

Supporting Information

One-Pot Synthesis of Isoxazole-Fused Tricyclic Quinazoline Alkaloid Derivatives via Intramolecular Cycloaddition of Methyl Azaarenes under Metal-free Conditions

Zhuo Wang¹, Yu-Han Zhao¹, Jia-Xin Chen¹, Meng-Yao Chen¹, Xue-Han Li¹, Ting Jiang¹, Fang Liu¹, Xi Yang¹, Yuan-Yuan Sun¹ and Yan-Ping Zhu^{1,2 *}

¹ Key Laboratory of Molecular Pharmacology and Drug Evaluation, Ministry of Education, Collaborative Innovation Center of Advanced Drug Delivery System and Biotech Drugs in Universities of Shandong, School of Pharmacy, Yantai University, Shandong, Yantai, 264005, China.

² Anhui Laboratory of Molecule-Based Materials, College of Chemistry and Materials Science, Anhui Normal University, Wuhu 241000, China

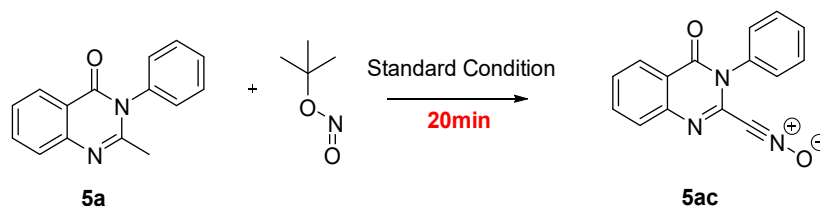
E-mail: chemzyp@foxmail.com; chemzyp@ytu.edu.cn,

Table of Contents

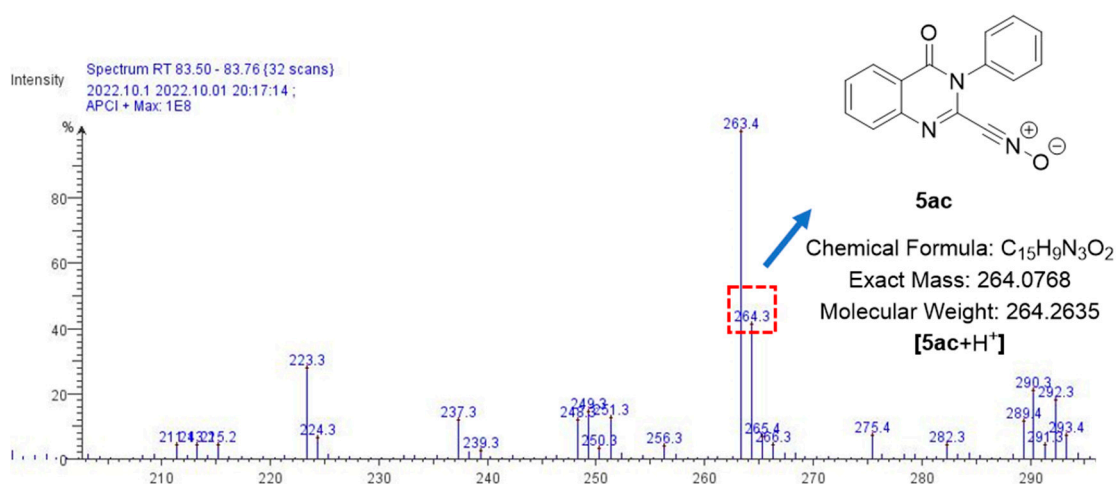
1. Evidence in support of the hypothetic mechanism	3
2. Copy of ^1H 、 ^{13}C NMR and HR-MS Spectra of Products.....	4

1. Evidence in support of the hypothetical mechanism

To gain further insight into the reaction mechanism, some control experiments were performed as illustrated in Scheme S1. To address the possible reaction intermediate, 2-methyl-3-phenylquinazolinone (**5a**) was reacted under the standard conditions for 20 mins, nitrile oxides (**5ac**) could be detected by MS (APCI).

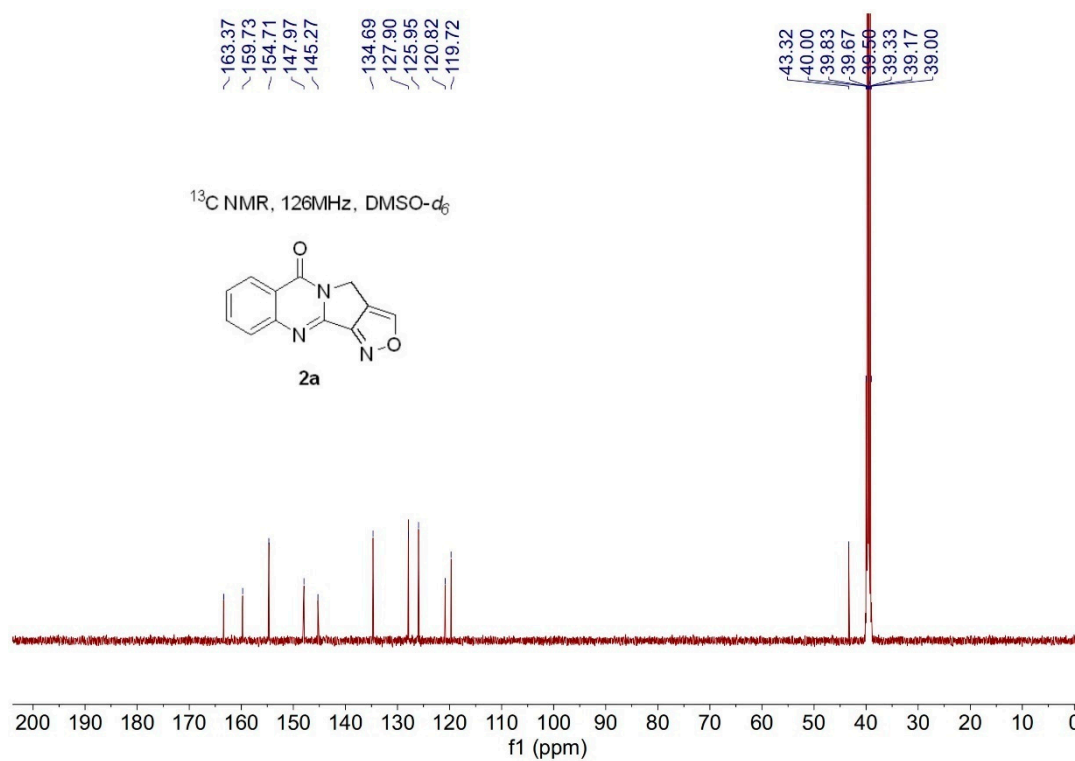
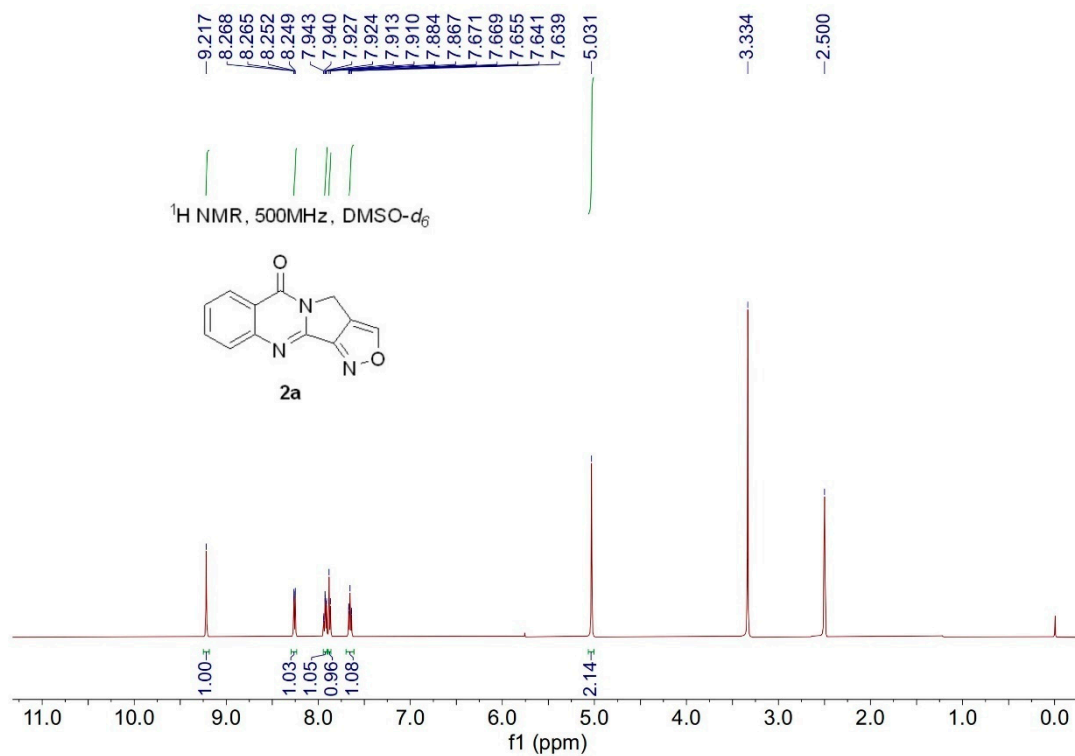


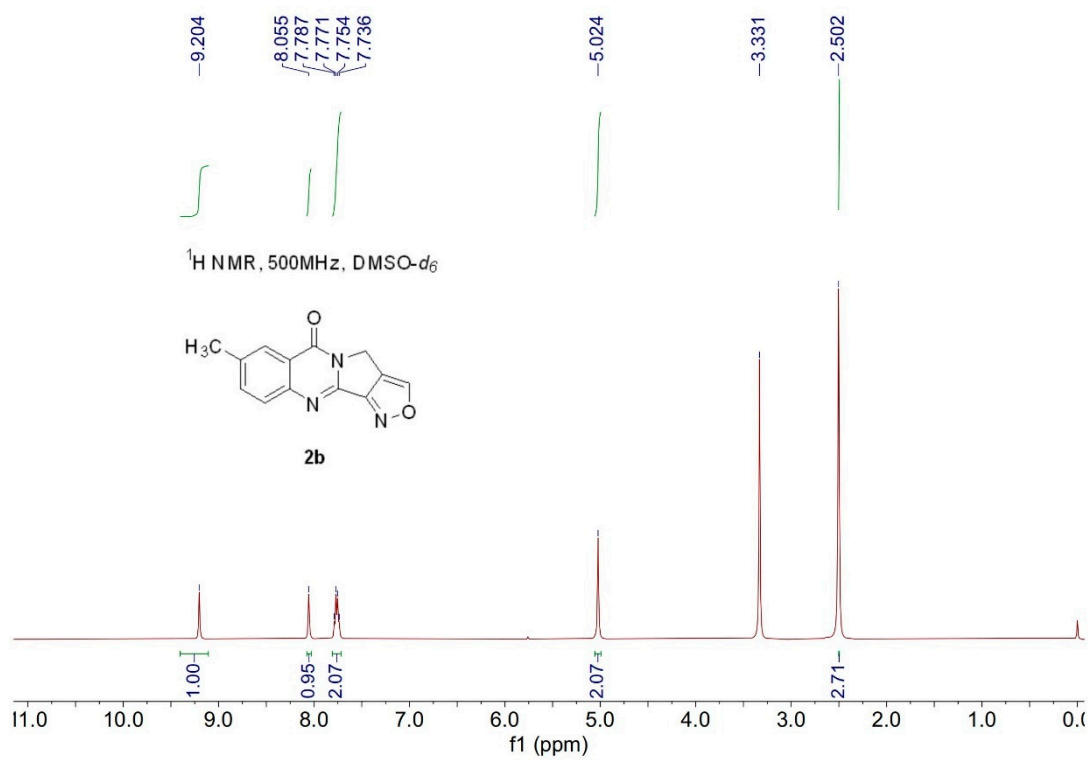
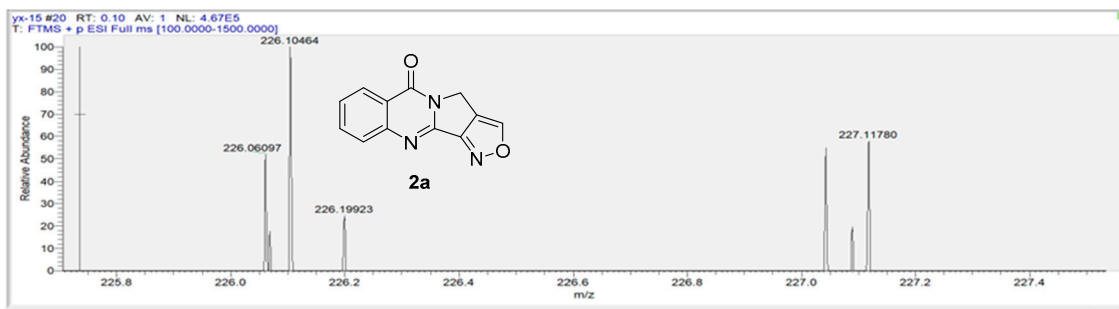
Scheme S1. Control experiment of **5a** with TBN.

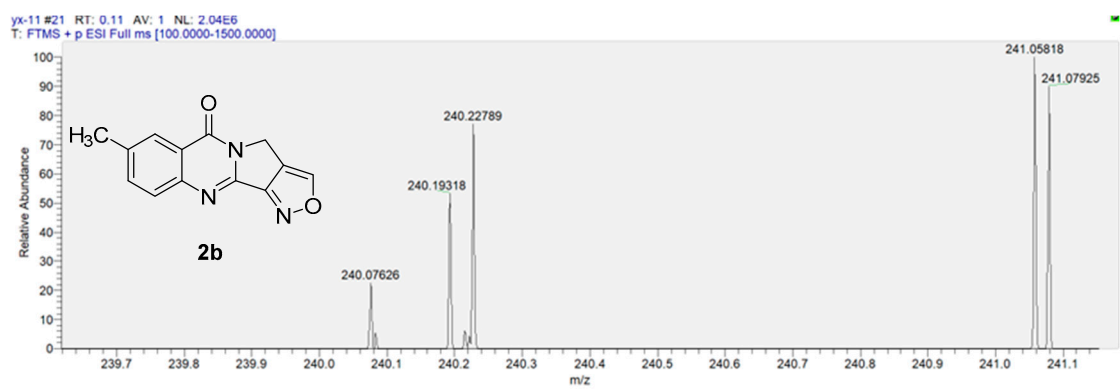
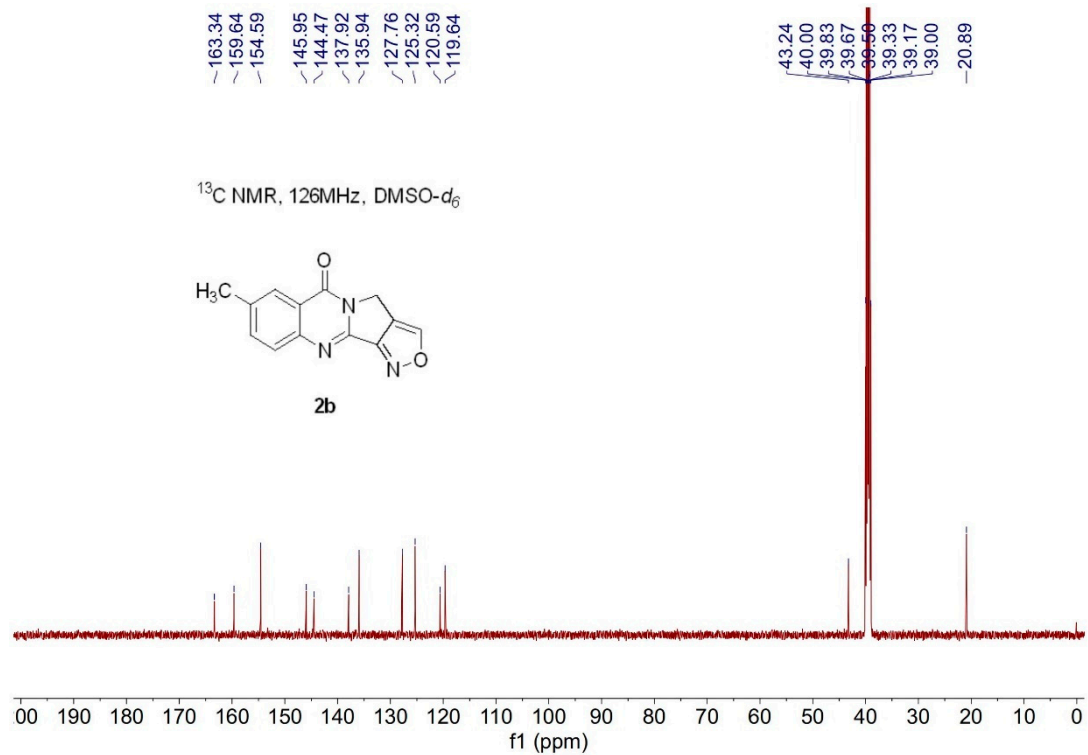


