Supplementary data for publication on line

Coordination variability of Cu^{I} in multidonor heterocyclic thioamides : synthesis, crystal structures, luminescent properties and ESI-mass studies of complexes

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ESI-Mass data of complexes

Complex. 1. Complete spectrum

Complex 1 $Cu(pyms)(PPh_3)_2$ $C_{40}H_{33}N_2CuP_2S$

m.wt: 699.24

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Analysis Info

Analysis Name	D:\Data\user data\TS LOBANA\AMS-18.d	Acquisition Date	7/13/2013 7:53:20 PM
Method	tune_wide.m	Operator	RAJESH VASHISTH
Sample Name		Instrument	micrOTOF-Q II 10356
Comment			

Acquisition Parameter

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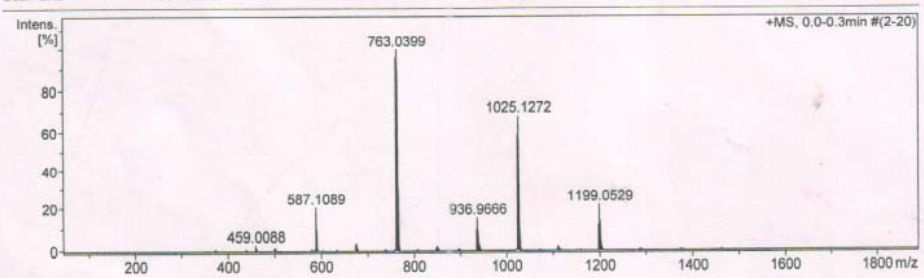
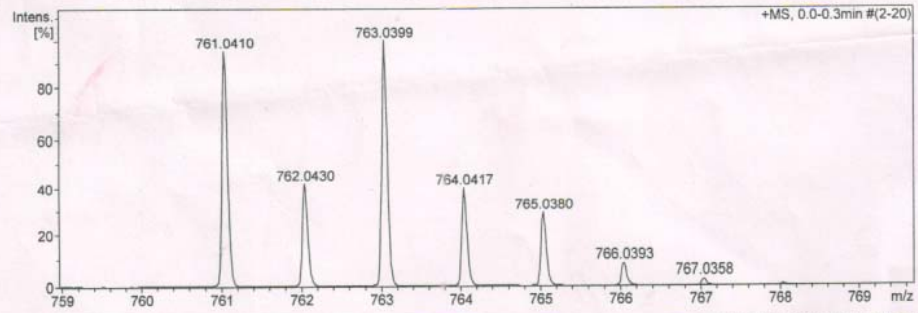
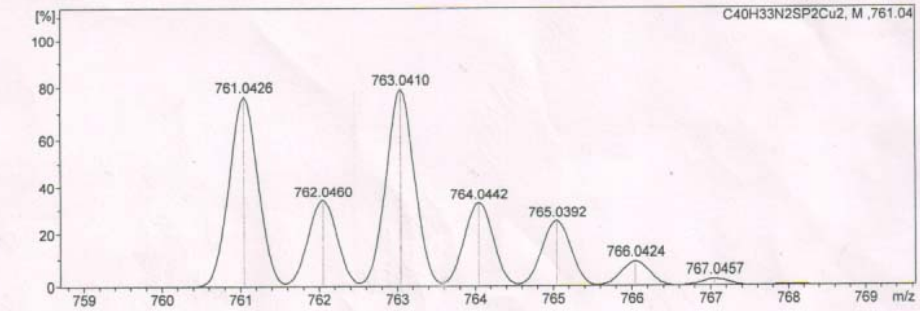
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste







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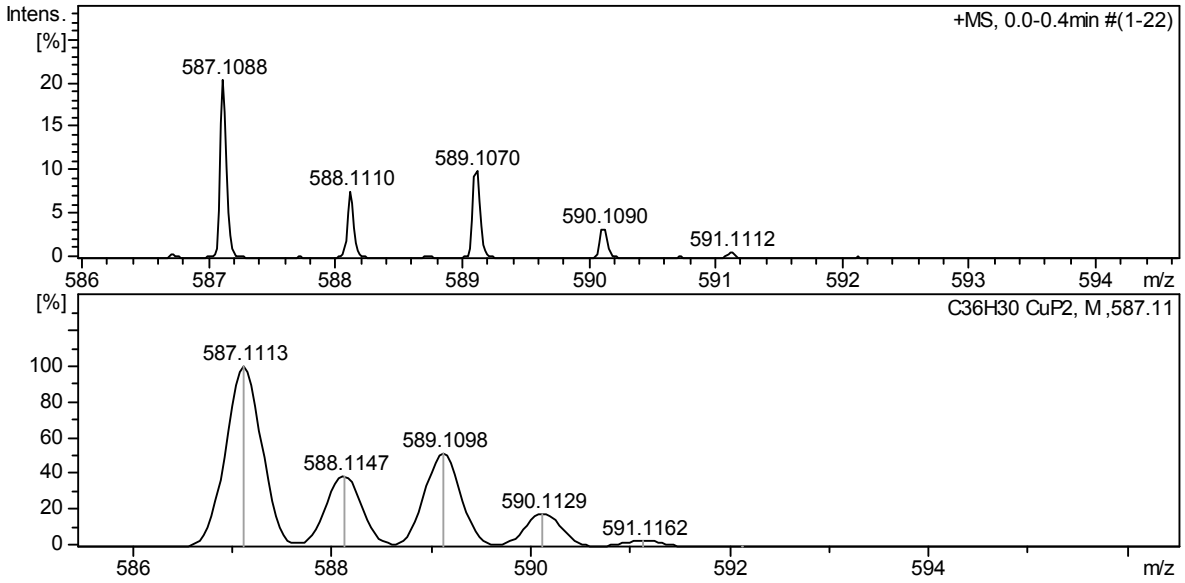
m/z observed 587.1- isotopic pattern



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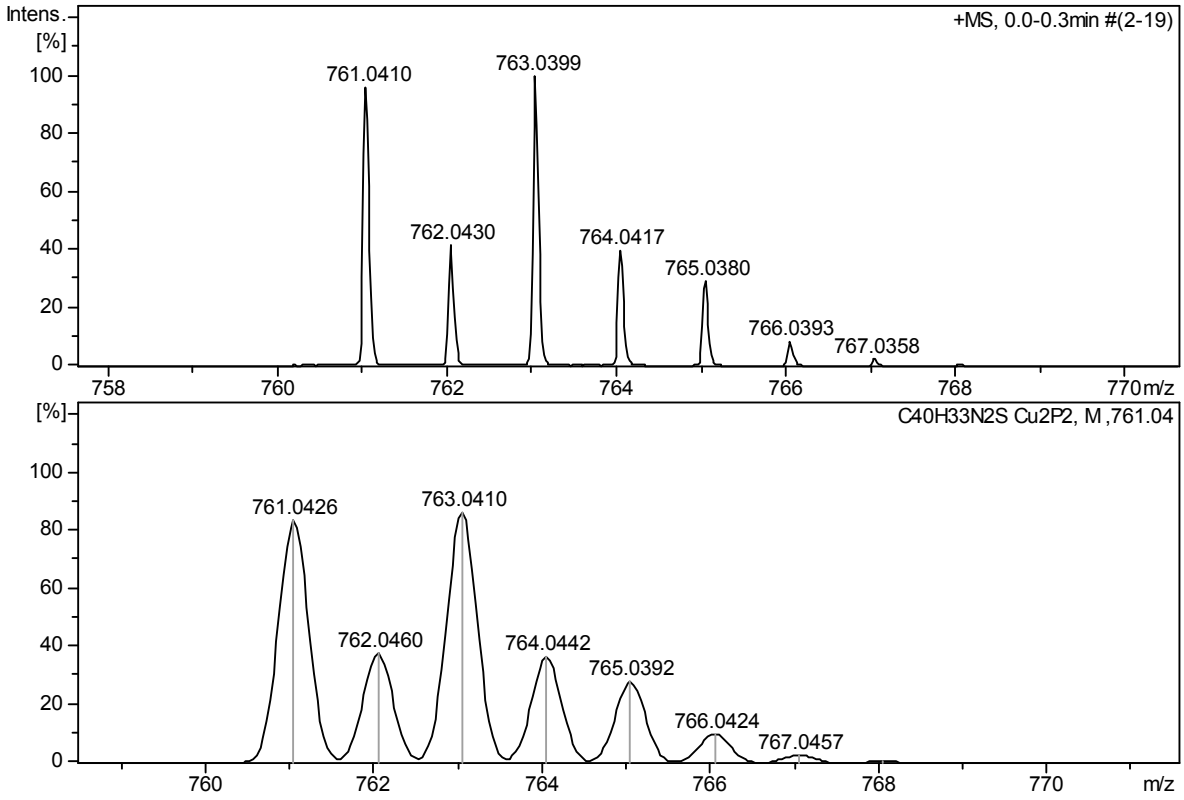

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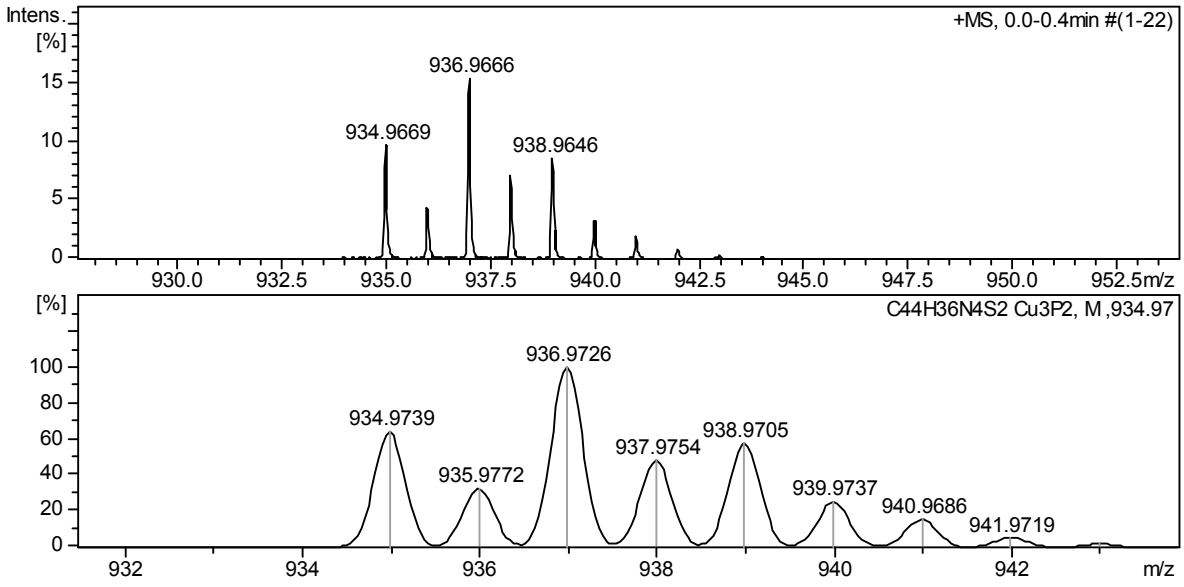

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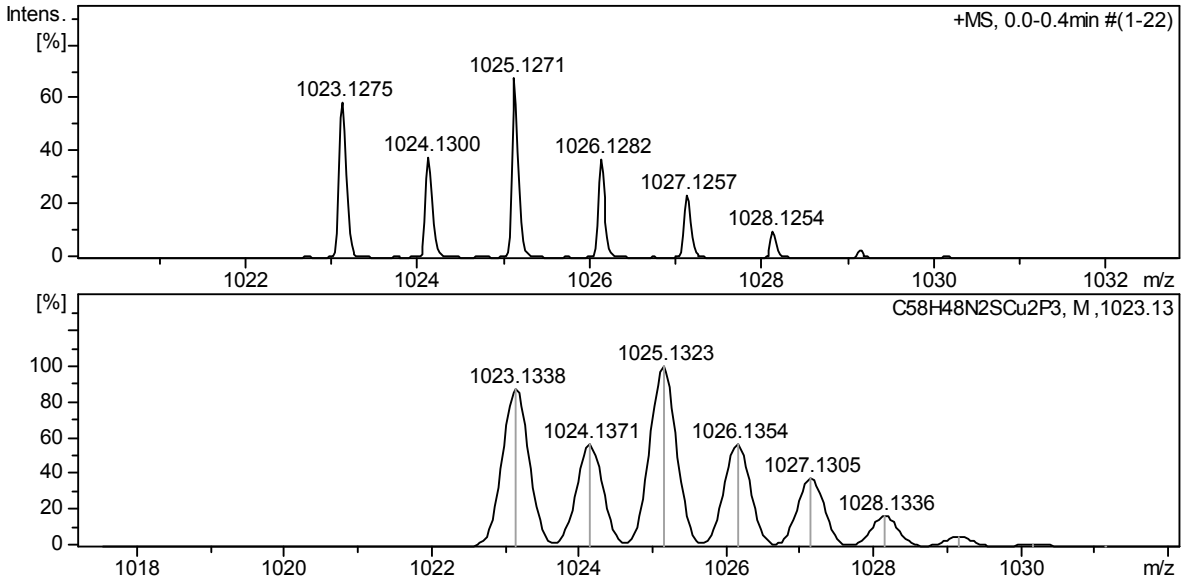

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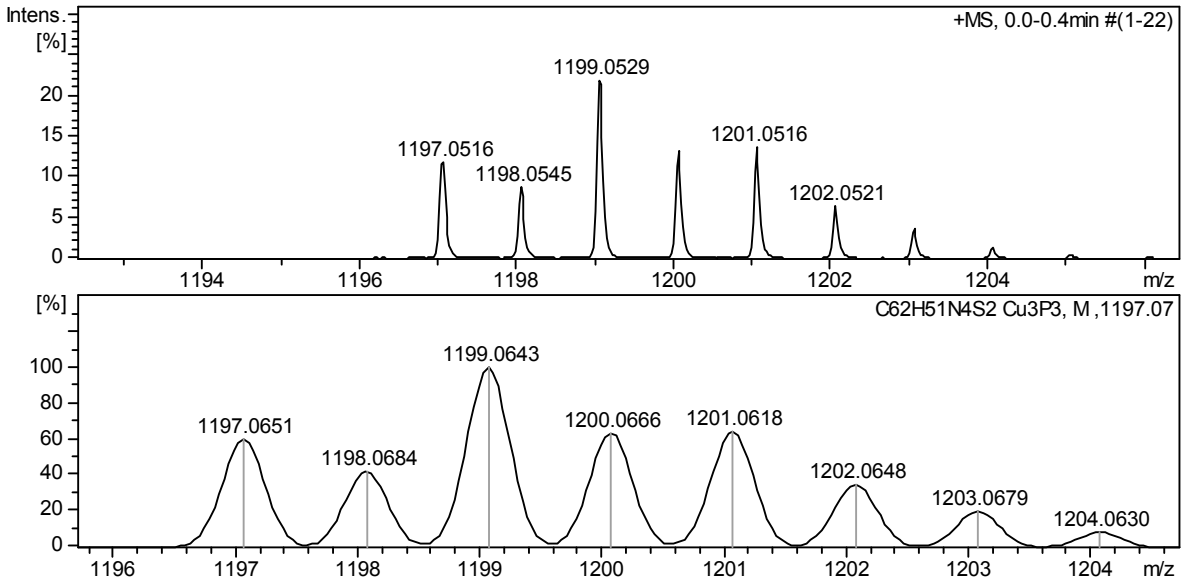

Complex 2 : Complete spectrum

$C_{42}H_{37}N_4OCuP_2S$ $Cu(pmss)(PPh_3)_2$

Mwt: 771

complex 2.

