

## Supporting information

### Rational Design and Synthesis of Novel Phenyltriazole Derivatives Targeting MRSA Cell Wall Biosynthesis

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Almaghrabi<sup>3</sup>, Marwa Alsulaimany<sup>3</sup>, Basmah Almohaywi<sup>4</sup>, Read Alghamdi<sup>3</sup>, Samar F. Miski<sup>5</sup>,  
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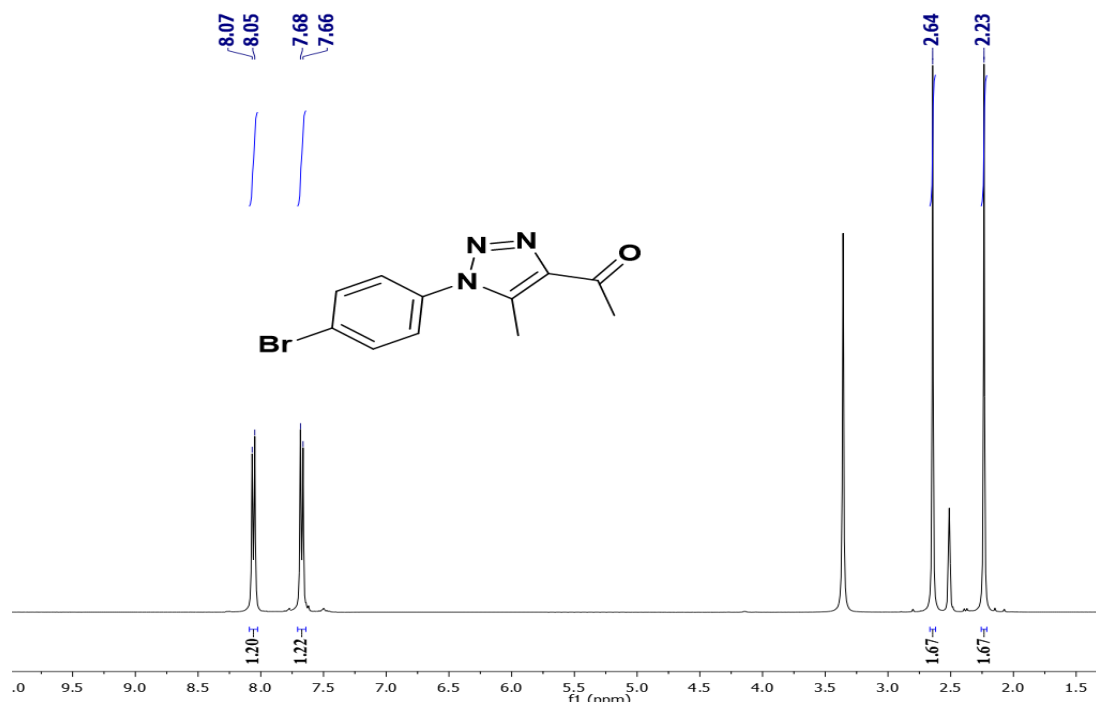
*E-mail address:* [m.elsebaei@azhar.edu.eg](mailto:m.elsebaei@azhar.edu.eg) , [heahmad@azhar.edu.eg](mailto:heahmad@azhar.edu.eg)

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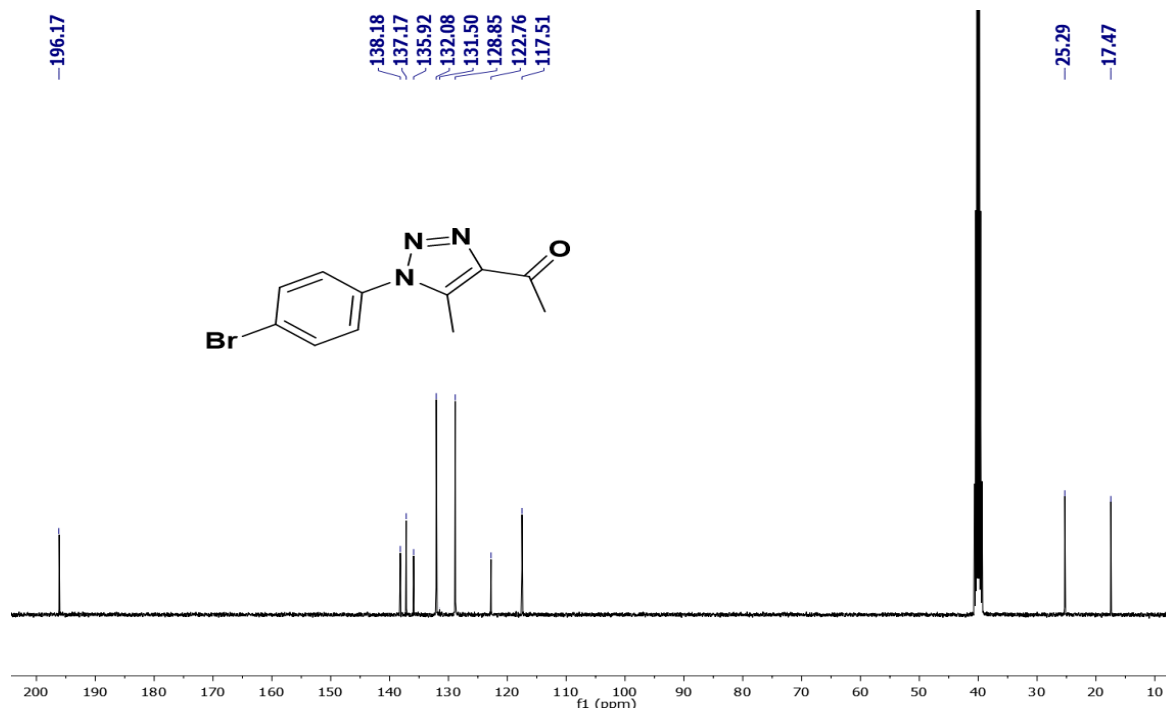
## **Table of Contents**

