

## Supporting Information

### 1,6-Conjugate addition of *in situ* generated aryldiazenes to *p*-quinone methides

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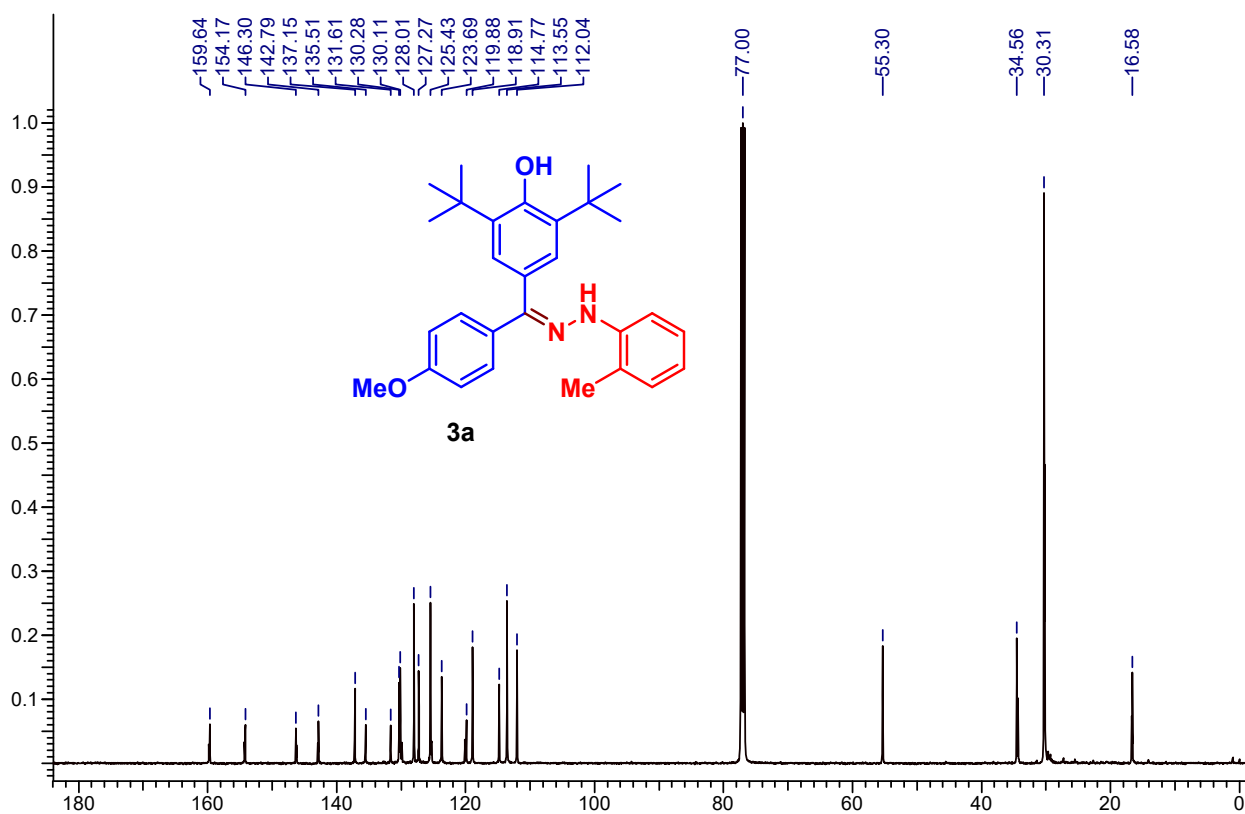
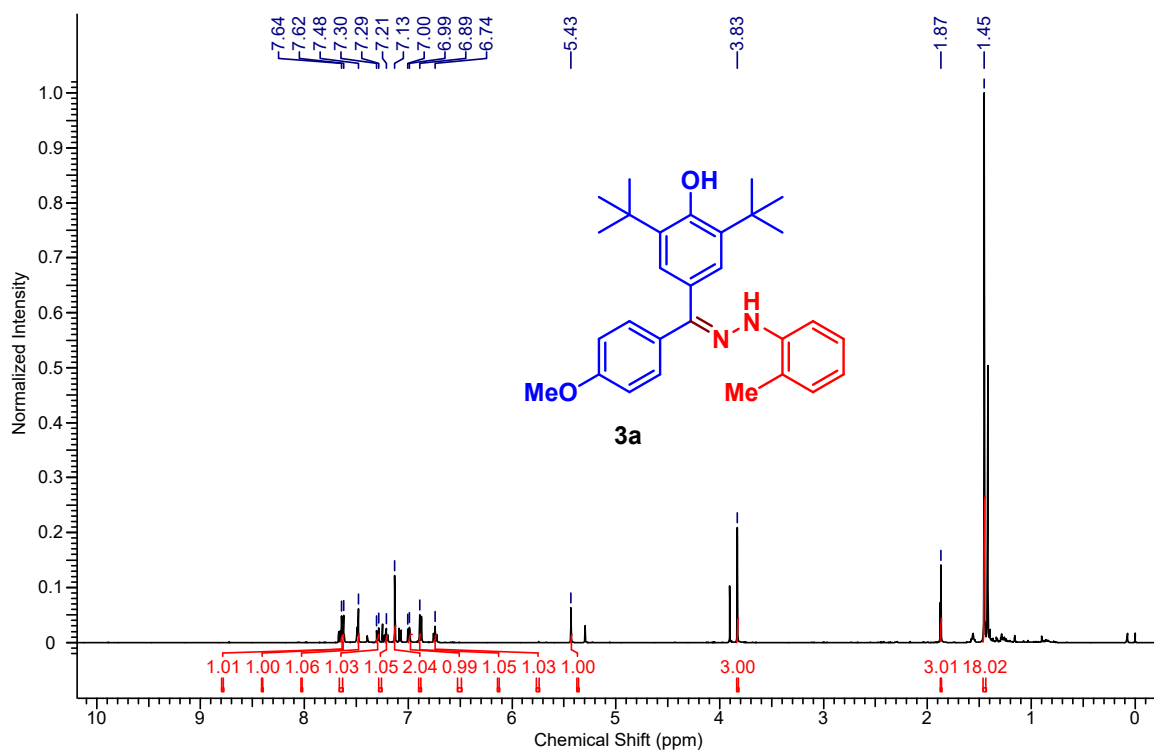
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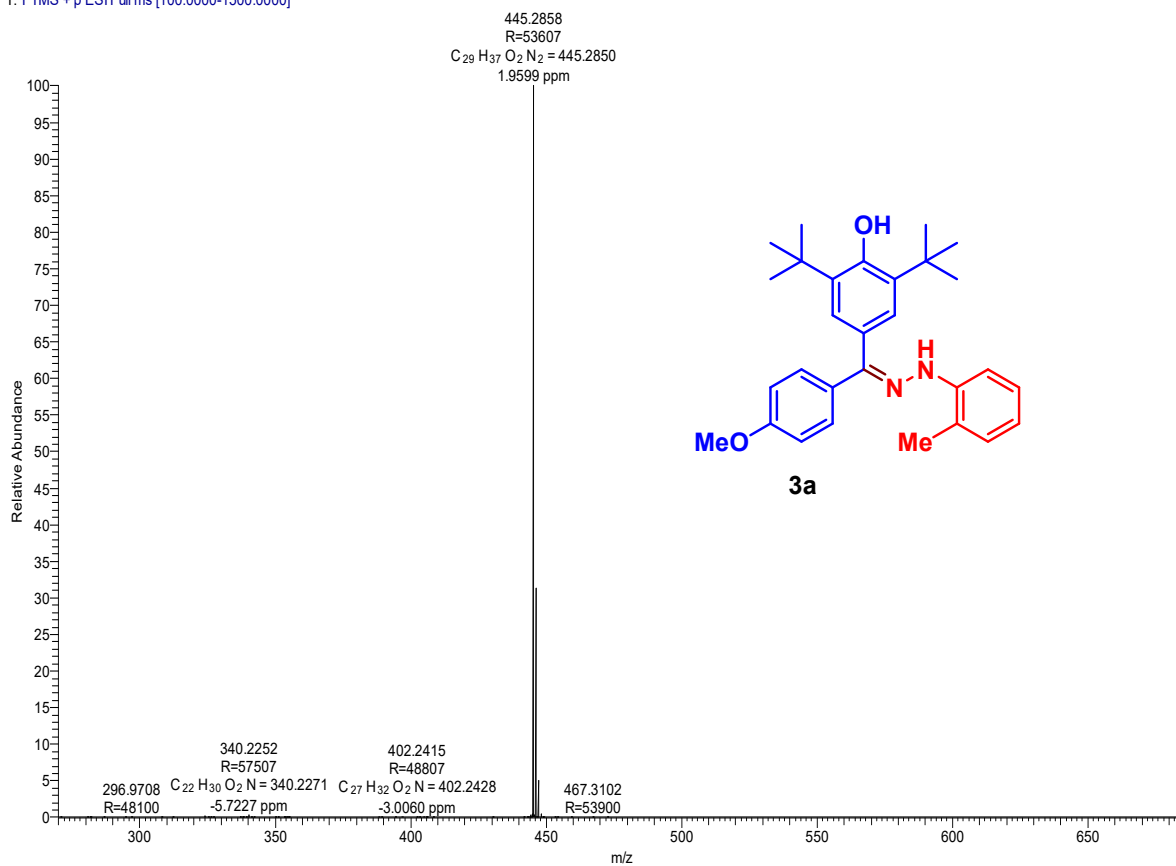
## 1. General information

All melting points were recorded on a Büchi melting point apparatus in open capillaries and are uncorrected. Commercially available reagents and dried solvents were used as received. Reactions were monitored by thin layer chromatography (TLC) using silica gel plates with visualization in UV lamp (254 nm) followed by exposing developed TLC plate to iodine (I<sub>2</sub>) vapor. Lastly, the developed TLC plates were visualized using phosphomolybdic acid as staining reagent. Flash chromatography was performed with CombiFlash *R<sub>f</sub>* 200i with UV/VIS and ELSD, Isco Teledyne Inc., USA using a RediSep® column (SiO<sub>2</sub>). Solvents used for column chromatography were distilled by the usual methods prior to use. <sup>1</sup>H NMR spectra were recorded on a Bruker 500 or 400 MHz spectrometer, <sup>13</sup>C NMR spectra were recorded at 126 or 101 MHz and <sup>19</sup>F spectra were recorded on a Bruker 376 MHz spectrometer, respectively. Chemical shifts are reported as  $\delta$  values (ppm) relative to residual solvent peak of CDCl<sub>3</sub> (7.26 ppm and 77.0 ppm for <sup>1</sup>H and <sup>13</sup>C NMR, respectively). Data for <sup>1</sup>H NMR spectra are reported as follows: chemical shift (ppm; s = singlet, d = doublet, t = triplet, dd = doublet of doublets, m = multiplet), coupling constant (Hz), and integration. Data for <sup>13</sup>C NMR are reported in terms of chemical shift (ppm). HRMS (ESI) spectra were recorded on an Orbitrap (quadrupole plus ion trap) and a TOF mass analyzer. The single crystal structure analysis of compounds **3c**, **3j** and **3s** was performed on a Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer equipped with Incoatech multilayer mirrors optics. The <sup>1</sup>H and <sup>13</sup>C NMR spectral data are given for the major isomers in the experimental data.

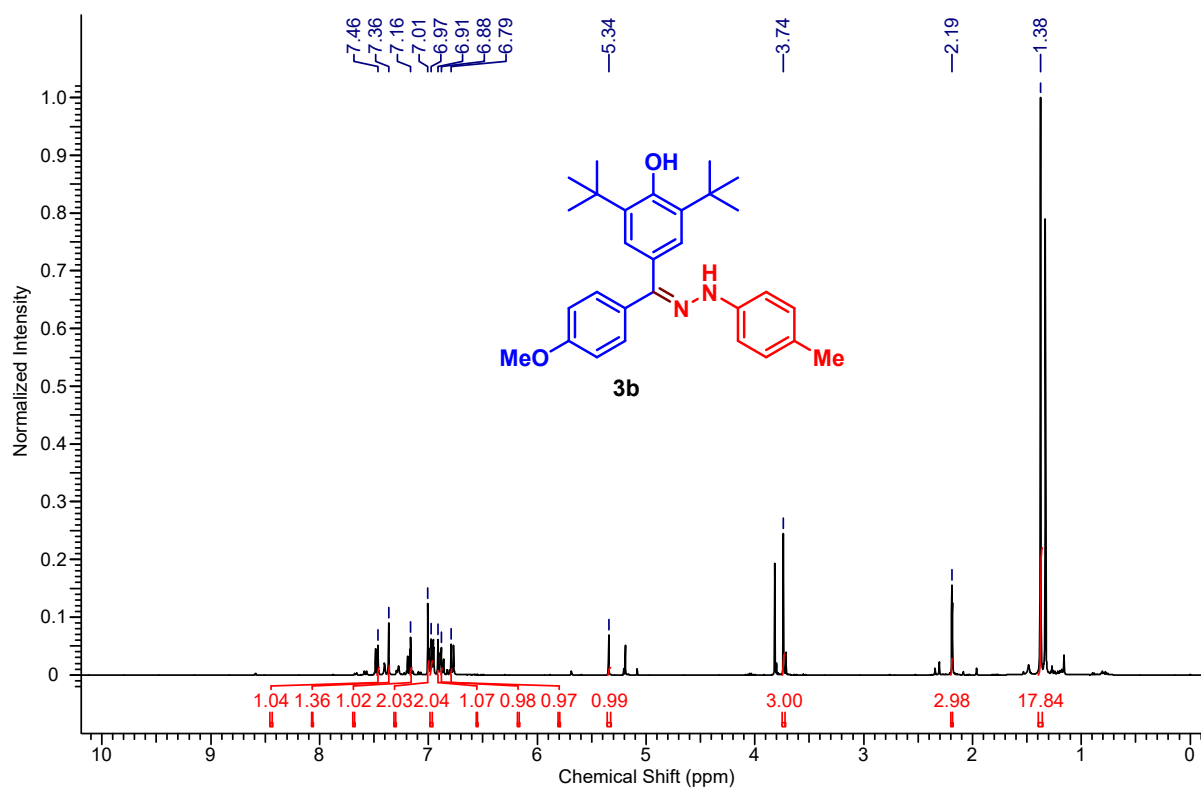
2. Copies of  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$  NMR and HRMS spectra of synthesized compounds:



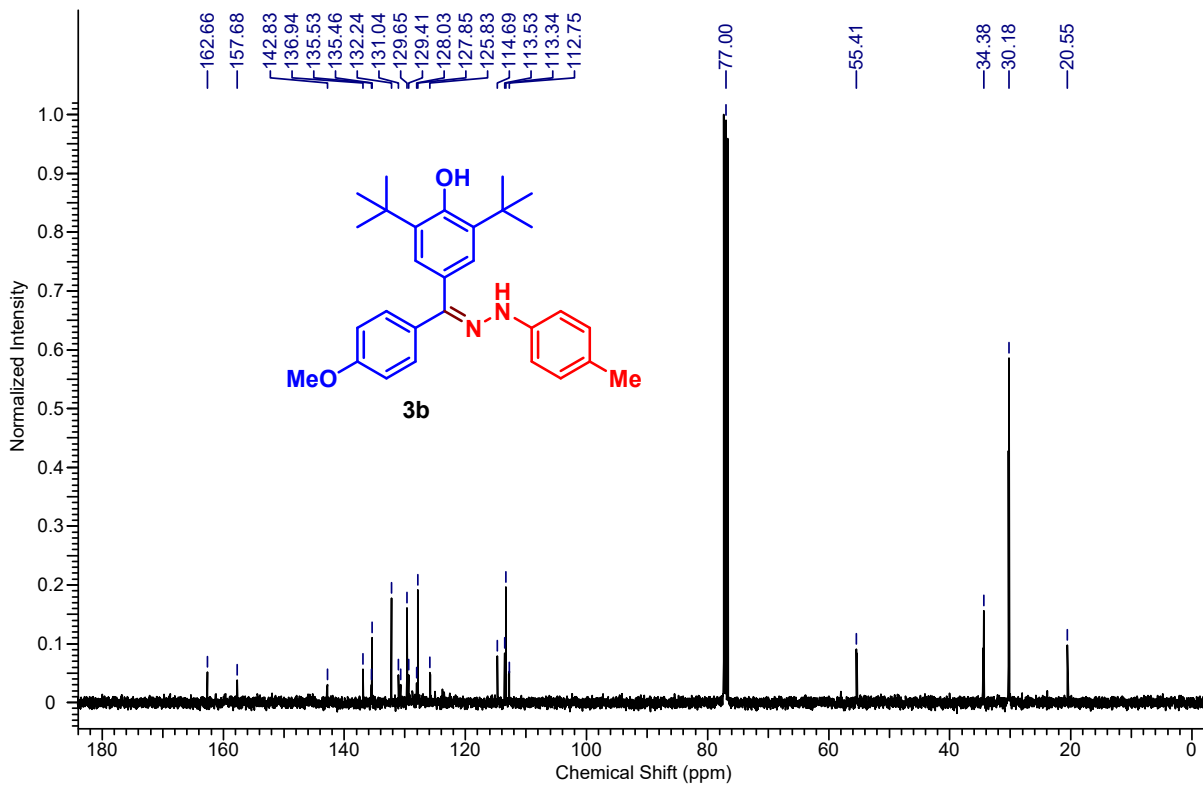
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T: FTMS + p ESI Full ms [100.0000-1500.0000]



### HRMS of Compound 3a

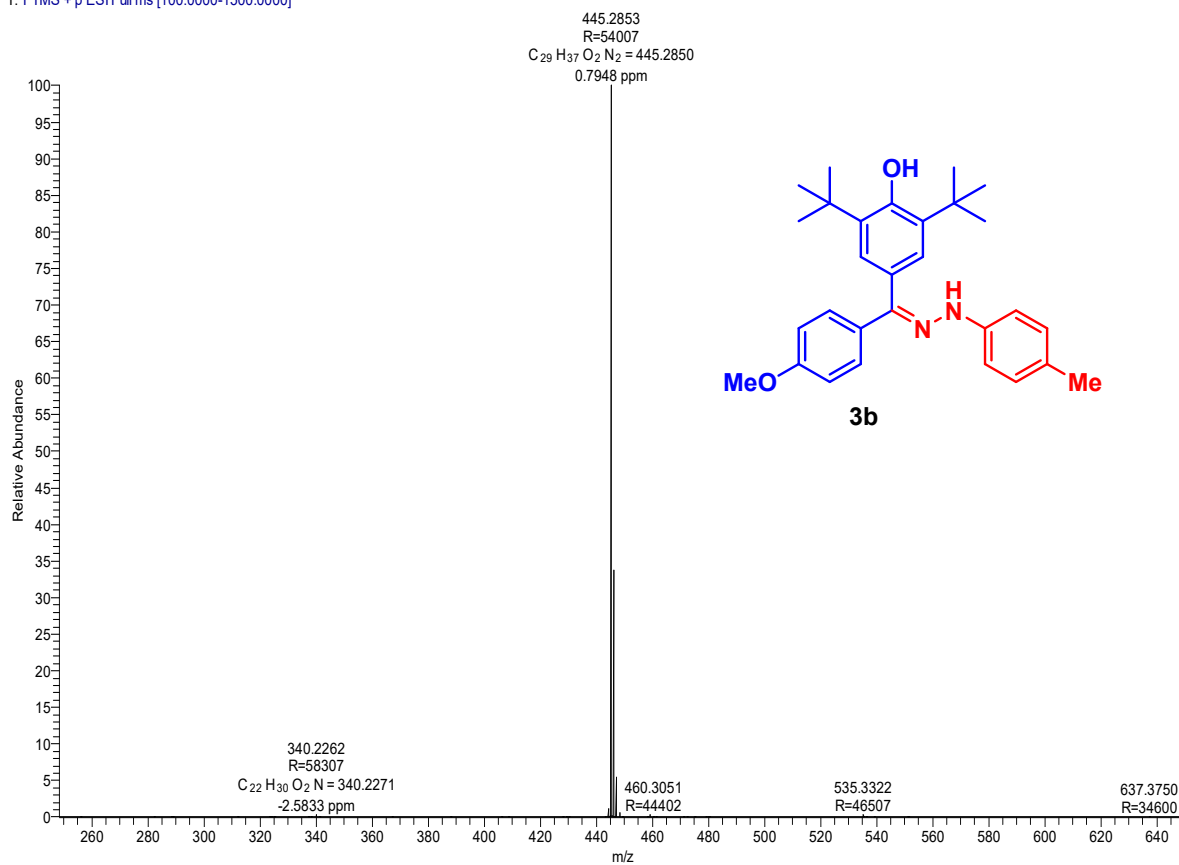


### <sup>1</sup>H NMR of Compound 3b [as 1:0.74 stereoisomeric mixture] (400 MHz, CDCl<sub>3</sub>)

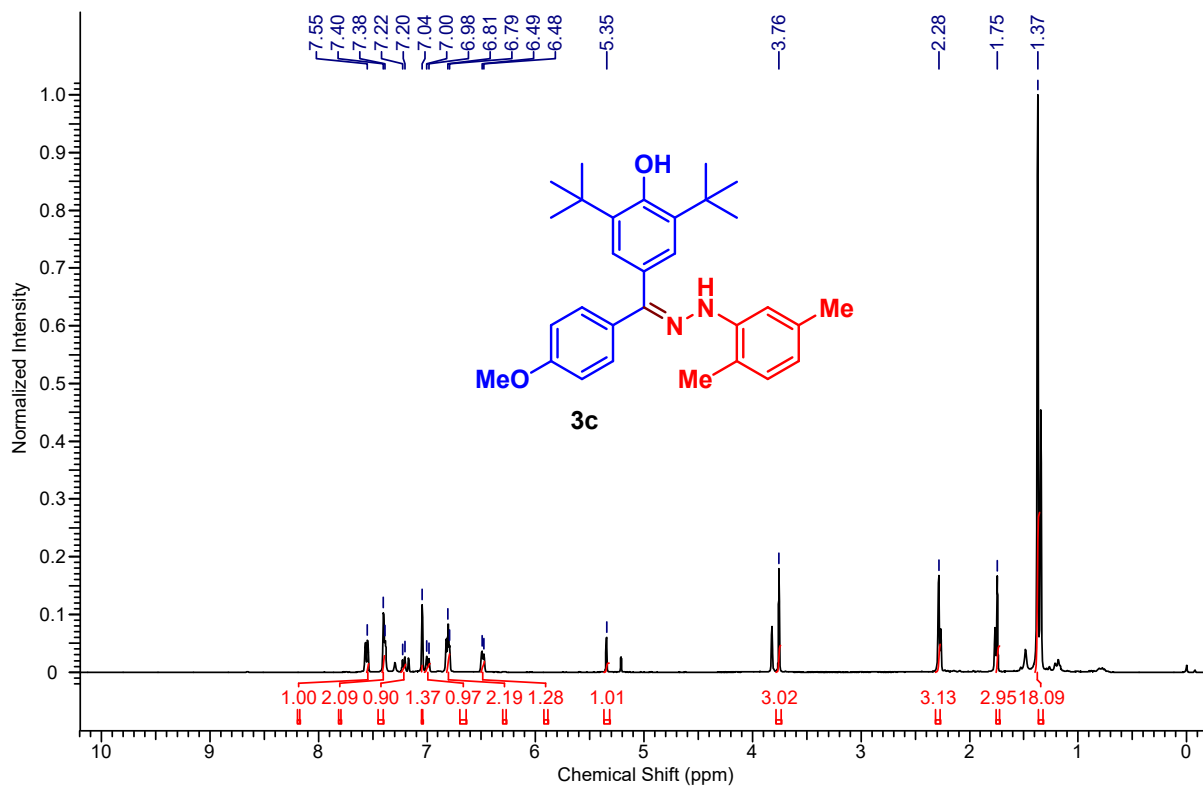


**13C NMR of Compound 3b [as 1:0.74 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)**

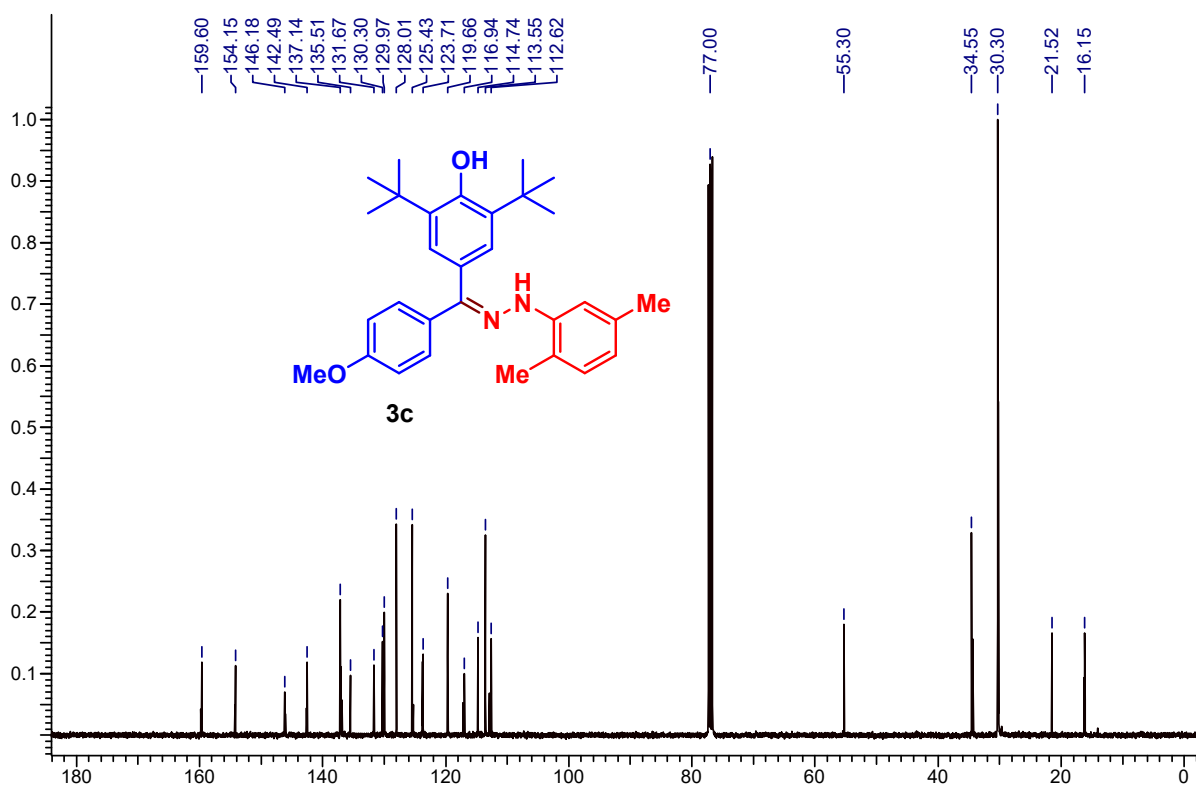
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**HRMS of Compound 3b**

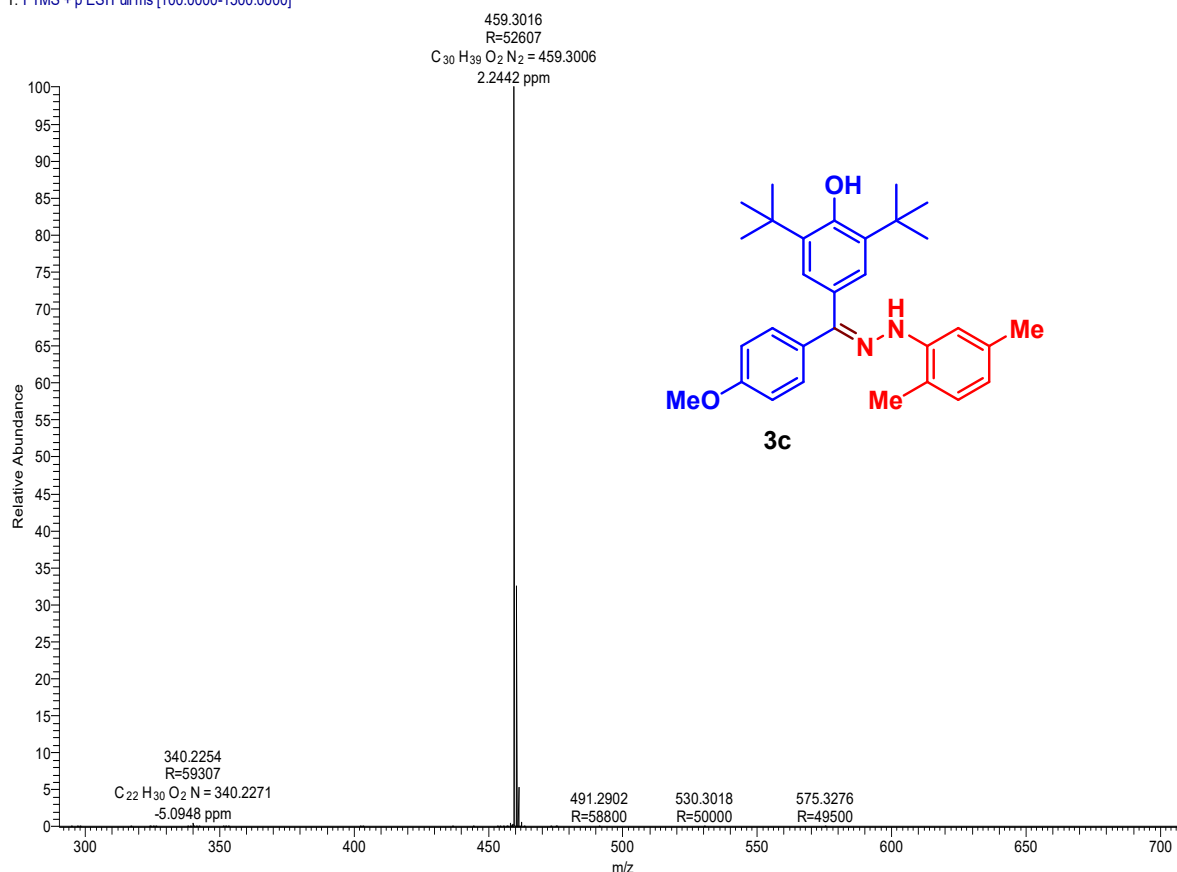


$^1\text{H}$  NMR of Compound 3c [as 1:0.45 stereoisomeric mixture] (400 MHz,  $\text{CDCl}_3$ )

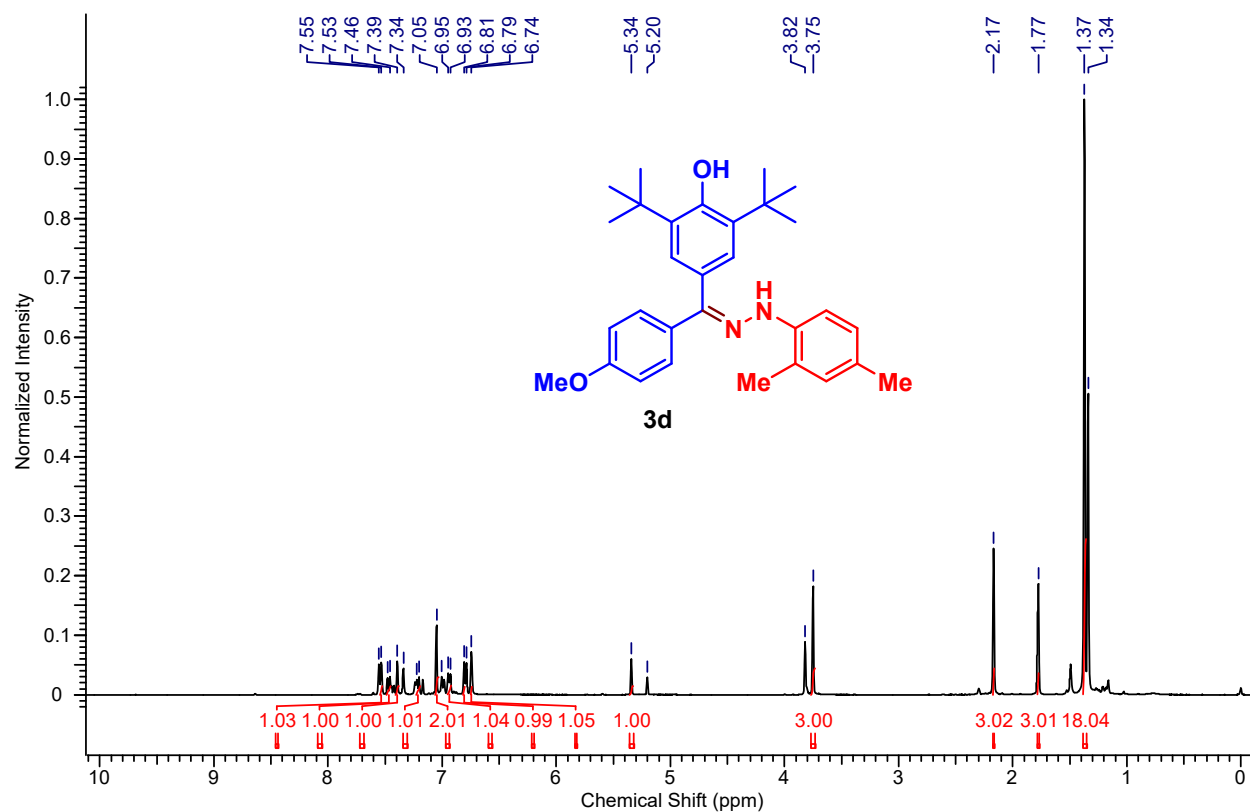


$^{13}\text{C}$  NMR of Compound 3c [as 1:0.45 stereoisomeric mixture] (101 MHz,  $\text{CDCl}_3$ )

