

**An Expedient Route to Highly Diversified [1,2,3]Triazolo[1,5-  
a][1,4]Benzodiazepines and their Evaluation for Antimicrobial,  
Antiproliferative and *In Silico* studies**

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Toyoake, Aichi 470-1192, Japan.*

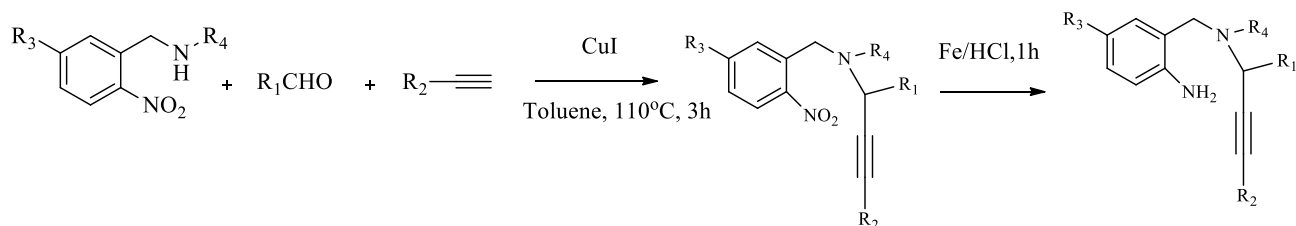
**Supplementary material**

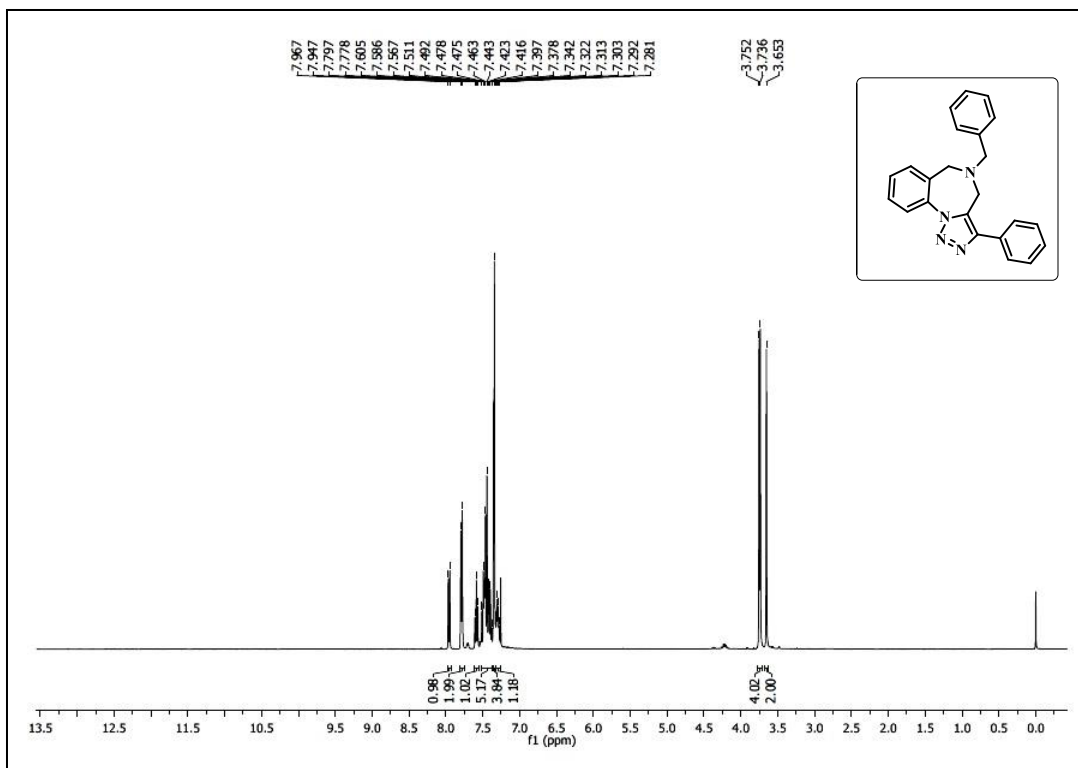
## General information:

Reagents and solvents were purchased from commercial sources (Aldrich and Merck) and used without further purification. Sodium azide (99% purity) and sodium nitrite (98% purity) were purchased from S. D. Fine-Chem Limited and used without purification. Copper (I) iodide (99.999 % purity) and was purchased from Sigma-Aldrich and used as such without further purification. All reactions were carried out in reaction vessels with magnetic stirring and no special precautions were taken to exclude air from the reaction vessels. The reactions were monitored by thin layer chromatography. Analytical TLC was performed on pre-coated aluminium sheets of silica gel 60F<sub>254</sub> of 0.2 mm thickness (Merck, Germany). Column chromatography was performed on silica gel (100-200mesh), SRL, India. Melting points were determined on Gallenkamp melting point apparatus using capillary tubes and are uncorrected. <sup>1</sup>HNMR (400MHz) and <sup>13</sup>CNMR (100MHz) spectra were recorded in CDCl<sub>3</sub>/ TMS solution with TMS as internal standard on a Bruker spectrometer. Mass spectra were recorded using ESI/HRMS at 60000 resolutions in Thermo scientific Exactive mass spectrometer. Elemental analyses were recorded using a ThermoFinnigan FLASH EA1112 CHN analyzer.

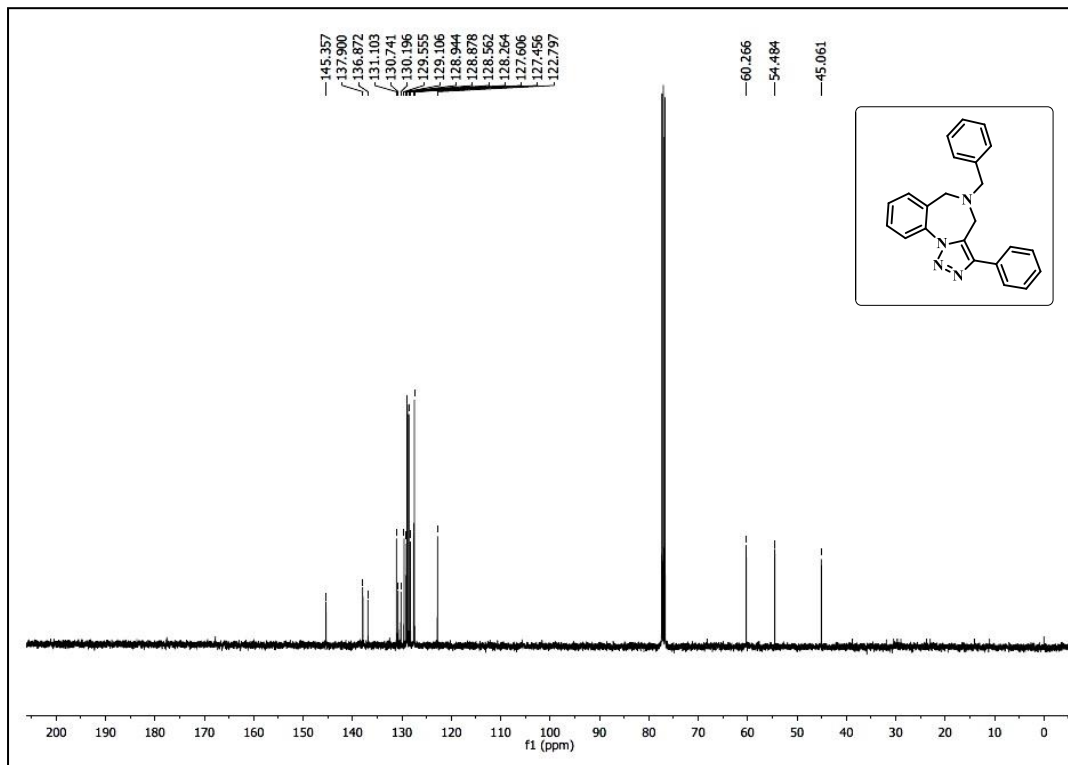
## Preparation of 2-amino-*N*-benzylpropargylamines:

The A<sup>3</sup>-coupling reaction of *N*-benzyl-1-(2-nitrophenyl)methanamine, aromatic aldehyde, alkyne affords 2-nitro-*N*-benzylpropargylamines which is reduced further to prepare 2-amino-*N*-benzylpropargylamines **1**.

