Supporting Information

One Step Synthesis of highly functionalized thiazolo[3,2-b][1,2,4]triazole, triazolo[1,5-a]pyrimidine and triazolo[3,4-b][1,3,4]thiadiazine.

Tariq A. Shah[a], Zubair Ahmad[a], Niyaz A. Mir[b], M. Muneer[a*], Nigam P. Rath[c] and Musheer Ahmad[d]

[a]*Department of Chemistry, Aligarh Muslim University, Aligarh – 202002, India,*

[b]*Solid State & Structural Chemistry Unit, IISC, Bangalore, Karnataka-560012,*

[c]*Department of Chemistry and Biochemistry and Center for Nanoscience, University of Missouri-St.Louis, St. Louis, MO 63121, USA,*

[d]*Supramolecular Lab, Department of Chemistry, Indian Institute of Technology, Kanpur – 208016, India*

*Corresponding author: readermuneer@gmail.com; m.muneer.ch@amu.ac.in

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1. General information

(a) Dibenzoylacetylene (DBA) **10** was synthesized by a reported protocol.[1] All other reagents were obtained from sigma Aldrich and used as such without further purification. Solvents used were dried by standard procedures prior to use. The progress of the reaction was monitored by thin-layer chromatography (TLC). ^{1}H NMR spectra were recorded on Bruker Avance II 400 spectrometer at 400 MHz using $CDCl_3$ or DMSO-d_6 as solvent and tetramethylsilane (TMS) as internal standard .^{13}C NMR spectra were run via the same instrument at 100 MHz. Melting points were recorded on Mel-Temp melting point apparatus and are uncorrected.

(b) *Preparation of thiazolo[3,2-b]triazole, triazolo[1,5-a]pyrimidine and triazolo[3,4-b][1,3,4]thiadiazine derivatives* ***(20-28).***

A general procedure for the preparation of **20-28** was to stir an equimolar mixture of the appropriate triazole/tetrazole derivative, for example **12** (0.177g, 1 mmol) with DBA **10** (0.234 g, 1 mmol) in acetonitrile (10 ml) at room temperature for 60 min. The progress of the reaction was monitored by TLC until a precipitate was obtained. The precipitate so obtained was filtered and crystallized in acetonitrile. The product **21** was obtained as brown colored solid, m.p 170-171 ^{0}C, 0.350 g, and yield 85%. Brown color needle shaped diffraction quality crystals were obtained from methanol.

(c) *Preparation of triazolo[5,1-b][1,3]thiazinone and triazolo[1,5-a]pyrimidinone derivatives* ***(33-35).***

General procedure for the preparation of **33-35** involves, stirring an equimolar mixture of appropriate triazole and dimethylacetylenedicarboxylate (DMAD) in 10 ml acetonitrile at room temperature. The precipitate so obtained was filtered and crystallized in appropriate solvents (acetonitrile/methanol). For example, to a magnetically stirred solution of **12** (0.177g, 1 mmol) in 10 ml of acetonitrile was added DMAD **30** (0.142g, 1 mmol) drop wise at room temperature and

stirred for 30 minutes. The precipitate so obtained was filtered, washed with acetonitrile and crystallized in methanol. The product **34** was obtained as white solid, m.p 178-179^{0}C, 0.238g, and yield 82%. Colorless block shaped diffraction quality crystals were obtained from acetonitrile and methanol (2:1).

(d) *Preparation of triazol-3-yl amino/thio acrylates and triazolo[5,1-b][1,3]thiazinone* ***(36-44).***

The general procedure for the synthesis of **36-44** involves, refluxing an equimolar (1 mmol each) mixture of triazole derivative (**11, 12, 14, 16, and 17)** and activated acetylene (methylpropiolate **31** and ethylphenylpropiolate **32**) in 10 ml solvent (acetonitrile/methanol) for 3-5 hours or as required for the completion of the reaction monitored by TLC. The solvent was removed under reduced pressure and the solid was crystallized in appropriate solvents (acetonitrile/methanol).

For example, for the synthesis of **36**, equimolar amounts of **31** (0.084 g, 1 mmol) and **11** (0.101 g, 1 mmol) in 10 mL acetonitrile were refluxed for 4 hours. The solvent was removed under reduced pressure and the solid was crystallized in acetonitrile. The product **36** was obtained as White solid, melting point 200-201^{o}C, 0.147 g and yield 79%. Colorless block shaped diffraction quality crystals were obtained from acetonitrile.

2. Characterization techniques.

(a) Single crystal X-ray diffraction Studies.

Single crystal X-ray data of compounds **21**, **24**, **27**, **36**, **41** were collected at 100K on a Brucker SMART APEX CCD diffractometer while as that of **25** and **34** were collected at 150K on *Rigaku Mercury 375/M CCD (XtaLAB mini)* using graphite monochromated MoK_α radiation (λ= 0.71073 Å). The linear absorption coefficients, scattering factors for the atoms and the

anomalous dispersion corrections were referred from the International Tables for X-ray Crystallography.[2]The data integration and reduction for **21**, **24**, **27**, **36**, **41** were worked out with SAINT [3] software while as that of **25** and **34** with *Rigaku crystal clear software.*[4] Empirical absorption correction was applied to the collected reflections with *SADABS*,[5] and the space group was determined using *XPREP.*[6] The structure was solved by the direct methods using *SHELXTL-97* [7] and refined on F^2 by full-matrix least-squares using the *SHELXTL-97* programme[8] package. All non-H atoms were refined anisotropically. The H-atoms attached to carbon atoms were positioned geometrically and treated as riding atoms using *SHELXL* default parameters. Structure solution and refinement for compounds **25** and **34** were performed using *SHELX-2013* [9] embedded in the WinGX suite[10] and refinement of coordinates and isotropic thermal parameters of non-hydrogen atoms were carried out by the full-matrix least-squares method. Mercury version 3.5 was used for molecular representations and packing diagrams.[11] The crystal and refinement data are collected in Table 1.

(b). Crystallization Details.

Crystallization Method**:** Solvent evaporation (at room temperature).

(i) Compound **21**: Brown colour needle shaped crystals, crystallised from methanol.

(ii) Compound **24**: Yellow colour block shaped diffraction quality crystals were obtained from acetonitrile.

(iii) Compound **25**: Green colour block shaped diffraction quality crystals were obtained from acetonitrile.

(iv) Compound **27**: Yellow colour block shaped diffraction quality crystals were obtained from acetonitrile.

(v) Compound **34**: Colourless block shaped diffraction quality crystals were obtained from acetonitrile and methanol (2:1).

(vi) Compound **36**: Colourless block shaped diffraction quality crystals were obtained from acetonitrile.

(vii) Compound **41**: Colourless rectangular shaped diffraction quality crystals were obtained from methanol.

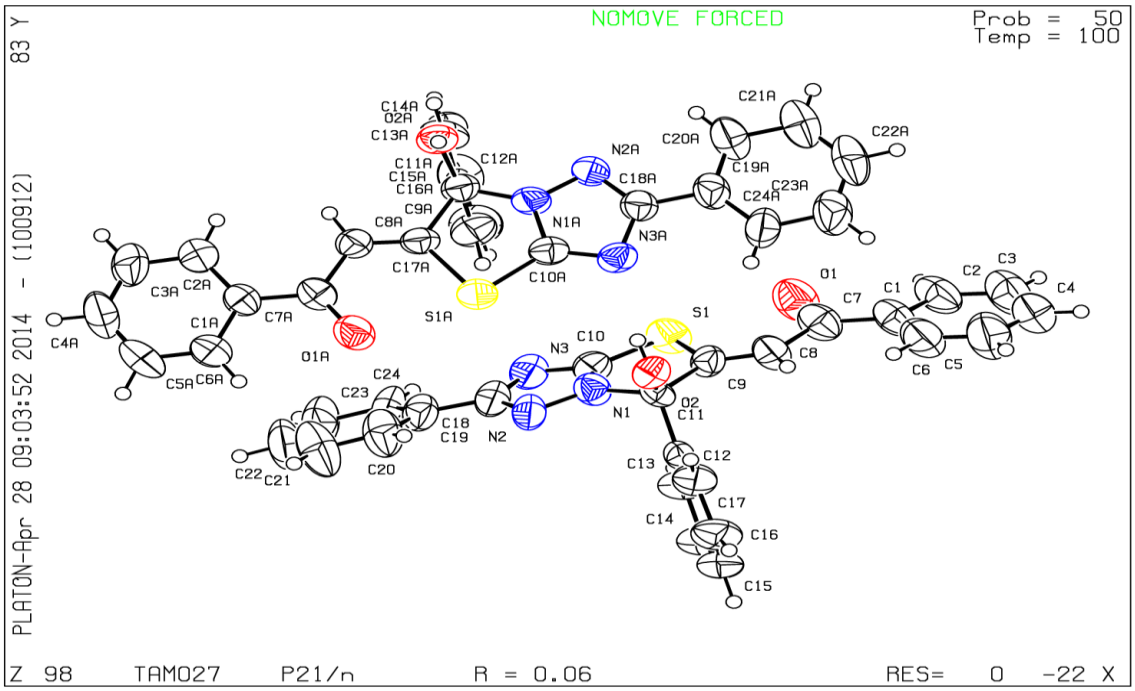
(C). Table 1. Crystallographic Information

Compound	**21**	**24**	**25**	**27**	**34**	**36**	**41**
CCDC No.	1410751	1410752	1410753	1410754	1410755	1410756	1410757
Molecular Formula	$C_{24}H_{17}N_3O_2S$	$C_{19}H_{14}N_4OS$	$C_{24}H_{16}N_4OS$	$C_{23}H_{16}N_4O_2S$	$C_{13}H_9N_3O_3S$	$C_6H_7N_3O_2S$	$C_{11}H_7N_3OS$
Formula Weight	411.48	346.40	408.47	412.47	287.29	185.21	229.26
Crystal System	Monoclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space Group	*P 2$_1$/n*	*P-1*	*P*2$_1$/n	*P 2$_1$/c*	*P*2$_1$/c	*P 2$_1$/n*	*P 2$_1$/n*
a (Å)	13.409(2)	9.337(4)	6.99200	13.1611(14)	7.1783(10)	5.4918(4)	6.9892(6)
b (Å)	22.777(3)	9.368(4)	14.61700	13.5100(15)	14.804(2)	16.0080(11)	10.5036(10)
c (Å)	13.401(2)	10.286(5)	19.05100	10.7868(10)	2.0251(19)	9.4419(7)	13.4268(13)
α (˚)	90	113.699(7)	90	90	90	90	90
β (˚)	99.1300	97.243(8)	95.5000	98.381(4)	97.835(6)	103.129(4)	104.277(4)
γ (˚)	90	97.258(8)	90	90	90	90	90
V (Å^3)	4041.0(10)	801.6(6)	1938.088	1897.5(3)	1266.0(3)	808.37(10)	955.24(15)
$\rho_{calc.}$ (g/cm^3)	1.353	1.435	1.400	1.444	1.507	1.522	1.594
Z	8	2	4	4	4	4	4
F(000)	1712	360	848	856	592	384.0	472
μ. (mm^{-1})	0.187	0.217	0.192	0.200	0.266	0.361	0.316
T (K)	100	100	150(2)	100	150(2)	100	100
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073

Unique Reflns.	6851	2902	4460	4283	2894	3867	3319
Completeness (%)	96.3	97.4	99.9	99.9	99.9	98.4	0.99
R_1 (F^2)	0.0590	0.0548	0.0541	0.0387	0.0464	0.0509	0.0495
wR_2(F^2)	0.2355	0.1741	0.1726	0.0868	0.1456	0.1563	0.1365
GooF	1.07	1.13	1.17	1.02	1.13	1.03	0.98

Note: CCDC No.'s **1410751, 1410752, 1410753, 1410754, 1410755, 1410756 and 1410757** for compounds **21**, **24**, **25**, **27**, **34**, **36** and **41** respectively contains the supplementary crystallographic data. These data can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.

(d) ORTEP PLOT of X-ray Crystal 21, 14, 25, 27, 34, 36, 41.



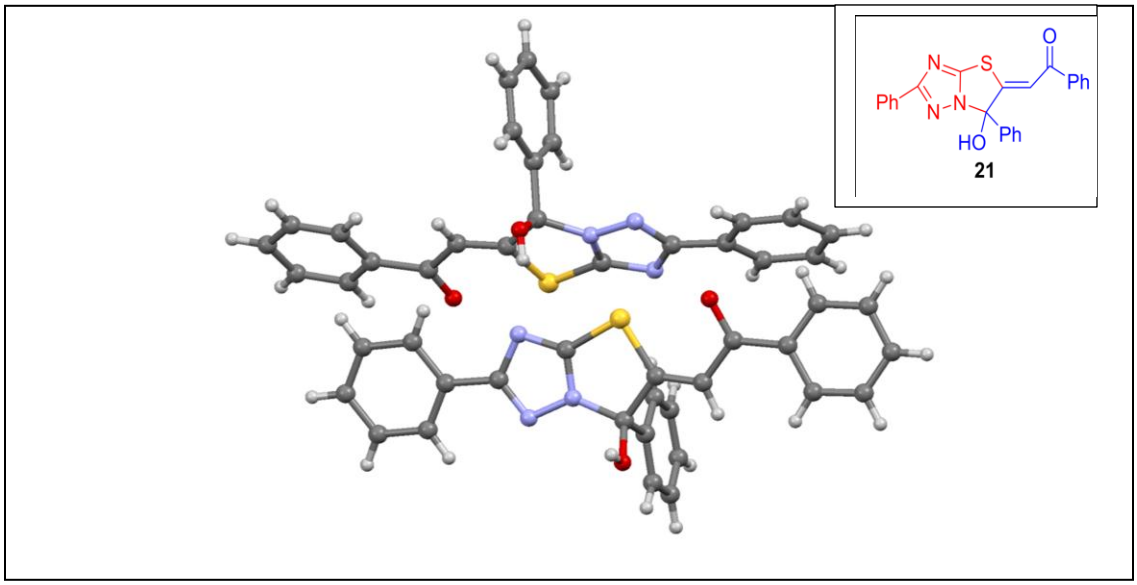
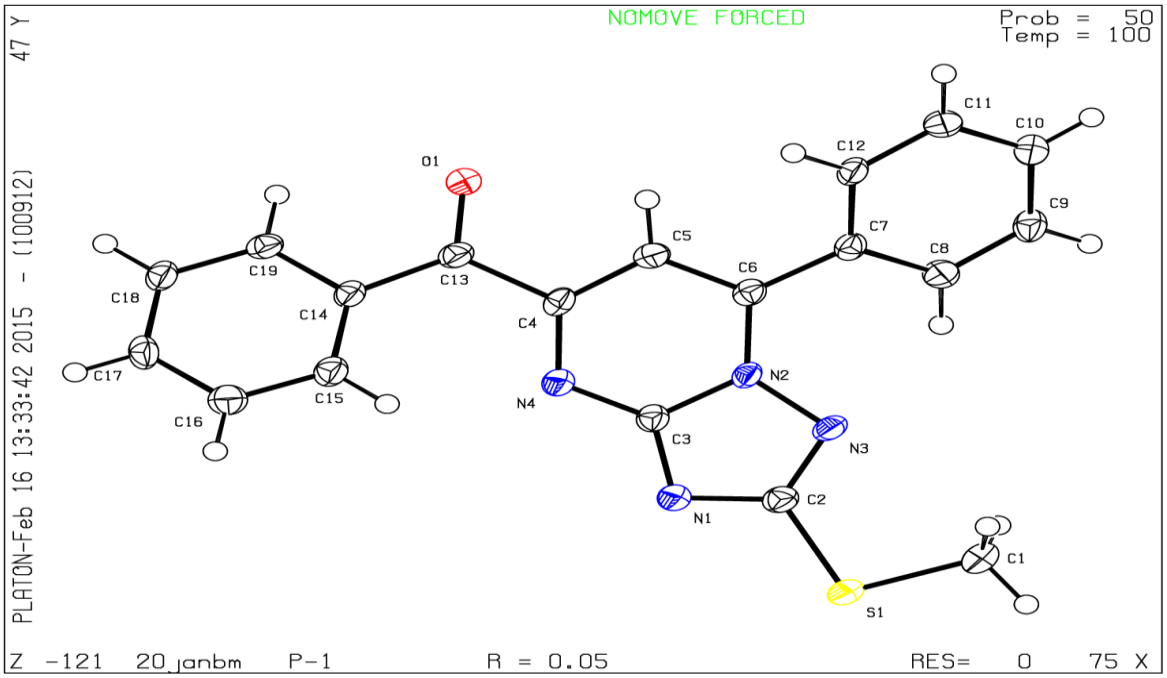


Figure 1. View of **21** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.



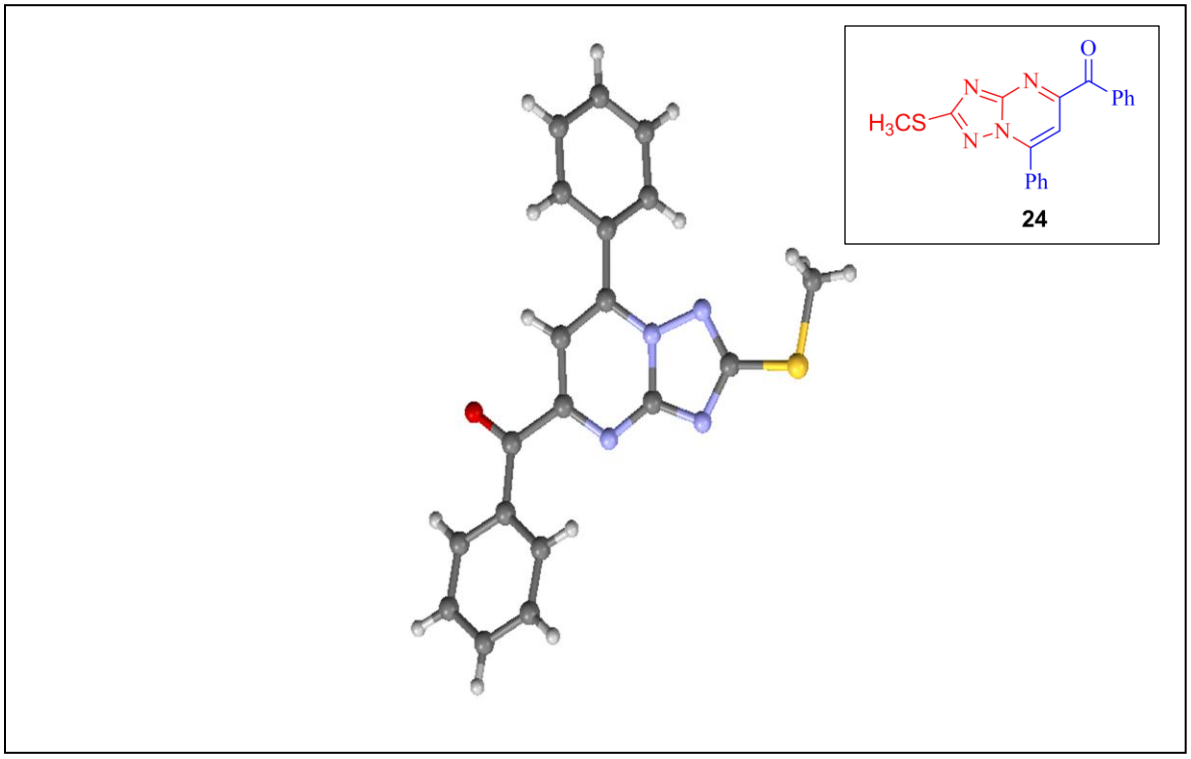


Figure 2. View of **24** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.

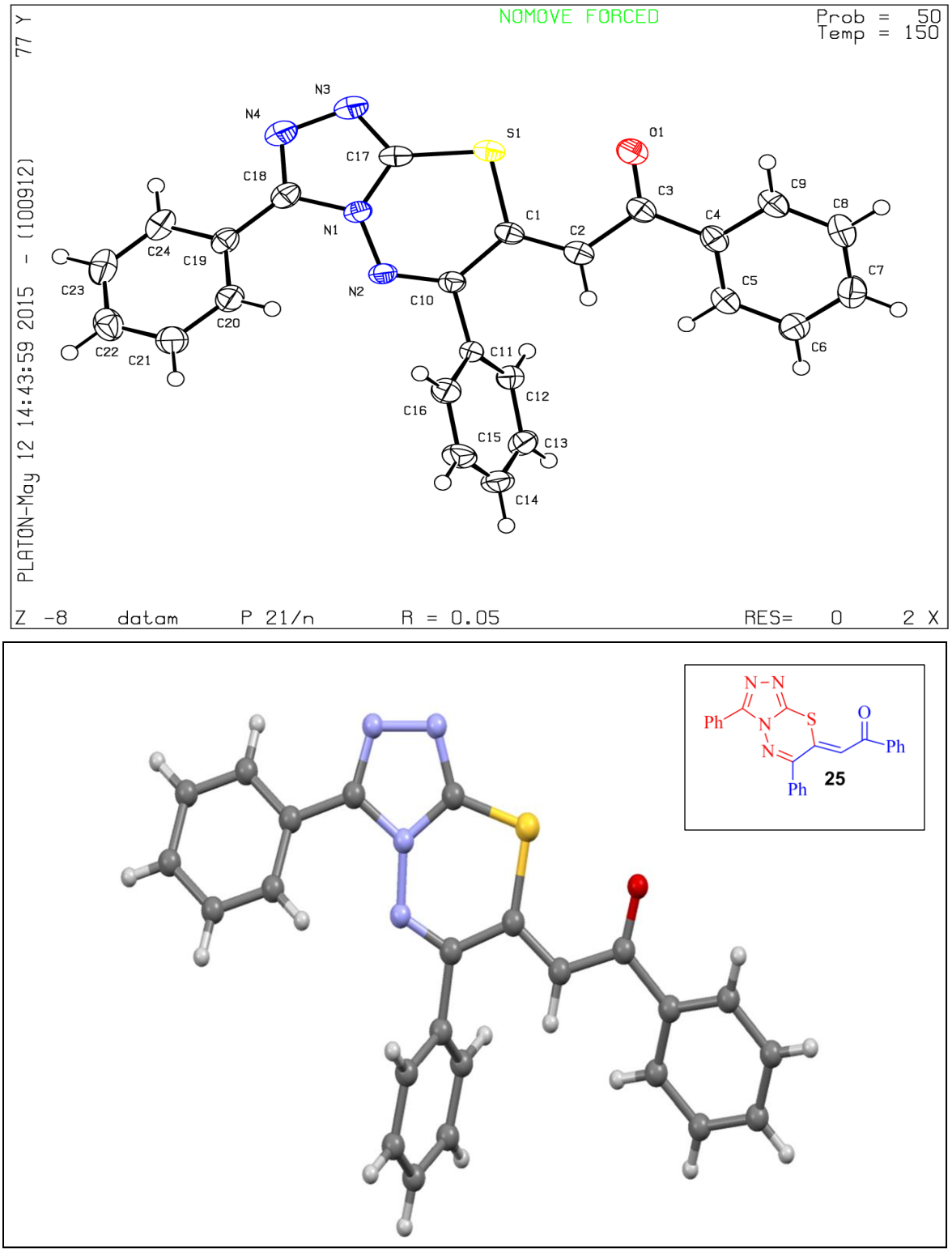
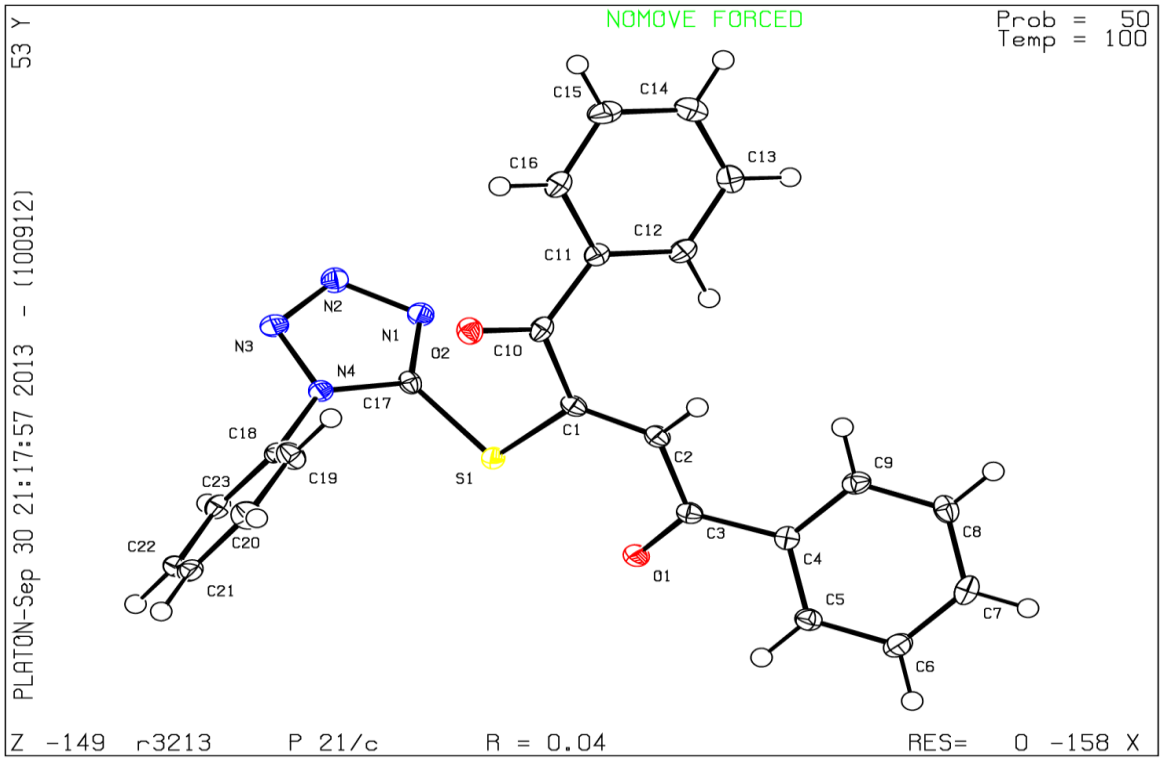


Figure 3. View of **25** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.



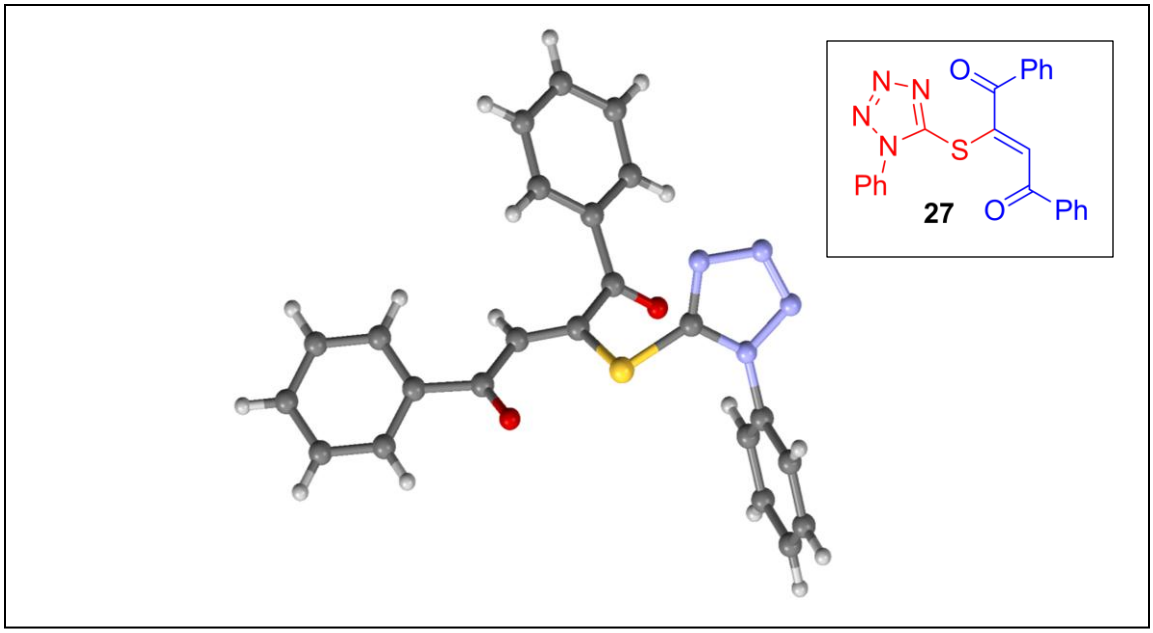


Figure 4. View of **27** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.

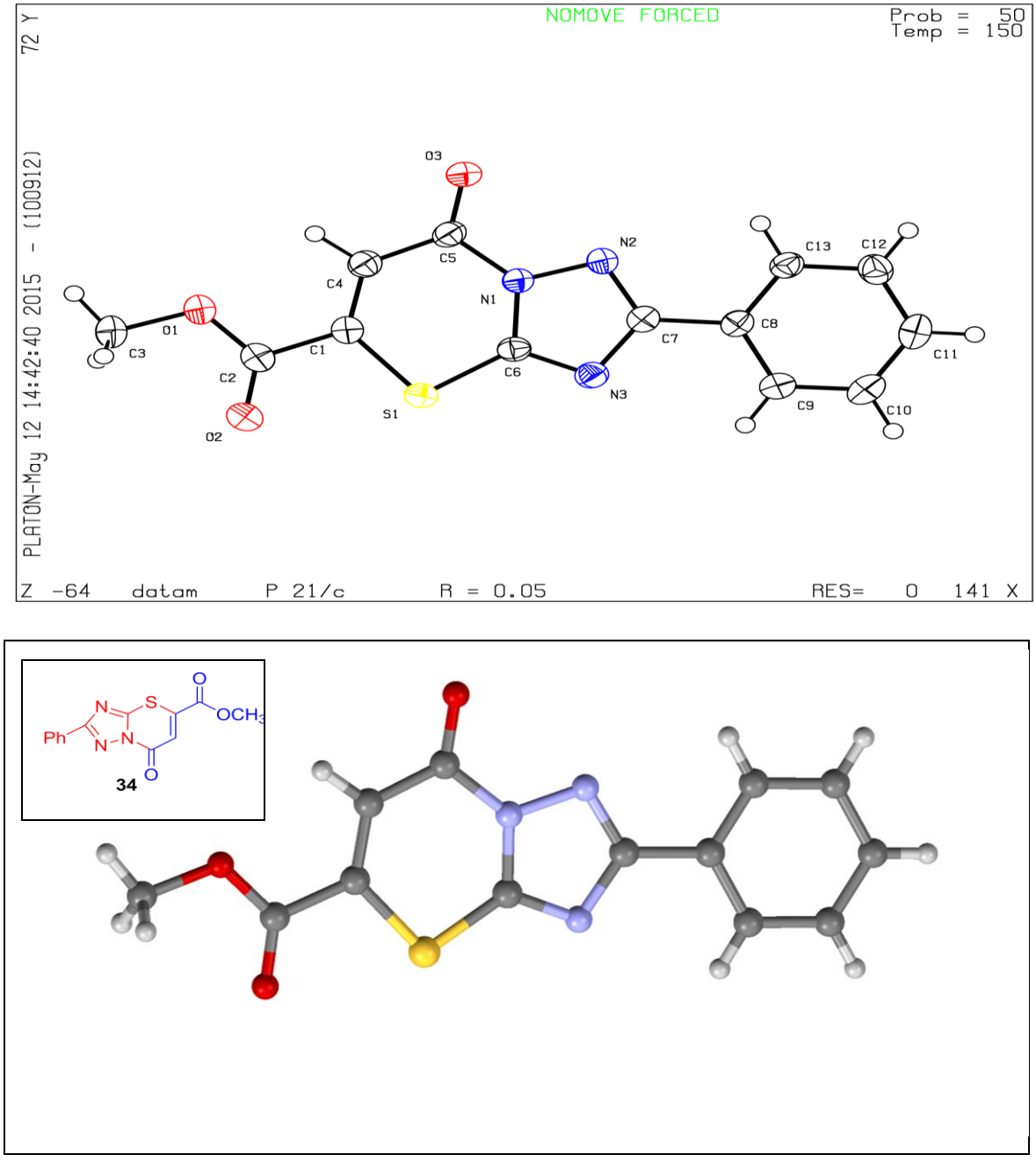
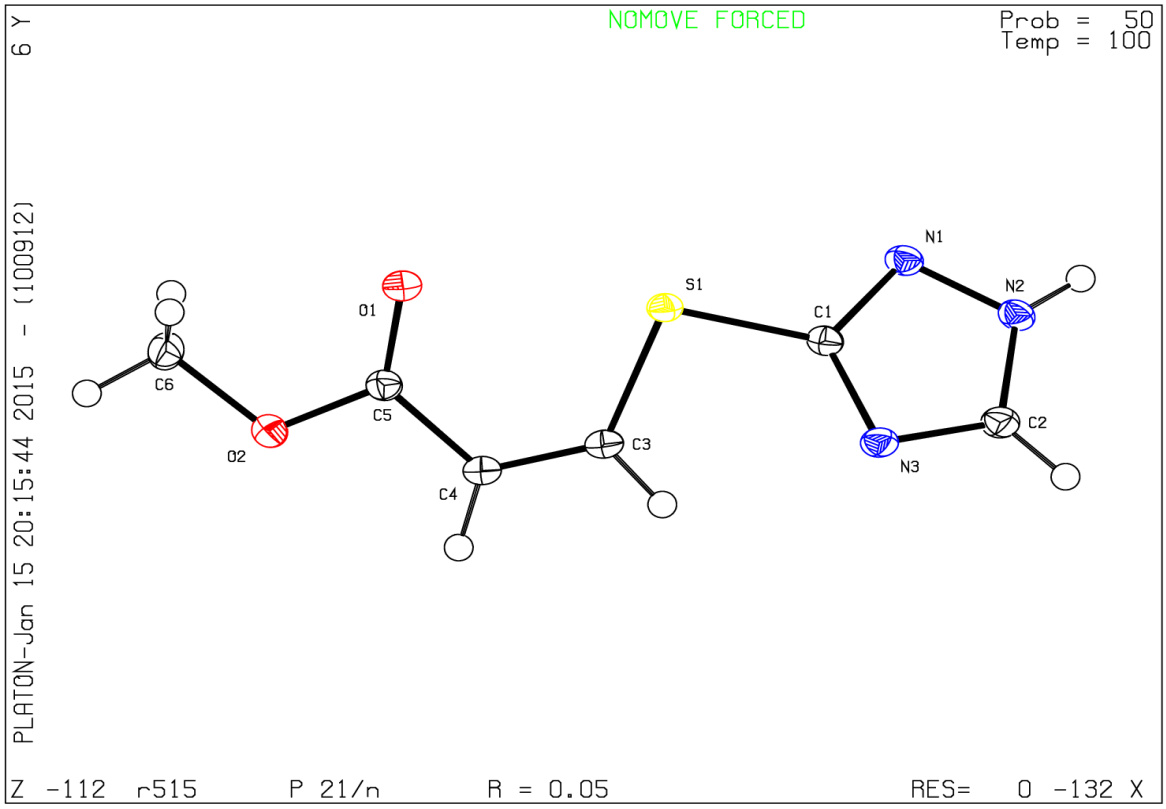


Figure 5. View of **34** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.



