

## Supporting Information

### Addition of Sulfonylphthalides to *para*-Quinone Methides: Selective 1,6-Additions and Oxidative Annulation

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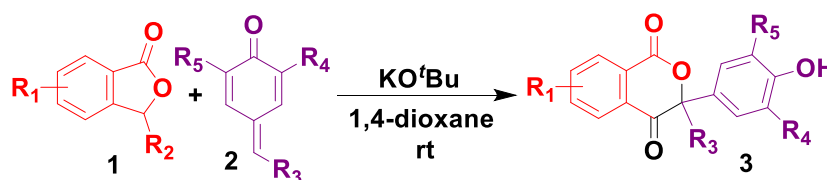
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## Material and Methods General Information

All reactions were carried out in oven-dried glassware and the compounds synthesized were fully characterized by spectroscopic data. The NMR spectra were recorded on JEOL - 400 spectrometers, ( $^1\text{H-NMR}$  400 MHz,  $^{13}\text{C-NMR}$  100 MHz) and were referenced to the residual peaks of  $\text{CDCl}_3$  at 7.26 ppm ( $^1\text{H-NMR}$ ) and  $\text{CDCl}_3$  at 77.23 ppm ( $^{13}\text{C-NMR}$ ). Chemical shifts ( $\delta$ ) are expressed in ppm, and  $J$  values are given in Hz. Data are reported as follows: Chemical shift in ppm ( $\delta$ ), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constant (Hz), and integration. The reactions were monitored by thin layer chromatography (TLC) using silica gel GF254. The melting points (m.p.) were determined on digital melting point apparatus and are uncorrected. Micromass Q-TOF mass spectrometer was used to record high resolution mass spectra 60-70 eV in ESI mode. Materials unless otherwise indicated, all reagents were obtained from commercial suppliers used without further purification.

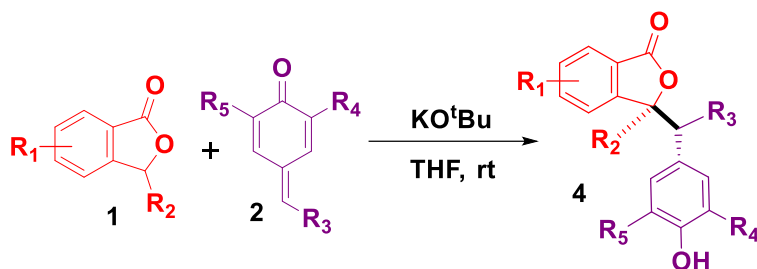
All the *p*-QMs and Sulfonylphthalide starting materials were synthesized using the procedure given in literature.<sup>1,2</sup>

### General Procedure for the preparation of isochroman-1,4-dione



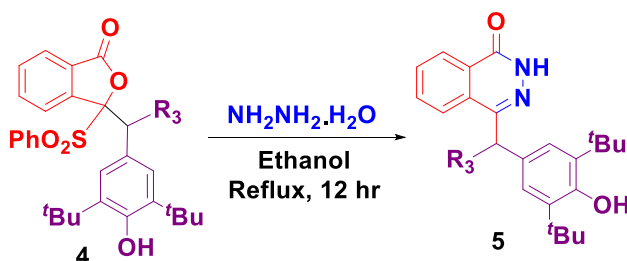
To a 25 mL reaction flask, was added sulfonylphthalide **1** (100 mg, 1 equiv., 0.364 mmol) *p*-quinone methide **2** (107 mg, 1 equiv. 0.364 mmol), potassium *tert*-butoxide (122.72 mg, 3.0 equiv., 1.093mmol) and 1,4-Dioxane (3 mL). The reaction mixture was stirred at room temperature for 15 minutes. Progress of the reaction was monitored by TLC. After the completion of the reaction, the mixture was quenched with water, extracted with ethyl acetate. The combined organic layers were dried over sodium sulfate, concentrated under reduced pressure and purified by column chromatography to afford product **3** as white solid.

### General procedure for the 1,6-addition of sulfonylphthalides to *p*-quinone methides



To a 25 mL reaction flask, was added sulfonylphthalide **1** (100 mg, 1 equiv., 0.364 mmol), *p*-quinone methide **2** (107 mg, 1 equiv. 0.364 mmol), potassium *tert*-butoxide (8.18 mg, 0.2 equiv., 0.0729 mmol) and THF (3 mL). The reaction mixture was stirred at room temperature for 15 minutes. The progress of reaction was monitored by TLC. After the completion of reaction, the mixture was quenched with water, extracted with ethyl acetate. The combined organic layers were dried over sodium sulfate and evaporated off the solvent under reduced pressure to get residue. This residue was washed with hexane (5 mL) to get the crude product as white solid. Recrystallization of this crude product using ethanol furnished the pure desired product **4**.

### General procedure for the preparation of phthalazinones



To a 25 mL reaction flask, was added **4** (100 mg, 1 equiv. 0.175 mmol) and hydrazine hydrate (28.1 mg, 5 equiv., 0.879 mmol) in ethanol (5 mL). The reaction mixture was refluxed. Progress of the reaction was monitored by TLC. After the completion of reaction, the mixture was quenched with water, extracted with ethyl acetate. The combined organic layers were dried over sodium sulphate and evaporated off the solvent under reduced pressure to get residue. The resulting crude was then purified by column chromatography to afford the product **5** as a white solid.

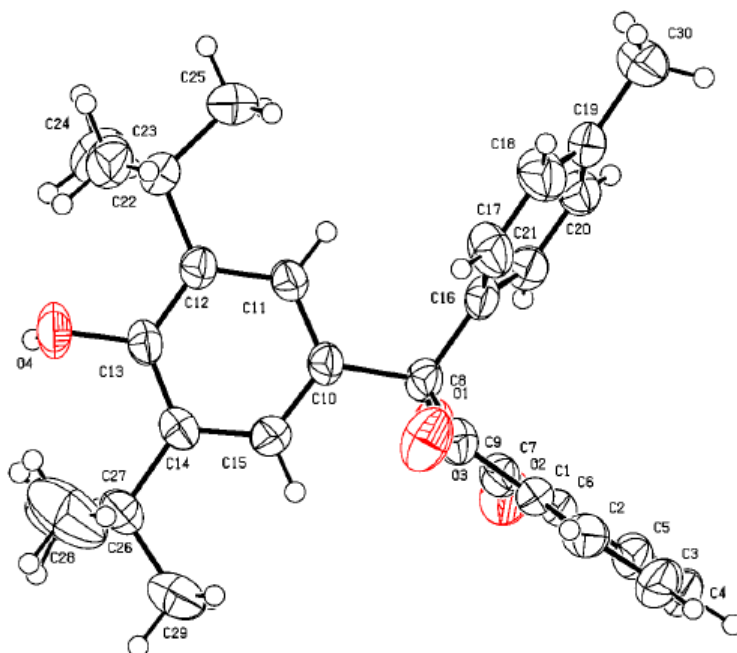
### References

1. S. H. Li, Y. Y. Liu, B. Huang, T. Zhou, H. M. Tao, Y. J. Xiao, L. Liu and J. L. Zhang, *ACS Catal.*, 2017, **7**, 2805,
2. M. Sakulsombat, M. Angelin and O. Ramstorm, *Tetrahedron Lett.*, 2010, **51**, 75.

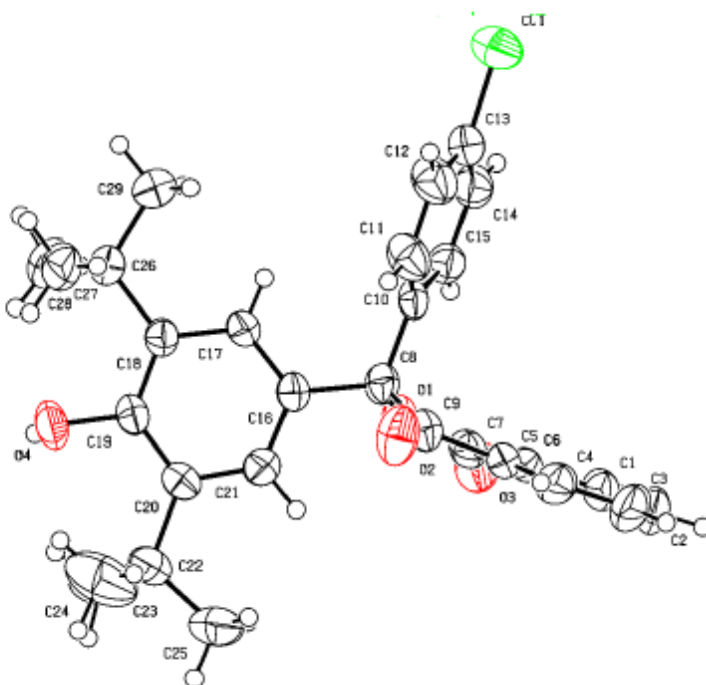
**Table 1: Crystal data and structure refinement of 3b, 3g and 4l.**

Parameters	<b>3b</b>	<b>3g</b>	<b>4l</b>
CCDC Number	2218203	2218202	2241101
Empirical formula	C <sub>30</sub> H <sub>32</sub> O <sub>4</sub>	C <sub>29</sub> H <sub>29</sub> ClO <sub>4</sub>	C <sub>35</sub> H <sub>35</sub> ClO <sub>5</sub> S
Formula weight	456.55	476.97	603.14
Crystal system	triclinic	triclinic	monoclinic
Space group	P-1	P-1	P-1
Temperature (K)	299 K	297 K	273 K
Unit cell dimensions	a = 9.895(2) Å b = 10.862(2) Å c = 12.428(3) Å	a = 9.9448(6) Å b = 10.8509(6) Å c = 12.3306(7) Å	a = 11.4676(18) Å b = 23.735(4) Å c = 24.998(3) Å
	$\alpha = 92.652(6)^\circ$ $\beta = 104.732(6)^\circ$ $\gamma = 95.795(6)^\circ$	$\alpha = 92.569(2)^\circ$ $\beta = 104.348(2)^\circ$ $\gamma = 96.070(2)^\circ$	$\alpha = 90(3)^\circ$ $\beta = 92.236(3)^\circ$ $\gamma = 90(3)^\circ$
volume (Å <sup>3</sup> )	1281.6(5)	1278.38(13)	6798.9(17)
Z	2	2	1
Radiation type (Mo-K $\alpha$ )/Å	0.71073	0.71073	0.71073
No. measured reflections	34408	15977	175457
Calculated density (mg/m <sup>3</sup> )	1.183	1.239	0.147 g/cm <sup>3</sup>
Absorption coefficient (mm <sup>-1</sup> )	0.077	0.181	0.026 mm <sup>-1</sup>
F(000)	488.0	504.0	318
$\theta$ range for data collection	1.699 to 24.998°	1.709 to 25.701°	1.90 to 28.29°
Limiting indices	-11 ≤ h ≤ 11 -12 ≤ h ≤ 12 -14 ≤ h ≤ 14	-12 ≤ h ≤ 12 -13 ≤ h ≤ 13 -14 ≤ h ≤ 15	-15 ≤ h ≤ 15 -31 ≤ k ≤ 31 -33 ≤ l ≤ 32
Refinement method	Full-matrix least squares on F <sup>2</sup>	Full-matrix least squares on F <sup>2</sup>	Full-matrix least squares on F <sup>2</sup>
Data / restraints / parameter	4486/0/314	4809/0/314	16842 / 0 / 794
Final R Indices[I > 2 $\sigma$ (I)]	R1 = 0.0686 wR2 = 0.1388	R1 = 0.0533 wR2 = 0.1215	R1 = 0.0546 wR2 = 0.1433
R indices (all data)	R1 = 0.0953 wR2 = 0.1579	R1 = 0.0707 wR2 = 0.1355	R1 = 0.0813 wR2 = 0.1640
Goodness of fit on F <sup>2</sup>	1.103	1.027	1.016
Largest diff. peak and hole (eÅ <sup>-3</sup> )	0.395 to -0.212	0.285 and -0.188	0.694 and -0.553
Reflections collected / unique	34408/4486 [R(int)=0.0375]	15977/4809 [R(int)=0.0396]	16842 [R(int) = 0.0675]

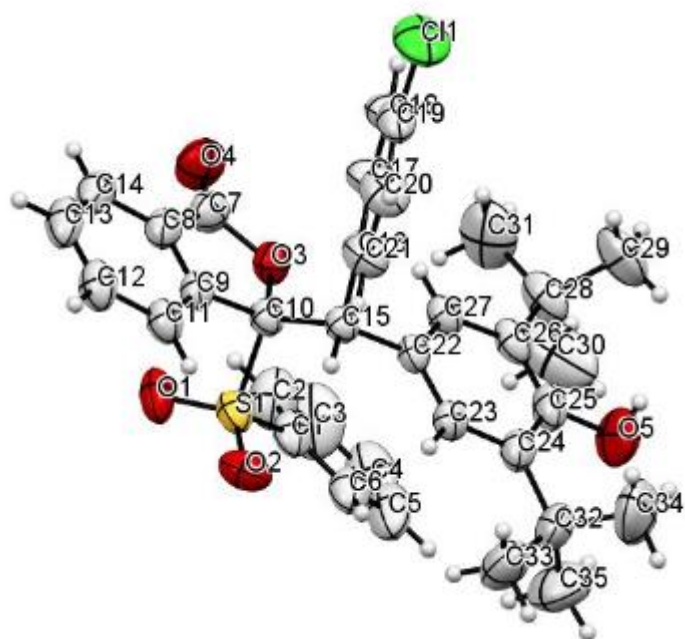
**Sample preparation for crystal growth:** Compound **3b**, **3g** and **4l** was dissolved in ethanol, while slow evaporation of solvent at room temperature needle type crystals were grown.



**Figure 1:** ORTEP diagram of compound of **3b** with 50% ellipsoid probability



**Figure 2:** ORTEP diagram of compound of **3g** with 50% ellipsoid probability

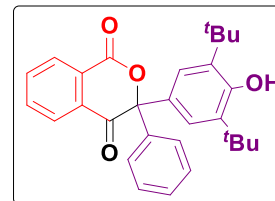


**Figure 3:** ORTEP diagram of compound of **4I** with 50% ellipsoid probability.

## **Analytical Data**

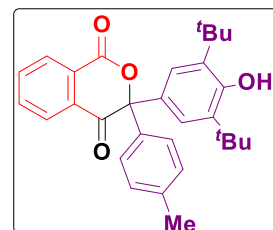
### **3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-phenylisochroman-1,4-dione (3a):**

White solid; m.p. 188 - 190 °C; Yield – 86% (138 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.28 (s, 18H), 5.30 (s, 1H), 7.08 (s, 2H), 7.32 - 7.42 (m, 5H), 7.76 - 7.82 (m, 2H), 8.09 – 8.14 (m, 1H), 8.18 – 8.24 (m, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.09, 34.41, 94.06, 124.71, 126.83, 127.28, 128.02, 128.35, 128.69, 129.37, 131.17, 131.93, 134.72, 135.11, 135.61, 138.90, 154.24, 162.60, 192.13; HRMS (ESI): m/z calcd for C<sub>29</sub>H<sub>30</sub>O<sub>4</sub> [M+1] 443.2217 found 443.2215.



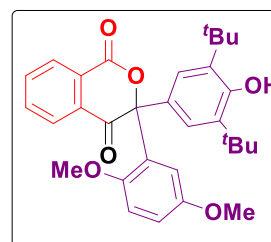
### **3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(*p*-tolyl)isochroman-1,4-dione (3b):**

White solid; m.p. 193 - 195 °C; Yield – 85% (141 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.35 (s, 18H), 2.32 (s, 3H), 5.29 (s, 1H), 7.08 – 7.17 (m, 4H), 7.23 - 7.27 (m, 2H), 7.75 - 7.80 (m, 2H), 8.08 – 8.12 (m, 1H), 8.18 – 8.22 (s, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 21.08, 30.13, 34.41, 94.10, 124.70, 126.81, 127.21, 128.09, 129.06, 129.48, 13.12, 131.99, 134.64, 135.00, 135.59, 136.05, 138.55, 154.19, 162.67, 192.24; HRMS (ESI): m/z calcd for C<sub>30</sub>H<sub>32</sub>O<sub>4</sub> [M + 1] 457.2373, found 457.2373.



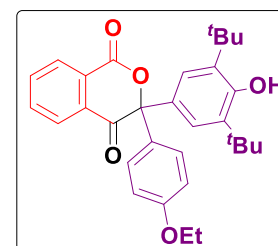
### **3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(2,5-dimethoxyphenyl)isochroman-1,4-dione (3c):**

White solid; m.p. 205 - 207 °C; Yield – 82% (150 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.39 (s, 18H), 3.51 (s, 3H), 3.62 (s, 3H), 5.33 (s, 1H), 6.27 – 6.30 (s, 1H), 6.84 – 6.86 (m, 2H), 7.43 (s, 2H), 7.75 – 7.80 (m, 2H), 8.11 – 8.15 (m, 1H), 8.22 – 8.26 (m, 1H), 8.00 (d, *J* = 8 Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.23, 34.57, 55.57, 56.20, 112.91, 114.65, 116.89, 124.03, 125.40, 126.47, 130.01, 131.74, 132.13, 134.24, 136.00, 151.42, 153.31, 154.30, 162.14, 190.98; HRMS (ESI): m/z calcd for C<sub>31</sub>H<sub>34</sub>O<sub>6</sub> [M + 1] 503.2428, found 503.2424.



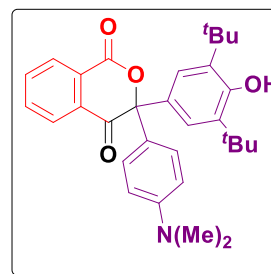
### **3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(4-ethoxyphenyl)isochroman-1,4-dione (3d):**

White solid; m.p. 187 - 189 °C; Yield – 84% (148 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.32 – 1.40 (m, 21H), 3.99 (q, *J* = 8 Hz, 2H), 5.28 (s, 1H), 6.80 – 6.85 (m, 2H), 7.07 (s, 2H), 7.22 – 7.25 (m, 2H), 7.75 – 7.80 (m, 2H), 8.07 – 8.11 (m, 1H), 8.15 – 8.21 (m, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 14.73, 30.13, 34.41, 63.44, 94.05, 114.19, 124.67, 126.82, 128.09, 128.71, 129.56, 130.10, 130.93, 131.97, 134.65, 135.00, 135.57, 154.18, 159.10, 162.72, 192.34; HRMS (ESI): m/z calcd for C<sub>31</sub>H<sub>34</sub>O<sub>5</sub> [M + 1] 487.2479, found 487.2479.

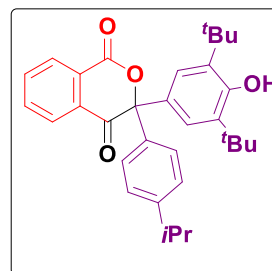


**3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(4-dimethylamino)phenyl)isochroman-1,4-dione (3e):**

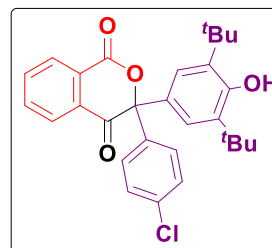
White solid; m.p. 196 - 198 °C; Yield – 81% (141 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.35 (s, 18H), 2.93 (s, 6H), 5.26 (s, 1H), 6.62 – 6.67 (m, 2H), 7.10 (s, 2H) 7.16 - 7.21 (m, 2H), 7.74 - 7.78 (m, 2H), 8.08 – 8.12 (m, 1H), 8.16 – 8.21 (m, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.17, 34.40, 40.28, 94.48, 111.81, 124.85, 126.81, 128.06, 128.20, 128.24, 129.83, 130.04, 132.13, 134.51, 134.80, 135.44, 154.09, 162.99, 192.50; HRMS (ESI): m/z calcd for C<sub>31</sub>H<sub>35</sub>NO<sub>4</sub> [M + 1] 486.2639, found 486.2637.

**3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(4-isopropylphenyl)isochroman-1,4-dione (3f):**

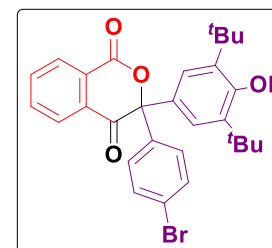
White solid; m.p. 202 – 204 °C; Yield – 76% (134 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.21 (d, *J* = 8Hz, 6H), 1.34 (s, 18H), 2.88 (sept, *J* = 8Hz, 1H), 5.28 (s, 1H), 7.08 (s, 2H) 7.17 – 7.21 (m, 2H), 7.24 – 7.29 (m, 2H), 7.75 - 7.79 (m, 2H), 8.08 – 8.13 (m, 1H), 8.17 – 8.22 (m, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 23.78, 30.11, 33.72, 34.41, 94.11, 124.63, 126.41, 126.83, 127.29, 128.12, 129.45, 130.13, 132.01, 134.63, 135.00, 135.58, 136.36, 149.42, 154.17, 162.66, 192.26; HRMS (ESI): m/z calcd for C<sub>32</sub>H<sub>36</sub>O<sub>4</sub> [M + 1] 485.2686, found 485.2688.

**3-(4-chlorophenyl)-3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)isochroman-1,4-dione (3g):**

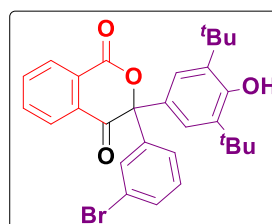
White solid; m.p. 186 - 188 °C; Yield – 75% (130 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.34 (s, 18H), 5.31 (s, 1H), 7.08 (s, 2H), 7.24 - 7.32 (m, 5H), 7.78 - 7.82 (m, 2H), 8.08 – 8.13 (m, 1H), 8.18 – 8.22 (m, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.10, 34.45, 93.36, 124.29, 126.85, 127.95, 128.47, 128.94, 129.07, 130.26, 131.80, 134.75, 135.28, 135.91, 137.66, 154.37, 162.31, 191.76; HRMS (ESI): m/z calcd for C<sub>29</sub>H<sub>29</sub>ClO<sub>4</sub> [M + 1] 477.1827, found 477.1825.

**3-(4-bromophenyl)-3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)isochroman-1,4-dione (3h):**

White solid; m.p. 198 - 200 °C; Yield – 73% (138 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.27 (s, 18H), 5.24 (s, 1H), 7.01 (s, 2H), 7.15 - 7.20 (m, 2H), 7.38 - 7.43 (m, 2H), 7.71 - 7.75 (m, 2H), 8.02 – 8.06 (m, 1H), 8.11 – 8.14 (m, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.10, 34.46, 93.38, 123.04, 124.27, 126.85, 127.96, 129.02, 129.23, 130.26, 131.43, 131.81, 134.84, 135.28, 135.94, 138.21, 154.38, 162.28, 191.67; HRMS (ESI): m/z calcd for C<sub>29</sub>H<sub>29</sub>BrO<sub>4</sub> [M + 1] 521.1322, found 521.1320.

**3-(3-bromophenyl)-3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)isochroman-1,4-dione (3i):**

White solid; m.p. 166 - 168 °C; Yield – 80% (151 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.51 (s, 18H), 5.48 (s, 1H), 7.26 (s, 2H), 7.35 – 7.47 (m, 2H), 7.61 – 7.65 (m, 1H), 7.731 – 7.735(m, 1H), 7.95 – 7.99 (m, 2H), 8.25 – 8.30 (m, 1H), 8.35 – 8.40 (m, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.10, 34.47, 93.08, 122.48, 124.24, 126.29, 126.90, 127.92, 128.90, 129.72,



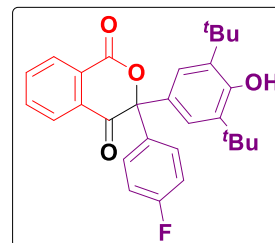


130.29, 130.49, 131.79, 134.87, 135.32, 135.97, 141.23, 154.41, 162.15, 191.44; HRMS (ESI):  $m/z$  calcd for  $C_{29}H_{29}BrO_4$  [ $M + 2$ ] 521.1322, found 523.1305.

### 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl) 3-(4-fluorophenyl)-isochroman-1,4-dione (3j):

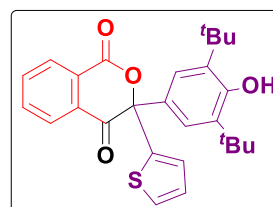
White solid; m.p. 193 - 195 °C; Yield – 78% (130 mg);  $^1H$ -NMR (400 MHz,  $CDCl_3$ );  $\delta$  = 1.34 (s, 18H), 5.31 (s, 1H), 7.00 – 7.09 (m, 4H), 7.31 – 7.37 (m, 2H), 7.78 – 7.83 (m, 2H), 8.00 – 8.14 (m, 1H), 8.20 – 8.23 (m, 1H);  $^{13}C$ -NMR (100 MHz,  $CDCl_3$ );  $\delta$  = 30.11, 34.45, 115.13, 115.35, 124.34, 126.85, 128.02, 129.26, 129.47, 129.55, 130.23, 131.86, 134.81, 135.02, 135.05, 135.22, 135.89, 154.34, 163.19 (d,  $J$  = 160 Hz) 191.99; HRMS (ESI):  $m/z$  calcd for  $C_{29}H_{29}FO_4$  [ $M + 1$ ] 461.2123, found 461.2125.

$^{19}F$ -NMR (376 MHz,  $CDCl_3$ ) :  $\delta$  = -112.97.



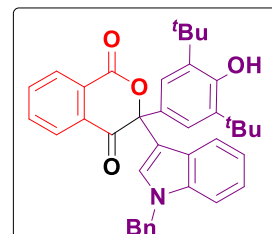
### 3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(thiophen-2-yl)isochroman-1,4-dione (3k):

White solid; m.p. 183 - 185 °C; Yield – 83% (135 mg);  $^1H$ -NMR (400 MHz,  $CDCl_3$ );  $\delta$  = 1.36 (s, 18H), 5.30 (s, 1H), 6.97 – 7.04 (m, 2H), 7.21 – 7.27 (m, 2H), 7.33 – 7.37 (m, 1H), 7.78 – 7.83 (m, 2H), 8.14 – 8.16 (m, 1H), 8.23 – 8.25 (m, 1H);  $^{13}C$ -NMR (100 MHz,  $CDCl_3$ );  $\delta$  = 30.11, 34.46, 91.42, 123.52, 126.60, 127.11, 127.76, 127.96, 129.33, 130.28, 131.45, 134.79, 135.27, 135.85, 142.57, 154.46, 161.89, 190.51; HRMS (ESI):  $m/z$  calcd for  $C_{27}H_{28}O_4S$  [ $M + 1$ ] 449.1781, found 449.1785.



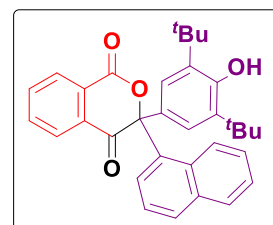
### 3-(1-benzyl-1*H*-indol-3-yl)-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)isochroman-1,4-dione (3l):

White solid; m.p. 198 - 200 °C; Yield – 40% (83 mg);  $^1H$ -NMR (400 MHz,  $CDCl_3$ );  $\delta$  = 1.32 (s, 18H), 5.25 (s, 2H), 6.91 (s, 1H), 7.00 – 7.07 (m, 3H), 7.11 – 7.27 (m, 8H), 7.45 - 7.49 (m, 1H), 7.77 – 7.81 (m, 2H), 8.11– 8.15 (m, 1H), 8.22– 8.25 (m, 1H);  $^{13}C$ -NMR (100 MHz,  $CDCl_3$ );  $\delta$  = 30.14, 34.41, 50.08, 91.93, 109.94, 114.86, 120.30, 121.23, 122.47, 124.23, 126.51, 127.02, 127.65, 128.20, 128.69, 128.74, 128.89, 13.07, 134.57, 134.92, 135.54, 136.95, 137.14, 154.17, 162.98, 191.38; HRMS (ESI):  $m/z$  calcd for  $C_{38}H_{37}NO_4$  [ $M + 1$ ] 572.2795, found 572.2798.



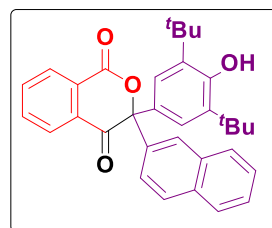
### 3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(naphthalen-2-yl)isochroman-1,4-dione (3o):

White solid; m.p. 189 - 191 °C; Yield – 68% (122 mg);  $^1H$ -NMR (400 MHz,  $CDCl_3$ );  $\delta$  = 1.38 (s, 18H), 5.36 (s, 1H), 6.81 – 6.85 (m, 1H), 7.28 – 7.46 (m, 5H), 7.68 – 7.70 (m, 1H), 7.81 – 7.88 (m, 4H), 8.15 – 8.19 (m, 1H), 8.24 – 8.28 (m, 1H);  $^{13}C$ -NMR (100 MHz,  $CDCl_3$ );  $\delta$  = 30.20, 34.58, 94.50, 124.17, 124.44, 125.51, 125.58, 126.49, 127.05, 127.36, 128.09, 128.92, 129.09, 130.40, 130.62, 130.91, 132.03, 134.45, 134.88, 135.08, 135.89, 136.29, 154.42, 162.76, 191.68; HRMS (ESI):  $m/z$  calcd for  $C_{35}H_{32}O_4$  [ $M + 1$ ] 493.2373, found 493.2377.



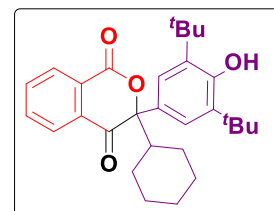
### 3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(naphthalen-1-yl)isochroman-1,4-dione (3p):

White solid; m.p. 174 - 176 °C; Yield – 73% (131 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.38 (s, 18H), 5.36 (s, 1H), 6.83 (d, *J* = 8Hz, 1H), 7.28 – 7.37 (m, 4H), 7.41 – 7.46 (m, 1H), 7.70 (d, *J* = 8Hz, 1H), 7.81 – 7.88 (m, 3H), 8.15 – 8.19 (m, 1H), 8.24 – 8.28 (m, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.20, 34.58, 94.49, 124.17, 124.44, 125.51, 125.58, 126.49, 127.06, 127.36, 128.93, 129.09, 130.40, 130.62, 134.88, 135.08, 135.90, 136.28, 154.42, 162.75, 191.67; HRMS (ESI): *m/z* calcd for C<sub>35</sub>H<sub>32</sub>O<sub>4</sub> [M + 1] 493.2373, found 493.2376.



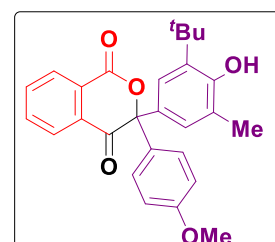
### 3-cyclohexyl-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)isochroman-1,4-dione (3q):

White solid; m.p. 210 - 212 °C; Yield – 78% (127 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.16-1.74 (m, 11H), 1.38 (s, 18H), 2.50-2.57 (m, 1H), 5.20 (s, 1H), 7.23 (s, 2H), 7.70 – 7.79 (m, 2H), 8.00 – 8.04 (m, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 25.10, 26.13, 26.47, 27.86, 30.20, 34.48, 46.79, 95.87, 121.83, 126.56, 127.70, 127.99, 129.93, 131.52, 134.44, 134.96, 135.95, 153.64, 163.07, 192.86; HRMS (ESI): *m/z* calcd for C<sub>29</sub>H<sub>36</sub>O<sub>4</sub> [M + 1] 449.2686, found 449.2688.



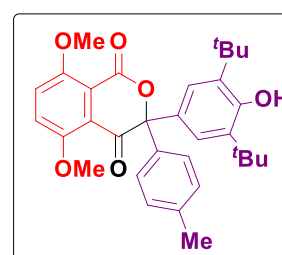
### 3-(3-(*tert*-butyl-4-hydroxy-5-methylphenyl)-3-phenylisochroman-1,4-dione (3r):

White solid; m.p. 216 – 218 °C; Yield – 80% (116 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.25 (s, 9H), 2.11 (s, 3H), 3.71 (s, 3H), 4.80 (s, 1H), 6.76 – 6.80 (m, 2H), 6.85 – 6.87 (m, 1H), 7.030 - 7.036 (m, 1H), 7.17- 7.21 (m, 2H), 7.70 – 7.74 (m, 2H), 8.02 – 8.06 (m, 1H), 8.10 – 8.14 (m, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 16.11, 29.55, 34.64, 55.25, 93.60, 113.71, 123.06, 124.50, 126.85, 127.73, 128.85, 130.02, 130.14, 131.16, 131.89, 134.70, 135.08, 135.34, 135.54, 153.13, 159.74, 162.66, 192.21; HRMS (ESI): *m/z* calcd for C<sub>27</sub>H<sub>26</sub>O<sub>4</sub> [M+1] 431.1826 found 431.1829.



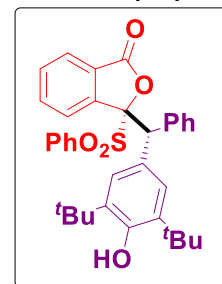
### 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)-5,8-dimethoxy-3-phenylisochroman-1,4-dione (3s):

White solid; m.p. 191 - 193 °C; Yield – 86% (129 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.33 (s, 18H), 2.31 (s, 3H), 3.90 (s, 6H), 5.23 (s, 1H), 6.70 (d, *J* = 4Hz, 1H), 7.03 (s, 2H), 7.10 - 7.14 (m, 2H), 7.21 – 7.25 (m, 1H), 7.27 – 7.29 (m, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 21.08, 30.14, 34.37, 56.03, 56.45, 93.40, 104.96, 105.45, 115.09, 124.86, 127.18, 128.84, 130.24, 131.65, 135.25, 136.62, 138.10, 153.88, 161.47, 163.12, 165.30, 188.95; HRMS (ESI): *m/z* calcd for C<sub>31</sub>H<sub>34</sub>O<sub>6</sub> [M+1] 503.2515 found 503.2519.



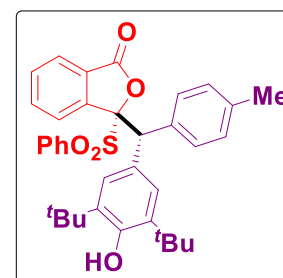
**3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(phenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3*H*)-one**

**(4a):** White solid; m.p. 142 - 144 °C; Yield – 96% (198 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.33 (s, 18H), 5.02 (s, 1H), 5.28 (s, 1H), 6.95 - 7.07 (m, 3H), 7.17 - 7.26 (m, 6H), 7.38 - 7.49 (m, 4H), 7.65 - 7.70 (m, 2H), 7.93 (d, *J* = 8.4Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.32, 34.18, 54.57, 103.22, 124.74, 125.64, 126.53, 127.06, 127.14, 128.03, 128.35, 128.45, 128.81, 130.10, 130.69, 133.64, 134.17, 135.65, 136.83, 138.98, 153.25, 168.04; HRMS (ESI): *m/z* calcd for C<sub>35</sub>H<sub>36</sub>SO<sub>5</sub> [M+Na] 591.2176 found 591.2174.



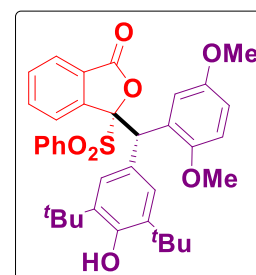
**3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(*p*-tolyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3*H*)-one**  
**(4b):**

White solid; m.p. 208 - 210 °C; Yield – 81% (171 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.31 (s, 18H), 2.10 (s, 3H), 4.99 (s, 1H), 5.24 (s, 1H), 6.83 - 6.88 (m, 2H), 7.10 - 7.12 (m, 6H), 7.36 - 7.50 (m, 4H), 7.65 - 7.70 (m, 2H), 7.92 (d, *J* = 8Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 20.81, 30.25, 34.11, 54.07, 103.28, 124.60, 125.68, 126.40, 127.02, 127.98, 128.17, 128.59, 128.85, 129.17, 130.03, 130.72, 133.64, 134.25, 135.42, 135.86, 136.71, 144.44, 153.15, 168.19; HRMS (ESI): *m/z* calcd for C<sub>36</sub>H<sub>38</sub>SO<sub>5</sub> [M + Na] 605.2332, found 605.2335.



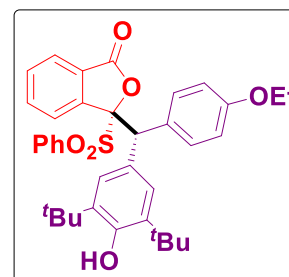
**3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(2,5-dimethoxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3*H*)-one**  
**(4c):**

White solid; m.p. 159 - 161 °C; Yield – 93% (213 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.34 (s, 18H), 3.57 (s, 3H), 3.76 (s, 3H), 5.00 (s, 1H), 6.12 (s, 1H), 6.40 – 6.48 (m, 2H), 7.16 – 7.24 (m, 4H), 7.36 – 7.68 (m, 6H), 7.73 (d, *J* = 8.0Hz, 1H), 8.00 (d, *J* = 8.0Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.29, 34.08, 55.29, 56.09, 103.97, 111.98, 114.22, 123.94, 125.38, 126.66, 126.80, 127.86, 128.12, 128.21, 128.79, 129.4, 130.07, 130.77, 133.53, 133.83, 135.29, 137.25, 144.41, 149.26, 153.08, 168.69; HRMS (ESI): *m/z* calcd for C<sub>37</sub>H<sub>40</sub>NaSO<sub>7</sub> [M + Na] 651.2387, found 651.2386.



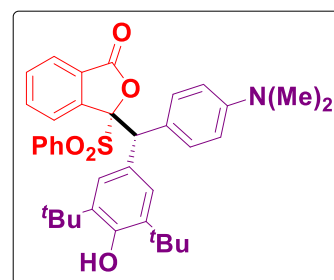
**3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(4-ethoxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3*H*)-one**  
**(4d):**

White solid; m.p. 145 - 147°C; Yield – 95% (211 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.24 - 1.36 (m, 21H), 3.82 (q, *J* = 8.0Hz, 2H), 5.01 (s, 1H), 5.23 (s, 1H), 6.56 (d, *J* = 8.0Hz, 2H), 7.11 - 7.24 (m, 6H), 7.37 - 7.51 (m, 4H), 7.68 (d, *J* = 8.0Hz, 2H), 7.92 (d, *J* = 7.6Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 14.67, 30.22, 34.09, 53.61, 63.14, 103.29, 114.26, 124.54, 125.70, 126.30, 126.92, 127.96, 128.30, 129.80, 129.97, 130.73, 133.65, 134.27, 135.39, 136.59, 144.45, 153.08, 157.71, 168.20; HRMS (ESI): *m/z* calcd for C<sub>37</sub>H<sub>40</sub>NaSO<sub>6</sub> [M + Na] 635.2438, found 635.2434.