NMR and HPLC spectra

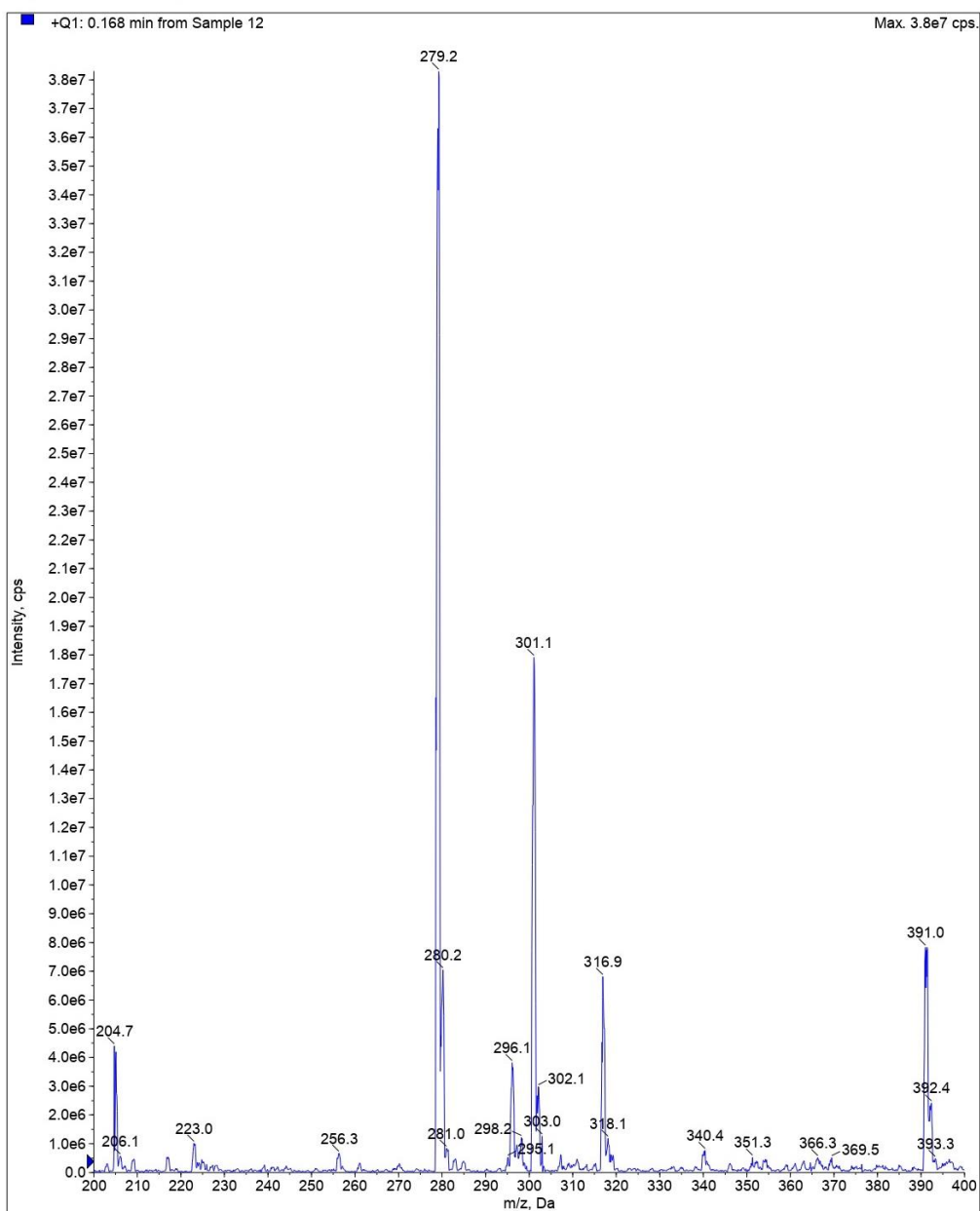
S3-S42



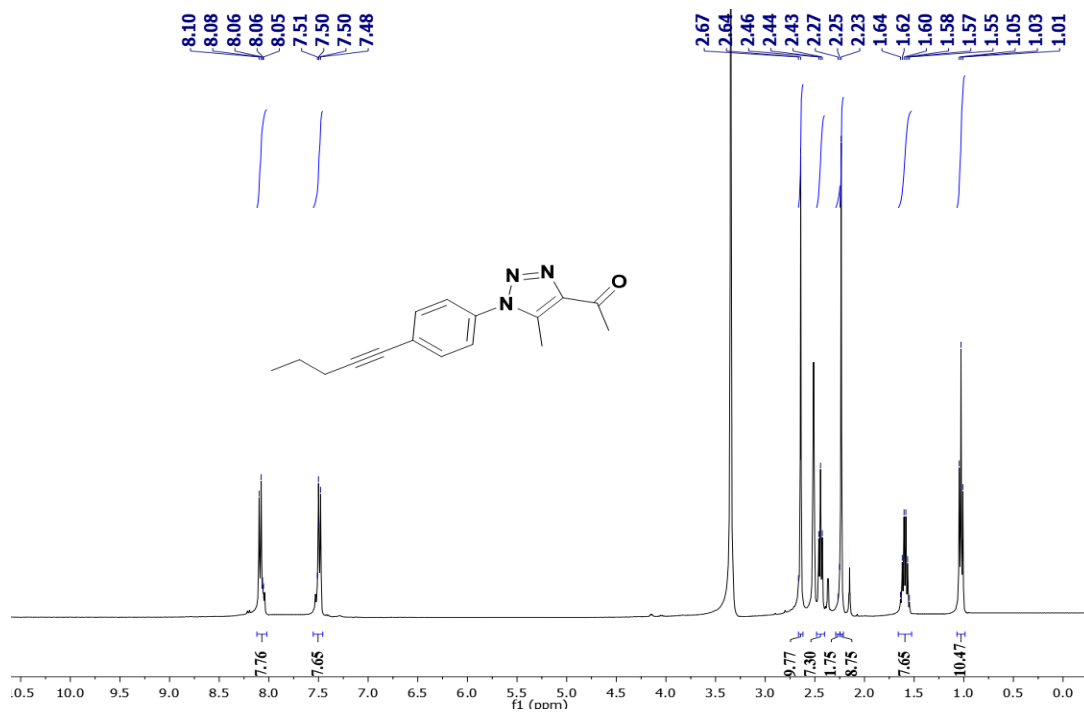
<sup>1</sup>H NMR of compound 4



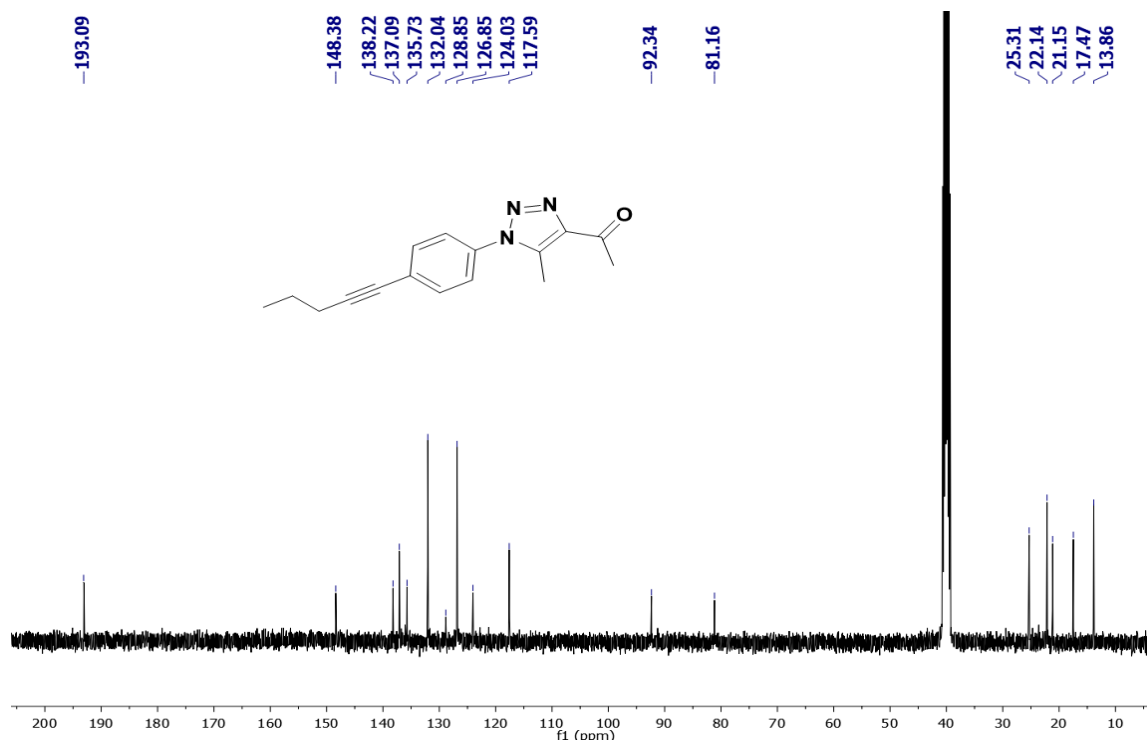
<sup>13</sup>C NMR of compound 4



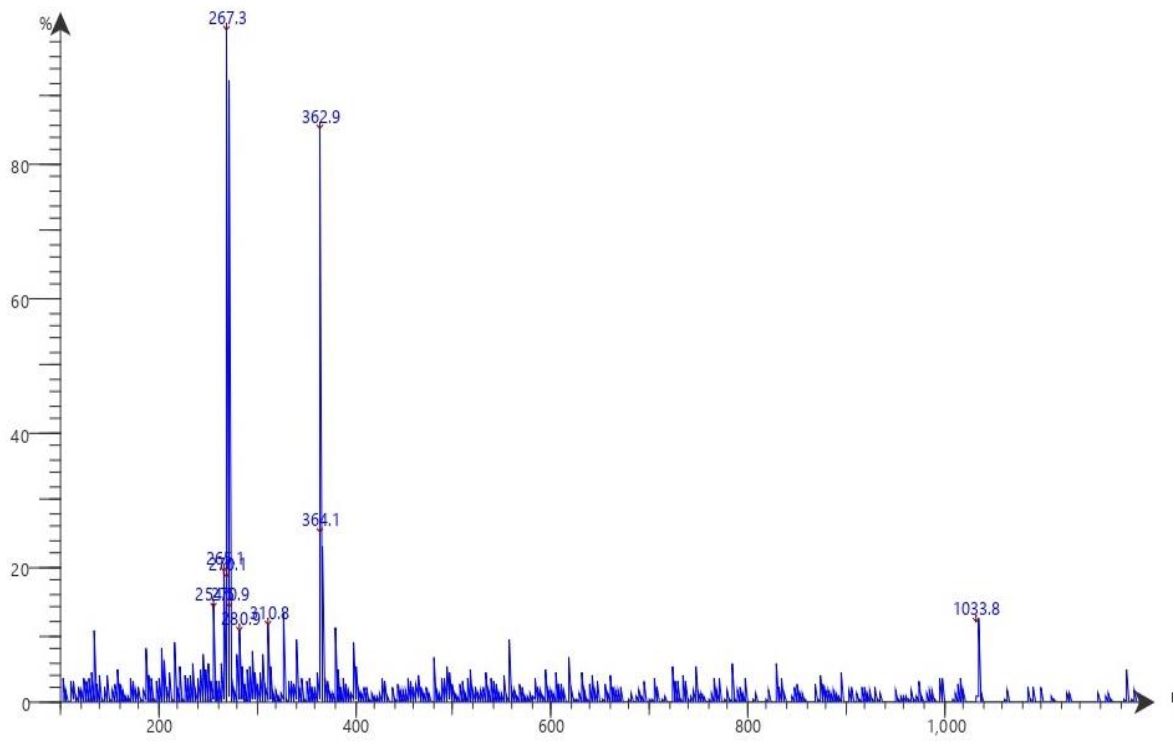
**Mass of Compound 4**



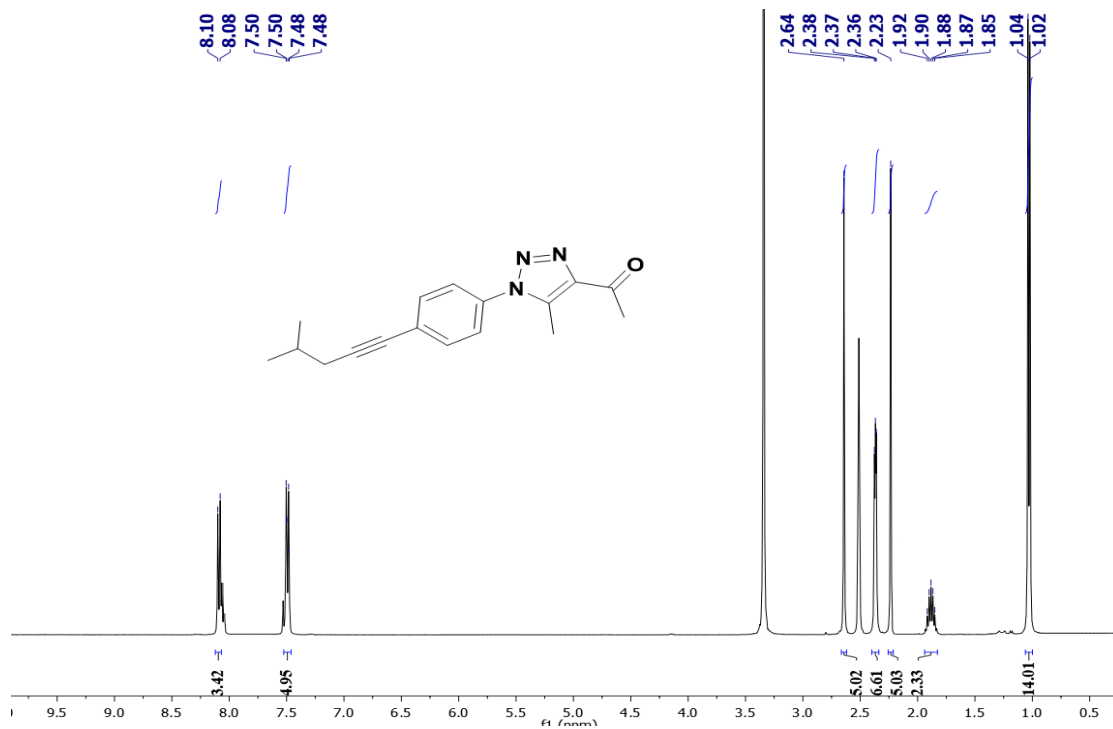
**<sup>1</sup>H NMR of compound 5**



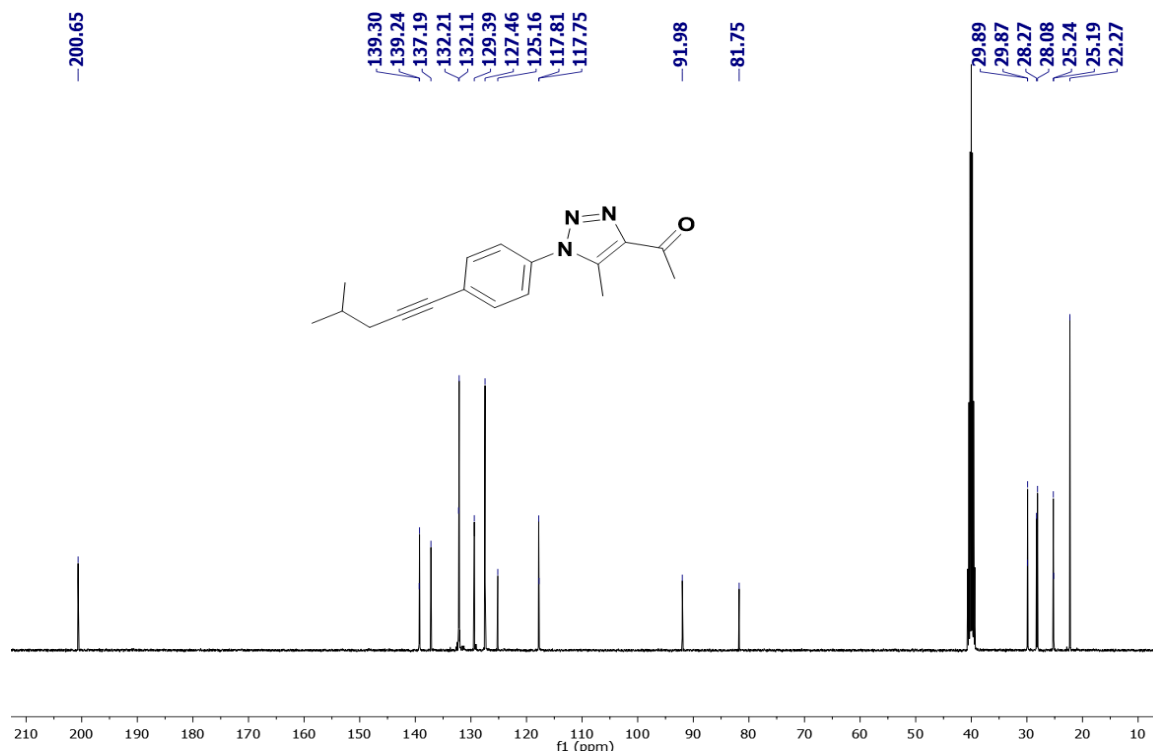
**<sup>13</sup>C NMR of compound 5**



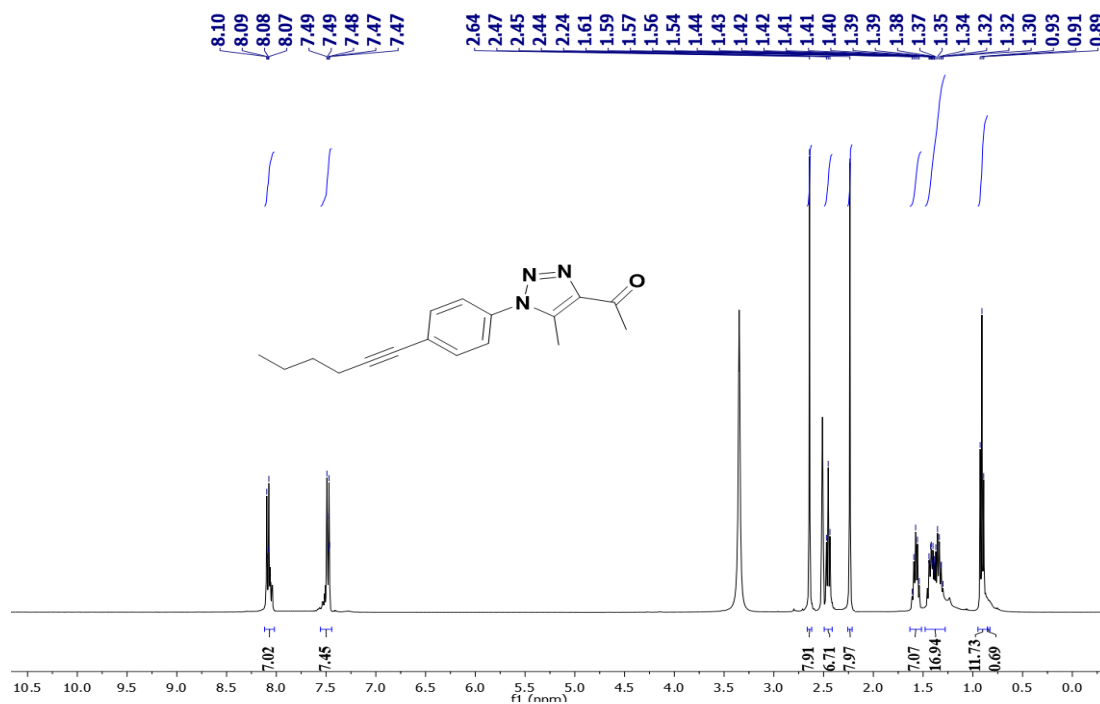
*Mass of compound 5*



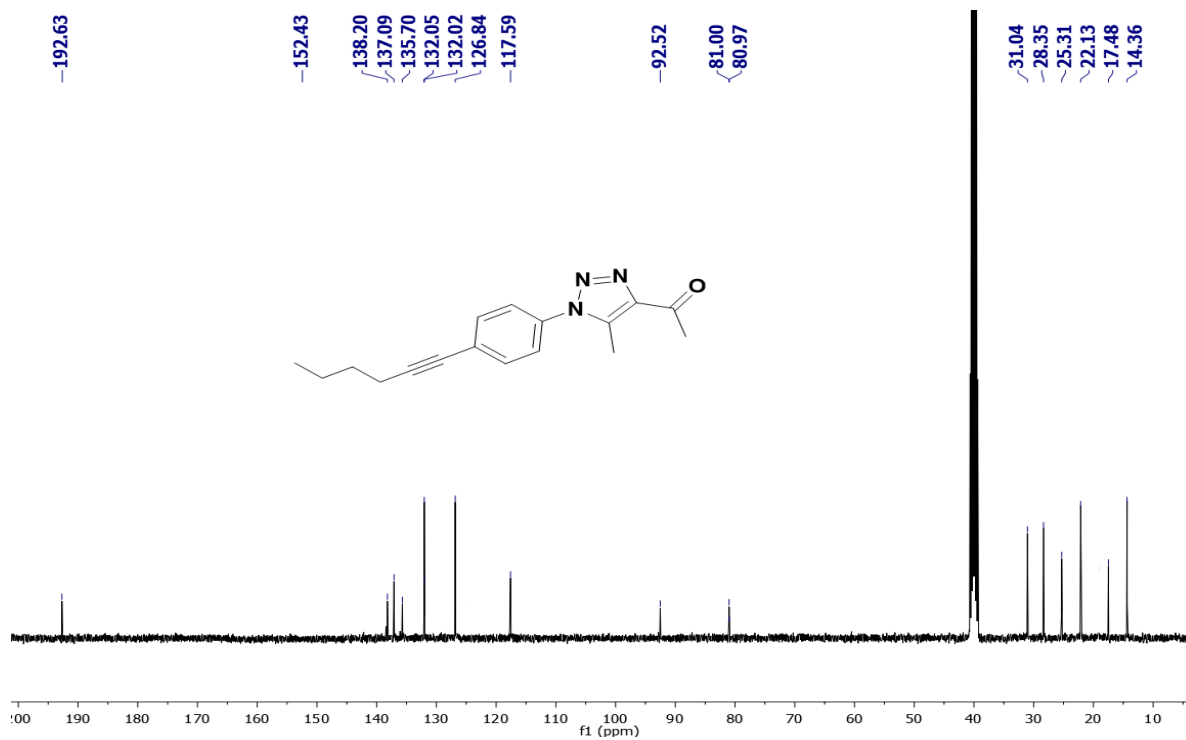
<sup>1</sup>H NMR of compound 6



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

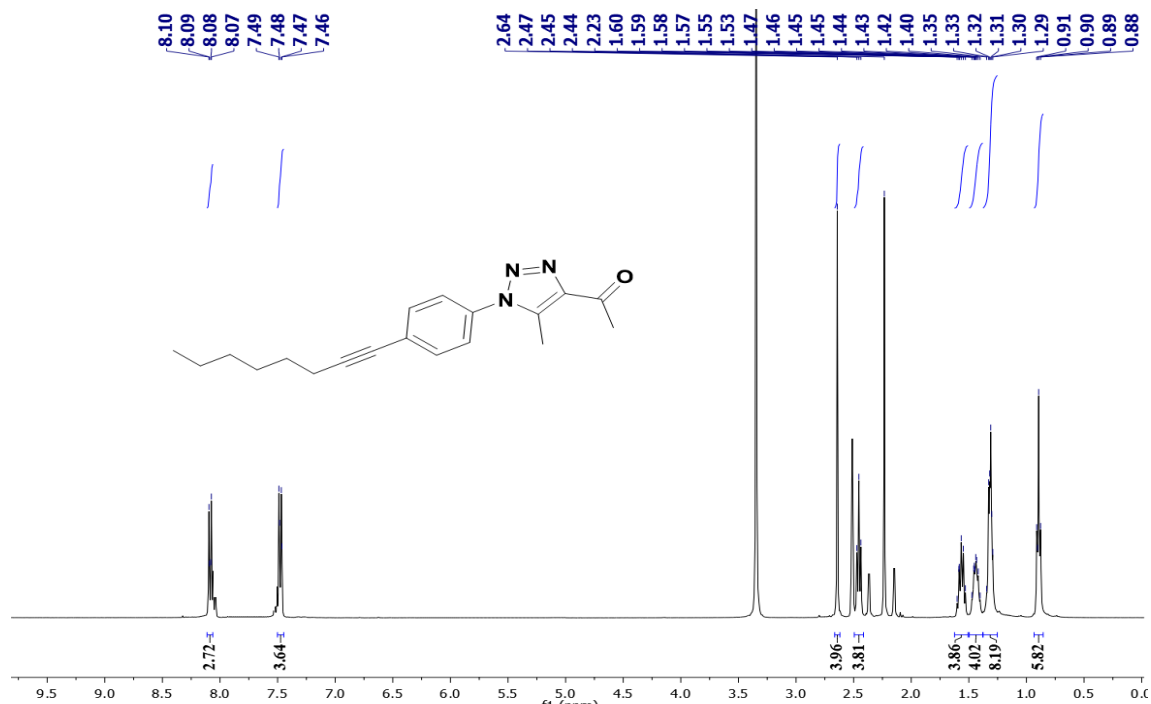


<sup>1</sup>H NMR of compound 7

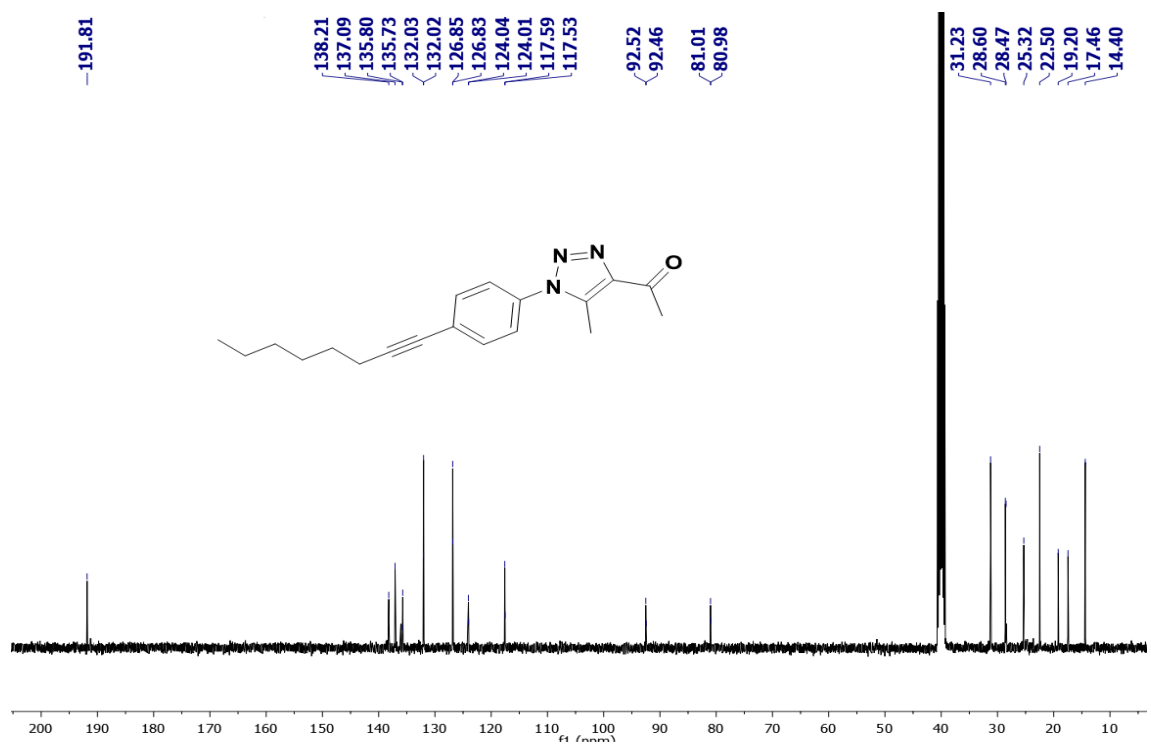


<sup>13</sup>C NMR of compound 7

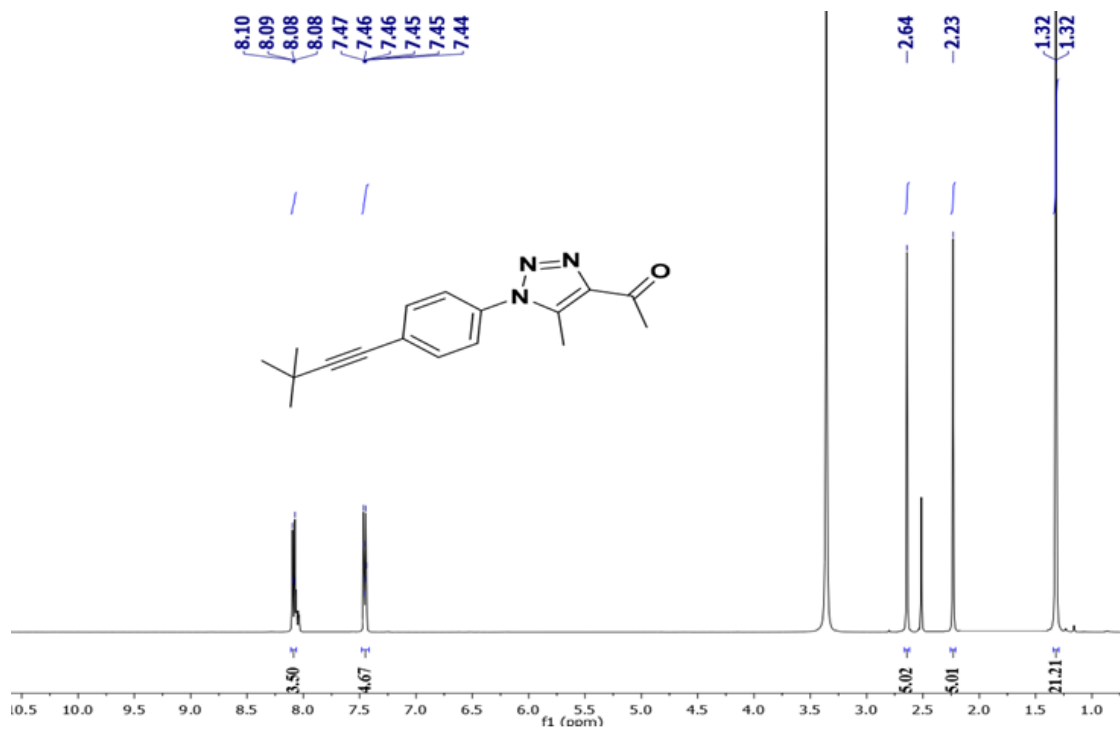




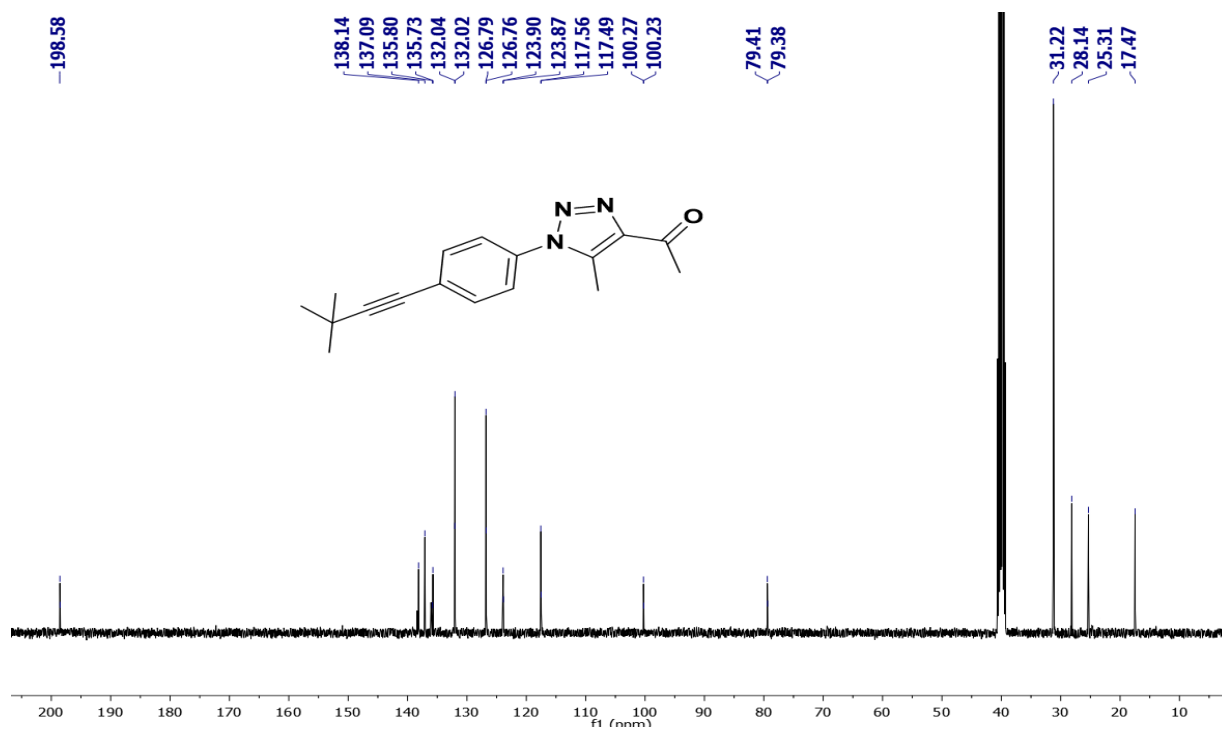
<sup>1</sup>H NMR of compound 8



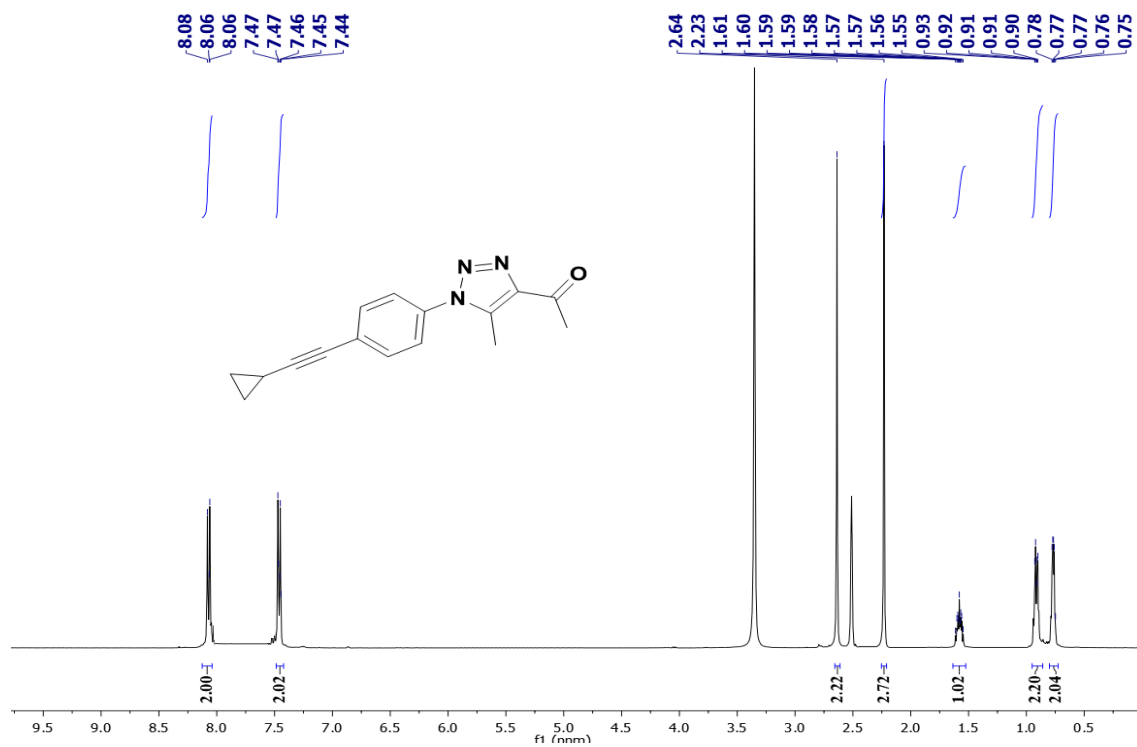
<sup>13</sup>C NMR of compound 8



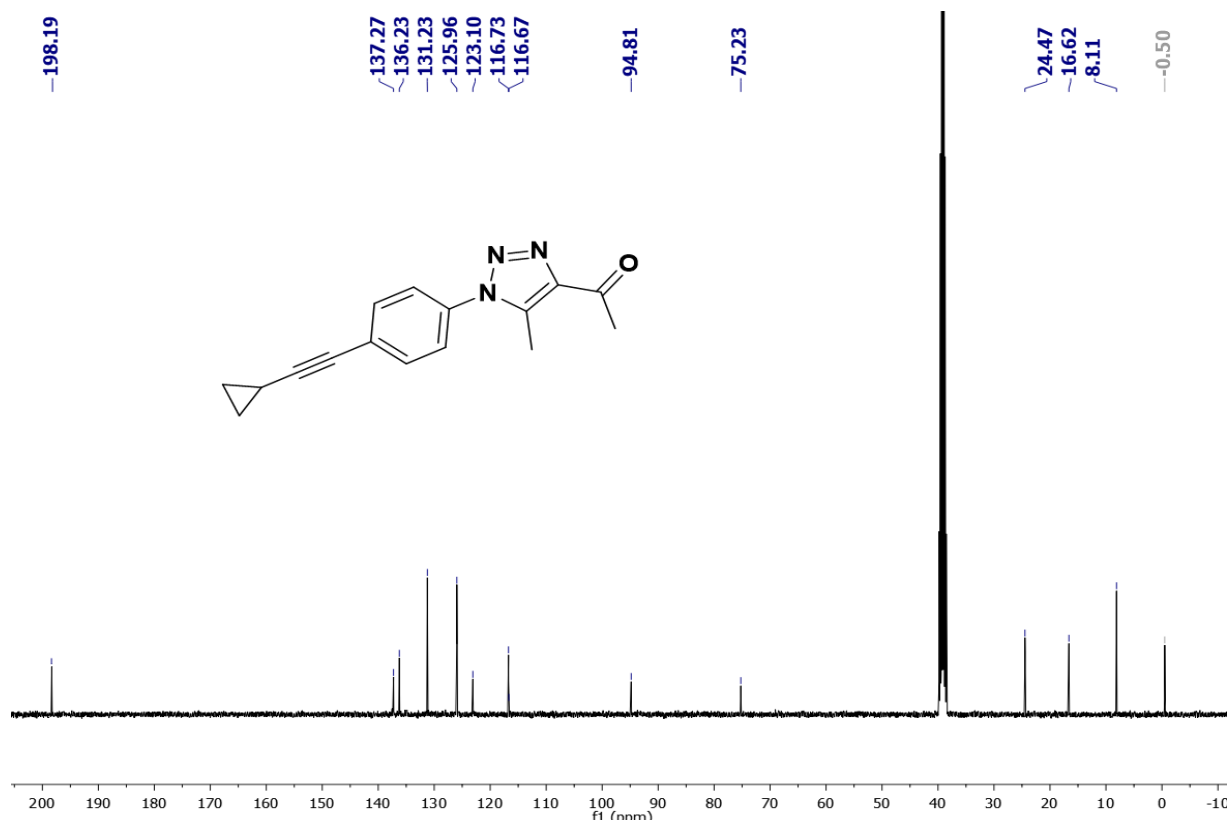
<sup>1</sup>H NMR of compound 9



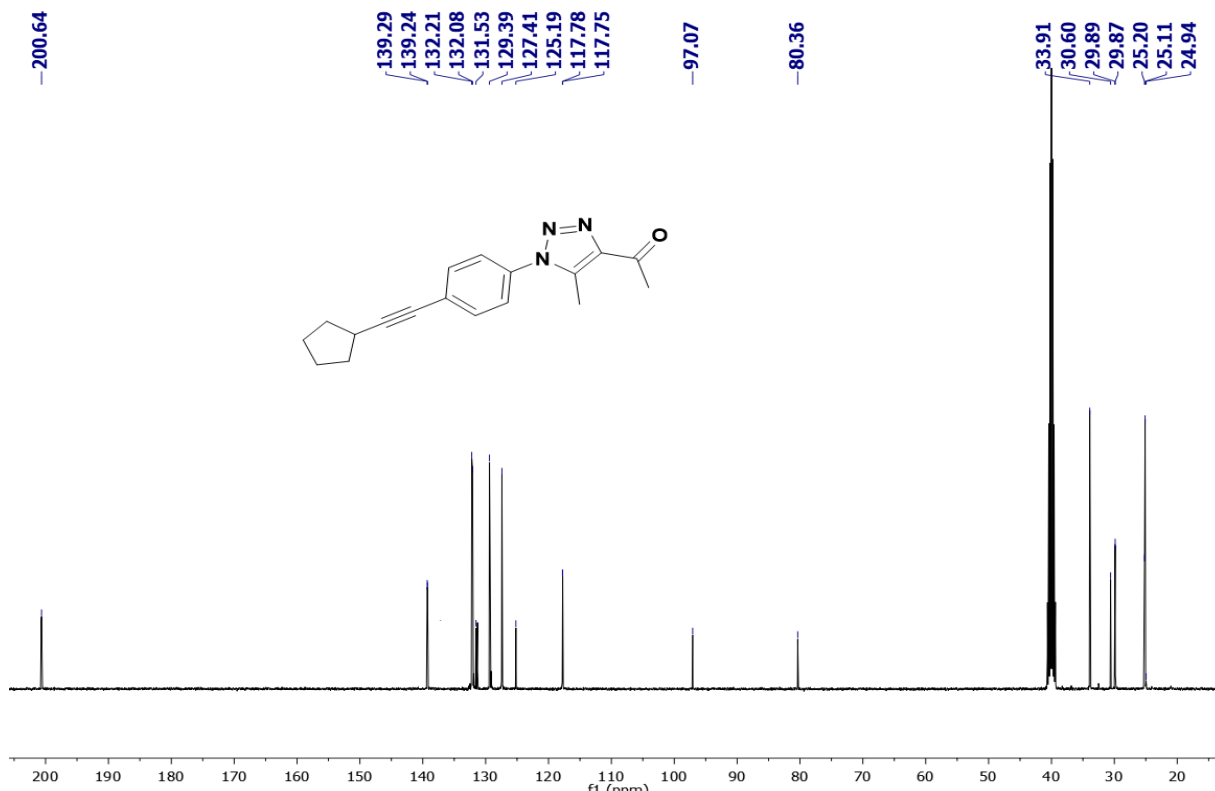
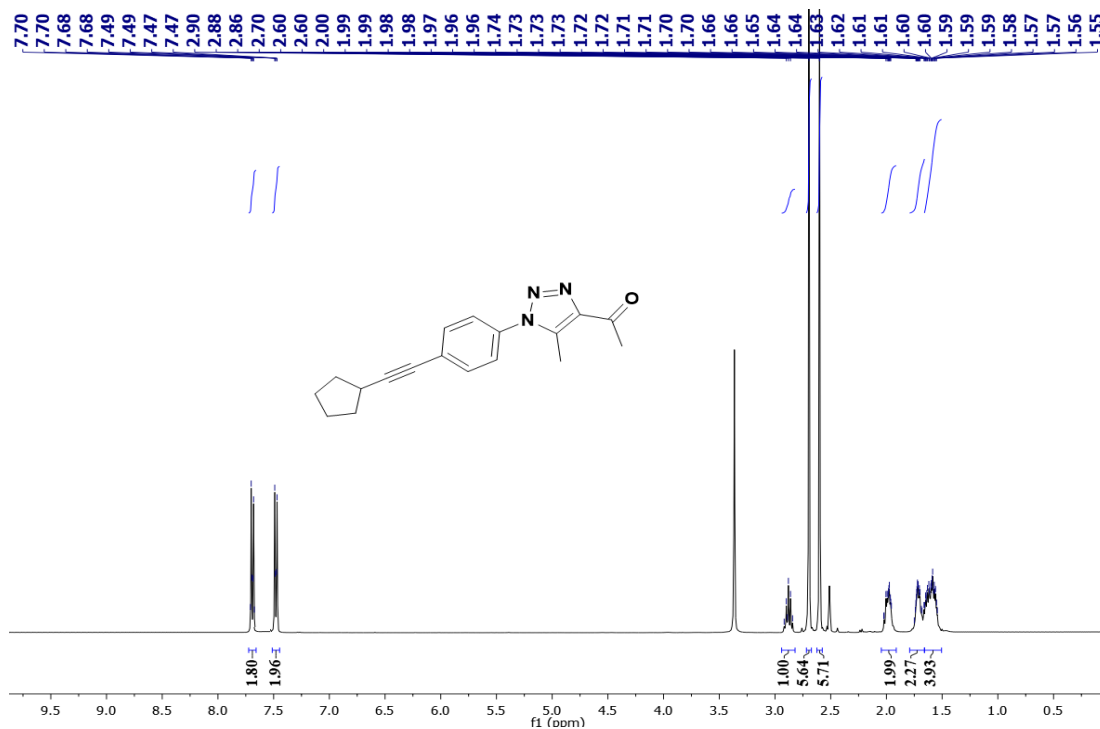
<sup>13</sup>C NMR of compound 9

