

**Supplementary information**

**Synthesis and biological evaluation of pyrazolo-triazole hybrids as  
cytotoxic and apoptosis inducing agents**

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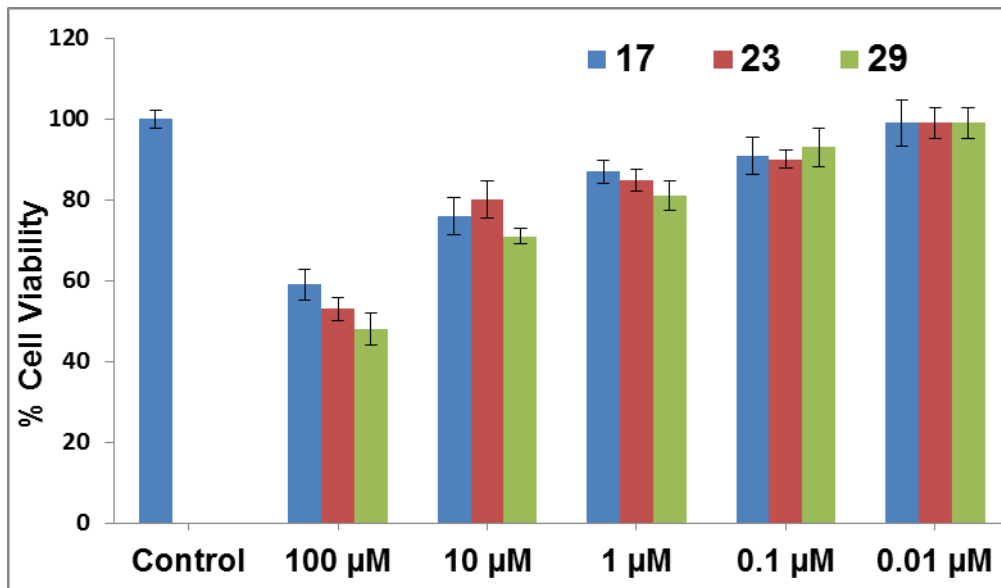
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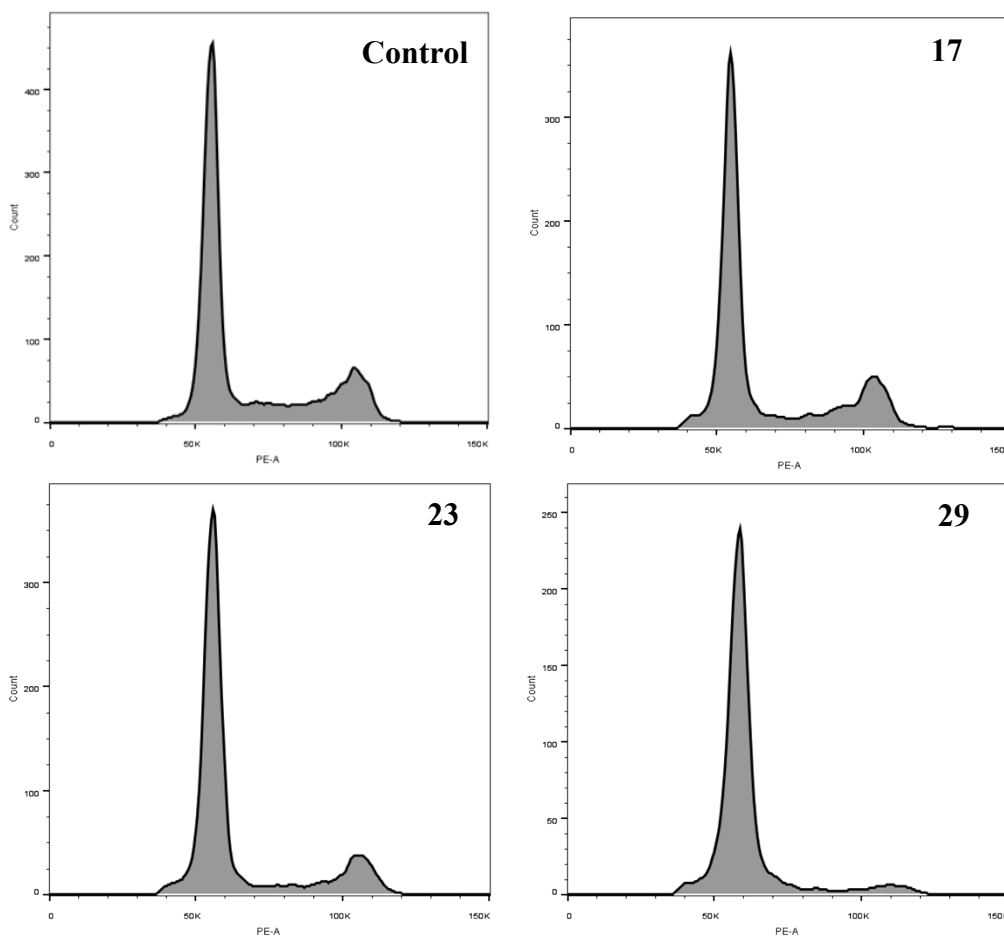
Phone: 0061 3 9925 2970; Fax: 0061 3 9925 2882

E-mail: [ahmedkamal@iict.res.in](mailto:ahmedkamal@iict.res.in)

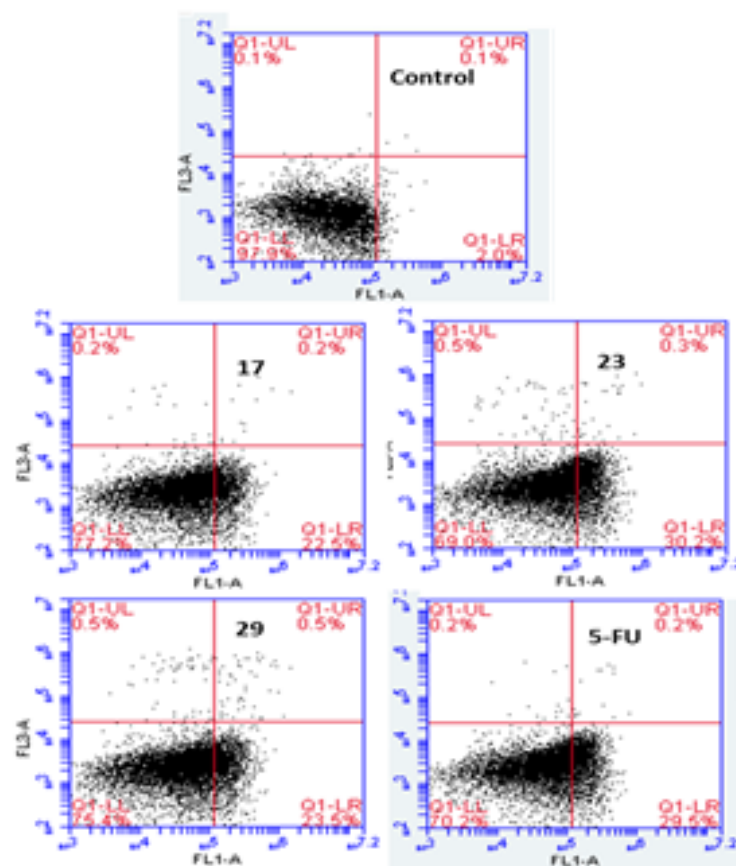
Phone: (+) 91-40-27193157; Fax: (+) 91-40-27193189;



**Figure S1** Effect of compounds **17**, **23** and **29** on cell viability of normal keratinocytes (HaCaT). Data are mean  $\pm$  SD from three independent experiments.

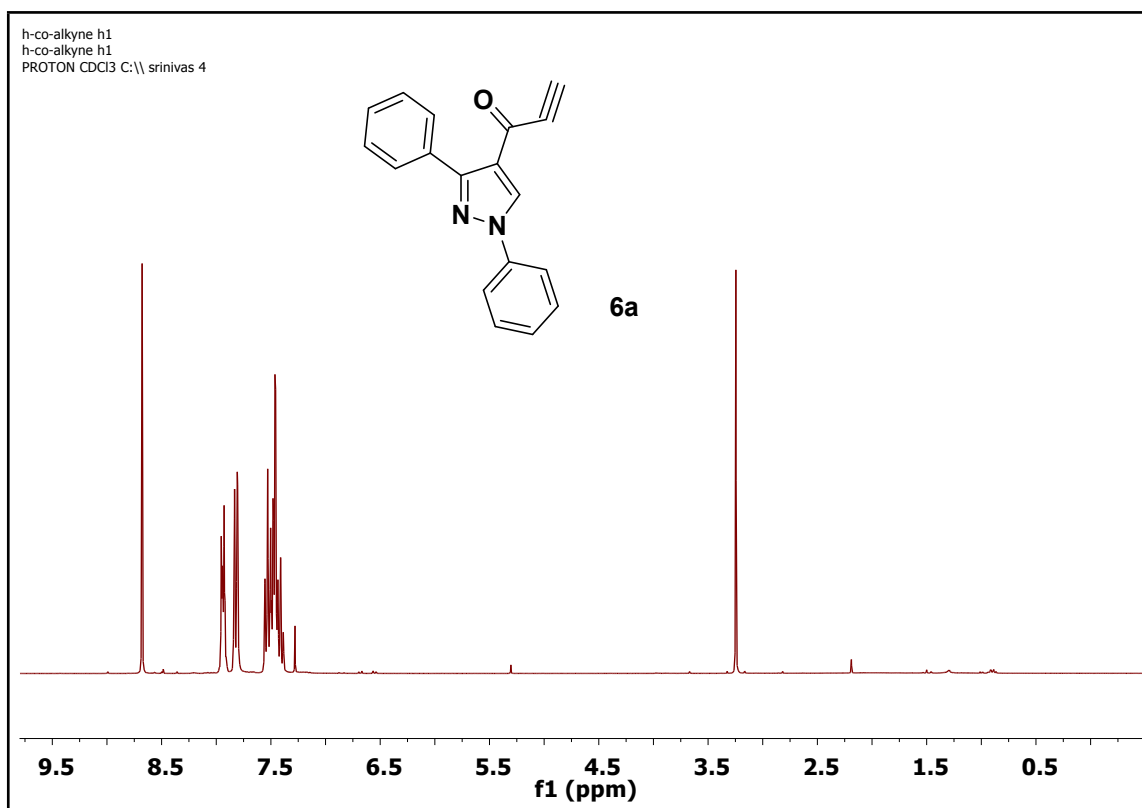


**Figure S2** Effect of compounds **17**, **23** and **29** on cell cell cycle arrest of U87MG cell

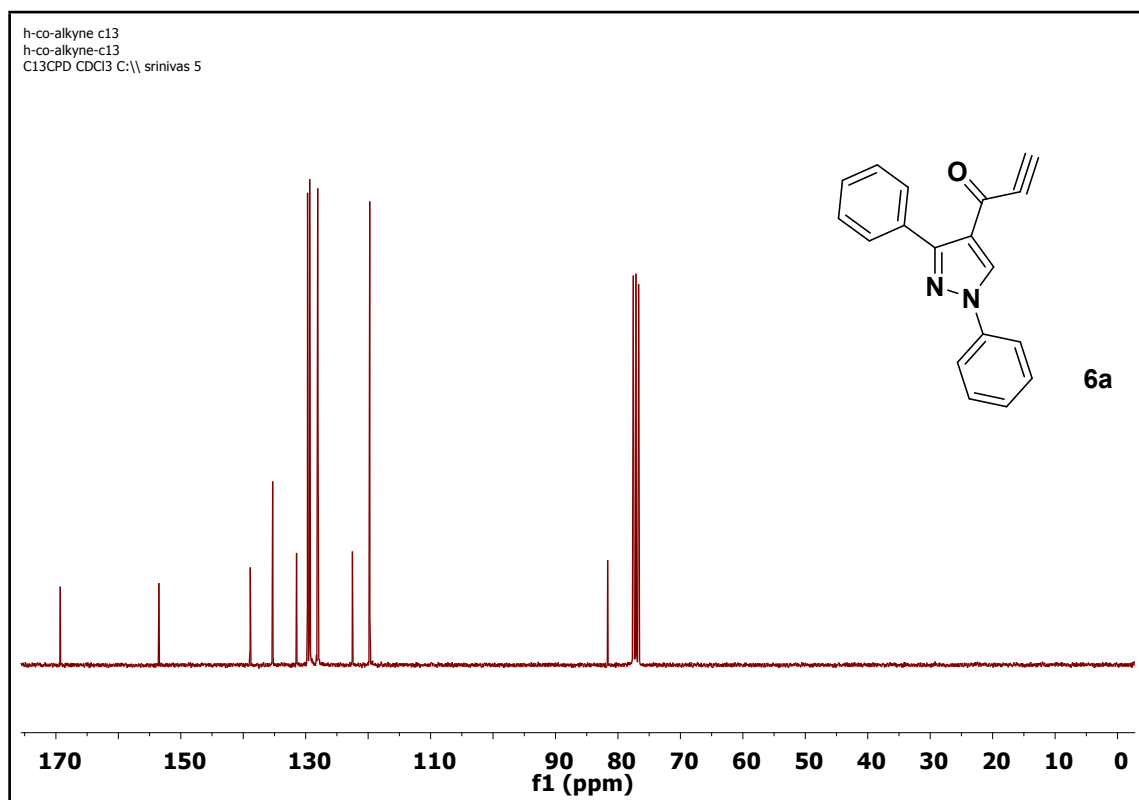


**Figure S3** Effect of compounds **17**, **23**, **29** and 5-Flurouracil on apoptosis of U87MG cells. Apoptotic cells were analyzed by flow-cytometry, after being stained with Annexin V-FITC/PI dual staining. The percentage of cells positive for PI and/or Annexin V-FITC is reported inside the quadrants. Cells in the Lower left quadrant (Q1-LL: AV-/PI-) : Live cells, lower right quadrant (Q1-LR: AV+/PI-) : Early apoptotic cells, upper right quadrant (Q1-UR: AV+/PI+) Late apoptotic, upper left quadrant (Q1-UL: AV-/PI+) : necrotic cells.

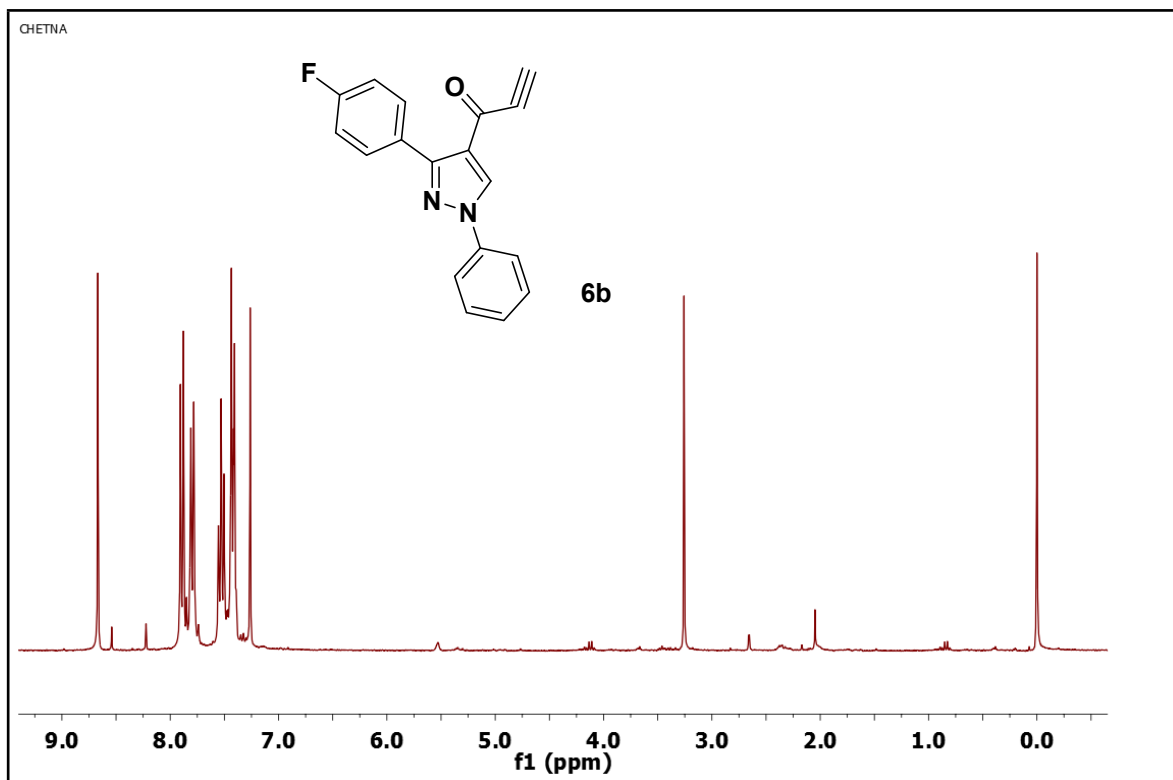
# $^1\text{H}$ , $^{13}\text{C}$ NMR and High Resolution Mass Spectra of New Compounds



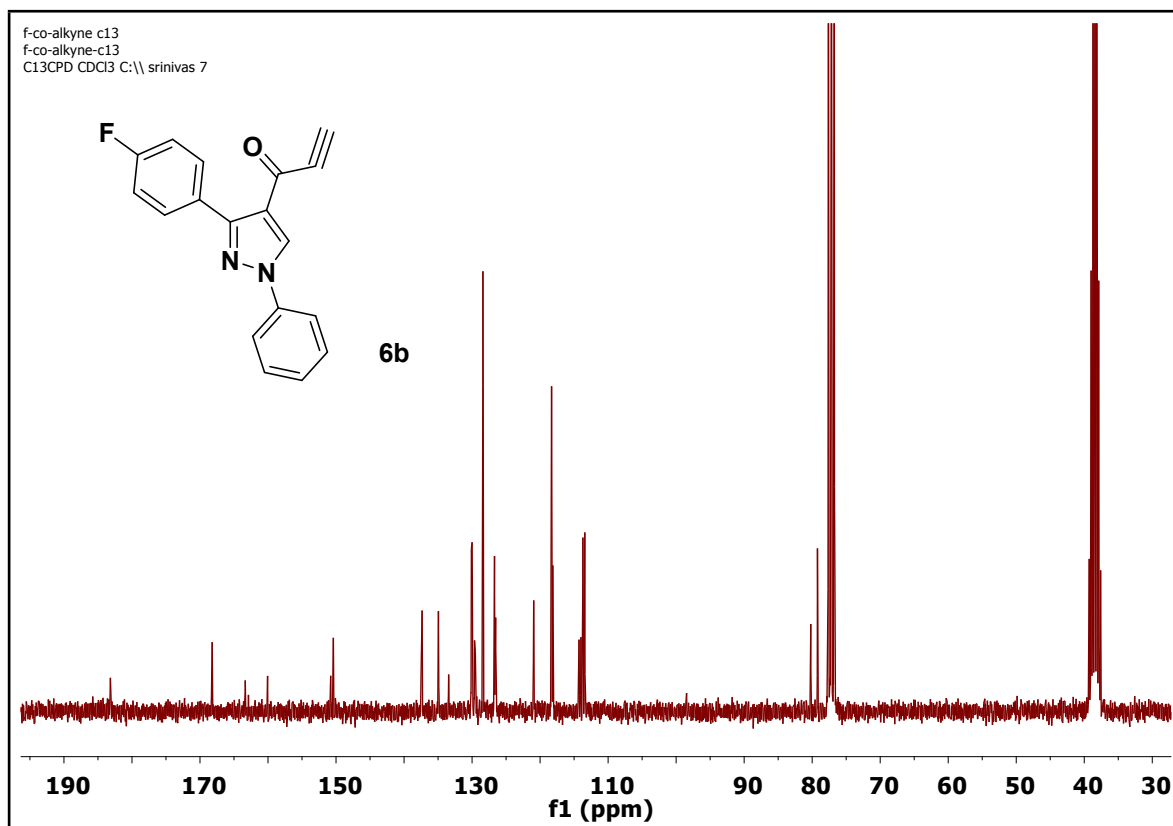
$^1\text{H}$  NMR spectra of compound 6a



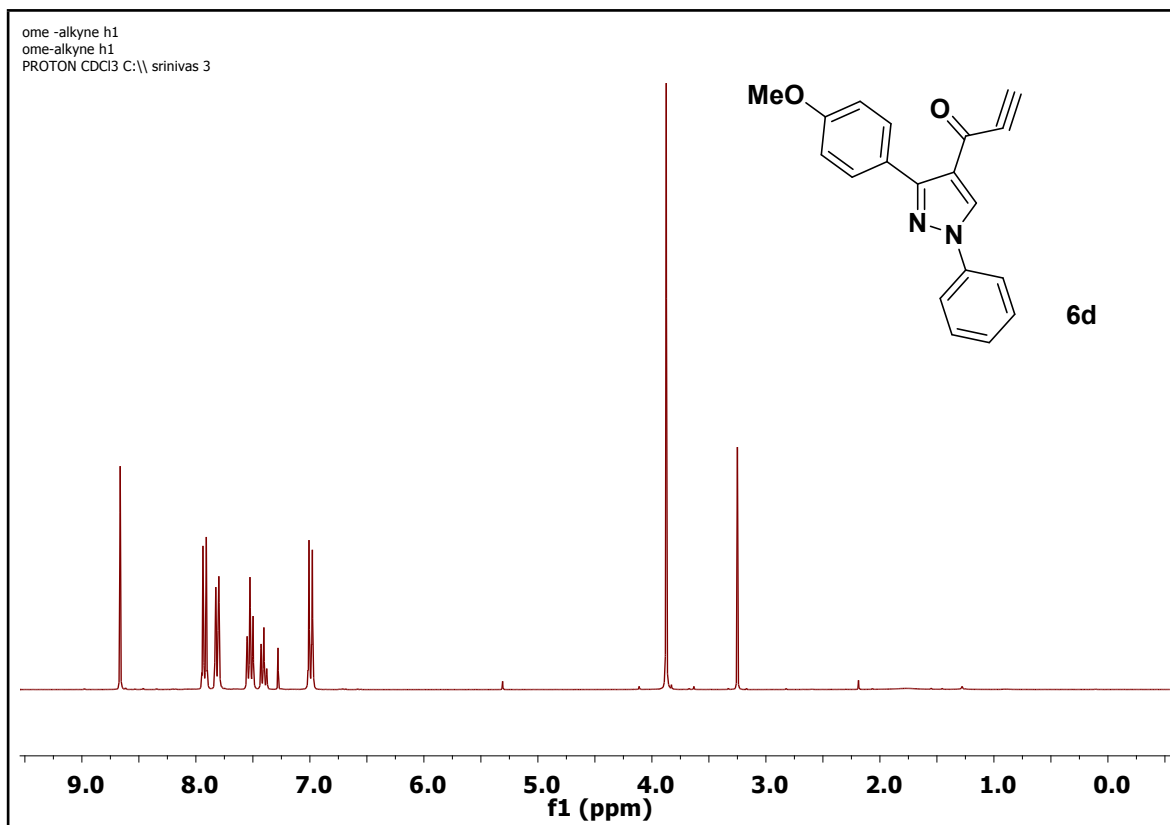
$^{13}\text{C}$  NMR spectra of compound 6a



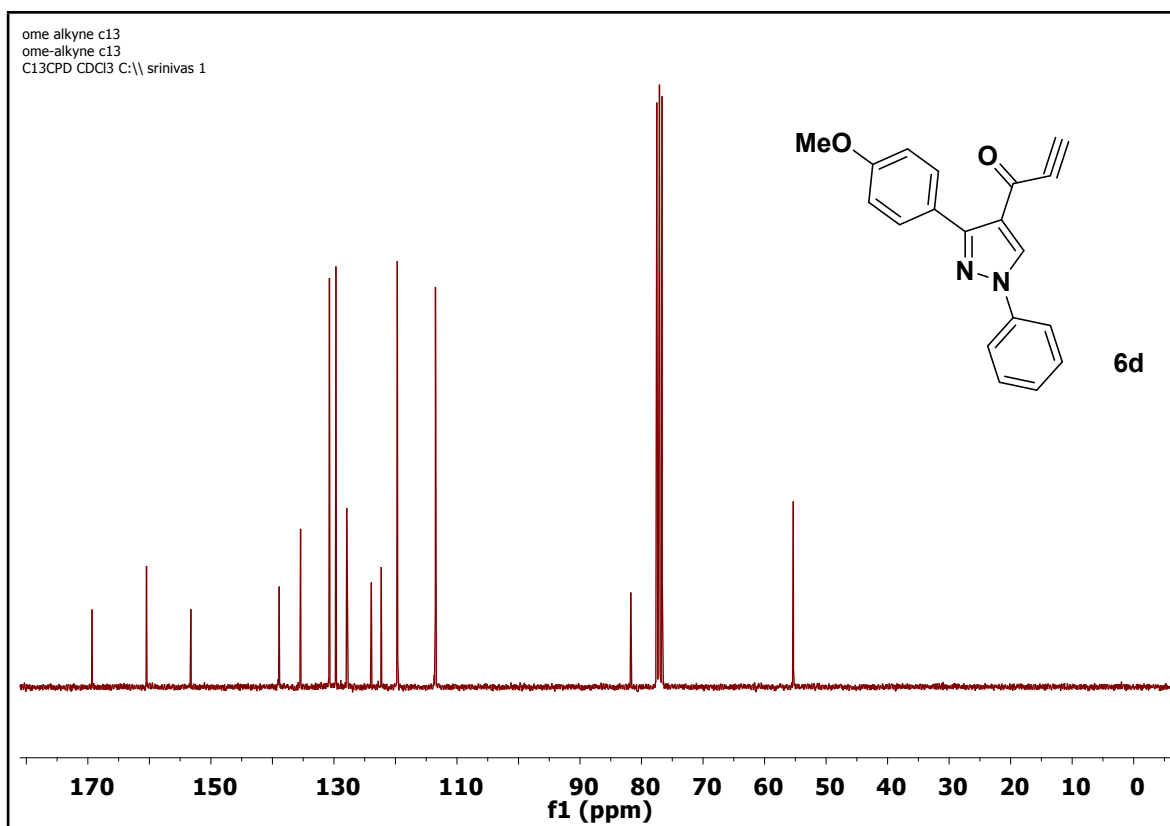
<sup>1</sup>H NMR spectra of compound **6b**



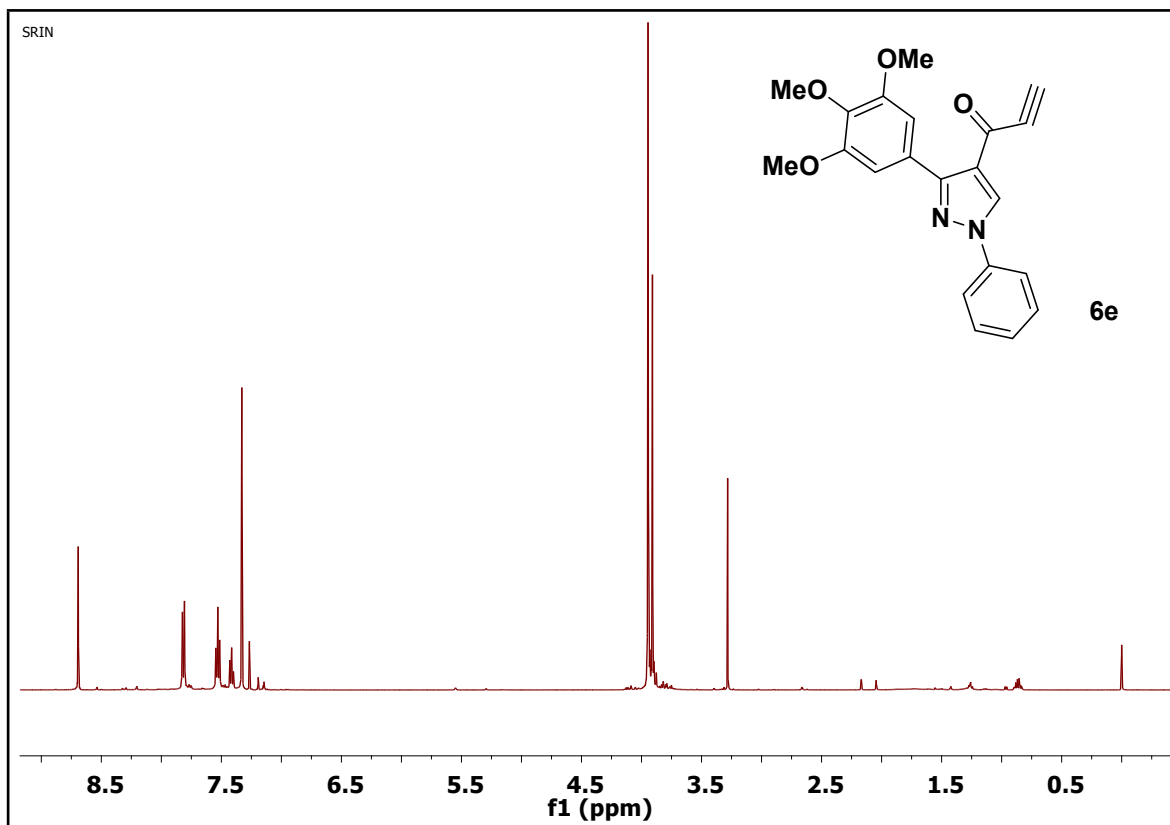
<sup>13</sup>C NMR spectra of compound **6b**



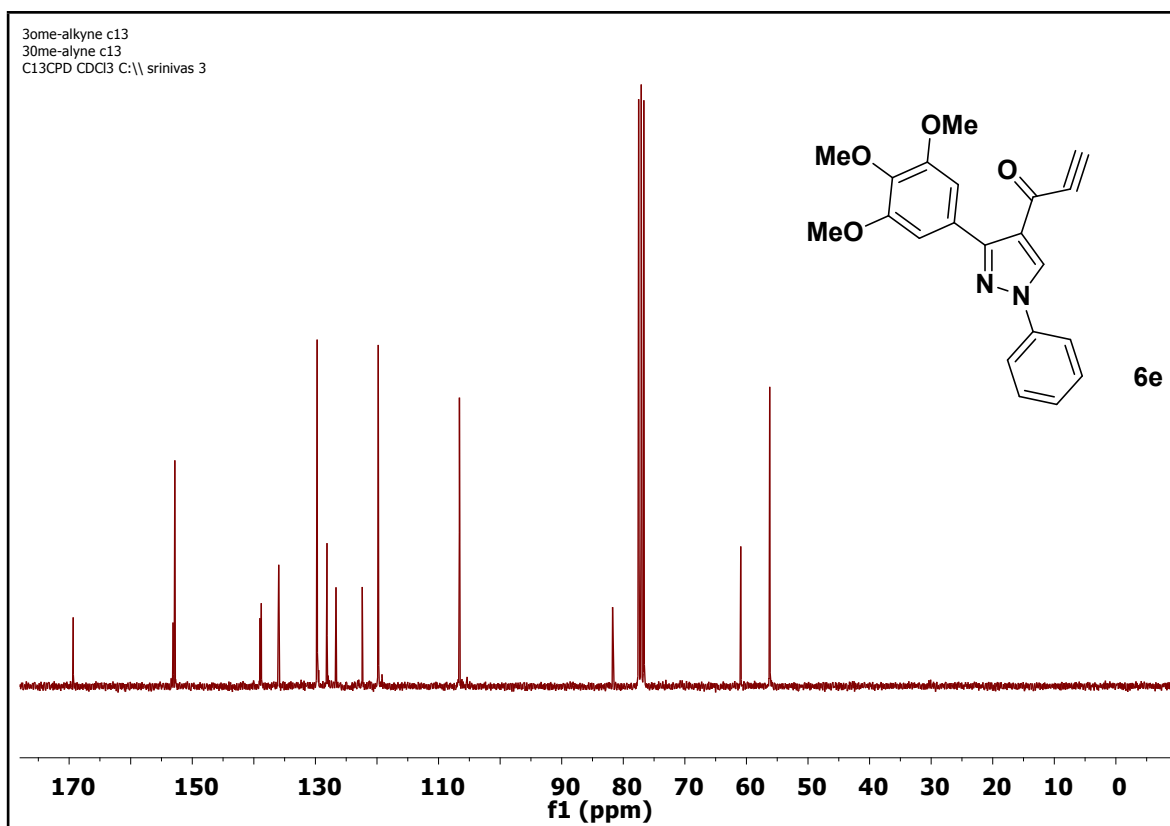
<sup>1</sup>H NMR spectra of compound 6d



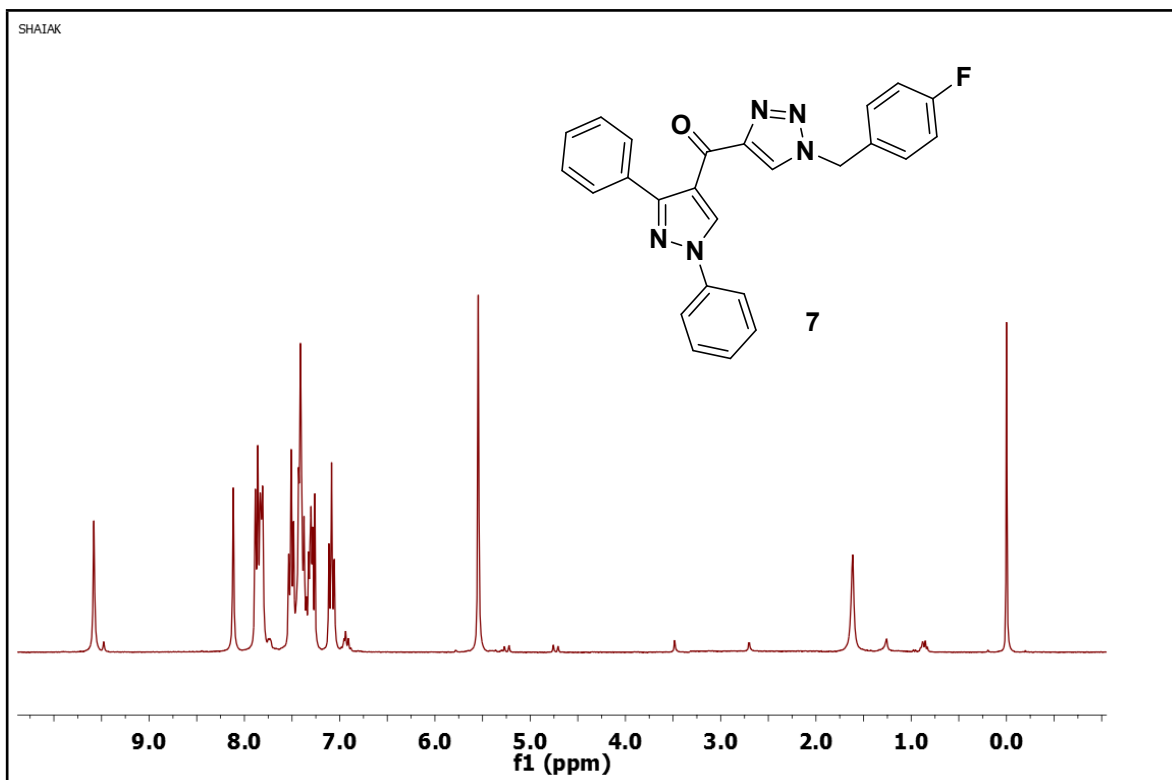
<sup>13</sup>C NMR spectra of compound 6d