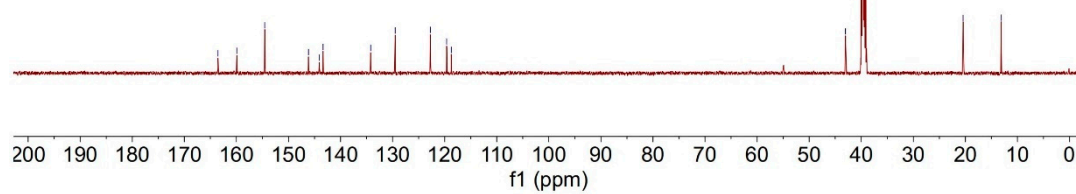
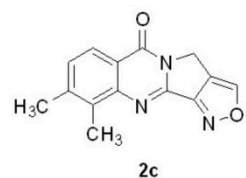
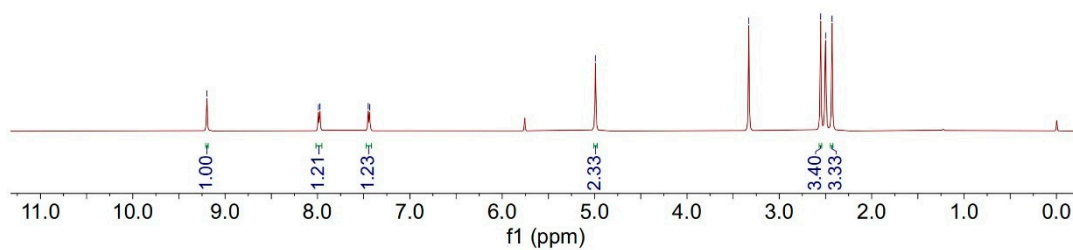
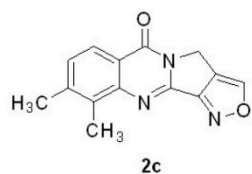
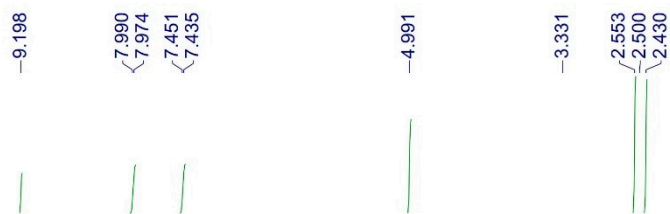
Scheme S2. The MS(APCI) results for the reaction of **5a** was reacted under the standard conditions for 20 mins.

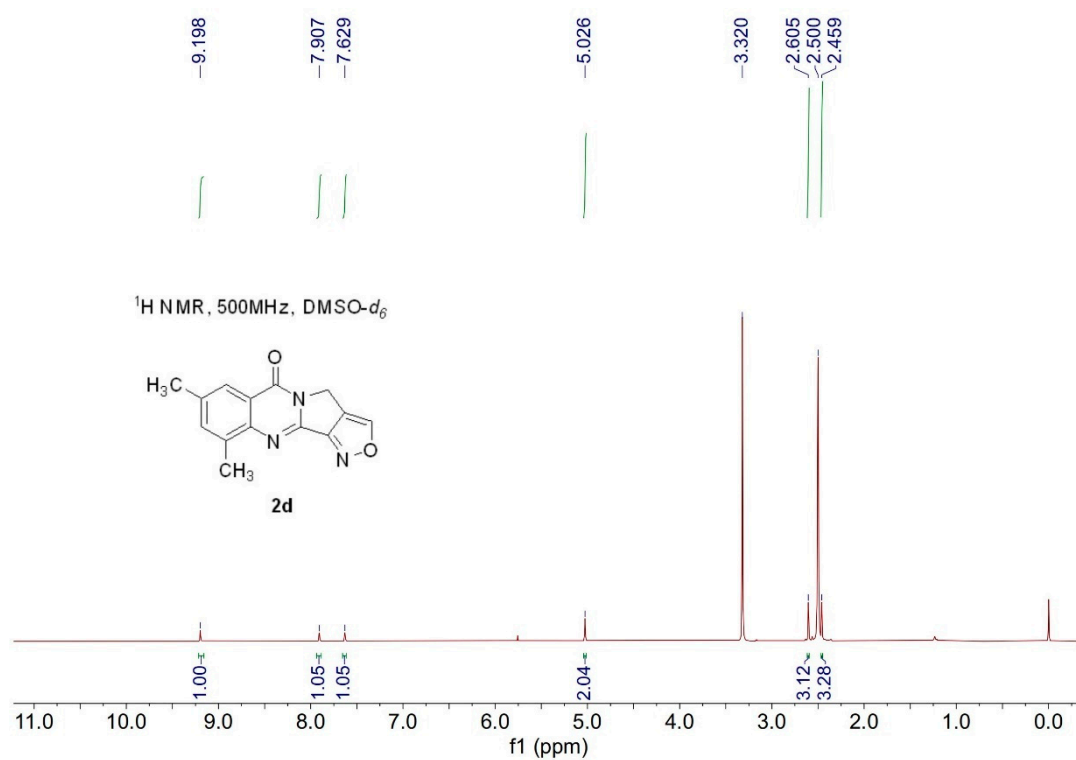
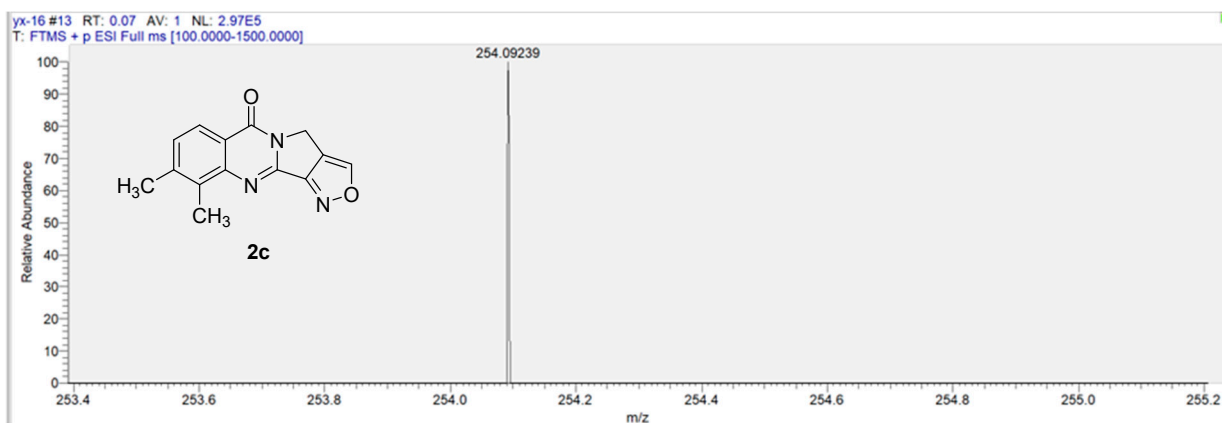
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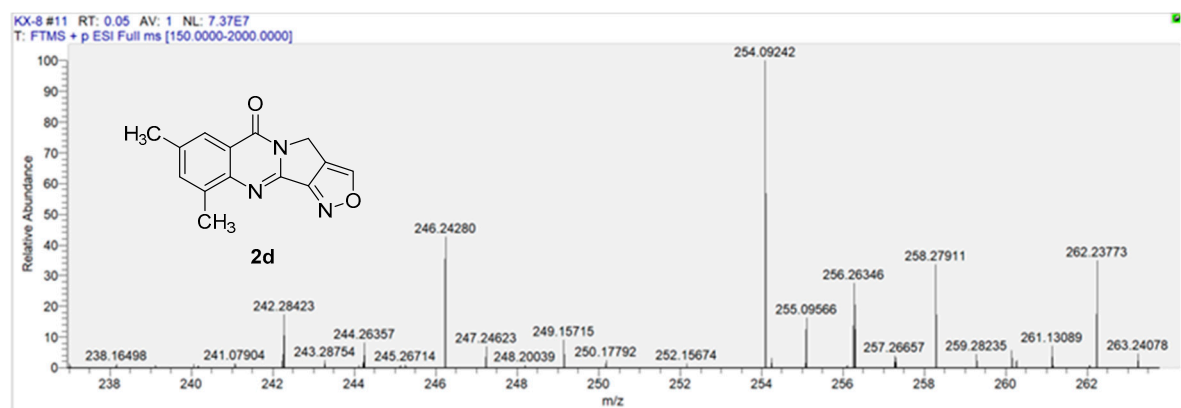
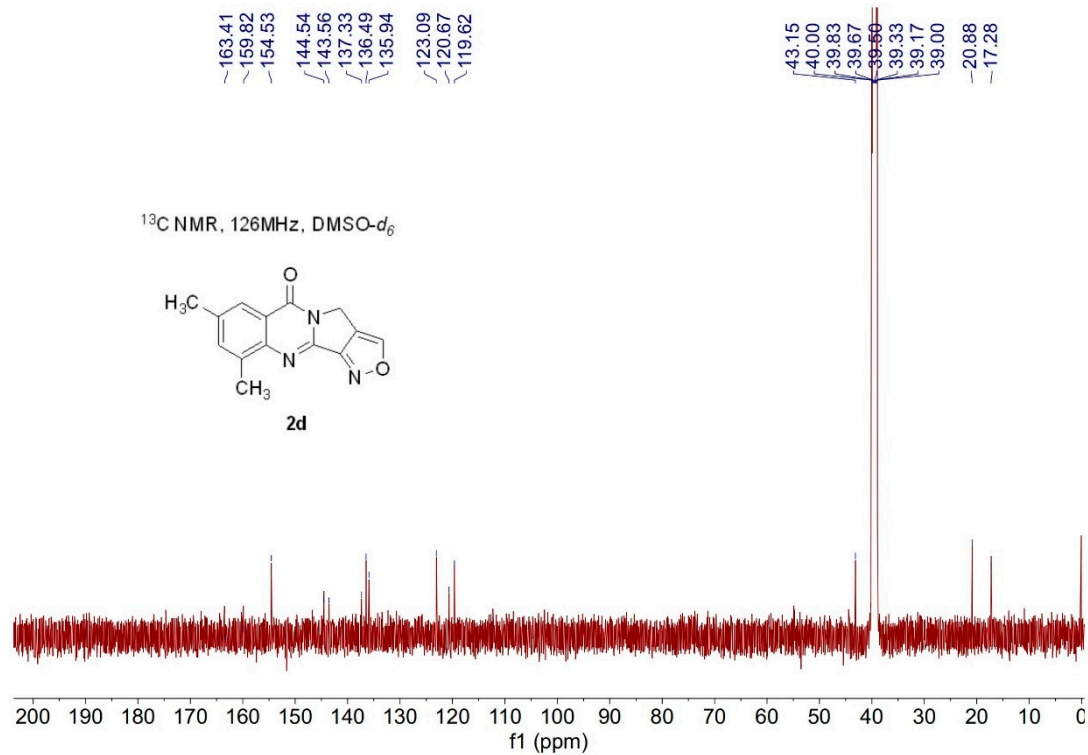


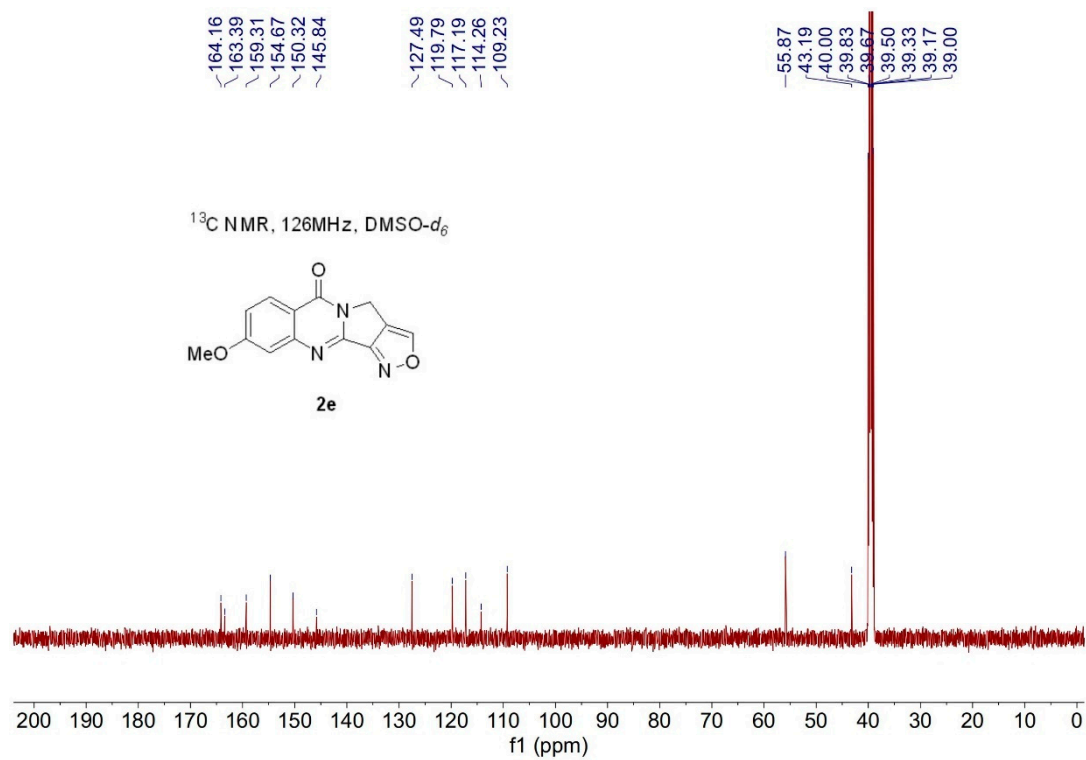
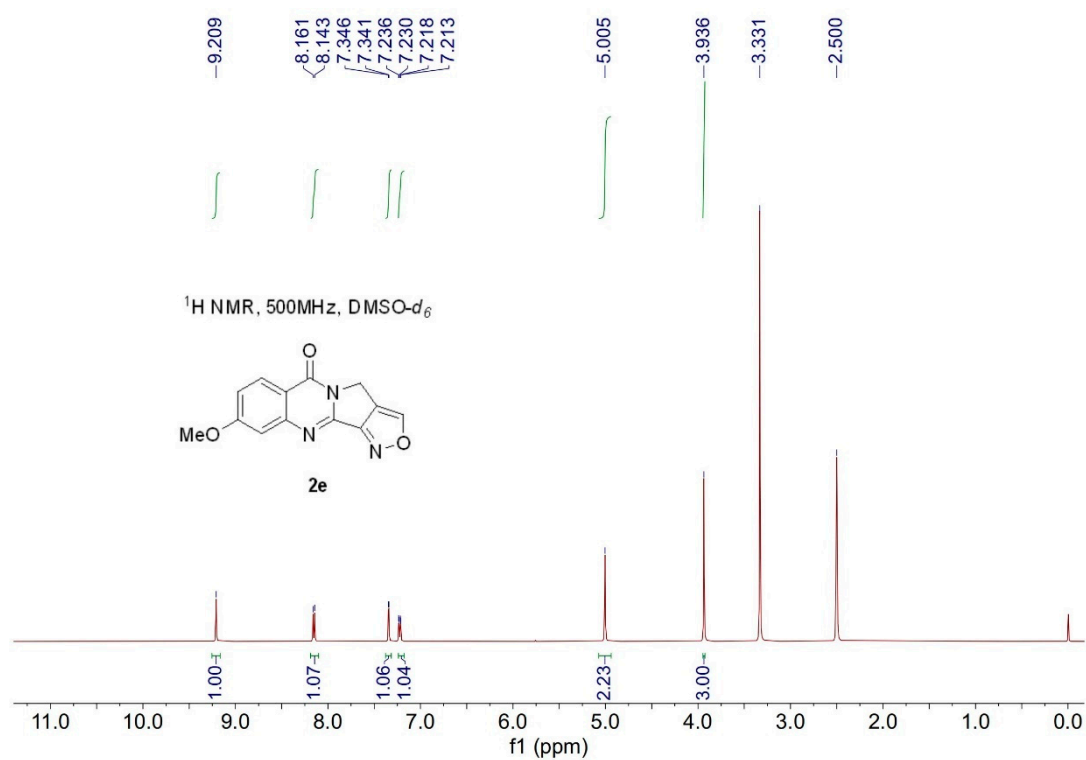


