

“Ultrasound Assisted Synthesis and *In Silico* Modelling of 1,2,4-triazole Coupled Acetamide Derivatives of 2-(4-isobutylphenyl) propanoic acid as Potential Anticancer Agents”

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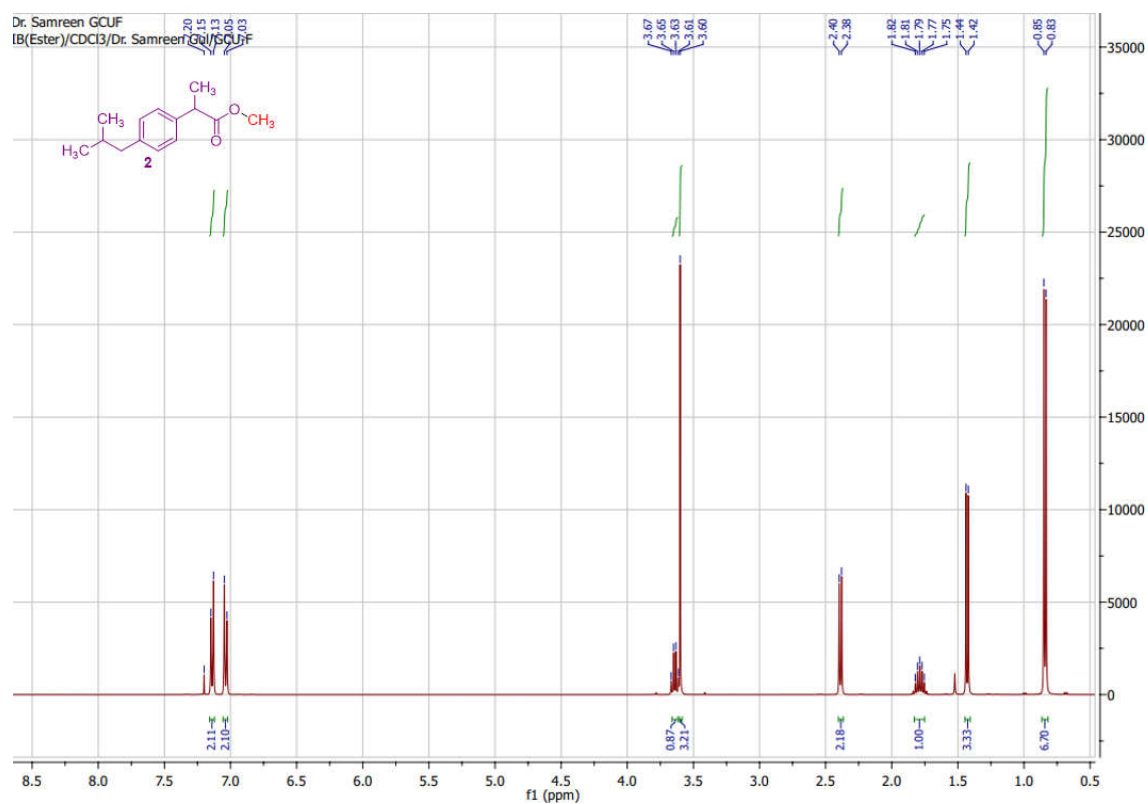


Figure S1: ¹H NMR spectrum of compound 2 (Full)

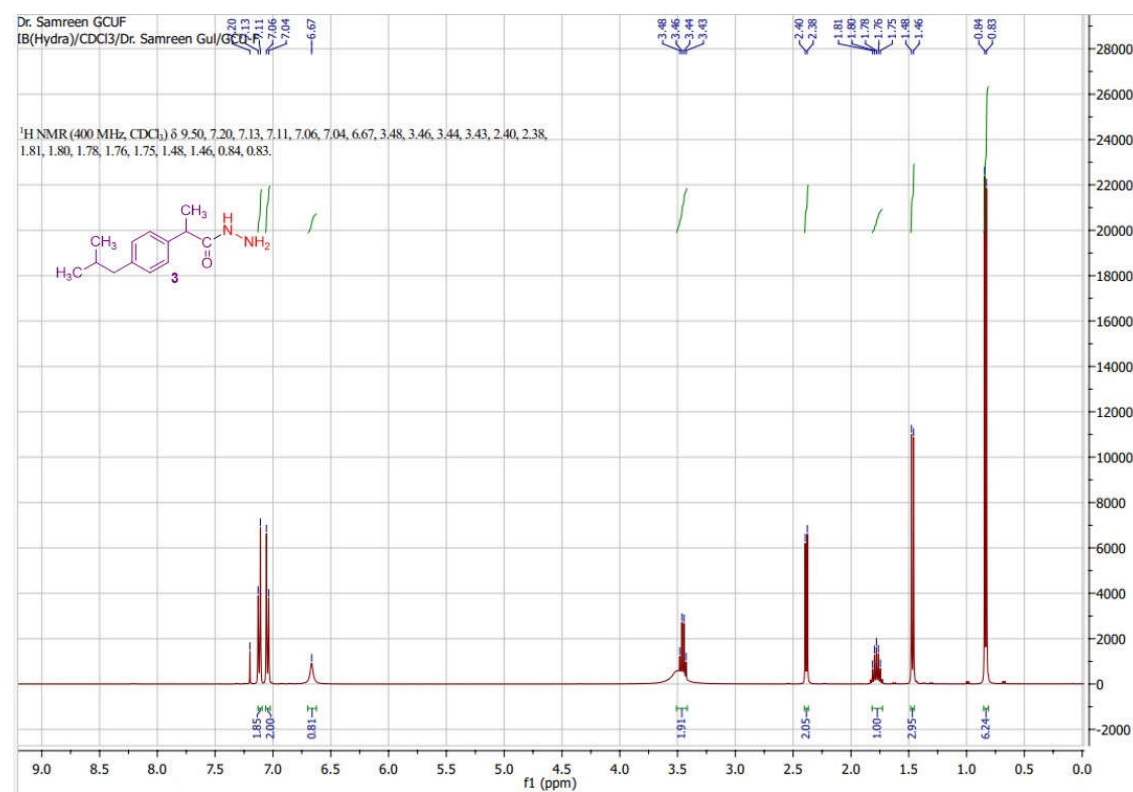
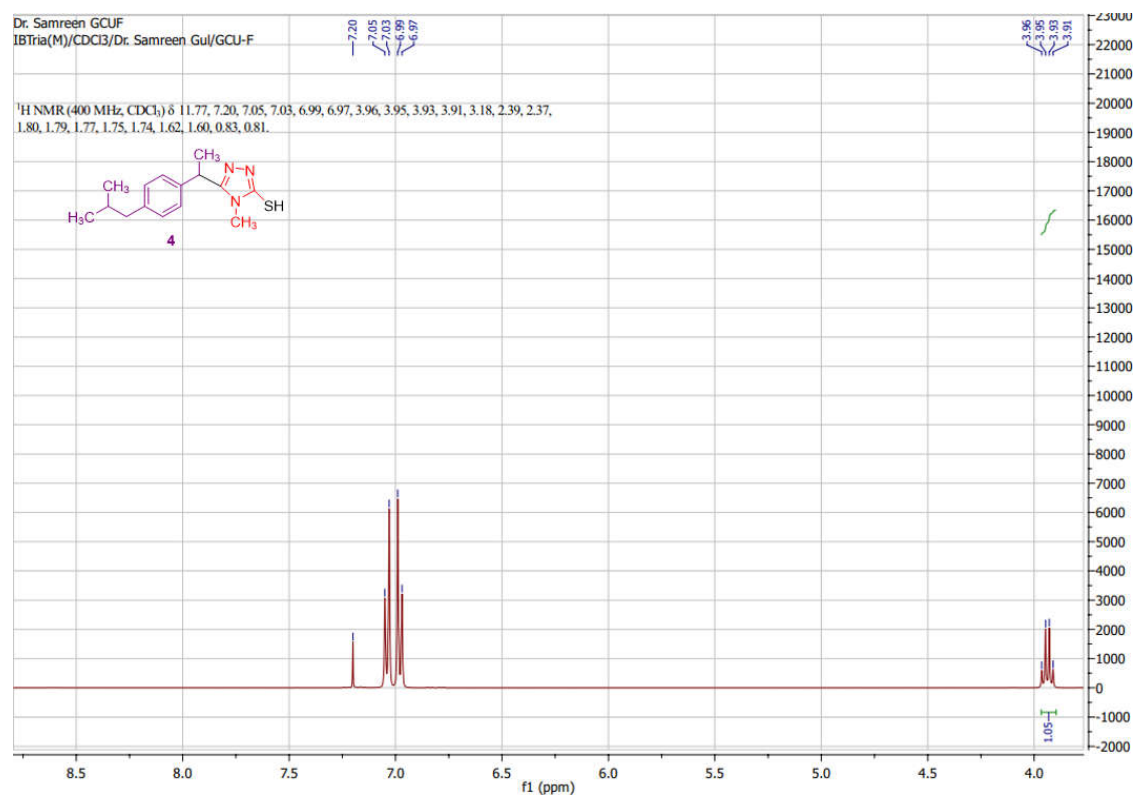
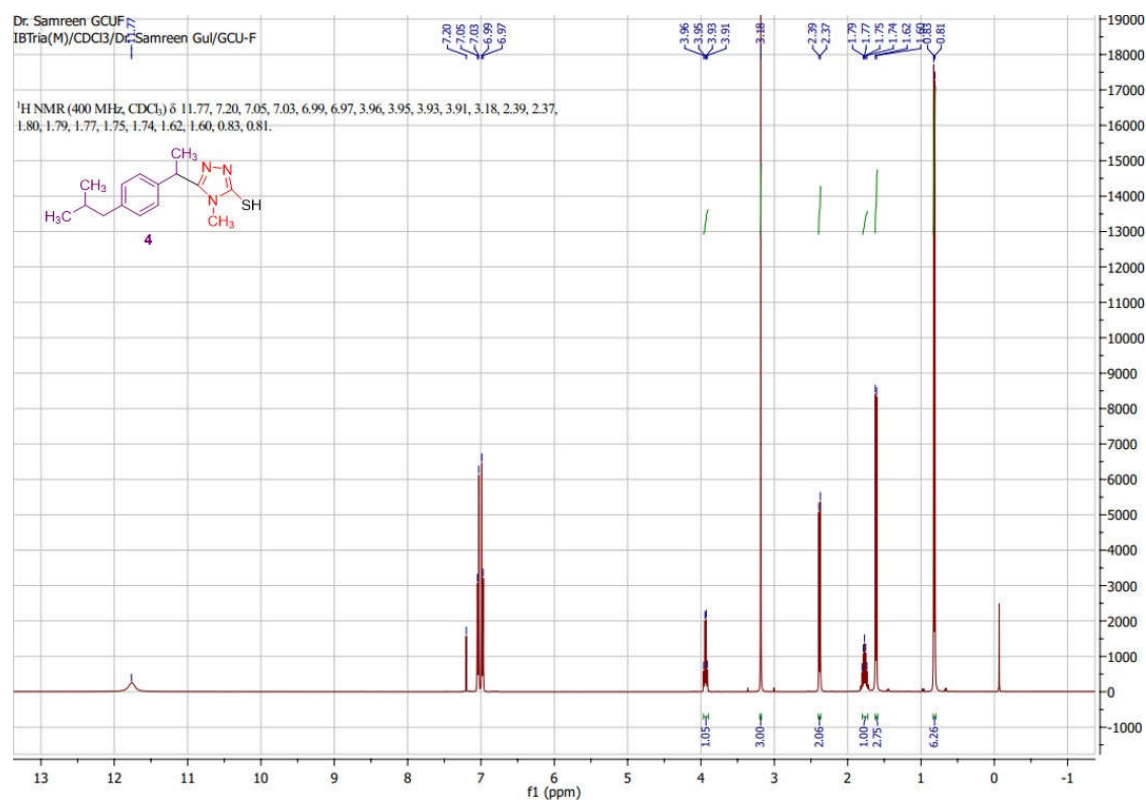


Figure S2: ¹H NMR spectrum of compound 3 (Full)



