

**Supplementary Material (ESI) for Organic & Biomolecular
Chemistry**

Supporting Information

**S_mI₂-mediated ketyl-arene coupling of β-arylthio ketones: a facile
and diastereoselective synthesis of thiochroman derivatives**

Hui Mao,^a Bing-Xin You,^a Lie-Jin Zhou,^a Ting-Ting Xie,^a Yi-Hang Wen,^a Xin Lv^a and
Xiao-Xia Wang*^{a,b}

^aDepartment of Chemistry, College of Chemistry and Life Sciences, Zhejiang Normal
University, Jinhua 321004, People's Republic of China. E-mail:
wangxiaoxia@zjnu.cn

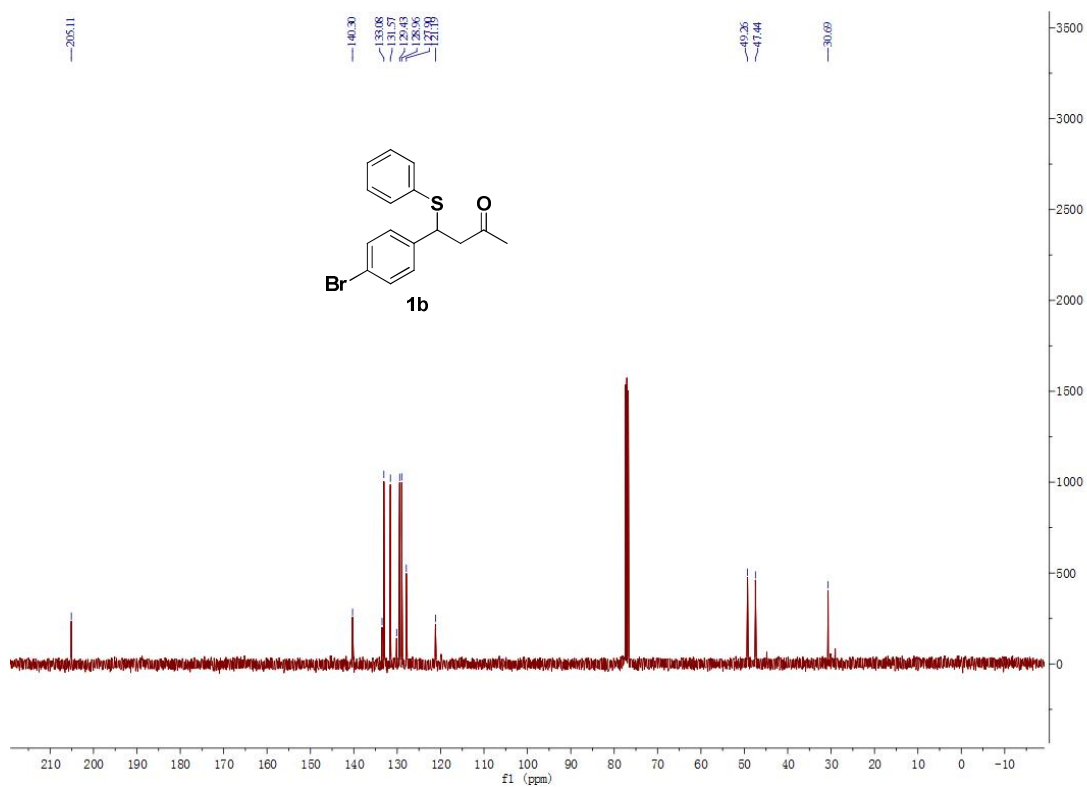
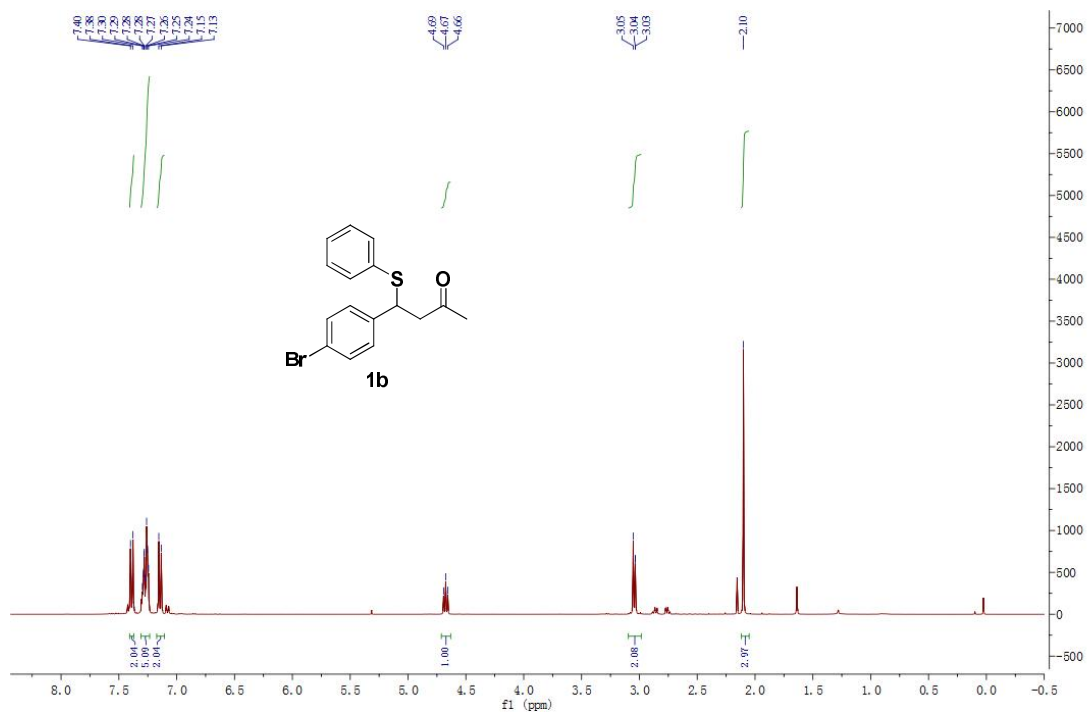
^bSchool of Environment and Civil Engineering, Dongguan University of Technology,
Dongguan, 523808, People's Republic of China.

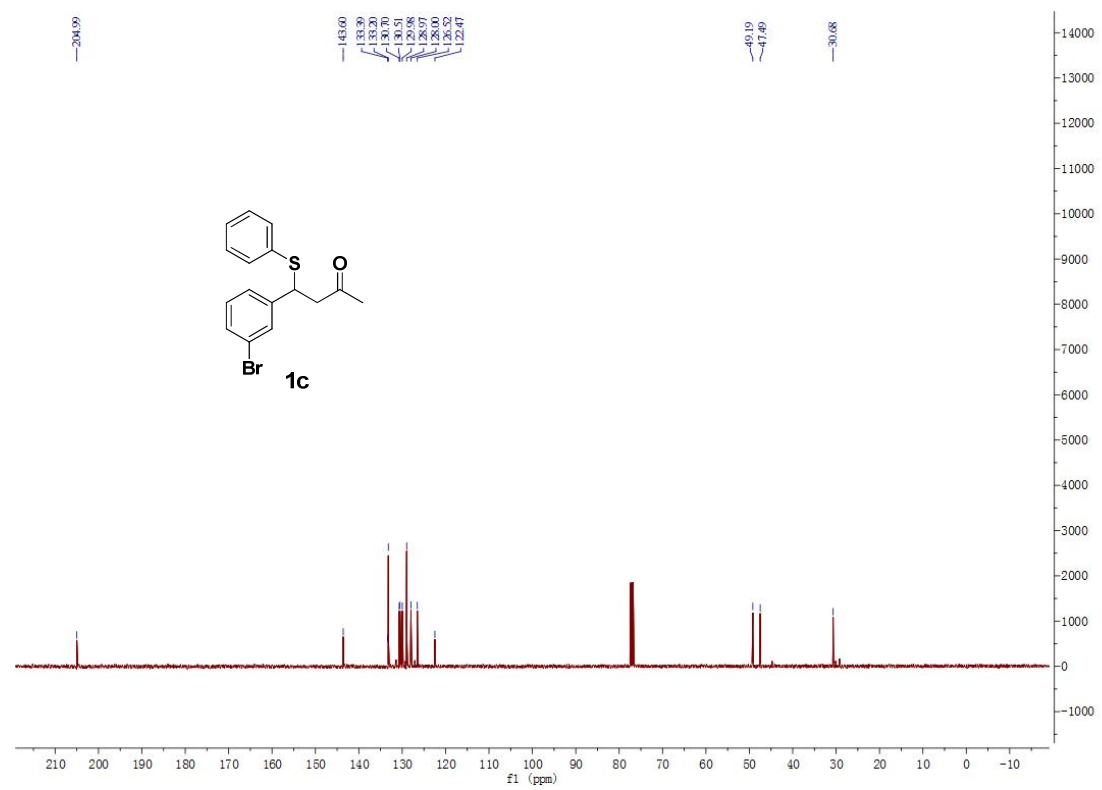
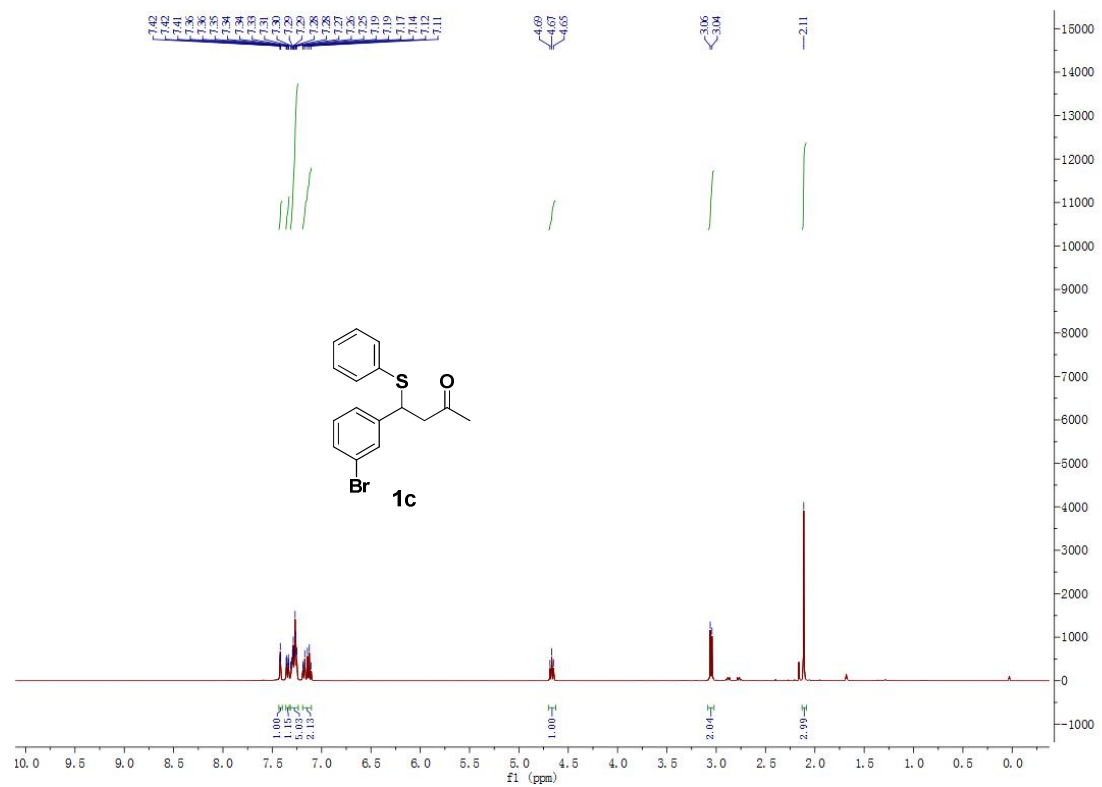
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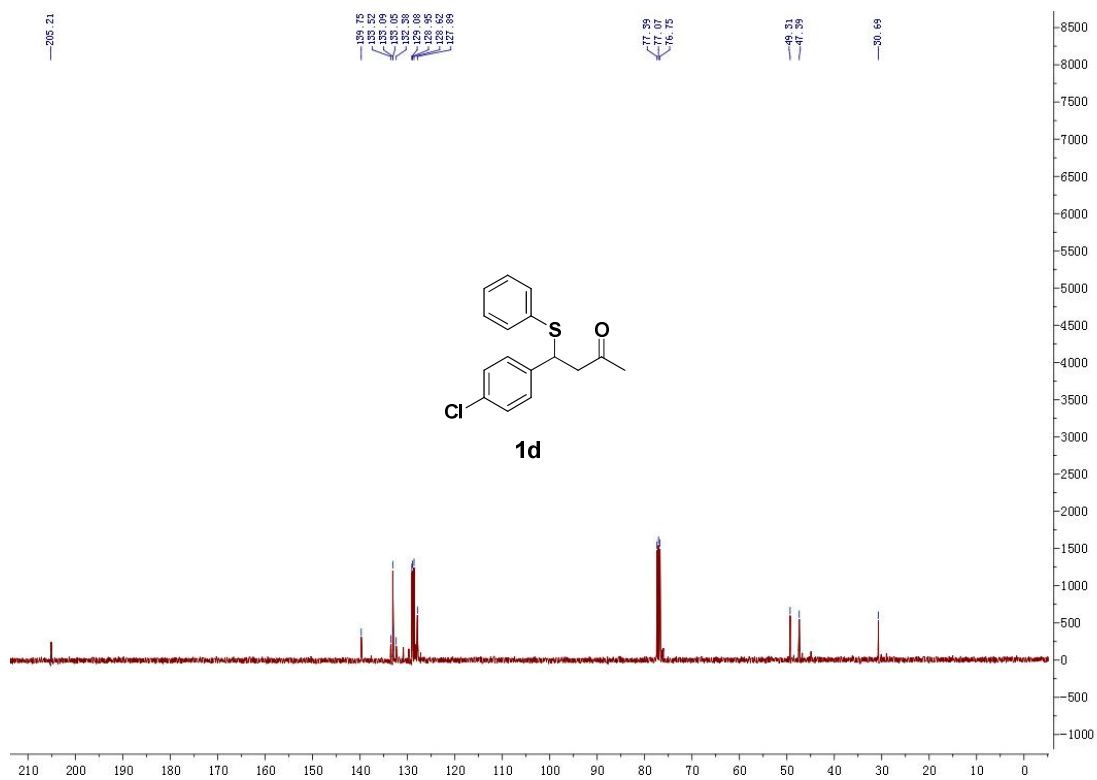
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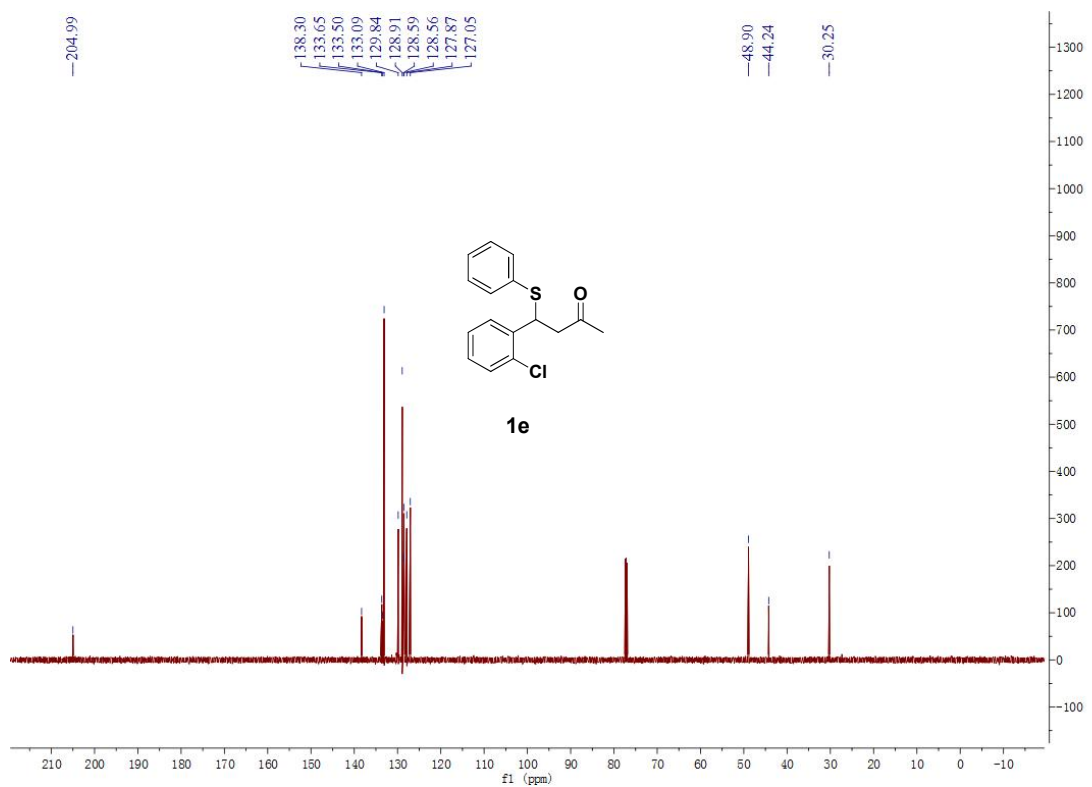
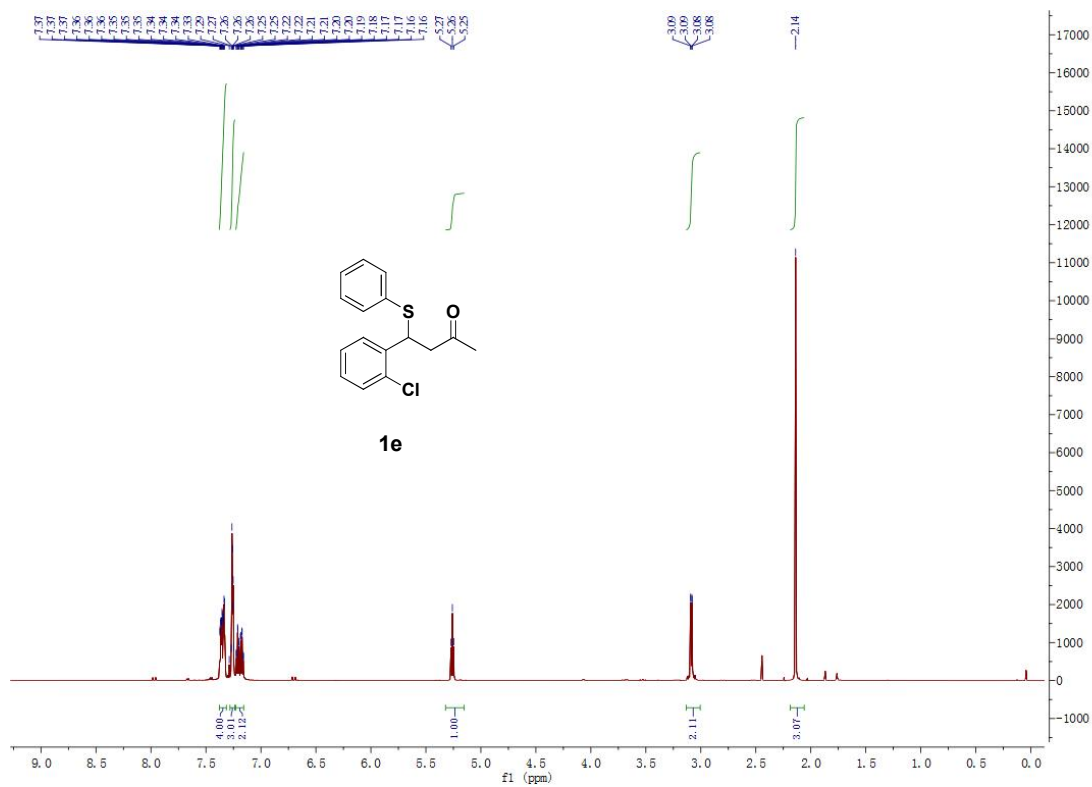
General Information. THF was distilled from sodium/benzophenone. Metallic samarium and other solvents were obtained from commercial sources, and used without further purification unless otherwise stated. All the cascade reactions were carried out under a nitrogen atmosphere in oven-dried flasks. All melting points are uncorrected. The ^1H and ^{13}C NMR spectra were recorded in CDCl_3 on a 400 or 600 MHz instrument with TMS as internal standard. Recorded shifts are reported in parts per million (δ) downfield from TMS. Data are represented as follows: Chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad), coupling constant (J , Hz) and integration. TLC was carried out with 0.2 mm thick silica gel plates (GF254). Visualization was accomplished by UV light. The columns were hand packed with silica gel 60 (300–400 mesh). Unknown products were additionally confirmed by high-resolution mass spectra (HRMS) using a TOF-MS instrument with an ESI or APCI source.

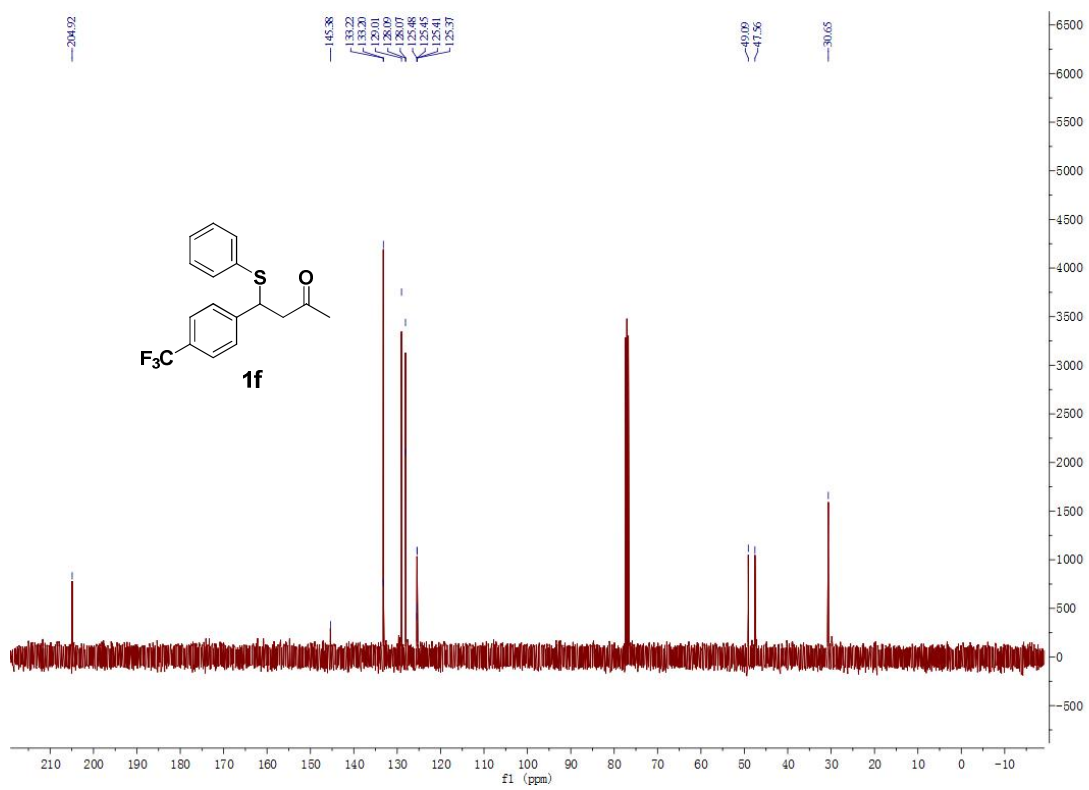
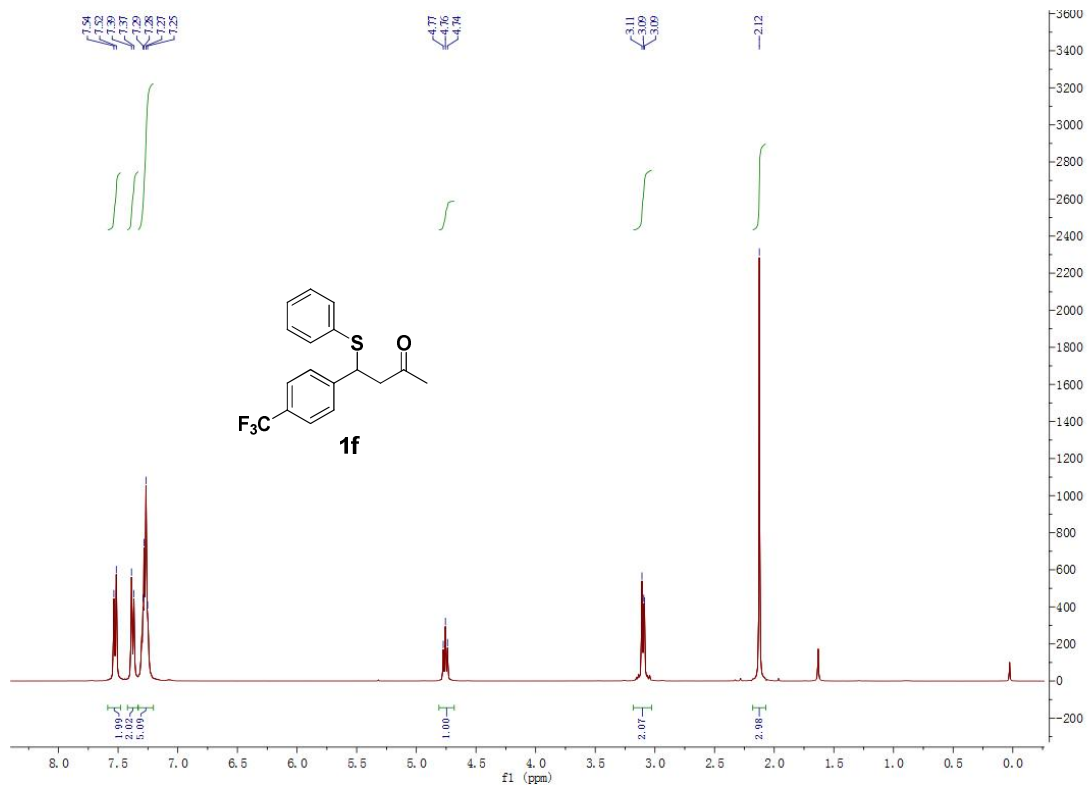
NMR Spectra for new substrates 1

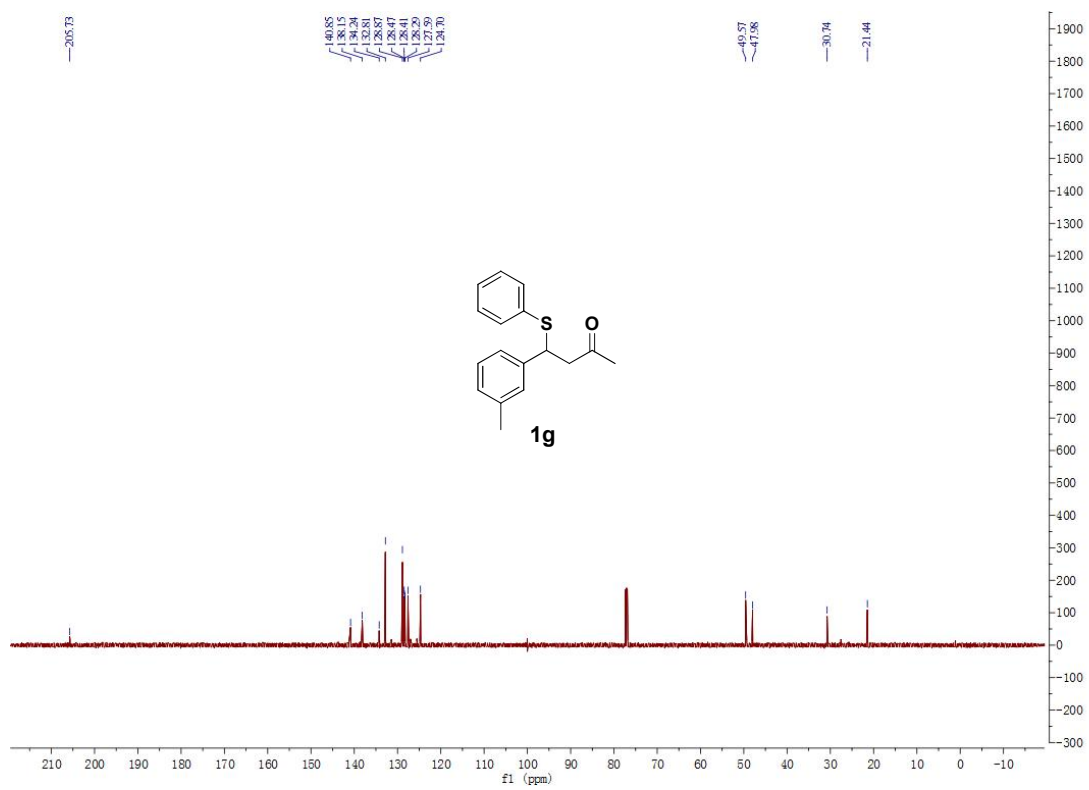
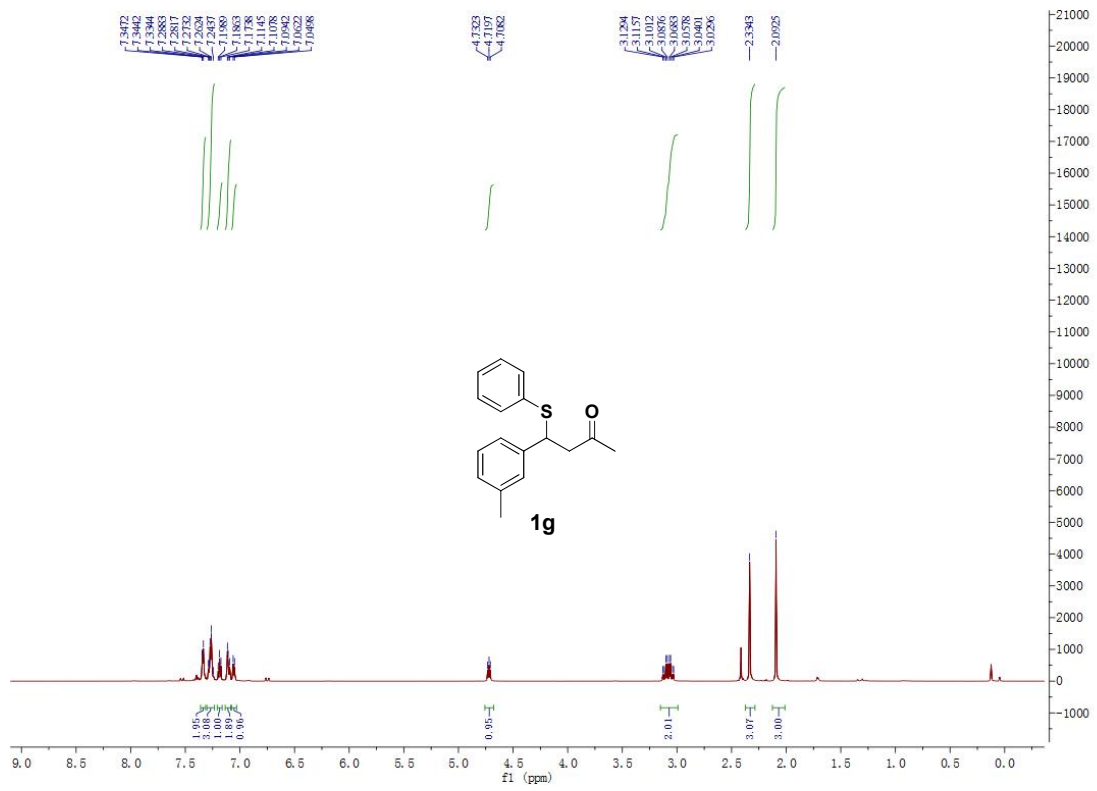


