

Supplementary Materials: Synthesis, Characterization and Molecular Docking of Novel Bioactive Thiazolyl-Thiazole Derivatives as promising Cytotoxic Antitumor Drug

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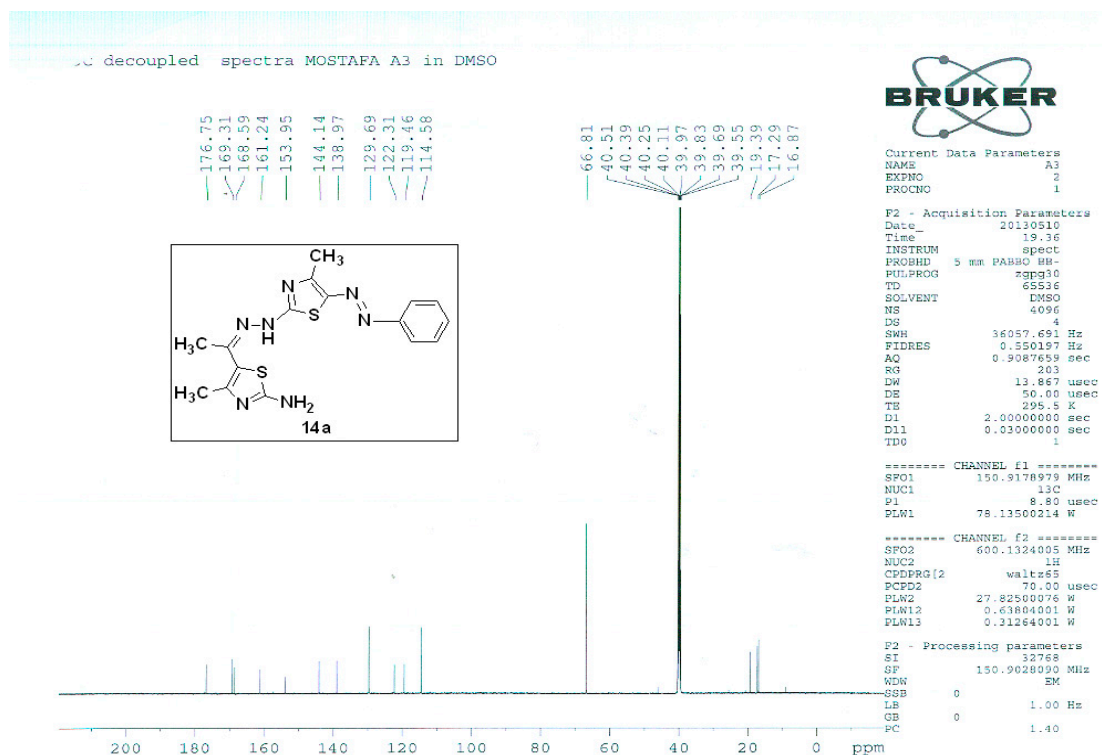


Figure S1. ¹³C-NMR of compound 14a.

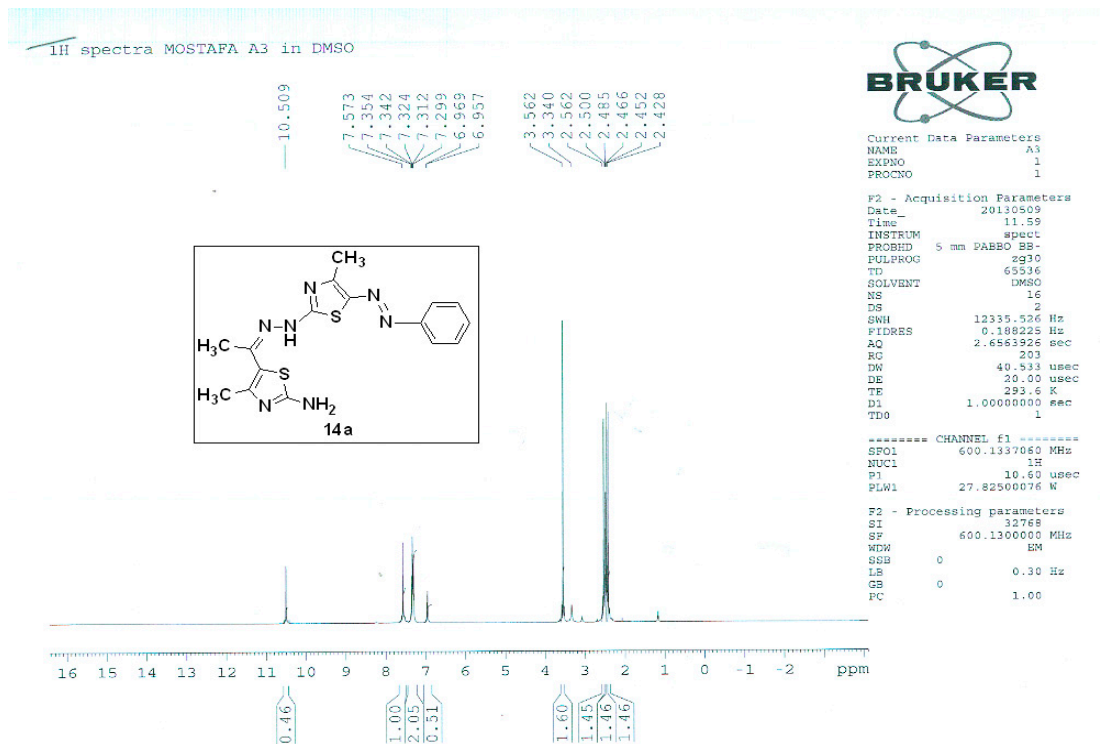
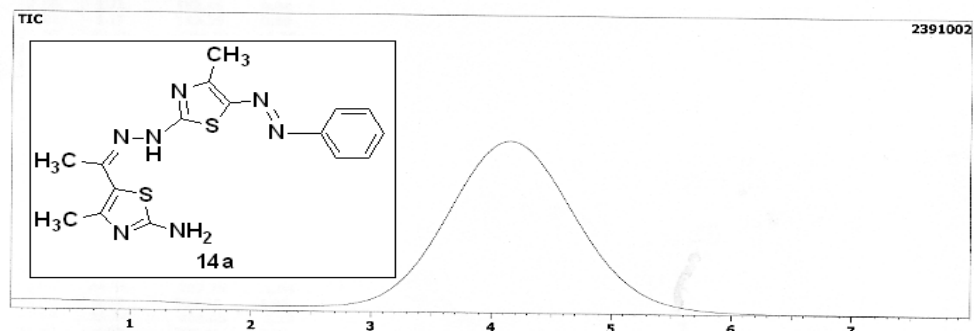
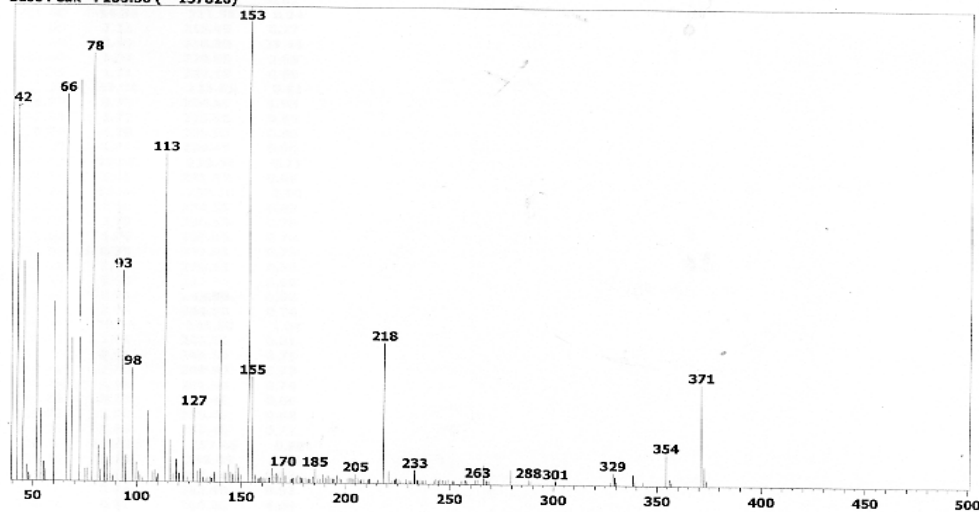


Figure S2. ¹H-NMR of compound 14a.