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Analysis Info

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Method	tune_wide.m	Operator	RAJESH VASHISTH
Sample Name	sh-35	Instrument	micrOTOF-Q II 10356
Comment			

Acquisition Parameter

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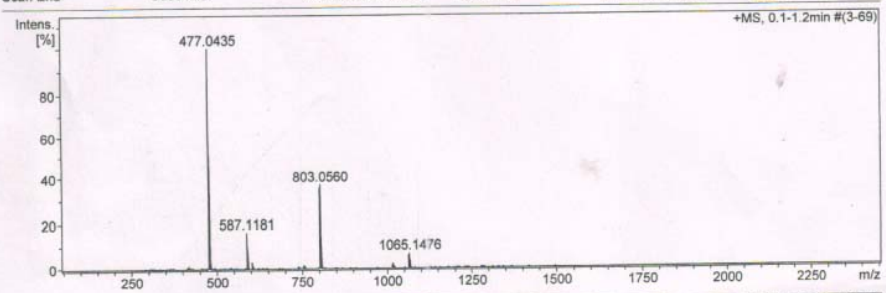
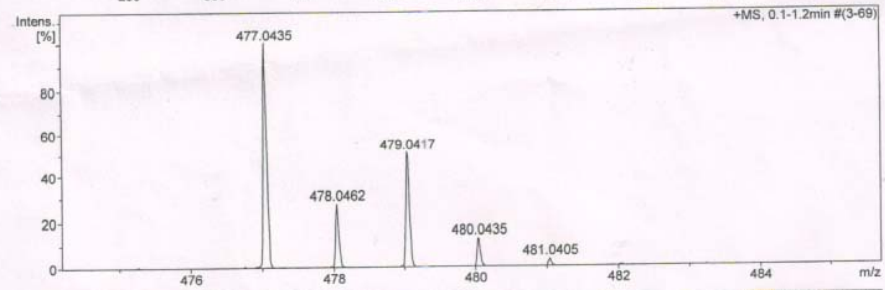
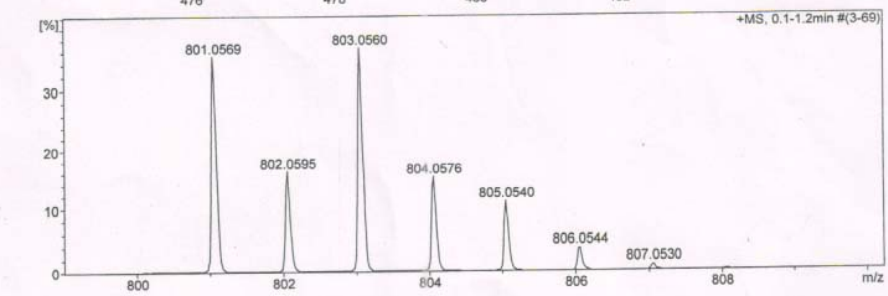
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste







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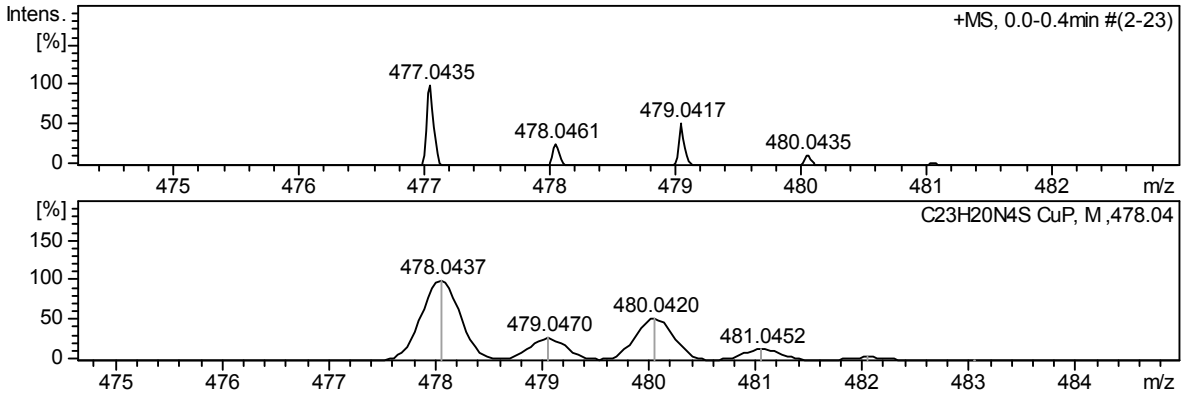
m/z observed 477.0- isotopic pattern



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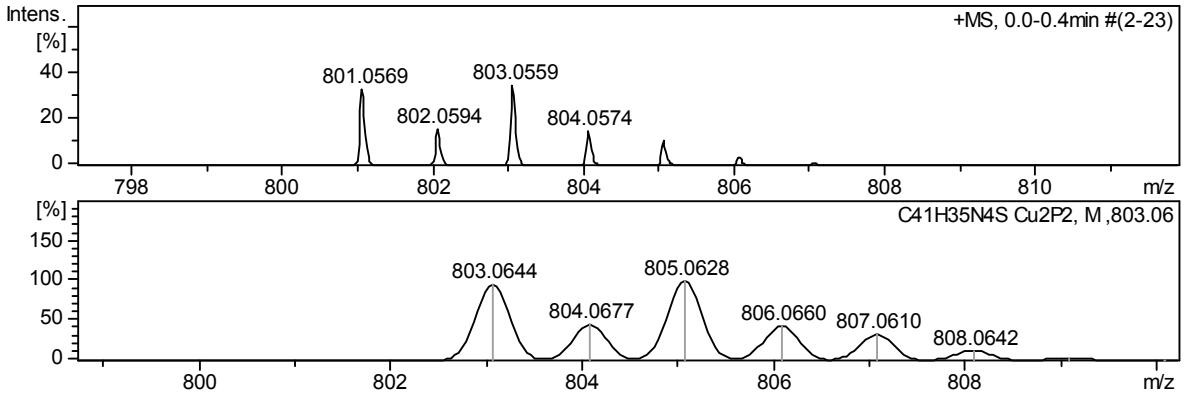

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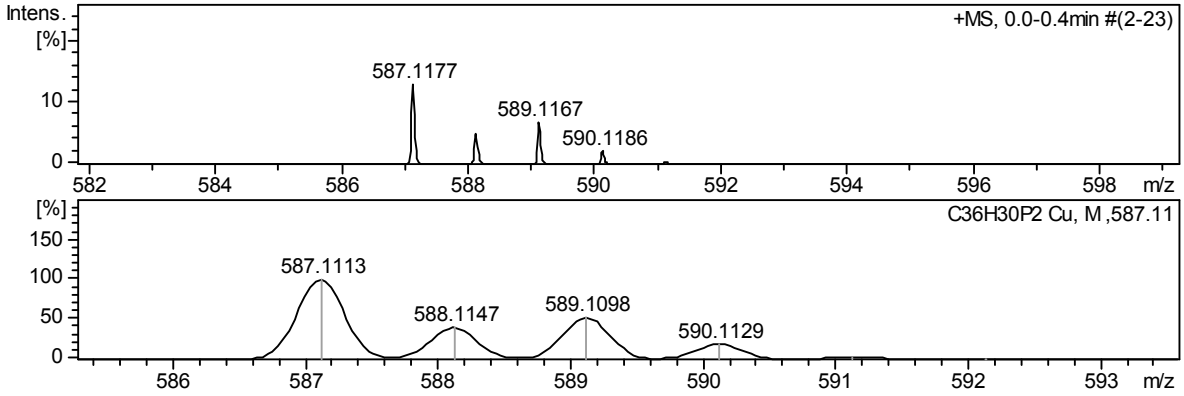
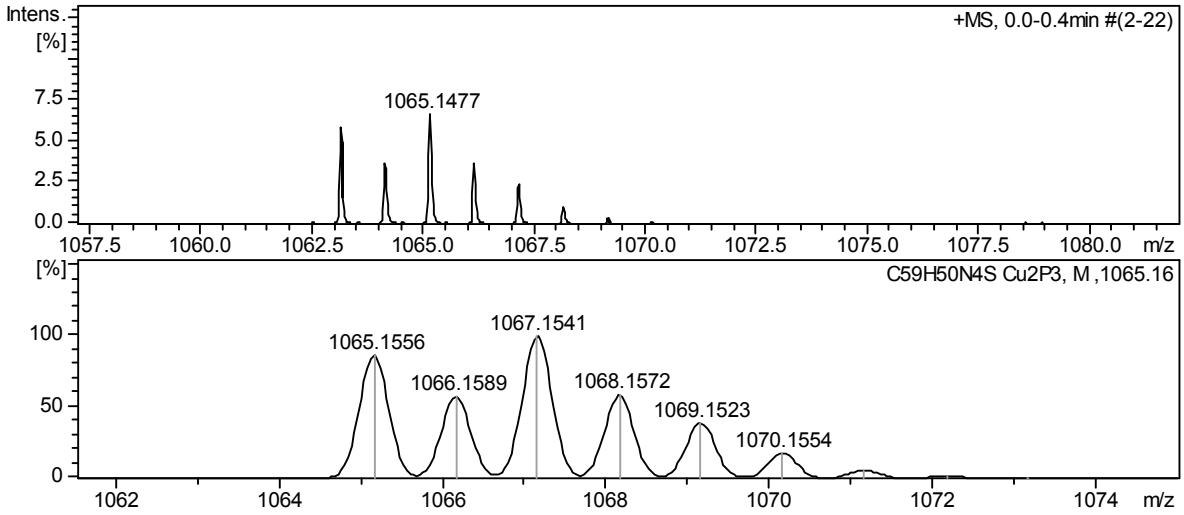
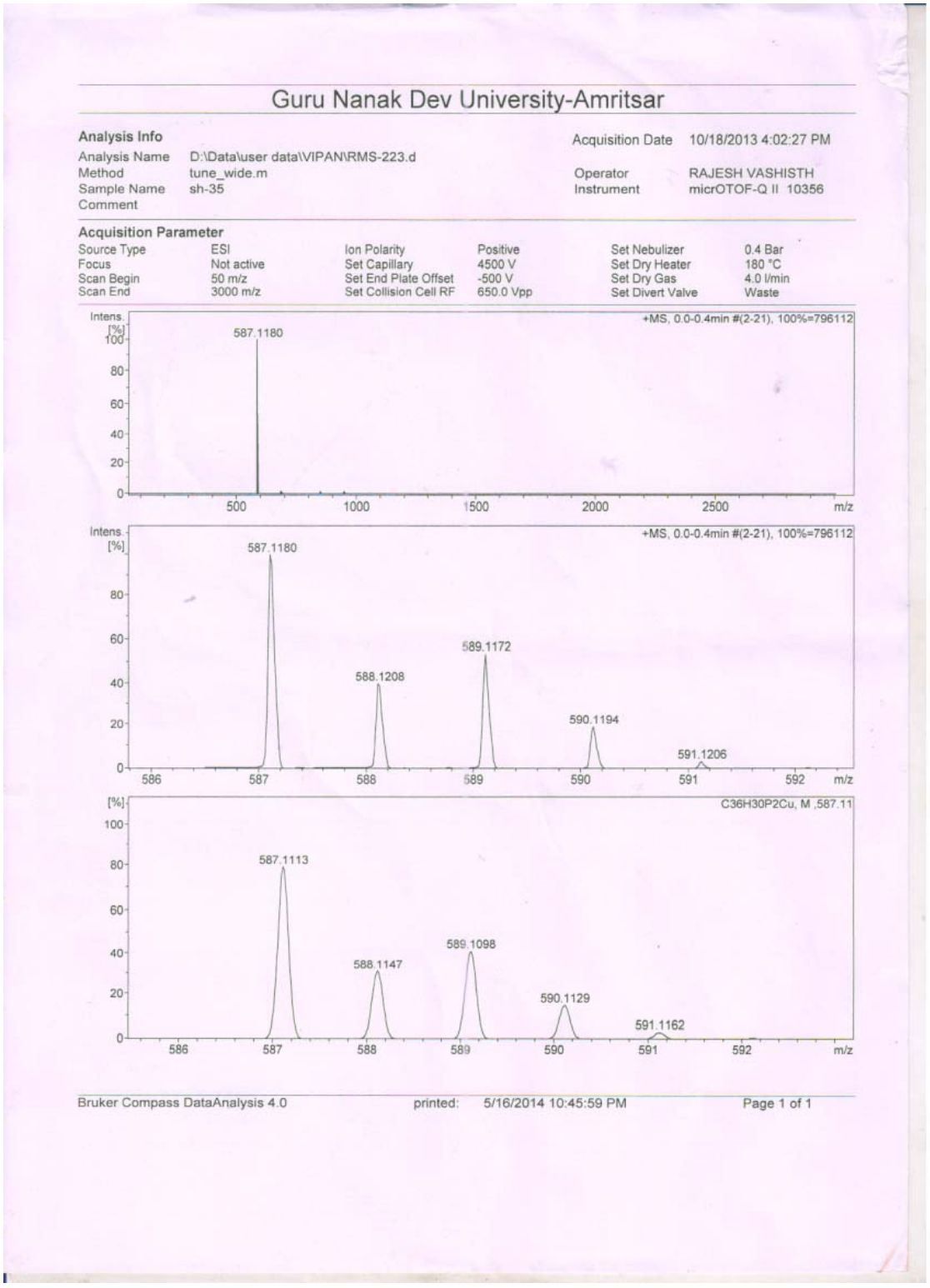


m/z observed 1065.1- isotopic pattern



Complex 3. Complete spectrum and m/z observed 587.1- isotopic pattern



Complex 5. Complete spectrum

$C_{76}H_{63}BrCu_2N_2P_4S_2$ $[Cu_2Br(dtucH)(PPh_3)_4]$

Mol. wt: 1399.27

Complex 5

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Analysis Info

Analysis Name	D:\Data\user data\VIPAN\V-340.d	Acquisition Date	10/18/2013 3:41:27 PM
Method	tune_wide.m	Operator	RAJESH VASHISTH
Sample Name	sh-35	Instrument	micrOTOF-Q II 10356
Comment			

Acquisition Parameter

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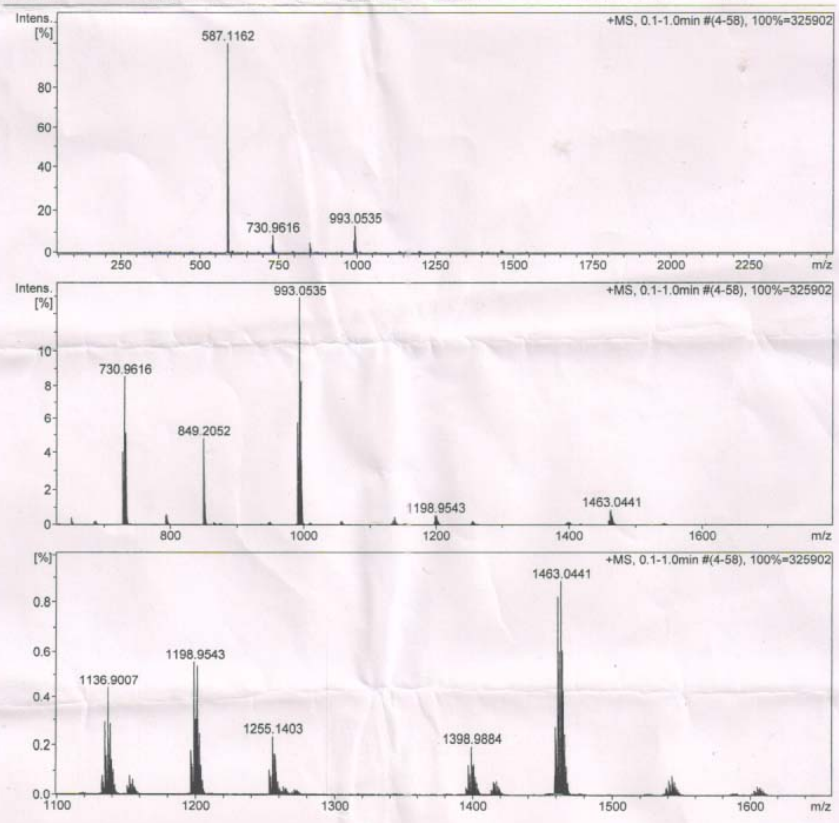
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