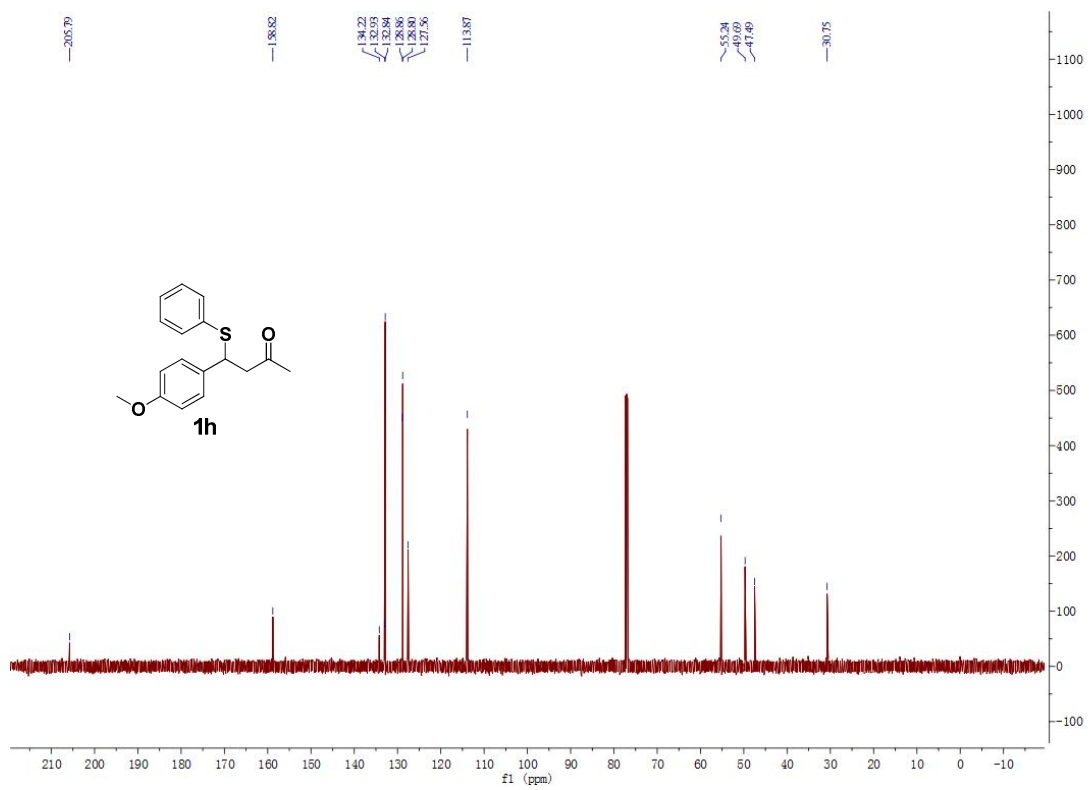
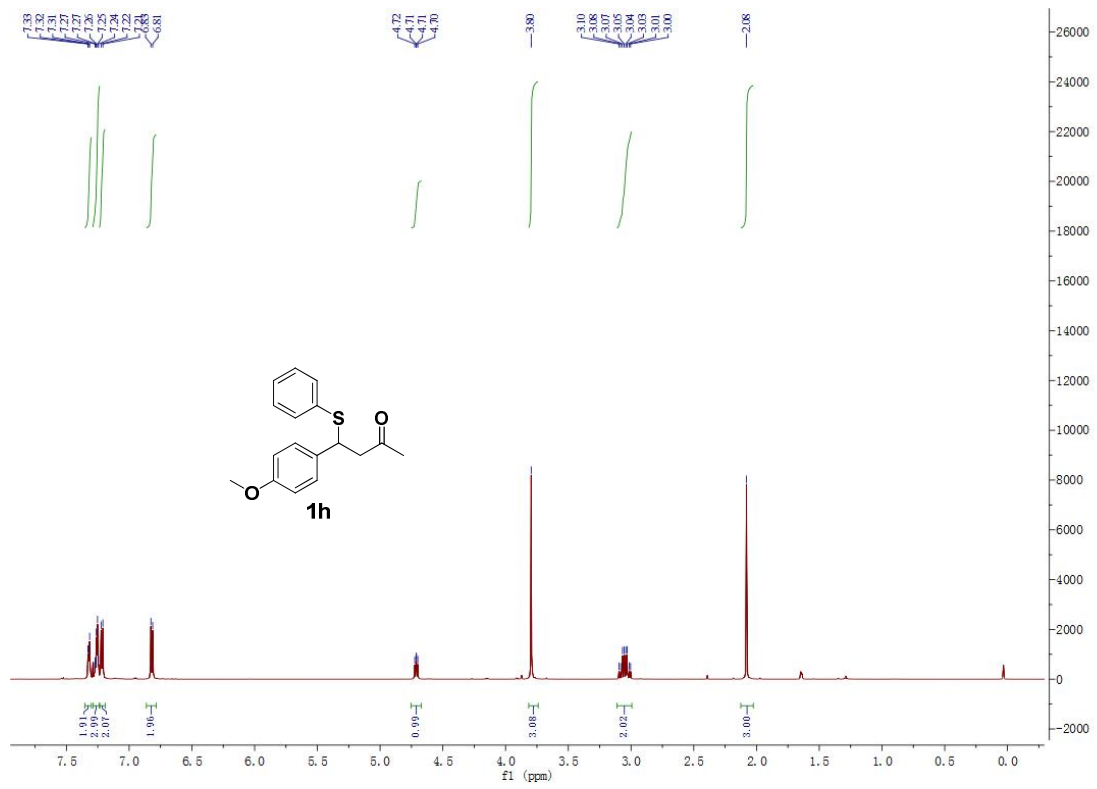


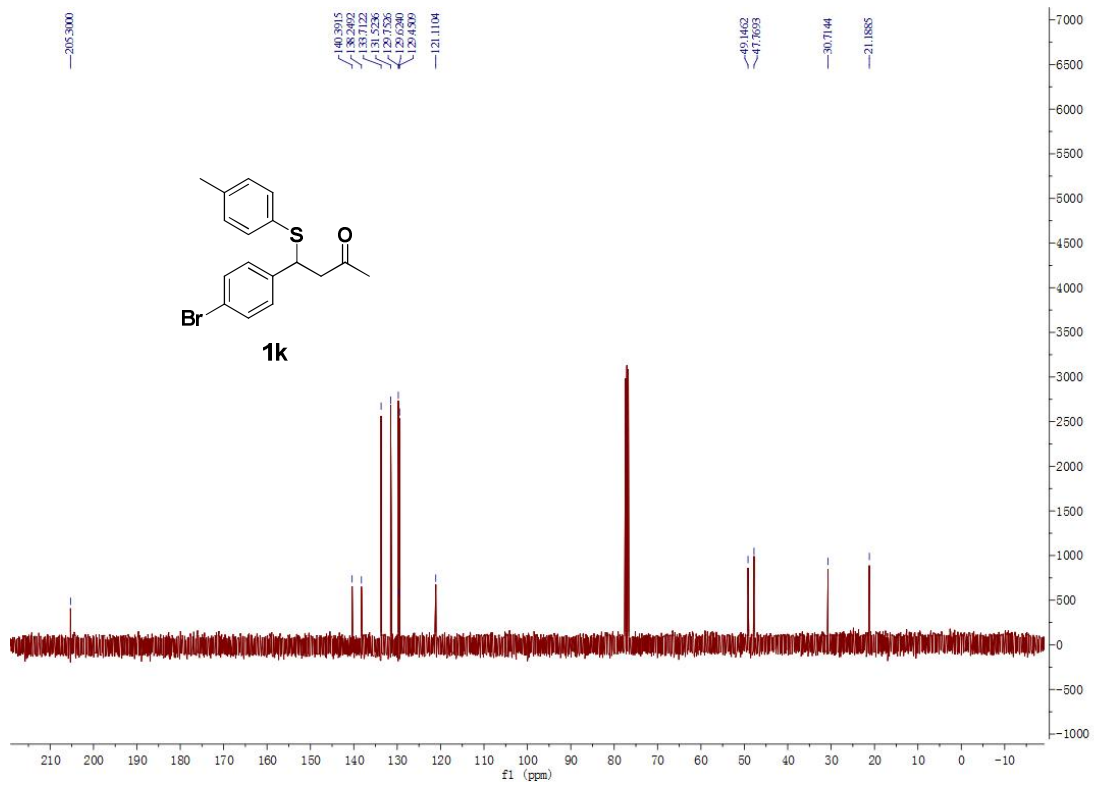
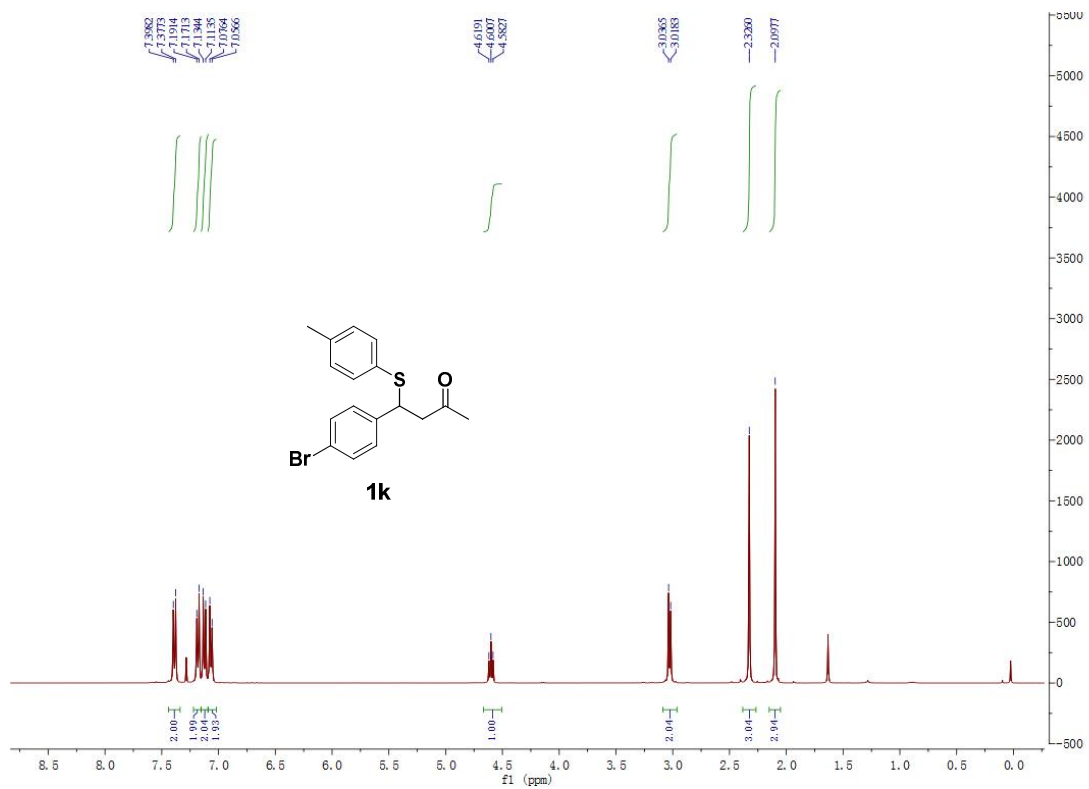


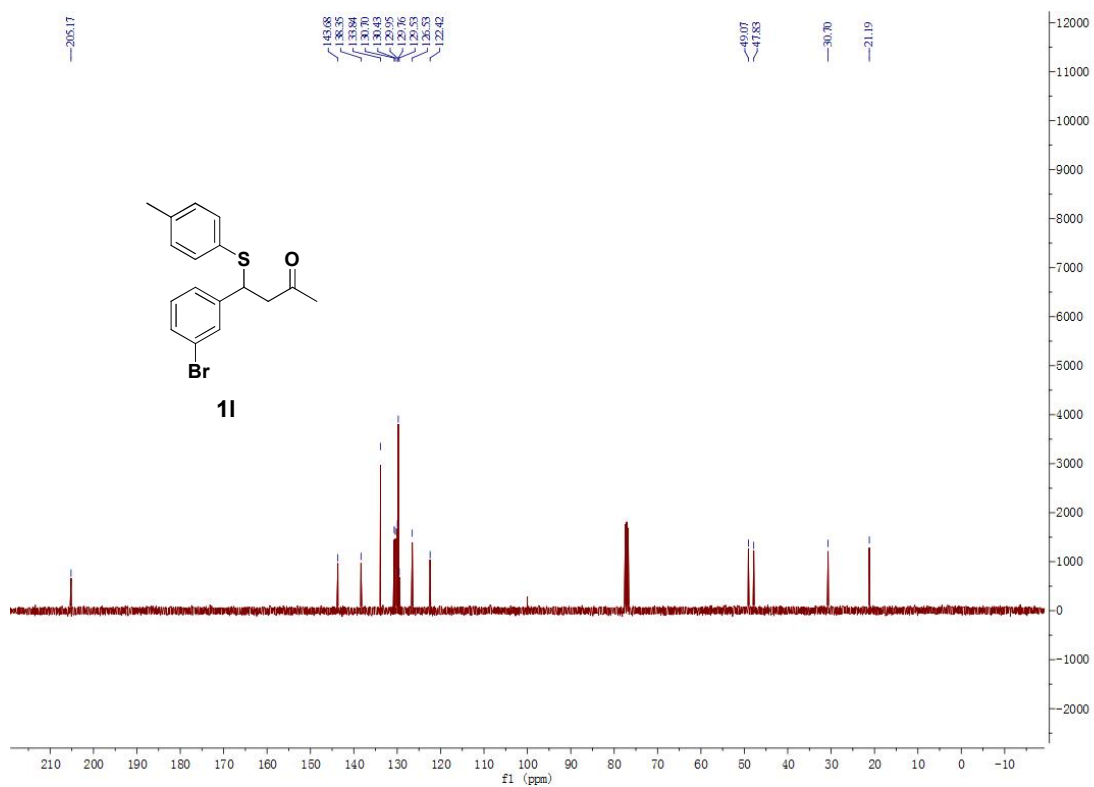
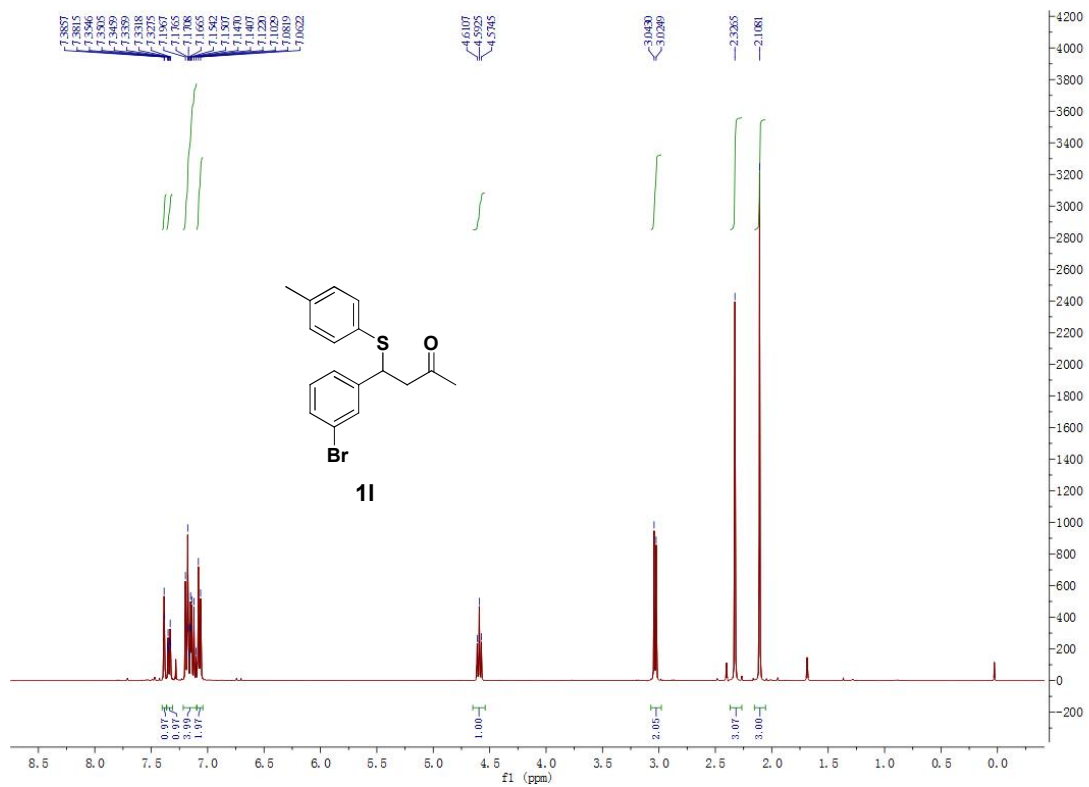


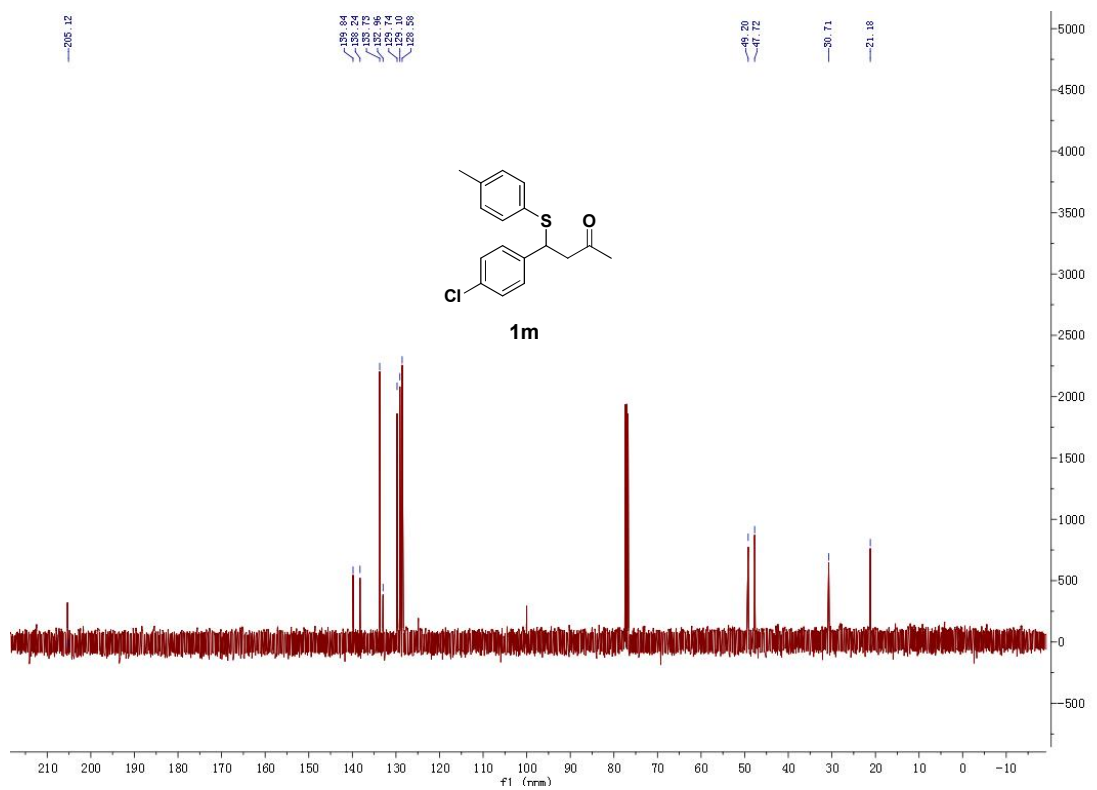
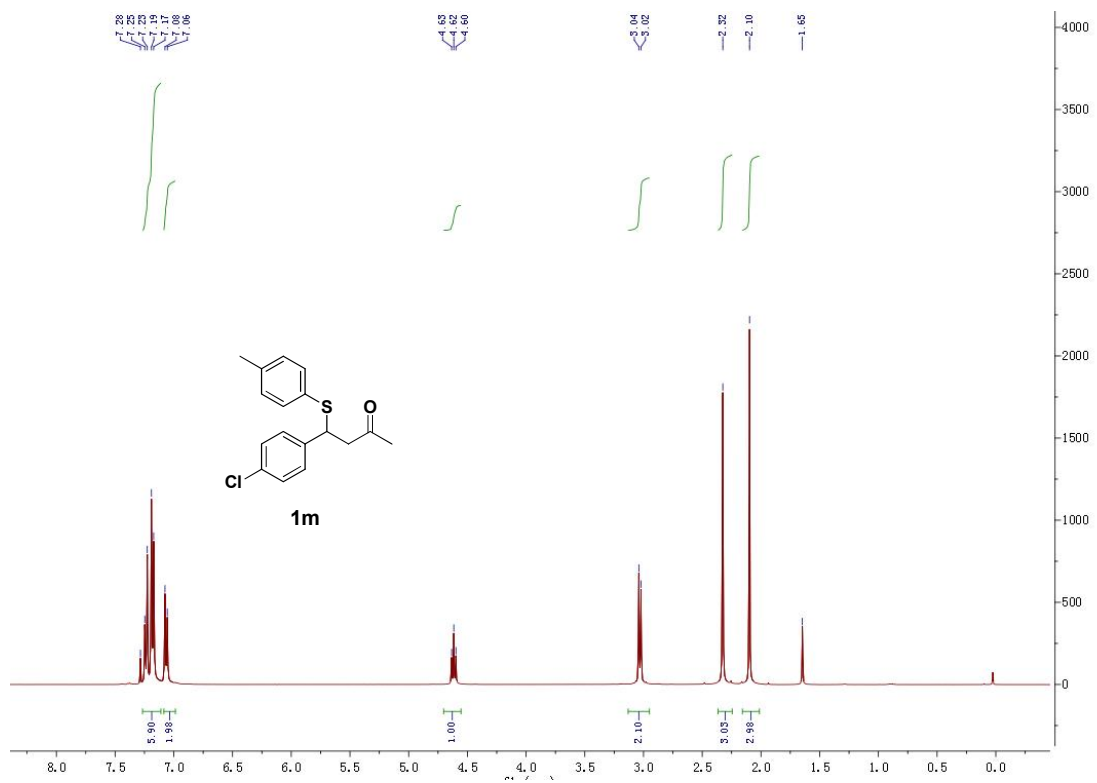


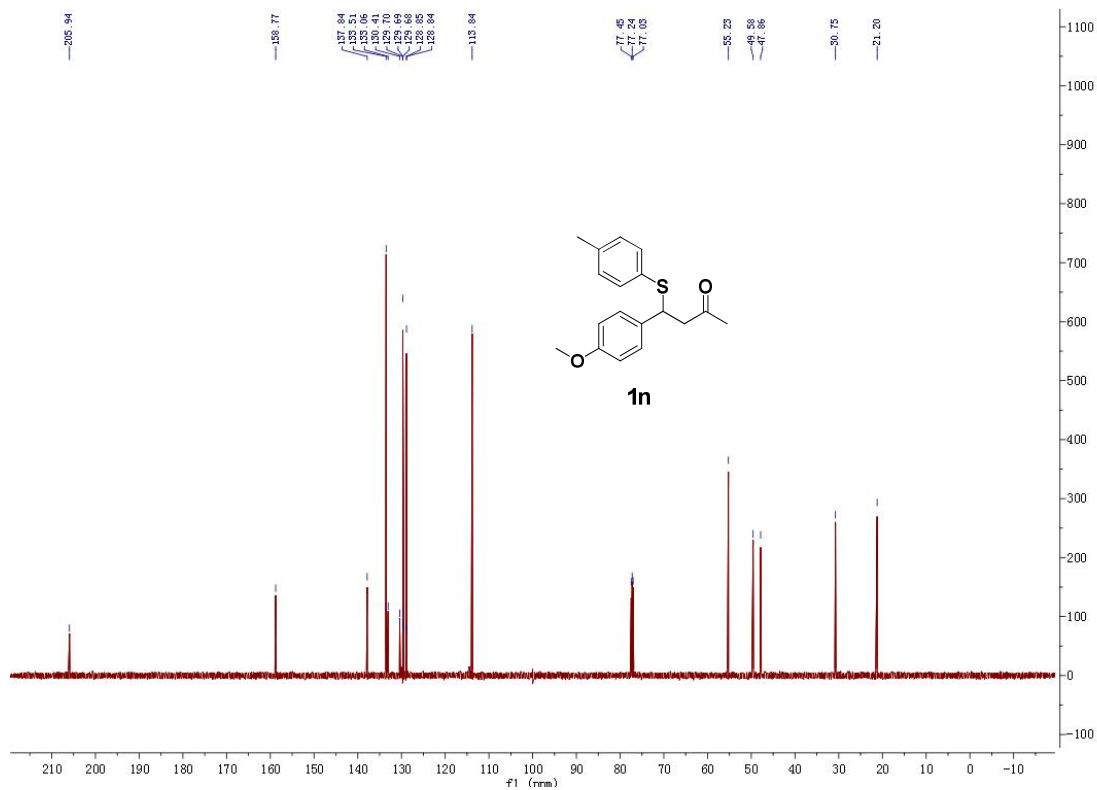
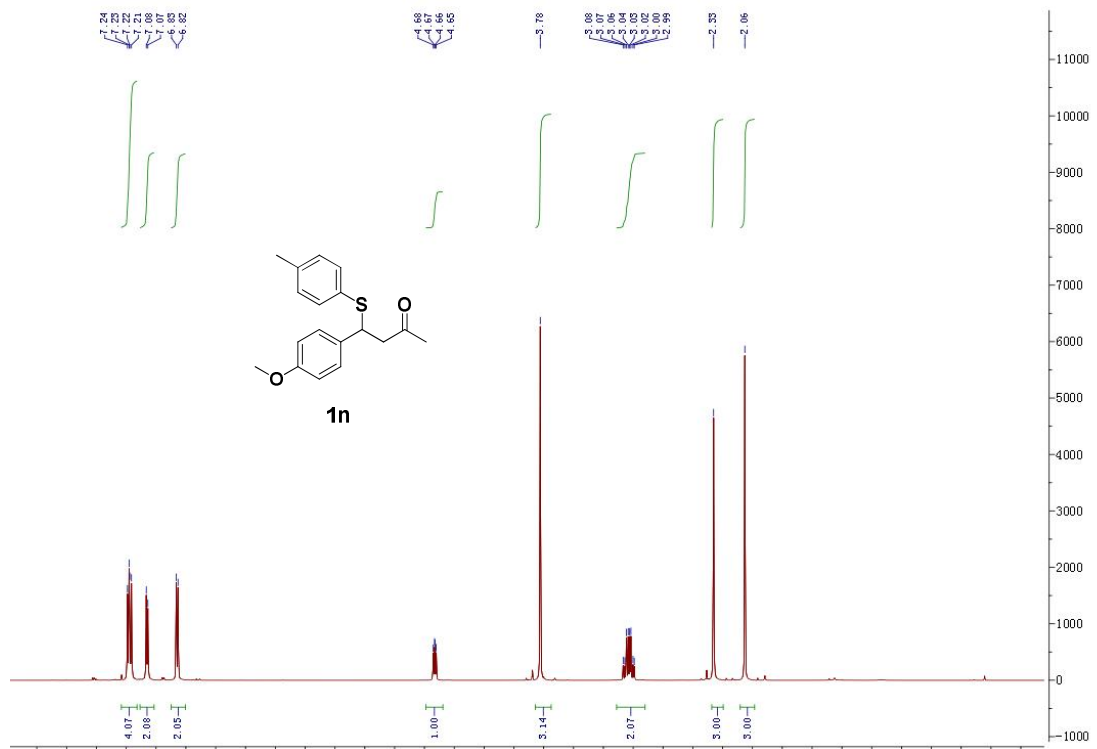


