

Electronic Supplementary Information for:

Converting drugs into gelators: supramolecular hydrogels from *N*-acetyl-L-cysteine and coinage-metal salts

Pablo Casuso, Pedro Carrasco, Iraida Loinaz, Hans J. Grande and Ibon Odriozola*

CIDETEC Centre for Electrochemical Technologies, New Materials Department, Paseo Miramón 196, 20009 Donostia-San Sebastián, Spain

* To whom correspondence should be addressed. E-mail: iodriozola@cidetec.es

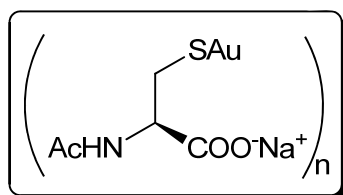
Purification of M-NAC hydrogels

Au-NAC and **Ag-NAC** hydrogels were dissolved by the addition of NaOH 1N and the resulting solutions were dialysed against ultrapure water for 3 days. Then, the solutions were freeze-dried to give the corresponding compounds as white solids. **Cu-NAC** was unstable to dialysis and it was purified as follows: the gel was diluted in HCl 0.001 N. The resulting suspension was then centrifuged and washed several times with HCl 0.001 N. The product was lyophilised to give **Cu-NAC** as a white solid.

Energy dispersive X-ray spectroscopy (EDS)

Analyses were performed on an INCA-300 model from OXFORD, operated at an accelerating voltage of 20 kV.

Au-NAC



Chemical Formula: C₅H₇AuNNaO₃S

Calculated elemental analysis (%): C, 15.76; H, 1.85; Au, 51.68; N, 3.67; Na, 6.03; O, 12.59; S, 8.41

All results in atomic percent:

	C	N	O	Na	S	Au	Total
zone 1	30.92	12.39	33.37	6.21	9.41	7.69	100.00
zone 2	31.80	12.94	32.89	6.19	8.98	7.20	100.00
zone 3	30.96	14.96	34.13	6.18	7.50	6.27	100.00

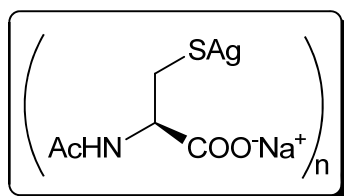
	C	N	O	Na	S	Au
Max.	31.80	14.96	34.13	6.21	9.41	7.69
Min.	30.92	12.39	32.89	6.18	7.50	6.27

All results in weight percent:

	C	N	O	Na	S	Au	Total
zone 1	12.22	5.71	17.57	4.70	9.93	49.86	100.00
zone 2	13.00	6.17	17.91	4.84	9.80	48.29	100.00
zone 3	13.55	7.63	19.89	5.17	8.76	45.00	100.00

	C	N	O	Na	S	Au
Max.	13.55	7.63	19.89	5.17	9.93	49.86
Min.	12.22	5.71	17.57	4.70	8.76	45.00

Ag-NAC



Chemical Formula: C₅H₇AgNNaO₃S

Calculated elemental analysis (%): C, 20.56; H, 2.42; Ag, 36.94; N, 4.80; Na, 7.87; O, 16.44; S, 10.98

All results in atomic percent:

	C	N	O	Na	S	Ag	Total
zone 1	22.29	19.70	32.84	6.75	9.10	9.31	100.00
zone 2	23.63	21.14	34.97	7.10	6.67	6.48	100.00
zone 3	21.80	22.24	34.39	6.54	7.58	7.44	100.00

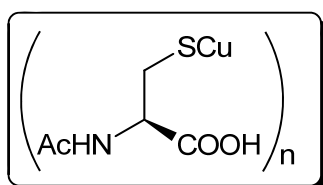
	C	N	O	Na	S	Ag
Max.	23.63	22.24	34.97	7.10	9.10	9.31
Min.	21.80	19.70	32.84	6.54	6.67	6.48

All results in weight percent:

	C	N	O	Na	S	Ag	Total
zone 1	10.62	10.95	20.85	6.16	11.58	39.84	100.00
zone 2	12.81	13.36	25.25	7.37	9.65	31.56	100.00
zone 3	11.29	13.43	23.72	6.49	10.48	34.60	100.00