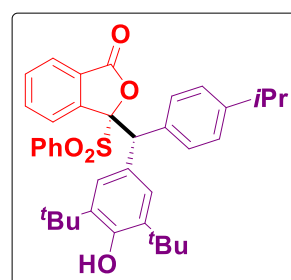
**3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(4-dimethylamino)phenyl)methyl-3-phenylsulfonyl)isobenzofuran-1(3*H*)-one (4e):**

White solid; m.p. 158 - 160 °C; Yield – 89% (198 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.31 (s, 18H), 2.77 (s, 6H), 4.96 (s, 1H), 5.18 (s, 1H), 6.39 (d, *J* = 8.4Hz, 2H), 7.09 (d, *J* = 8.0Hz, 2H), 7.14 - 7.22 (m, 4H), 7.36 - 7.51 (m, 4H), 7.66 - 7.72 (m, 2H), 7.94 (d, *J* = 8.0Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.24, 34.07, 40.21, 53.58, 103.59, 112.20, 124.63, 125.65, 126.29, 127.05, 127.21, 127.93, 128.70, 129.53, 130.00, 130.63, 133.56, 134.17, 134.56, 135.25, 136.74, 144.64, 152.95, 168.37; HRMS (ESI): *m/z* calcd for C<sub>37</sub>H<sub>41</sub>NSO<sub>5</sub> [M + 1] 612.2778, found 612.2776.



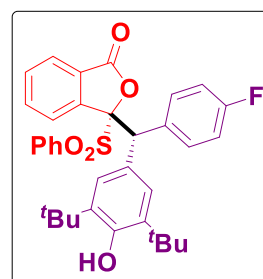
**3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(4-isopropylphenyl)methyl)-3-phenylsulfonyl)isobenzofuran-1(3*H*)-one (4f)**

White solid; m.p. 208 - 210 °C; Yield – 83% (184 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.05 (d, *J* = 7.0Hz, 6H), 1.33 (s, 18H), 2.66 (sept, *J* = 7.0Hz, 1H), 5.01 (s, 1H), 5.24 (s, 1H), 6.89 (d, *J* = 8.0Hz, 2H), 7.12 - 7.23 (m, 6H), 7.37 - 7.49 (m, 4H), 7.64 - 7.71 (m, 2H), 7.92 (d, *J* = 8.0Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 23.65, 30.26, 33.33, 34.12, 54.17, 103.30, 124.62, 125.58, 126.43, 126.53, 127.00, 127.98, 128.10, 128.69, 130.01, 130.62, 133.63, 134.21, 135.36, 135.90, 136.71, 144.45, 147.51, 153.16, 168.09; HRMS (ESI): *m/z* calcd for C<sub>38</sub>H<sub>42</sub>KSO<sub>5</sub> [M + K] 649.2385, found 649.2380.



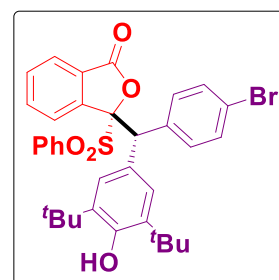
**3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(4-fluorophenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3*H*)-one (4i):**

White solid; m.p. 166 - 168 °C; Yield – 45% (95 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.33 (s, 18H), 5.05 (s, 1H), 5.29 (s, 1H), 6.71 - 6.78 (m, 2H), 7.16 - 7.25 (m, 6H), 7.38 - 7.53 (m, 4H), 7.67 - 7.73 (m, 2H), 7.91 (d, *J* = 8.0Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.22, 34.13, 53.60, 102.89, 115.24, 115.46, 124.49, 125.83, 126.28, 127.76, 128.03, 130.00, 130.36, 130.90, 133.78, 134.41, 135.60, 136.41, 144.25, 153.27, 160.36, 161.59 (d, *J* = 145 Hz) 162.82, 167.95; <sup>19</sup>F-NMR (376 MHz, CDCl<sub>3</sub>): δ = -114.85, -115.36; HRMS (ESI): *m/z* calcd for C<sub>35</sub>H<sub>35</sub>FSNaO<sub>5</sub> [M + Na] 609.2081, found 609.2084.



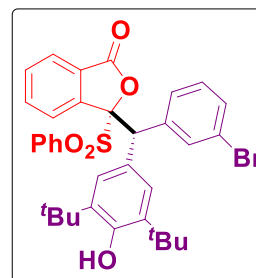
**3-((4-chlorophenyl)(3,5-di-*tert*-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3*H*)-one (4j):**

White solid; m.p. 168 - 170 °C; Yield – 68% (160 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.32 (s, 18H), 5.05 (s, 1H), 5.25 (s, 1H), 7.10 - 7.22 (m, 5H), 7.40 - 7.53 (m, 5H), 7.62 - 7.81 (m, 4H), 7.88 - 8.01 (m, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.20, 34.12, 53.75, 90.48, 102.64, 121.21, 124.45, 125.55, 126.26, 128.04, 129.20, 129.77, 13.00, 130.00, 131.60, 133.80, 134.92, 135.67, 136.37, 144.11, 153.33, 167.89; HRMS (ESI): *m/z* calcd for C<sub>35</sub>H<sub>35</sub>BrNaSO<sub>5</sub> [M + Na] 669.1281, found 669.1282.



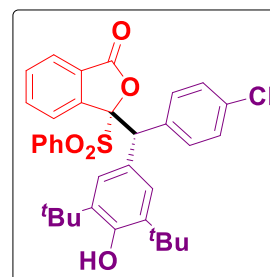
**3-((4-chlorophenyl)3,5-di-*tert*-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3*H*)-one (4k):**

White solid; m.p. 160 - 162 °C; Yield – 50% (117 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.33 (s, 18H), 5.07 (s, 1H), 5.23 (s, 1H), 6.18 (s, 2H), 6.84 – 7.22 (m, 3H), 7.35 – 7.52 (m, 4H), 7.62 – 8.01 (m, 6H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.20, 34.14, 53.93, 90.48, 102.62, 124.96, 126.04, 126.41, 126.91, 128.04, 129.19, 129.76, 130.00, 131.02, 131.42, 132.22, 133.80, 134.92, 135.67, 136.38, 139.39, 140.91, 144.02, 153.40, 167.53; HRMS (ESI): m/z calcd for C<sub>35</sub>H<sub>35</sub>BrKSO<sub>5</sub> [M + K] 685.1020, found 685.1023.



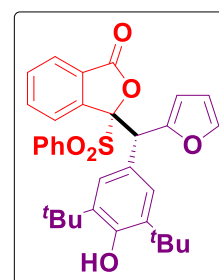
**3-((4-chlorophenyl)3,5-di-*tert*-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3*H*)-one (4l):**

White solid; m.p. 138 - 140 °C; Yield – 45% (98 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.32 (s, 18H), 5.04 (s, 1H), 5.27 (s, 1H), 7.00 - 7.04 (m, 2H), 7.15 - 7.23 (m, 6H), 7.38 - 7.53 (m, 4H), 7.67 – 7.73 (m, 2H), 7.90 (d, *J* = 8 Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.22, 34.14, 53.71, 90.49, 102.74, 124.46, 125.92, 126.28, 127.51, 128.05, 128.67, 129.22, 130.01, 131.01, 133.81, 134.49, 134.94, 135.66, 136.39, 137.38, 144.15, 153.34, 167.92; HRMS (ESI): m/z calcd for C<sub>35</sub>H<sub>35</sub>ClKSO<sub>5</sub> [M + K] 641.1525, found 641.1525.



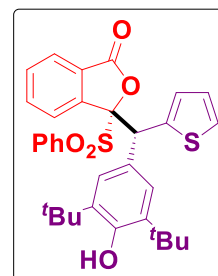
**3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(furan-2-yl)methyl)-3(phenylsulfonyl)isobenzofuran-1(3*H*)-one (4m):**

White solid; m.p. 142 - 144 °C; Yield – 86% (175 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.24 (s, 18H), 5.03 (s, 1H), 5.38 (s, 1H), 6.30 – 6.32 (m, 1H), 6.37 – 6.40 (m, 1H), 7.01 (s, 2H), 7.22 (t, *J* = 8Hz, 1H), 7.39 – 7.54 (m, 7H), 7.776 – 7.821 (m, 1H), 8.23 (d, *J* = 8Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.08, 34.06, 47.50, 100.73, 110.34, 110.67, 124.52, 125.05, 126.15, 127.00, 127.50, 128.24, 130.17, 130.66, 133.97, 134.06, 134.59, 135.22, 142.32, 142.95, 149.96, 153.31, 166.89; HRMS (ESI): m/z calcd for C<sub>33</sub>H<sub>34</sub>KNSO<sub>6</sub> [M + K] 597.1708, found 597.1705.



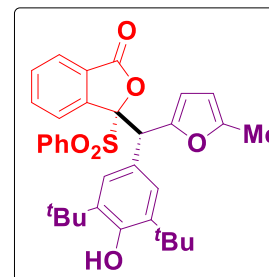
**3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(thiophen-2-yl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3*H*)-one (4n):**

White solid; m.p. 157 - 159 °C; Yield – 89% (186 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.33 (s, 18H), 5.06 (s, 1H), 5.59 (s, 1H), 6.66 (t, *J* = 4Hz, 1H), 6.82 (d, *J* = 3.6Hz, 1H), 6.96 (d, *J* = 5.2Hz, 1H), 7.17 - 7.24 (m, 4H), 7.38 – 7.44 (m, 3H), 7.49 – 7.56 (m, 1H), 7.68 – 7.78 (m, 2H), 8.03 (d, *J* = 8Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.20, 34.13, 50.18, 102.38, 124.50, 125.31, 125.72, 126.13, 126.78, 127.12, 127.23, 127.99, 129.92, 130.93, 133.69, 134.34, 135.39, 136.37, 140.61, 144.06, 153.40, 16.84; HRMS (ESI): m/z calcd for C<sub>33</sub>H<sub>34</sub>S<sub>2</sub>NaO<sub>5</sub> [M + Na] 597.1740, found 597.1739.



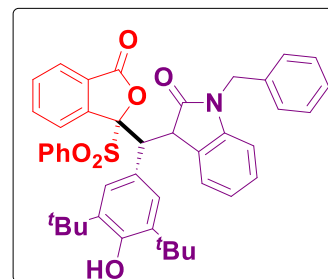
**3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(5-methylfuran-2-yl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4o):**

White solid; m.p. 142 - 144 °C; Yield – 85% (177 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.24 (s, 18H), 2.26 (s, 3H), 5.29 (s, 1H), 5.87 (s, 1H), 6.22 (d, *J* = 4 Hz, 1H), 7.02 (s, 2H), 7.20 - 7.24 (m, 3H), 7.41 - 7.54 (m, 5H), 7.77 - 7.82 (m, 1H), 8.23 (d, *J* = 8 Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 13.56, 30.10, 34.10, 47.62, 100.80, 106.50, 111.10, 124.78, 125.02, 126.15, 127.05, 127.56, 128.23, 130.18, 130.61, 133.79, 134.01, 134.78, 135.12, 143.17, 147.92, 151.83, 153.25, 167.03; HRMS (ESI): *m/z* calcd for C<sub>34</sub>H<sub>36</sub>NaSO<sub>6</sub> [M + Na] 595.2125, found 595.2128.



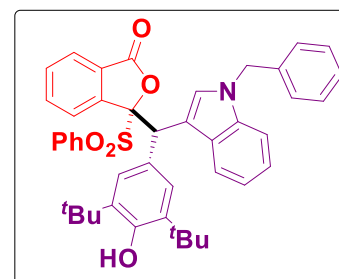
**1-benzyl-2-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-2-(3-oxo-1 (phenylsulfonyl)1,3dihydroisobenzofuran-1-yl)indolin-3-one (4p):**

White solid; m.p. 199 - 201 °C; Yield – 63% (164 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.18 (s, 18H), 4.82 (d, *J* = 16 Hz, 1H), 5.05 (s, 1H), 5.29 (s, 1H), 5.28 (d, *J* = 16 Hz, 1H), 6.71 - 6.79 (m, 2H), 7.07 - 7.13 (m, 3H), 7.27 - 7.38 (m, 7H), 7.40 - 7.49 (m, 5H), 7.75 - 7.84 (m, 2H), 8.99 (d, *J* = 7.6 Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 29.93, 34.44, 44.45, 57.77, 102.17, 109.29, 121.75, 122.08, 122.20, 124.70, 126.02, 126.51, 126.68, 126.92, 127.66, 127.75, 128.38, 128.73, 129.03, 129.71, 130.58, 133.69, 133.73, 134.73, 135.65, 136.09, 142.40, 143.48, 153.29, 167.40, 172.29; HRMS (ESI): *m/z* calcd for C<sub>43</sub>H<sub>41</sub>SNNaO<sub>6</sub> [M + Na] 722.2547, found 722.2544.



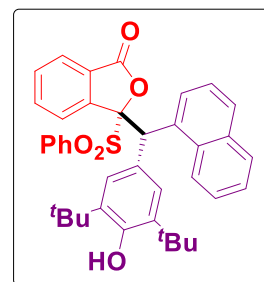
**3-((1-benzyl-1H-indol-3-yl)(3,5-di-*tert*-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-(3H)-one (4q):**

White solid; m.p. 158 - 160 °C; Yield – 63% (160 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.31 (s, 18H), 4.97 (s, 1H), 5.07 (s, 2H), 5.62 (s, 1H), 6.66 - 6.71 (m, 2H), 6.97 - 7.09 (m, 4H), 7.16 - 7.25 (m, 7H), 7.35 - 7.59 (m, 5H), 7.64 - 7.76 (m, 2H), 7.98 (d, *J* = 8 Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.25, 34.06, 45.45, 49.81, 103.57, 109.47, 113.92, 118.41, 119.41, 121.91, 123.52, 125.36, 126.38, 126.73, 126.94, 127.07, 127.49, 127.86, 128.54, 128.61, 129.91, 130.48, 133.43, 134.42, 135.01, 135.14, 136.98, 144.90, 152.95, 168.68; HRMS (ESI): *m/z* calcd for C<sub>44</sub>H<sub>44</sub>SNO<sub>5</sub> [M + 1] 698.2935, found 698.2936.



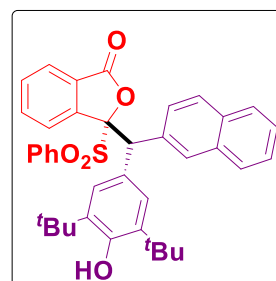
**3-((3,5-di-tert-butyl-4-hydroxyphenyl)(naphthalen-1-yl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4r):**

White solid; m.p. 165 - 167 °C; Yield – 85% (191 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.33 (s, 18H), 5.00 (s, 1H), 6.41 (s, 1H), 7.12 – 7.32 (m, 5H), 7.41 – 7.47 (m, 5H), 7.51 – 7.77 (m, 7H), 8.56 (d, *J* = 12Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.22, 34.10, 45.26, 104.22, 122.48, 123.35, 124.56, 125.46, 125.97, 126.50, 126.69, 127.57, 127.97, 128.26, 129.15, 129.58, 130.09, 130.71, 133.25, 133.62, 133.72, 134.11, 135.36, 135.70, 136.30, 136.94, 144.16, 153.11, 168.64; HRMS (ESI): *m/z* calcd for C<sub>39</sub>H<sub>38</sub>NaSO<sub>5</sub> [M + Na] 641.2332, found 641.2337.



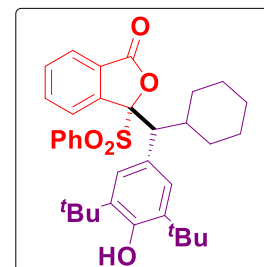
**3-((3,5-di-tert-butyl-4-hydroxyphenyl)(naphthalen-2-yl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4s):**

White solid; m.p. 169 - 171 °C; Yield – 84% (189 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.33 (s, 18H), 5.00 (s, 1H), 6.42 (s, 1H), 6.97 – 7.07 (m, 1H), 7.12 – 7.25 (m, 1H), 7.27 – 7.45 (m, 4H), 7.46 – 7.67 (m, 7H), 7.70 – 7.81 (m, 3H), 7.95 – 8.00 (m, 1H), 8.57 (d, *J* = 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.23, 34.10, 45.27, 104.22, 122.48, 123.37, 124.57, 125.46, 126.49, 126.70, 127.57, 127.97, 129.15, 129.59, 130.09, 130.70, 133.62, 134.10, 135.37, 136.31, 136.95, 144.17, 153.11, 168.63; HRMS (ESI): *m/z* calcd for C<sub>39</sub>H<sub>38</sub>NaSO<sub>5</sub> [M + Na] 641.2332, found 641.2337.



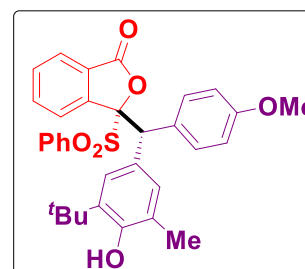
**3-(cyclohexyl(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4t):**

White solid; m.p. 105 - 107 °C; Yield – 66% (138 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 0.67 – 1.48 (s, 29H), 3.92 (s, 1H), 5.01 (s, 1H), 6.73 - 7.34 (m, 9H), 7.67 - 7.99 (m, 4H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 25.59, 26.33, 26.59, 28.89, 30.35, 40.71, 52.97, 105.60, 124.26, 124.44, 126.05, 126.85, 127.16, 127.88, 129.85, 131.11, 133.36, 134.40, 134.72, 137.06, 144.73, 152.98, 168.26; HRMS (ESI): *m/z* calcd for C<sub>35</sub>H<sub>42</sub>SNaO<sub>5</sub> [M + Na] 597.2645, found 597.2646.



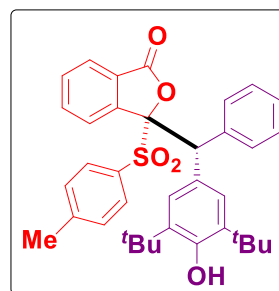
**3-((3-tert-butyl-4-hydroxy-5-methylphenyl)(4-methoxyphenyl)methyl)-3-phenylsulfonyl)isobenzofuran-1(3H)-one (4u):**

White solid; m.p. 150 - 152 °C; Yield – 82% (166 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.38 (s, 9H), 1.87 (s, 3H), 3.59 (s, 3H), 4.61 (s, 1H), 5.15 (s, 1H), 6.51 – 6.55 (m, 2H), 6.97 – 7.01 (m, 1H), 7.07 – 7.23 (m, 5H), 7.3 – 7.52 (m, 4H), 7.66 – 7.74 (m, 2H), 7.98 (d, *J* = 8Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 15.95, 29.67, 34.14, 53.60, 54.98, 103.46, 113.74, 122.68, 124.39, 125.81, 127.10, 127.91, 128.75, 129.02, 129.67, 129.77, 130.42, 130.83, 132.96, 134.41, 136.84, 144.45, 152.00, 158.31, 168.47; HRMS (ESI): *m/z* calcd for C<sub>33</sub>H<sub>32</sub>SO<sub>6</sub> [M+1] 557.1812, found 557.1815.



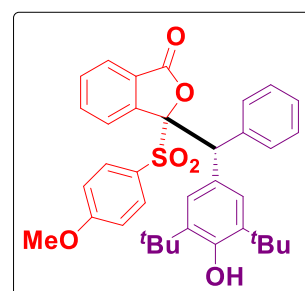
### 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(phenyl)methyl)-3-tosylisobenzofuran-1(3*H*)-one (4aa):

White solid; m.p. 149 - 151 °C; Yield – 75% (151 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.33 (s, 18H), 2.28 (s, 3H), 5.01 (s, 1H), 5.27 (s, 1H), 6.95 - 7.25 (m, 8H), 7.42 - 7.46 (m, 1H), 7.64 - 7.69 (m, 2H), 7.91 (d, *J* = 7.2Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 21.75, 30.20, 34.10, 54.43, 103.16, 124.59, 125.64, 126.64, 126.97, 127.02, 127.99, 128.45, 128.71, 128.84, 130.05, 130.65, 133.84, 134.21, 135.41, 138.97, 144.47, 144.55, 153.19, 168.24; HRMS (ESI): *m/z* calcd for C<sub>36</sub>H<sub>38</sub>SO<sub>5</sub> [M + Na] 605.2332, found 605.2336.



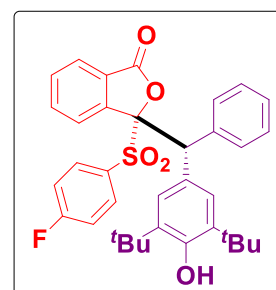
### 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(phenyl)methyl)-3-((4-methoxyphenyl)sulfonyl)isobenzofuran-1(3*H*)-one (4ab):

White solid; m.p. 151 - 153 °C; Yield – 93% (196 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.34 (s, 18H), 3.76 (s, 3H), 5.03 (s, 1H), 5.26 (s, 1H), 6.60 – 6.43 (m, 2H), 6.93 - 7.06 (m, 3H), 7.21 – 7.24 (m, 3H), 7.34 (m, 3H), 7.63 – 7.70 (m, 2H), 7.90 (d, *J* = 8Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.20, 34.11, 54.48, 55.30, 102.95, 113.37, 124.51, 125.65, 126.40, 126.94, 126.98, 127.95, 128.14, 128.45, 128.65, 130.61, 132.21, 134.40, 135.49, 139.08, 144.67, 153.09, 163.38, 168.34; HRMS (ESI): *m/z* calcd for C<sub>36</sub>H<sub>38</sub>SKO<sub>6</sub> [M + K] 637.2021, found 637.2025.



### 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(phenyl)methyl)-3-((4-fluorophenyl)sulfonyl)isobenzofuran-1(3*H*)-one (4ac):

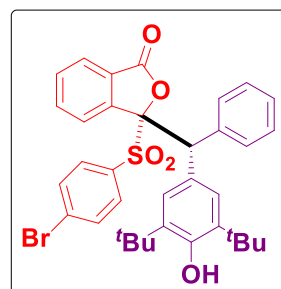
White solid; m.p. 154 - 156 °C; Yield – 72% (144 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.33 (s, 18H), 5.07 (s, 1H), 5.24 (s, 1H), 6.71 - 6.78 (m, 2H), 7.17 - 7.25 (m, 6H), 7.38 - 7.52 (m, 4H), 7.67 - 7.73 (m, 2H), 7.91 (d, *J* = 8Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.23, 34.11, 54.61, 90.50, 103.26, 115.33, 115.56, 116.82, 124.38, 125.83, 126.47, 127.11, 128.55, 130.87, 132.88, 134.42, 135.66, 138.82, 144.23, 153.35, 161.59, 165.21 (d, *J* = 255 Hz), 168.10; <sup>19</sup>F-NMR (376 MHz, CDCl<sub>3</sub>); δ = -100.44, -102.11; HRMS (ESI): *m/z* calcd for C<sub>35</sub>H<sub>35</sub>FN<sub>5</sub>SO<sub>5</sub> [M + Na] 609.2081, found 609.2083.





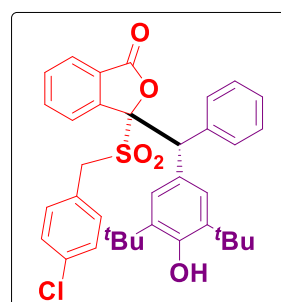
**3-((4-bromophenyl)sulfonyl)-3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(phenyl)methyl)isobenzofuran-1(3*H*)-one (4ad):**

White solid; m.p. 165 - 167 °C; Yield – 65% (119 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.35 (s, 18H), 5.08 (s, 1H), 5.23 (s, 1H), 6.93 – 7.06 (m, 3H), 7.20 – 7.34 (m, 8H), 7.45 – 7.52 (m, 1H), 7.65 – 7.74 (m, 2H), 7.91 (d, *J* = 8Hz, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.27, 34.14, 54.55, 103.60, 124.33, 125.88, 126.56, 126.78, 127.13, 127.67, 128.47, 128.57, 129.29, 130.94, 131.33, 131.39, 134.47, 135.62, 136.18, 138.79, 144.06, 153.45, 168.07; HRMS (ESI): *m/z* calcd for C<sub>35</sub>H<sub>35</sub>BrKSO<sub>5</sub> [M + K] 685.1020, found 685.1022.



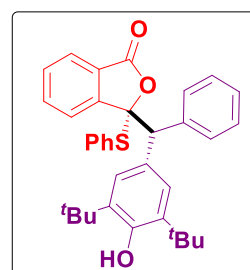
**3-((4-chlorobenzyl)sulfonyl)-3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(phenyl)methyl)isobenzofuran-1(3*H*)-one (4ae):**

White solid; m.p. 183 - 185 °C; Yield – 71% (135 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.50 (s, 18H), 2.81 (d, *J* = 12.8Hz, 1H), 3.99 (d, *J* = 13.2Hz, 1H), 5.25 (s, 1H), 5.32 (s, 1H), 6.98 – 7.12 (m, 5H), 7.22 – 7.27 (m, 2H), 7.33 – 7.46 (m, 3H), 7.56 – 7.62 (m, 1H), 7.74 – 7.78 (m, 4H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.37, 34.48, 54.73, 56.88, 103.44, 123.72, 124.15, 125.99, 126.55, 127.26, 127.34, 127.78, 128.24, 128.78, 128.82, 130.90, 130.70, 134.56, 135.27, 136.87, 138.56, 143.57, 154.04, 168.11; HRMS (ESI): *m/z* calcd for C<sub>36</sub>H<sub>37</sub>ClNaO<sub>5</sub> [M + Na] 639.1942, found 639.1943.



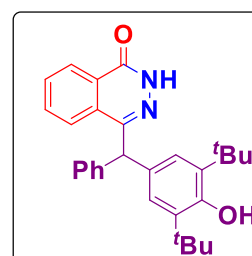
**3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(phenyl)methyl)-3-(phenylthio)isobenzofuran-1(3*H*)-one (4af):**

White solid; m.p. 192 - 194 °C; Yield – 76% (168 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.19 (s, 18H), 4.76 (s, 1H), 4.91 (s, 1H), 6.80 (s, 1H), 6.95 - 7.21 (m, 7H), 7.31 - 7.61 (m, 4H), 7.67 - 7.71 (m, 1H), 7.90 – 7.94 (m, 2H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 29.98, 34.04, 60.71, 99.59, 122.90, 124.32, 126.38, 126.52, 127.36, 127.69, 128.38, 128.40, 128.59, 129.06, 129.30, 130.17, 133.14, 134.91, 136.36, 139.07, 150.51, 152.45, 168.56; HRMS (ESI): *m/z* calcd for C<sub>35</sub>H<sub>36</sub>SNaO<sub>3</sub> [M + Na] 559.2277, found 559.2279.



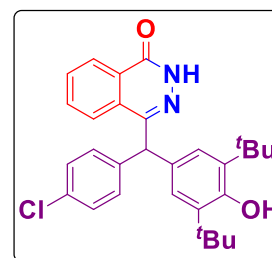
**4-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(phenyl)methyl)phthalazin-1(2*H*)-one (5a):**

White solid; m.p. 263 – 265 °C; Yield – 85% (65mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.36 (s, 18H), 5.14 (s, 1H), 5.29 (s, 1H), 5.89 (s, 1H), 7.00 (s, 2H), 7.20 - 7.24 (m, 2H), 7.28 - 7.33 (m, 2H), 7.68 – 7.76 (m, 2H) 7.83 – 7.87 (m, 1H), 8.43 – 8.48 (m, 1H), 10.08 (s, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.27, 34.33, 52.91, 125.33, 126.03, 126.76, 126.95, 128.24, 128.42, 129.19, 130.06, 130.91, 131.13, 133.44, 135.69, 141.60, 148.97, 152.62, 159.89; HRMS (ESI): *m/z* calcd for C<sub>29</sub>H<sub>33</sub>N<sub>2</sub>O<sub>2</sub> [M + 1] 441.2537, found 441.2533.



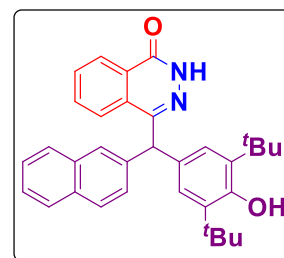
**4-((4-chlorophenyl)3,5-di-*tert*-butyl-4-hydroxyphenyl)(phenyl)methyl)phthalazin-1(2H)-one (5b):**

White solid; m.p. 222 – 224 °C; Yield – 80% (62 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.35 (s, 18H), 5.15 (s, 1H), 5.84 (s, 1H), 6.97 (s, 2H), 7.10 - 7.15 (m, 2H), 7.24 - 7.29 (m, 2H), 7.70 – 7.81 (m, 3H) 8.43 – 8.47 (m, 1H), 9.99 (s, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.26, 34.35, 52.31, 125.18, 125.82, 127.06, 128.27, 128.55, 129.89, 130.51, 130.58, 131.27, 132.57, 133.52, 135.95, 140.26, 148.50, 152.79, 159.83; HRMS (ESI): m/z calcd for C<sub>29</sub>H<sub>31</sub>ClN<sub>2</sub>O<sub>2</sub> [M + 1] 475.2143, found 475.2146.



**4-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(naphthalene-2-yl)methyl)phthalazin-1(2H)-one (5c):**

White solid; m.p. 211 – 213 °C; Yield – 65% (51 mg); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>); δ = 1.35 (s, 18H), 5.15 (s, 1H), 6.55 (s, 1H), 7.03 - 7.06 (m, 3H), 7.34 - 7.50 (m, 3H), 7.70 – 7.91 (m, 6H) 8.45 – 8.49 (m, 1H), 9.79 (s, 1H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>); δ = 30.31, 34.35, 49.30, 123.38, 125.08, 125.37, 125.51, 126.34, 126.43, 127.08, 127.25, 127.67, 129.03, 130.00, 131.25, 133.72, 135.94, 138.08, 149.09, 152.81, 159.85; HRMS (ESI): m/z calcd for C<sub>33</sub>H<sub>34</sub>N<sub>2</sub>O<sub>2</sub> [M + 1] 491.2632, found 491.2635.



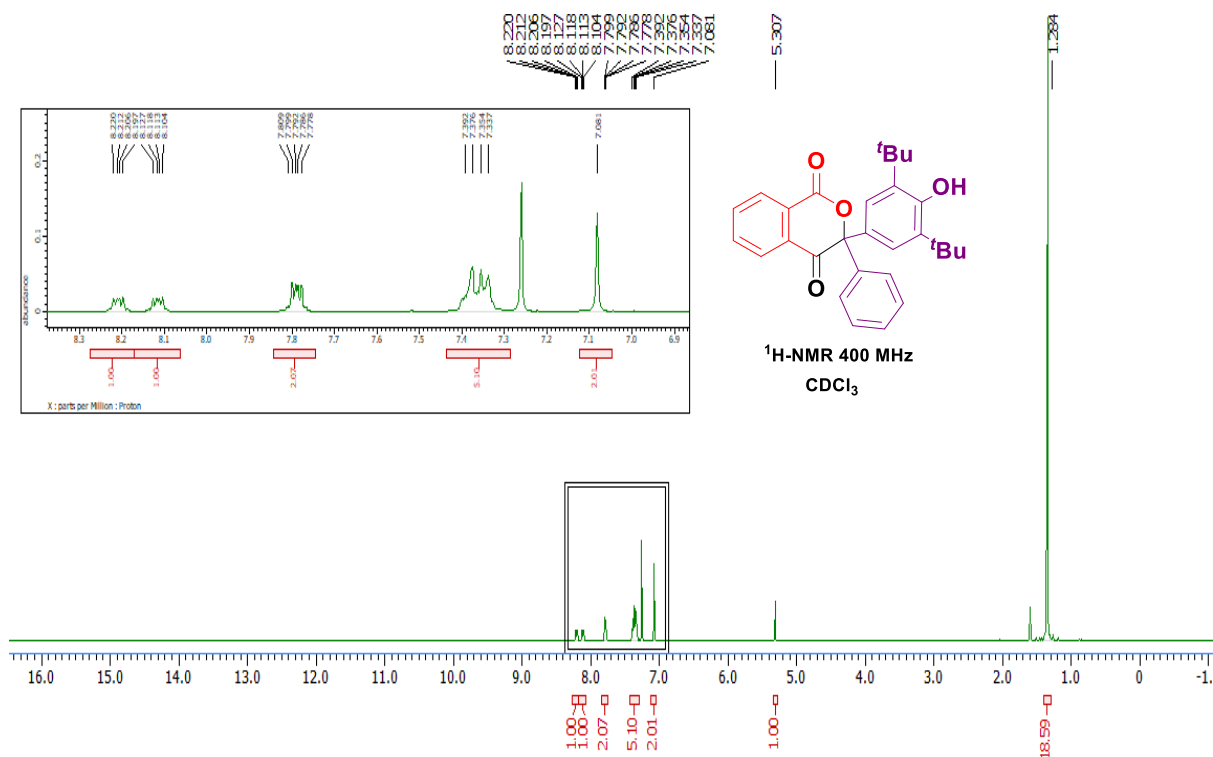


Fig. 1: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)-3-phenylisochroman-1,4-dione (3a)

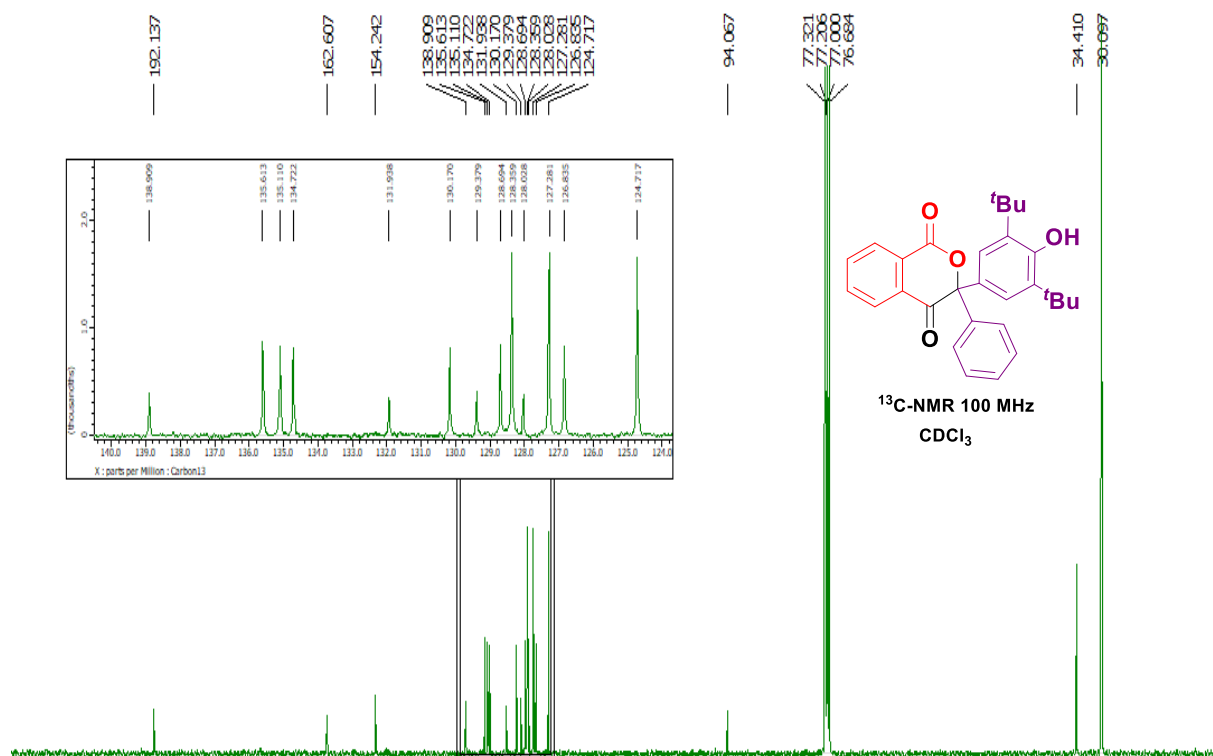
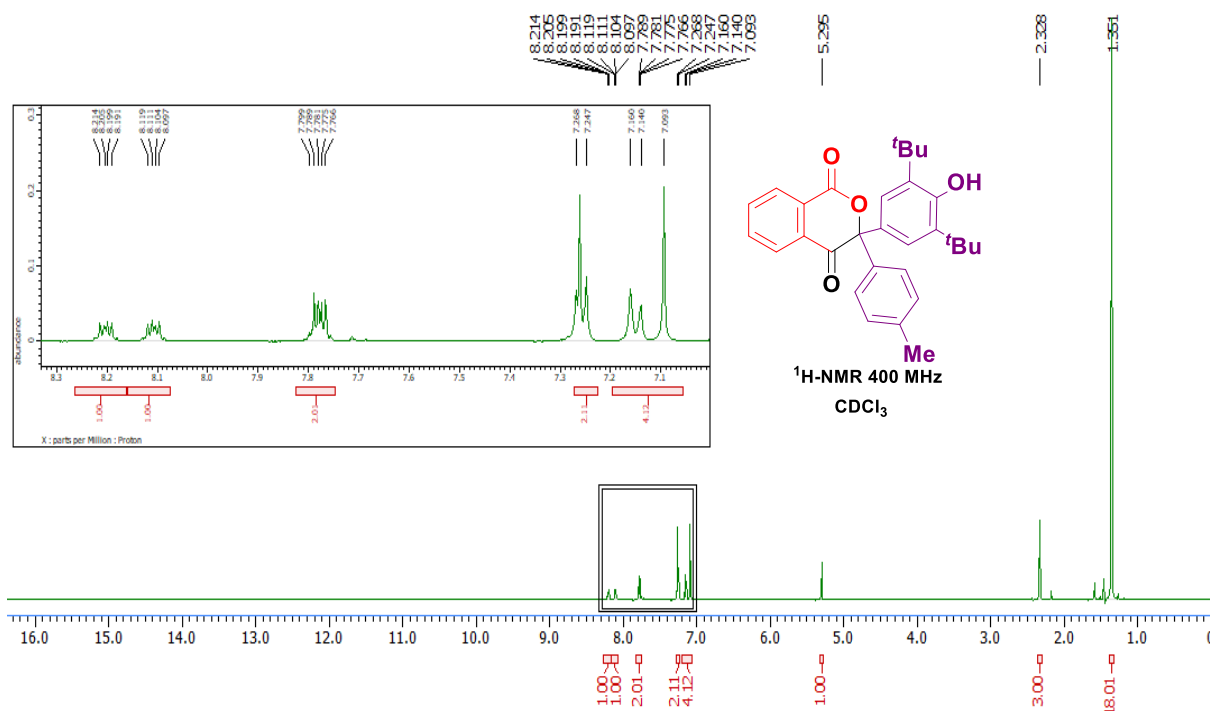
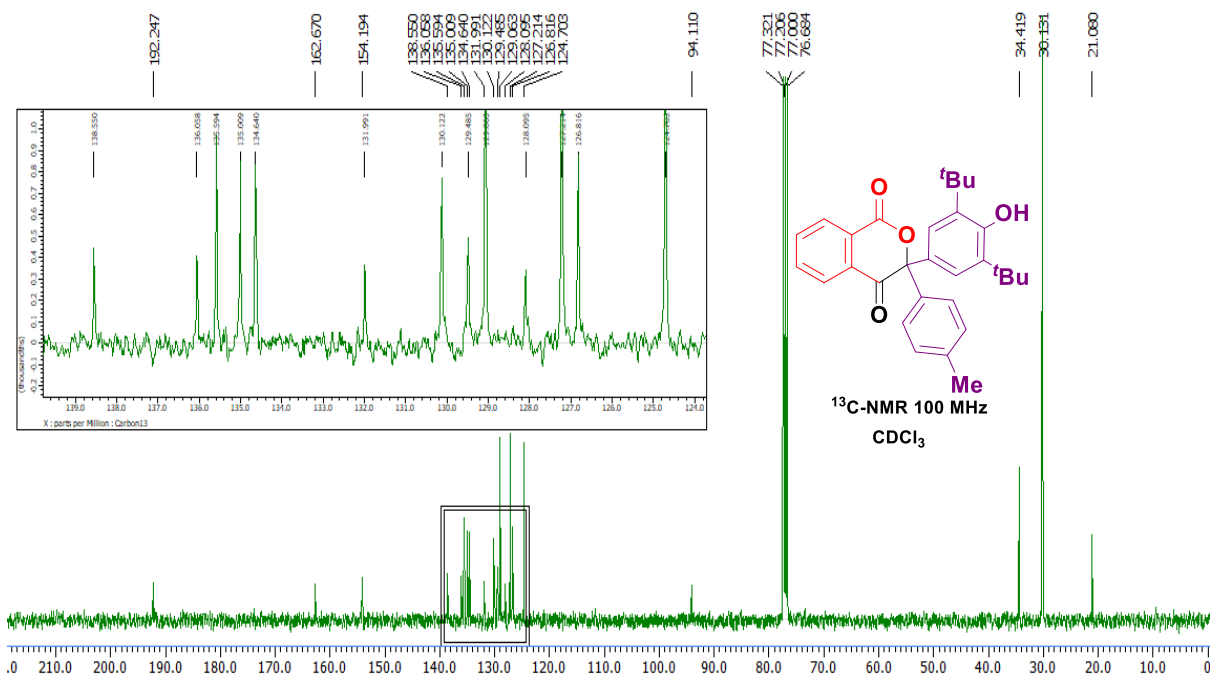