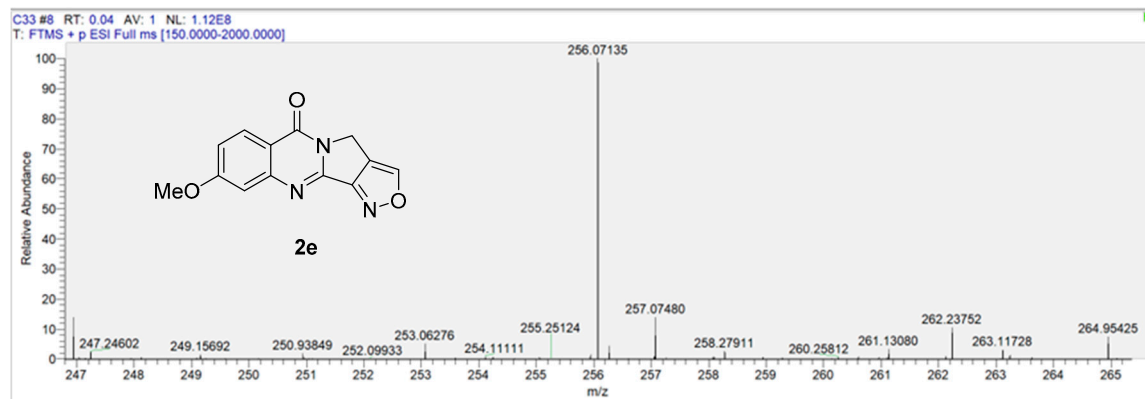




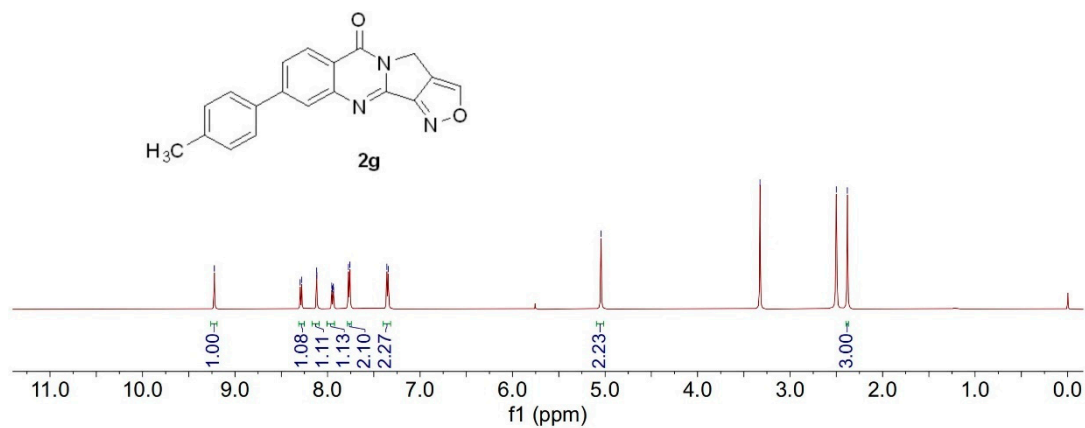


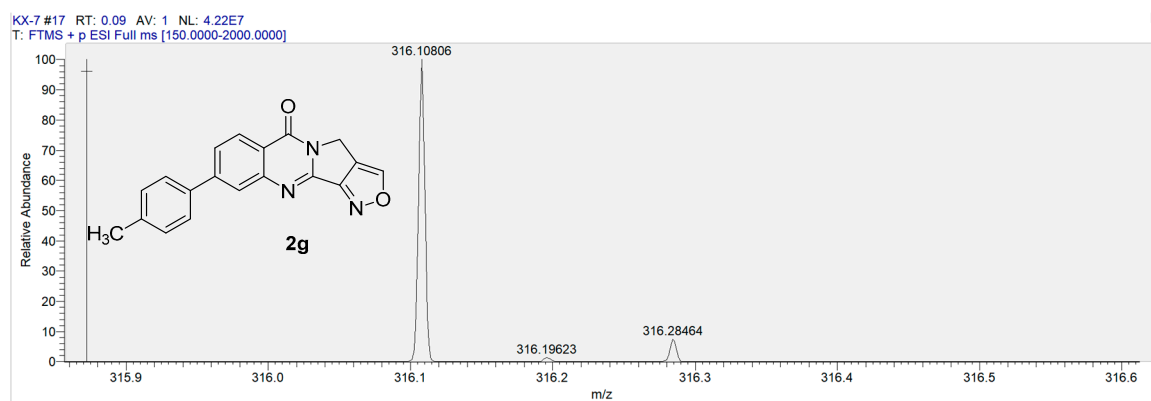
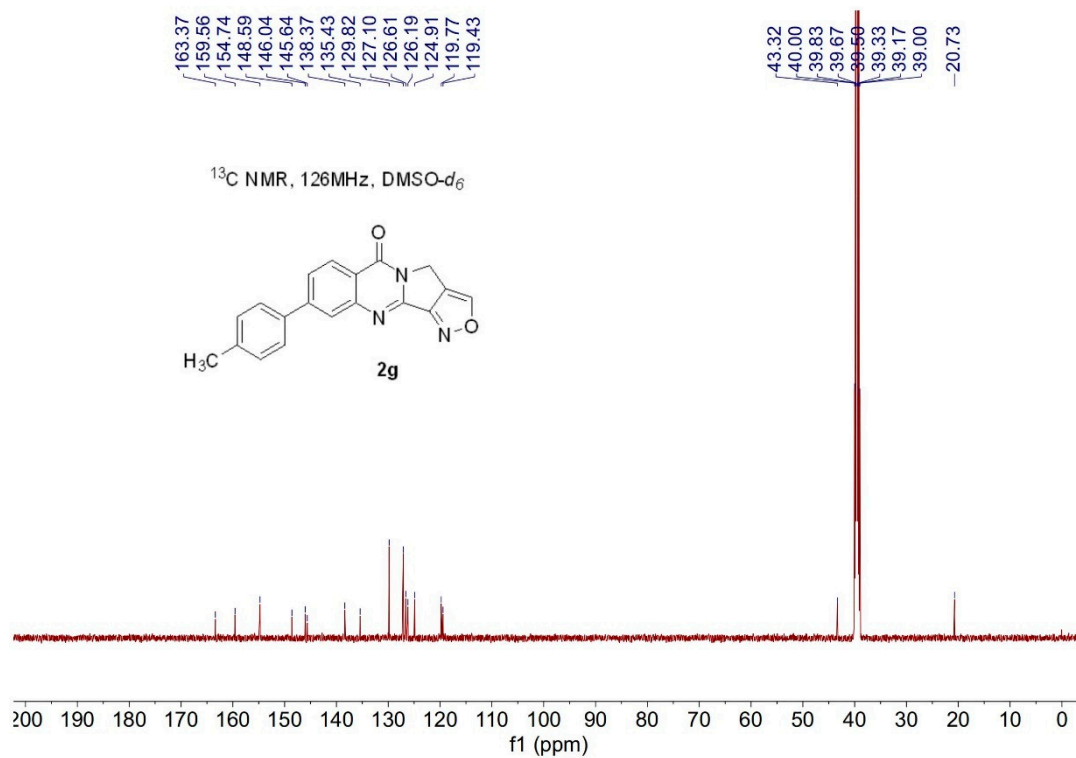


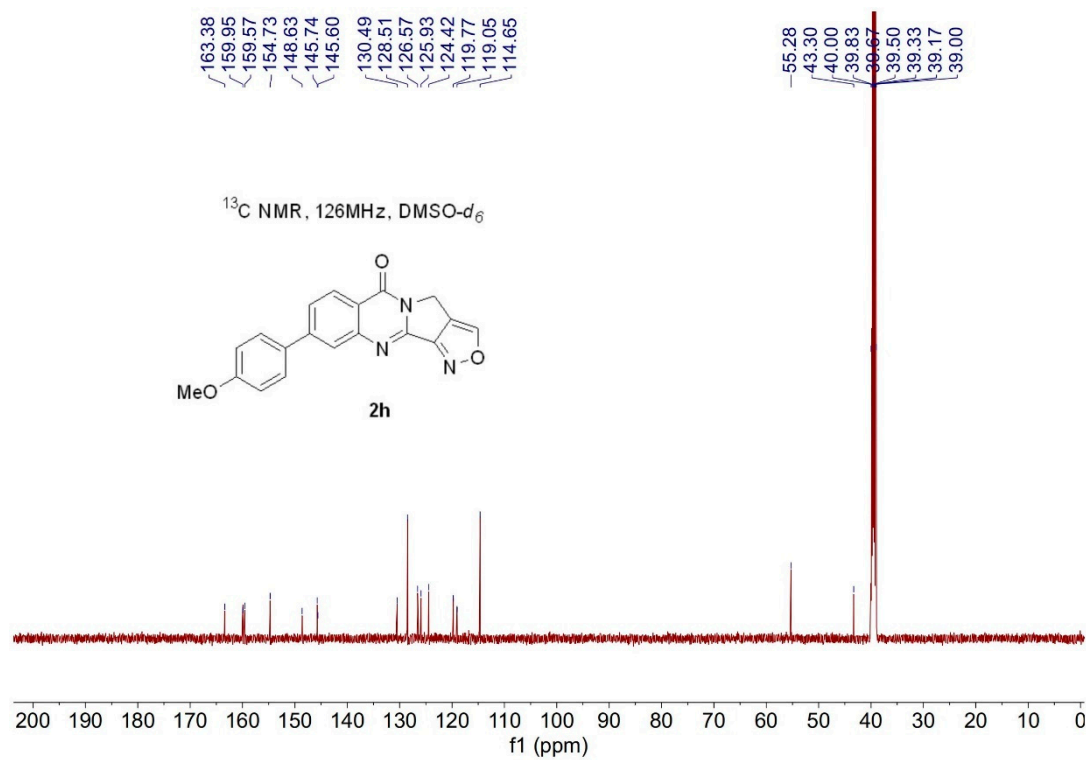
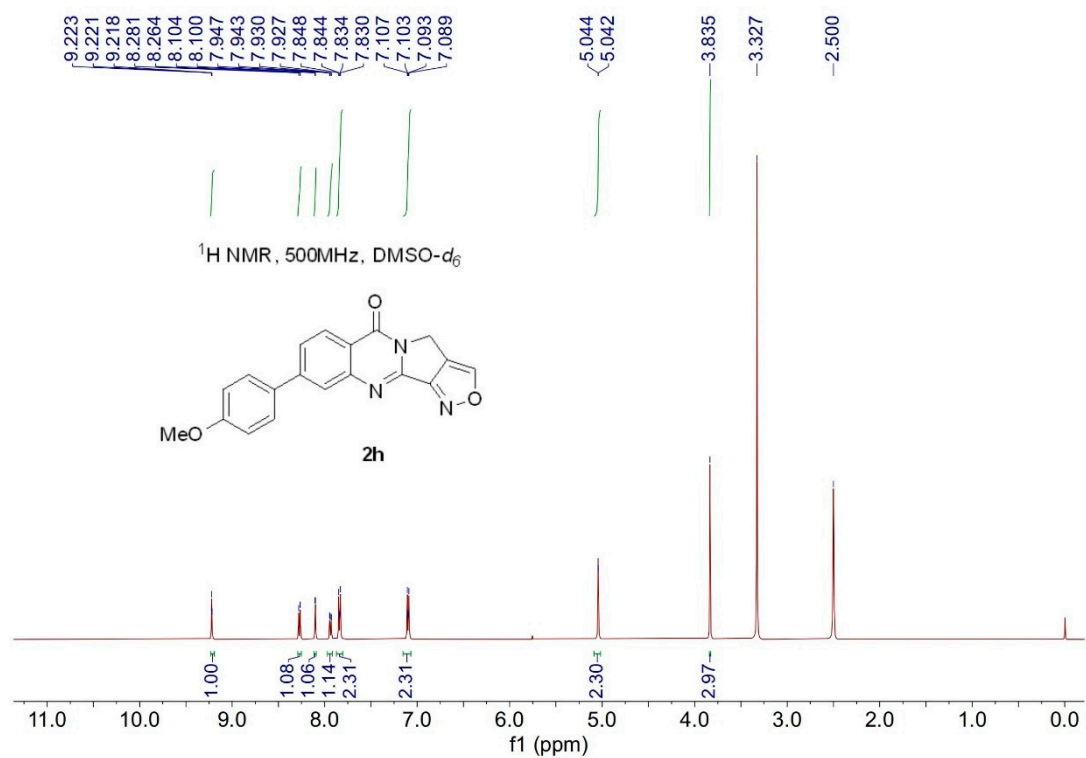


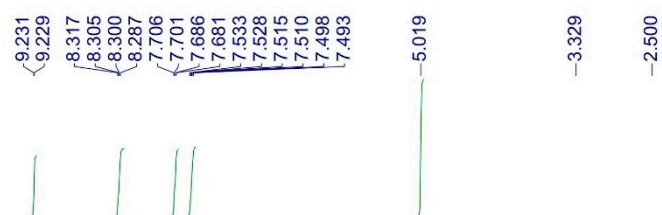
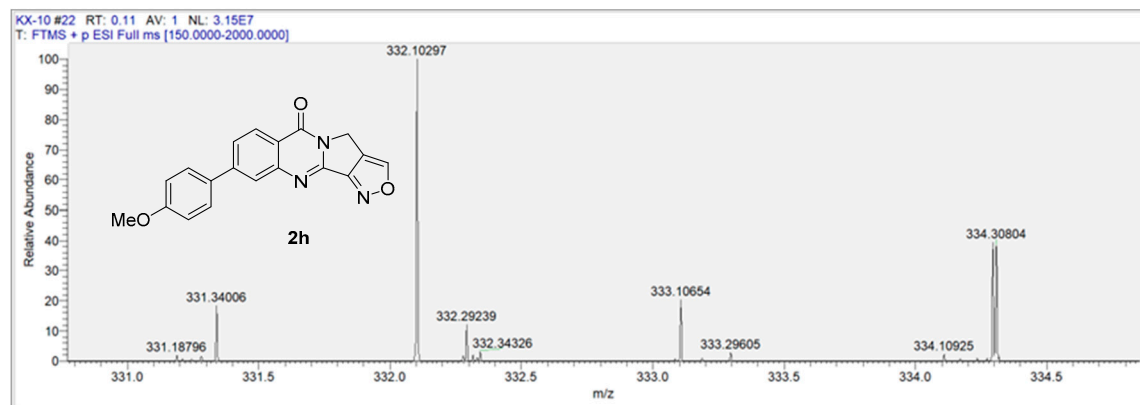