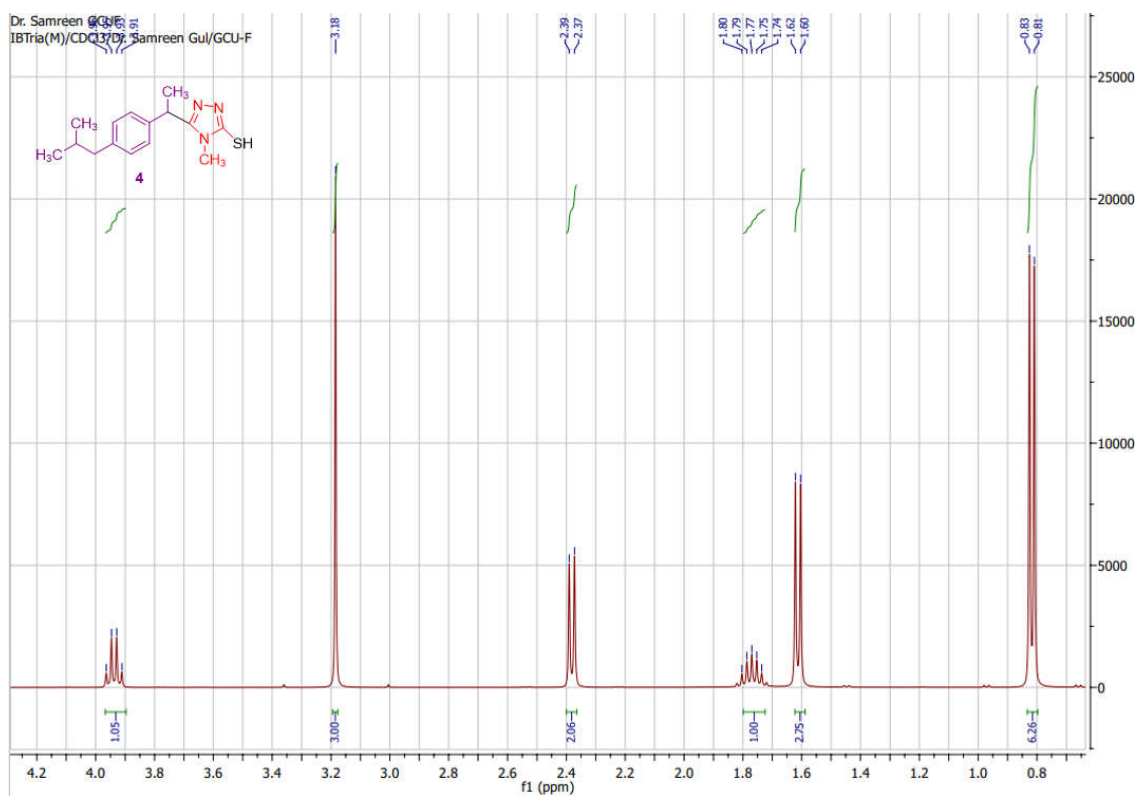


Figure S5. ¹H NMR spectrum of compound 4 (aliphatic region)

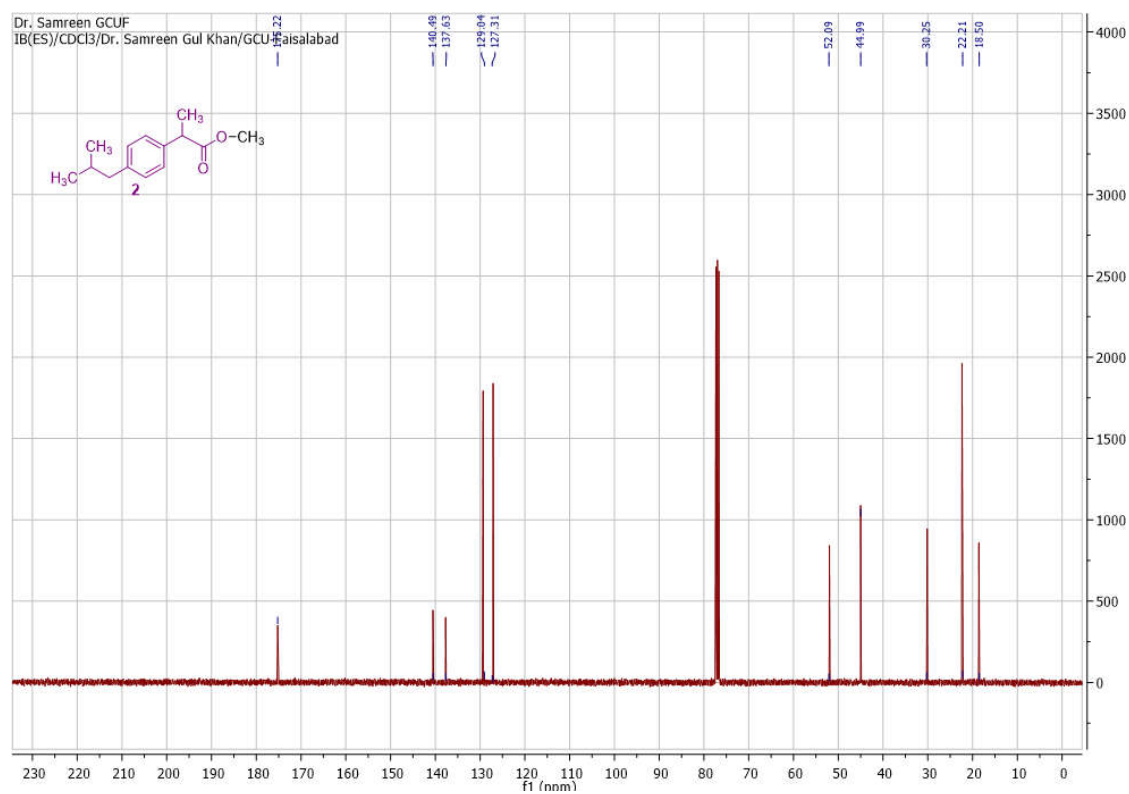


Figure S6. ¹³C NMR spectrum of compound 2

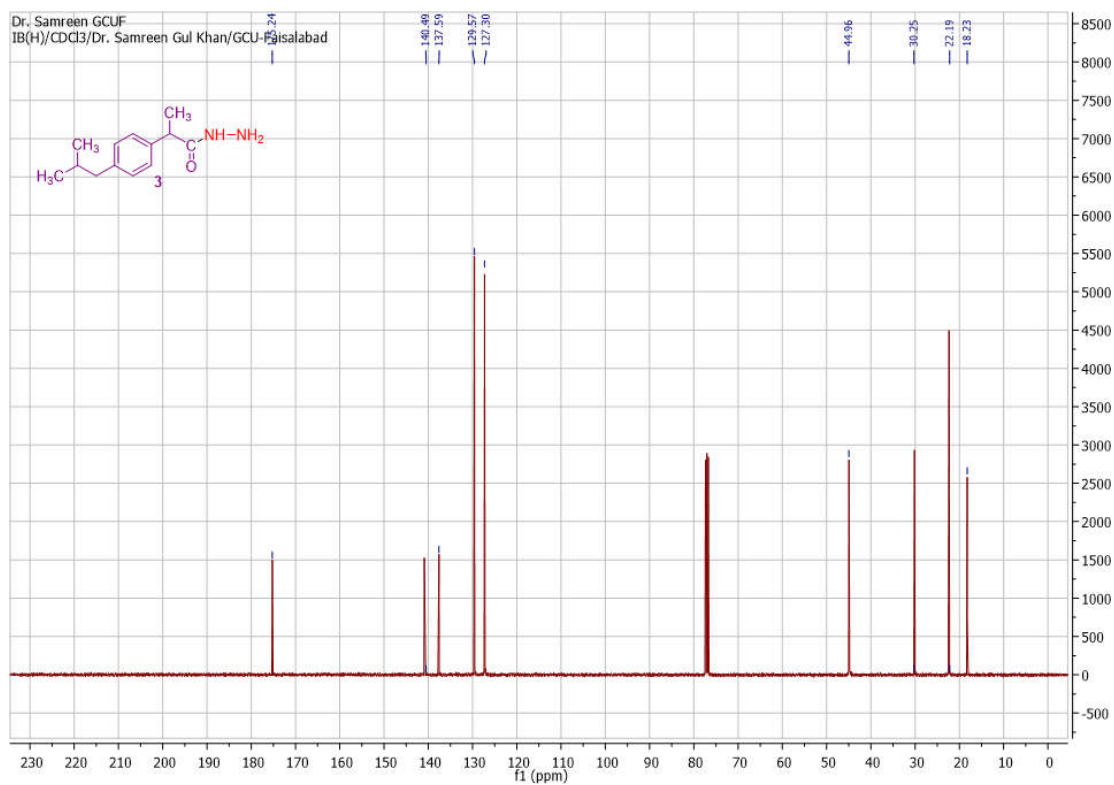


Figure S7. ¹³C NMR spectrum of compound 3

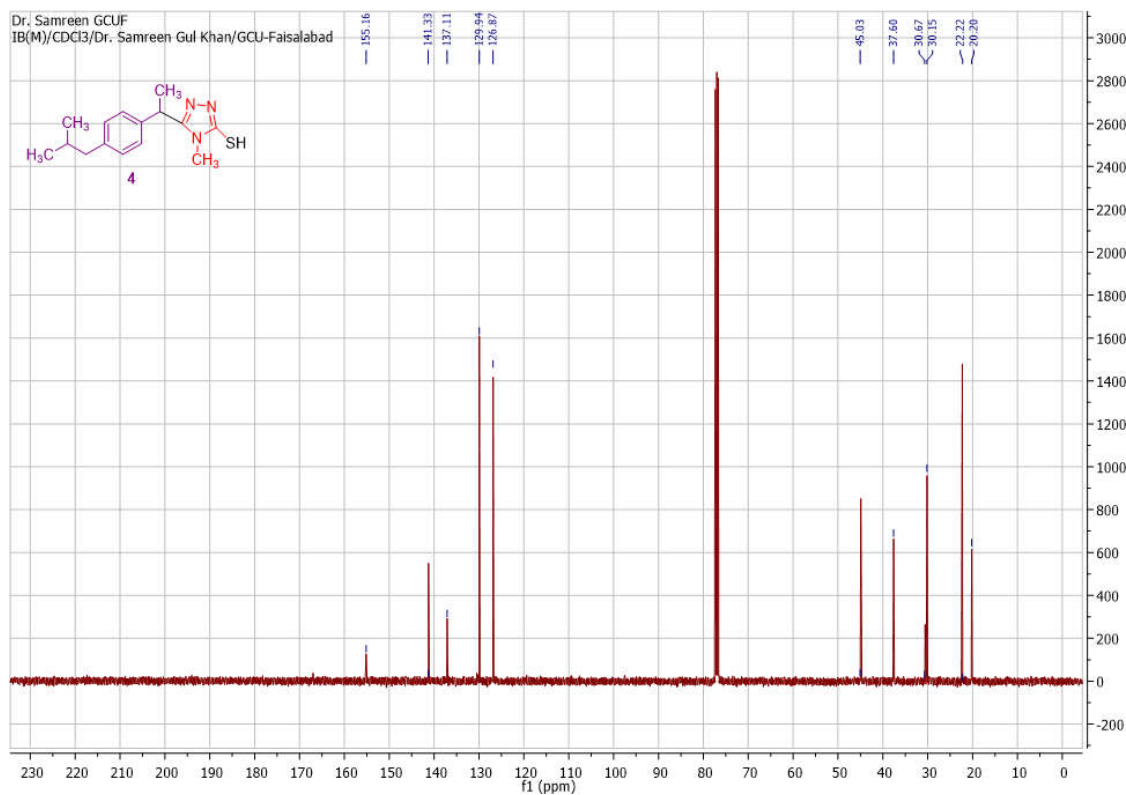


Figure S8. ¹³C NMR spectrum of compound 4

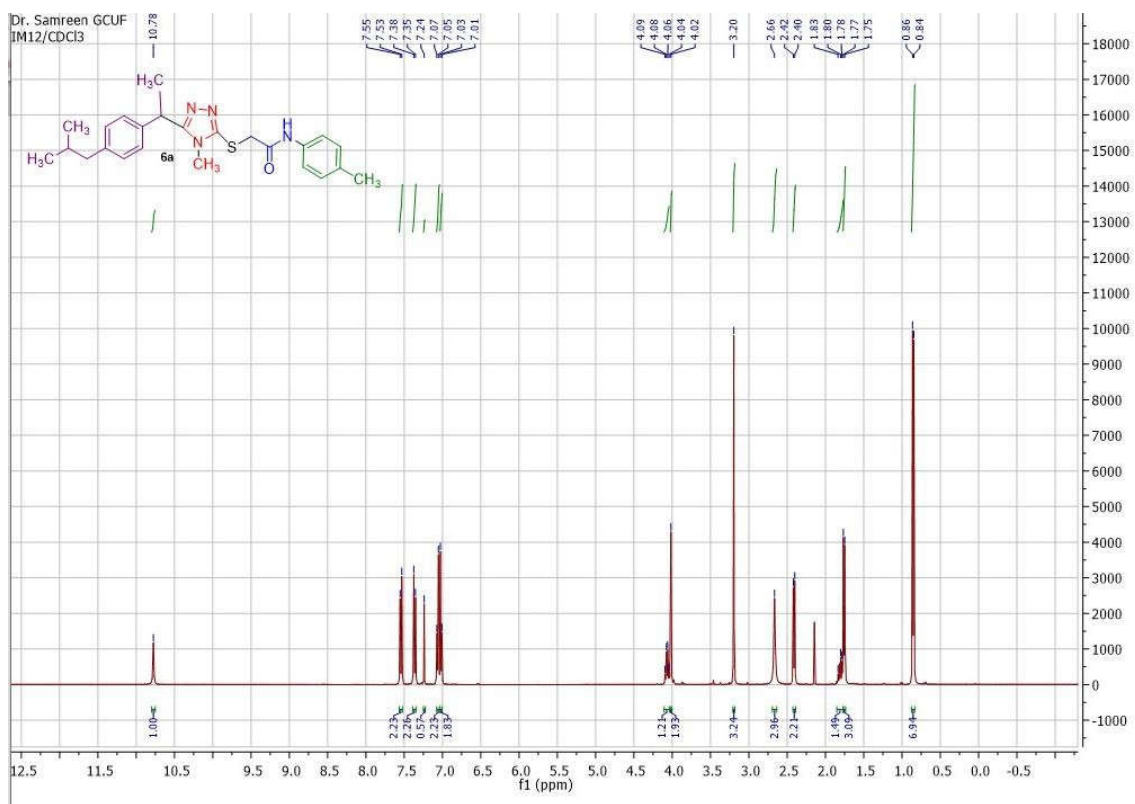


Figure S9: ¹H NMR spectrum of compound **6a** (Full)

