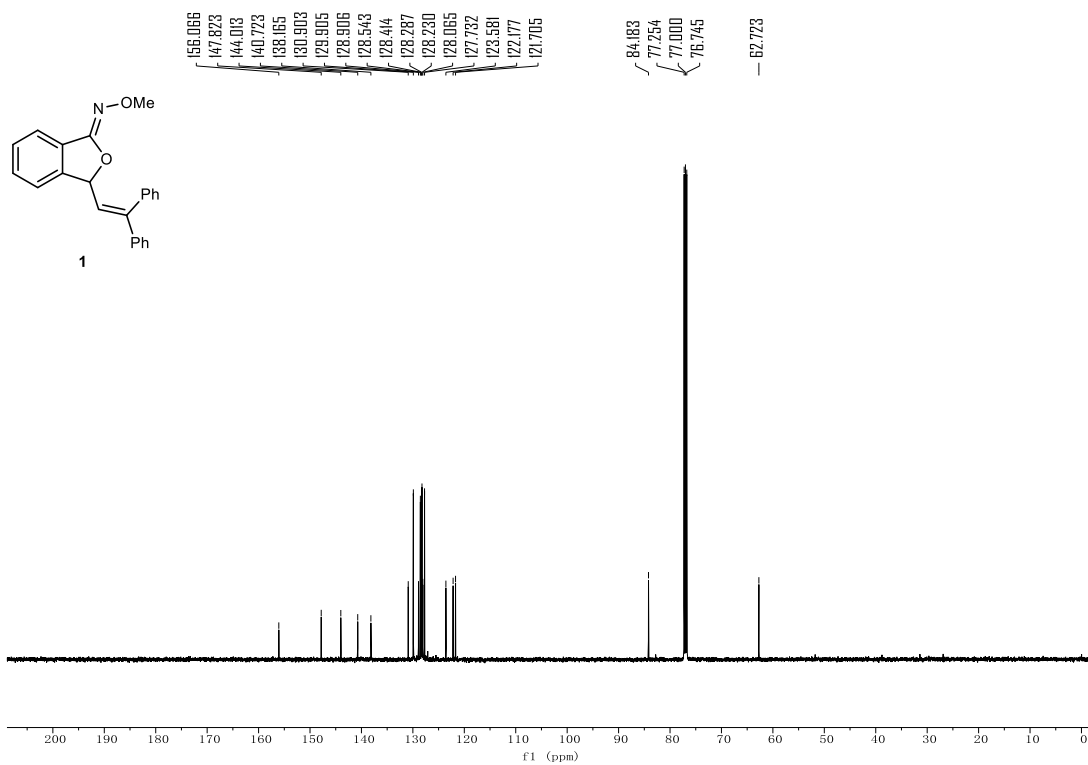
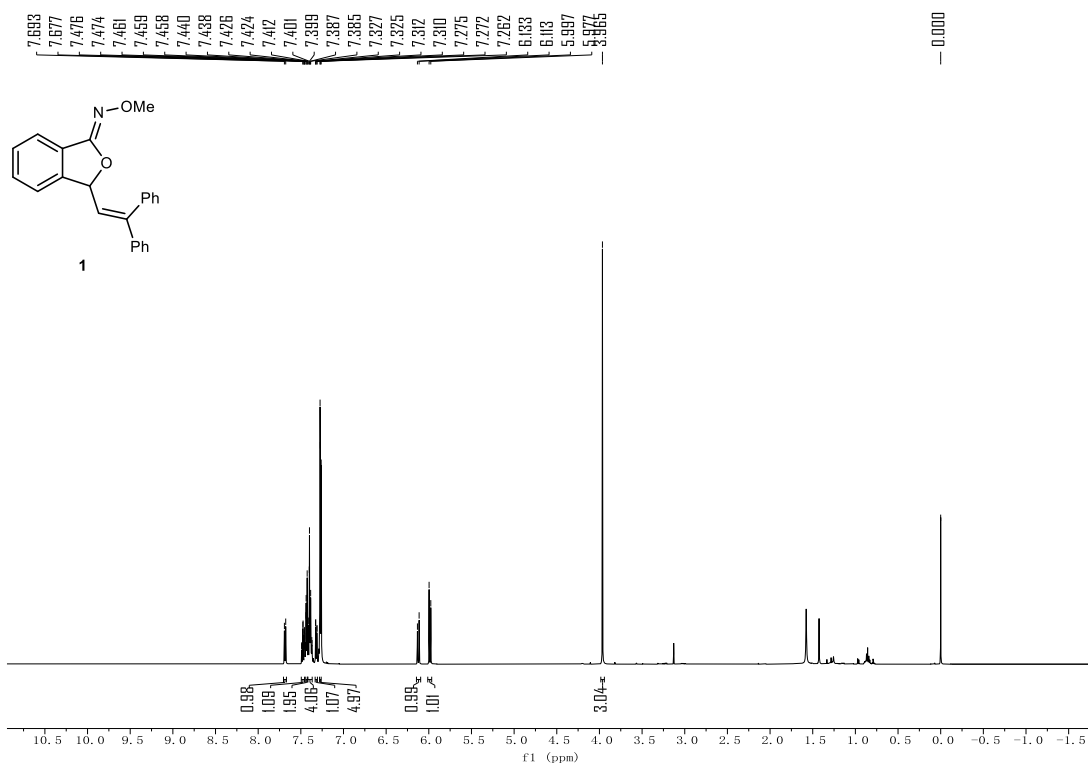
[S20] Marenich, A. V.; Cramer, C. J.; Truhlar, D. G., Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the

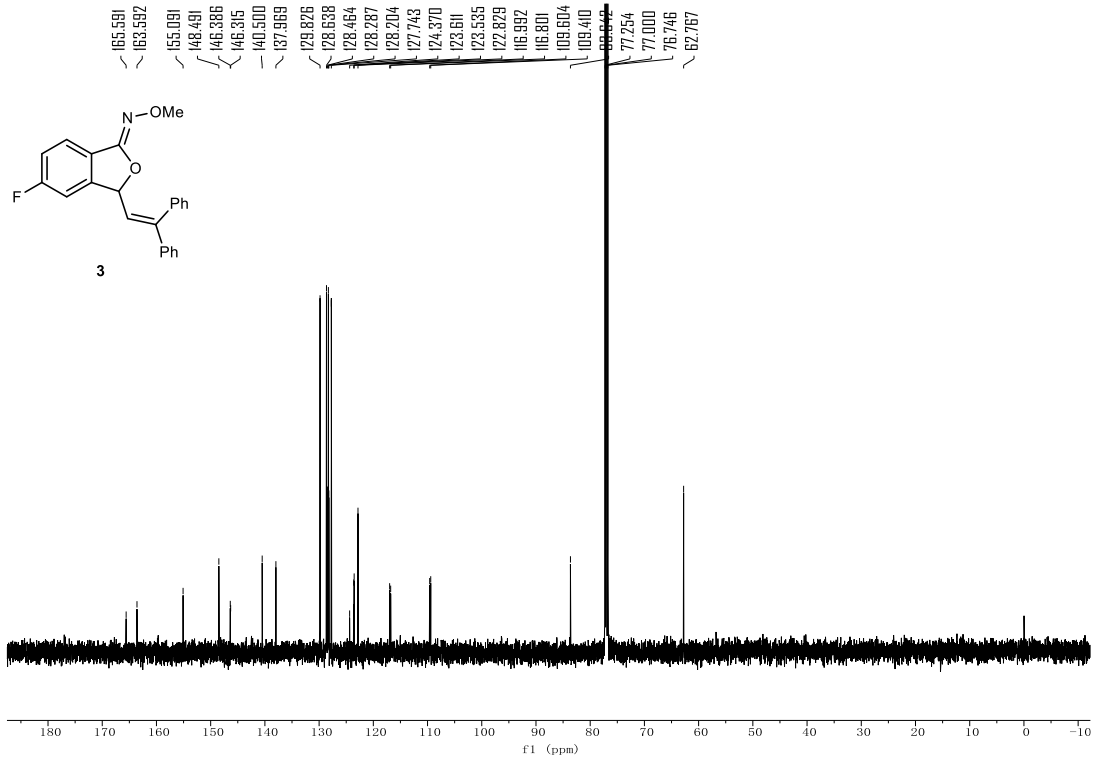
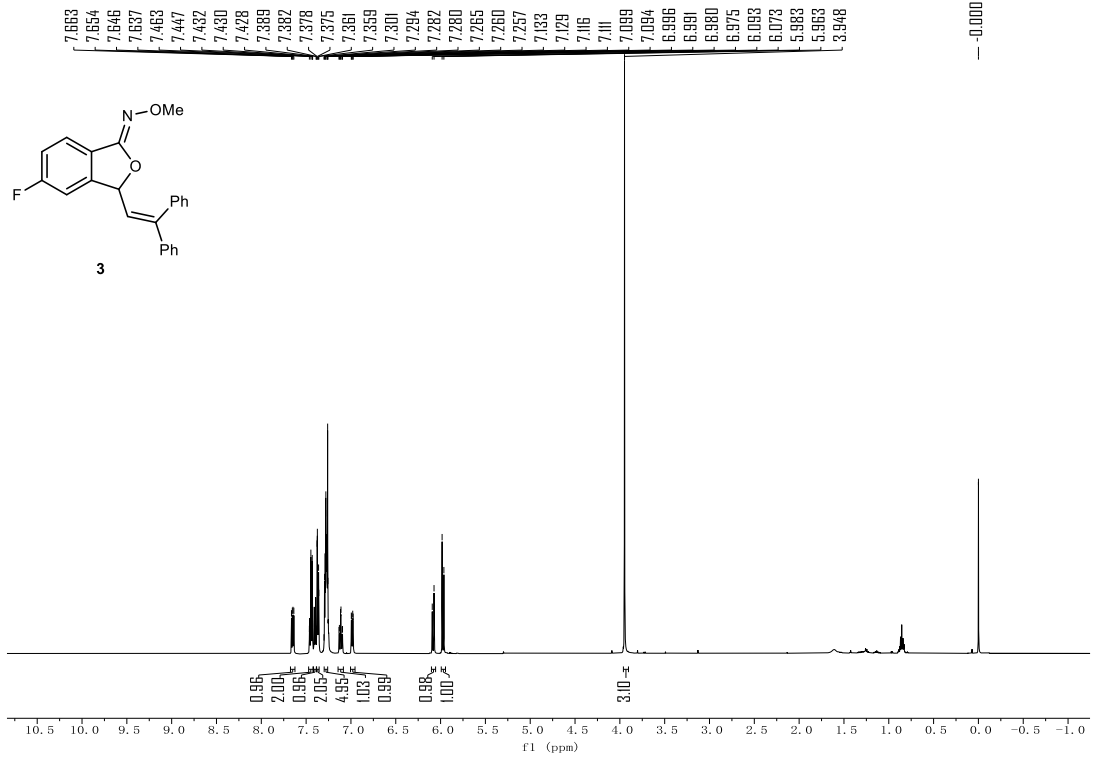
Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B.* **2009**, *113*, 6378-6396.

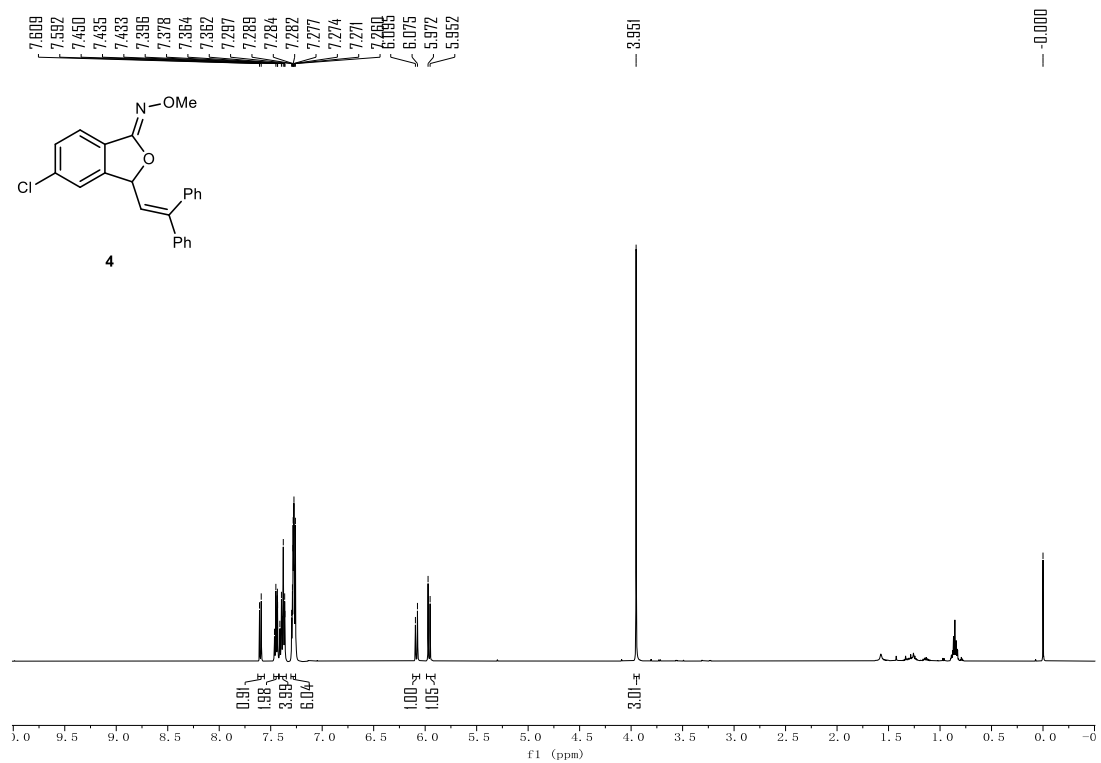
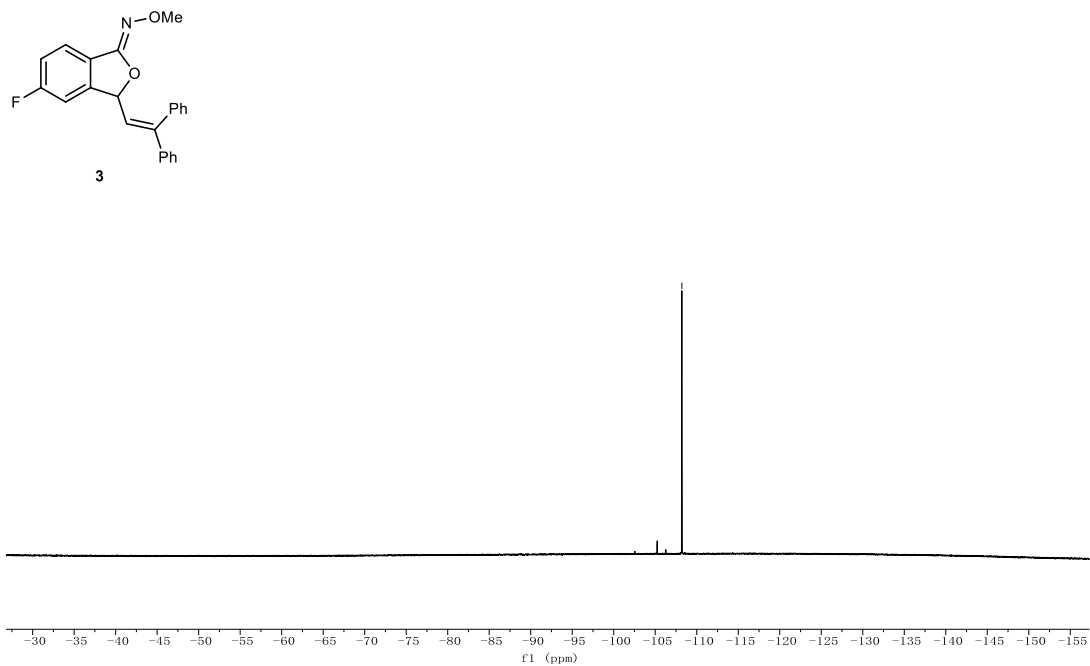
[S21] Zhao, Y.; Truhlar, D. G., A New Local Density Functional for Main-Group Thermochemistry, Transition Metal Bonding, Thermochemical Kinetics, and Noncovalent Interactions. *J. Chem. Phys.* **2006**, *125*, 194101.

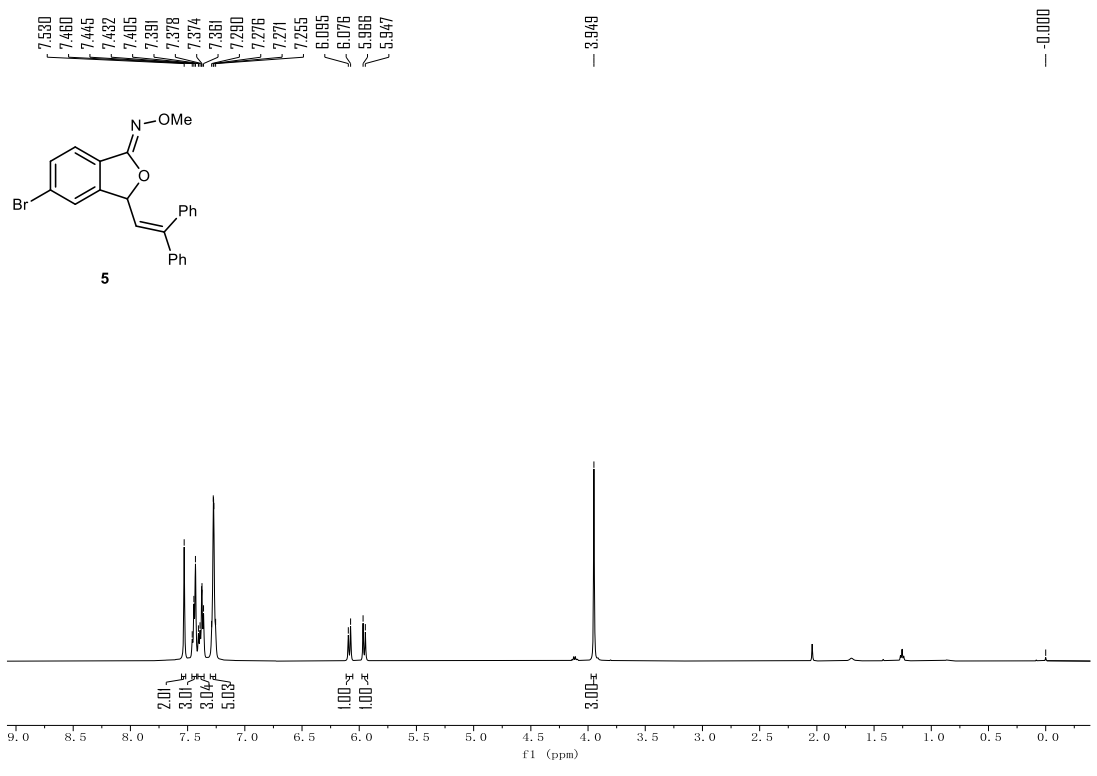
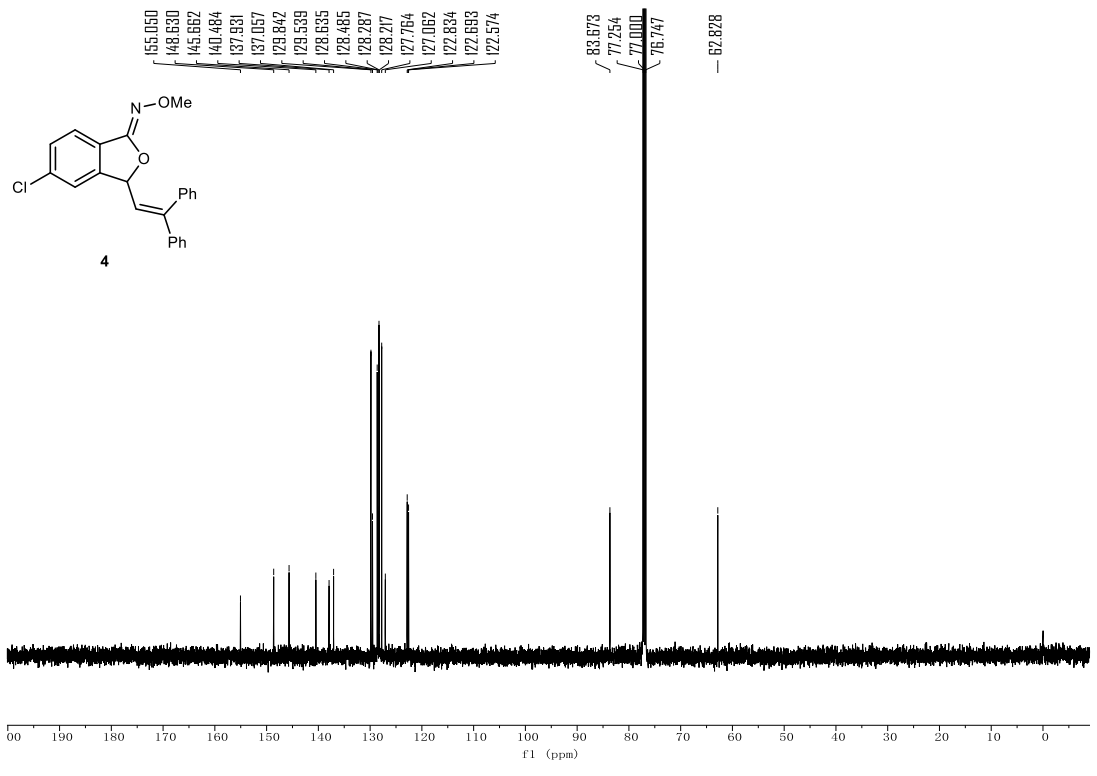
[S22] Legault, C. Y. CYLview, 1.0b; Université de Sherbrooke, **2009**, (<http://www.cylview.org>).