Fig. 2: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)-3-phenylisochroman-1,4-dione (3a)



**Fig. 3:** <sup>1</sup>H-NMR spectrum of 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(*p*-tolyl)isochroman-1,4-dione (**3b**)



**Fig. 4:** <sup>13</sup>C-NMR spectrum of 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(*p*-tolyl)isochroman-1,4-dione (**3b**)

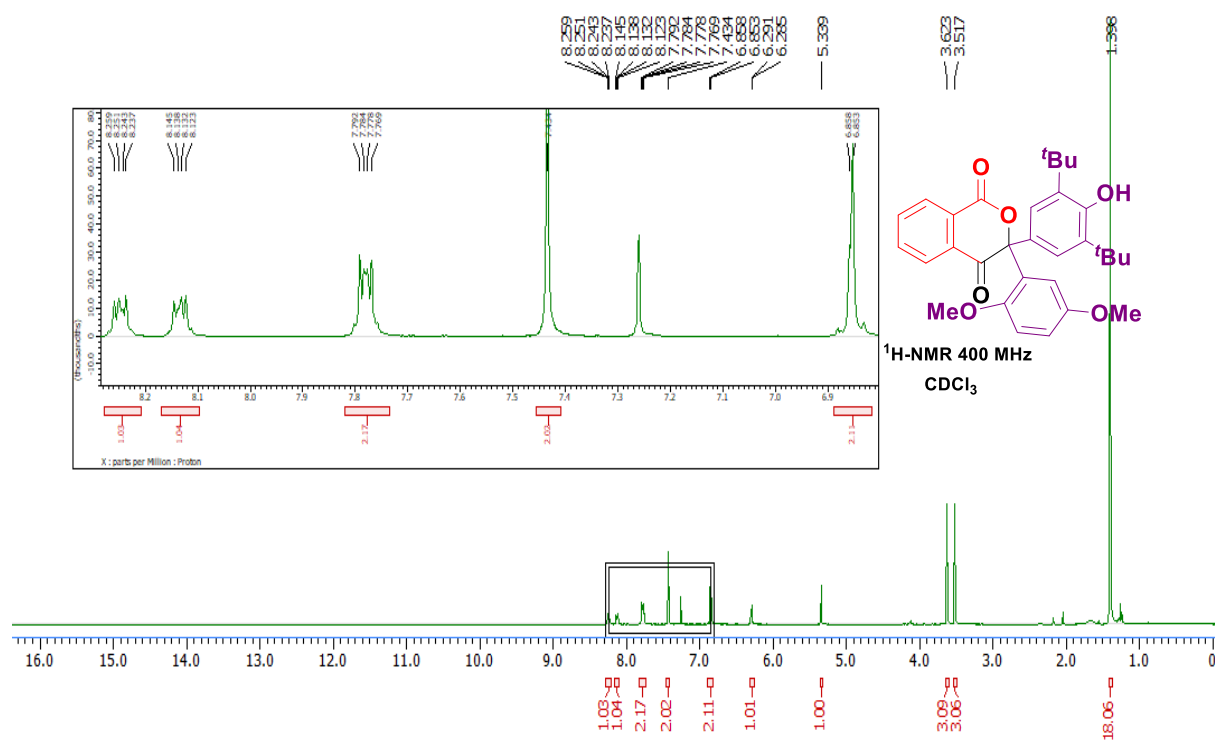


Fig. 5: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(2,5-dimethoxyphenyl)isochroman-1,4-dione (**3c**)

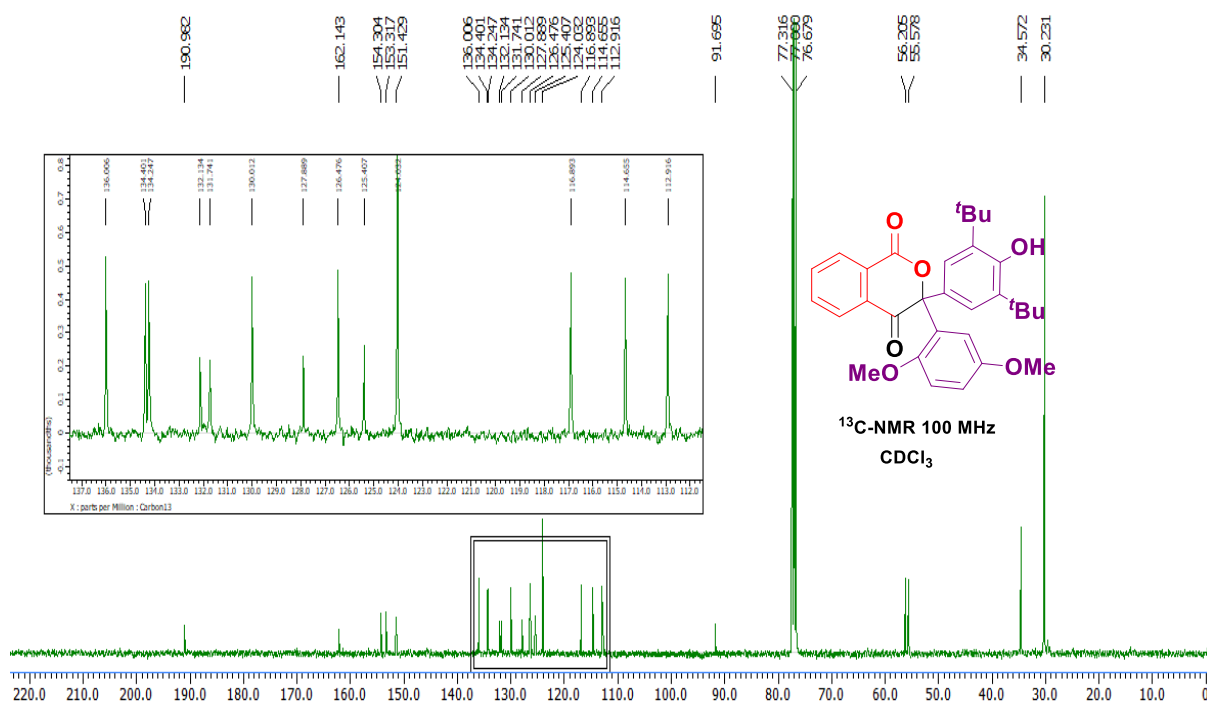


Fig. 6: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(*p*-tolyl)isochroman-1,4-dione (**3c**)

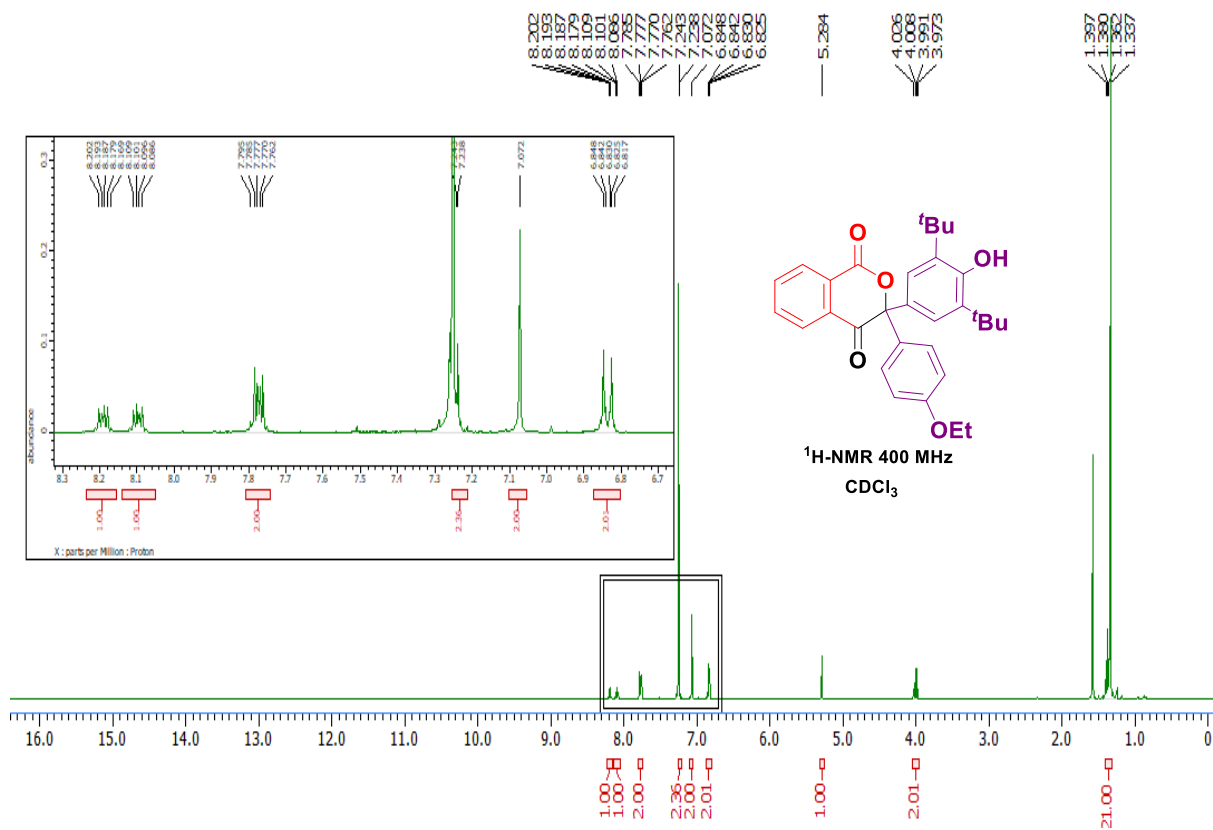


Fig. 7: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)-3-(4-ethoxyphenyl)isochroman-1,4-dione (3d)

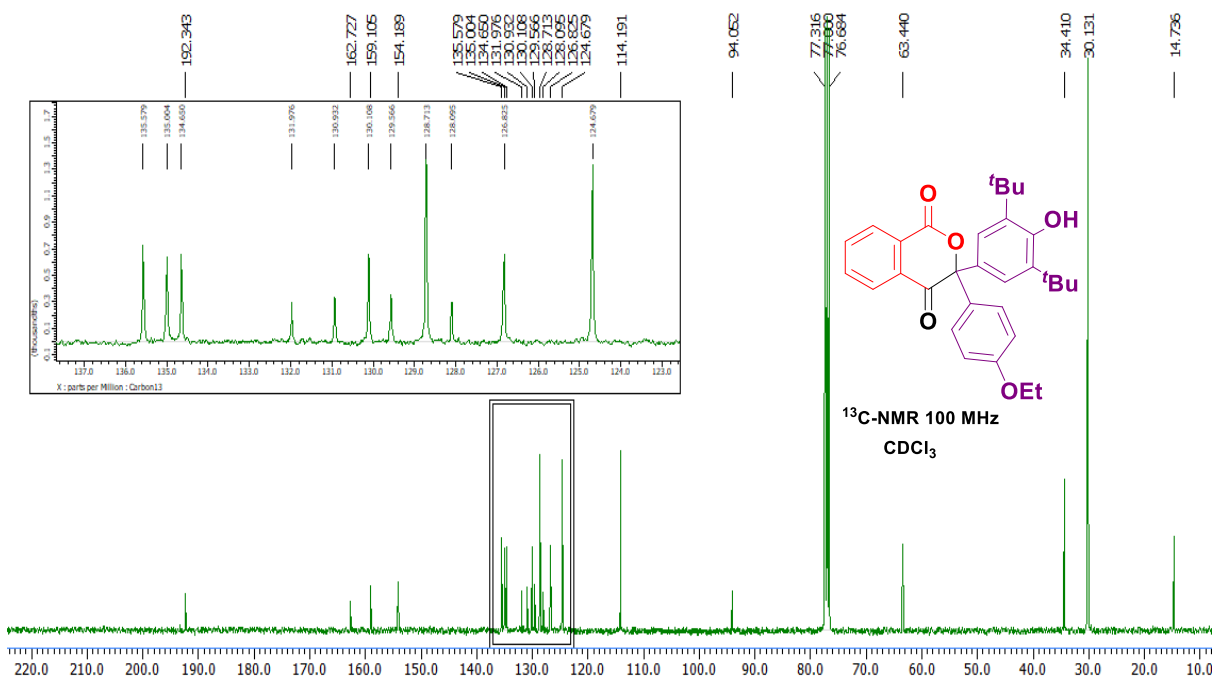
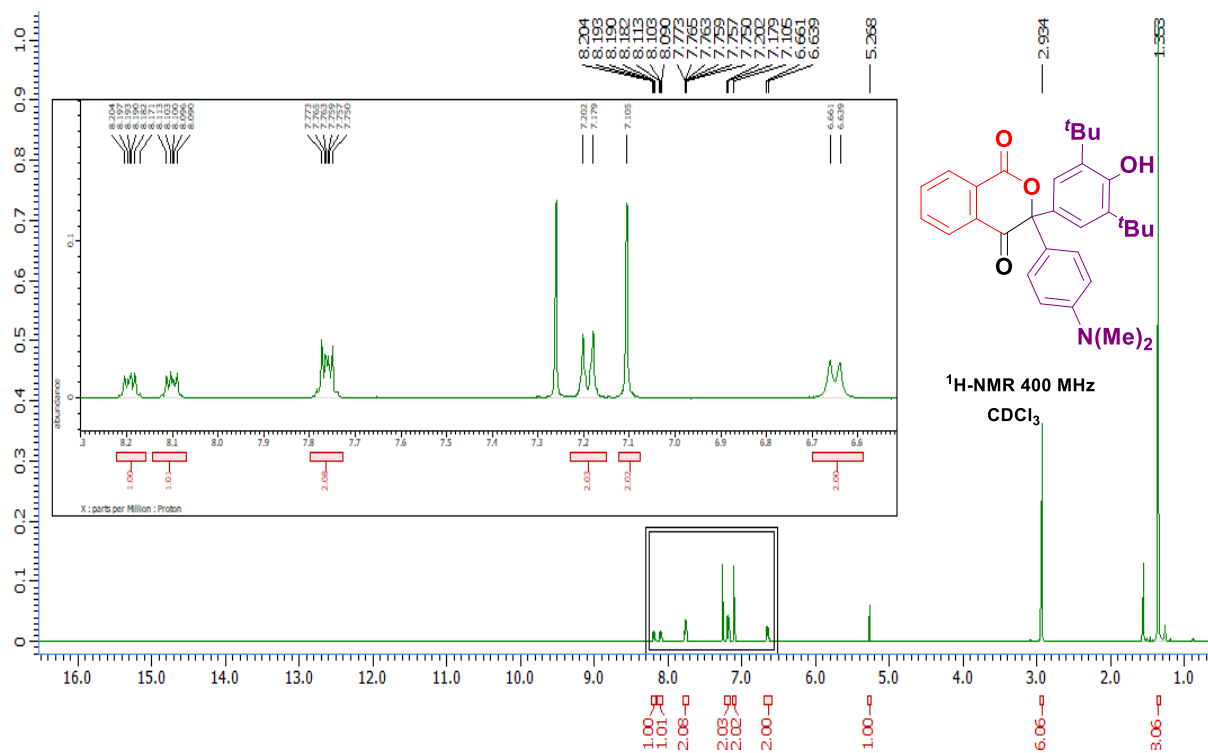
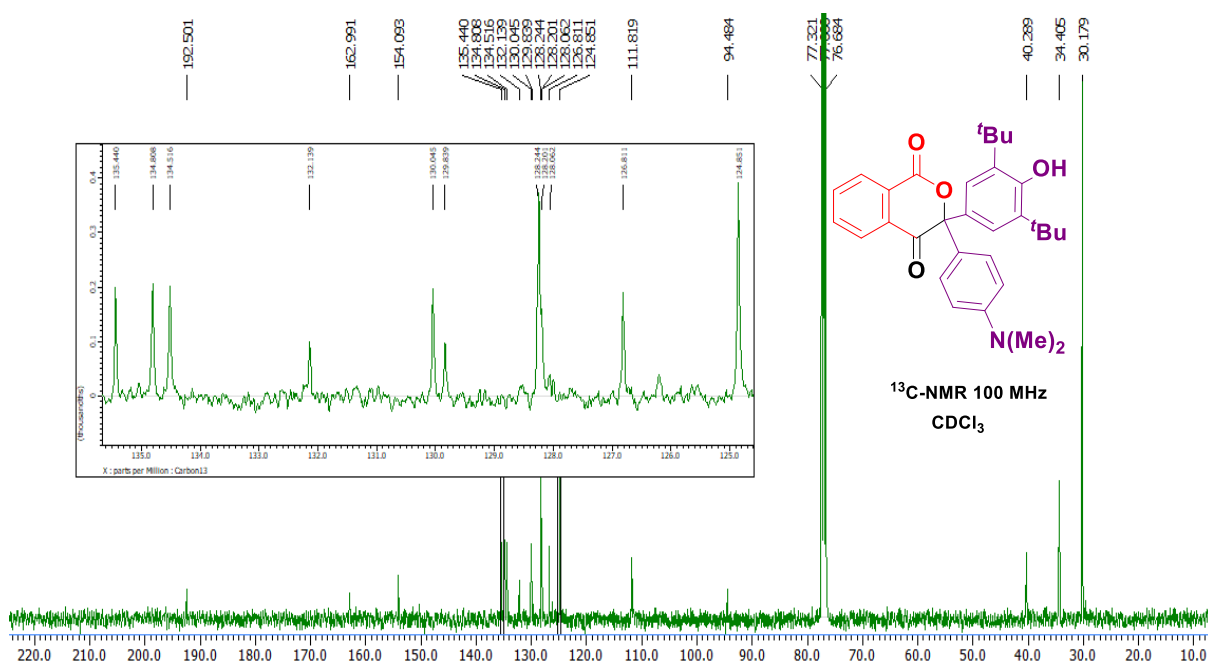


Fig. 8: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)-3-(4-ethoxyphenyl)isochroman-1,4-dione (3d)



**Fig. 9: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(4-dimethylamino)phenyl)isochroman-1,4-dione (3e)**

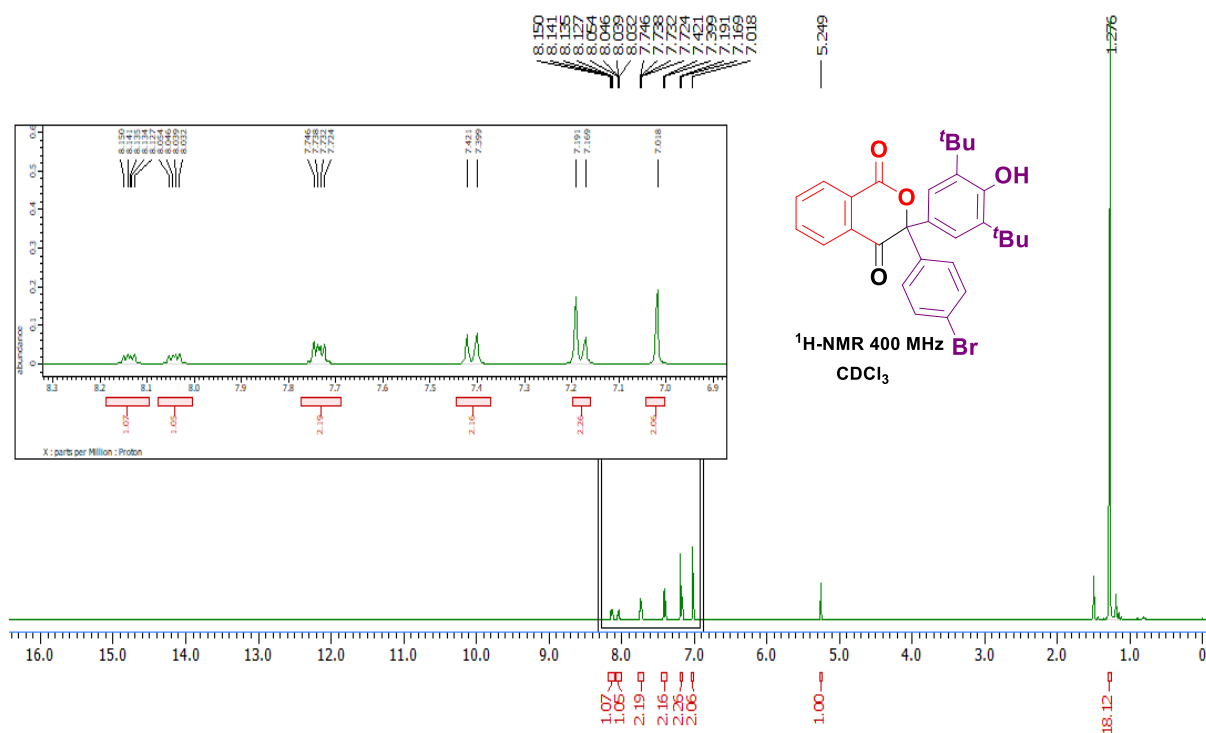


**Fig. 10: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(4-dimethylamino)phenyl)isochroman-1,4-dione (3e)**

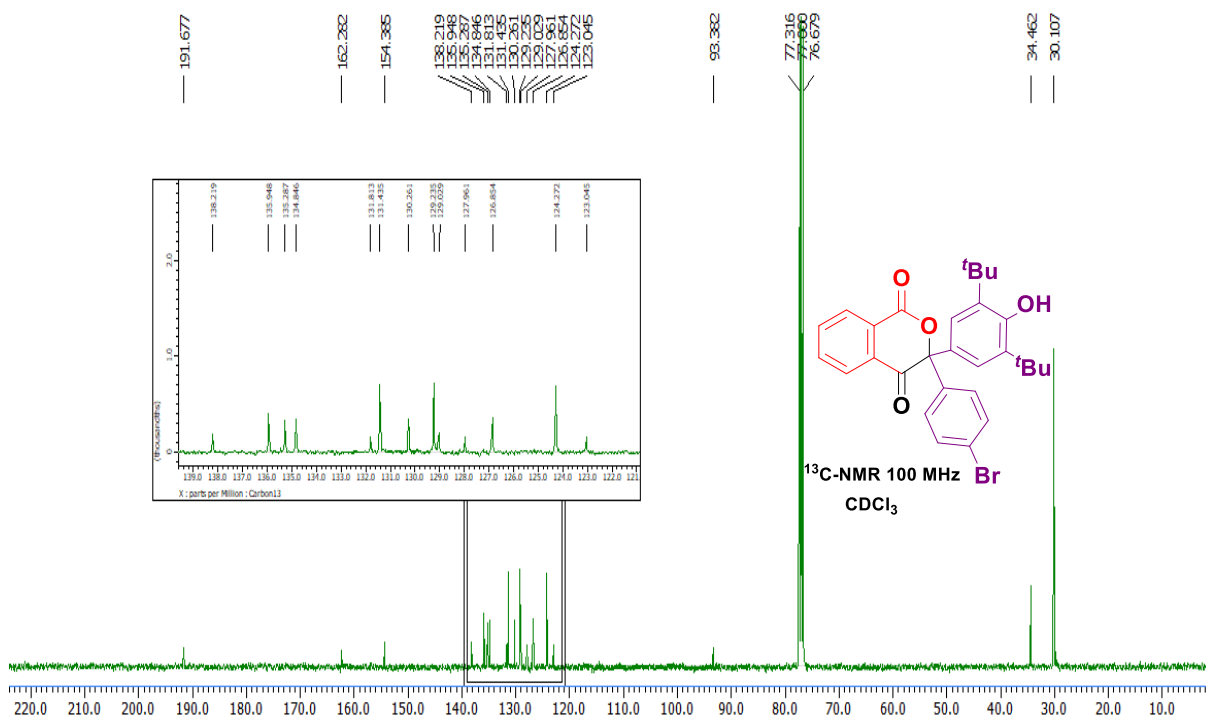






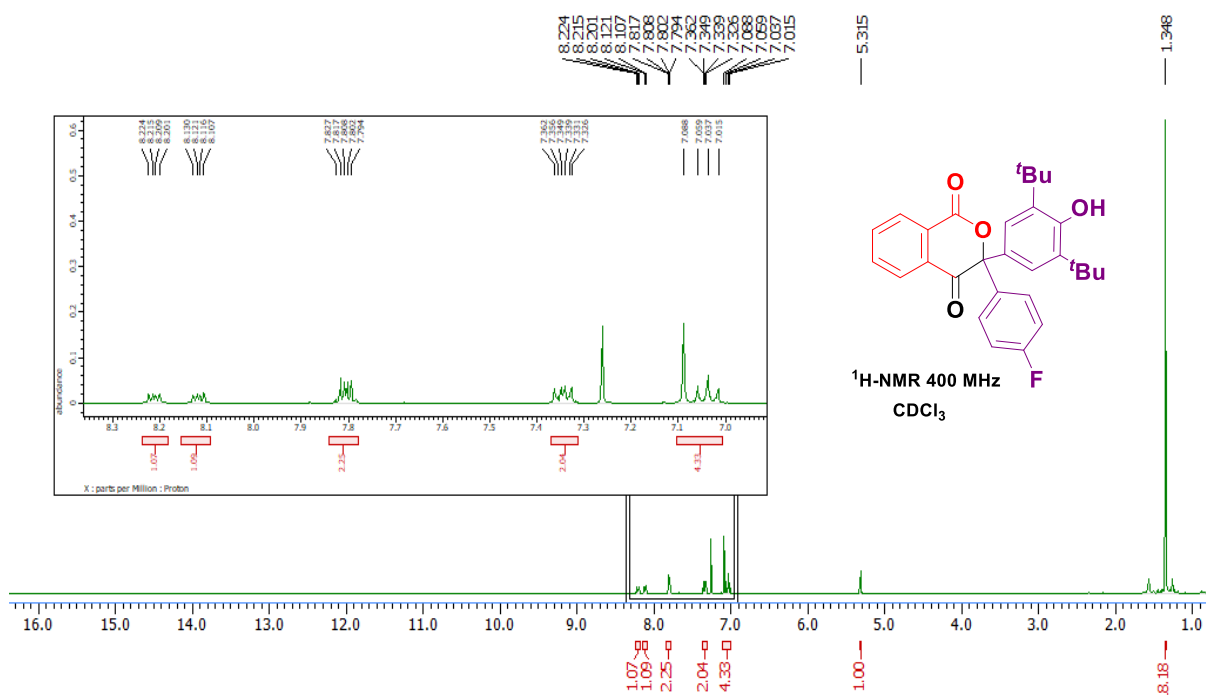


**Fig. 15: <sup>1</sup>H-NMR spectrum of 3-(4-bromophenyl)-3-((3,5-di-tert-butyl-4-hydroxyphenyl)isochroman-1,4-dione (*3h*)**

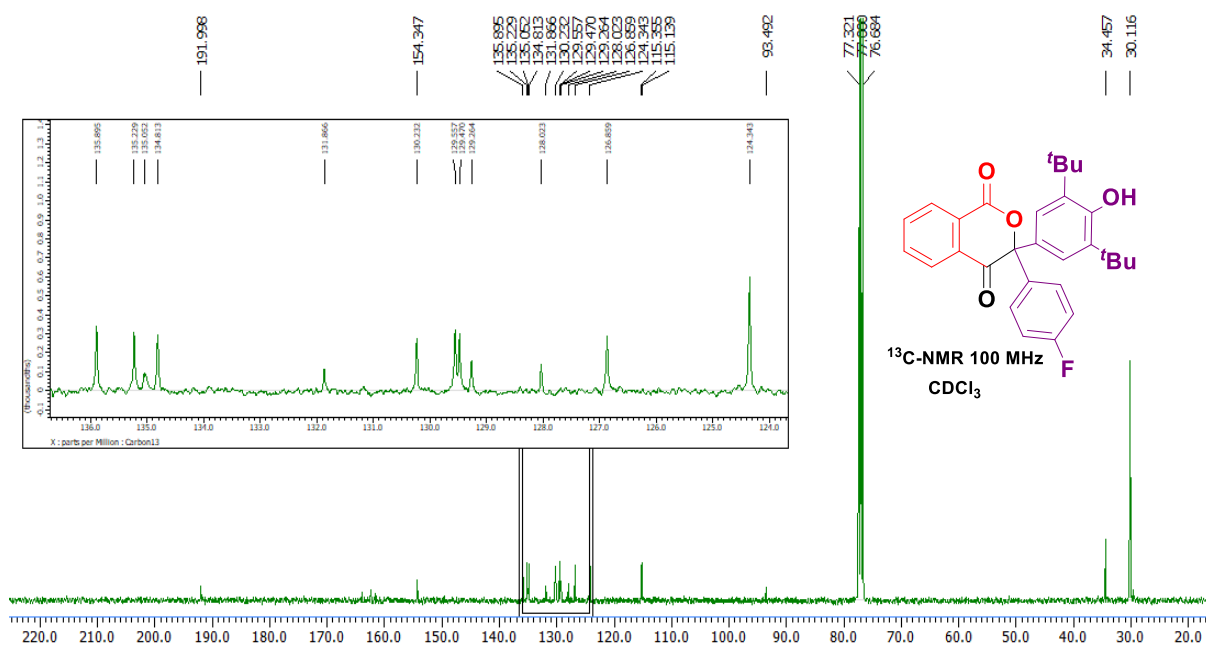


**Fig. 16: <sup>13</sup>C-NMR spectrum of 3-(4-bromophenyl)-3-((3,5-di-tert-butyl-4-hydroxyphenyl)isochroman-1,4-dione (*3h*)**

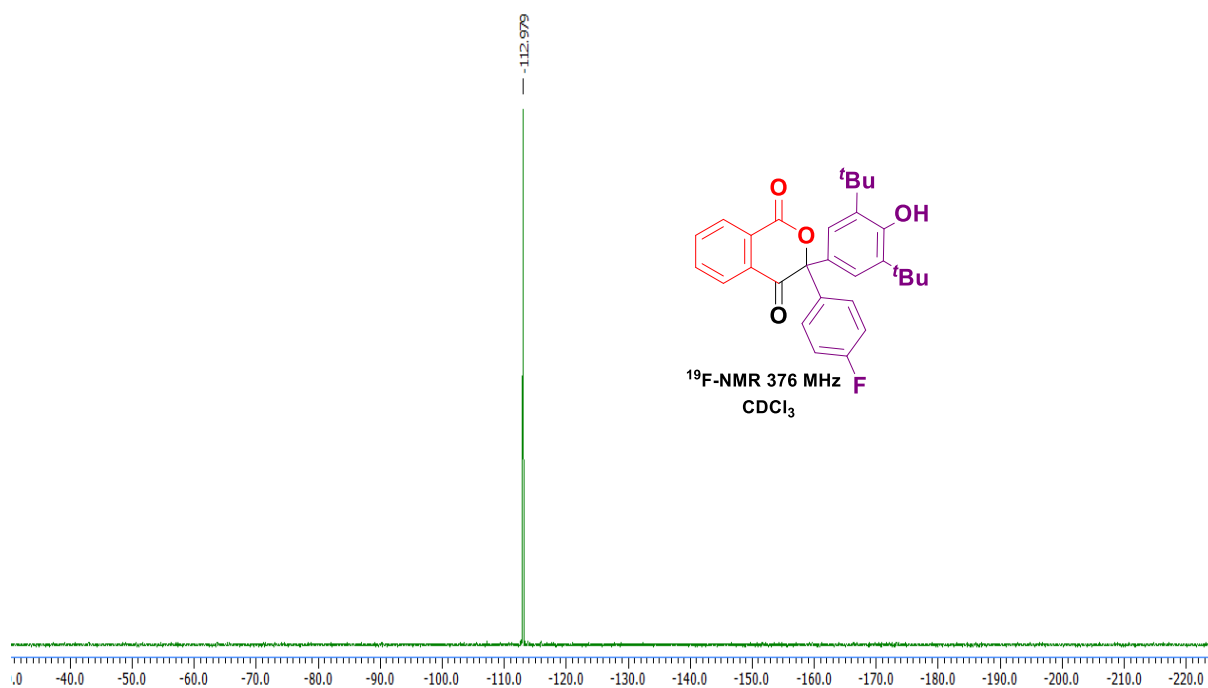




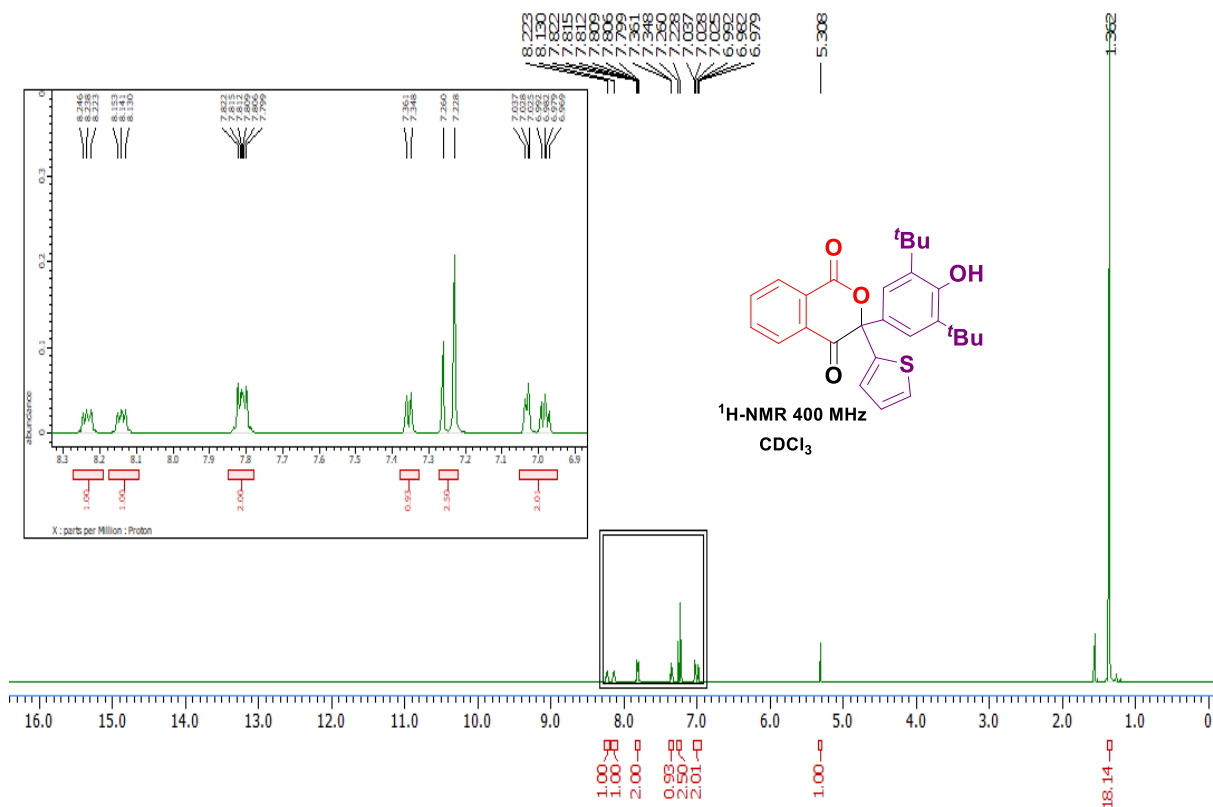
**Fig. 19: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl) 3-(4-fluorophenyl)-isochroman-1,4-dione (3j)**



