molecules

MDPI

Supplementary Materials

Synthesis and α-Glucosidase Inhibition Activity of 2-[3-(Benzoyl/4-bromobenzoyl)-4-hydroxy-1,1-dioxido-2*H*-benzo[*e*][1,2]thiazin-2-yl]-*N*-arylacetamides: An *In Silico* and Biochemical Approach

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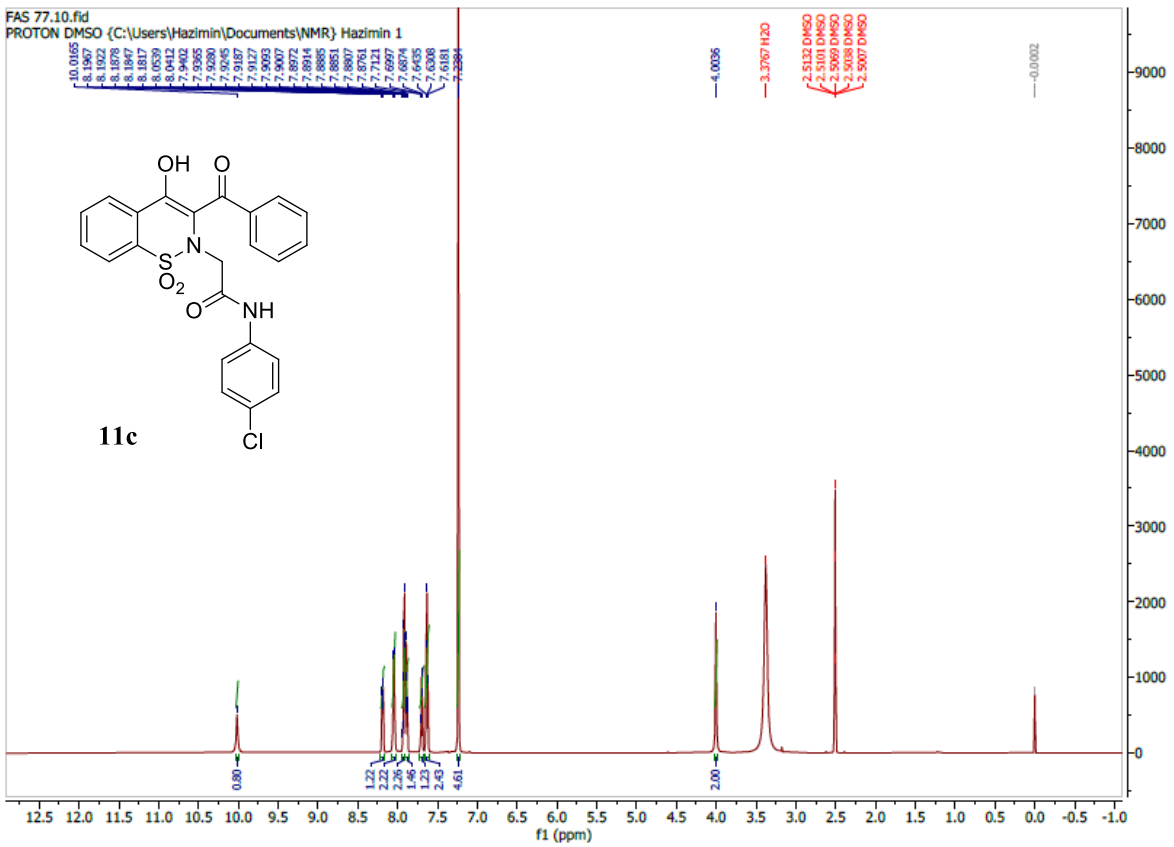
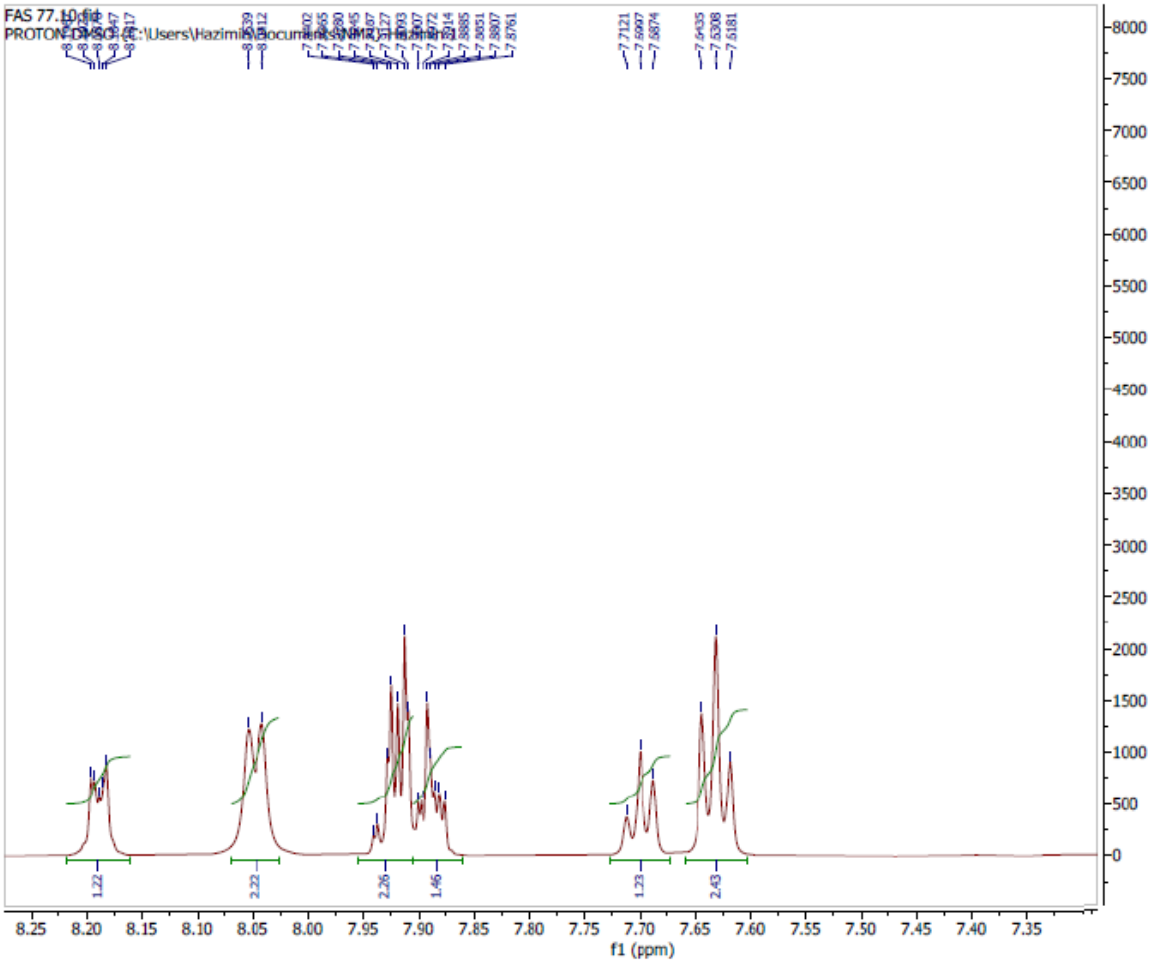
(Supplementary Data File)

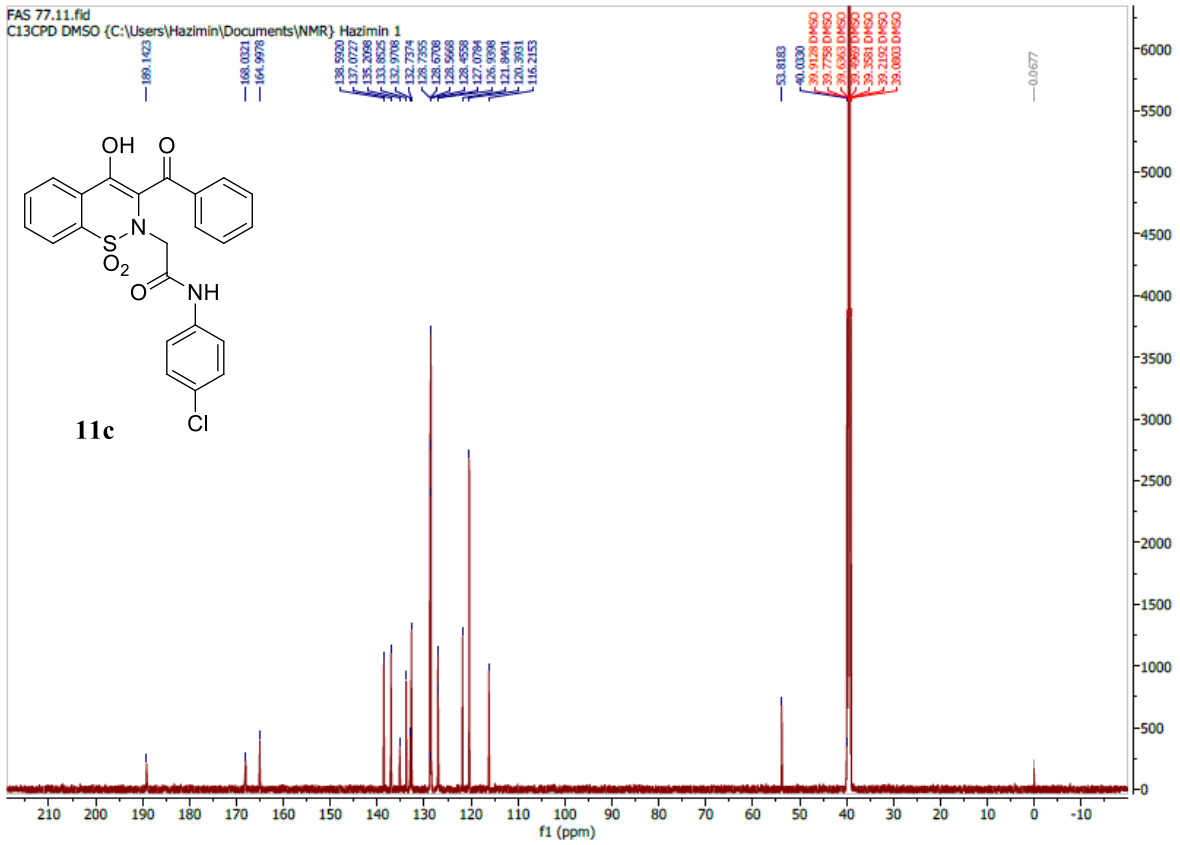
^{1}H NMR, ^{13}C NMR and MS Spectra of potent compounds



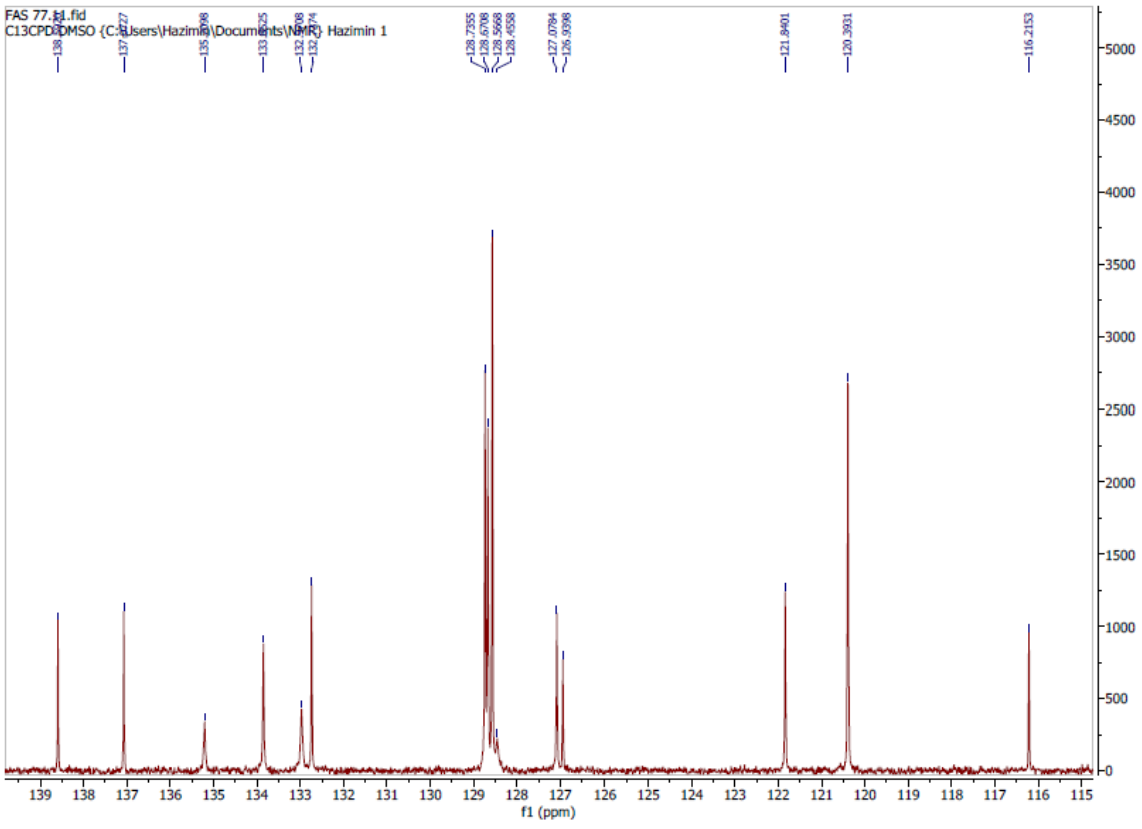
^{1}H NMR Spectrum of compound **11c**.



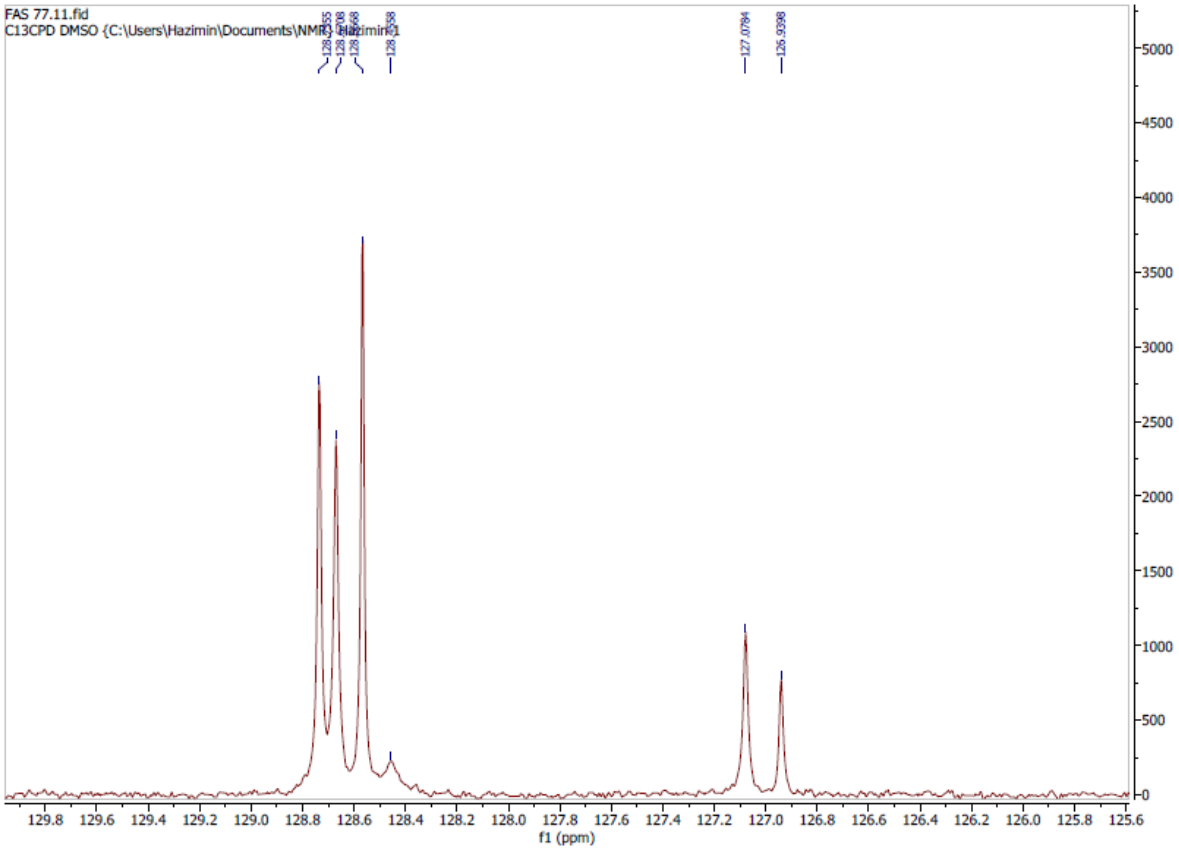
Expanded form of ^{1}H NMR Spectrum of compound **11c** (region 7.60-8.25 ppm).



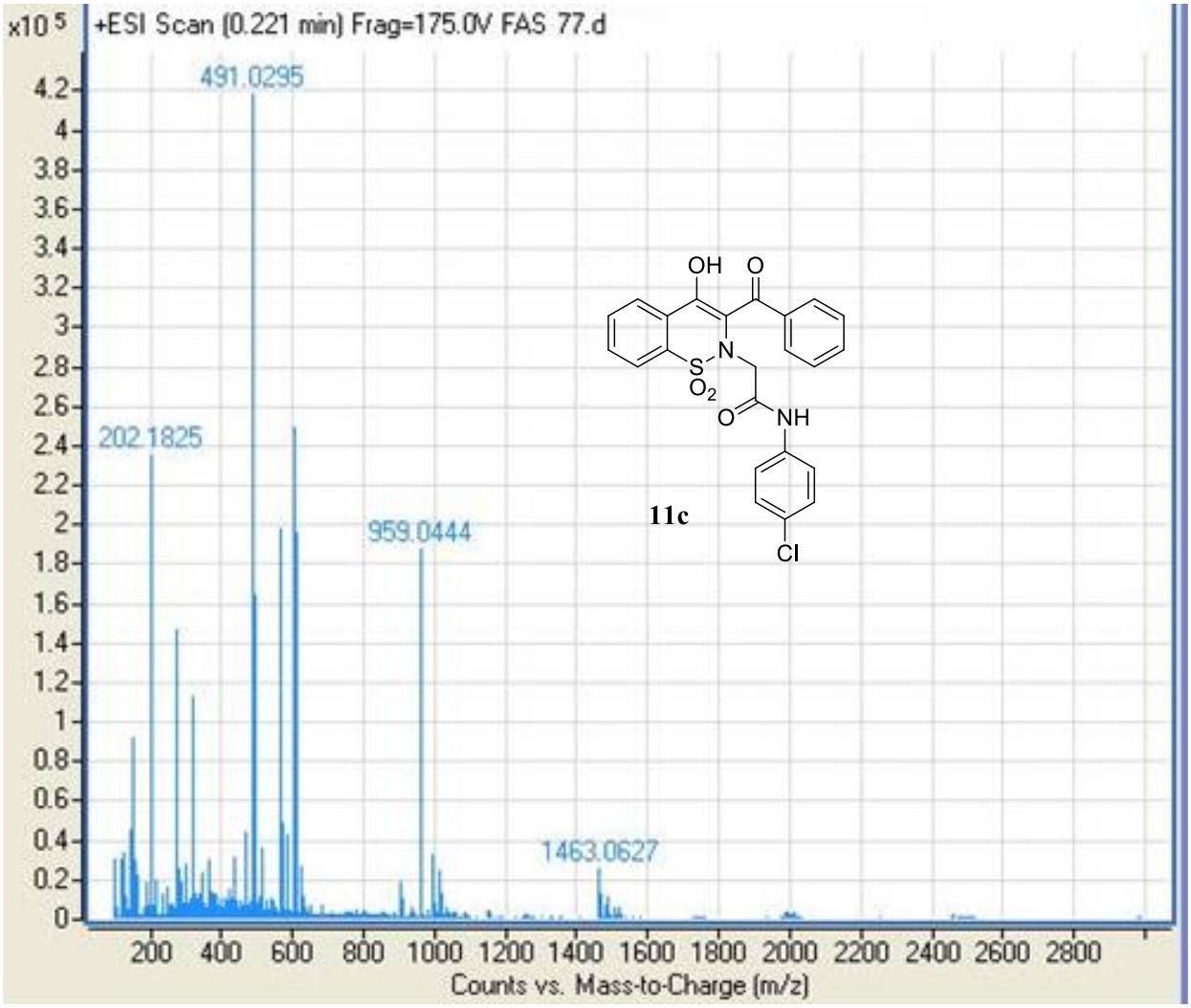
^{13}C NMR Spectrum of compound **11c.**



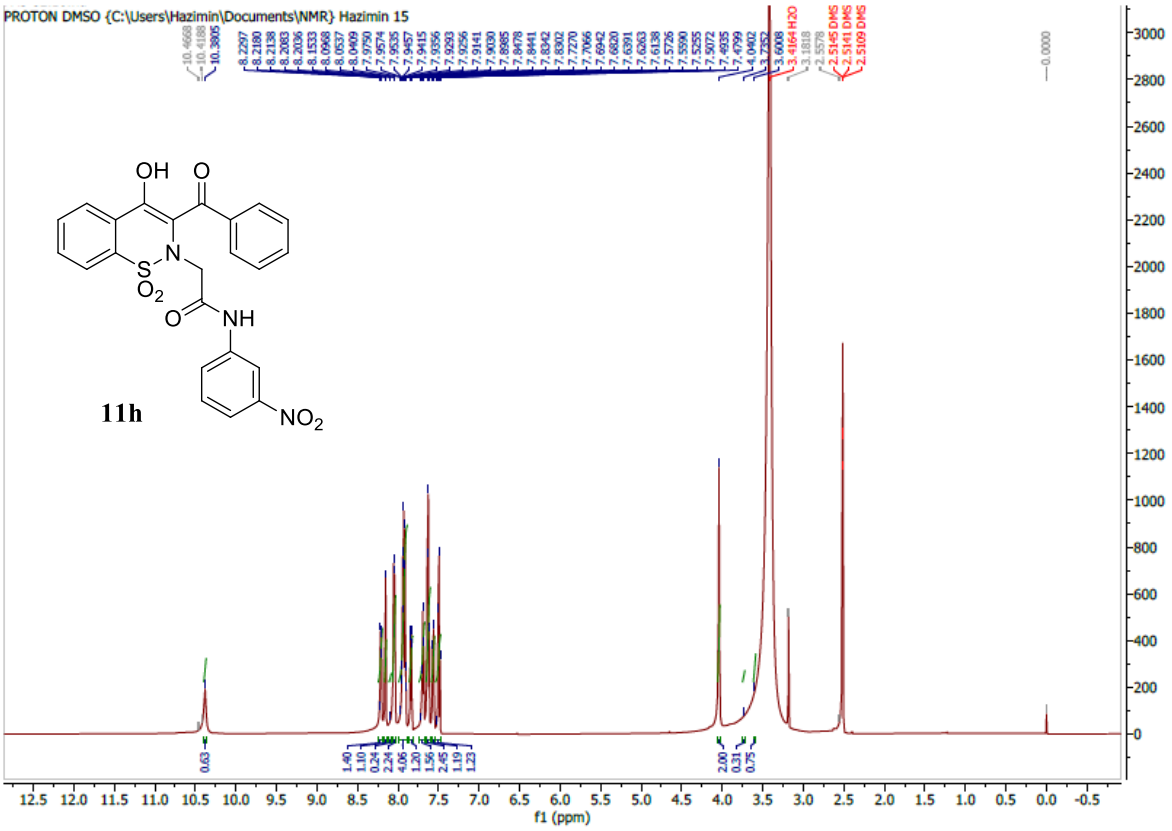
Expanded form of ^{13}C NMR Spectrum of compound **11c** (region 116-139 ppm).