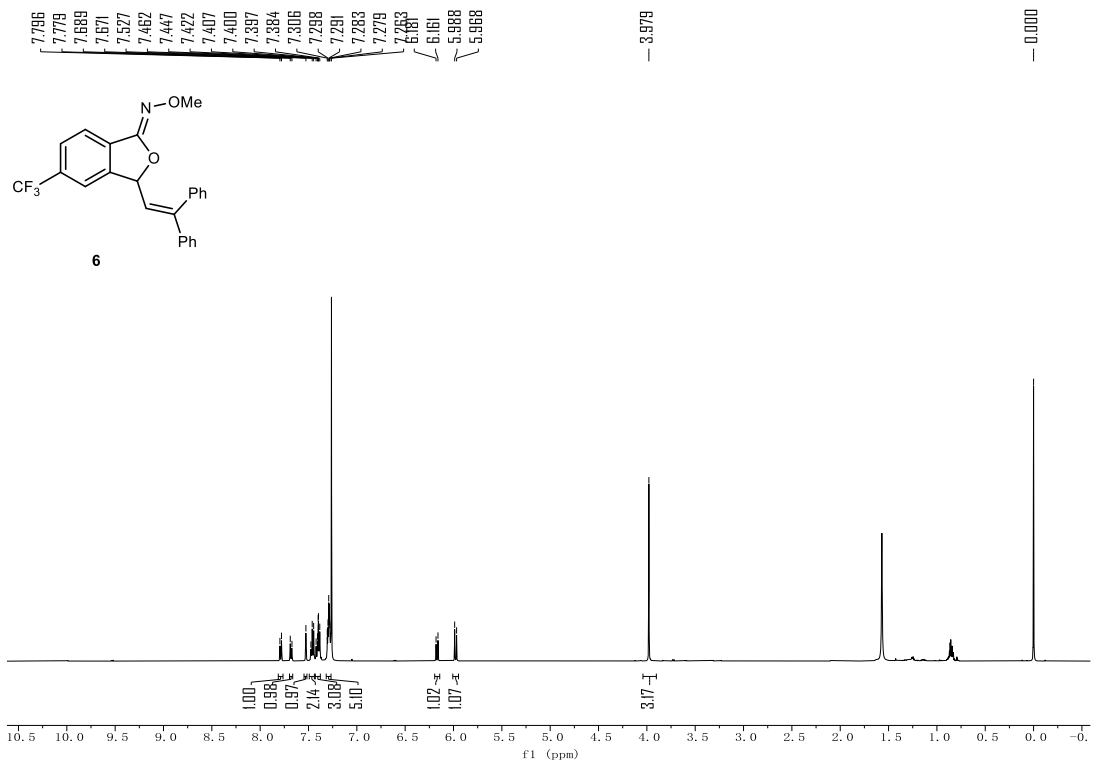
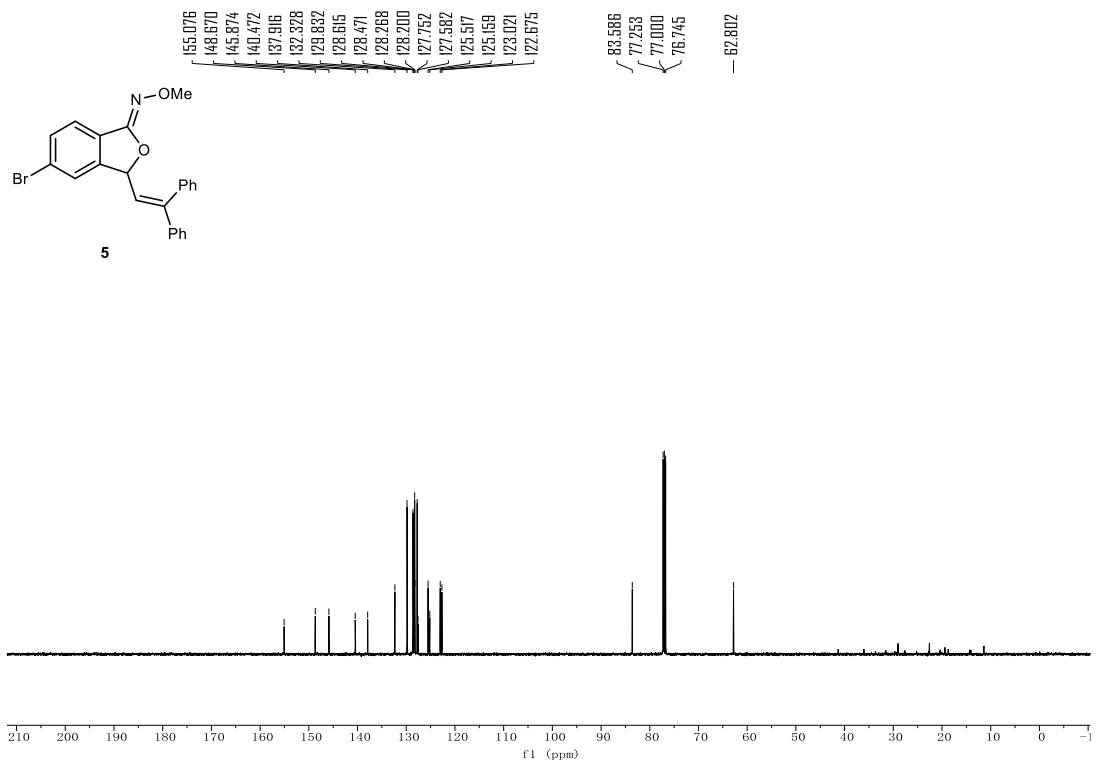
## 4. <sup>1</sup>H NMR, <sup>13</sup>C NMR, and <sup>19</sup>F NMR Spectra



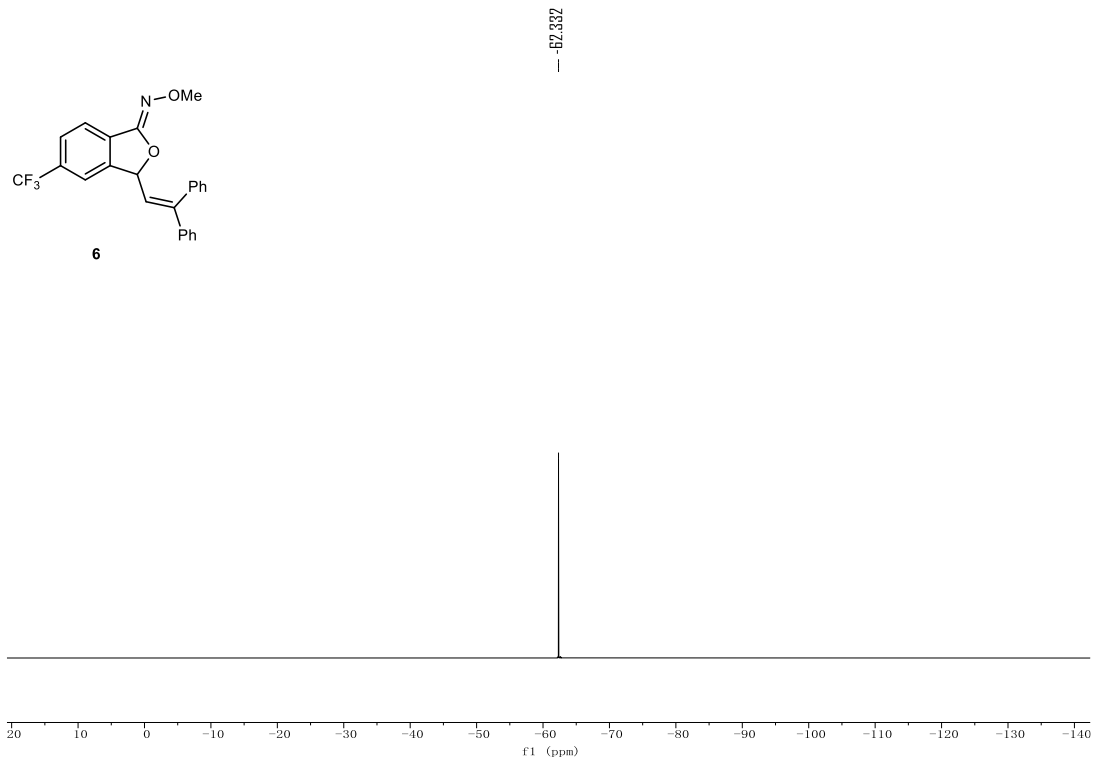
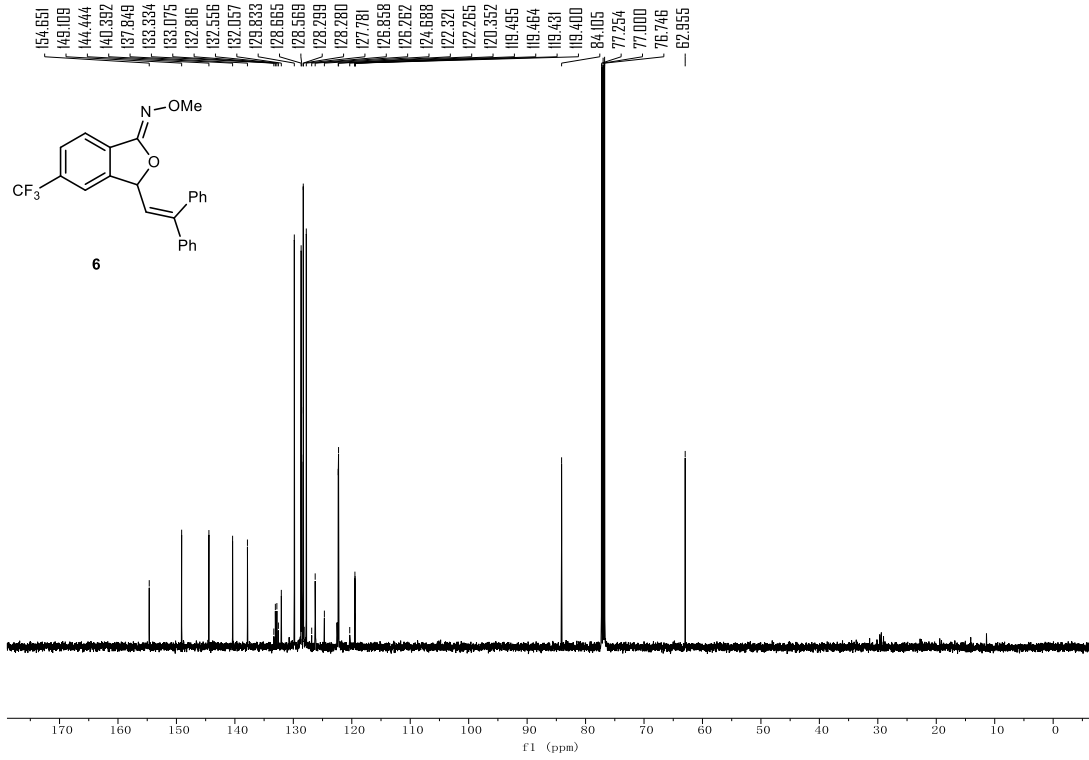


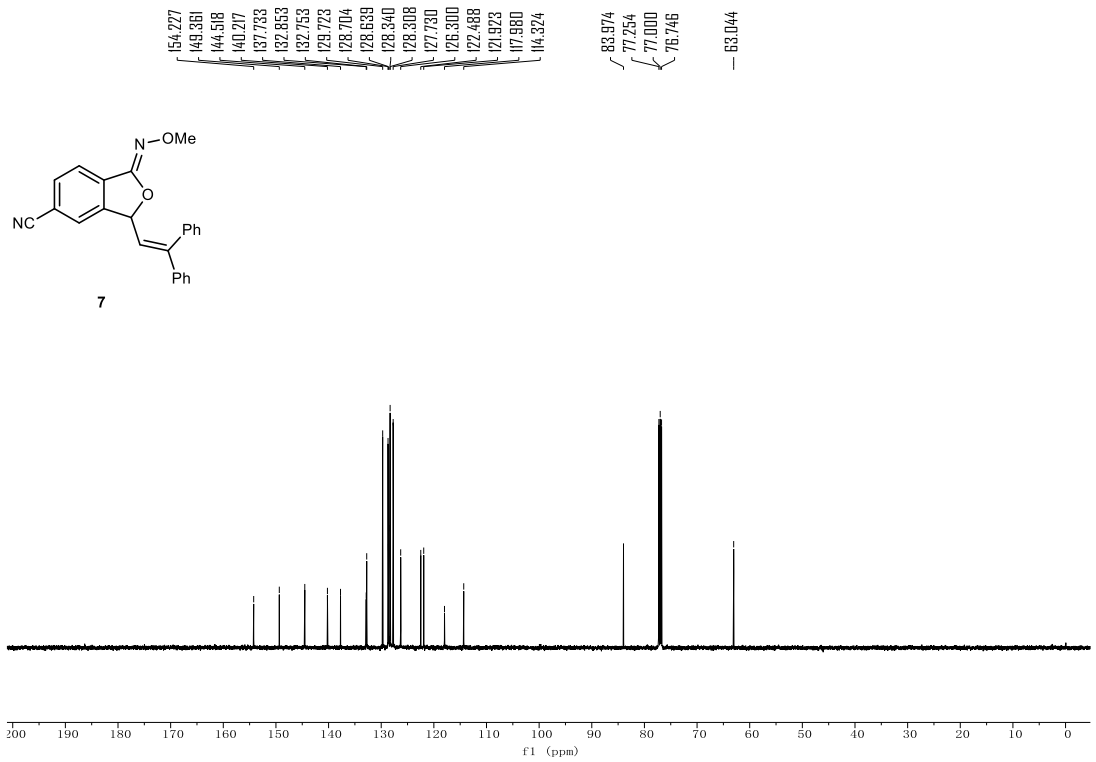
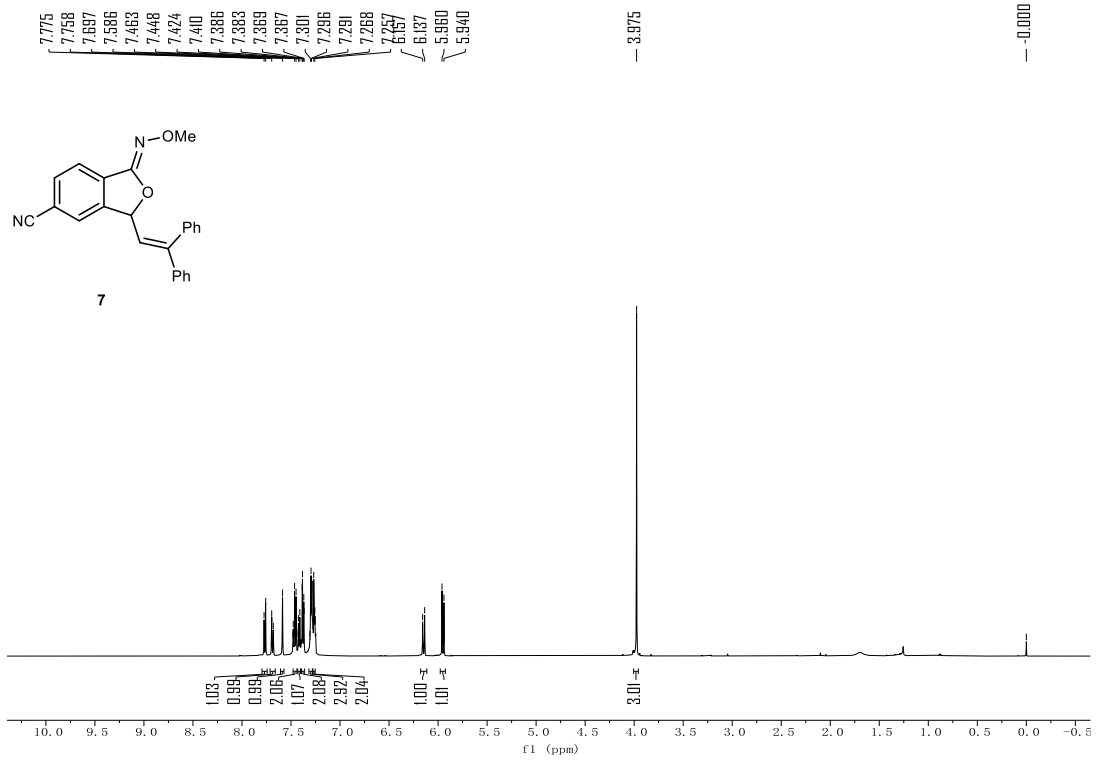