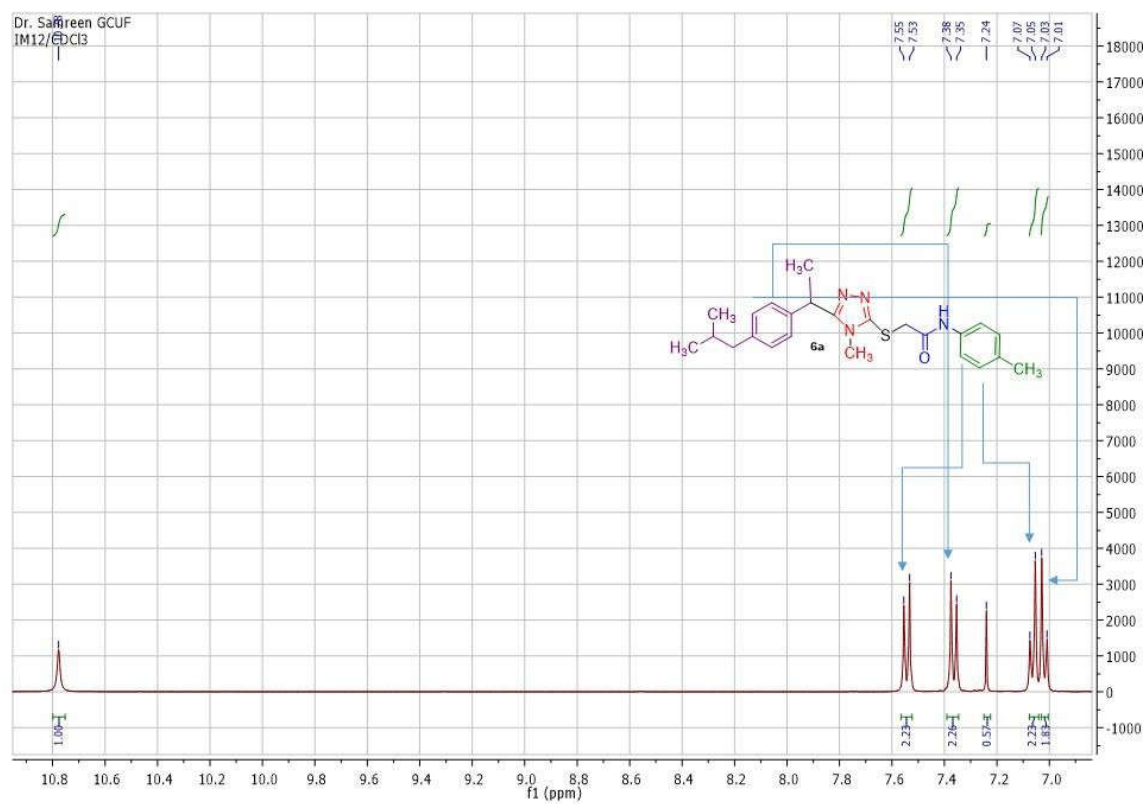


Figure S10. ¹H NMR spectrum of compound **6a** (aromatic region)

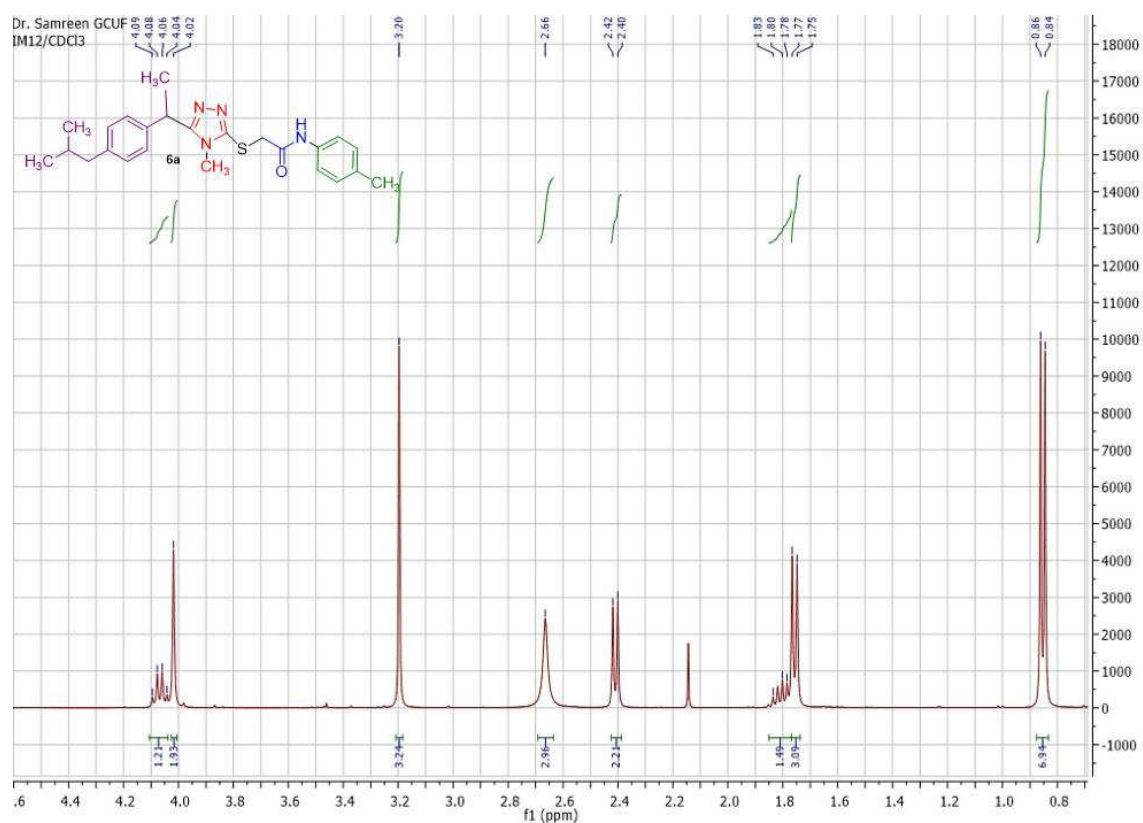


Figure S11. ¹H NMR spectrum of compound **6a** (aliphatic region)

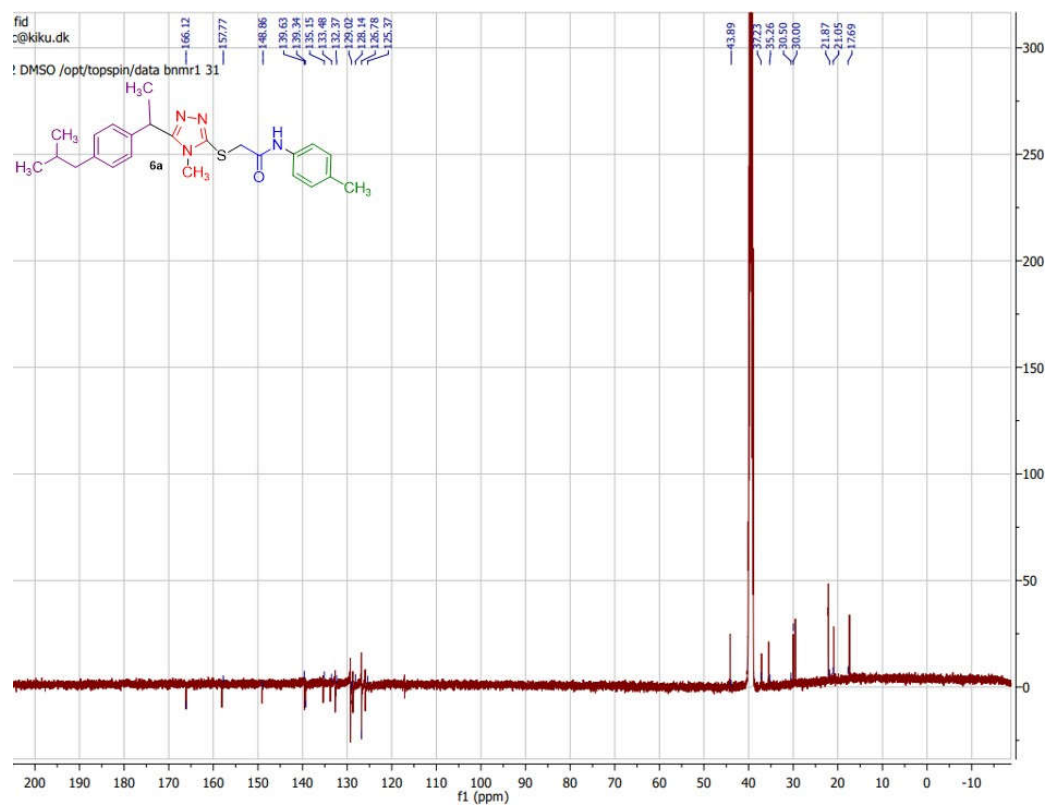


Figure S12. ¹³C NMR spectrum of compound **6a** (Full spectrum)

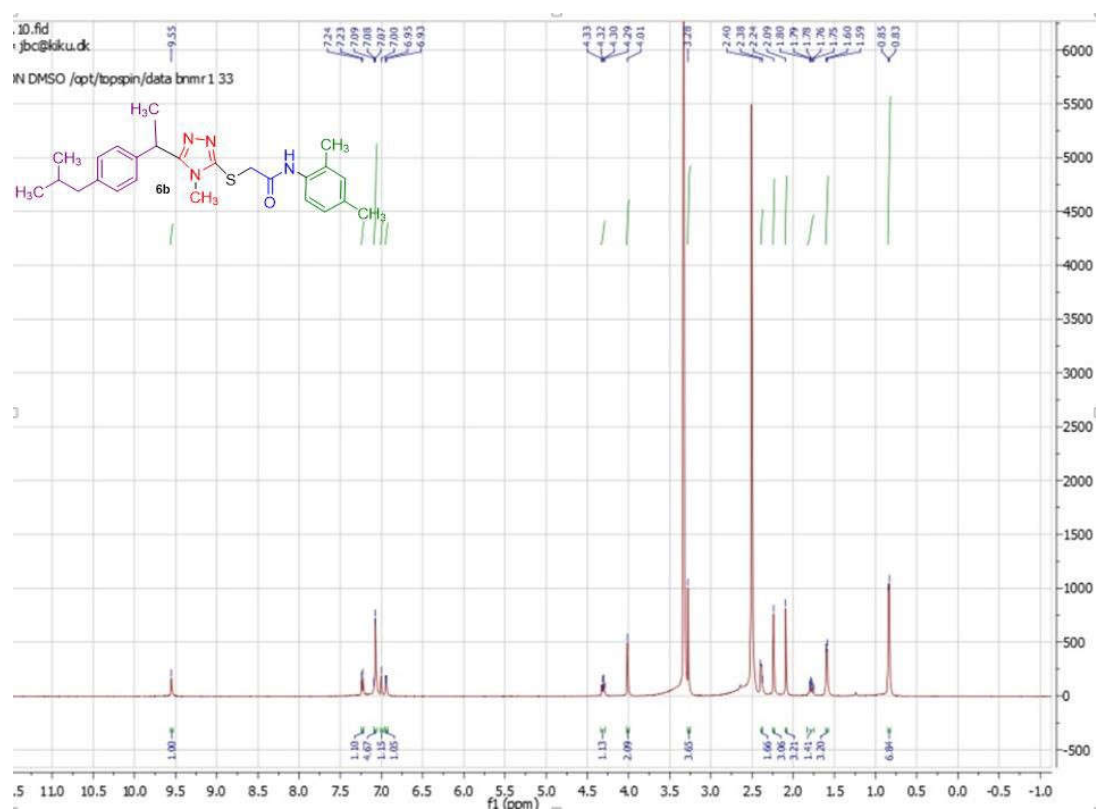


Figure S13. ^1H NMR spectrum of compound **6b** (Full spectrum)