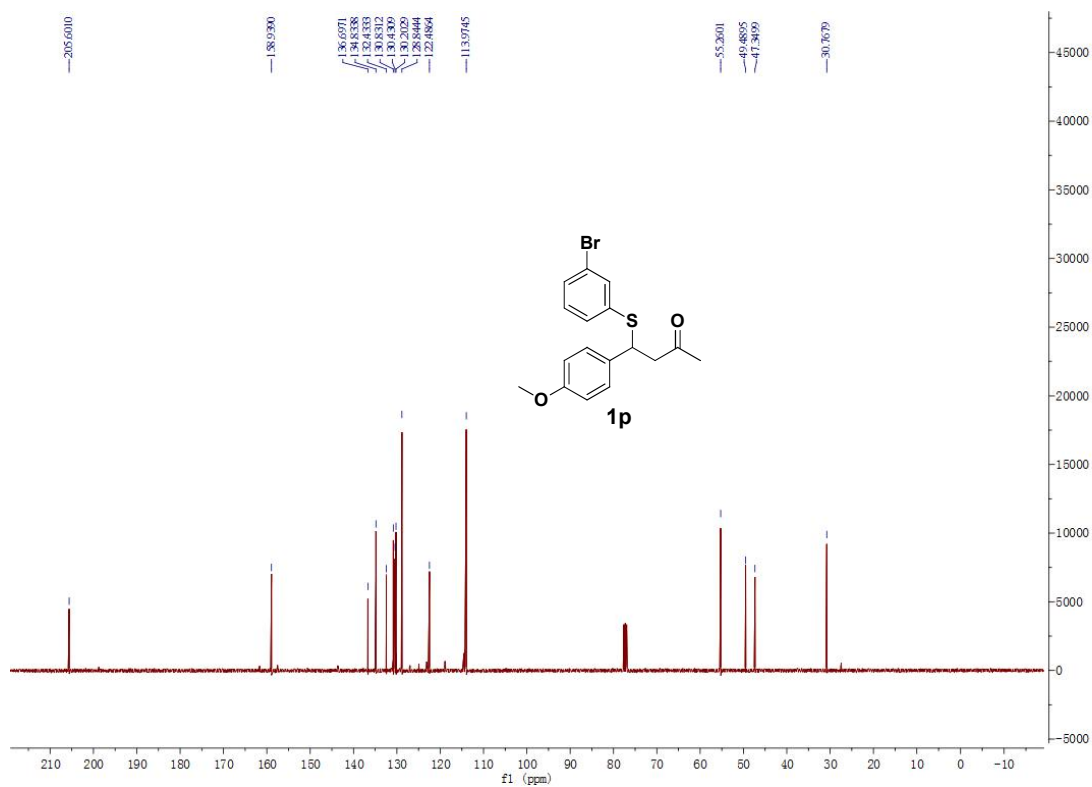
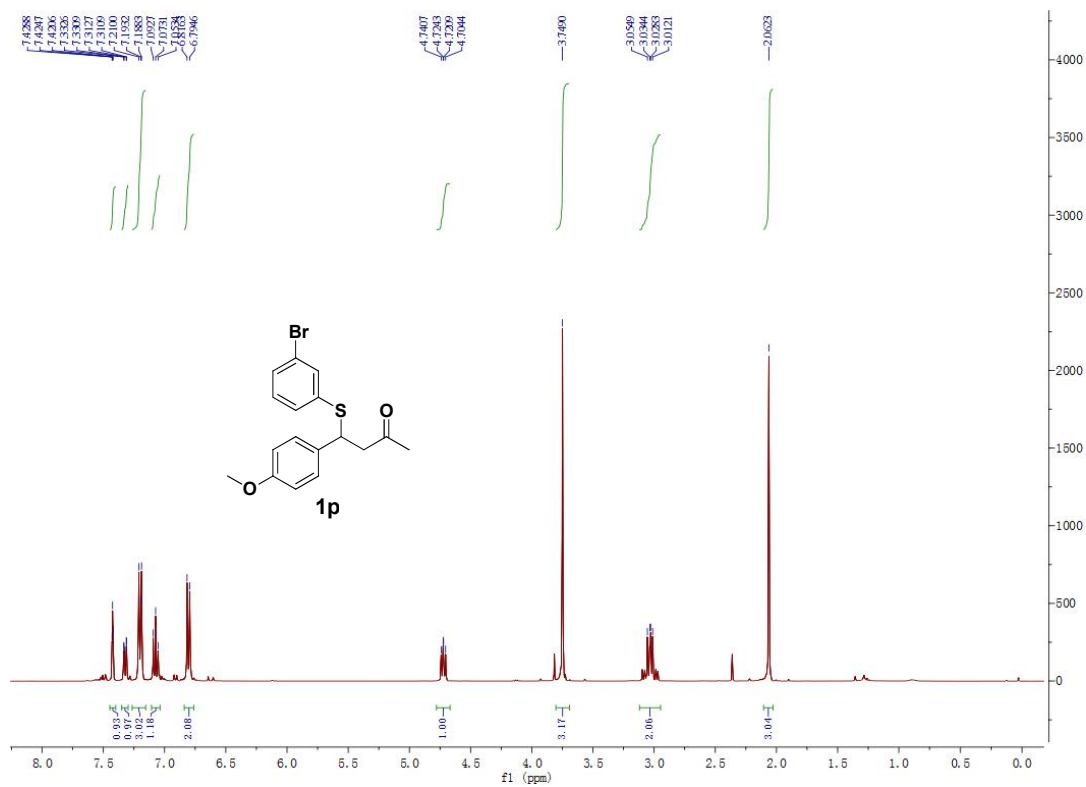


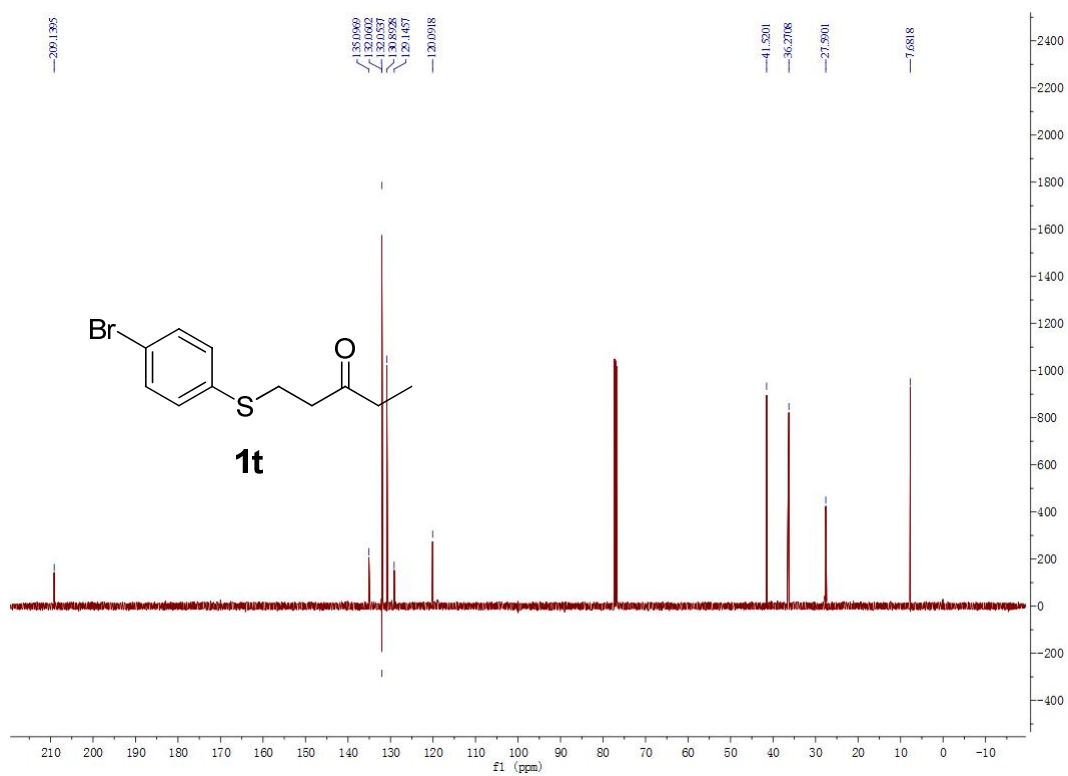
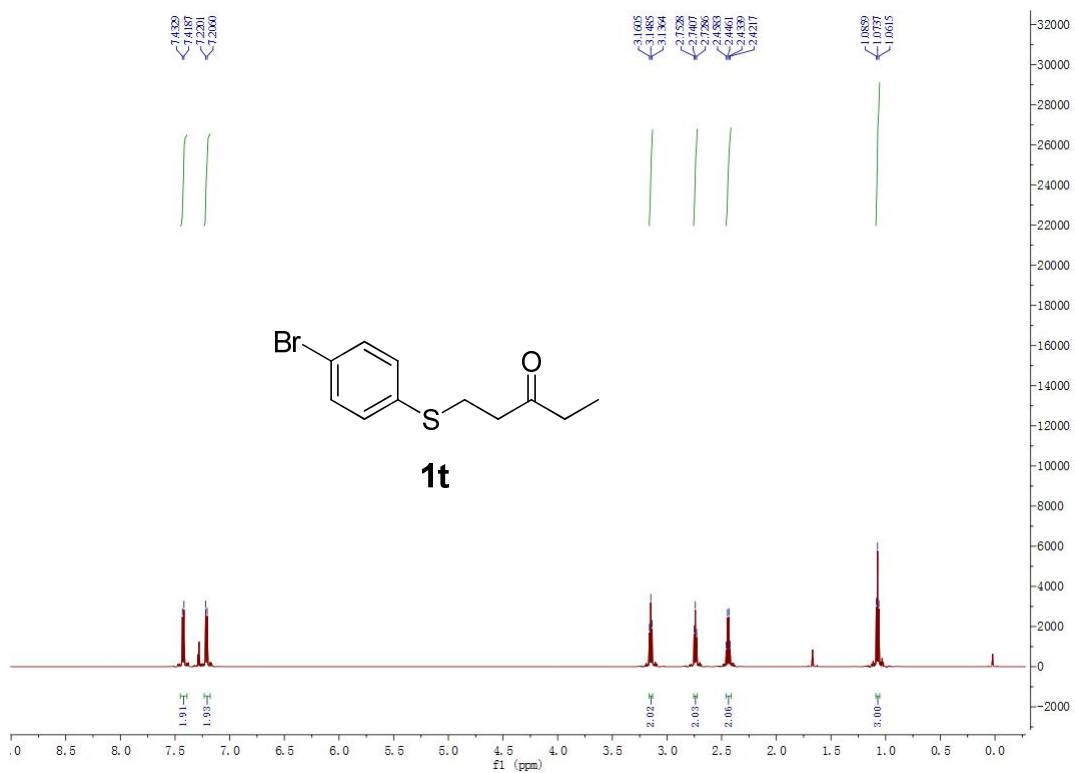


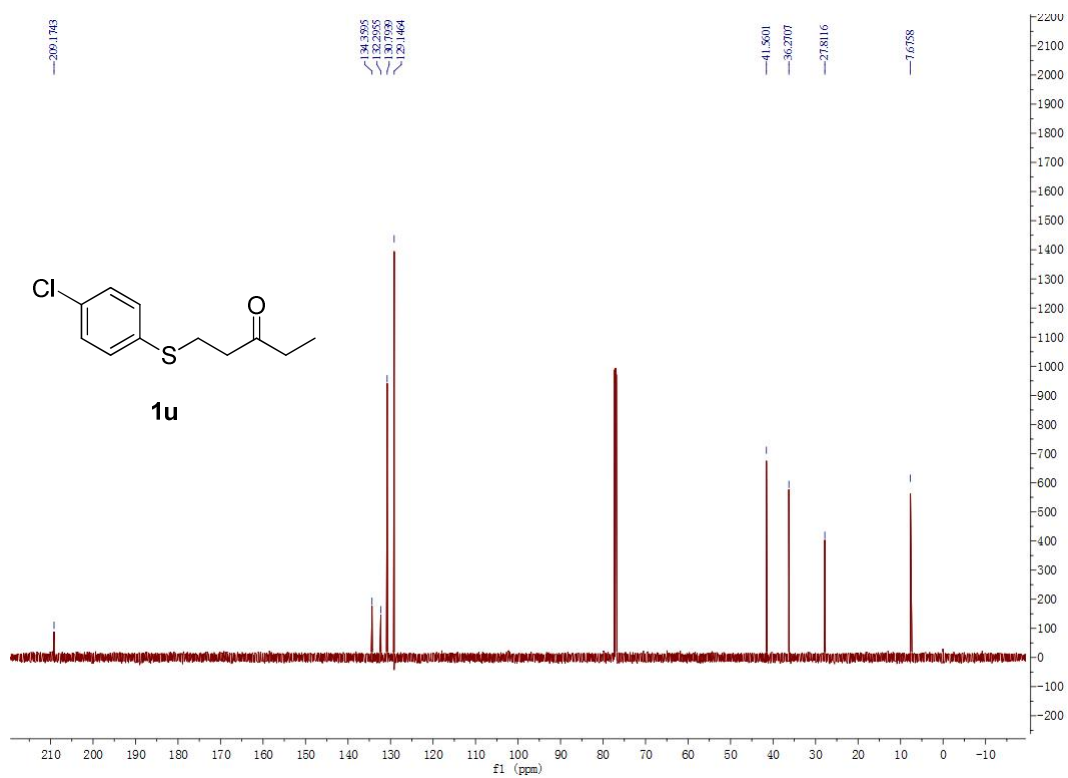
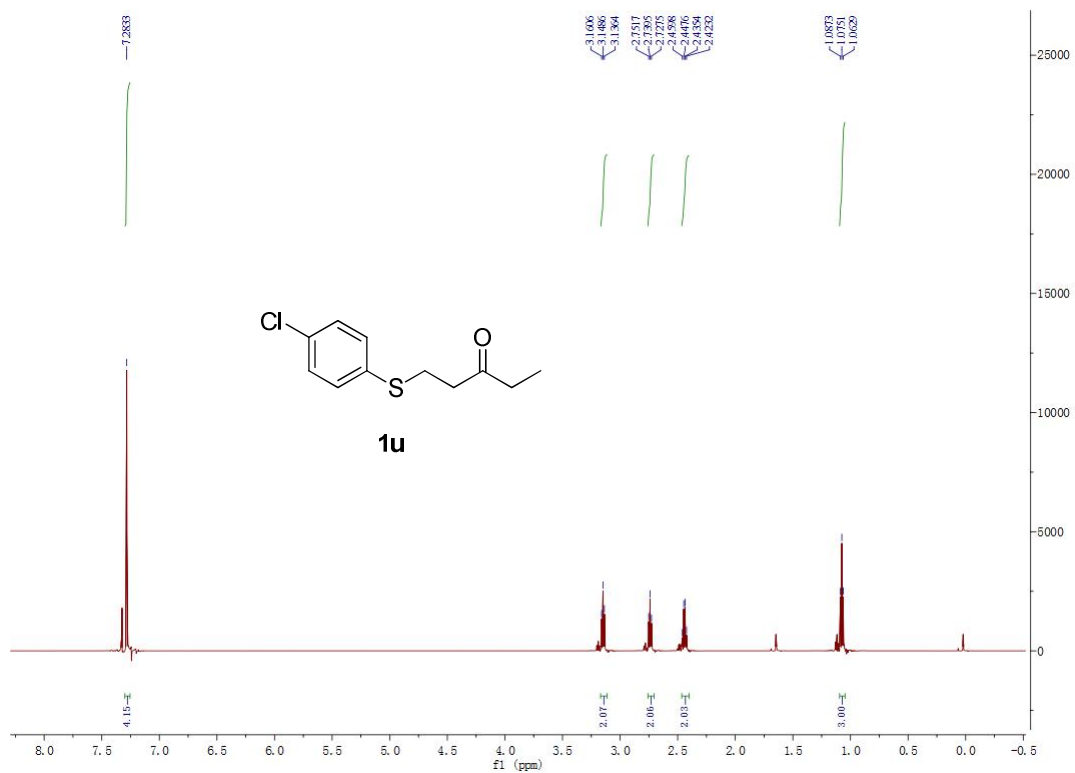


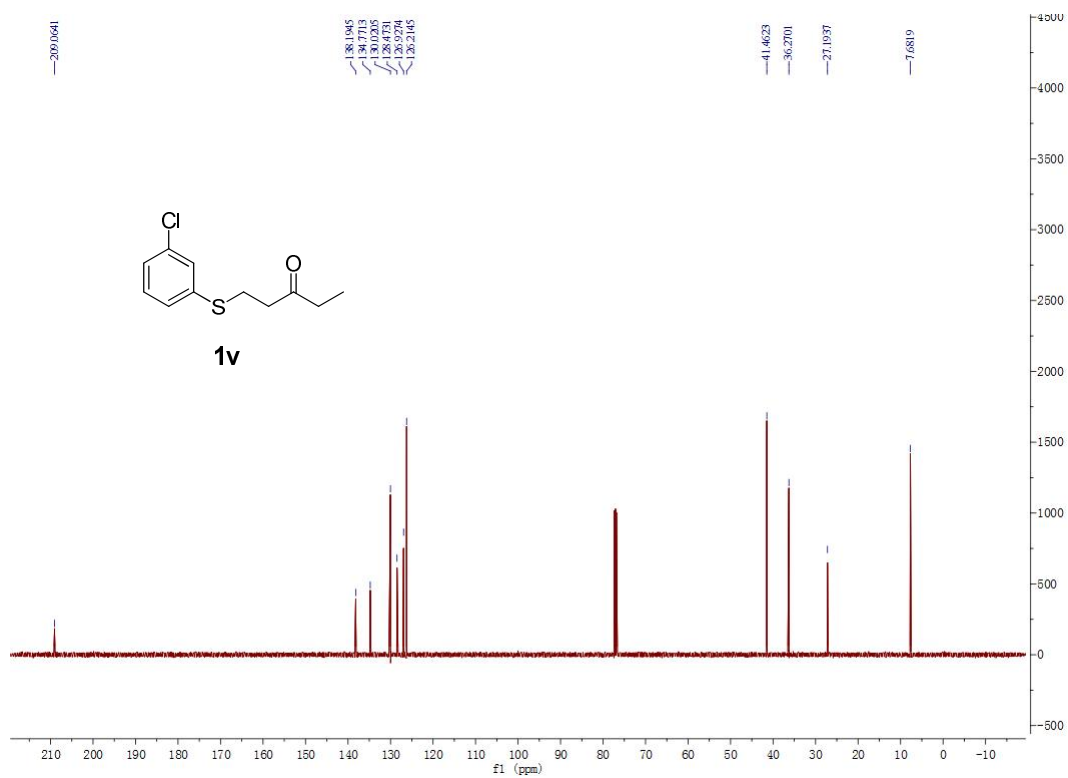
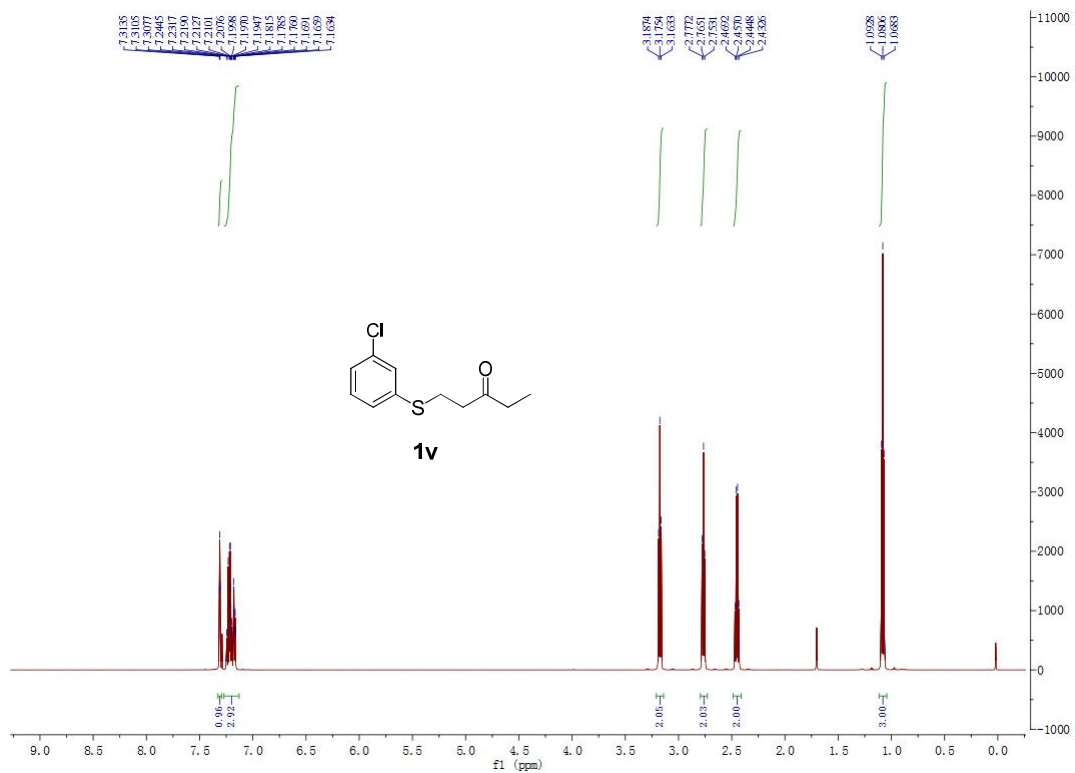


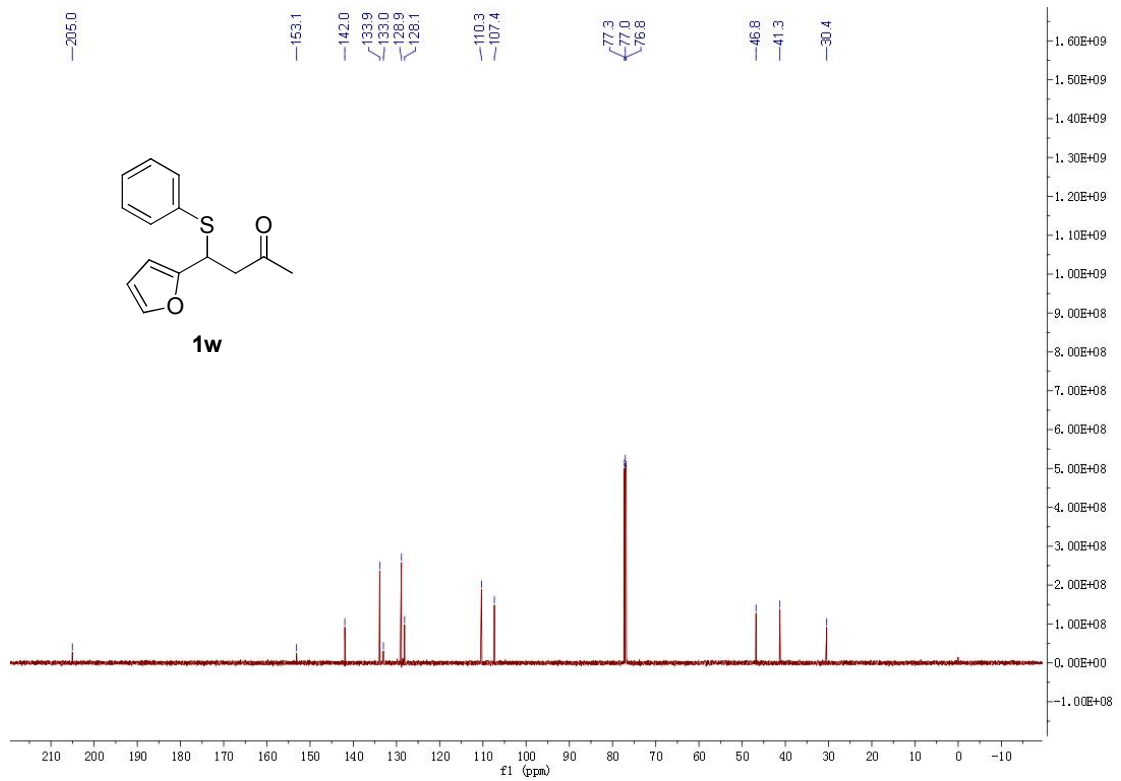
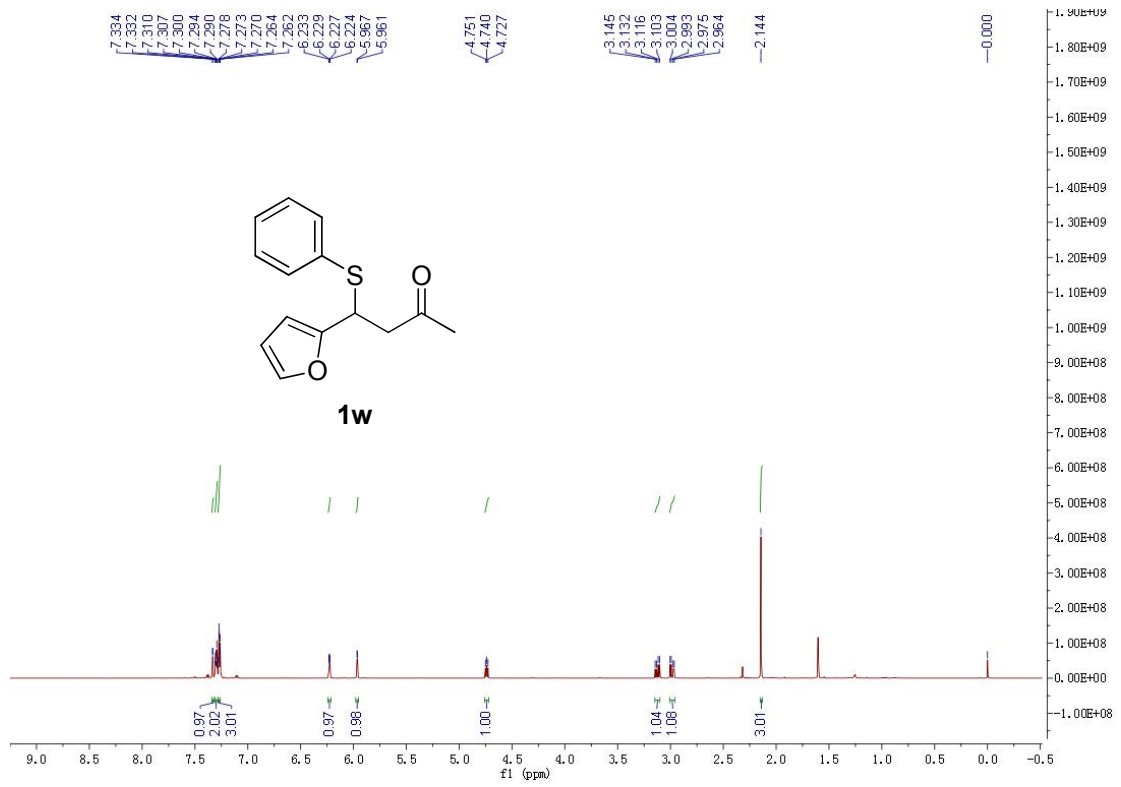