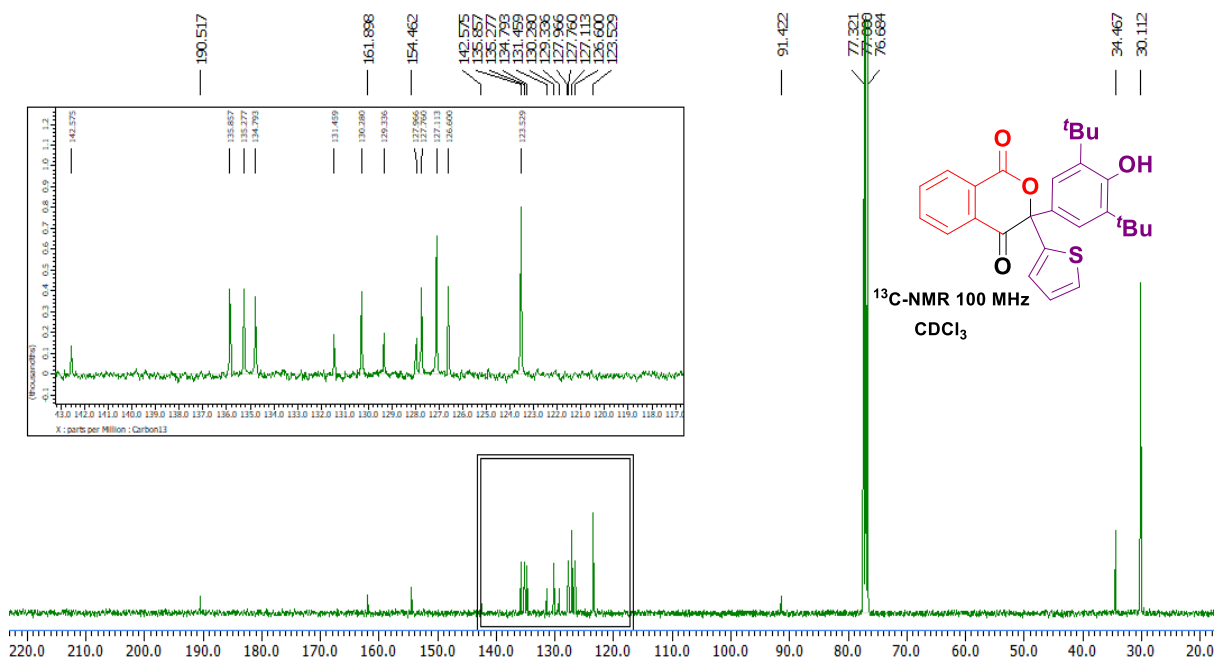
**Fig. 20: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl) 3-(4-fluorophenyl)-isochroman-1,4-dione (3j)**



**Fig. 21:**  $^{19}\text{F-NMR}$  spectrum of 3-((3,5-di-*tert*-butyl-4-hydroxyphenyl) 3-(4-fluorophenyl)-isochroman-1,4-dione (3j)



**Fig. 22:** <sup>1</sup>H-NMR spectrum of 3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(thiophen-2-yl)isochroman-1,4-dione (**3k**)



**Fig. 23:** <sup>13</sup>C-NMR spectrum of 3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-3-(thiophen-2-yl)isochroman-1,4-dione (**3k**)

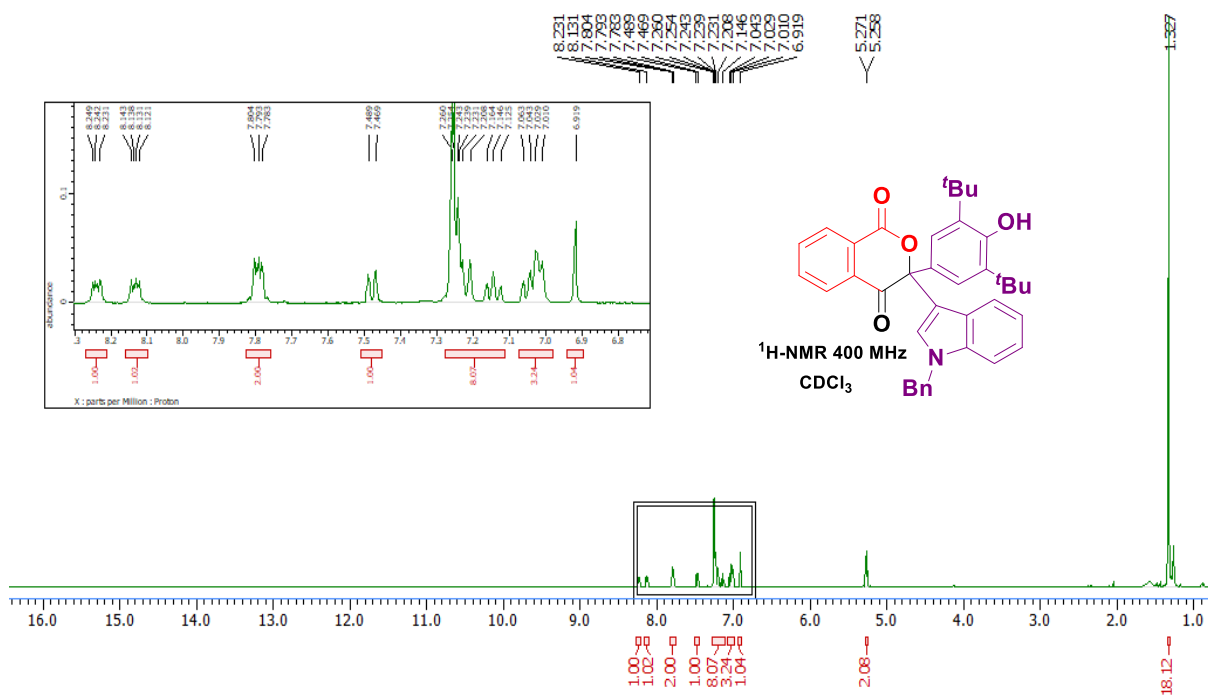


Fig. 24: <sup>1</sup>H-NMR spectrum of 3-(1-benzyl-1H-indol-3-yl)-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)isochroman-1,4-dione (3l)

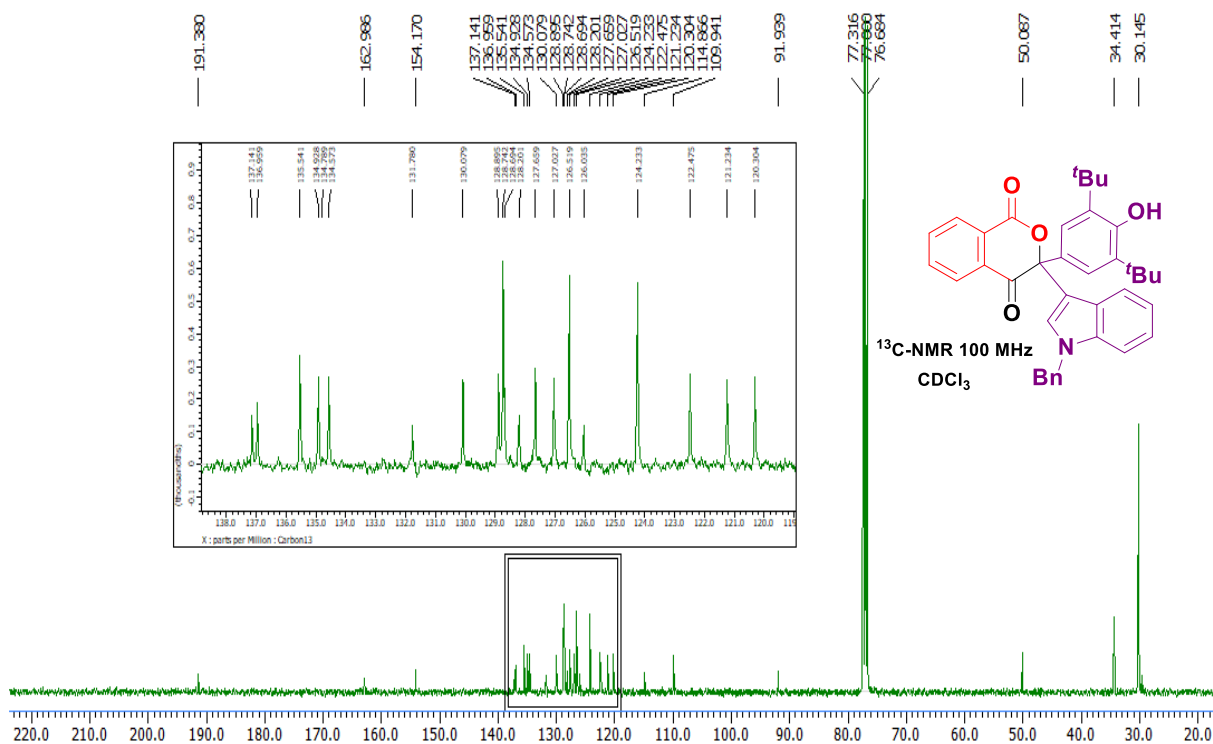
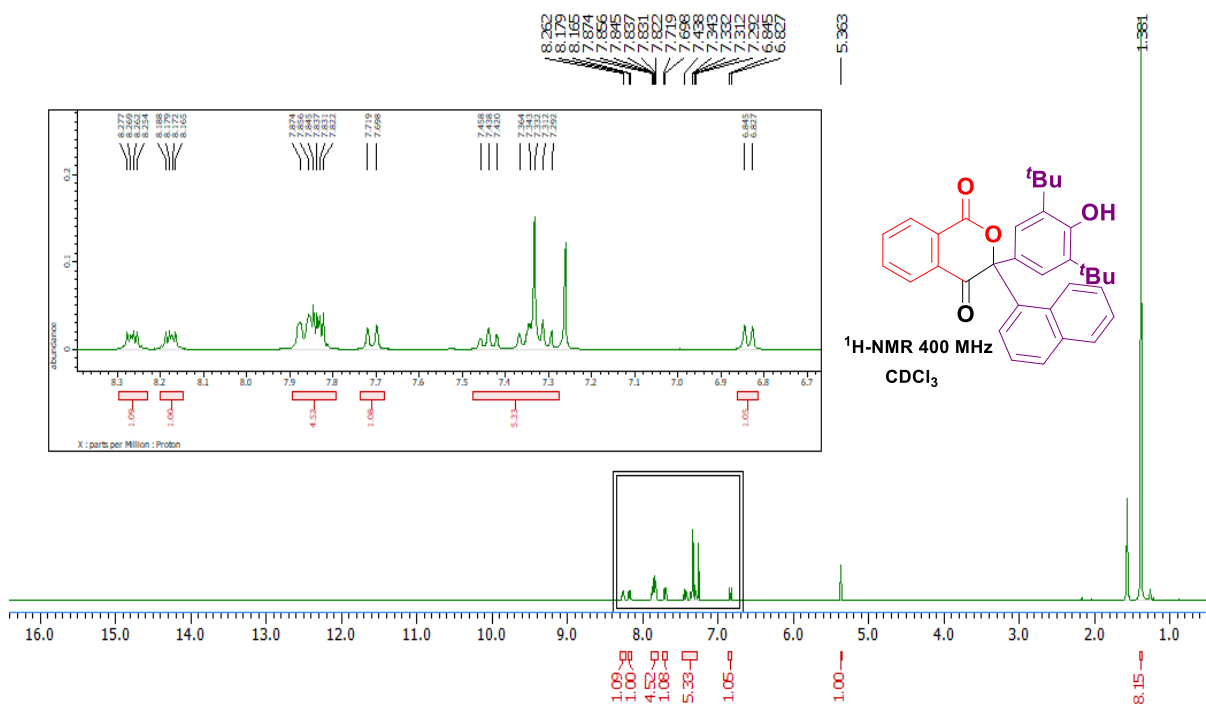
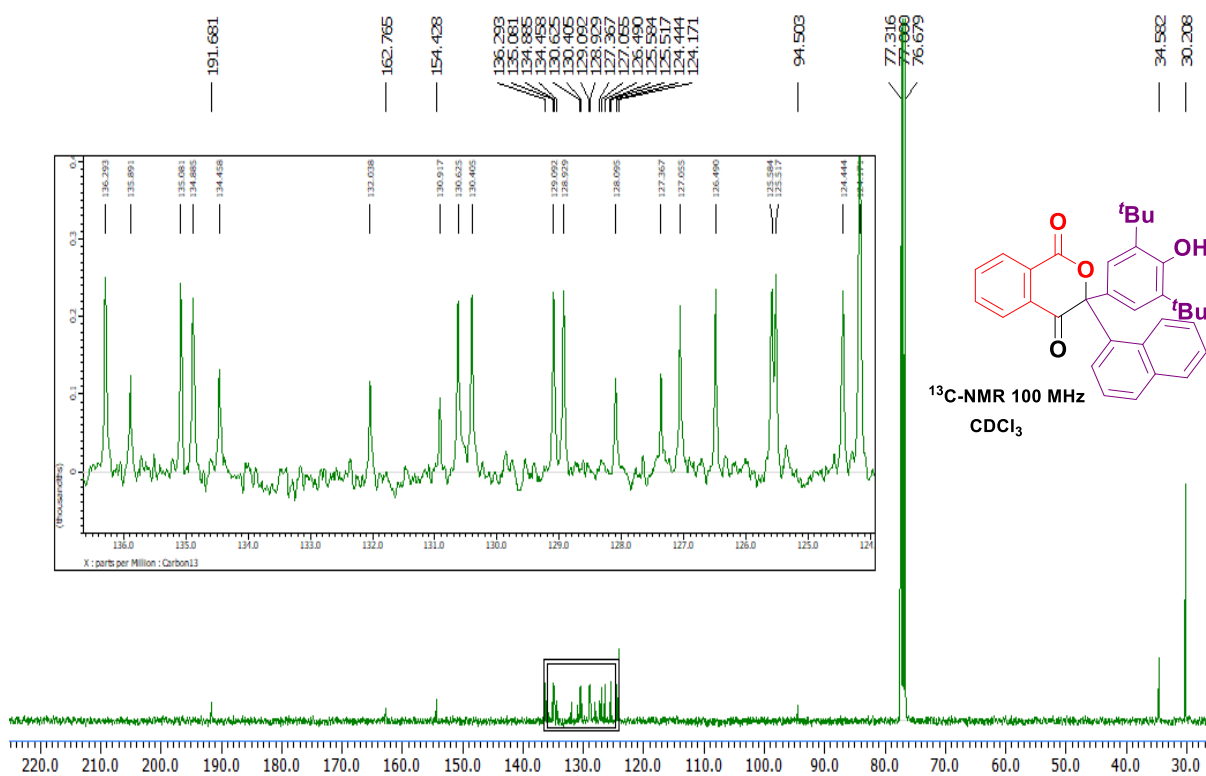


Fig. 25: <sup>13</sup>C-NMR spectrum of 3-(1-benzyl-1H-indol-3-yl)-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)isochroman-1,4-dione (3l)

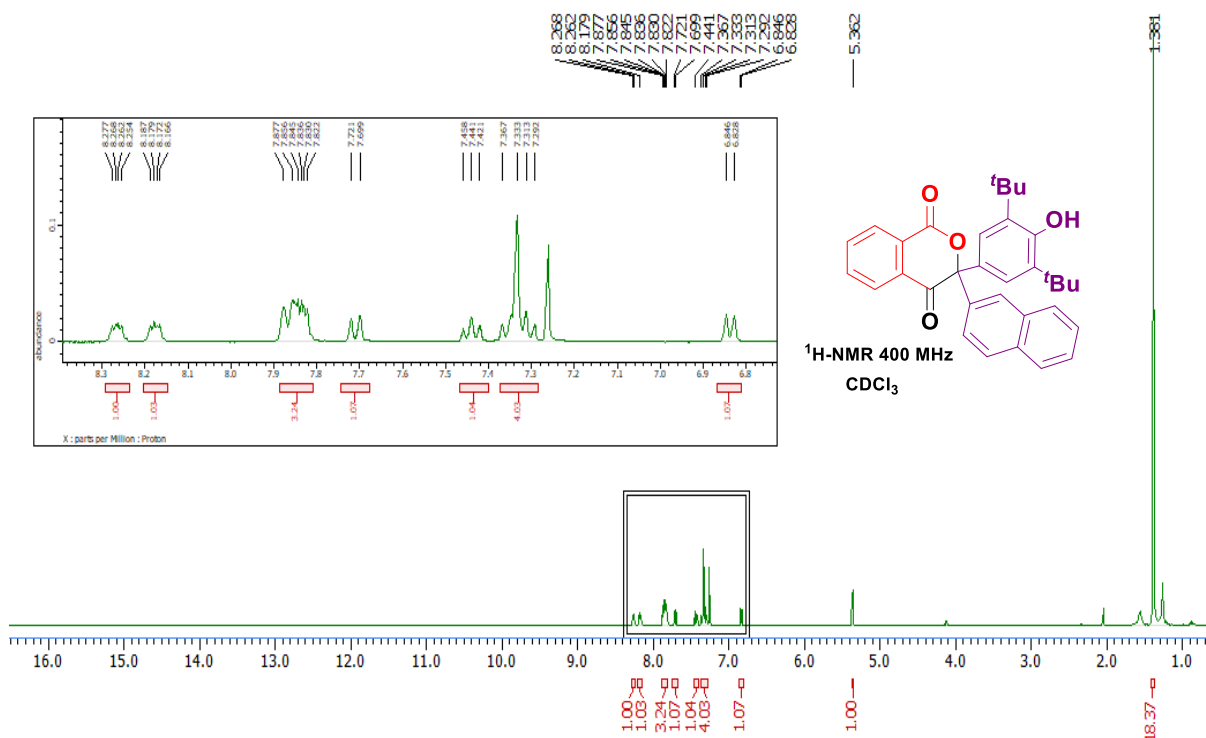


**Fig. 26: <sup>1</sup>H-NMR spectrum of 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-3-(naphthalen-1-yl)isochroman-1,4-dione (3o)**

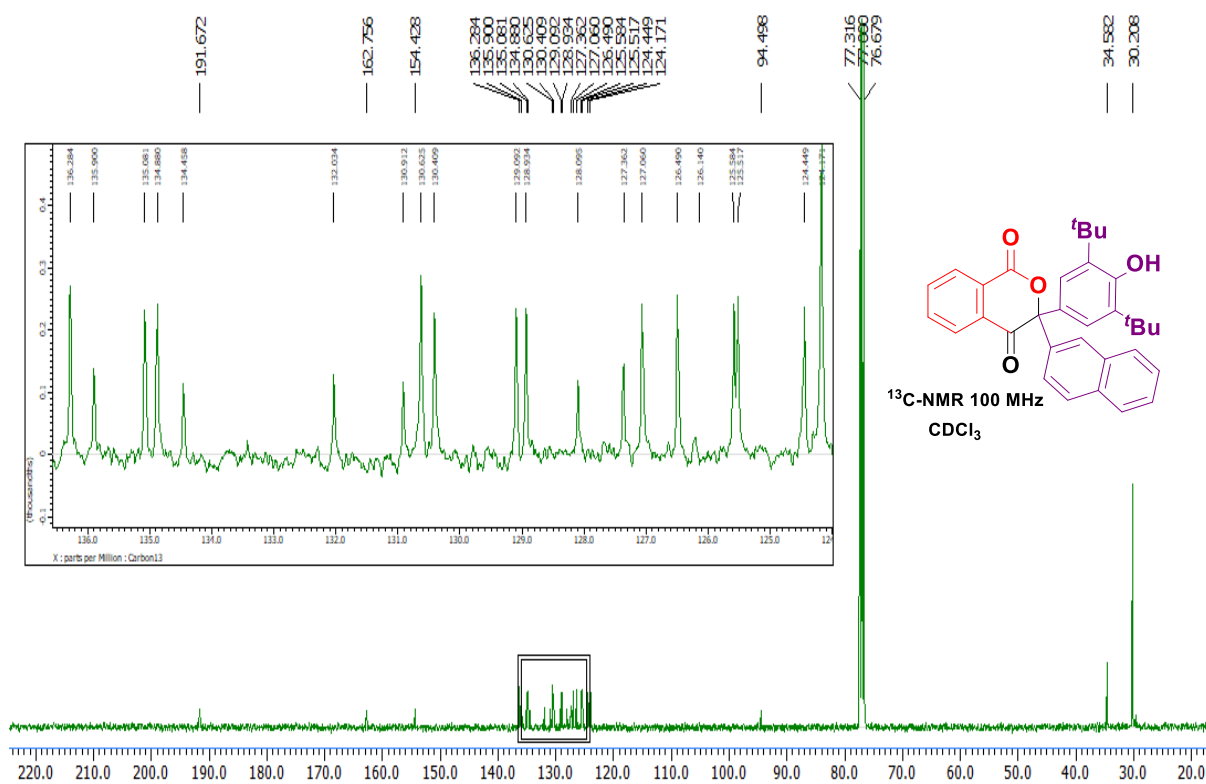


**Fig. 27: <sup>13</sup>C-NMR spectrum of 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-3-(naphthalen-1-yl)isochroman-1,4-dione (3o)**





**Fig. 28: <sup>1</sup>H-NMR spectrum of 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-3-(naphthalen-2-yl)isochroman-1,4-dione (3p)**



**Fig. 29: <sup>13</sup>C-NMR spectrum of 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-3-(naphthalen-2-yl)isochroman-1,4-dione (3p)**

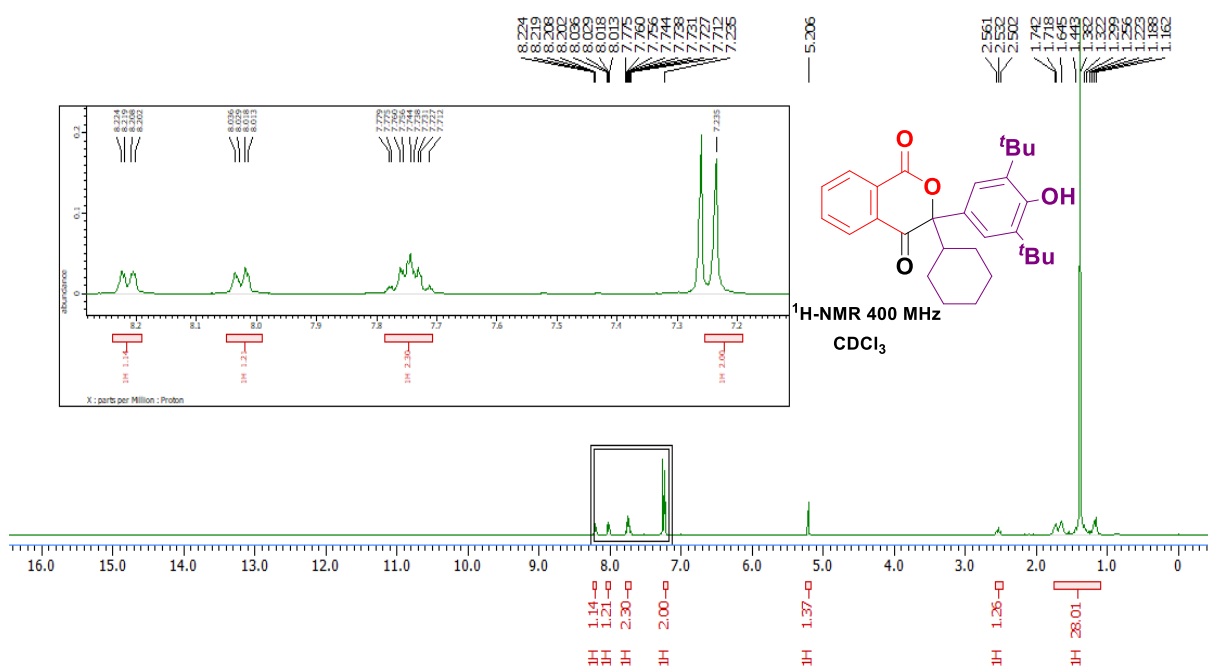


Fig. 30: <sup>1</sup>H-NMR spectrum of 3-cyclohexyl-3-(3,5-di-tert-butyl-4-hydroxyphenyl)isochroman-1,4-dione (3q)

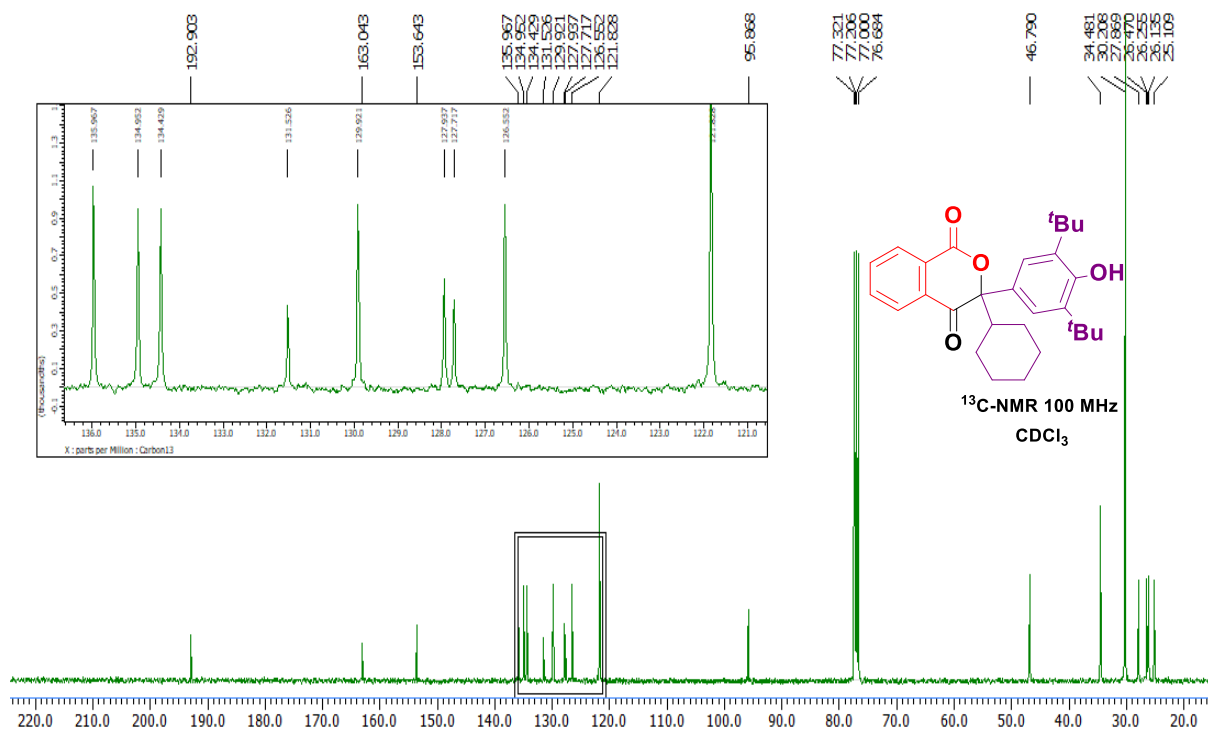
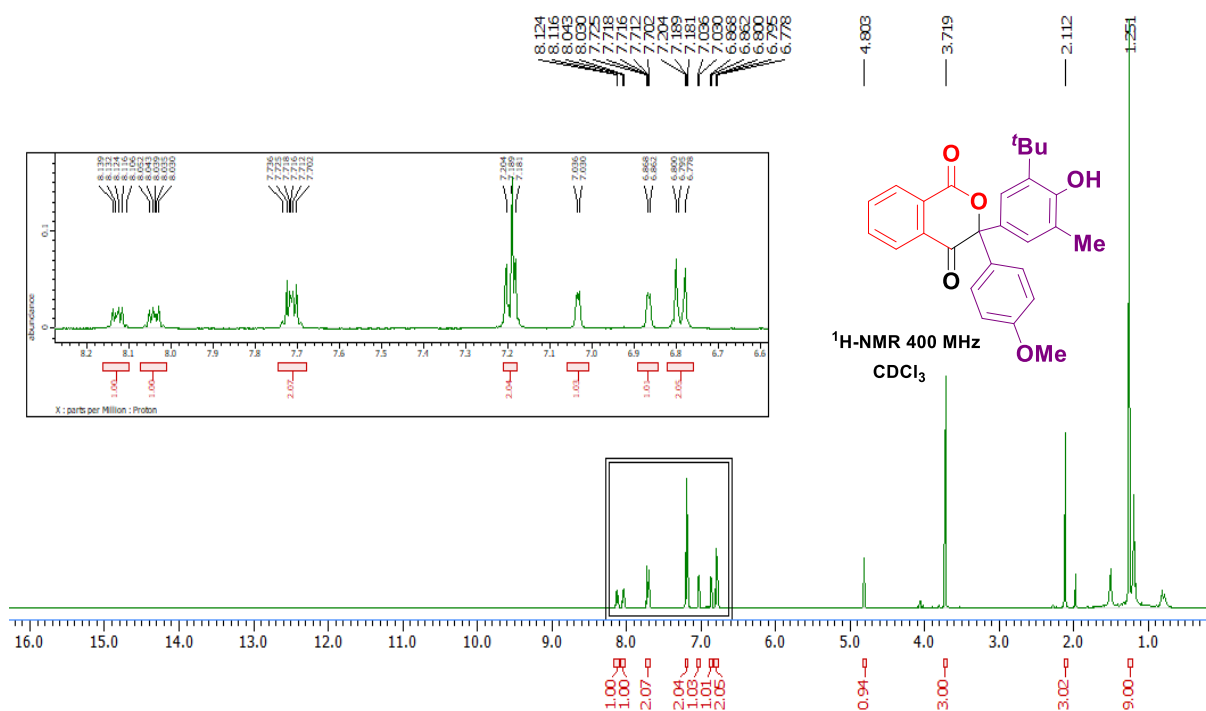
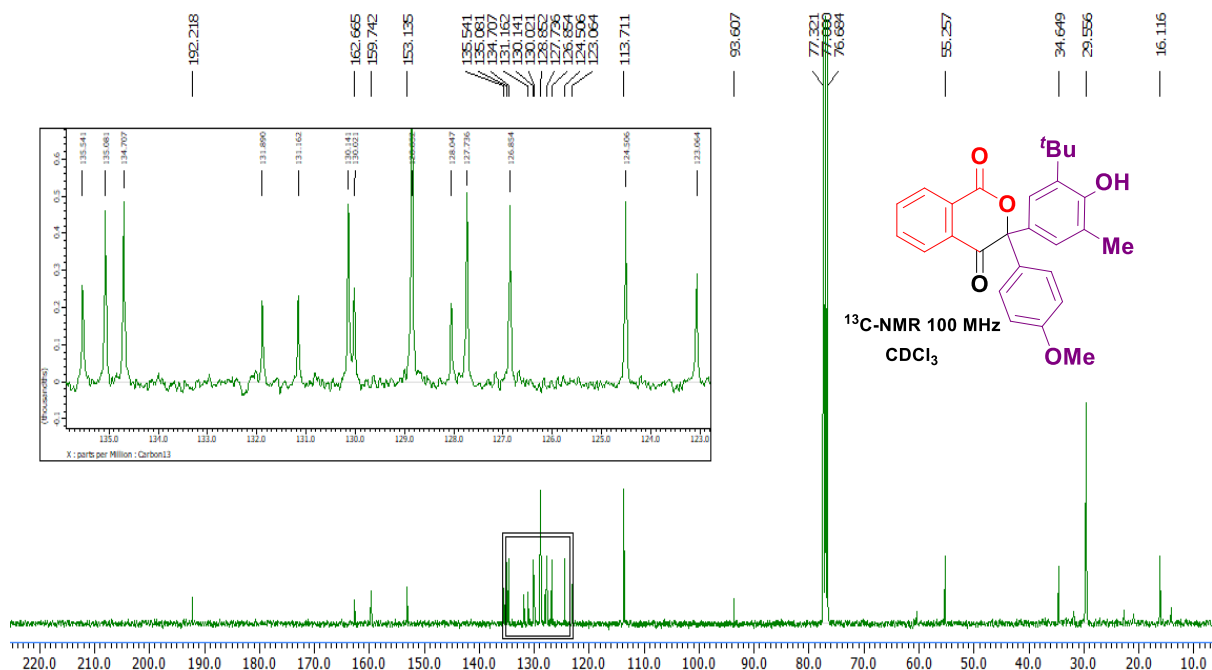


Fig. 31: <sup>13</sup>C-NMR spectrum of 3-cyclohexyl-3-(3,5-di-tert-butyl-4-hydroxyphenyl)isochroman-1,4-dione (3q)



**Fig. 32: <sup>1</sup>H-NMR spectrum of 3-(3-(*tert*-butyl-4-hydroxy-5-methylphenyl))-3-phenylisochroman-1,4-dione (**3r**)**



**Fig. 33: <sup>13</sup>C-NMR spectrum of 3-(3-(*tert*-butyl-4-hydroxy-5-methylphenyl))-3-phenylisochroman-1,4-dione (**3r**)**

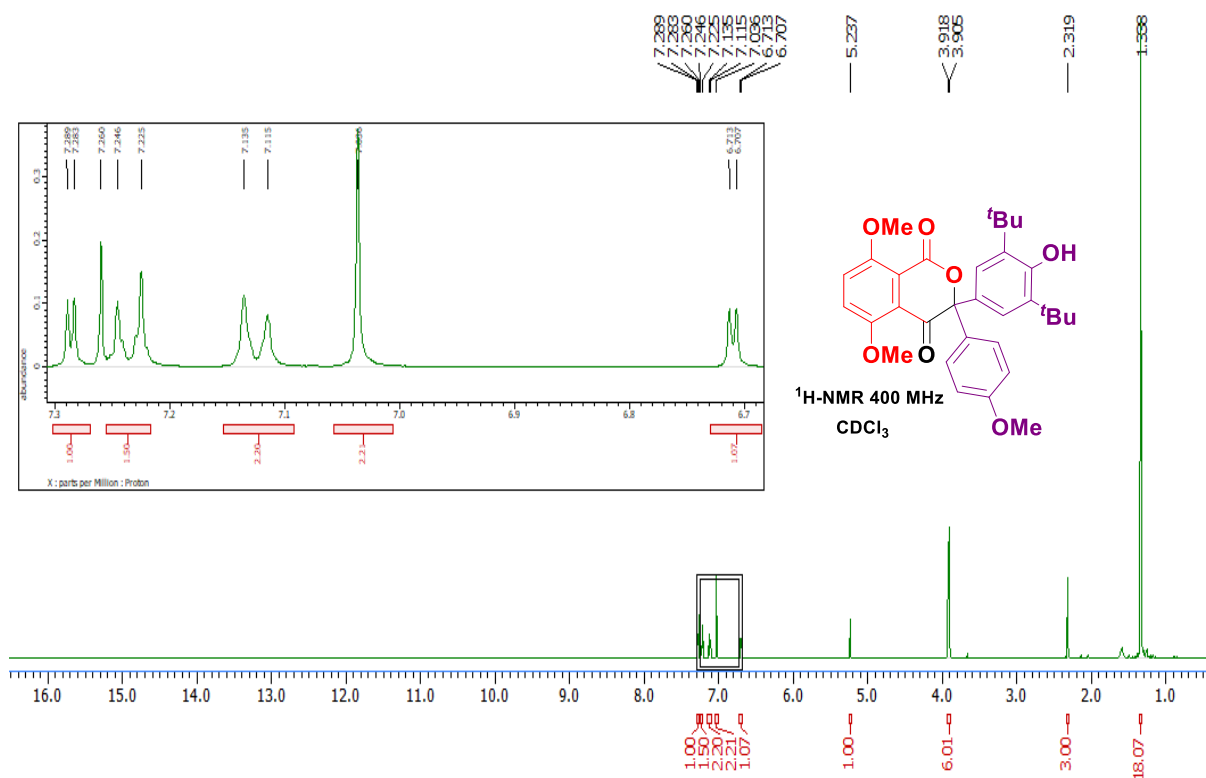


Fig. 34: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)-5,8-dimethoxy-3-phenylisochroman-1,4-dione (3s)

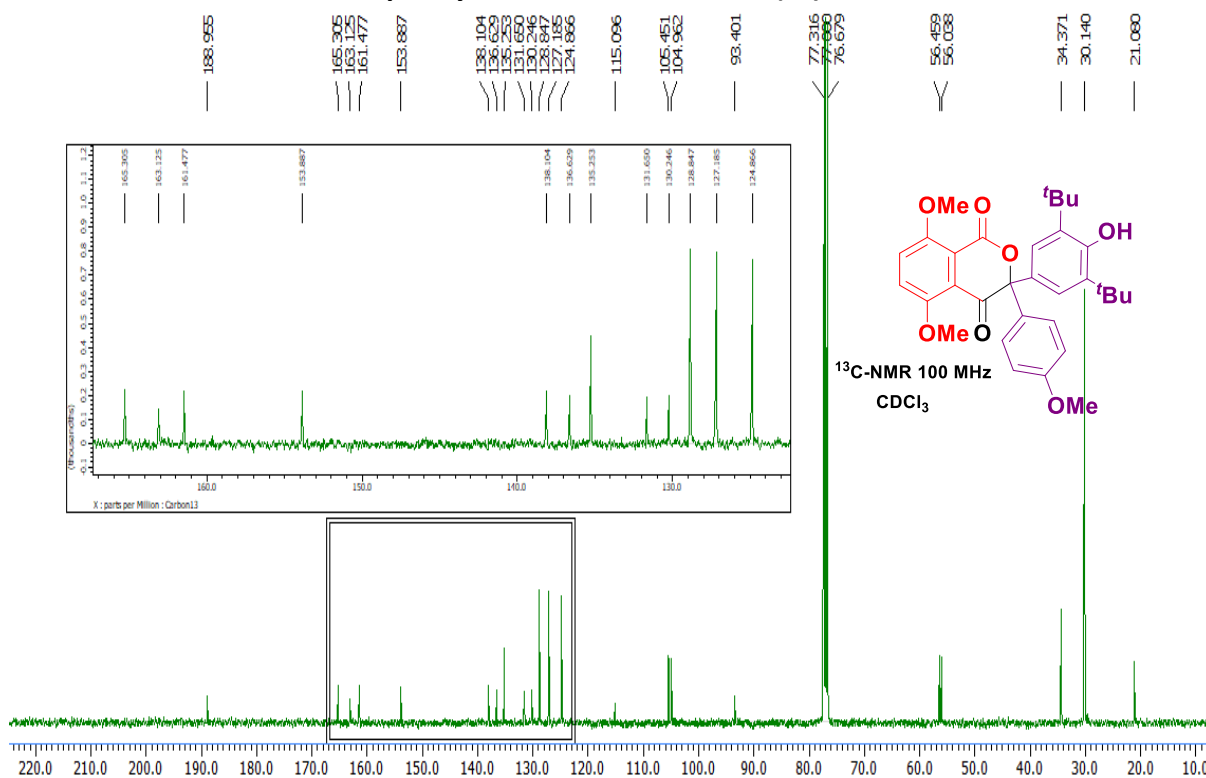


Fig. 35: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)-5,8-dimethoxy-3-phenylisochroman-1,4-dione (3s)

