SUPPLEMENTARY DATA
For

Visible-light Prompted Synthesis and Binding Studies of 5,6-Dihydroimidazo[2,1-*b*]thiazoles With BSA and DNA Using Biophysical and Computational Methods

Ranjana Aggarwal,[a,b]* Mona Hooda,[a] Prince Kumar,[a] Naman Jain,[a] Gyan Prakash Dubey,[a] Heerak Chugh,[c] Ramesh Chandra,[c]

[a]Department of Chemistry, Kurukshetra University, Kurukshetra-136119, Haryana, India

[b]CSIR-National Institute of Science Communication and Policy Research, New Delhi 110012, India

[c]Department of Chemistry, University of Delhi, New Delhi 110007, India

*Corresponding author:

Prof. Ranjana Aggarwal, CSIR- National Institute of Science Communication and Policy Research, New Delhi, India. Tel: +91-9896740740

E-mails: *ranjana67in@yahoo.com*, *ranjanaaggarwal67@gmail.com*

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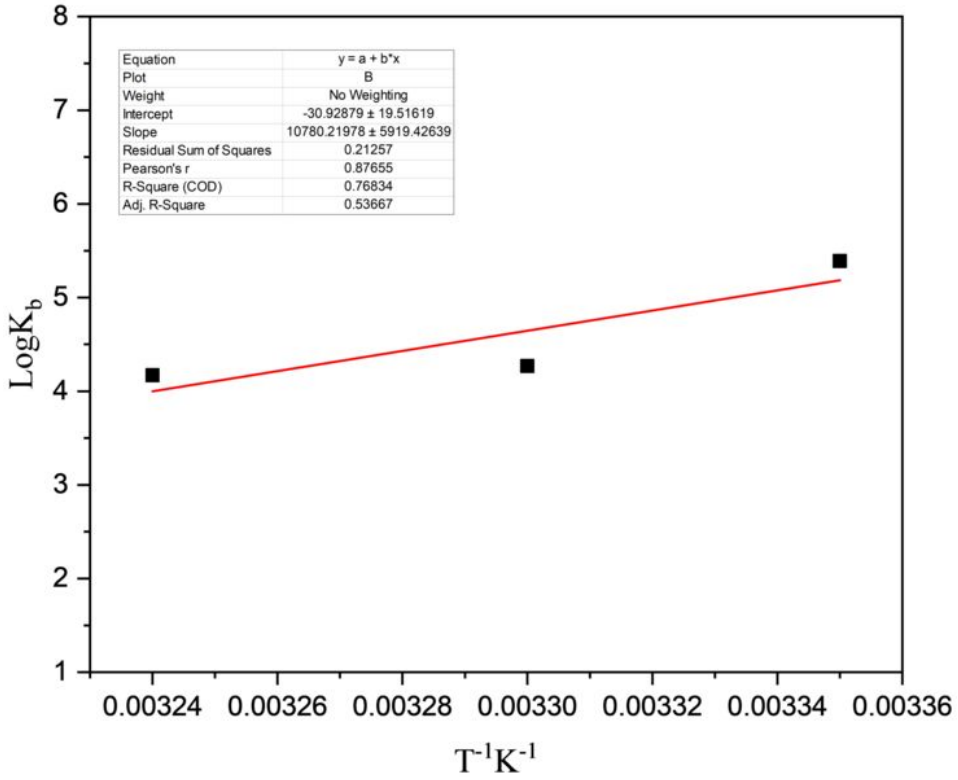

Fig S1. Van't Hoff plot of Log K vs 1/T for binding of **3i** with BSA.

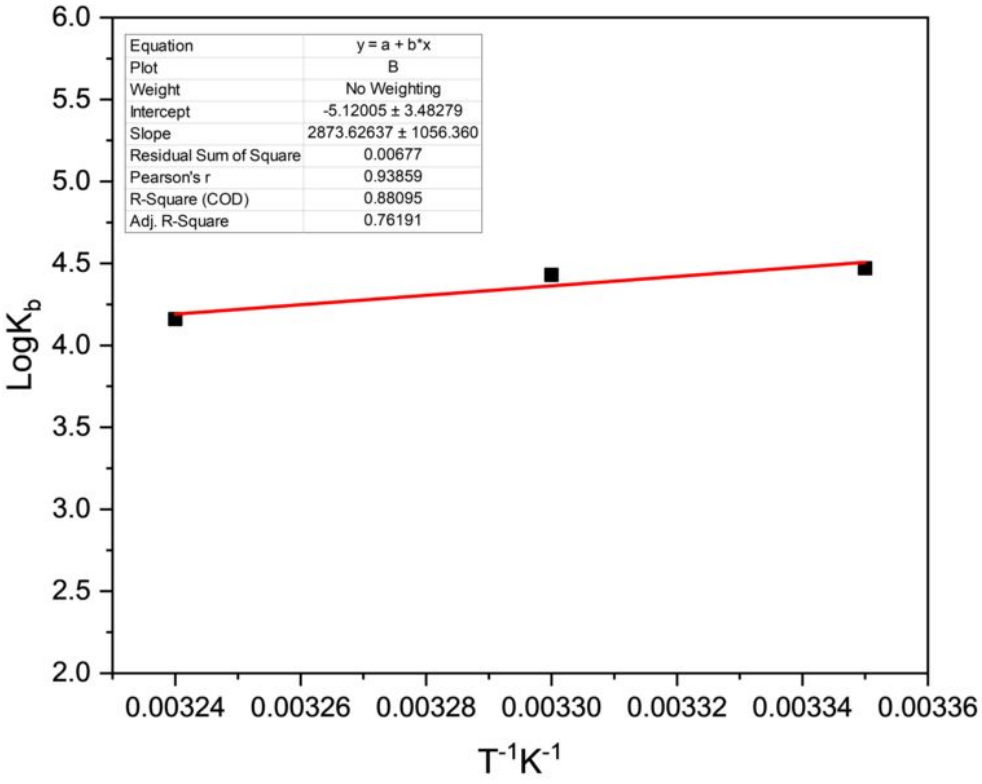

Fig S2. Van't Hoff plot of Log K vs 1/T for binding of **3i** with DNA.

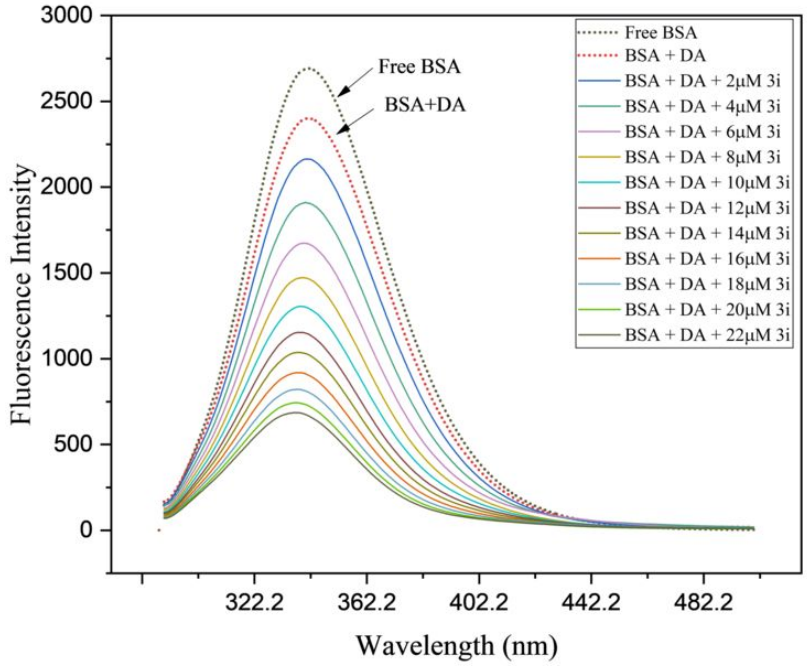

Fig S3. Displacement of Dansylamide (DA) from BSA-Dansylamide complex by **3i**. [Dansylamide] = [BSA] = 15 μM and [**3i**] = 0 – 22 μM, λex = 280 nm

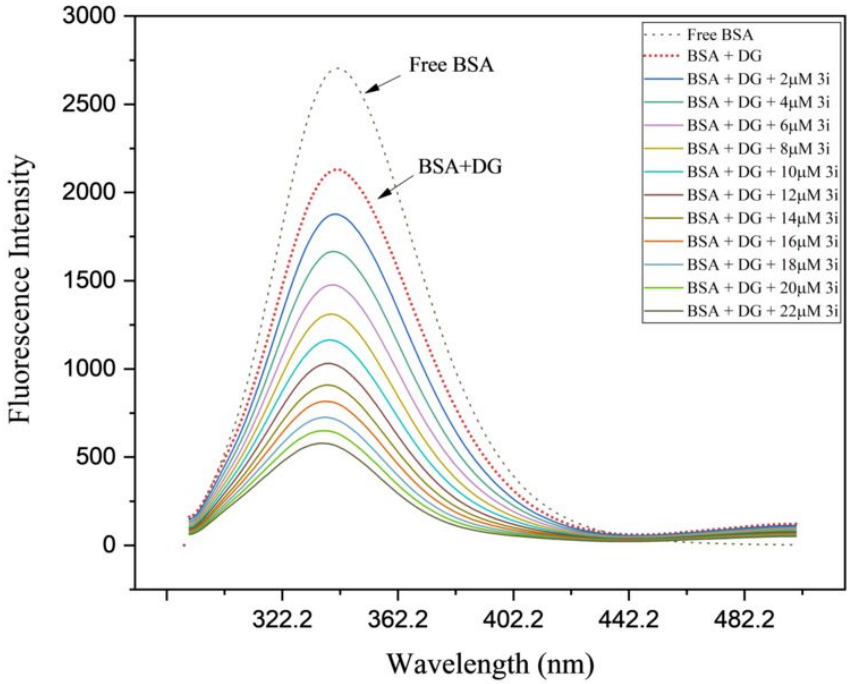

Fig S4. Displacement of Dansylglycine (DG) from BSA-Dansylglycine complex by **3i**. [Dansylglycine] = [BSA] = 15 μM and [**3i**] = 0 – 22 μM, λex = 280 nm

Characterization of Final Compounds

^{1}H NMR, ^{13}C{1H} NMR, HMQC, HMBC and HRMS Spectrum of Final Compounds

1. 2-(4-Methylbenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3a)**

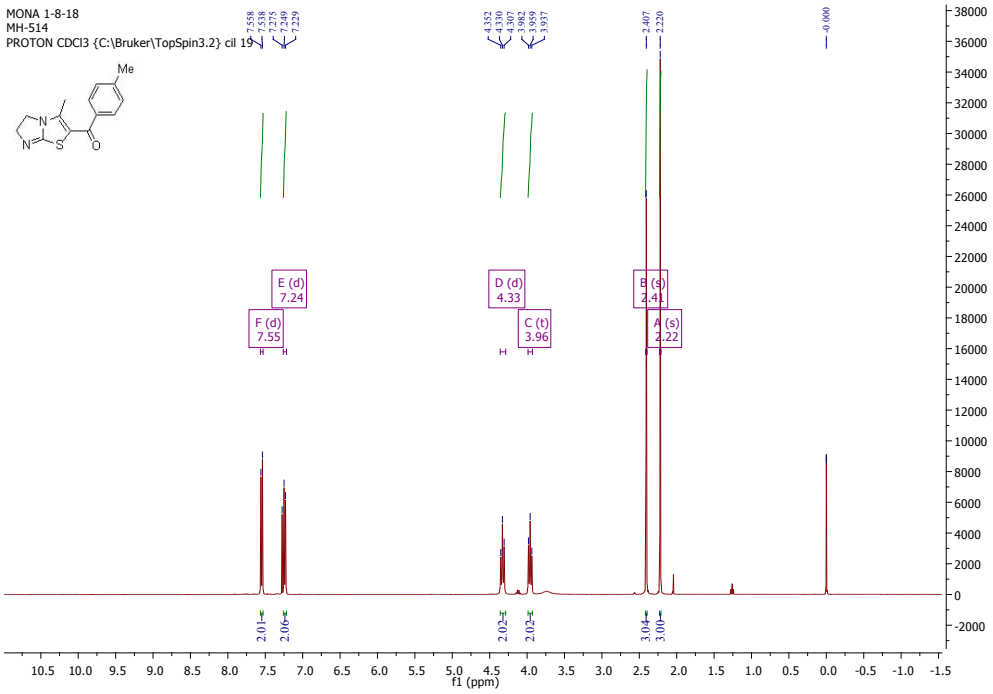

Figure S5a. ^{1}H NMR spectrum of **3a** in $CDCl_3$ (400 MHz).