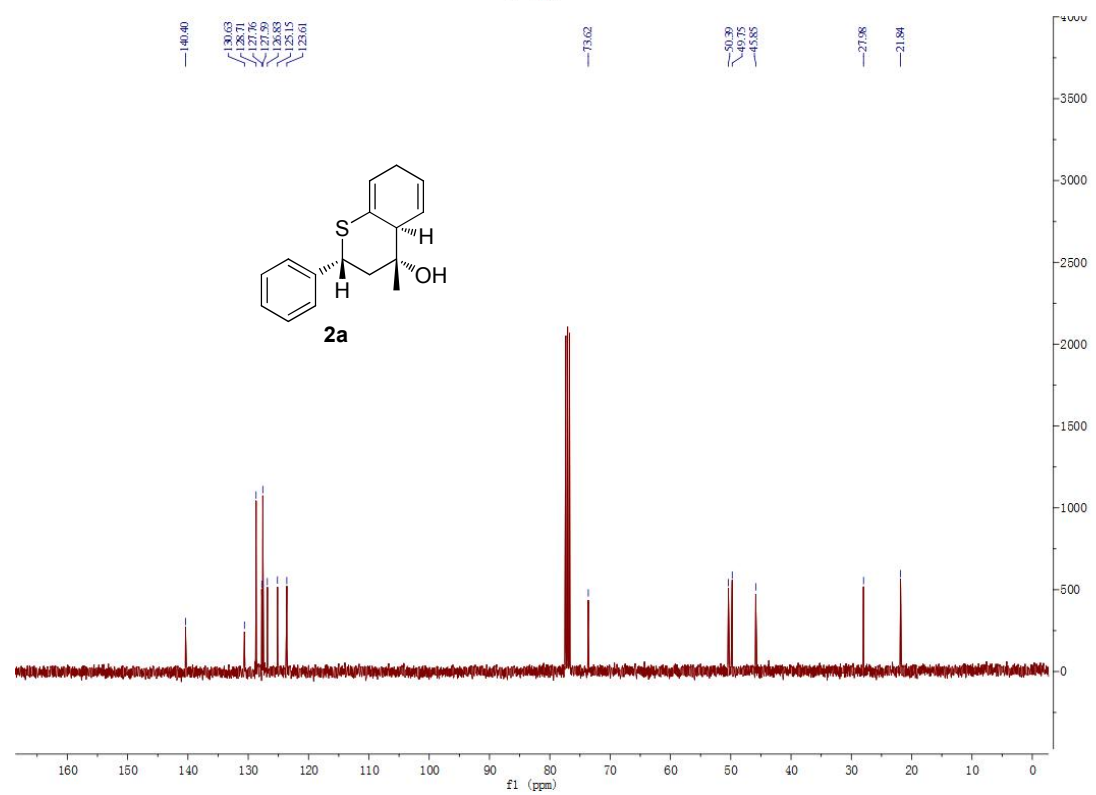
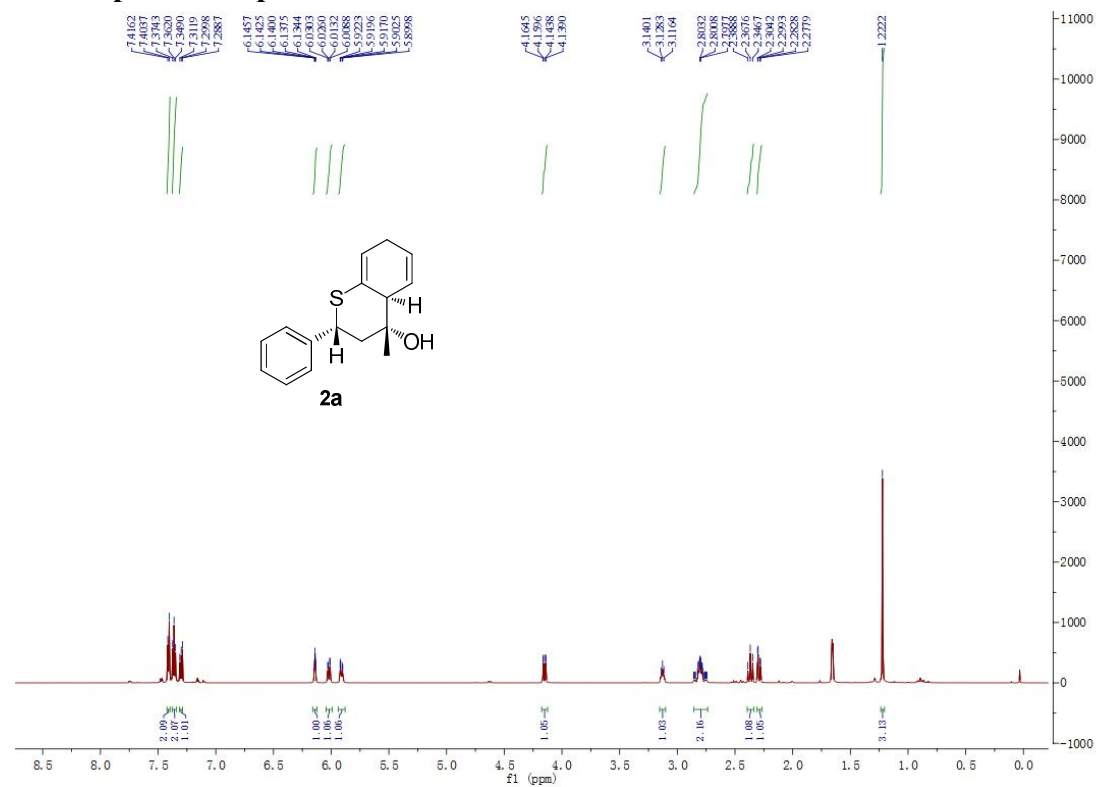


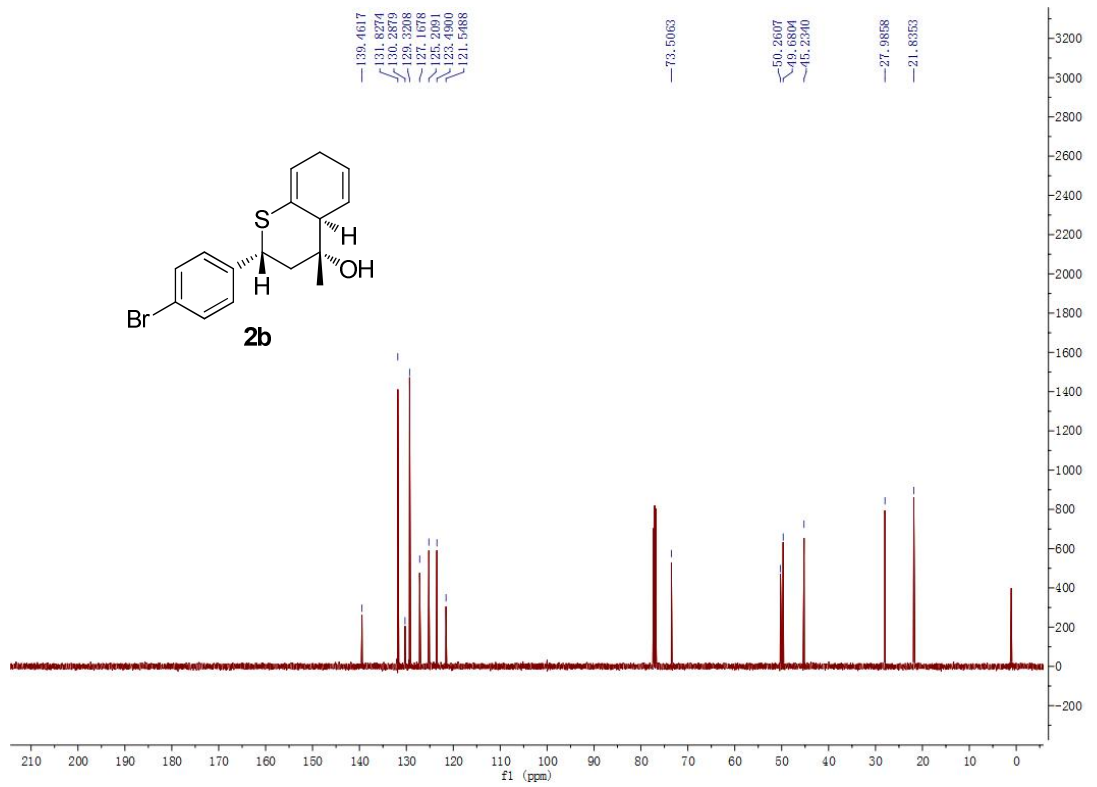
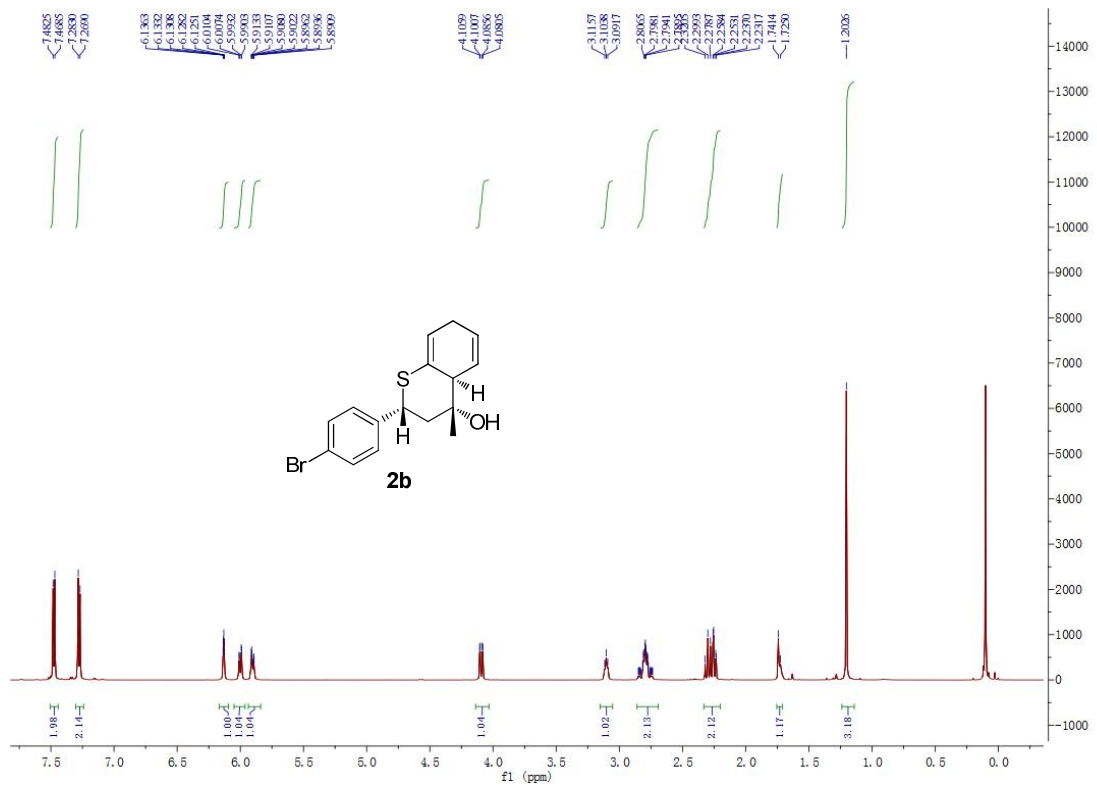


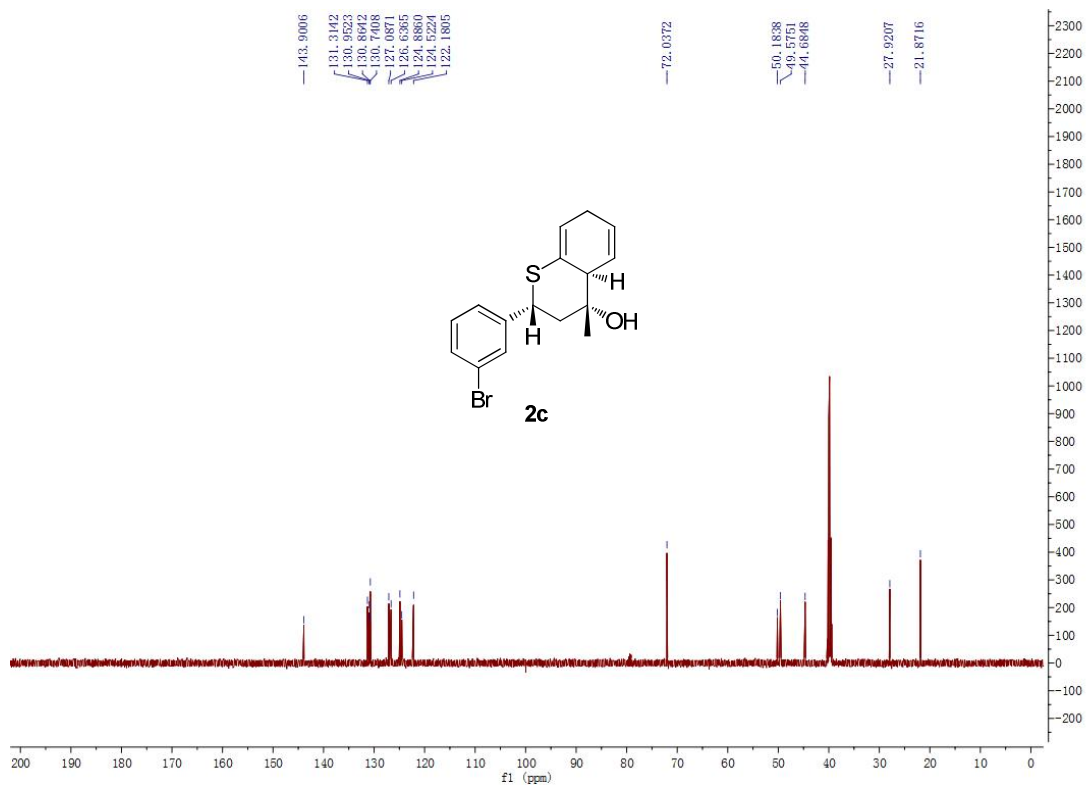
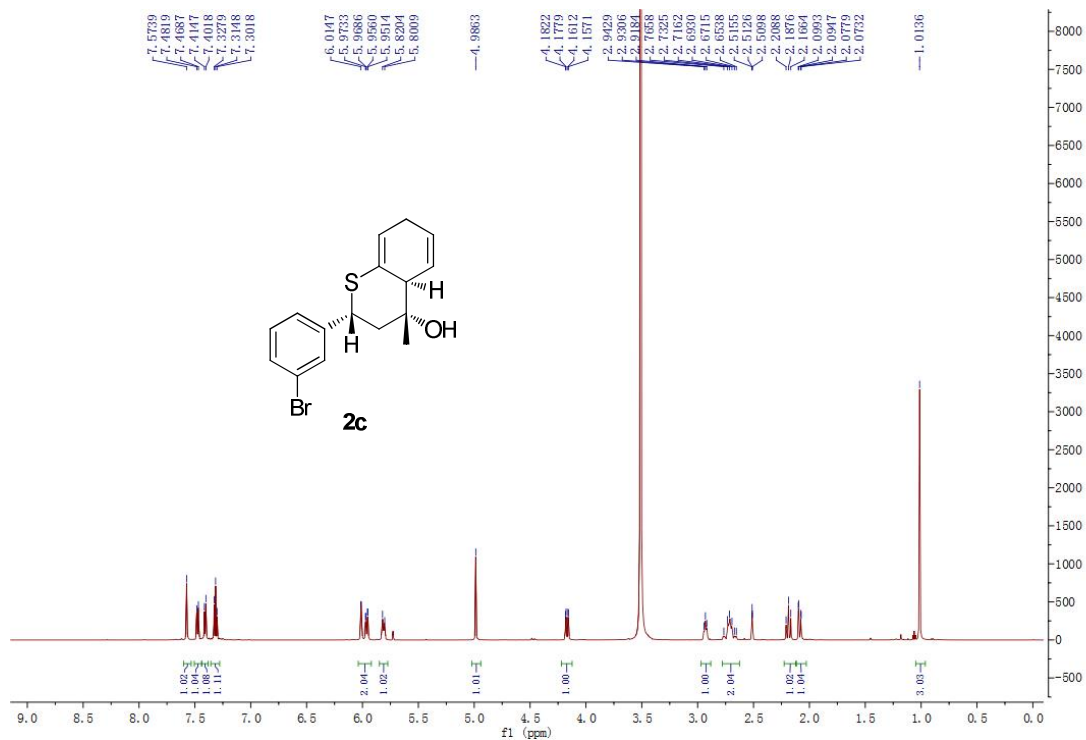


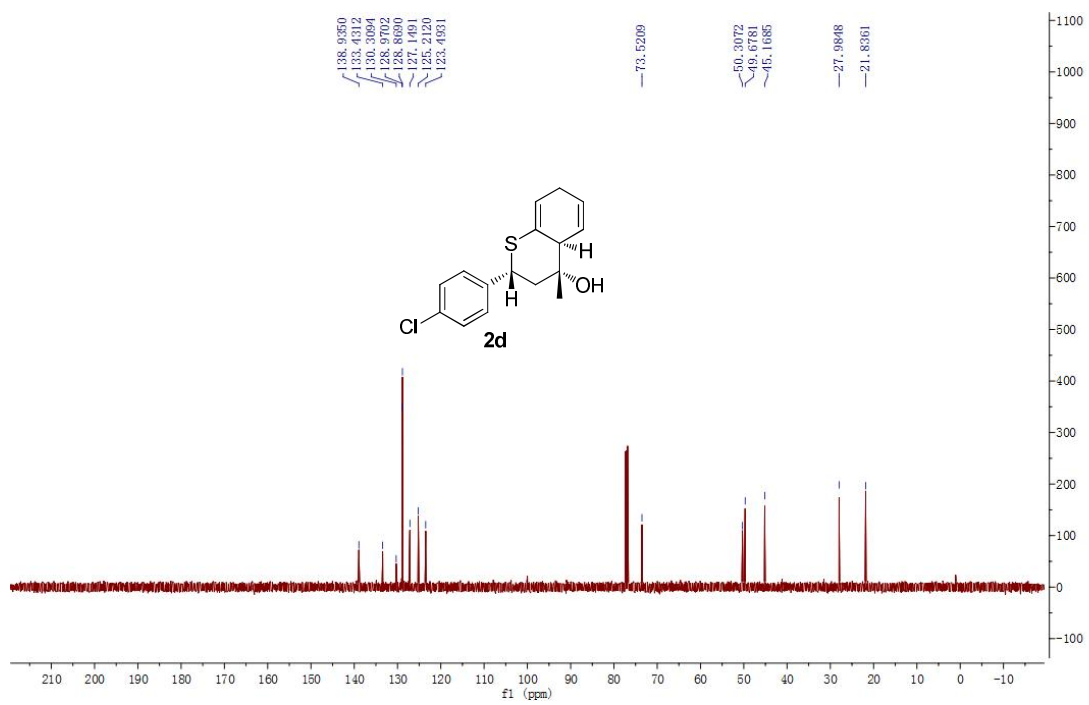
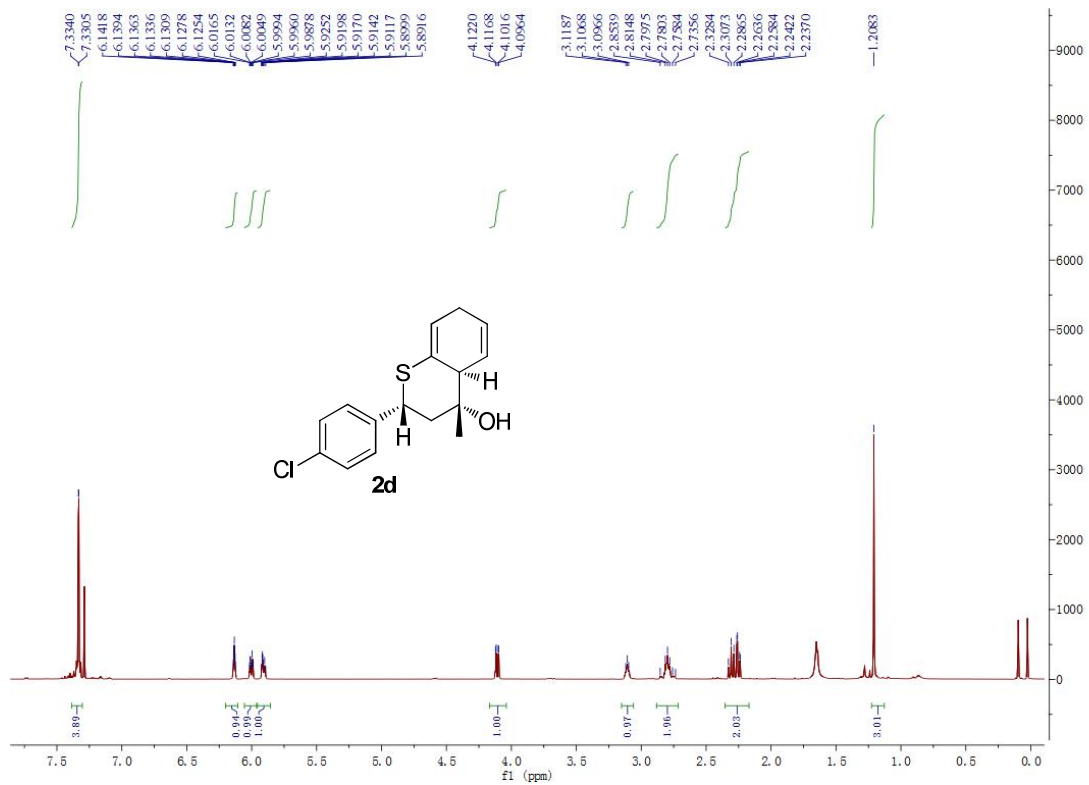


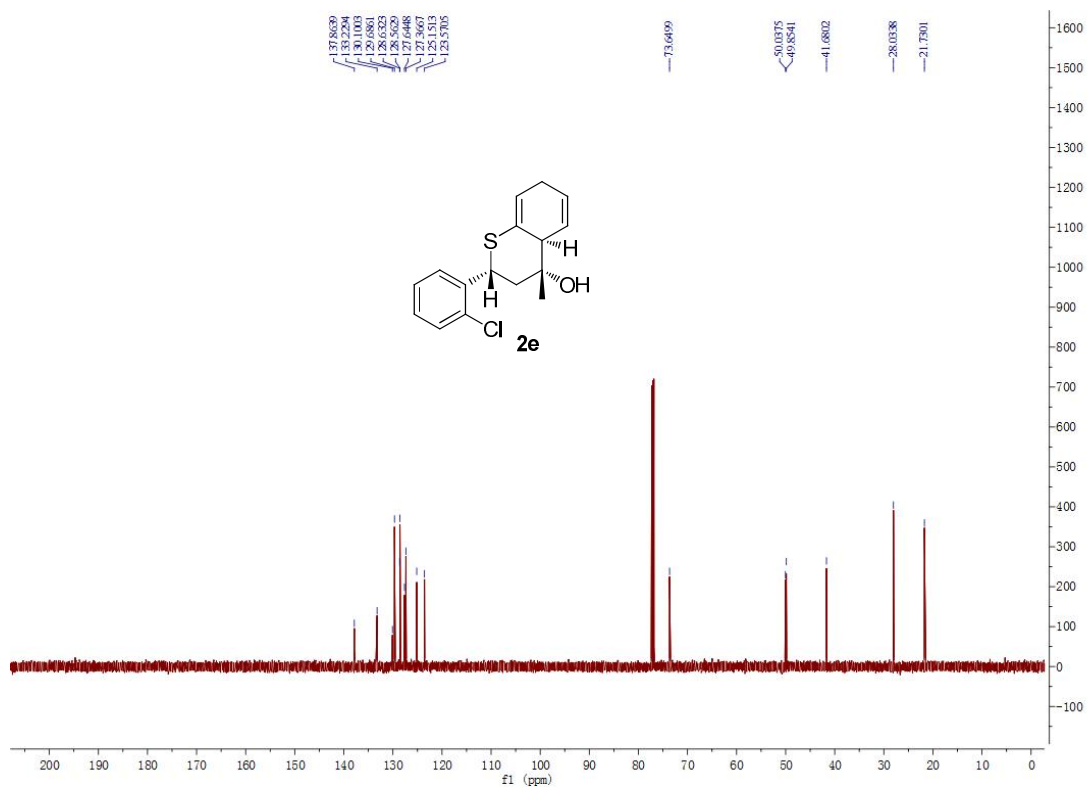
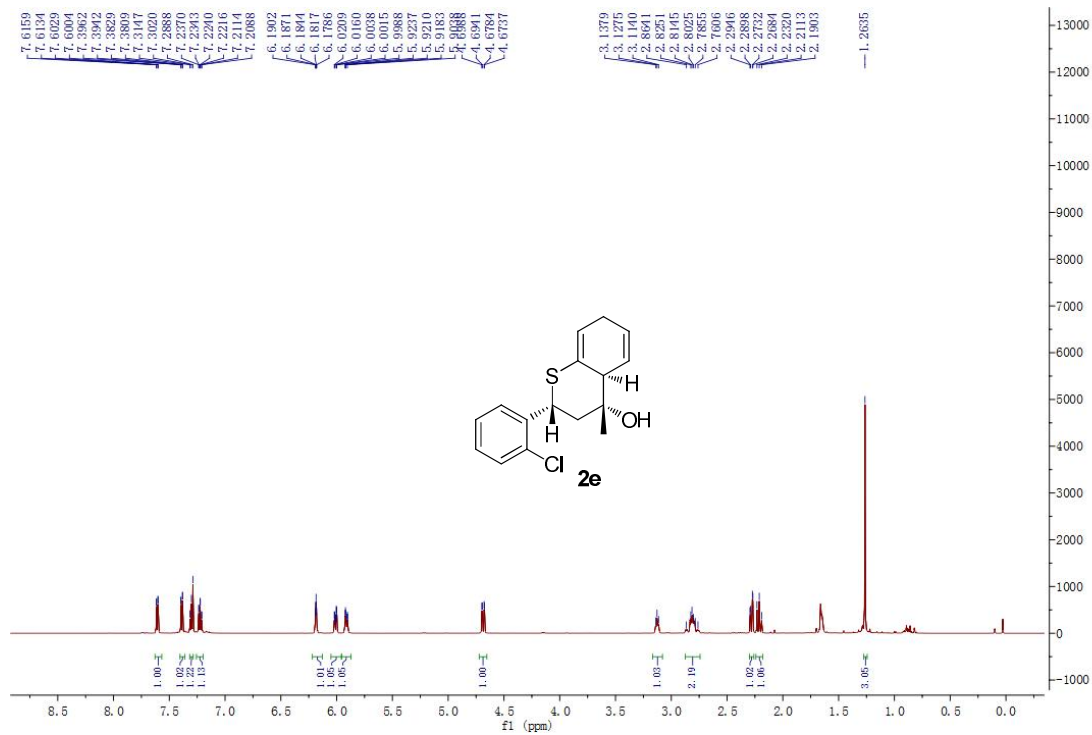
NMR Spectra for products 2

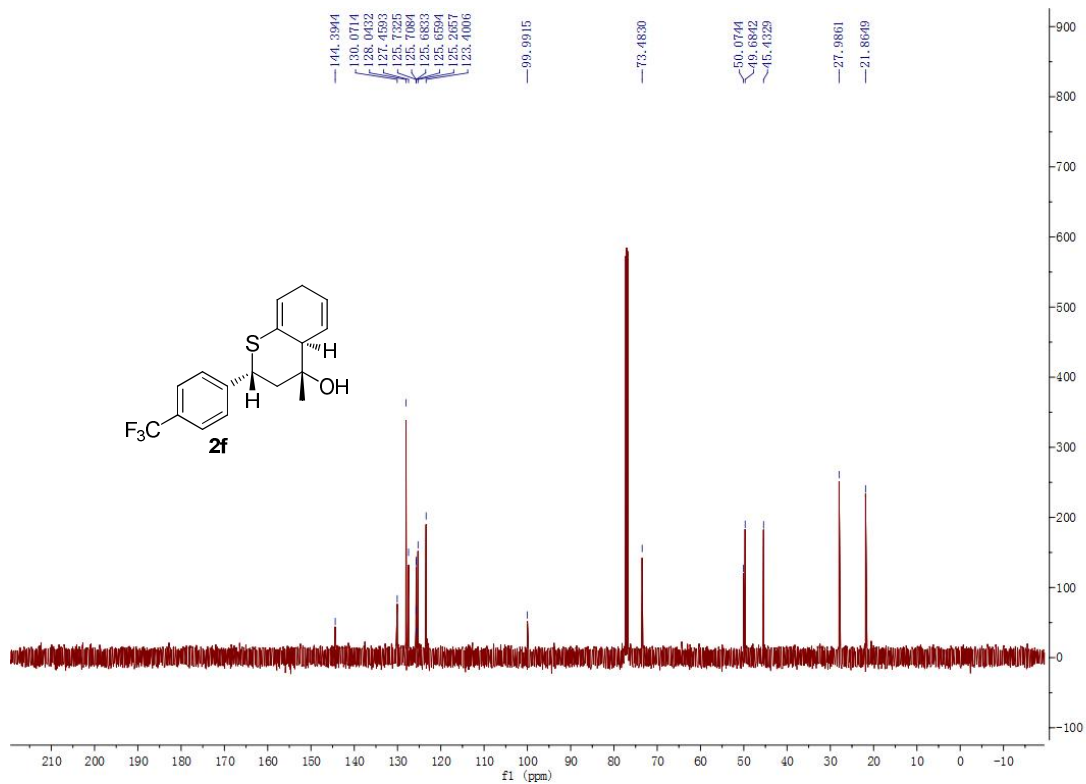
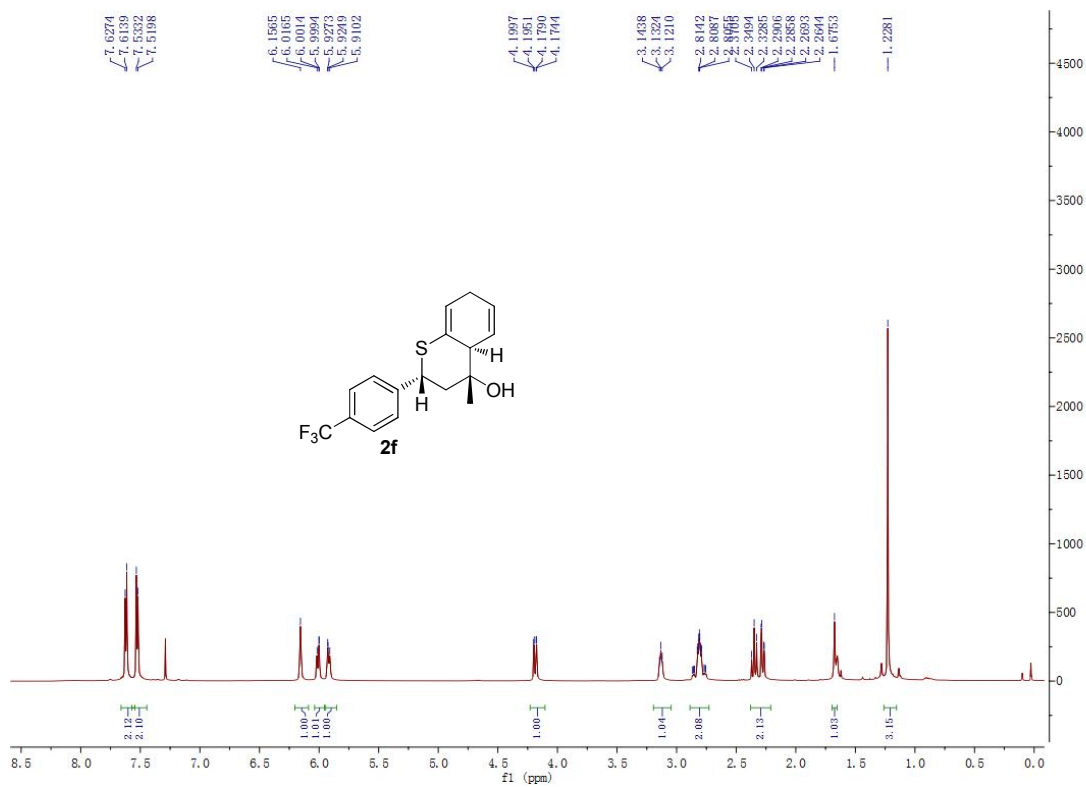




