

## Supporting Information

### Design, synthesis, molecular docking and biological evaluation of 1,2,4 triazole derivatives possessing a hydrazone moiety as anti-breast cancer agents

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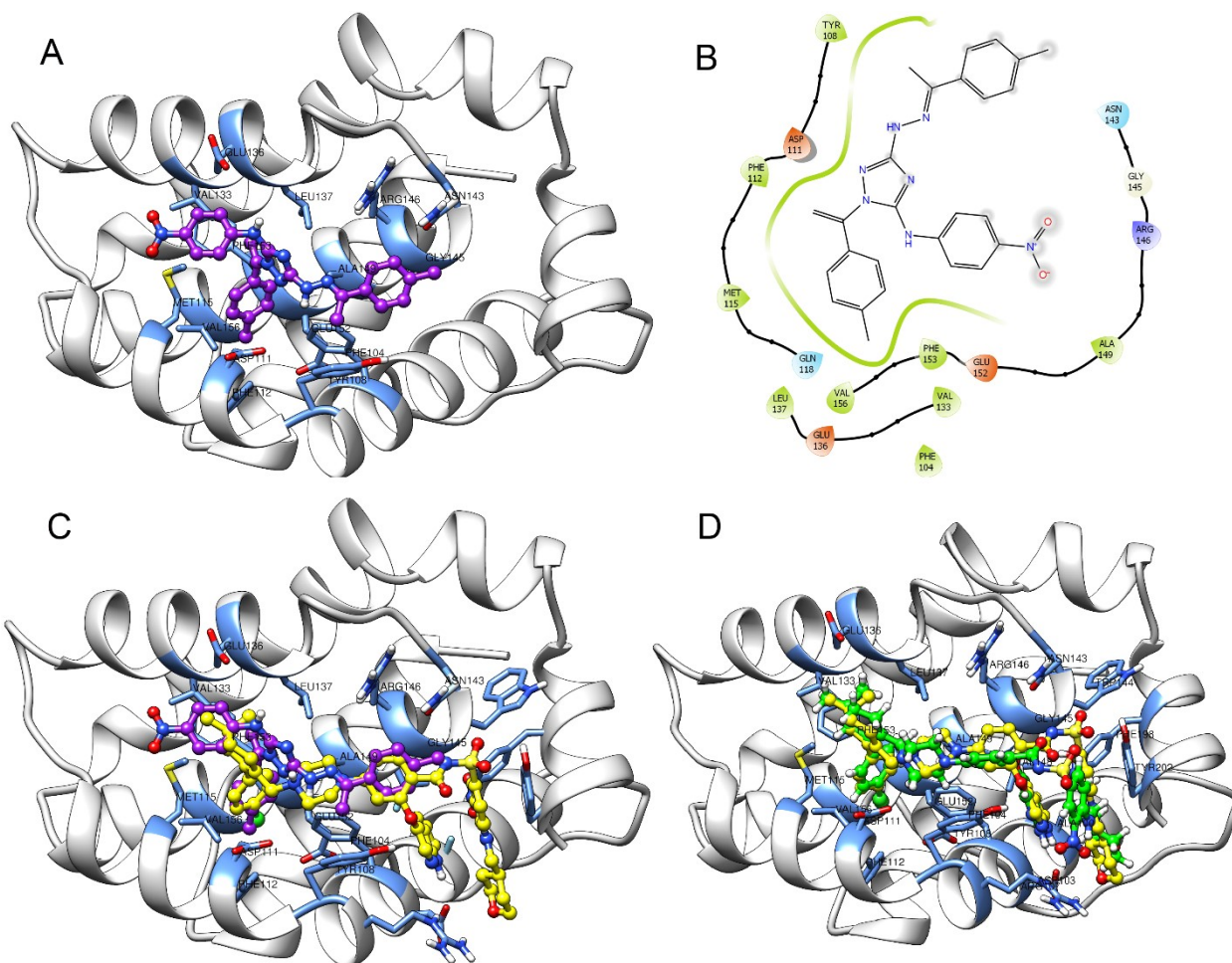
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Crystallographic data with CCDC reference number 2155032 **BIH2** has been deposited within the Cambridge Crystallographic Data Center via [www.ccdc.cam.ac.uk/deposit](http://www.ccdc.cam.ac.uk/deposit). Crystallographic data and refinement details of the data collection are presented in supporting information.

**Table 1.** Crystal data and structure refinement details for **BIH2**.

Compound	<b>BIH2</b>
CCDC	2155032
Empirical formula	C <sub>24</sub> H <sub>21</sub> N <sub>7</sub> O <sub>2</sub>
Formula weight/g. mol <sup>-1</sup>	439.48
Temperature/K	298
Radiation, Wavelength (Å)	MoKα (λ = 0.71073)
Crystal system	Monoclinic
Space group	C2/c
a/Å	26.325(4)
b/Å	8.6403(14)
c/Å	22.014(4)
α/°	90
β/°	117.940(2)
γ/°	90
Volume/Å <sup>3</sup>	4423.7(12)
Z	8
ρ <sub>calcd</sub> (g. cm <sup>-3</sup> )	1.320
μ (mm <sup>-1</sup> )	0.089
F(000)	1840
2θ range for data collection (°)	3.502 to 49.992
h/k/l	-31 ≤ h ≤ 31, -10 ≤ k ≤ 10, -26 ≤ l ≤ 26
Reflections collected	13333
Independent reflections	3877 [R <sub>int</sub> = 0.0735, R <sub>sigma</sub> = 0.0710]
Data/restraints/parameters	3877/0/300
Goodness-of-fit on F <sup>2</sup> (S)	1.060
Final R indices [I > 2σ(I)]	R <sub>1</sub> = 0.0528, wR <sub>2</sub> = 0.1299
R indices (all data)	R <sub>1</sub> = 0.0939, wR <sub>2</sub> = 0.1460
Largest diff. peak/hole / e Å <sup>-3</sup>	0.22/-0.16



**Fig. S2.** Molecular docking results of most active compound BIH4 and cocystal ligand of apoptosis regulator Bcl-2 (PDB ID: 6O0K). (A) Binding poses of BIH4 at Bcl-2 active site, (B) Schematic protein-ligand 2D interaction diagram of BIH4, (C) Superimposition of docked compound BIH4 (purple) and cocystal ligand of Bcl-2 (yellow), and (D) Natural binding pose (yellow) of and re-docking pose (green) of cocystal ligand (RMSD: 1.57 Å).

# Copies of $^1\text{H}$ and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compounds

## BI1

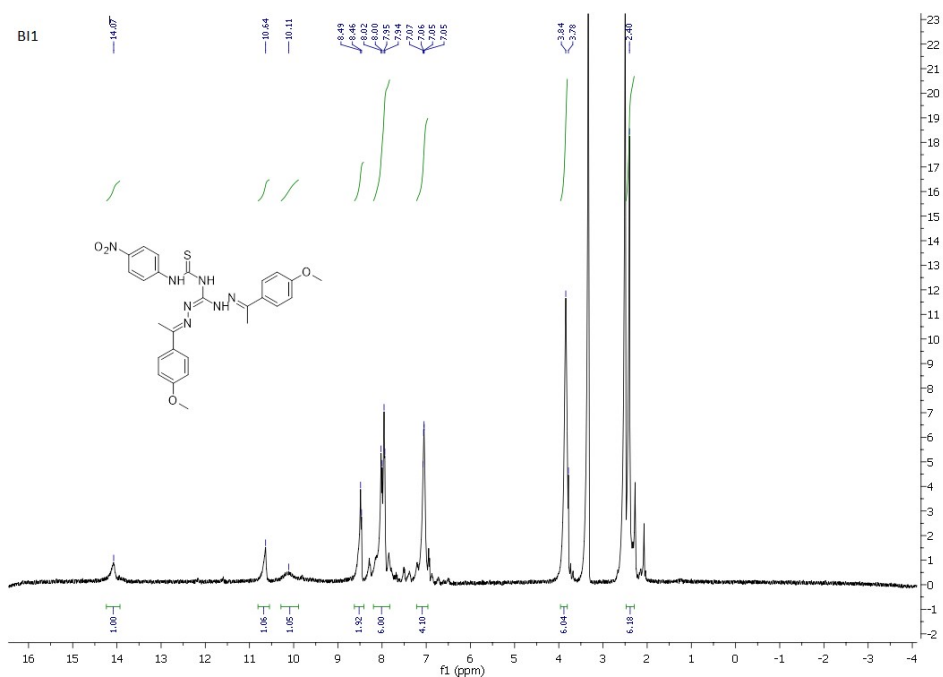
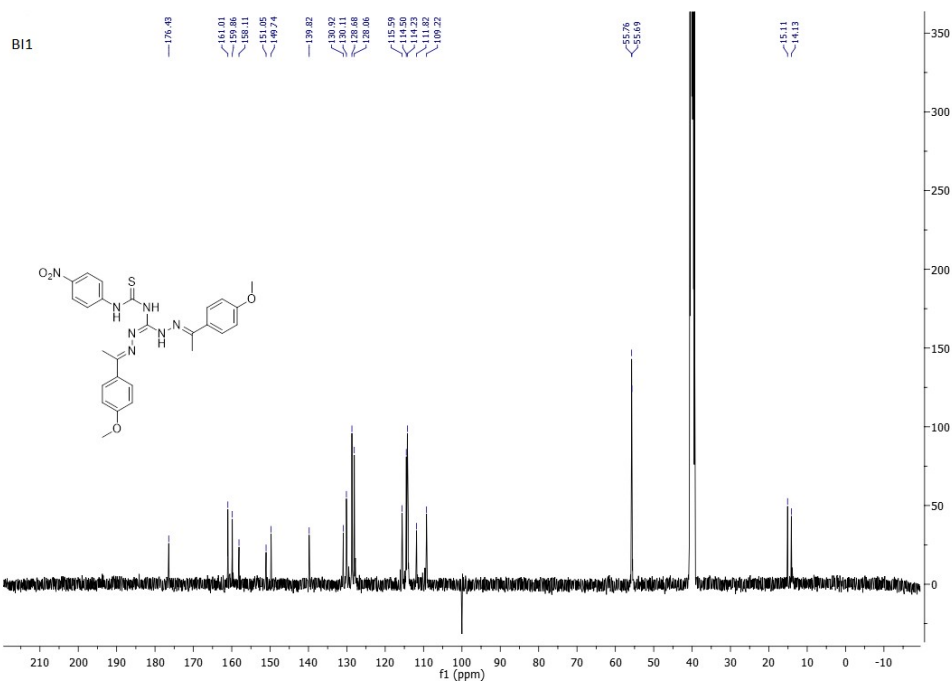
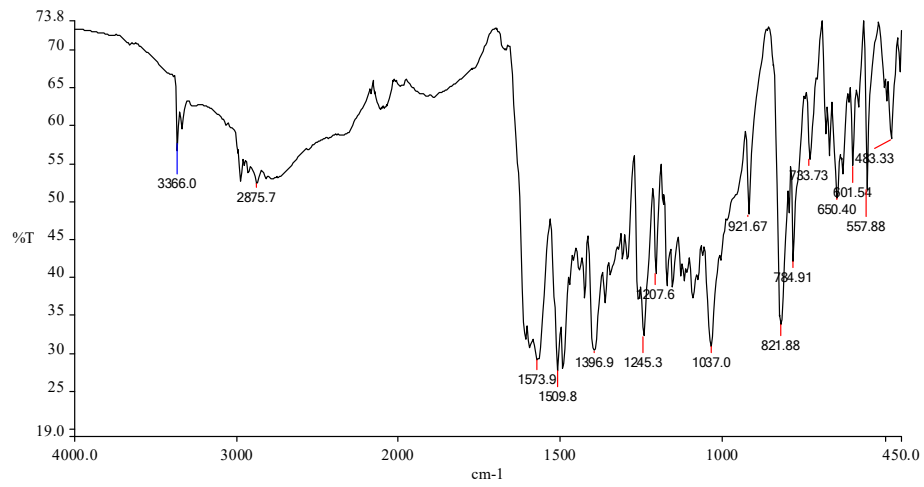