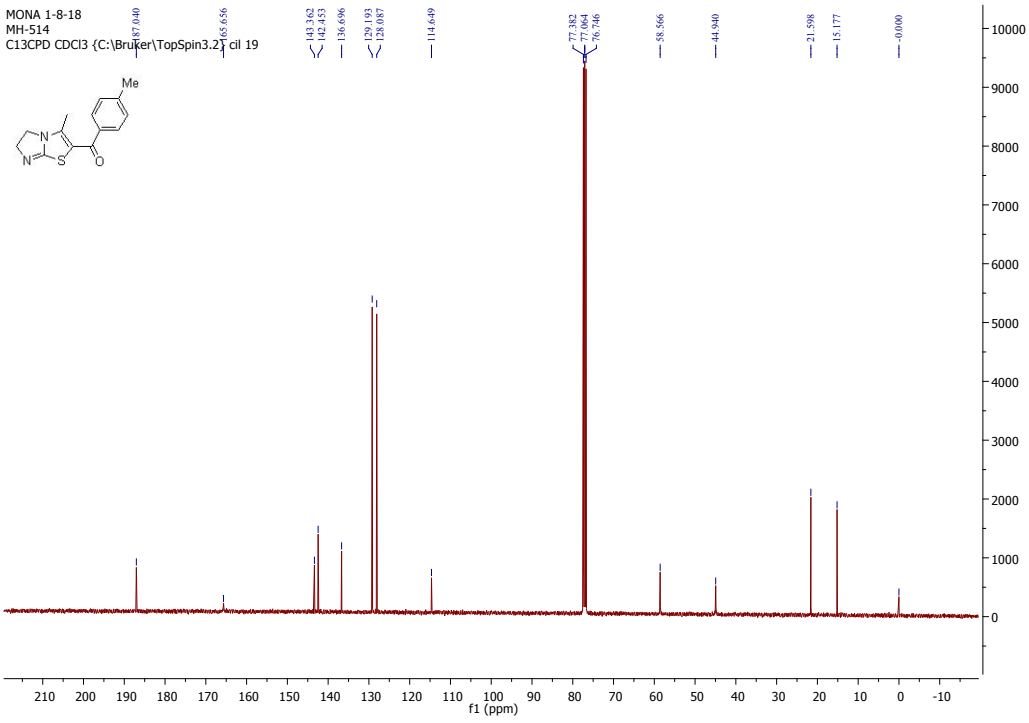

Figure S5b. ^{13}C{^{1}H} NMR spectrum of **3a** in $CDCl_3$ (100 MHz).

2. 2-(2-Methoxybenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3b)**

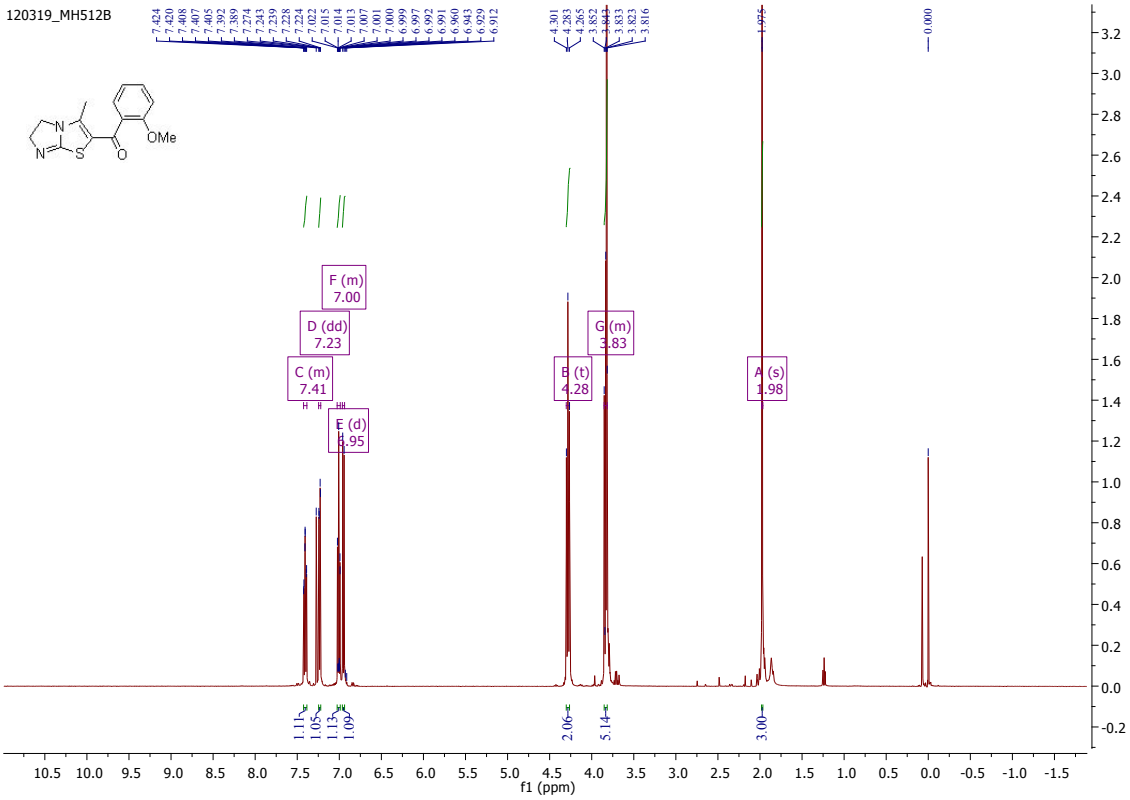

Figure S6a. ^{1}H NMR spectrum of **3b** in $CDCl_3$ (500 MHz).

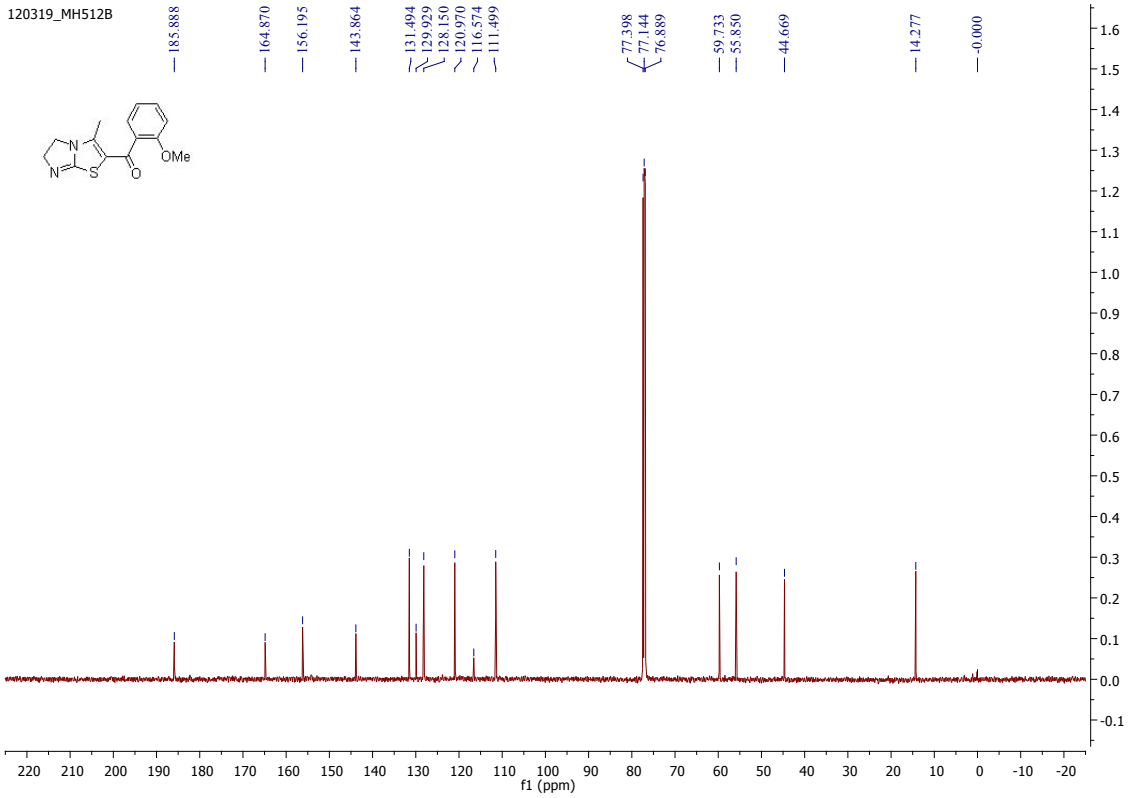

Figure S6b. ^{13}C{^{1}H} NMR spectrum of **3b** in $CDCl_3$ (125 MHz).

3. 2-(3-Methoxybenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3c)**

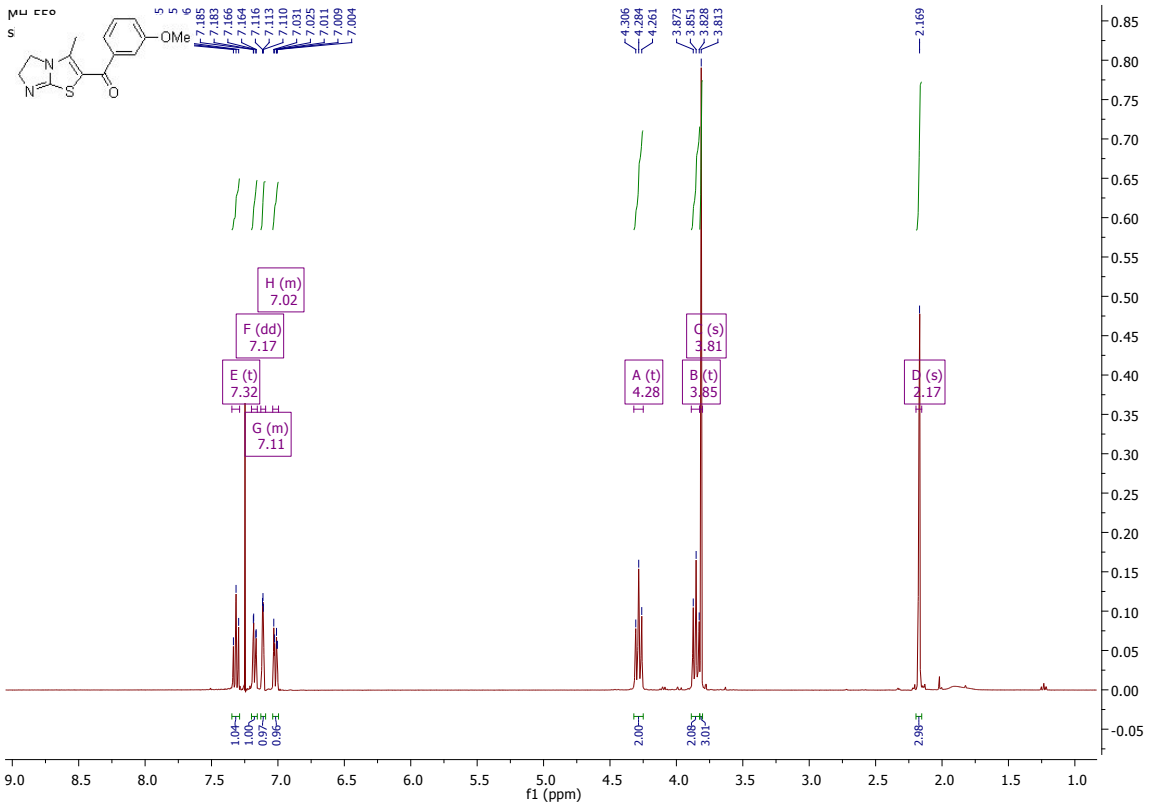

Figure S7a. ^{1}H NMR spectrum of **3c** in $CDCl_3$ (400 MHz).

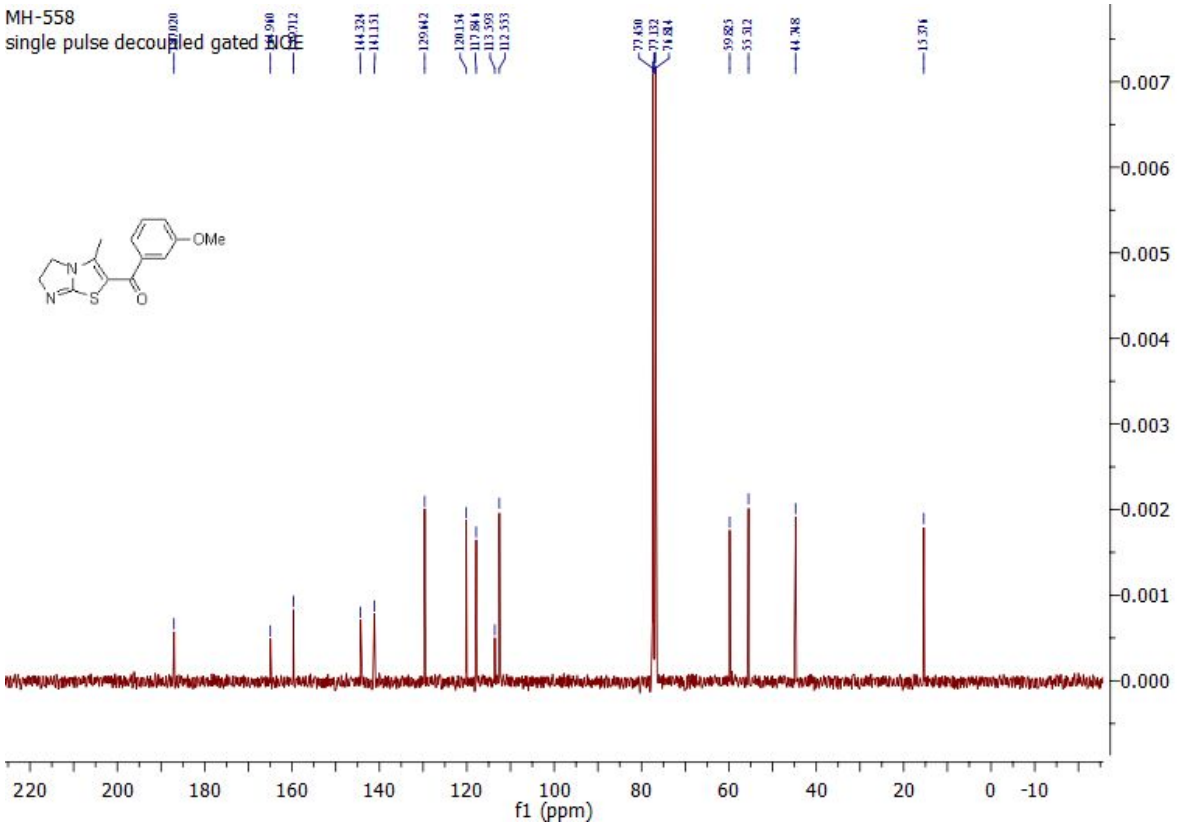

Figure S7b. $^{13}C\{^{1}H\}$ NMR spectrum of **3c** in $CDCl_3$ (100 MHz).

