

## Supporting information

### Novel 3-Arylethynyl-substituted Thieno[3,4-*b*]pyrazine Derivatives as a Human Transglutaminase 2 Inhibitors.

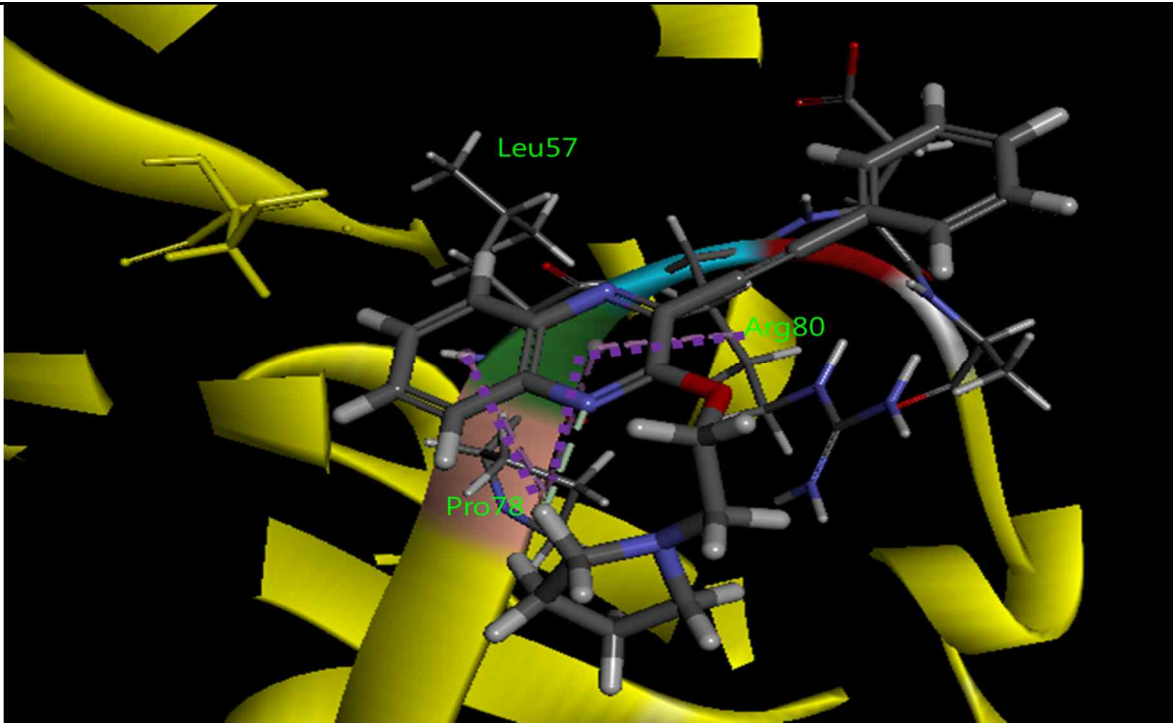
*Nayeon Kim,<sup>a</sup> Se Hun Kwak,<sup>a</sup> Seon-Hyeong Lee,<sup>b</sup> Se-Jin Kim,<sup>b</sup> Vinayak Juvekar,<sup>a</sup> Hee-Chul Ahn,<sup>c</sup>*

*Soo-Youl Kim,<sup>b,\*</sup> Young-Dae Gong<sup>a,\*</sup>*

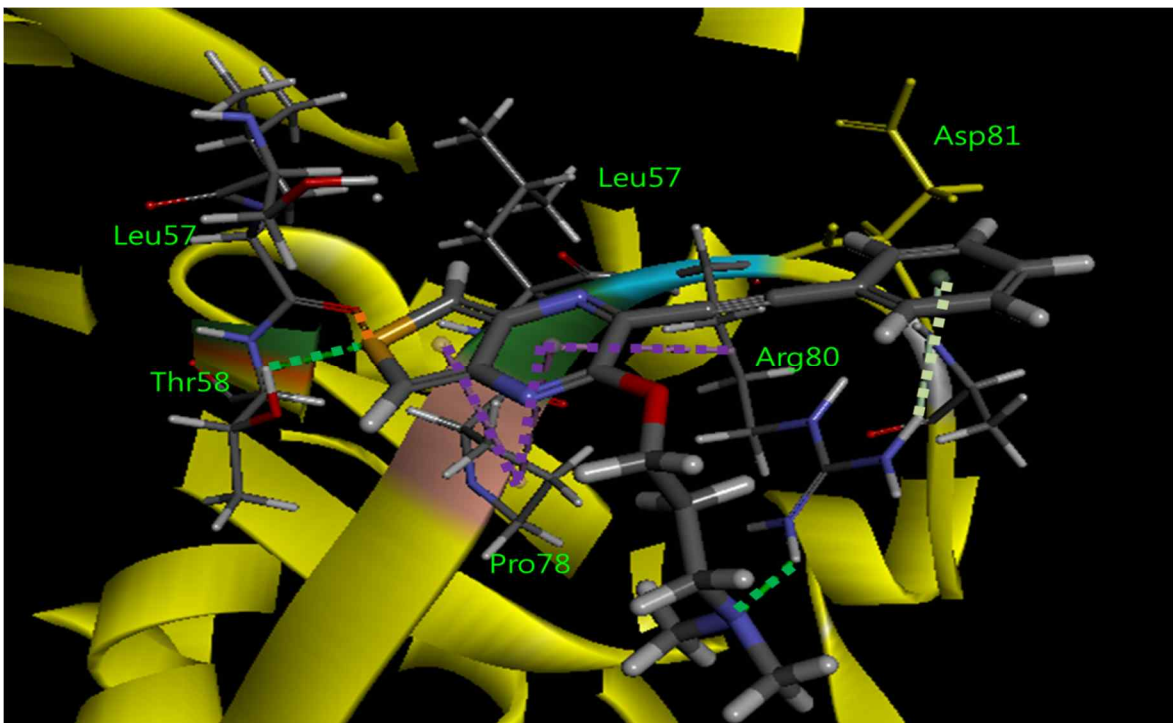
<sup>a</sup>Innovative Drug Library Research Center, Dongguk University, Pil-dong 3-ga, Jung-gu, Seoul 100-715, Republic of Korea, <sup>b</sup>Cancer Cell and Molecular Biology Branch, Division of Cancer Biology, Division of Translational & Clinical Research I, Research Institute, 323 Ilsandong-gu, Goyang 410-749, Republic of Korea, and <sup>c</sup>Department of Pharmacy, College of Pharmacy, Dongguk University, Goyang, Gyeonggi 410-820, Korea

Co-corresponding author's E-Mail : [ydgon@dongguk.edu](mailto:ydgon@dongguk.edu); [kimsooyoul@gmail.com](mailto:kimsooyoul@gmail.com)

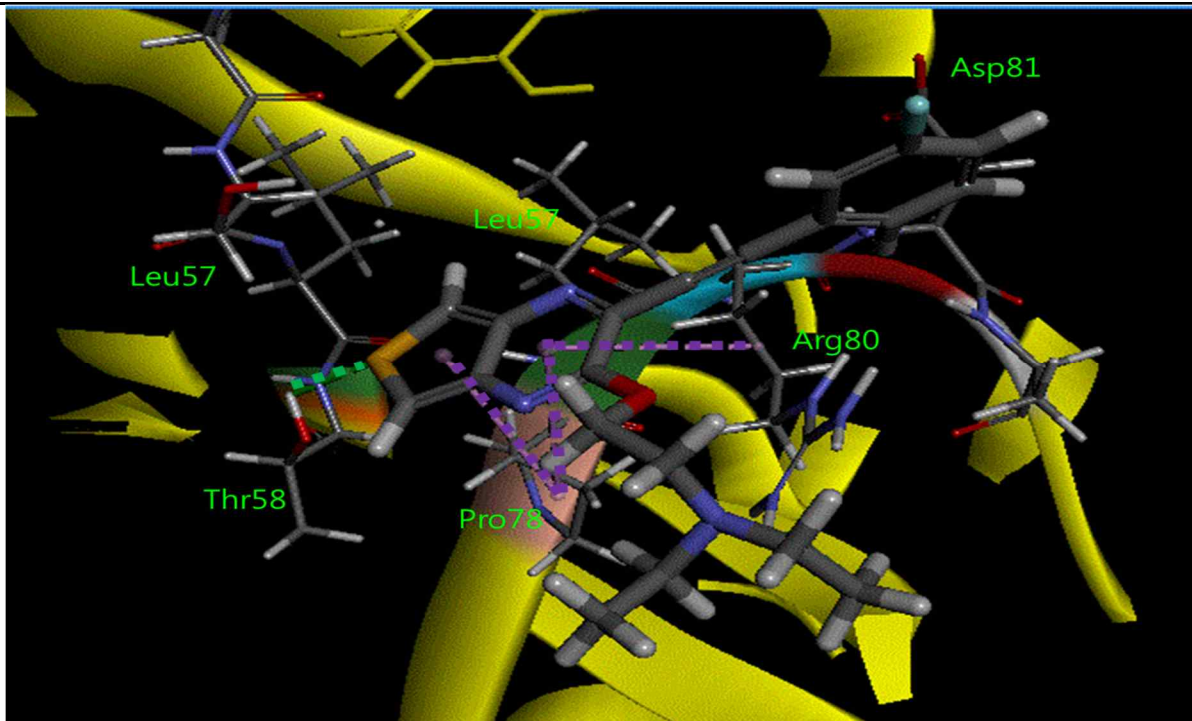
	<b>Content</b>	<b>Page No.</b>
1.	3D Structure presented Docking results of GK-13 and the compounds <b>GK-419,421,423,425,428,</b>	S2-S4
2.	The viewing 3D-molecular volume and IC <sub>50</sub> of chosen thieno[3,4- <i>b</i> ]pyrazine derivatives from 1st screening using the SRB test	S5
3.	<sup>1</sup> H & <sup>13</sup> C NMR, LC/MS and High Resolution Mass Spectrum of <b>GK-428,</b> representative lead compound	S6–S8
4.	<sup>1</sup> H & <sup>13</sup> C NMR, LC/MS data of the intermediates of <b>GK-428,</b> <b>2-4 compounds</b>	S9-S113
5.	<sup>1</sup> H & <sup>13</sup> C NMR, LC/MS and High Resolution Mass Spectrum of Figure 3 compounds <b>GK-414–430</b>	S14-S52



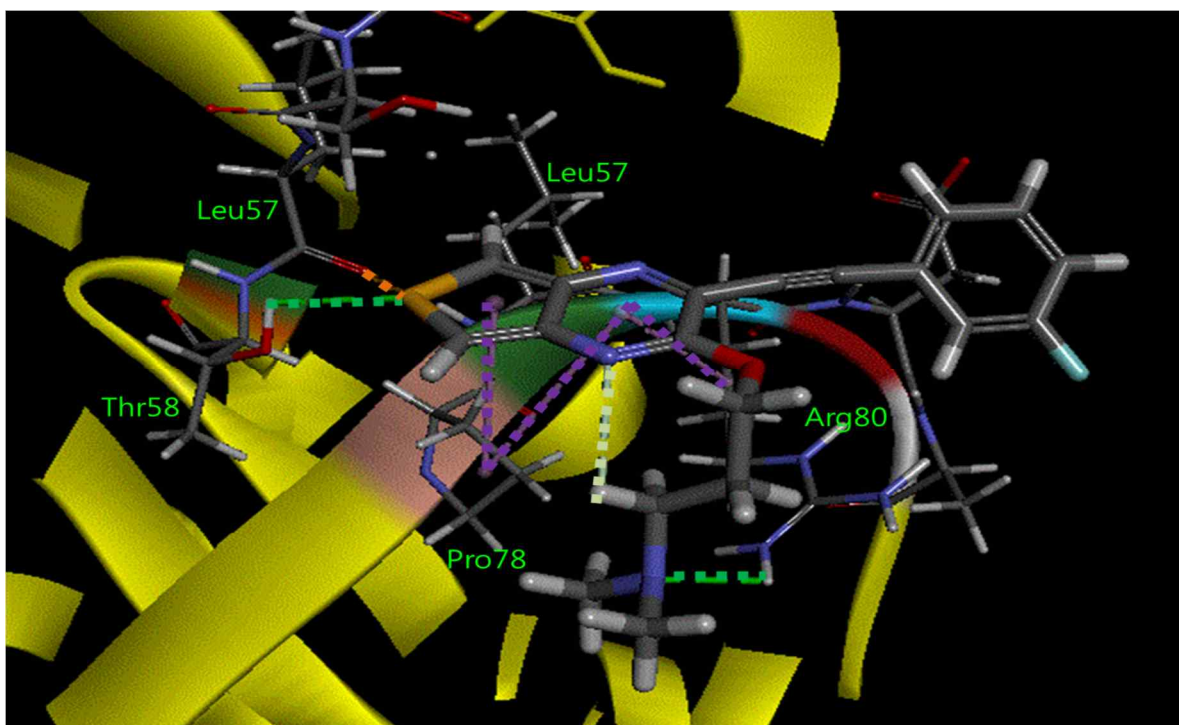
3D Structure presented Docking results of **GK-13**



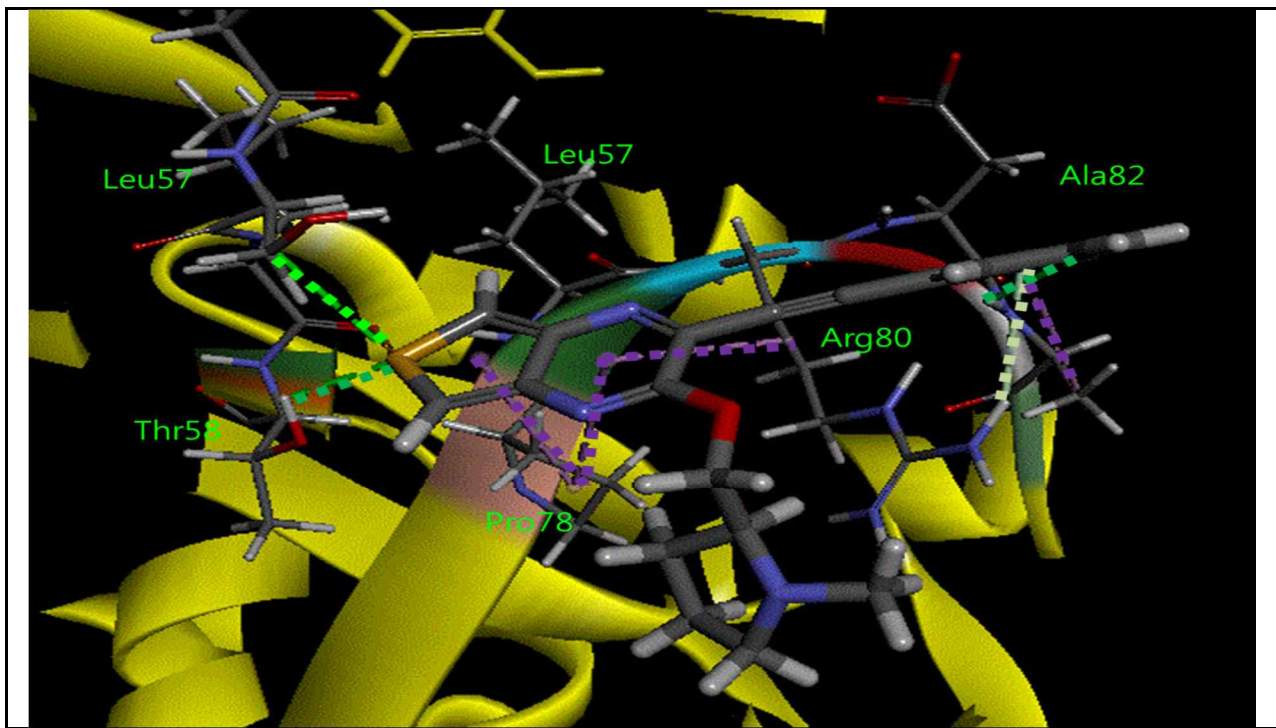
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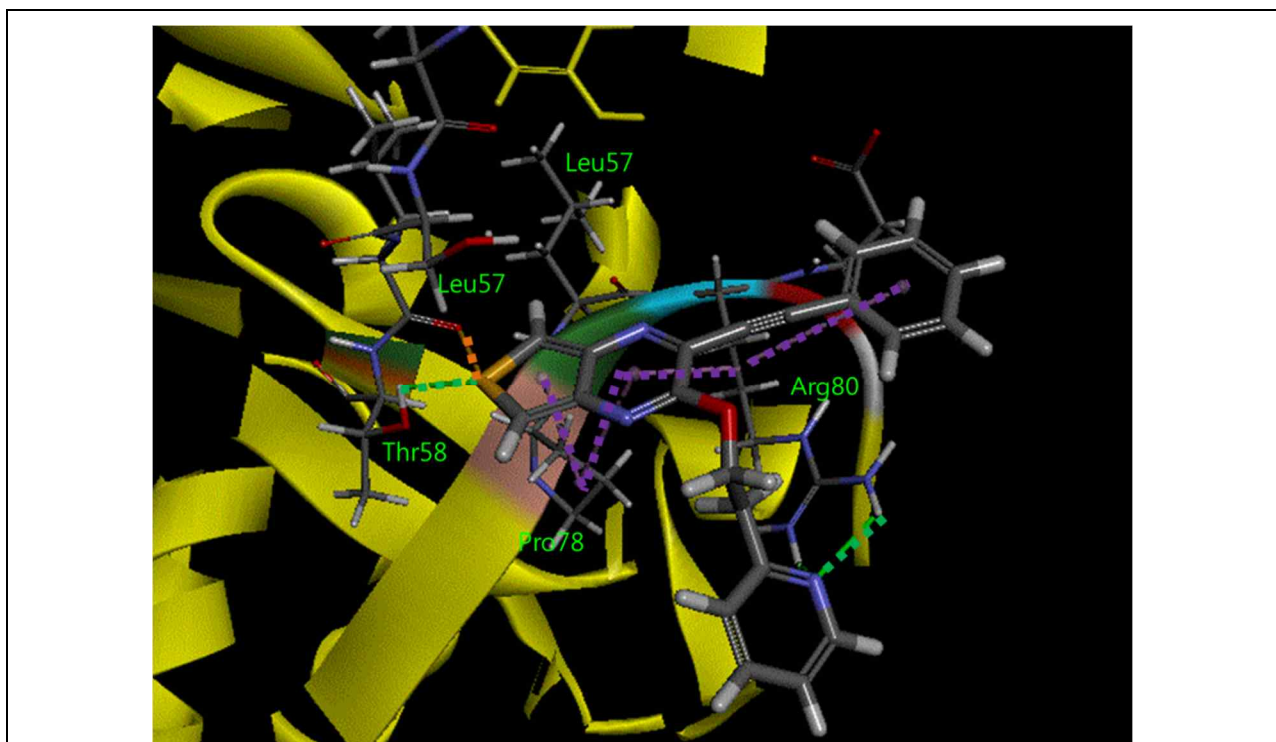
3D Structure presented Docking results of **GK-419**



3D Structure presented Docking results of **GK-421**



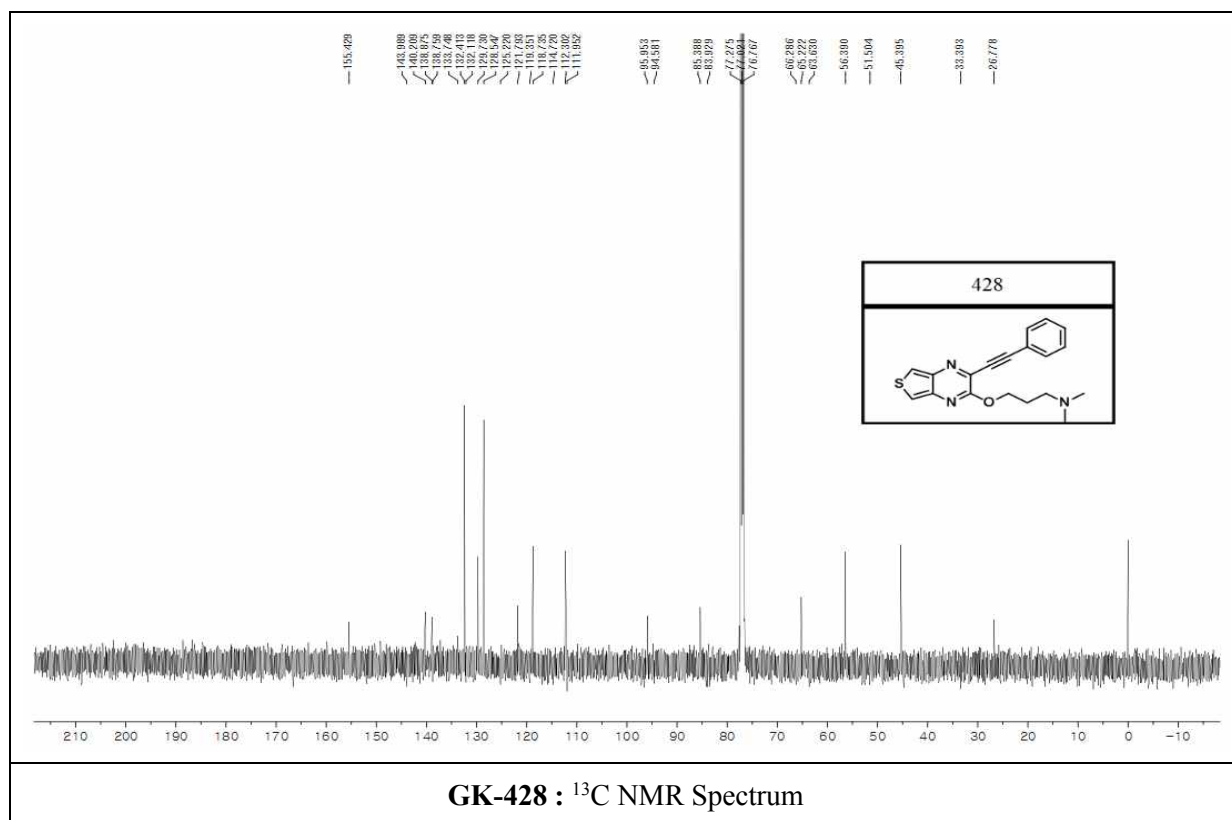
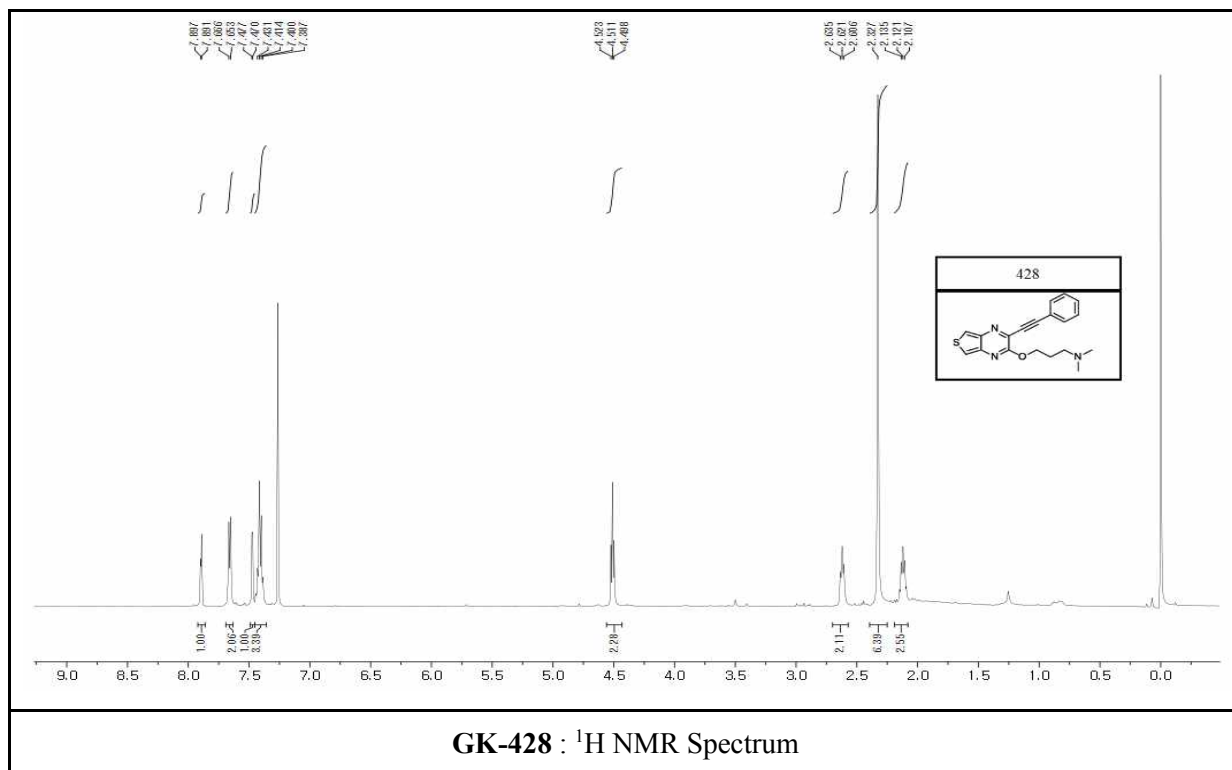
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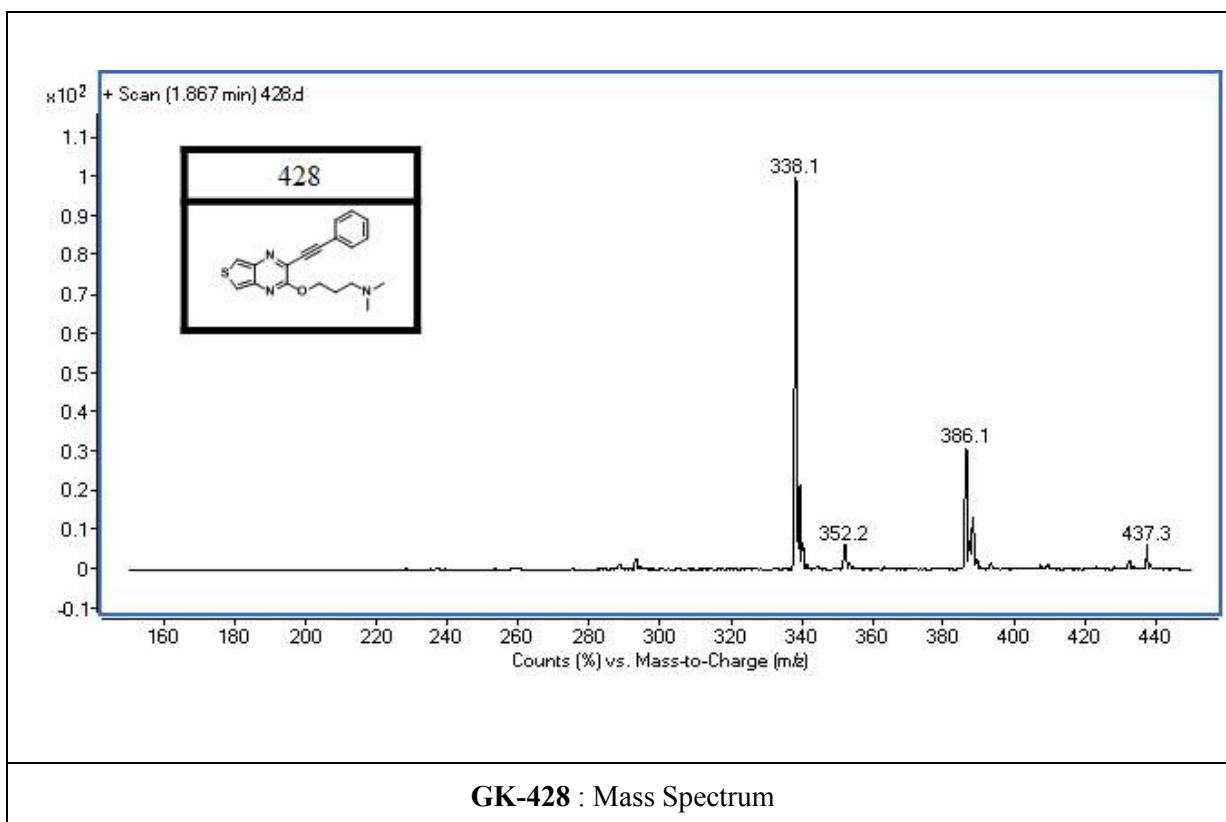
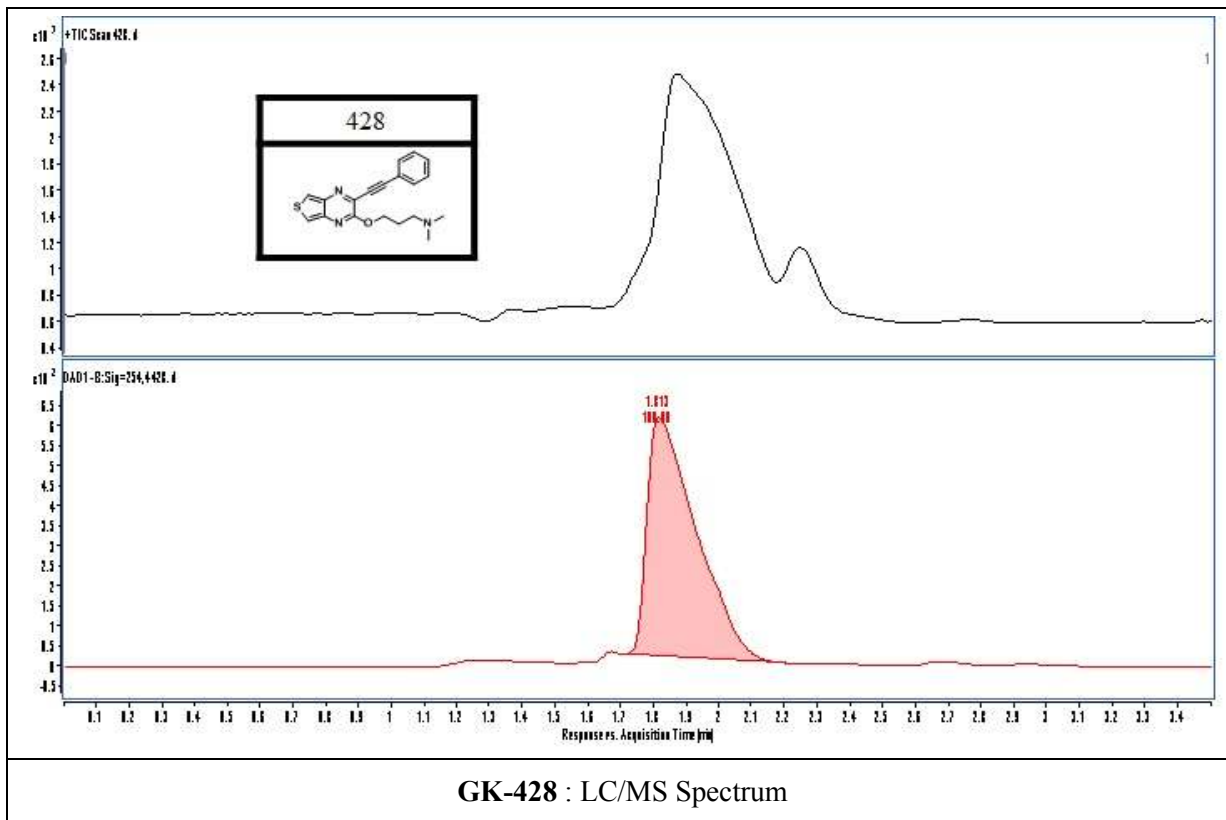


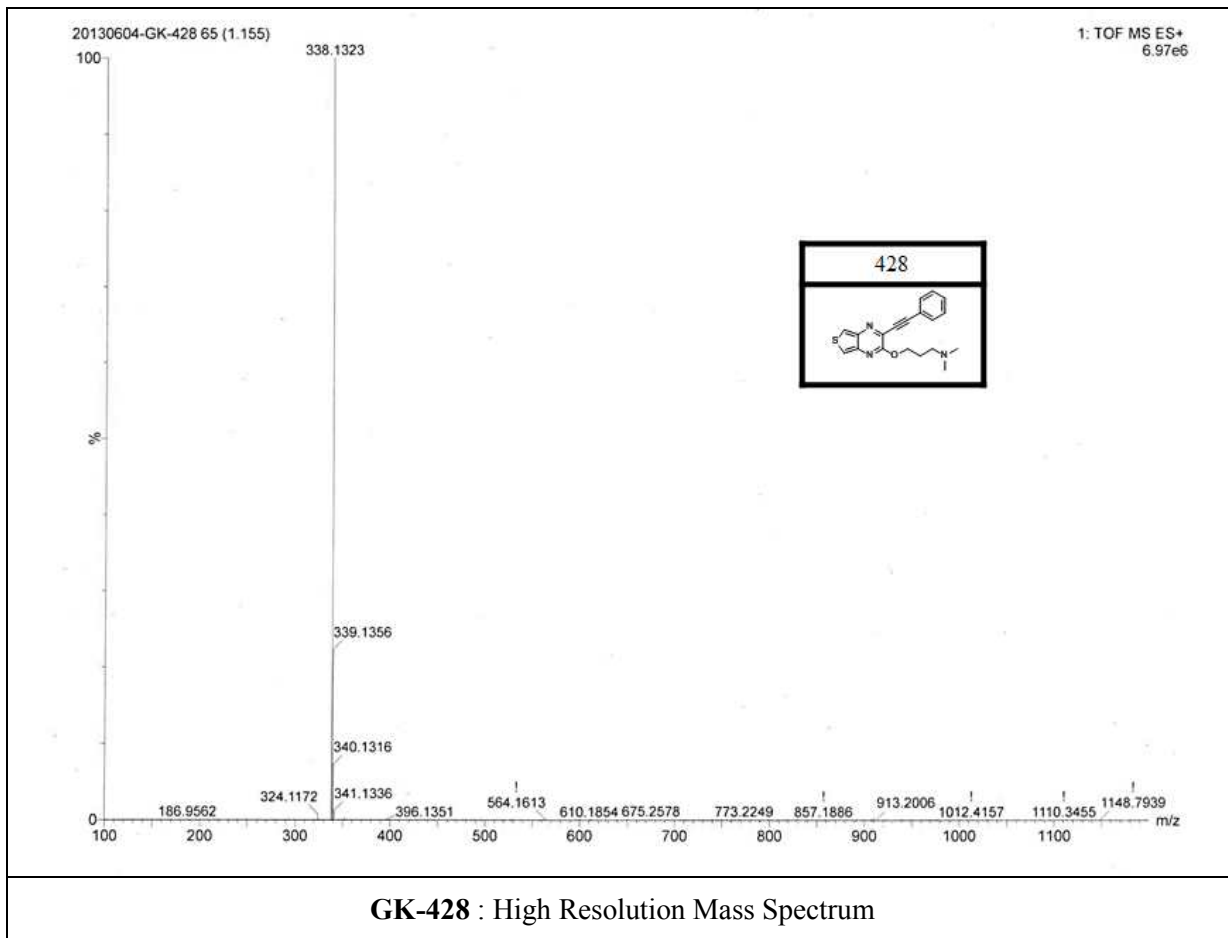
3D Structure presented Docking results of **GK-425**