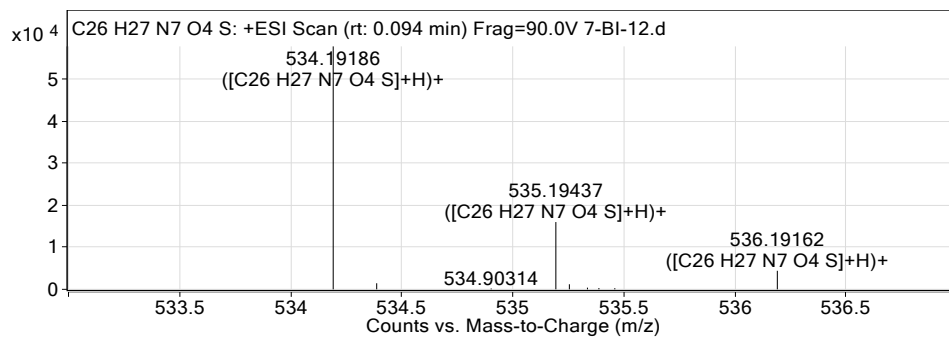
Figure 1.  $^1\text{H}$ -NMR spectrum of compound BI1



**Figure 2.**  $^{13}\text{C}$ -NMR spectrum of compound **BI1**

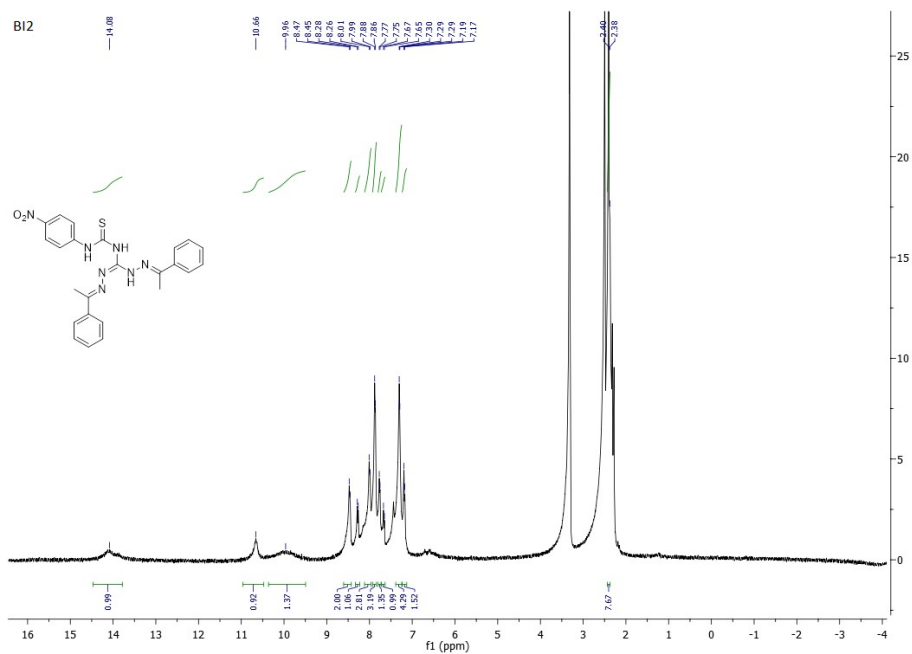


**Figure 3.** IR spectrum of compound **BI1**

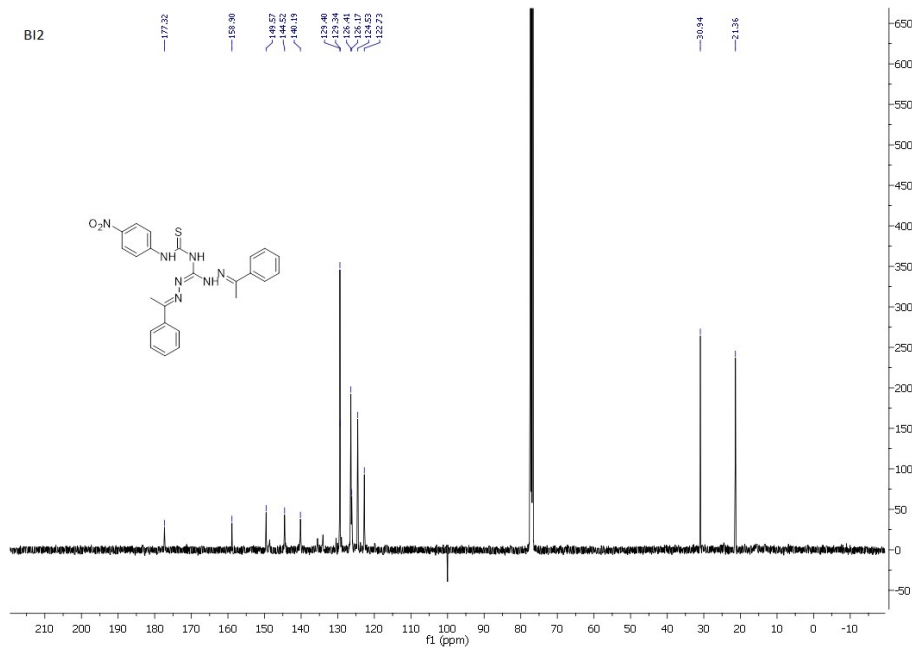


**Figure 4.** Mass spectrum of compound **BI2**

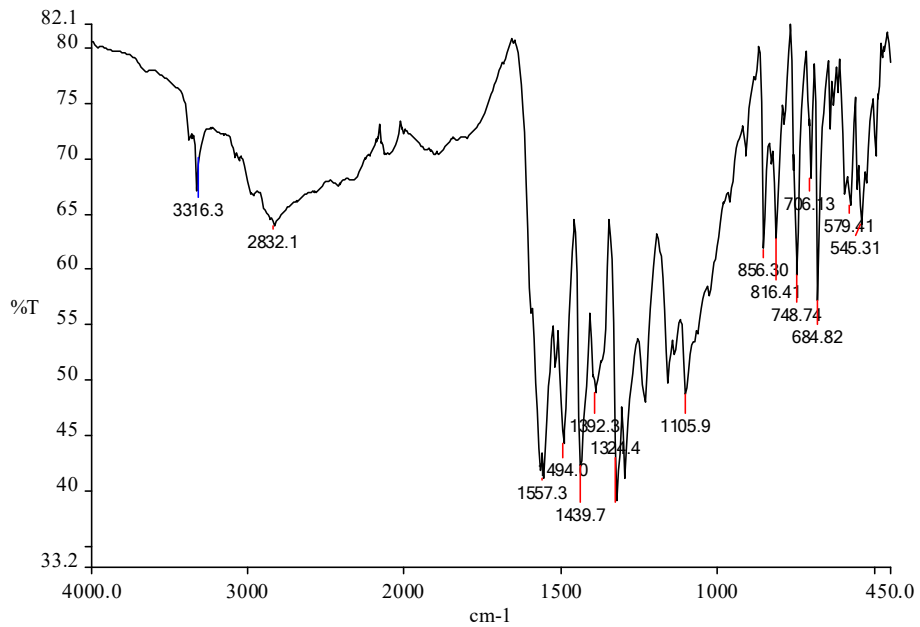
**BI2**



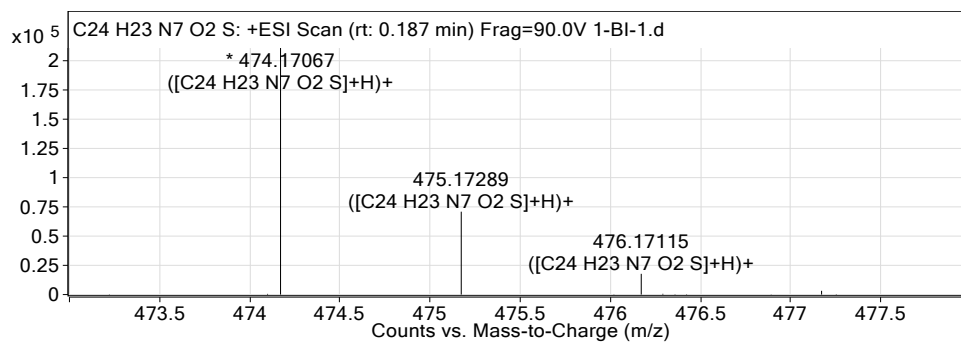
**Figure 5.** <sup>1</sup>H-NMR spectrum of compound **BI2**