4. 2-(4-Methoxybenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3d)**

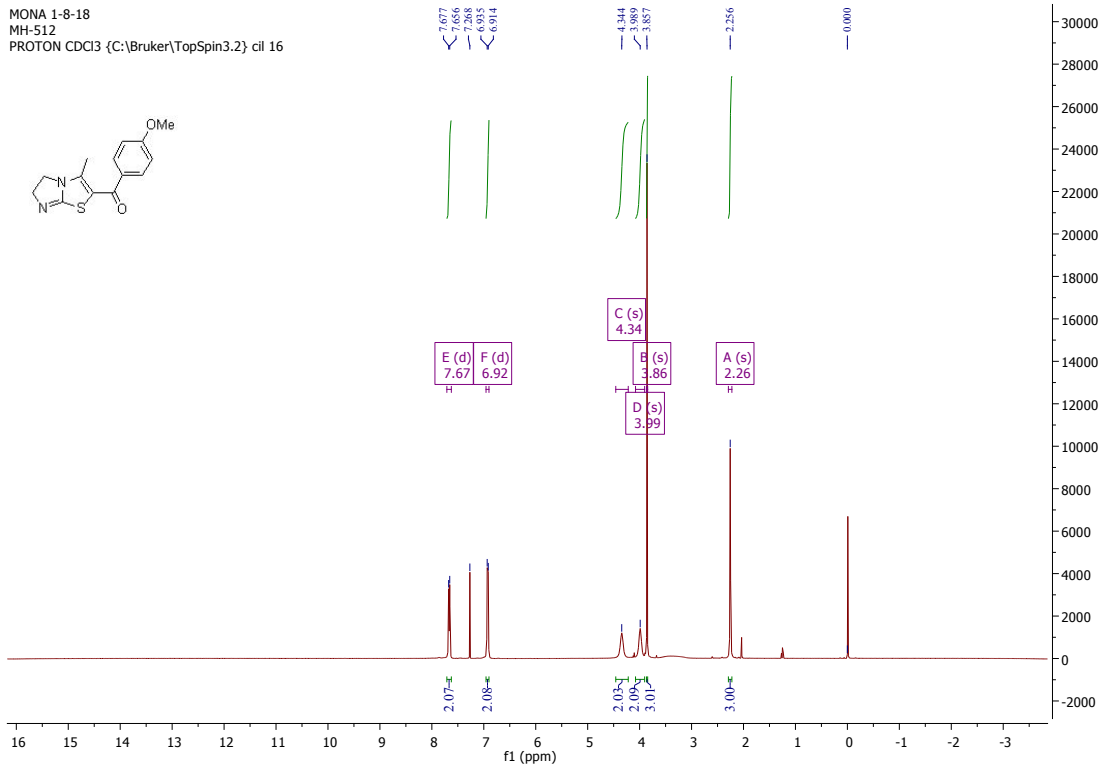

Figure S8a. ^{1}H NMR spectrum of **3d** in $CDCl_3$ (400 MHz).

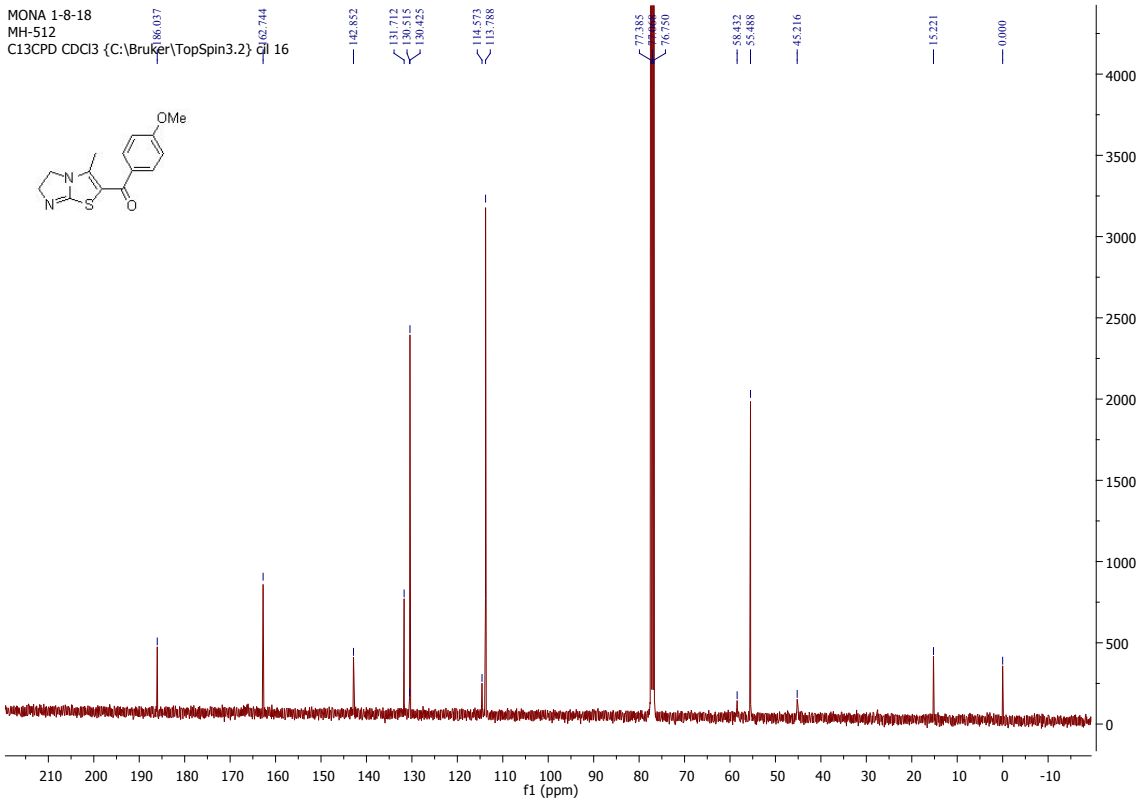

Figure S8b. $^{13}C\{^{1}H\}$ NMR spectrum of **3d** in $CDCl_3$ (100 MHz).

5. 2-Benzoyl-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3e)**

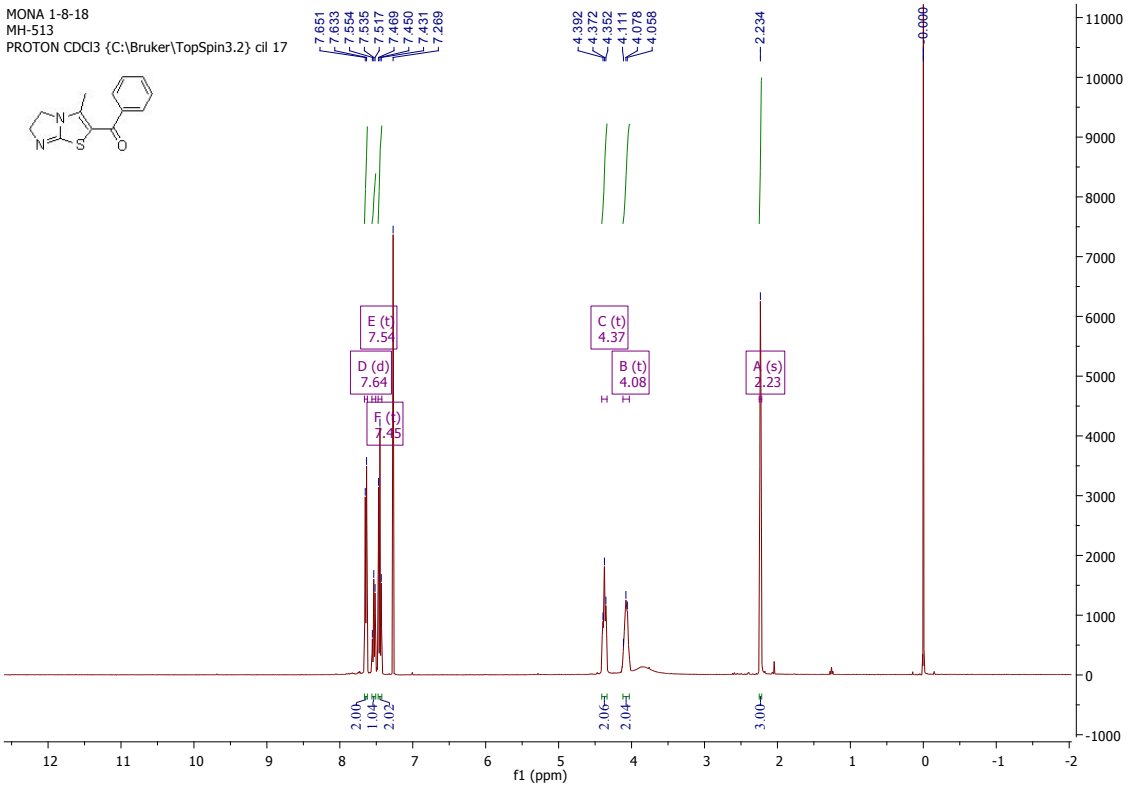

Figure S9a. ^{1}H NMR spectrum of **3e** in $CDCl_3$ (400 MHz).

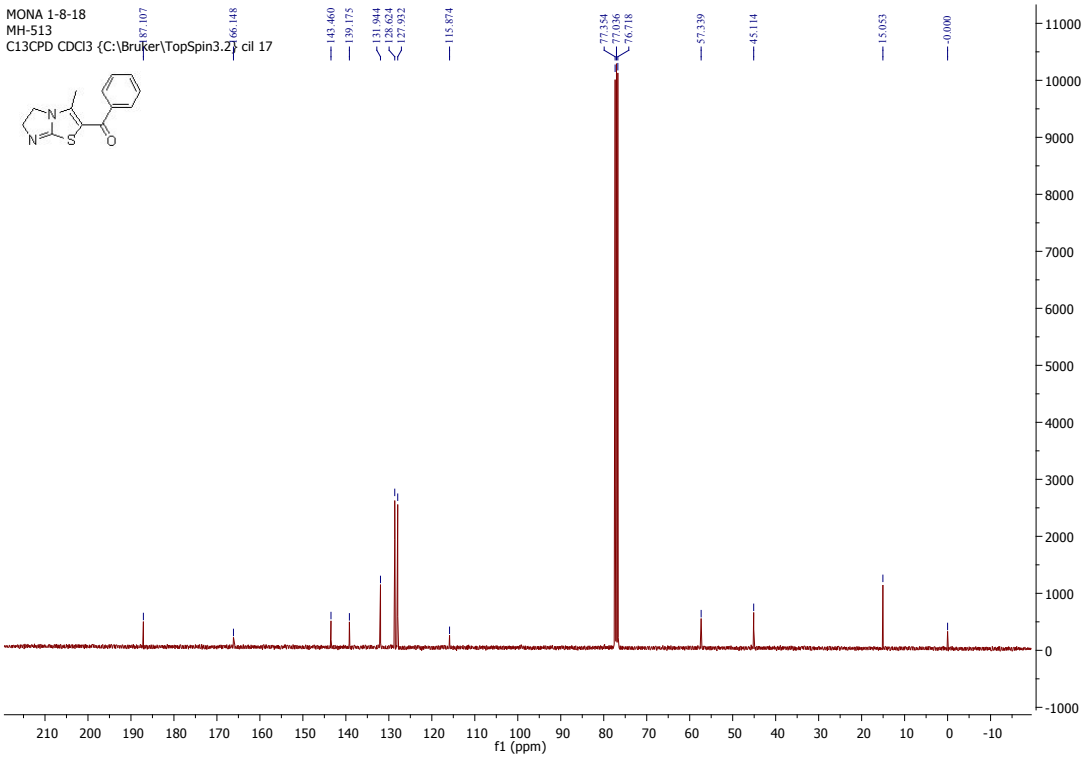

Figure S9b. ^{13}C{^{1}H} NMR spectrum of **3e** in $CDCl_3$ (100 MHz).

