

New Journal of Chemistry

NBS/DMSO-Mediated synthesis of (2,3-dihydrobenzo[*b*][1,4]oxathiin-3-yl)methanols from aryloxymethylthiiranes

Jun Dong, and Jiaxi Xu*

State Key Laboratory of Chemical Resource Engineering, Department of Organic Chemistry,
Faculty of Science, Beijing University of Chemical Technology, Beijing 100029, People's Republic of
China

Supporting Information

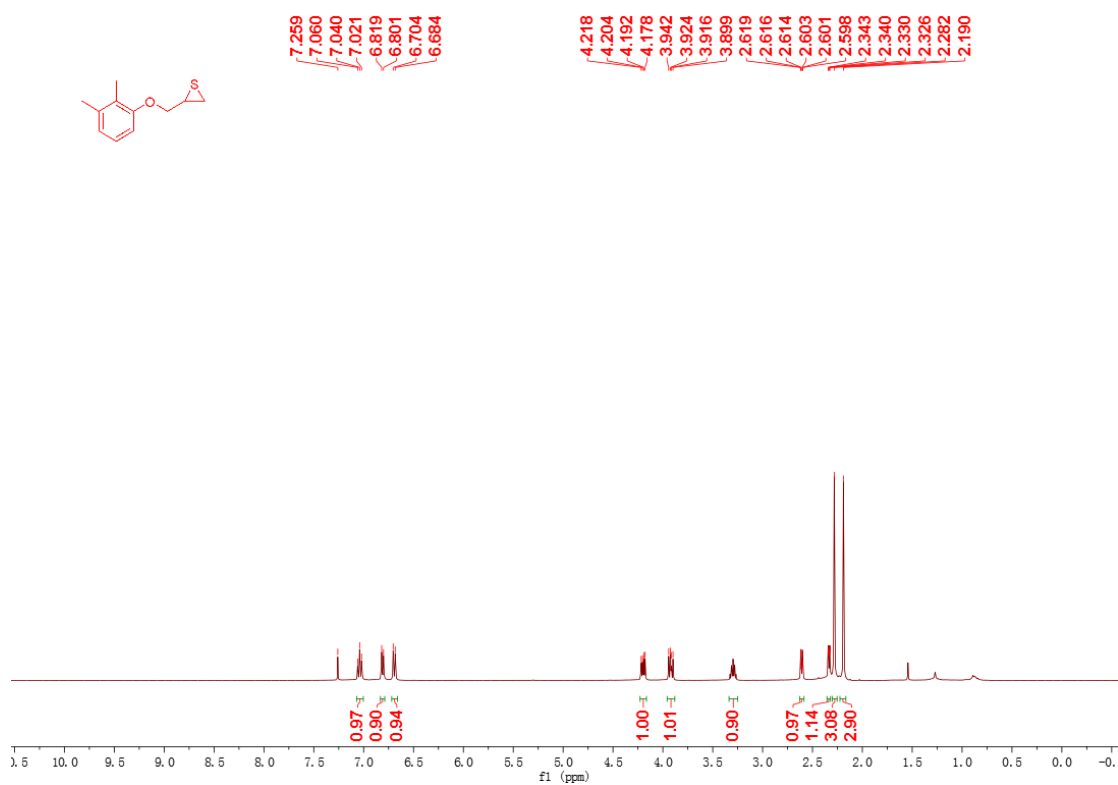
Contents

Copies of ¹ H and ¹³ C NMR spectra of unknown products 1, 2, and 3.....	S2
Copies of mass spectra of byproducts in reaction mixtures.....	S23

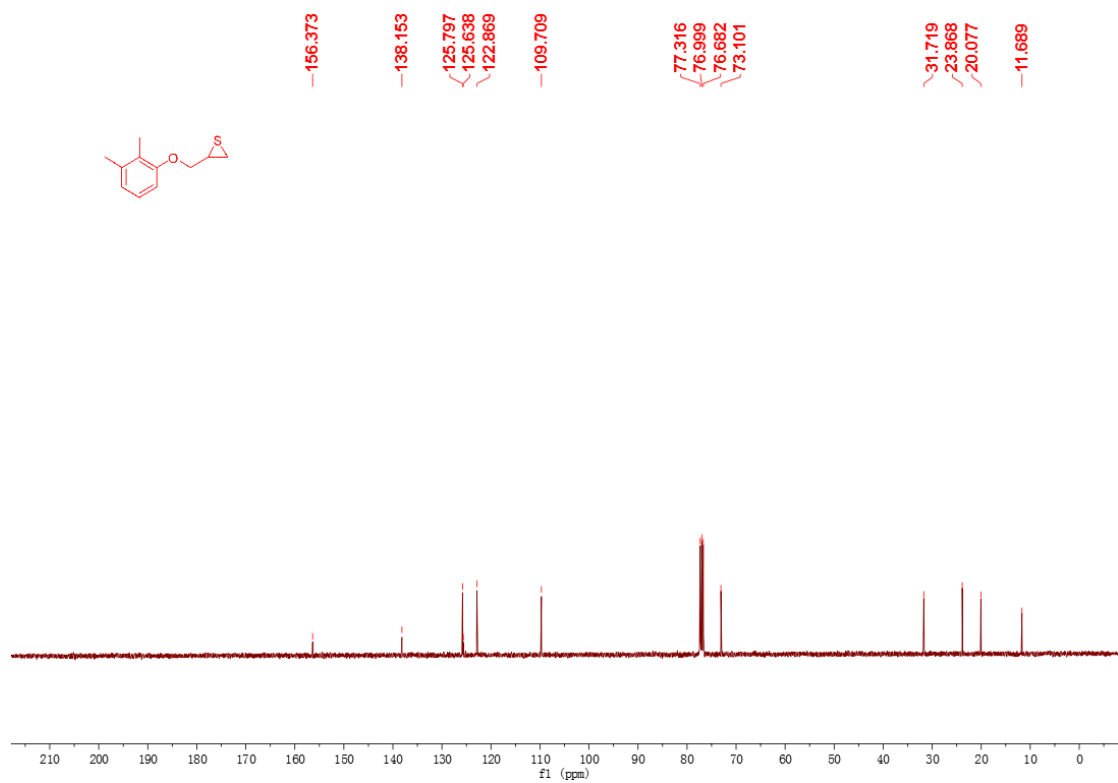
* Corresponding author. Tel.: +0-8610-6443-5565; fax: +0-8610-6443-5565; e-mail: jxxu@mail.buct.edu.cn

Copies of ^1H and ^{13}C NMR spectra of unknown products 1, 2, and 3

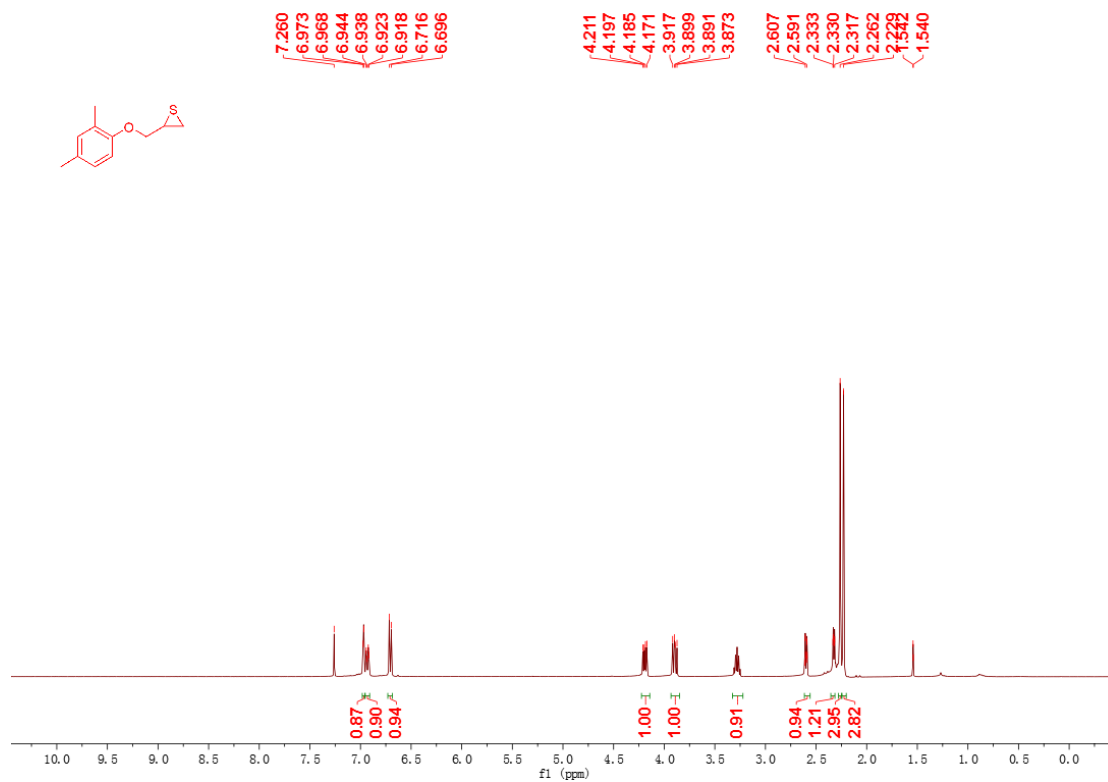
^1H NMR (400 MHz, CDCl_3) of compound **1f**



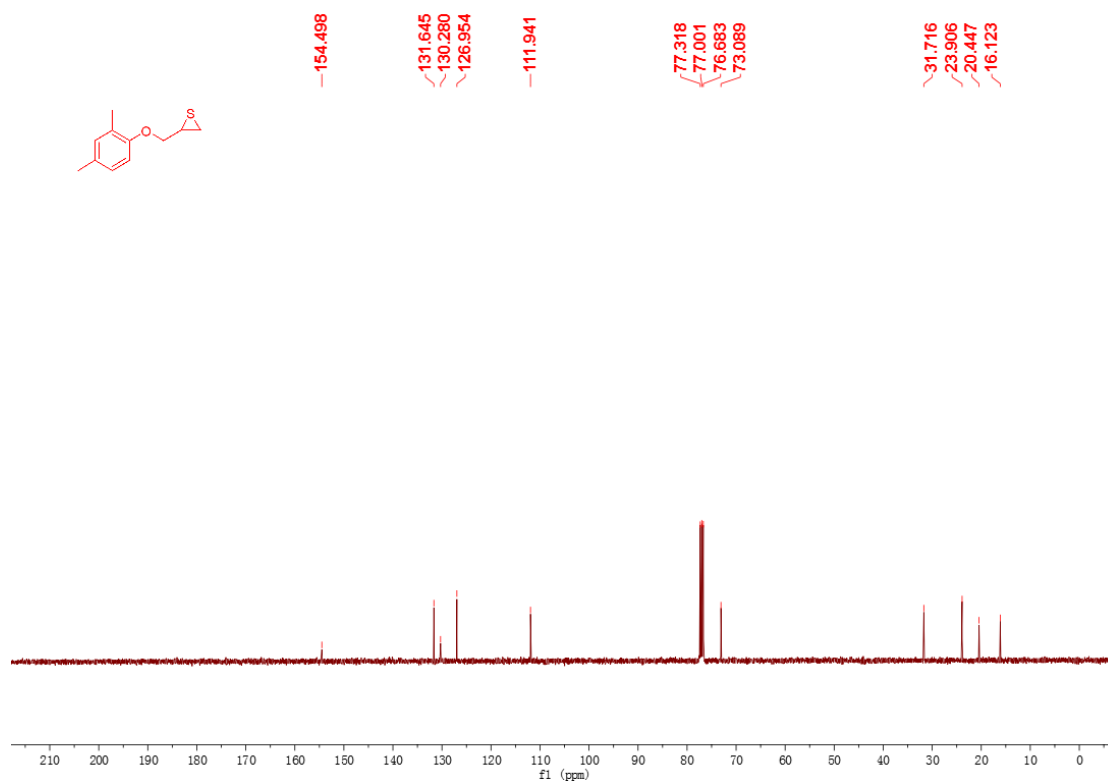
^{13}C NMR (101 MHz, CDCl_3)



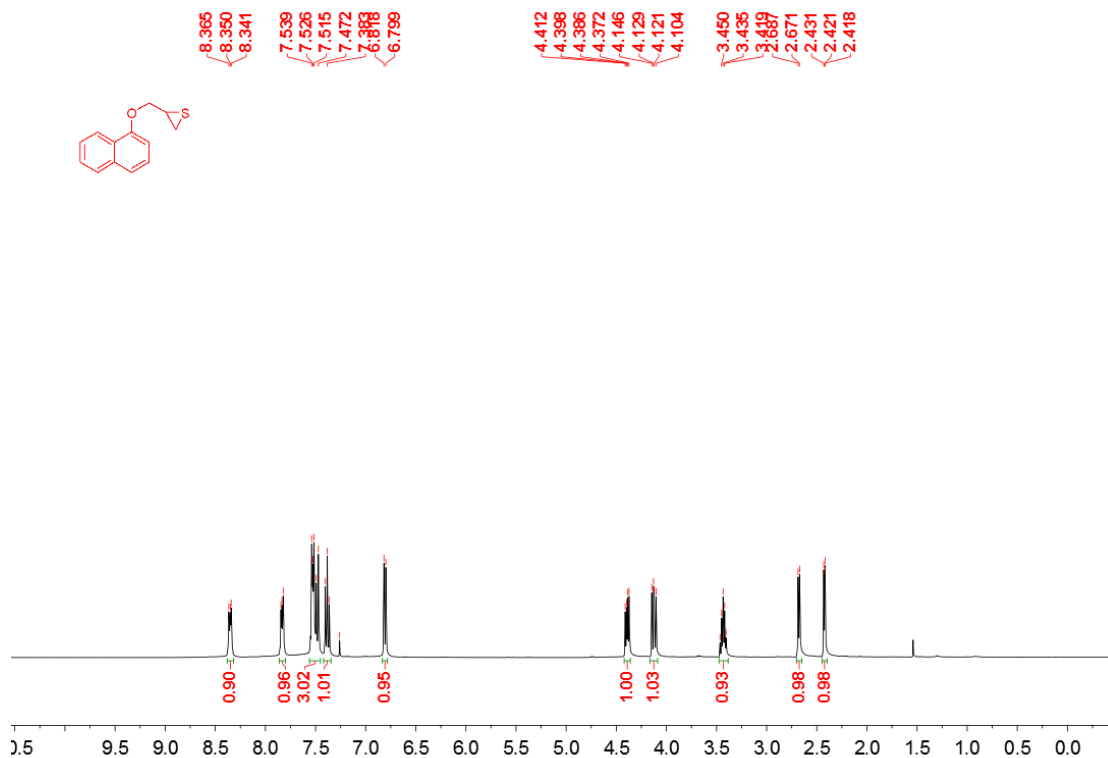
^1H NMR (400 MHz, CDCl_3) of compound **1g**