<b>The viewing 3D-molecular volume and IC50 of chosen thieno[3,4-b]pyrazine derivatives from 1<sup>st</sup> screening using the SRB test</b>		
<b>Code</b>	<b>3D-molecular volume</b>	<b>IC50</b>
GK-13	278.85	16.4
GK-414	295.32	
GK-416	293.26	
GK-417	279.88	
GK-418	267.19	
GK-419	294.63	28.1
GK-421	279.2	11.7
GK-422	303.55	
GK-423	287.09	18.7
GK-424	290.17	
GK-425	275.08	6.3
GK-426	257.24	
GK-427	287.43	
GK-428	278.51	3.8
GK-430	278.51	

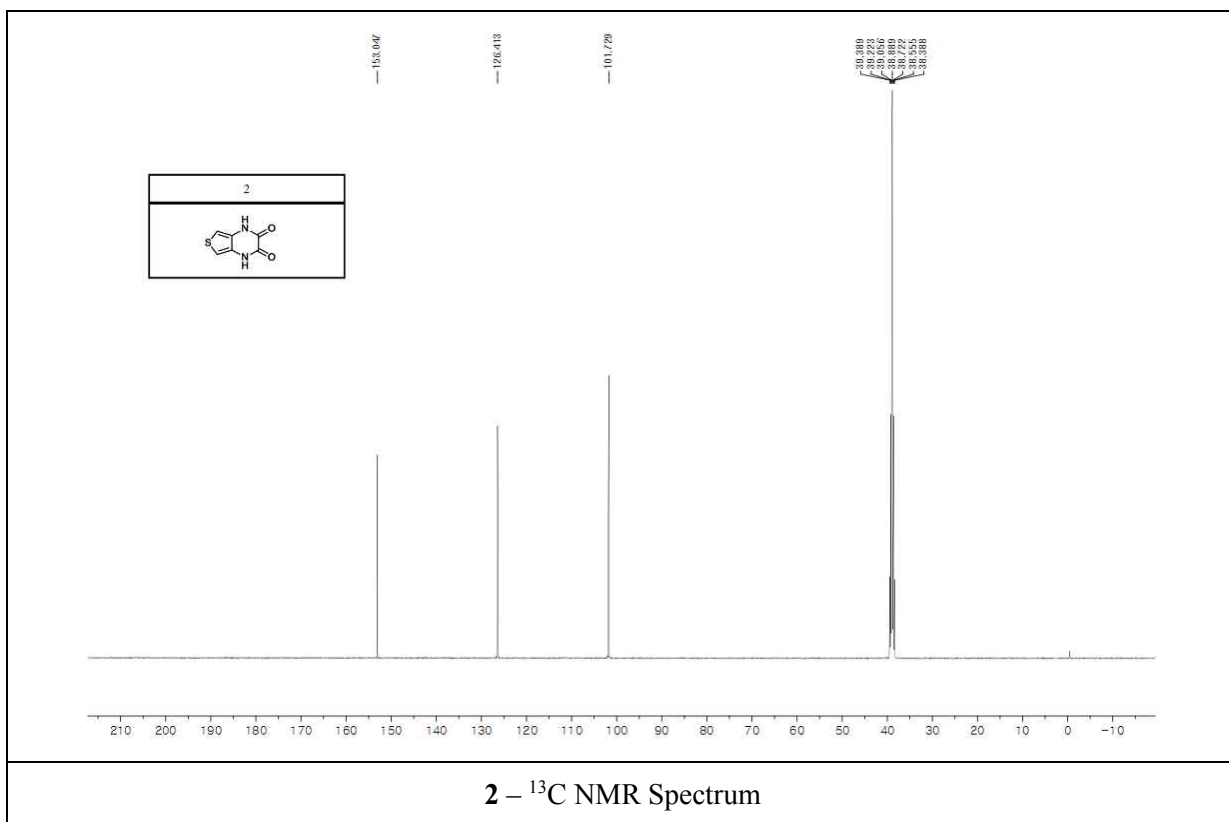
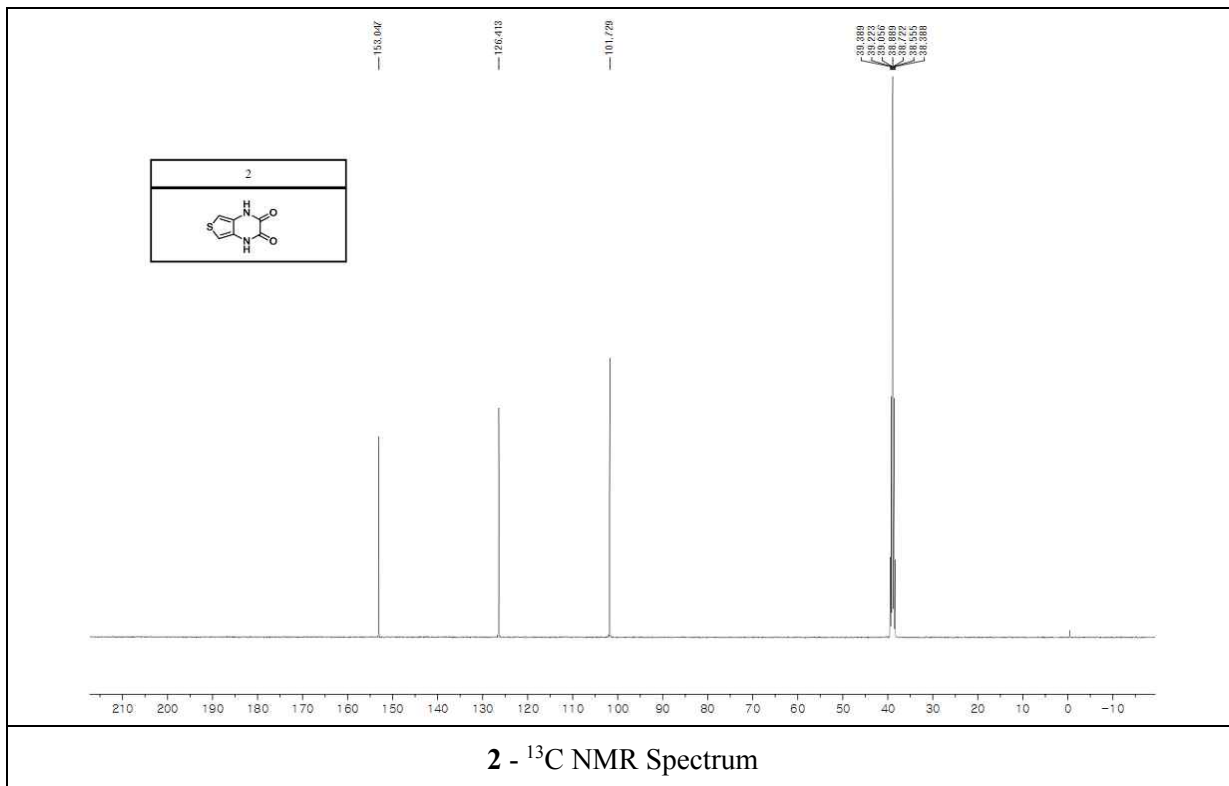
\*3D-molecular volume calculated by using the software Discovery studio 4.0

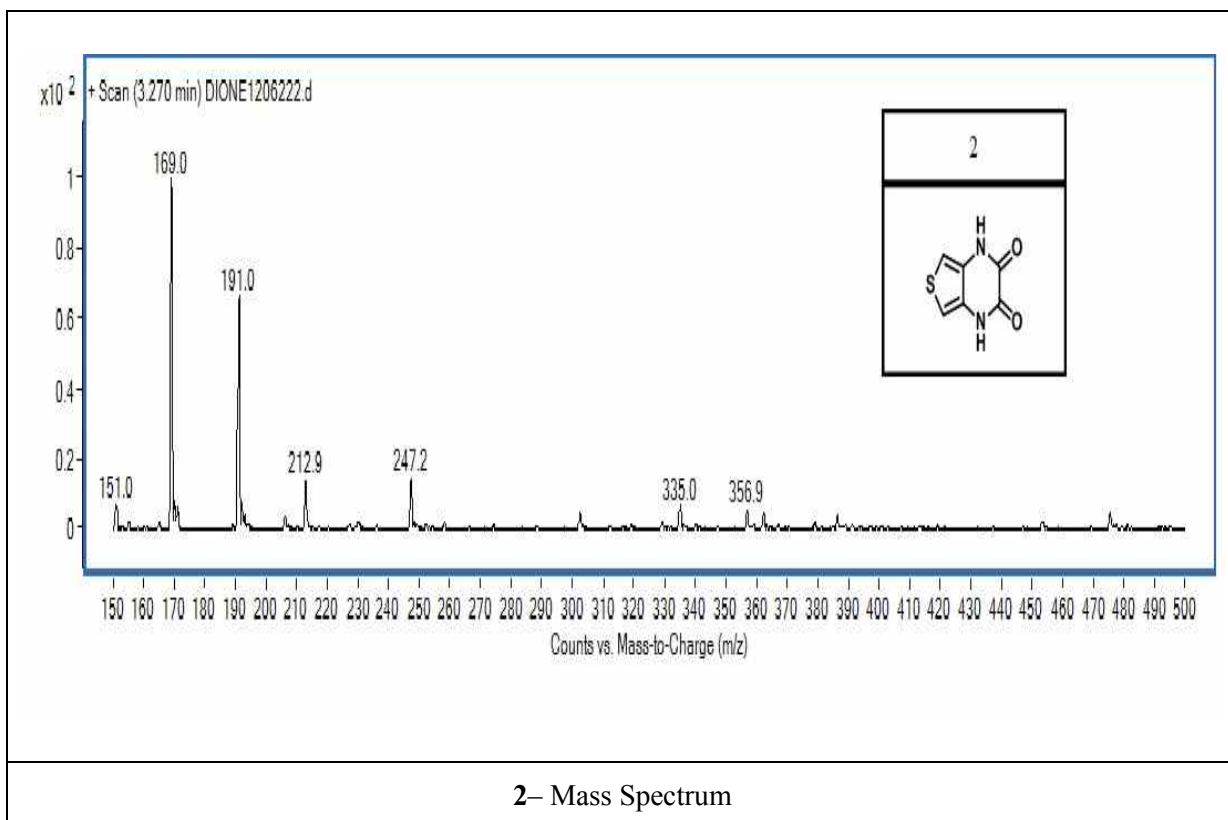
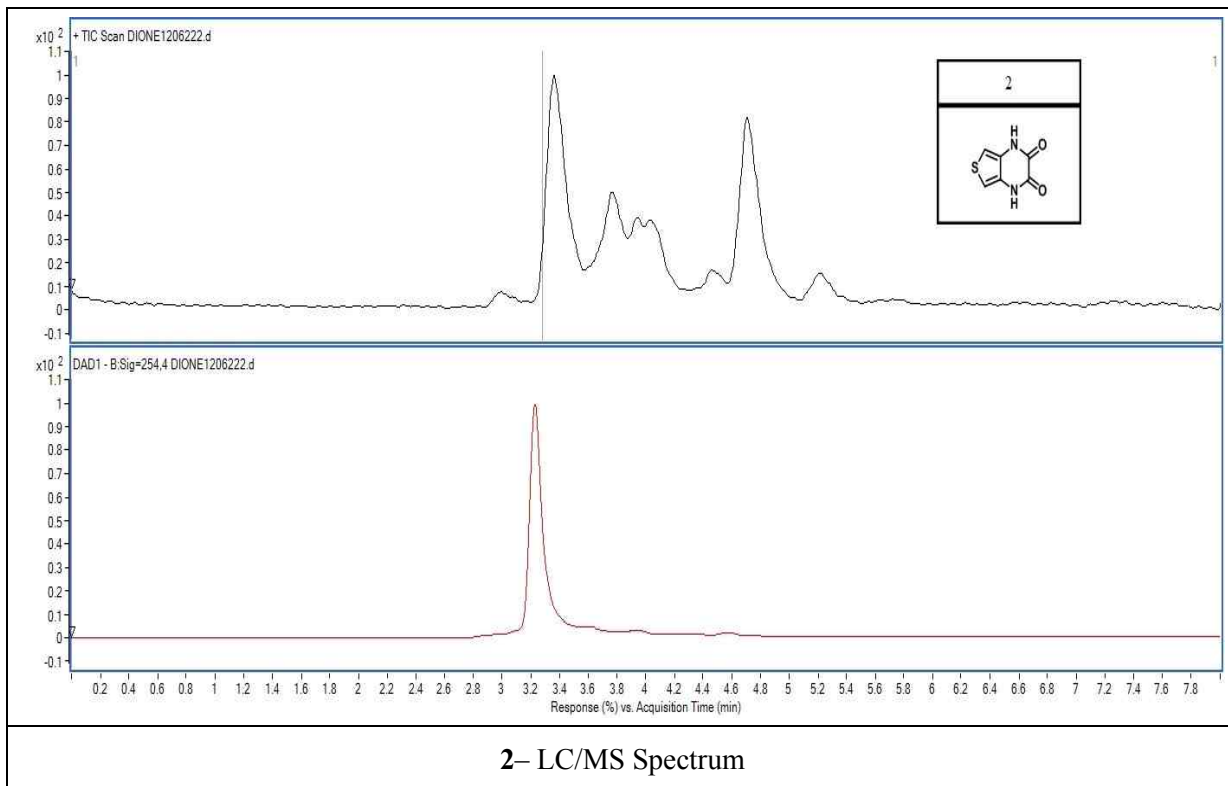


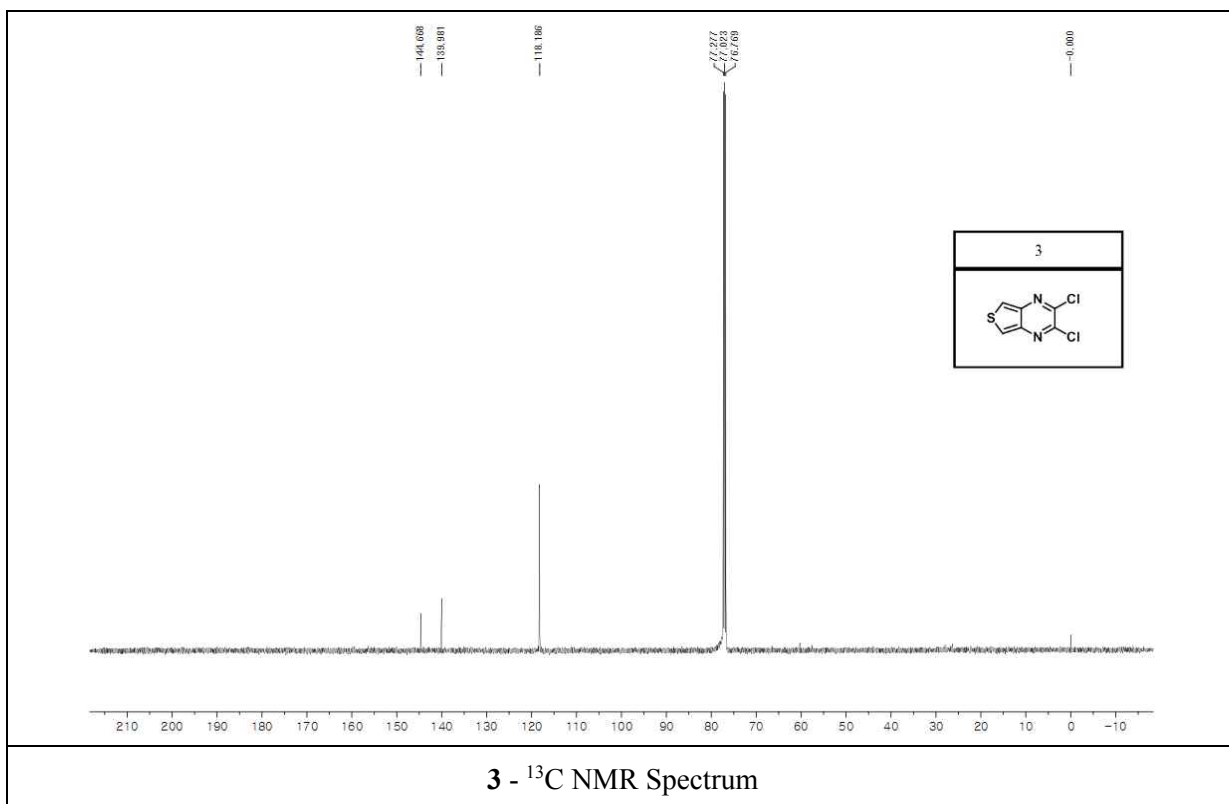
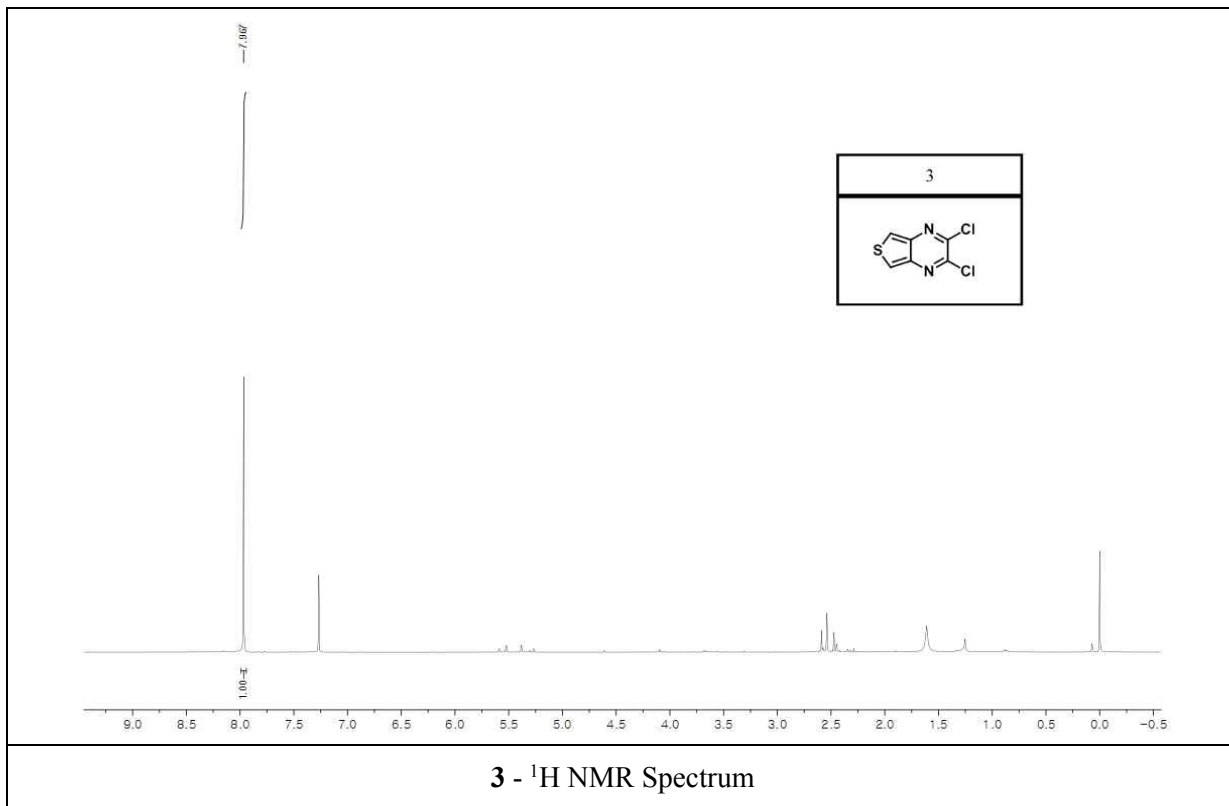


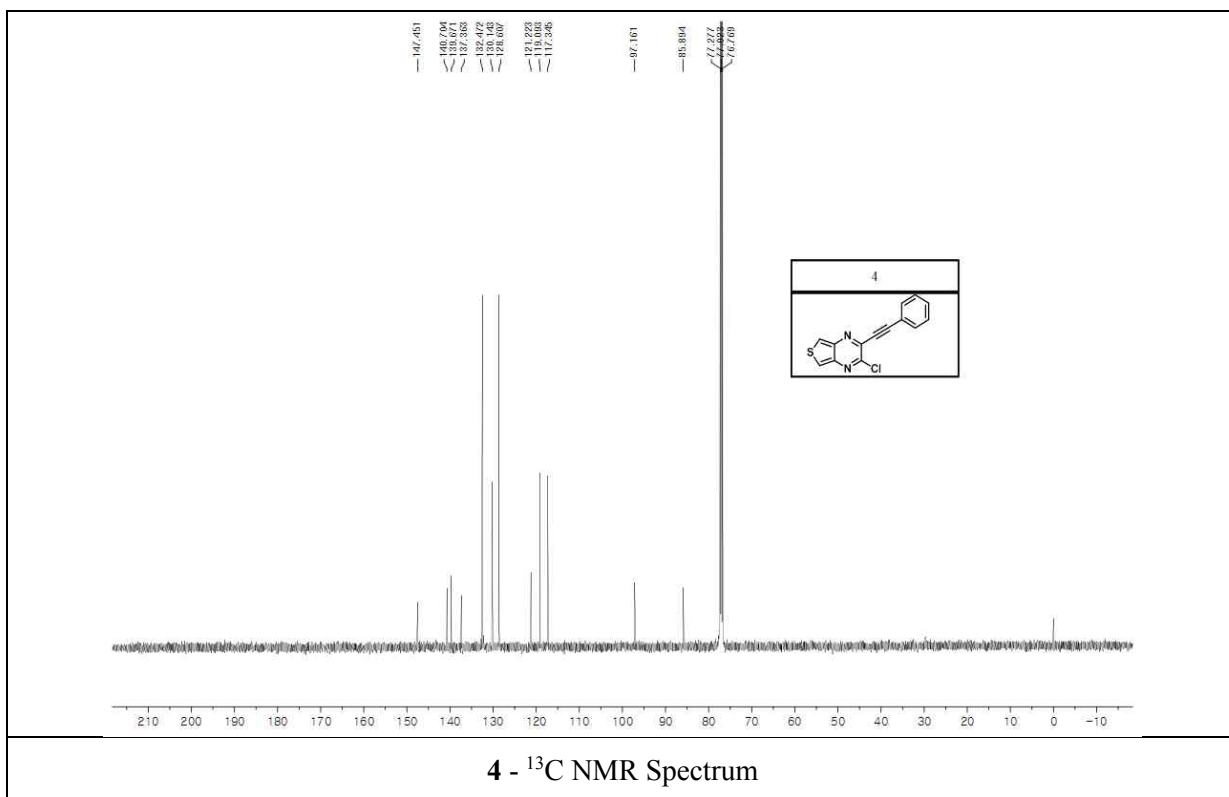
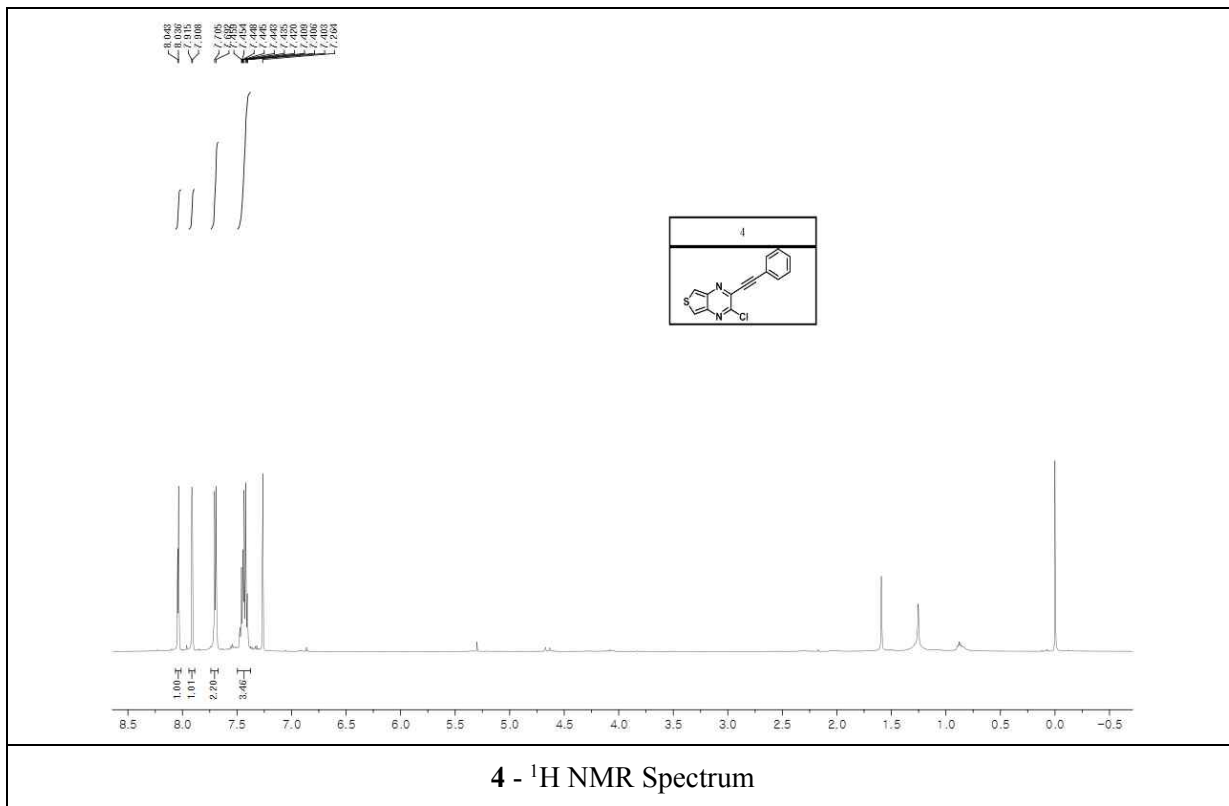


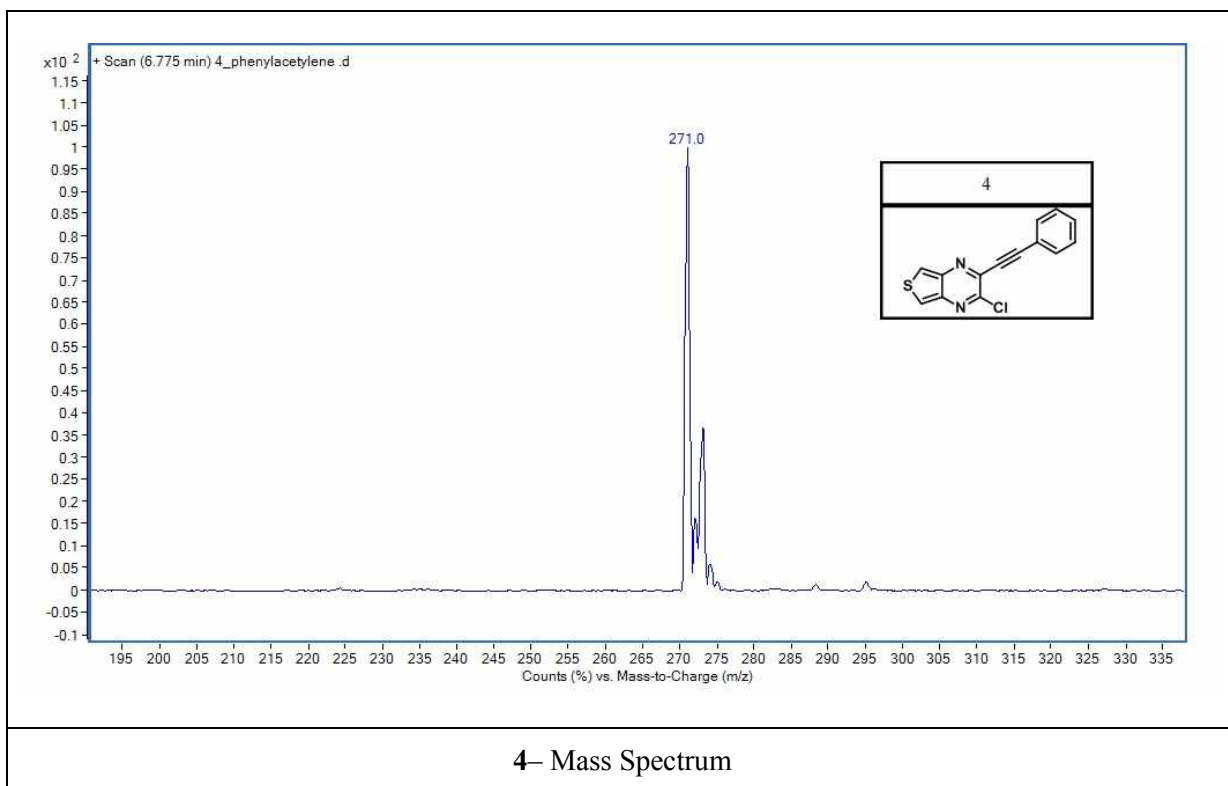
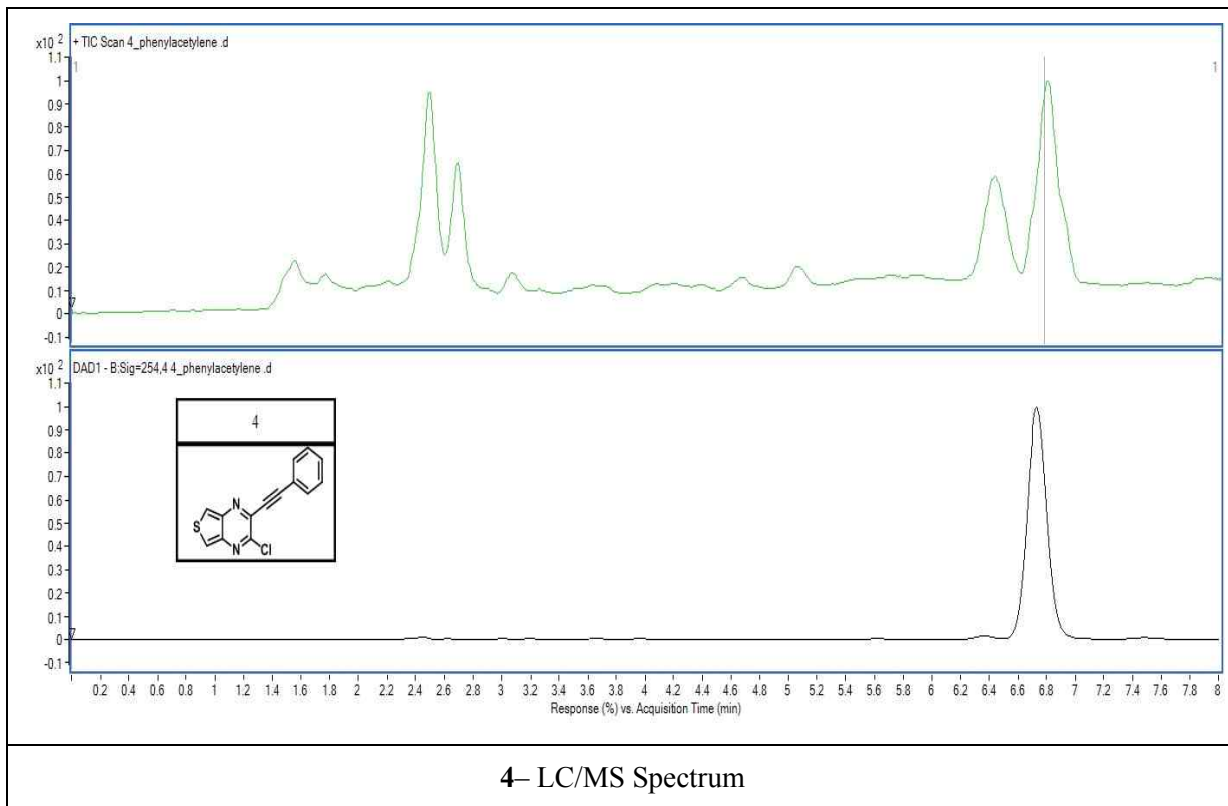