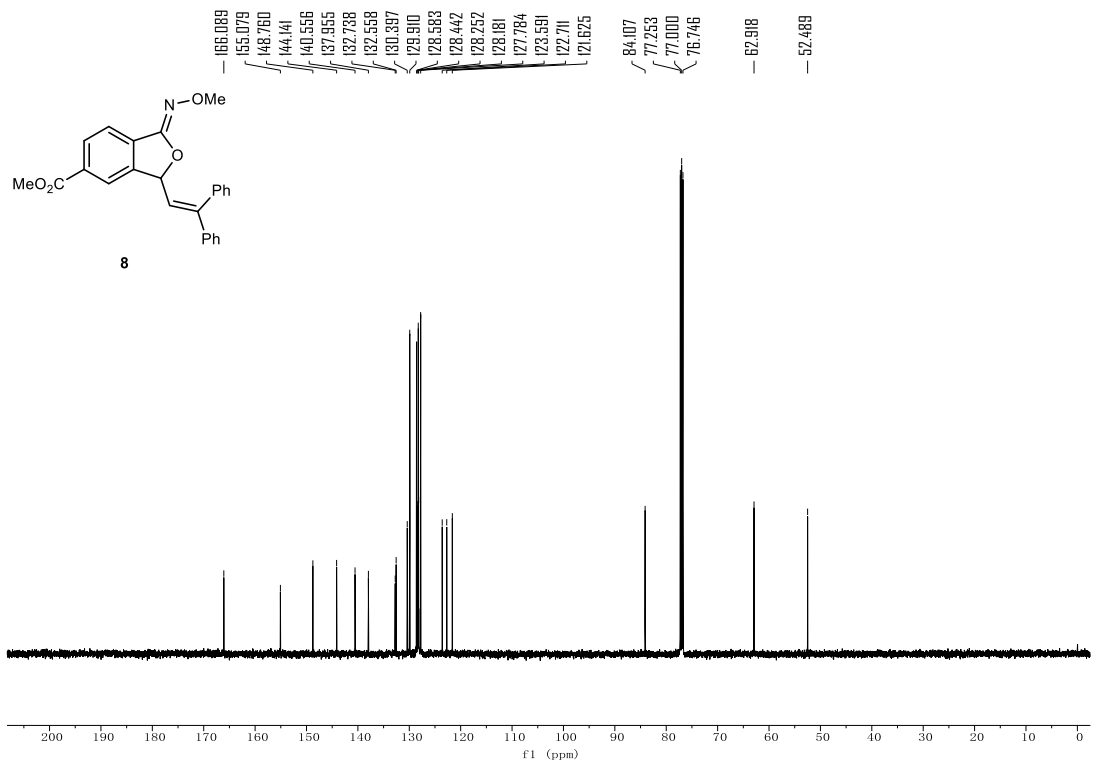
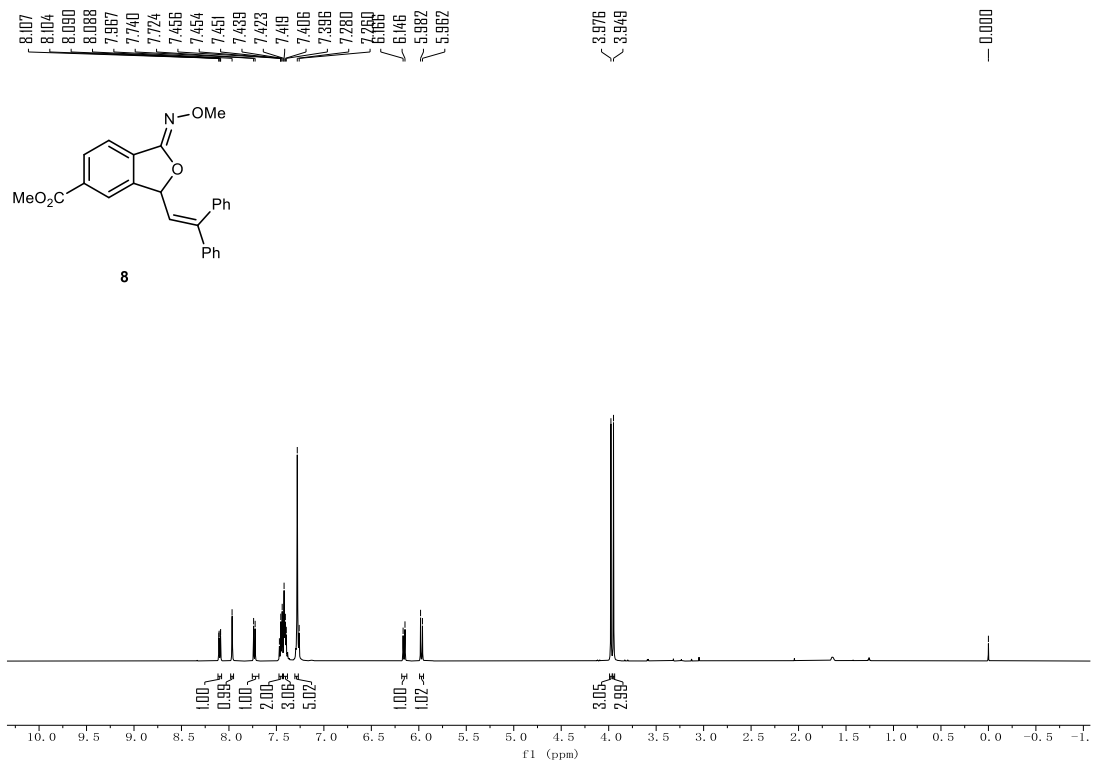


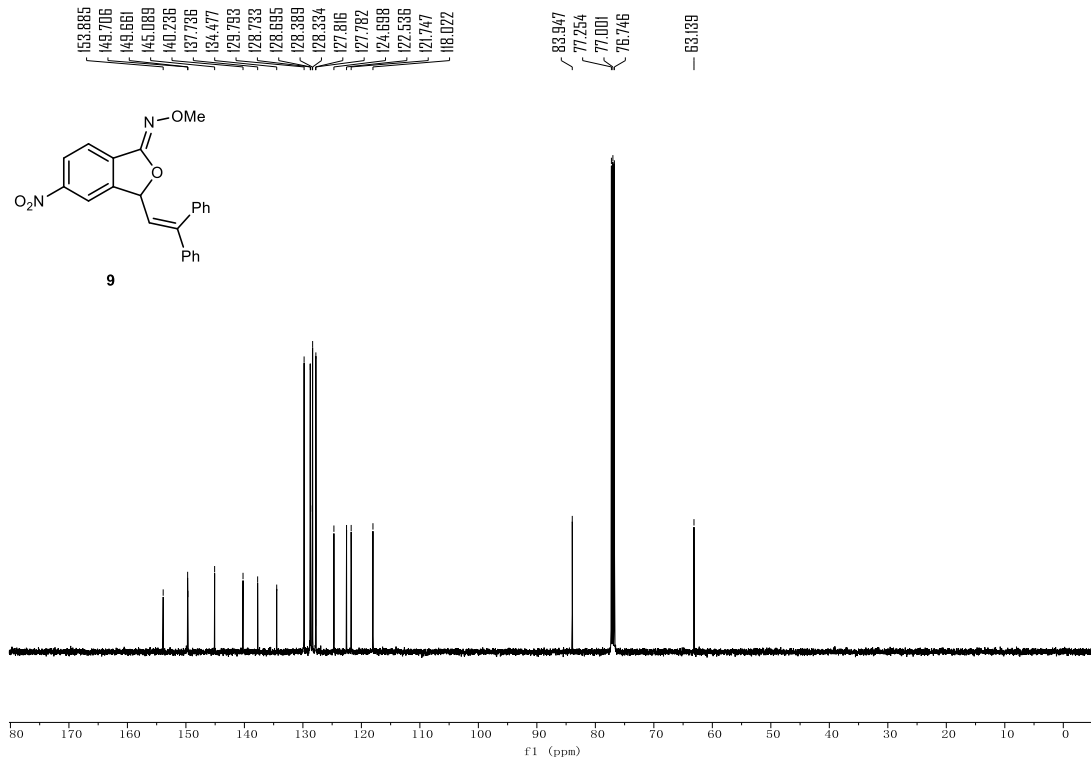
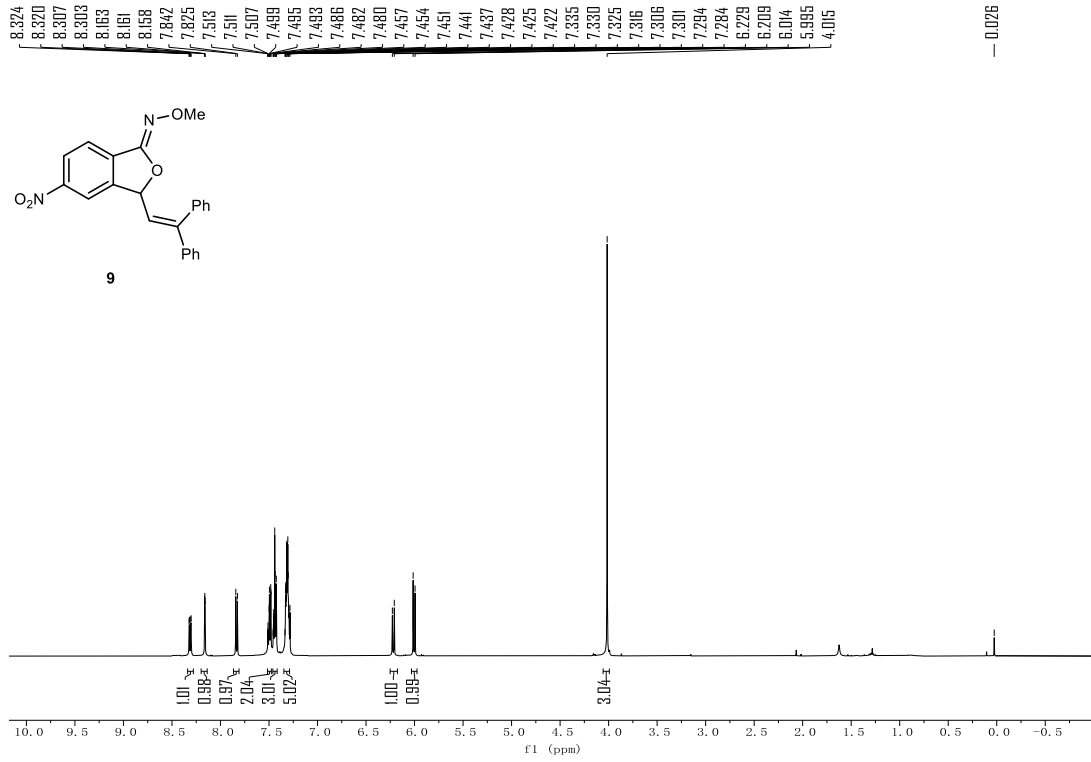


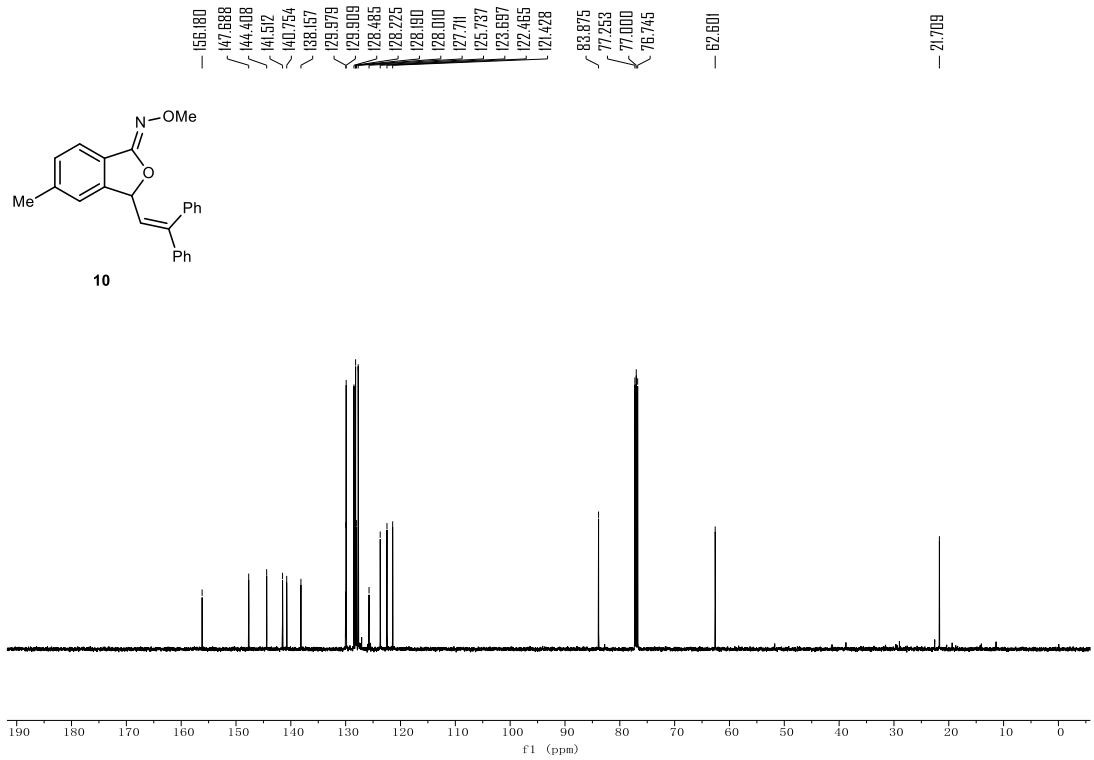
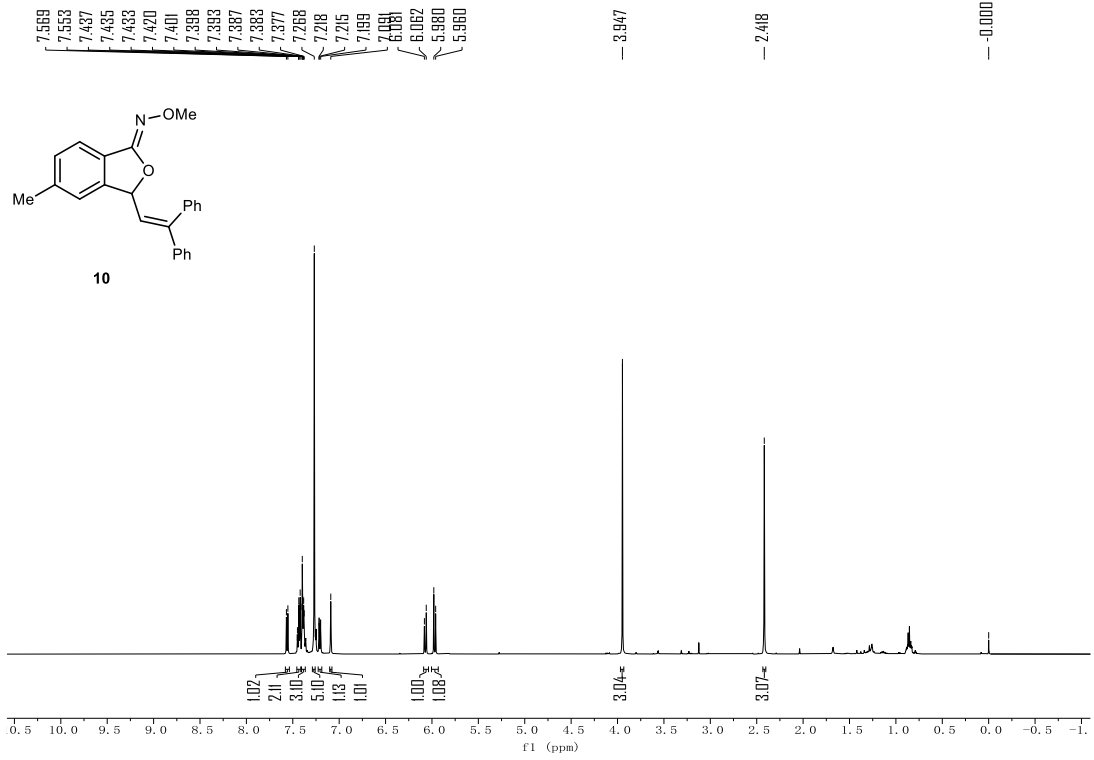


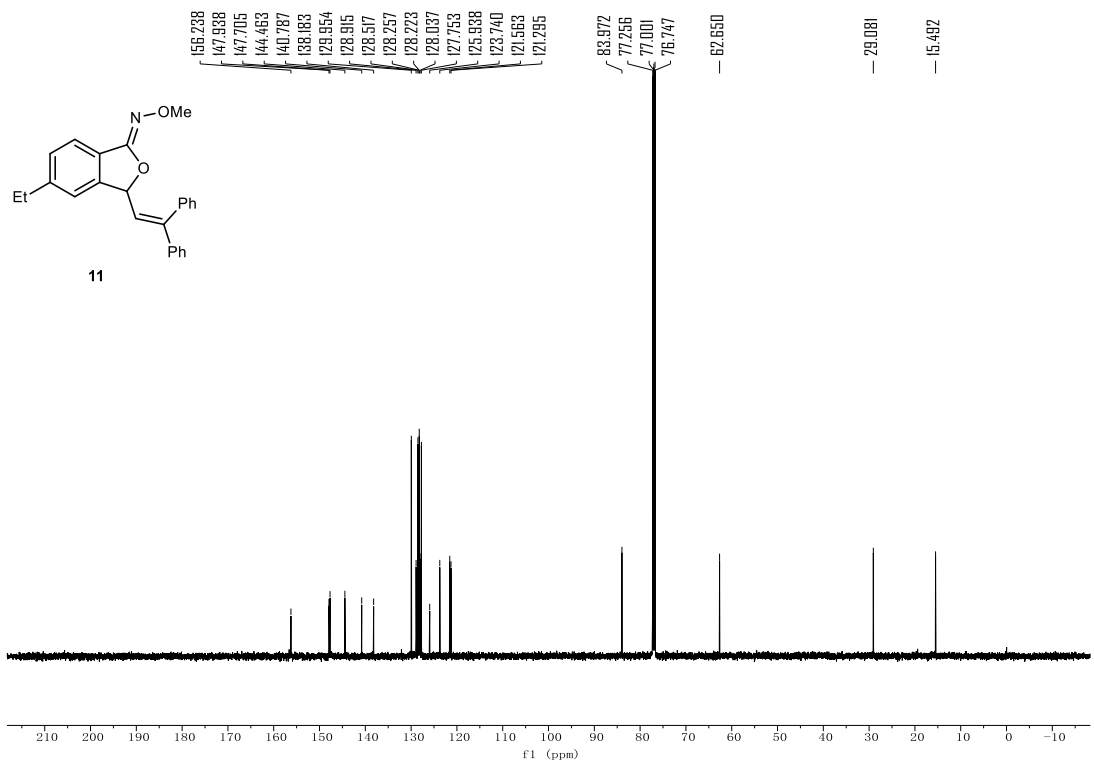
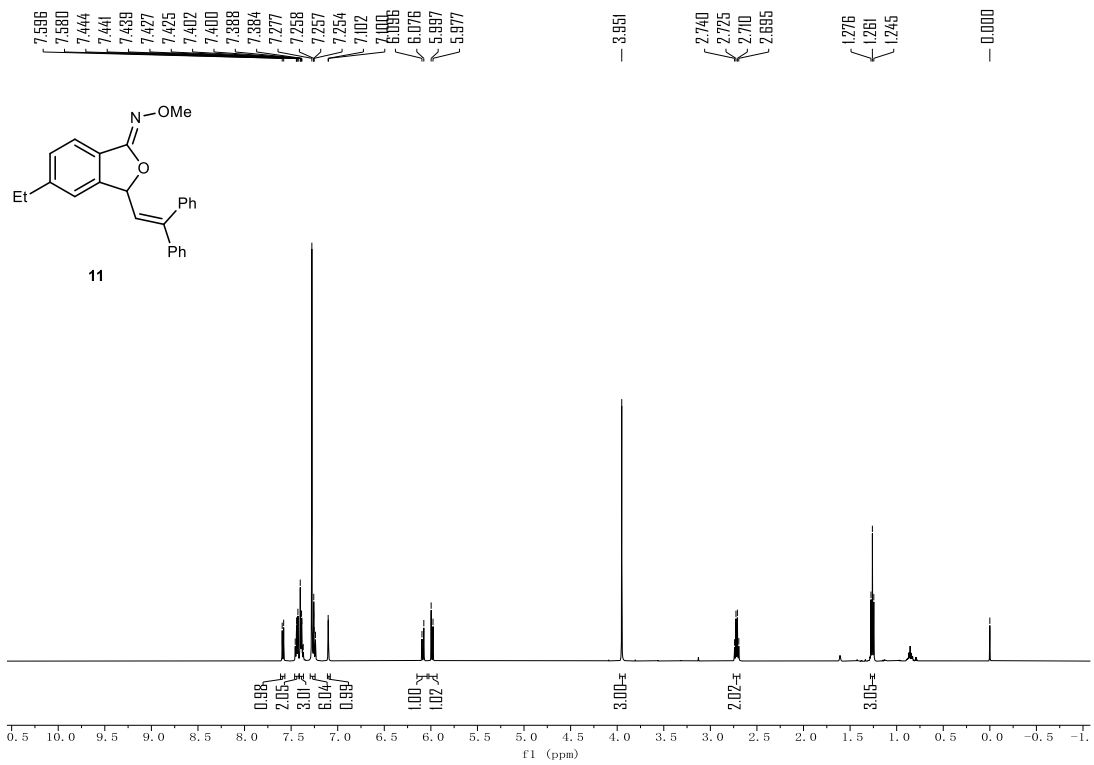


