

Benzilic acid based new 2-aryl-1,3-thiazolidin-4-one derivatives: synthesis and anticancer activity

Özlen GÜZEL-AKDEMİR ¹ , Kübra DEMİR-YAZICI ^{1*} 

¹ Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Istanbul University, Fatih 34116 Istanbul, Turkey.

* Corresponding Author. E-mail: kubra.demir@istanbul.edu.tr (K.D.-Y.); Tel. +90-212-440 00 00/13462.

(Supplementary Material)

Table of Contents	Page
Figure S1: IR (KBr) Spectrum of Compound 3a	4
Figure S2: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3a	5
Figure S3: IR (KBr) Spectrum of Compound 3b	6
Figure S4: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3b	7
Figure S5: IR (KBr) Spectrum of Compound 3c	8
Figure S6: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3c	9
Figure S7: ¹³ C-NMR (125.6 MHz, APT (decoupled)) Spectrum of Compound 3c	10
Figure S8: MS-APCI(-) (150 eV, m/z, %) Spectrum of Compound 3c	11
Figure S9: IR (KBr) Spectrum of Compound 3d	12
Figure S10: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3d	13
Figure S11: IR (KBr) Spectrum of Compound 3e	14
Figure S12: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3e	15
Figure S13: ¹³ C-NMR (125.6 MHz, APT (decoupled)) Spectrum of Compound 3e	16
Figure S14: MS-APCI(-) (150 eV, m/z, %) Spectrum of Compound 3e	17
Figure S15: IR (KBr) Spectrum of Compound 3f	18
Figure S16: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3f	19
Figure S17: ¹³ C-NMR (125.6 MHz, APT (decoupled)) Spectrum of Compound 3f	20
Figure S18: IR (KBr) Spectrum of Compound 3g	21
Figure S19: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3g	22
Figure S20: IR (KBr) Spectrum of Compound 3h	23
Figure S21: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3h	24
Figure S22: IR (KBr) Spectrum of Compound 3i	25
Figure S23: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3i	26
Figure S24: IR (KBr) Spectrum of Compound 3j	27
Figure S25: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3j	28
Figure S26: IR (KBr) Spectrum of Compound 3k	29
Figure S27: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3k	30
Figure S28: IR (KBr) Spectrum of Compound 3l	31
Figure S29: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3l	32
Figure S30: IR (KBr) Spectrum of Compound 3m	33
Figure S31: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3m	34
Figure S32: IR (KBr) Spectrum of Compound 3n	35
Figure S33: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3n	36
Figure S34: IR (KBr) Spectrum of Compound 3o	37
Figure S35: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3o	38
Figure S36: IR (KBr) Spectrum of Compound 3p	39
Figure S37: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 3p	40
Figure S38: IR (KBr) Spectrum of Compound 4a	41
Figure S39: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4a	42
Figure S40: IR (KBr) Spectrum of Compound 4b	43
Figure S41: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4b	44
Figure S42: IR (KBr) Spectrum of Compound 4c	45
Figure S43: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4c	46
Figure S44: IR (KBr) Spectrum of Compound 4d	47
Figure S45: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4d	48
Figure S46: IR (KBr) Spectrum of Compound 4e	49
Figure S47: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4e	50
Figure S48: IR (KBr) Spectrum of Compound 4f	51
Figure S49: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4f	52
Figure S50: IR (KBr) Spectrum of Compound 4g	53
Figure S51: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4g	54
Figure S52: IR (KBr) Spectrum of Compound 4h	55
Figure S53: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4h	56
Figure S54: IR (KBr) Spectrum of Compound 4i	57

Figure S55: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4i	58
Figure S56: IR (KBr) Spectrum of Compound 4j	59
Figure S57: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4j	60
Figure S58: IR (KBr) Spectrum of Compound 4k	61
Figure S59: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4k	62
Figure S60: IR (KBr) Spectrum of Compound 4l	63
Figure S61: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4l	64
Figure S62: IR (KBr) Spectrum of Compound 4m	65
Figure S63: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4m	66
Figure S64: IR (KBr) Spectrum of Compound 4n	67
Figure S65: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4n	68
Figure S66: ¹³ C-NMR (125.6 MHz, APT (decoupled)) Spectrum of Compound 4n	69
Figure S67: MS-APCI(-) (150 eV, m/z, %) Spectrum of Compound 4n	70
Figure S68: IR (KBr) Spectrum of Compound 4o	71
Figure S69: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4o	72
Figure S70: IR (KBr) Spectrum of Compound 4p	73
Figure S71: ¹ H-NMR (500 MHz, DMSO- <i>d</i> ₆) Spectrum of Compound 4p	74
Figure S72: ¹³ C-NMR (125.6 MHz, APT (decoupled)) Spectrum of Compound 4p	75
Figure S73: MS-APCI(-) (150 eV, m/z, %) Spectrum of Compound 4p	76