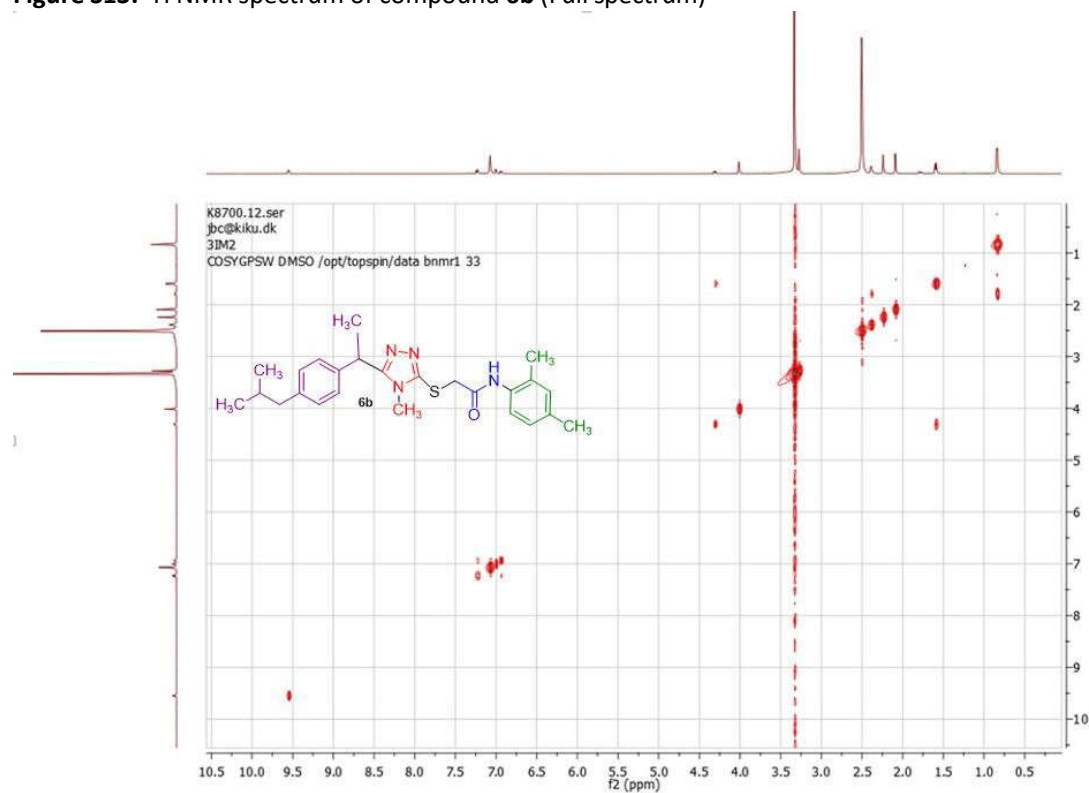
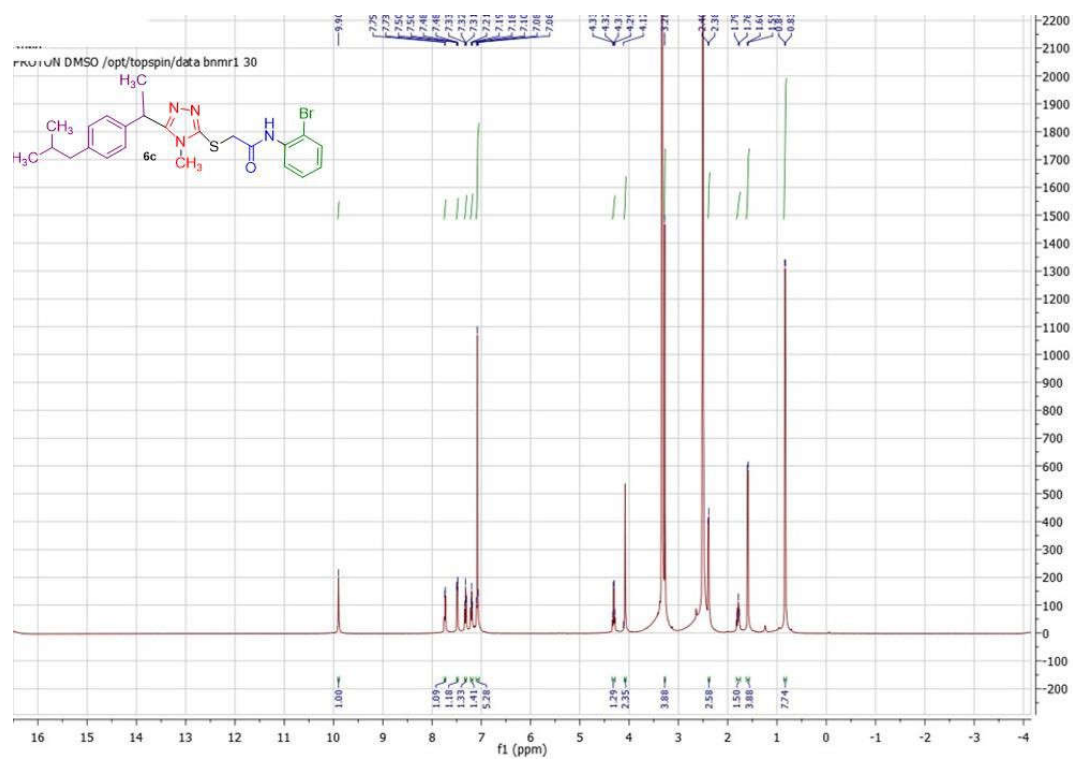
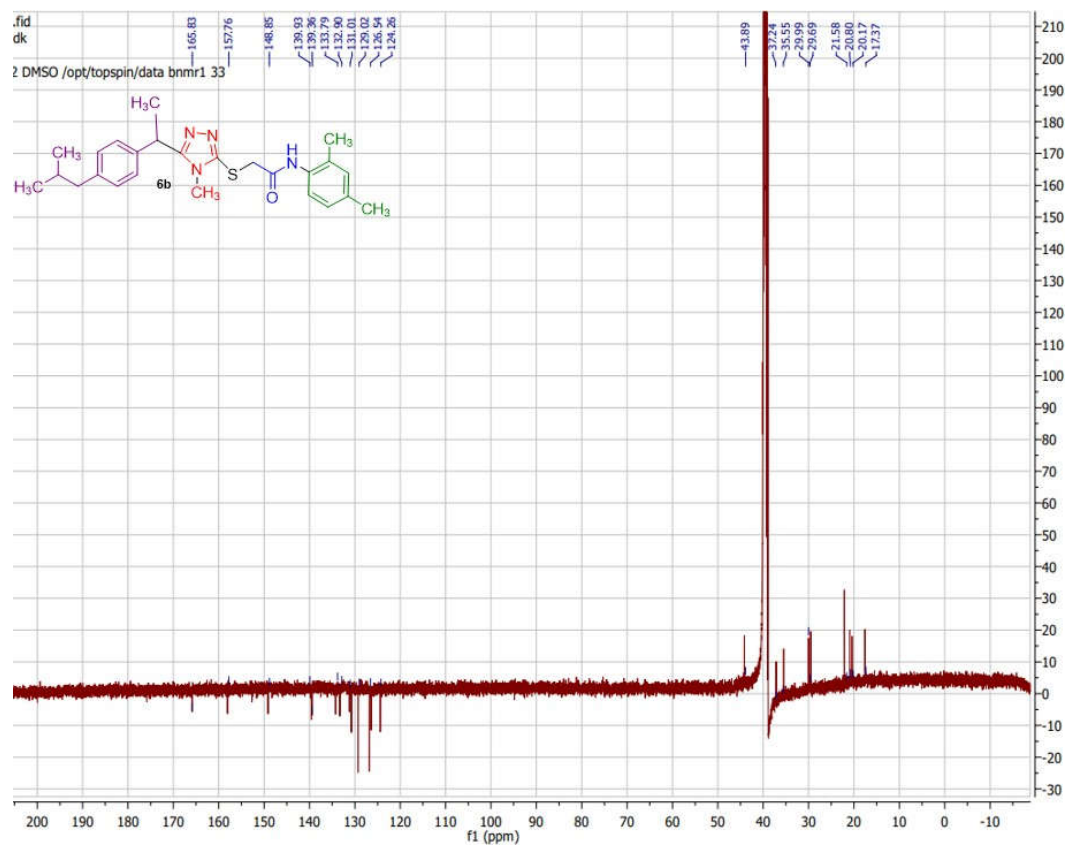
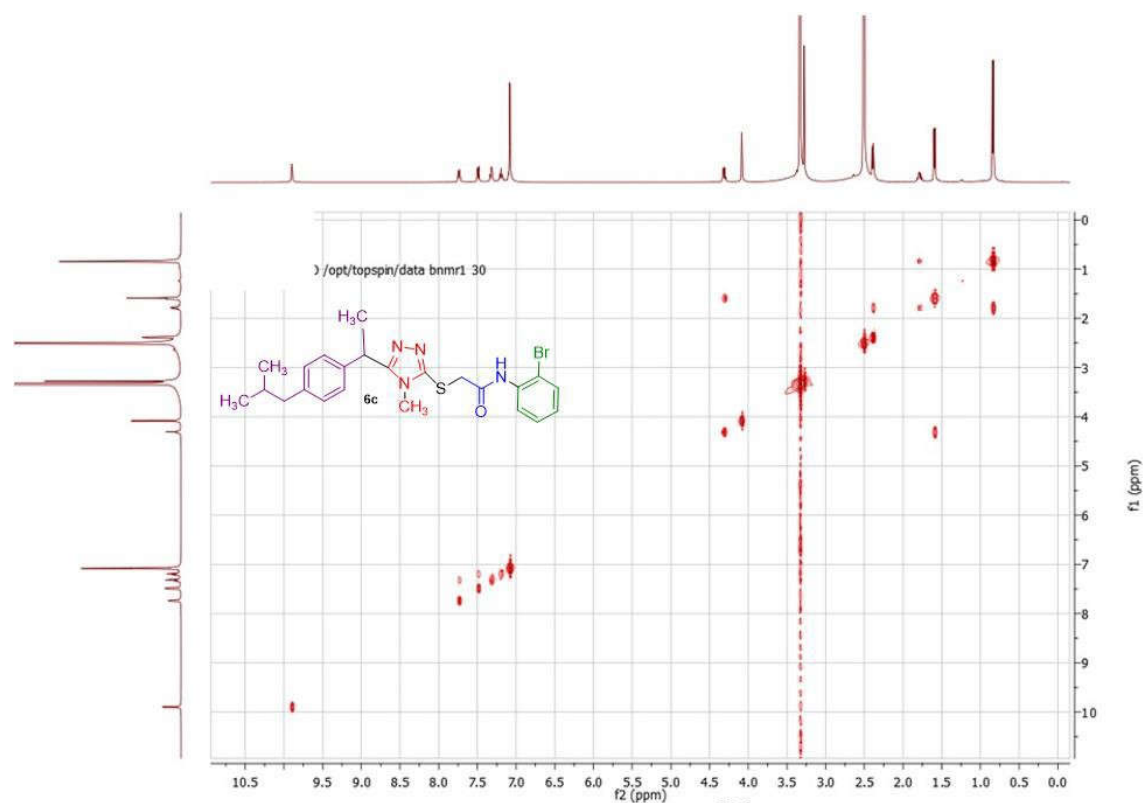
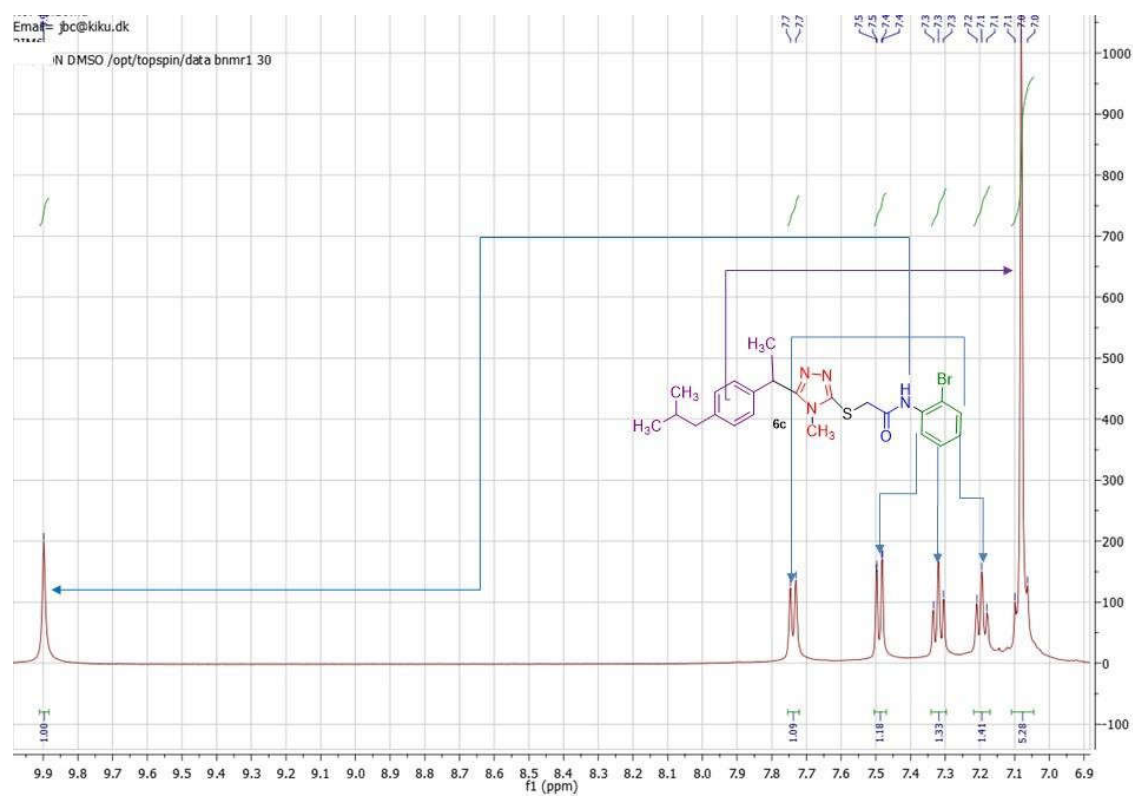