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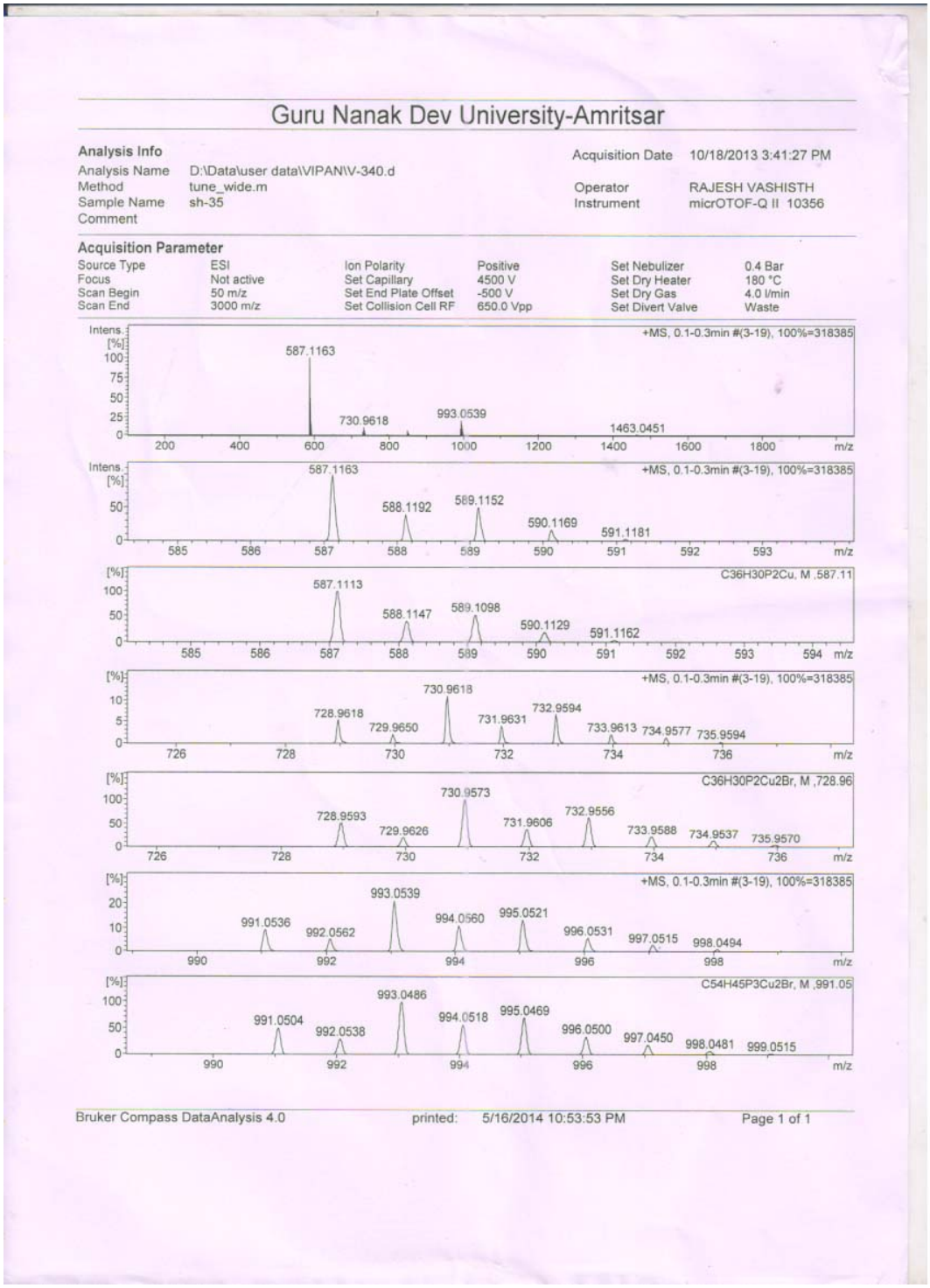
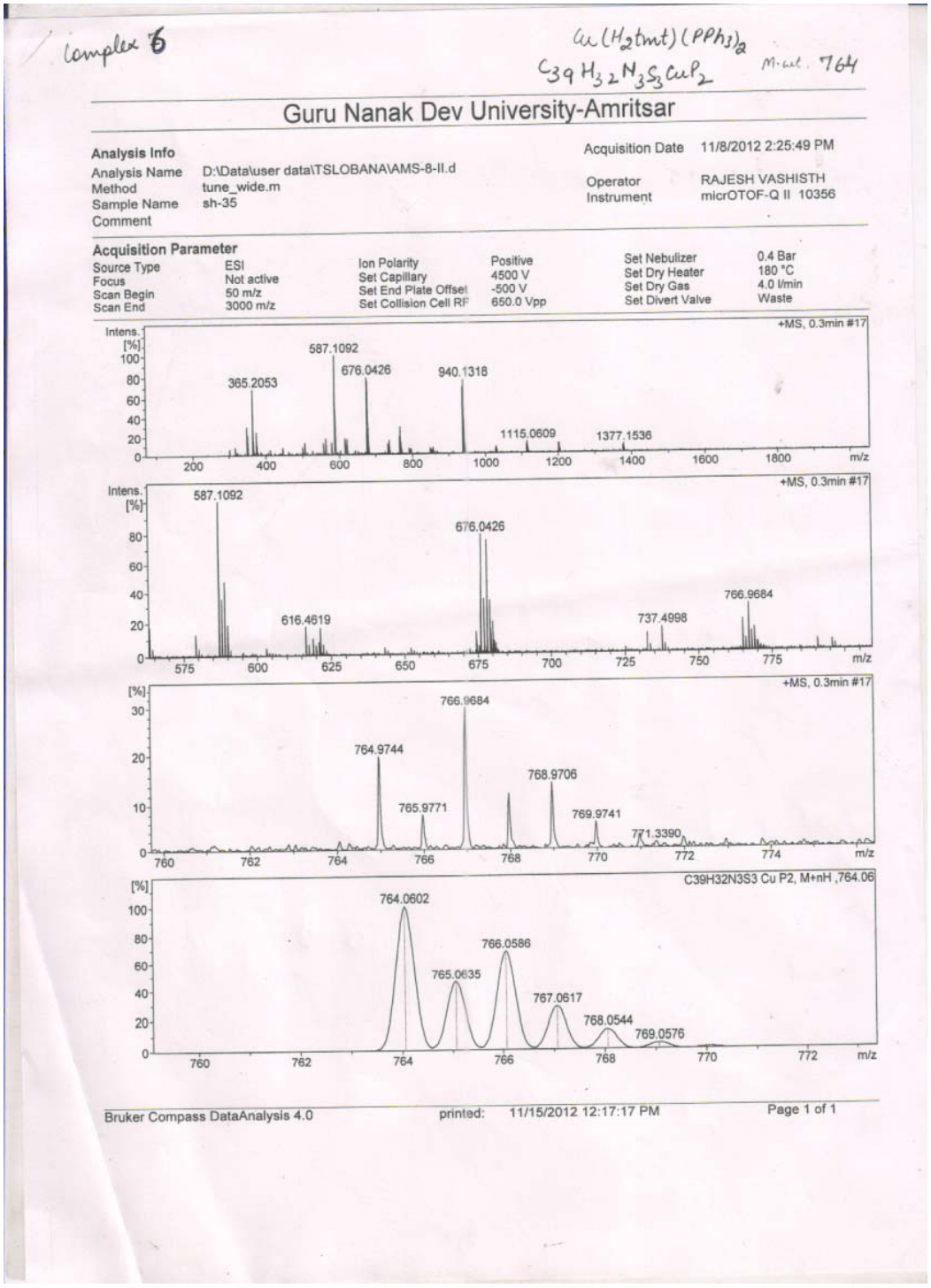
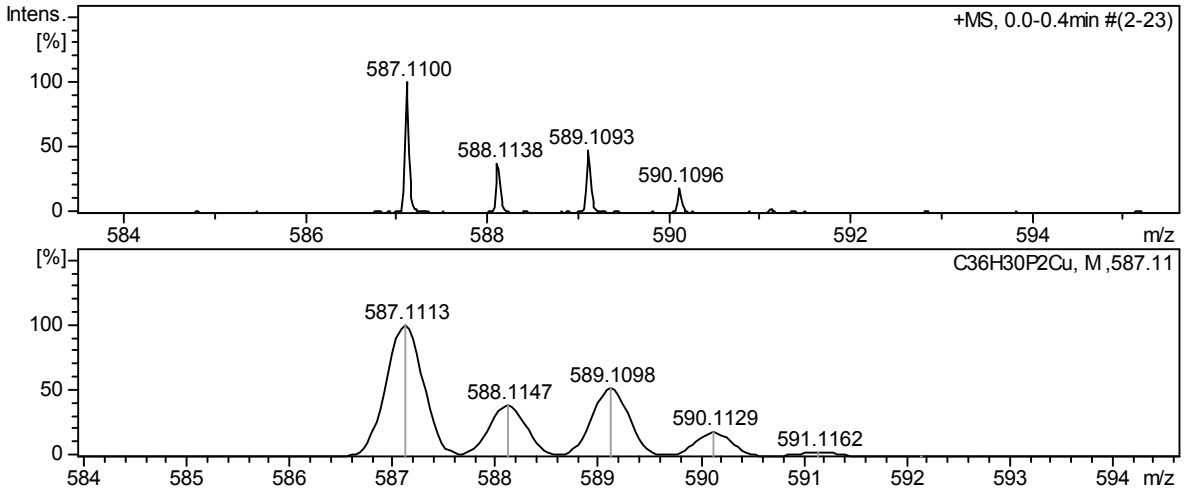
Species identified with isotopic patterns in same graph below.



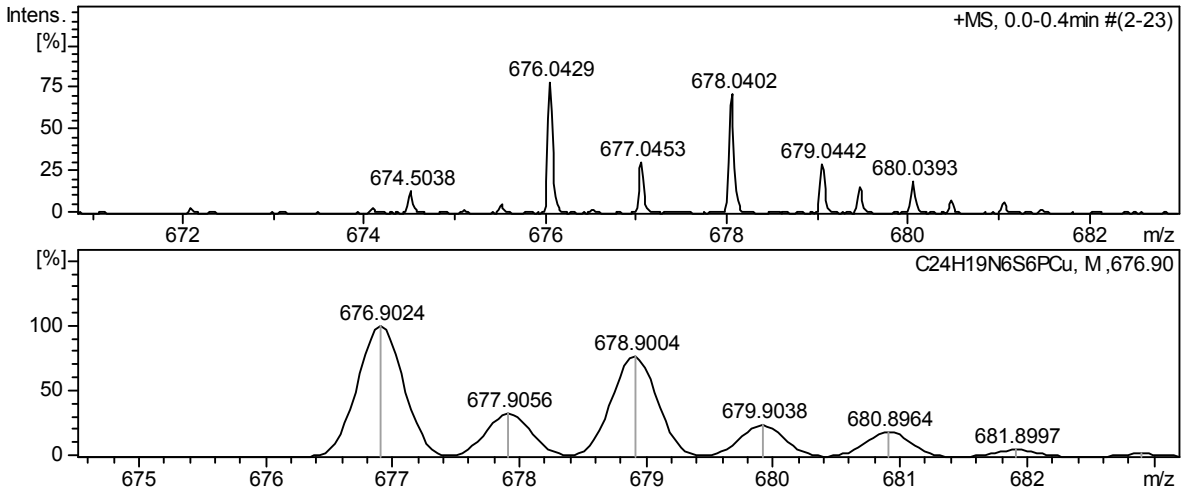
Complex 6. Complete spectrum



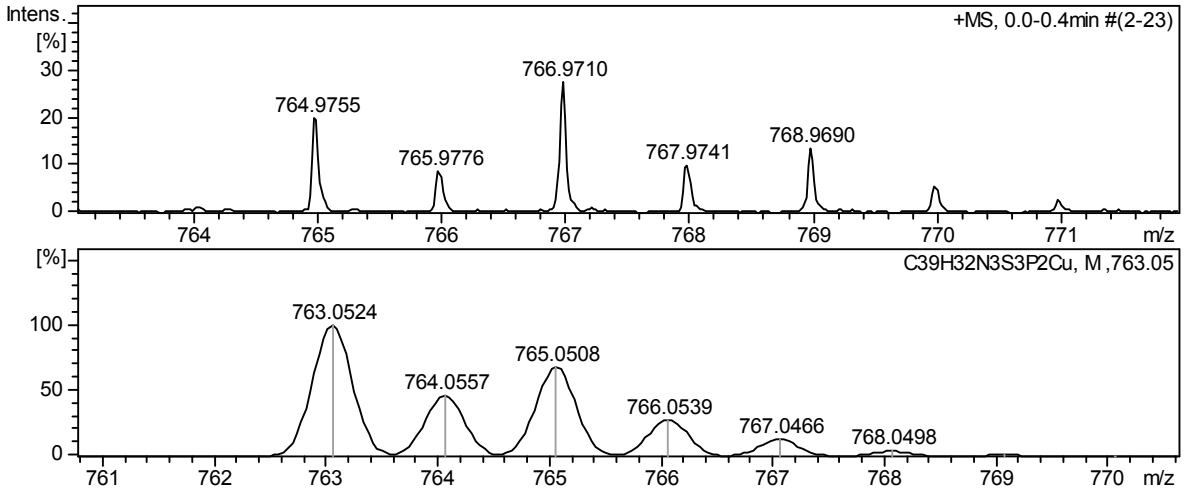
m/z observed 587.1- isotopic pattern



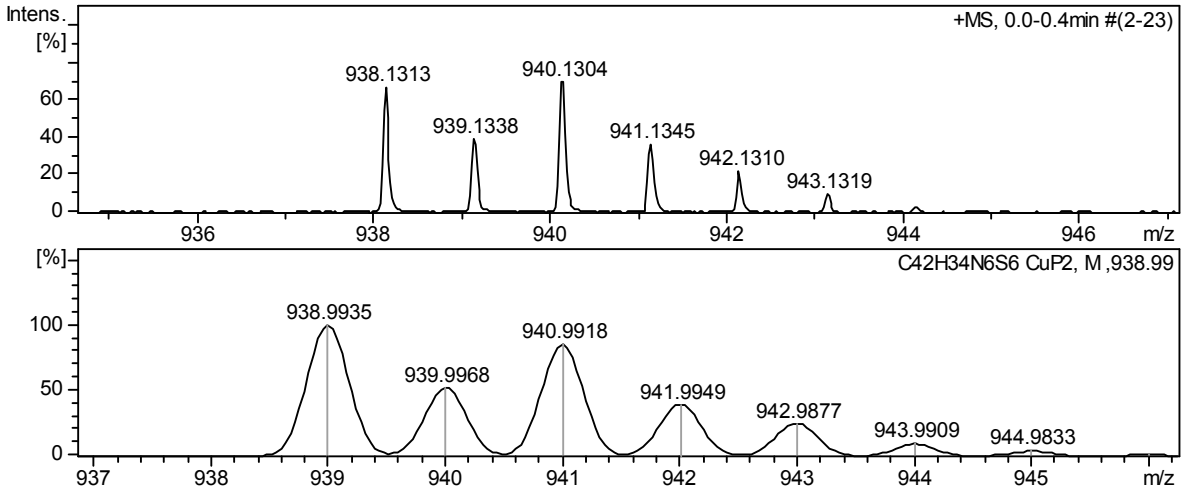
m/z observed 676.90- isotopic pattern



m/z observed 763.05- isotopic pattern



m/z observed 938.99- isotopic pattern



Complex 7. Complete spectrum

$C_{111}H_{92}Br_2Cu_3N_3P_6S_3$ $[Cu_3Br_2(H_2tmt)(PPh_3)_6]$

Complex 7 Mol wt: 2100.32

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Analysis Info

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Method	tune_wide.m	Operator	RAJESH VASHISTH
Sample Name	sh-35	Instrument	micrOTOF-Q II 10356
Comment			

Acquisition Parameter

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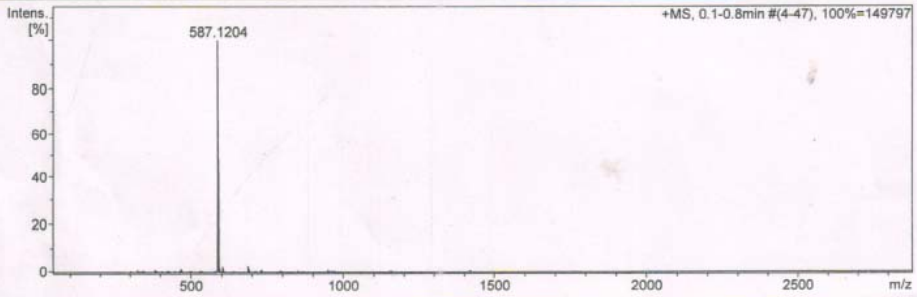
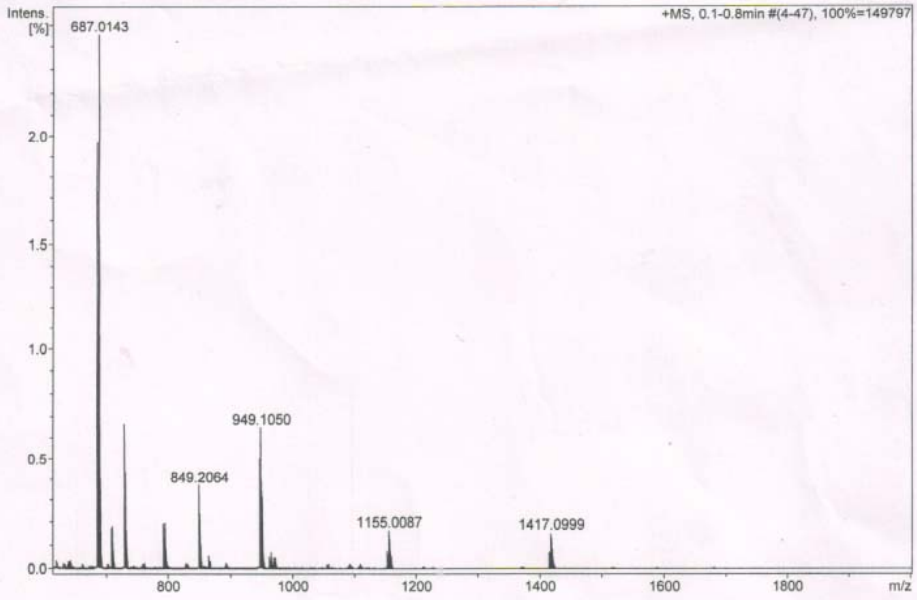
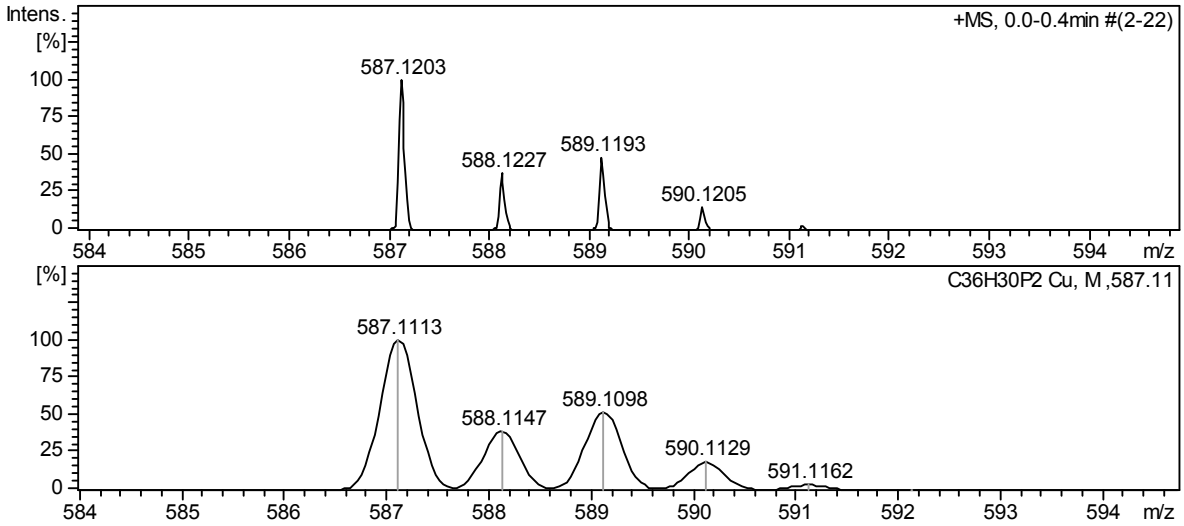
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste