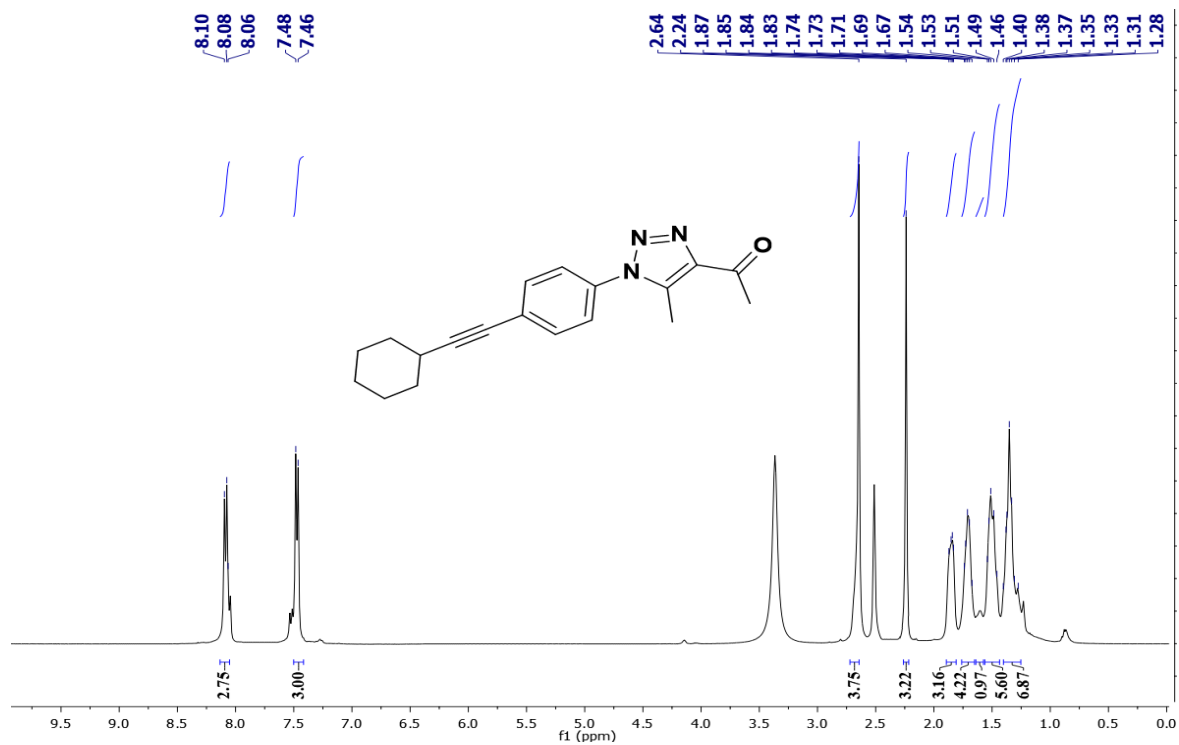


<sup>1</sup>H NMR of compound 10

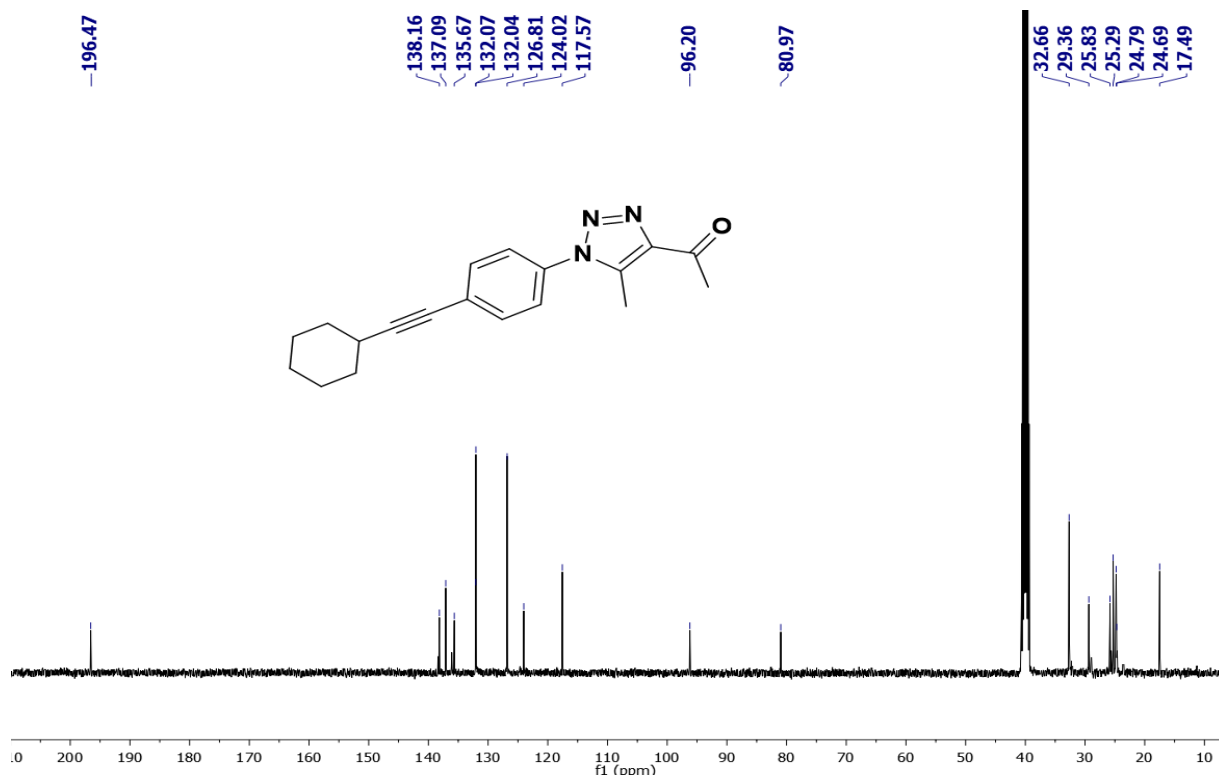


<sup>13</sup>C NMR of compound 10

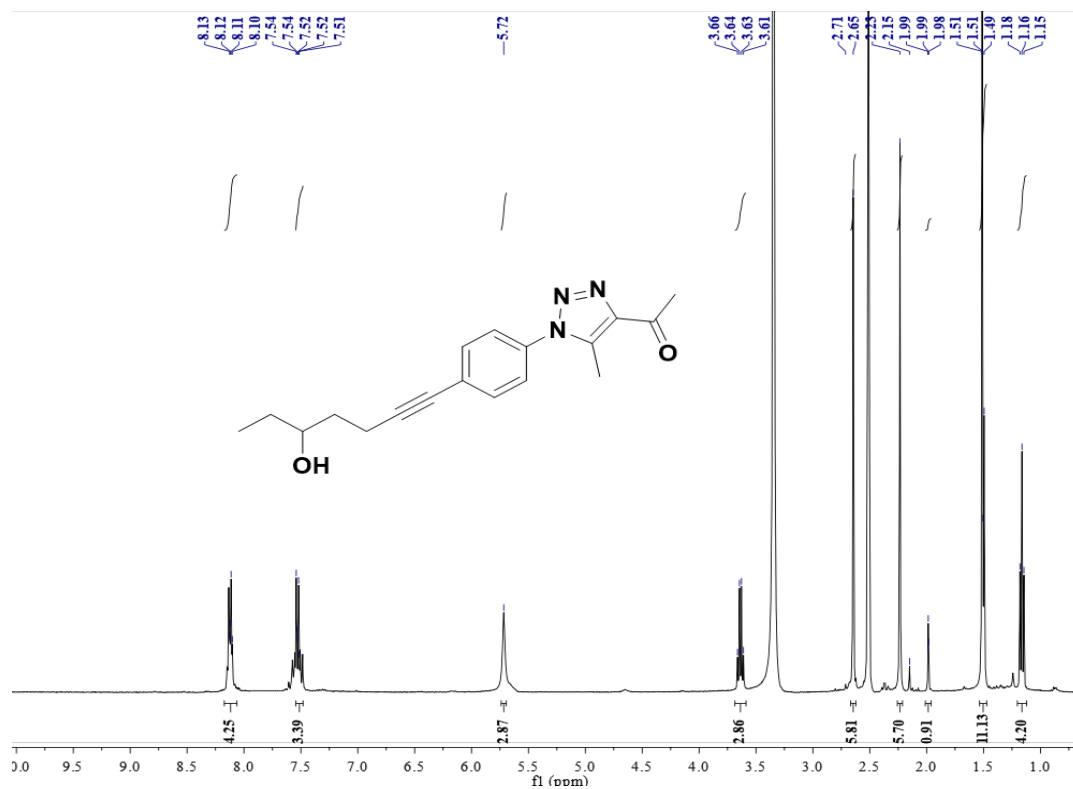




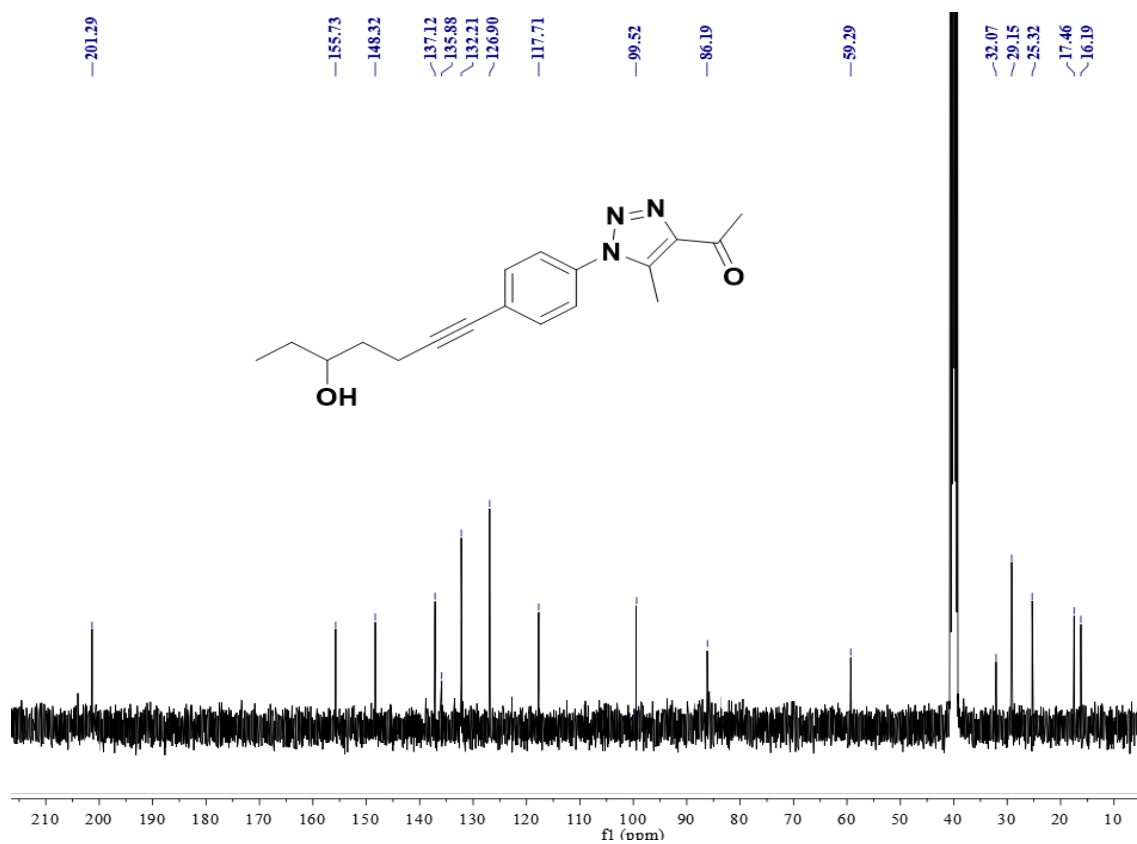
<sup>1</sup>H NMR of compound 12



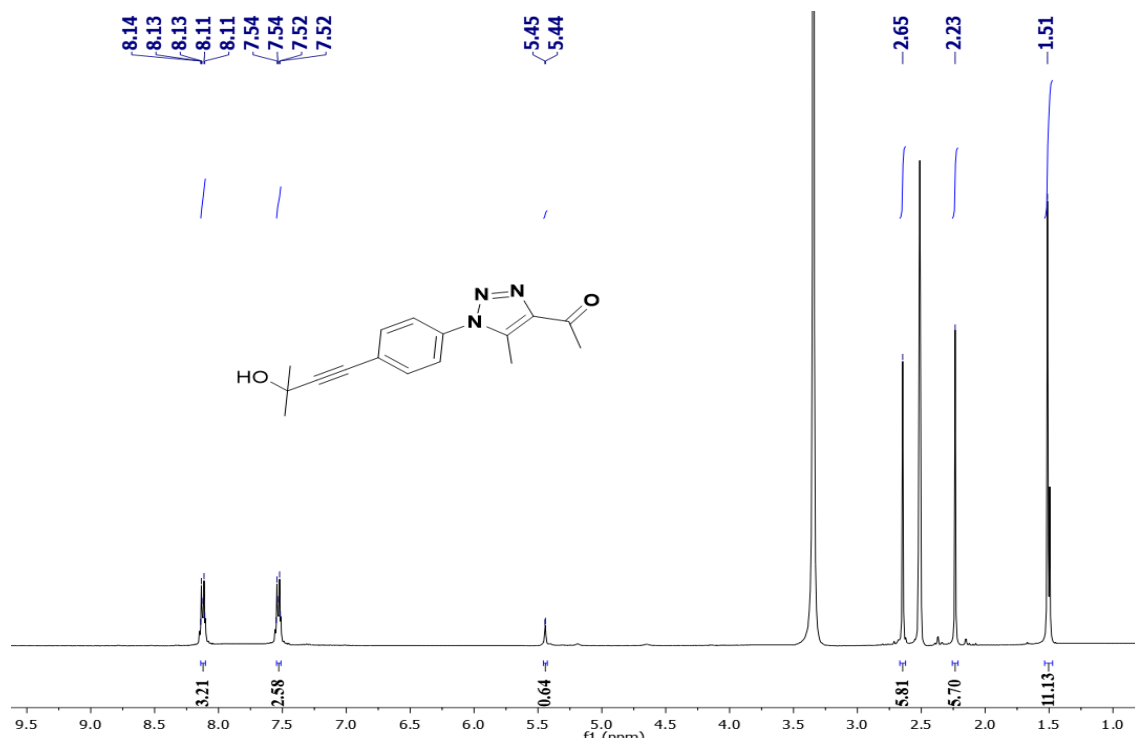
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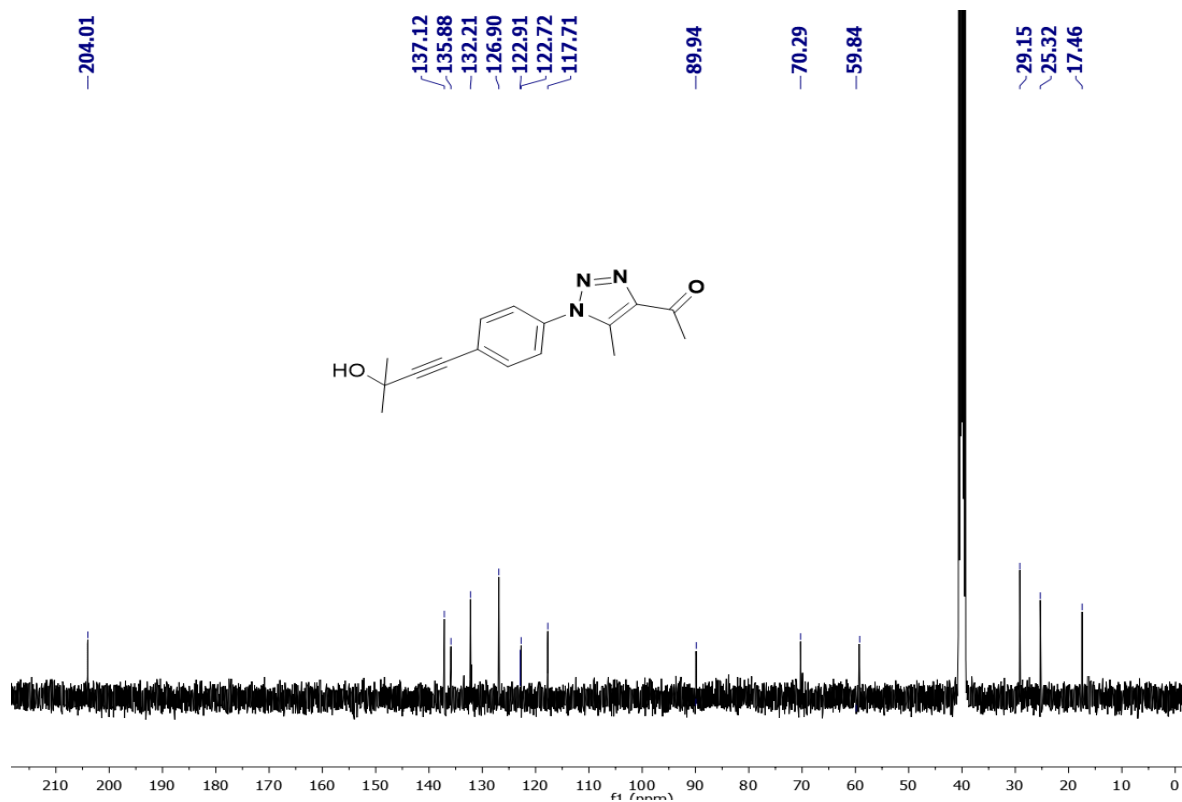
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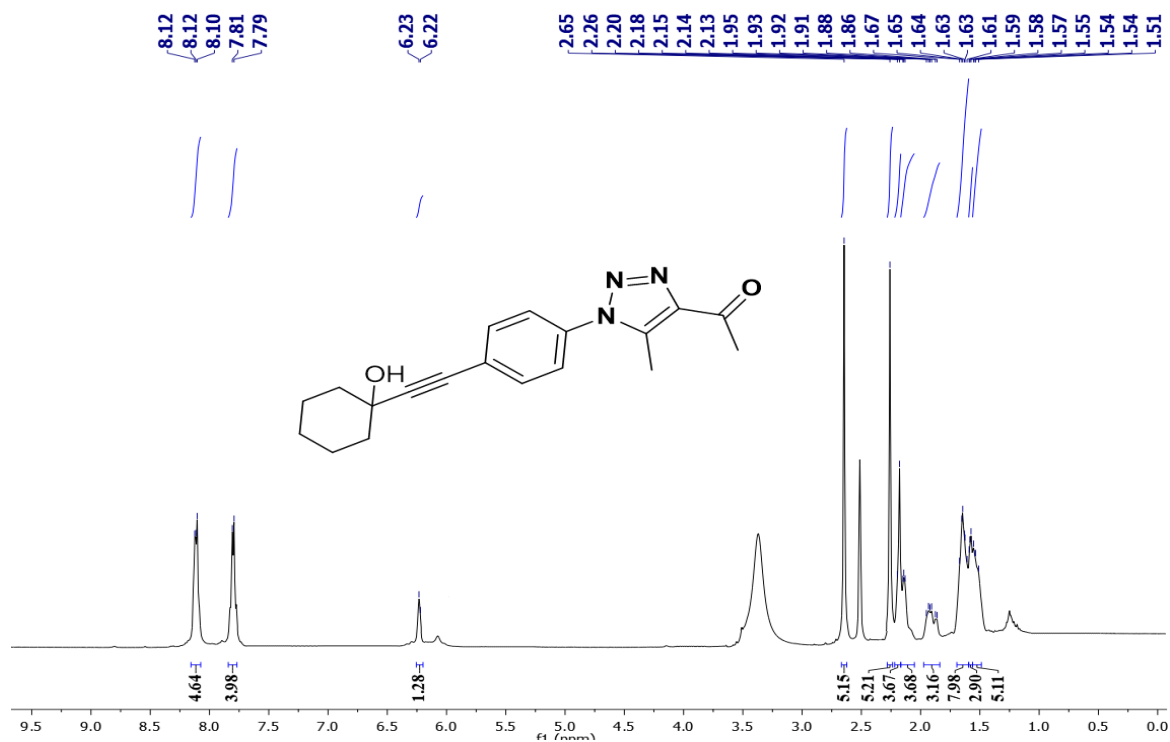
**<sup>13</sup>C NMR of compound 13**



