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One-pot synthesis and antimicrobial activity of new 4,6-disubstituted-3,4-dihydropyrimidine-2(1*H*)-thiones

Mahmoud Al-Refai [1,*], Mohammad Ibrahim [1], Abdullah Al-Fawwaz [2] and Armin Geyer [3]

[1] *Department of Chemistry, Faculty of Science, Al Al-Bayt University, Al-Mafraq, 25113, Jordan*
[2] *Department of Biological Sciences, Faculty of Science, Al Al-Bayt University, Al-Mafraq, 25113, Jordan*
[3] *Faculty of Chemistry, Philipps University Marburg, Hans-Meerwein-Straße 4, Marburg, 35032, Germany*

** Corresponding author at: Department of Chemistry, Faculty of Science, Al Al-Bayt University, Al-Mafraq, 25113, Jordan. Tel.: +962.2.6297000/2141. Fax: +962.2.6297021. E-mail address: mahmoud_alrefai@aabu.edu.jo (M. Al-Refai).*

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ABSTRACT

A series of 3,4-dihydropyrimidine-2(1*H*)-thiones (3a-i) were synthesized in moderate yields *via* a one-pot reaction of 3-acetyl-2,5-diclorothiophene (1), aryl aldehydes (2a-i) and thiourea in methanolic solution of potassium hydroxide under reflux conditions. All newly synthesized compounds were characterized by extensive NMR analysis, including ^{1}D NMR experiments (^{1}H and ^{13}C) and 2D NMR experiments (COSY, HMBC and HSQC), as well as ESI-MS and HRESI-MS data. The antimicrobial activity of all new compounds (3a-f) was tested against bacteria and fungi. Thione derivative (3c) only showed activity against *Staphylococcus aureus*, *Bacillus subtilis* and *Aspergillus niger*.

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Supplementary materials

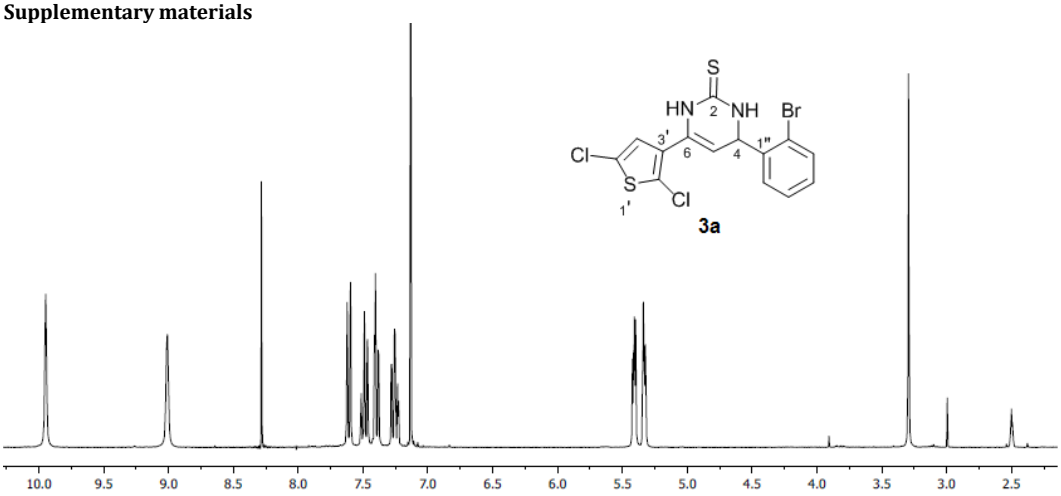

Figure S1. ^{1}H NMR spectrum of compound **3a**.

http://dx.doi.org/10.5155/eurjchem.8.1.96-100.1543

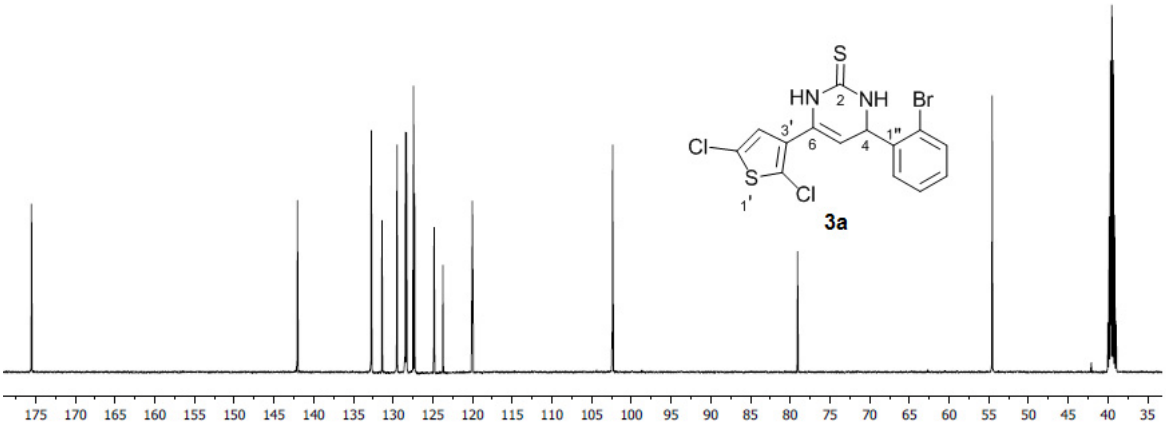

Figure S2. ^{13}C NMR spectrum of compound **3a**.

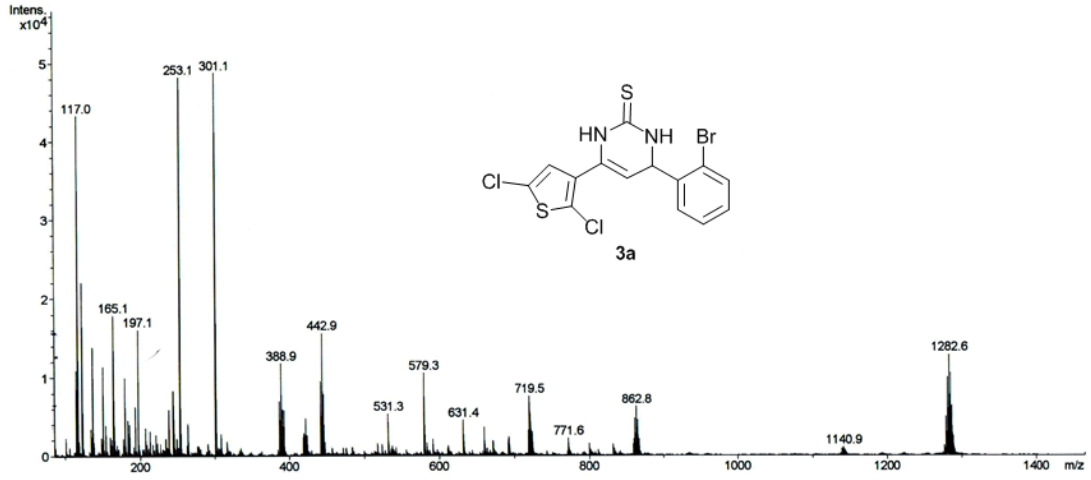

Figure S3. (+)-ESIMS spectrum of compound **3a**.

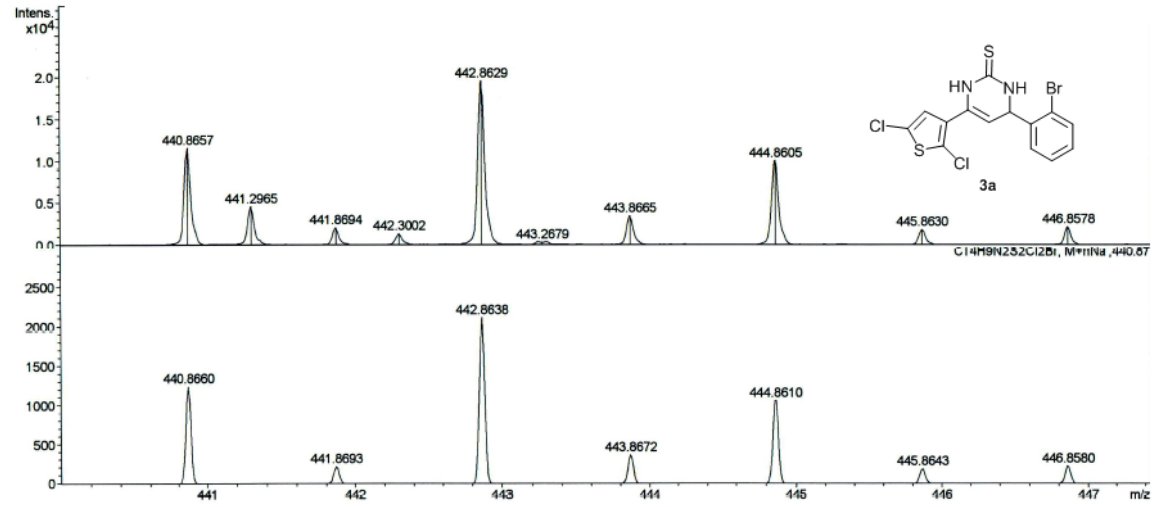

Figure S4. (+)-HRESIMS spectrum of compound **3a**.