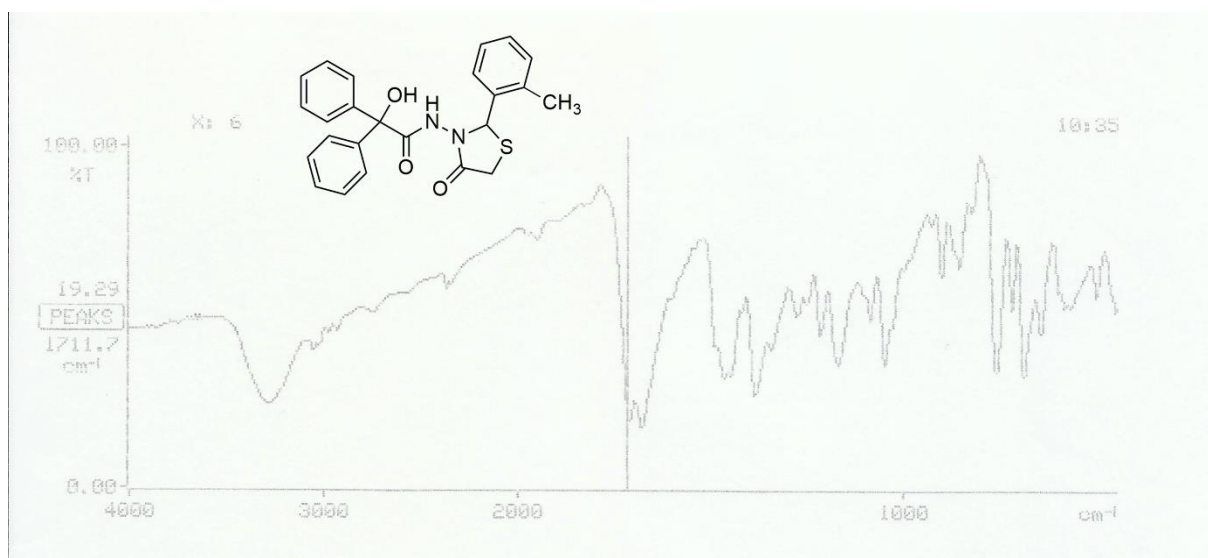


Figure S1: IR (KBr) Spectrum of Compound **3a**

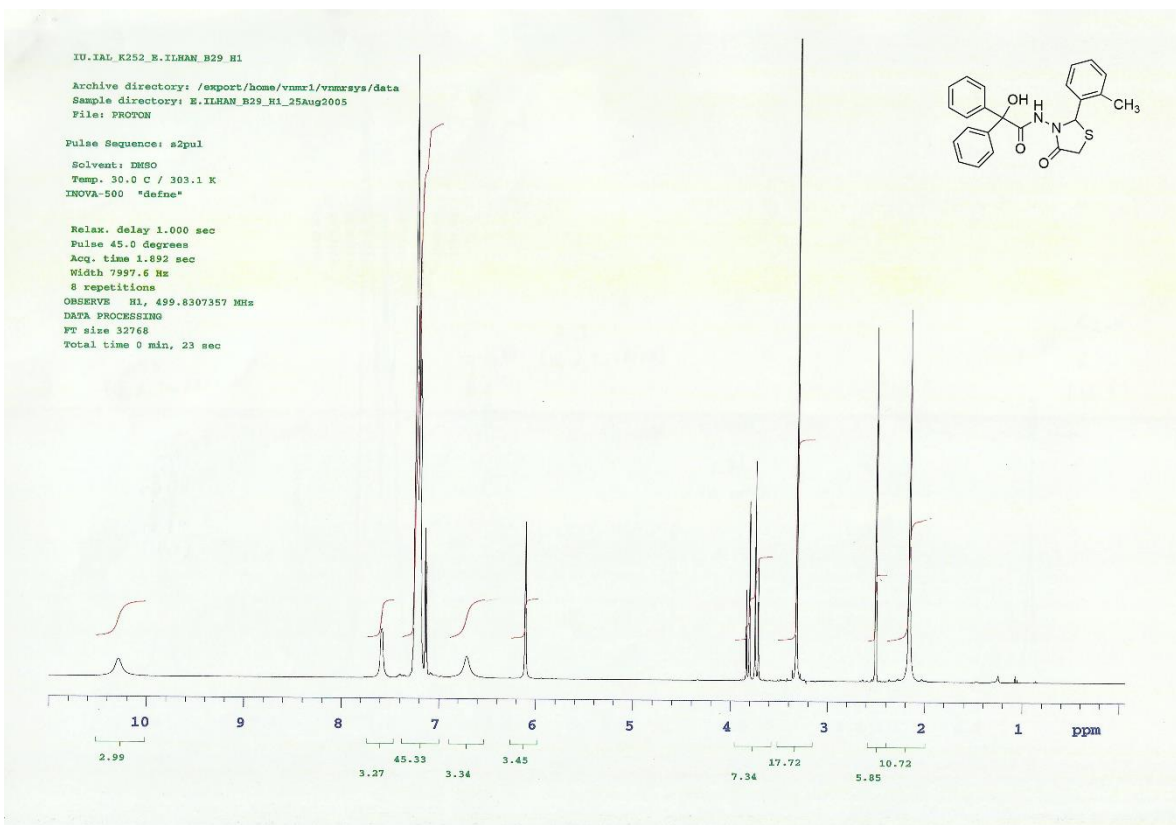


Figure S2: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **3a**

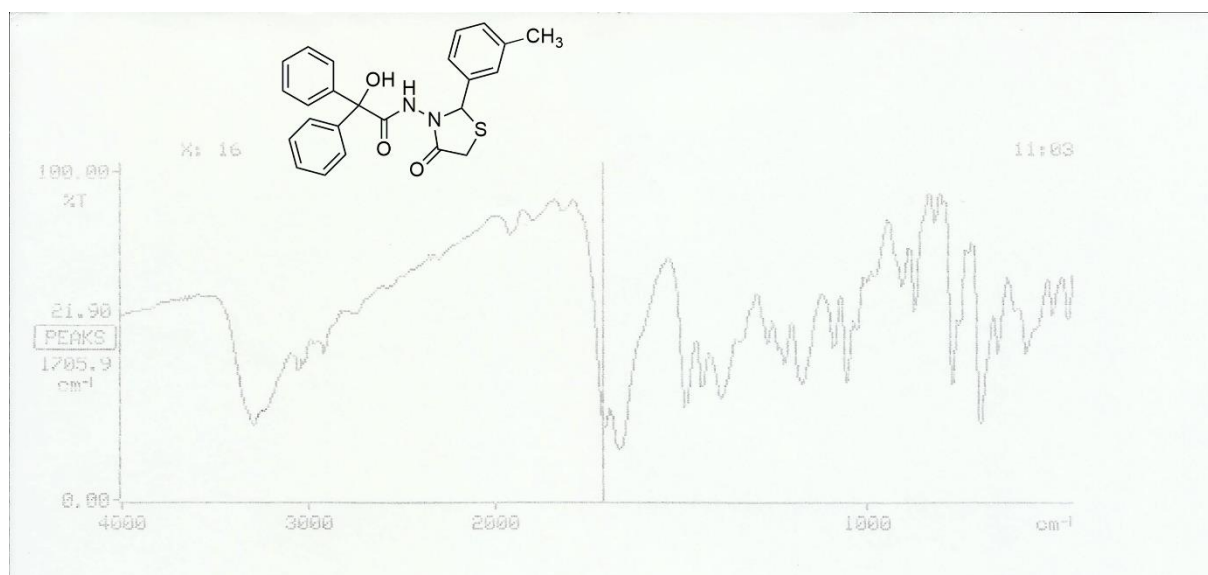


Figure S3: IR (KBr) Spectrum of Compound **3b**

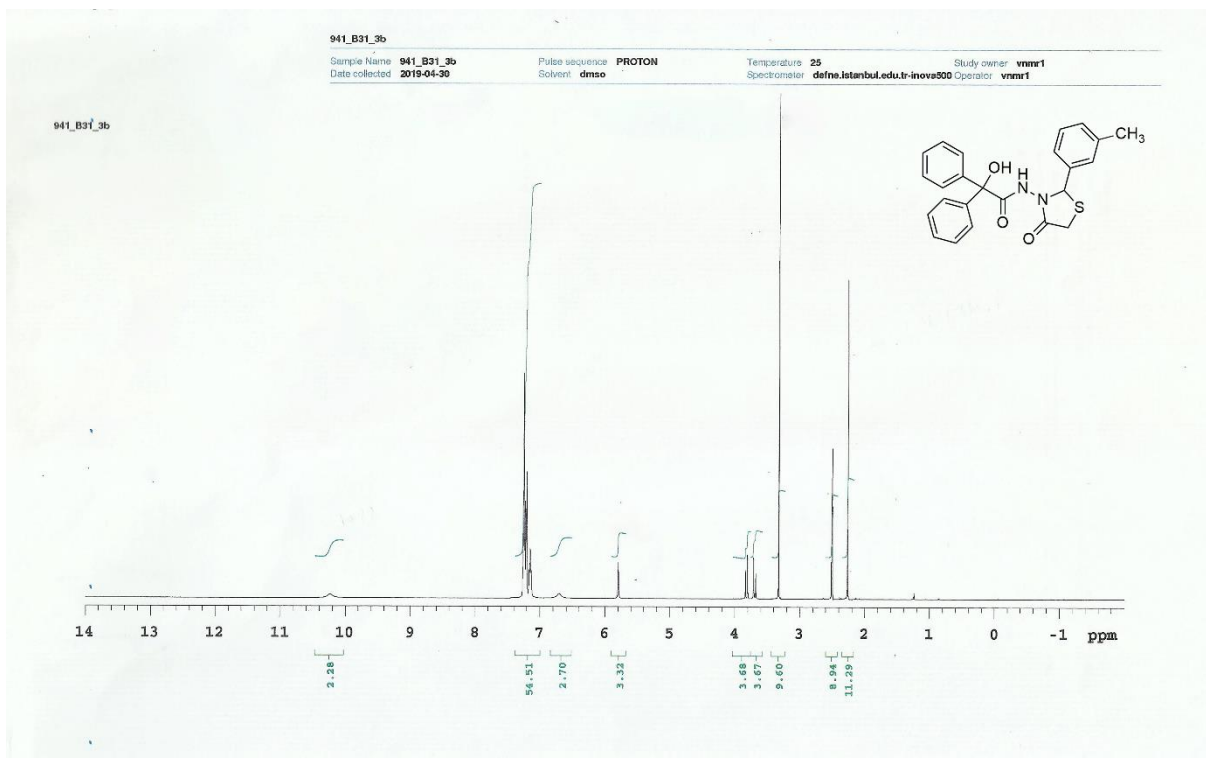


Figure S4: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **3b**

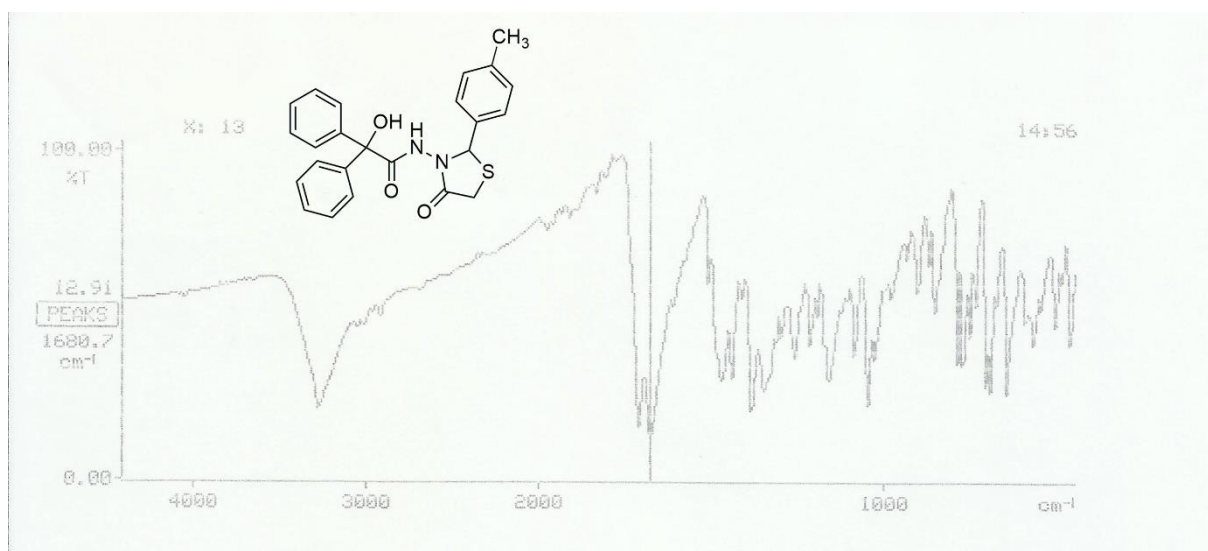


Figure S5: IR (KBr) Spectrum of Compound **3c**

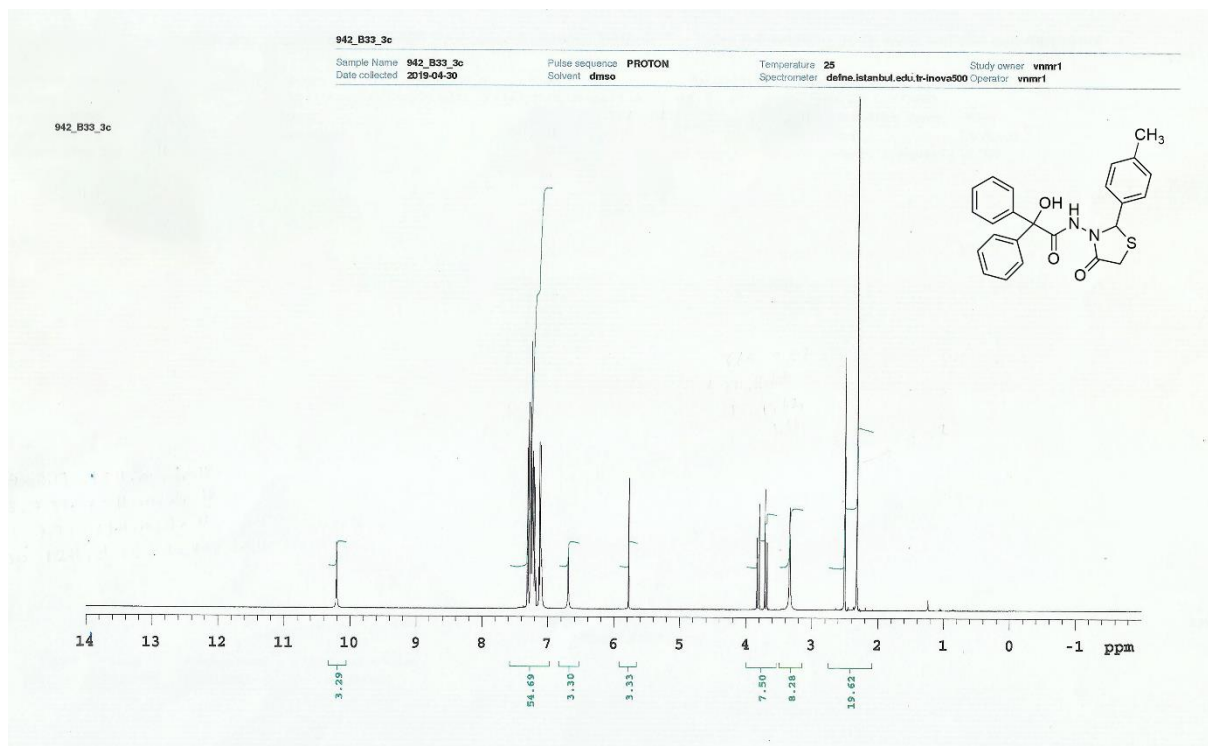


Figure S6: ¹H-NMR (500 MHz, DMSO-*d*₆) Spectrum of Compound **3c**

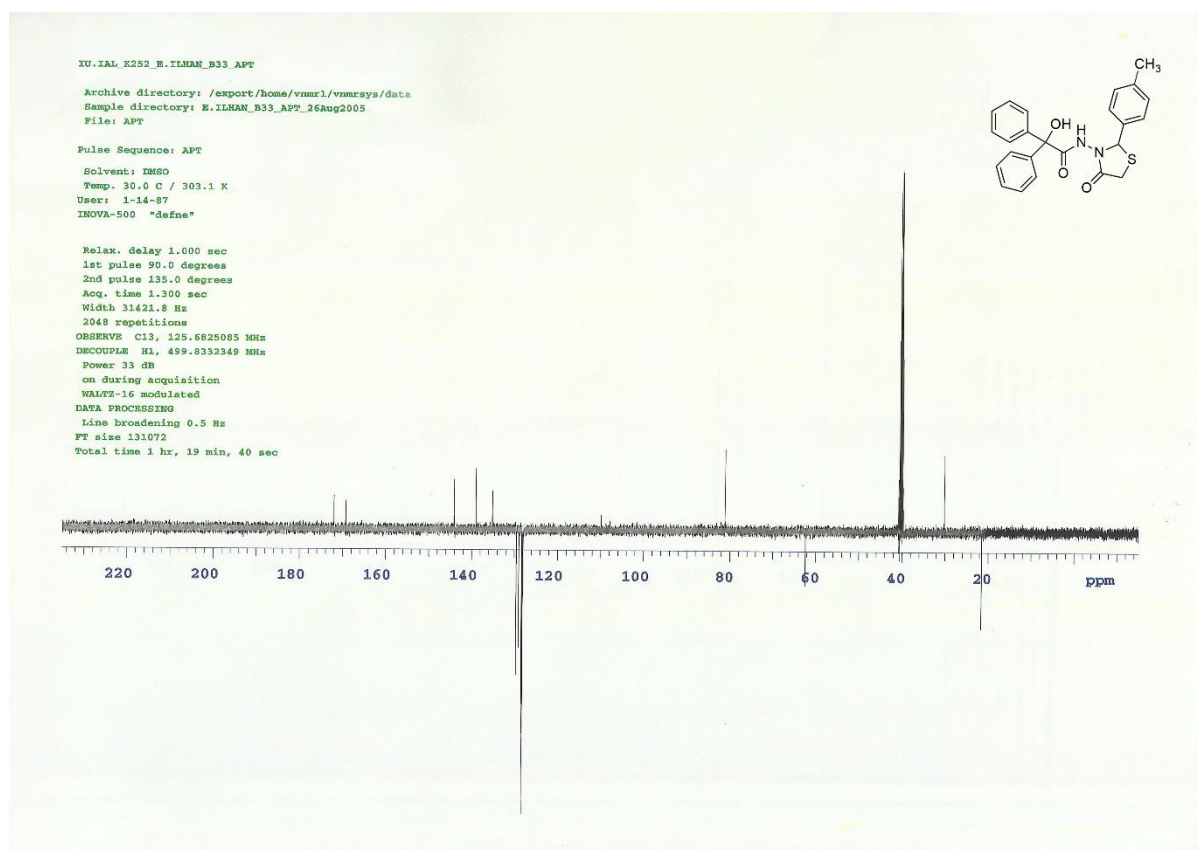


Figure S7: ^{13}C -NMR (125.6 MHz, APT (decoupled)) Spectrum of Compound **3c**

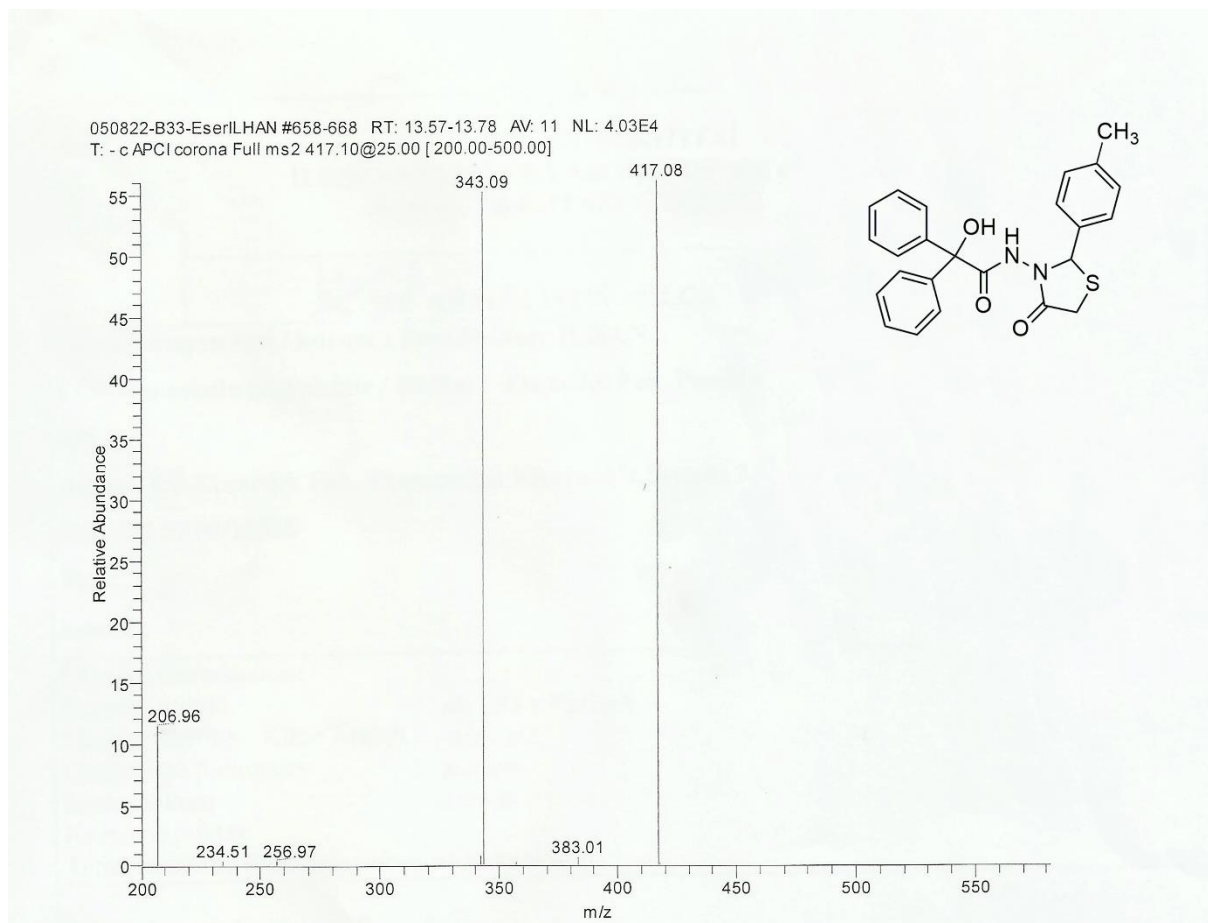


Figure S8: MS-APCI(-) (150 eV, m/z, %) Spectrum of Compound **3c**

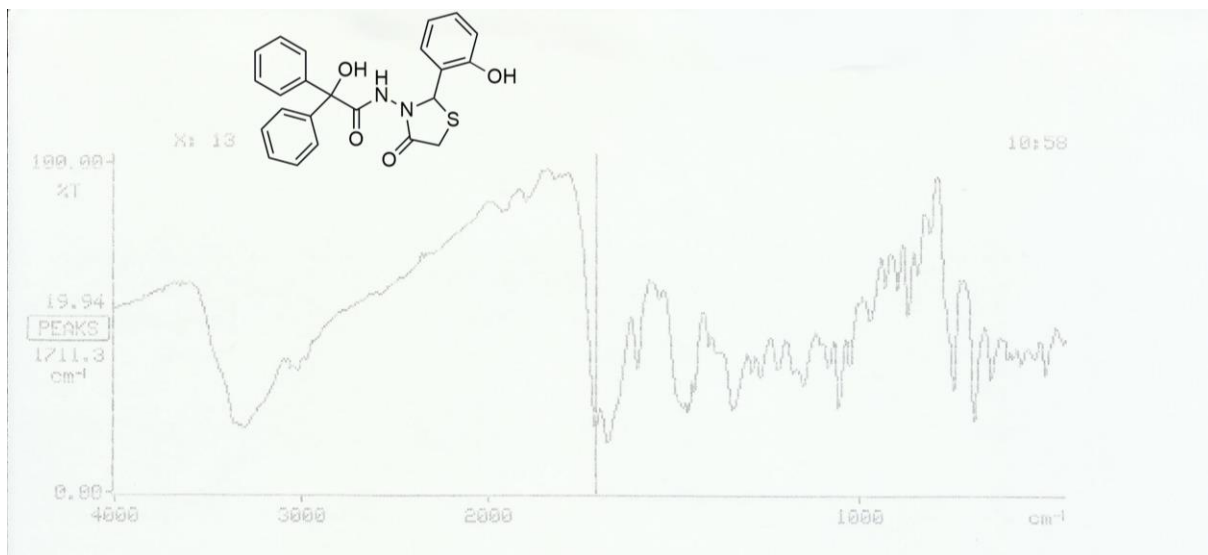


Figure S9: IR (KBr) Spectrum of Compound **3d**

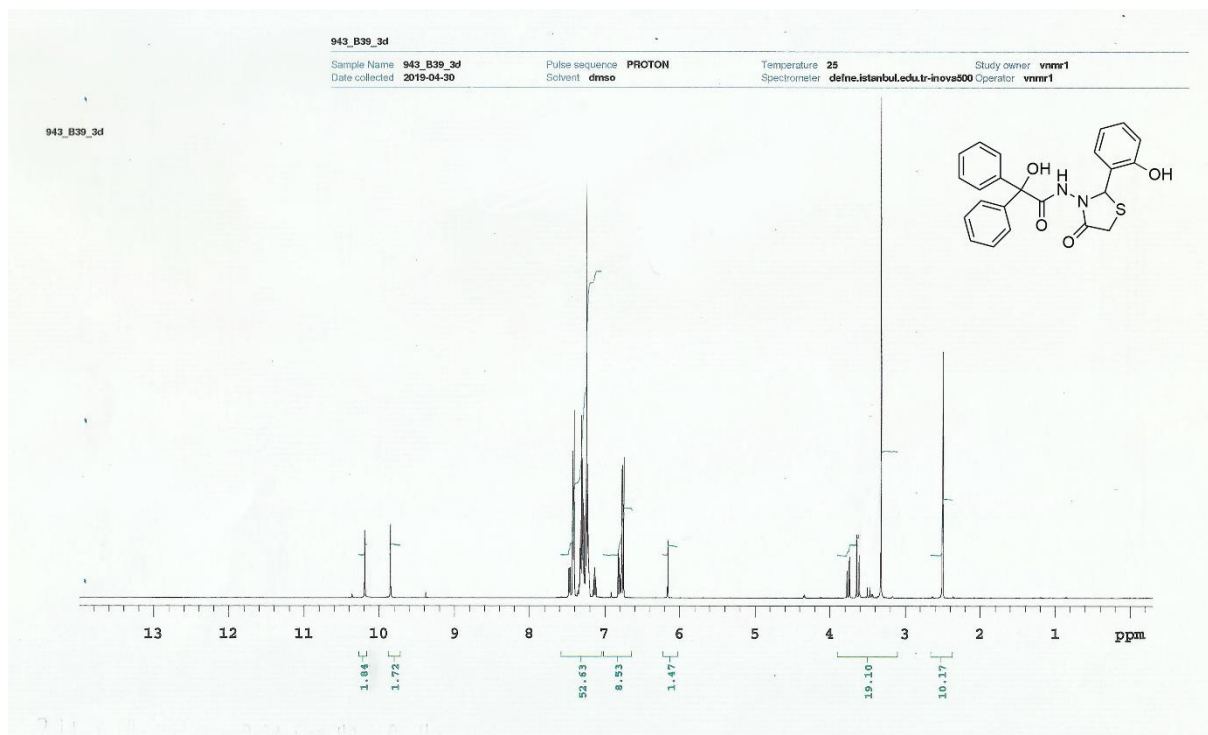


Figure S10: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **3d**

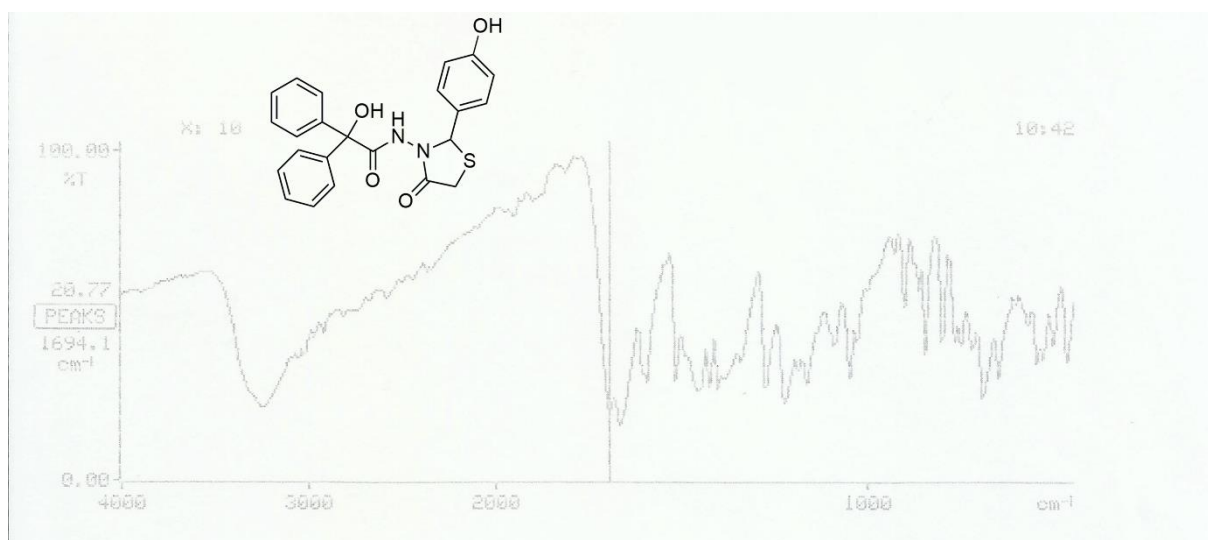