m/z observed 587.1- isotopic pattern



NMR data of complexes

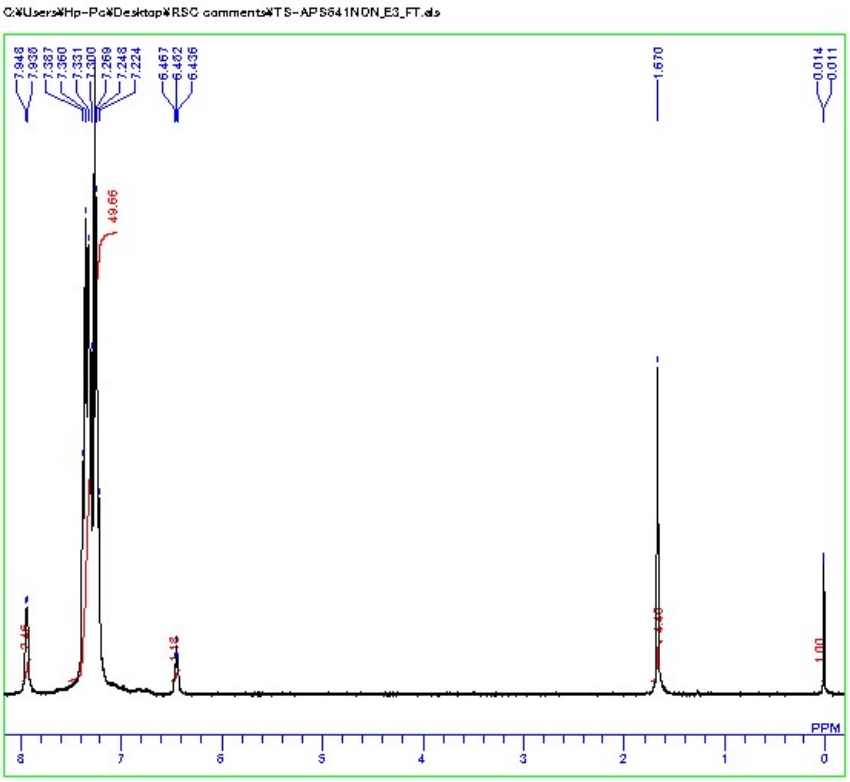


Fig. 1a.S. ^{1}H spectrum of [Cu(κ^{1}N, κ^{1}S-pymS)(PPh$_3$)$_2$] (1)

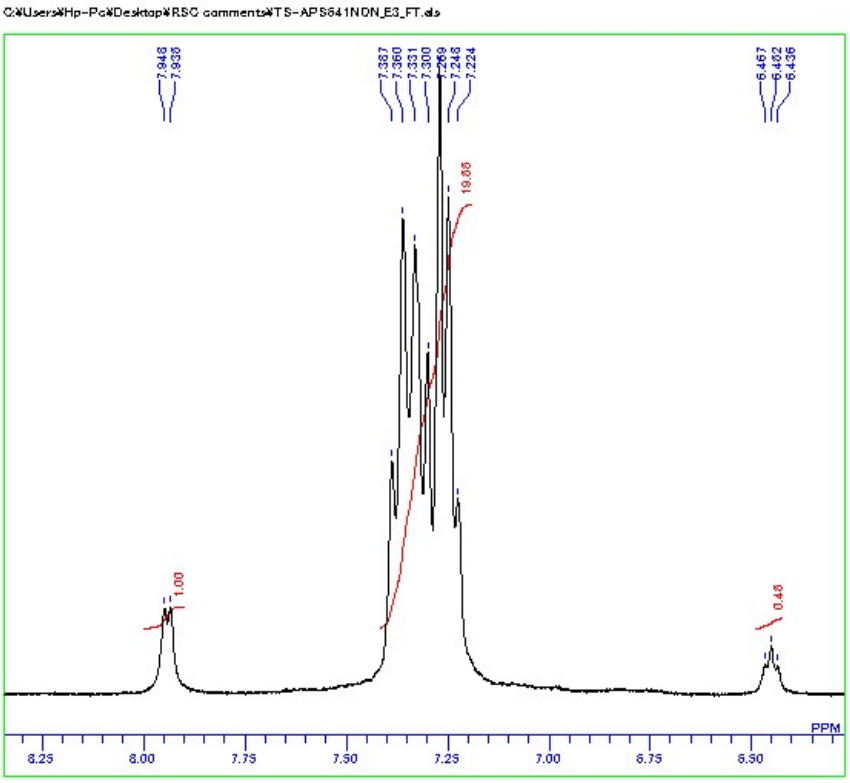


Fig.ure 1b.S. Expanded ^{1}H spectrum of [Cu(κ^{1}N, κ^{1}S-pymS)(PPh$_3$)$_2$] (1)

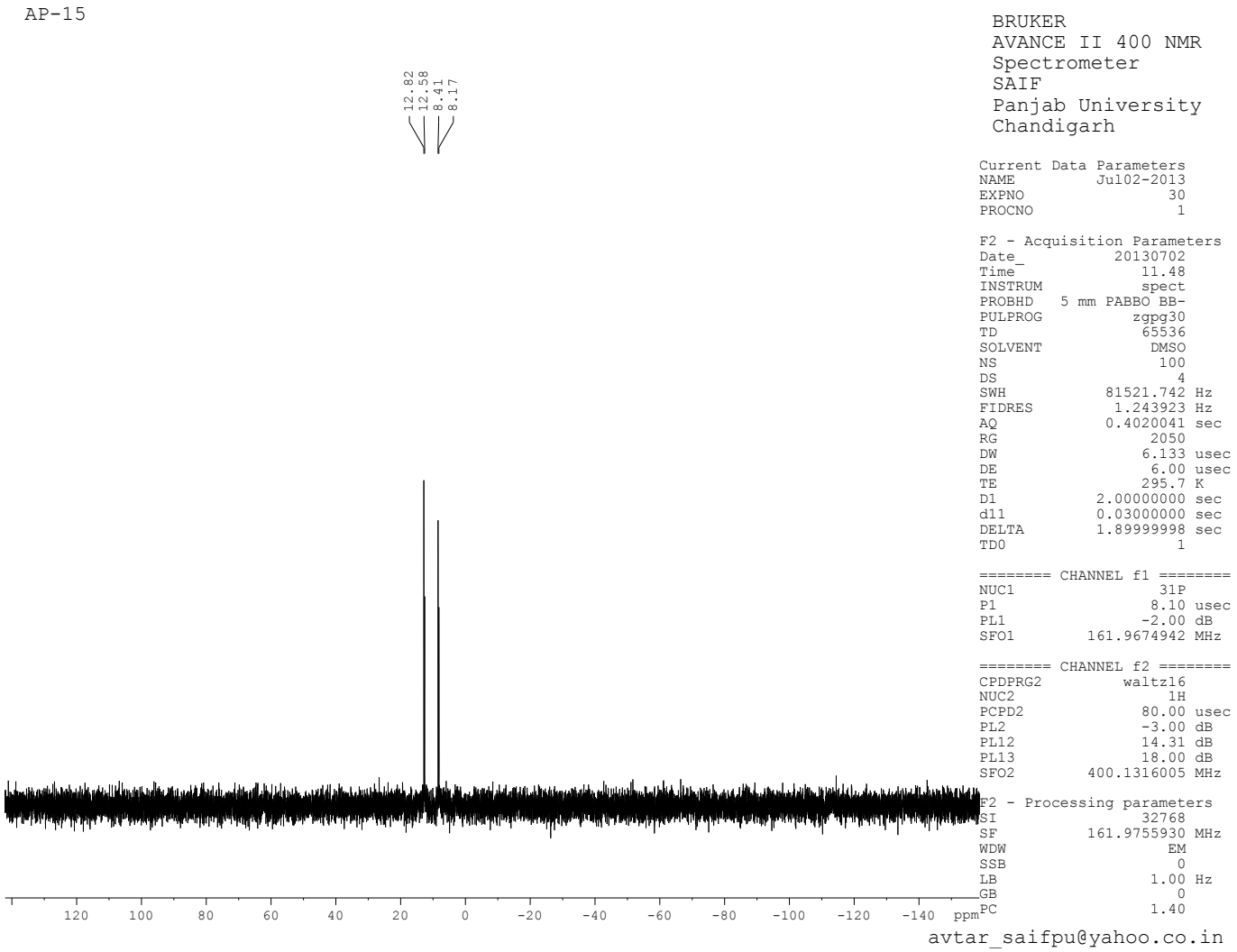


Fig.1c.S. ^{31}P spectrum of [Cu(κ^{1}N, κ^{1}S-pymS)(PPh$_3$)$_2$] (1)

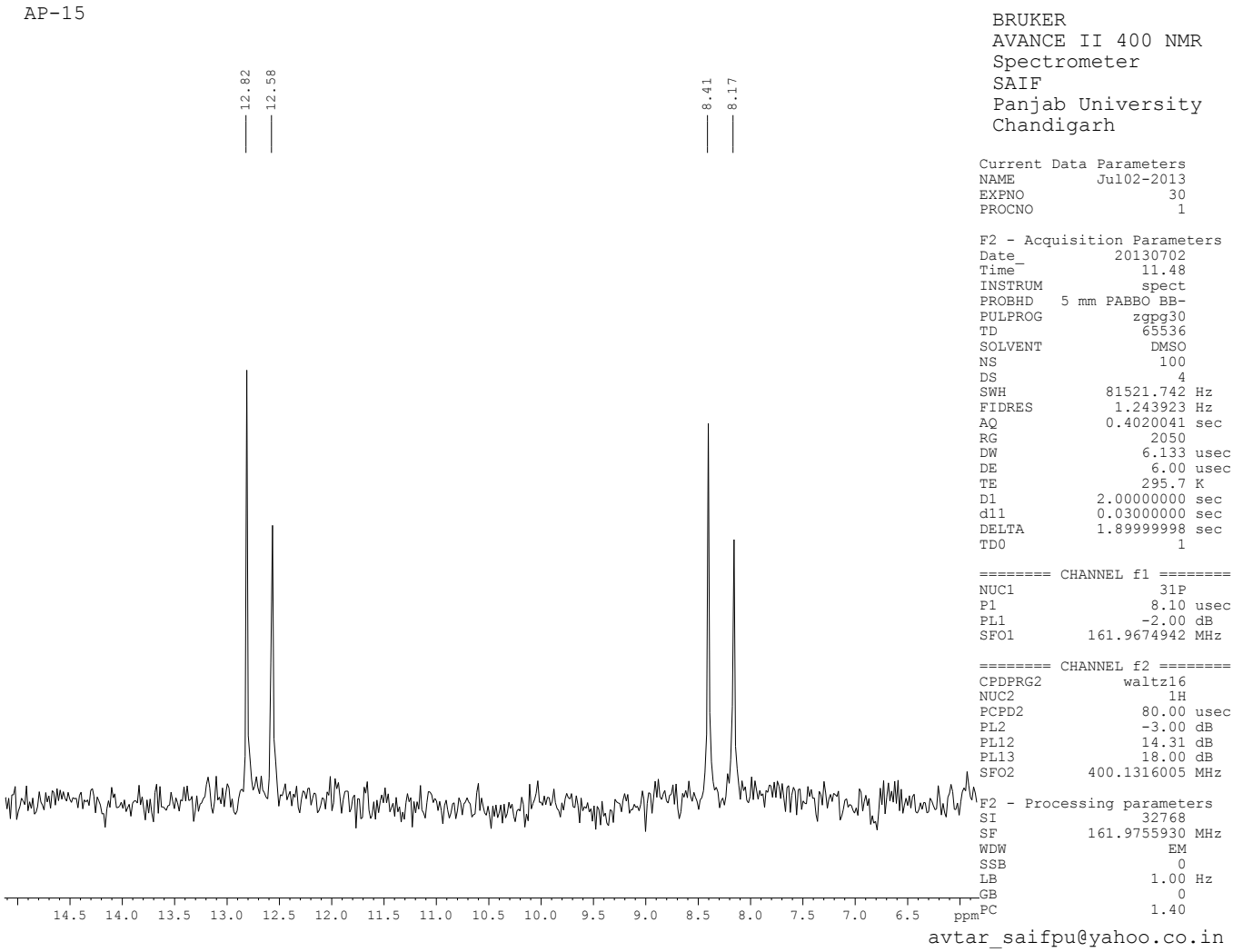


Fig.1d.S. Expanded ^{31}P spectrum of [Cu(κ^{1}N, κ^{1}S-pymS)(PPh$_3$)$_2$] (1)

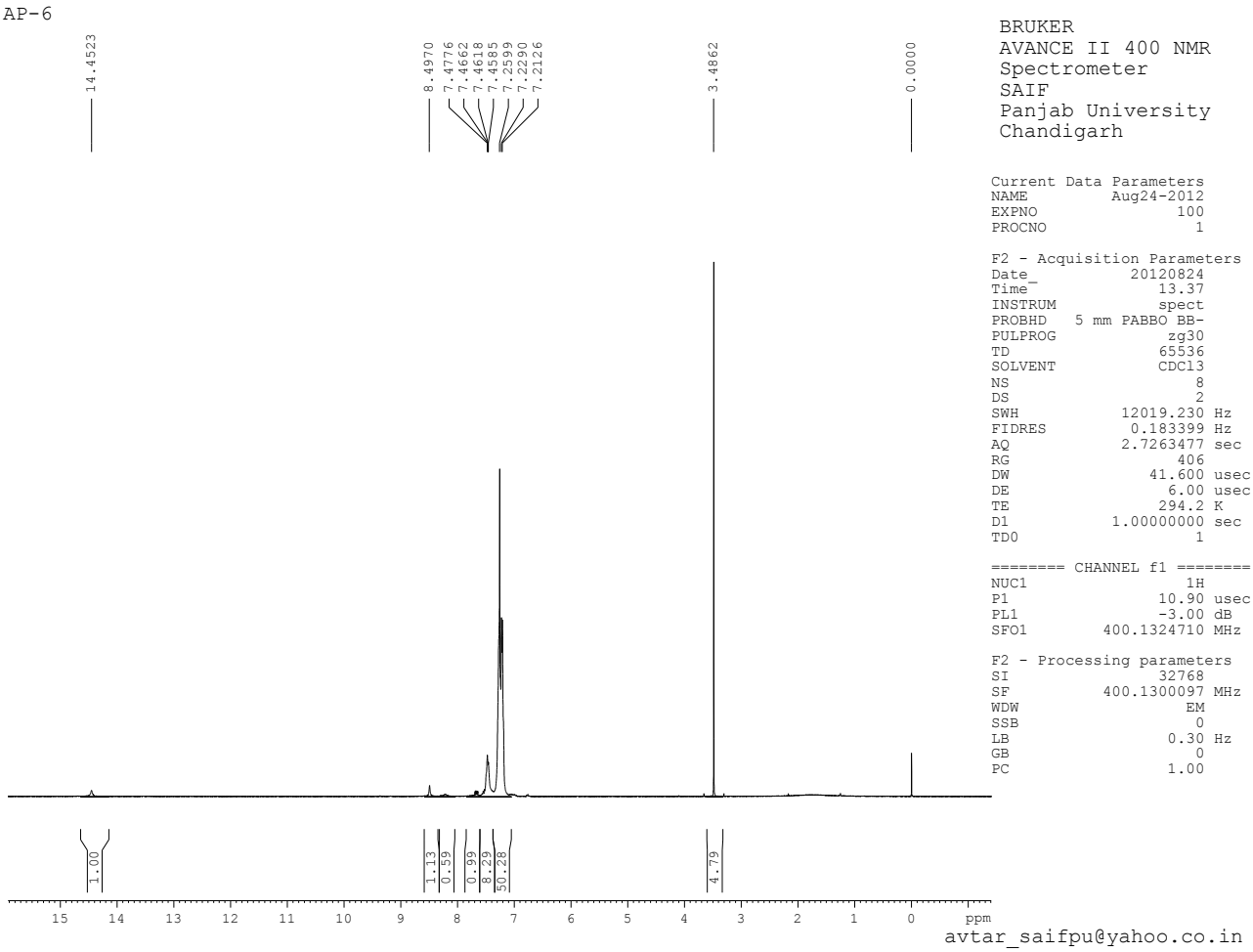


Fig.2a.S. ^{1}H spectrum of [Cu(κ^{1}N,κ^{1}S-purSH)(PPh_3)$_2$]·CH_3OH (2a)

