

Supporting Information for

Complexity-Building ESIPT-Assisted Synthesis of Fused Polyheterocyclic Sulfonamides.

Srinivas Beduru and Andrei G. Kutateladze*

Department of Chemistry and Biochemistry, University of Denver, USA, 80208

*Correspondence: Andrei.Kutateladze@du.edu

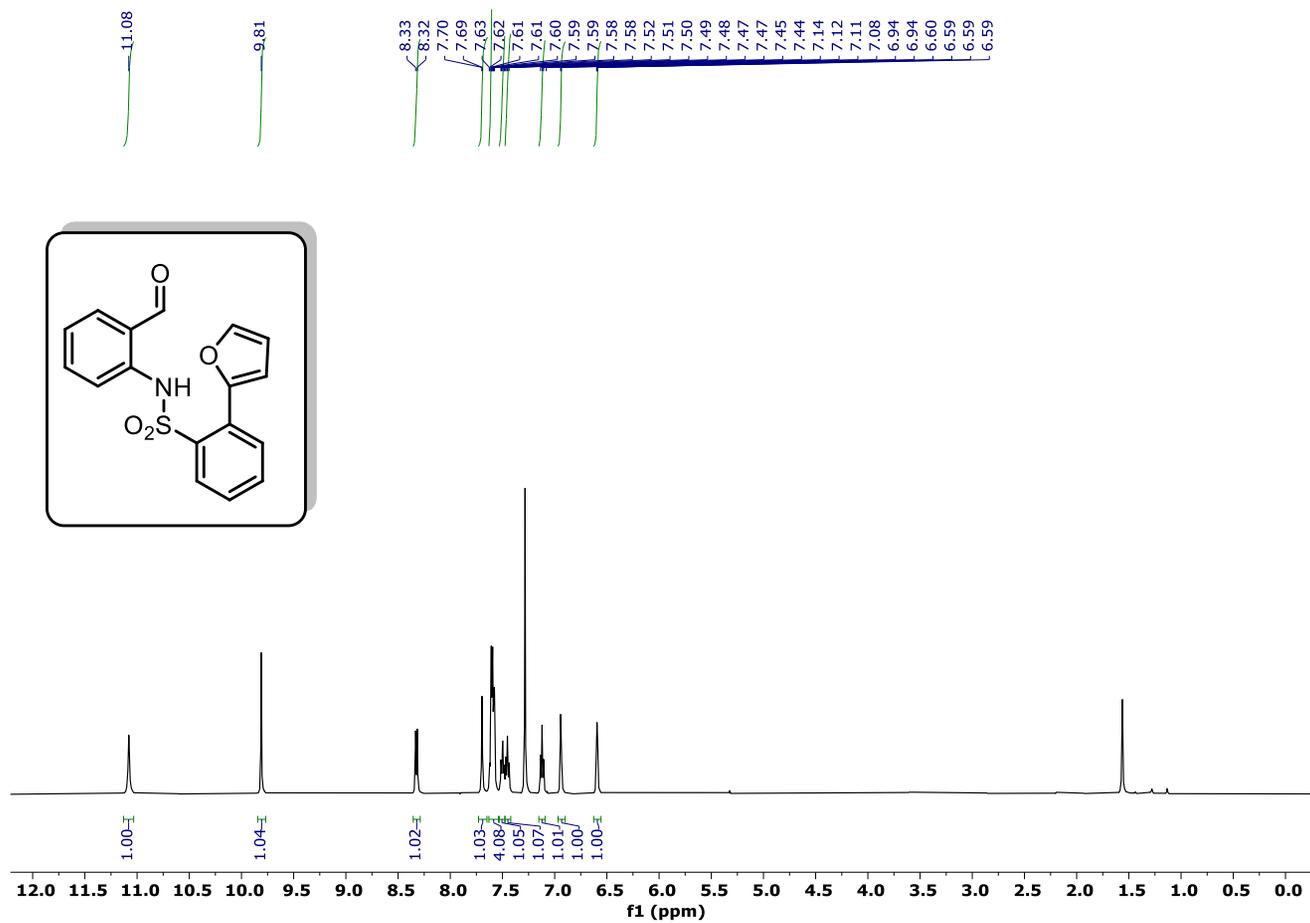
NMR spectra	Page
<i>N</i> -(2-Formylphenyl)-2-(furan-2-yl)benzenesulfonamide (8a)	
¹ H NMR spectrum	S5
¹³ C NMR spectrum	S6
<i>N</i> -(2-Formylphenyl)-2-(thiophen-2-yl)benzenesulfonamide (8b)	
¹ H NMR spectrum	S7
¹³ C NMR spectrum	S8
<i>N</i> -(2-Formylphenyl)-2-(furan-2-yl)-4,5-dimethoxybenzenesulfonamide (8c)	
¹ H NMR spectrum	S9
¹³ C NMR spectrum	S10
<i>N</i> -(2-Formylphenyl)-4,5-dimethoxy-2-(thiophen-2-yl)benzenesulfonamide (8d)	
¹ H NMR spectrum	S11
¹³ C NMR spectrum	S12
2-(Furan-2-yl)- <i>N</i> -(8-oxo-5,6,7,8-tetrahydronaphthalen-1-yl)benzenesulfonamide (10c)	
¹ H NMR spectrum	S13
¹³ C NMR spectrum	S14
(5 <i>S</i> ,6 <i>S</i> ,8 <i>aS</i>)-5-Hydroxy-5,6-dihydro-6,8 <i>a</i> -epoxybenzo[<i>g</i>]benzo[4,5]isothiazolo[2,3- <i>a</i>]azocine 13,13-dioxide (11a)	
¹ H NMR spectrum	S15
¹³ C NMR spectrum	S16
HSQC spectrum	S17
(4 <i>bR</i> ,7 <i>aS</i> ,8 <i>R</i>)-8-Hydroxy-7 <i>a</i> ,8-dihydrobenzo[4,5]isothiazolo[2,3- <i>a</i>]thieno[2,3- <i>b</i>]quinoline 14,14-dioxide (11b)	
¹ H NMR spectrum	S18
¹³ C NMR spectrum	S19
HSQC spectrum	S20
(5 <i>R</i> ,6 <i>R</i> ,8 <i>aR</i>)-5-Hydroxy-10,11-dimethoxy-5,6-dihydro-6,8 <i>a</i> -epoxybenzo[<i>g</i>]benzo[4,5]isothiazolo[2,3- <i>a</i>]azocine 13,13-dioxide (11c)	
¹ H NMR spectrum	S21

¹³ C NMR spectrum	S22
HSQC spectrum	S23
<i>(4bR,7aS,8R)</i> -8-Hydroxy-2,3-dimethoxy-7a,8-dihydrobenzo[4,5]isothiazolo[2,3-a]thieno[2,3-b]quinoline 14,14-dioxide (11d)	
¹ H NMR spectrum	S24
¹³ C NMR spectrum	S25
HSQC spectrum	S26
<i>(4bR,7aS,8S)</i> -8-Hydroxy-8-methyl-7a,8-dihydrobenzo[4,5]isothiazolo[2,3-a]furo[2,3-b]quinoline 14,14-dioxide (11e)	
¹ H NMR spectrum	S27
¹³ C NMR spectrum	S28
HSQC spectrum	S29
<i>(5R,6S,8aS)</i> -5-Hydroxy-5-methyl-5,6-dihydro-6,8a-epoxybenzo[<i>g</i>]benzo[4,5]isothiazolo[2,3-a]azocine 13,13-dioxide (11ea)	
¹ H NMR spectrum	S30
¹³ C NMR spectrum	S31
HSQC spectrum	S32
<i>(4bR,7aS,8R)</i> -8-Hydroxy-8-methyl-7a,8-dihydrobenzo[4,5]isothiazolo[2,3-a]thieno[2,3-b]quinoline 14,14-dioxide (11f)	
¹ H NMR spectrum	S33
¹³ C NMR spectrum	S34
HSQC spectrum	S35
<i>(3aR,15aS,15bS)</i> -15a-Hydroxy-14,15,15a,15b-tetrahydro-13H-benzo[<i>de</i>]benzo[4,5]isothiazolo[2,3-a]furo[2,3-b]quinoline 8,8-dioxide (11g)	
¹ H NMR spectrum	S36
¹³ C NMR spectrum	S37
HSQC spectrum	S38
<i>(5aR,17aS,17bS)</i> -17a-Hydroxy-2-methylene-1,2,4a,16,17,17a,17b,17c-octahydro-3H,15H-benzo[<i>de</i>]benzo[4,5]isothiazolo[2,3-a]pyrano[3',2':4,5]furo[2,3-b]quinolin-3-one 10,10-dioxide (12)	
¹ H NMR spectrum	S39
¹³ C NMR spectrum	S40
HSQC spectrum	S41

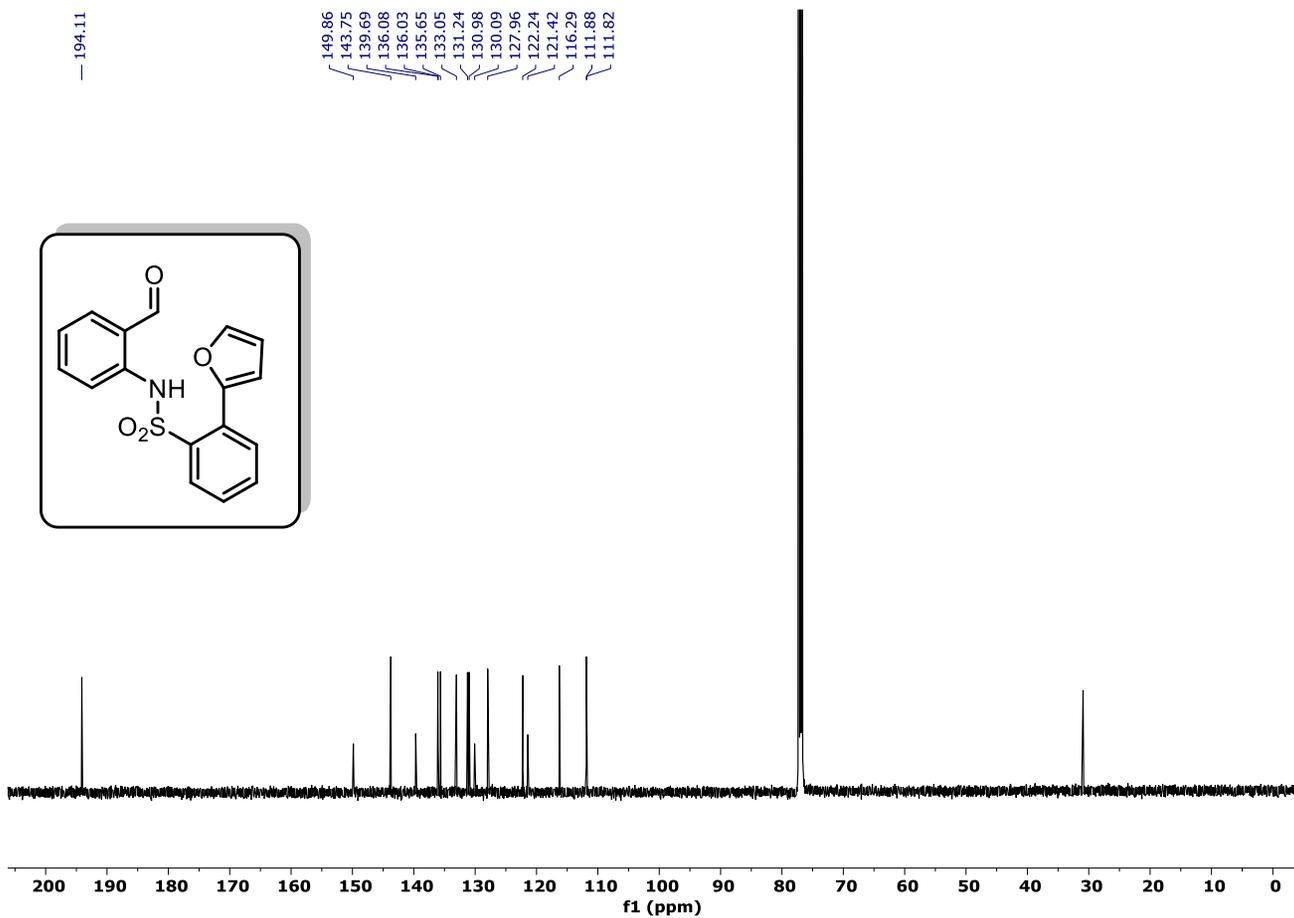
(5aR,17aS,17bS)-17a-Hydroxy-2-methylene-1,2,4a,16,17,17a,17b,17c-octahydro-3H,15H-benzo[de]benzo[4,5]isothiazolo[2,3-a]pyrano[3',2':4,5]furo[2,3-b]quinolin-3-one 10,10-dioxide (13)

¹ H NMR spectrum	S42
¹³ C NMR spectrum	S43
HSQC spectrum	S44
NOESY spectrum	S45
UV Spectra of photoprecursors	S46

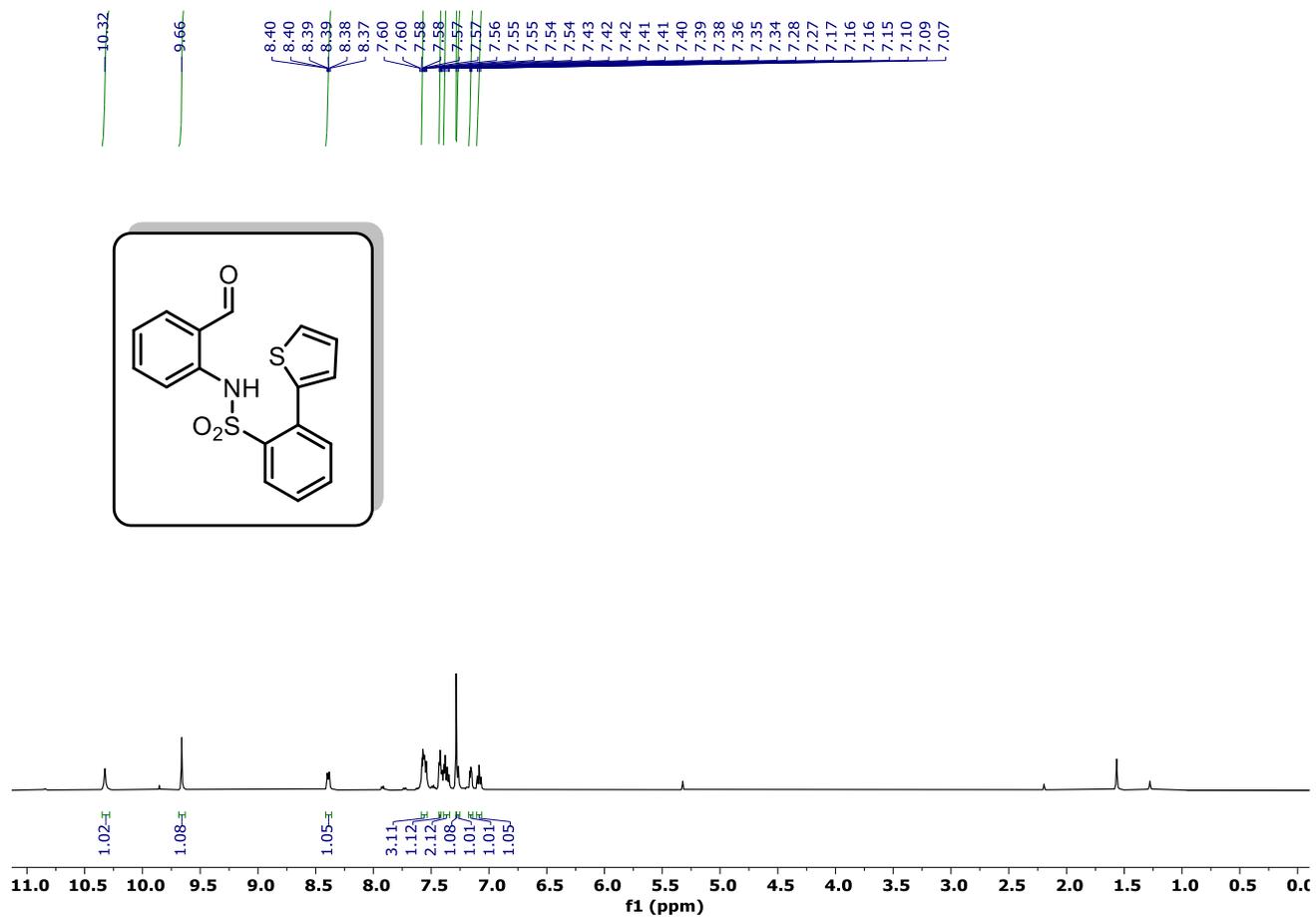
^1H NMR spectrum of **8a** (500 MHz, CDCl_3)



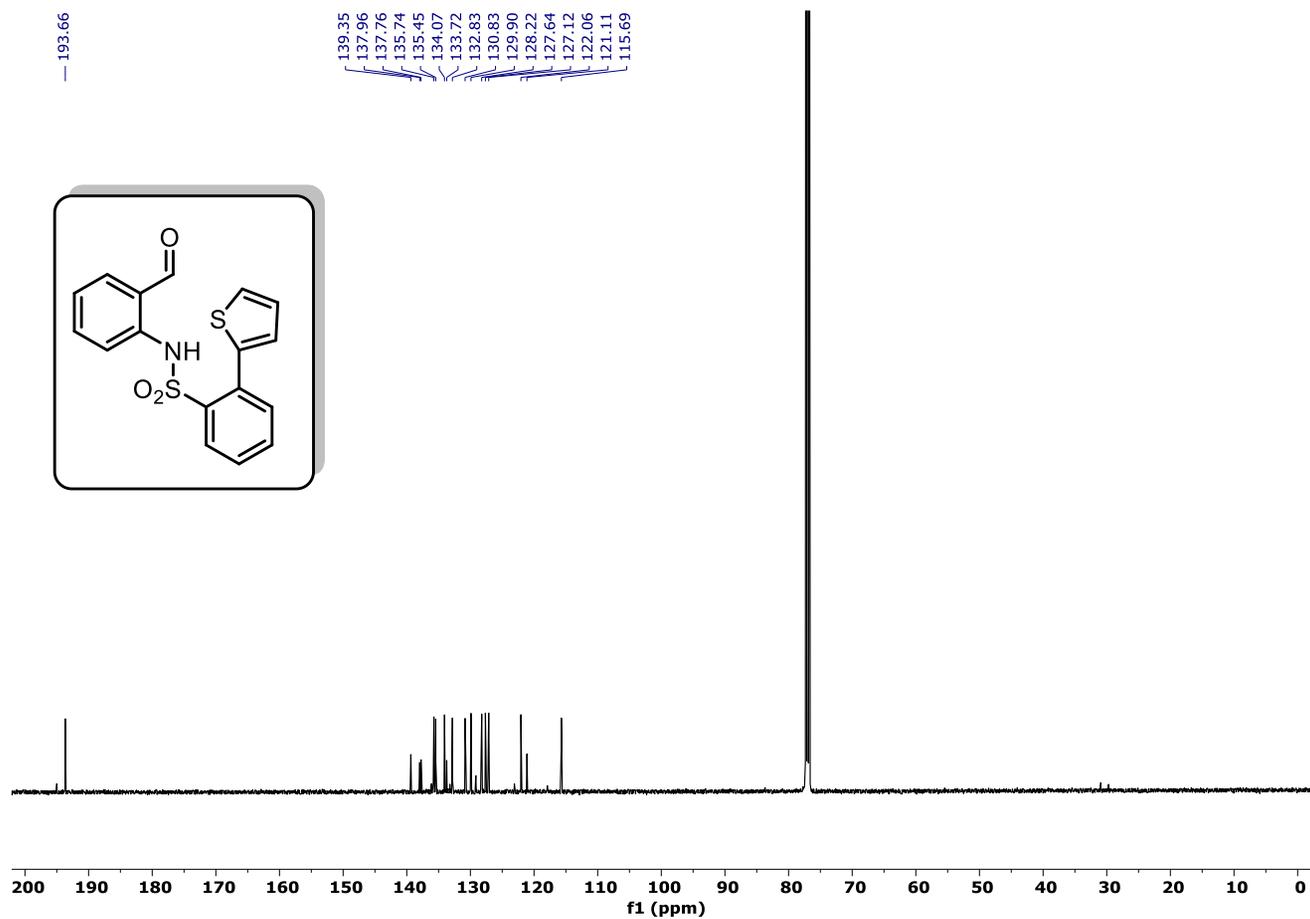
^{13}C NMR spectrum of **8a** (126 MHz, CDCl_3)