Figure S11: IR (KBr) Spectrum of Compound **3e**

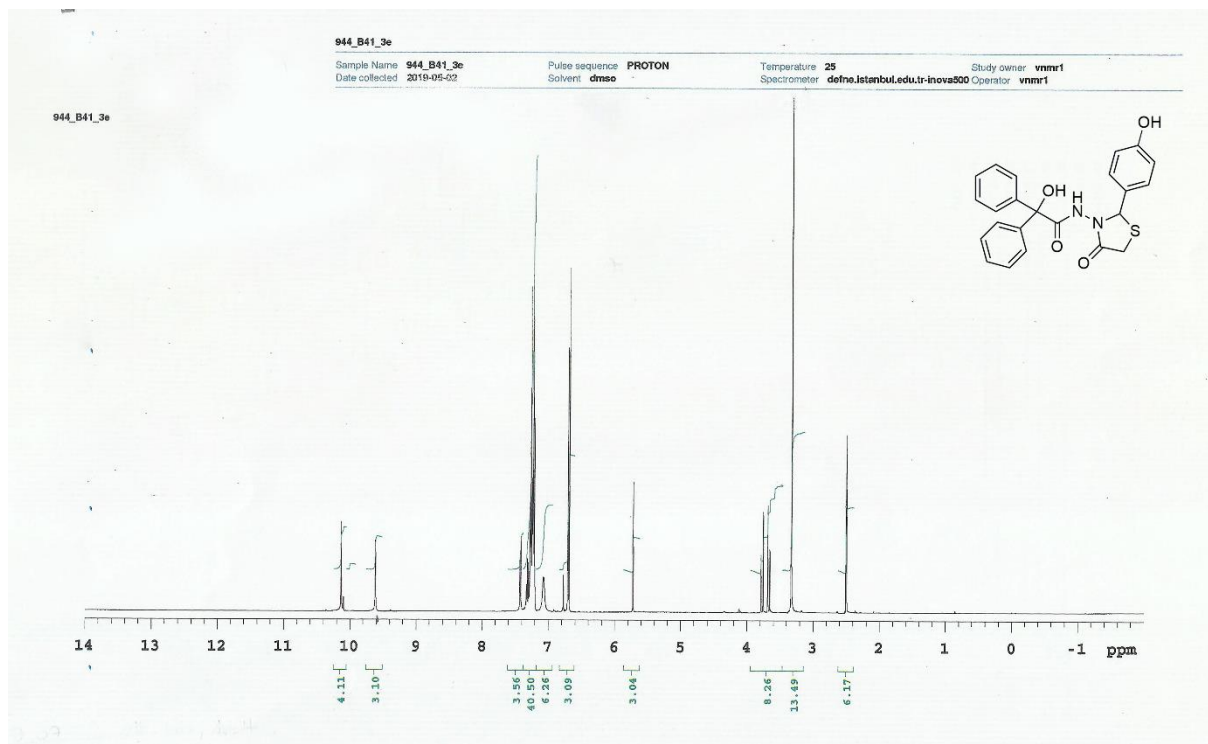


Figure S12: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **3e**

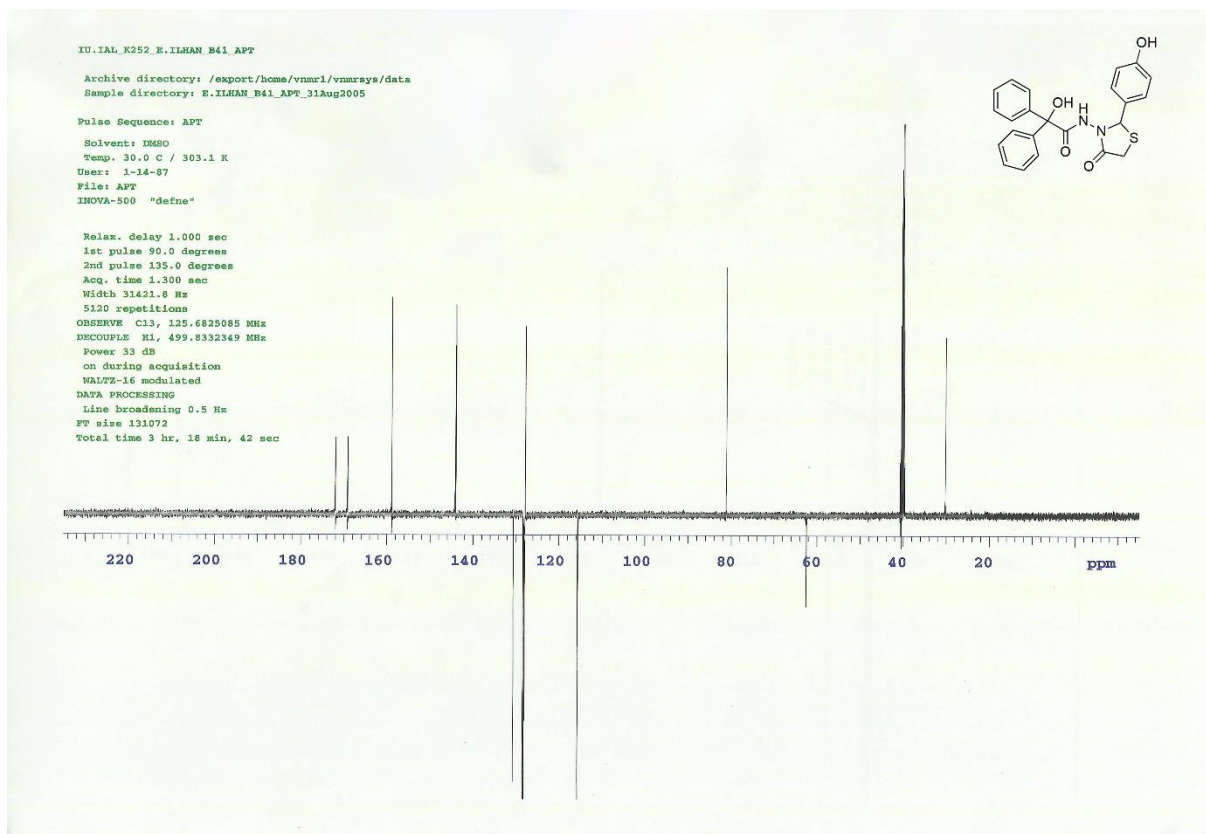


Figure S13: ^{13}C -NMR (125.6 MHz, APT (decoupled)) Spectrum of Compound **3e**

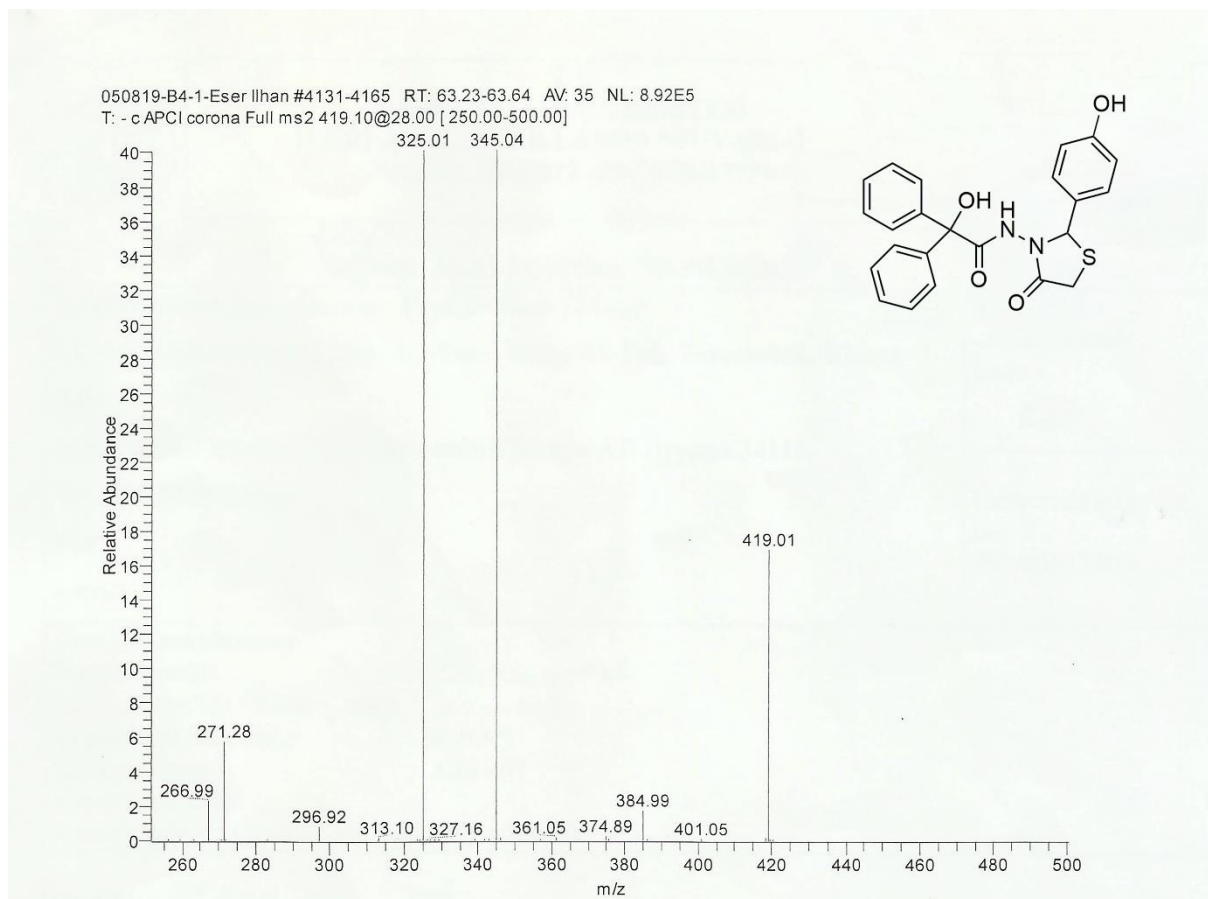


Figure S14: MS-APCI(-) (150 eV, m/z, %) Spectrum of Compound **3e**

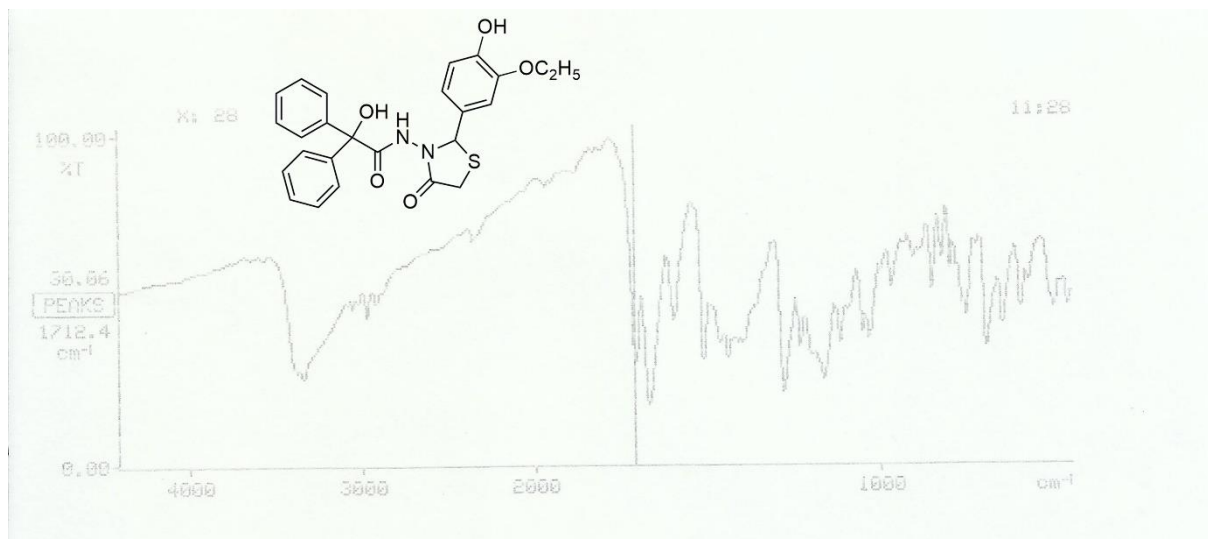


Figure S15: IR (KBr) Spectrum of Compound **3f**

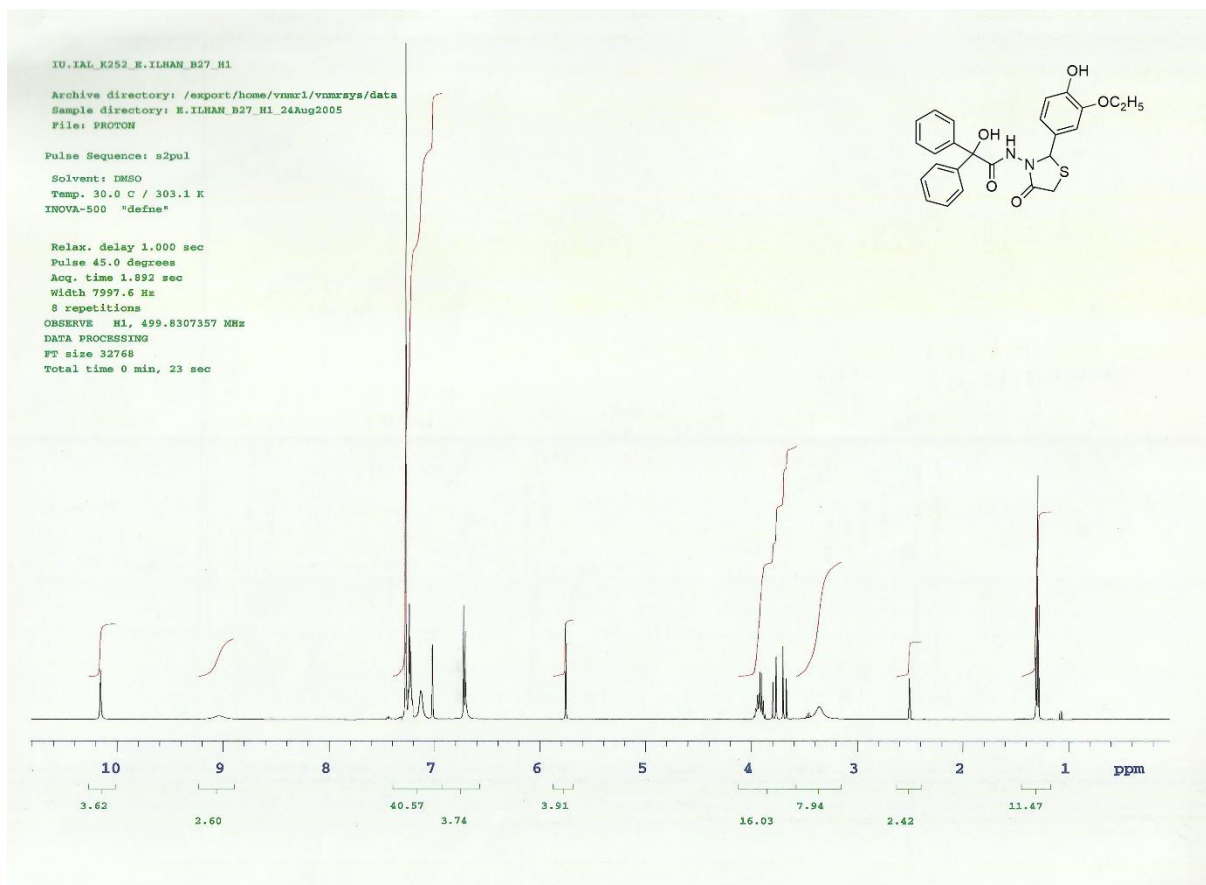


Figure S16: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **3f**

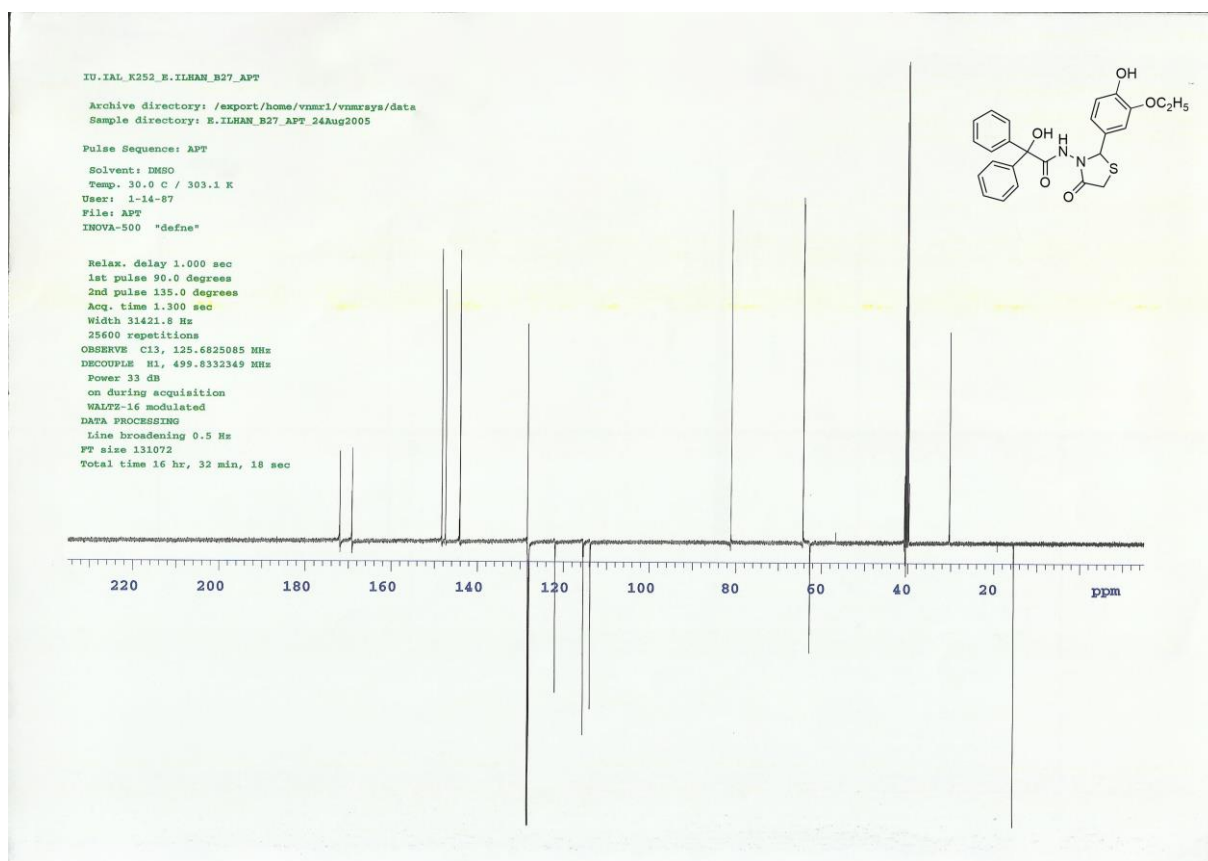


Figure S17: ^{13}C -NMR (125.6 MHz, APT (decoupled)) Spectrum of Compound **3f**

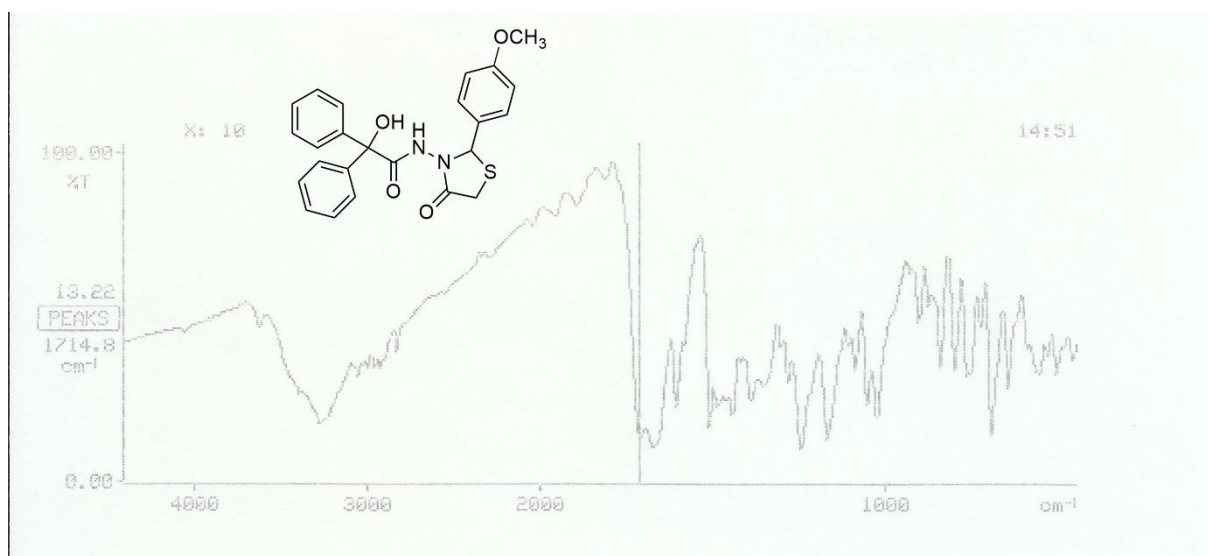


Figure S18: IR (KBr) Spectrum of Compound **3g**

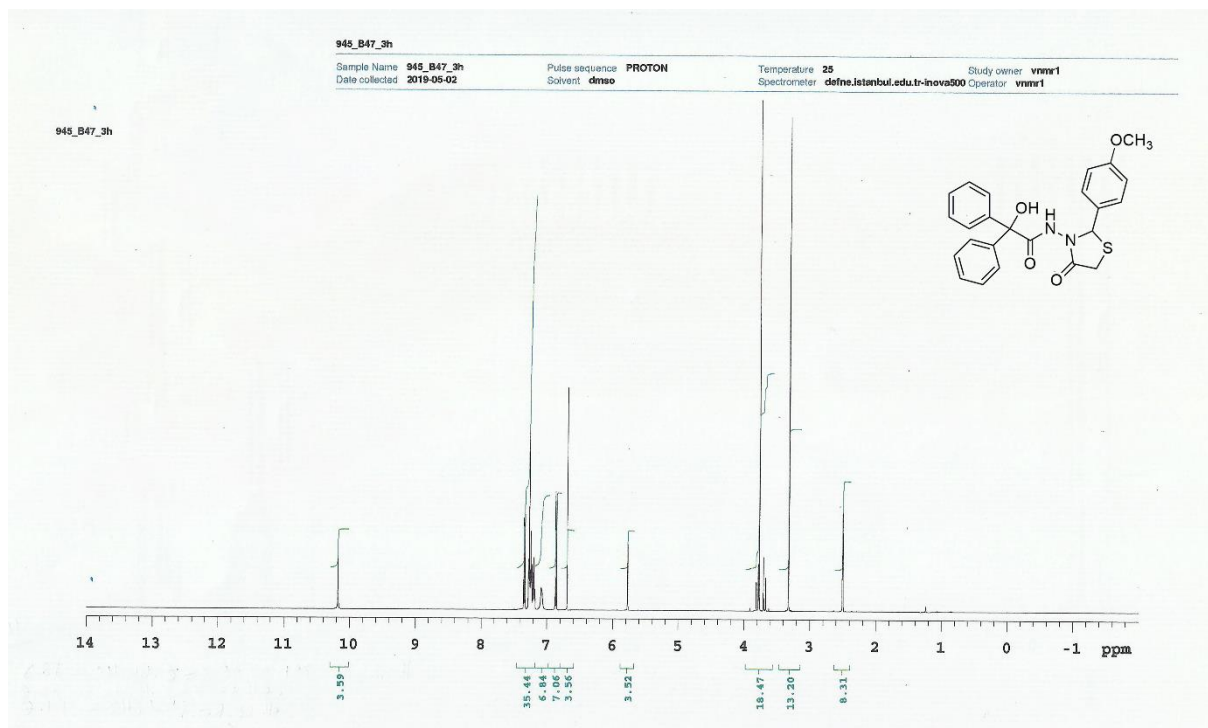


Figure S19: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **3g**

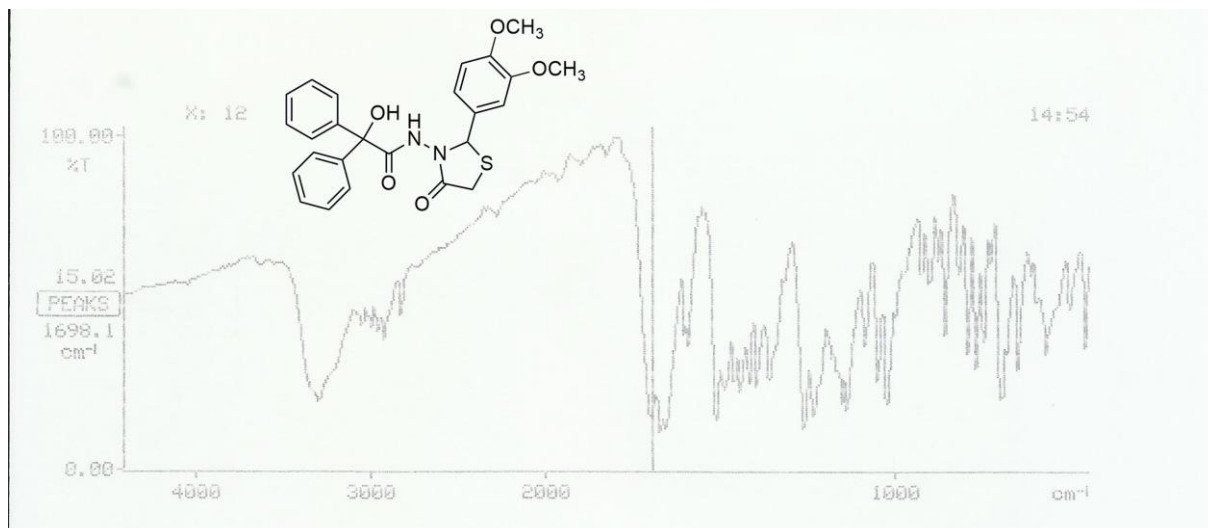


Figure S20: IR (KBr) Spectrum of Compound **3h**

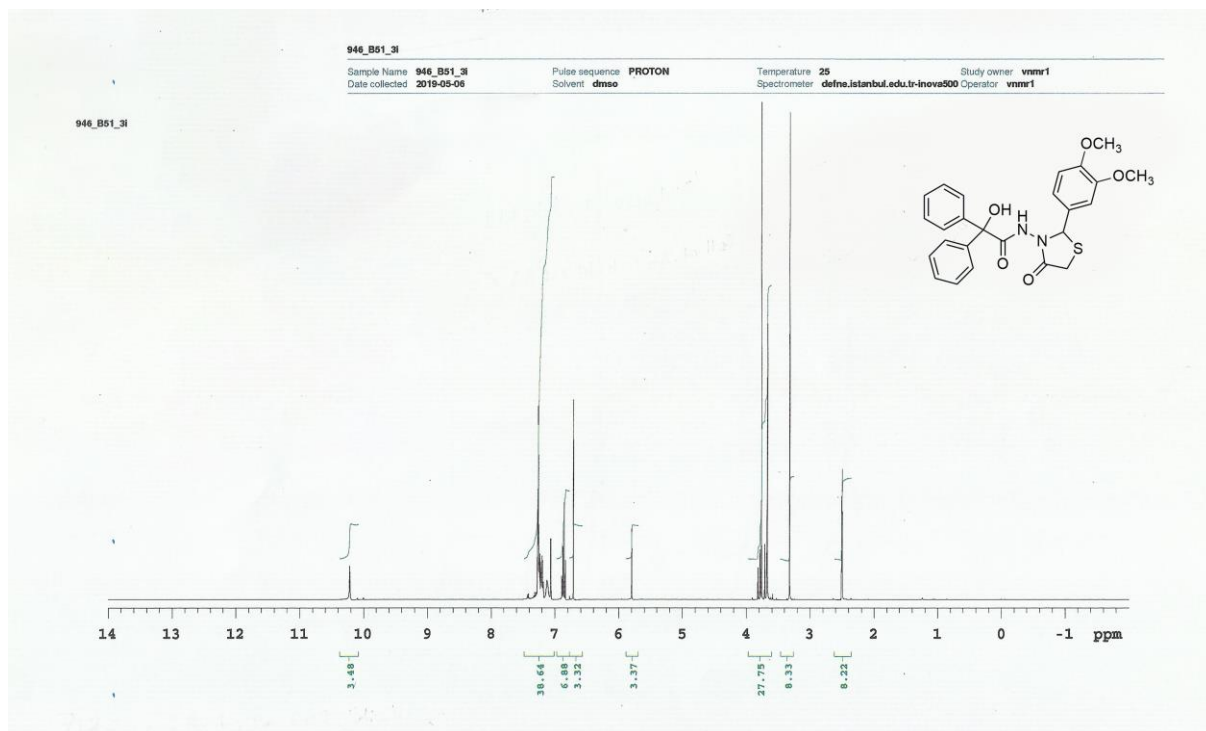


Figure S21: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **3h**