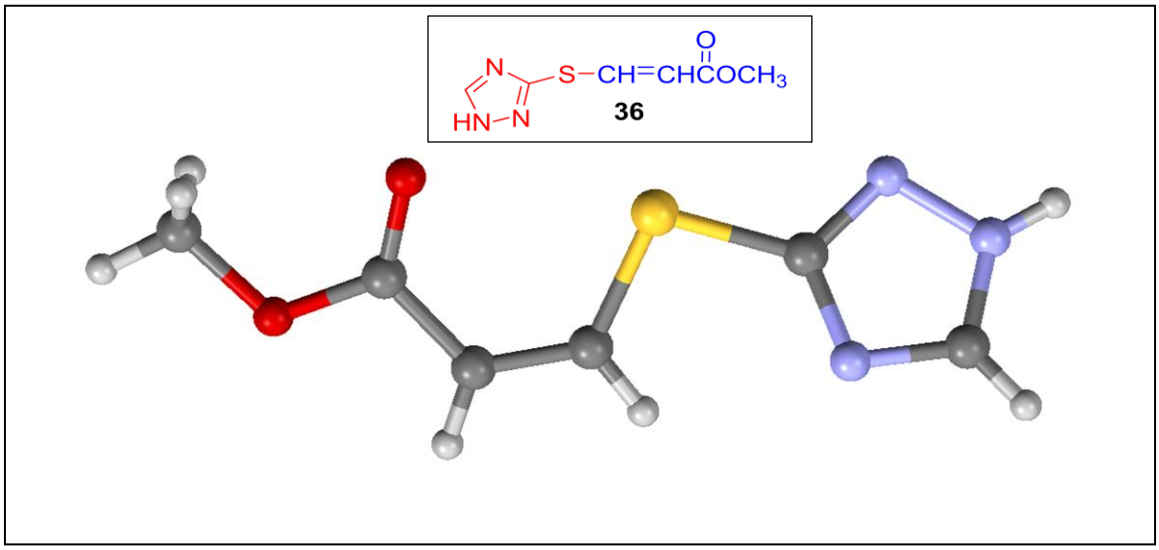
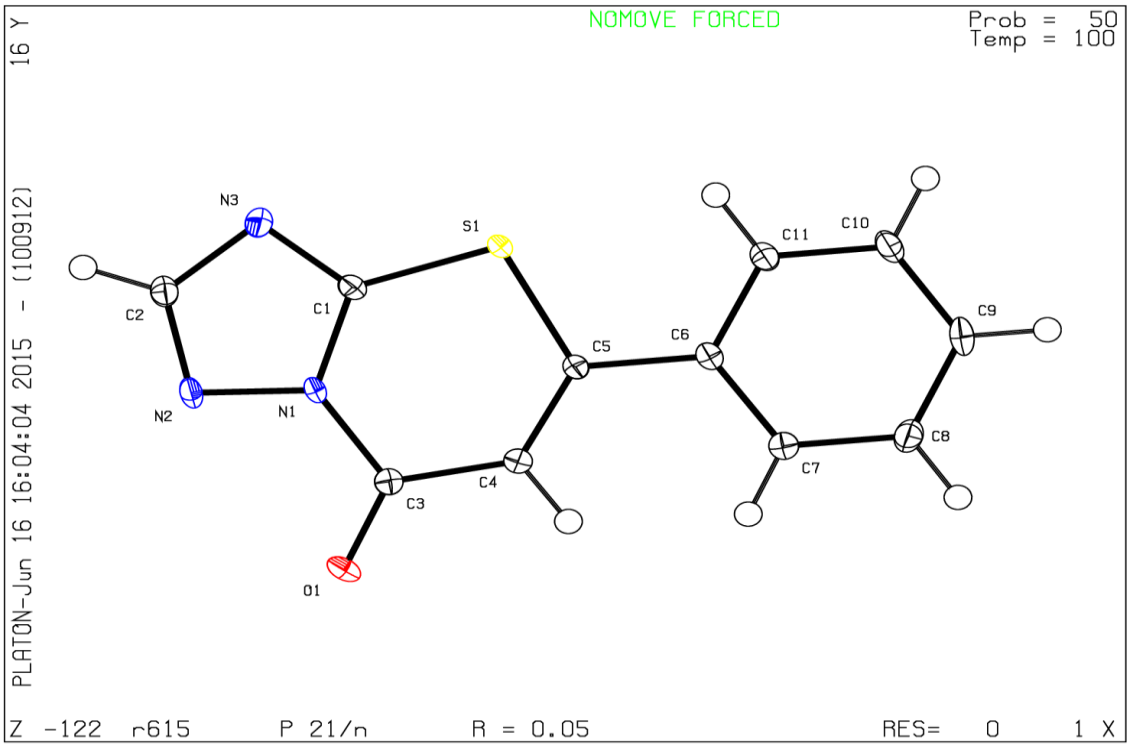


Figure 6. View of **36** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.



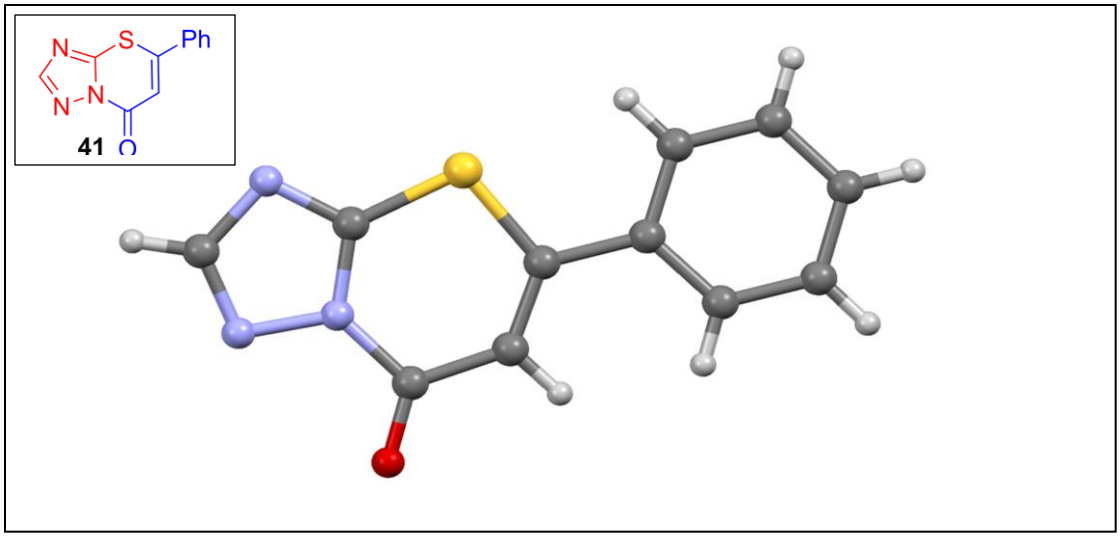
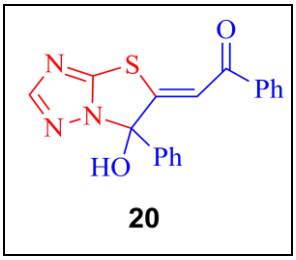


Figure 7. View of **41** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.

4. Spectral data of synthesized compounds:

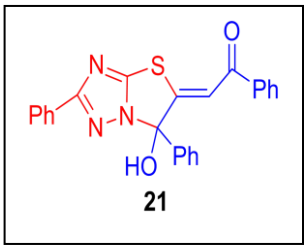
2-(6-hydroxy-6-phenylthiazolo[3,2-b][1,2,4]triazol-5(6H)-ylidene)-1-phenylethanone (20)



20

Light-brown solid, **M.P** 168-169 ^{o}C, 0.261 g, yield 77%. **IR** (KBr): ν_{cm}^{-1}: 1563 (C=C), 1591 (C=N), 1646 (C=O), 3067 (aromatic-CH). **^{1}H NMR** (400 MHZ, DMSO): δ 3.40 (1H, s, OH), 6.63 (1H, s, olefinic), 7.13 - 8.09 (10H, m, aromatic), 8.78 (1H, s, triazole). **^{13}C NMR** (100 MHZ, DMSO): δ 187.8 (C=O), 166.4, 157.1, 155.4, 139.7, 135.9, 133.4, 129.3, 129.0, 128.7, 128.5, 128.1, 127.9, 124.9, 117.2, **ESI-MS**: 336.1 $[M+H]^{+}$.

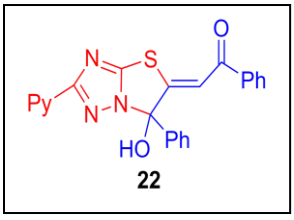
2-(6-hydroxy-2,6-diphenylthiazolo[3,2-b][1,2,4]triazol-5(6H)-ylidene)-1-phenylethanone (21)



21

Light-brown solid, **M.P** 170-171^{o}C, 0.350 g, yield 85%. **IR** (KBr): ν_{cm}^{-1}: 1589 (C=C), 1640 (C=O), 3151 (aromatic-CH), 3609 (OH). **^{1}H NMR** (400 MHZ, DMSO): δ 3.28(1H, s, OH), 6.67 (1H, s, olefinic), 7.31 – 8.44 (15H, m, aromatic). **^{13}C NMR** (100 MHZ, DMSO): δ 187.5 (C=O), 167.6, 165.12, 156.26, 141.0, 139.5, 136.06, 133.29, 130.35, 129.76, 129.30, 129.15, 128.58, 128.49, 128.23, 127.80, 117.2, 91.2. **ESI –MS**: 412.11 $[M+H]^{+}$.

2-(6-hydroxy-6-phenyl-2-(pyridin-4-yl)thiazolo[3,2-b][1,2,4]triazol-5(6H)-ylidene)-1-phenylethanone (22)

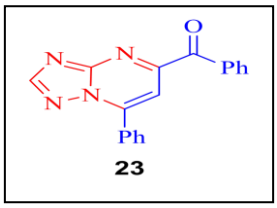


22

Light-green solid, **M.P** 168-169 ^{o}C, 0.347 g, yield 84%. **IR** (KBr): ν_{cm}^{-1}: 1506 (C=C), 1639 (C=O), 3061(aromatic-CH), 3386 (OH).**^{1}H NMR** (400 MHZ; DMSO): δ 3.46 (1H, s, OH), 6.68 (1H, s, Olefinic), 7.31 –8.03 (10H, m, aromatic), 8.54-8.68 (4H, m, pyridyl). **^{13}C NMR** (100 MHZ, DMSO): δ 191.0 (C=O), 165.4,

164.6, 156.9, 150.2, 140.9, 137.4, 134.6, 133.6, 129.5, 128.8, 128.7, 128.3, 128.1, 120.0, 119.6, 117.6. **ESI-MS**: 412.02 $(M+H)^+$.

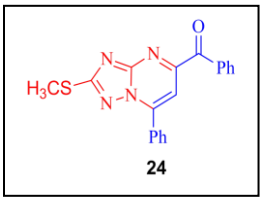
Phenyl-(7-phenyl-[1,2,4]triazolo[1,5-a]pyrimidin-5-yl)methanone (23)



23

Light Yellow solid, **M.P** 176-177 ^oC, 0.239 g, yield 79%. **IR** (KBr): ν_{cm}^{-1}: 1550 (C=C), 1612 (C=N), 1666 (C=O), 3107 (aromatic-CH). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.26 - 8.2 (11H, m, aromatic), 8.49 (triazole-H). **^{13}C NMR** (100 MHZ, $CDCl_3$): δ 186.4 (C=O), 162.0, 157.0, 143.7, 135.9, 135.5, 134.1, 132.0, 130.1, 129.28, 127.9, 106.8. **ESI-MS:** 301.00 $[M+H]^+$.

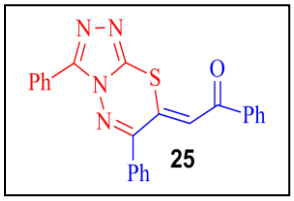
2-(methylthio)-7-phenyl-[1,2,4]triazolo[1,5-a]pyrimidin-5-yl(phenyl)methanone (24)



24

Yellow solid, **M.P** 182-183 ^oC, 0.321 g, yield 96%. **IR** (KBr): ν_{cm}^{-1}: 1534 (C=C), 1589 (C=N), 1649 (C=O), 2924 ($-CH_3$), 3071 (aromatic-CH). **^{1}H NMR** (400 MHZ, DMSO): δ 2.73 (3H, s, $-CH_3$), 7.53 -8.25 (11H, m, aromatic). **^{13}C NMR** (100 MHz, DMSO): δ 190.7 (C=O), 170.1, 156.3, 155.0, 147.14, 134.4, 133.3, 131.7, 130.6, 129.1, 129.0, 128.5, 128, 127.9, 107.6, 13.4. **ESI-MS**: 333.12 $[M+H]^+$.

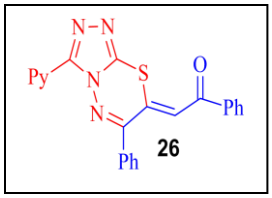
2-(3,6-diphenyl-7H-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazin-7-ylidene)-1-phenylethanone (25)



25

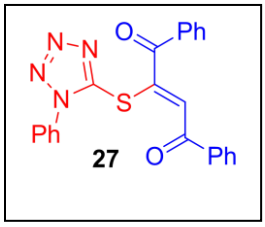
Light-green solid, **M.P** 220-221 ^oC, 0.401 g, yield 98%. **IR** (KBr): ν_{cm}^{-1}: 1575 (C=C), 1596 (C=N), 1631 (C=O), 3059 (aromatic –CH). **^{1}H NMR** (400 MHZ, $CDCl_3$): 7.26 (1H, s, Olefinic), 7.43-8.15 (15H, m, aromatic). **^{13}C NMR** (100 MHz, $CDCl_3$): δ 189.0 (C=O), 153.0, 151.8, 136.7, 135.7, 134.9, 133.7, 130.9, 130.5, 129.2, 129.0, 128.6, 128.5, 128.2, 125.5, 123.4, **ESI $^-$MS:** 409.0 $[M+H]^+$.

1-phenyl-2-(6-phenyl-3-(pyridin-4-yl)-7H-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazin-7-ylidene)ethanone (26)



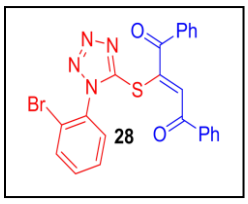
Yellow solid, **M.P** 241-242 ^{o}C, 0.389 g, yield 95%. **IR** (KBr): ν_{cm}^{-1}: 1555 (C=C), 1605 (C=N), 1641 (C=O). 3259 (aromatic-CH).**^{1}H NMR** (400 MHZ, DMSO): δ 5.9 (1H, s, olefinic), 7.25-7.9 (10H, m, aromatic), 8.0-8.7 (4H, m, pyridyl). **^{13}C NMR** (100 MHZ, DMSO): δ 188.7 (C=O), 152.1, 150.1, 149.9, 149.9, 145.7, 138.3, 136.8, 133.2, 132.8, 129.0, 128.88, 128.1, 127.8, 126.2, 120.8, 116.4. **ESI $^{-}$MS:** 410.01 $[M+H]^{+}$.

1, 4-diphenyl-2-((1-phenyl-1H-tetrazol-5-yl)thio)but-2-ene-1,4-dione (27)



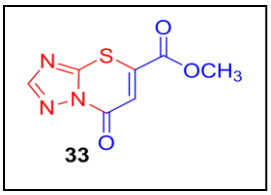
Light yellow solid, **M.P** 156-157 ^{o}C, 0.359 g, yield 87%. **IR** (KBR): ν_{cm}^{-1}: 1547 (C=C), 1591 (C=N), 1638, 1661 (2C=O), 3035 (aromatic-CH). **^{1}H NMR** (400 MHZ, $CDCl_3$): δ 7.26 (1H, s, olefinic), 7.26-7.95 (15H, m, aromatic). **^{13}C NMR** (100 MHZ, $CDCl_3$): δppm 191.0, 188.7 (2C=O), 150.8, 150.7, 136.3, 135.3, 134.3, 134.1, 133.4, 130.6, 130.1, 129.7, 129.0, 128.8, 128.5, 124.9, 124.6, **ESI $^{-}$MS:** 413.2 $[M+H]^{+}$.

2-((1-(2-bromophenyl)-1H-tetrazol-5-yl)thio)-1,4-diphenylbut-2-ene-1,4-dione (28)



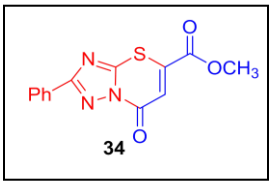
Yellow solid, **M.P** 172-173 ^{o}C, 0.422 g, yield 85%. **IR** (KBR): ν_{cm}^{-1}: 1524 (C=C), 1612 & 1675 (2C=O), 3064 (aromatic-CH). **^{1}H NMR** (400 MHZ, $CDCl_3$): δ 7.25 (1H, s, olefinic), 7.34-8.33 (14H, m, aromatic). **^{13}C NMR** (100 MHZ, $CDCl_3$): δppm 187.7, 187.5 (2C=O), 164.6, 144.1, 136.5, 135.1, 134.4, 134.4, 134.3, 132.1, 131.9, 129.1, 129.1, 129.0, 128.9, 127.6, 127.1, 122.3,115. **ESI $^{-}$MS:** 496.0 $[M+H]^{+}$.

methyl 7-oxo-7H-[1,2,4]triazolo[5,1-b][1,3]thiazine-5-carboxylate (33)



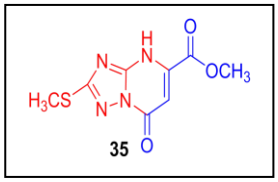
Yellow solid, **M.P** 184-185 ^{o}C, 0.157 g, yield 74%. **IR** (KBR): ν_{cm}^{-1}: 1592 (C=C), 1720 (C=O), 2956 (-CH_3), 3070 (aromatic-CH). **^{1}H NMR** (400 MHZ, DMSO): δ 4.10 (3H, s, methyl), 8.1 (1H, s, thiazinone), 8.3 (1H, s, triazole). **^{13}C NMR** (100 MHZ, DMSO): δppm 165.0, 164.9 (2C=O), 159.8, 156.4, 126.3, 125.1, 54.0. **ESI $^{-}$MS:** 212.3 $[M+H]^{+}$.

methyl 7-oxo-2-phenyl-7H-[1,2,4]triazolo[5,1-b][1,3]thiazine-5-carboxylate (34)



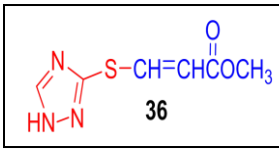
White solid, **M.P** 178-179 ^{o}C, 0.237 g, yield 82%. **IR** (KBR): ν_{cm}^{-1}: 1592 (C=C), 1715 (C=O), 2955 (-CH_3), 3070 (aromatic-CH). **^{1}H NMR** (400 MHZ, DMSO): δ 4.03 (3H, s, methyl), 8.1 (1H, s, thiazinone), 7.52-8.21 (5H, m, aromatic). **^{13}C NMR** (100 MHZ, DMSO): δppm 163.1, 161.1 (2C=O), 154.8, 152.2, 139.1, 130.8, 128.7, 128.3, 126.9, 122.0, 54.3. **ESI $^{-}$MS:** 288.0 $[M+H]^{+}$.

methyl 2-(methylthio)-7-oxo-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-5-carboxylate (35)



Light-yellow solid, **M.P** 165-166 ^{o}C, 0.196 g, yield 81%. **IR** (KBR): ν_{cm}^{-1}: 1580 (C=C), 1691, 1753 (2C=O), 2953 (-CH_3), 3018 (aromatic-CH). **^{1}H NMR** (400 MHZ, DMSO): δ 2.57 (3H, s, -CH_3), 3.96 (3H, s, -OCH_3), 6.5(1H, s, pyrimidine), 13.4 (1H, s, pyrimidine-NH). **^{13}C NMR** (100 MHZ, DMSO): δppm 163.85, 156.97 (2C=O), 158.8, 151.45, 136.7, 108.9, 53.4, 13.3. **ESI $^{-}$MS:** 241.0 $[M+H]^{+}$.

methyl 3-((1H-1,2,4-triazol-3-yl)thio)acrylate (36)

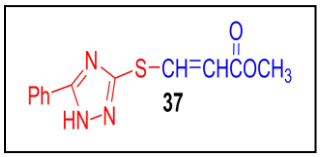


White solid, **M.P** 200-201^{o}C, 0.147 g, yield 79%. **IR** (KBR): ν_{cm}^{-1}: 1229 (O-C), 1595 (C=C), 1699 (C=O), 2910 (-CH_3), 3117(triazole-NH). **^{1}H NMR** (400 MHZ, DMSO): δ 3.08 (3H, s, -CH_3), 6.09 (1H, d, =CHCOO-), 7.96(1H, d, -

SCH=), 8.34(1H, s, triazole), 13.4 (1H, s, triazole-NH). **^{13}C NMR** (100 MHZ, DMSO): δppm 167.1(C=O), 145.4, 143.1, 117.8, 114.6, 51.9. **ESI $^{-}$MS:** 186.2 $[M+H]^{+}$.

methyl 3-((5-phenyl-1H-1,2,4-triazol-3-yl)thio)acrylate (37)

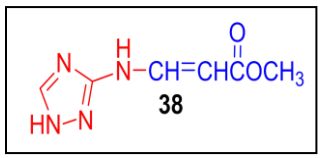
White solid, **M.P** 196-197 ^{o}C, 0.224 g, yield 85%. **IR** (KBR): ν_{cm}^{-1}: 1229(O-C), 1569 (C=C), 1683 (C=O), 2951 (-CH_3), 3256 (triazole-NH). **^{1}H NMR** (400 MHZ, DMSO): δ 3.04 (3H, s, -CH_3), 6.91 (1H, d, =CHCOO-), 7.80(1H, d, -SCH=), 7.48-7.25 (5H, m, phenyl), 13.5 (1H, s, triazole-NH). **^{13}C NMR** (100 MHZ, DMSO): δppm 163.5 (C=O), 155.7, 152.1, 134.7, 131.0, 128.7, 127.6, 118.0, 50.6. **ESI $^{-}$MS**: 262.30 $[M+H]^{+}$.



37

methyl 3-((1H-1,2,4-triazol-3-yl)amino)acrylate (38)

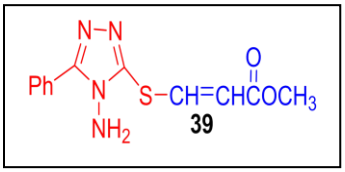
White solid, **M.P** 183-184, 0.133 g, yield 78%. **IR** (KBR): ν_{cm}^{-1}: 1234 (O-C), 1585 (C=C), 1687 (C=O), 2924 (-CH_3), 3217(triazole-NH). **^{1}H NMR** (400 MHZ, DMSO): δ 3.77 (3H, s, -CH_3), 5.89 (1H, d, =CHCOO-), 6.23 (1H, s, -NH), 7.41(1H, d, -NCH=), 8.36(1H, s, triazole), 13.4 (1H, s, triazole-NH). **^{13}C NMR** (100 MHZ, DMSO): δppm 168.8(C=O), 153.8, 147.4, 136.2, 109.2, 51.4. **ESI $^{-}$MS:** 169.3 $[M+H]^{+}$.



38

methyl 3-((4-amino-5-phenyl-4H-1,2,4-triazol-3-yl)thio)acrylate (39)

Light-yellow solid, **M.P** 191-192 ^{o}C, 0.252 g, yield 91%. **IR** (KBR): ν_{cm}^{-1}: 1243(C-O), 1589 (C=C), 1697 (C=O), 2947 (-CH_3), 3284 & 3356 (triazole-NH_2). **^{1}H NMR** (400 MHZ,DMSO): δ 3.76 (3H, s, -CH_3), 6.1 (2H, s, NH_2), 6.25 (1H, d, =CHCOO-), 8.07-7.48 (5H, m, aromatic), 8.15(1H, d, -SCH=).**^{13}C NMR** (100 MHZ, DMSO): δppm 166.2 (C=O), 154.6,

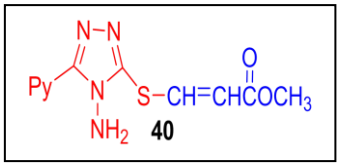


39

152.1, 141.9, 129.5, 128.2, 127.8, 126.4, 114.9, 51.3. **ESI $^{-}$MS:** 277.31 $[M+H]^{+}$.

methyl-3-((4-amino-5-(pyridin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acrylate (40)

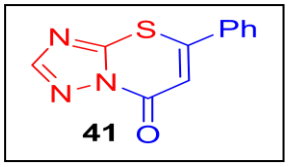
Light-yellow solid, **M.P** 196-197 ^{o}C, 0.242 g, yield 87%. **IR** (KBR): ν_{cm}^{-1}: 1227 (C-O), 1589 (C=C), 1697 (C=O), 2953 (-CH_3), 3044 (aromatic =CH), 3297 & 3354 (triazole-NH_2). **^{1}H NMR** (400 MHZ,DMSO): δ 3.76 (3H, s, -CH_3), 6.34 (2H, s, NH_2), 6.29 (1H, d, =CHCOO-), 8.09-8.04 (4H, m, pyridyl), 8.73(1H, d, -SCH=).**^{13}C NMR** (100 MHZ, DMSO): δppm 166.2 (C=O), 153.4, 152.5, 149.9, 141.5, 133.6, 121.3, 115.2, 51.4. **ESI $^{-}$MS:** 278.30 $[M+H]^{+}$.



40

5-phenyl-7H-[1,2,4]triazolo[5,1-b][1,3]thiazin-7-one (41)

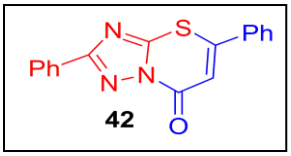
Light-yellow solid, **M.P** 270-271^{o}C, 0.191 g, yield 83%. **IR** (KBR): ν_{cm}^{-1}: 1698 (C=O), 3061 (aromatic CH). **^{1}H NMR** (400 MHZ, DMSO): δ 6.9 (1H, s, thiazinone), 7.51-7.64 (5H, m, phenyl), 8.3 (1H, s, triazole). **^{13}C NMR** (100 MHZ, DMSO): δppm 155.5, 153.1, 151.4, 133.9, 132.1, 129.6, 126.8, 114.3. **ESI $^{-}$MS:** 230.0 $[M+H]^{+}$.



41

2, 5-diphenyl-7H-[1,2,4]triazolo[5,1-b][1,3]thiazin-7-one (42)

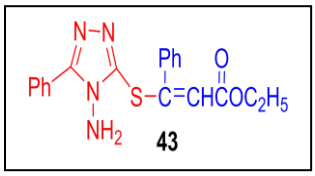
Light-yellow solid, **M.P** 221-222 ^{o}C, 0.262 g, yield 85%. **IR** (KBR): ν_{cm}^{-1}: 1701 (C=O), 3056 (aromatic -CH). **^{1}H NMR** (400 MHZ, DMSO): δ 7.2 (1H, s, thiazinone), 7.52-8.22 (10H, m, phenyl). **^{13}C NMR** (100 MHZ, DMSO): δppm 162.5 (C=O), 155.2, 152.1, 149.5, 133.6, 131.8, 130.6, 129.4, 128.7, 128.6, 126.8, 126.8, 114.4. **ESI $^{-}$MS:** 307.0 $[M+H]^{+}$.



42

methyl 3-((4-amino-5-phenyl-4H-1,2,4-triazol-3-yl)thio)-3-phenylacrylate (43)

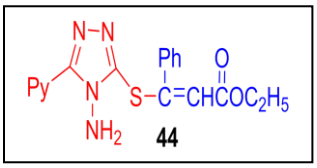
Light-yellow solid, **M.P** 162-163 ^{o}C, 0.319 g, yield 88%. **IR** (KBR): ν_{cm}^{-1}: 1182 (O-CH_2), 1698 (C=O), 2925 (-CH_3), 3057 (aromatic CH), 3262 & 3324 (-NH_2). **^{1}H NMR** (400 MHZ, $CDCl_3$): δ 1.34 (3H, t, -CH_3), 4.28 (2H, q, -CH_2), 4.45 (2H, s, -NH2), 6.20 (1H, s, =CHCO-), 7.22-7.69 (10H, m, phenyl). **^{13}C NMR** (100 MHZ, $CDCl_3$): δppm 165.7 (C=O), 154.4, 154.3, 147.9, 136.9, 130.2, 129.8, 128.5, 1284, 128.1, 127.8, 126.0, 117.7, 60.9, 14.29. **ESI –MS:** 363.0 $[M+H]^{+}$.



43

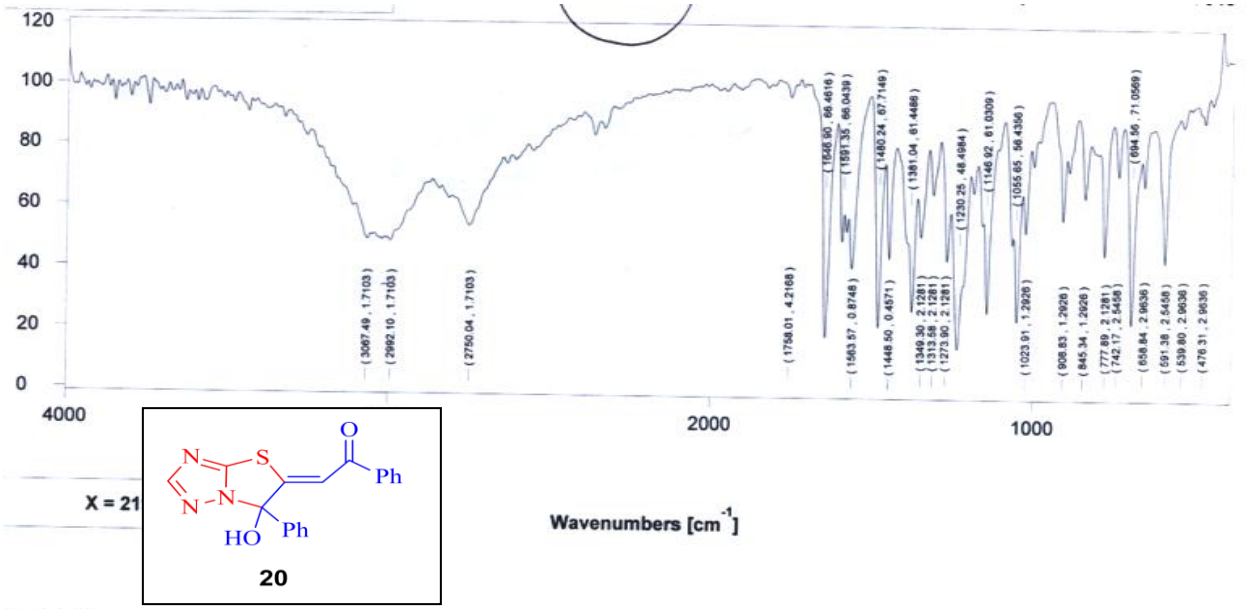
ethyl 3-((4-amino-5-(pyridin-4-yl)-4H-1,2,4-triazol-3-yl)thio)-3-phenylacrylate (44)

Light-yellow solid, **M.P** 208-209 ^{o}C, 0.314 g, yield 86%. **IR** (KBR): ν_{cm}^{-1}: 1187(O-C), 1694 (C=O), 2928 (-CH_3), 3057(aromatic CH), 3320 & 3434 (-NH_2). **^{1}H NMR** (400 MHZ, DMSO): δ 1.31 (3H, t, -CH_3), 4.25 (2H, q, -CH_2), 6.19 (2H, s, -NH2), 6.22 (1H, s, =CHCO-), 7.17-7.31 (5H, m, phenyl), 7.83-8.66 (4H, m, pyridyl). **^{13}C NMR** (100 MHZ, DMSO): δppm 164.9 (C=O), 155.1, 151.3, 149.7, 149.7, 137.0, 133.5, 128.8, 127.8, 127.6, 121.3, 117.1, 60.1, 14.08. **ESI –MS:** 365.0 $[M+H]^{+}$.