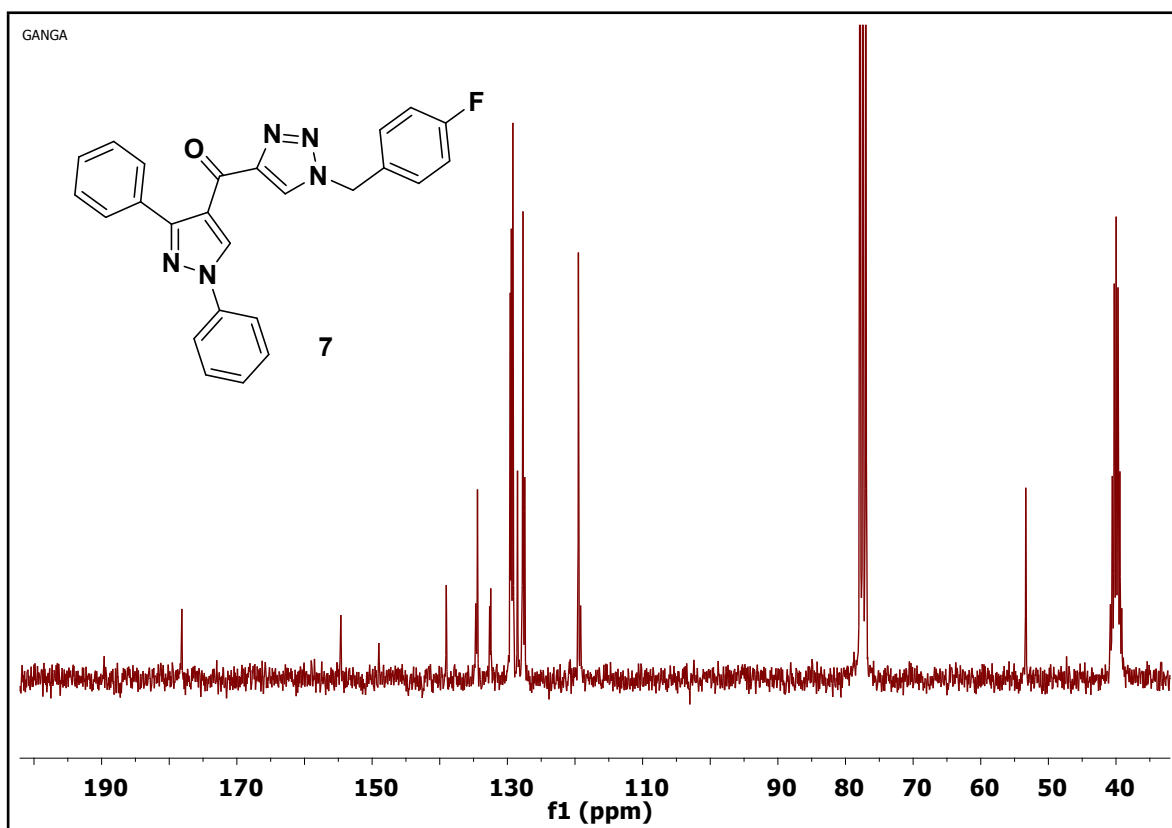
$^1\text{H}$  NMR spectra of compound 6e



$^{13}\text{C}$  NMR spectra of compound 6e

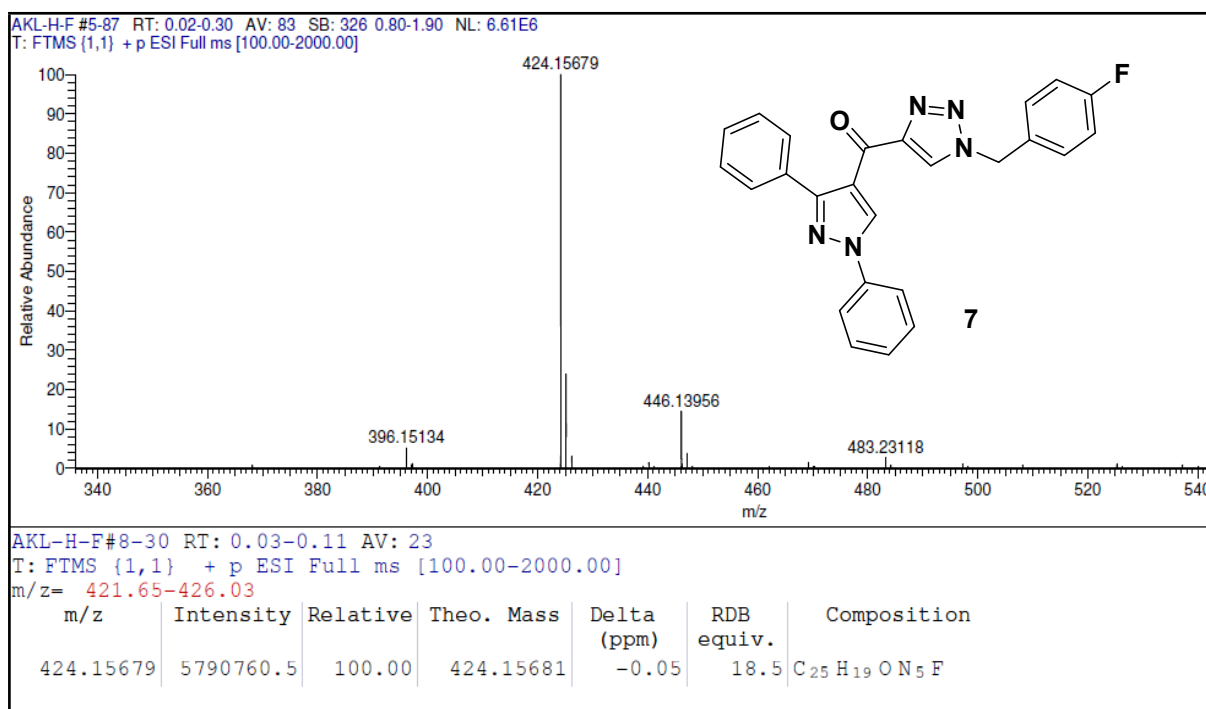


$^1\text{H}$  NMR spectra of compound 7

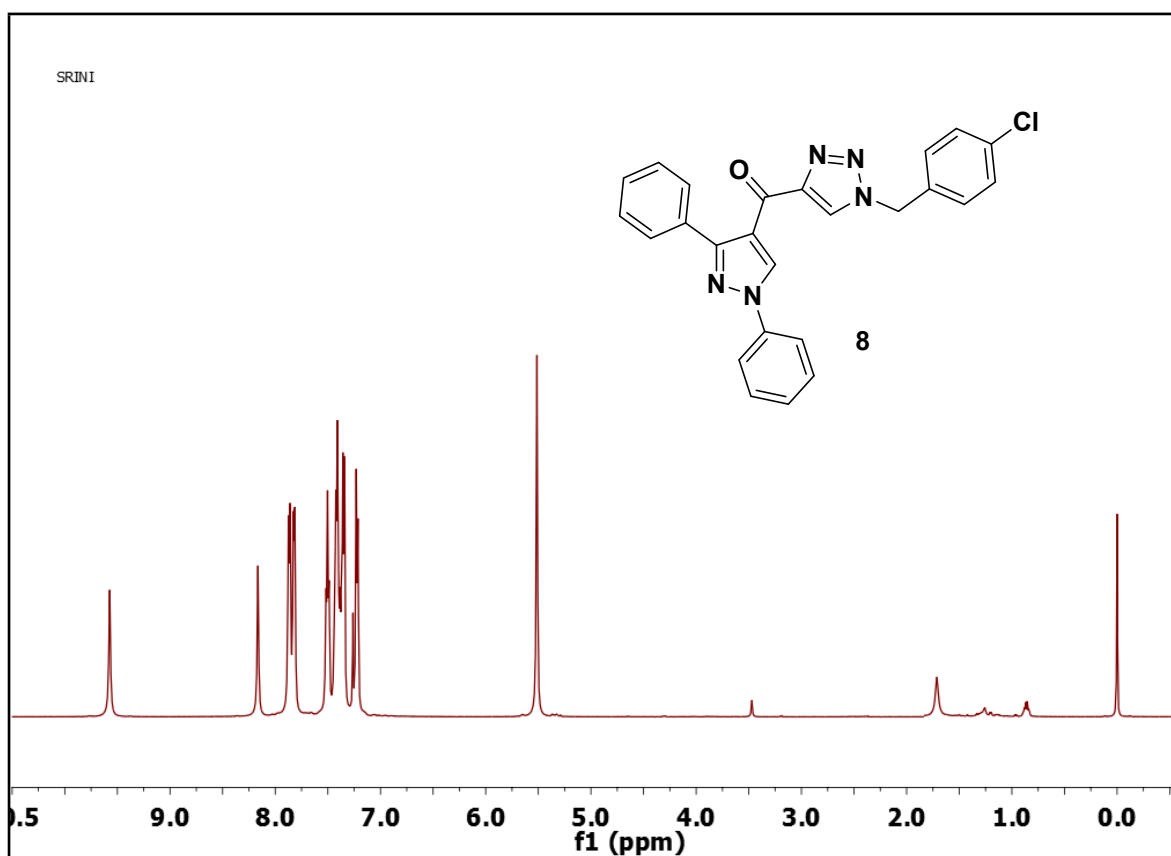


$^{13}\text{C}$  NMR spectra of compound 7

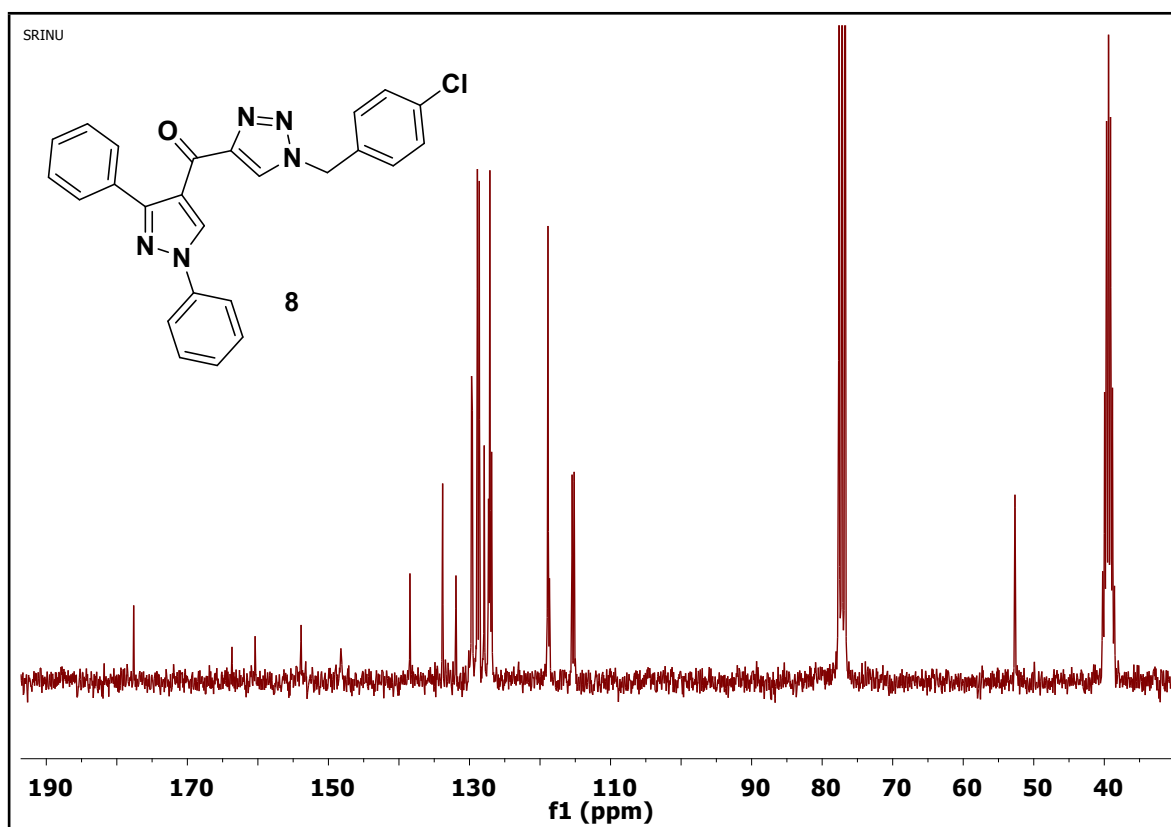




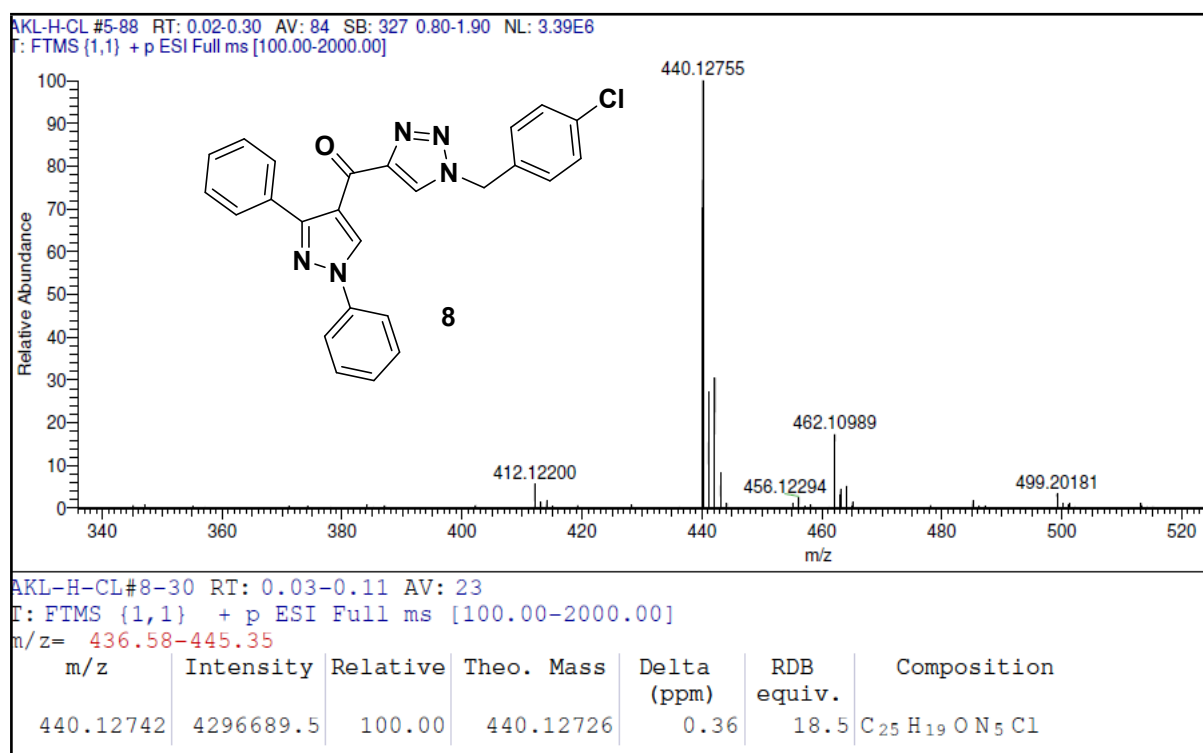
HRMS Spectra of compound 7



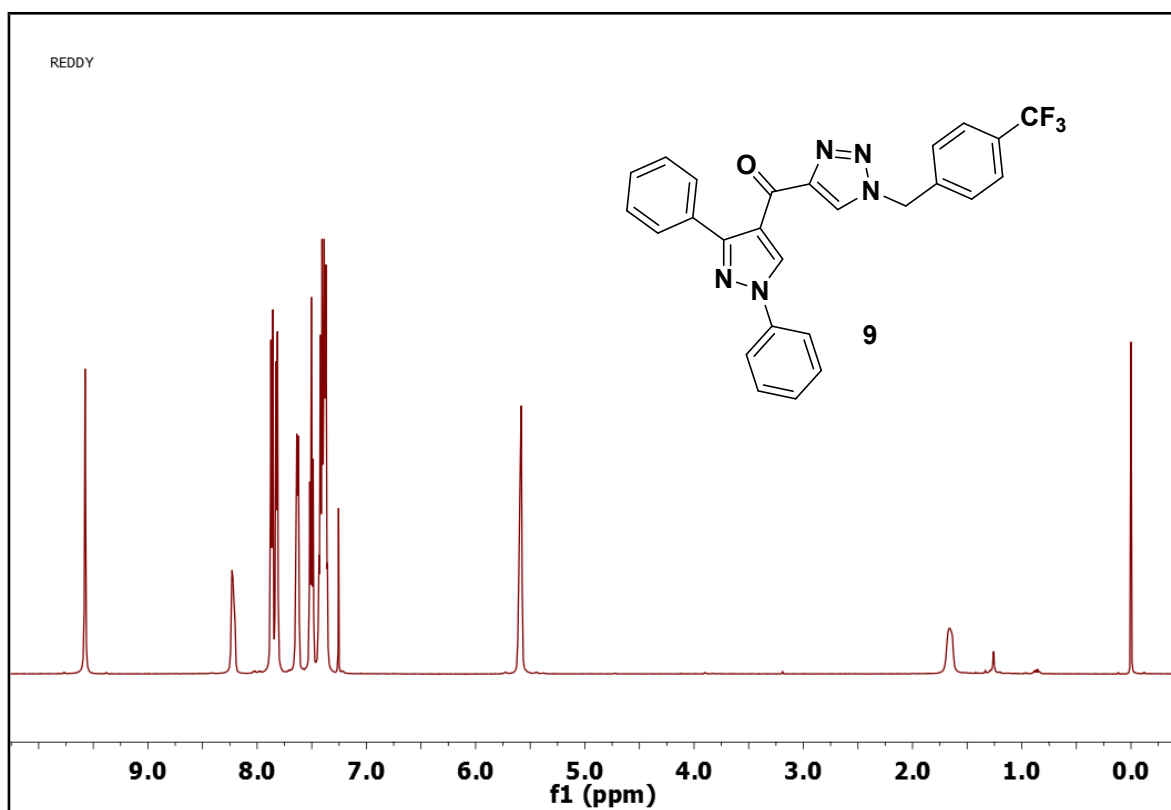
<sup>1</sup>H NMR spectra of compound 8



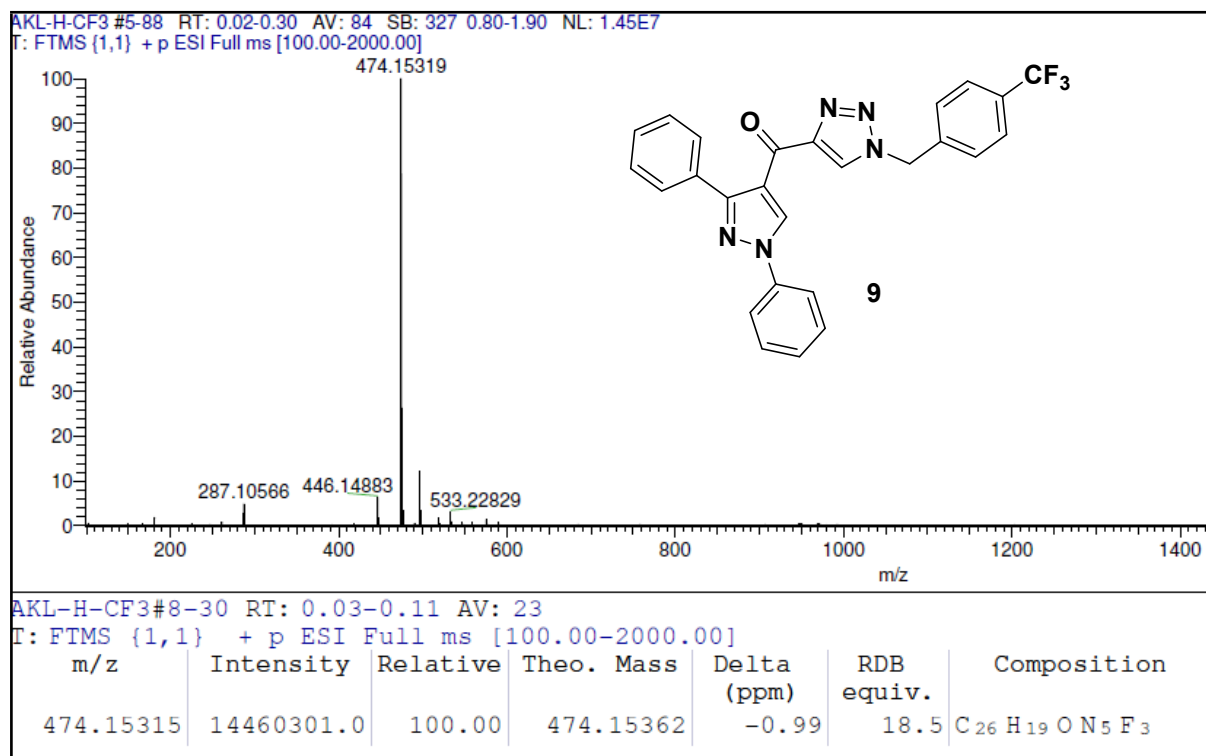
<sup>13</sup>C NMR spectra of compound 8



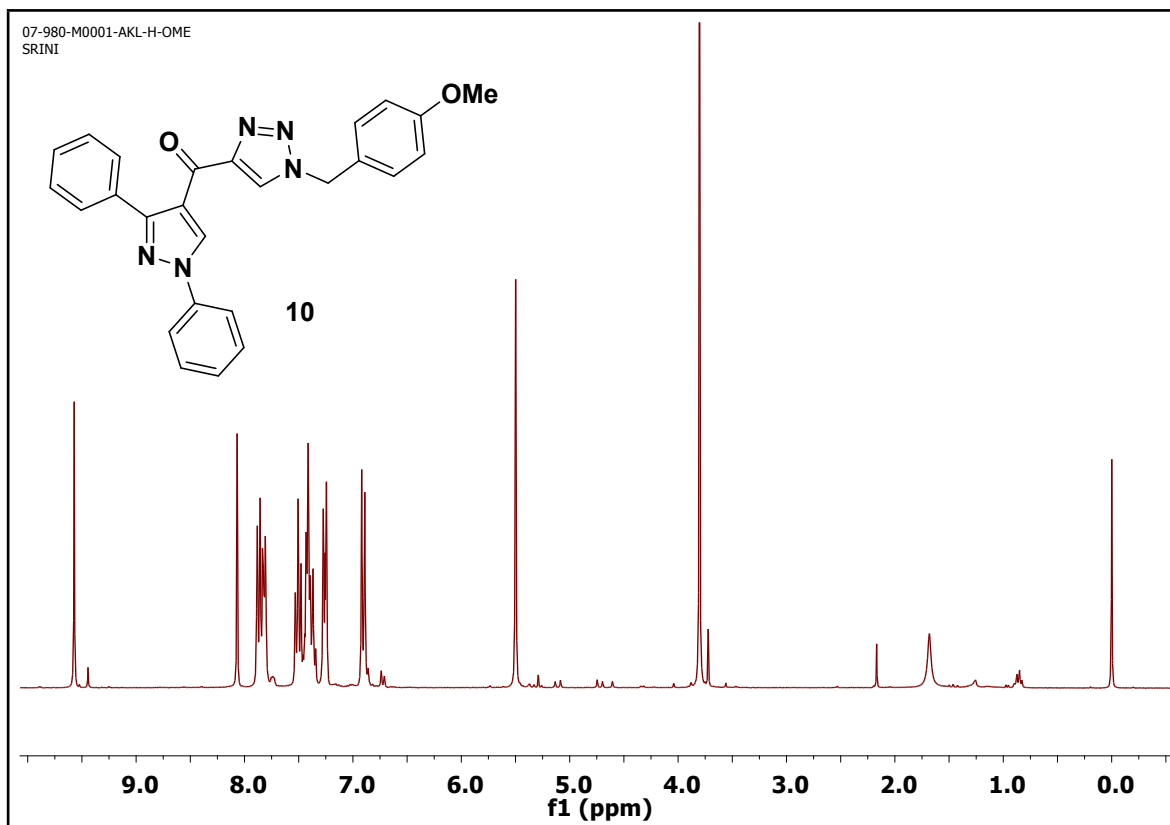
HRMS Spectra of compound 8



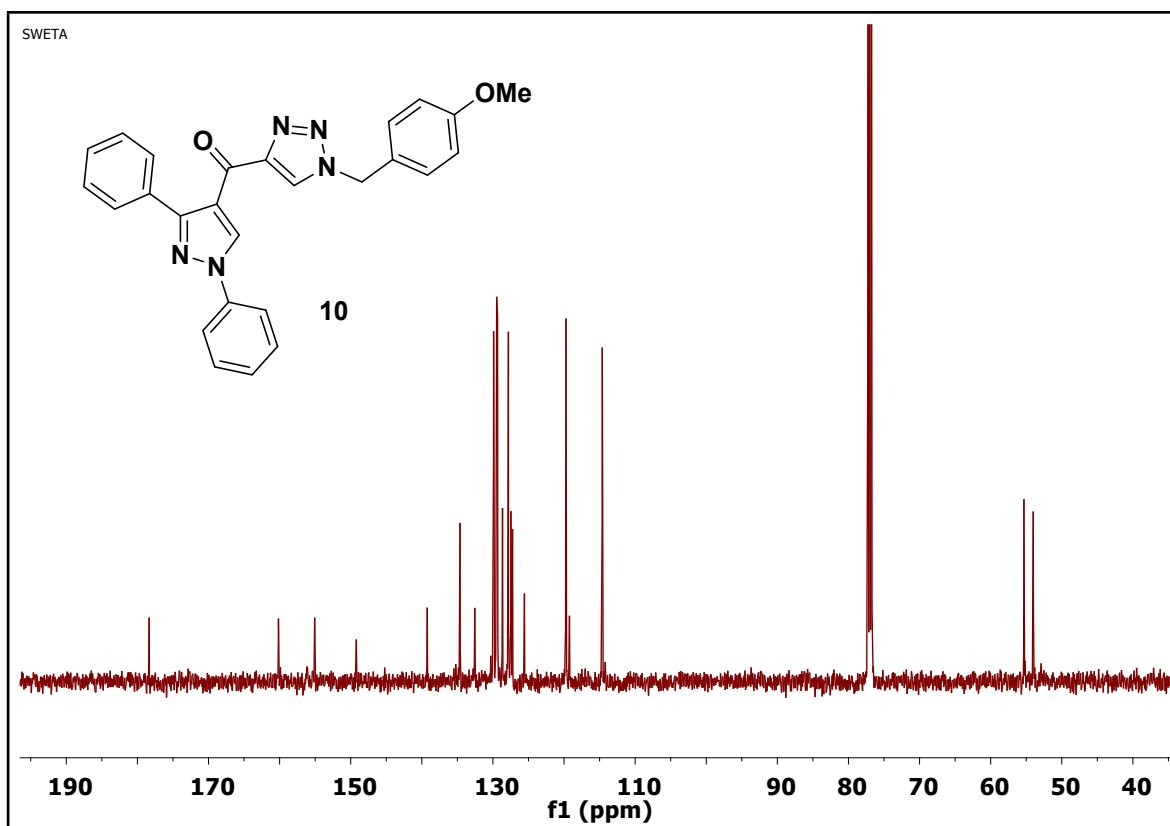
<sup>1</sup>H NMR spectra of compound 9



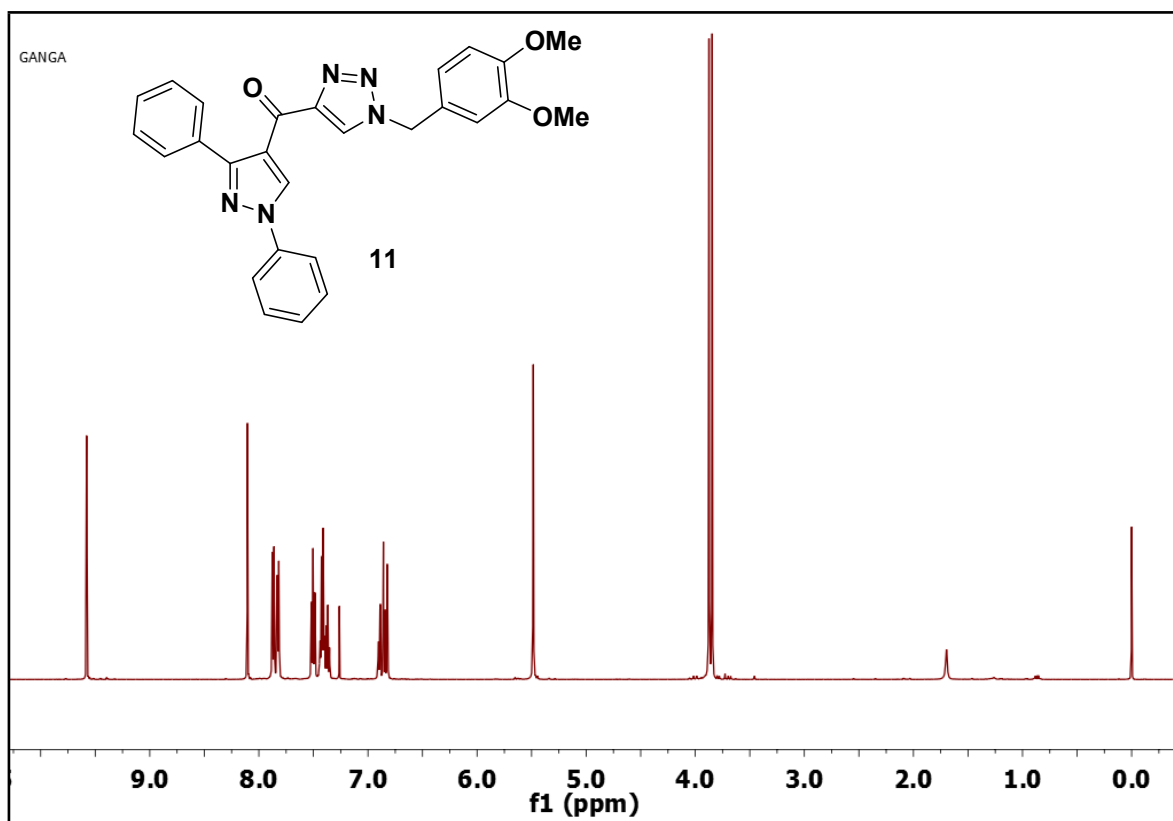
HRMS Spectra of compound 9



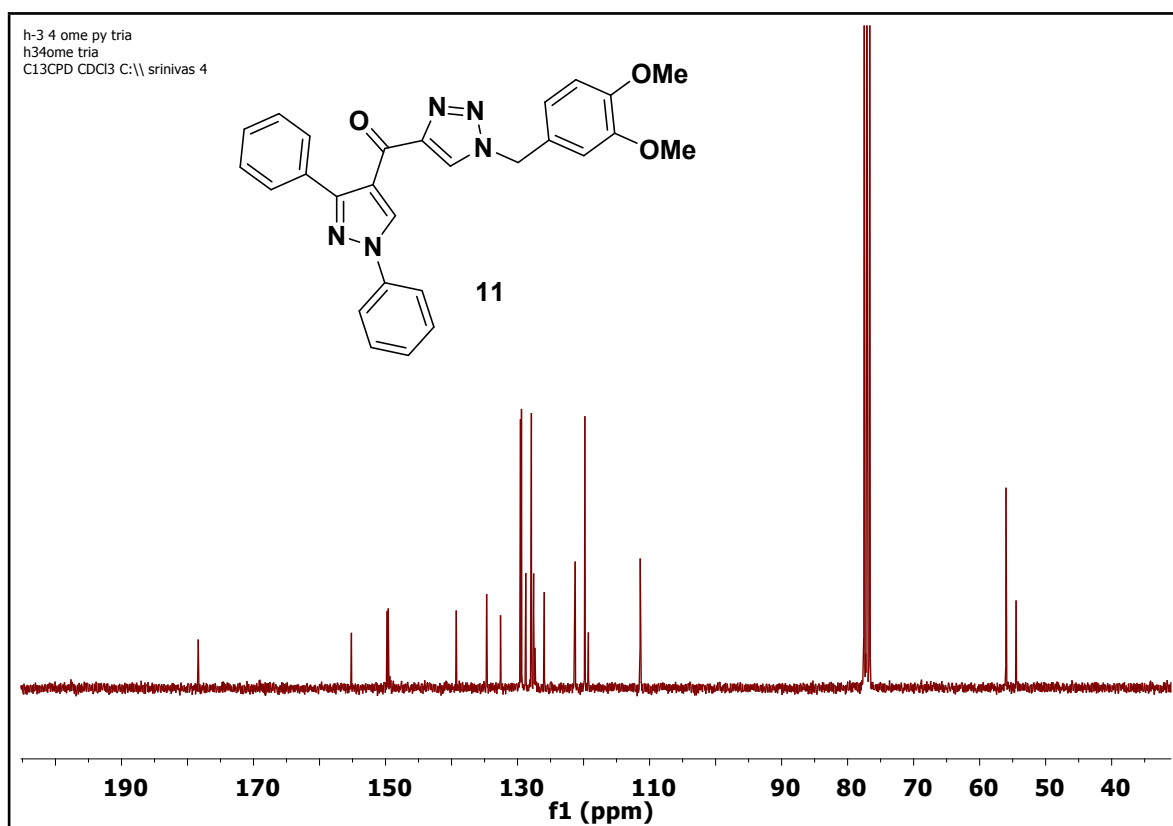
$^1\text{H}$  NMR spectra of compound **10**



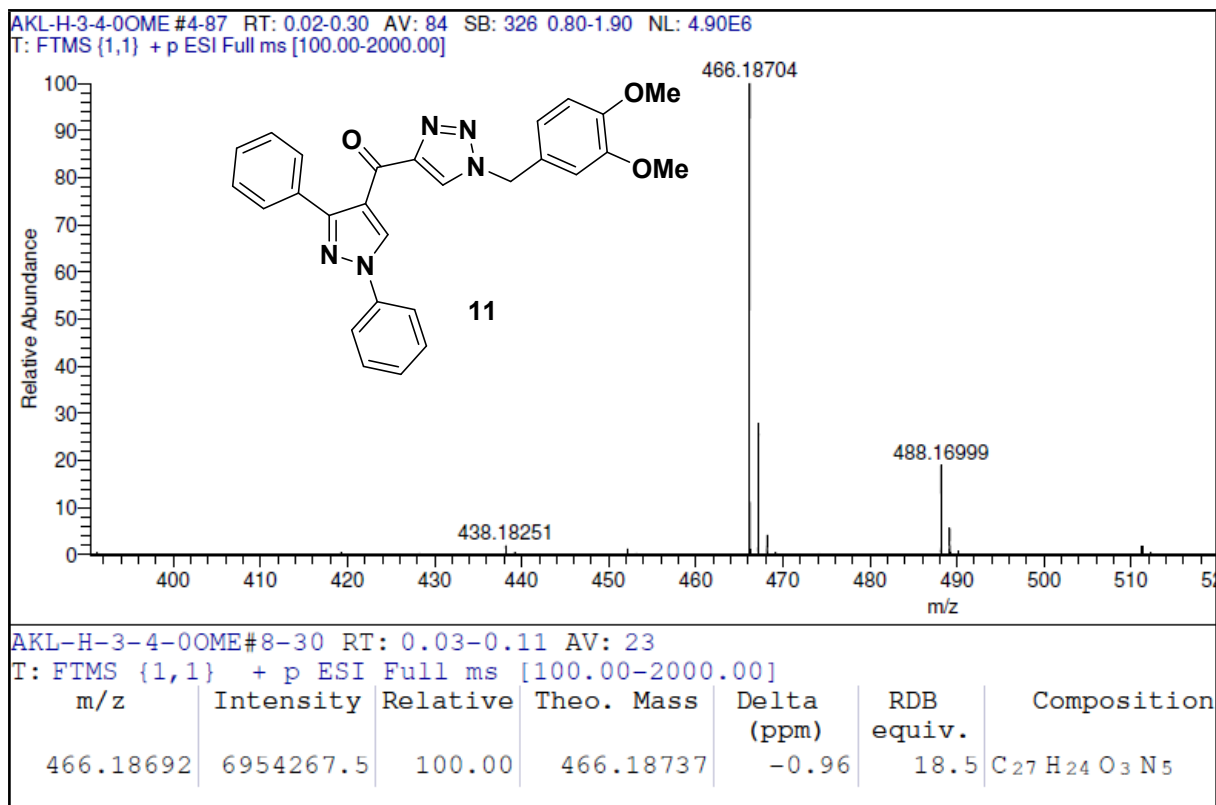
$^{13}\text{C}$  NMR spectra of compound **10**