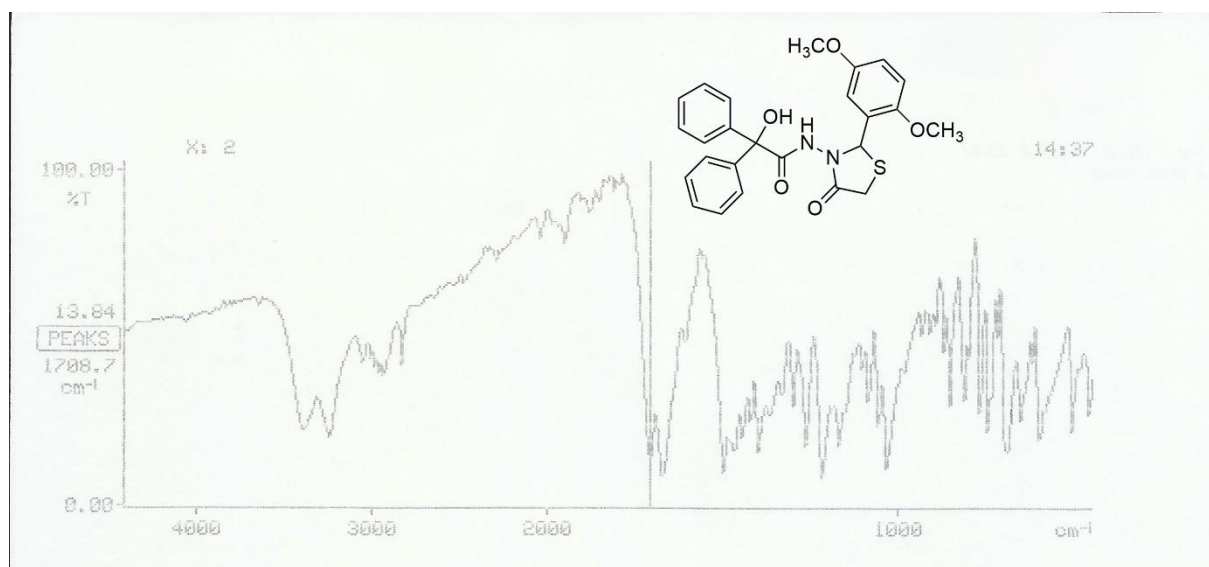


Figure S22: IR (KBr) Spectrum of Compound **3i**

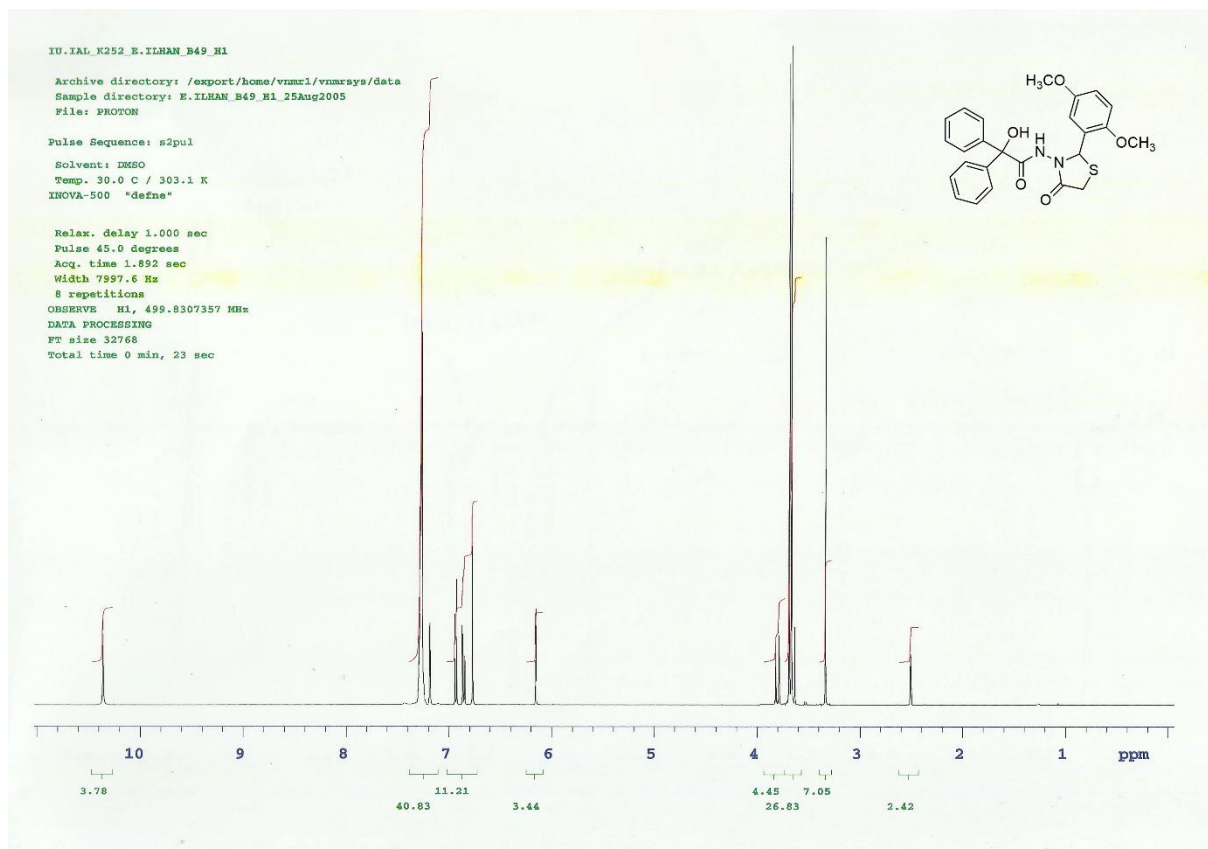


Figure S23: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **3i**

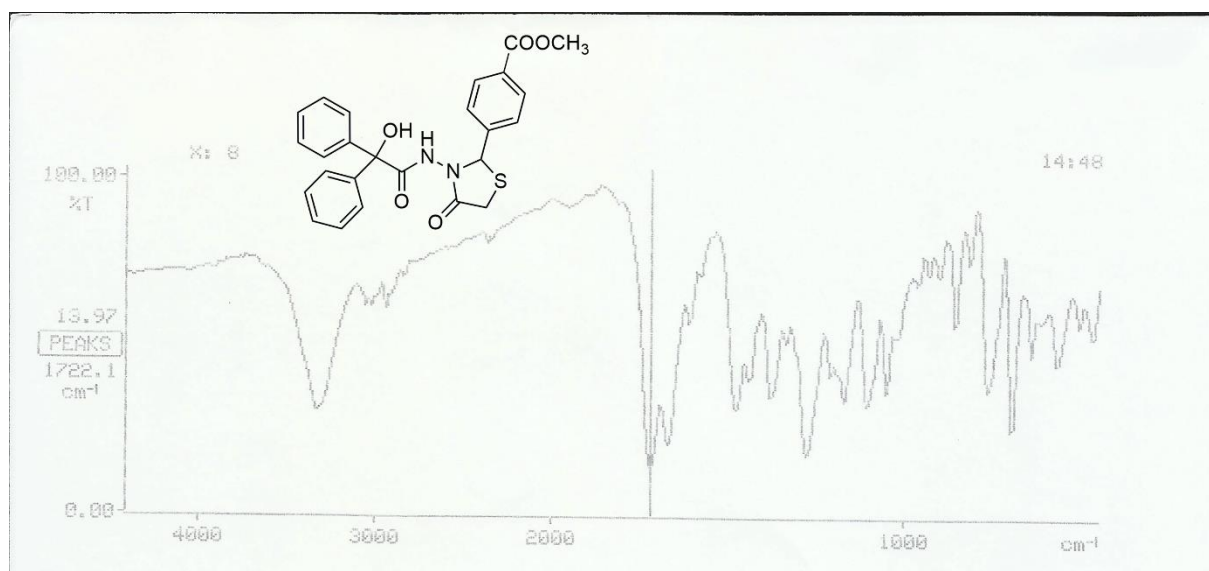


Figure S24: IR (KBr) Spectrum of Compound 3j

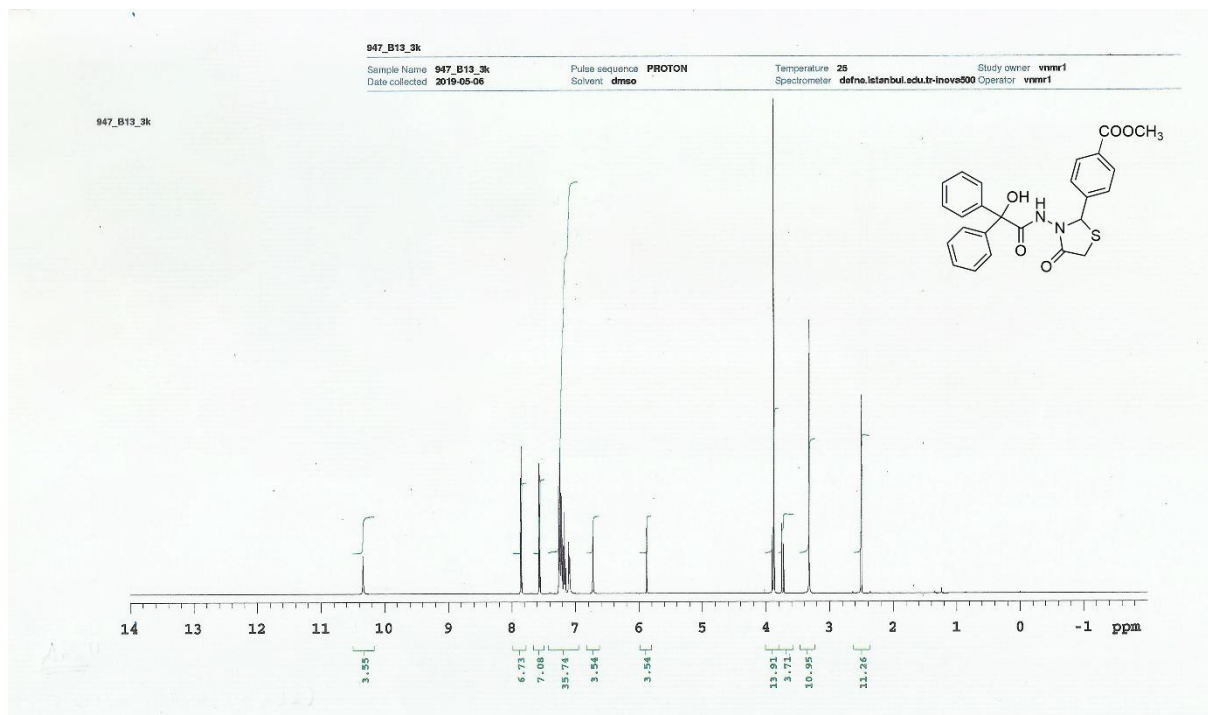


Figure S25: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **3j**

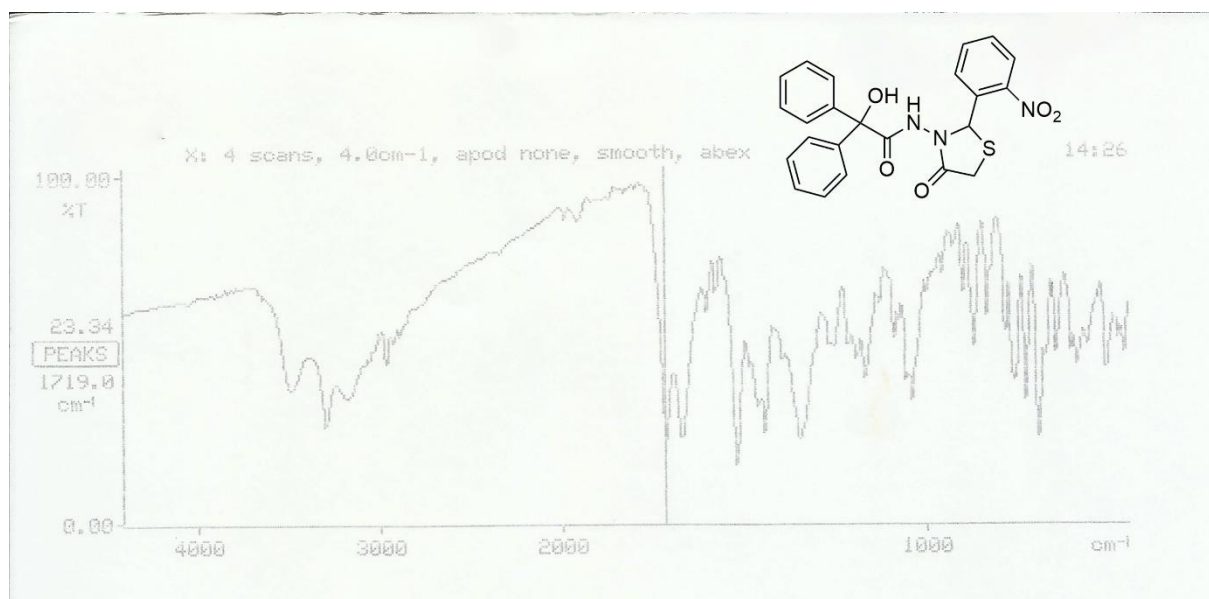


Figure S26: IR (KBr) Spectrum of Compound **3k**

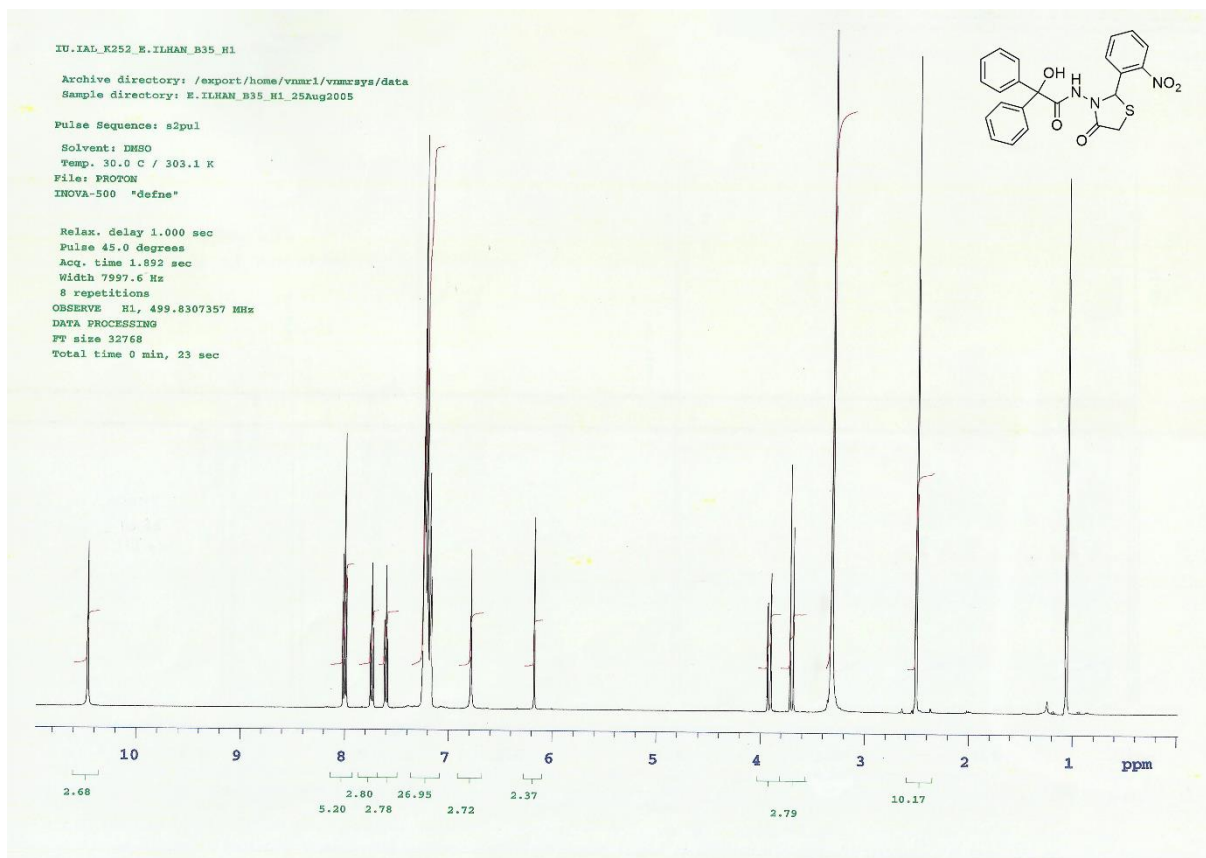


Figure S27: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **3k**

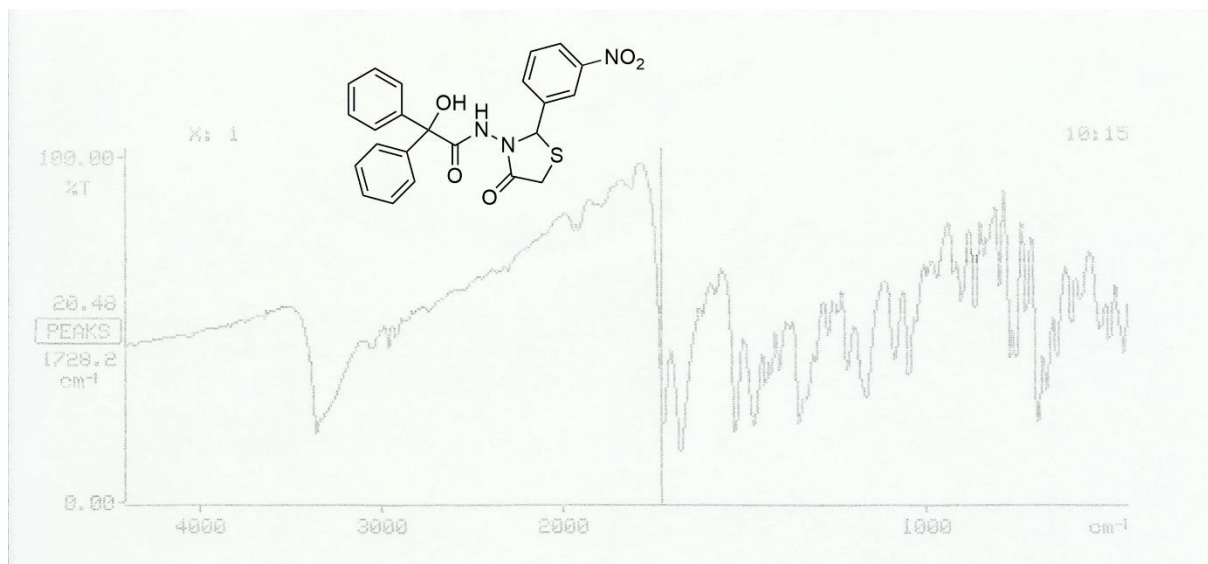


Figure S28: IR (KBr) Spectrum of Compound 31

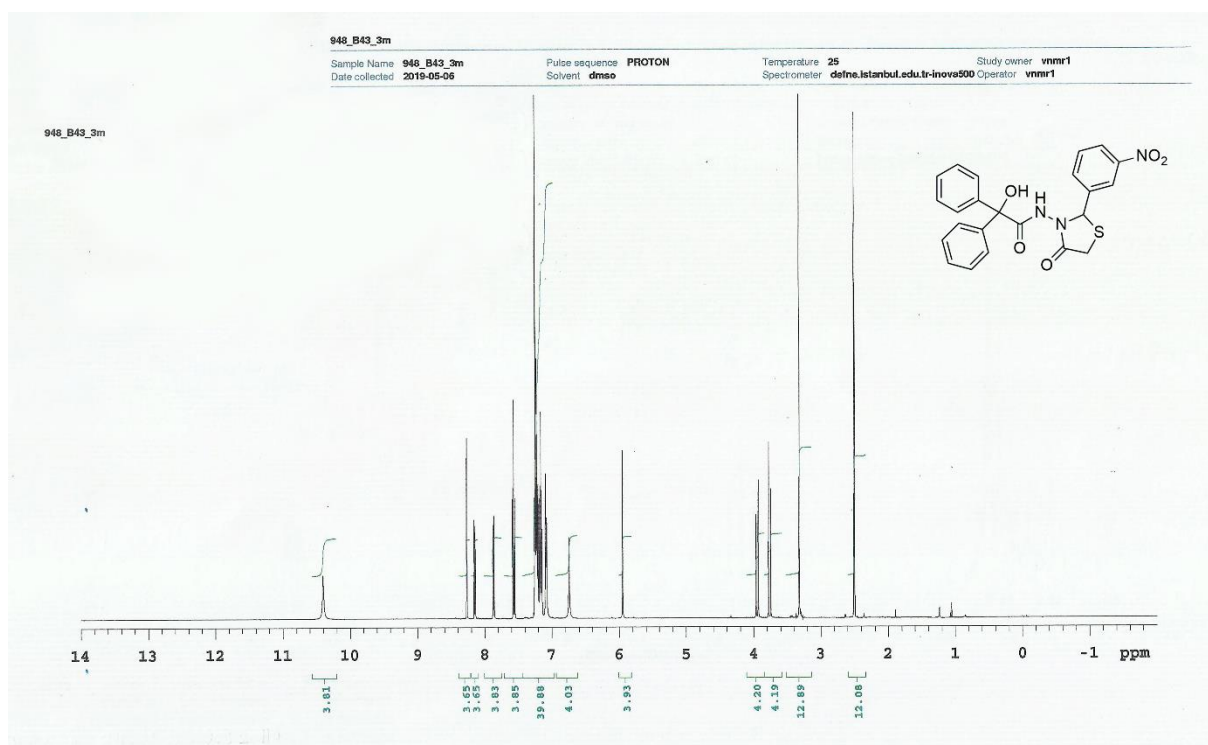


Figure S29: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **31**

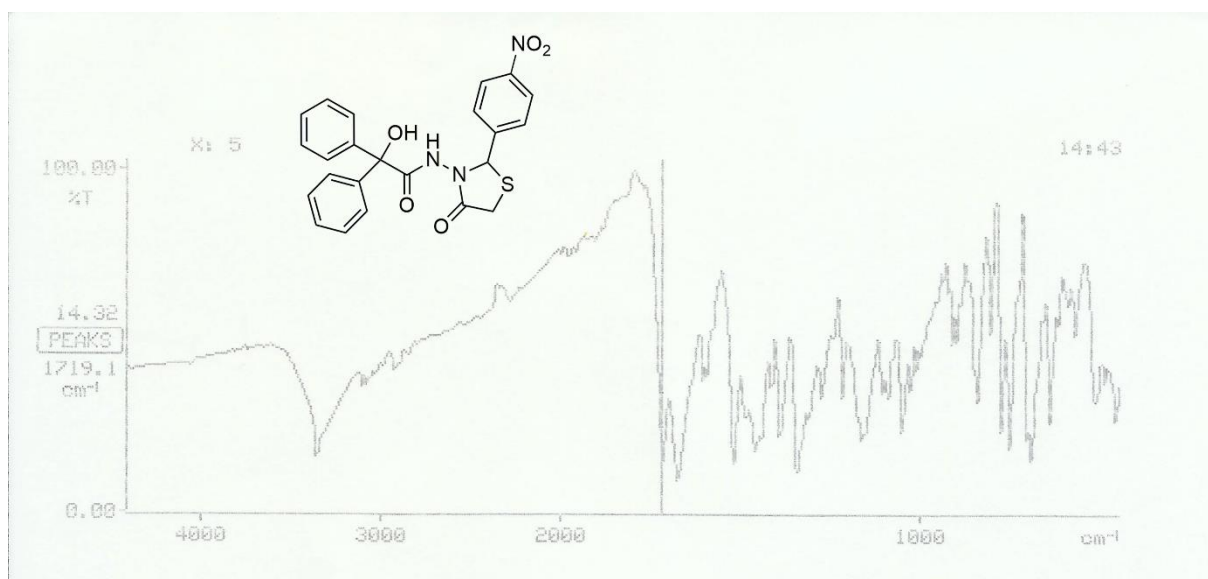


Figure S30: IR (KBr) Spectrum of Compound **3m**

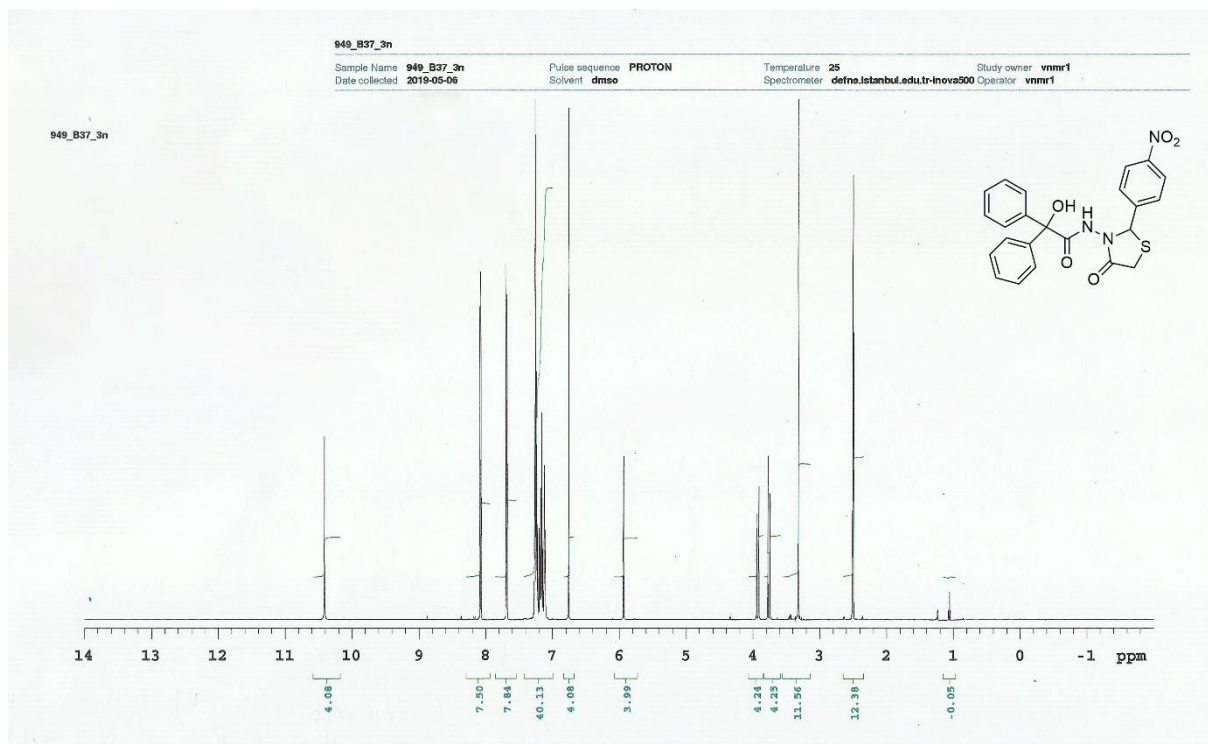


Figure S31: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **3m**

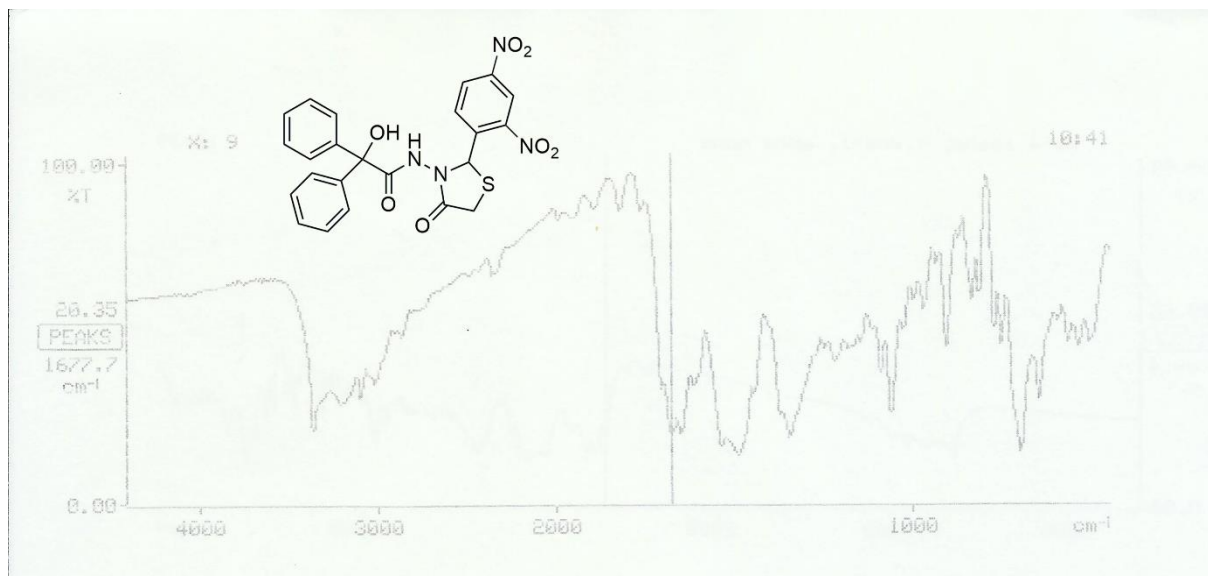