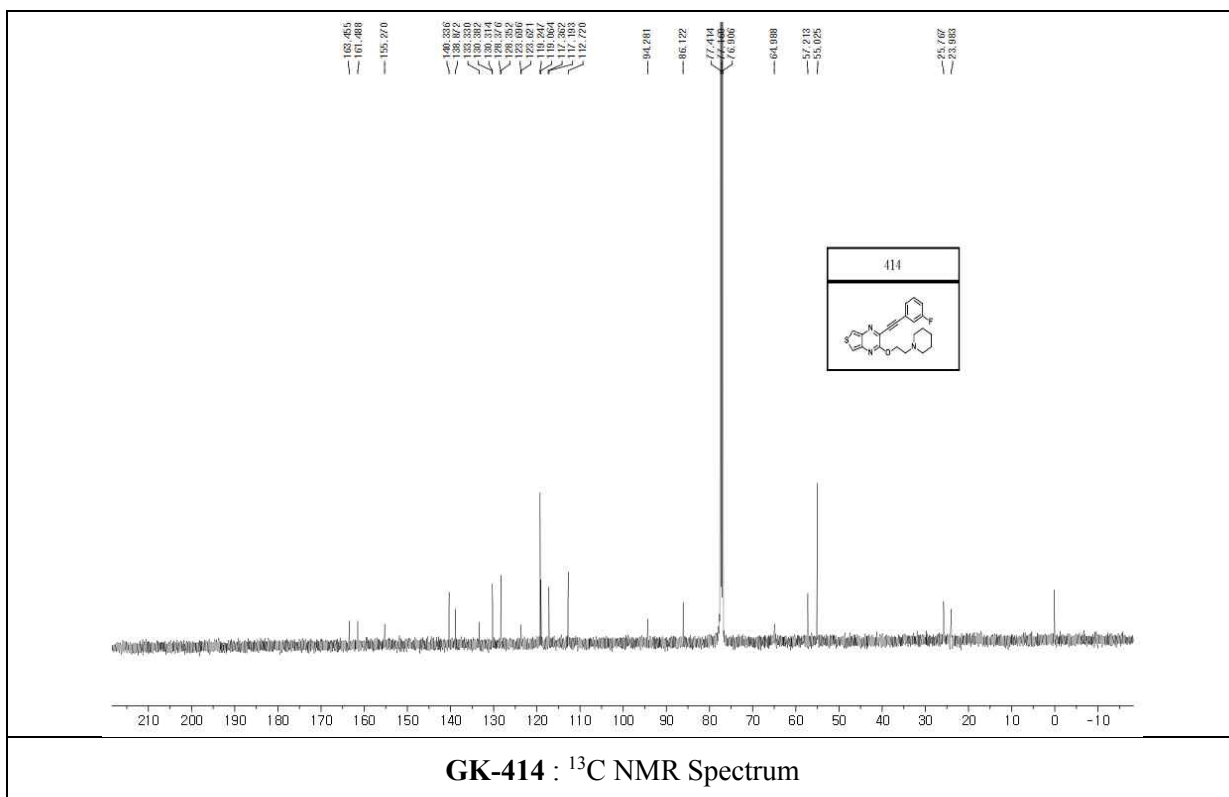
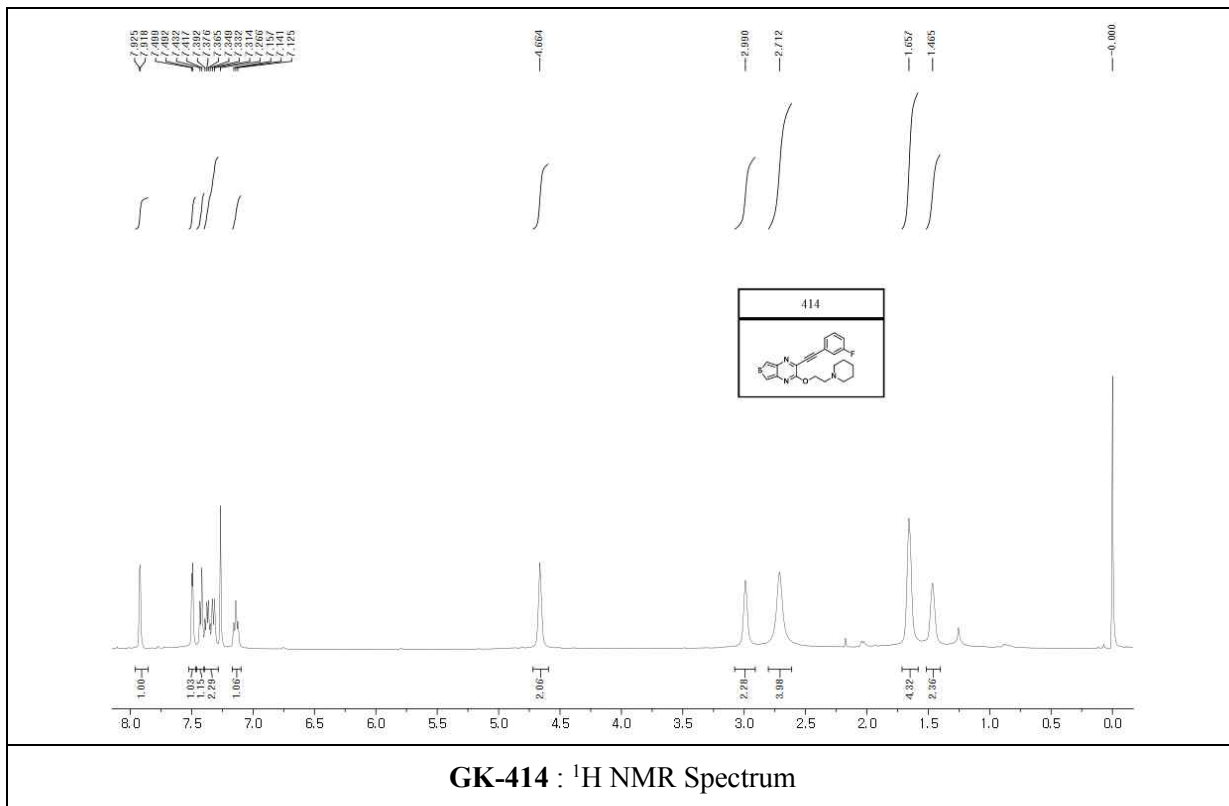


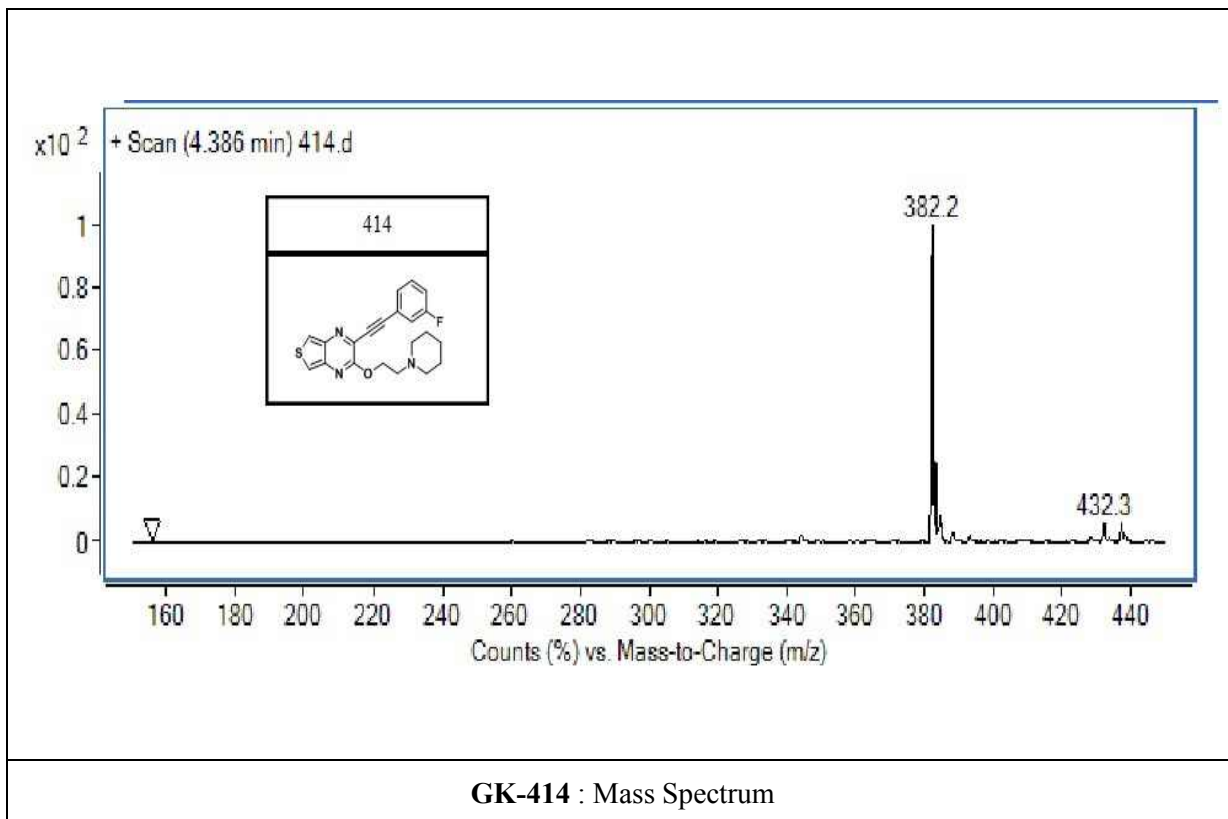
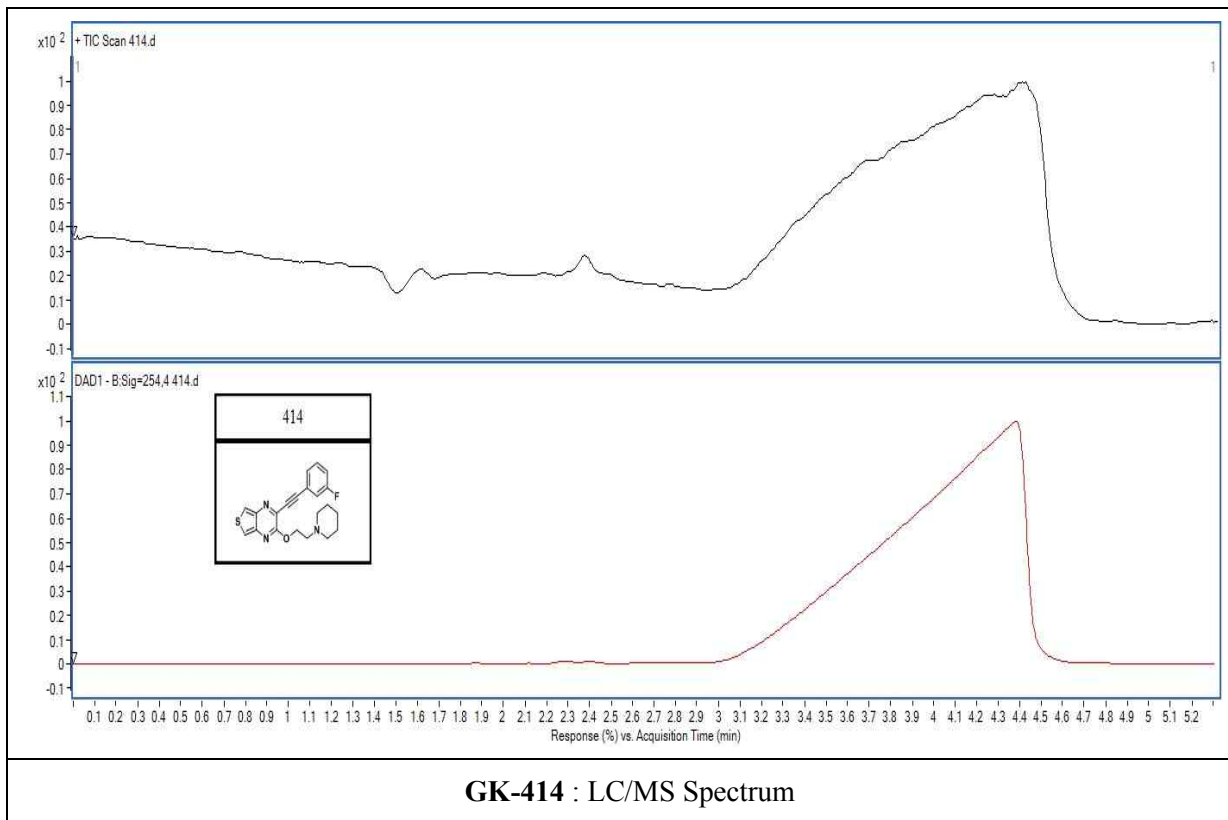


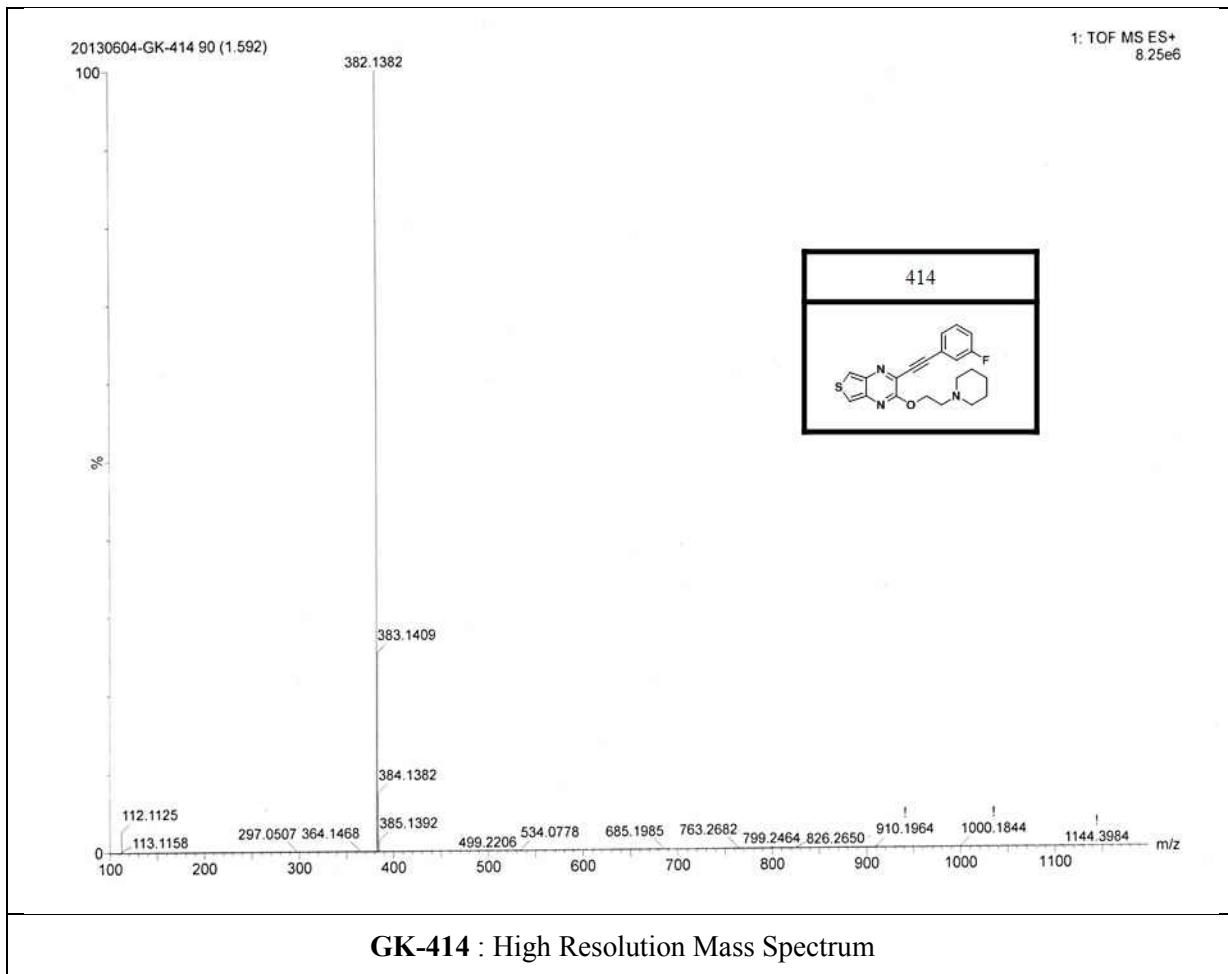




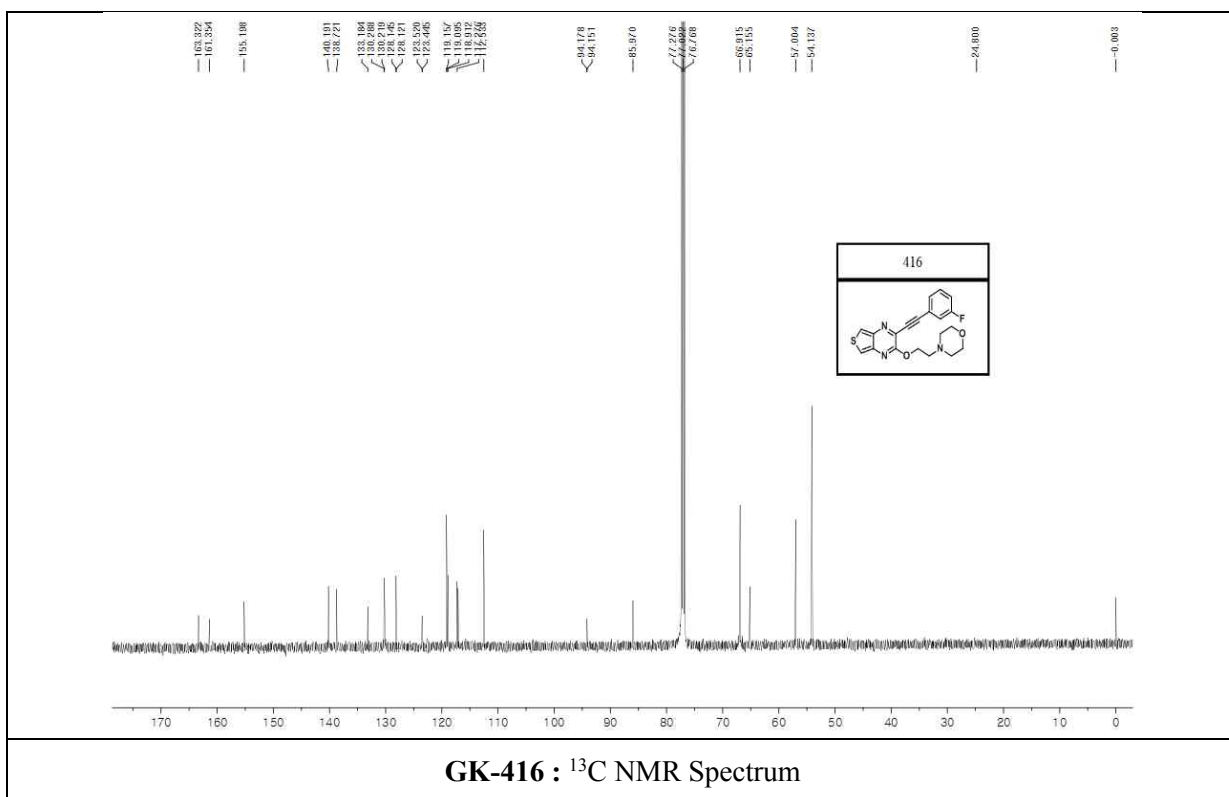
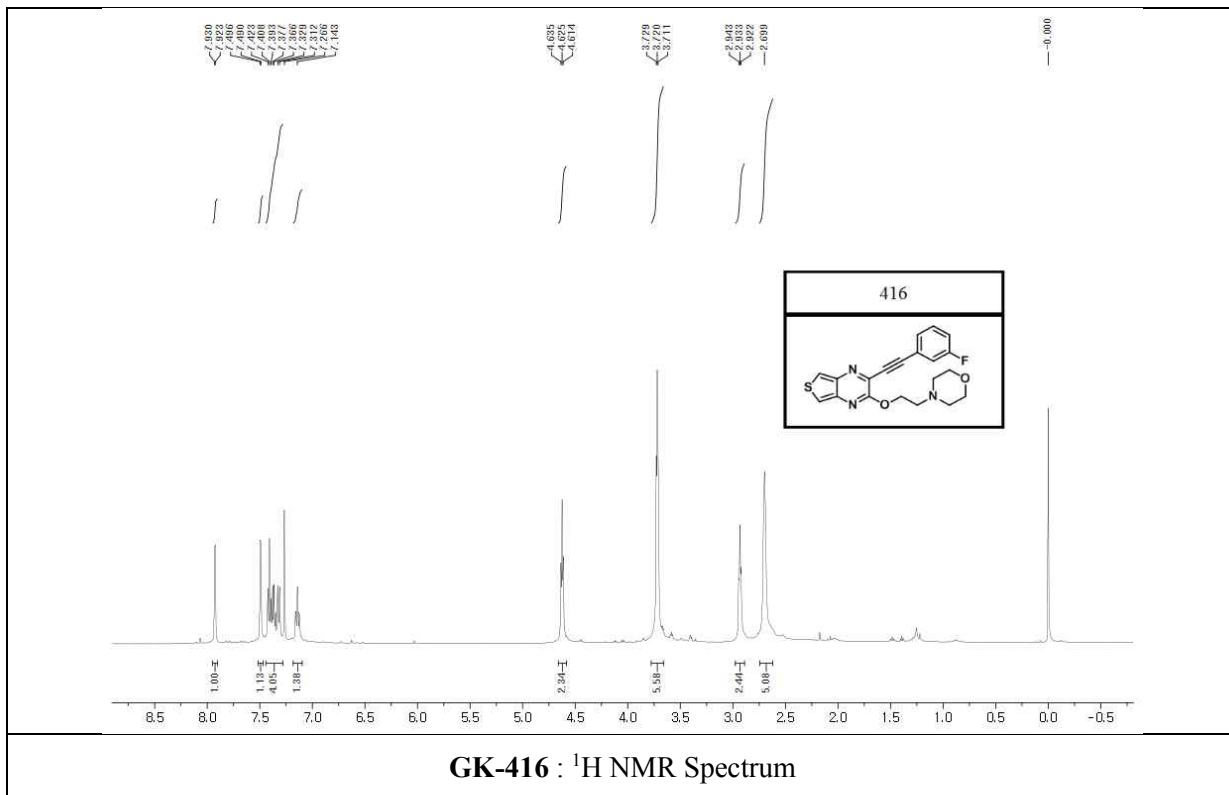


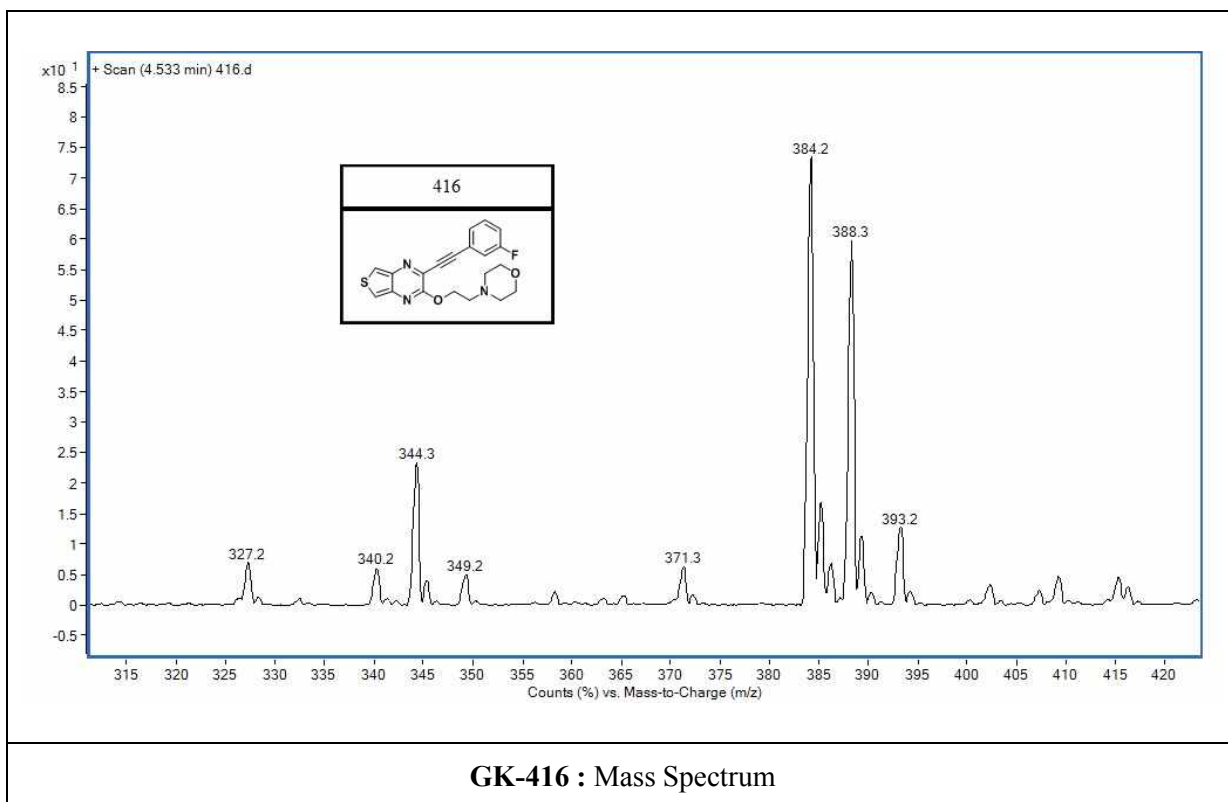
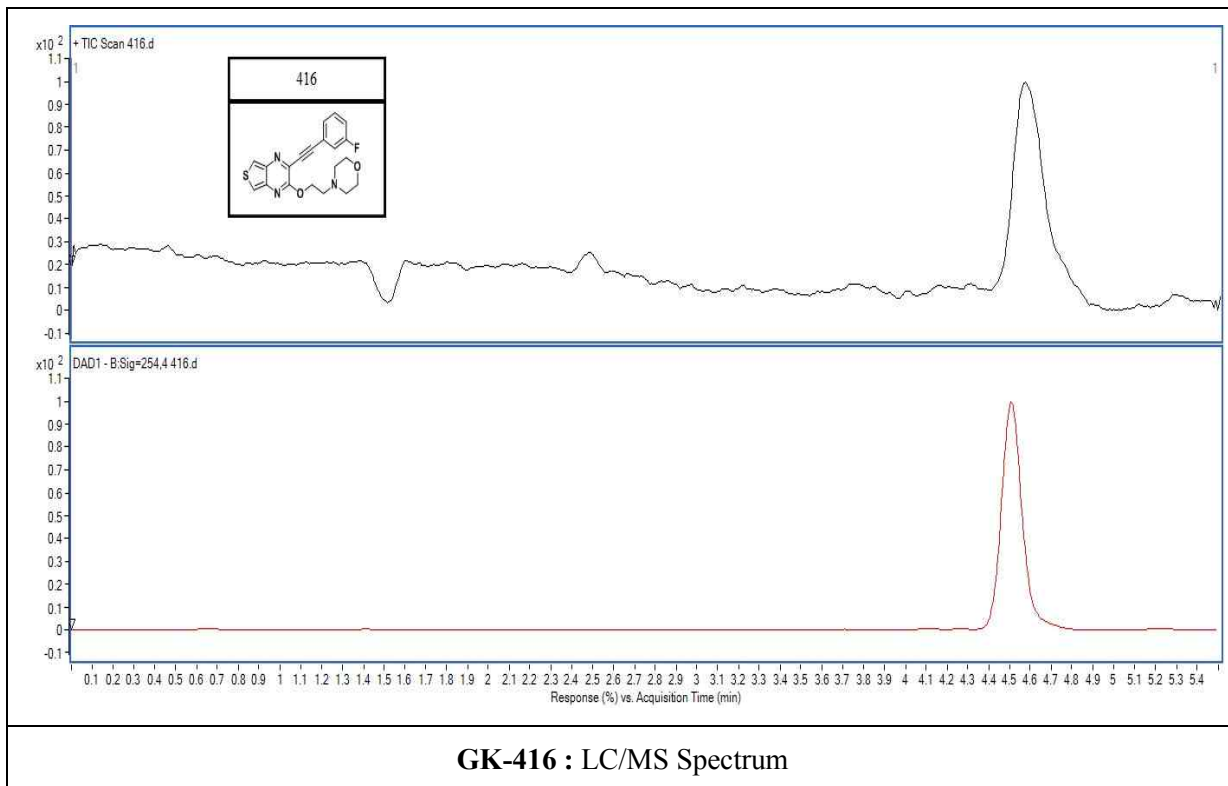


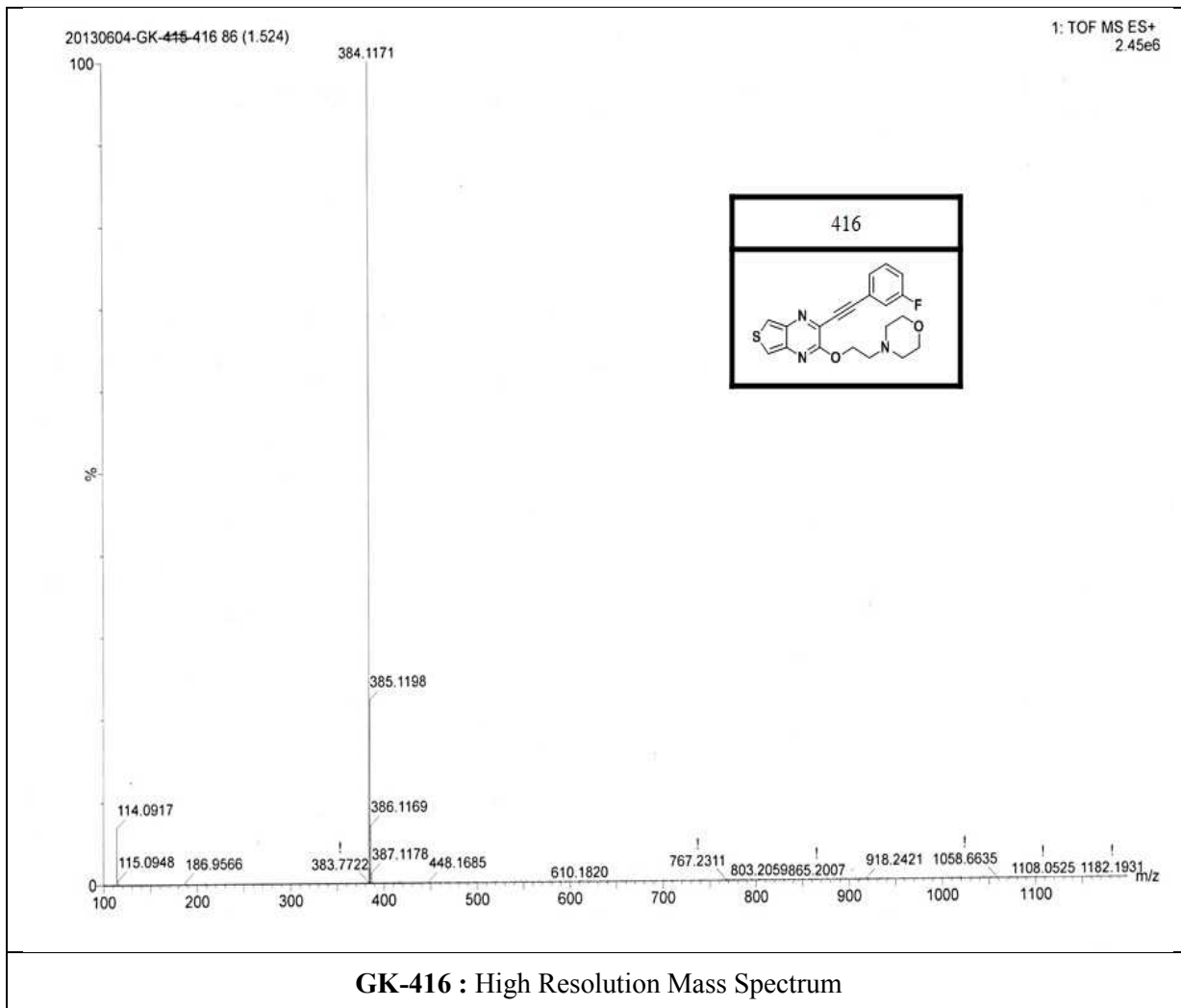


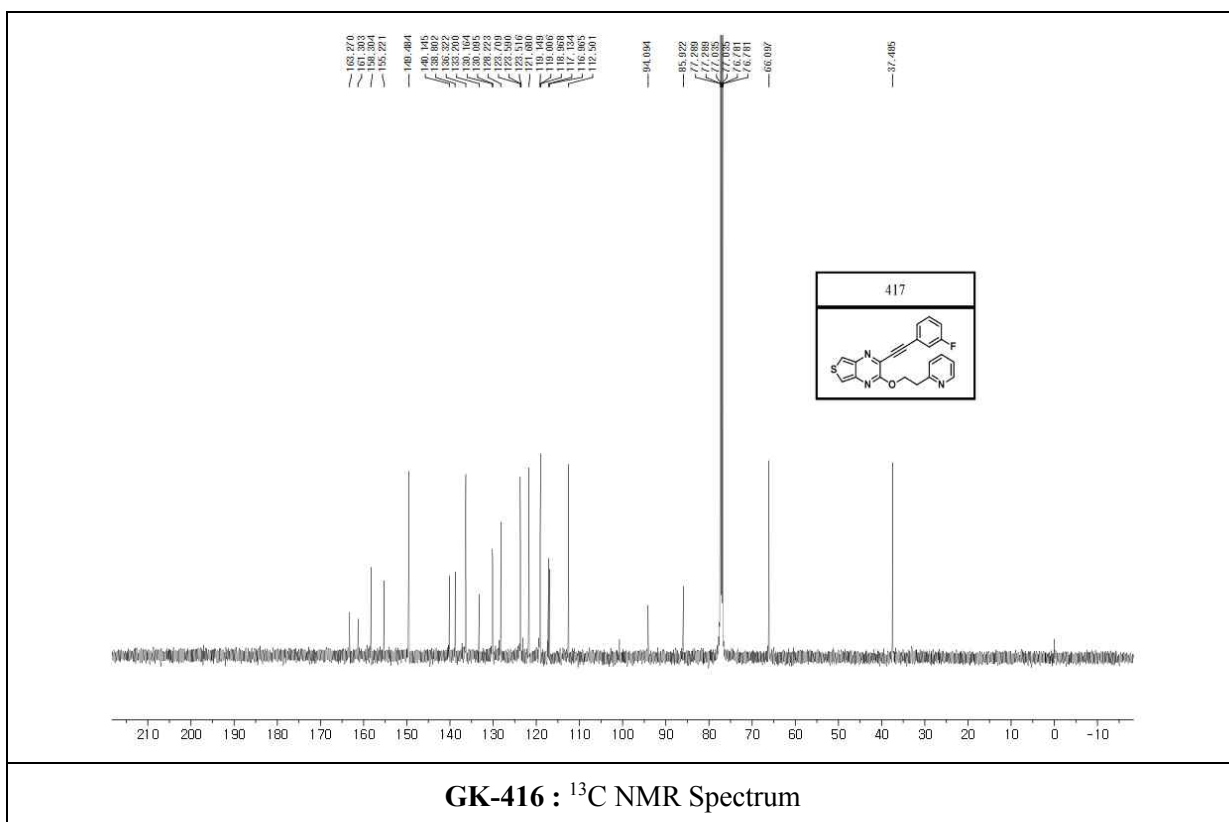
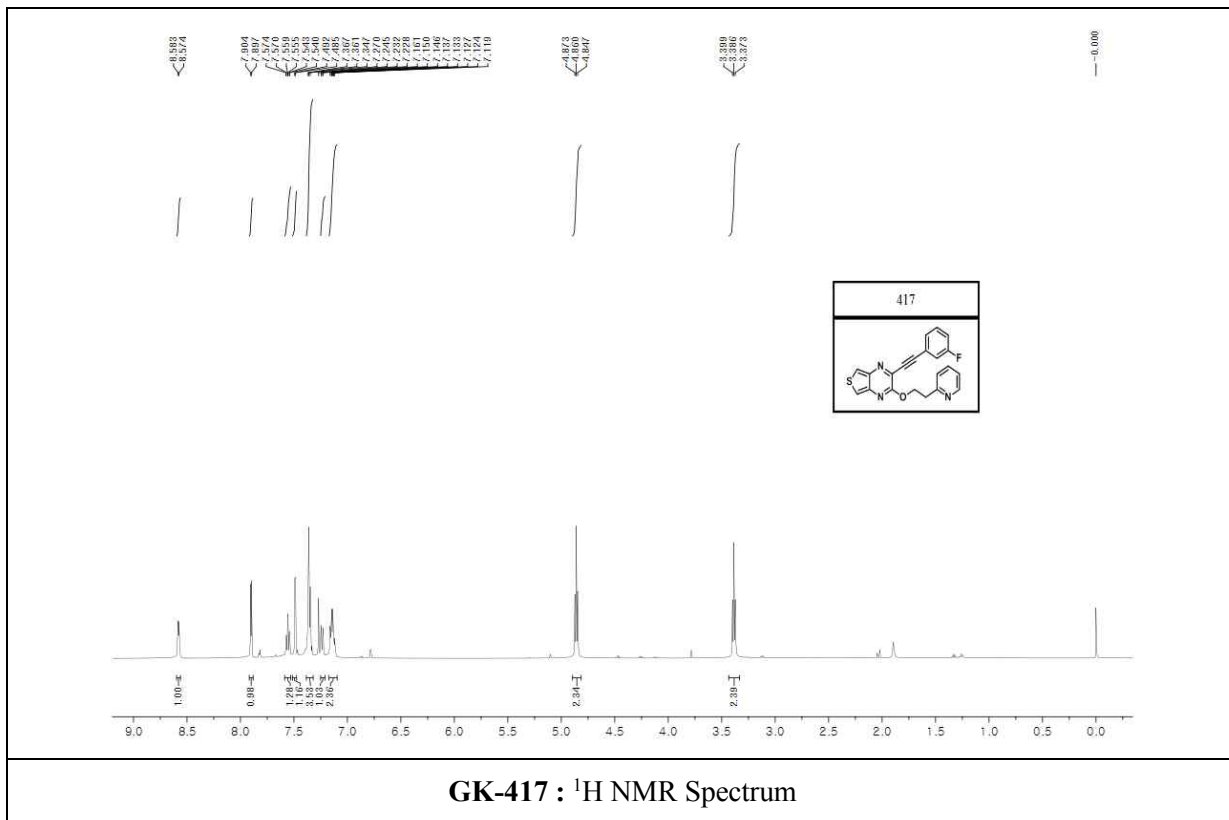