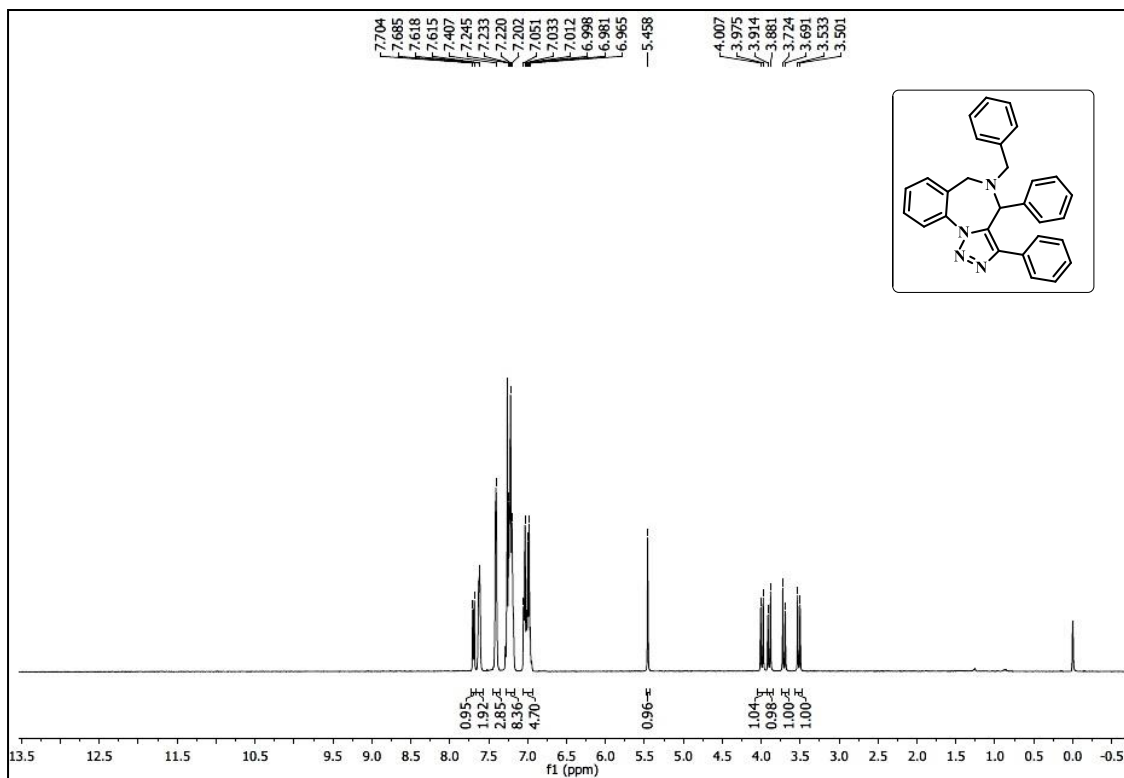




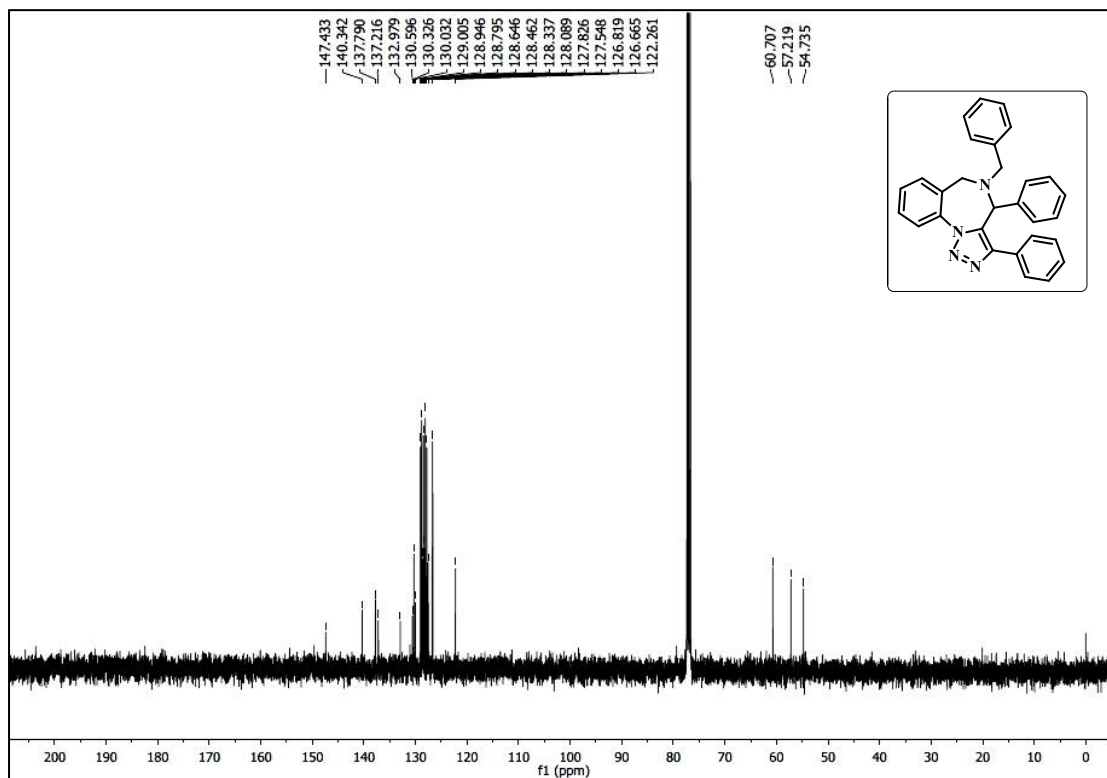
**<sup>1</sup>H NMR of 2a**



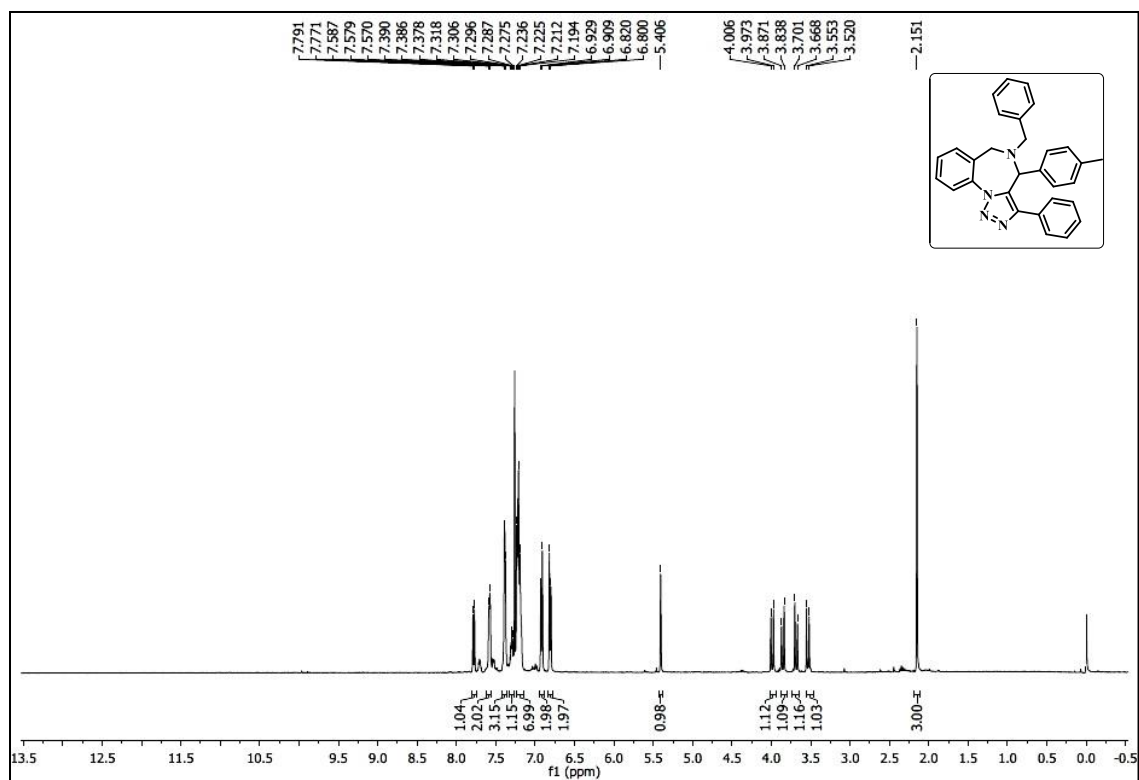
**<sup>13</sup>C NMR of 2a**



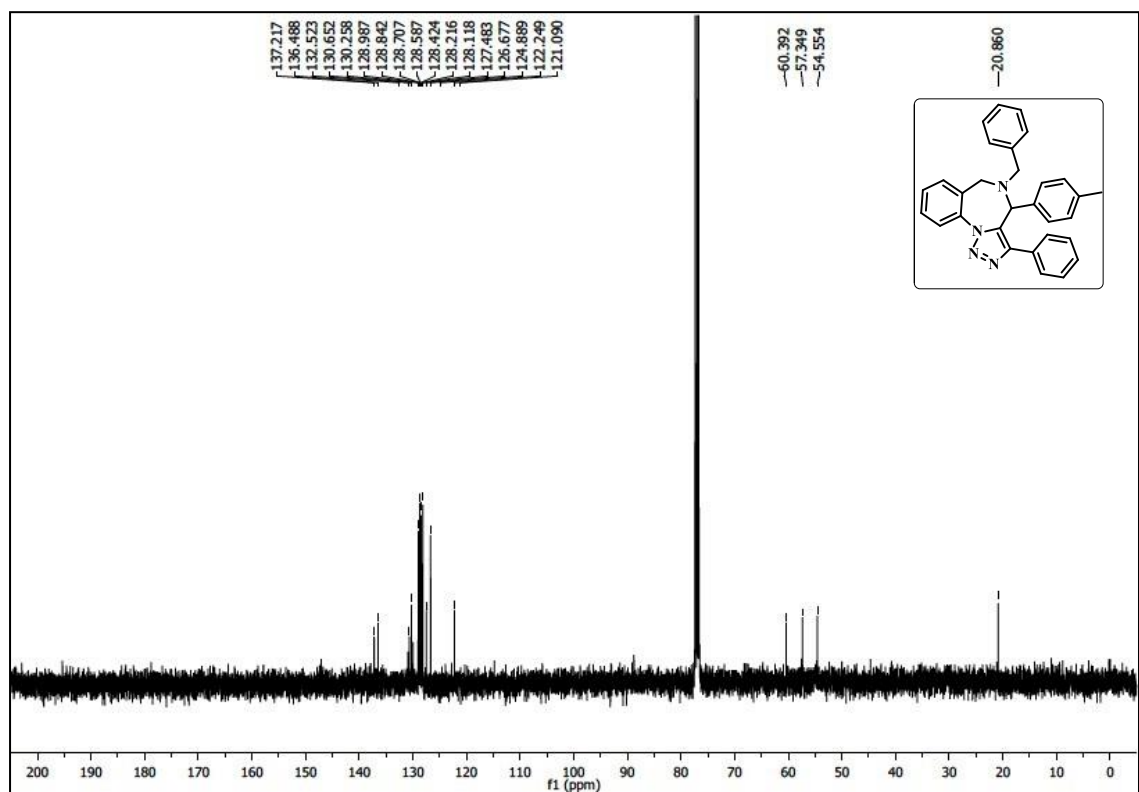
**<sup>1</sup>H NMR of 2b**



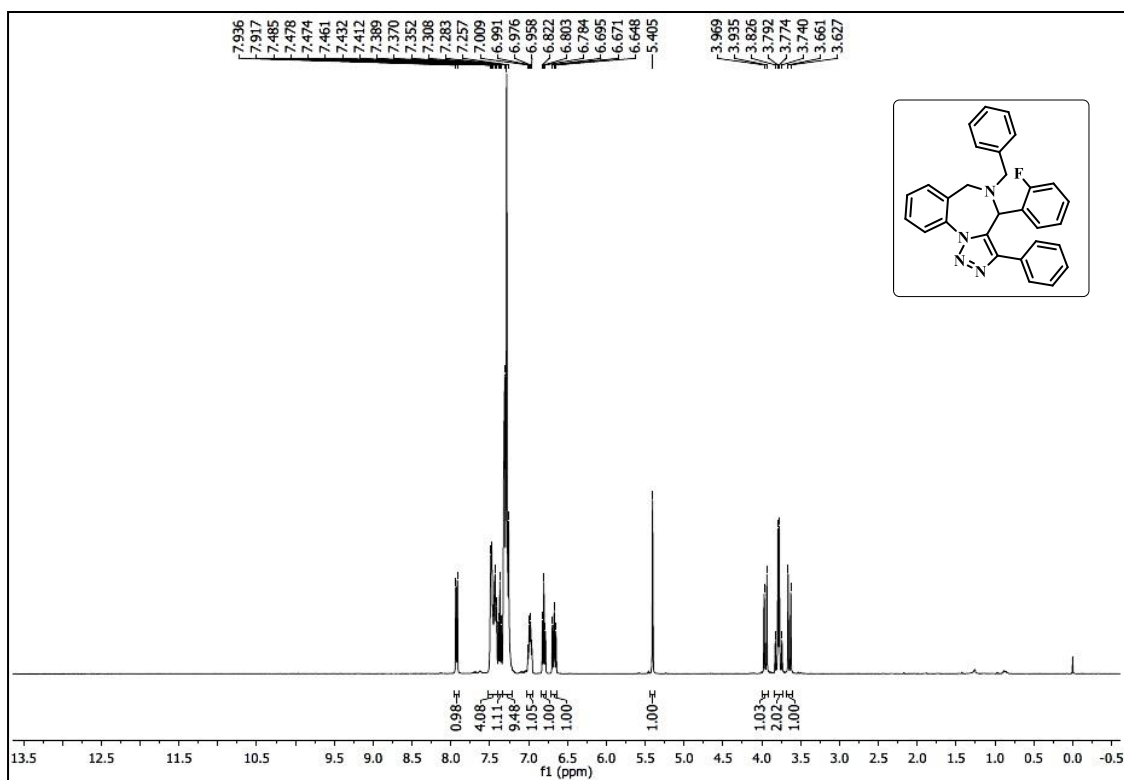
**<sup>13</sup>C NMR of 2b**



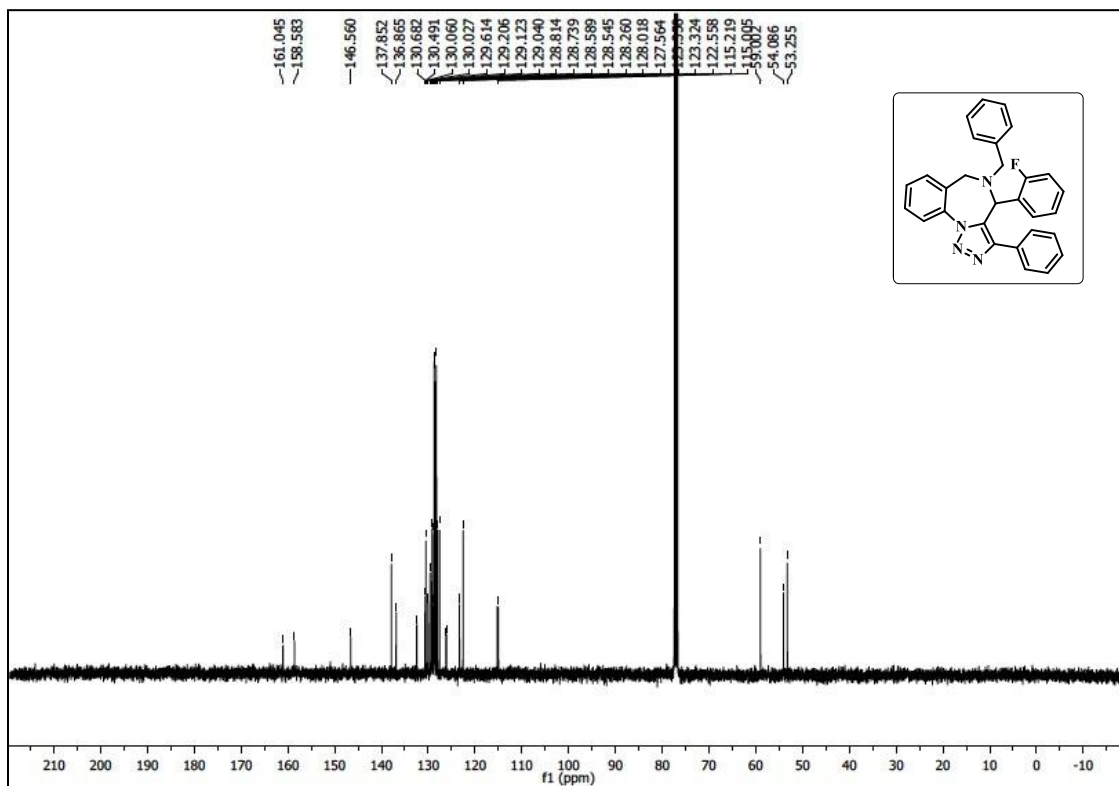