Figure S32: IR (KBr) Spectrum of Compound **3n**

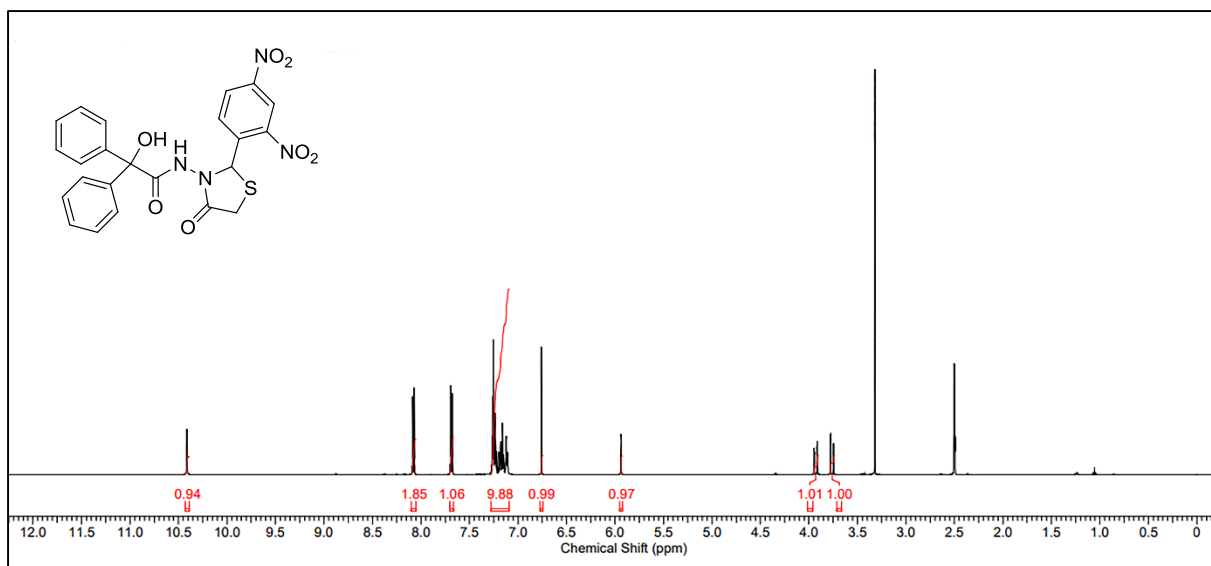


Figure S33: ¹H-NMR (500 MHz, DMSO-*d*₆) Spectrum of Compound 3n

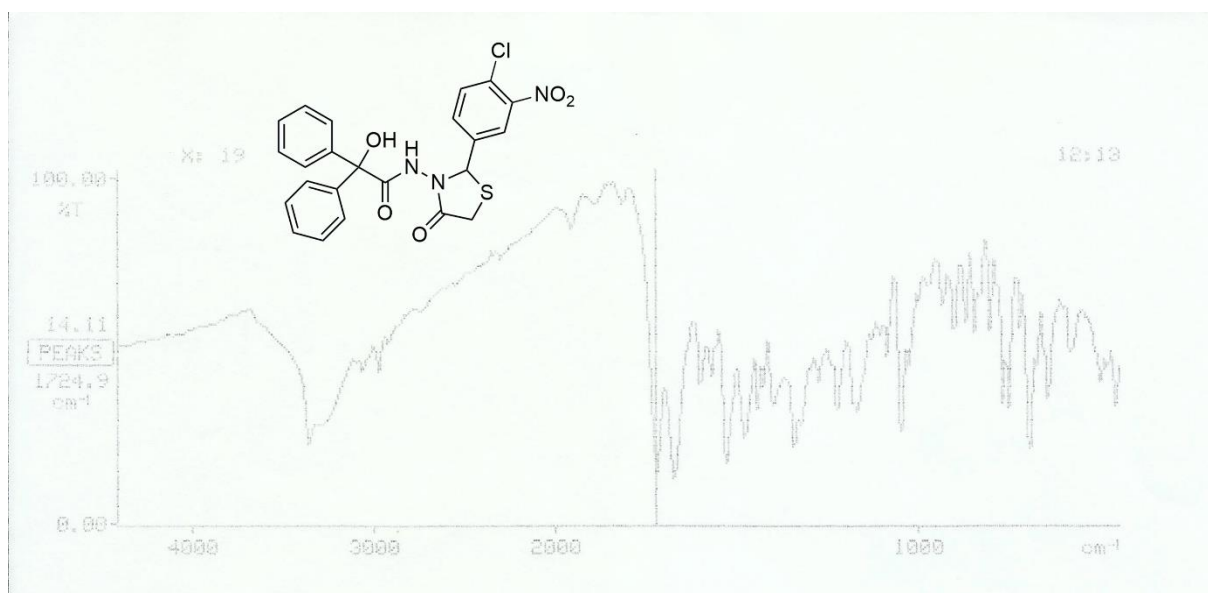


Figure S34: IR (KBr) Spectrum of Compound **30**

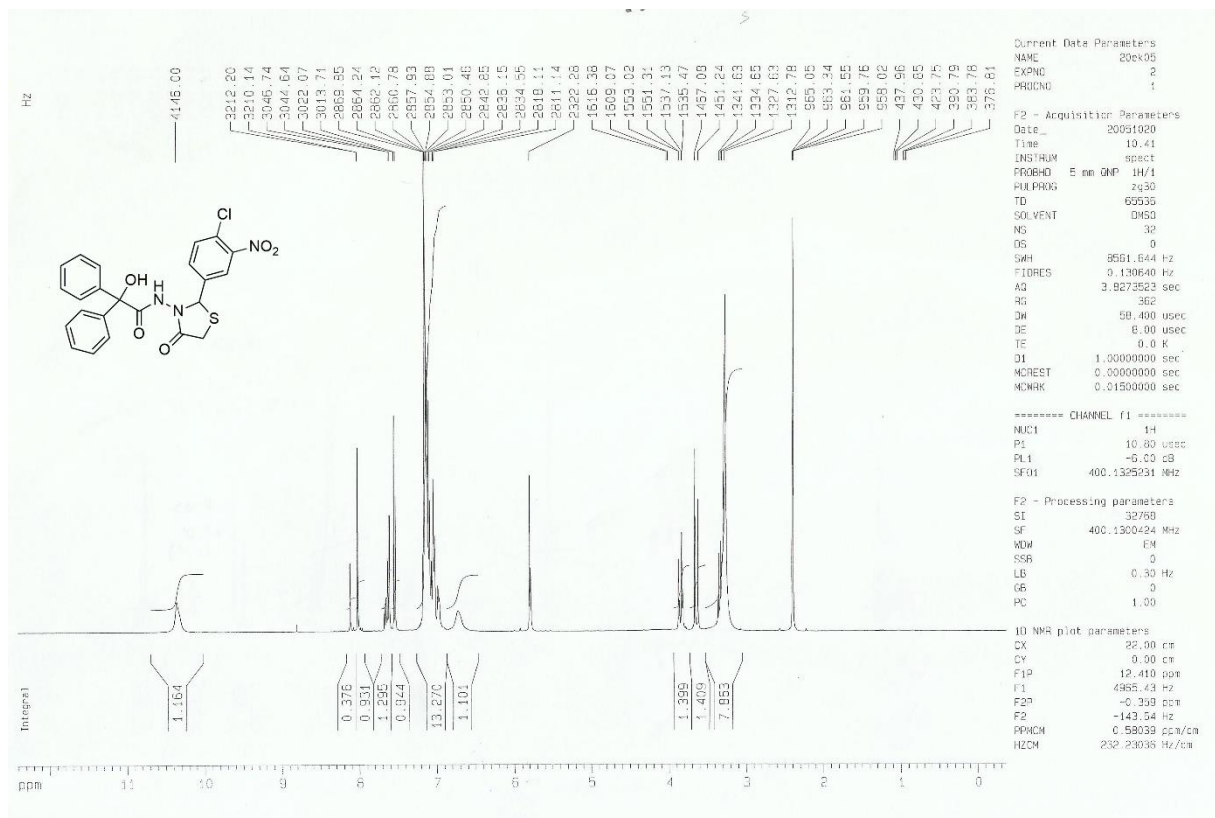


Figure S35: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound 3o

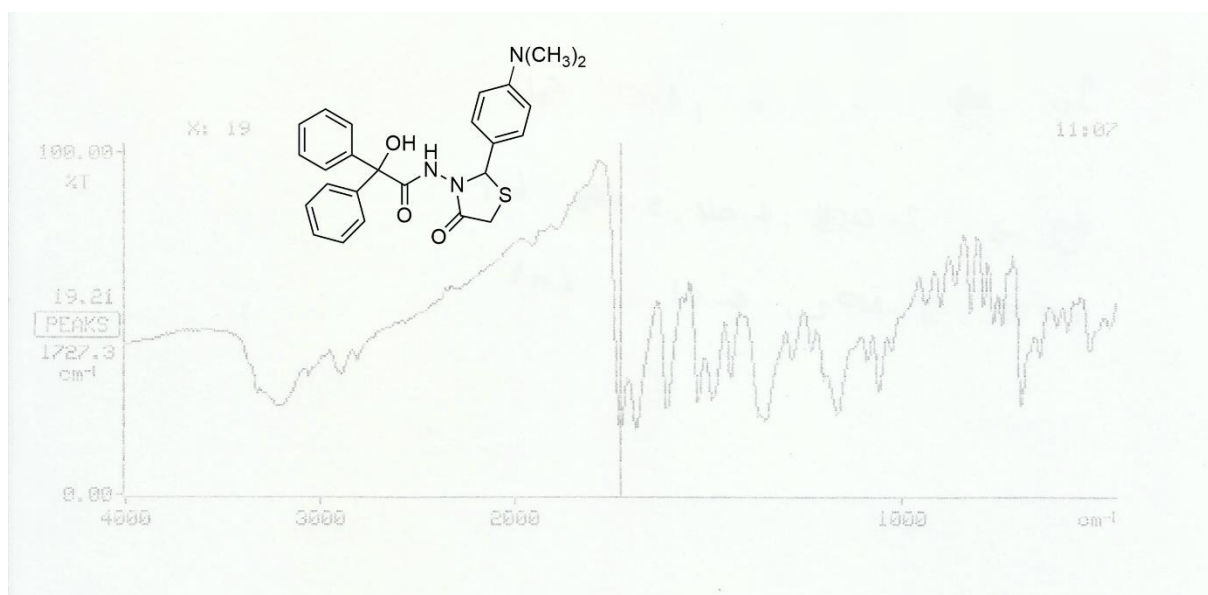


Figure S36: IR (KBr) Spectrum of Compound **3p**

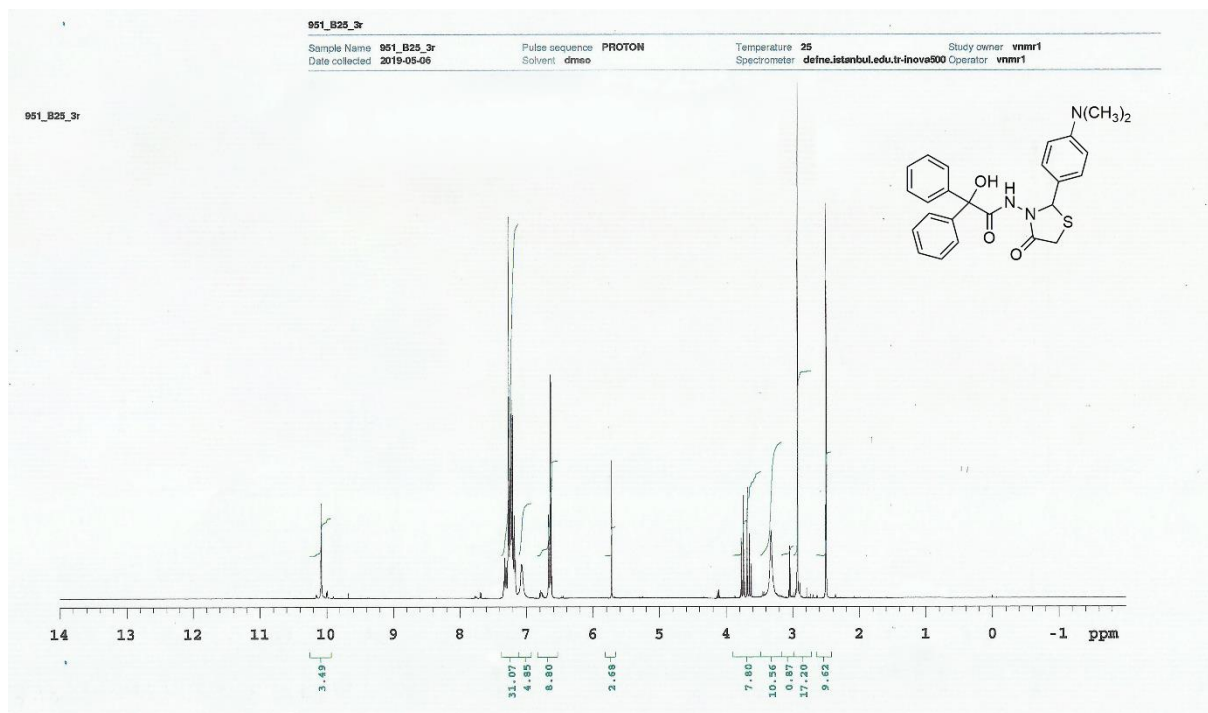


Figure S37: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **3p**

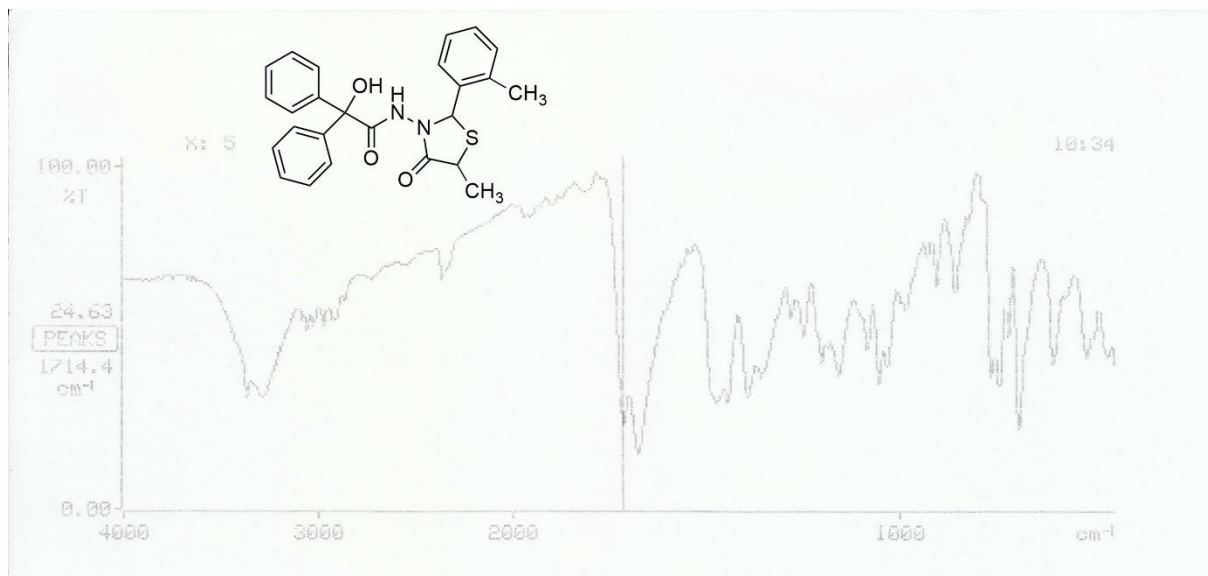


Figure S38: IR (KBr) Spectrum of Compound **4a**

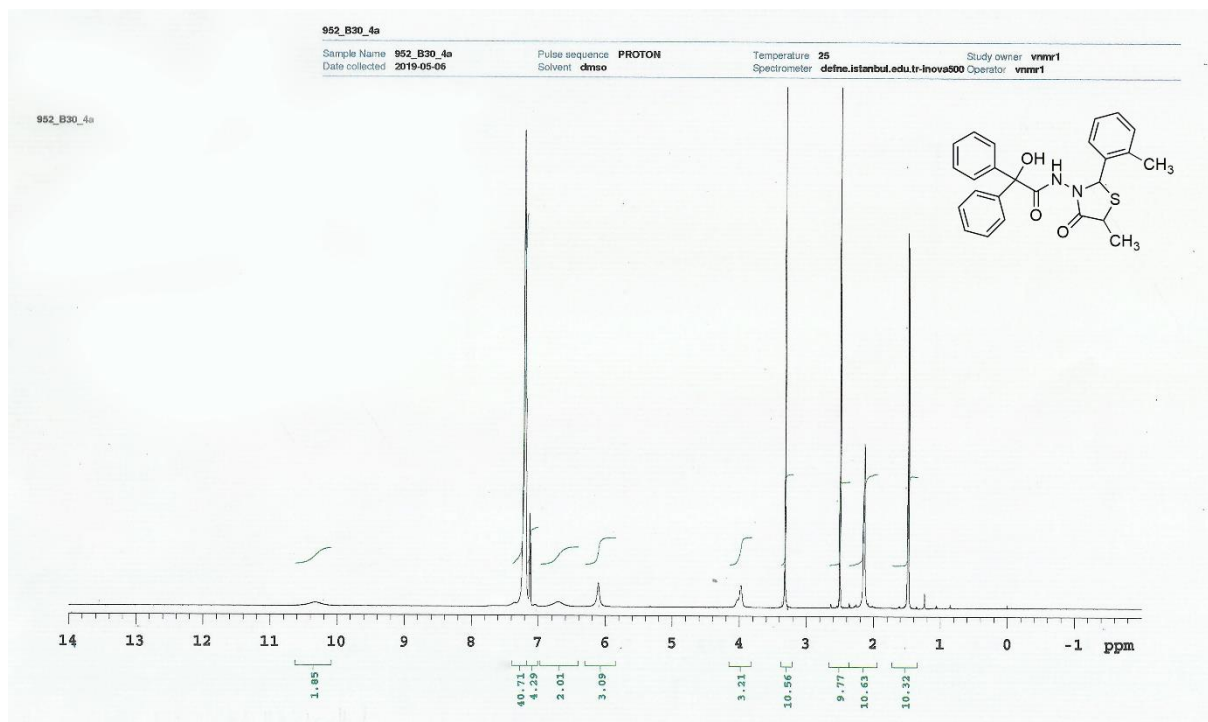


Figure S39: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4a**

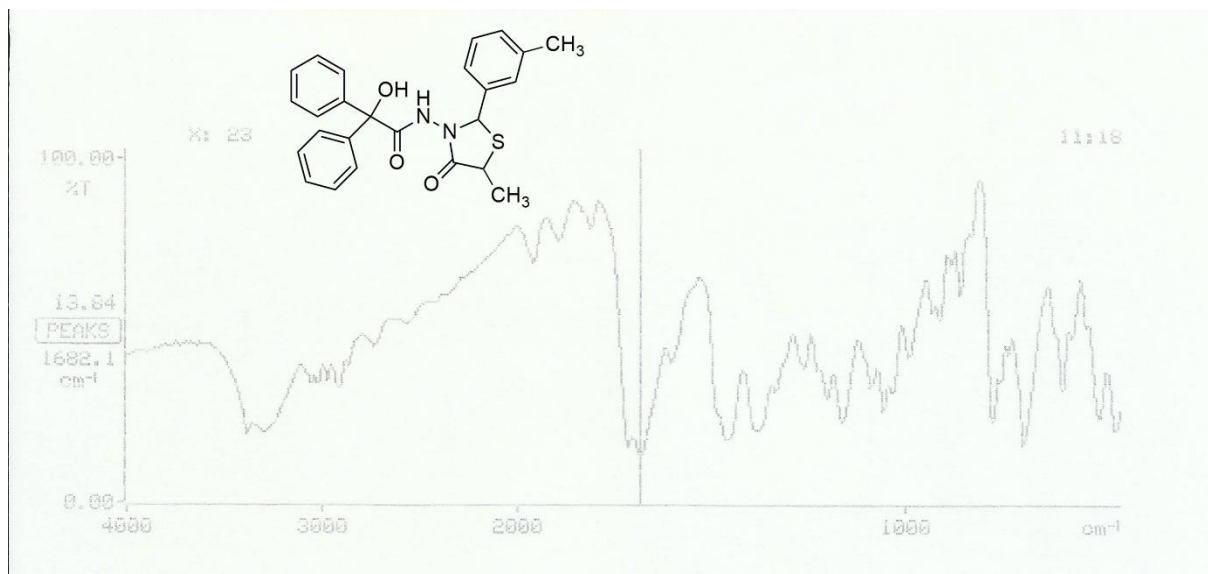


Figure S40: IR (KBr) Spectrum of Compound **4b**

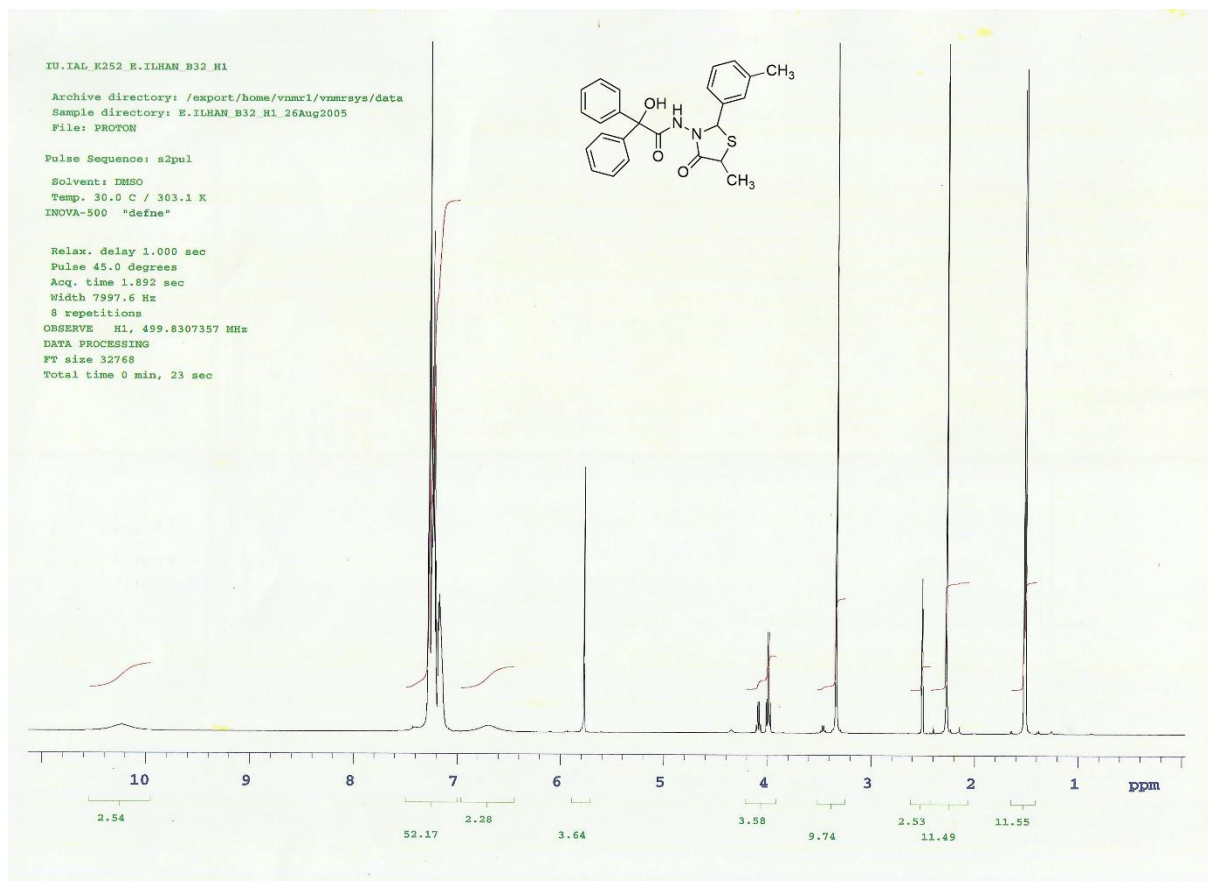


Figure S41: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4b**

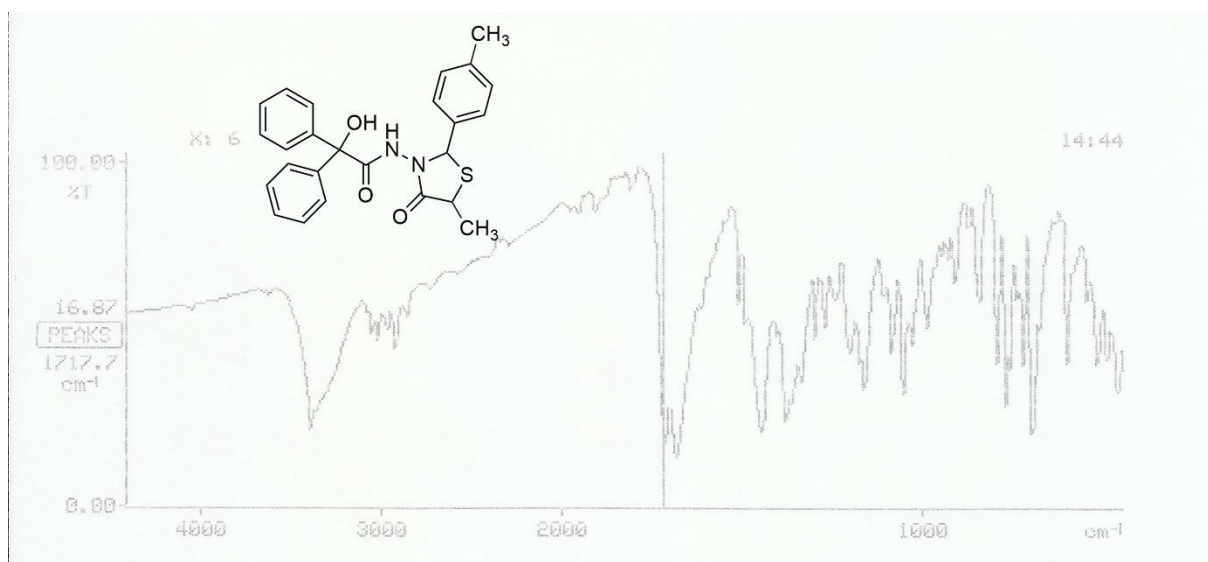


Figure S42: IR (KBr) Spectrum of Compound **4c**

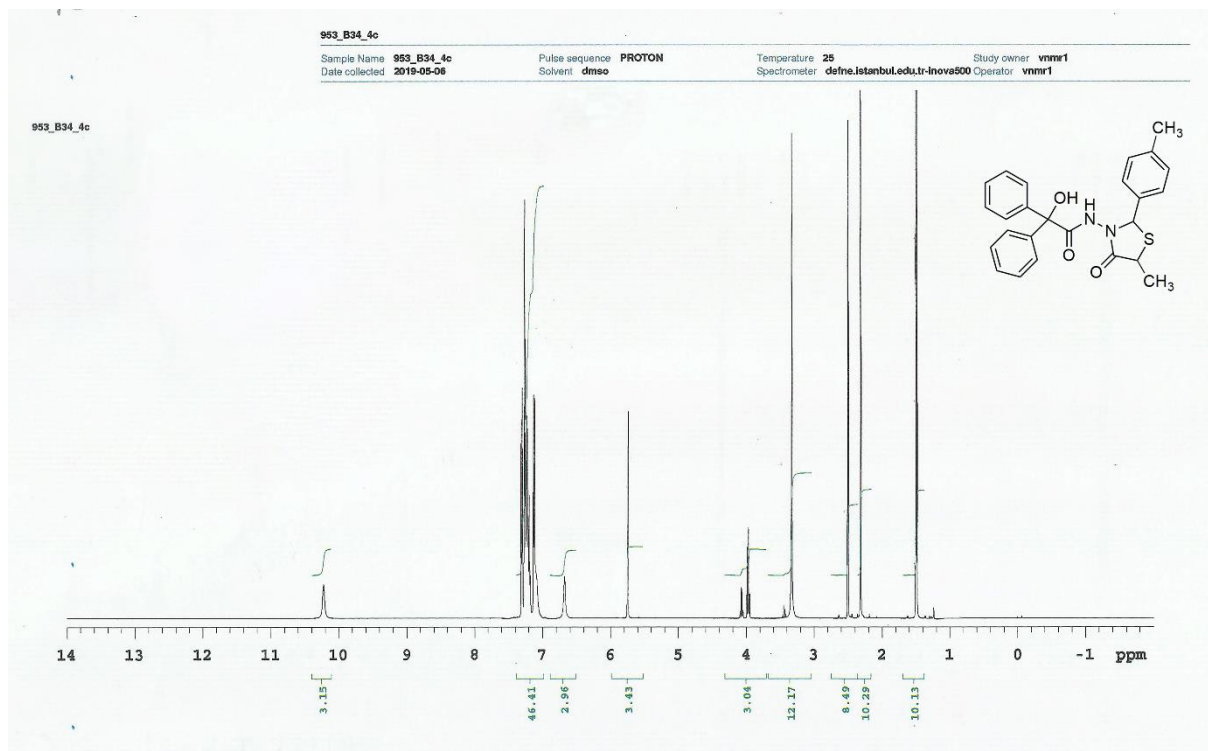


