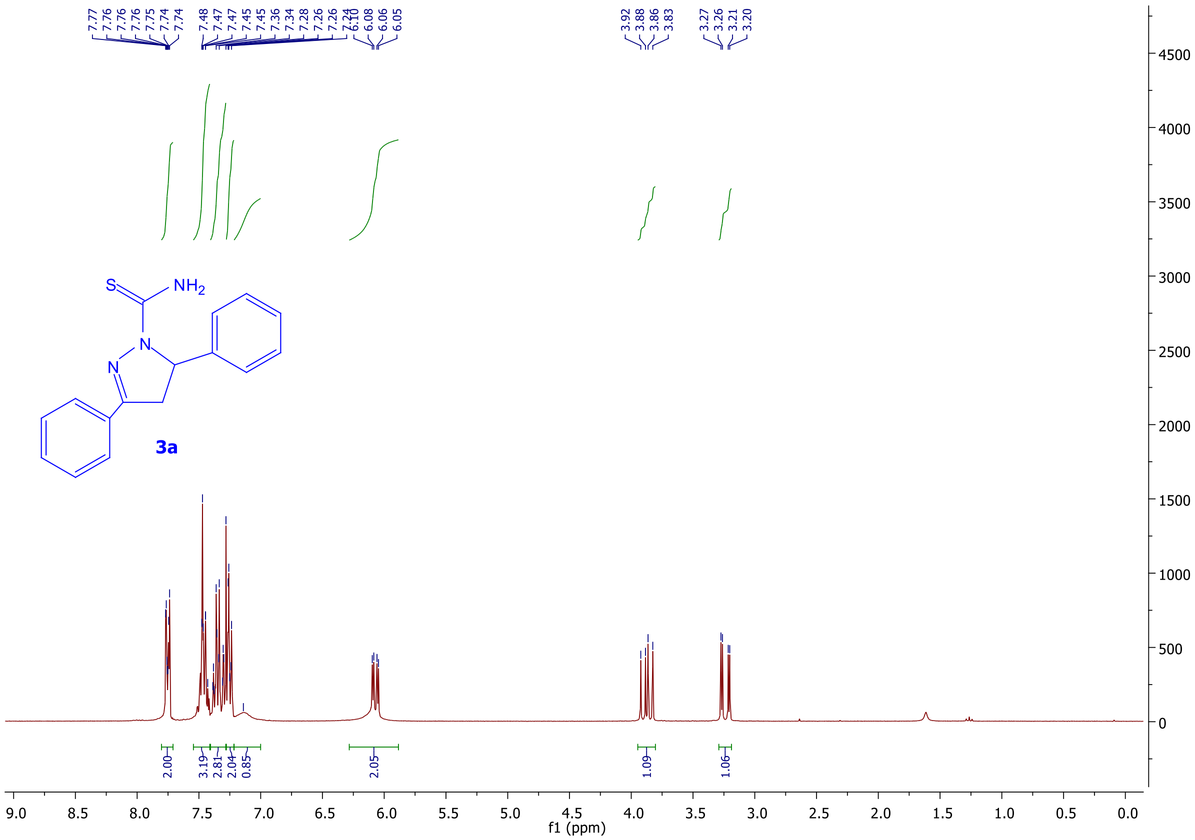
Synthesis, antioxidant activity and molecular doking of some new thiazolyl-pyrazolinyl-pyran-2-one derivatives

D. Hikem-Oukacha[a], S. Tellal[a,b], A. Amar[c], K. Ould Lamara[a], A. Rabahi[d], A. Benazzouz[a], S. Bouaziz-Terrachet[e], M. Makhloufi-Chebli[a], B. Jismy[b] and M. Abarbri[b,]*

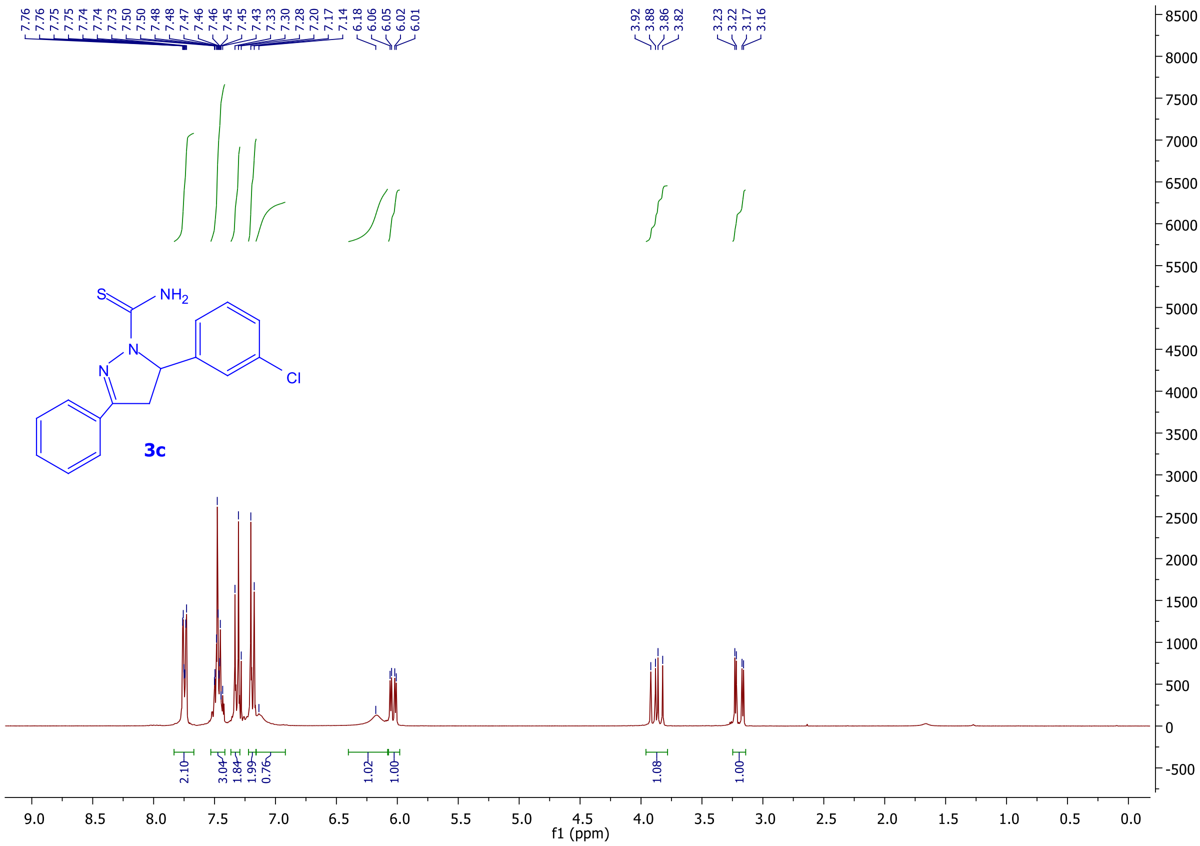
[a] *Laboratory of Physics and Chemistry Materials LPCM, Department of Chemistry, Faculty of Sciences, University Mouloud Mammeri, 15000, Tizi-Ouzou, Algeria.*
[b] *Laboratory of Physico-Chemistry of Materials and Electrolytes for Energy (PCM2E). EA 6299, Faculty of Sciences, avenue Monge Parc de Grandmont, 37200 Tours, France.*
[c] *LPCQ Laboratory, Department of Chemistry, Faculty of Sciences, University Mouloud Mammeri, 15000, Tizi-Ouzou, Algeria.*
[d] *Laboratory of Applied Organic Chemistry, Faculty of Chemistry, University of Science and Technology Houari Boumediene, BP 32, El Alia, 16111 Bab Ezzouar, Algiers, Algeria.*
[e] *Department of Chemistry, Faculty of Sciences, University Mohamed Bouguerra, Boumerdes, Algeria.*

Table of Contents

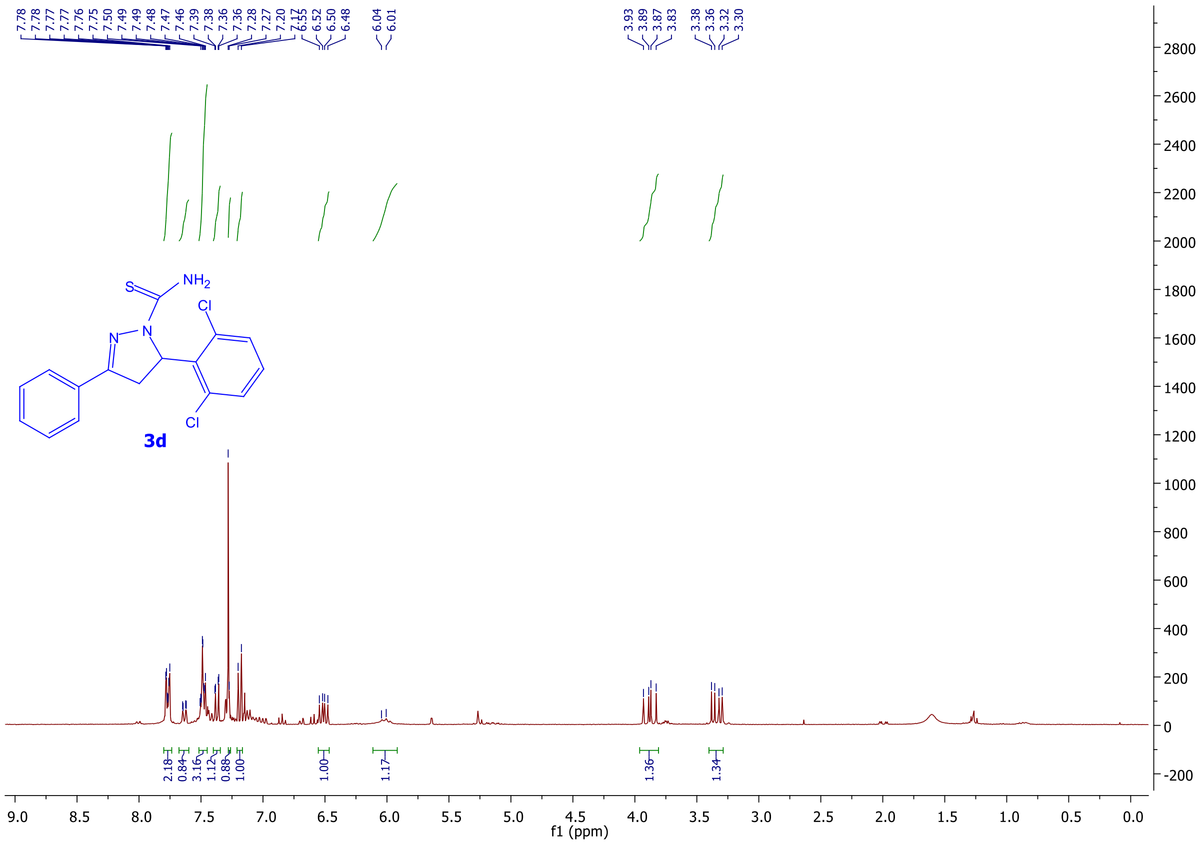
[1]H NMR of product **3a** in $CDCl_3$ (300 MHz)