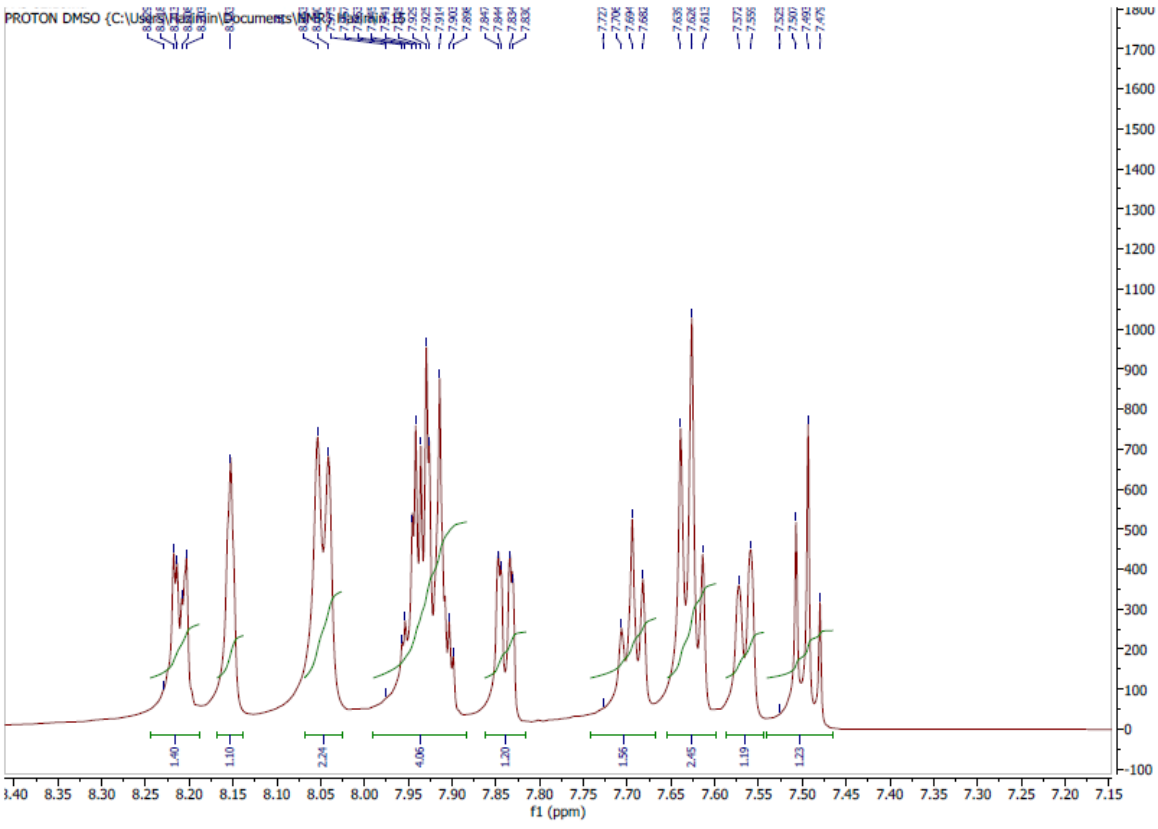
Expanded form of ^{13}C NMR Spectrum of compound **11c** (region 126.8-129.0 ppm).



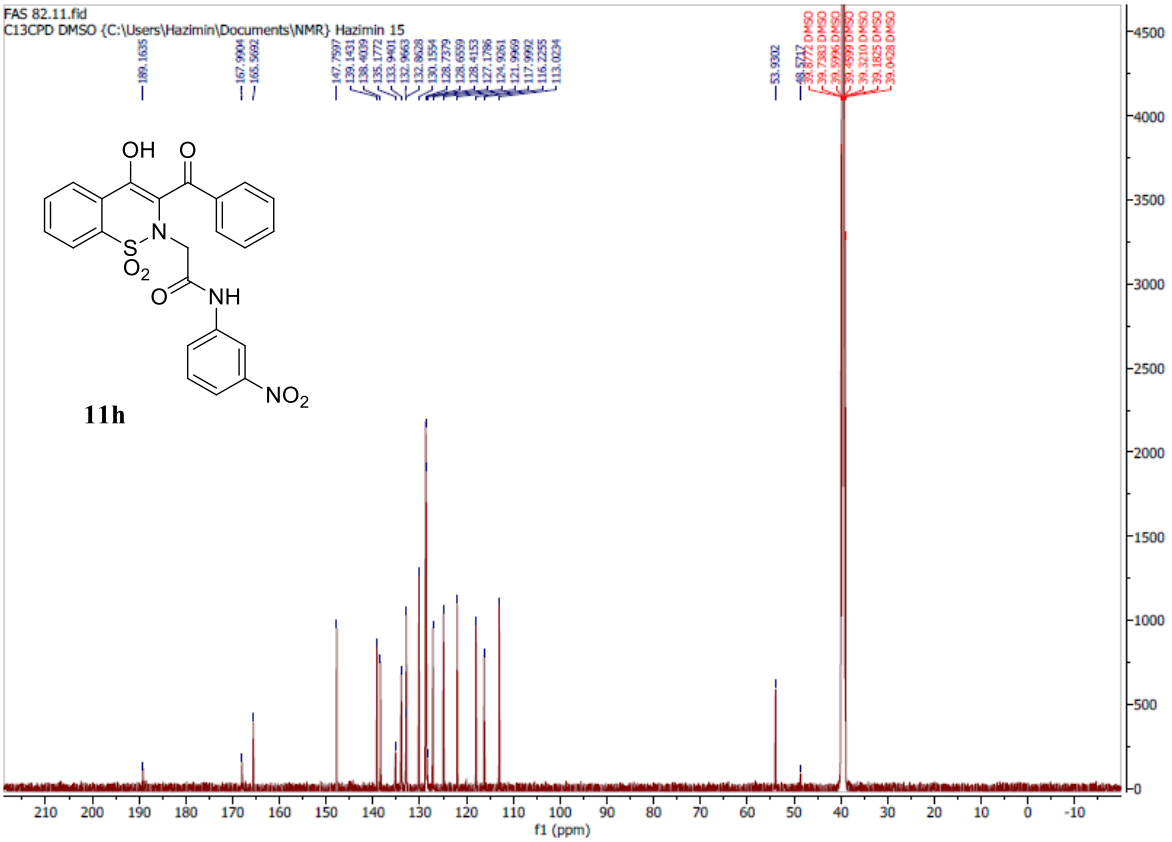
MS Spectrum of compound **11c.**



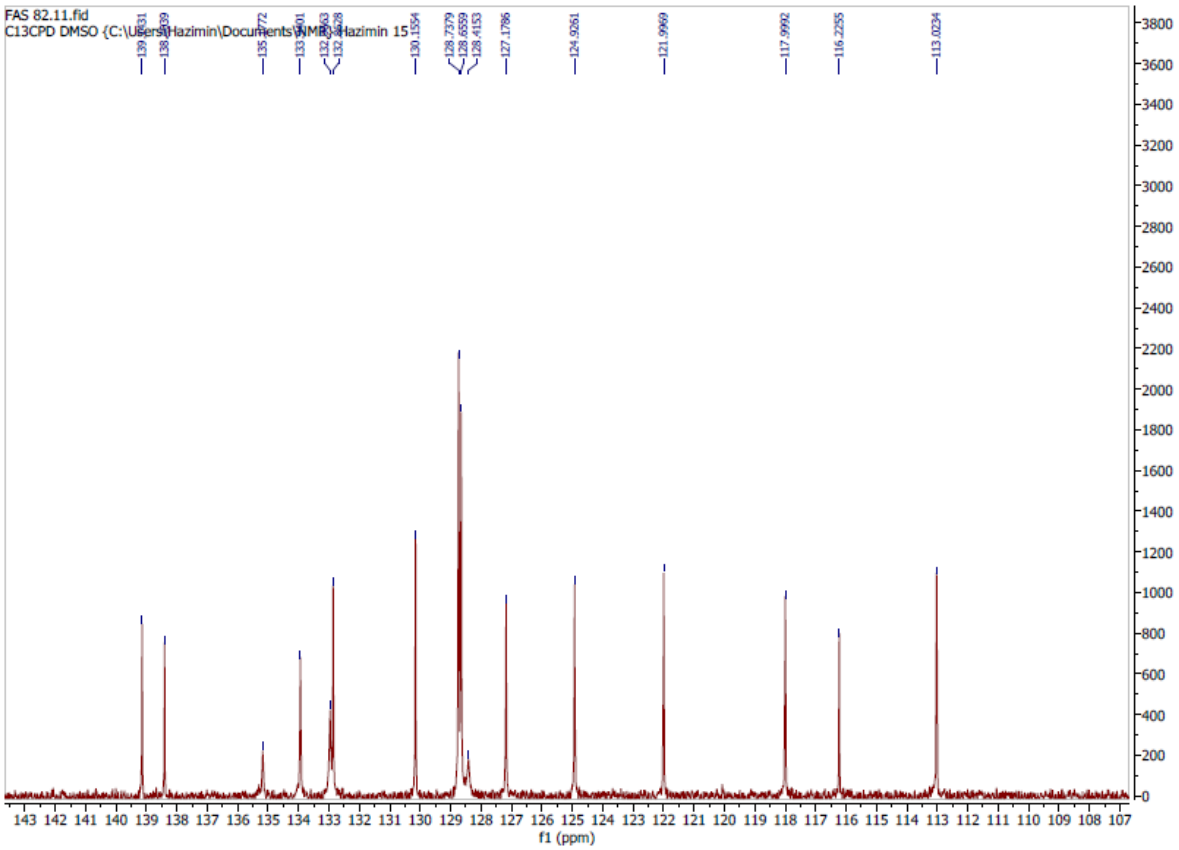
^{1}H NMR Spectrum of compound **11h**.



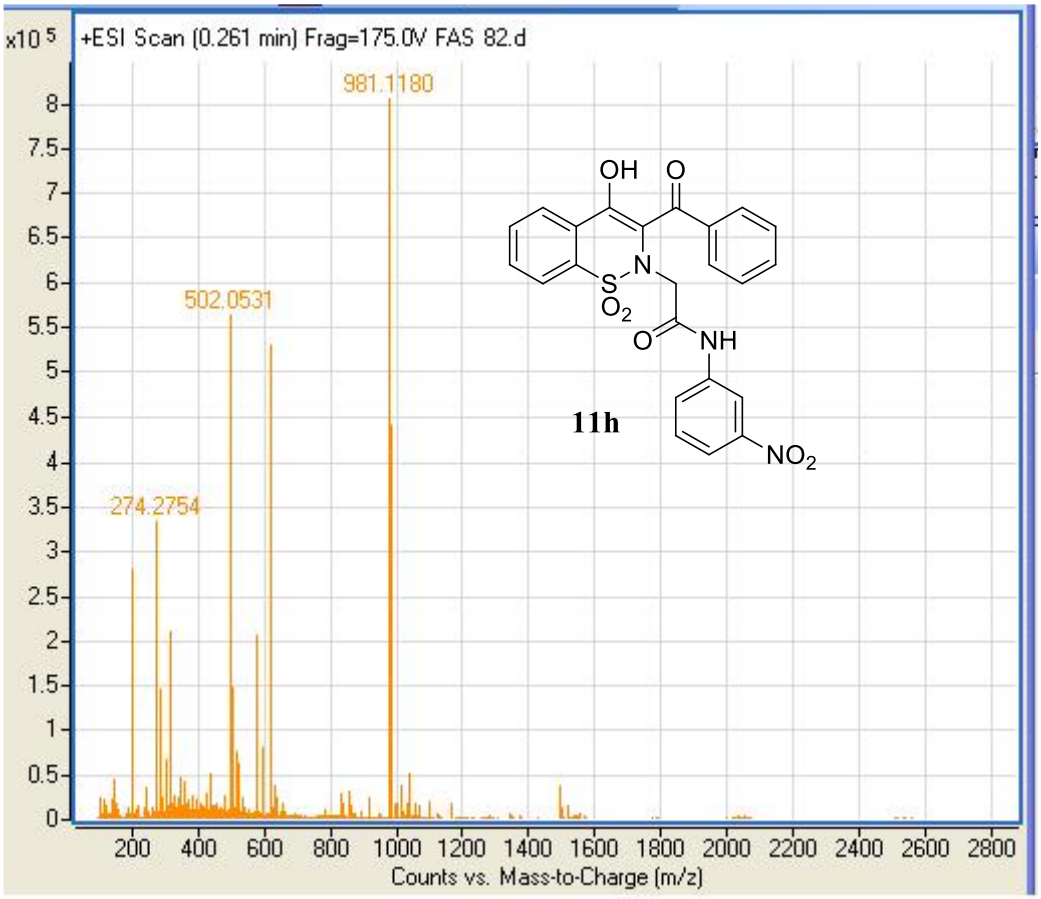
Expanded form of ^{1}H NMR Spectrum of compound **11h** (region 7.45-8.25 ppm).



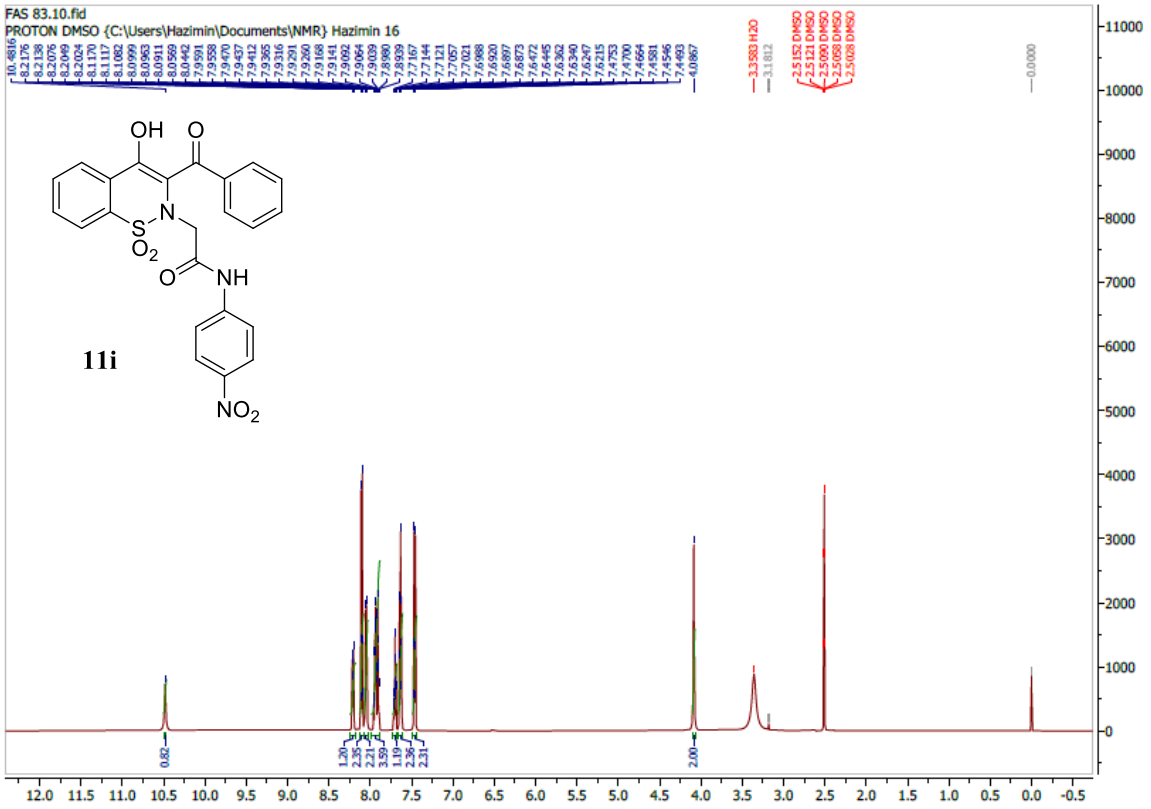
^{13}C NMR Spectrum of compound **11h.**



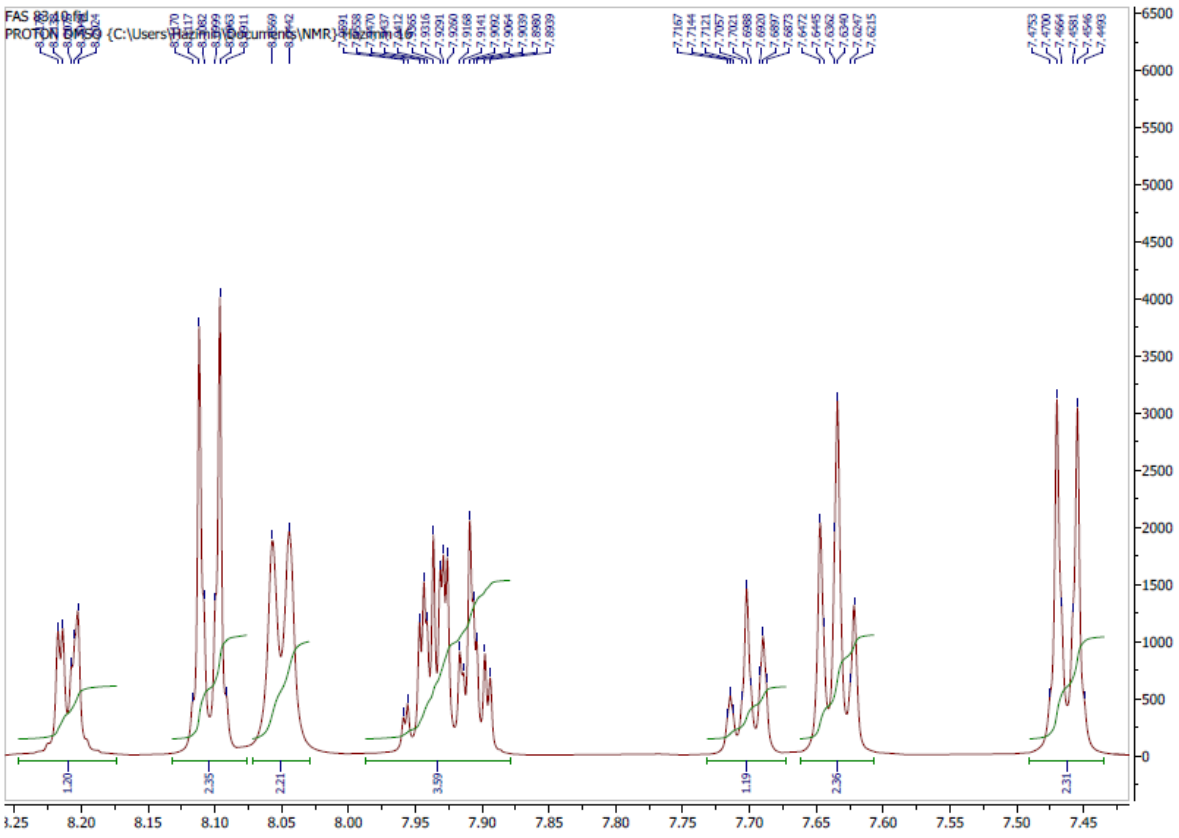
Expanded form of ^{13}C NMR Spectrum of compound **11h** (region 113-140 ppm).