6. 2-(4-Fluorobenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3f)**

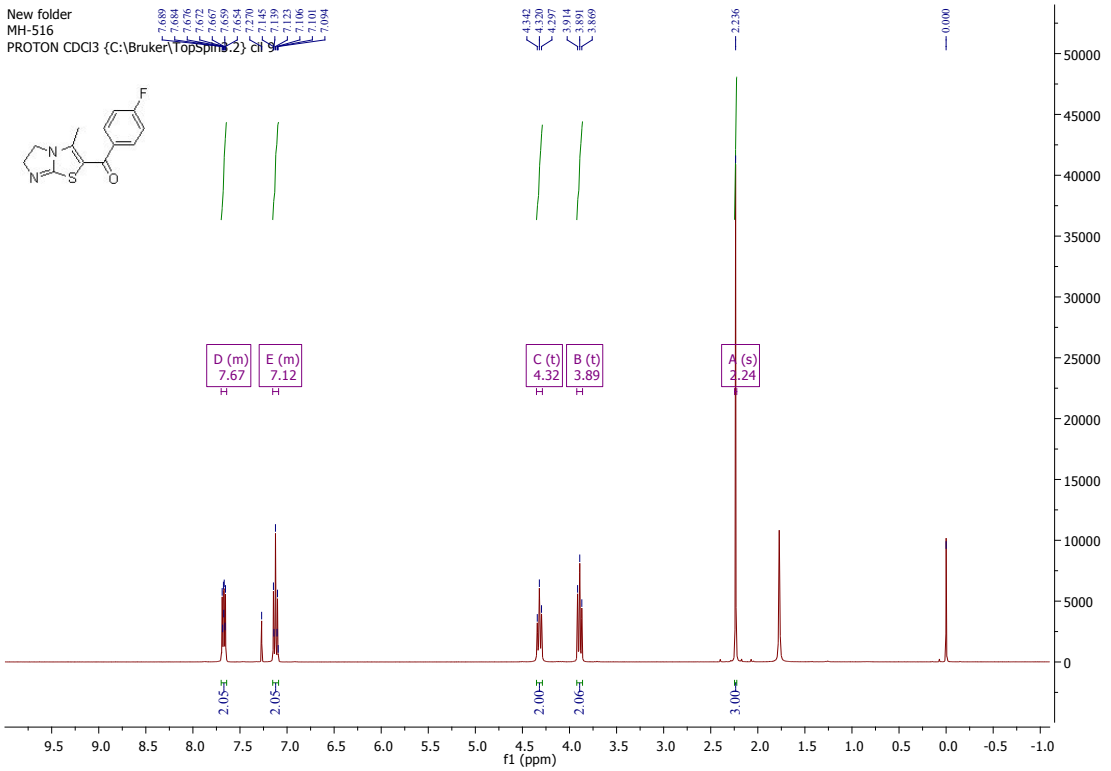

Figure S10a. ^{1}H NMR spectrum of **3f** in $CDCl_3$ (400 MHz).

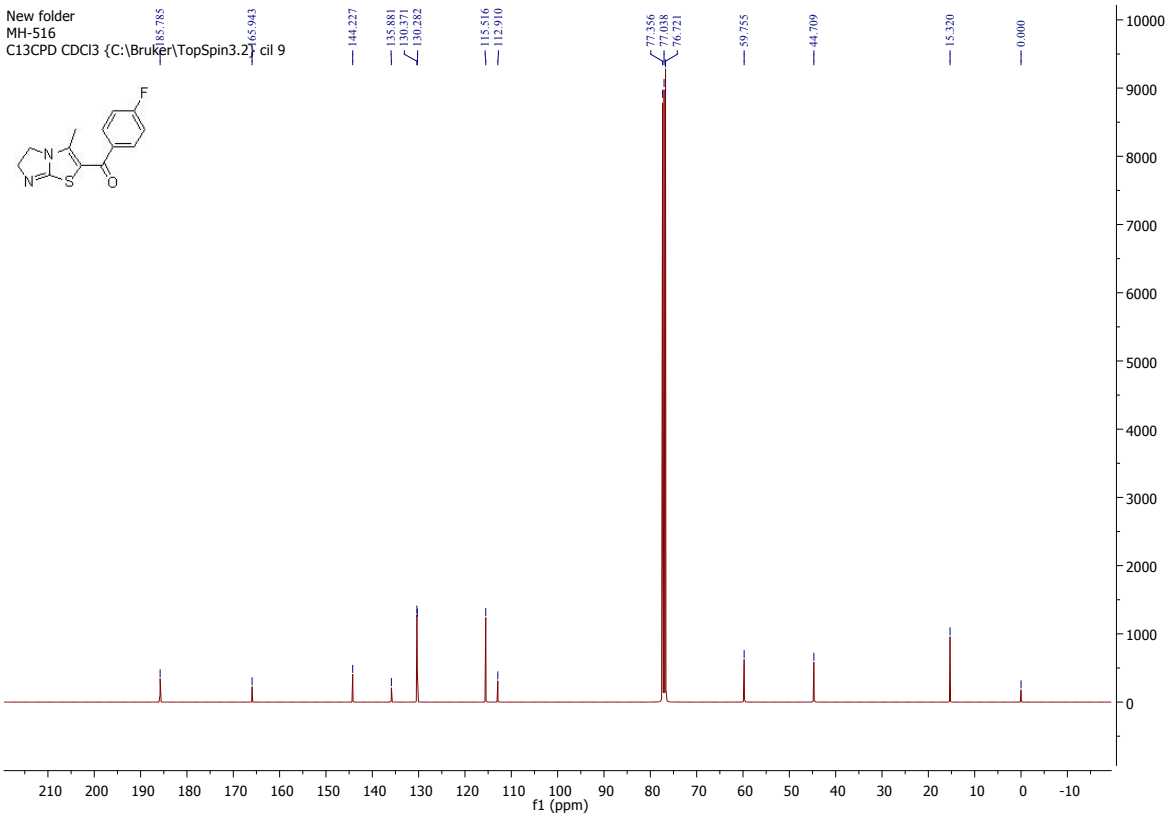

Figure S10b. $^{13}C\{^{1}H\}$ NMR spectrum of **3f** in $CDCl_3$ (100 MHz).

7. 2-(4-Chlorobenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3g)**

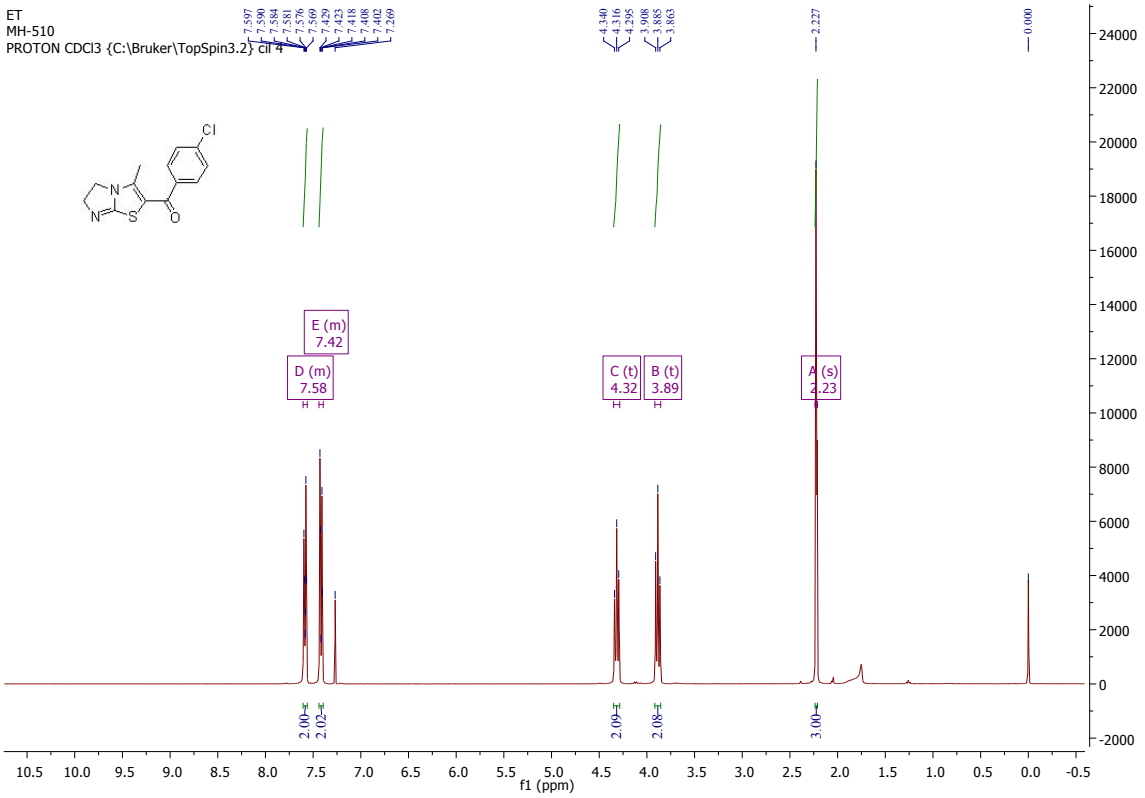

Figure S11a. ^{1}H NMR spectrum of **3g** in $CDCl_3$ (400 MHz).

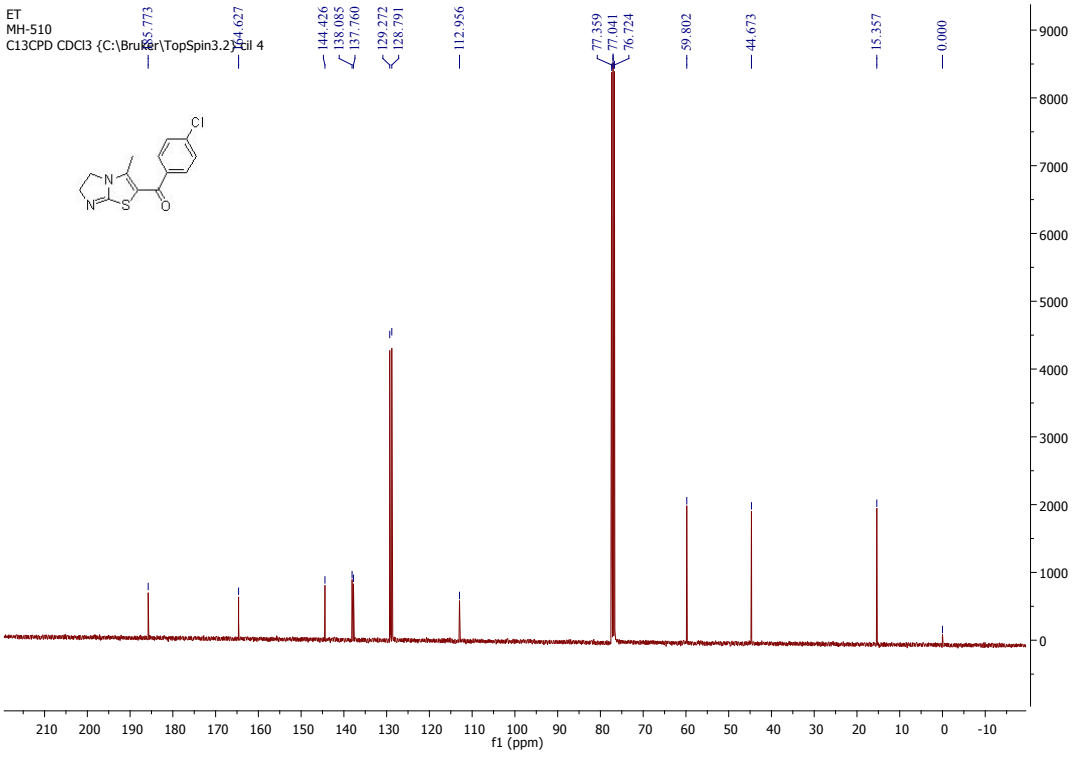

Figure S11b. $^{13}C\{^{1}H\}$ NMR spectrum of **3g** in $CDCl_3$ (100 MHz).

8. 2-(4-Bromobenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3h)**

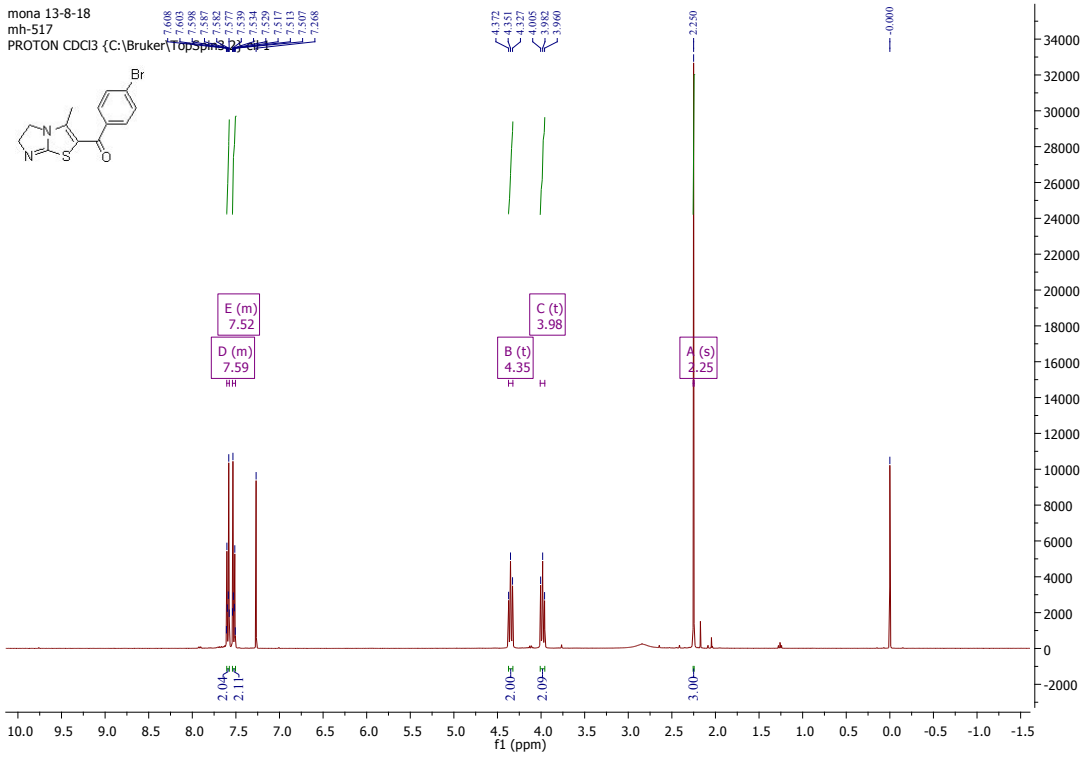

Figure S12a. ^{1}H NMR spectrum of **3h** in $CDCl_3$ (400 MHz).