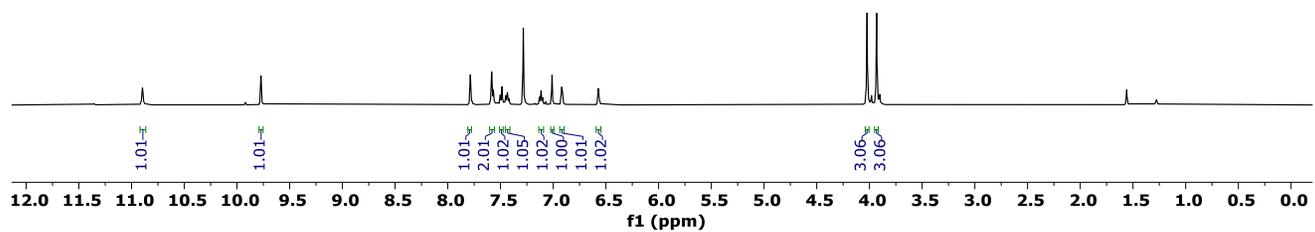
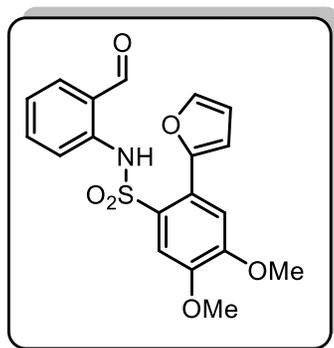
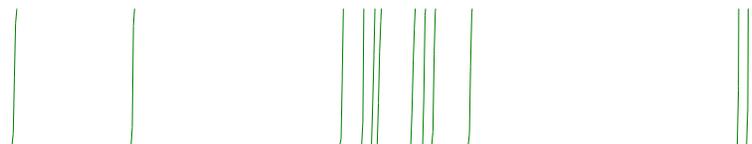
^1H NMR spectrum of **8b** (500 MHz, CDCl_3)



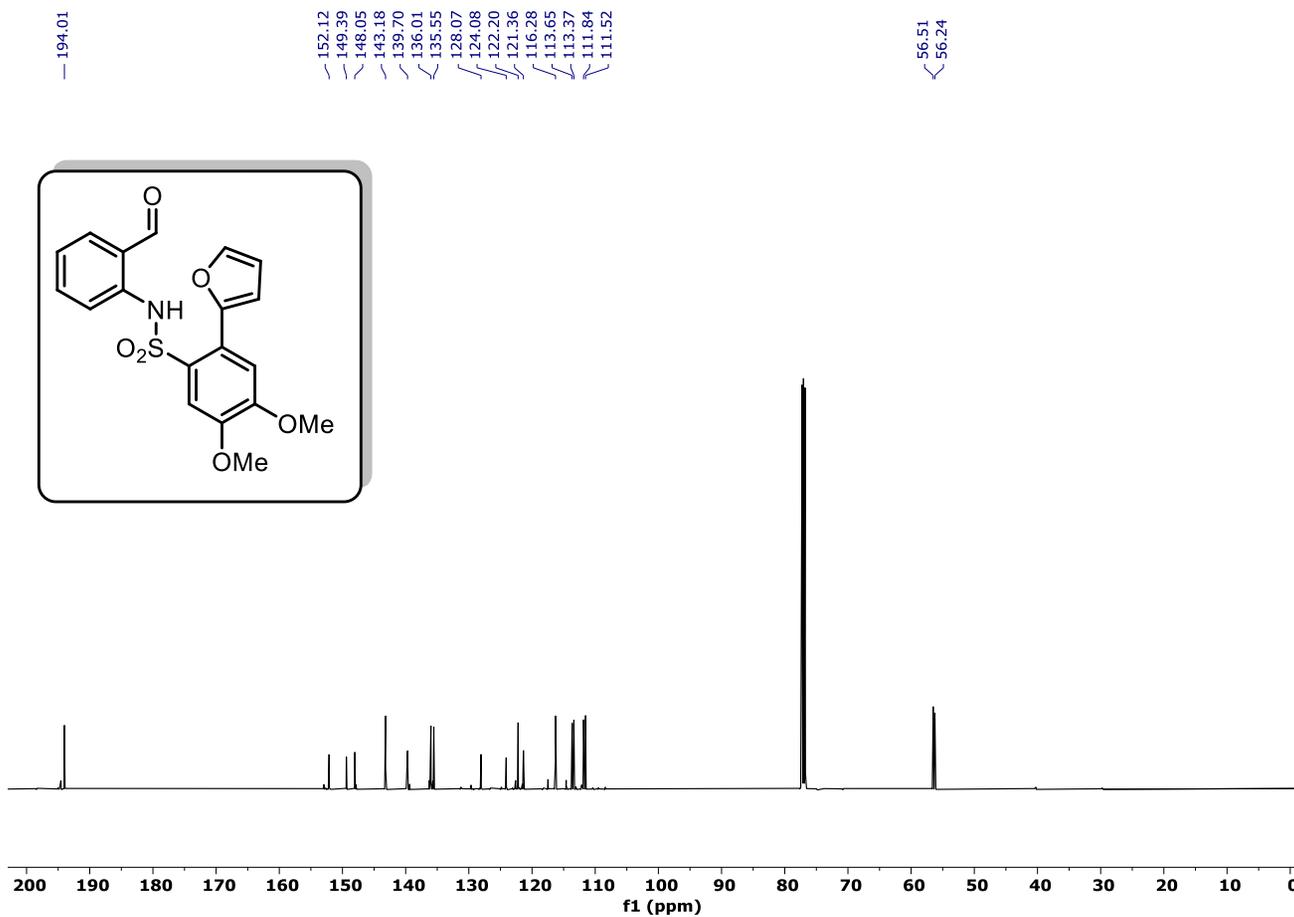
^{13}C NMR spectrum of **8b** (126 MHz, CDCl_3)



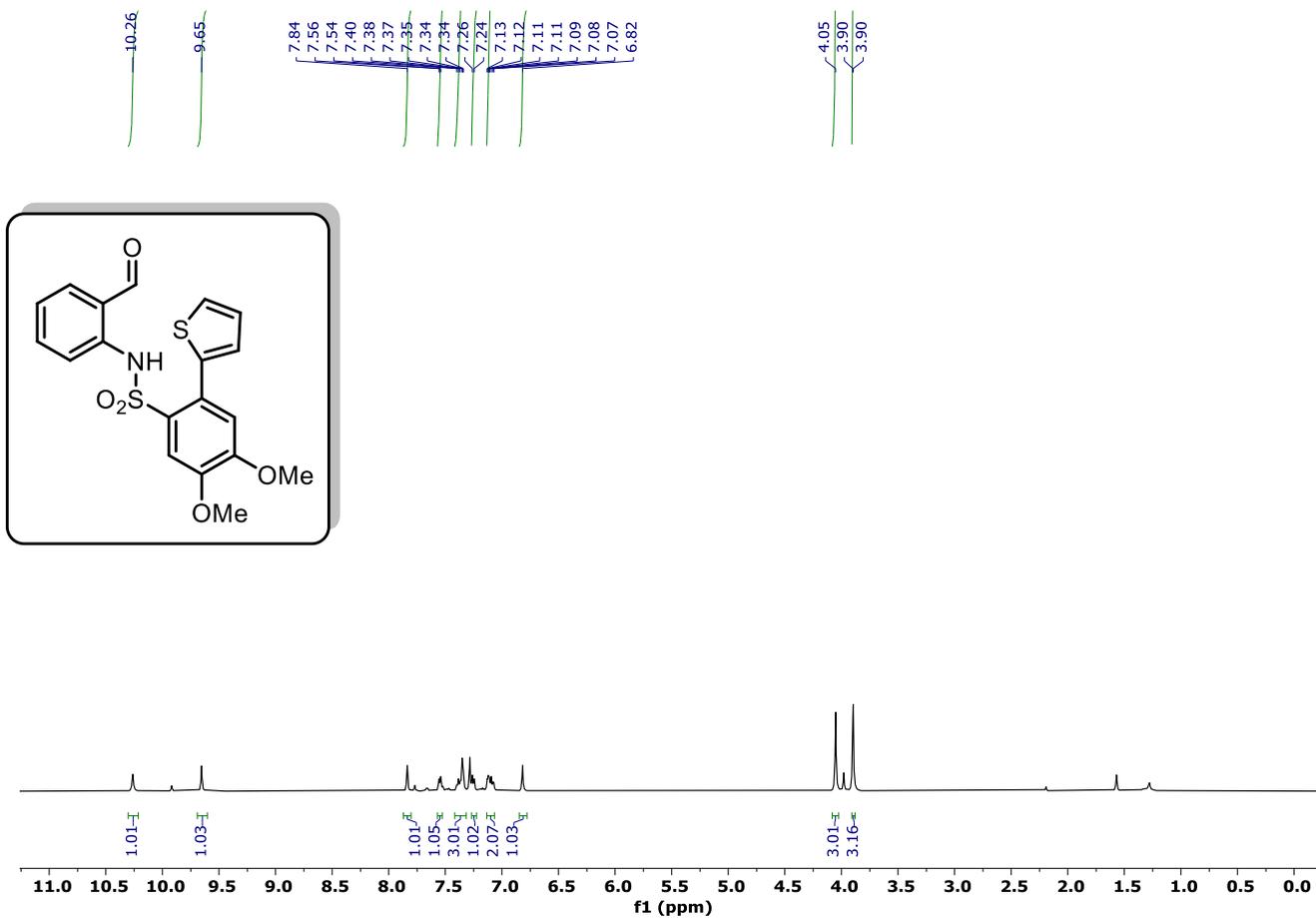
^1H NMR spectrum of **8c** (500 MHz, CDCl_3)



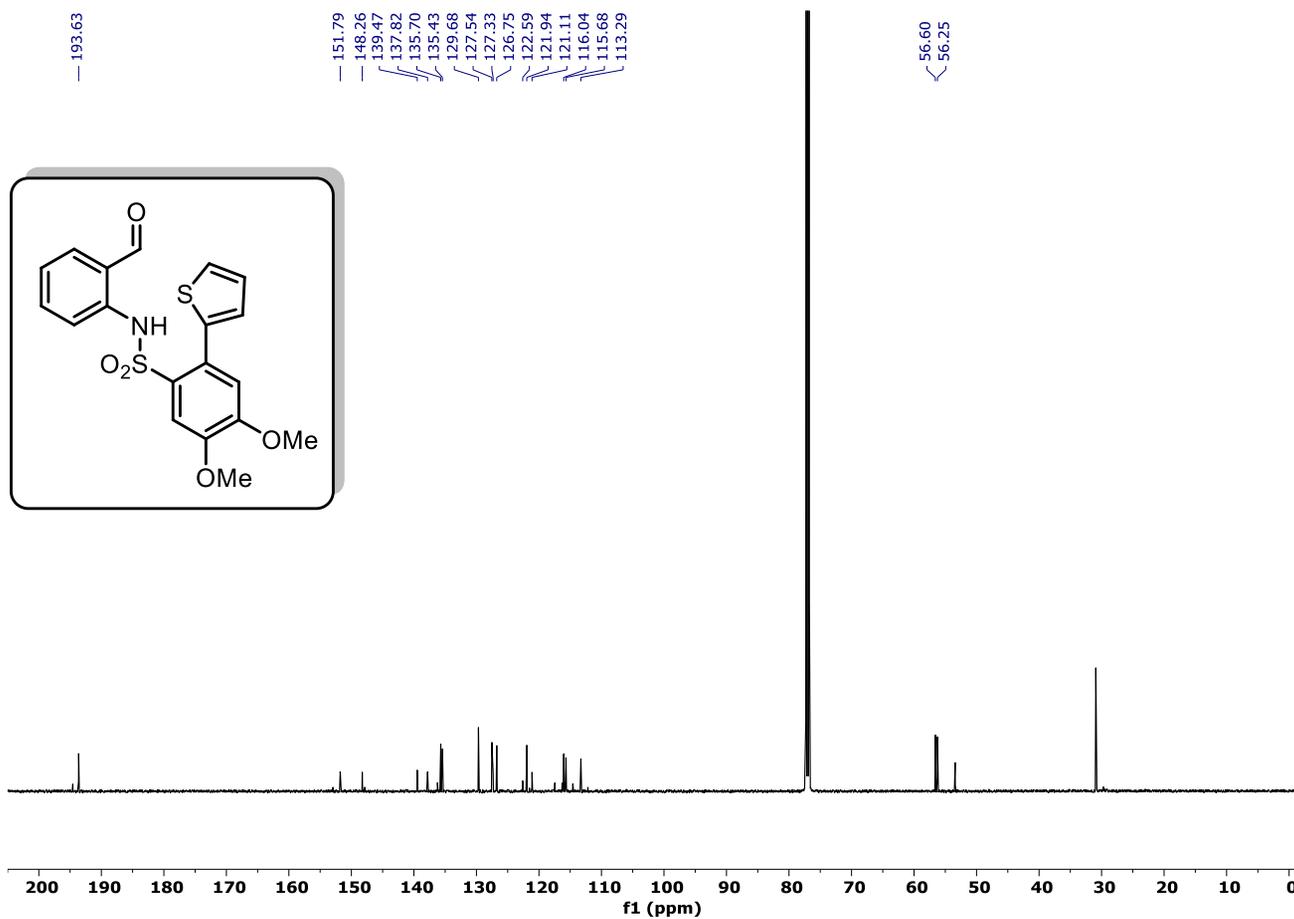
^{13}C NMR spectrum of **8c** (126 MHz, CDCl_3)



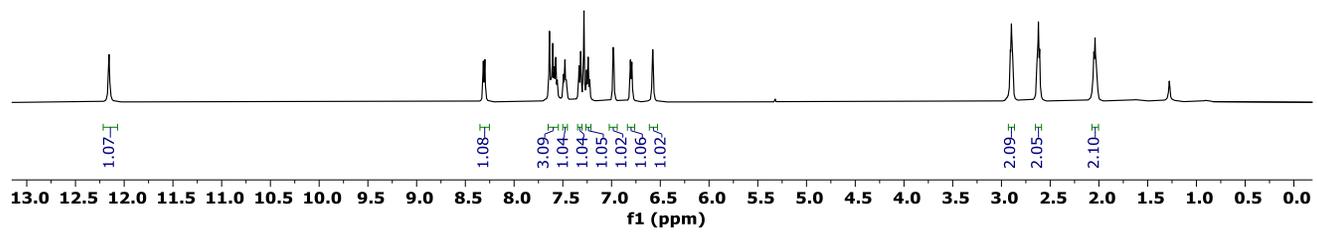
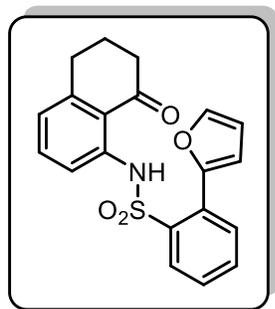
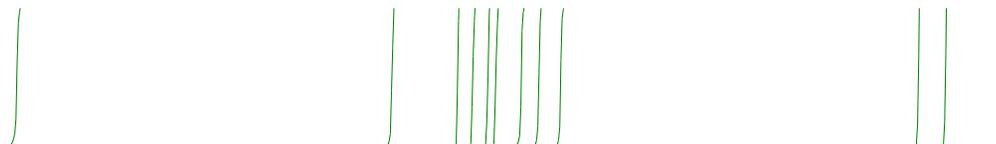
^1H NMR spectrum of **8d** (500 MHz, CDCl_3)



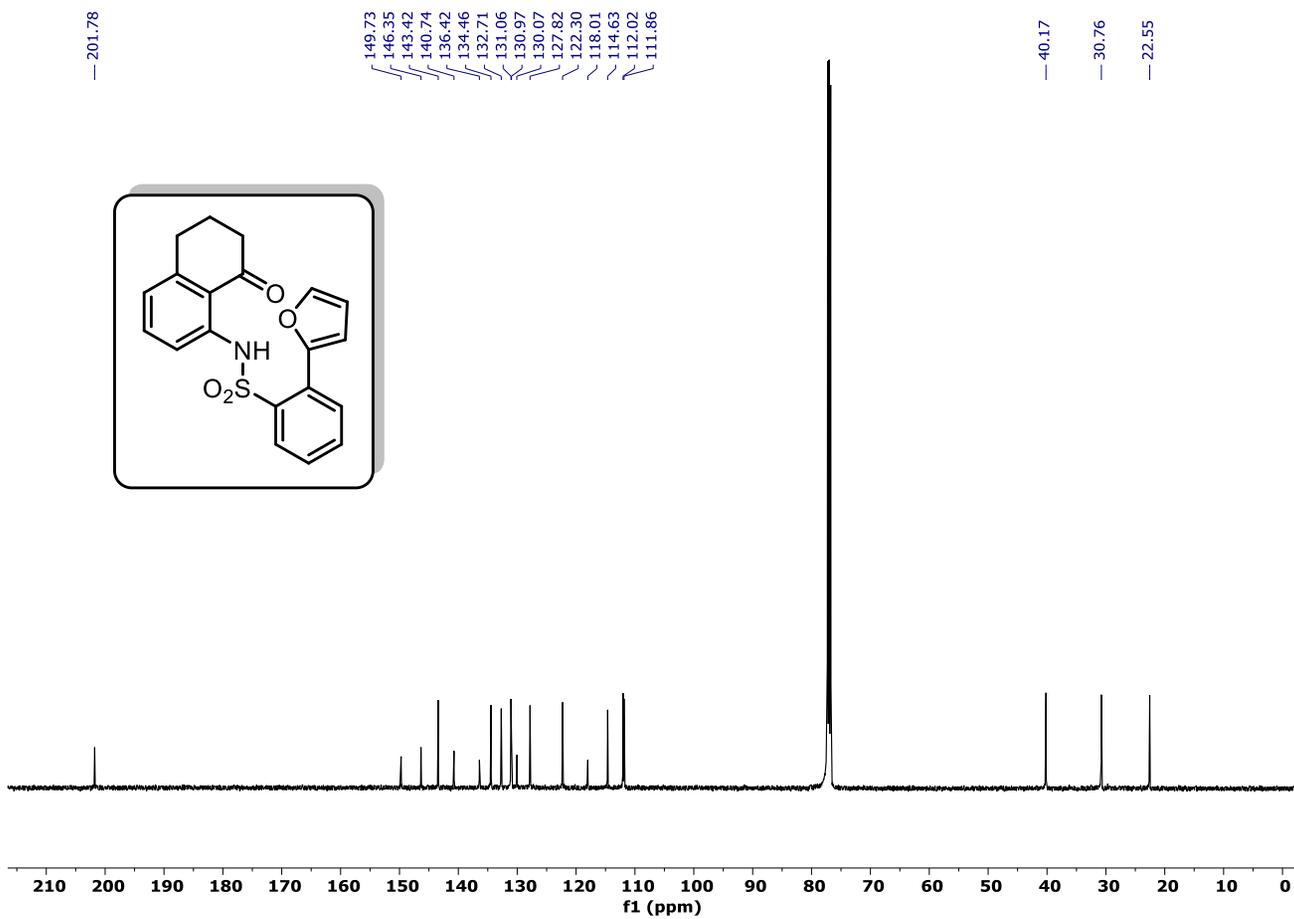
^{13}C NMR spectrum of **8d** (126 MHz, CDCl_3)