^1H NMR, 500MHz, $\text{DMSO}-d_6$

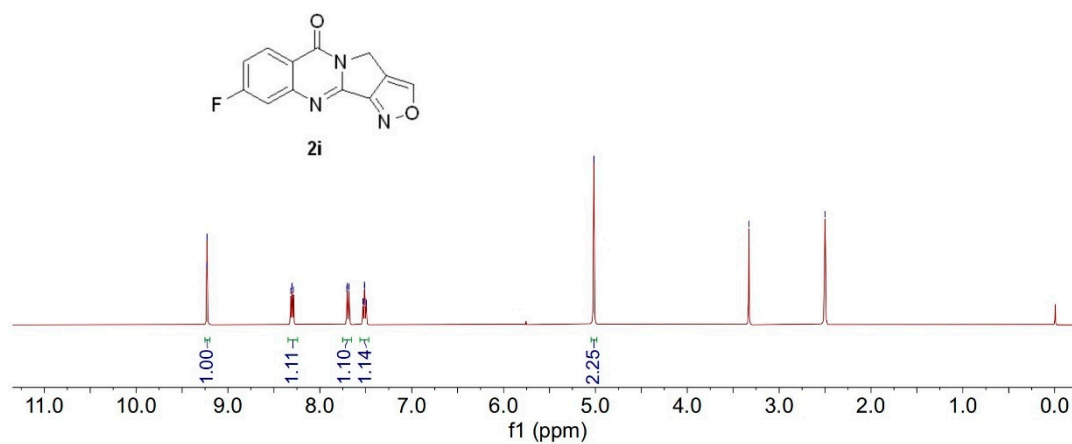


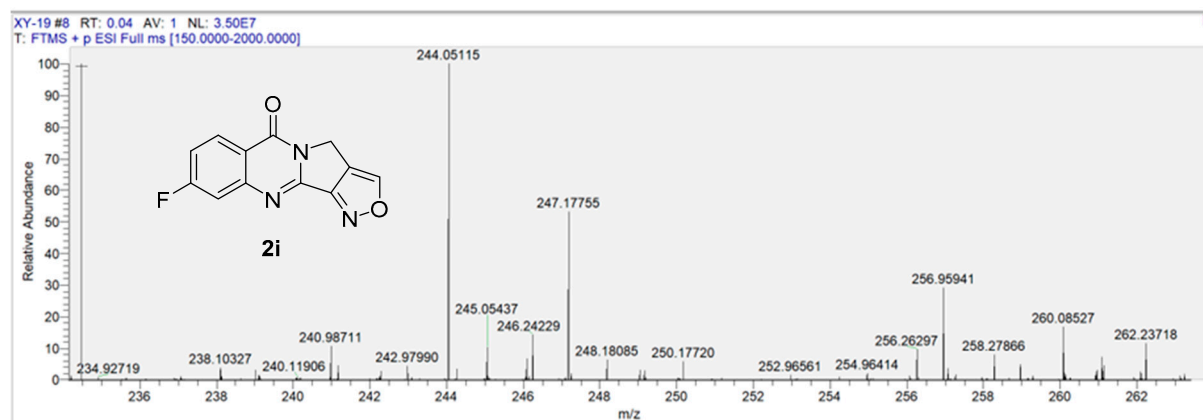
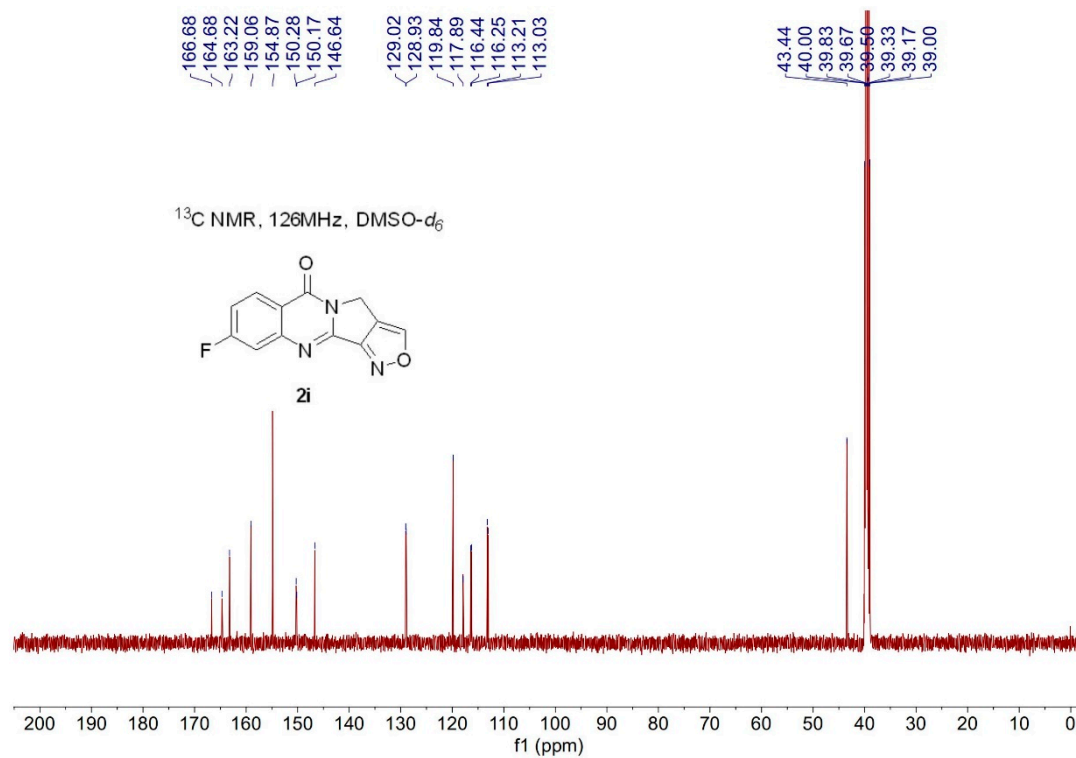


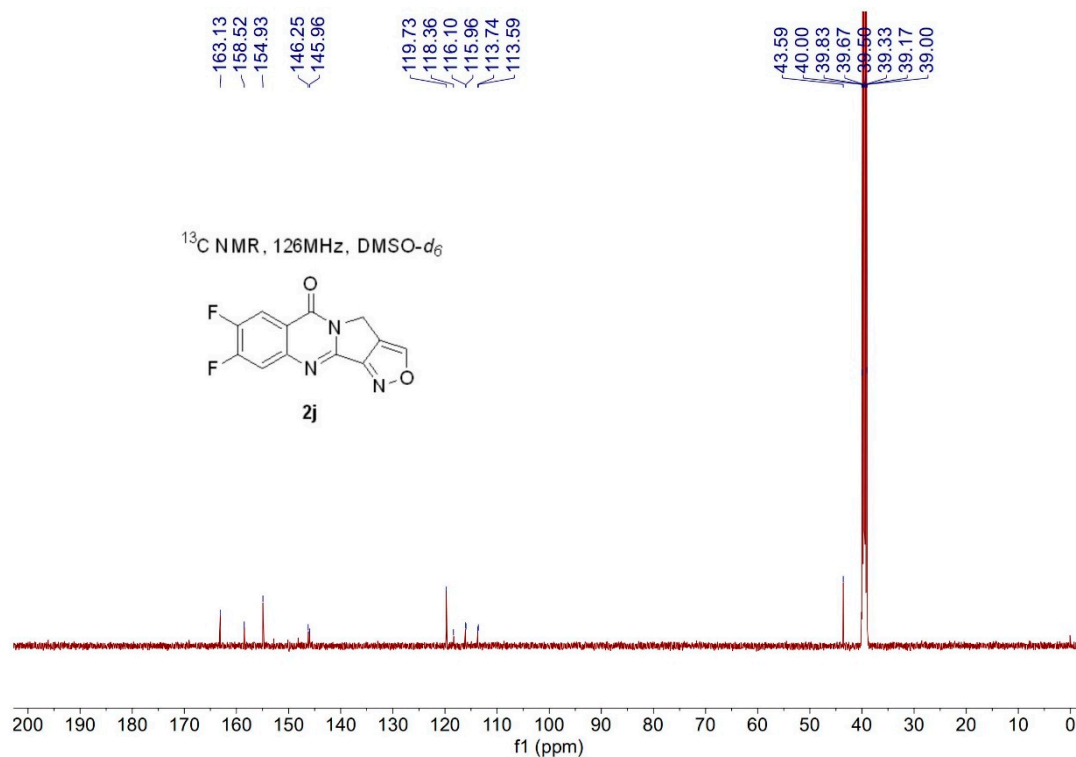
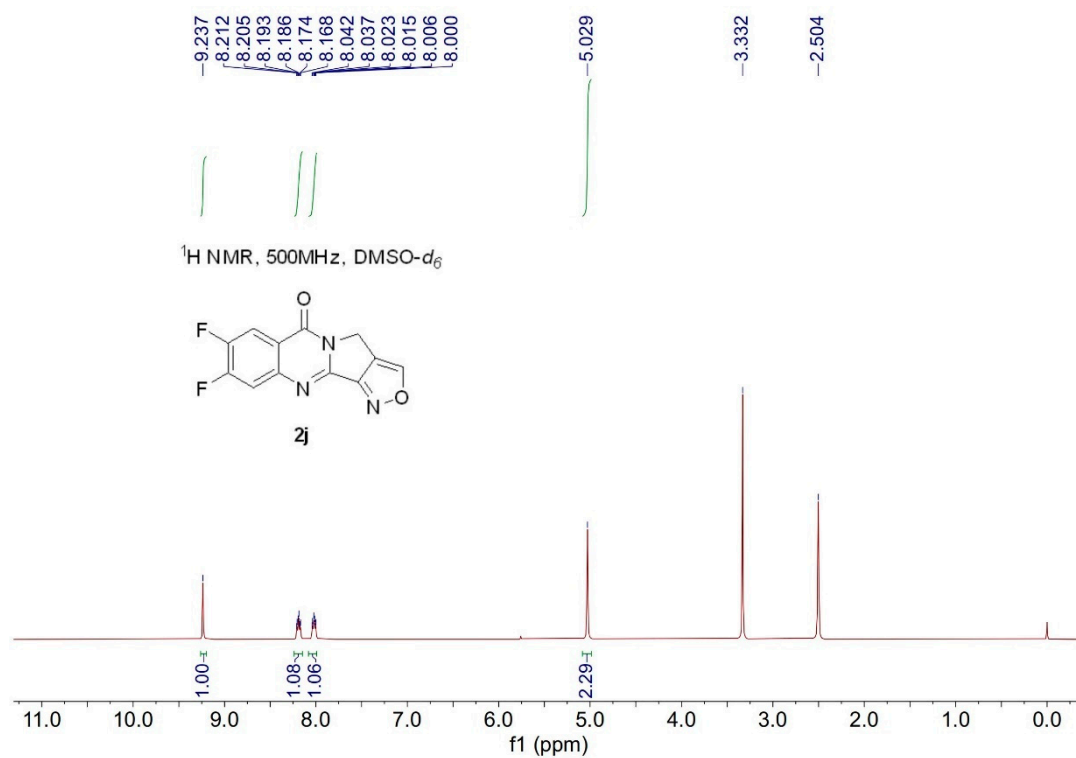


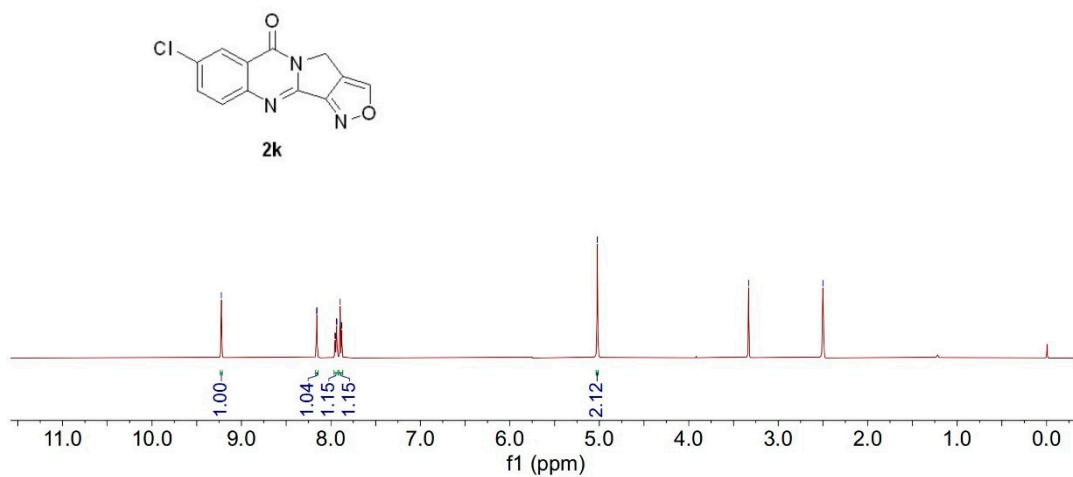
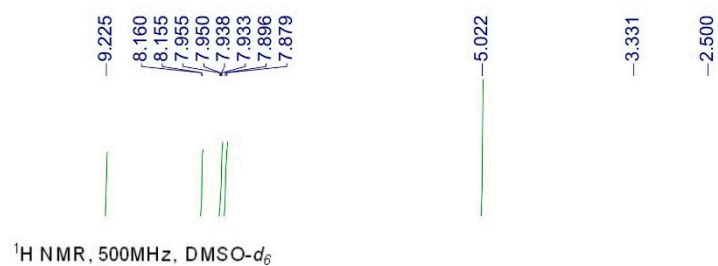
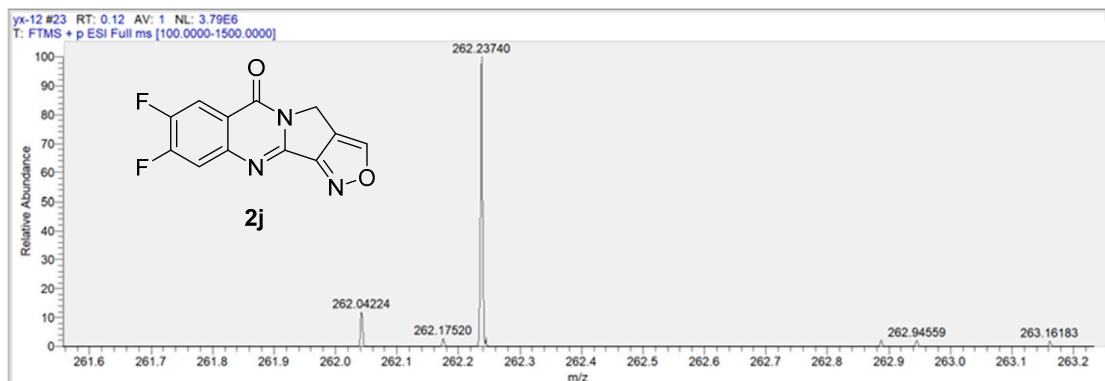


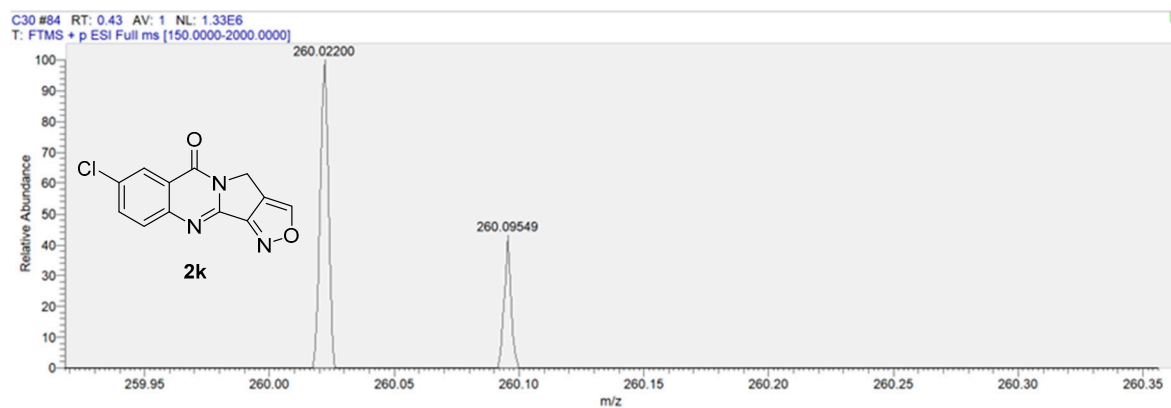
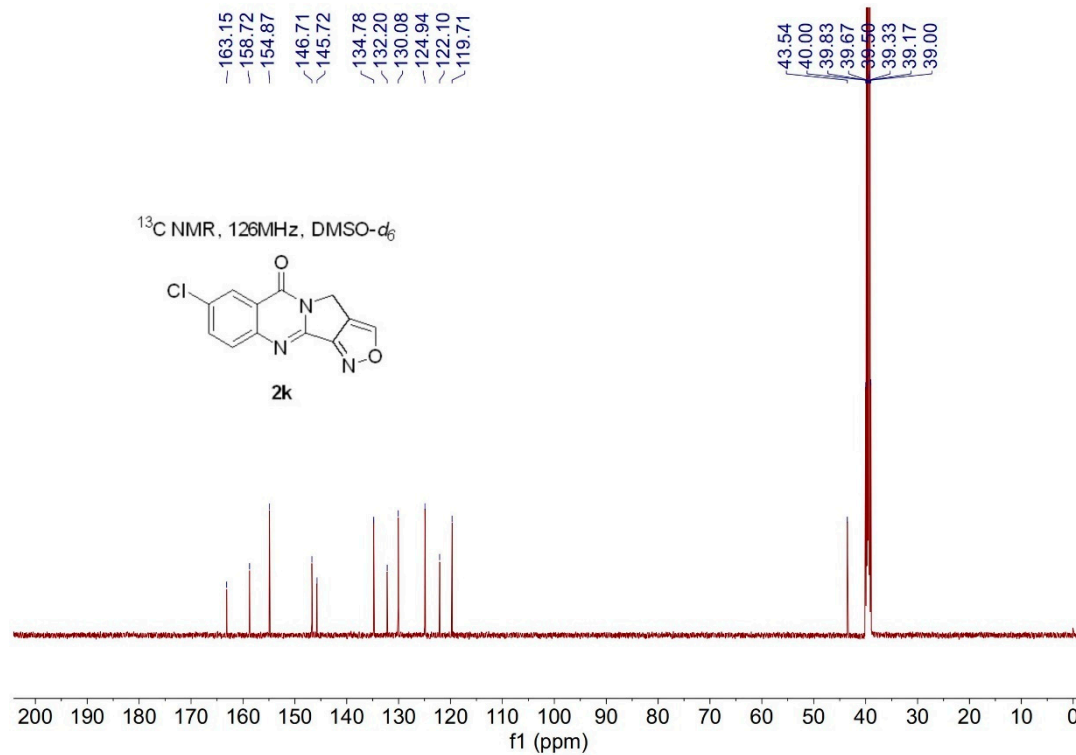
¹H NMR, 500MHz, DMSO-*d*₆