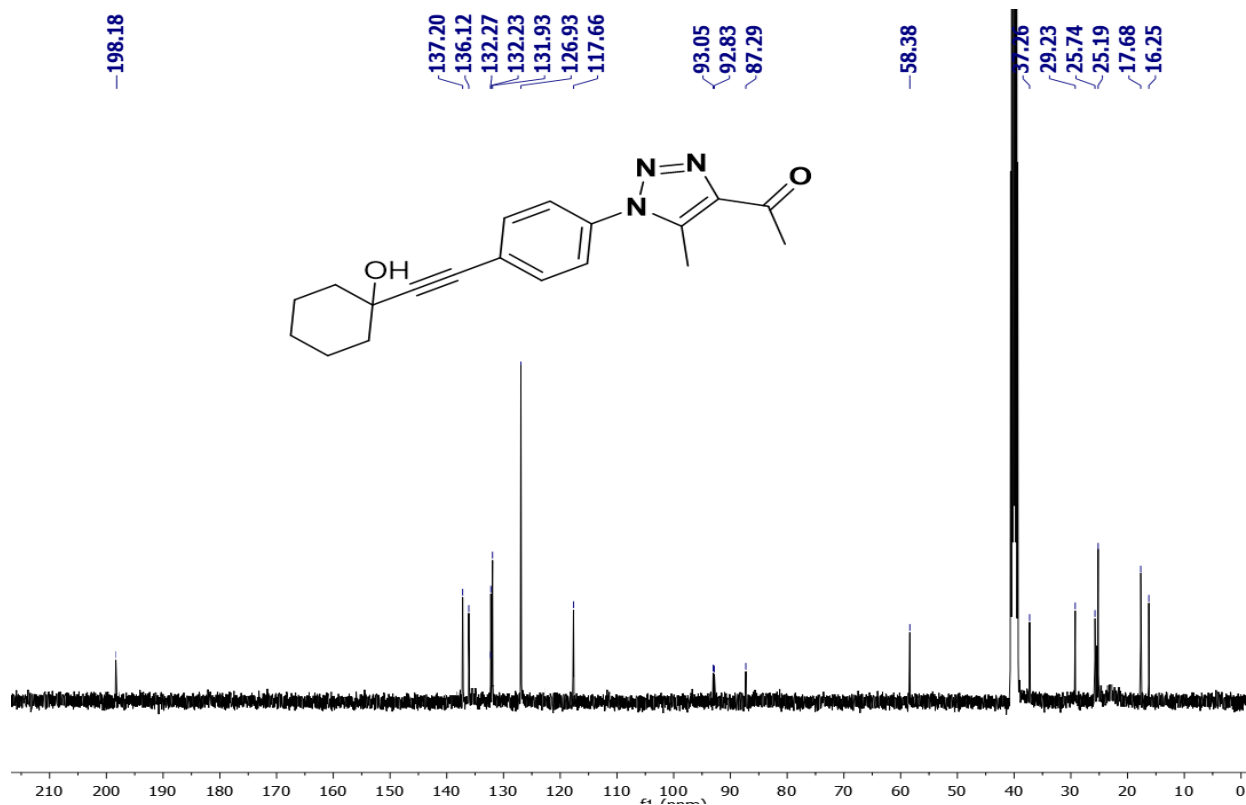
<sup>1</sup>H NMR of compound 14



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

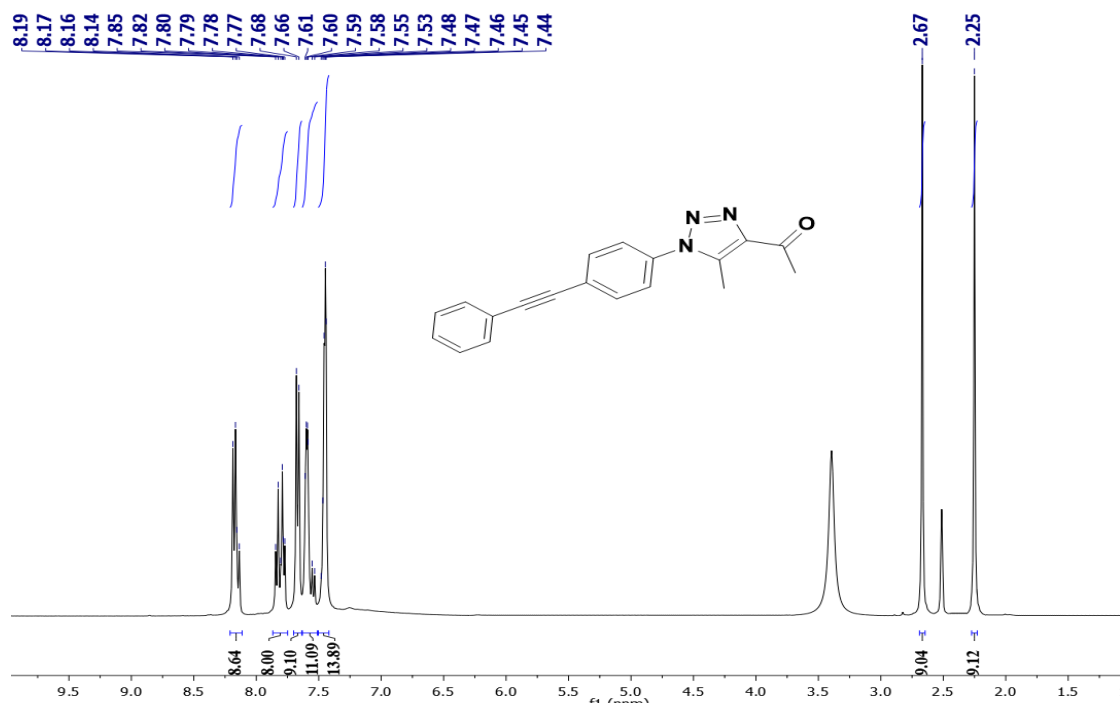


<sup>1</sup>H NMR of compound 15

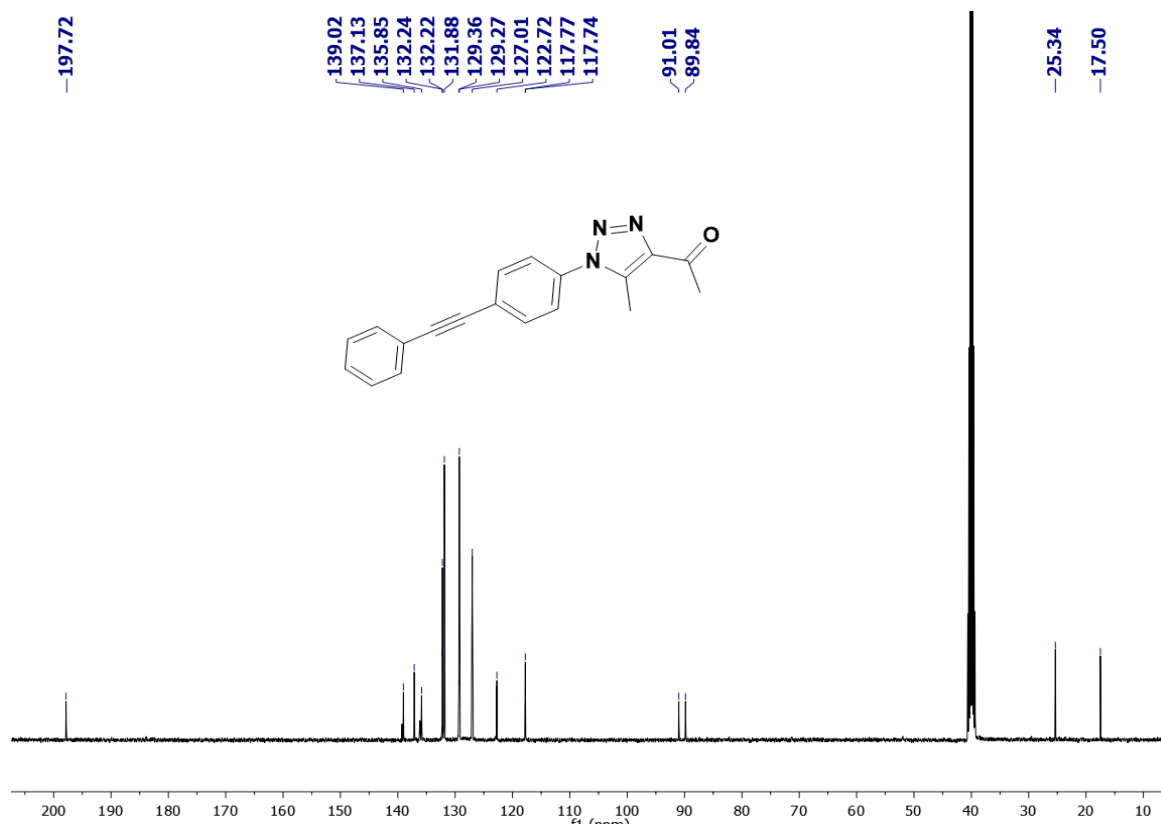


<sup>13</sup>C NMR of compound 15

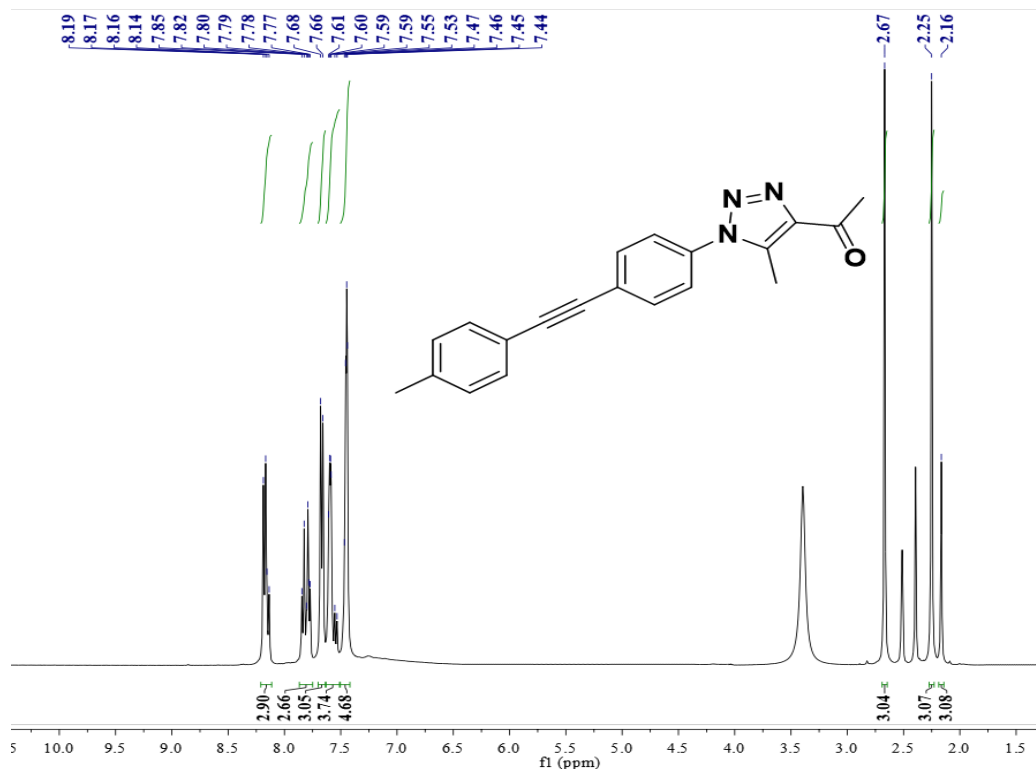




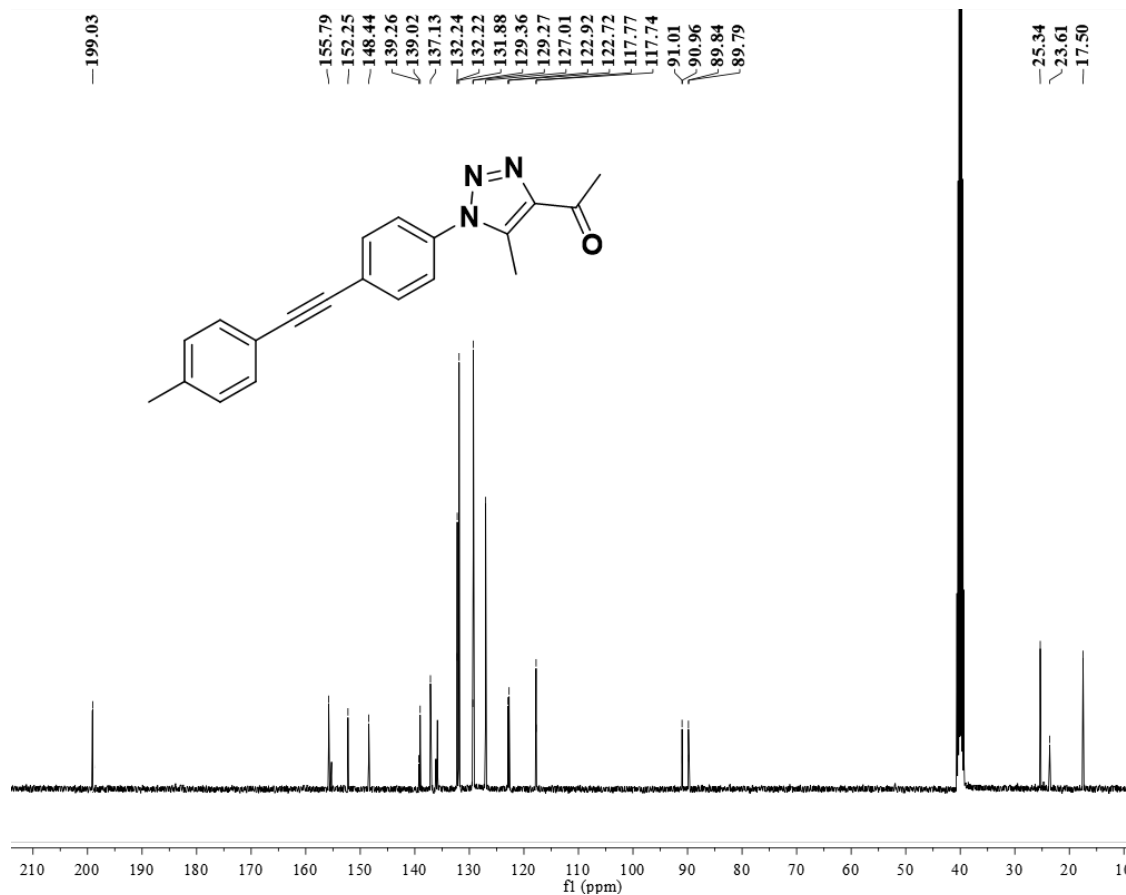
<sup>1</sup>H NMR of compound 16



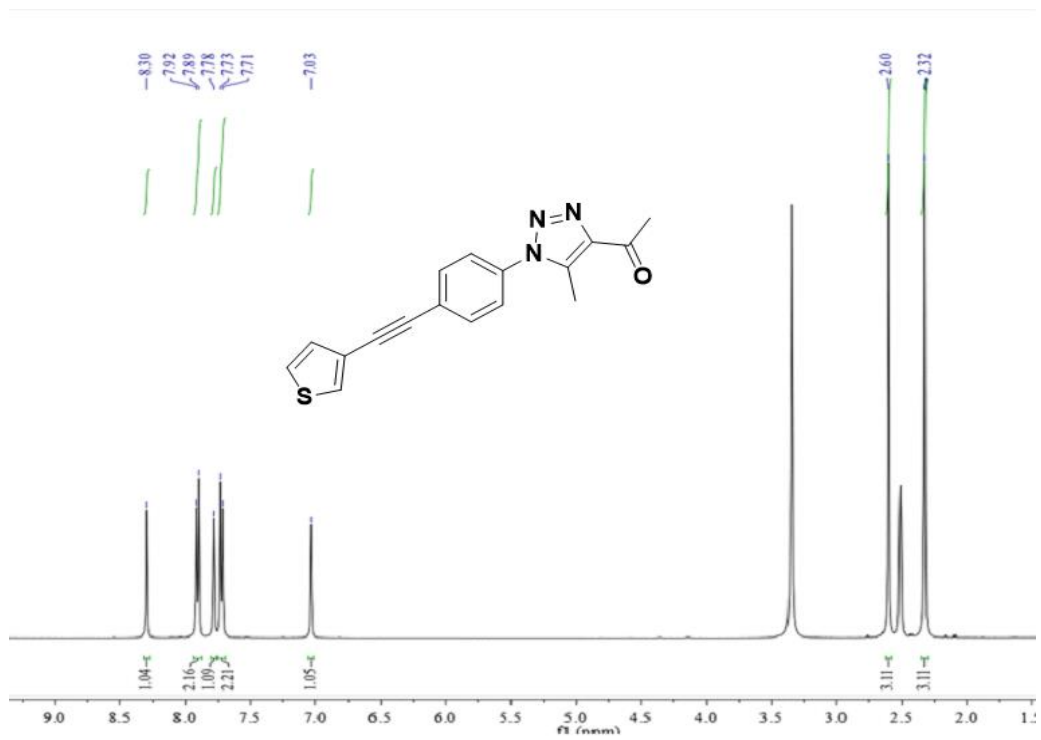
<sup>13</sup>C NMR of compound 16



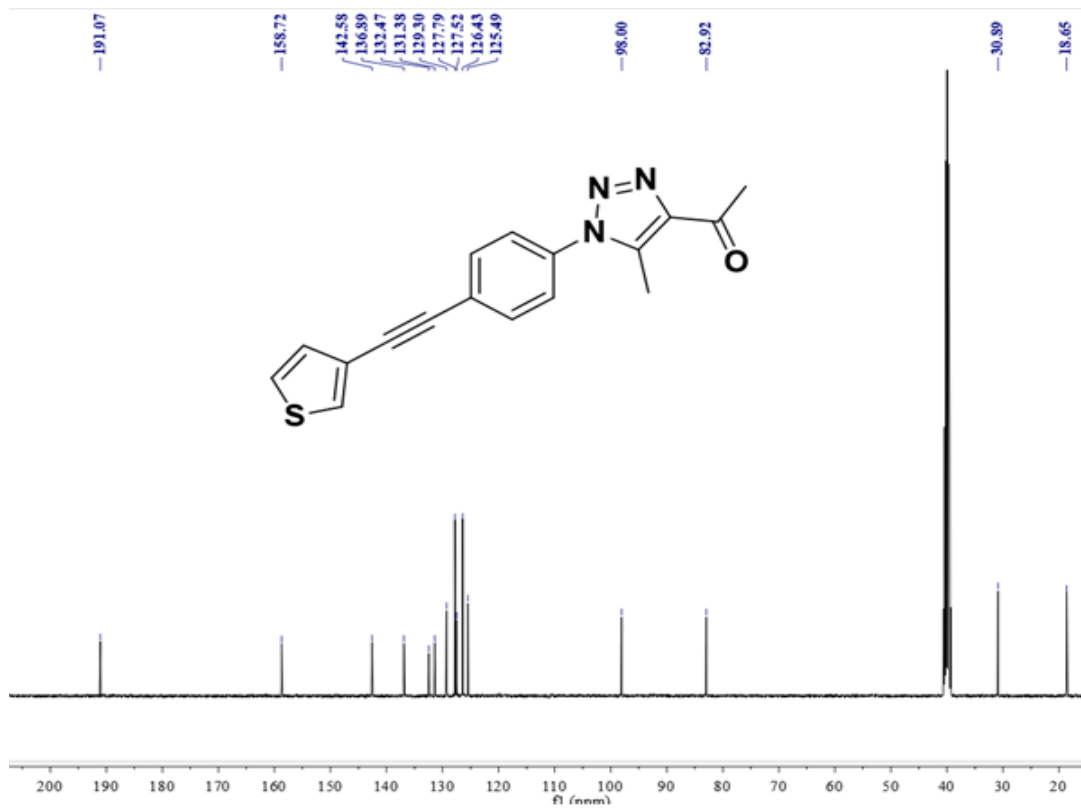
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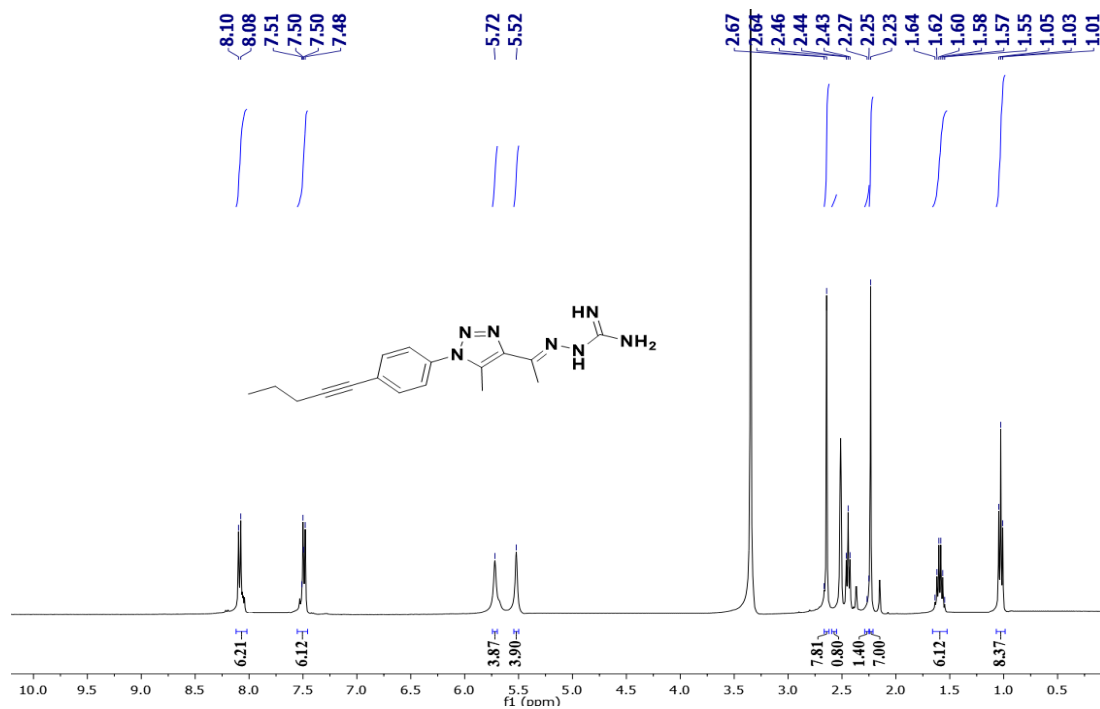
**<sup>13</sup>C NMR of compound 17**