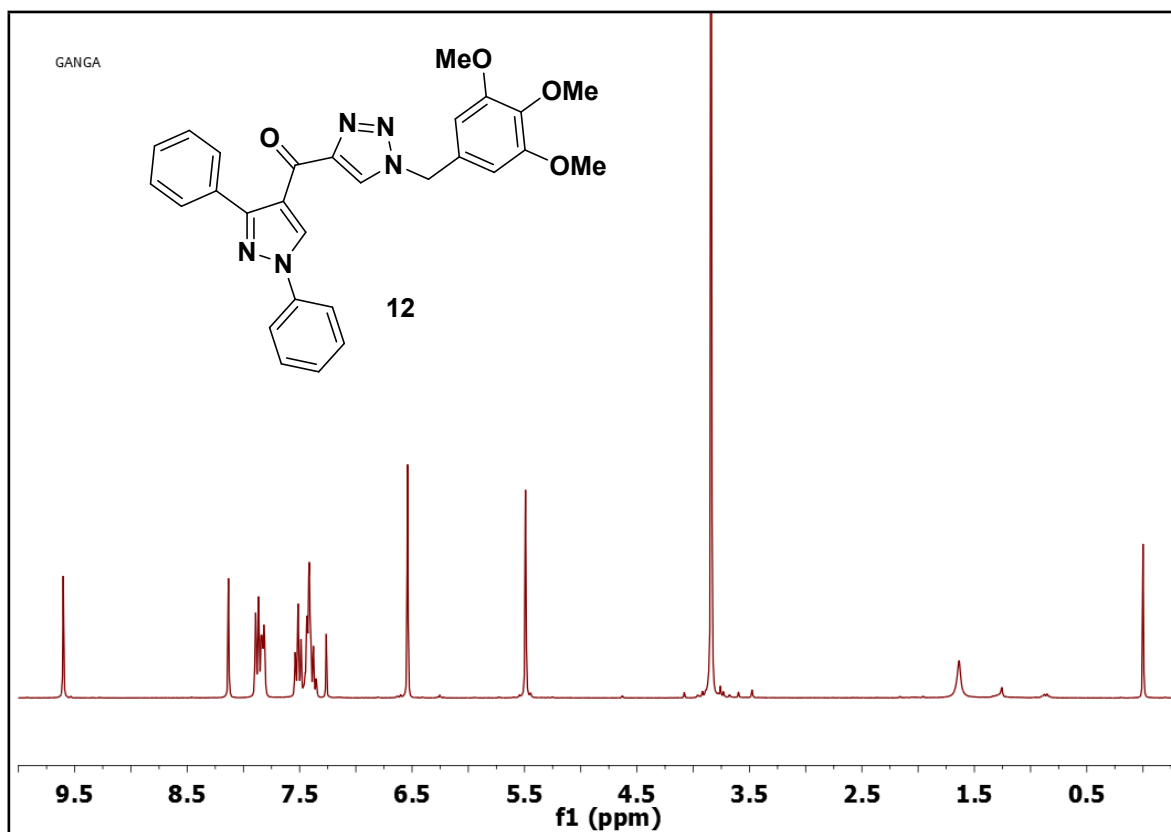
$^1\text{H}$  NMR spectra of compound 11



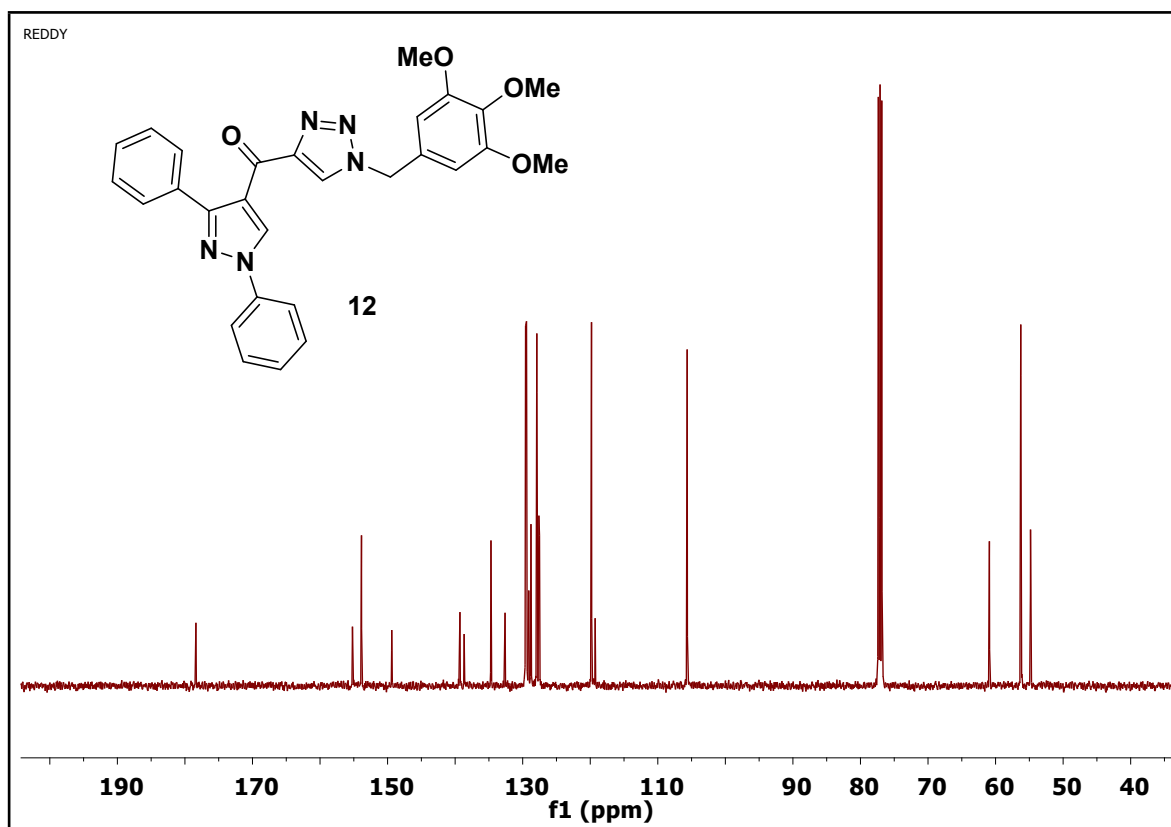
$^{13}\text{C}$  NMR spectra of compound 11



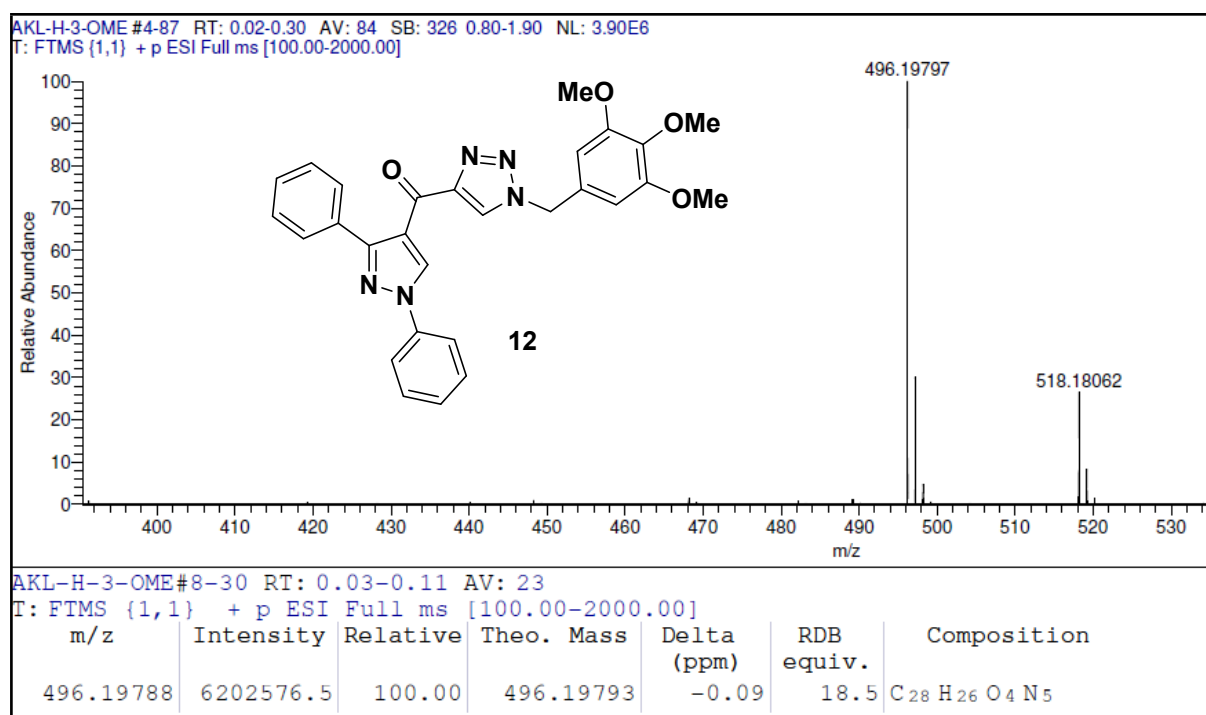
HRMS Spectra of compound **11**



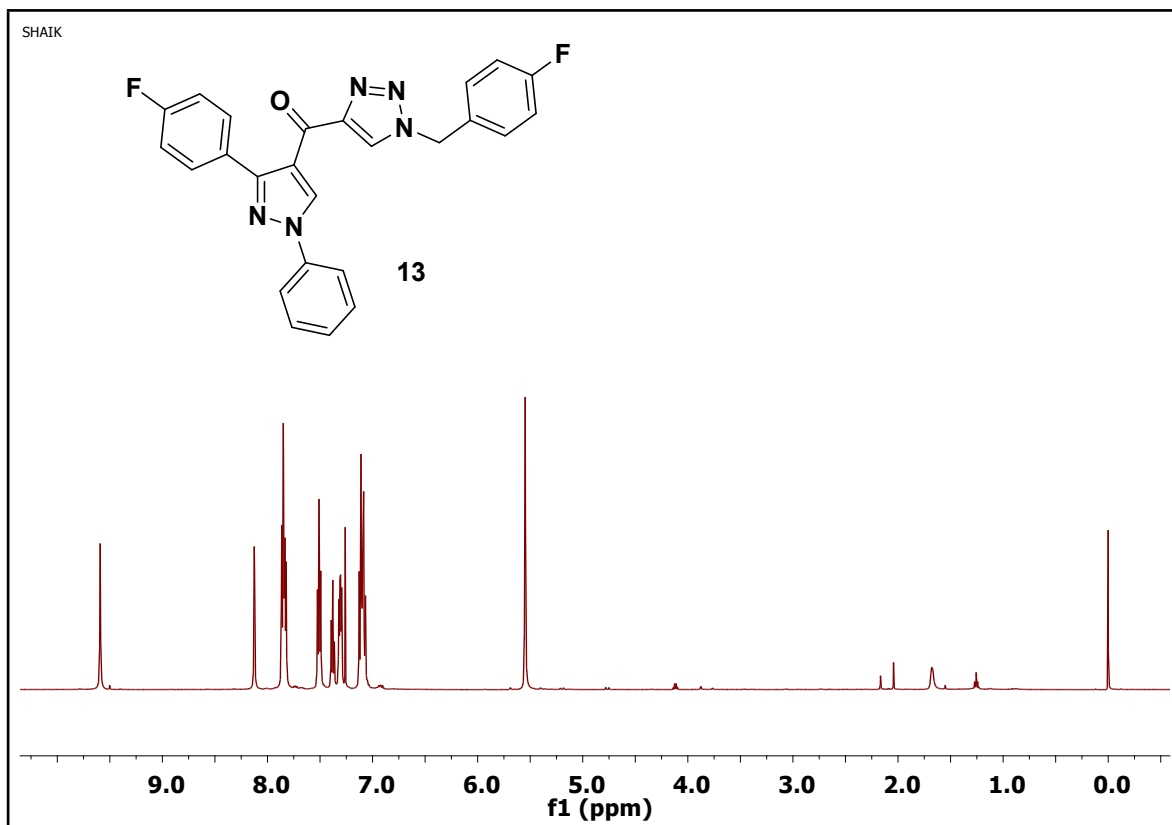
<sup>1</sup>H NMR spectra of compound **12**



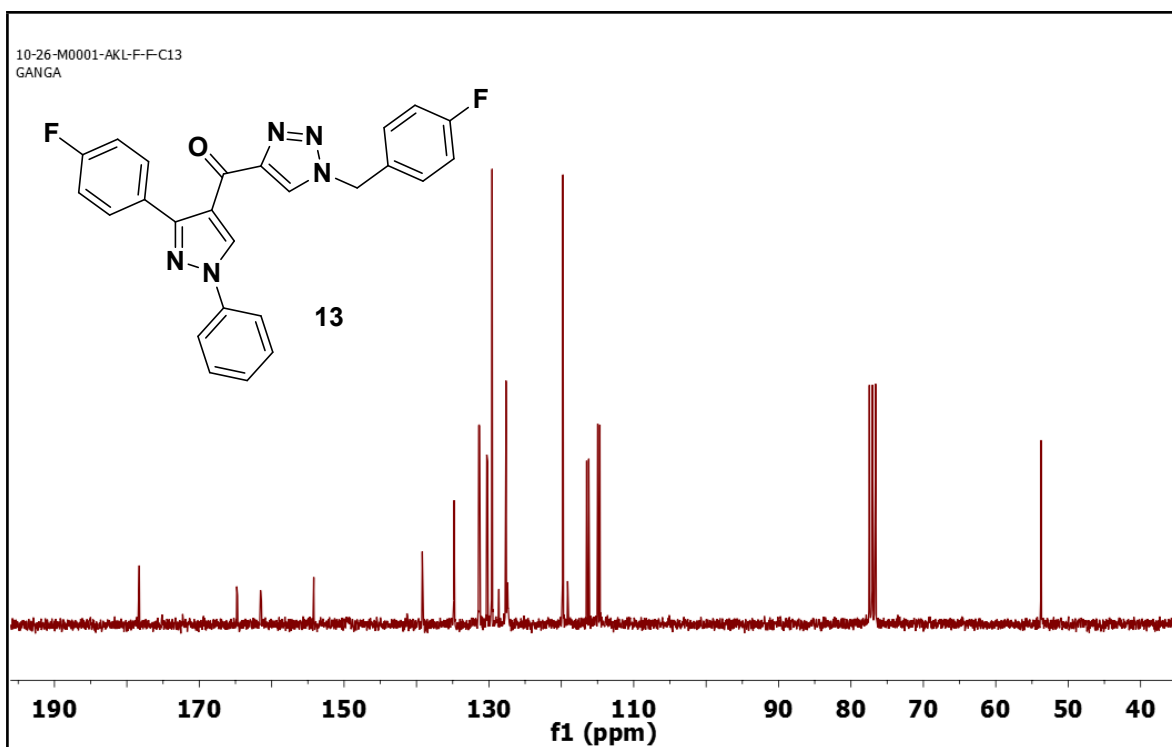
$^{13}\text{C}$  NMR spectra of compound 12



HRMS Spectra of compound 12

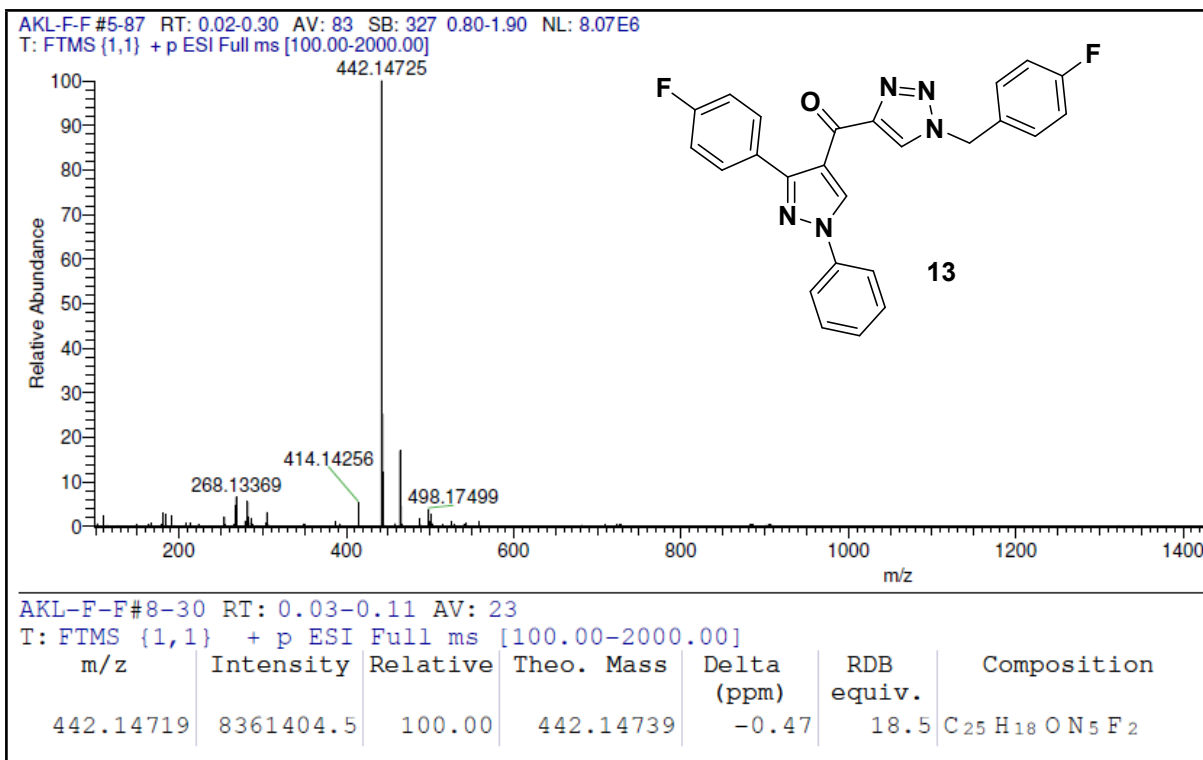


$^1\text{H}$  NMR spectra of compound 13

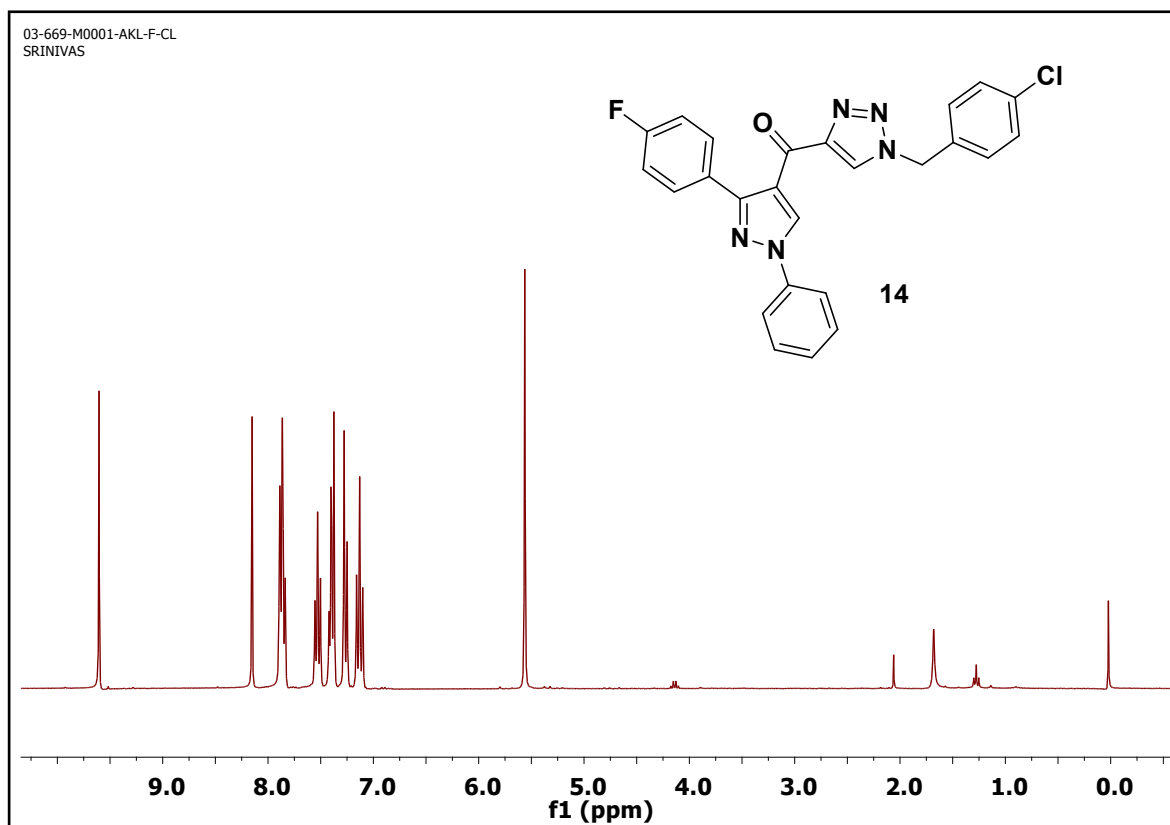


$^{13}\text{C}$  NMR spectra of compound 13

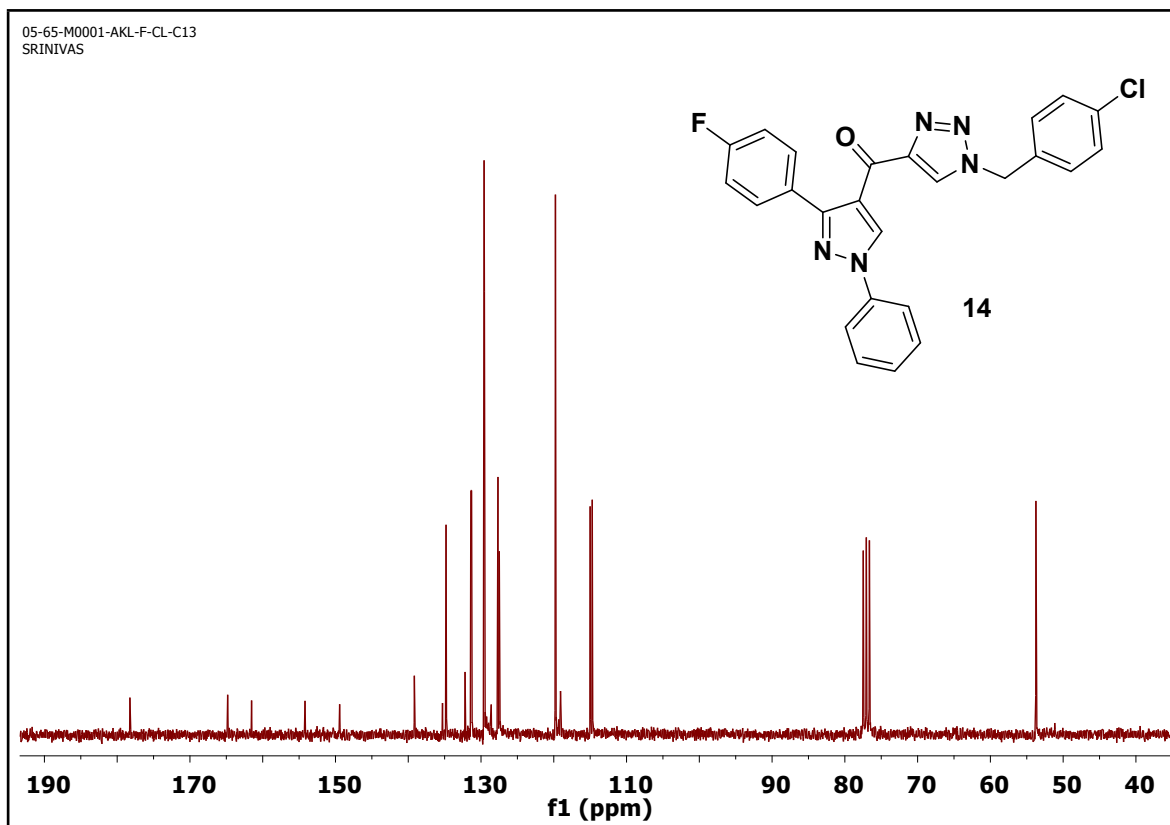




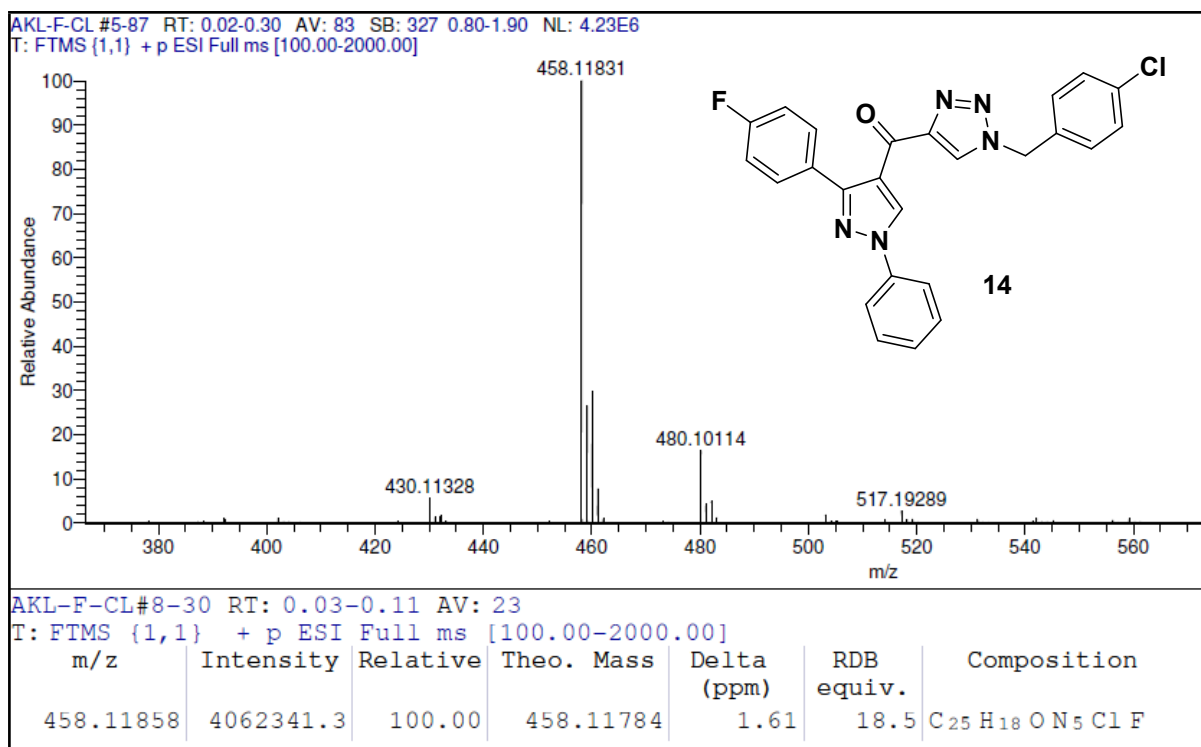
HRMS Spectra of compound 13



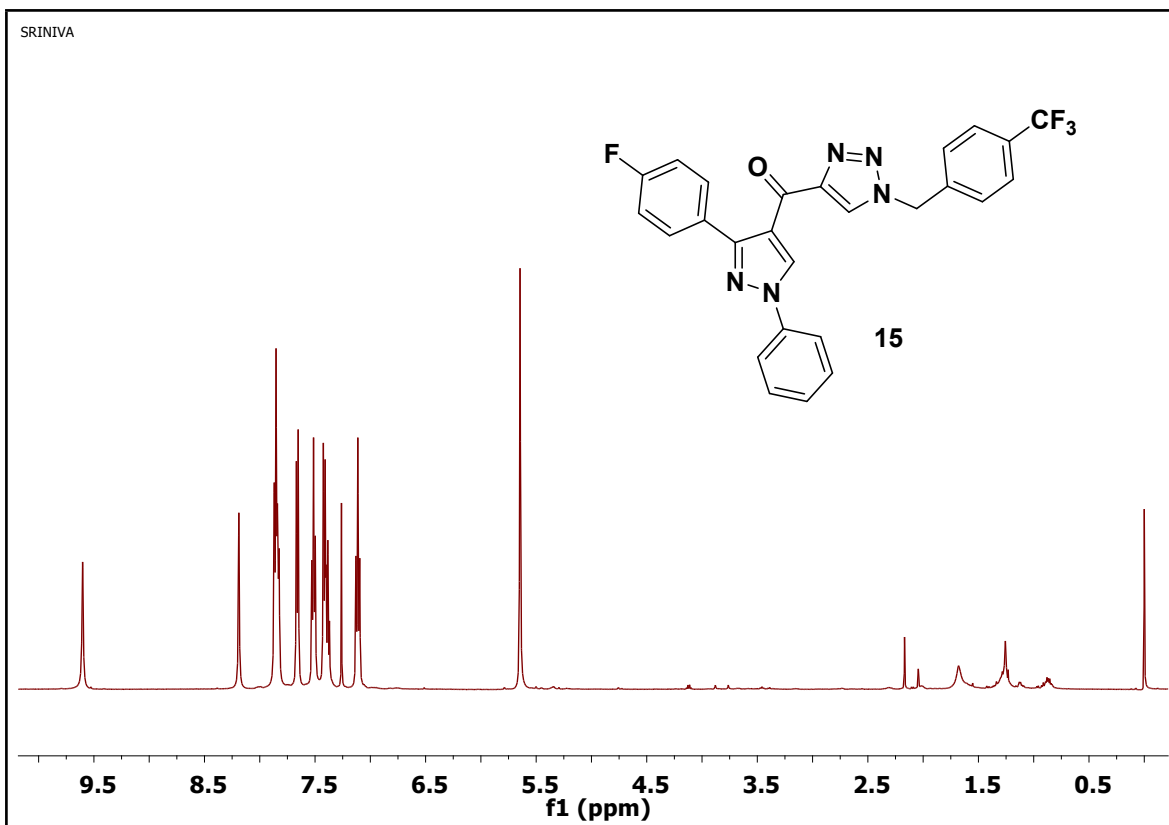
<sup>1</sup>H NMR spectra of compound 14



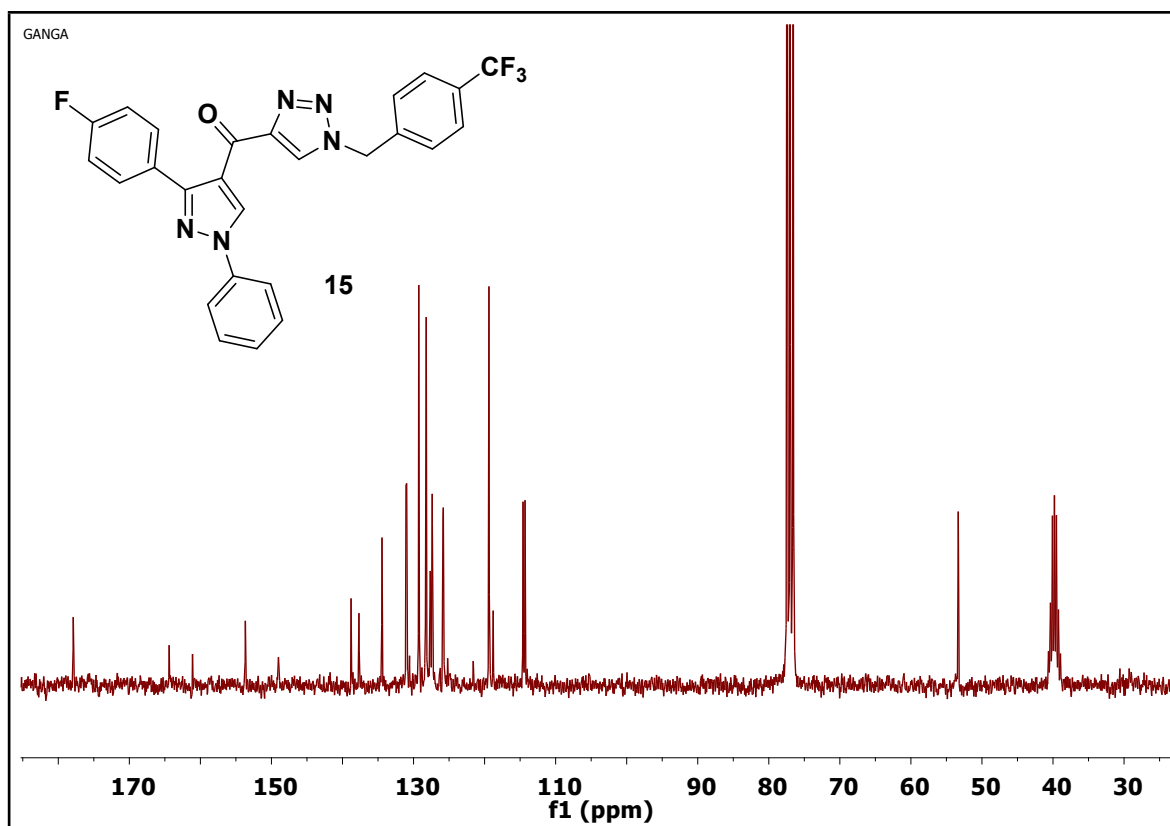
<sup>13</sup>C NMR spectra of compound 14