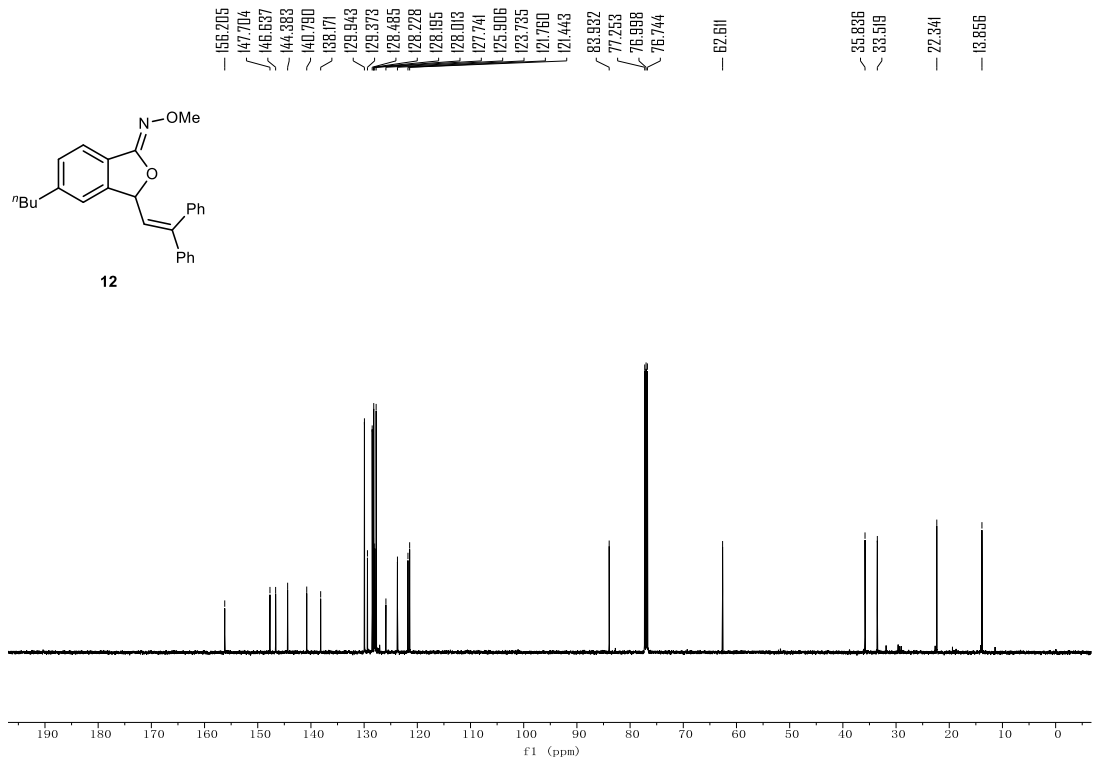
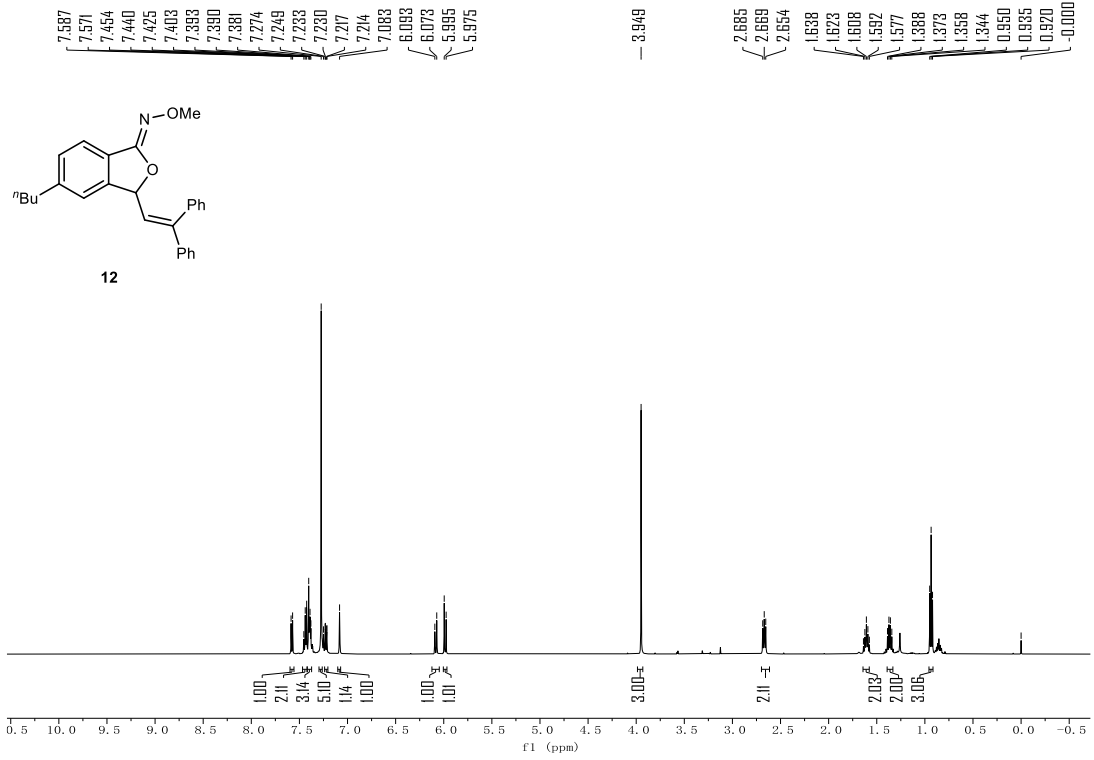


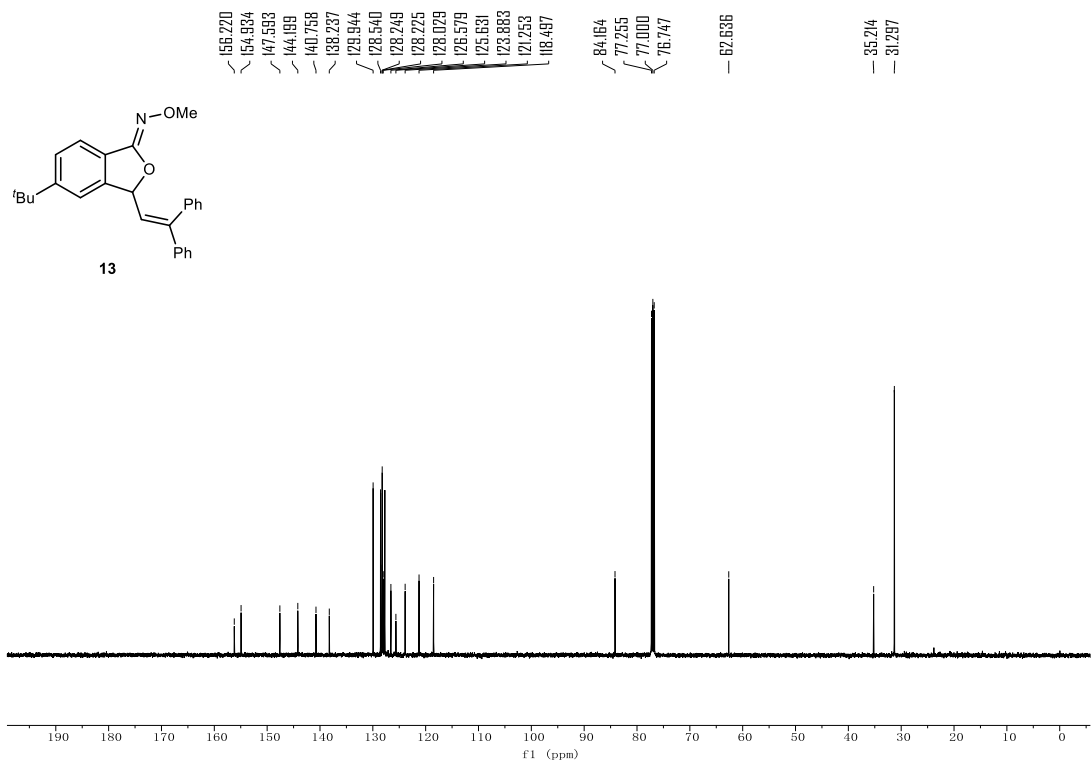
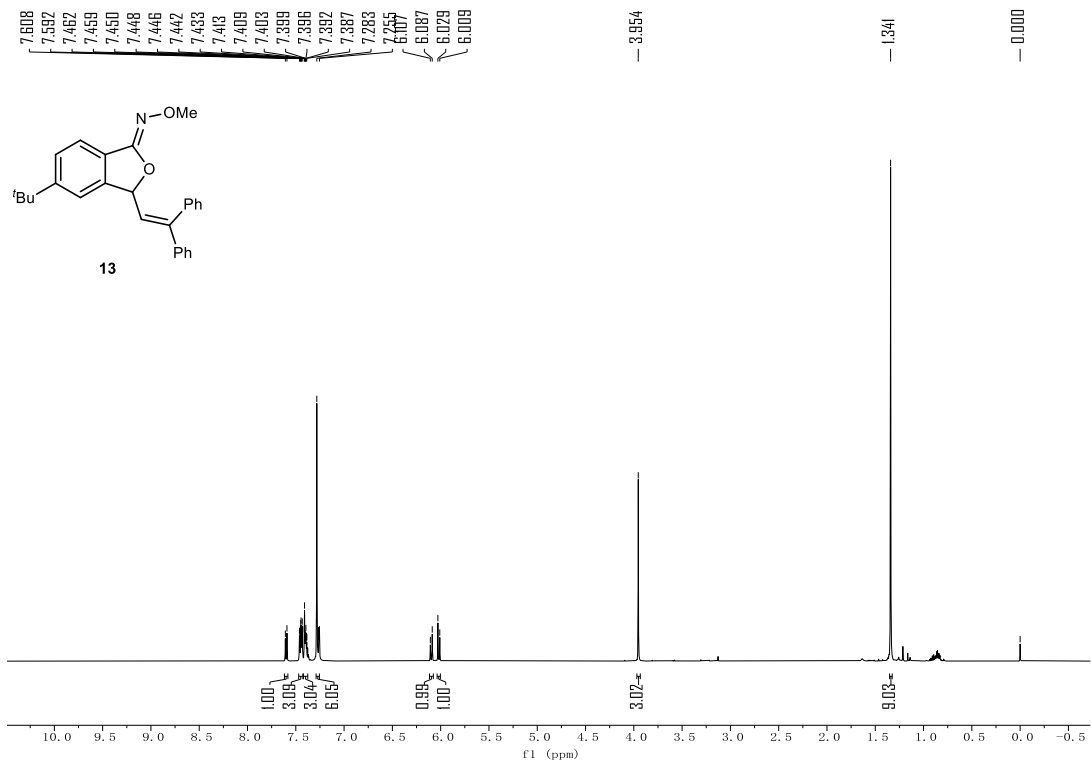




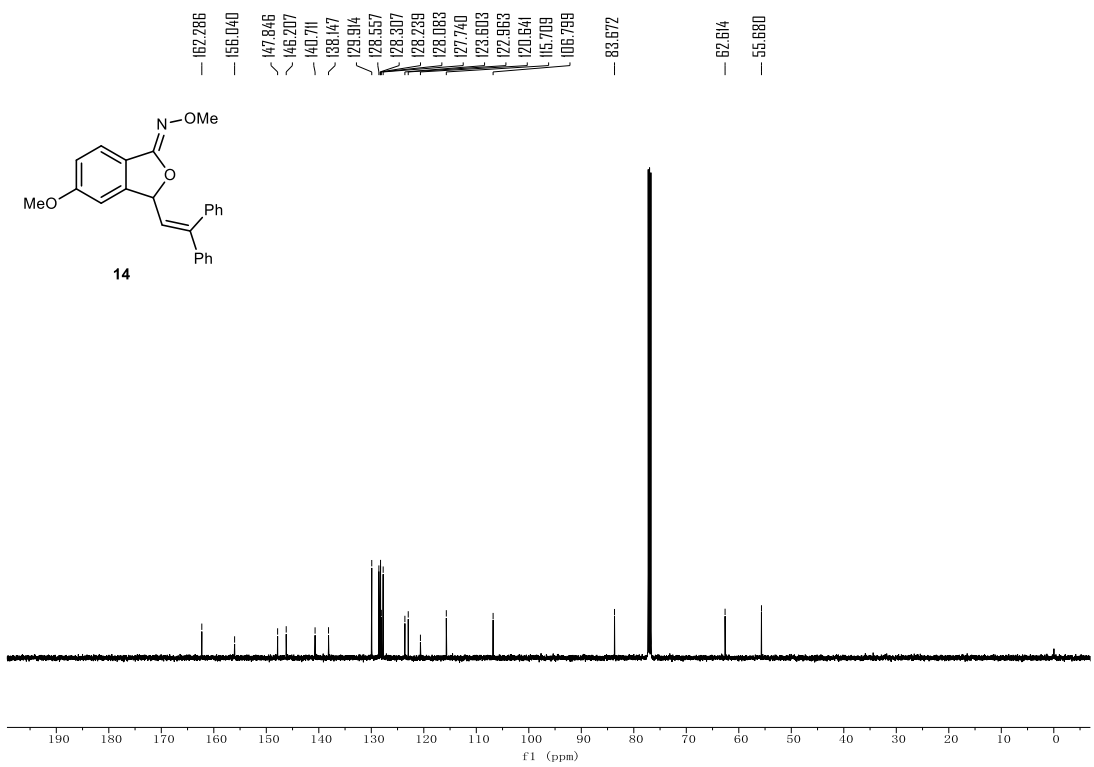
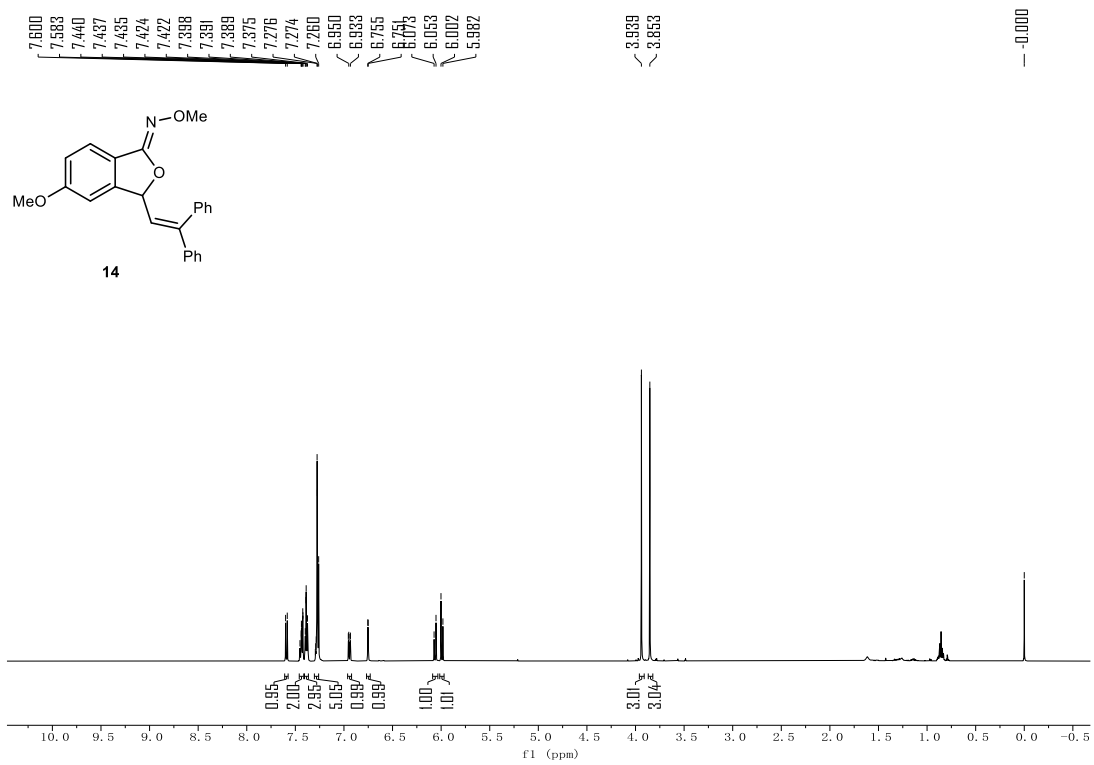


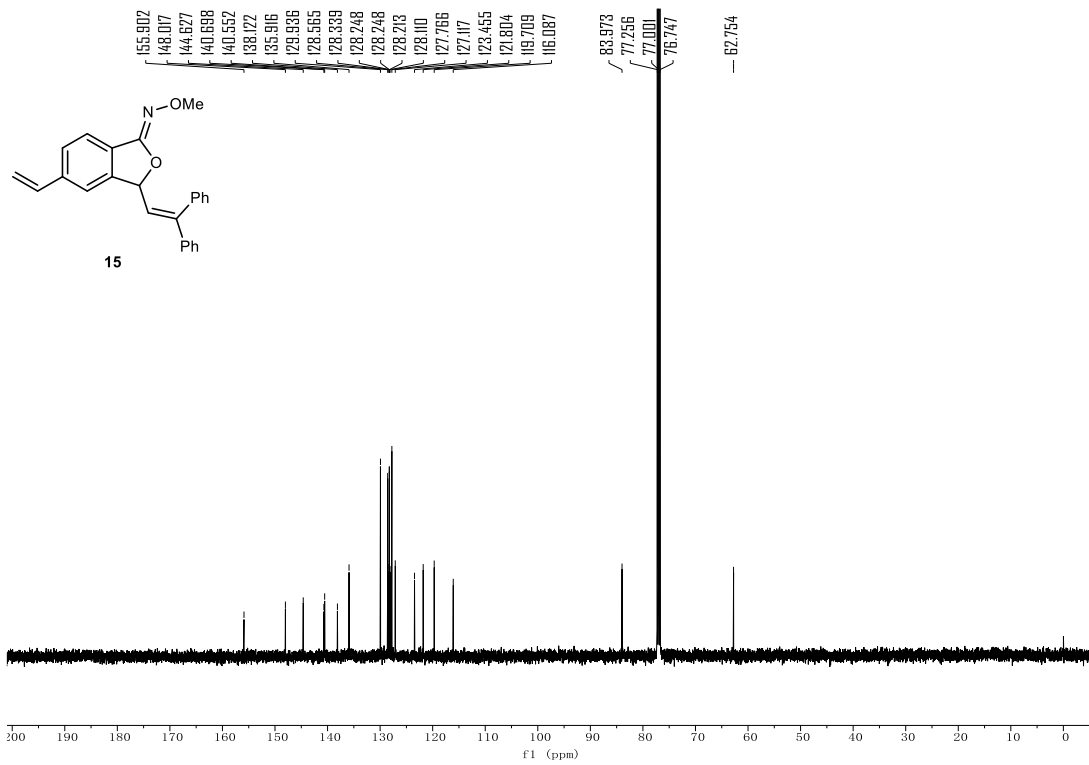
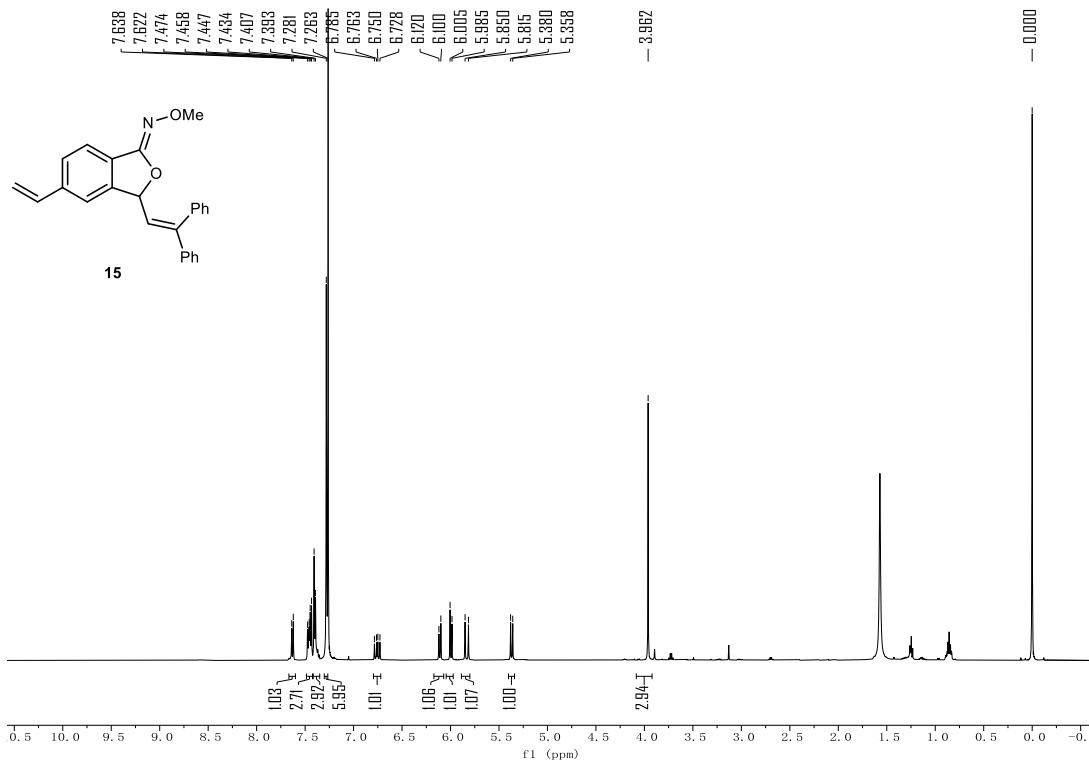


