Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Towards the Synthesis of Sugar Amino Acid Containing Antimicrobial Noncytotoxic CAP Conjugates with Gold Nanoparticles and Their Mechanistic Study Towards Cell Disruption[§]

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Supporting Information

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General Procedure for Attachment of Thiol functionalized AuNP in toluene to the Synthesized Peptides: Peptide **1** (10 mg) was taken in a 5 ml pear shaped flask. To it 0.5 mL of dry MeOH was added. Then 0.5 mL of octanethiol functionalized Au nanoparticle in toluene (2-4 nm, 2% w/v; from Sigma-Aldrich) was added to the solution and incubated at room temperature for 4 days. Thereafter, the supernatant liquid was decanted and the precipitated particles were washed with MeOH. Now, supernatant liquid and washings were combined and concentrated. The solid residue was re-dissolved in dry MeOH, vortexed and centrifuged to remove any unreacted Au nanoparticles. The supernatant liquid was decanted and the residue washed with dry MeOH. The combined clear MeOH solution was concentrated and the solid residue was washed with hexane to remove any trace of liberated octanethiol. The solid compound was then dried, dissolved in water to prepare the required concentrated AuNP attached aqueous peptide solution and submitted for the biological activity.

N.B.- A blank test was carried out to see if the octanethiol stabilized AuNPs were stable in methanol solution or not. A 0.5 mL of octanethiol stabilized AuNP solution was taken in a 5 mL pear shaped flask, concentrated and dried. 1mL dry MeOH was added and kept at room temperature for 4 days. No AuNP had come to the MeOH solution (detected by TEM). This indicated that our peptide (which contains the thiol functionality) was responsible to take the AuNP to polar solvent like MeOH or water.

General methods For RP-HPLC: an analytical Supelco C_5 column (4.6 mm i.d. × 250 mm, 5 μm particle size) was used in combination with elutants A (0.1% TFA in H_2O) and B (0.1% TFA in MeCN).

HPLC data

Peptide1

Linear gradient 20→85% B in 25 mins, total run 30 mins, t_R= 2.117 min

Peptide 2

Linear gradient 20→70% B in 30 mins, t_R= 4.315 min

Peptide 3

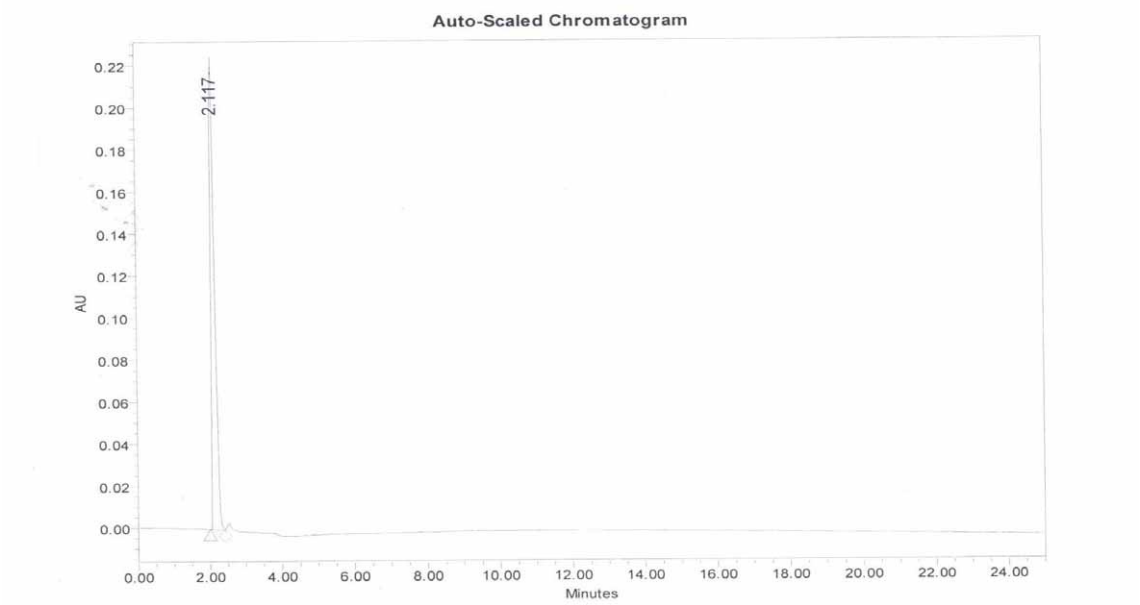
Linear gradient 30→85% B in 30 mins, t_R= 13.466 min

