

Supplementary data for

Blue Copper Protein Analogue: Synthesis and Characterization of Copper Complexes of the NSNS Macrocyclic 1,8-dithia-4,11- diazacyclotetradecane

Tia L. Walker^{*a}, Sam Mula^b, Wilhelm Malasi^c, James T. Engle^c, Christopher J. Ziegler^c, A. van der Est^b, Jody Modarelli^d and Michael J. Taschner^c

Department of Chemistry, Physics and Astronomy

Indiana University Northwest

Gary, IN 46408, USA

Email: tialwalk@iun.edu

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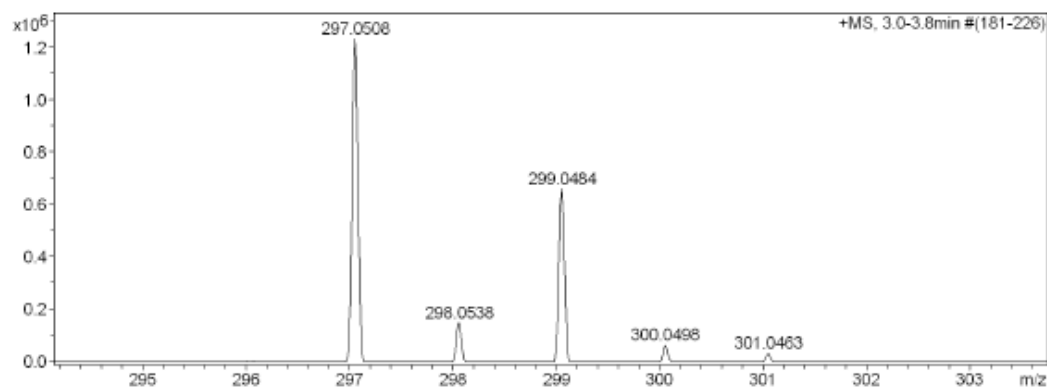
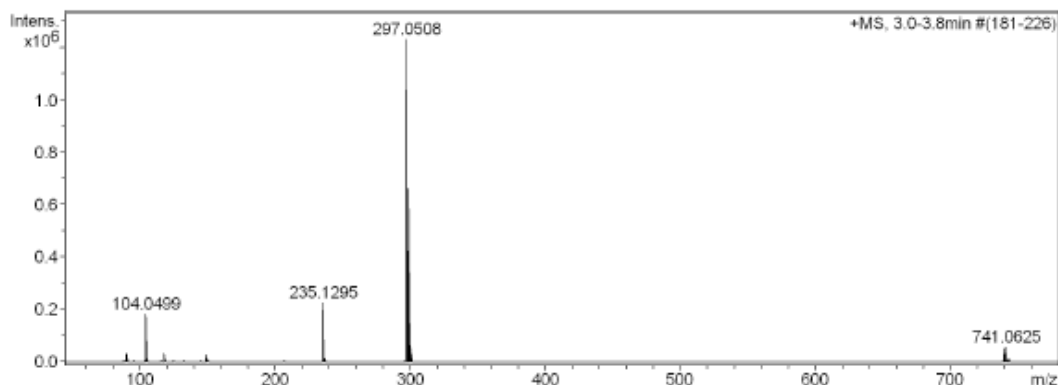
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General information

Instrumentation: All ¹H and ¹³C-NMR spectra were obtained using a Varian Mercury 300 spectrometer, operating at either 300 MHz (¹H) or 75 MHz (¹³C). Chemical shifts were referenced relative to the residual solvent peak.