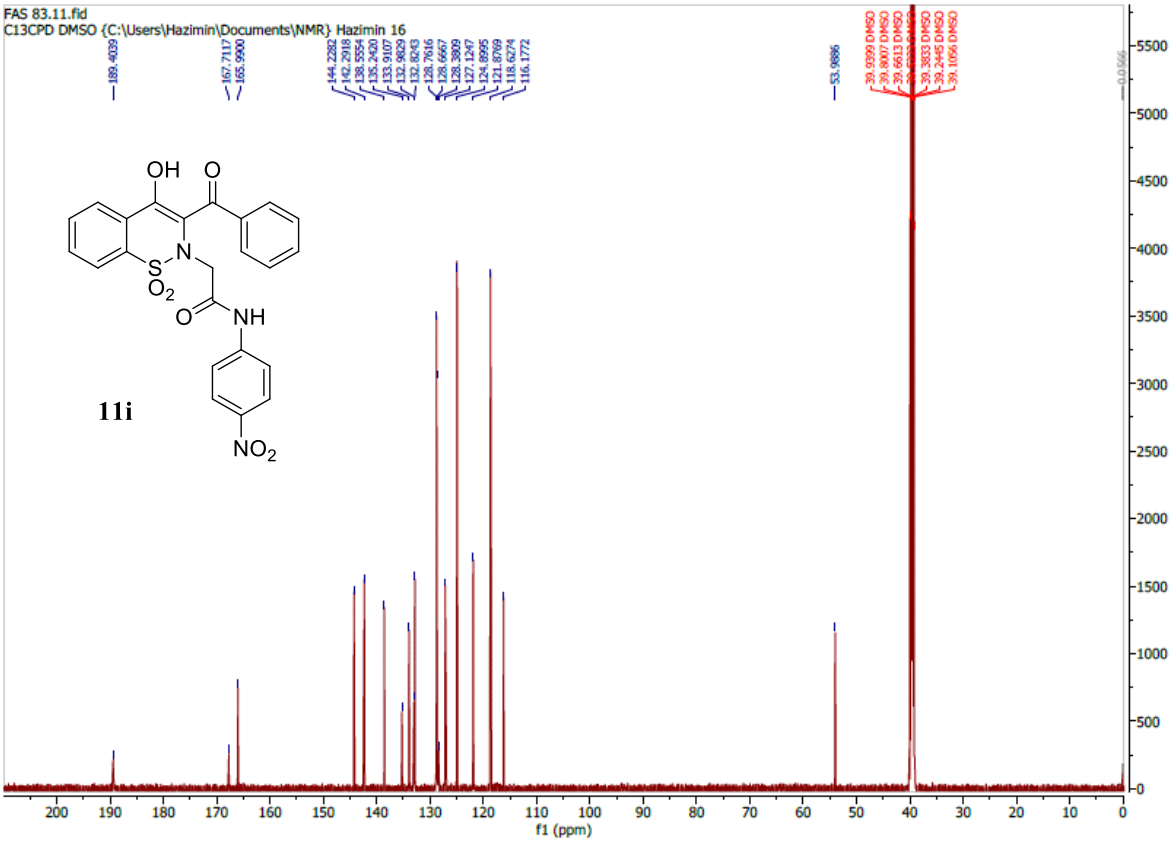
MS Spectrum of compound **11h.**



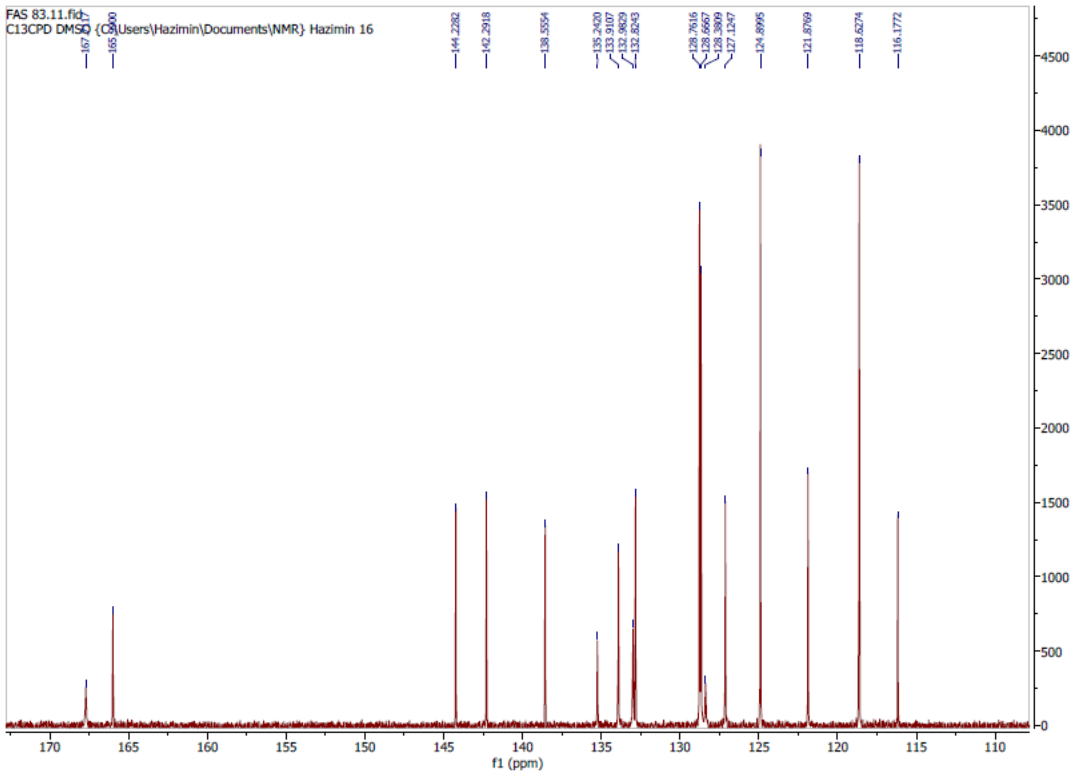
^{1}H NMR Spectrum of compound **11i**.



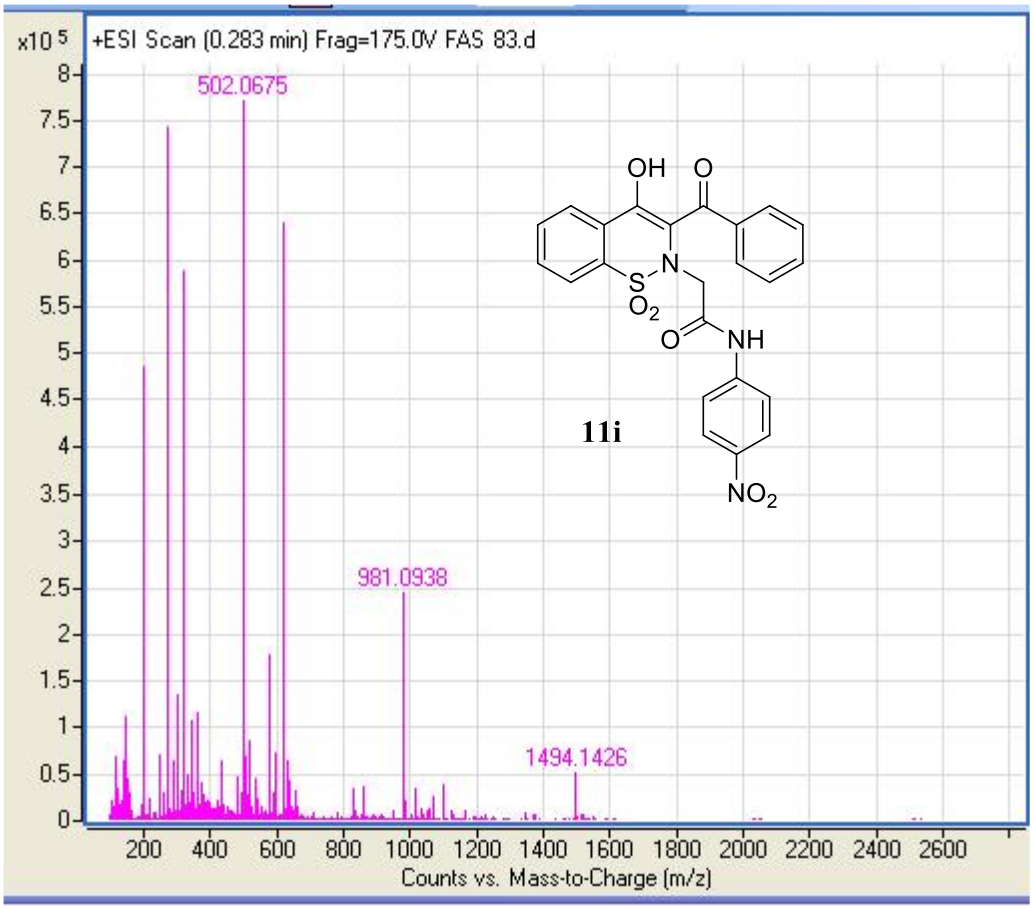
Expanded form of ^{1}H NMR Spectrum of compound **11i** (region 7.43-8.23 ppm).



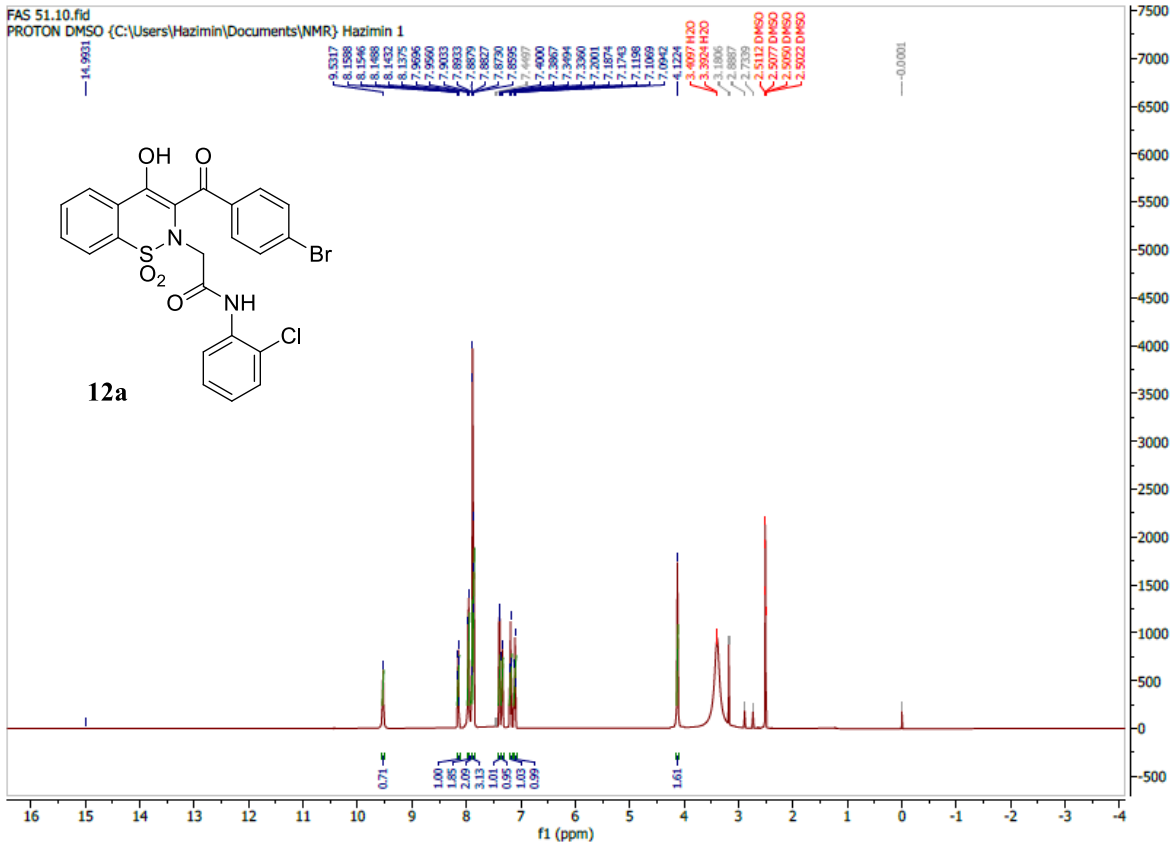
^{13}C NMR Spectrum of compound **11i.**



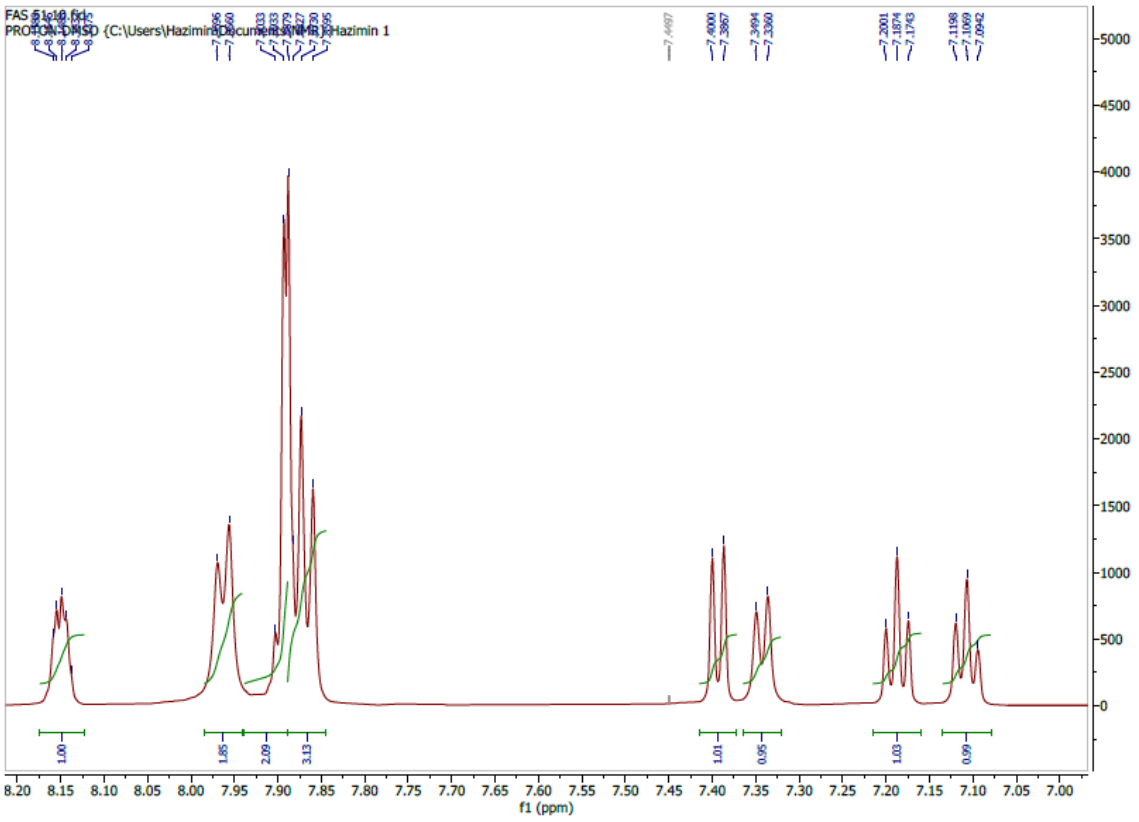
Expanded form of ^{13}C NMR Spectrum of compound **11i** (region 115-145 ppm).



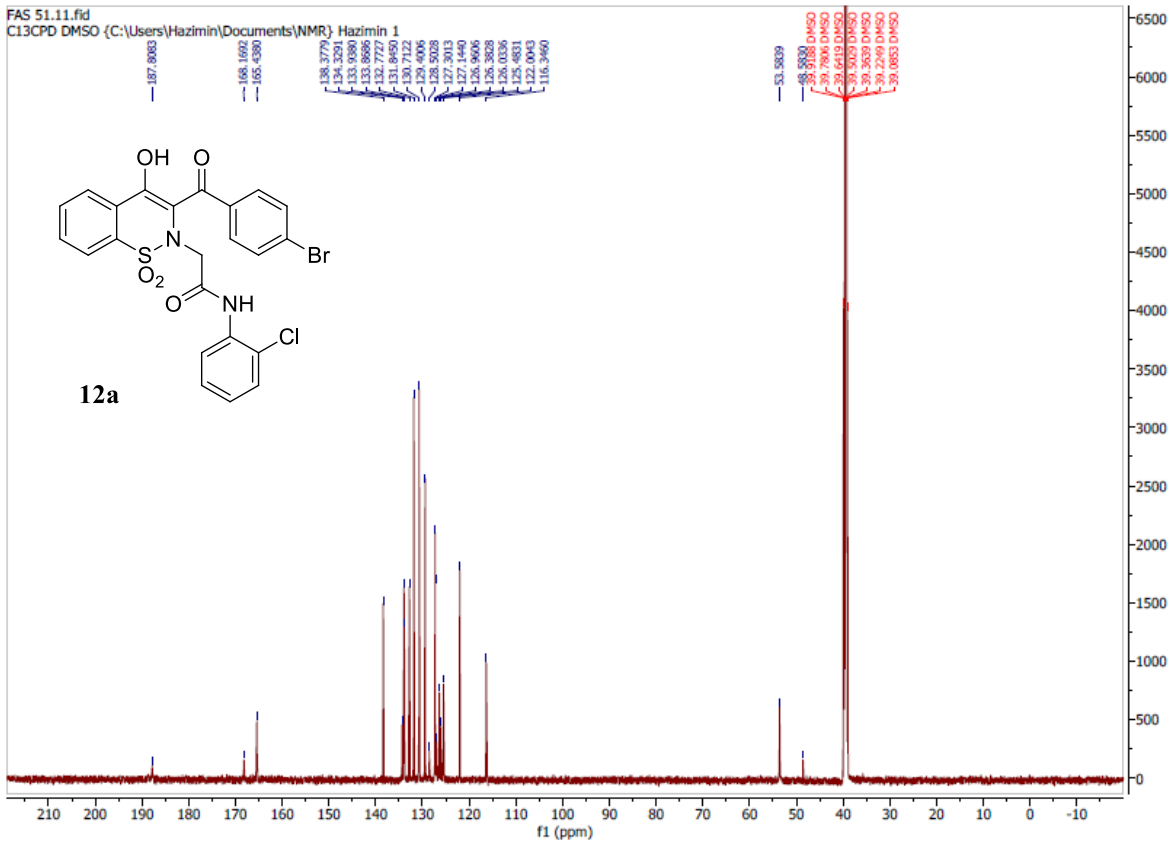
MS Spectrum of compound **11i.**



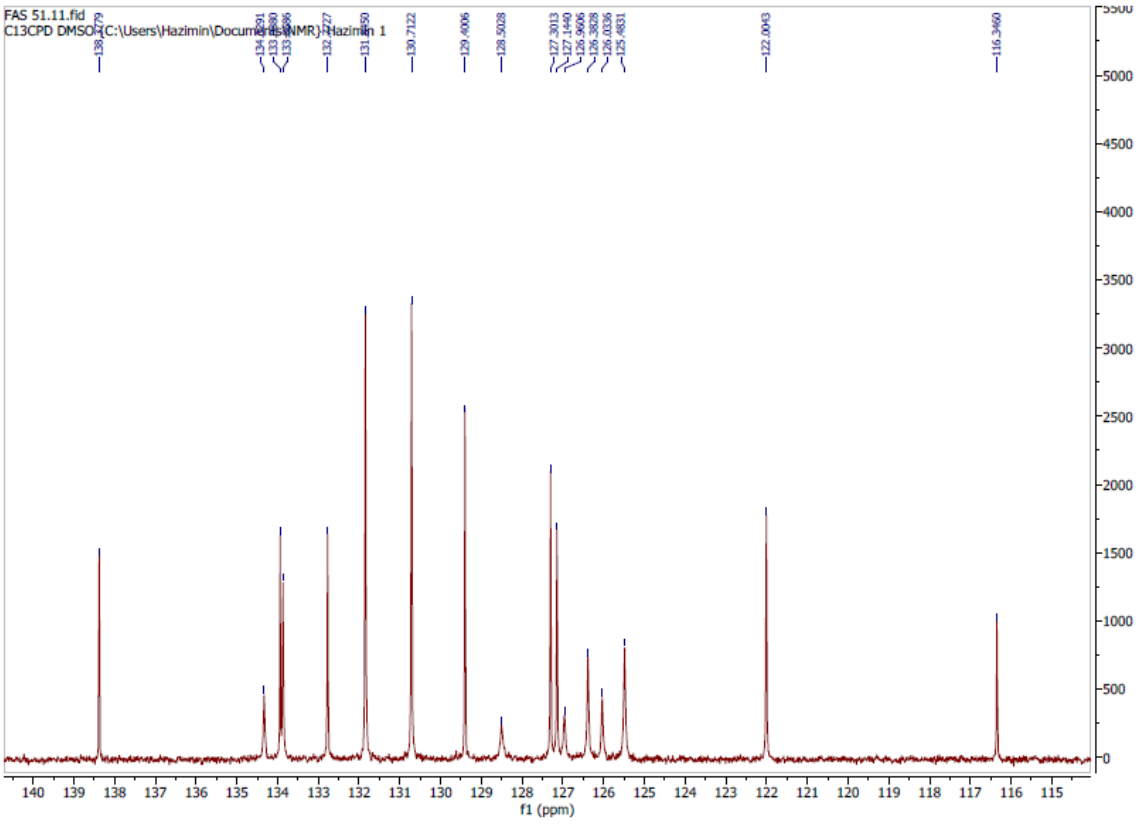
^{1}H NMR Spectrum of compound **12a**.