<sup>1</sup>H NMR of 2c



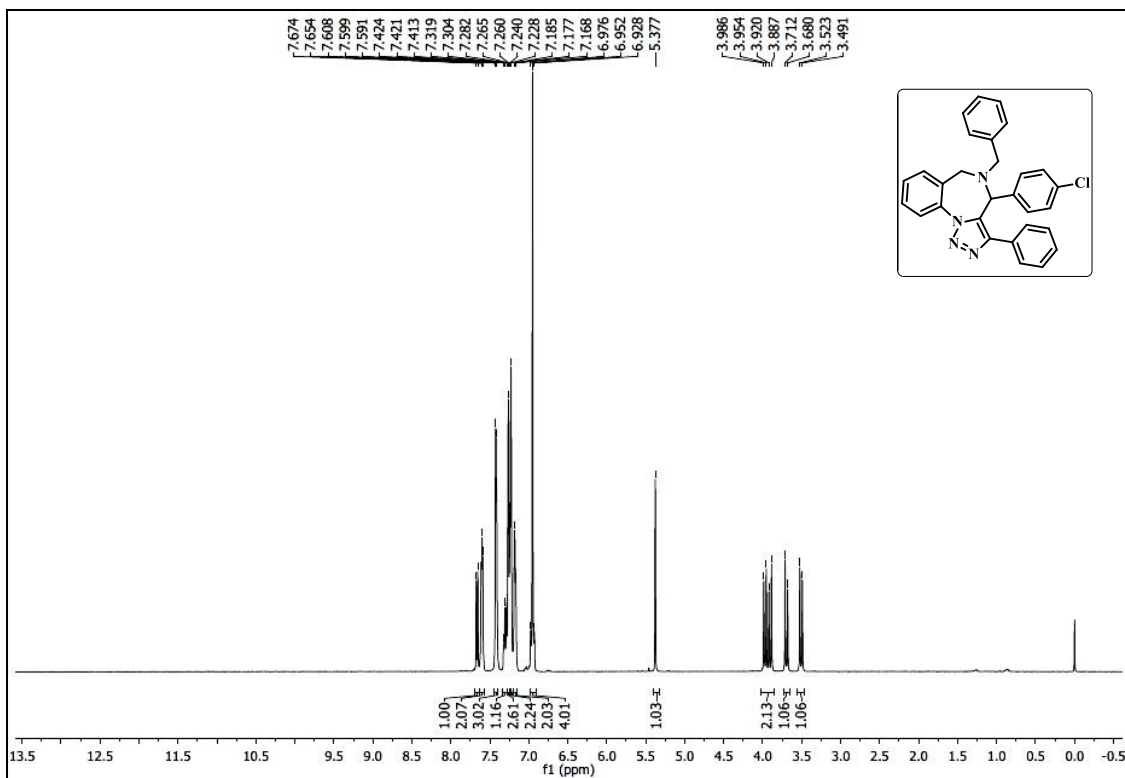
<sup>13</sup>C NMR of 2c



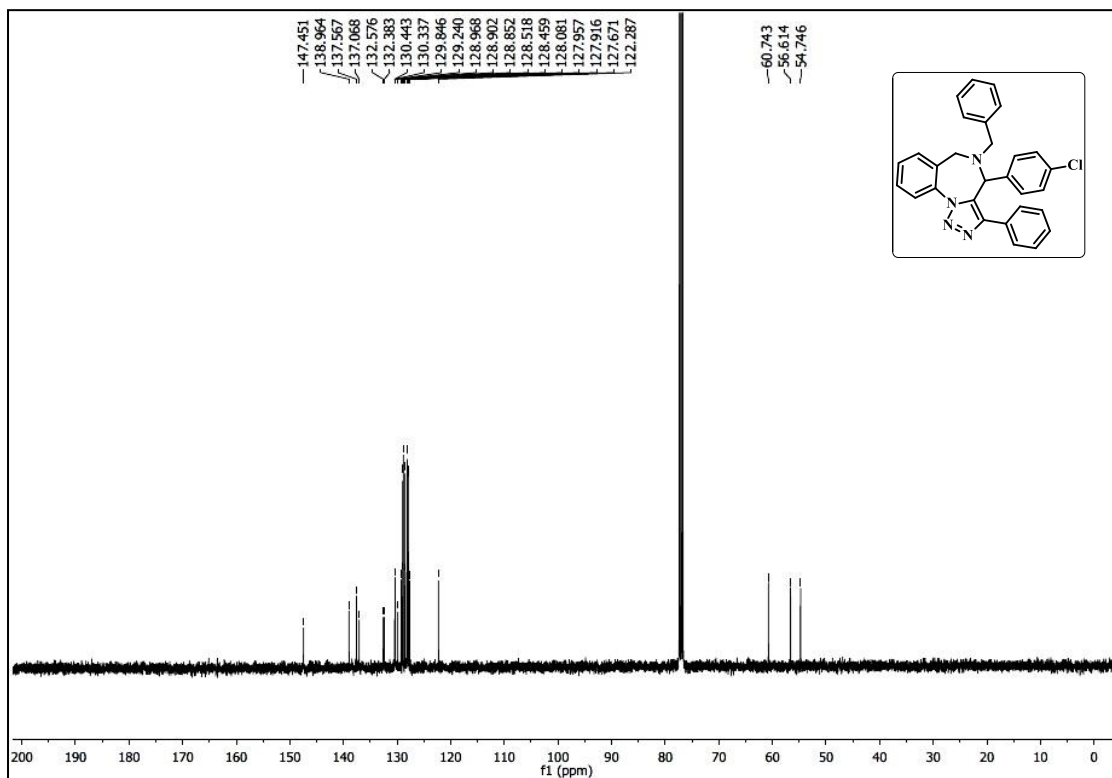
**<sup>1</sup>H NMR of 2d**



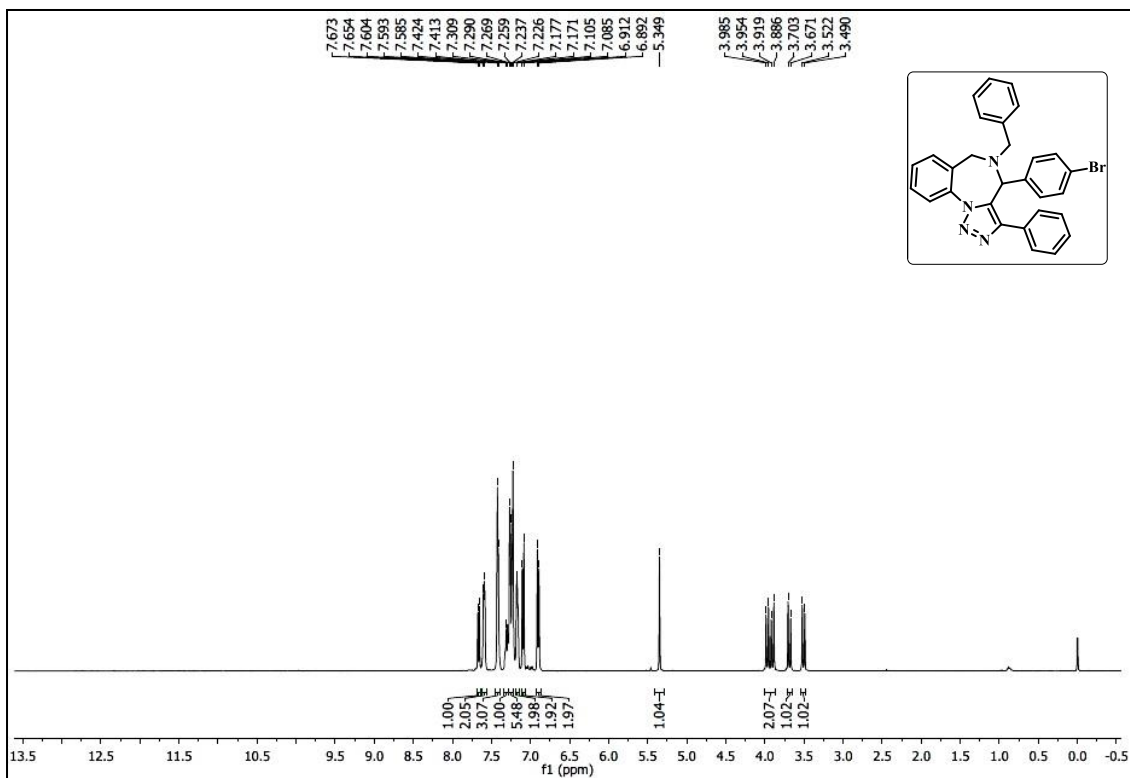
**<sup>13</sup>C NMR of 2d**



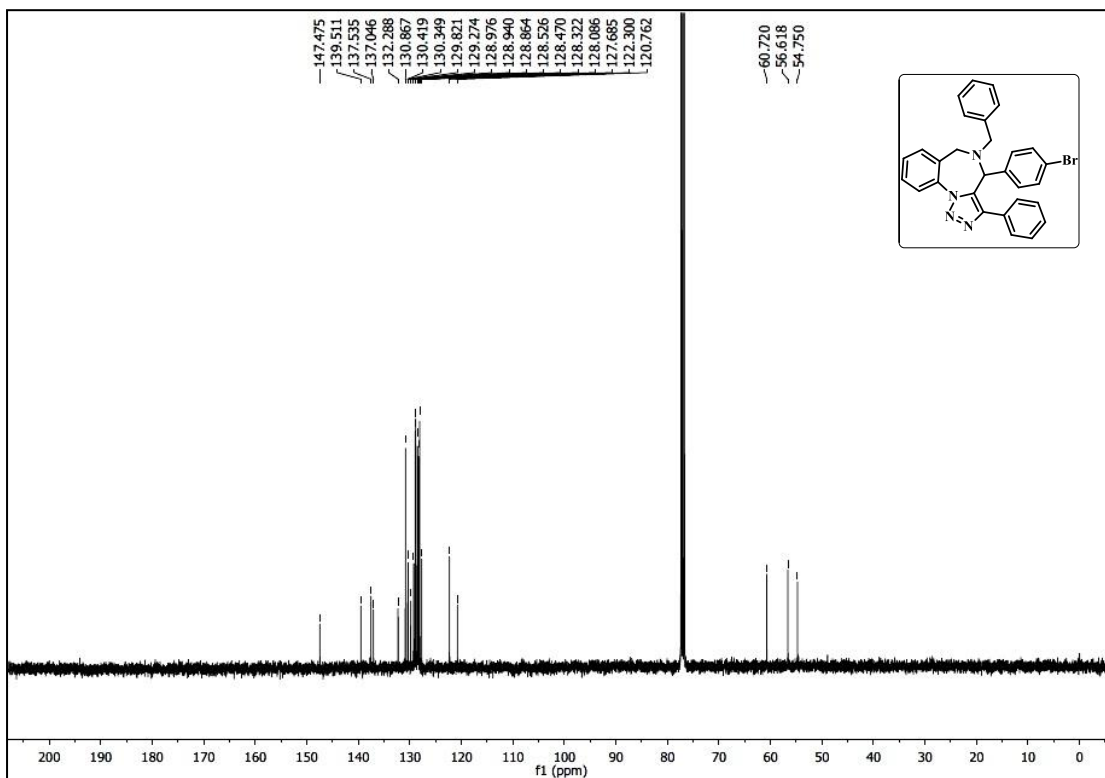
**<sup>1</sup>H NMR of 2e**



**<sup>13</sup>C NMR of 2e**

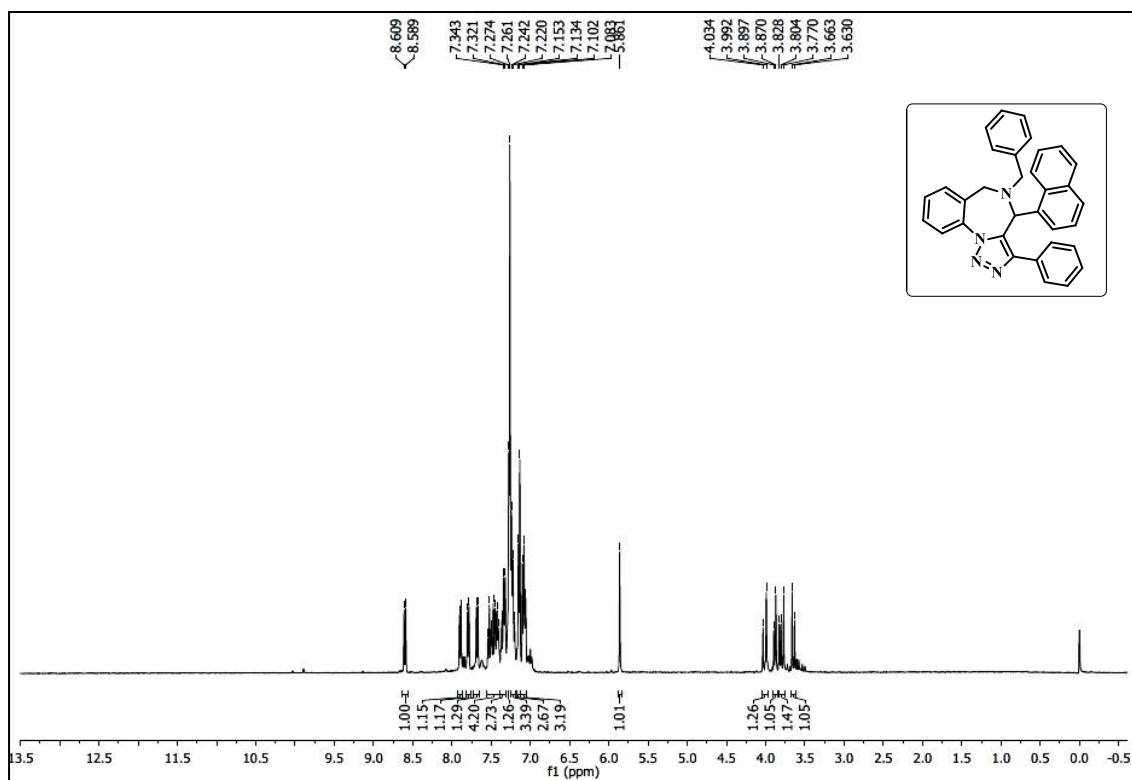