*** CLASS-5000 *** Report No. = 1 Data : A3.D03 13/02/27 10:00:49
 Sample : Dr/ Sobhy
 ID : A 3
 Sample Amount : 0
 Dilution Factor : 0
 Type : Unknown
 Operator :
 Method File Name : DI.MET



Scan # 486
 Mass Peak # : 164 Ret. Time : 4.050
 Base Peak : 153.30 (157826)



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Figure S3. Mass of compound 14a.

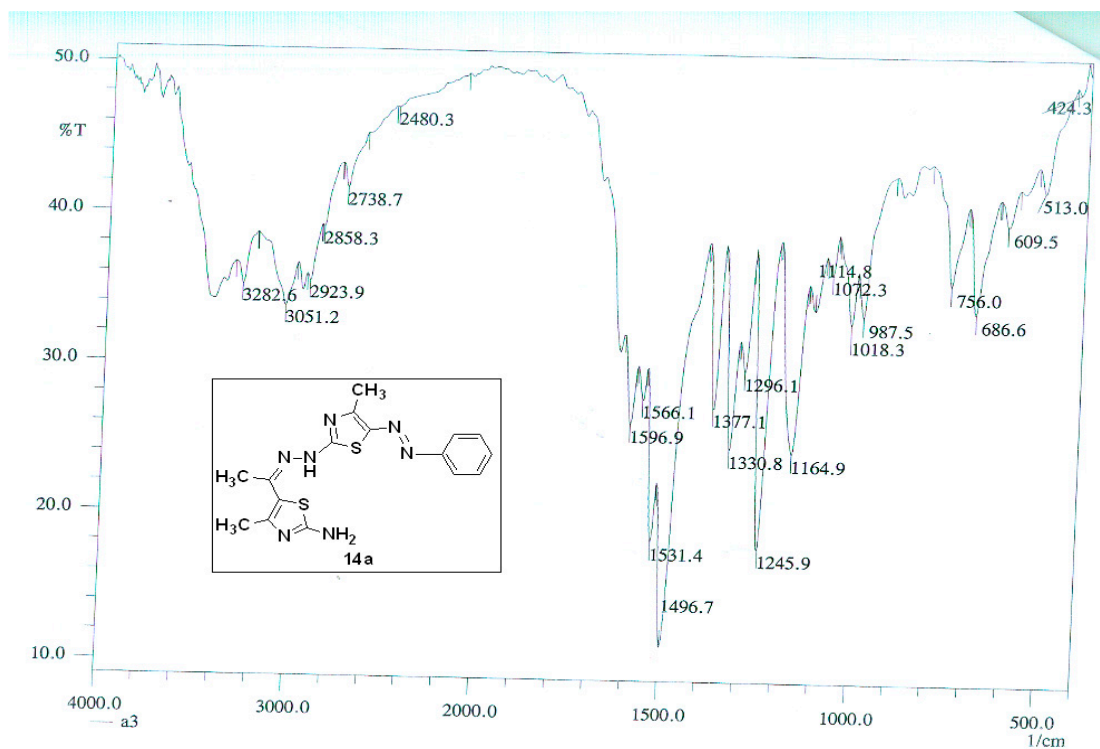


Figure S4. IR of compound 14a.

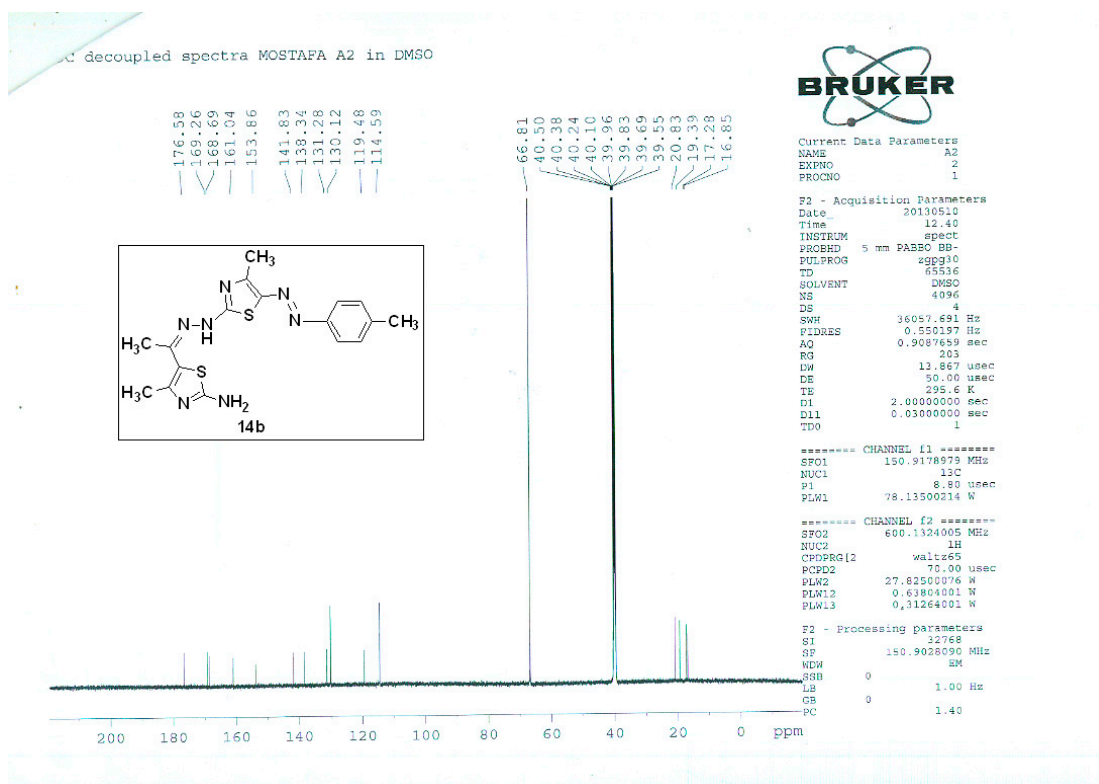


Figure S5. ¹³C-NMR of compound 14b.