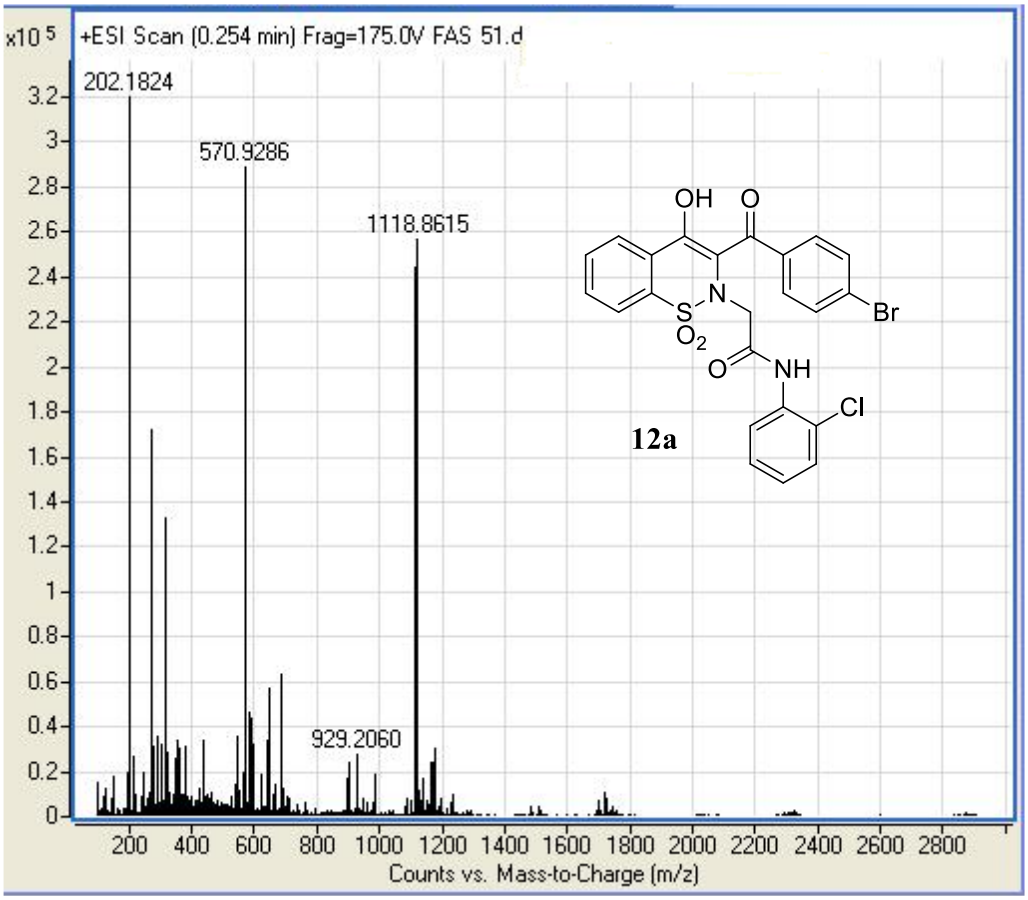
Expanded form of ^{1}H NMR Spectrum of compound **12a** (region 7.05-8.20 ppm).



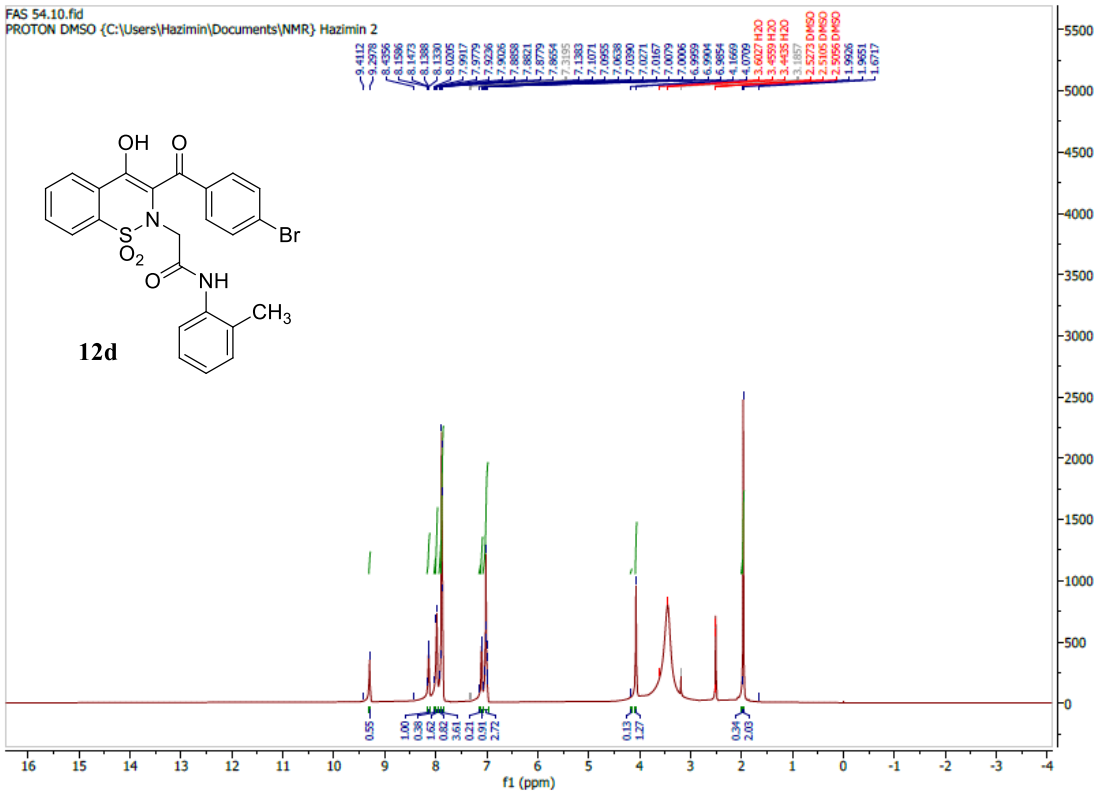
^{13}C NMR Spectrum of compound **12a.**



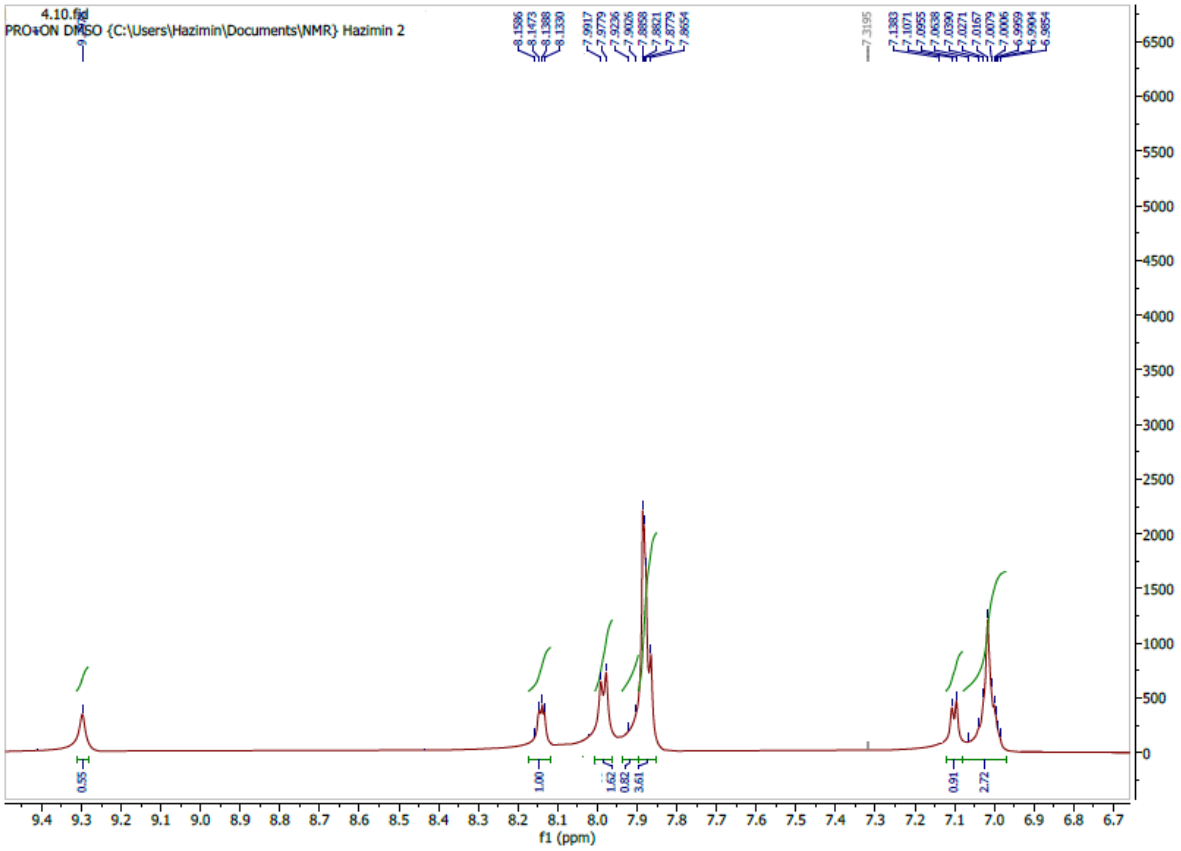
Expanded form of ^{13}C NMR Spectrum of compound **12a** (region 116-139 ppm).



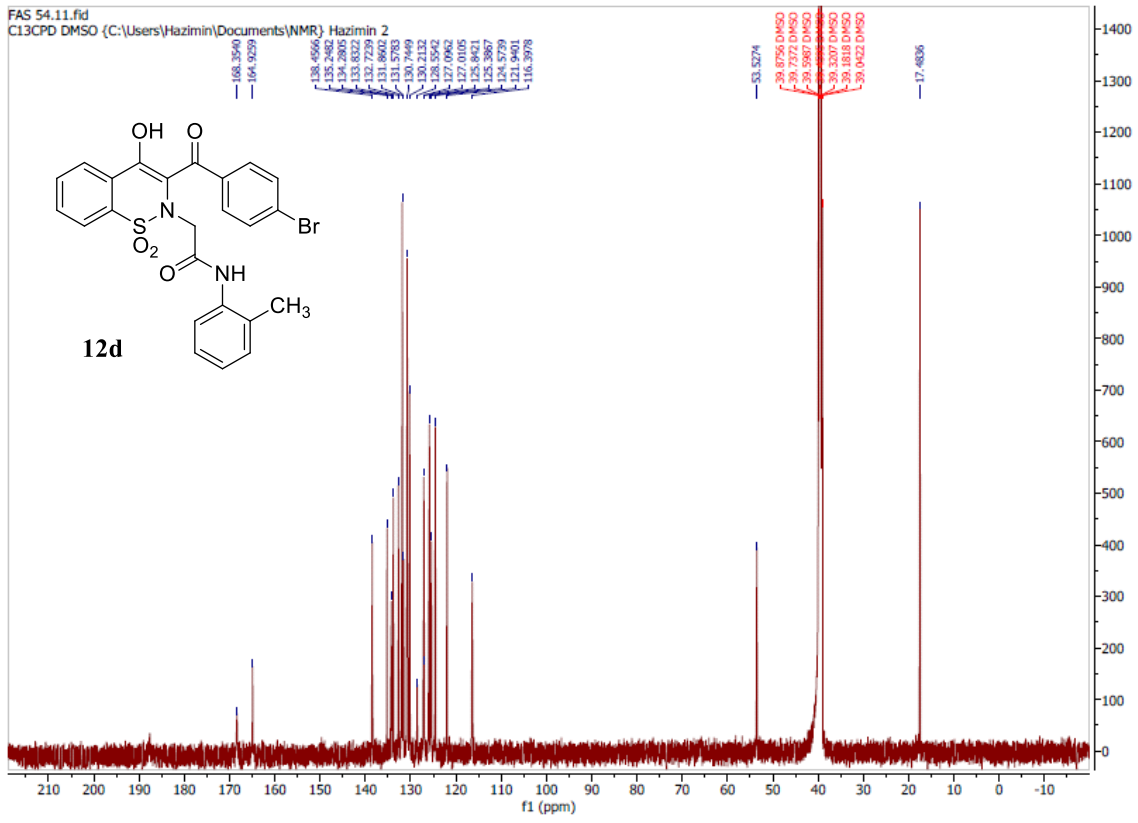
MS Spectrum of compound **12a.**



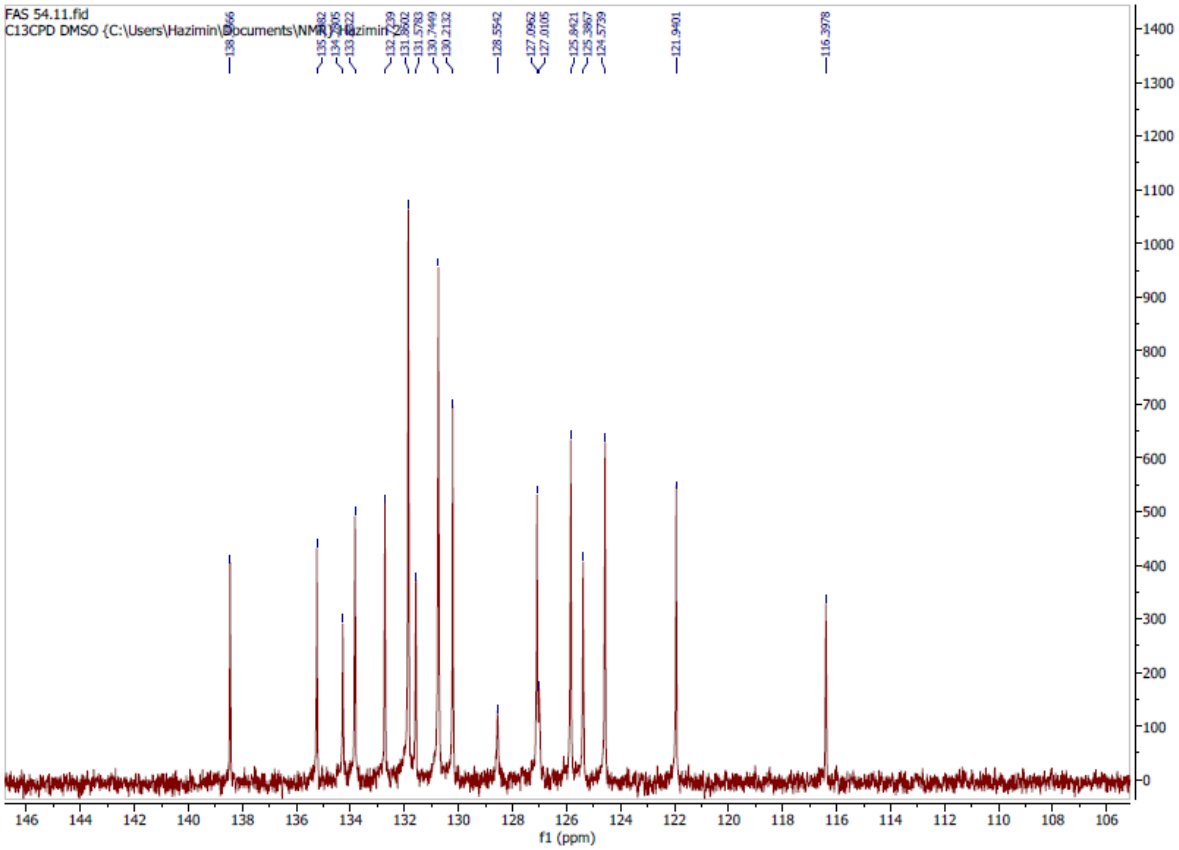
^{1}H NMR Spectrum of compound **12d**.



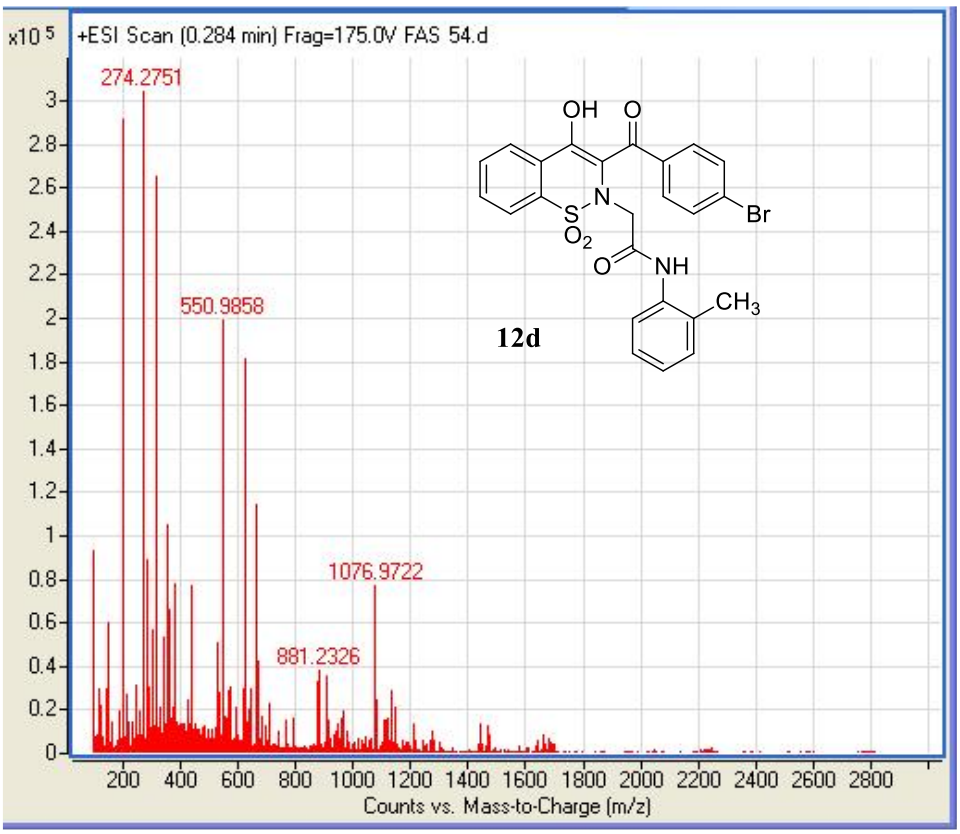
Expanded form of ^{1}H NMR Spectrum of compound **12d** (region 6.90-8.20 ppm).



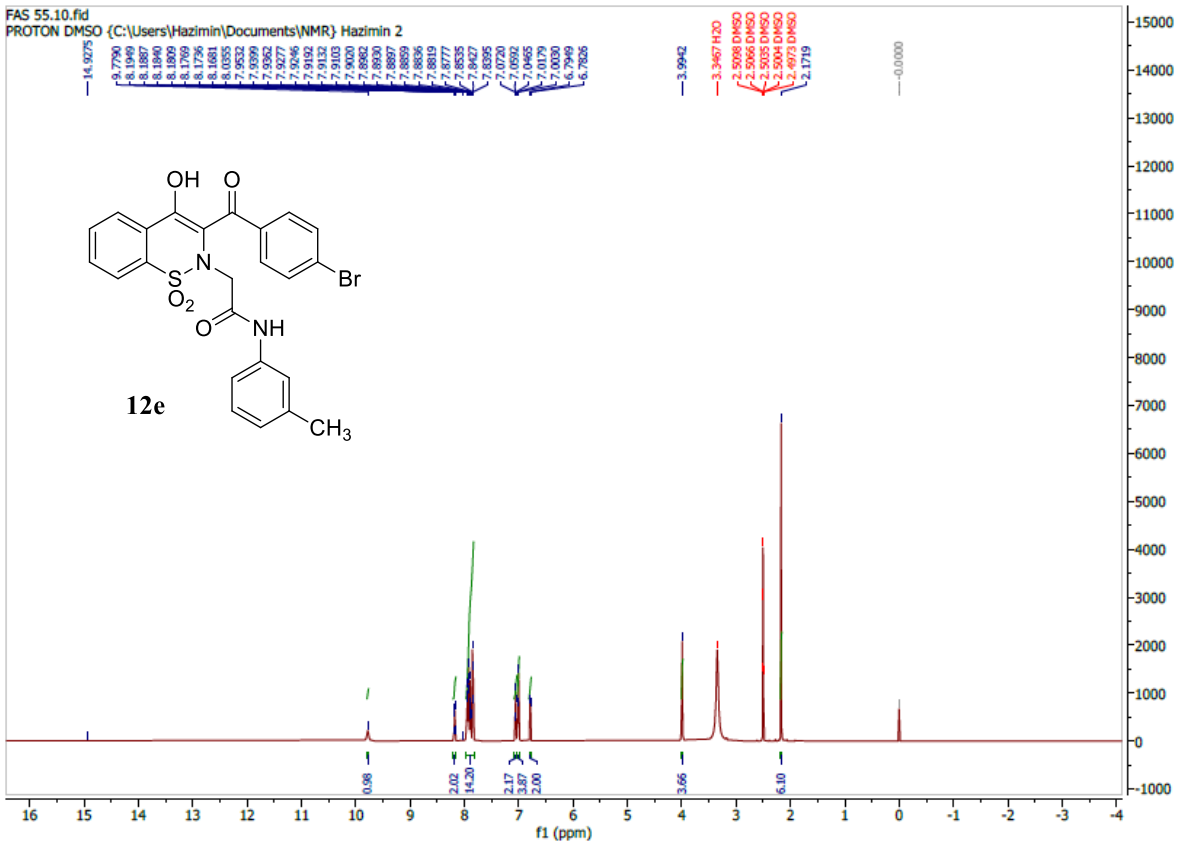
^{13}C NMR Spectrum of compound **12d.**



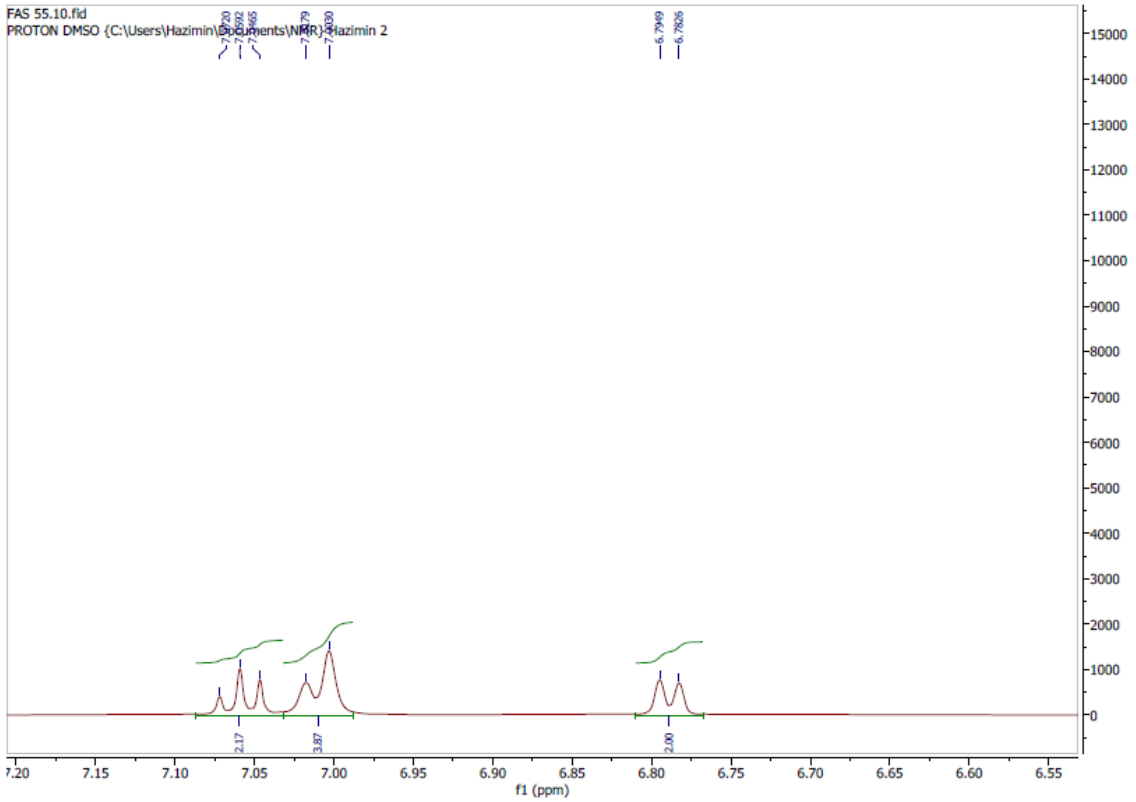
Expanded form of ^{13}C NMR Spectrum of compound **12d** (region 116-140 ppm).