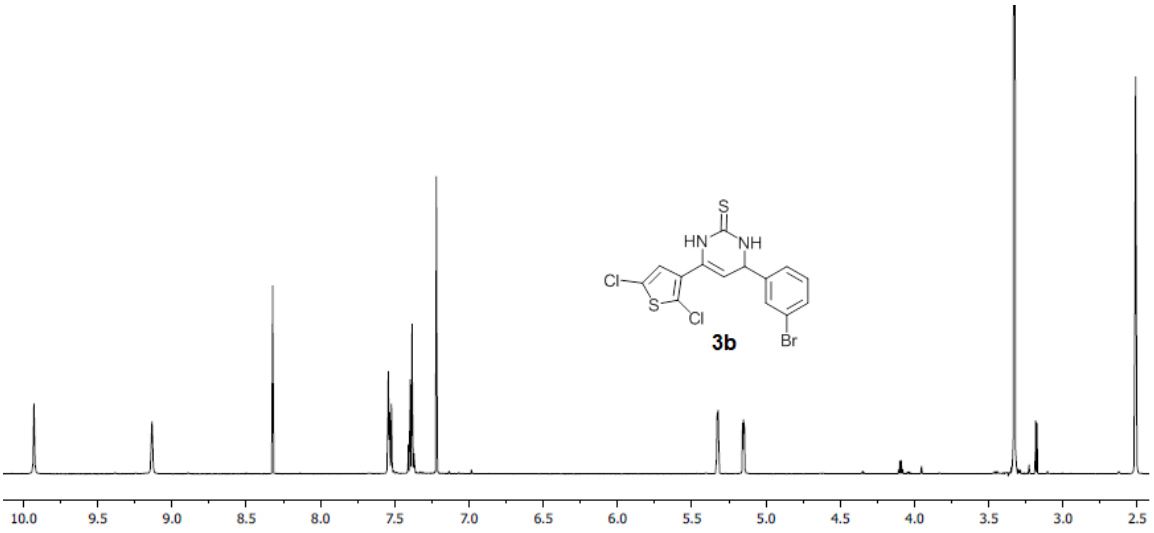

Figure S5. ^{1}H NMR spectrum of compound **3b**.

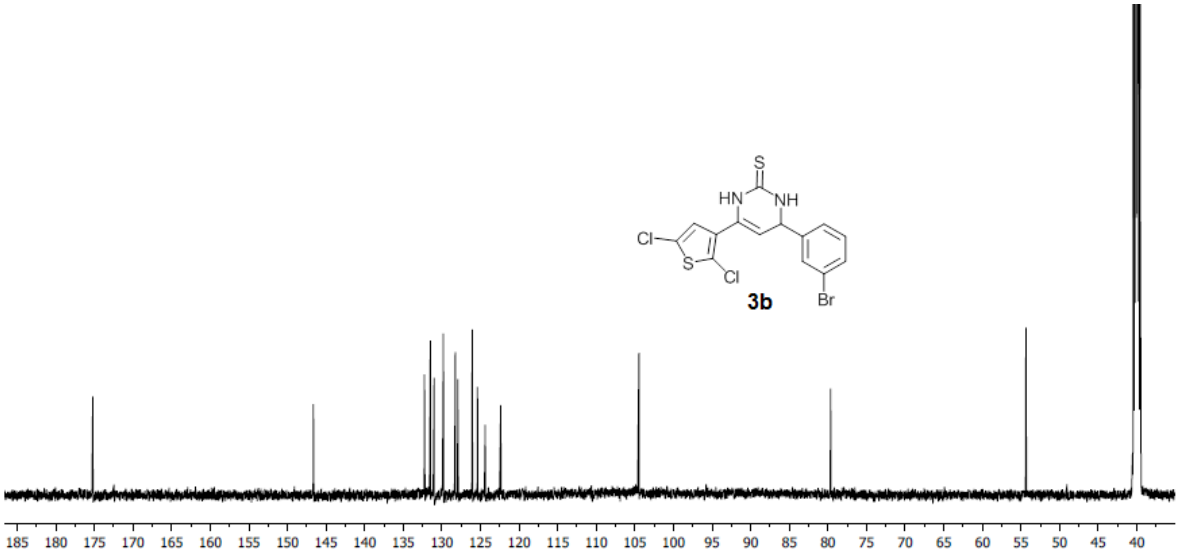

Figure S6. ^{13}C NMR spectrum of compound **3b**.

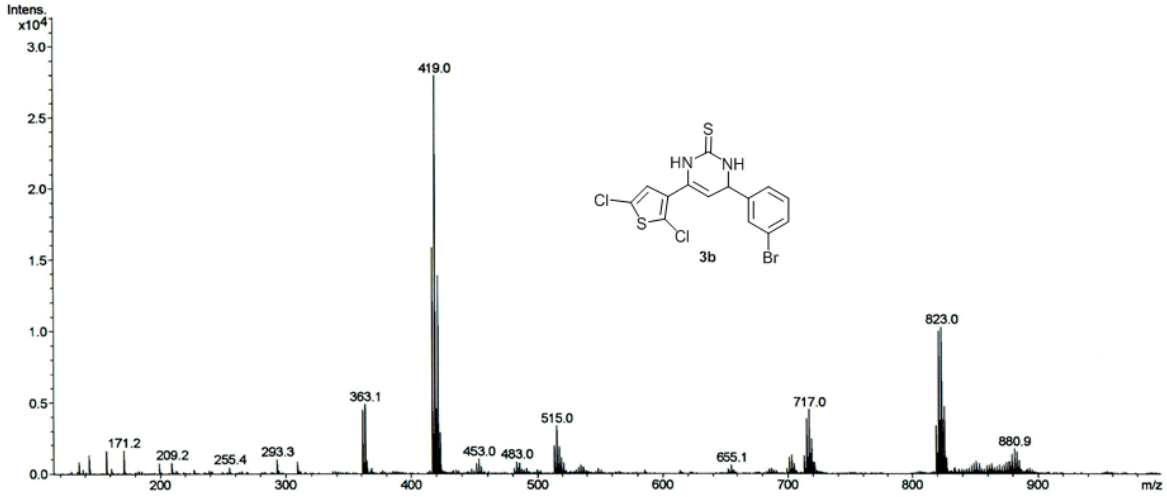

Figure S7. (-)-ESIMS spectrum of compound **3b**.

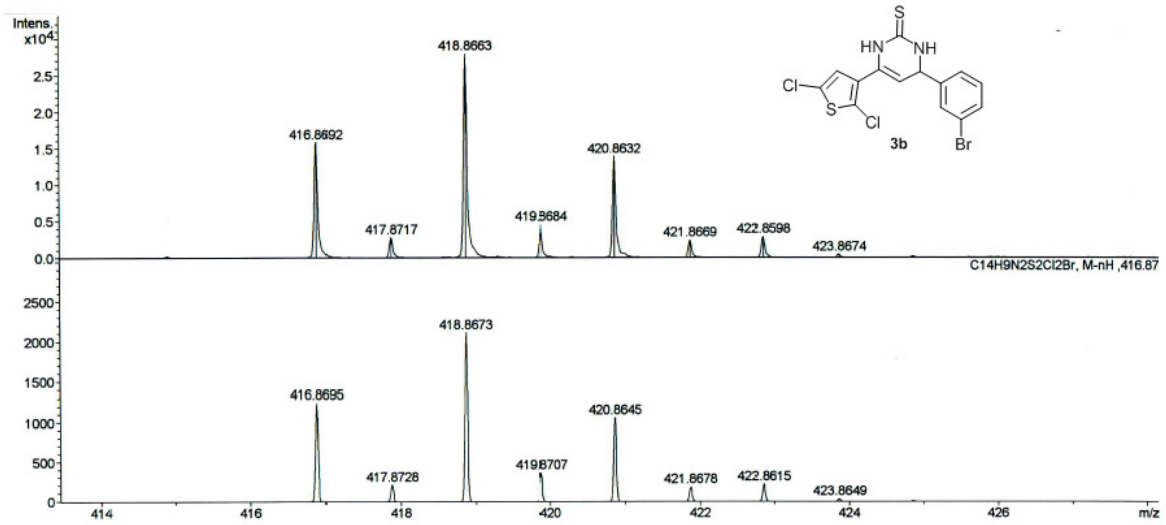

Figure S8. (-)-HRESIMS spectrum of compound **3b**.

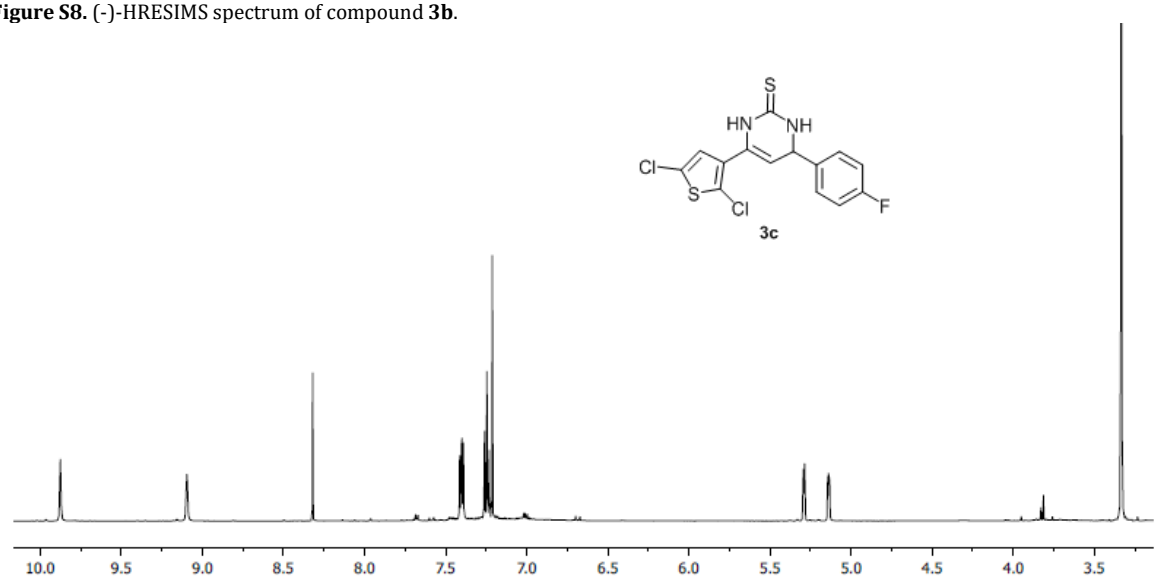

Figure S9. ^{1}H NMR spectrum of compound **3c**.