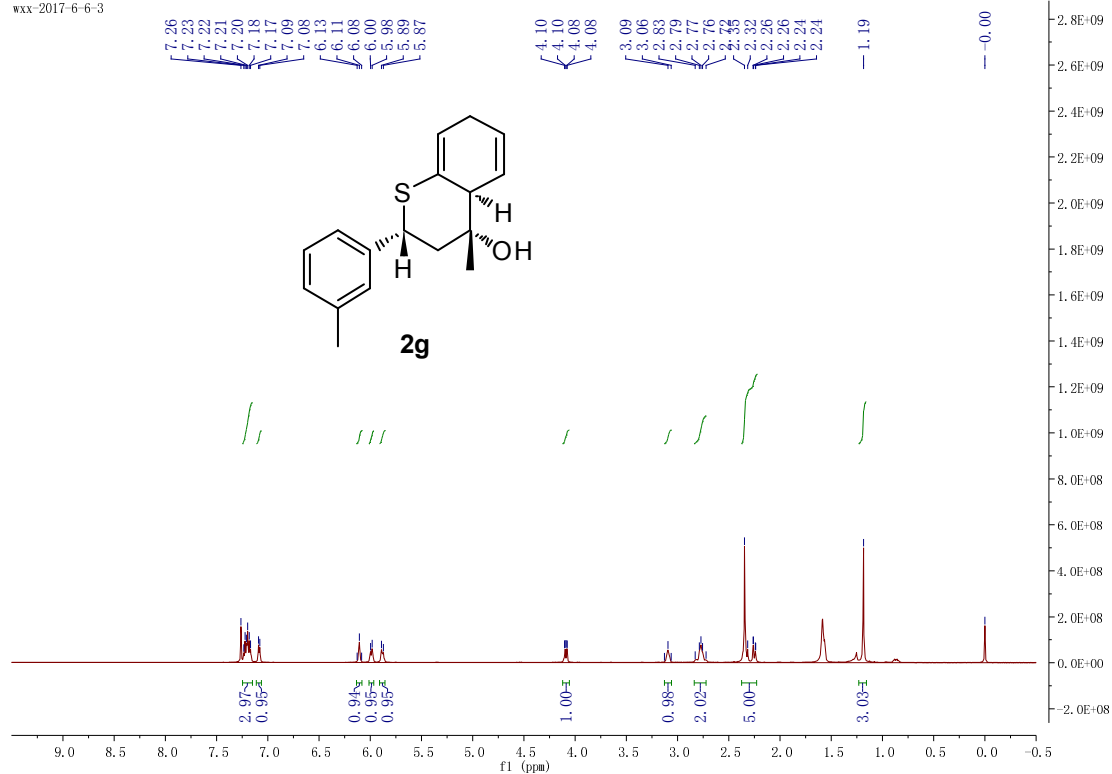




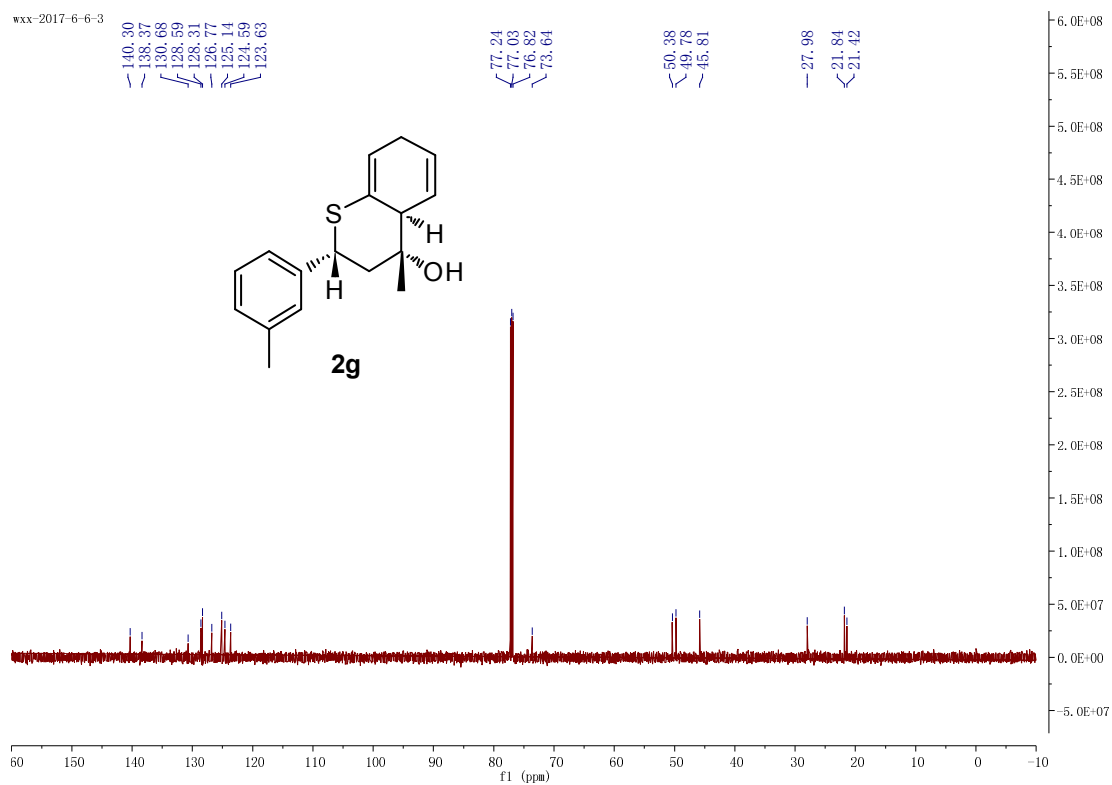


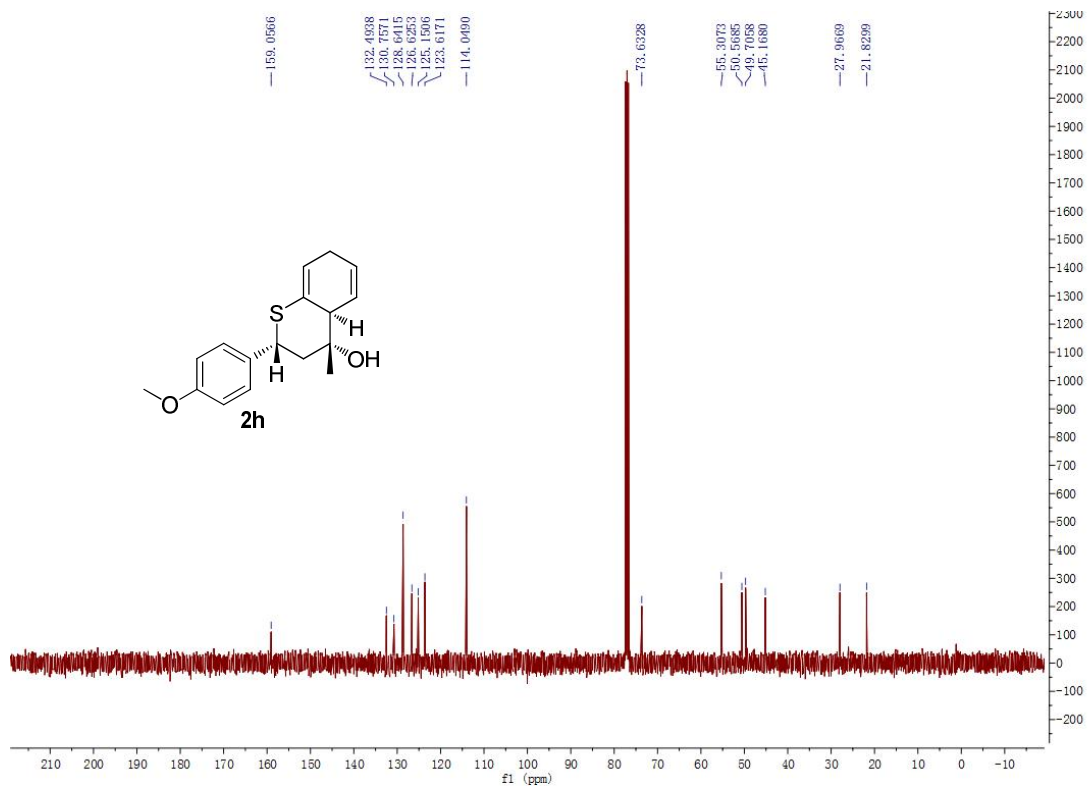
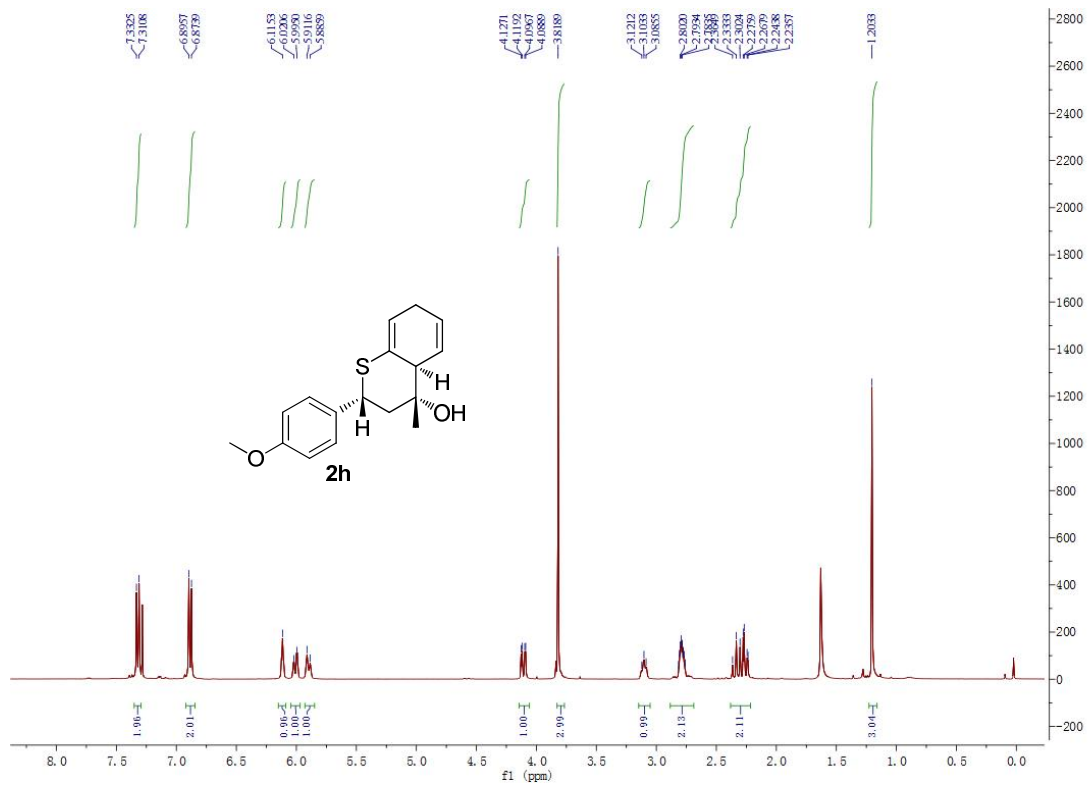


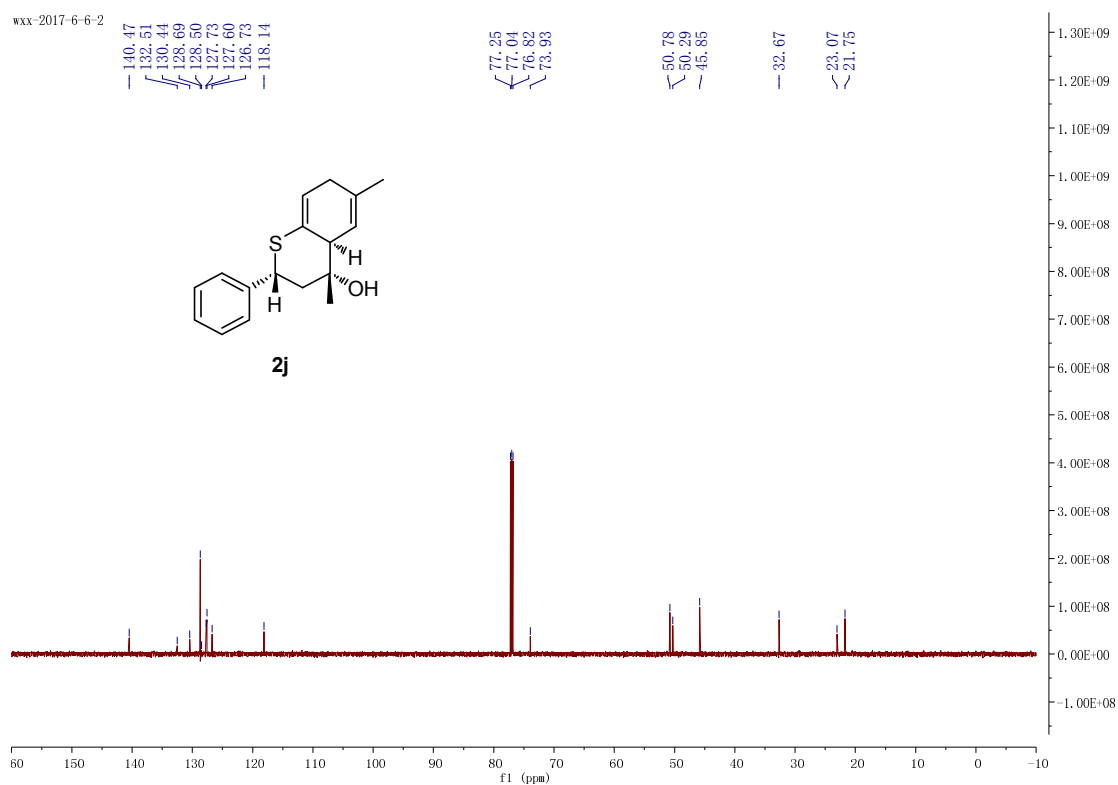
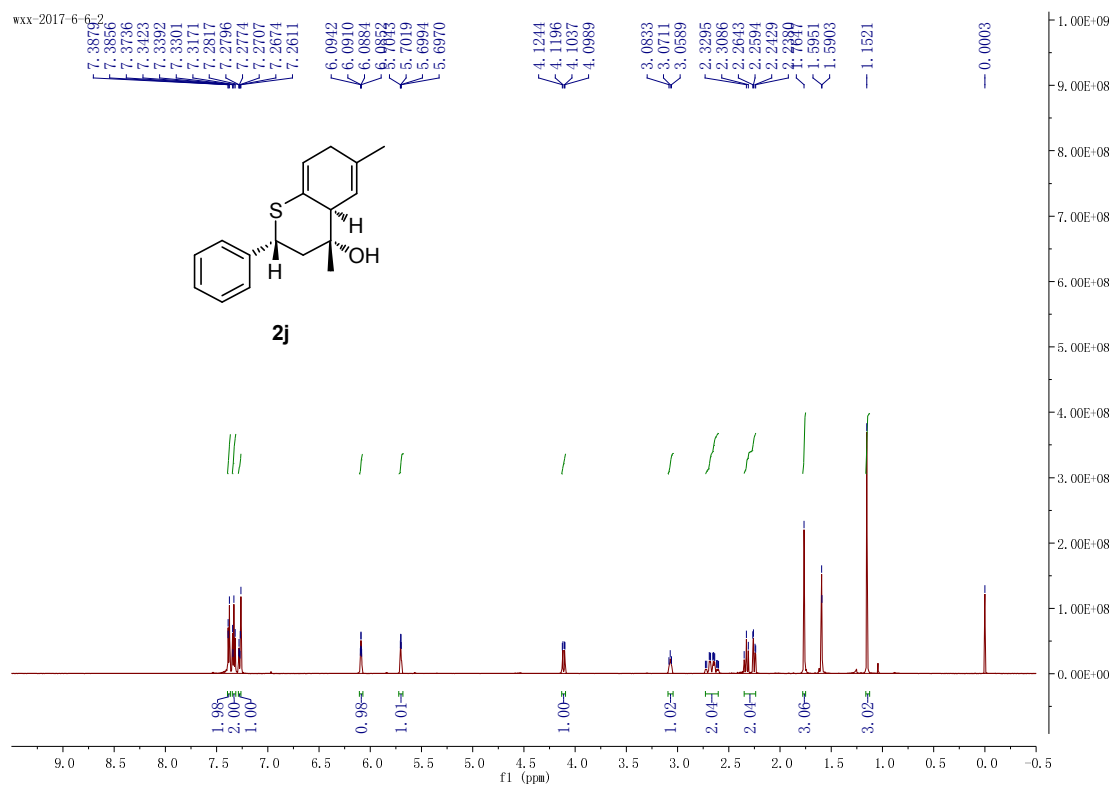
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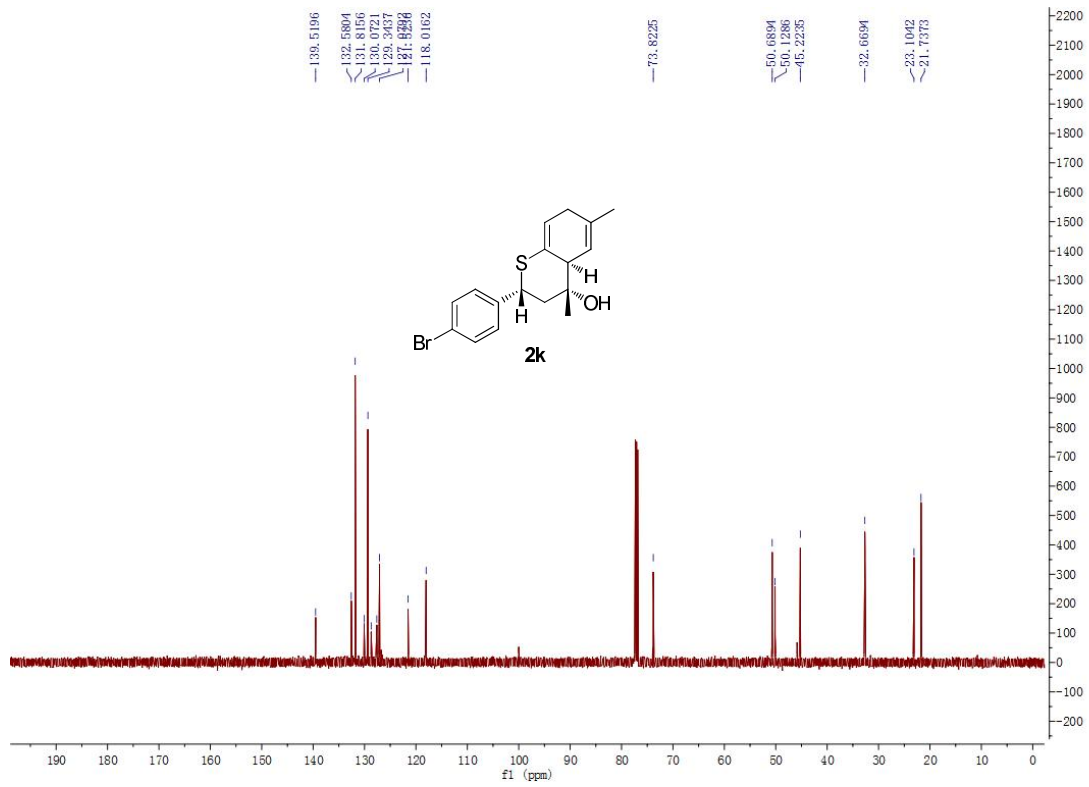
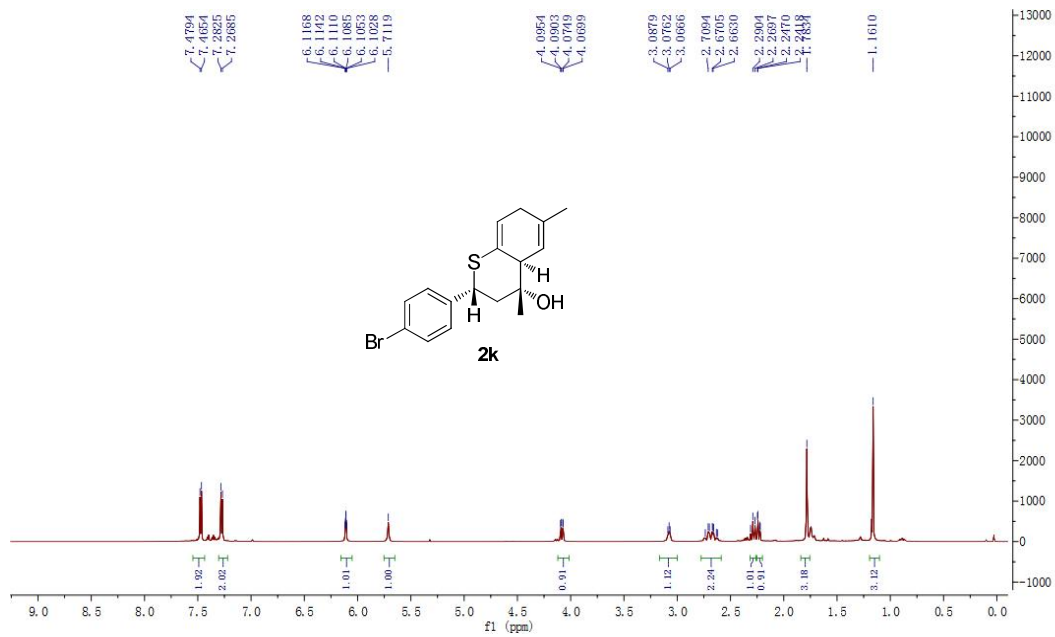


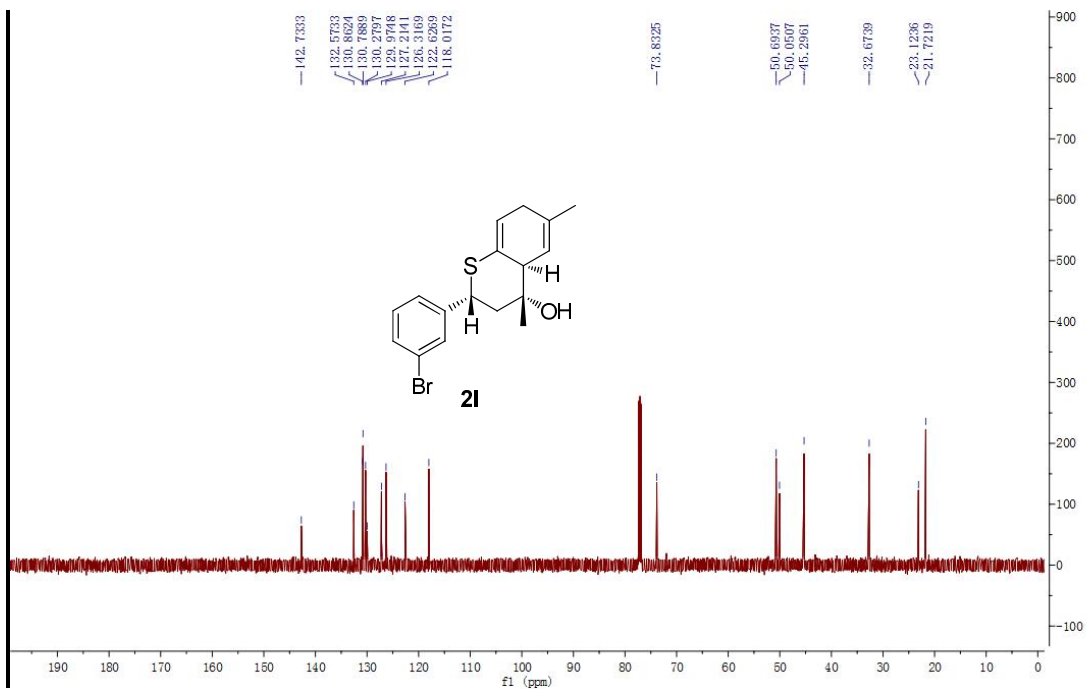
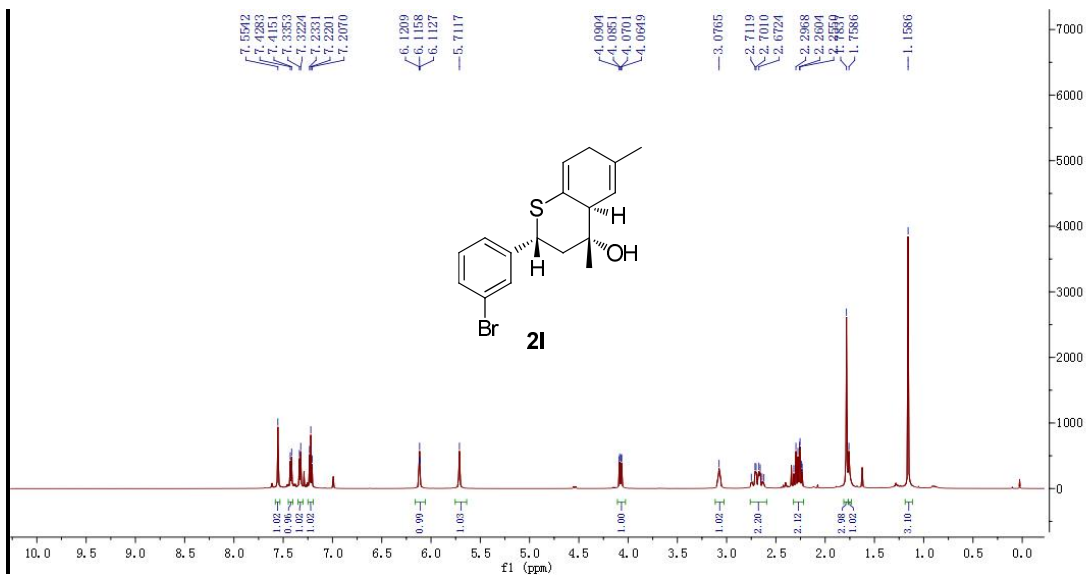
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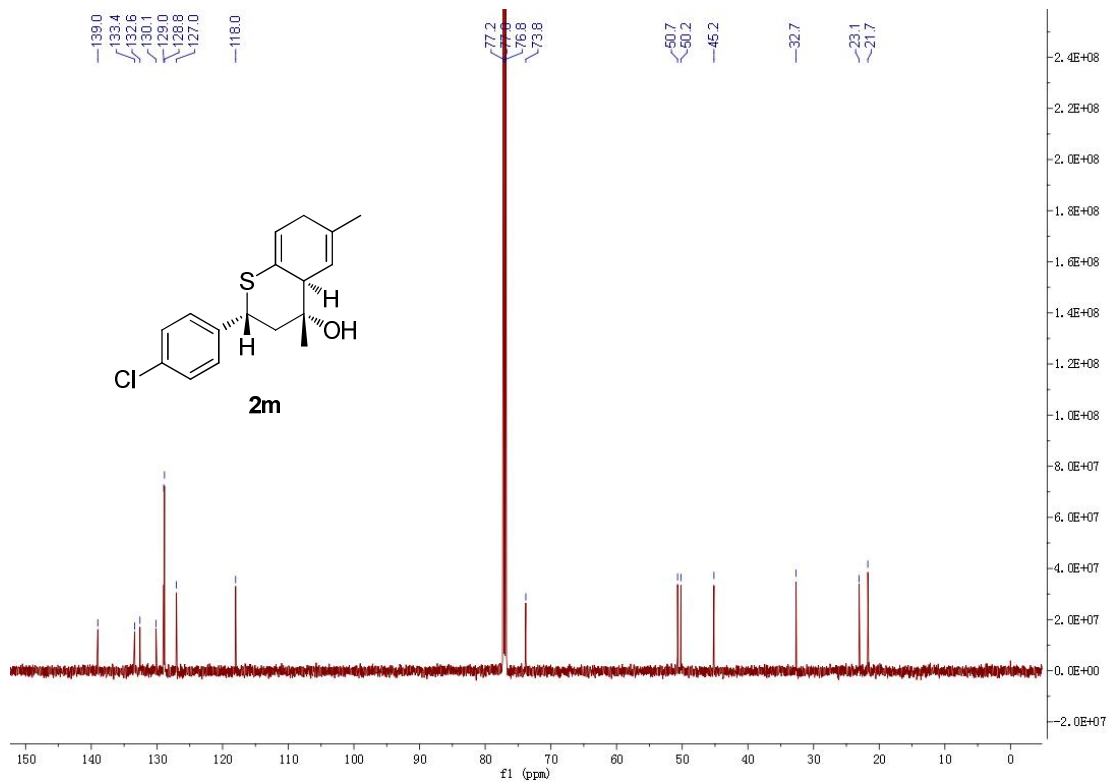
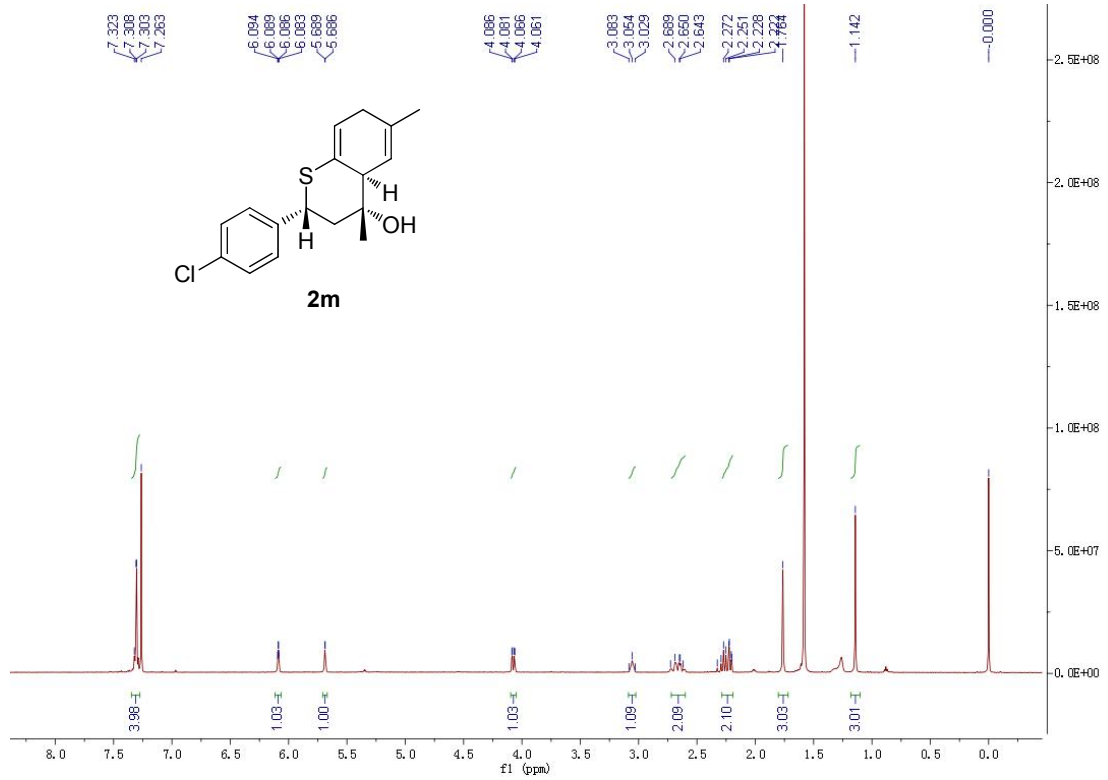