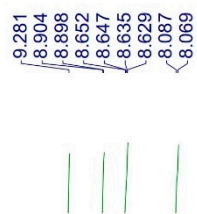




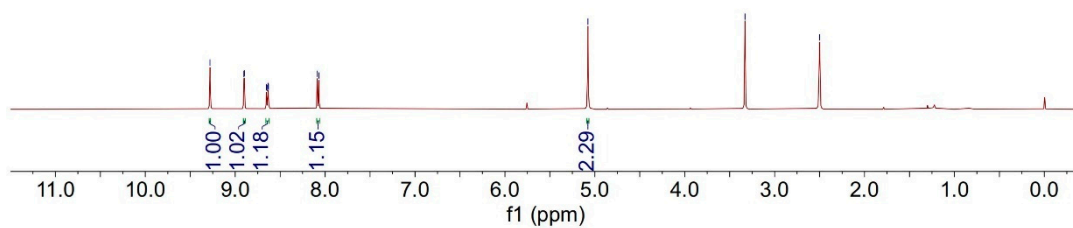
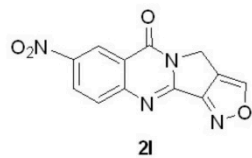




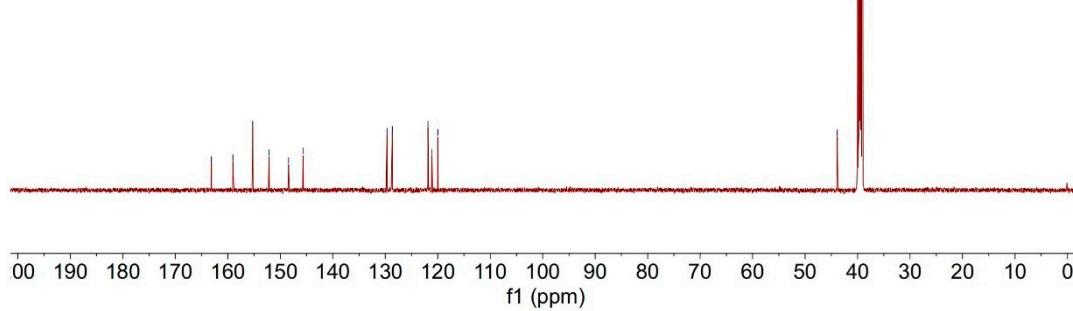
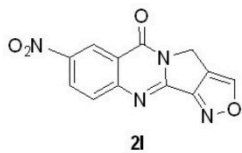


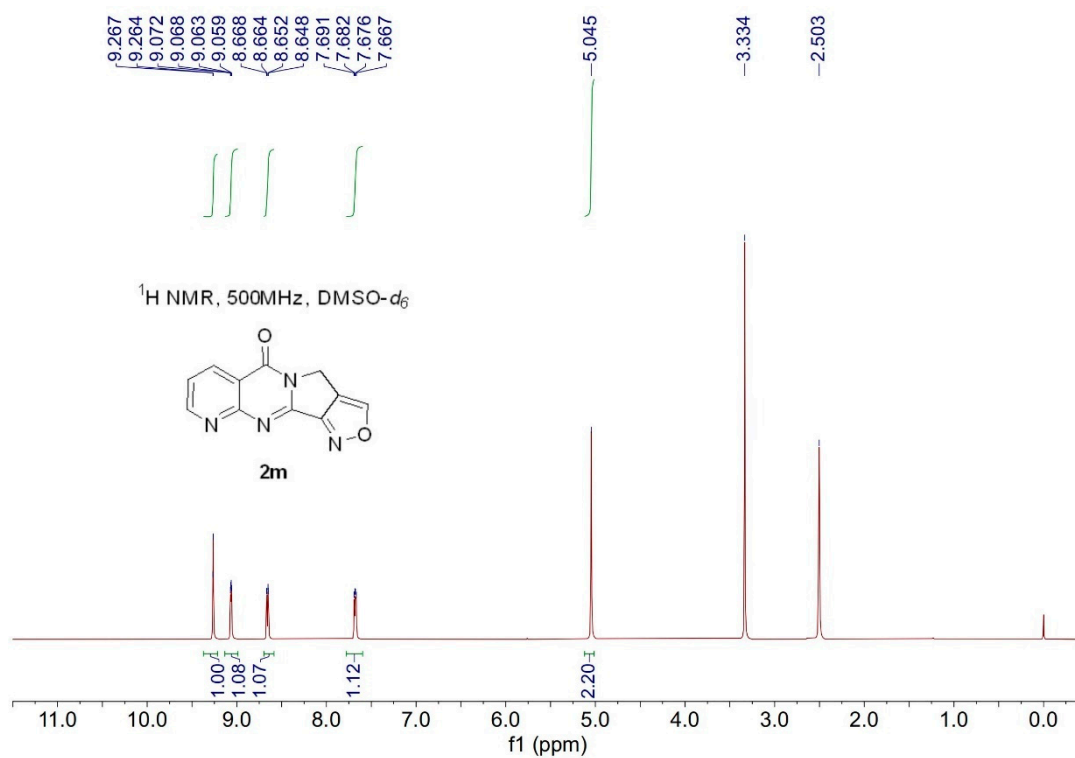
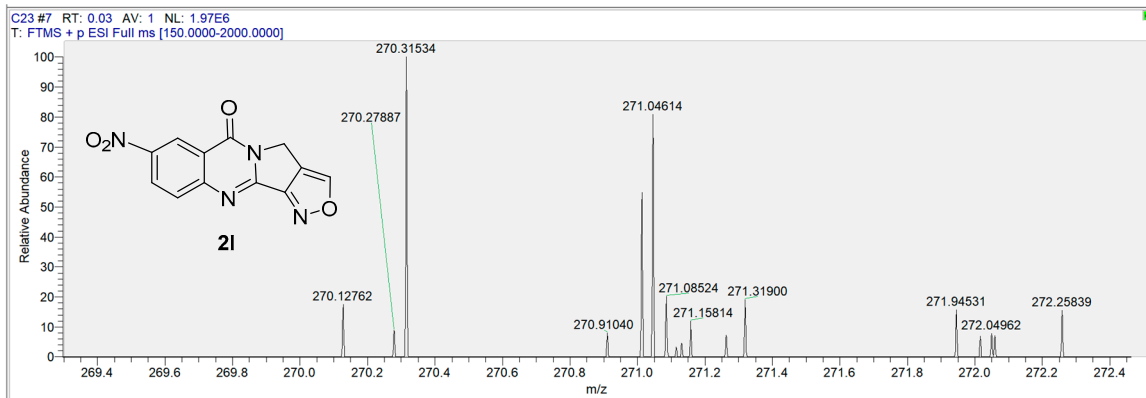


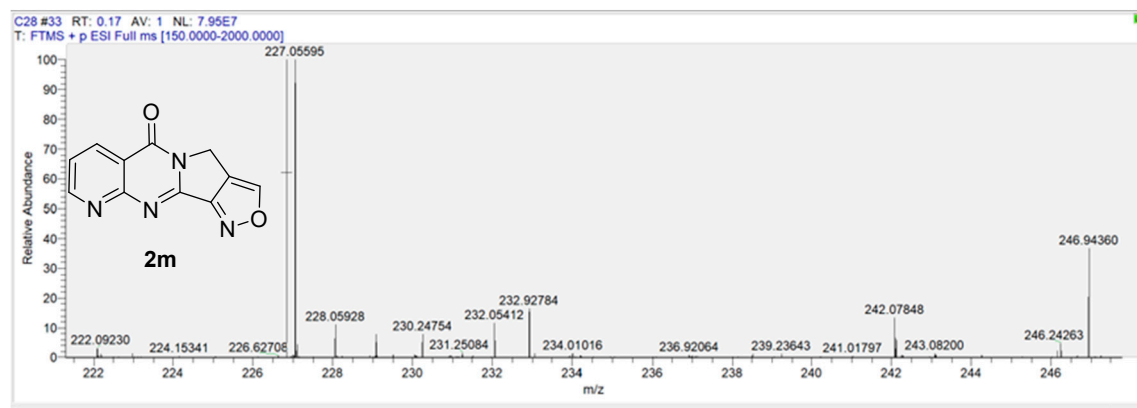
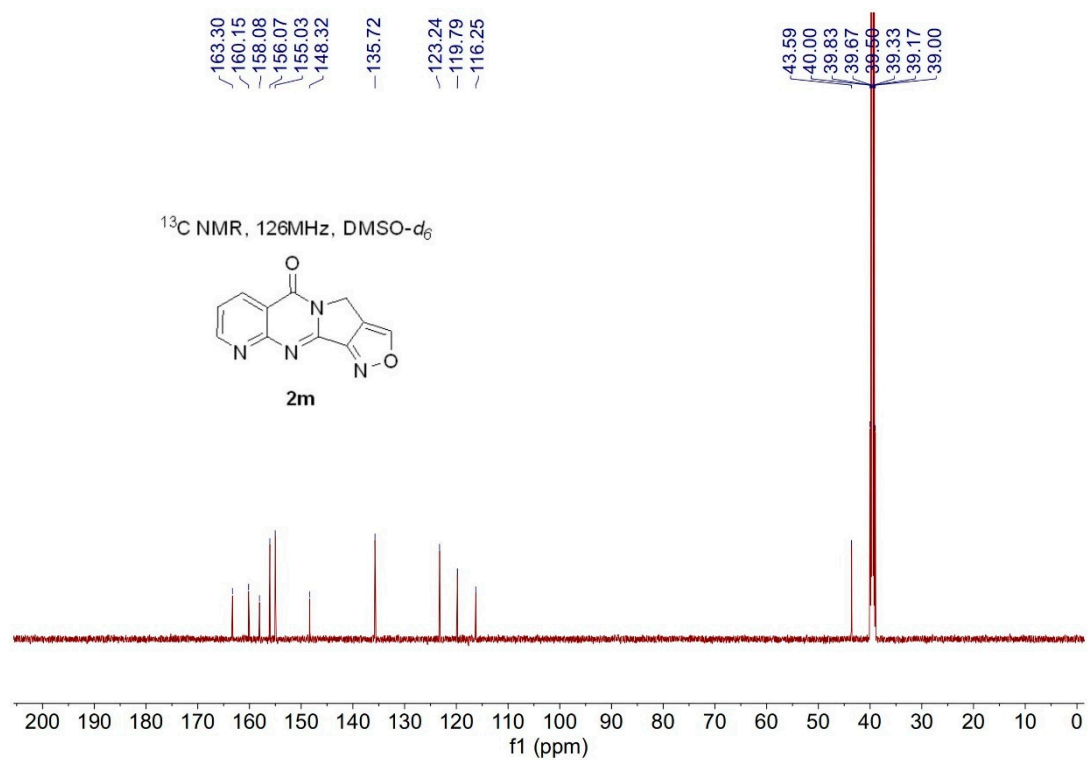
^1H NMR, 500MHz, $\text{DMSO}-d_6$

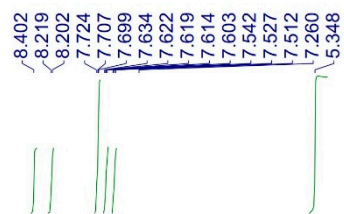


^{13}C NMR, 126MHz, $\text{DMSO}-d_6$

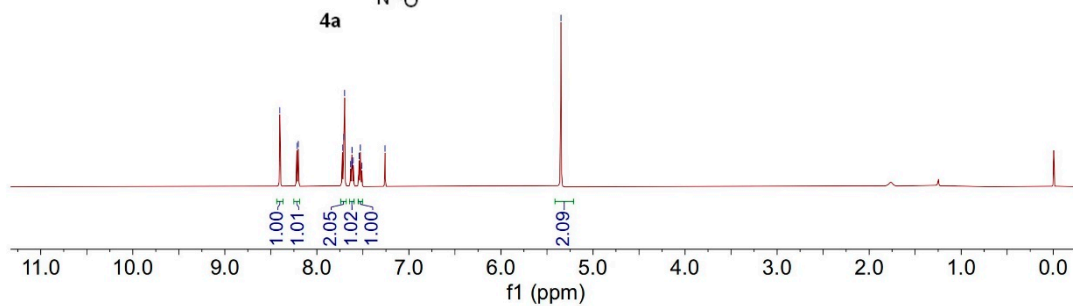
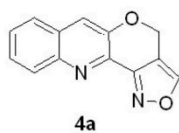




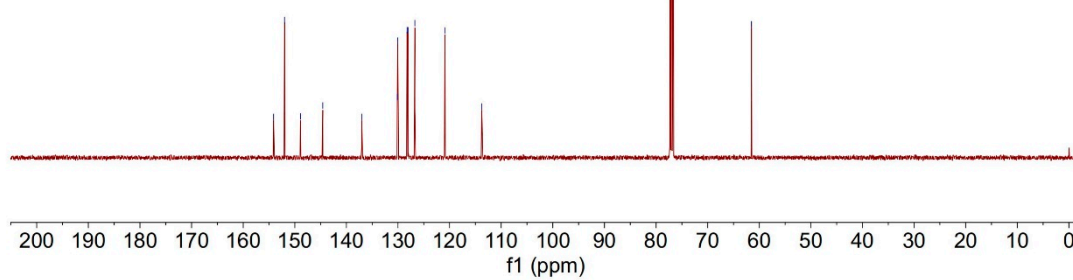
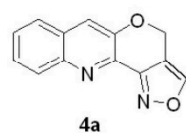


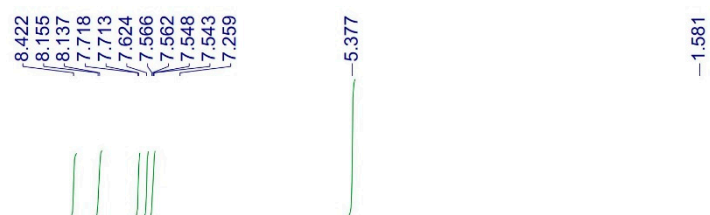
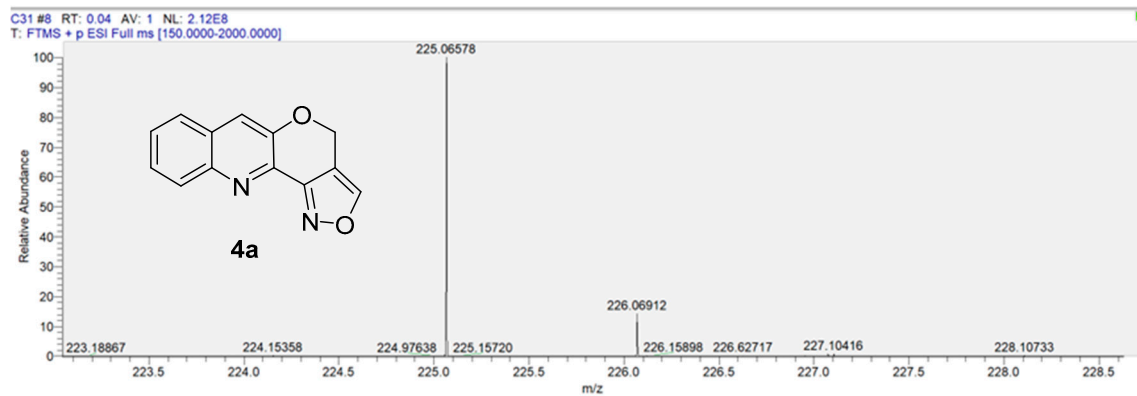