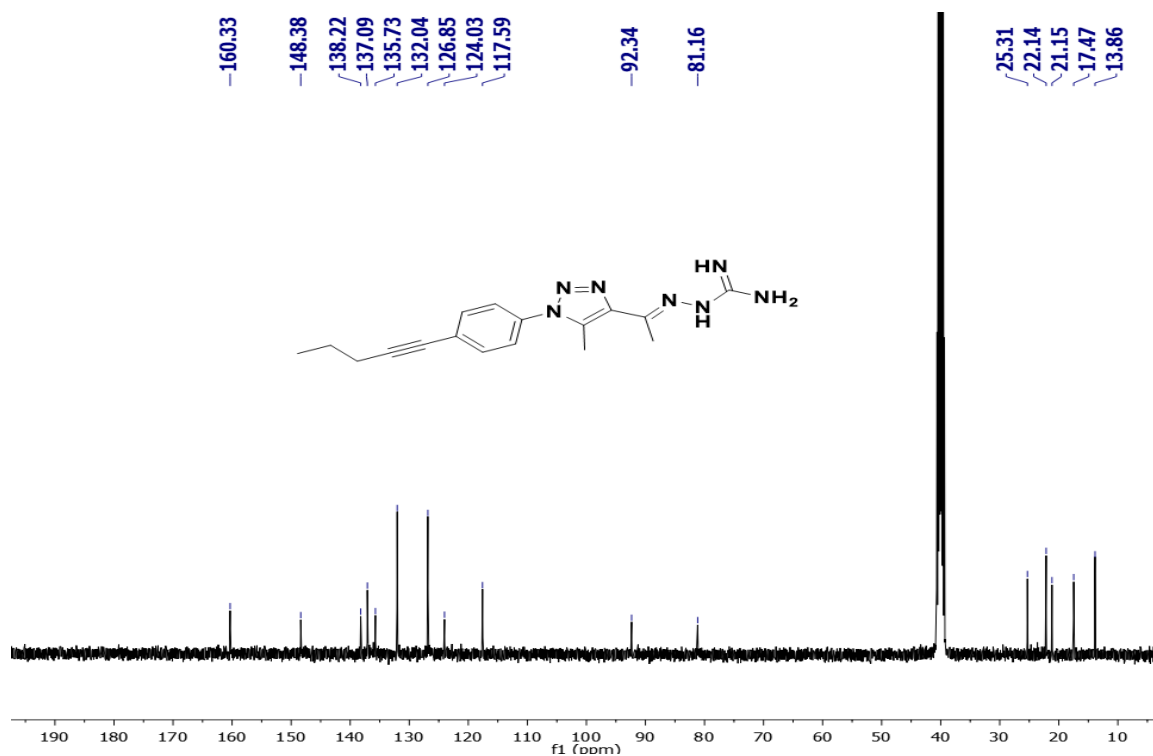
<sup>1</sup>H NMR of compound 18



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



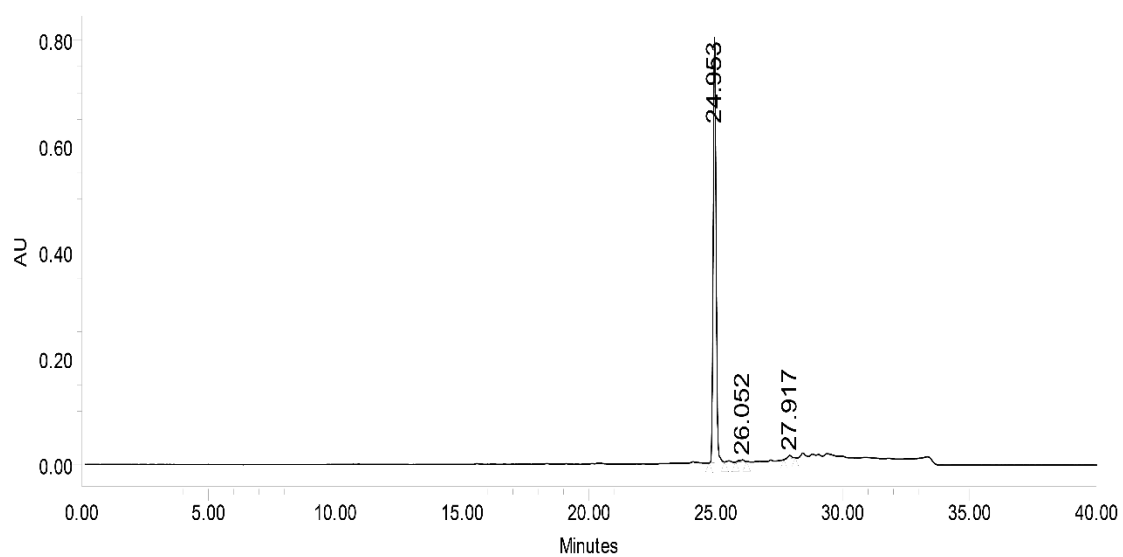
<sup>1</sup>H NMR of compound 19



<sup>13</sup>C NMR of compound 19

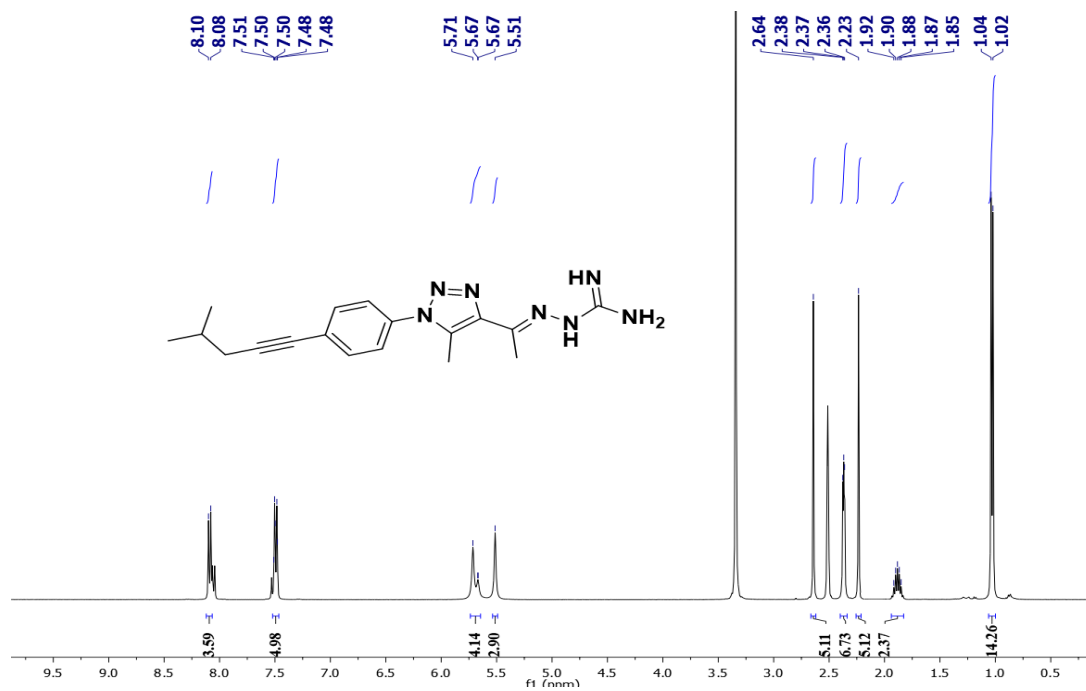
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Injection Volume:	10.00 ul	Channel Name:	380.0nm
Run Time:	40.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 380.0 nm (PDA 210.0 to 400.0 nm)
Date Acquired:	9/23/2021 10:14:12 AM EEST		
Date Processed:	9/25/2021 10:10:19 AM EEST		

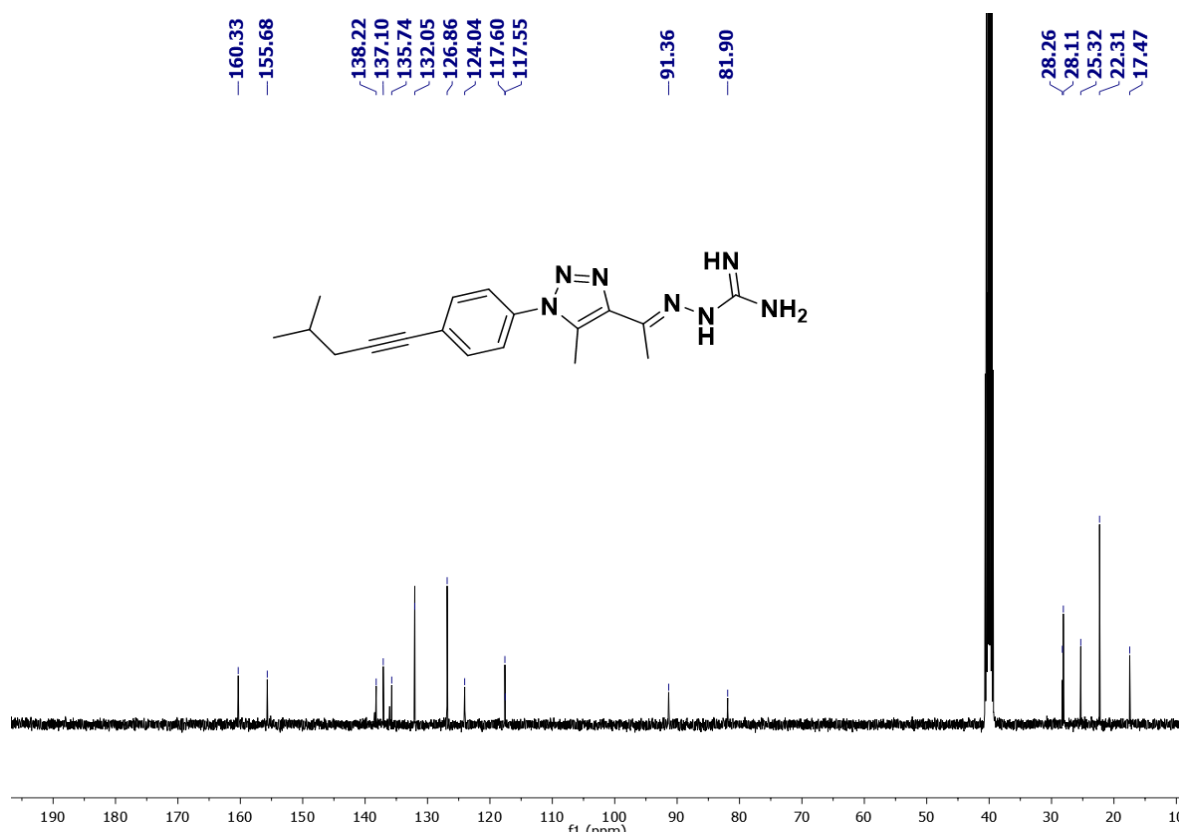


	RT	Area	% Area	Height
1	24.953	6307513	98.07	801049
2	26.052	54696	0.85	3763
3	27.917	69272	1.08	5877

### HPLC of compound 19



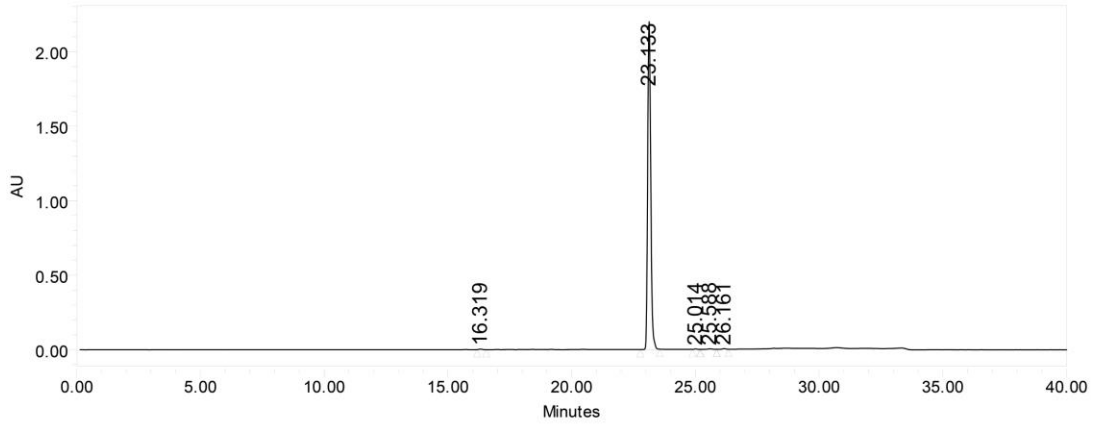
<sup>1</sup>H NMR of compound 20



<sup>13</sup>C NMR of compound 20

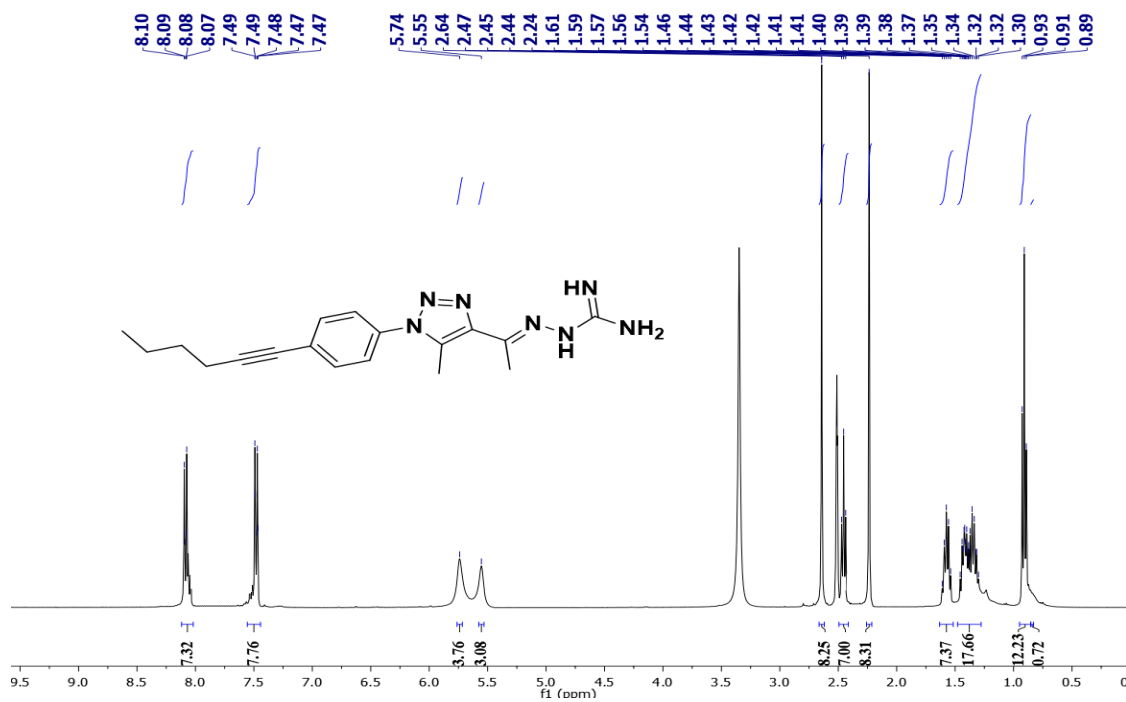
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Sample Type:	Unknown	Sample Set Name:	dsrtrr
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Injection Volume:	10.00 ul	Channel Name:	380.0nm
Run Time:	40.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 380.0 nm (PDA 210.0 tc
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Date Processed:	9/25/2021 10:10:49 AM EEST		

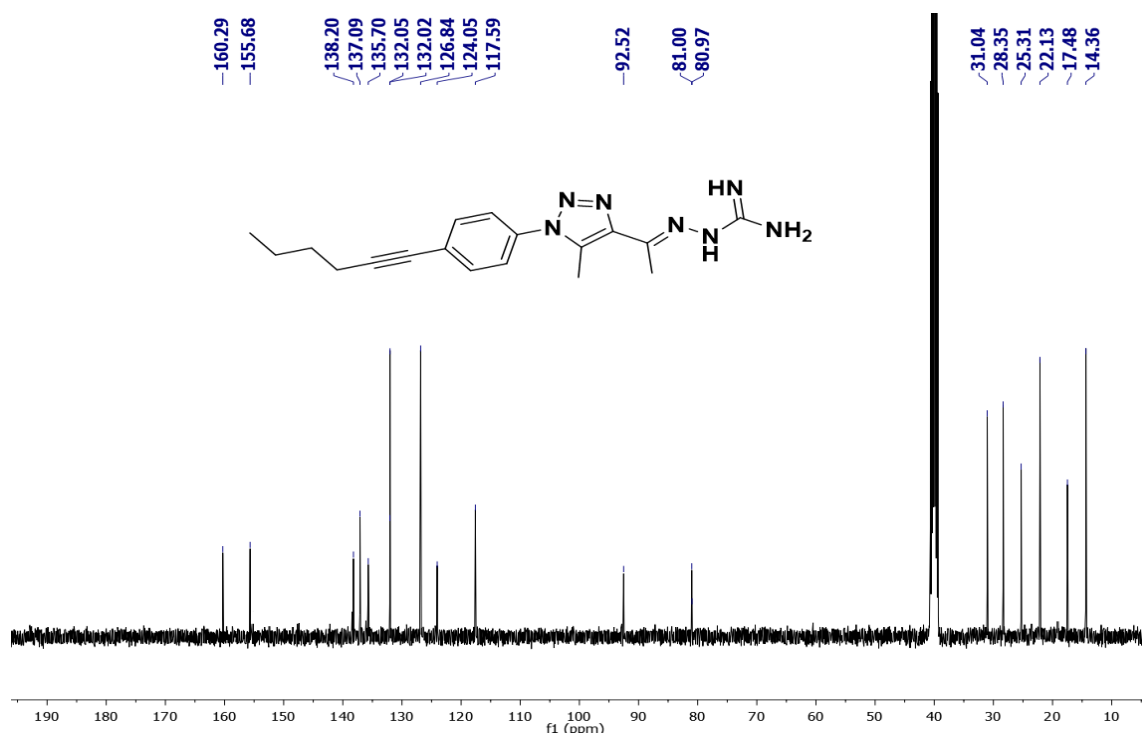


	RT	Area	% Area	Height
1	16.319	26071	0.14	3249
2	23.133	19029581	99.33	2195283
3	25.014	22557	0.12	2996
4	25.588	43357	0.23	3816
5	26.161	37042	0.19	3854

### HPLC of compound 20



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

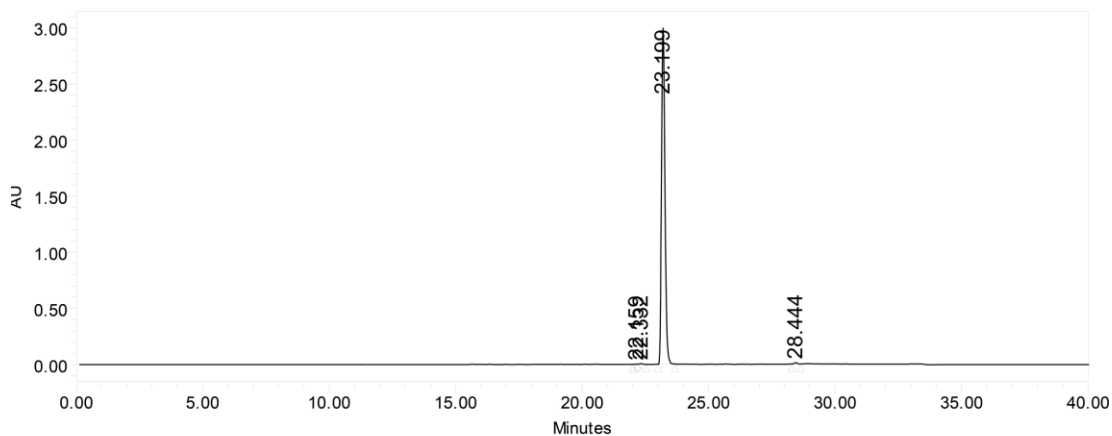


<sup>13</sup>C NMR of compound 21



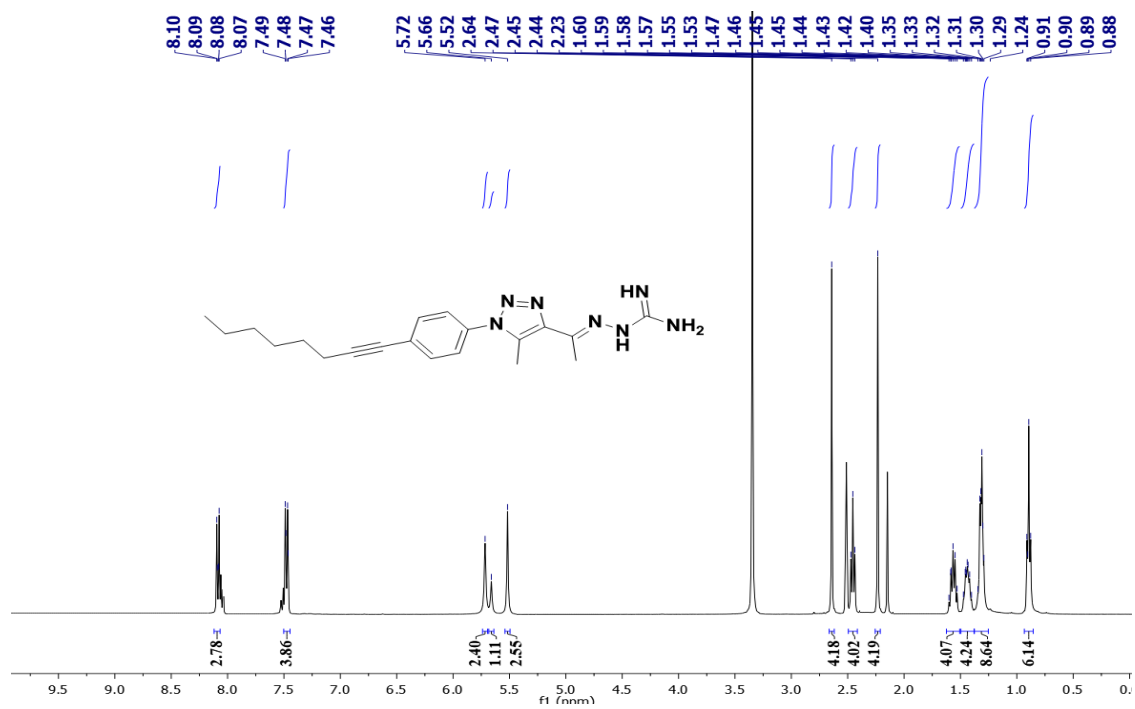
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Sample Type:	Unknown	Sample Set Name:	dsrtrr
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Injection #:	1	Processing Method:	Default
Injection Volume:	10.00 ul	Channel Name:	380.0nm
Run Time:	40.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 380.0 nm (PDA 210.0 tc
Date Acquired: 9/23/2021 2:20:14 PM EEST			
Date Processed: 9/25/2021 10:12:42 AM EEST			

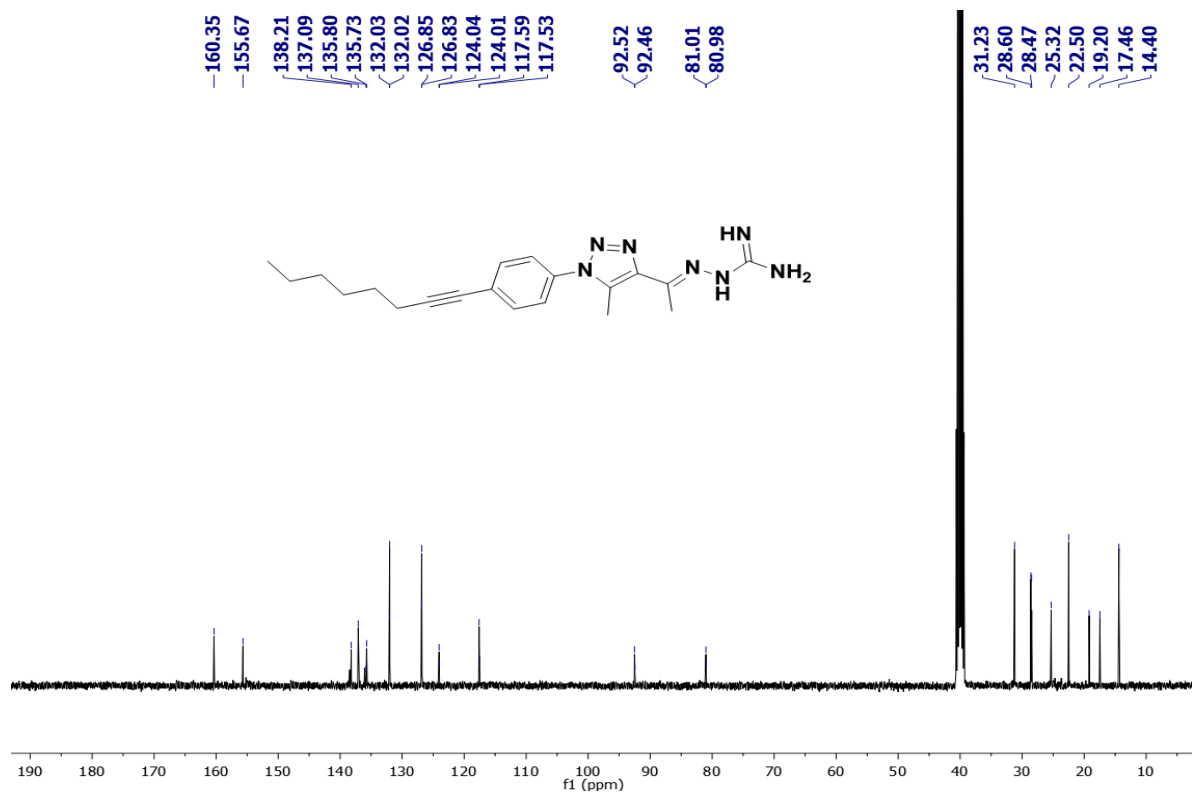


	RT	Area	% Area	Height
1	22.159	22642	0.08	3184
2	22.332	66747	0.23	6423
3	23.199	28255253	99.33	3003594
4	28.444	101149	0.36	12102