	C	N	O	Na	S	Ag
Max.	12.81	13.43	25.25	7.37	11.58	39.84
Min.	10.62	10.95	20.85	6.16	9.65	31.56

Cu-NAC



Chemical Formula: $C_5H_8CuNO_3S$

Calculated elemental analysis (%): C, 26.60; H, 3.57; Cu, 28.15; N, 6.20; O, 21.26; S, 14.20

All results in atomic percent:

	C	N	O	S	Cu	Total
zone 1	32.15	9.84	41.02	7.95	9.04	100.00
zone 2	31.38	12.70	37.25	8.98	9.68	100.00
zone 3	31.79	10.54	42.66	7.71	7.31	100.00

	C	N	O	S	Cu
Max.	32.15	12.70	42.66	8.98	9.68
Min.	31.38	9.84	37.25	7.71	7.31

All results in weight percent:

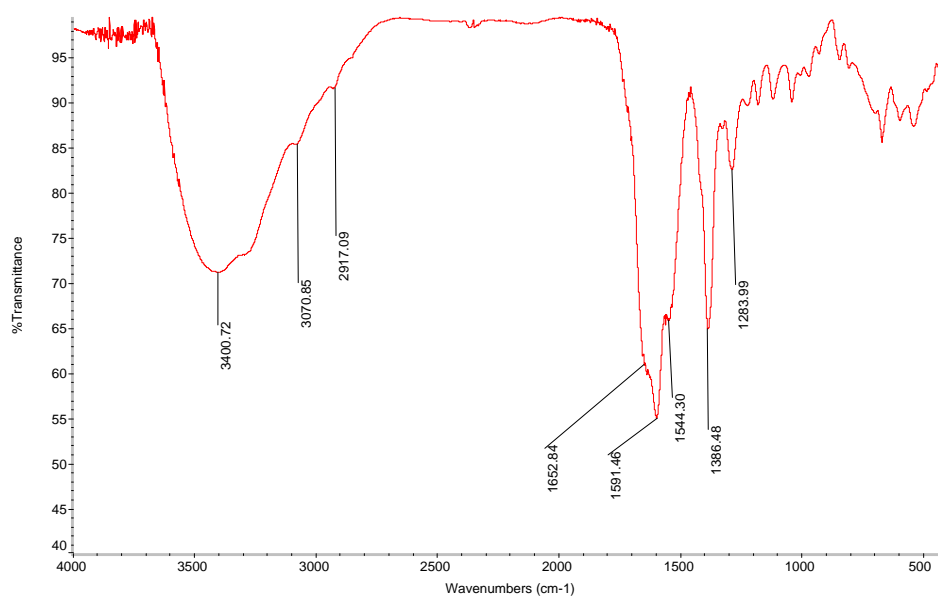
	C	N	O	S	Cu	Total
zone 1	19.21	6.86	32.66	12.68	28.59	100.00
zone 2	18.35	8.66	29.02	14.01	29.95	100.00
zone 3	19.85	7.67	35.48	12.84	24.15	100.00