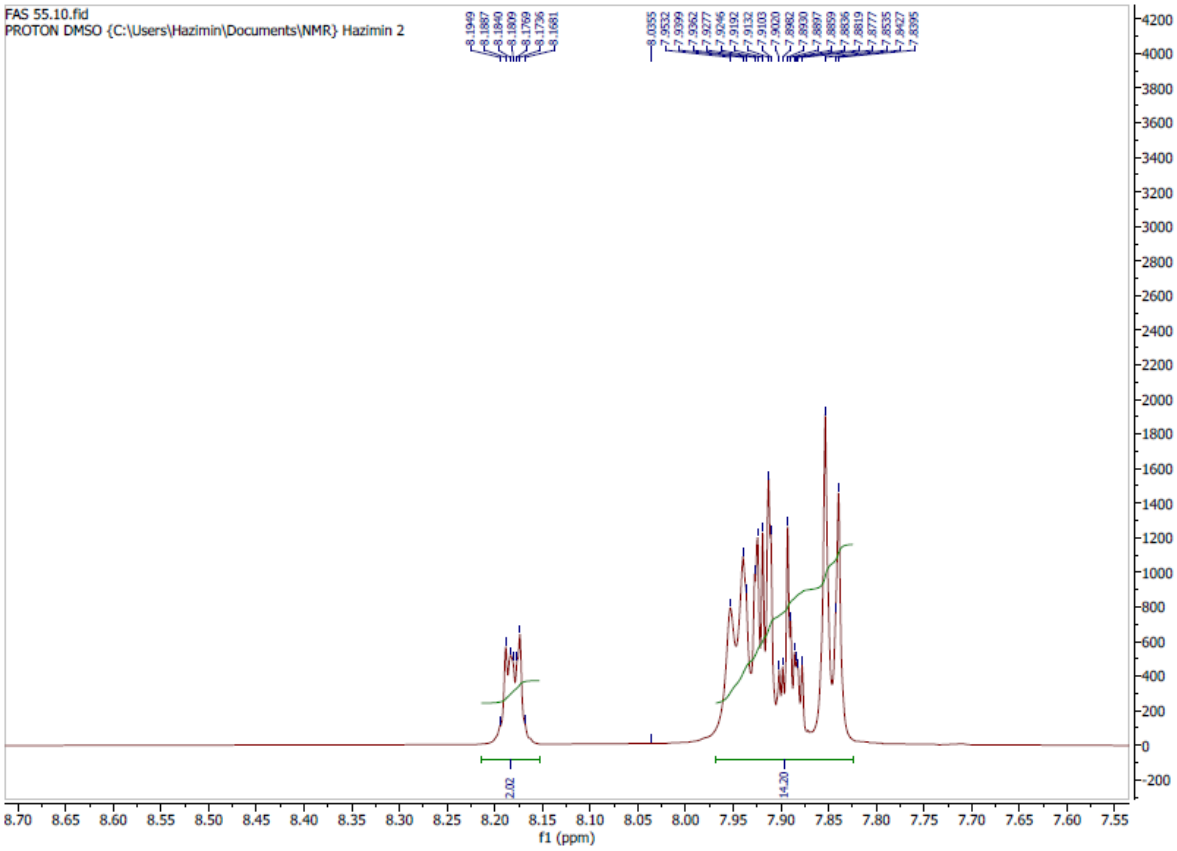
MS Spectrum of compound **12d.**



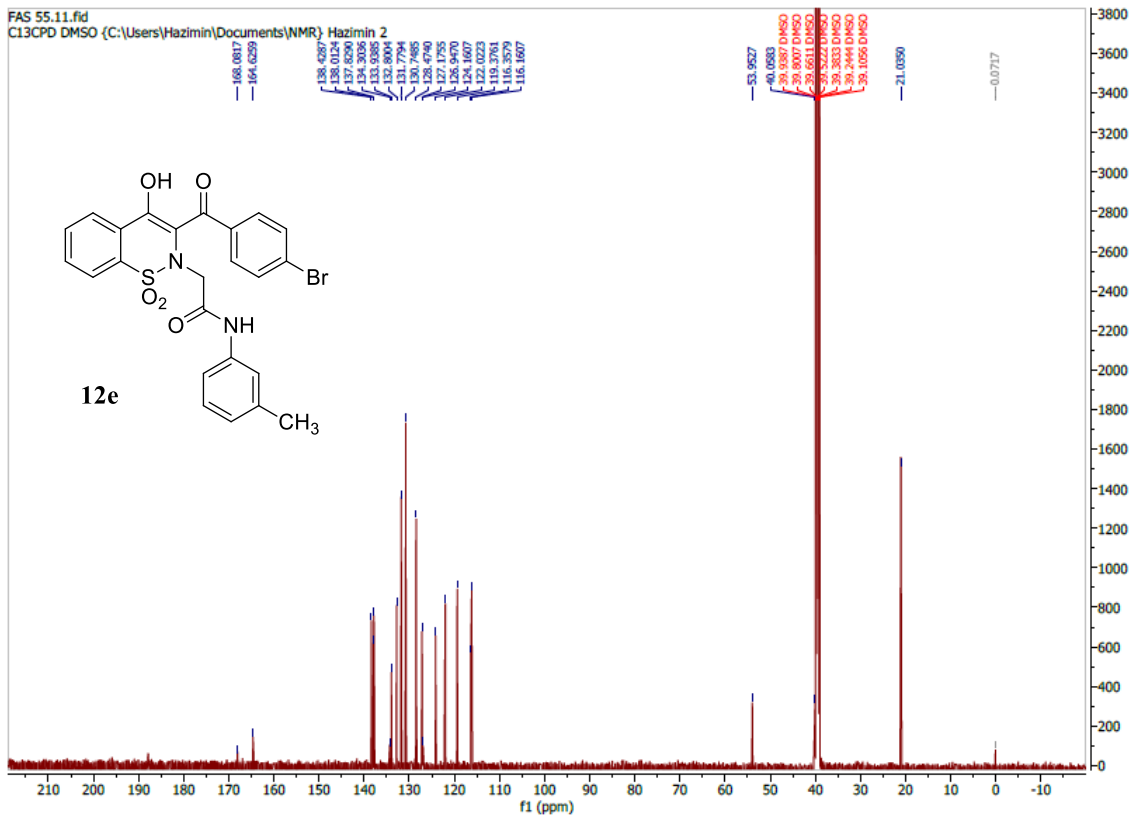
^{1}H NMR Spectrum of compound **12e**.



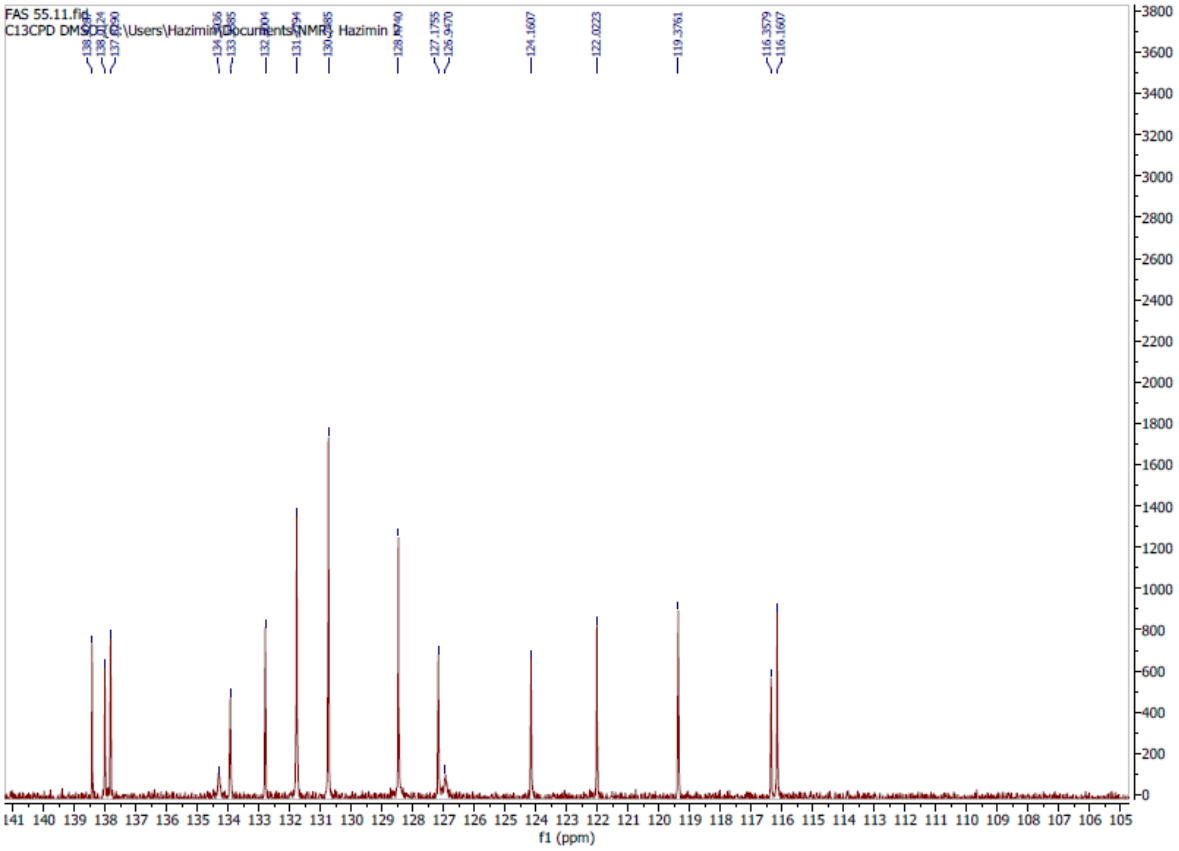
Expanded form of ^{1}H NMR Spectrum of compound **12e** (region 6.75-7.10 ppm).



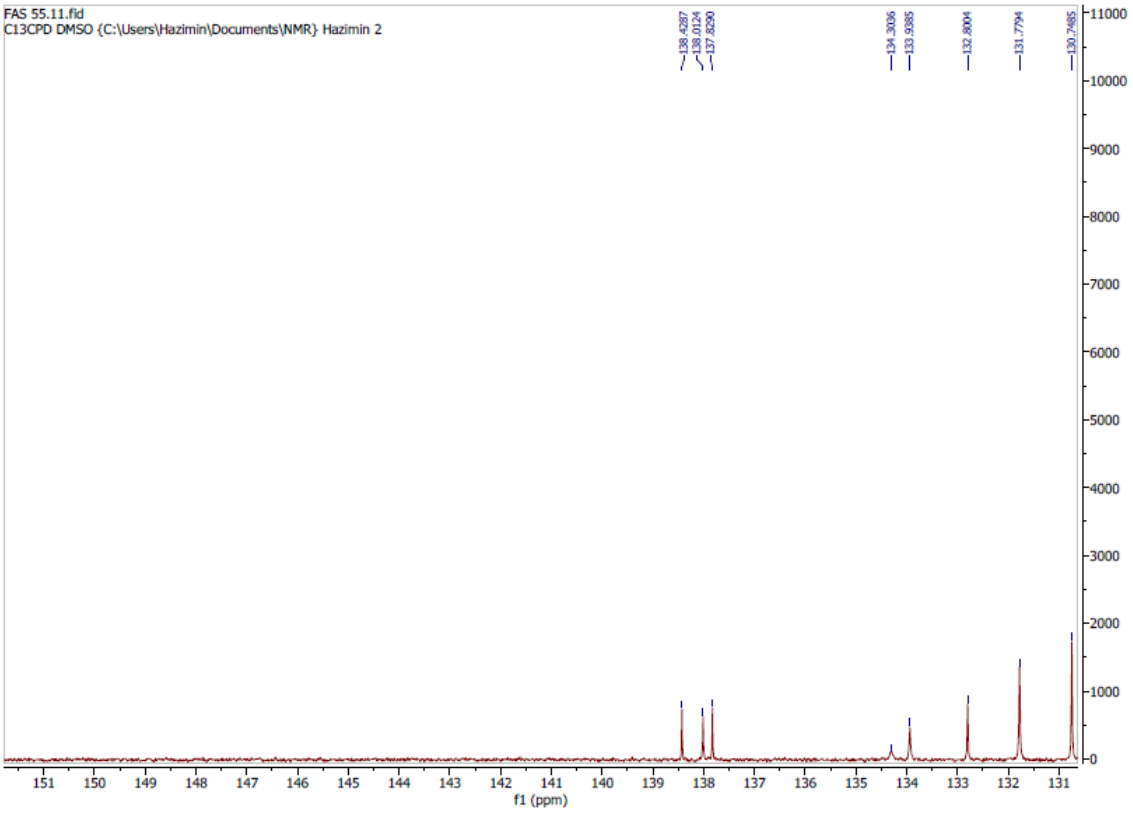
Expanded form of ^{1}H NMR Spectrum of compound **12e** (region 7.80-8.25 ppm).



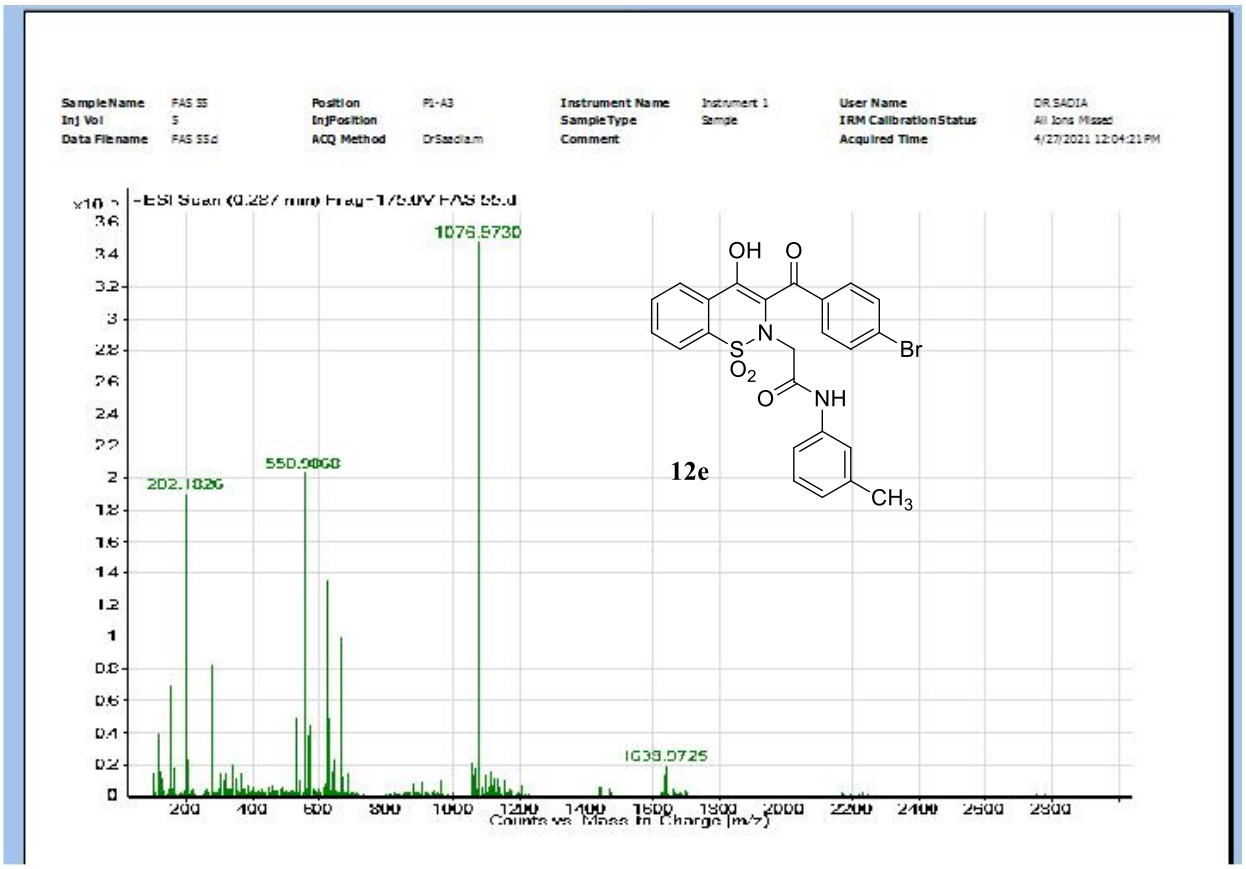
^{13}C NMR Spectrum of compound **12e.**



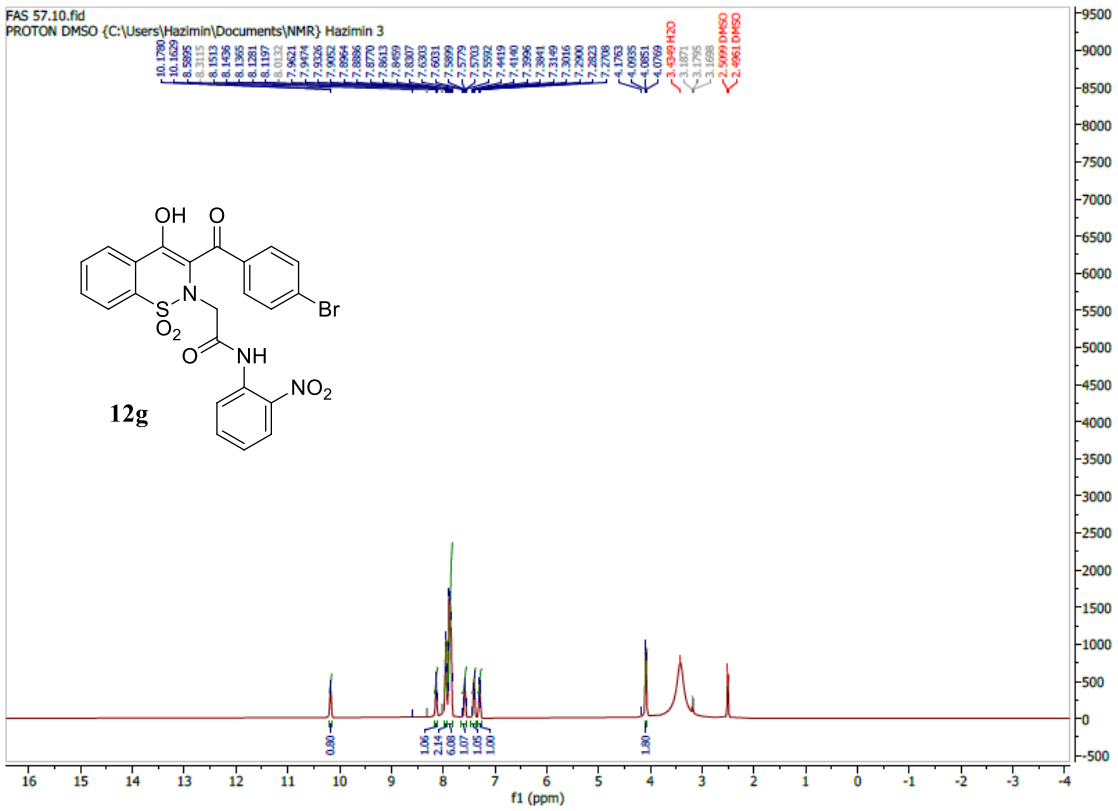
Expanded form of ^{13}C NMR Spectrum of compound **12e** (region 116-139 ppm).