Cu High Resolution Mass Spectrometry: [Cu+(14aneNSNS)]PF₆⁻

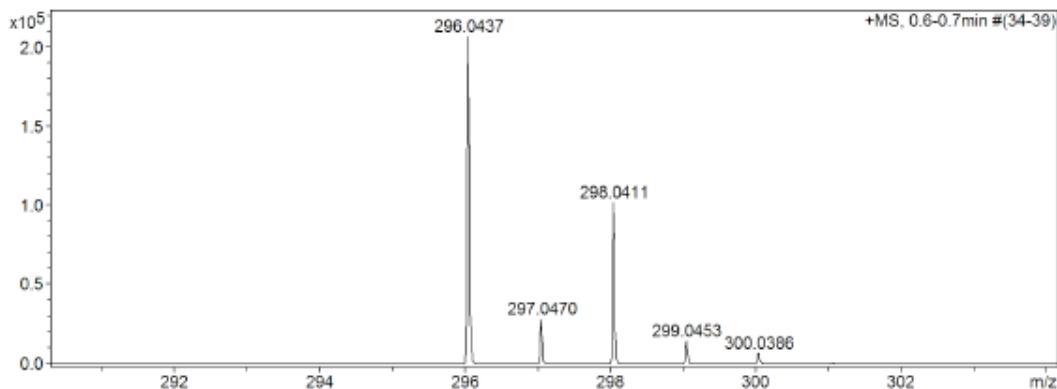
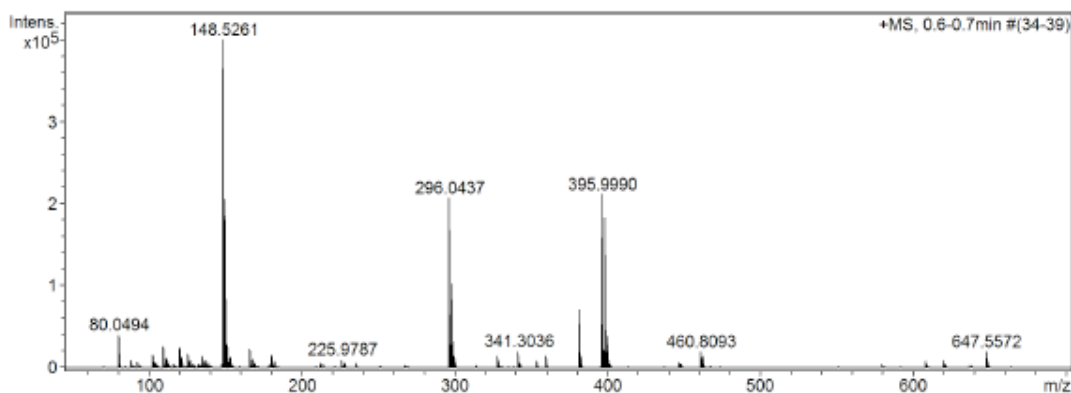
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Acquisition Parameter			
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Focus	Not active	Set Capillary	4500 V
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Scan End	3000 m/z	n/a	n/a