	C	N	O	S	Cu
Max.	19.85	8.66	35.48	14.01	29.95
Min.	18.35	6.86	29.02	12.68	24.15

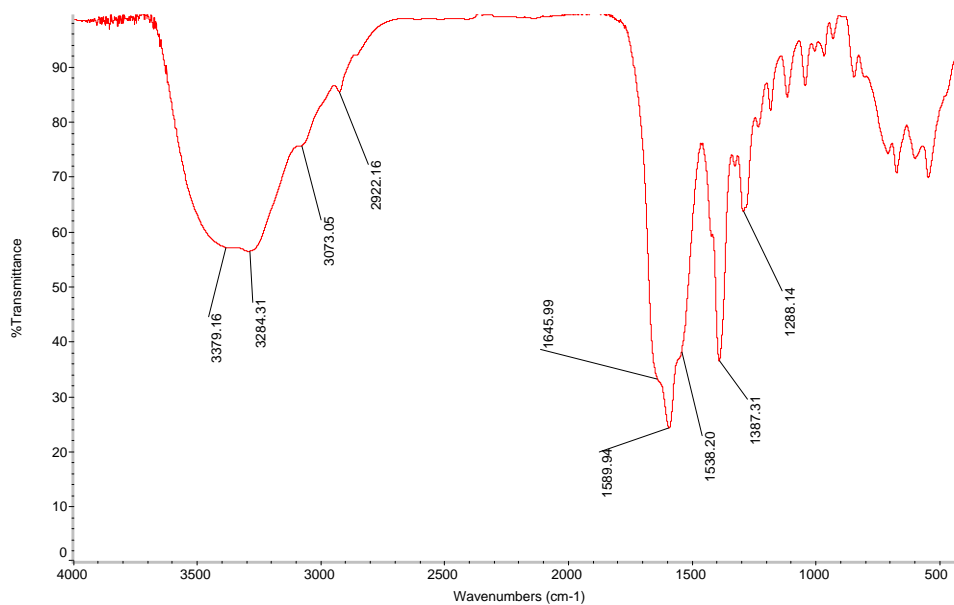
FT-IR Spectra

Fourier Transformed Infra-Red Spectroscopy (FT-IR) spectra were taken from a Nicolet Avatar 360 apparatus. All samples were measured in KBr disks.