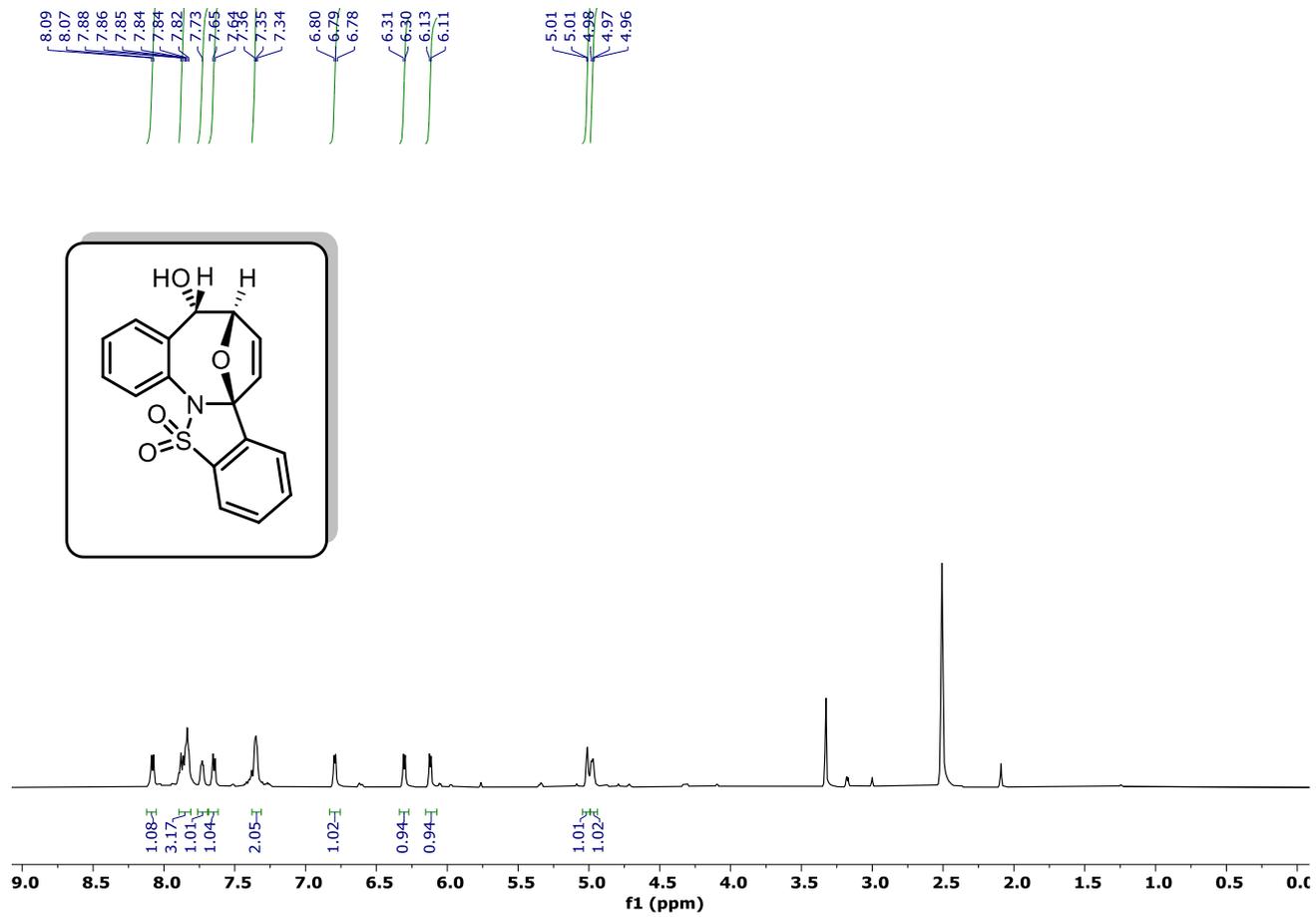
^1H NMR spectrum of **10c** (500 MHz, CDCl_3)



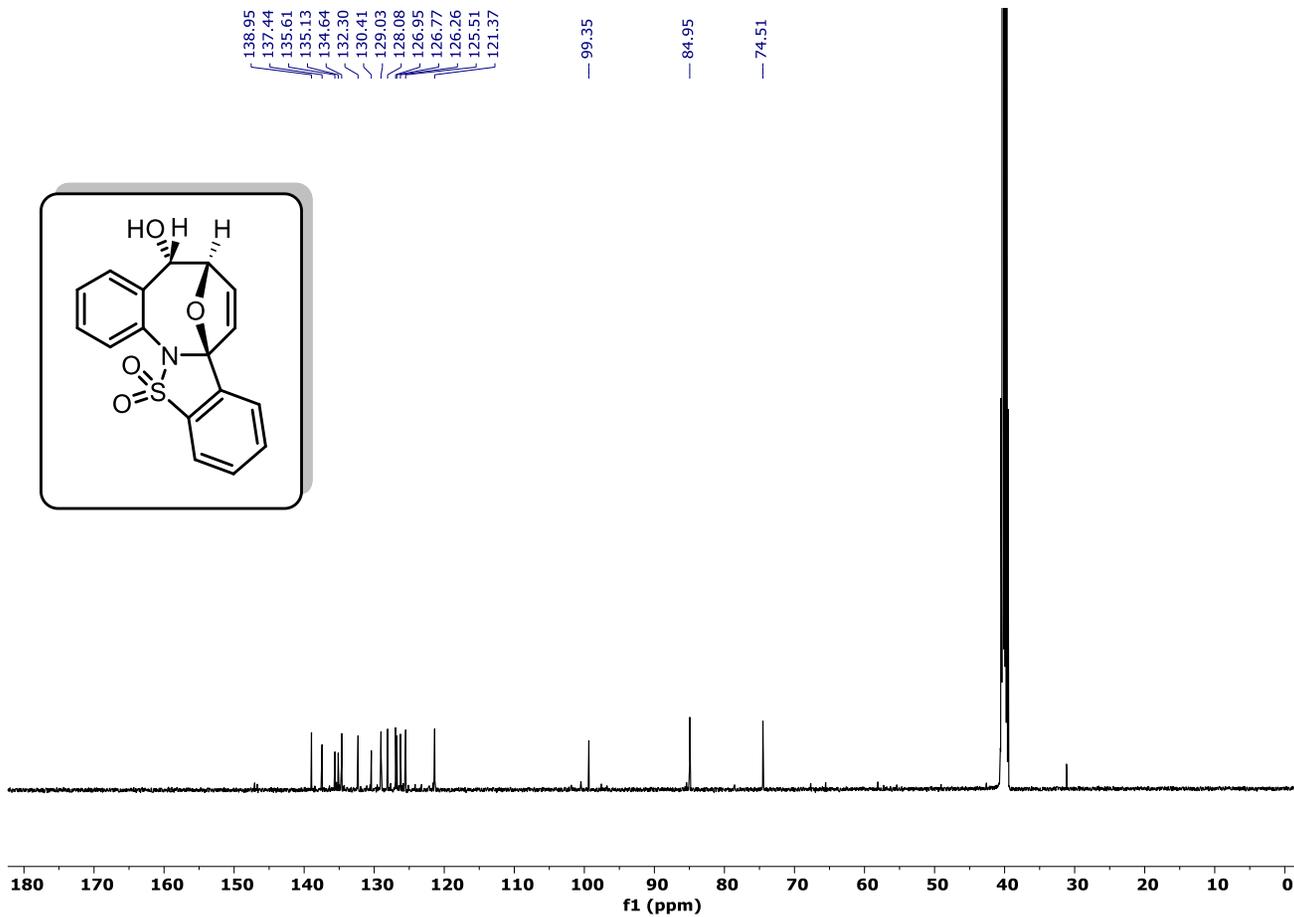
^{13}C NMR spectrum of **10c** (126 MHz, CDCl_3)



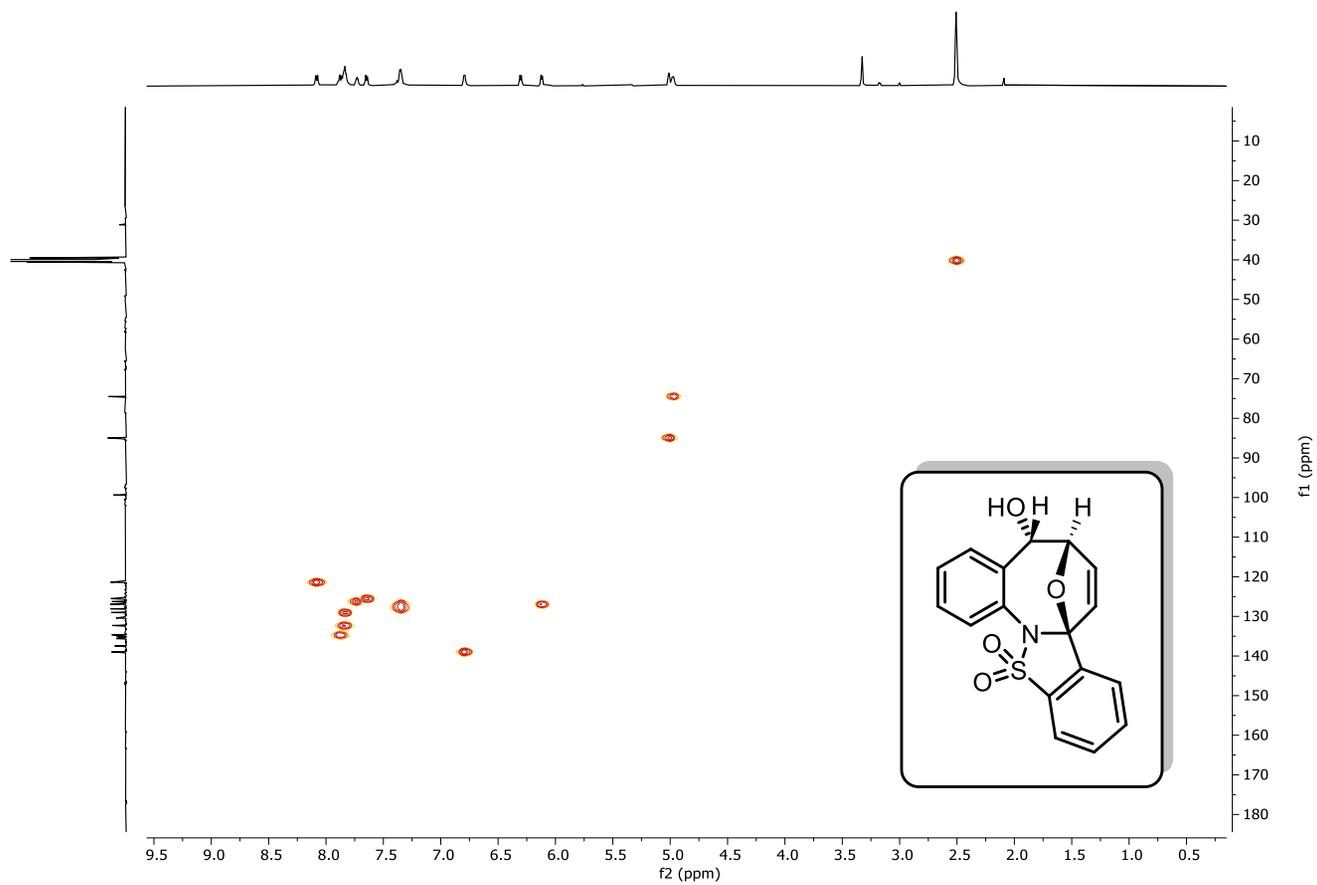
^1H NMR spectrum of **11a** (500 MHz, $\text{DMSO-}d_6$)



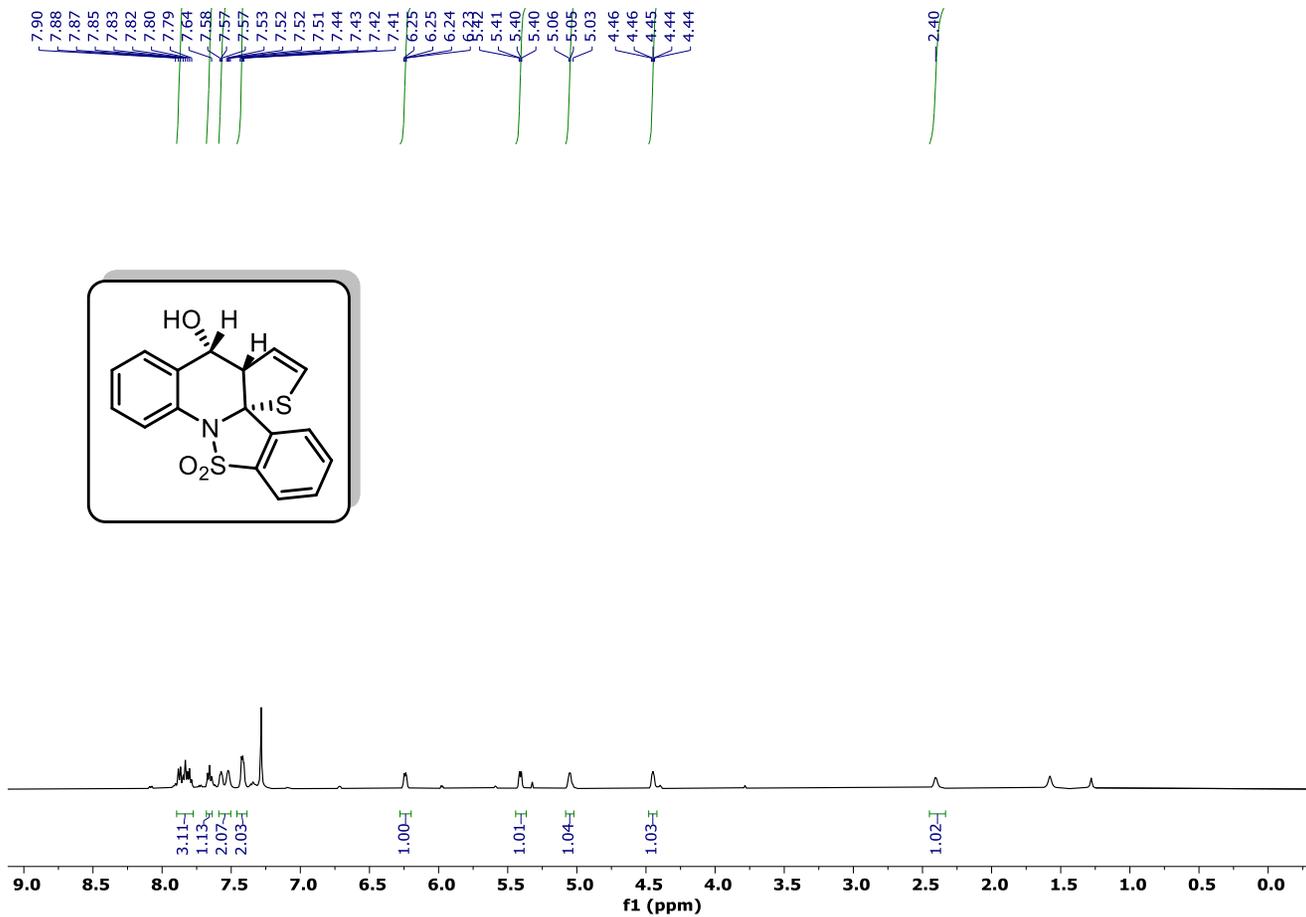
^{13}C NMR spectrum of **11a** (126 MHz, $\text{DMSO-}d_6$)



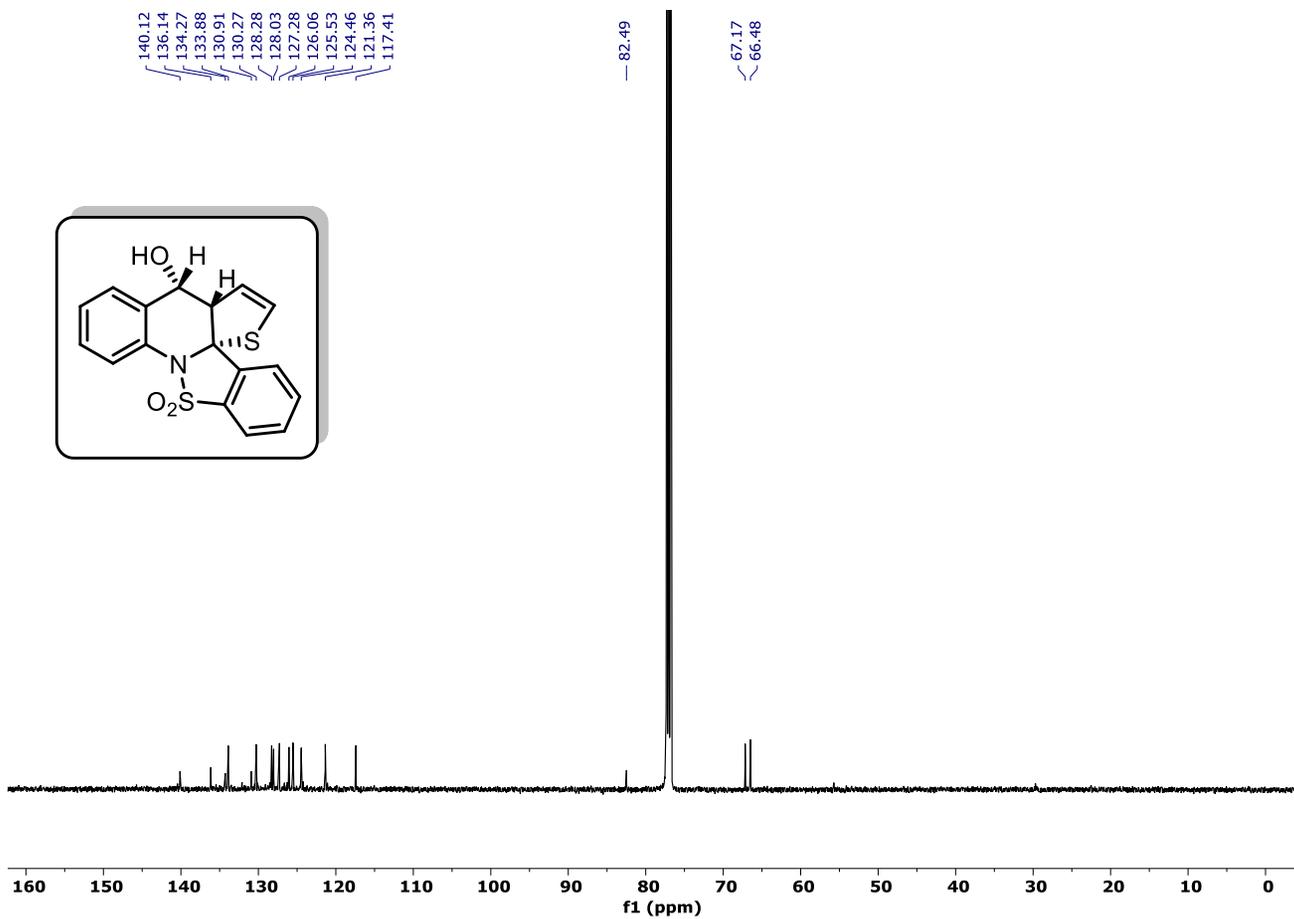
HSQC spectrum of **11a** (DMSO-*d*₆)



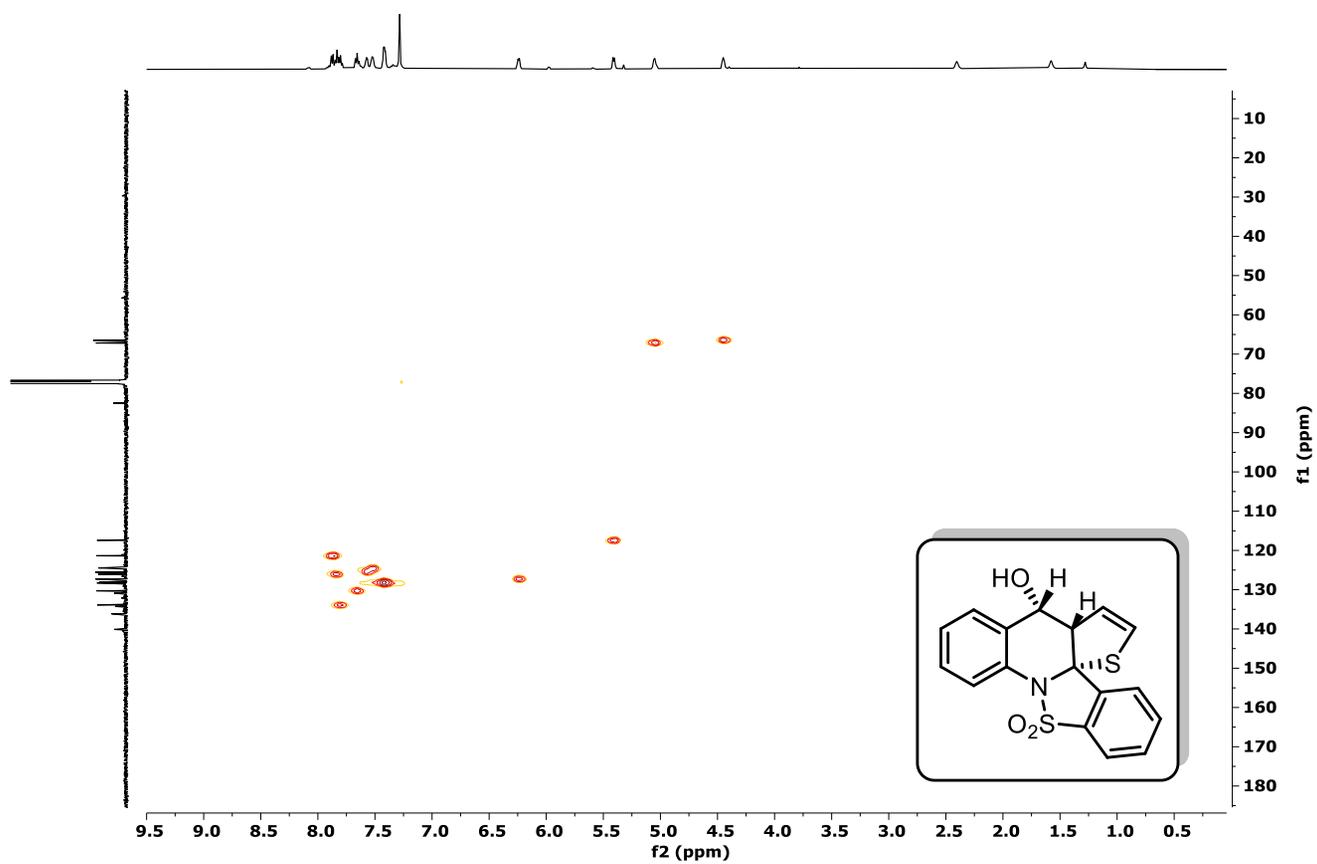
^1H NMR spectrum of **11b** (500 MHz, CDCl_3)