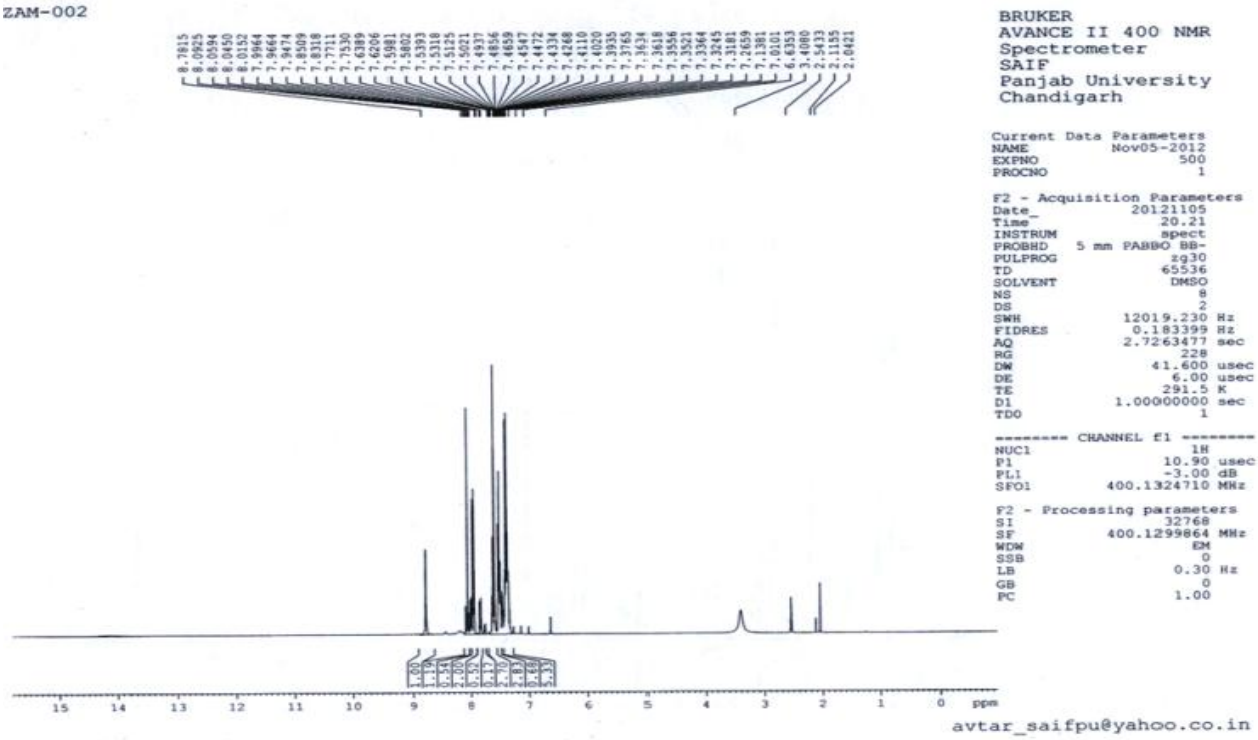


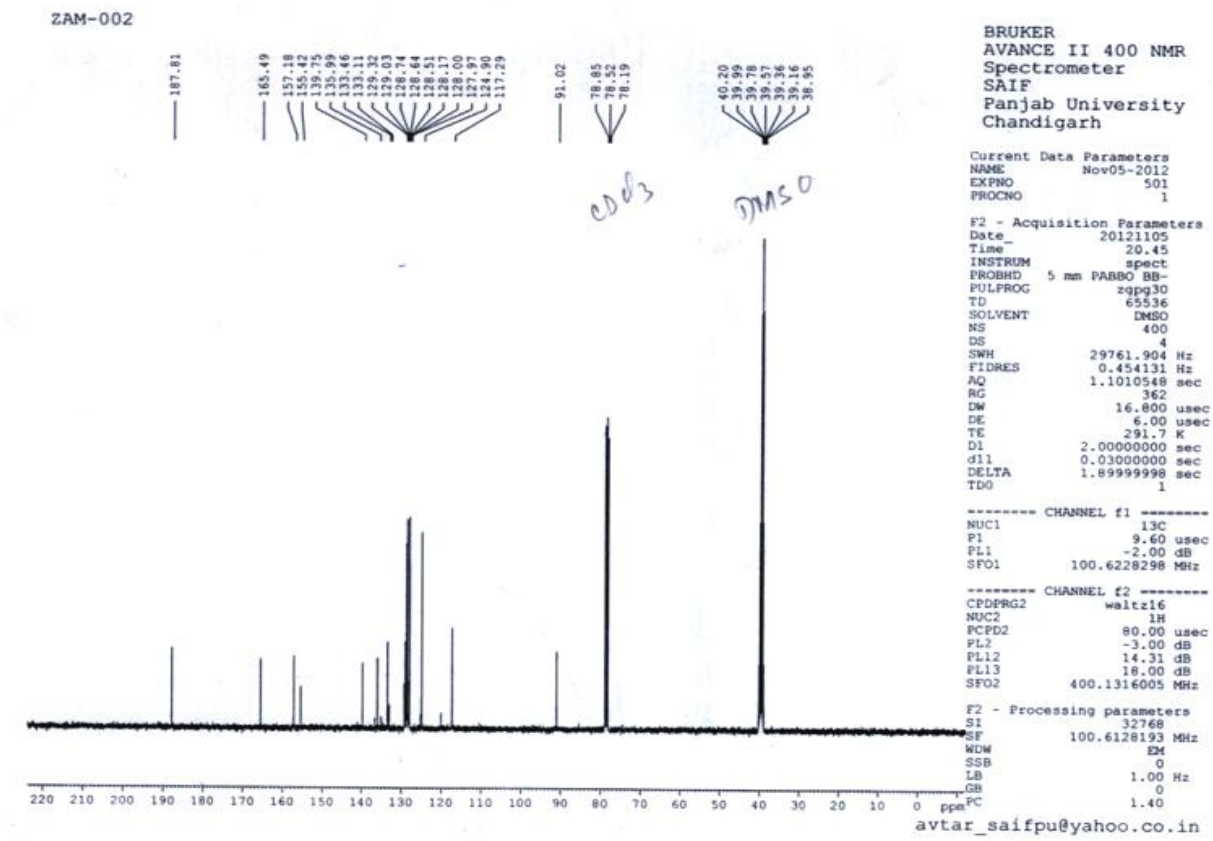
44

5. Spectra of synthesized compounds.



20

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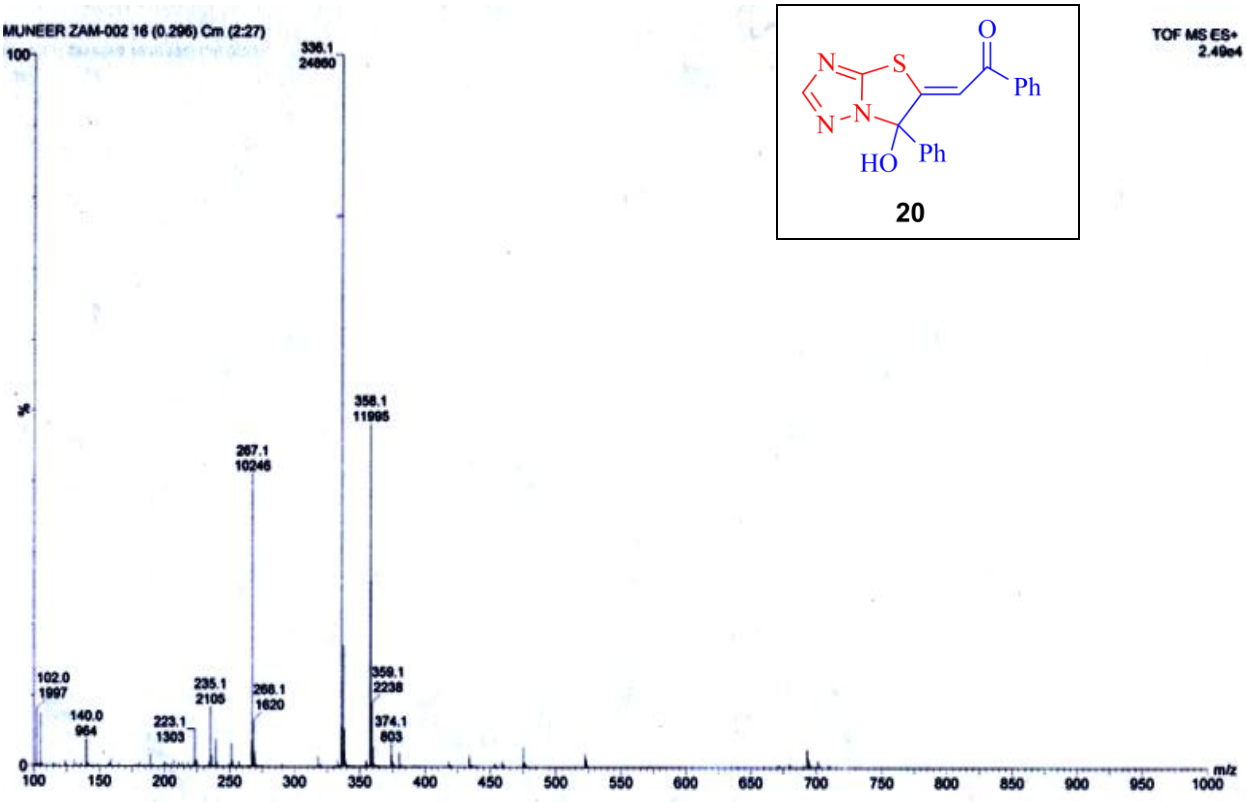
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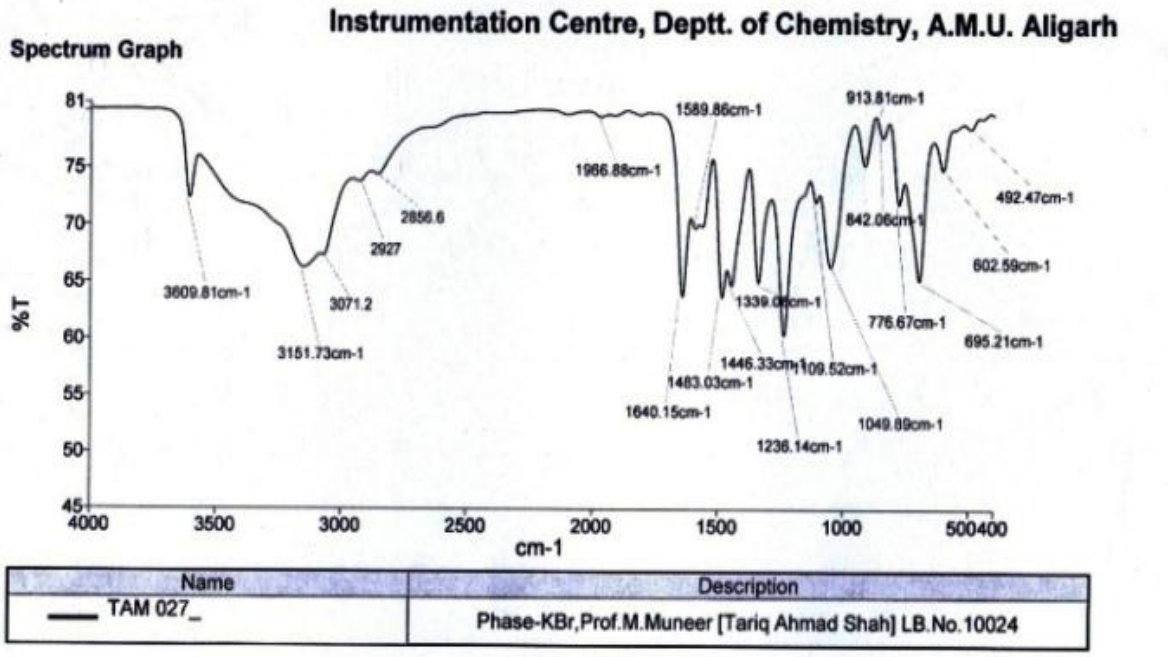
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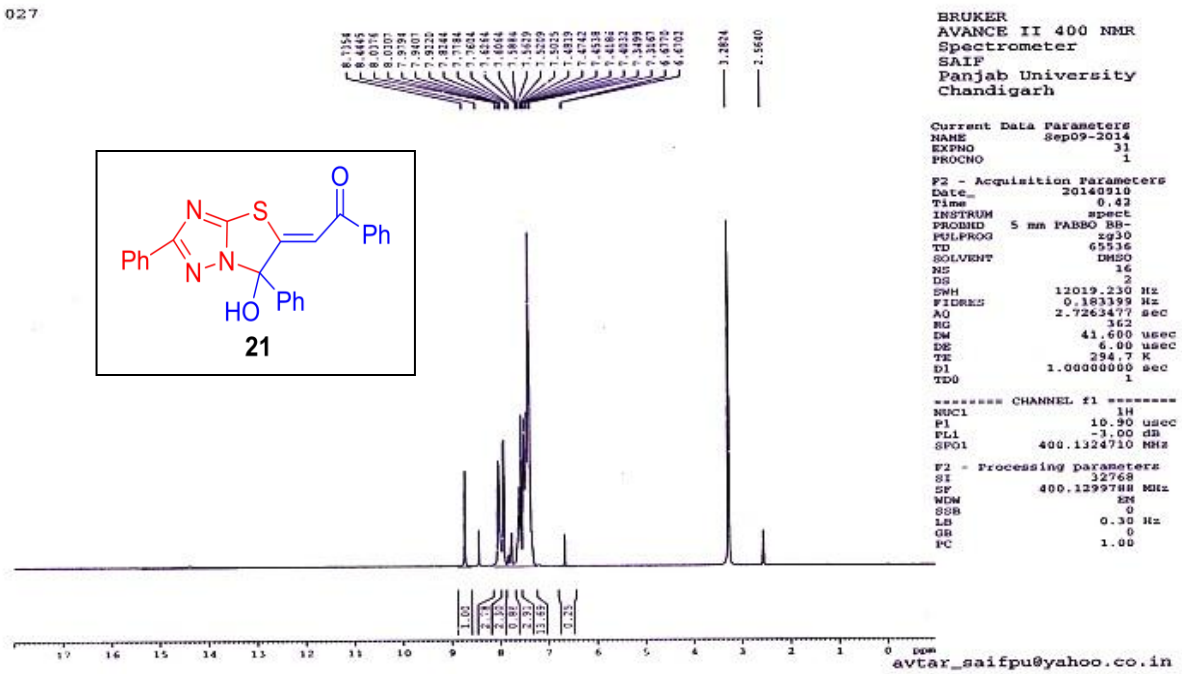
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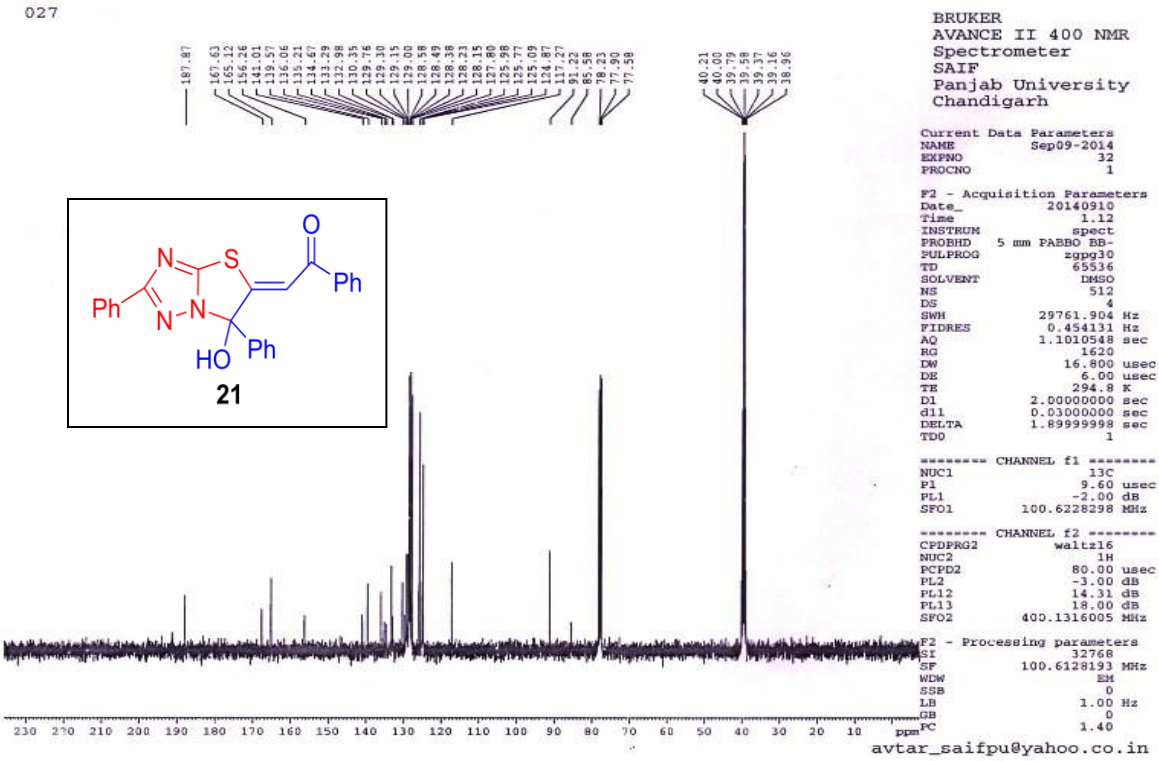
Panjab University
Chandigarh
avtar_saifpu@yahoo.co.in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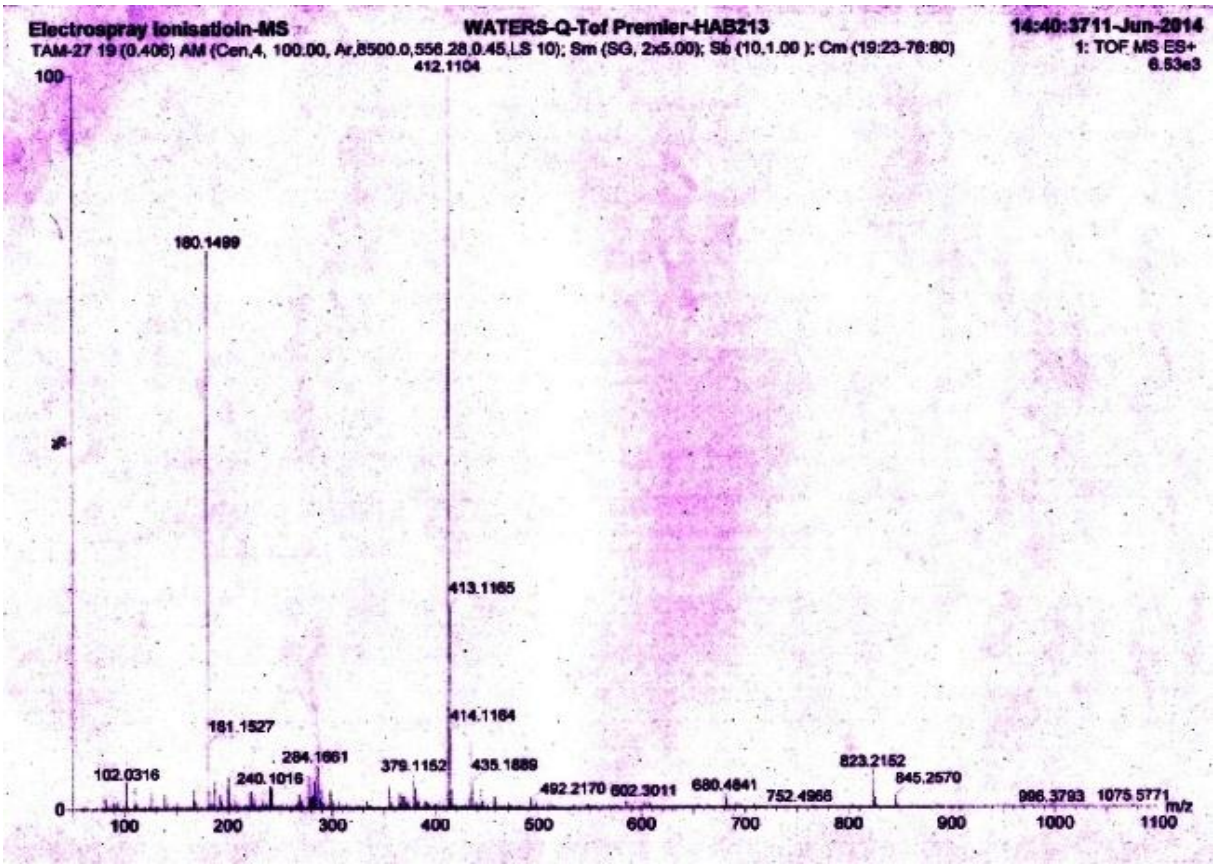
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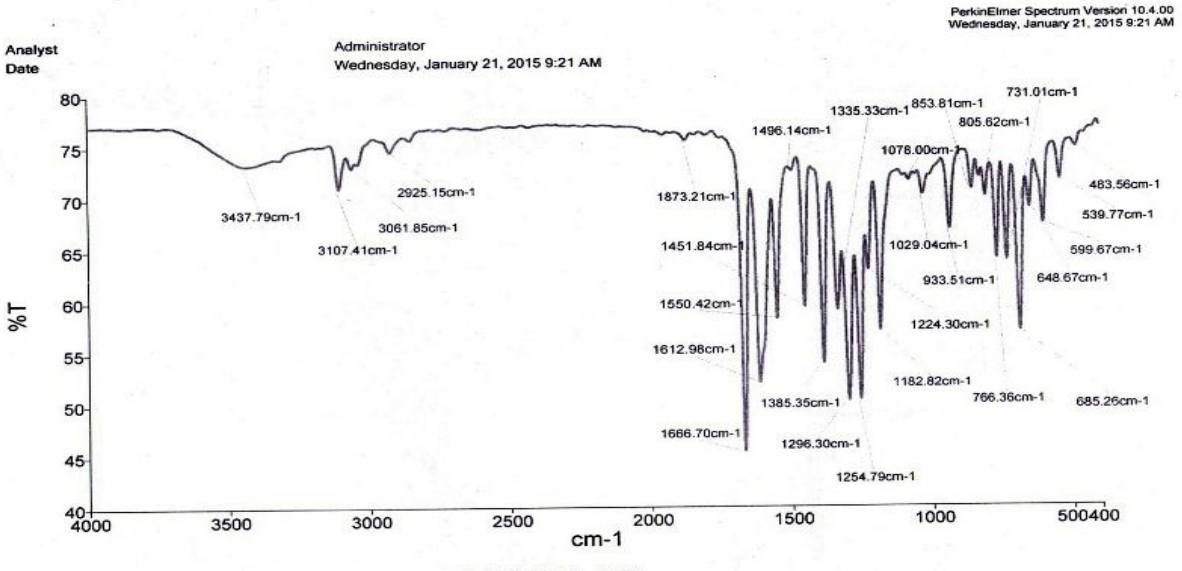
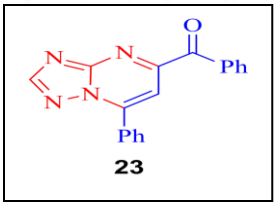
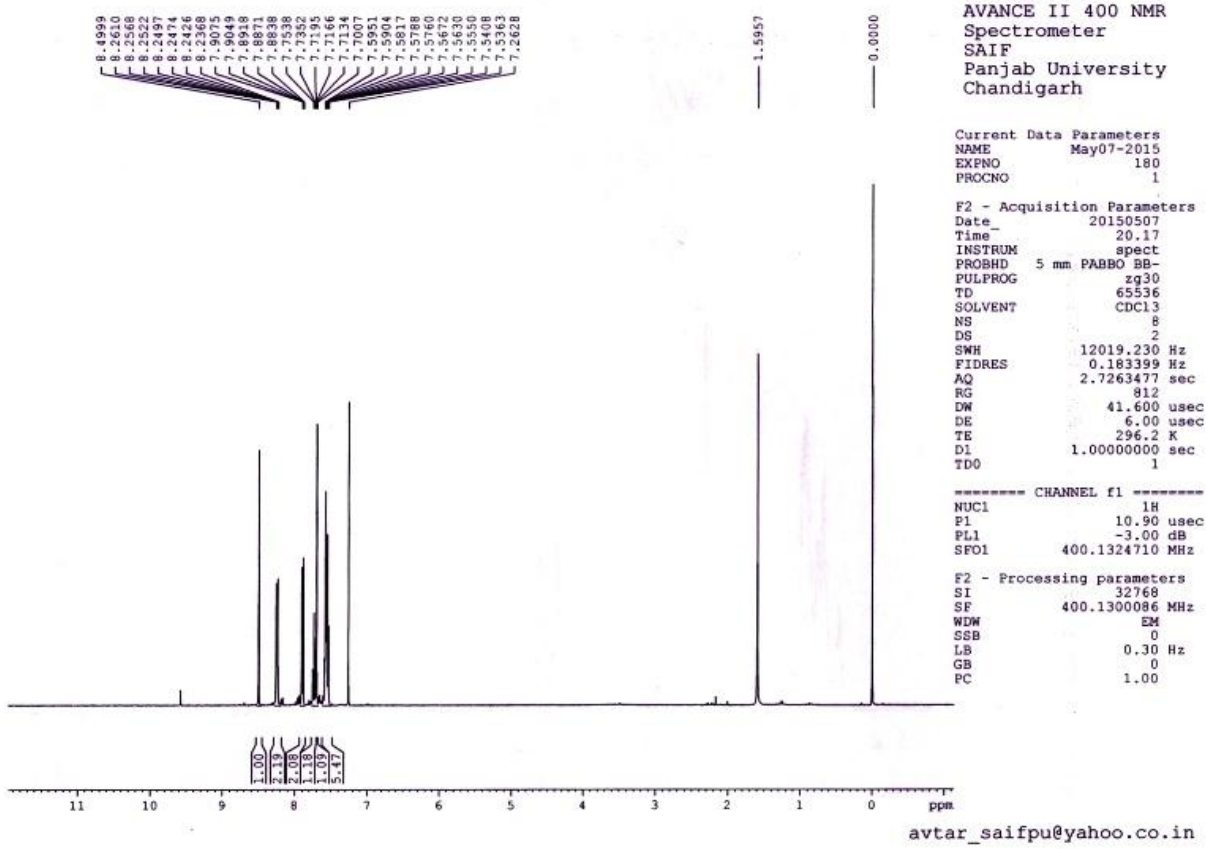
823.2152
845.2570
996.3793
1075.5771
m/z





23

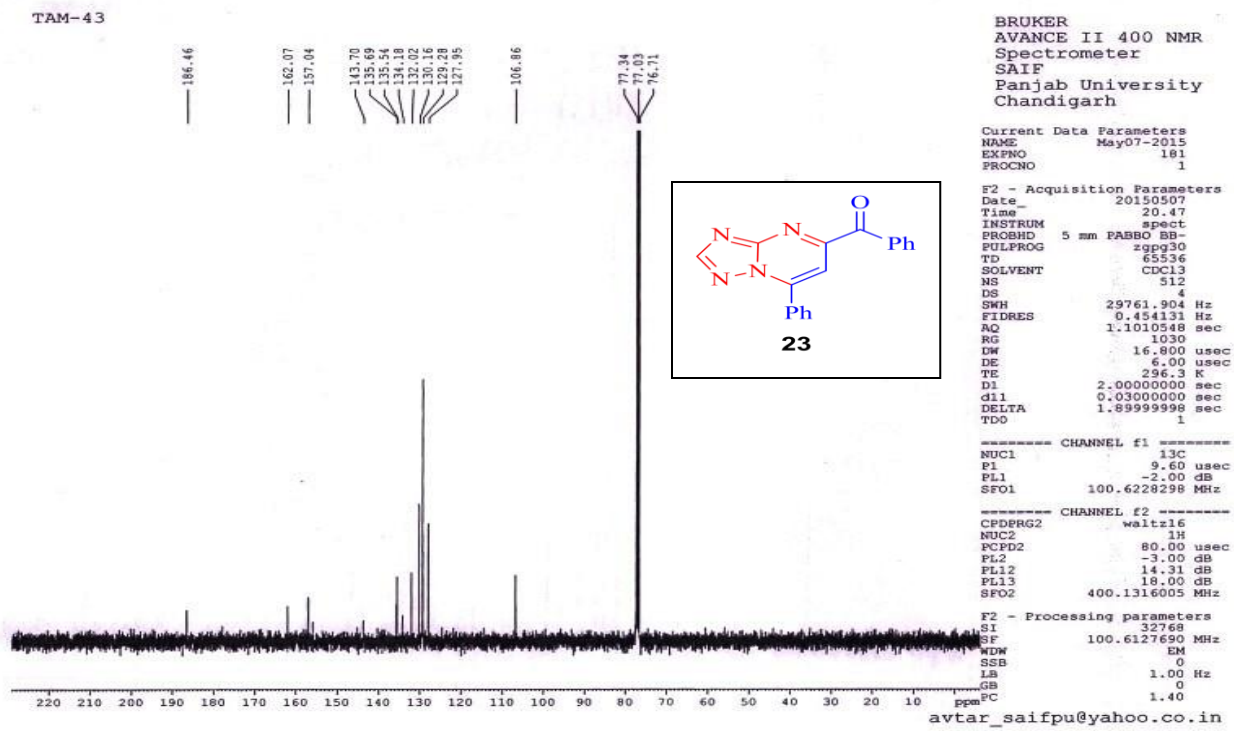
TAM-43

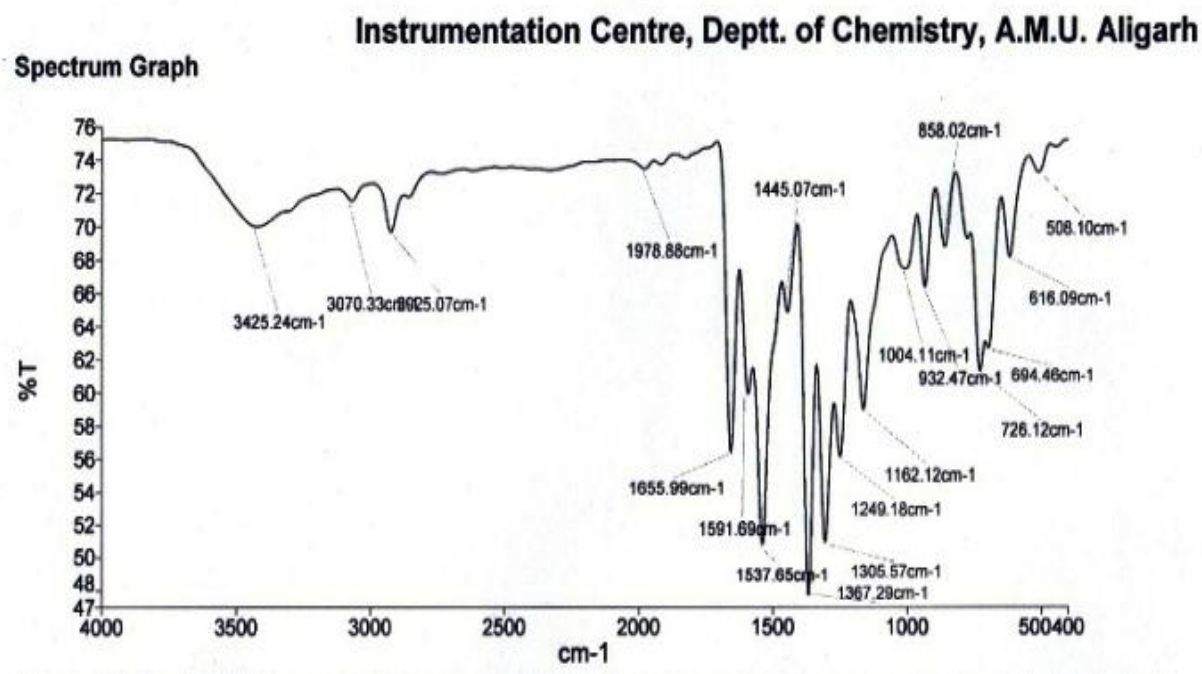


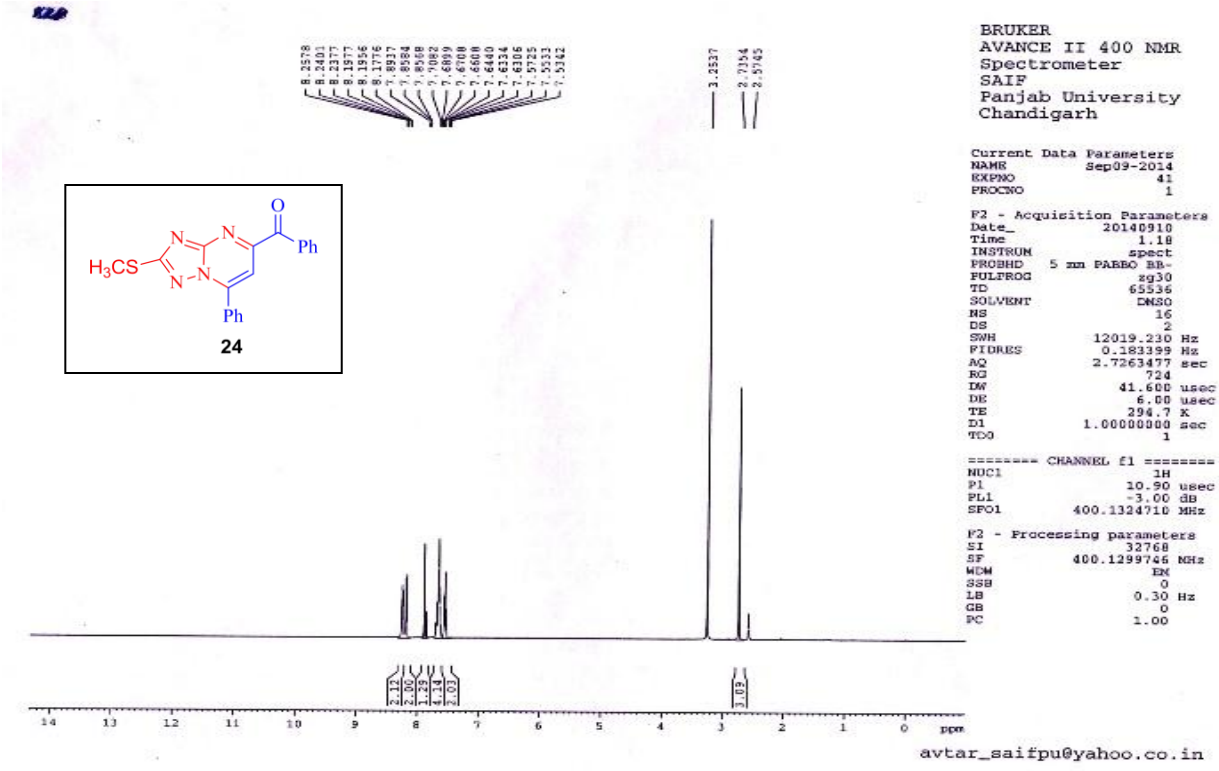
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