¹H spectra MOSTAFA A2 in DMSO

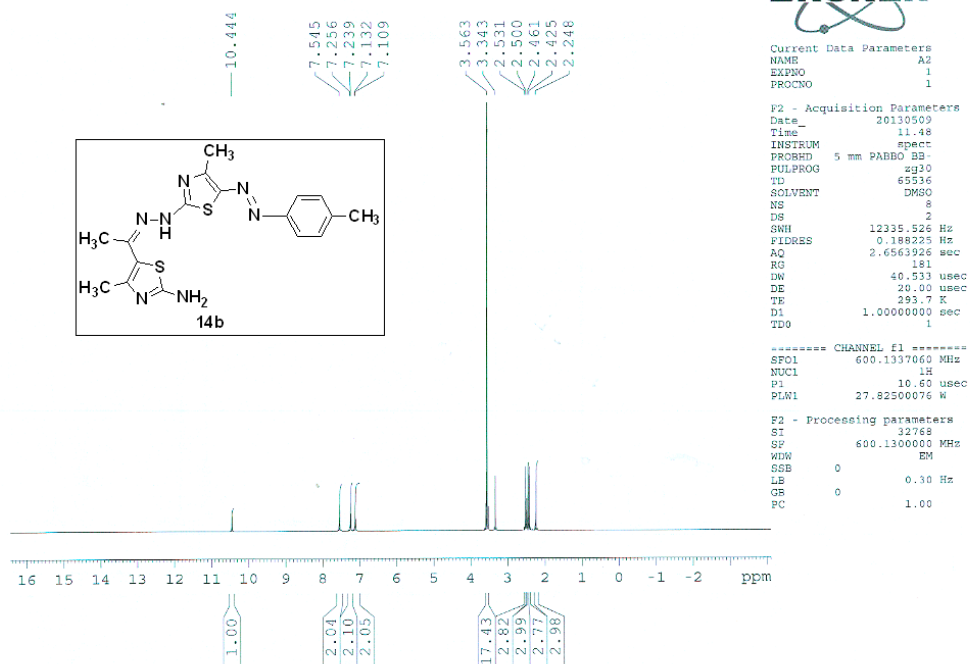
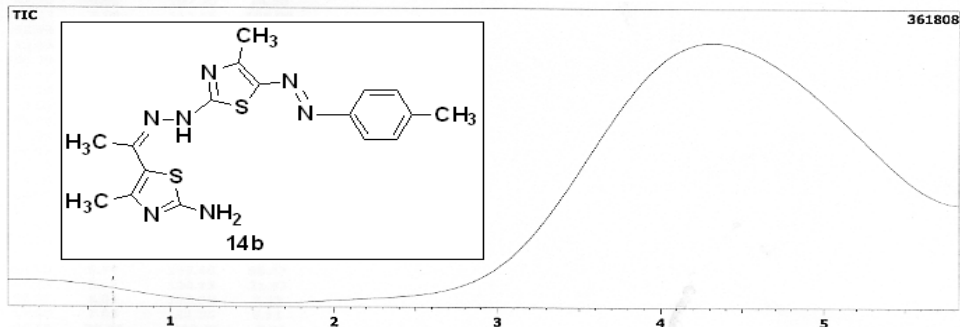


Figure S6. ¹H-NMR of compound 14b.

Data : A2SOBHY.D11 13/02/24 14:10:49
 Sample : Dr/ Sobhy
 ID : A2
 Operator :
 Method File Name : DI.MET



Scan # : 448
 Mass Peak # : 58 Ret. Time : 3.733
 Base Peak : 113.55 (20107)

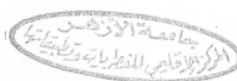
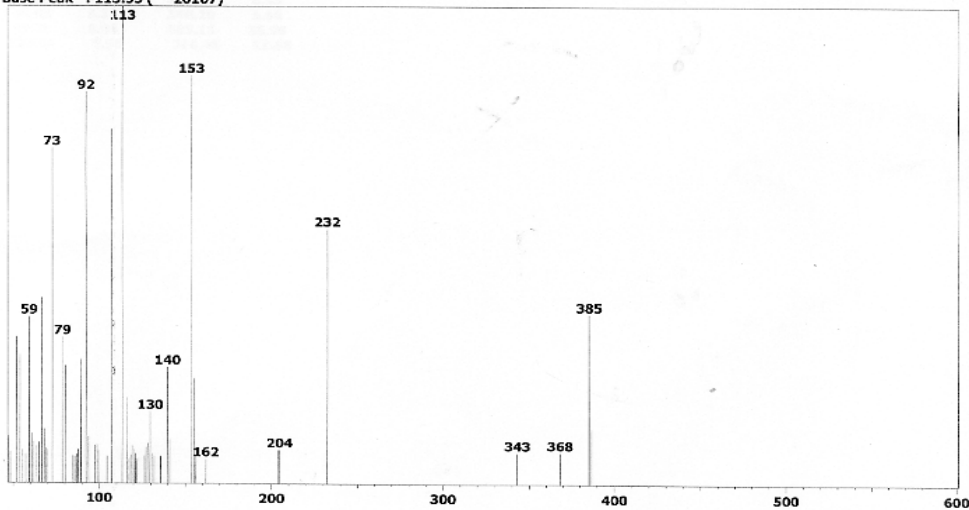


Figure S7. Mass of compound 14b.

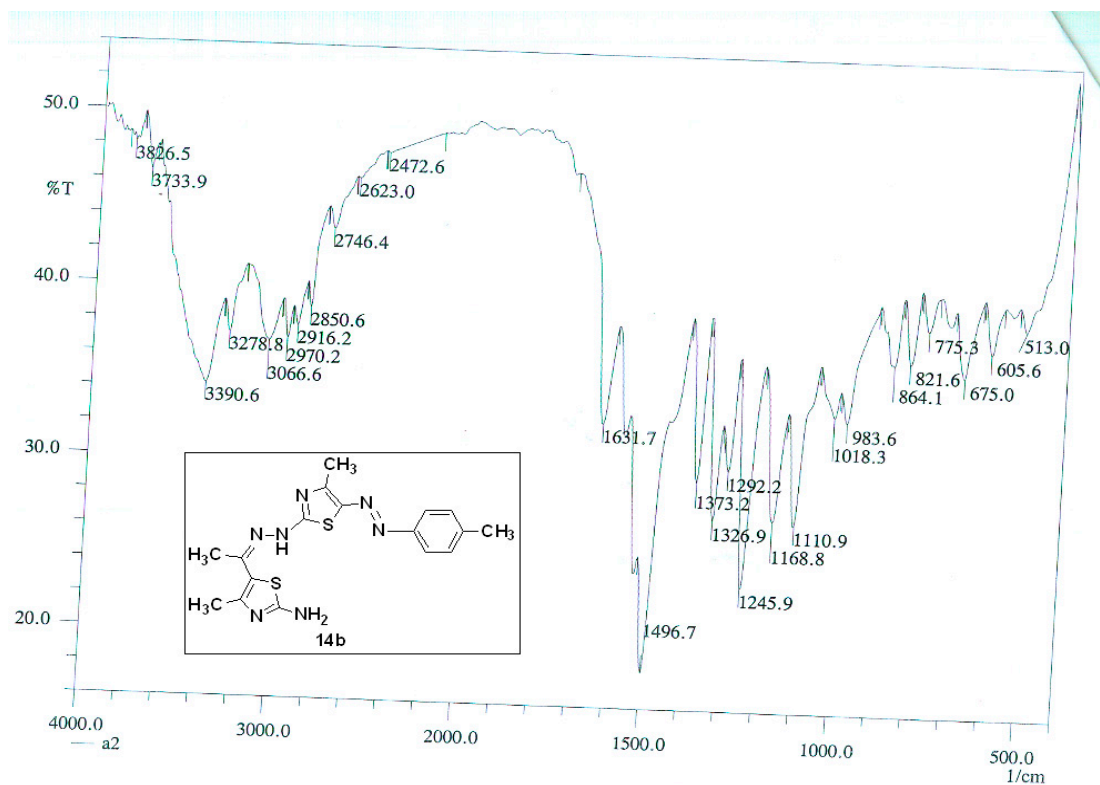


Figure S8. IR of compound 14b.