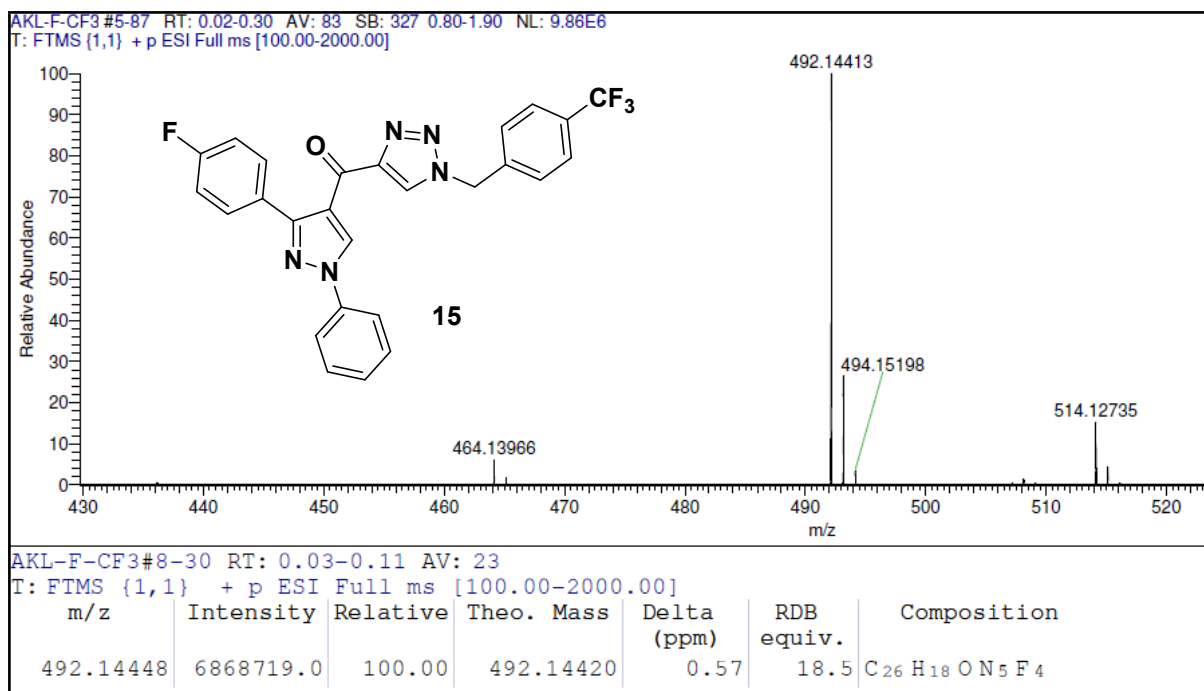
HRMS Spectra of compound 14



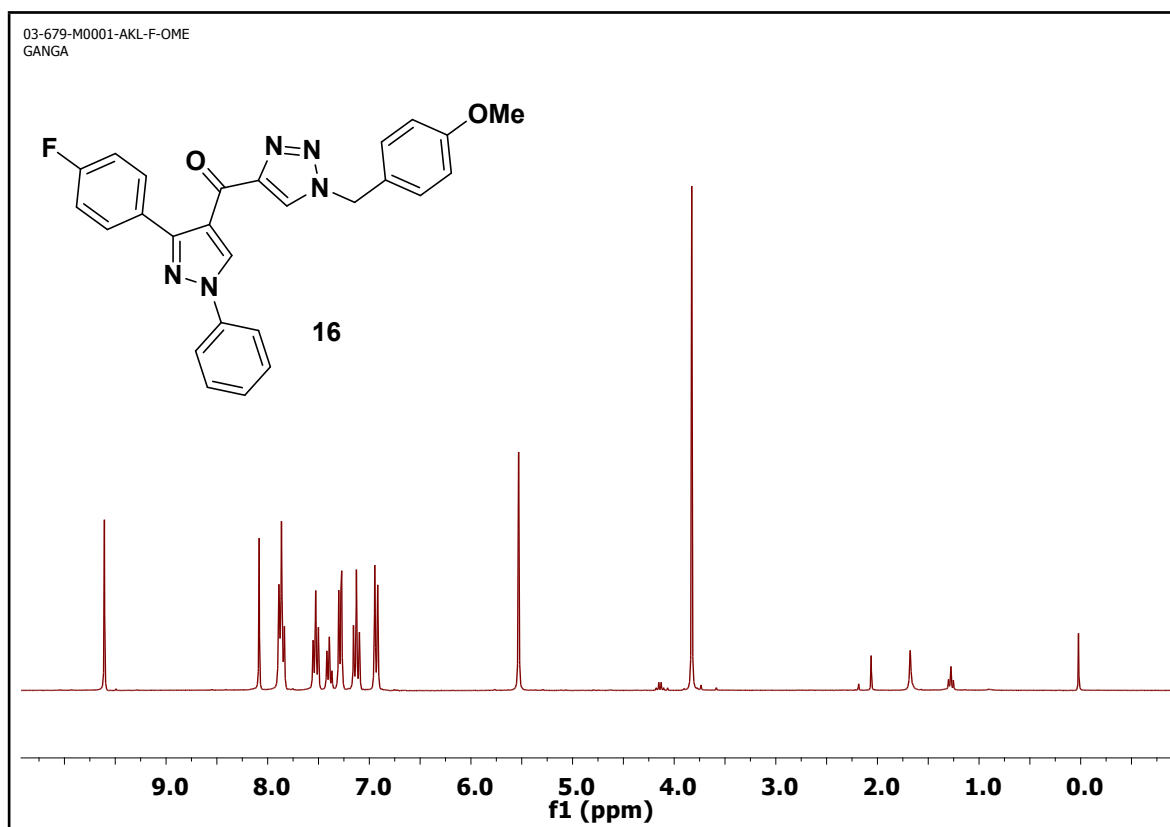
$^1\text{H}$  NMR spectra of compound 15



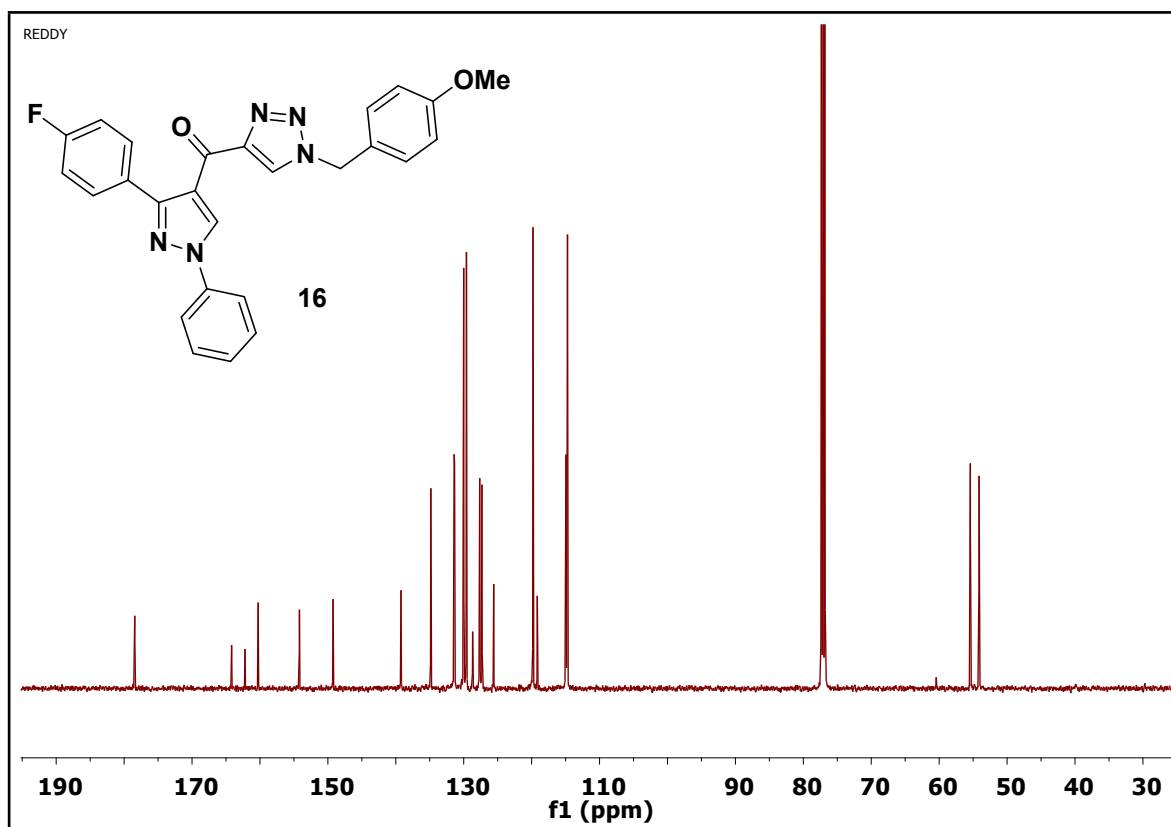
$^{13}\text{C}$  NMR spectra of compound 15



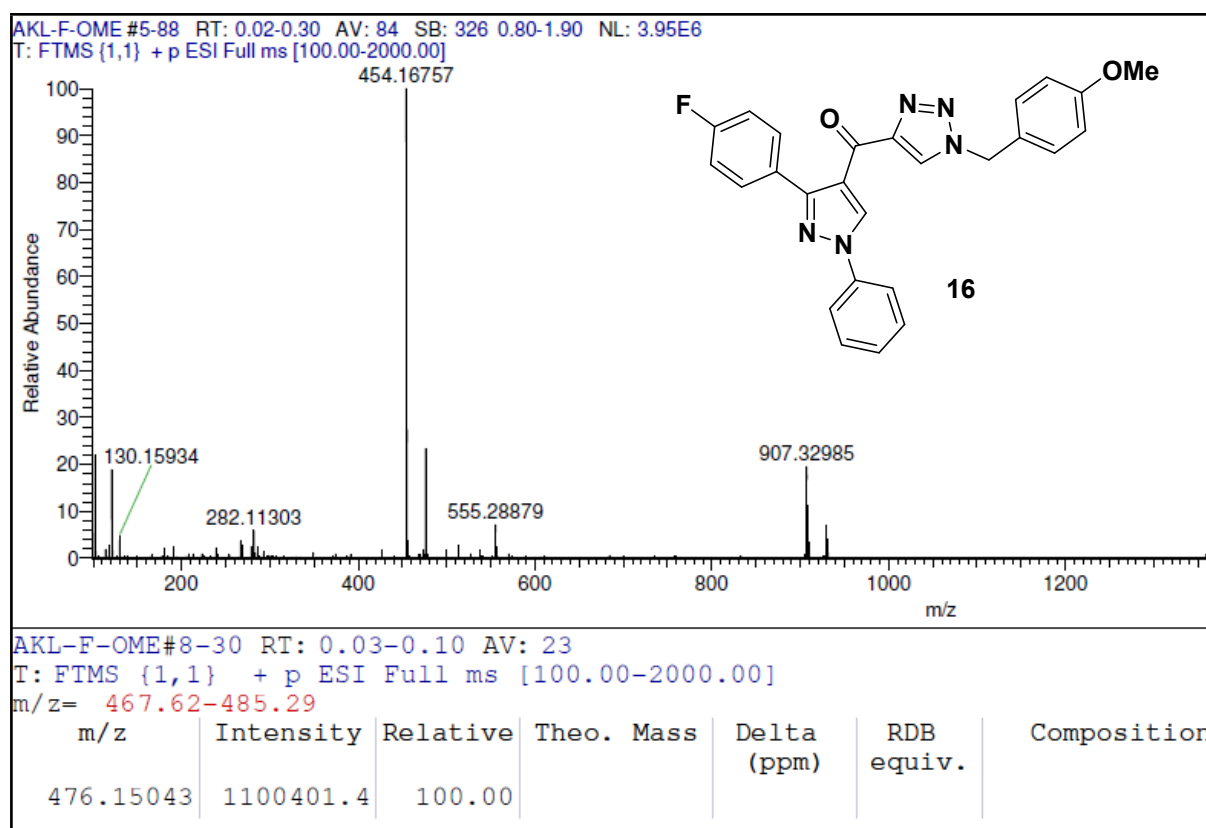
HRMS Spectra of compound 15



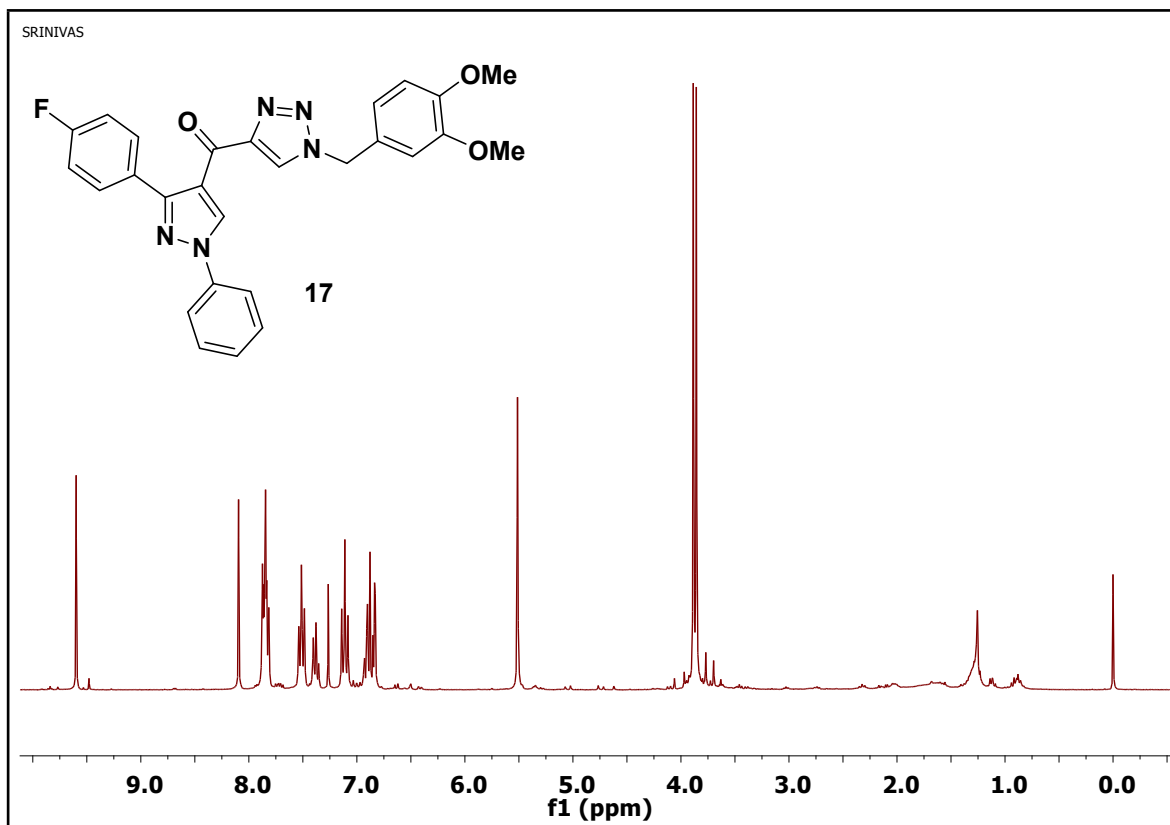
<sup>1</sup>H NMR spectra of compound 16



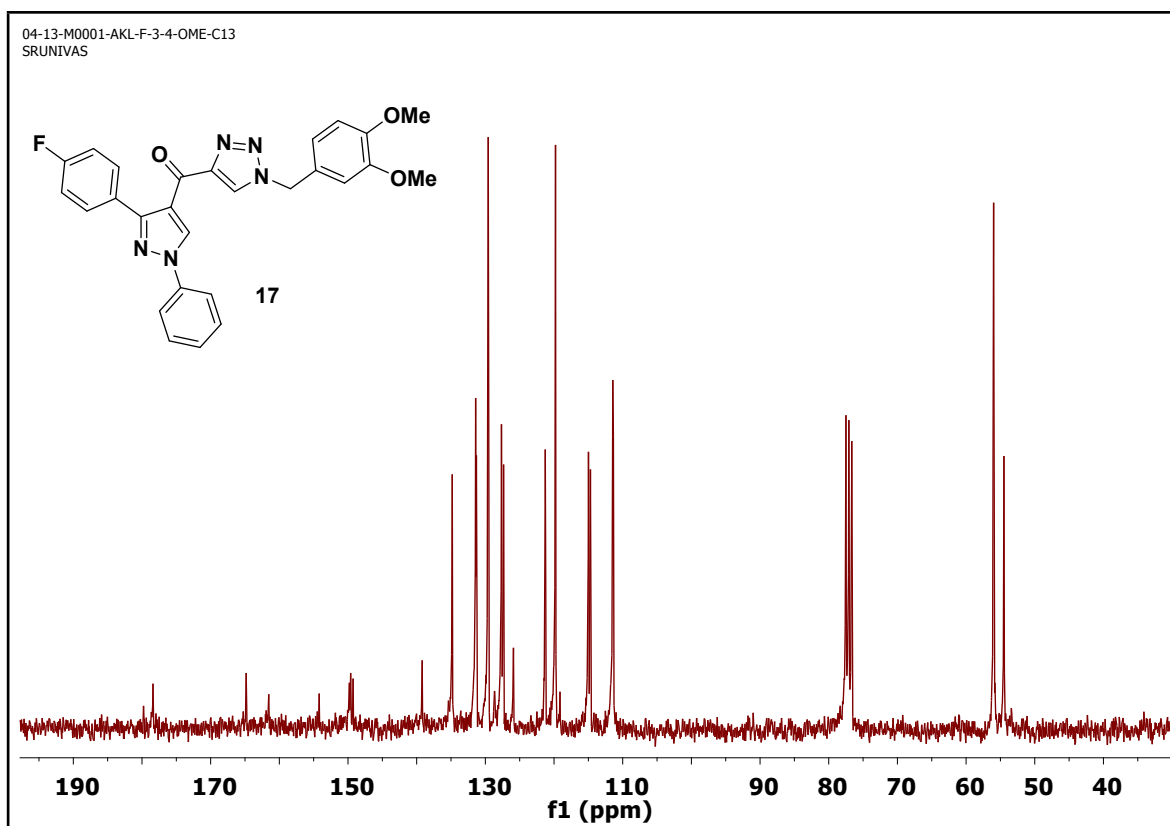
<sup>13</sup>C NMR spectra of compound 16



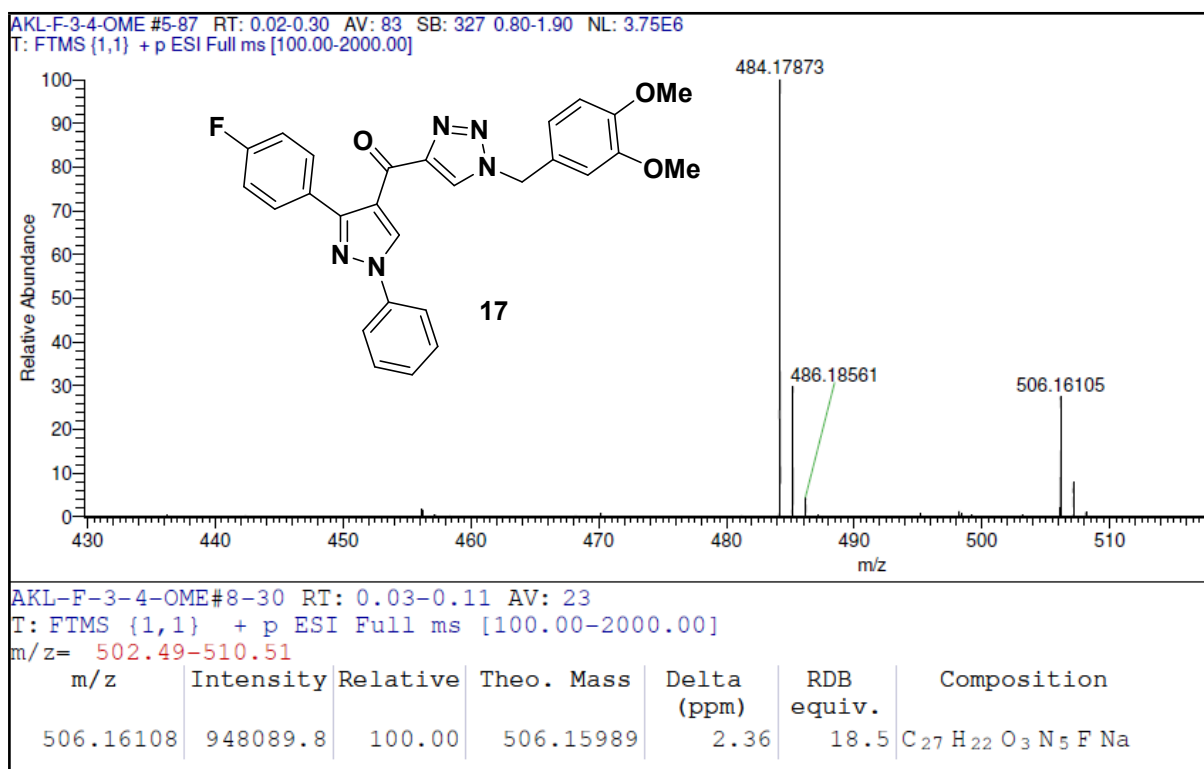
HRMS Spectra of compound 16



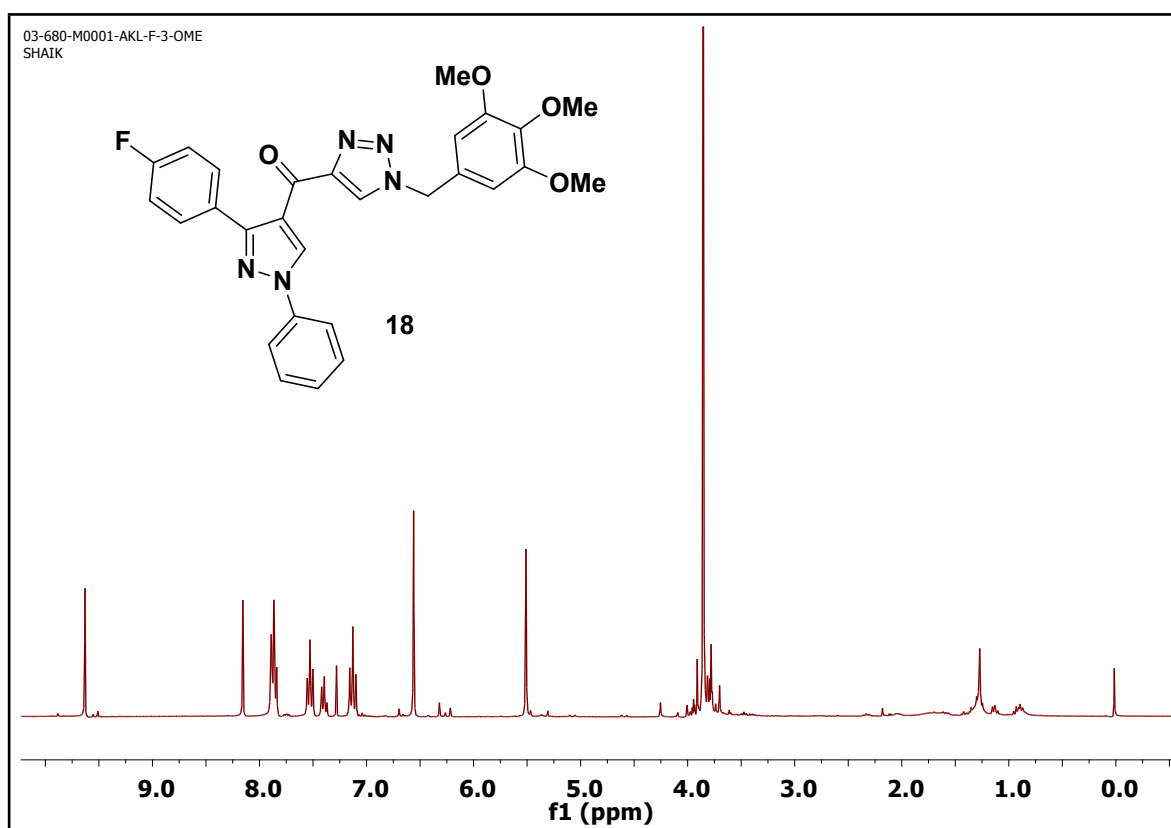
$^1\text{H}$  NMR spectra of compound 17



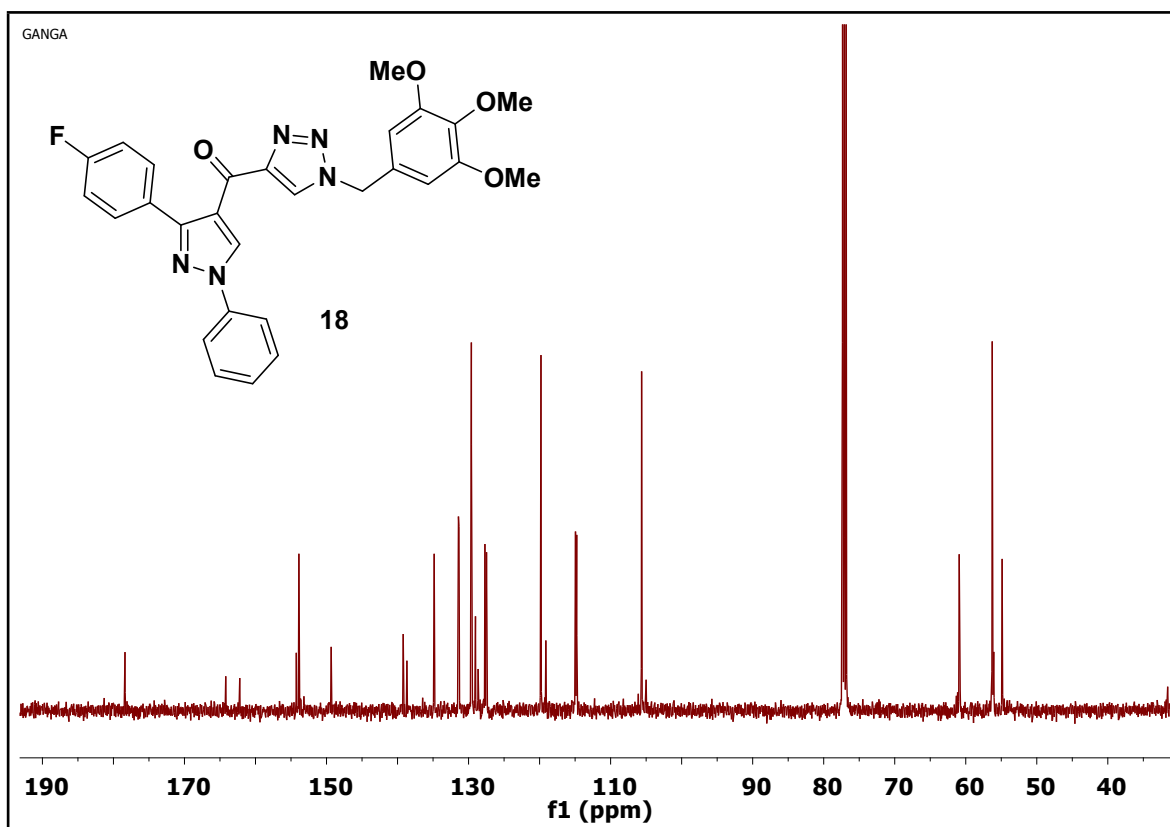
$^{13}\text{C}$  NMR spectra of compound 17



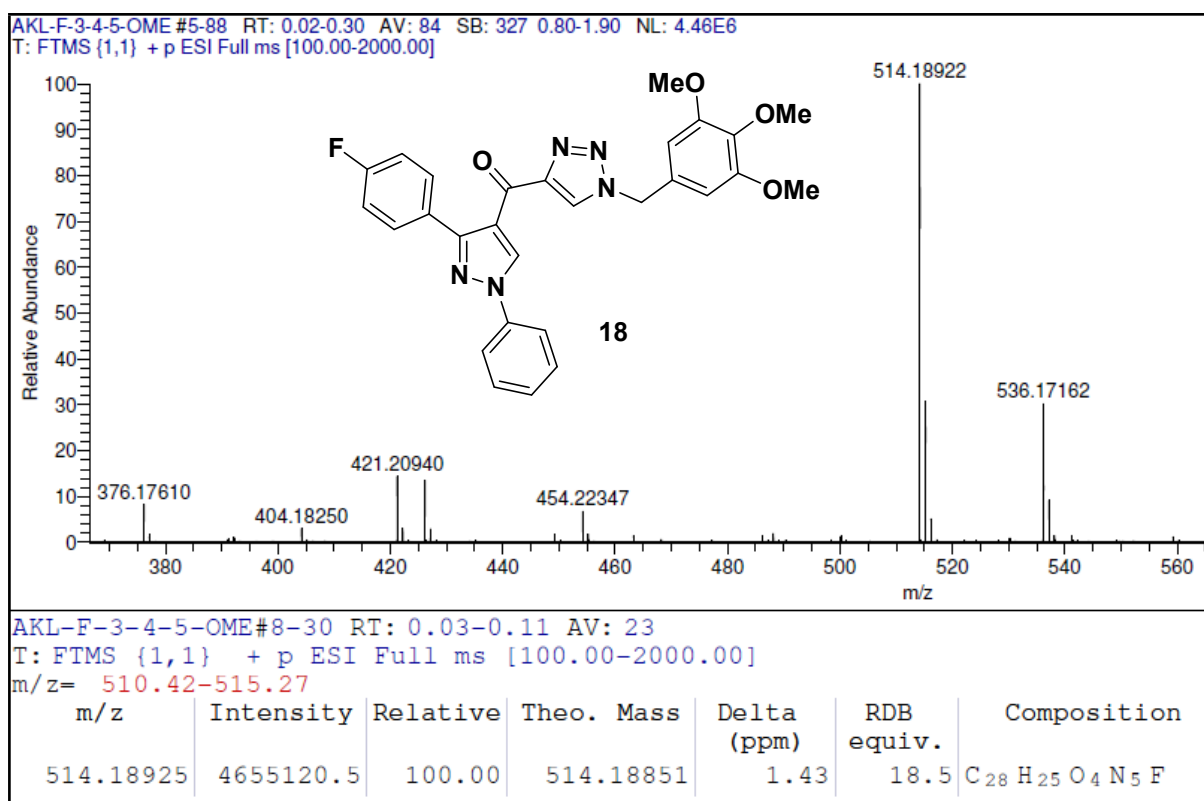
HRMS Spectra of compound 17



<sup>1</sup>H NMR spectra of compound 18

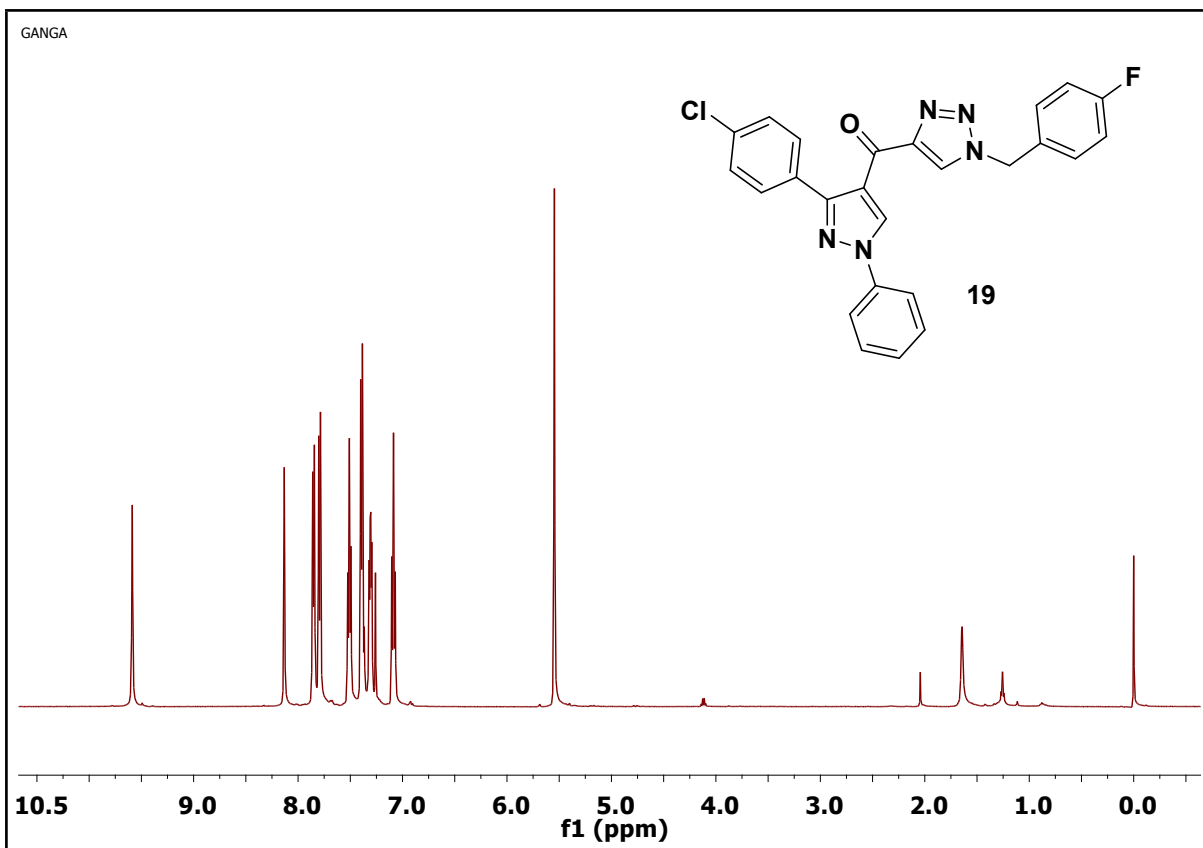


<sup>13</sup>C NMR spectra of compound **18**

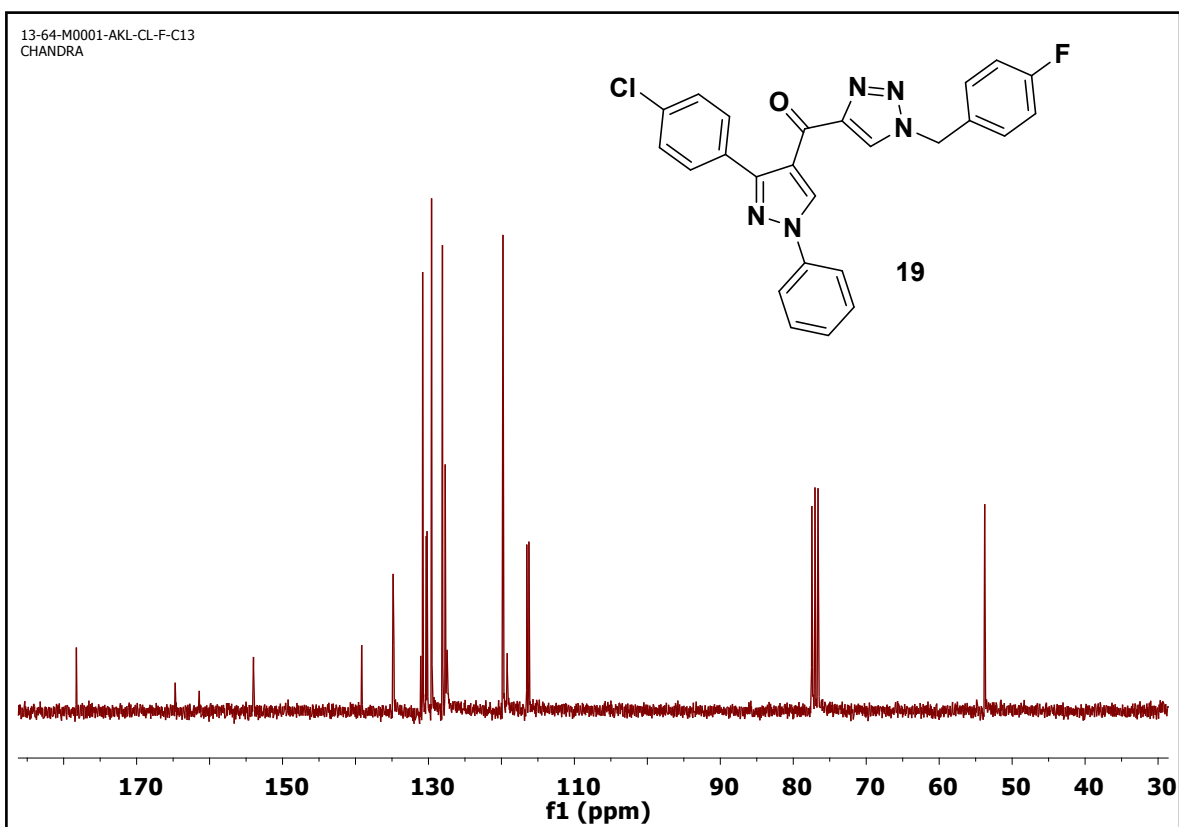


HRMS Spectra of compound **18**

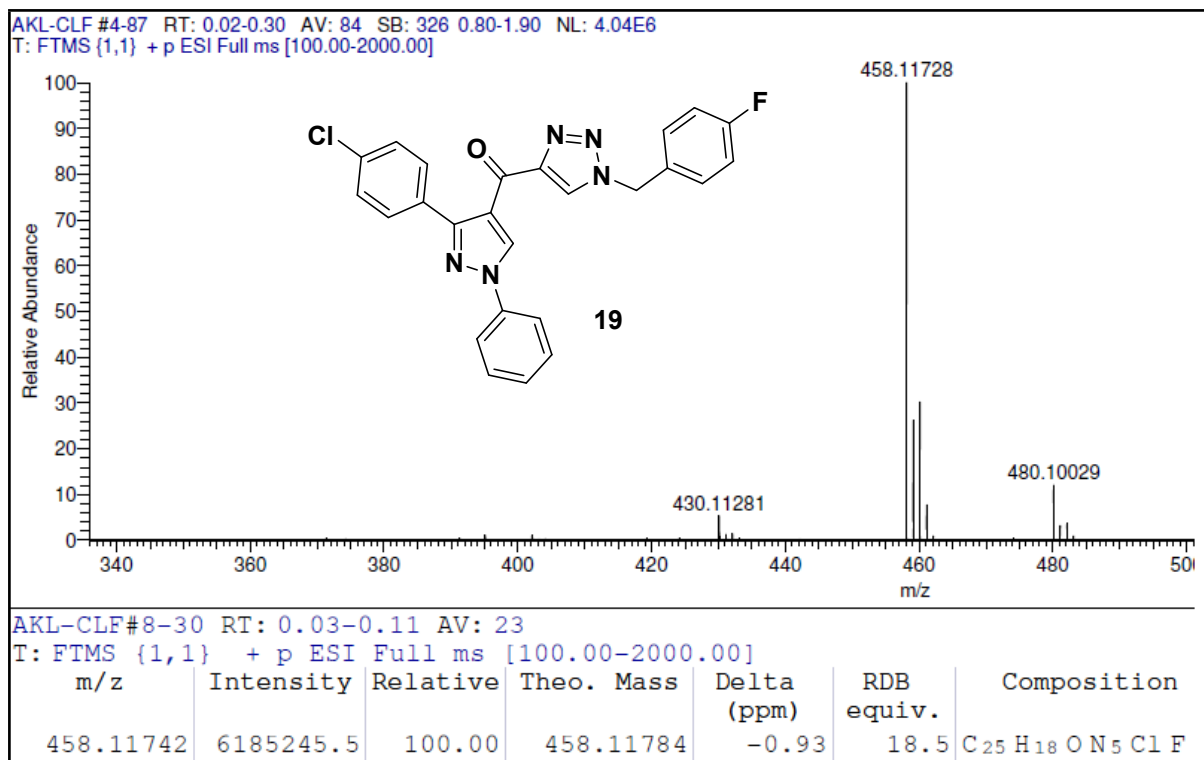




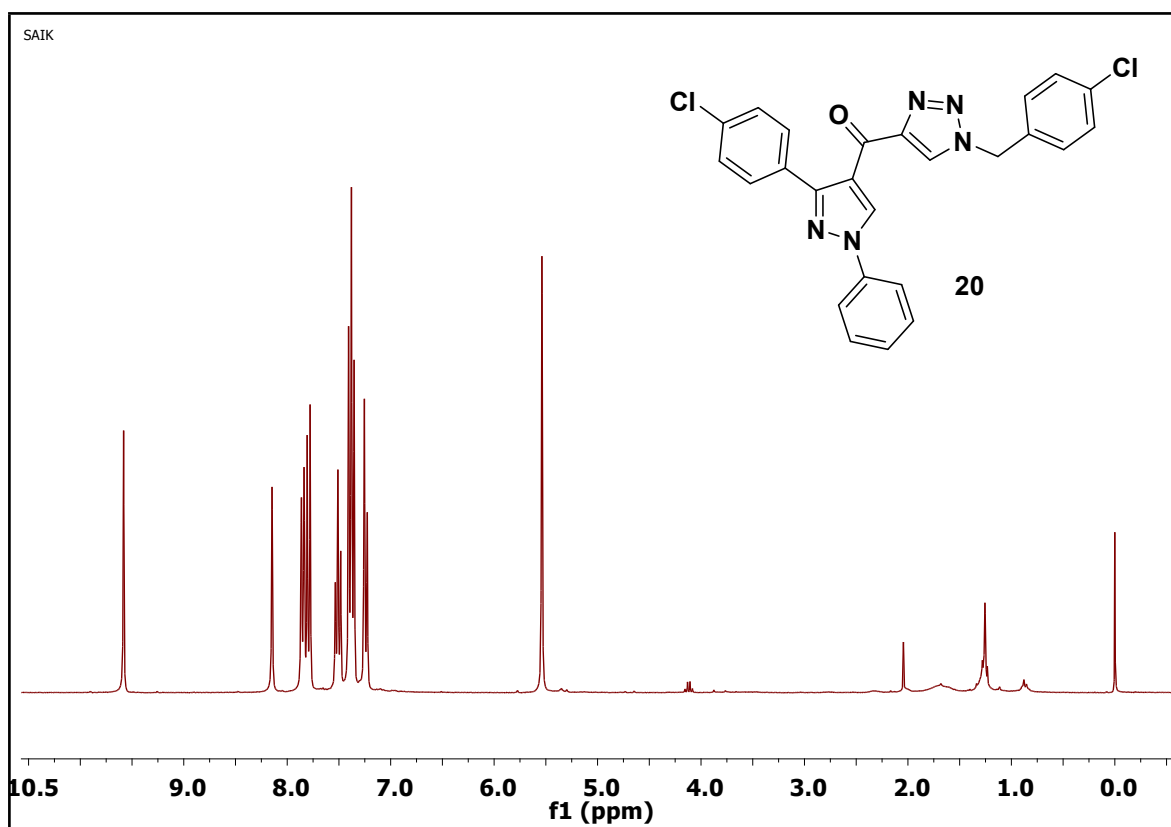
$^1\text{H}$  NMR spectra of compound 19