Figure S14. COSY- ^1H NMR spectrum of compound **6b**





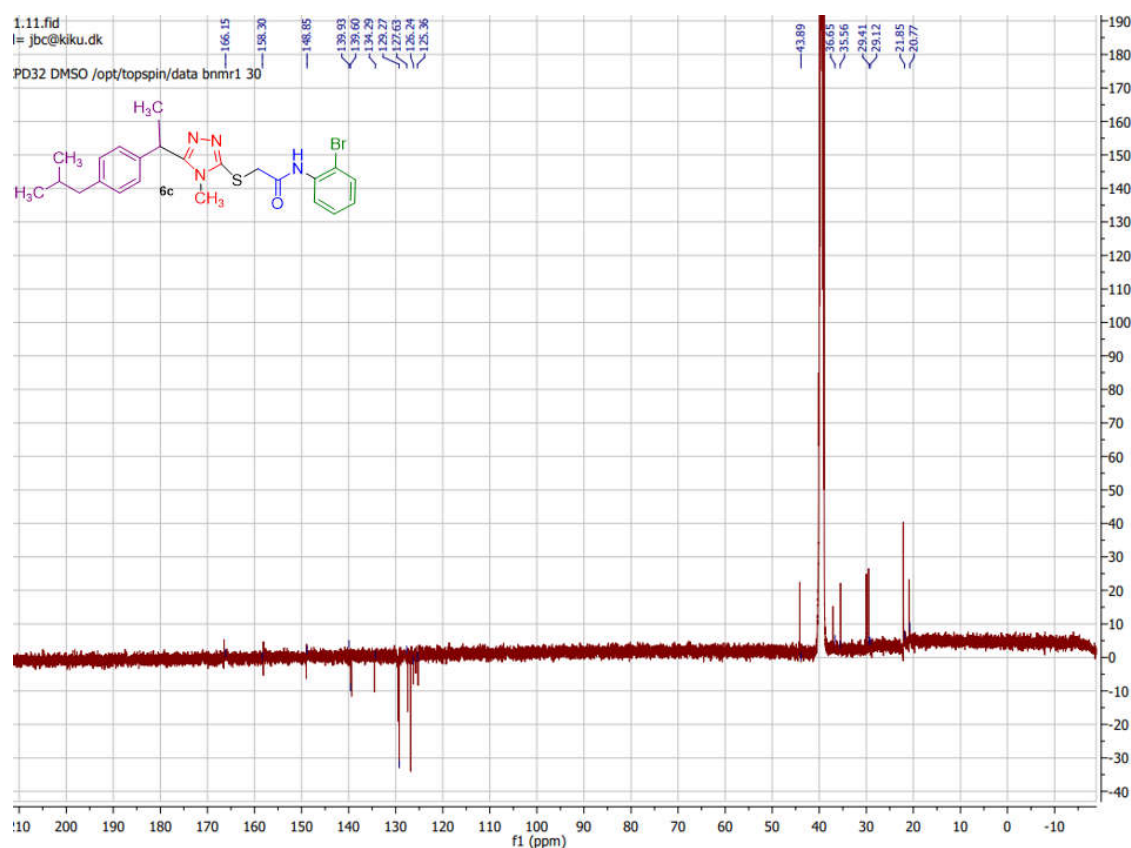


Figure S19. ^{13}C NMR spectrum of compound **6c** (Full spectrum)

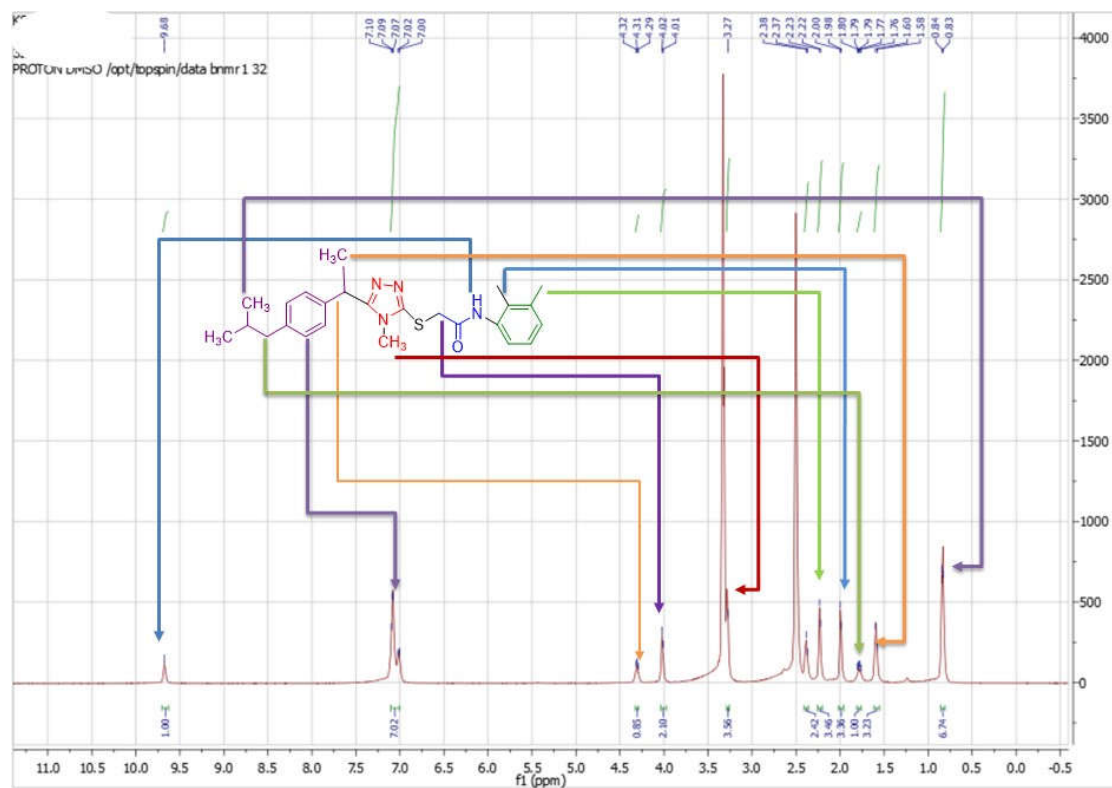


Figure S20. ^1H NMR spectrum of compound **6d** (Full spectrum)

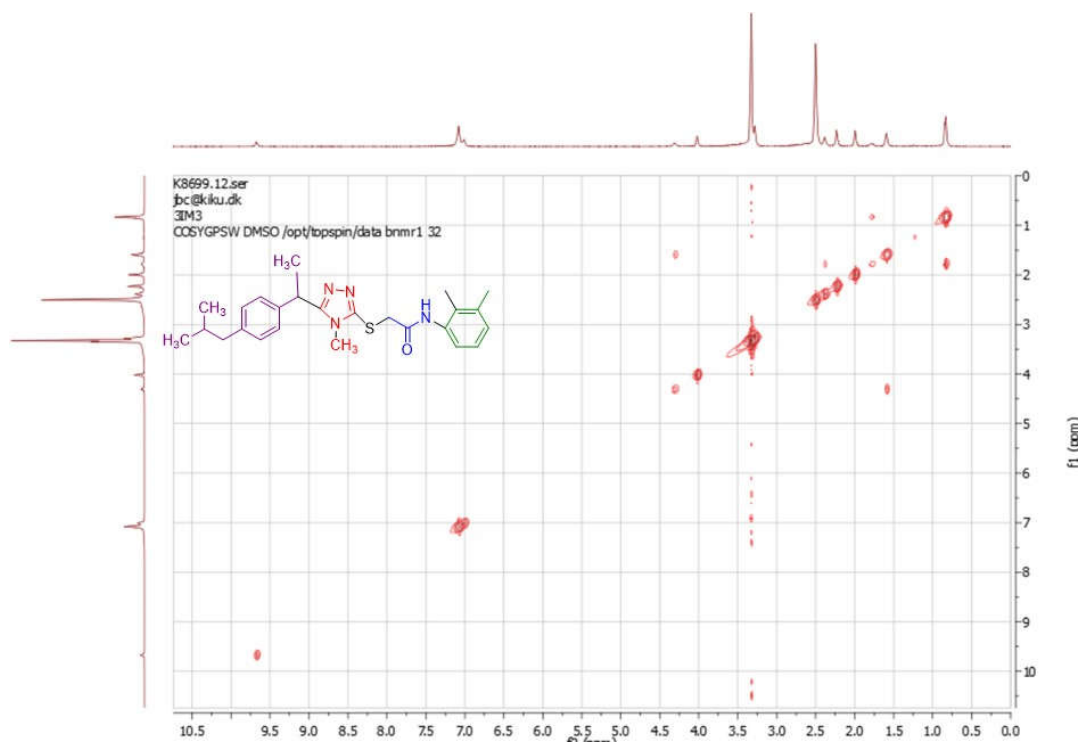


Figure S21. COSY ^1H NMR spectrum of compound **6d**

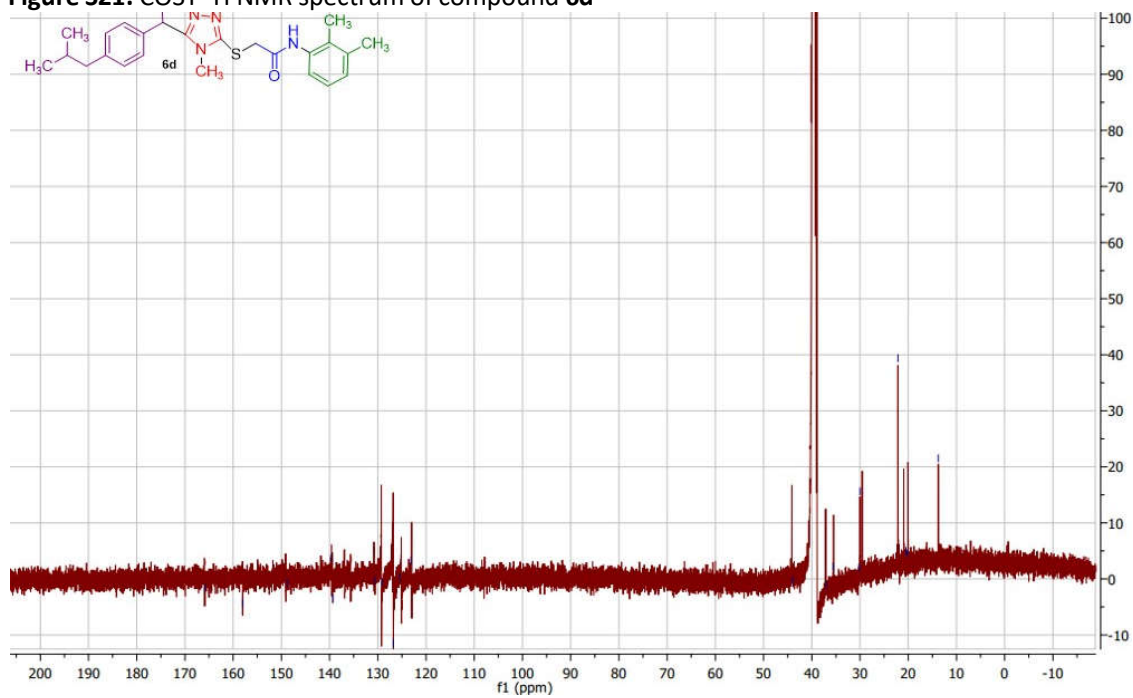


Figure S22. ^{13}C NMR spectrum of compound **6d** (Full spectrum)