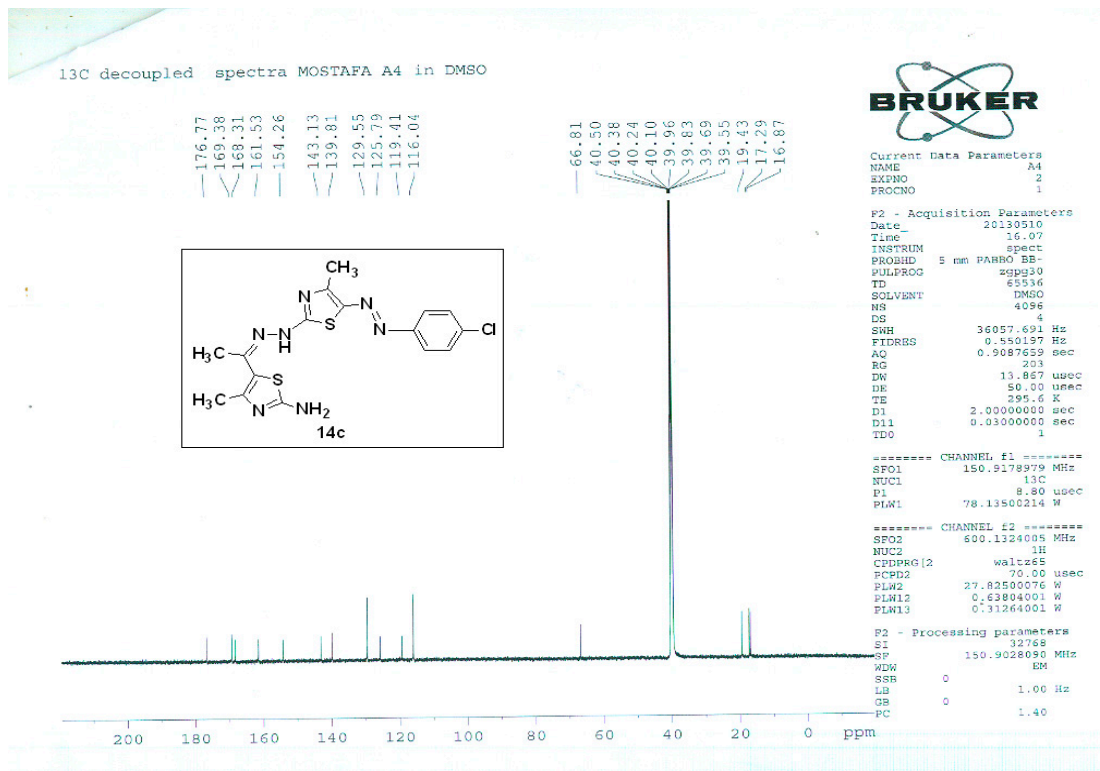


Figure S9. ¹³C-NMR of compound 14c.

¹H spectra MOSTAFA A4 in DMSO

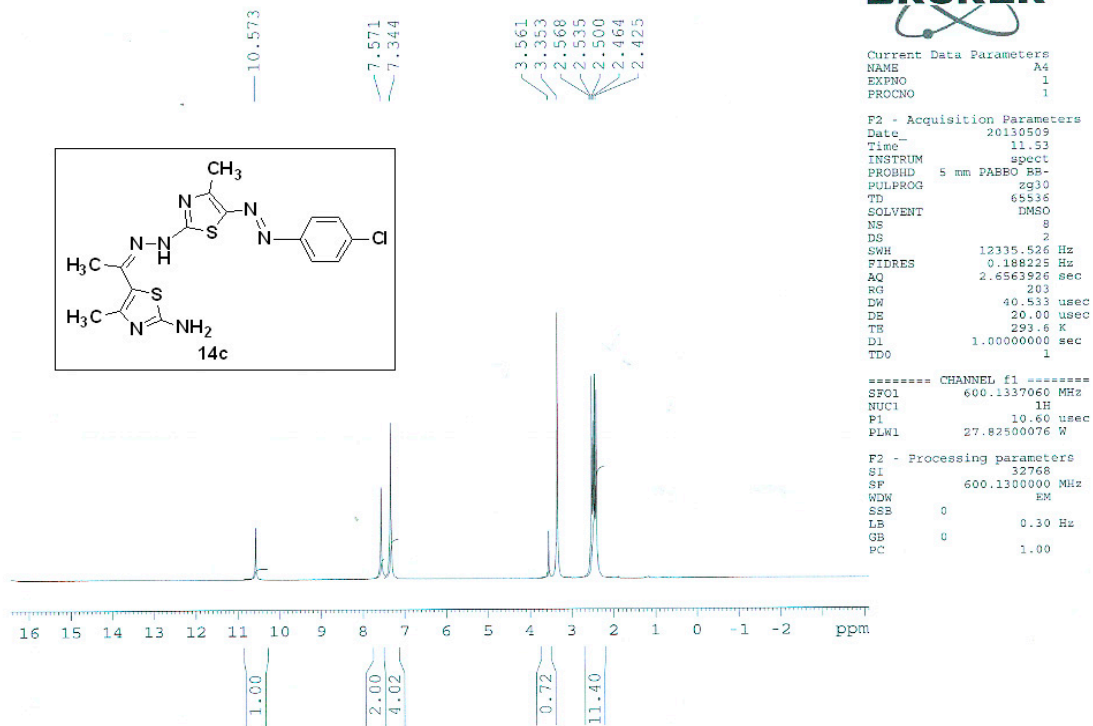
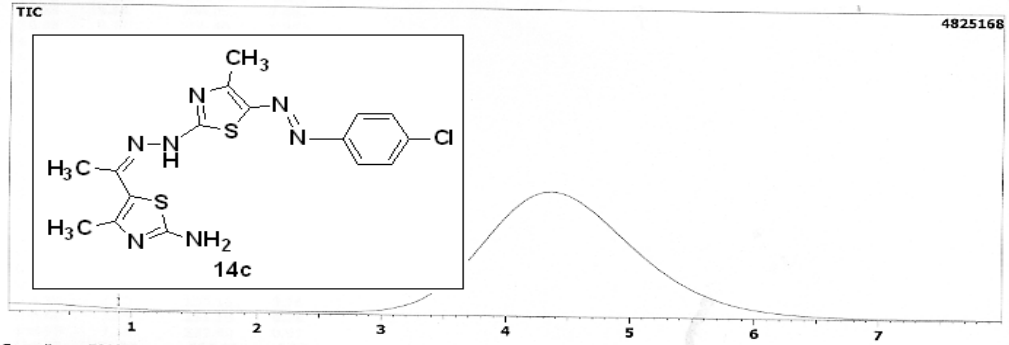
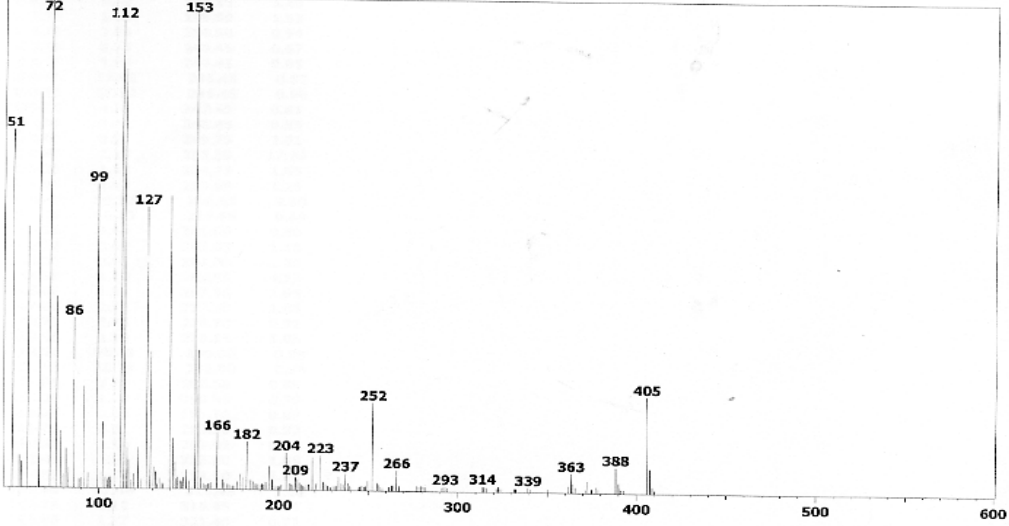


Figure S10. ¹H-NMR of compound 14c.

Data : A4.D03 13/C_/27 10:31:34
Sample : Dr/ Sobhy
ID : A 4
Operator :
Method File Name : DI.MET



Scan # : 5221
Mass Peak # : 174 Ret. Time : 4.350
Base Peak : 72.45 (158344)



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Figure S11. Mass of compound 14c.