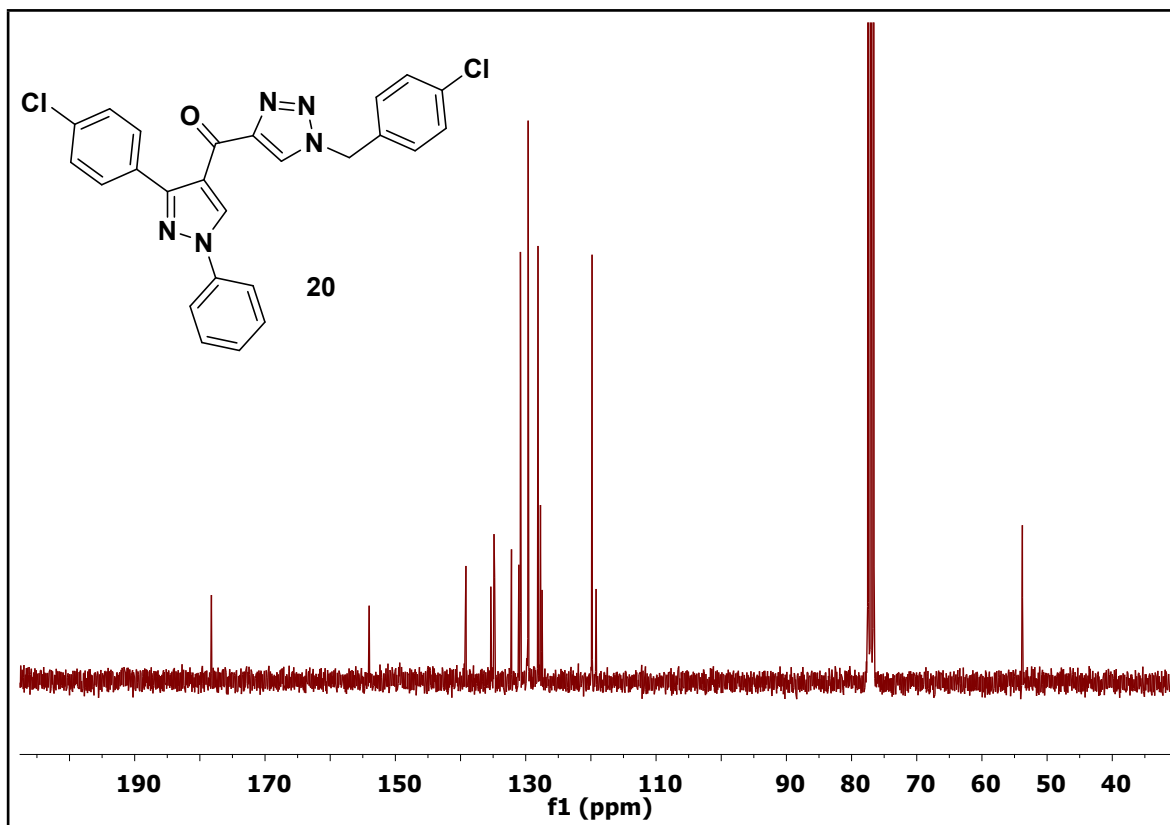
$^{13}\text{C}$  NMR spectra of compound 19



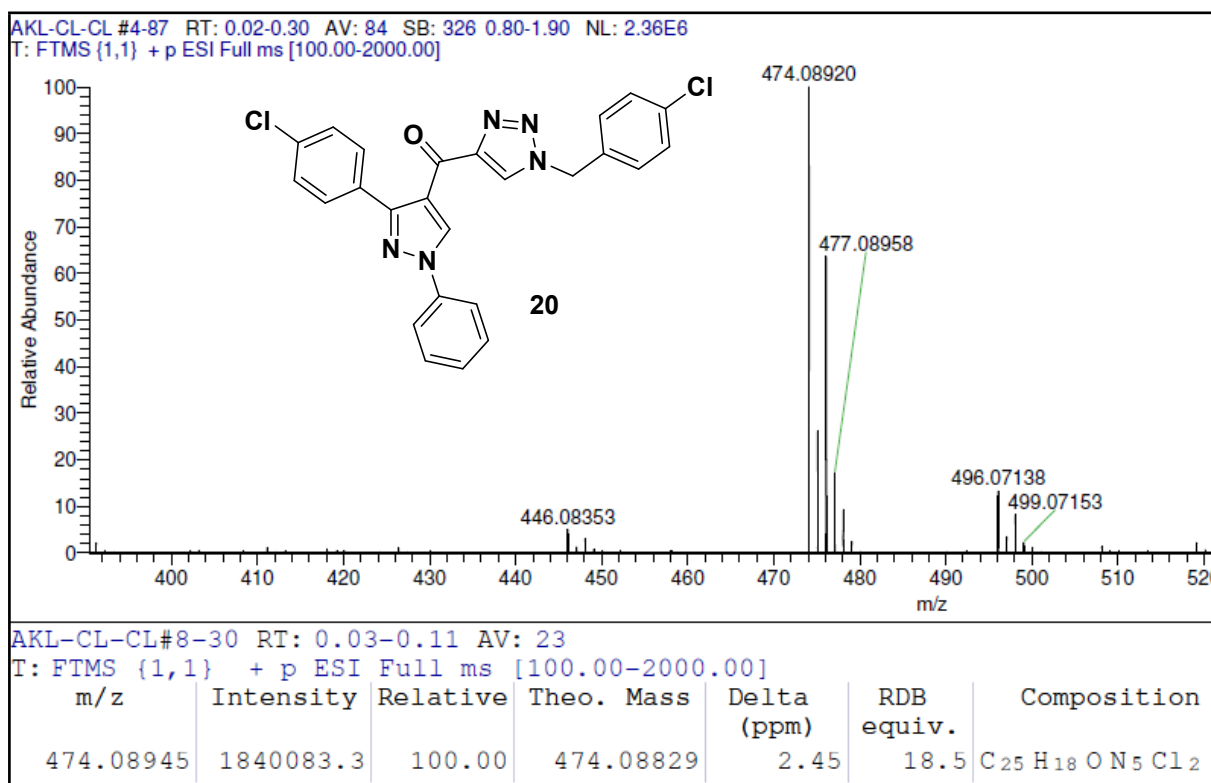
HRMS spectra of compound 19



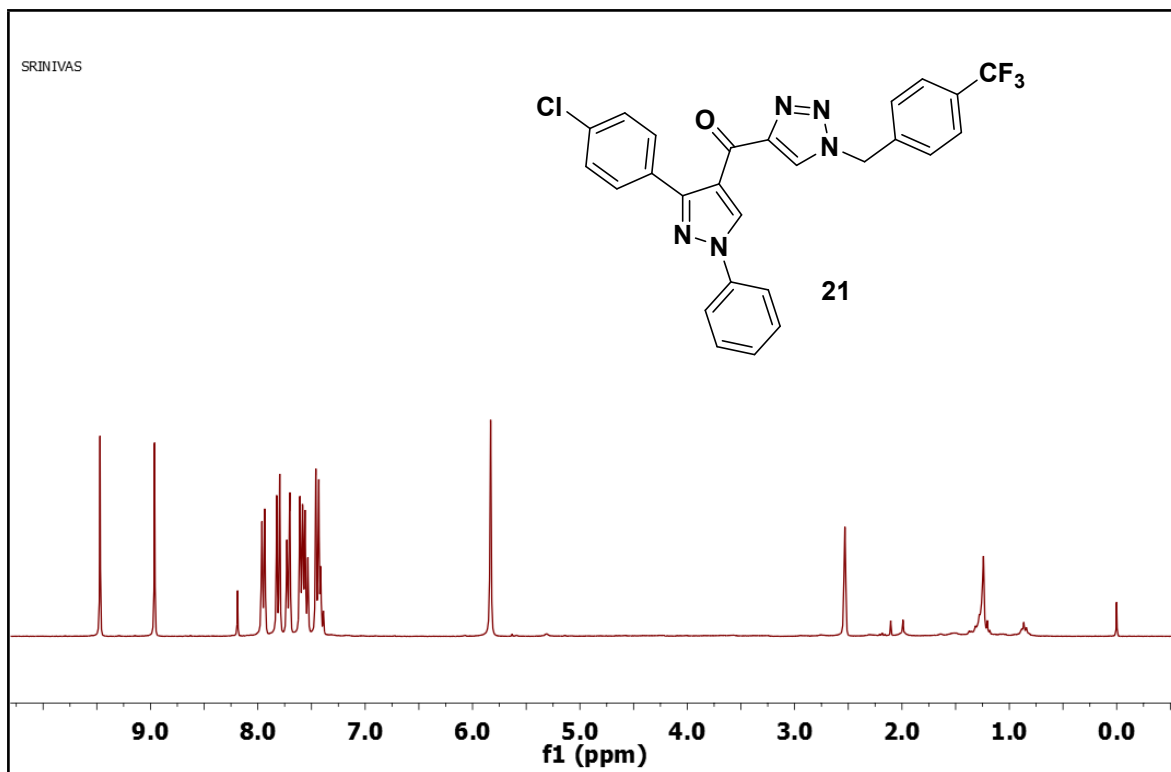
<sup>1</sup>H NMR spectra of compound 20



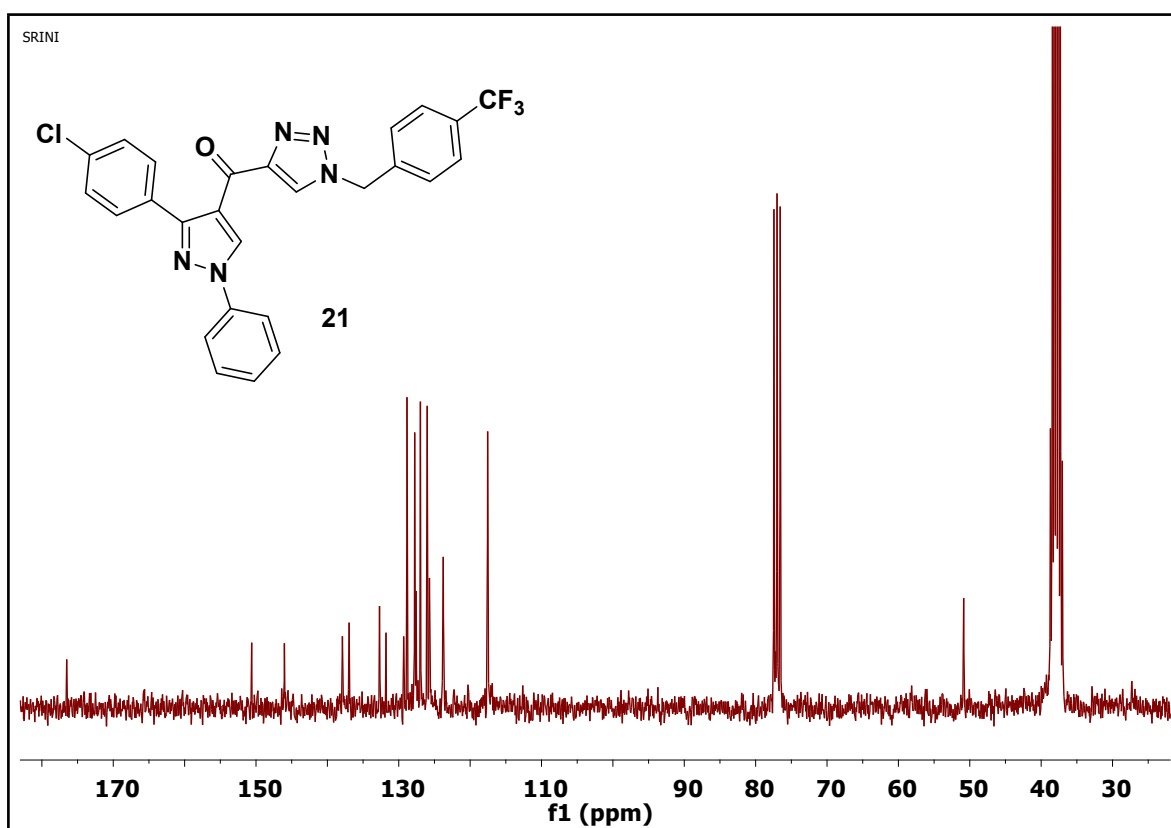
$^{13}\text{C}$  NMR spectra of compound **20**



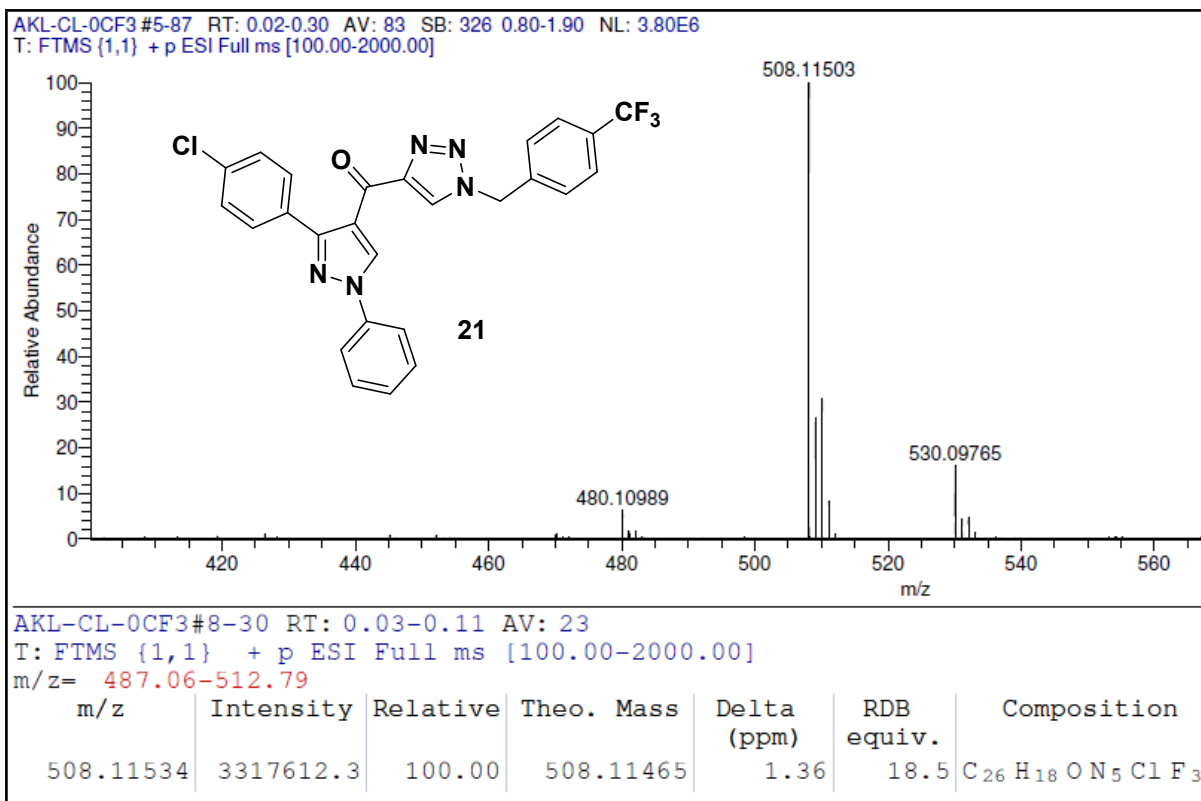
HRMS Spectra of compound **20**



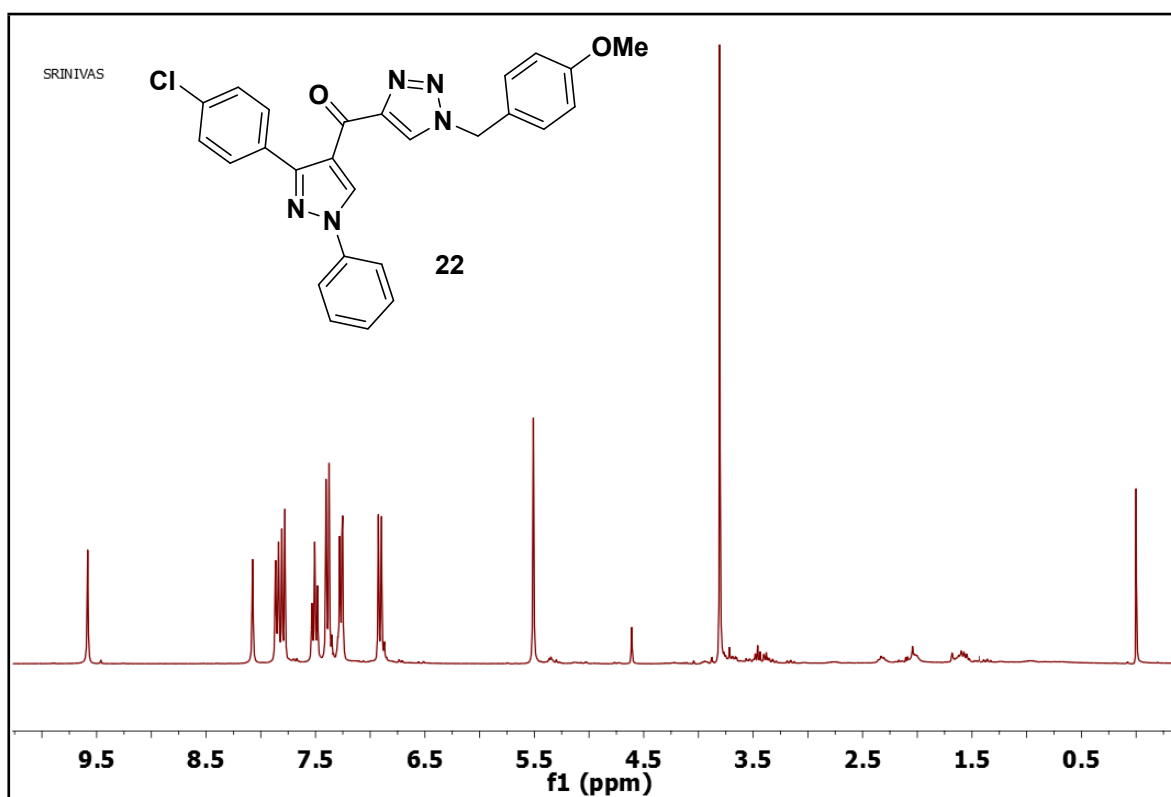
<sup>1</sup>H NMR spectra of compound 21



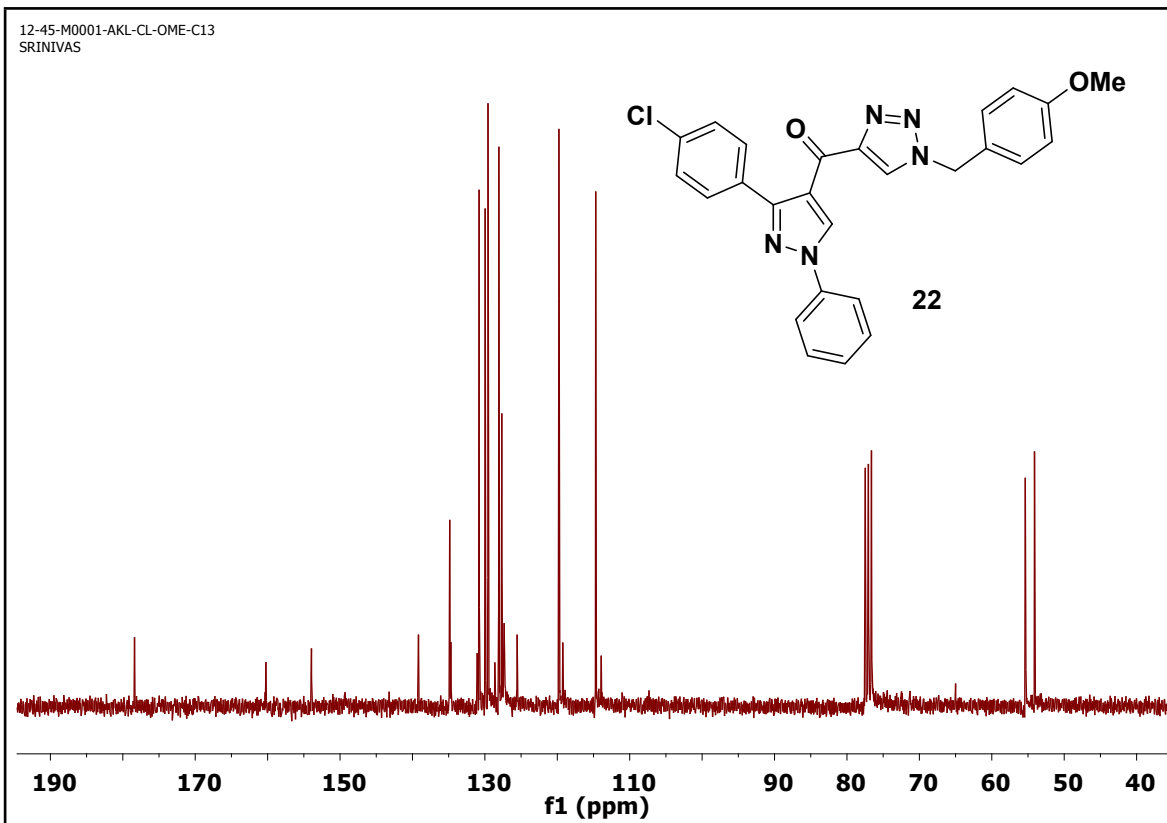
<sup>13</sup>C NMR spectra of compound 21



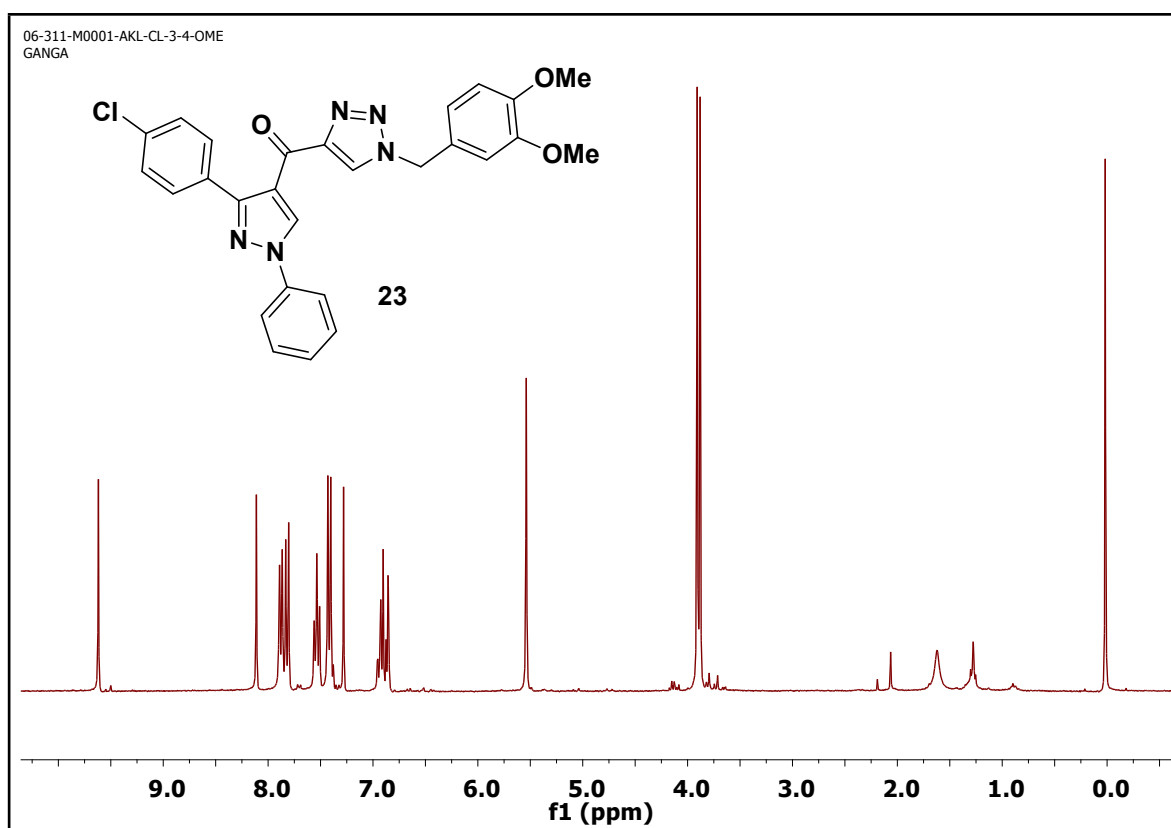
HRMS Spectra of compound 21



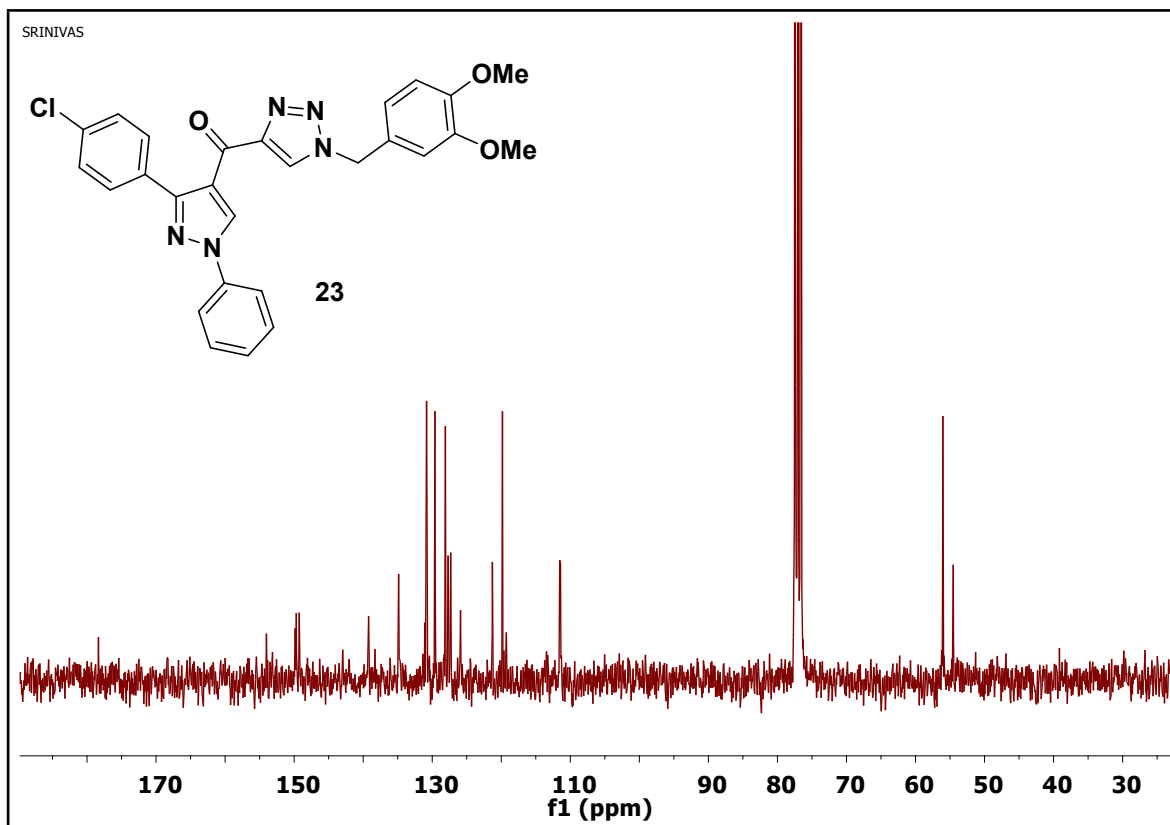
<sup>1</sup>H NMR spectra of compound 22



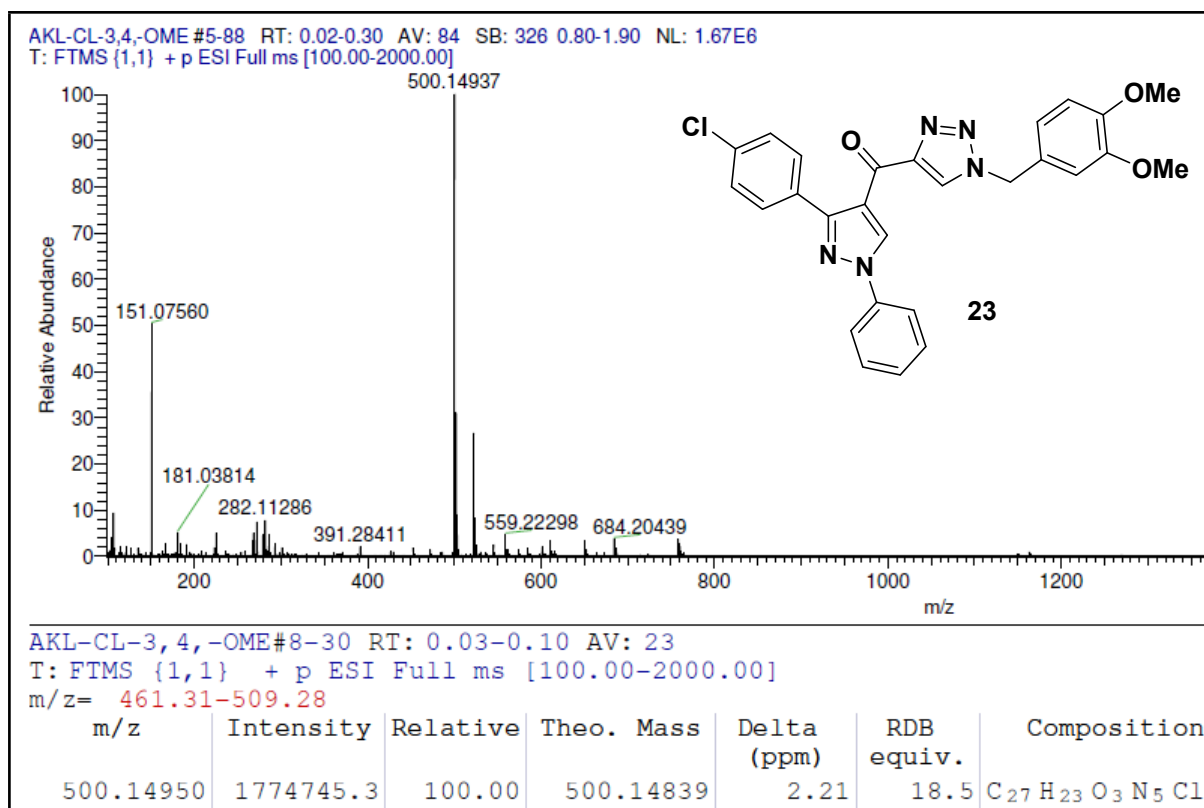
$^{13}\text{C}$  NMR spectra of compound 22