		Set Nebulizer	0.3 Bar
		Set Dry Heater	180 °C
		Set Dry Gas	4.0 l/min
		Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule
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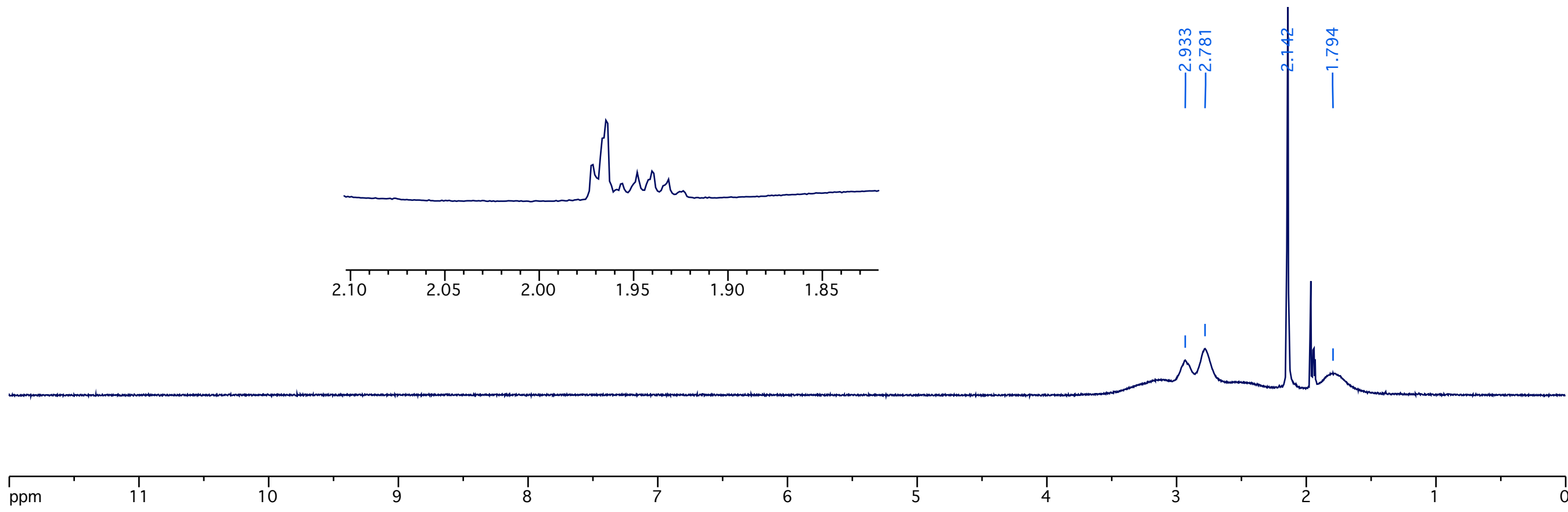
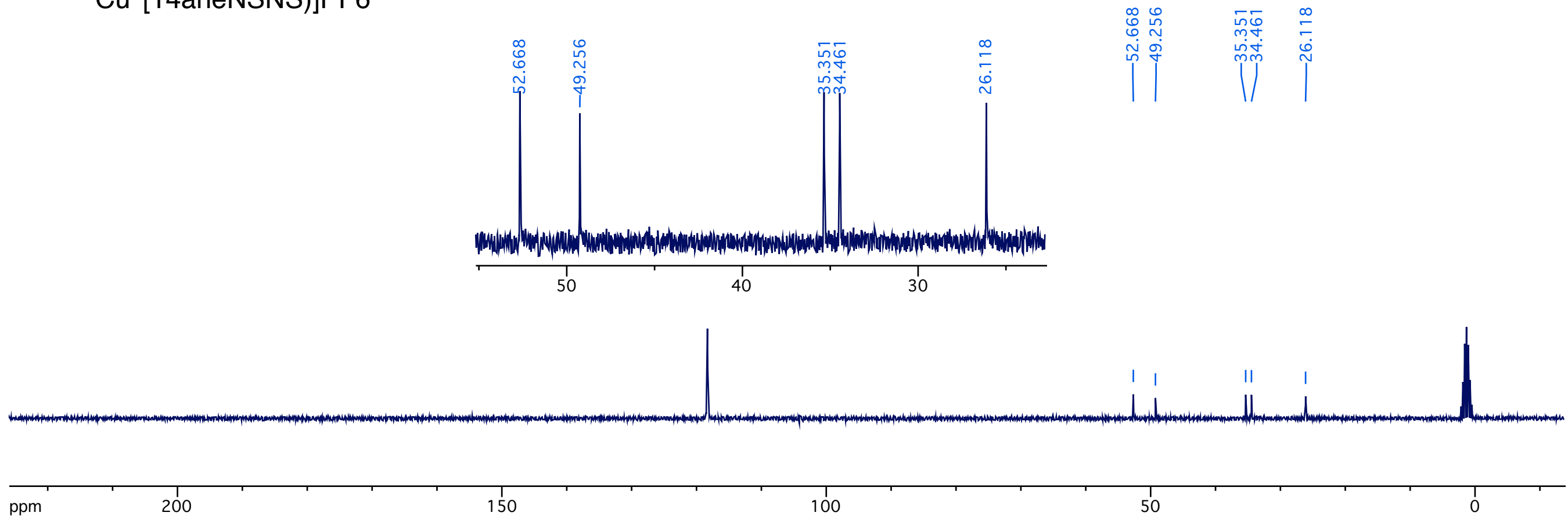
Cu High Resolution Mass Spectrometry: [Cu²⁺(14aneNSNS)]ClO₄⁻