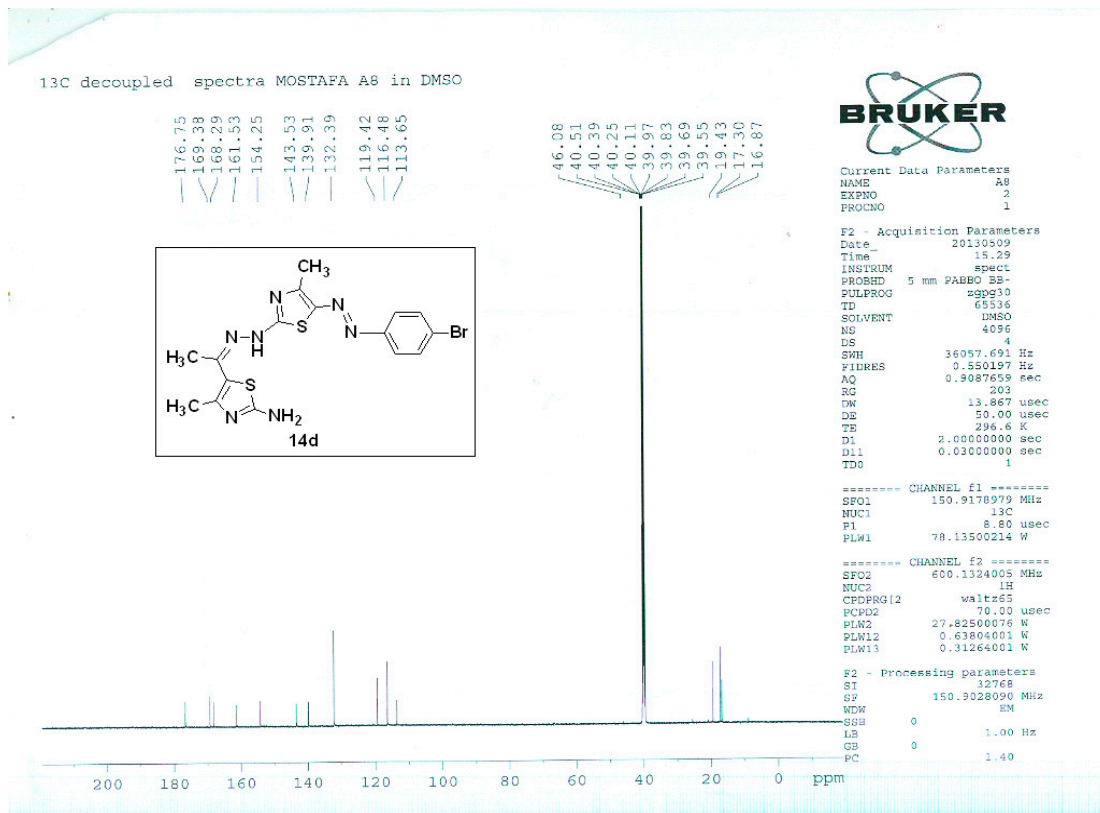
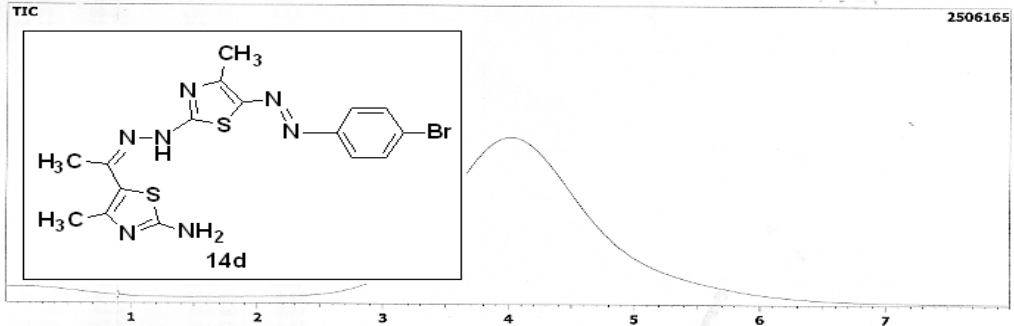
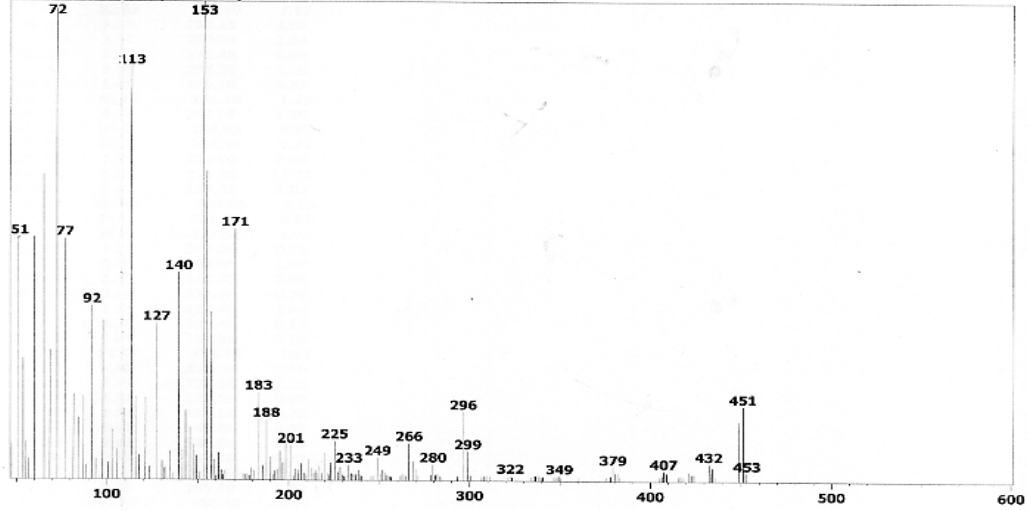


Figure S12. ¹³C-NMR of compound 14d.

Data : AS.D03 13/02/27 10:48:15
Sample : Dr/ Sobhy
ID : A 8
Operator :
Method File Name : DI.MET



Scan # : 464
Mass Peak # : 178 Ret. Time : 3.867
Base Peak : 153.35 (142214)



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Figure S13. Mass of compound 14d.

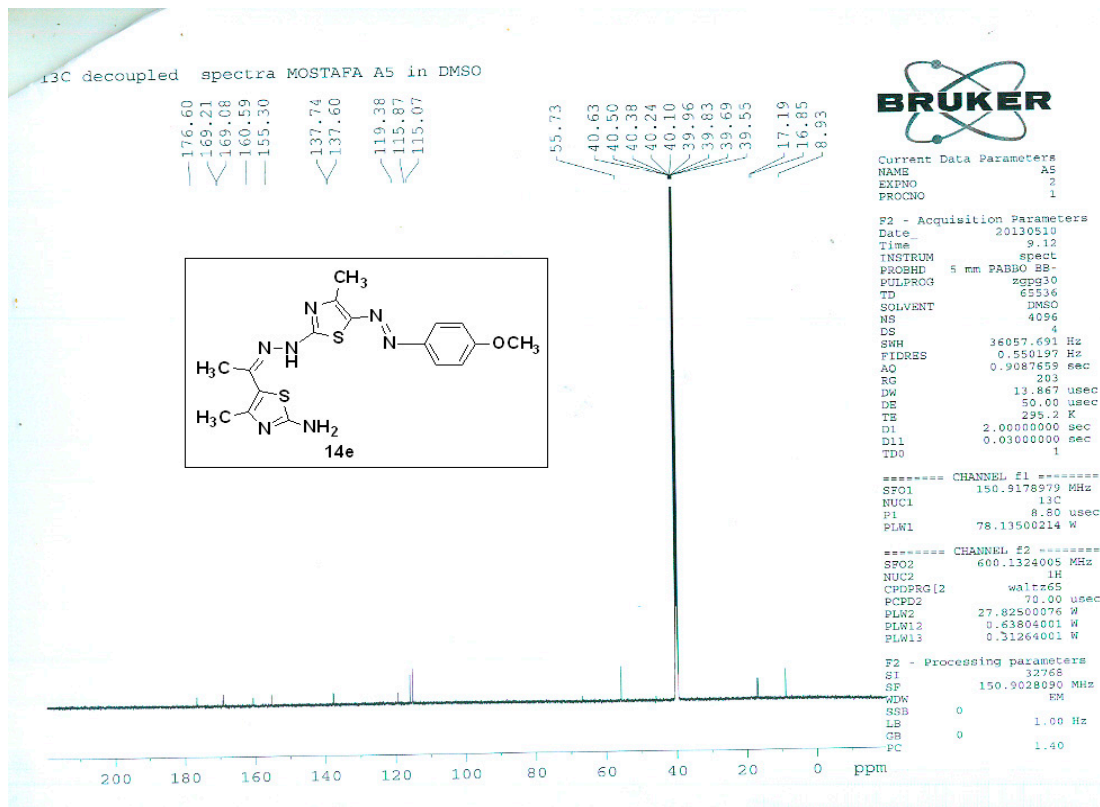


Figure S14. ¹³C-NMR of compound 14e.