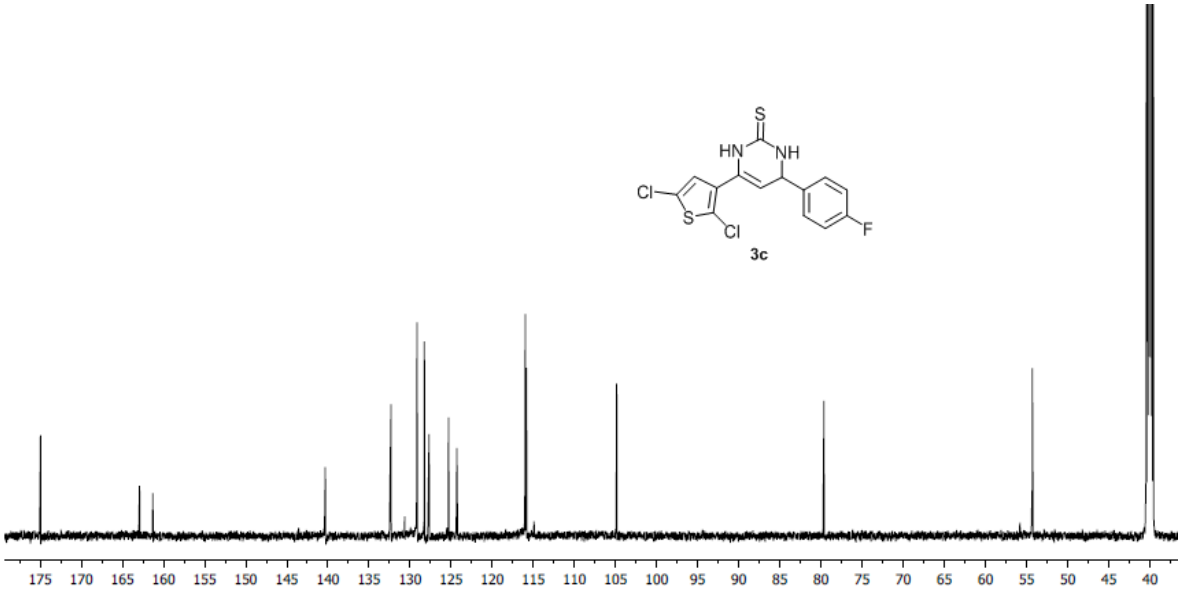

Figure S10. ^{13}C NMR spectrum of compound **3c**.

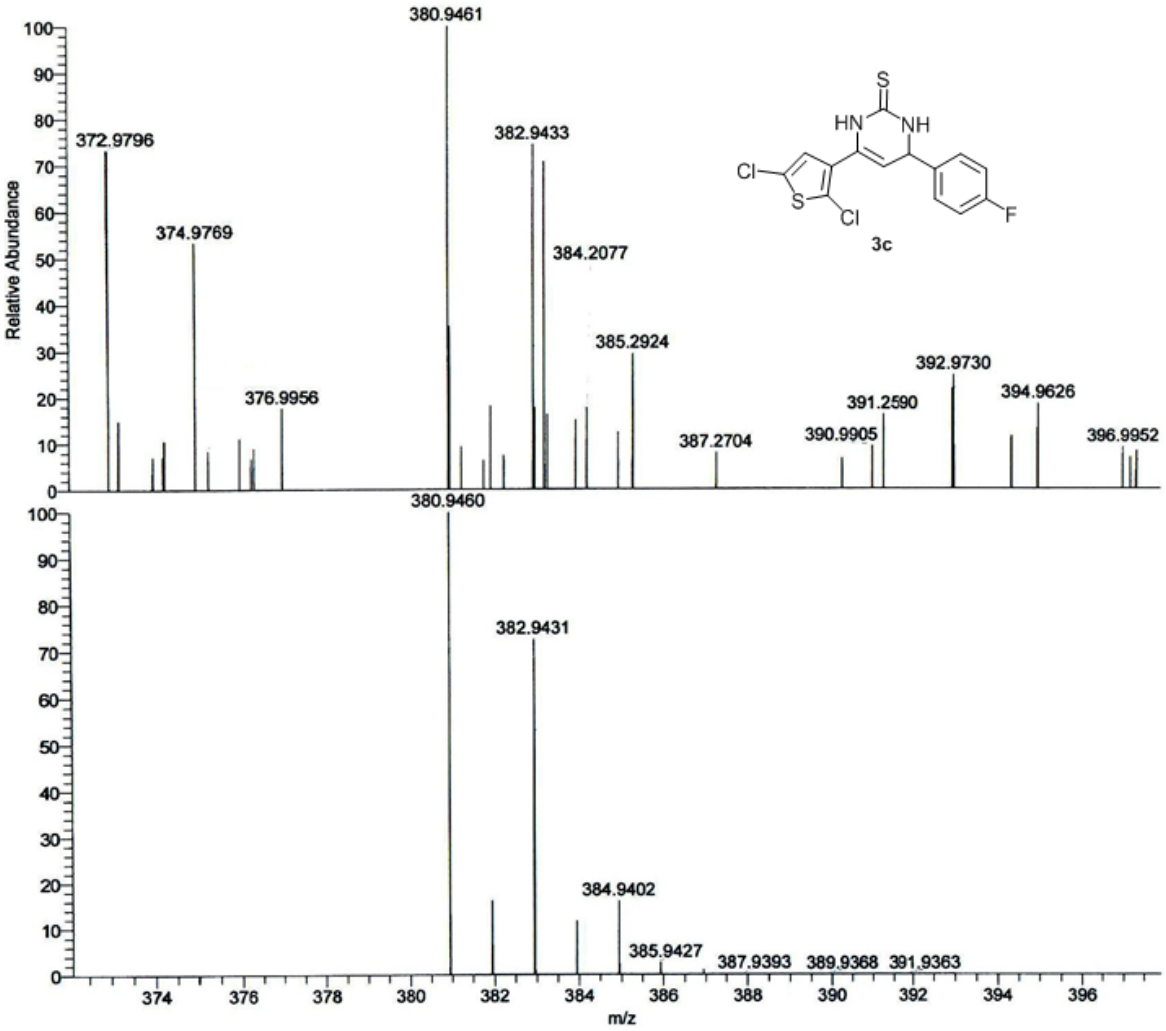

Figure S11. (+)-HRESIMS spectrum of compound **3c**.

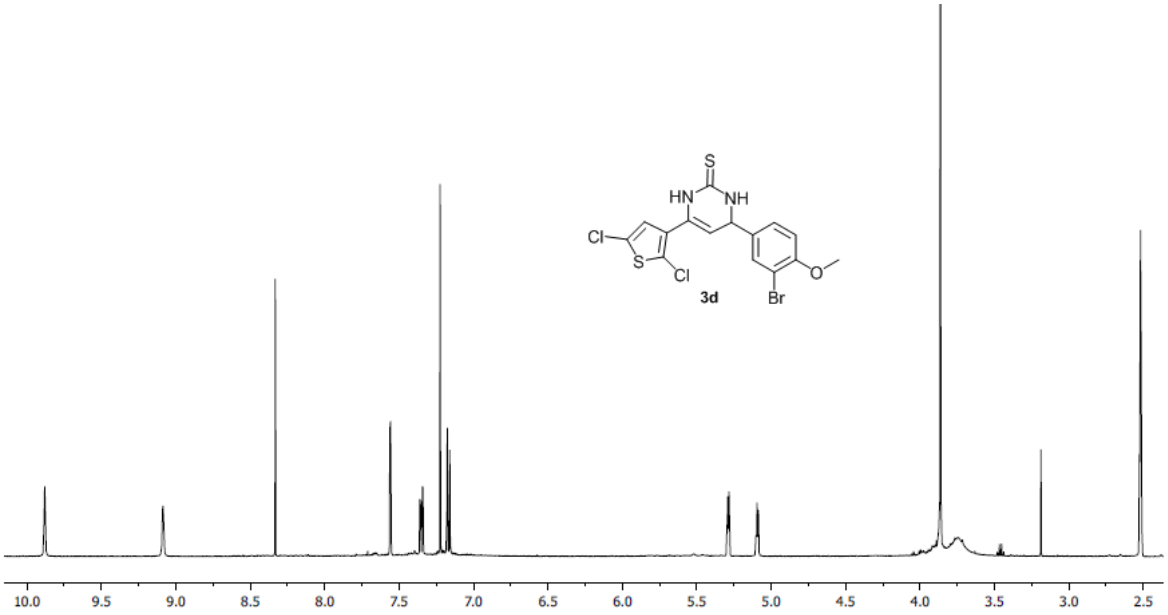

Figure S12. ^{1}H NMR spectrum of compound **3d**.

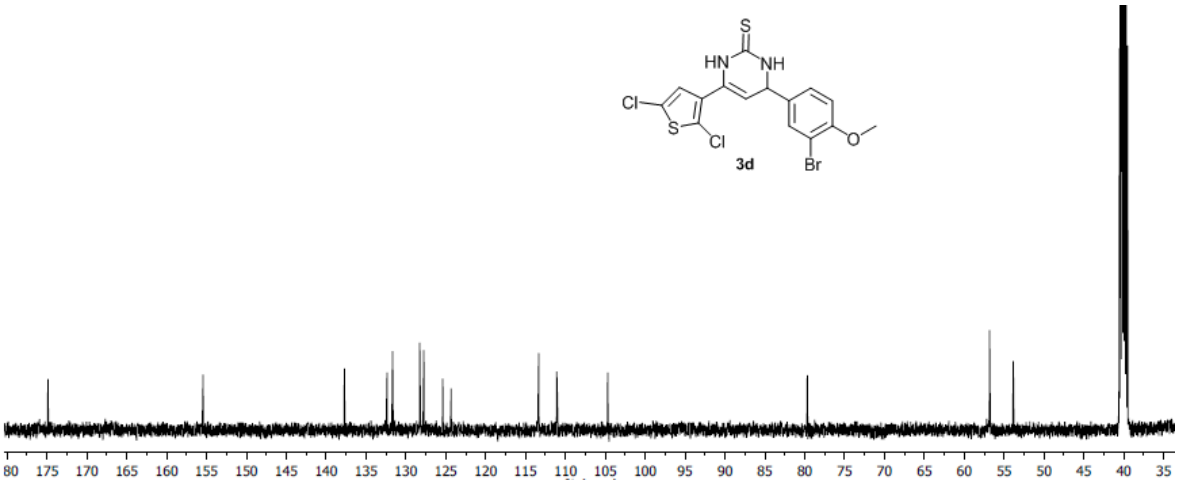

Figure S13. ^{13}C NMR spectrum of compound **3d**.