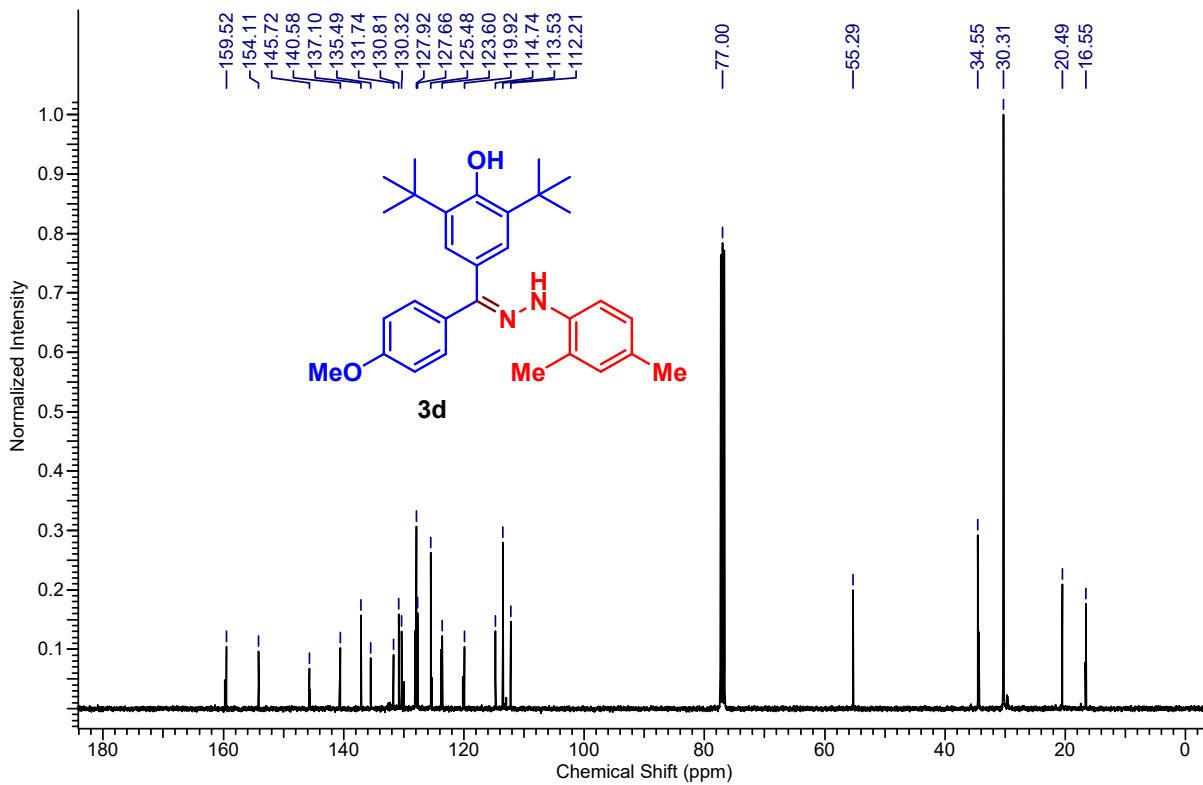
5E #902 RT: 5.00 AV: 1 NL: 5.77E9  
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HRMS of Compound 3c

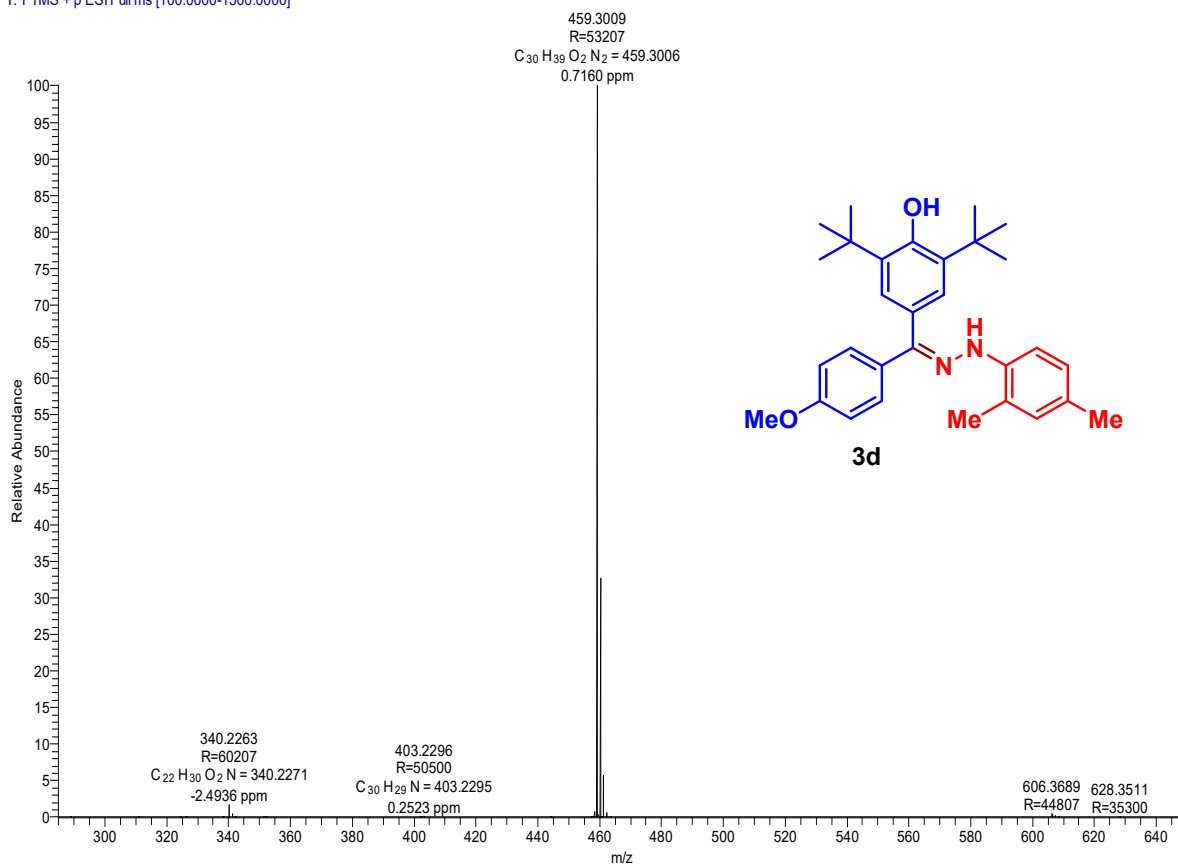


<sup>1</sup>H NMR of Compound 3d [as 1:0.53 stereoisomeric mixture] (400 MHz, CDCl<sub>3</sub>)



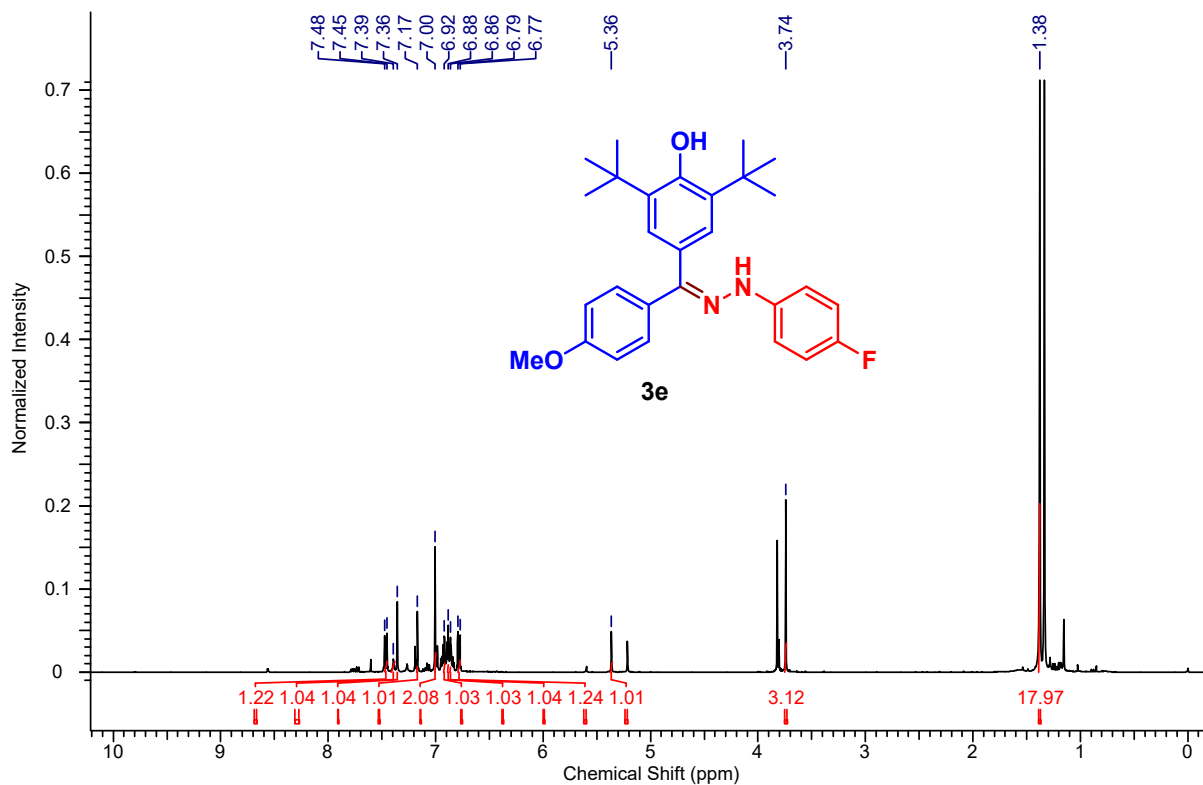
**<sup>13</sup>C NMR of Compound 3d [as 1:0.53 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)**

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T: FTMS + p ESI Full ms [100.0000-1500.0000]

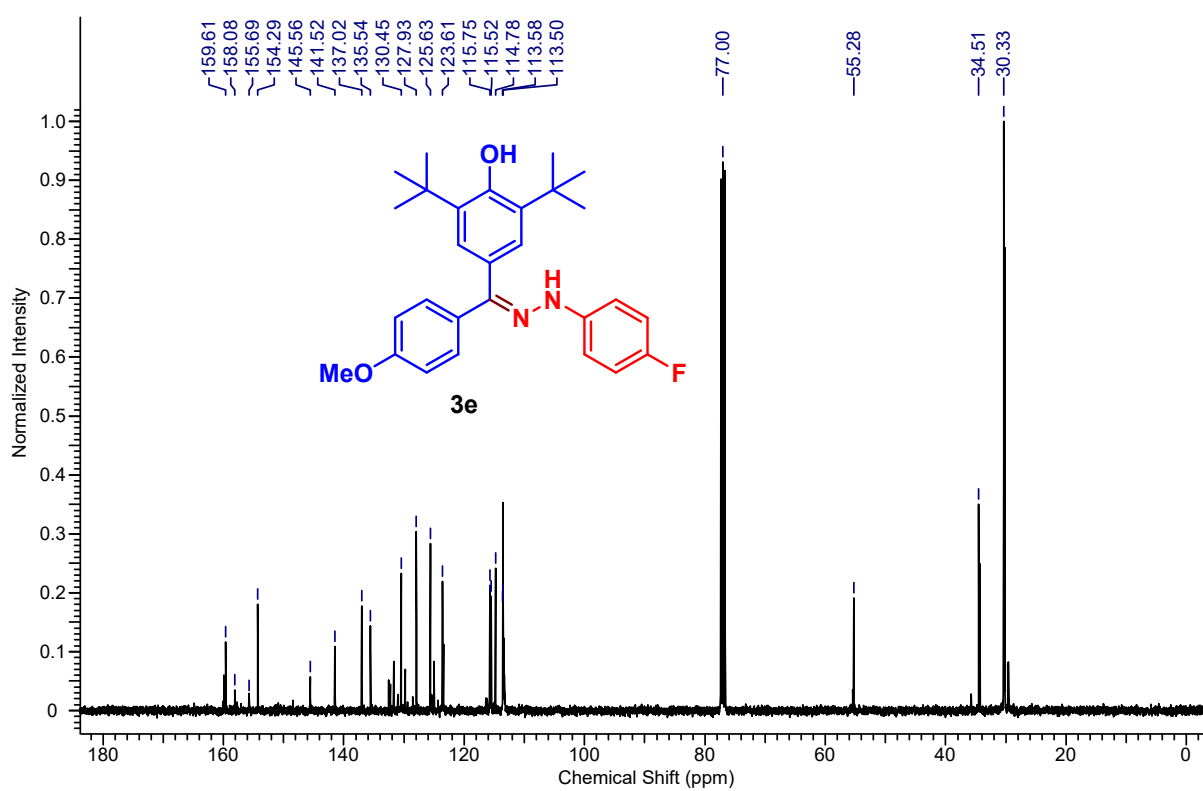


**HRMS of Compound 3d**

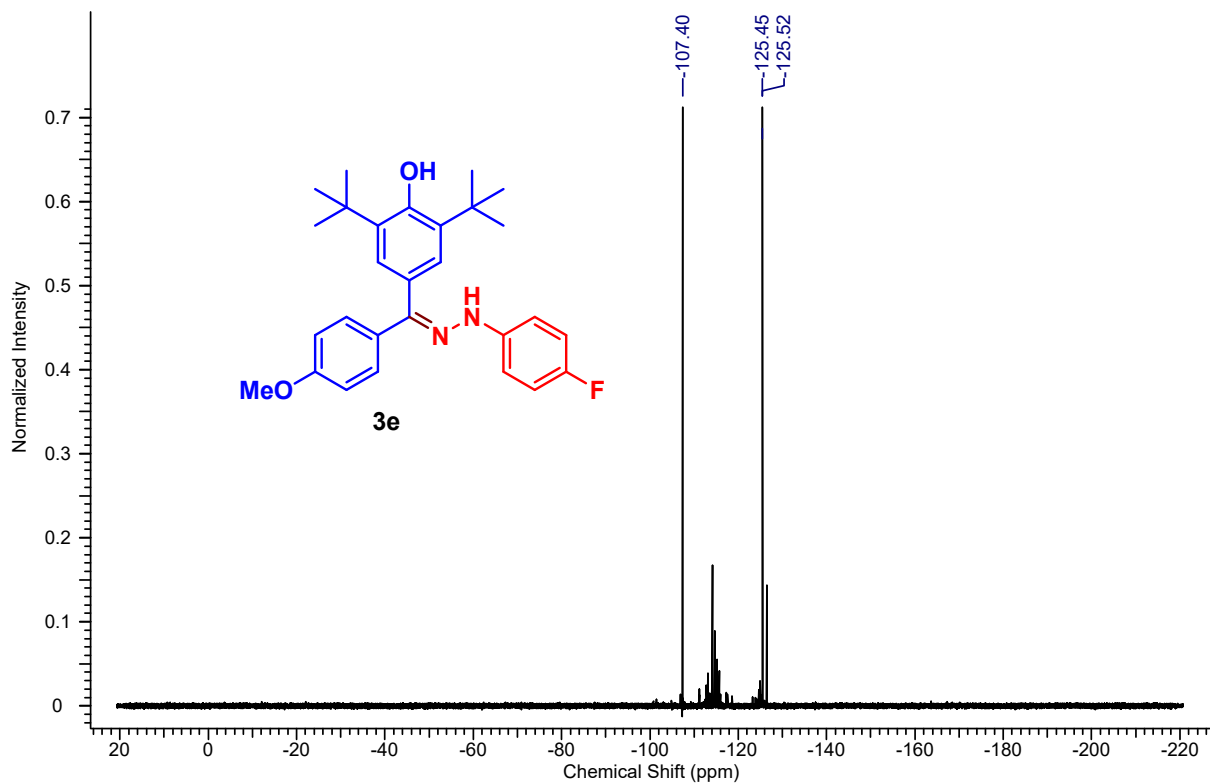




**<sup>1</sup>H NMR of Compound 3e [as 1:0.77 stereoisomeric mixture] (400 MHz, CDCl<sub>3</sub>)**

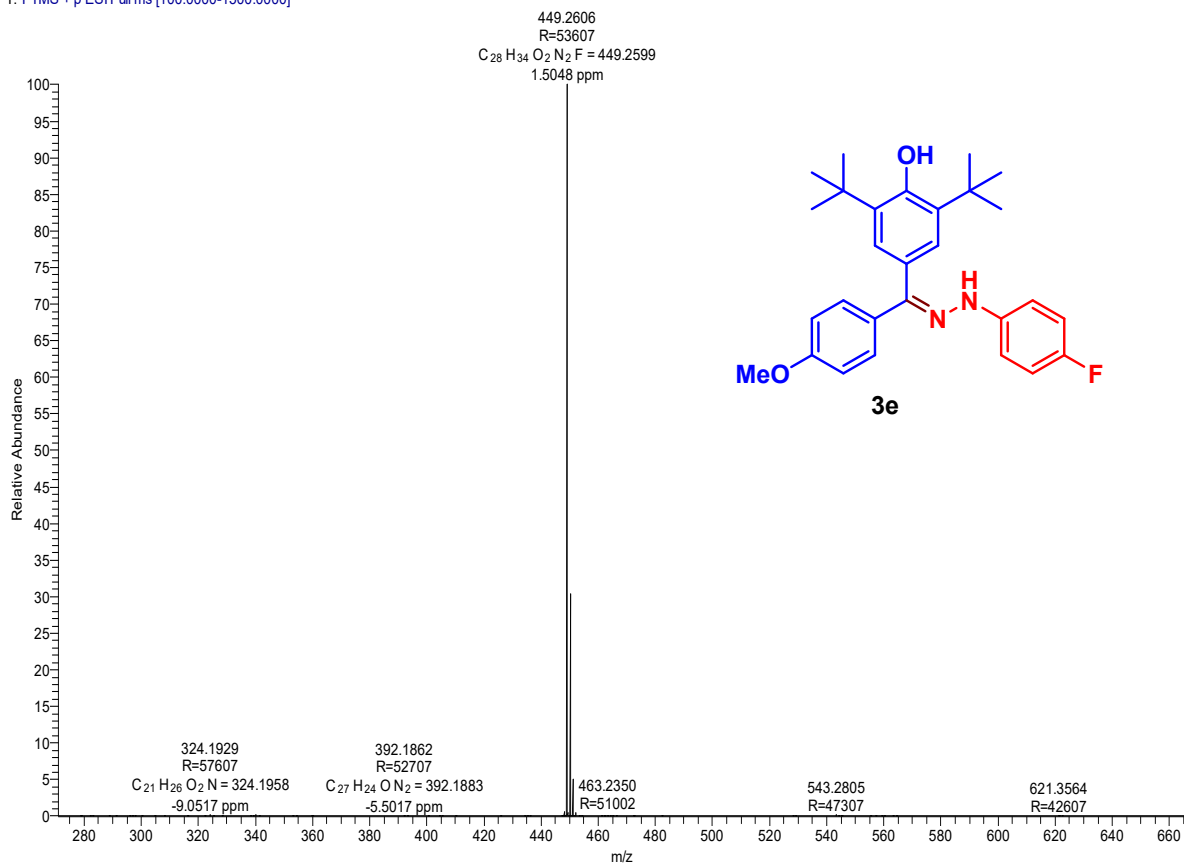


**<sup>13</sup>C NMR of Compound 3e [as 1:0.77 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)**

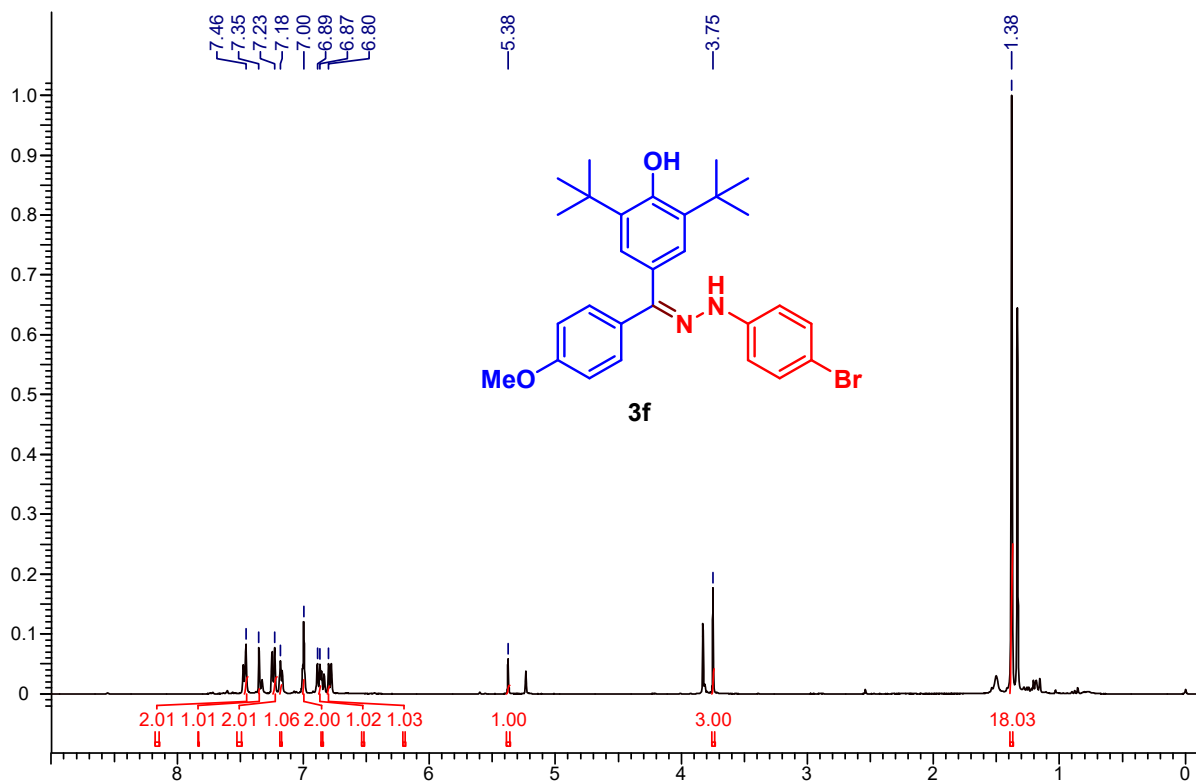


### <sup>19</sup>F NMR of Compound 3e [as 1:0.77 stereoisomeric mixture] (376 MHz, CDCl<sub>3</sub>)

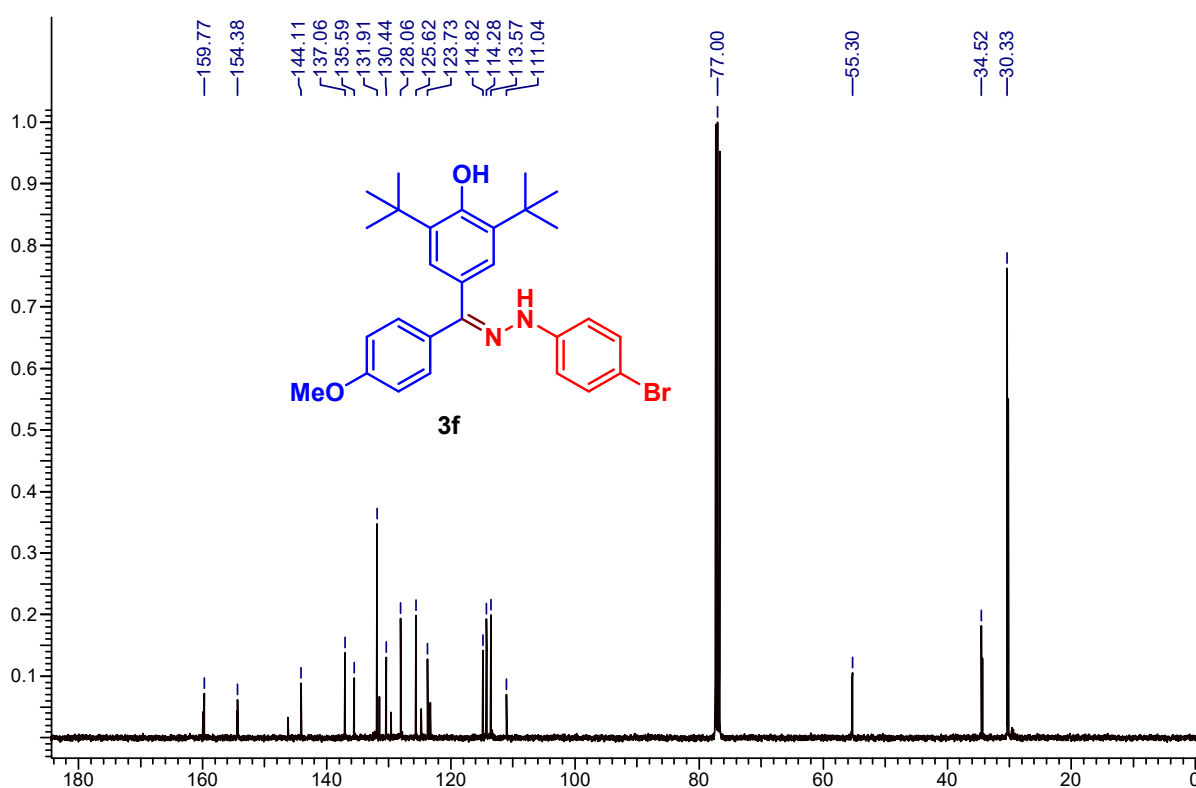
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### HRMS of Compound 3e

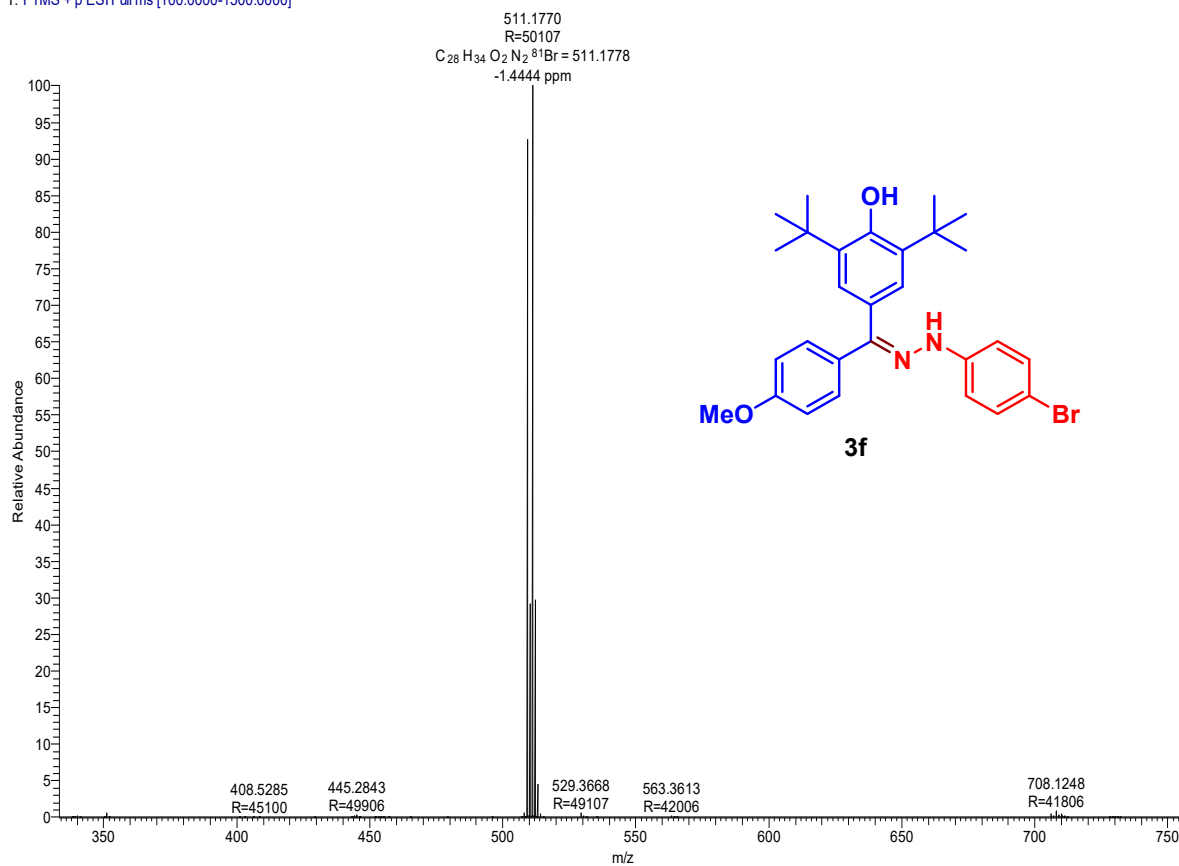


**<sup>1</sup>H NMR of Compound 3f [as 1:0.67 stereoisomeric mixture] (400 MHz, CDCl<sub>3</sub>)**

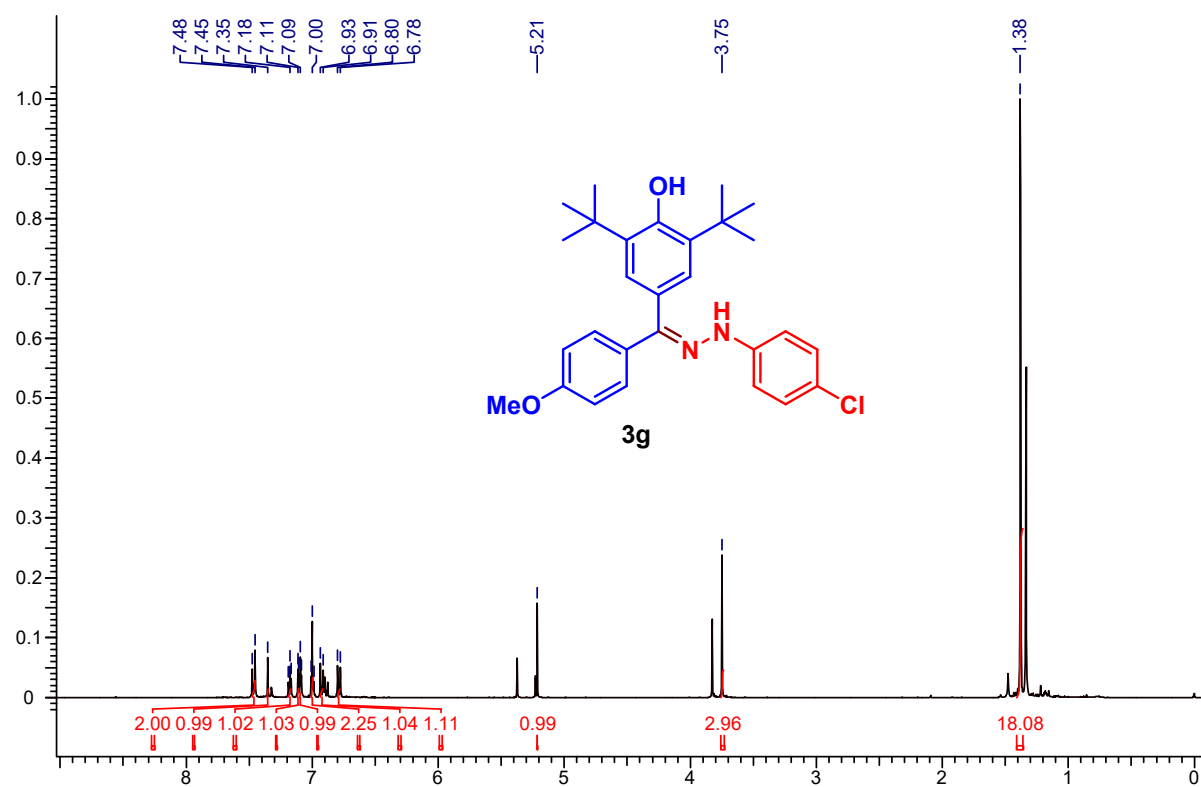


**<sup>13</sup>C NMR of Compound 3f [as 1:0.67 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)**

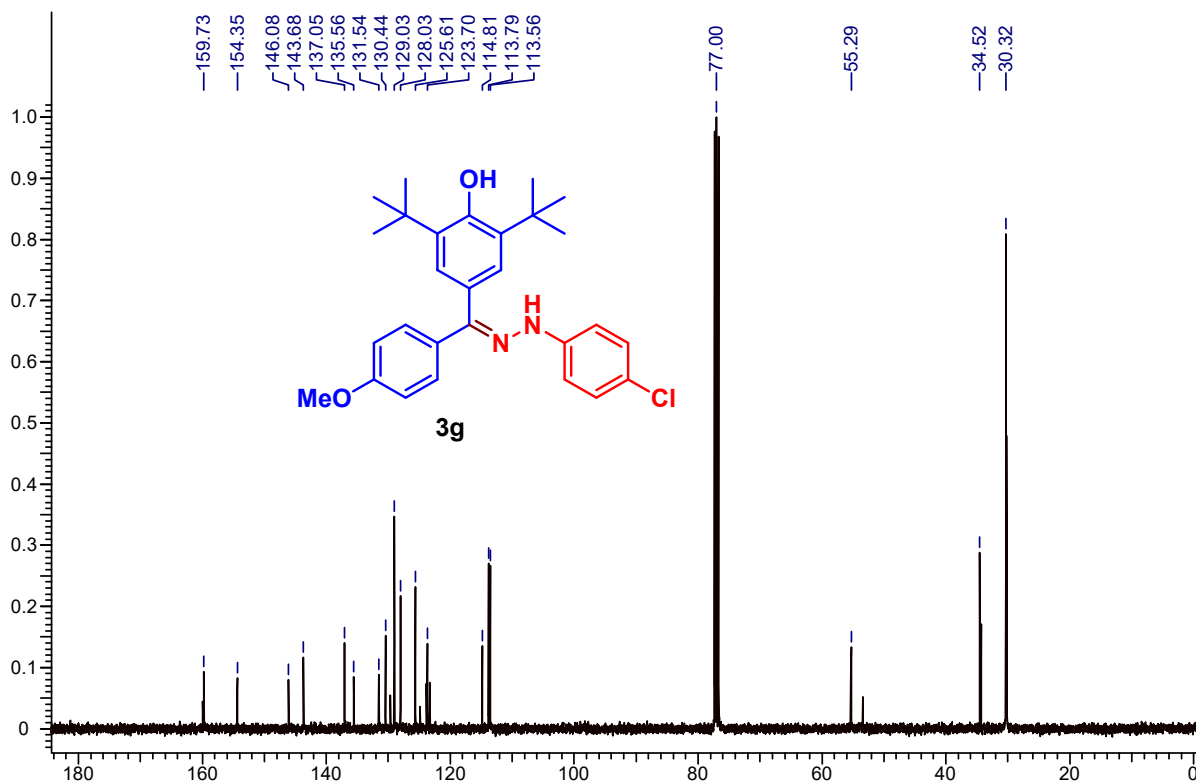
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T: FTMS + p ESI Full ms [100.0000-1500.0000]