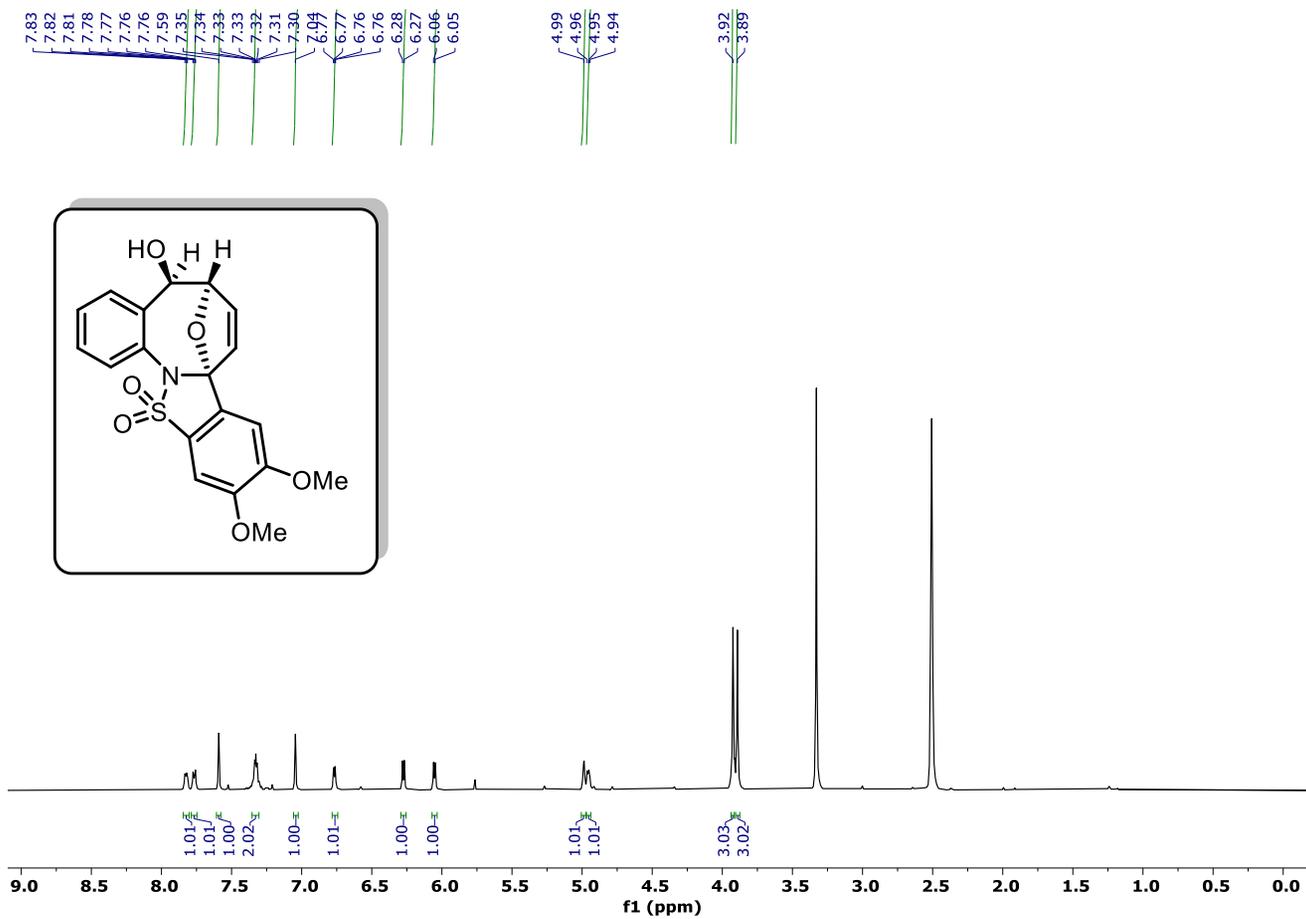
^{13}C NMR spectrum of **11b** (126 MHz, CDCl_3)



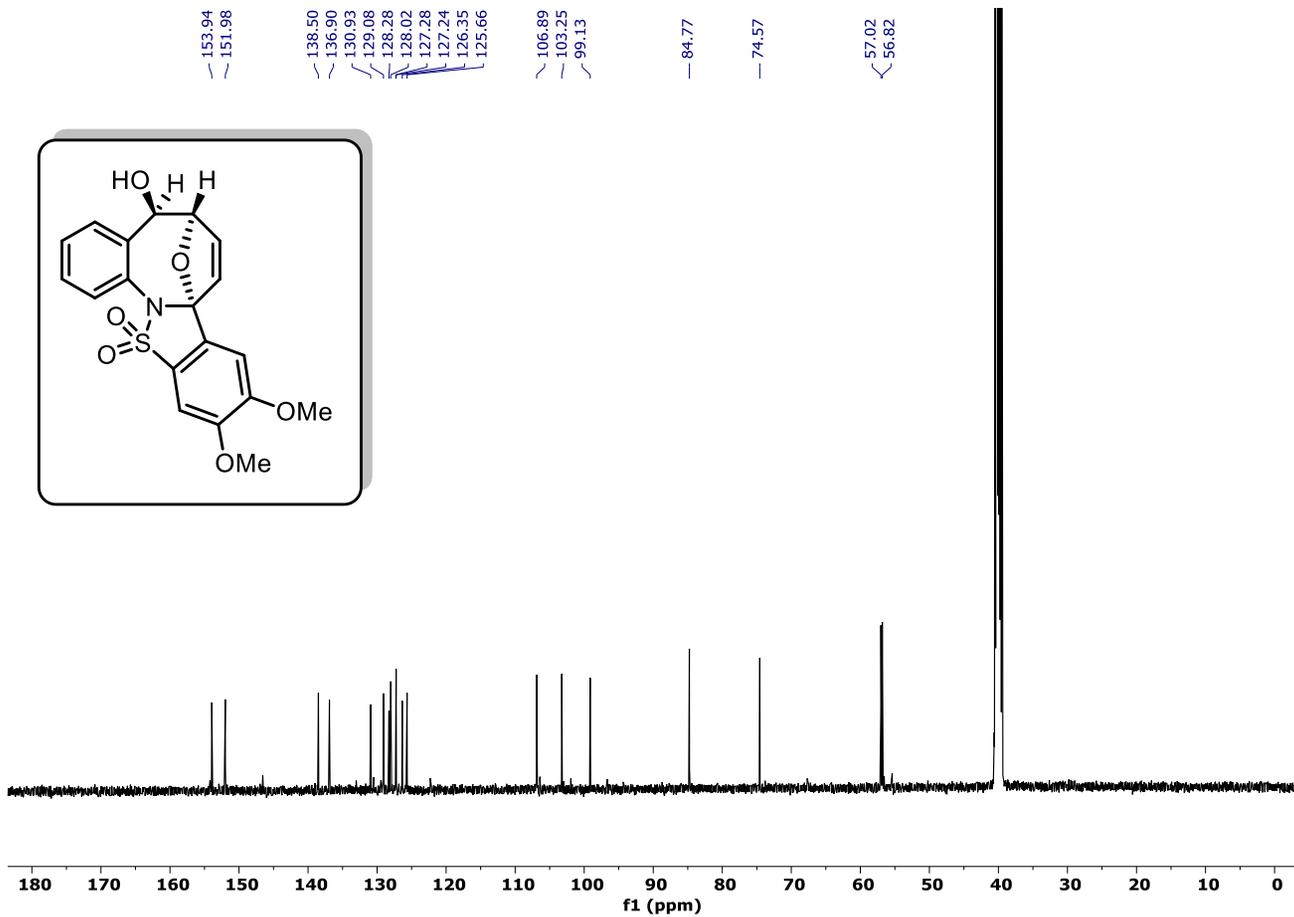
HSQC spectrum of **11b** (CDCl₃)



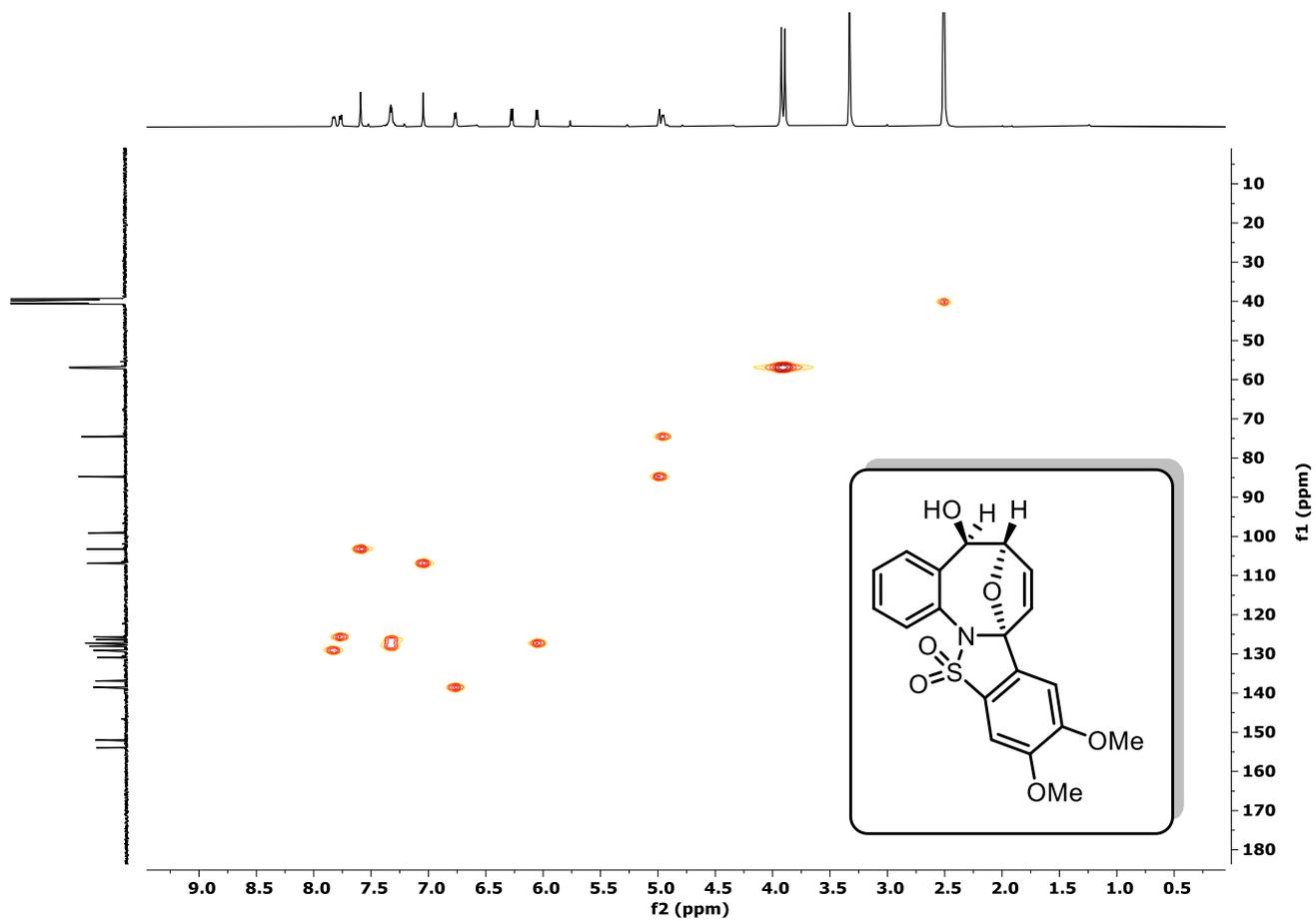
^1H NMR spectrum of **11c** (500 MHz, $\text{DMSO-}d_6$)



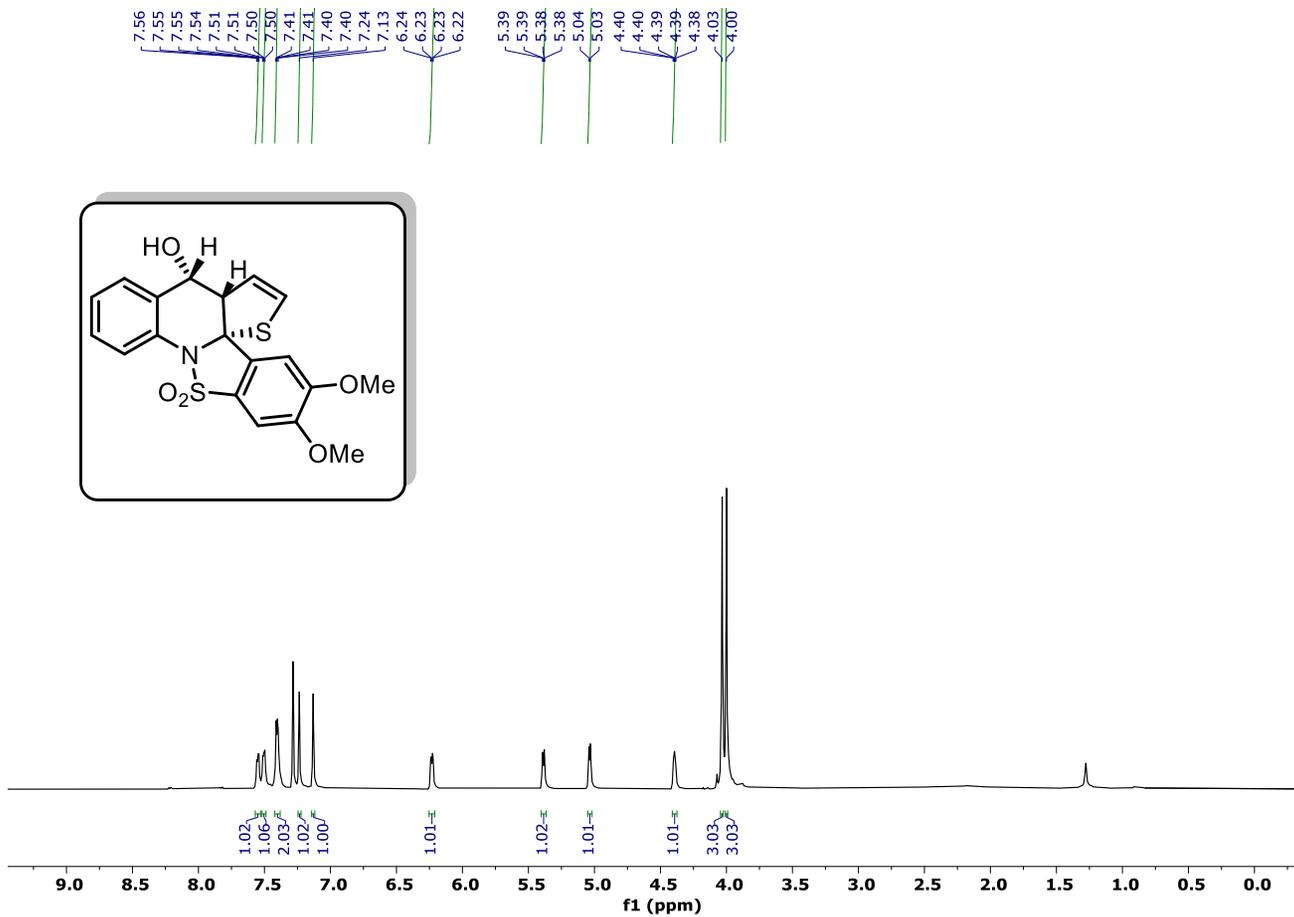
^{13}C NMR spectrum of **11c** (126 MHz, $\text{DMSO-}d_6$)



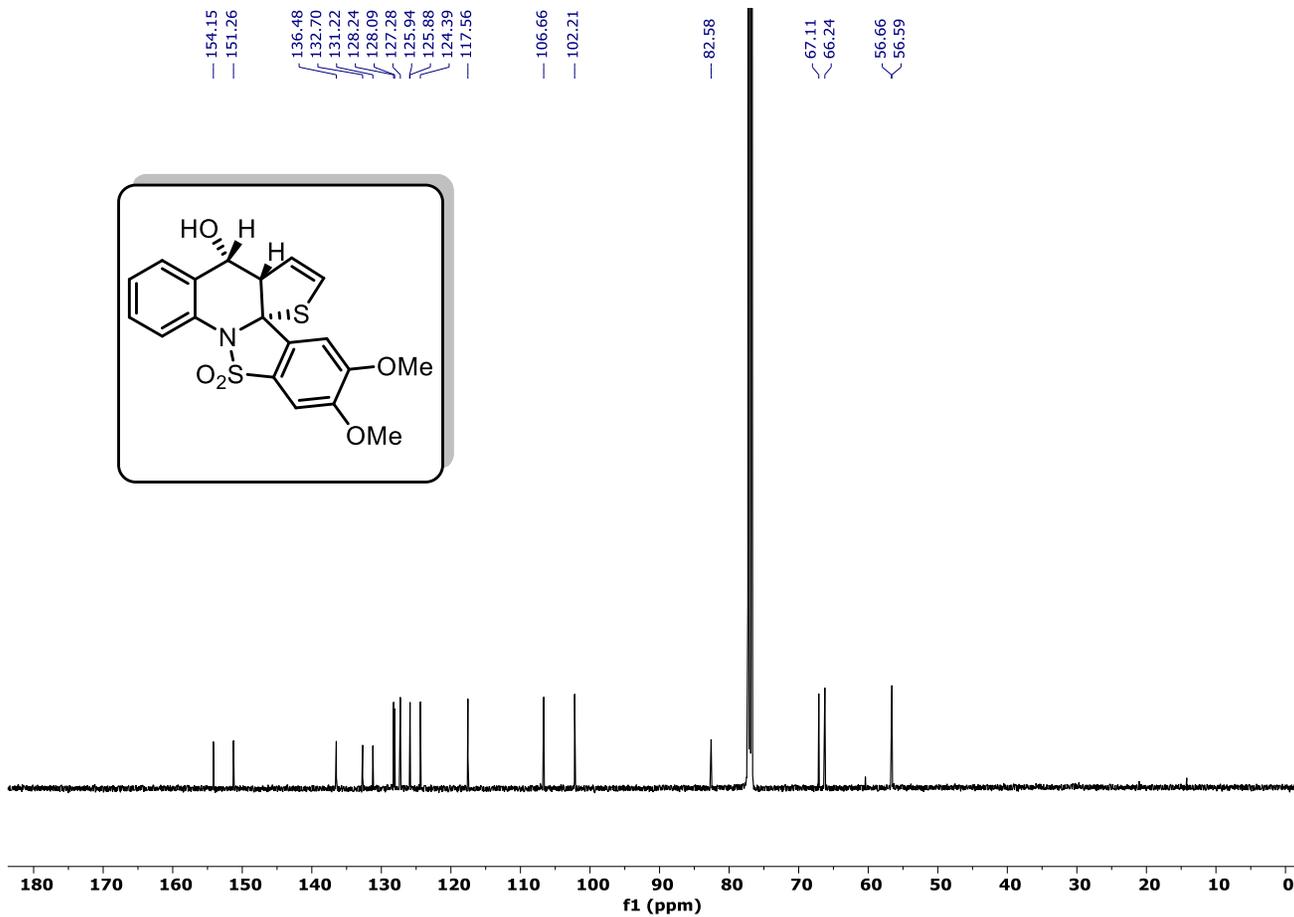
HSQC spectrum of **11c** (DMSO-*d*₆)