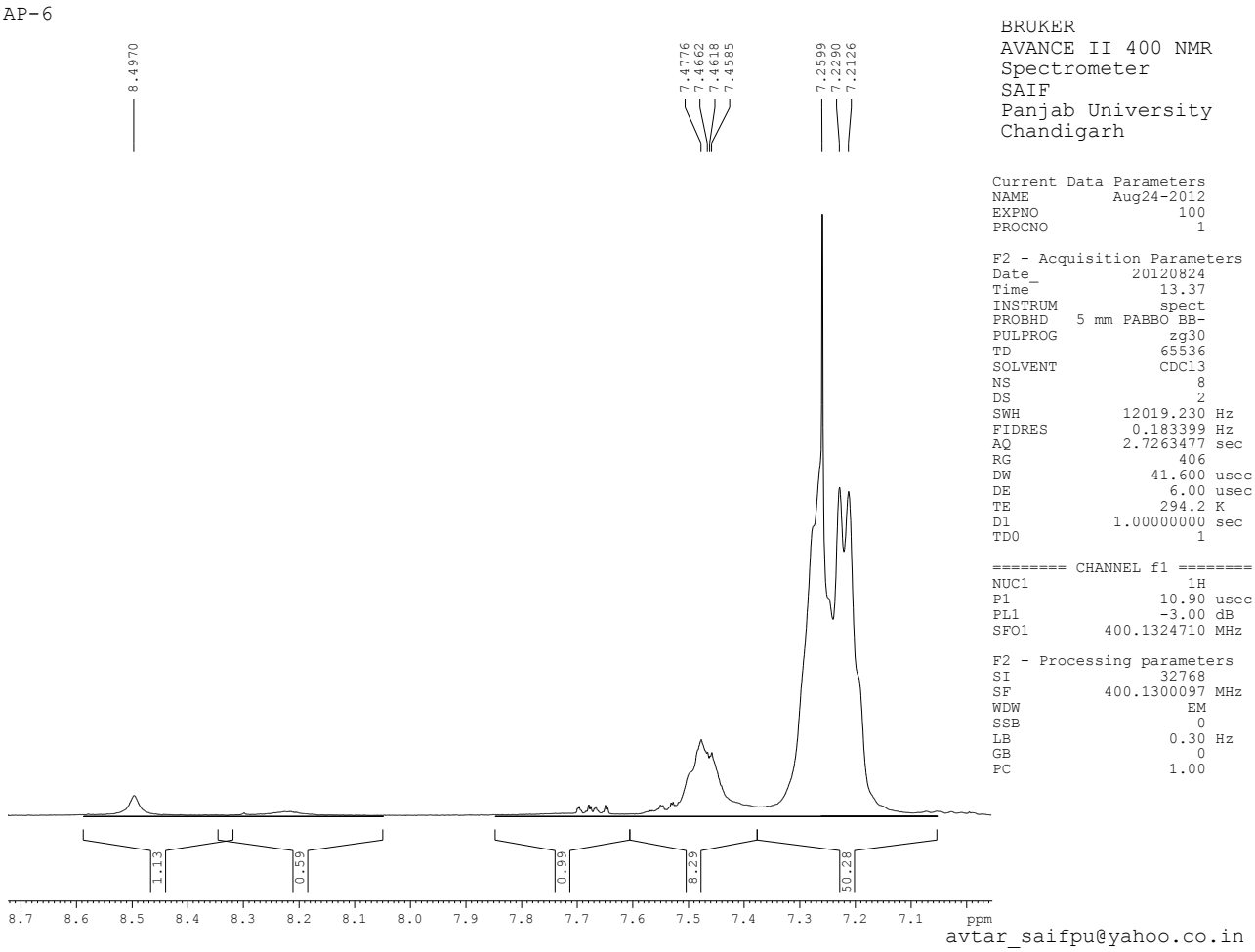


Fig. 2b.S. Expanded ^{1}H spectrum of [Cu(κ^{1}N,κ^{1}S-purSH)(PPh$_3$)$_2$]·CH$_3$OH (2a)

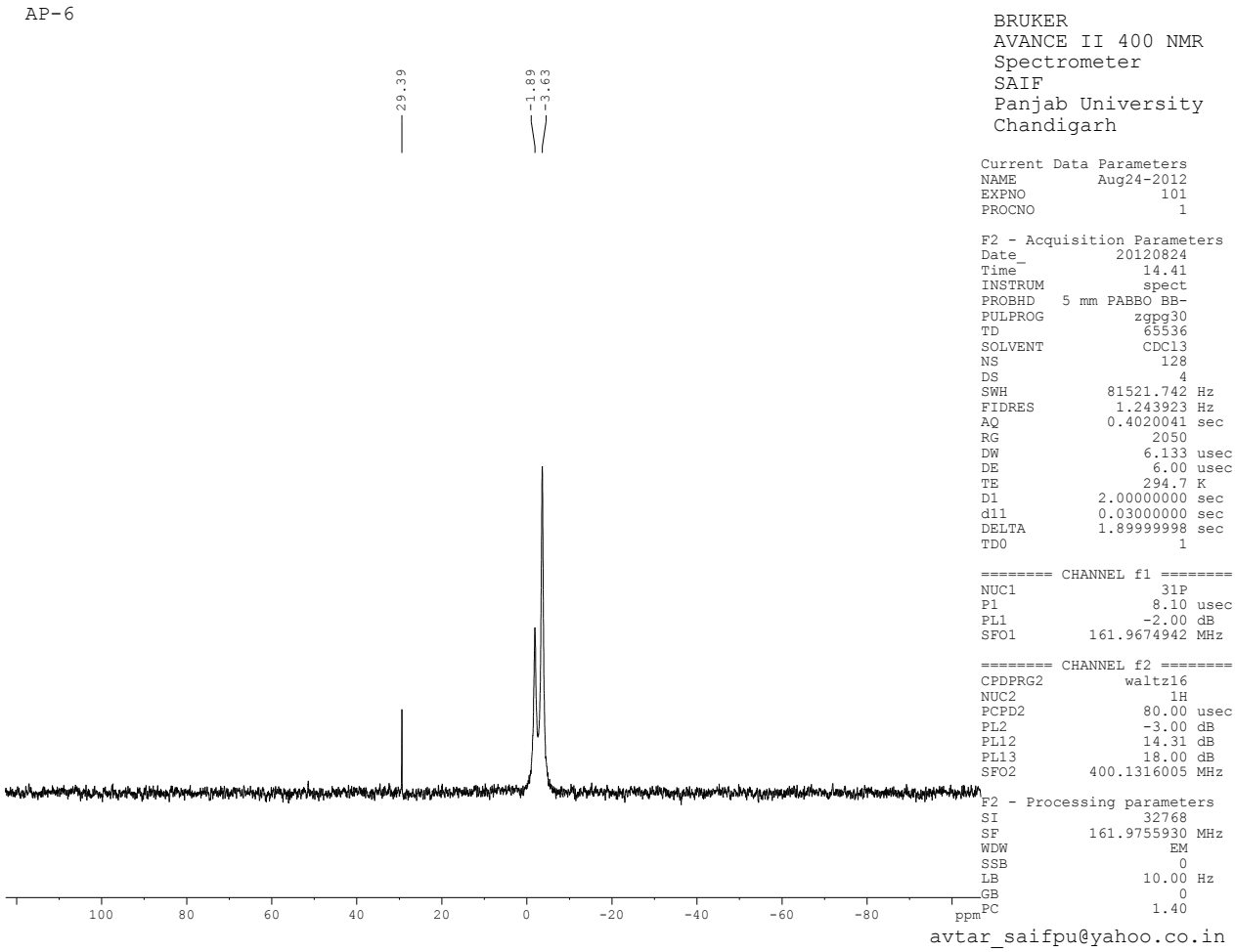


Fig.2c.S. ^{31}P spectrum of [Cu(κ^{1}N,κ^{1}S-purSH)(PPh$_3$)$_2$]·CH$_3$OH (2a)

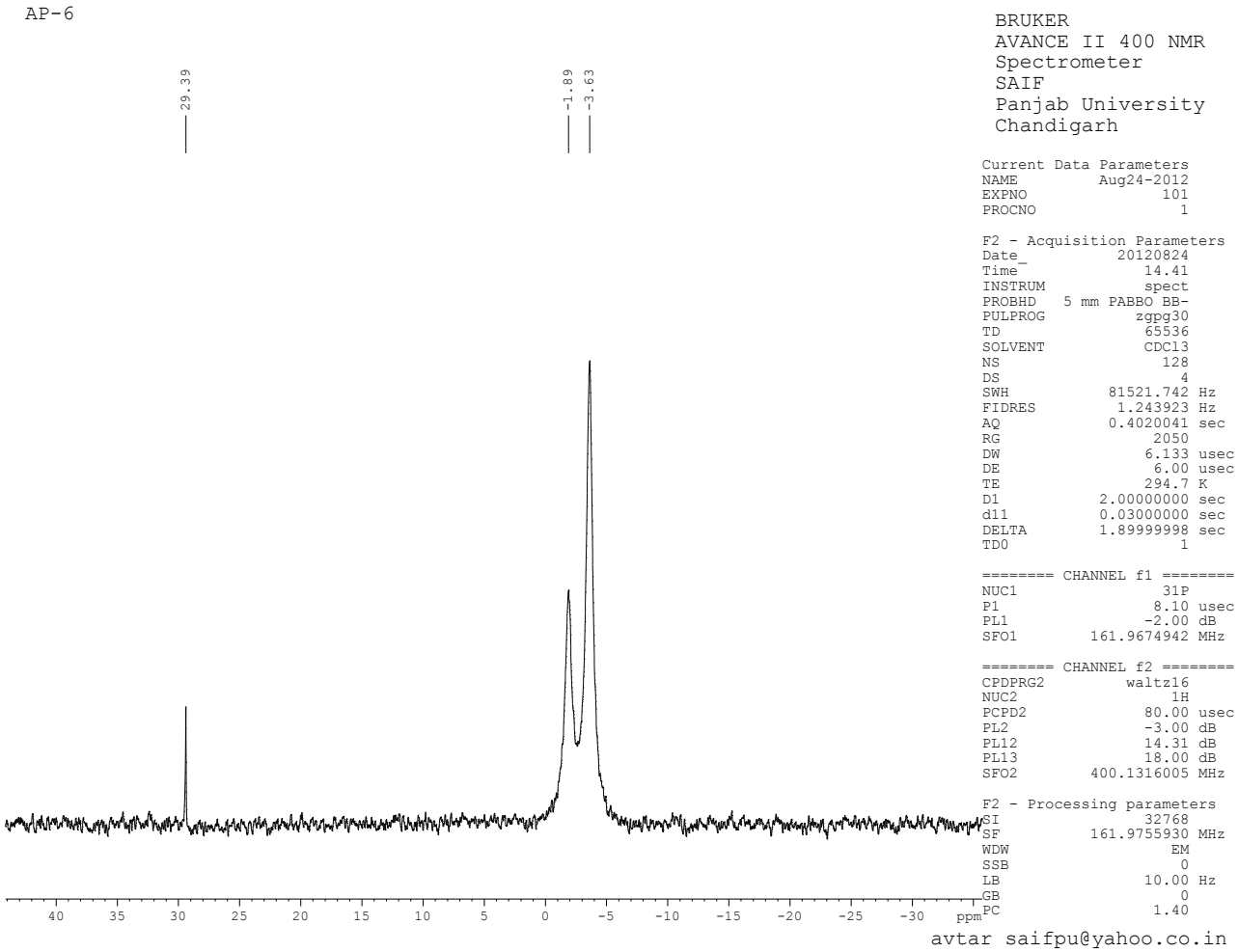


Fig.2d.S. Expanded ^{31}P spectrum of $[Cu(\kappa^1N,\kappa^1S\text{-purSH})(PPh_3)_2]\cdot CH_3OH$ (2a)

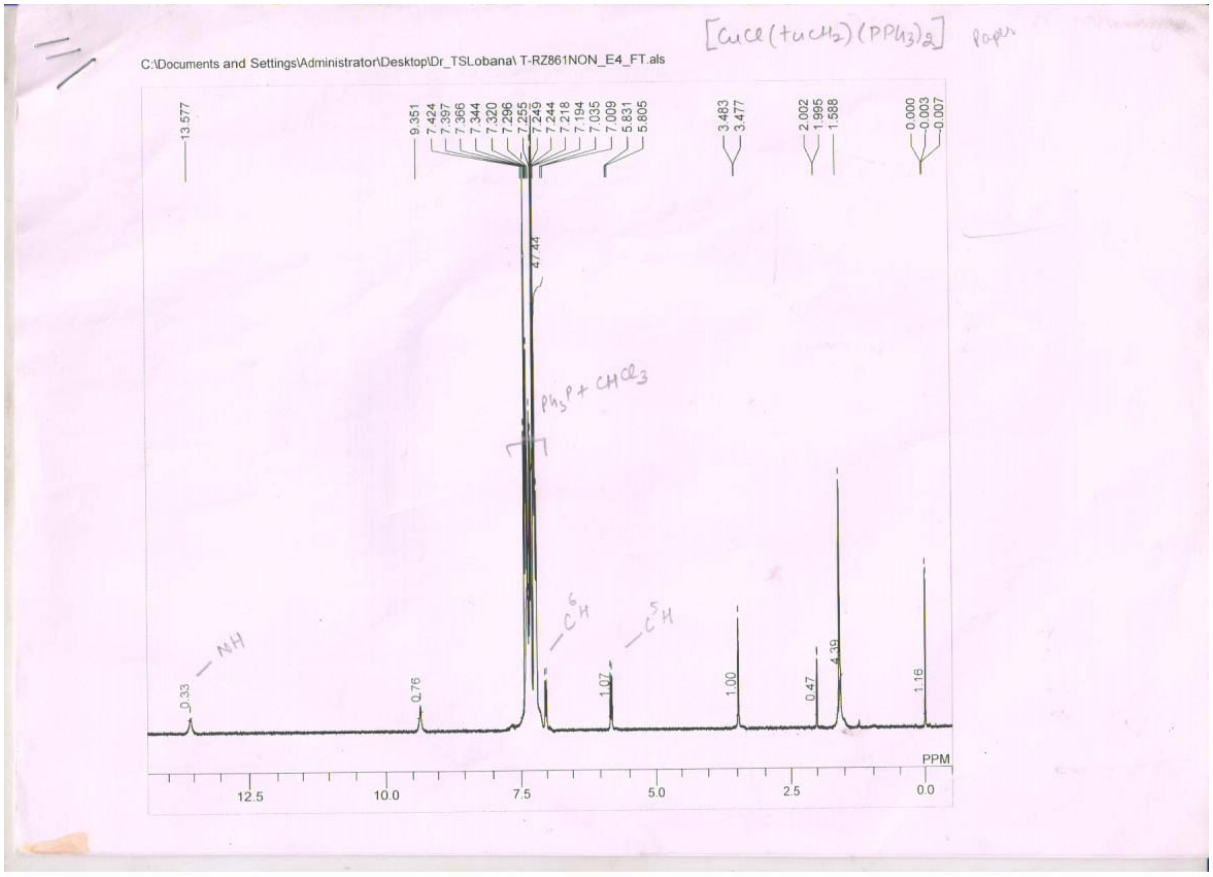


Fig.3a.S. ^{1}H spectrum of [CuCl(κ^{1}S-tucH$_2$)(PPh$_3$)$_2$](3)