^1H NMR, 500 MHz, CDCl_3

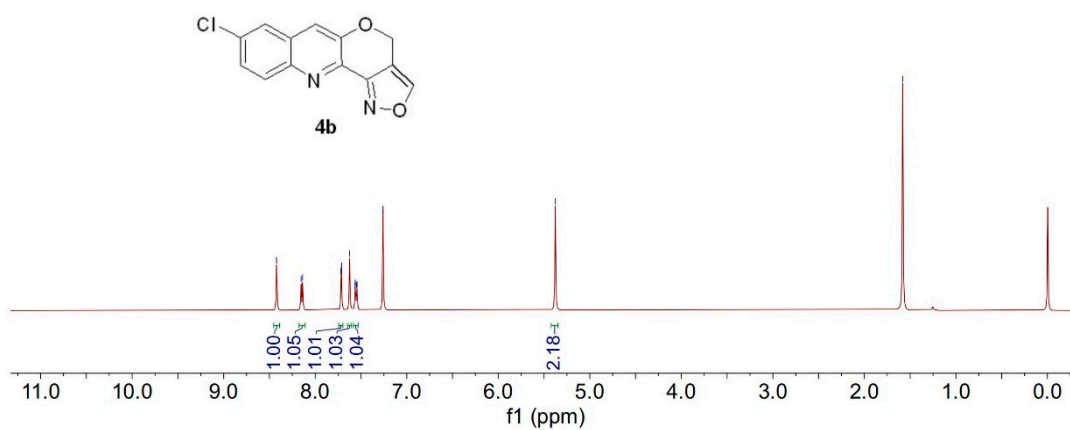


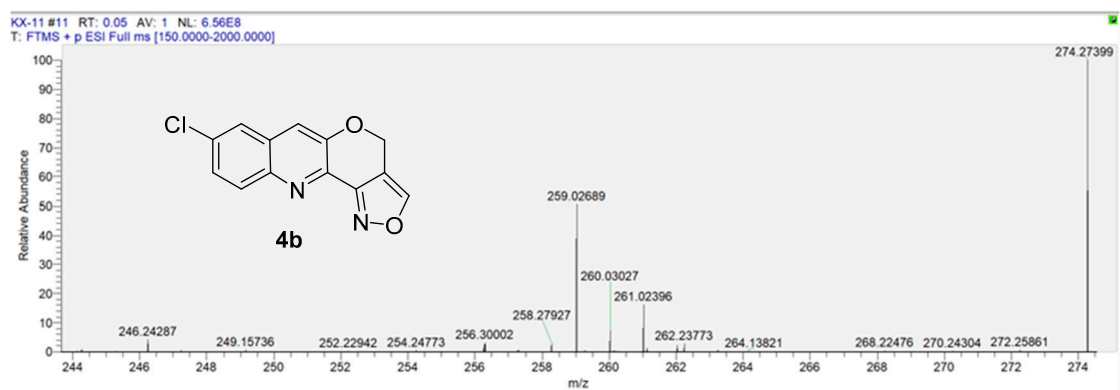
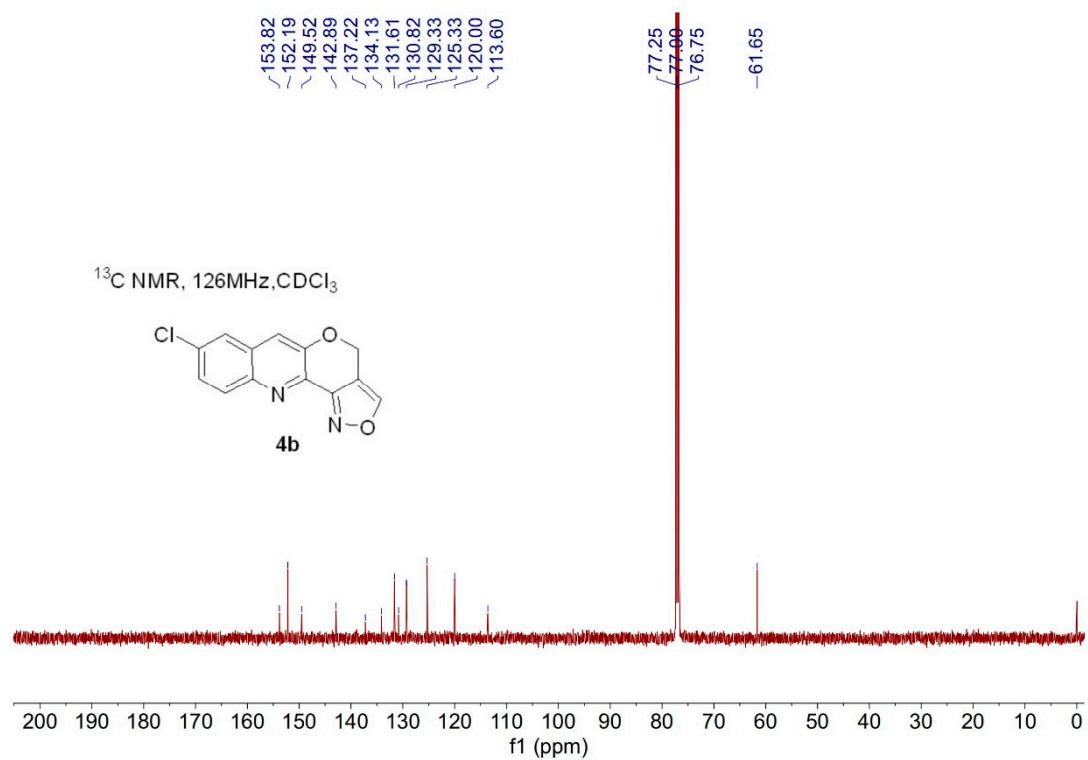
^{13}C NMR, 126MHz, CDCl_3





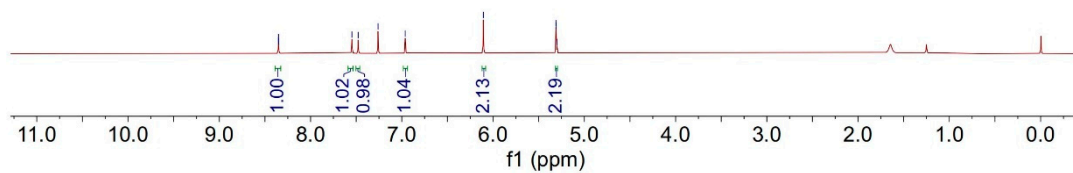
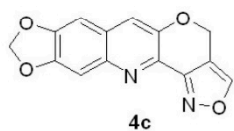
¹H NMR, 500 MHz, CDCl₃



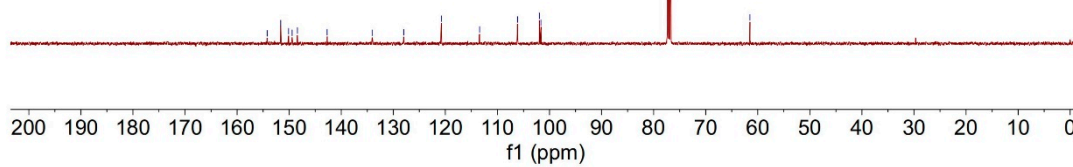
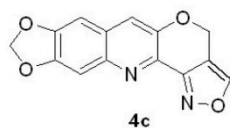


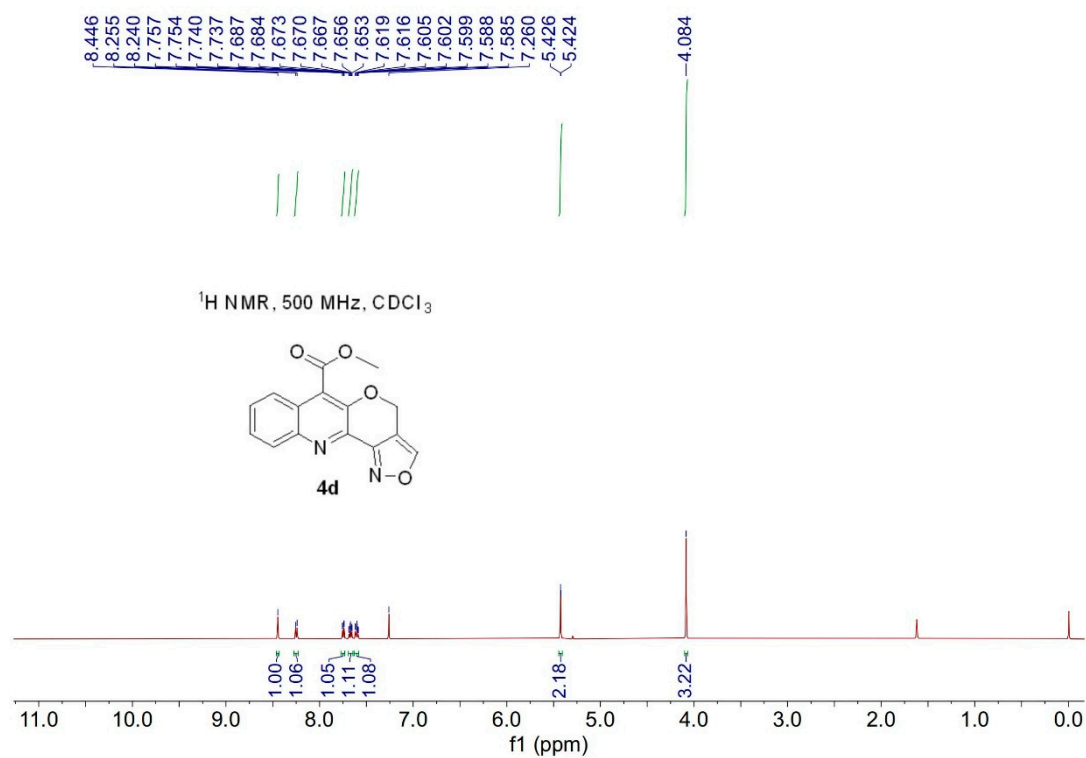
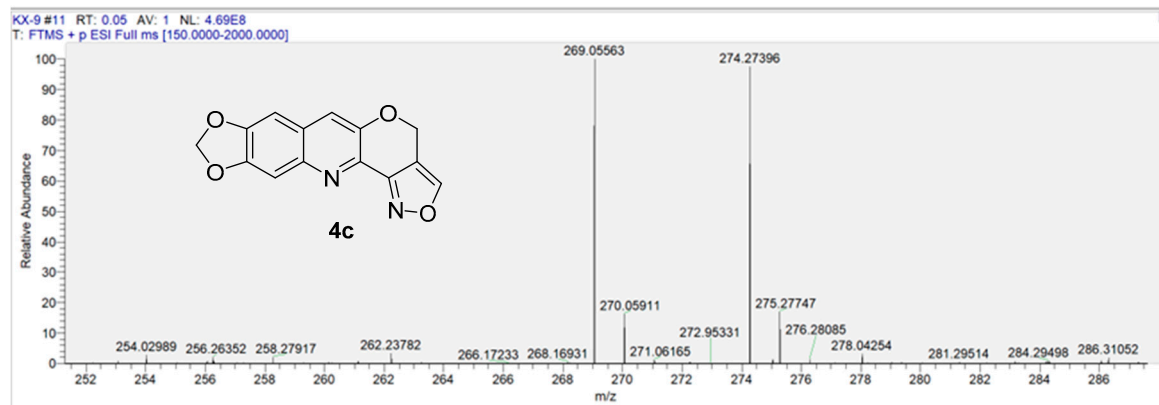


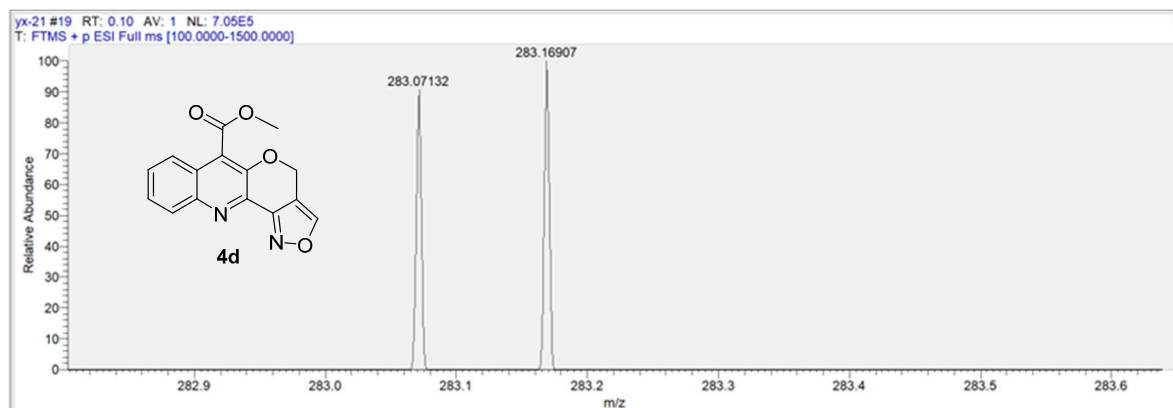
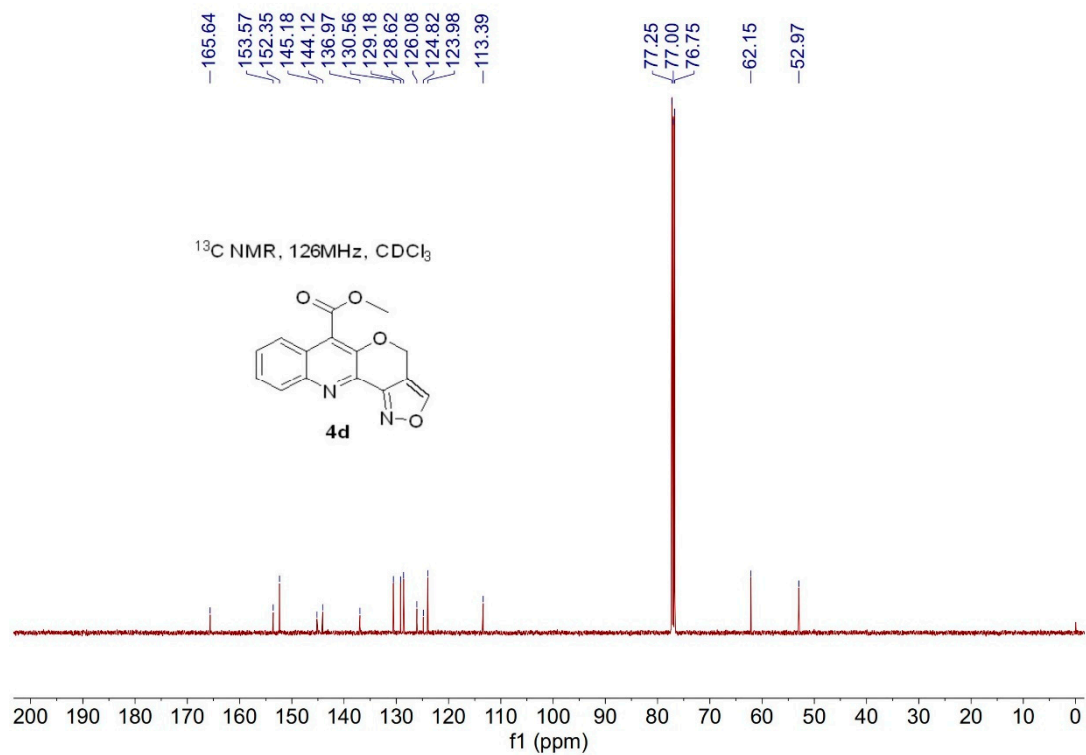
^1H NMR, 500 MHz, CDCl_3