**<sup>1</sup>H NMR of 2f**

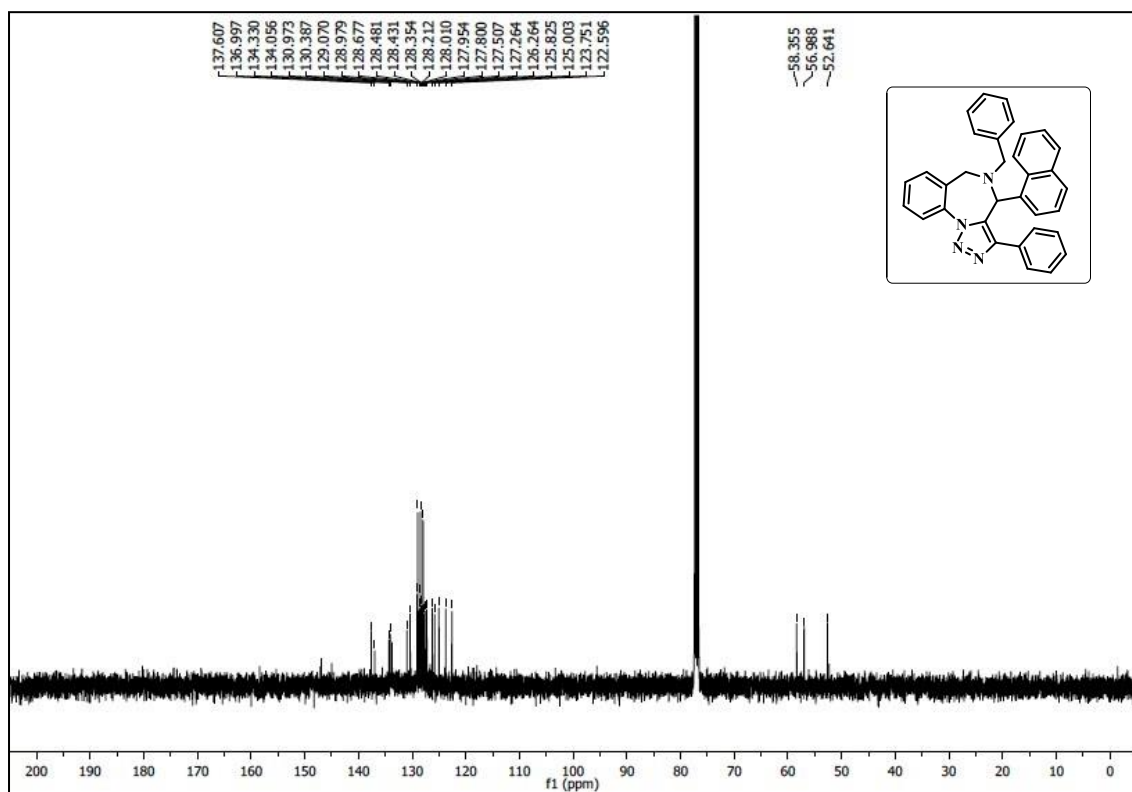


**<sup>13</sup>C NMR of 2f**

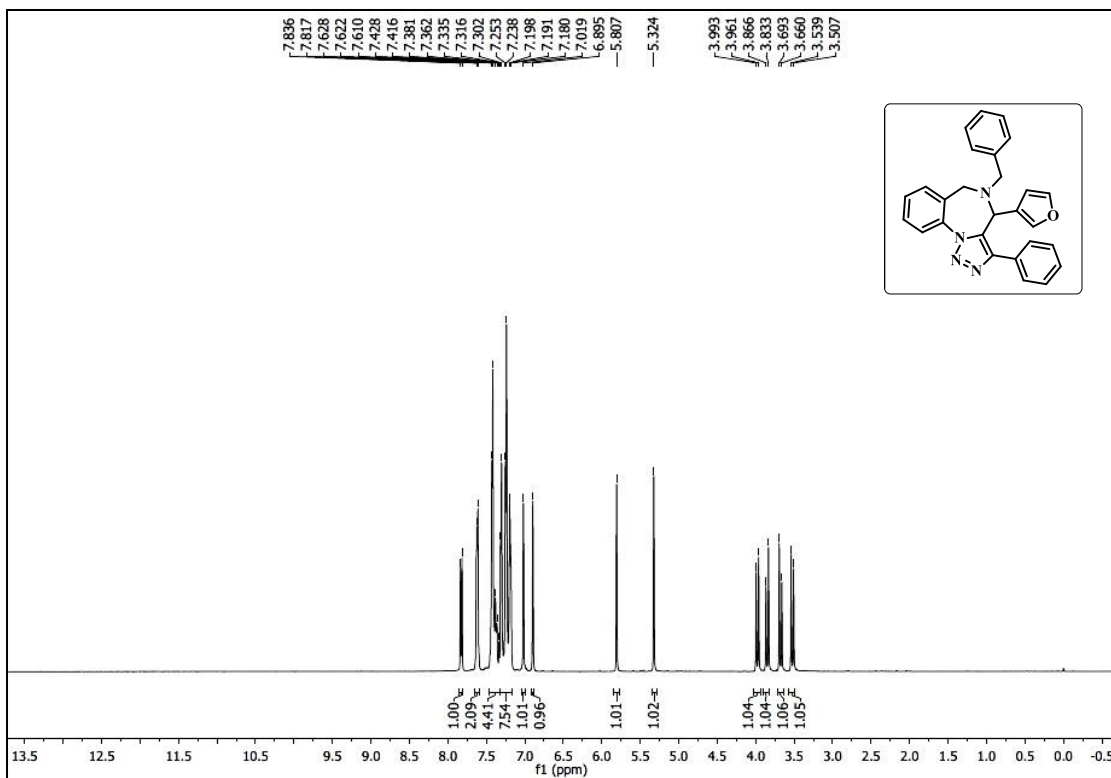




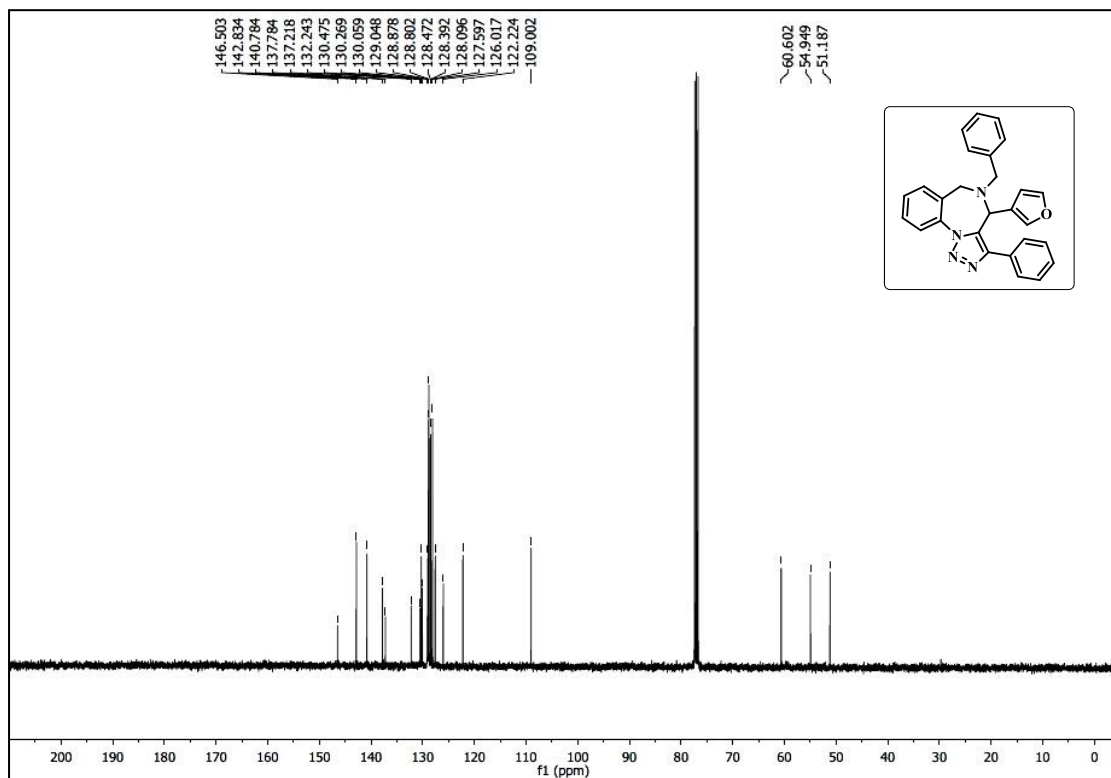
**<sup>1</sup>H NMR of 2g**



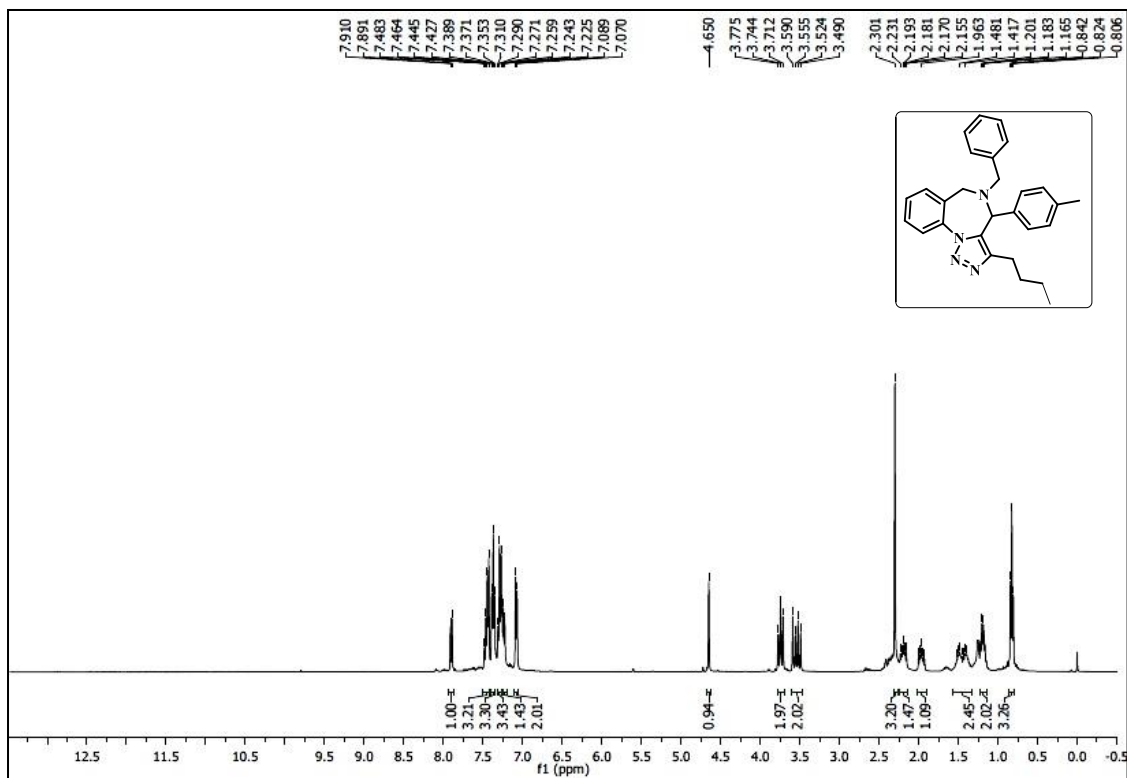
**<sup>13</sup>C NMR of 2g**



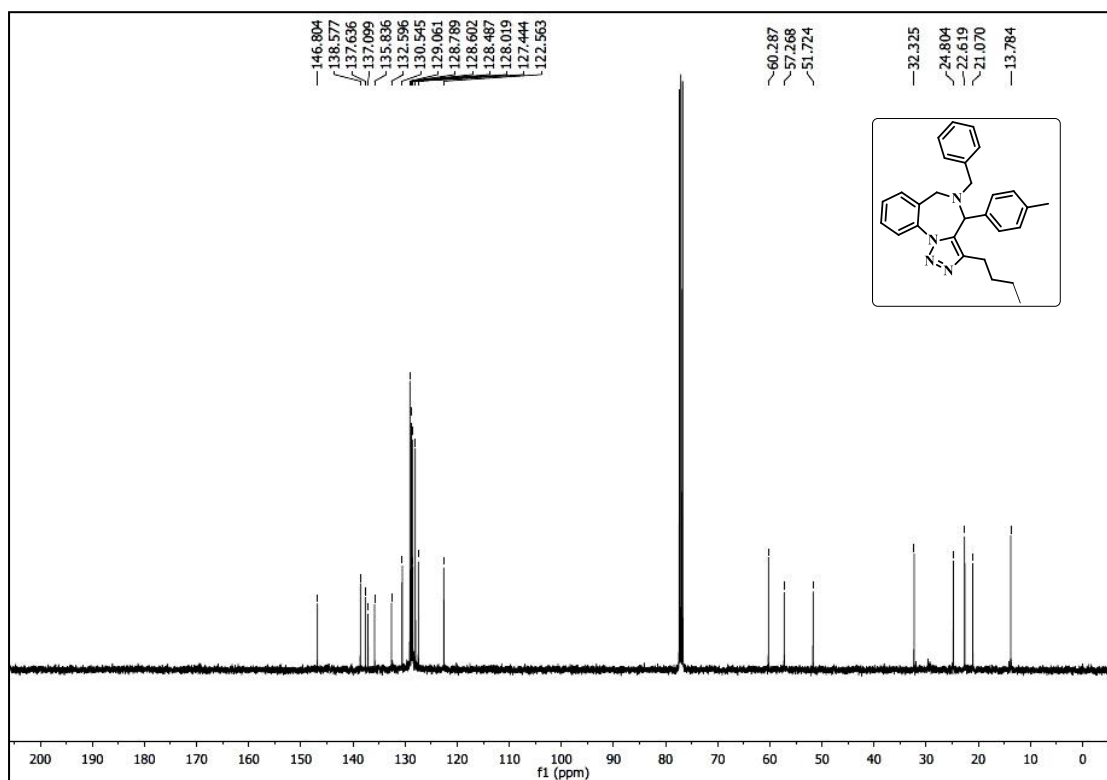