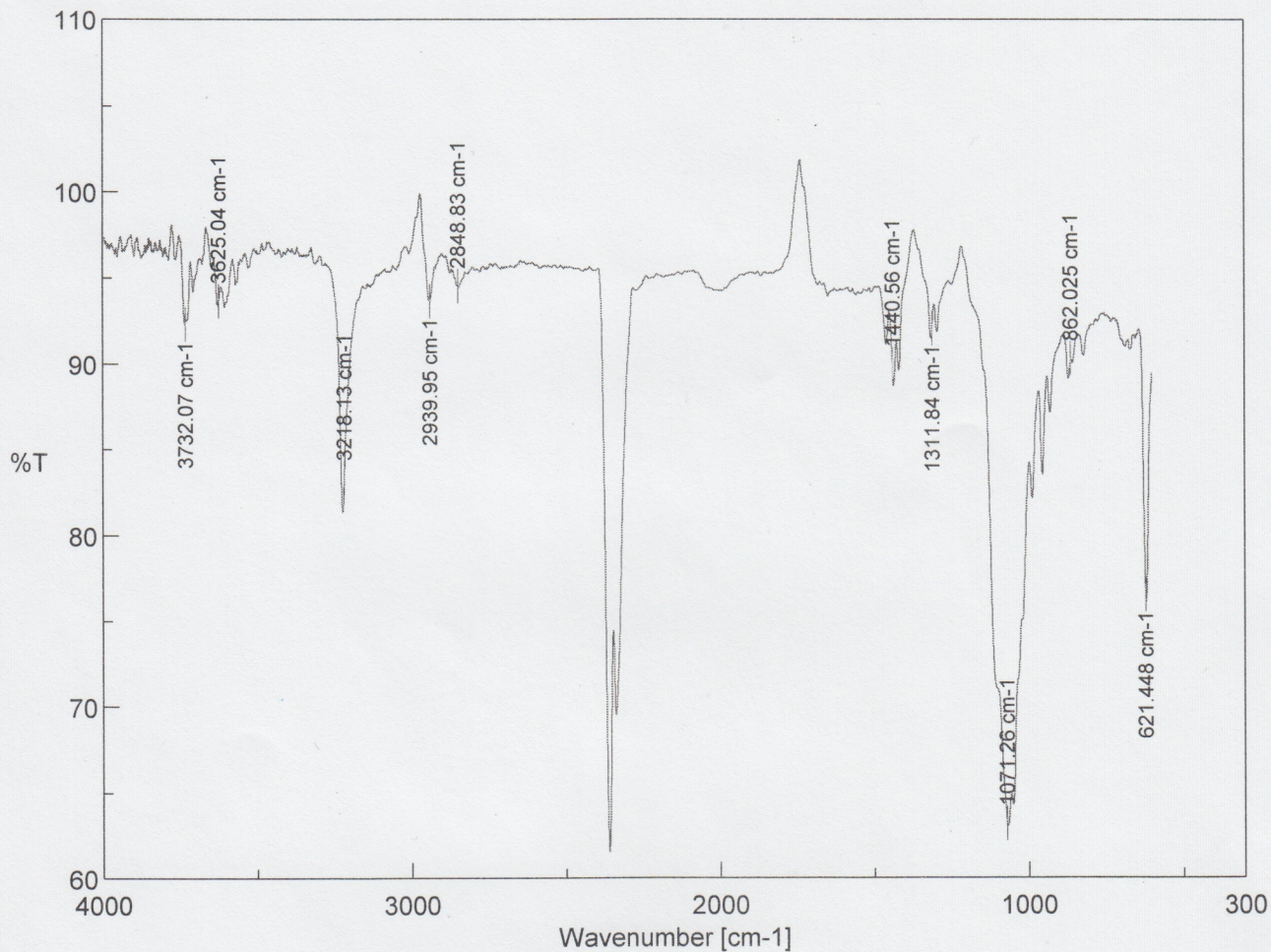
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Method	tune_low.m			Instrument / Ser#	micrOTOF-Q 10195
Sample Name	N2S2Cu-II				
Comment	N2S2Cu-II in acetonitrile at 4 ul/min				
Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



Meas. #	Formula	m/z	err [ppm]	Mea n err [ppm]	rdb	N-R ul e	e ⁻ Co nf	mSi gma	Std l	Std Me an m/z	Std l Va rN or m	Std m/z Diff	Std Com b Dev
296.0437	1 C 13 H 17 Cu N 2 S	296.0403	-11.3	-10.7	8.0	ok	odd	10.4	14.5	3.2	5.5	0.6	994.6
	2 C 10 H 21 Cu N 2 S 2	296.0437	0.1	0.6	1.0	ok	odd	21.5	28.1	0.4	7.4	0.7	872.3

Cu⁺[14aneNSNS)]PF₆⁻





Memory-8

[Comment]

Sample Name
 Comment
 User
 Division
 Company Indiana U.

[Measurement Information]

Model Name FT/IR-4200typeA
 Serial Number B008361018

Accessory ATR PRO450-S
 Accessory S/N A098261272

Light Source Standard
 Detector TGS
 Accumulation 100
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 Zero Filling On
 Apodization Cosine
 Gain Auto (16)
 Aperture Auto (5 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Data Information]

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 Data points 7054