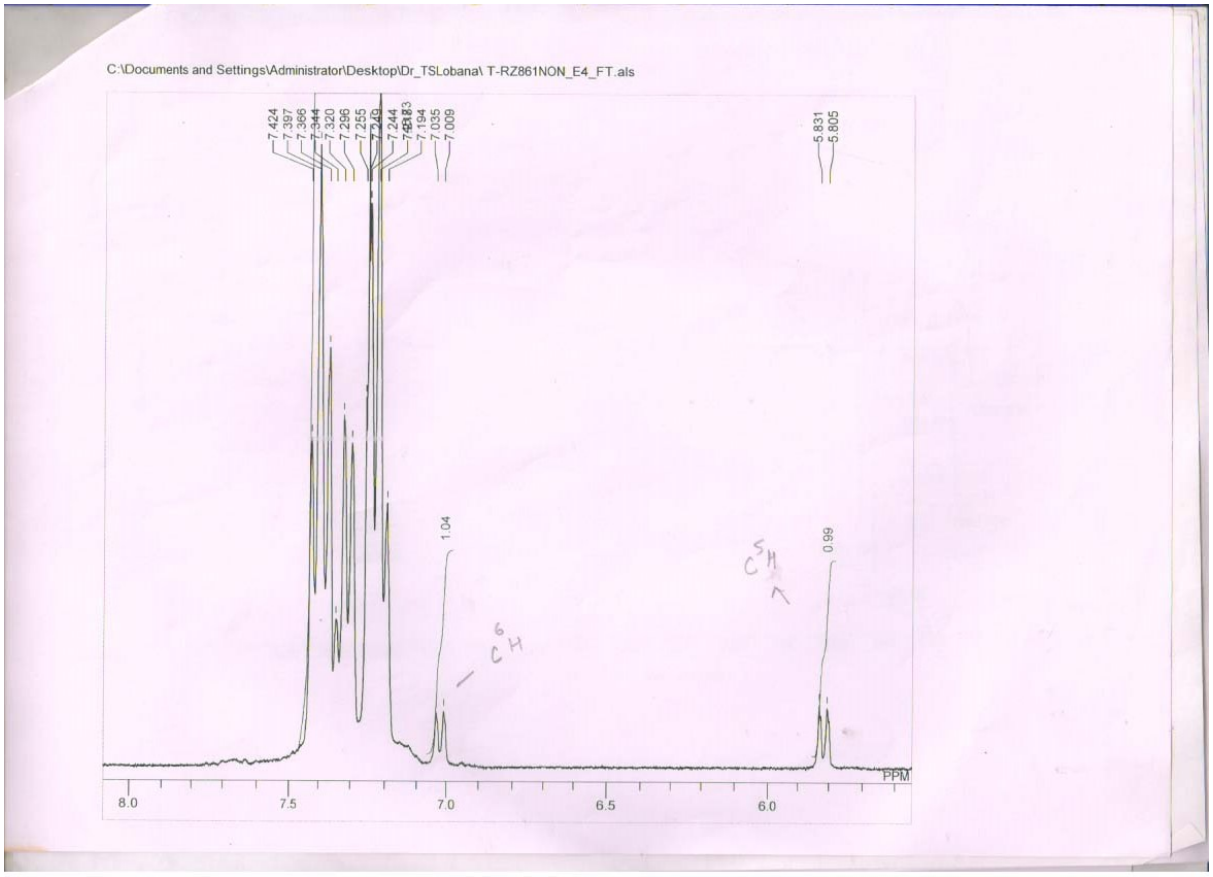


Fig.3b.S. Expanded ^{1}H spectrum of [CuCl(κ^{1}S-tucH$_2$)(PPh$_3$)$_2$](3)

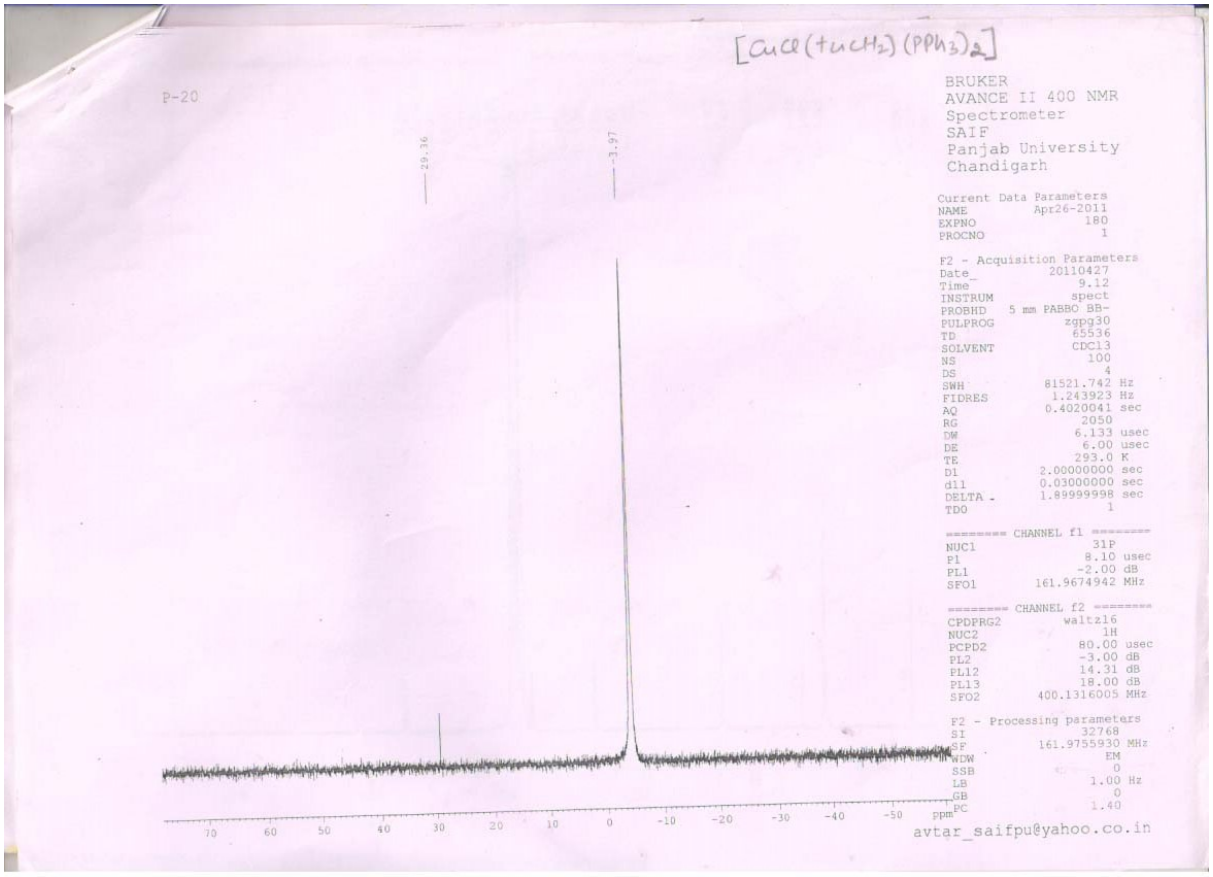


Fig.3c.S. ^{31}P spectrum of [CuCl(κ^{1}S-tucH$_2$)(PPh$_3$)$_2$](3)

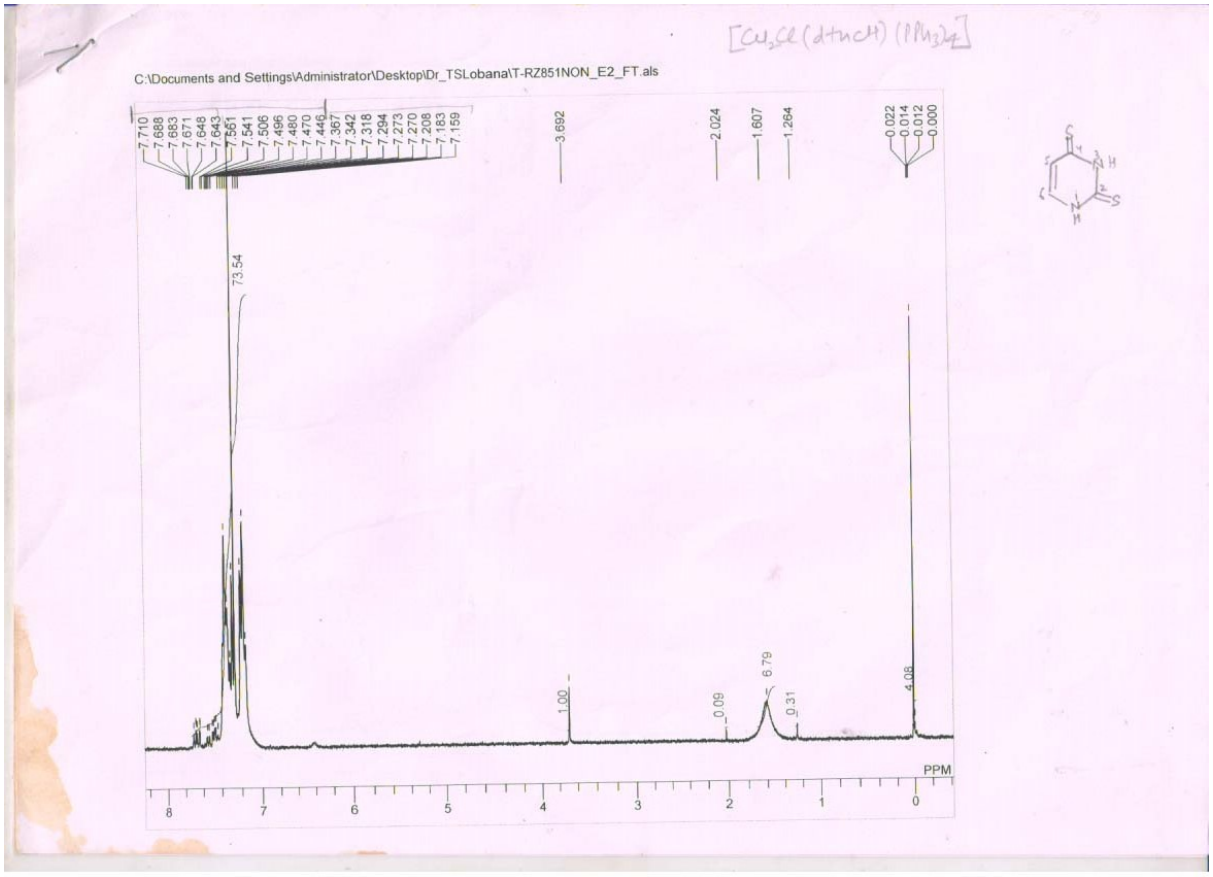


Fig.4a.S. ^{1}H spectrum of $[Cu_2(\kappa^2Cl)(\kappa^1S,\kappa^1S\text{-dtucH})(PPh_3)_4]$ (4)

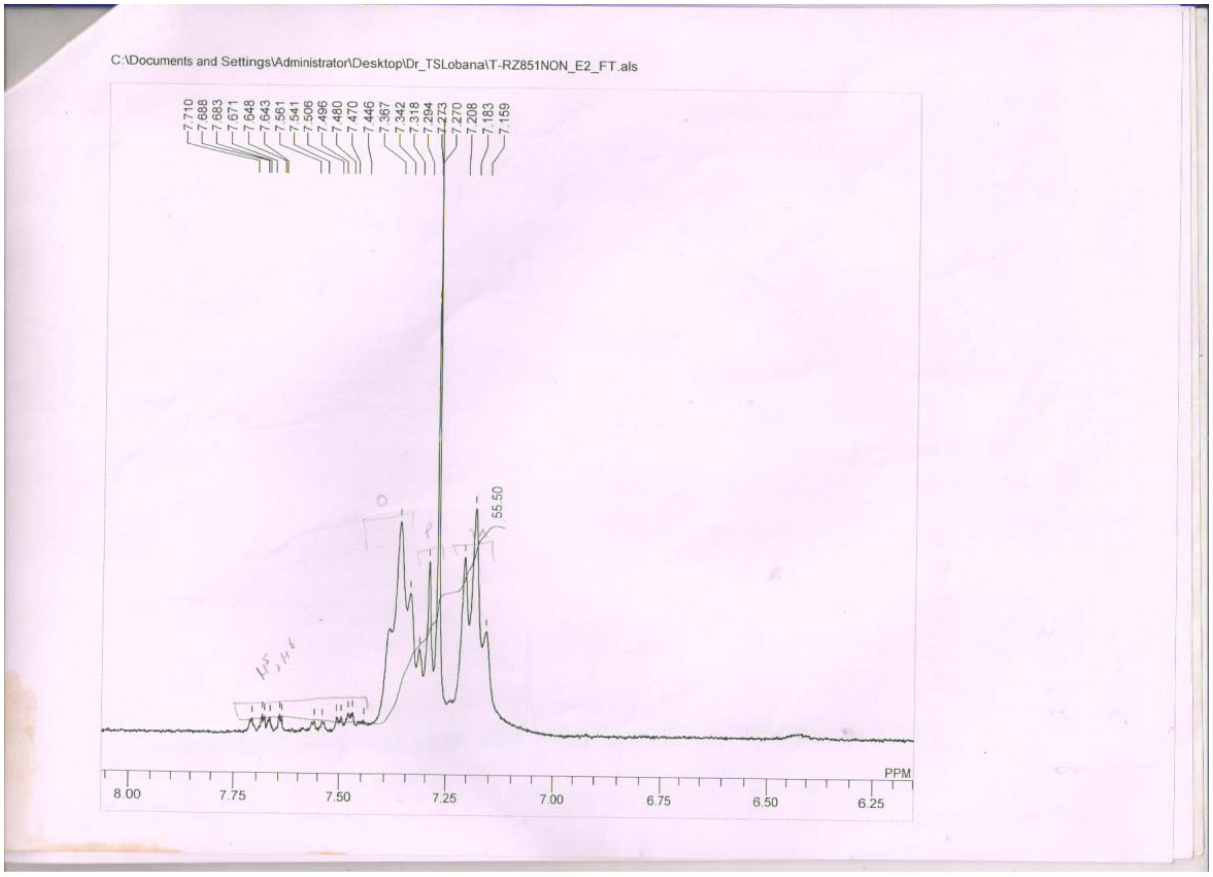


Fig.4b.S. Expanded ^{1}H spectrum of $[Cu_2(\kappa^2Cl)(\kappa^1S,\kappa^1S\text{-dtucH})(PPh_3)_4]$ (4)

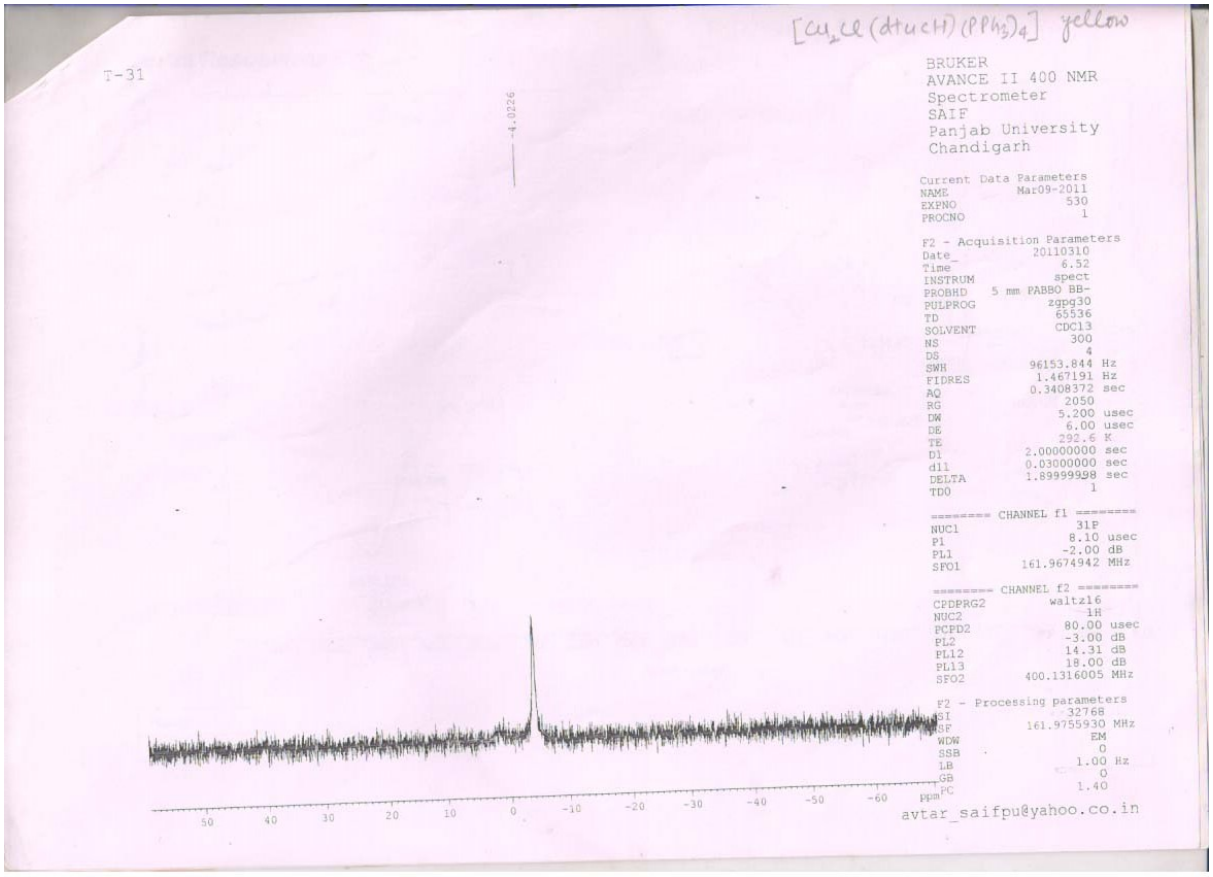


Fig.4c.S. ^{31}P spectrum of $[Cu_2(\kappa^2Cl)(\kappa^1S,\kappa^1S\text{-dtucH})(PPh_3)_4]$ (4)