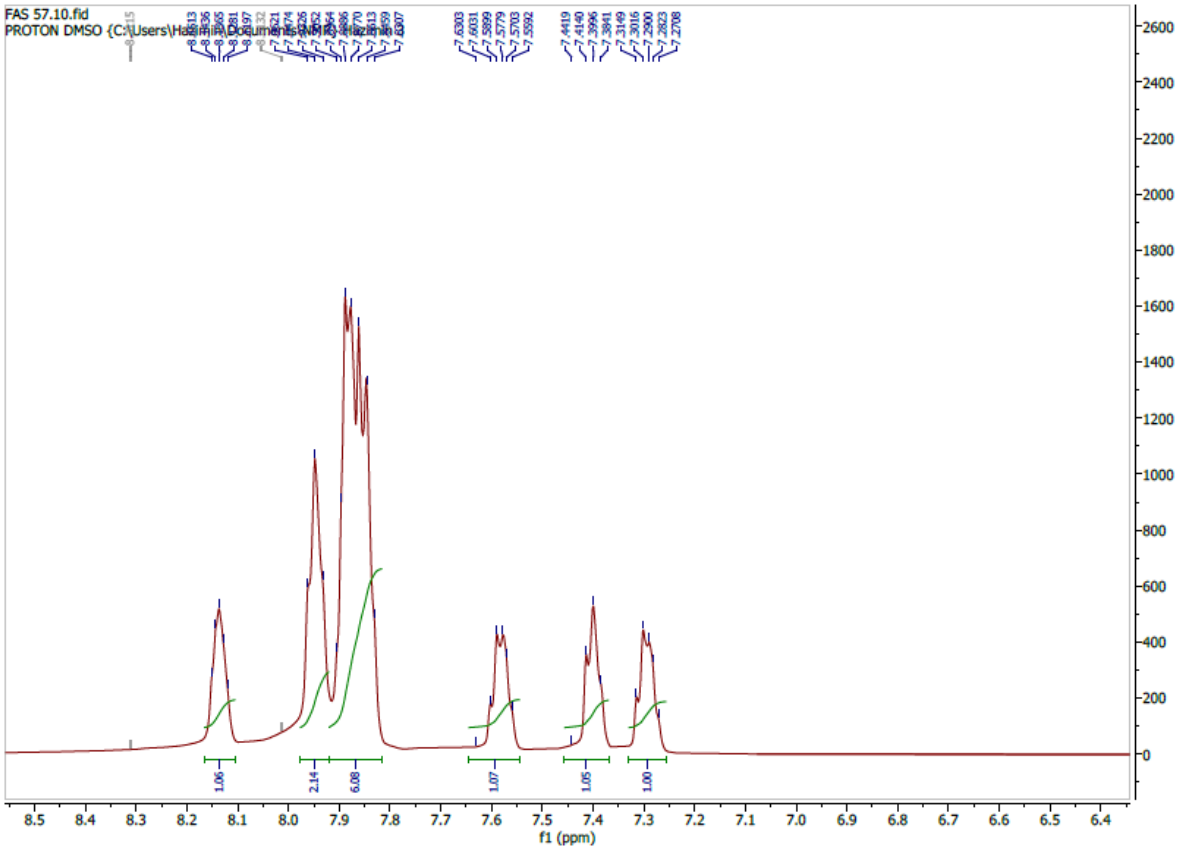
Expanded form of ^{13}C NMR Spectrum of compound **12e** (region 130-139 ppm).



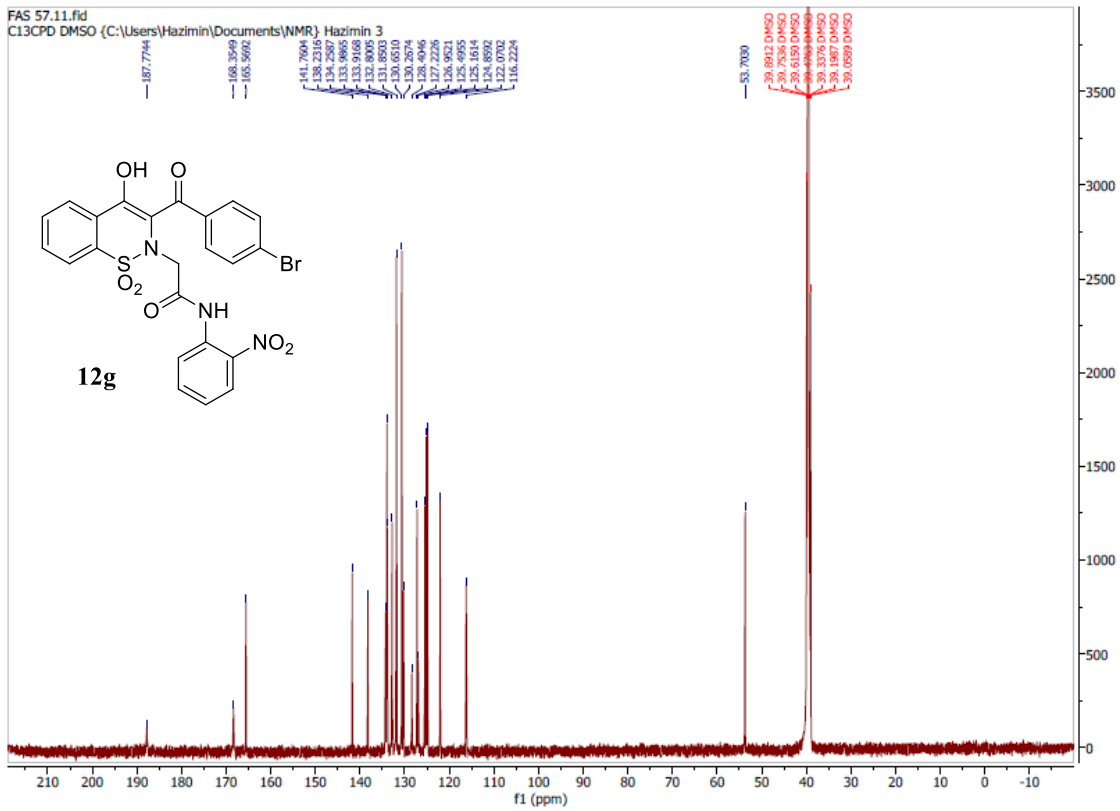
MS Spectrum of compound **12e.**



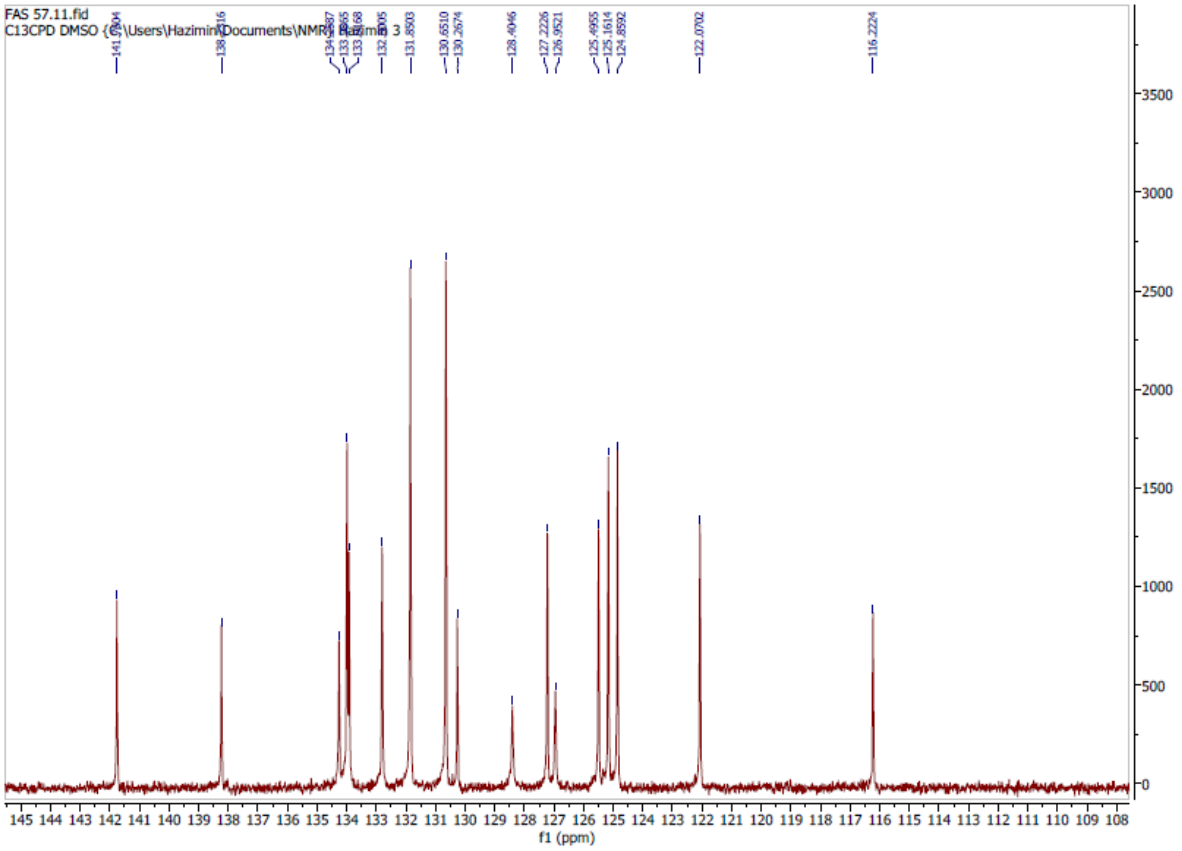
^{1}H NMR Spectrum of compound **12g**.



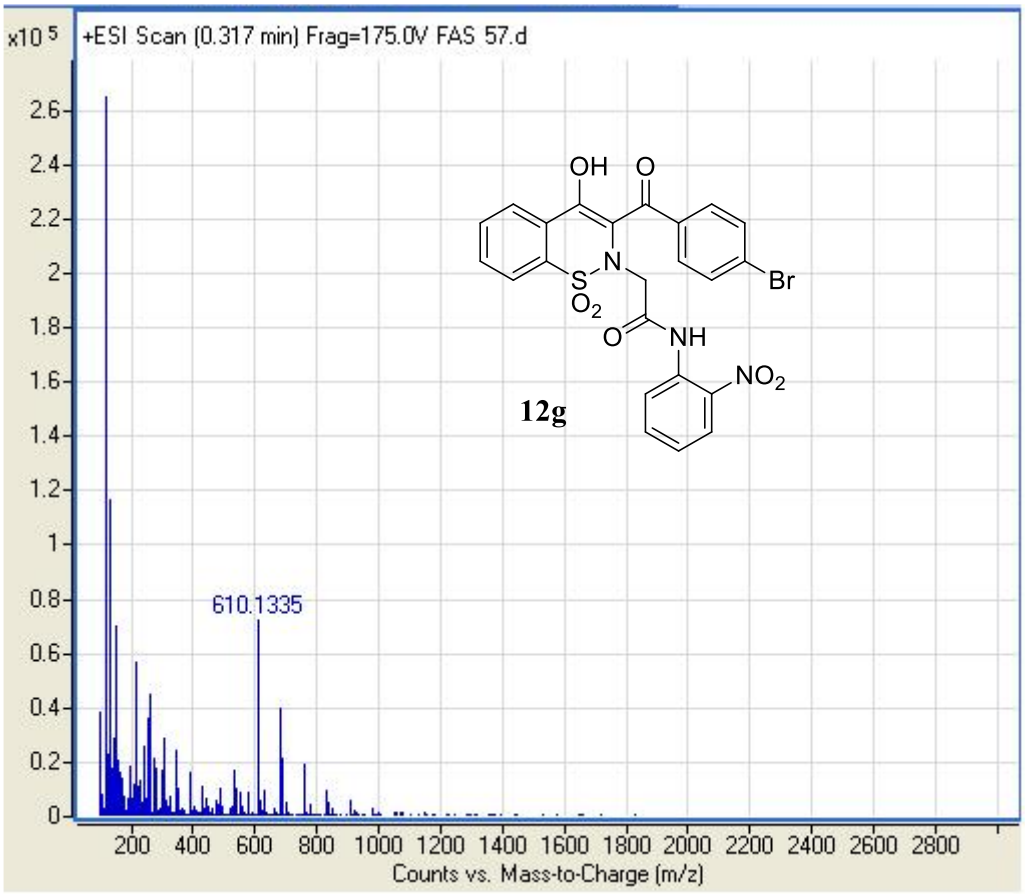
Expanded form of ^{1}H NMR Spectrum of compound **12g** (region 7.20-8.20 ppm).



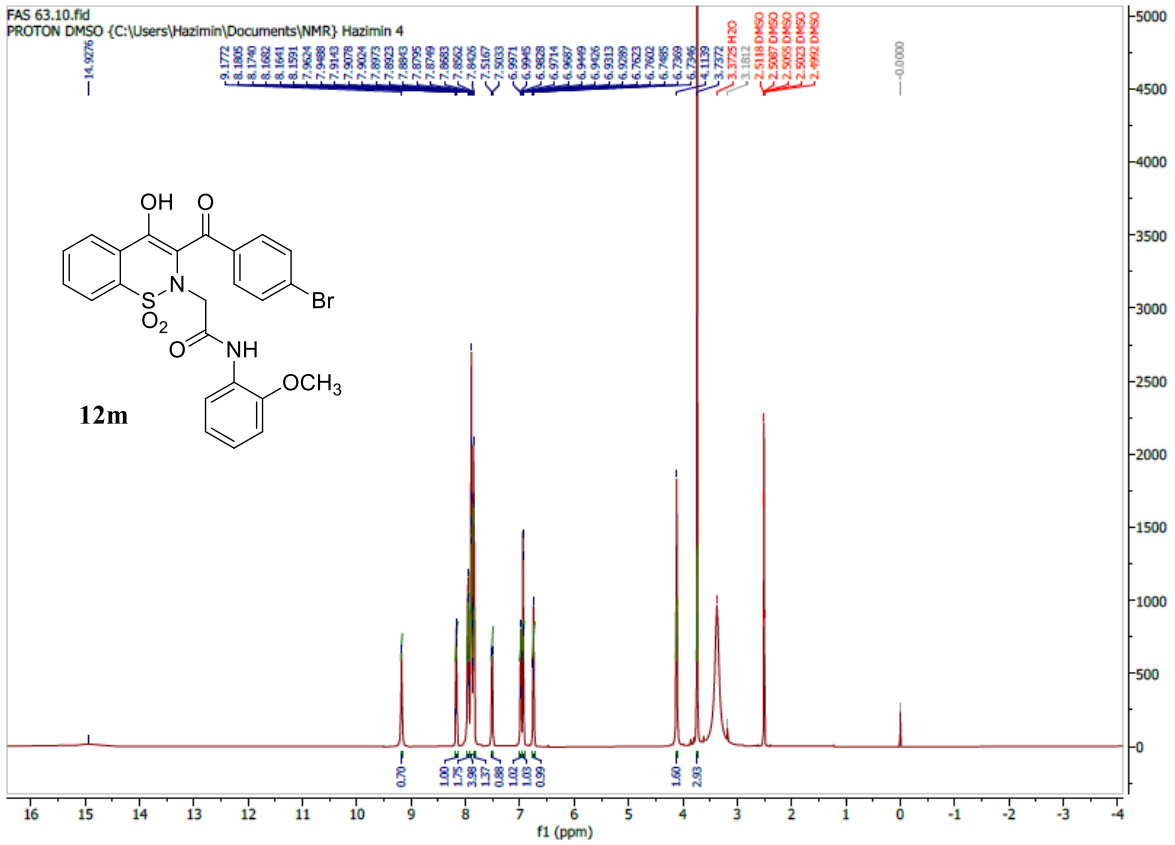
^{13}C NMR Spectrum of compound **12g.**



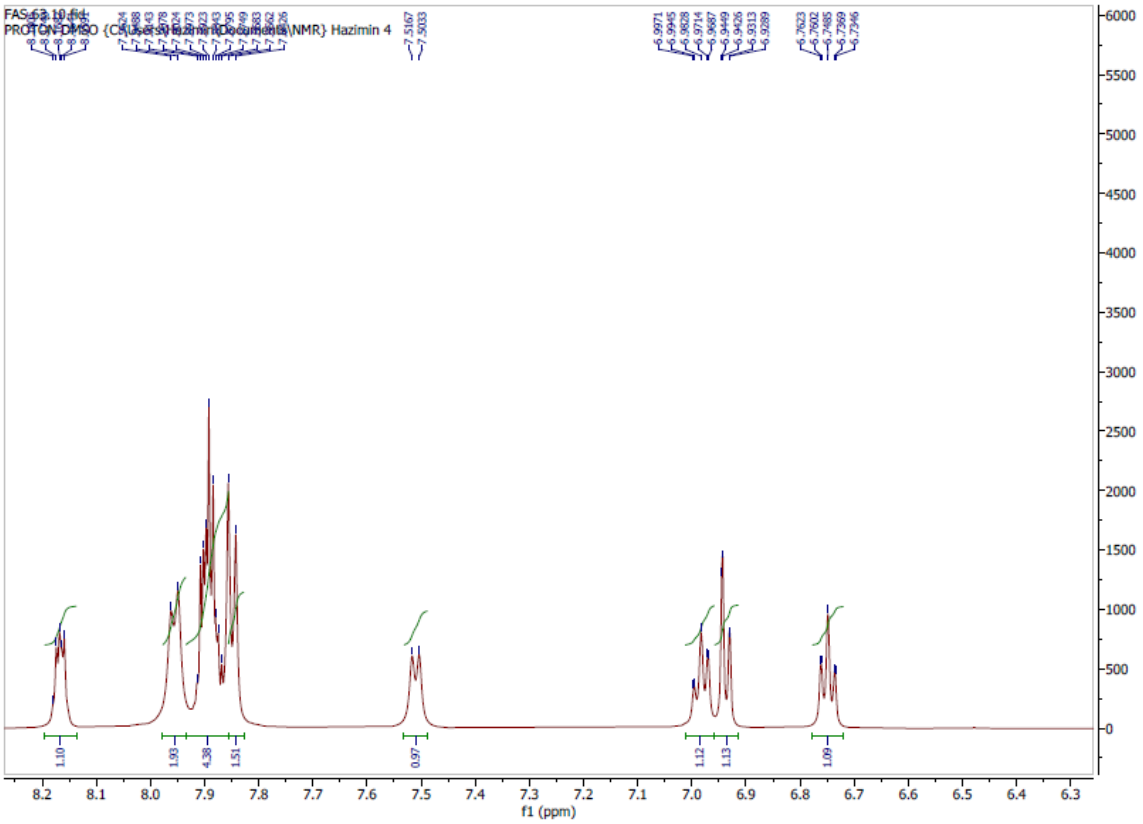
Expanded form of ^{13}C NMR Spectrum of compound **12g** (region 116-142 ppm).



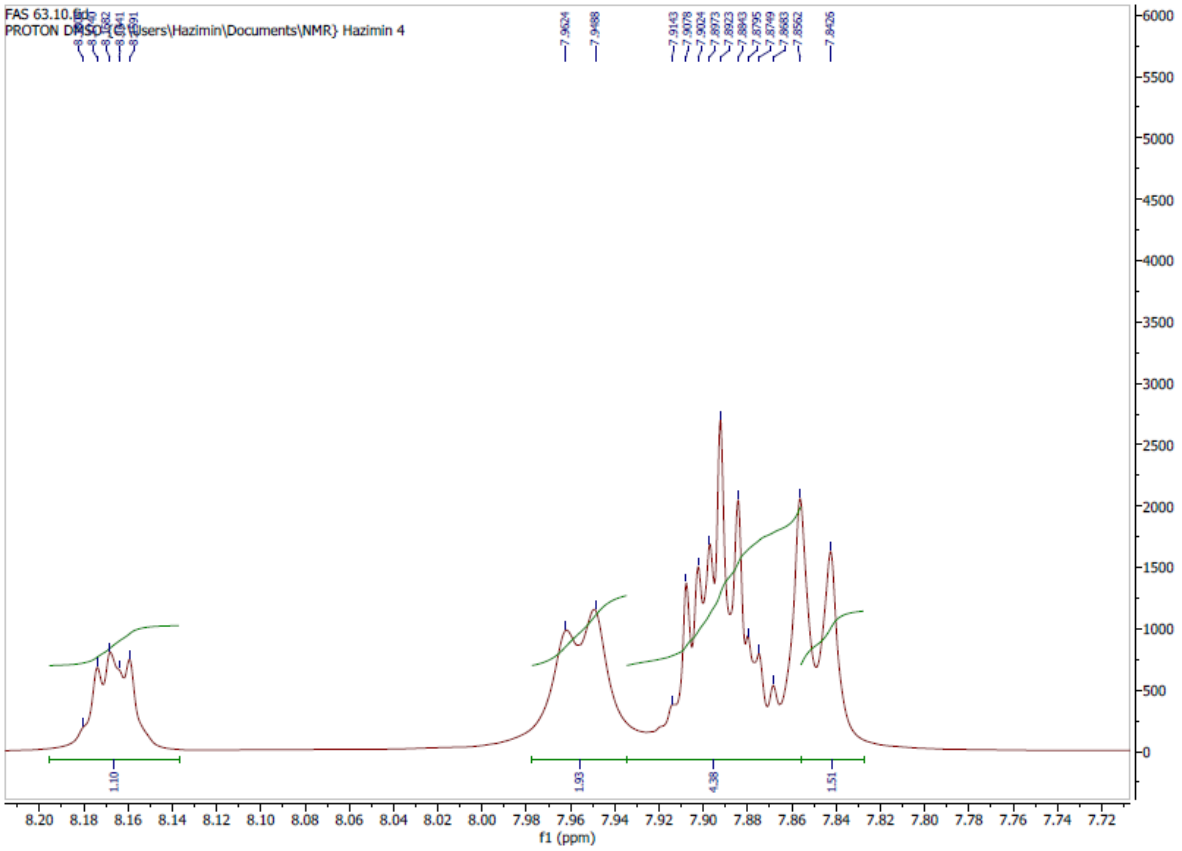
MS Spectrum of compound **12g.**



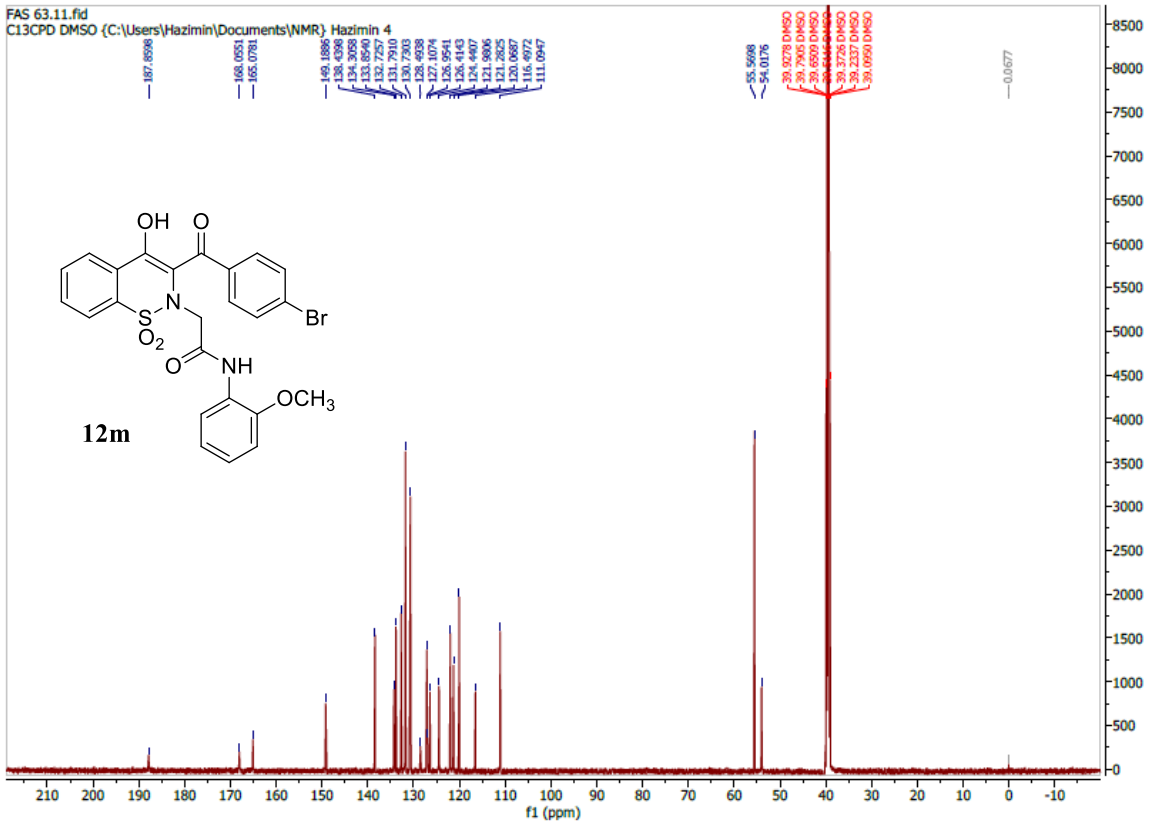
^{1}H NMR Spectrum of compound **12m**.