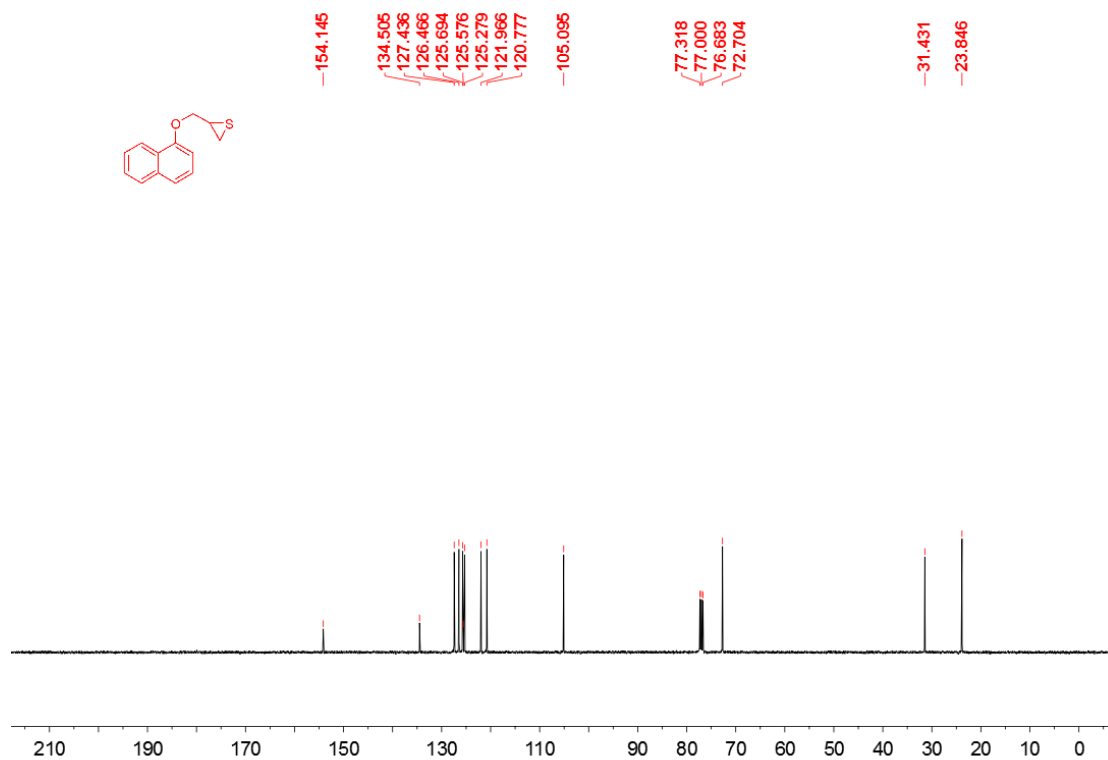
^{13}C NMR (101 MHz, CDCl_3)



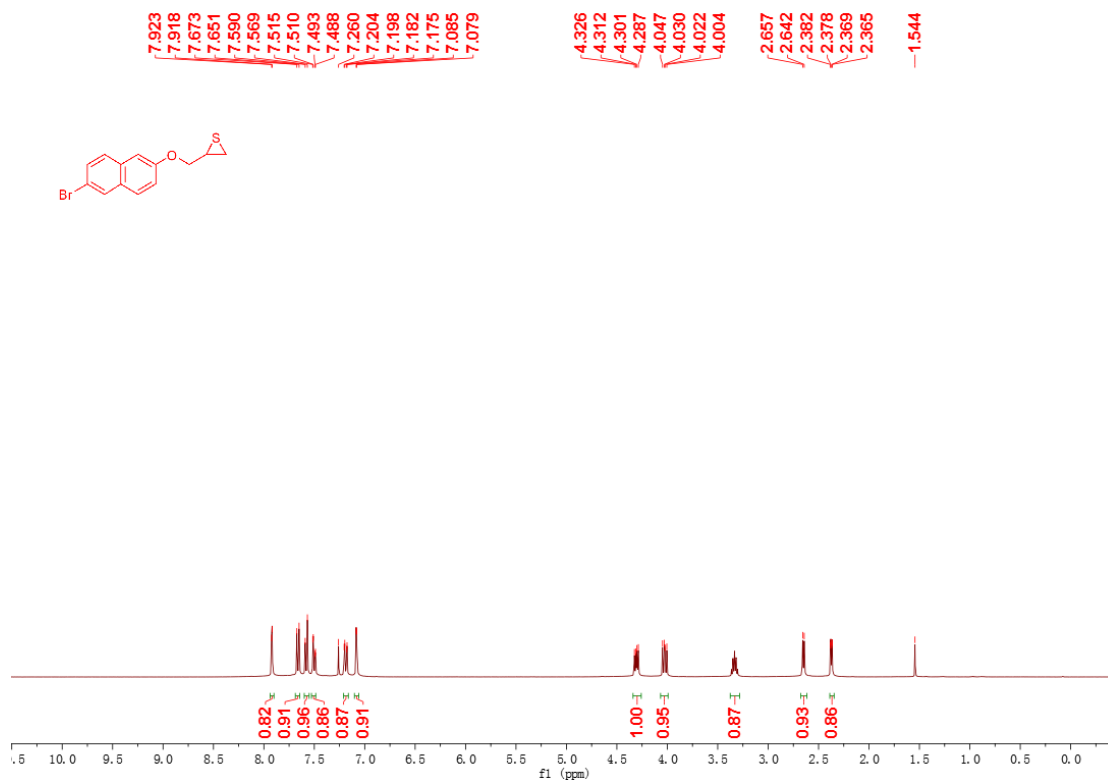
^1H NMR (400 MHz, CDCl_3) of compound **1h**



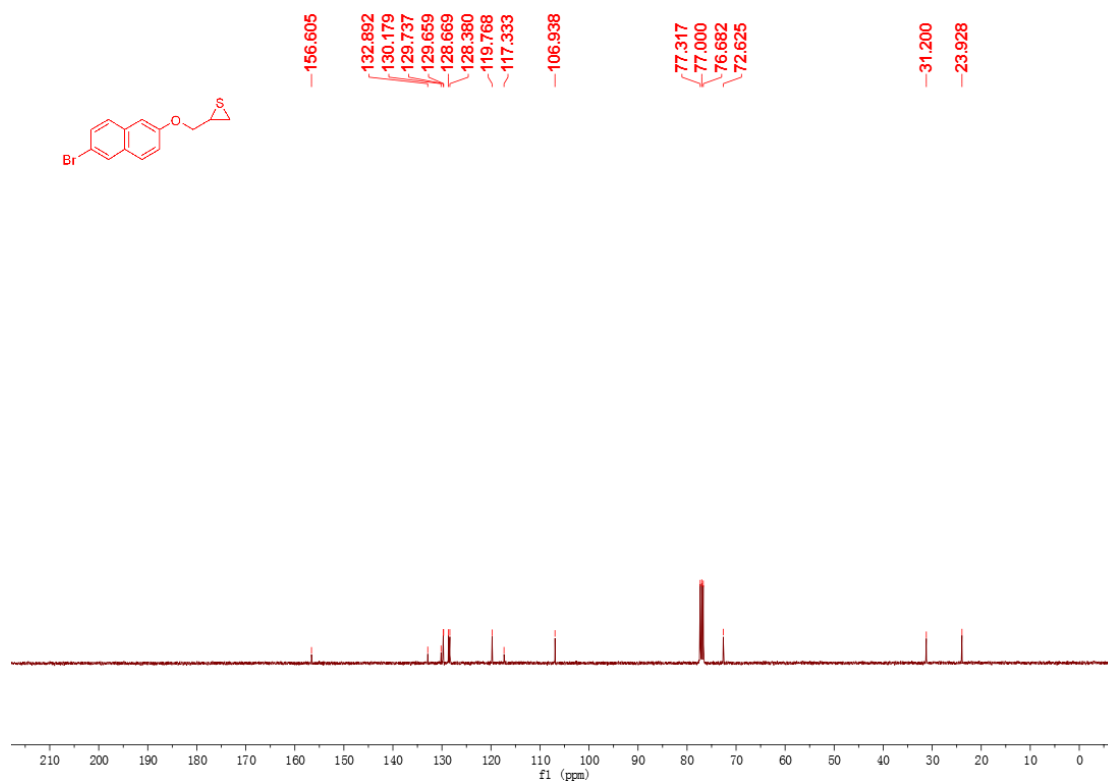
^{13}C NMR (101 MHz, CDCl_3)



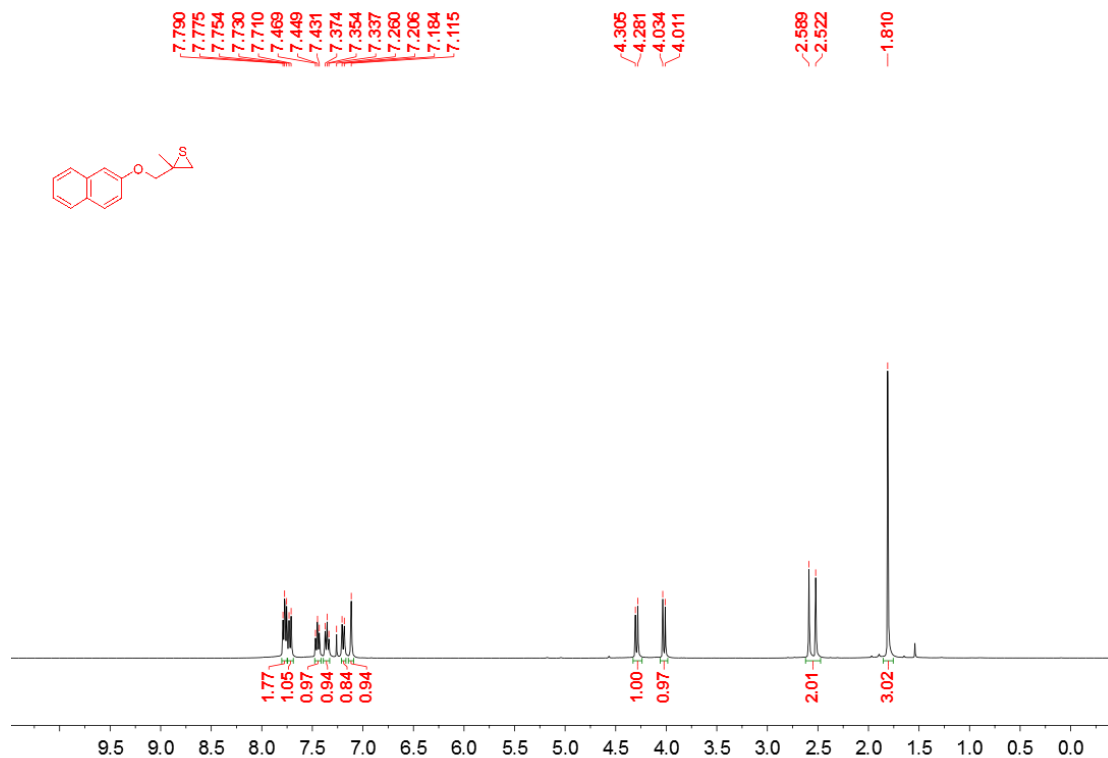
^1H NMR (400 MHz, CDCl_3) of compound **1j**



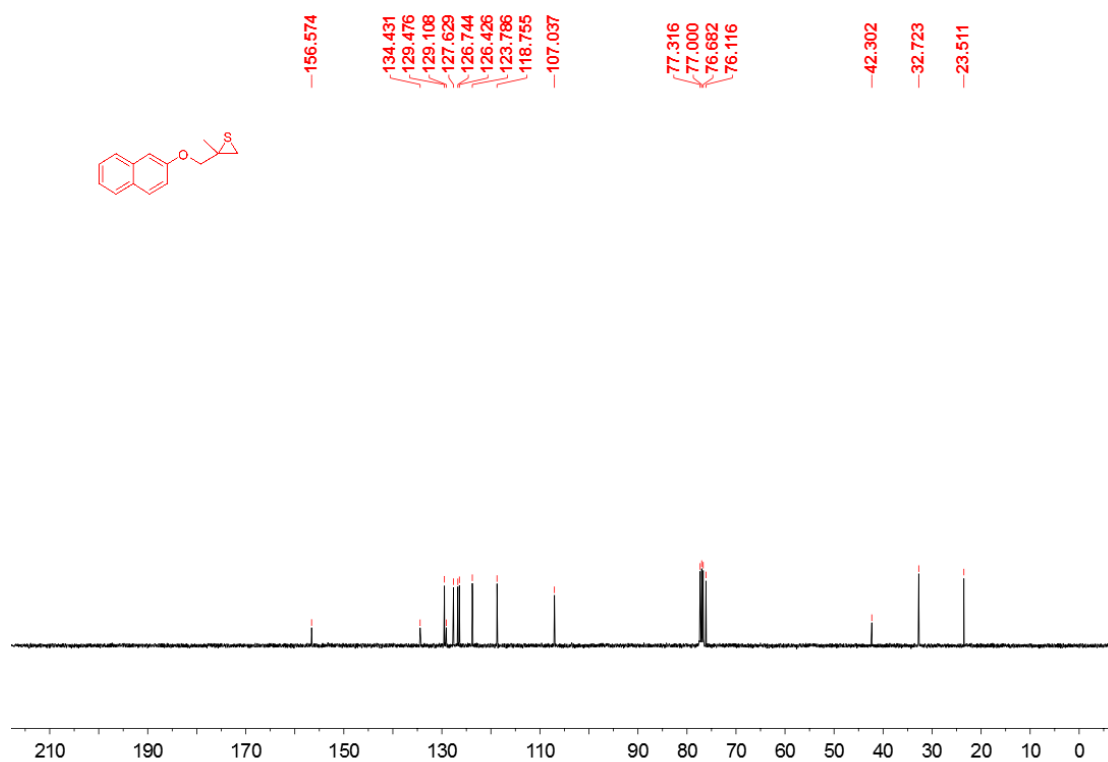
^{13}C NMR (101 MHz, CDCl_3)



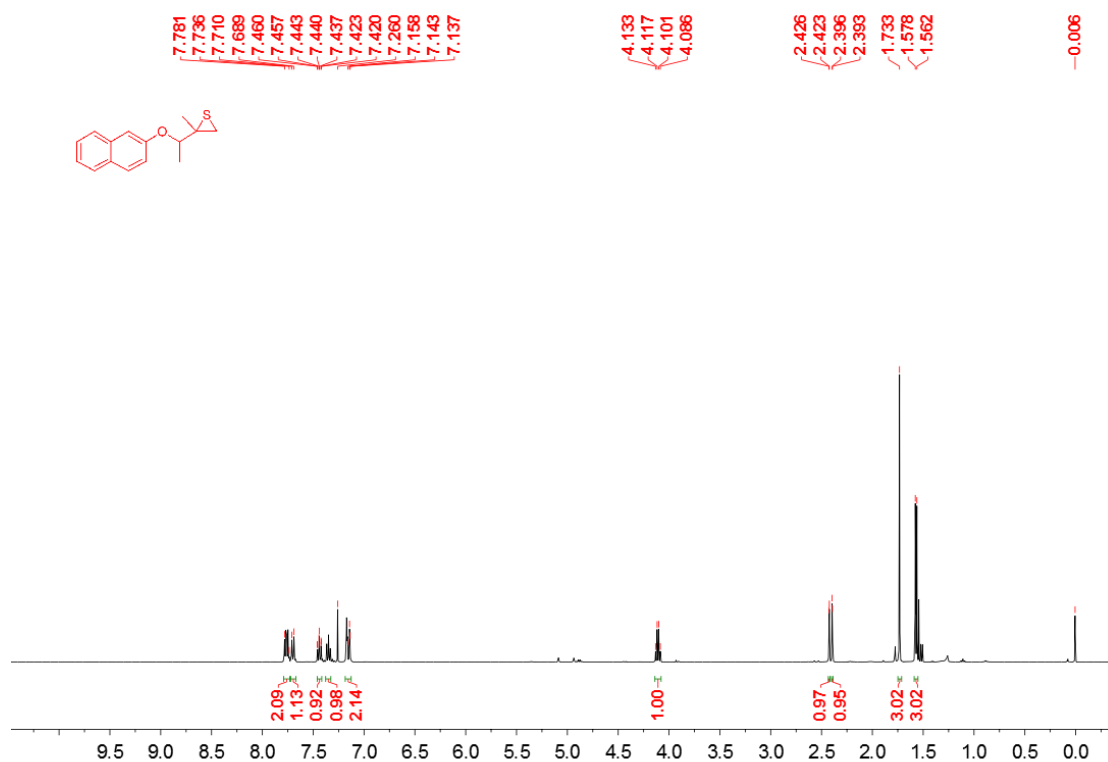
^1H NMR (400 MHz, CDCl_3) of compound **1n**