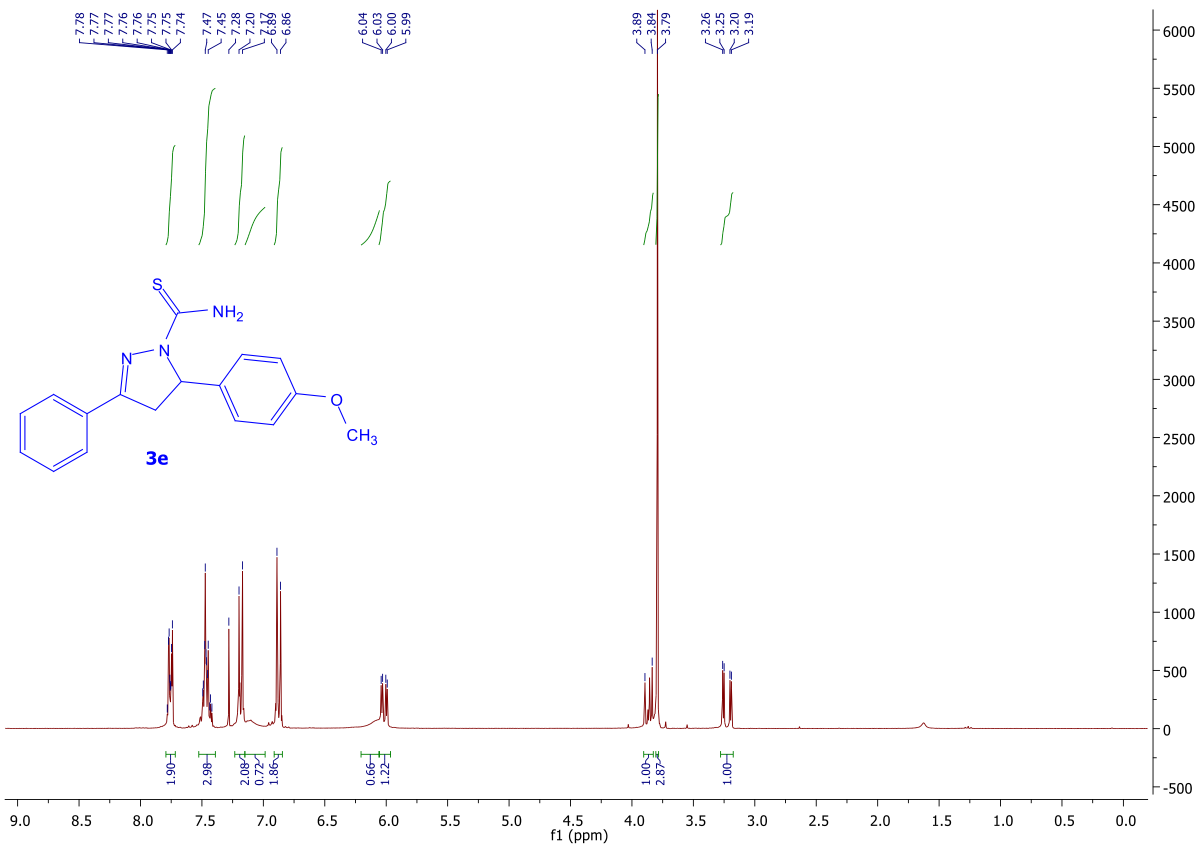
[1]H NMR of product **3c** in $CDCl_3$ (300 MHz)



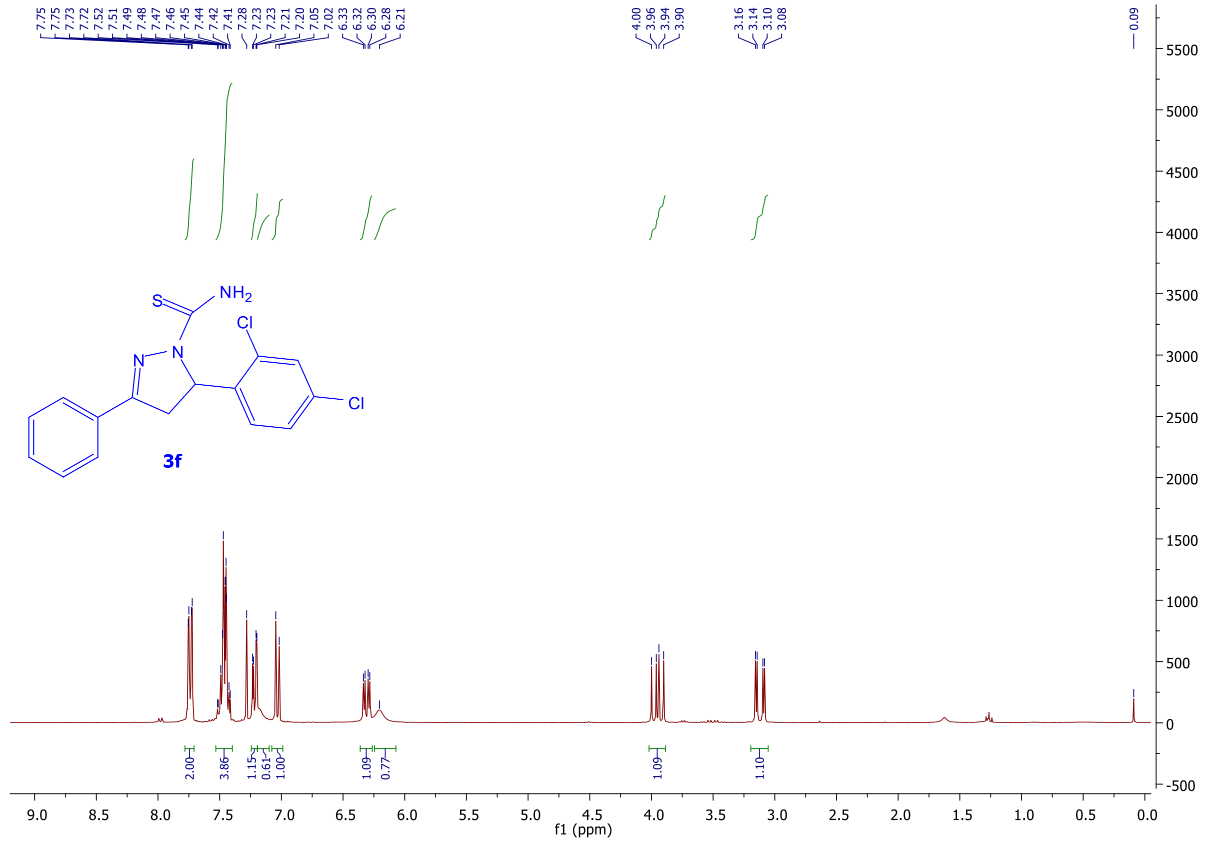
^{1}H NMR of product **3d** in $CDCl_3$ (300 MHz)



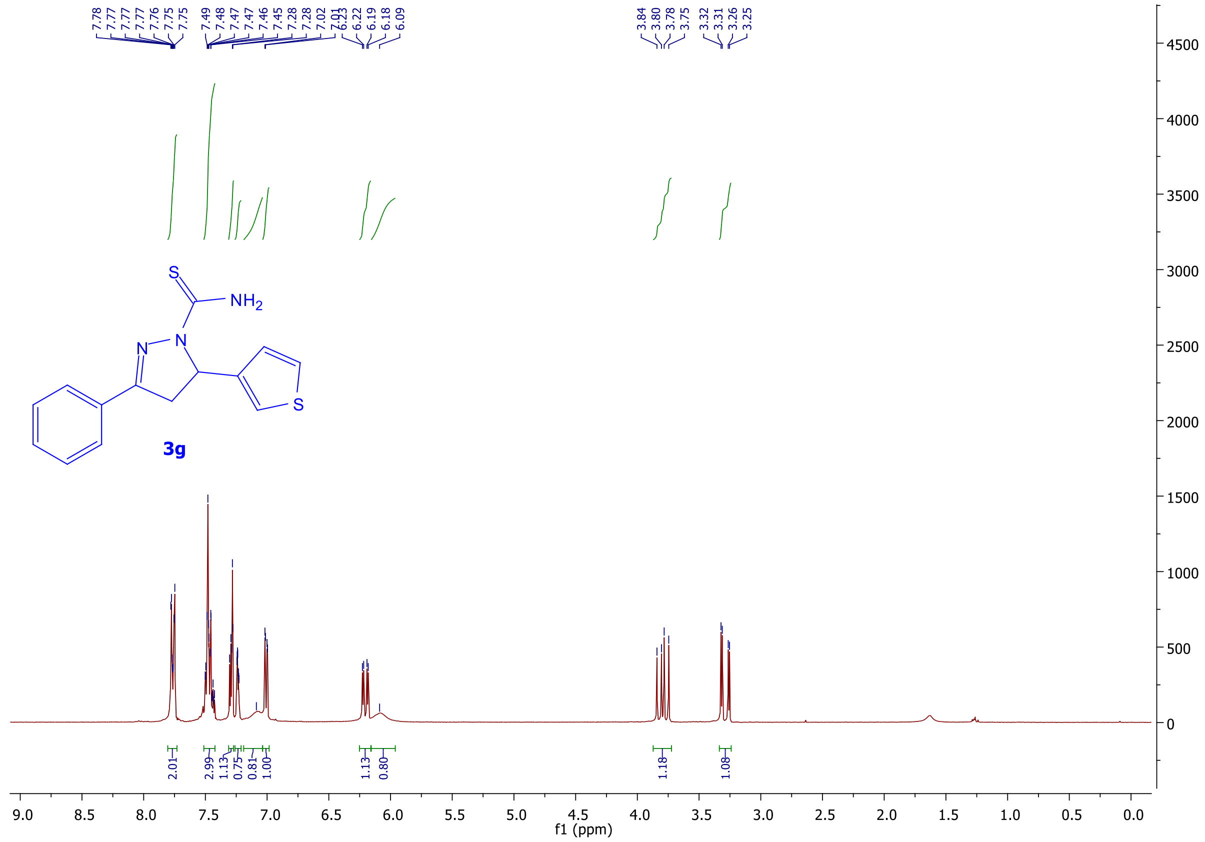
^{1}H NMR of product **3e** in $CDCl_3$ (300 MHz)