**<sup>1</sup>H NMR of 2h**



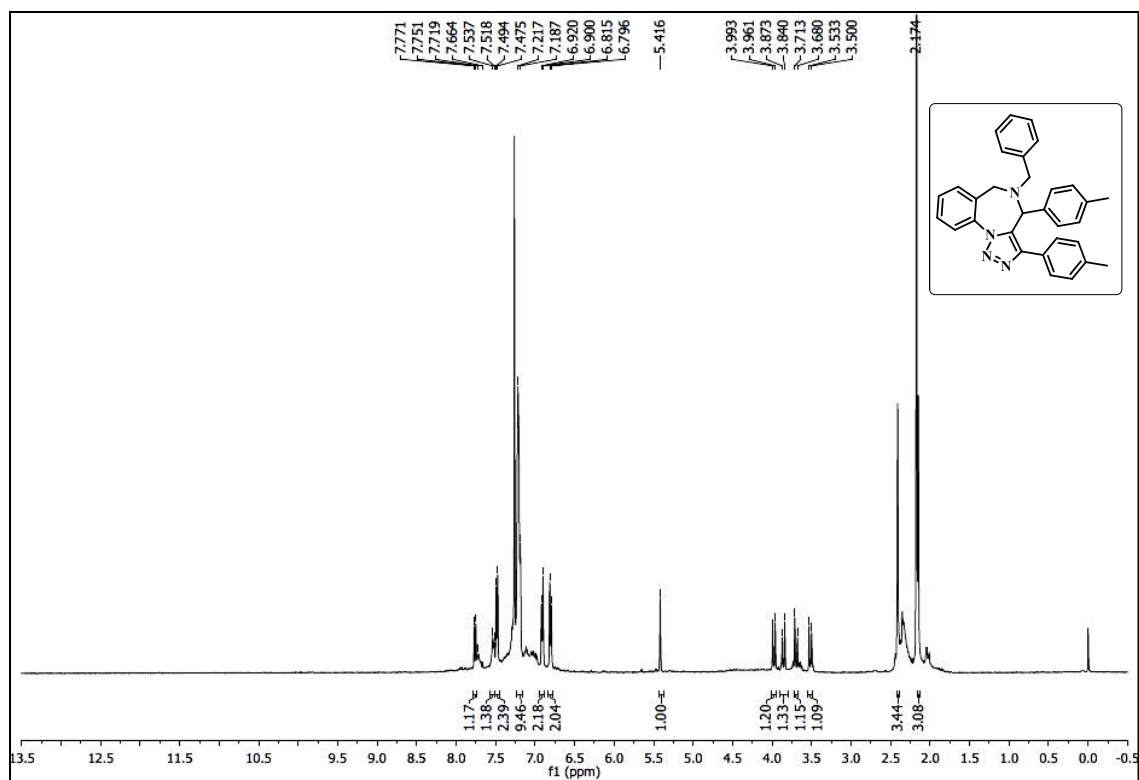
**<sup>13</sup>C NMR of 2h**



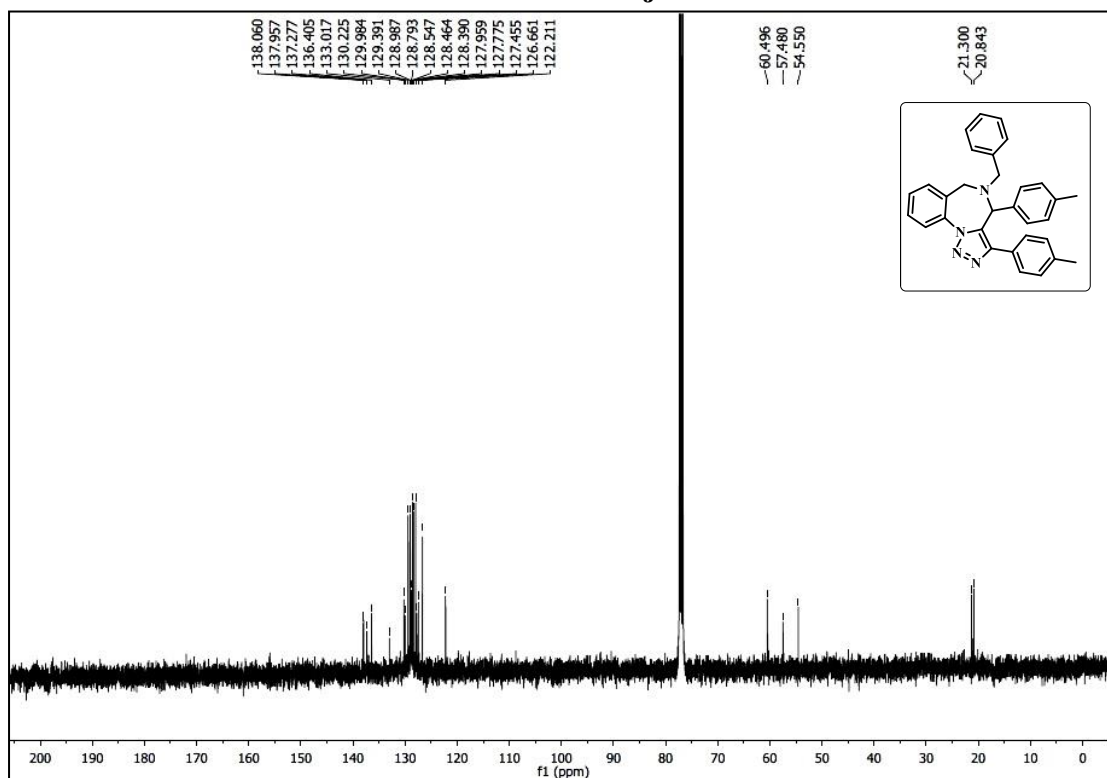
**<sup>1</sup>H NMR of 2i**



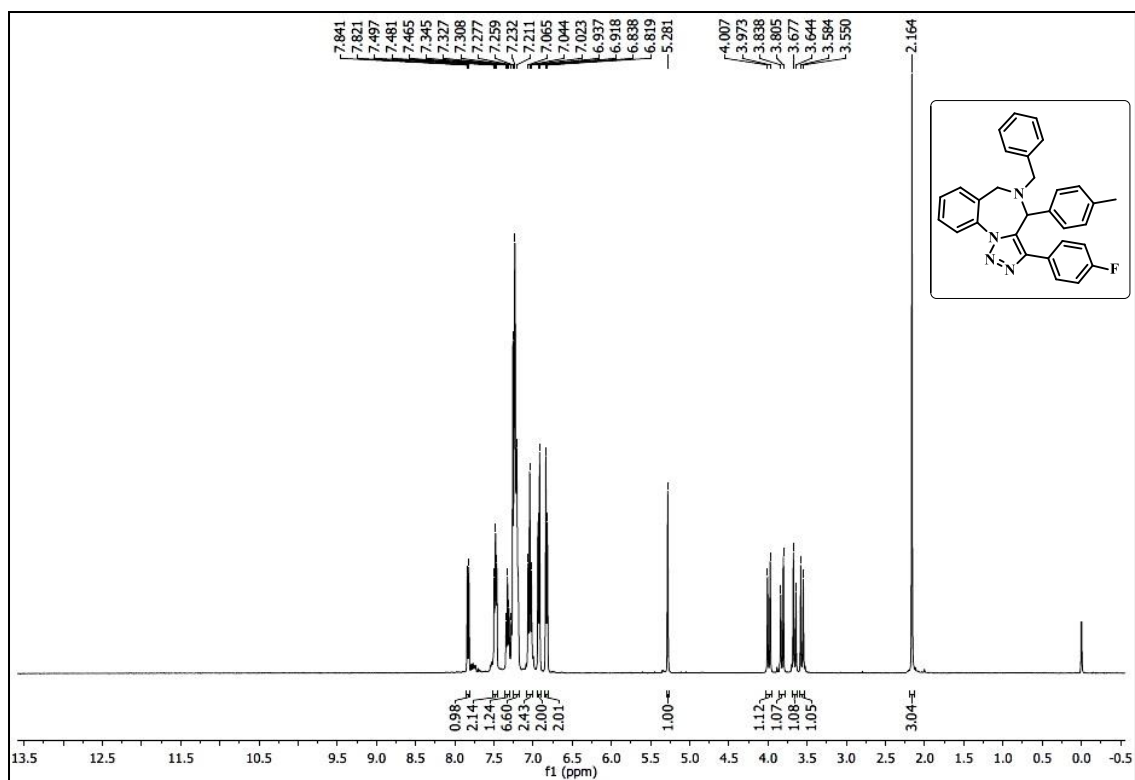
**<sup>13</sup>C NMR of 2i**



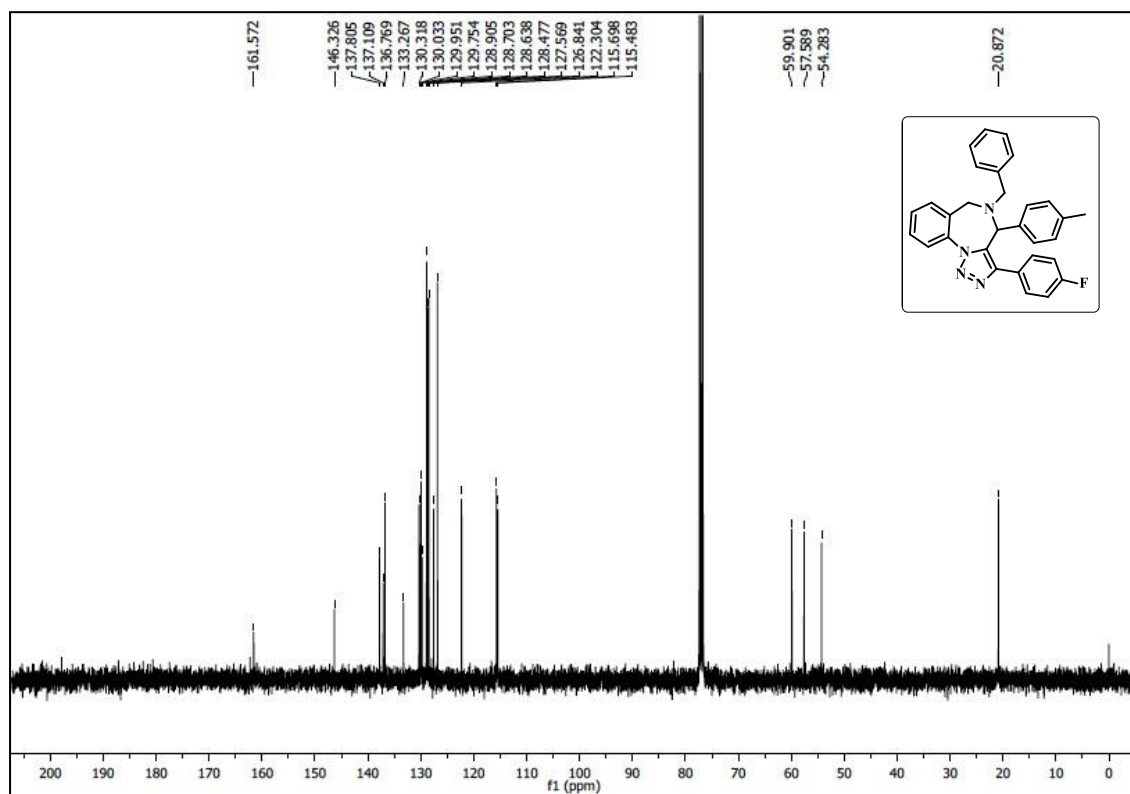
**<sup>1</sup>H NMR of 2j**



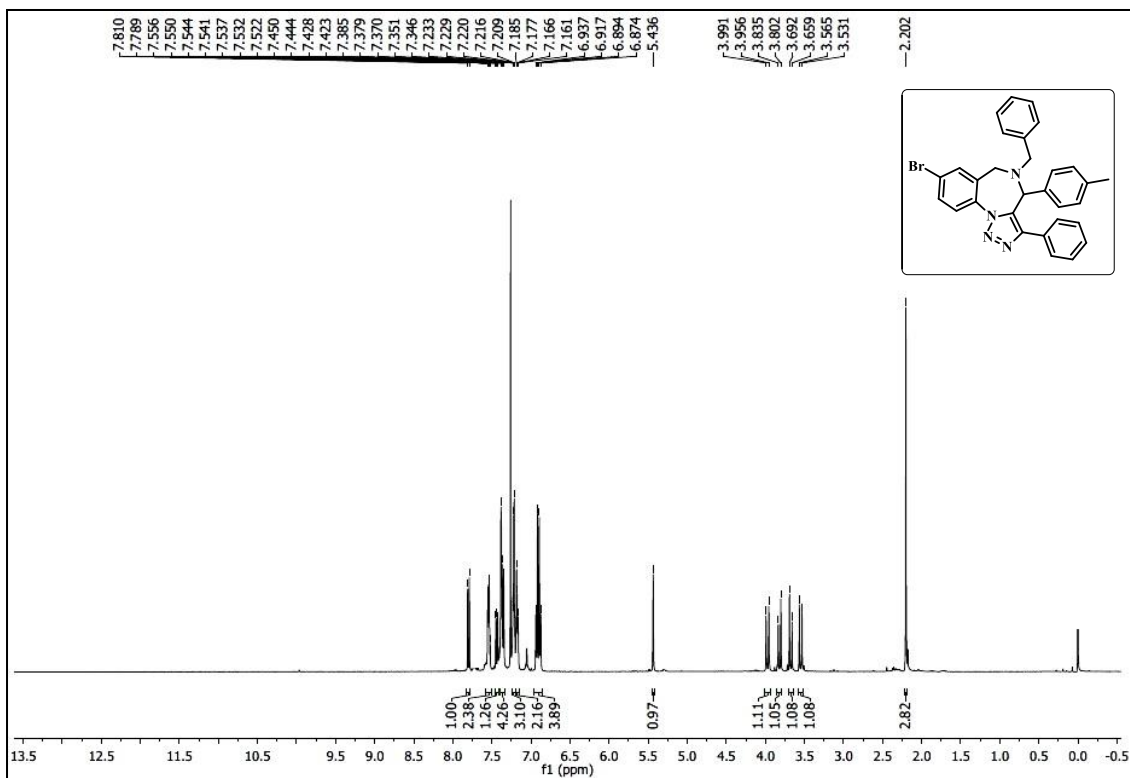