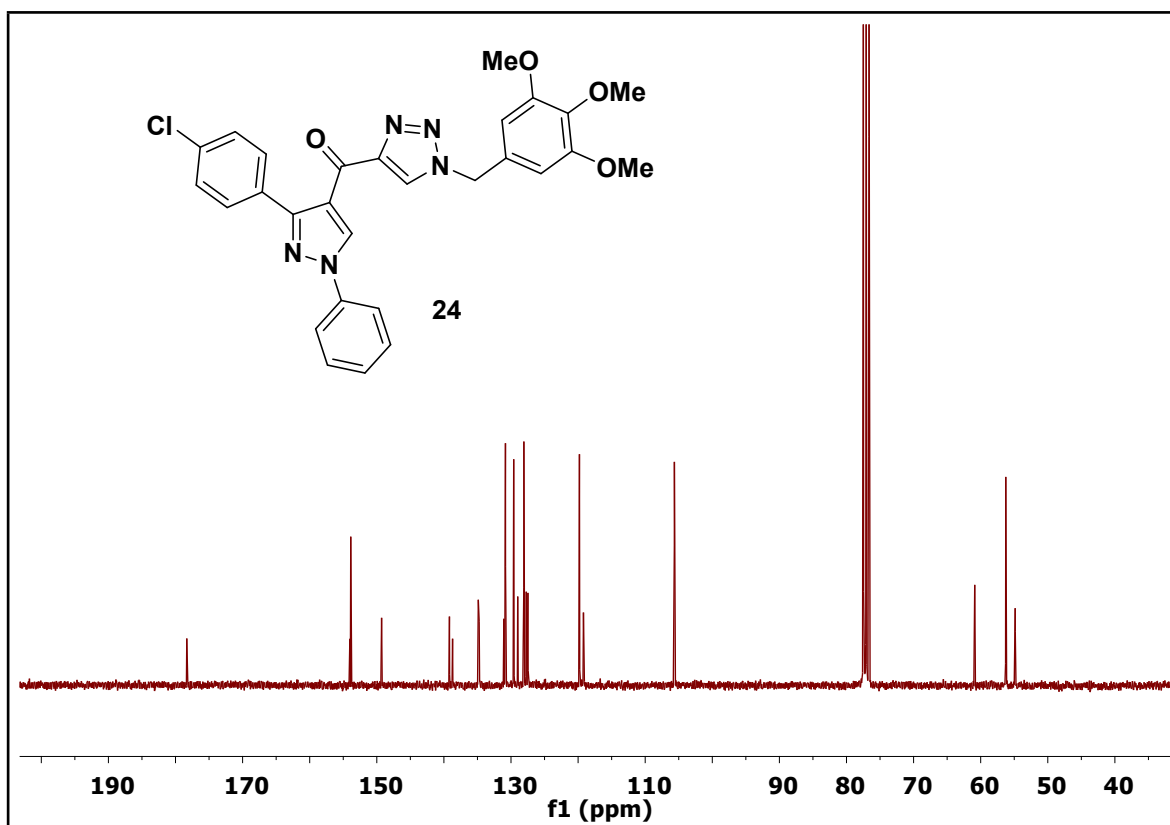
$^1\text{H}$  NMR spectra of compound 23



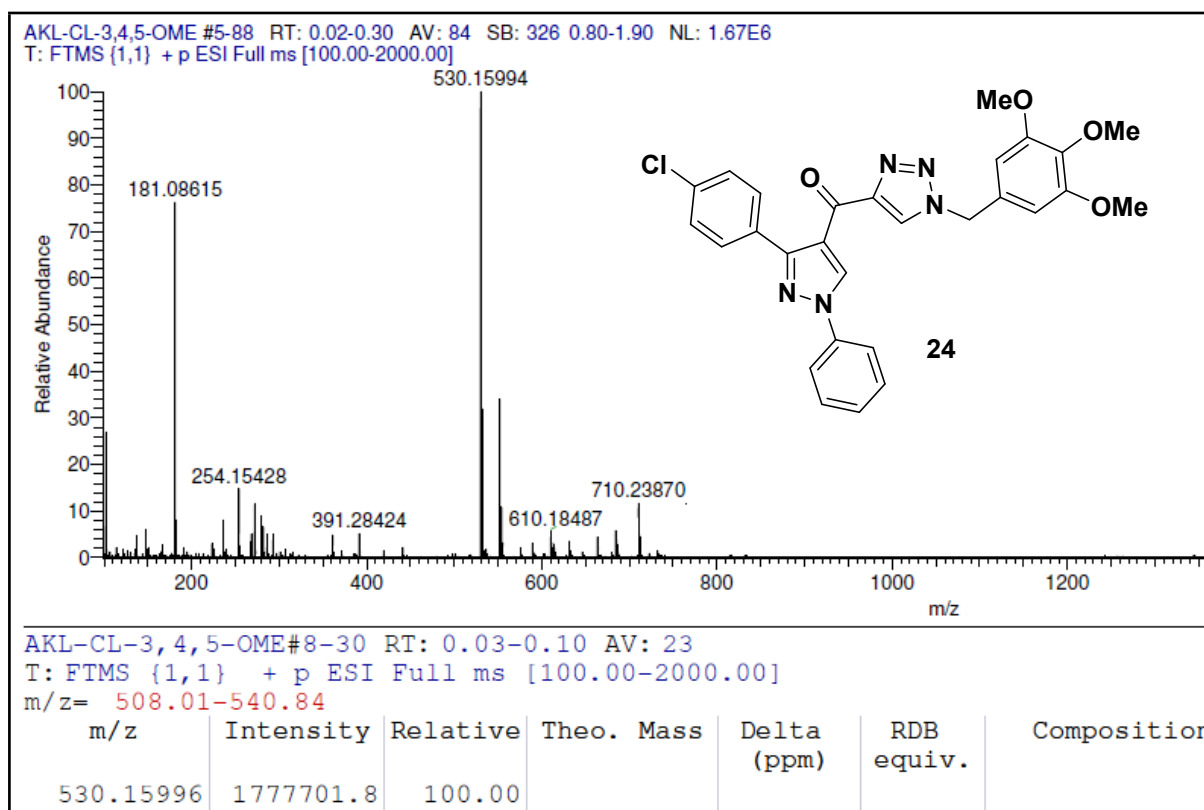
$^{13}\text{C}$  NMR spectra of compound 23



HRMS Spectra of compound 23

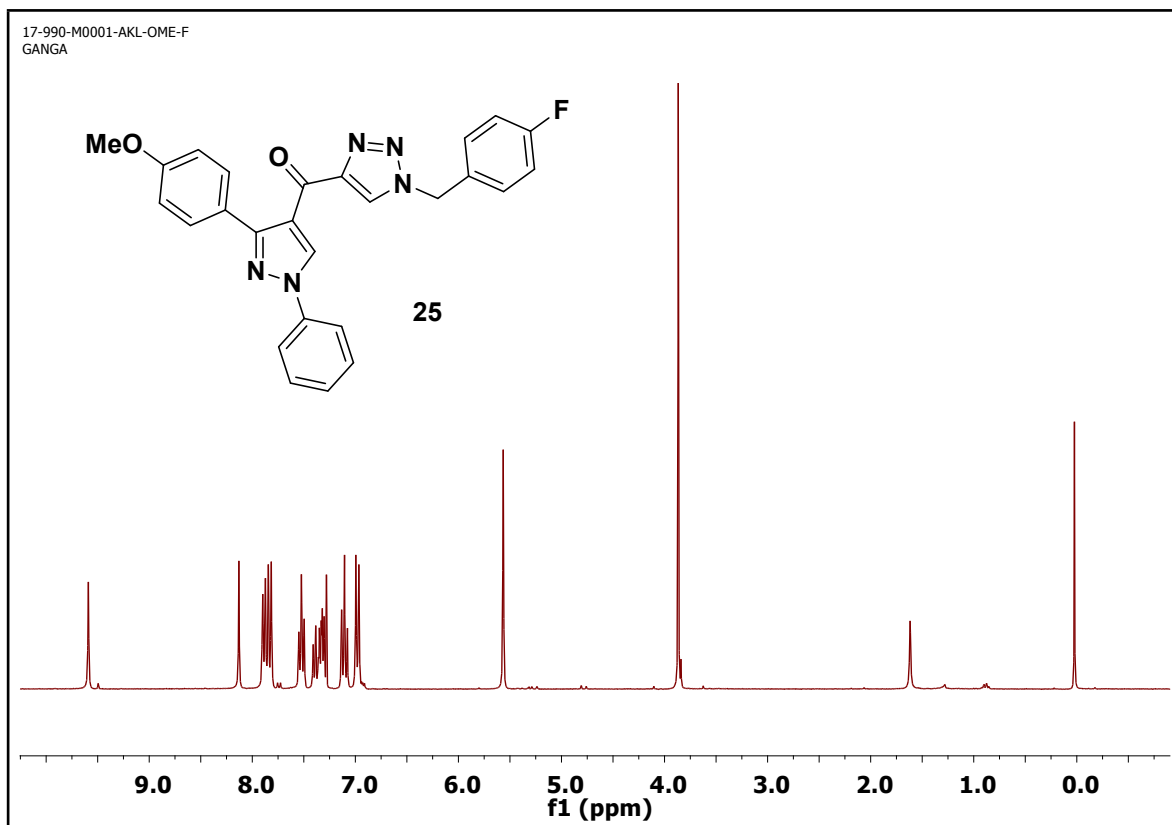


<sup>13</sup>C NMR spectra of compound 24

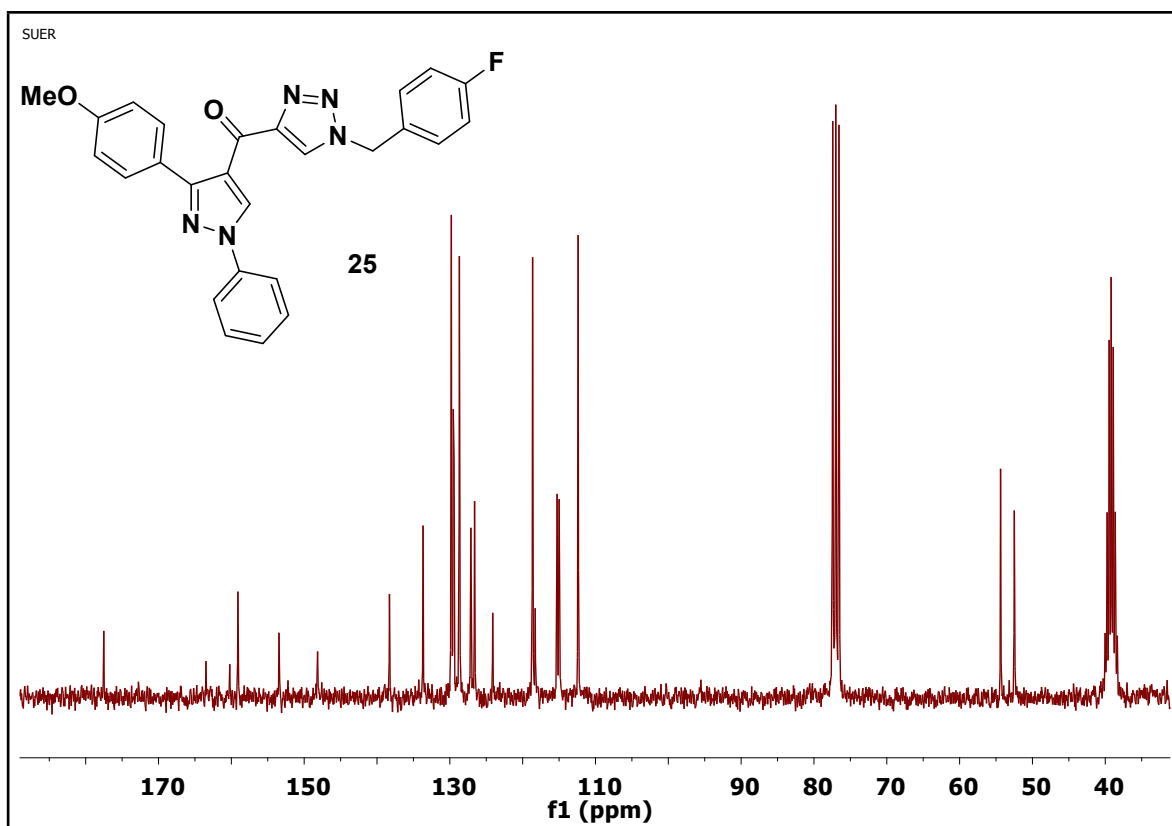


HRMS Spectra of compound 24



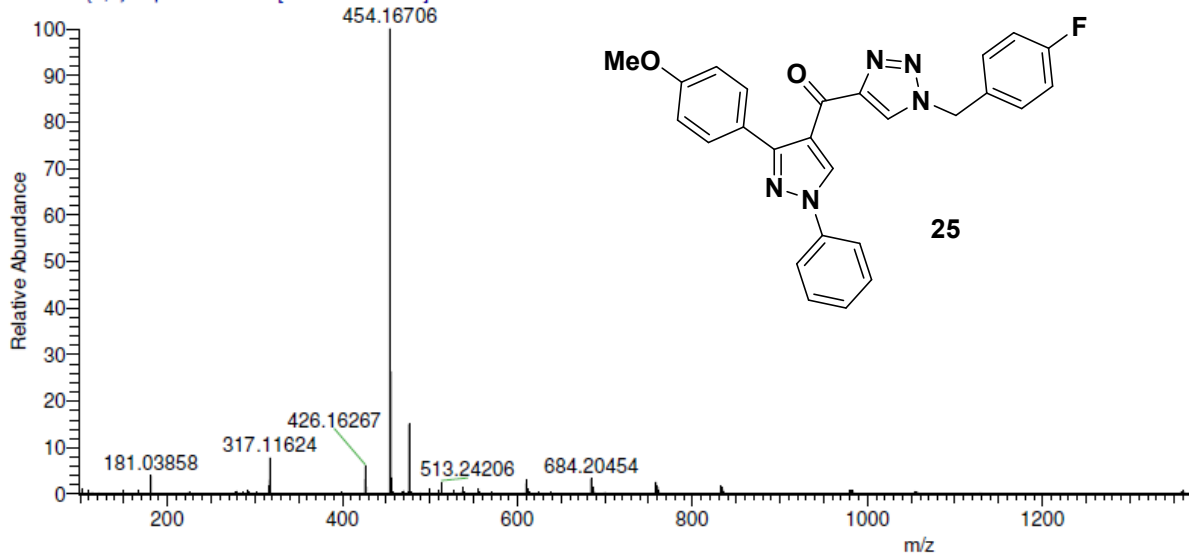


$^1\text{H}$  NMR spectra of compound 25



$^{13}\text{C}$  NMR spectra of compound 25

AKL-OME-F#5-88 RT: 0.02-0.30 AV: 84 SB: 326 0.80-1.90 NL: 8.59E6  
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

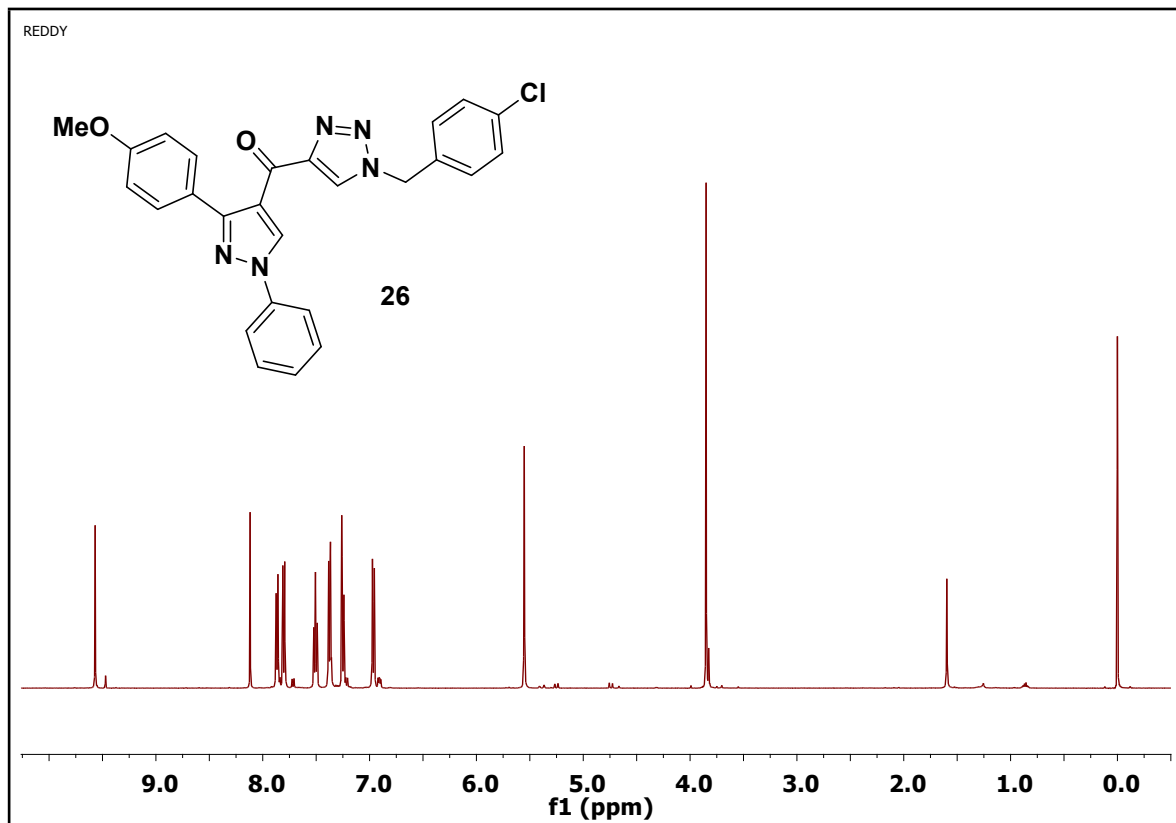


AKL-OME-F#8-30 RT: 0.03-0.10 AV: 23  
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

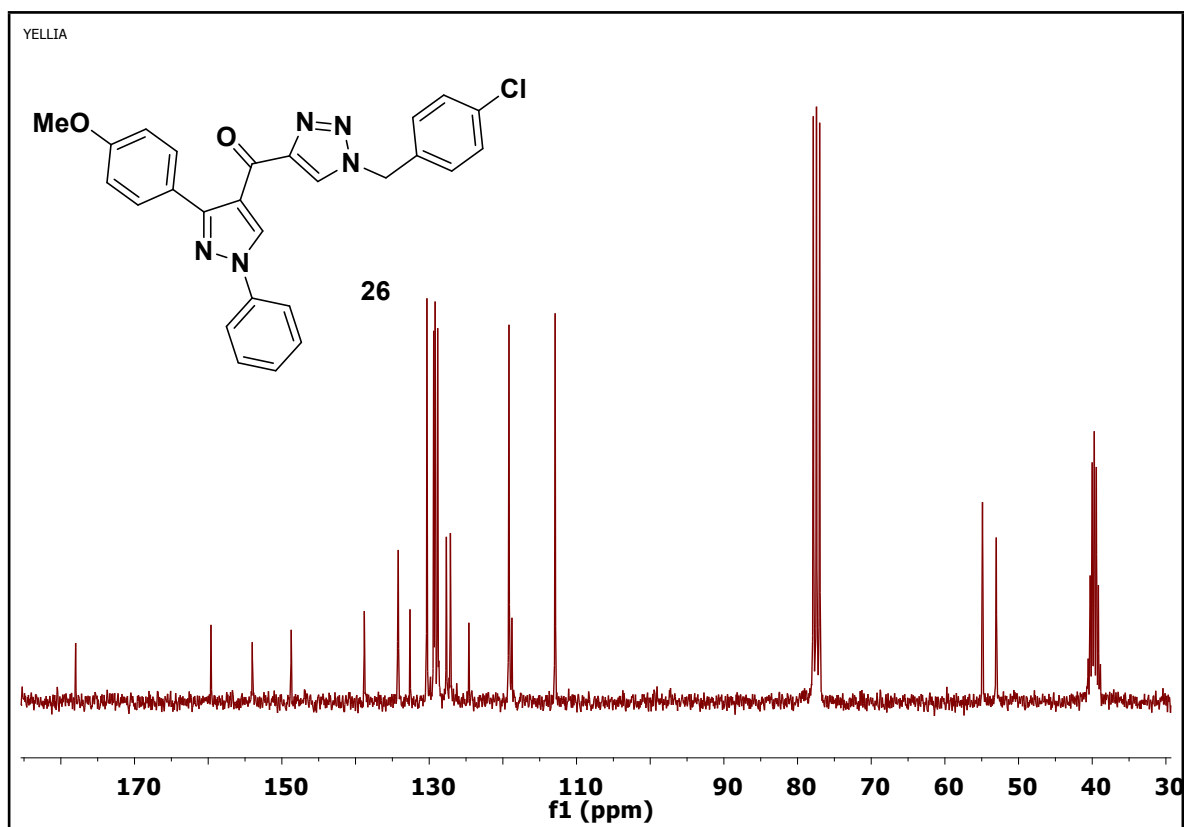
m/z= 439.84-468.88

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
454.16696	9715468.0	100.00	454.16738	-0.92	18.5	C <sub>26</sub> H <sub>21</sub> O <sub>2</sub> N <sub>5</sub> F

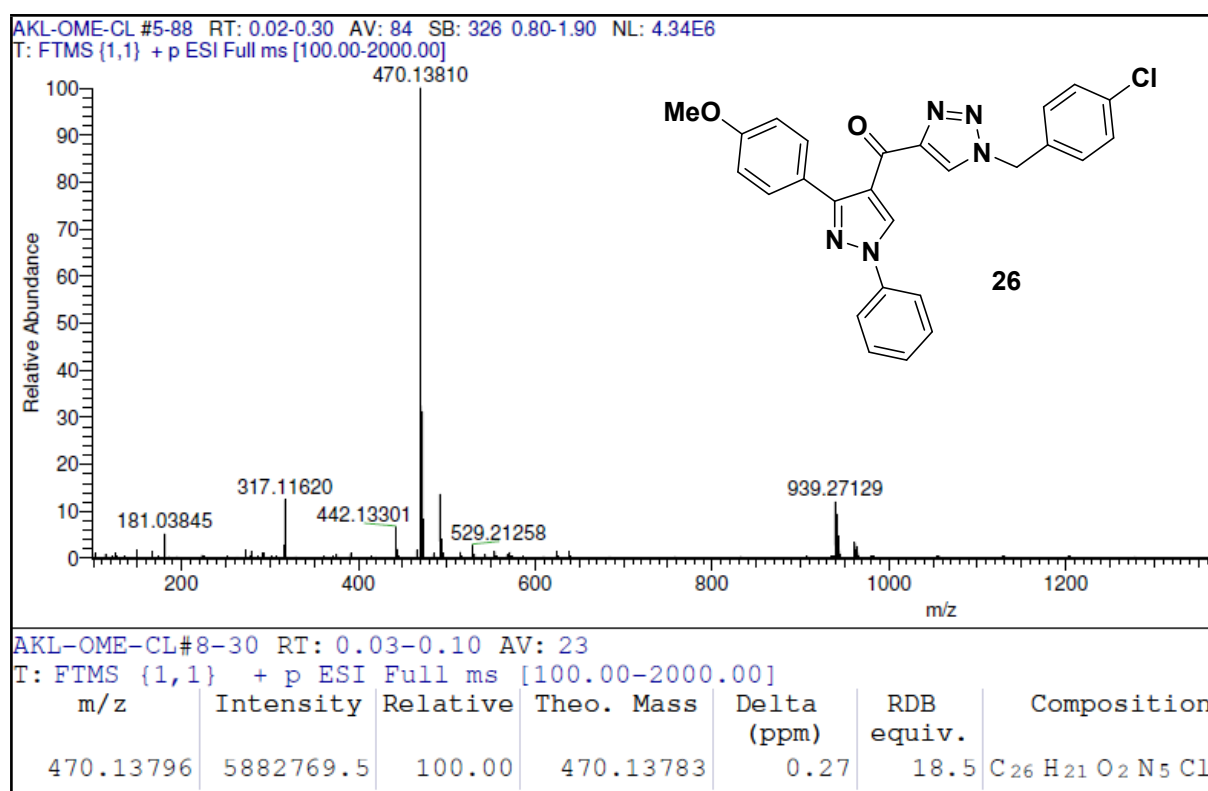
HRMS Spectra of compound 25



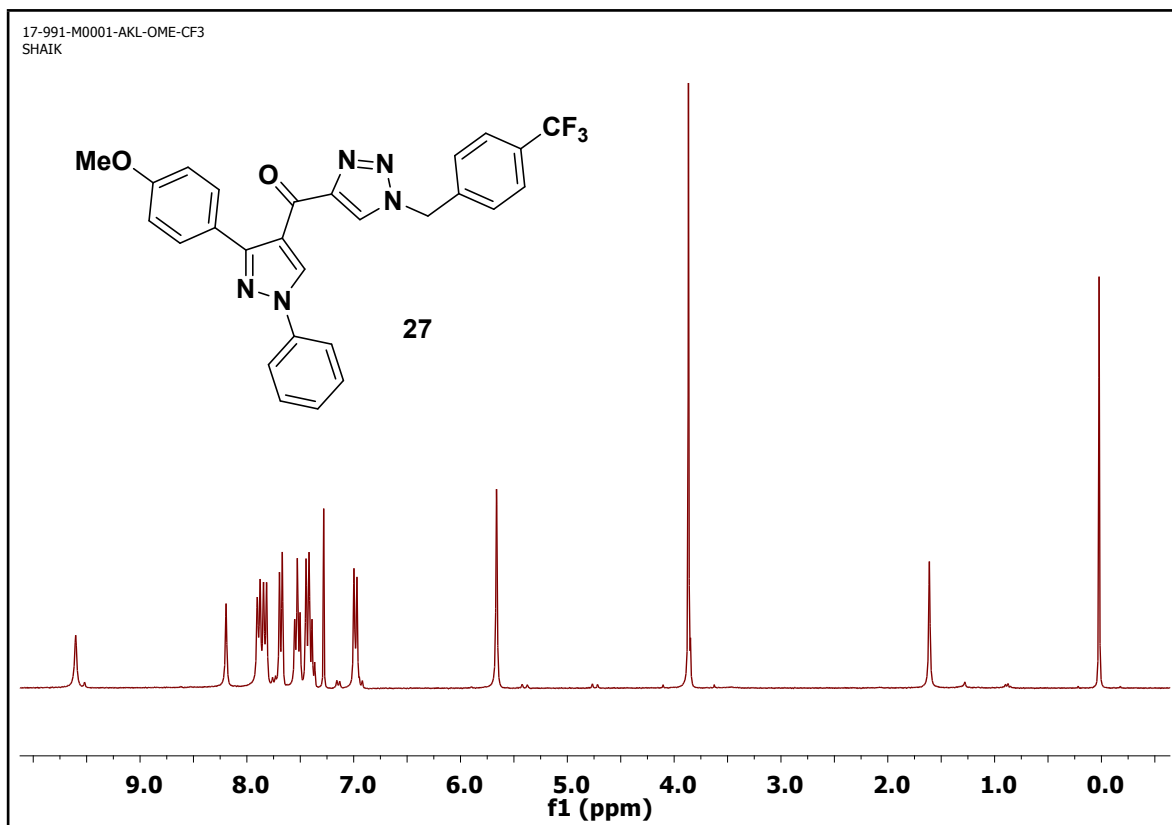
<sup>1</sup>H NMR spectra of compound 26



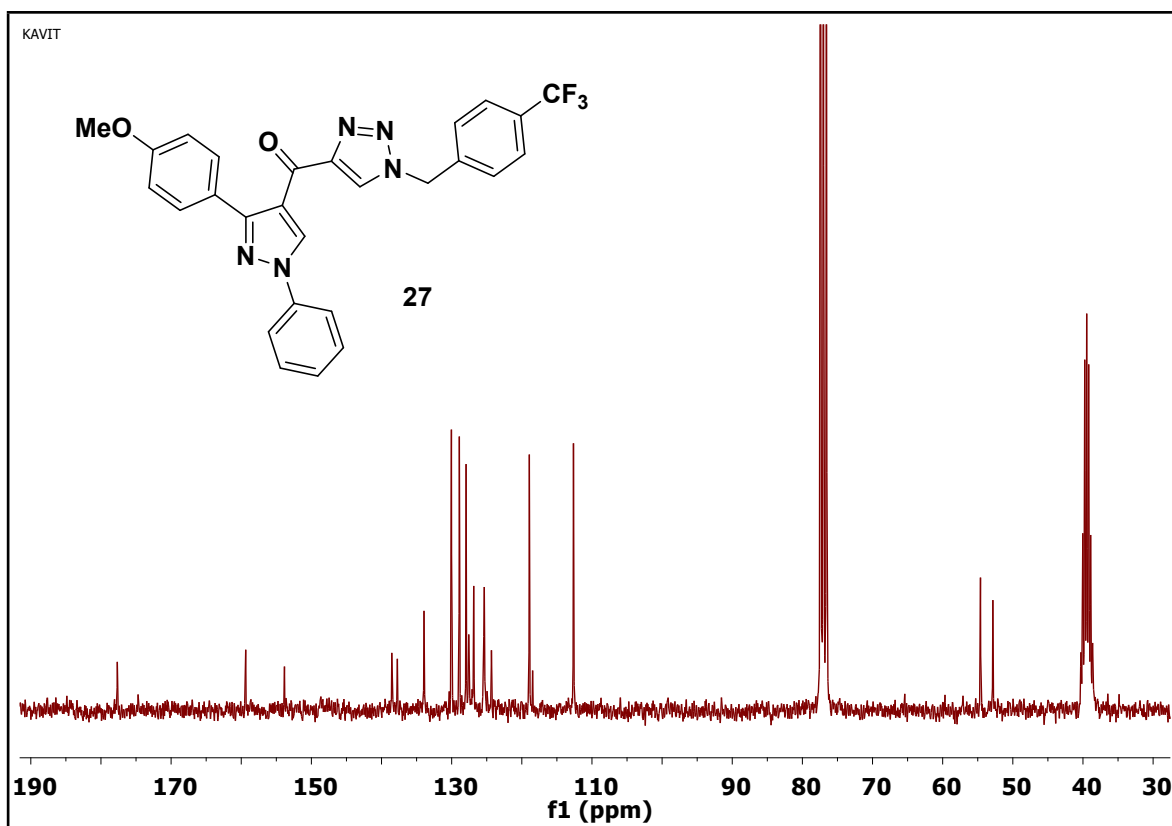
<sup>13</sup>C NMR spectra of compound 26



HRMS Spectra of compound 26

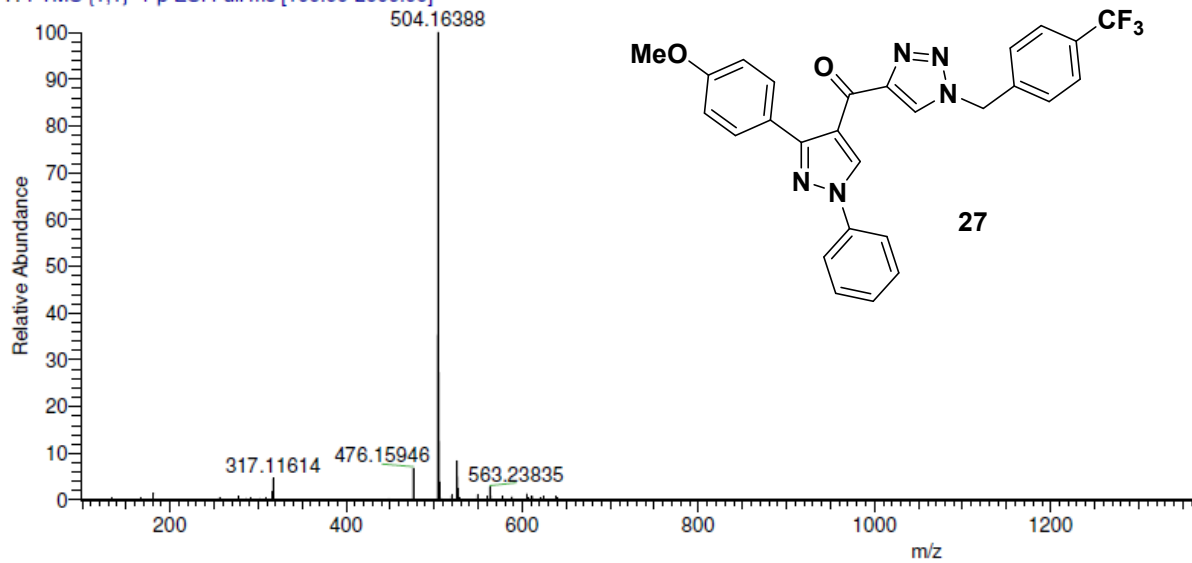


$^1\text{H}$  NMR spectra of compound 27



$^{13}\text{C}$  NMR spectra of compound 27

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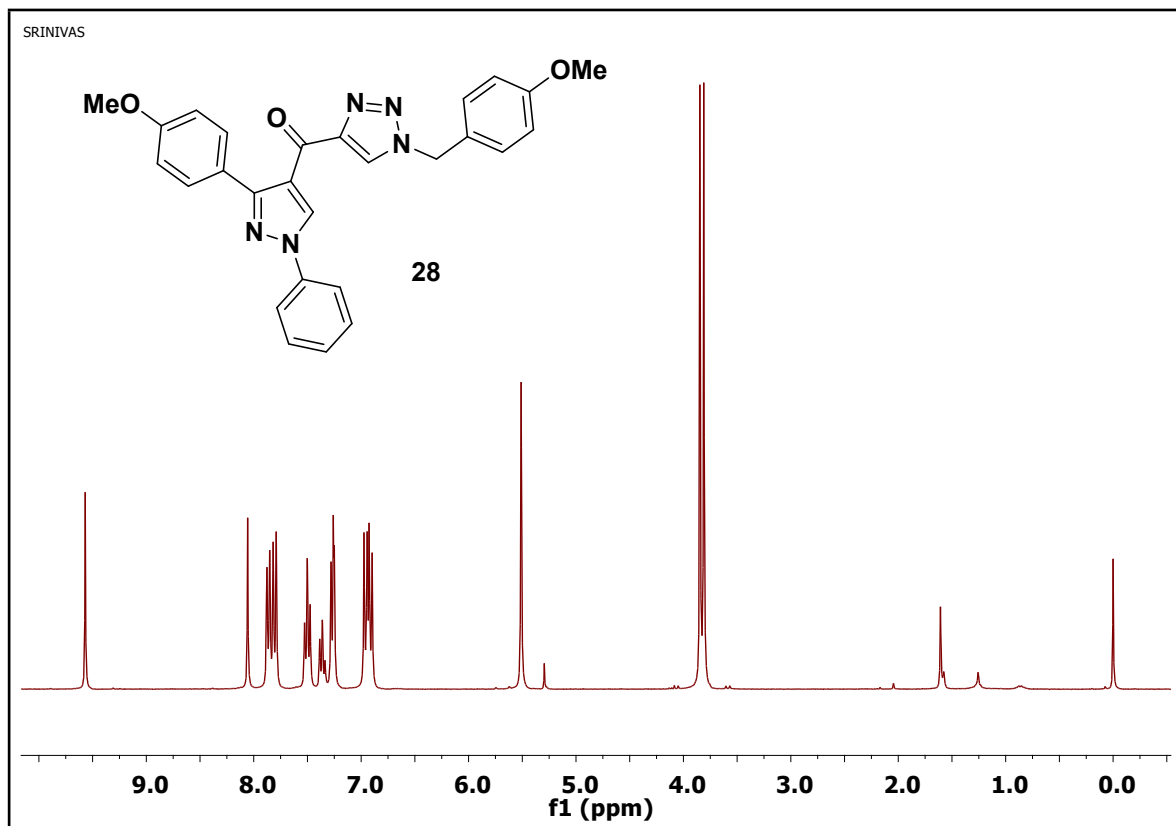