**Figure 6.** <sup>13</sup>C-NMR spectrum of compound **BI2**



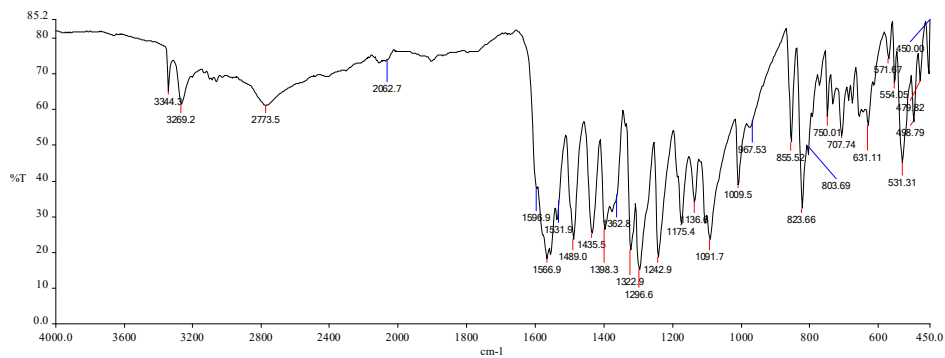
**Figure 7.** IR spectrum of compound BI2



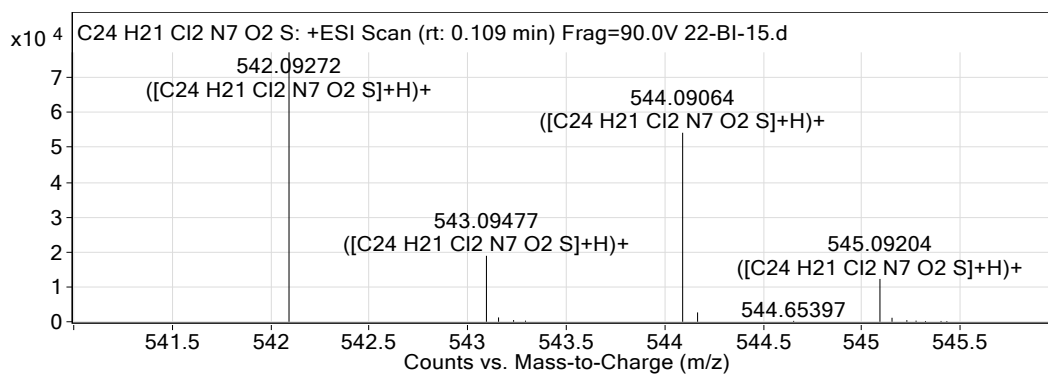
**Figure 8.** Mass spectrum of compound BI2







**Figure 11.** IR spectrum of compound BI3



**Figure 12.** Mass spectrum of compound BI3

# BI4

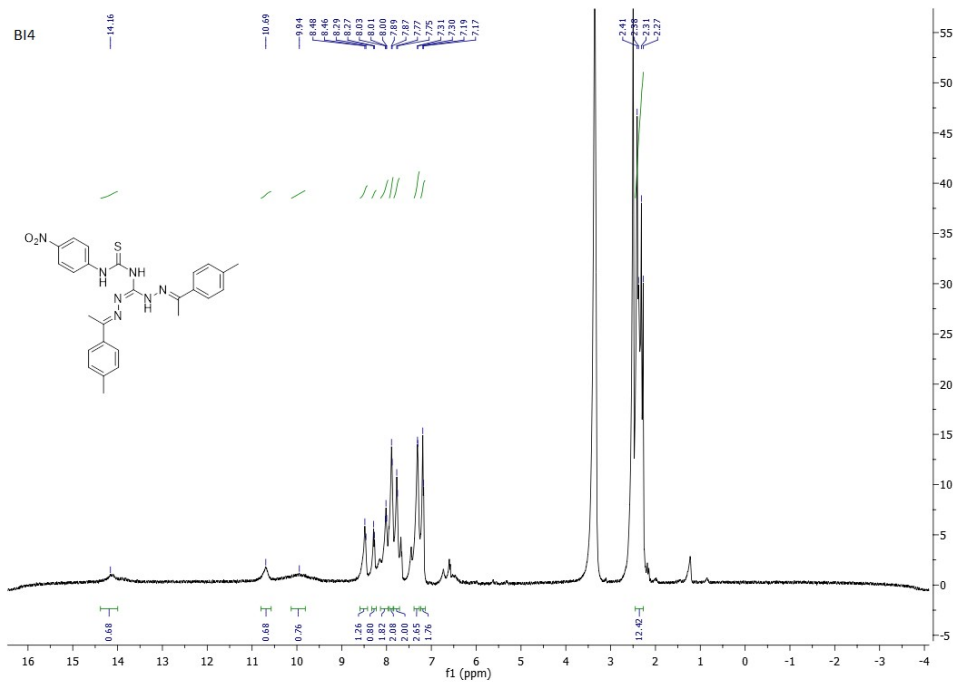


Figure 13. <sup>1</sup>H-NMR spectrum of compound BI4

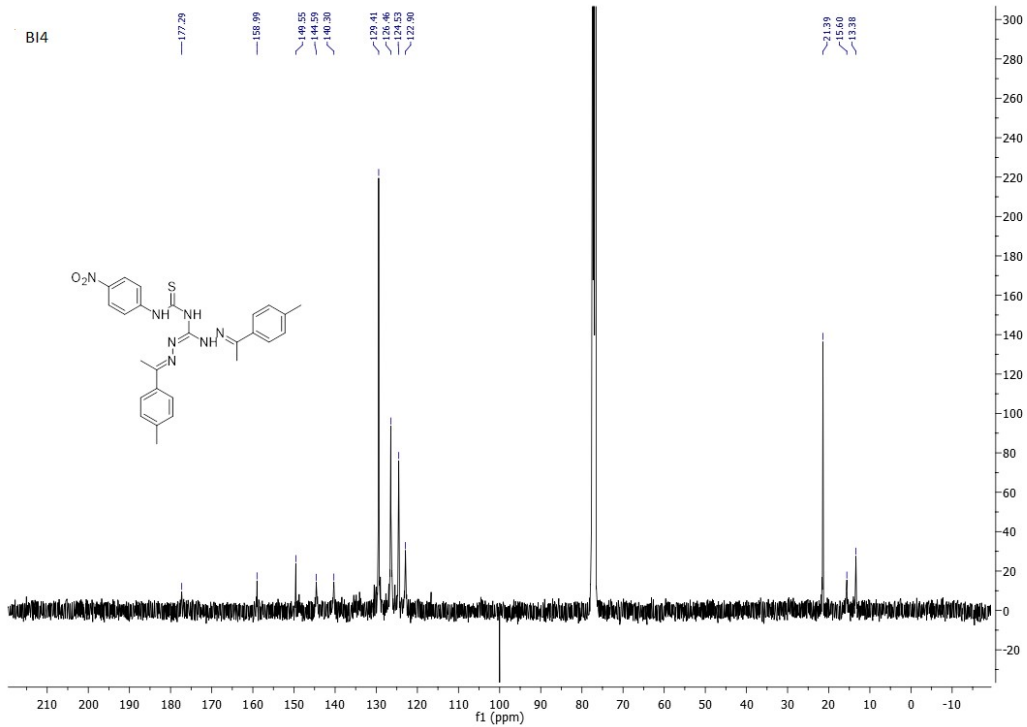
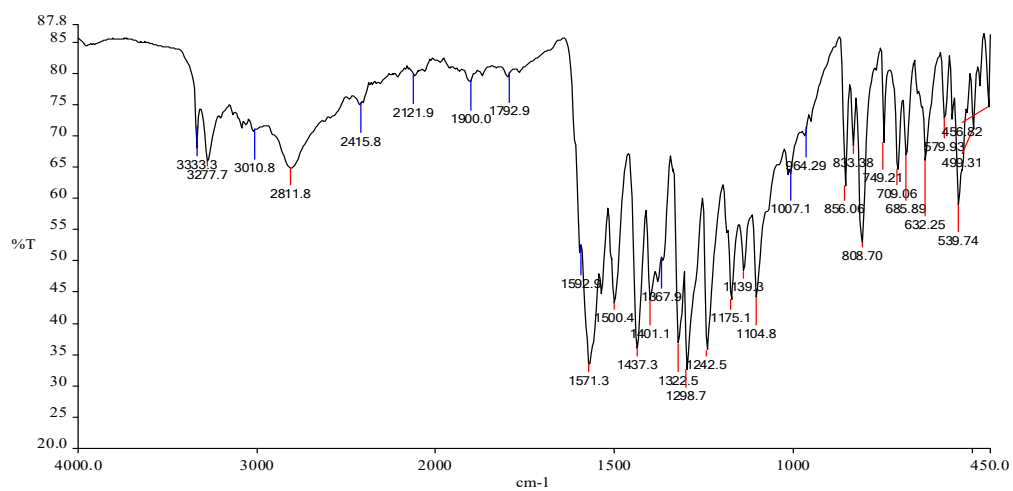
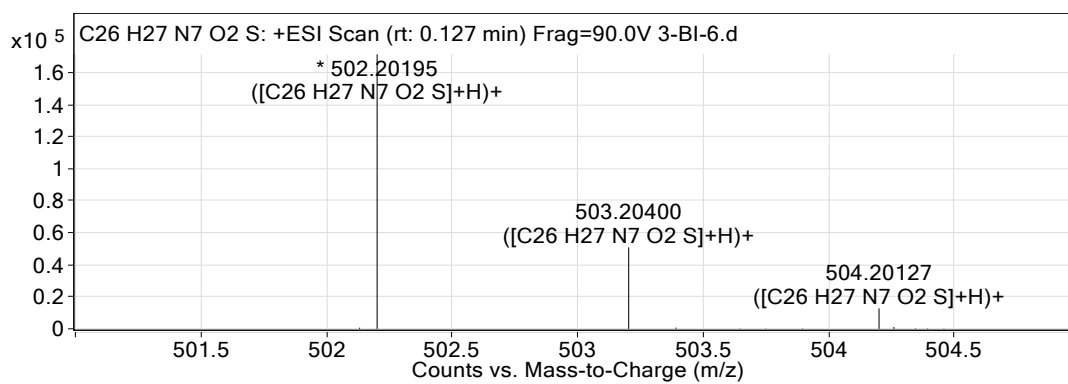