Peptide 4

Linear gradient 50→90% B in 10 mins, total run 20 mins, t_R= 18.701 min

HPLC chromatogram of

1

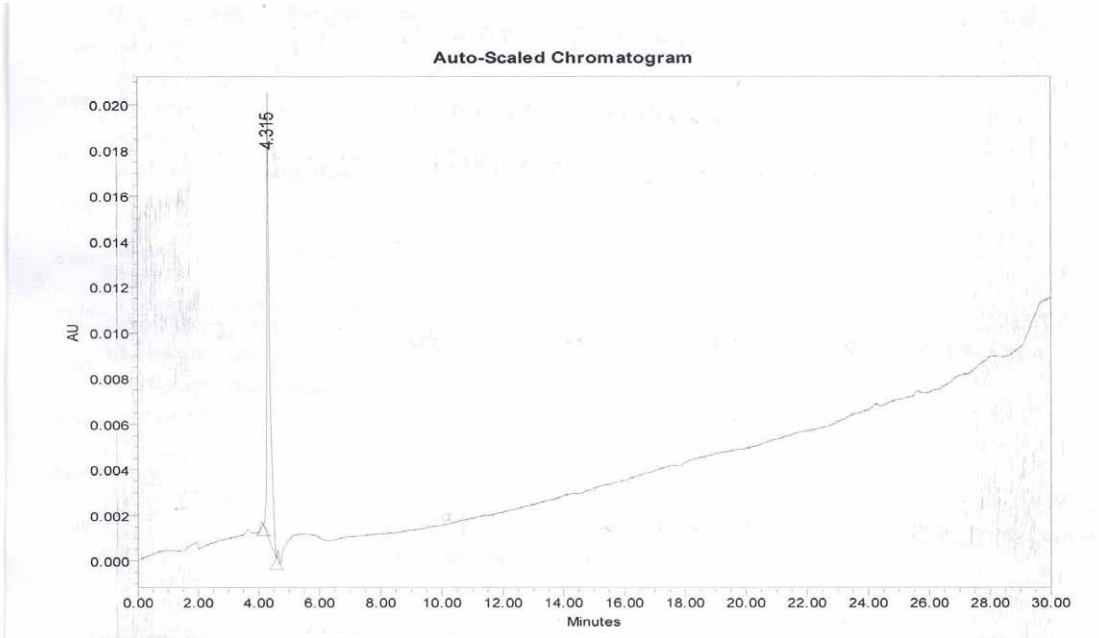


Peak Results

	Name	RT	Area	Height	% Area
1		2.117	1653953	220774	100.00

HPLC chromatogram of