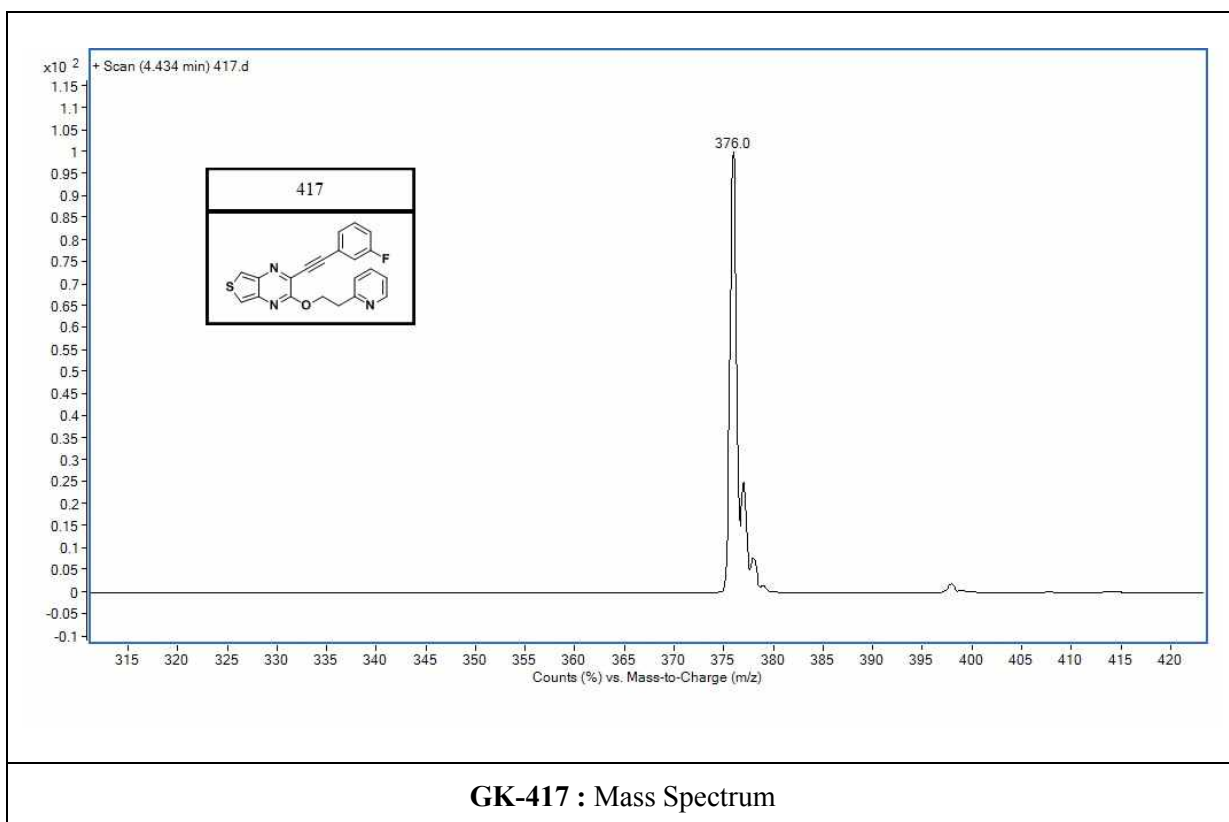
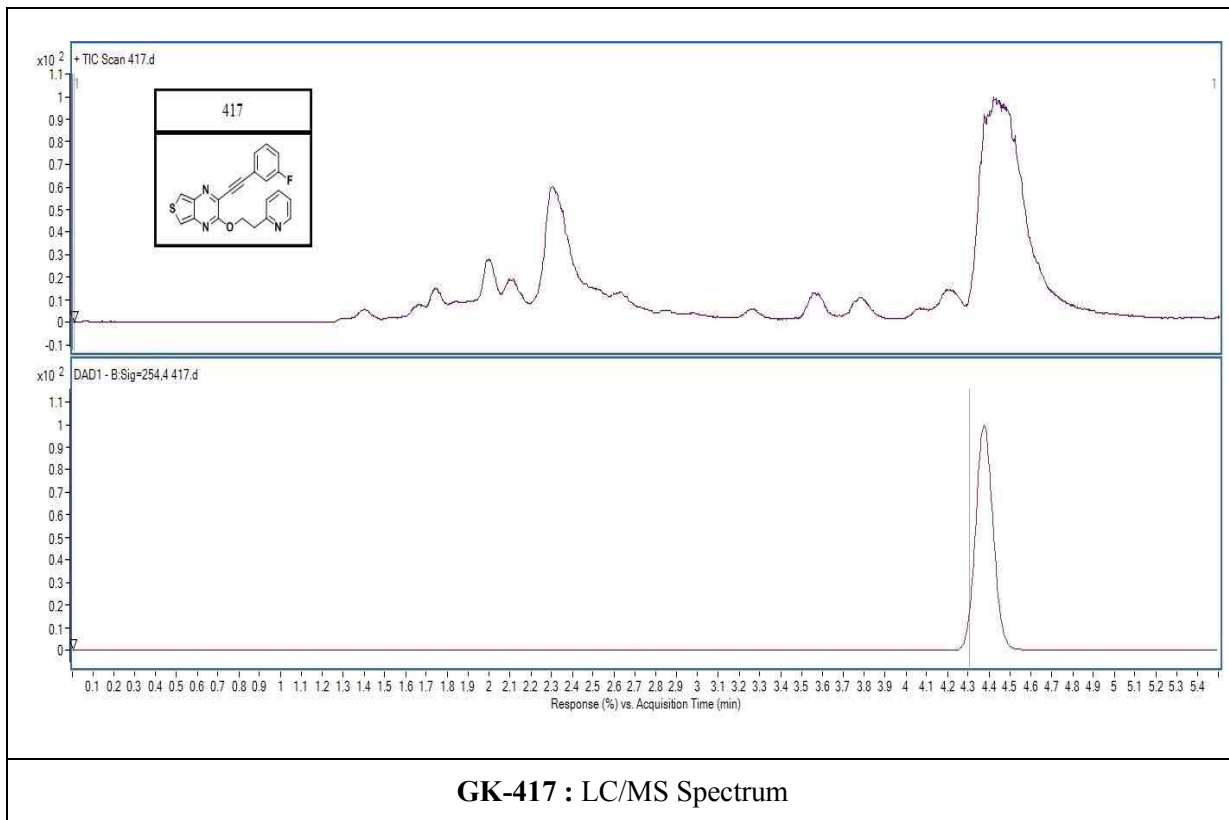






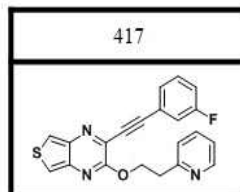
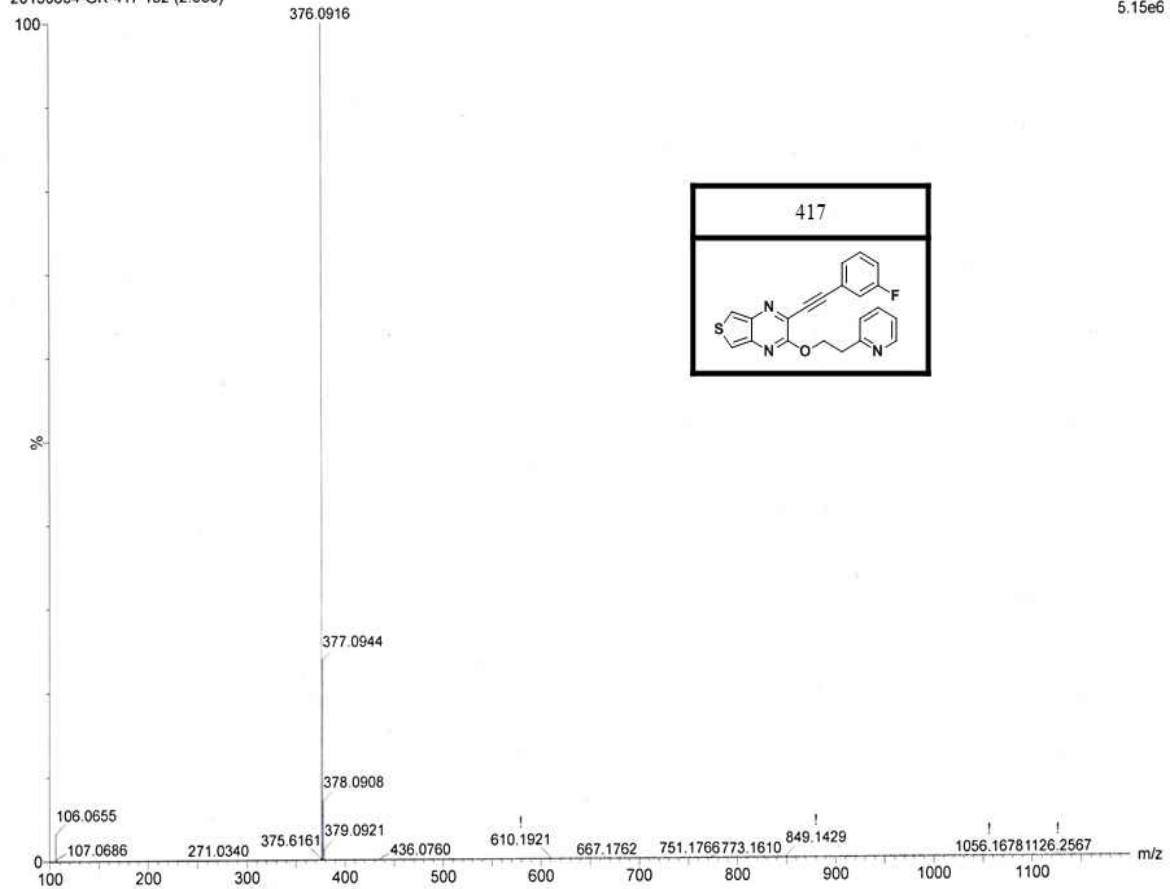




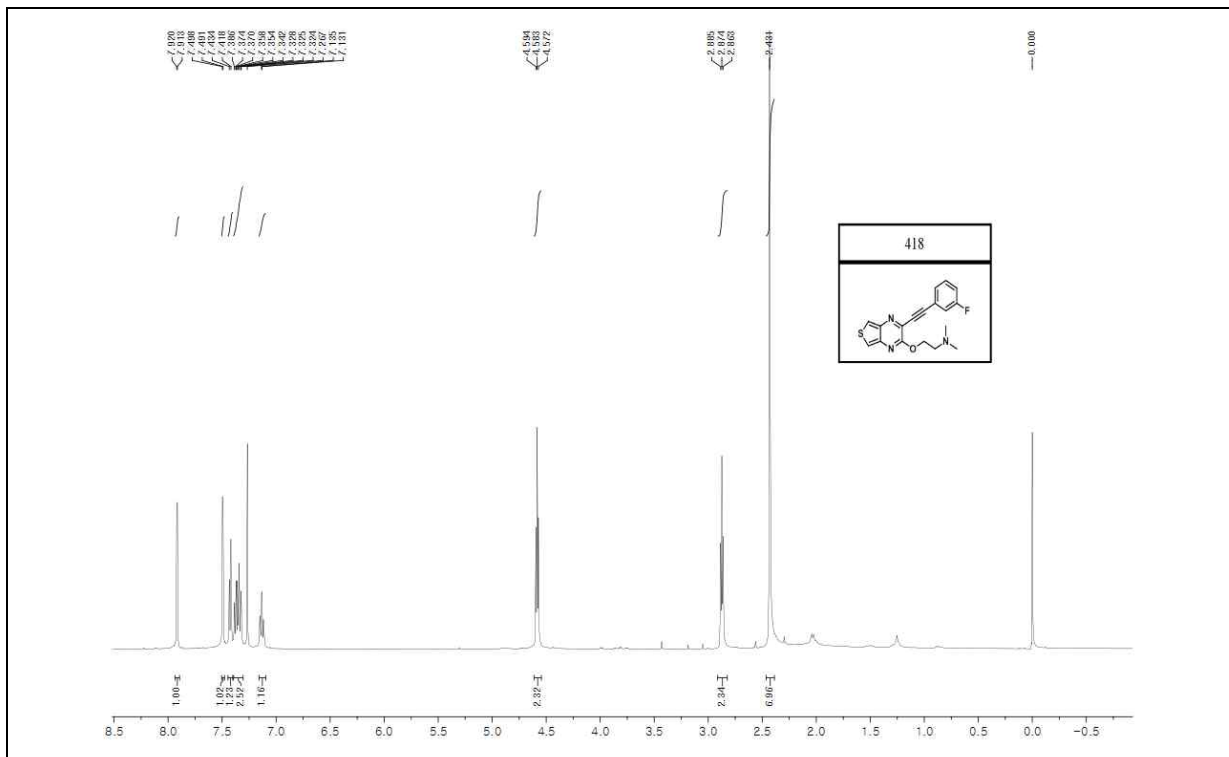


20130604-GK-417 152 (2.680)

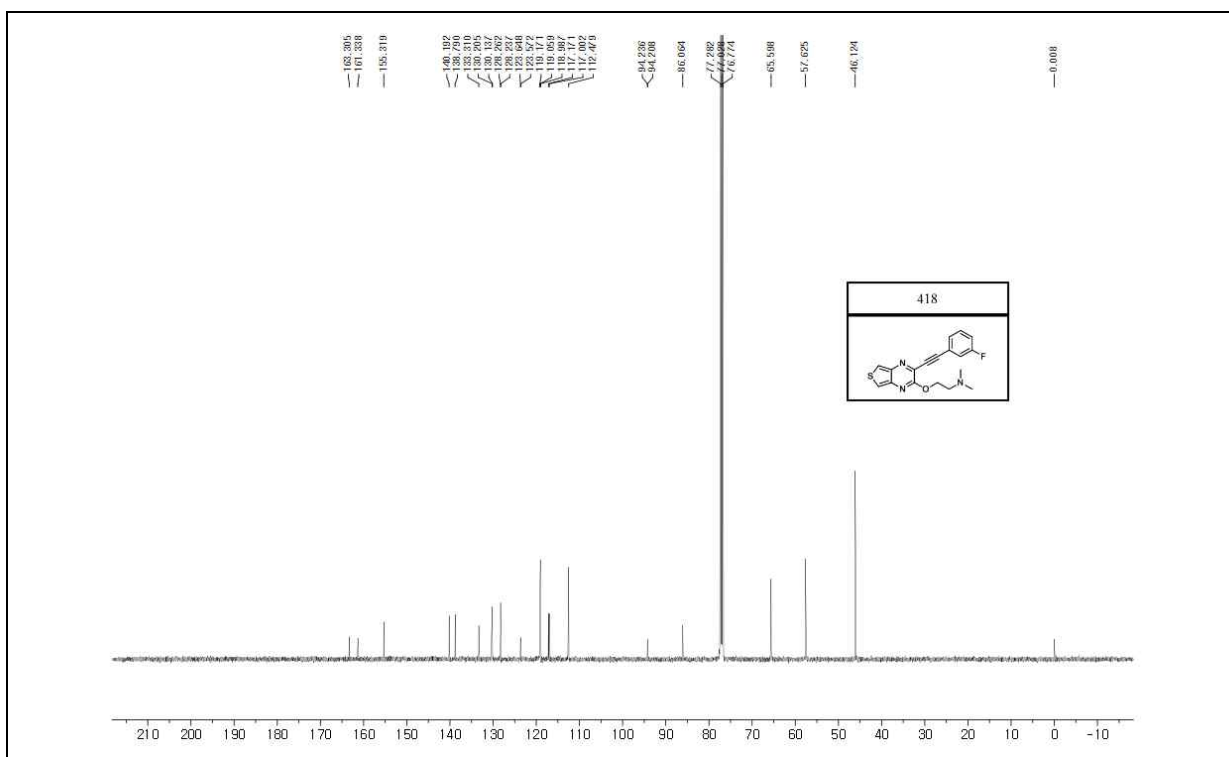
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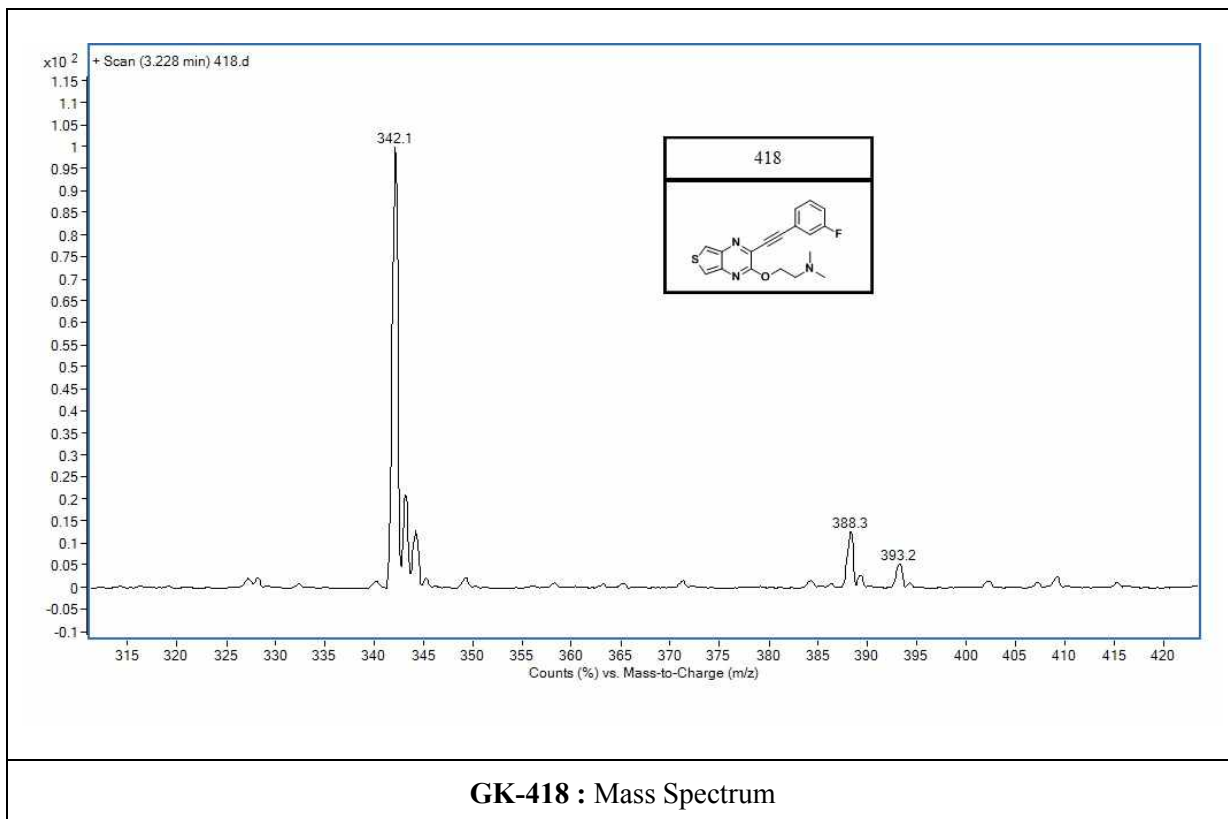
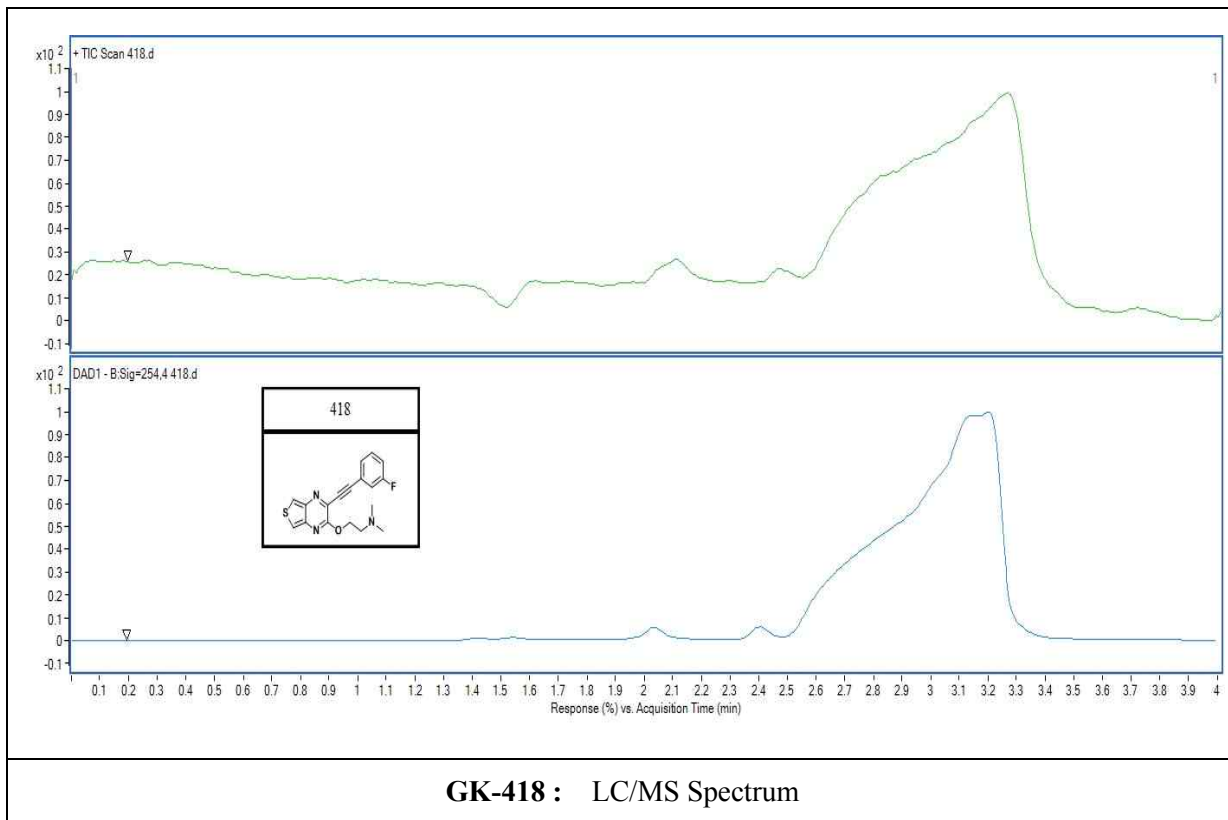
**GK-417** : High Resolution Mass Spectrum



**GK-418 : <sup>1</sup>H NMR Spectrum**



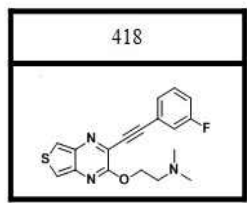
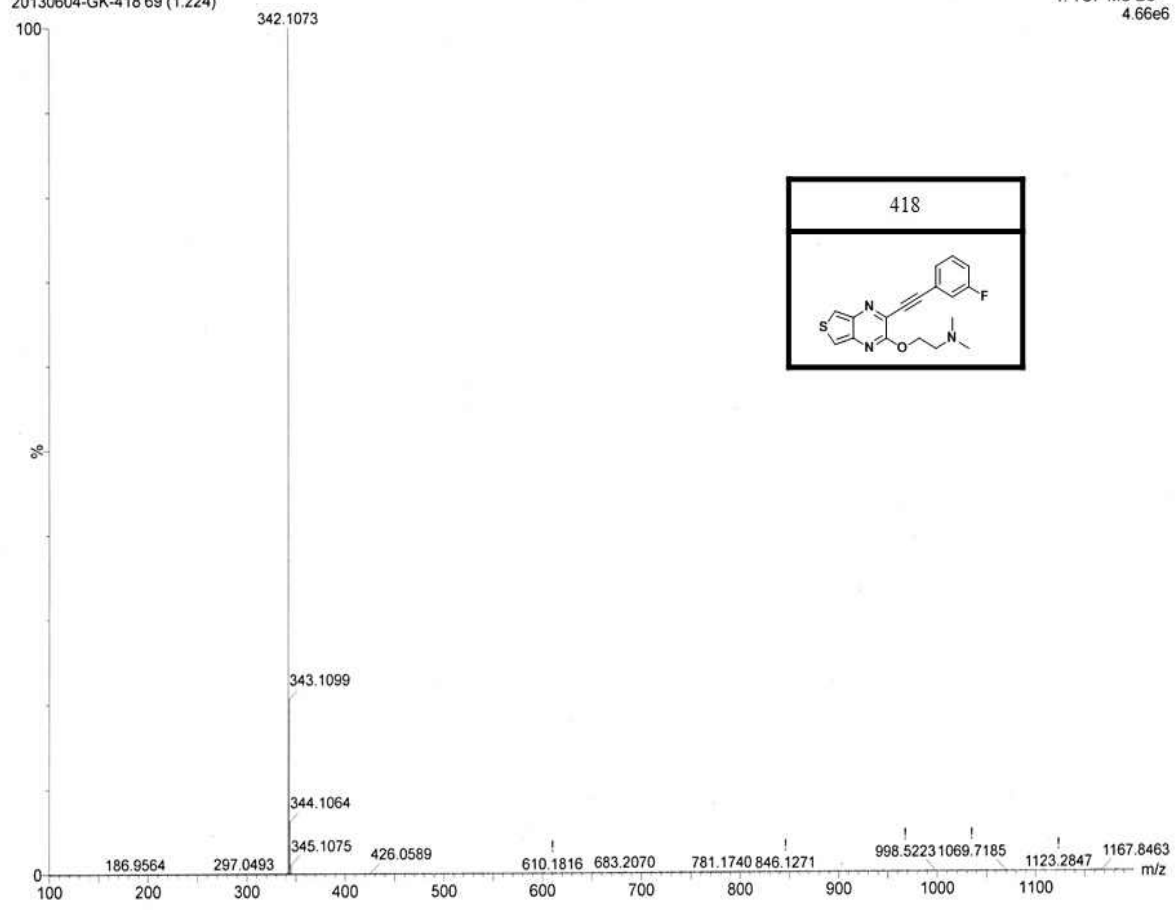
**GK-418 : <sup>13</sup>C NMR Spectrum**





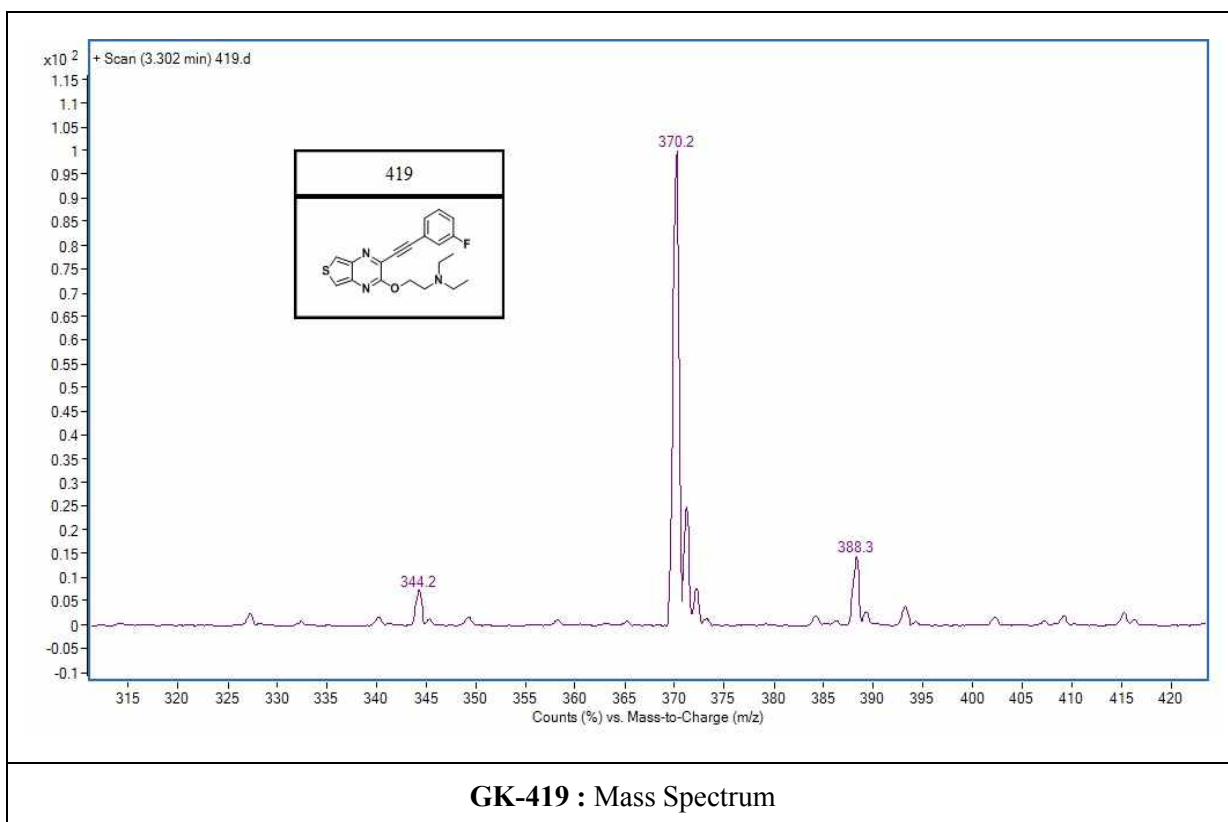
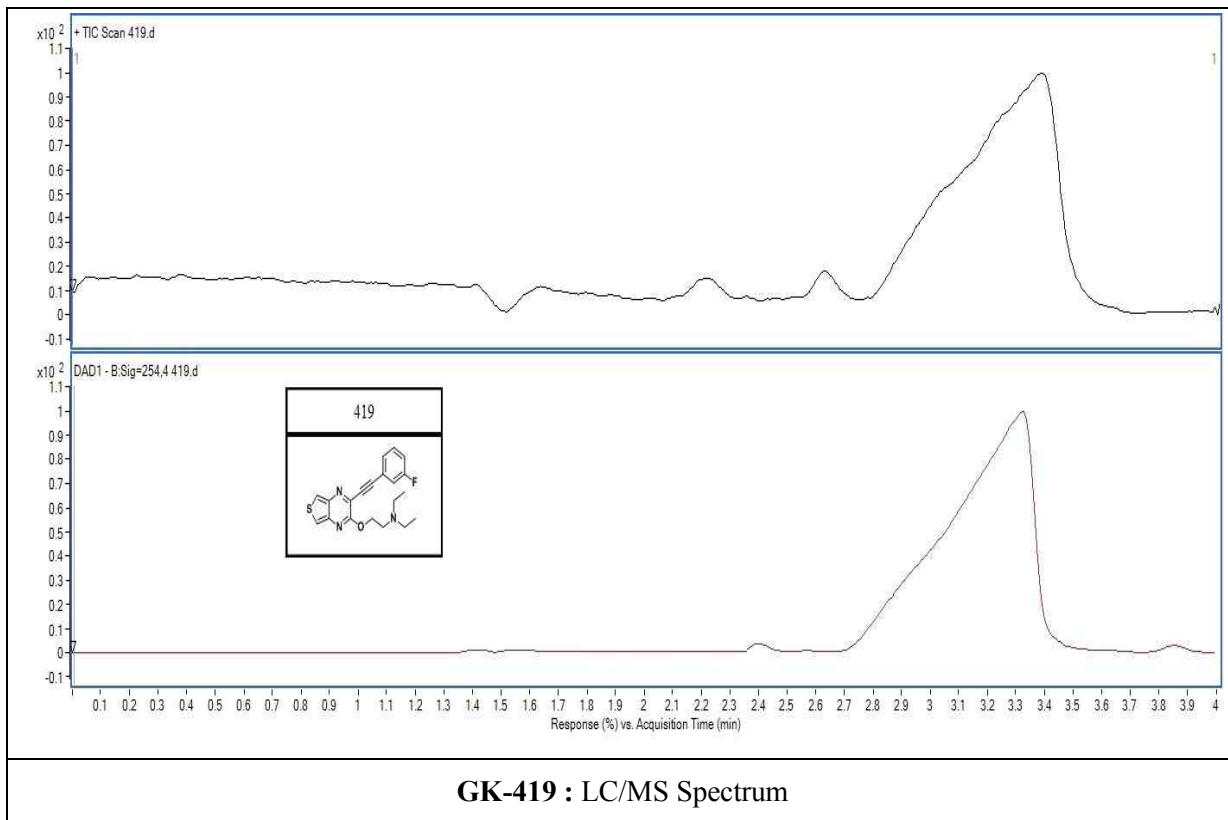
20130604-GK-418 69 (1.224)