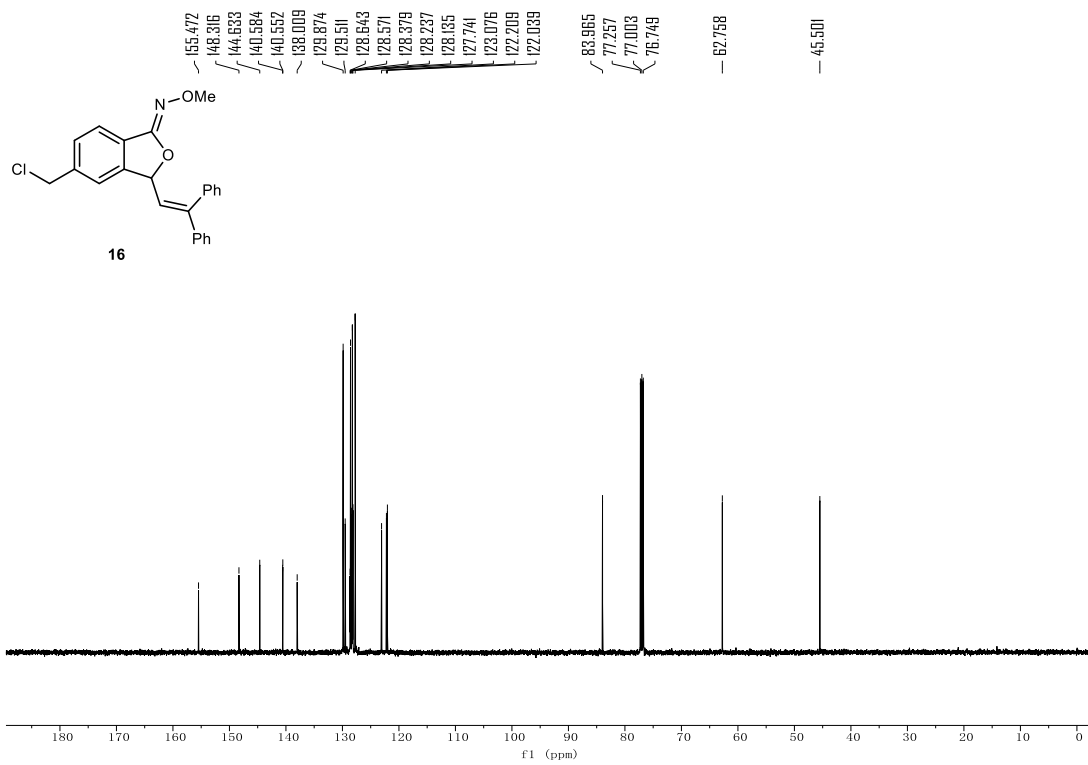
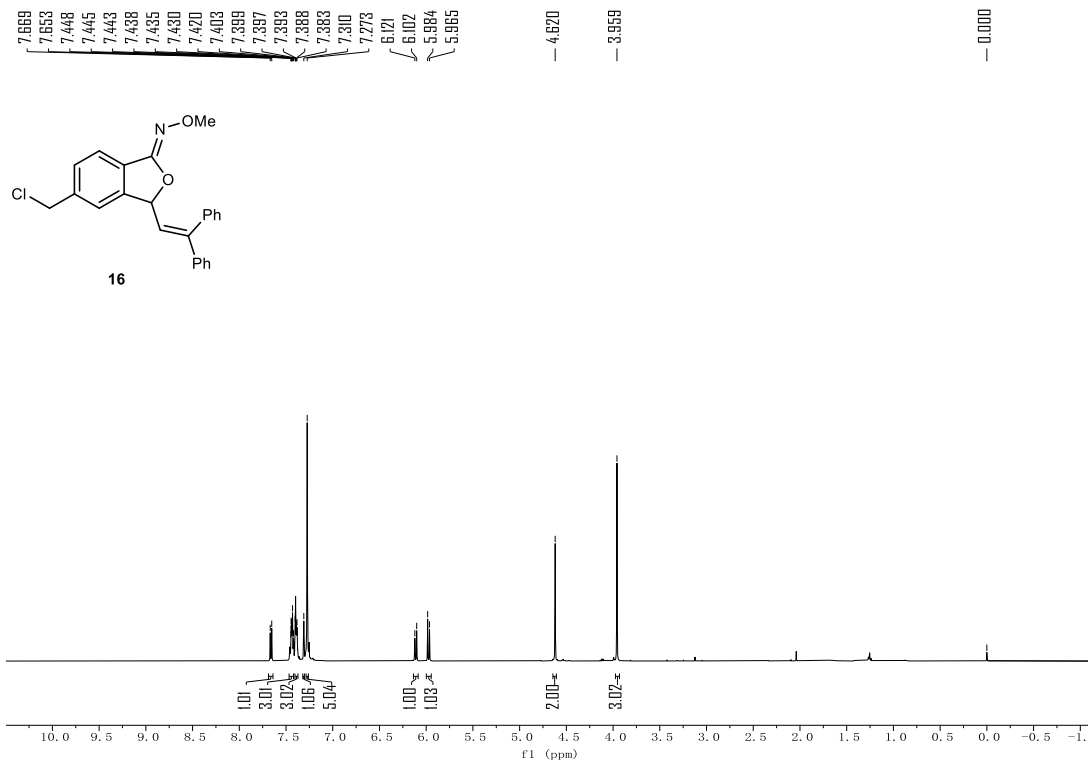


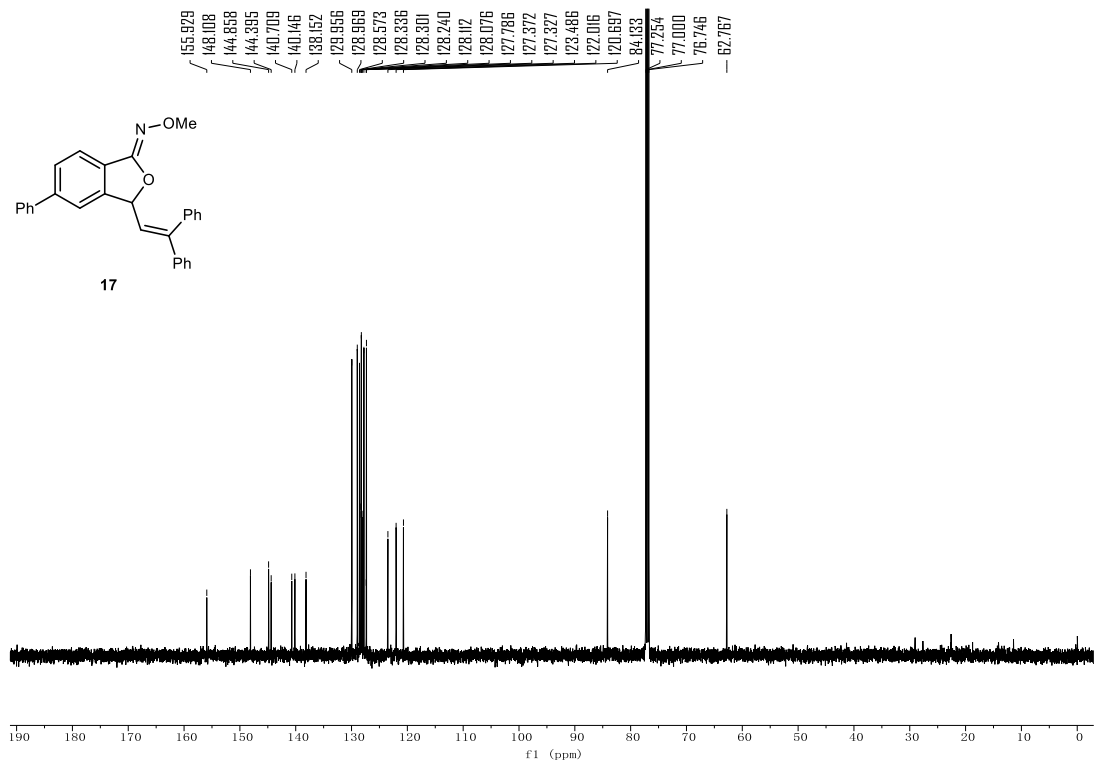
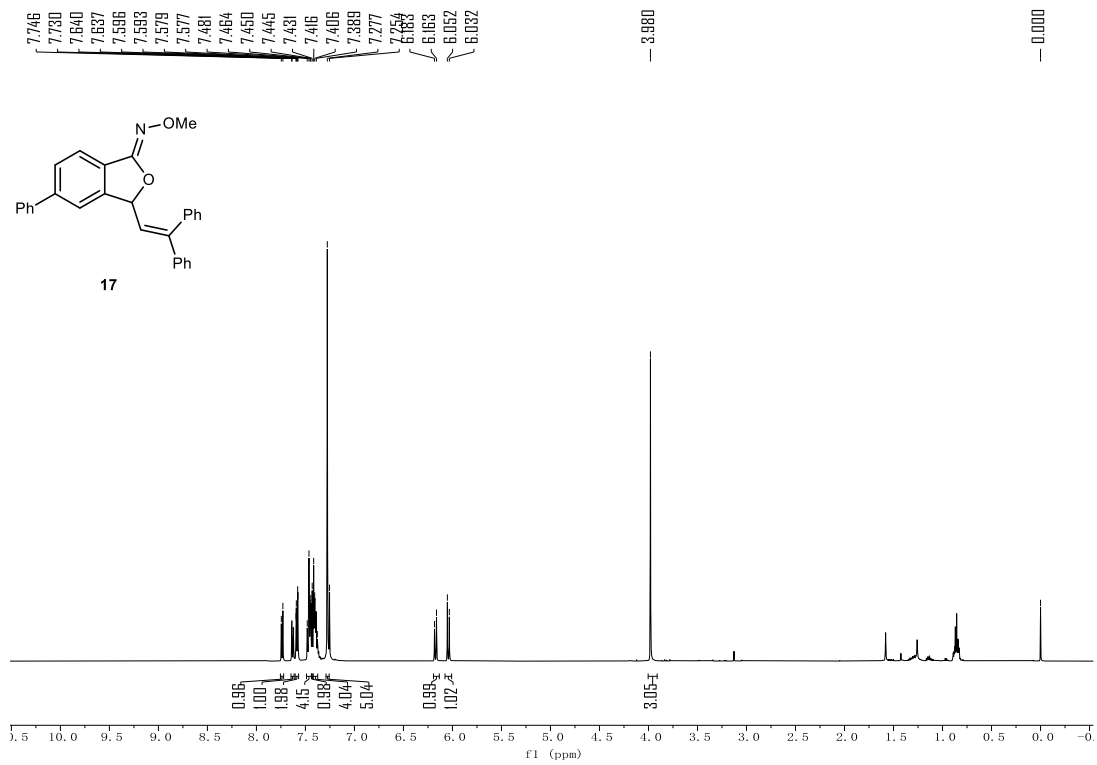


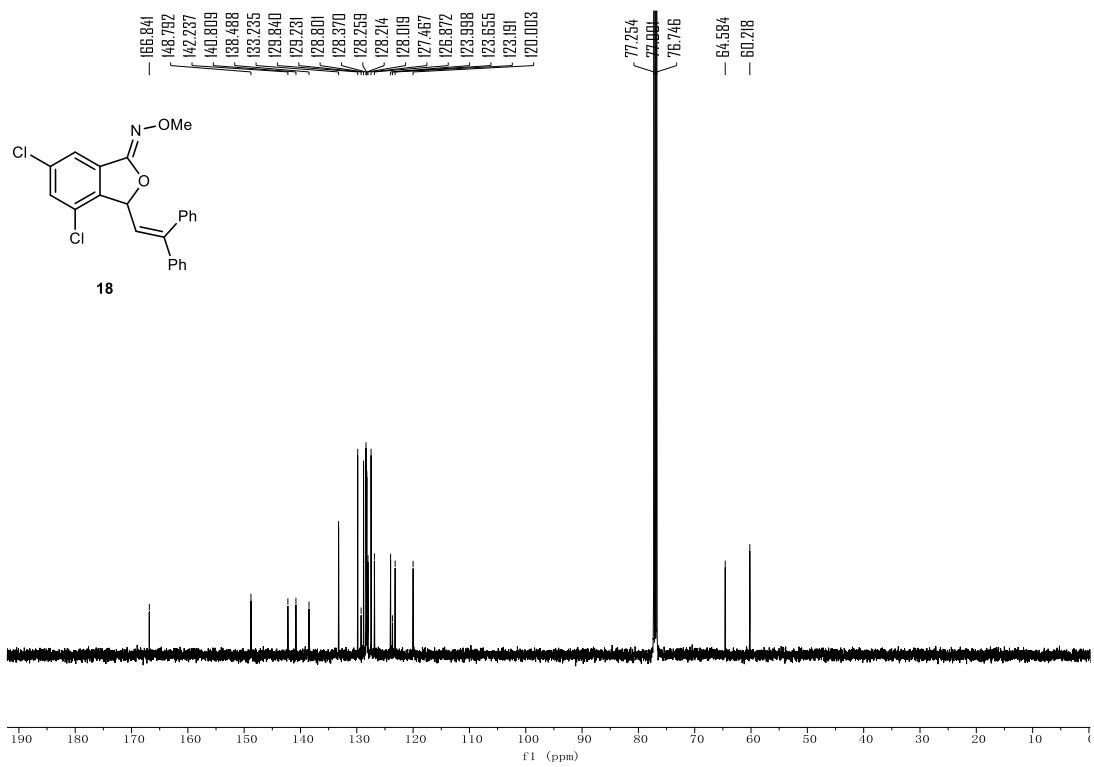
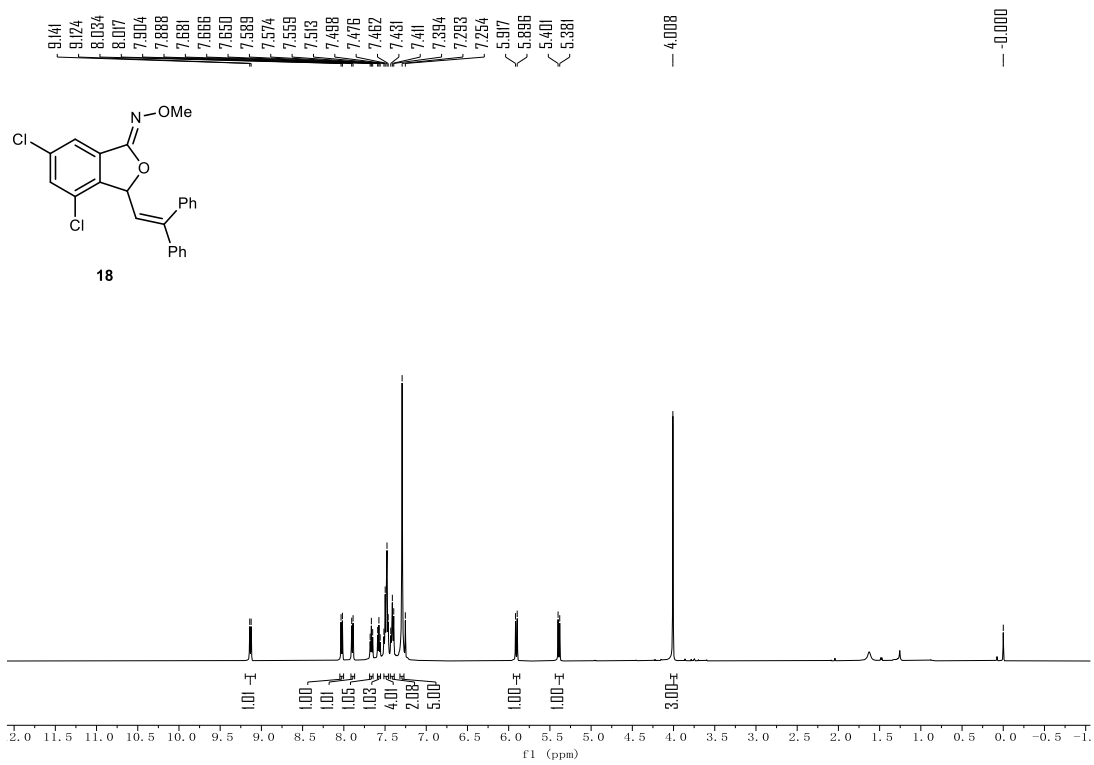