### HRMS of Compound 3f

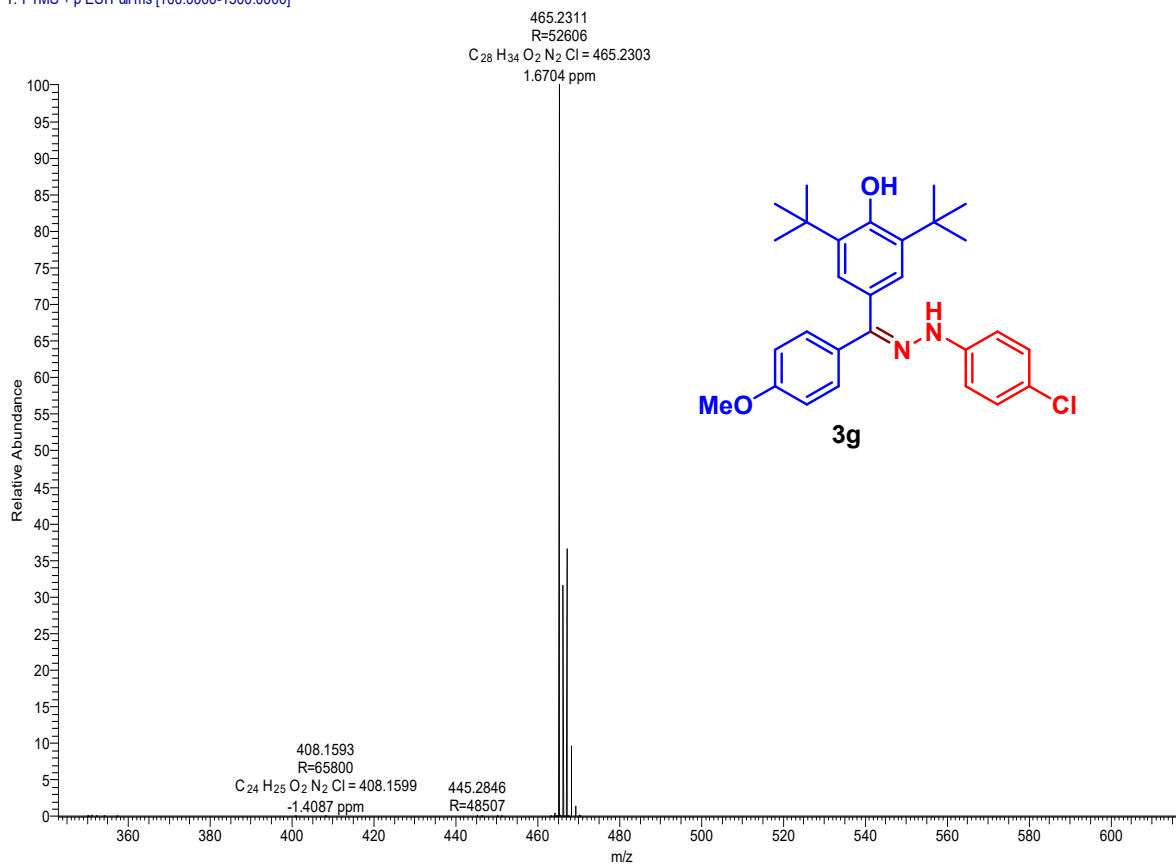


### <sup>1</sup>H NMR of Compound 3g [as 1:0.65 stereoisomeric mixture] (400 MHz, CDCl<sub>3</sub>)

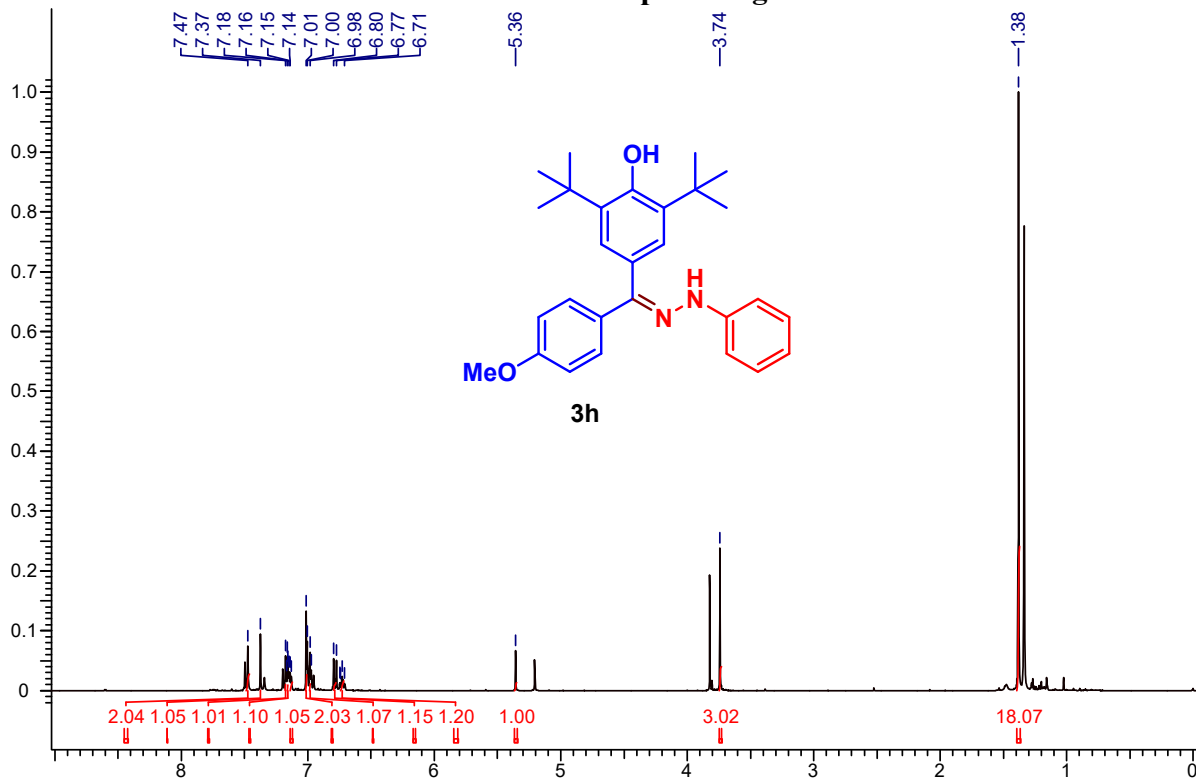


**<sup>13</sup>C NMR of Compound 3g [as 1:0.65 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)**

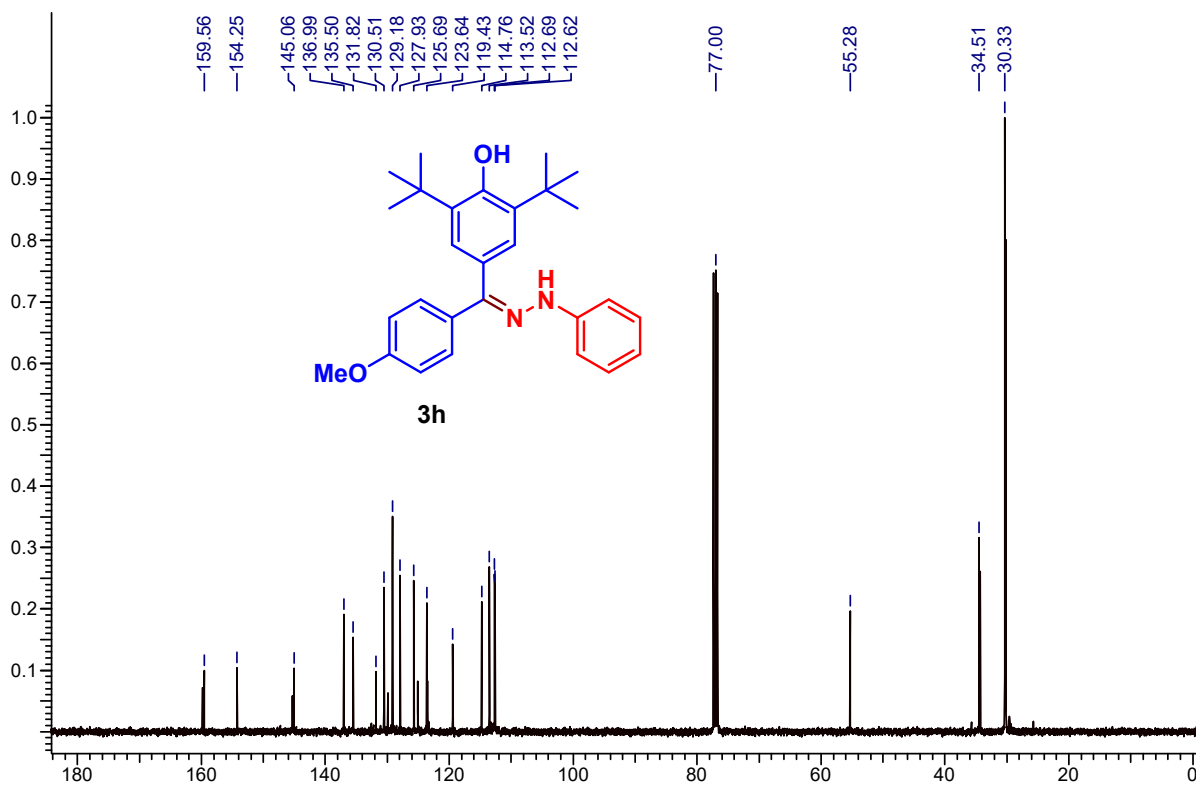
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### HRMS of Compound 3g

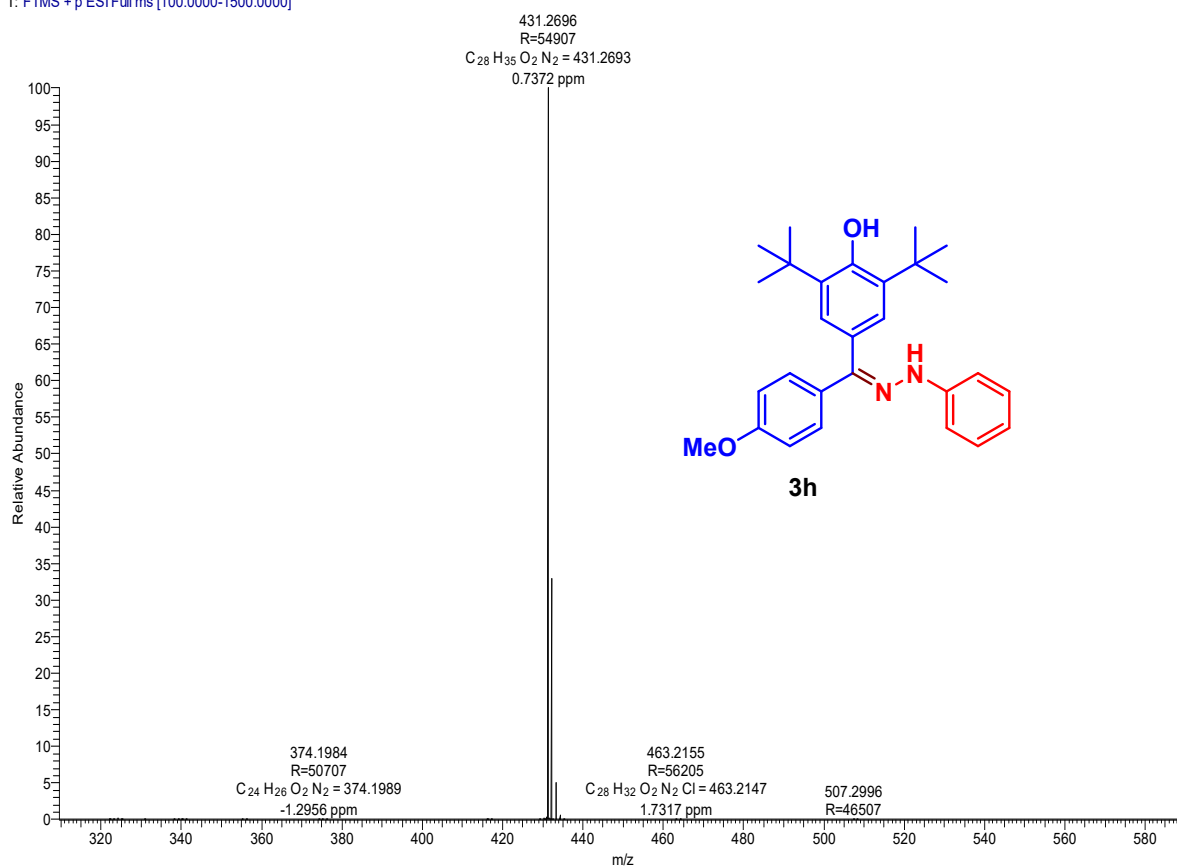


### <sup>13</sup>C NMR of Compound 3h [as 1:0.81 stereoisomeric mixture] (400 MHz, CDCl<sub>3</sub>)

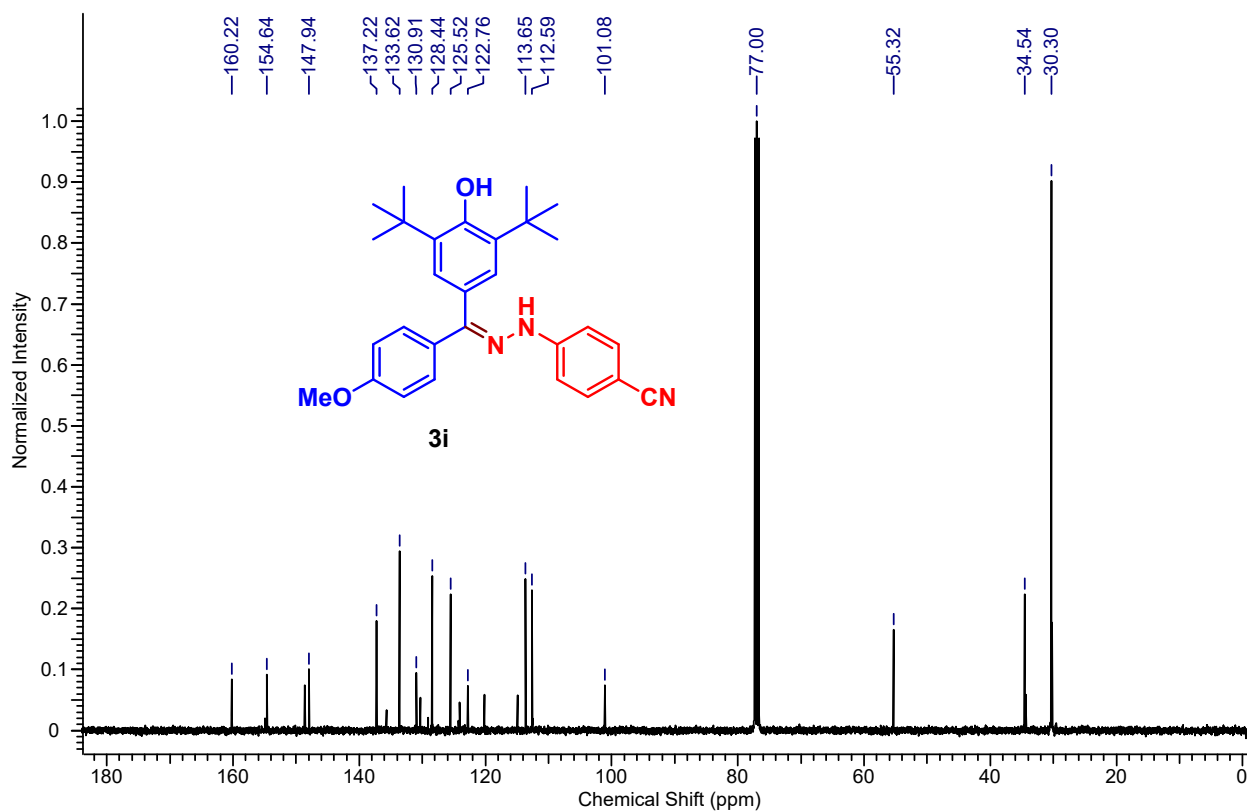
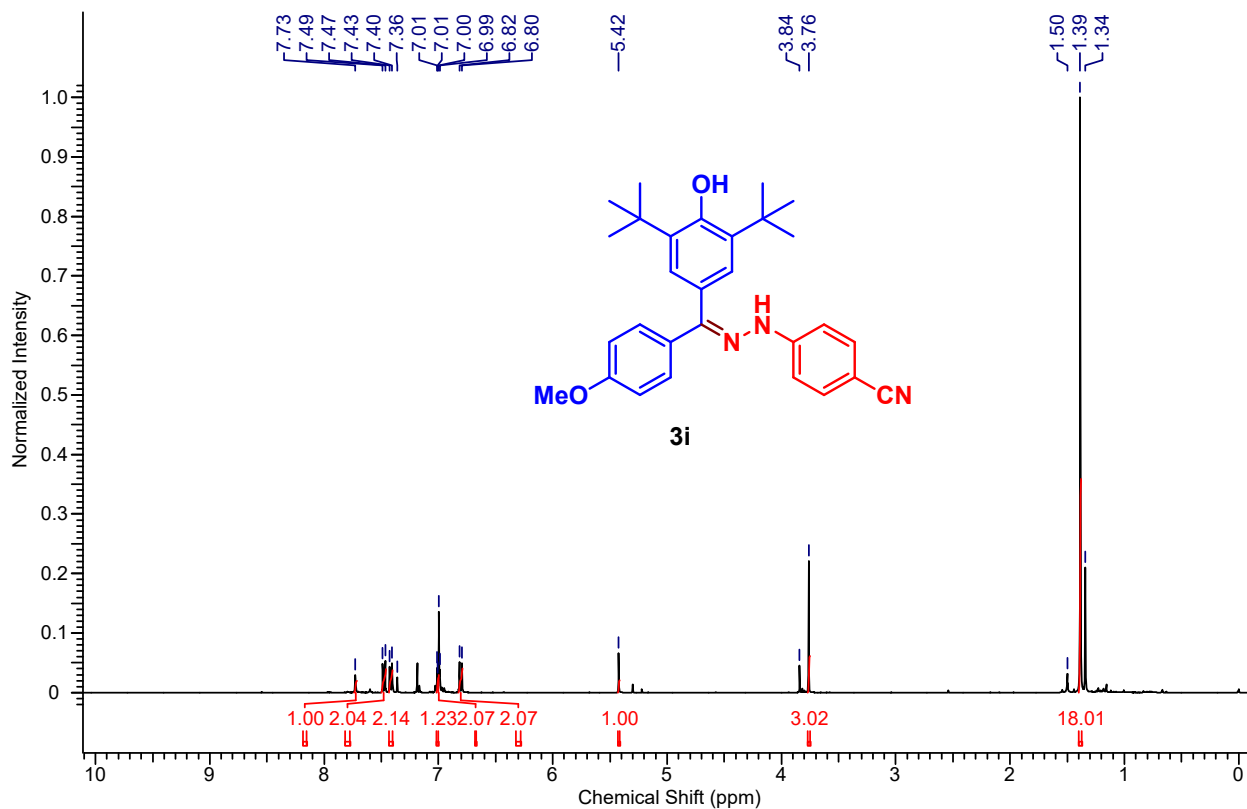


# <sup>13</sup>C NMR of Compound 3h [as 1:0.81 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)

5J#741 RT: 3.31 AV: 1 NL: 8.36E9  
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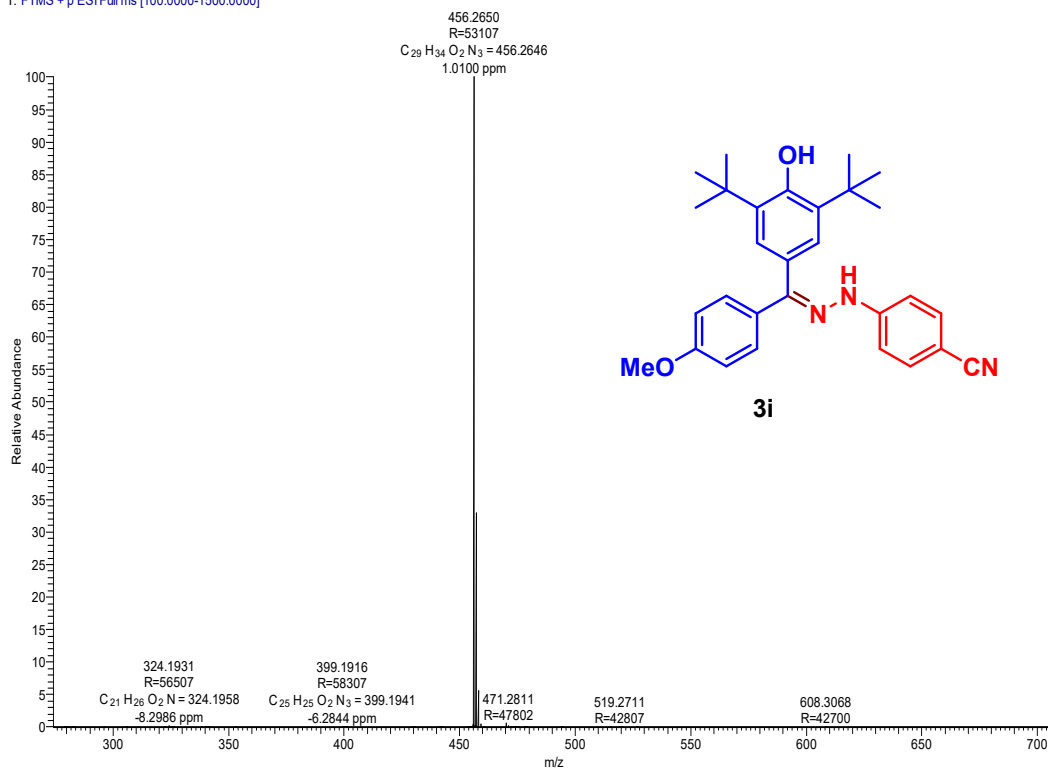


HRMS of Compound 3h

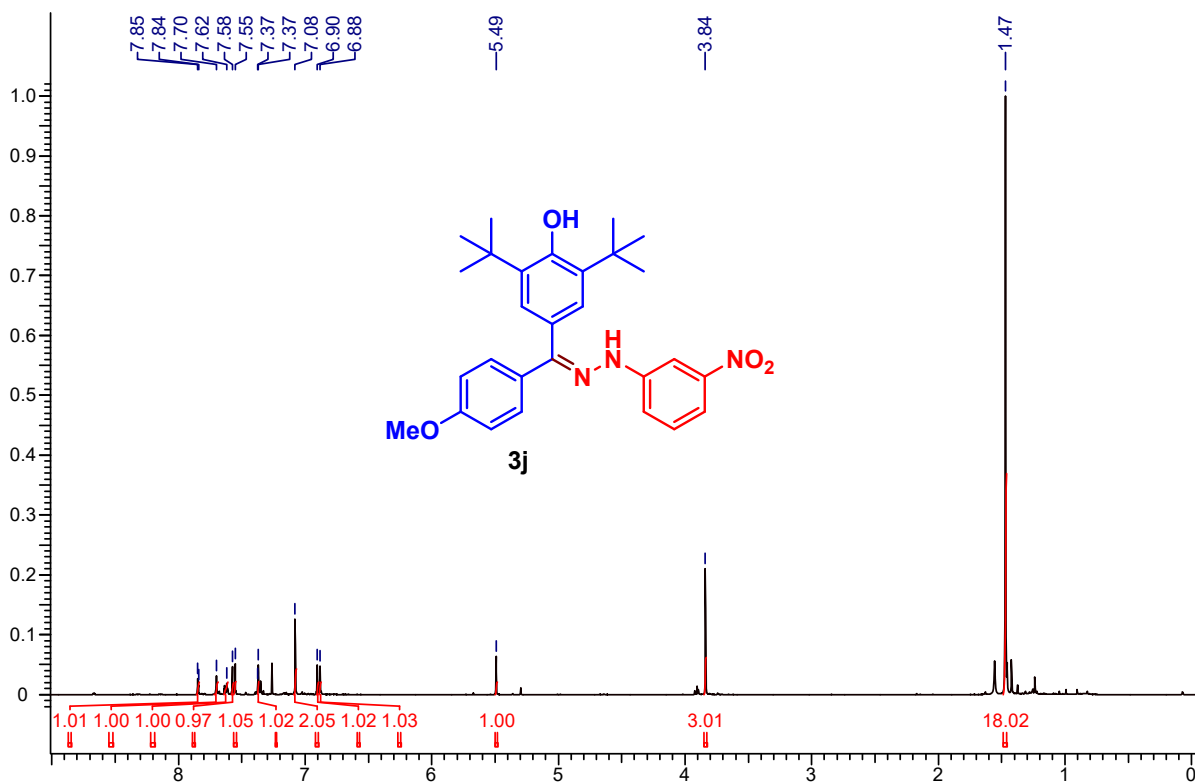




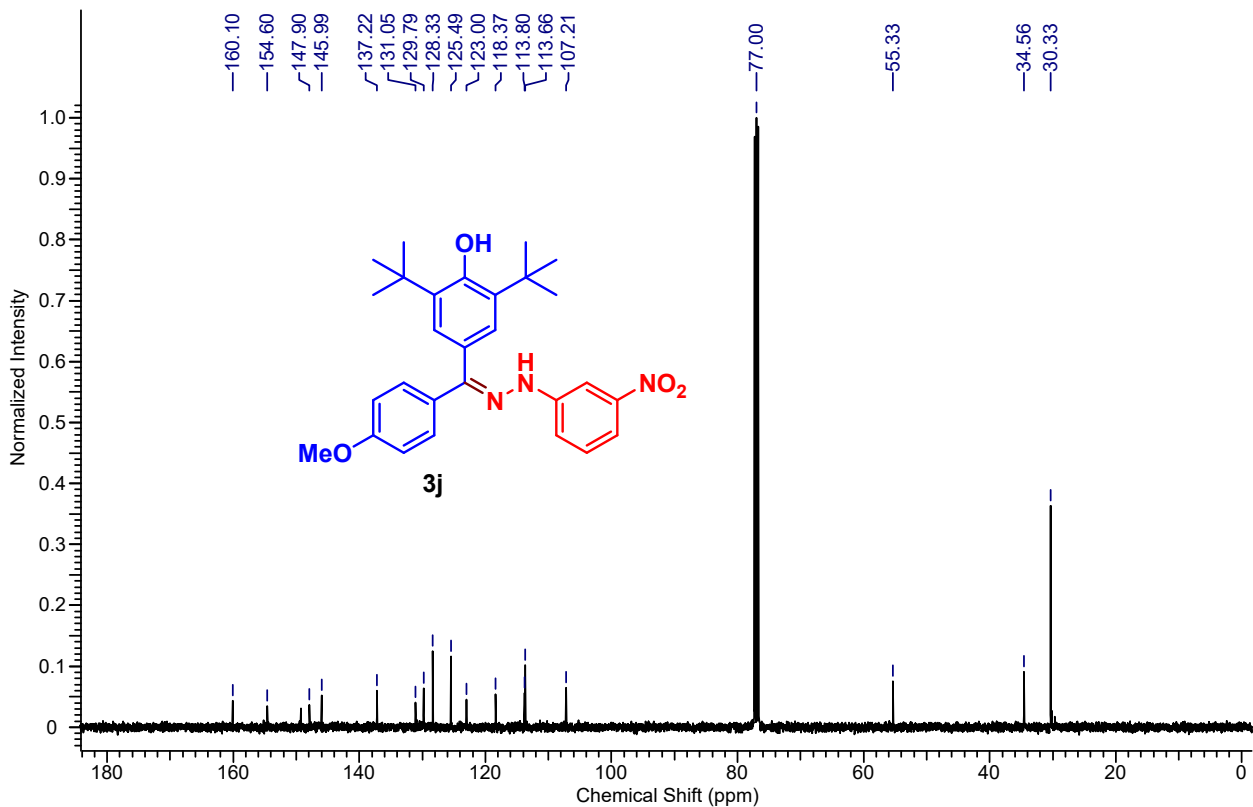
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### HRMS of Compound 3i