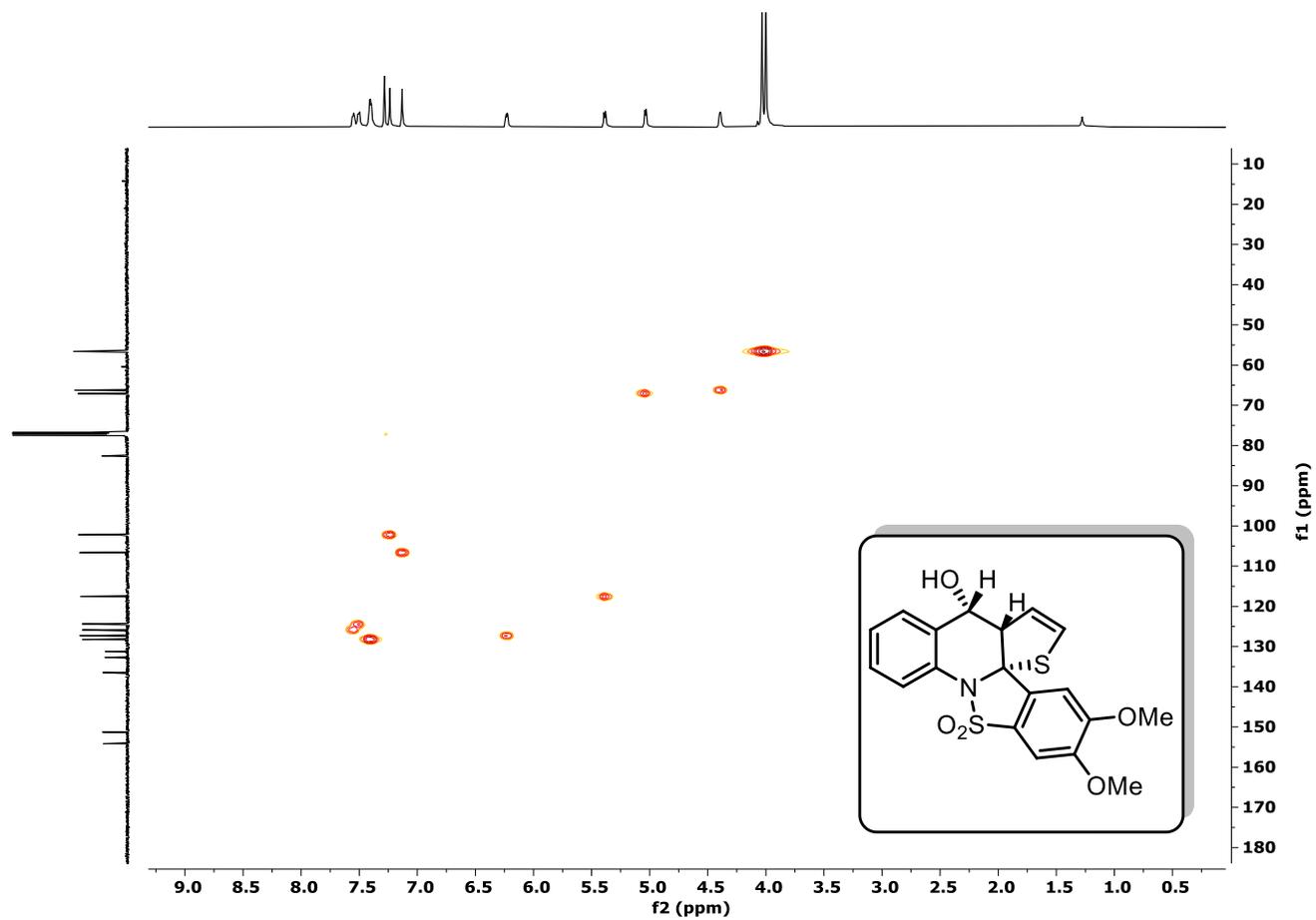
^1H NMR spectrum of **11d** (500 MHz, CDCl_3)



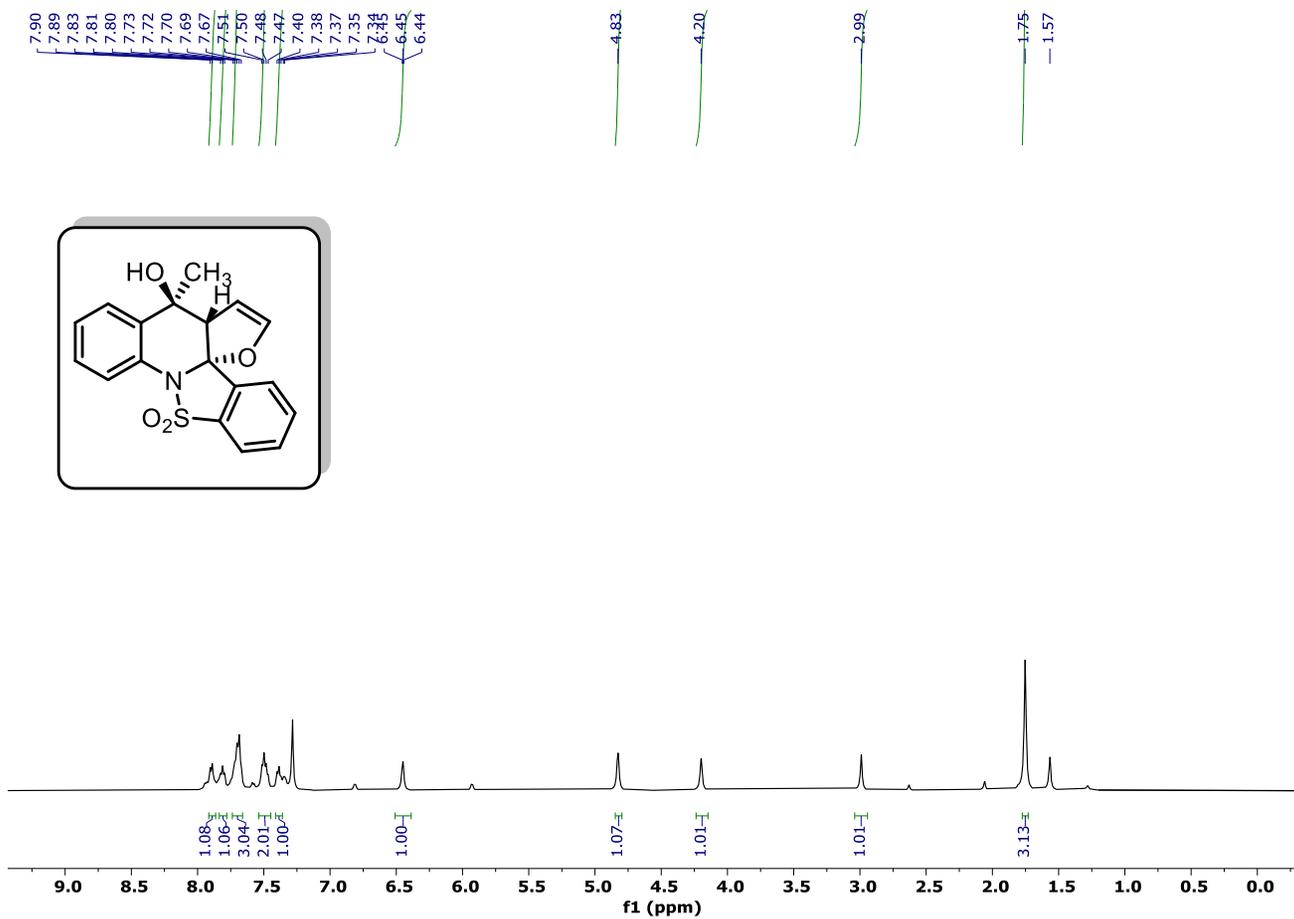
^{13}C NMR spectrum of **11d** (126 MHz, CDCl_3)



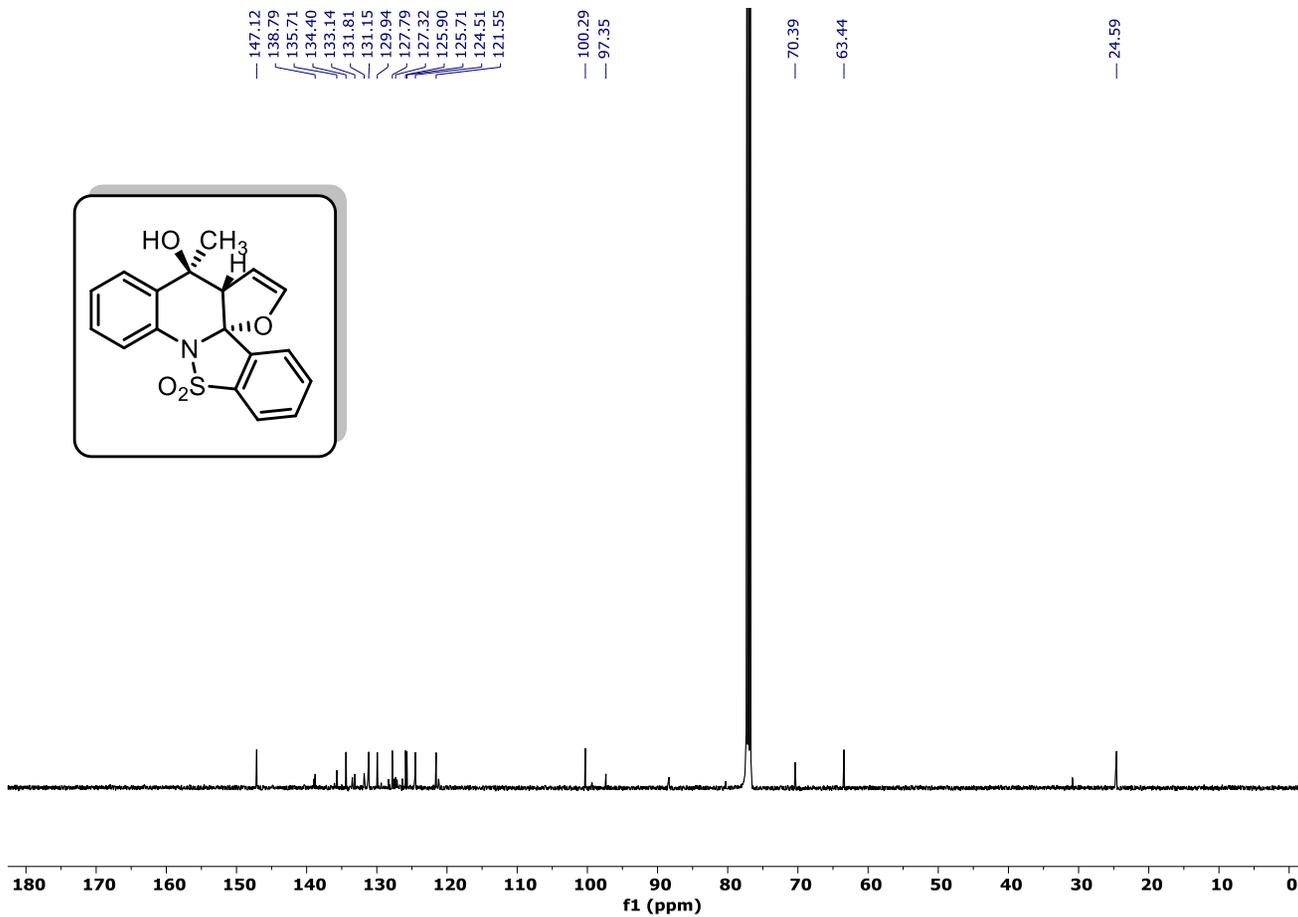
HSQC spectrum of **11d** (CDCl₃)



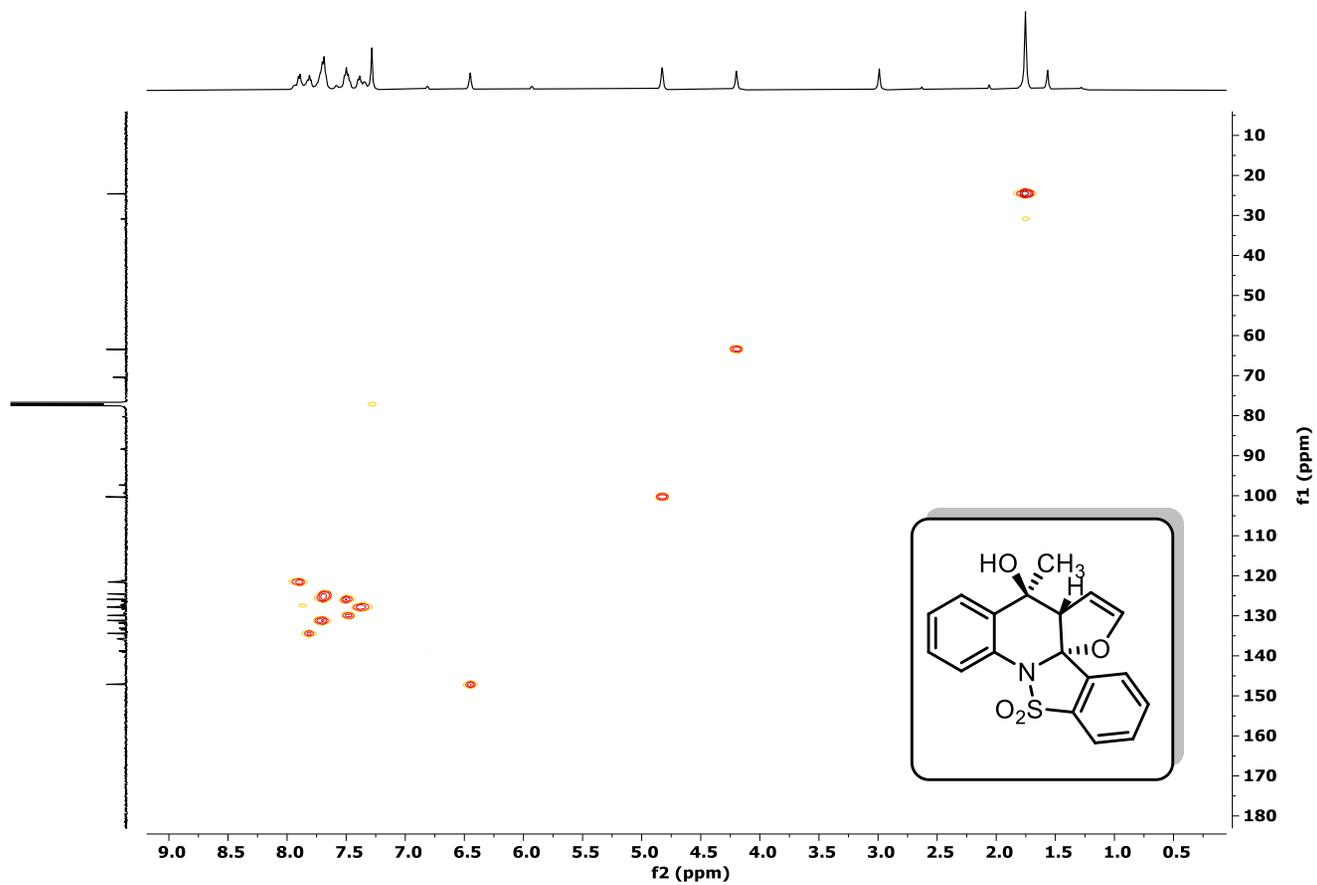
^1H NMR spectrum of **11e** (Major; 500 MHz, CDCl_3)



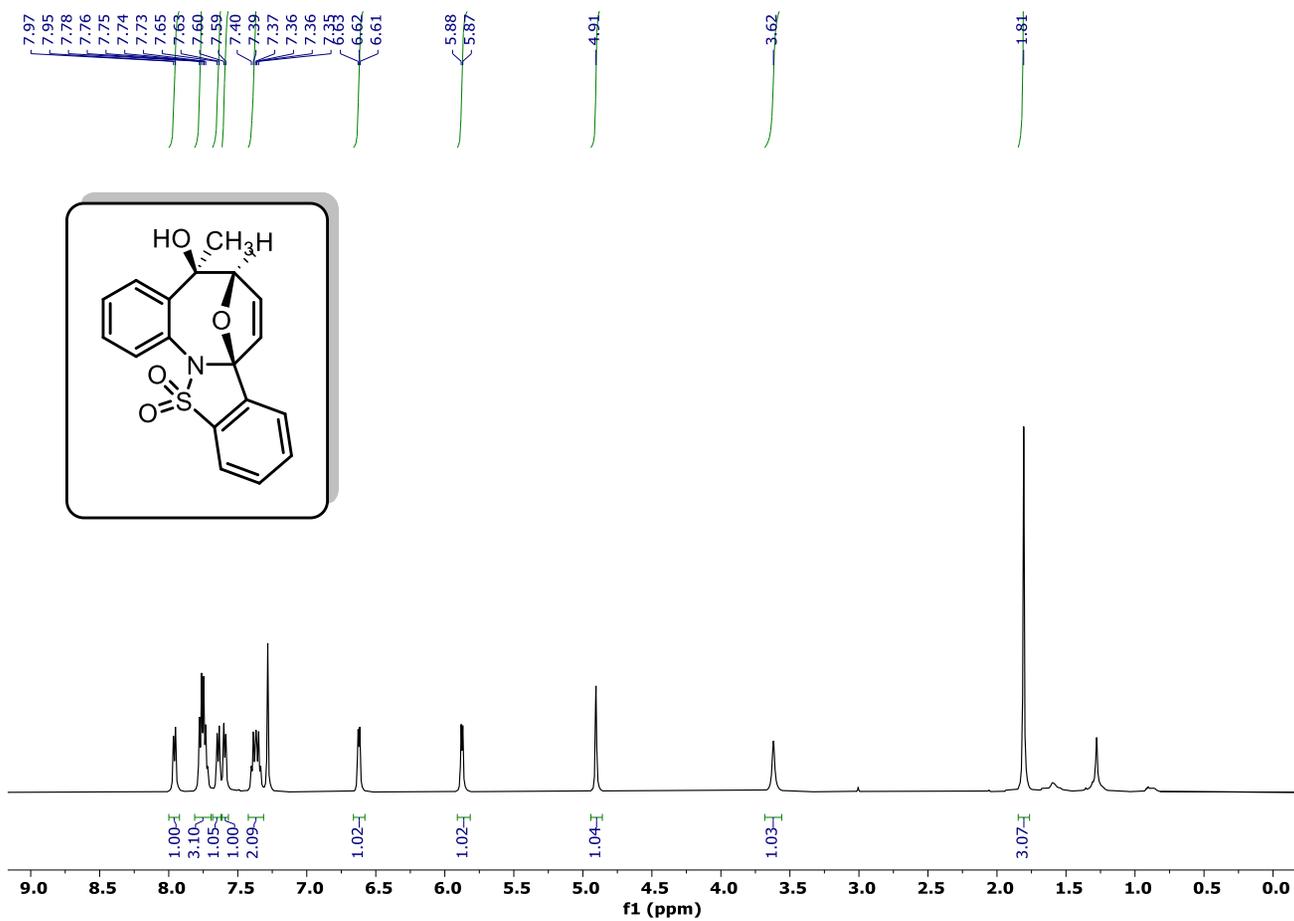
^{13}C NMR spectrum of **11e** (126 MHz, CDCl_3)