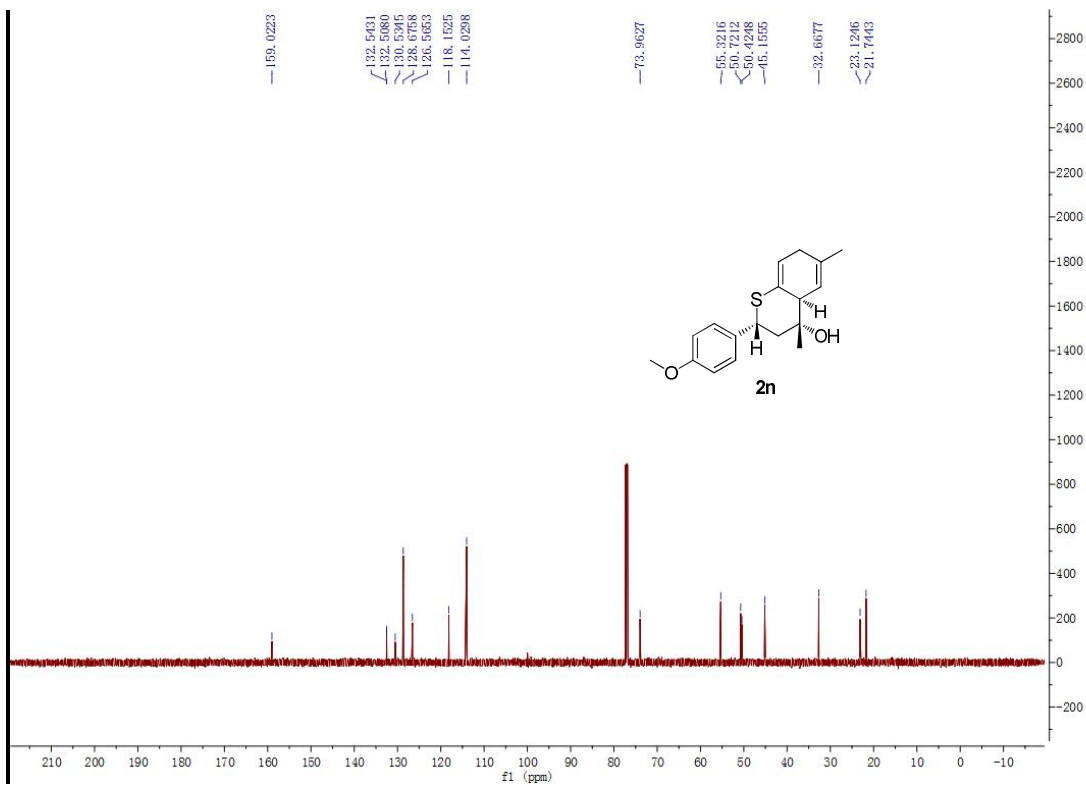
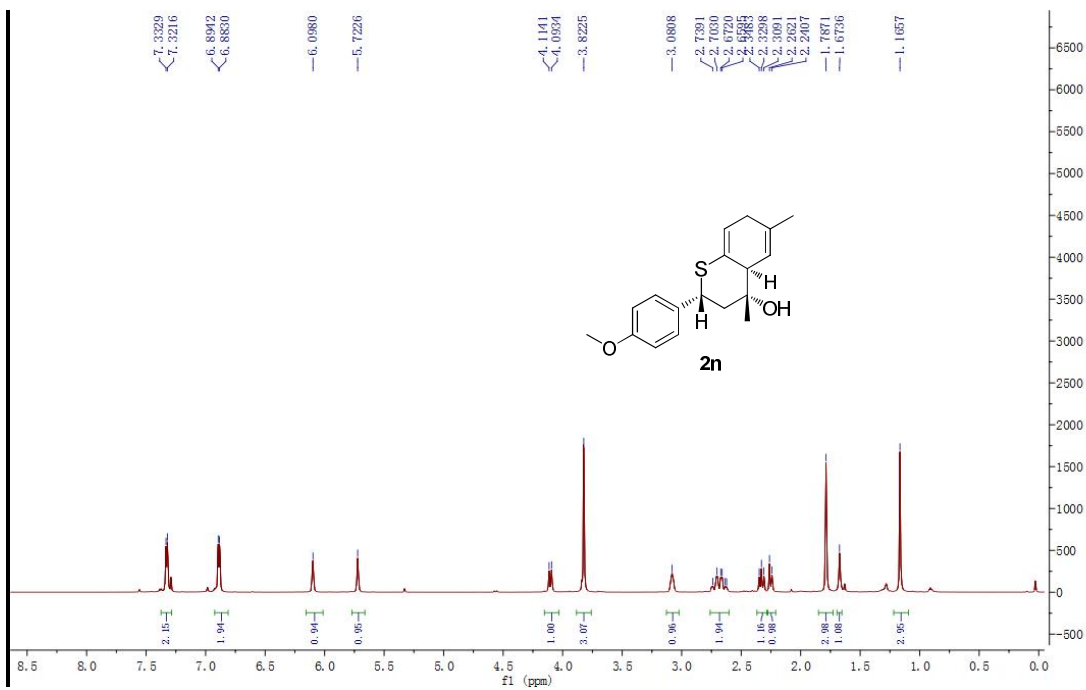


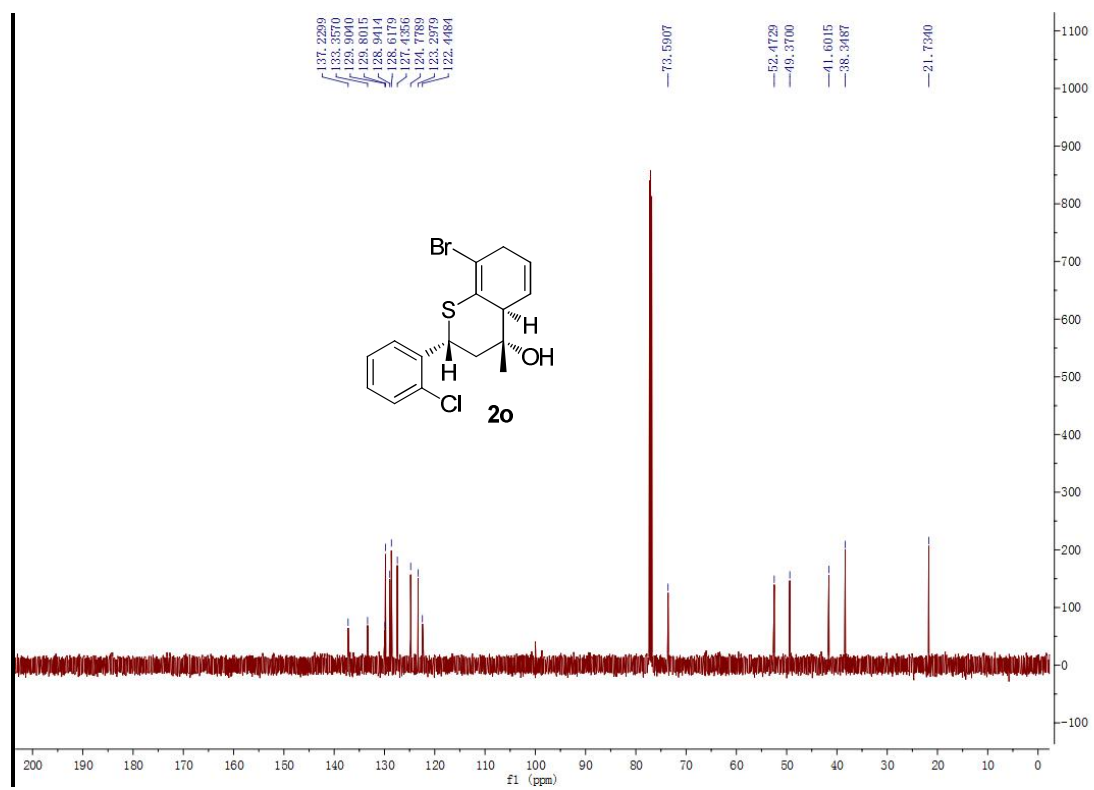
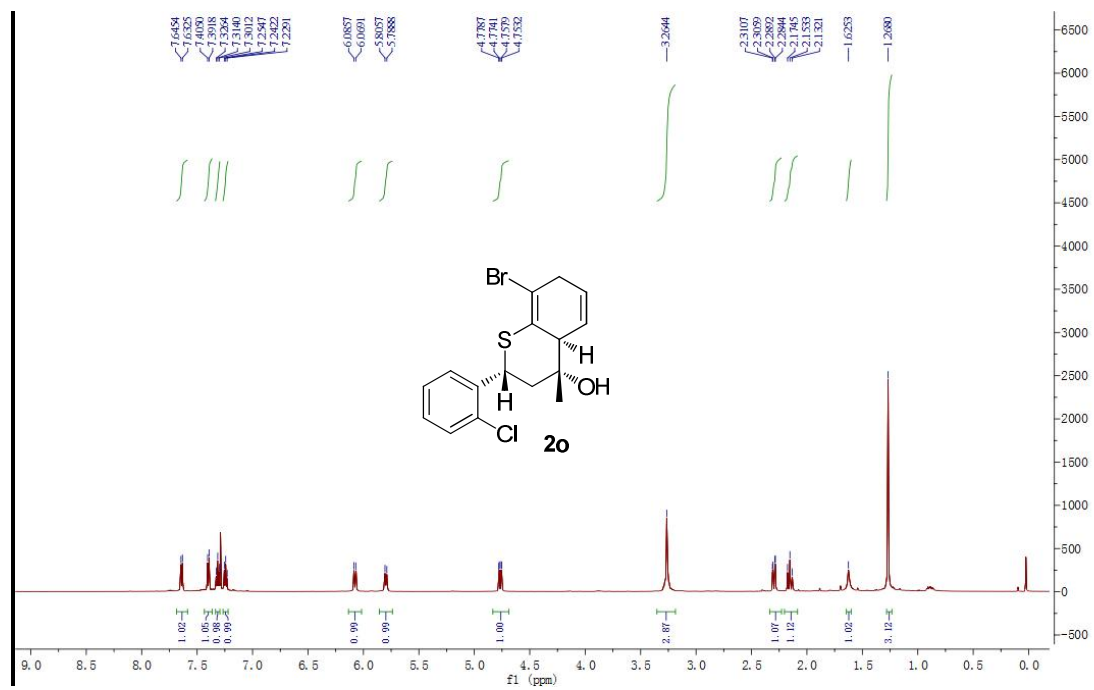


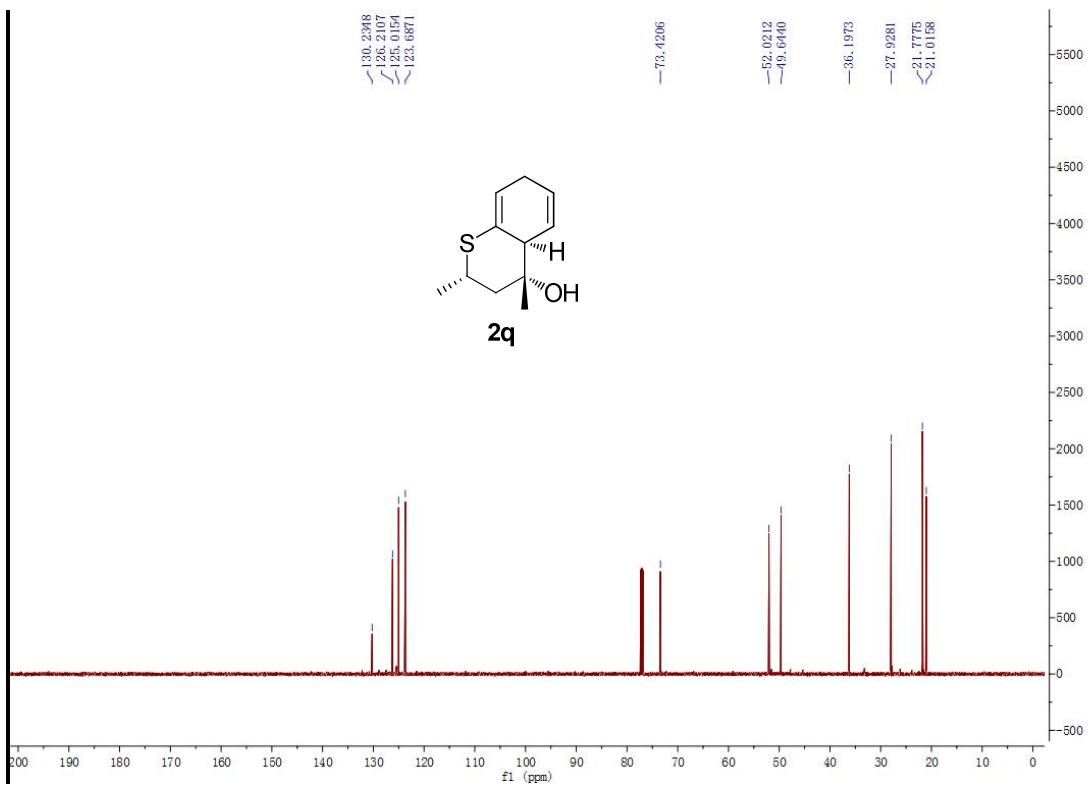
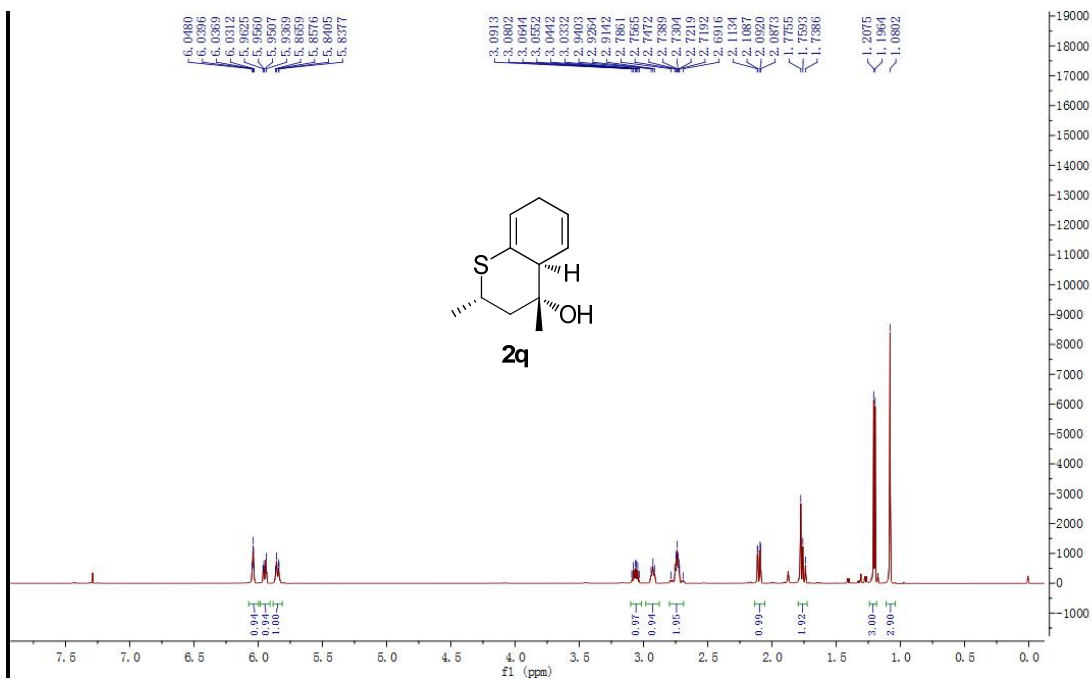


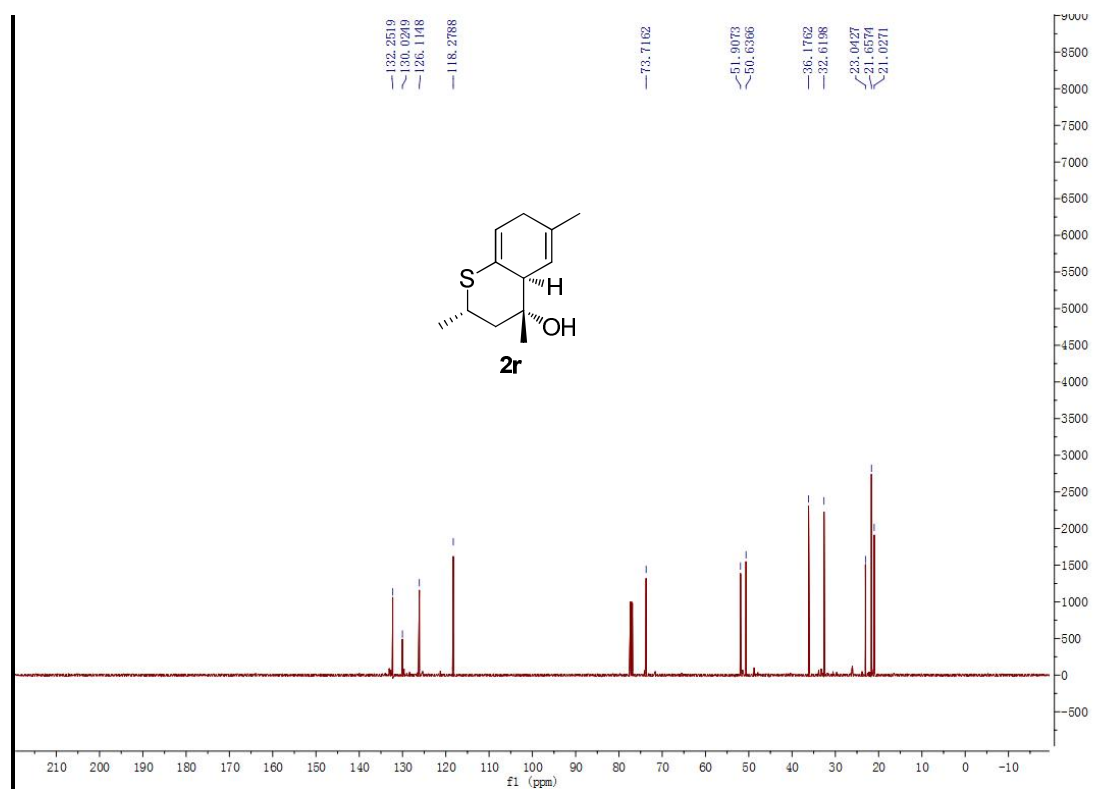
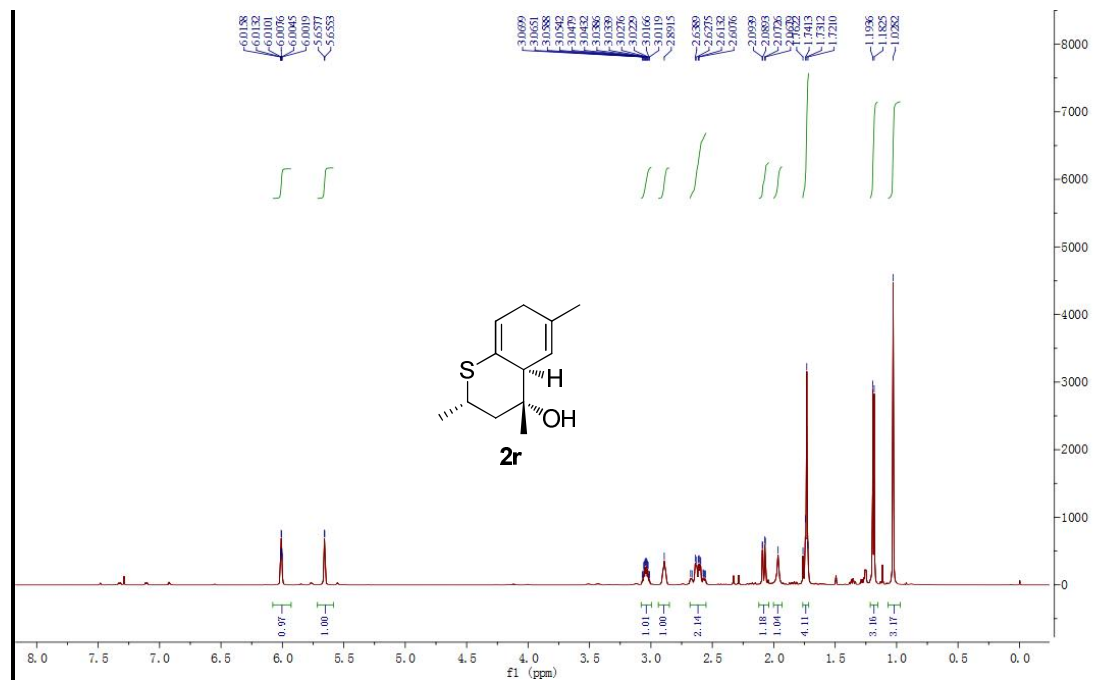


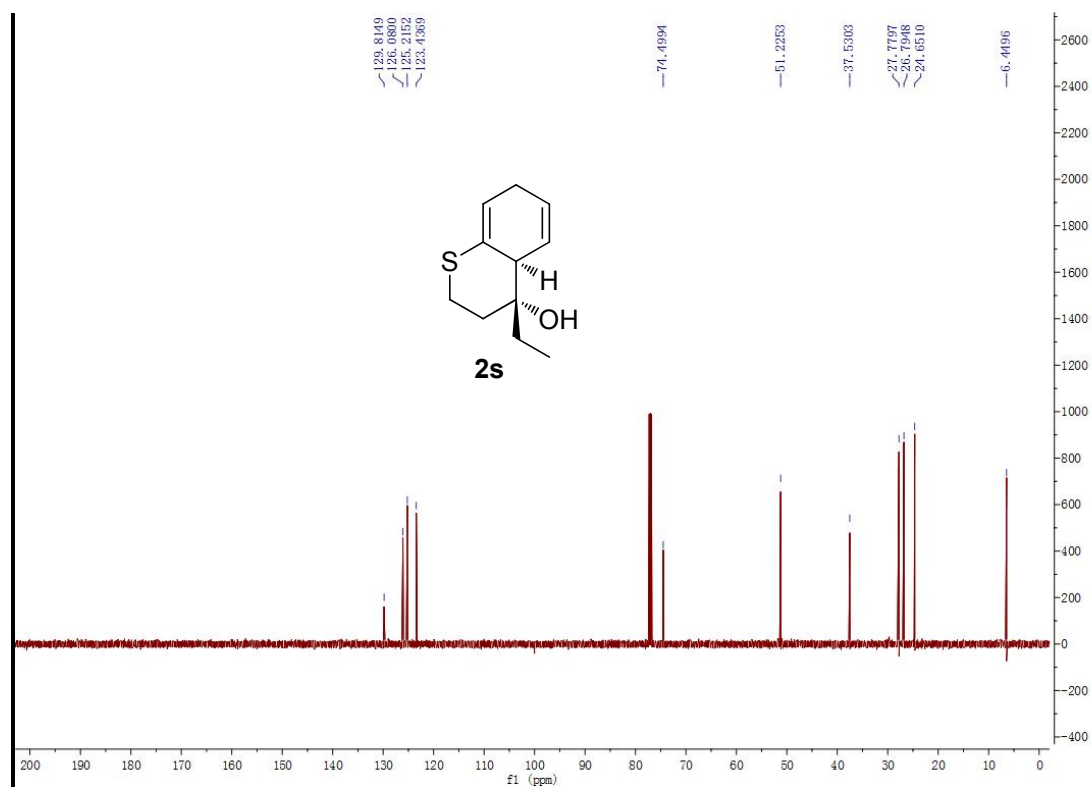
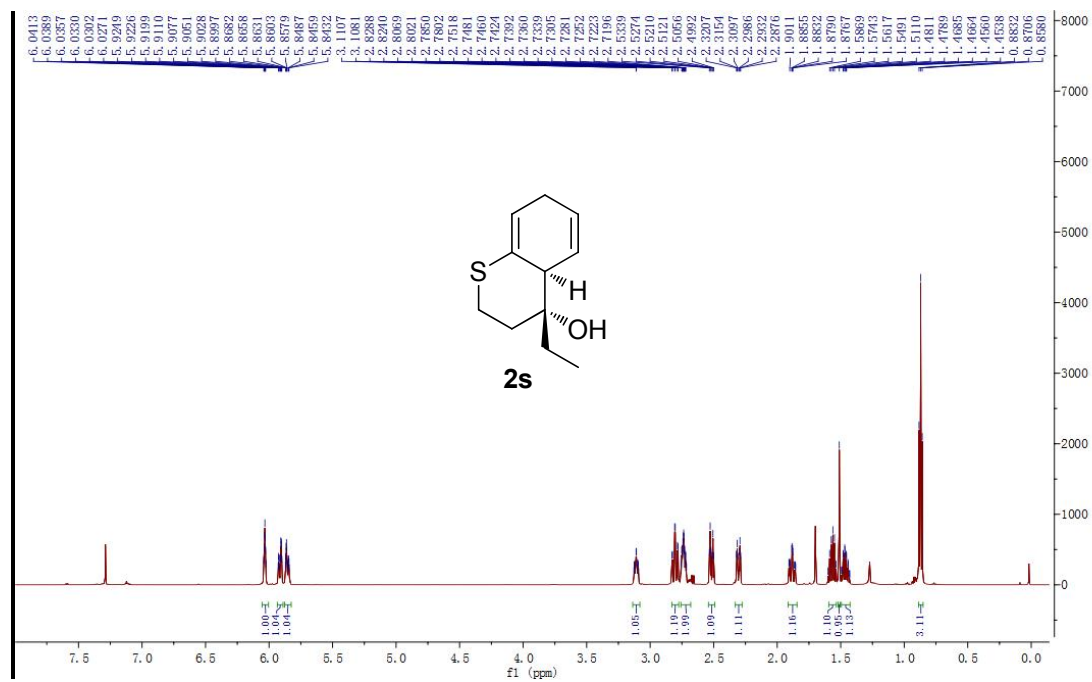