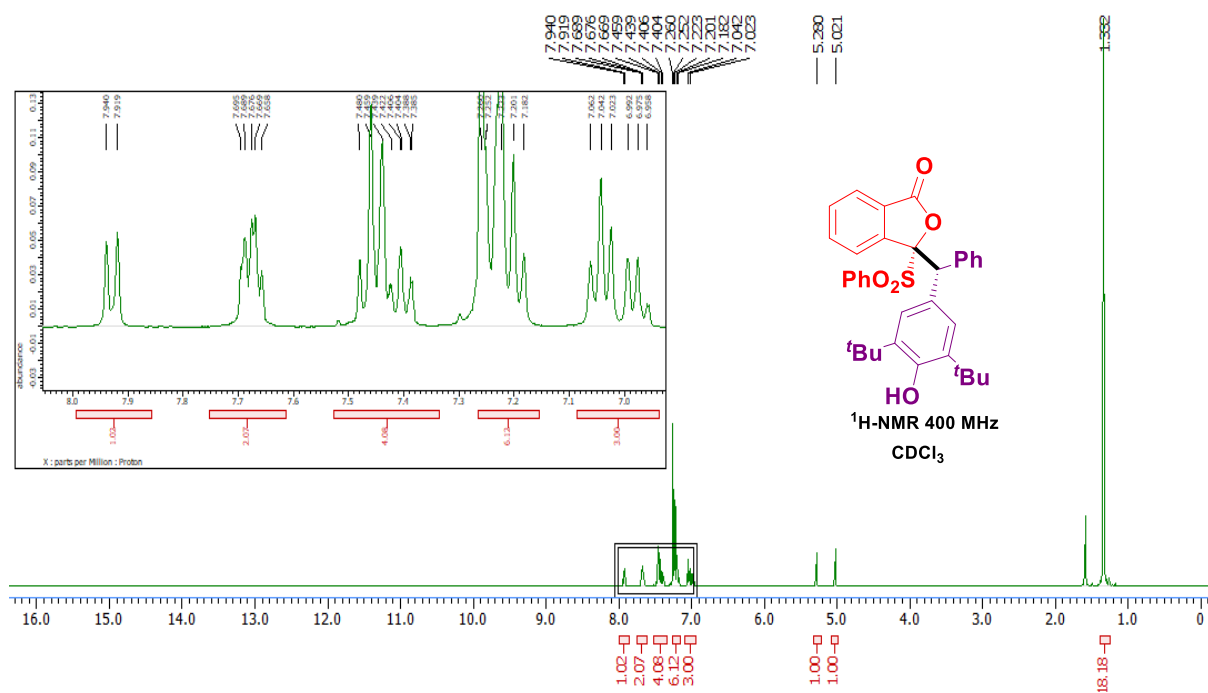


Fig. 36: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4a)

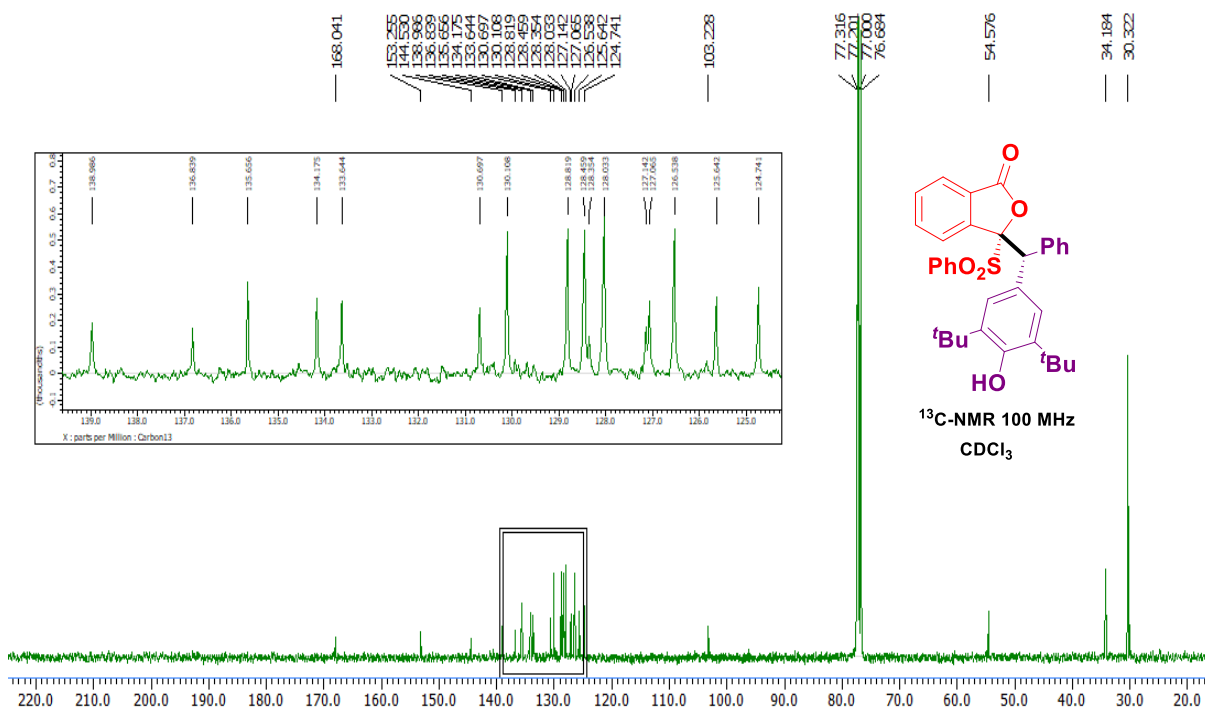


Fig. 37: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4a)

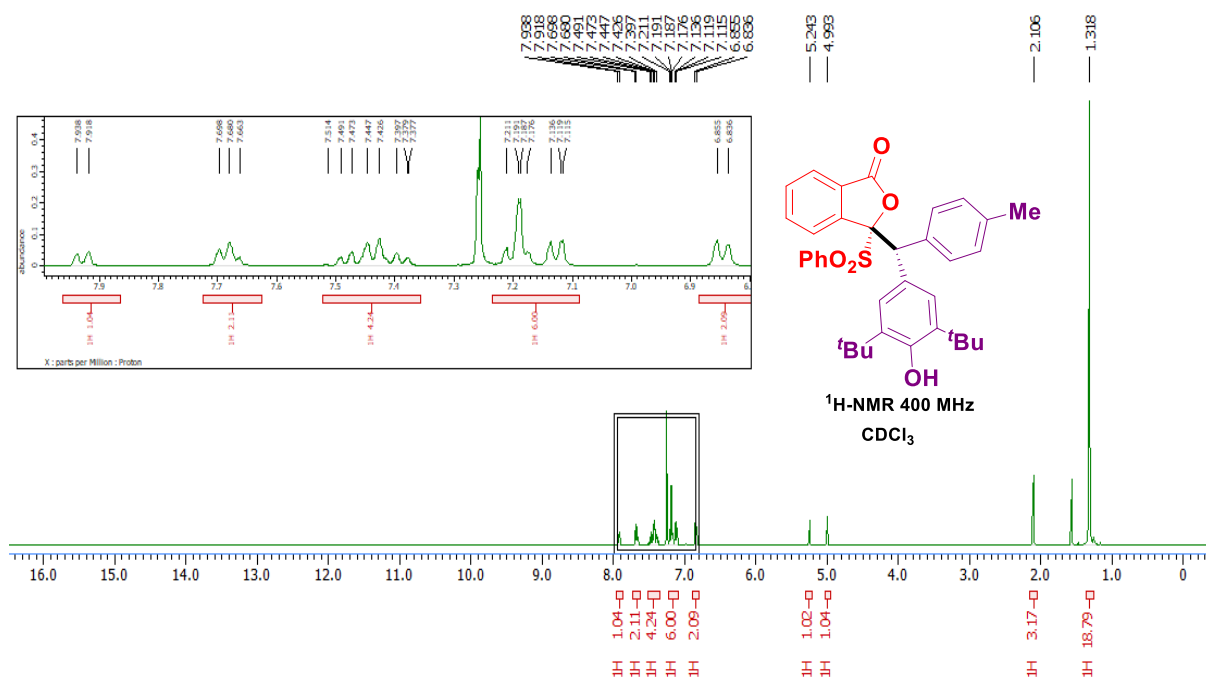


Fig. 38: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(p-tolyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (**4b**)

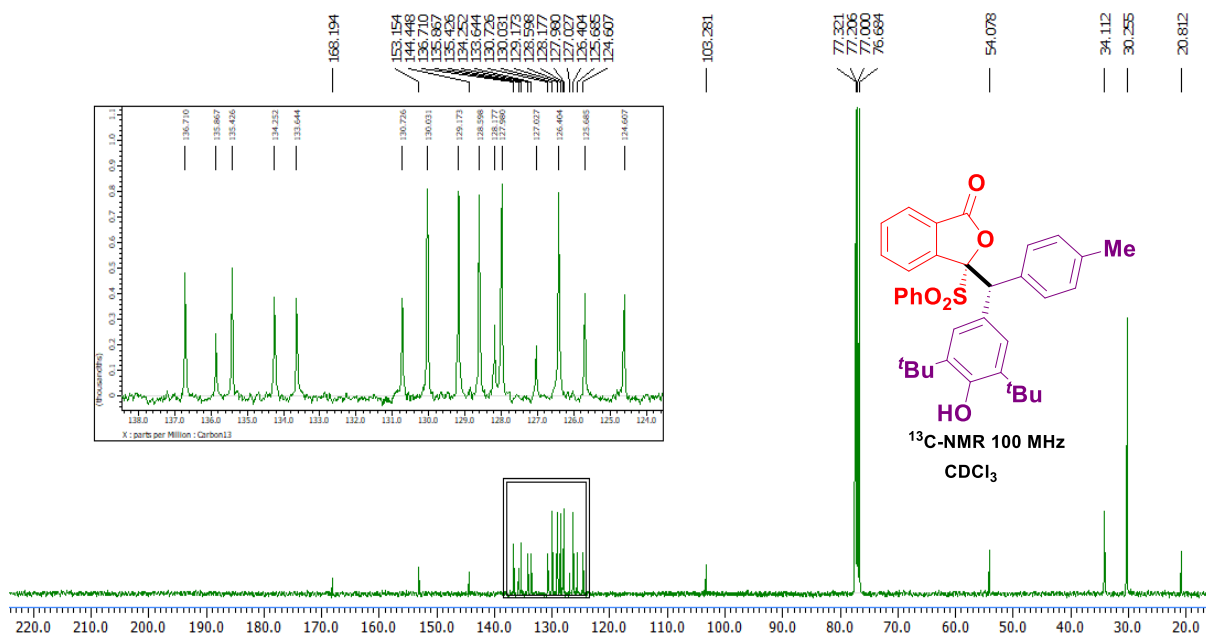
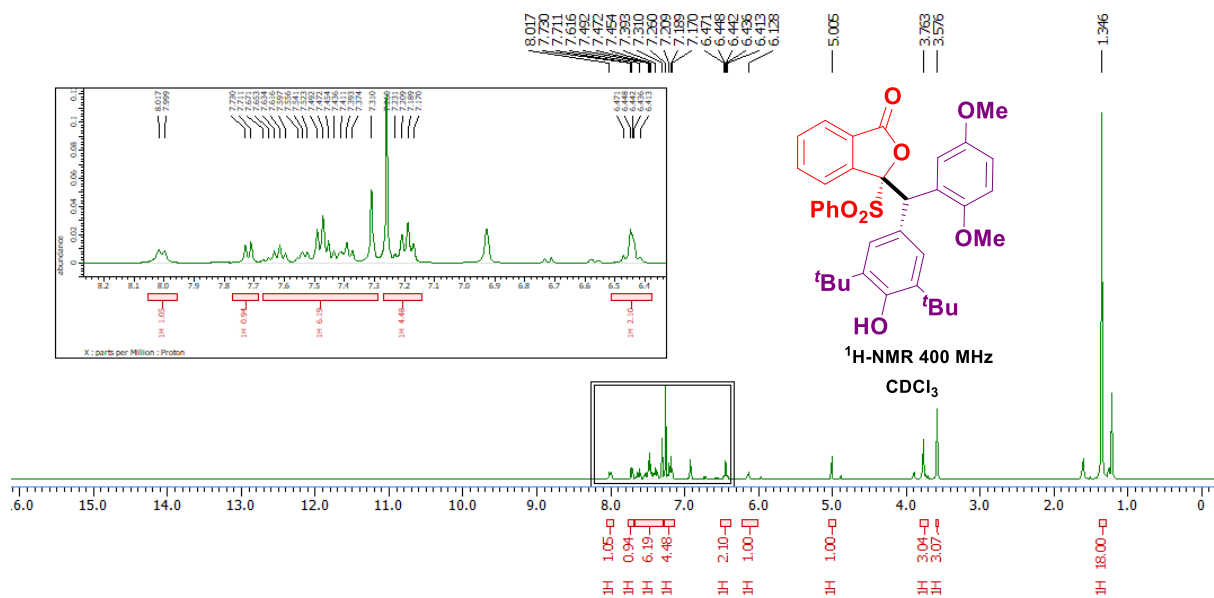
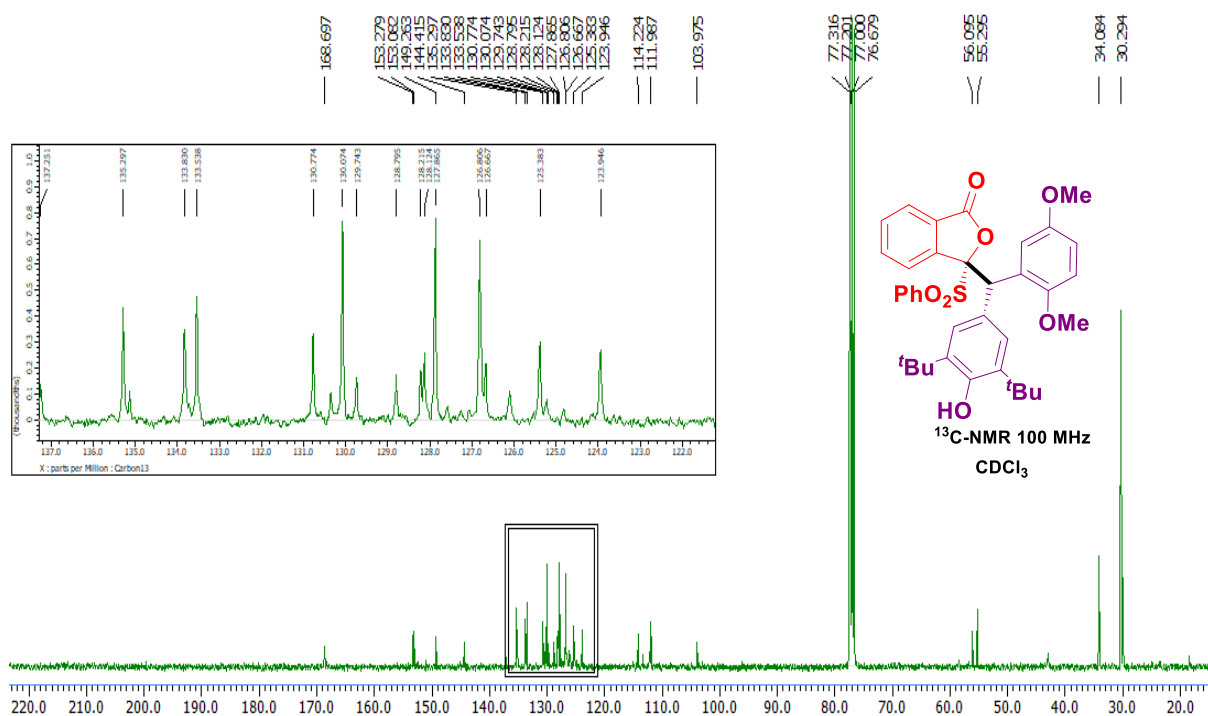


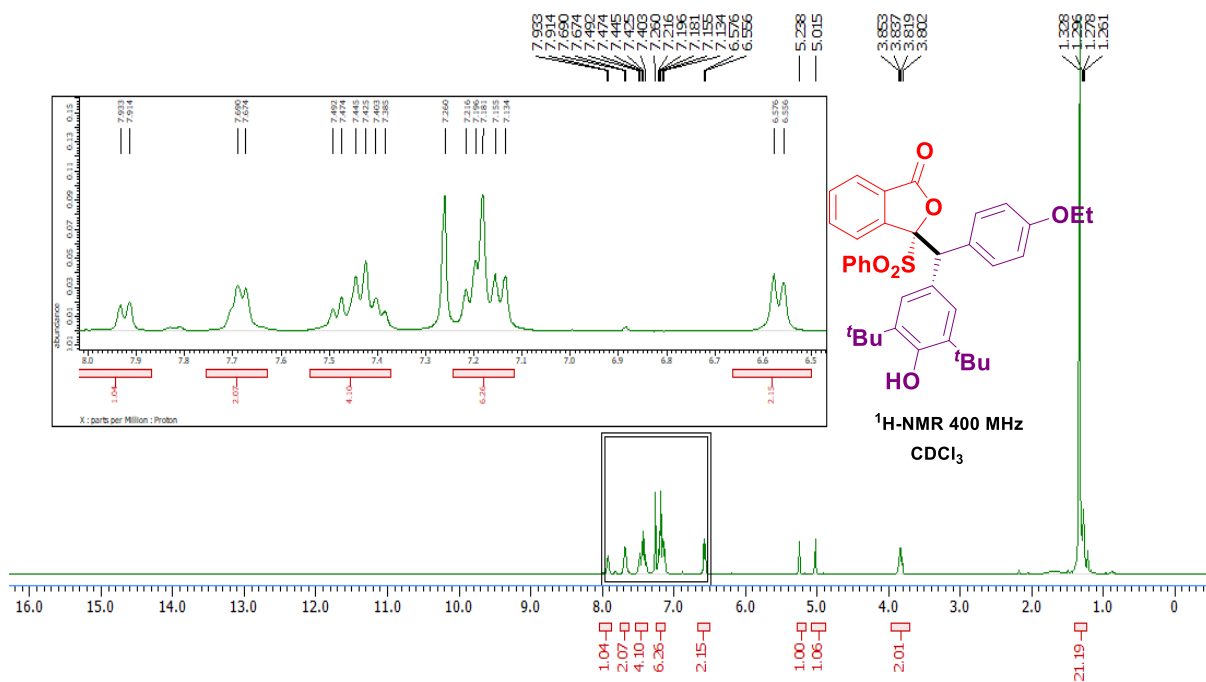
Fig. 39: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(p-tolyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (**4b**)



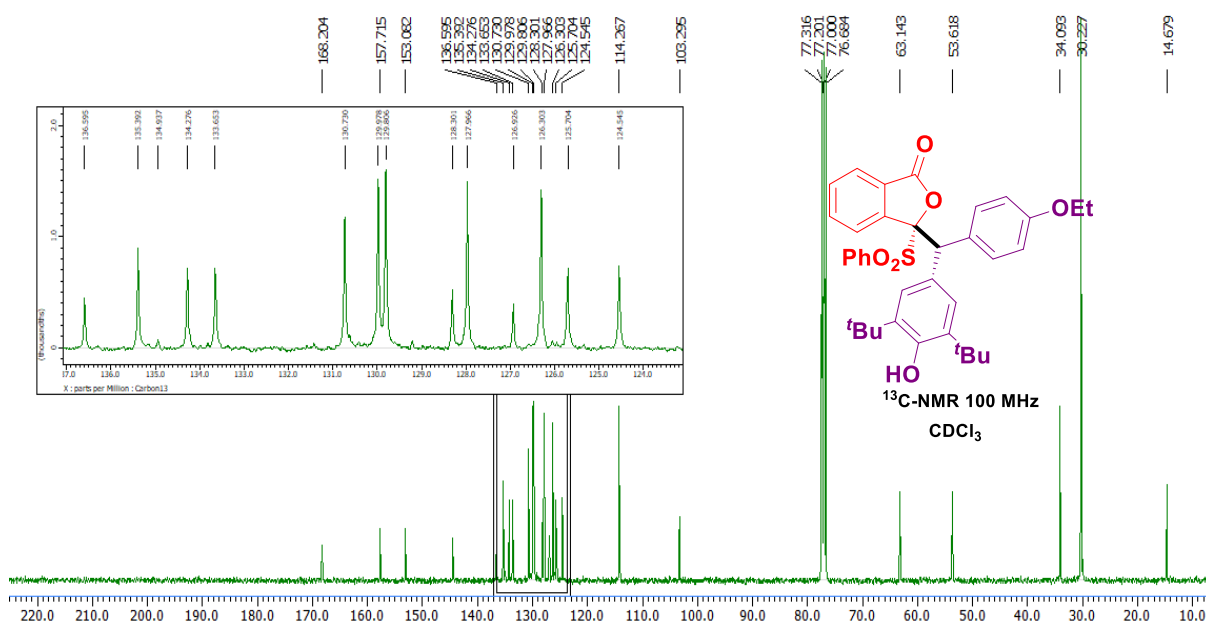
**Fig. 40:** <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(2,5-dimethoxyphenyl)methyl)-3-(phenylsulfonylisobenzofuran-1(3H)-one (4c)



**Fig. 41:** <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(2,5-dimethoxyphenyl)methyl)-3-(phenylsulfonylisobenzofuran-1(3H)-one (4c)

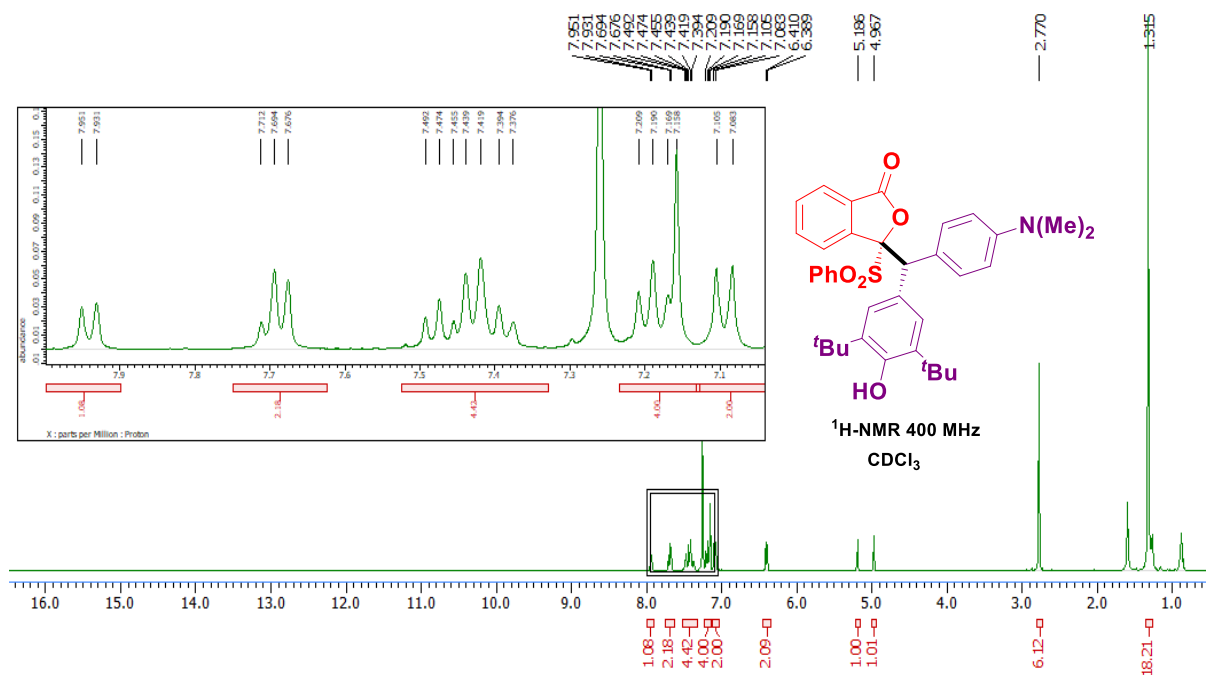


**Fig. 42:** <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(4-ethoxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4d)

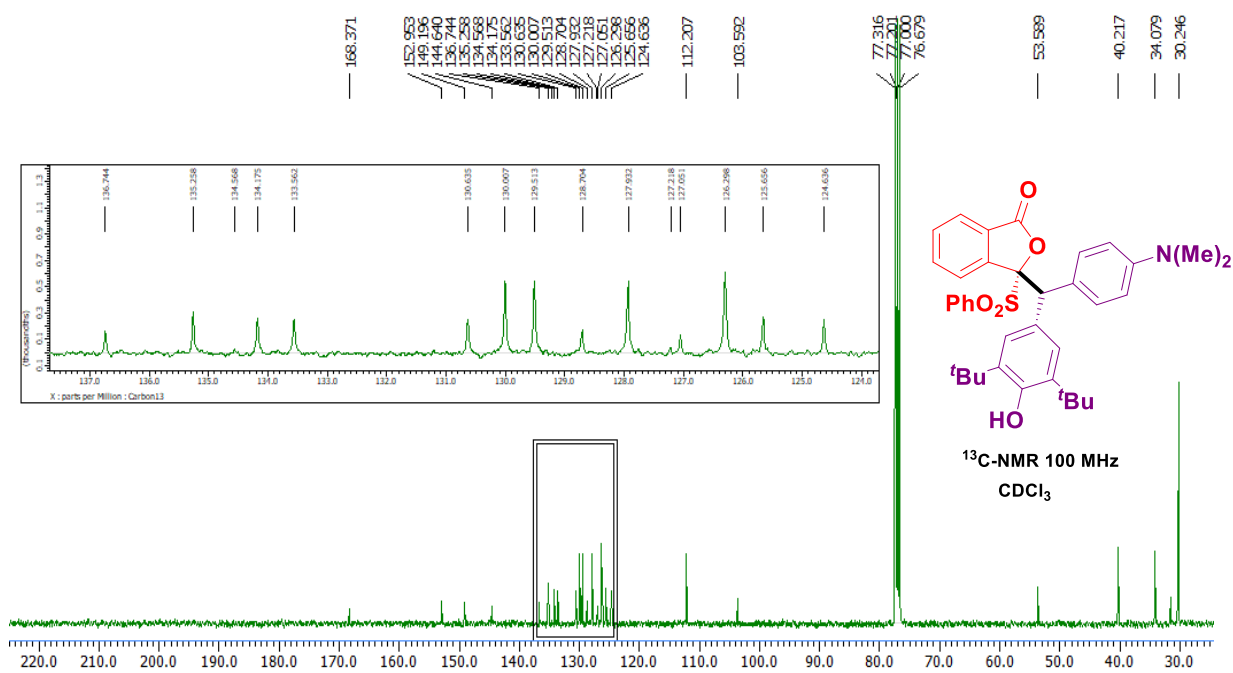


**Fig. 43:** <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(4-ethoxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4d)





**Fig. 44: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(4-dimethylamino)phenyl)methyl-3-henylsulfonyl)isobenzofuran-1(3H)-one (4e)**



**Fig. 45: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(4-dimethylamino)phenyl)methyl-3-henylsulfonyl)isobenzofuran-1(3H)-one (4e)**

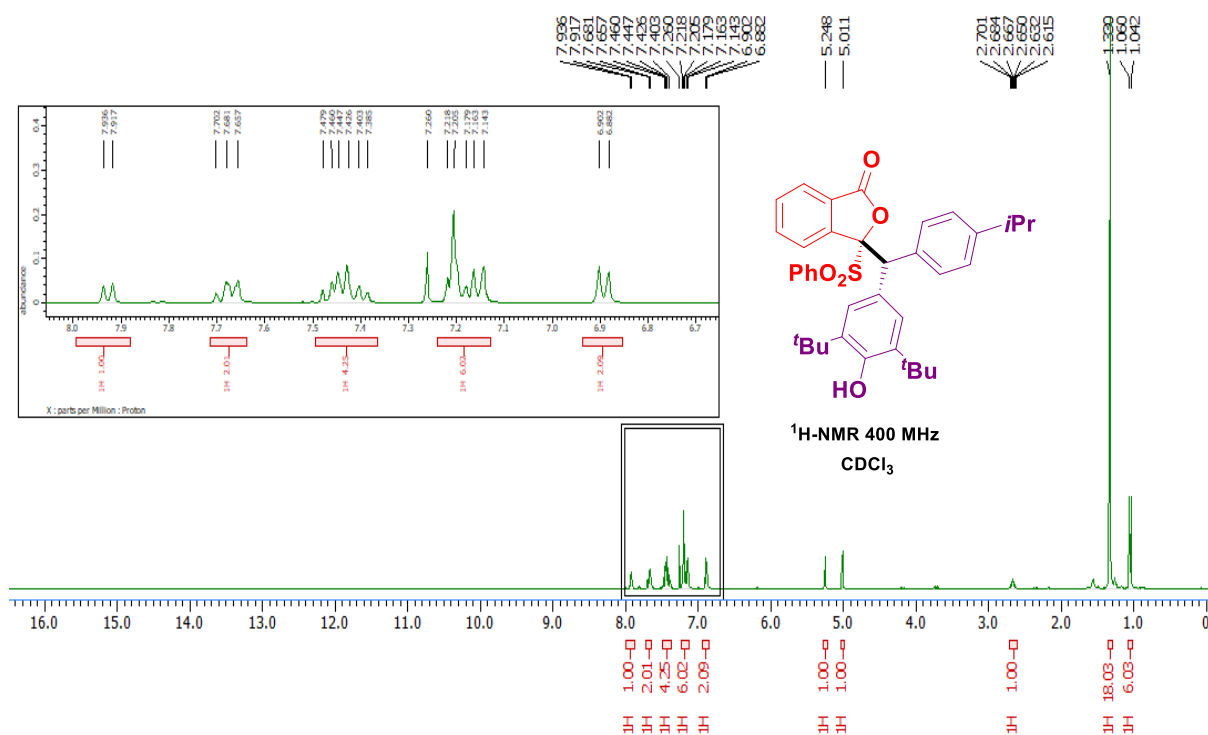


Fig. 46: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(4-isopropylphenyl)methyl)-3-henylsulfonyl)isobenzofuran-1(3H)-one (4f)

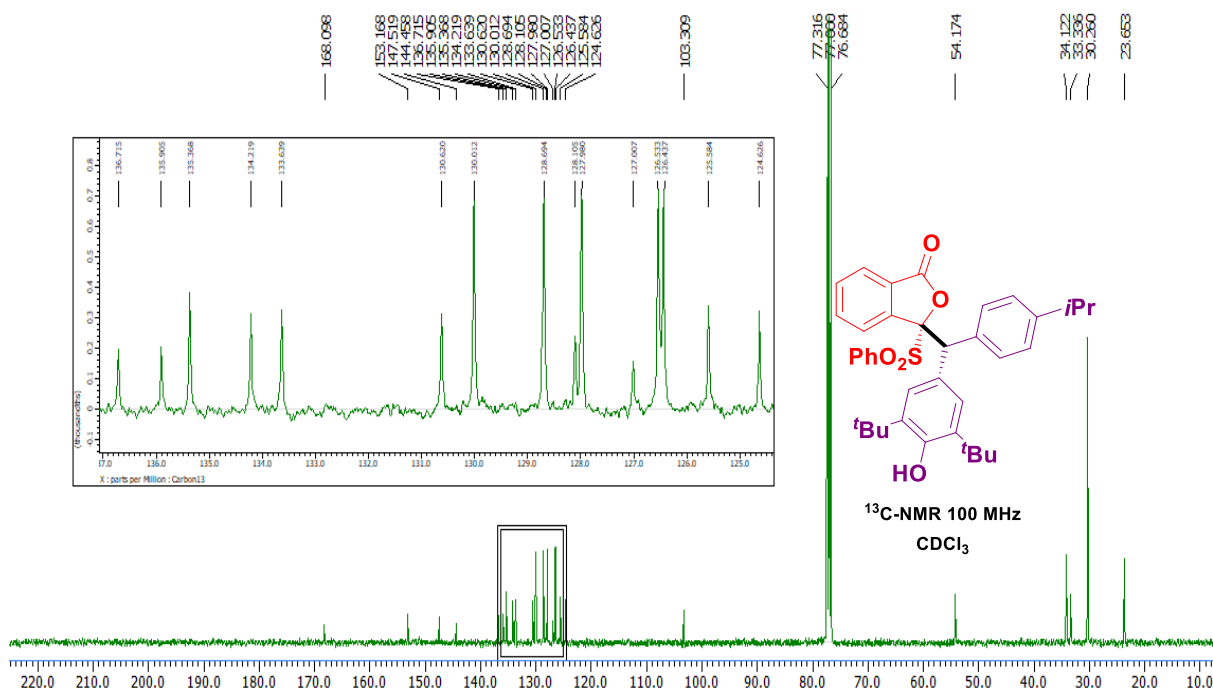
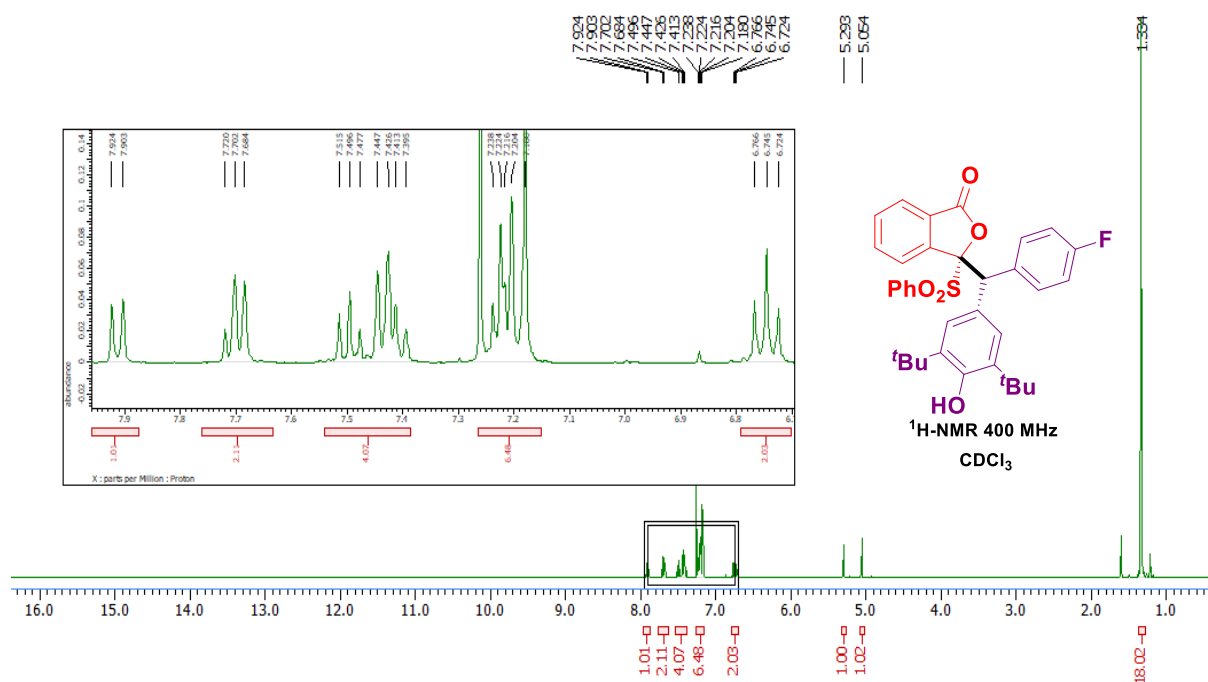
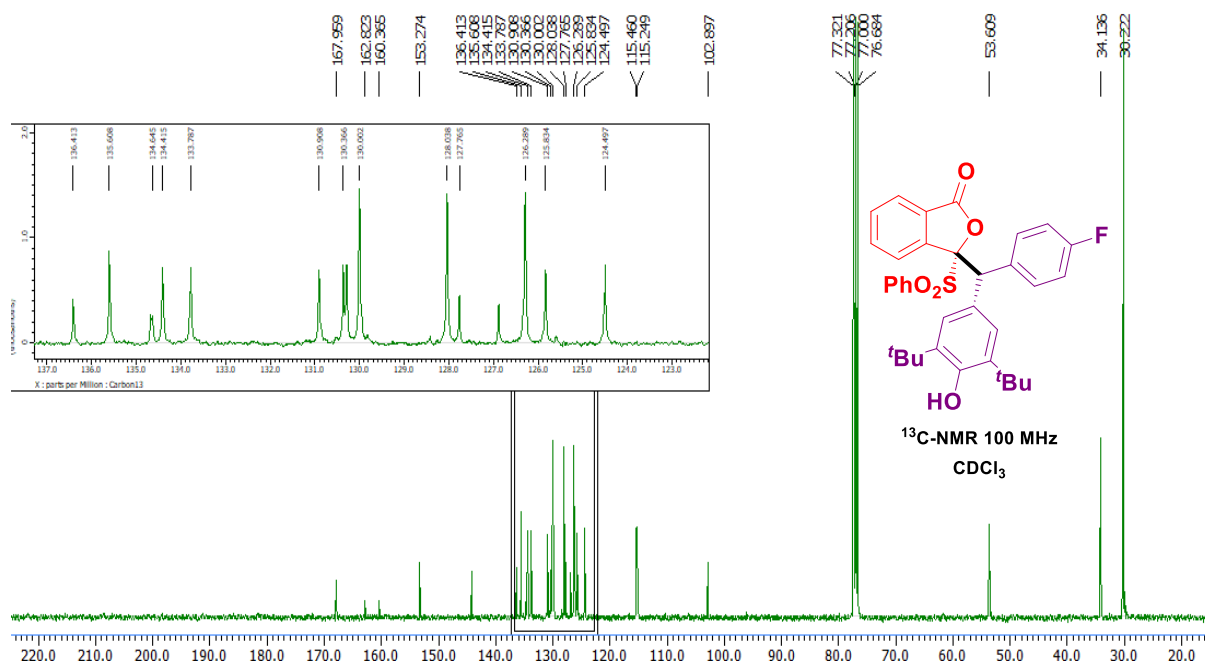