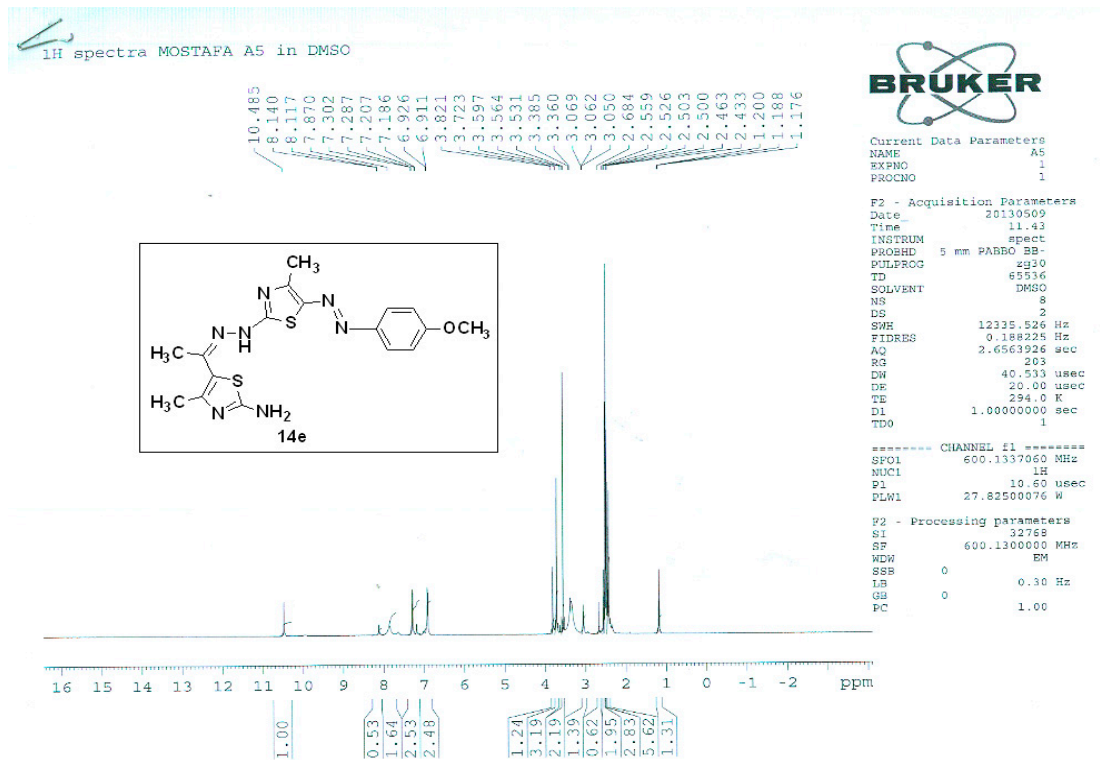
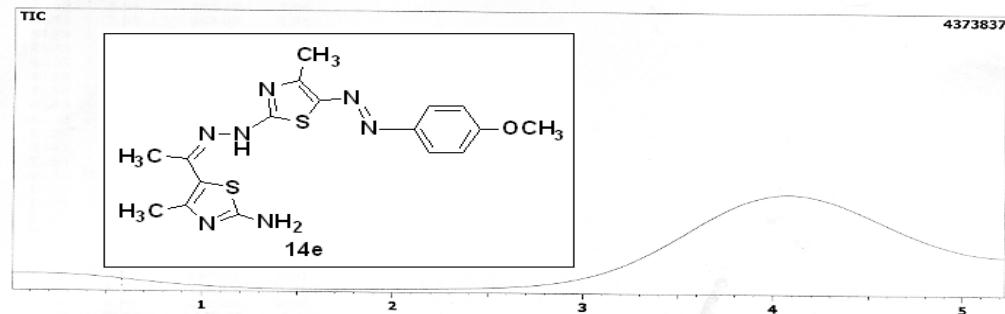


Figure S15. ¹H-NMR of compound 14e.

Data : A5.D03 13/02/27 10:58:05
 Sample : Dr/ Sobhy
 ID : A 5
 Operator :
 Method File Name : D1.MET



Scan # : (306 - 626)
 Mass Peak # : 178 Ret. Time : (2.545 - 5.216)
 Base Peak : 43.75 (67723)

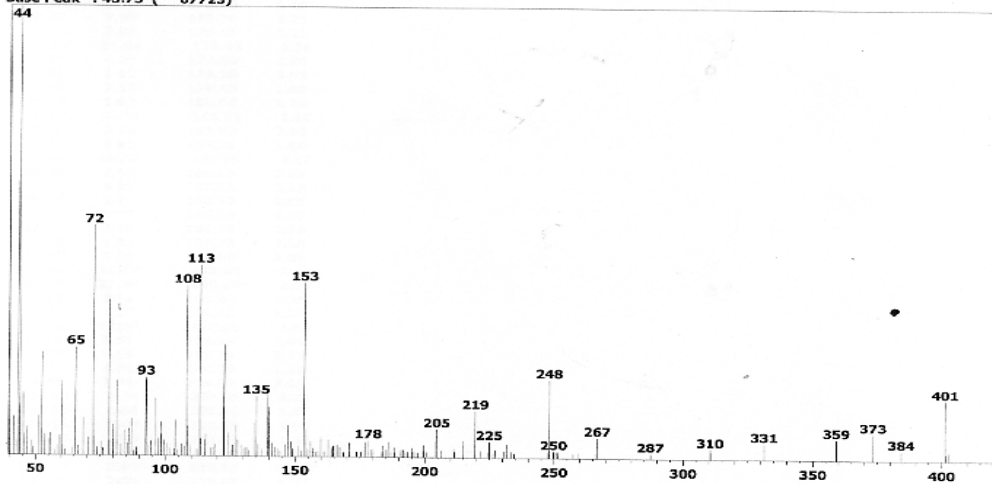


Figure S16. Mass of compound 14e.

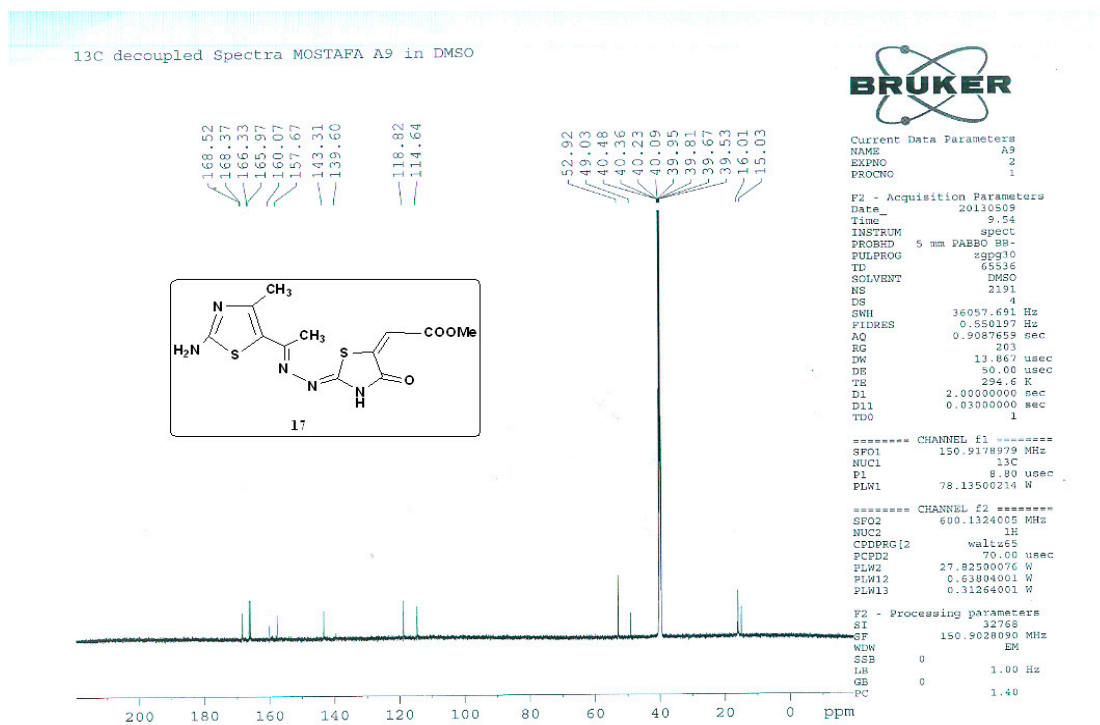


Figure S17. ¹³C-NMR of compound 17.