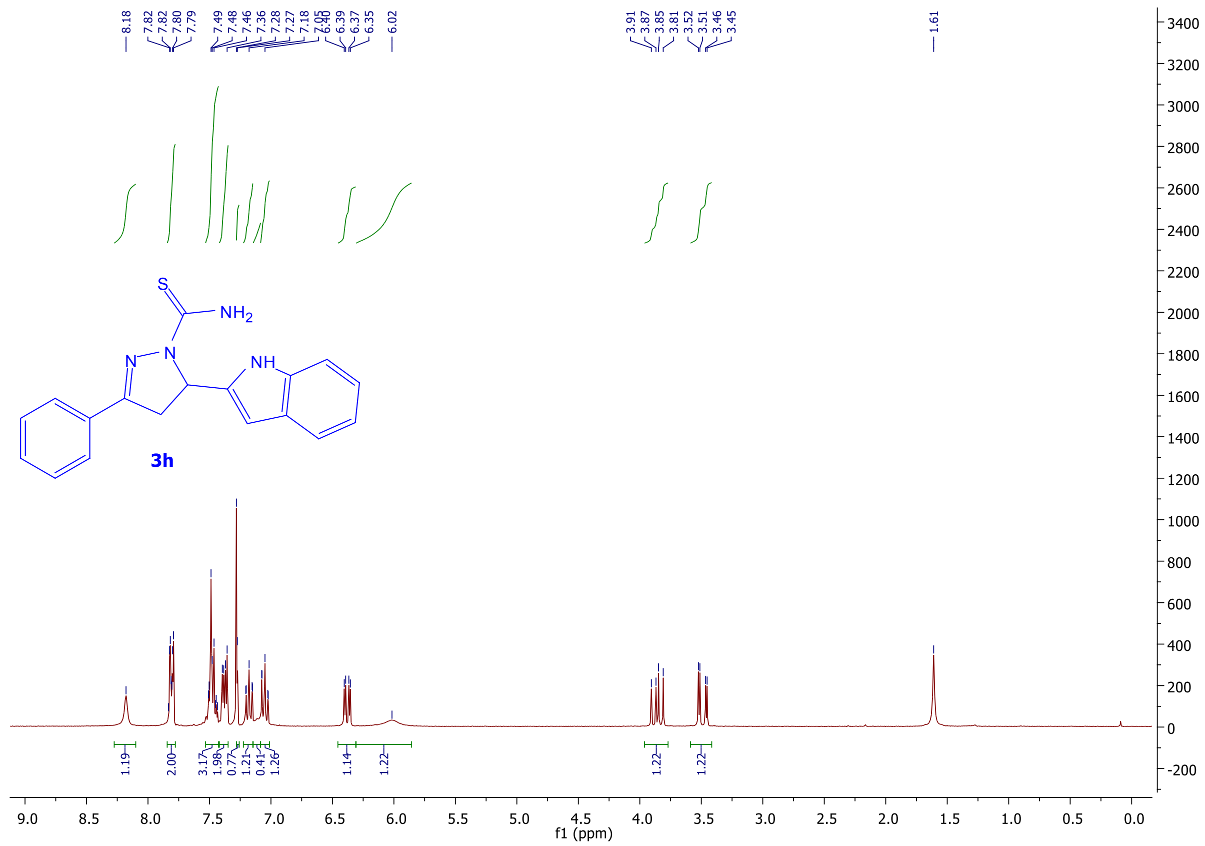
^{1}H NMR of product **3f** in $CDCl_3$ (300 MHz)



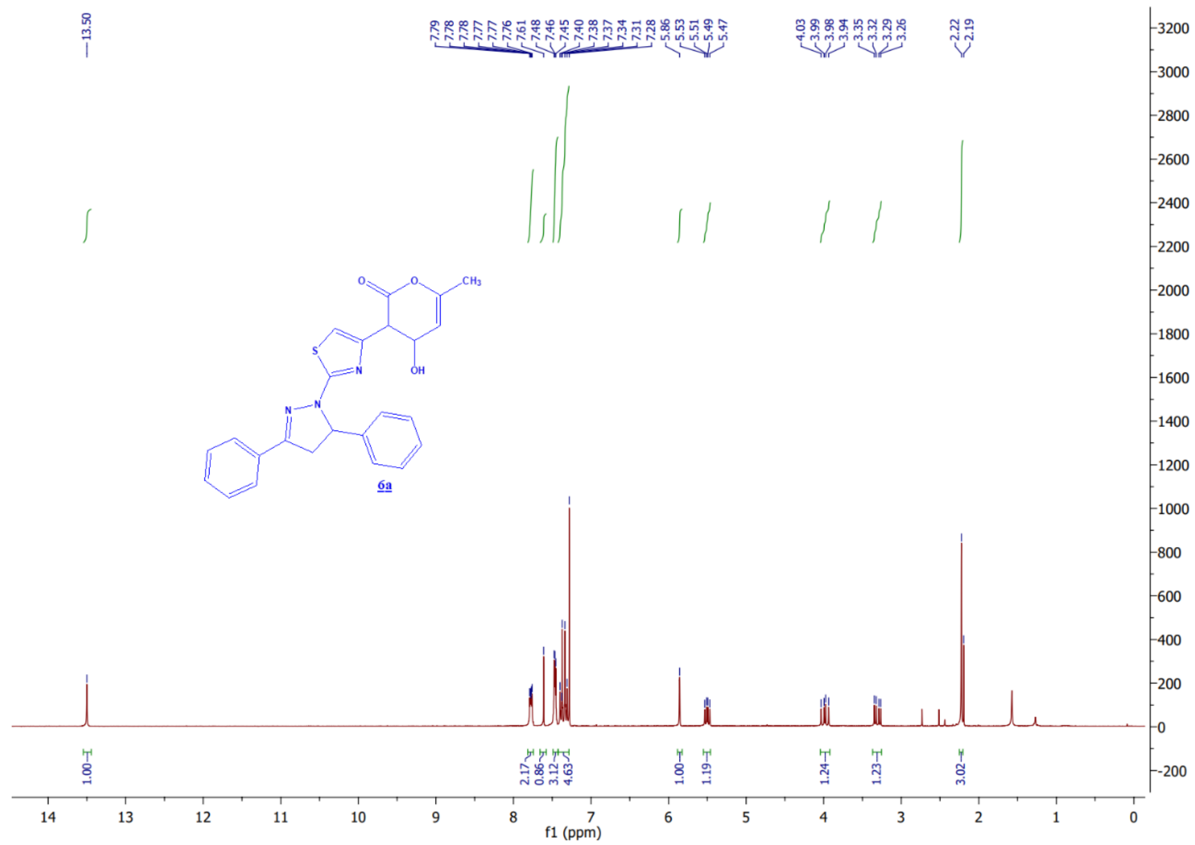
^{1}H NMR of product **3g** in $CDCl_3$ (300 MHz)



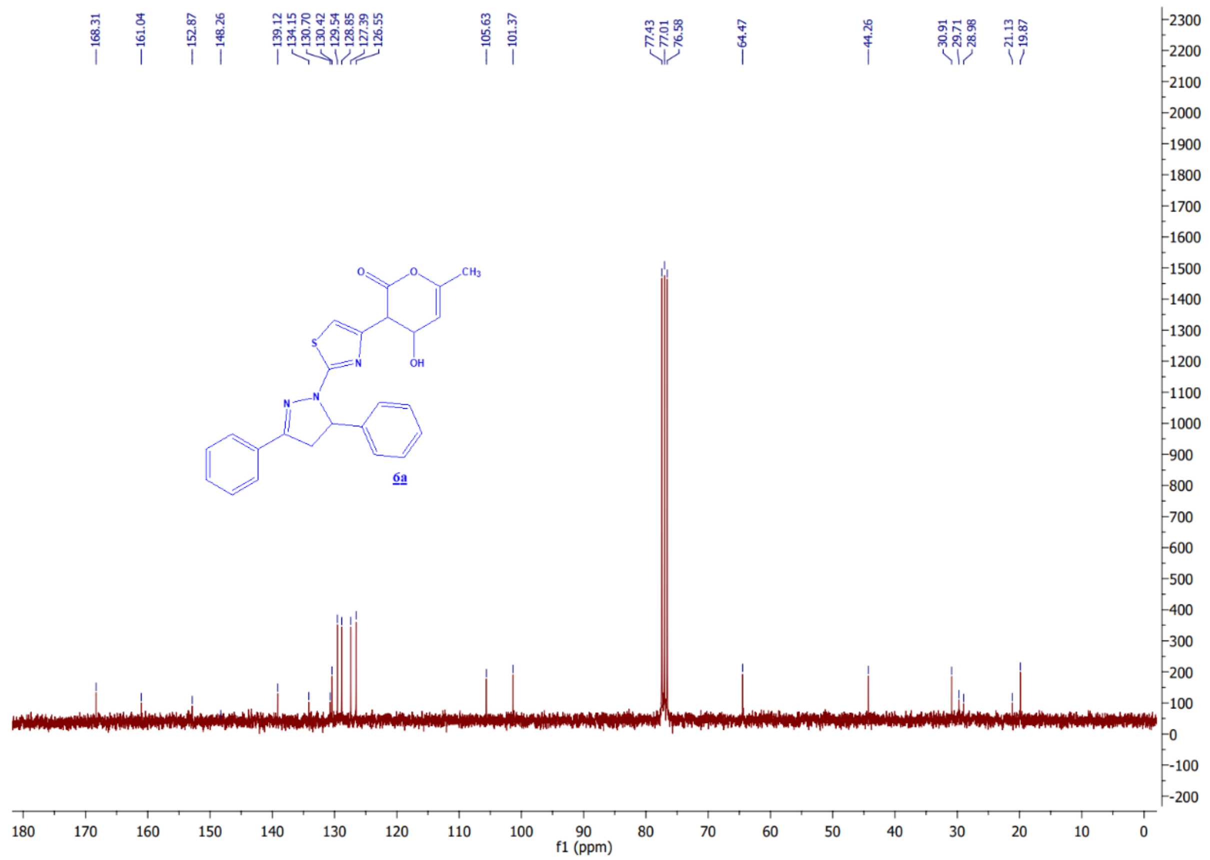
[1]H NMR of product **3h** in CDCl₃ (300 MHz)