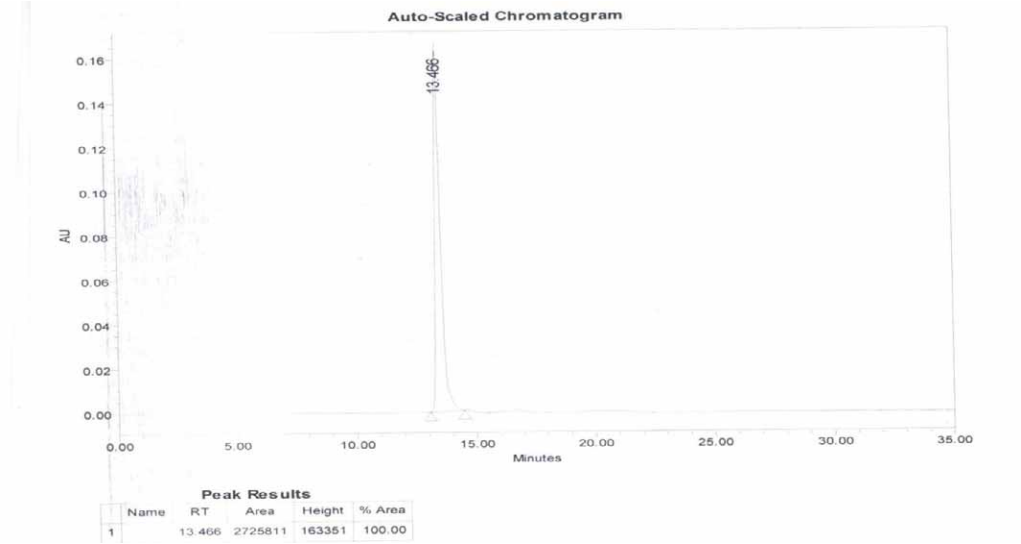
2



Peak Results

	Name	RT	Area	Height	% Area
1		4.315	122370	19124	100.00

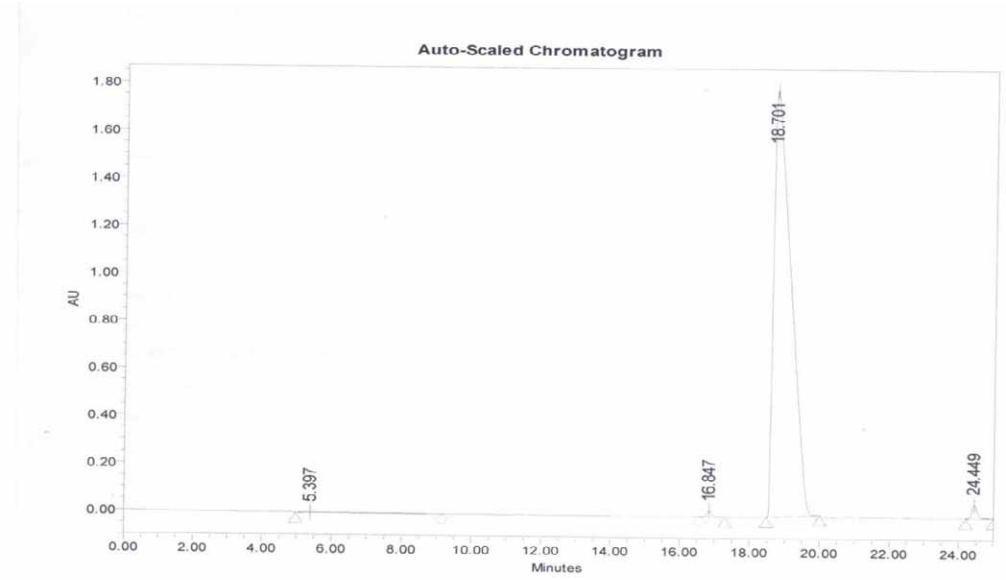
HPLC chromatogram of **3**



Peak Results

	Name	RT	Area	Height	% Area
1		13.466	2725811	163351	100.00