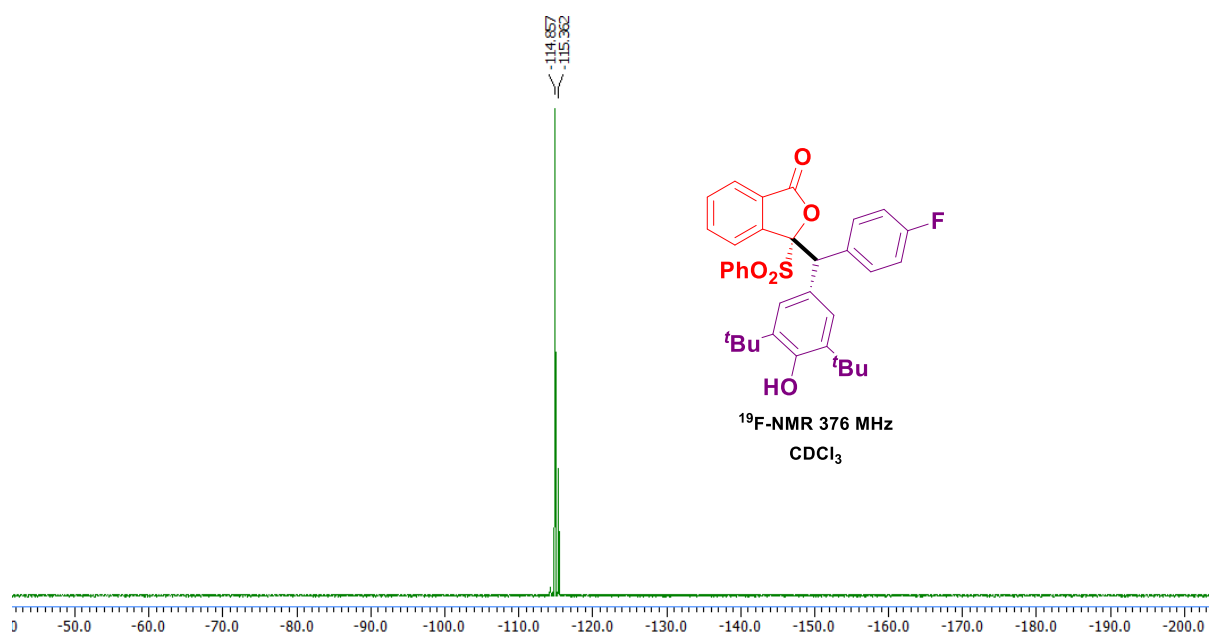
Fig. 47: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(4-isopropylphenyl)methyl)-3-henylsulfonyl)isobenzofuran-1(3H)-one (4f)



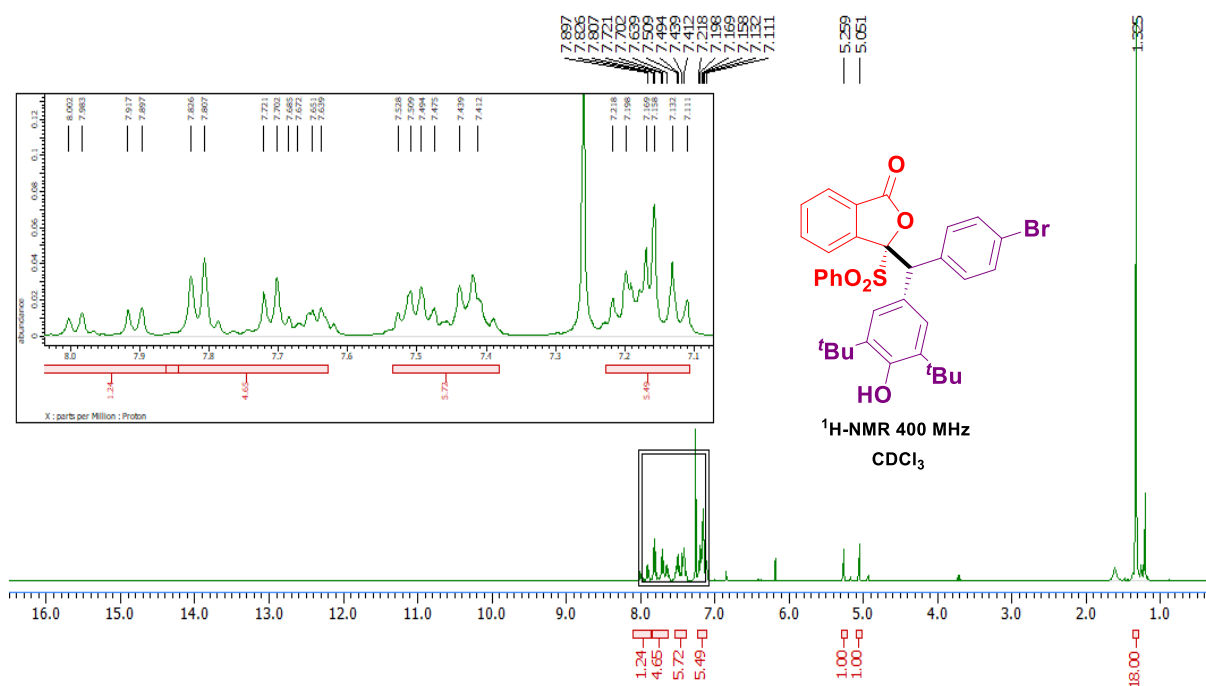
**Fig. 48: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(4-fluorophenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4i)**



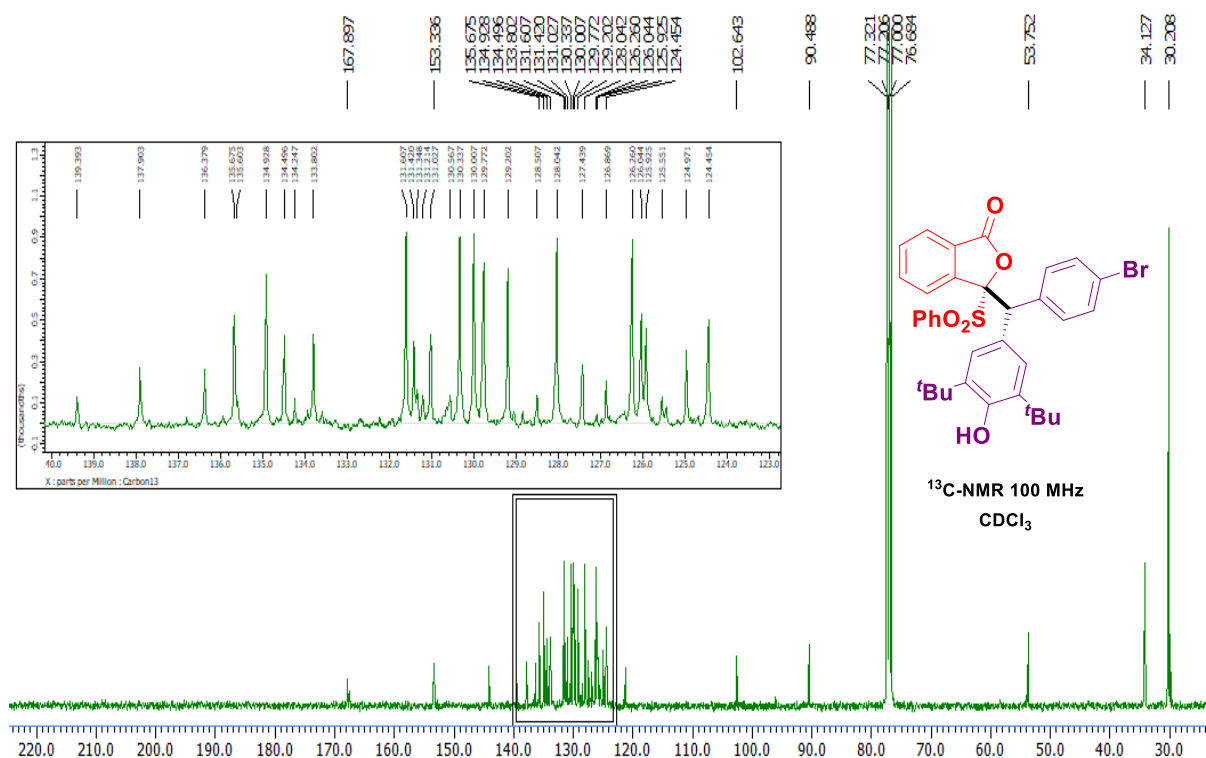
**Fig. 49: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(4-fluorophenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4i)**



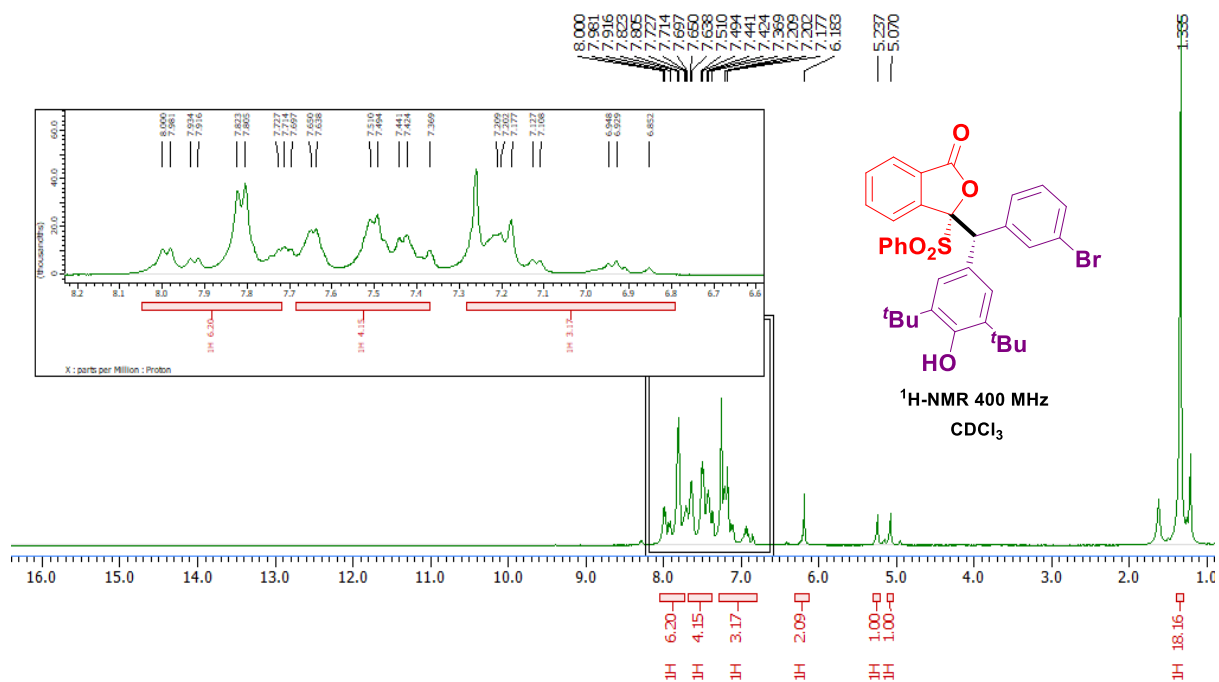
**Fig. 50:**  $^{19}\text{F-NMR}$  spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(4-fluorophenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4i)



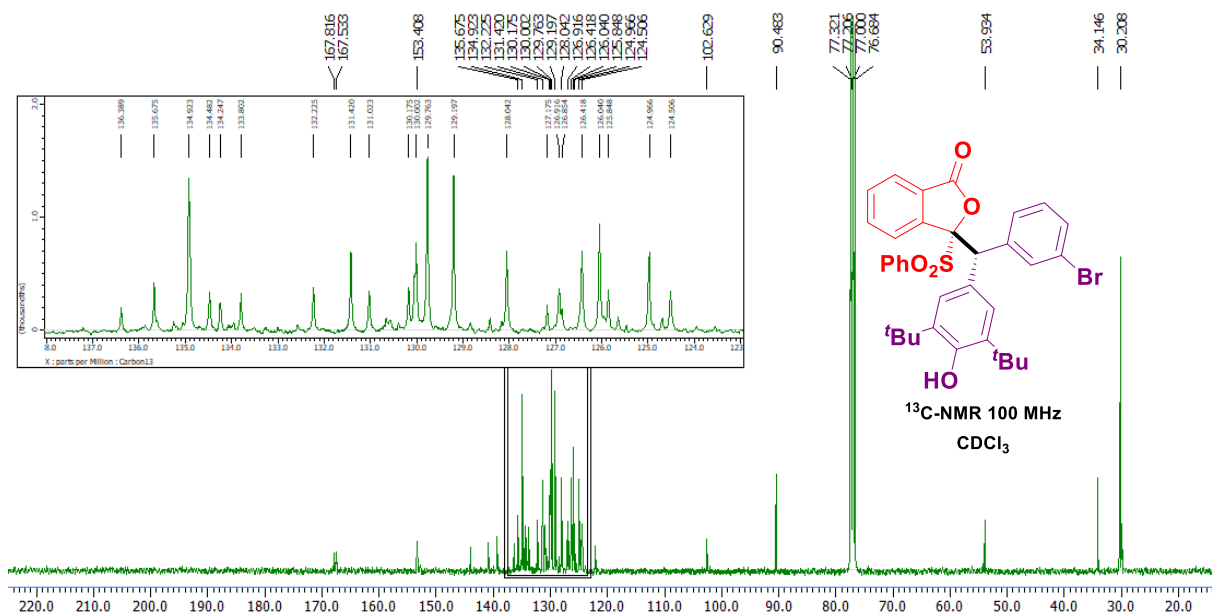
**Fig. 51: <sup>1</sup>H-NMR spectrum of 3-((4-bromophenyl)(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4j)**



**Fig. 52: <sup>13</sup>C-NMR spectrum of 3-((4-bromophenyl)(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4j)**



**Fig. 53:** <sup>1</sup>H-NMR spectrum of 3-((3-bromophenyl)(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4k)



**Fig. 54:** <sup>13</sup>C-NMR spectrum of 3-((3-bromophenyl)(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4k)

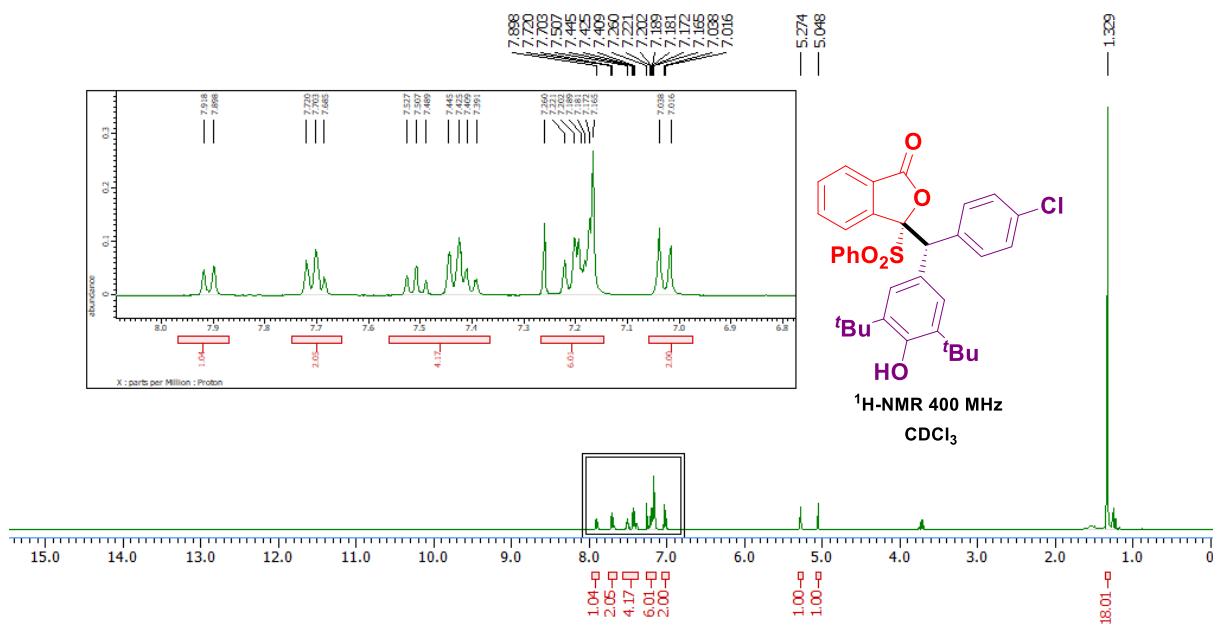


Fig. 55: <sup>1</sup>H-NMR spectrum of 3-((4-chlorophenyl)3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl) isobenzofuran-1(3H)-one (4l)

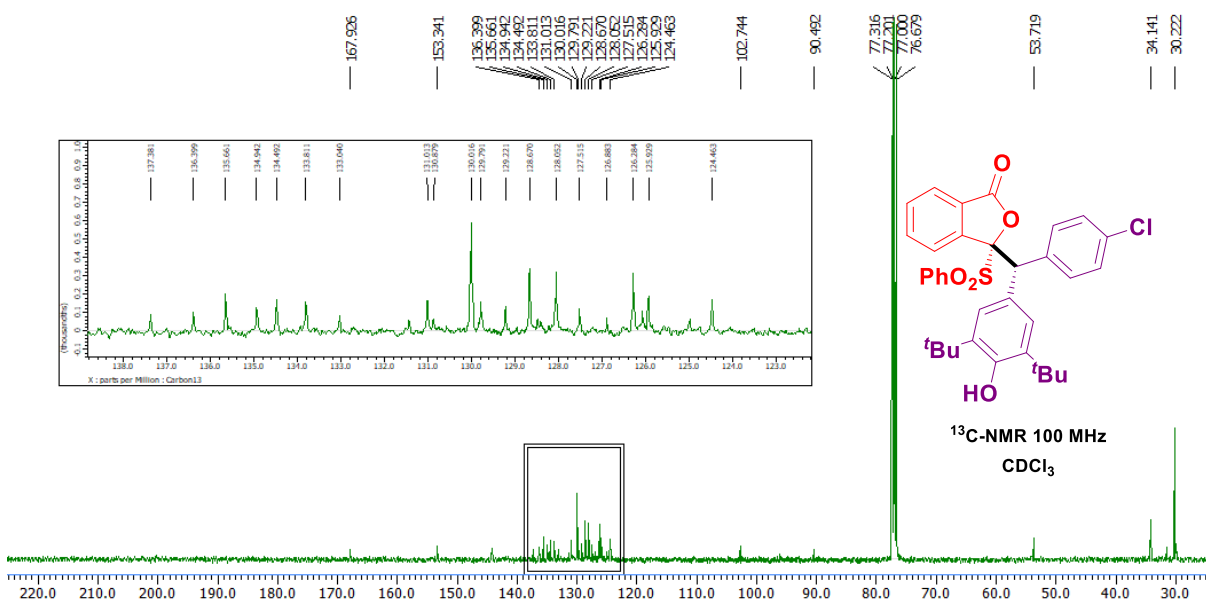


Fig. 56: <sup>13</sup>C-NMR spectrum of 3-((4-chlorophenyl)3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl) isobenzofuran-1(3H)-one (4l)

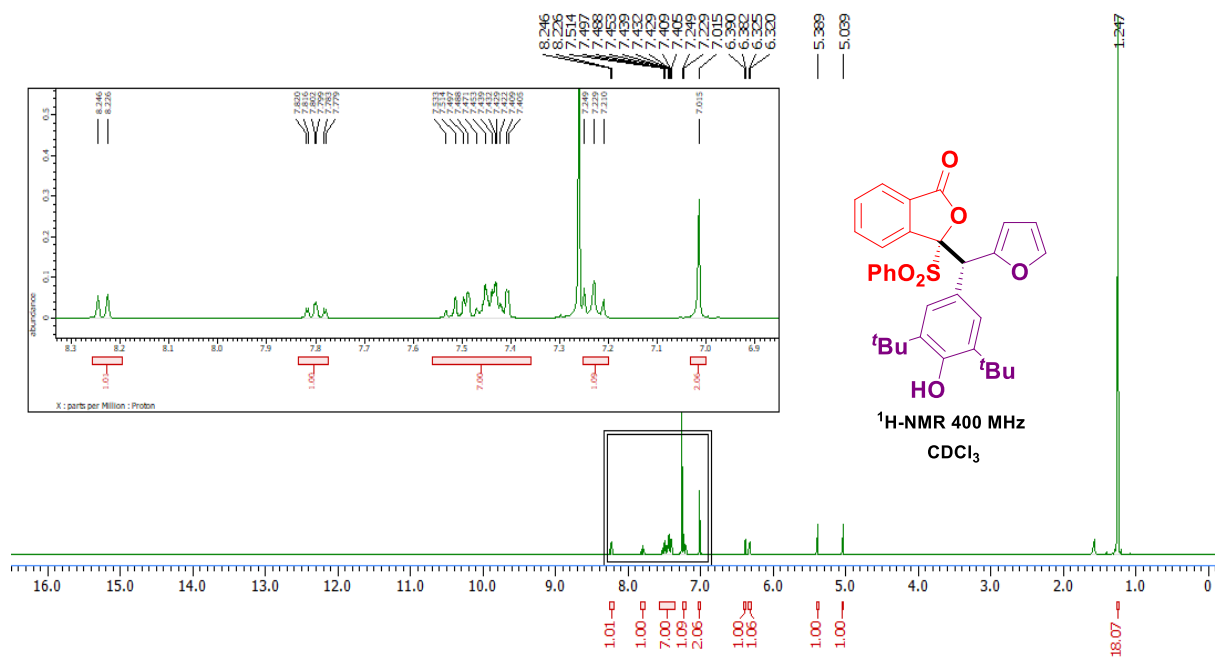


Fig. 57: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(furan-2-yl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4m)

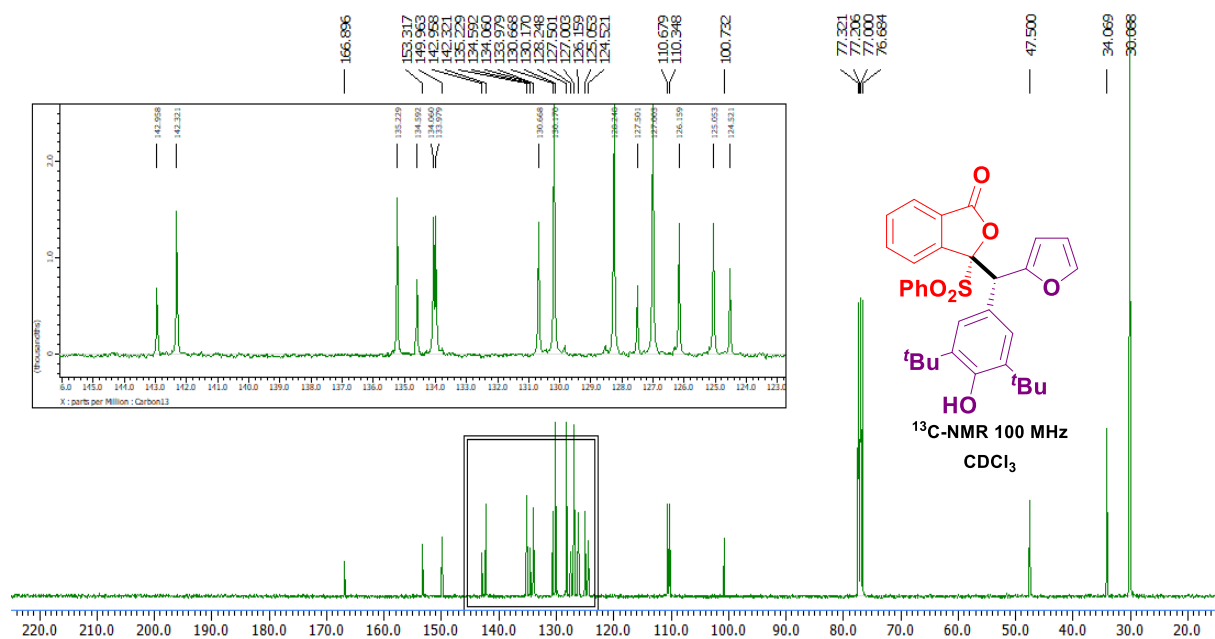


Fig. 58: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(furan-2-yl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4m)



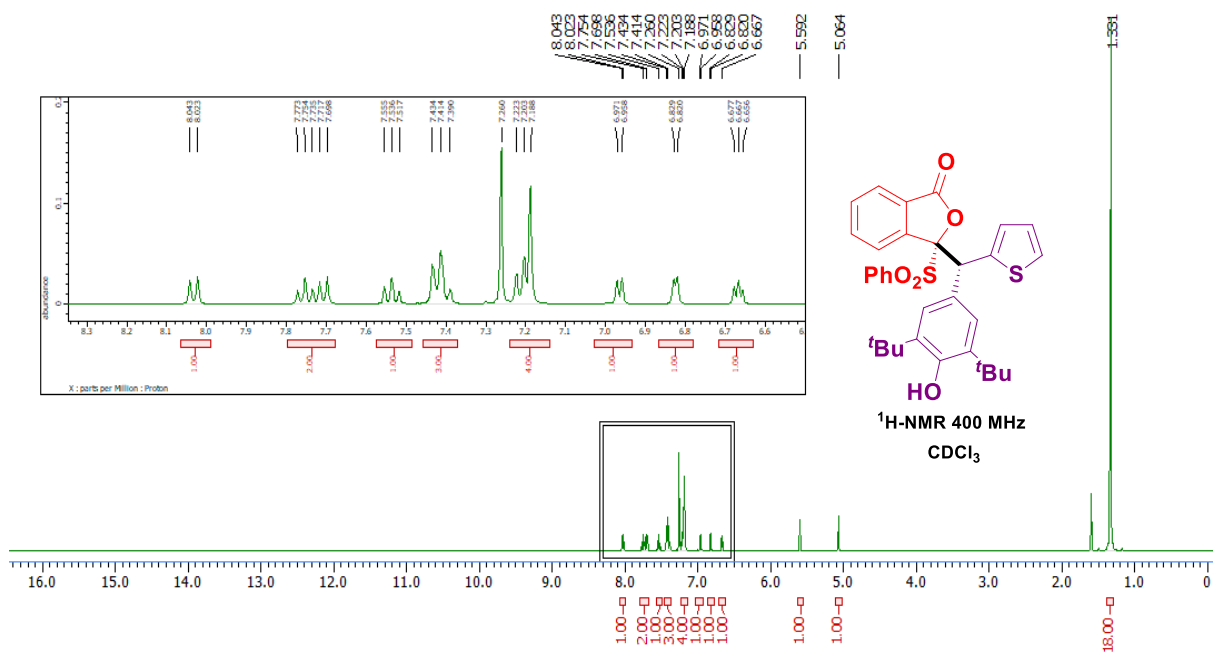


Fig. 59: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(thiophen-2-yl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4n)

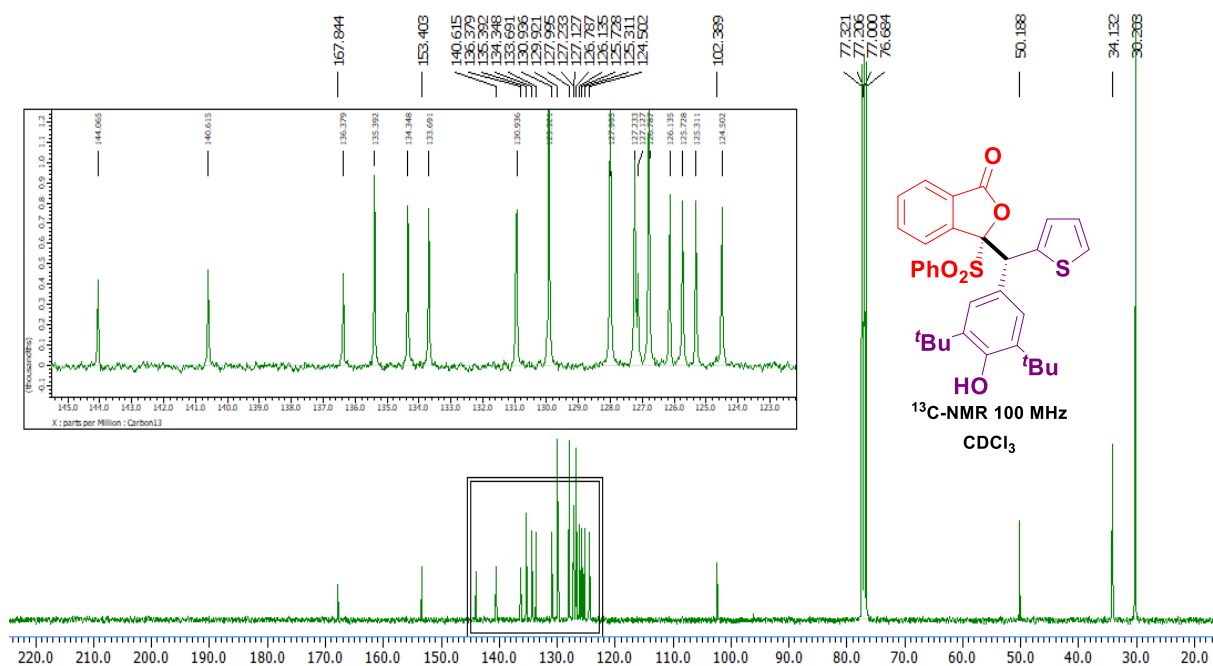


Fig. 60: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(thiophen-2-yl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4n)

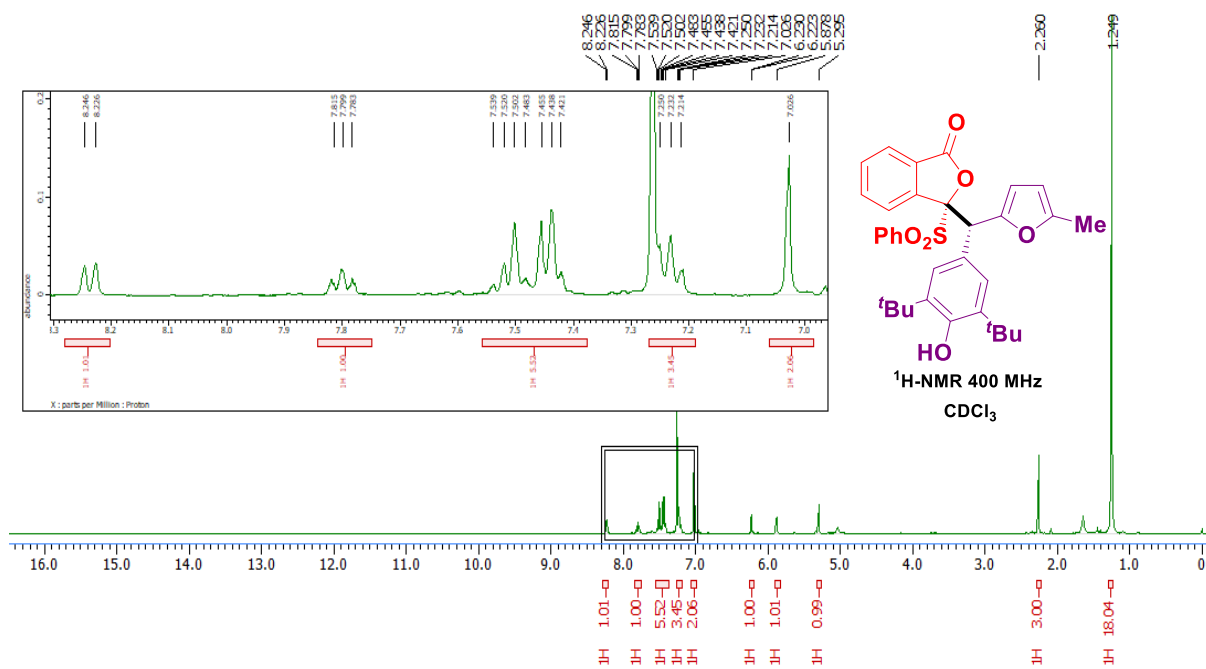


Fig. 61: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(5-methylfuran-2-yl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4o)

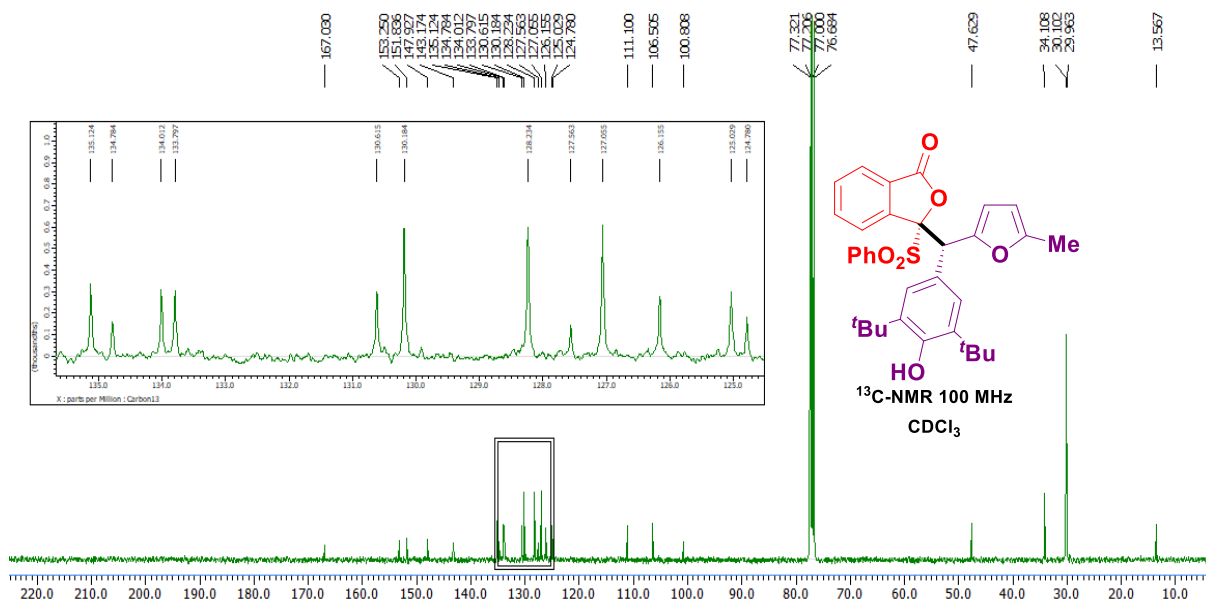


Fig. 62: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(5-methylfuran-2-yl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4o)

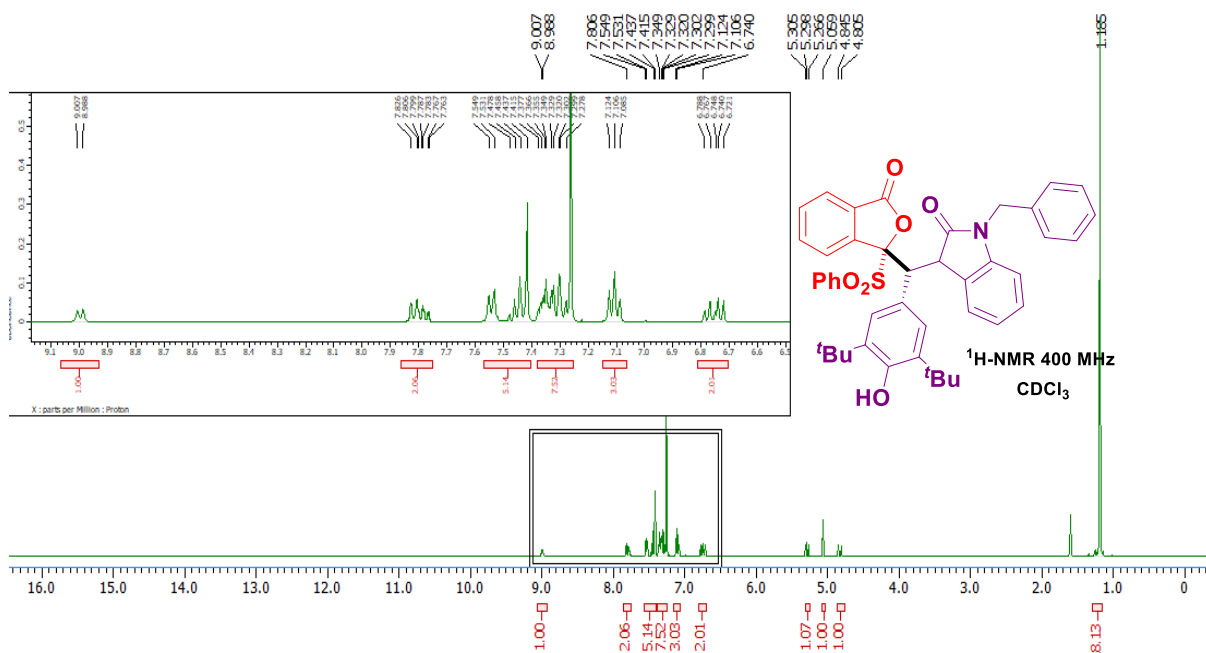


Fig. 63: <sup>1</sup>H-NMR spectrum of 1-benzyl-2-(3,5-di-tert-butyl-4-hydroxyphenyl)-2-(3-oxo-1-(phenylsulfonyl)1,3dihydroisobenzofuran-1-yl)indolin-3-one (4p)