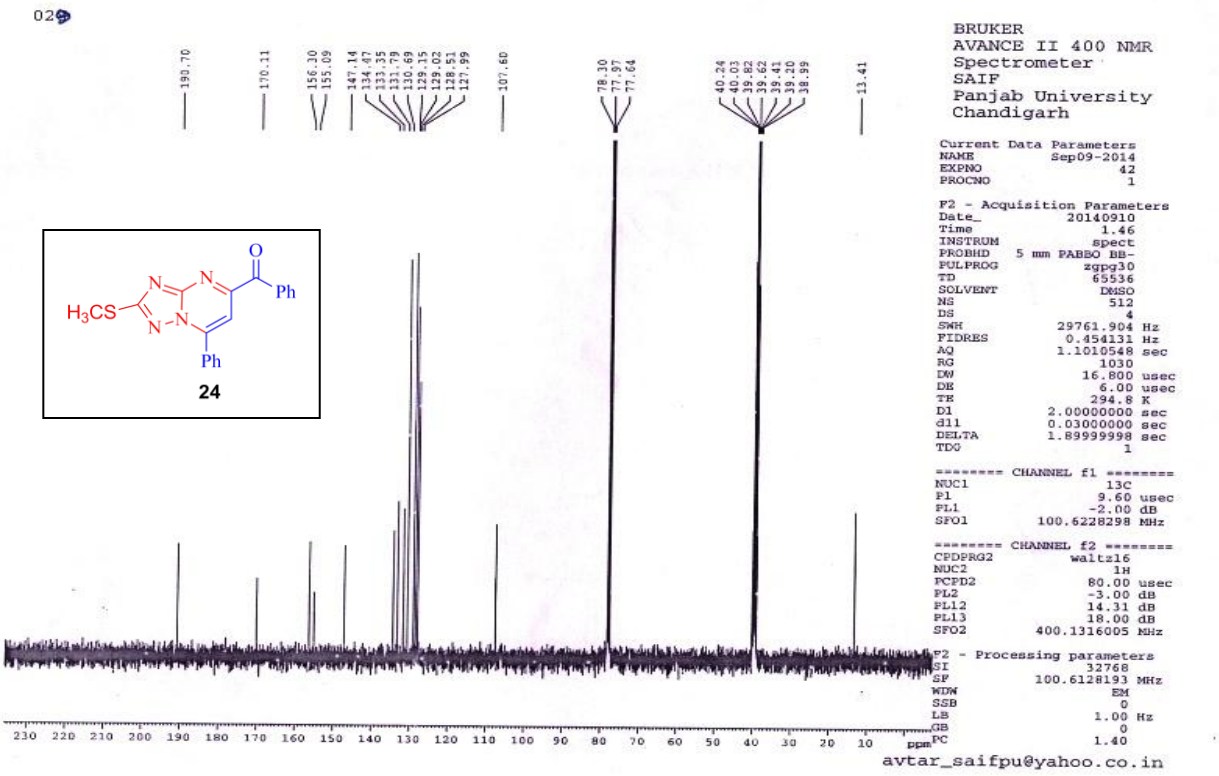
Current Data Parameters	
NAME	May07-2015
EXPNO	180
PROCNO	1
F2 - Acquisition Parameters	
Date_	20150507
Time	20.17
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	812
DW	41.600 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	32768
SF	400.1300086 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

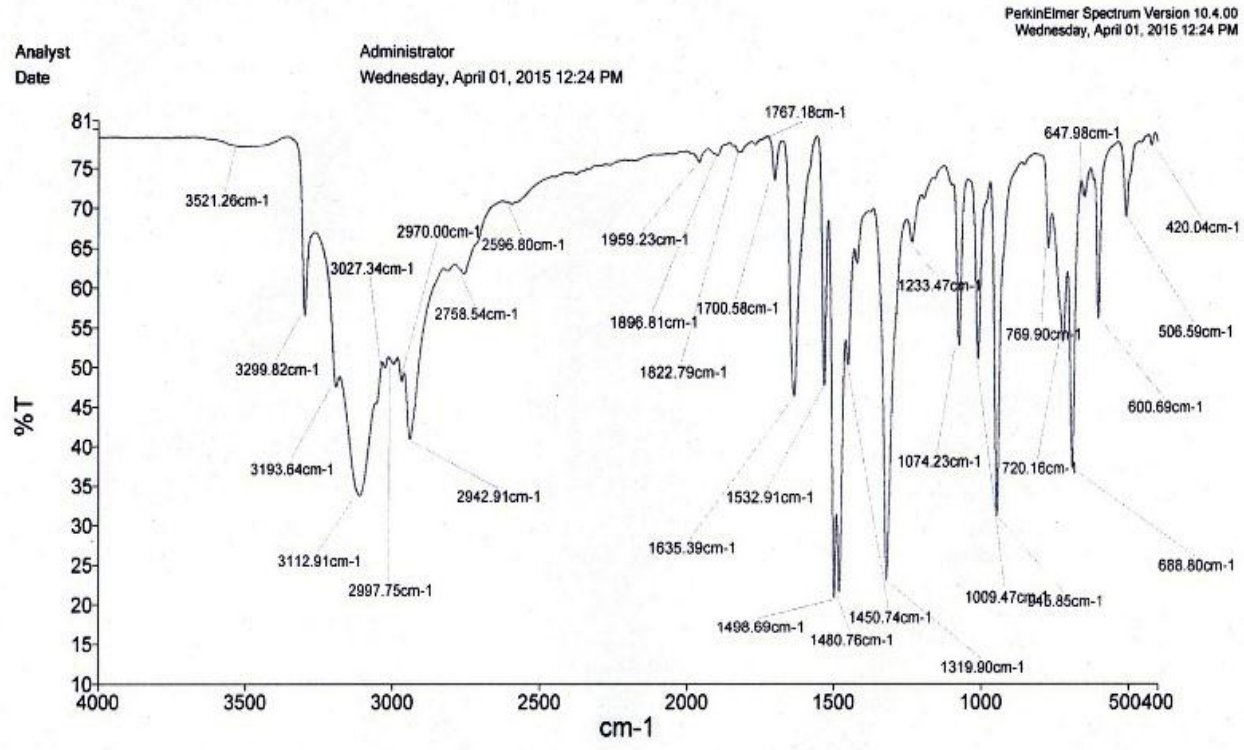
avtar_saifpu@yahoo.co.in

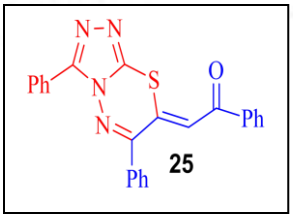

TAM-43
186.46
162.07
157.04
143.70
135.69
135.54
134.18
132.02
130.16
129.28
127.95
106.86
77.34
77.03
76.71
O
Ph
N
N
N
Ph
23
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME May07-2015
EXPNO 181
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150507
Time 20.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 296.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
avtar_saifpu@yahoo.co.in


Instrumentation Centre, Deptt. of Chemistry, A.M.U. Aligarh
Spectrum Graph
%T
cm-1
3425.24cm-1
3070.33cm-1
2925.07cm-1
1978.88cm-1
1655.99cm-1
1591.69cm-1
1537.65cm-1
1445.07cm-1
1367.29cm-1
1305.57cm-1
1249.18cm-1
1162.12cm-1
1004.11cm-1
932.47cm-1
858.02cm-1
726.12cm-1
694.46cm-1
616.09cm-1
508.10cm-1

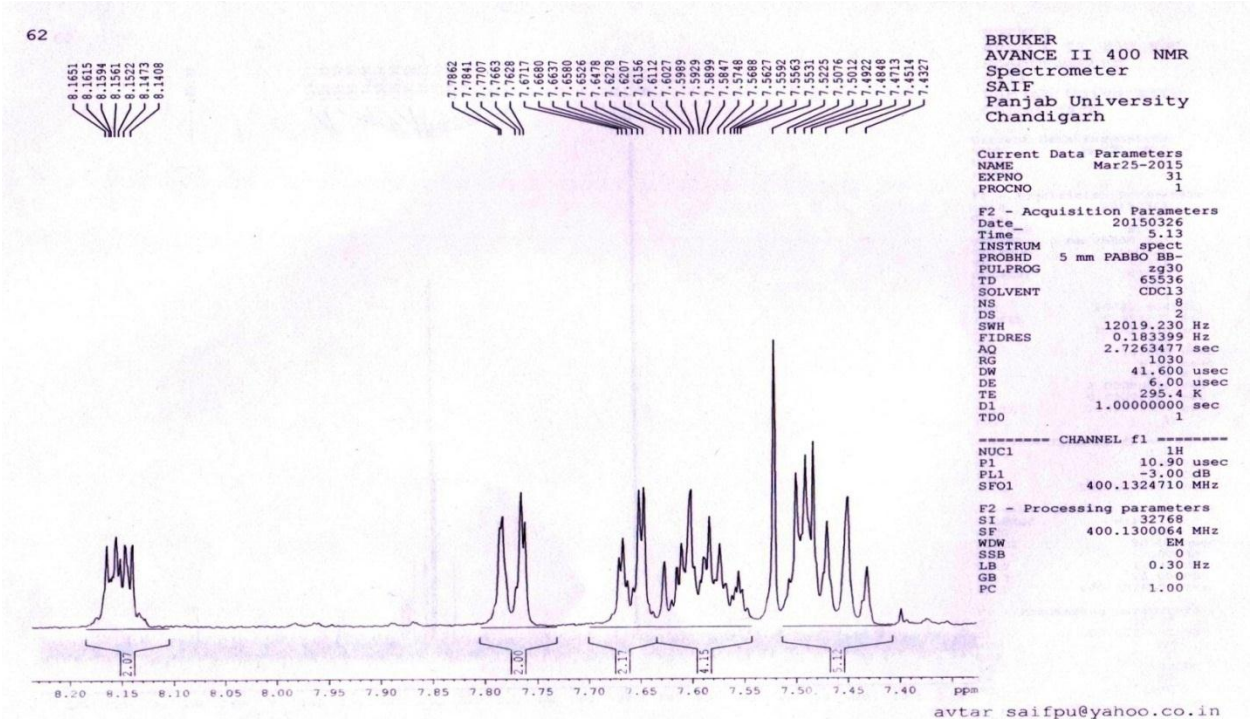

BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME Sep09-2014
EXPNO 41
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140910
Time 1.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 724
DW 41.600 usec
DE 6.00 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1299746 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
H3CS
Ph
Ph
O
24
ppm
avtar_saifpu@yahoo.co.in

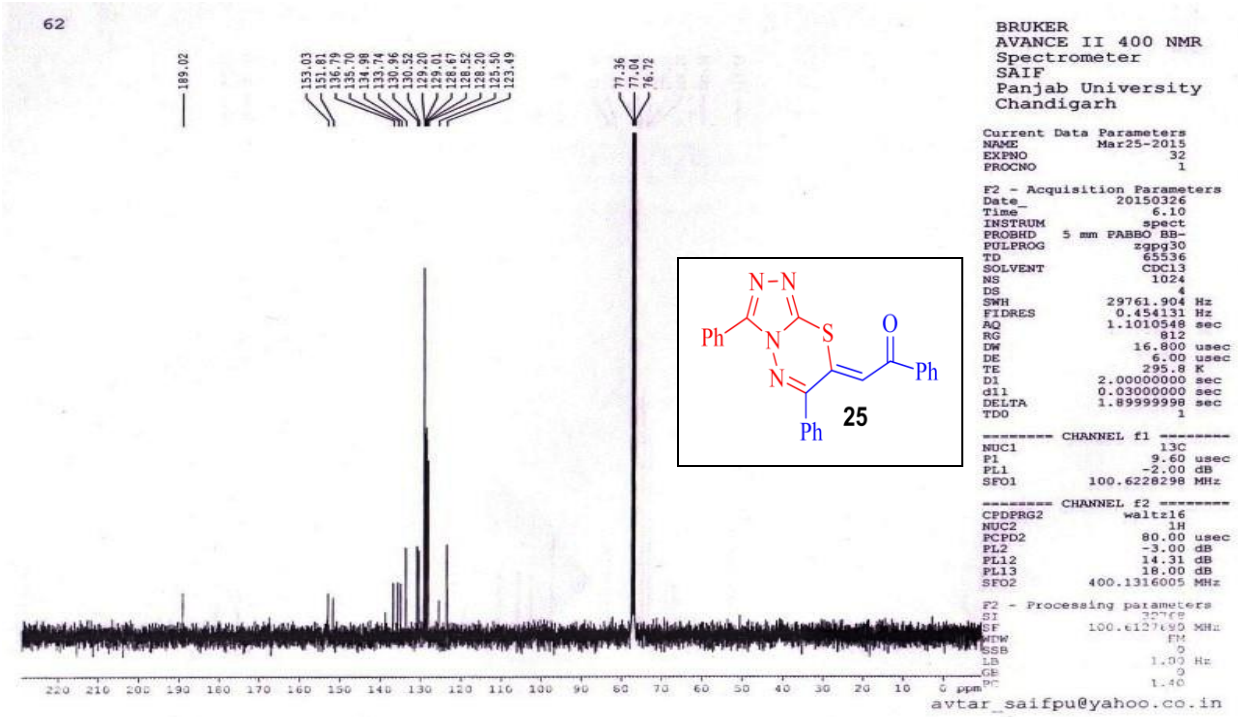

02
190.70
170.11
156.30
155.09
147.14
134.47
133.35
131.79
130.69
129.35
129.02
128.51
127.99
107.60
78.30
77.97
77.64
40.24
40.03
39.82
39.62
39.41
39.20
38.99
13.41
H3CS
N
N
N
N
O
Ph
Ph
24
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME Sep09-2014
EXPNO 42
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140910
Time 1.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 294.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
avtar_saifpu@yahoo.co.in

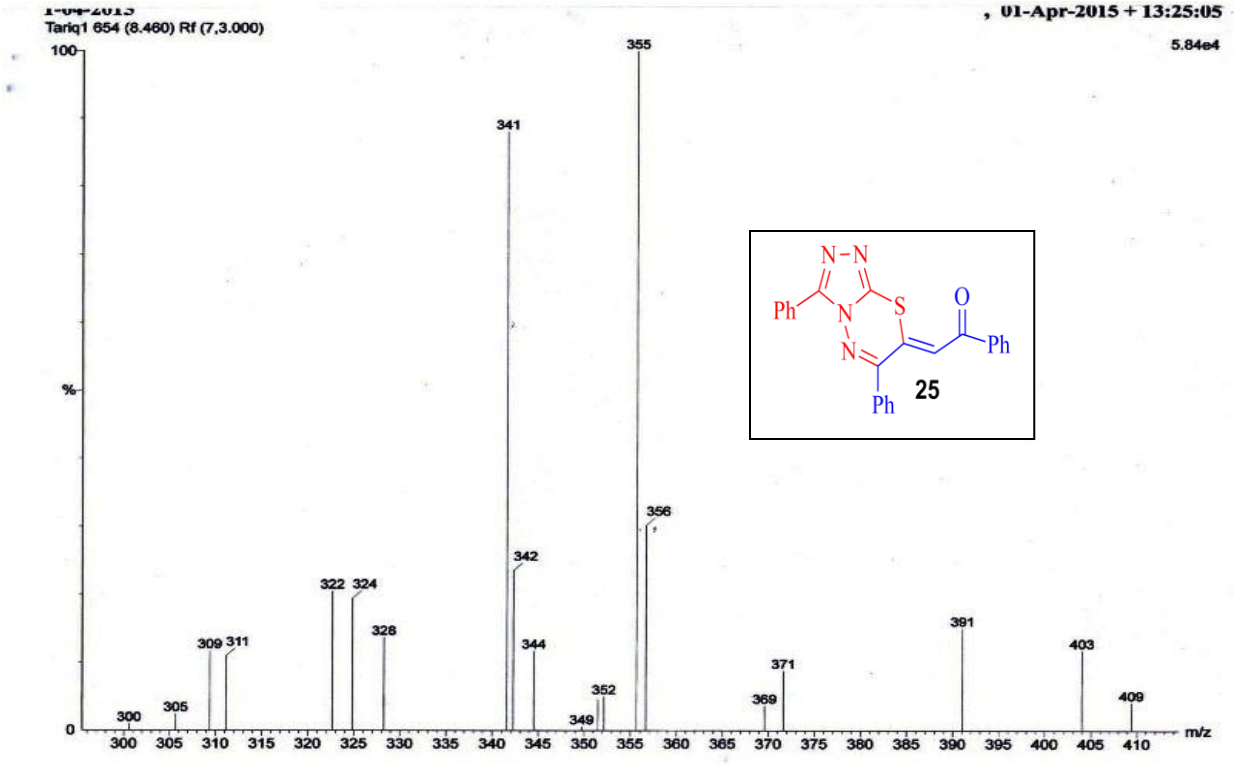

PerkinElmer Spectrum Version 10.4.00
Wednesday, April 01, 2015 12:24 PM
Analyst
Administrator
Date
Wednesday, April 01, 2015 12:24 PM
%T
cm-1
3521.26cm-1
3299.82cm-1
3193.64cm-1
3112.91cm-1
3027.34cm-1
2997.75cm-1
2970.00cm-1
2942.91cm-1
2758.54cm-1
2596.80cm-1
1959.23cm-1
1896.81cm-1
1822.79cm-1
1767.18cm-1
1700.58cm-1
1635.39cm-1
1532.91cm-1
1498.69cm-1
1480.76cm-1
1450.74cm-1
1319.90cm-1
1233.47cm-1
1074.23cm-1
1009.47cm-1
945.85cm-1
769.90cm-1
720.16cm-1
647.98cm-1
600.69cm-1
506.59cm-1
420.04cm-1
688.80cm-1
Code- 62-S, Phase- KBr. Prof. M. Muneer [Mr. Tariq Ahmad Shah] L.B. No. 11128

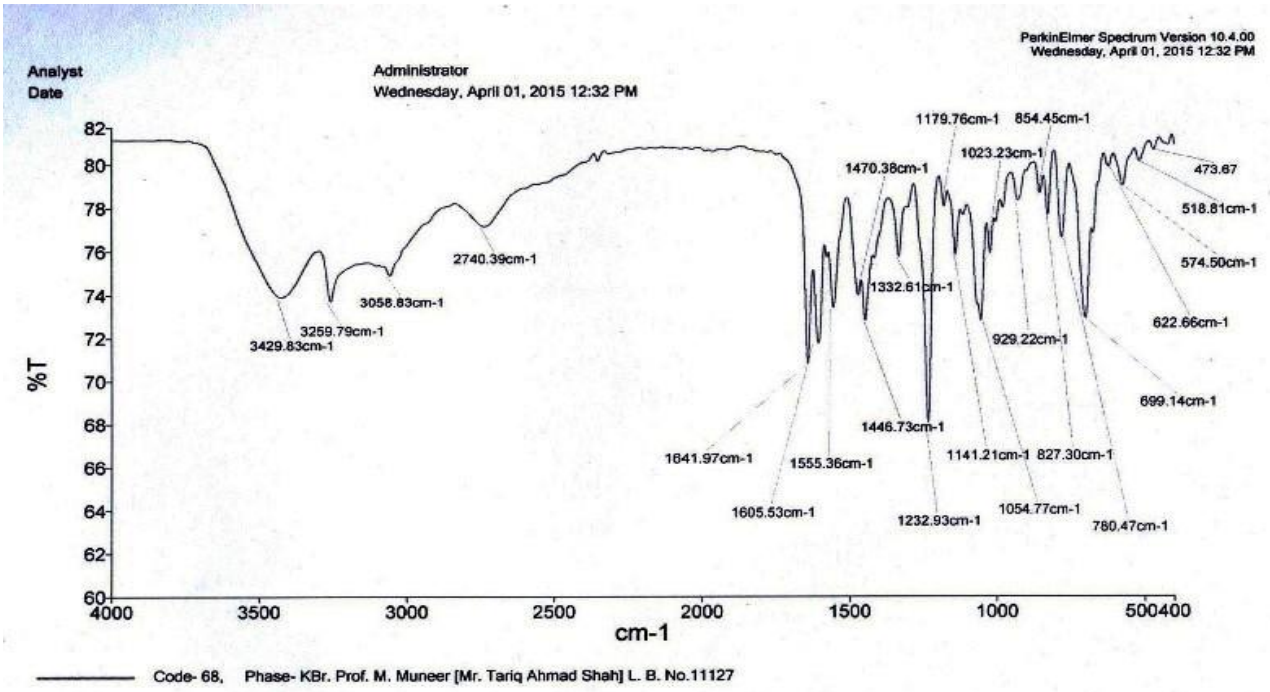

N-N
Ph
N
S
O
Ph
N
Ph

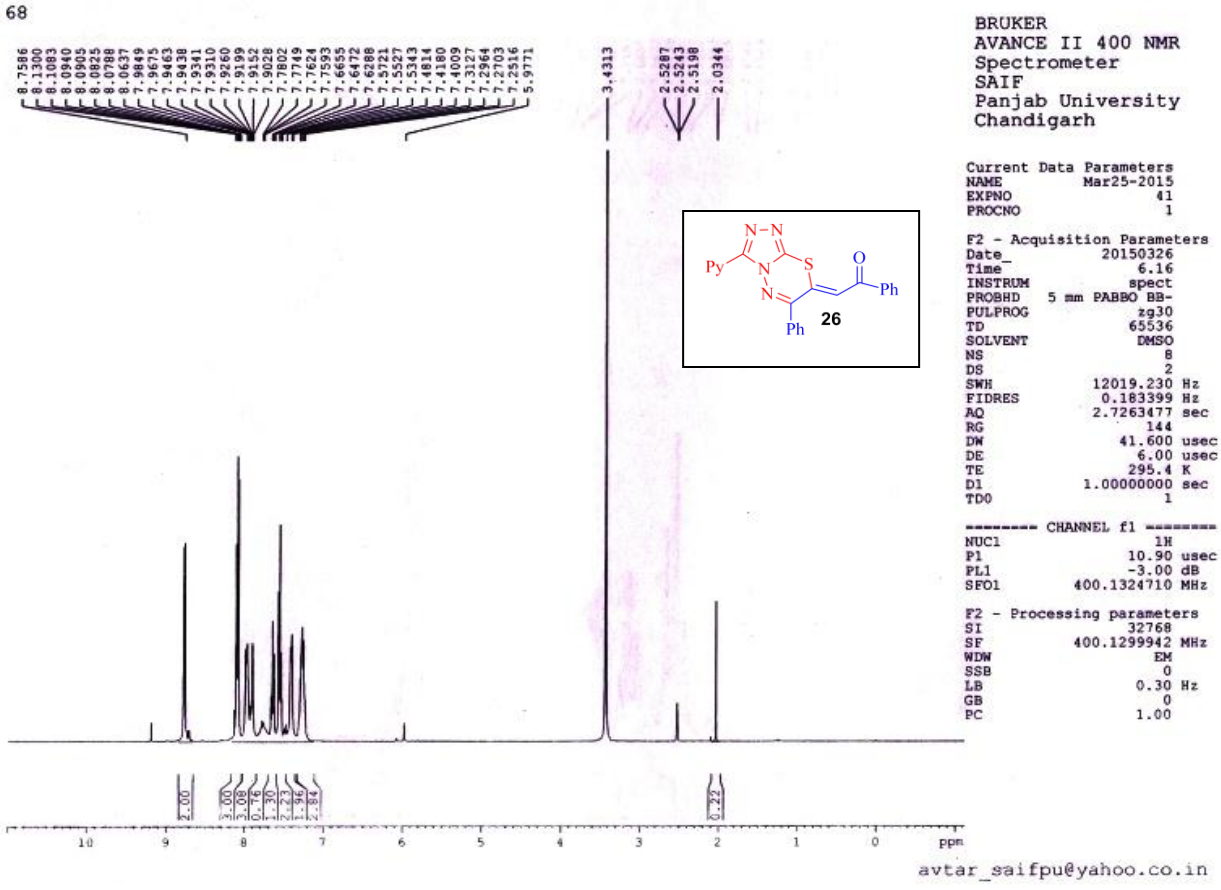
25

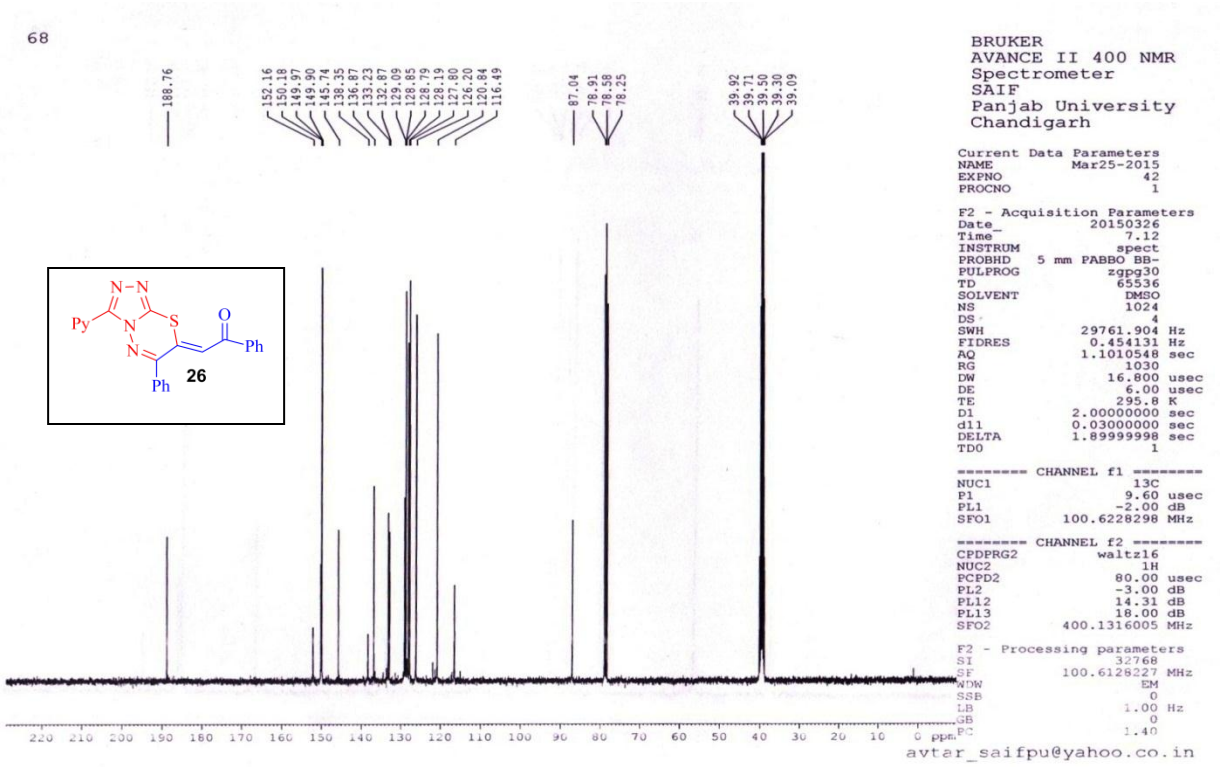

62
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME Mar25-2015
EXPNO 31
PROCNO 1
F2 - Acquisition Parameters
Date 20150326
Time 5.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 1030
DW 41.600 usec
DE 6.00 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300064 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm
avtar saifpu@yahoo.co.in

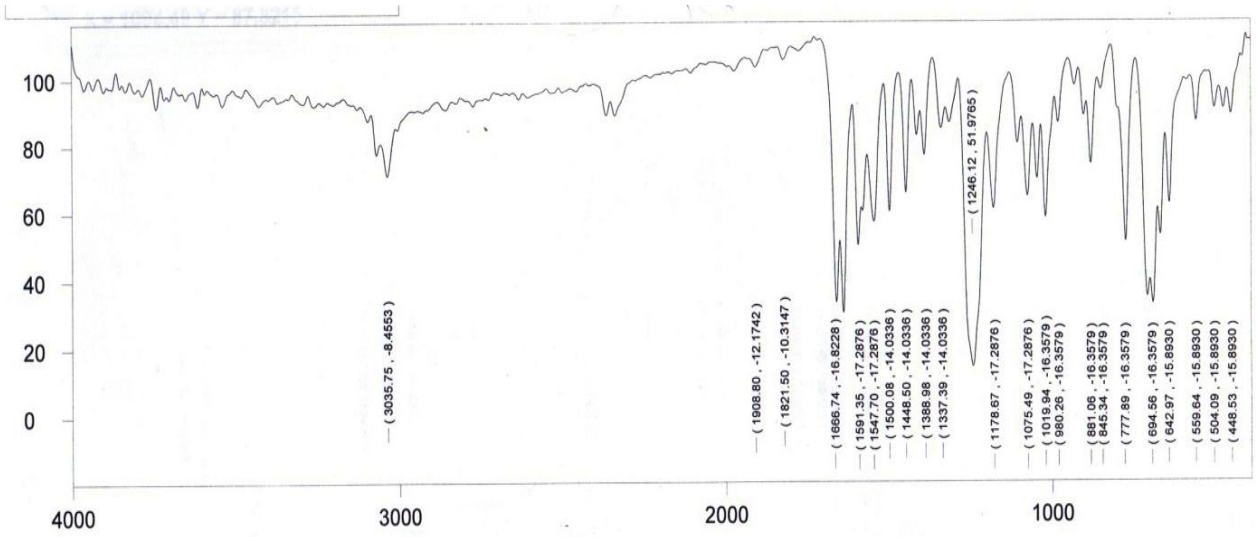

62
189.02
153.03
151.81
136.79
135.70
134.98
133.74
130.96
130.52
129.20
129.01
128.67
128.52
128.20
126.50
123.49
77.36
77.04
76.72
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME Mar25-2015
EXPNO 32
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150326
Time 6.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 812
DW 16.800 usec
DE 6.00 usec
TE 295.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
MDW FM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N-N
Ph
N
S
O
Ph
N
Ph
25
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
avtar_saifpu@yahoo.co.in


Tariq1 654 (8.460) Rf (7,3.000)
, 01-Apr-2015 + 13:25:05
5.84e4
100
%
0
355
341
356
342
322
324
328
309
311
344
352
349
371
369
391
403
409
300
305
m/z
300 305 310 315 320 325 330 335 340 345 350 355 360 365 370 375 380 385 390 395 400 405 410
N-N
Ph
N
S
O
Ph
N
Ph
25


PerkinElmer Spectrum Version 10.4.00
Wednesday, April 01, 2015 12:32 PM
Analyst
Date
Administrator
Wednesday, April 01, 2015 12:32 PM
%T
cm-1
3429.83cm-1
3259.79cm-1
3058.83cm-1
2740.39cm-1
1641.97cm-1
1605.53cm-1
1555.36cm-1
1470.38cm-1
1446.73cm-1
1332.61cm-1
1232.93cm-1
1179.76cm-1
1141.21cm-1
1054.77cm-1
1023.23cm-1
929.22cm-1
854.45cm-1
827.30cm-1
780.47cm-1
699.14cm-1
622.66cm-1
574.50cm-1
518.81cm-1
473.67
Code- 68, Phase- KBr. Prof. M. Muneer [Mr. Tariq Ahmad Shah] L. B. No.11127

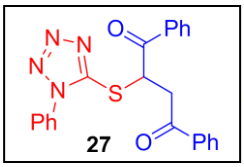

68
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Py
Ph
Ph
26
Current Data Parameters
NAME Mar25-2015
EXPNO 41
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150326
Time 6.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 144
DW 41.600 usec
DE 6.00 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1299942 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm
avtar_saifpu@yahoo.co.in