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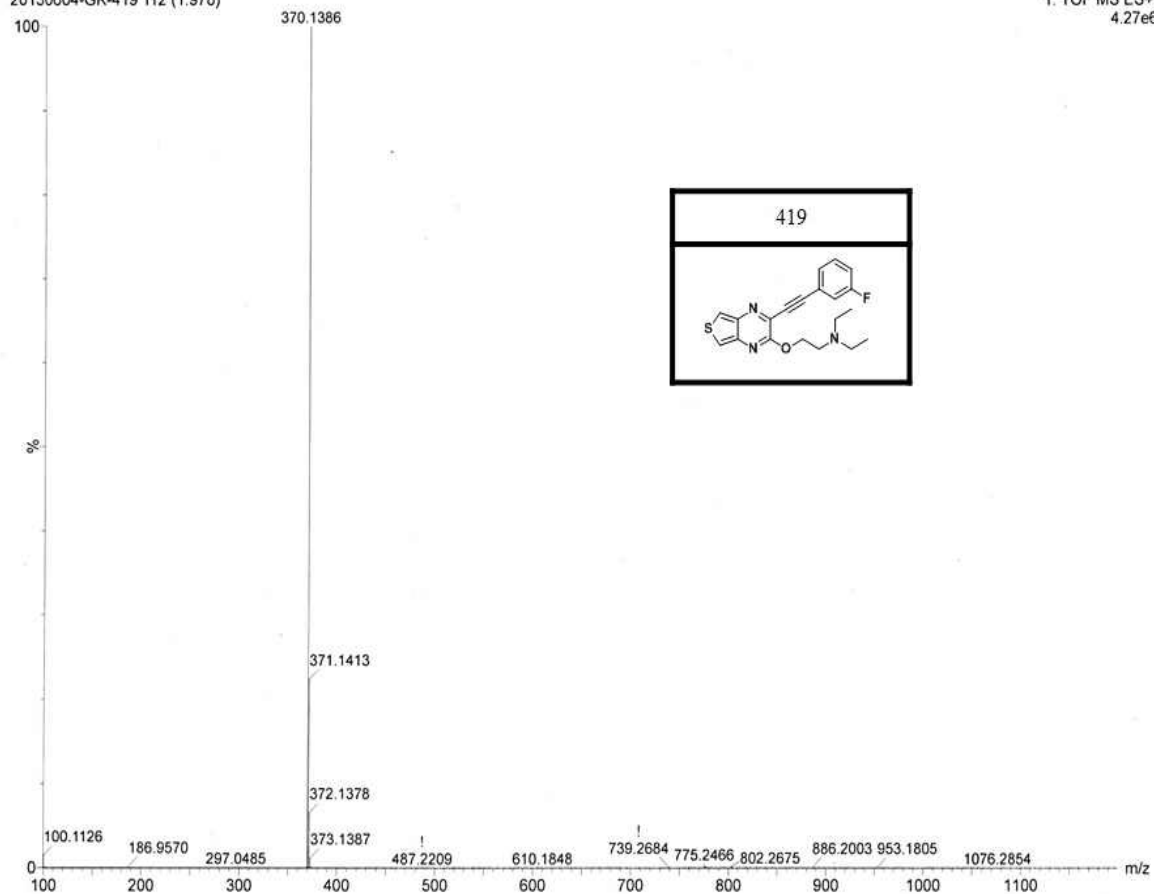
**GK-418 : High Resolution Mass Spectrum**



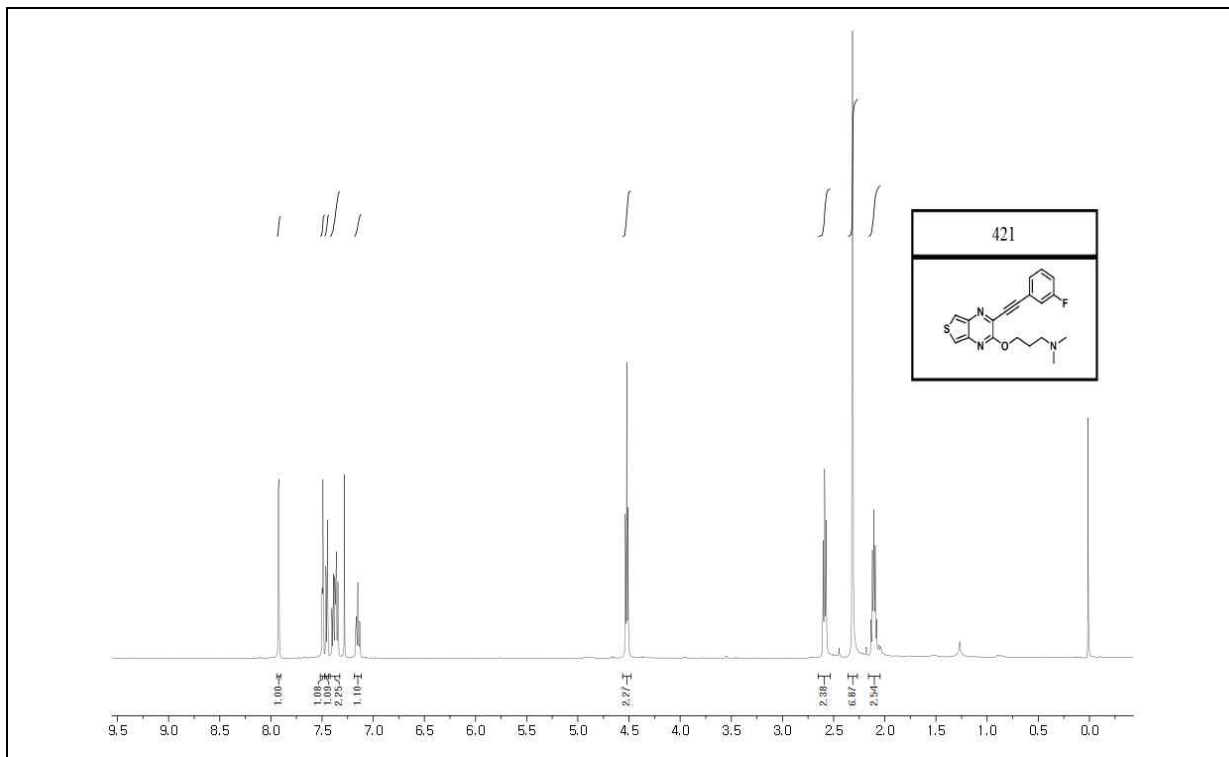


20130604-GK-419 112 (1.978)

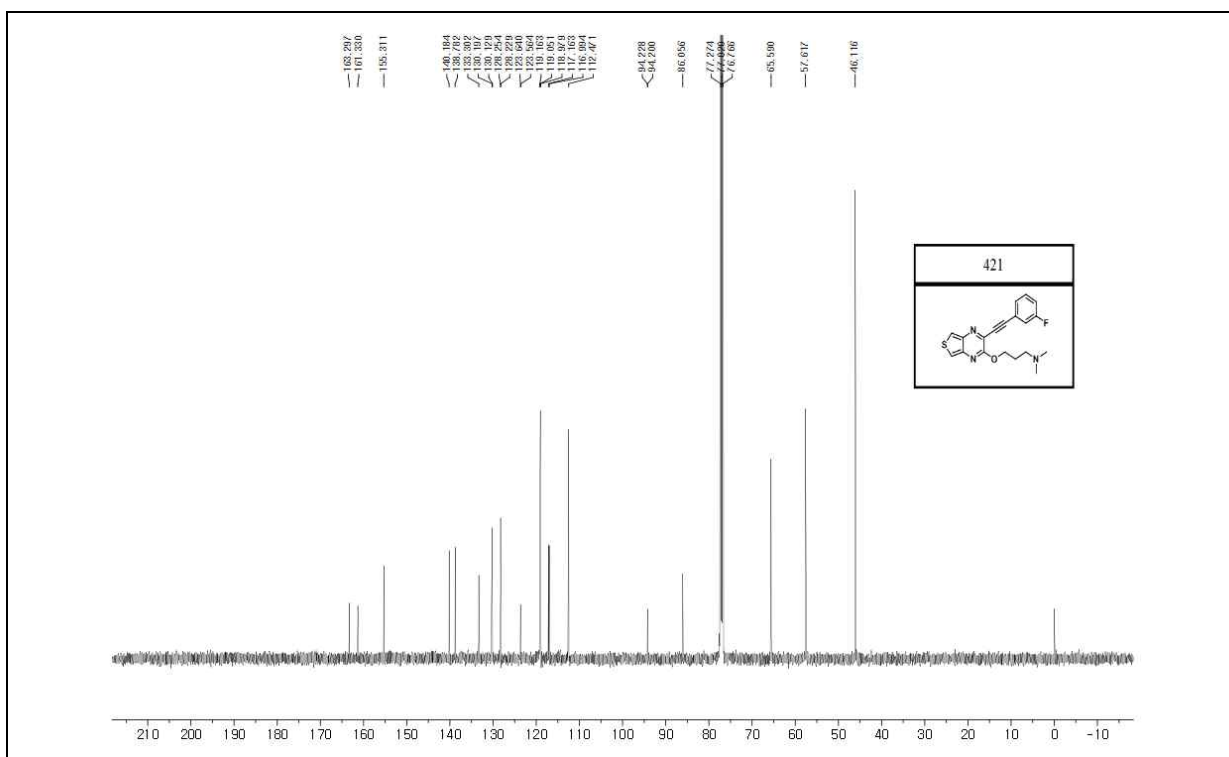
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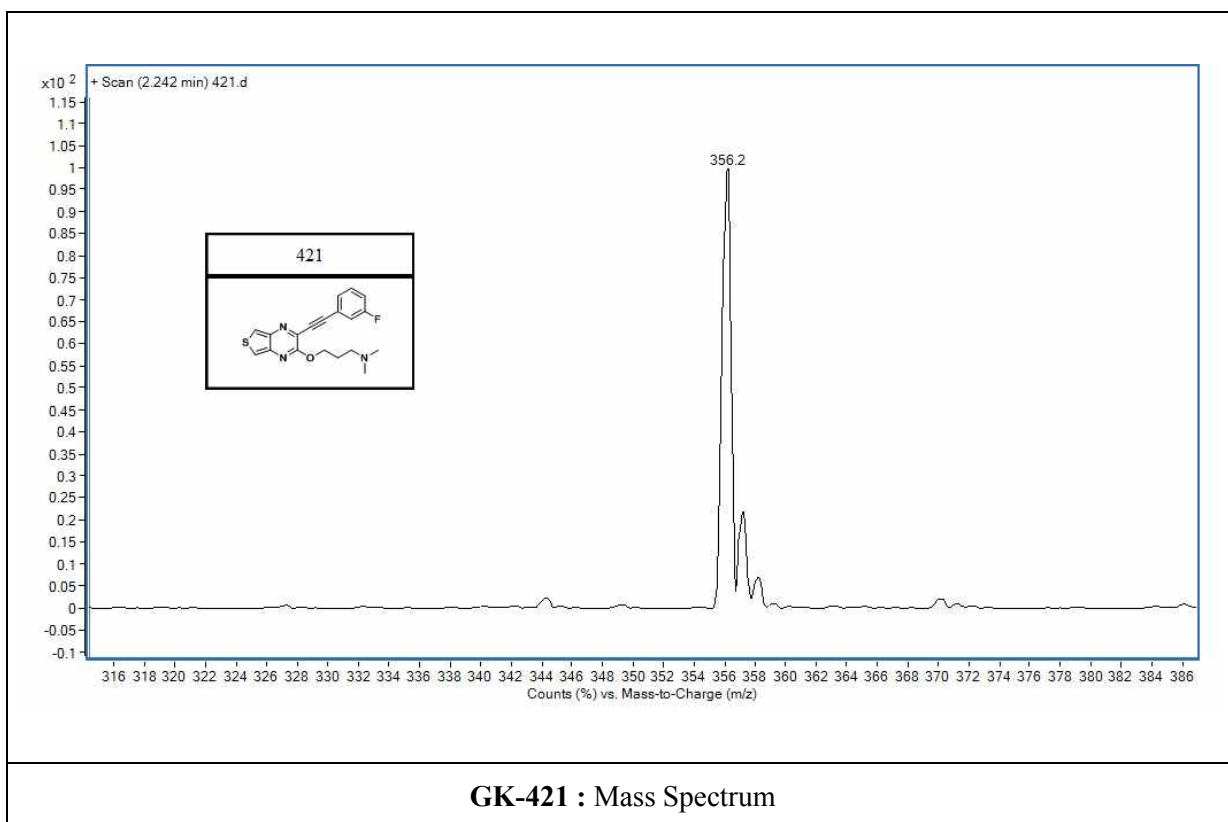
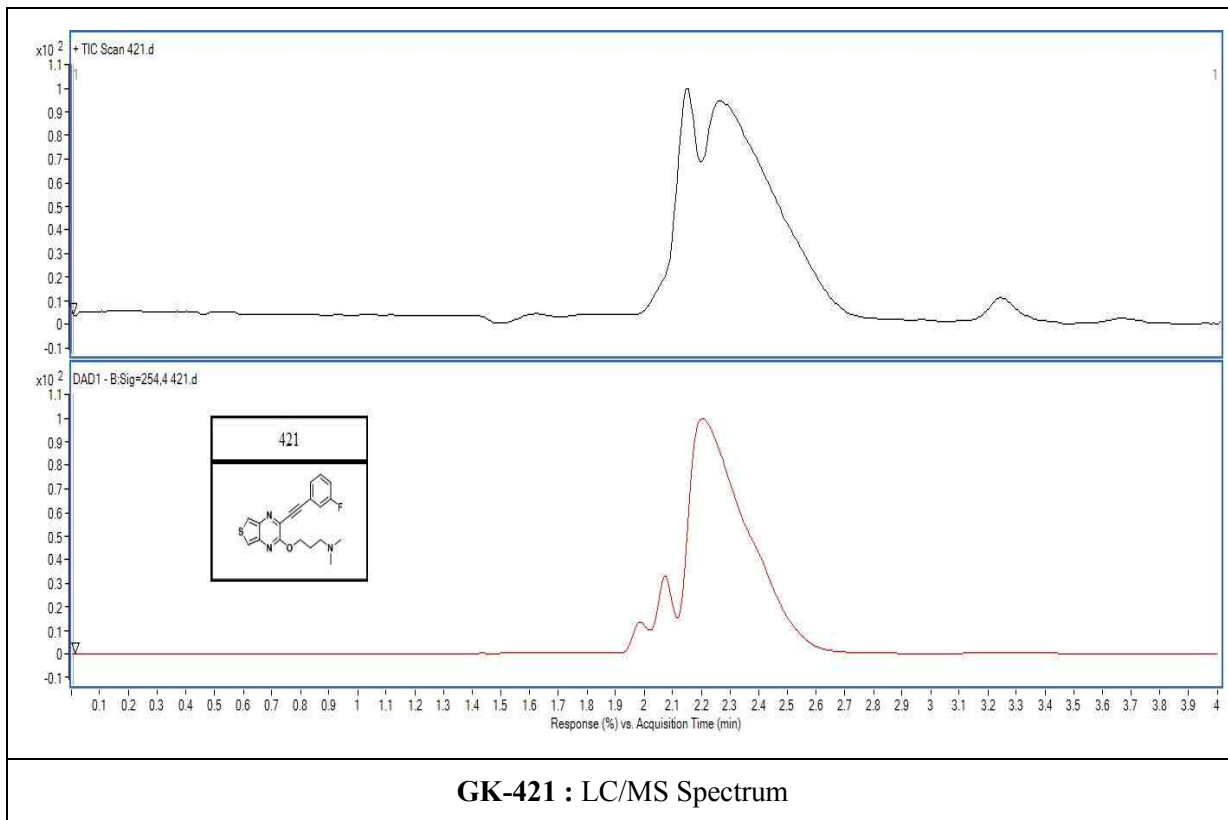
**GK-419 : High Resolution Mass Spectrum**

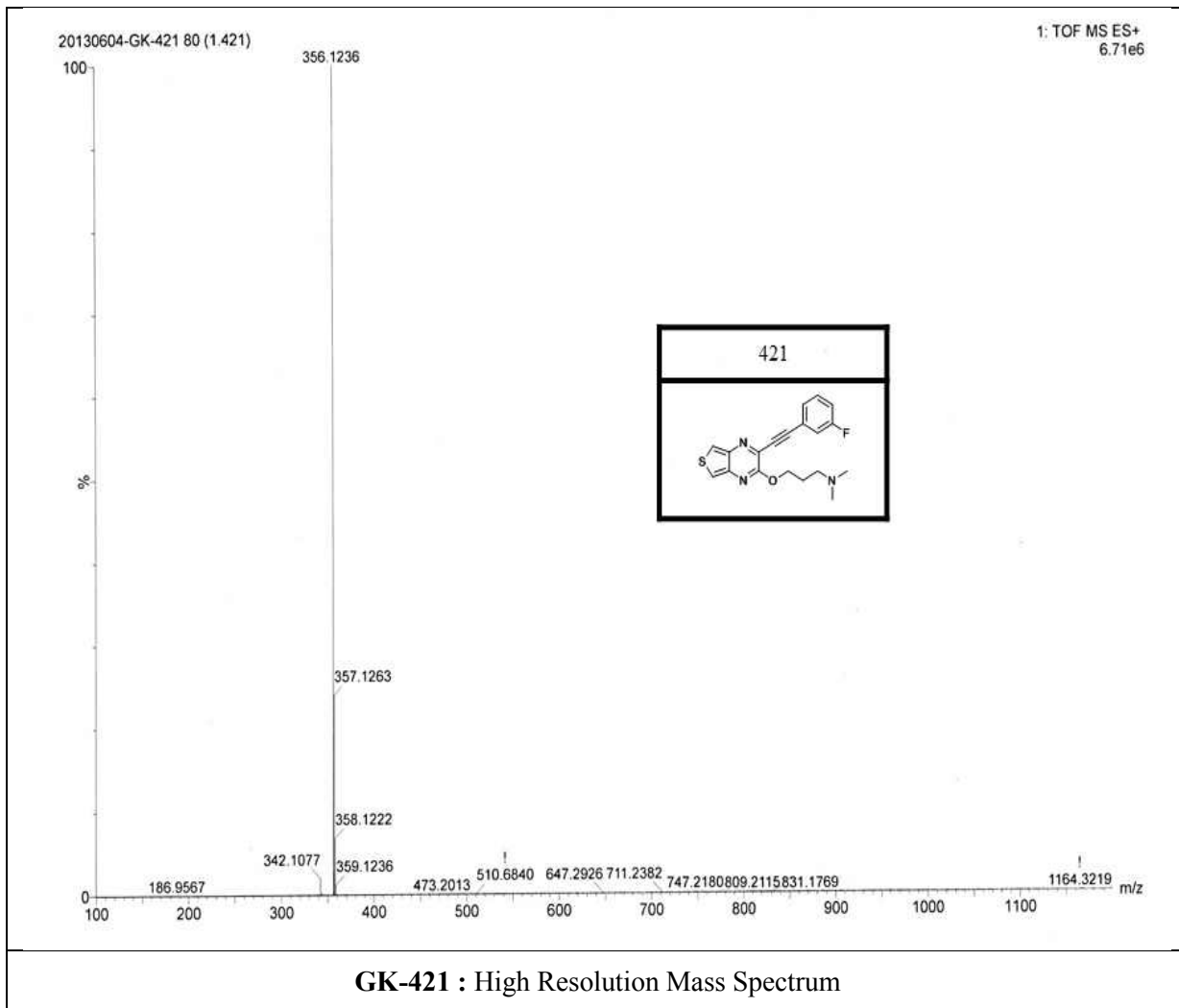


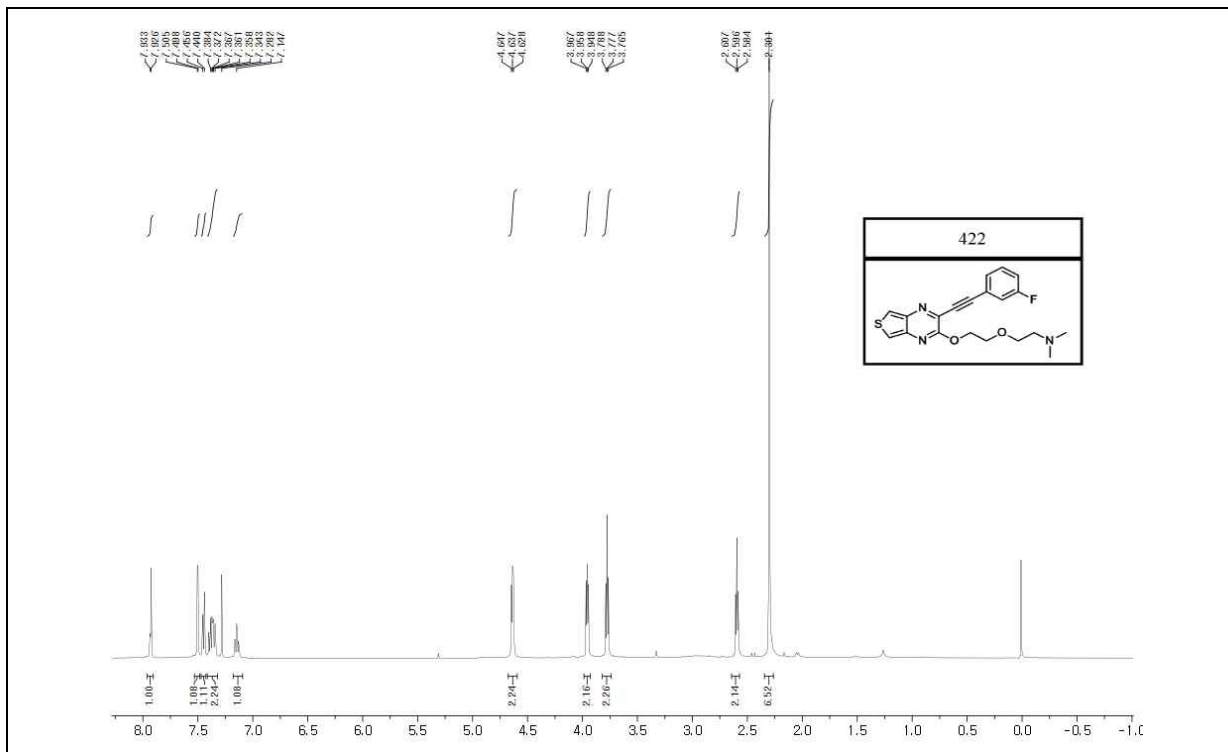
GK-421 : <sup>1</sup>H NMR Spectrum



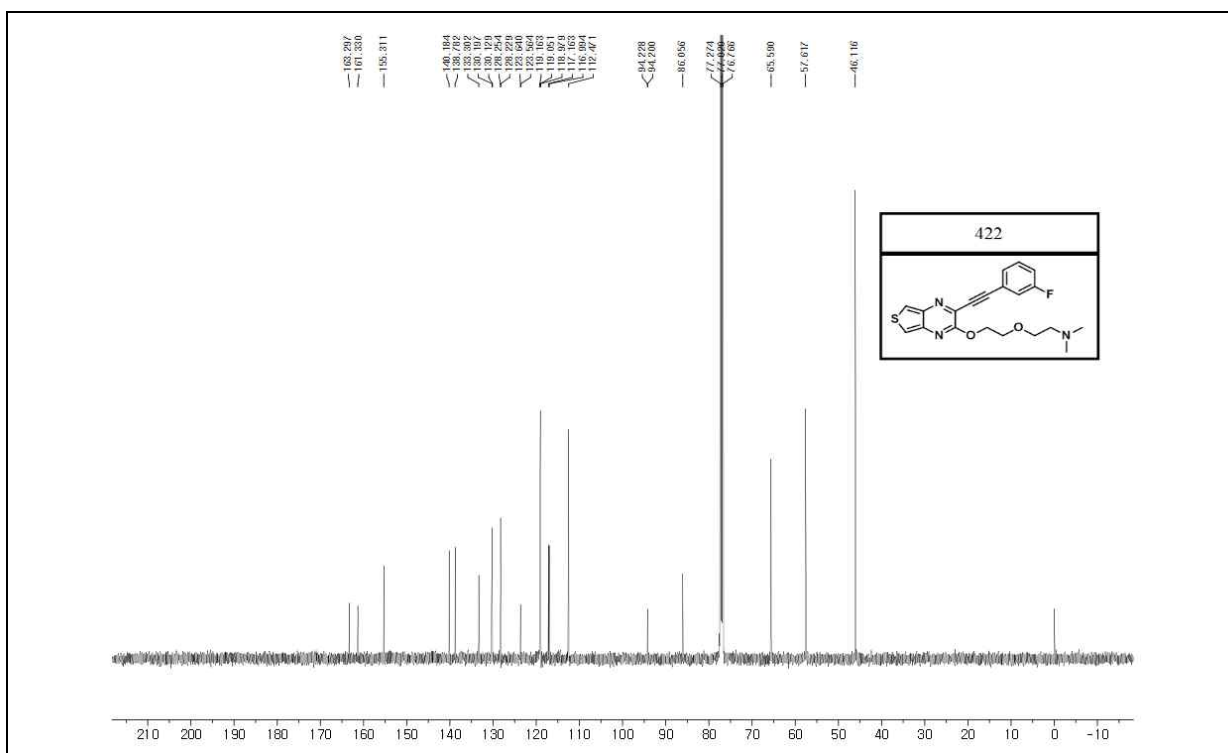
GK-421 : <sup>13</sup>C NMR Spectrum





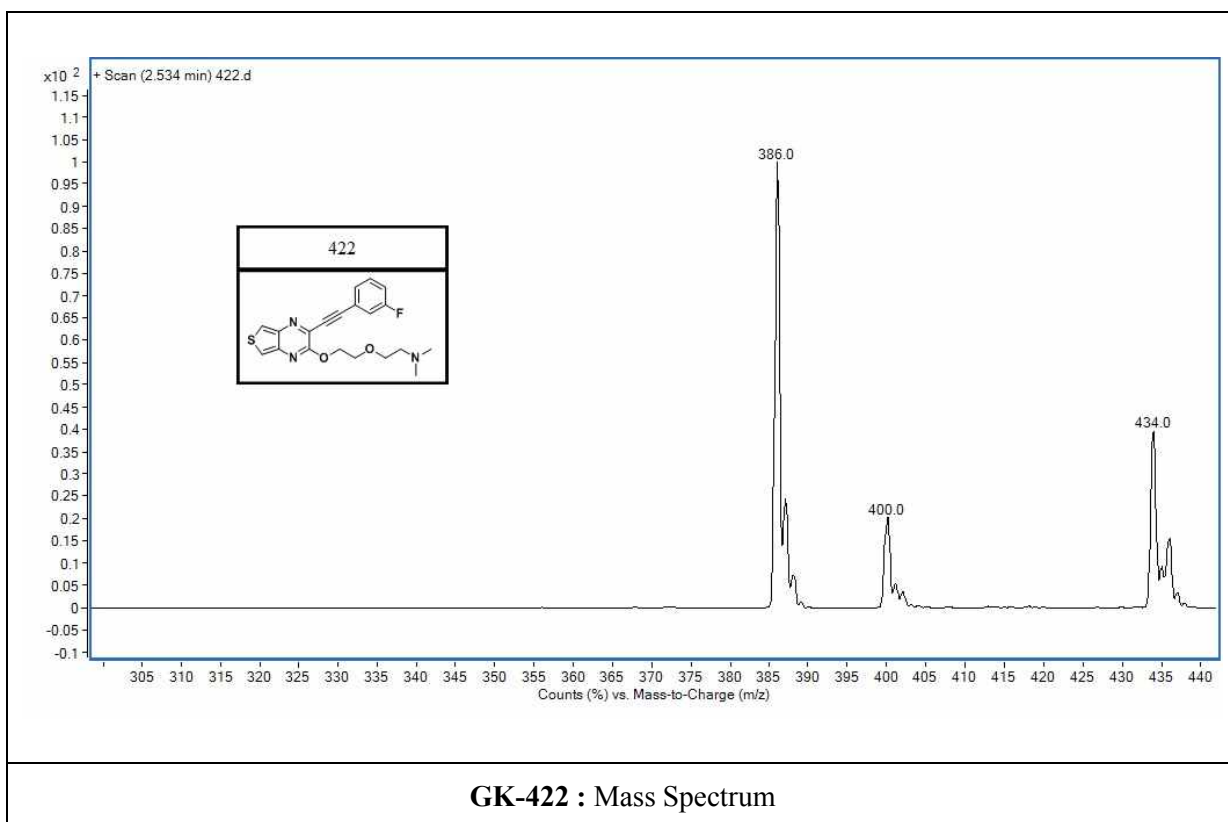
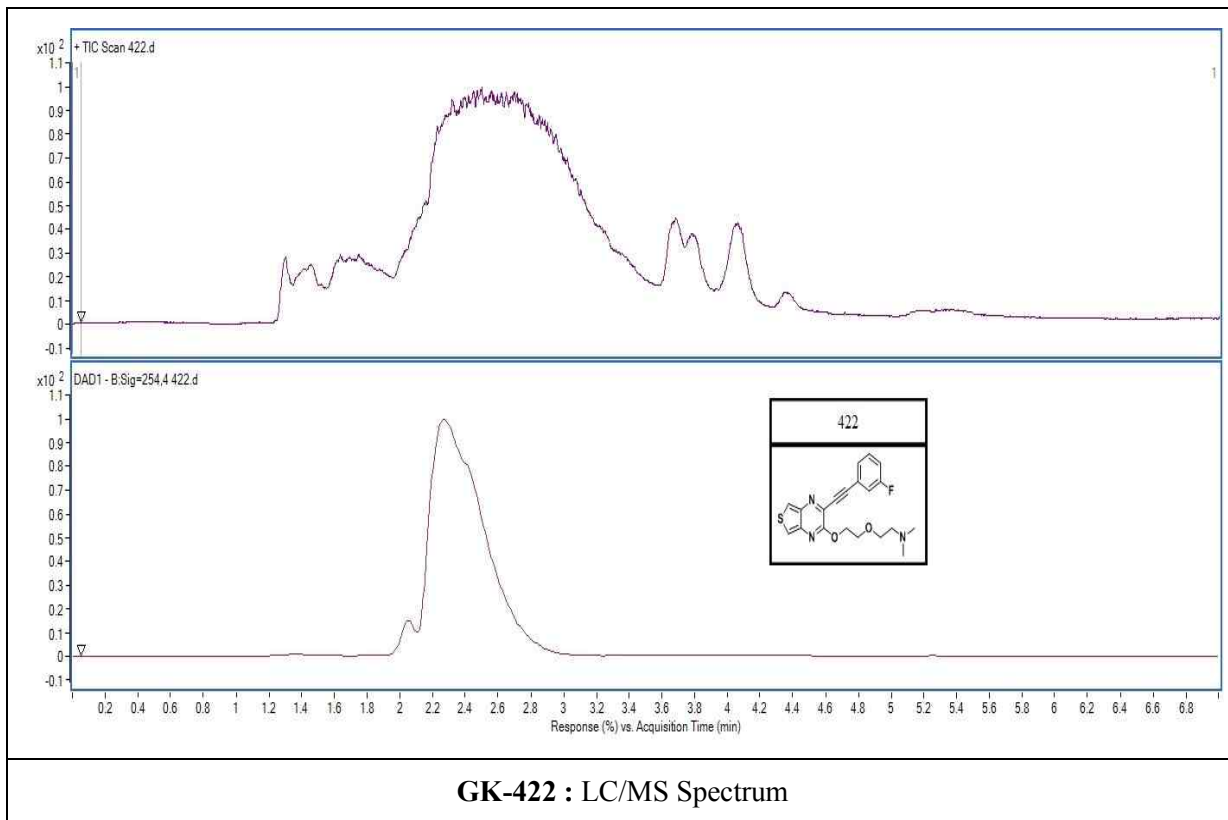