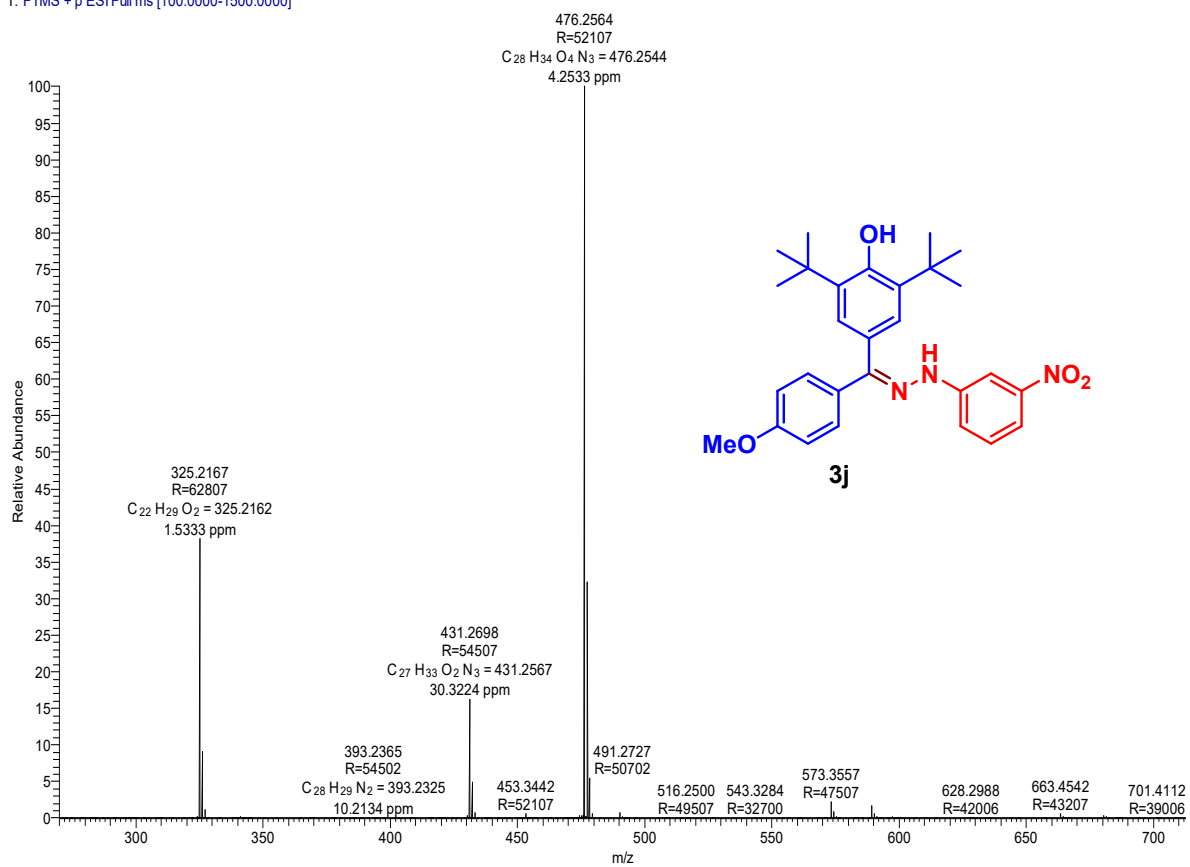


### <sup>1</sup>H NMR of Compound 3j [as 1:0.11 stereoisomeric mixture] (400 MHz, CDCl<sub>3</sub>)

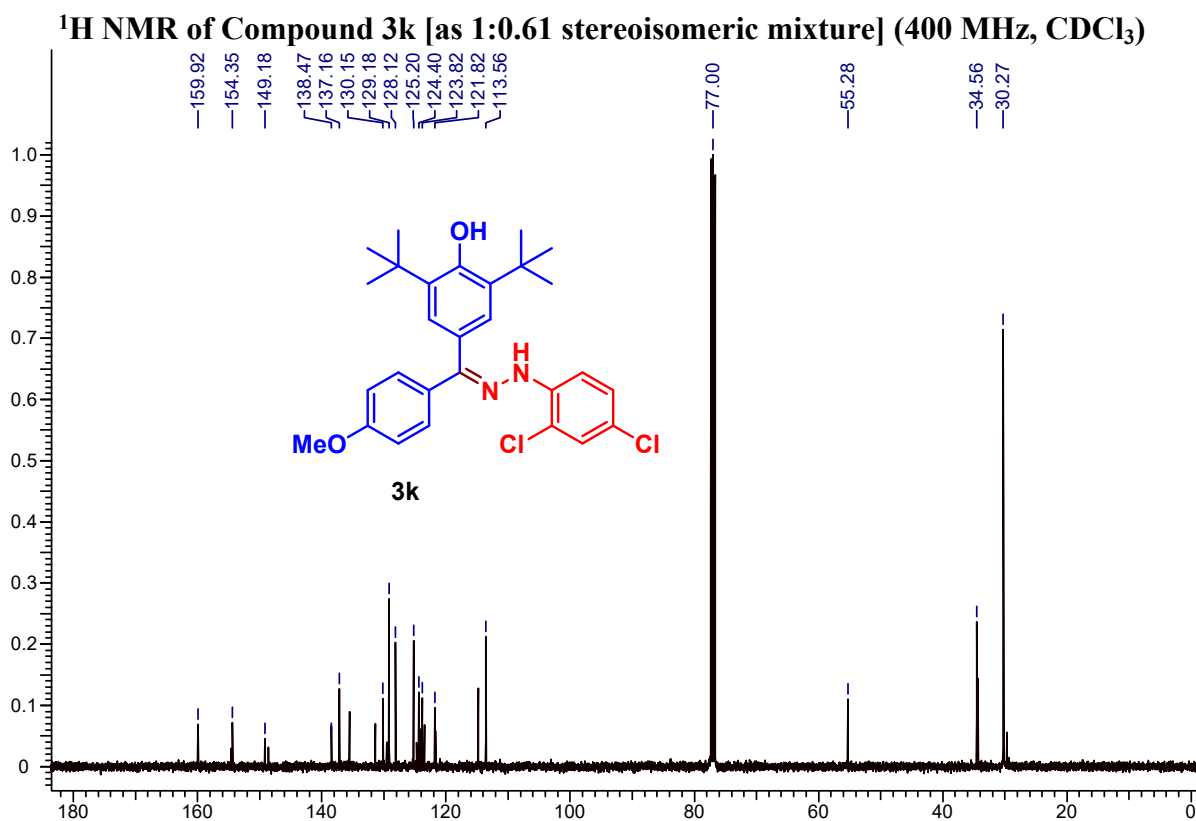
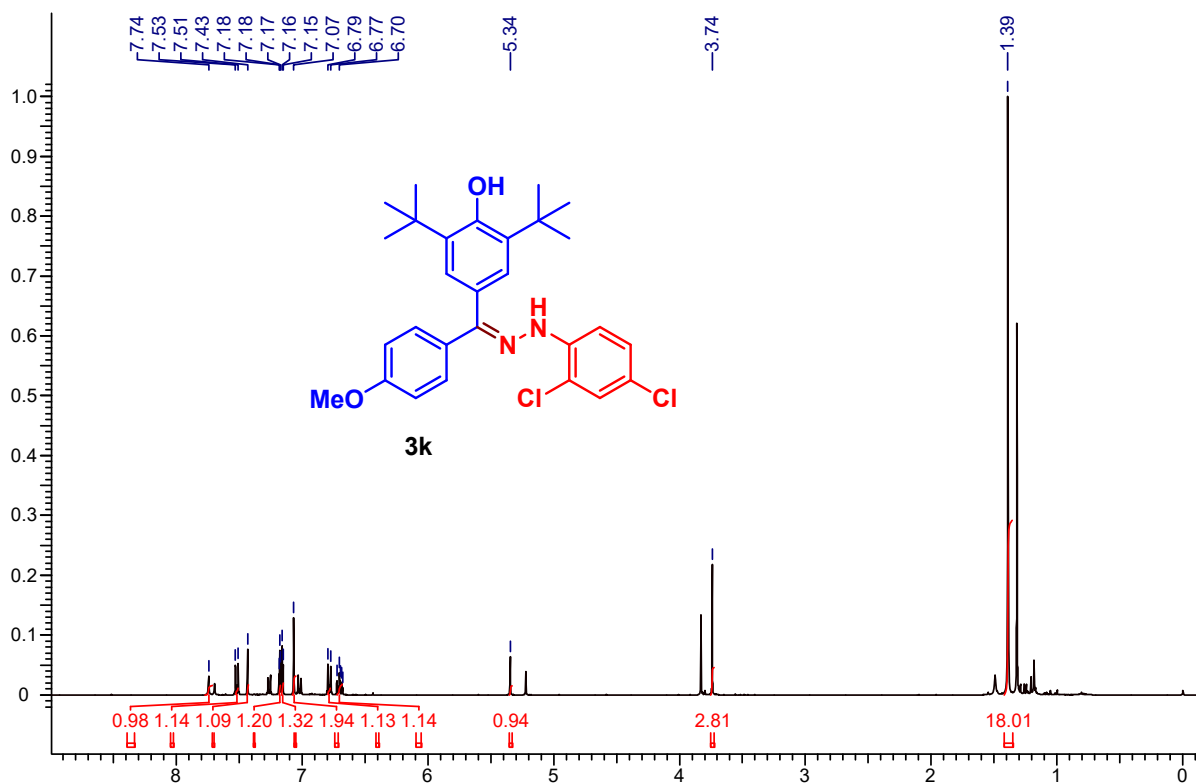


**<sup>13</sup>C NMR of Compound 3j [as 1:0.11 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)**

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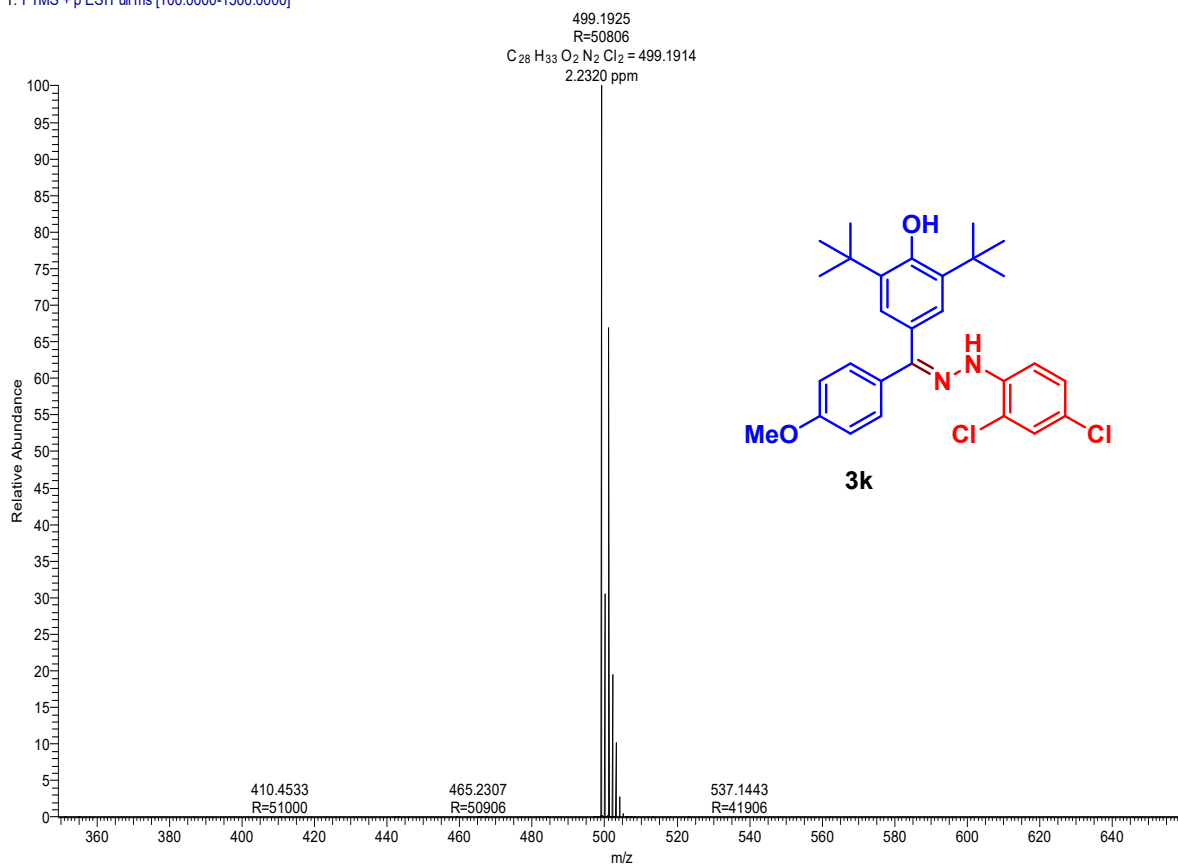


**HRMS of Compound 3j**

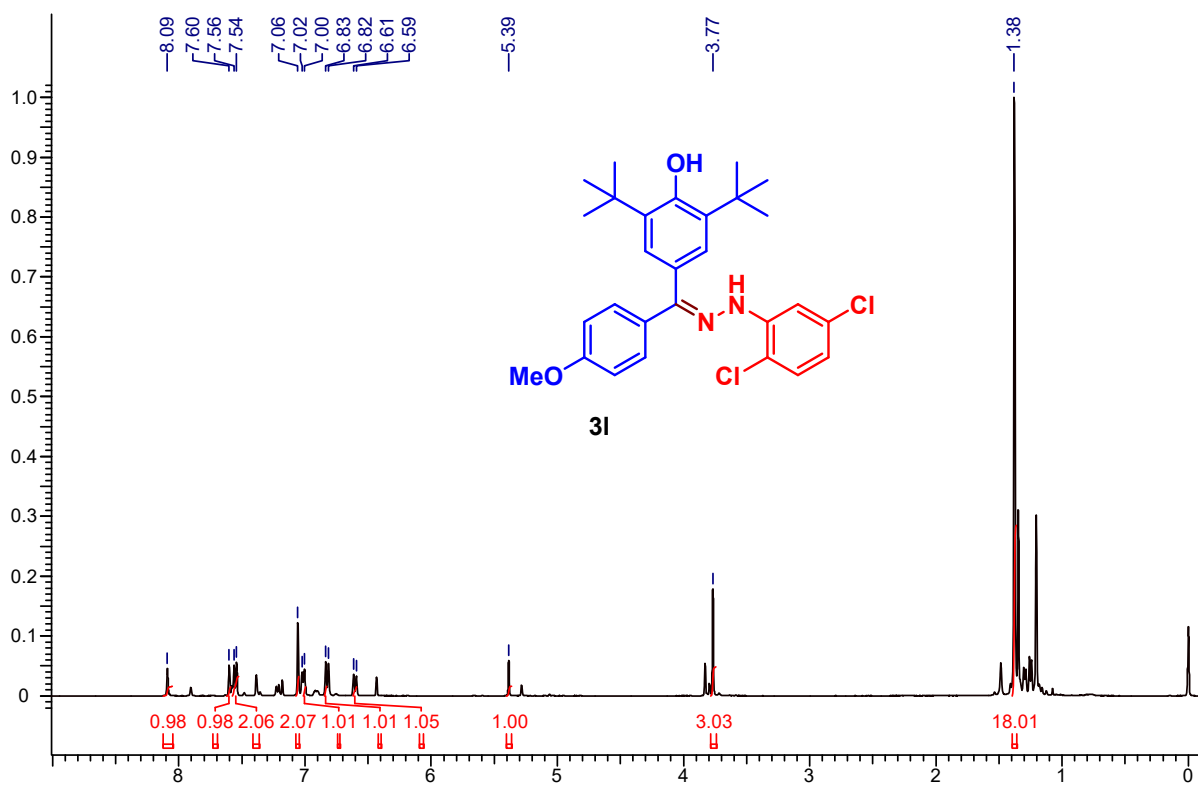


**<sup>13</sup>C NMR of Compound 3k [as 1:0.61 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)**

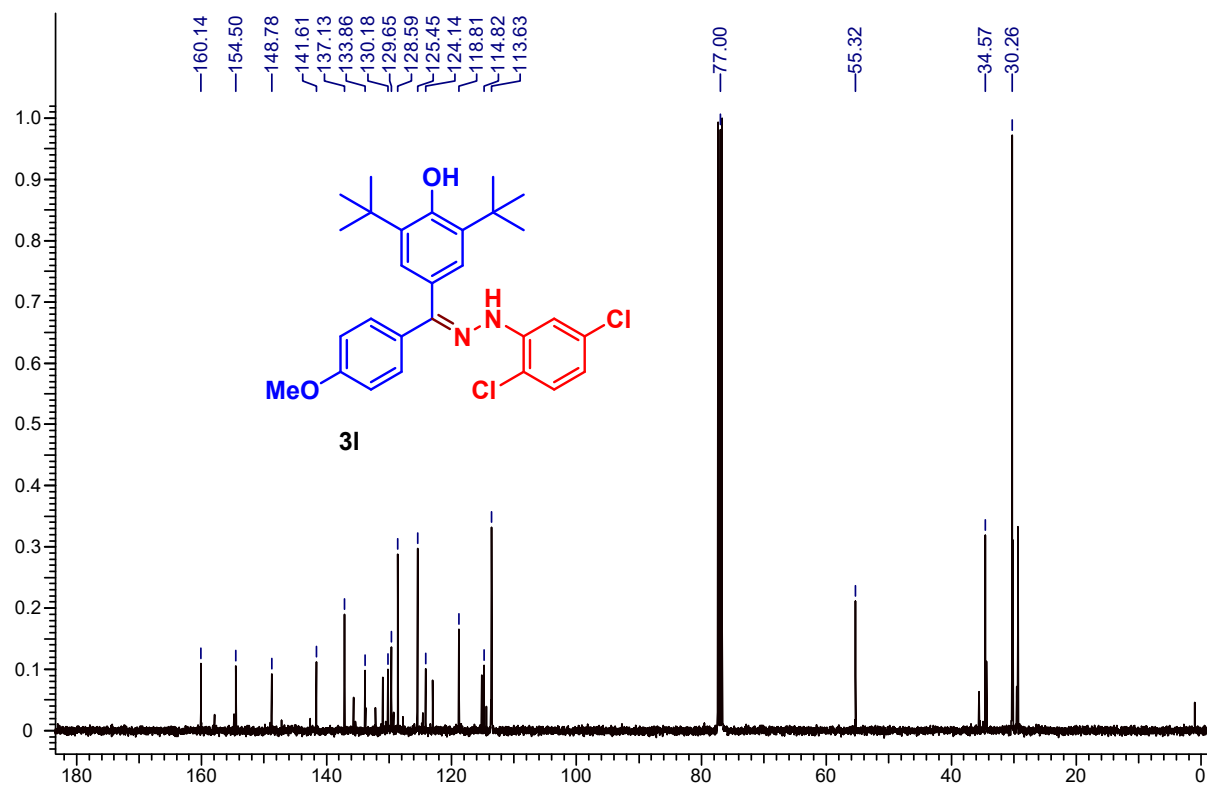
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### HRMS of Compound 3k

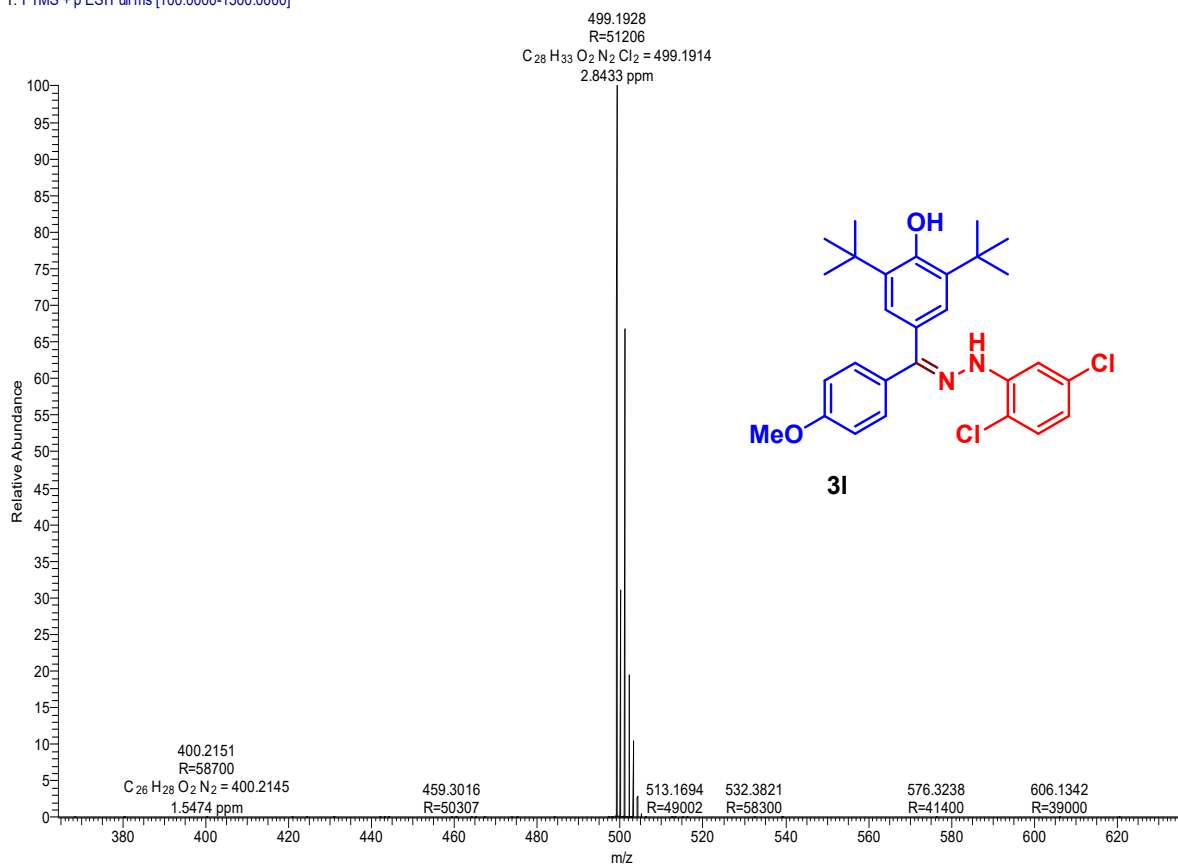


**<sup>1</sup>H NMR of Compound 3I [as 1:0.30 stereoisomeric mixture] (400 MHz, CDCl<sub>3</sub>)**

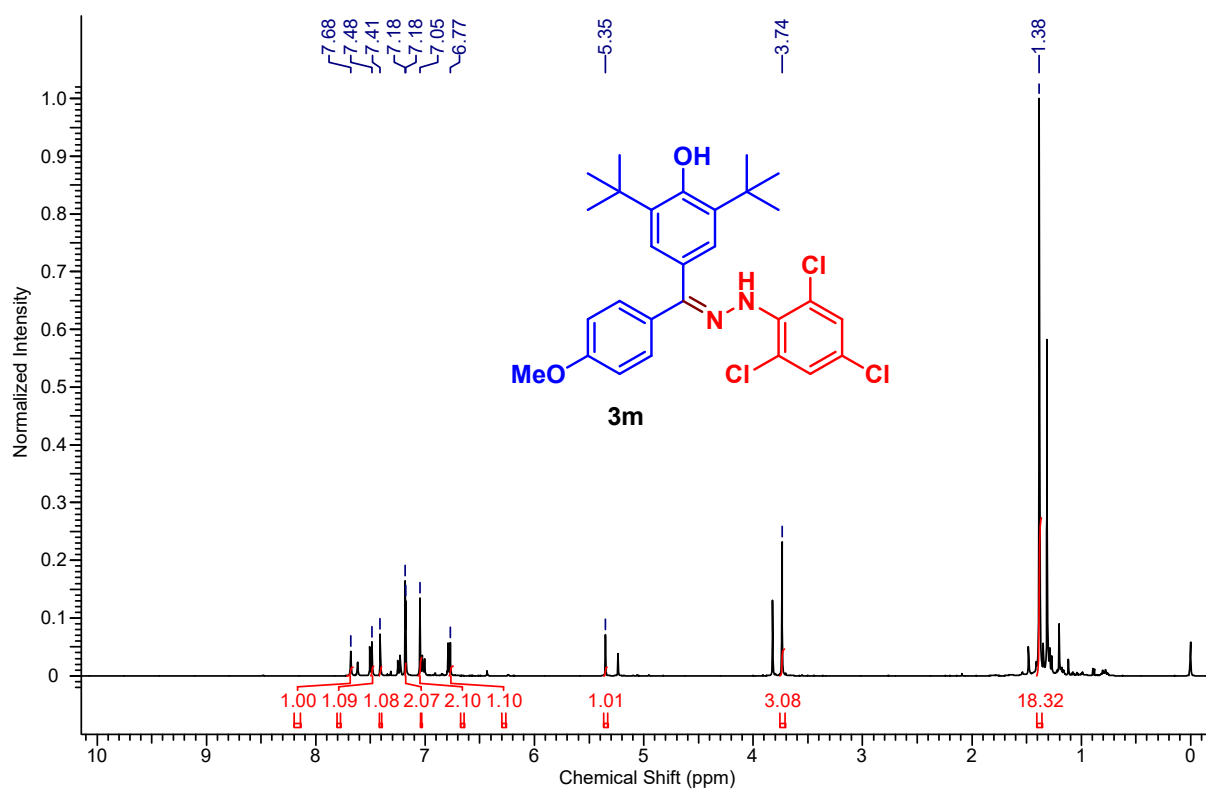


**<sup>13</sup>C NMR of Compound 3I [as 1:0.30 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)**

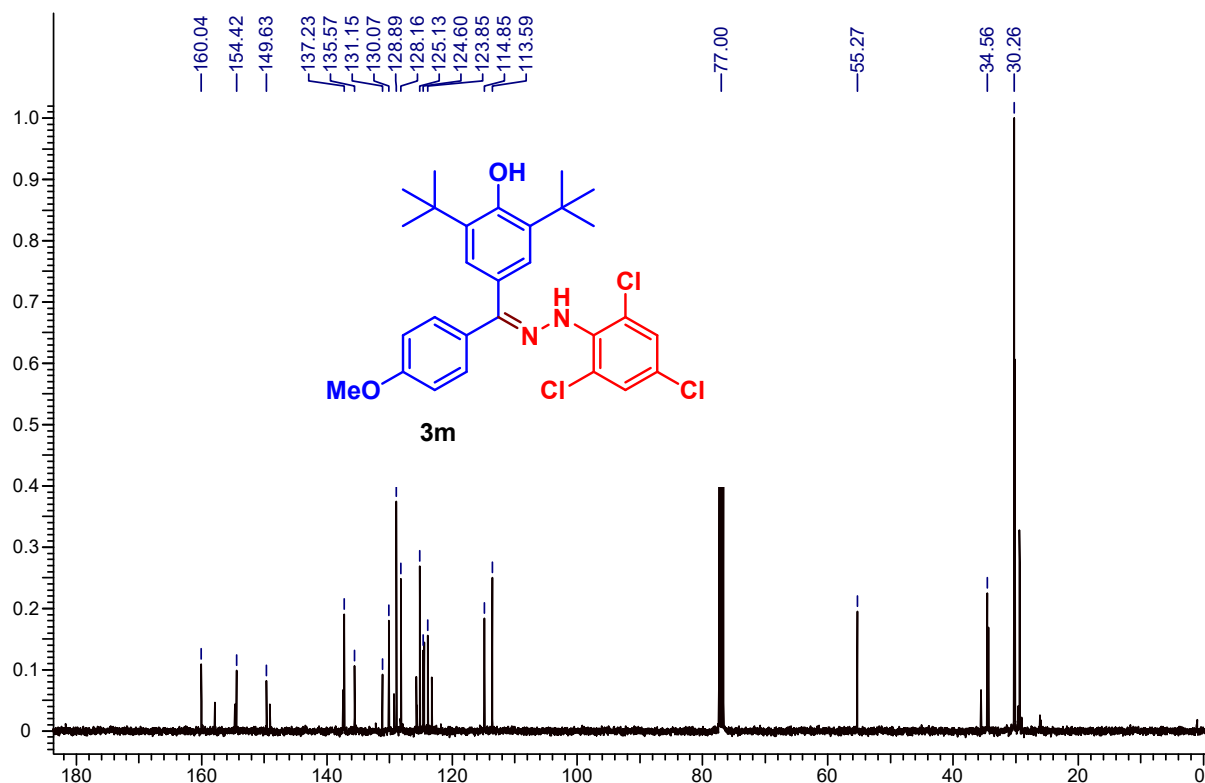
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### HRMS of Compound 3l