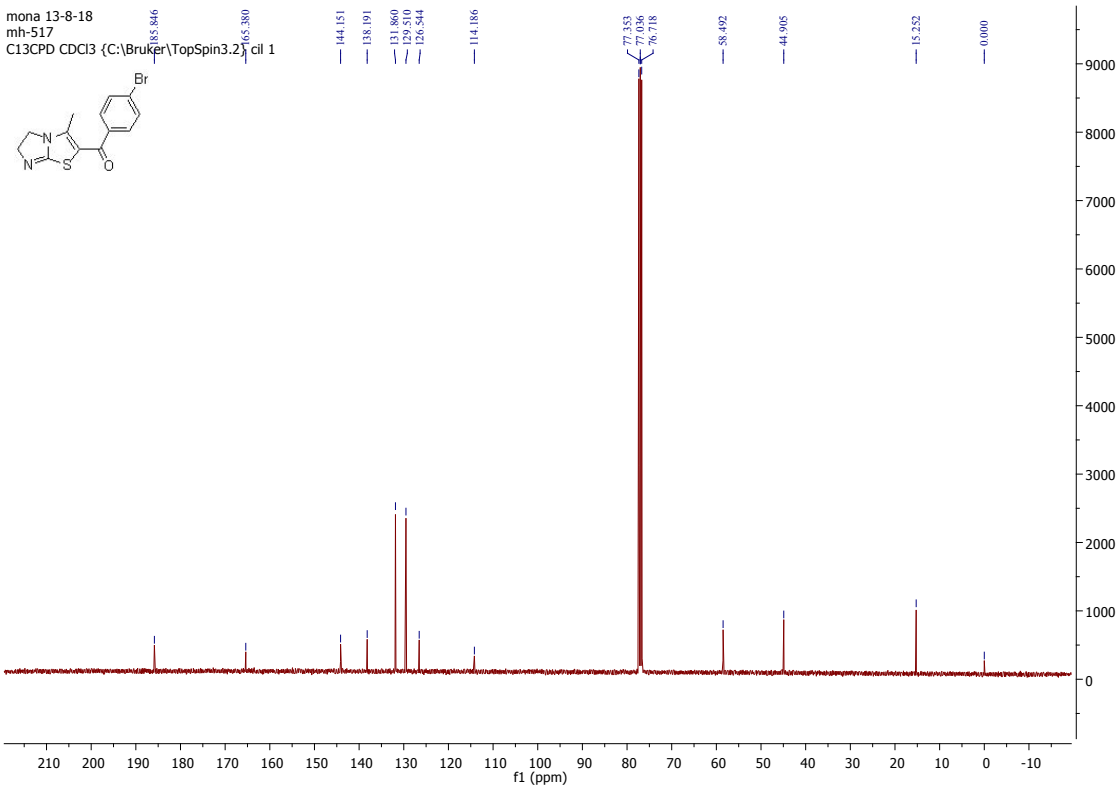

Figure S12b. $^{13}C\{^{1}H\}$ NMR spectrum of **3h** in $CDCl_3$ (100 MHz).

9. 2-(2,4-Dichlorobenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3i)**

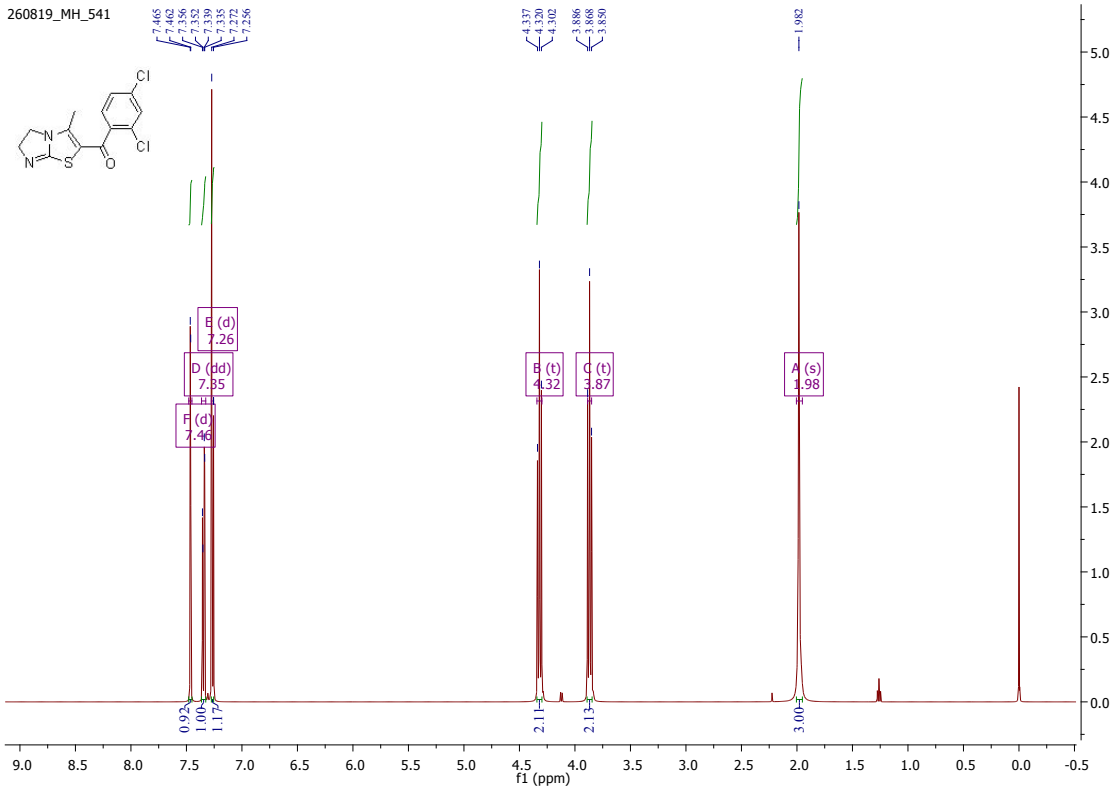

Figure S13a. ^{1}H NMR spectrum of **3i** in $CDCl_3$ (500 MHz).

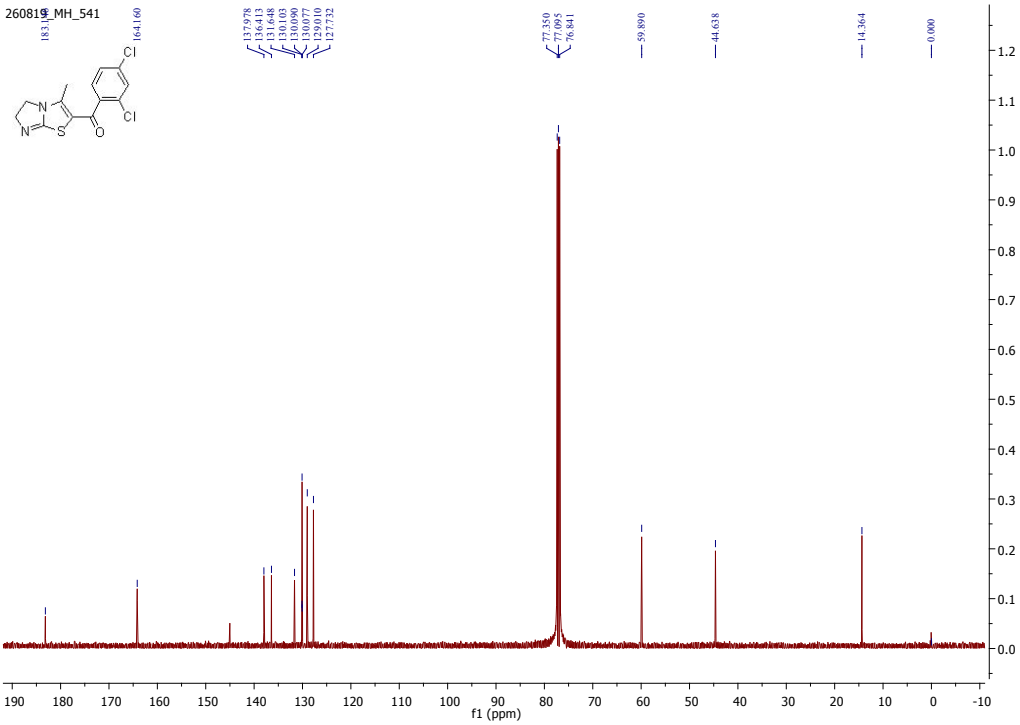

Figure S13b. $^{13}C\{^{1}H\}$ NMR spectrum of **3i** in $CDCl_3$ (125 MHz).

10. 2-Thienoyl-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3j)**

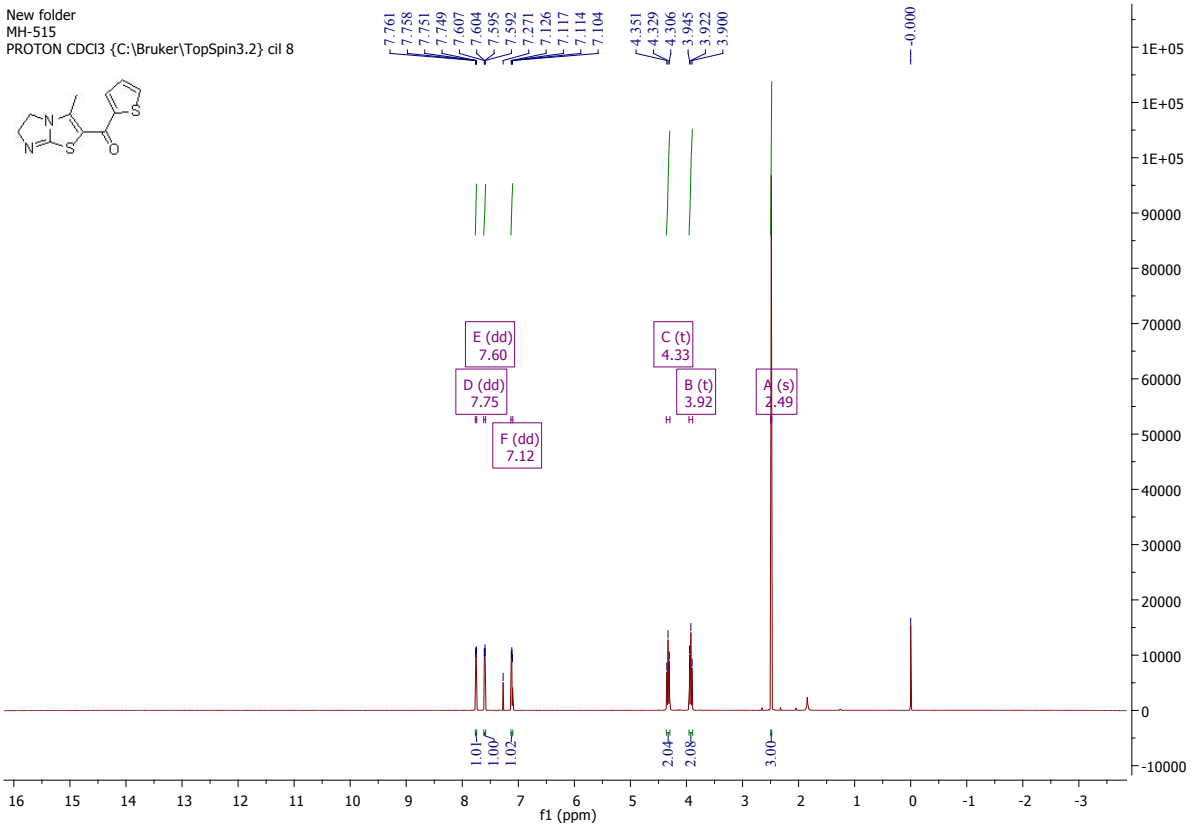

Figure S14a. ^{1}H NMR spectrum of **3j** in $CDCl_3$ (400 MHz).