GK-422 : <sup>1</sup>H NMR Spectrum



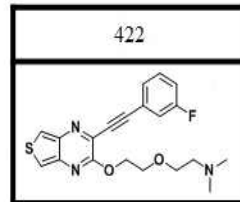
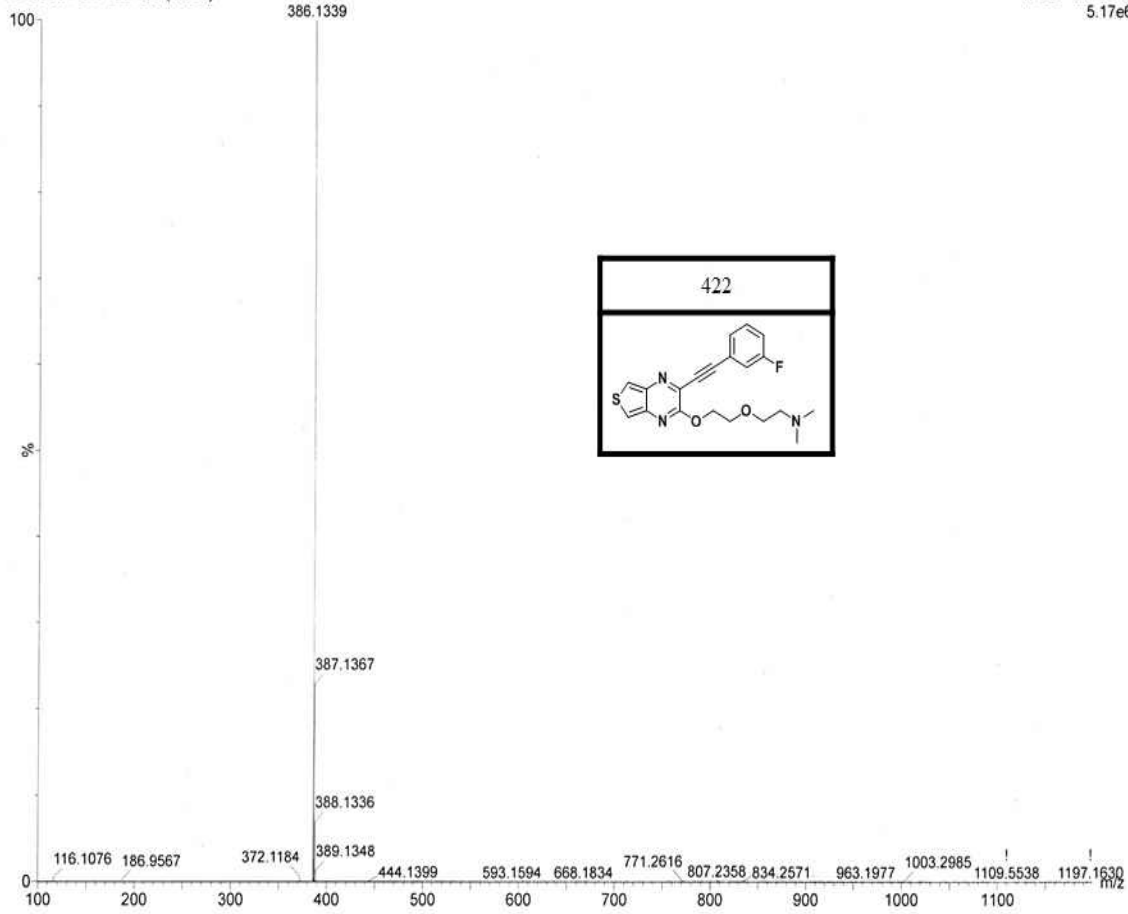
GK-422 : <sup>13</sup>C NMR Spectrum



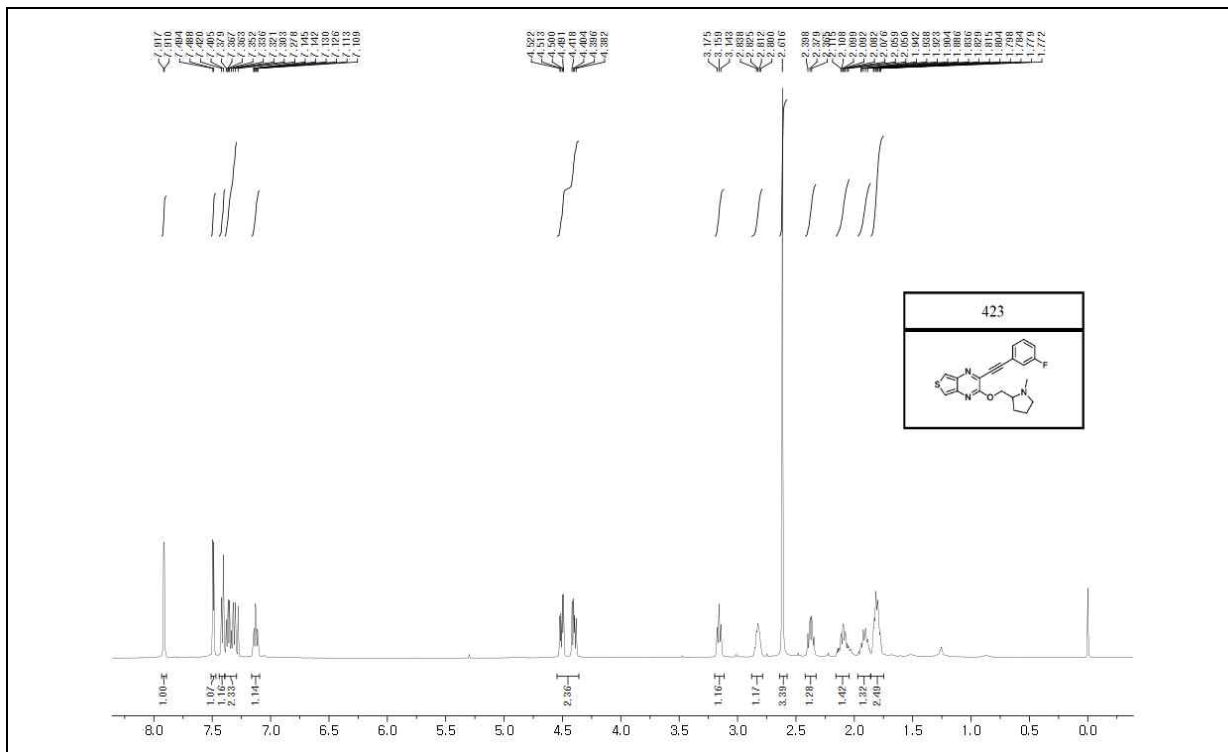


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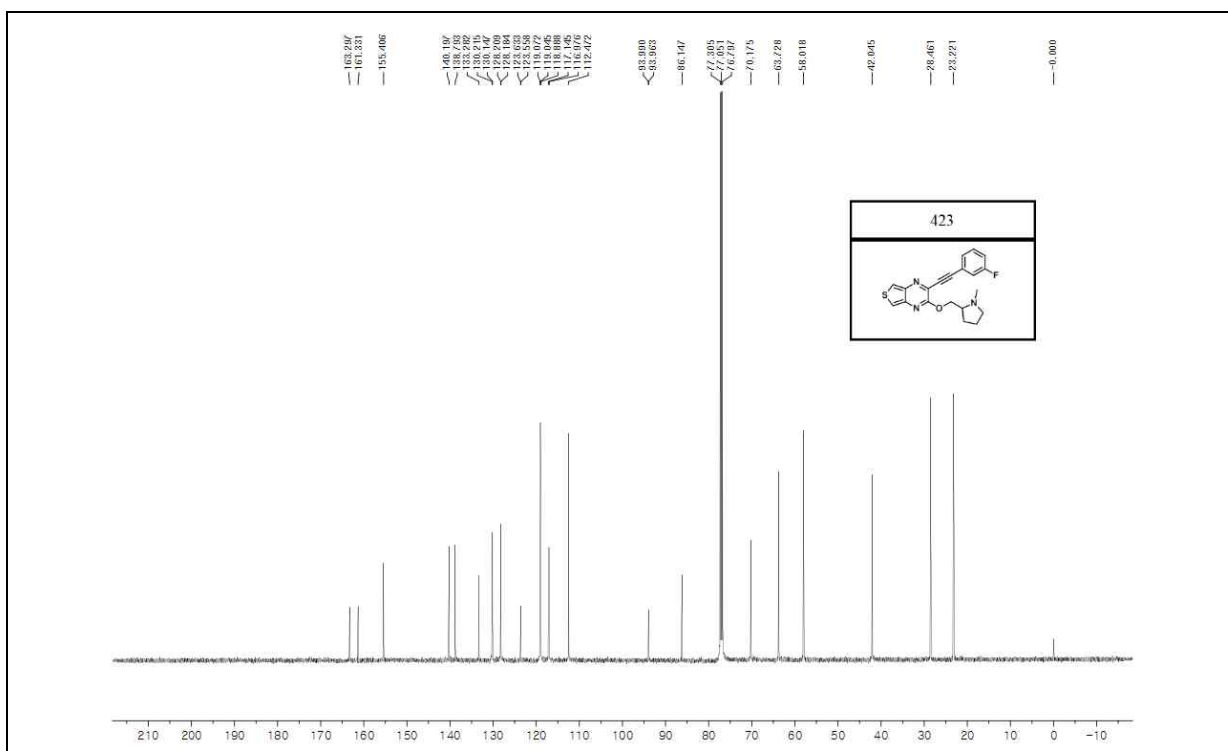
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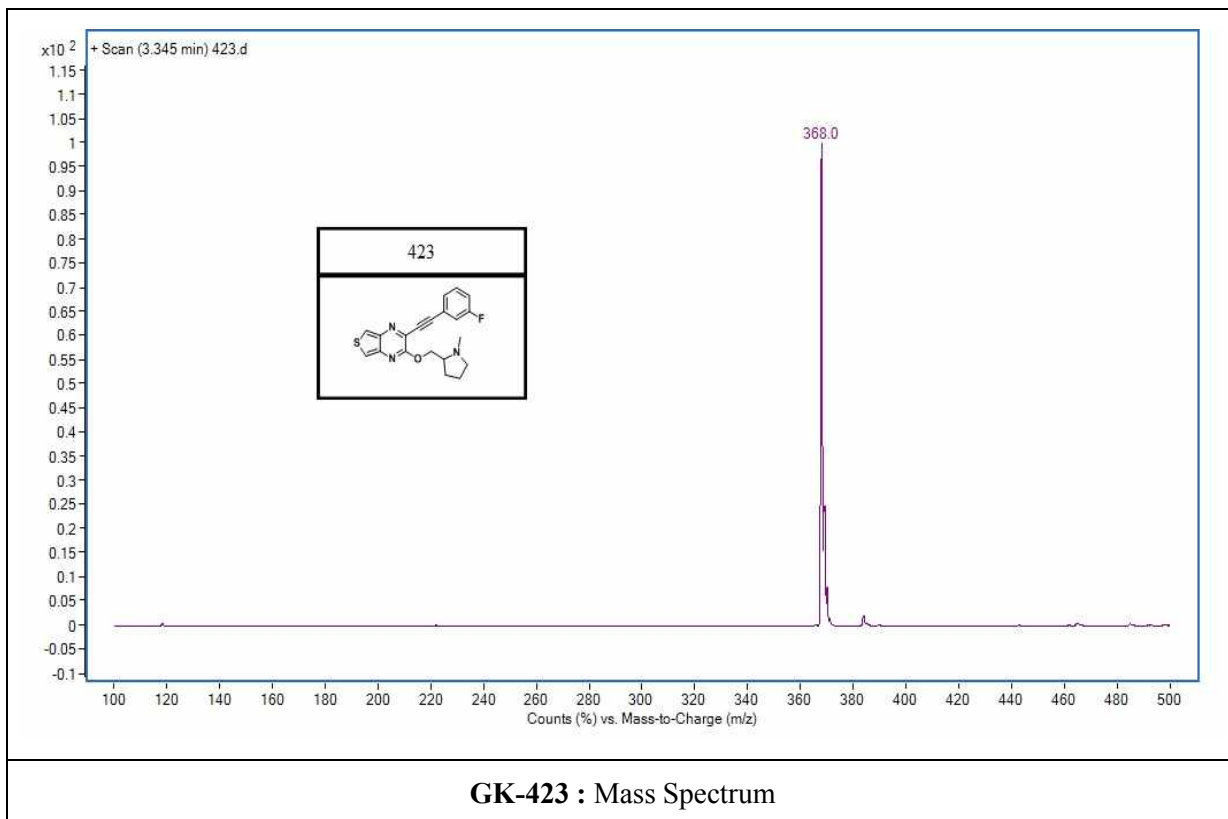
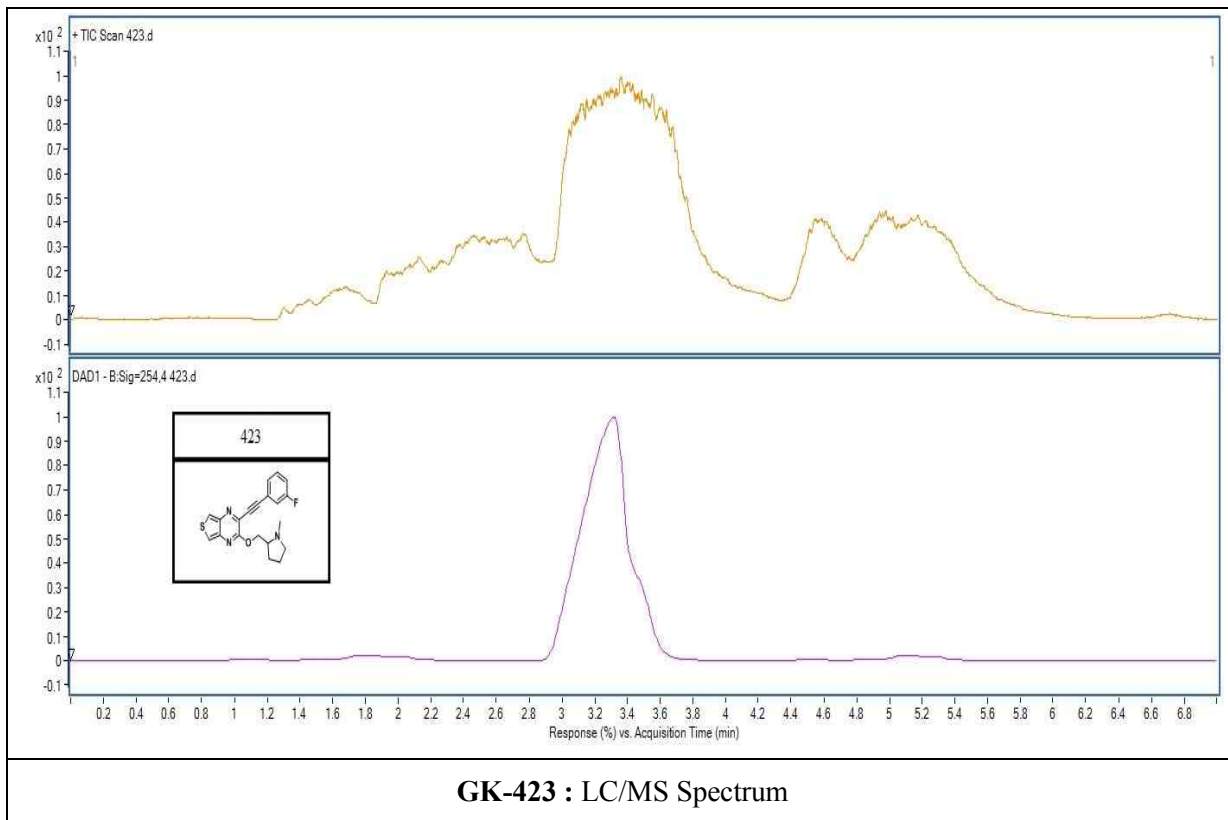
**GK-422 : High Resolution Mass Spectrum**

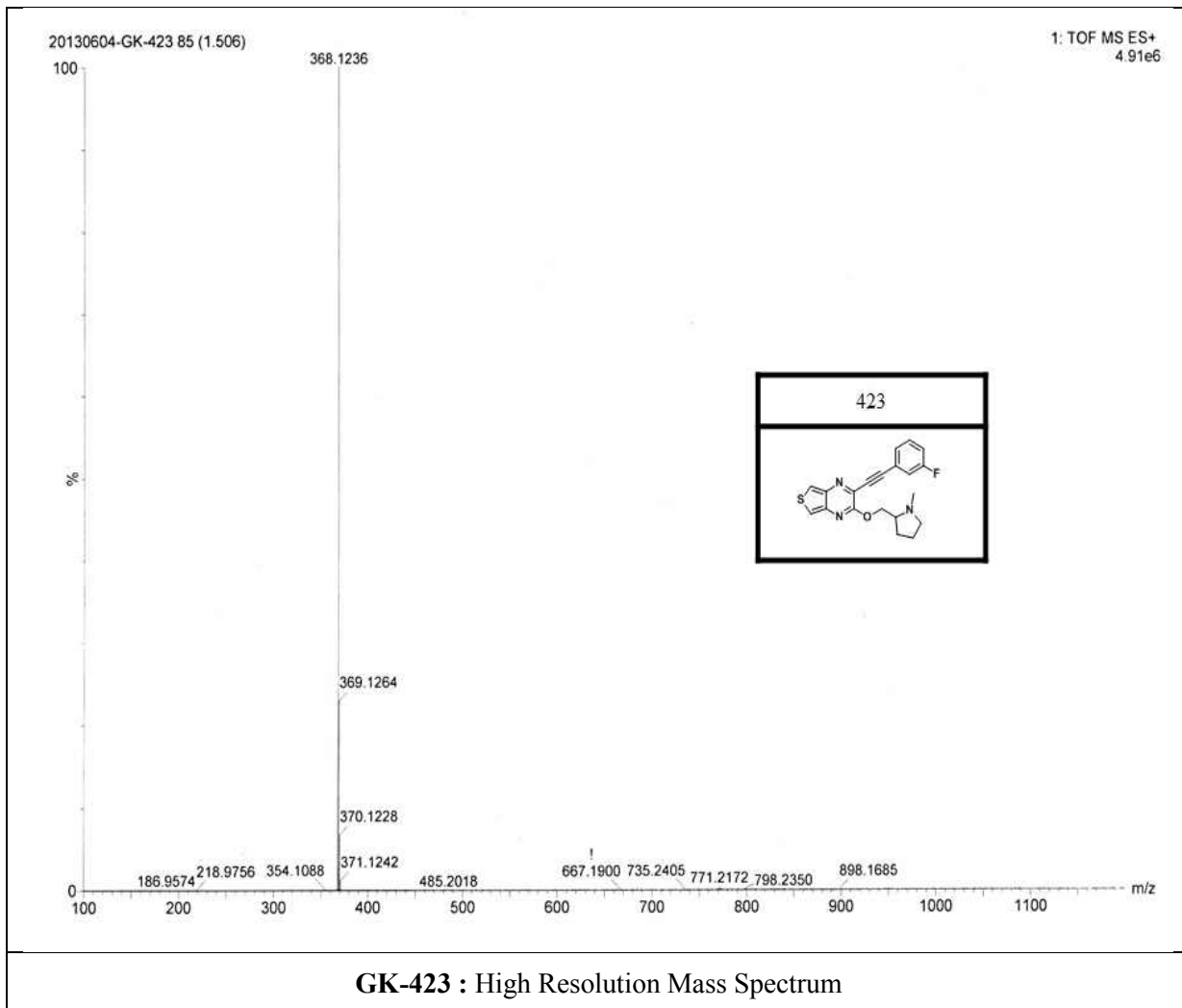


GK-423 : <sup>1</sup>H NMR Spectrum

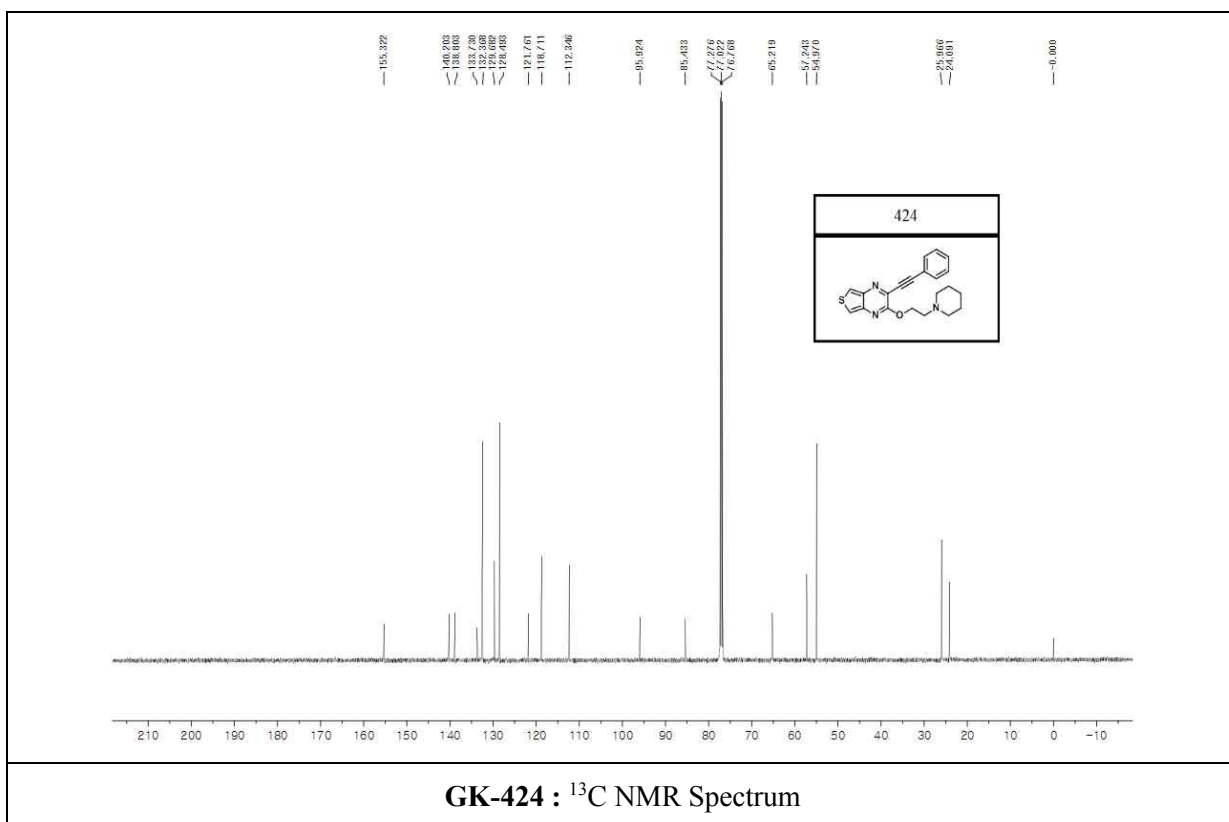
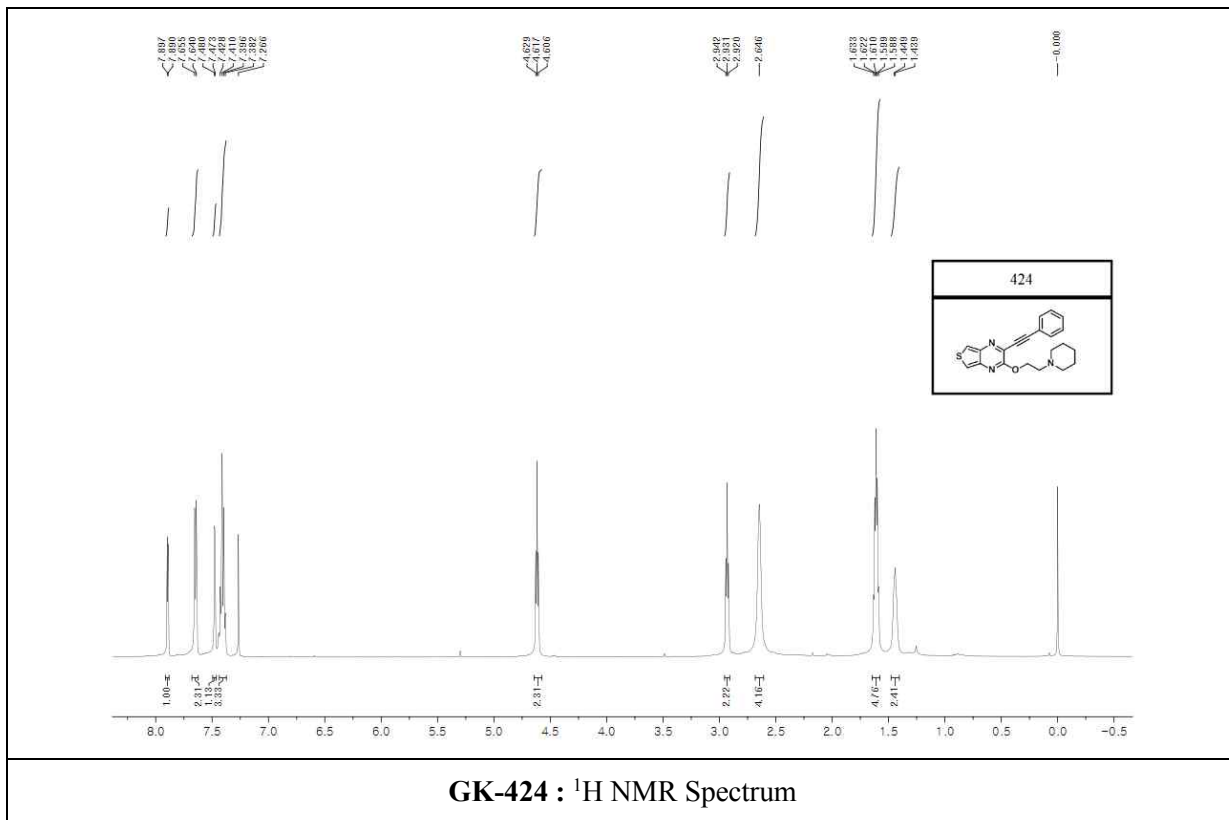


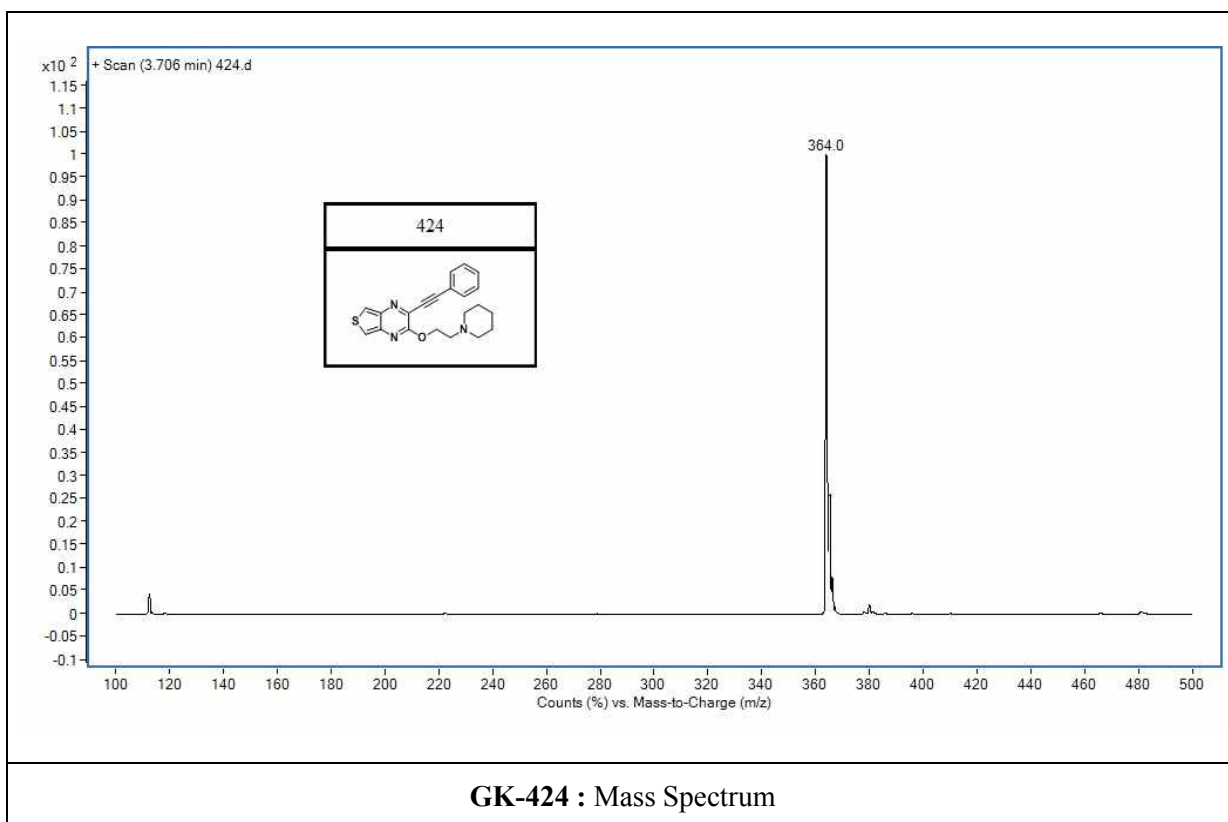
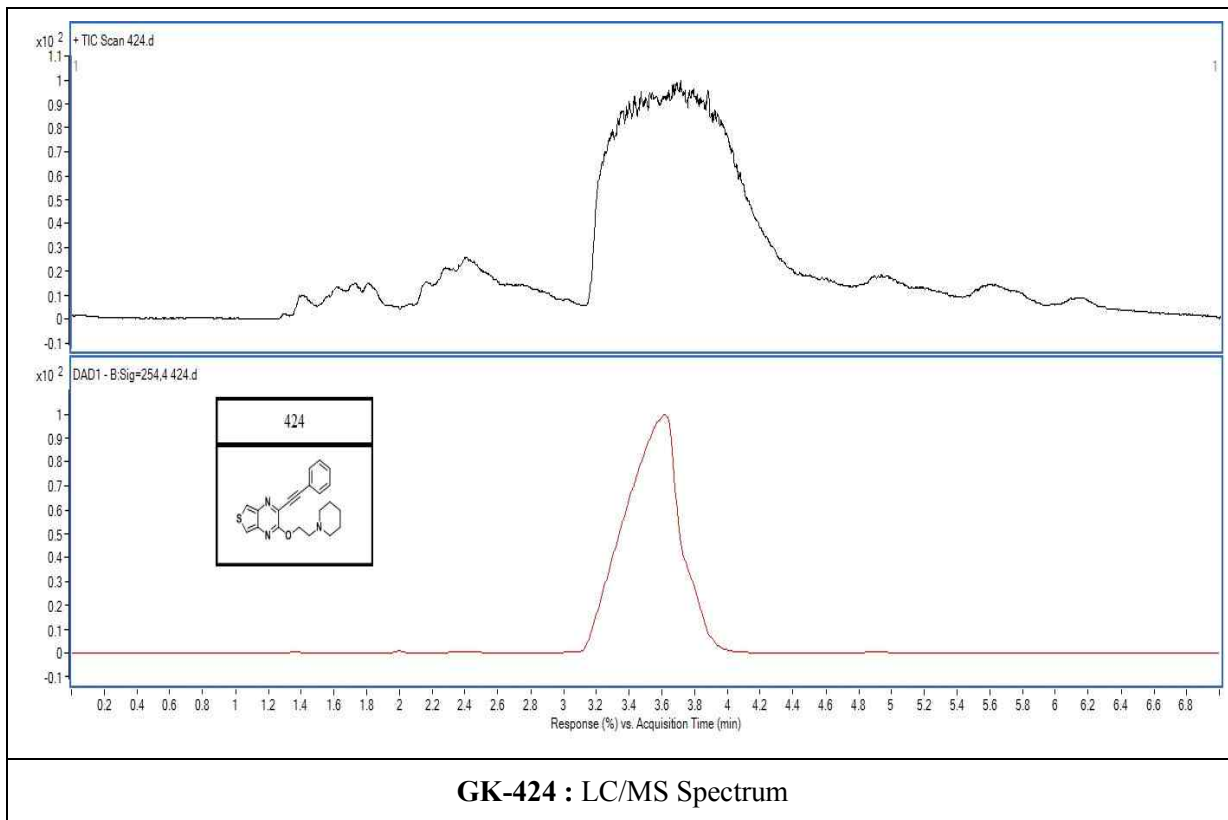
GK-423 : <sup>13</sup>C NMR Spectrum