AKL-OME-CF3 #8-30 RT: 0.03-0.10 AV: 23  
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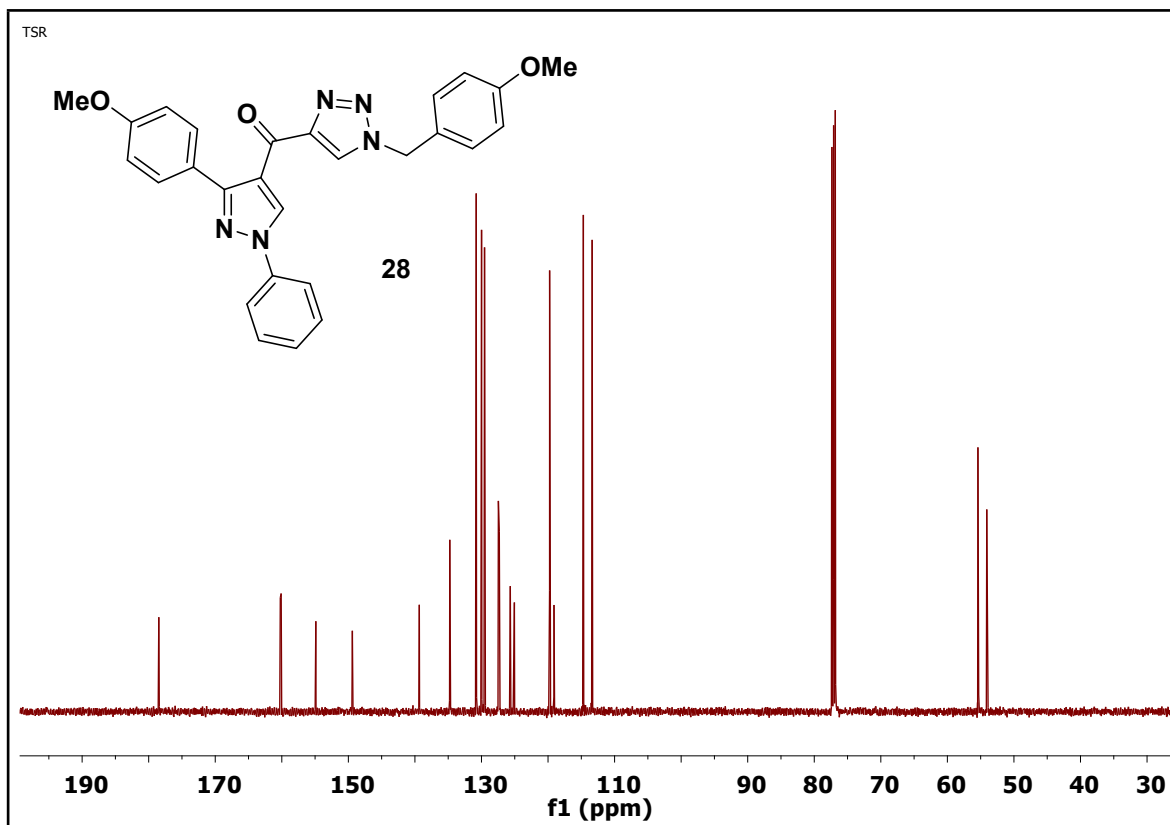
m/z= 519.37-533.26

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
526.14693	981816.1	100.00				

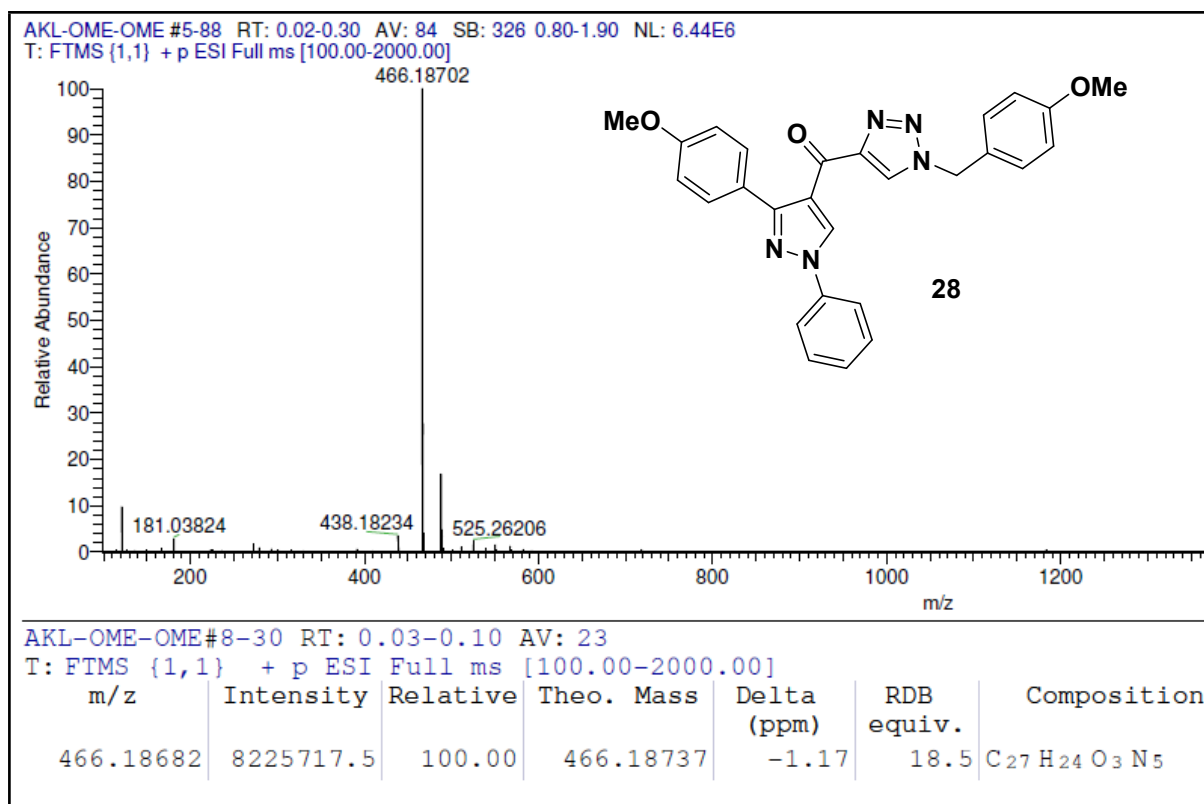
HRMS Spectra of compound 27



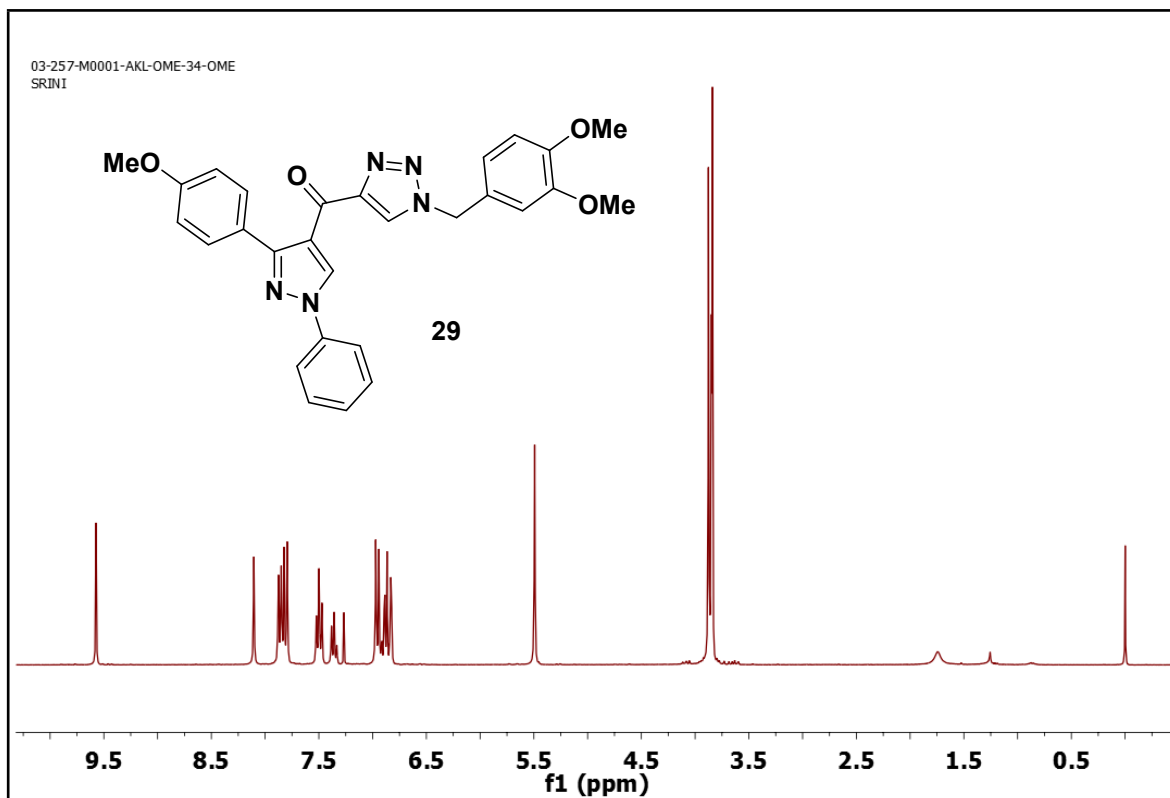
<sup>1</sup>H NMR spectra of compound 28



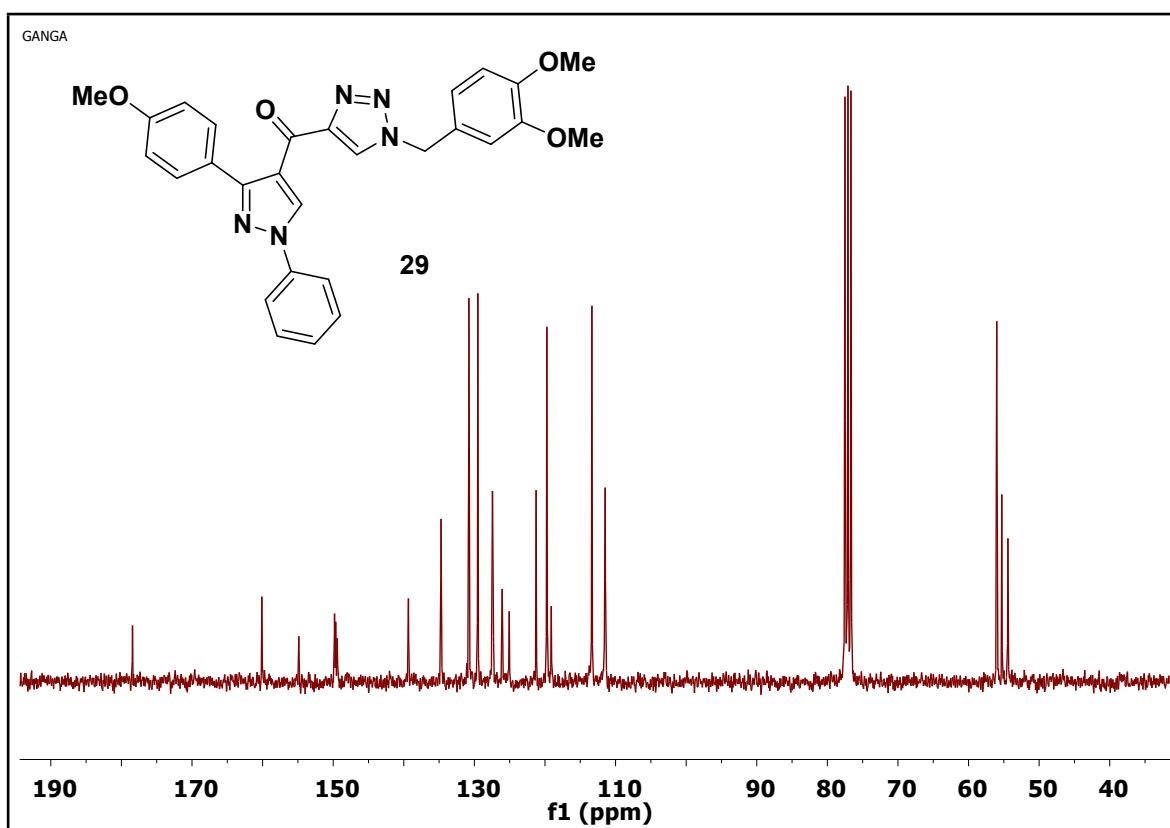
<sup>13</sup>C NMR spectra of compound **28**



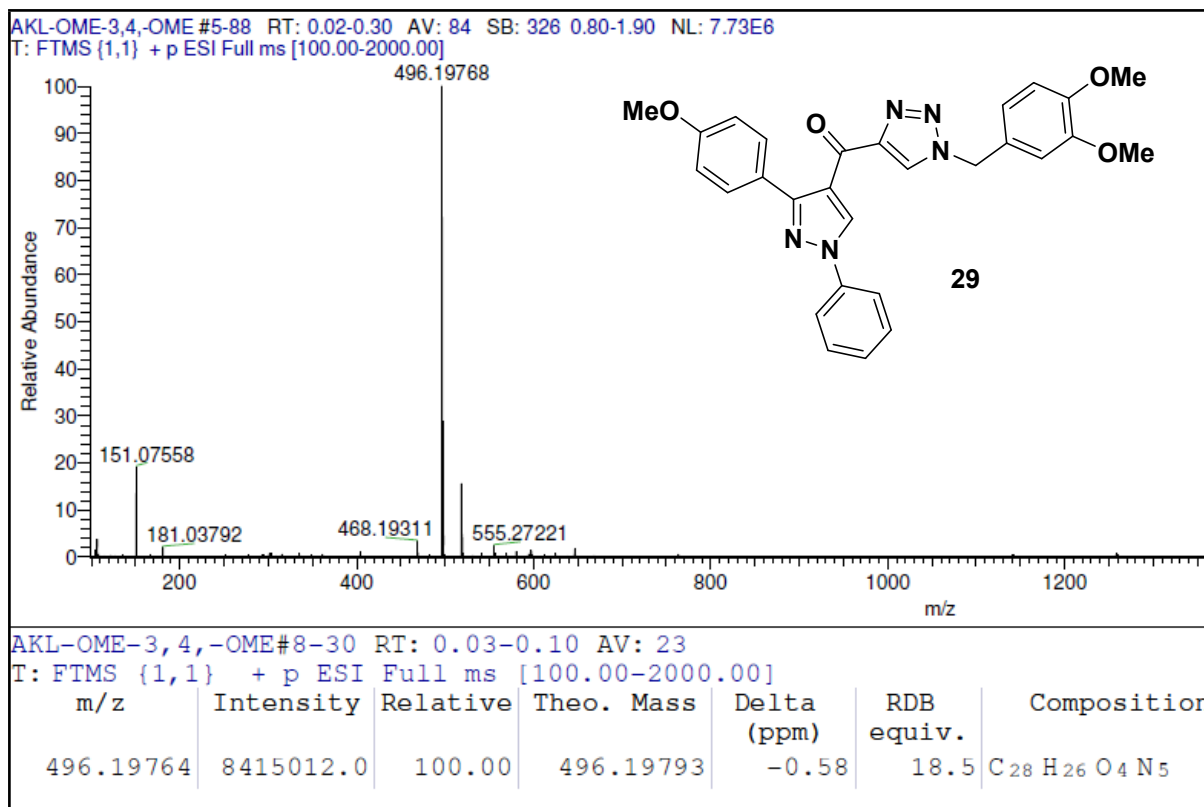
HRMS Spectra of compound **28**



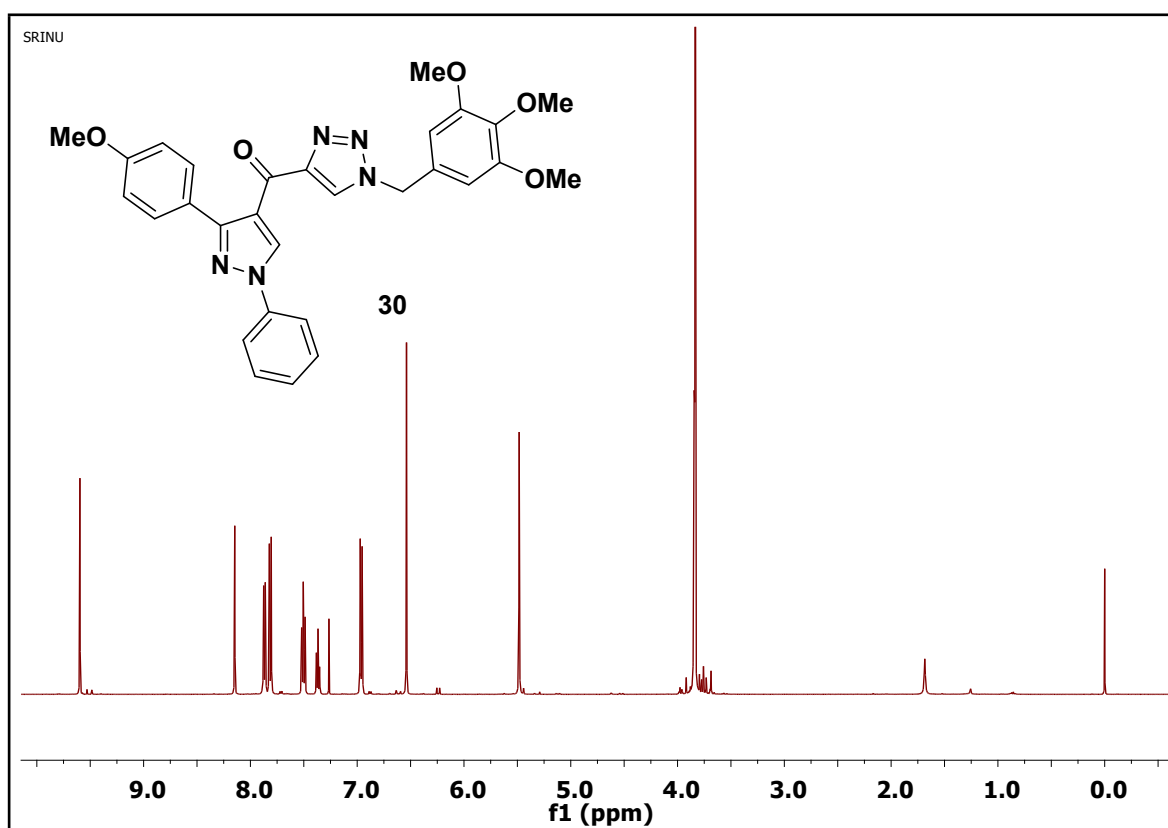
$^1\text{H}$  NMR spectra of compound 29



$^{13}\text{C}$  NMR spectra of compound 29

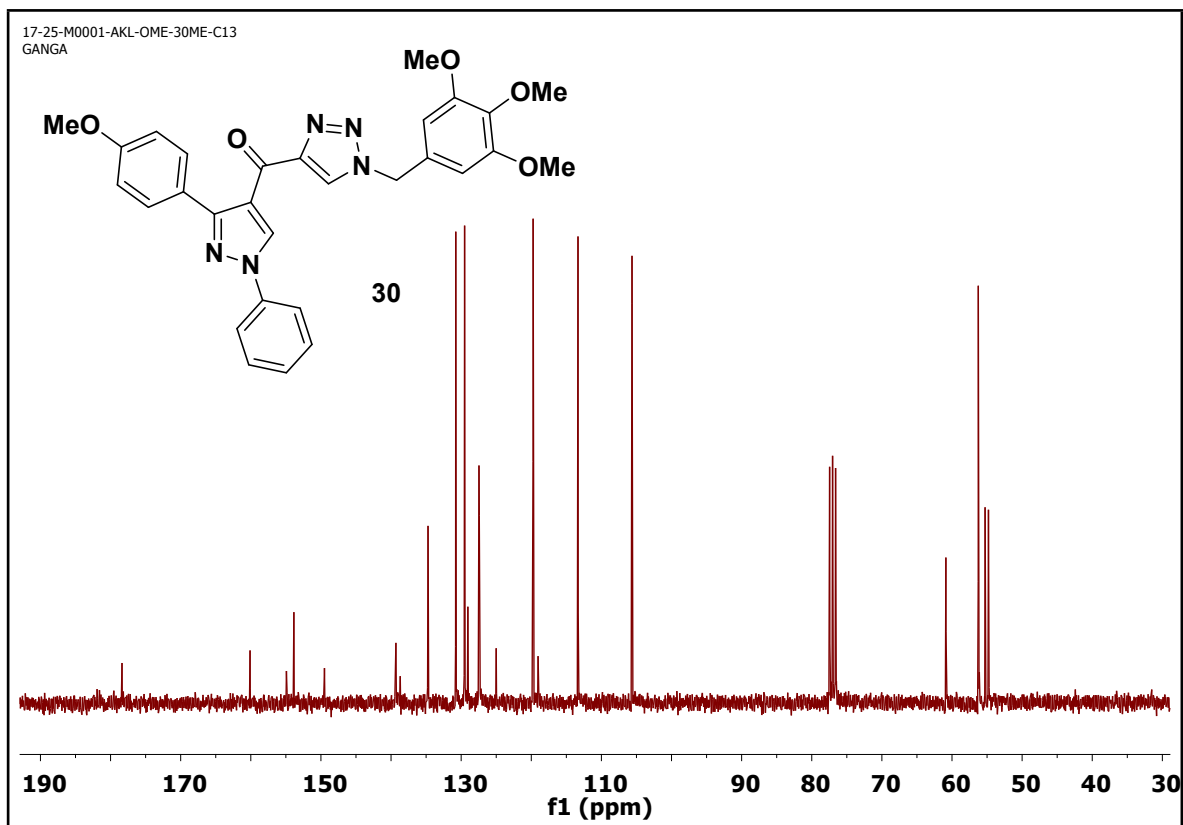


HRMS Spectra of compound 29

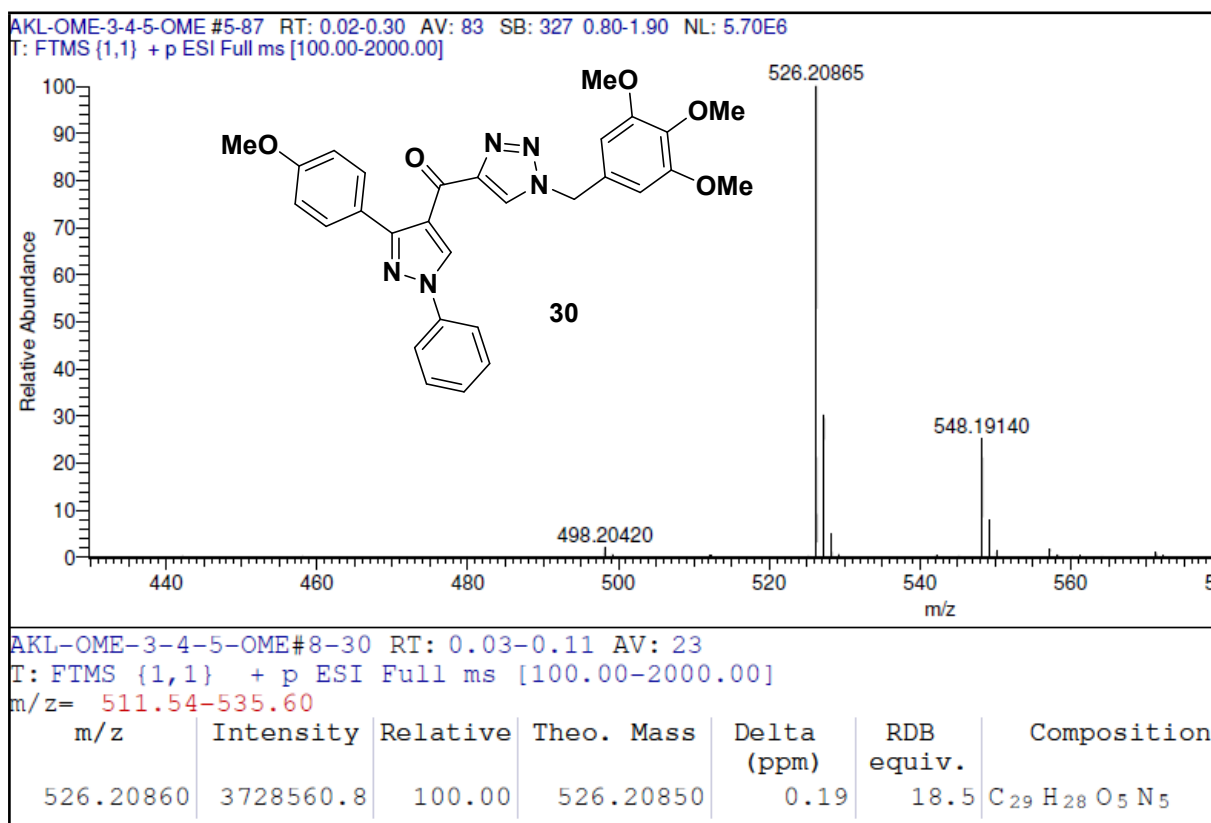


<sup>1</sup>H NMR spectra of compound 30

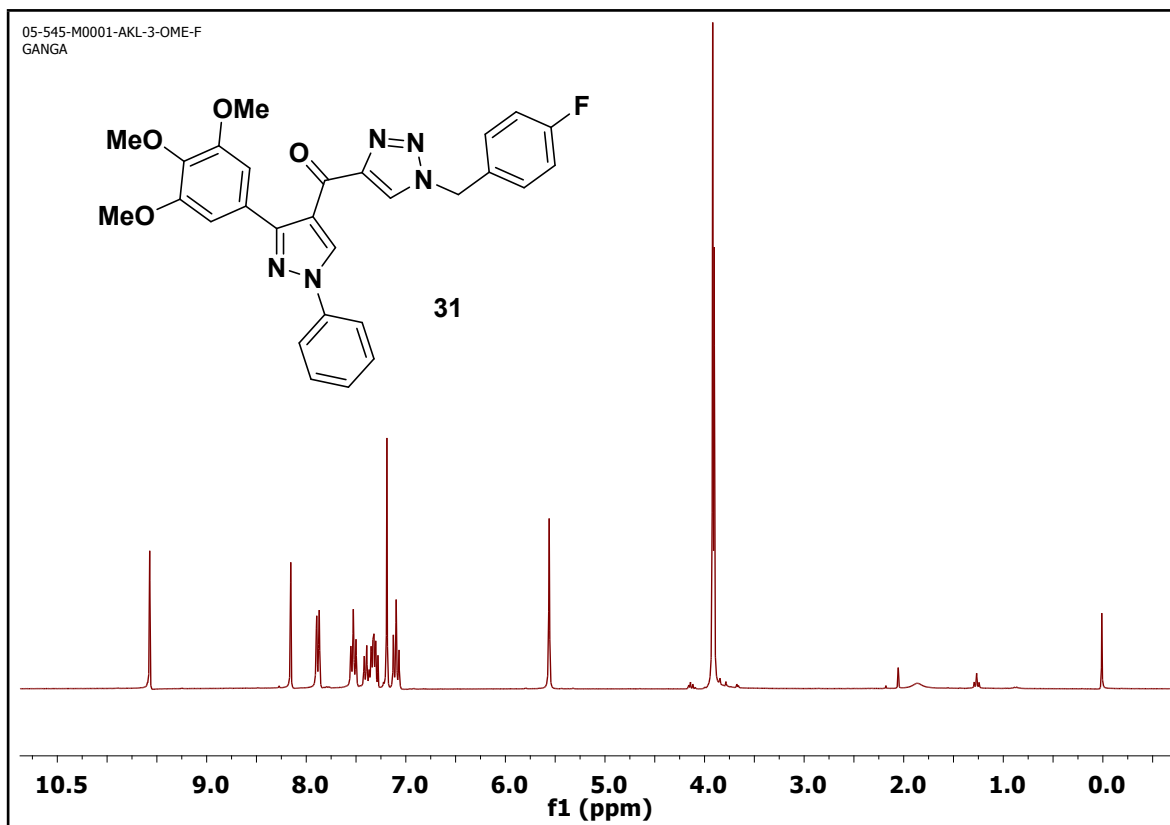




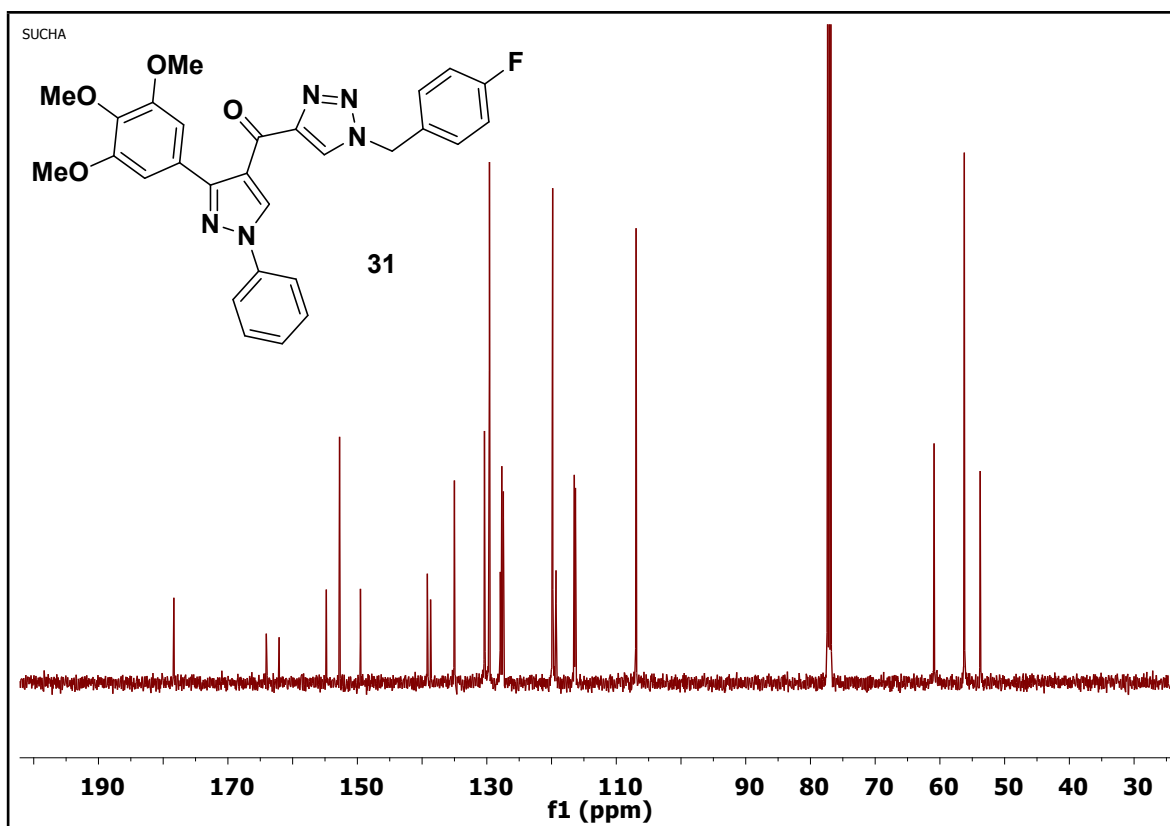
$^{13}\text{C}$  NMR spectra of compound **30**



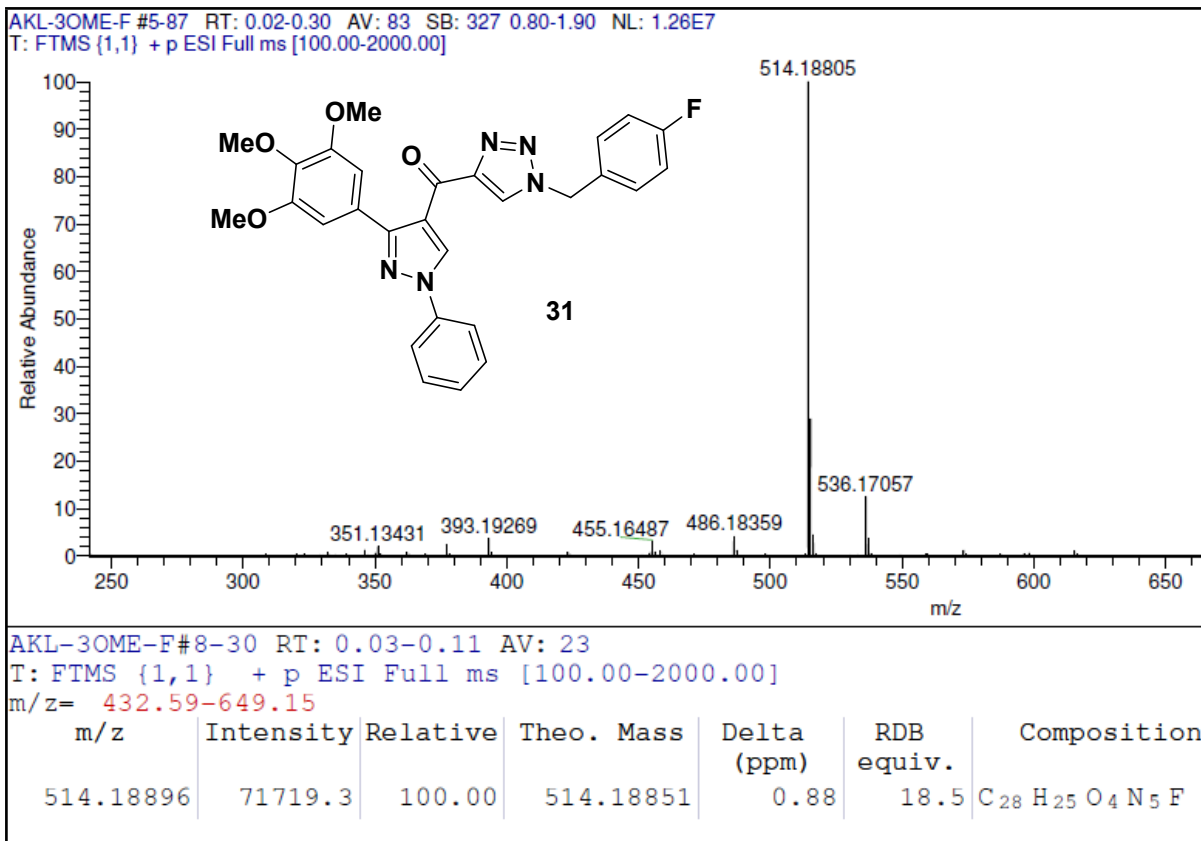
HRMS Spectra of compound **30**



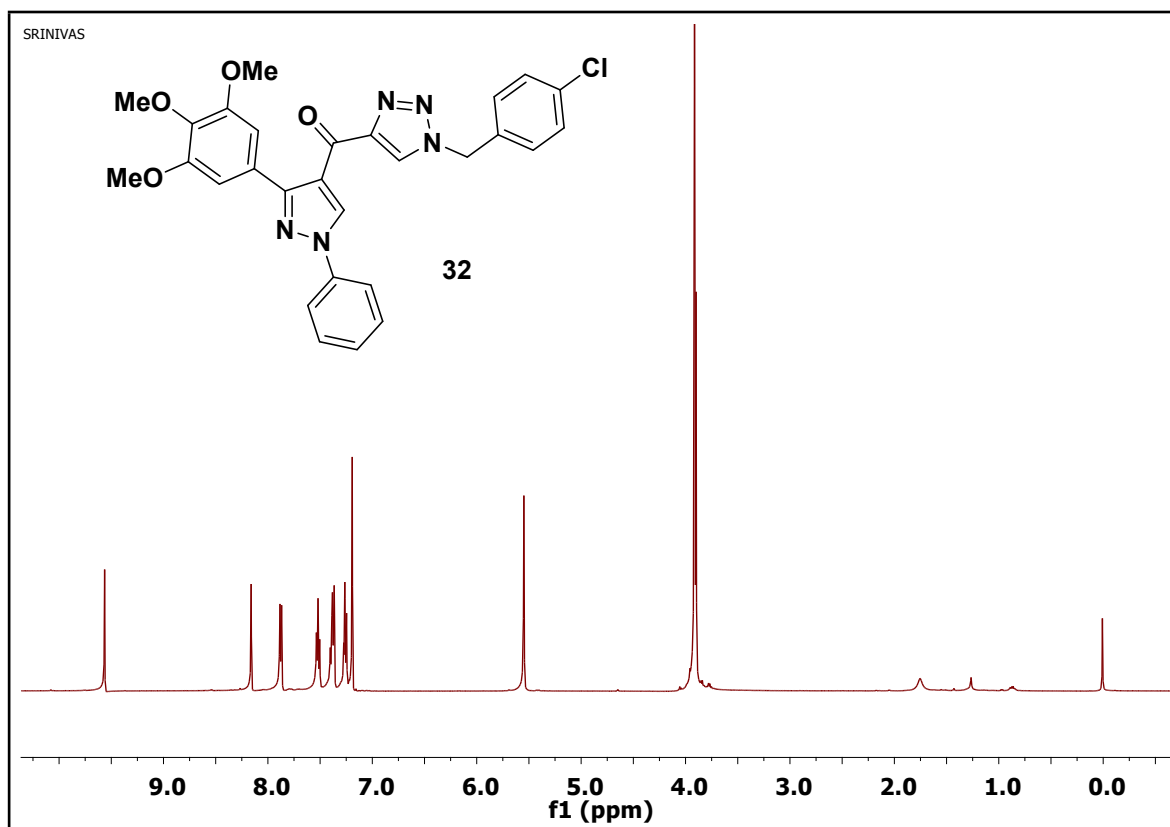
$^1\text{H}$  NMR spectra of compound 31