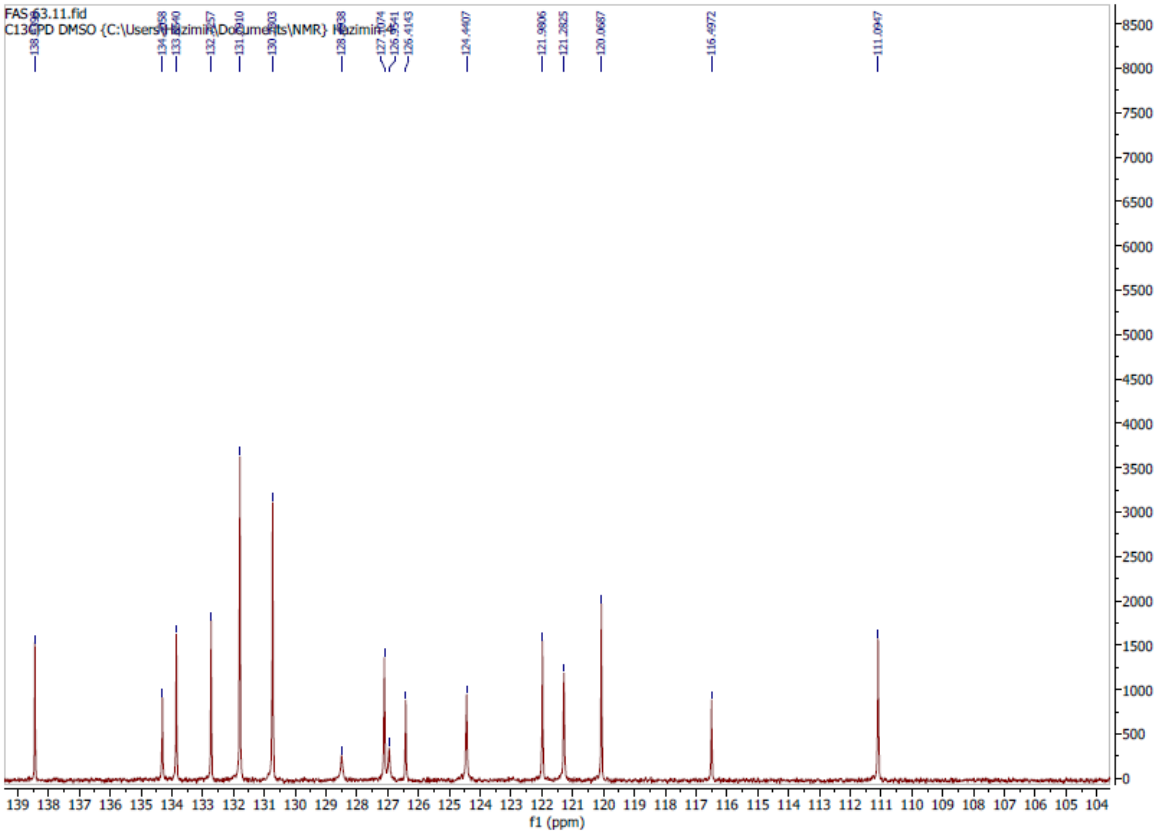
Expanded form of ^{1}H NMR Spectrum of compound **12m** (region 6.70-7.60 ppm).



Expanded form of ^{1}H NMR Spectrum of compound **12m** (region 7.82-8.20 ppm).



^{13}C NMR Spectrum of compound **12m.**



Expanded form of ^{13}C NMR Spectrum of compound **12m** (region 110-139 ppm).

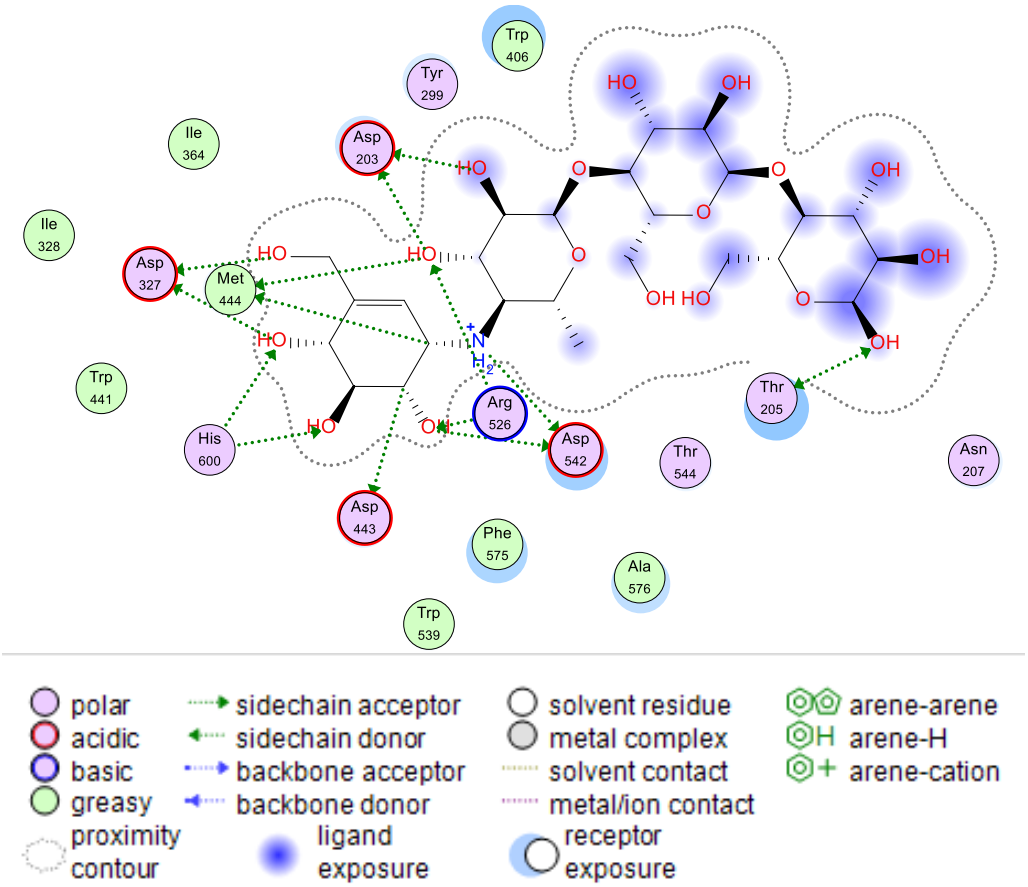
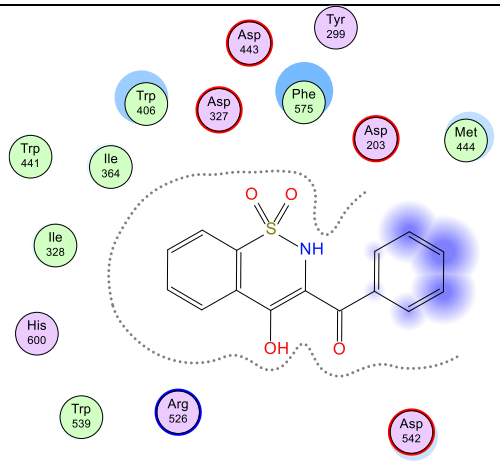
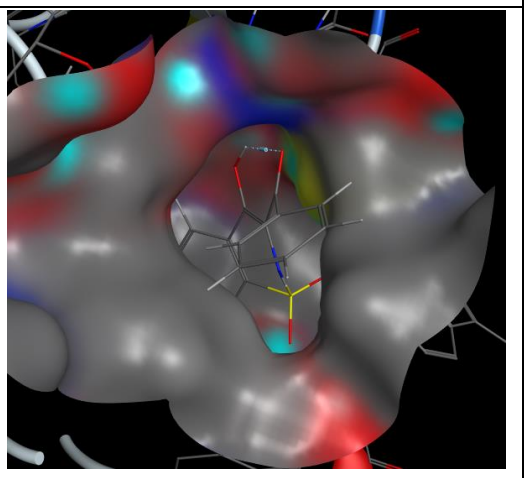
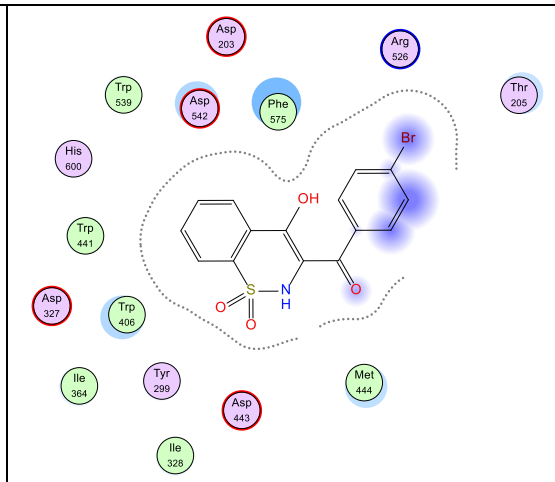
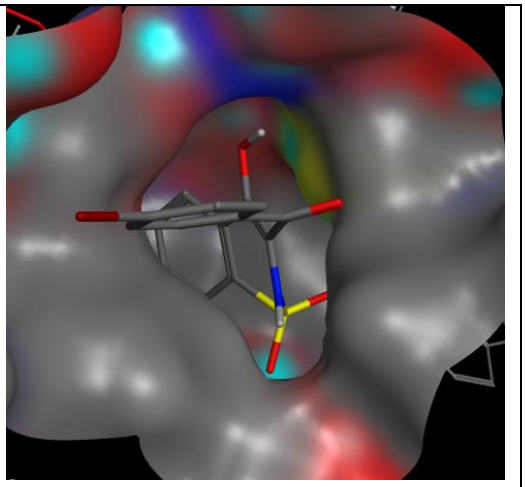
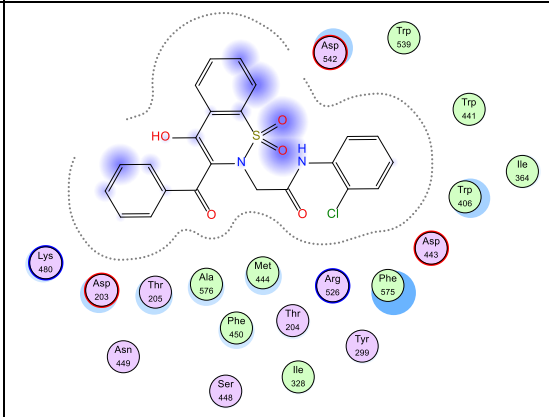
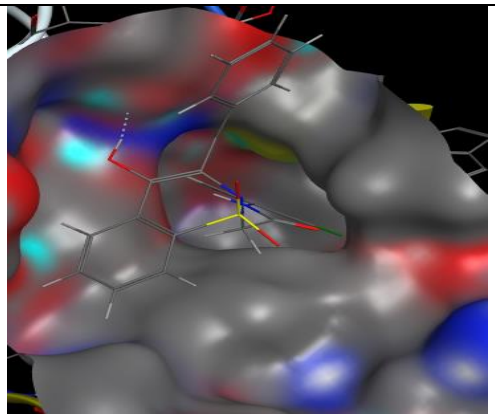
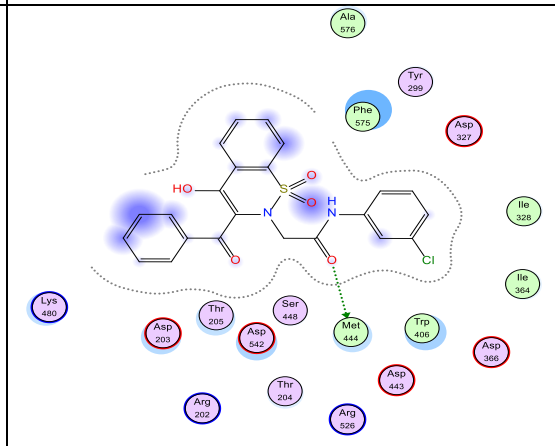
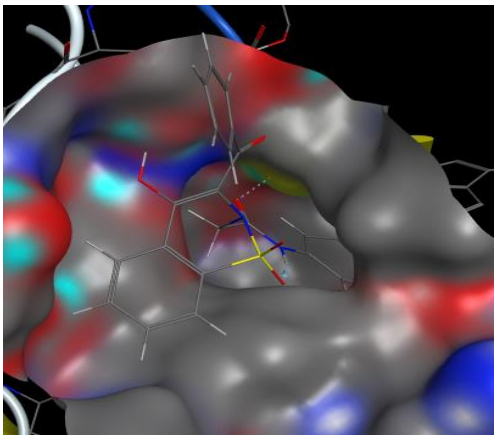
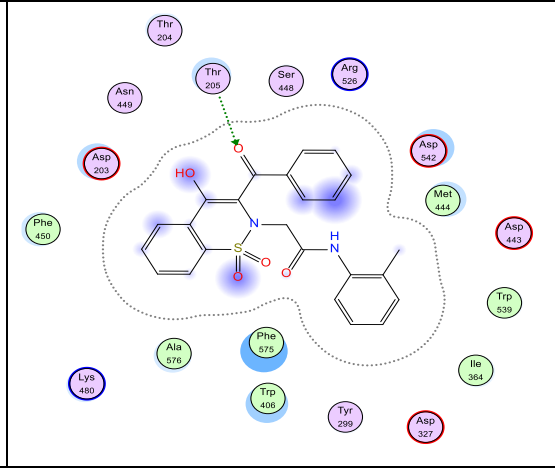
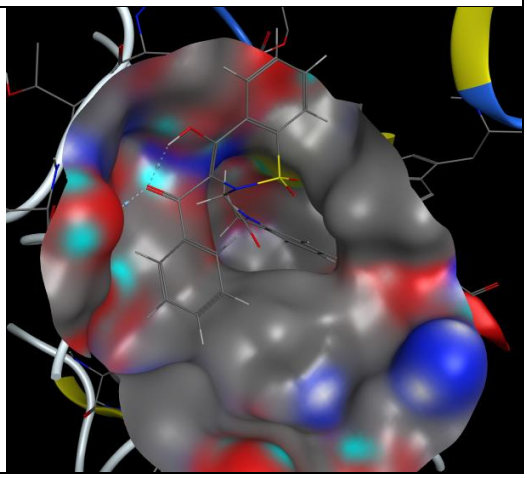
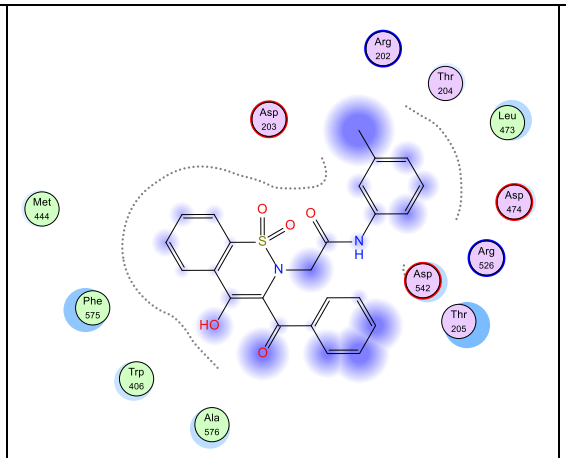
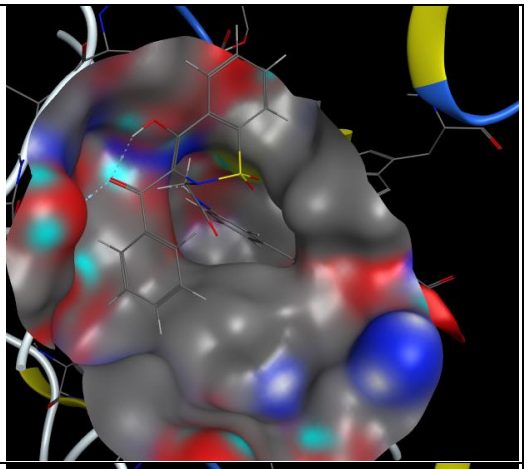
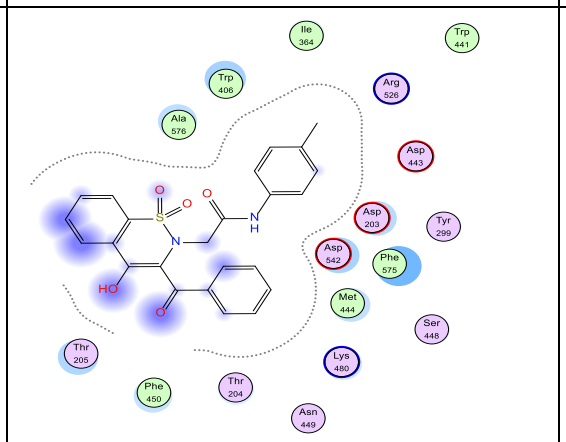
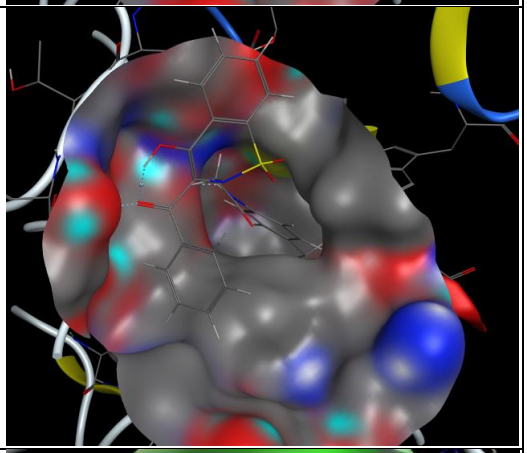
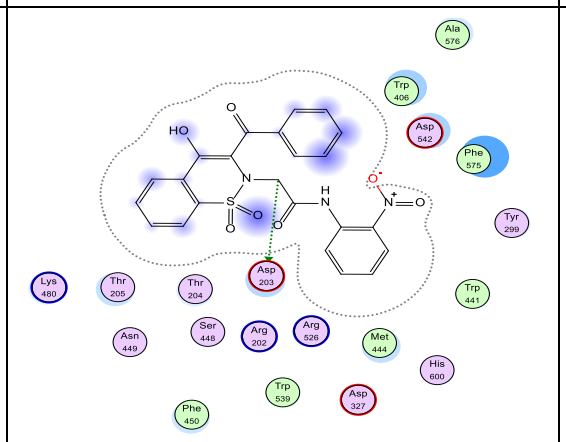
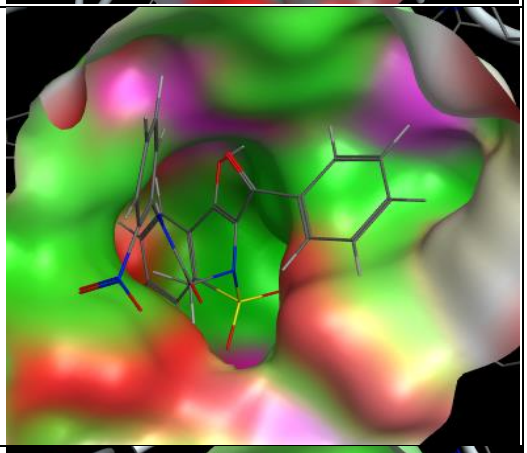
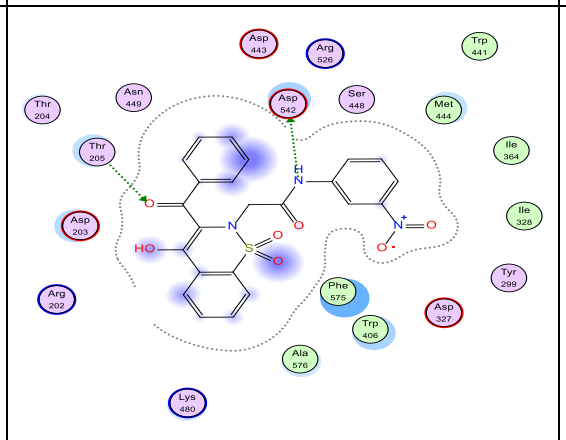
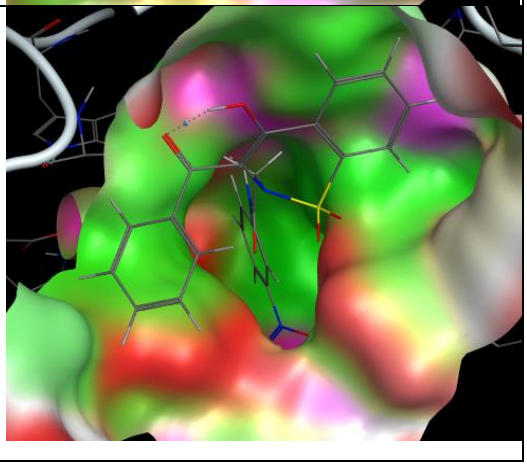