### HPLC of compound 21



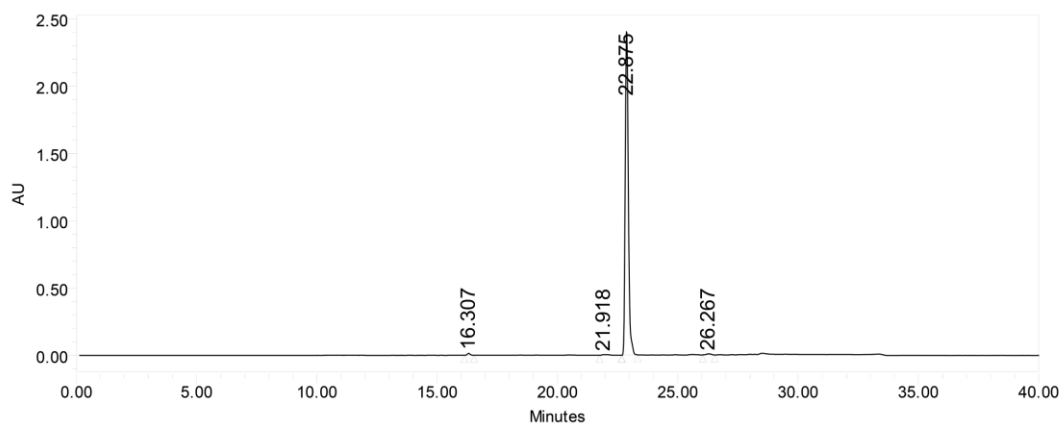
**<sup>1</sup>H NMR of compound 22**



**<sup>13</sup>C NMR of compound 22**

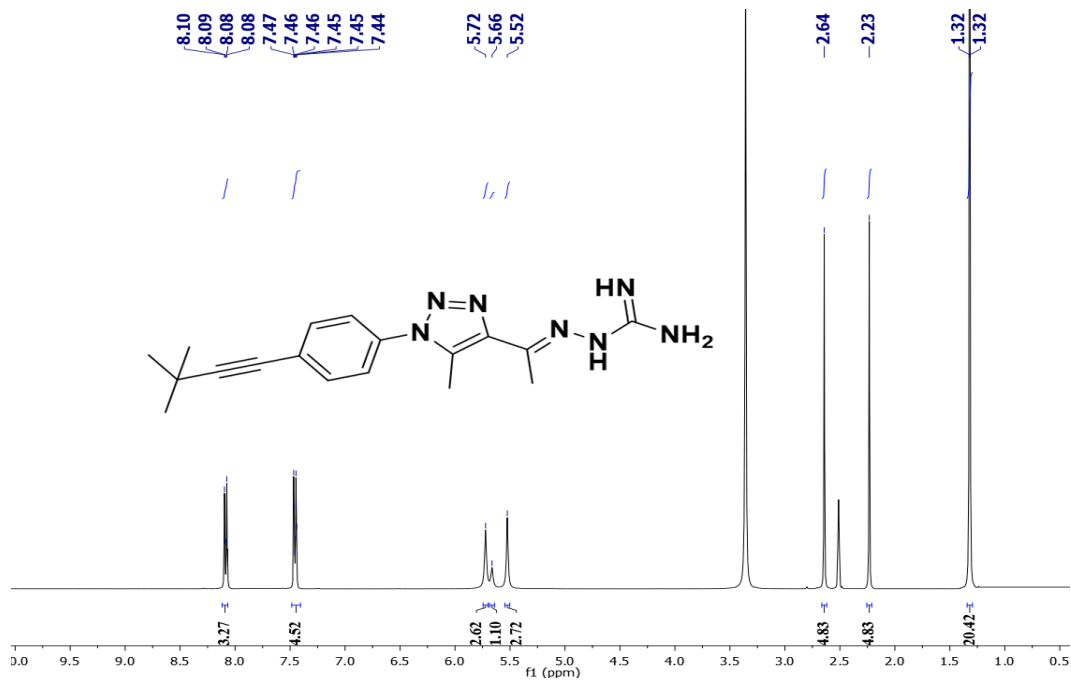
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Run Time:	40.0 Minutes	Proc. Chnl. Descr.:	W2996 FDA 380.0 nm (FDA 210.0 to
Date Acquired:	9/23/2021 11:36:12 AM EEST		
Date Processed:	9/25/2021 10:11:19 AM EEST		

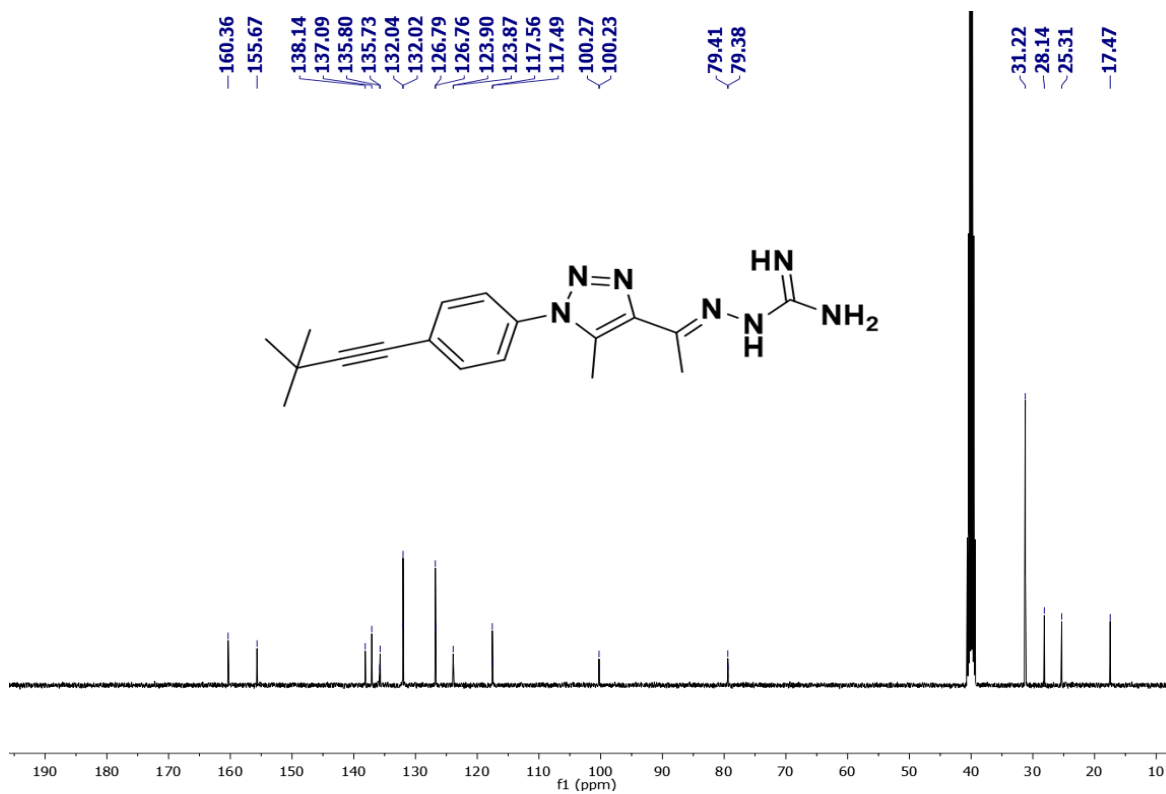


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1	16.307	116481	0.53	14105
2	21.918	86390	0.39	4221
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4	26.267	104513	0.47	7530

### HPLC of compound 22



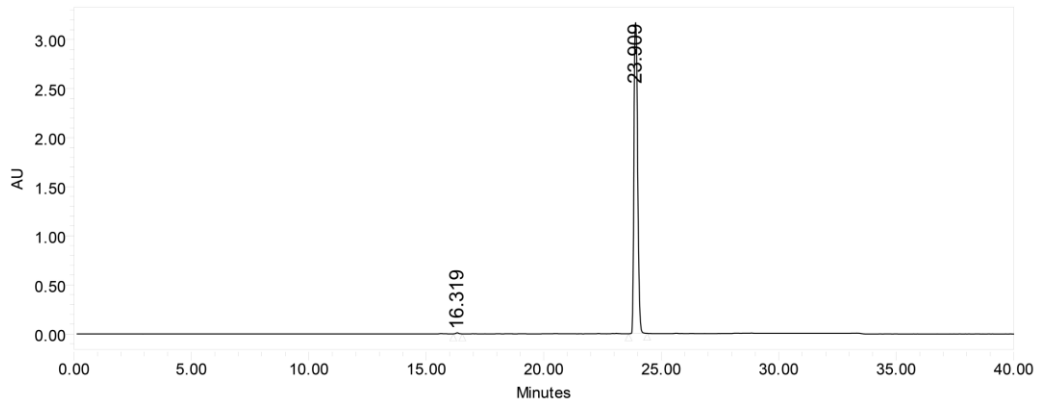
<sup>1</sup>H NMR of compound 23



<sup>13</sup>C NMR of compound 23

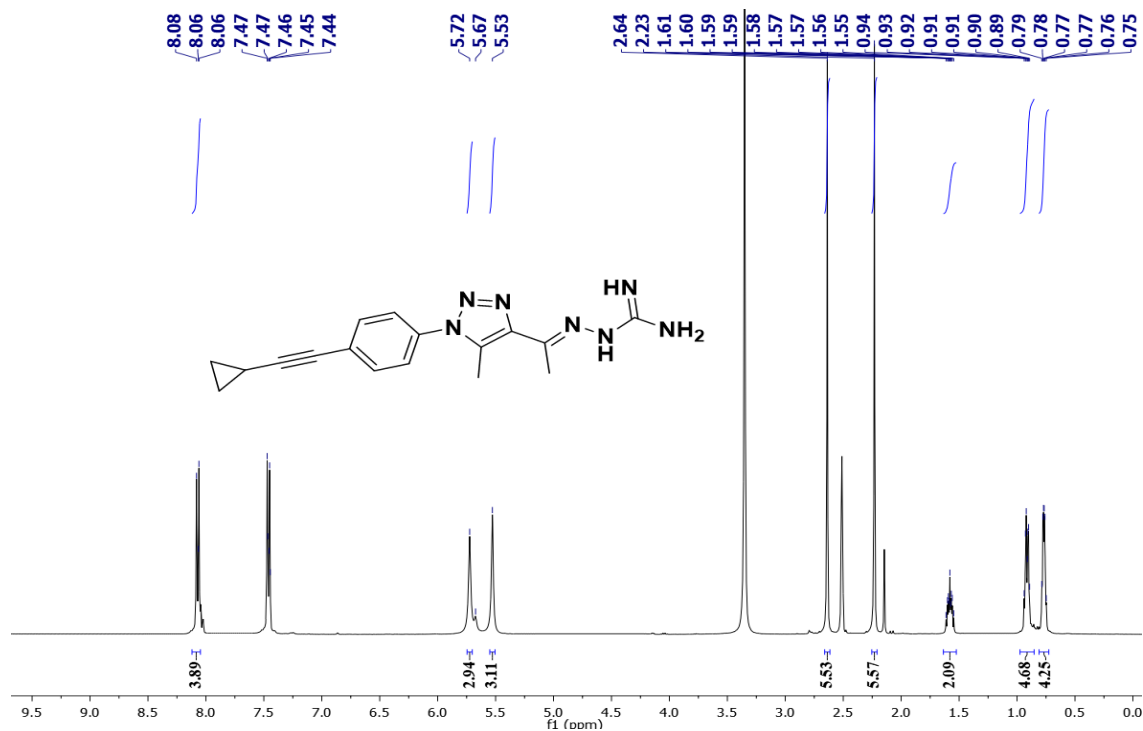
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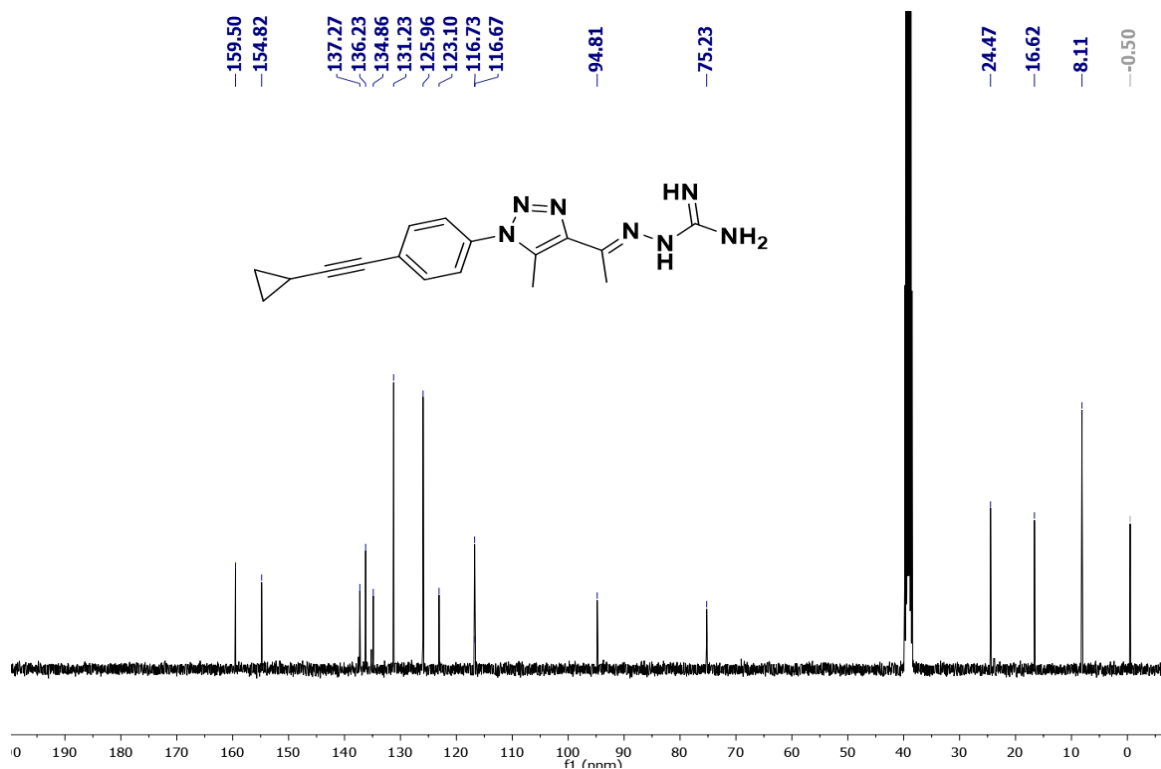


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1	16.319	87894	0.26	10420
2	23.909	34345973	99.74	3180506

### HPLC of compound 23



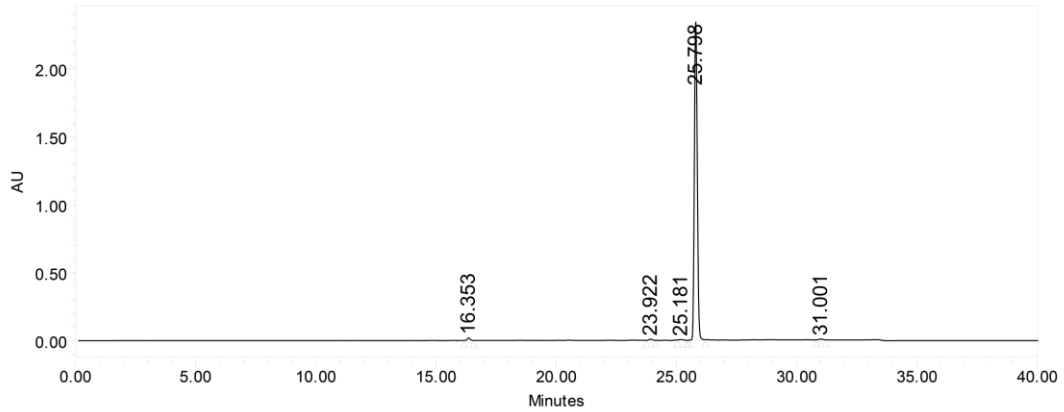
**<sup>1</sup>H NMR of compound 24**



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

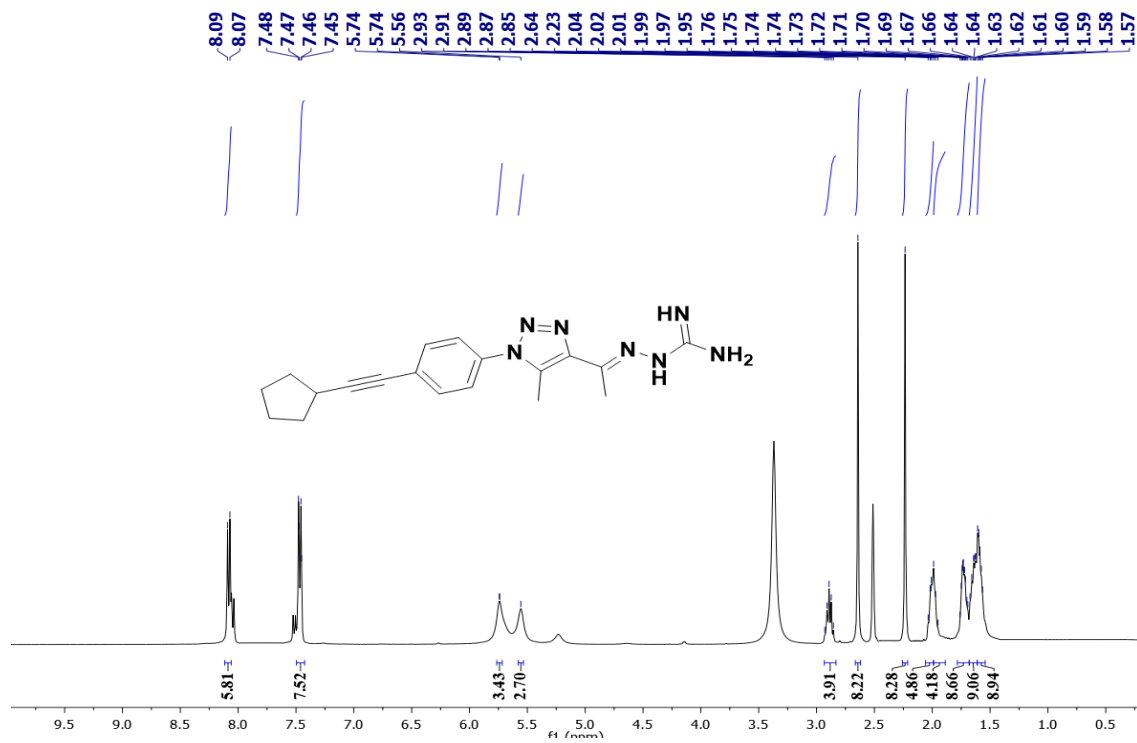
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Injection #:	1	Processing Method:	Default
Injection Volume:	10.00 ul	Channel Name:	380.0nm
Run Time:	40.0 Minutes	Proc. Chnl. Descr.:	W2996 FDA 380.0 nm (FDA 210.0 to
Date Acquired:	9/23/2021 3:42:14 PM EEST		
Date Processed:	9/25/2021 10:13:22 AM EEST		

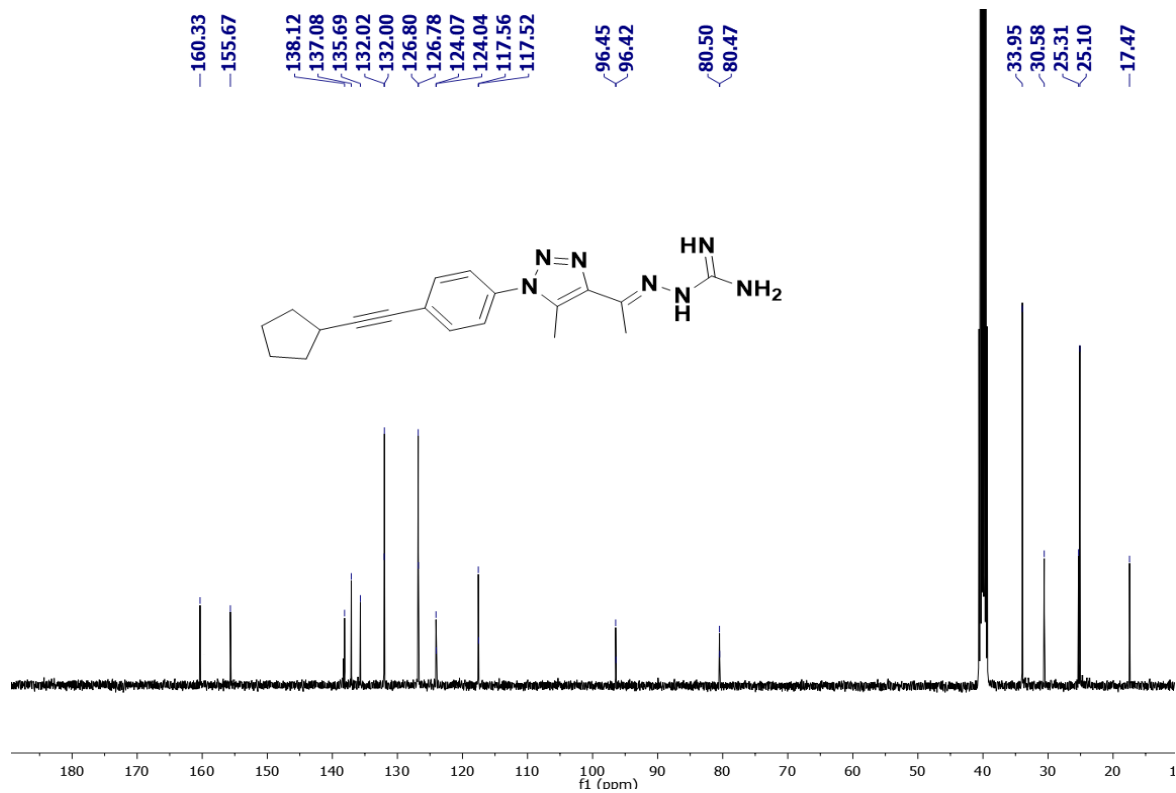


	RT	Area	% Area	Height
1	16.353	153971	0.76	18345
2	23.922	83008	0.41	9528
3	25.181	52962	0.26	4640
4	25.798	19911687	98.23	2336748
5	31.001	68107	0.34	6330