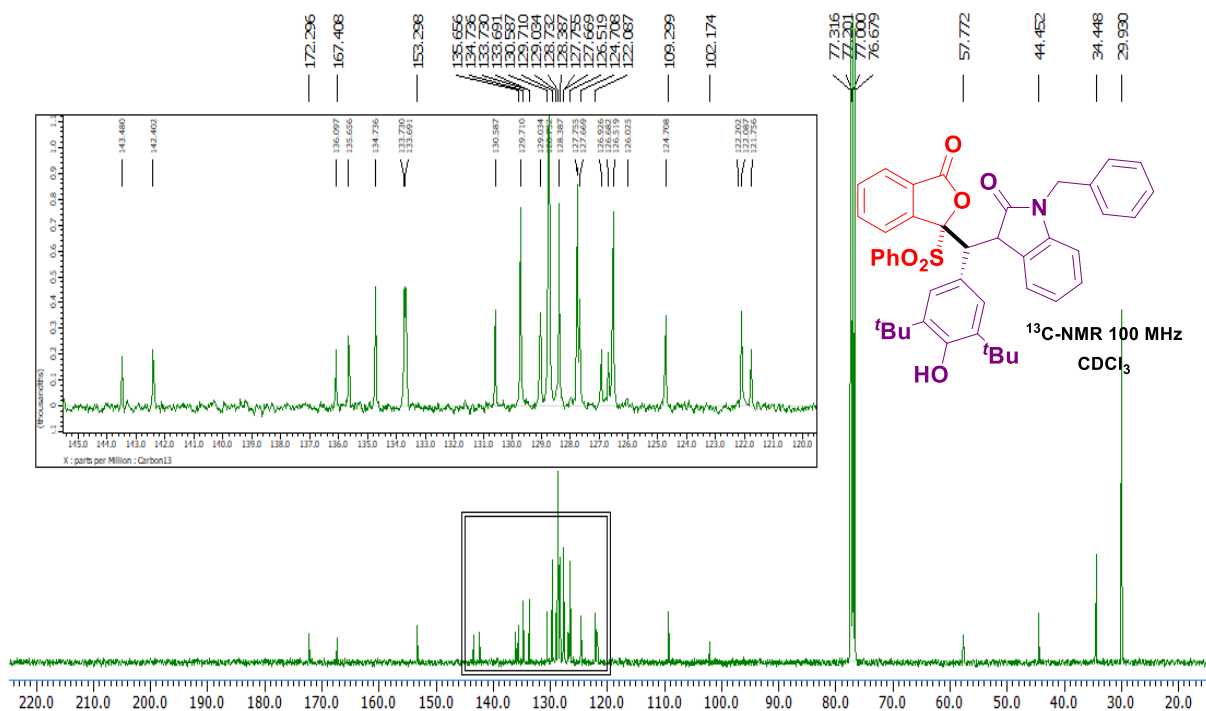
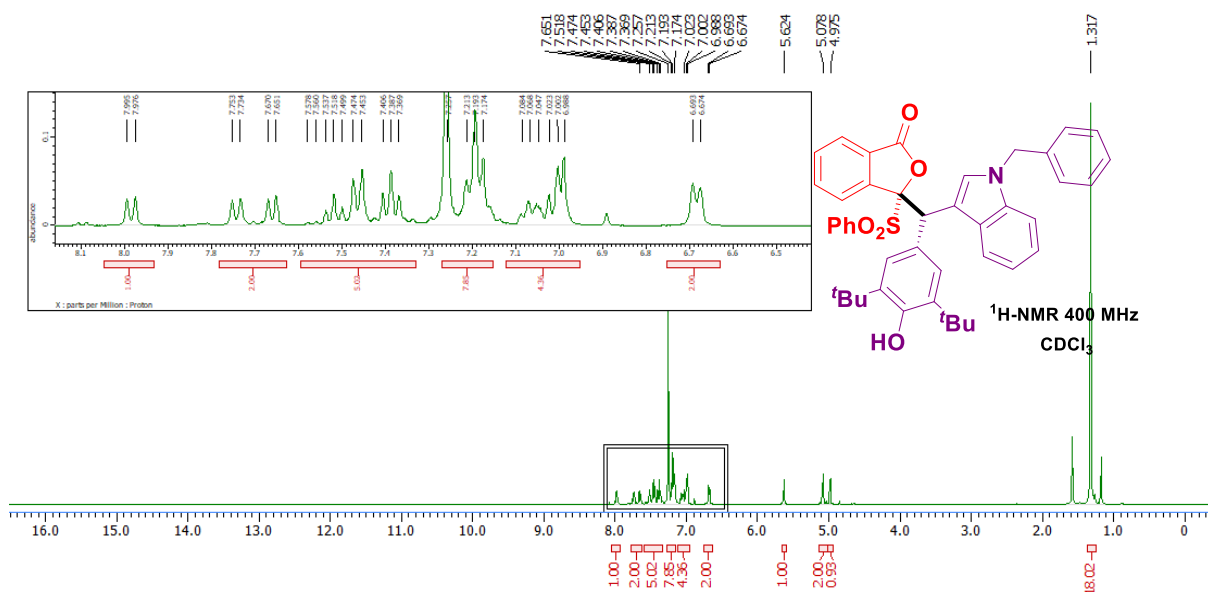
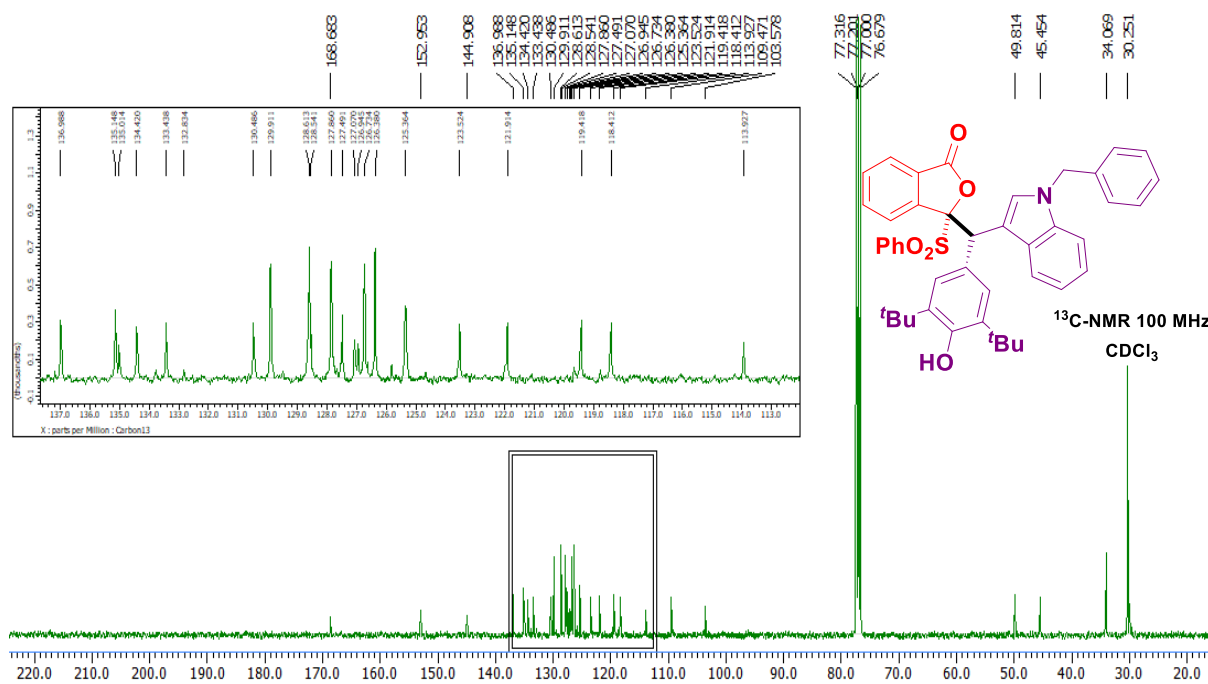


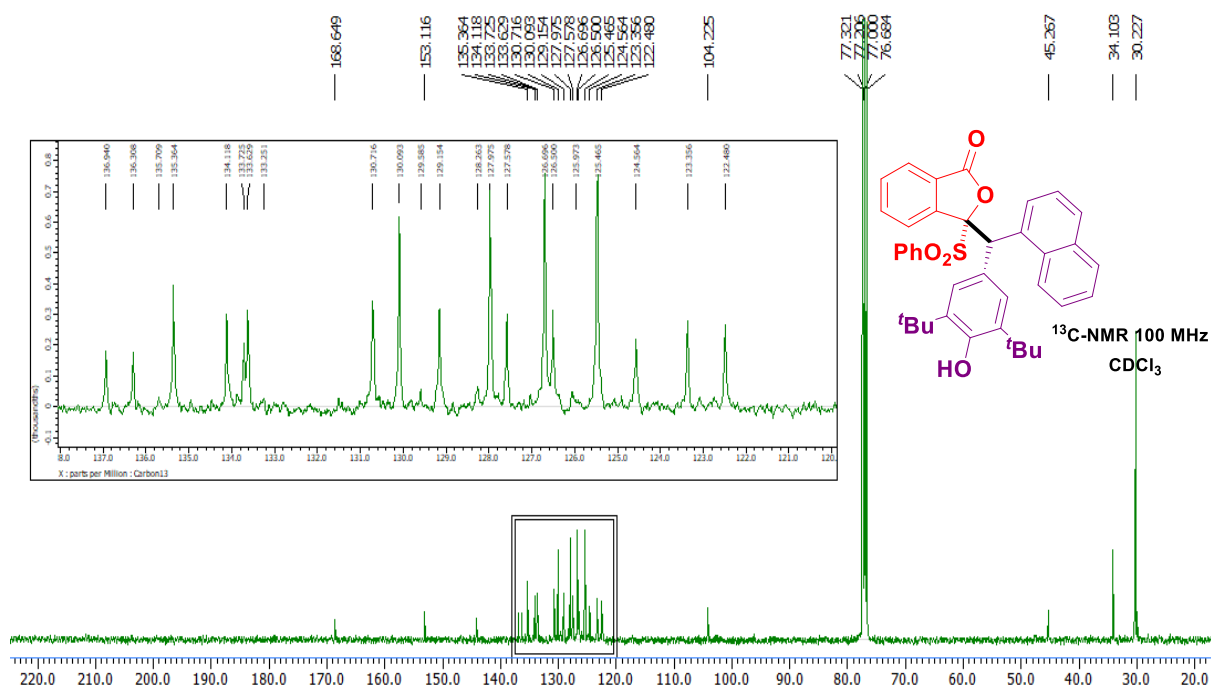
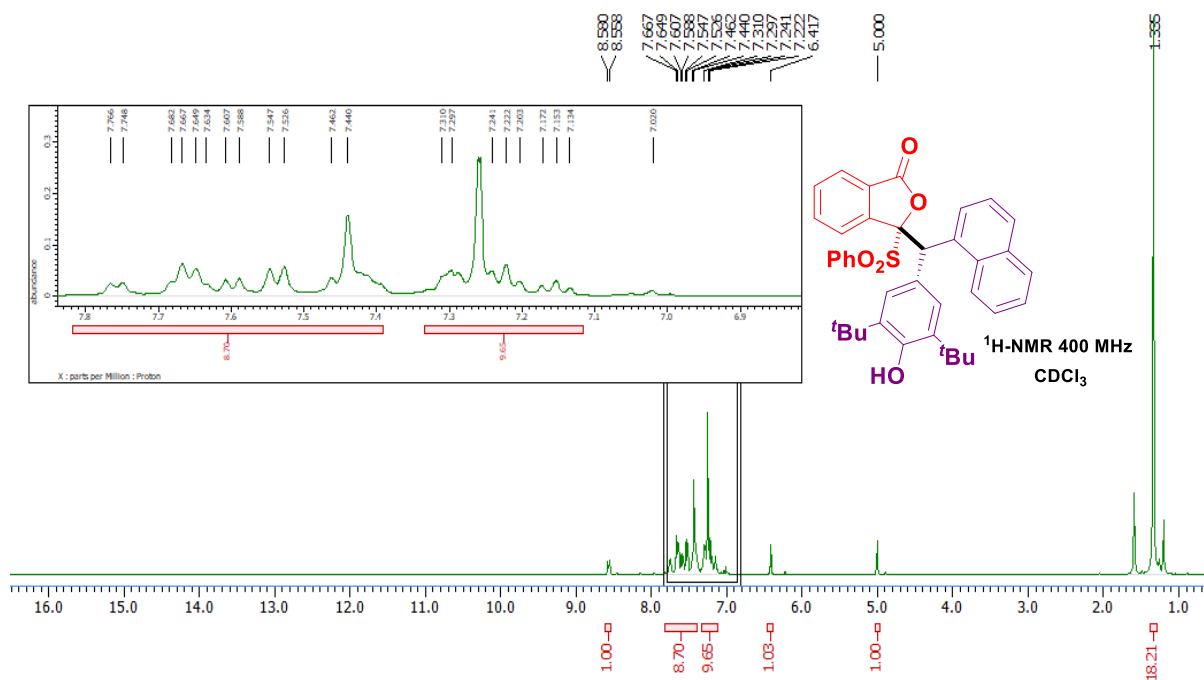
Fig. 64: <sup>13</sup>C-NMR spectrum of 1-benzyl-2-(3,5-di-tert-butyl-4-hydroxyphenyl)-2-(3-oxo-1-(phenylsulfonyl)1,3dihydroisobenzofuran-1-yl)indolin-3-one (4p)

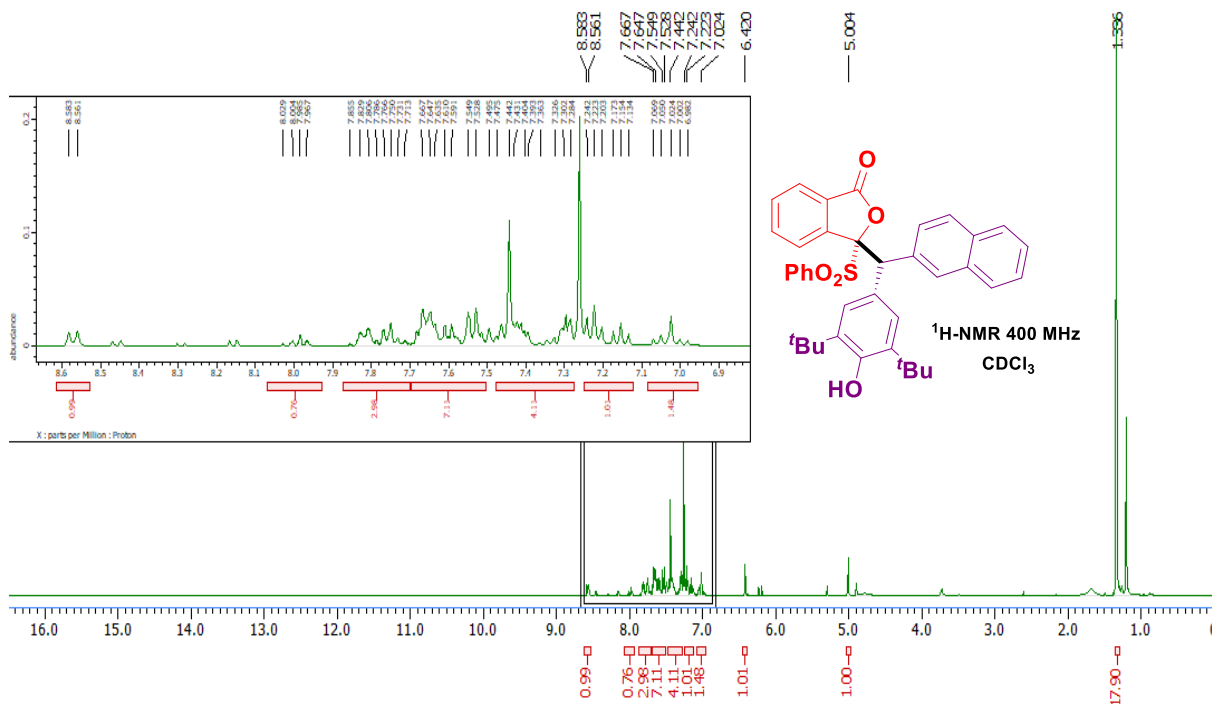


**Fig. 65: <sup>1</sup>H-NMR spectrum of 3-((1-benzyl-1H-indol-3-yl)(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-(3H)-one (4q)**

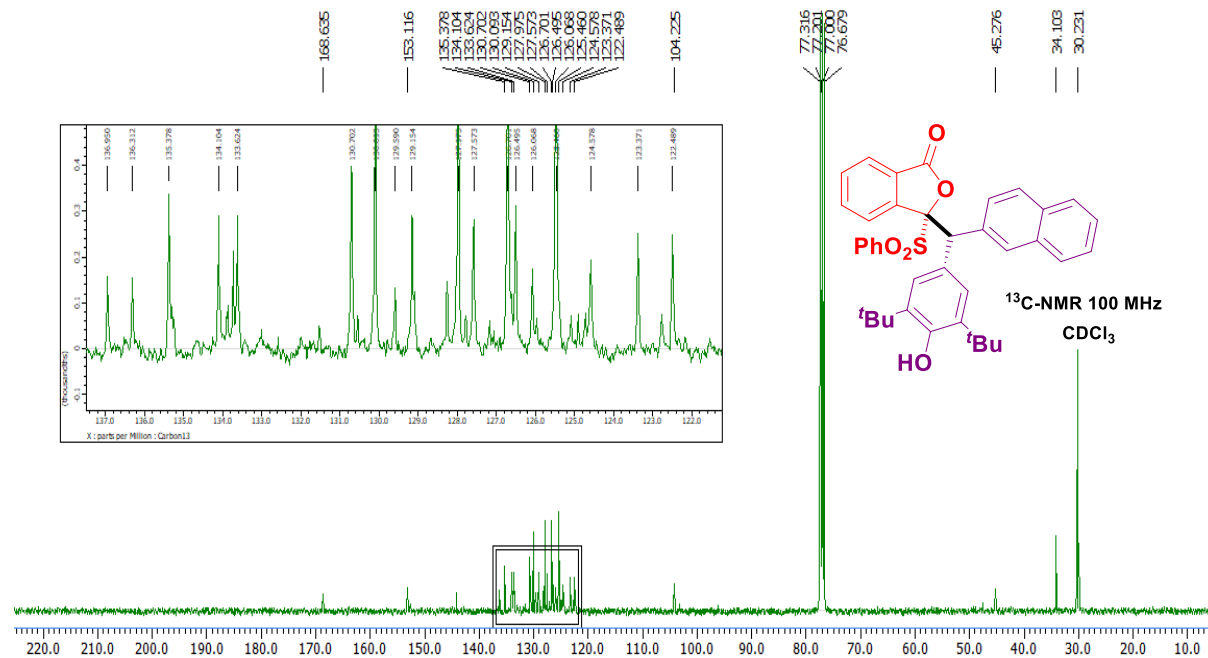


**Fig. 66: <sup>13</sup>C-NMR spectrum of 3-((1-benzyl-1H-indol-3-yl)(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-(3H)-one (4q)**





**Fig. 69:** <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(naphthalene -2-yl)methyl)-3-(phenylsulfonyl) isobenzofuran-1(3H)-one (4s)



**Fig. 70:** <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(naphthalene -2-yl)methyl)-3-(phenylsulfonyl) isobenzofuran-1(3H)-one (4s)

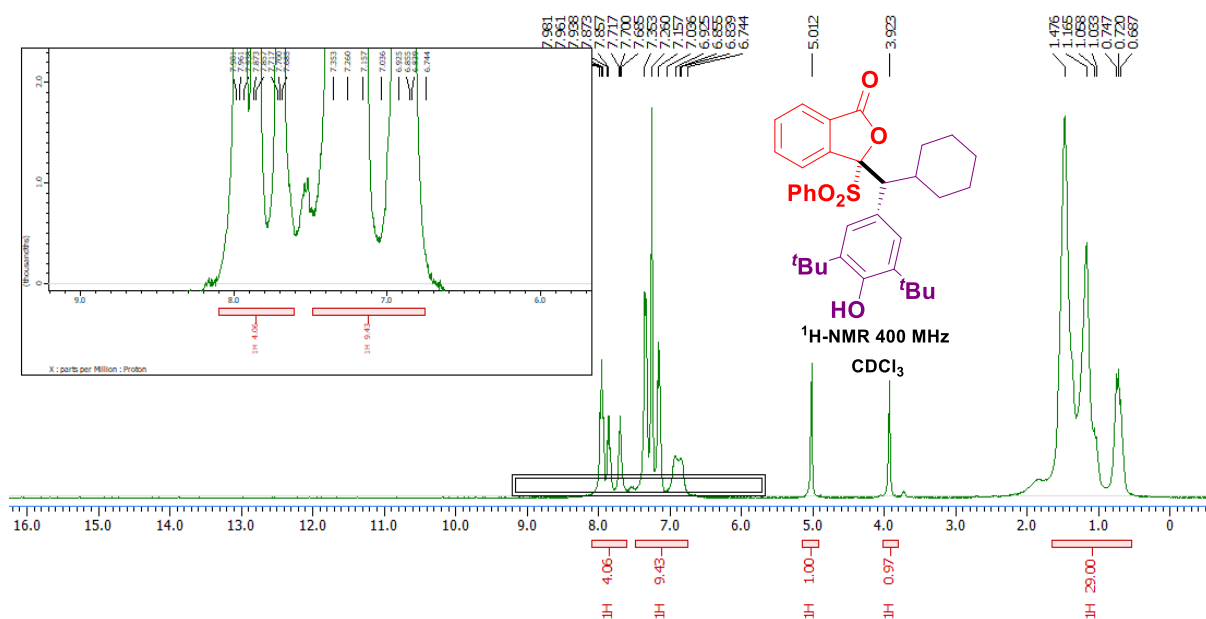


Fig. 71: <sup>1</sup>H-NMR spectrum of 3-(cyclohexyl (3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4t)

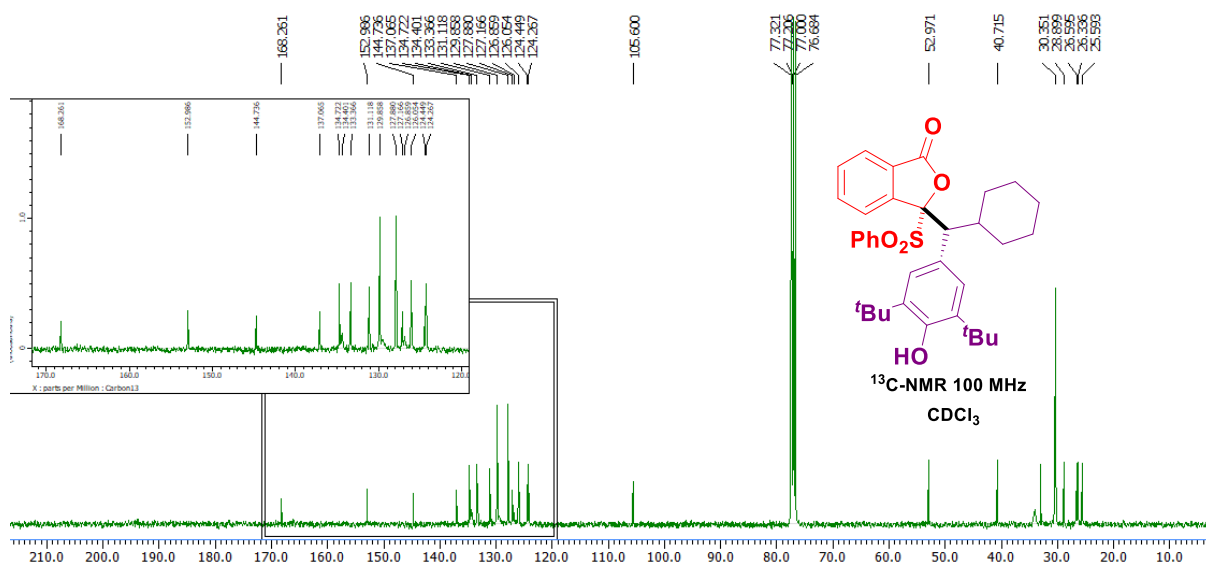
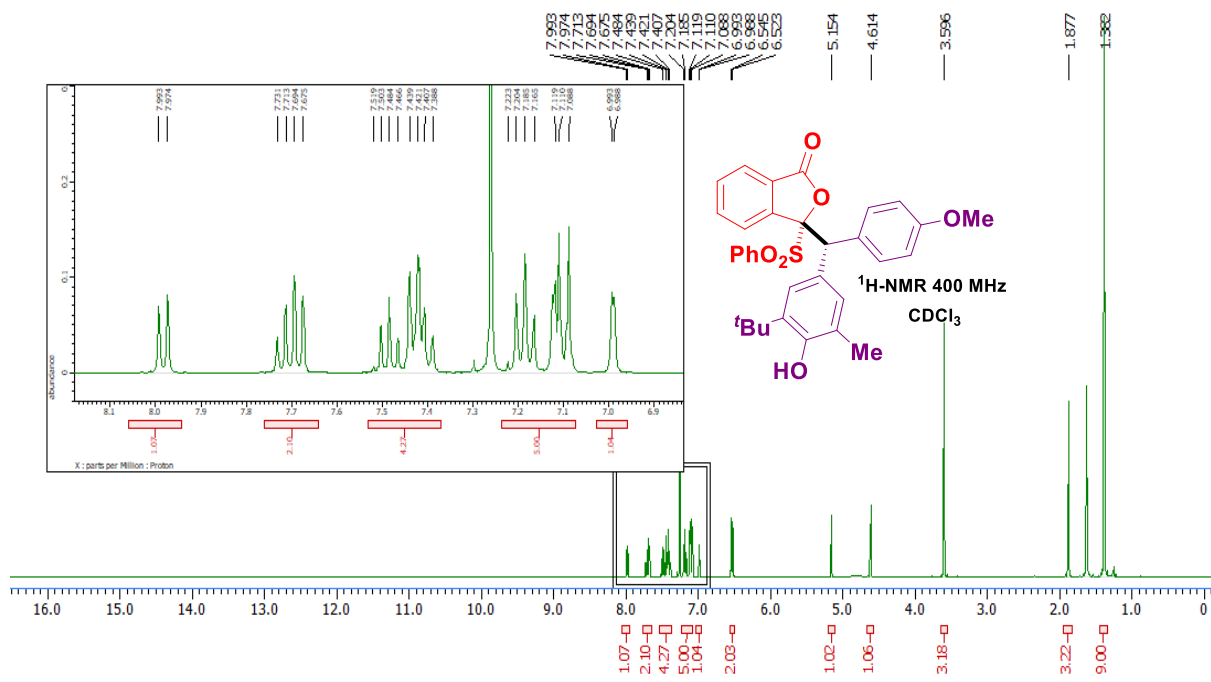
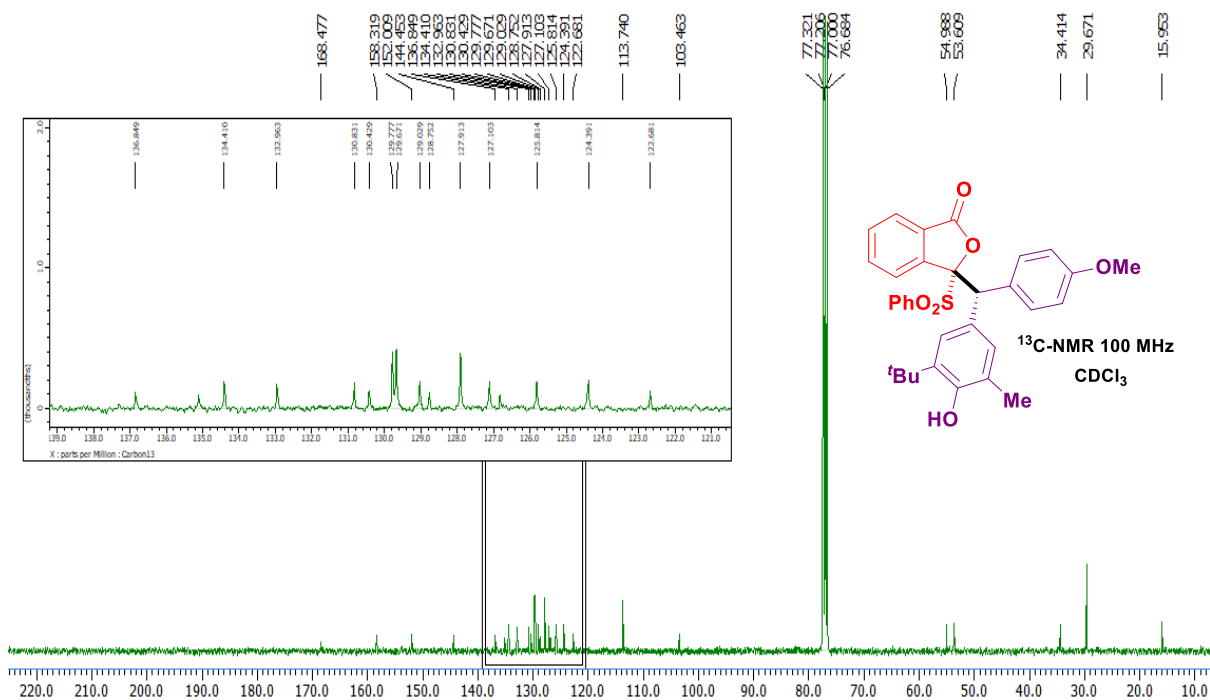


Fig. 72: <sup>13</sup>C-NMR spectrum of 3-(cyclohexyl(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-3-(phenylsulfonyl)isobenzofuran-1(3H)-one (4t)

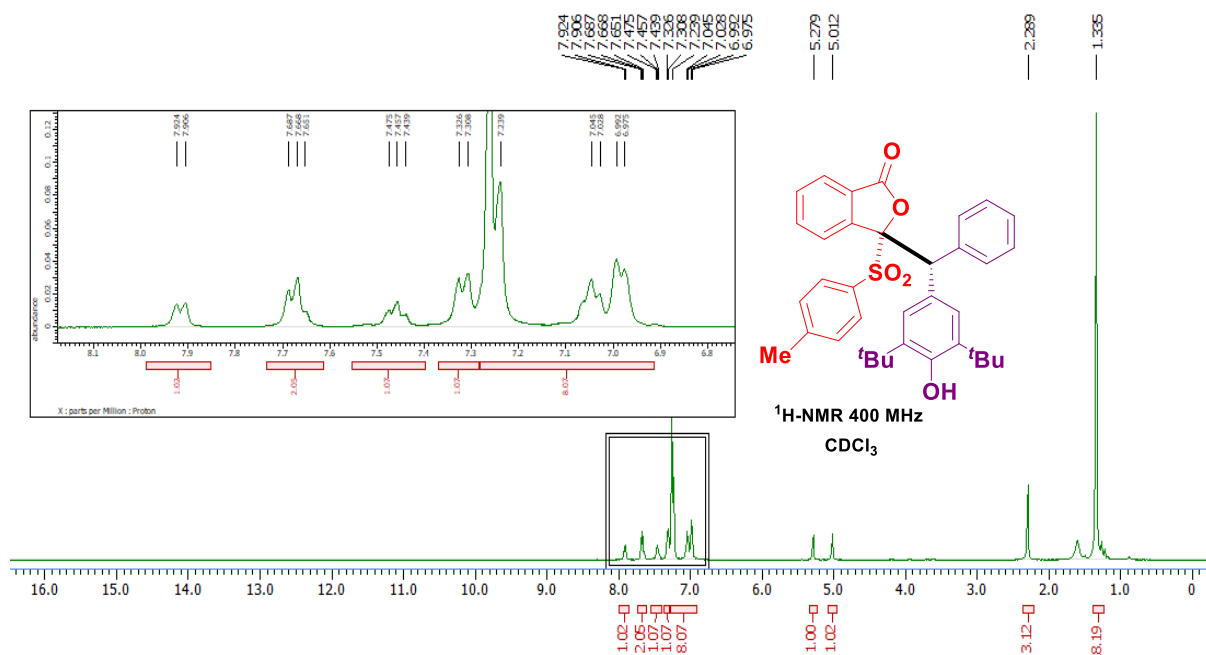


**Fig. 73:** <sup>1</sup>H-NMR spectrum of 3-((3-(tert-butyl)-4-hydroxy-5-methylphenyl)(4-methoxyphenyl)methyl)-3-phenylsulfonylisobenzofuran-1(3H)-one (4u)

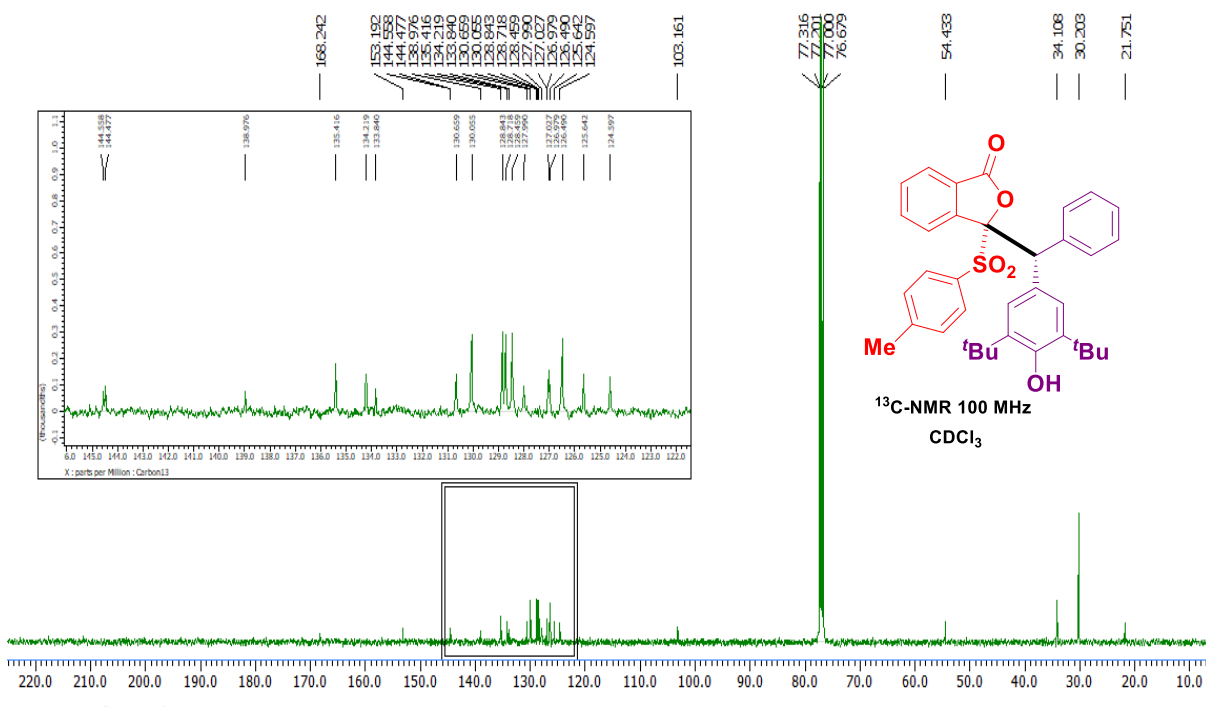


**Fig. 74:** <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-3-phenylsulfonylisobenzofuran-1(3H)-one (4u)





**Fig. 75: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-3-tosylisobenzofuran-1(3H)-one (4aa)**



**Fig. 76: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-3-tosylisobenzofuran-1(3H)-one (4aa)**

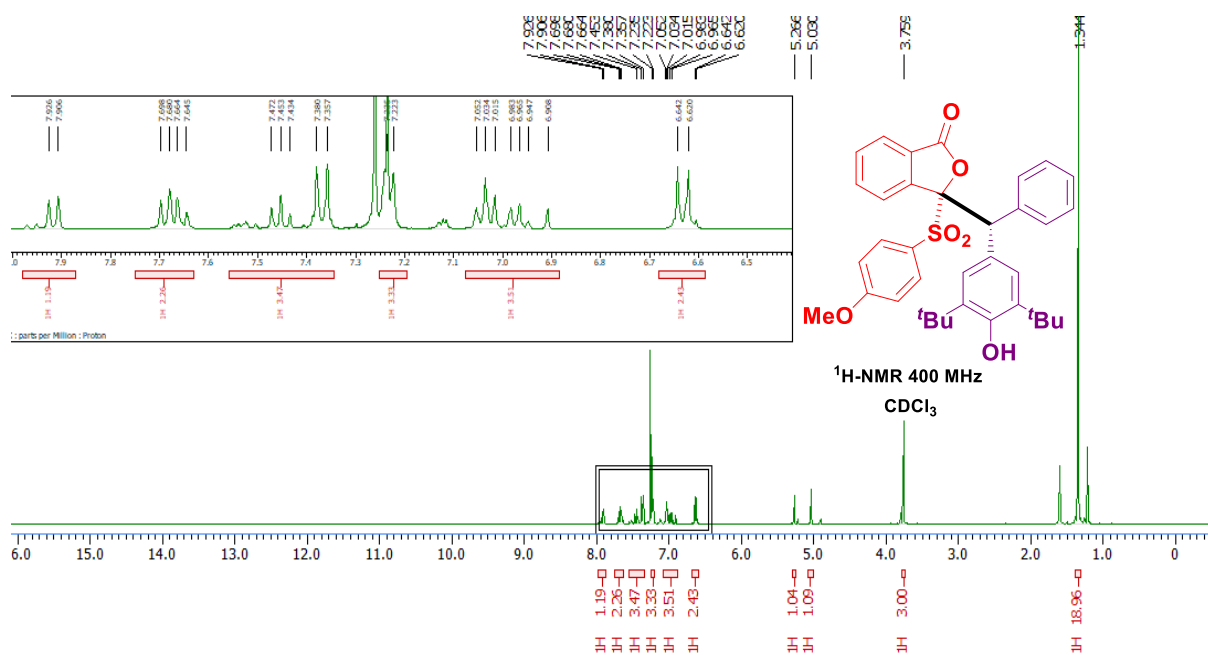


Fig. 77: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-3-((4-methoxyphenyl)sulfonyl)isobenzofuran-1(3H)-one (4ab)