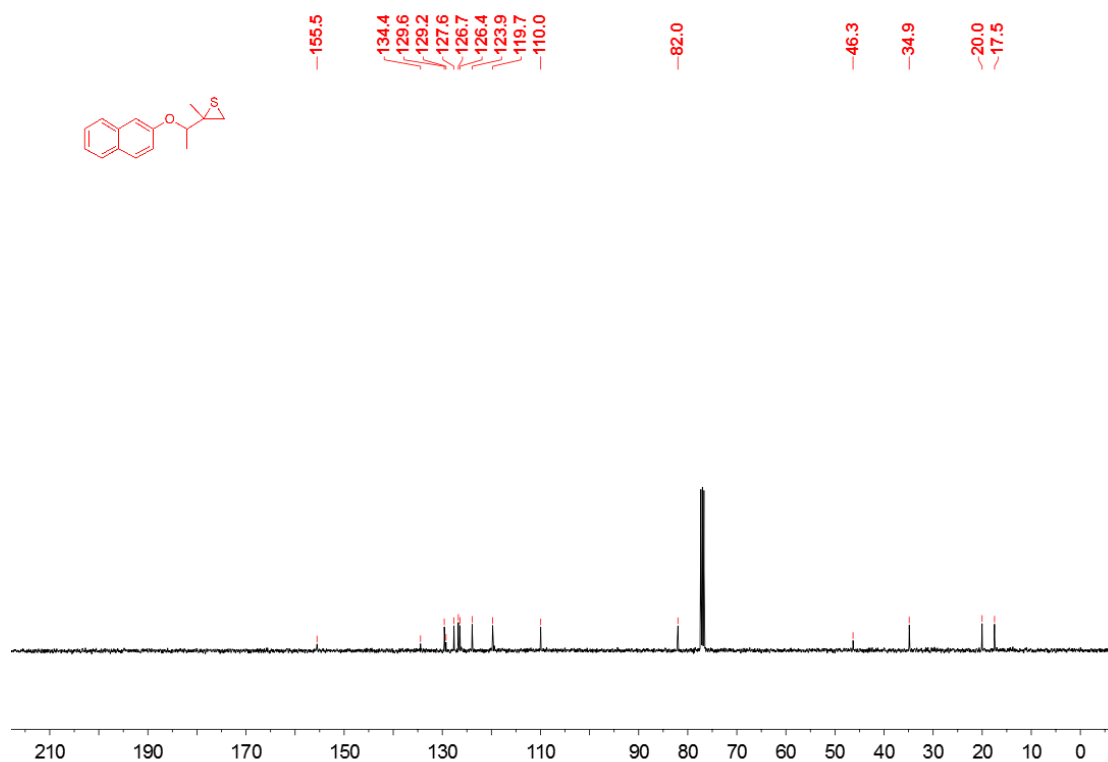
^{13}C NMR (101 MHz, CDCl_3)



^1H NMR (400 MHz, CDCl_3) of compound **1o**



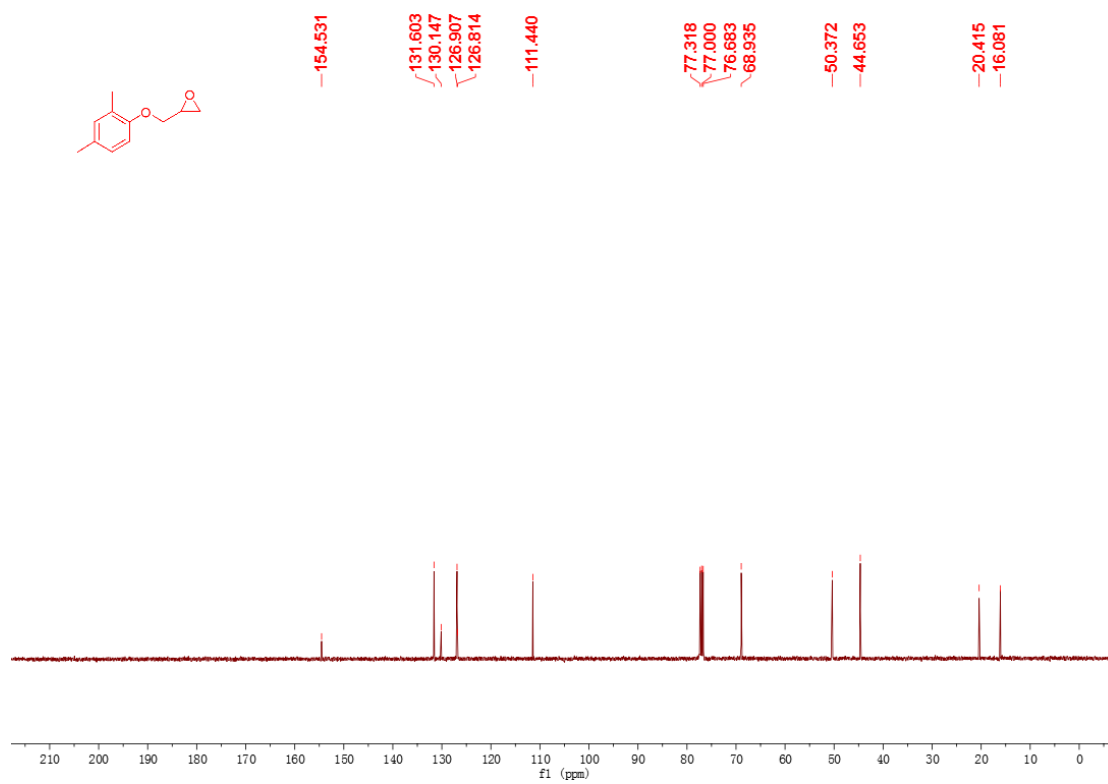
^{13}C NMR (101 MHz, CDCl_3)



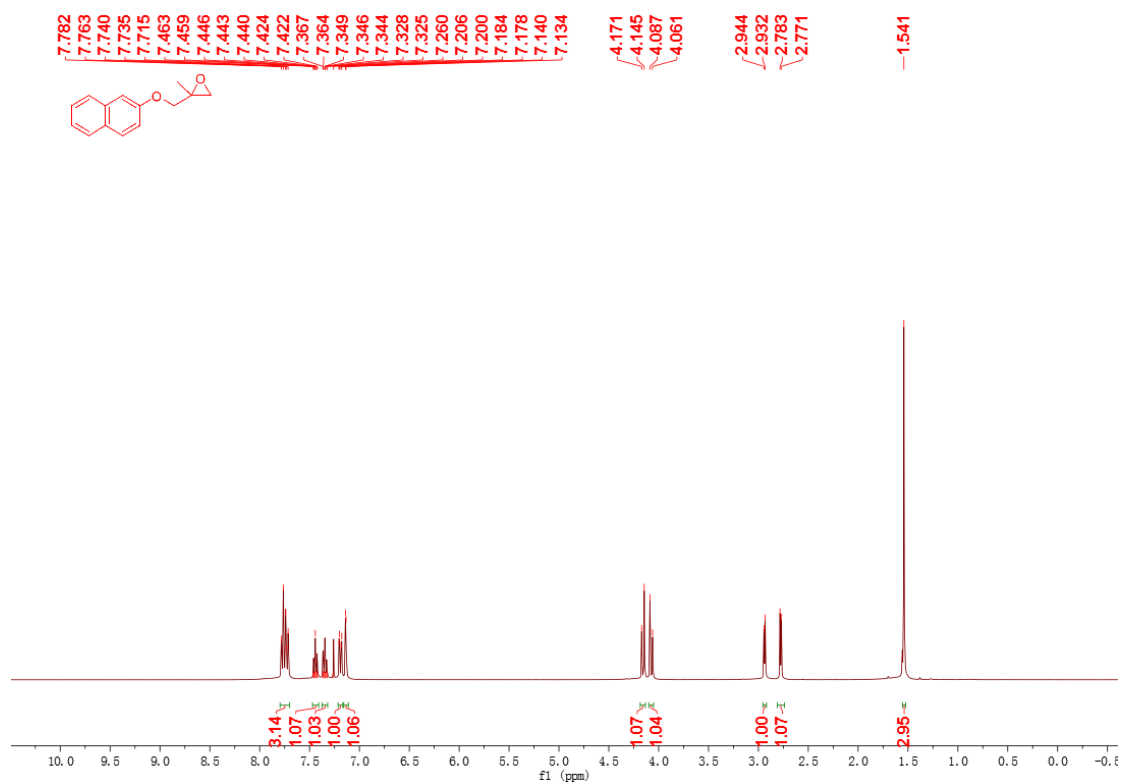
¹H NMR (400 MHz, CDCl₃) of compound **3g**



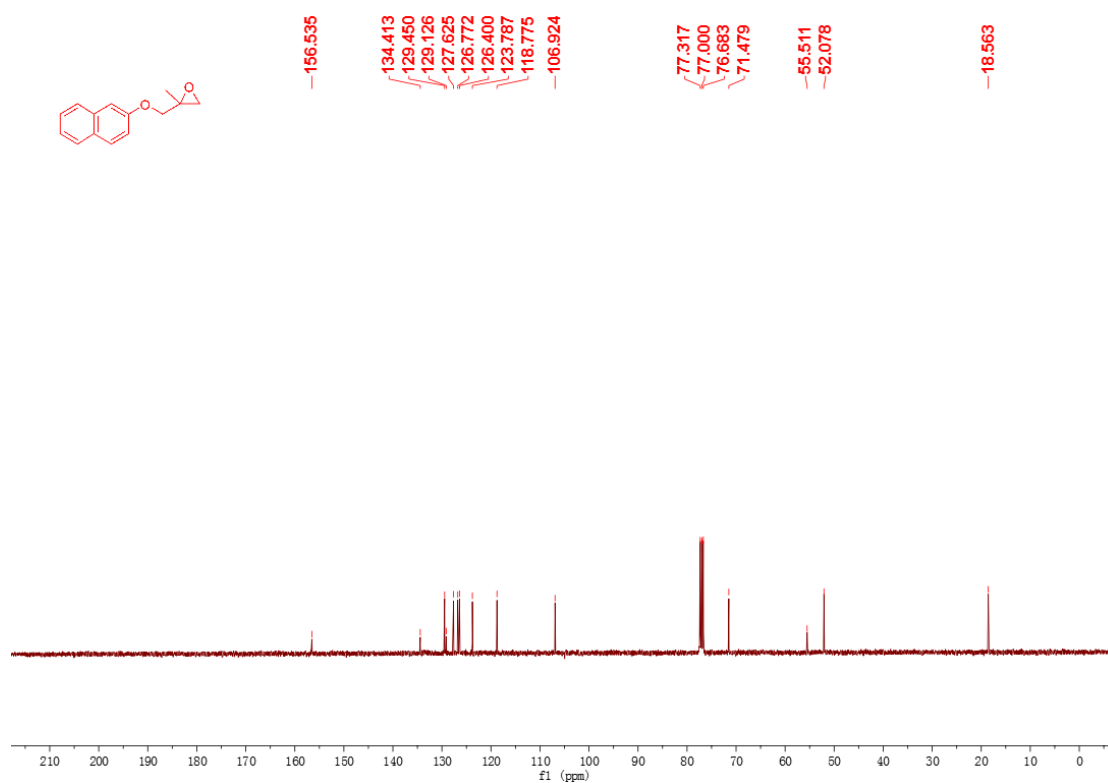
¹³C NMR (101 MHz, CDCl₃)



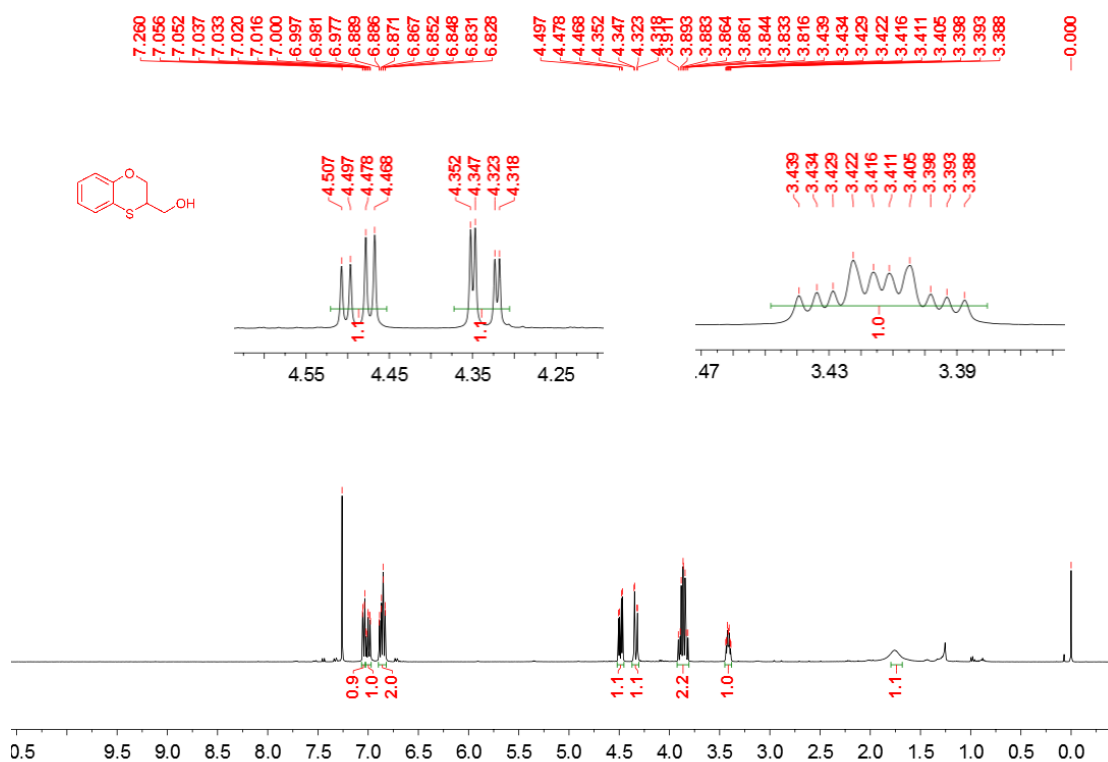
^1H NMR (400 MHz, CDCl_3) of compound **3n**



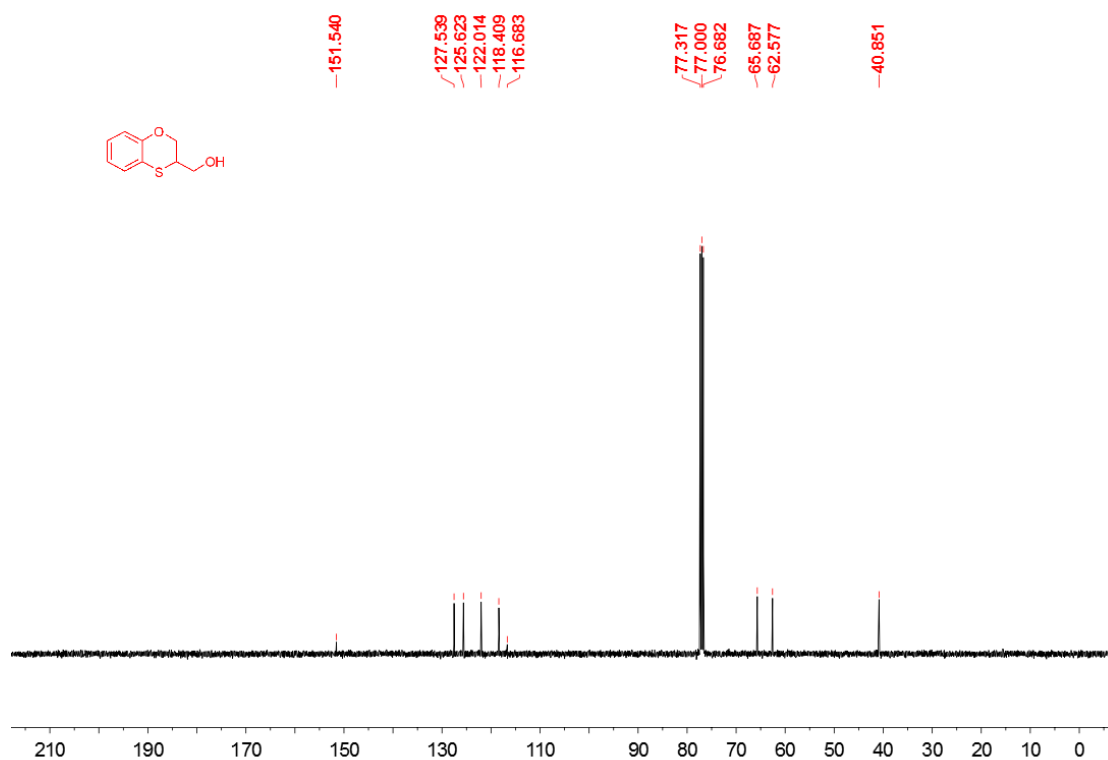
^{13}C NMR (101 MHz, CDCl_3)