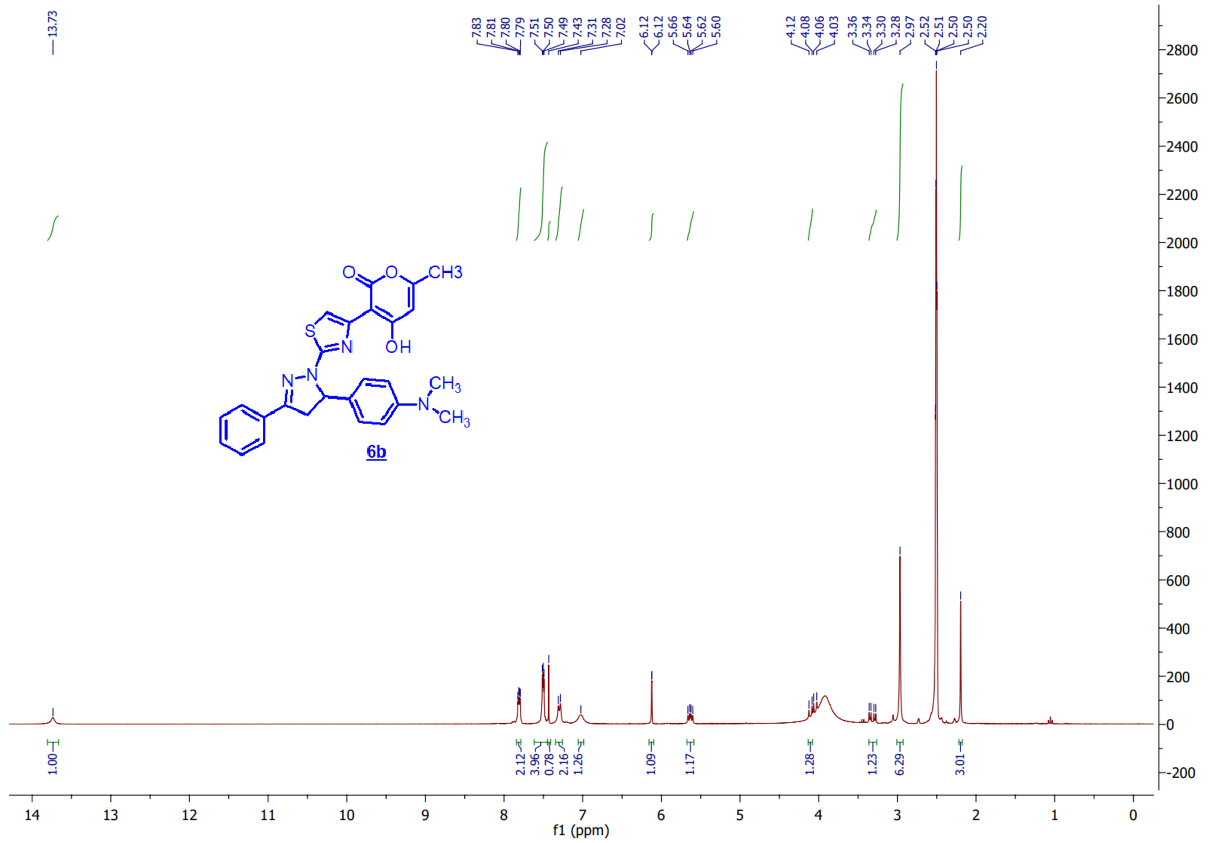
[1]H NMR of product **6a** in CDCl₃ (300 MHz)



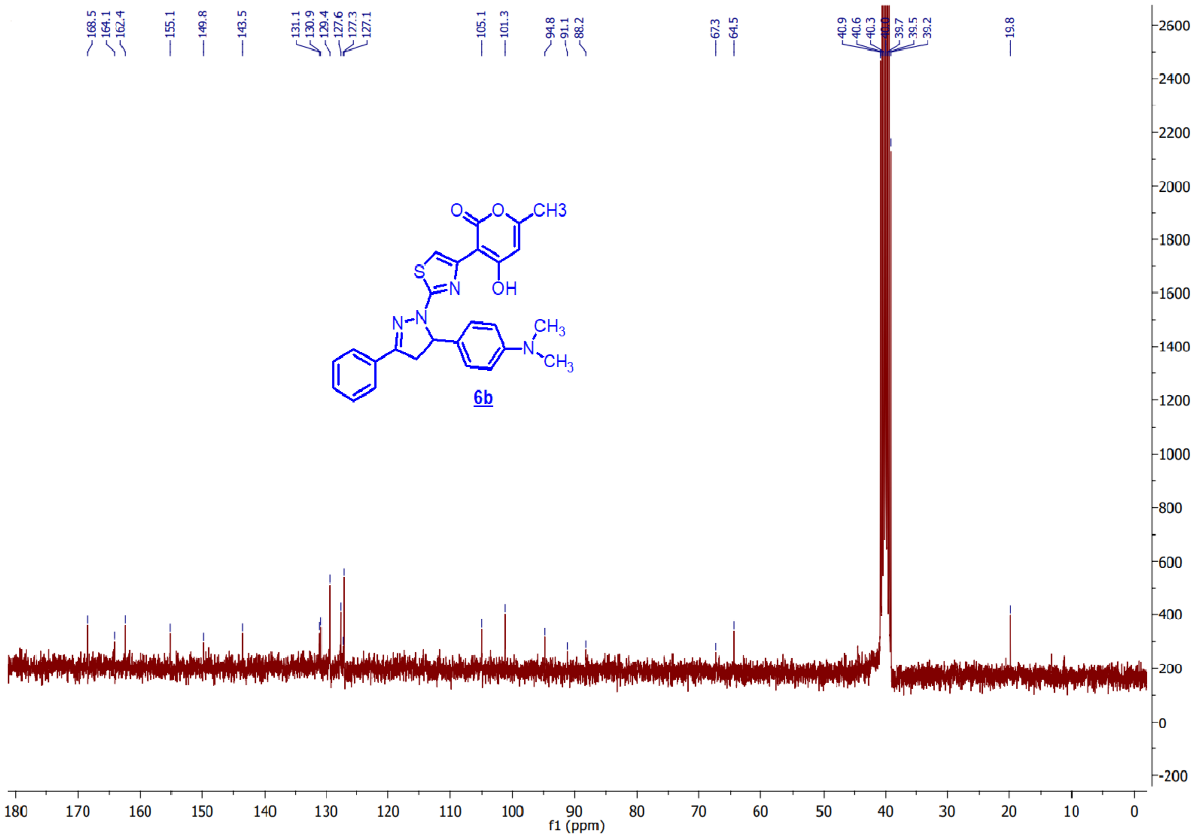
^{13}C NMR of product **6a** in $CDCl_3$ (75 MHz)