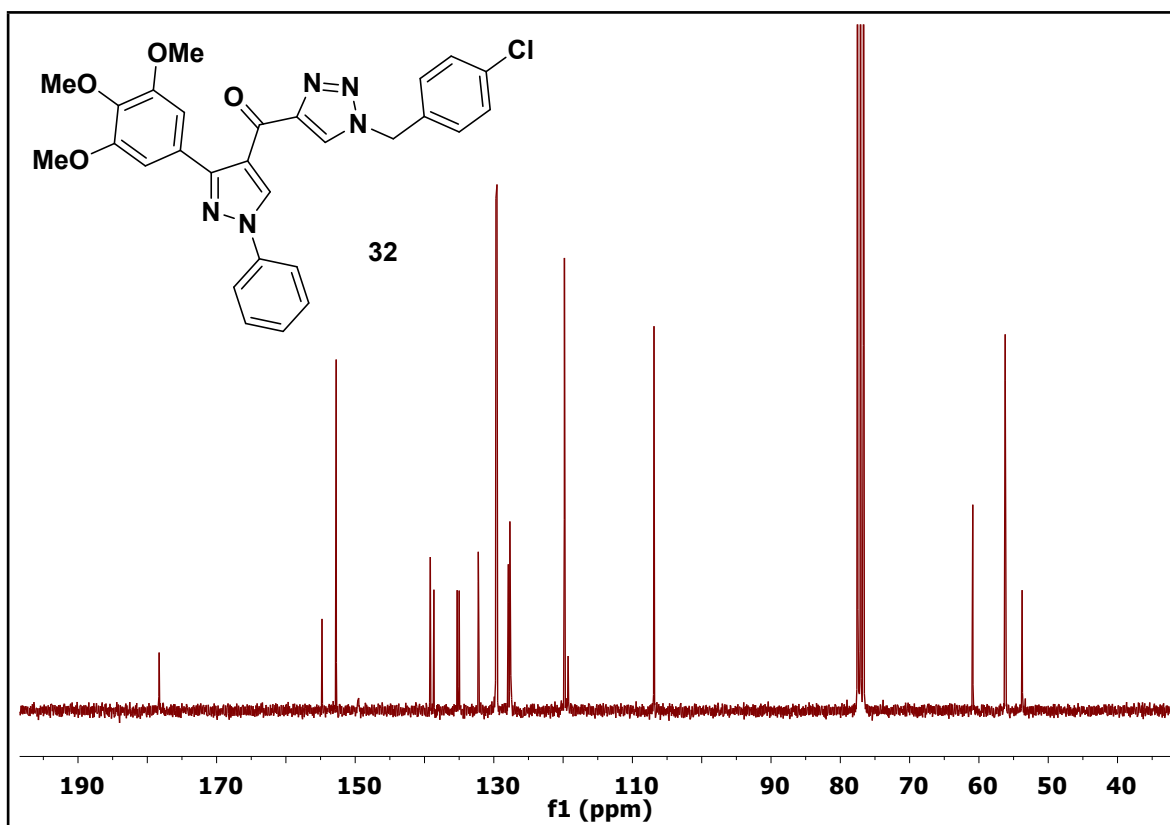
$^{13}\text{C}$  NMR spectra of compound 31



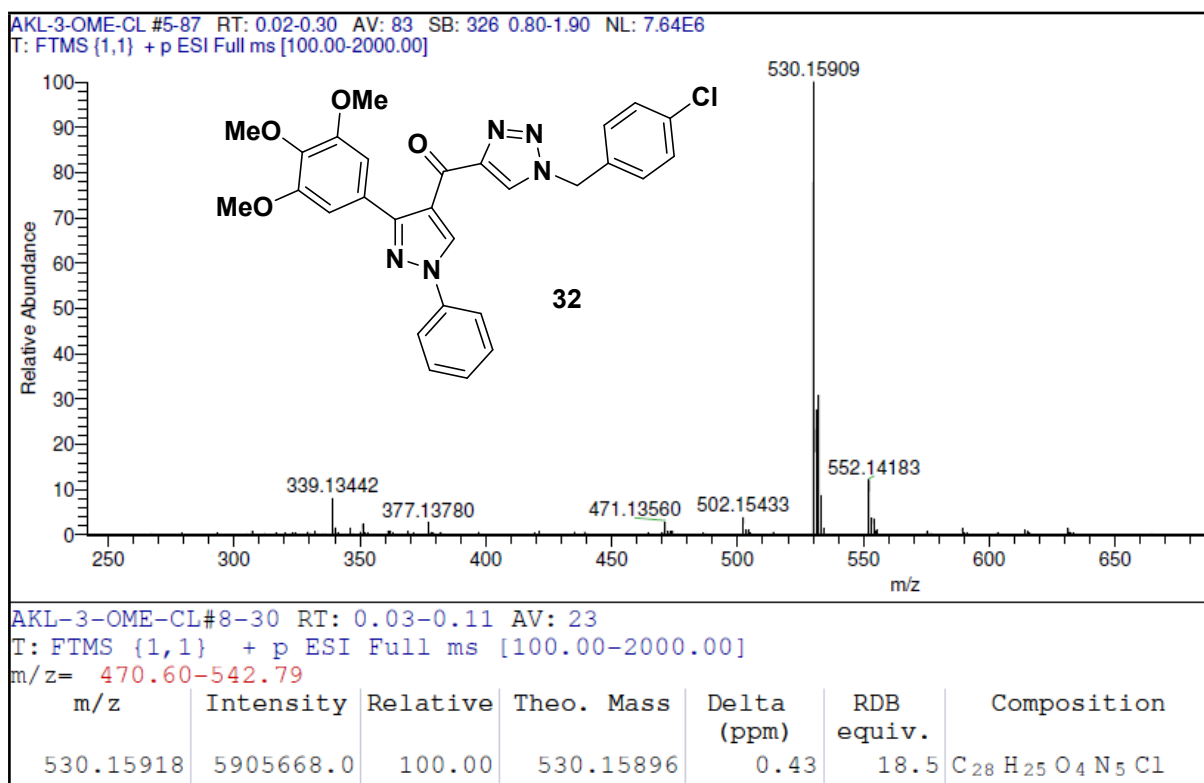
HRMS Spectra of compound 31



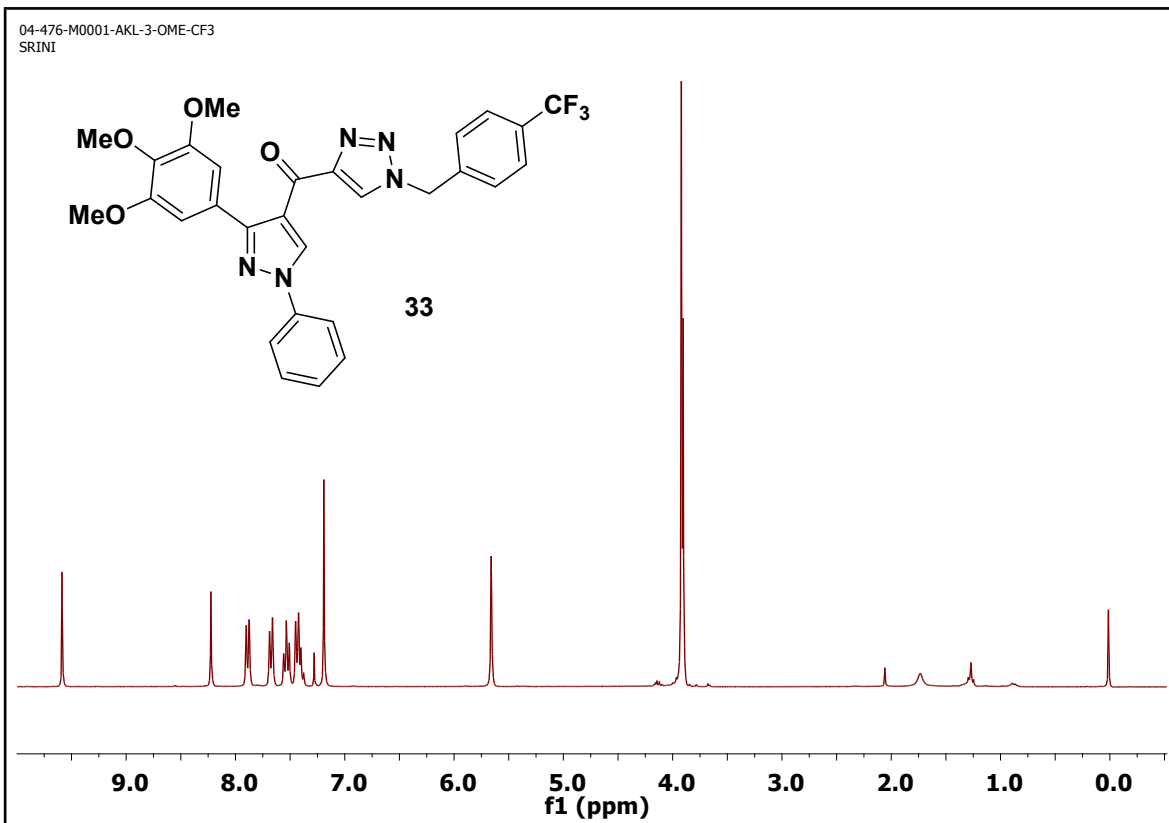
<sup>1</sup>H NMR spectra of compound 32



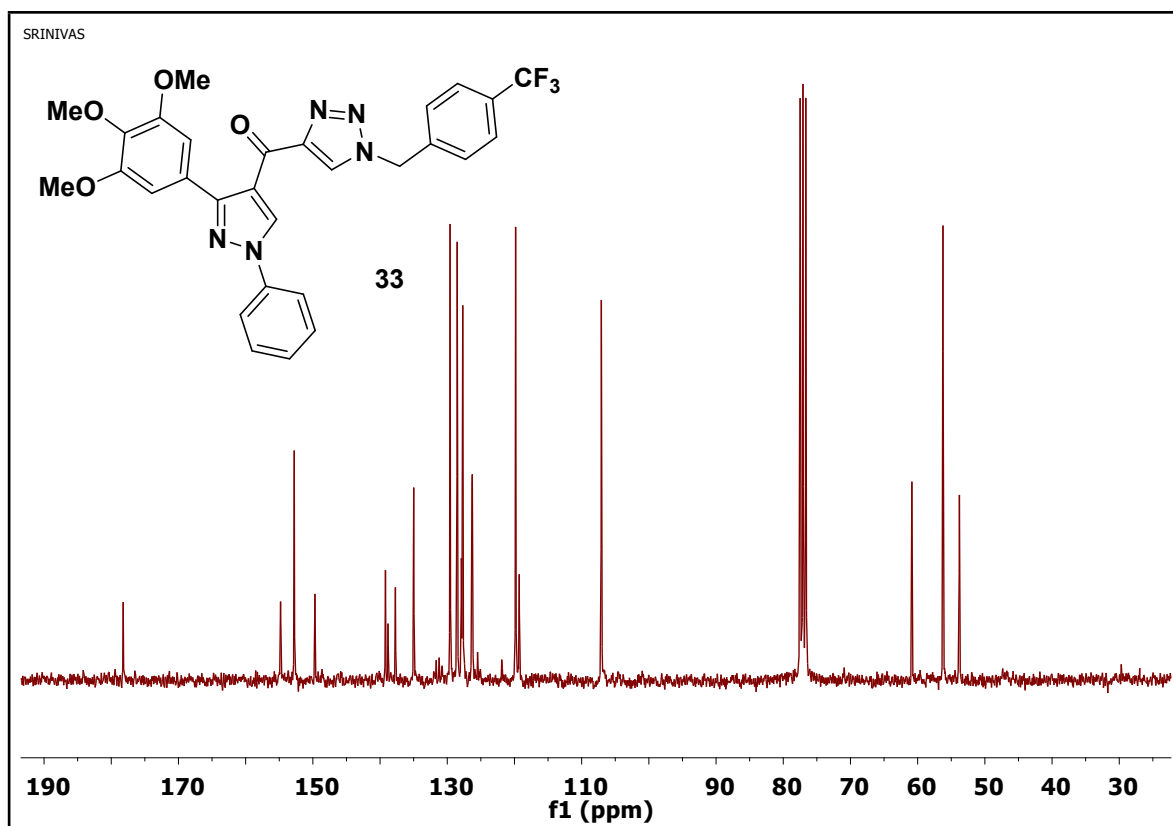
<sup>13</sup>C NMR spectra of compound 32



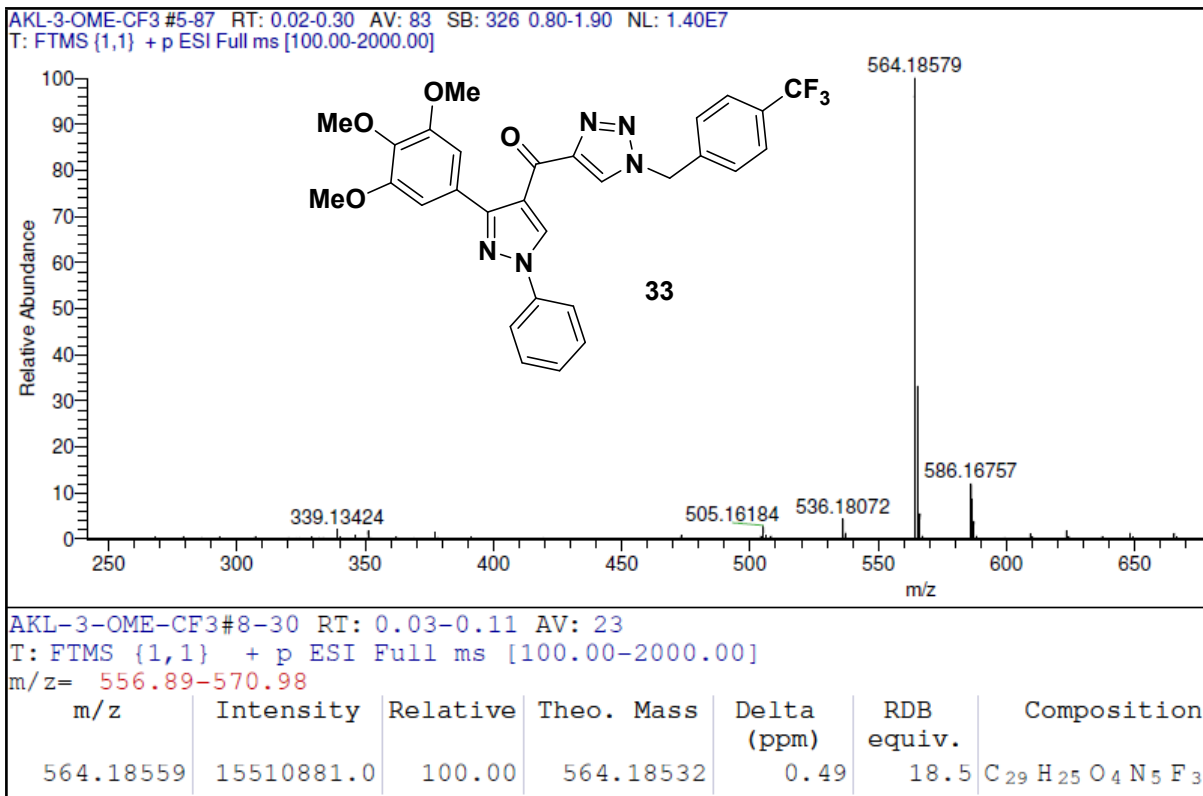
HRMS Spectra of compound 32



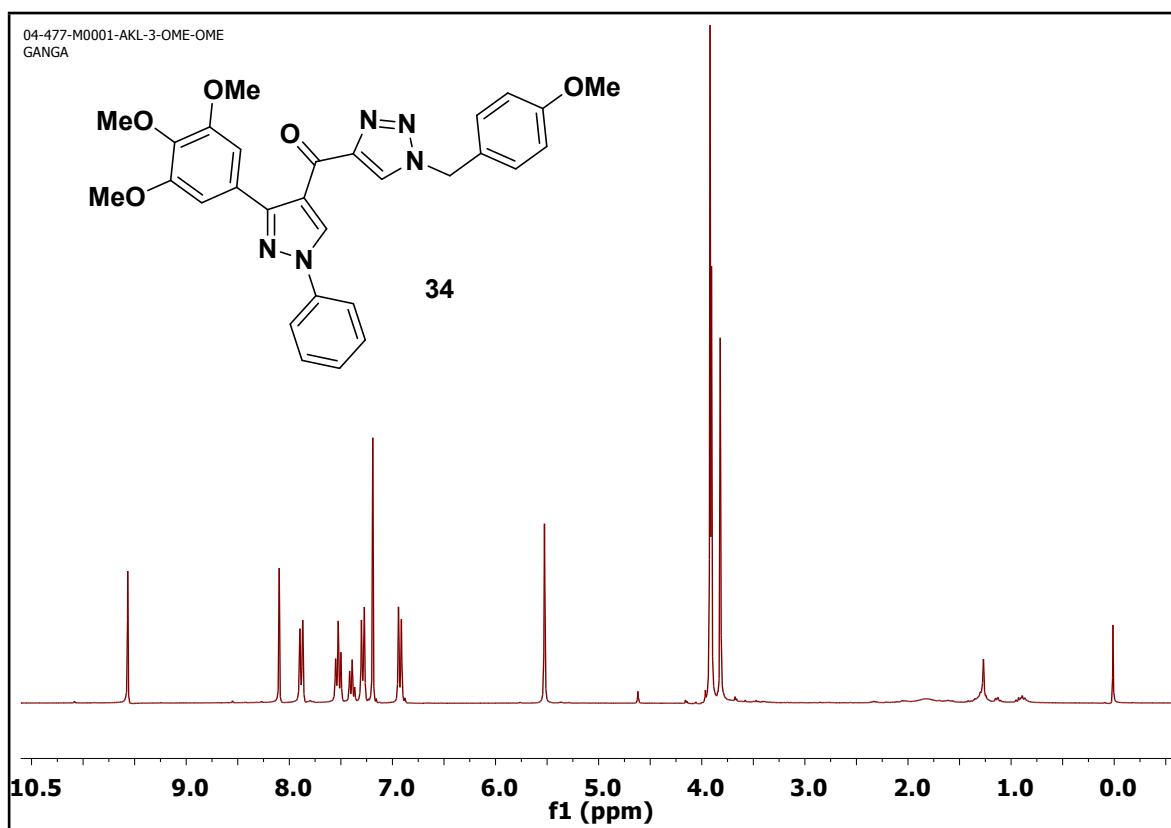
$^1\text{H}$  NMR spectra of compound 33



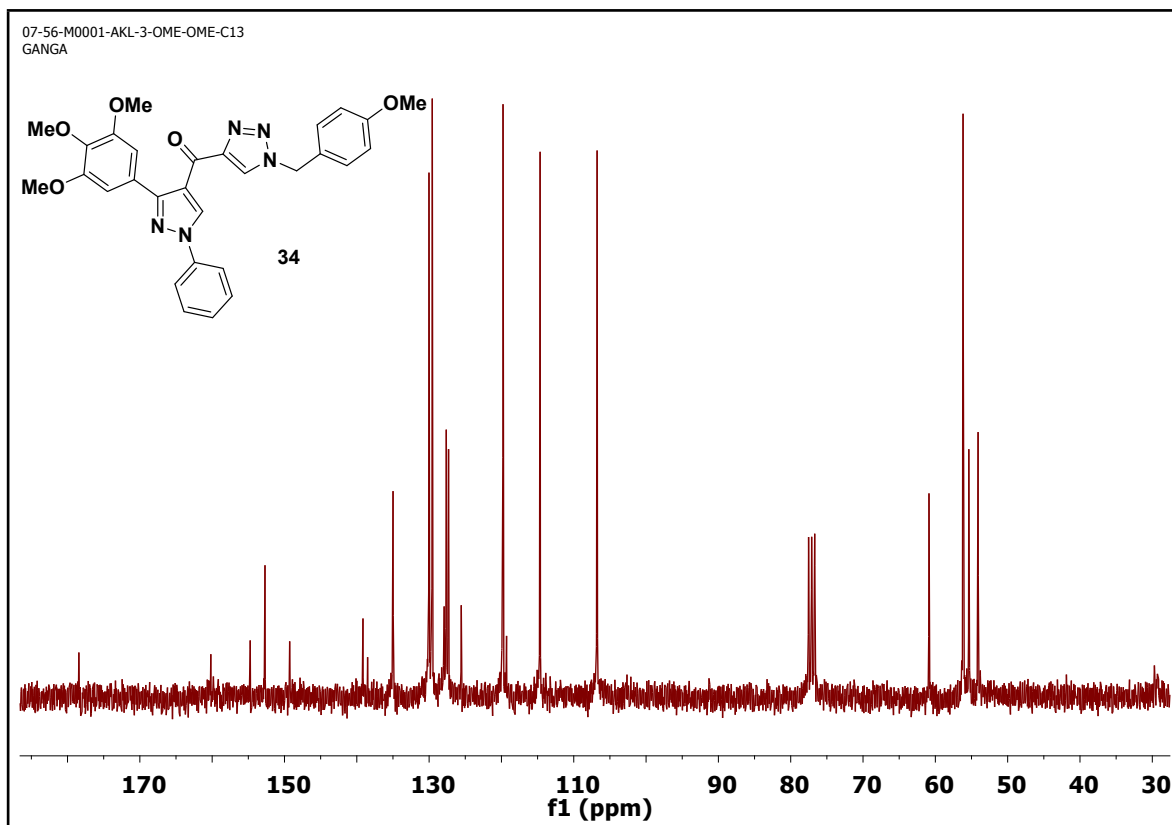
$^{13}\text{C}$  NMR spectra of compound 33



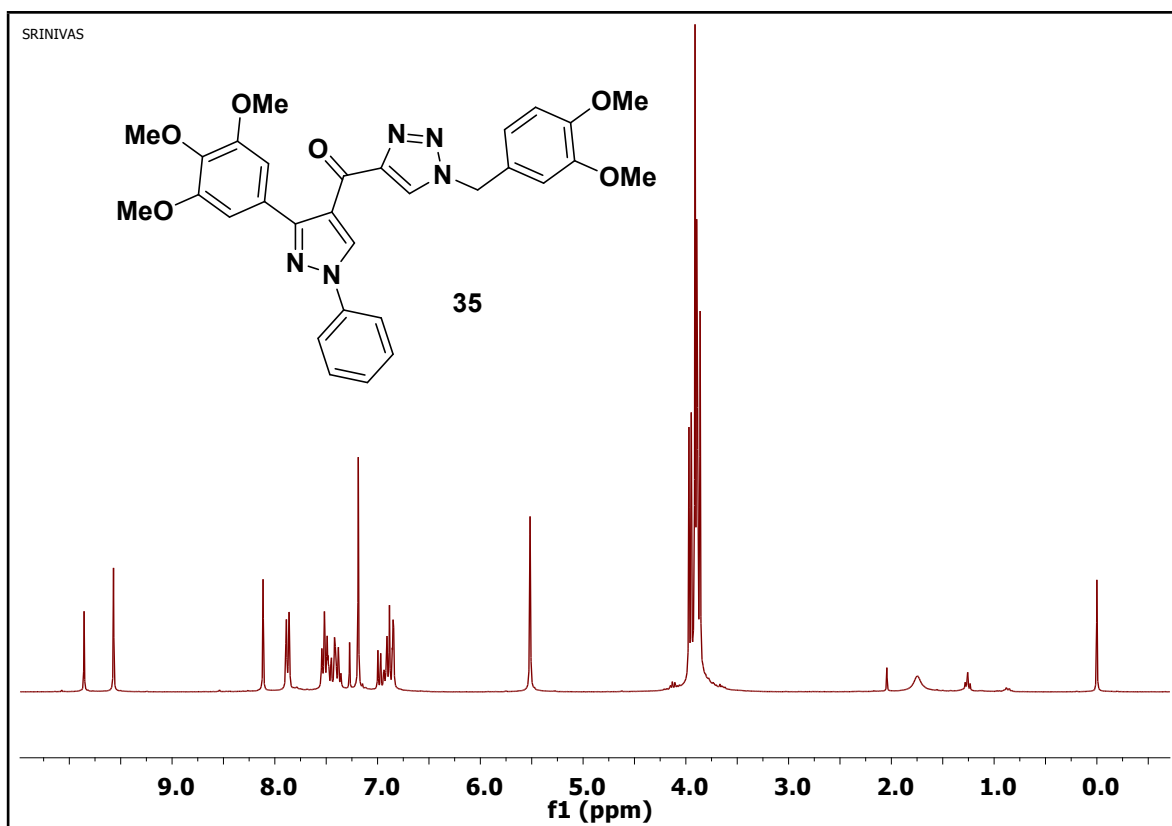
HRMS Spectra of compound 33



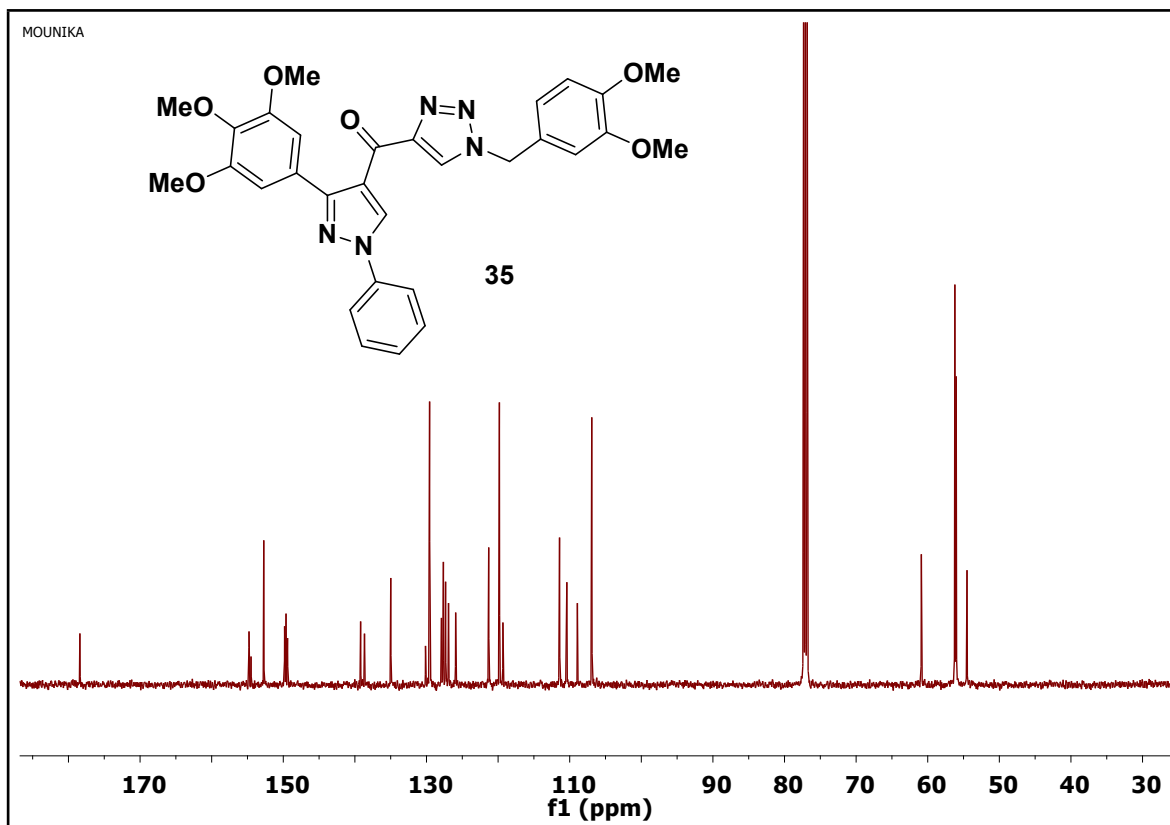
<sup>1</sup>H NMR spectra of compound 34



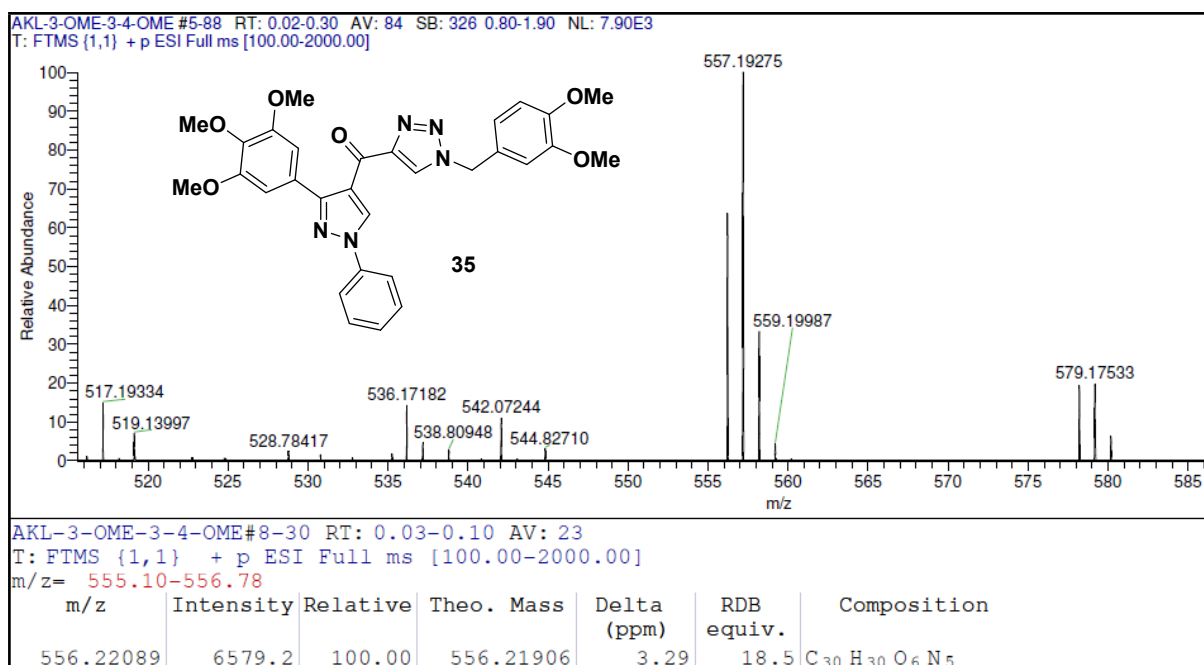
$^{13}\text{C}$  NMR spectra of compound 34



$^1\text{H}$  NMR spectra of compound 35

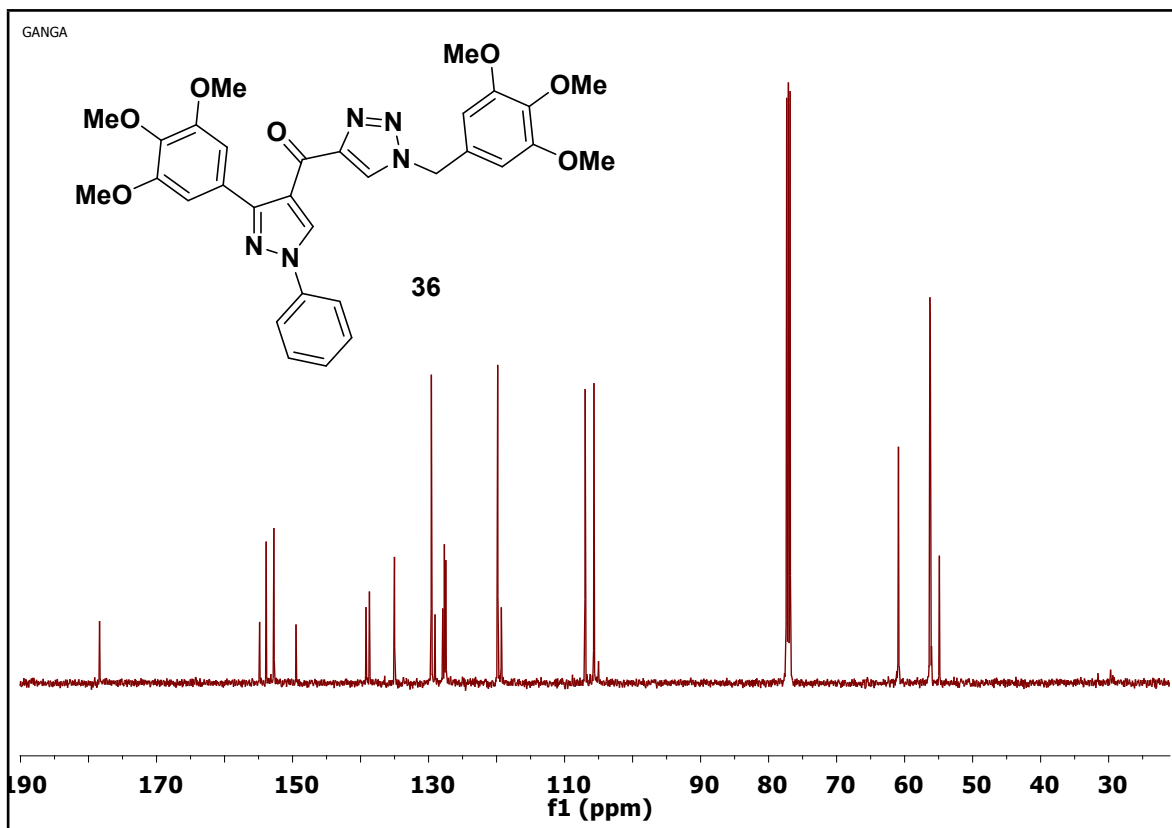


$^{13}\text{C}$  NMR spectra of compound **35**



HRMS Spectra of compound **35**





$^{13}\text{C}$  NMR spectra of compound 36

F