Figure 14. <sup>13</sup>C-NMR spectrum of compound BI4



**Figure 15.** IR spectrum of compound **B14**



**Figure 16.** Mass spectrum of compound **B14**

# BI5

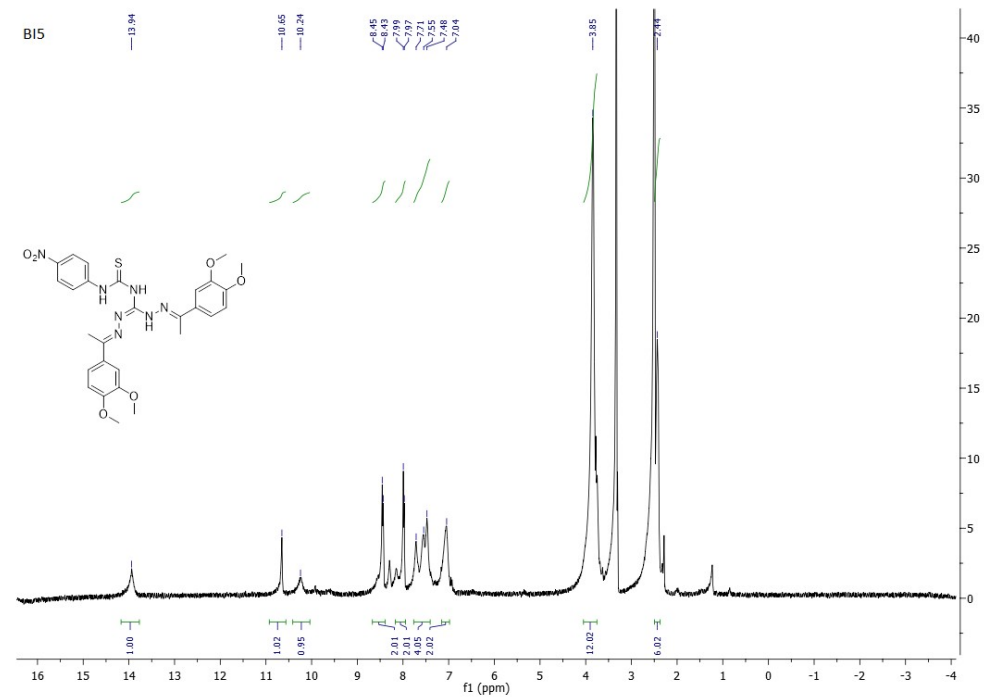


Figure 17. <sup>1</sup>H-NMR spectrum of compound BI5

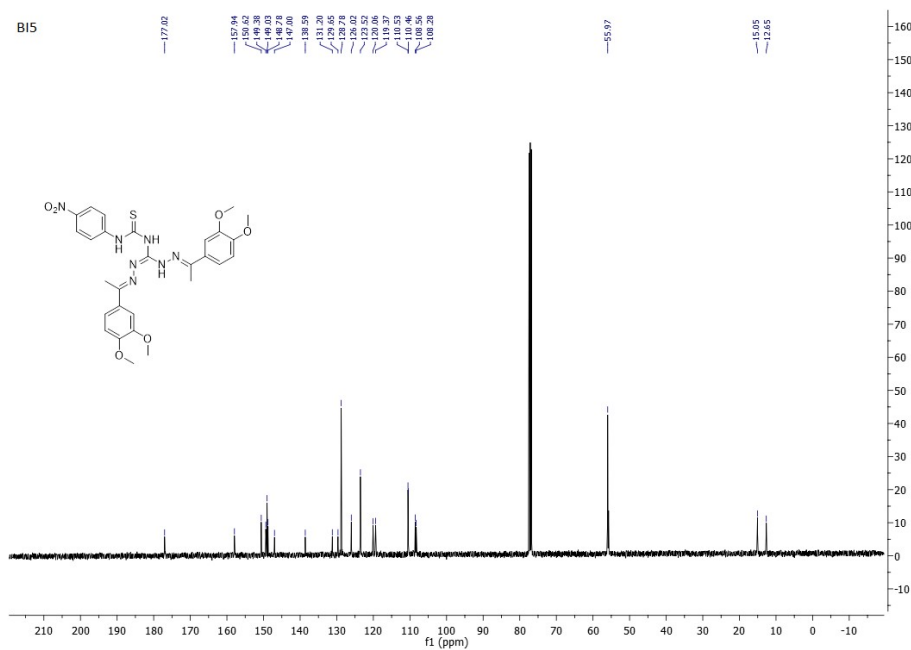
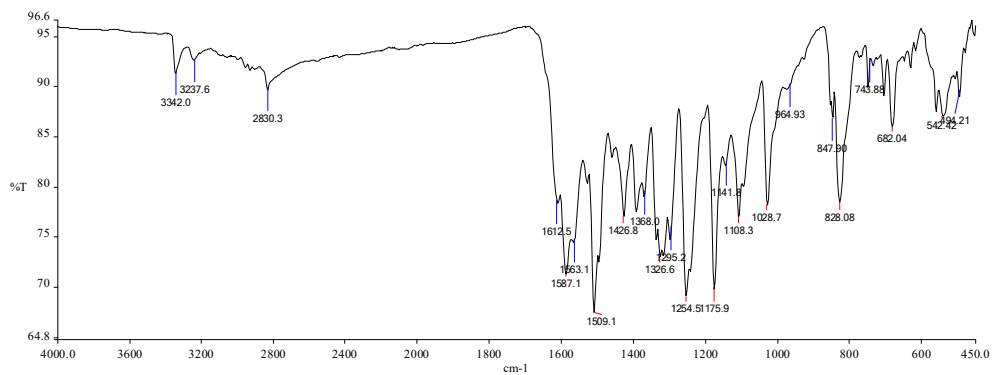
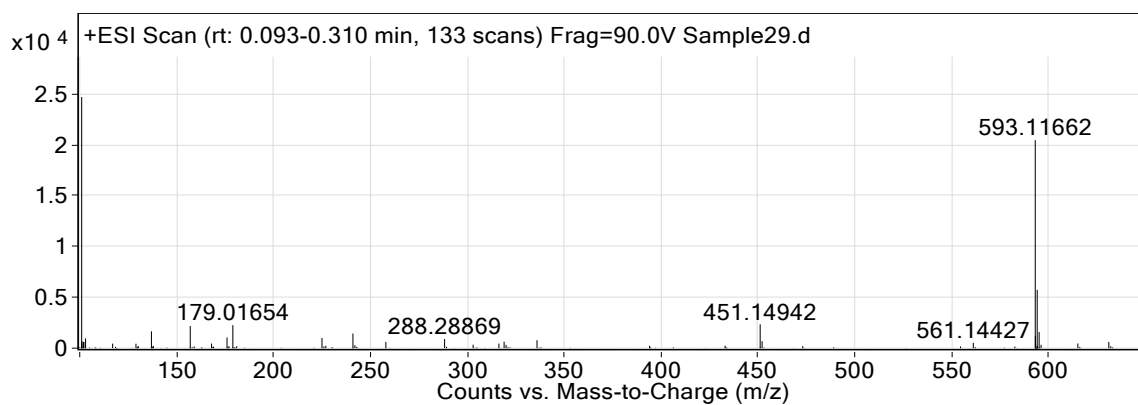