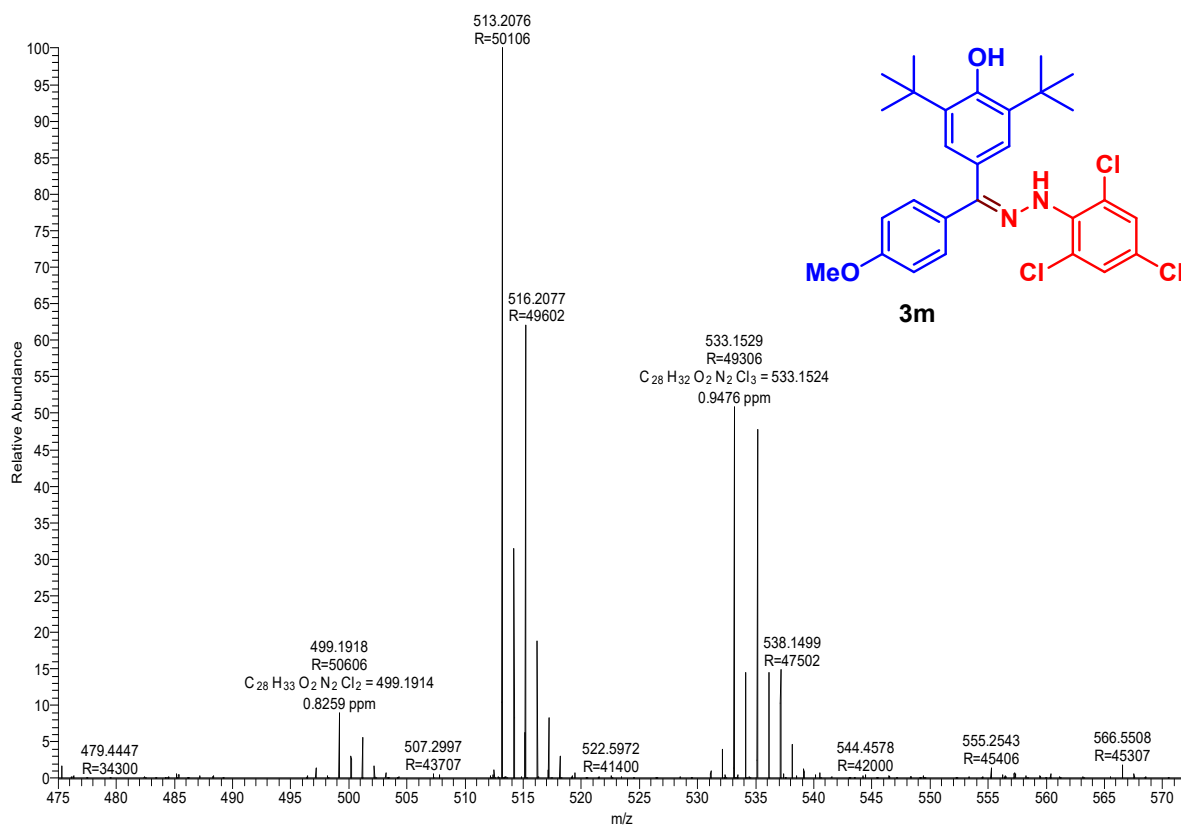


### <sup>1</sup>H NMR of Compound 3m [as 1:0.59 stereoisomeric mixture] (400 MHz, CDCl<sub>3</sub>)

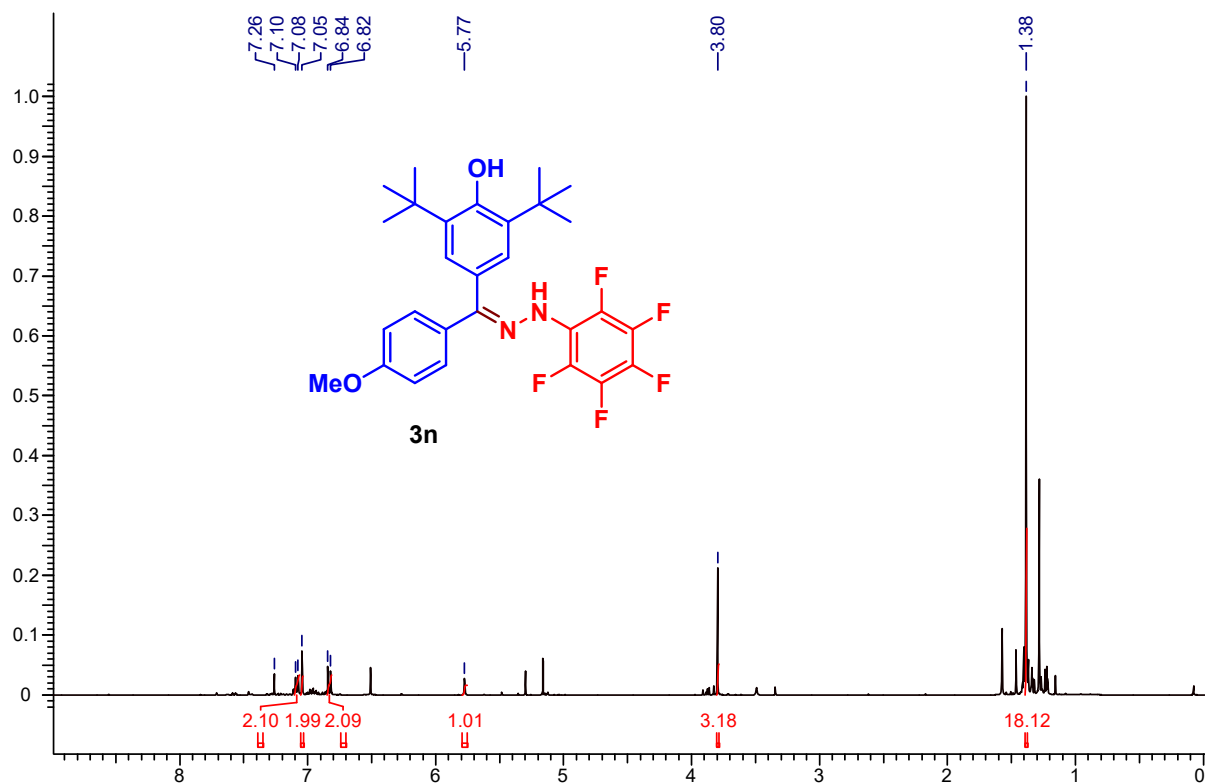


### <sup>13</sup>C NMR of Compound 3m [as 1:0.59 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)

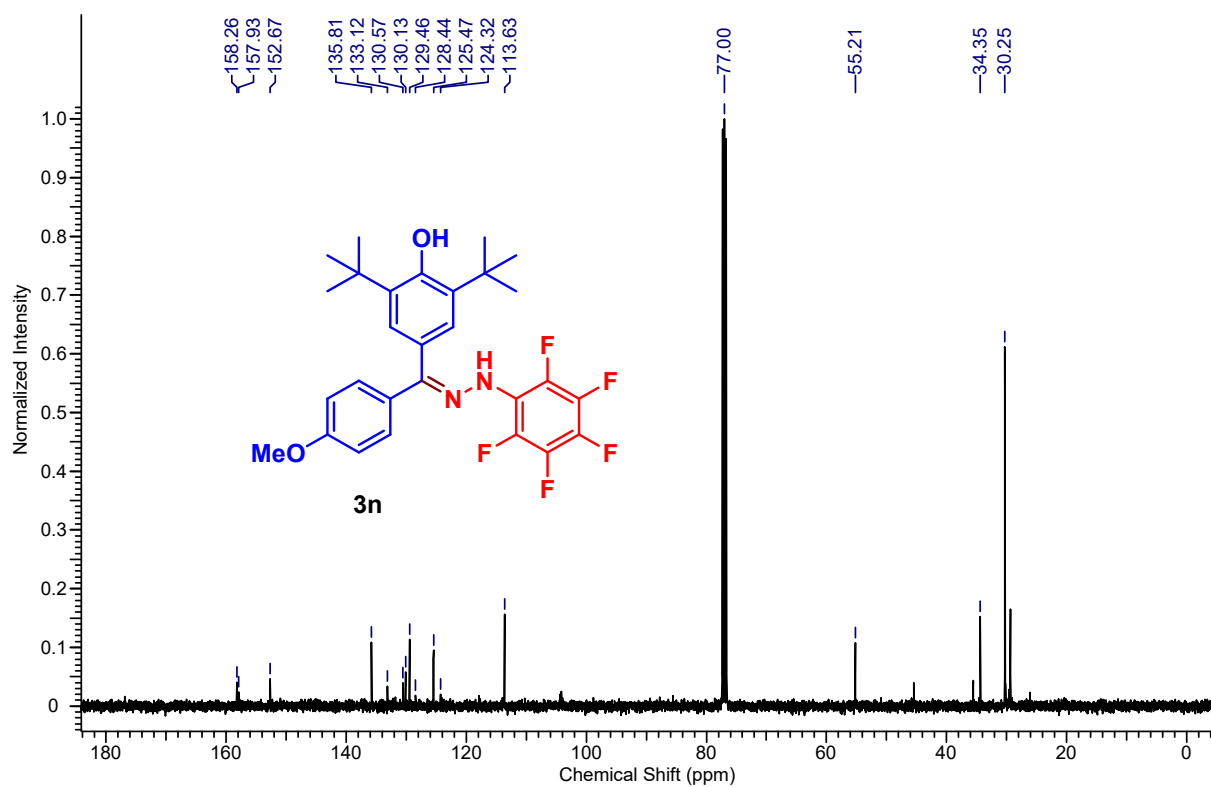
50\_230626141631 #889 RT: 3.97 AV: 1 NL: 3.43E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]



### HRMS of Compound 3m

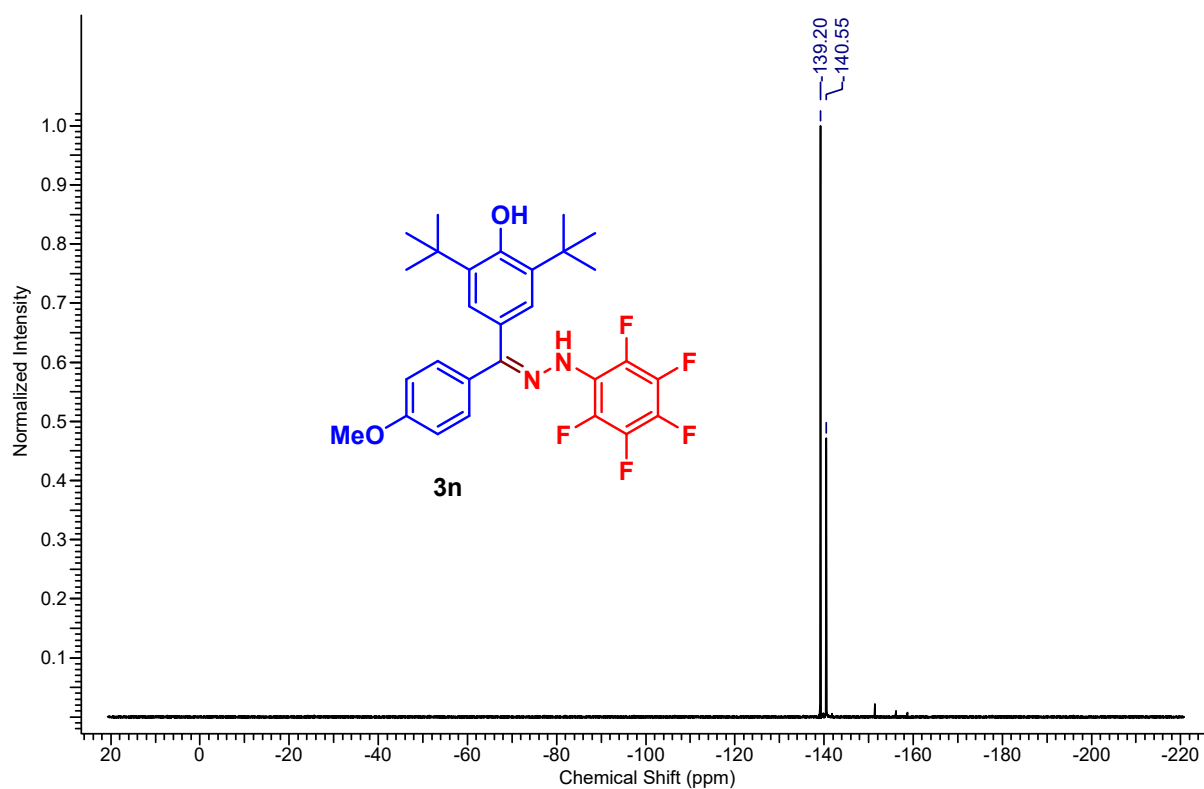


### <sup>1</sup>H NMR of Compound 3n (400 MHz, CDCl<sub>3</sub>)

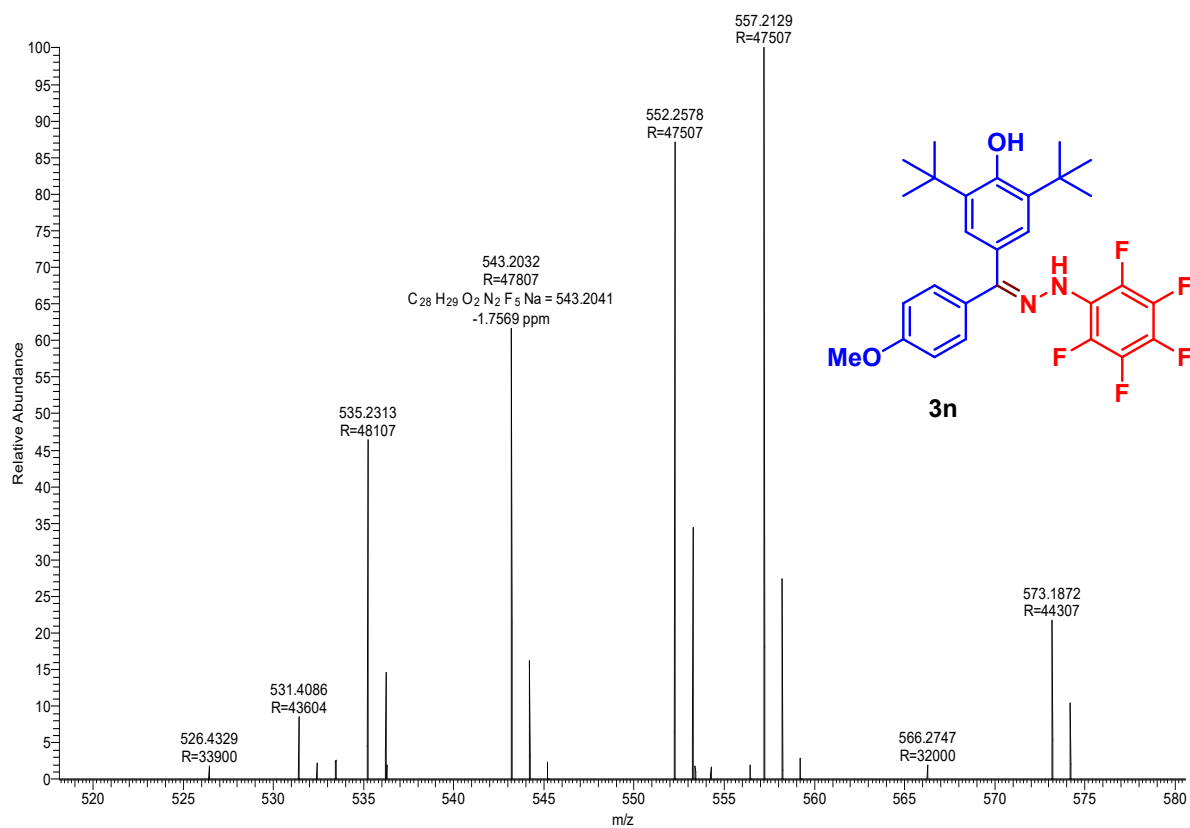




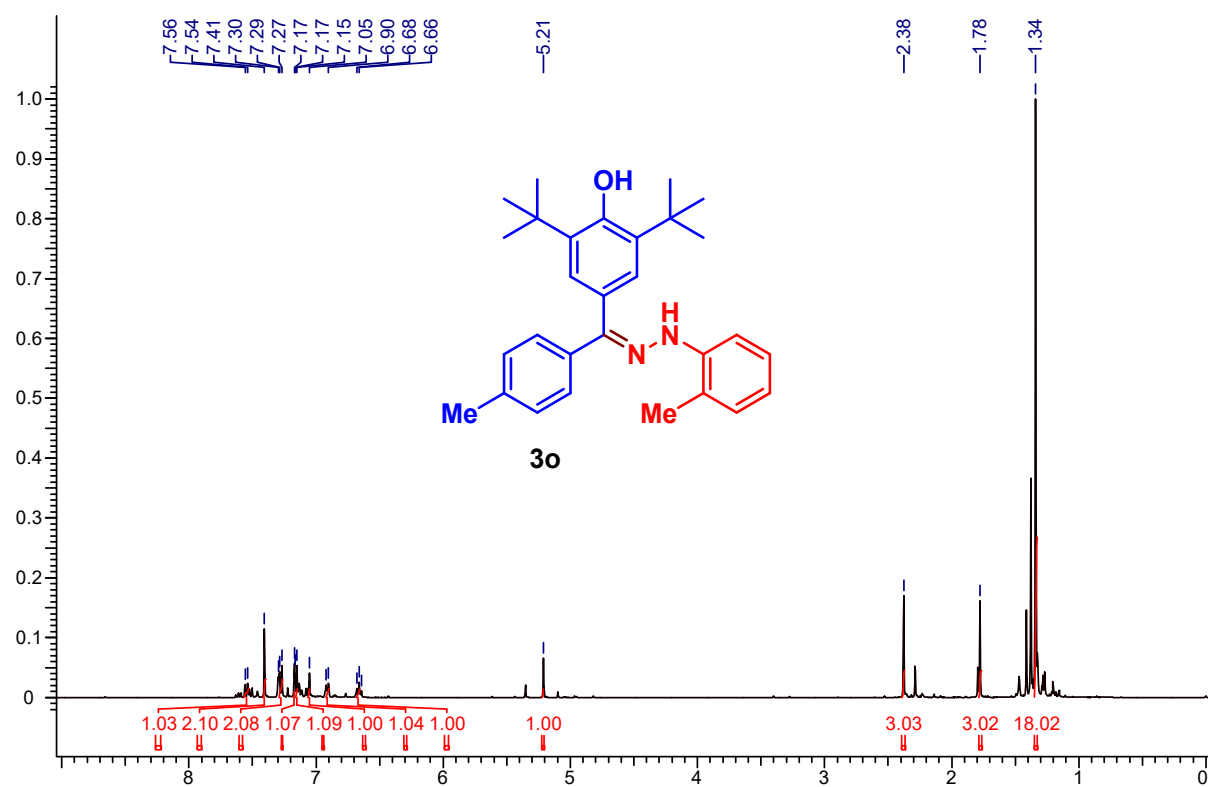
### $^{13}\text{C}$ NMR of Compound 3n (101 MHz, $\text{CDCl}_3$ )



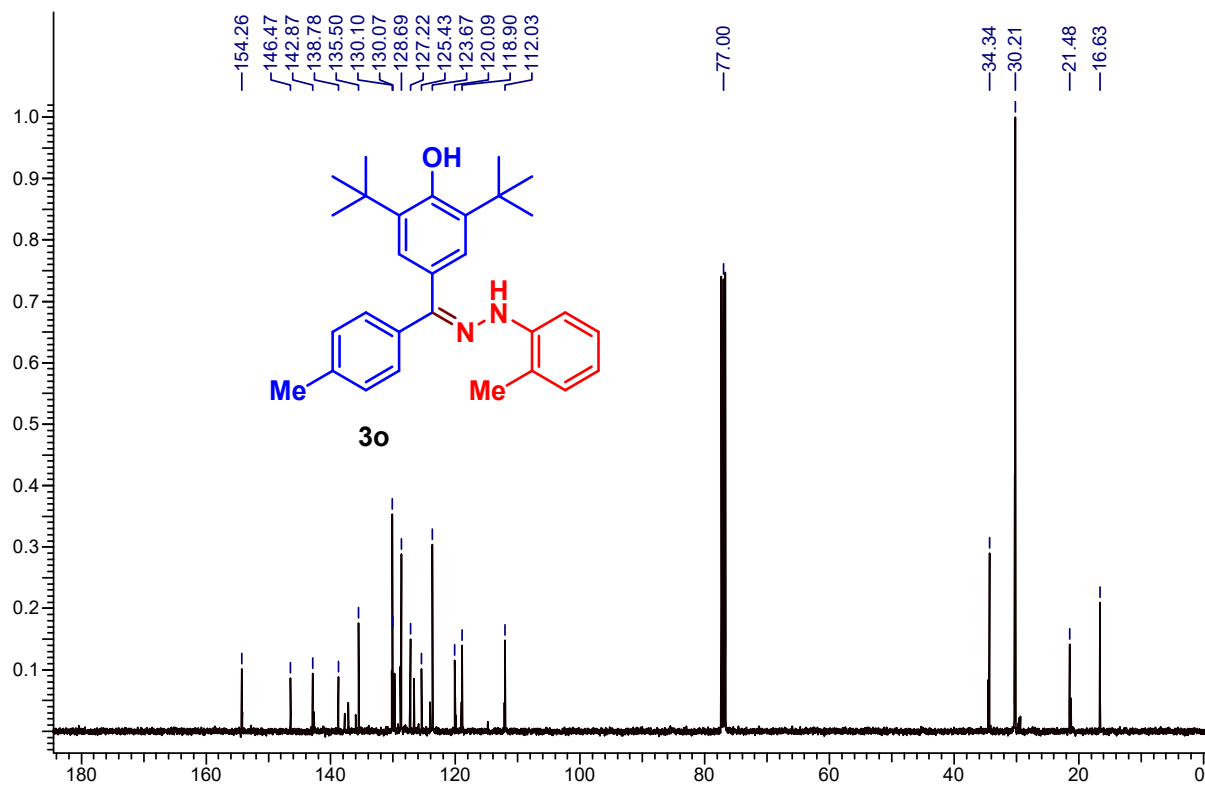
### $^{19}\text{F}$ NMR of Compound 3n (376 MHz, $\text{CDCl}_3$ )



### HRMS of Compound 3n

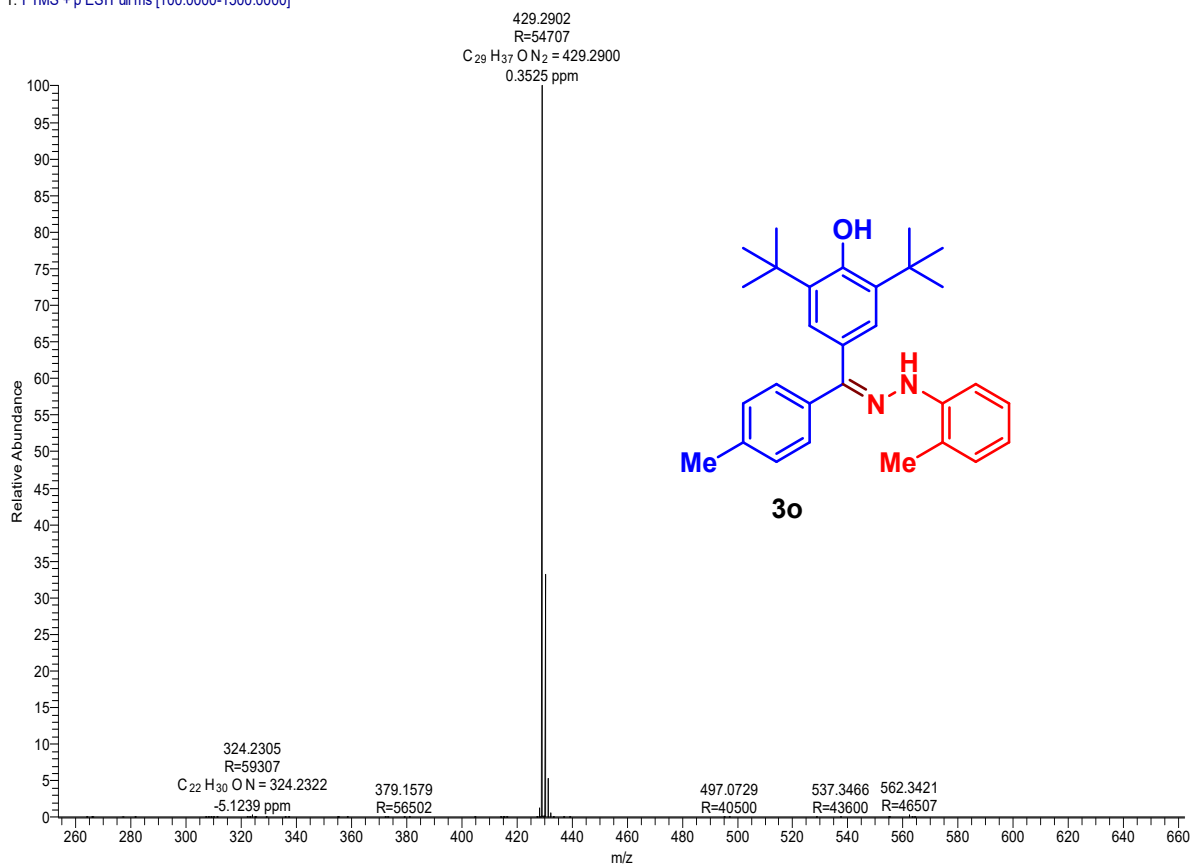


**<sup>1</sup>H NMR of Compound 3o [as 1:0.27 stereoisomeric mixture] (400 MHz, CDCl<sub>3</sub>)**

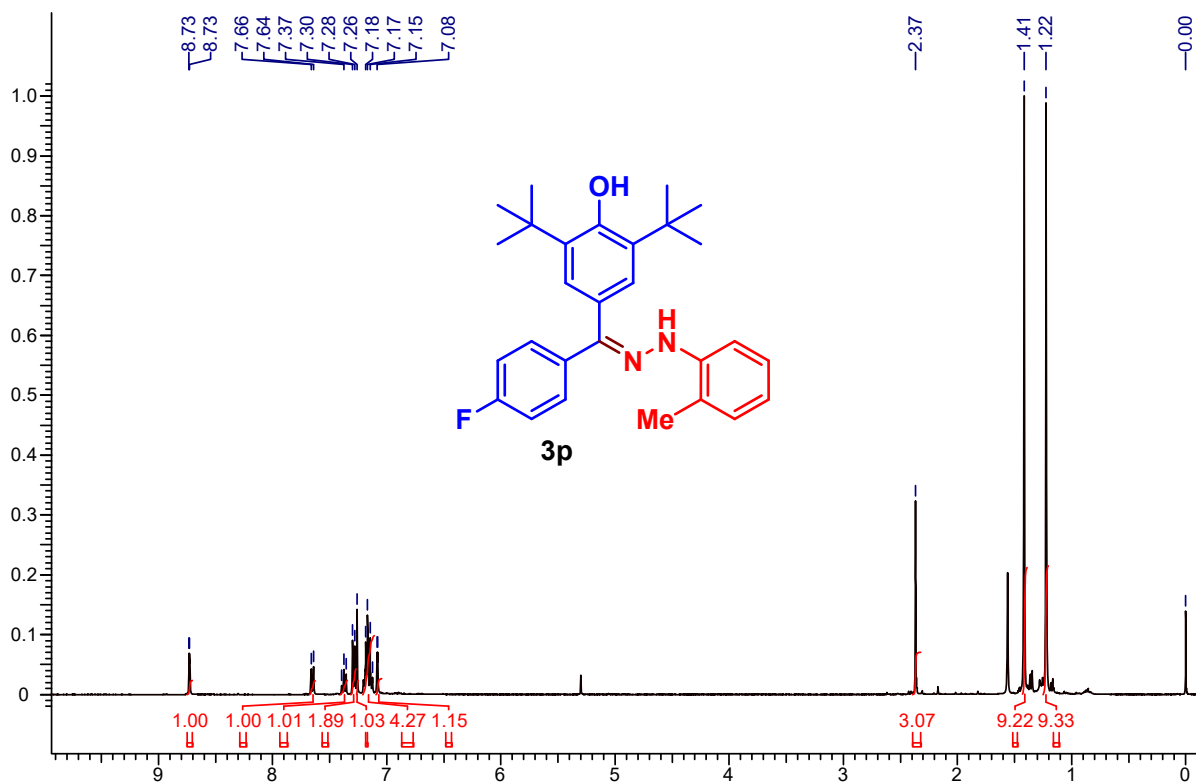


**<sup>13</sup>C NMR of Compound 3o [as 1:0.27 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)**

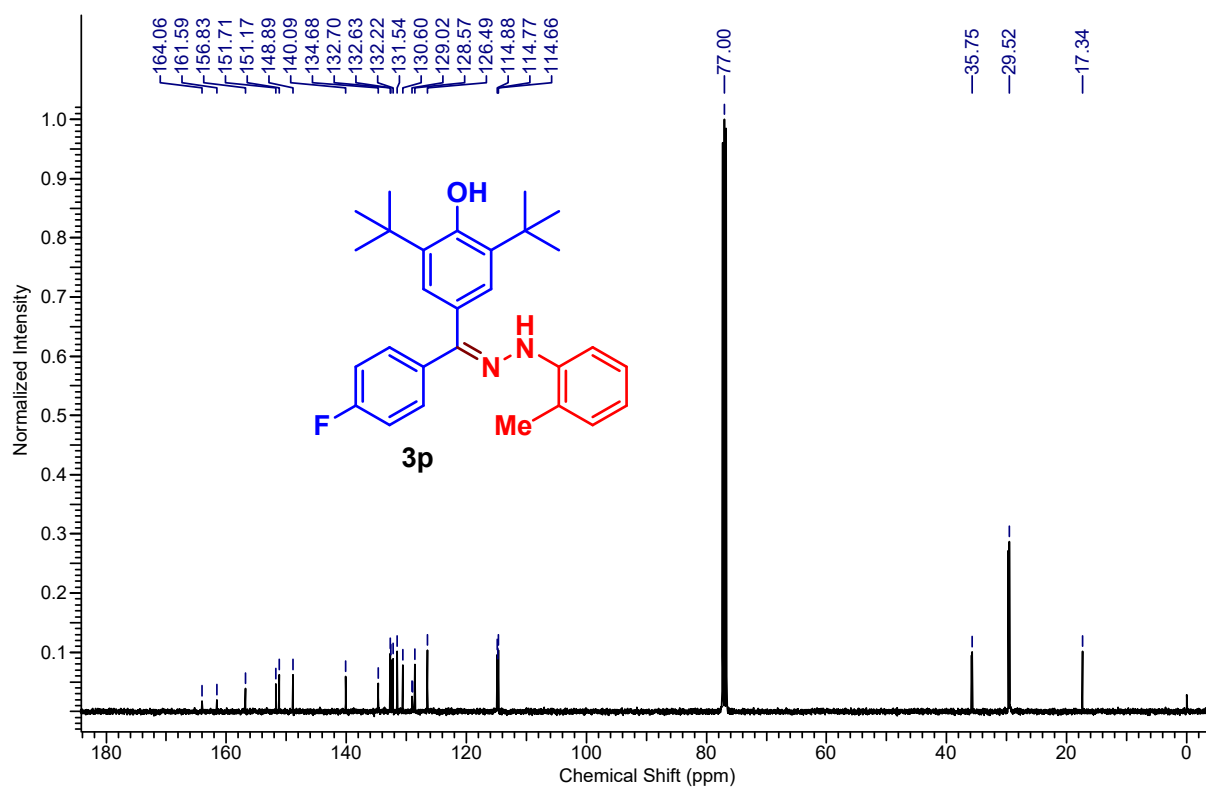
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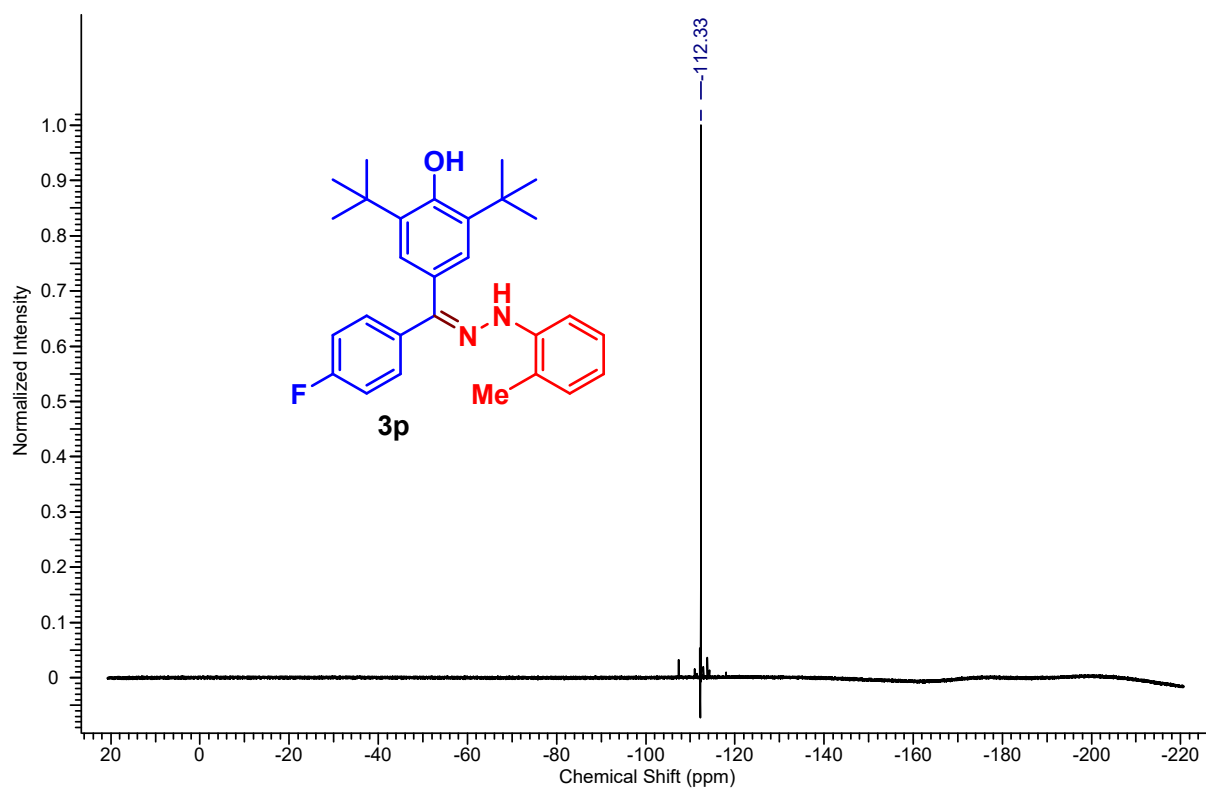
### HRMS of Compound 3o