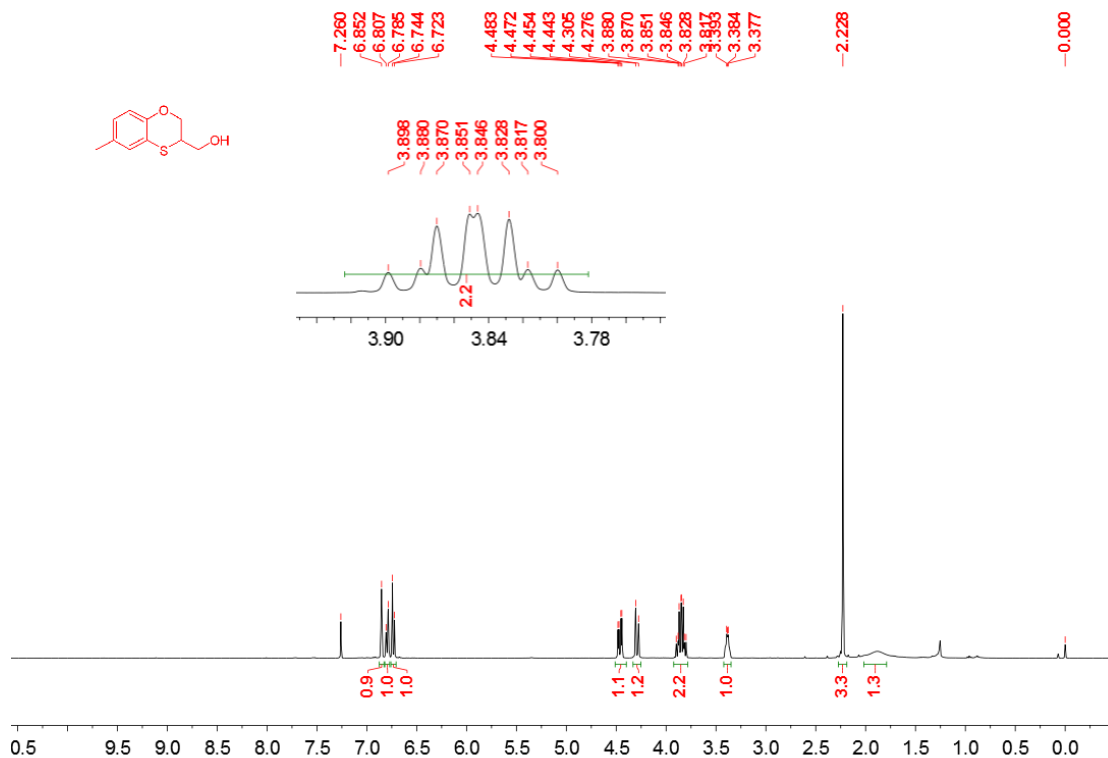
¹H NMR (400 MHz, CDCl₃) of compound **2a**



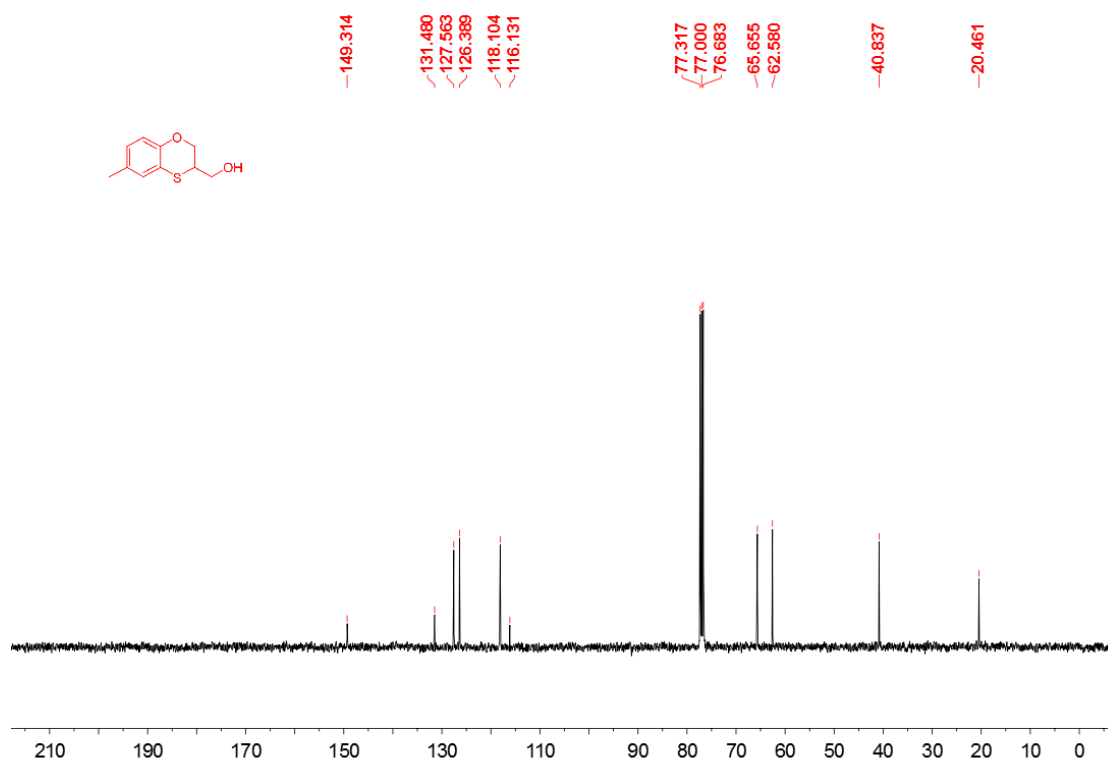
¹³C NMR (101 MHz, CDCl₃)



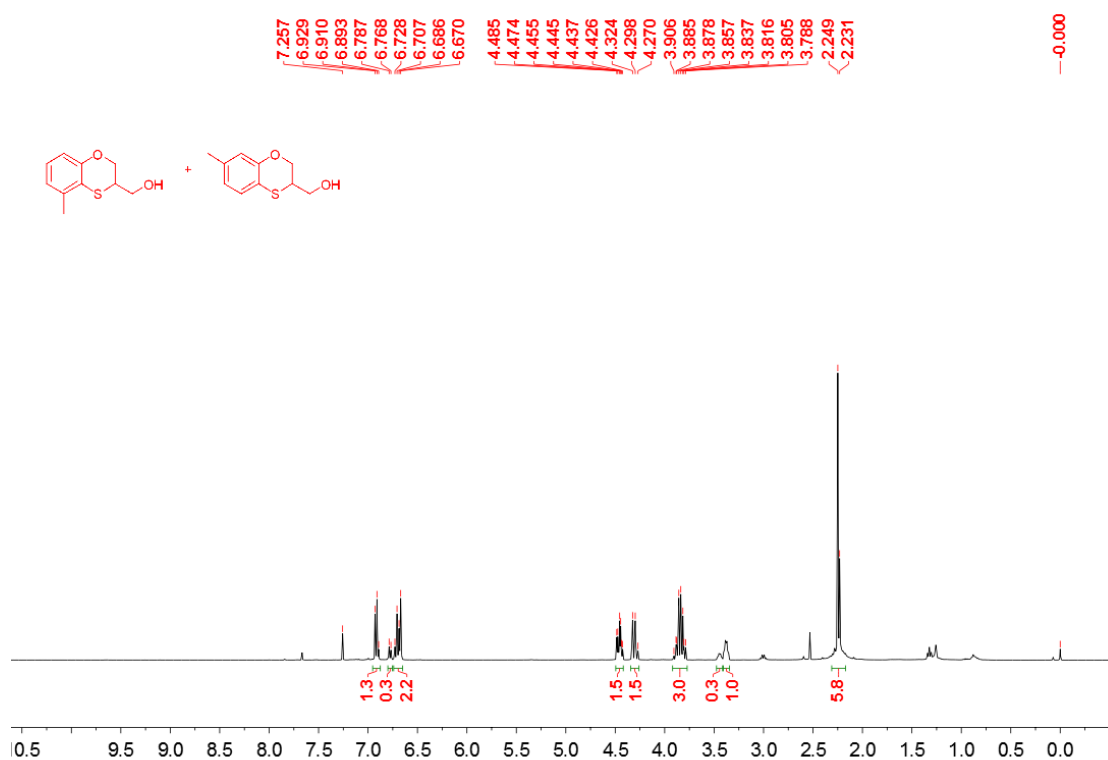
^1H NMR (400 MHz, CDCl_3) of compound **2b**



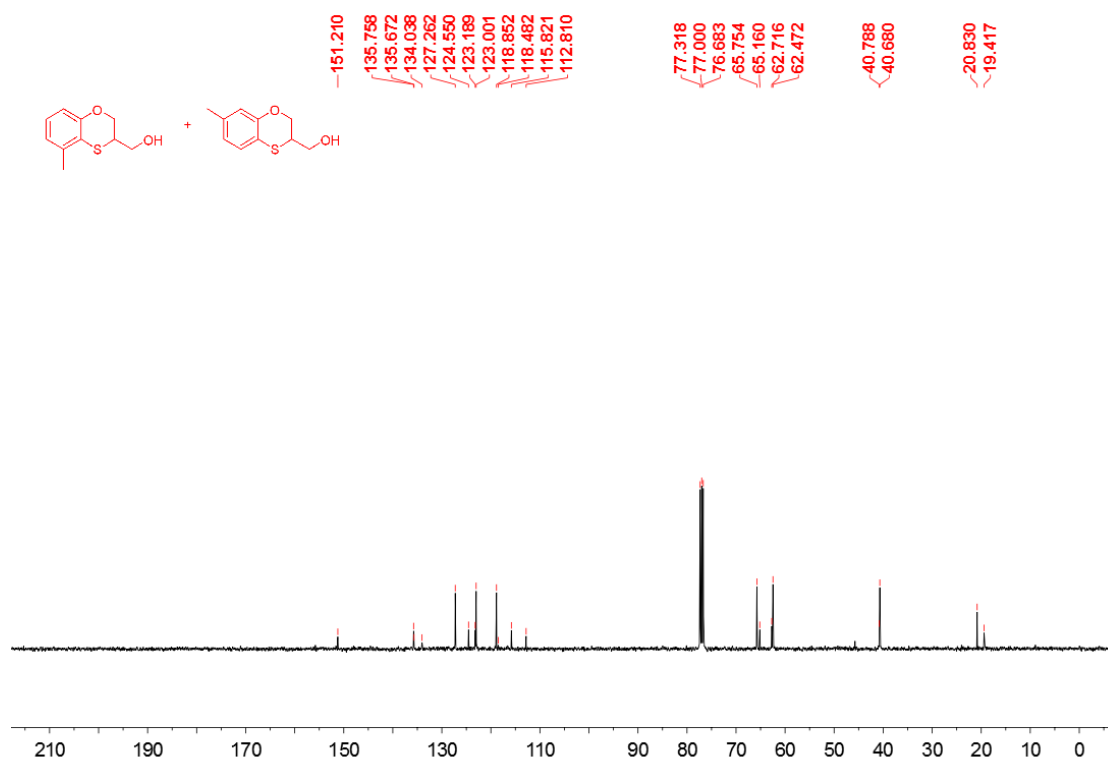
^{13}C NMR (101 MHz, CDCl_3)



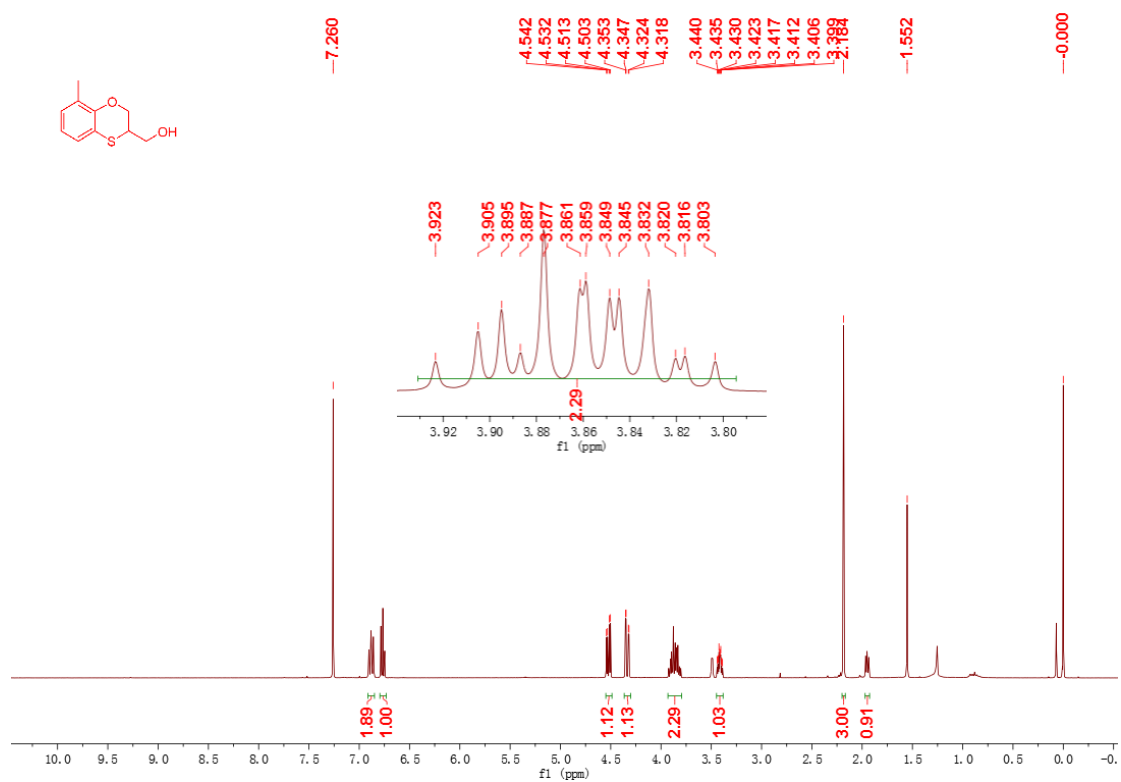
^1H NMR (400 MHz, CDCl_3) of compound **2c**



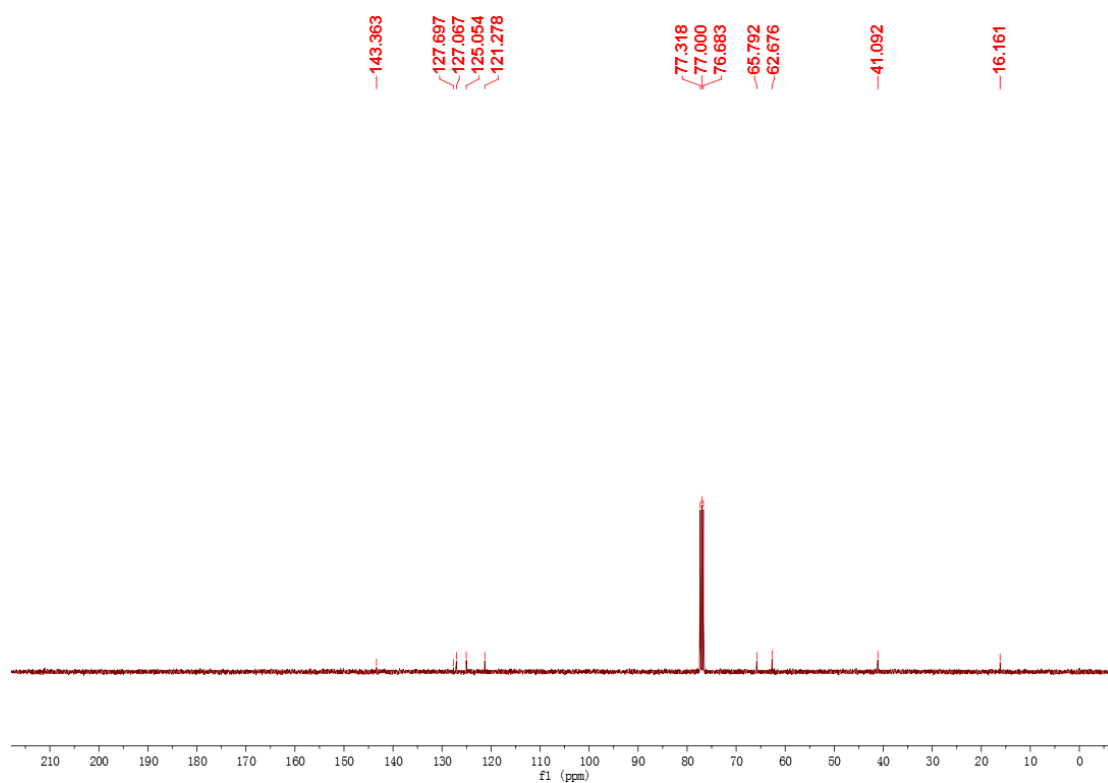
^{13}C NMR (101 MHz, CDCl_3)