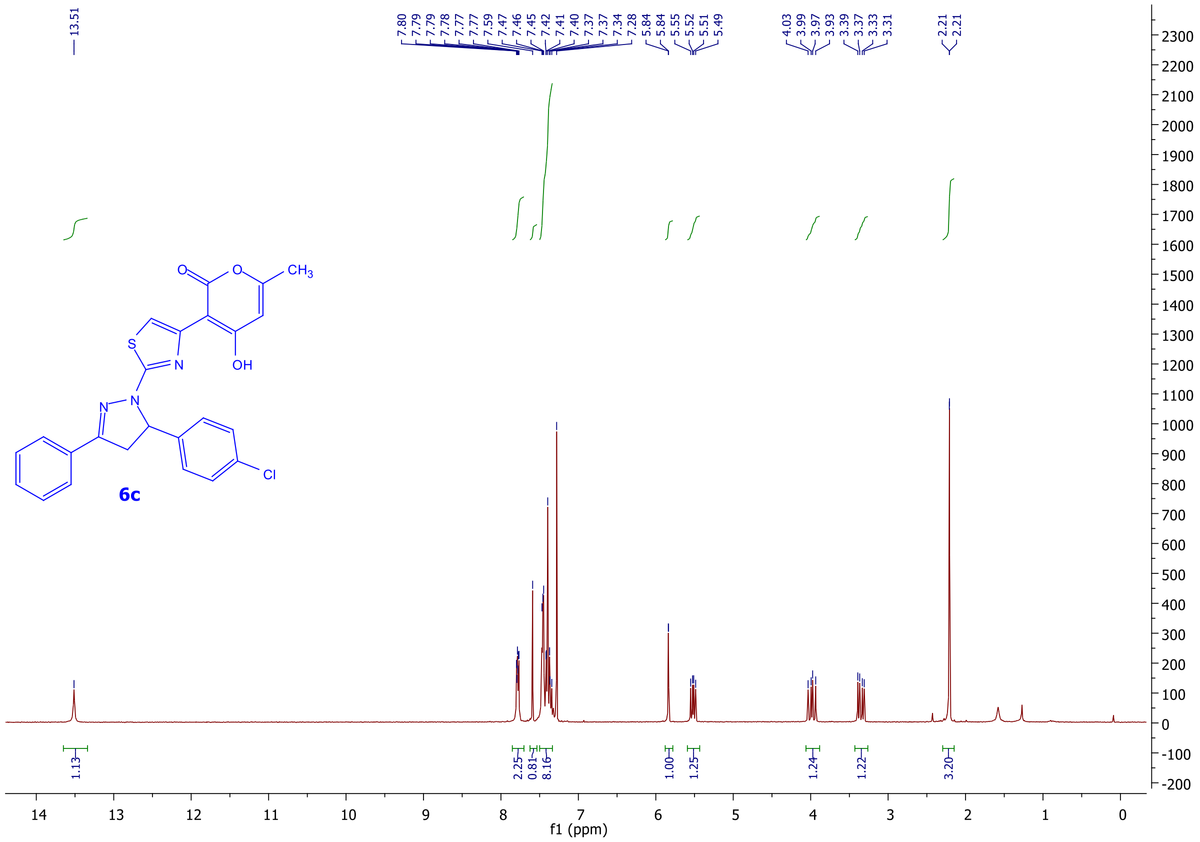
^{1}H NMR of product **6b** in DMSO (300 MHz)



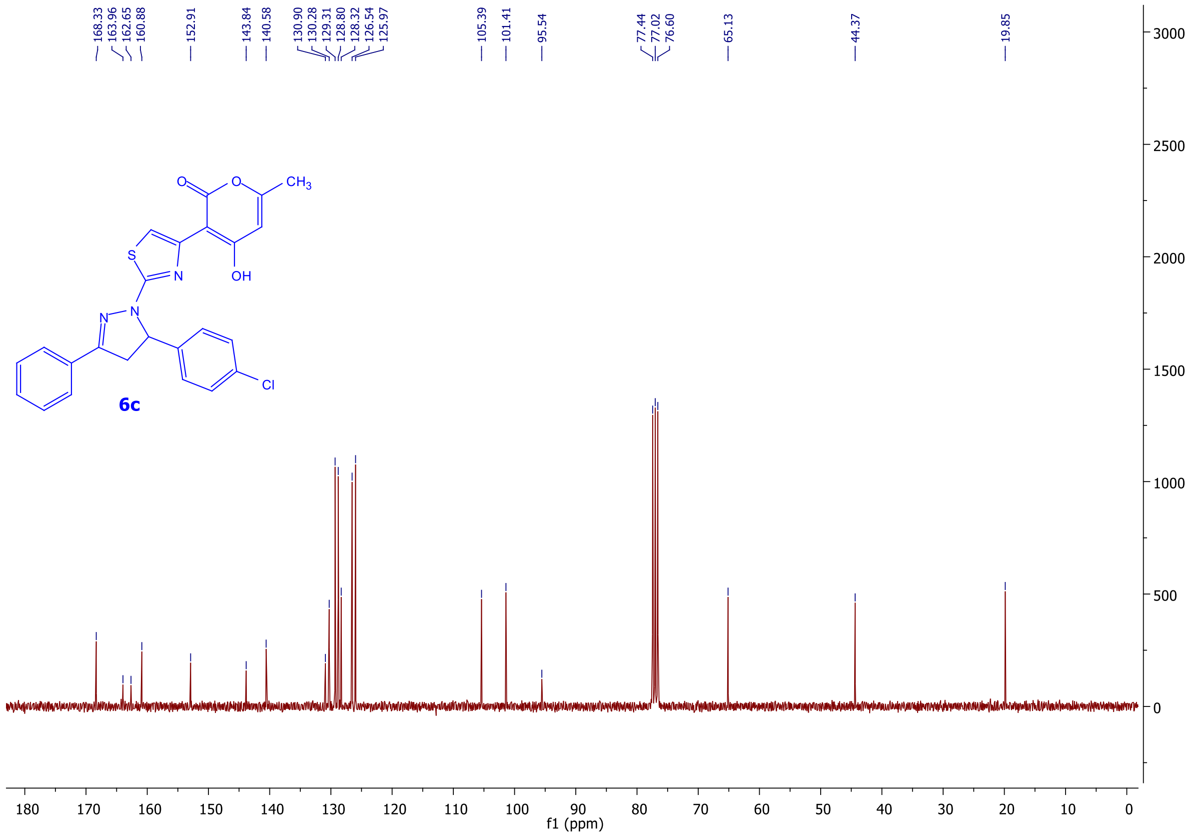
^{13}C NMR of product **6b** in DMSO (75 MHz)



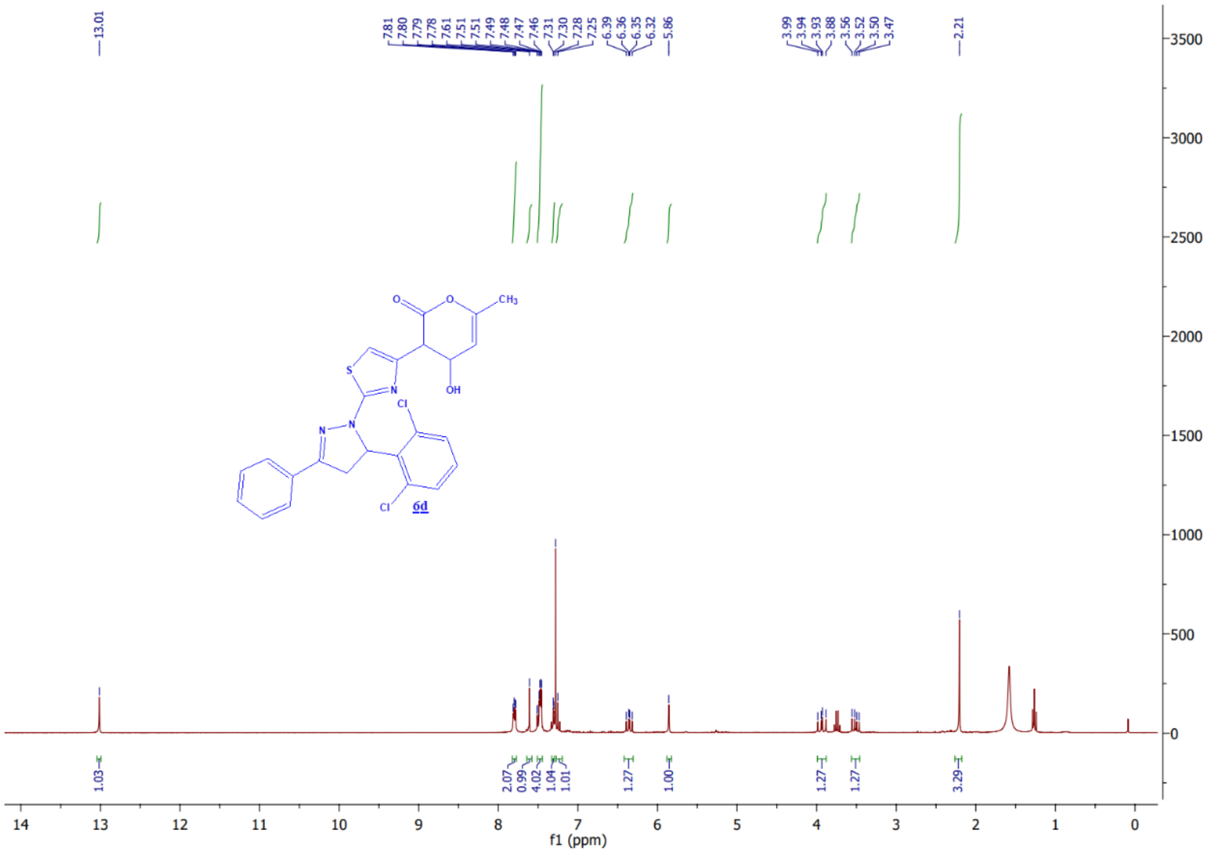
^{1}H NMR of product **6c** in $CDCl_3$ (300 MHz)