Figure S43: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4c**

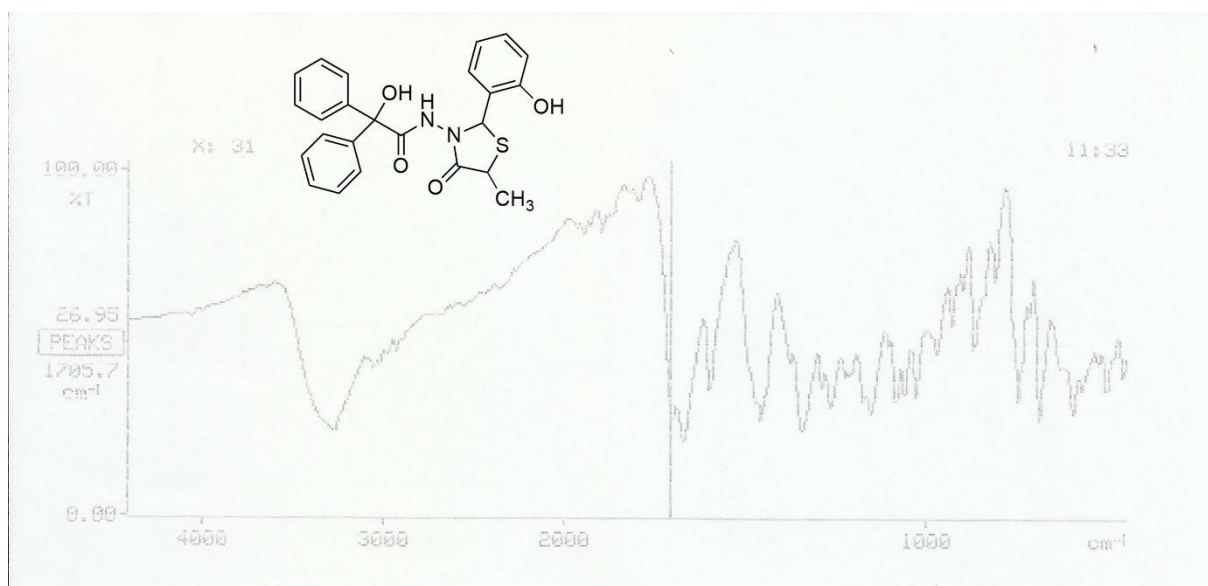


Figure S44: IR (KBr) Spectrum of Compound **4d**

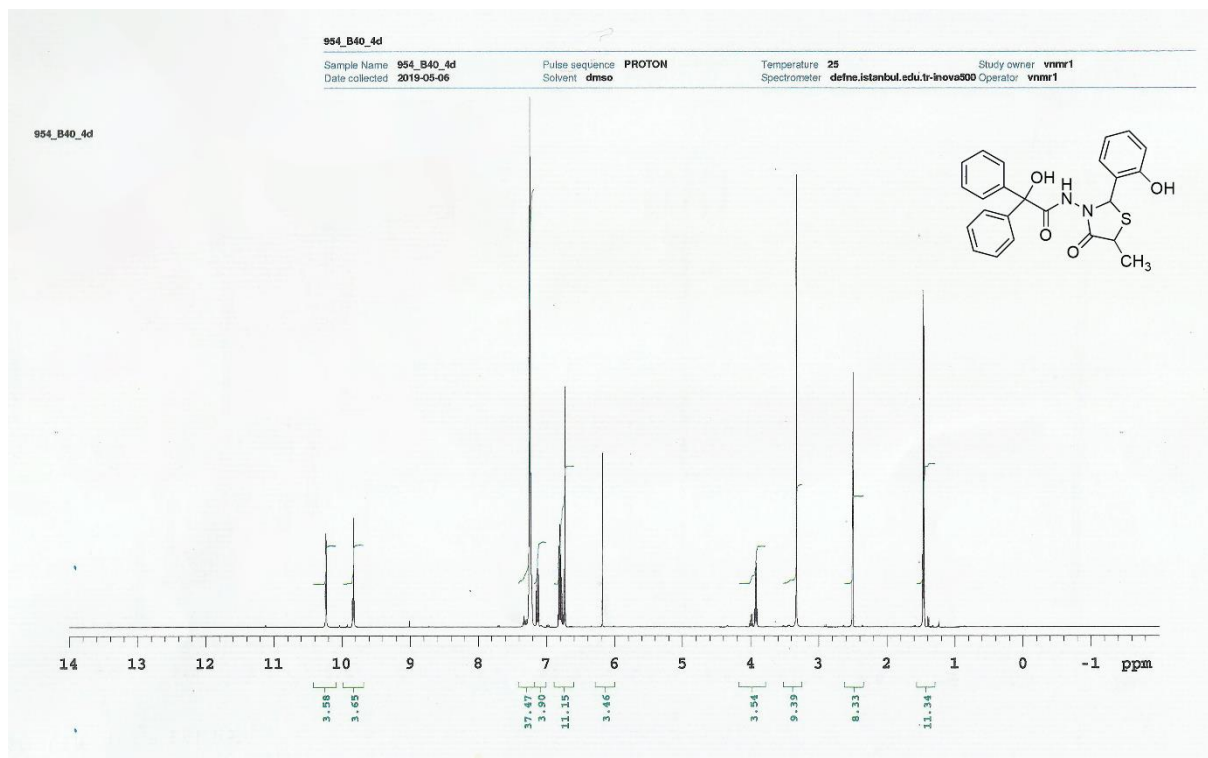


Figure S45: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4d**

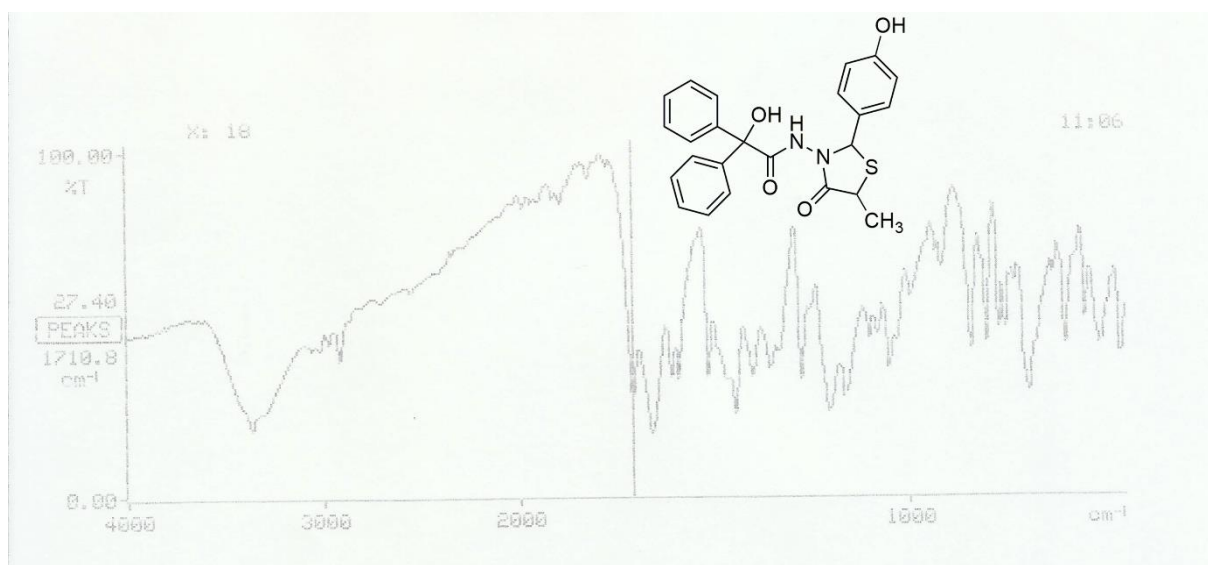


Figure S46: IR (KBr) Spectrum of Compound **4e**

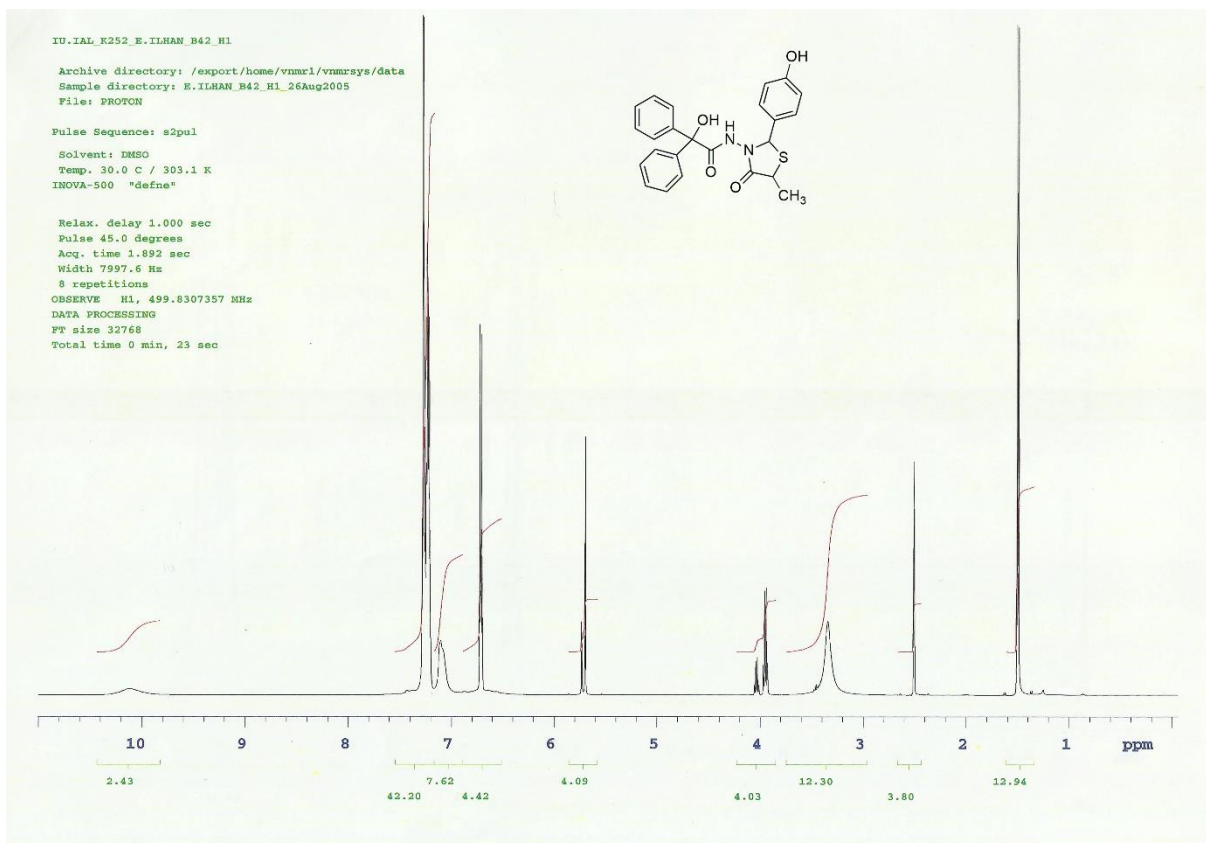


Figure S47: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4e**

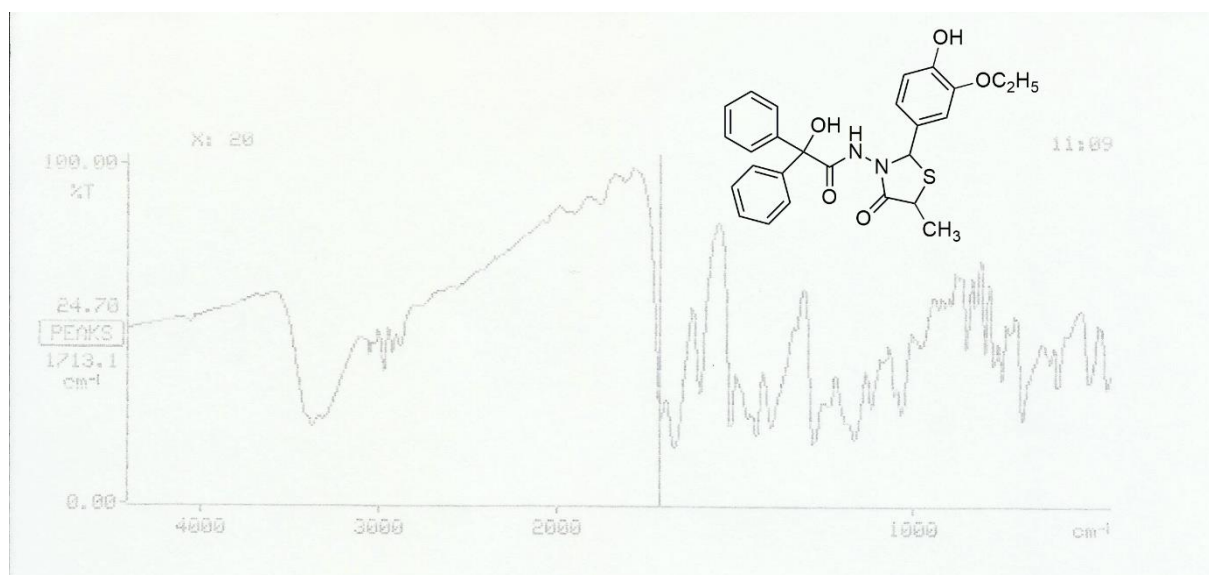


Figure S48: IR (KBr) Spectrum of Compound **4f**

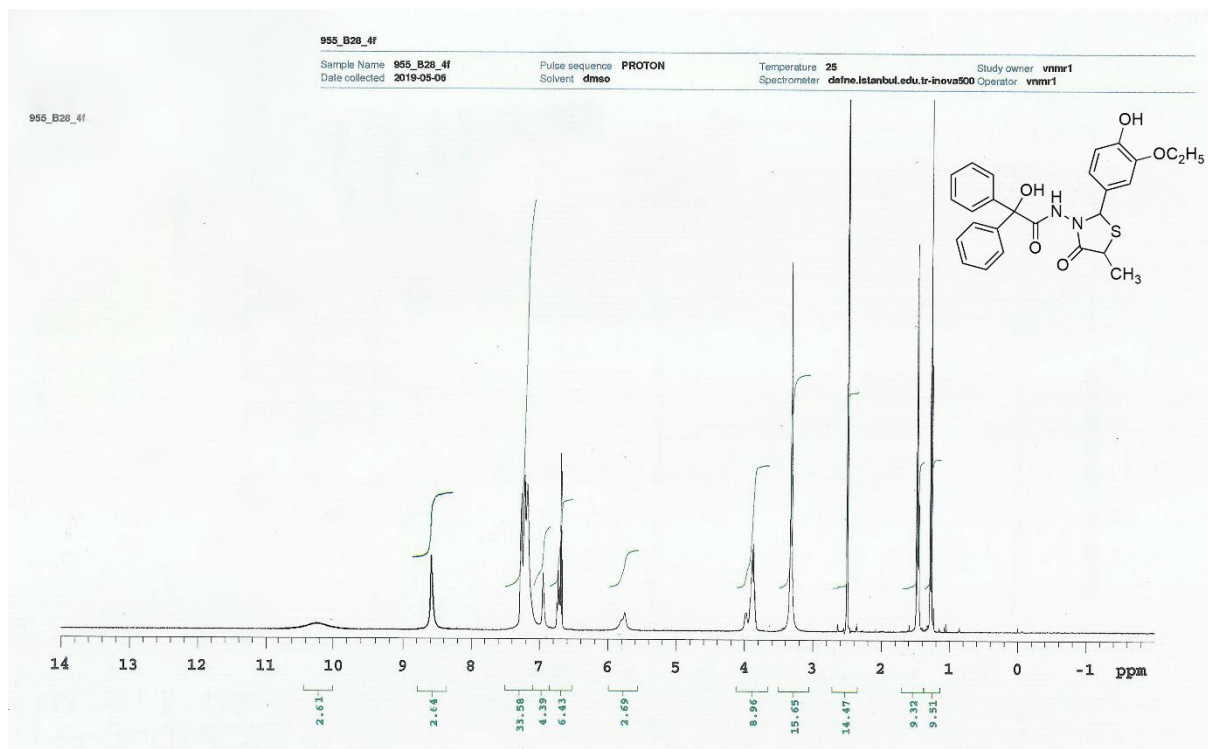


Figure S49: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4f**

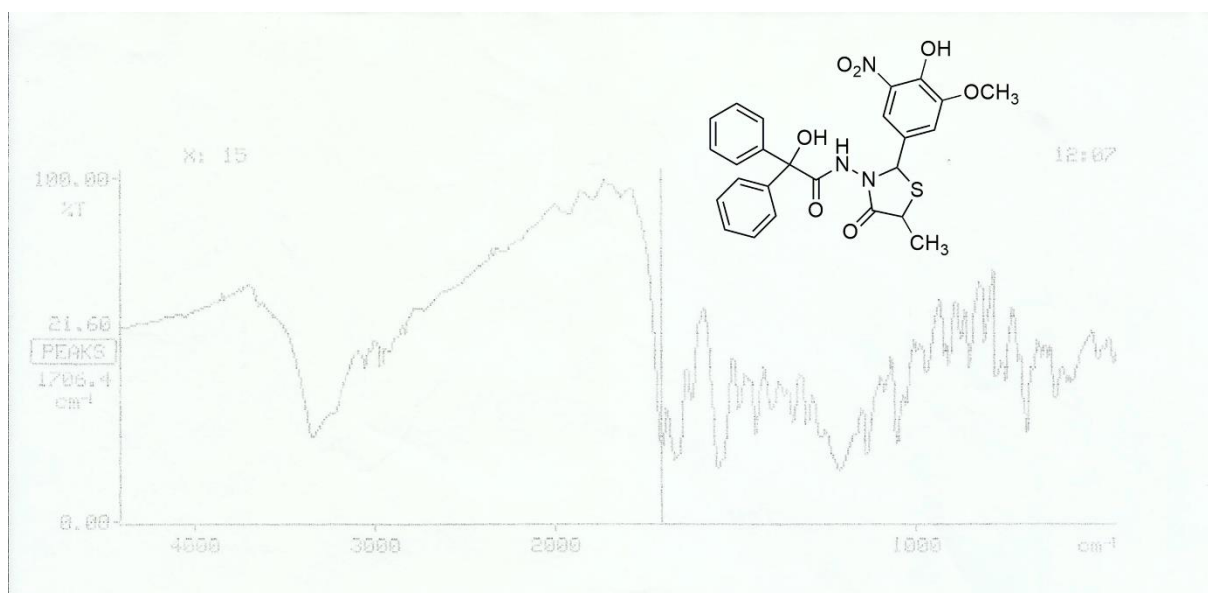


Figure S50: IR (KBr) Spectrum of Compound **4g**

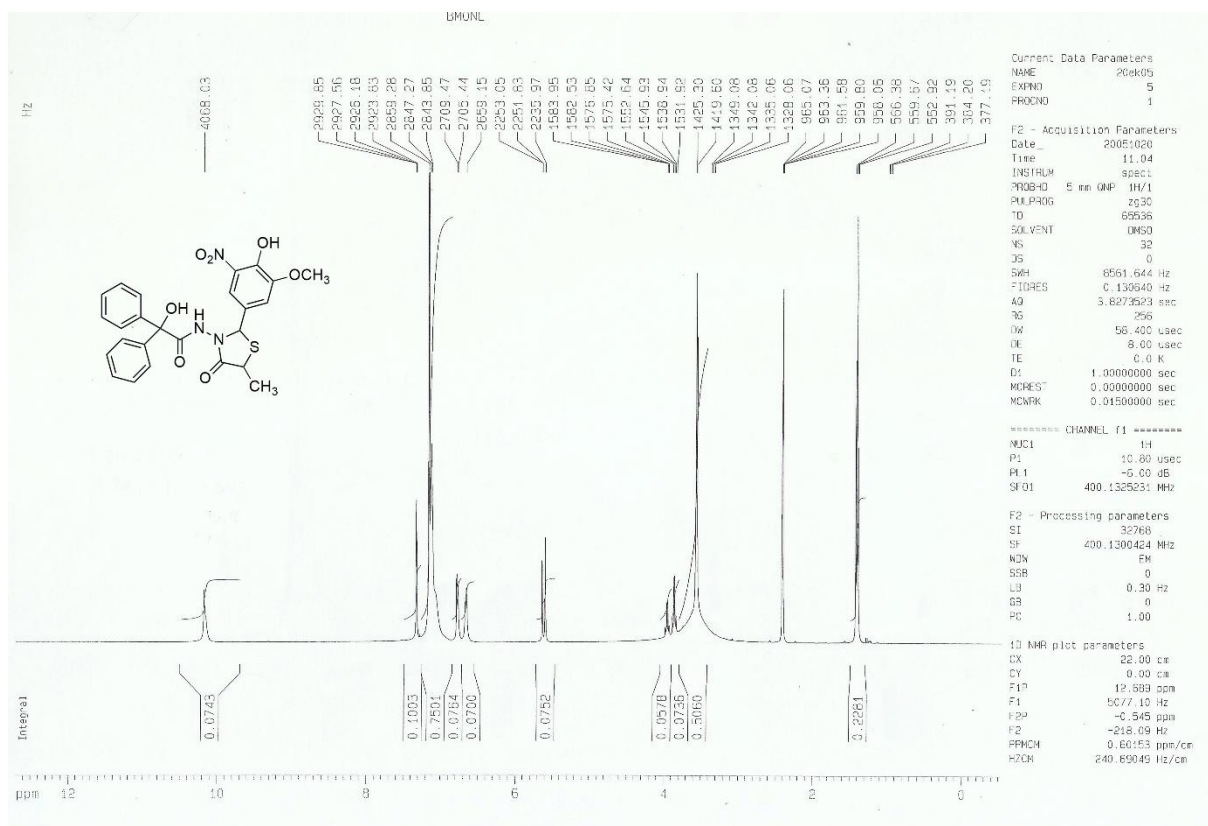


Figure S51: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4g**

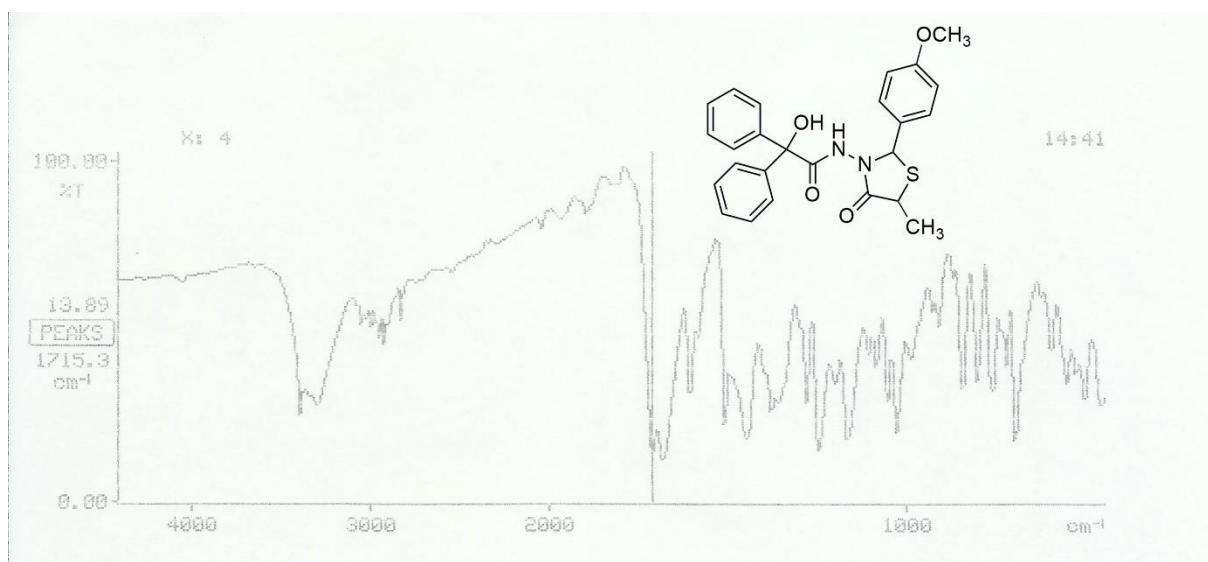


Figure S52: IR (KBr) Spectrum of Compound **4h**

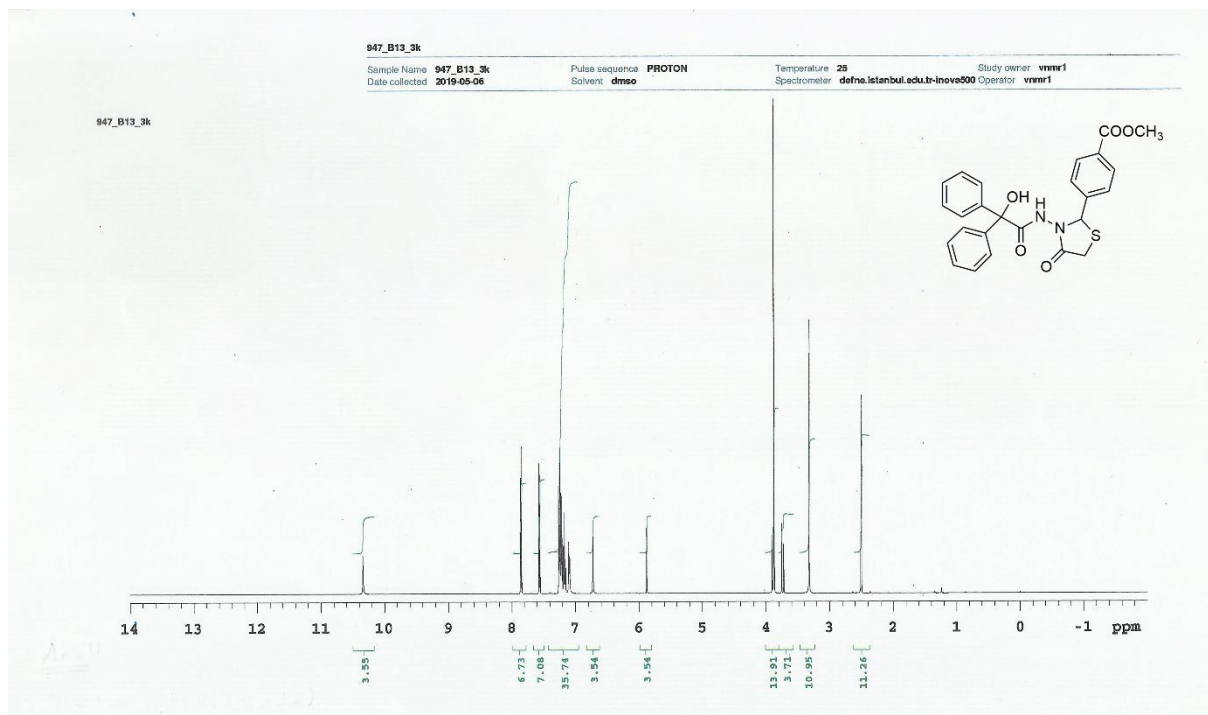


Figure S53: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4h**

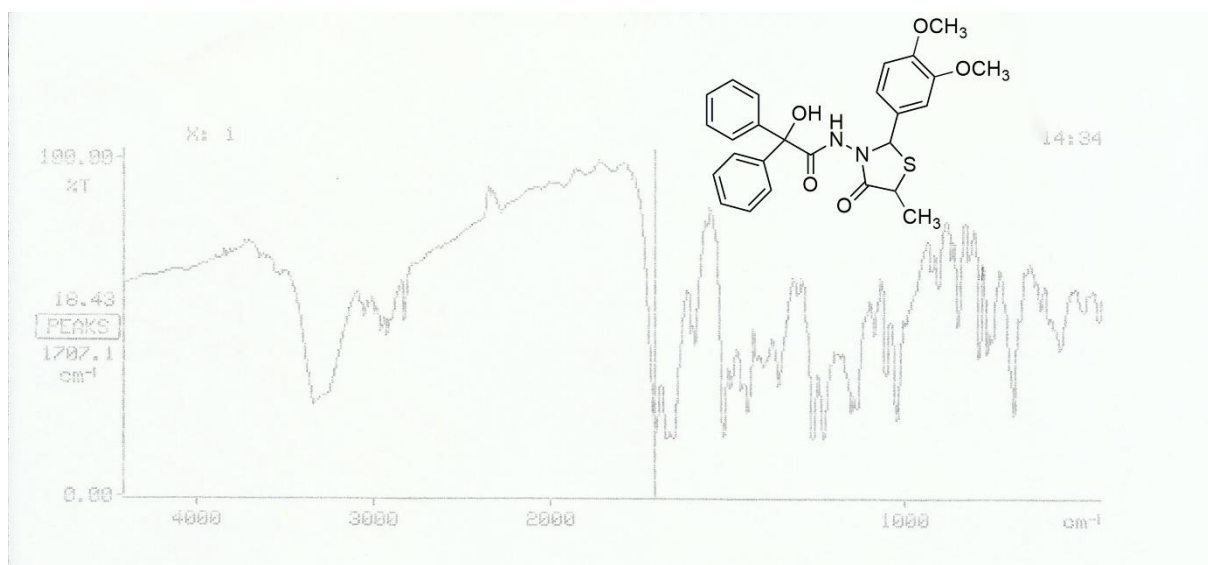