Figure 18. <sup>13</sup>C-NMR spectrum of compound BI5



**Figure 19.** IR spectrum of compound **B15**



**Figure 20.** Mass spectrum of compound **B15**

# BI6

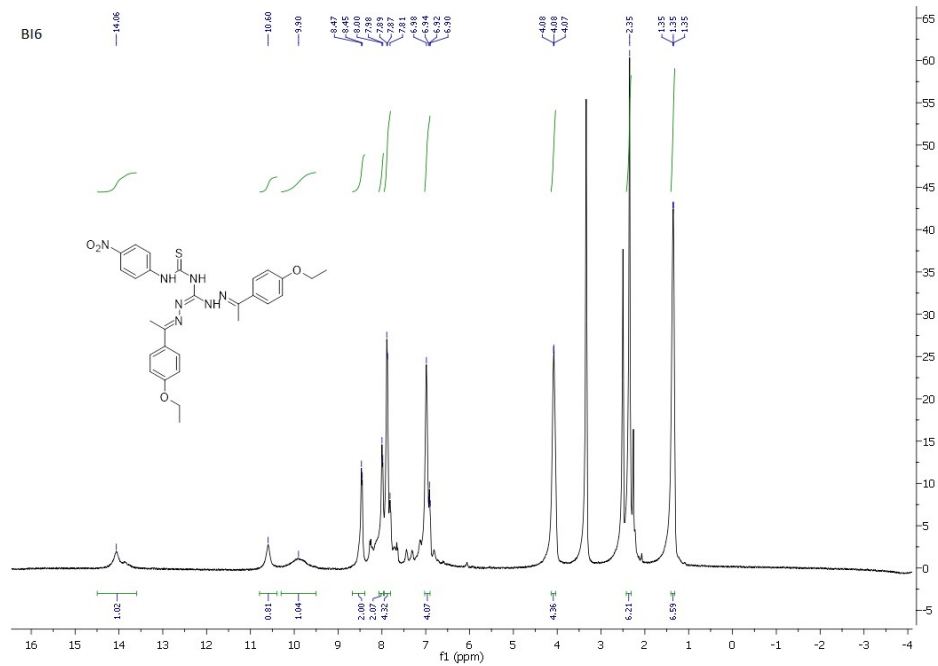


Figure 21. <sup>1</sup>H-NMR spectrum of compound BI6

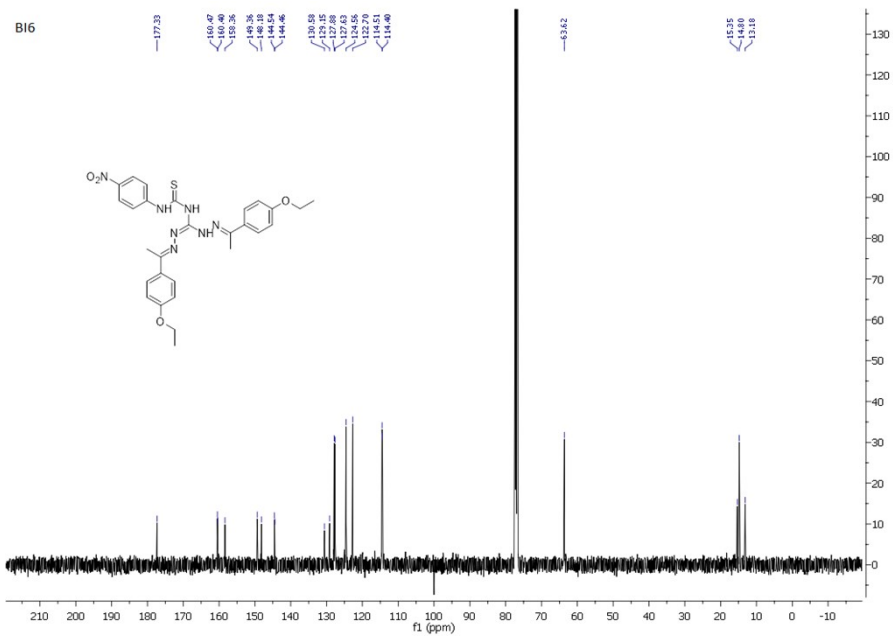


Figure 22. <sup>13</sup>C-NMR spectrum of compound BI6

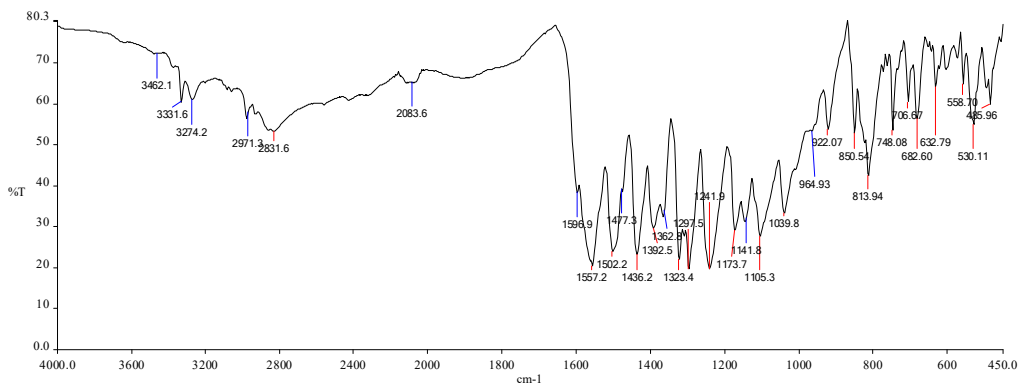


Figure 23. IR spectrum of compound BI6

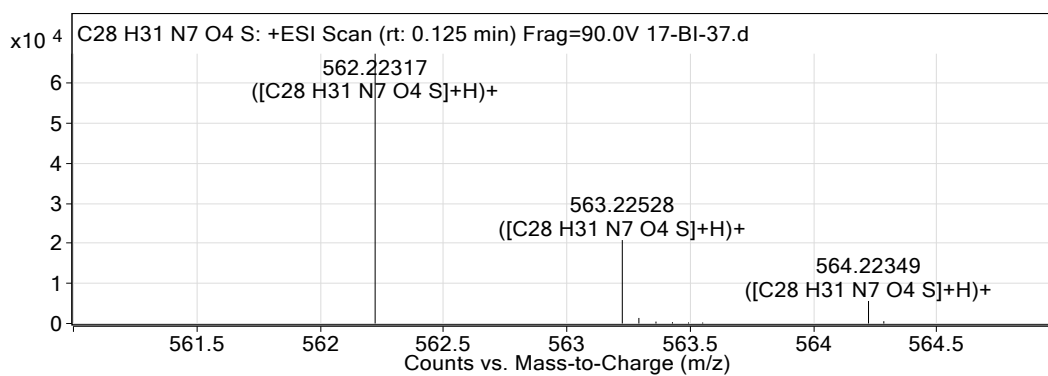


Figure 24. Mass spectrum of compound BI6



# BIH1

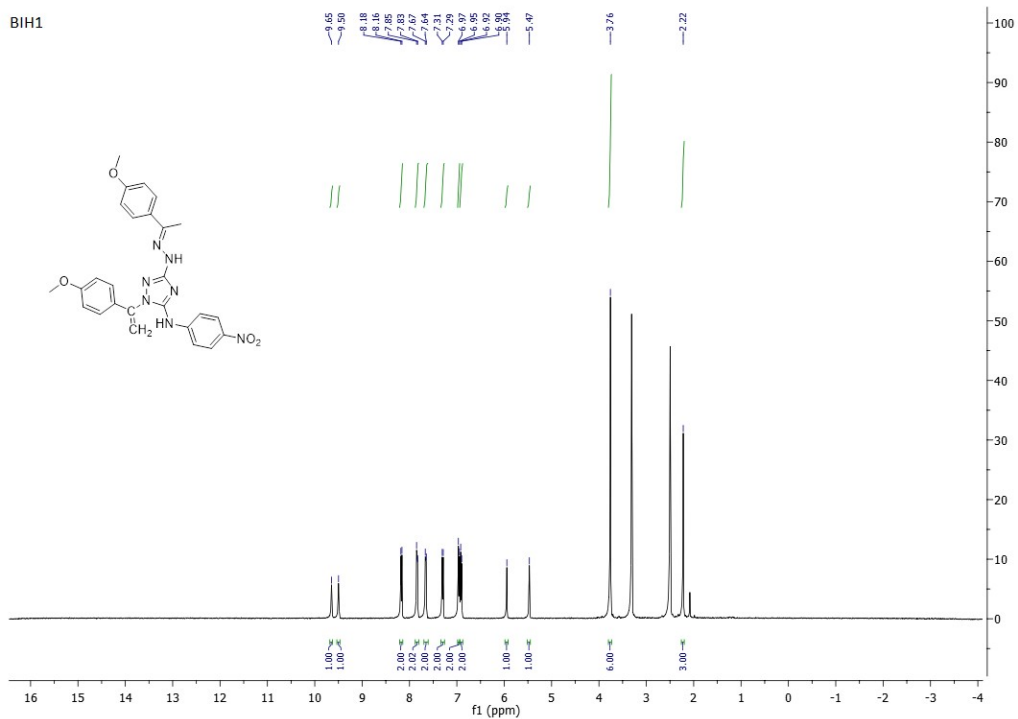


Figure 25.  $^1\text{H}$ -NMR spectrum of compound BIH1

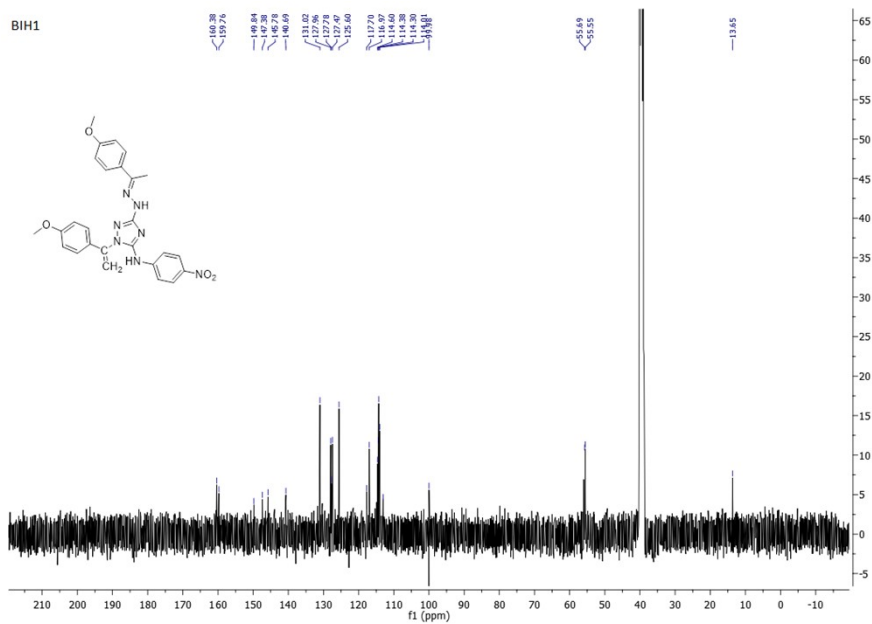
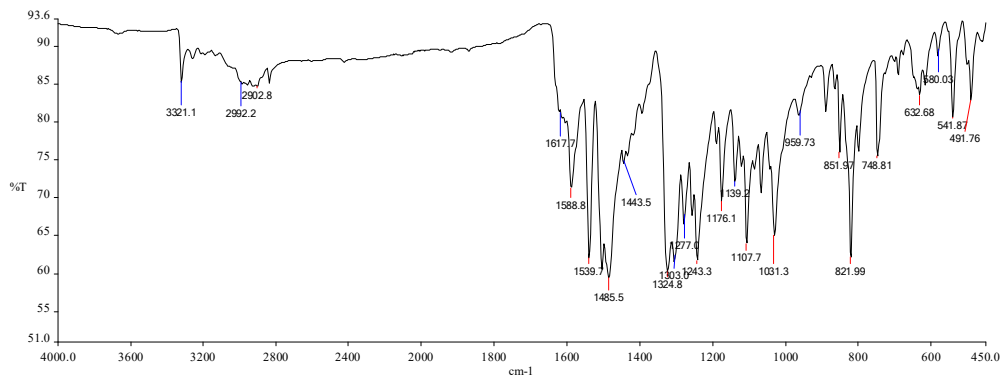
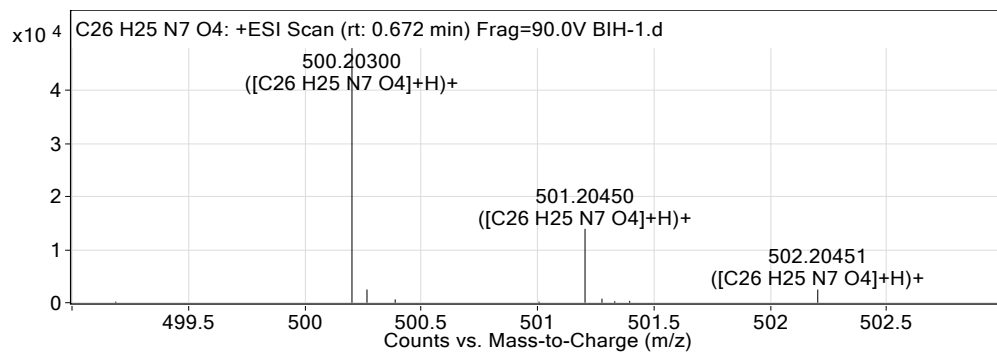