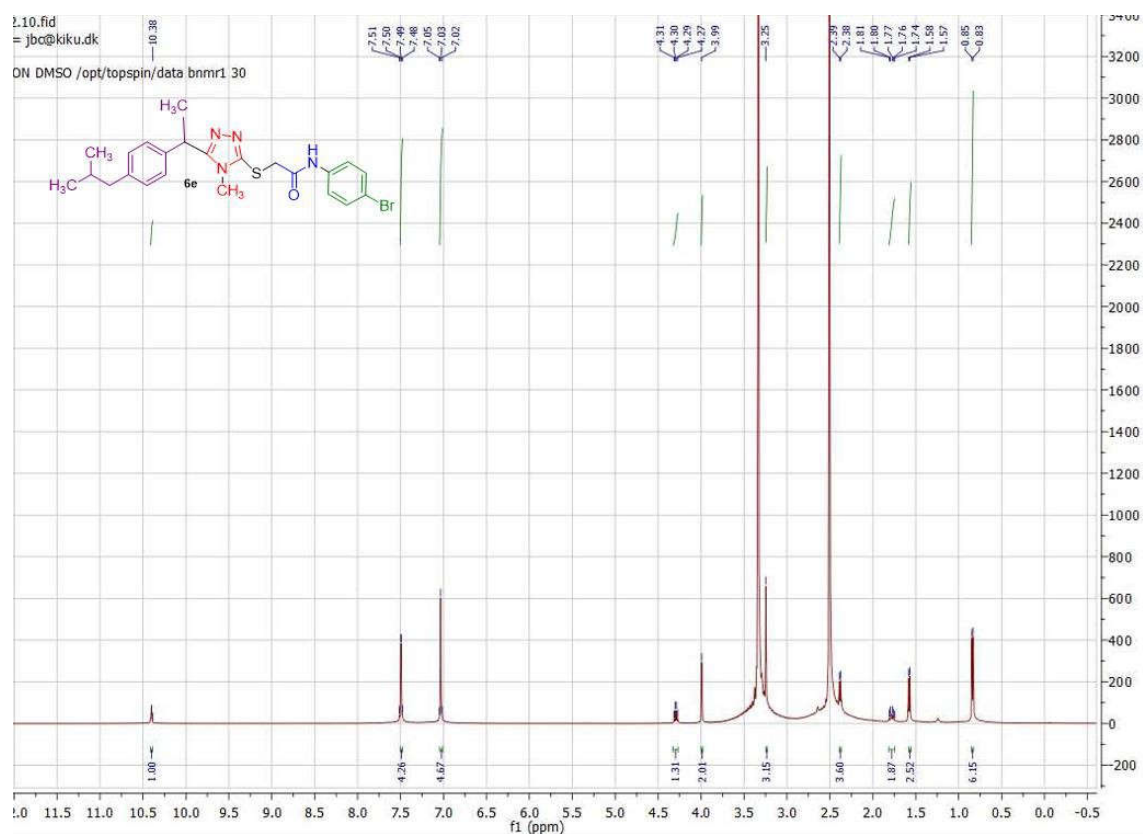


Figure S23. ^1H NMR spectrum of compound **6e** (Full)

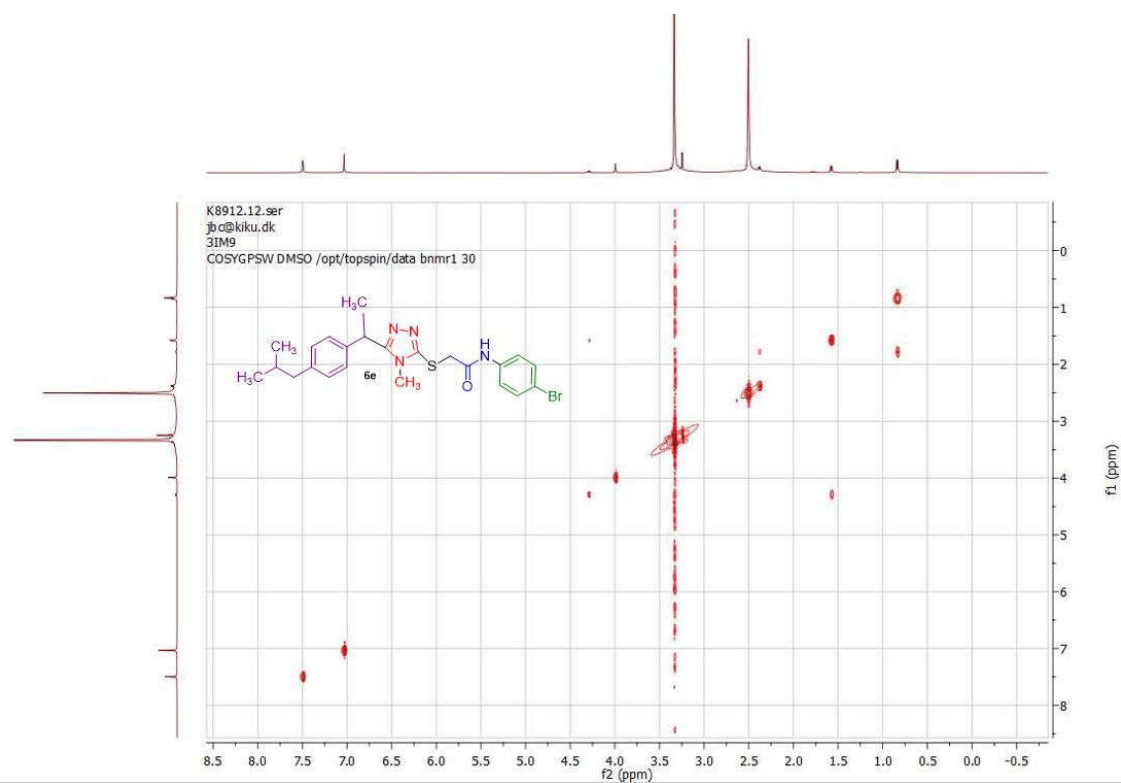


Figure S24. COSY ^1H NMR spectrum of compound **6e**

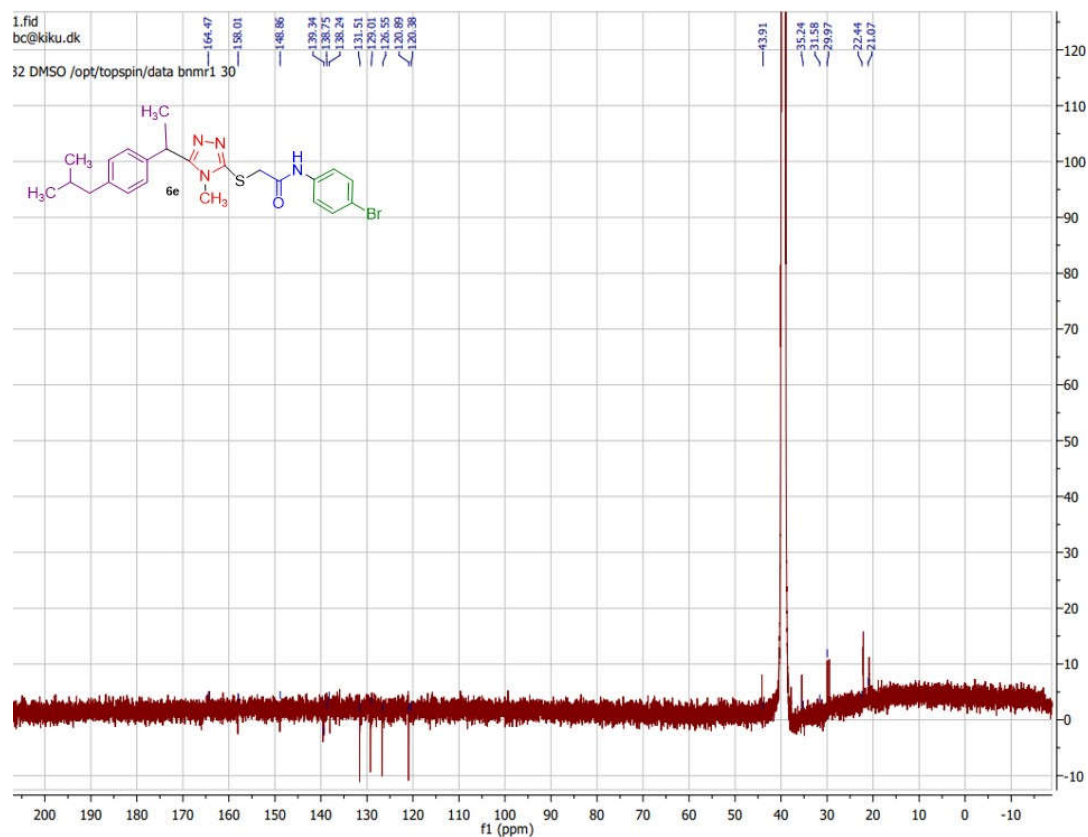


Figure S25. ^{13}C NMR spectrum of compound **6e** (Full spectrum)

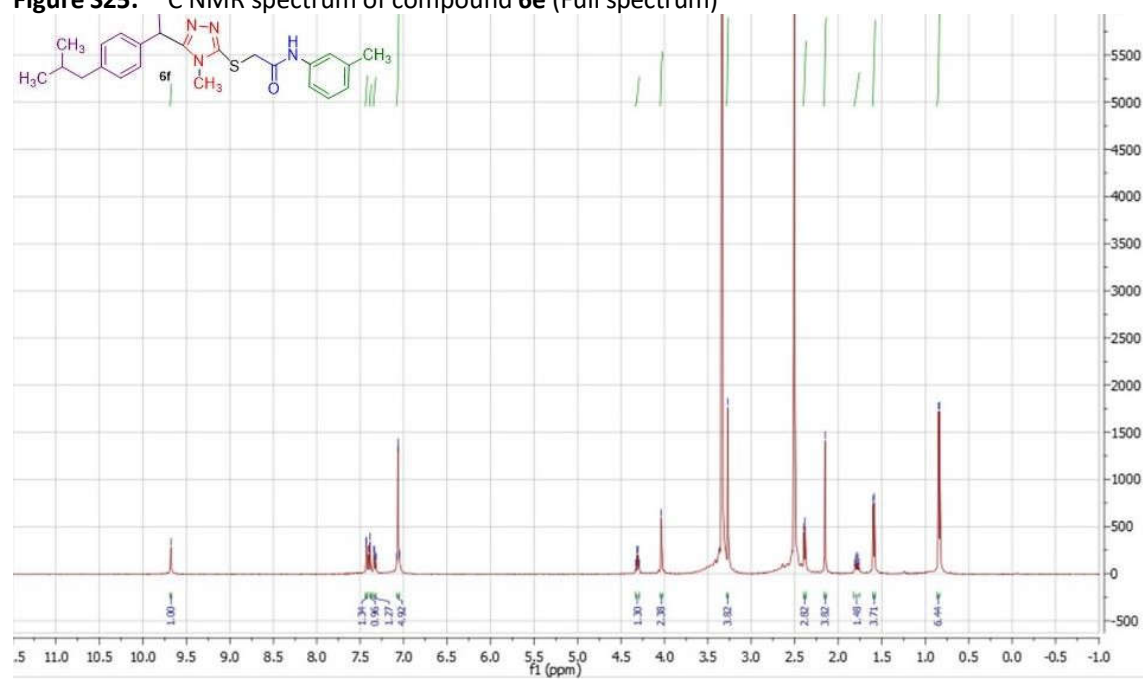


Figure S26. ^1H NMR spectrum of compound **6f** (Full Spectrum)