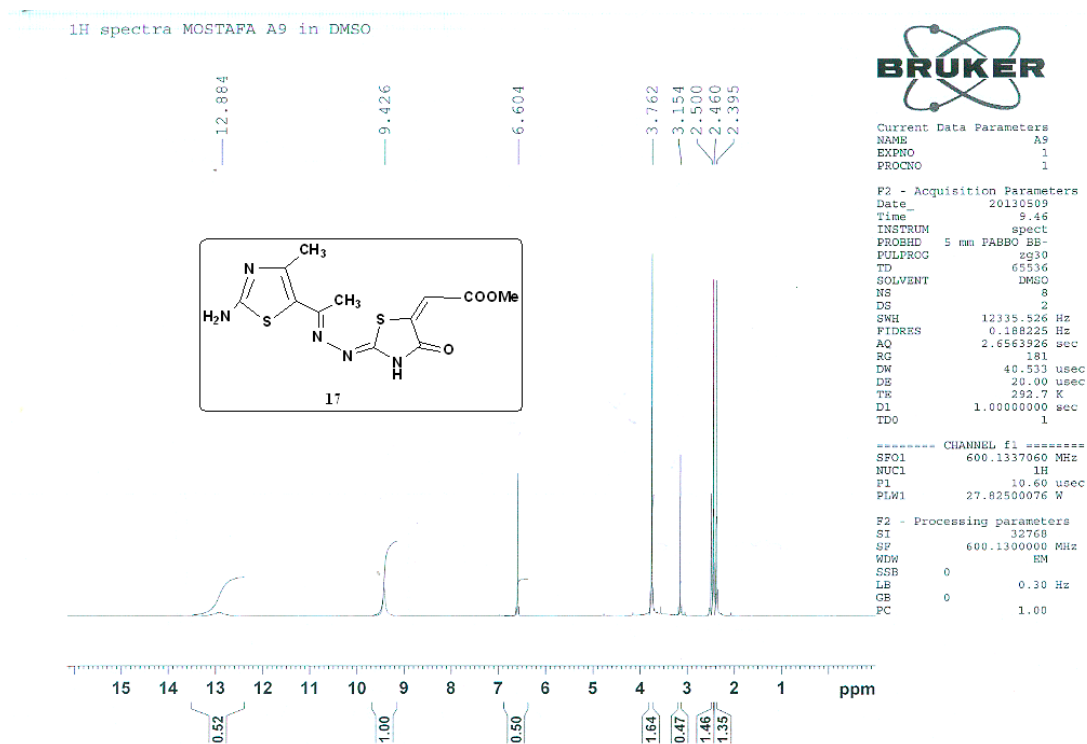
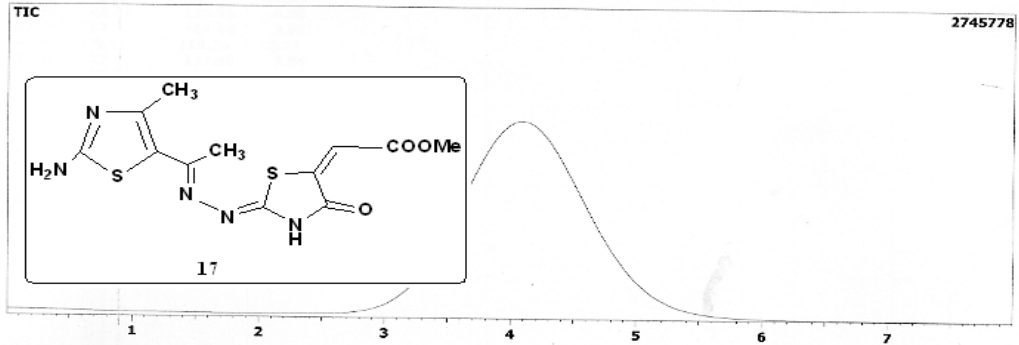
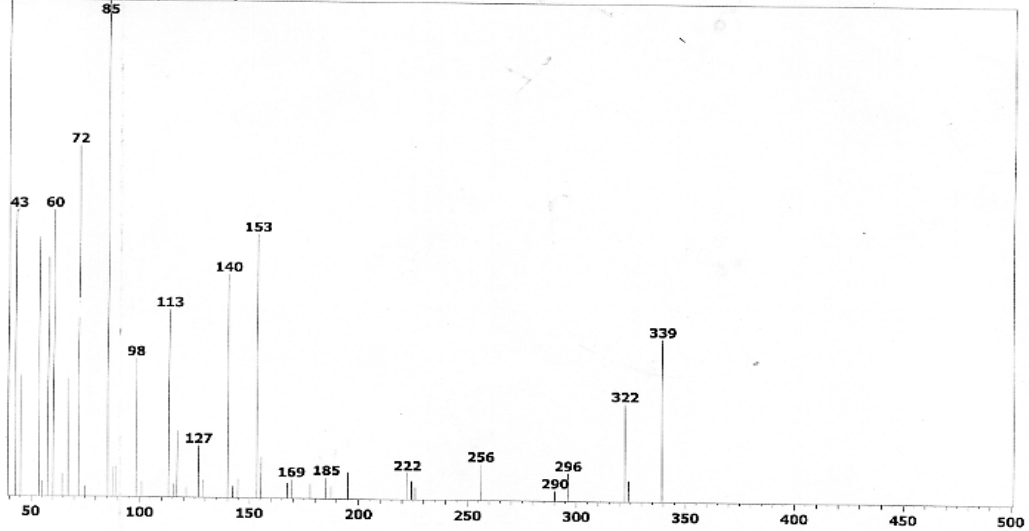


Figure S18. ¹H-NMR of compound 14e.

*** CLASS-5000 *** Report No. = 1 Data : A9.D03 13/02/27 10:18:13
Sample : Dr/ Sobhy
ID : A 9
Sample Amount : 0
Dilution Factor : 0
Type : Unknown
Operator :
Method File Name : DI.MET



Scan # : 500
Mass Peak # : 42 Ret. Time : 4.167
Base Peak : 85.30 (150179)



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Figure S19. Mass of compound 17.