Figure 26.  $^{13}\text{C}$ -NMR spectrum of compound BIH1



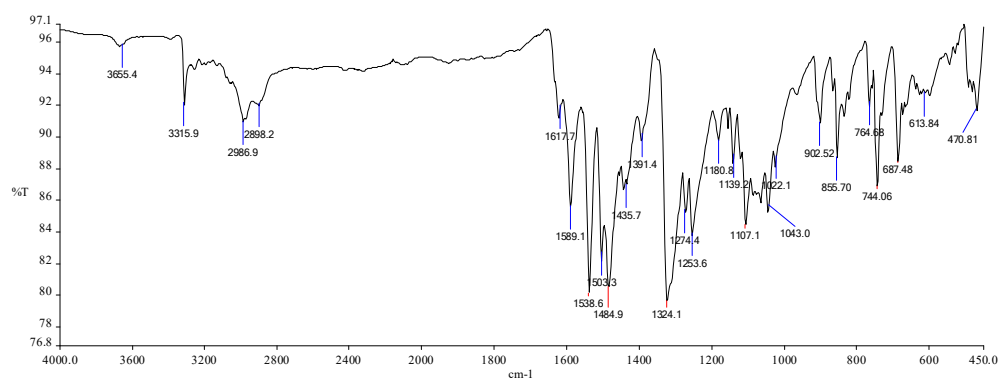
**Figure 27.** IR spectrum of compound **BIH1**



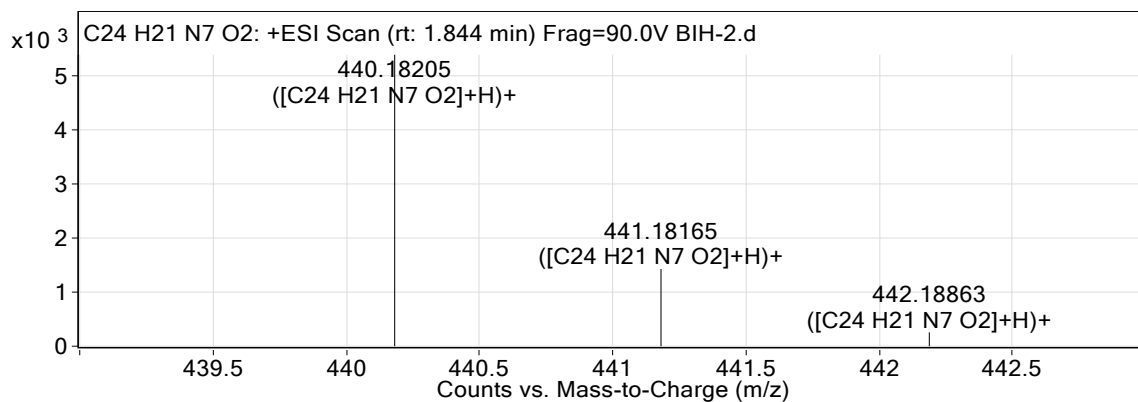
**Figure 28.** Mass spectrum of compound **BIH1**

**BIH2**





**Figure 31.** IR spectrum of compound **BIH2**



**Figure 32.** Mass spectrum of compound **BIH2**

# BIH3

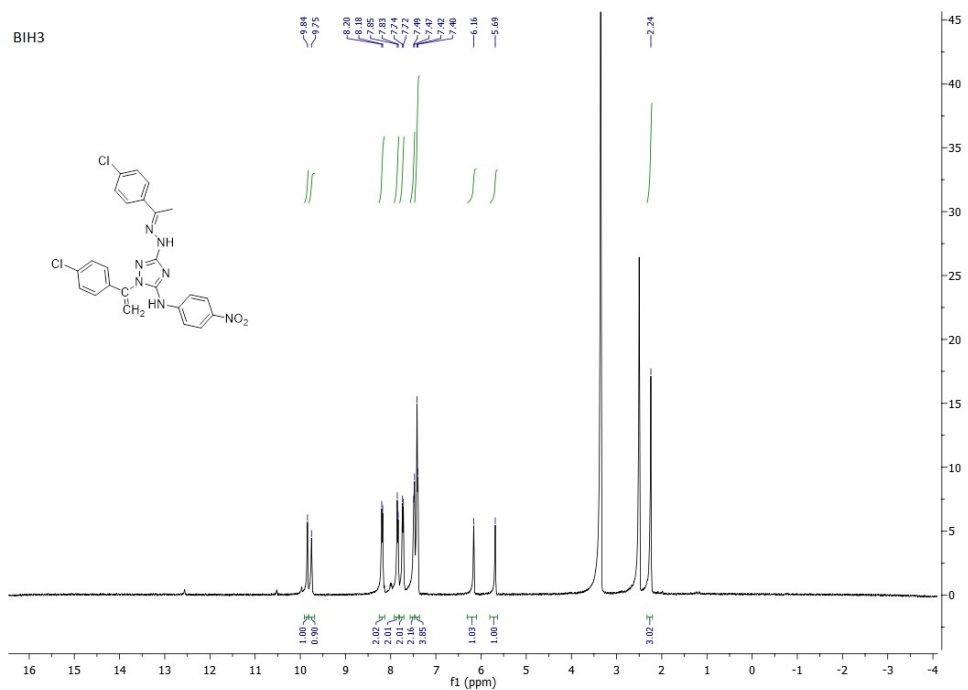


Figure 33. <sup>1</sup>H-NMR spectrum of compound BIH3

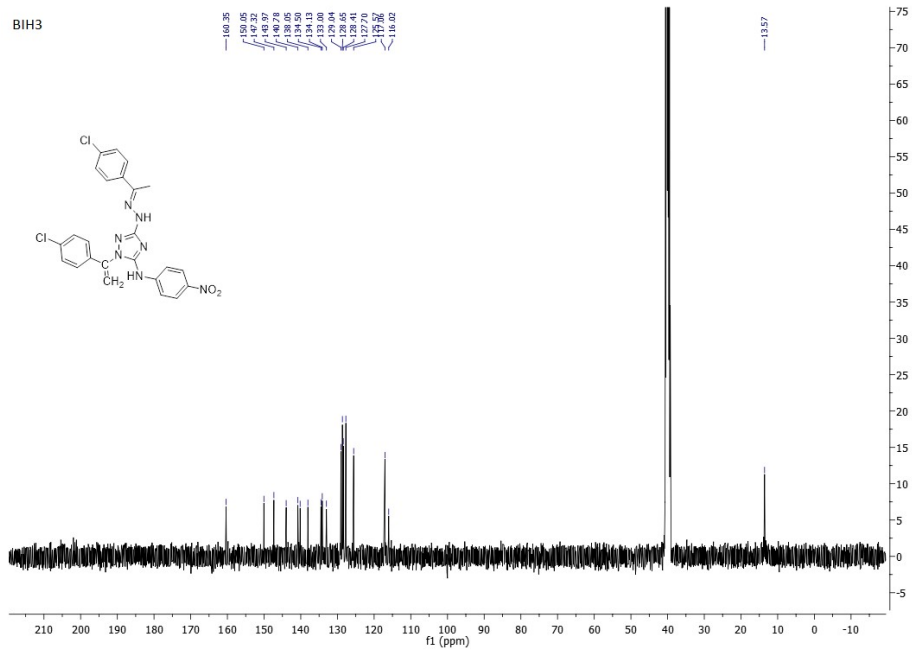
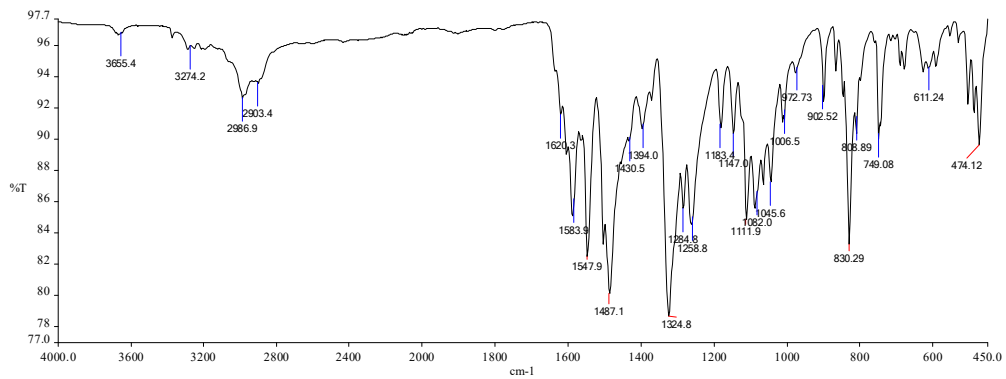
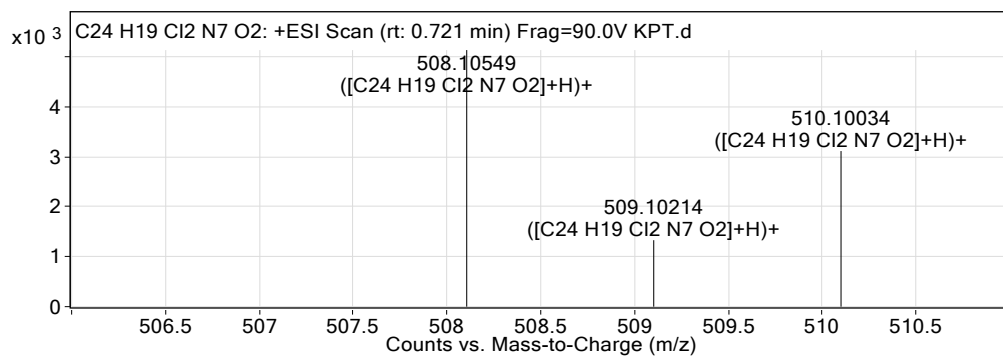