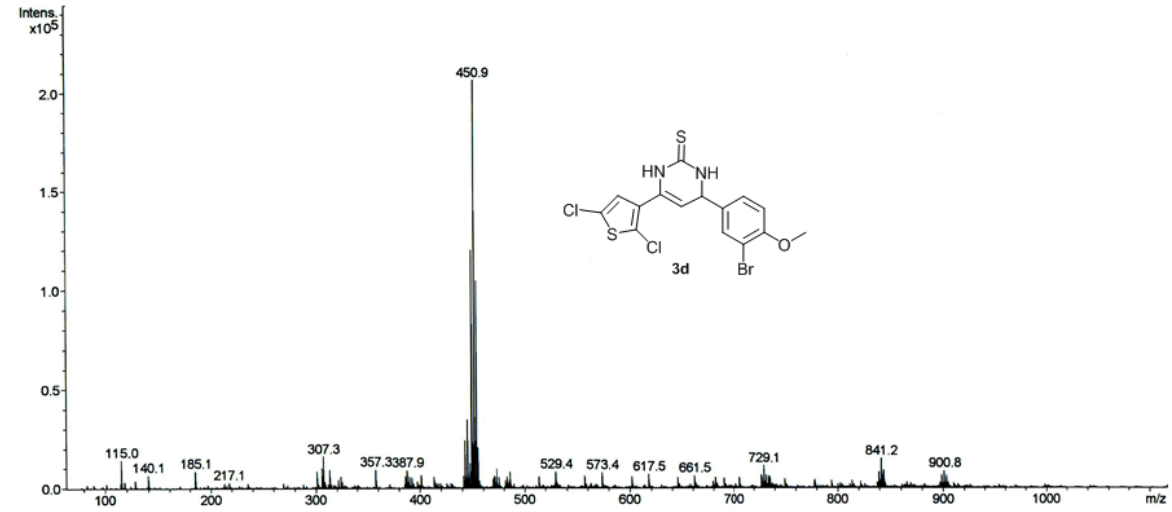

Figure S14. (+)-ESIMS spectrum of compound **3d**.

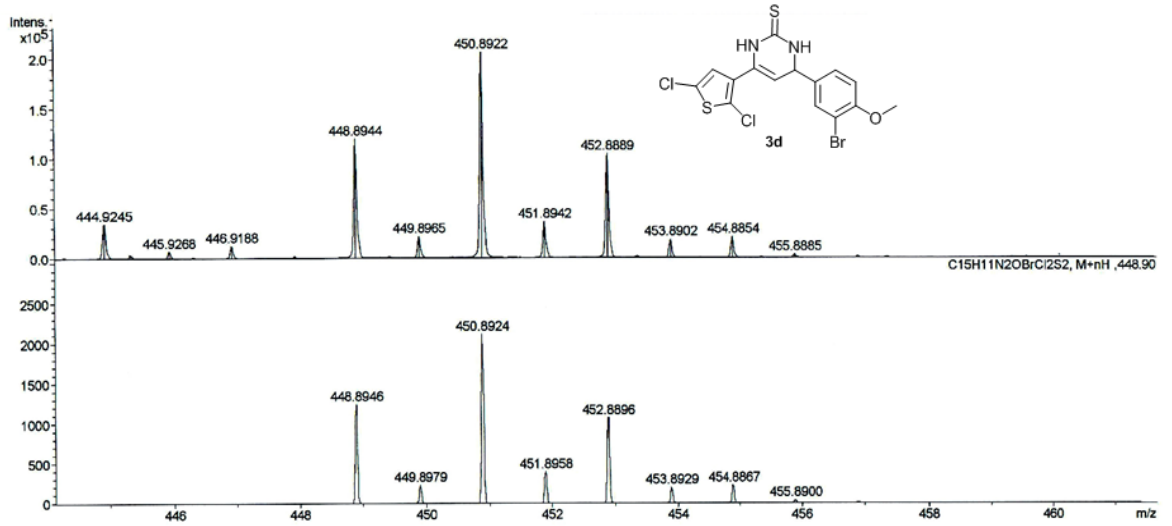

Figure S15. (+)-HRESIMS spectrum of compound **3d**.

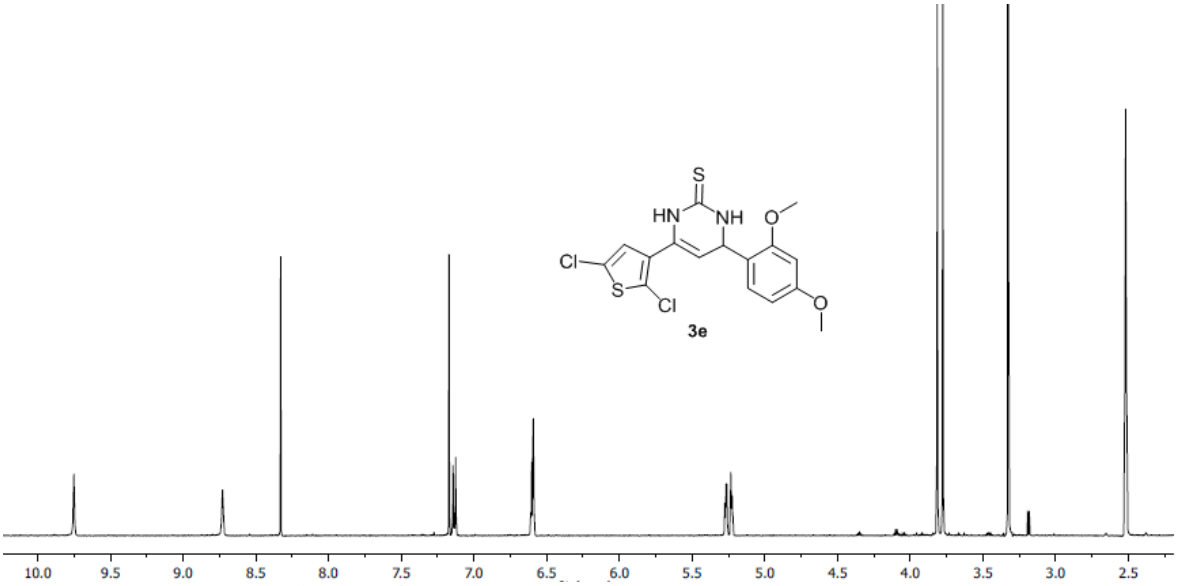

Figure S16. ^{1}H NMR spectrum of compound **3e**.

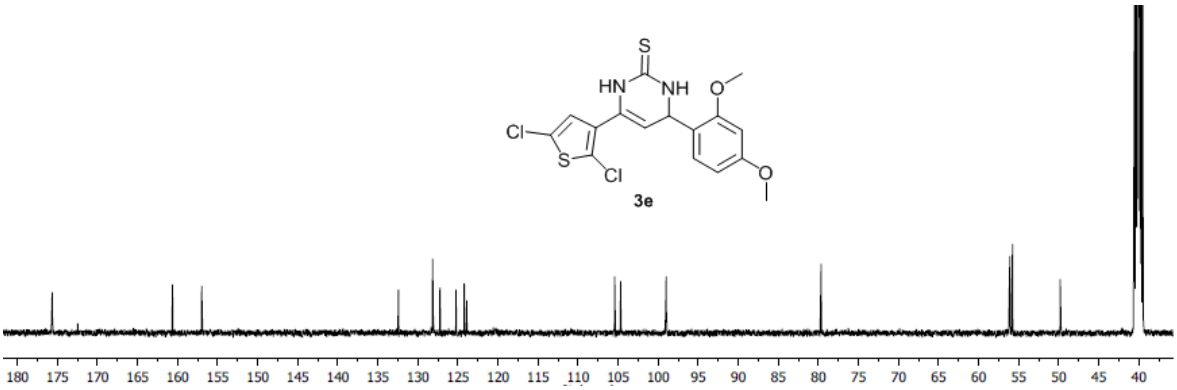

Figure S17. ^{13}C NMR spectrum of compound **3e**.

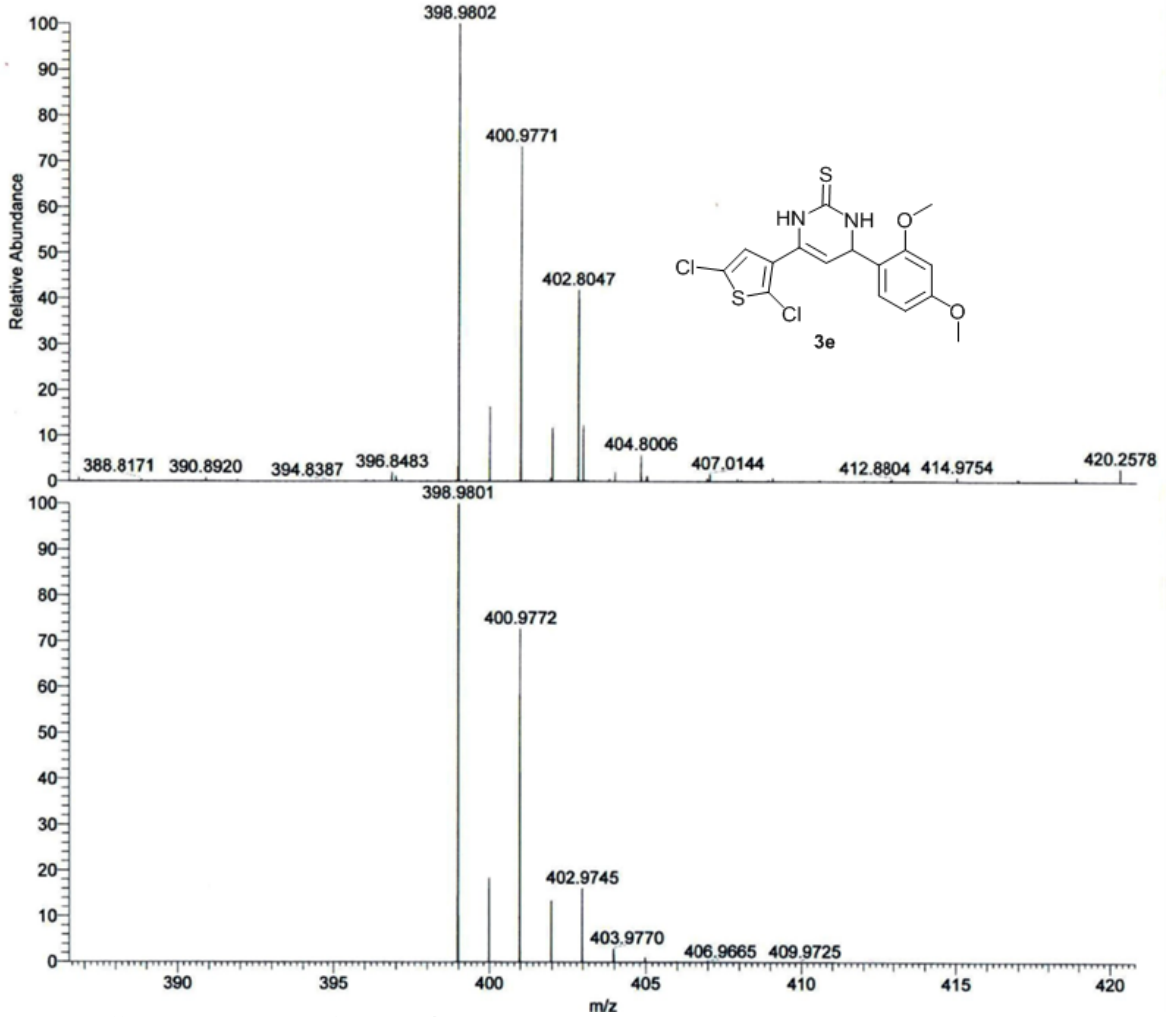

Figure S18. (-)-HRESIMS spectrum of compound **3e**.