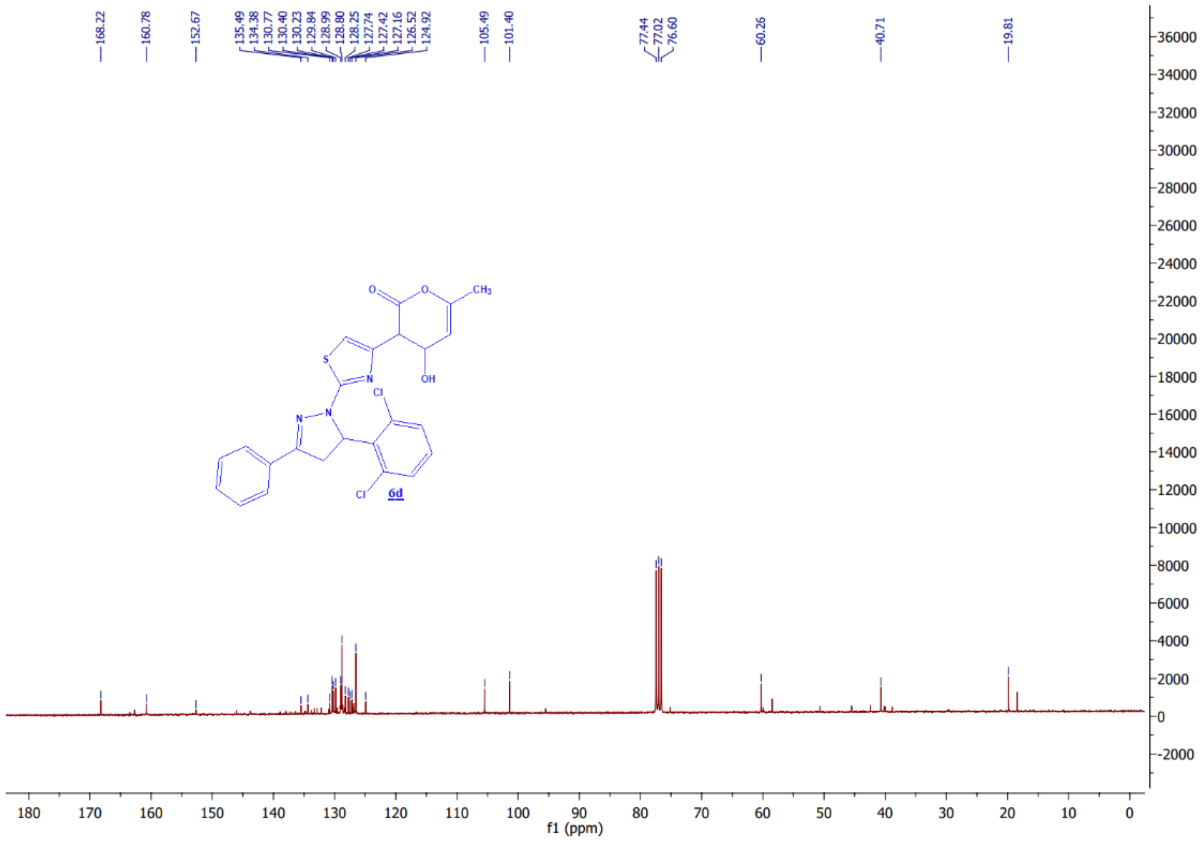
^{13}C NMR of product **6c** in $CDCl_3$ (75 MHz)



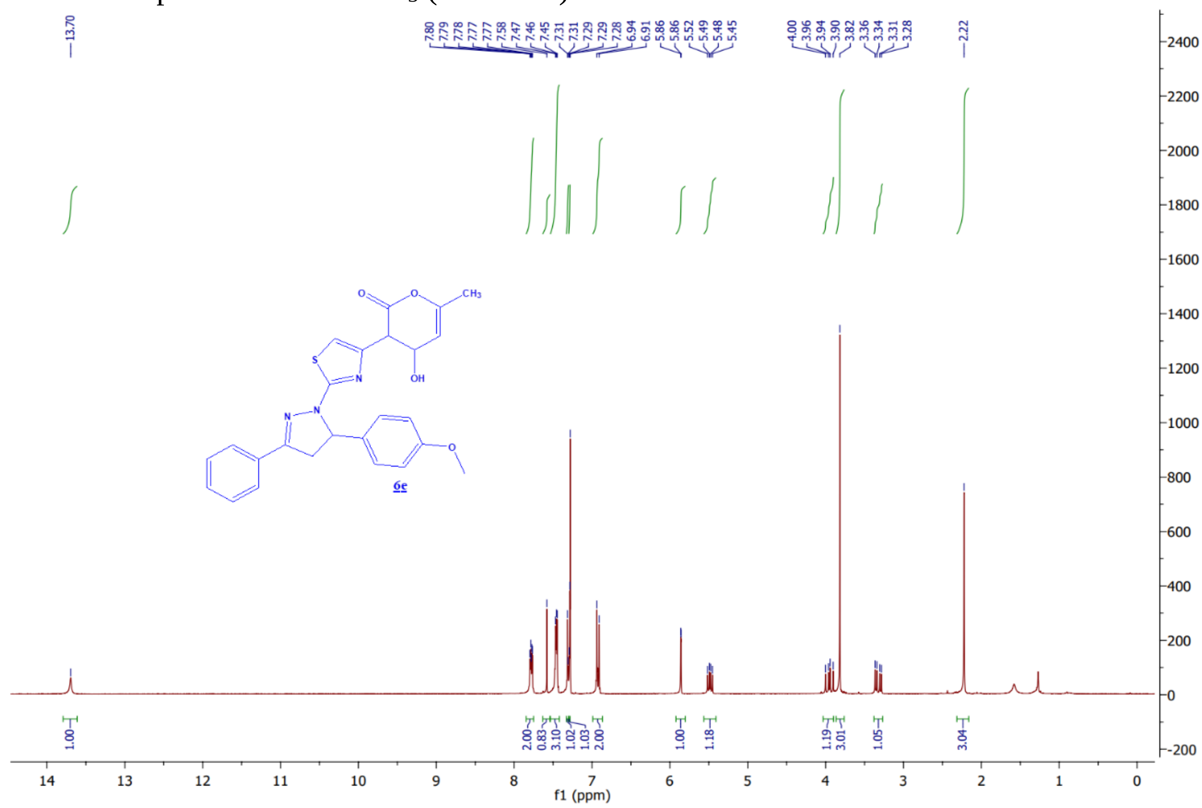
^{1}H NMR of product **6d** in $CDCl_3$ (300 MHz)



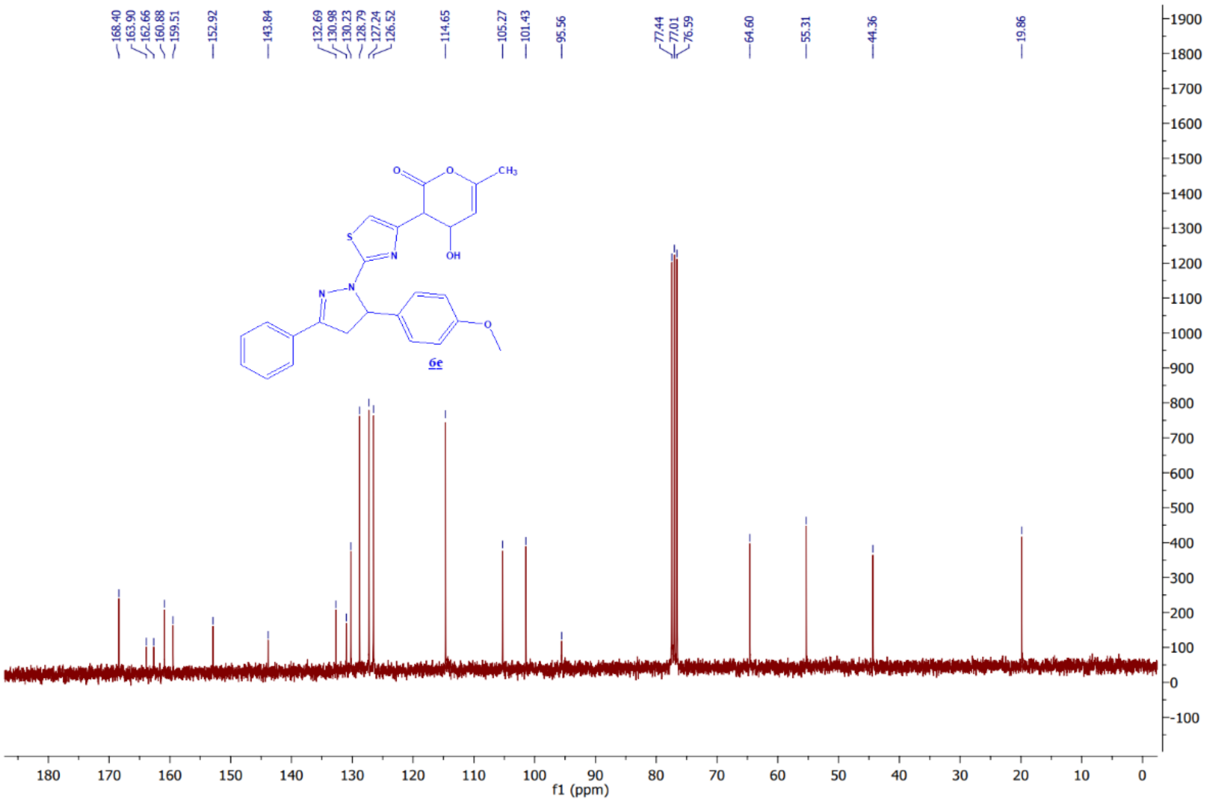
^{13}C NMR of product **6d** in $CDCl_3$ (75 MHz)



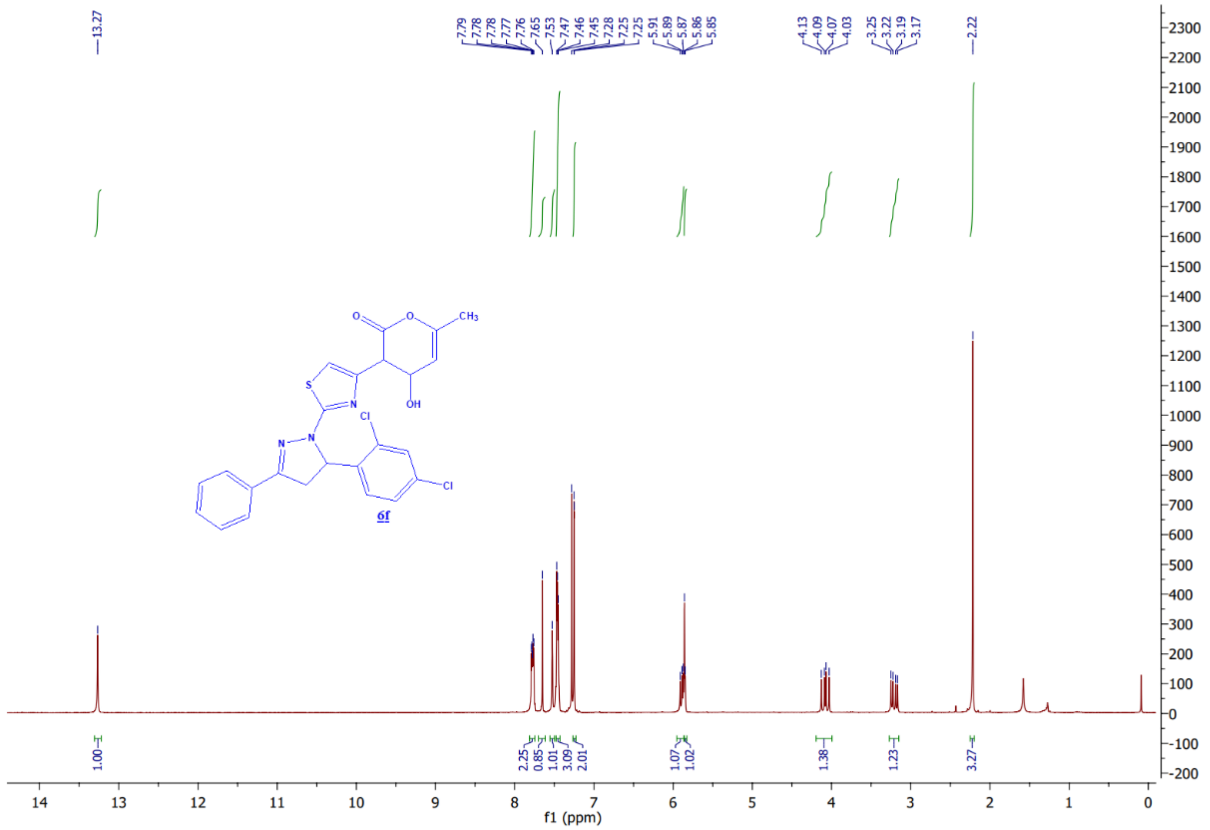
^{1}H NMR of product **6e** in $CDCl_3$ (300 MHz)