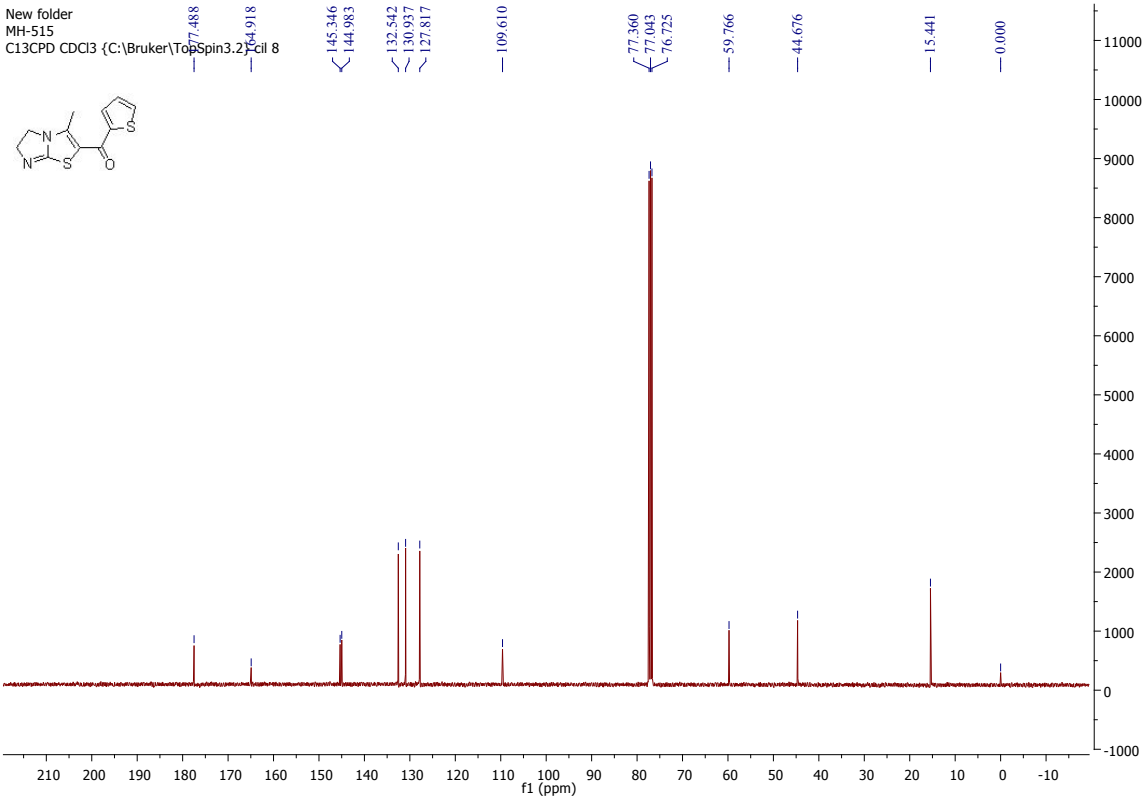

Figure S14b. $^{13}C\{^{1}H\}$ NMR spectrum of **3j** in $CDCl_3$ (100 MHz).

2D NMR (HMBC & HMQC)

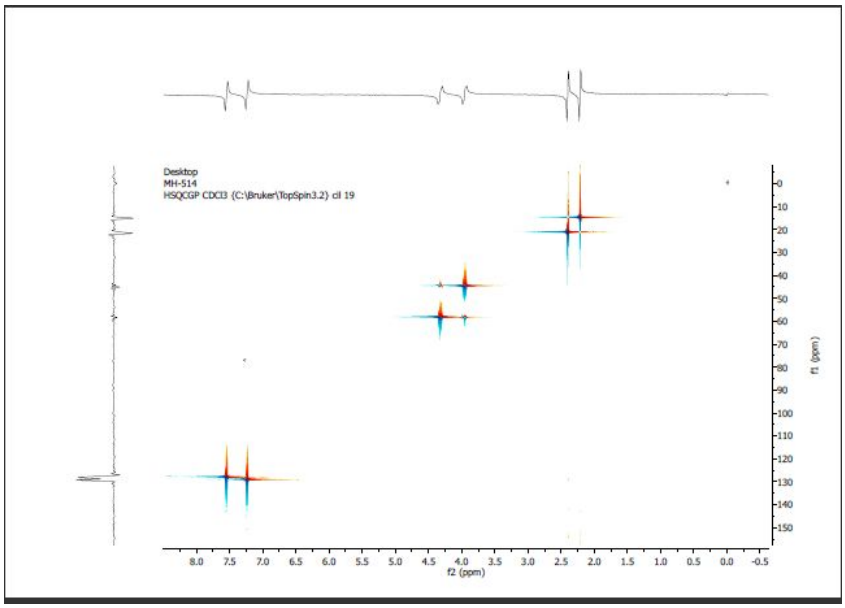

Figure S15a. HMQC of **3a**

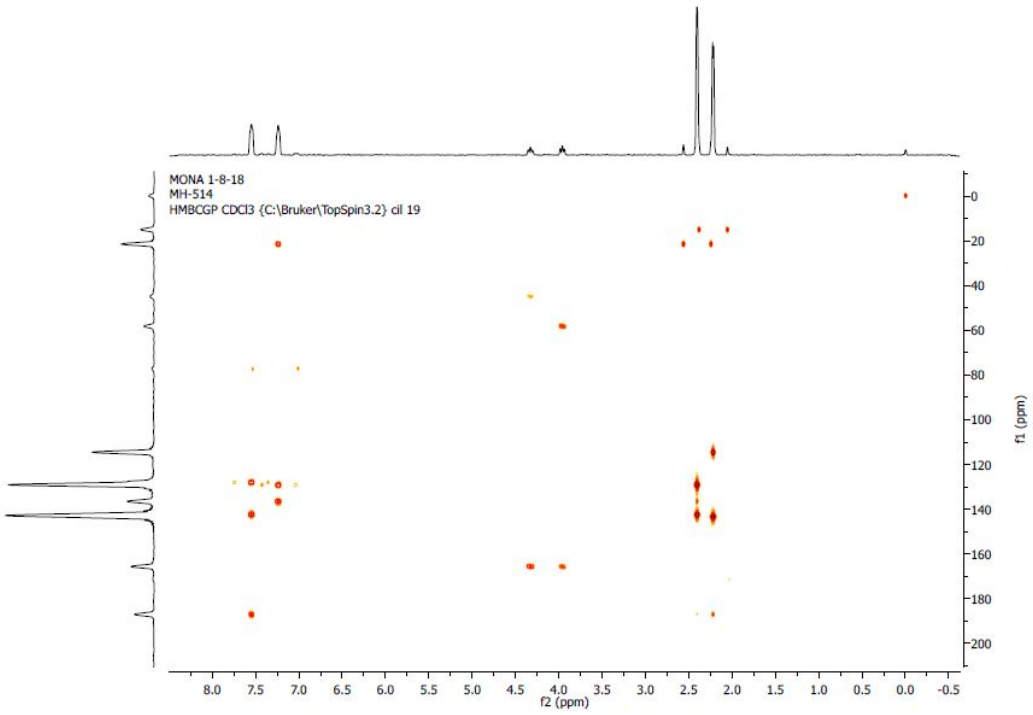

Figure S15b. HMBC of **3a**

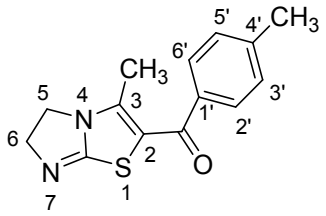

Table S1: 2D NMR correlation results for compound **3a**

Chemical shifts (δ in ppm)	**gs-HMQC correlation**	**gs-HMBC correlation**	**Assignments**
187.0	---	7.55 (H2′/H6′)	CO
		2.22 (3-CH_3)	
165.6	---	4.33 (H5)	C8
		3.96 (H6)	
143.3	---	2.22 (3-CH_3)	C3
142.4	---	7.55 (H2′/H6′)	C4′
		2.41 (4-$CH_3C_6H_4$)	
136.7	---	7.24 (H3′/H5′)	C1′
129.1	7.24 (H3′/H5′)	7.24 (H3′/H5′)	C3′/C5′
		2.41 (4-$CH_3C_6H_4$)	
128.0	7.55 (H2′/H6′)	7.55 (H2′/H6′)	C2′/C6′
114.6	---	2.22 (3-CH_3)	C2
58.55	4.33 (H5)	3.96 (H6)	C5
44.9	3.96 (H6)	4.33 (H5)	C6
21.6	2.41 (4-$CH_3C_6H_4$)	7.24 (H3′/H5′)	4- $CH_3C_6H_4$
15.6	2.22 (3-CH_3)		3-CH_3

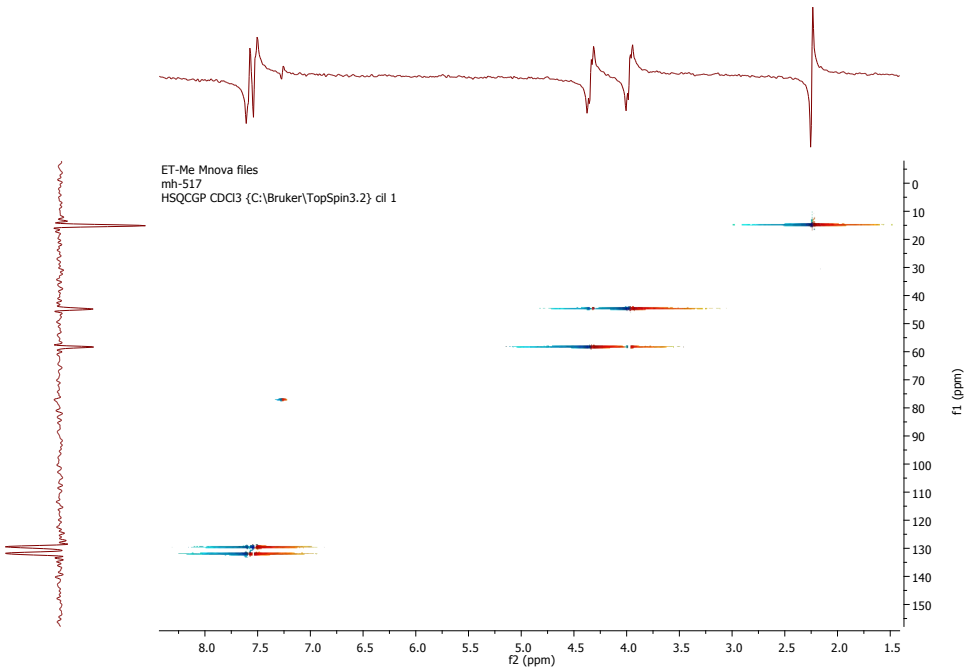

Figure S16a. HMQC of **3h**

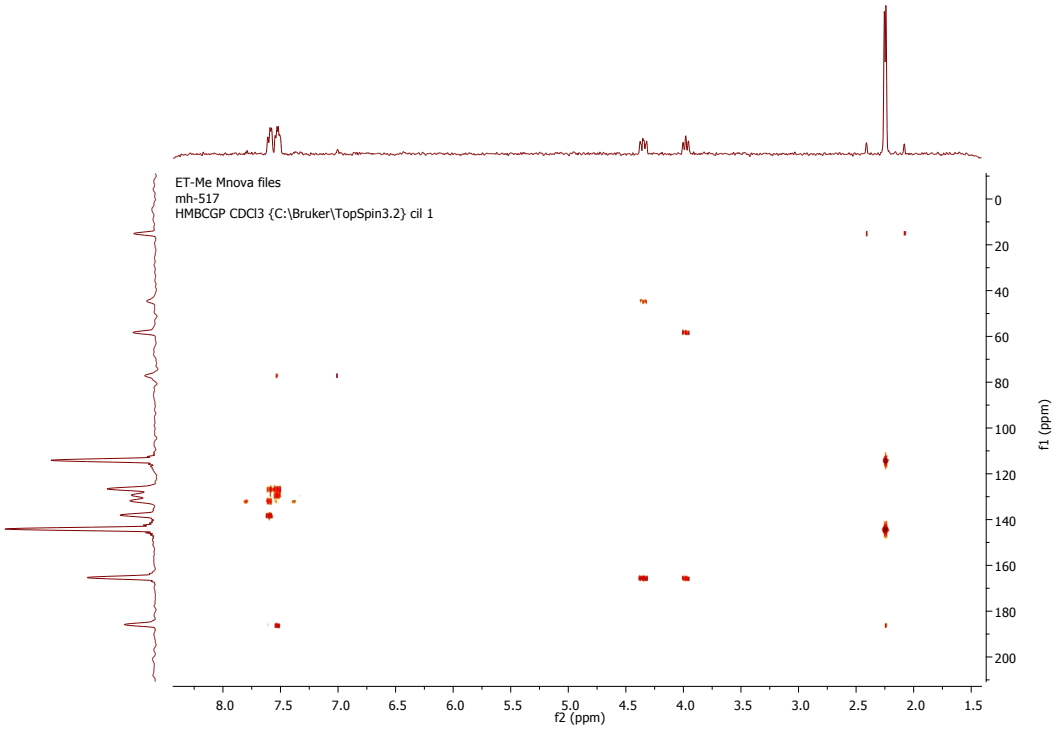

Figure S16b. HMBC of **3h**

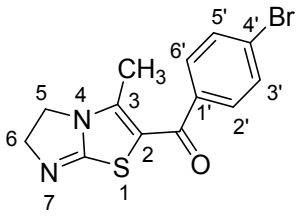

Table S2: 2D NMR correlation results for compound **3h**

Chemical shifts (δ in ppm)	**gs-HMQC correlation**	**gs-HMBC correlation**	**Assignments**
185.8	---	7.60 (H2′/H6′) 2.25 (3-CH_3)	CO
165.3	---	4.35 (H5) 3.98 (H6)	C8
144.1	---	2.25 (3-CH_3)	C3
138.1	---	7.60 (H2′/H6′)	C4′
131.8	---	7.54 (H3′/H5′)	C1′
129.5	7.54 (H3′/H5′)	7.54 (H3′/H5′)	C3′/C5′
126.5	7.60 (H2′/H6′)	7.60 (H2′/H6′)	C2′/C6′
114.1	---	2.25 (3-CH_3)	C2
58.4	4.35 (H5)	3.98 (H6)	C5
44.9	3.98 (H6)	4.35 (H5)	C6
15.2	2.25 (3-CH_3)		3-CH_3