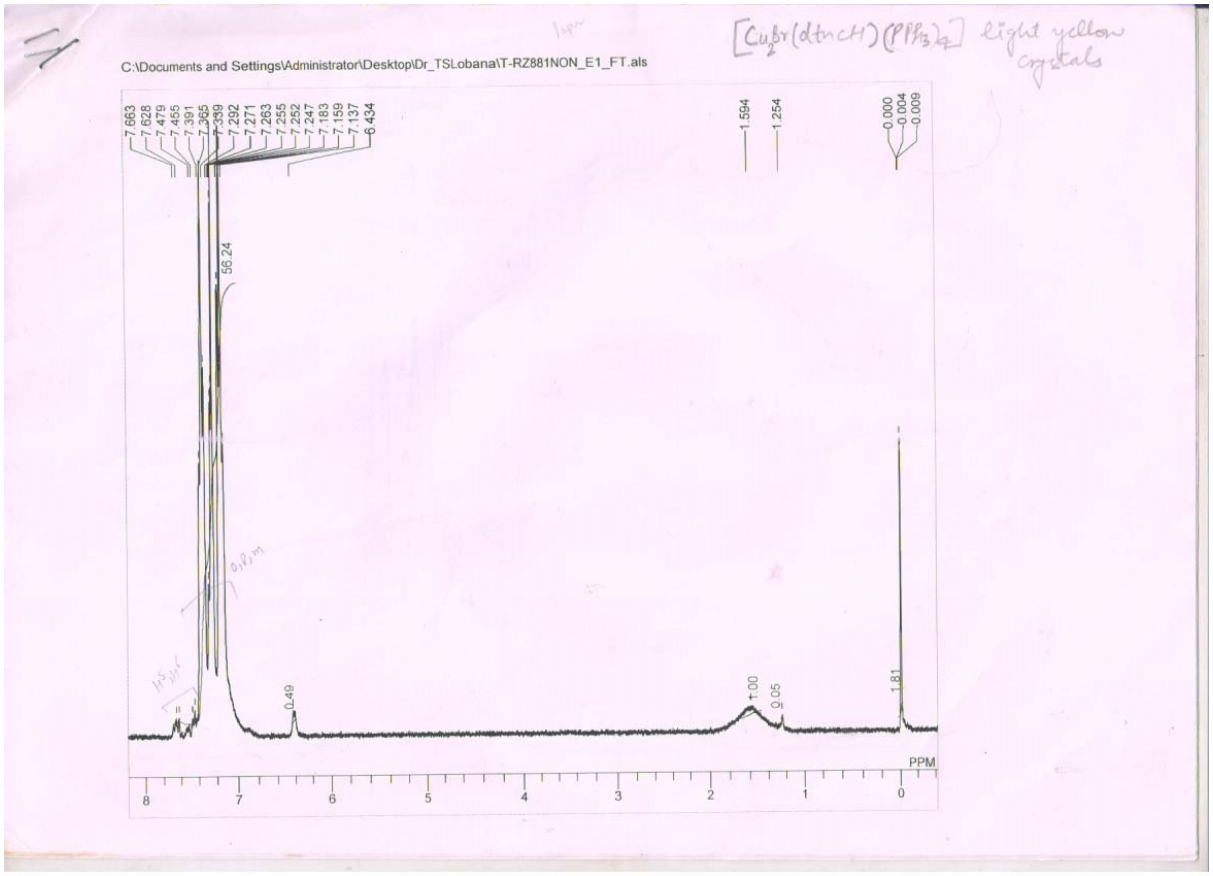


Fig.5a.S. ^{1}H spectrum of $[Cu_2(\kappa^2Br)(\kappa^1S,\kappa^1S\text{-dtucH})(PPh_3)_4]$ (5)

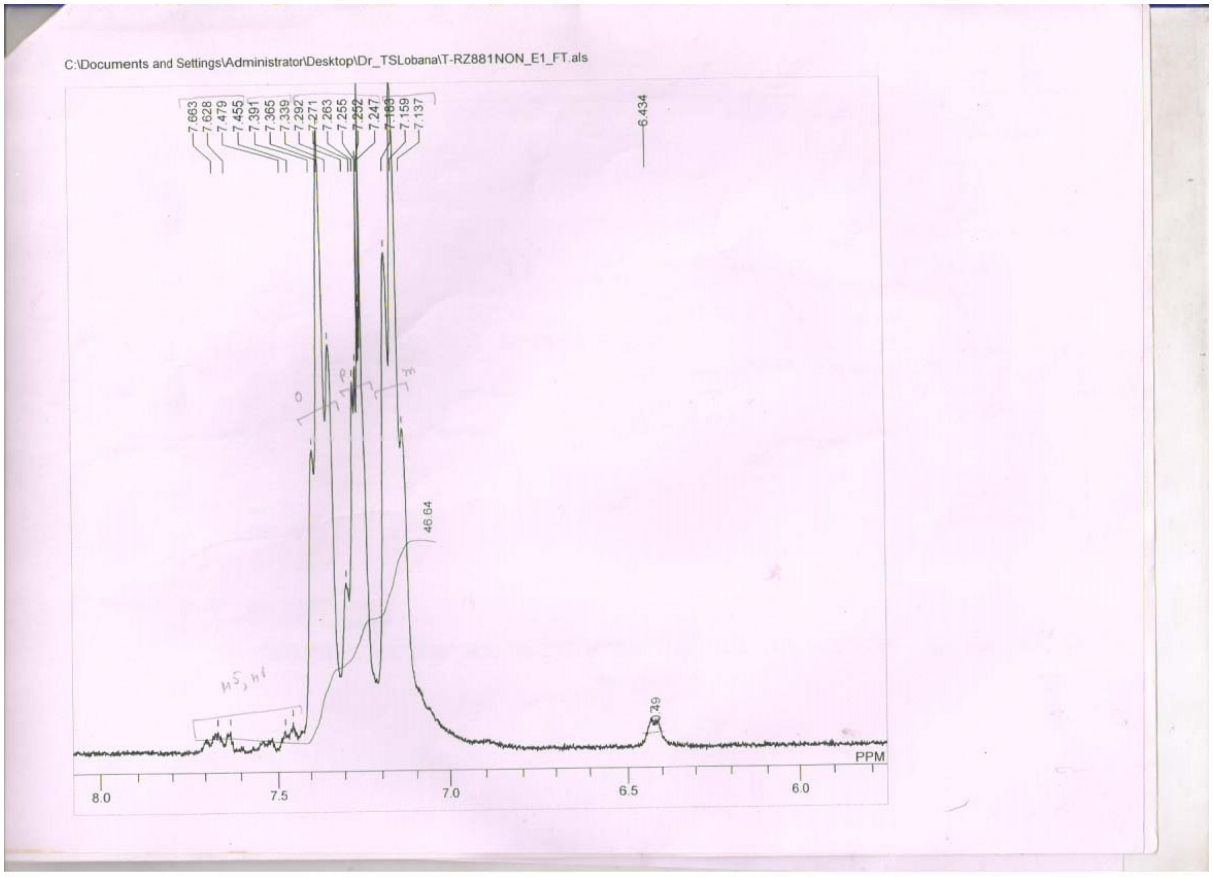


Fig.5b.S. Expanded ^{1}H spectrum of $[Cu_2(\kappa^2Br)(\kappa^1S,\kappa^1S\text{-dtucH})(PPh_3)_4]$ (5)

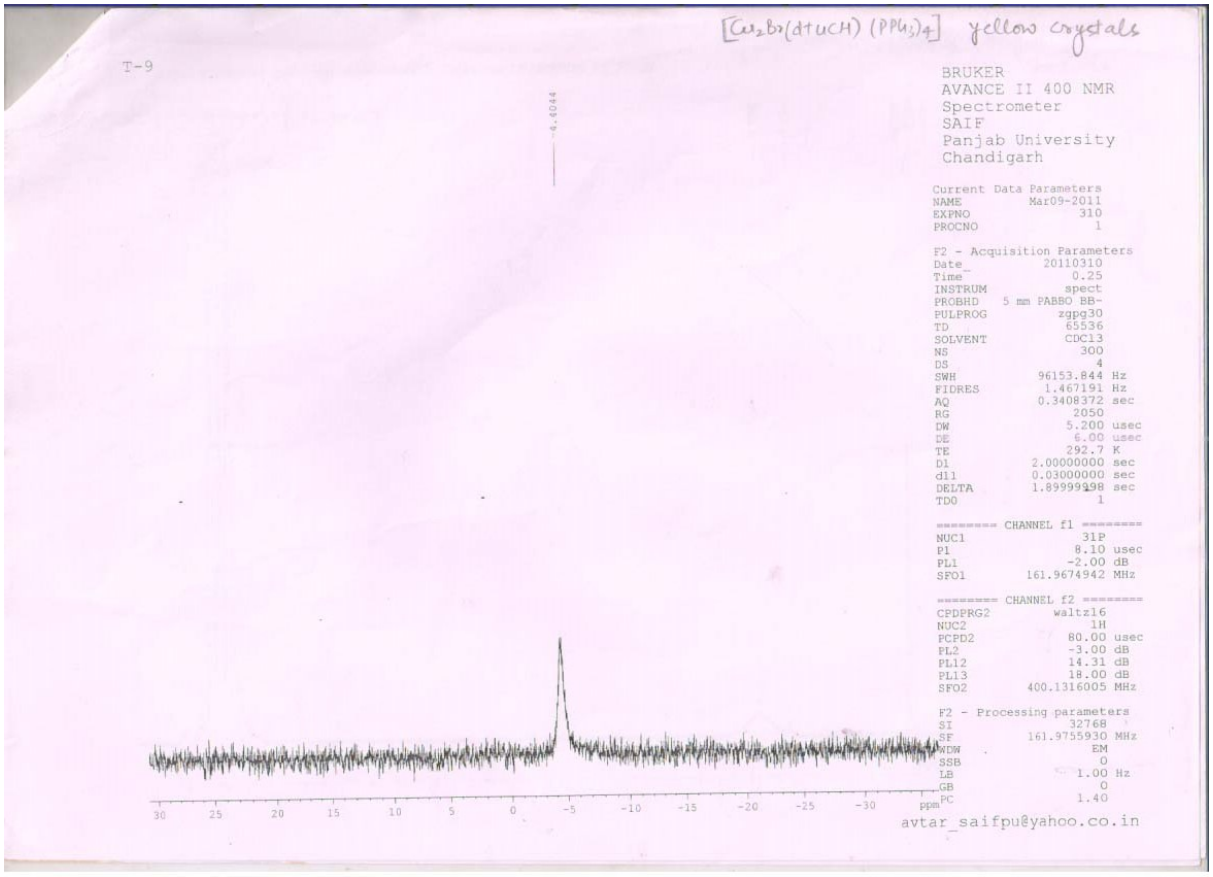
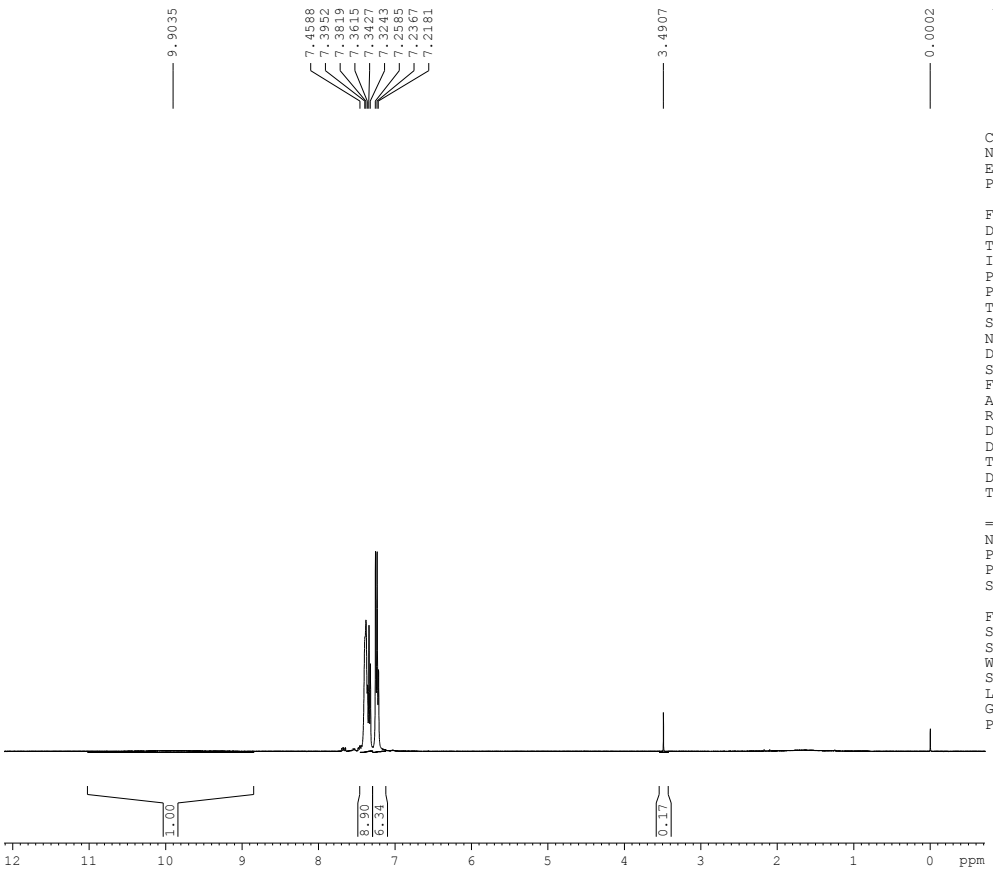


Fig.5c.S. ^{31}P spectrum of $[Cu_2(\kappa^2Br)(\kappa^1S,\kappa^1S\text{-dtucH})(PPh_3)_4]$ (5)

AP-5



BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME Aug24-2012
EXPNO 90
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120824
Time 13.30
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 406
DW 41.600 usec
DE 6.00 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

avtar_saifpu@yahoo.co.in

Fig.6a.S. ^{1}H spectrum of $[Cu(tmtH_2)(PPh_3)_2]\cdot 0.5H_2O$ (6)

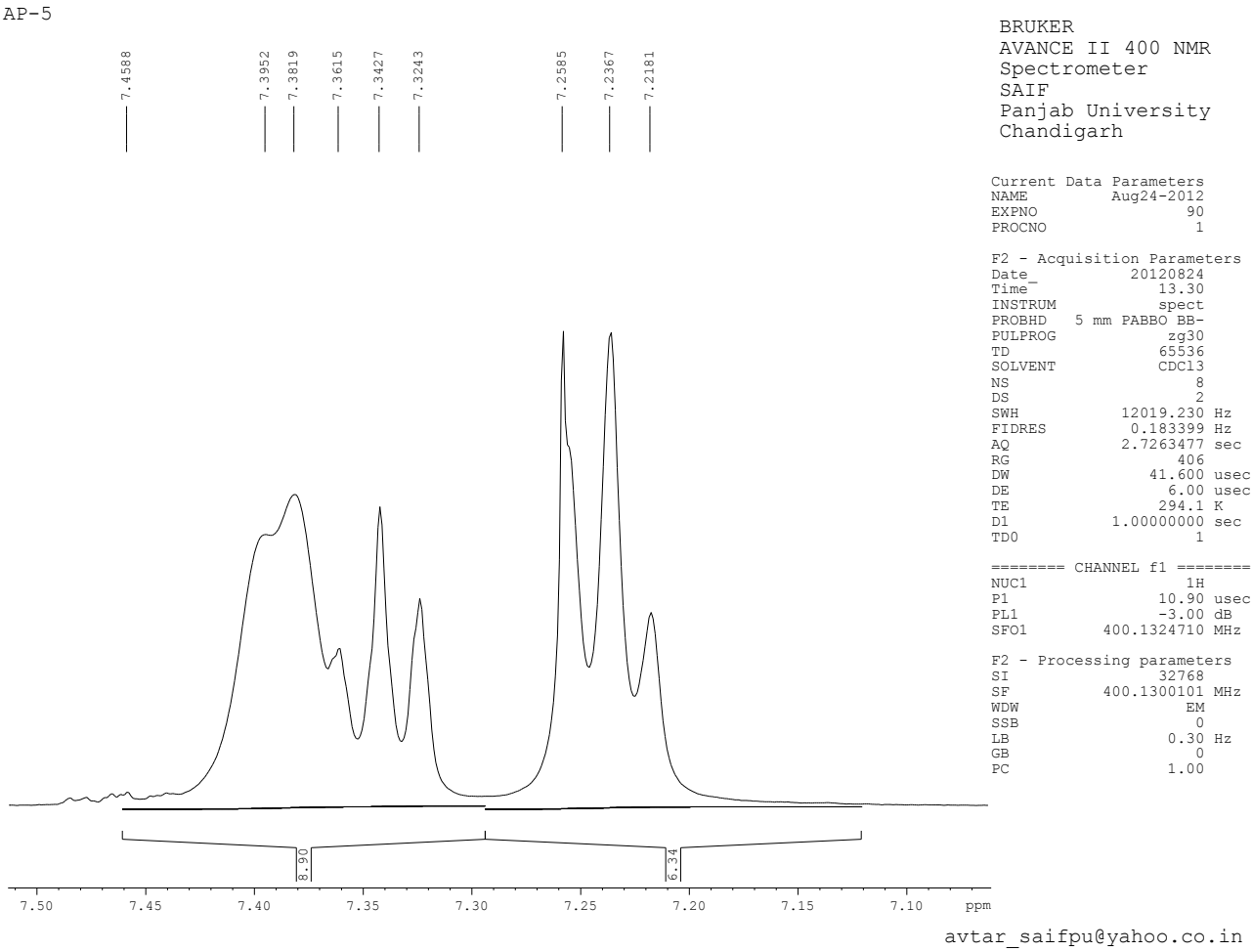

Fig.6b.S. Expanded ^{1}H spectrum of $[Cu(tmtH_2)(PPh_3)_2]\cdot 0.5H_2O$ (6)