**<sup>13</sup>C NMR of 2j**



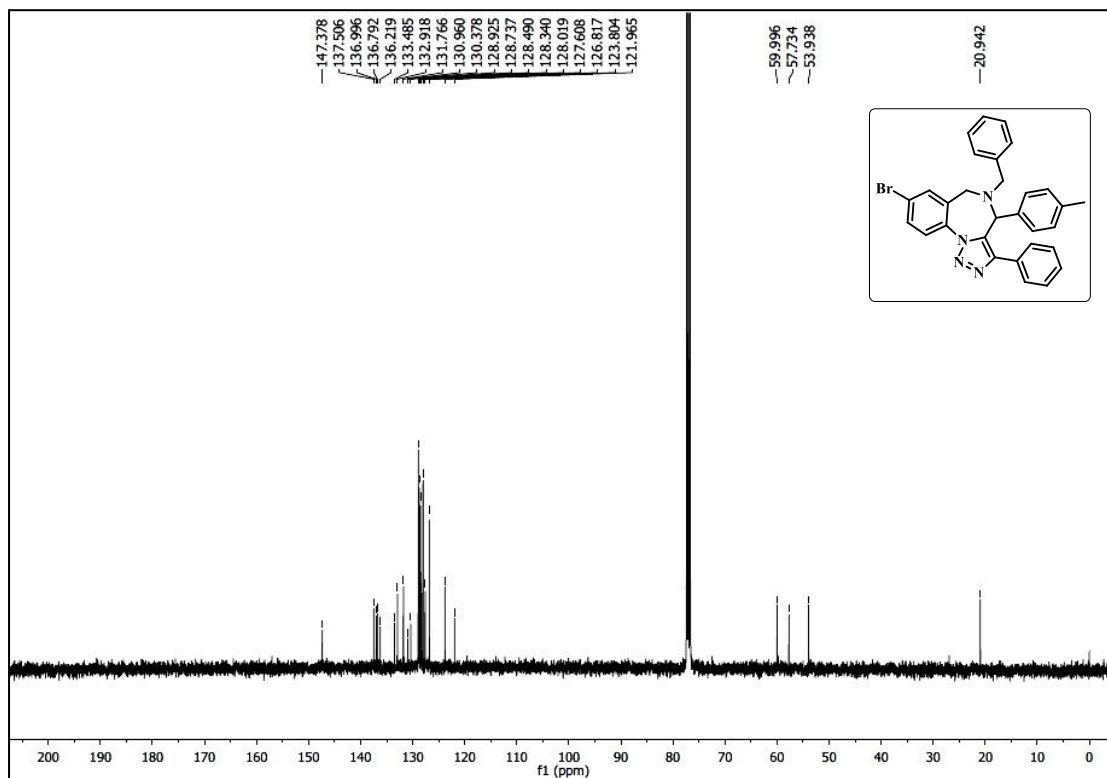
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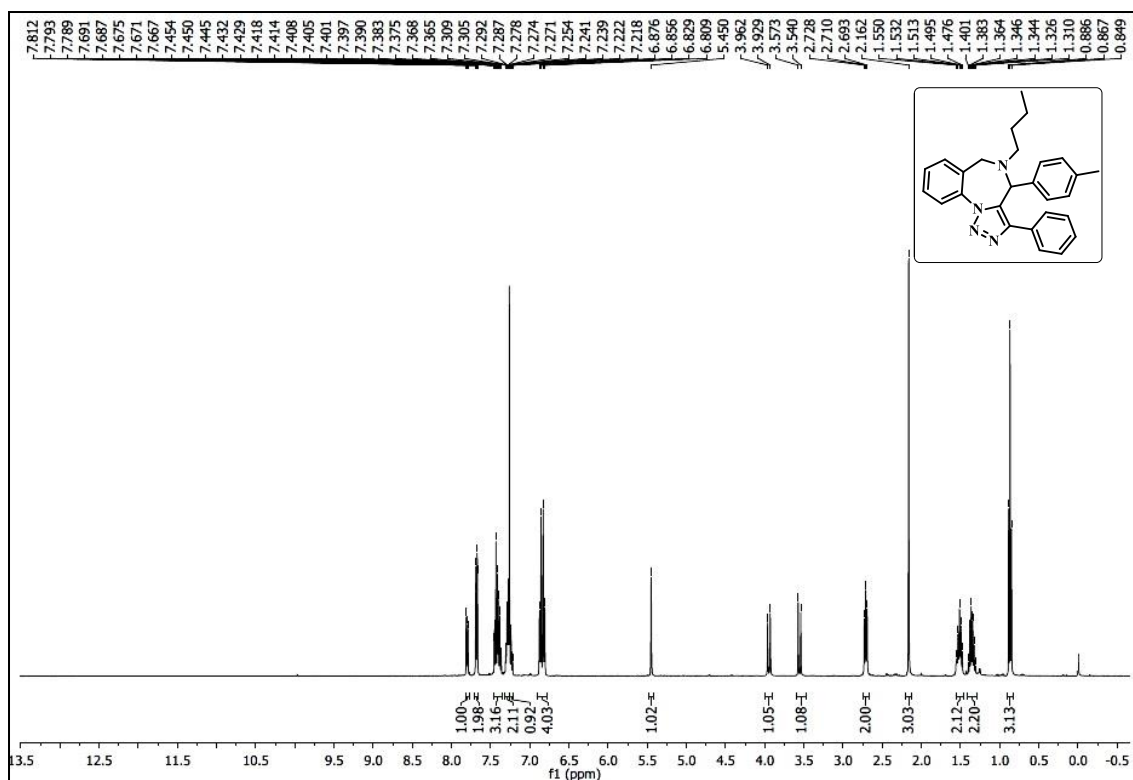
**<sup>13</sup>C NMR of 2k**



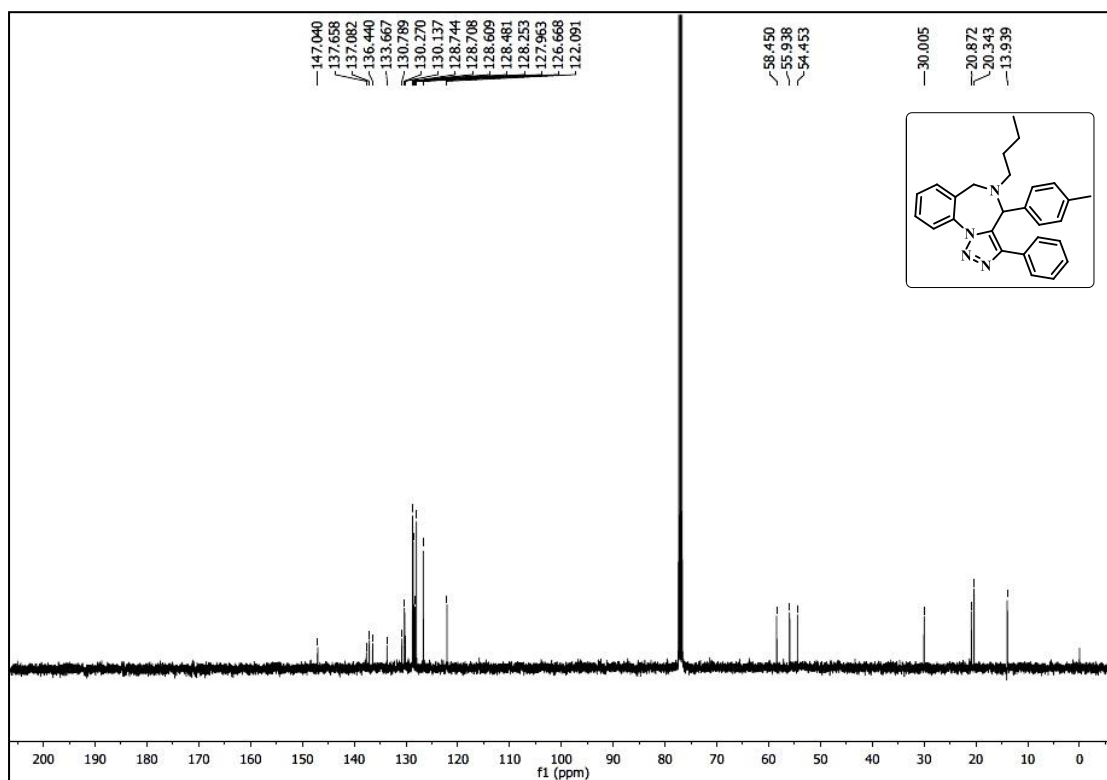
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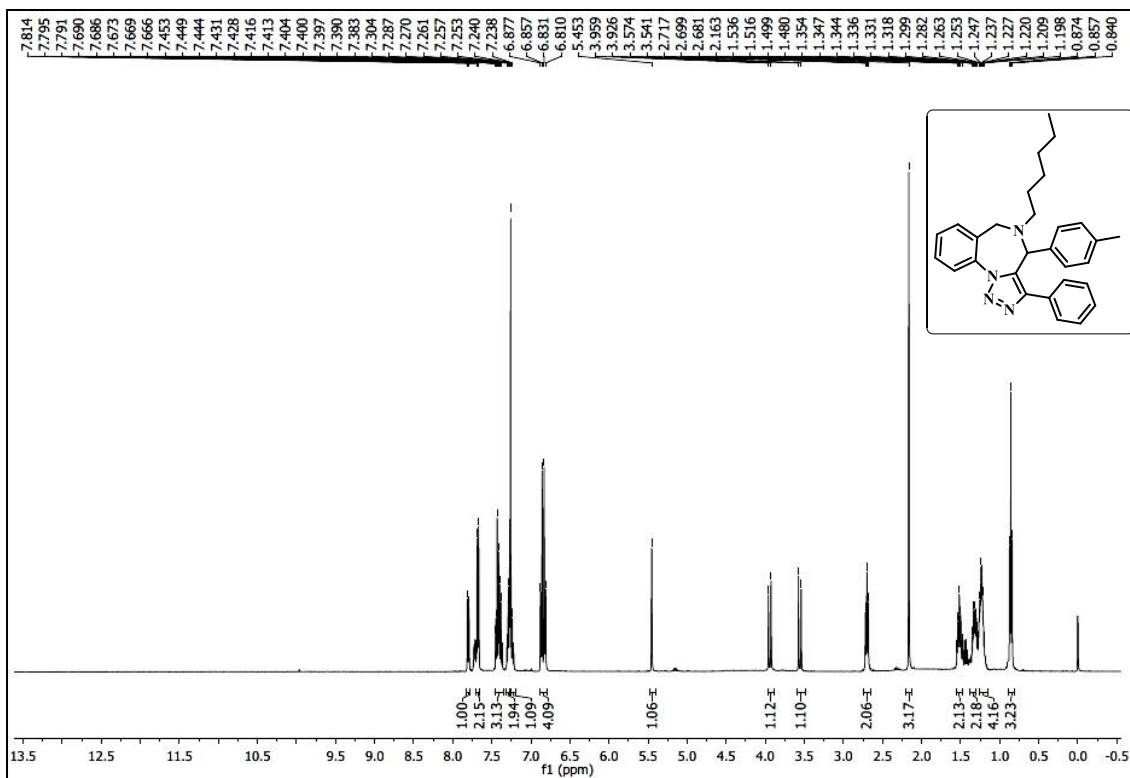
**<sup>13</sup>C NMR of 21**