### <sup>1</sup>H NMR of Compound 3p (400 MHz, CDCl<sub>3</sub>)

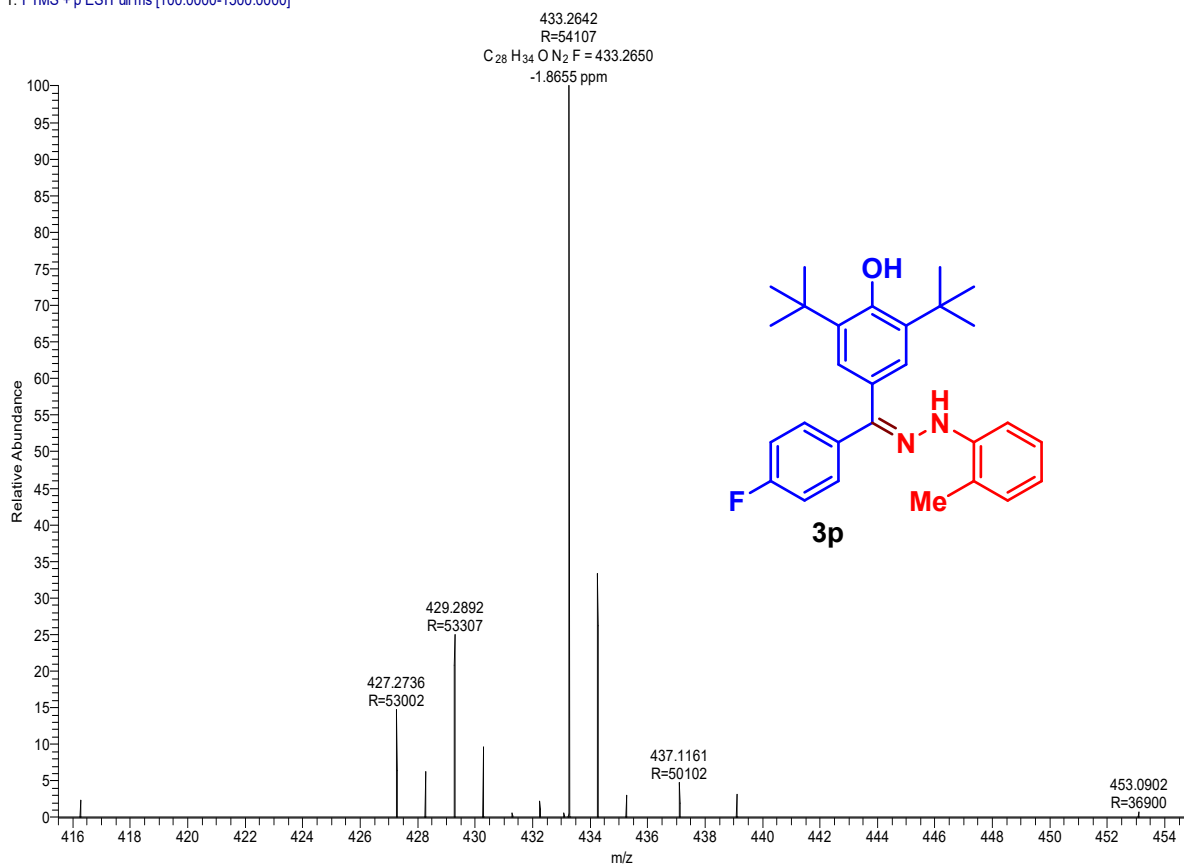


### <sup>13</sup>C NMR of Compound 3p (101 MHz, CDCl<sub>3</sub>)

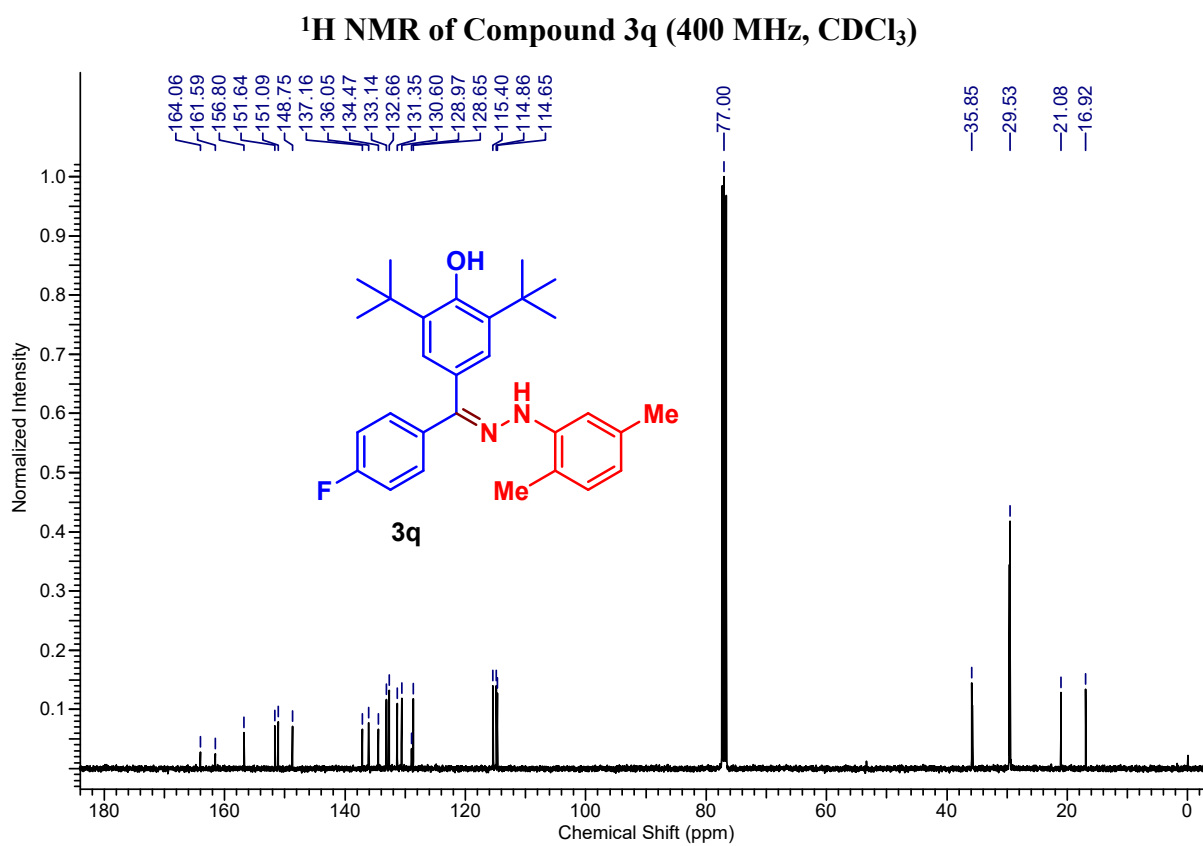
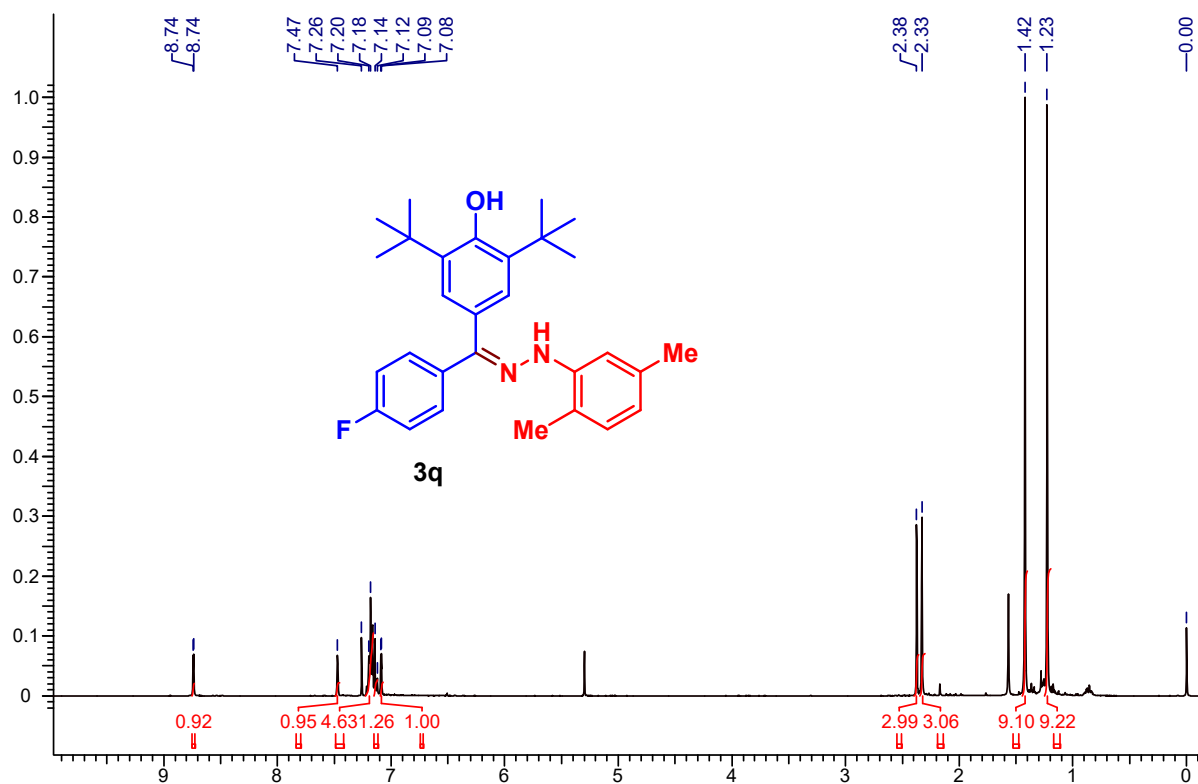


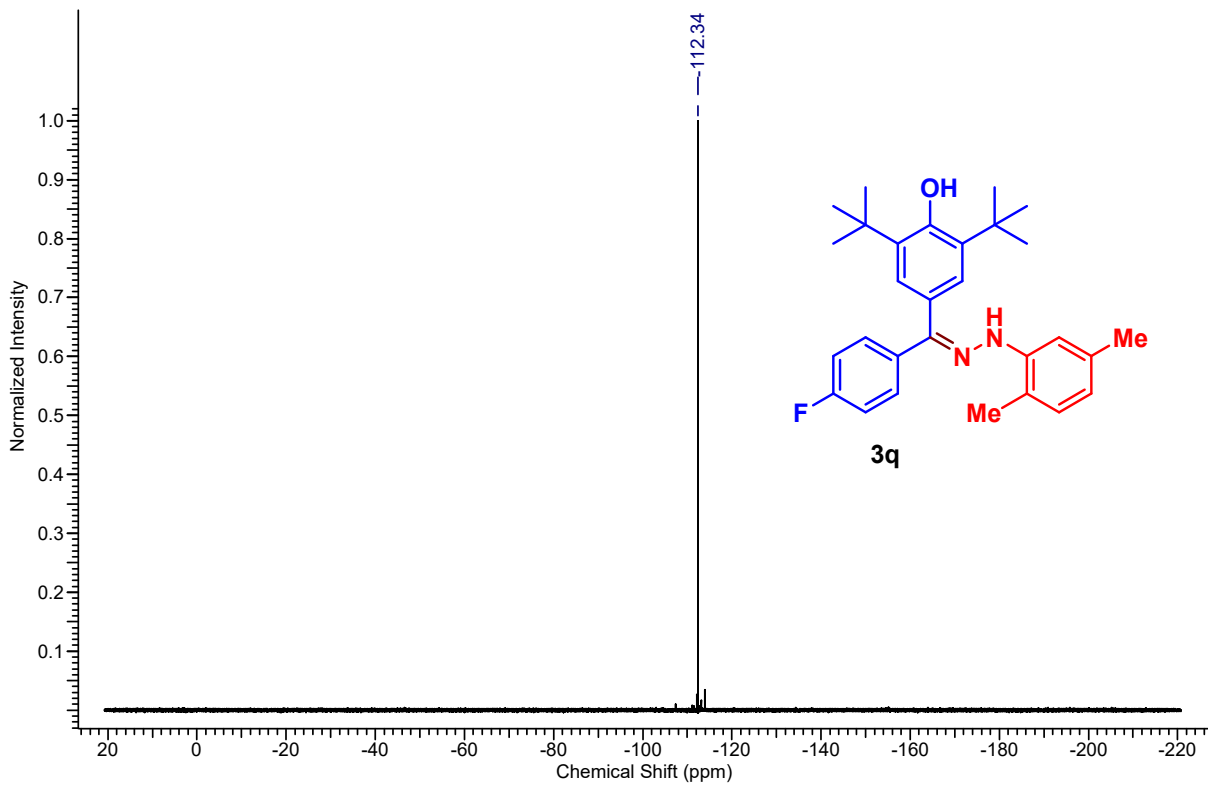
# <sup>19</sup>F NMR of Compound 3p (376 MHz, CDCl<sub>3</sub>)

5AW #918 RT: 4.09 AV: 1 NL: 2.14E7  
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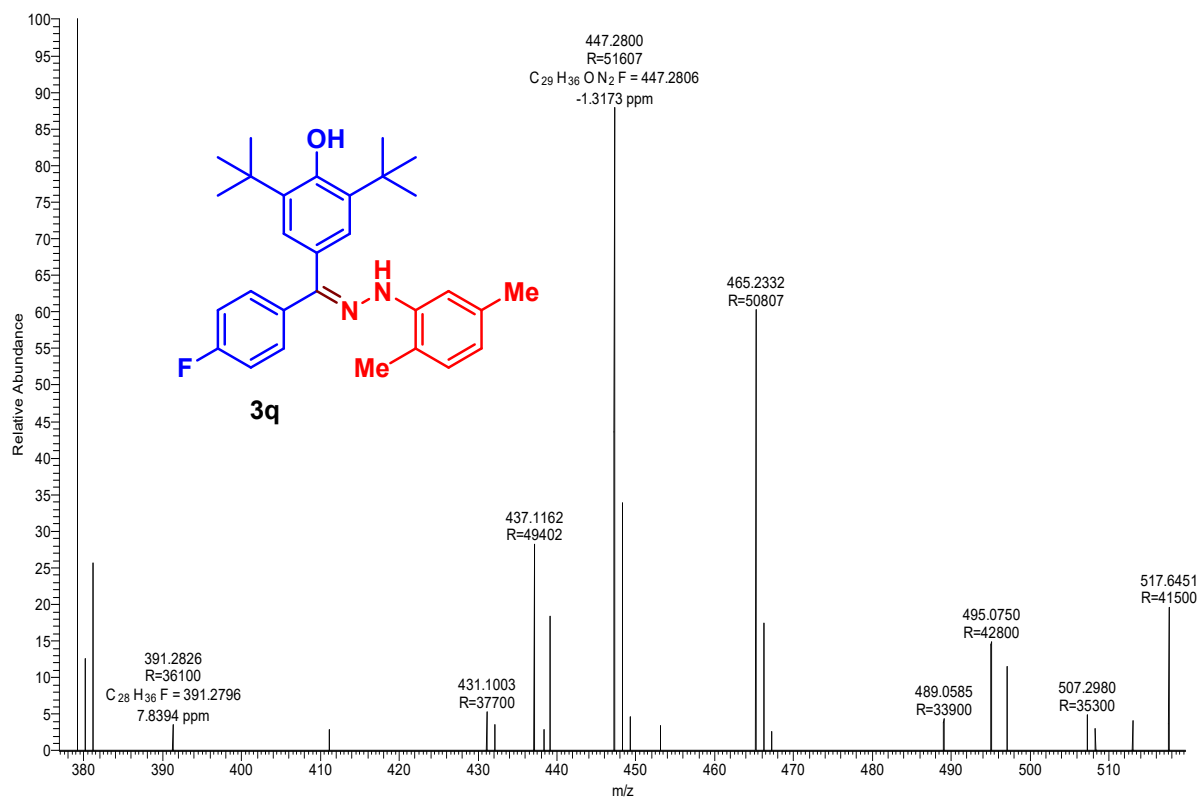
## HRMS of Compound 3p





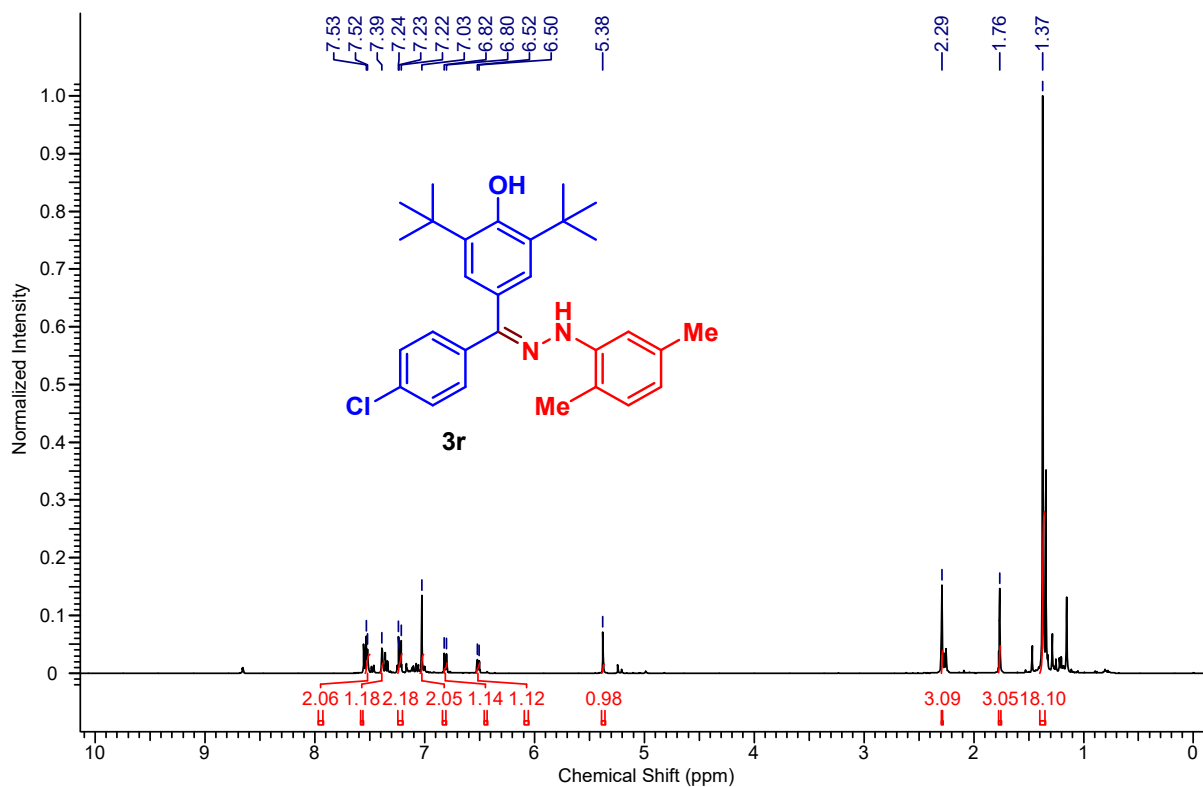
### $^{19}\text{F}$ NMR of Compound 3q (376 MHz, $\text{CDCl}_3$ )

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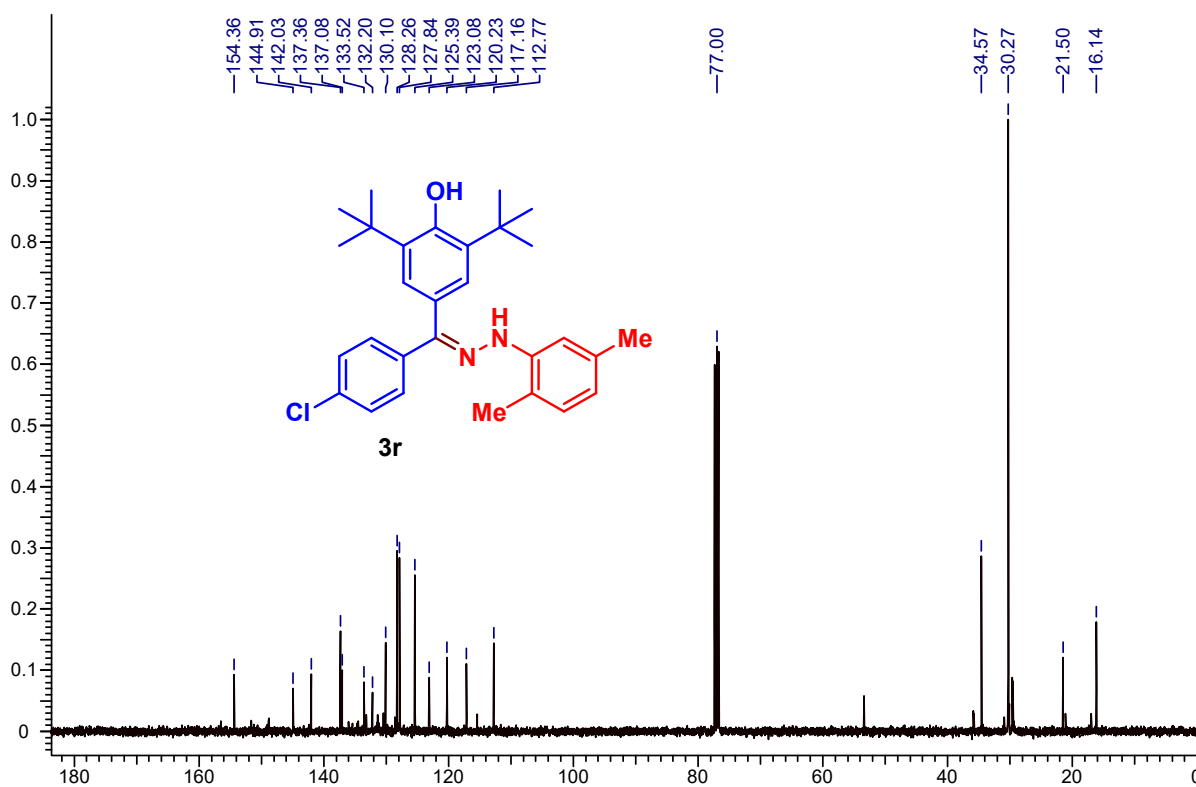




### HRMS of Compound 3q

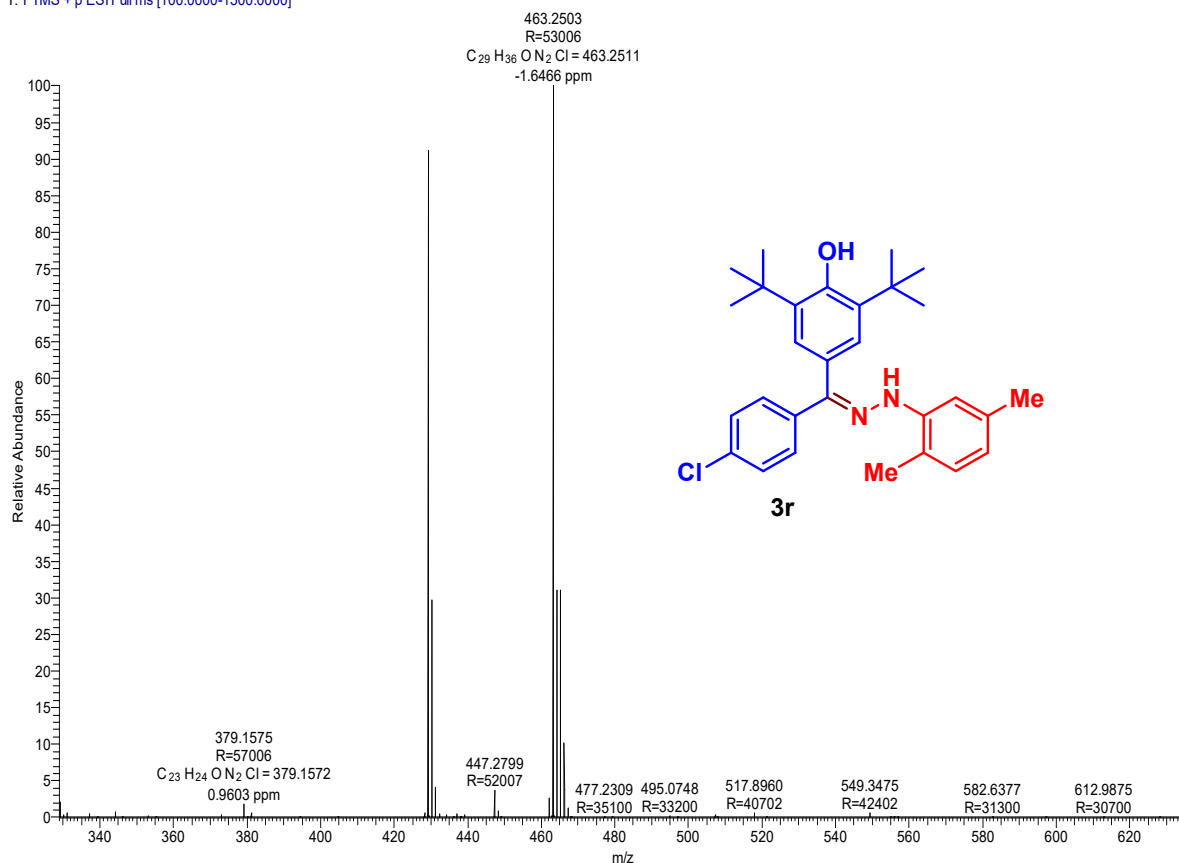


### <sup>13</sup>C NMR of Compound 3r [as 1:0.20 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)

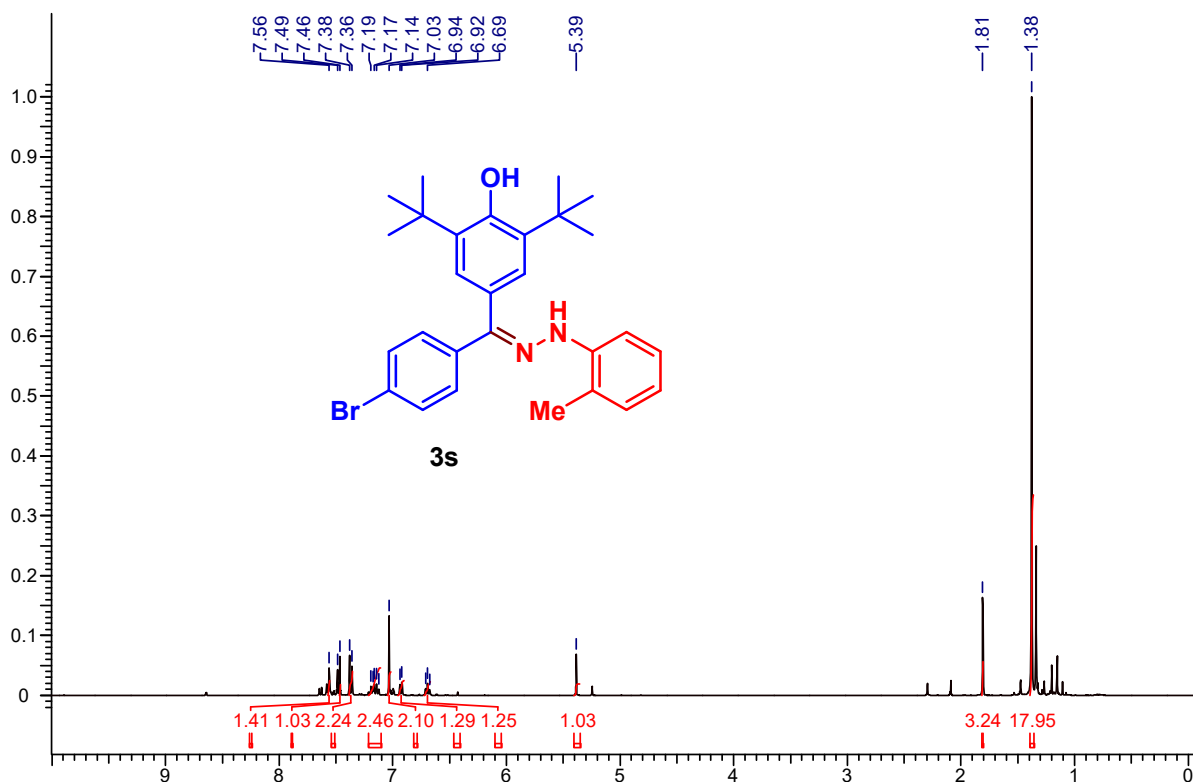


### <sup>13</sup>C NMR of Compound 3r [as 1:0.20 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)

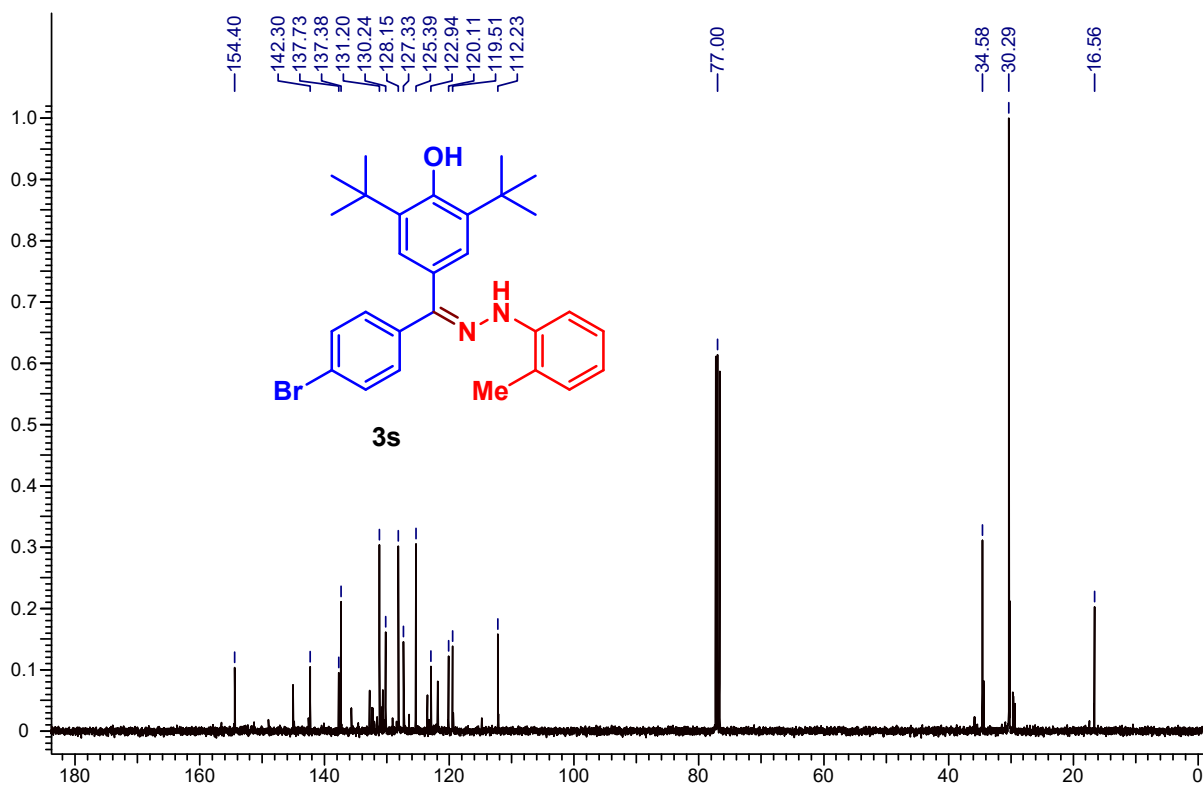
5AZ#994 RT: 4.43 AV: 1 NL: 1.60E8  
T: FTMS + p ESI Full ms [100.0000-1500.0000]