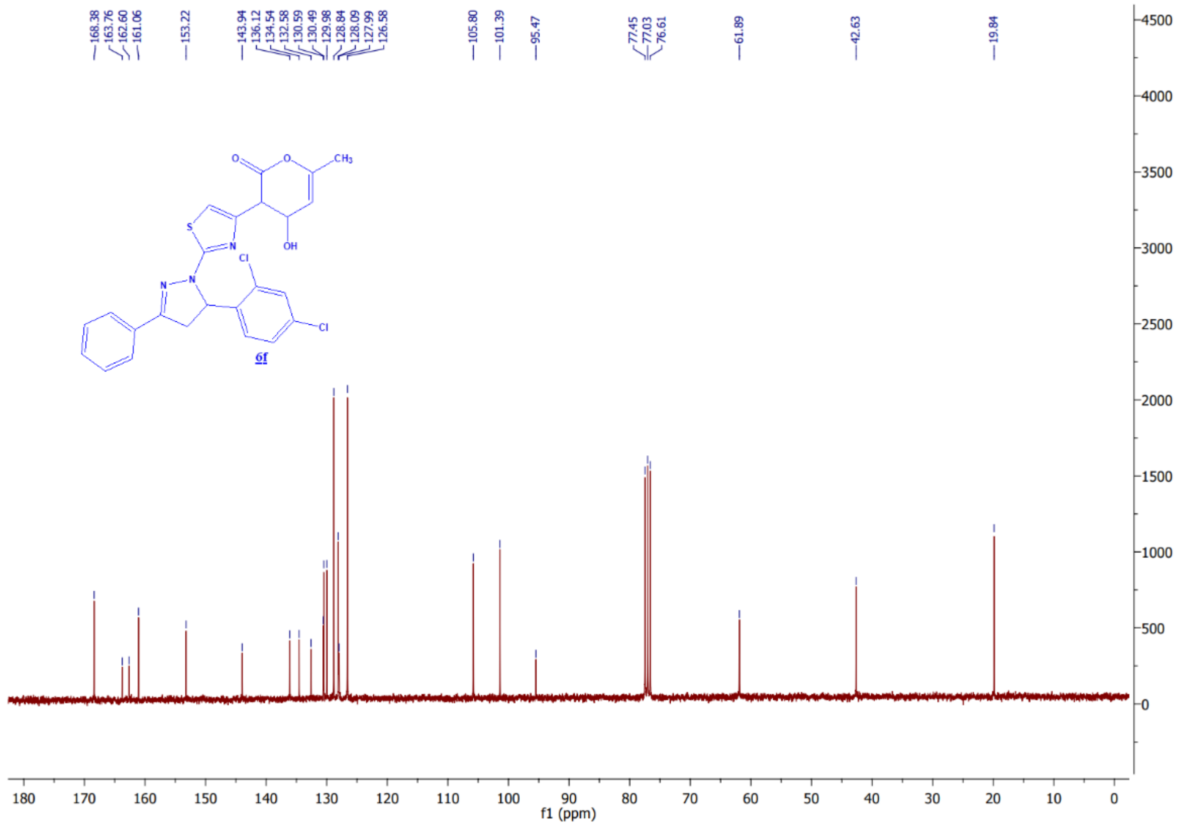
^{13}C NMR of product **6e** in $CDCl_3$ (75 MHz)



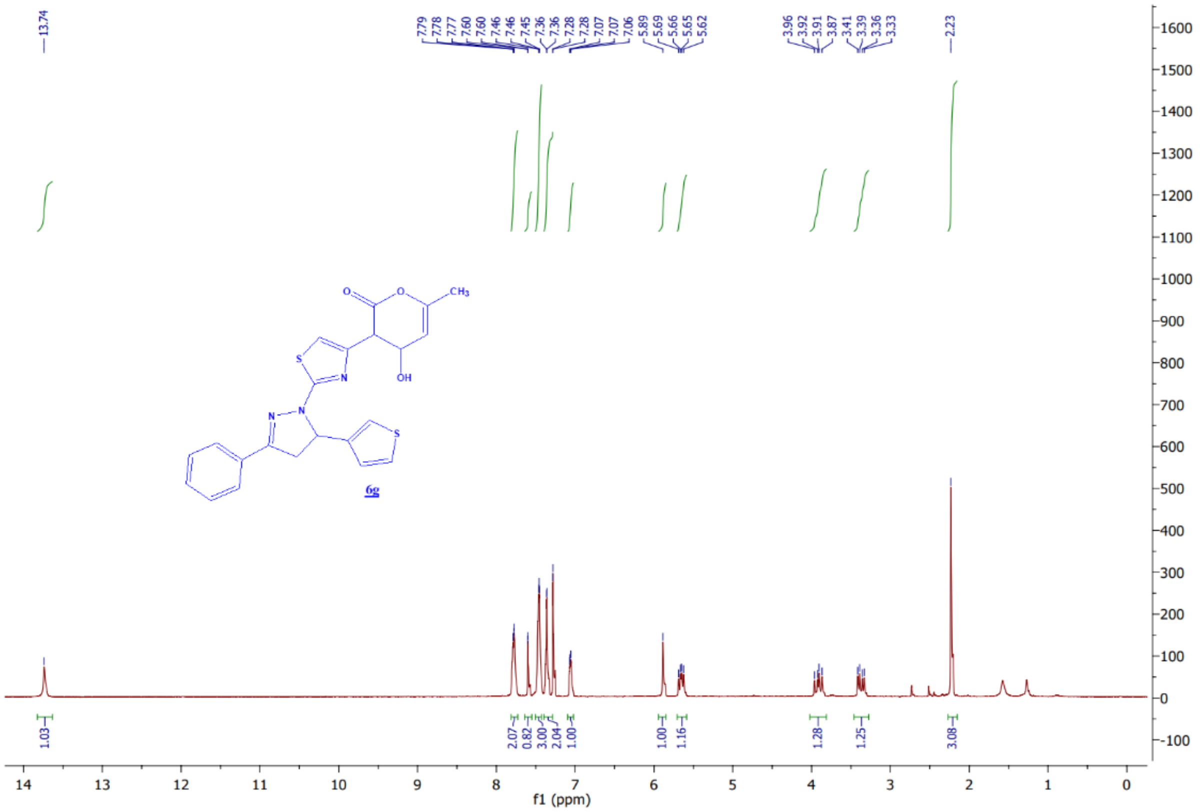
^{1}H NMR of product **6f** in $CDCl_3$ (300 MHz)



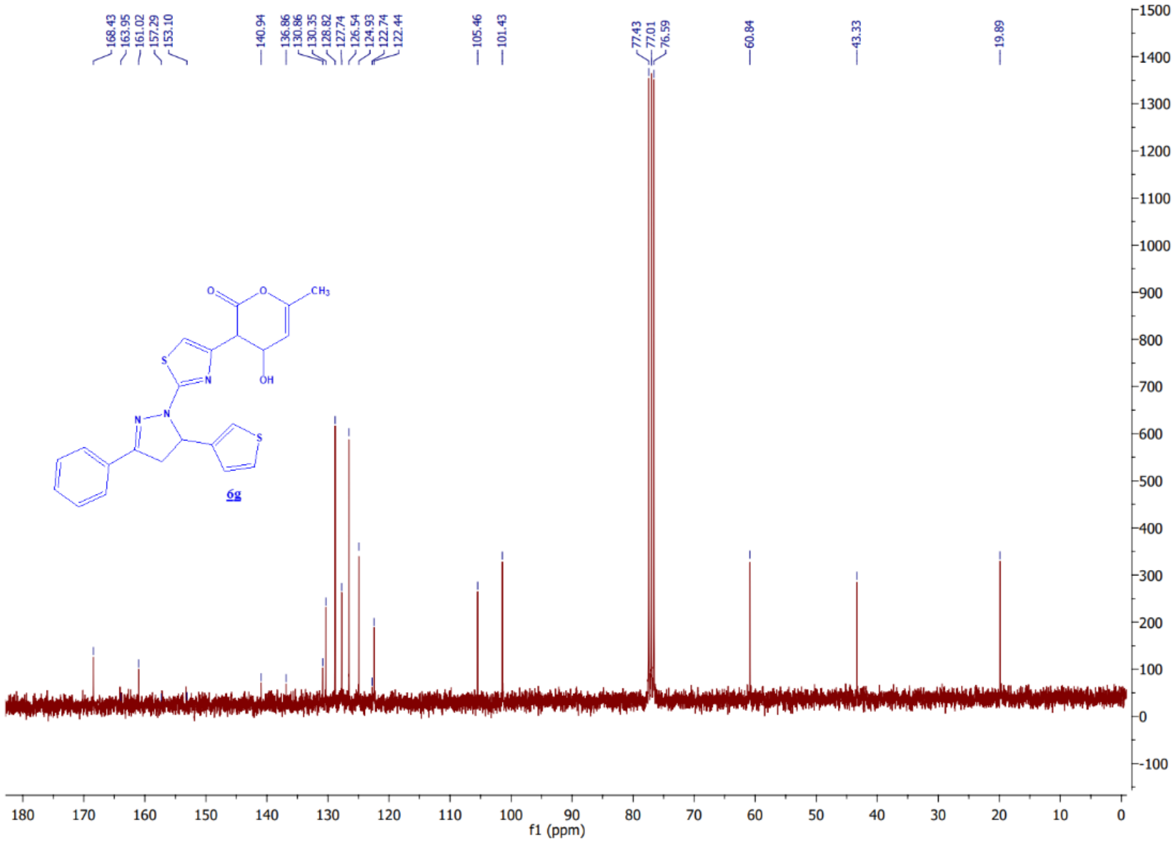
^{13}C NMR of product **6f** in $CDCl_3$ (75 MHz)