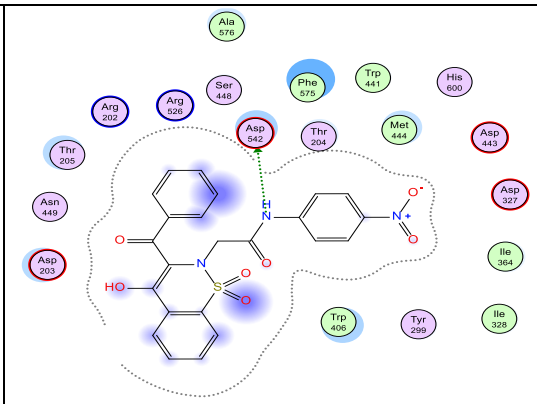
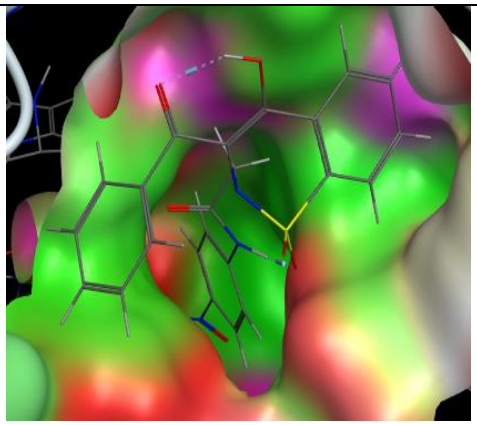
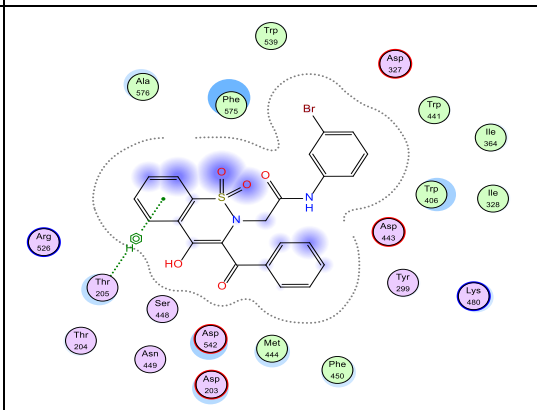
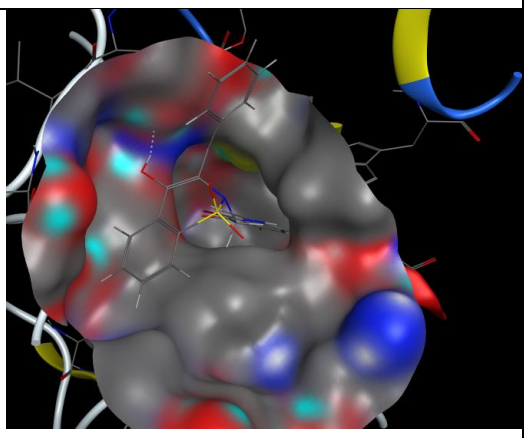
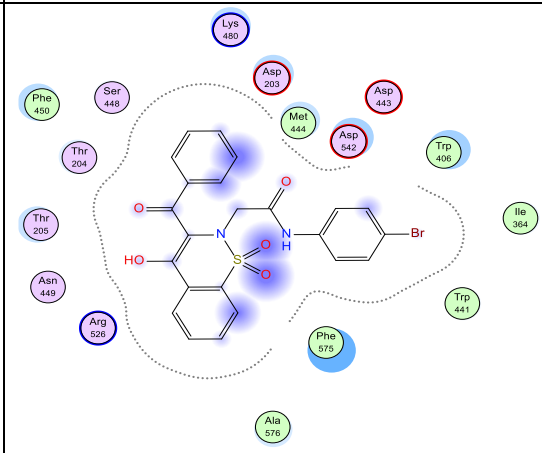
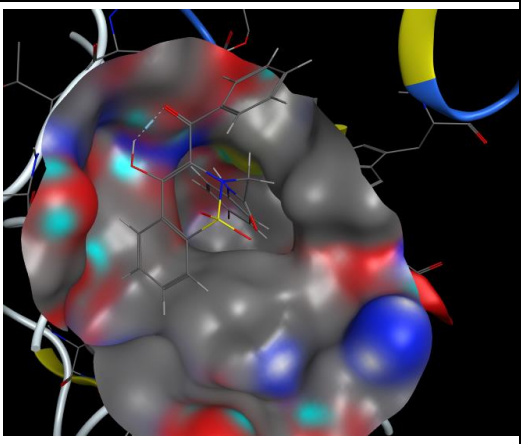
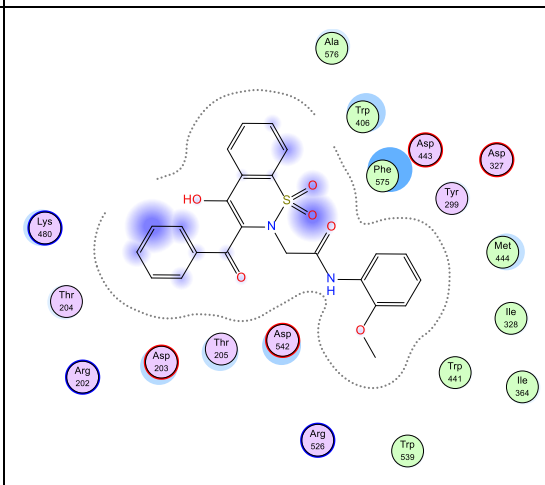
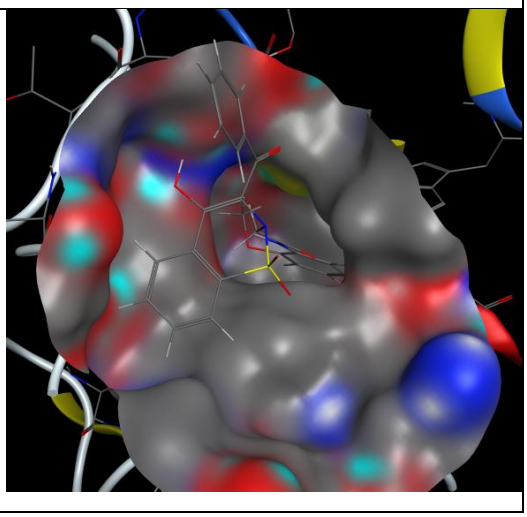
Figure S1. Selected (reference) residues. Computed acarbose interactions.

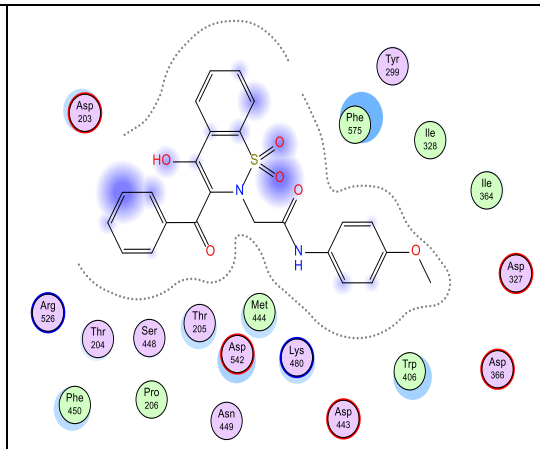
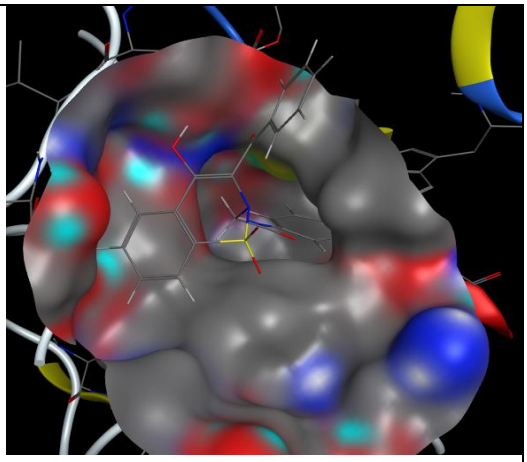
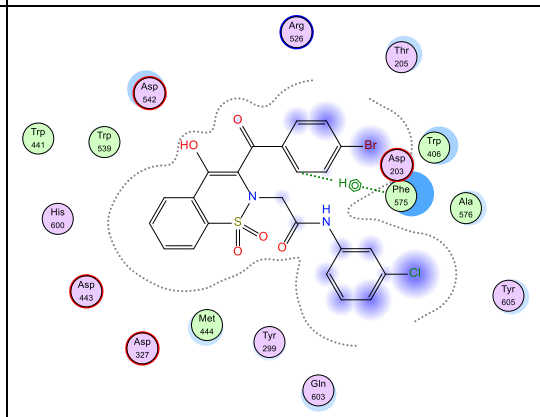
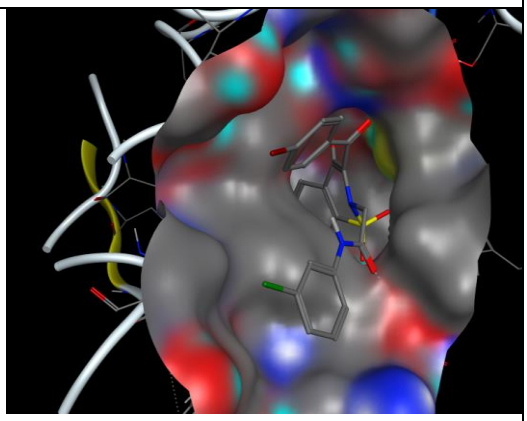
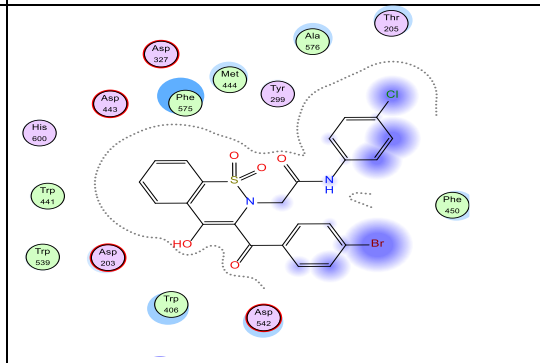
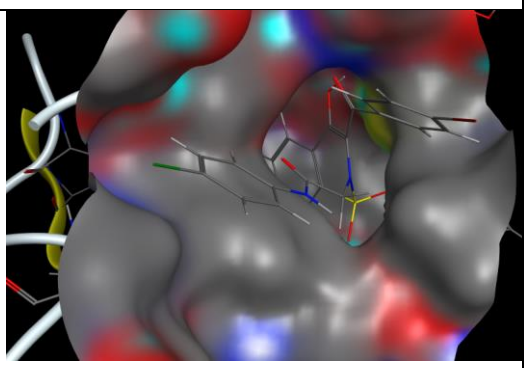
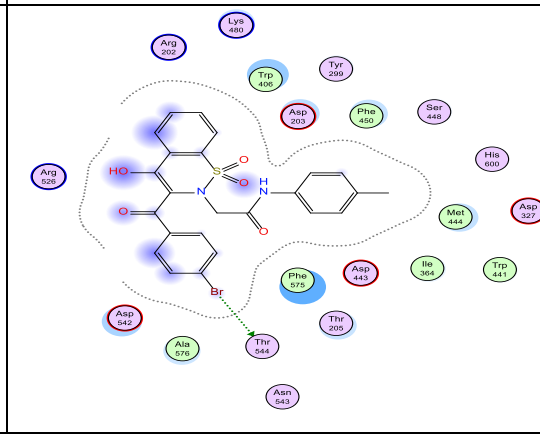
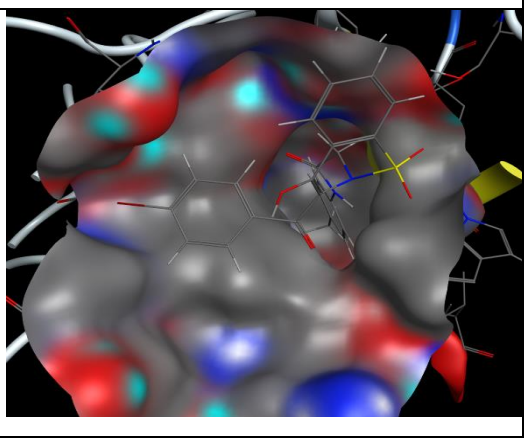
Table S1. 2D and 3D interaction modes of compounds **9a,b; 11(a,b,d-m)** and **12(b,c,f,h-m)**. In 2D interaction modes the blue color indicates ligand exposure and green color dotted line indicates the interactions of receptor enzyme with ligands. In 3D interaction modes the colored portions show pocket selected and red portion indicates the ligand exposure points.

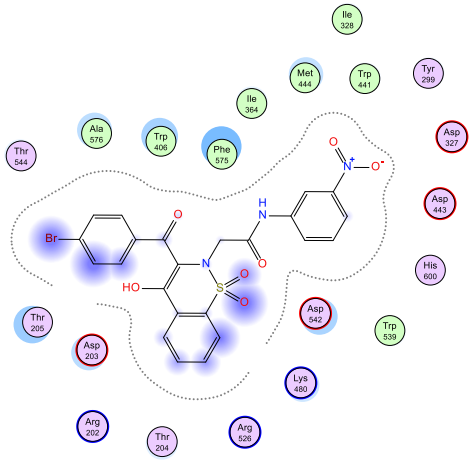
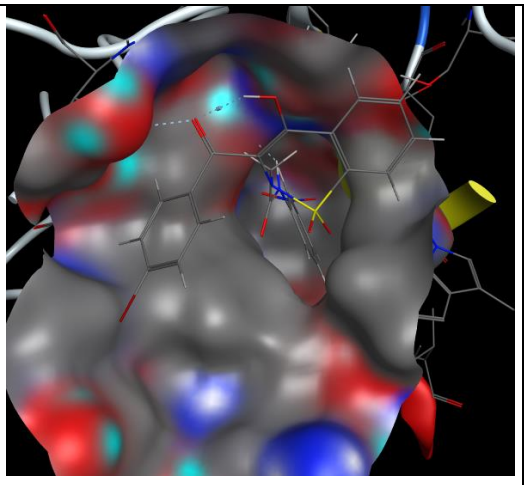
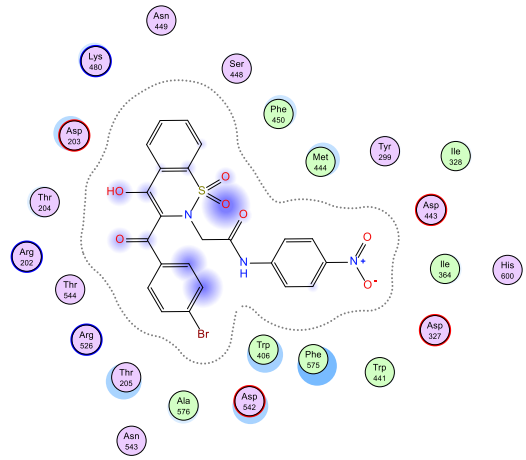
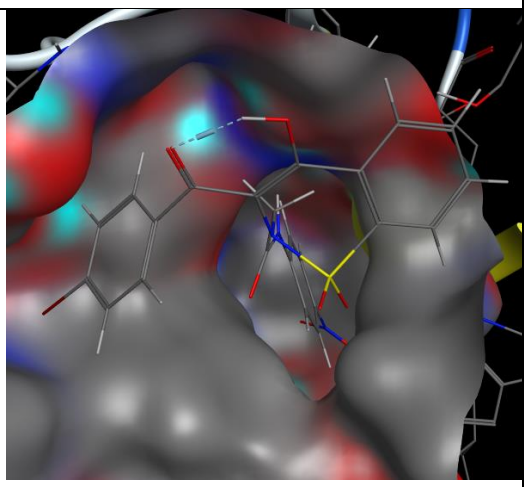
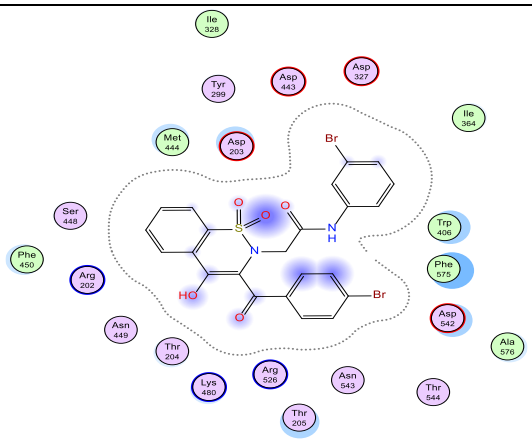
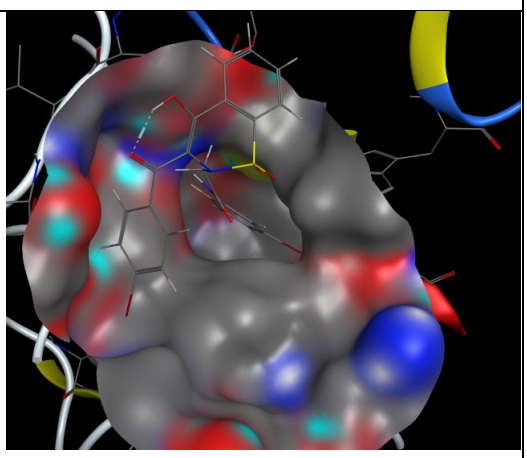
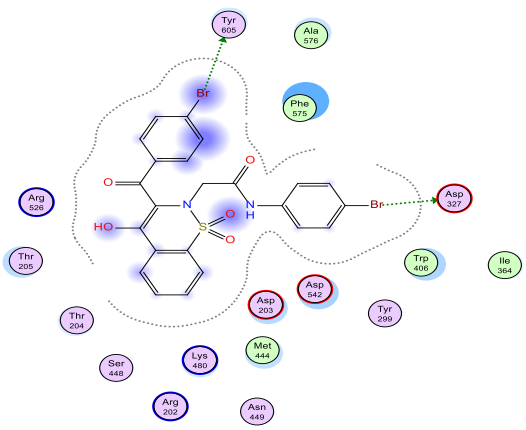
Comp.	2D-interaction mods	3D-maps
9a		

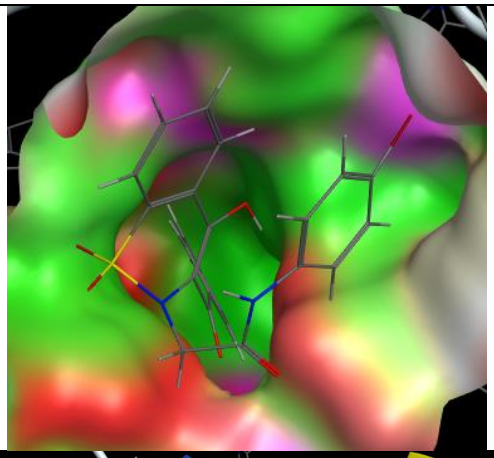
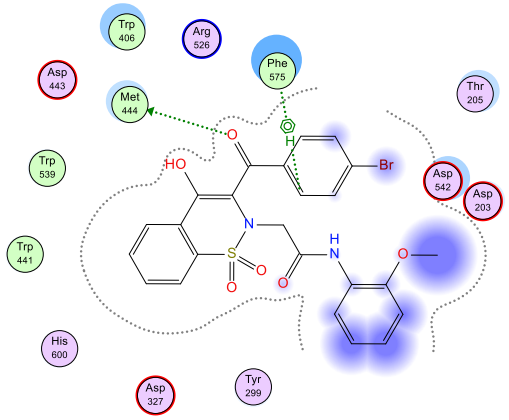
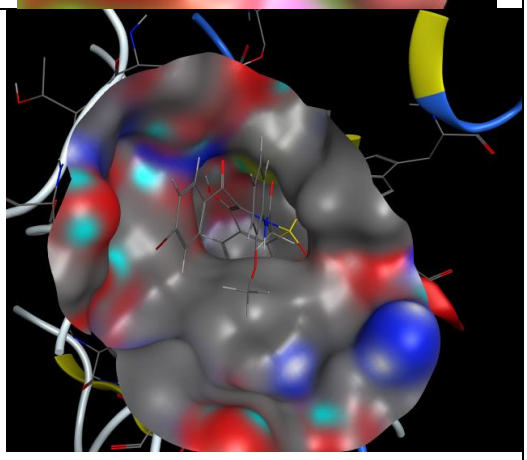
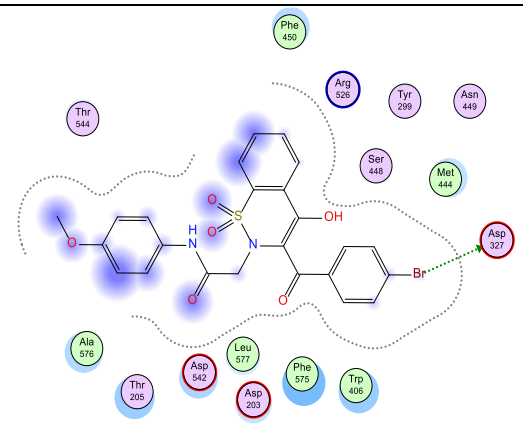
9b		
11a		
11b		
11d		

11e		
11f		
11g		
11h		

11i		
11j		
11k		
11l		

11m		
12b		
12c		
12f		

12h		
12i		
12j		
12k		

		
12l	 Trp 406 Arg 526 Asp 443 Phe 575 Met 444 Thr 205 Trp 539 Asp 542 Asp 203 Trp 441 His 600 Asp 327 Tyr 299	
12m	 Phe 450 Arg 526 Tyr 299 Asn 449 Thr 544 Ser 448 Met 444 Asp 327 Ala 576 Leu 577 Asp 542 Phe 575 Trp 406 Thr 205 Asp 203