### HPLC of compound 24



<sup>1</sup>H NMR of compound 25

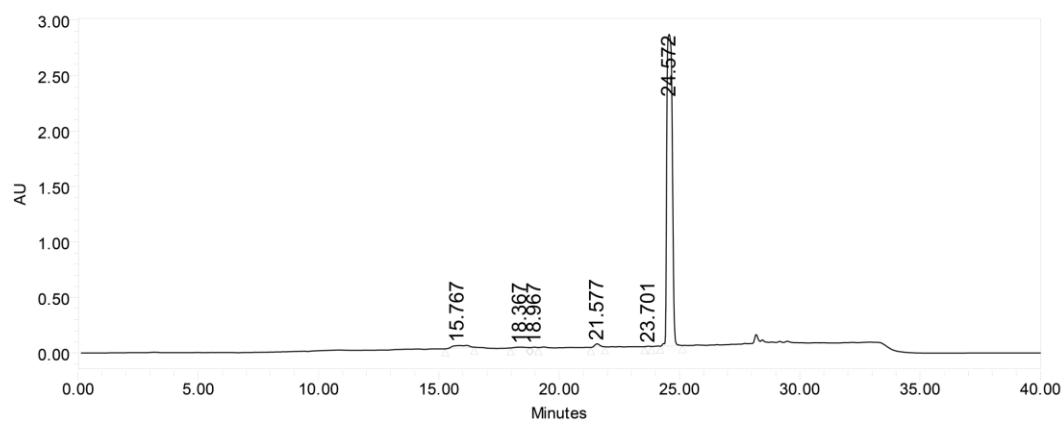


<sup>13</sup>C NMR of compound 25



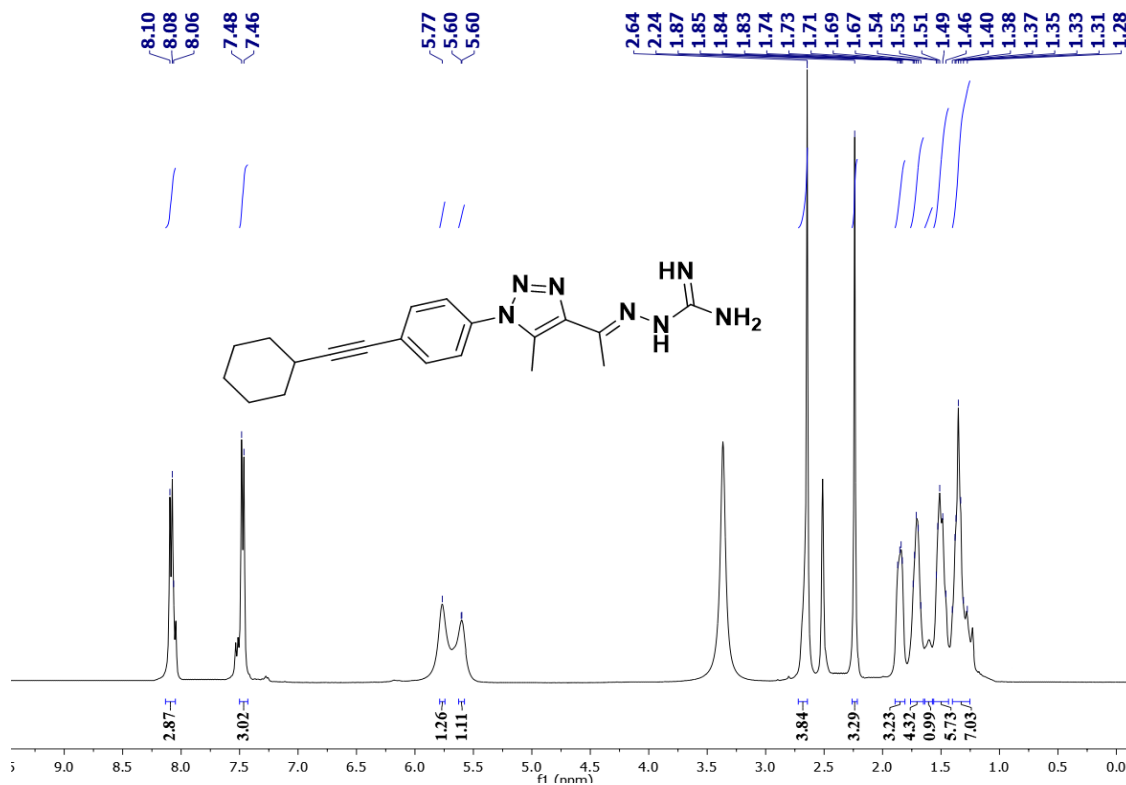
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Injection #: 1	Processing Method: Default
Injection Volume: 10.00 ul	Channel Name: 300.0nm
Run Time: 40.0 Minutes	Proc. Chnl. Descr.: W2996 PDA 300.0 nm (PDA 210.0 to
Date Acquired: 9/23/2021 4:23:14 PM EEST	
Date Processed: 9/25/2021 10:14:21 AM EEST	

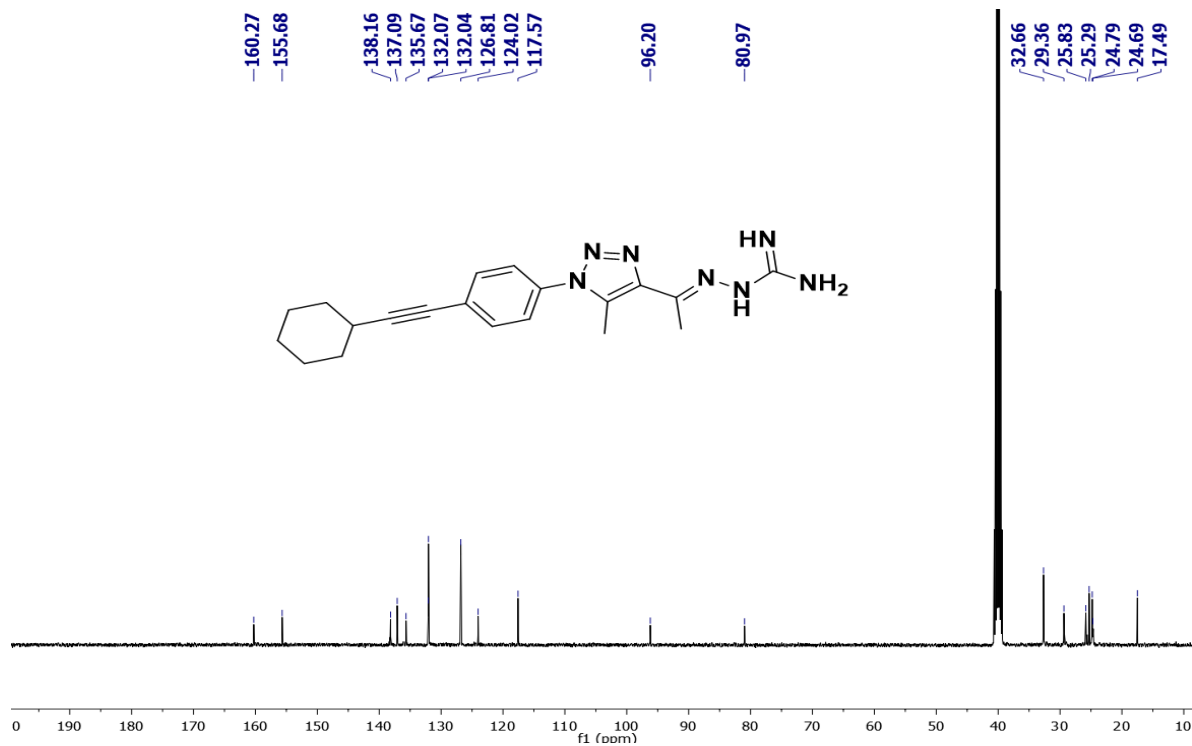


	RT	Area	% Area	Height
1	15.767	1017649	2.23	22382
2	18.367	189445	0.42	6558
3	18.967	44091	0.10	4311
4	21.577	434099	0.95	29567
5	23.701	28443	0.06	3885
6	24.572	43850569	96.24	2806716

### HPLC of compound 25



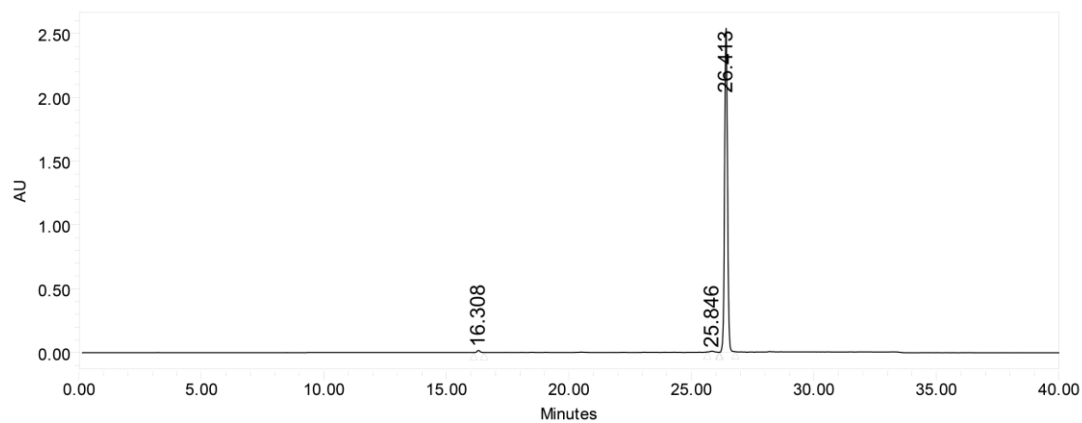
<sup>1</sup>H NMR of compound 26



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

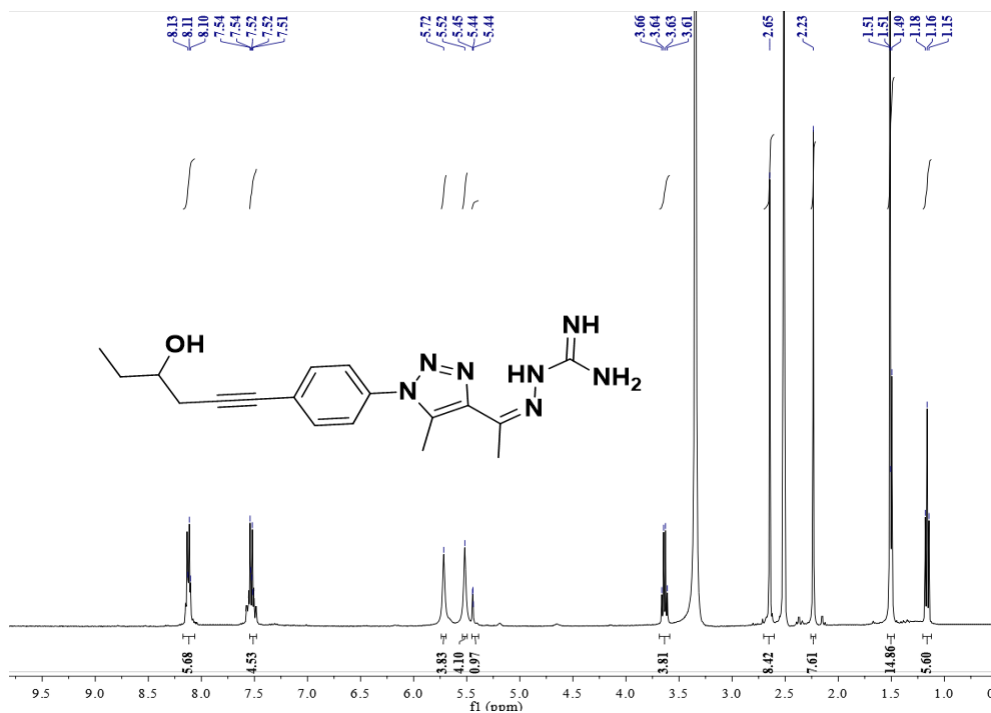
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Injection Volume:	10.00 ul	Channel Name:	375.0nm
Run Time:	40.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 375.0 nm (PDA 210.0 to 400.0 nm)
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Date Processed:	9/25/2021 10:15:04 AM EEST		

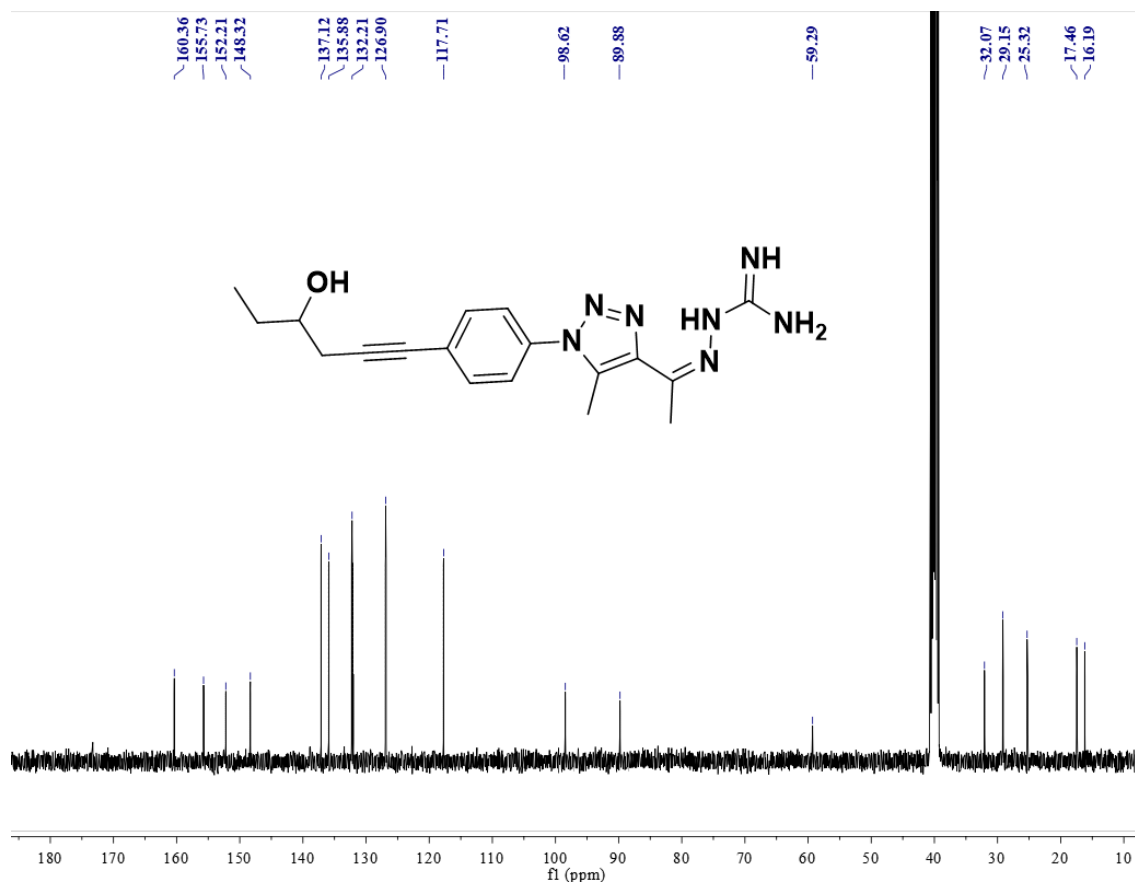


	RT	Area	% Area	Height
1	16.308	136166	0.64	16002
2	25.846	81675	0.39	7243
3	26.413	20966280	98.97	2545583

### HPLC of compound 26



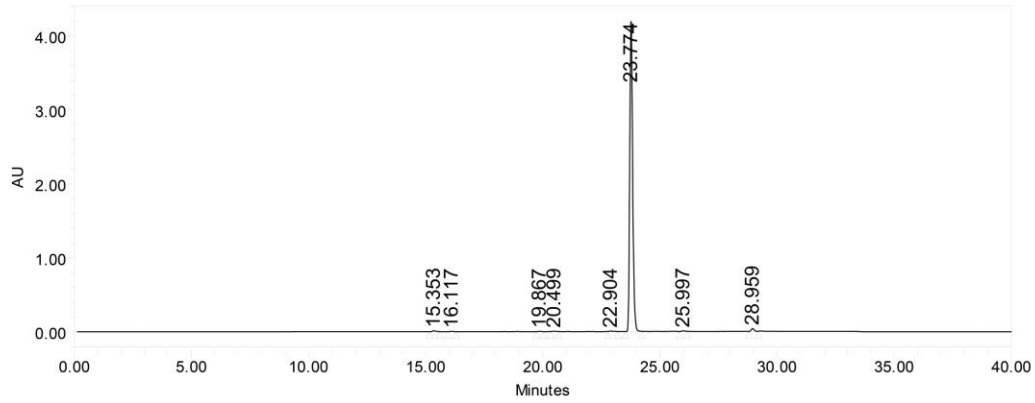
<sup>1</sup>H NMR of compound 27



<sup>13</sup>C NMR of compound 27

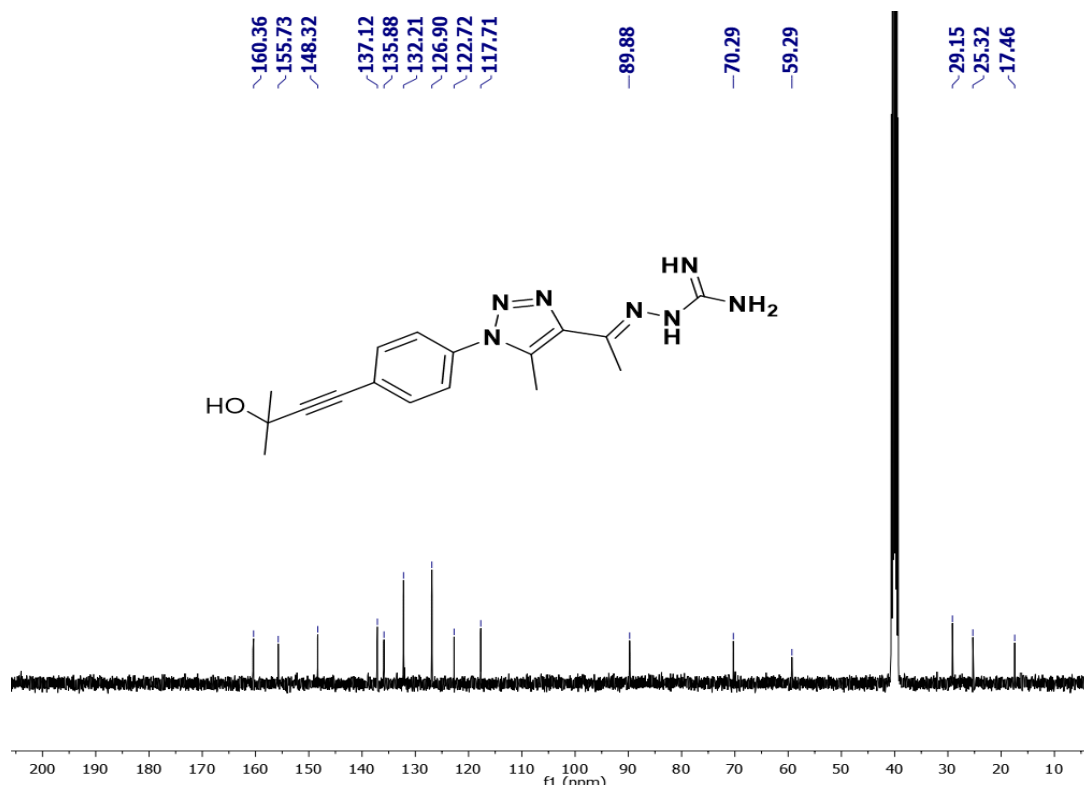
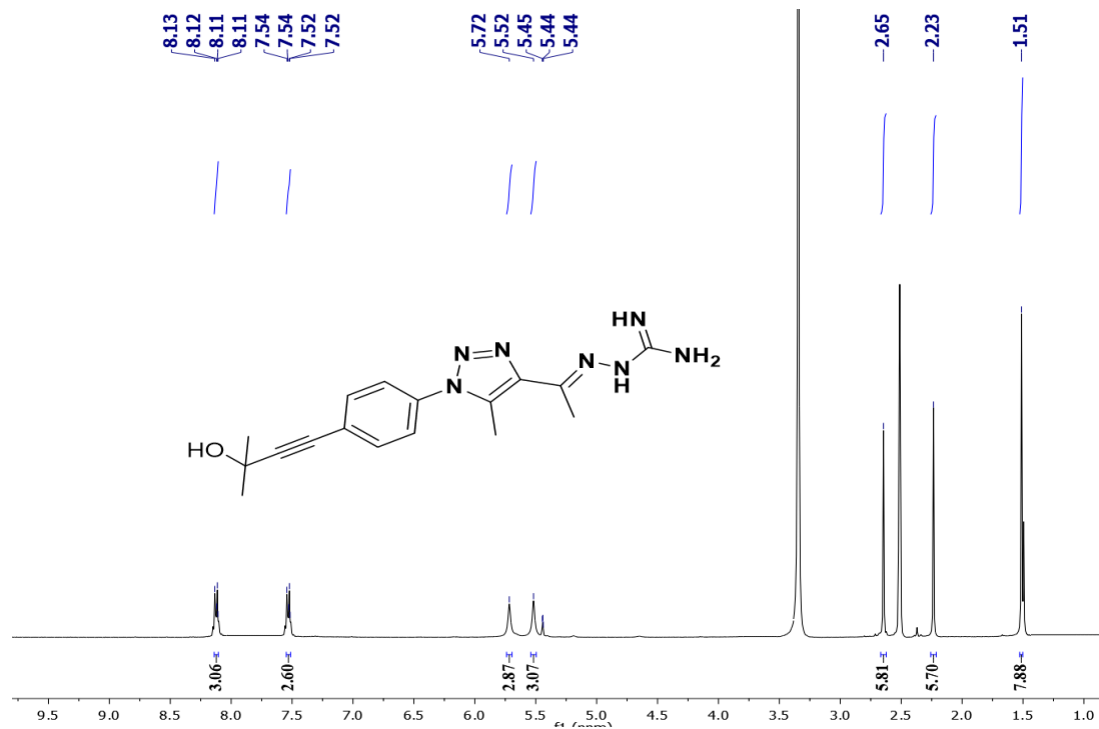
## SAMPLE INFORMATION

Sample Name: 3SN-9	Acquired By: System
Sample Type: Unknown	Sample Set Name: dsrtr
Vial: 38	Acq. Method Set: Trial 1 gradient
Injection #: 1	Processing Method: Default
Injection Volume: 10.00 ul	Channel Name: 380.0nm
Run Time: 40.0 Minutes	Proc. Chnl. Descr.: W2996 PDA 380.0 nm (PDA 210.0 to 400.0 nm)
Date Acquired: 9/23/2021 7:07:13 PM EEST	
Date Processed: 9/25/2021 10:19:57 AM EEST	



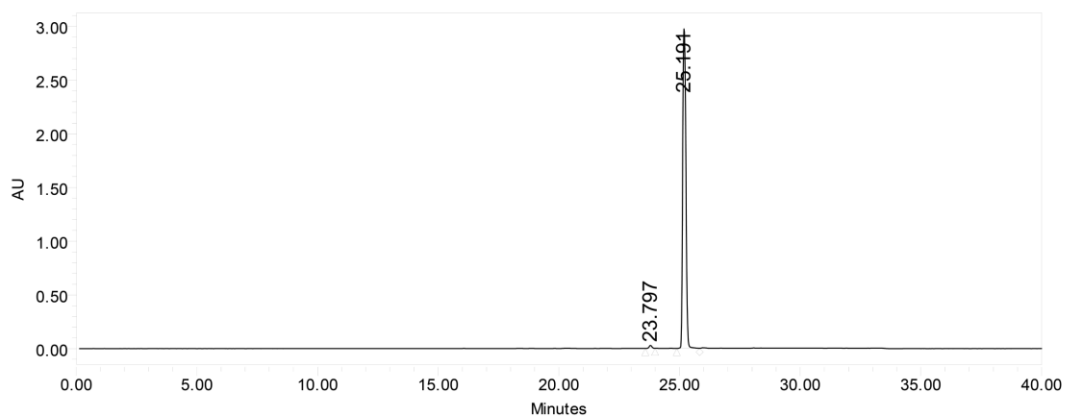
	RT	Area	% Area	Height
1	15.353	117024	0.32	11146
2	16.117	36635	0.10	4562
3	19.867	31563	0.08	3911
4	20.499	37627	0.10	3876
5	22.904	82488	0.22	6670
6	23.774	36457192	98.16	4214363
7	25.997	67127	0.18	8156
8	28.959	309113	0.83	37863