68
188.76
152.16
150.18
149.97
149.90
145.74
138.35
136.87
133.23
132.87
129.09
128.85
128.79
128.19
127.80
126.20
120.84
116.49
87.04
78.91
78.58
78.25
39.92
39.71
39.50
39.30
39.09
Py
Ph
Ph
O
26
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME Mar25-2015
EXPNO 42
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150326
Time 7.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 295.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128227 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
avtar_saifpu@yahoo.co.in



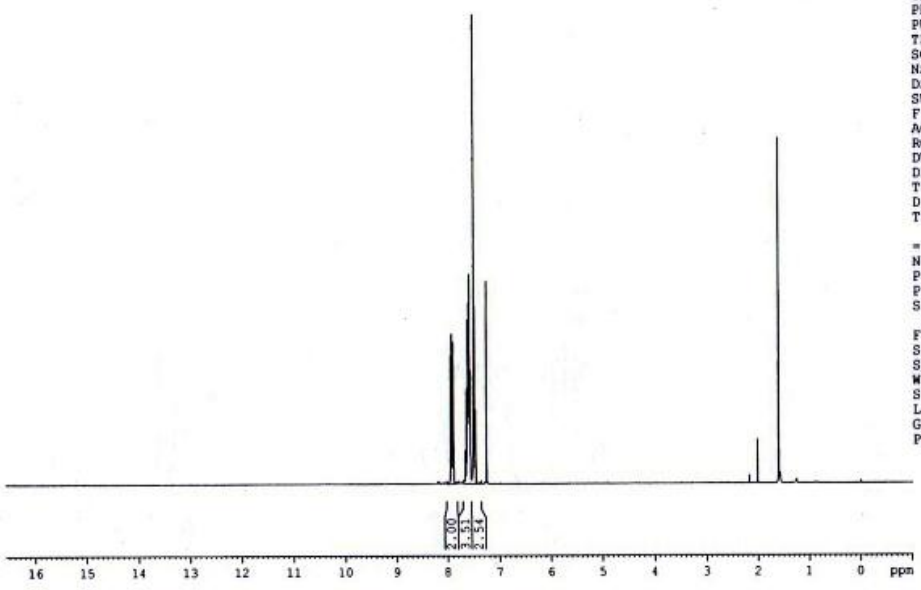
X = 2194.51 Y = 101.309

Wavenumbers [cm^{-1}]



27

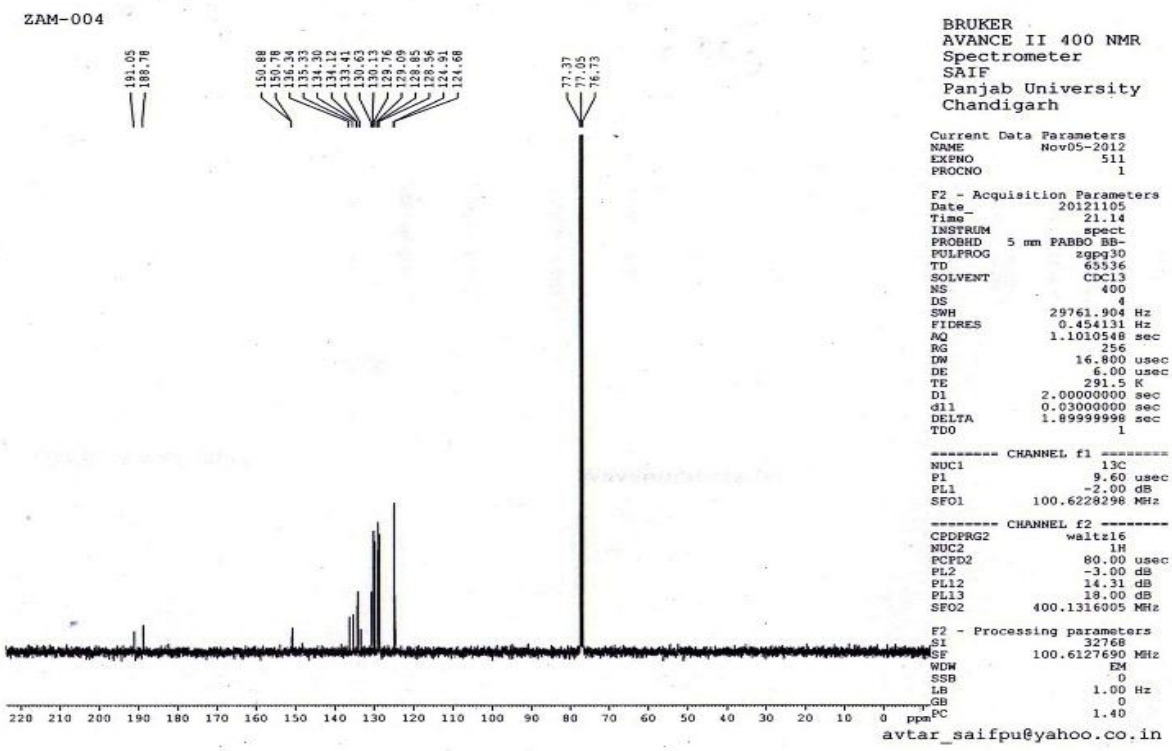
ZAM-004

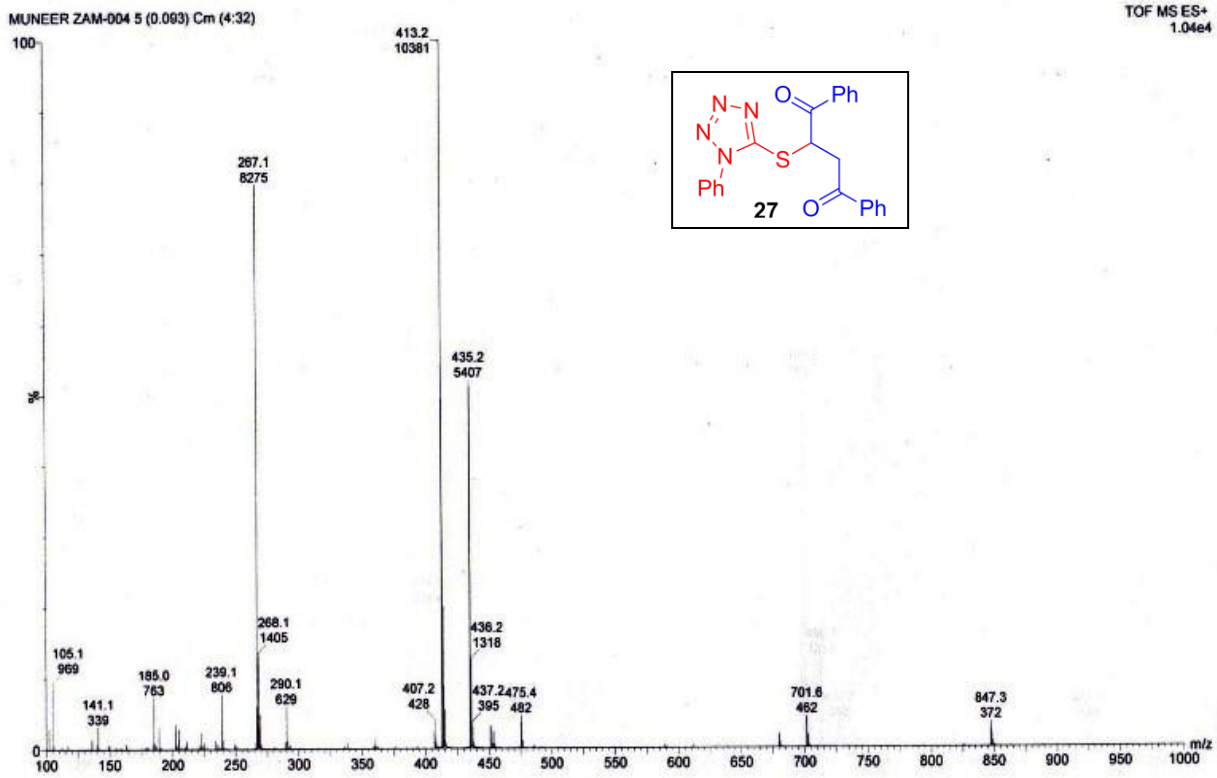


BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters	
NAME	Nov05-2012
EXPNO	510
PROCNO	1
F2 - Acquisition Parameters	
Date_	20121105
Time	20.51
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	456
DW	41.600 usec
DE	6.00 usec
TE	291.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	32768
SF	400.1300077 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

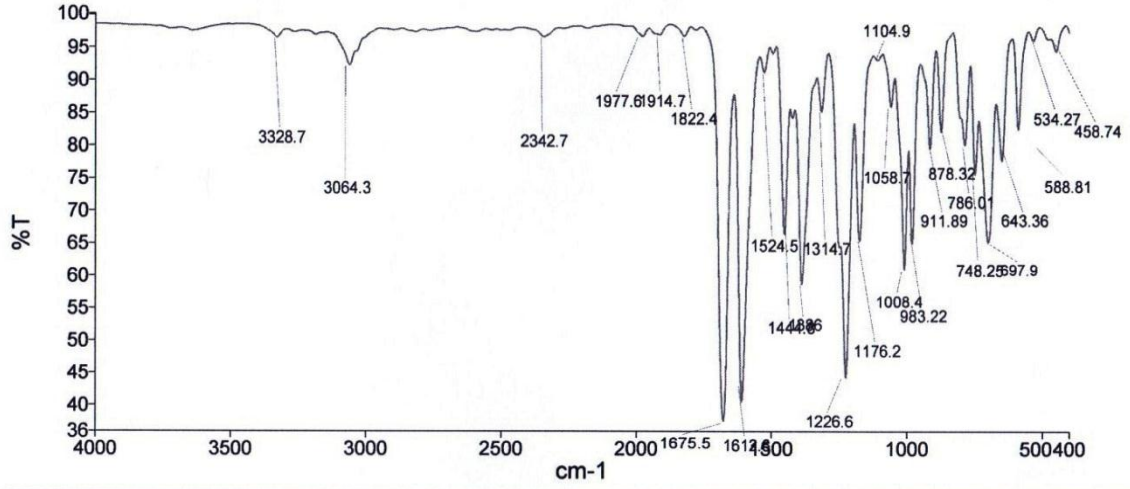
avtar_saifpu@yahoo.co.in


ZAM-004
191.05
188.78
150.88
150.78
136.34
135.33
134.30
134.12
133.41
130.63
130.13
129.76
129.09
128.85
128.56
124.91
124.68
77.37
77.05
76.73
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME Nov05-2012
EXPNO 511
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121105
Time 21.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 256
DW 16.800 usec
DE 6.00 usec
TE 291.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
avtar_saifpu@yahoo.co.in

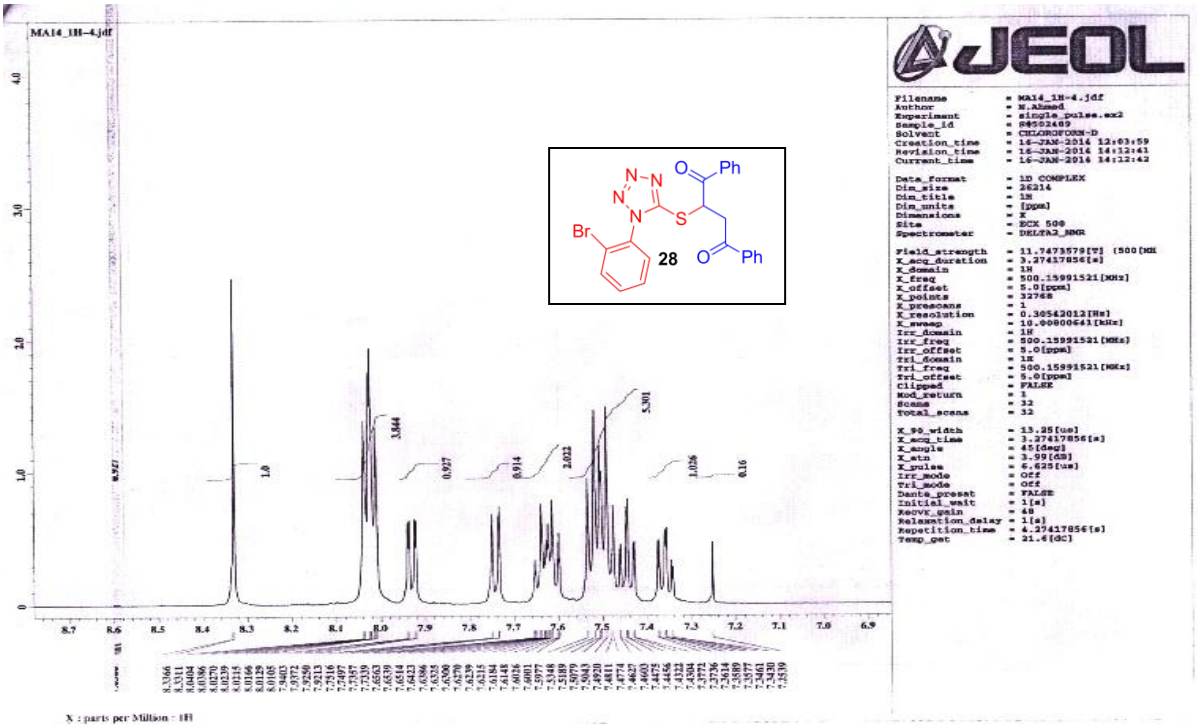

MUNEER ZAM-004 5 (0.093) Cm (4:32)
TOF MS ES+
1.04e4
100
%
0
413.2
10381
267.1
8275
435.2
5407
268.1
1405
436.2
1318
105.1
969
185.0
763
239.1
806
141.1
339
290.1
629
407.2
428
437.2
395
475.4
482
701.6
462
847.3
372
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z
N
N
N
Ph
S
O
Ph
O
Ph
27

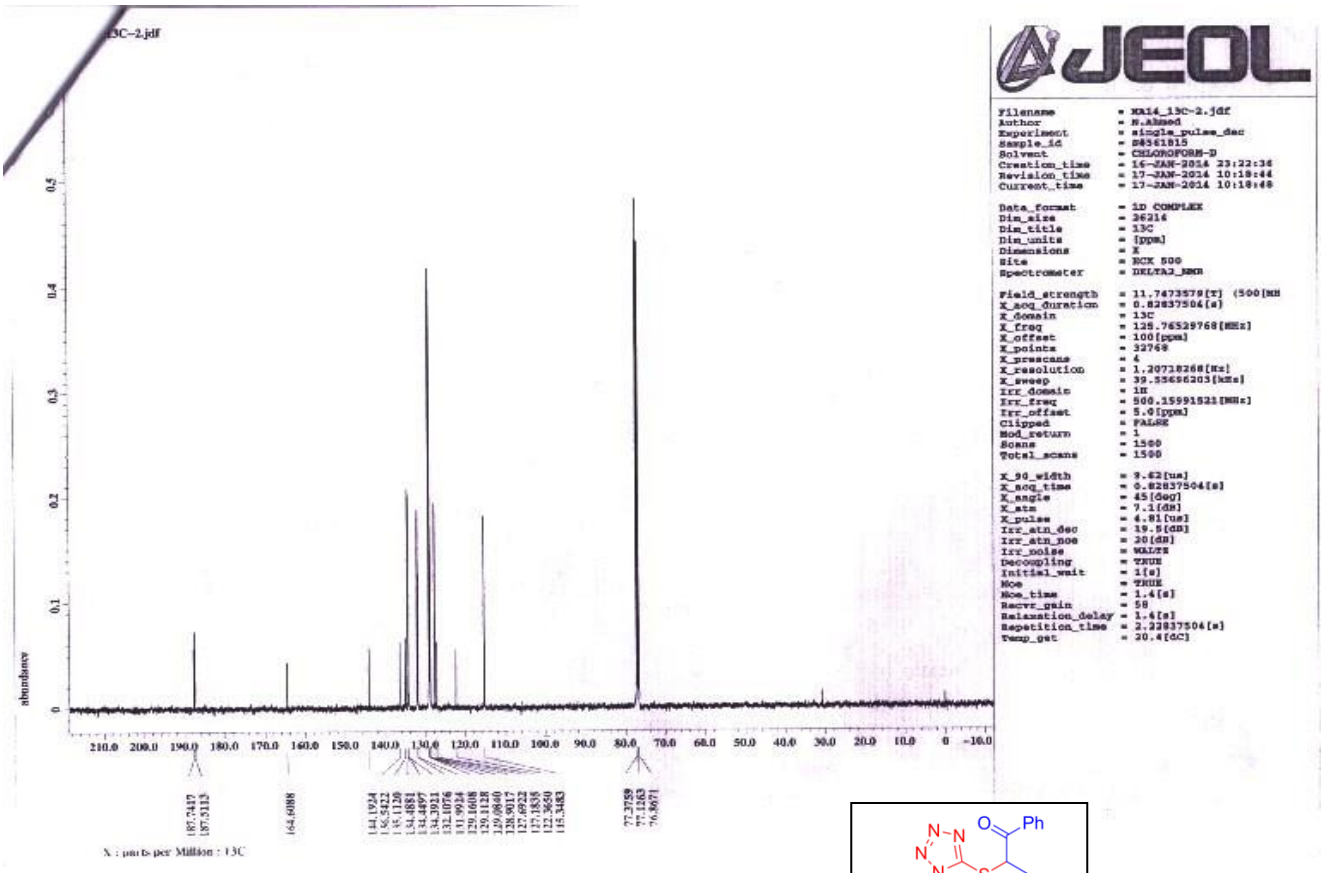
Instrumentation Centre, Deptt. of Chemistry, A.M.U. Aligarh

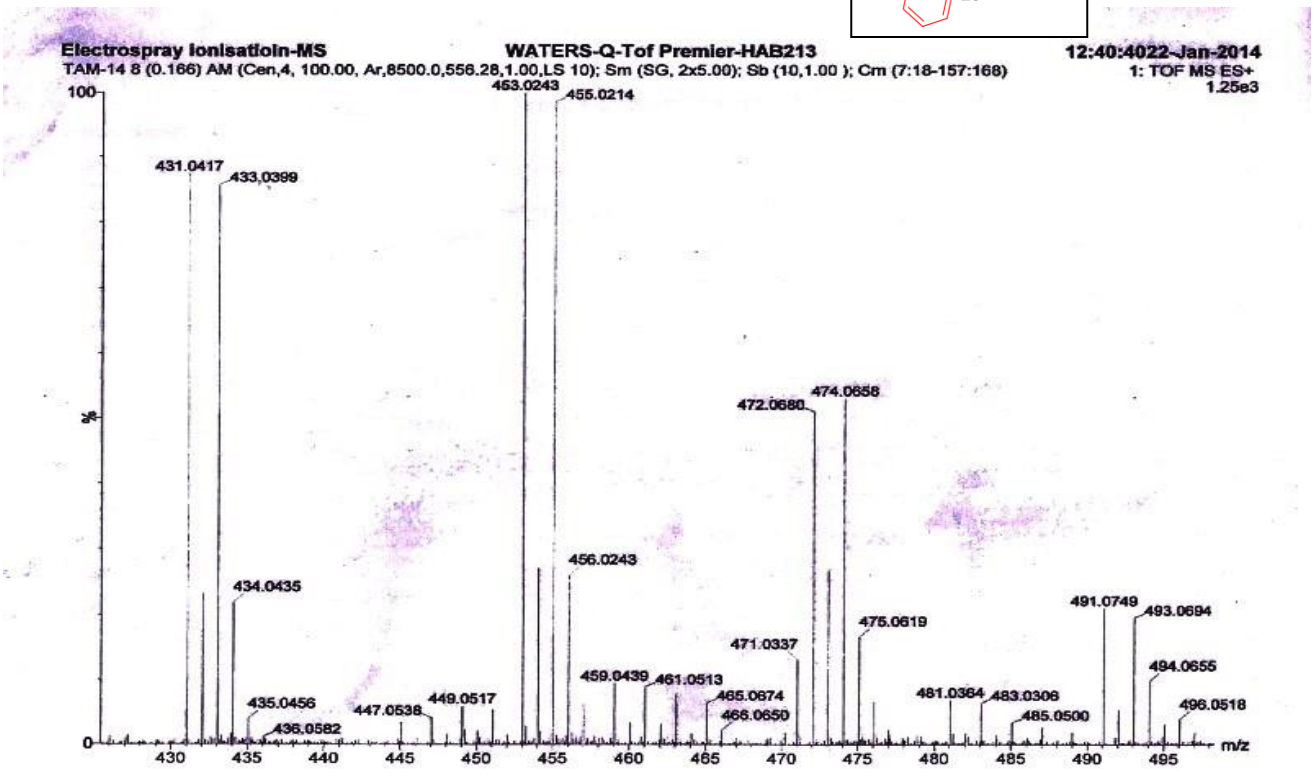
Spectrum Graph



Name	Description
TAM-014	Phas-KBr, Tariq A.S[Prof.M.Munir] L.B.No.8594

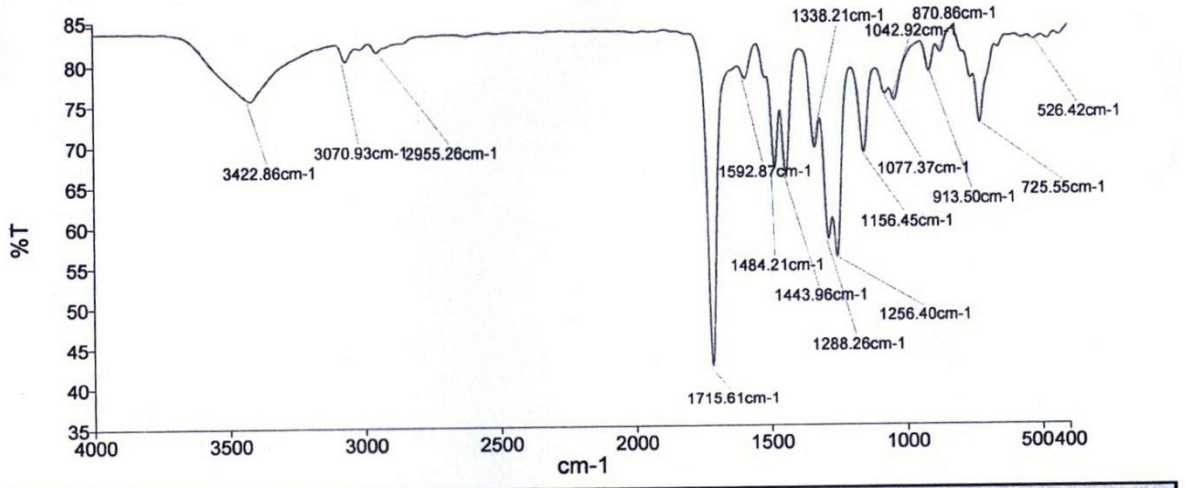



13C-2.jdf
abundance
X : parts per Million : 13C
Filename = xm14_13C-2.jdf
Author = N.Ahmed
Experiment = single_pulse_dec
Sample_id = 84561815
Solvent = CHLOROFORM-D
Creation_time = 16-JAN-2014 23:22:36
Revision_time = 17-JAN-2014 10:18:44
Current_time = 17-JAN-2014 10:18:48
Data_format = 1D COMPLEX
Dim_size = 36214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = RCX 500
Spectrometer = DELTA2_NMR
Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.82837504[s]
X_domain = 13C
X_freq = 125.76529768[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.20718268[Hz]
X_sweep = 39.55696203[kHz]
Irr_domain = 1H
Irr_freq = 500.35991521[MHz]
Irr_offset = 5.0[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1560
Total_scans = 1560
X_90_width = 9.62[us]
X_acq_time = 0.82837504[s]
X_angle = 45[deg]
X_atn = 7.1[dB]
X_pulse = 4.81[us]
Irr_atn_dec = 19.5[dB]
Irr_atn_noe = 20[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 1.4[s]
Recvr_gain = 58
Relaxation_delay = 1.4[s]
Repetition_time = 2.22837504[s]
Temp_get = 20.4[dC]
Br
O
Ph
N
S
28

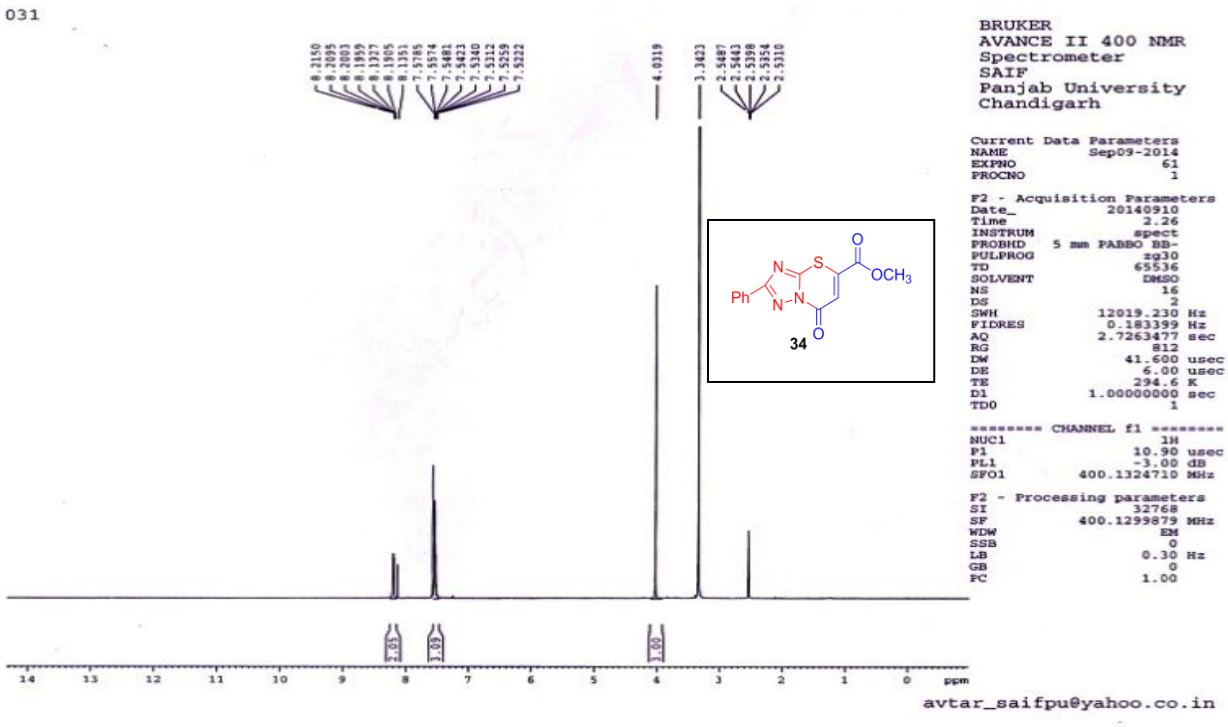

Electrospray Ionisation-MS
WATERS-Q-Tof Premier-HAB213
12:40:4022-Jan-2014
TAM-14 8 (0.166) AM (Cen,4, 100.00, Ar,8500.0,556.28,1.00,LS 10); Sm (SG, 2x5.00); Sb (10,1.00); Cm (7:18-157:168)
1: TOF MS ES+
1.25e3
%
m/z
453.0243
455.0214
431.0417
433.0399
474.0658
472.0680
456.0243
434.0435
475.0619
471.0337
491.0749
493.0694
459.0439
461.0513
494.0655
481.0364
483.0306
465.0674
466.0650
435.0456
447.0538
449.0517
436.0582
496.0518
485.0500

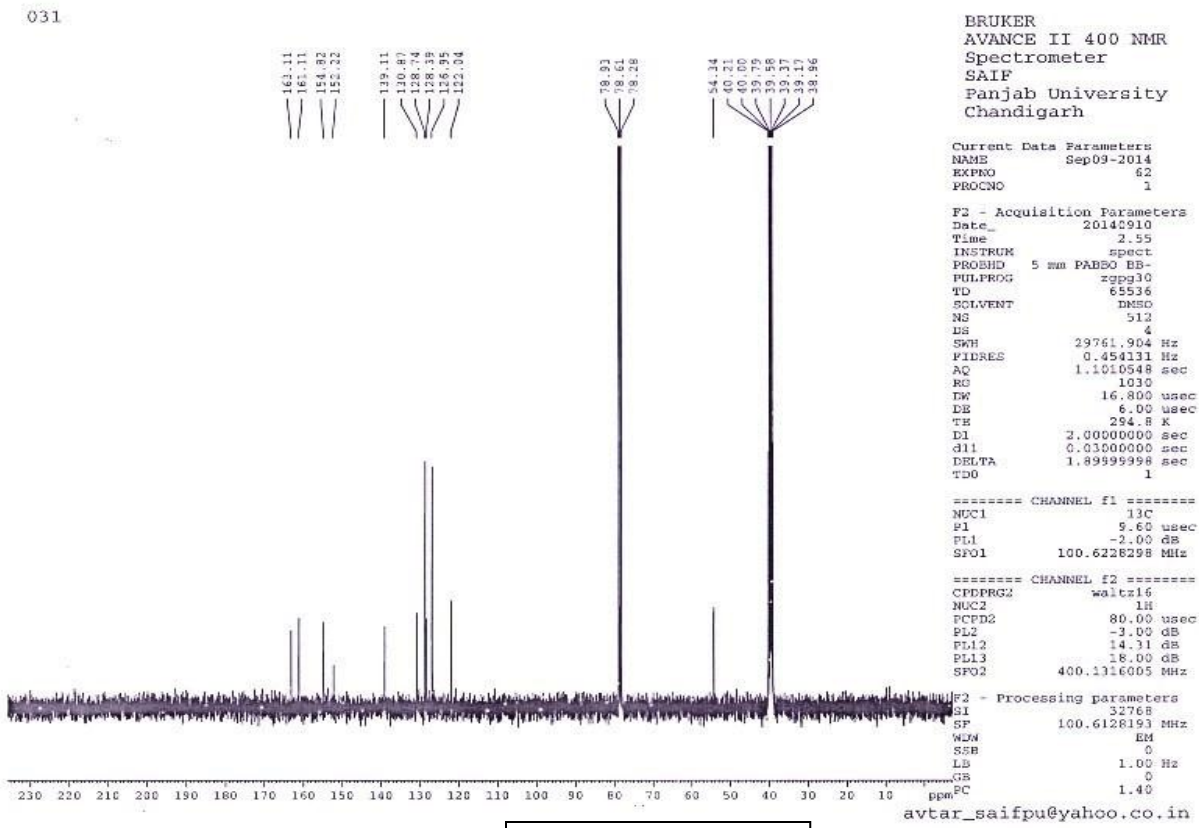
Instrumentation Centre, Deptt. of Chemistry, A.M.U. Aligarh

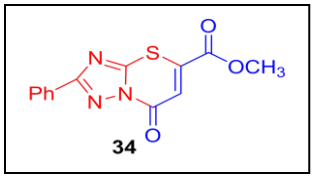
Spectrum Graph



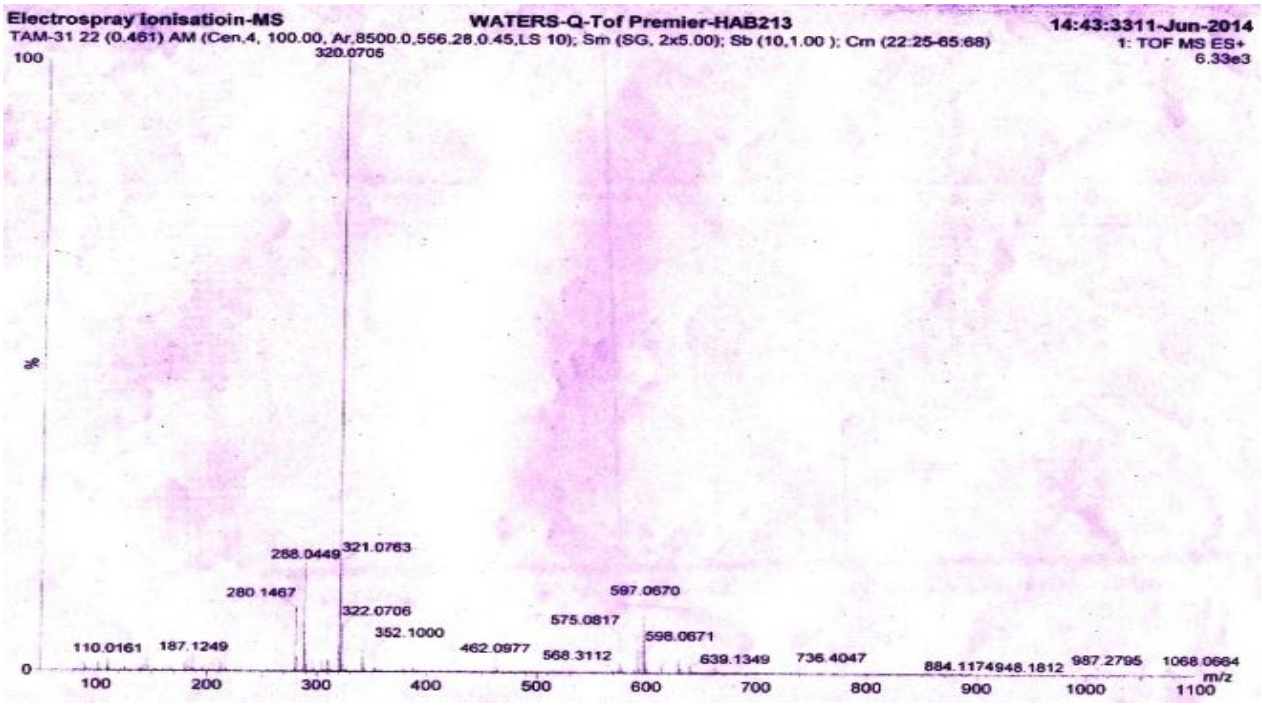
Name	Description
____ TAM 031_	Phase-KBr,Prof.M.Muneer [Mr.Tariq Shah] LB.No.10136