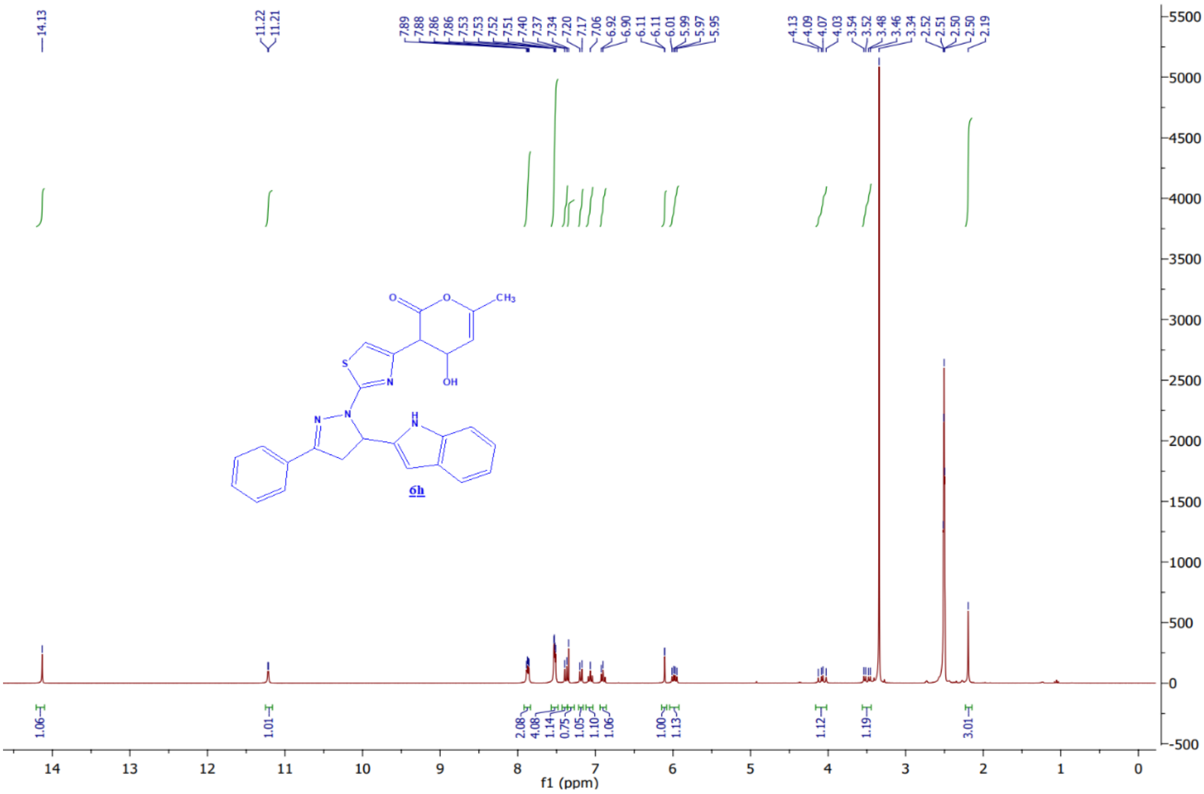
^{1}H NMR of product **6g** in $CDCl_3$ (300 MHz)



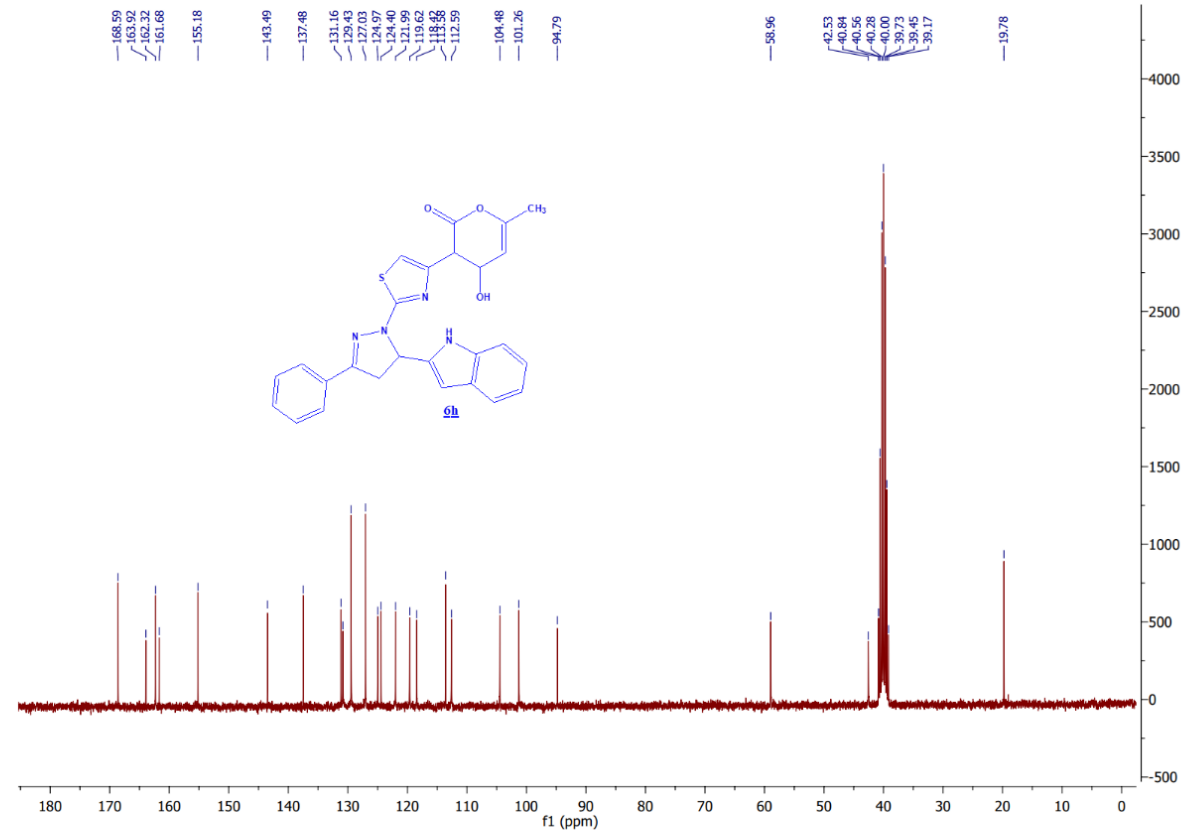
^{13}C NMR of product **6g** in $CDCl_3$ (75 MHz)



^{1}H NMR of product **6h** in DMSO (300 MHz)



^{13}C NMR of product **6h** in DMSO (75 MHz)



Summary table HRMs analysis of products **6a-h** in MeOH:CH_2Cl_2 (50:50 vol)

Name	Formula	M + 1 Calc.	M+ 1 Exp.	δ ppm	M - 1 Calc.	M - 1 Exp.	δ ppm	Validation
6a	$C_{24}H_{19}N_3O_3S$	430.12199	430.12444	5.69226	428.10744	428.10819	1.75516	**yes**
6b	$C_{26}H_{24}N_4O_3S$	473.16419	473.16669	5.29077	471.14963	471.15038	1.57338	**yes**
6c	$C_{24}H_{18}{}^{35}ClN_3O_3S$	464.08302	464.08562	5.61973	462.06846	462.06951	2.26676	**yes**
	$C_{24}H_{18}{}^{37}ClN_3O_3S$	466.08007	466.08243	5.06419	464.06551	464.06643	1.97319	
6d	$C_{24}H_{17}{}^{35}Cl_2N_3O_3S$	498.04404	498.04665	5.22345	496.02949	496.03061	2.24693	**yes**
	$C_{24}H_{17}{}^{35}Cl^{37}ClN_3O_3S$	500.04109	500.04363	5.07233	498.02654	498.02773	2.37883	
	$C_{24}H_{17}{}^{37}Cl_2N_3O_3S$	502.03814	502.04043	4.54566	500.02359	500.02495	2.71911	
6e	$C_{25}H_{21}N_3O_4S$	460.13255	460.13519	5.72056	458.11800	458.11896	2.09204	**yes**
6f	$C_{24}H_{17}{}^{35}Cl_2N_3O_3S$	498.04404	498.04666	5.25508	496.02949	496.03048	1.98908	**yes**
	$C_{24}H_{17}{}^{35}Cl^{37}ClN_3O_3S$	500.04109	500.04360	5.00372	498.02654	498.02746	1.85366	
	$C_{24}H_{17}{}^{37}Cl_2N_3O_3S$	502.03814	502.04046	4.62134	500.02359	500.02456	1.93536	
6g	$C_{22}H_{17}N_3O_3S_2$	436.07841	436.08081	5.50565	434.06386	434.06464	1.79831	**yes**
6h	$C_{26}H_{20}N_4O_3S$	469.13289	469.13550	5.56904	467.11833	467.11908	1.60358	**yes**