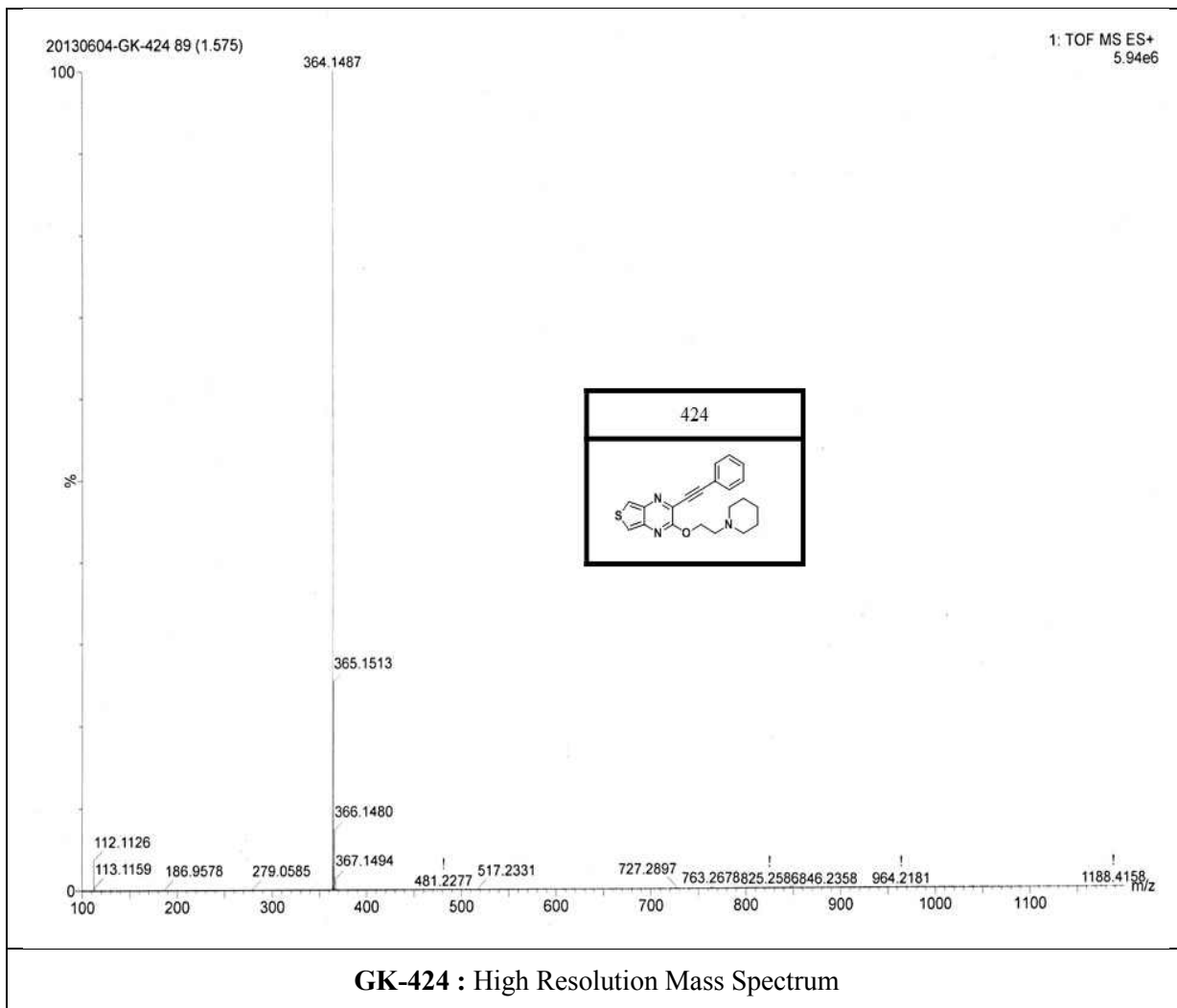




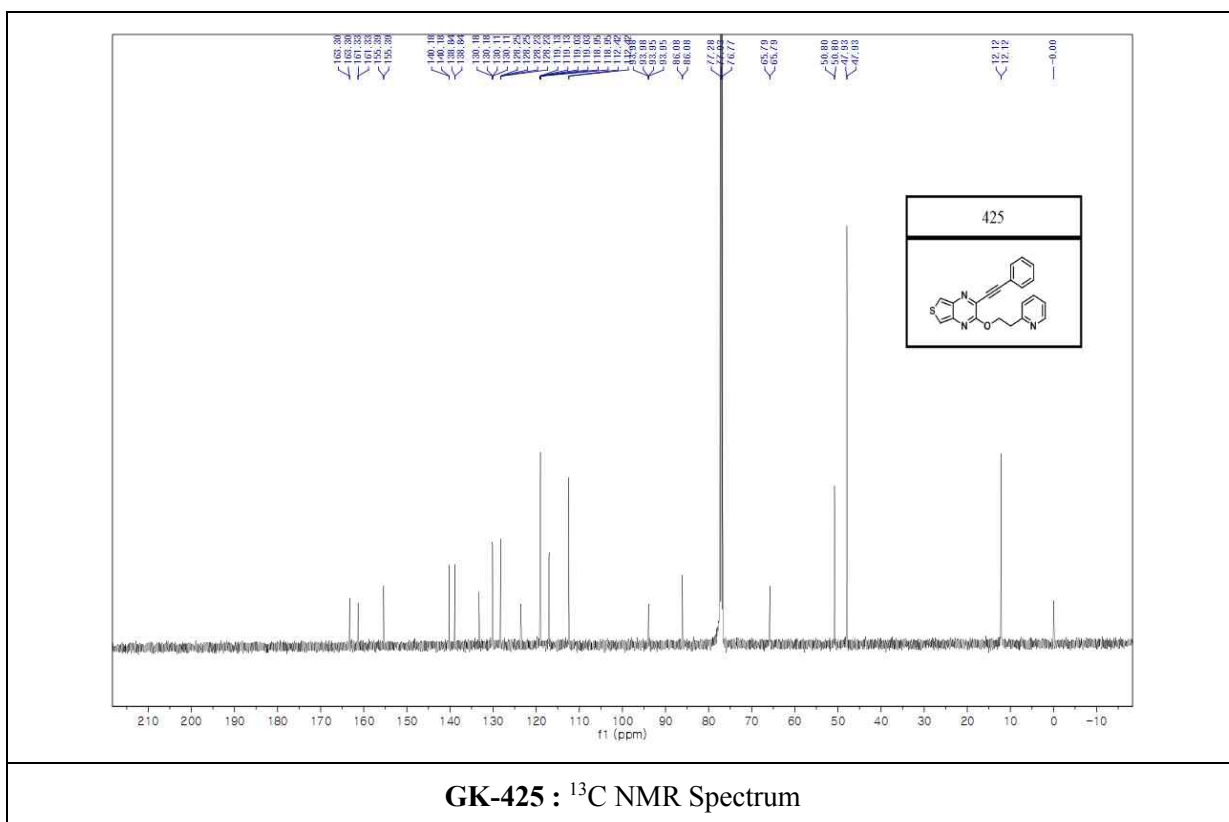
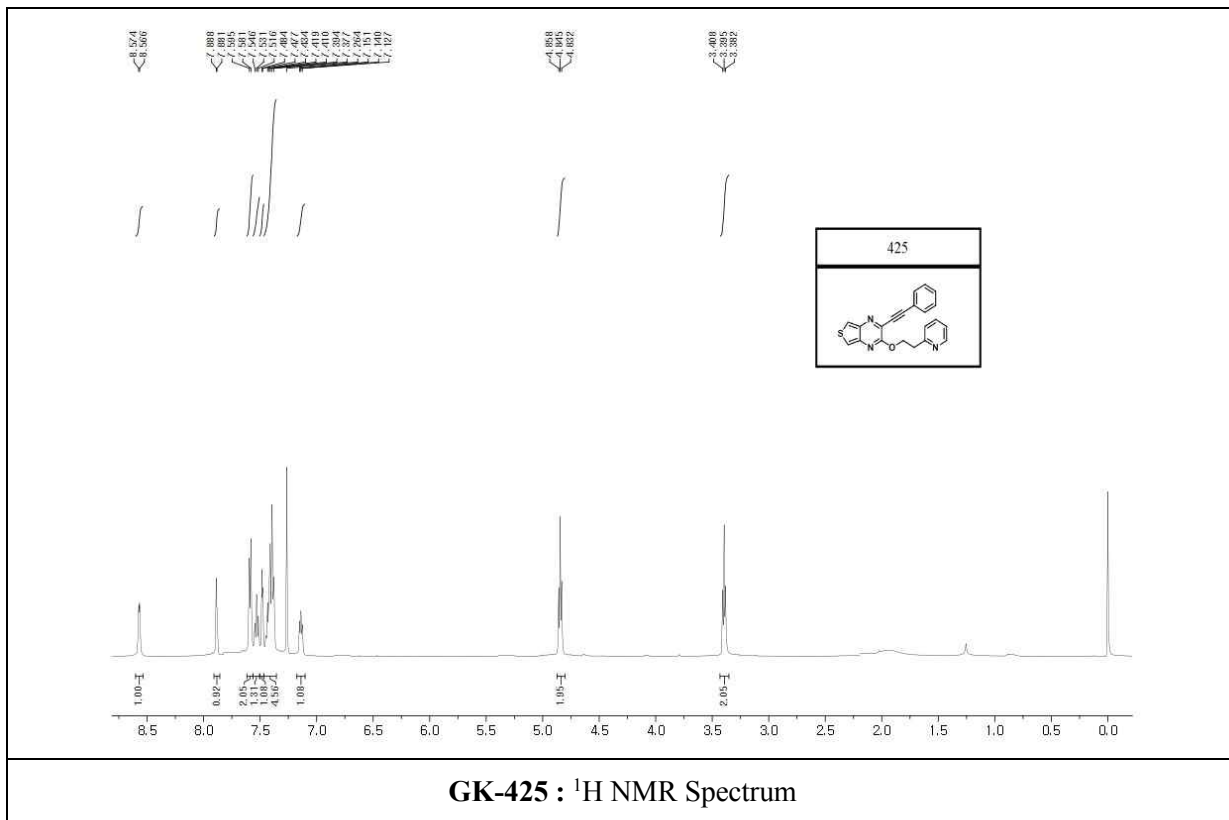
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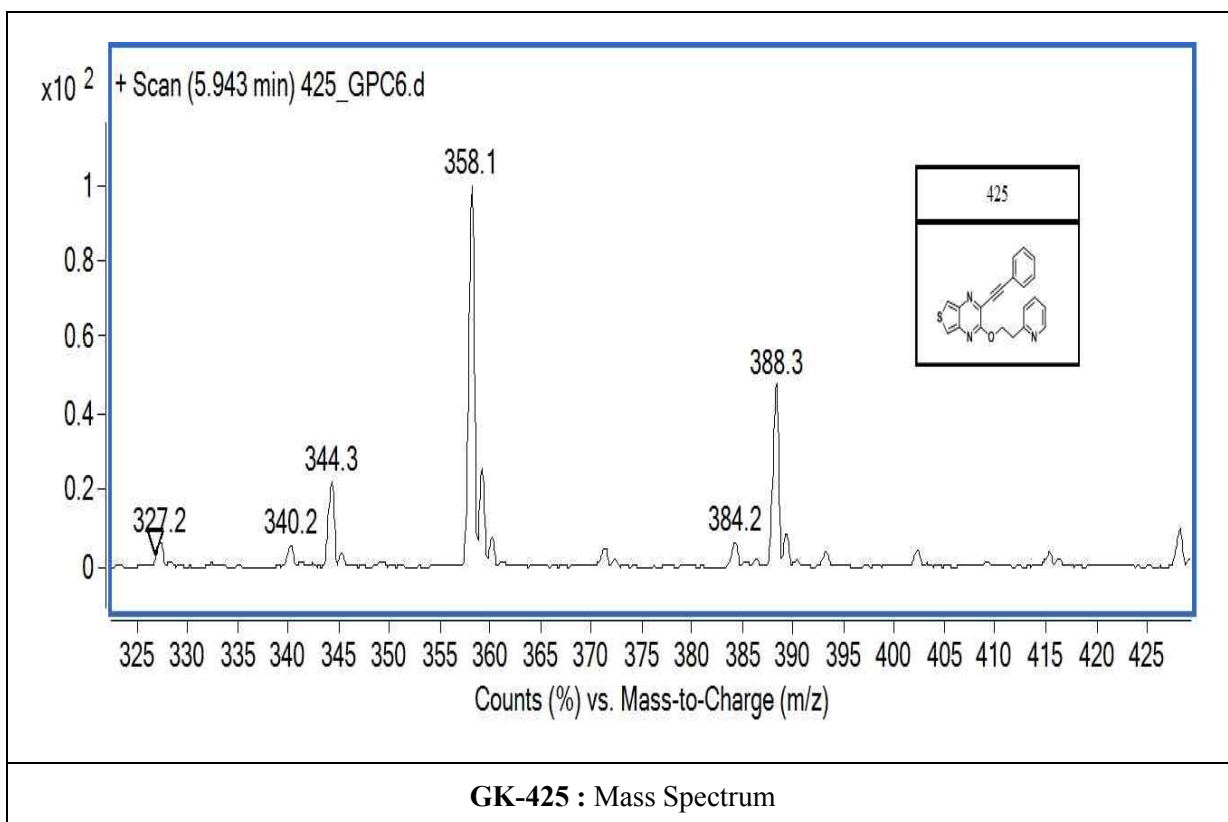
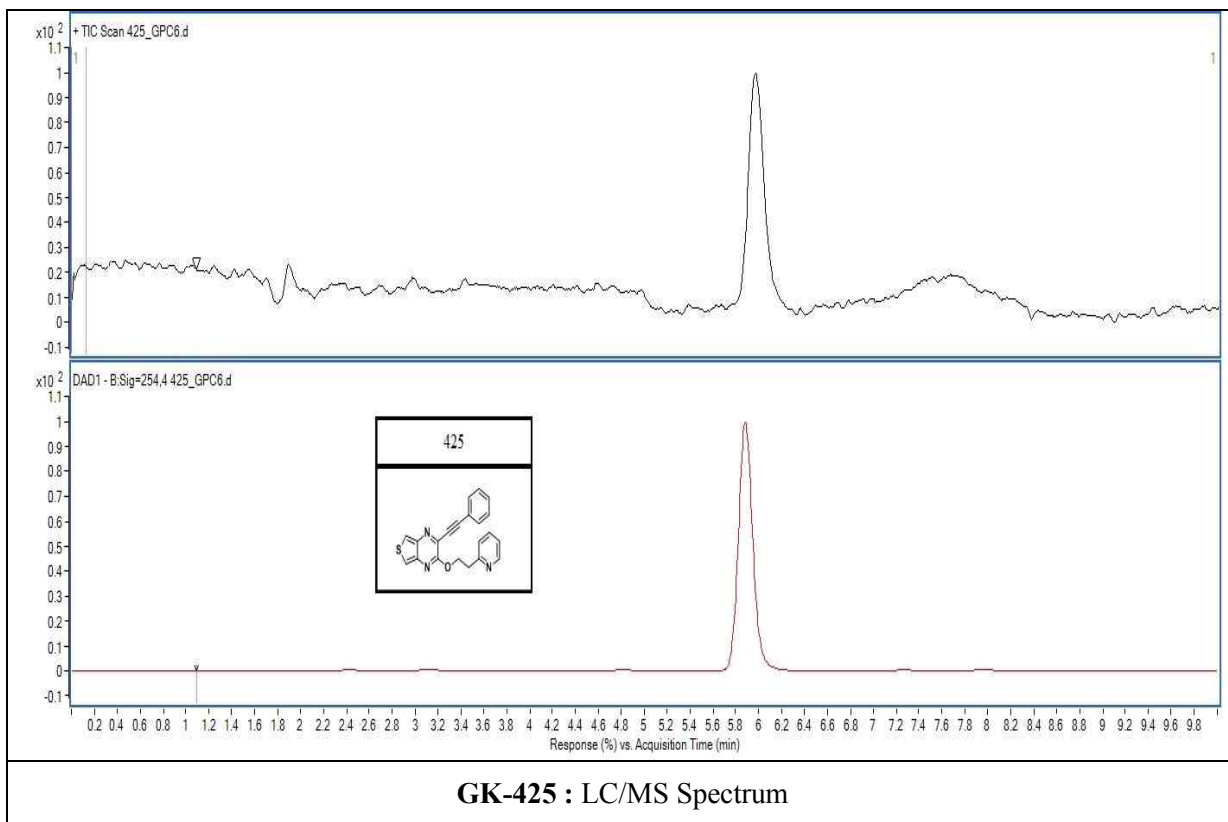


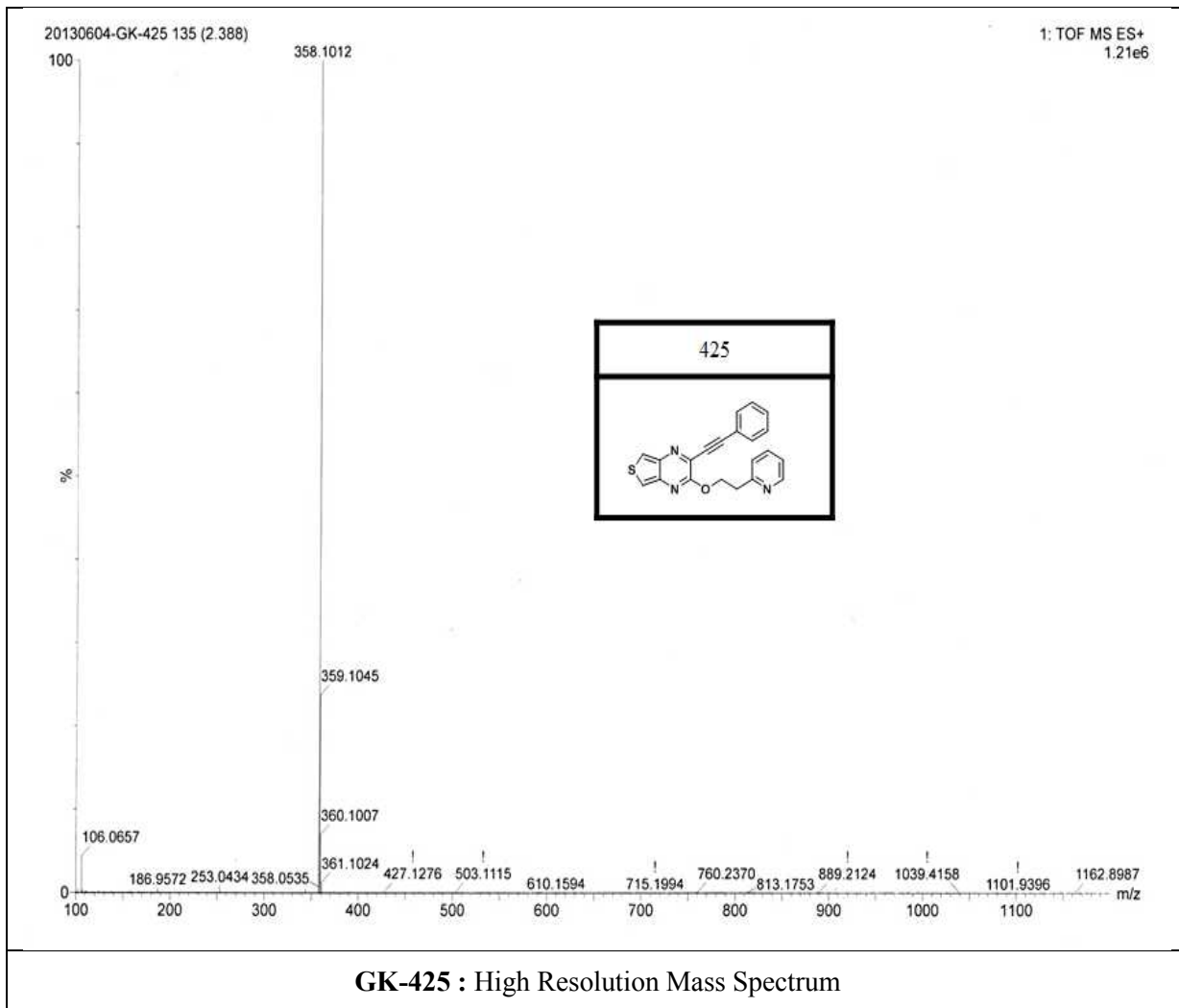


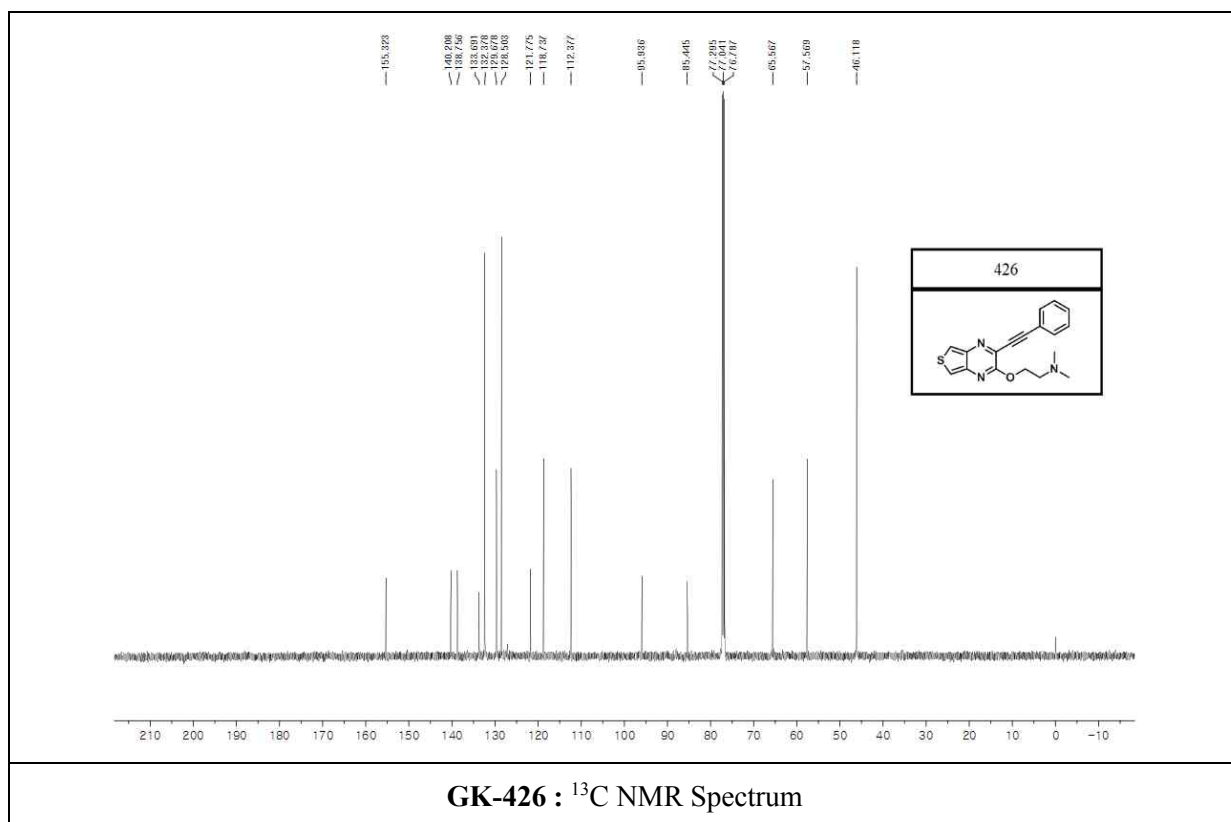
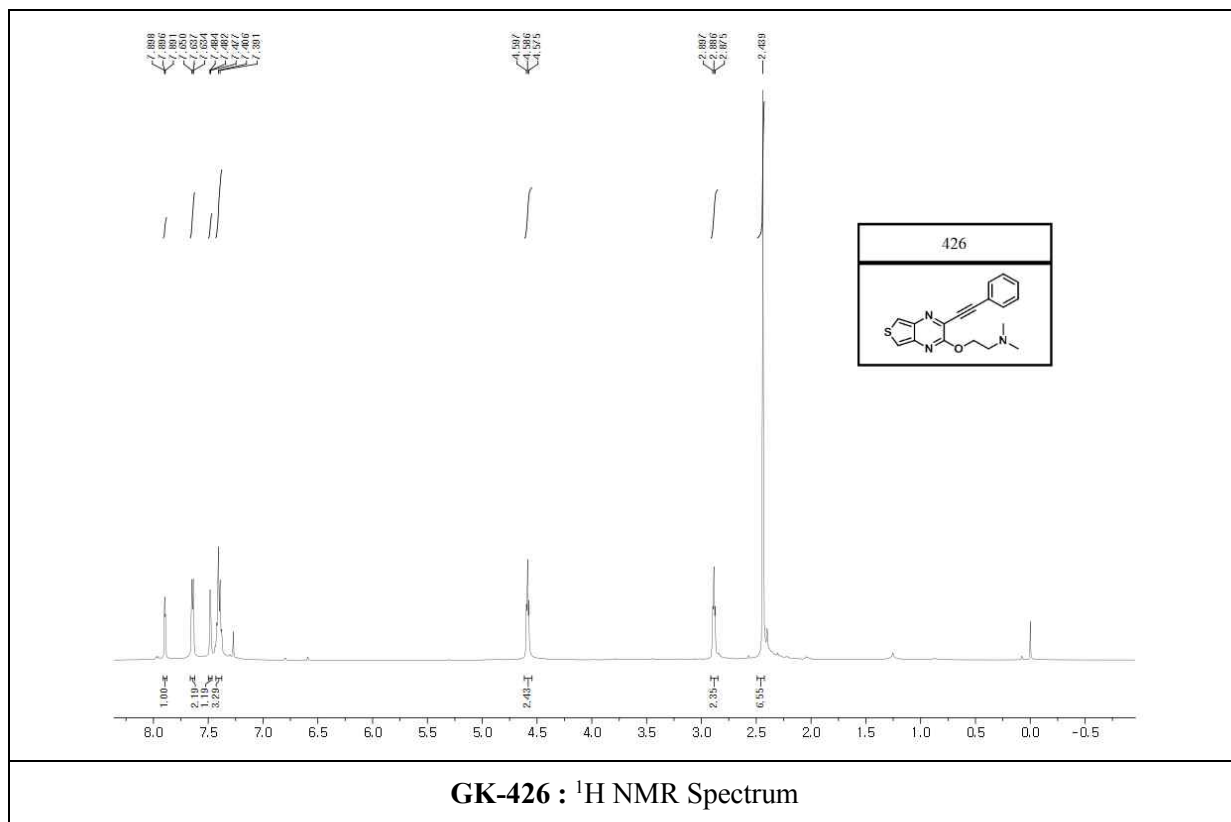


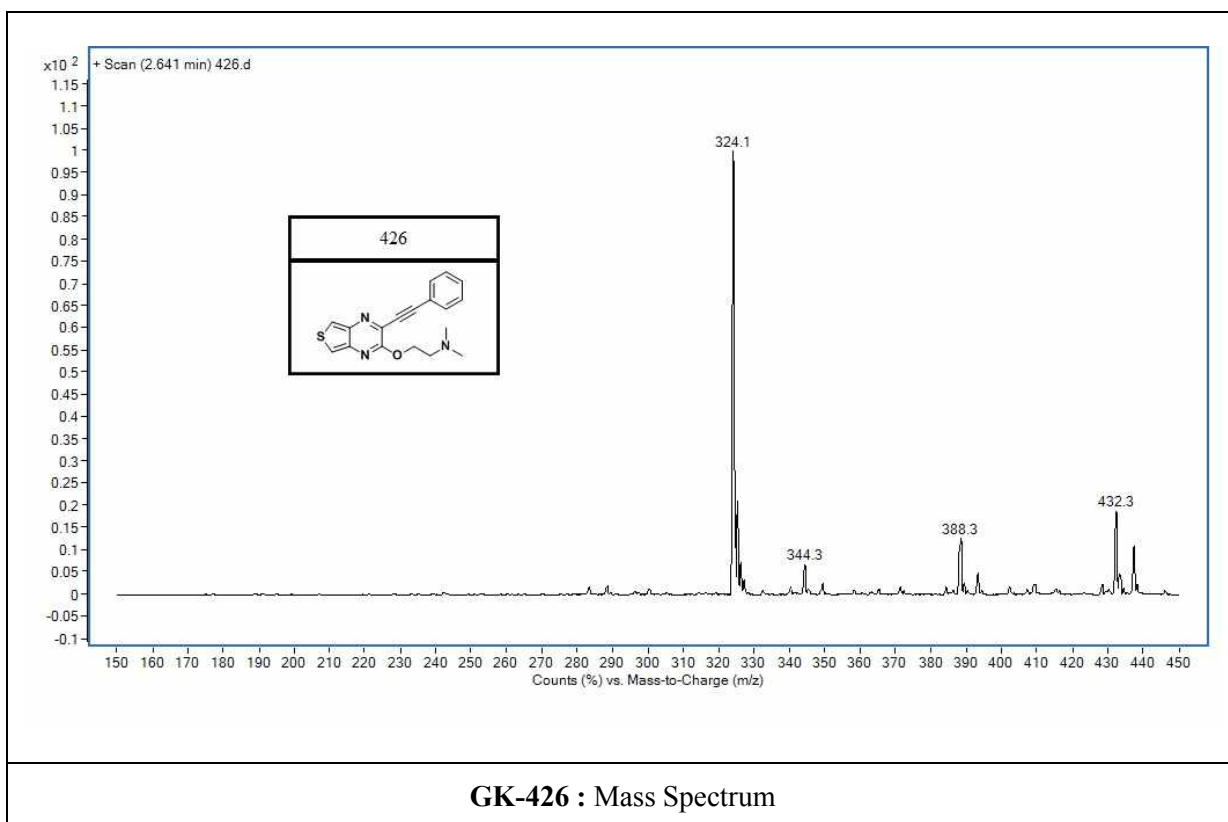
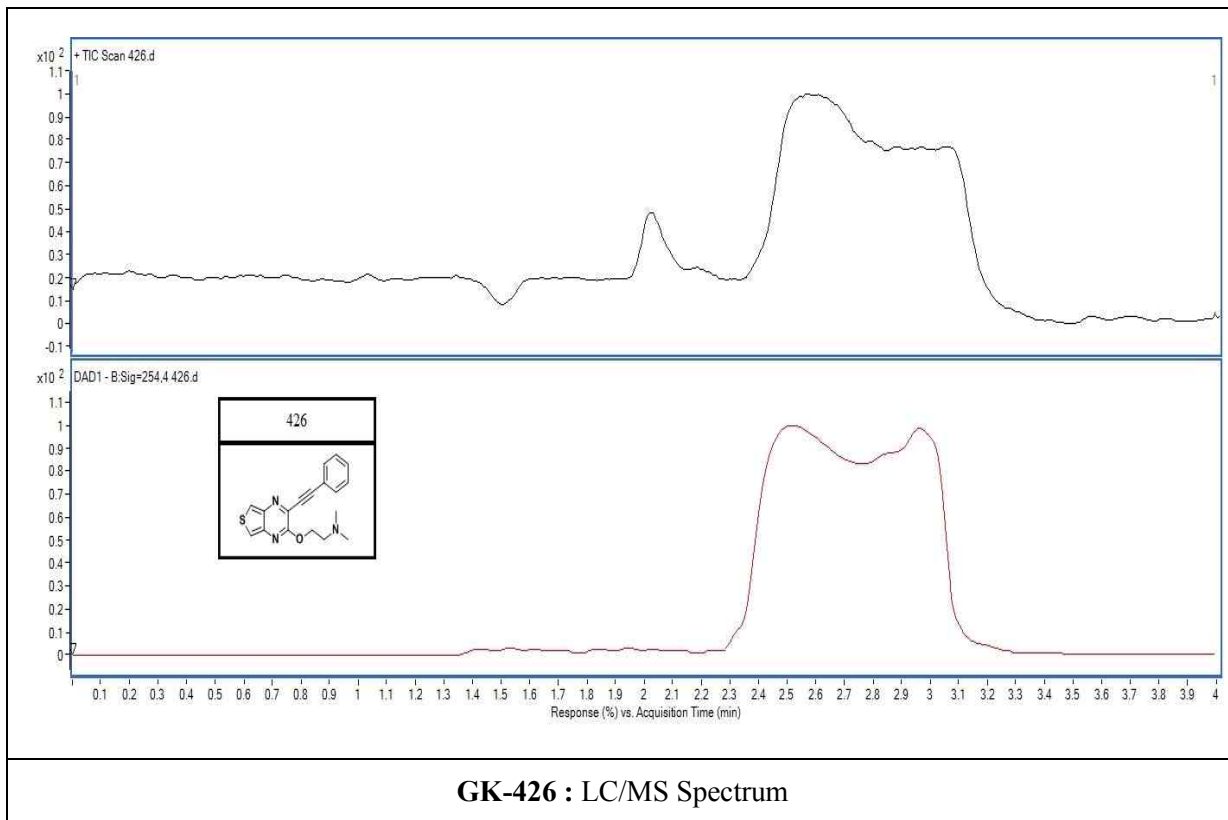