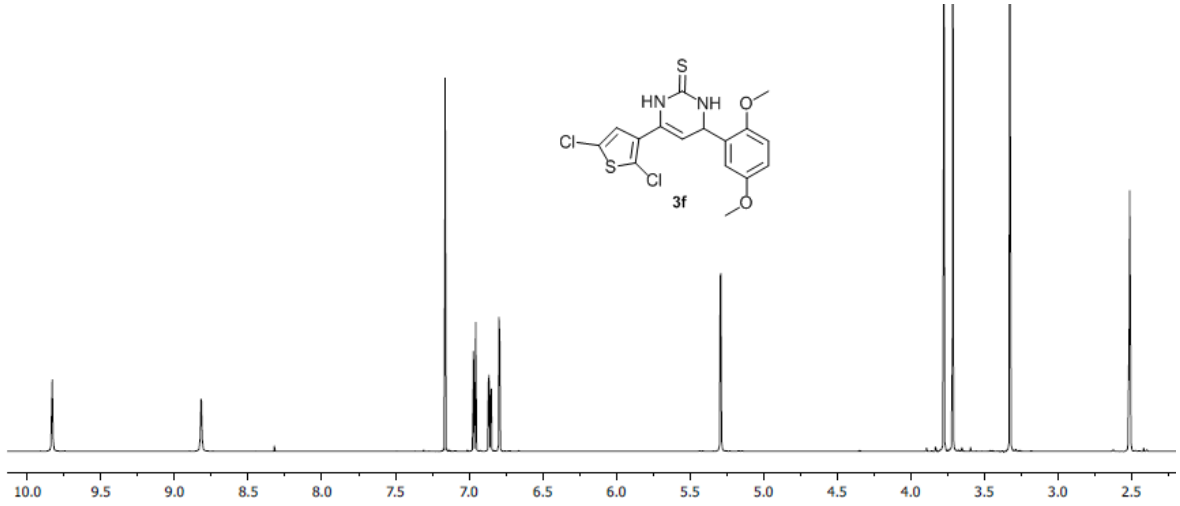

Figure S19. ^{1}H NMR spectrum of compound **3f**.

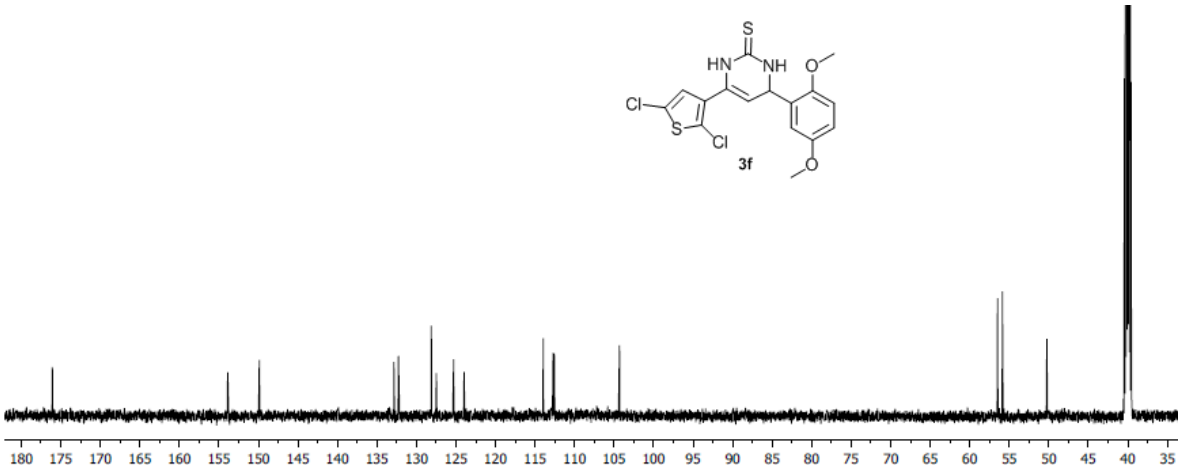

Figure S20. ^{13}C NMR spectrum of compound **3f**.

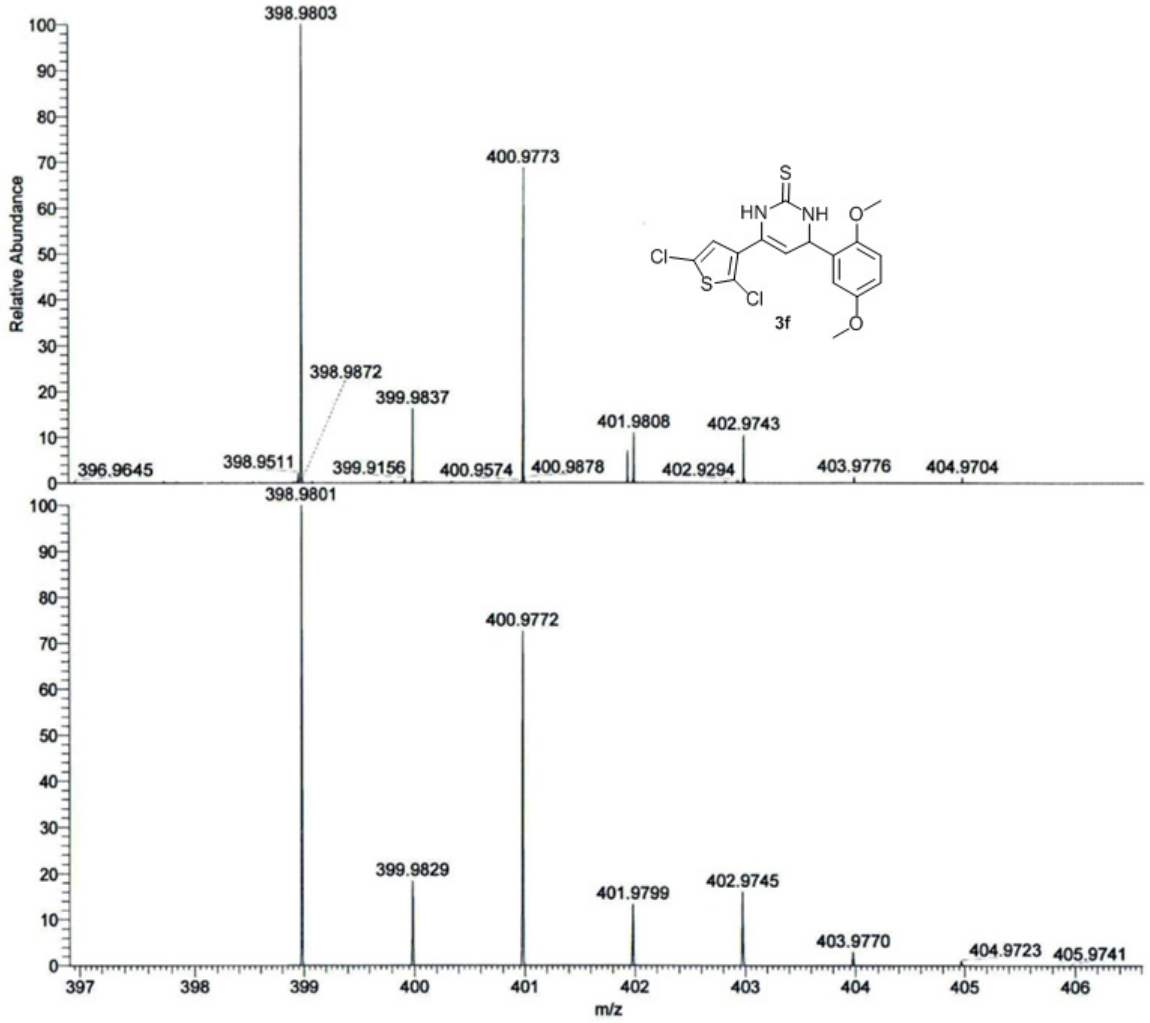

Figure S21. (-)-HRESIMS spectrum of compound **3f**.