031
161.11
161.11
154.82
152.22
139.11
130.87
128.74
128.39
126.95
122.04
78.93
78.61
78.28
54.34
40.21
40.00
39.79
39.58
39.37
39.17
38.96
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME Sep09-2014
EXPNO 62
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140910
Time 2.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 294.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
avtar_saifpu@yahoo.co.in

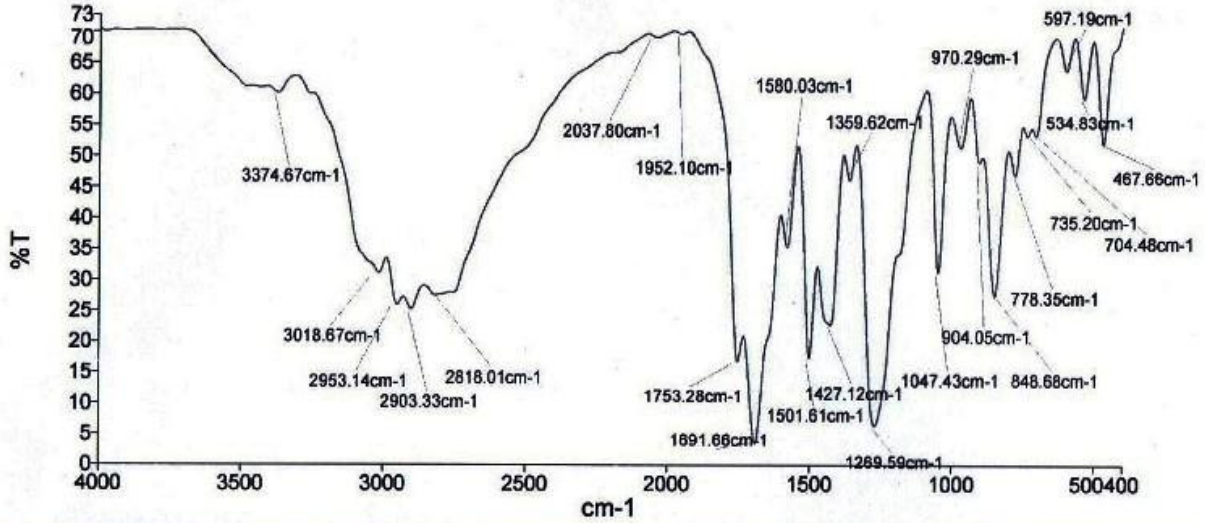

Ph
N
S
N
N
O
OCH3
O

34

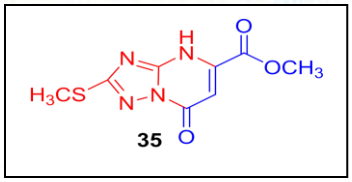

Electrospray Ionisatioin-MS
WATERS-Q-Tof Premier-HAB213
14:43:3311-Jun-2014
TAM-31 22 (0.461) AM (Cen,4, 100.00, Ar,8500.0,556.28,0.45,LS 10); Sm (SG, 2x5.00); Sb (10,1.00); Cm (22:25-65:68)
1: TOF MS ES+
6.33e3
100
%
0
320.0705
321.0763
258.0449
280.1467
322.0706
352.1000
597.0670
575.0817
598.0671
110.0161
187.1249
462.0977
568.3112
639.1349
736.4047
884.1174
948.1812
987.2795
1068.0664
100 200 300 400 500 600 700 800 900 1000 1100
m/z

Instrumentation Centre, Deptt. of Chemistry, A.M.U. Aligarh

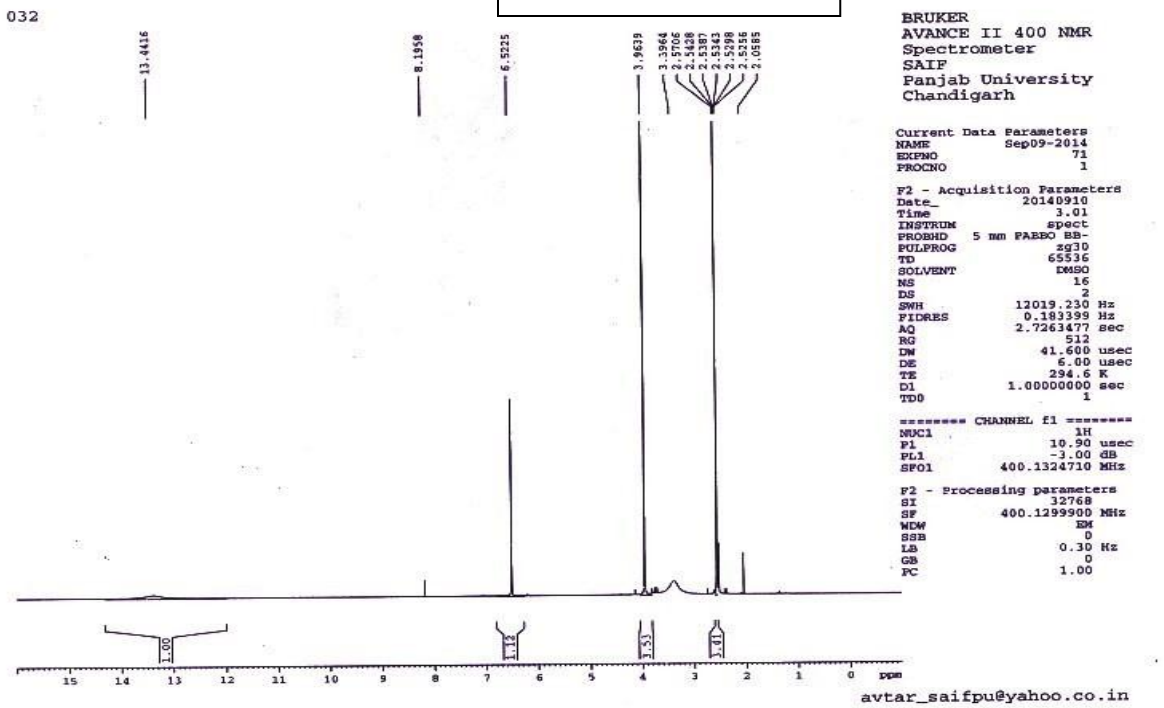
Spectrum Graph



Name	Description
TAM 032_	Phase-KBr,Prof.M.Muneer [Mr.Tariq Shah] LB.No.10137



35



BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

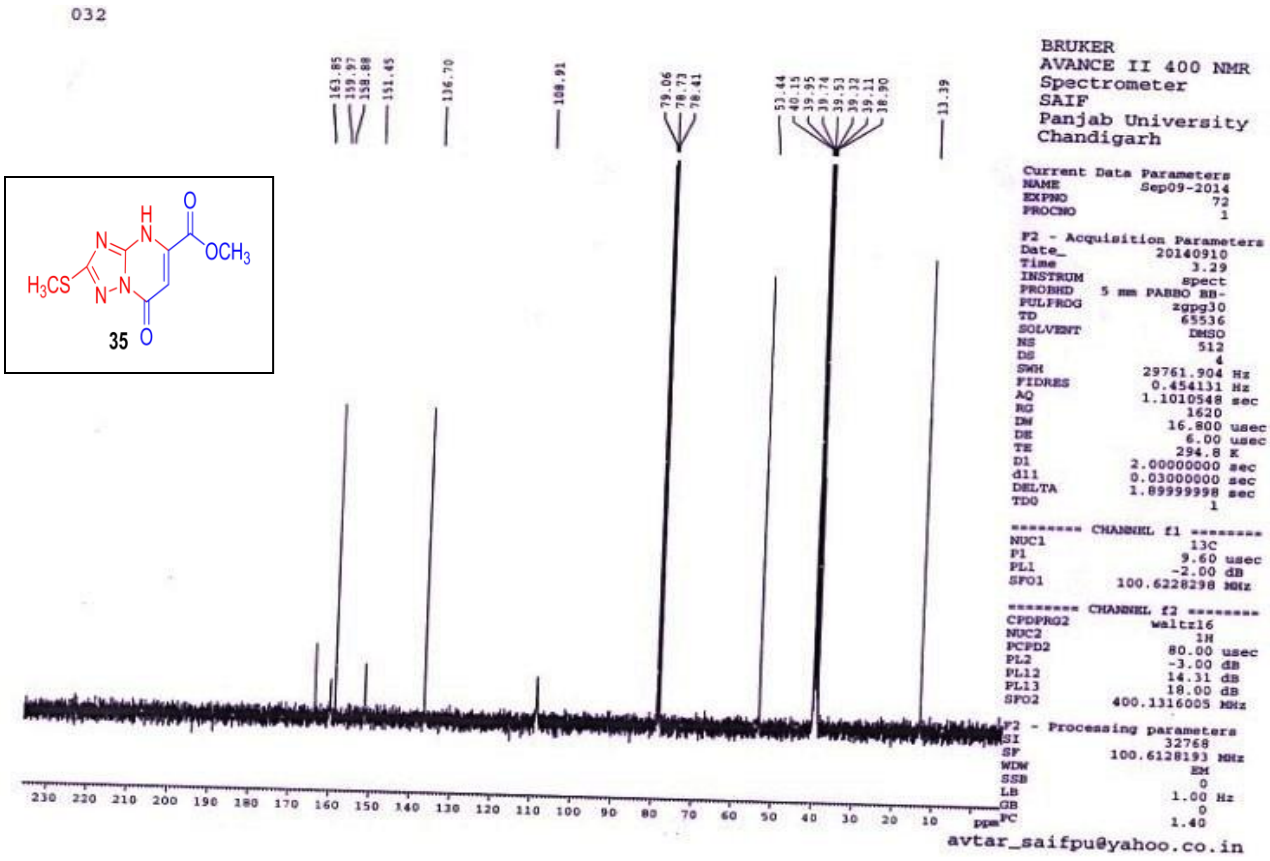
Current Data Parameters
NAME Sep09-2014
EXPNO 71
PROCNO 1

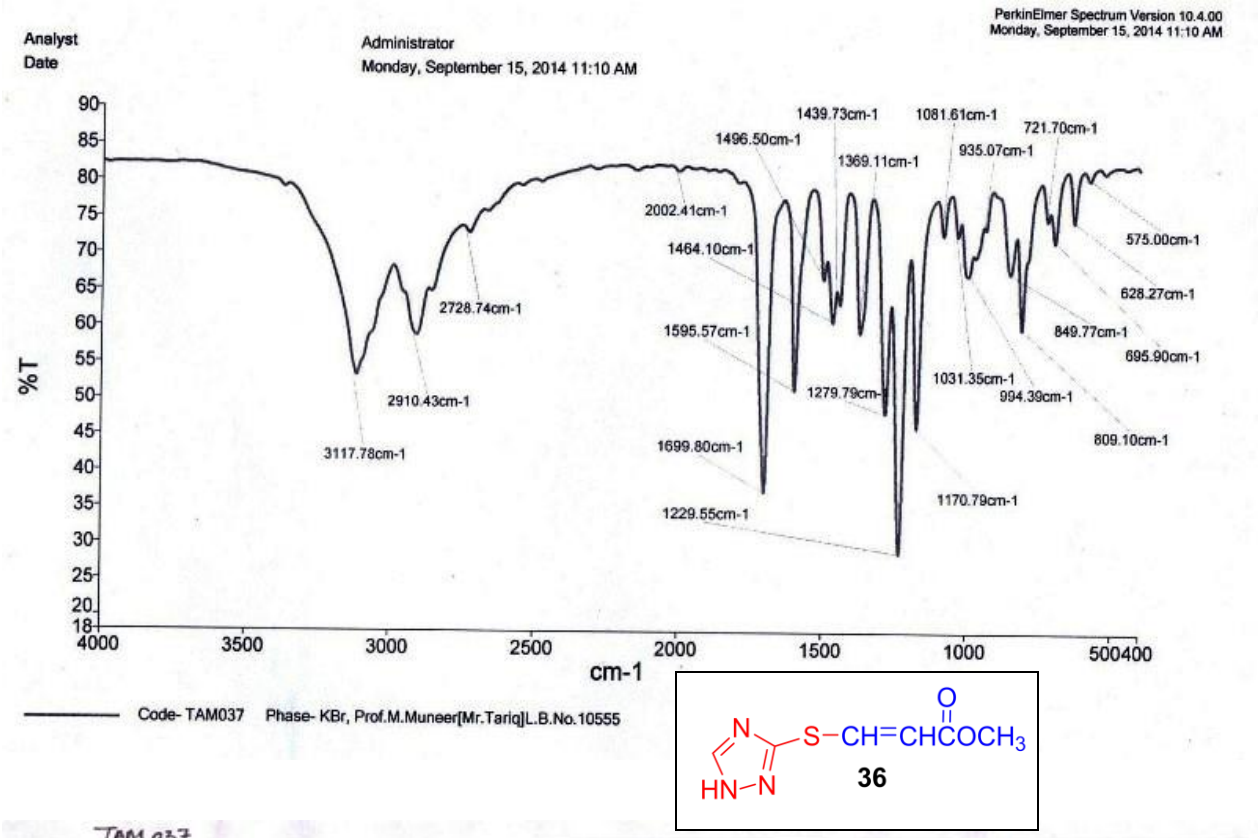
F2 - Acquisition Parameters
Date_ 20140910
Time 3.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 512
DW 41.600 usec
DE 6.00 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299900 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

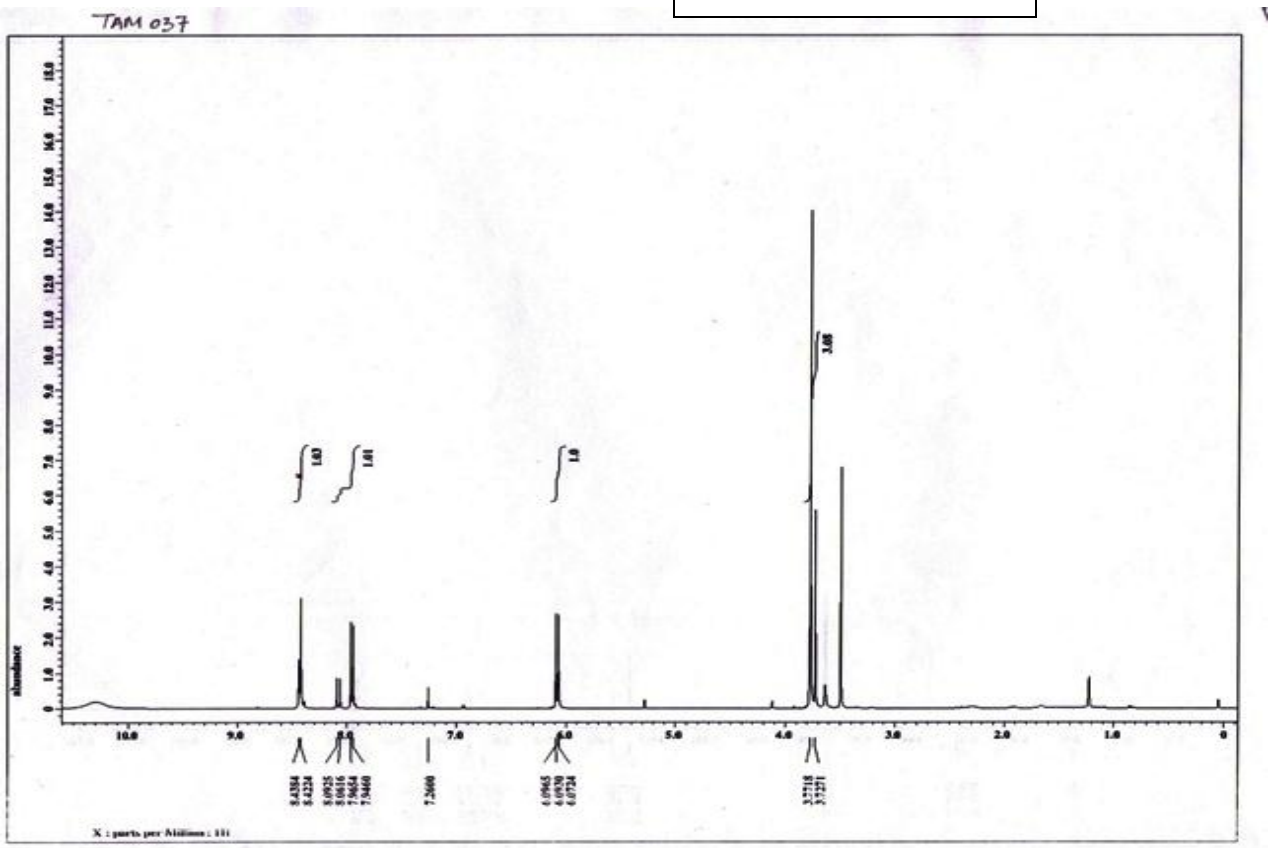
avtar_saifpu@yahoo.co.in

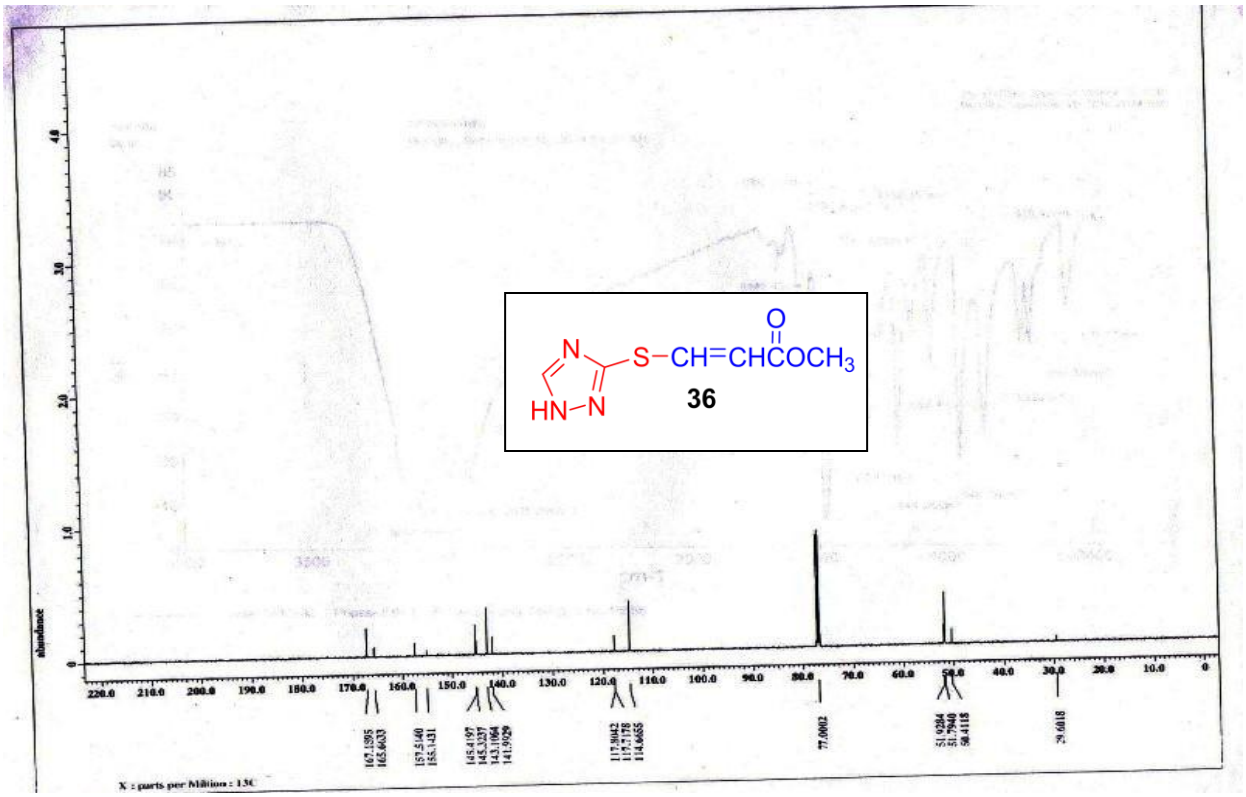

032
161.85
159.97
158.88
151.45
136.70
108.91
79.06
78.73
78.41
53.44
40.15
39.95
39.74
39.53
39.32
39.11
38.90
13.39
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME Sep09-2014
EXPNO 72
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140910
Time 3.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1620
DW 16.800 usec
DE 6.00 usec
TE 294.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
avtar_saifpu@yahoo.co.in
H
N
N
N
O
O
OCH3
H3CS
35

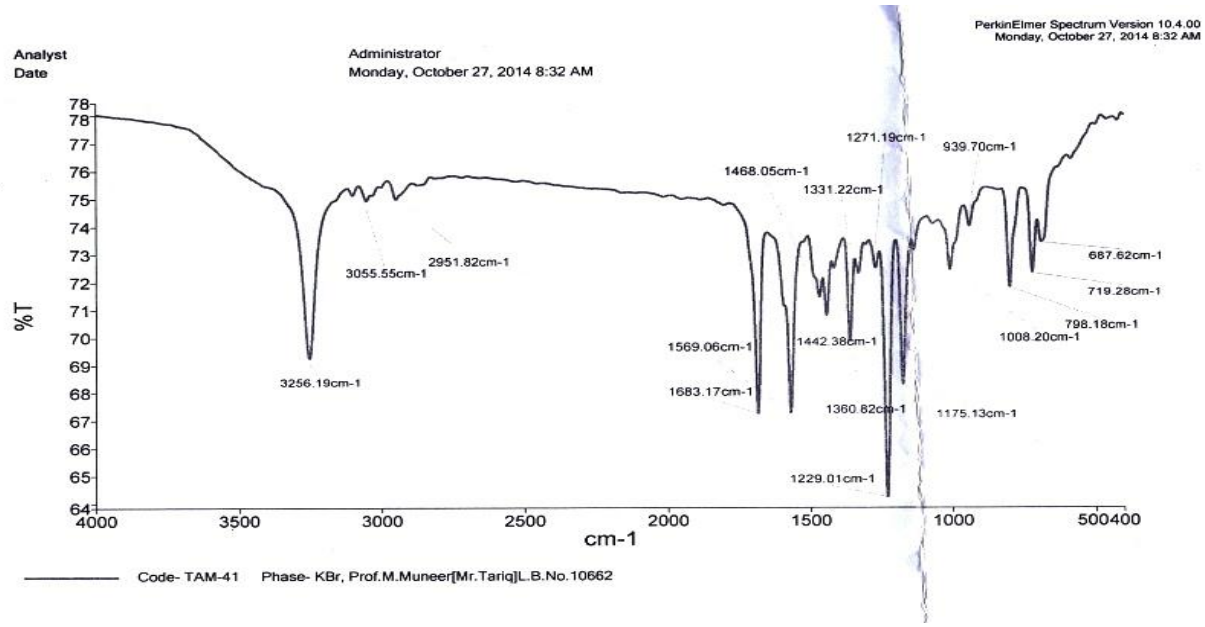

PerkinElmer Spectrum Version 10.4.00
Monday, September 15, 2014 11:10 AM
Analyst
Date
Administrator
Monday, September 15, 2014 11:10 AM
%T
cm-1
3117.78cm-1
2910.43cm-1
2728.74cm-1
2002.41cm-1
1699.80cm-1
1595.57cm-1
1496.50cm-1
1464.10cm-1
1439.73cm-1
1369.11cm-1
1279.79cm-1
1229.55cm-1
1170.79cm-1
1081.61cm-1
1031.35cm-1
994.39cm-1
935.07cm-1
849.77cm-1
809.10cm-1
721.70cm-1
695.90cm-1
628.27cm-1
575.00cm-1
Code- TAM037 Phase- KBr, Prof.M.Muneer[Mr.Tariq]L.B.No.10555

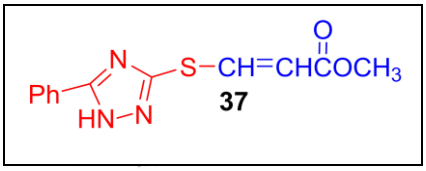
O
N
S–CH=CHCOCH3
HN–N

36

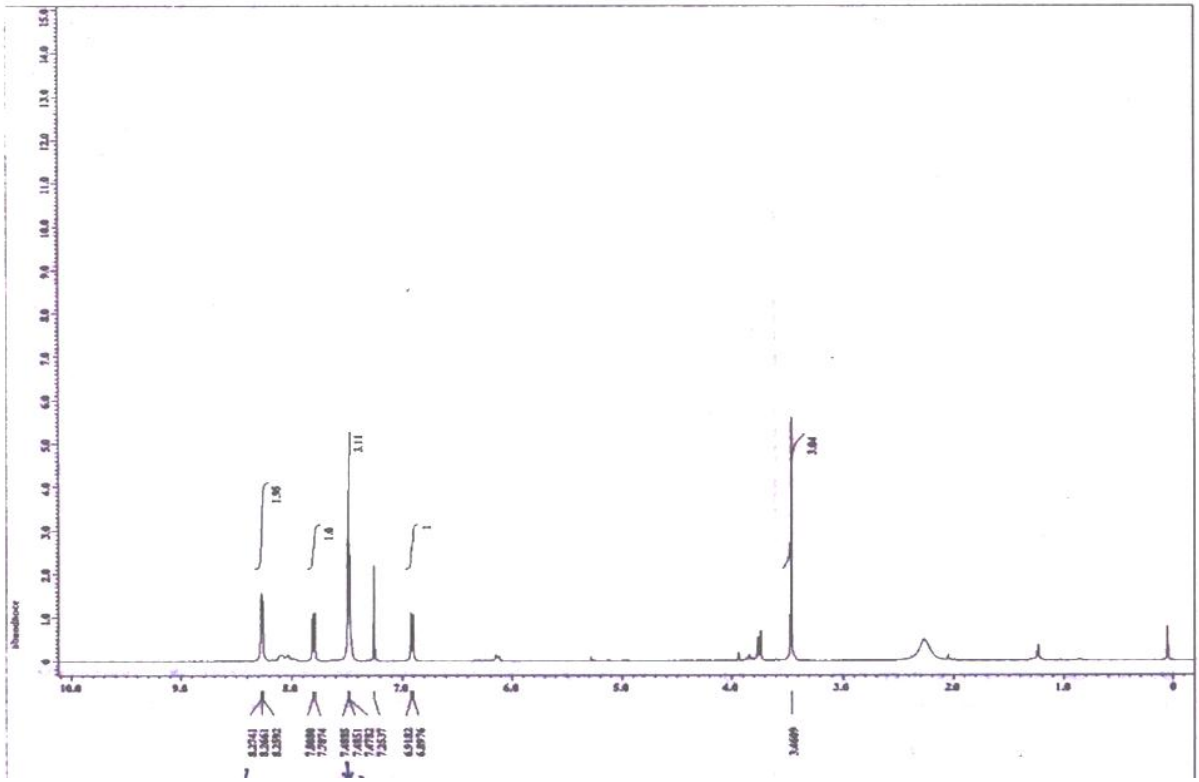

TAM 037

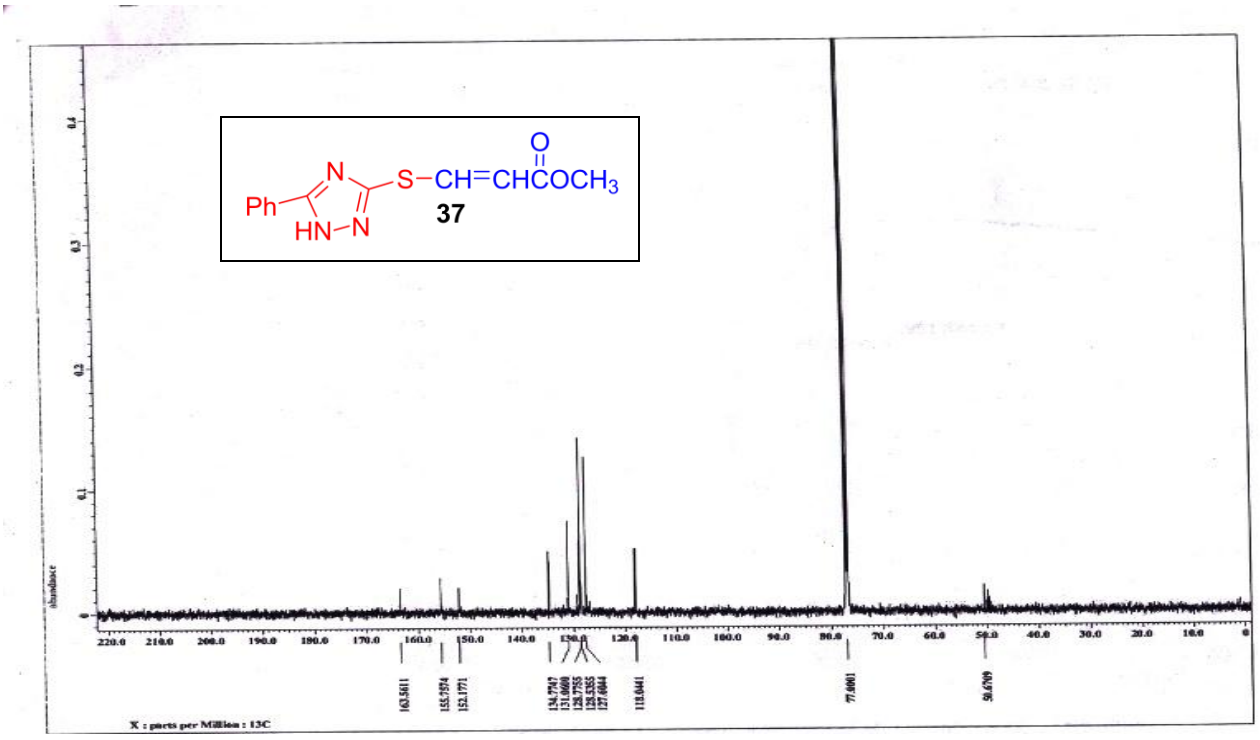

O
N
S–CH=CHCOCH3
HN–N
36
Abundance
X : parts per Million : 150
167.1595
165.6633
157.5140
155.1431
145.4197
145.3337
143.1064
141.9029
117.8042
117.7178
114.6655
77.0002
51.9284
51.7940
50.4118
29.6818

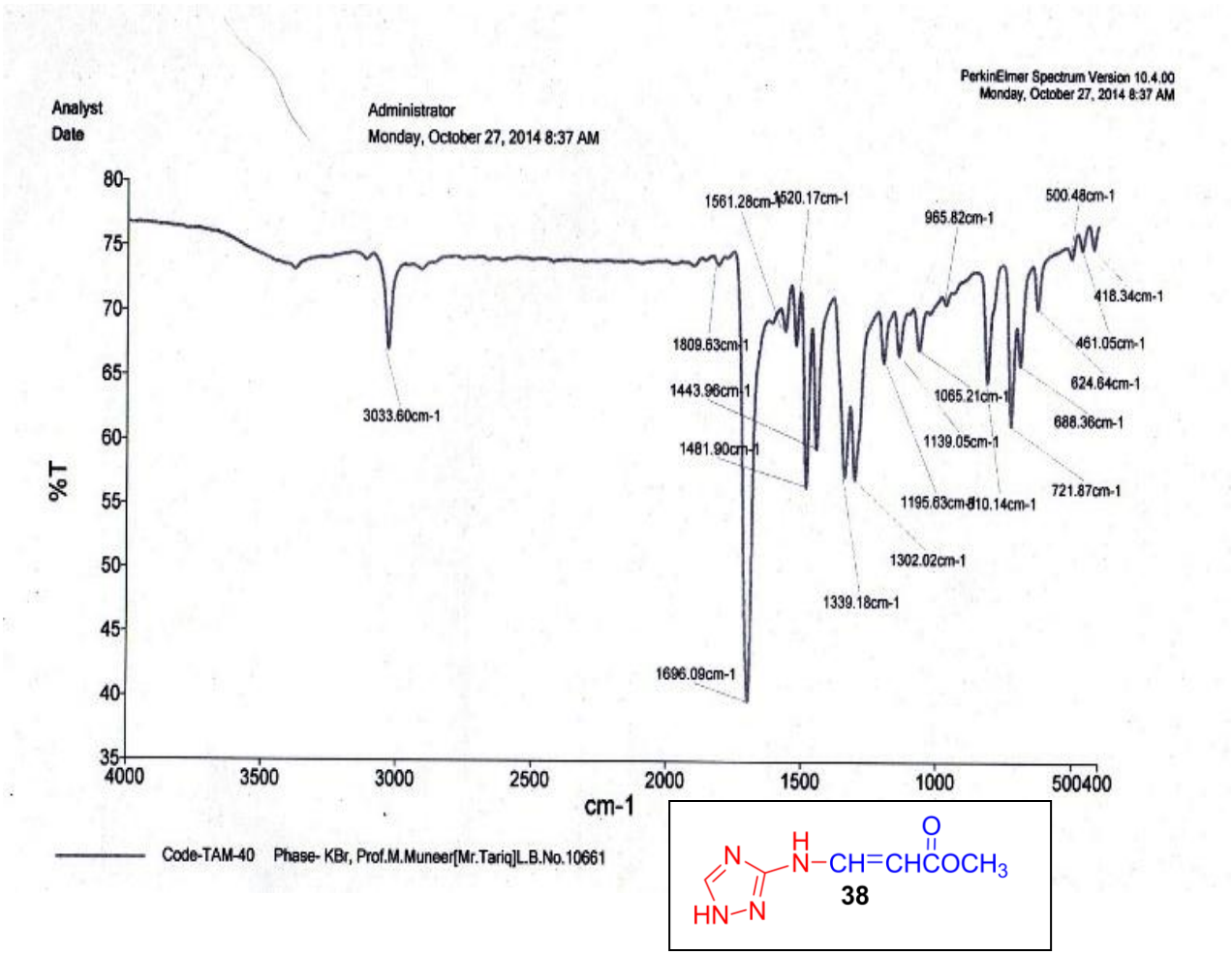

PerkinElmer Spectrum Version 10.4.00
Monday, October 27, 2014 8:32 AM
Analyst
Date
Administrator
Monday, October 27, 2014 8:32 AM
%T
cm-1
3256.19cm-1
3055.55cm-1
2951.82cm-1
1569.06cm-1
1683.17cm-1
1468.05cm-1
1442.38cm-1
1360.82cm-1
1331.22cm-1
1271.19cm-1
1229.01cm-1
1175.13cm-1
1008.20cm-1
939.70cm-1
798.18cm-1
719.28cm-1
667.62cm-1
Code- TAM-41 Phase- KBr, Prof.M.Muneer[Mr.Tariq]L.B.No.10662