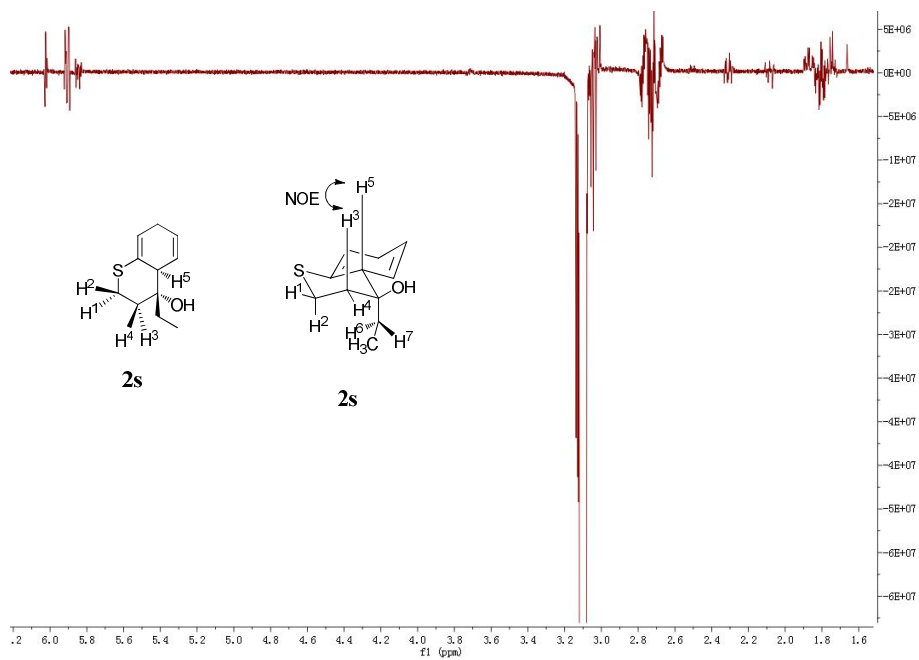




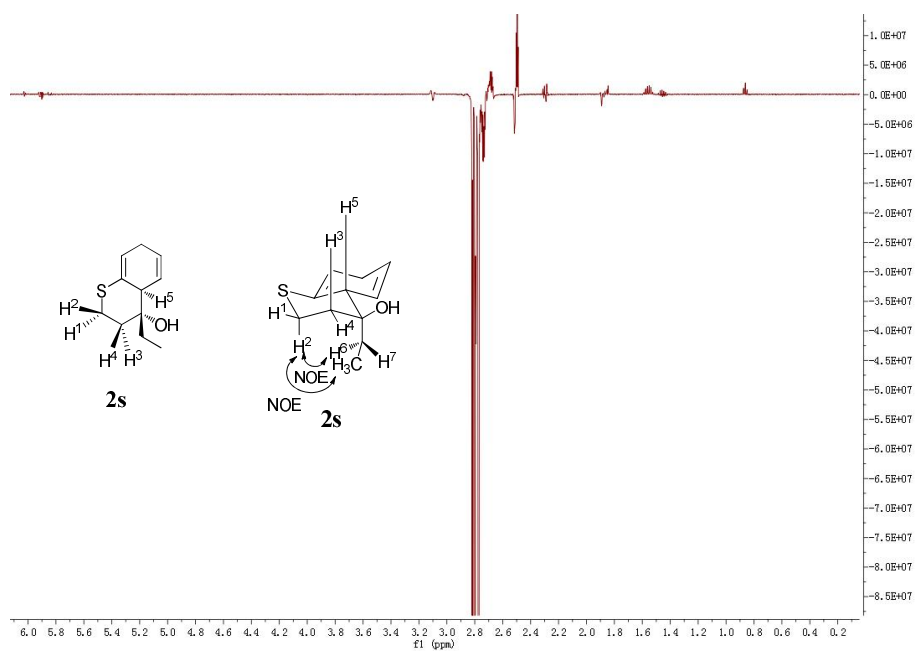


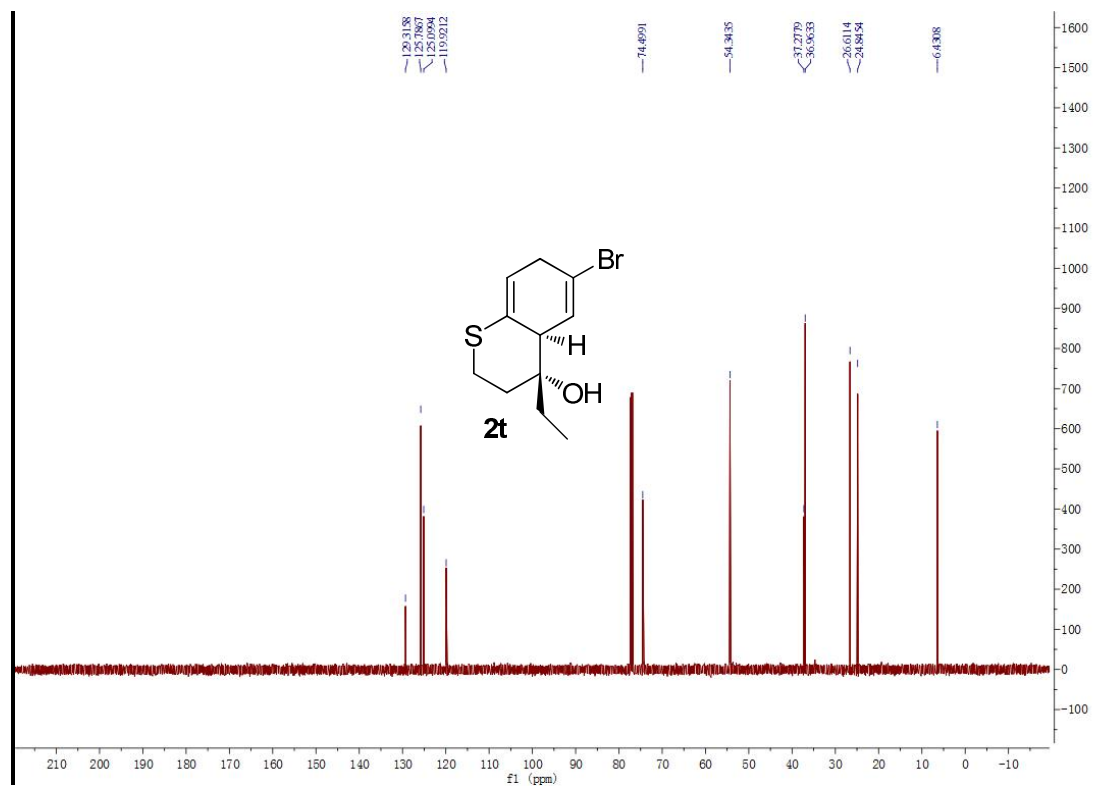
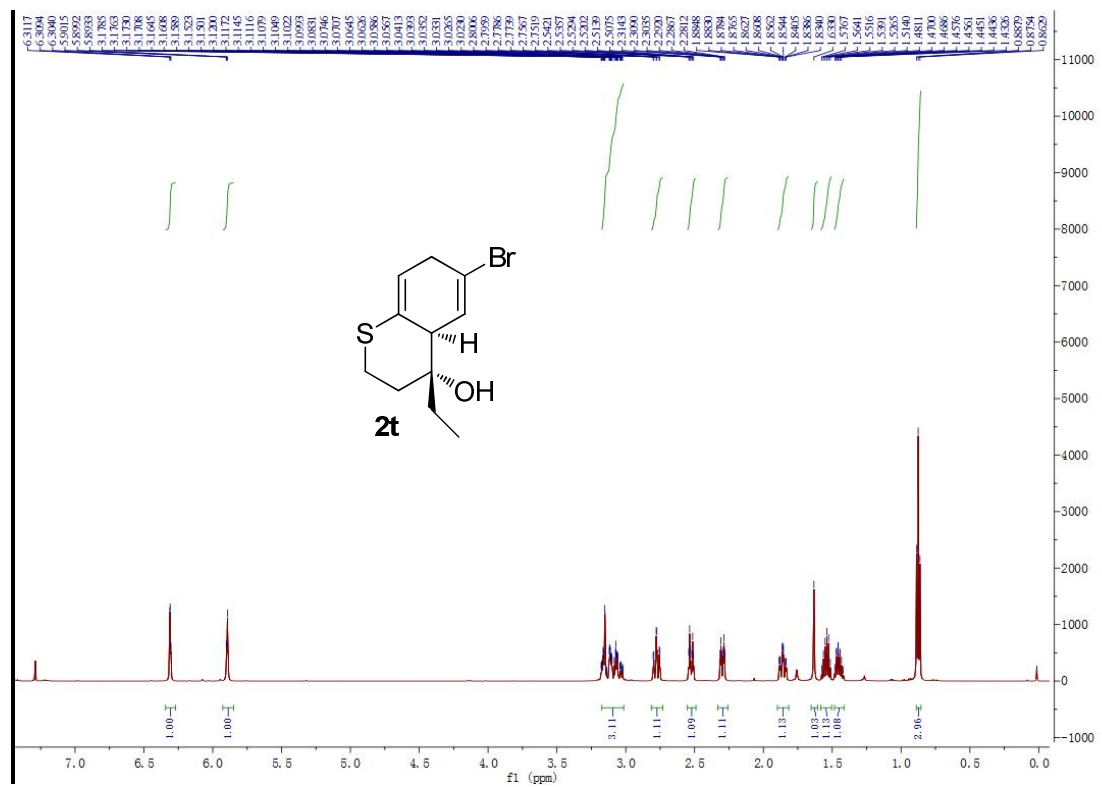
NOE effect for 2S

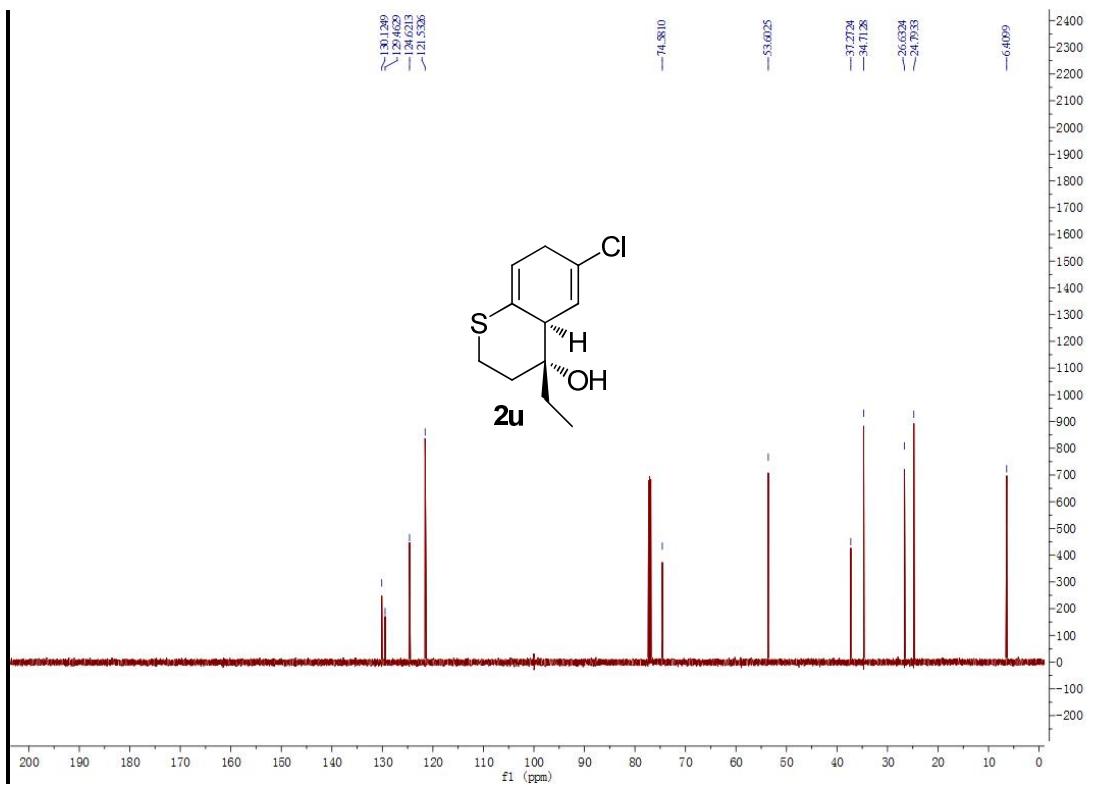
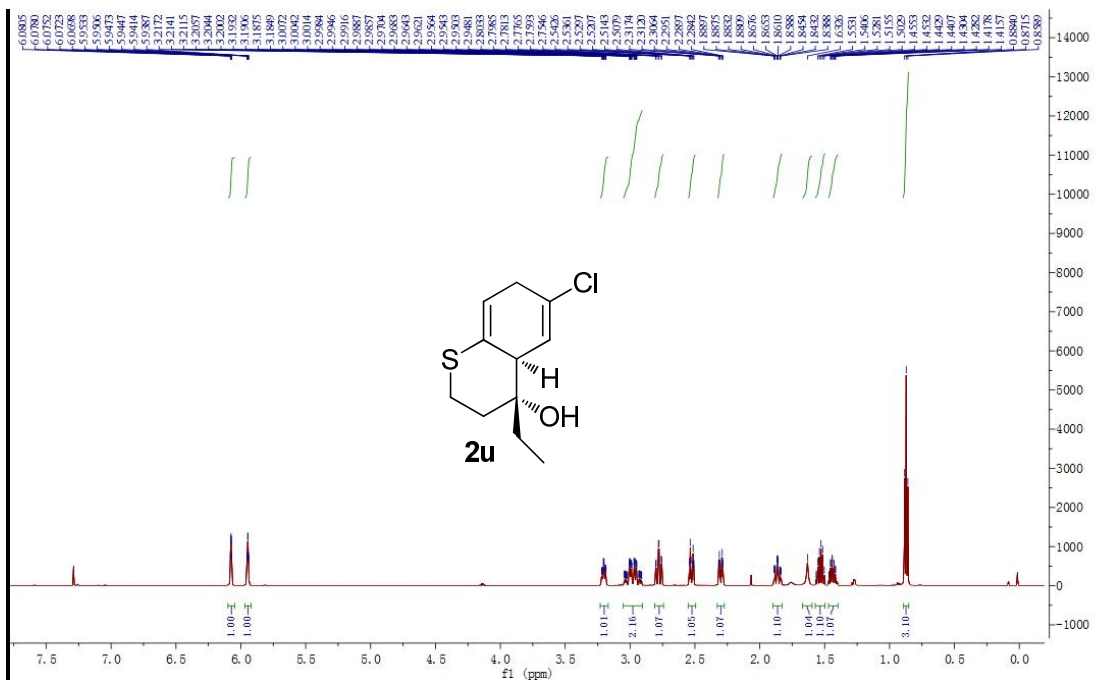
1) Irradiation of H⁵ and NOE with H³

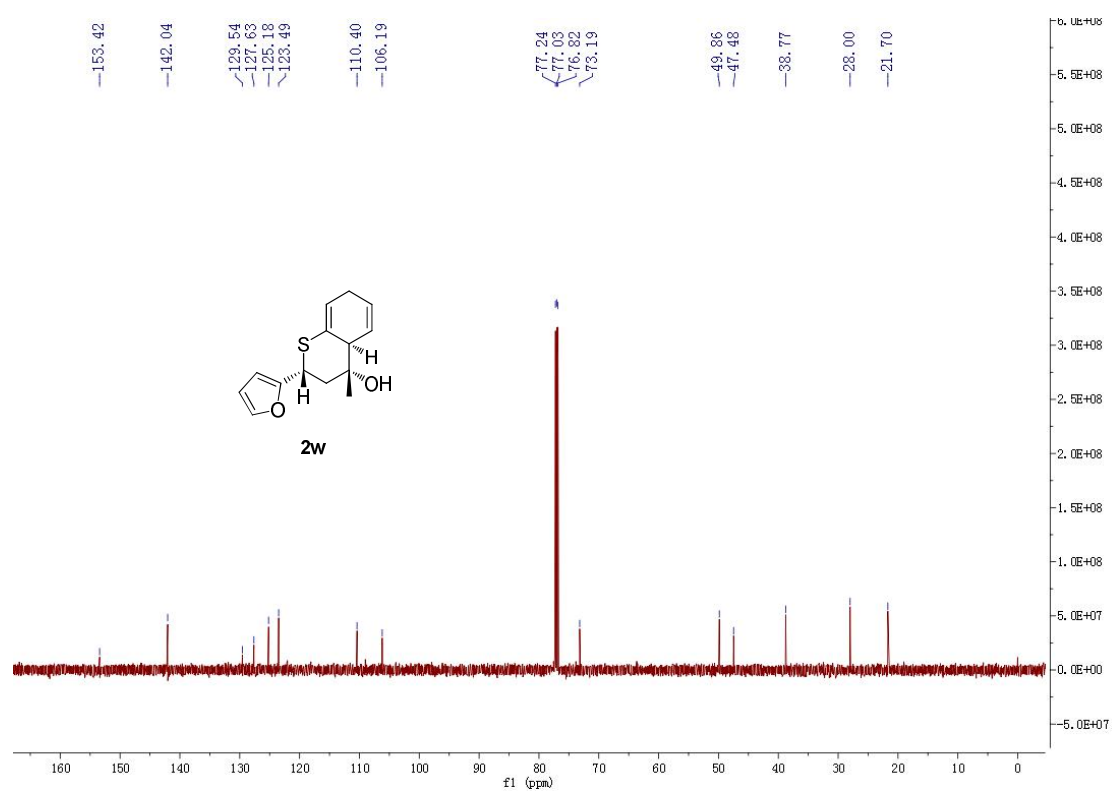
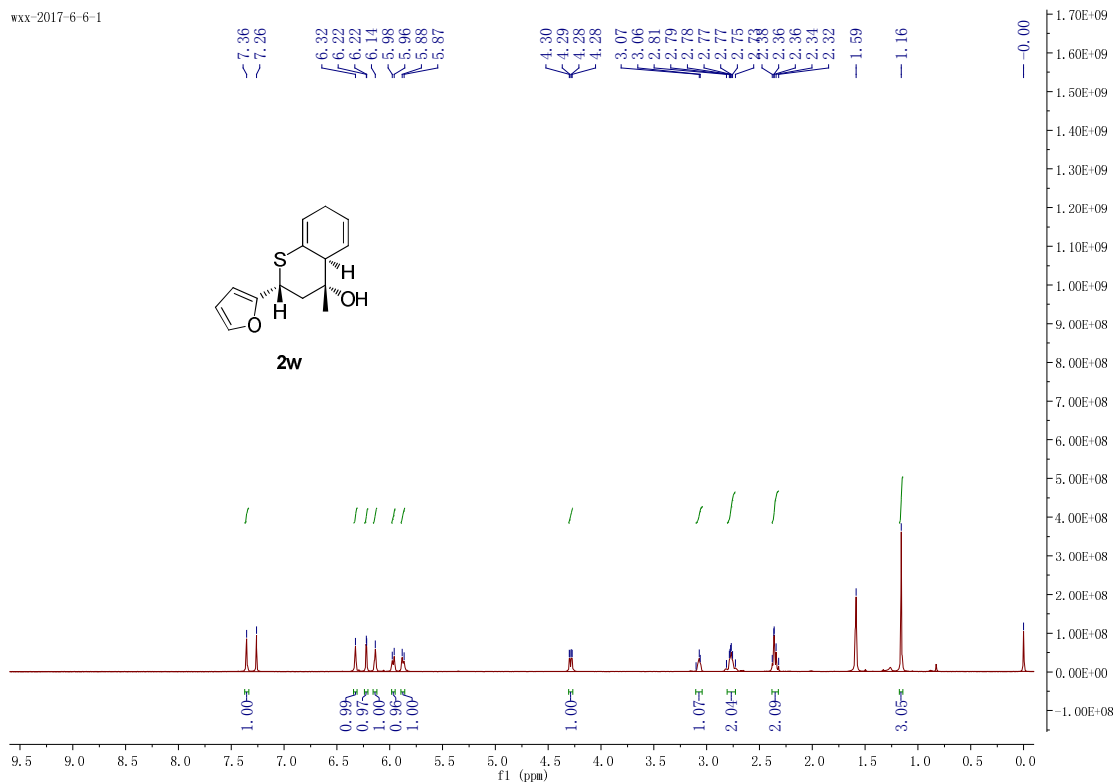


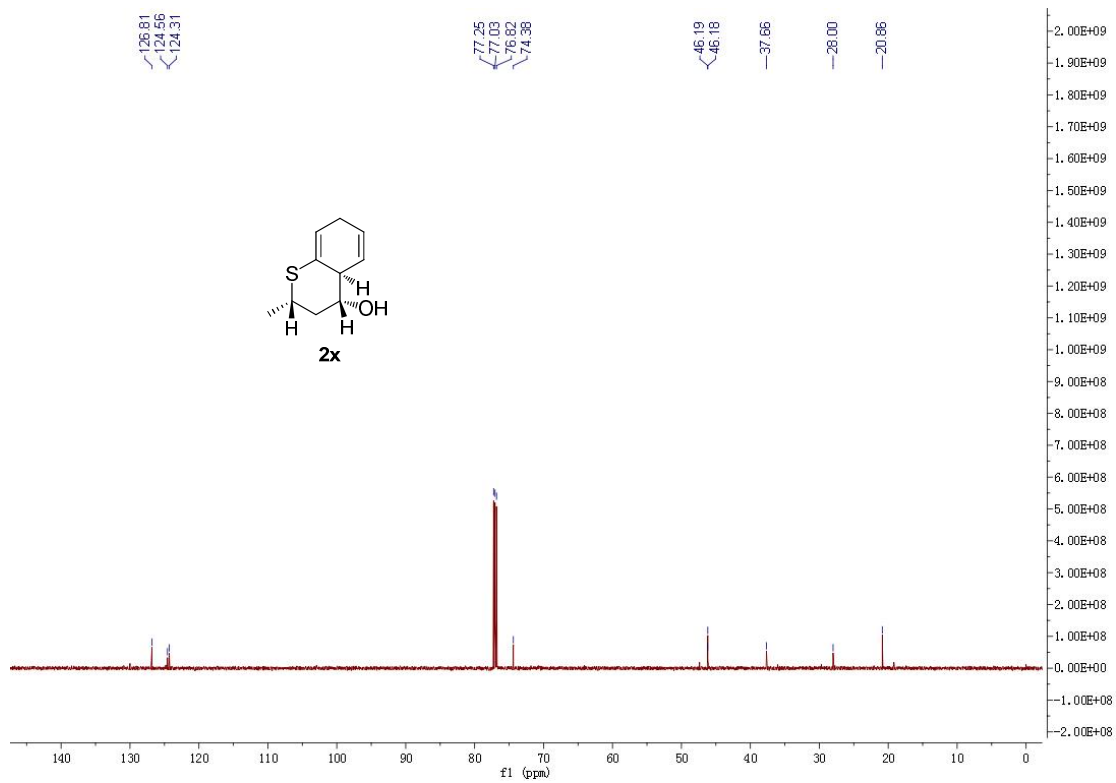
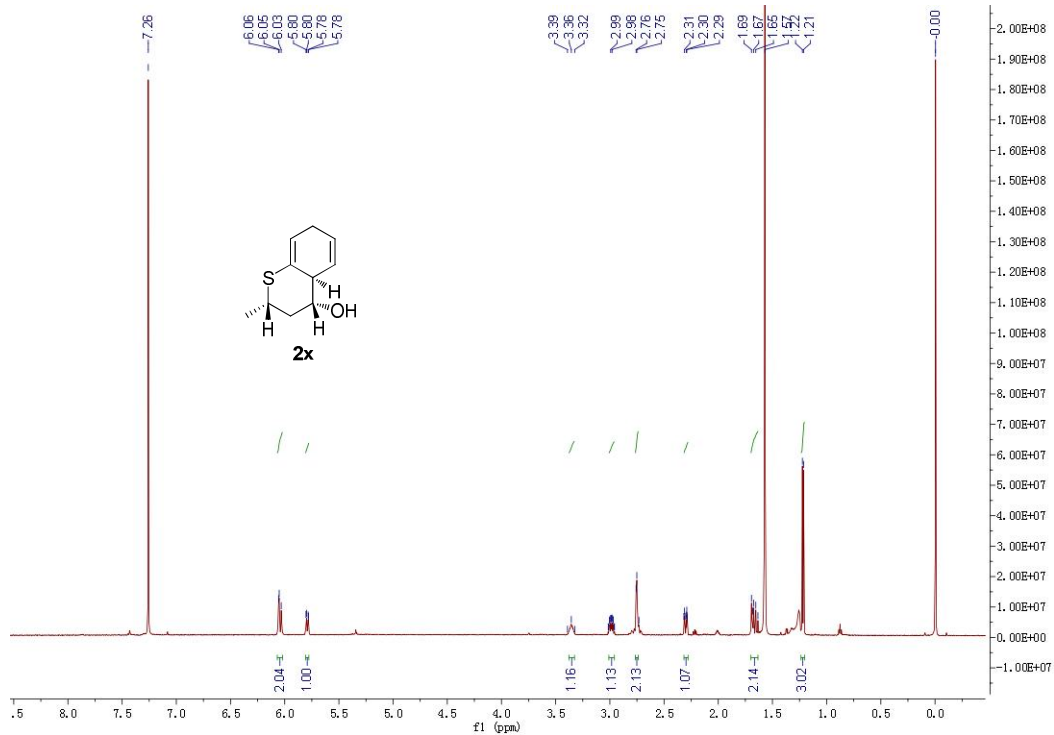
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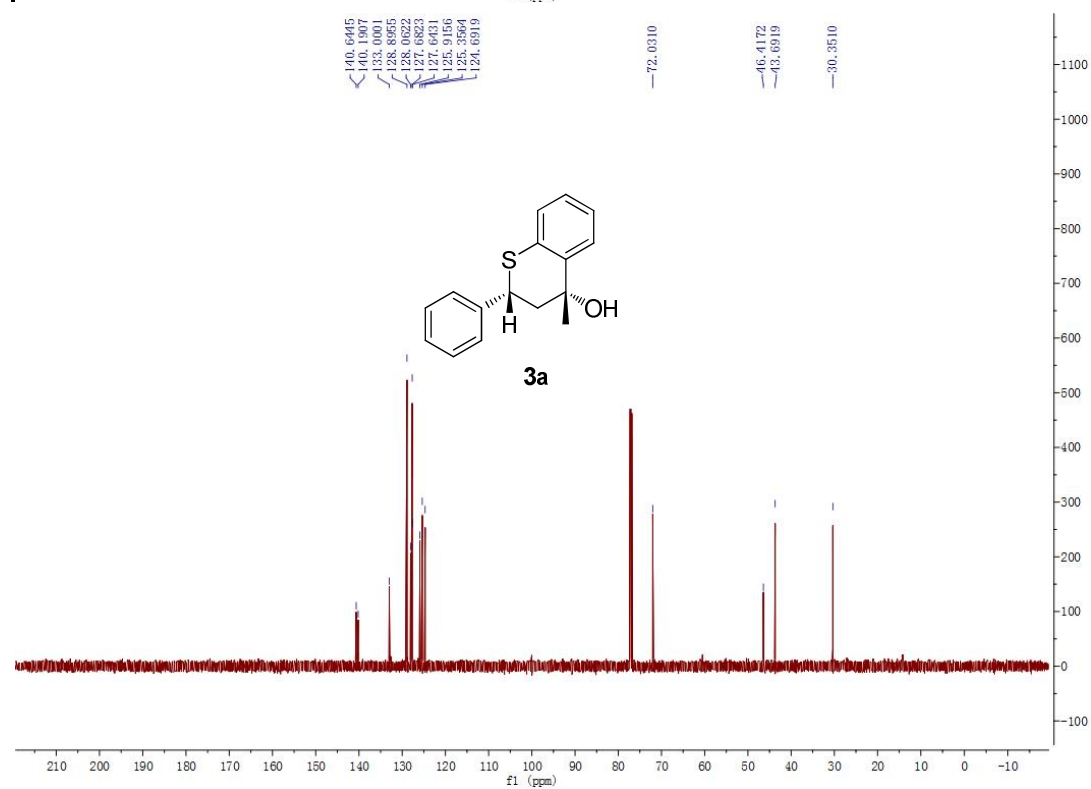
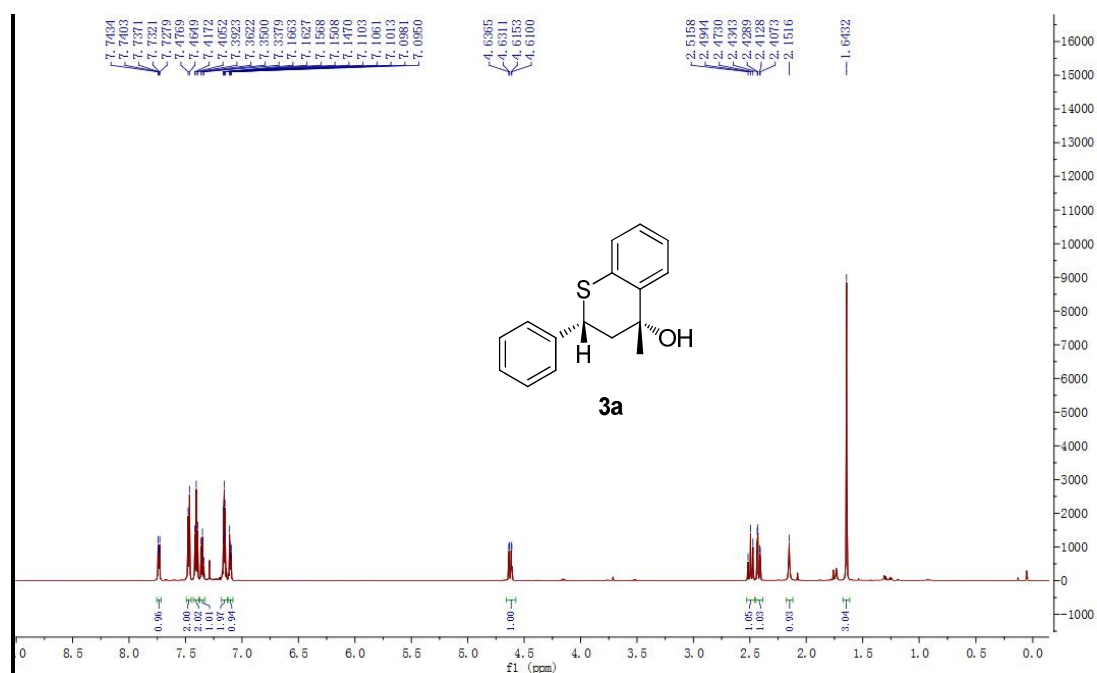