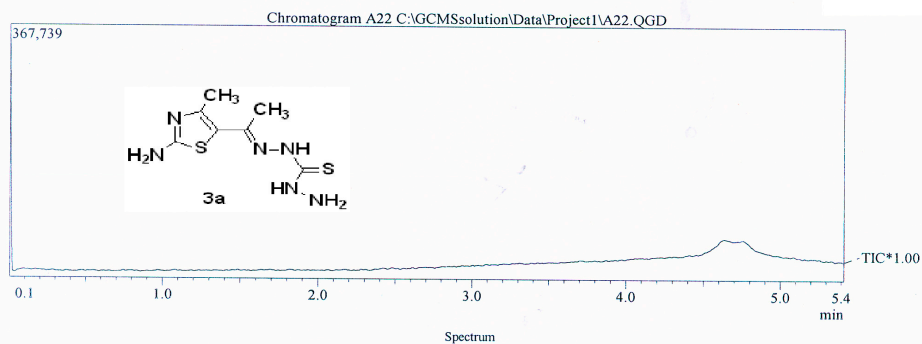
**Cairo University
Micro Analytical Center**

**DI Analysis
Shimadzu Qp-2010 Plus**

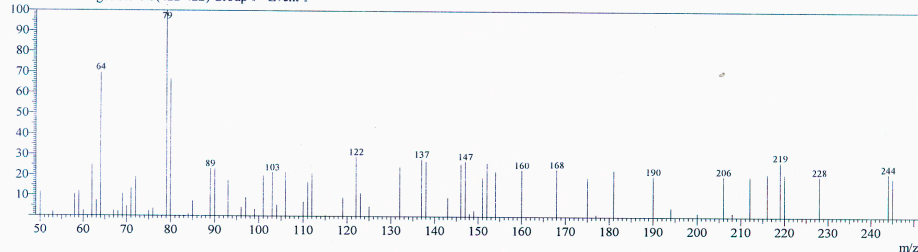
Sample Information
 Analyzed by : A.GABR
 Analyzed : 15/09/2013 01:44:16 م
 Sample Name : A22
 Sample ID :
 Customer Name : صديقي محمد - علوم القاهرة
 Data File : C:\GCMSsolution\Data\Project1\A22.QGD
 Org Data File : C:\GCMSsolution\Data\Project1\A22.QGD
 Method File : C:\GCMSsolution\Data\Project1\A.GABR.qgm
 Org Method File : C:\GCMSsolution\Data\Project1\A.GABR.qgm
 Report File :
 Tuning File : C:\GCMSsolution\System1\Tune1_default1.qgt
 SEndIfSModified by : A.GABR
 Modified : 15/09/2013 01:49:45 م

Method
 Analytical Line 1
 IonSourceTemp : 250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time : 0.00min
 End Time : 10.00min
 ACQ Mode : Scan
 Event Time : 0.50sec
 Scan Speed : 526
 Start m/z : 50.00
 End m/z : 300.00
 Electron Voltage : 70 eV
 Ionization Mode : EI

C:\GCMSsolution\Data\Project1\A22.QGD



Line# 1 R.Time:3.5(Scan#:426)
 MassPeaks:66
 RawMode:Single 3.5(426) BasePeak:79(272)
 BG Mode:Averaged 3.5-3.5(422-422) Group 1 - Event 1



Mass Table

Line# 1 R.Time:3.5(Scan#:426)

MassPeaks:66

RawMode:Single 3.5(426) BasePeak:79(272)

BG Mode:Averaged 3.5-3.5(422-422) Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	32	11.76	4	59.00	33	12.13	7	63.00	21	7.72
2	53.00	6	2.21	5	60.00	7	2.57	8	63.95	190	69.85
3	58.00	29	10.66	6	62.00	68	25.00	9	67.00	7	2.57

Figure S20. Mass of compound 3a.

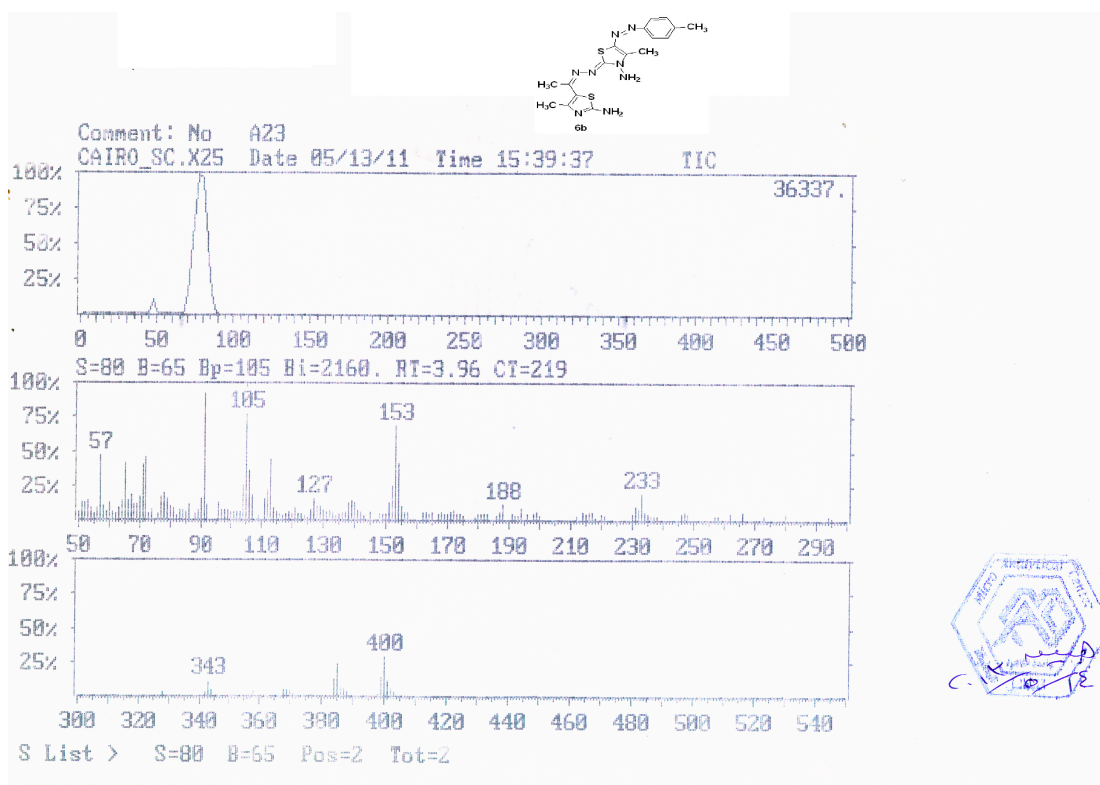


Figure S21. Mass of compound 6b

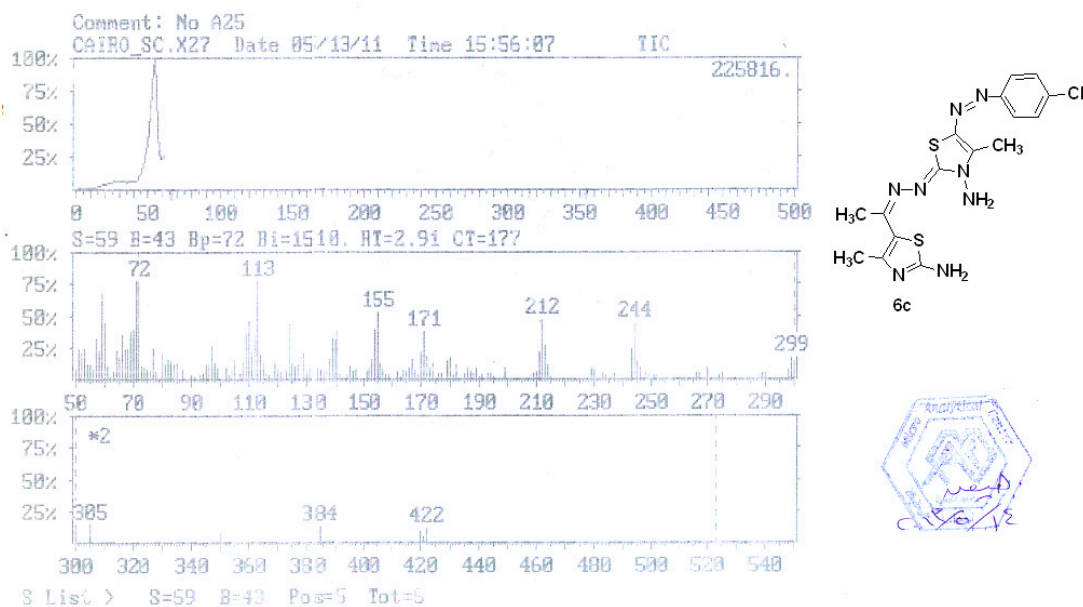


Figure S22. Mass of compound 6c.