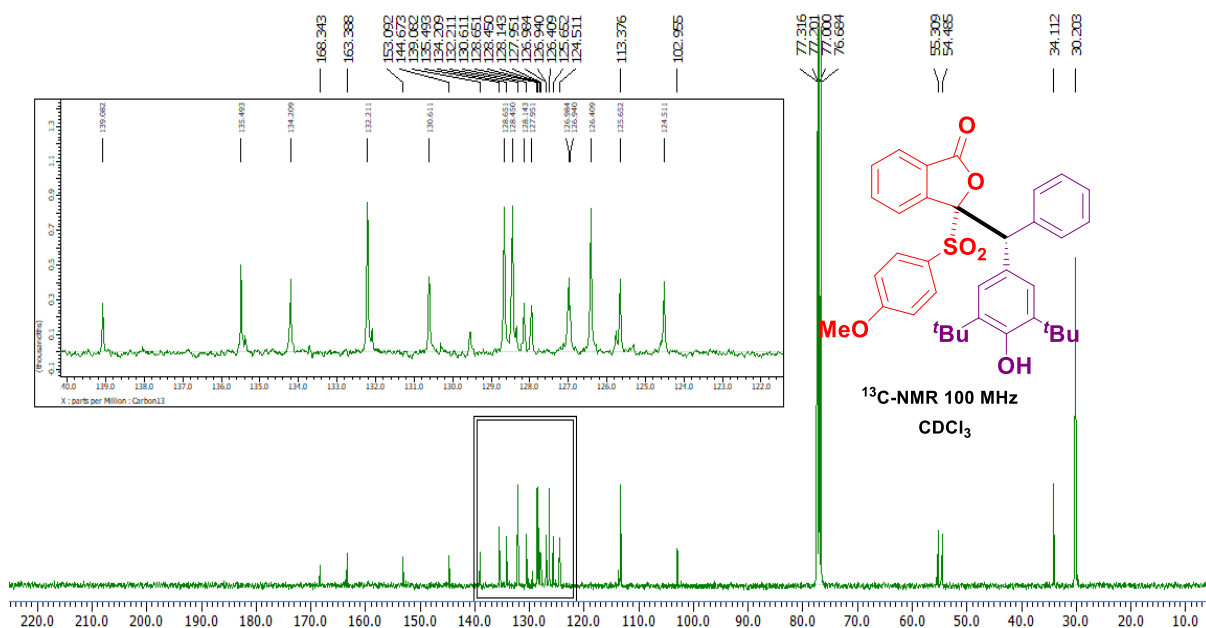


Fig. 78: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-3-((4-methoxyphenyl)sulfonyl)isobenzofuran-1(3H)-one (4ab)

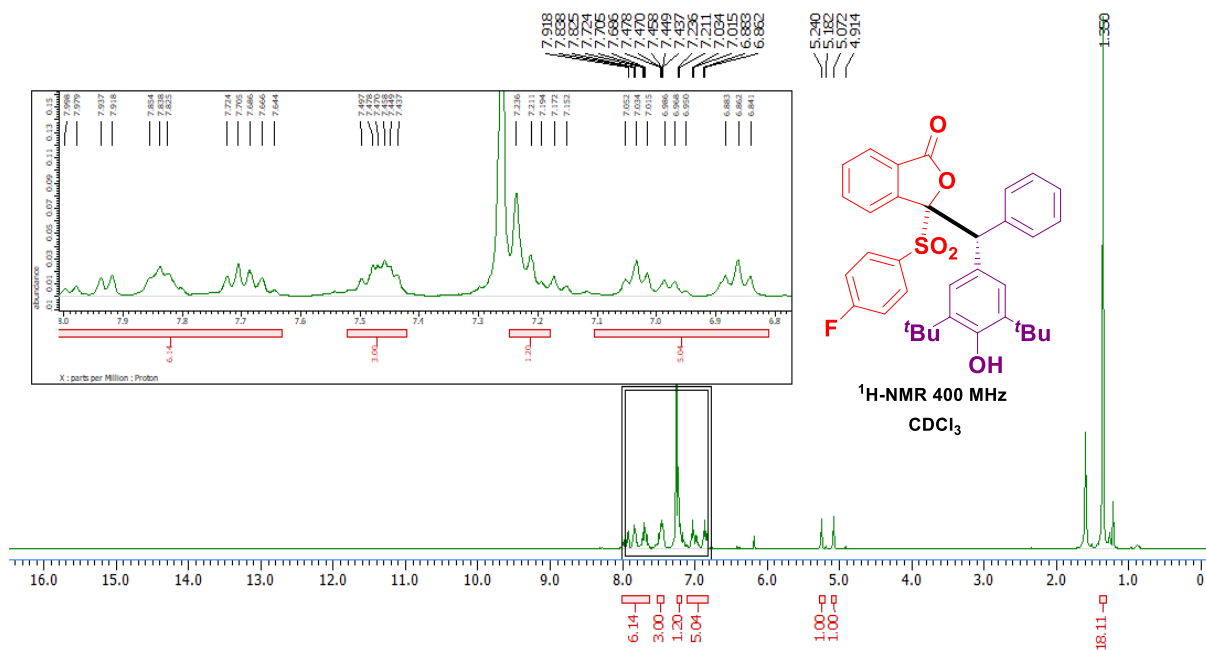


Fig. 79: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-3-((4-fluorophenyl)sulfonyl)-isobenzofuran-1(3H)-one (4ac)

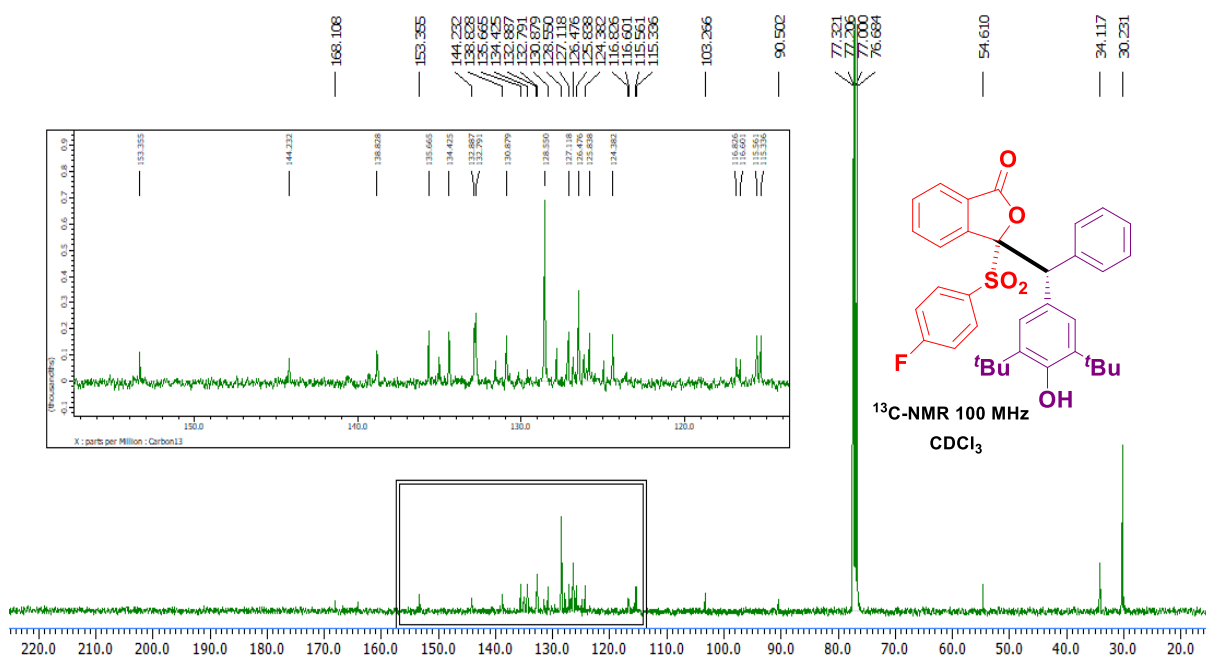
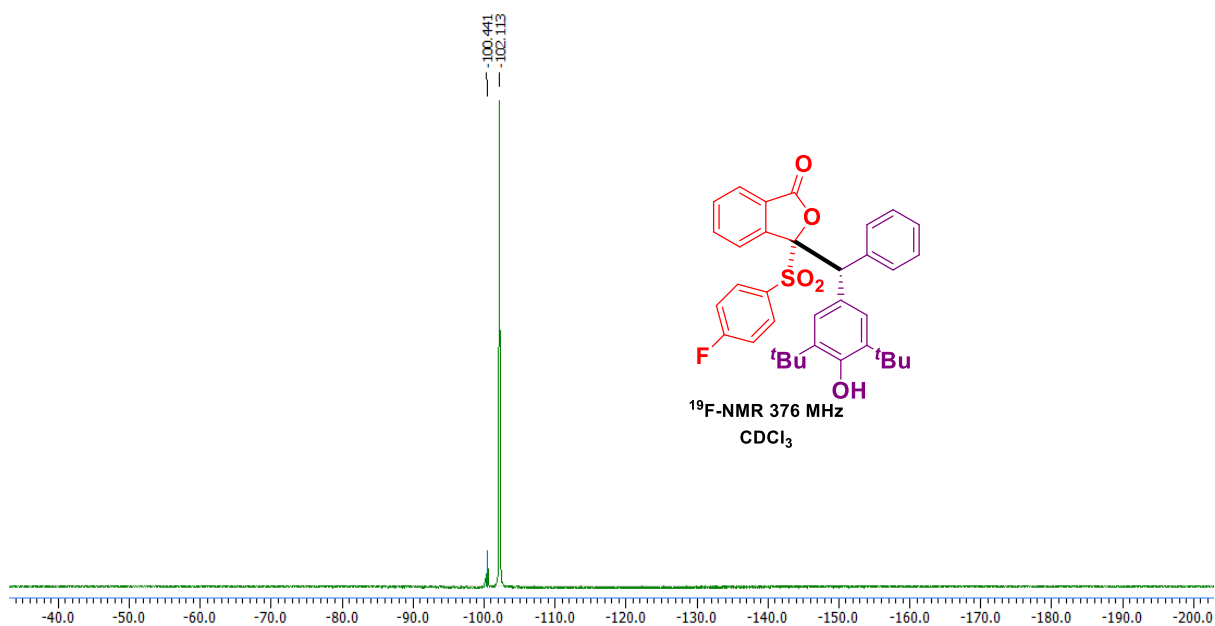


Fig. 80: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-3-((4-fluorophenyl)sulfonyl)-isobenzofuran-1(3H)-one (4ac)



**Fig. 81:**  $^{13}\text{C}$ -NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-3-((4-fluorophenyl)sulfonyl)-isobenzofuran-1(3H)-one (*4ac*)

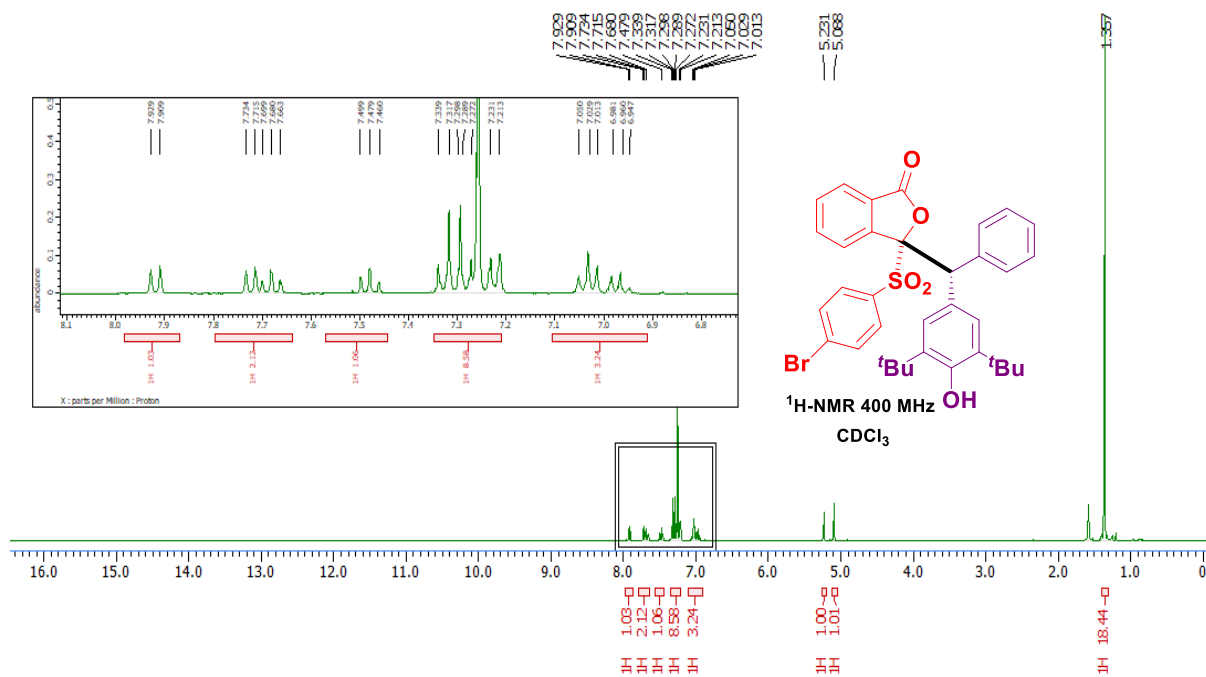


Fig. 82: <sup>1</sup>H-NMR spectrum of 3-((4-bromophenyl) sulfonyl)-3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-isobenzofuran-1(3H)-one (4ad)

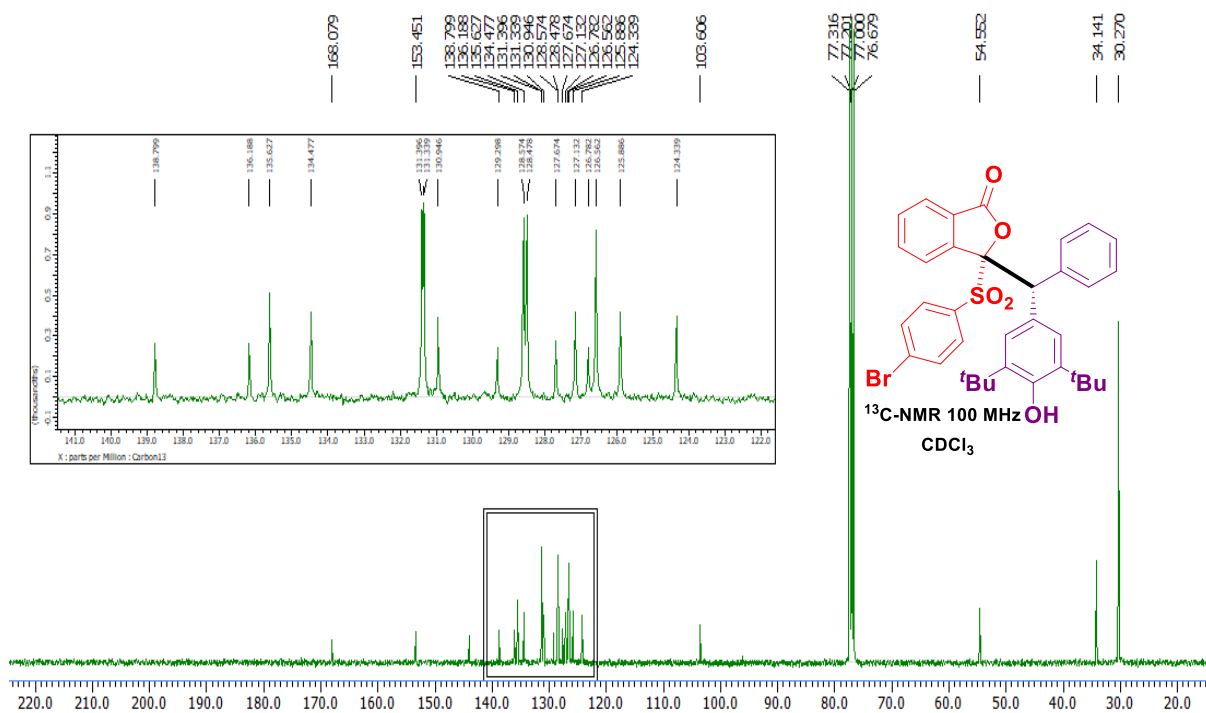
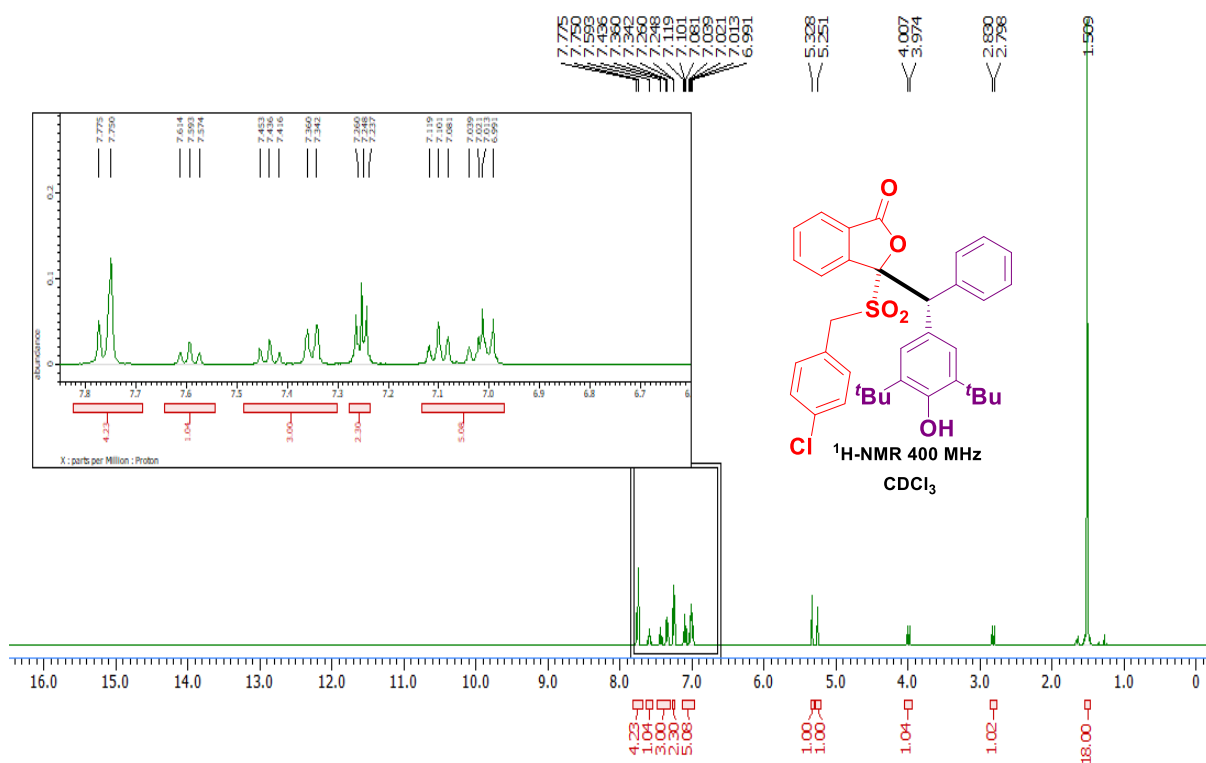
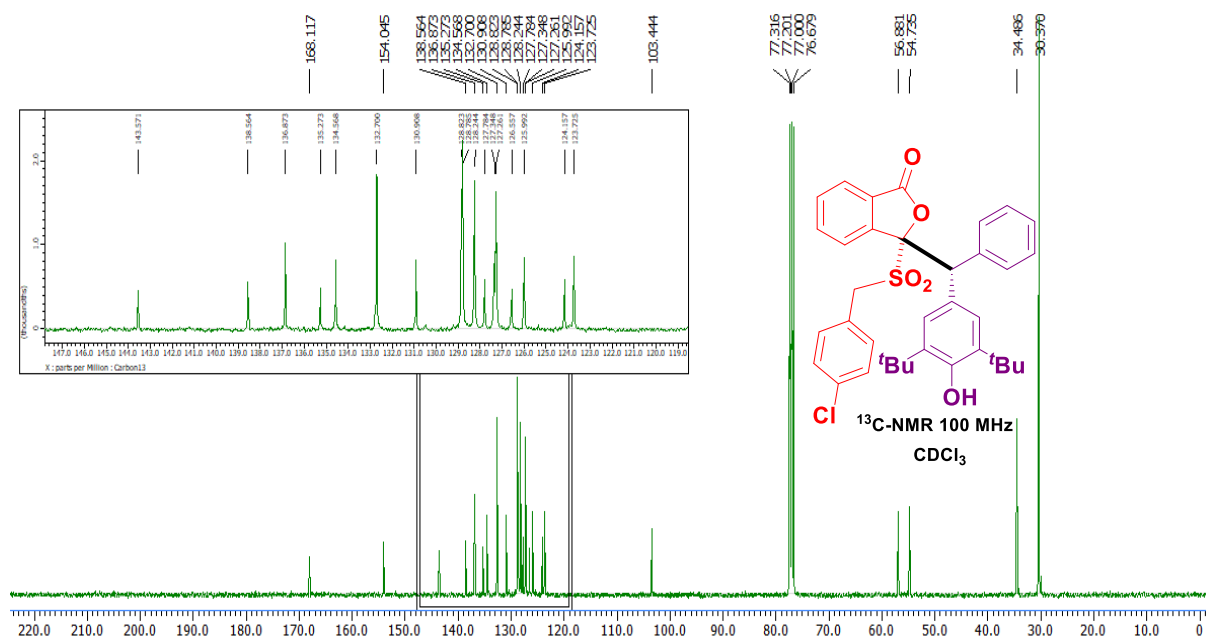


Fig. 83: <sup>13</sup>C-NMR spectrum of 3-((4-bromophenyl) sulfonyl)-3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-isobenzofuran-1(3H)-one (4ad)



**Fig. 84:** <sup>1</sup>H-NMR spectrum of 3-((4-chlorobenzyl)sulfonyl)-3((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)isobenzofuran-1(3H)-one (4ae)



**Fig. 85:** <sup>13</sup>C-NMR spectrum of 3-((4-chlorobenzyl)sulfonyl)-3((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)isobenzofuran-1(3H)-one (4ae)

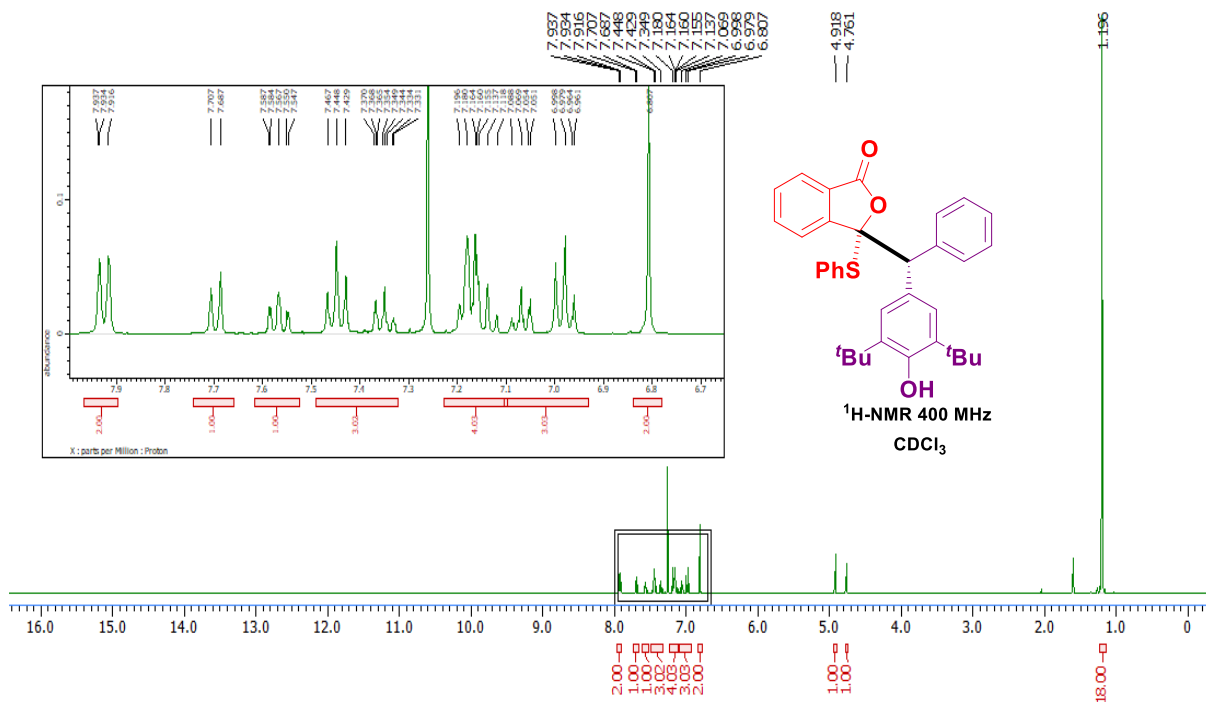


Fig. 86: <sup>1</sup>H-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-(phenylthio) 3-isobenzofuran-1(3H)-one (4af)

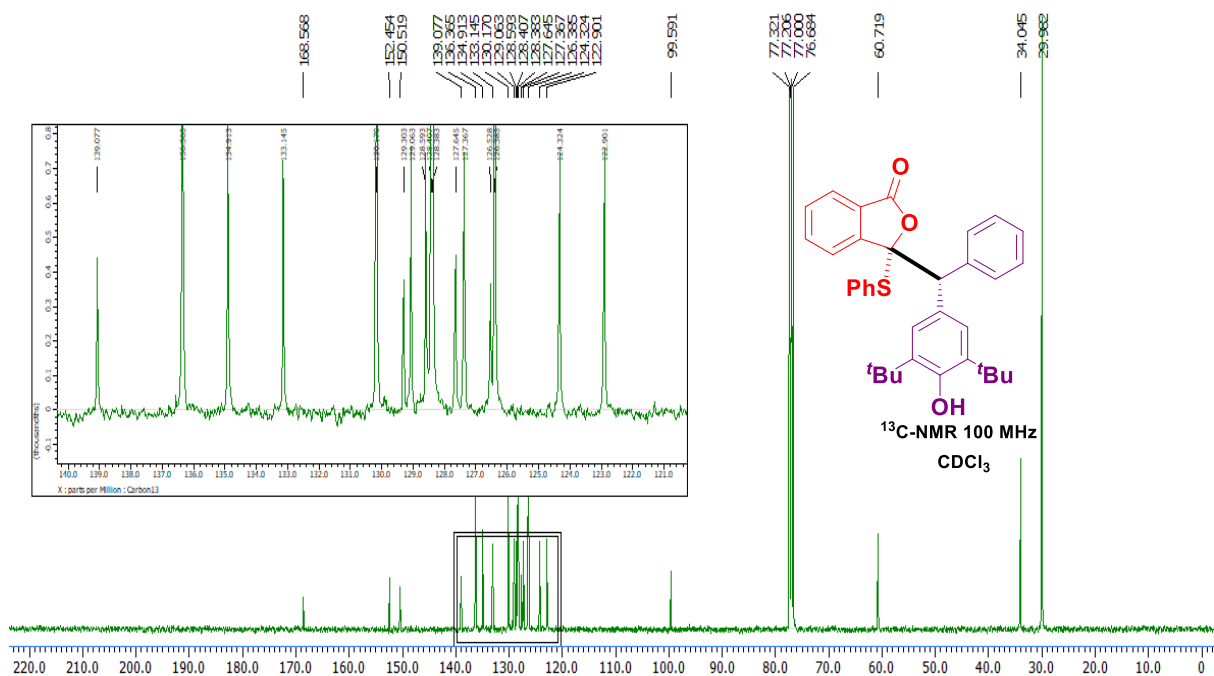


Fig. 87: <sup>13</sup>C-NMR spectrum of 3-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-(phenylthio) 3-isobenzofuran-1(3H)-one (4af)

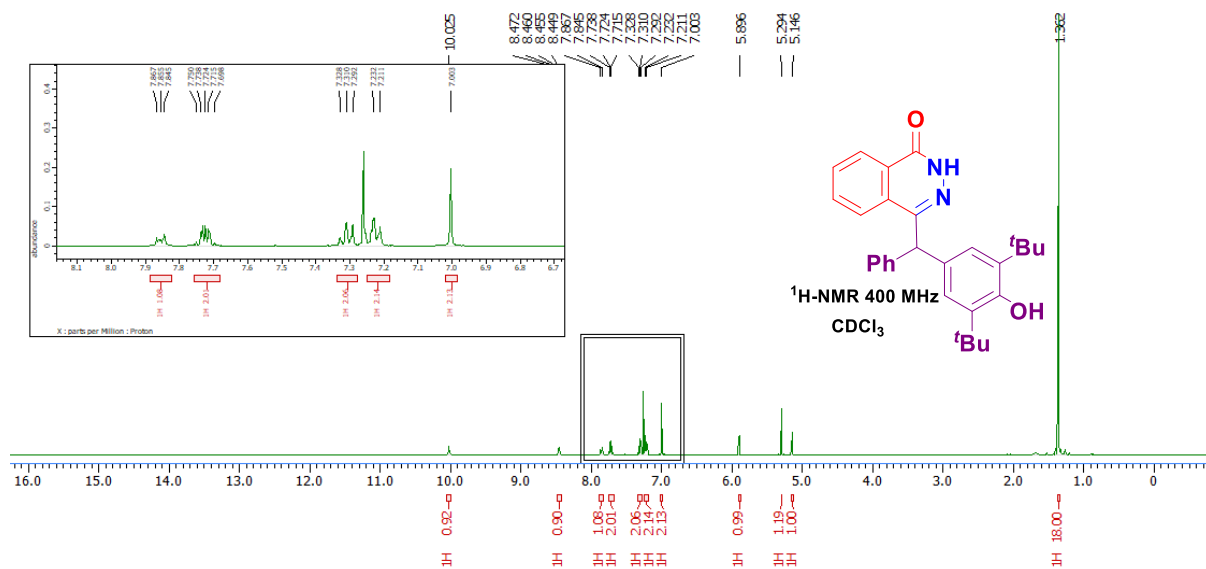


Fig. 88: <sup>1</sup>H-NMR spectrum of 4-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(phenyl)methyl)phthalazin-1(2H)-one (5a)

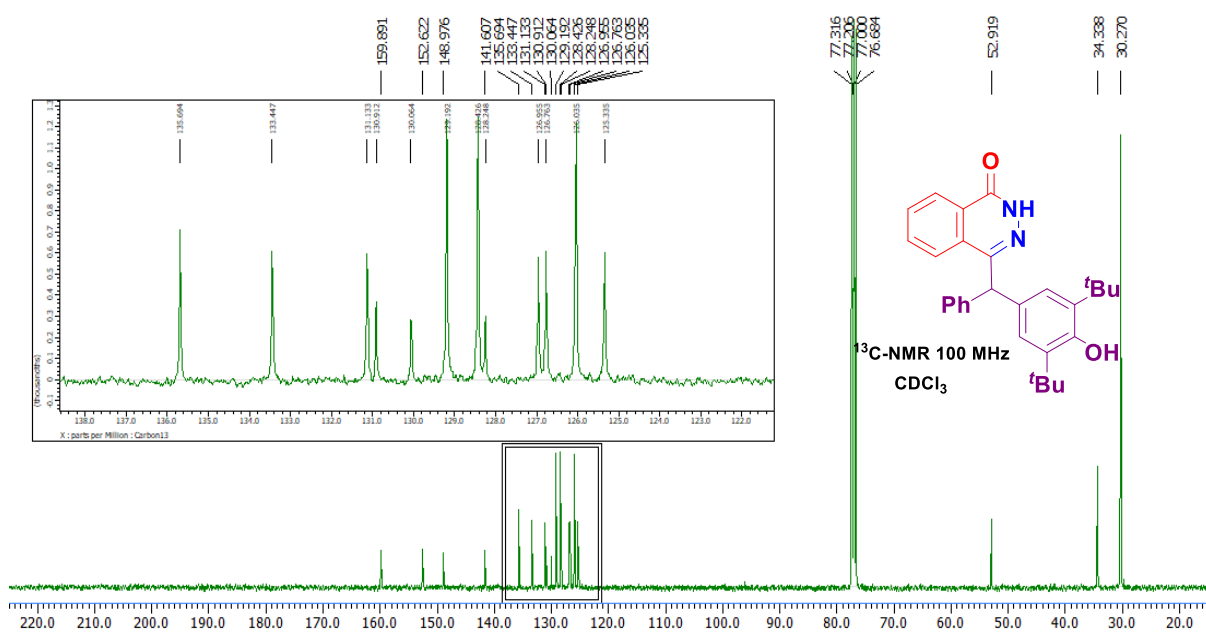
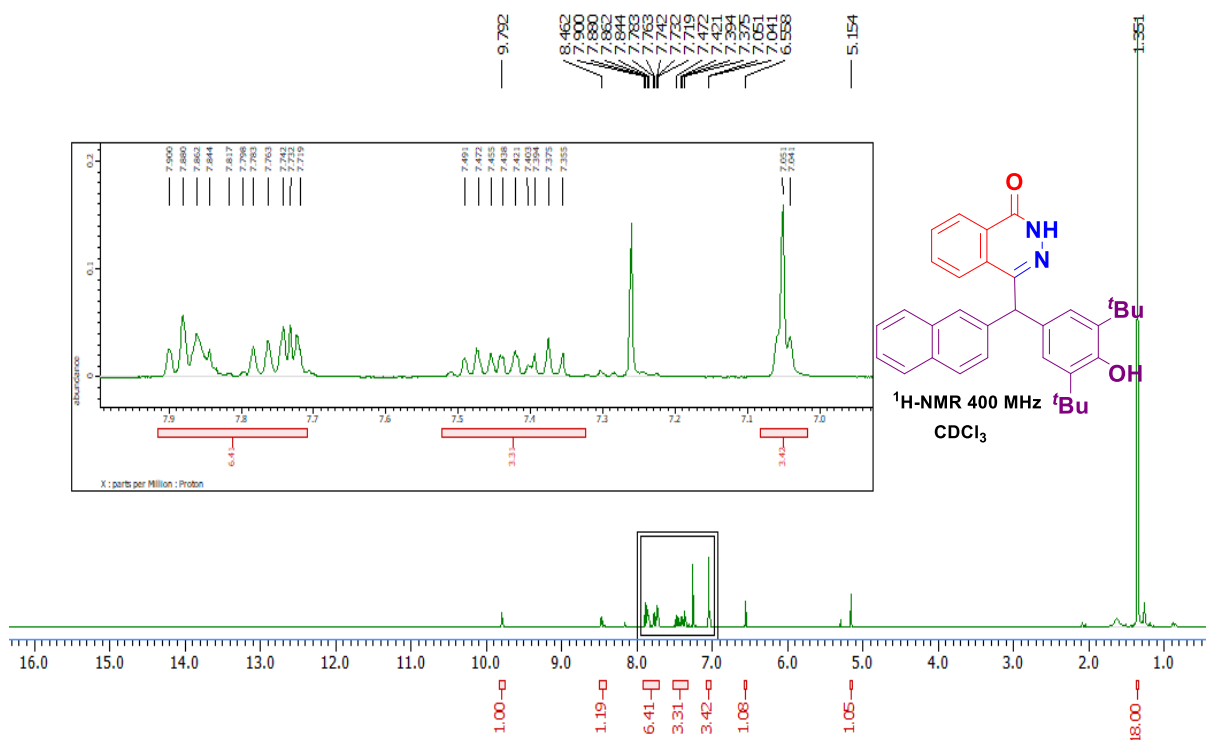


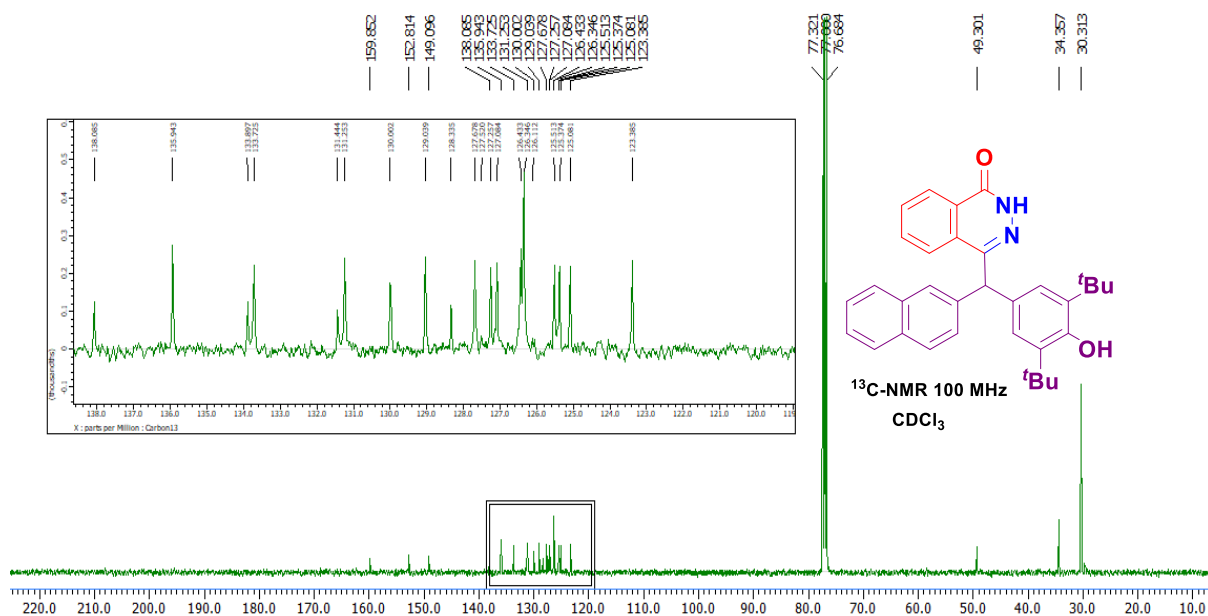
Fig. 89: <sup>13</sup>C-NMR spectrum of 4-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(phenyl)methyl)phthalazin-1(2H)-one (5a)







**Fig. 92: <sup>1</sup>H-NMR spectrum of 4-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(naphthalene-2-yl)methyl)phthalazin-1(2*H*)-one (5c)**



**Fig. 93: <sup>13</sup>C-NMR spectrum of 4-((3,5-di-*tert*-butyl-4-hydroxyphenyl)(naphthalene-2-yl)methyl)phthalazin-1(2*H*)-one (5c)**