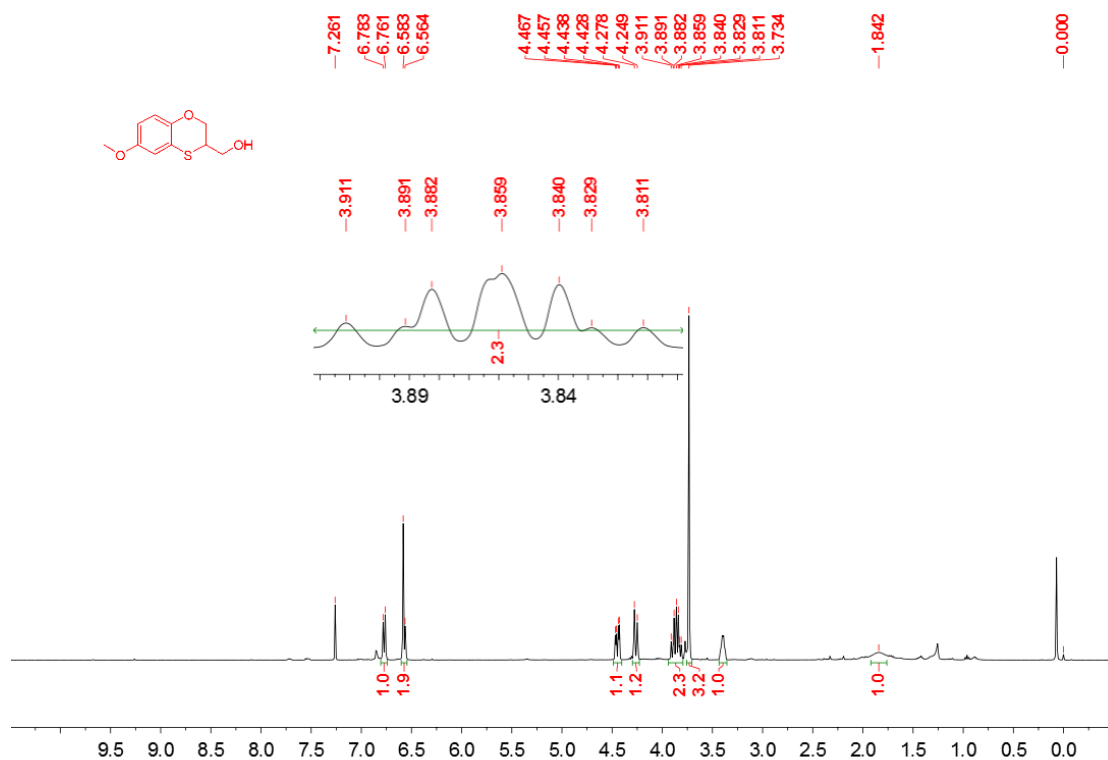
^1H NMR (400 MHz, CDCl_3) of compound **2d**



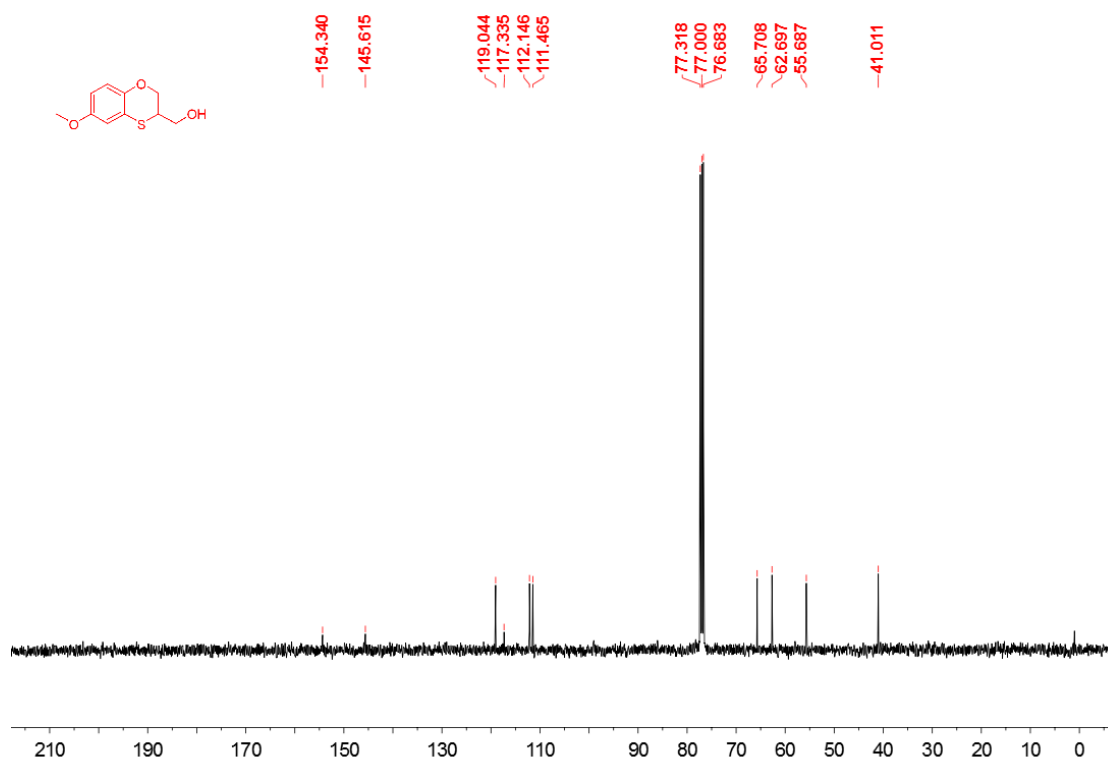
^{13}C NMR (101 MHz, CDCl_3)



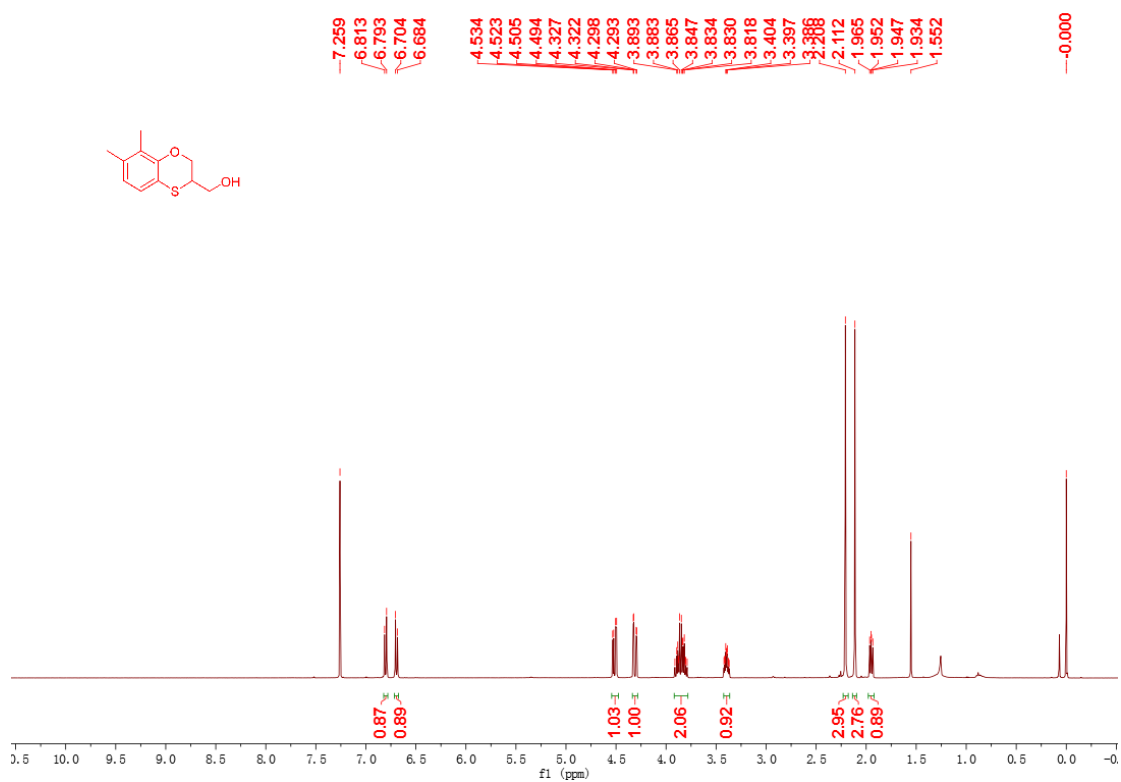
^1H NMR (400 MHz, CDCl_3) of compound **2e**



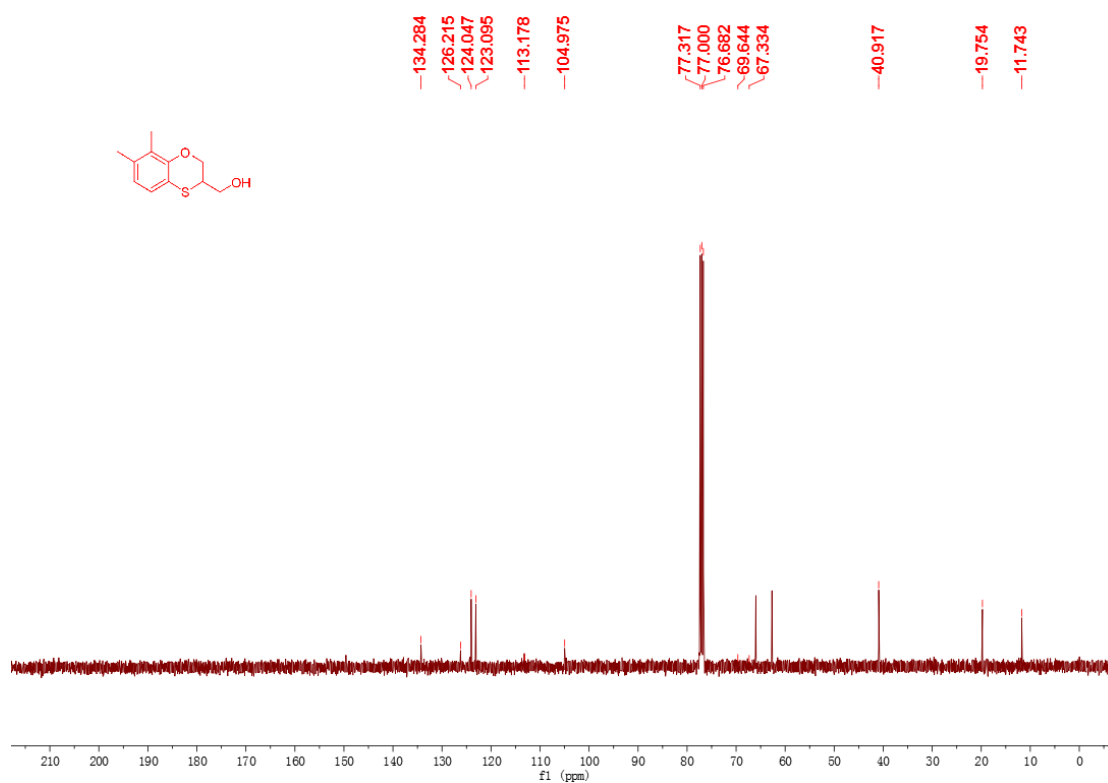
^{13}C NMR (101 MHz, CDCl_3)



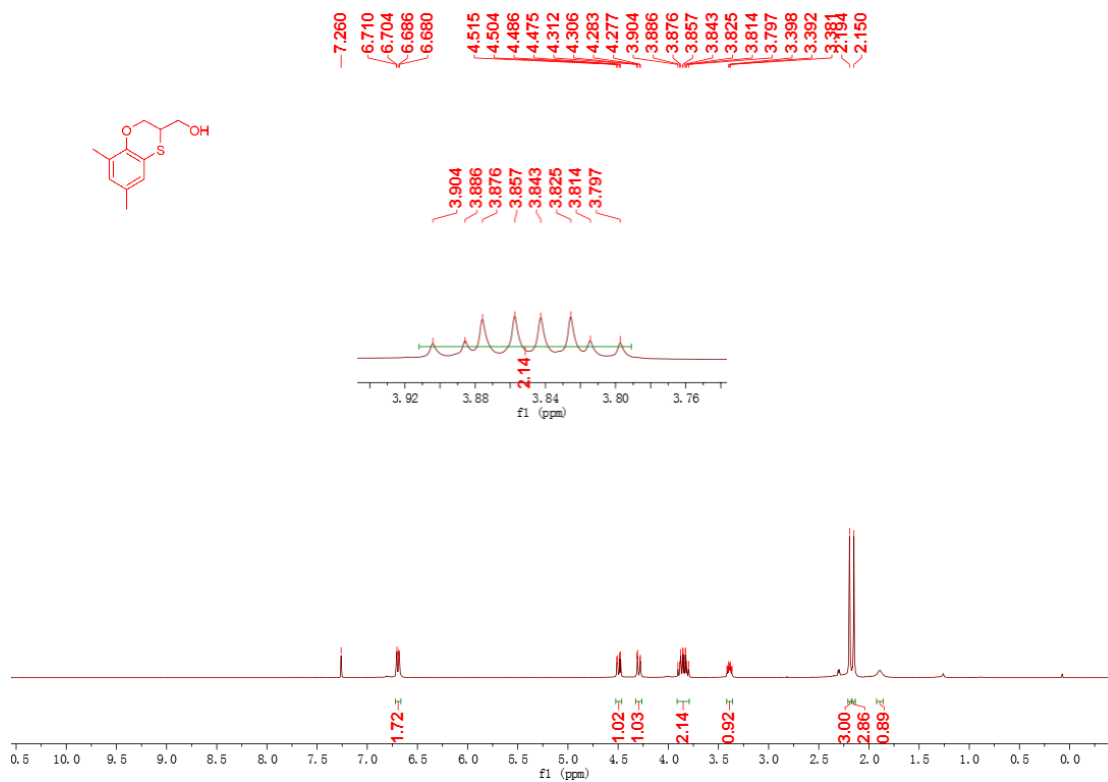
^1H NMR (400 MHz, CDCl_3) of compound **2f**



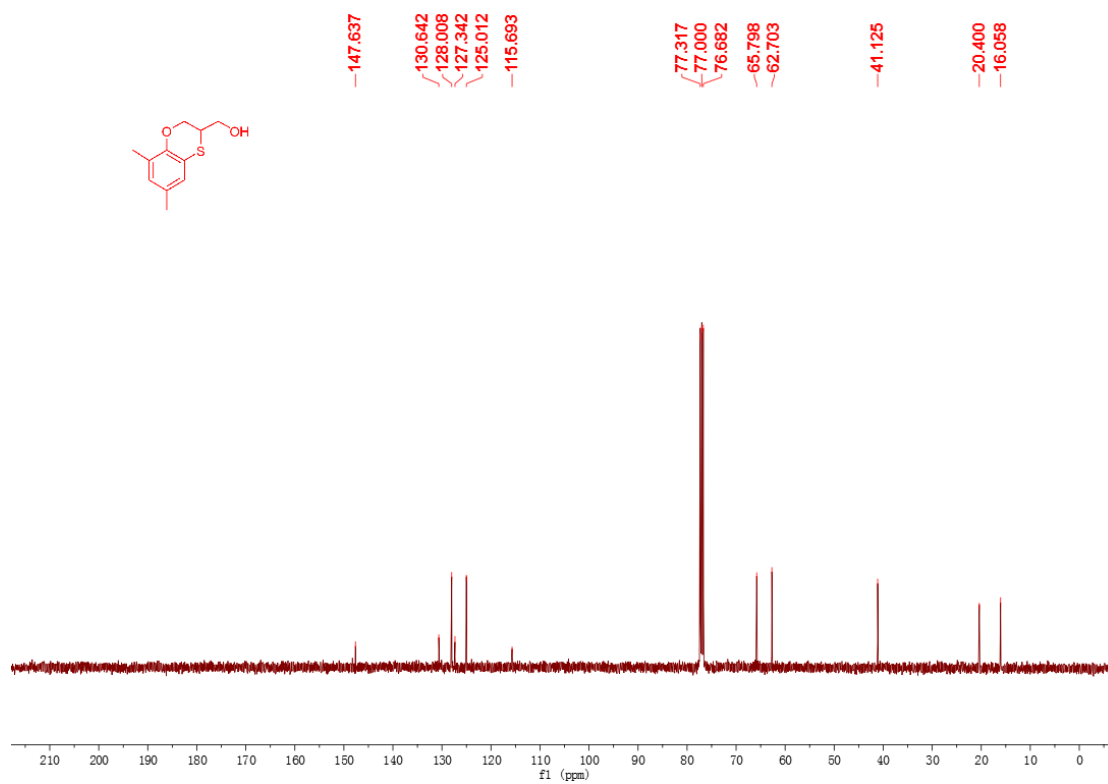
^{13}C NMR (101 MHz, CDCl_3)