Figure S54: IR (KBr) Spectrum of Compound **4i**

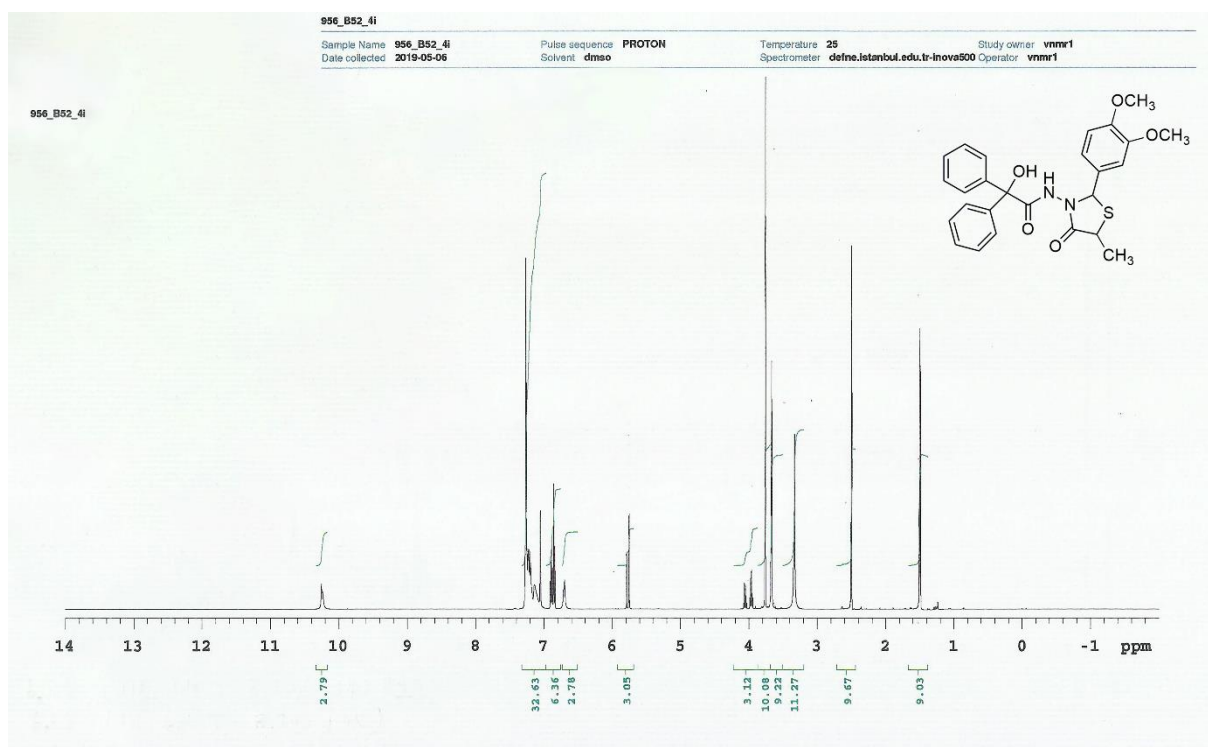


Figure S55: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4i**

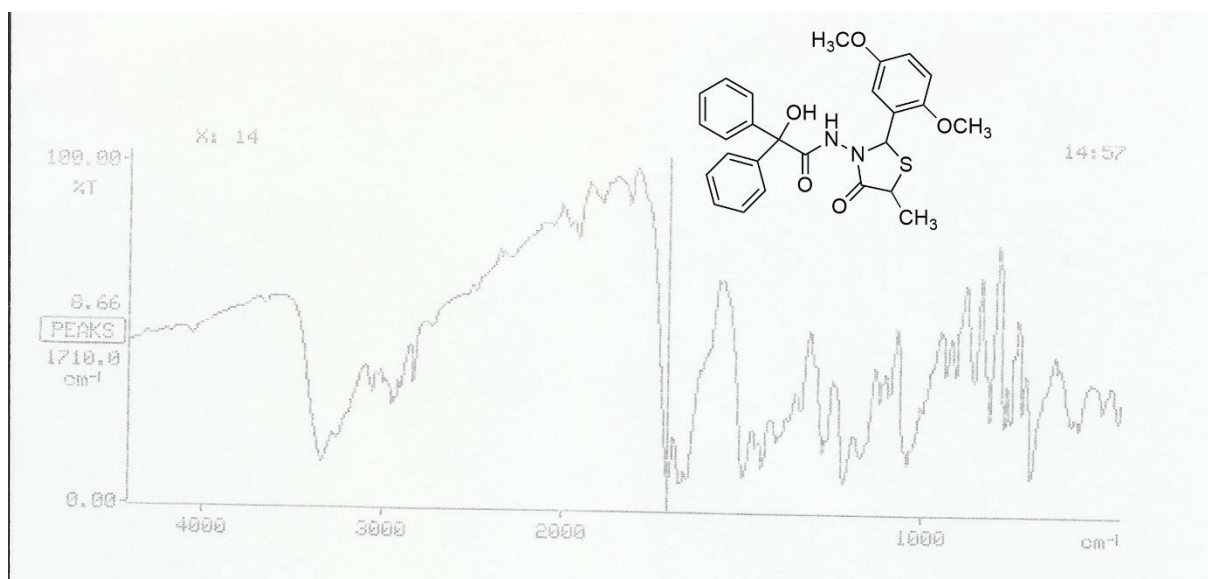


Figure S56: IR (KBr) Spectrum of Compound **4j**

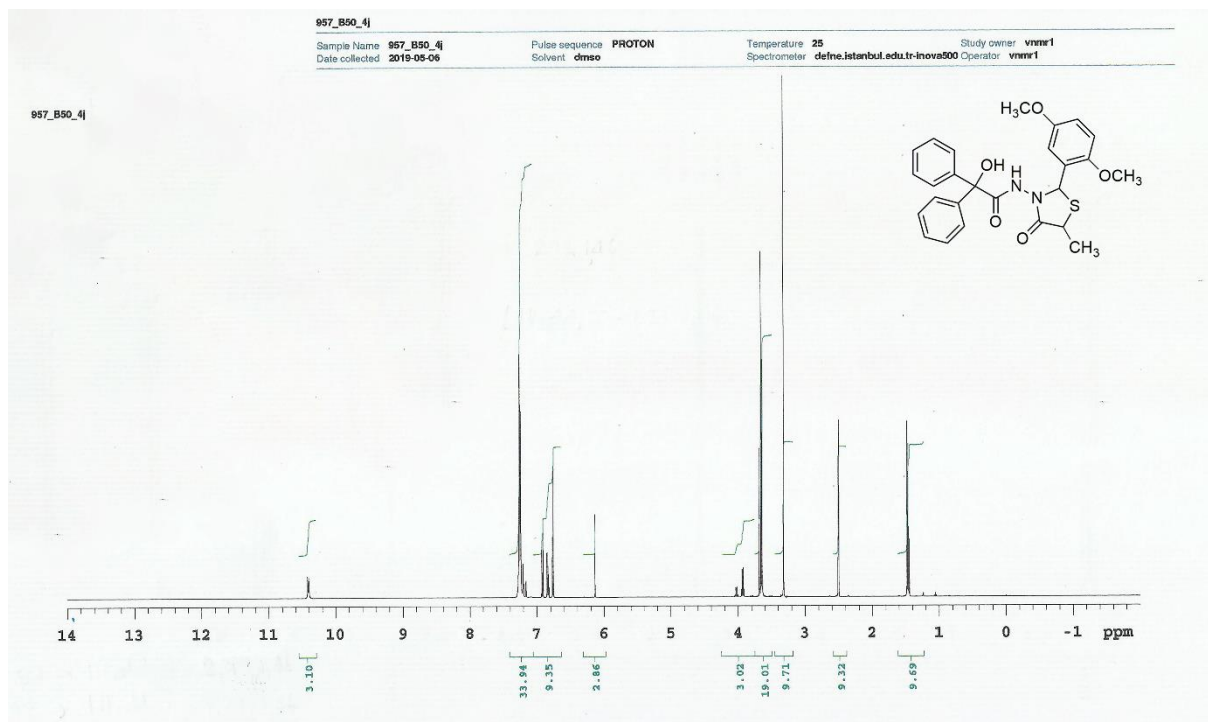


Figure S57: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4j**

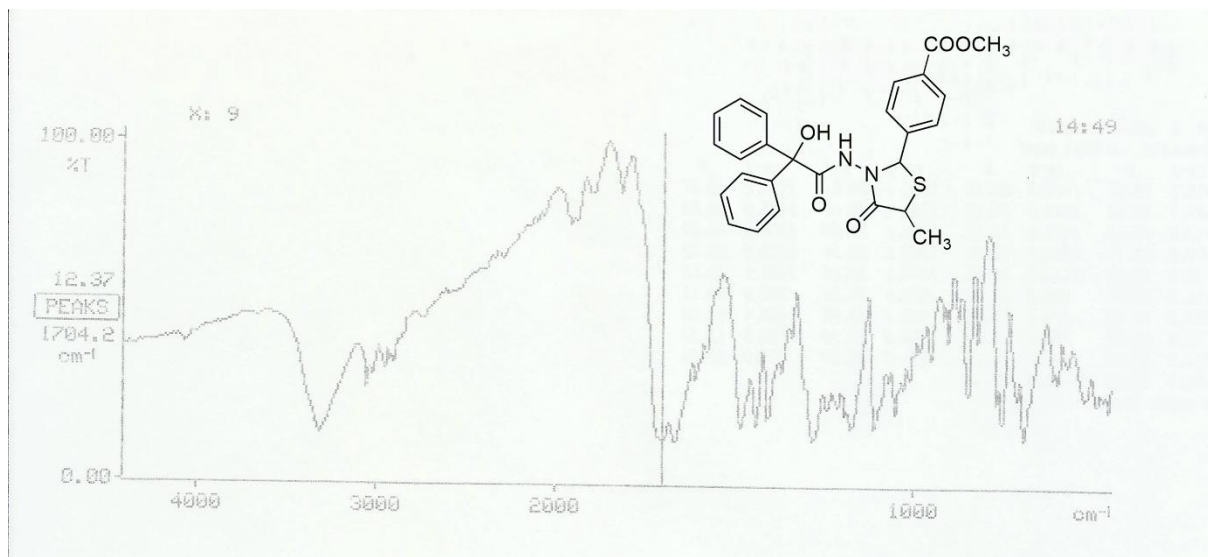


Figure S58: IR (KBr) Spectrum of Compound **4k**

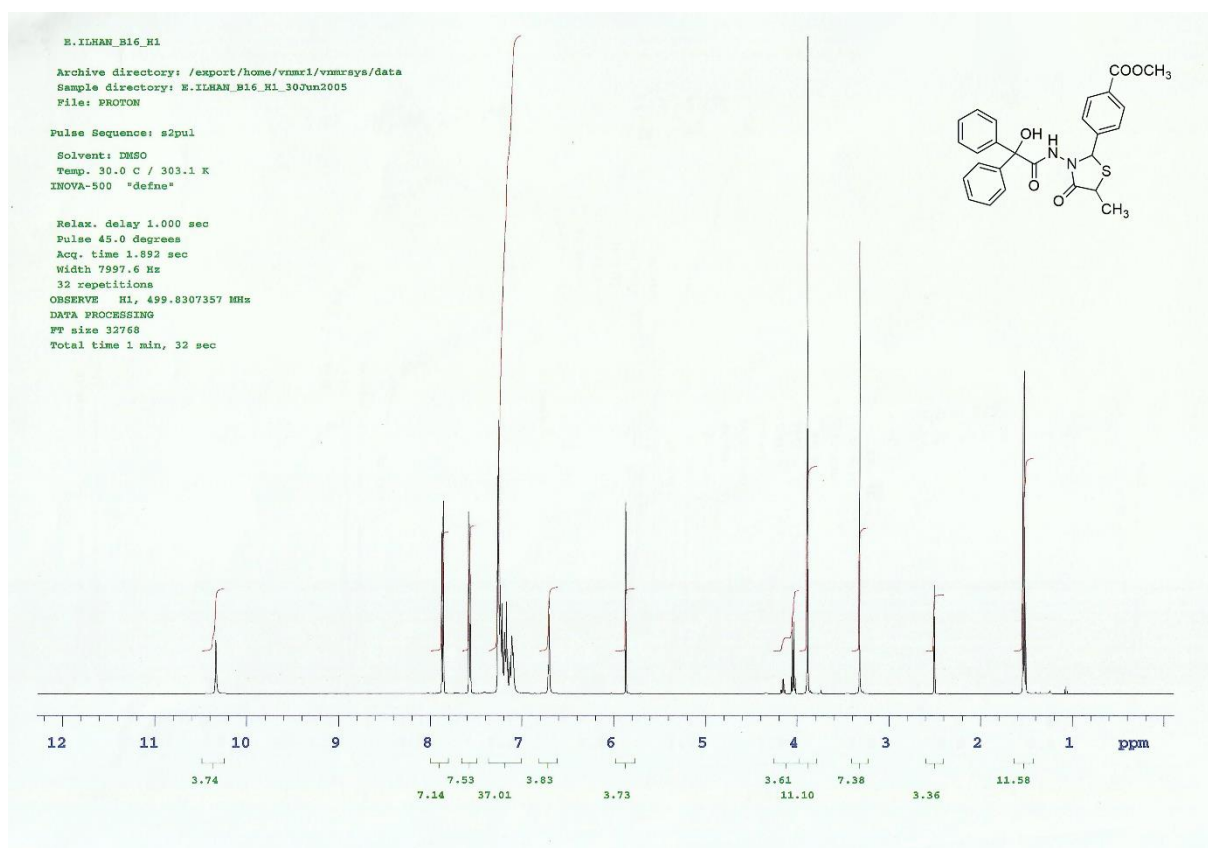


Figure S59: IR (KBr) Spectrum of Compound 4k

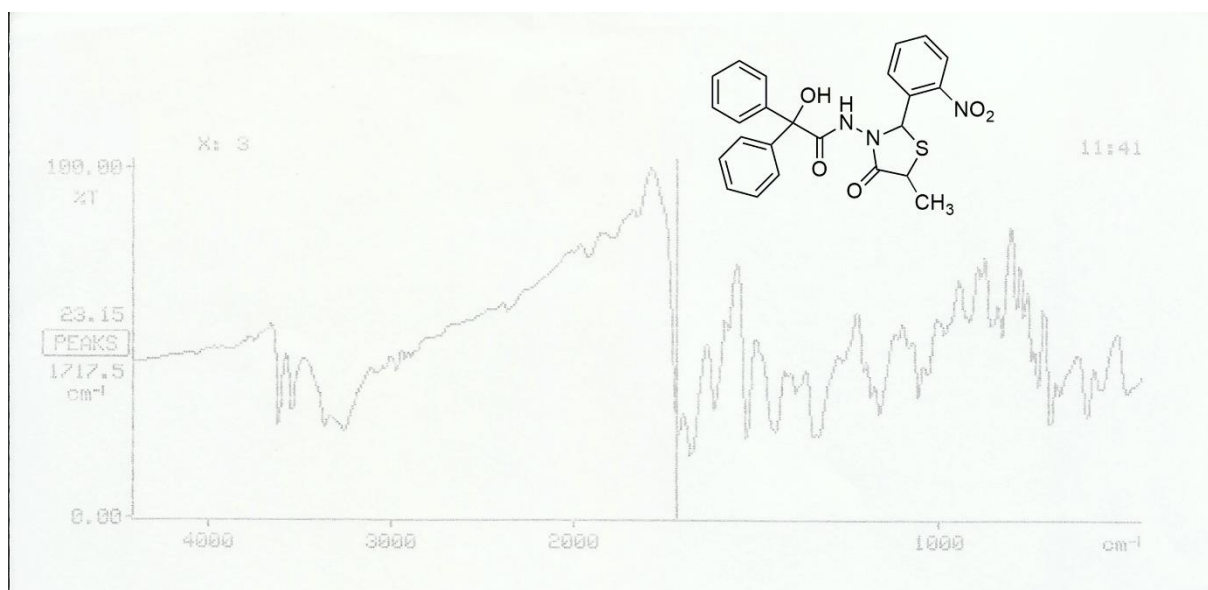


Figure S60: IR (KBr) Spectrum of Compound 41

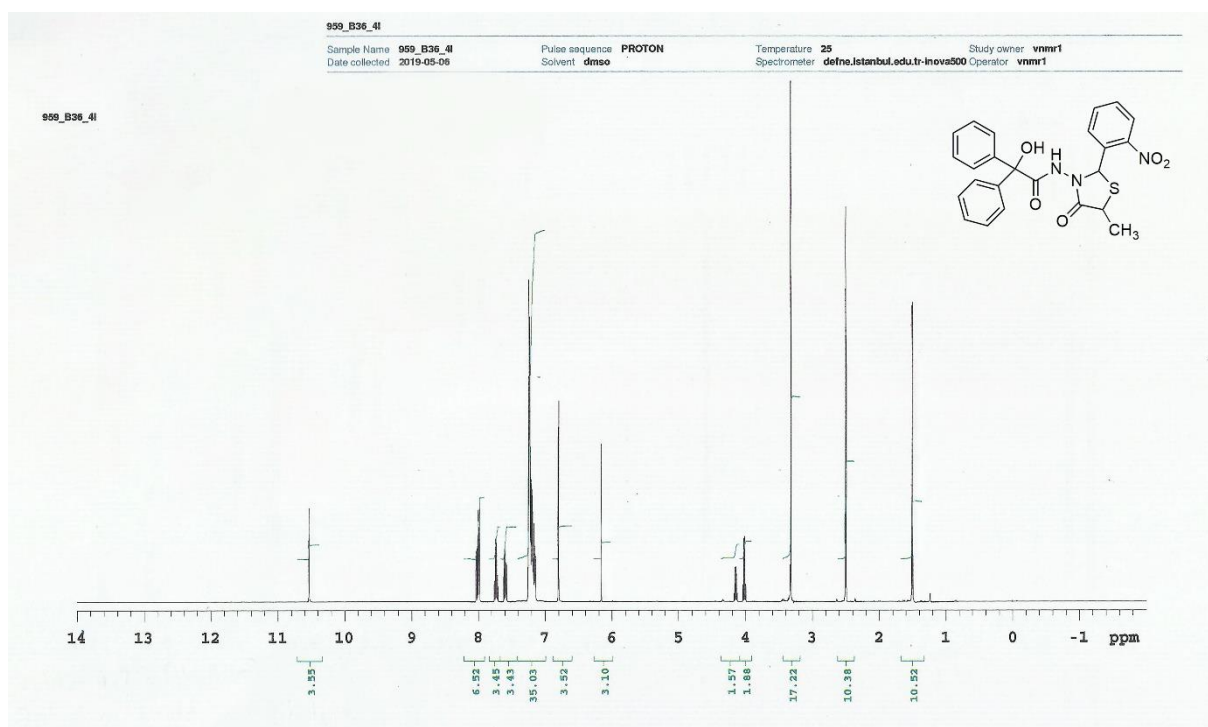


Figure S61: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4I**

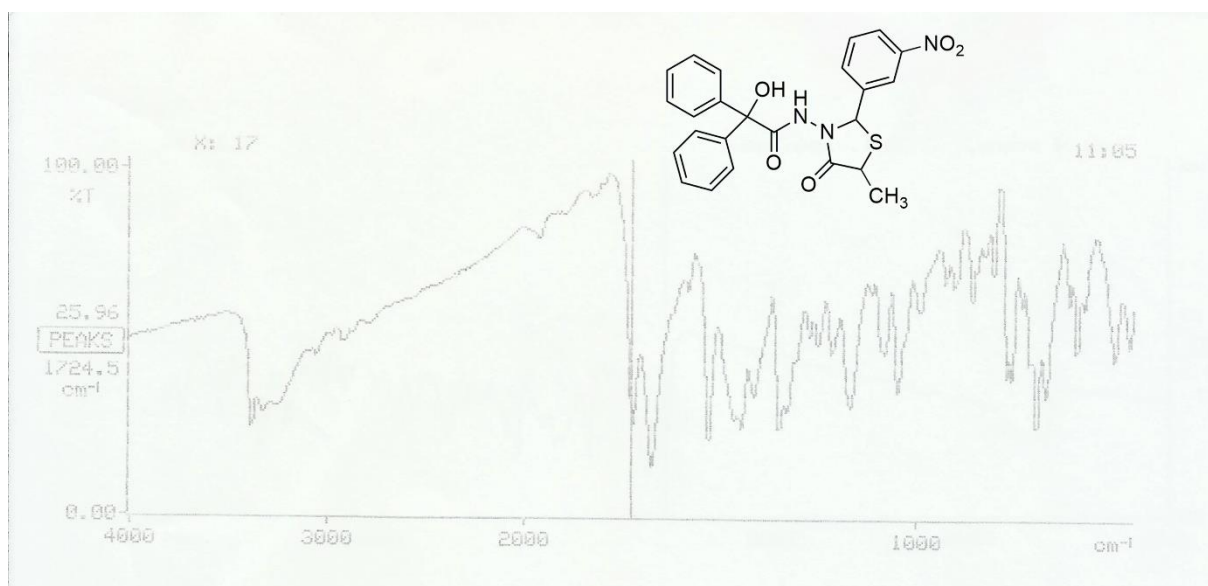


Figure S62: IR (KBr) Spectrum of Compound **4m**

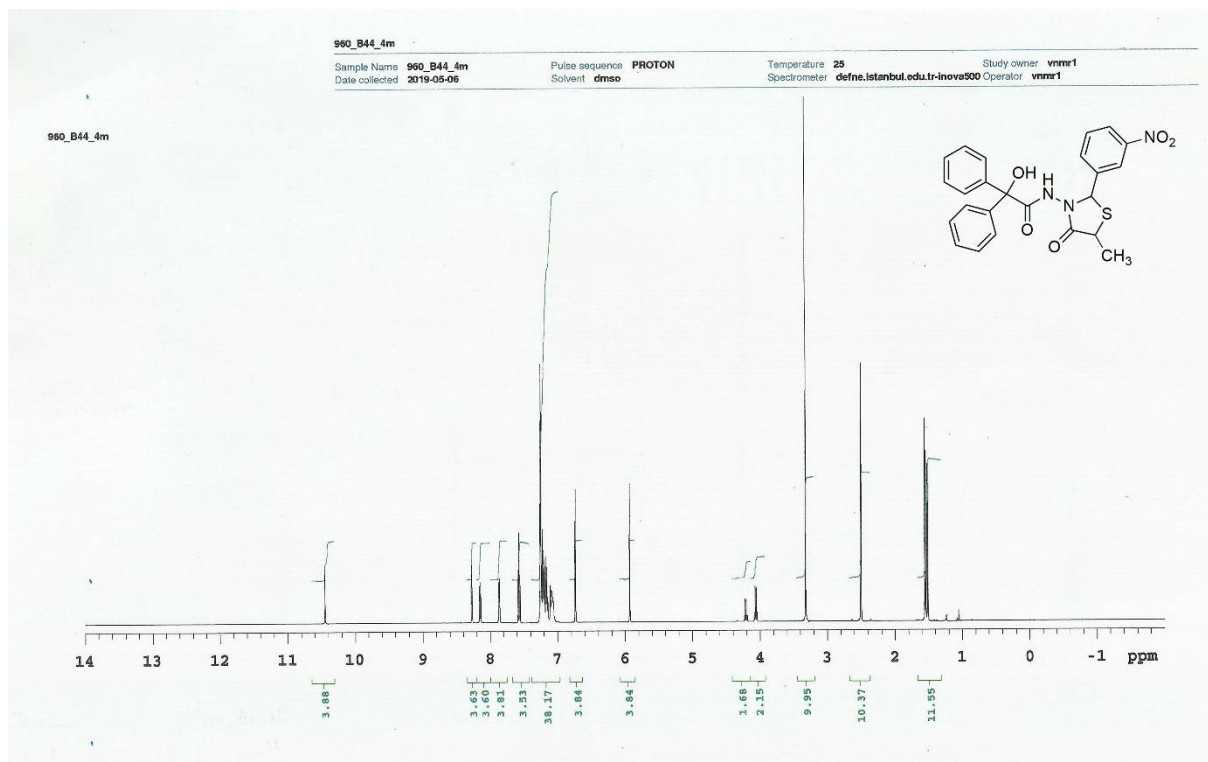


Figure S63: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4m**

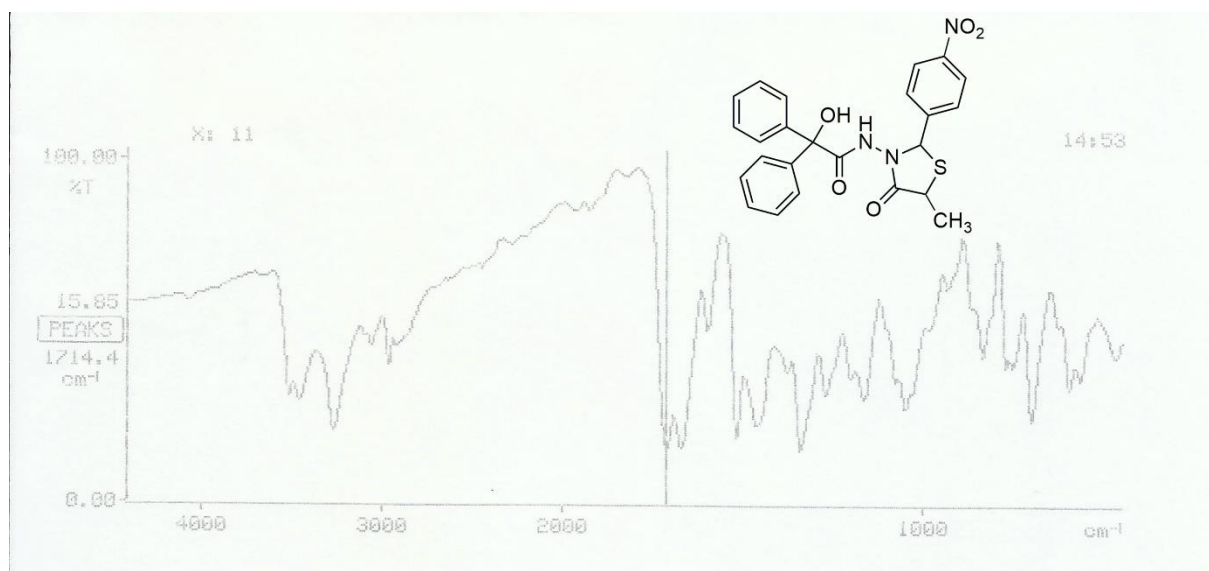


Figure S64: IR (KBr) Spectrum of Compound **4n**

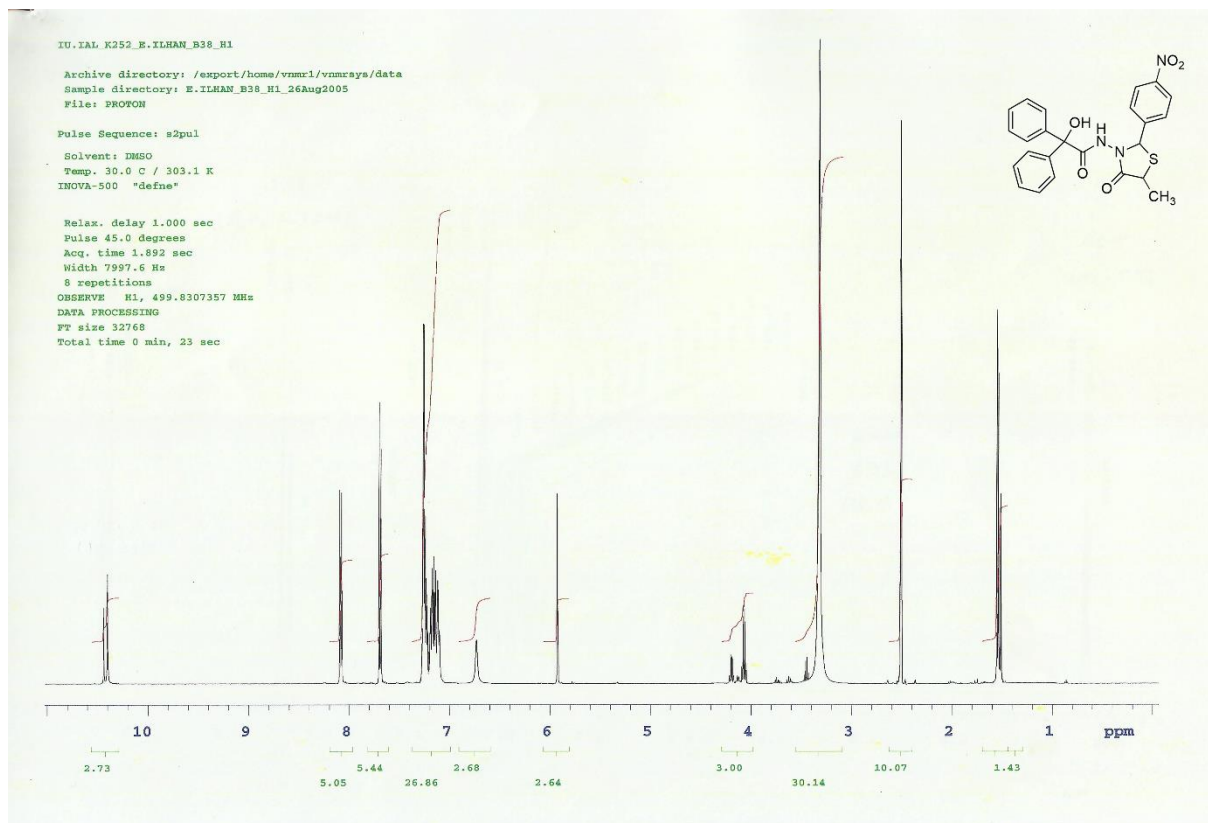