HRMS

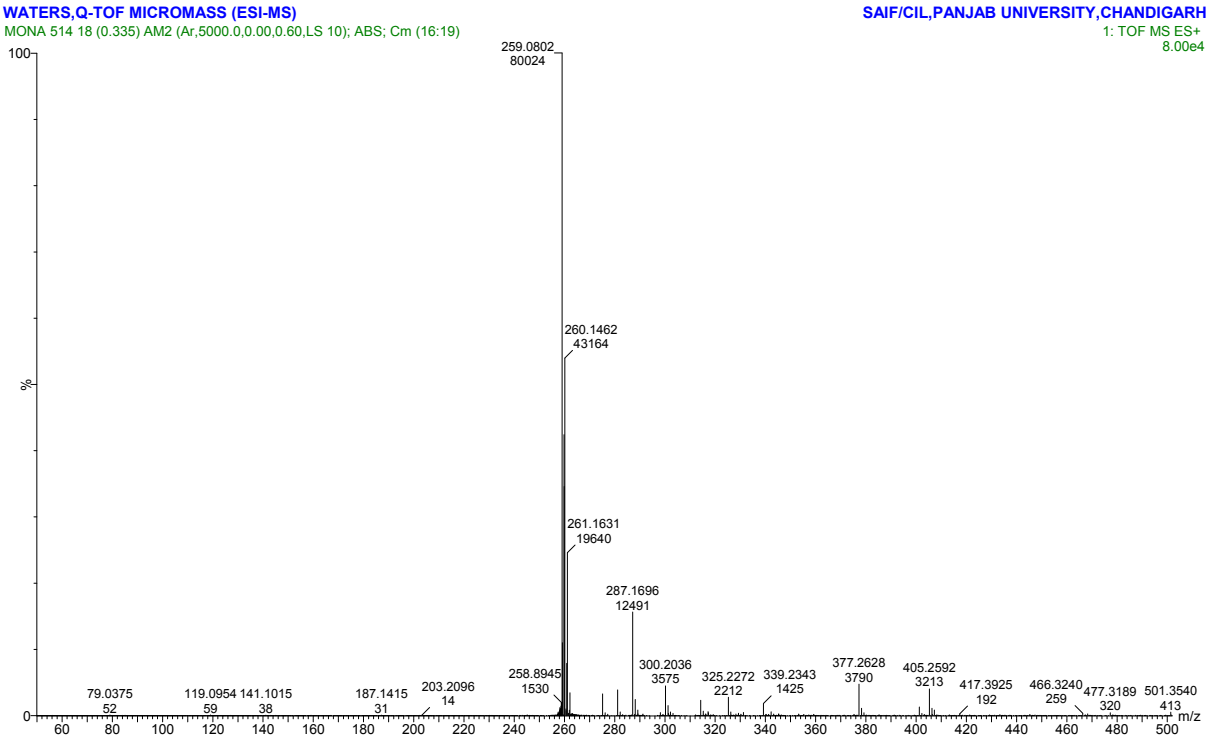

Figure S17. HRMS of 2-(4-Methylbenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3a)**

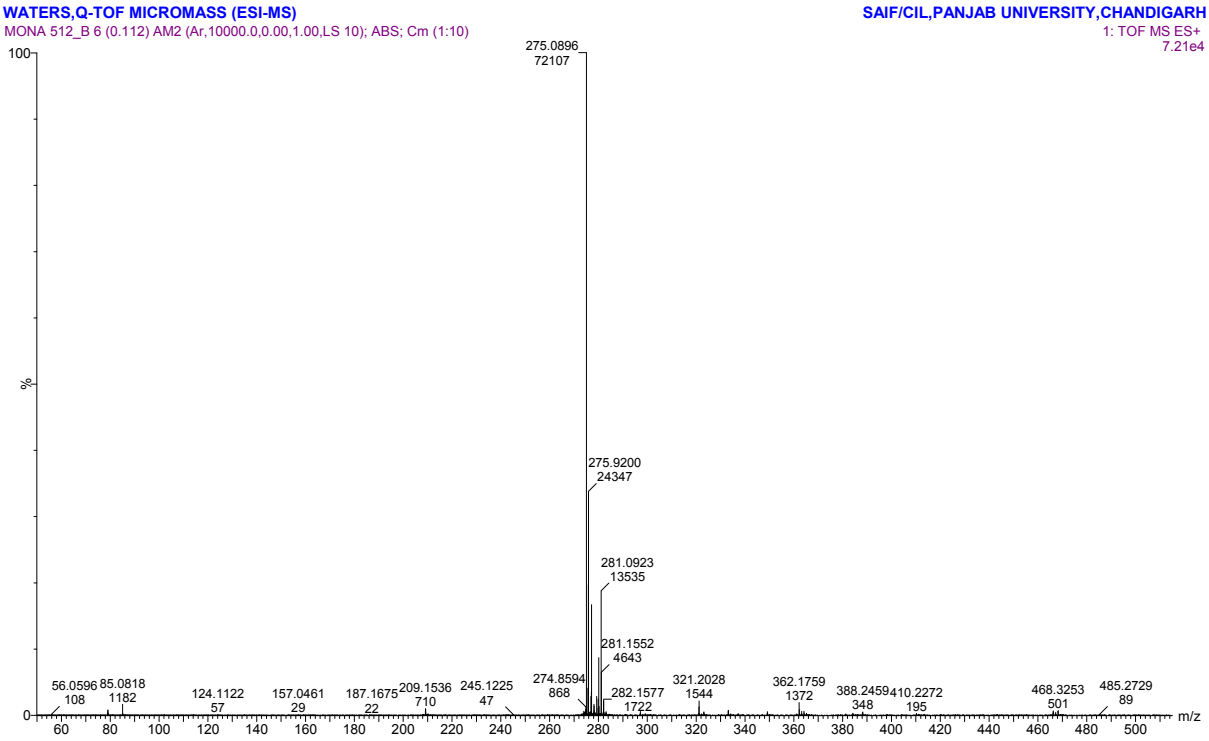

Figure S18. HRMS of 2-(2-Methoxybenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3b)**

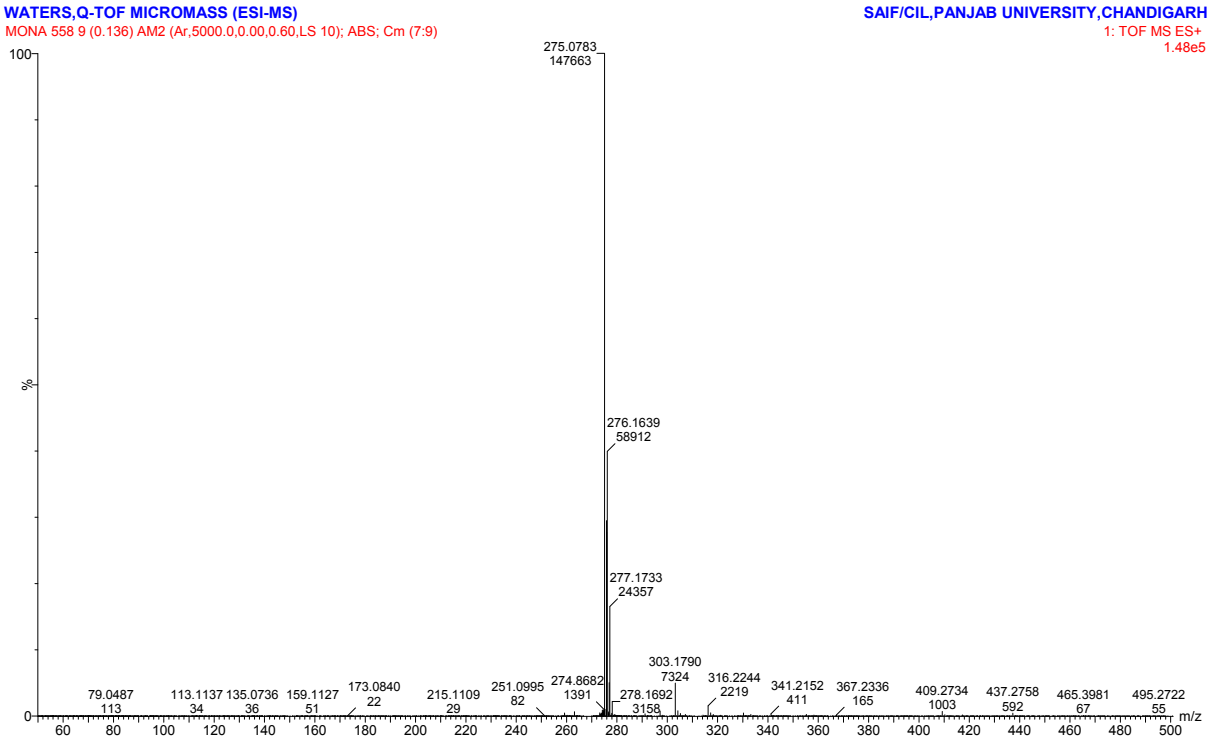

Figure S19. HRMS of 2-(3-Methoxybenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3c)**

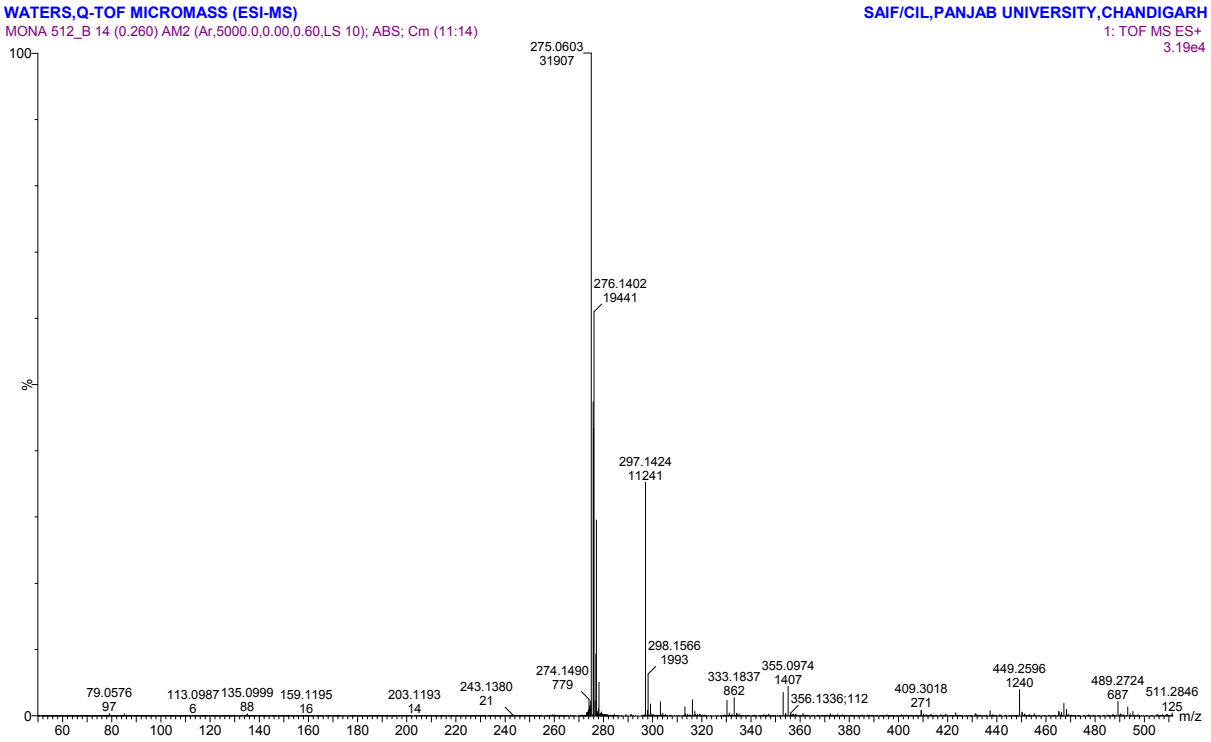

Figure S20. HRMS of 2-(4-Methoxybenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3d)**