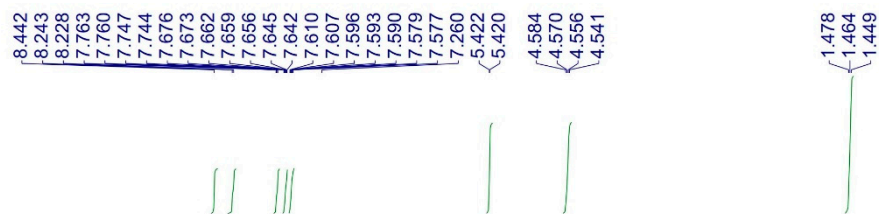


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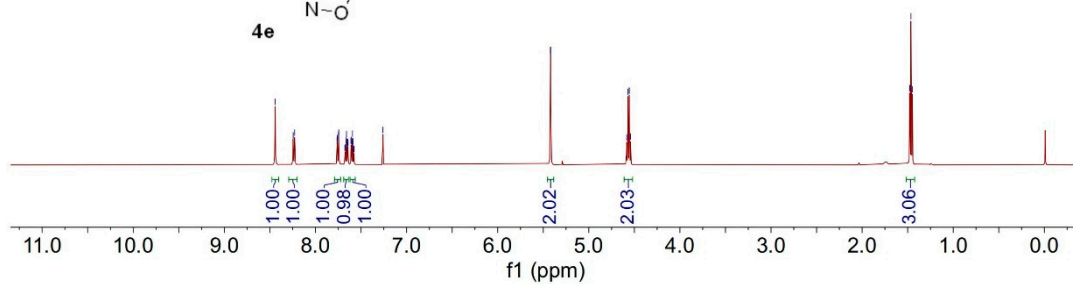
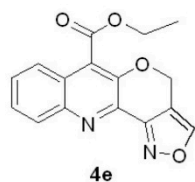




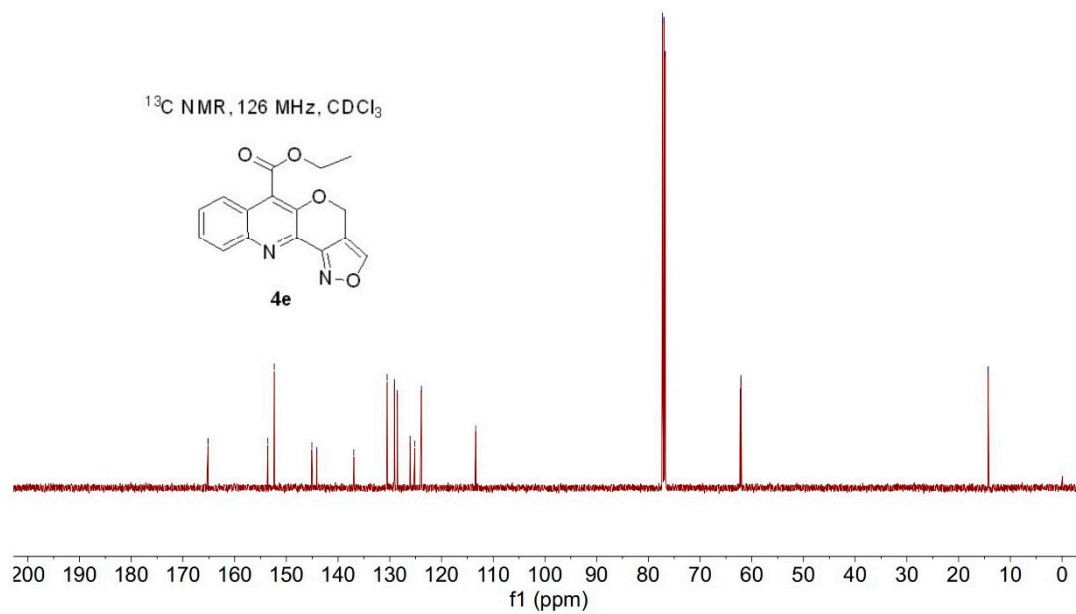
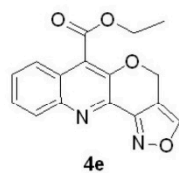


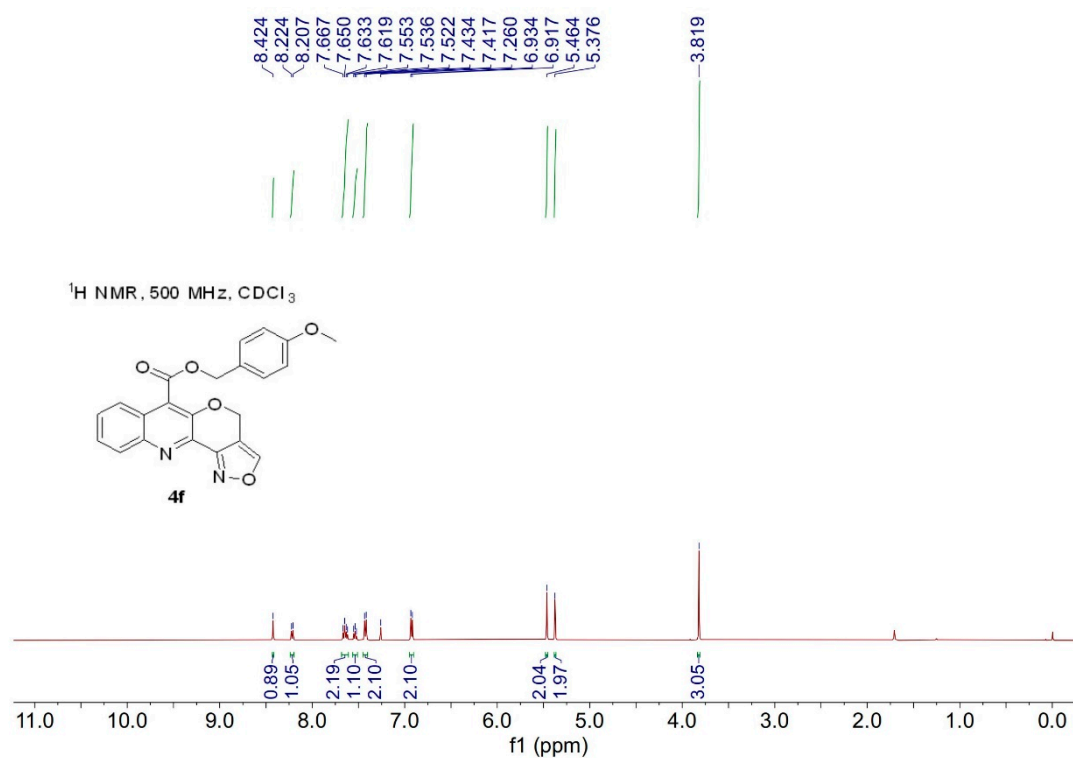
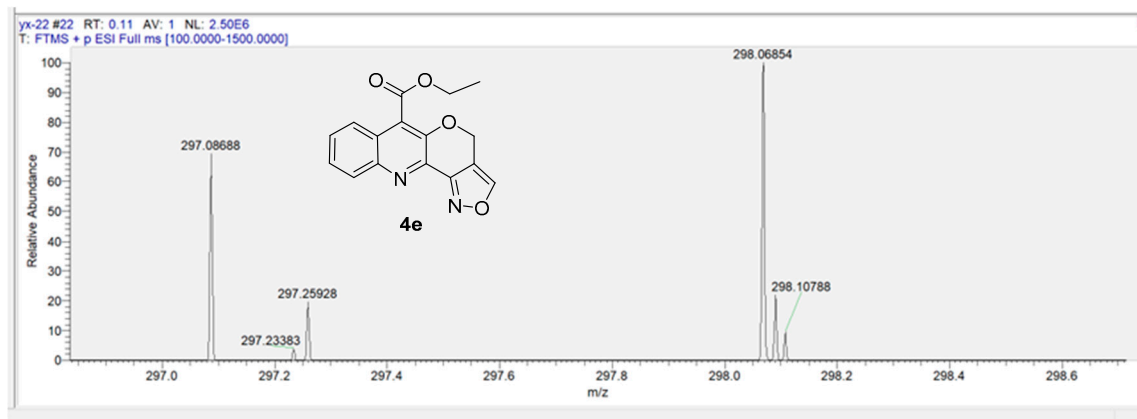


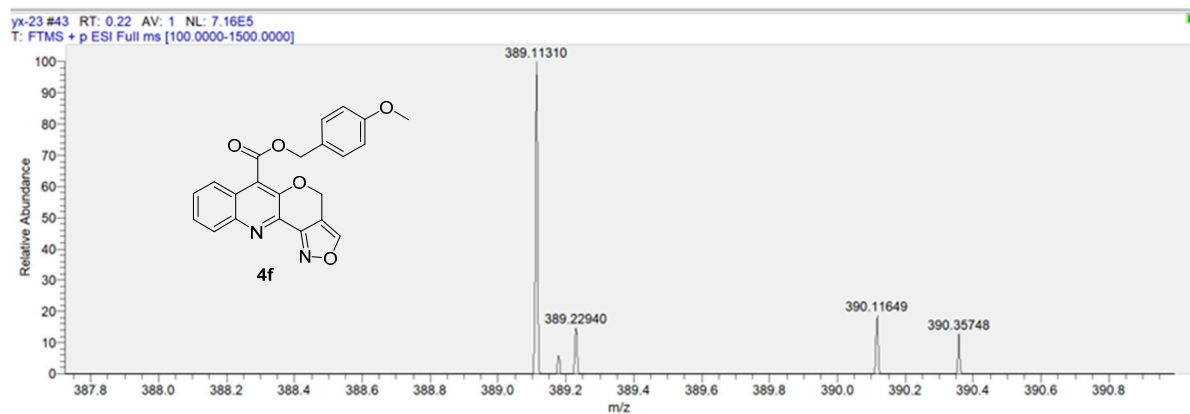
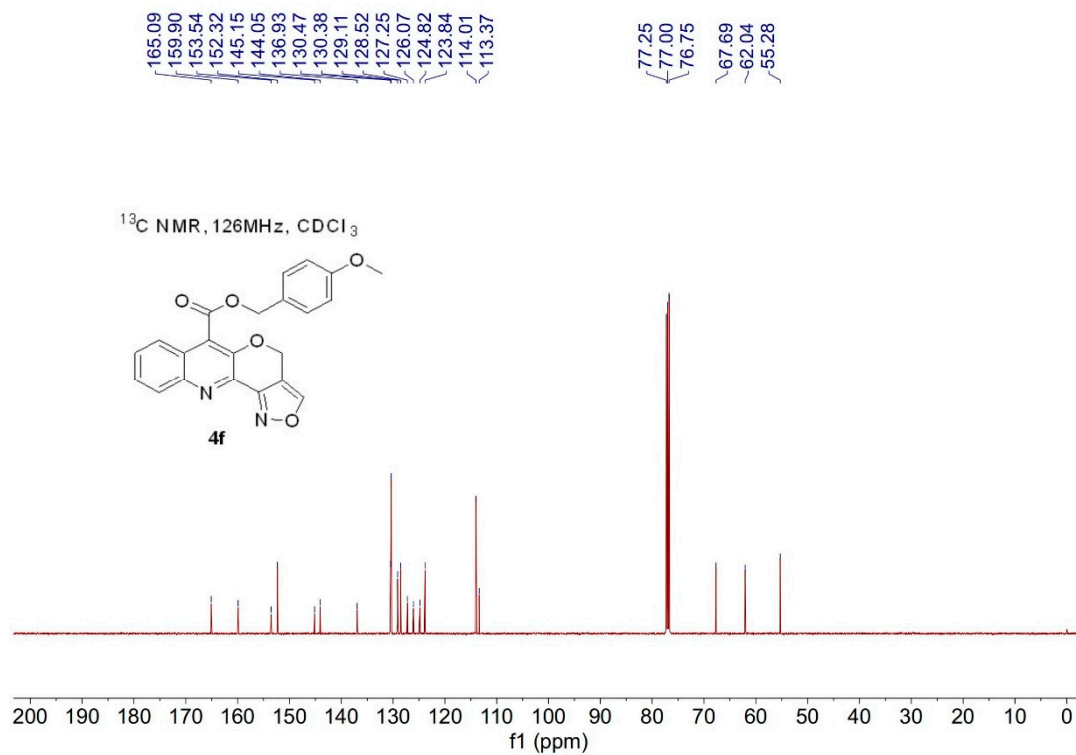
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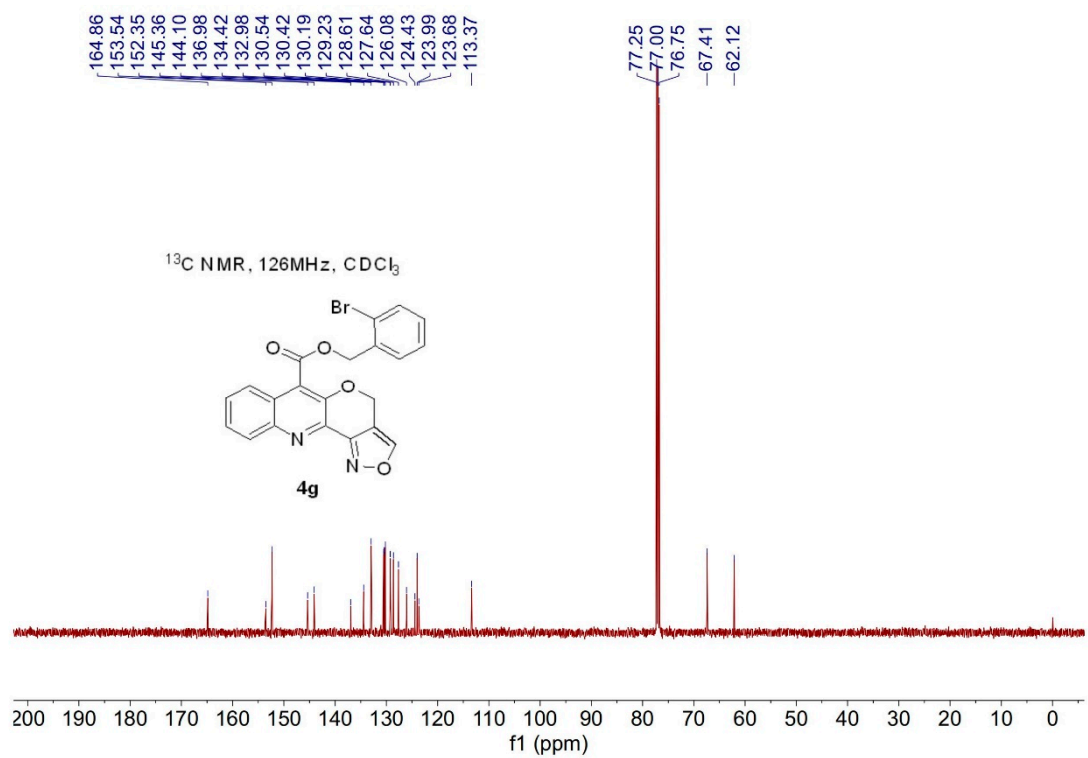
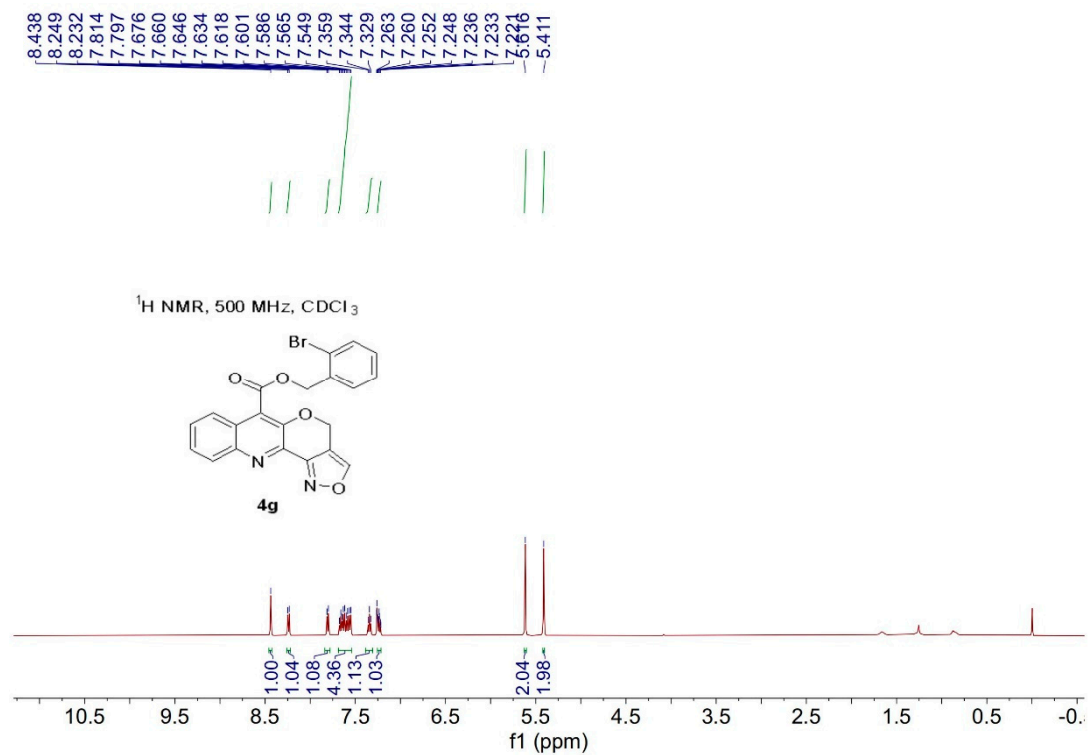