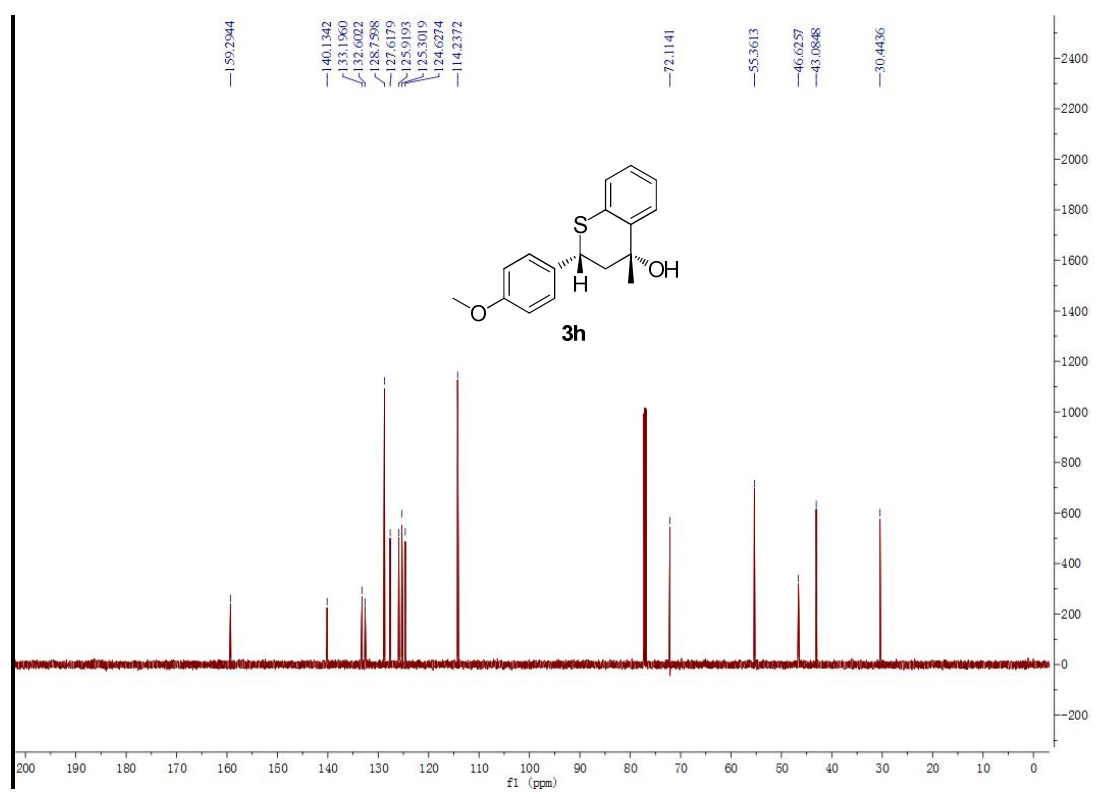
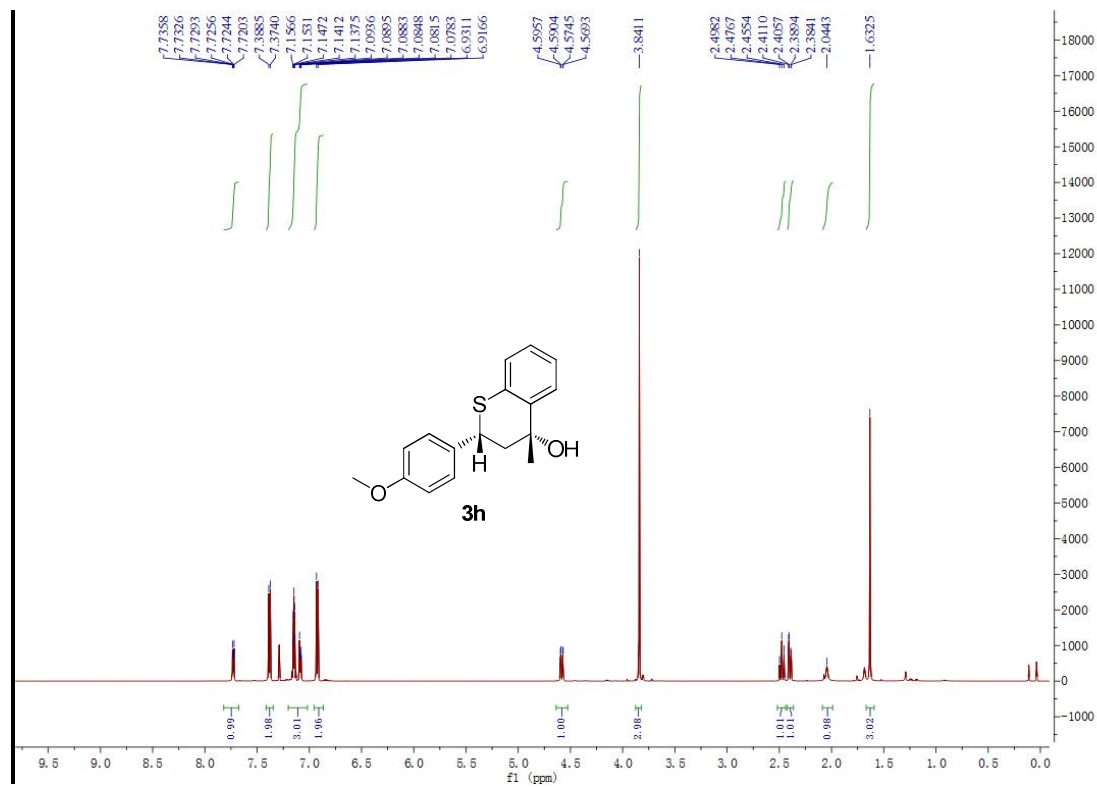


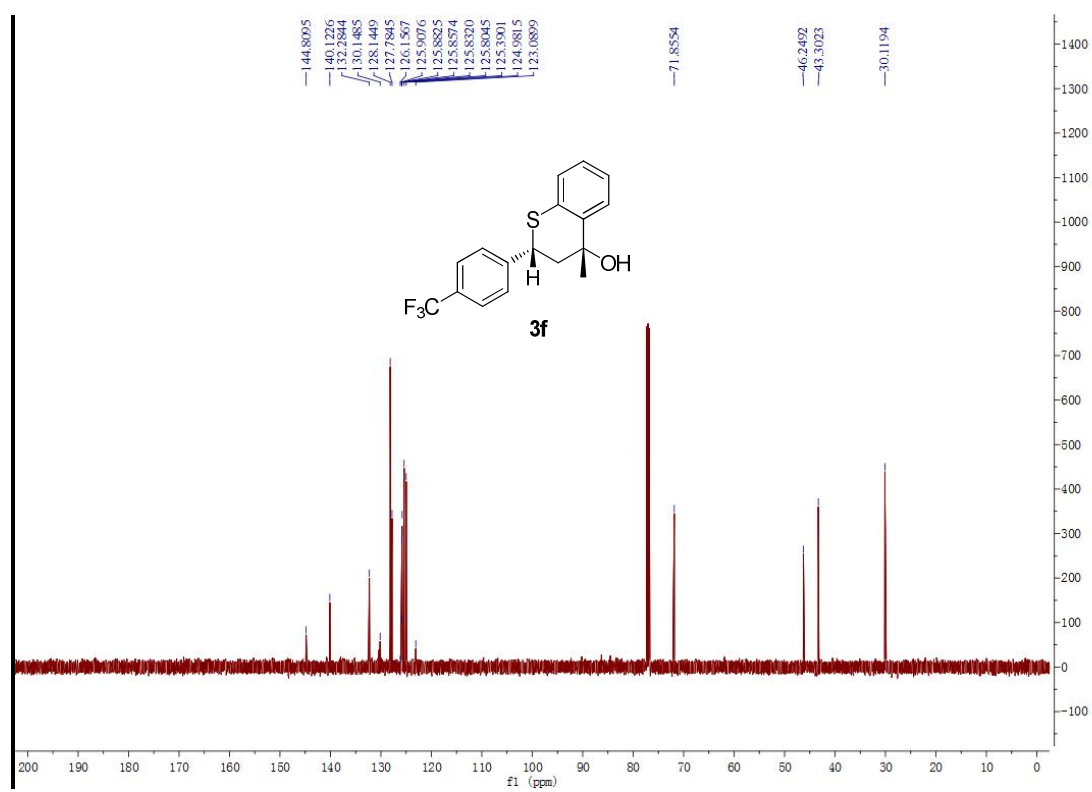
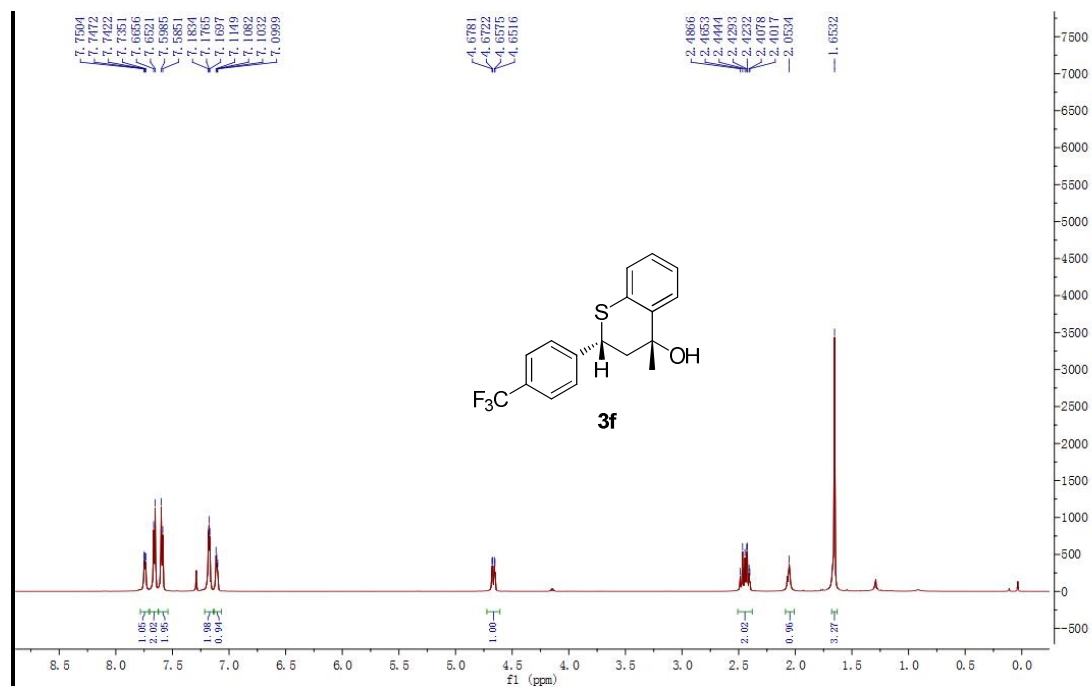


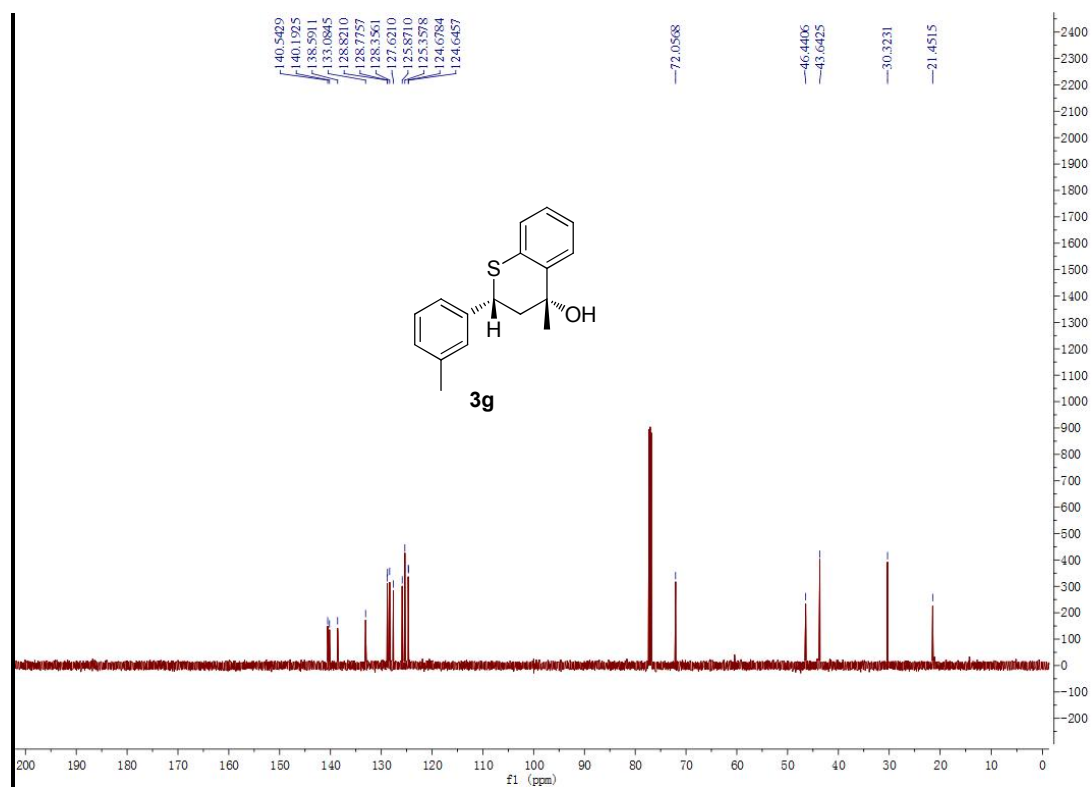
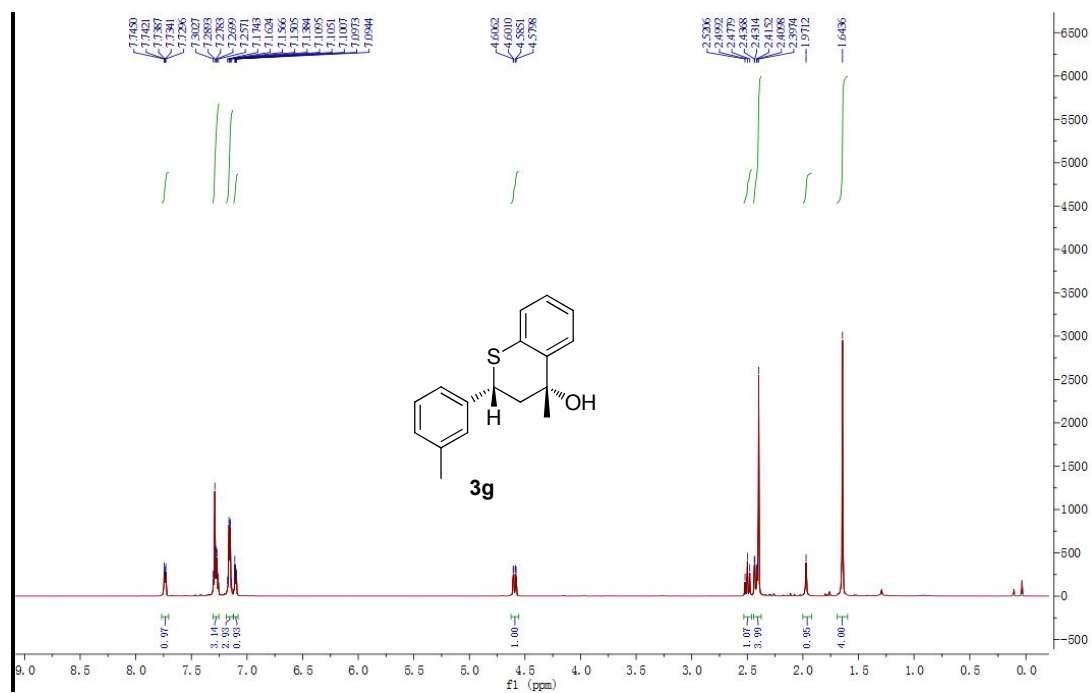


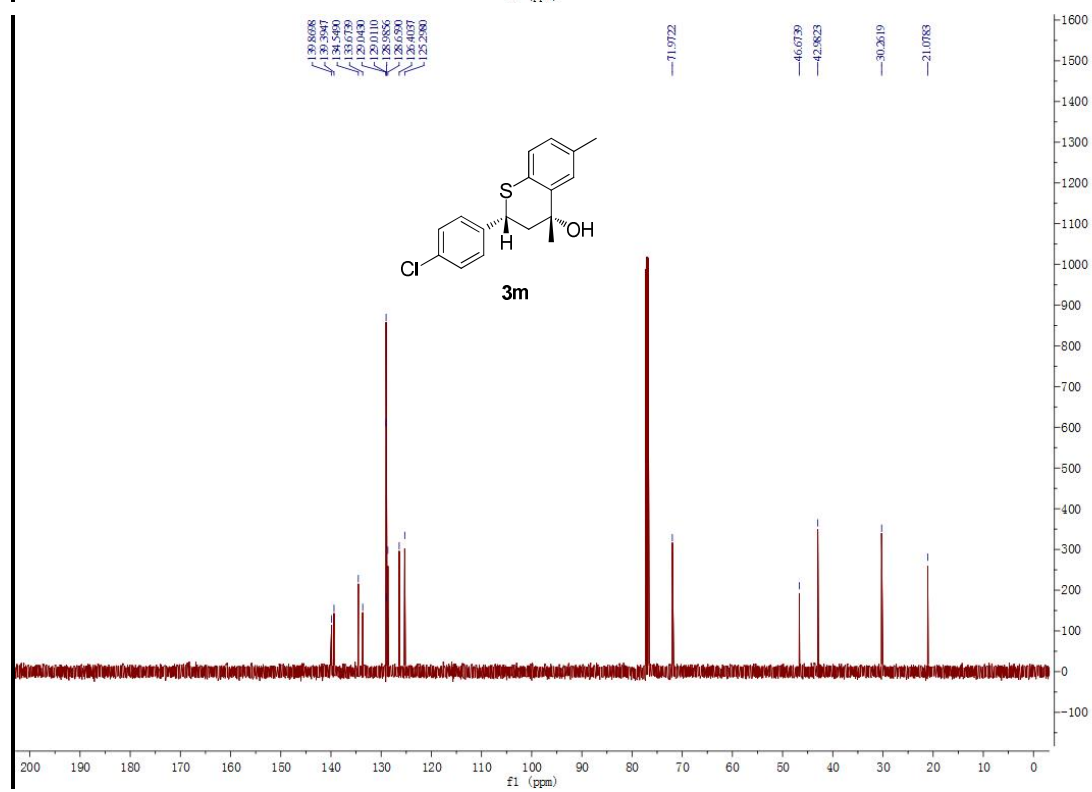
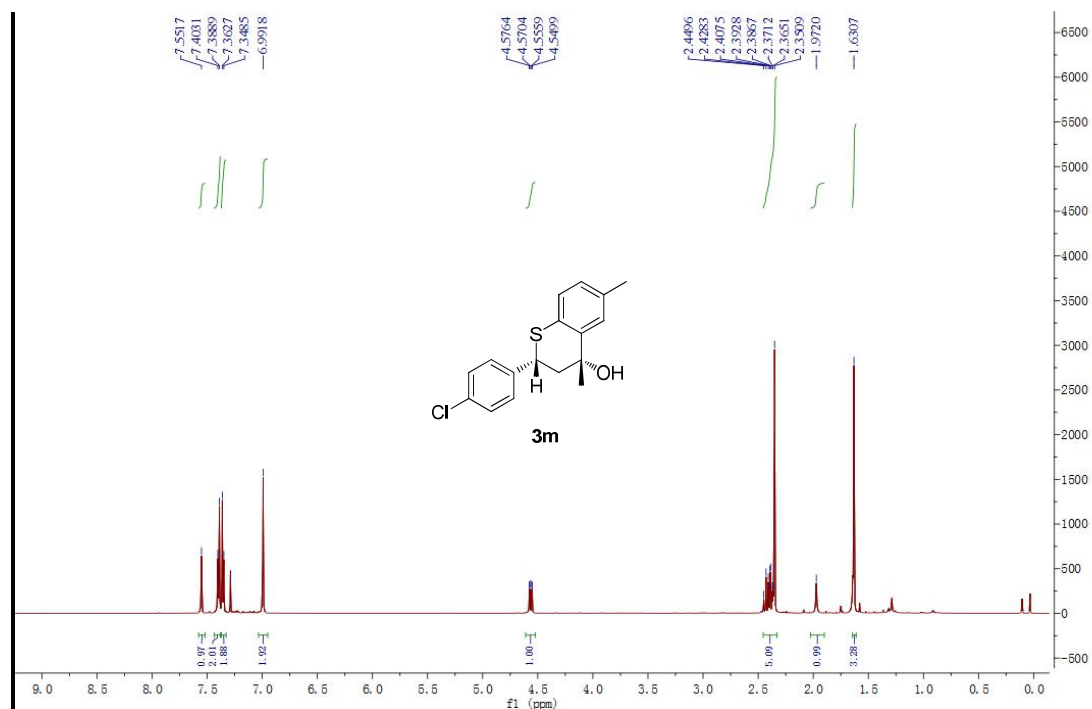
NMR spectra for products 3



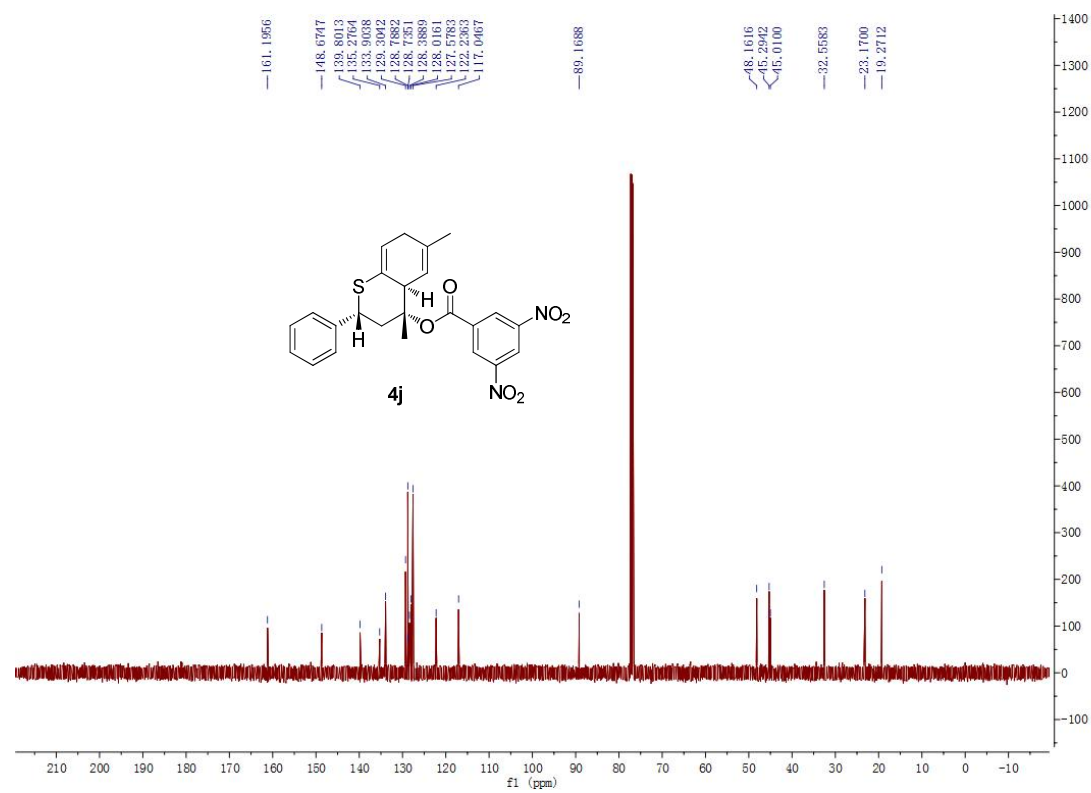
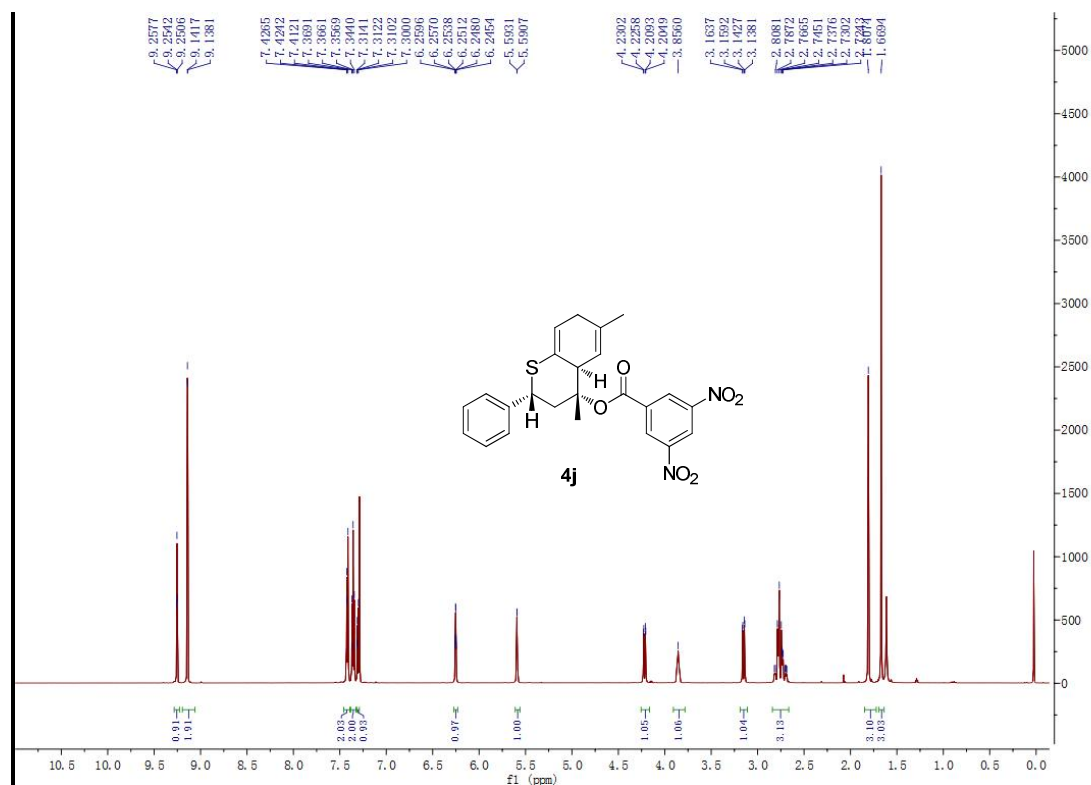




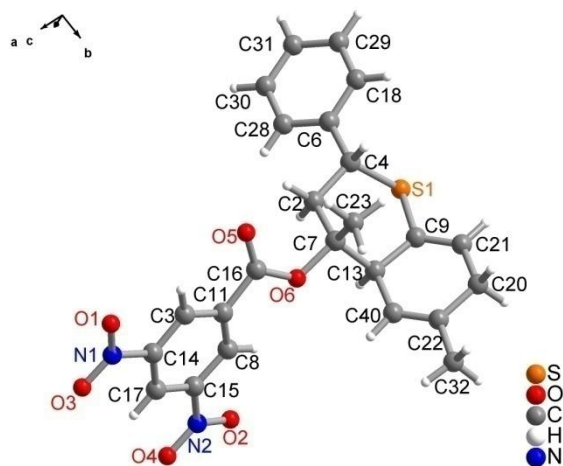




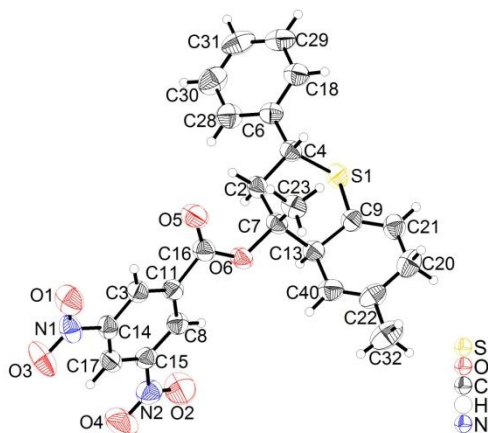
NMR Spectra and X-Ray Crystal Structure of for product 4j



X-Ray Crystal Structure of 4j' :



The thermal ellipsoid plot for the crystal structure of 4j' (50% ellipsoid contour percent probability level):



For more details please see the CIF file. The crystal data of **4j'** has already been deposited at Cambridge Crystallographic Data Center, UK, and the CCDC reference number is 1470852.