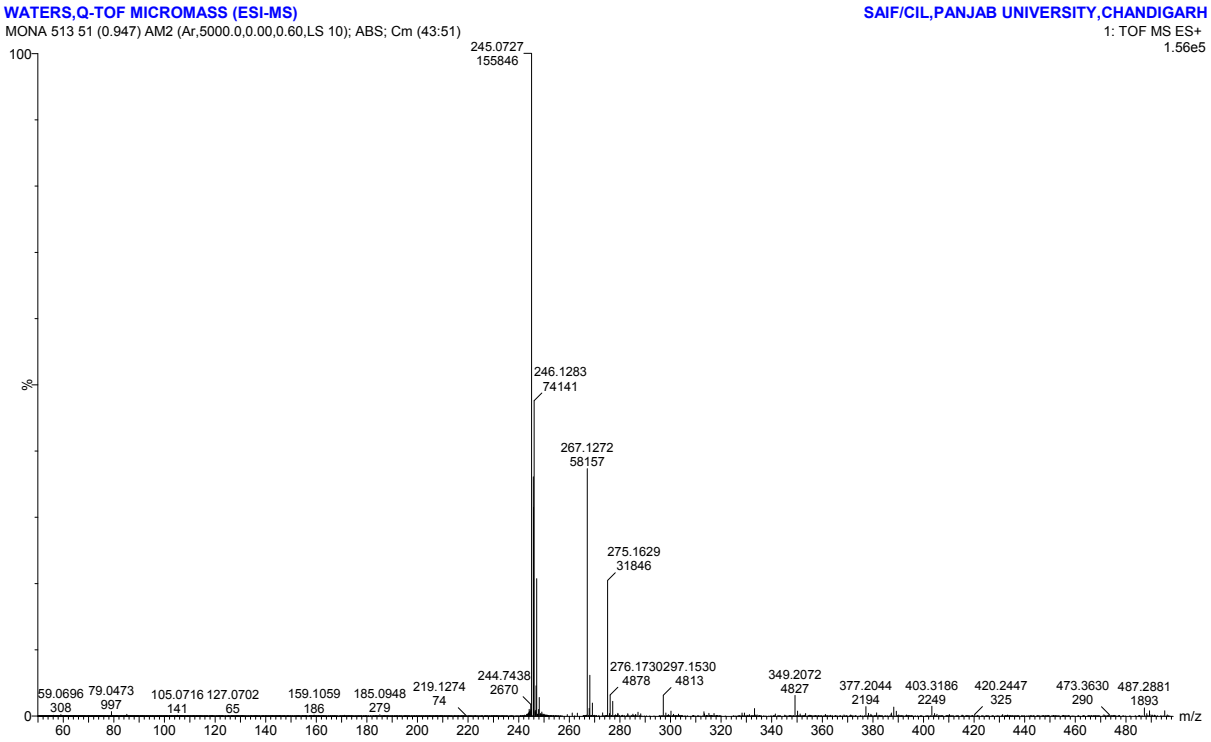

Figure S21. HRMS of 2-Benzoyl-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3e)**

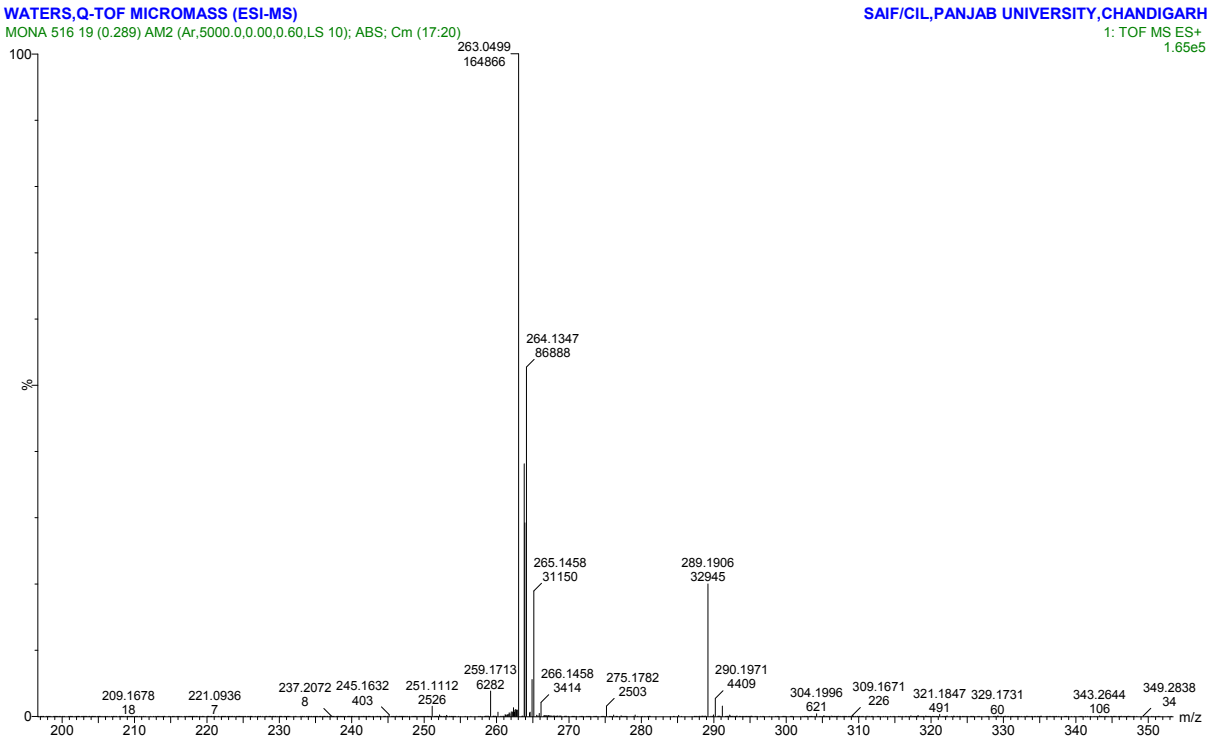

Figure S22. HRMS of 2-(4-Fluorobenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3f)**

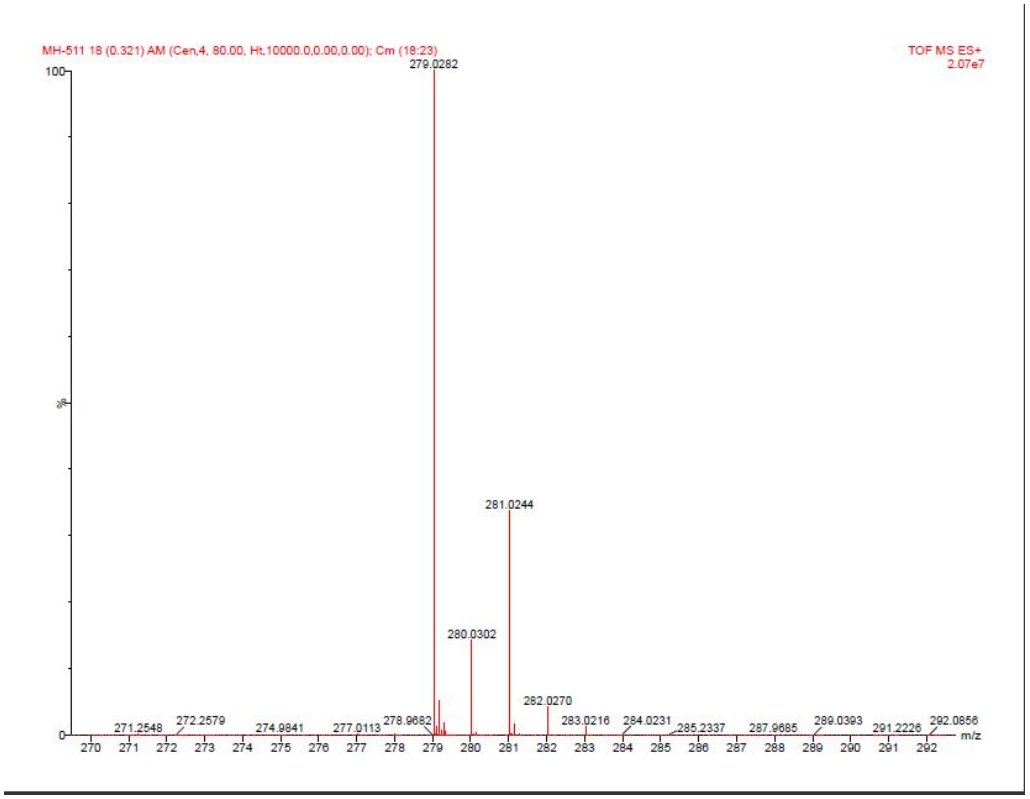

Figure S23. HRMS of 2-(4-Chlorobenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3g)**

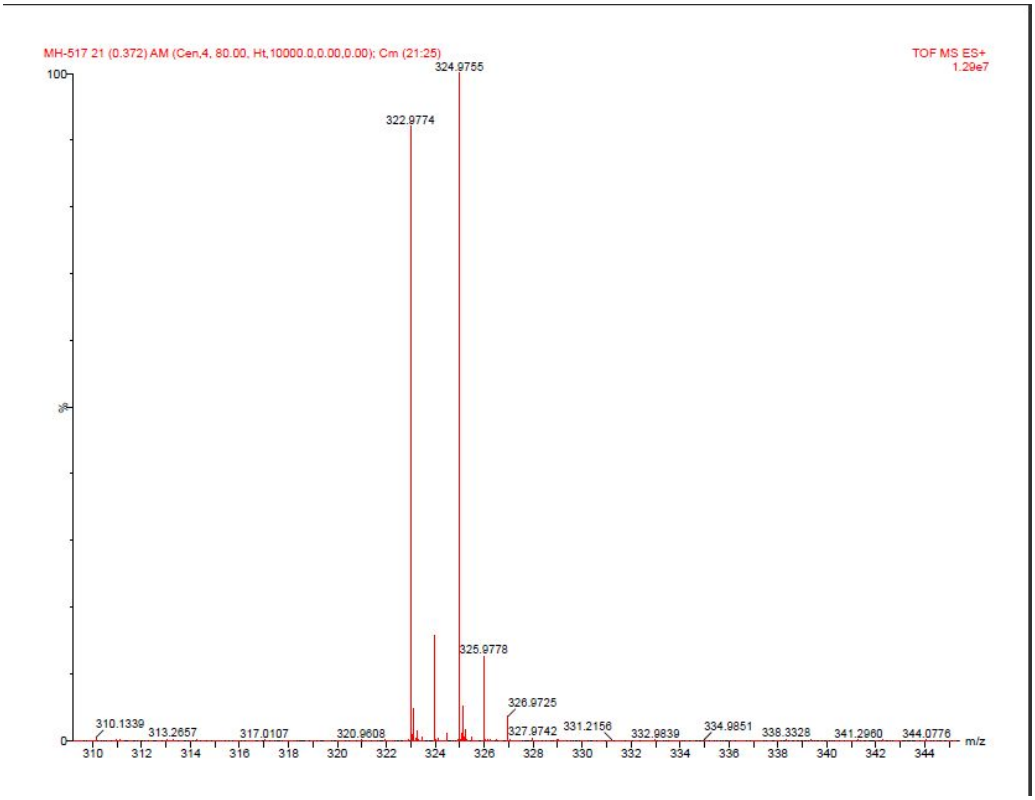

Figure S24. HRMS 2-(4-Bromobenzoyl)-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3h)**

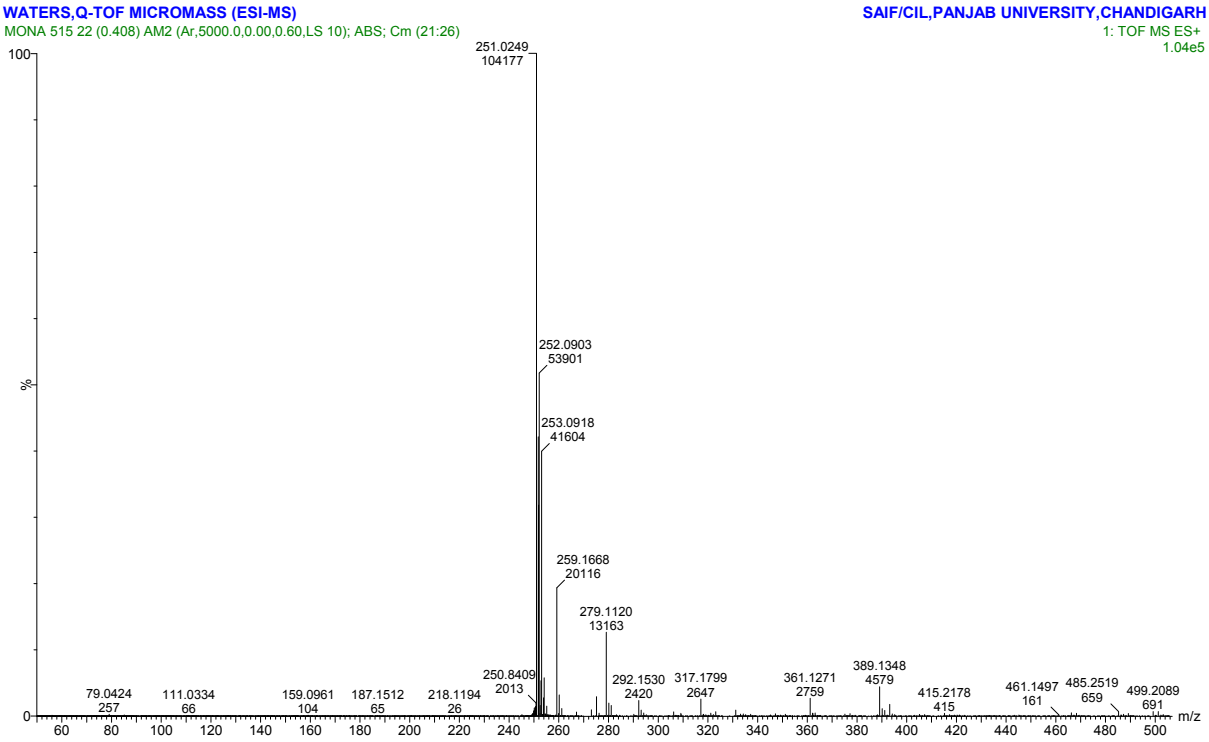

Figure S25. HRMS of 2-Thienoyl-3-methyl-5,6-dihydroimidazo[2,1-*b*]thiazole **(3j)**