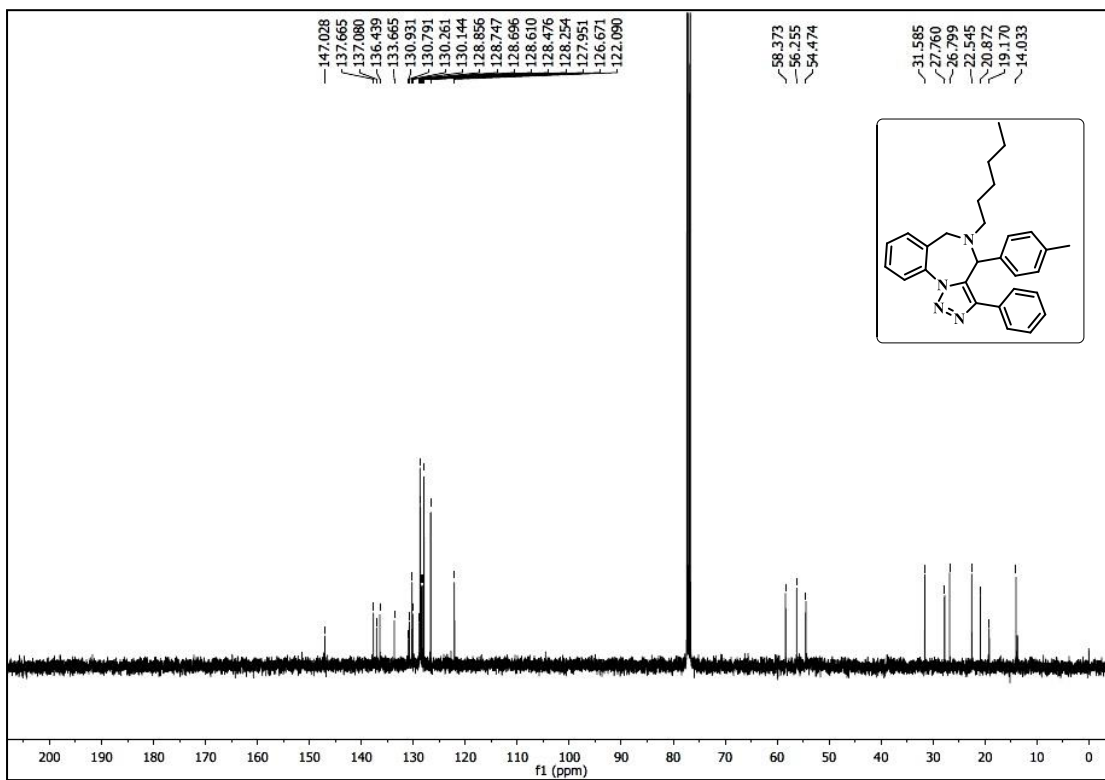
**<sup>1</sup>H NMR of 2m**



**<sup>13</sup>C NMR of 2m**

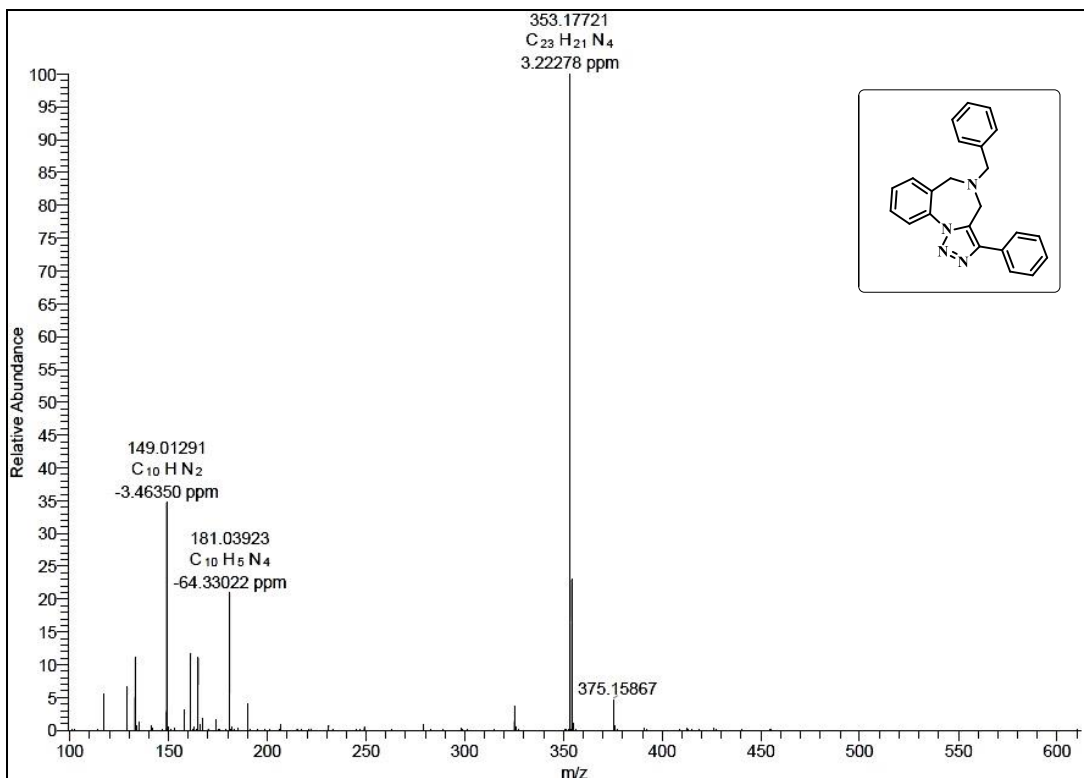


**<sup>1</sup>H NMR of 2n**

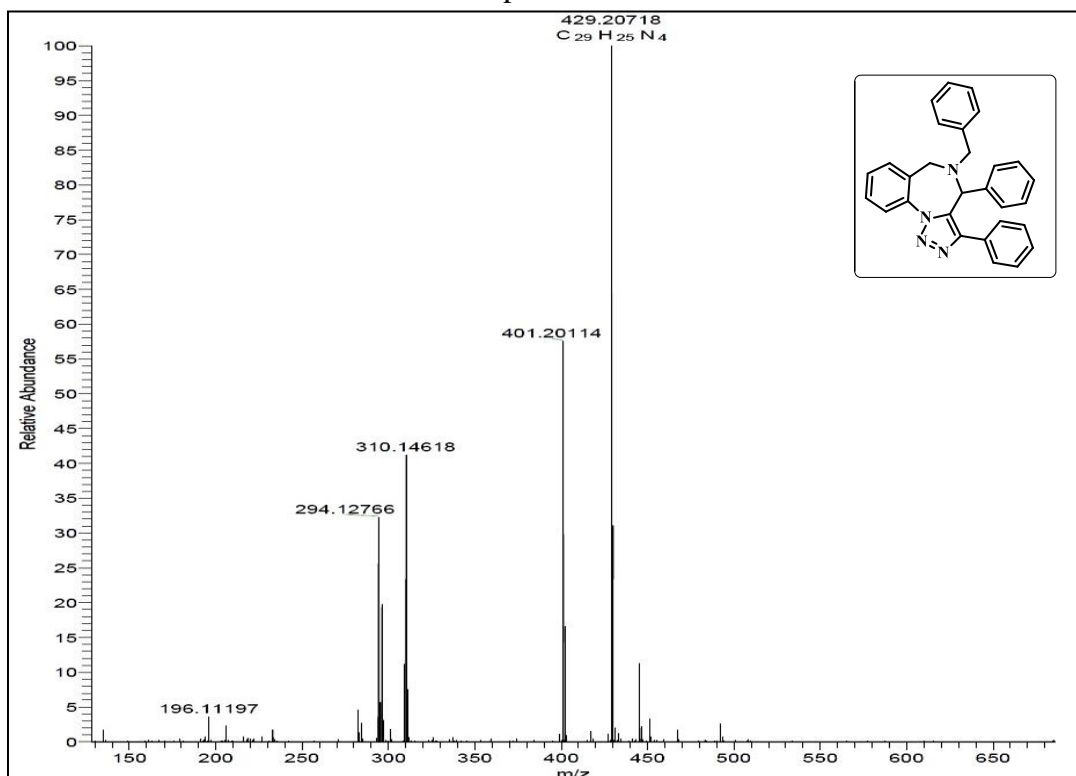


**<sup>13</sup>C NMR of 2n**

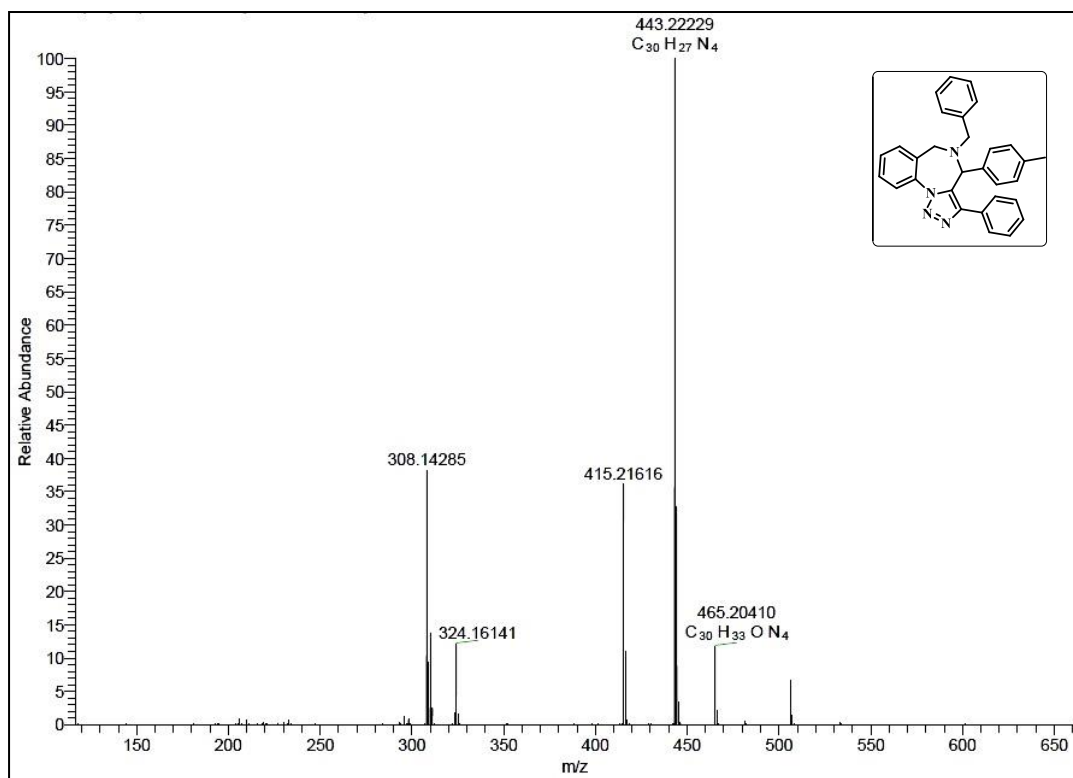




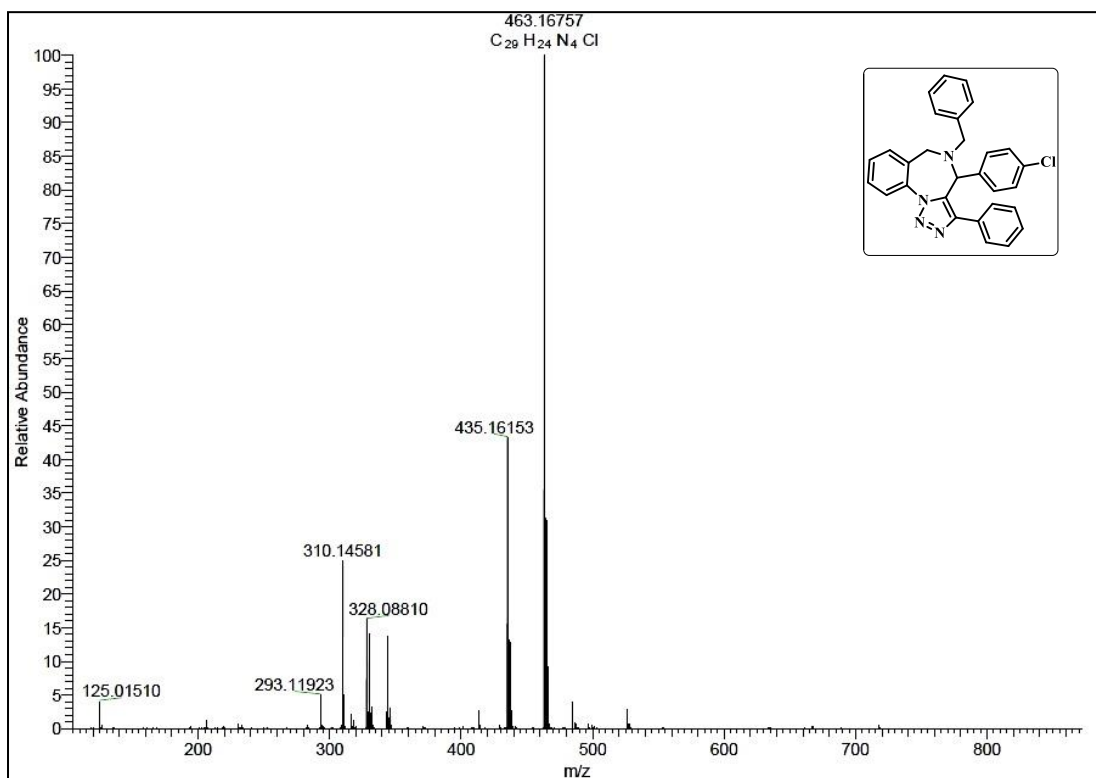
Mass spectrum of **2a**



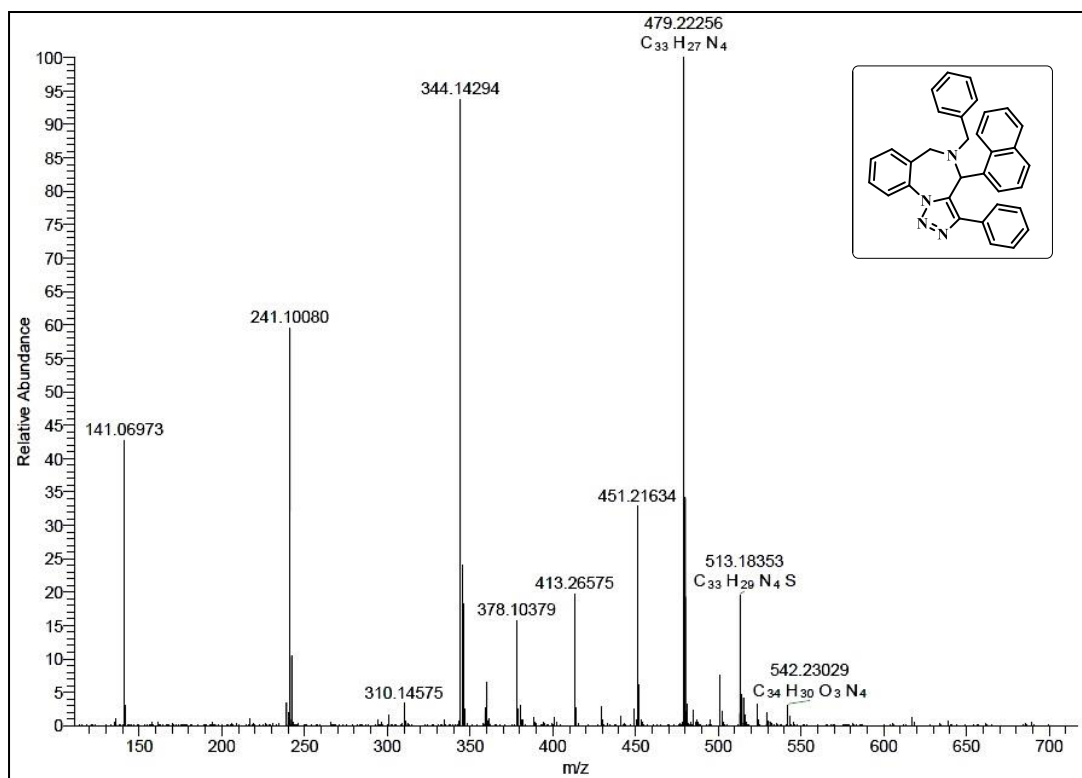
Mass spectrum of **2b**



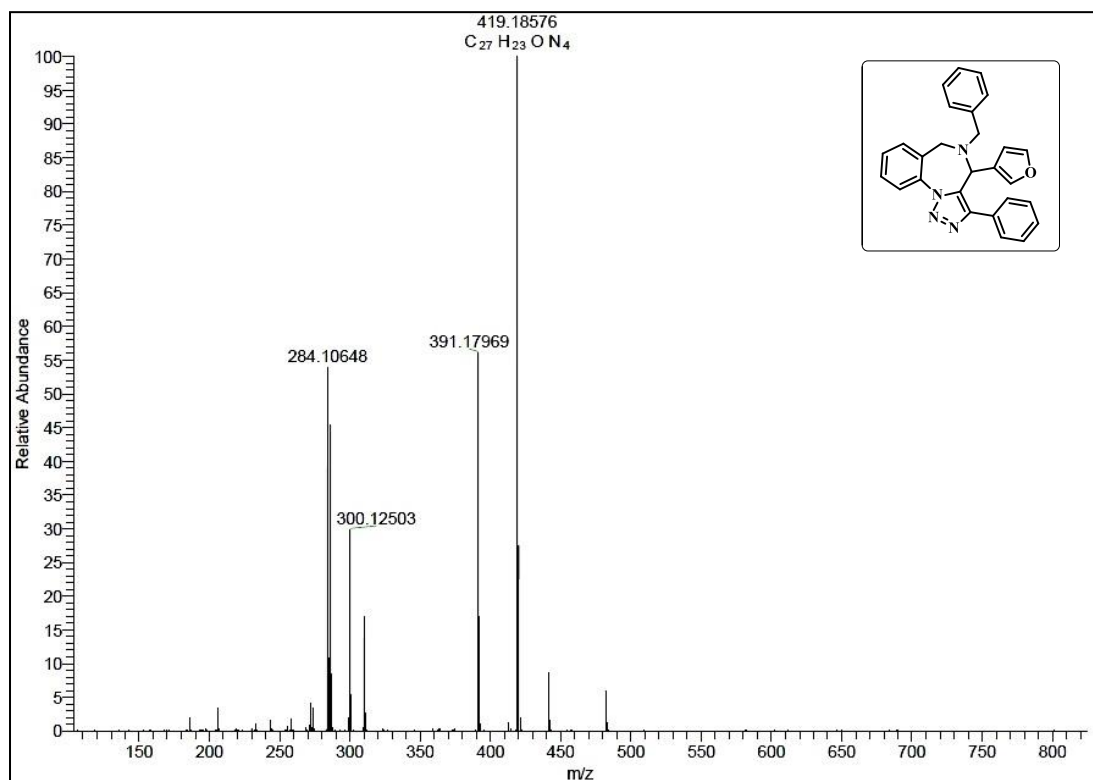
Mass spectrum of **2c**



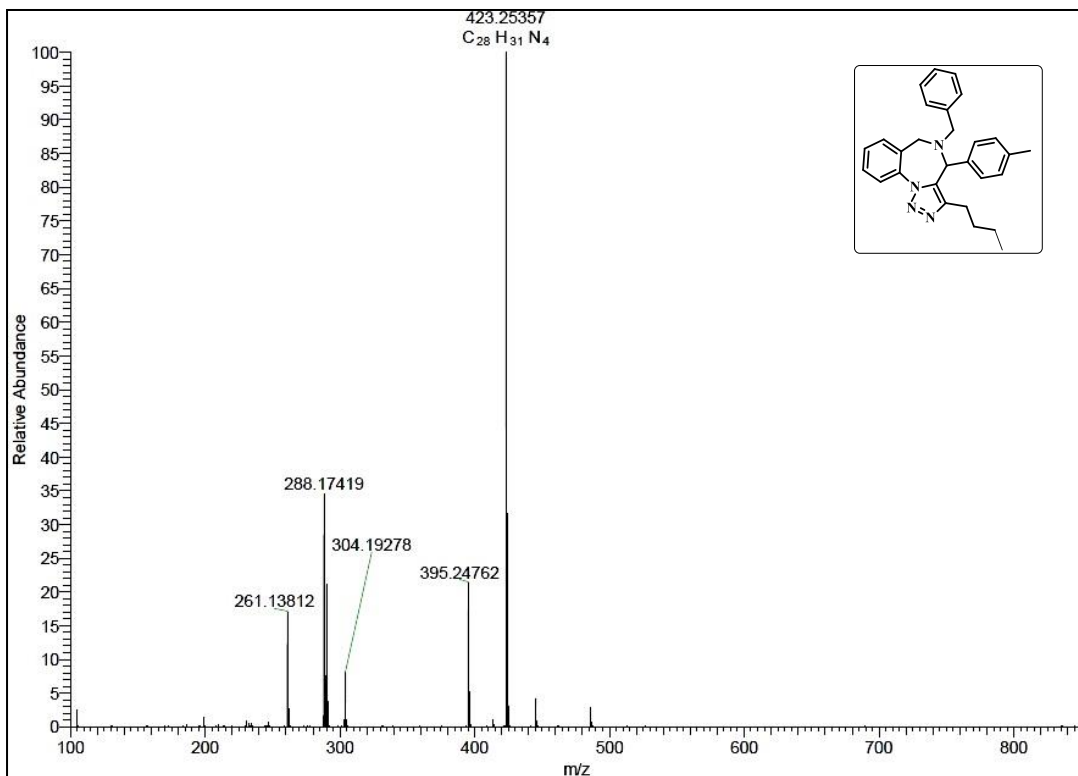
Mass spectrum of **2e**



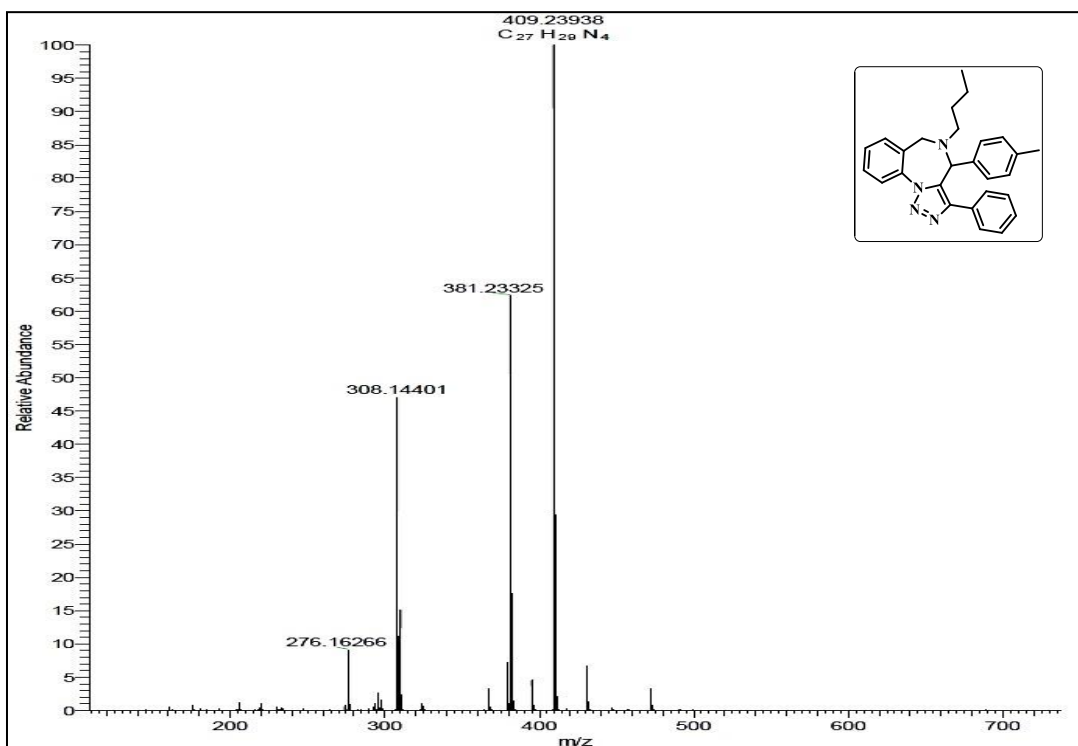
Mass spectrum of **2g**



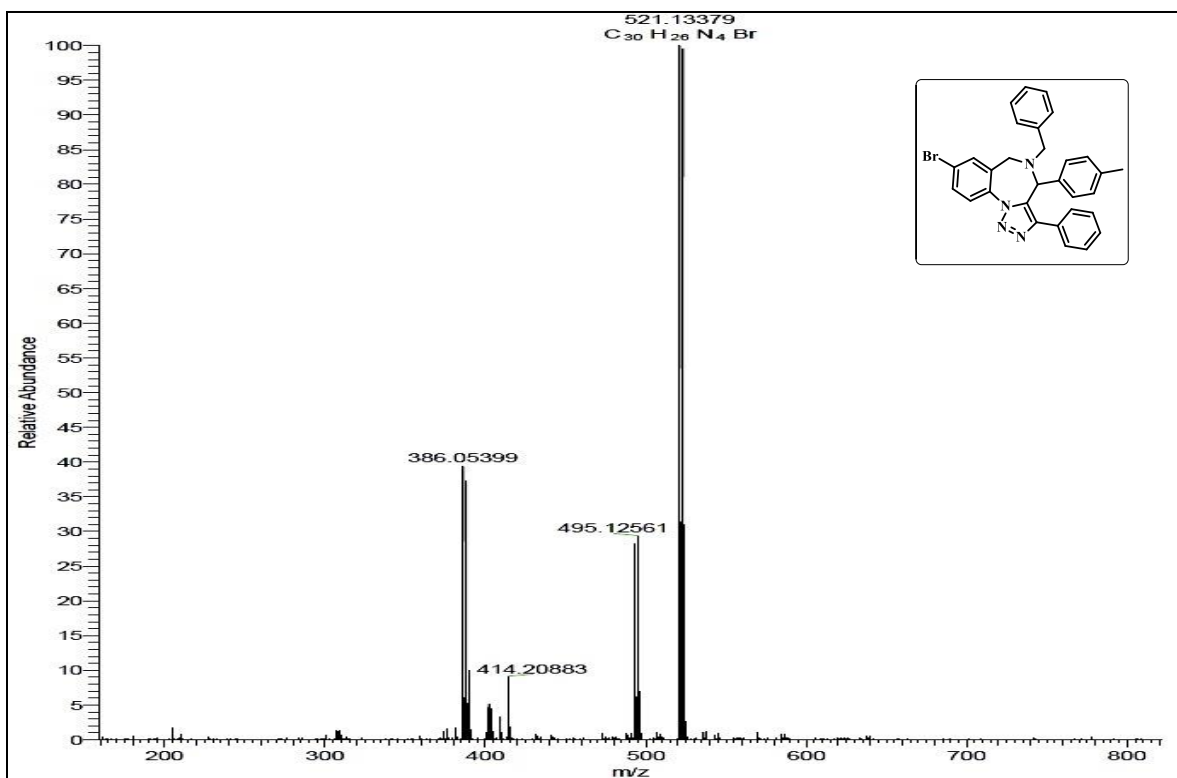
Mass spectrum of **2h**