Ph
HN
N
N
S
CH=CHCOCH3
O

37

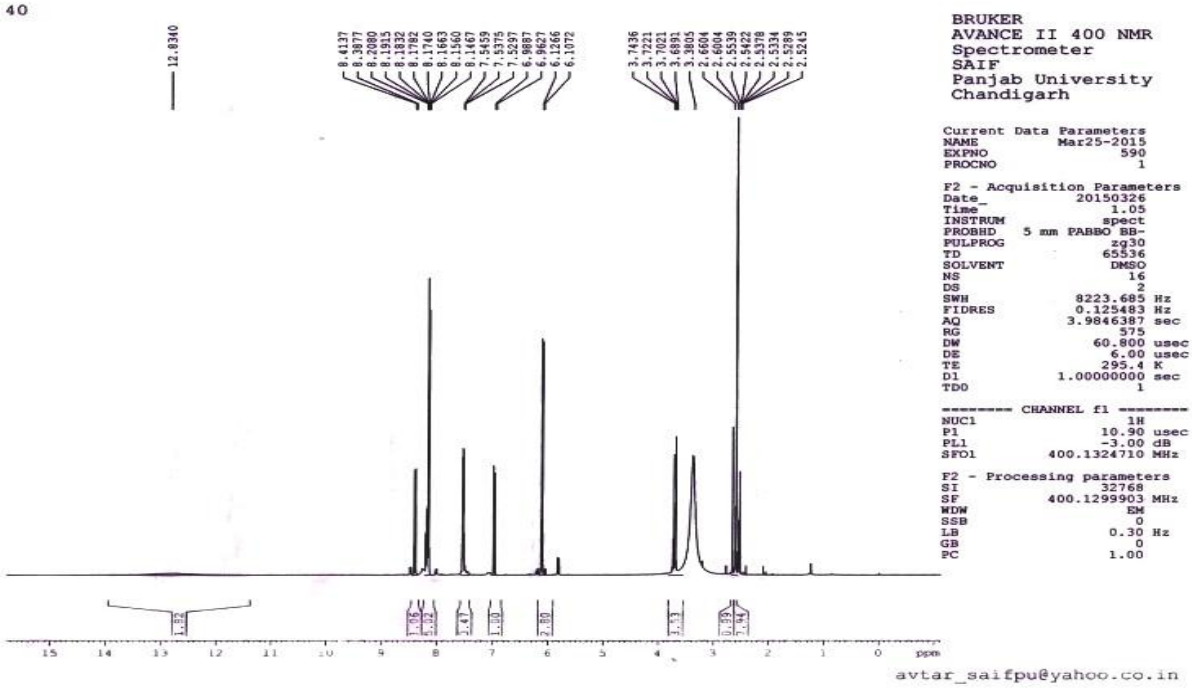



Ph
HN
N
N
S
CH=CHCOCH3
O
37
X : parts per Million : 13C

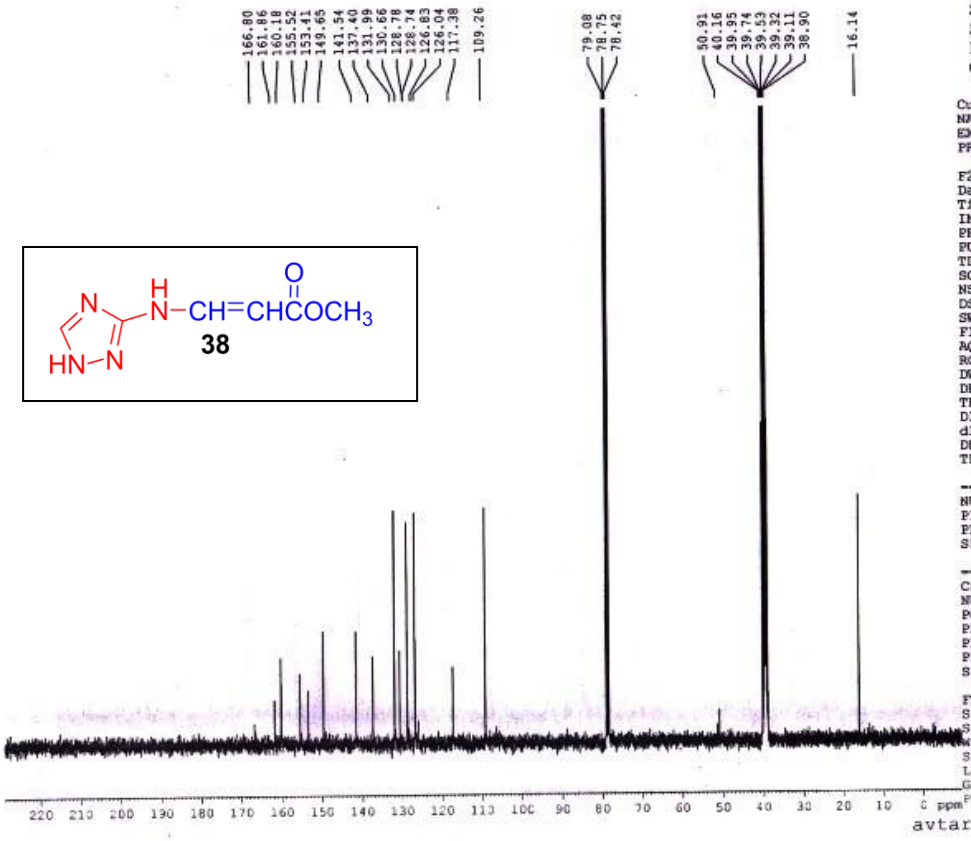

PerkinElmer Spectrum Version 10.4.00
Monday, October 27, 2014 8:37 AM
Analyst
Date
Administrator
Monday, October 27, 2014 8:37 AM
%T
cm-1
3033.60cm-1
1809.63cm-1
1561.28cm-1
1520.17cm-1
1443.96cm-1
1481.90cm-1
1696.09cm-1
1339.18cm-1
1302.02cm-1
1195.63cm-1
1139.05cm-1
1065.21cm-1
965.82cm-1
810.14cm-1
721.87cm-1
688.36cm-1
624.64cm-1
500.48cm-1
461.05cm-1
418.34cm-1
Code-TAM-40 Phase- KBr, Prof.M.Muneer[Mr.Tariq]L.B.No.10661

38

40


BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME Mar25-2015
EXPNO 590
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150326
Time 1.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 575
DW 60.800 usec
DE 6.00 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1299903 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
avtar_saifpu@yahoo.co.in

40

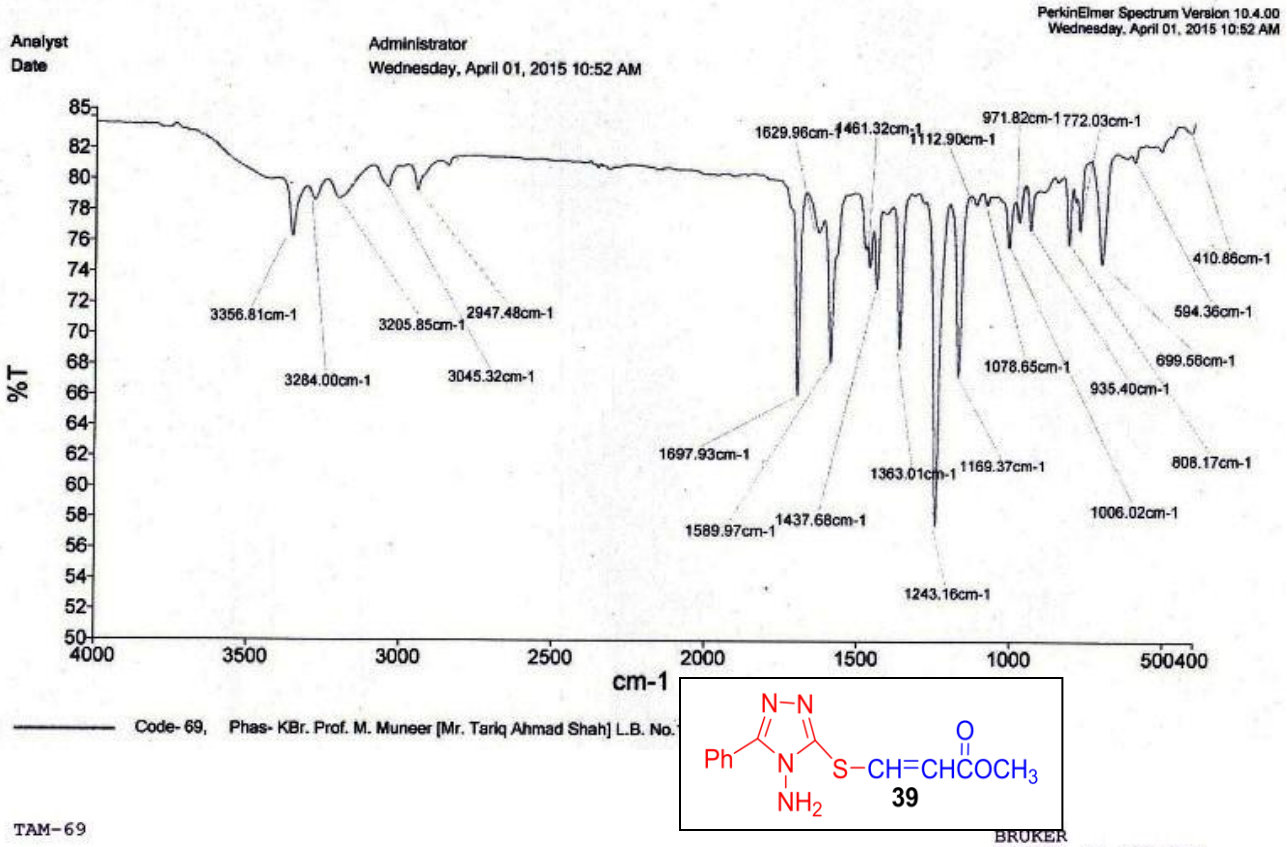


38

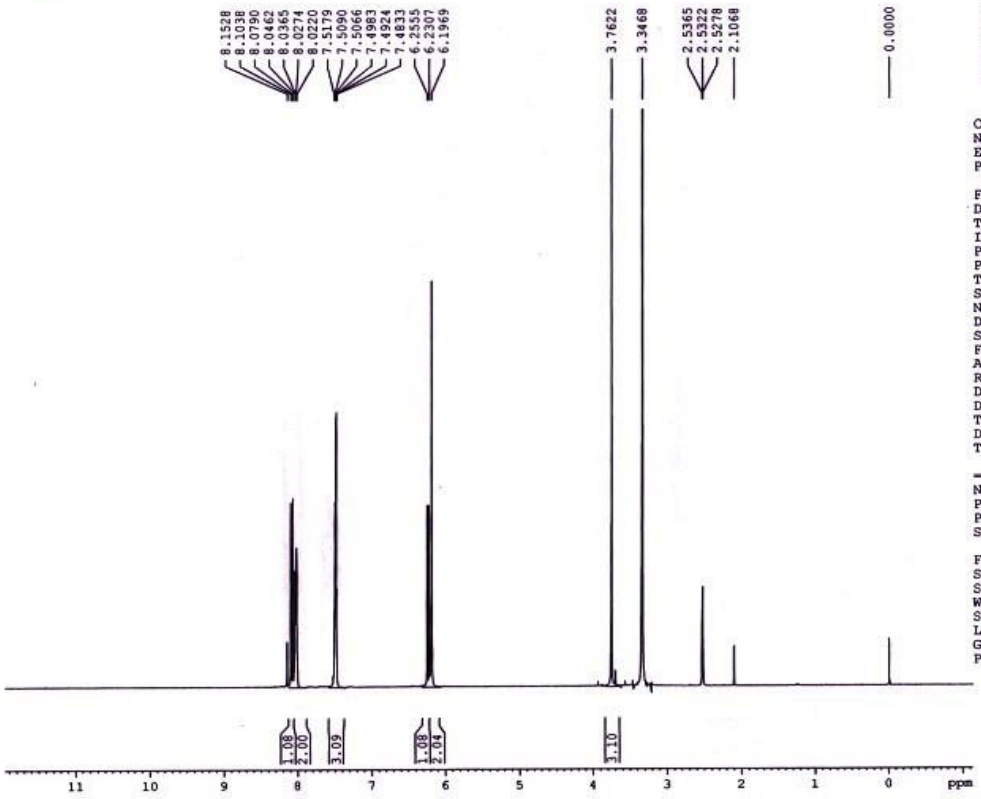
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters	
NAME	Mar25-2015
EXPNO	591
PROCNO	1
F2 - Acquisition Parameters	
Date_	20150326
Time	2.01
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	912
DW	16.800 usec
DE	6.00 usec
TE	295.5 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6128193 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

avtar_saifpu@yahoo.co.in



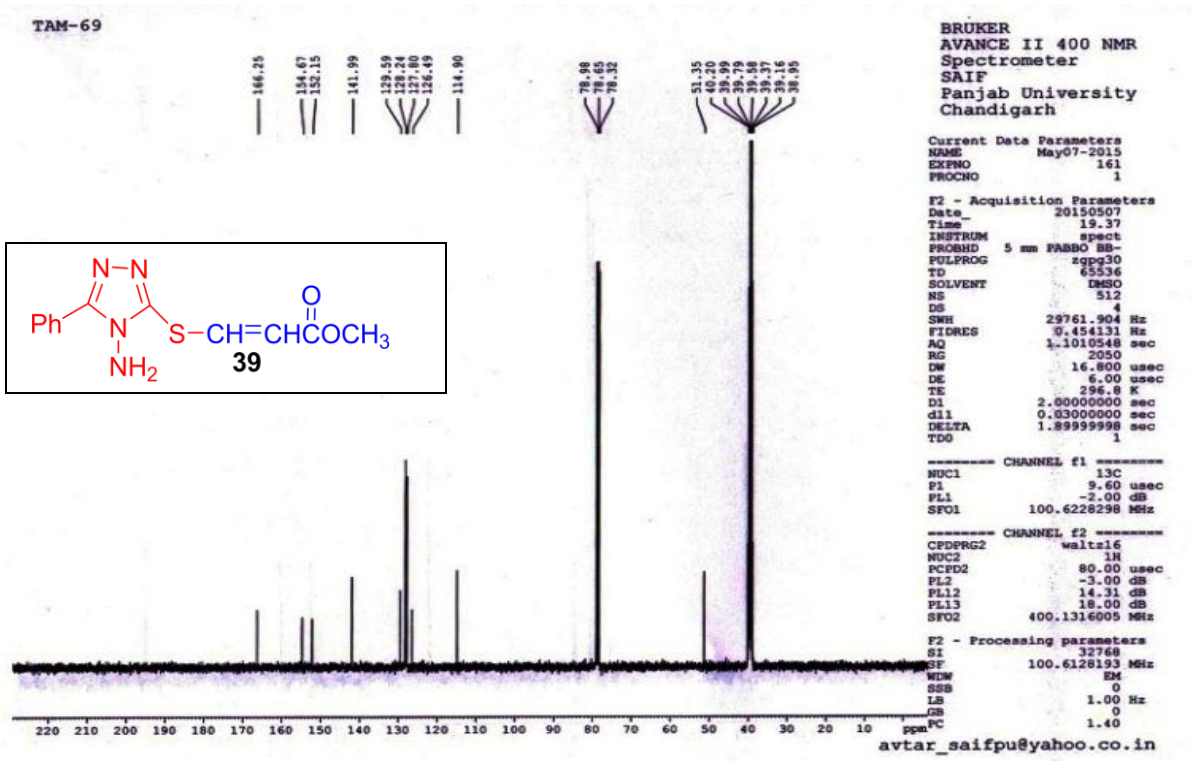
TAM-69

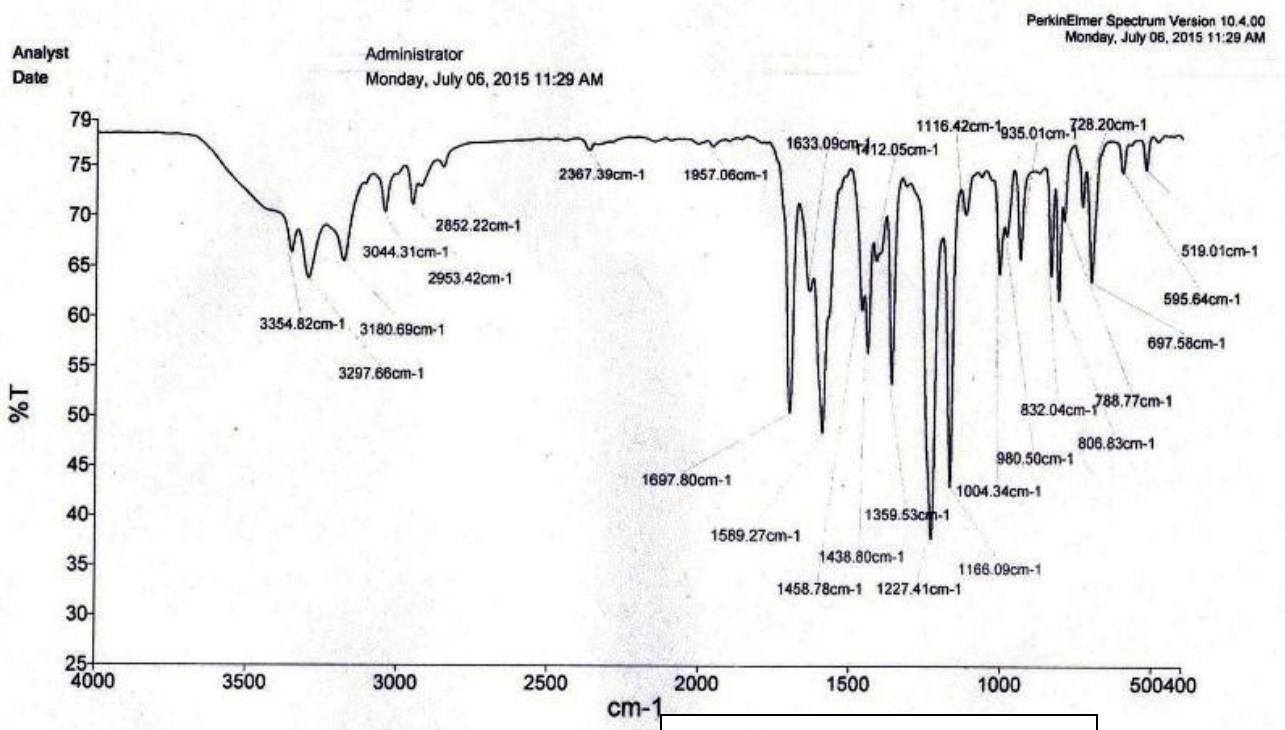


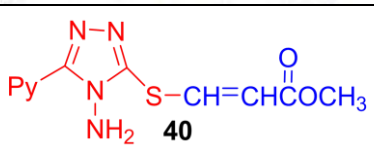
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters	
NAME	May07-2015
EXPNO	160
PROCNO	1
F2 - Acquisition Parameters	
Date_	20150507
Time	19.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	512
DW	41.600 usec
DE	6.00 usec
TE	296.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	32768
SF	400.1299909 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

avtar_saifpu@yahoo.co.in

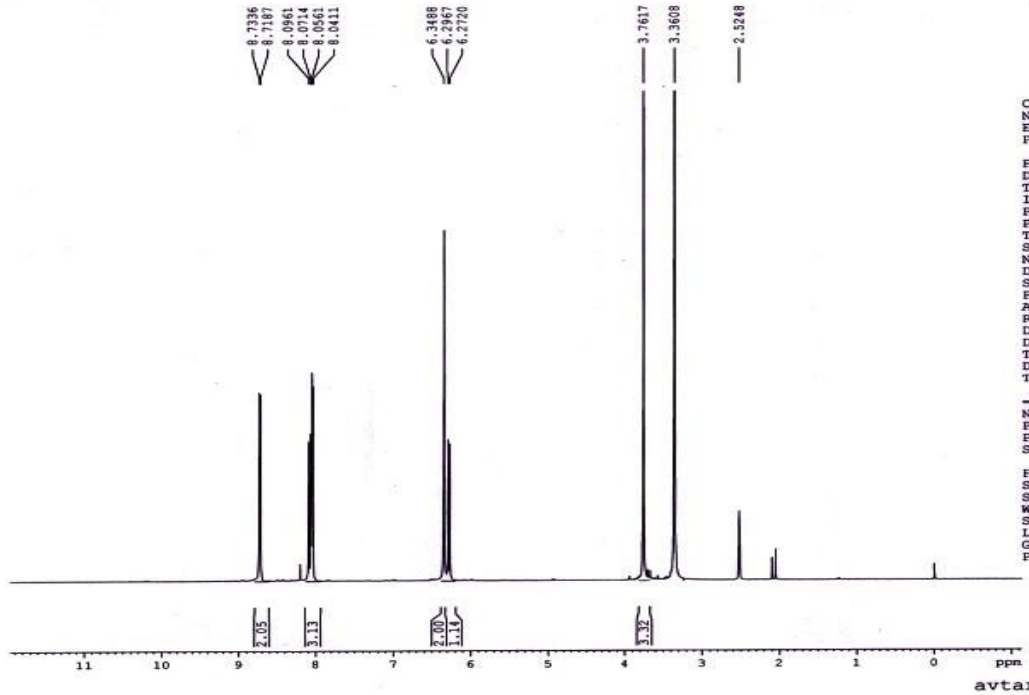

TAM-69
166.25
154.67
152.15
141.99
129.59
128.24
127.80
126.49
114.90
78.98
78.65
78.32
51.35
40.20
39.99
39.79
39.58
39.37
39.16
38.95
Ph
N–N
S–CH=CHCOCH3
NH2
O
39
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME May07-2015
EXPNO 161
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150507
Time 19.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.00 usec
TE 296.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
avtar_saifpu@yahoo.co.in





40

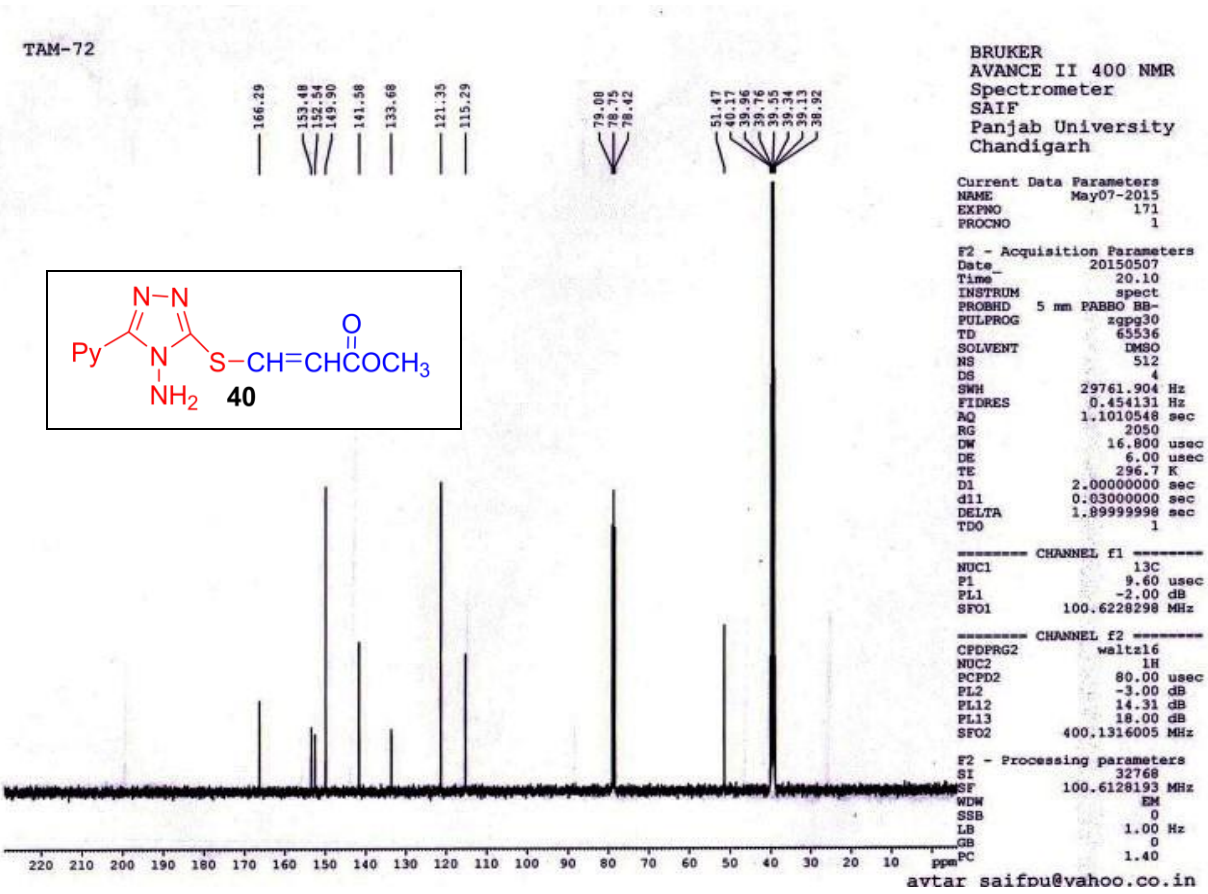
TAM-72

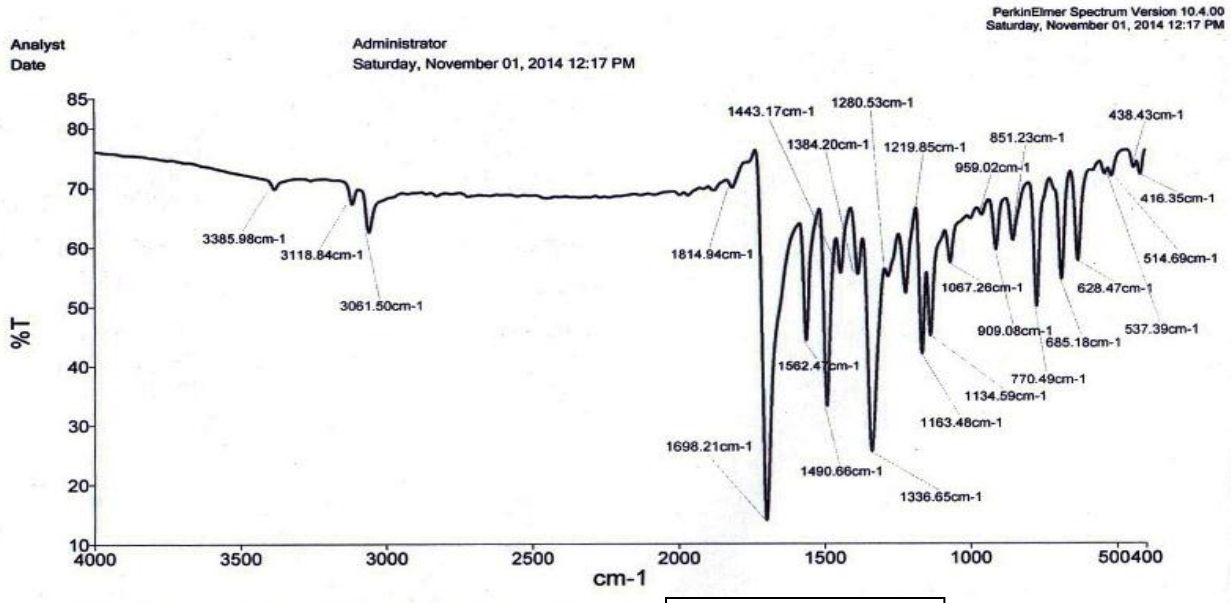


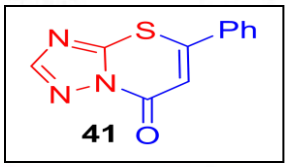
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters	
NAME	May07-2015
EXPNO	170
PROCNO	1
F2 - Acquisition Parameters	
Date_	20150507
Time	19.42
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	287
DW	41.600 usec
DE	6.00 usec
TE	296.5 K
D1	1.00000000 sec
TD0	1
-------- CHANNEL f1 --------	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	32768
SF	400.1299938 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

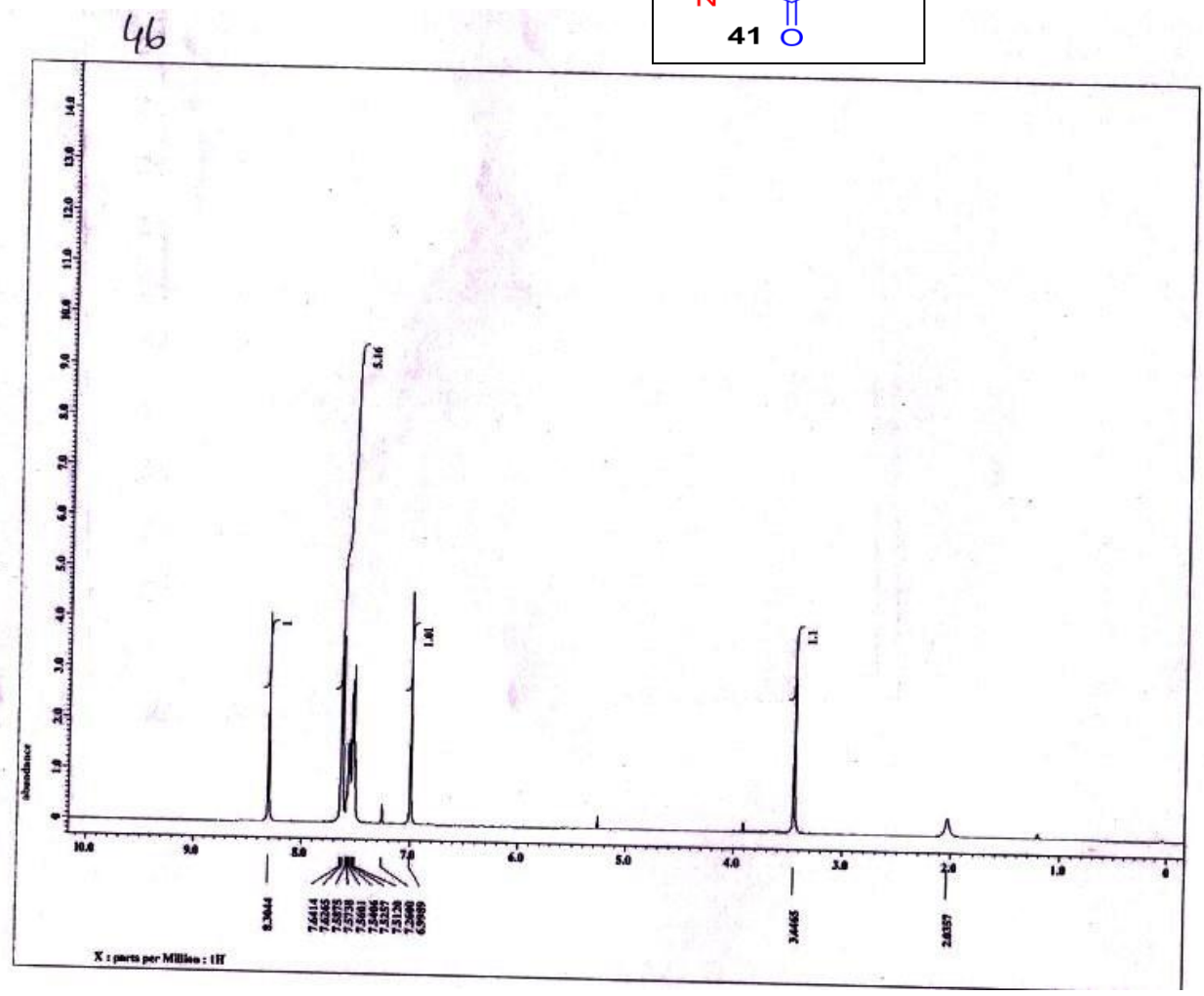
avtar_saifpu@yahoo.co.in

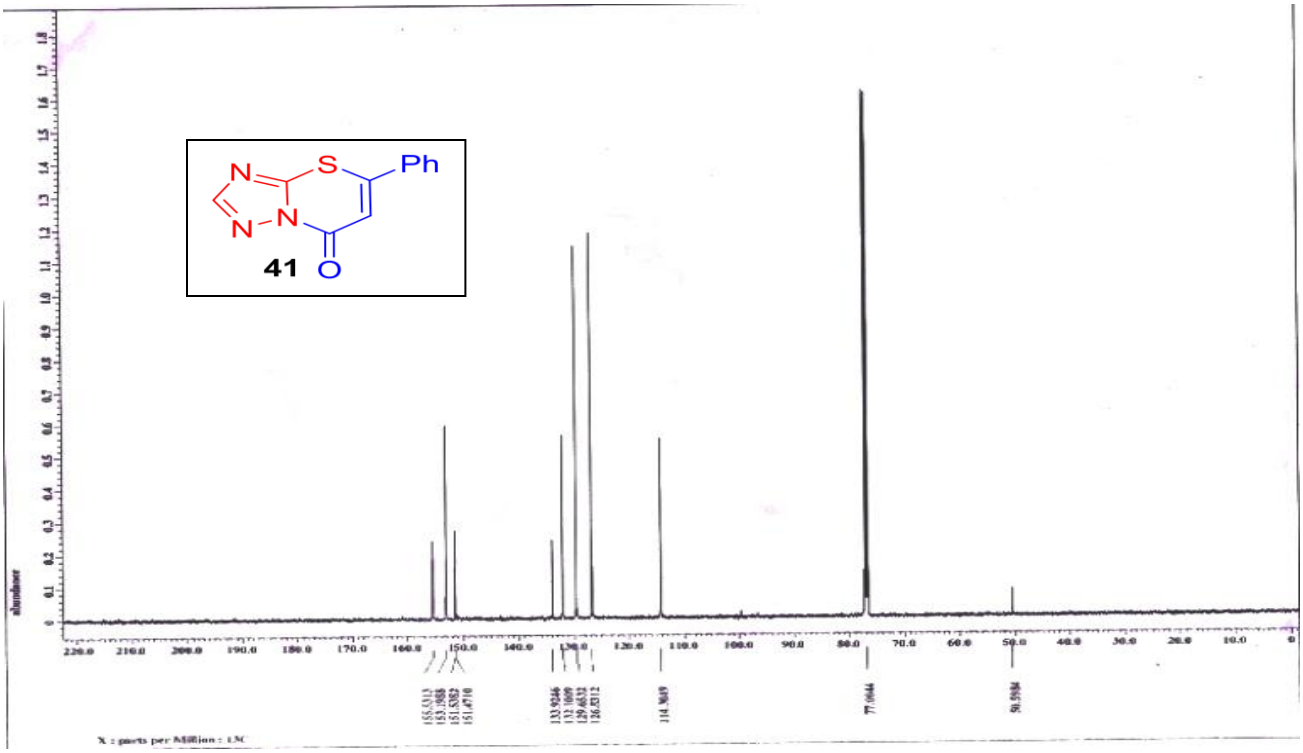

TAM-72
166.29
153.48
152.54
149.90
141.58
133.68
121.35
115.29
79.08
78.75
78.42
51.47
40.17
39.96
39.76
39.55
39.34
39.13
38.92
Py
N
N
NH2
S–CH=CHCOCH3
O
40
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME May07-2015
EXPNO 171
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150507
Time 20.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.00 usec
TE 296.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
avtar saifpu@yahoo.co.in