Figure 34. <sup>13</sup>C-NMR spectrum of compound BIH3



**Figure 35.** IR spectrum of compound **BIH3**



**Figure 36.** Mass spectrum of compound **BIH3**

# BIH4

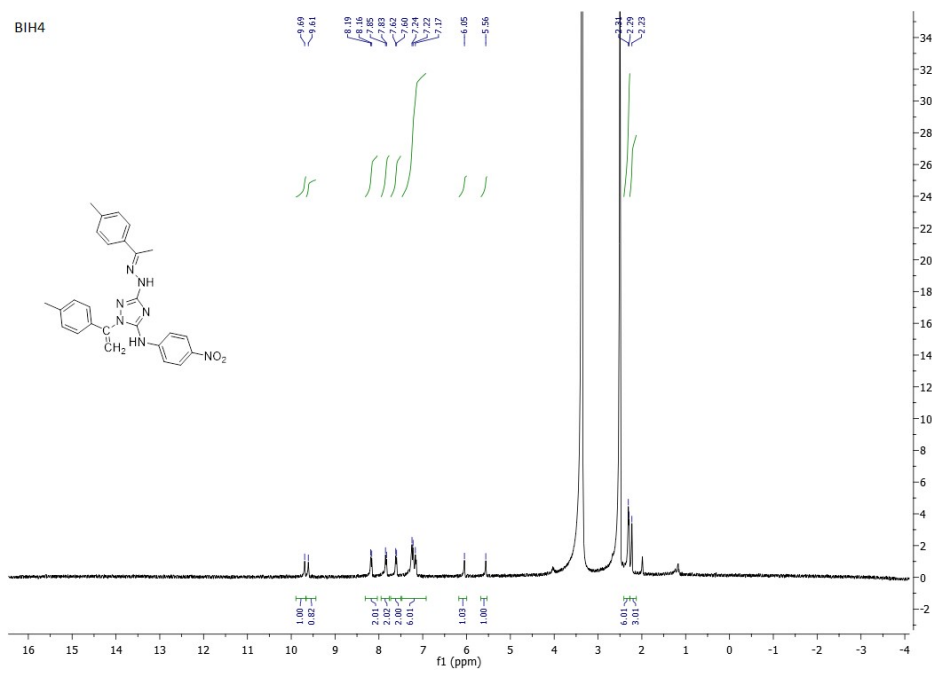


Figure 37.  $^1\text{H}$ -NMR spectrum of compound BIH4

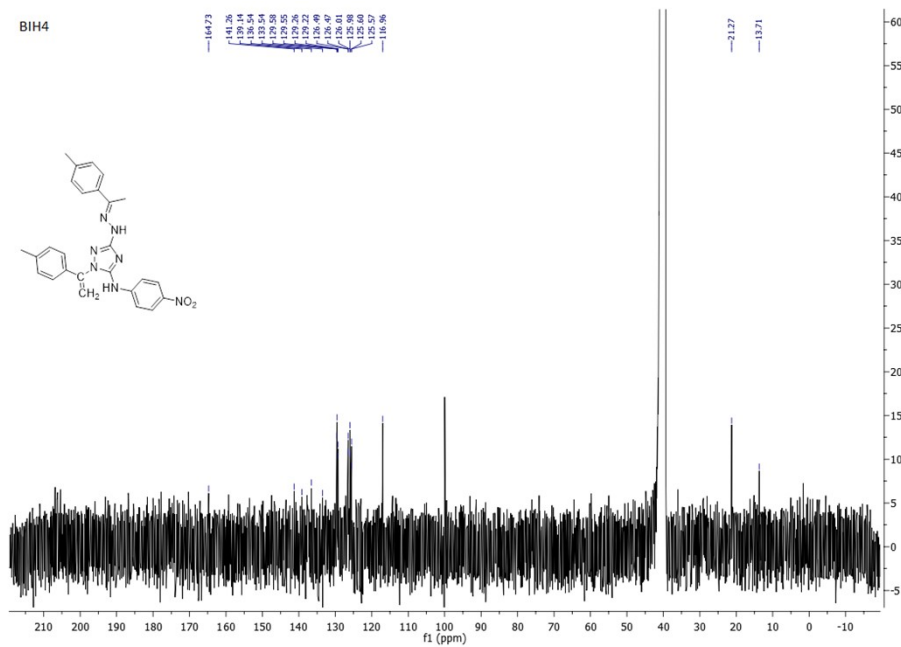
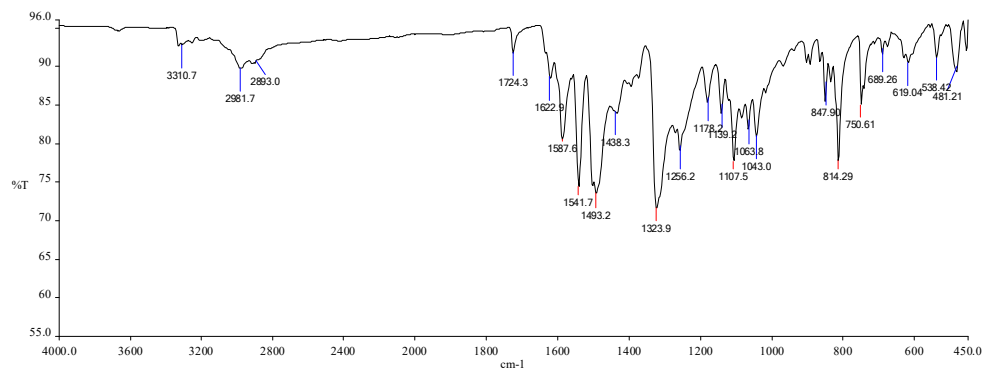
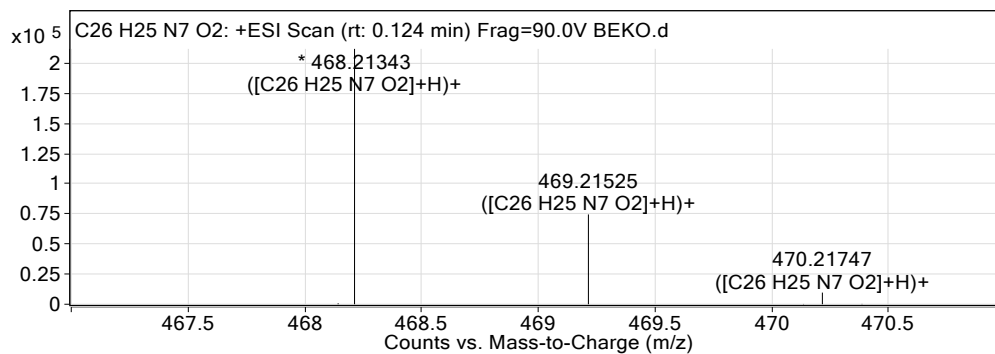