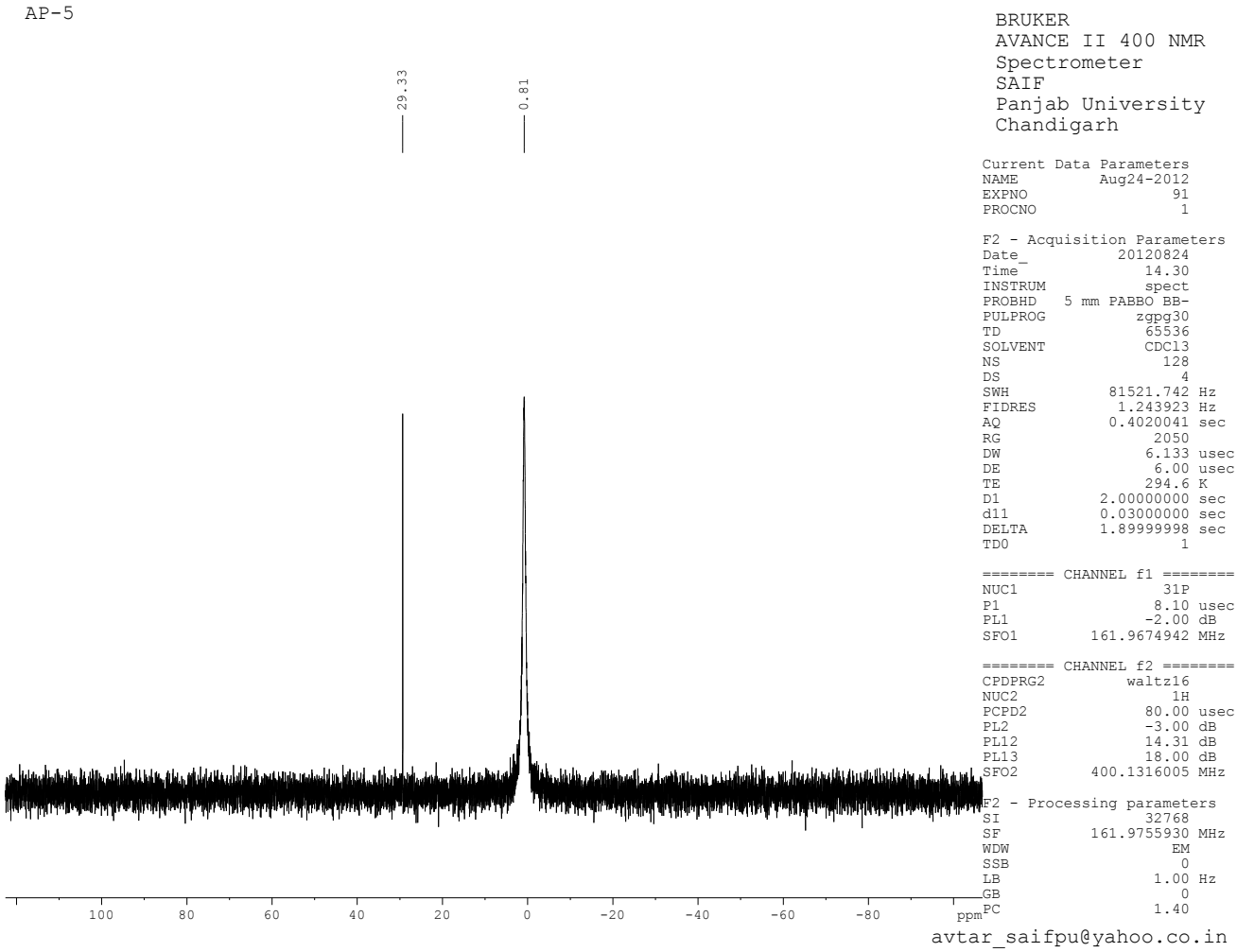

Fig.6c.S. ^{31}P spectrum of $[Cu(tmtH_2)(PPh_3)_2]\cdot 0.5H_2O$ (6)

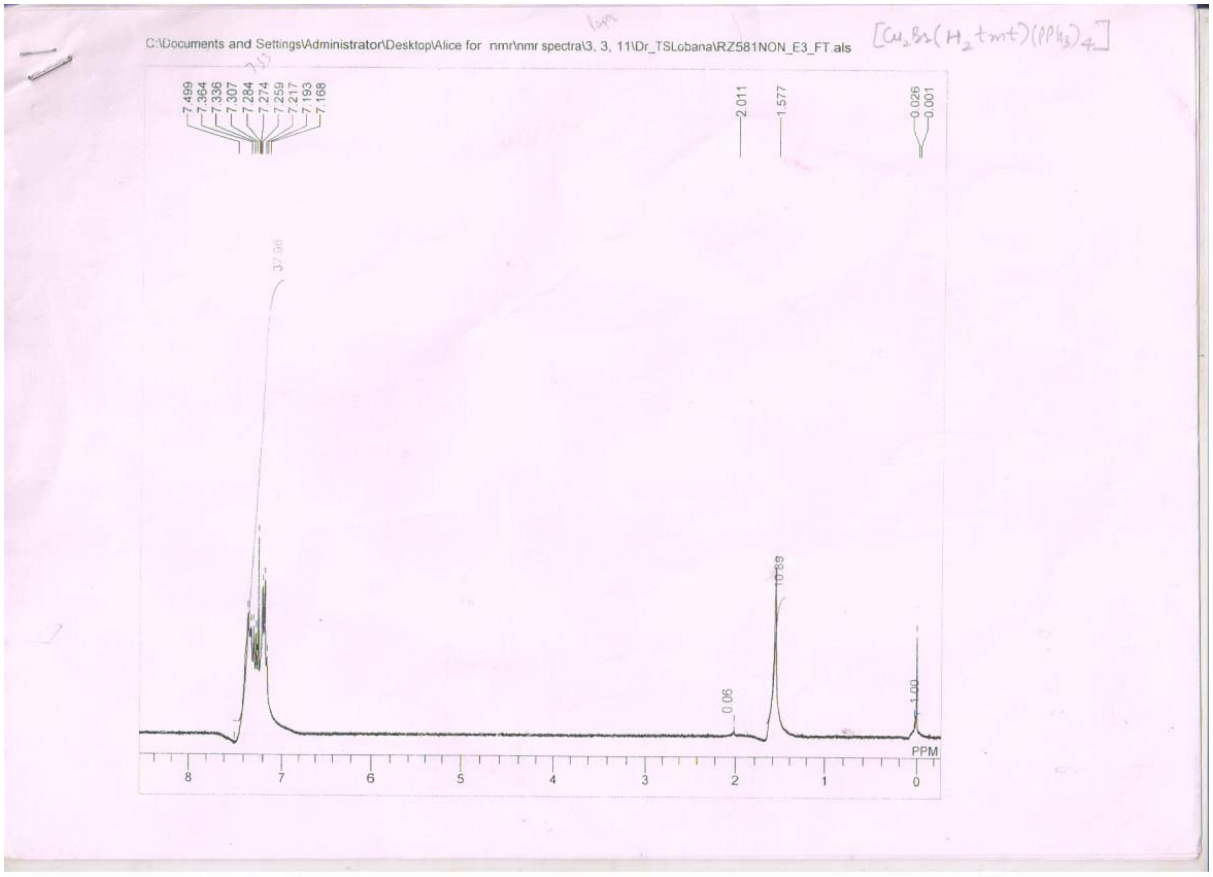

Fig.7a.S.^{1}H spectrum of $[Cu_3Br_2(\kappa^1N,\kappa^1S,\kappa^2S\text{-}tmtH_2)(PPh_3)_6]$(7)

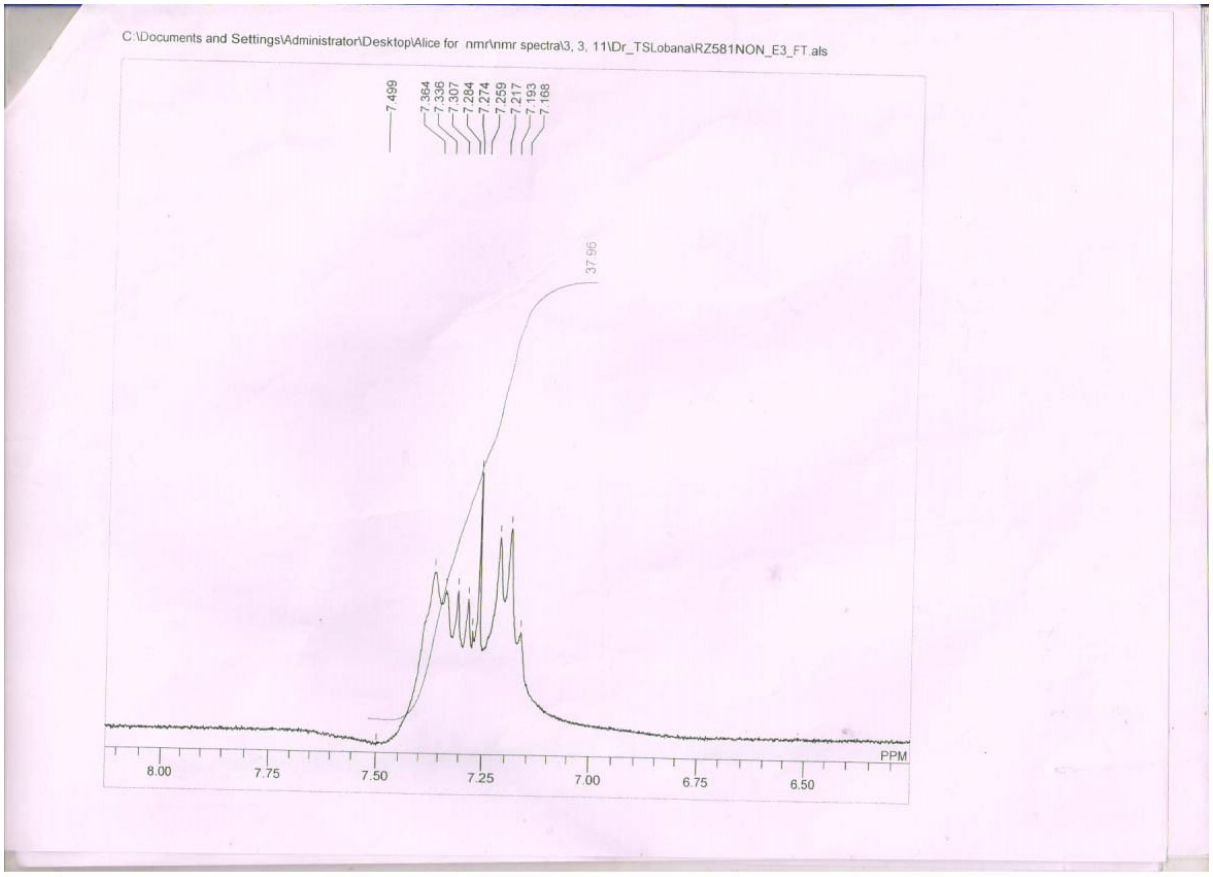

Fig. 7b.S. Expanded ^{1}H spectrum of $[Cu_3Br_2(\kappa^1N,\kappa^1S,\kappa^2S\text{-}tmtH_2)(PPh_3)_6]$(7)

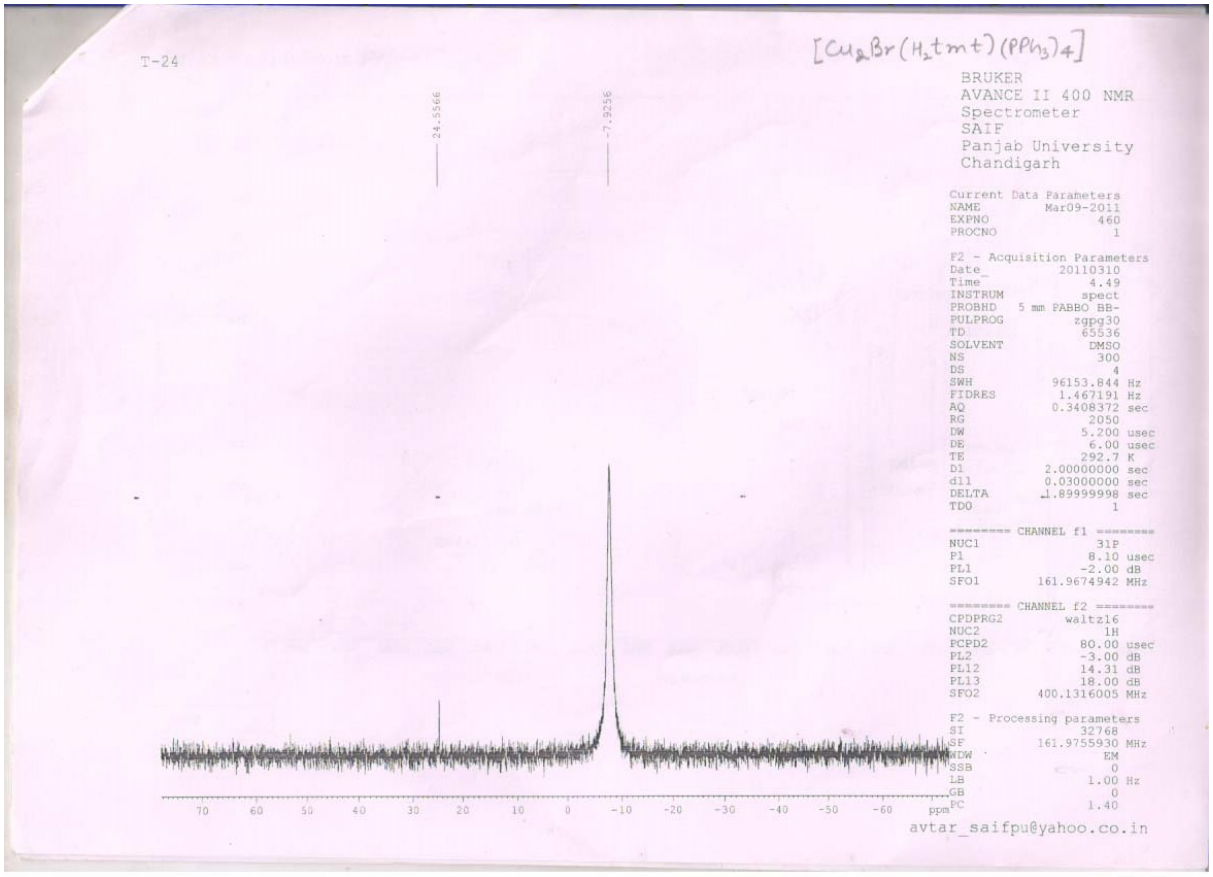

Fig. 7c.S. ^{31}P spectrum of $[Cu_3Br_2(\kappa^1N,\kappa^1S,\kappa^2S\text{-}tmtH_2)(PPh_3)_6]$(7)

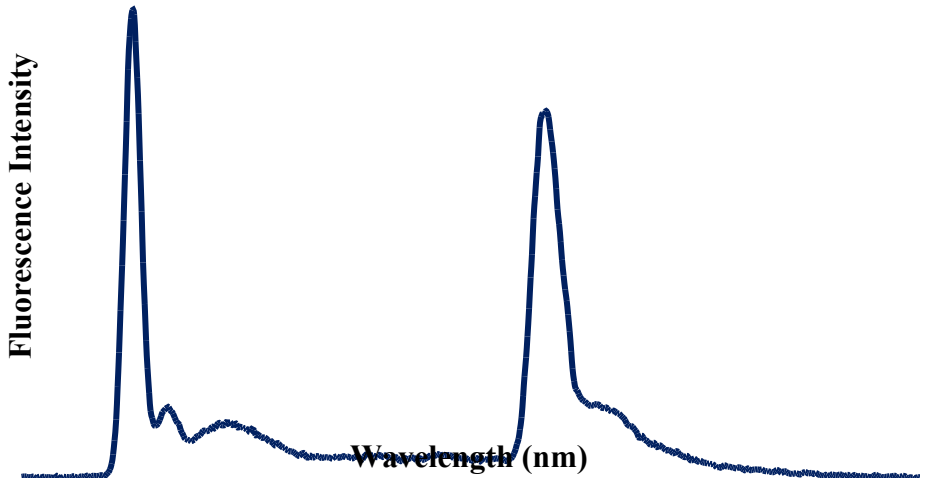

Figure 8. Fluorescence spectrum of DMSO ; λ_{ex} =276 nm