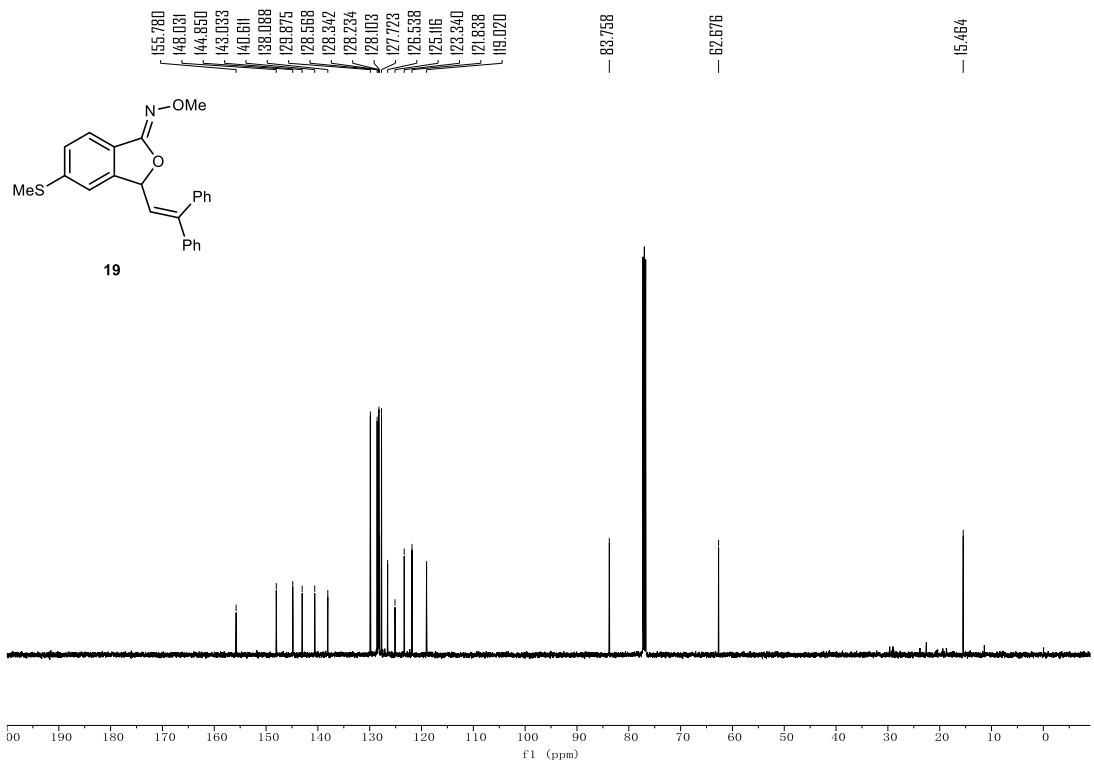
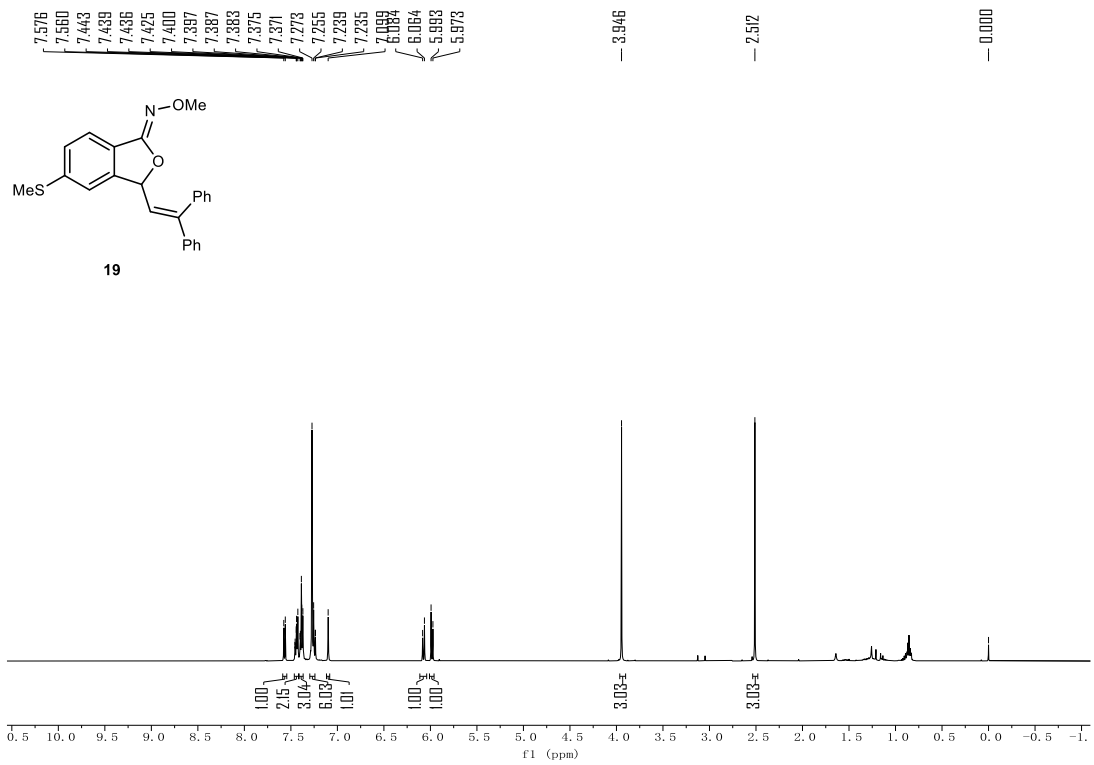






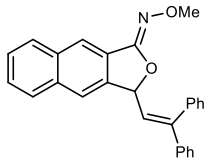




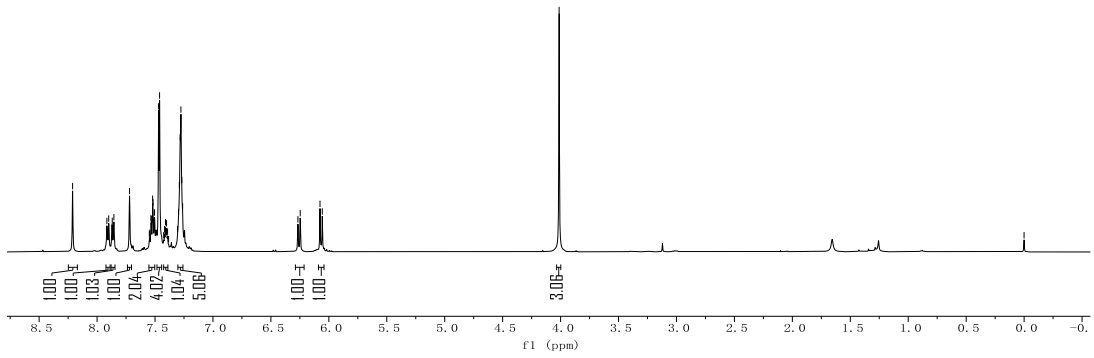


8.211  
7.915  
7.900  
7.869  
7.855  
7.720  
7.549  
7.546  
7.535  
7.532  
7.521  
7.517  
7.504  
7.469  
7.461  
7.425  
7.418  
7.409  
7.400  
7.392  
7.383  
7.315  
7.297  
7.290  
7.283  
7.276  
7.269  
7.262  
6.267  
6.247  
6.076  
6.056  
4.013

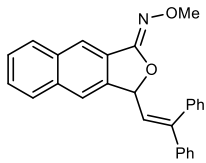
0.000



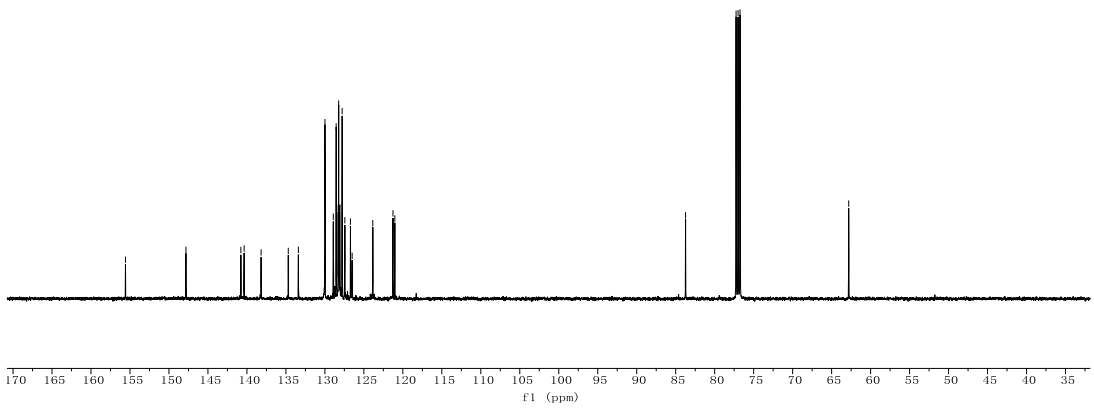
20

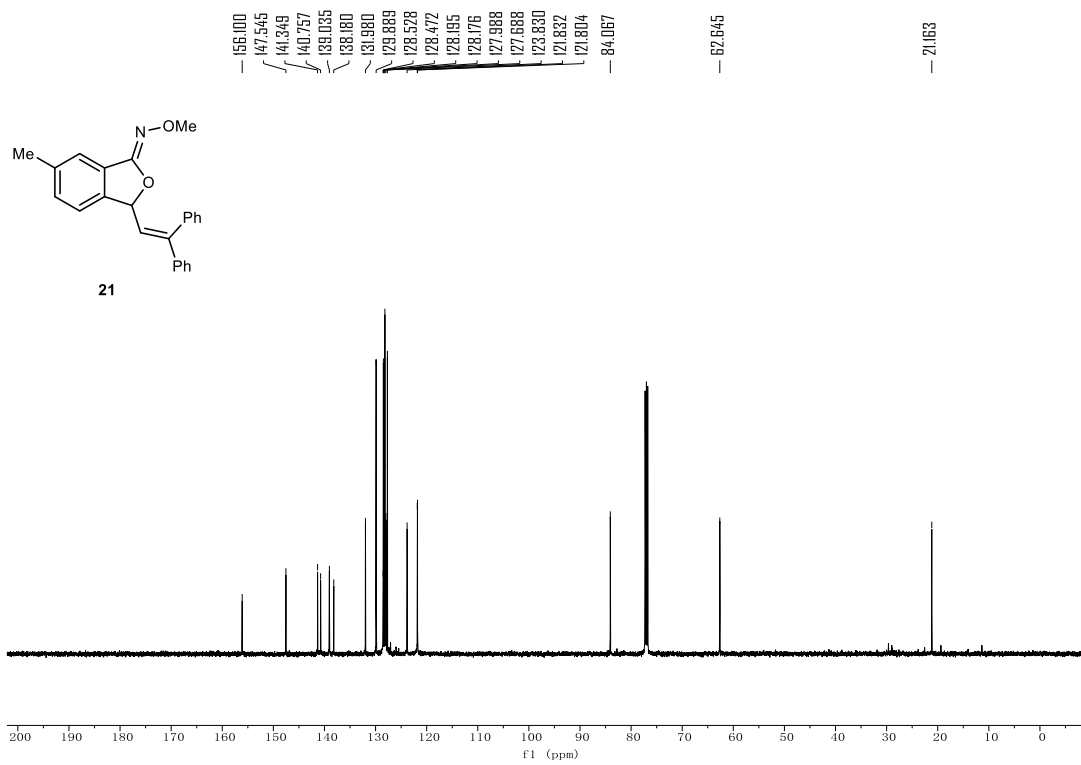
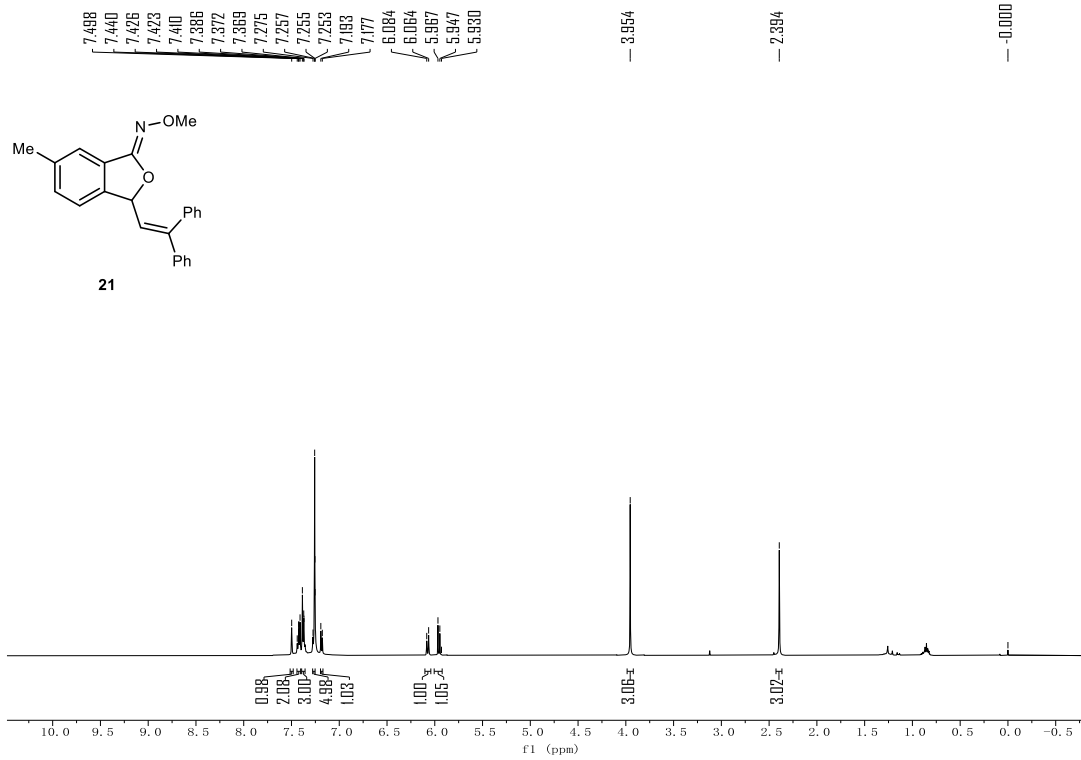


155.577  
147.818  
140.776  
140.357  
138.181  
134.655  
133.399  
129.990  
128.916  
128.551  
128.282  
128.229  
128.109  
128.070  
127.784  
127.440  
126.718  
125.503  
123.852  
121.263  
121.026  
83.734  
77.256  
77.001  
76.748  
67.809

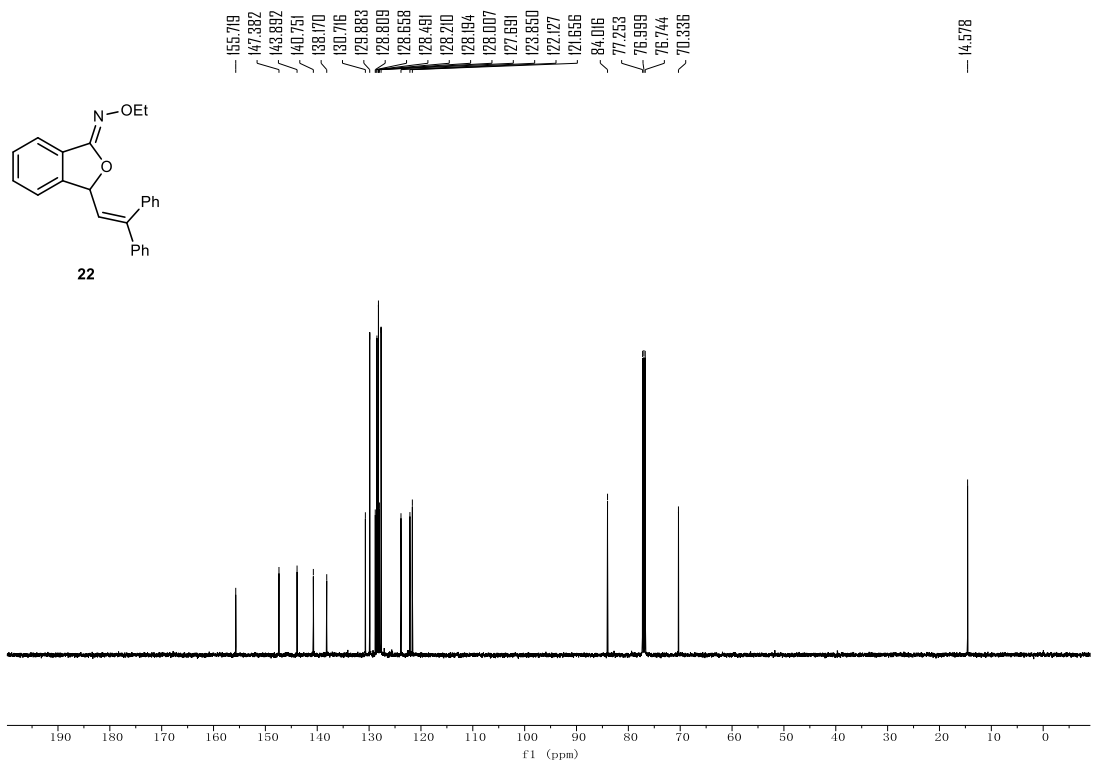
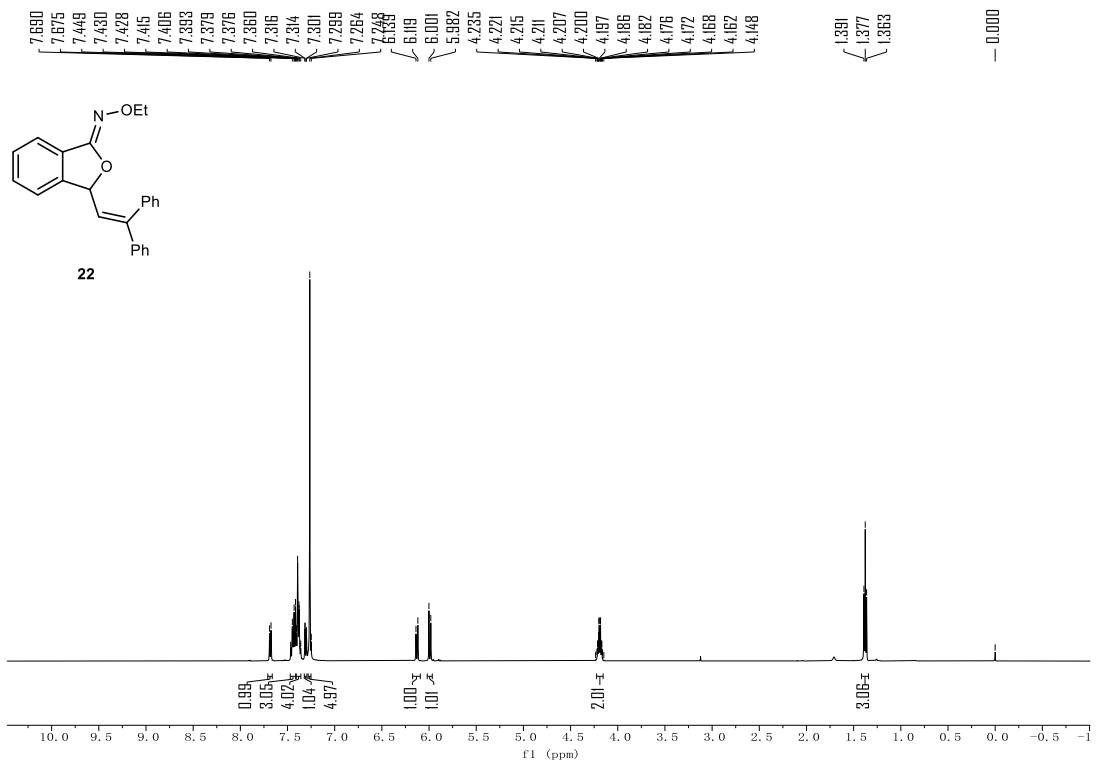