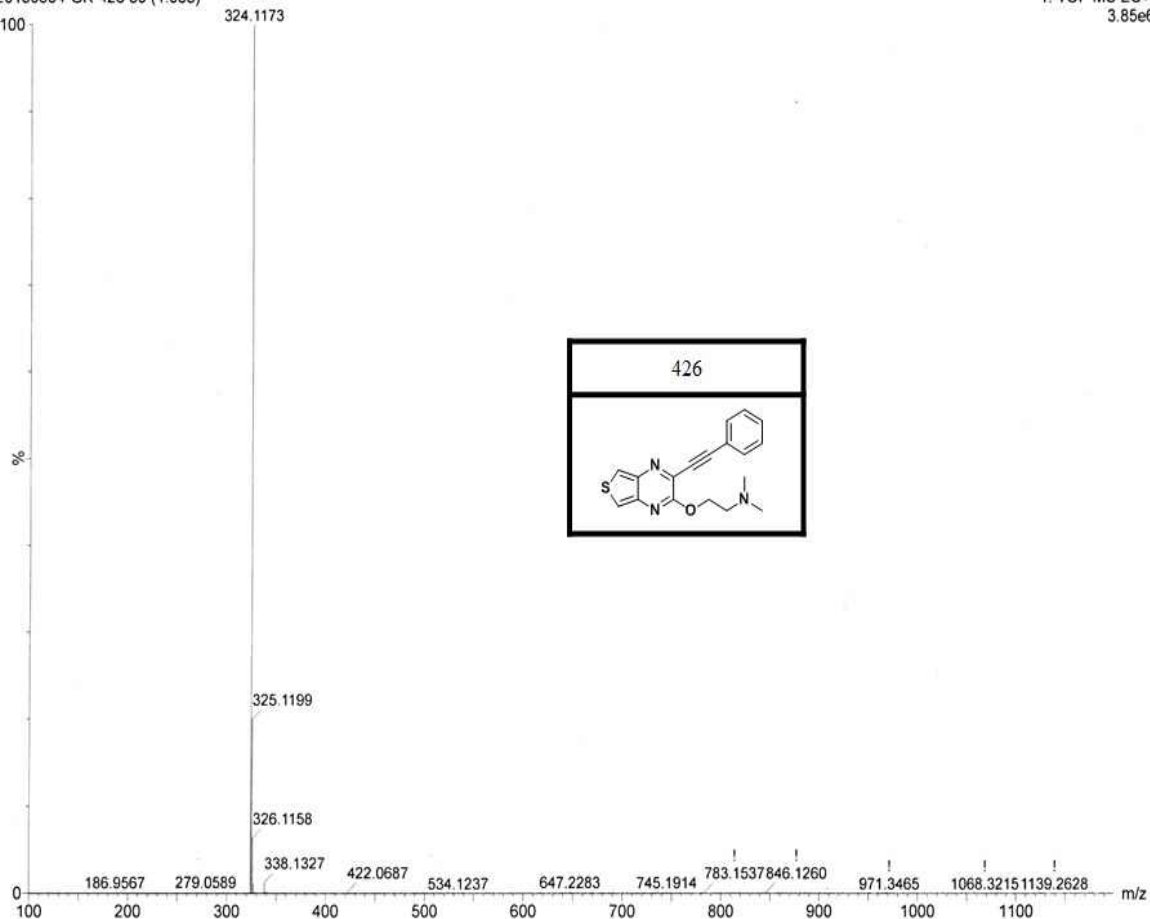




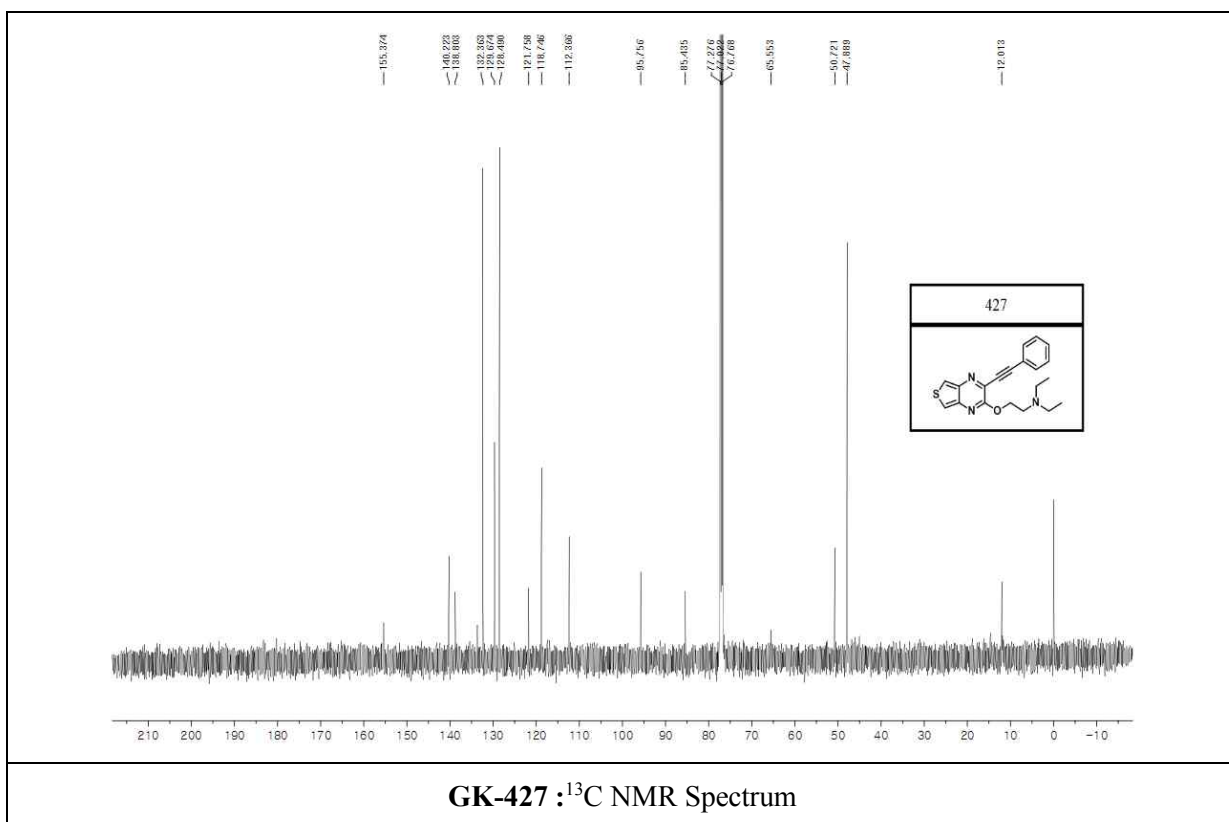
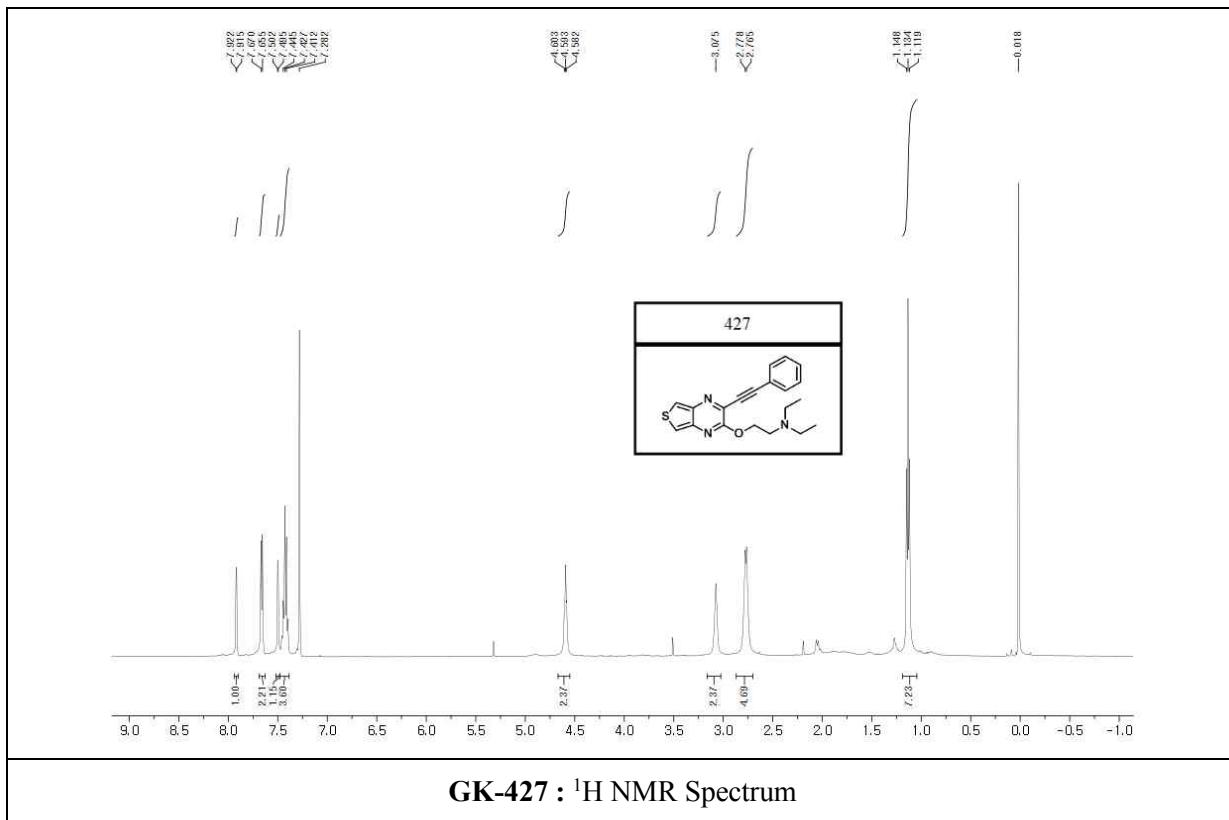


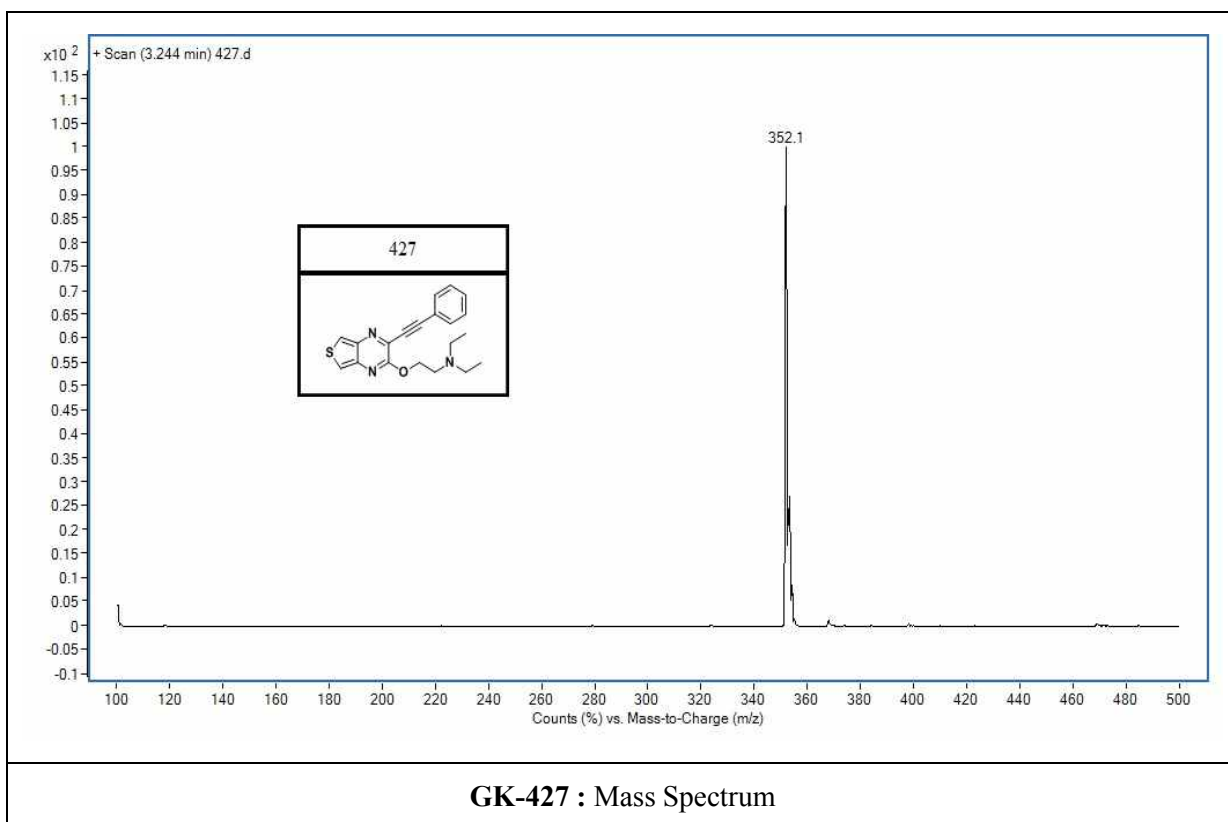
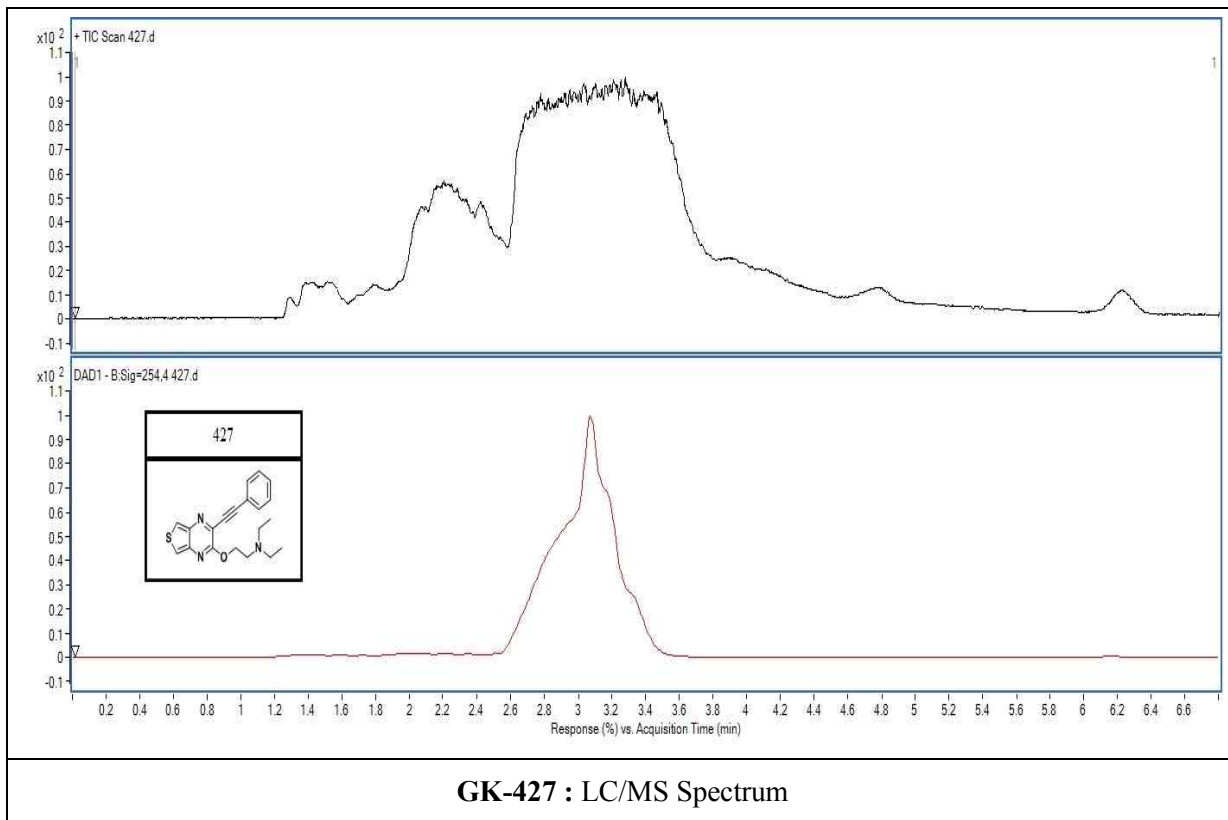
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1: TOF MS ES+  
3.85e6

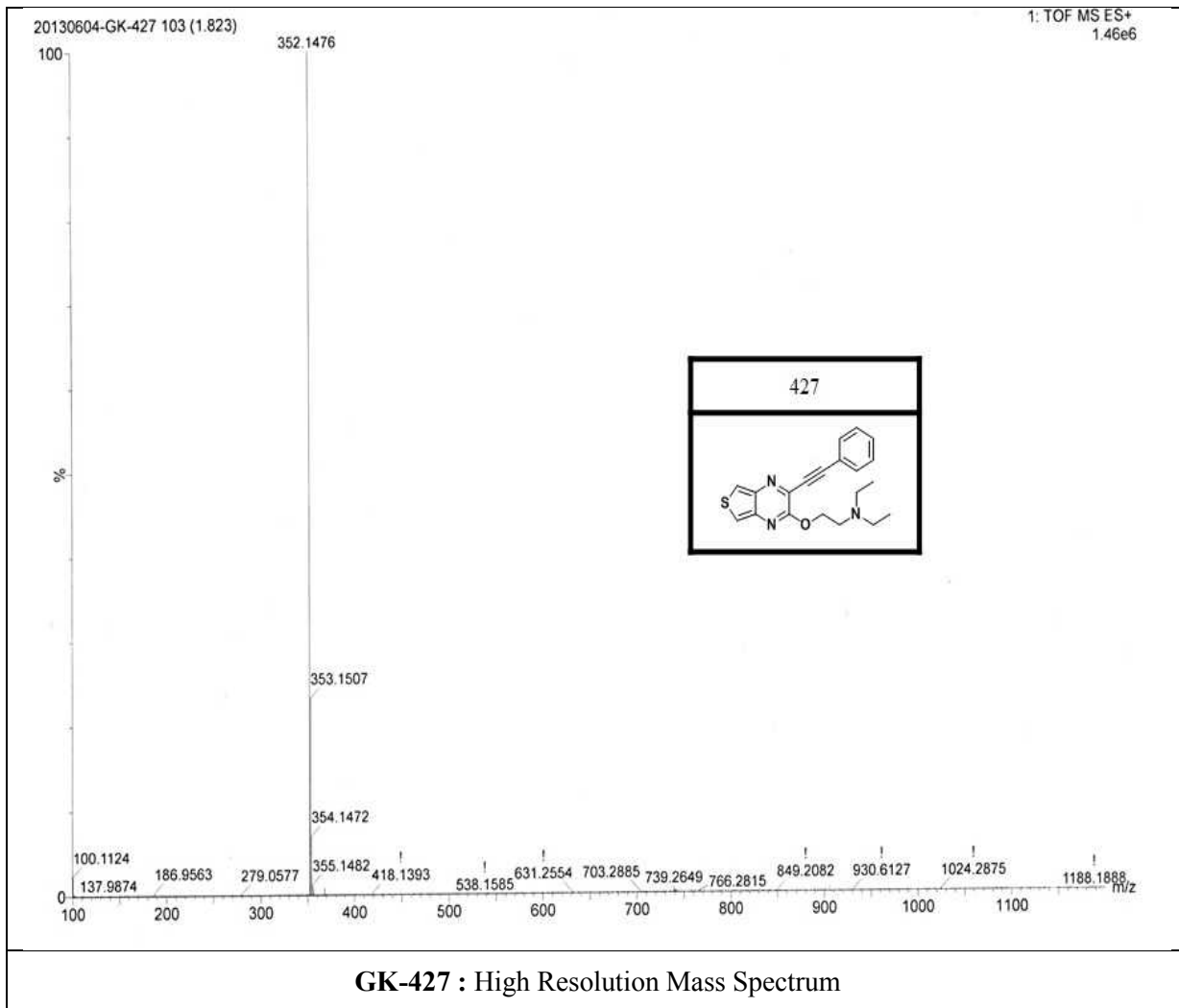


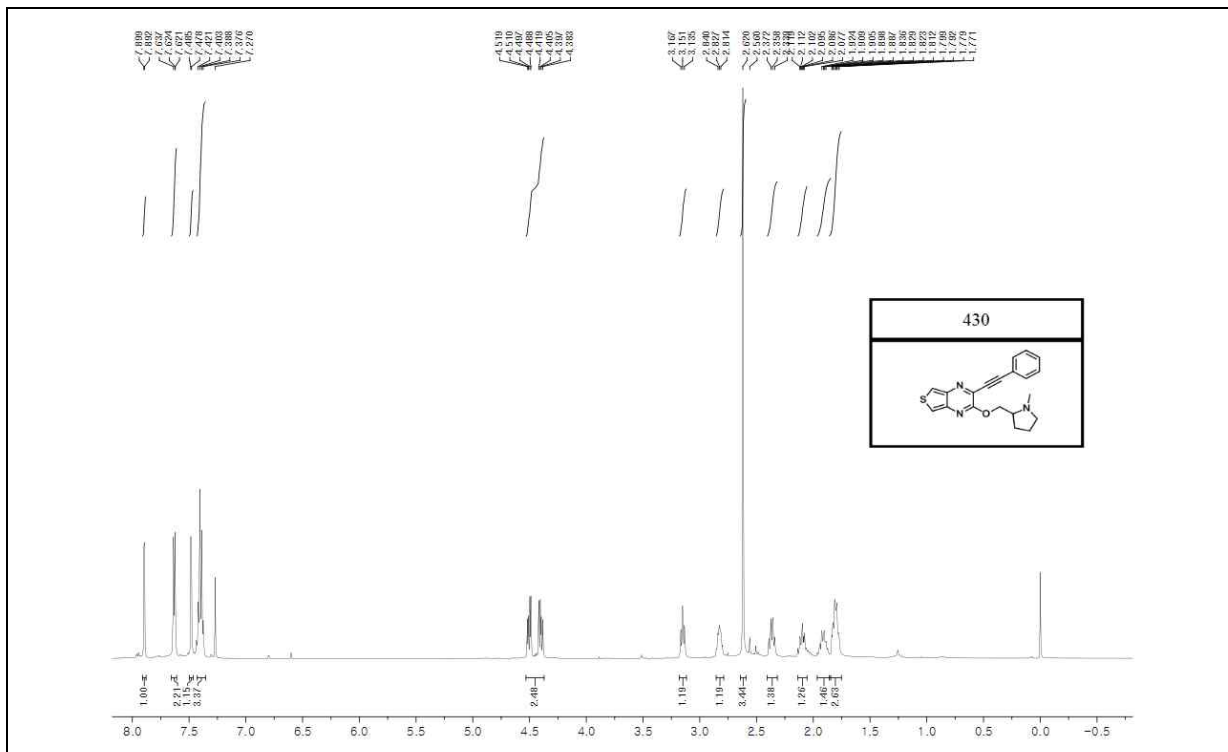
**GK-426 : High Resolution Mass Spectrum**



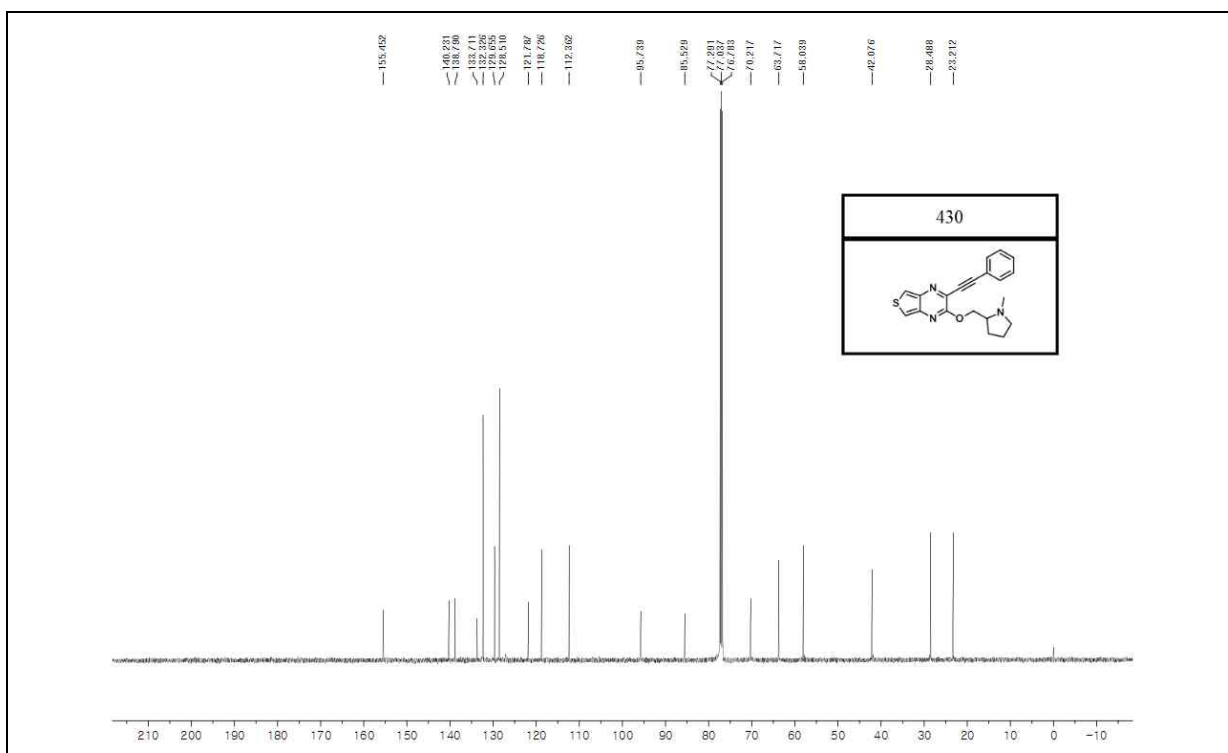




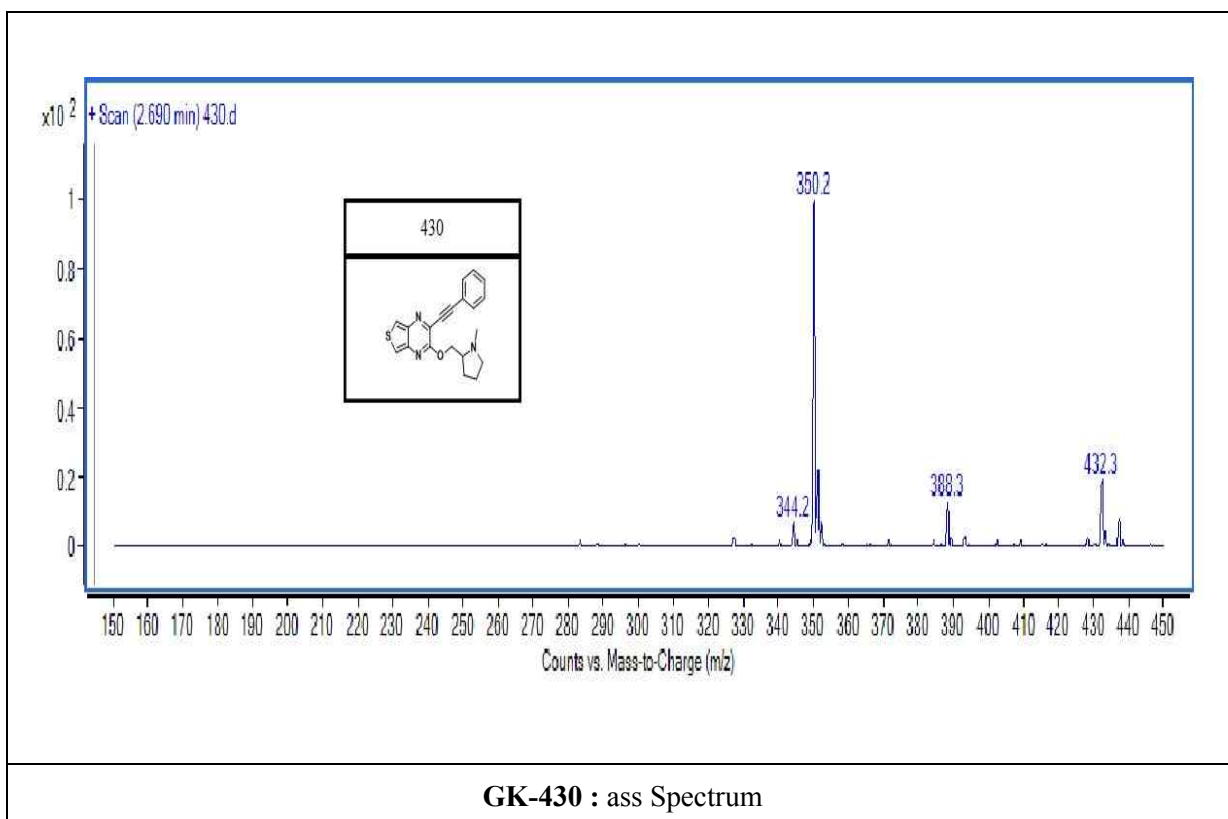
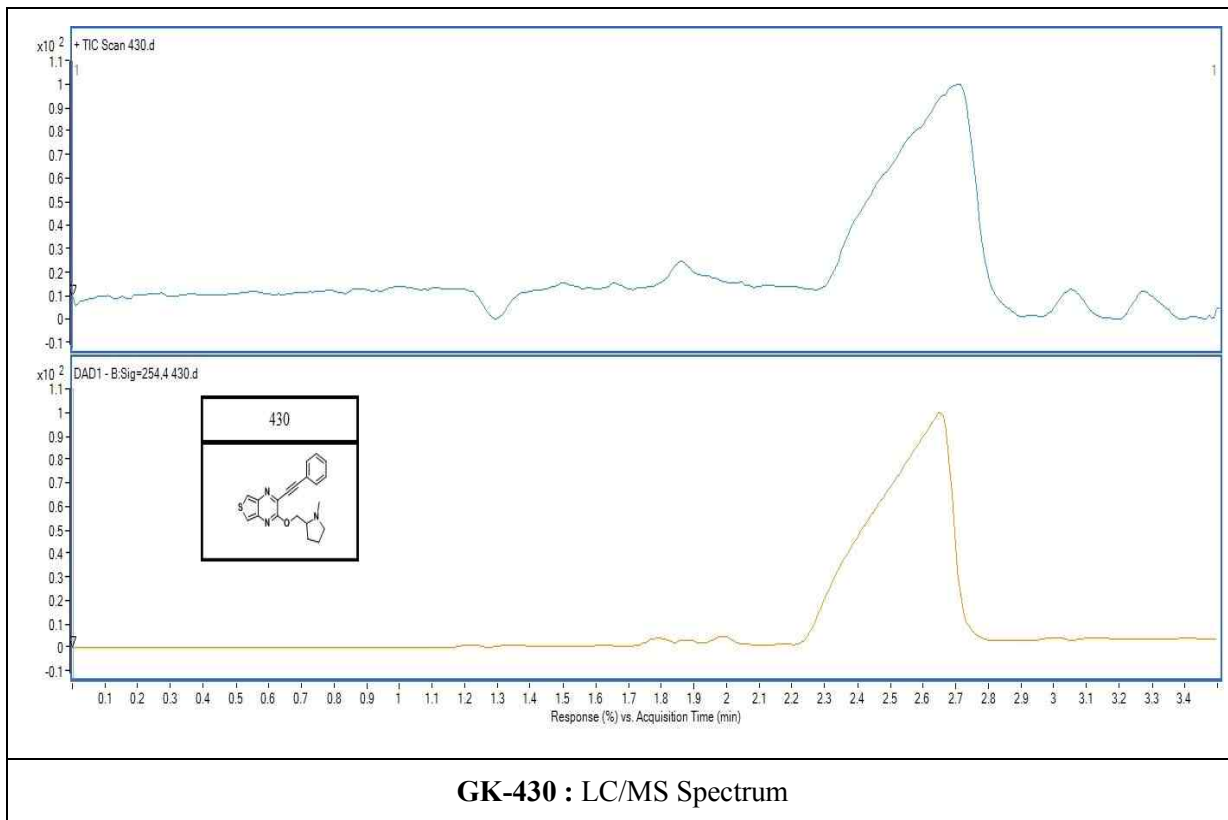




GK-430 : <sup>1</sup>H NMR Spectrum

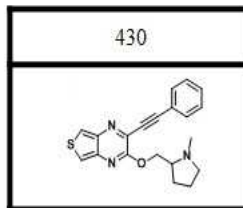
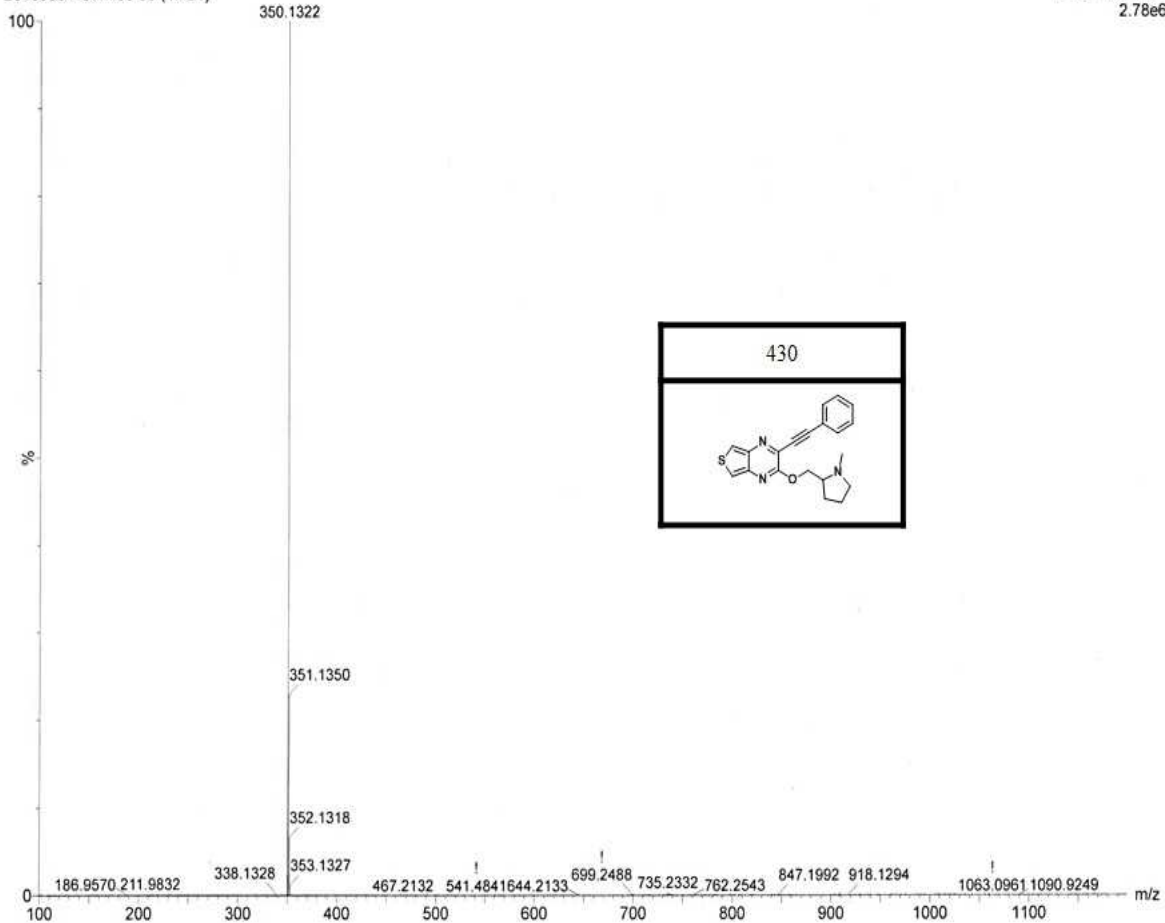


GK-430 : <sup>13</sup>C NMR Spectrum



20130604-GK-430 80 (1.421)

1: TOF MS ES+  
2.78e6



GK-430 : High Resolution Mass Spectrum