### HPLC of compound 27



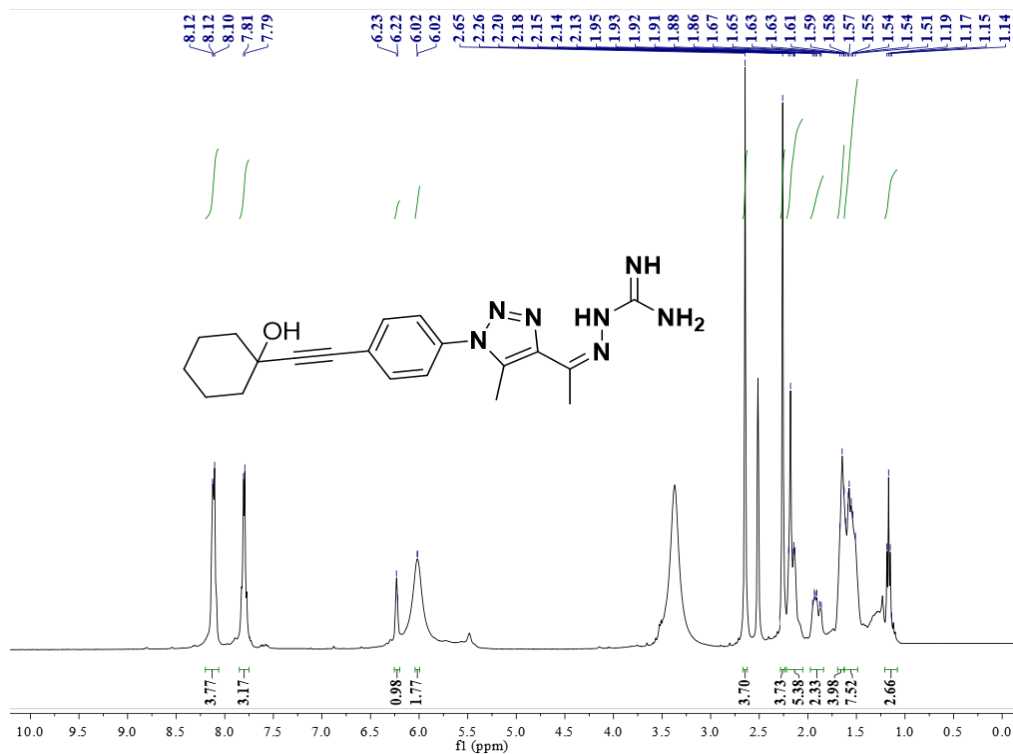
### SAMPLE INFORMATION

Sample Name:	3SN-5	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	dsrtrr
Vial:	39	Acq. Method Set:	Trial 1 gradient
Injection #:	1	Processing Method:	Default
Injection Volume:	10.00 ul	Channel Name:	380.0nm
Run Time:	40.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 380.0 nm (PDA 210.0 to
Date Acquired:	9/23/2021 7:48:13 PM EEST		
Date Processed:	9/25/2021 10:20:36 AM EEST		

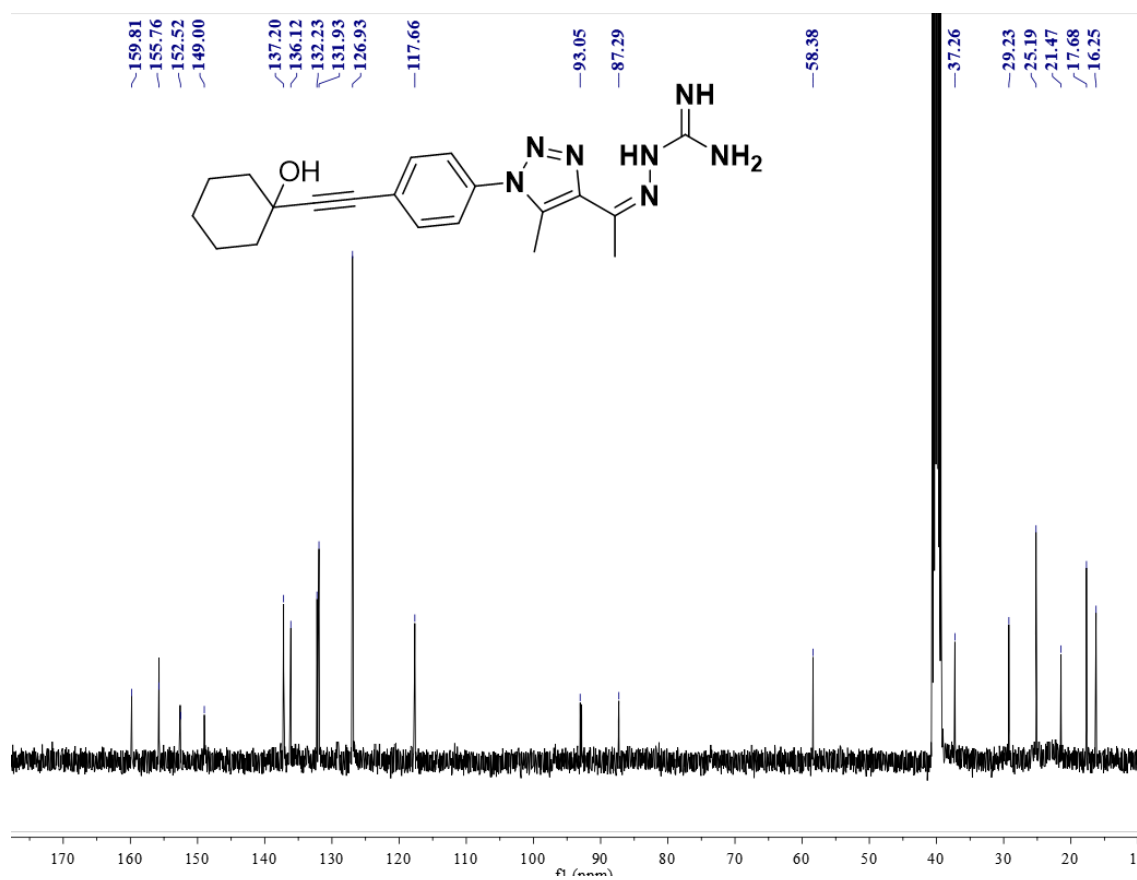


	RT	Area	% Area	Height
1	23.797	216931	0.79	26969
2	25.191	27288792	99.21	2992930

### HPLC of compound 28



**<sup>1</sup>H NMR of compound 29**

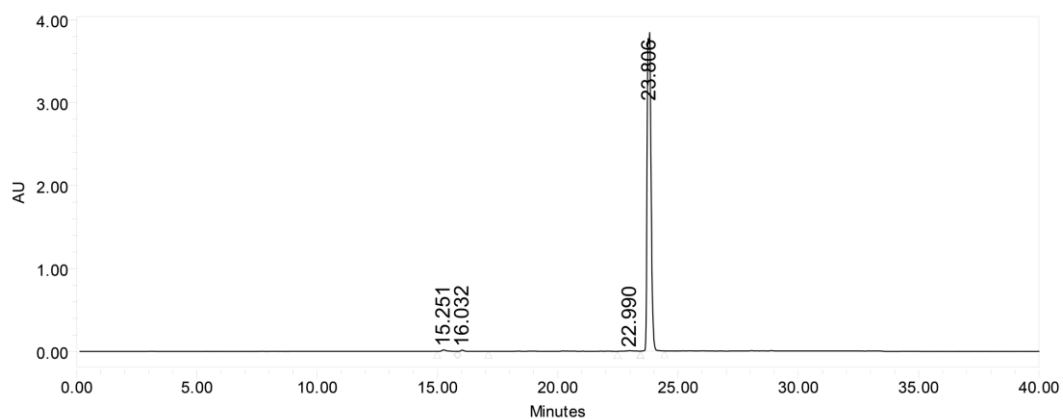


**<sup>13</sup>C NMR of compound 29**



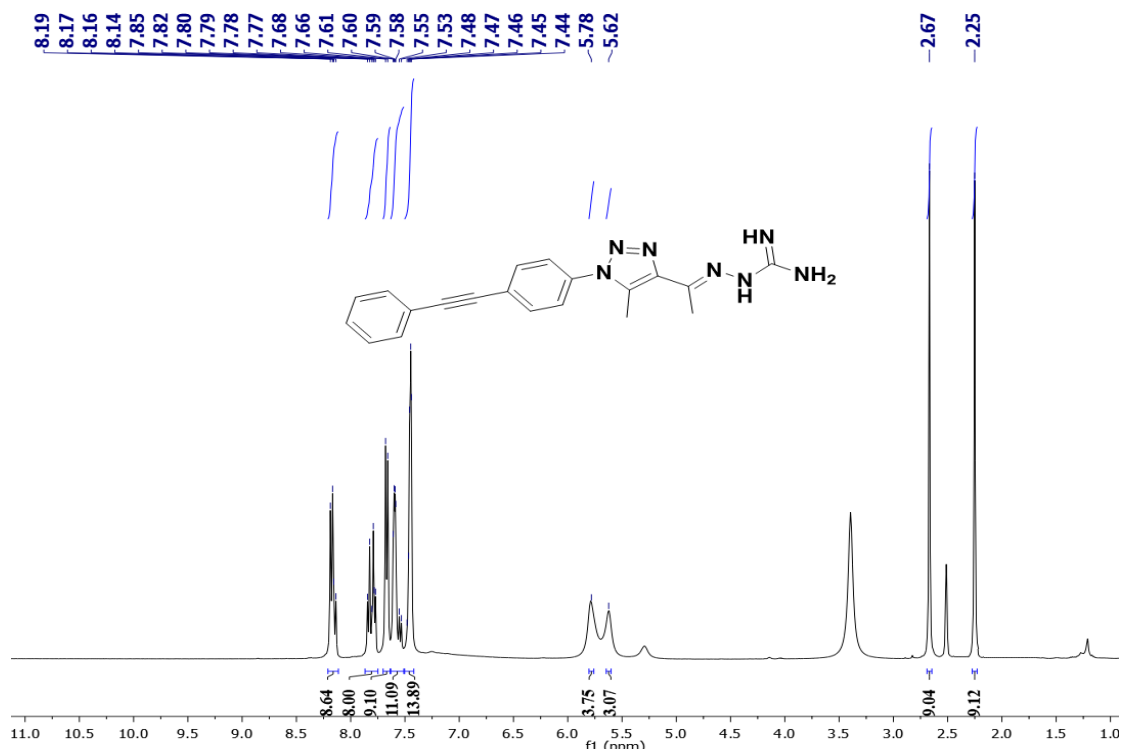
## SAMPLE INFORMATION

Sample Name: SN-3	Acquired By: System
Sample Type: Unknown	Sample Set Name: dsrtrr
Vial: 41	Acq. Method Set: Trial 1 gradient
Injection #: 1	Processing Method: Default
Injection Volume: 10.00 ul	Channel Name: 380.0nm
Run Time: 40.0 Minutes	Proc. Chnl. Descr.: W2996 PDA 380.0 nm (PDA 210.0 tc
Date Acquired: 9/23/2021 9:10:13 PM EEST	
Date Processed: 9/25/2021 10:21:44 AM EEST	

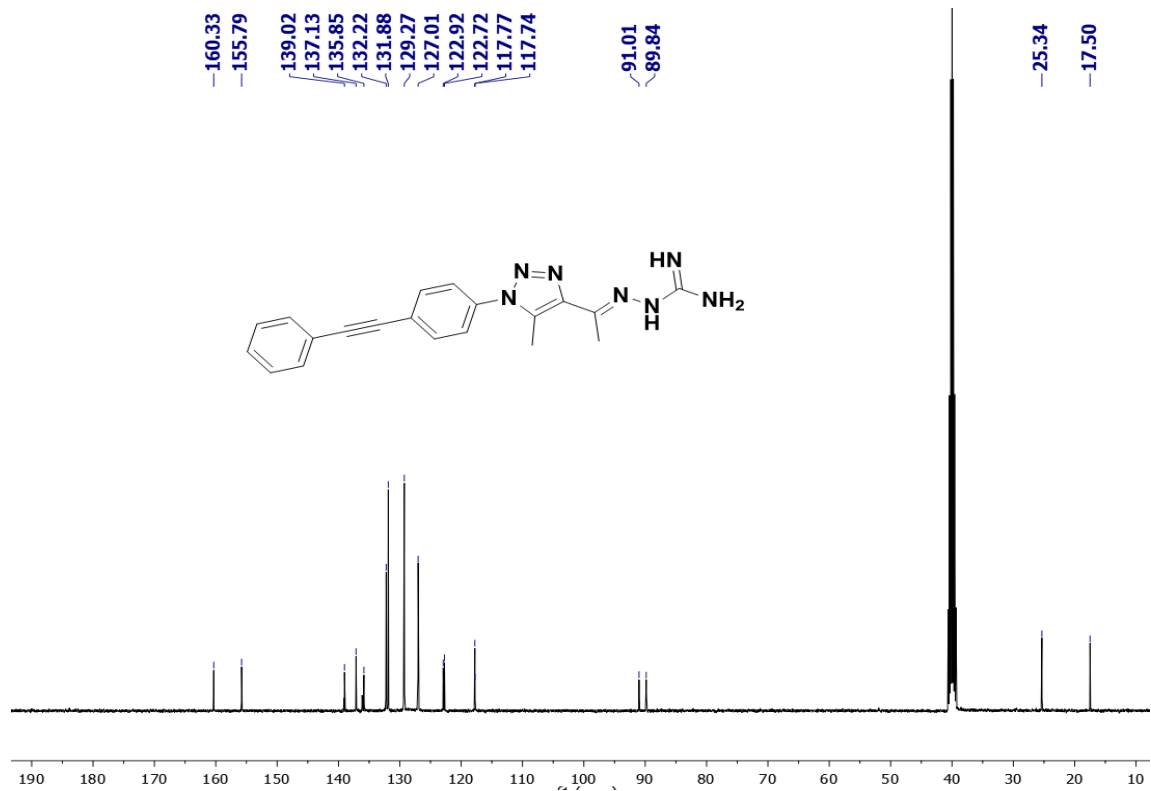


	RT	Area	% Area	Height
1	15.251	212107	0.49	17149
2	16.032	135351	0.31	14260
3	22.990	84749	0.19	5648
4	23.806	43255800	99.01	3841452

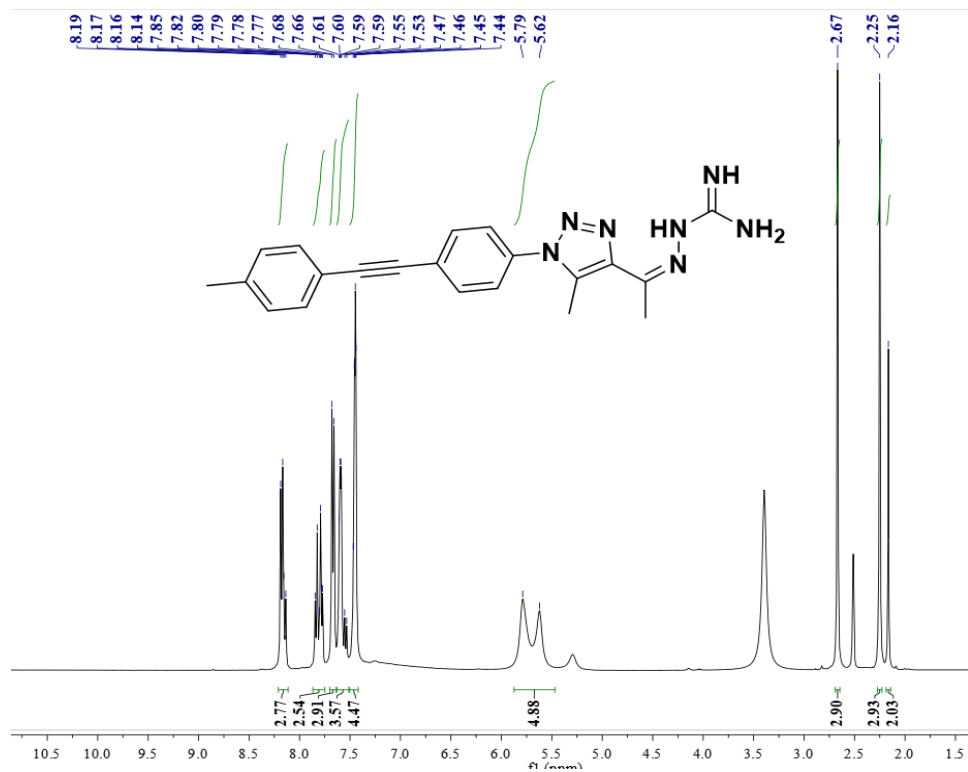
### HPLC of compound 29



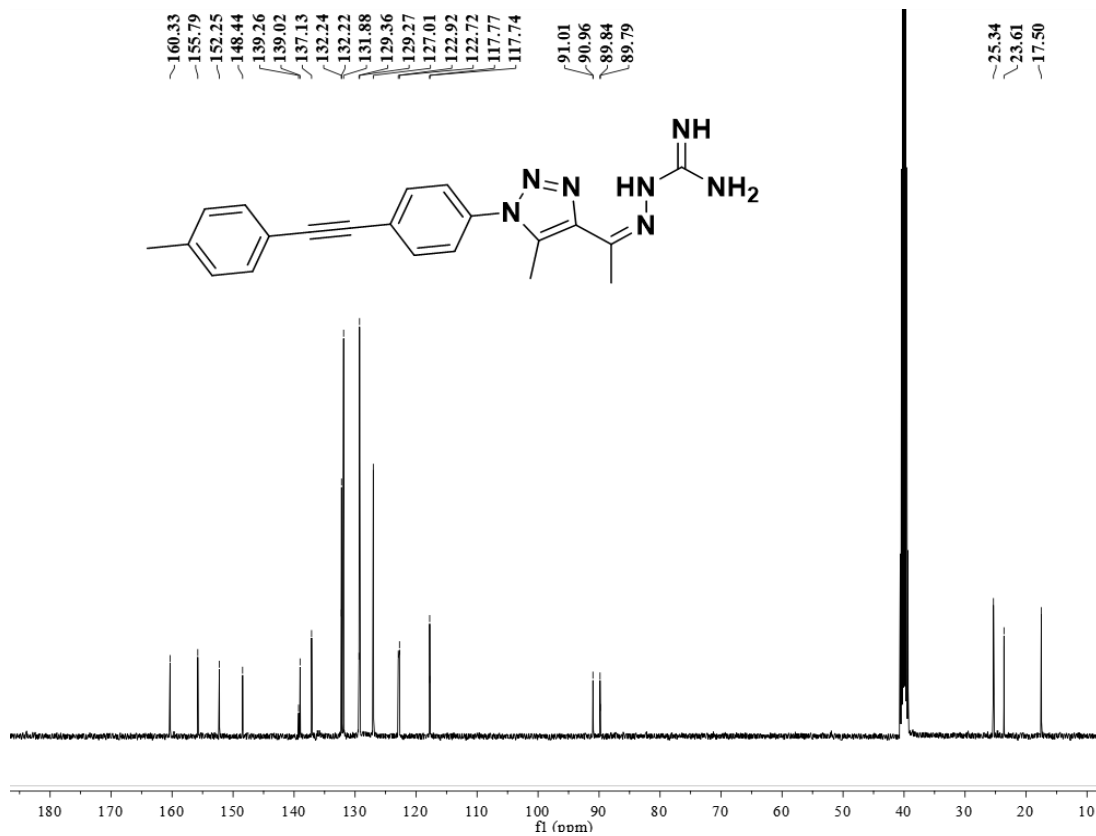
<sup>1</sup>H NMR of compound 30



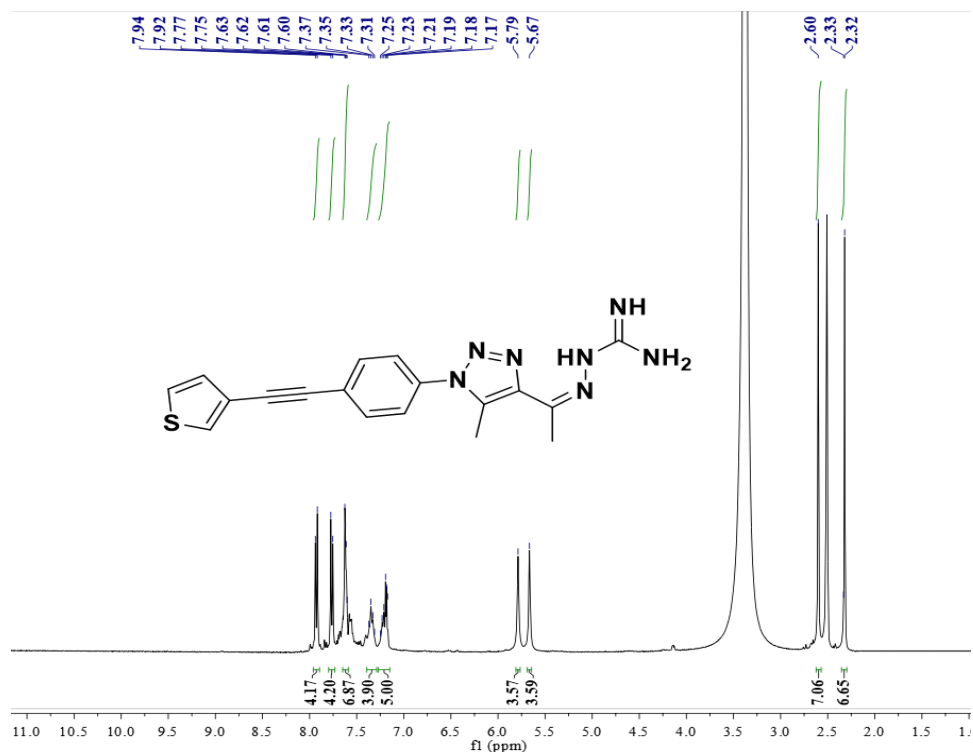
<sup>13</sup>C NMR of compound 30



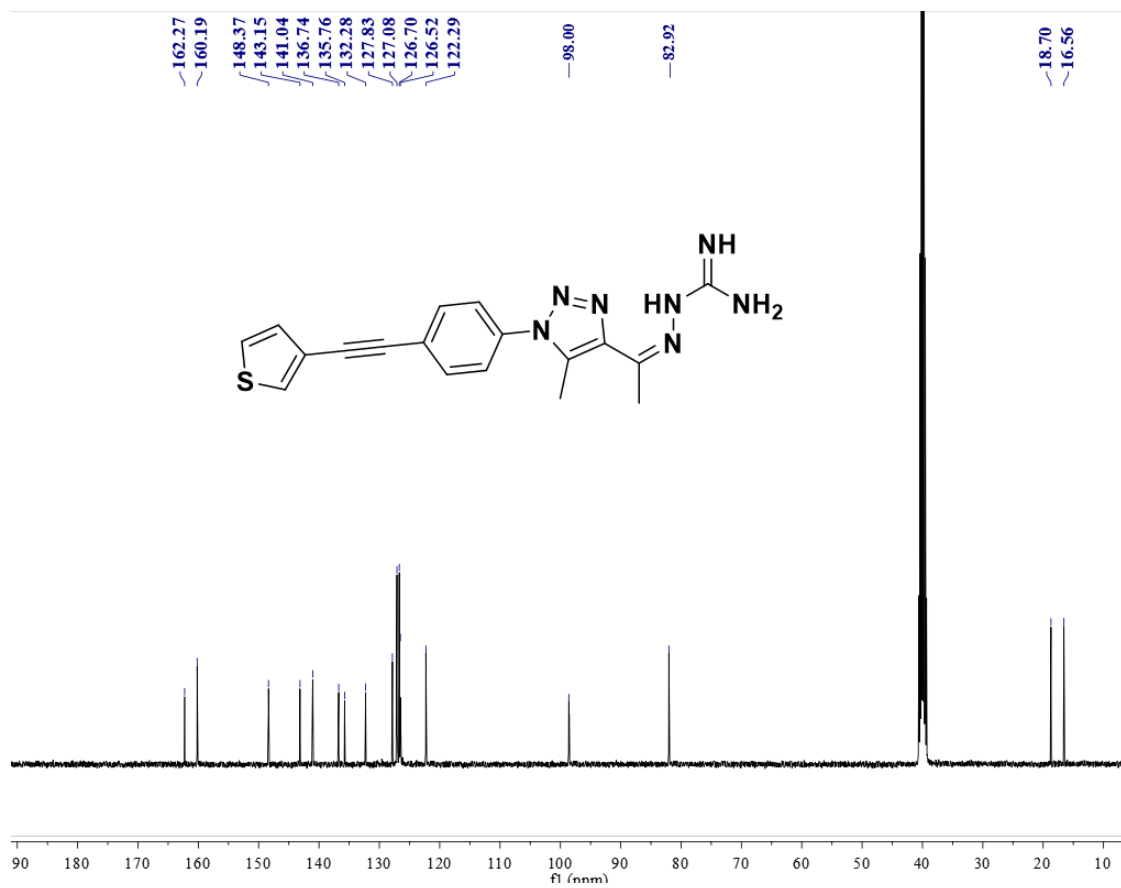
<sup>1</sup>H NMR of compound 31



<sup>13</sup>C NMR of compound 31



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



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