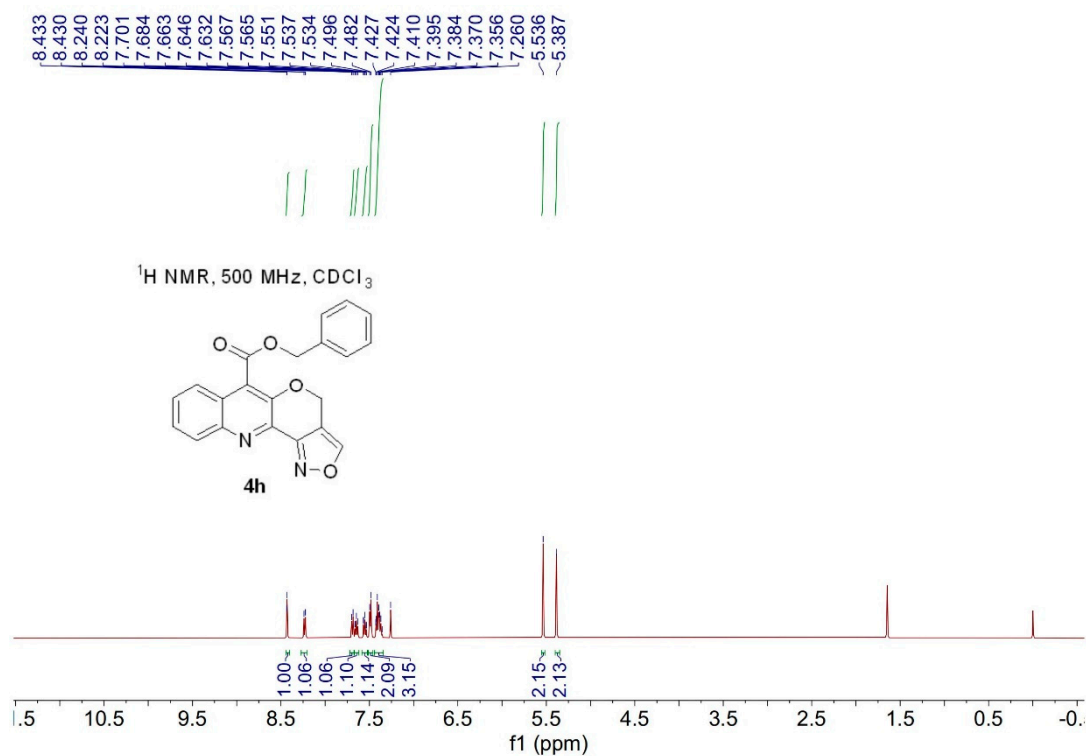
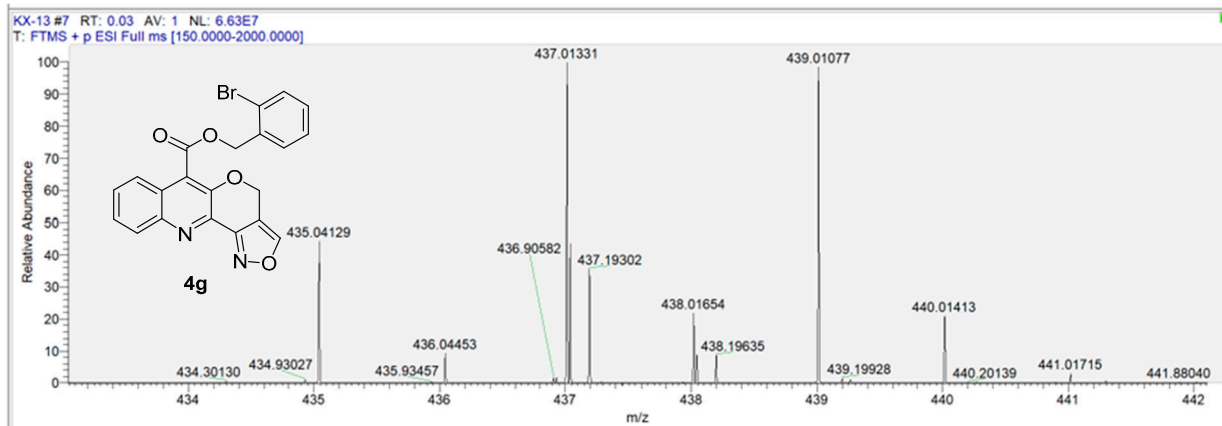
^{13}C NMR, 126 MHz, CDCl_3

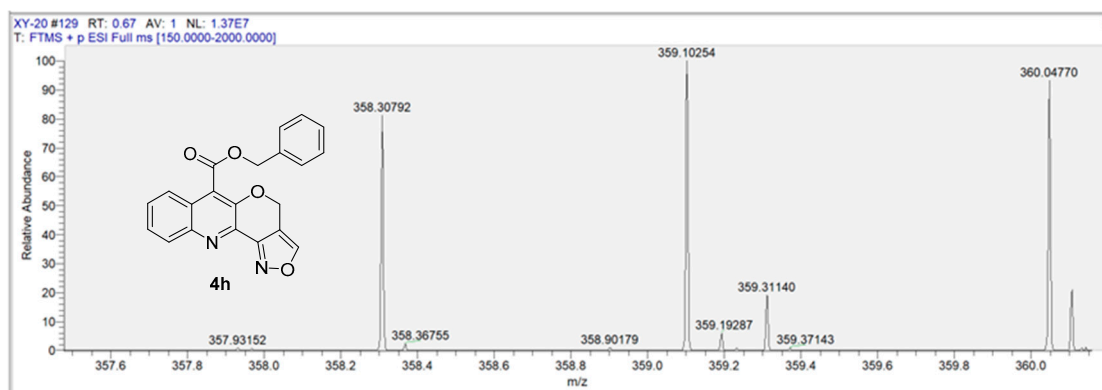
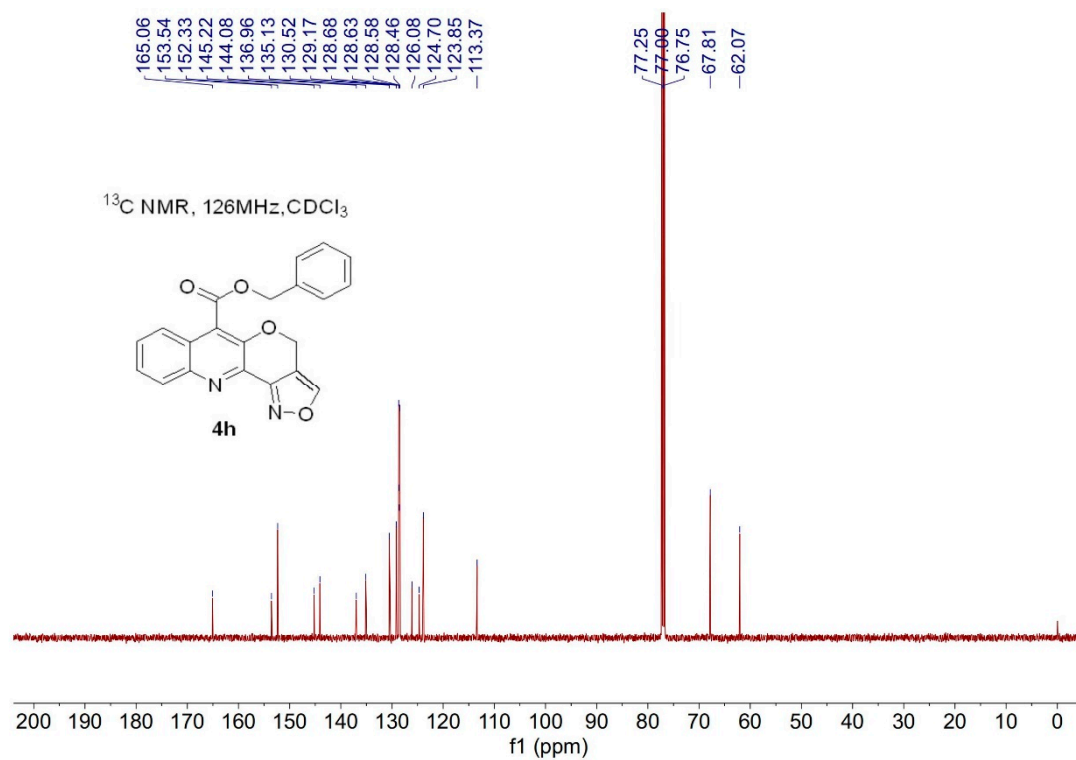


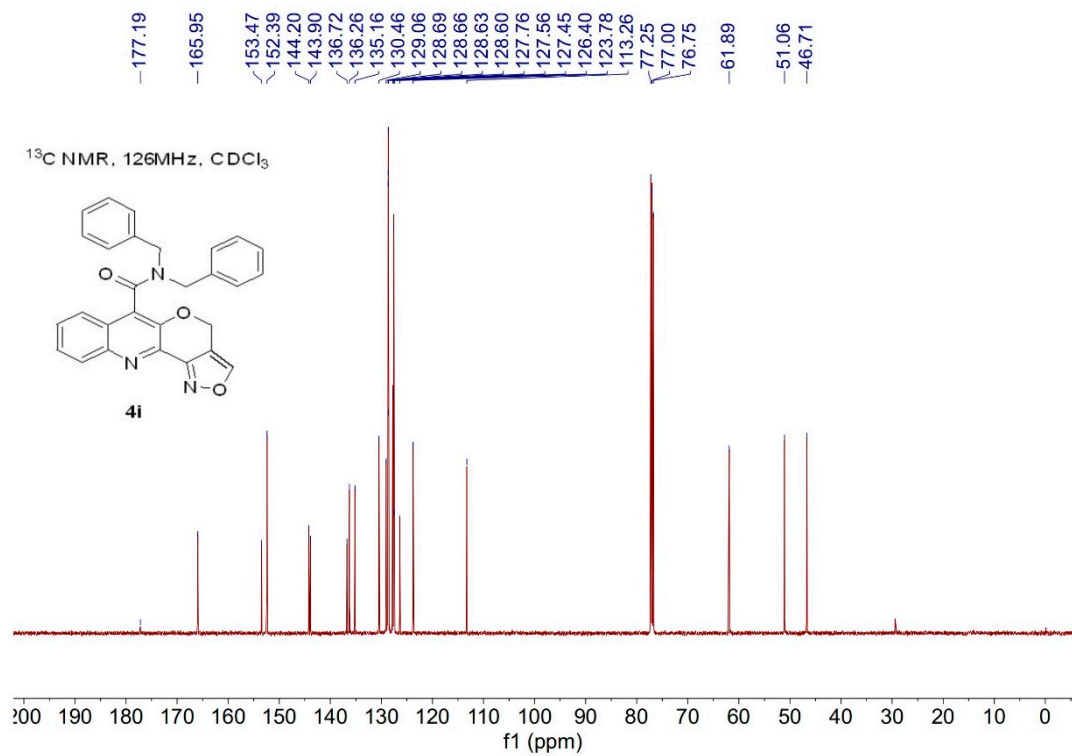
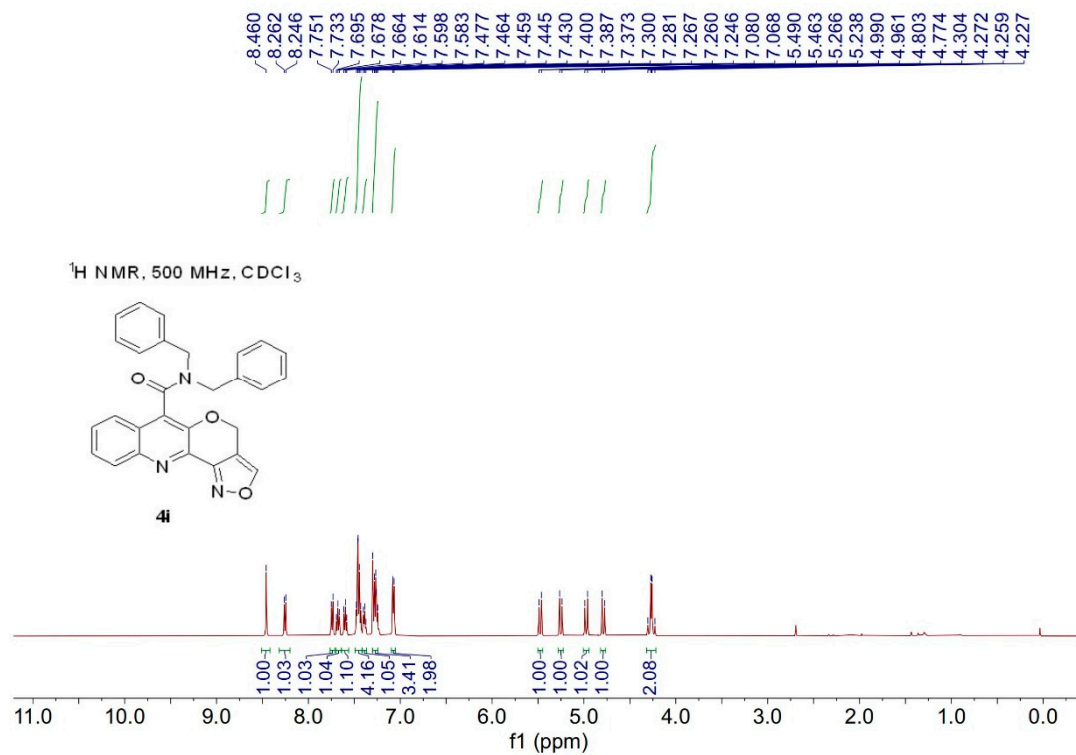


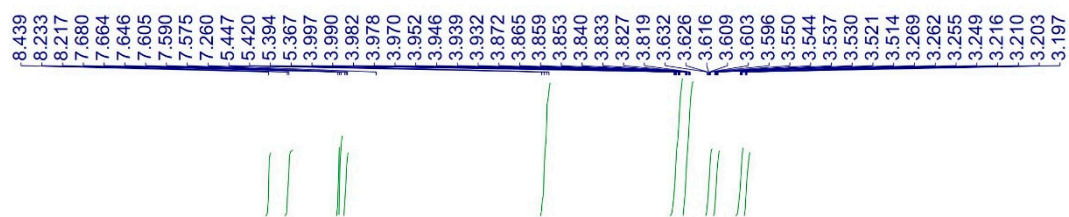
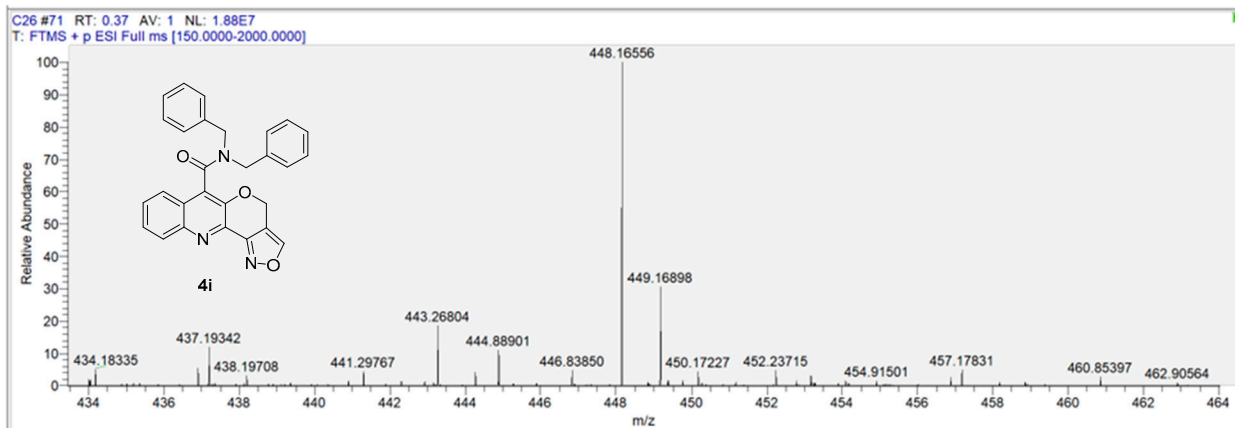












¹H NMR, 500 MHz, CDCl₃