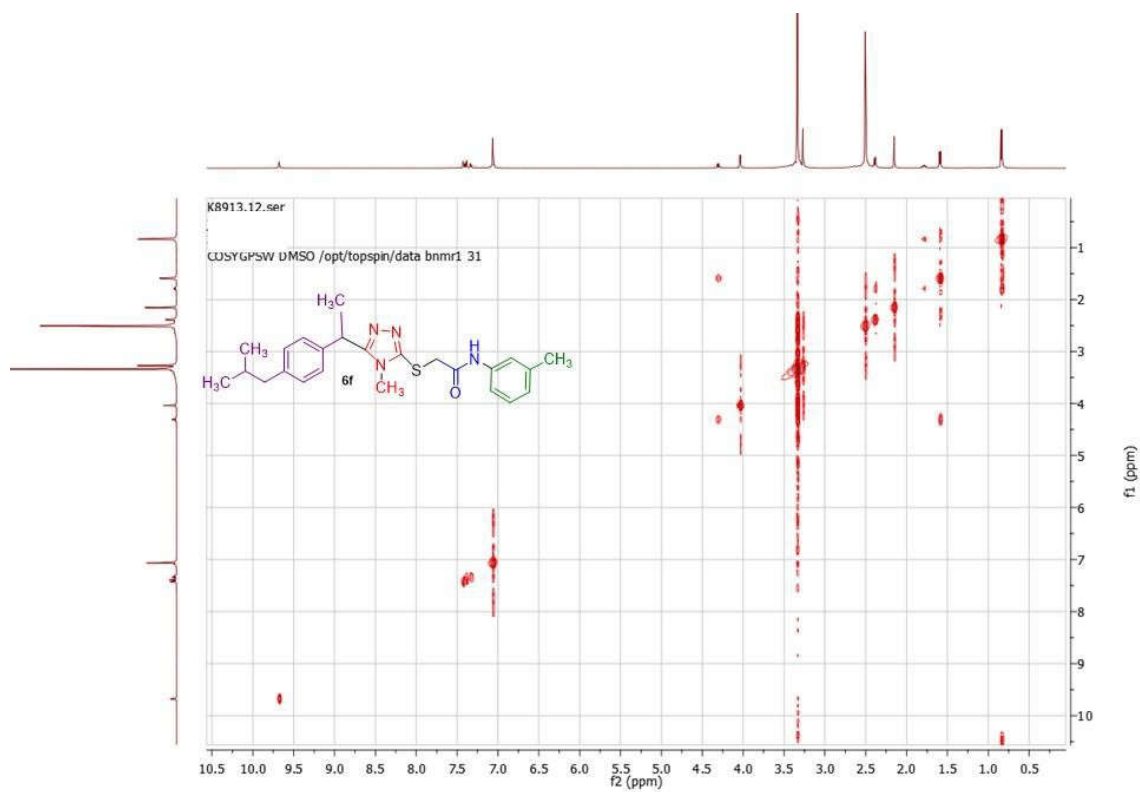


Figure S27. COSY ^1H NMR spectrum of compound **6f**

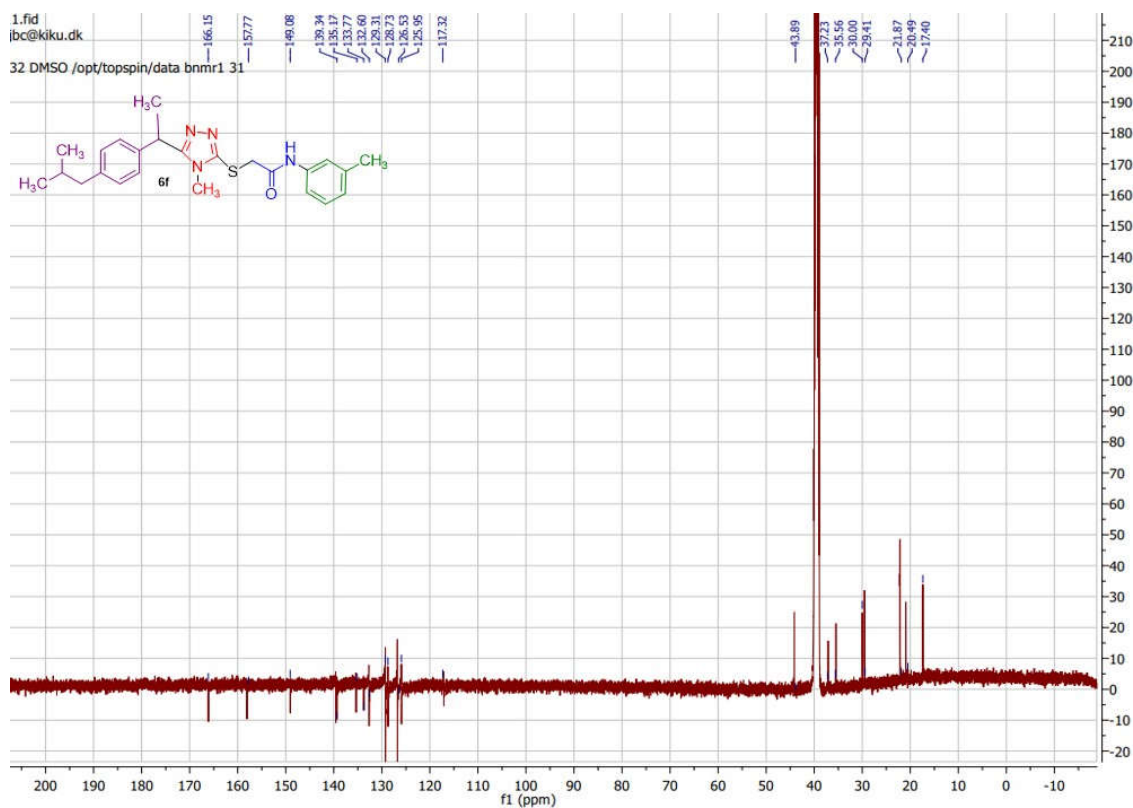


Figure S28. ^{13}C NMR spectrum of compound **6f**

Generic Display Report

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Method 10800

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Comment

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Operator

Instrument solarIX XR

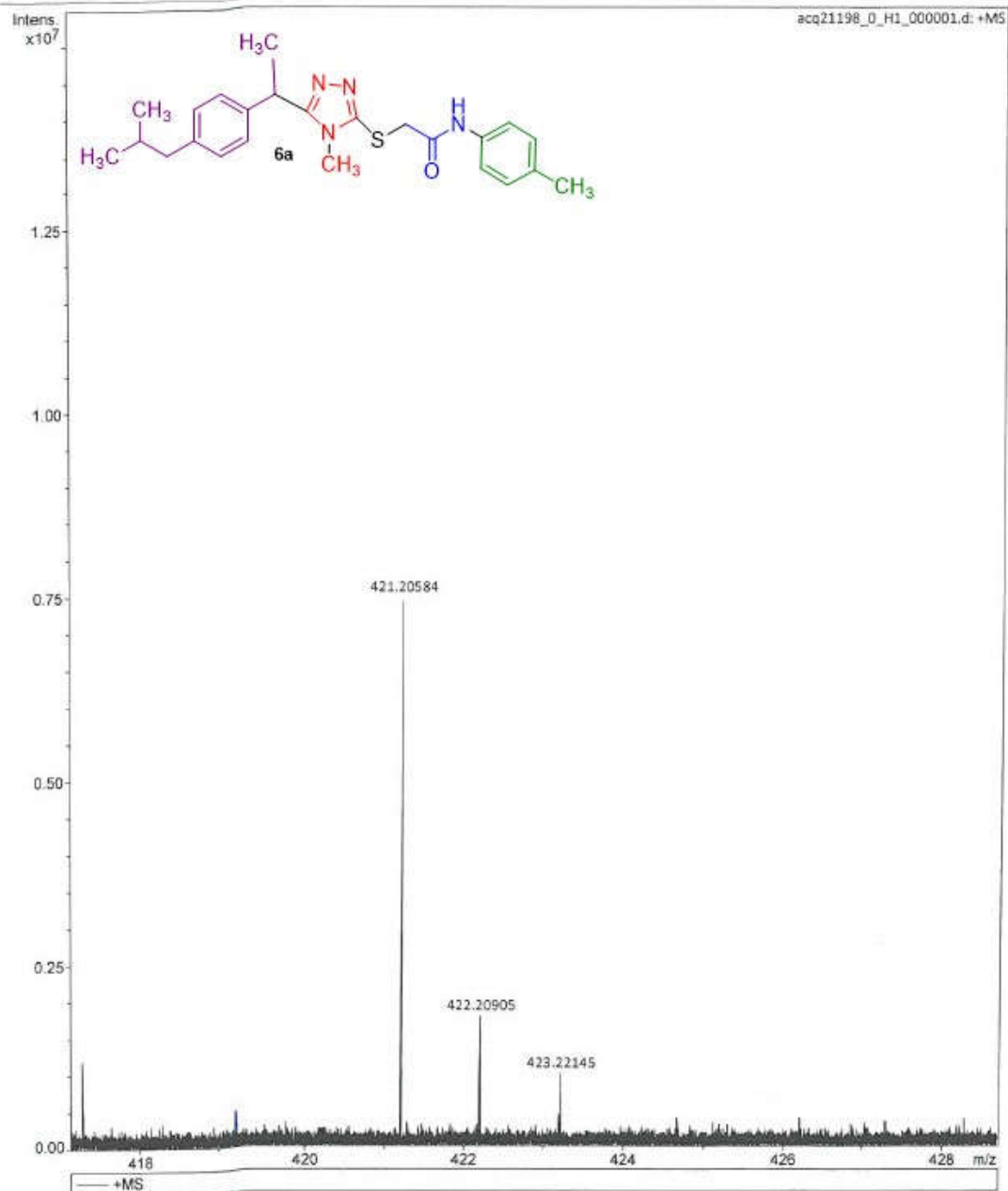


Figure S29. Mass Spectrum of compound 6a

Generic Display Report

Analysis Info

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Operator
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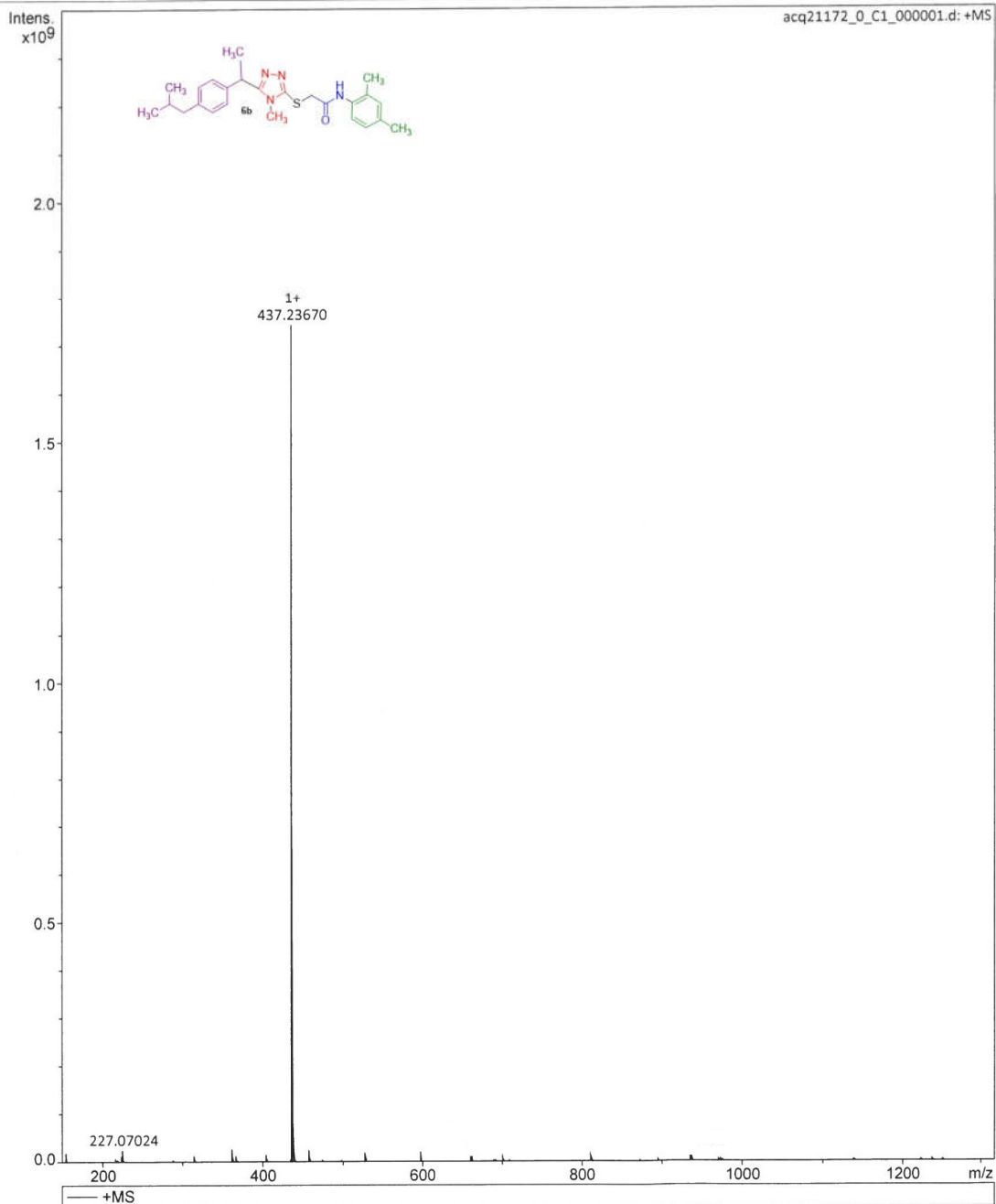