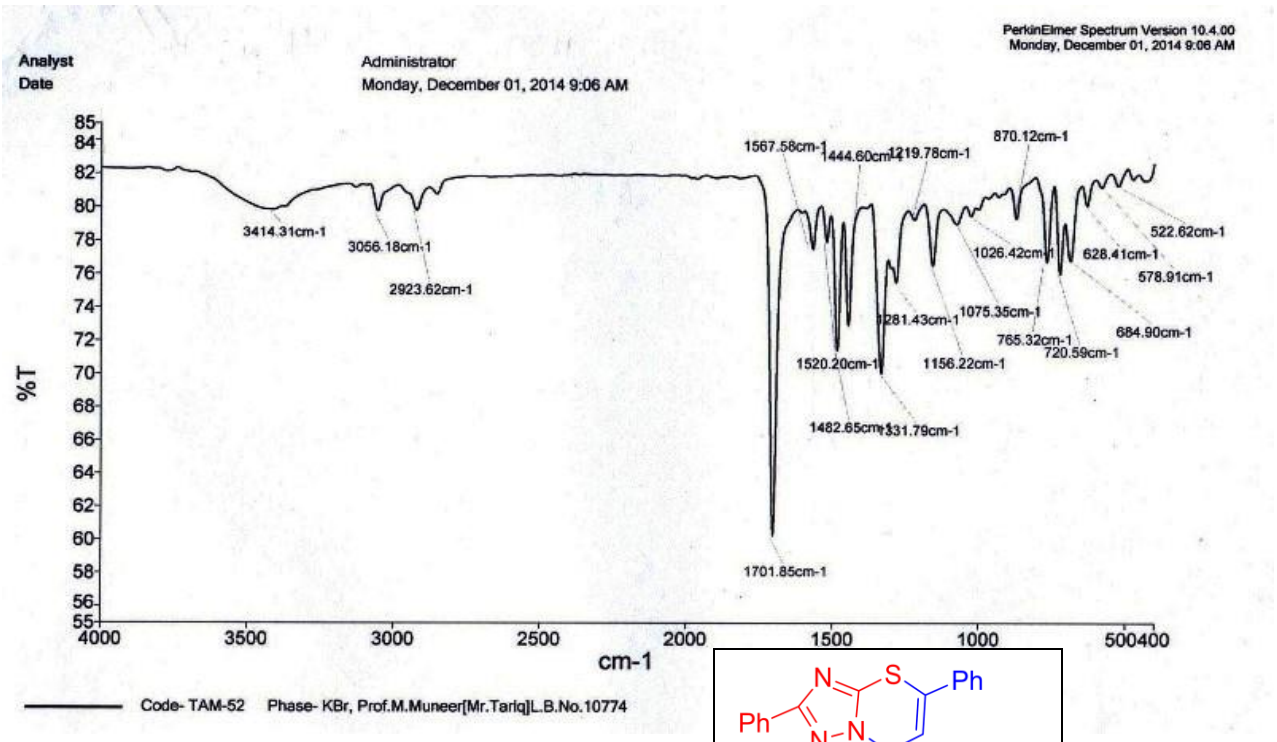

PerkinElmer Spectrum Version 10.4.00
Saturday, November 01, 2014 12:17 PM
Analyst
Date
Administrator
Saturday, November 01, 2014 12:17 PM
%T
cm-1
3385.98cm-1
3118.84cm-1
3061.50cm-1
1814.94cm-1
1443.17cm-1
1384.20cm-1
1280.53cm-1
1219.85cm-1
1698.21cm-1
1562.47cm-1
1490.66cm-1
1336.65cm-1
1163.48cm-1
1134.59cm-1
1067.26cm-1
959.02cm-1
851.23cm-1
770.49cm-1
685.18cm-1
909.08cm-1
628.47cm-1
537.39cm-1
514.69cm-1
438.43cm-1
416.35cm-1
Code- TAM 46 Phase- KBr, Prof.M.Muneer [Mr. Tariq]L.B.No.10687


N
S
Ph
N
N
O

41

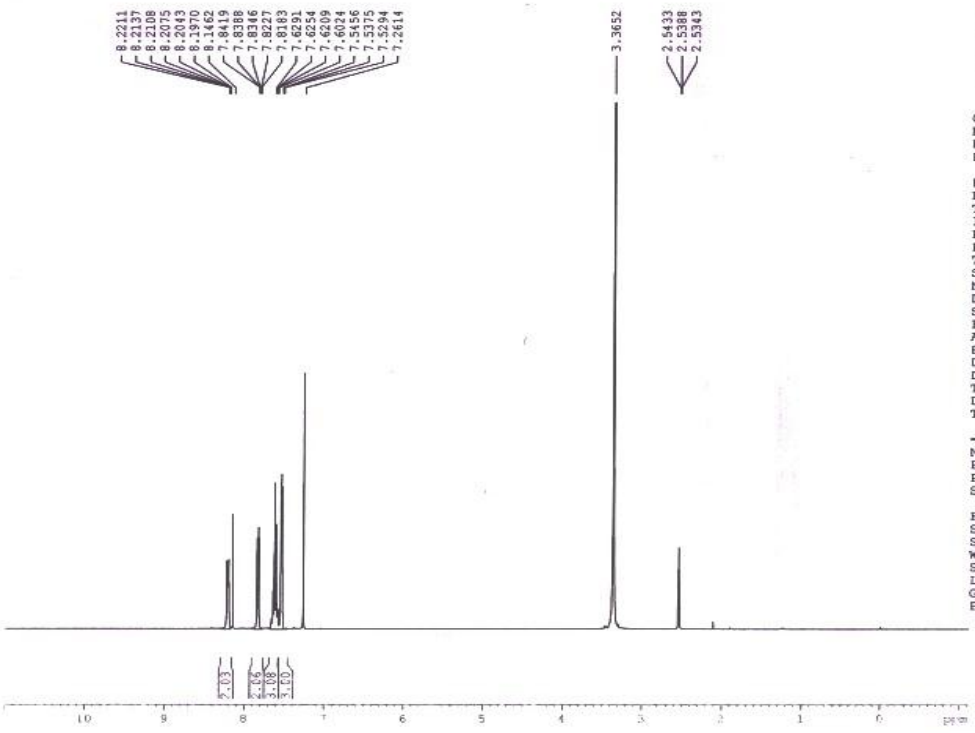

46
5.16
1.01
1.1
1
8.3044
7.6414
7.6245
7.5875
7.5739
7.5681
7.5466
7.5357
7.5139
7.3760
6.9989
3.4465
2.0357
X : parts per Million : 1H


N
S
Ph
N
N
O
41



42

52



AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters

NAME	Mar25-2015
EXPNO	21
PROCNO	1

F2 - Acquisition Parameters

Date_	20150326
Time	4.11
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	322
DW	41.600 usec
DE	6.00 usec
TE	295.4 K
D1	1.00000000 sec
TD0	1

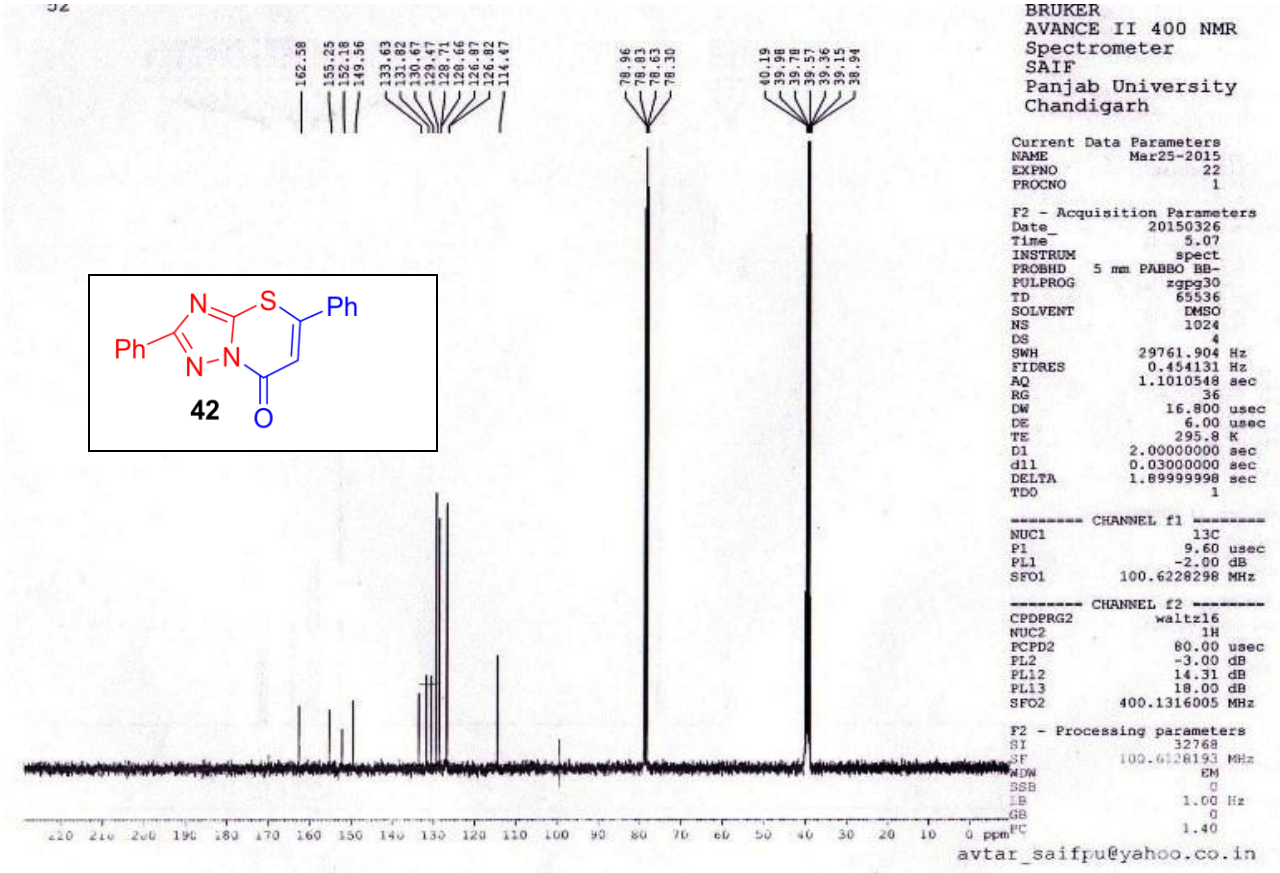
-------- CHANNEL f1 --------

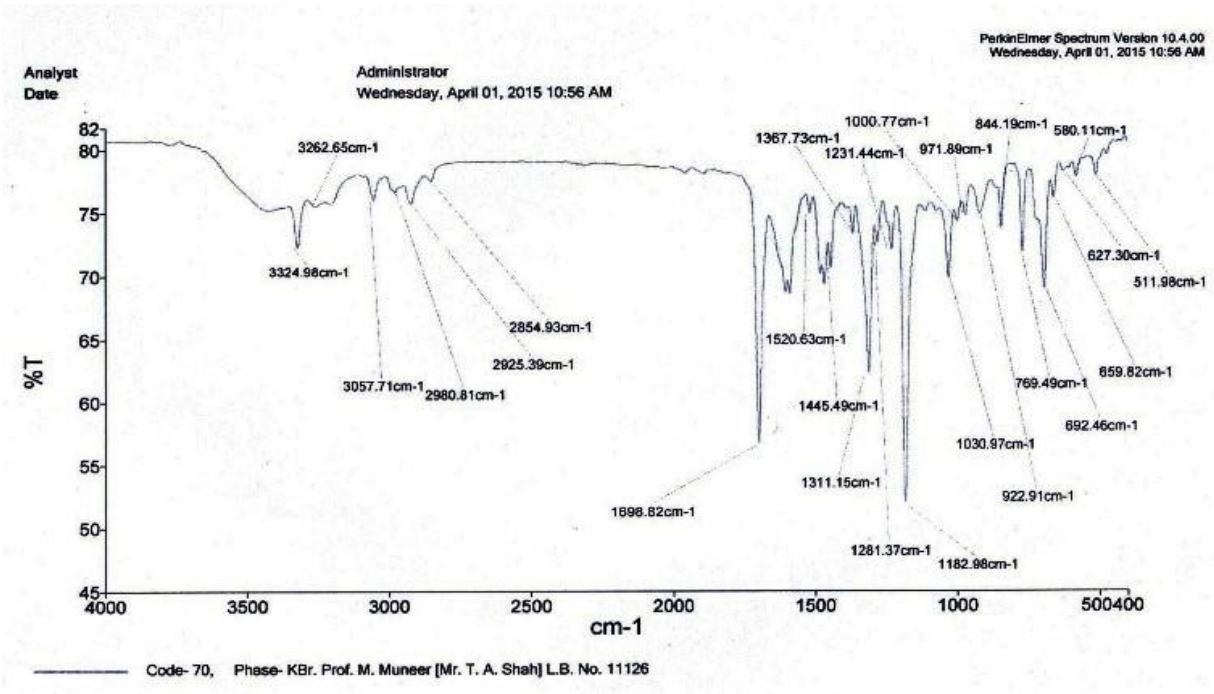
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz

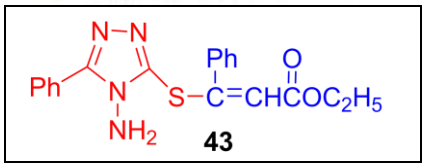
F2 - Processing parameters

SI	32768
SF	400.1299883 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

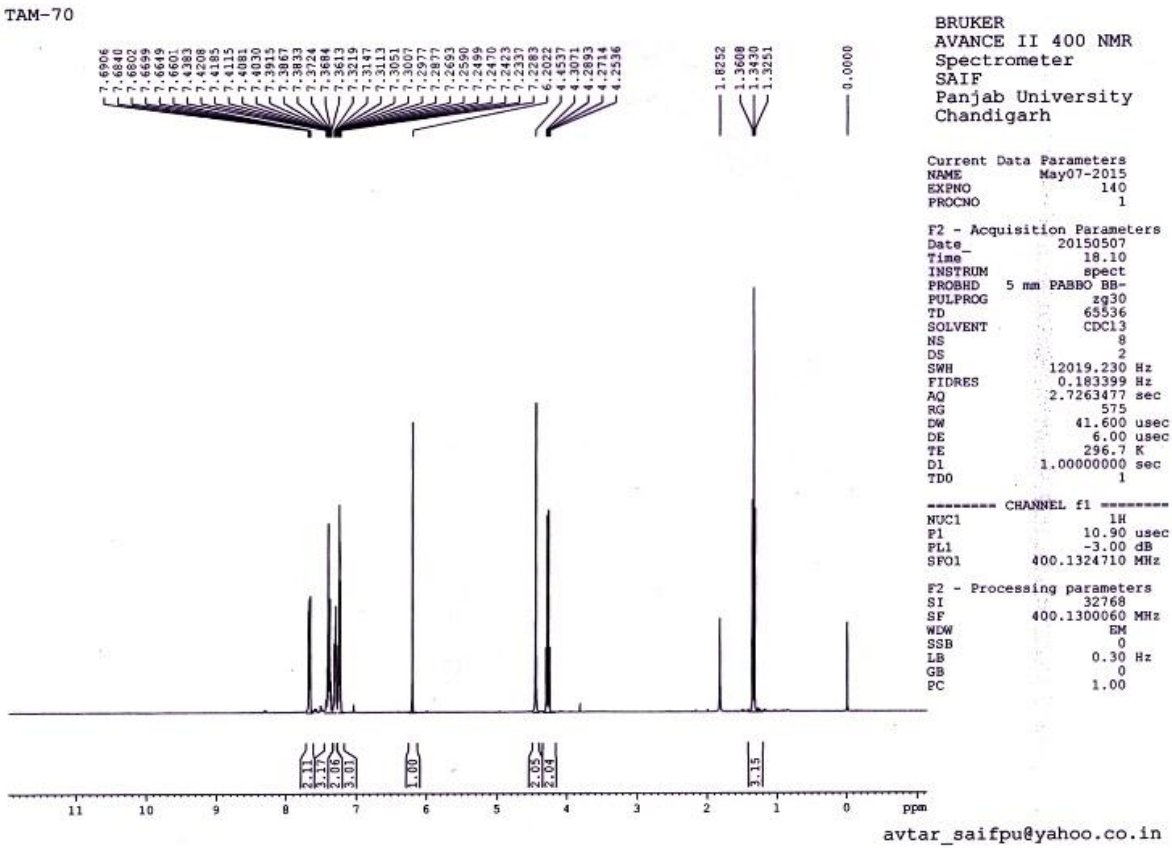
avtar saifpu@yahoo.co.in

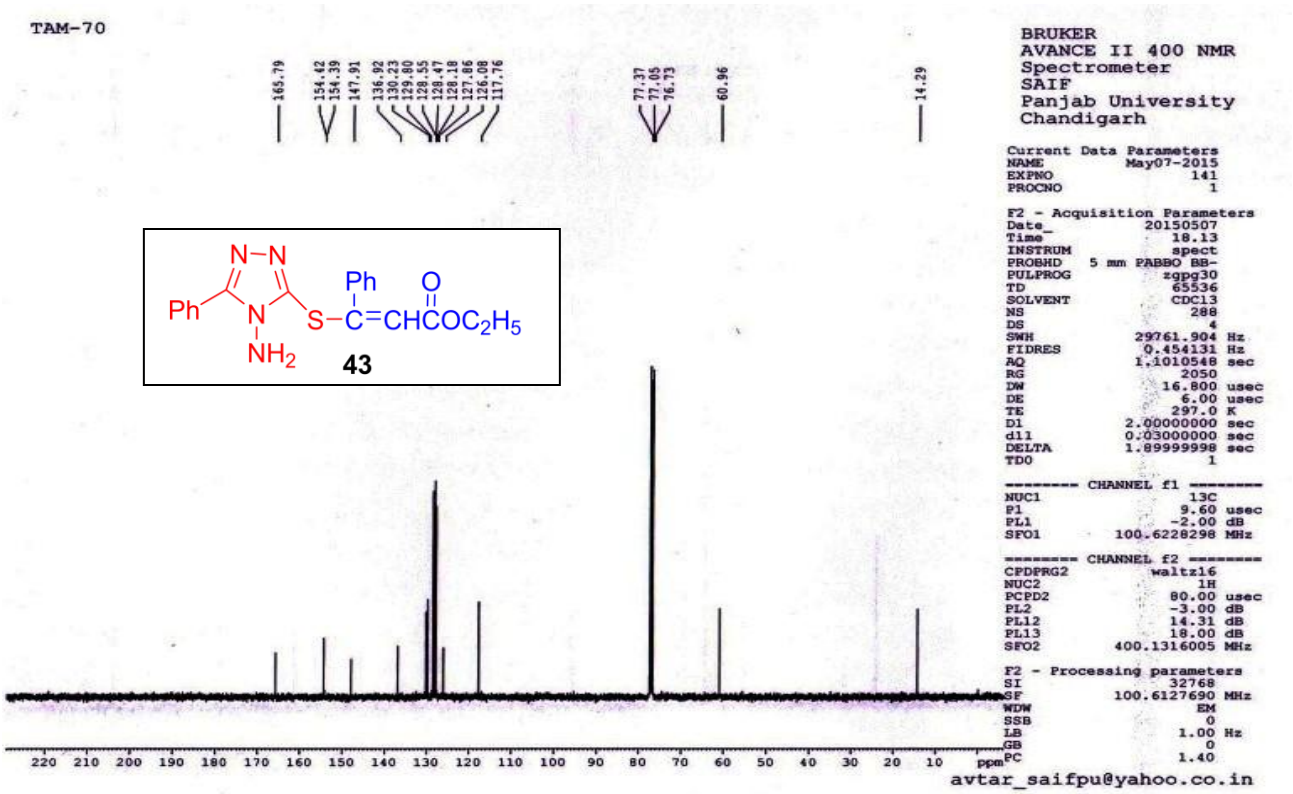

162.58
155.25
152.18
149.56
133.63
131.82
130.67
129.47
128.71
128.66
126.87
126.82
114.47
78.96
78.83
78.63
78.30
40.19
39.98
39.78
39.57
39.36
39.15
38.94
Ph
Ph
N
S
N
N
O
42
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME Mar25-2015
EXPNO 22
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150326
Time 5.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
avtar_saifpu@yahoo.co.in

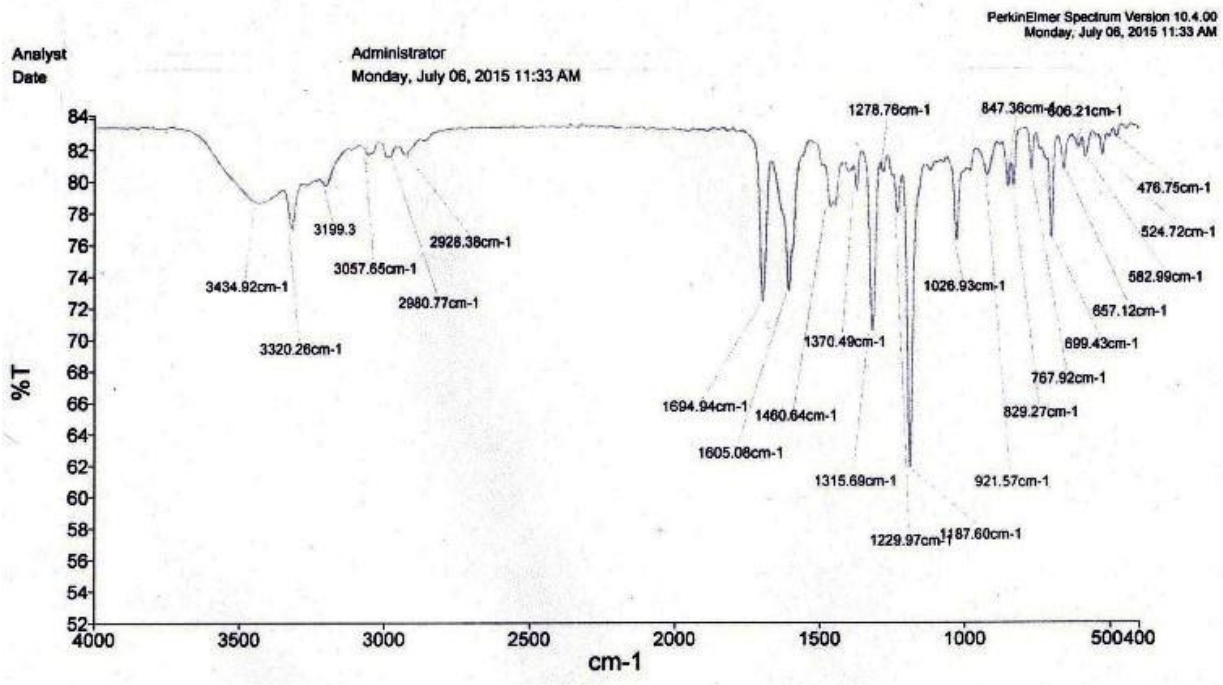

PerkinElmer Spectrum Version 10.4.00
Wednesday, April 01, 2015 10:56 AM
Analyst
Date
Administrator
Wednesday, April 01, 2015 10:56 AM
%T
cm-1
3262.65cm-1
3324.98cm-1
3057.71cm-1
2980.81cm-1
2925.39cm-1
2854.93cm-1
1898.82cm-1
1520.63cm-1
1445.49cm-1
1367.73cm-1
1311.15cm-1
1281.37cm-1
1231.44cm-1
1182.98cm-1
1000.77cm-1
971.89cm-1
1030.97cm-1
922.91cm-1
844.19cm-1
769.49cm-1
692.46cm-1
659.82cm-1
627.30cm-1
580.11cm-1
511.98cm-1
Code- 70, Phase- KBr. Prof. M. Muneer [Mr. T. A. Shah] L.B. No. 11126

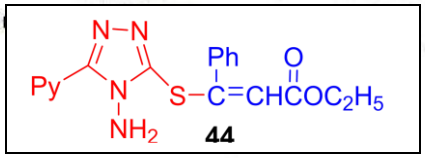

N–N
Ph
Ph
N
S–C=CHCOC2H5
NH2
O

43

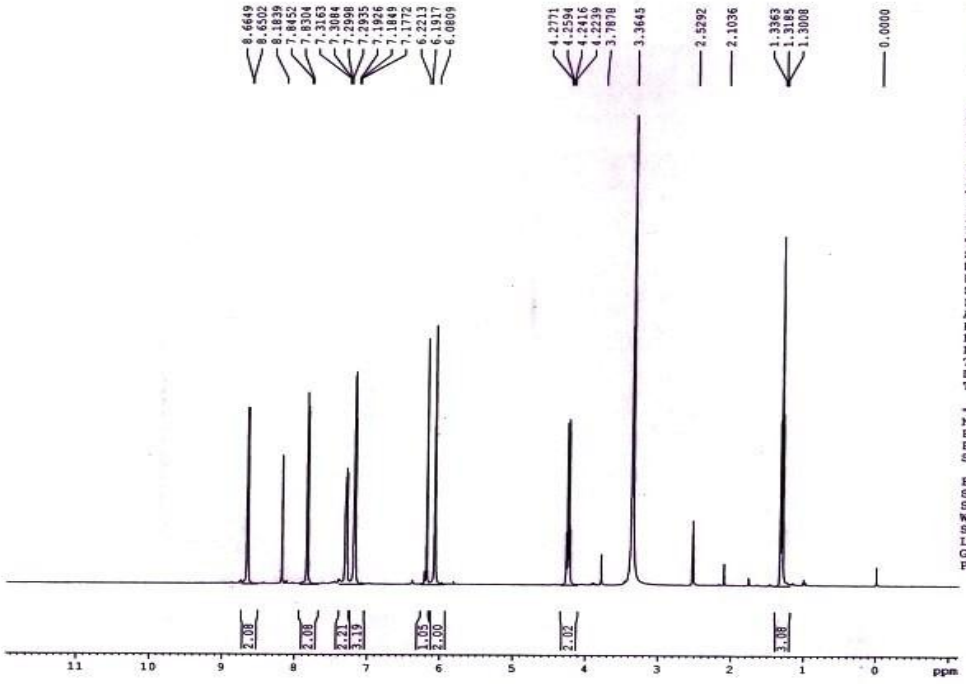

TAM-70
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME May07-2015
EXPNO 140
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150507
Time 18.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 575
DW 41.600 usec
DE 6.00 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm
avtar_saifpu@yahoo.co.in


TAM-70
165.79
154.42
154.39
147.91
136.92
130.23
129.80
128.55
128.47
128.18
127.86
126.08
117.76
77.37
77.05
76.73
60.96
14.29
Ph
N–N
N
NH2
S–C=CHCOC2H5
Ph
O
43
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME May07-2015
EXPNO 141
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150507
Time 18.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 288
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.00 usec
TE 297.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
avtar_saifpu@yahoo.co.in





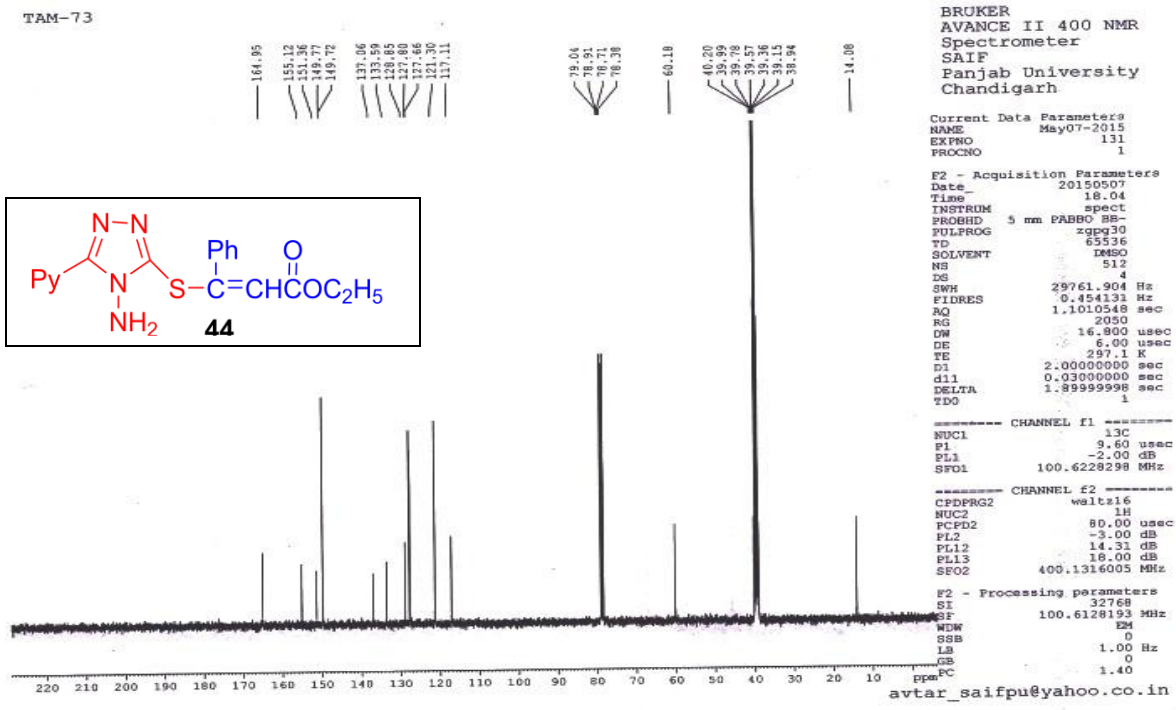
TAM-73



BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters	
NAME	May07-2015
EXPNO	130
PROCNO	1
F2 - Acquisition Parameters	
Date_	20150507
Time	17.35
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	287
DW	41.600 usec
DE	6.00 usec
TE	296.7 K
D1	1.00000000 sec
TD0	1
-------- CHANNEL f1 --------	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	32768
SF	400.1299921 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

avtar_saifpu@yahoo.co.in


TAM-73
164.95
155.12
151.36
149.77
149.72
137.06
133.59
128.85
128.60
127.66
121.30
117.11
79.04
78.91
78.71
78.38
60.18
40.20
39.99
39.78
39.57
39.36
39.15
38.94
14.08
N–N
Py
N
S–C=CHCOC2H5
Ph
O
NH2
44
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME May07-2015
EXPNO 131
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150507
Time 18.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.00 usec
TE 297.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
avtar_saifpu@yahoo.co.in

References

1. Lutz, R.E.; Smithey, W. R. *J. Org. Chem*. **1951**, 16, 51.

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