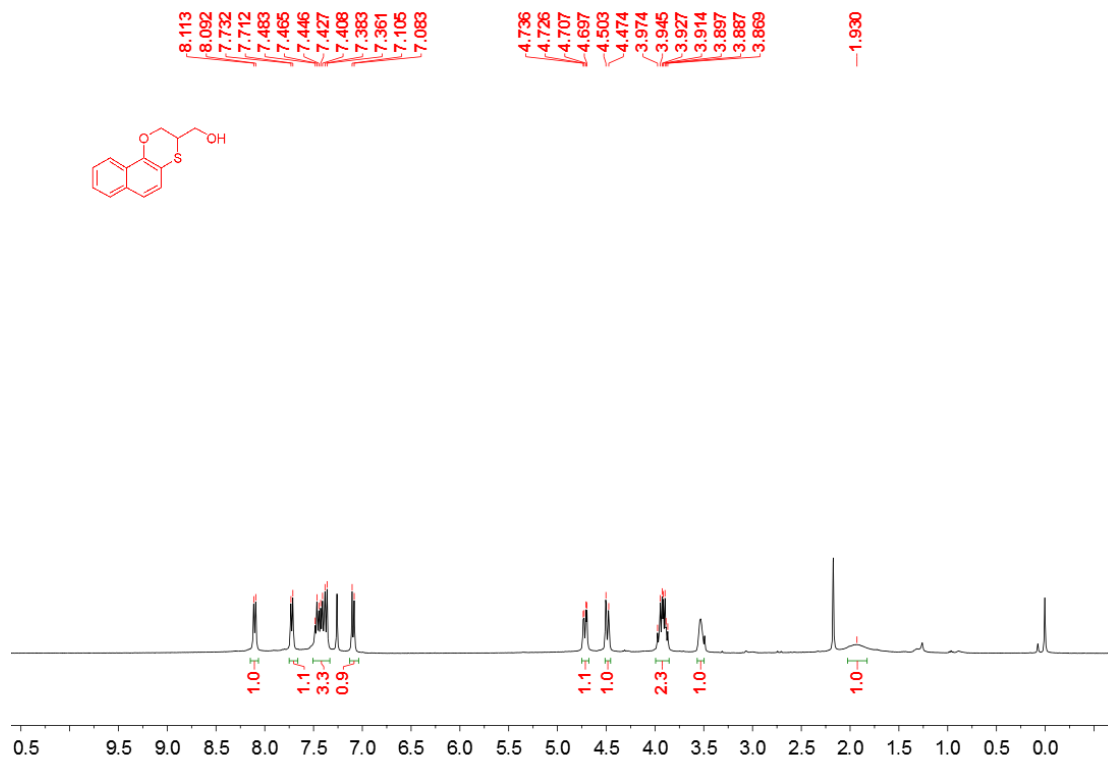
^1H NMR (400 MHz, CDCl_3) of compound **2g**



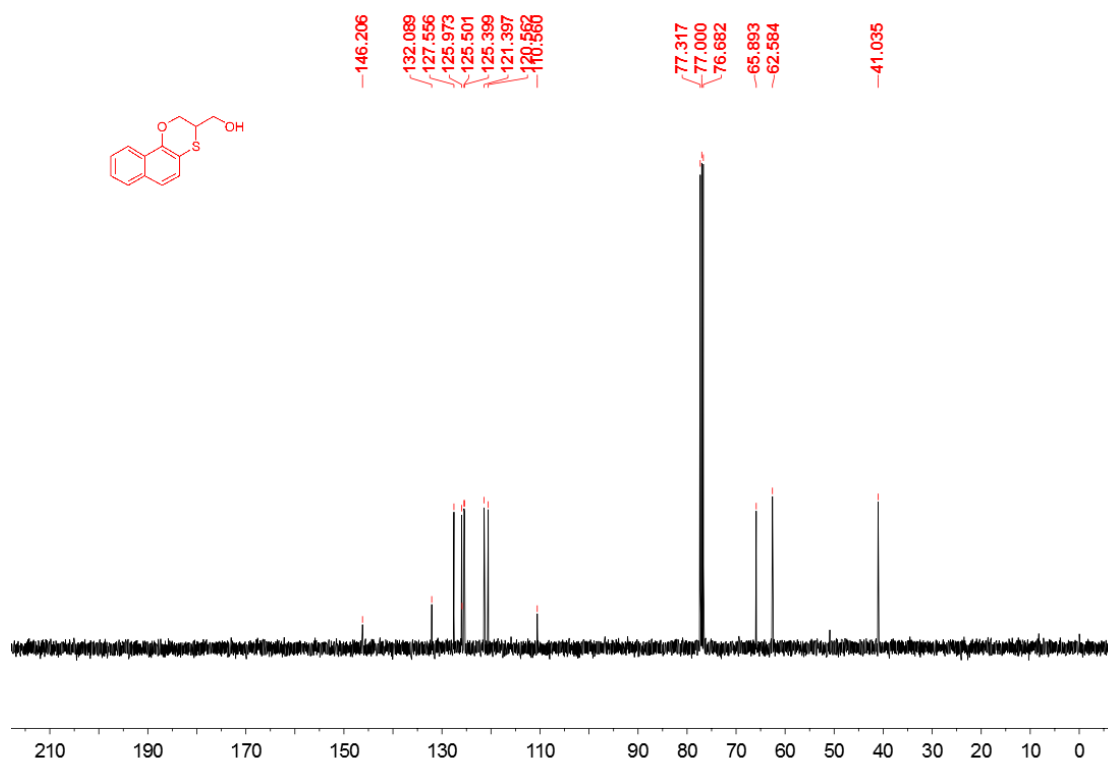
^{13}C NMR (101 MHz, CDCl_3)



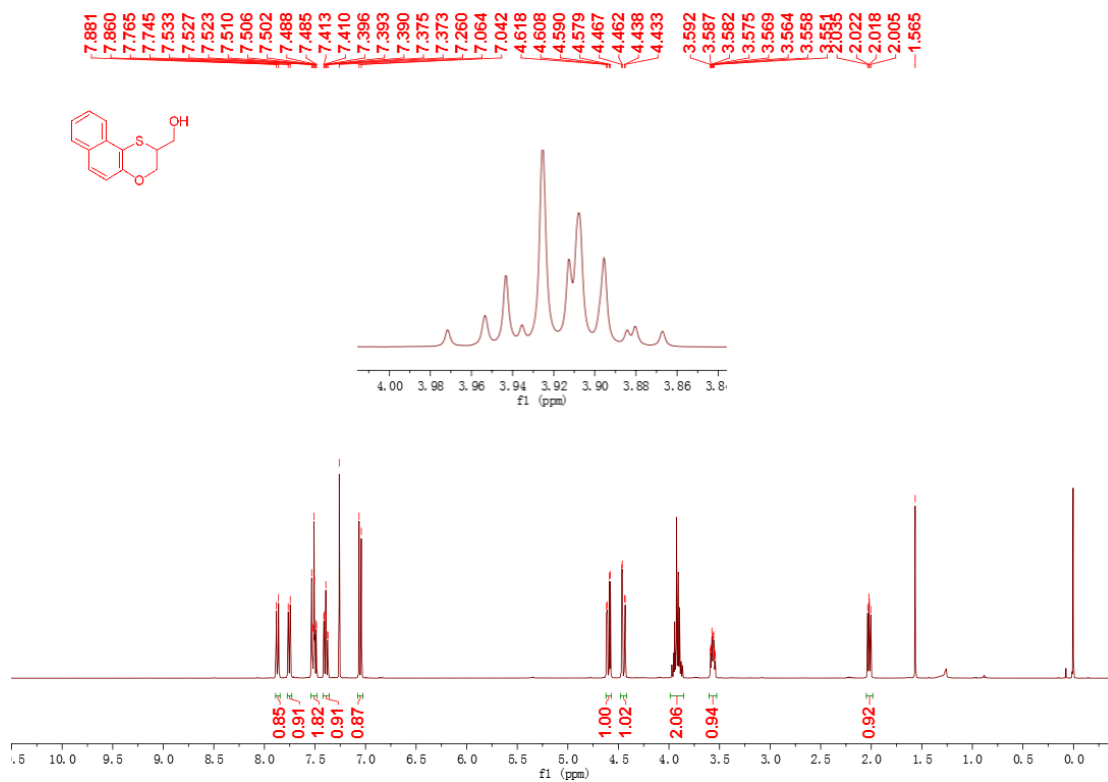
^1H NMR (400 MHz, CDCl_3) of compound **2h**



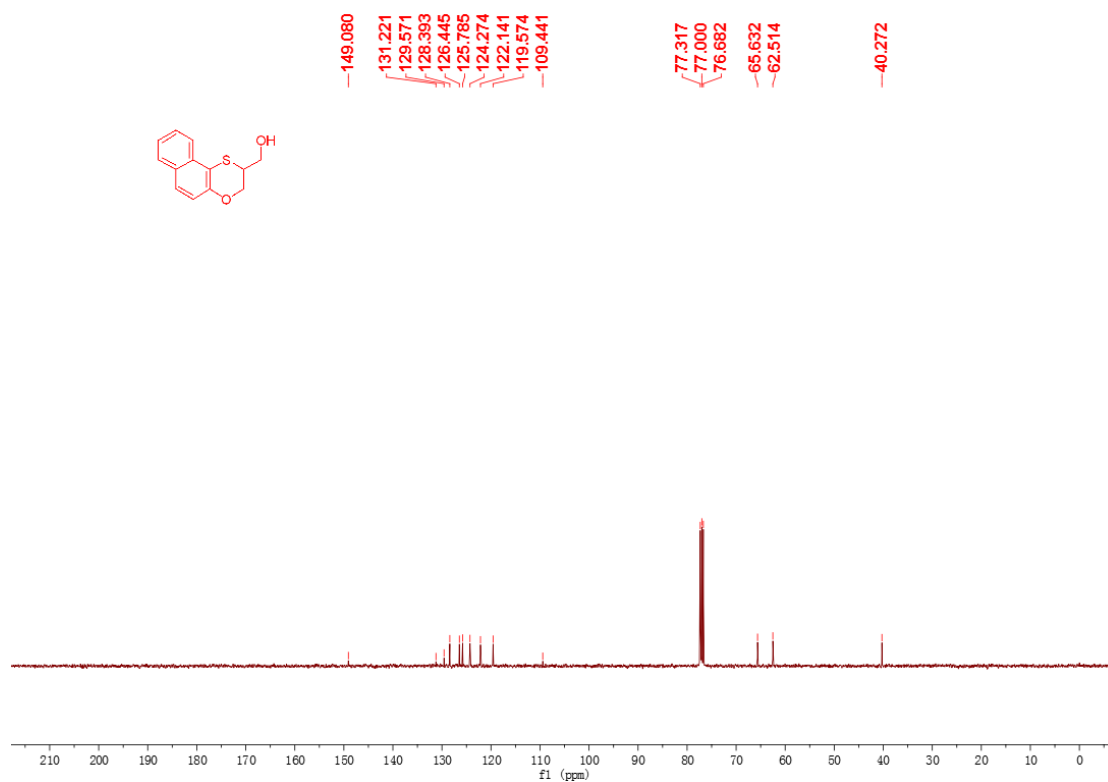
^{13}C NMR (101 MHz, CDCl_3)



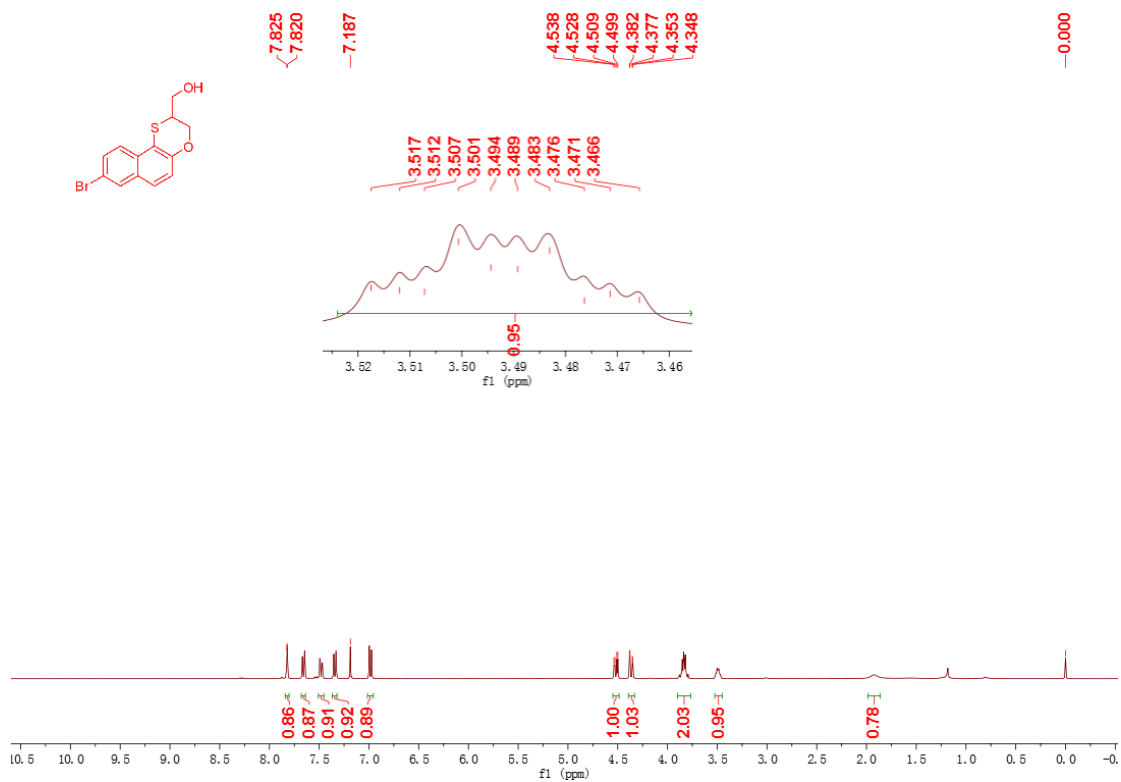
^1H NMR (400 MHz, CDCl_3) of compound **2i**