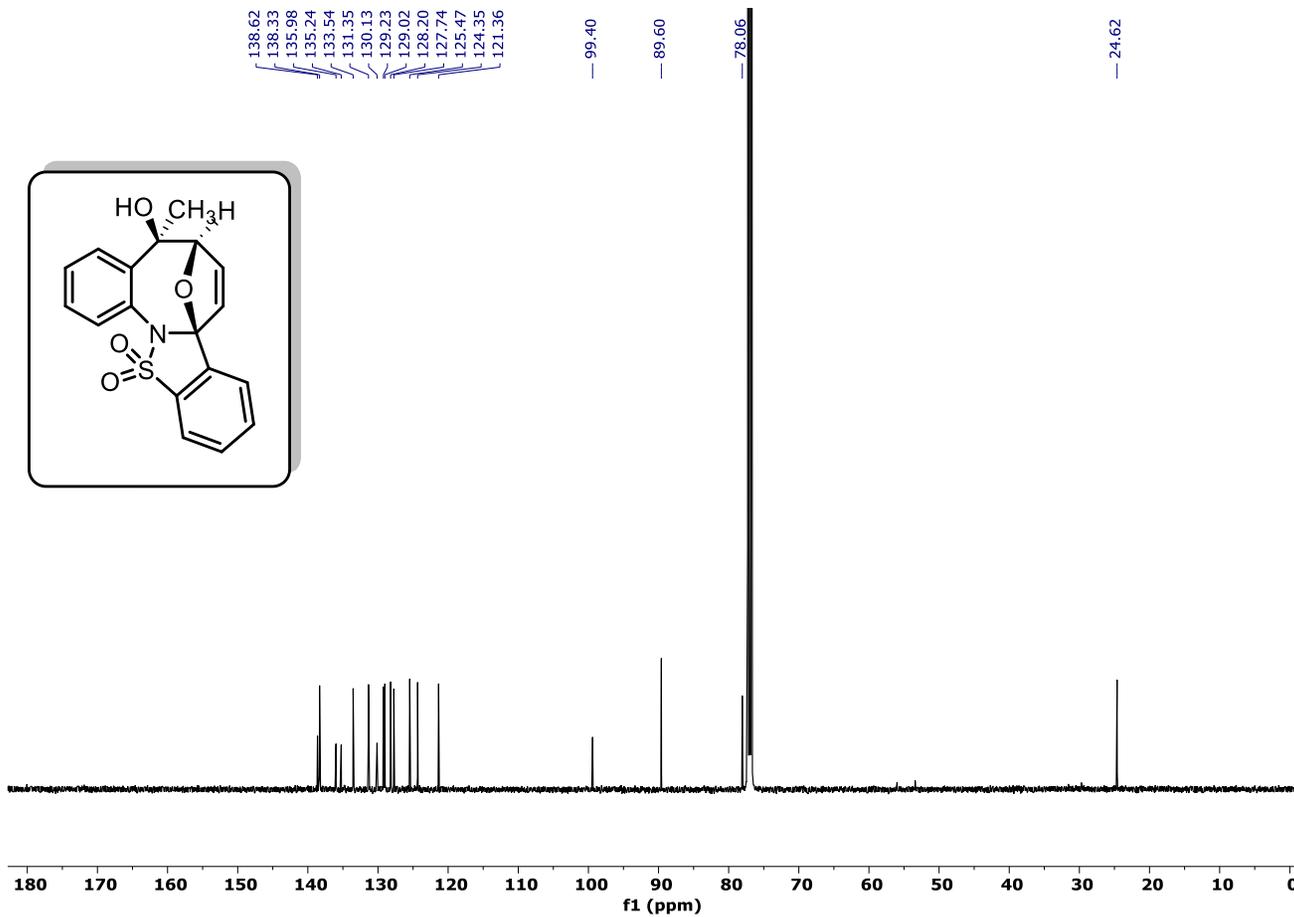
HSQC spectrum of **11e** (CDCl₃)



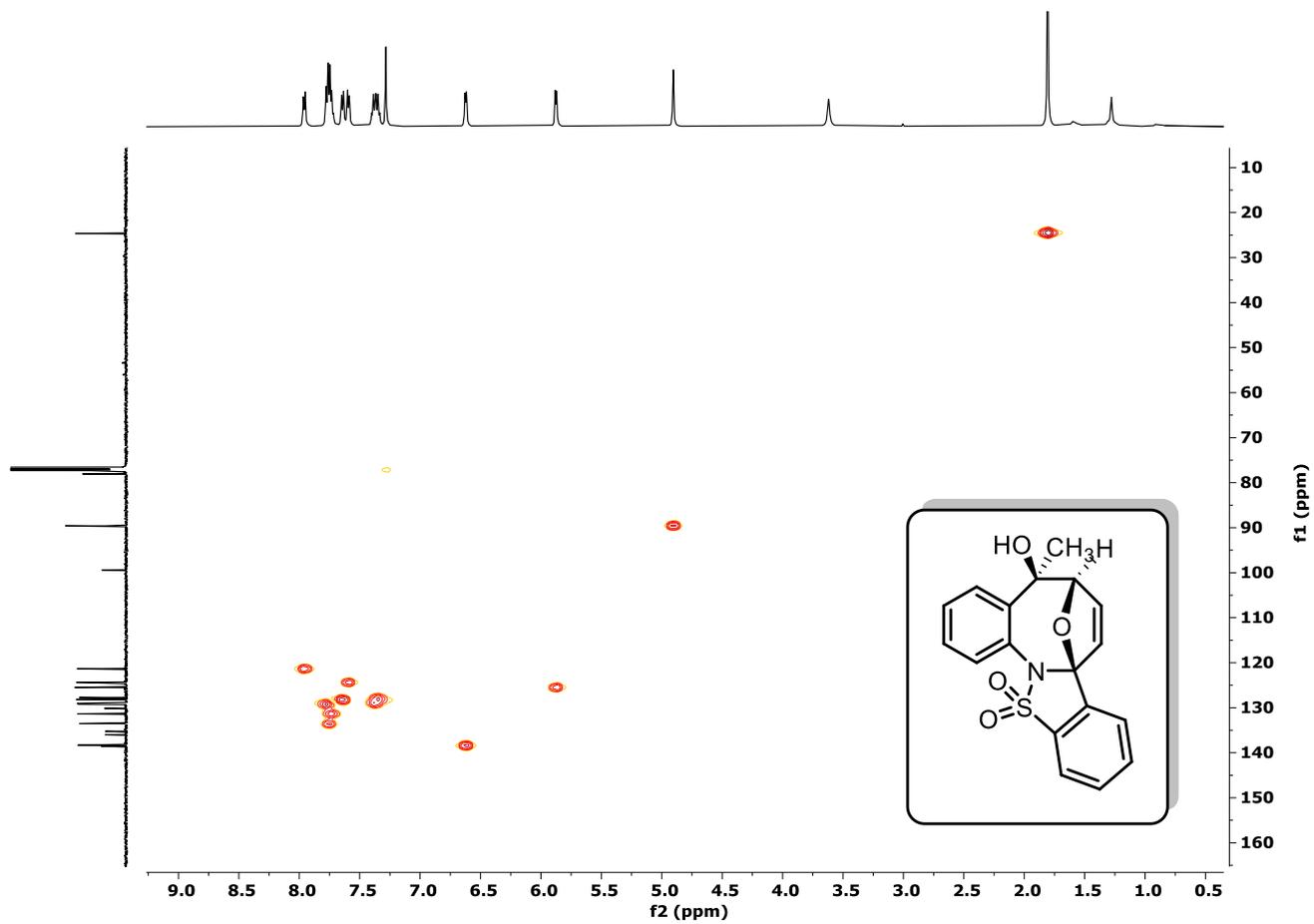
^1H NMR spectrum of **11ea** (500 MHz, CDCl_3)



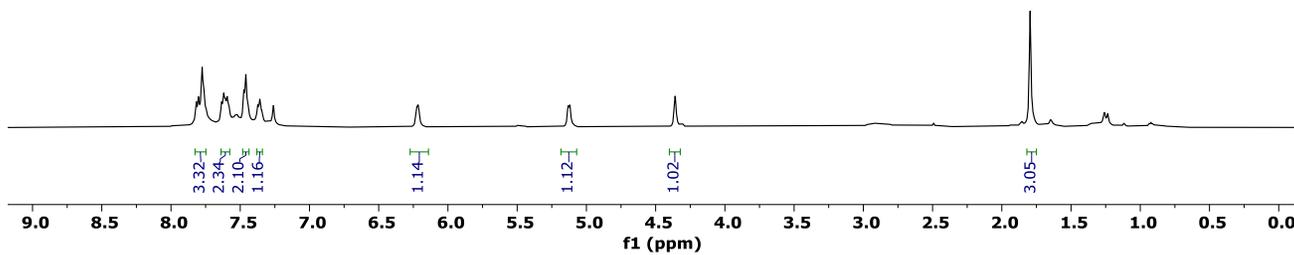
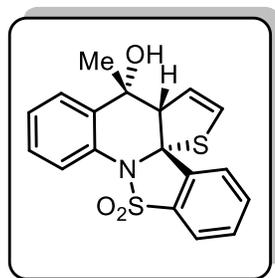
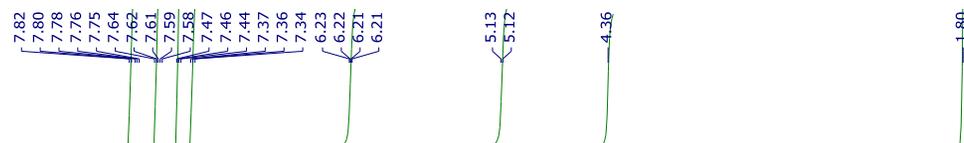
^{13}C NMR spectrum of **11ea** (126 MHz, CDCl_3)



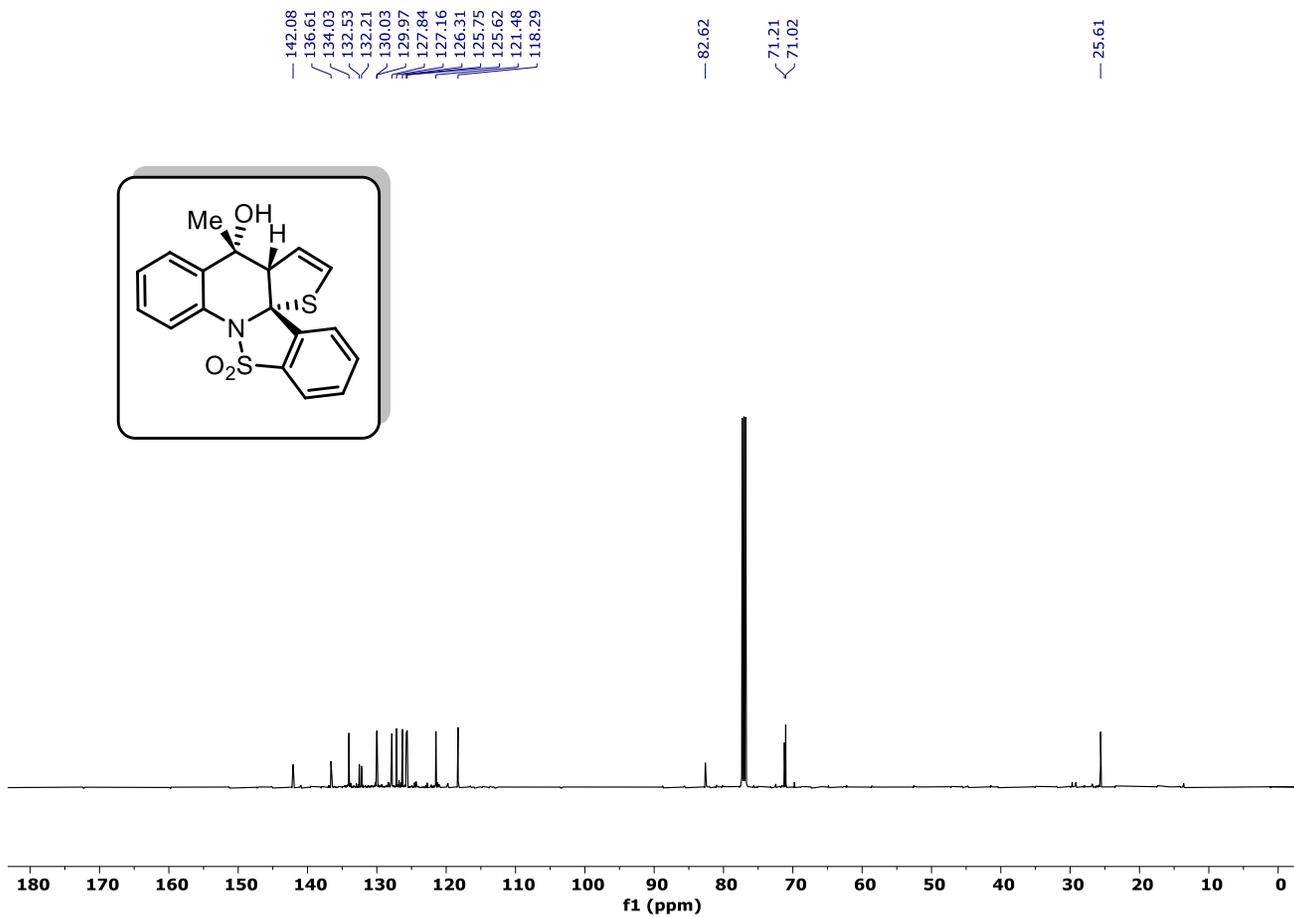
HSQC spectrum of **11ea** (CDCl₃)



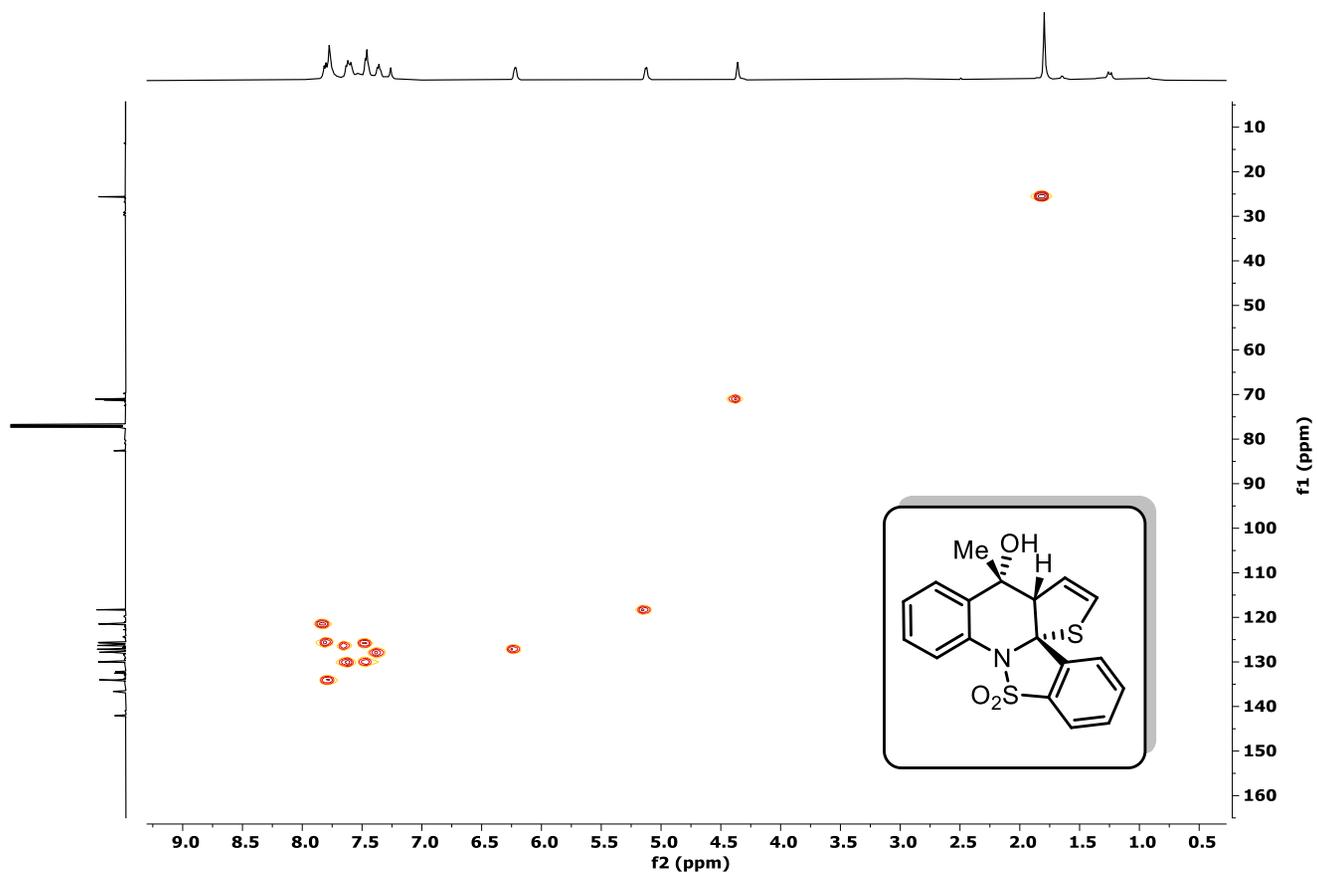
^1H NMR spectrum of **11f** (500 MHz, CDCl_3)



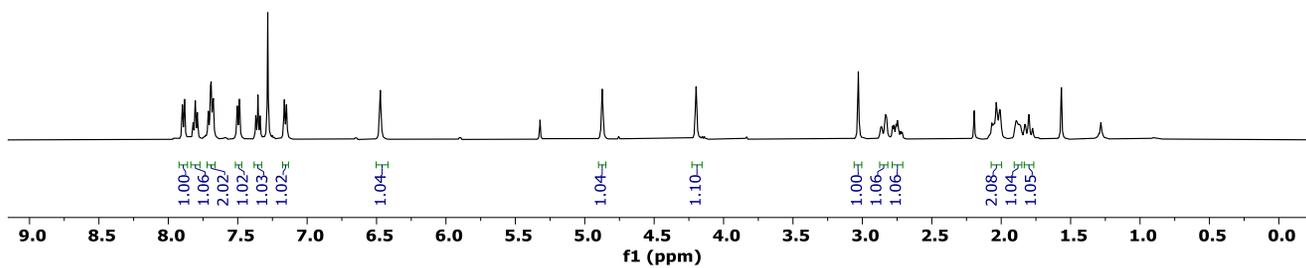
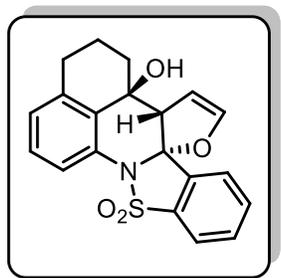
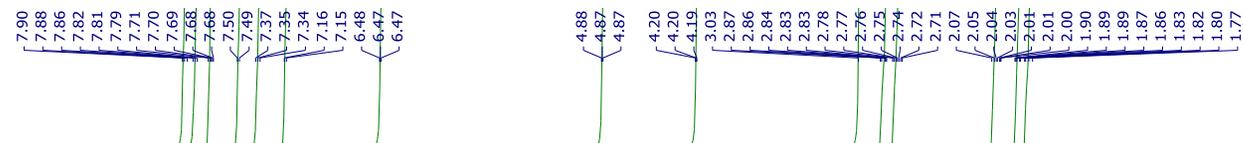
^{13}C NMR spectrum of **11f** (126 MHz, CDCl_3)