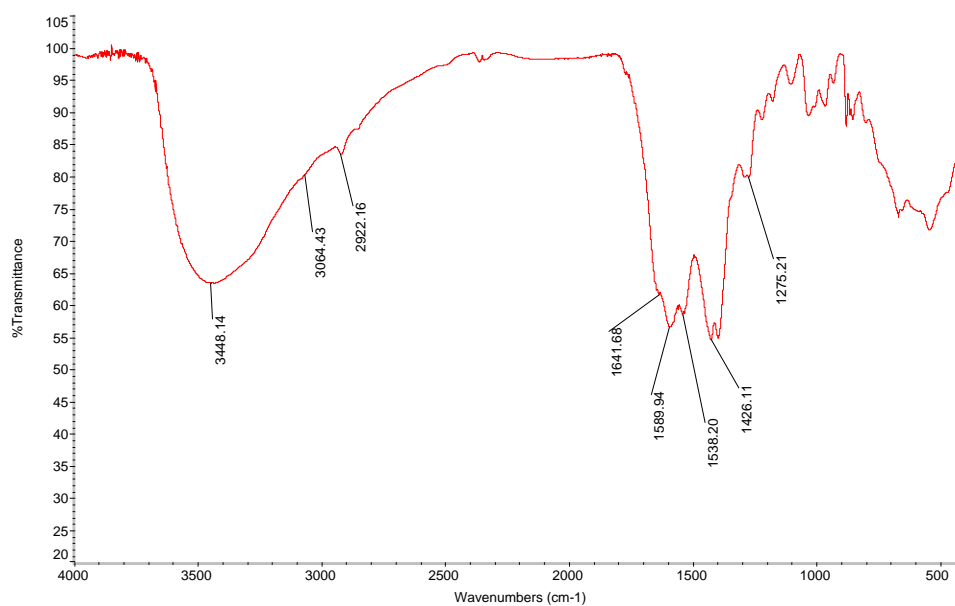
Au-NAC



Ag-NAC



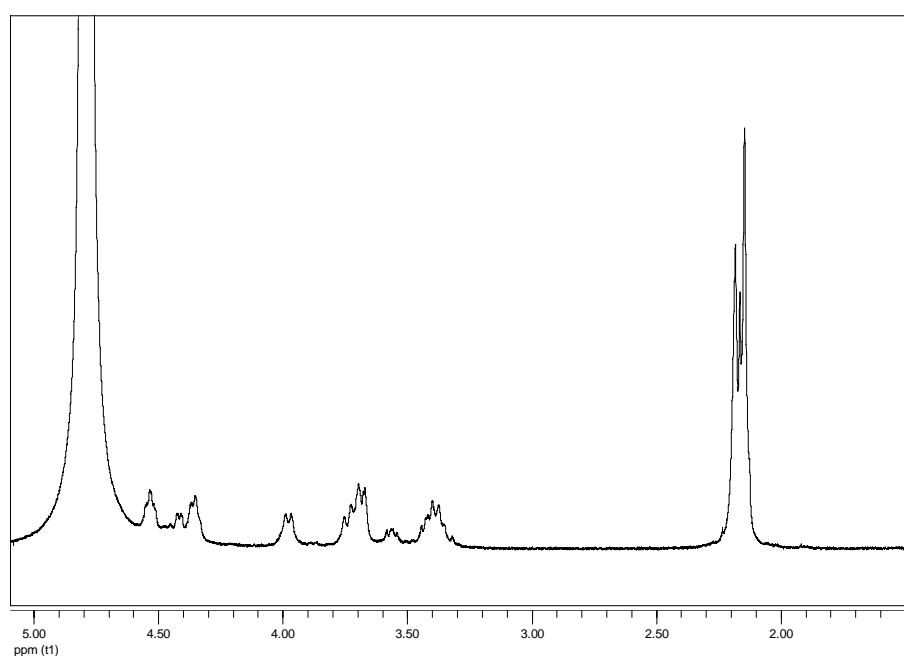
Cu-NAC



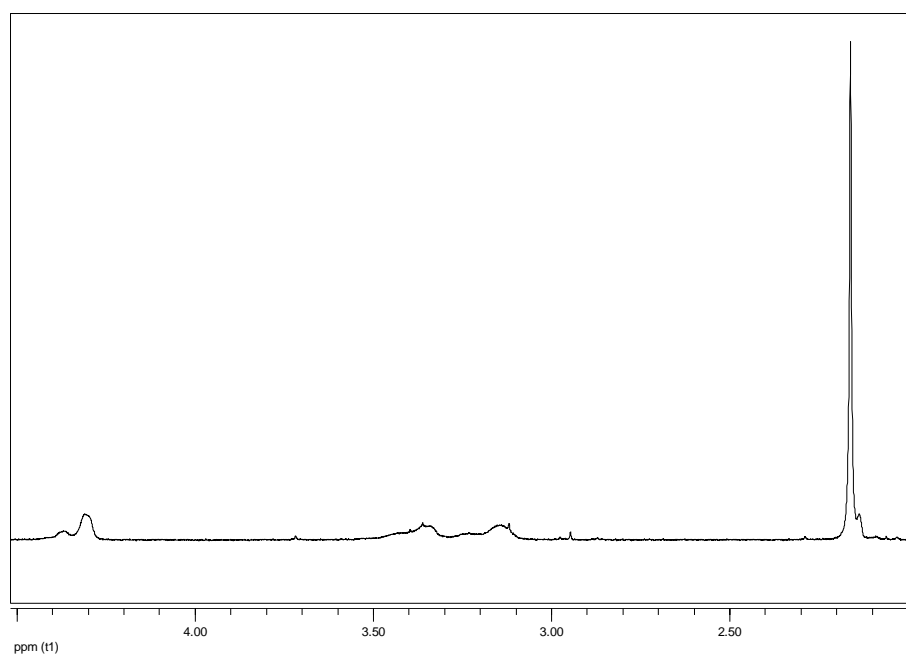
¹H NMR Spectra

Proton nuclear magnetic resonance (¹H NMR) experiments were performed on a Bruker AVANCE III spectrometer at 500 MHz. All samples were measured at room temperature in D₂O.