Figure S30. Mass Spectrum of compound 6b

Generic Display Report

Analysis Info

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Acquisition Date 7/6/2022

Operator
Instrument solariX XR

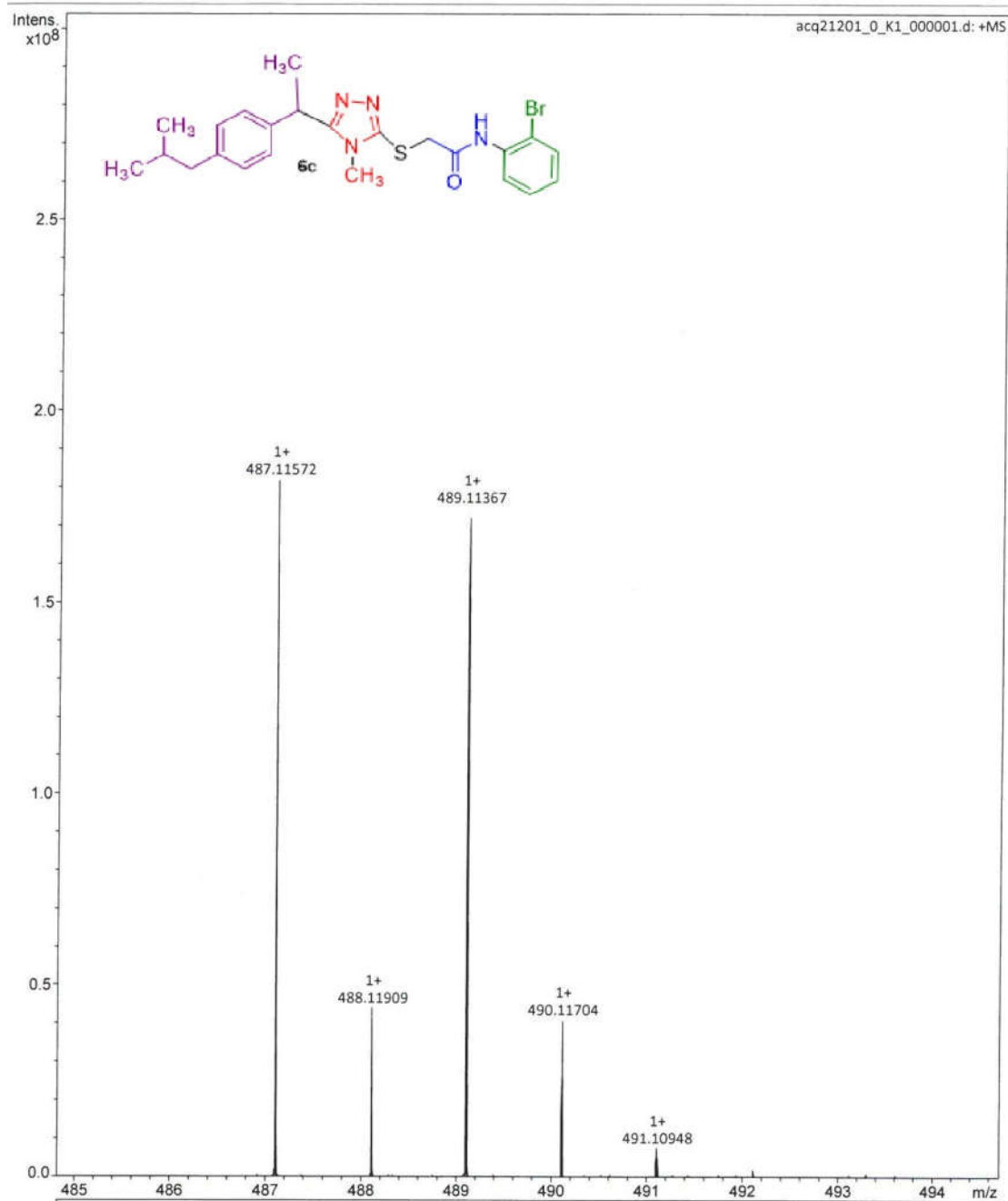


Figure S31. Mass Spectrum of compound 6c

Generic Display Report

Analysis Info

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Operator

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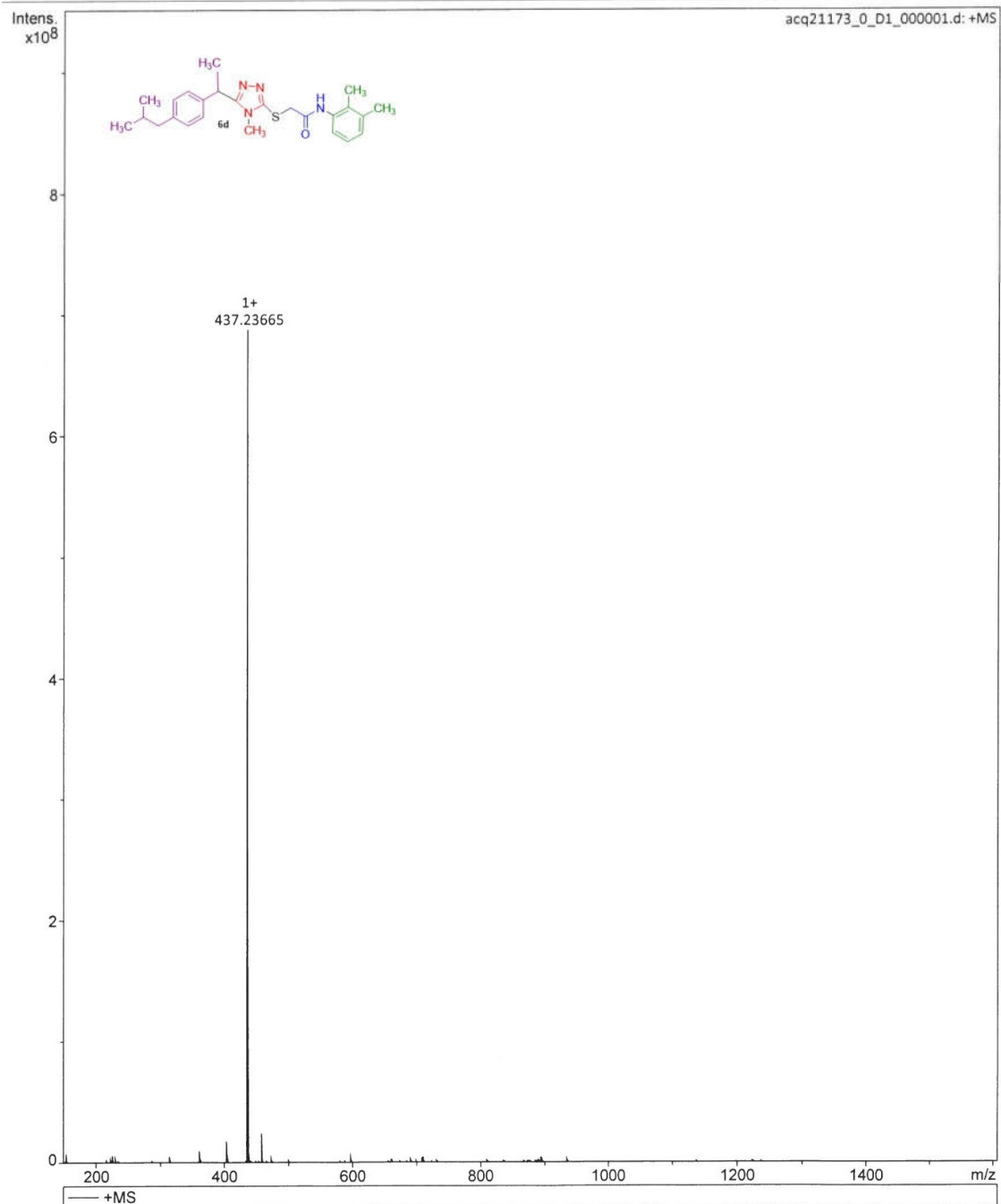


Figure S32. Mass Spectrum of compound 6d

Generic Display Report

Analysis Info

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Sample Name IM5
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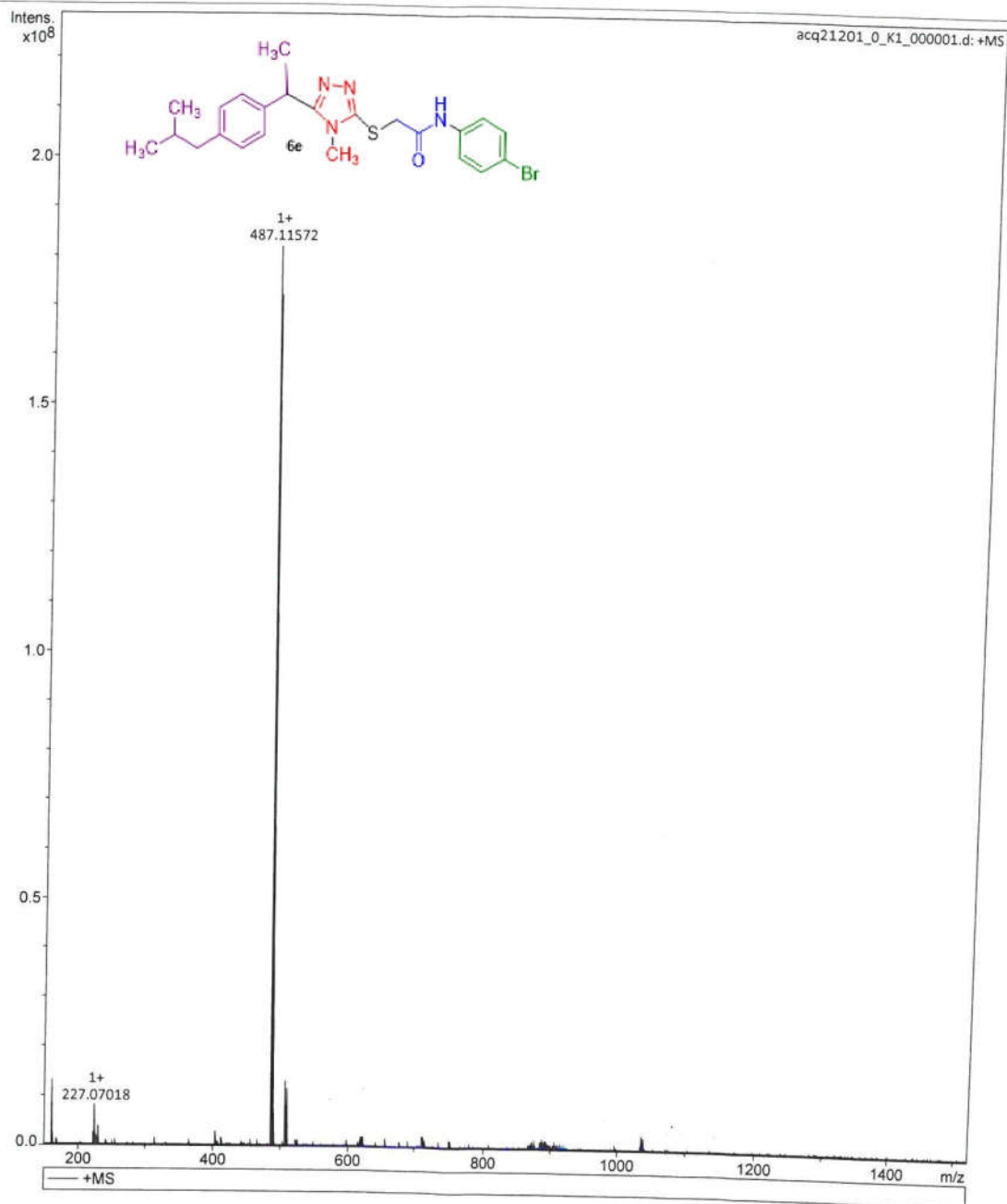


Figure S33. Mass Spectrum of compound 6e

Generic Display Report

Analysis Info

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Sample Name IM10

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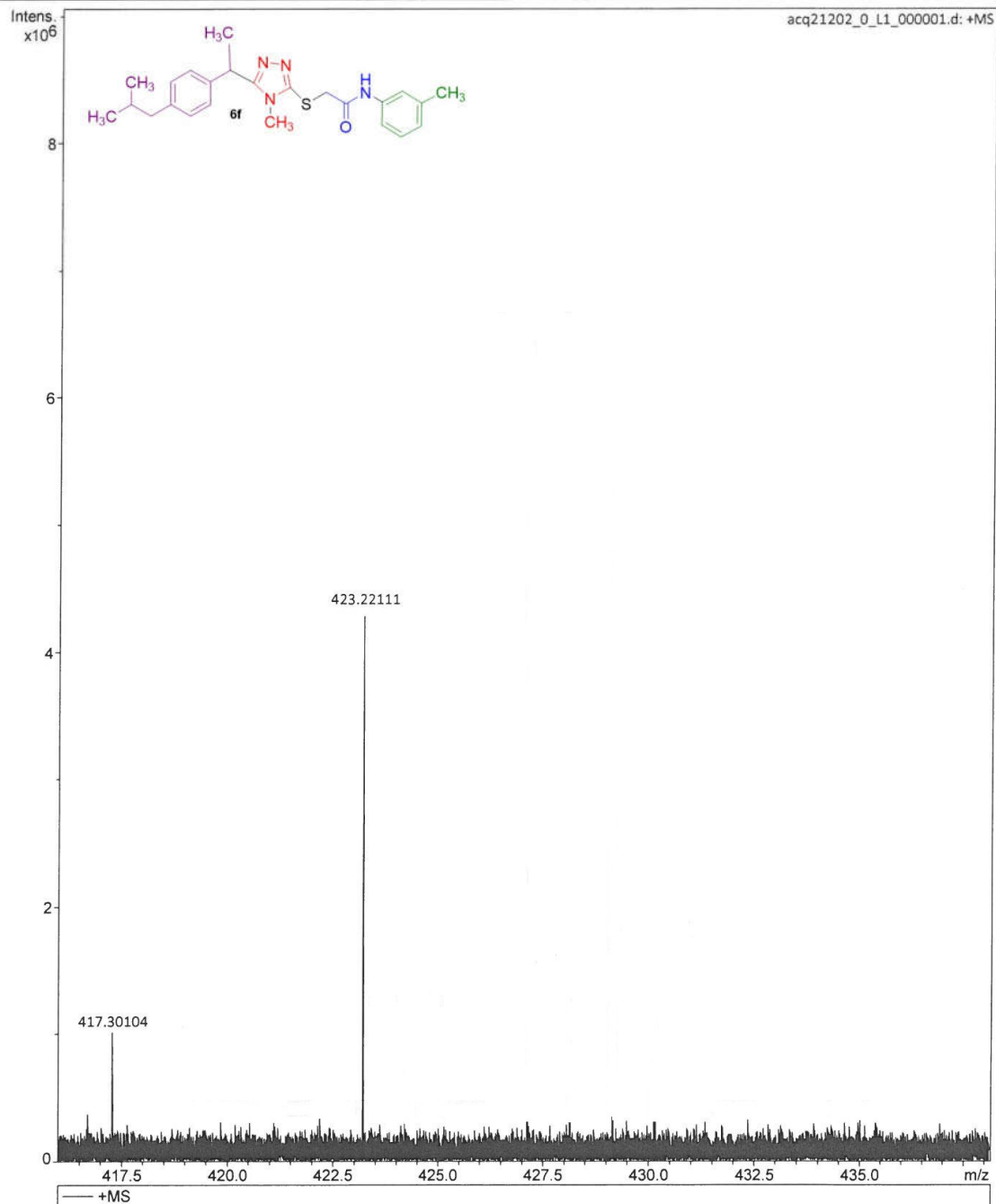


Figure S34. Mass Spectrum of compound 6f