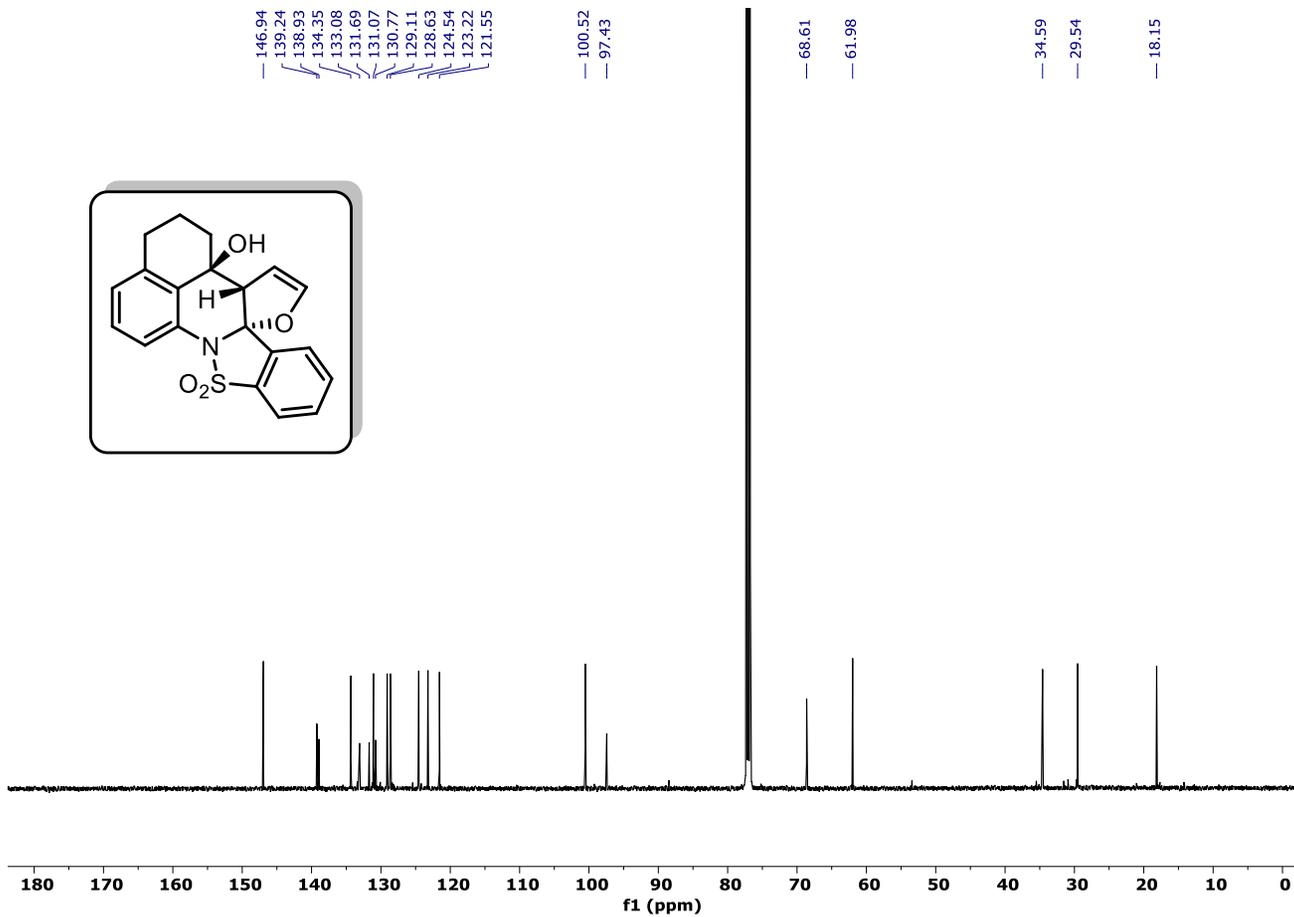
HSQC spectrum of **11f** (CDCl₃)



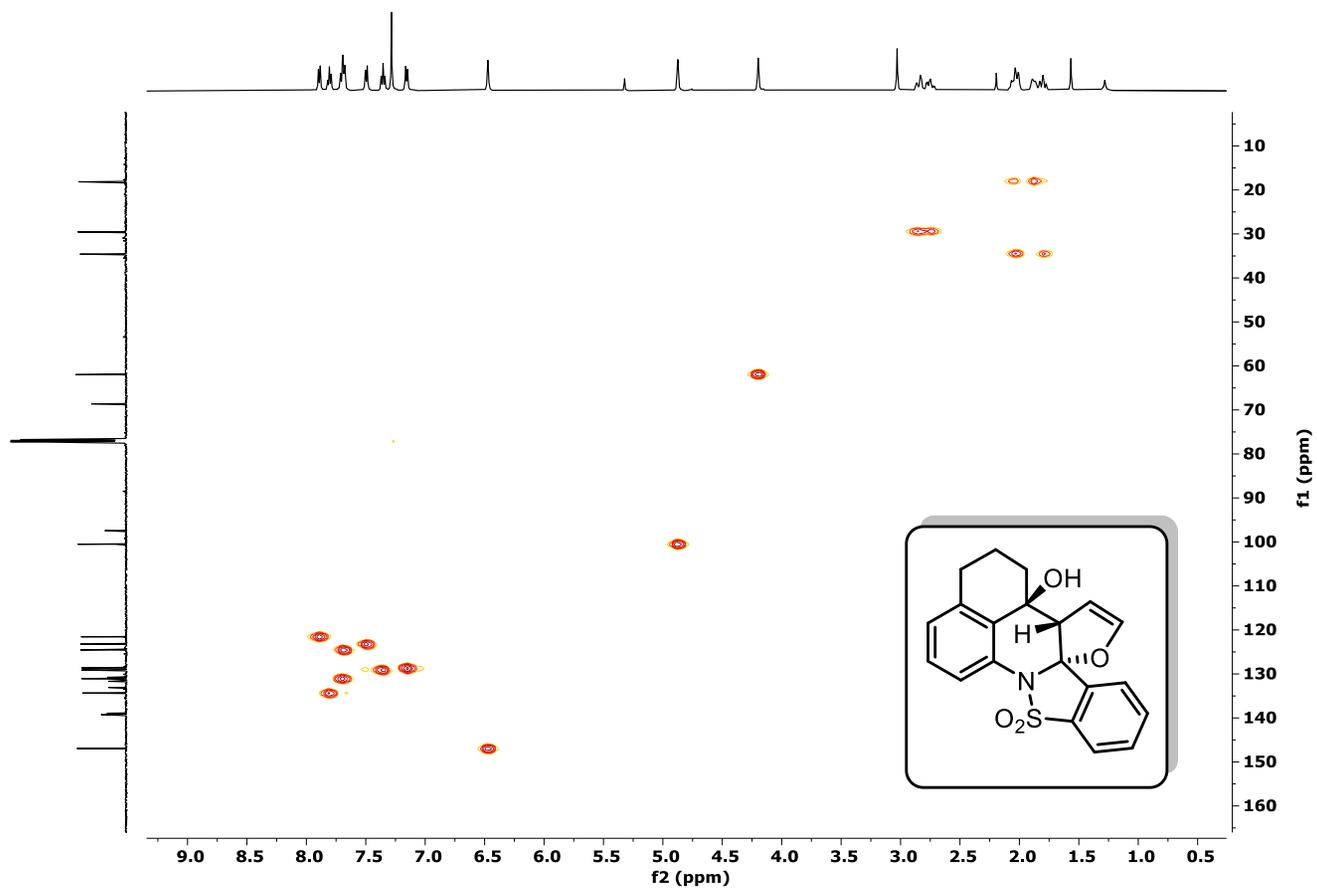
^1H NMR spectrum of **11g** (500 MHz, CDCl_3)



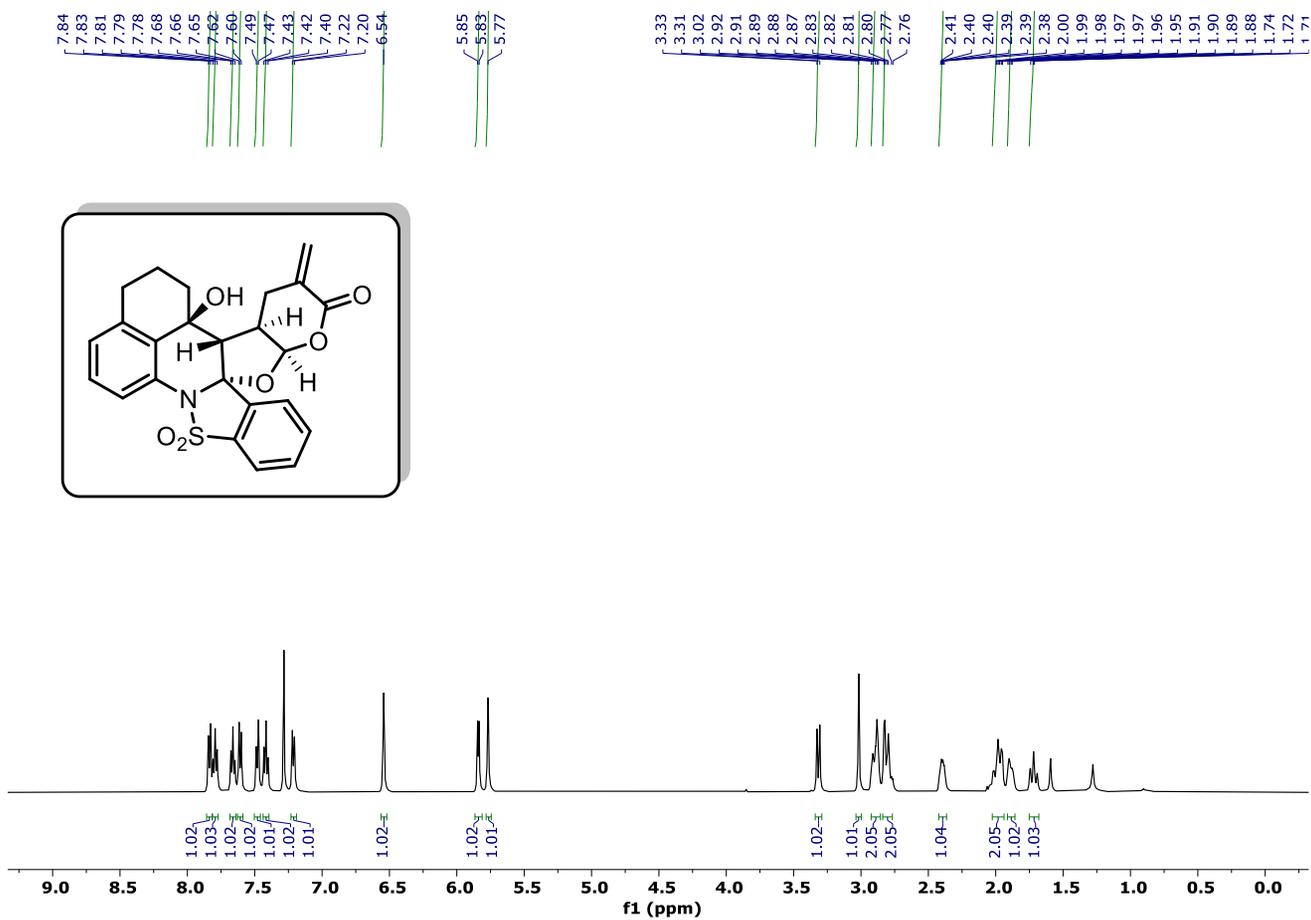
^{13}C NMR spectrum of **11g** (126 MHz, CDCl_3)



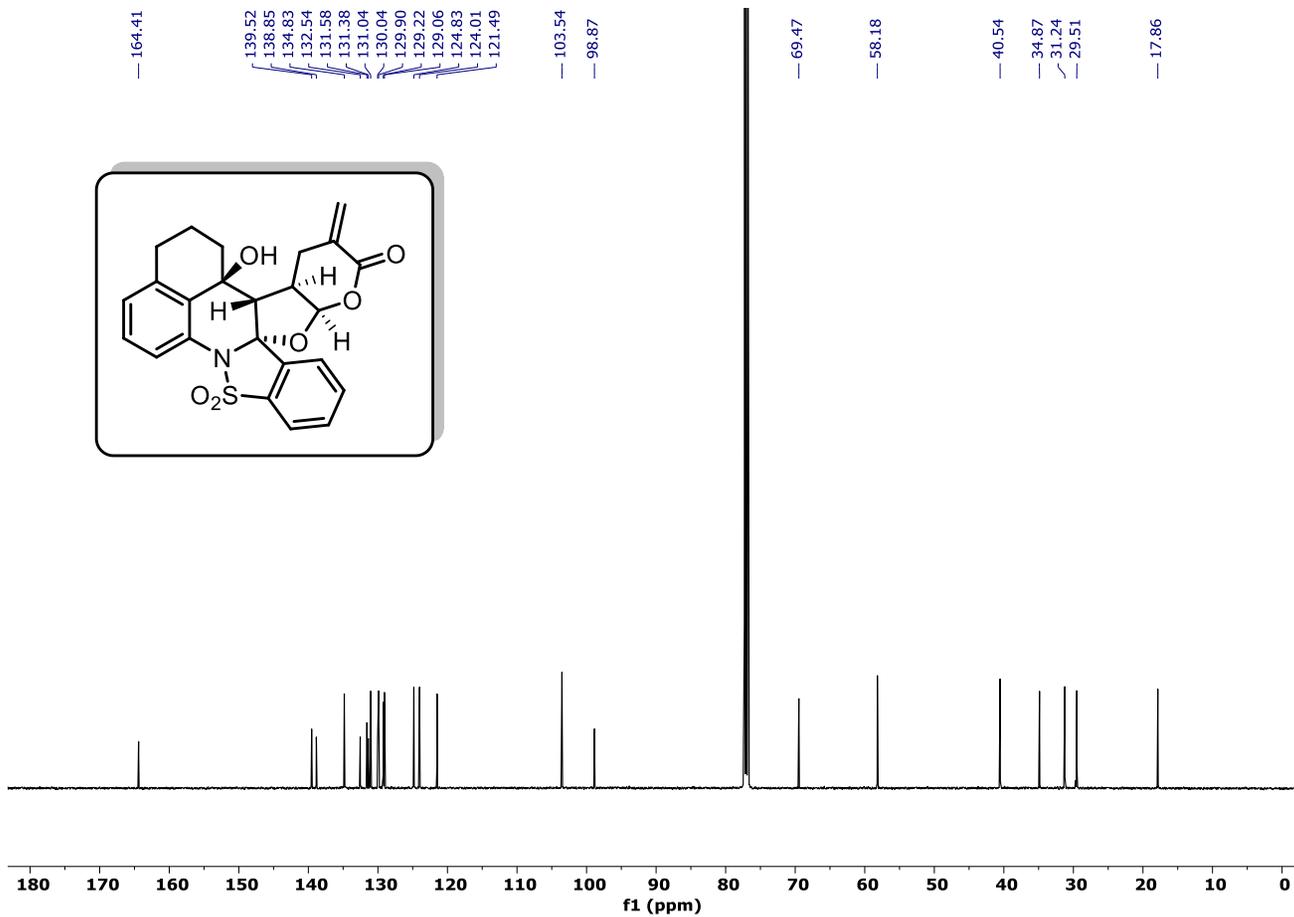
HSQC spectrum of **11g** (CDCl₃)



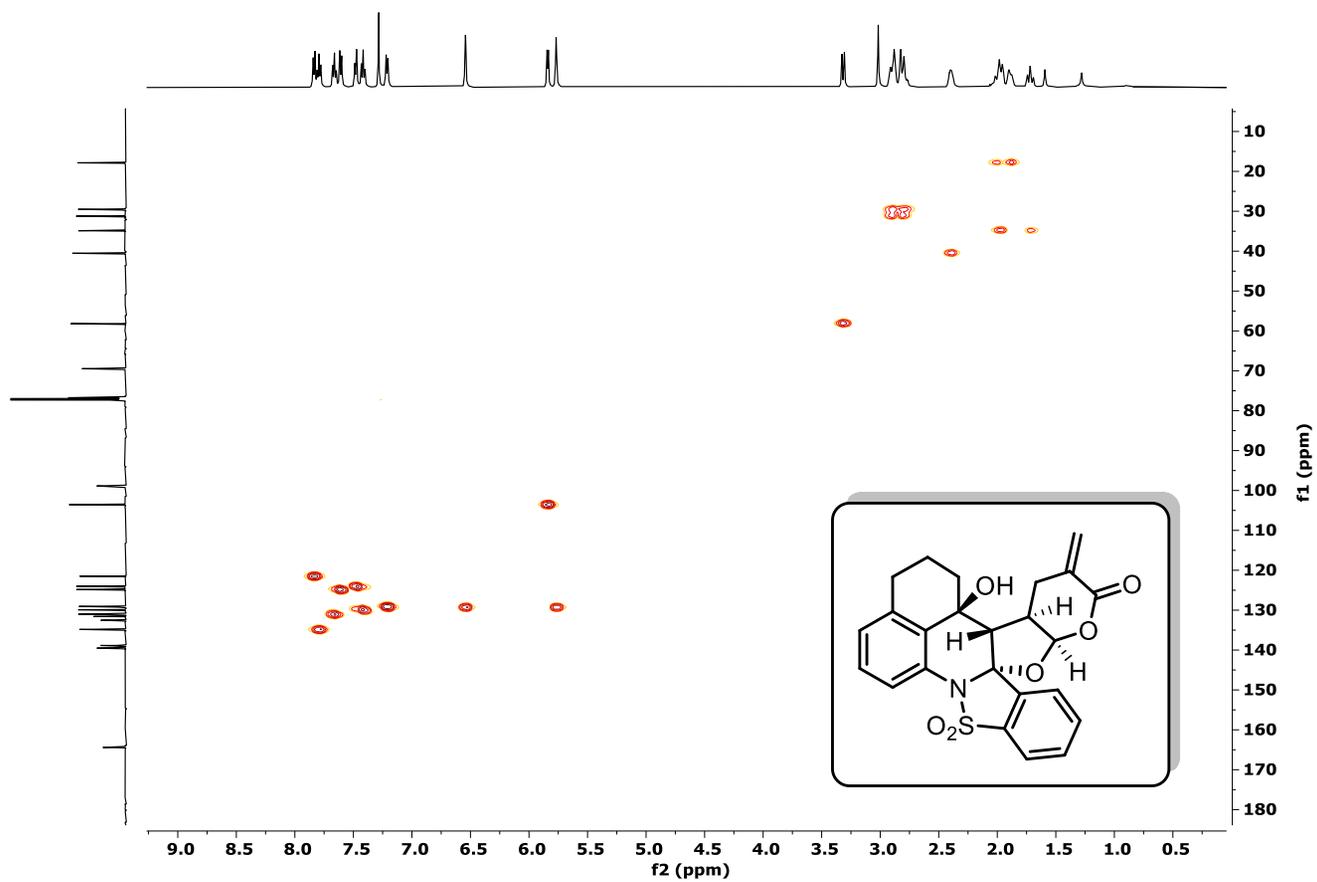
^1H NMR spectrum of **12** (500 MHz, CDCl_3)



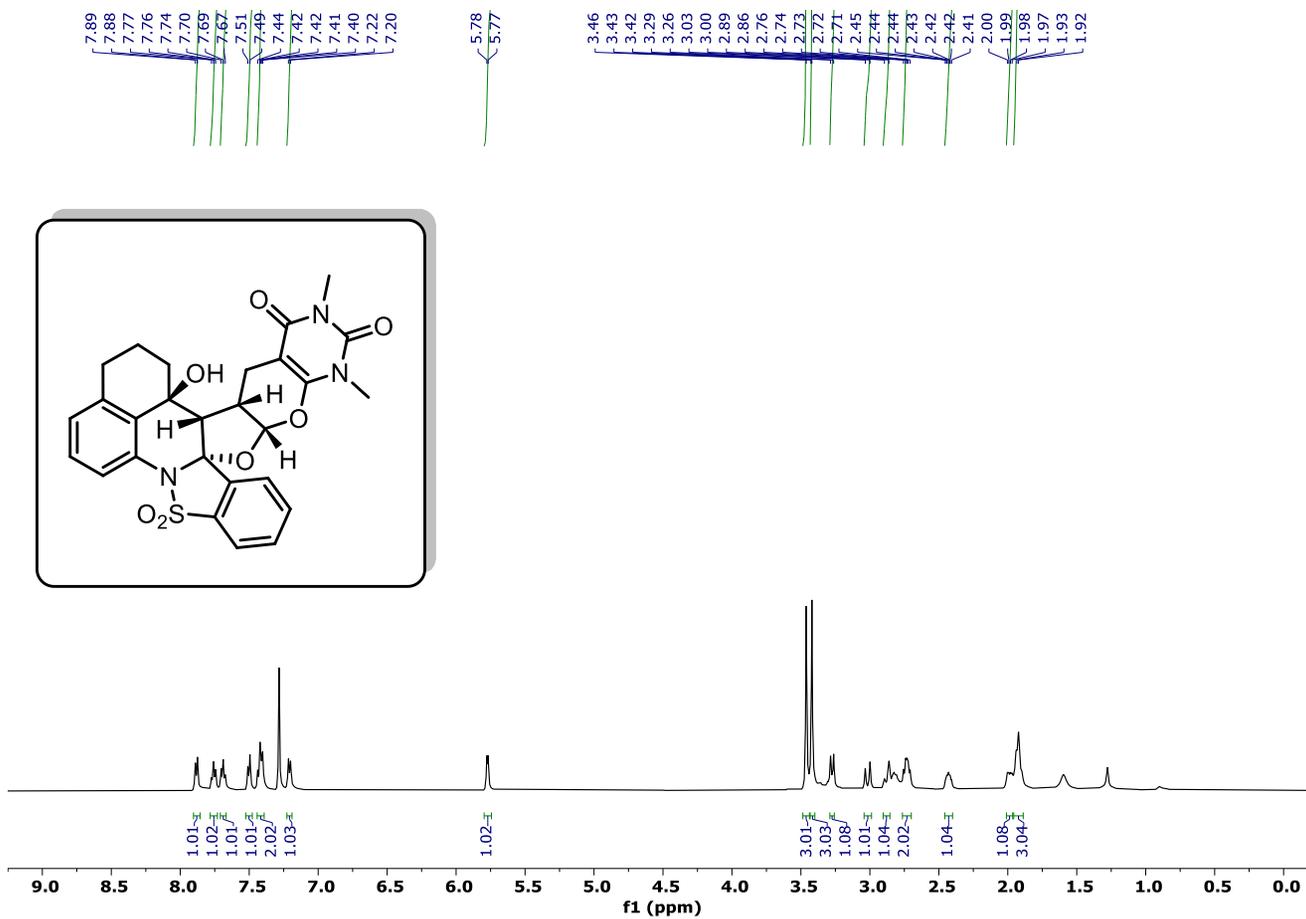
^{13}C NMR spectrum of **12** (126 MHz, CDCl_3)