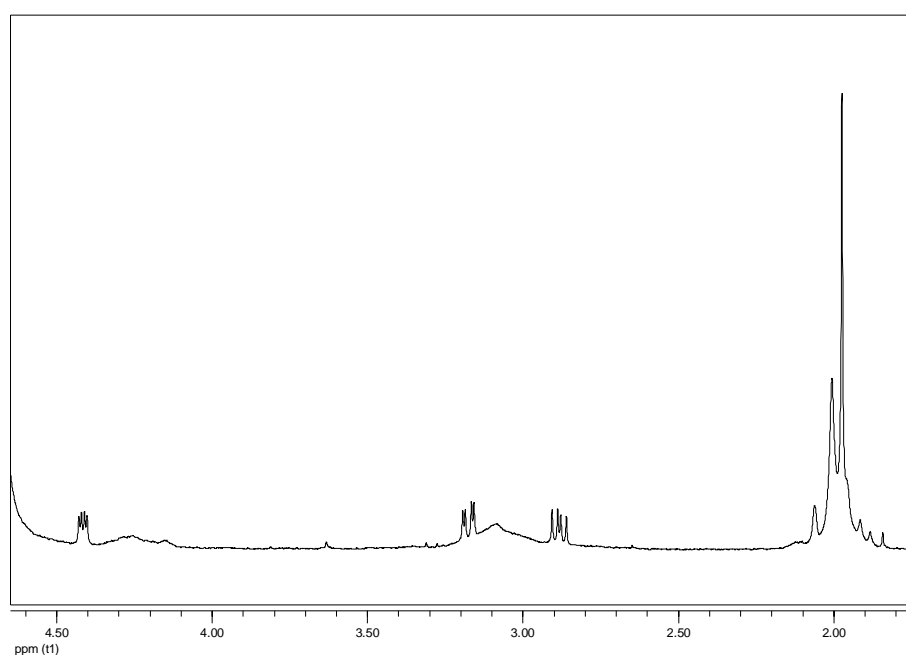
Au-NAC



Ag-NAC



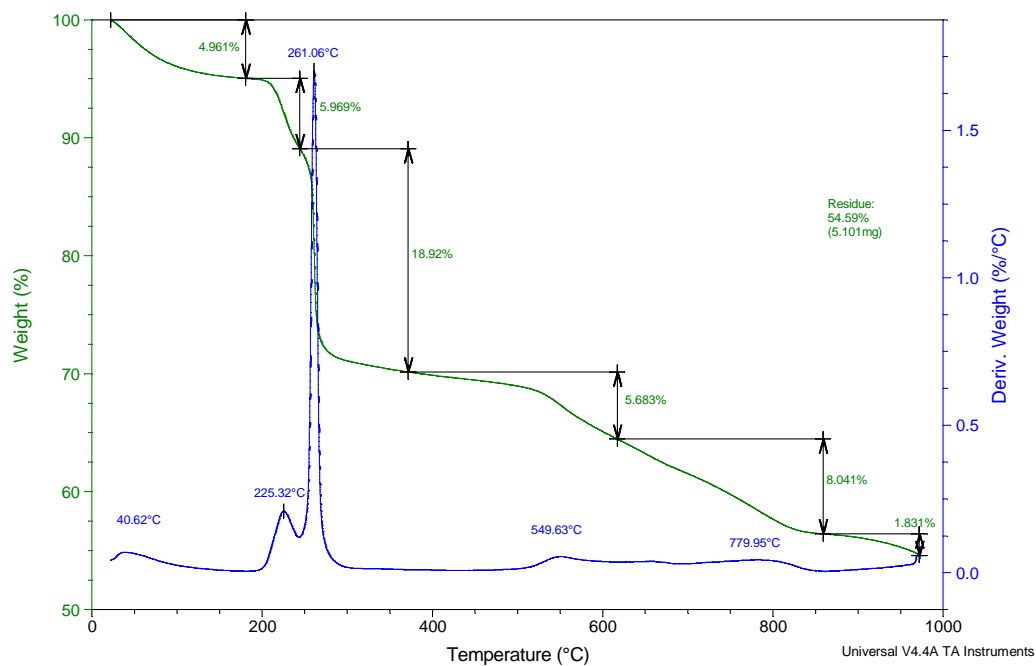
Cu-NAC



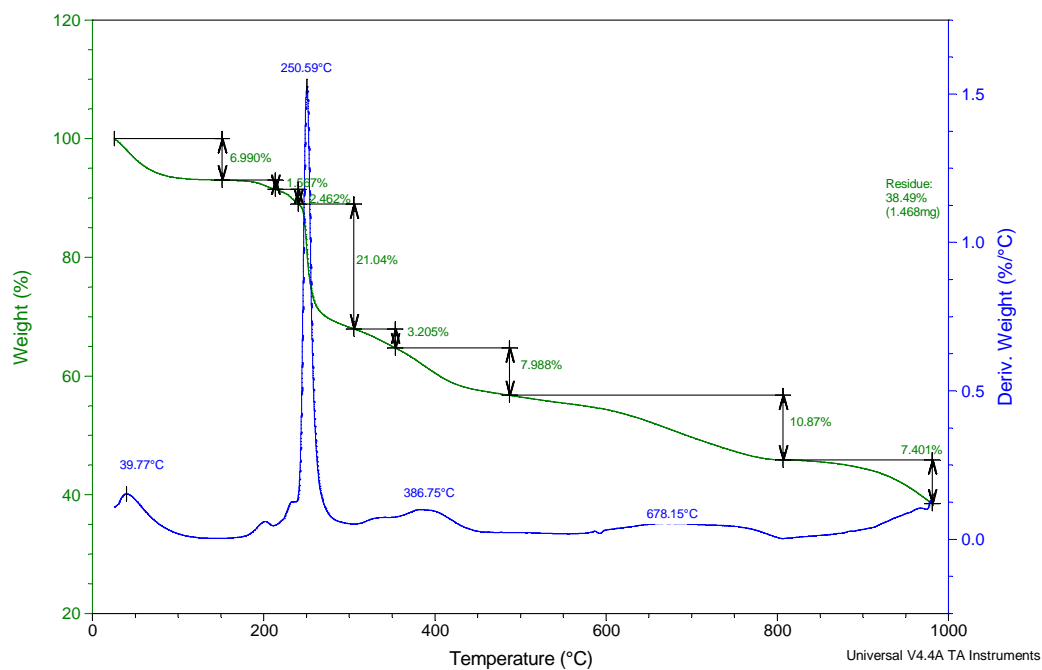
TGA Spectra

Thermogravimetric analyses (TGA) were performed on a Q500 apparatus from TA Instruments. The analyses were run under nitrogen, from room-temperature to 1000 °C at a rate of 10 °C min⁻¹.