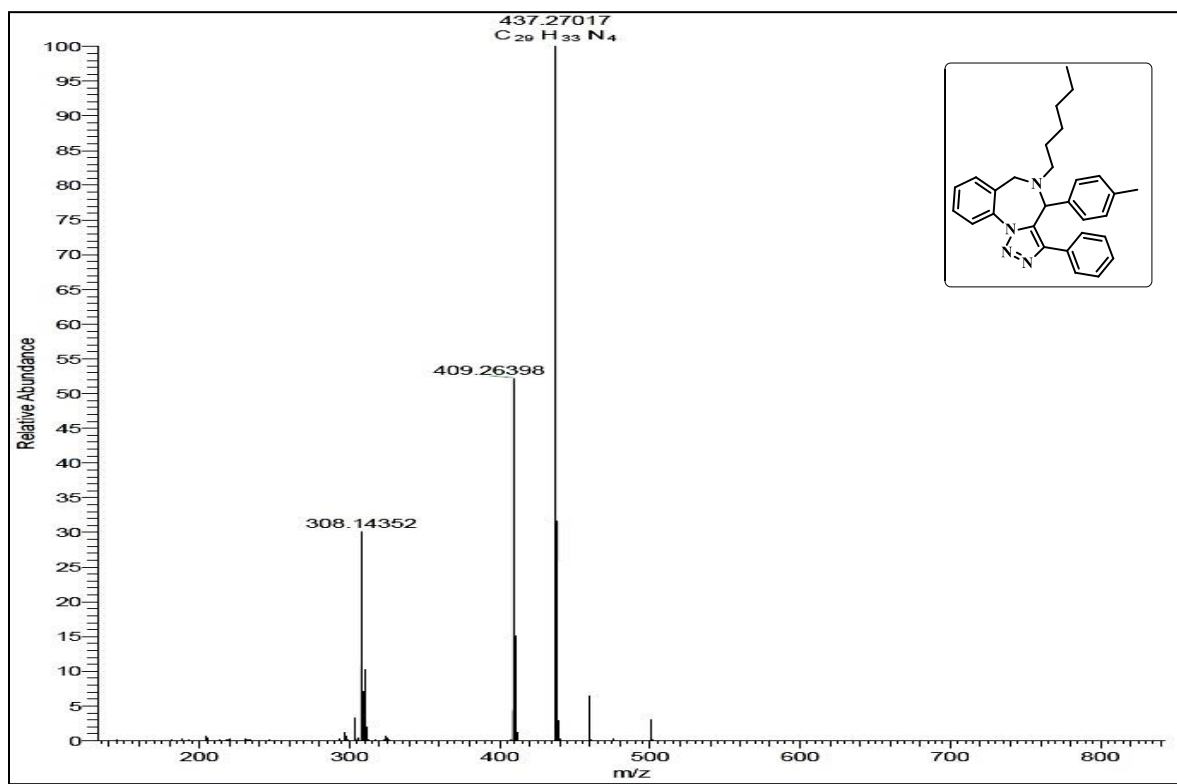
Mass spectrum of **2i**



Mass spectrum of **2m**



Mass spectrum of **2l**



Mass spectrum of **2n**

## Binding energy and the interaction of ligands with the DNA Gyrase and ALK receptor

Compound	Binding energy (kcal/mol) <sup>a</sup>	
	DNA Gyrase (2XCS)	ALK (2XP2)
2a	-10.24	-7.70
2b	-10.66	-8.58
2c	-9.79	-8.89
2d	-10.60	-8.65
2e	-9.93	-8.95
2f	-10.24	-9.07
2g	-11.07	-10.07
2h	-9.84	-8.24
2i	-9.32	-8.17
2j	-10.24	-8.37
2k	-9.75	-8.42
2l	-10.48	-8.94
2m	-9.13	-7.77
2n	-9.48	-8.24
Crystallized ligand	-13.81	-8.40
Standard drug	-7.94 <sup>b</sup>	-5.85 <sup>c</sup>

<sup>a</sup>Calculated by Autodock; <sup>b</sup>Streptomycin;

<sup>c</sup>Ciprofloxacin