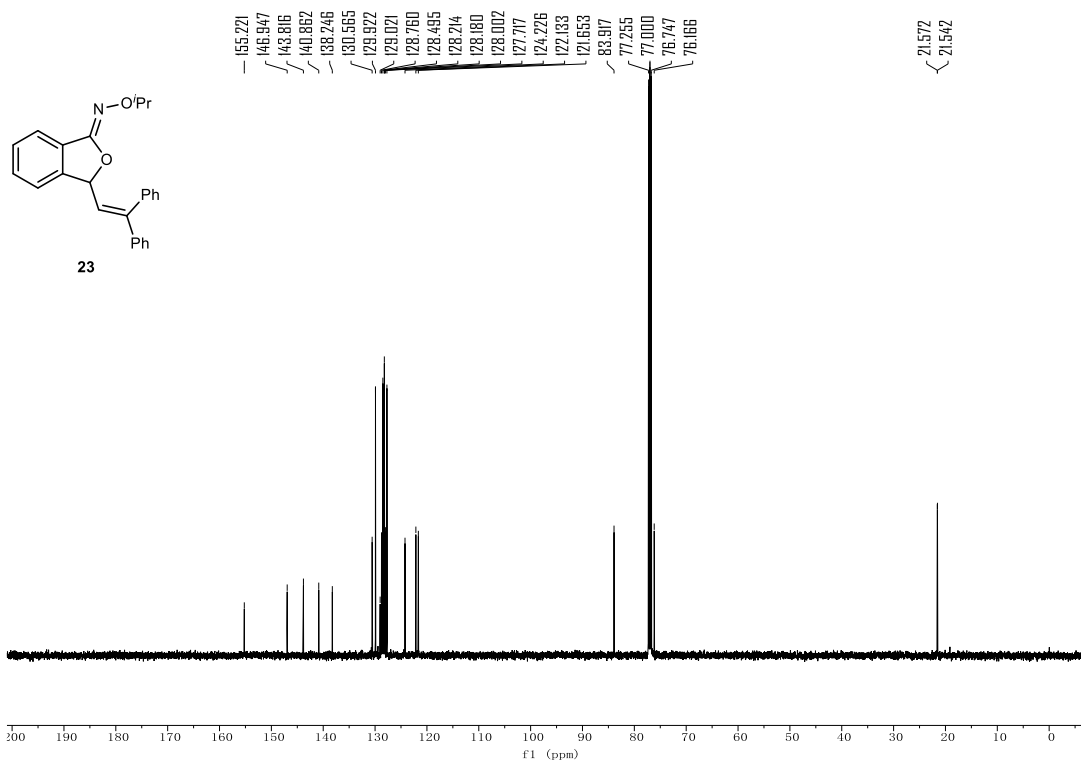
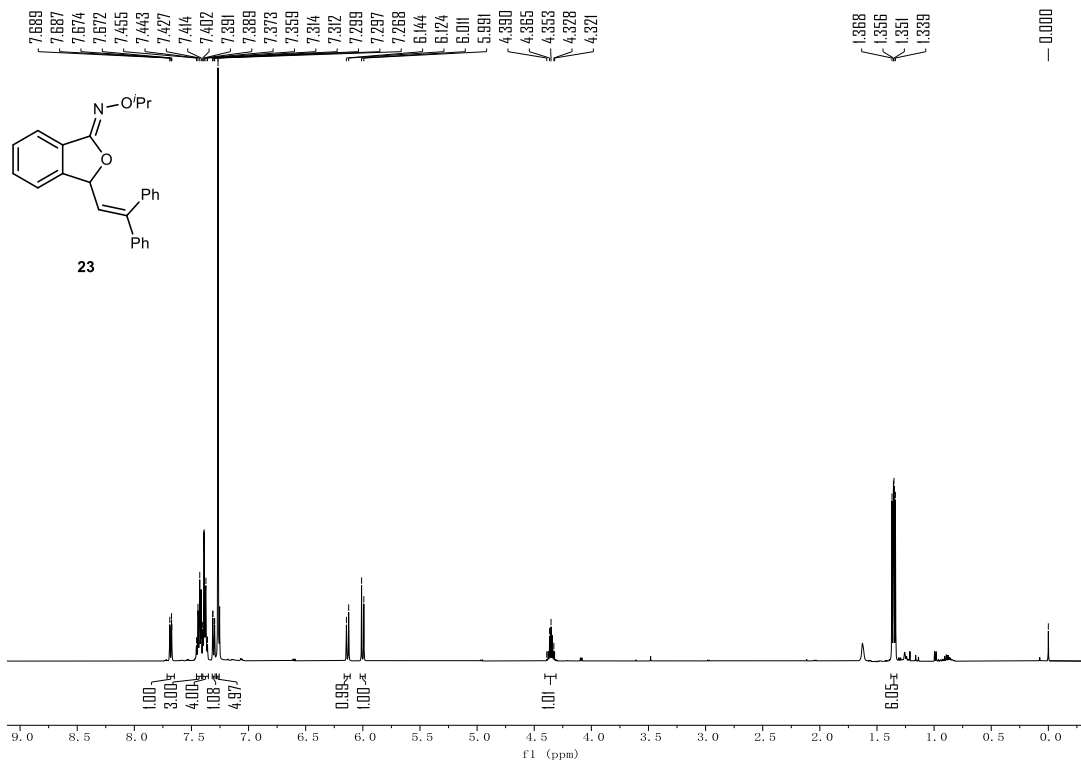
20

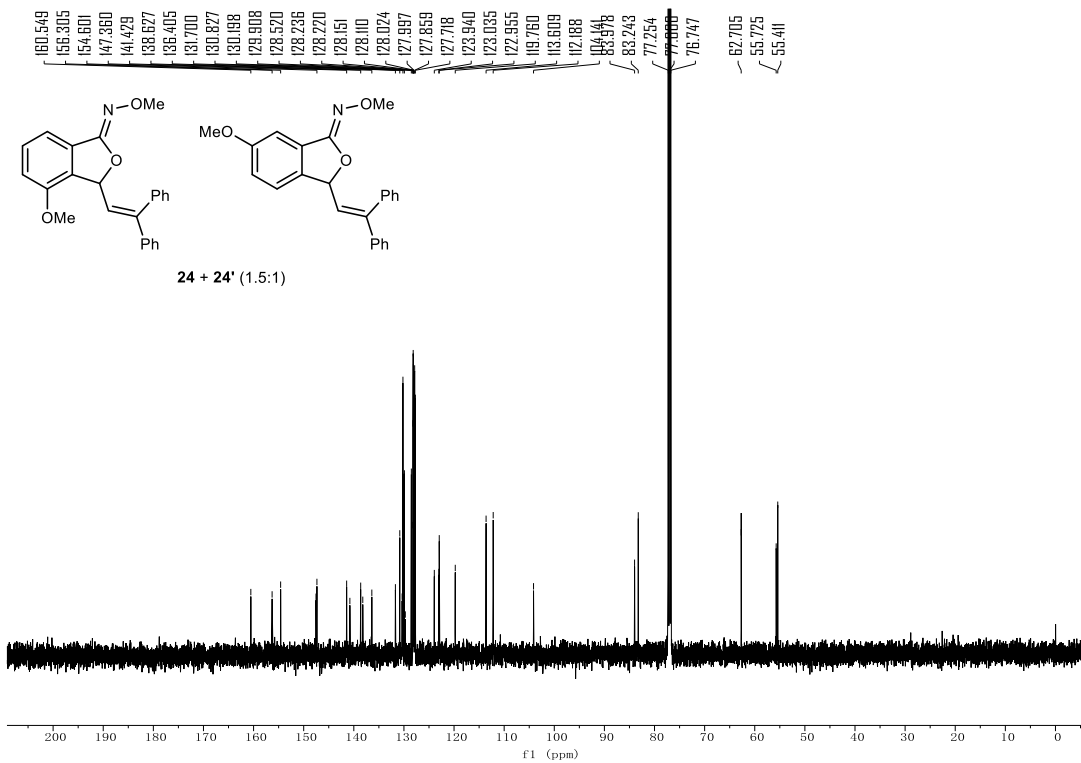
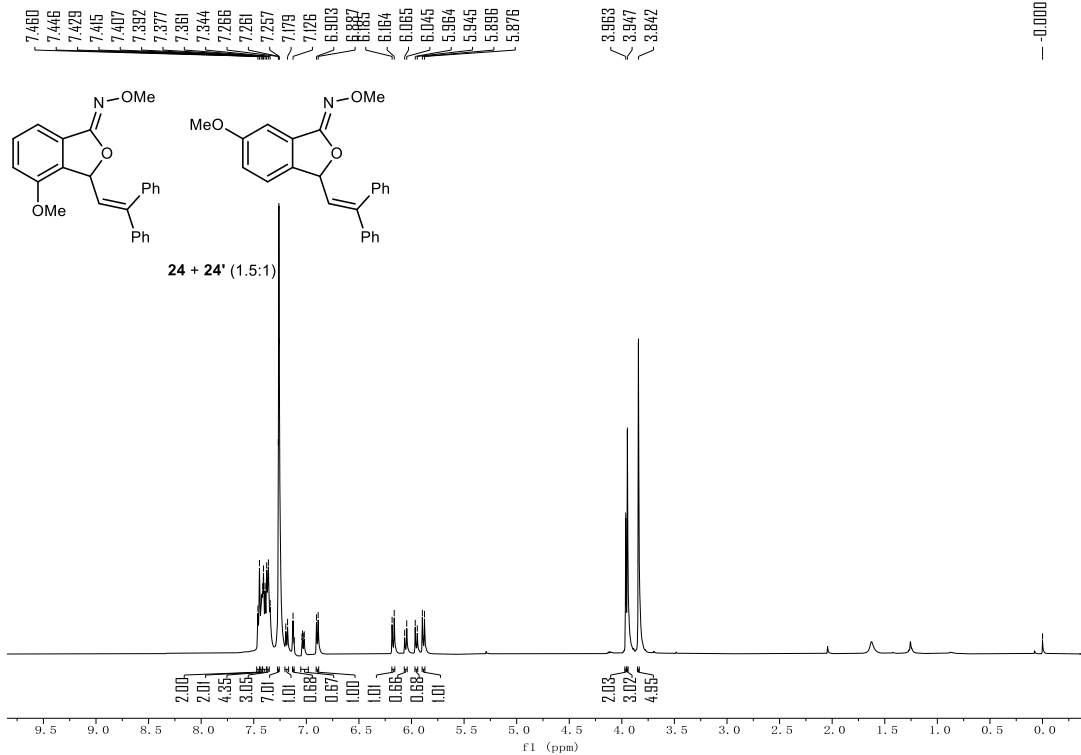


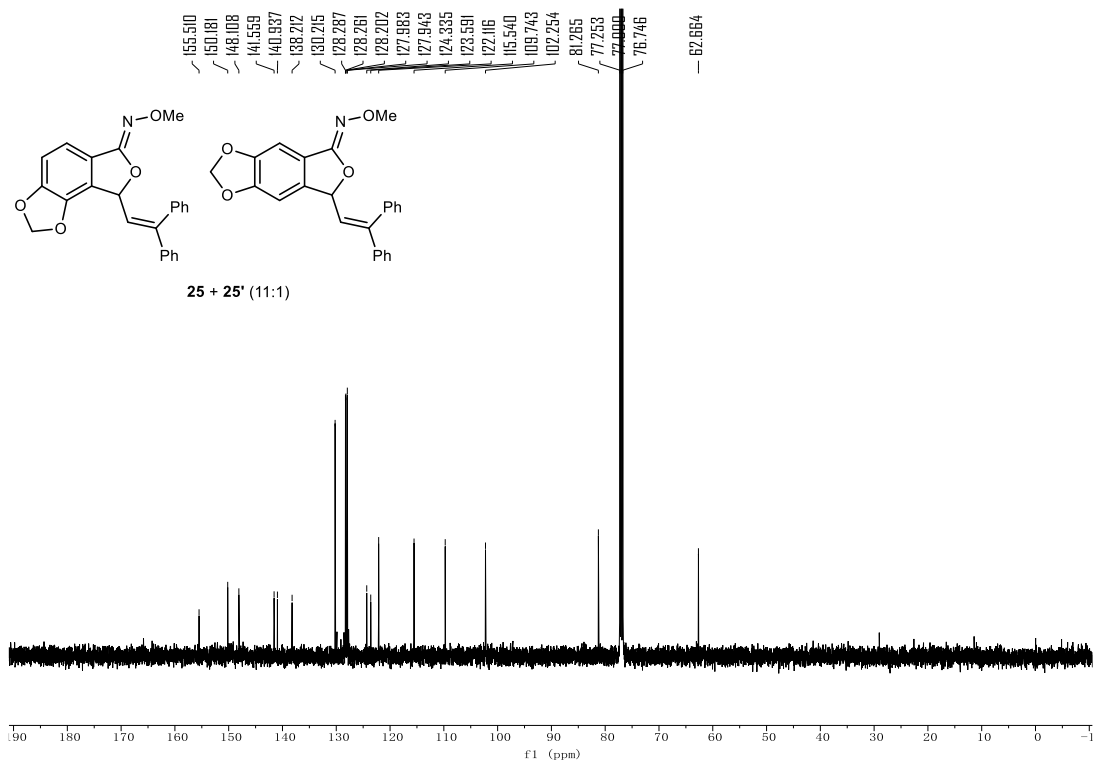
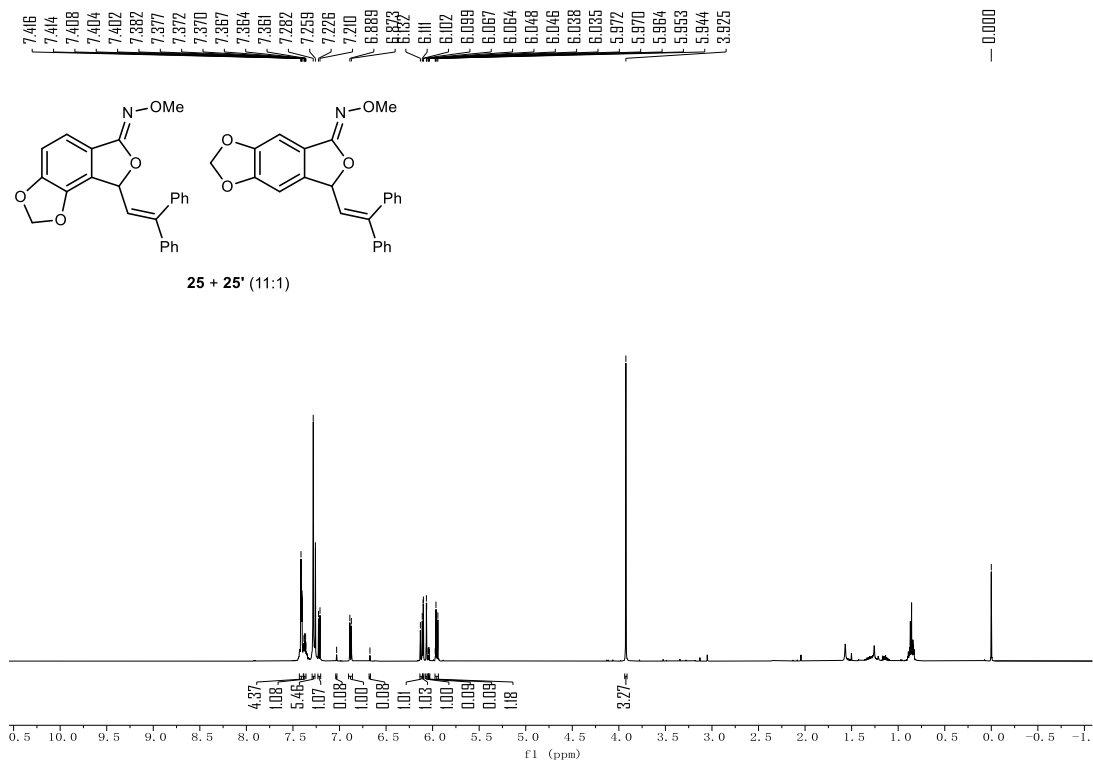


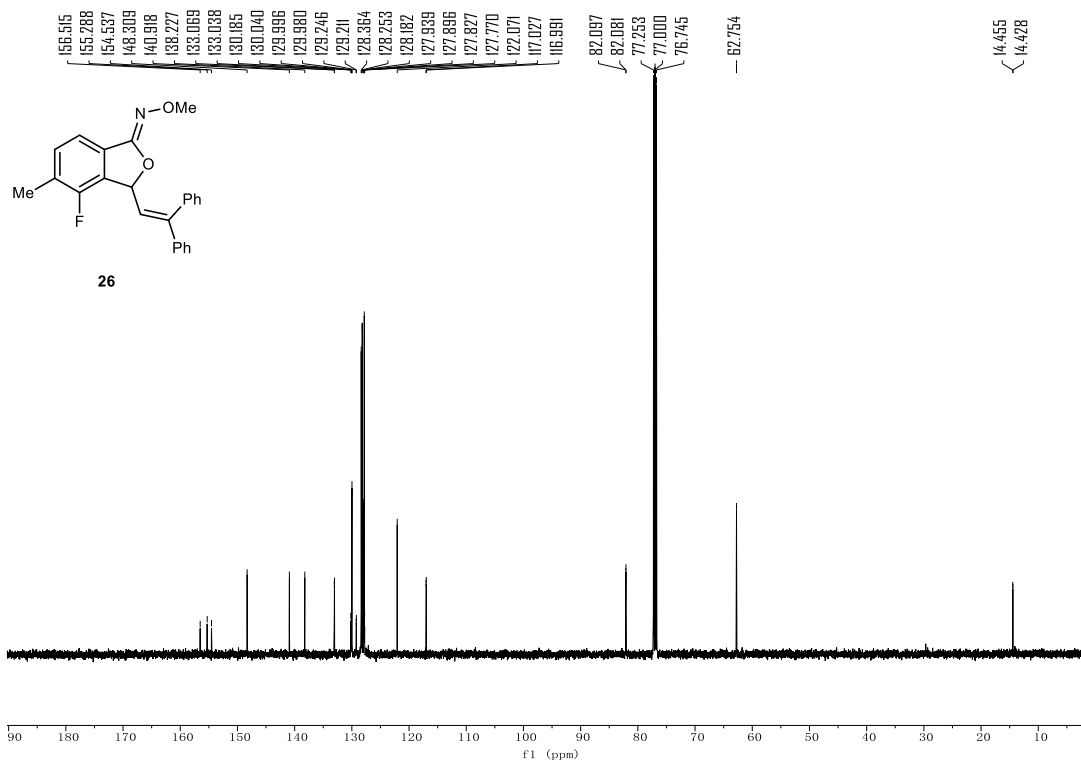
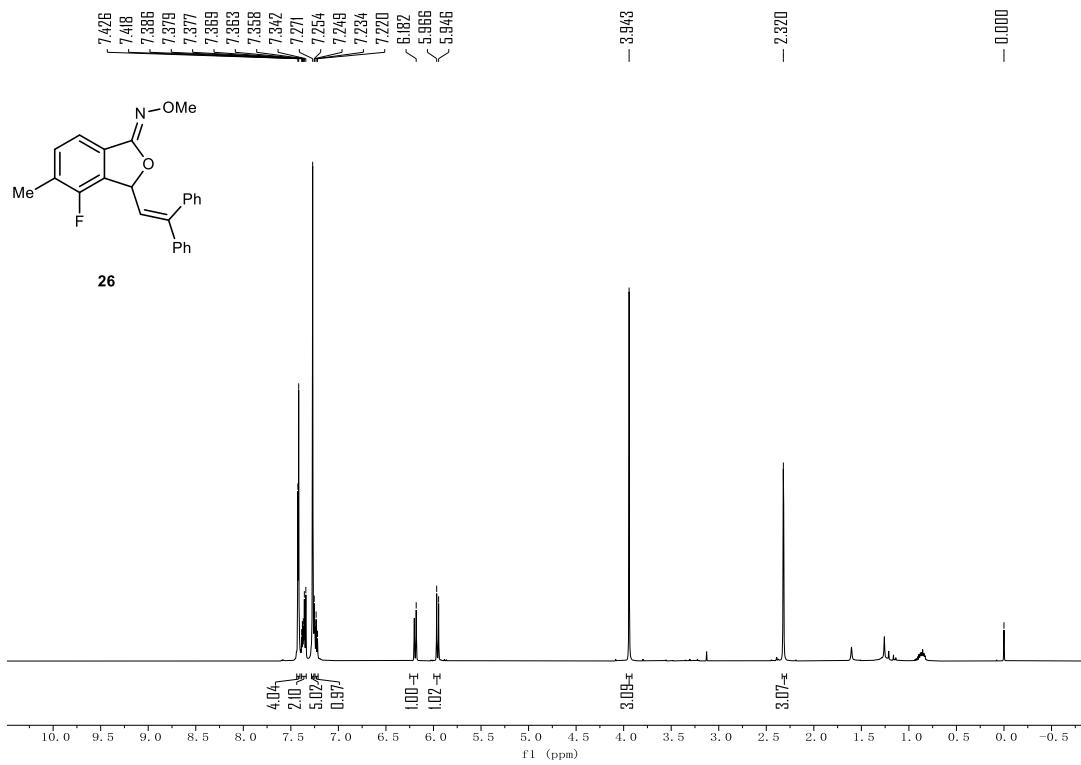