Figure S65: ¹H-NMR (500 MHz, DMSO-*d*₆) Spectrum of Compound **4n**

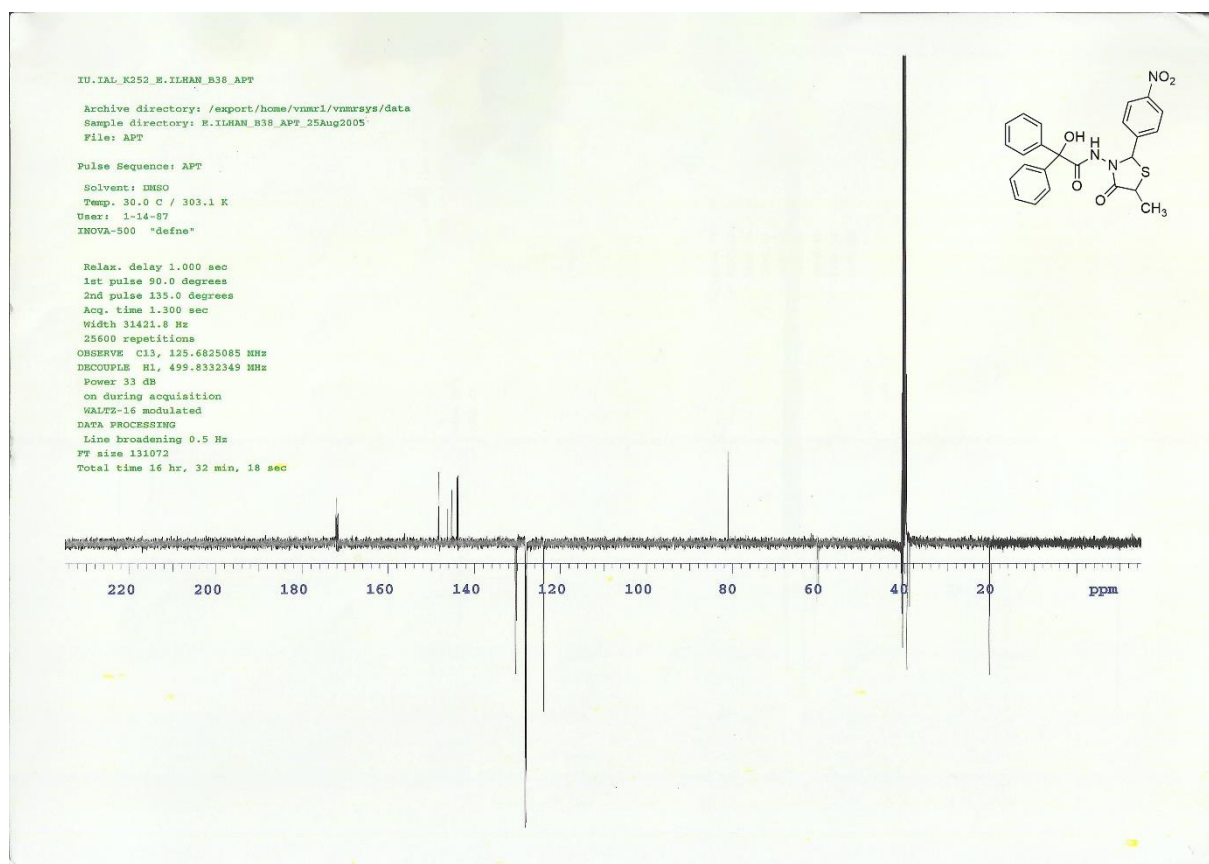


Figure S66: ^{13}C -NMR (125.6 MHz, APT (decoupled)) Spectrum of Compound **4n**

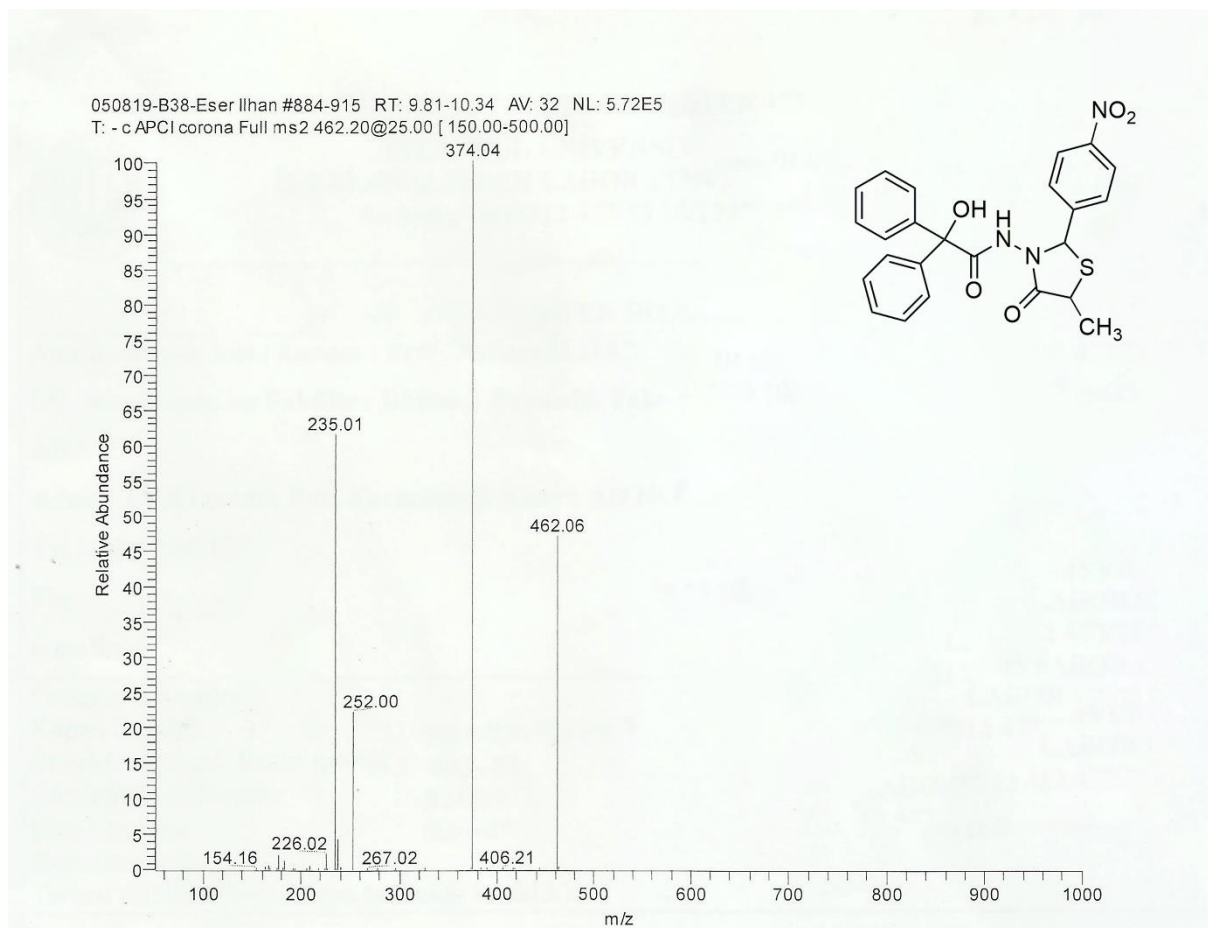


Figure S67: MS-APCI(-) (150 eV, m/z, %) Spectrum of Compound **4n**

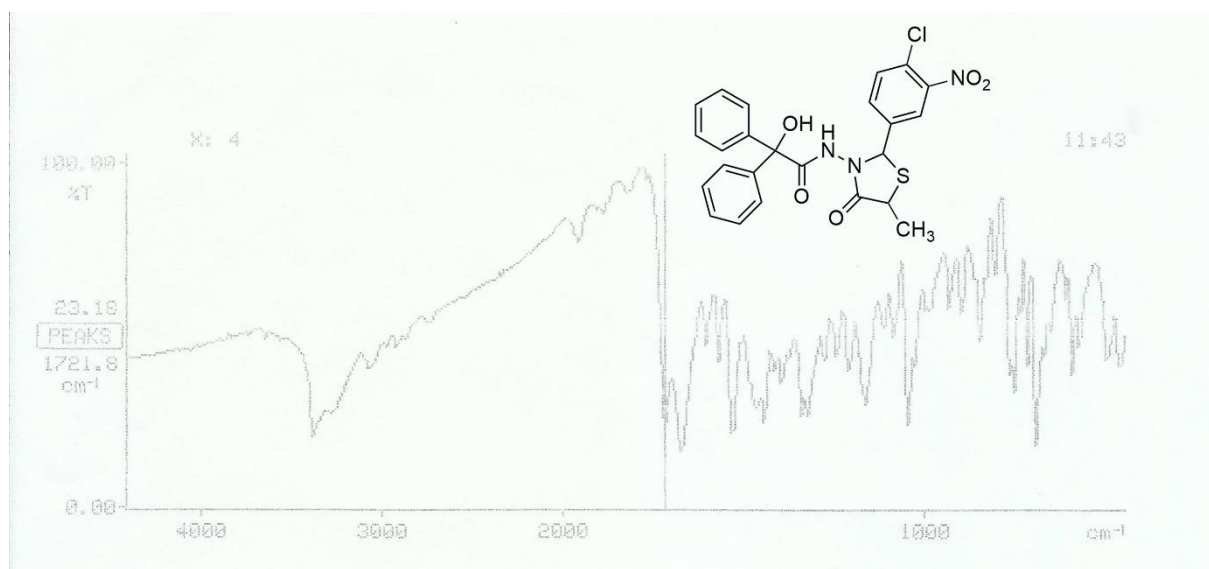


Figure S68: IR (KBr) Spectrum of Compound **4o**

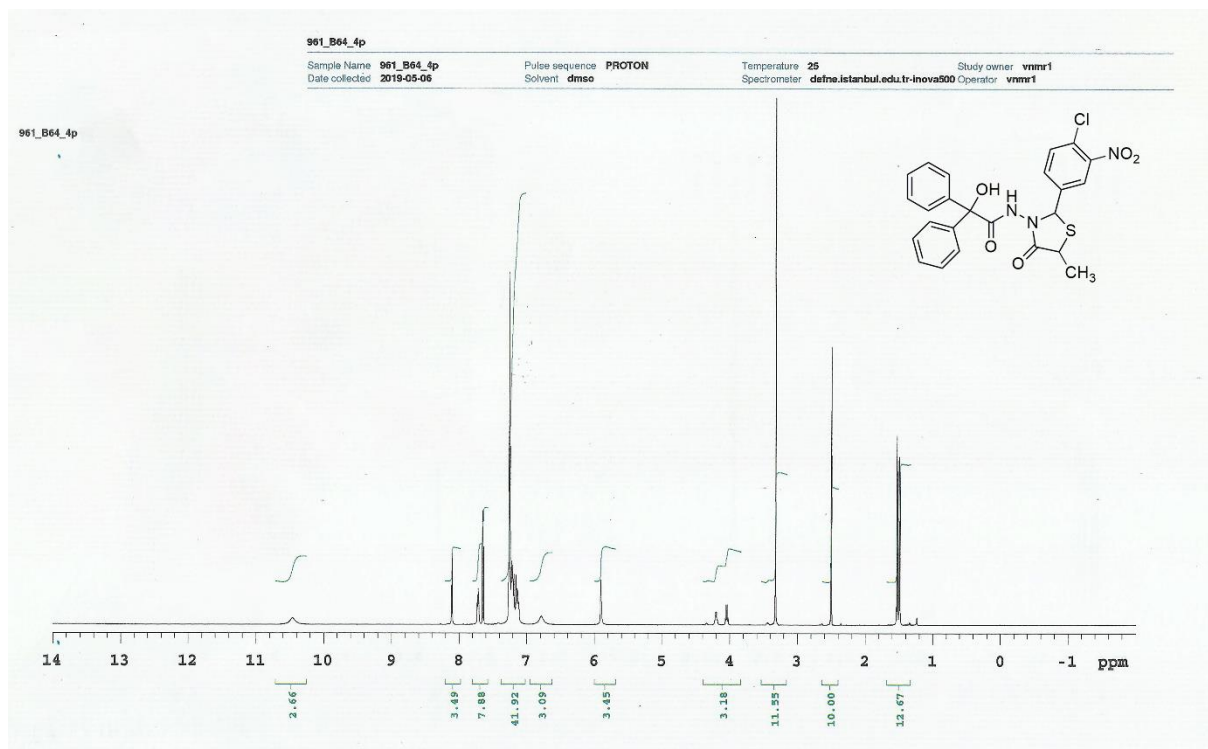


Figure S69: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4o**

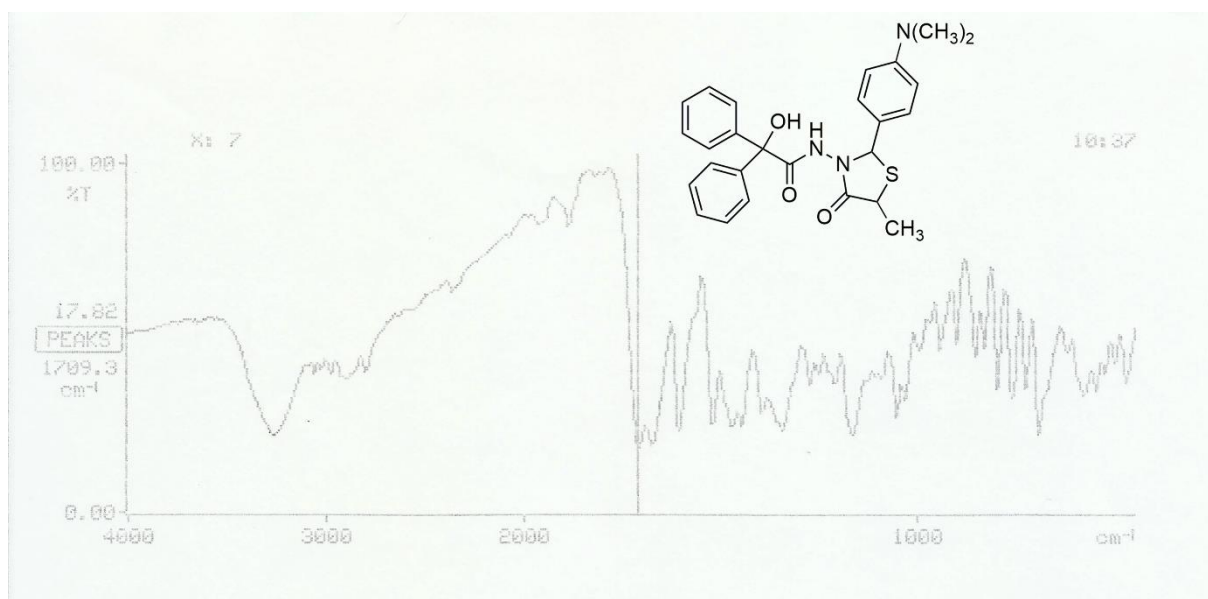


Figure S70: IR (KBr) Spectrum of Compound **4p**

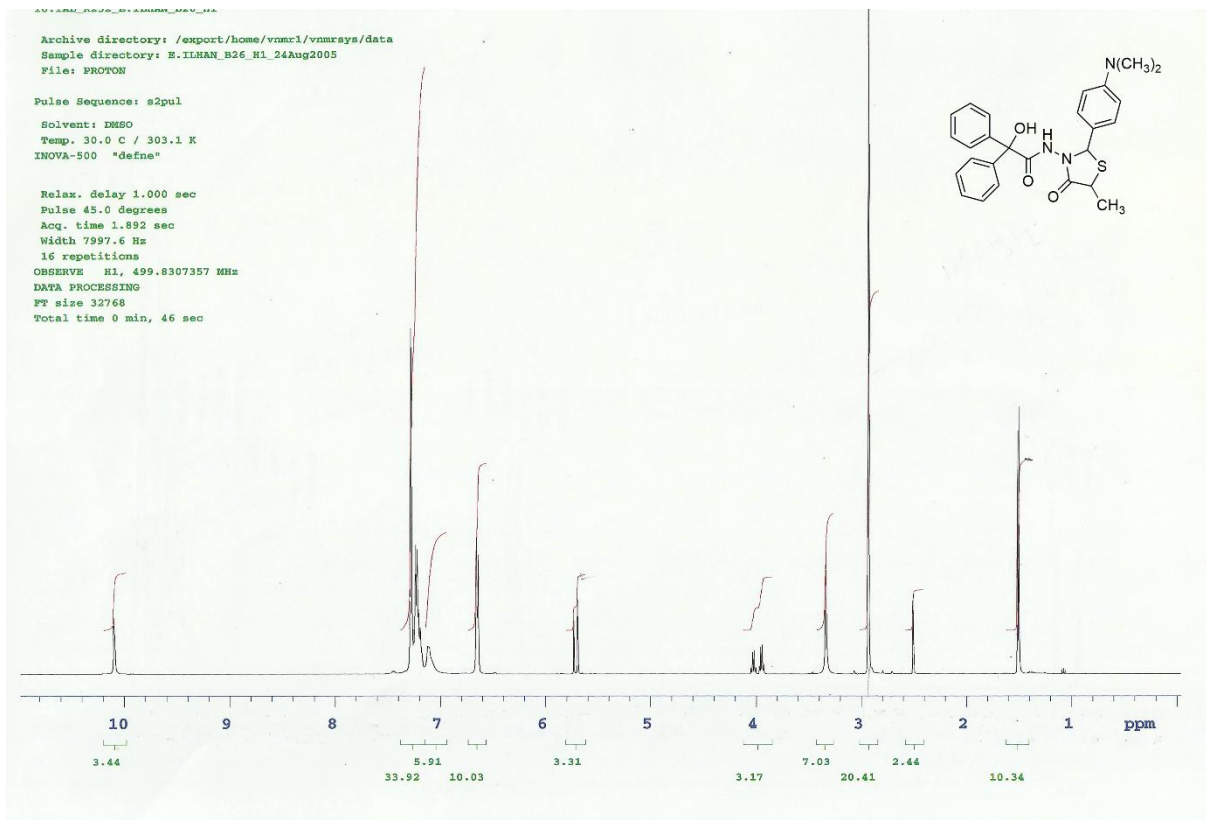


Figure S71: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **4p**

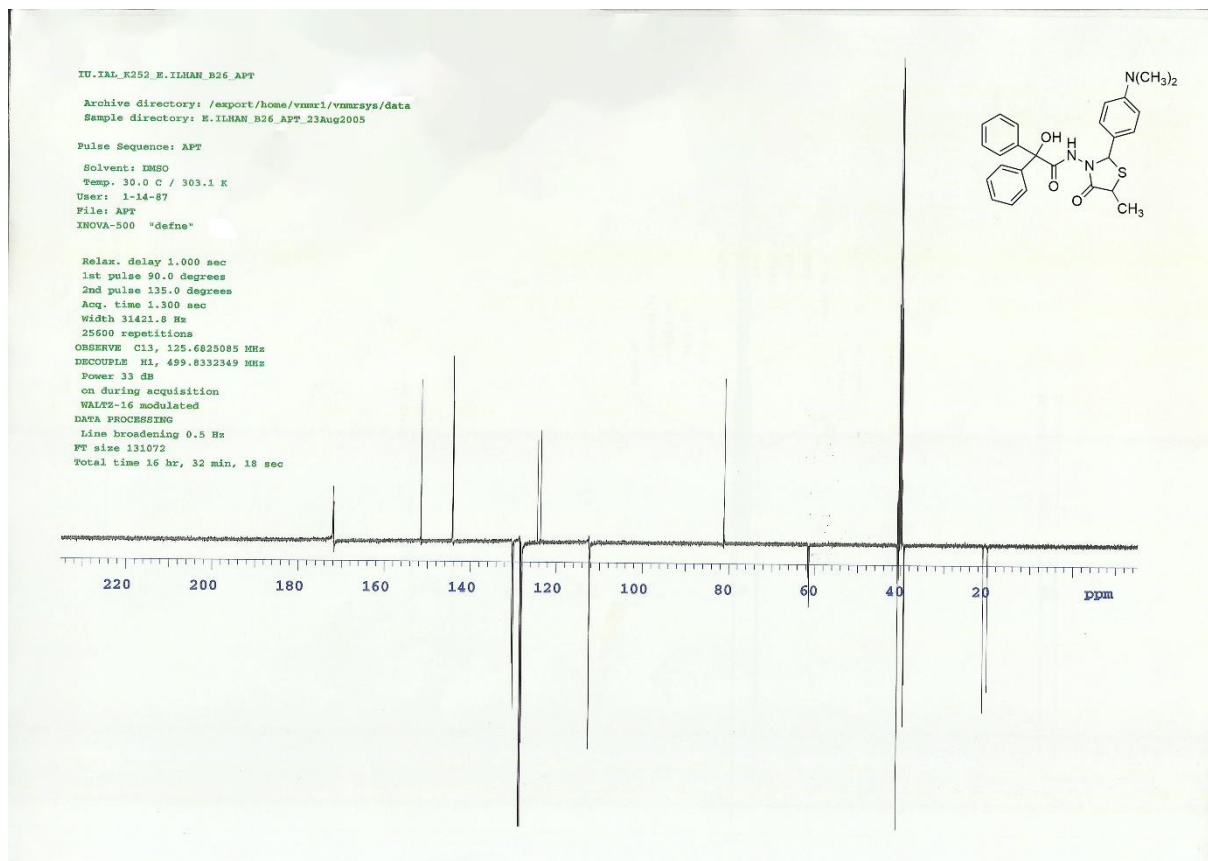


Figure S72: ^{13}C -NMR (125.6 MHz, APT (decoupled)) Spectrum of Compound **4p**

050819-B26-Eser Ilhan #143-164 RT: 2.75-3.20 AV: 22 NL: 2.69E5
T: - c APCI corona Full ms2 460.20@25.00 [150.00-500.00]

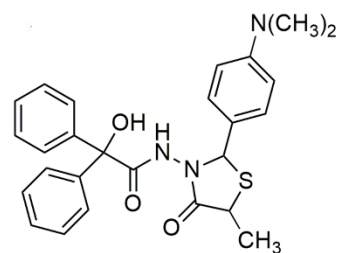
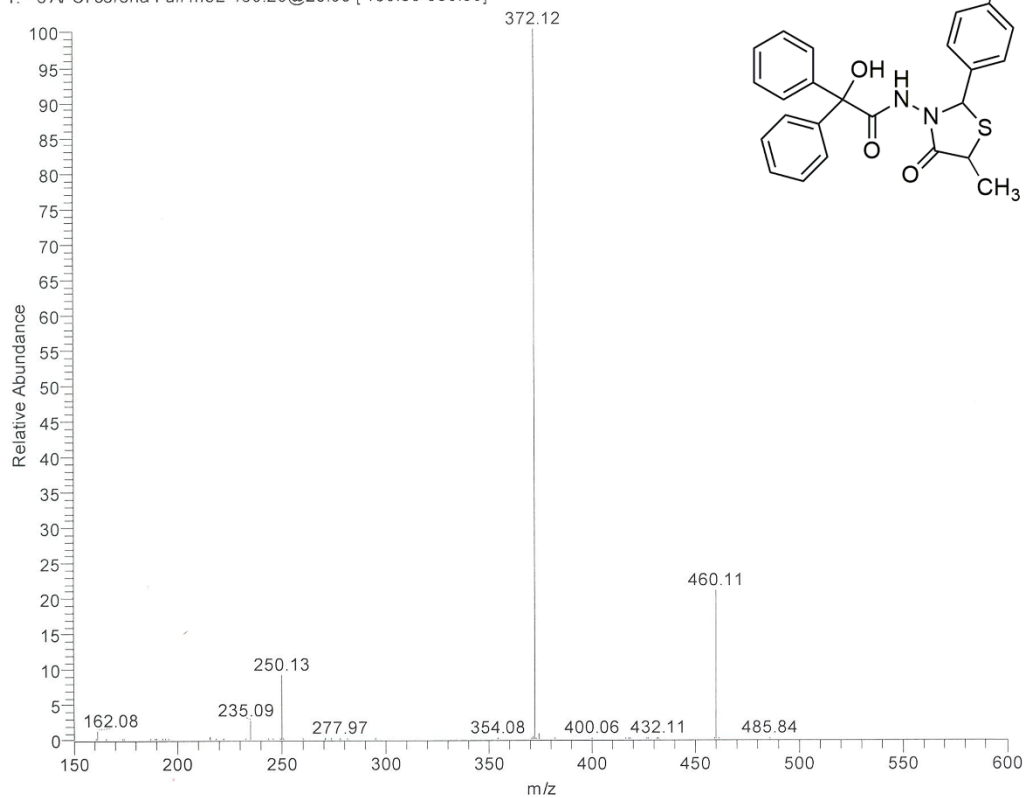


Figure S73: MS-APCI(-) (150 eV, m/z, %) Spectrum of Compound **4p**