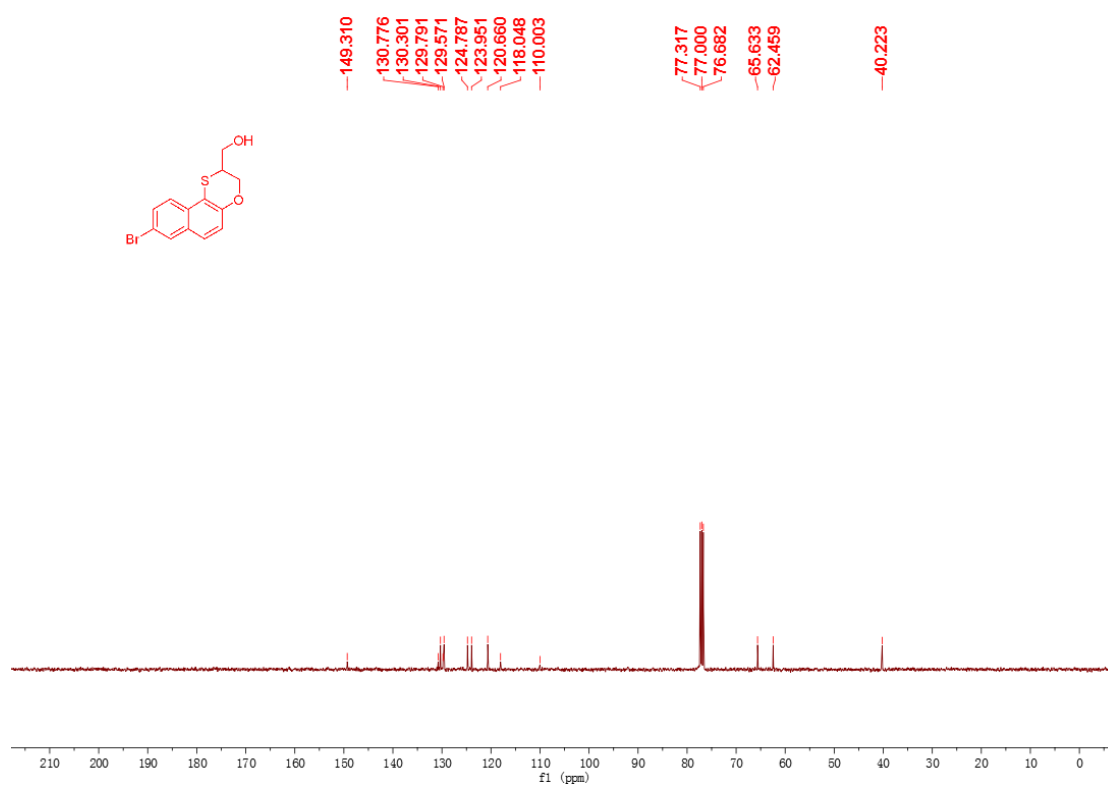
^{13}C NMR (101 MHz, CDCl_3)



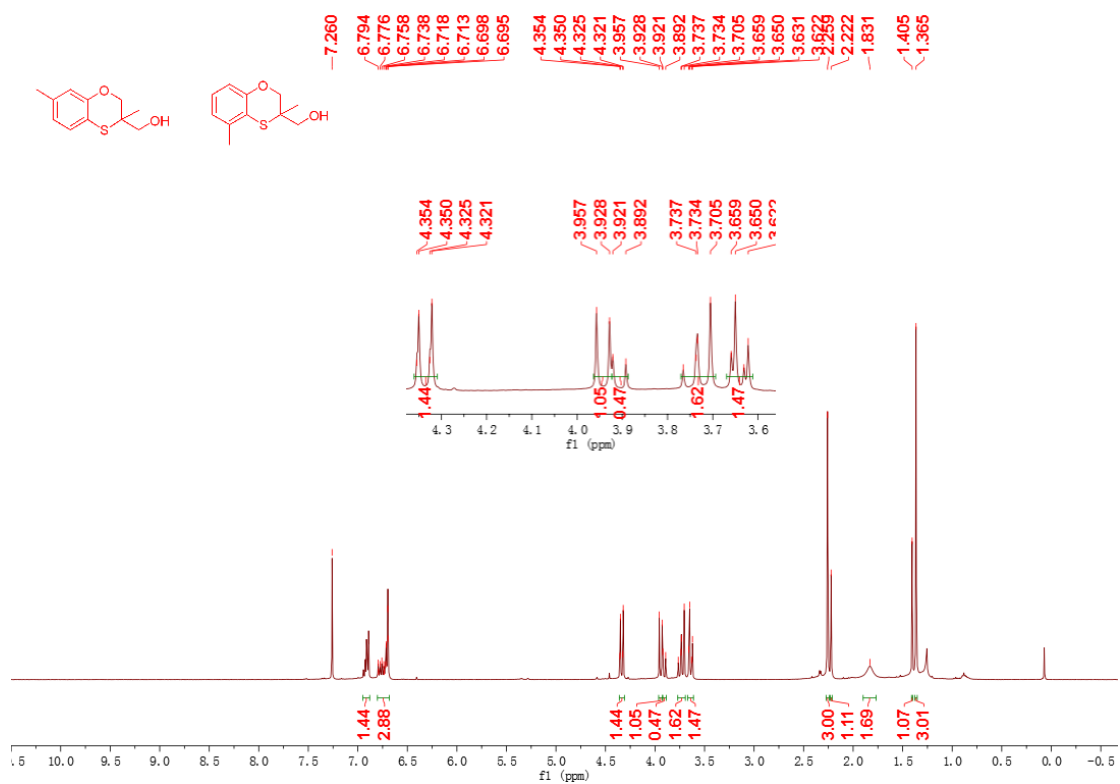
^1H NMR (400 MHz, CDCl_3) of compound **2j**



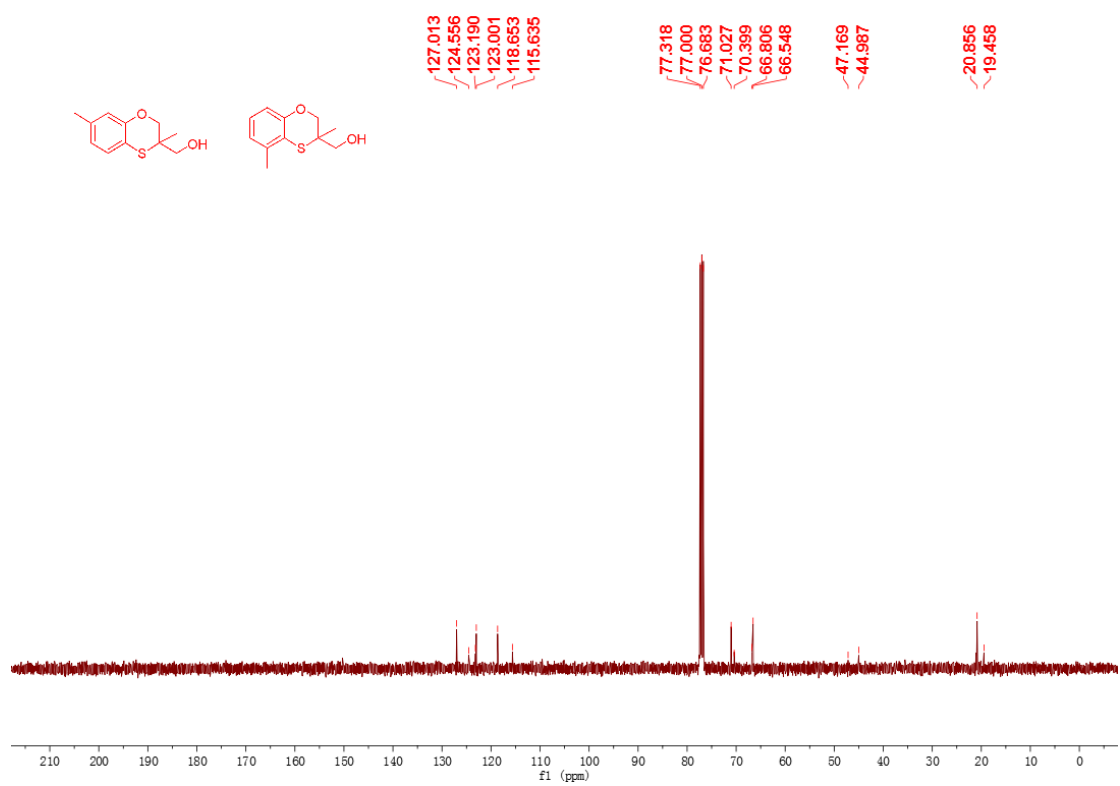
^{13}C NMR (101 MHz, CDCl_3)



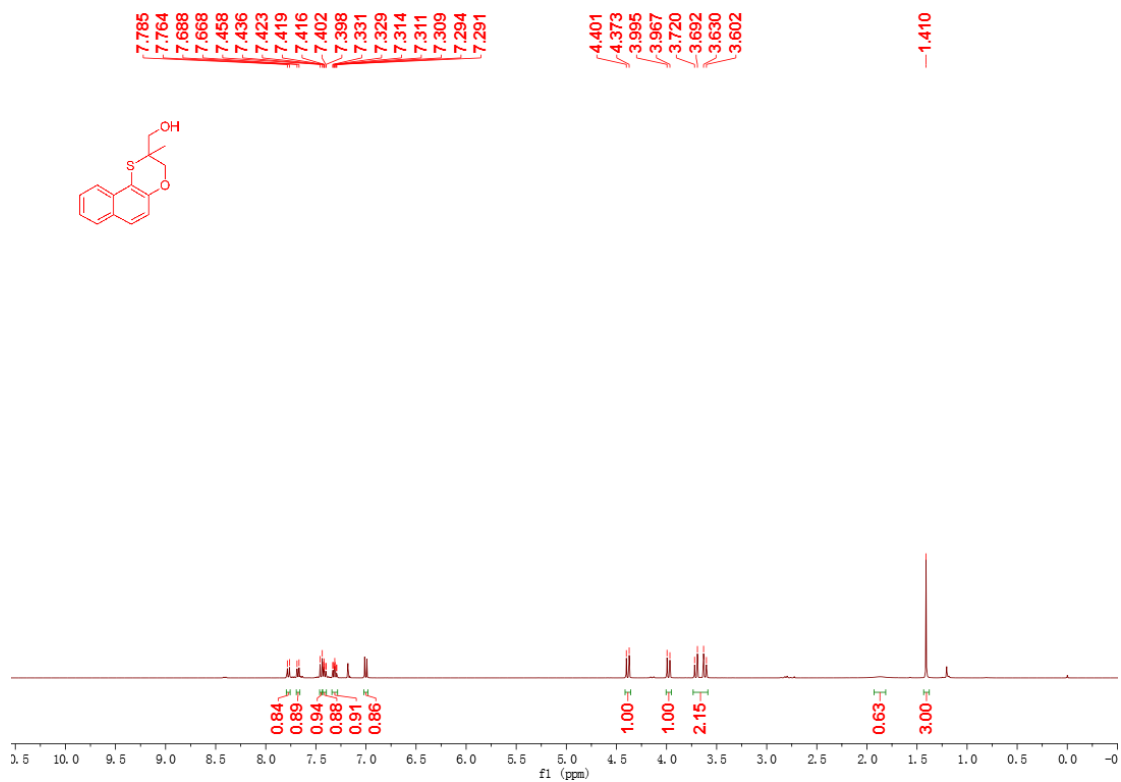
^1H NMR (400 MHz, CDCl_3) of compound **2m**



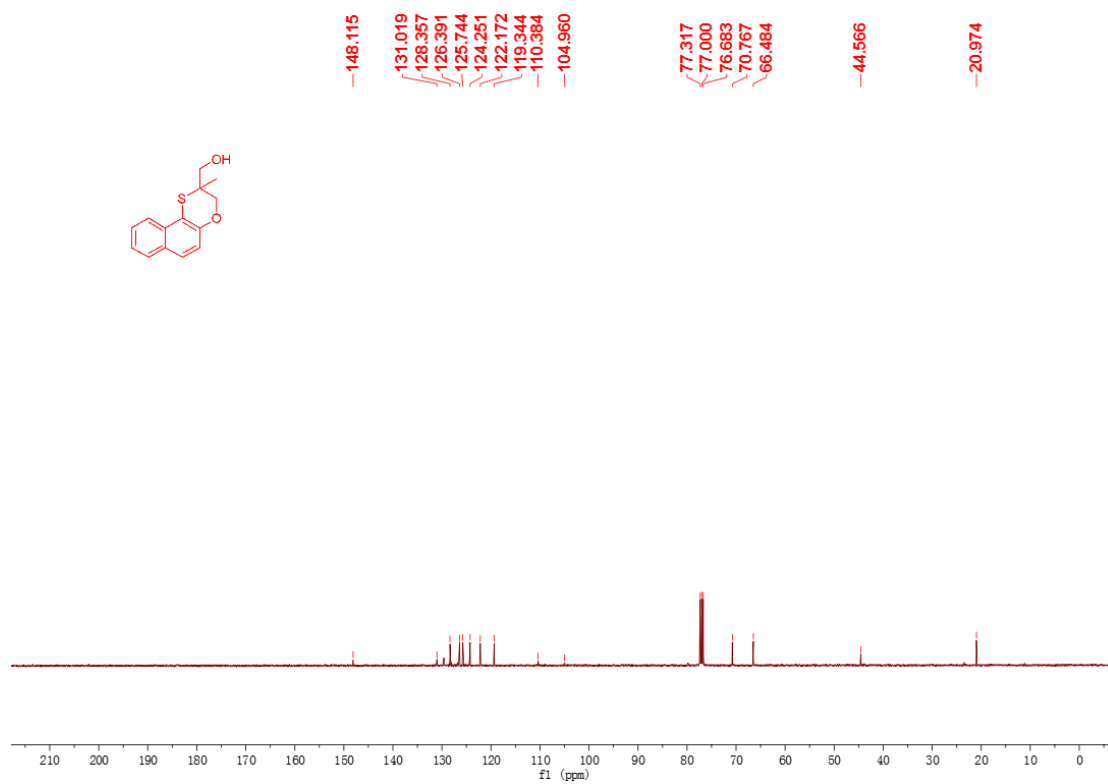
^{13}C NMR (101 MHz, CDCl_3)



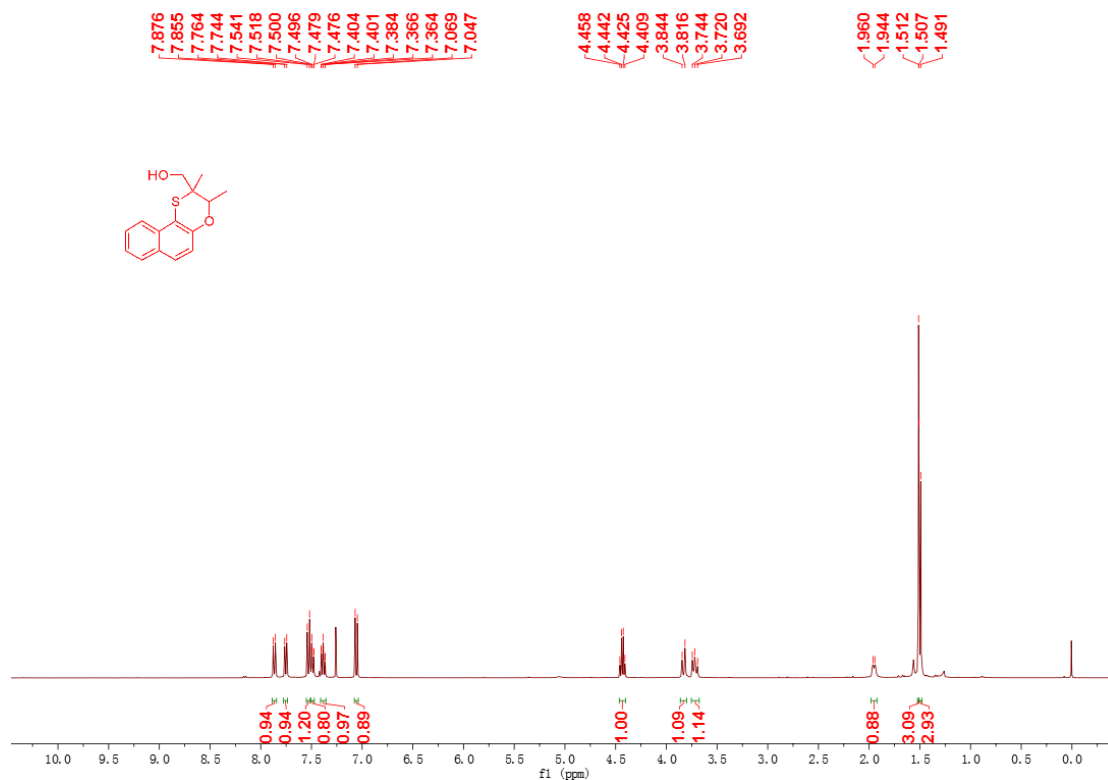
^1H NMR (400 MHz, CDCl_3) of compound **2n**