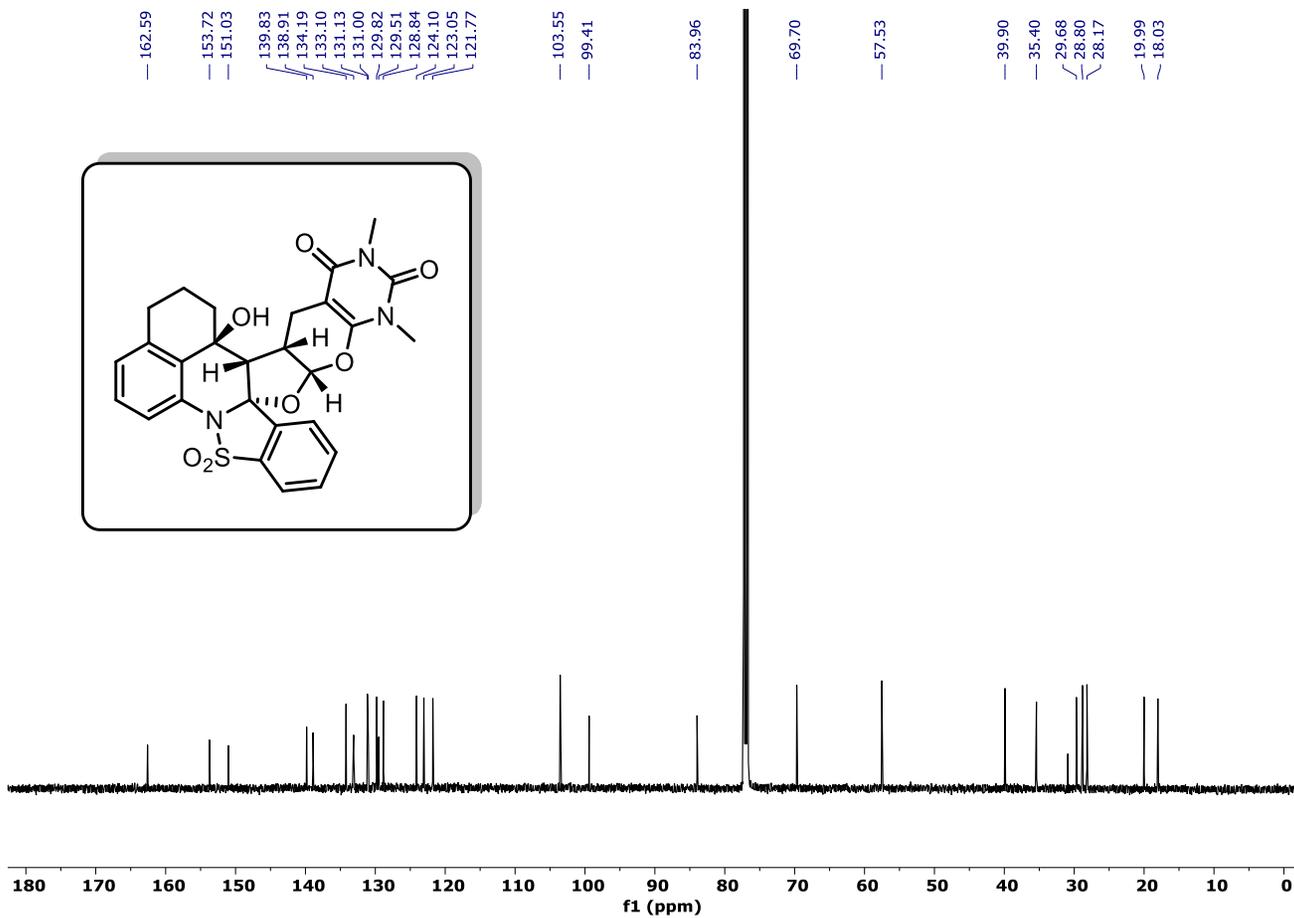
HSQC spectrum of **12** (CDCl₃)



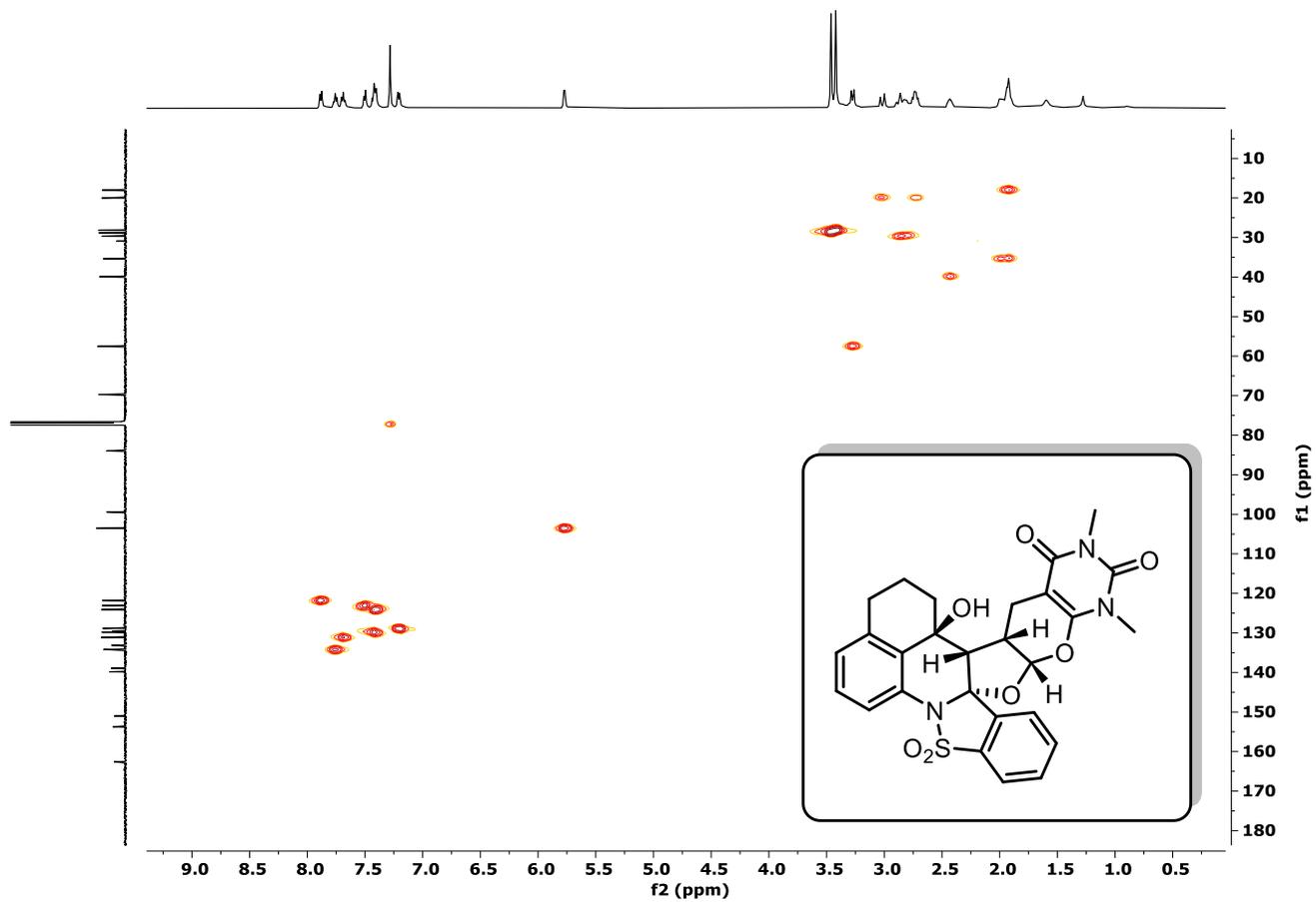
^1H NMR spectrum of **13** (500 MHz, CDCl_3)



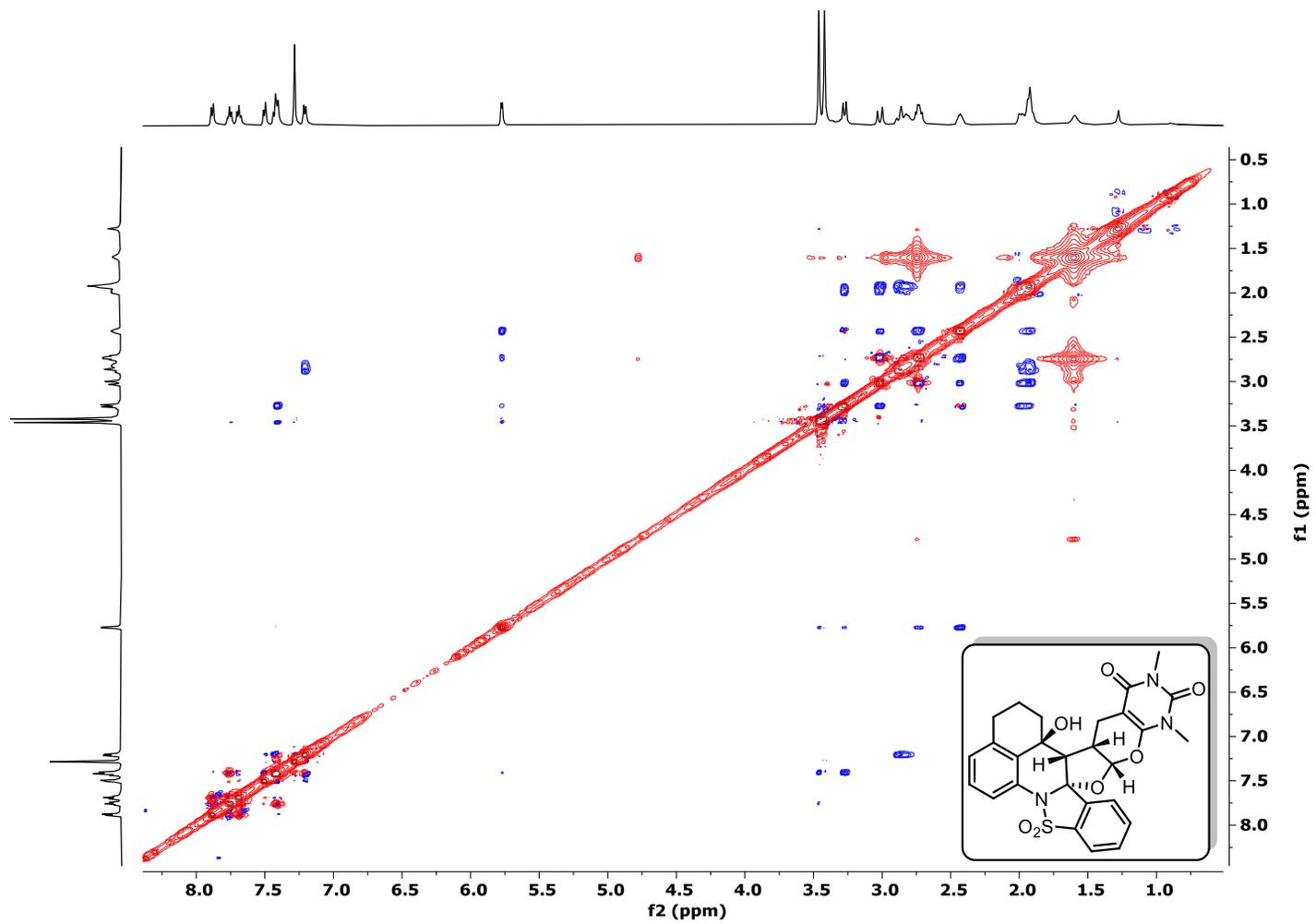
^{13}C NMR spectrum of **13** (126 MHz, CDCl_3)



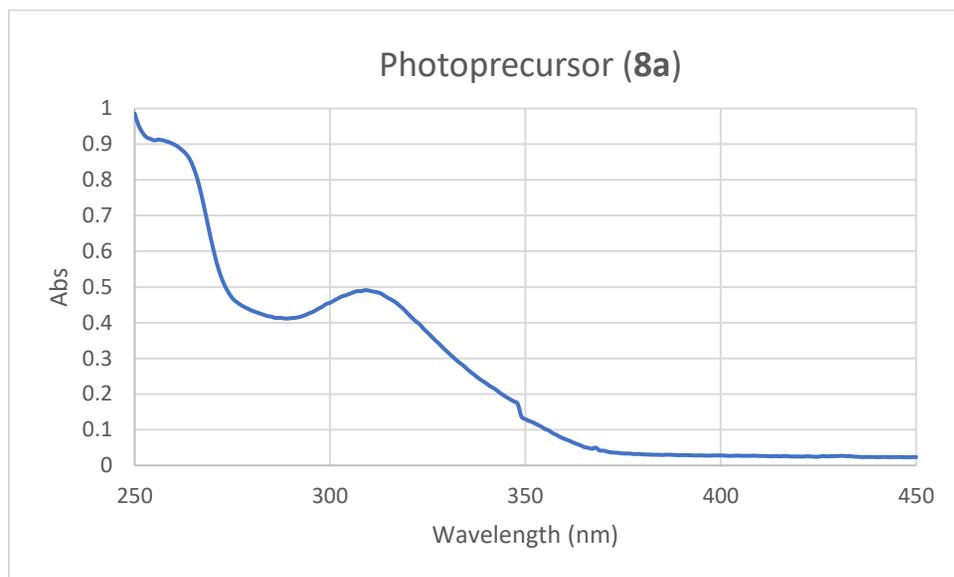
HSQC spectrum of **13** (CDCl₃)

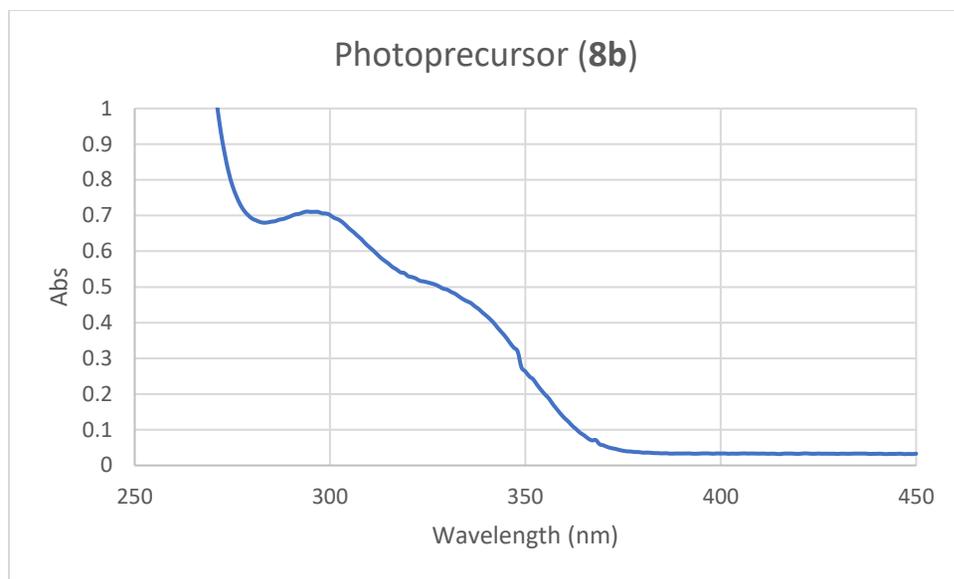


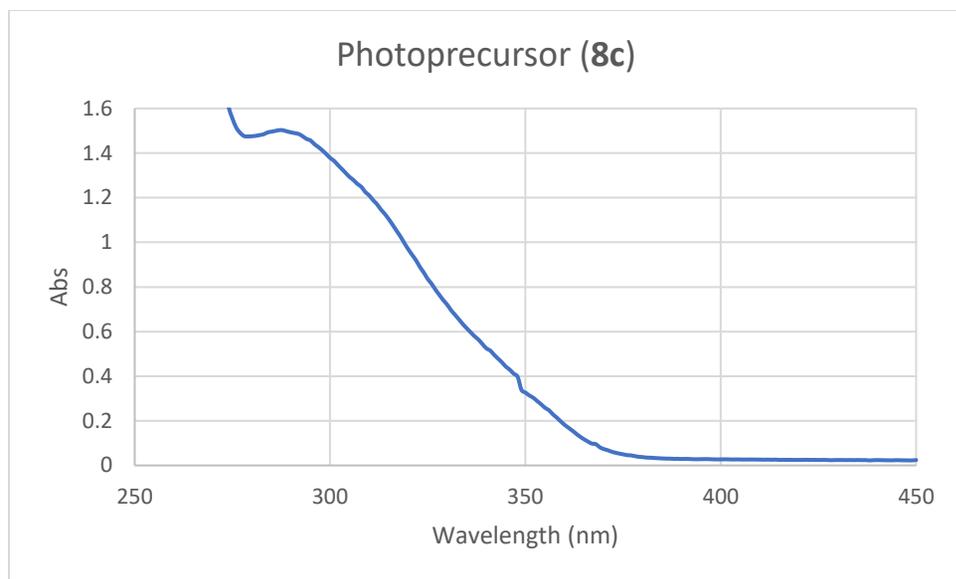
NOESY spectrum of **13** (CDCl₃)

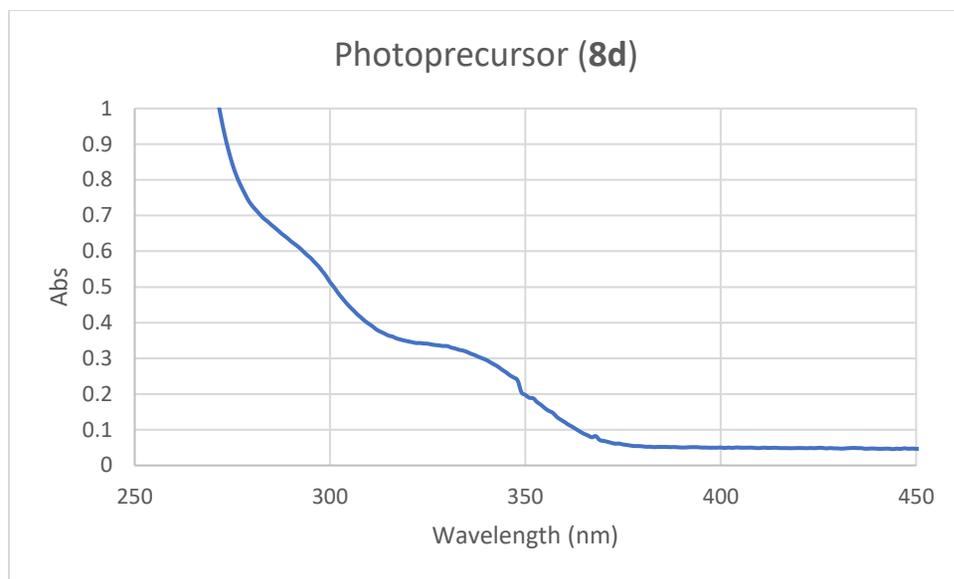


UV Spectra of photoprecursors









Photoprecursor (**8e**)