Figure 38.  $^{13}\text{C}$ -NMR spectrum of compound BIH4



**Figure 39.** IR spectrum of compound **BIH4**



**Figure 40.** Mass spectrum of compound **BIH4**



# BIH5

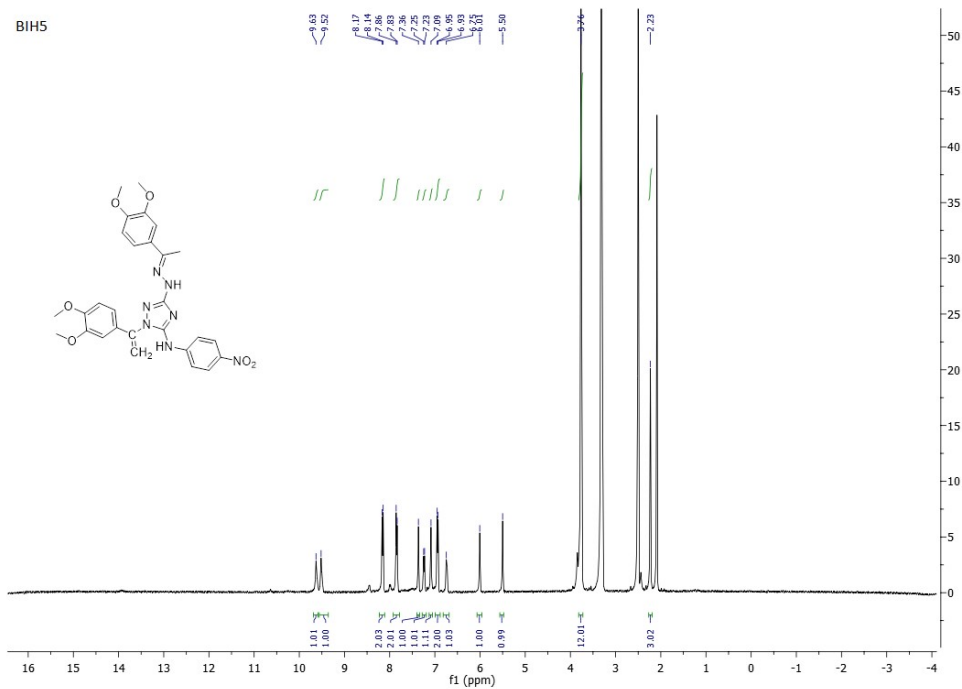


Figure 41.  $^1\text{H}$ -NMR spectrum of compound BIH5

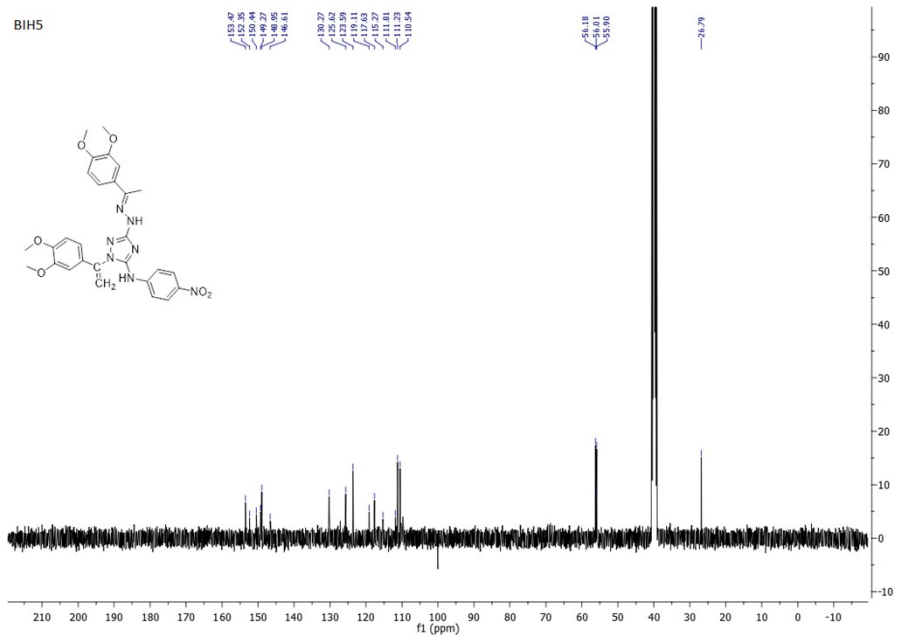
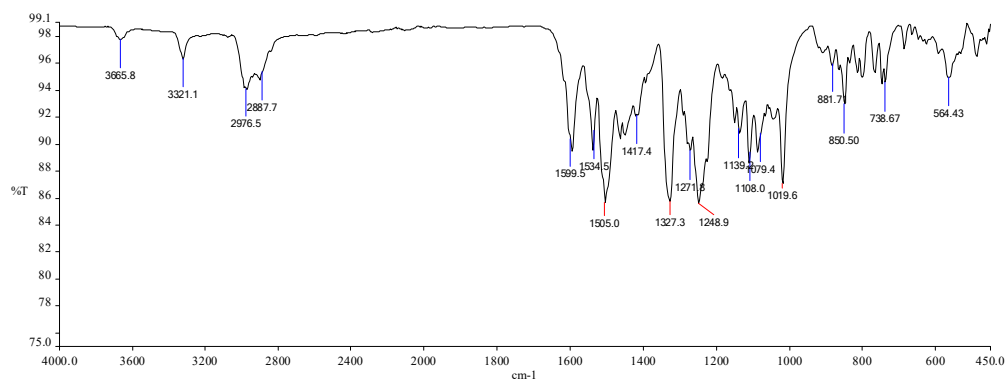
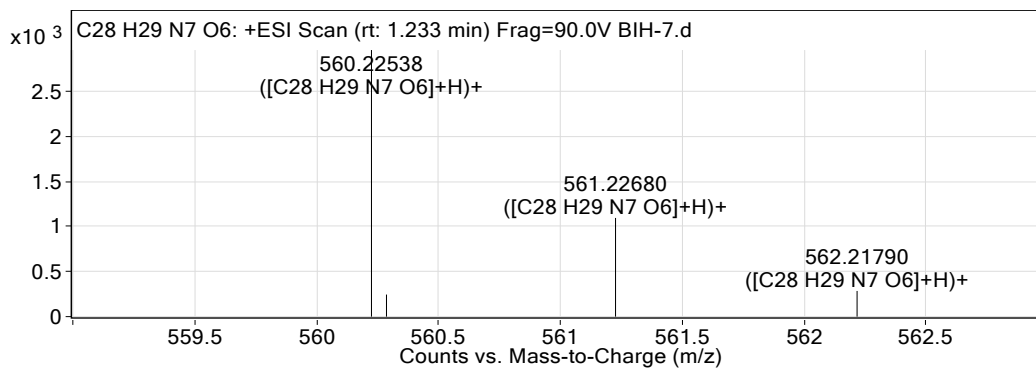


Figure 42.  $^{13}\text{C}$ -NMR spectrum of compound BIH5



**Figure 43.** IR spectrum of compound **BIH5**



**Figure 44.** Mass spectrum of compound **BIH5**

# BIH6

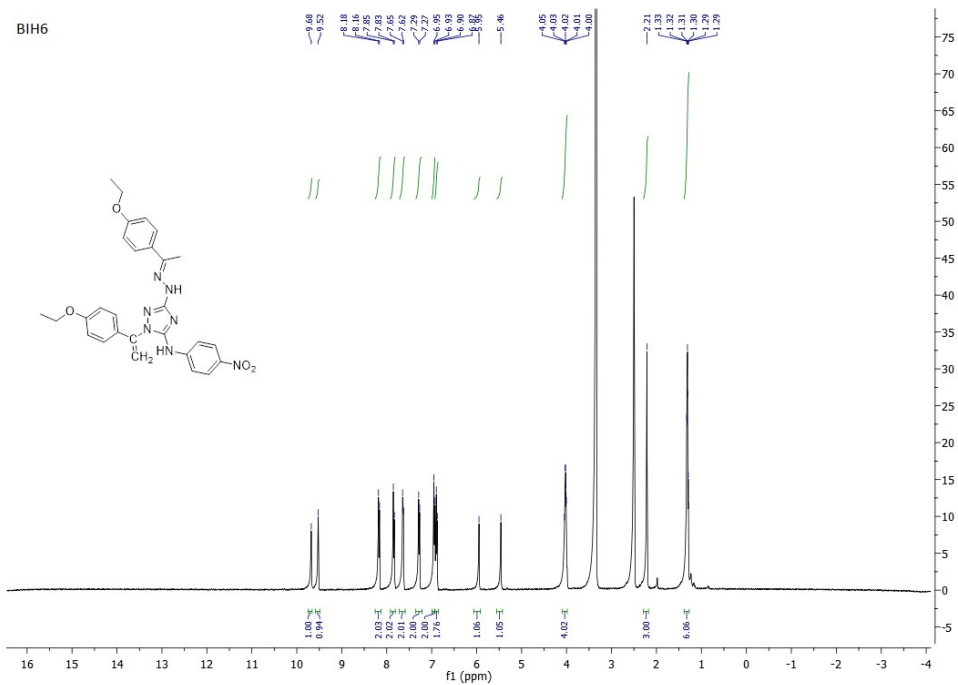


Figure 45. <sup>1</sup>H-NMR spectrum of compound BIH6

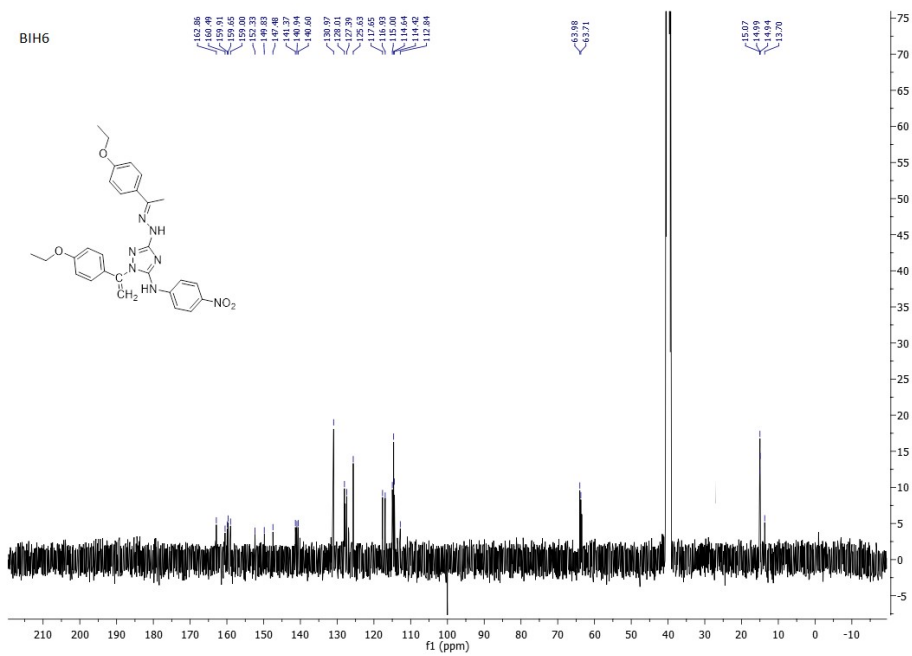
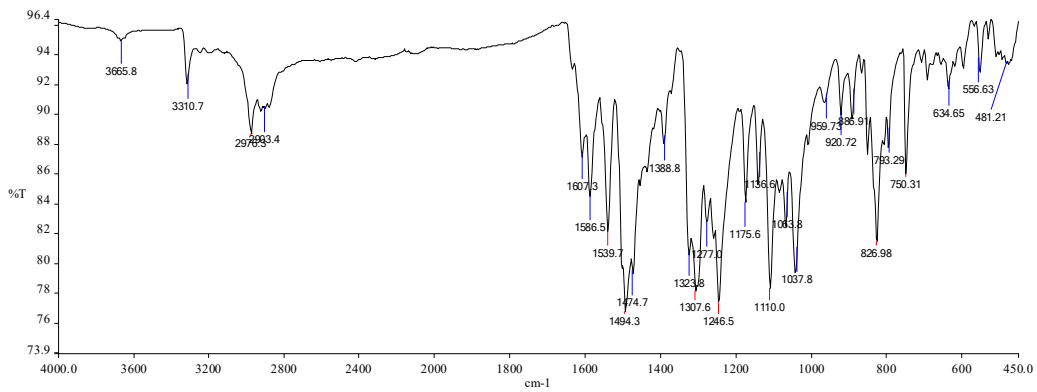
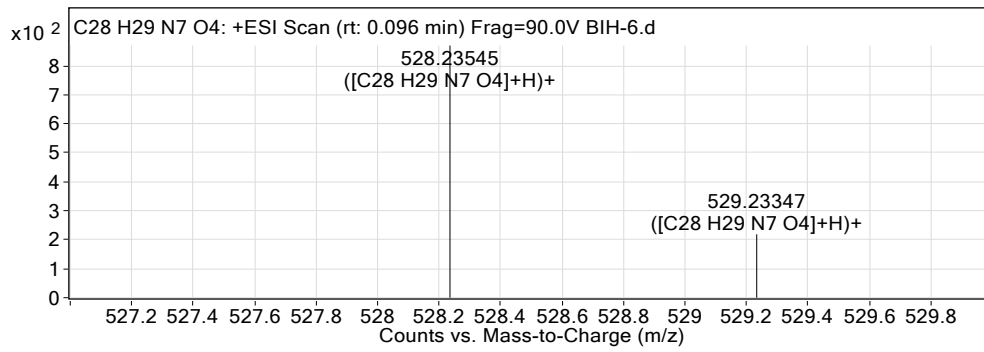


Figure 46. <sup>13</sup>C-NMR spectrum of compound BIH6



**Figure 47.** IR spectrum of compound **BIH6**



**Figure 48.** Mass spectrum of compound **BIH6**