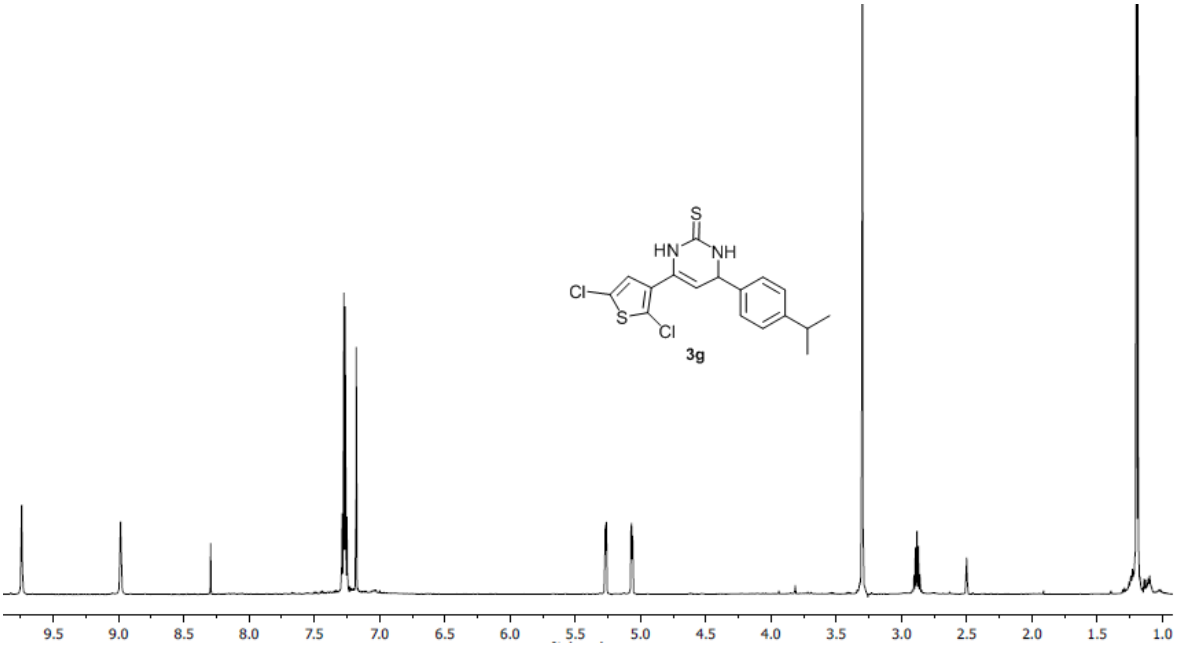

Figure S22. ^{1}H NMR spectrum of compound **3g**.

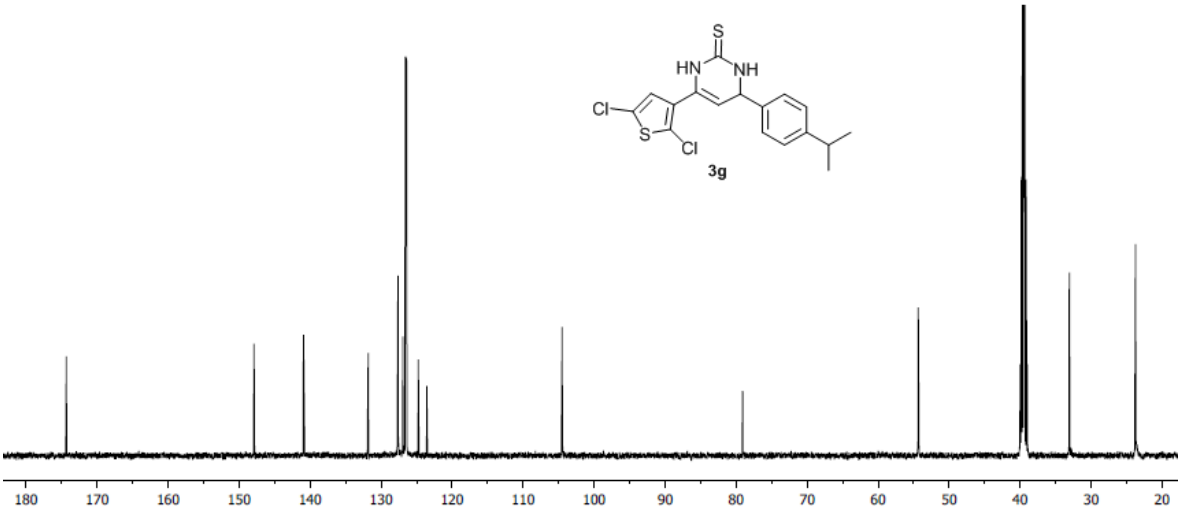

Figure S23. ^{13}C NMR spectrum of compound **3g**.

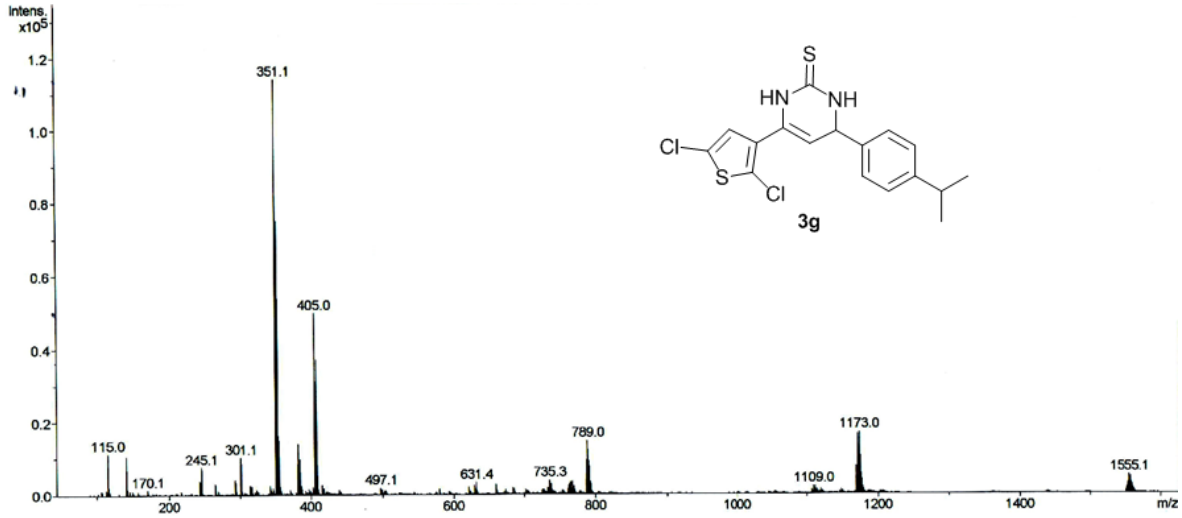

Figure S24. (+)-ESIMS spectrum of compound **3g**.

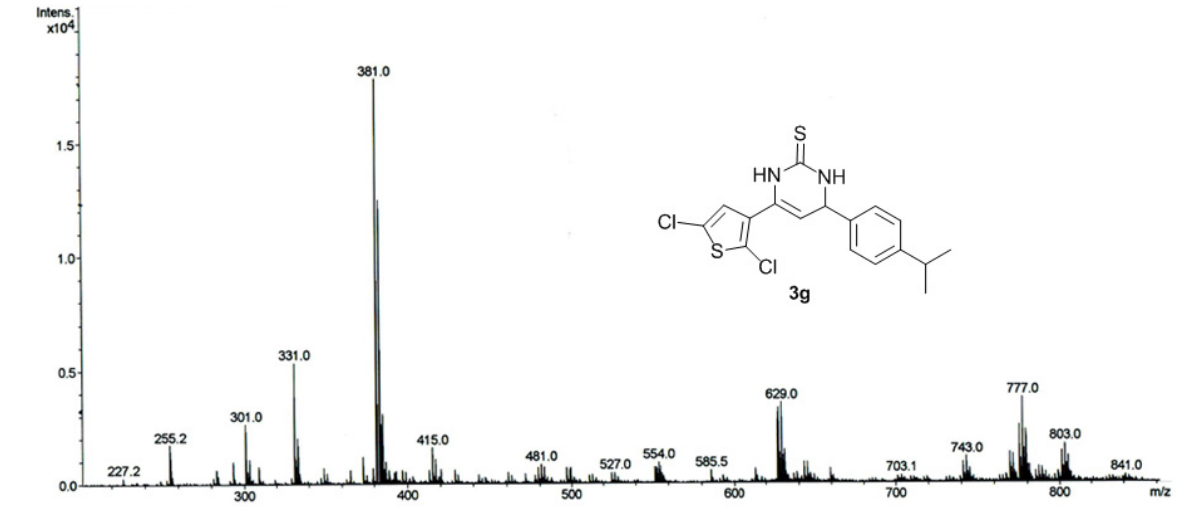

Figure S25. (-)-ESIMS spectrum of compound **3g**.

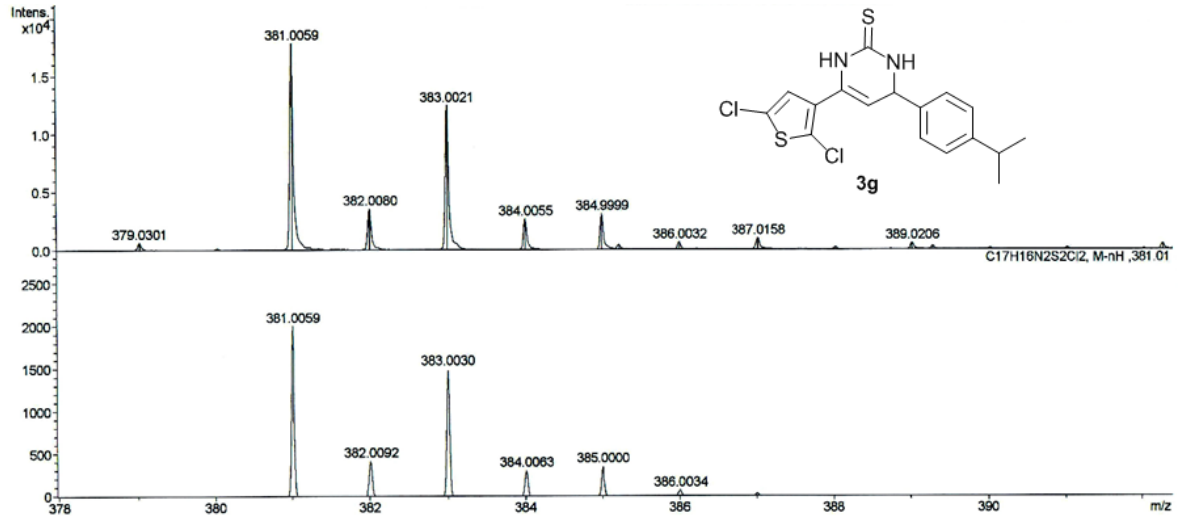

Figure S26. (-)-HRESIMS spectrum of compound **3g**.