### HRMS of Compound 3r

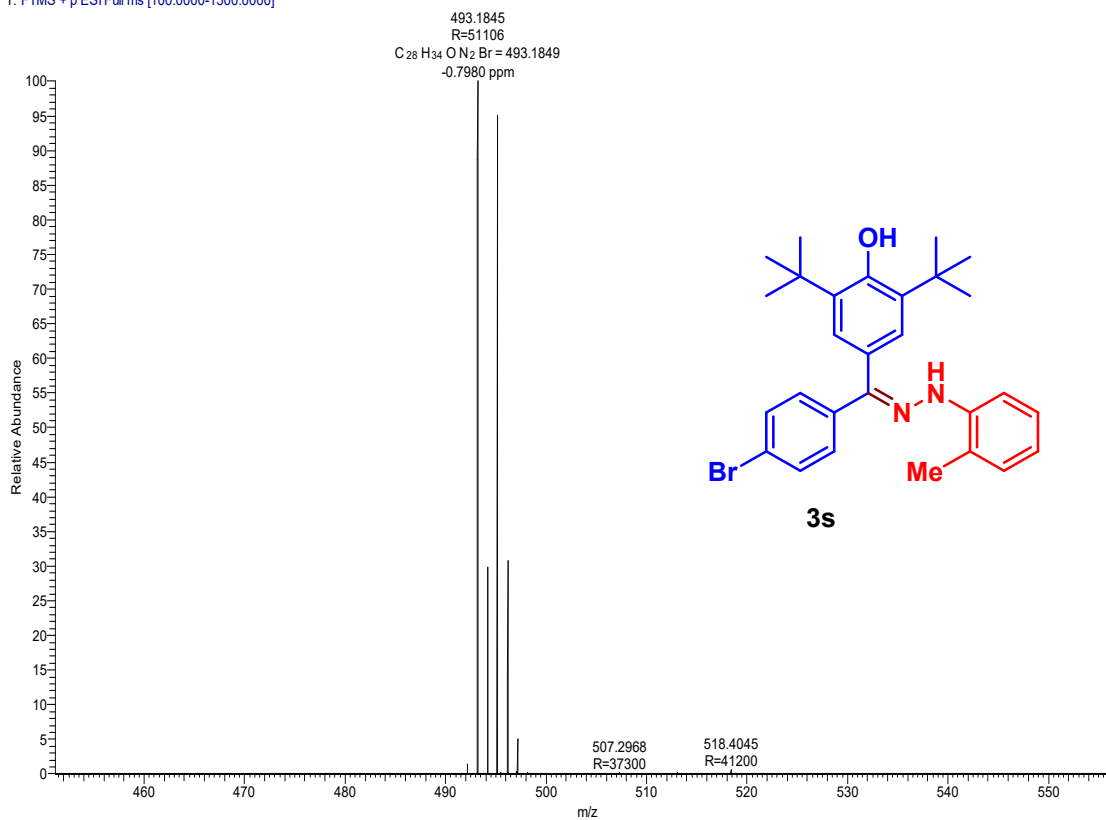


### <sup>1</sup>H NMR of Compound 3s [as 1:0.21 stereoisomeric mixture] (400 MHz, CDCl<sub>3</sub>)

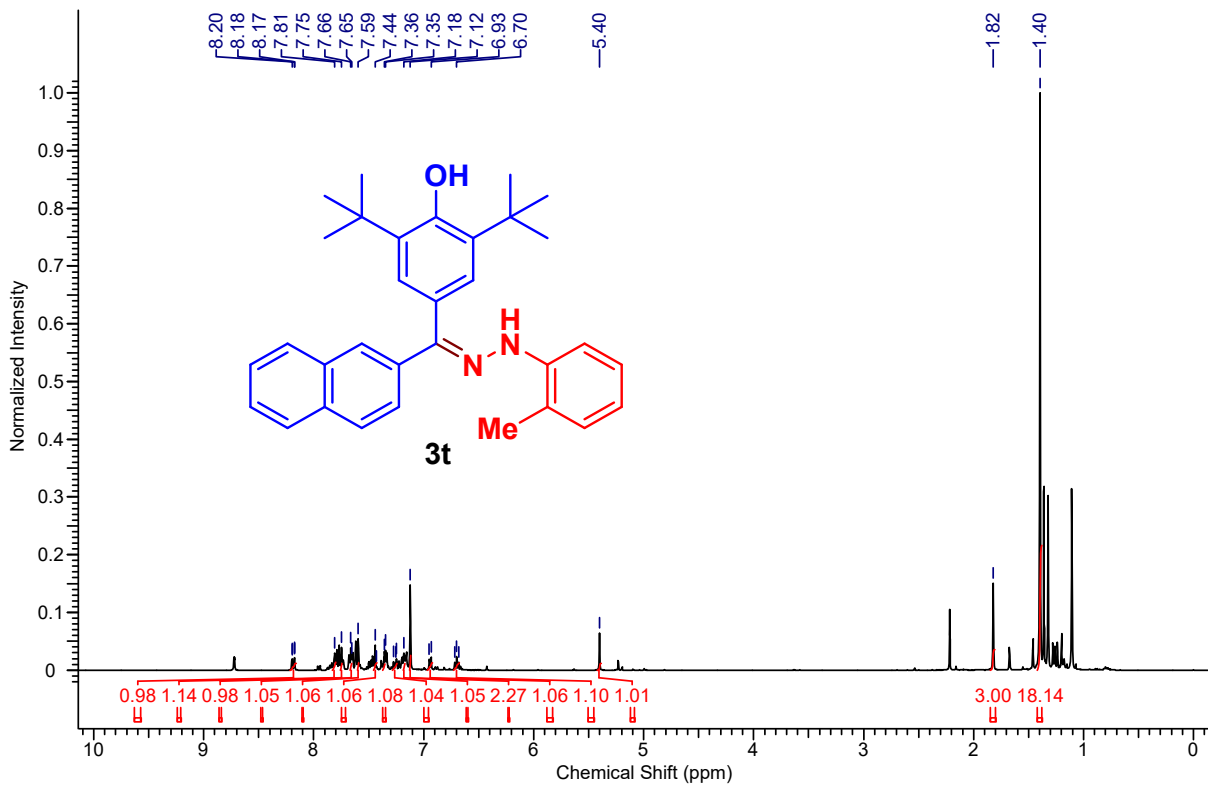


**<sup>13</sup>C NMR of Compound 3s [as 1:0.21 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)**

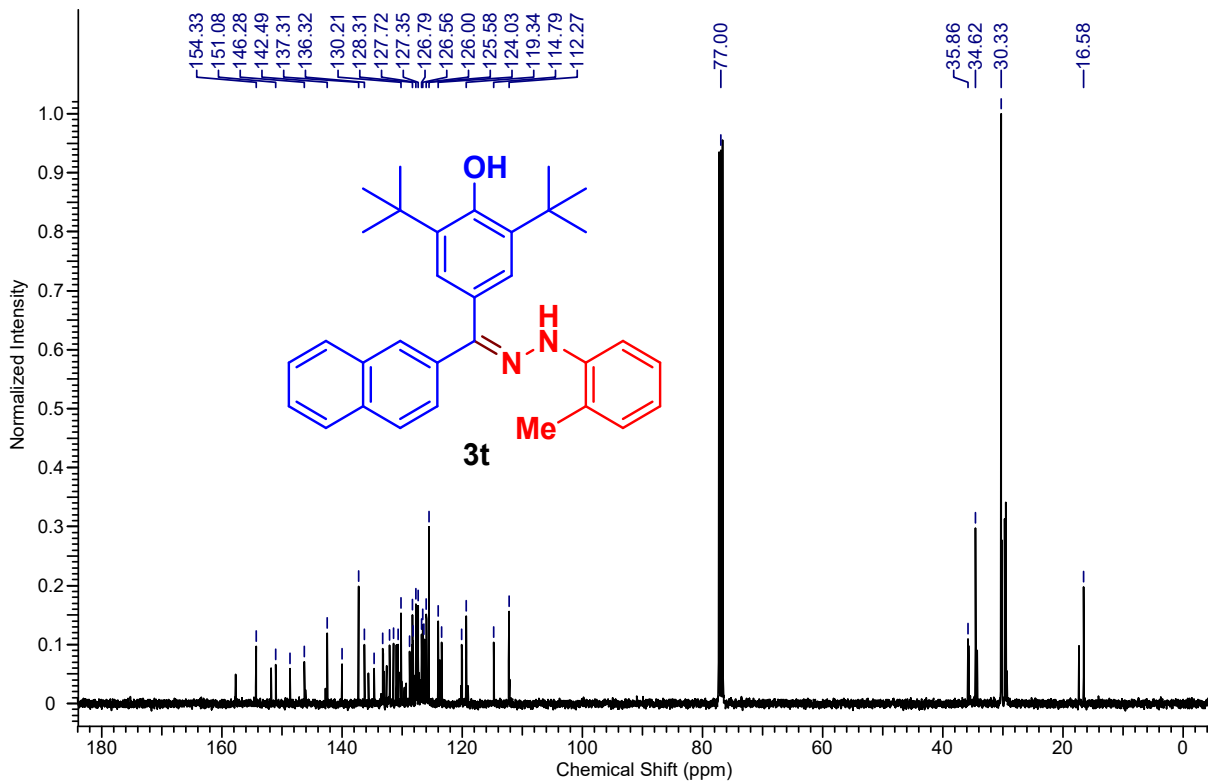
5AAA #928 RT: 4.13 AV: 1 NL: 1.10E8  
T: FTMS + p ESI Full ms [100.0000-1500.0000]



### HRMS of Compound 3s

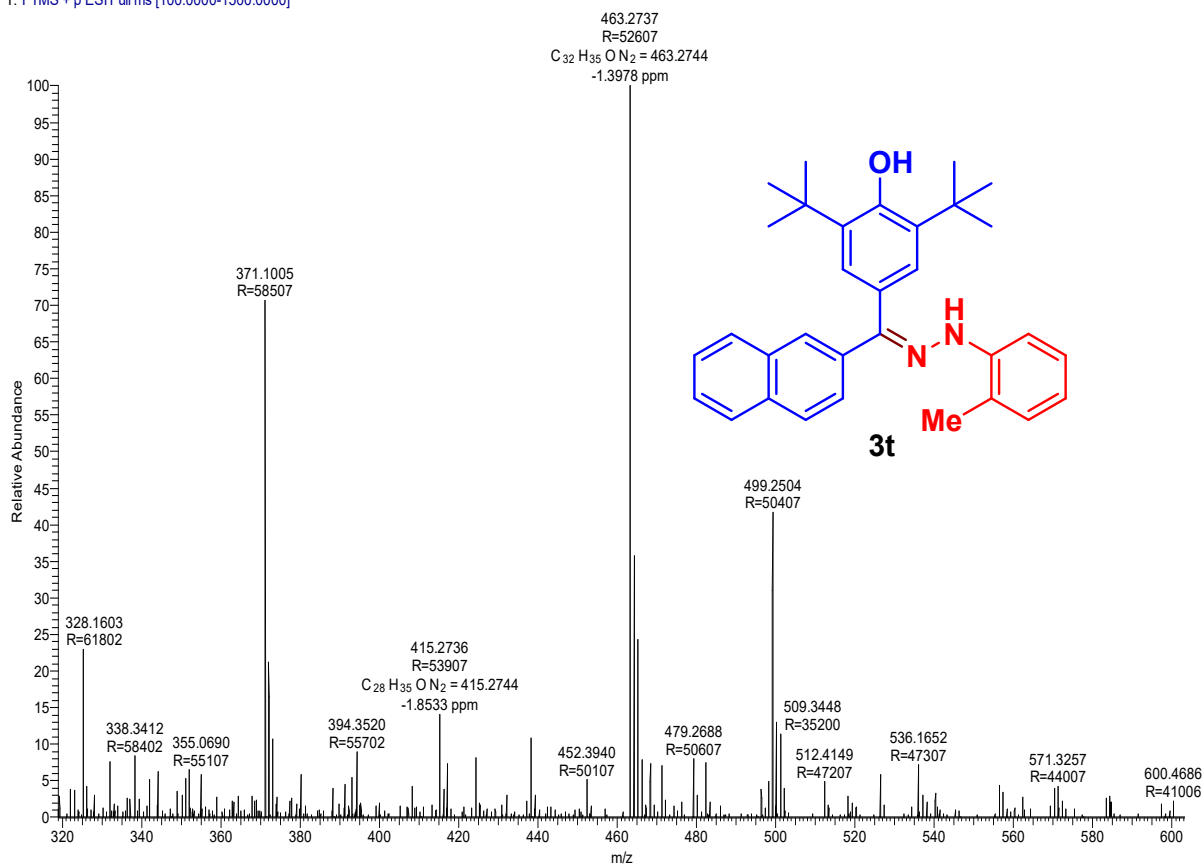


**<sup>1</sup>H NMR of Compound 3t [as 1:0.25 stereoisomeric mixture] (400 MHz, CDCl<sub>3</sub>)**

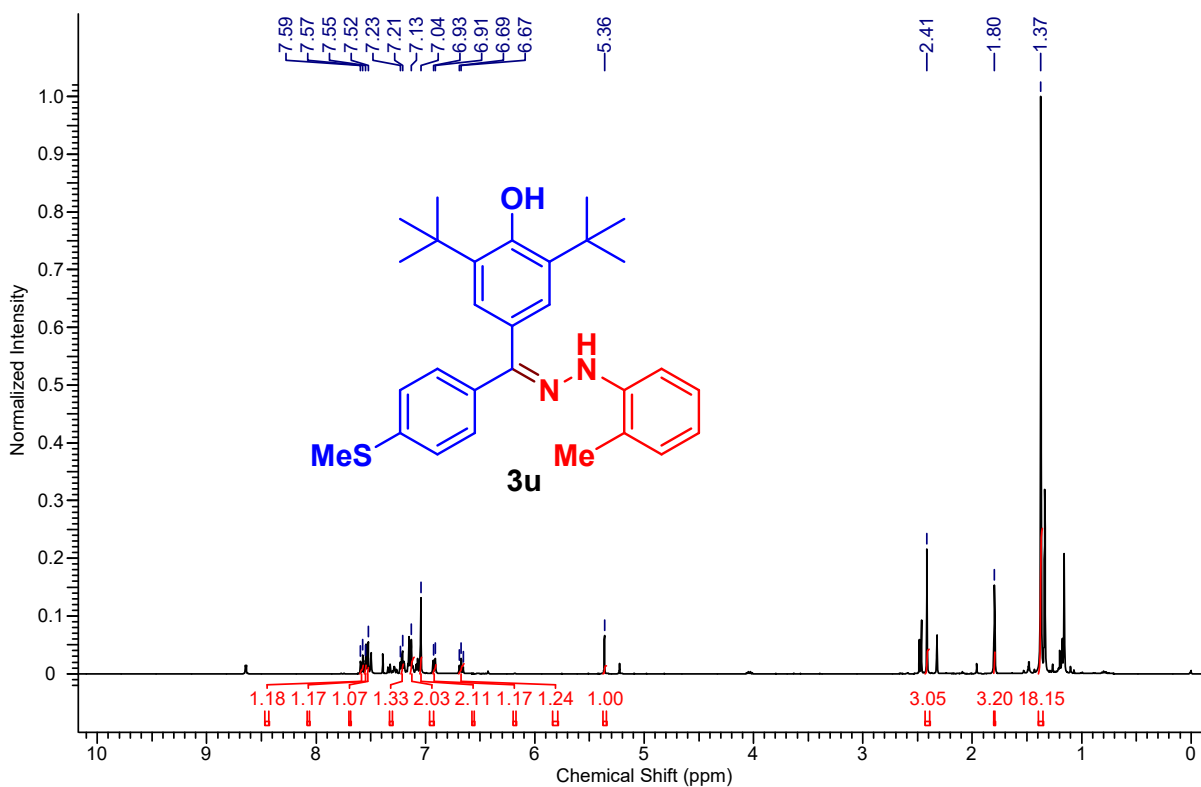


**<sup>13</sup>C NMR of Compound 3t [as 1:0.25 stereoisomeric mixture] (101 MHz, CDCl<sub>3</sub>)**

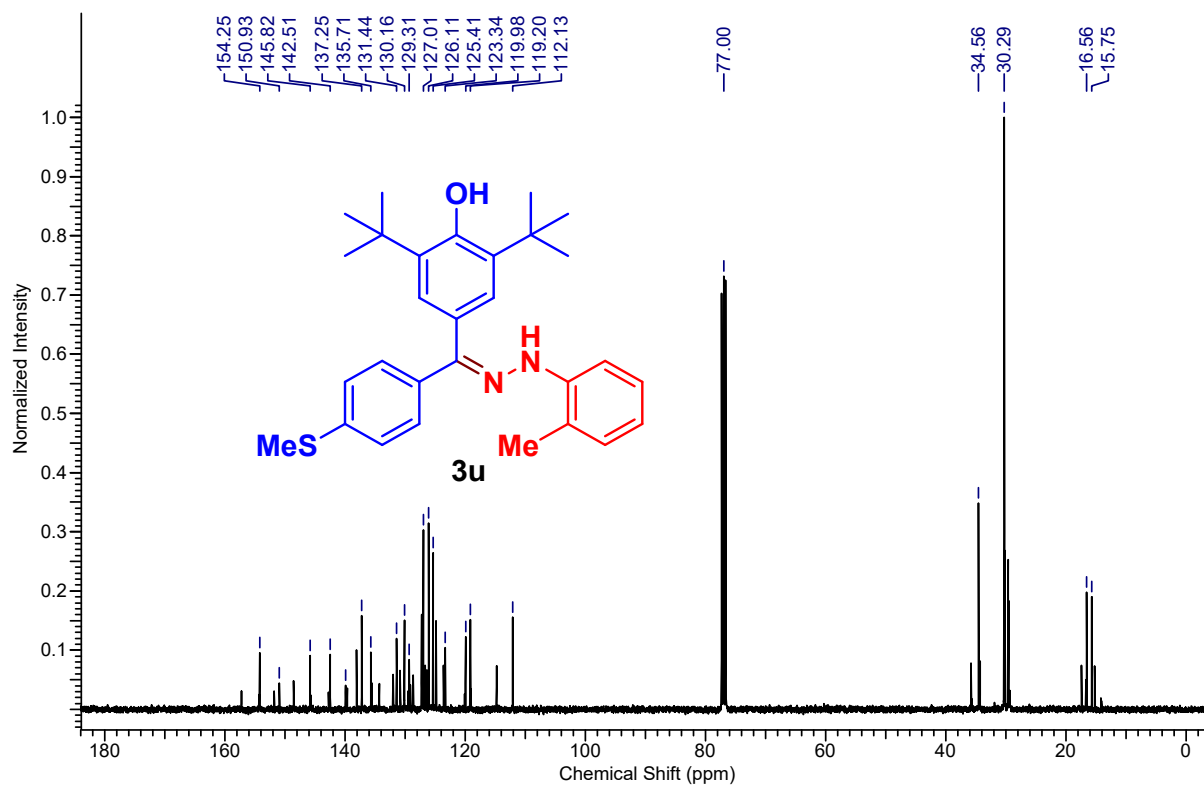
AR-88 #675 RT: 4.98 AV: 1 NL: 1.03E6  
T: FTMS + p ESI Full ms [100.0000-1500.0000]



### HRMS of Compound 3t

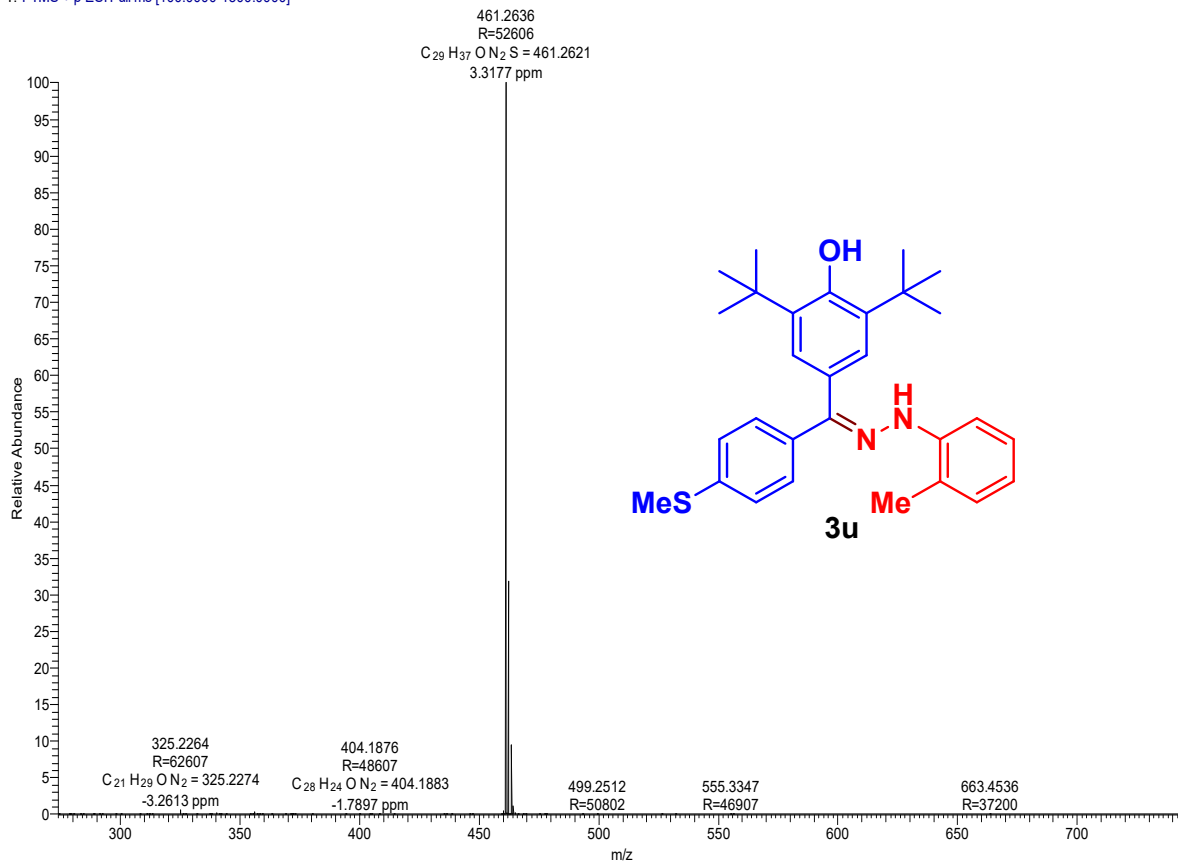


**$^1\text{H}$  NMR of Compound 3u [as 1:0.26 stereoisomeric mixture] (400 MHz,  $\text{CDCl}_3$ )**

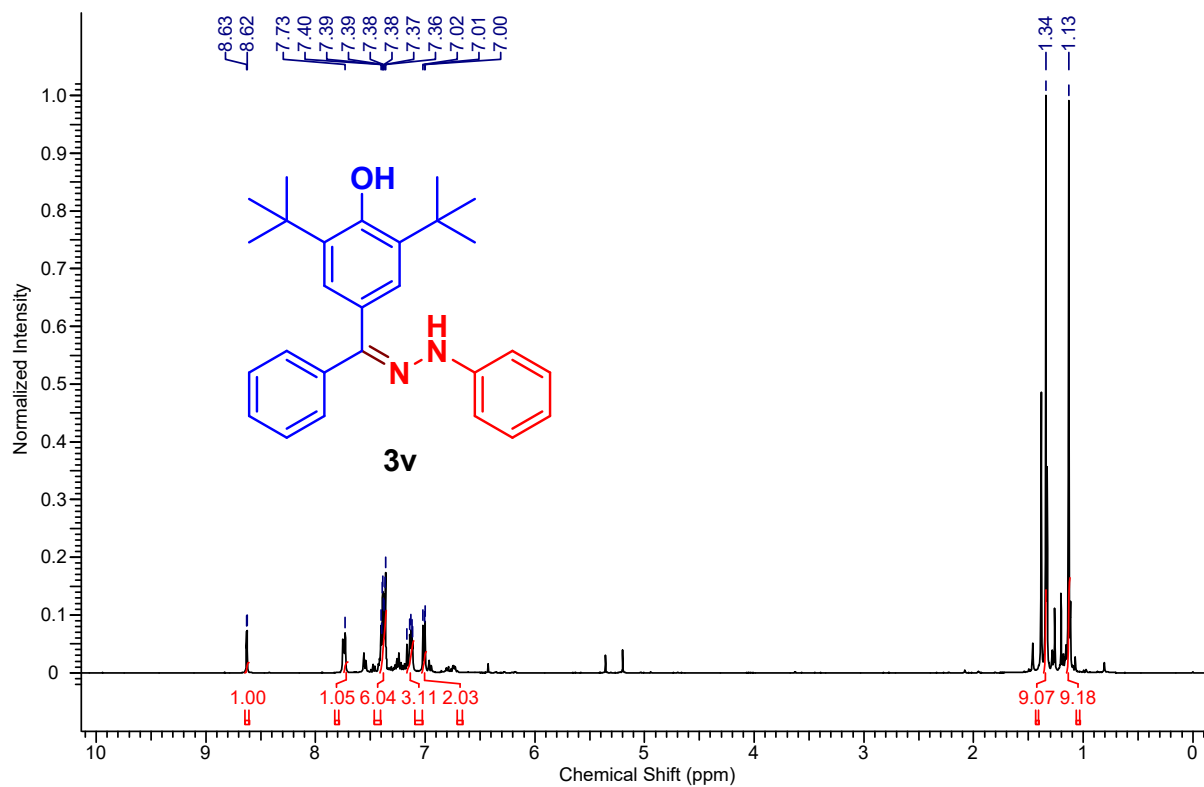


**$^{13}\text{C}$  NMR of Compound 3u [as 1:0.26 stereoisomeric mixture] (101 MHz,  $\text{CDCl}_3$ )**

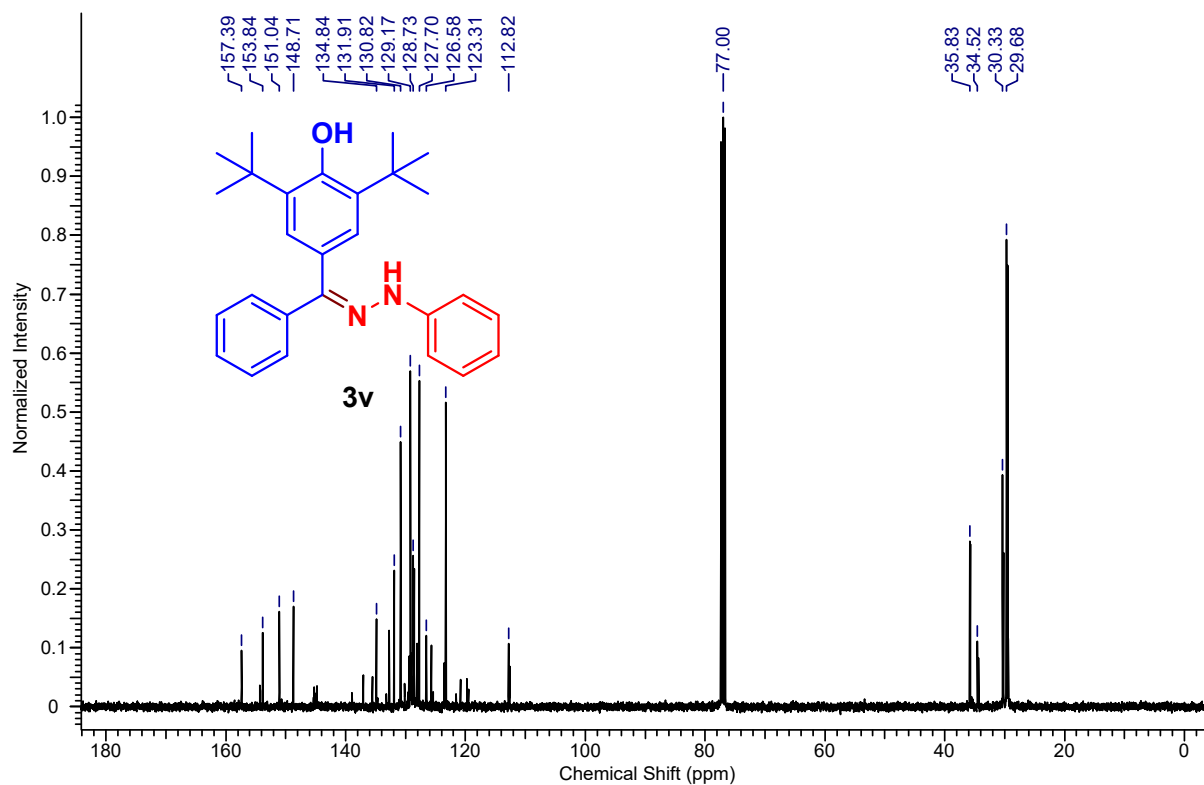
AR-89#683 RT: 4.44 AV: 1 NL: 9.31E8  
T: FTMS + p ESI Full ms [100.0000-1500.0000]



### HRMS of Compound 3u

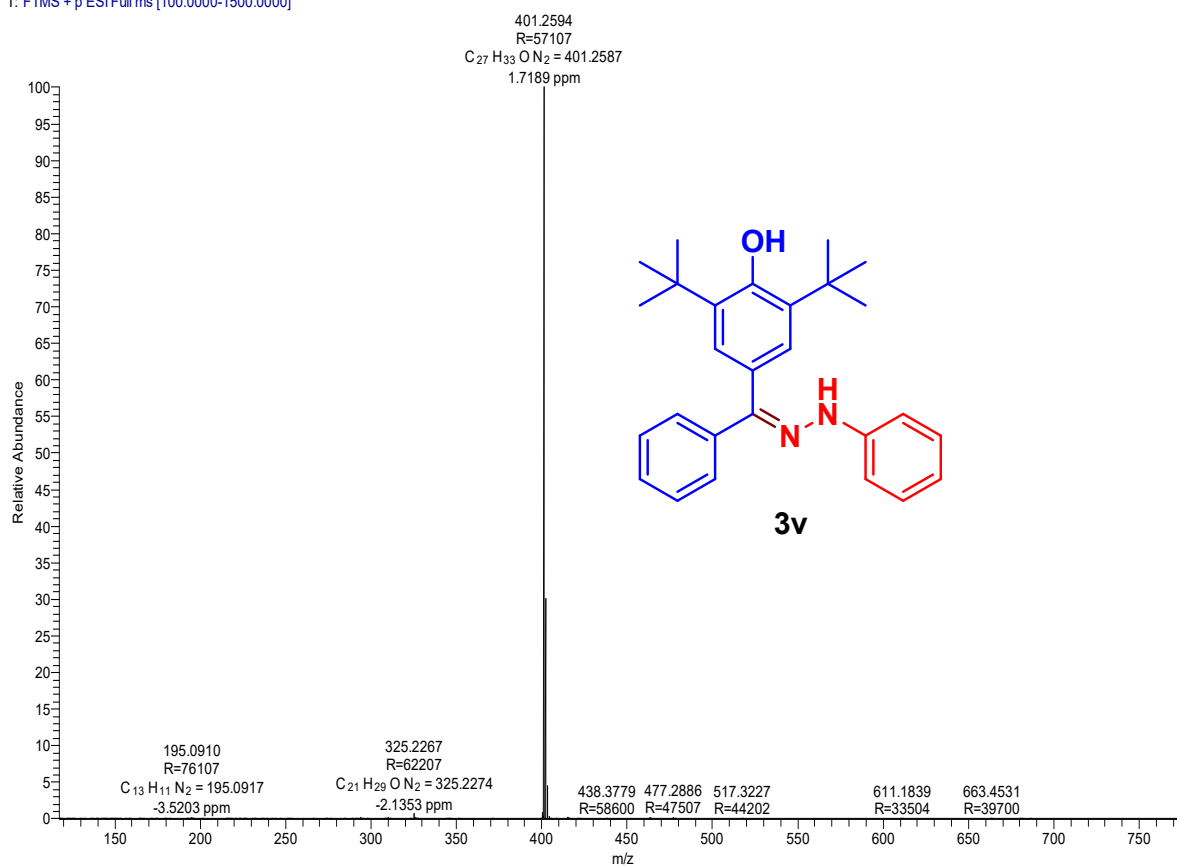


### <sup>1</sup>H NMR of Compound 3v [Z/E Mixture] (400 MHz, CDCl<sub>3</sub>)



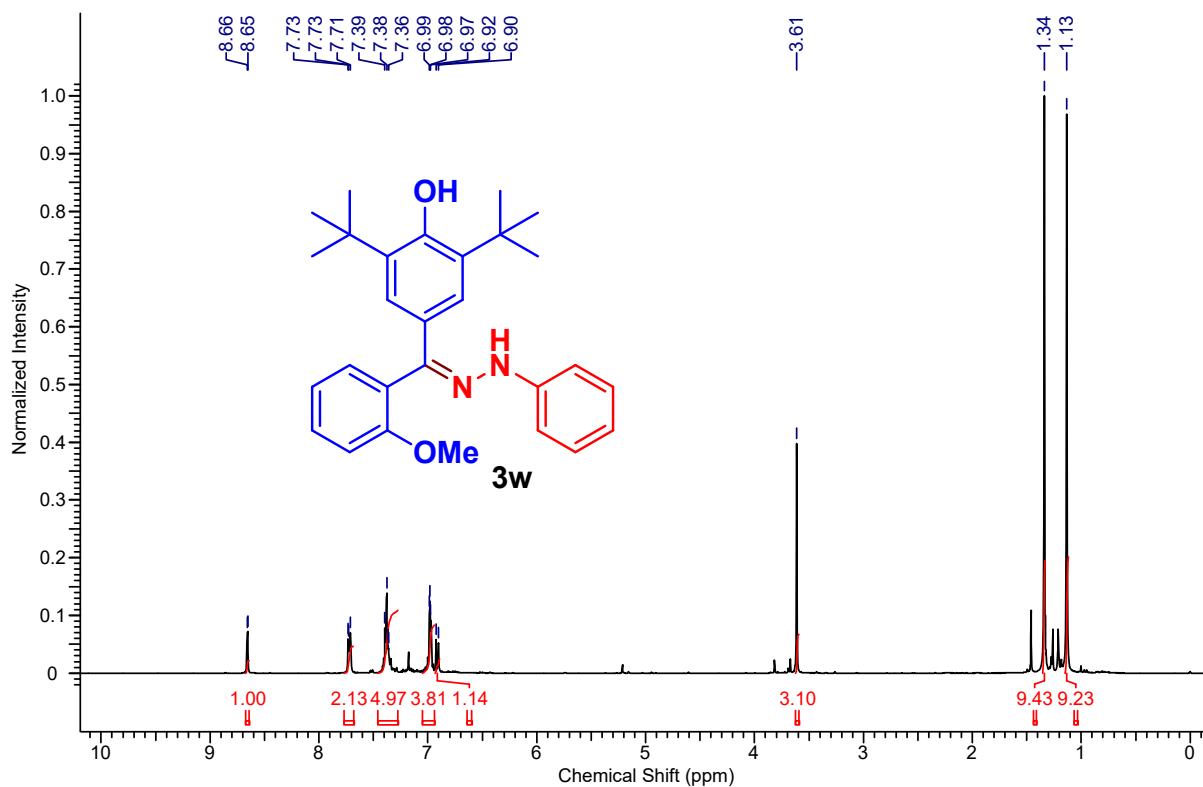
### <sup>13</sup>C NMR of Compound 3v [Z/E Mixture] (101 MHz, CDCl<sub>3</sub>)