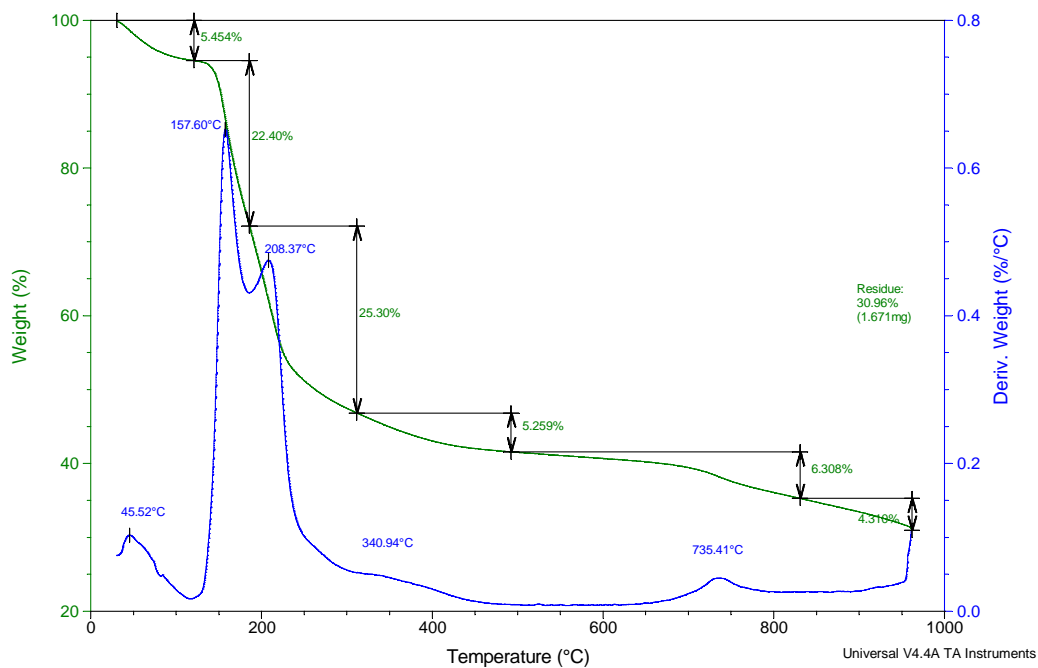
Au-NAC



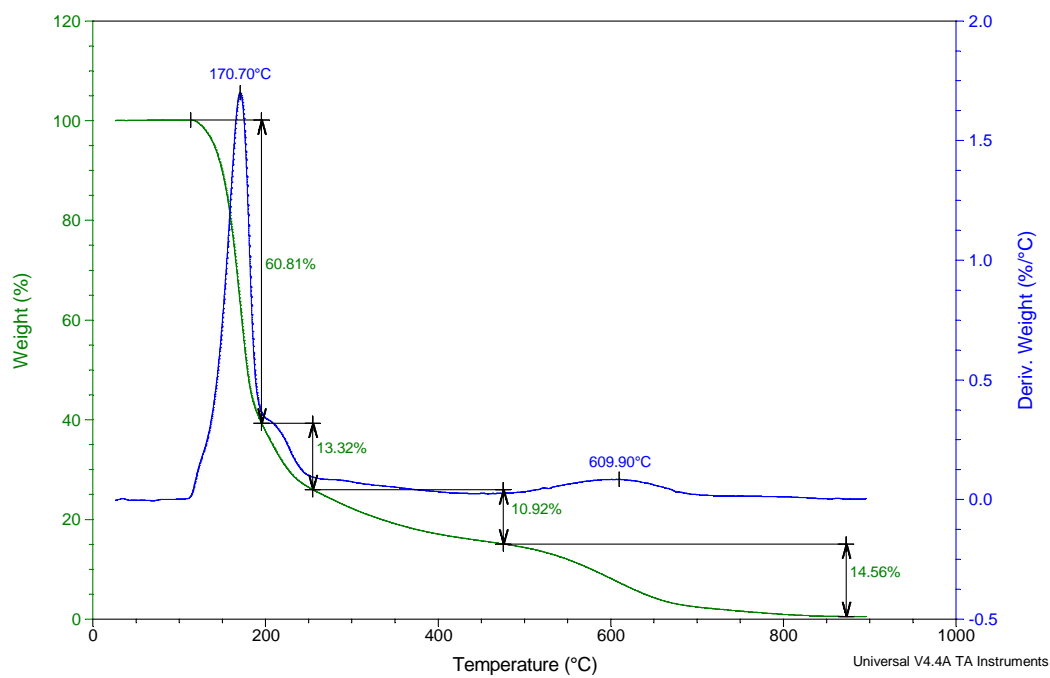
Ag-NAC



Cu-NAC



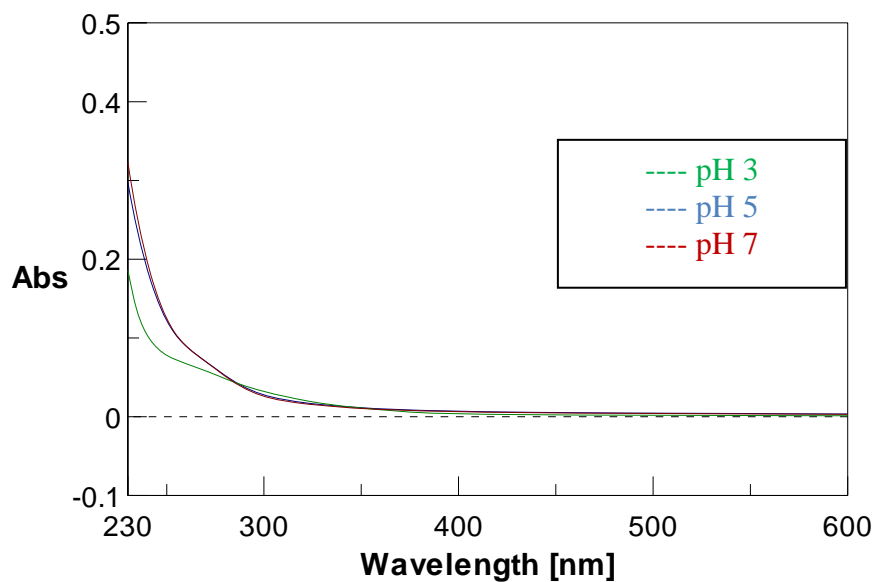
N-acetyl-L-cysteine



UV-vis Spectra

Spectra were acquired on a JASCO V-570 spectrophotometer at room temperature.

Ag-NAC



Cu-NAC