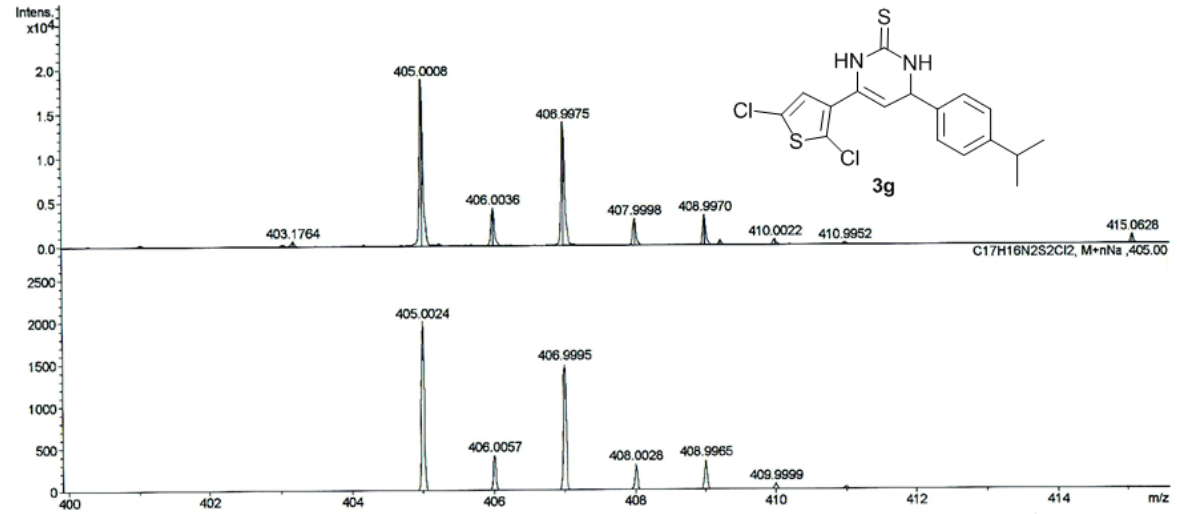

Figure S27. (+)-HRESIMS spectrum of compound **3g**.

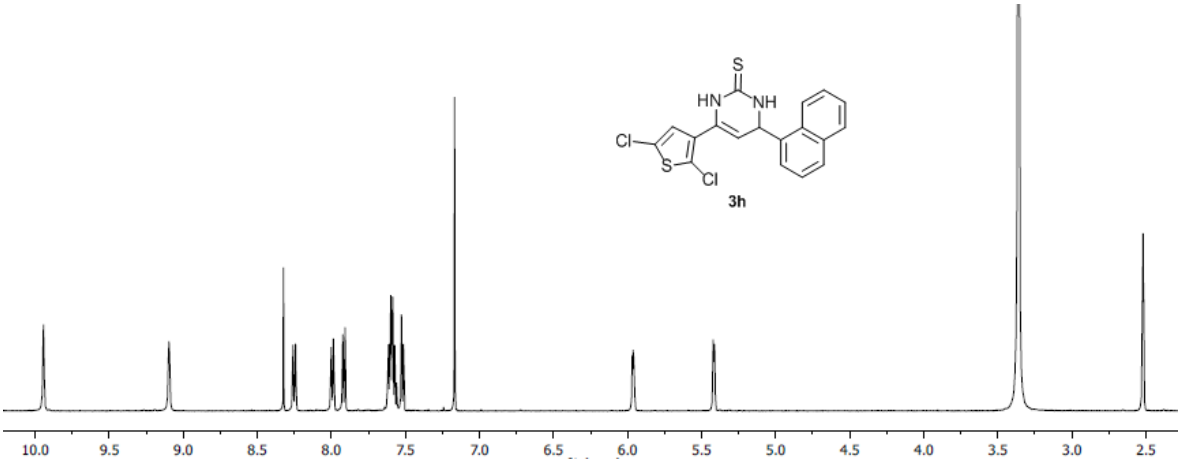

Figure S28. [1]H NMR spectrum of compound **3h**.

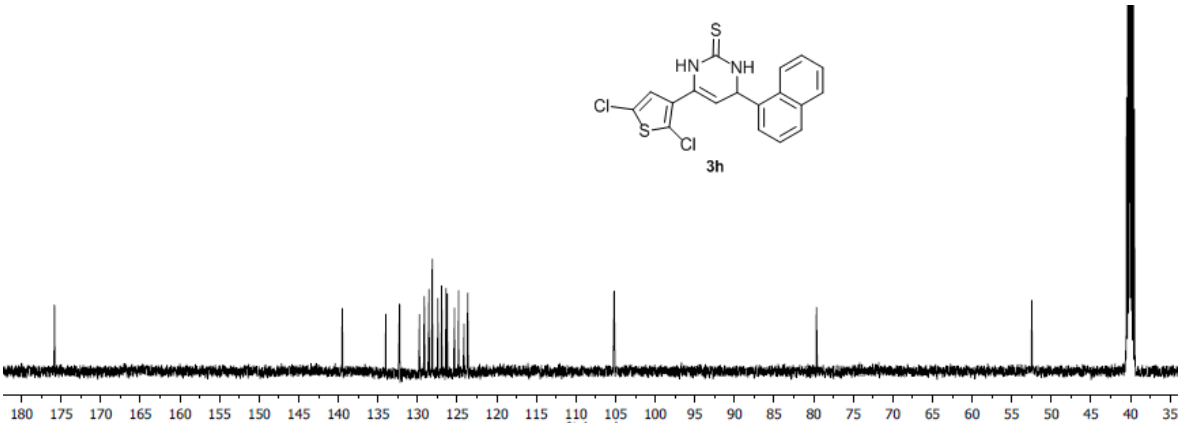

Figure S29. [13]C NMR spectrum of compound **3h**.

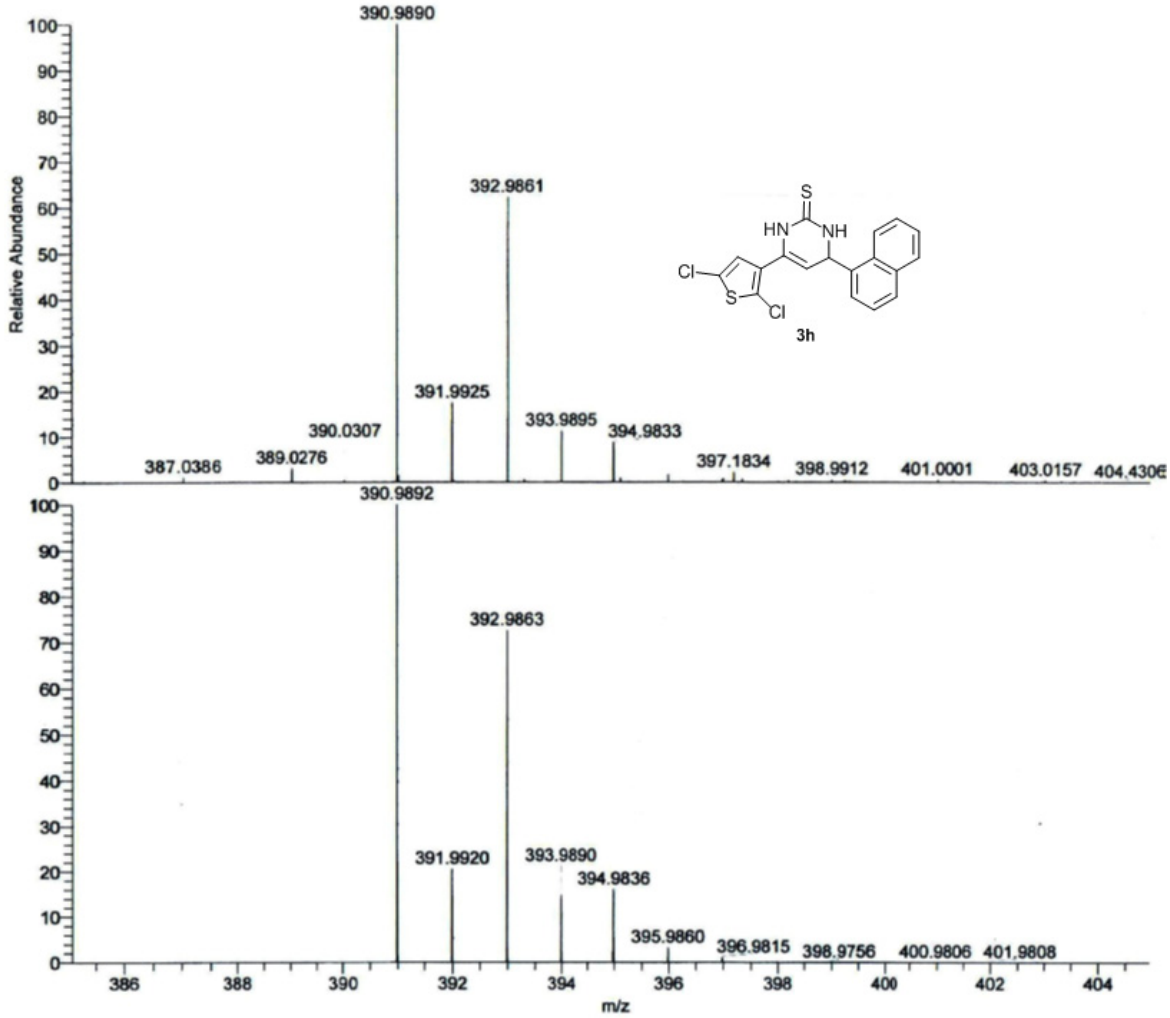

Figure S30. (+)-HRESIMS spectrum of compound **3h**.