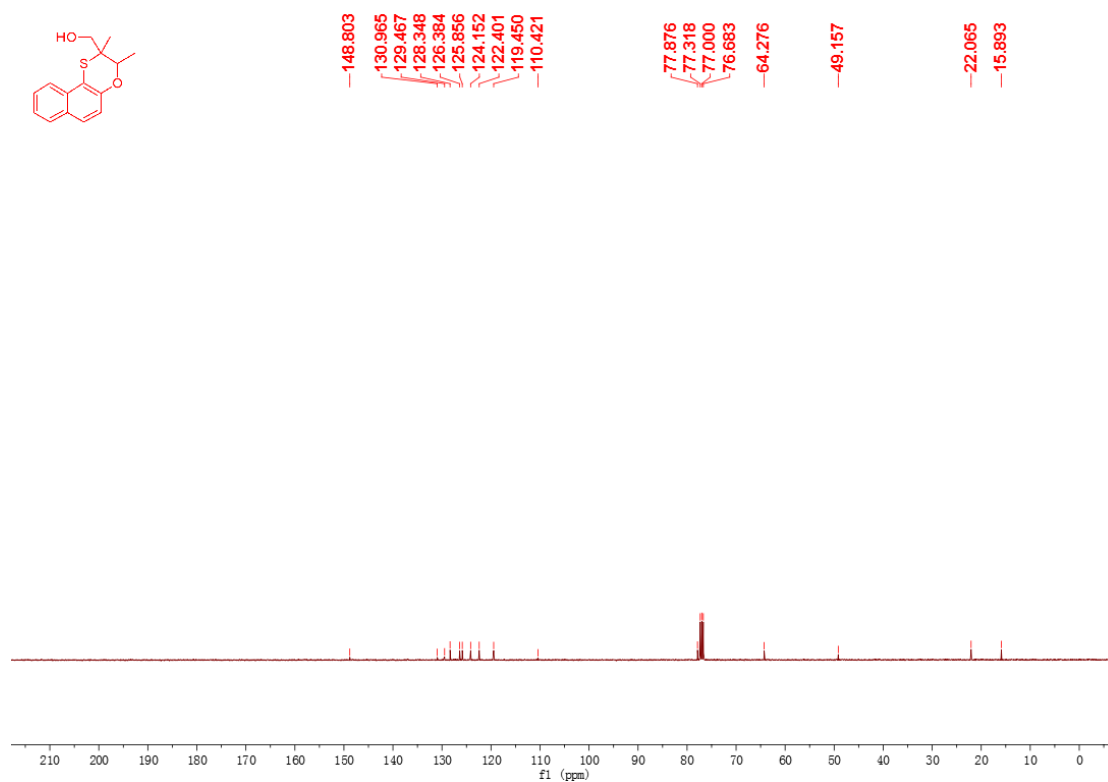
^{13}C NMR (101 MHz, CDCl_3)



^1H NMR (400 MHz, CDCl_3) of compound **2o**



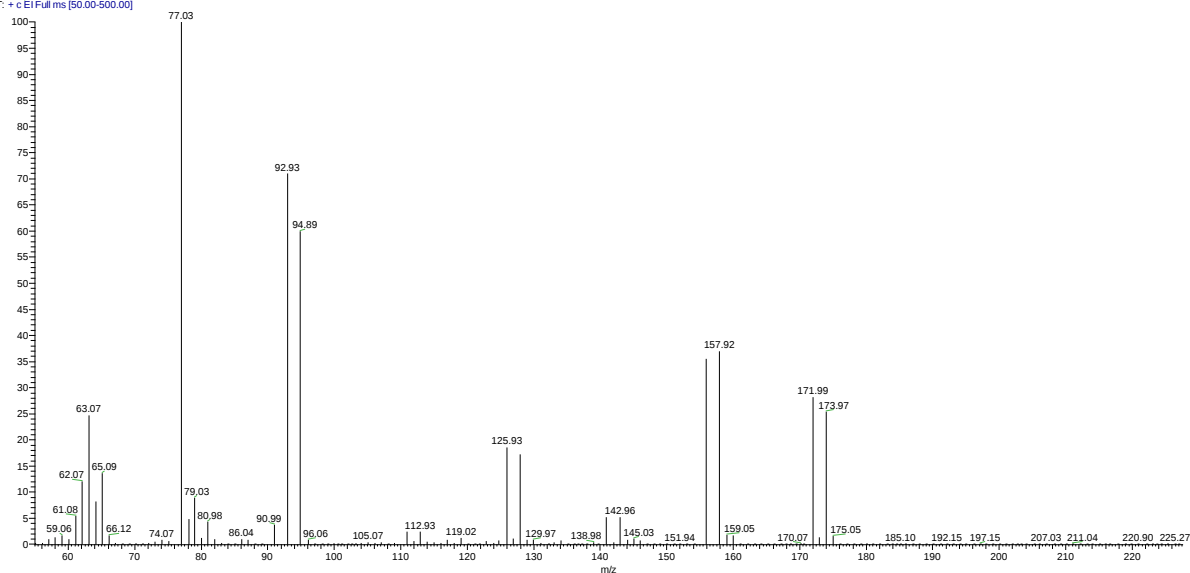
^{13}C NMR (101 MHz, CDCl_3)



Copies of mass spectra of byproducts in reaction mixtures

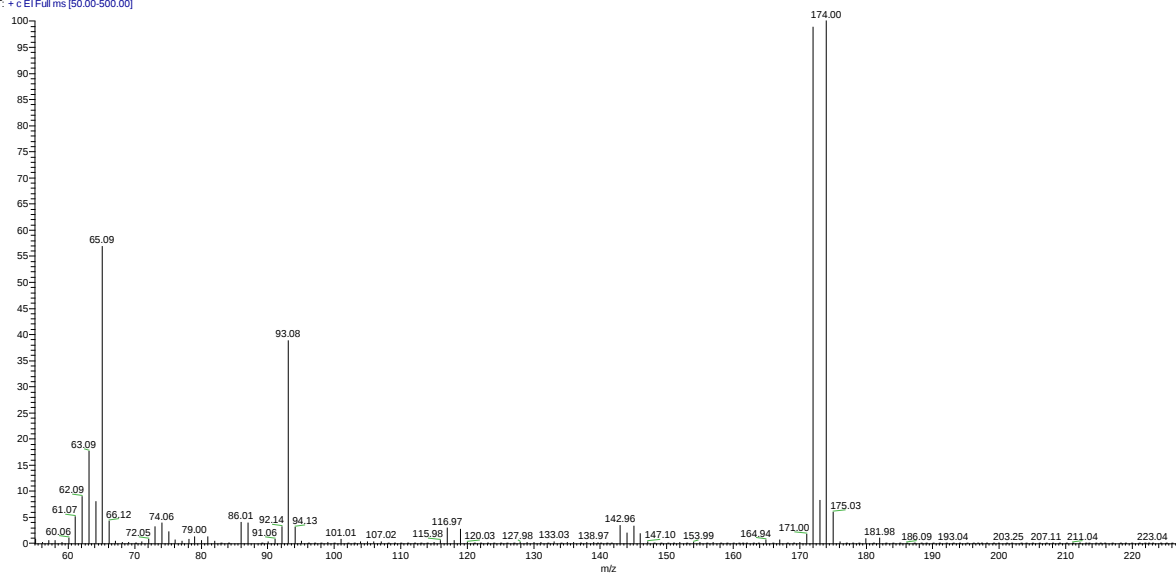
4-Bromophenol

Dongji750-b #1042 RT: 6.54 AV: 1 NL: 1.05E8
T: + c EI Full ms [50.00-500.00]



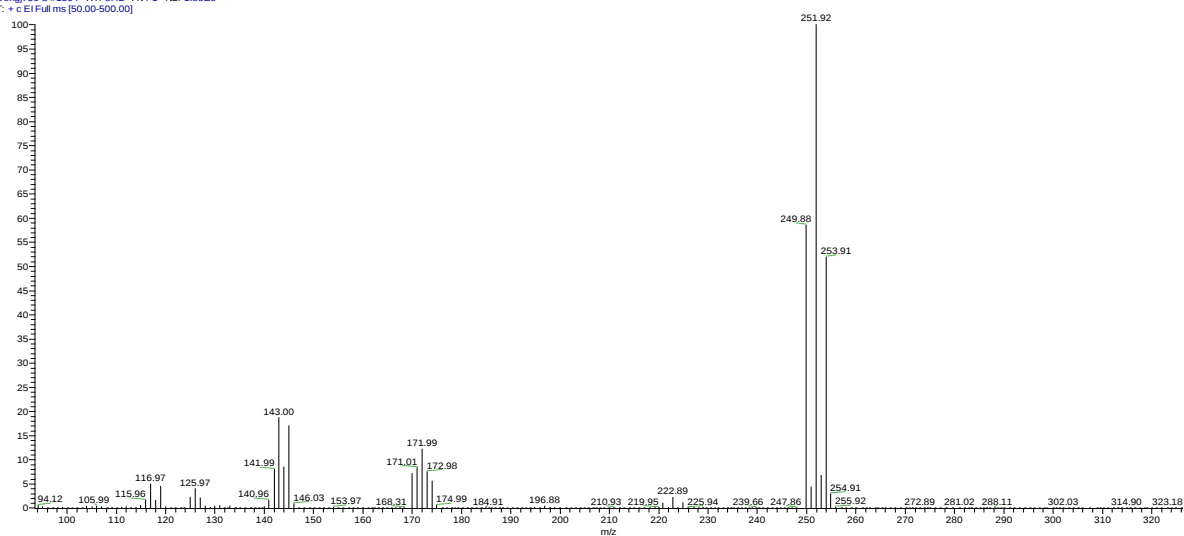
2-Bromophenol

Dongji750-b #1456 RT: 7.95 AV: 1 NL: 1.81E8
T: + c EI Full ms [50.00-500.00]



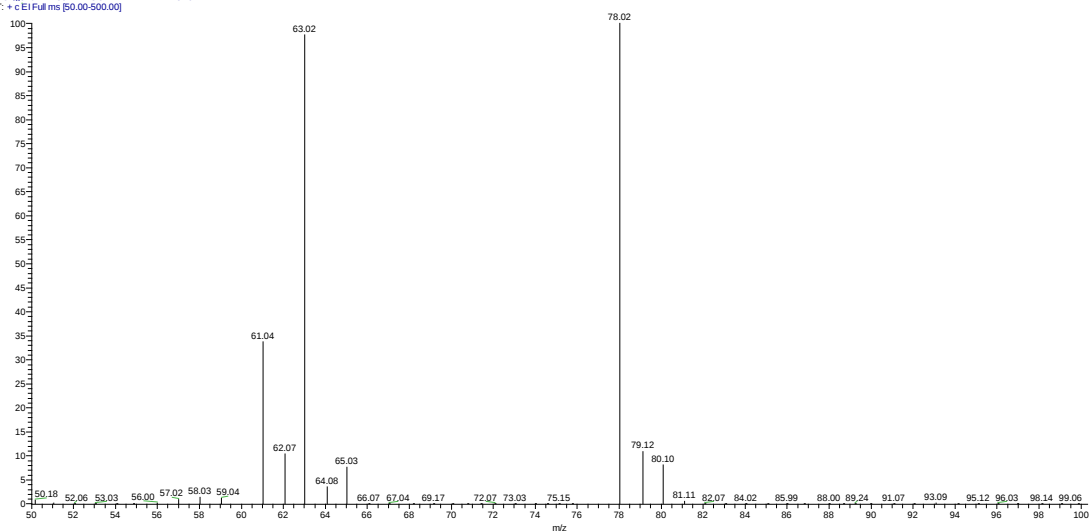
2,4-Dibromophenol

Dongji750-b #1594 RT: 8.42 AV: 1 NL: 1.88E8
T: + c EI Full ms [50.00-500.00]



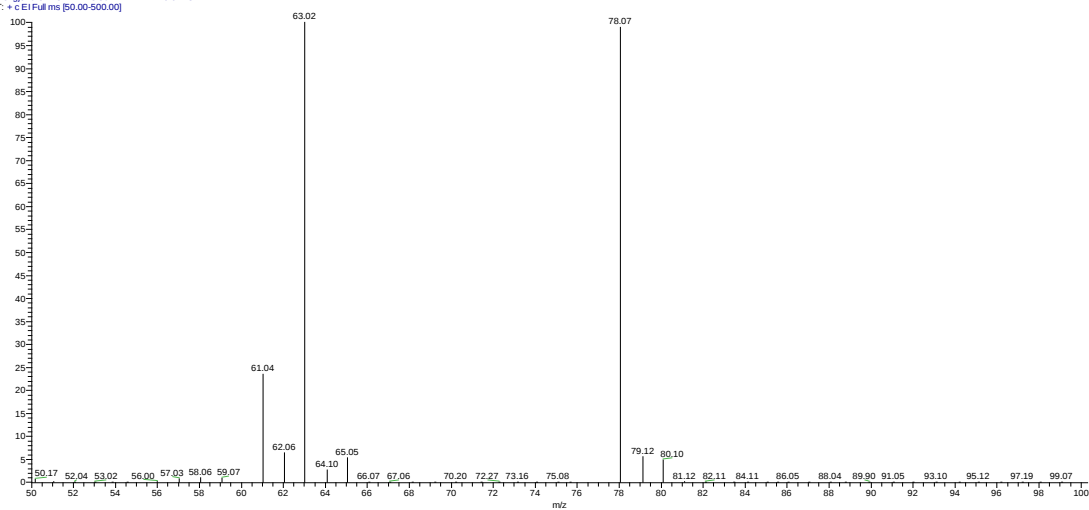
O¹⁸-riched DMSO obtained in the H₂O¹⁸ experiment

Dongji620-2 #286 RT: 3.97 AV: 1 NL: 1.15E9
T: + c EI Full ms [50.00-500.00]



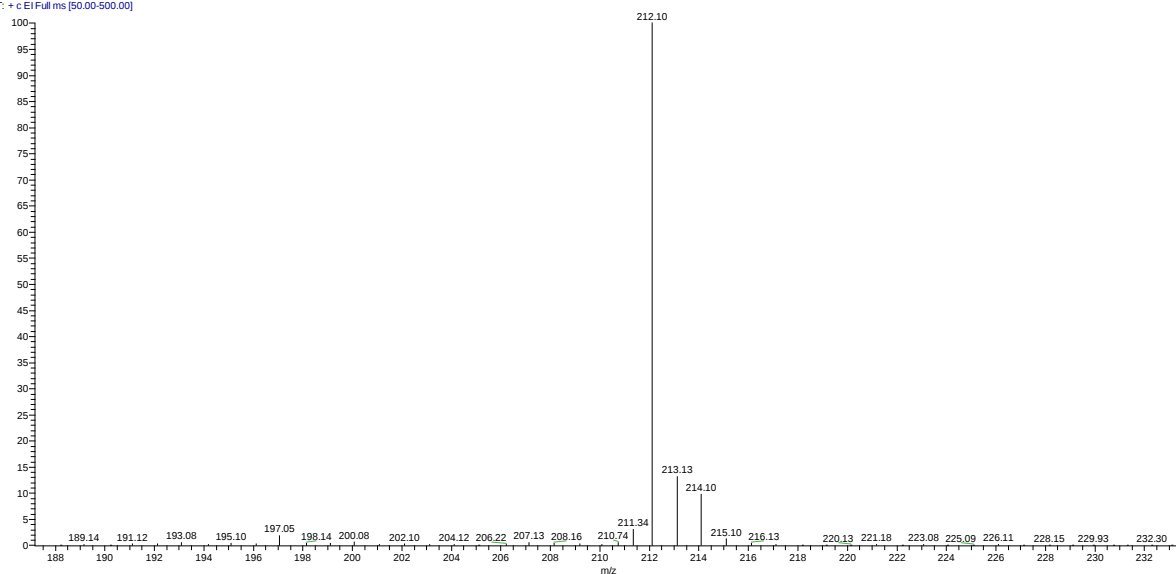
Normal DMSO

Dongji620-3 #237 RT: 3.80 AV: 1 NL: 9.91E8
T: + c EI Full ms [50.00-500.00]



1,2-Dibenzylhydrazine

Dongji750-b #2412 RT: 11.20 AV: 1 NL: 3.13E7
T: + c EI Full ms [50.00-500.00]



1,2-Diphenyldisulfane

Dongji750-c #2601 RT: 11.84 AV: 1 NL: 5.22E6
T: + c EI Full ms [50.00-500.00]