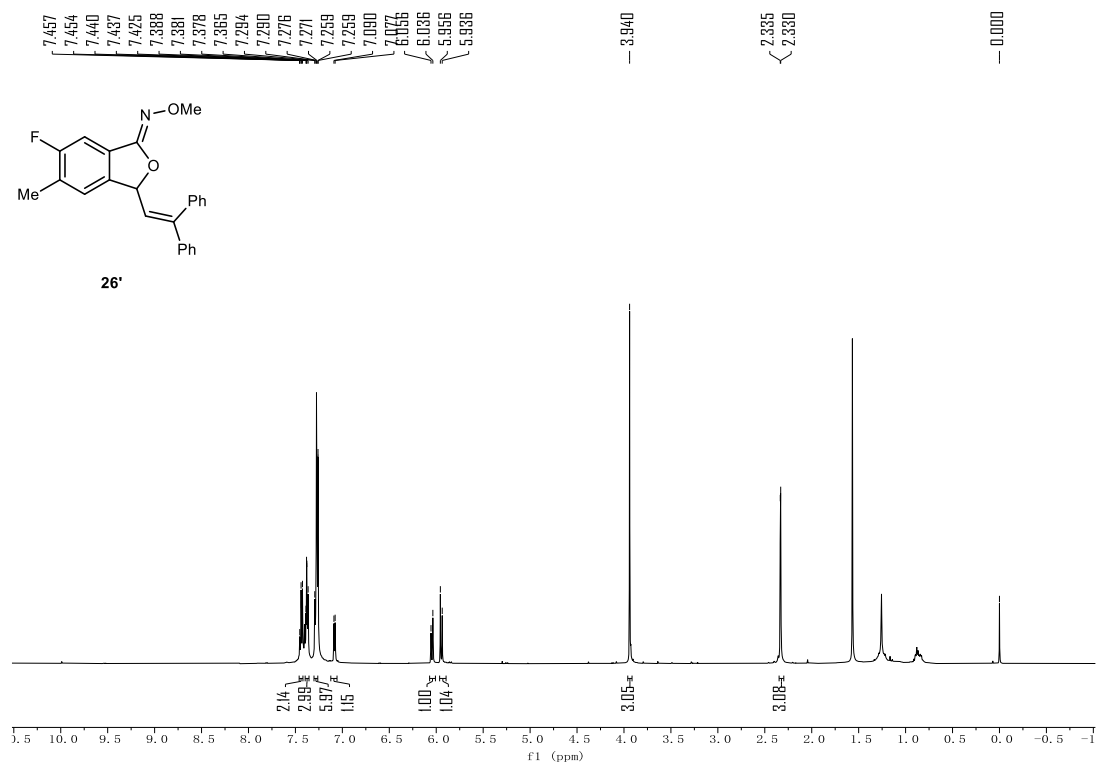
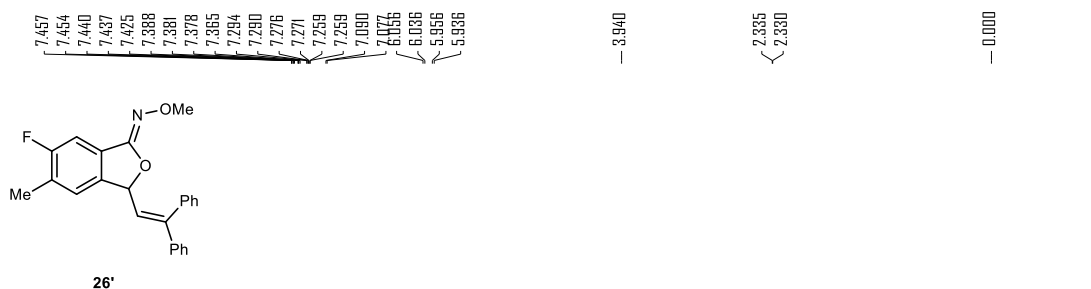
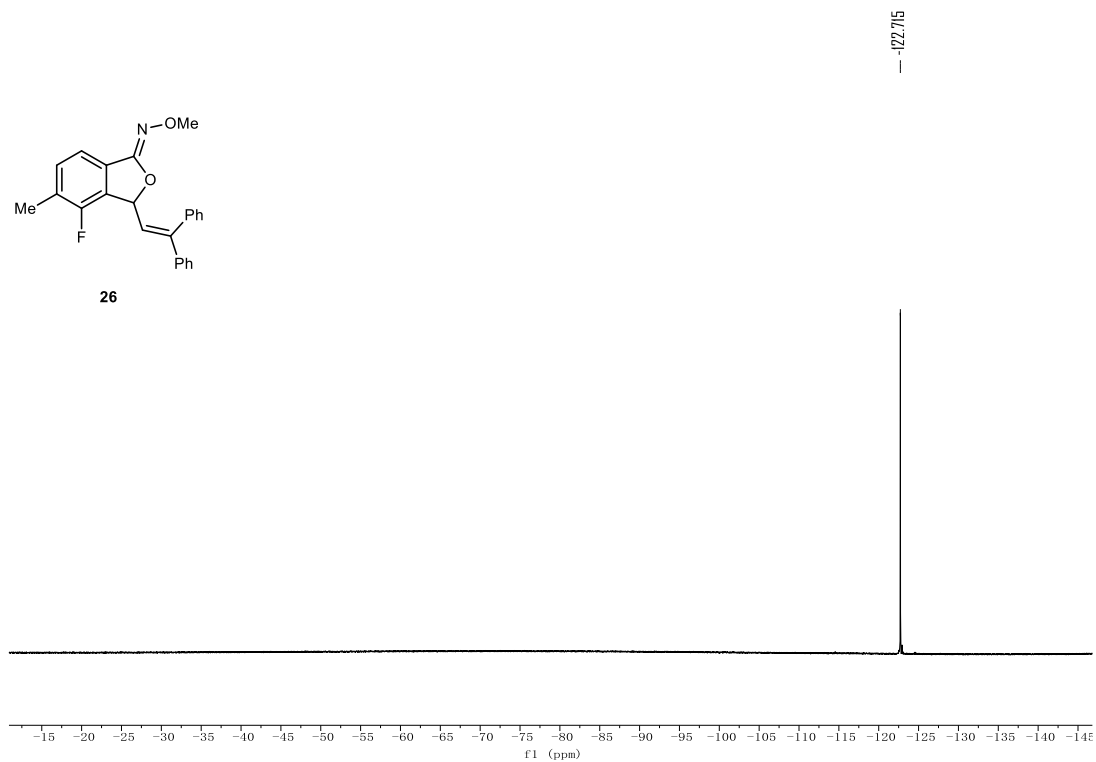
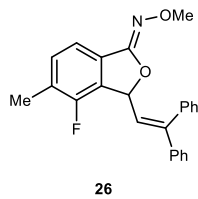


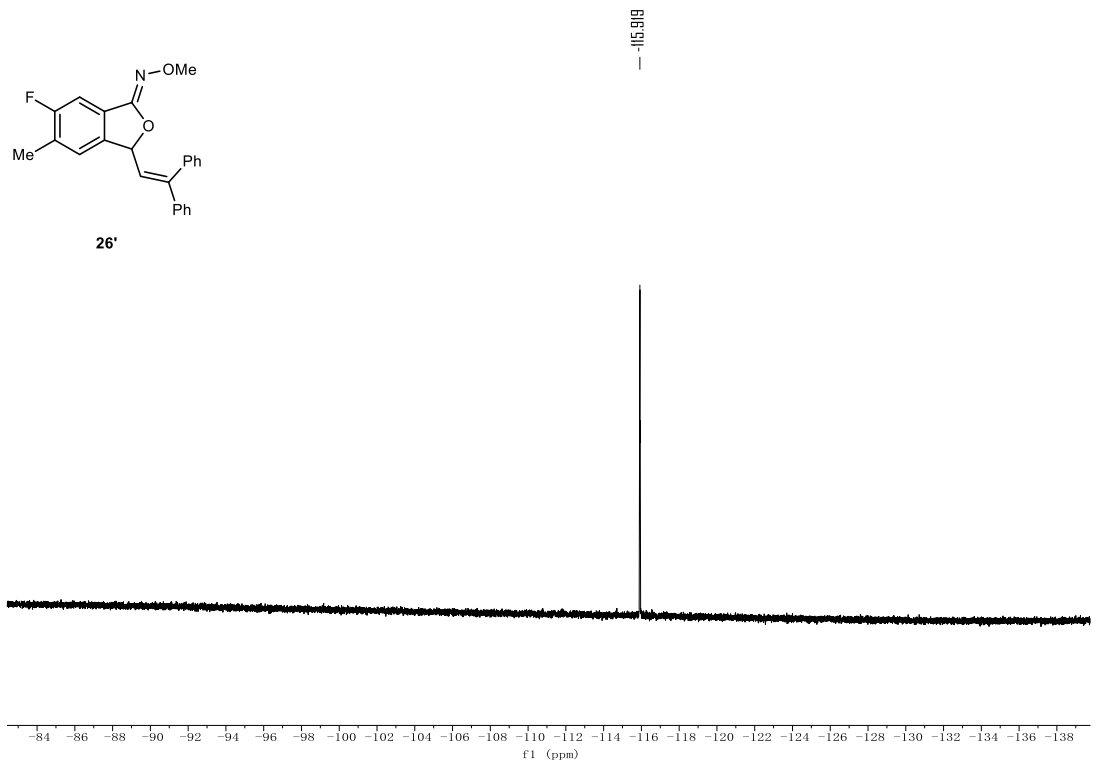
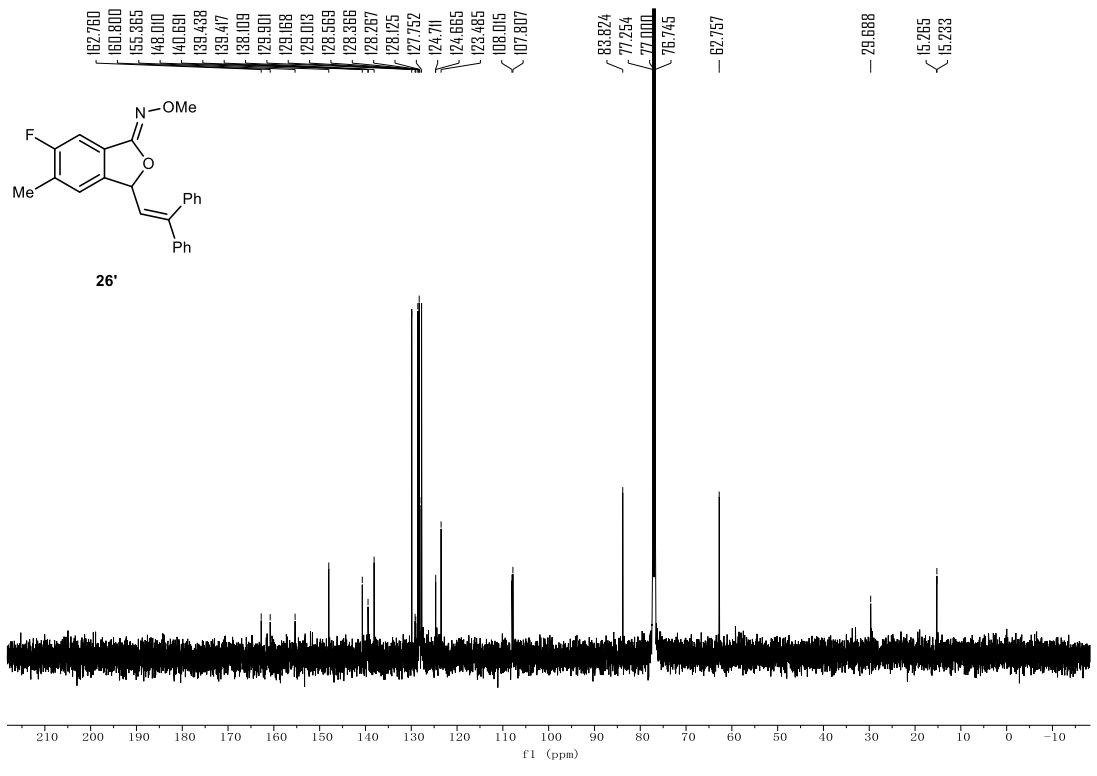


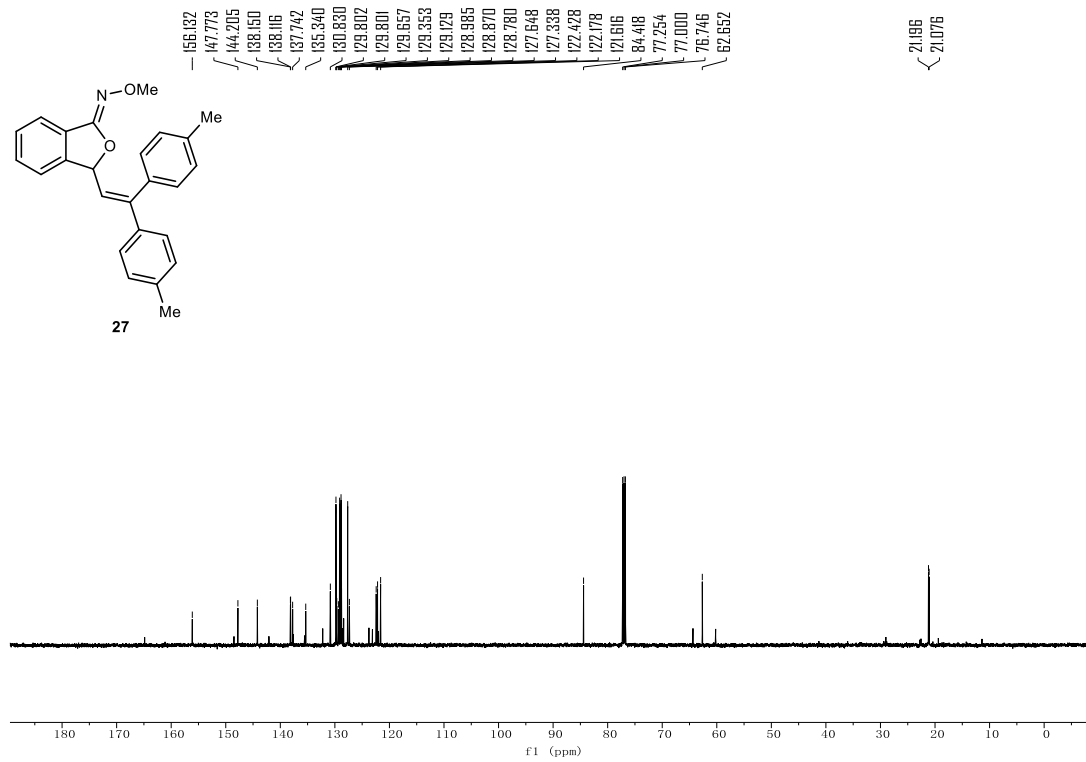
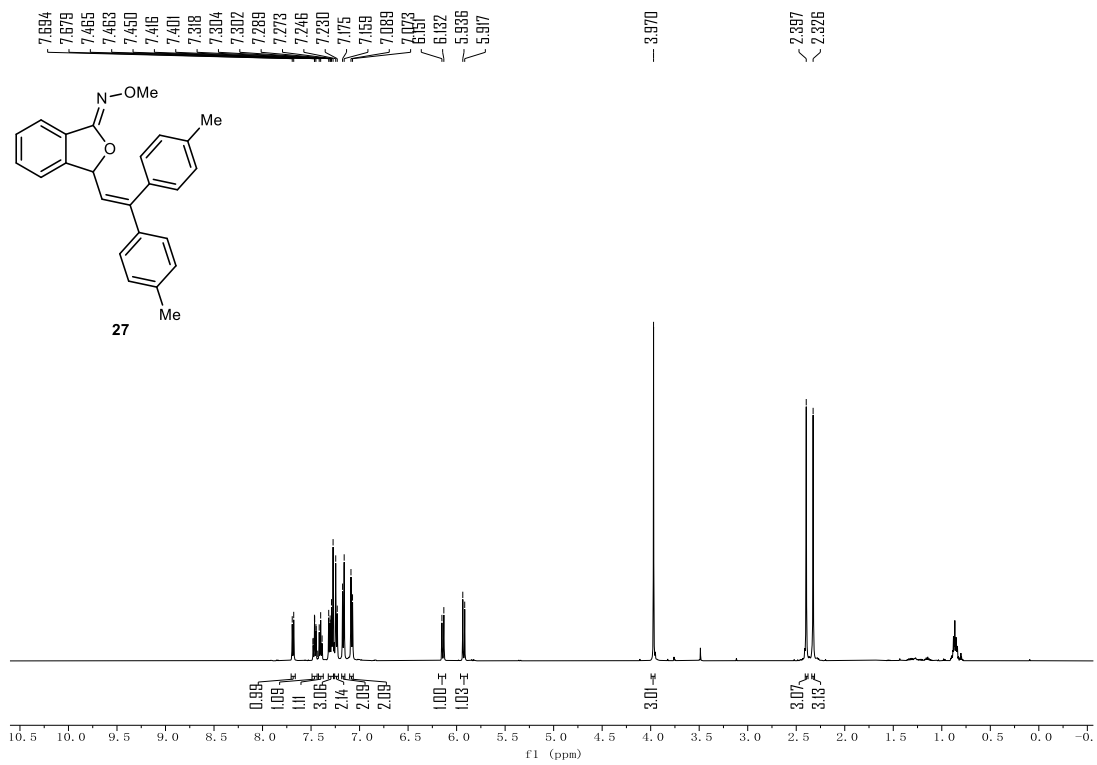








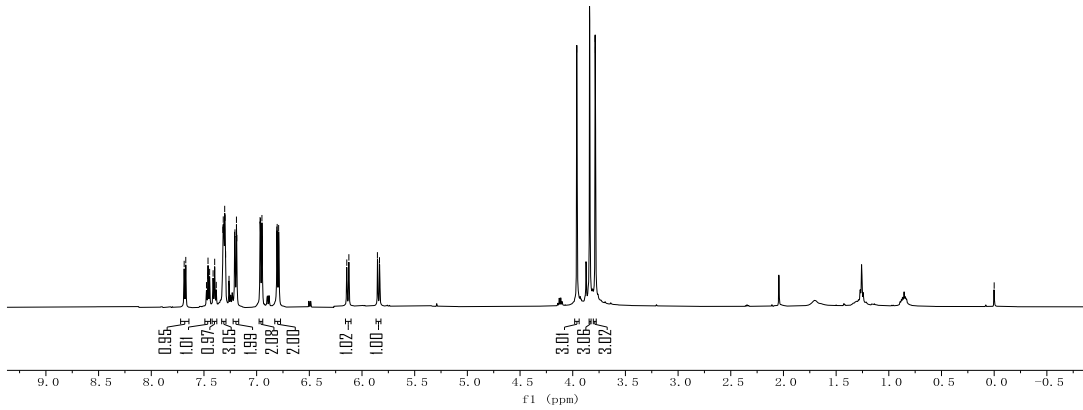
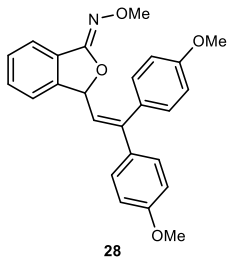






7.688  
7.673  
7.476  
7.464  
7.462  
7.458  
7.449  
7.446  
7.413  
7.398  
7.383  
7.320  
7.317  
7.31  
7.308  
7.303  
7.299  
7.295  
7.262  
7.209  
7.206  
7.192  
7.188  
6.967  
6.954  
6.950  
6.946  
6.809  
6.805  
6.791  
6.144  
6.125  
5.854  
5.834  
3.962  
3.841  
3.787  
3.785

-0.000



158.712  
158.378  
156.159  
147.394  
144.331  
133.718  
132.419  
131.167  
130.629  
129.087  
128.771  
128.411  
122.157  
121.402  
118.805  
118.455  
84.636  
77.255  
77.000  
76.746  
62.754  
62.553  
55.315  
55.146