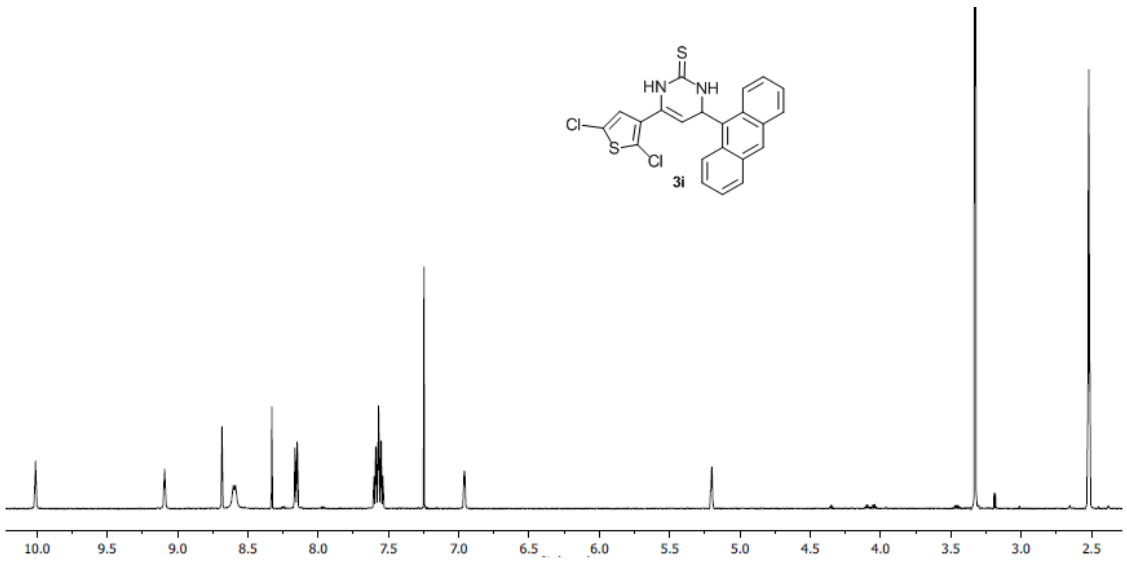

Figure S31. ^{1}H NMR spectrum of compound **3i**.

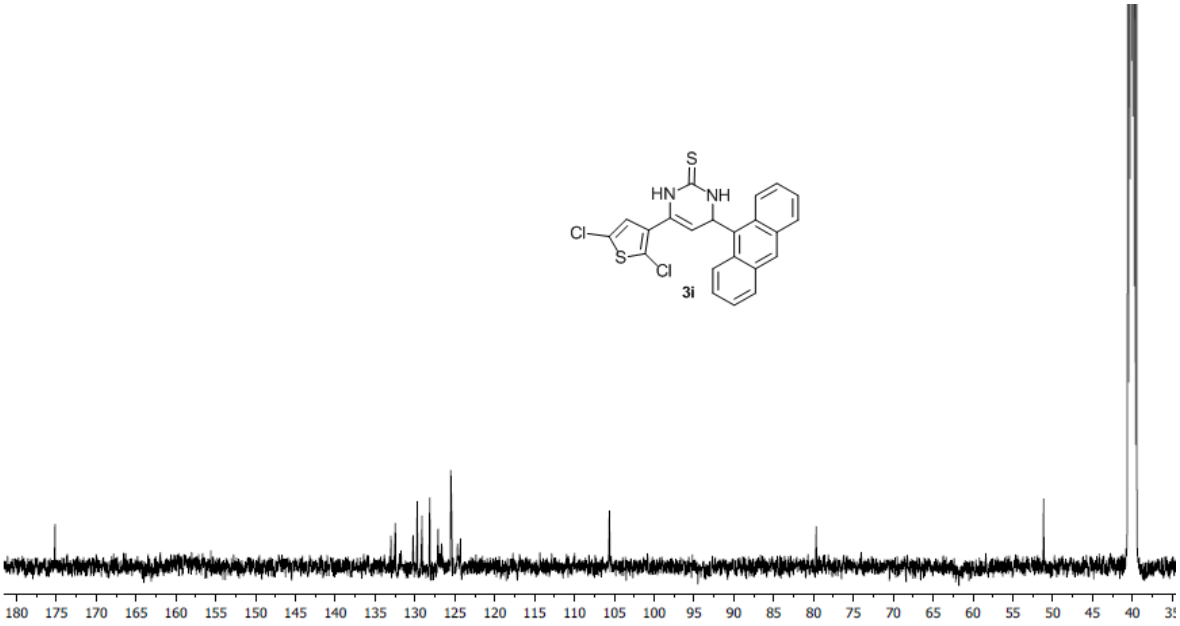

Figure S32. ^{13}C NMR spectrum of compound **3i**.

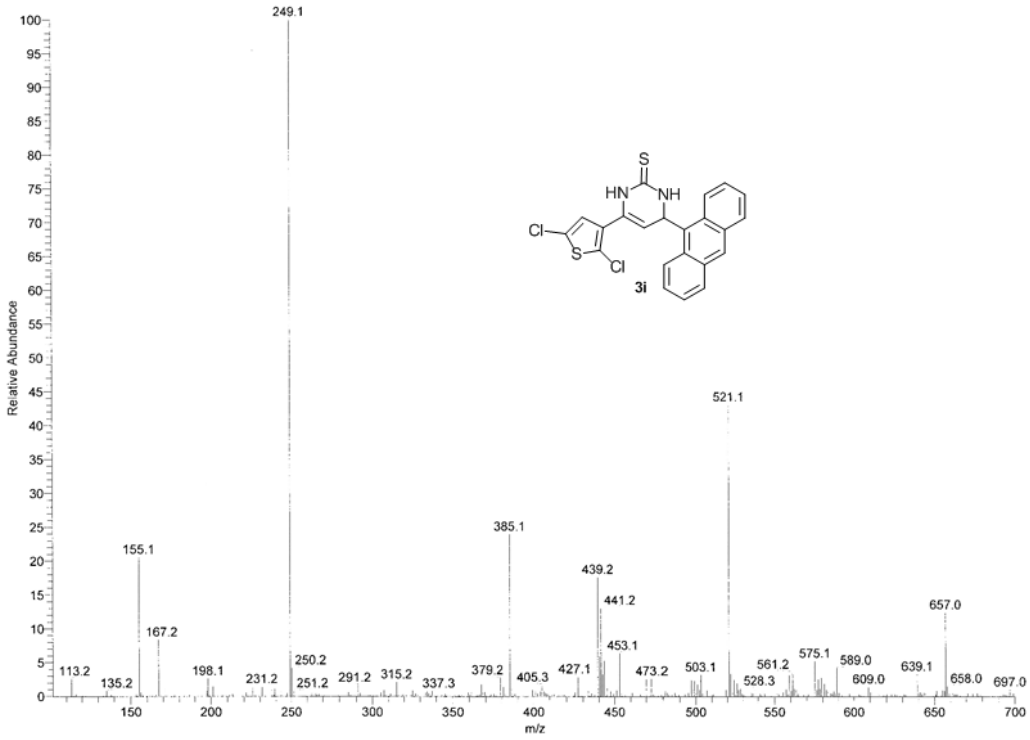

Figure S33. (-)-ESIMS spectrum of compound **3i**.

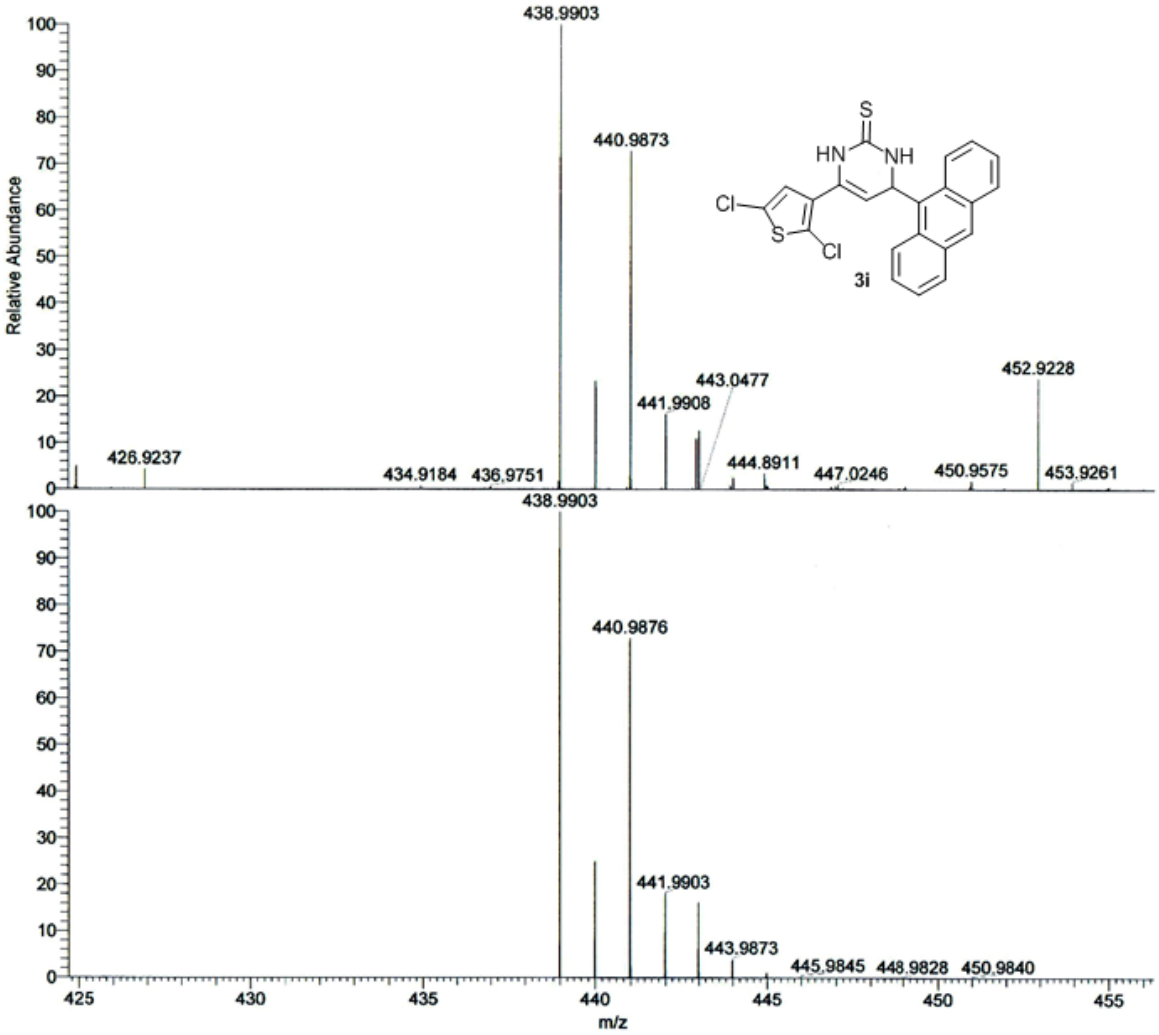

Figure S34. (-)-HRESIMS spectrum of compound **3i**.