AR-91 #608 RT: 3.67 AV: 1 NL: 1.13E9  
T: FTMS + p ESI Full ms [100.0000-1500.0000]

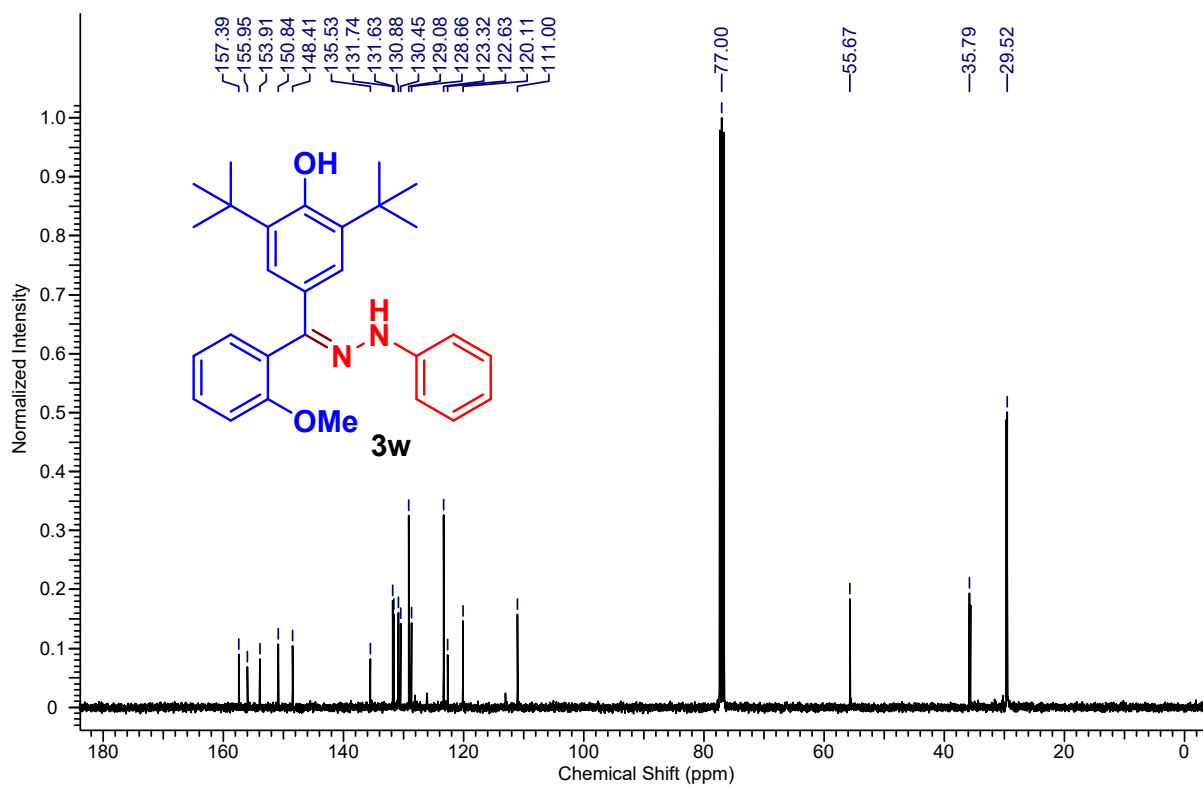




### HRMS of Compound 3v

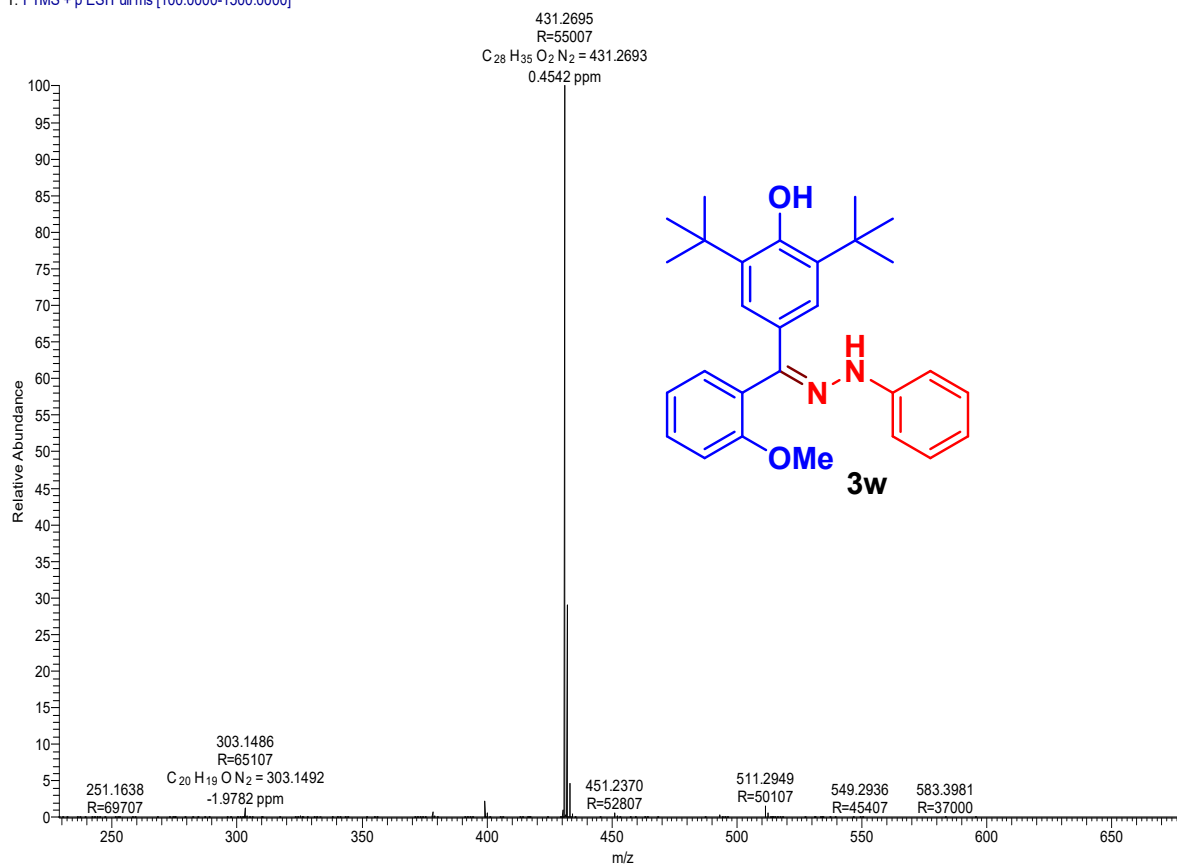


### <sup>13</sup>C NMR of Compound 3w (400 MHz, CDCl<sub>3</sub>)



# <sup>13</sup>C NMR of Compound 3w (101 MHz, CDCl<sub>3</sub>)

AR-95 #440 RT: 2.64 AV: 1 NL: 3.68E8  
T: FTMS + p ESI Full ms [100.0000-1500.0000]



## HRMS of Compound 3w

### 3. X-ray data of compounds 3c, 3j and 3s:

Single crystal X-ray diffraction data for compounds **3c**, **3j** and **3s** were collected using a Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer equipped with Incoatech multilayer mirrors optics. The intensity measurements were carried out with Mo micro-focus sealed tube diffraction source ( $\text{MoK}_\alpha = 0.71073 \text{ \AA}$ ) at low temperature. The X-ray data collection was monitored by APEX3 program (Bruker, 2016)<sup>[S1]</sup>. All the data were corrected for Lorentzian, polarization and absorption effects using SAINT and SADABS programs (Bruker, 2016). Using the APEX3 (Bruker) program suite, the structure was solved with the ShelXS-97 (Sheldrick, 2008)<sup>[S2]</sup> structure solution program, using direct methods. The model was refined with a version of ShelXL-2018/3 (Sheldrick, 2015)<sup>[S3]</sup> using Least Squares minimization. All the hydrogen atoms were placed in a geometrically idealized position and constrained to ride on their parent atoms. An *ORTEP* III<sup>[S4]</sup> view of the compounds was drawn with 50% probability displacement ellipsoids, and H atoms are shown as small spheres of arbitrary radii.

#### Single crystal X-ray of 3c:

Crystallization of compound **3c** was carried out at room temperature by the Solvent Evaporation Method using ethyl acetate and Pet ether (1:9) as a solvent system.

A specimen of  $\text{C}_{30}\text{H}_{38}\text{N}_2\text{O}_2$ , approximate dimension 0.110 mm x 0.130 mm x 0.200 mm and has an orthorhombic unit cell, was used for the X-ray crystallographic analysis.

Bond precision:	C-C = 0.0025 Å	Wavelength=0.71073	
Cell:	a=18.1645(7)	b=11.6514(4)	c=25.2936(10)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	5353.2(3)	5353.2(3)	
Space group	P b c a	P b c a	
Hall group	-P 2ac 2ab	-P 2ac 2ab	
Moiety formula	C30 H38 N2 O2	C30 H38 N2 O2	

Sum formula	C <sub>30</sub> H <sub>38</sub> N <sub>2</sub> O <sub>2</sub>	C <sub>30</sub> H <sub>38</sub> N <sub>2</sub> O <sub>2</sub>
Mr	458.62	458.62
D <sub>x</sub> , g cm <sup>-3</sup>	1.138	1.138
Z	8	8
Mu (mm <sup>-1</sup> )	0.071	0.071
F <sub>000</sub>	1984.0	1984.0
F <sub>000</sub> '	1984.76	
h, k, l max	24,15,33	24,15,33
Nref	6664	6650
T <sub>min</sub> ,T <sub>max</sub>	0.989,0.992	0.650,0.746
T <sub>min</sub> '	0.986	

Correction method= # Reported T Limits: T<sub>min</sub>=0.650 T<sub>max</sub>=0.746

Abs Corr = MULTI-SCAN

Data completeness= 0.998

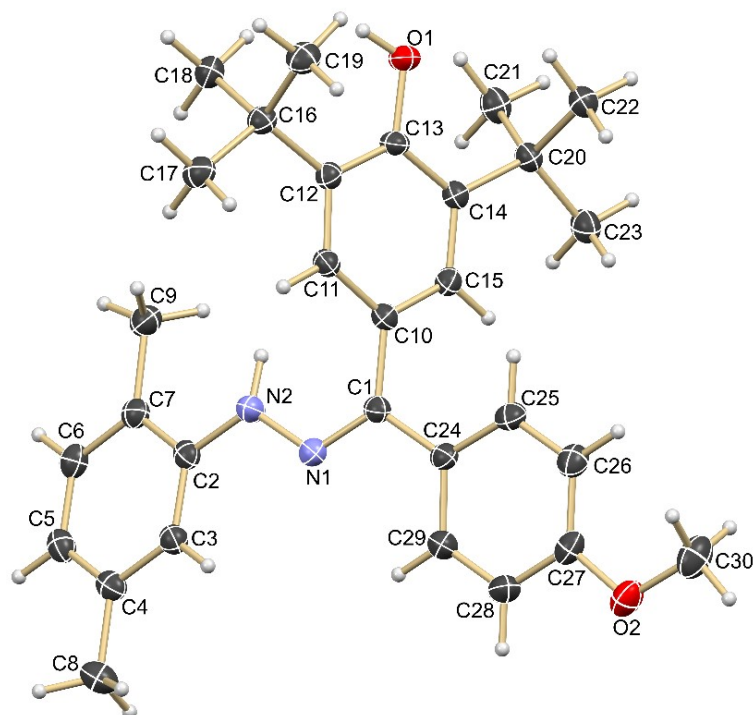
Theta(max)= 28.309

R(reflections)= 0.0487(4036)

wR2(reflections)=0.1264(6650)

S = 1.047

Npar= 325



CCDC No. 2289315

**Figure (S1):** ORTEP diagram of 3c

**Single crystal X-ray of 3j:**

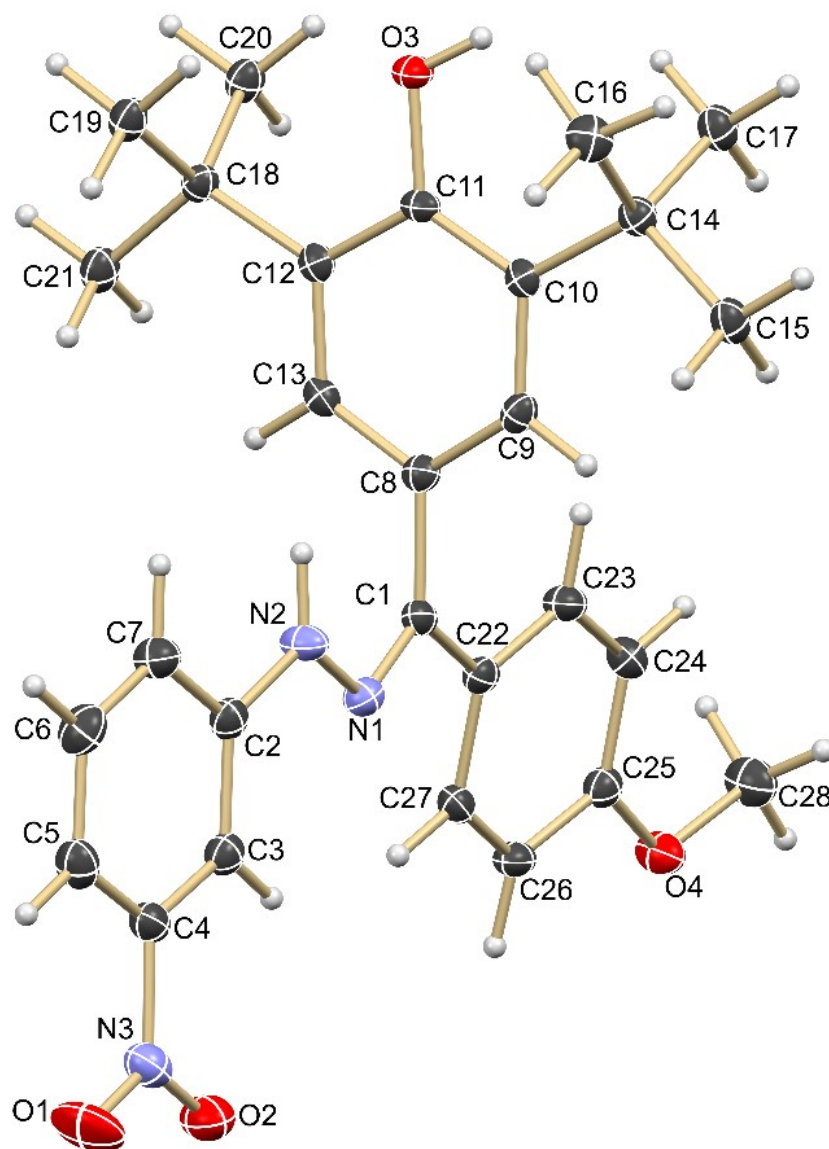
Crystallization of compound 3j was carried out at room temperature by the Solvent Evaporation Method using ethyl acetate and Pet ether (1:9) as a solvent system.

A specimen of C<sub>28</sub>H<sub>33</sub>N<sub>3</sub>O<sub>4</sub>, approximate dimension 0.100 mm x 0.120 mm x 0.130 mm and has a monoclinic unit cell, was used for the X-ray crystallographic analysis.

Bond precision:	C-C = 0.0020 Å	Wavelength=0.71073	
Cell:	a=12.2116(9)	b=19.3030(17)	c=10.9565(9)
	alpha=90	beta=106.653(2)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	2474.4(4)	2474.3(4)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C <sub>28</sub> H <sub>33</sub> N <sub>3</sub> O <sub>4</sub>	C <sub>28</sub> H <sub>33</sub> N <sub>3</sub> O <sub>4</sub>	
Sum formula	C <sub>28</sub> H <sub>33</sub> N <sub>3</sub> O <sub>4</sub>	C <sub>28</sub> H <sub>33</sub> N <sub>3</sub> O <sub>4</sub>	
Mr	475.57	475.57	
Dx,g cm <sup>-3</sup>	1.277	1.277	
Z	4	4	
Mu (mm <sup>-1</sup> )	0.086	0.086	
F000	1016.0	1016.0	
F000'	1016.44		
h,k,l max	16,25,14	16,25,14	
Nref	6201	6174	
Tmin,Tmax	0.989,0.991	0.175,0.209	
Tmin'	0.989		
Correction method=	# Reported T Limits: Tmin=0.175 Tmax=0.209		
AbsCorr =	MULTI-SCAN		
Data completeness=	0.996	Theta(max)= 28.364	
R(reflections)=	0.0450(4263)	wR2(reflections)= 0.1151(6174)	

S = 1.030

Npar= 331



CCDC No. 2289316

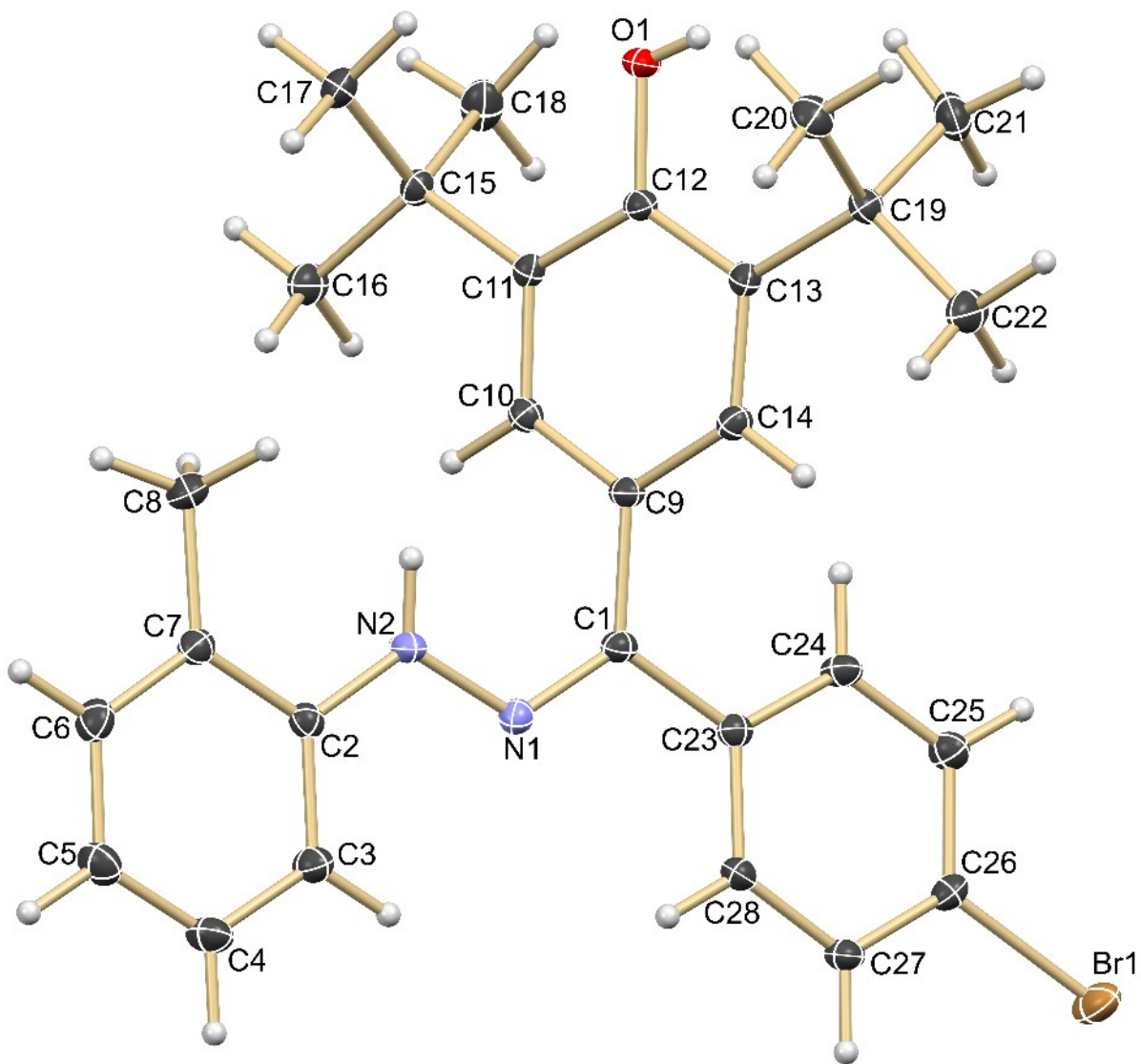
Figure (S2): ORTEP diagram of 3j

### Single crystal X-ray of 3s:

Crystallization of compound 3s was carried out at room temperature by the Solvent Evaporation Method using ethyl acetate and Pet ether (1:9) as a solvent system.

A specimen of  $C_{28}H_{33}BrN_2O$ , approximate dimension 0.080 mm x 0.110 mm x 0.140 mm and has a triclinic unit cell, was used for the X-ray crystallographic analysis.

Bond precision:	C-C = 0.0019 Å	Wavelength=0.71073	
Cell:	a=10.0089(4)	b=11.1233(5)	c=12.0576(5)
	alpha=104.087(1)	beta=108.984(1)	gamma=90.413(2)
Temperature:	100 K		
	Calculated	Reported	
Volume	1225.74(9)	1225.74(9)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C <sub>28</sub> H <sub>33</sub> Br N <sub>2</sub> O	C <sub>28</sub> H <sub>33</sub> Br N <sub>2</sub> O	
Sum formula	C <sub>28</sub> H <sub>33</sub> Br N <sub>2</sub> O	C <sub>28</sub> H <sub>33</sub> Br N <sub>2</sub> O	
Mr	493.46	493.47	
Dx,g cm <sup>-3</sup>	1.337	1.337	
Z	2	2	
Mu (mm <sup>-1</sup> )	1.699	1.699	
F000	516.0	516.0	
F000'	515.59		
h,k,l max	13,15,16	13,15,16	
Nref	6400	6362	
Tmin,Tmax	0.799,0.873	0.627,0.746	
Tmin'	0.788		
Correction method= # Reported T Limits: Tmin=0.627 Tmax=0.746			
AbsCorr = MULTI-SCAN			
Data completeness= 0.994	Theta(max)= 28.787		
R(reflections)= 0.0263(5760)	wR2(reflections)= 0.0689(6362)		
S = 1.057	Npar= 303		

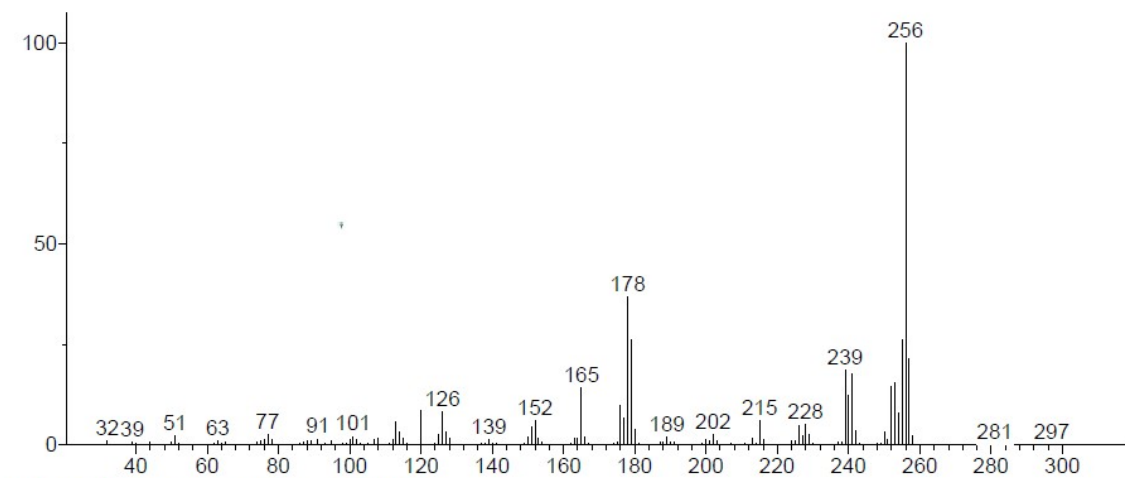


CCDC No. 2289314

Figure (S3): ORTEP diagram of 3s



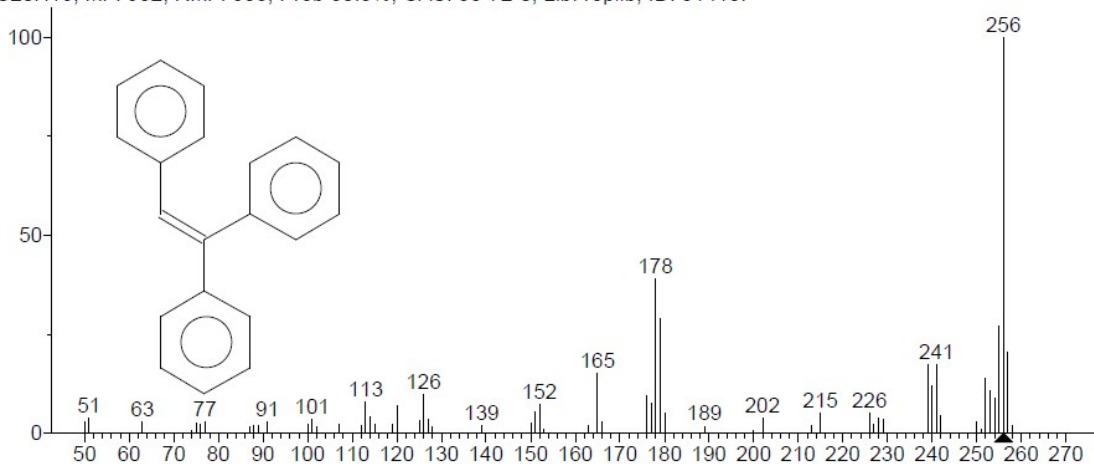
#### 4. Radical Trapping Experiment Data in Presence of 1,1-Diphenylethylene:



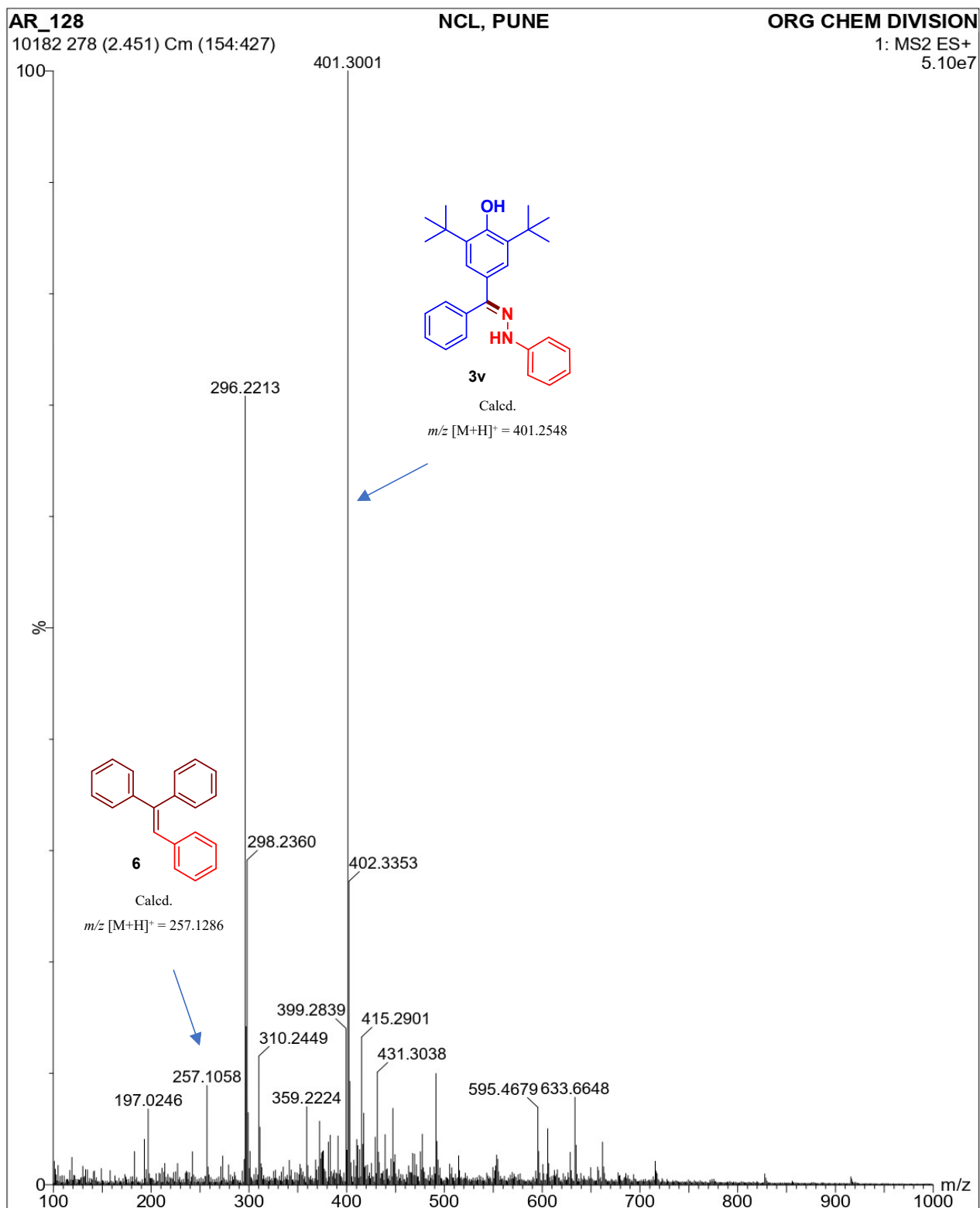
Name: + Scan (rt: 25.568 min) AR 128.D

MW: N/A ID#: 19739 DB: Text File

Hit 1 : Benzene, 1,1',1''-(1-ethenyl-2-ylidene)tris-  
C<sub>20</sub>H<sub>16</sub>; MF: 932; RMF: 955; Prob 83.3%; CAS: 58-72-0; Lib: replib; ID: 31413.



**Fig S4.** The GC-MS spectrum of the reaction mixture in the presence of 1,1-diphenylethylene.



**Fig S5.** The LC-MS spectrum of the reaction mixture in the presence of 1,1-diphenylethylene.

## 5. References:

- [S1] Bruker, *APEX3*, *SAINTE* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA. **2016**.
- [S2] Sheldrick, G. M. A Short History of SHELX. *Acta Crystallogr.* **2008**, A64, 112-122.
- [S3] Sheldrick, G. M. Crystal Structure Refinement with SHELXL. *Acta Crystallogr.* **2015**, C71, 3-8.
- [S4] Farrugia, L. J. WinGX and ORTEP for Windows: an update. *J. Appl. Crystallogr.* **2012**, 45, 84-854.