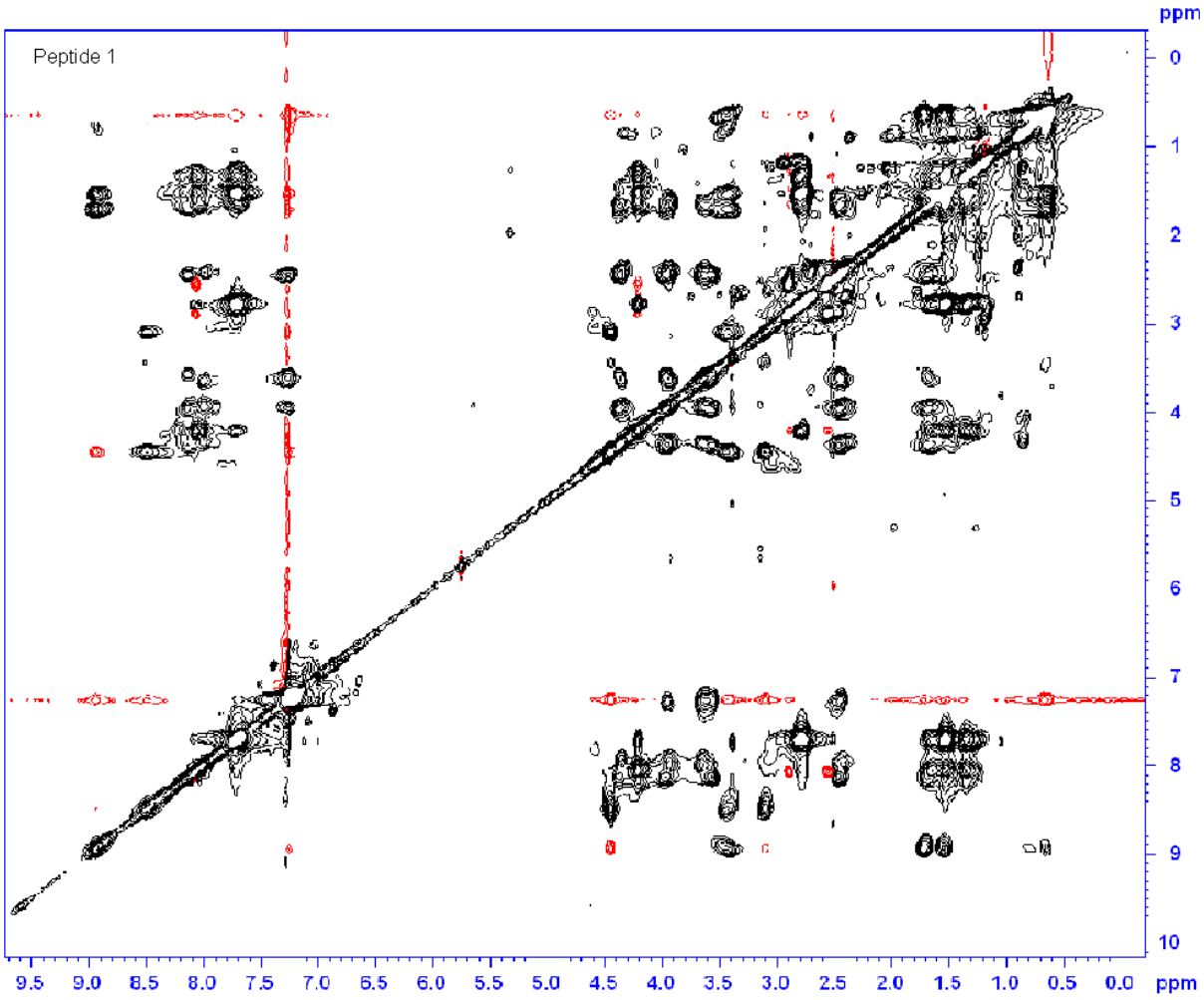
HPLC chromatogram of **4**



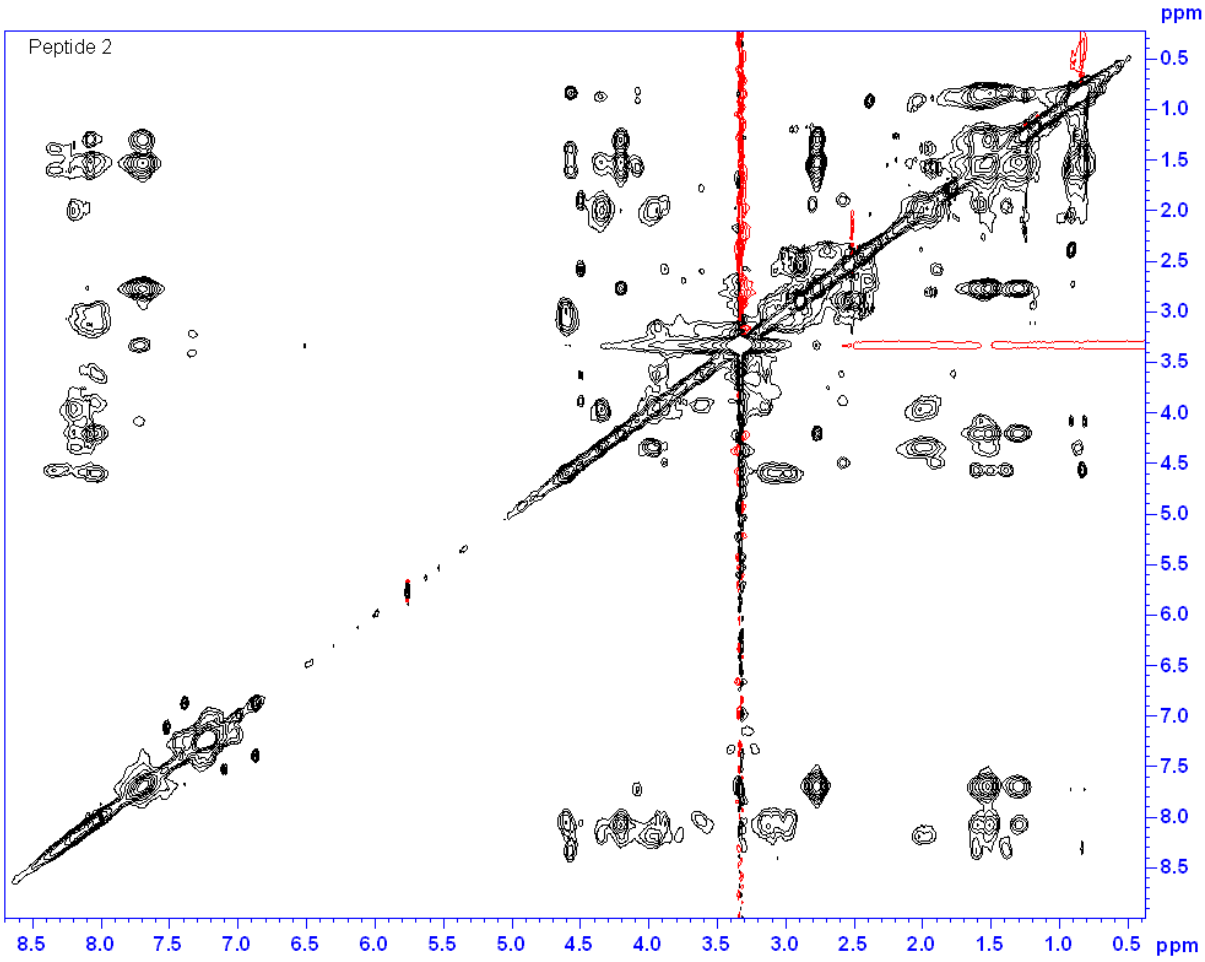
Peak Results

	Name	RT	Area	Height	% Area
1		5.397	248871	2160	0.40
2		16.847	218383	23613	0.35
3		18.701	60754101	1787315	98.20
4		24.449	647155	57531	1.05

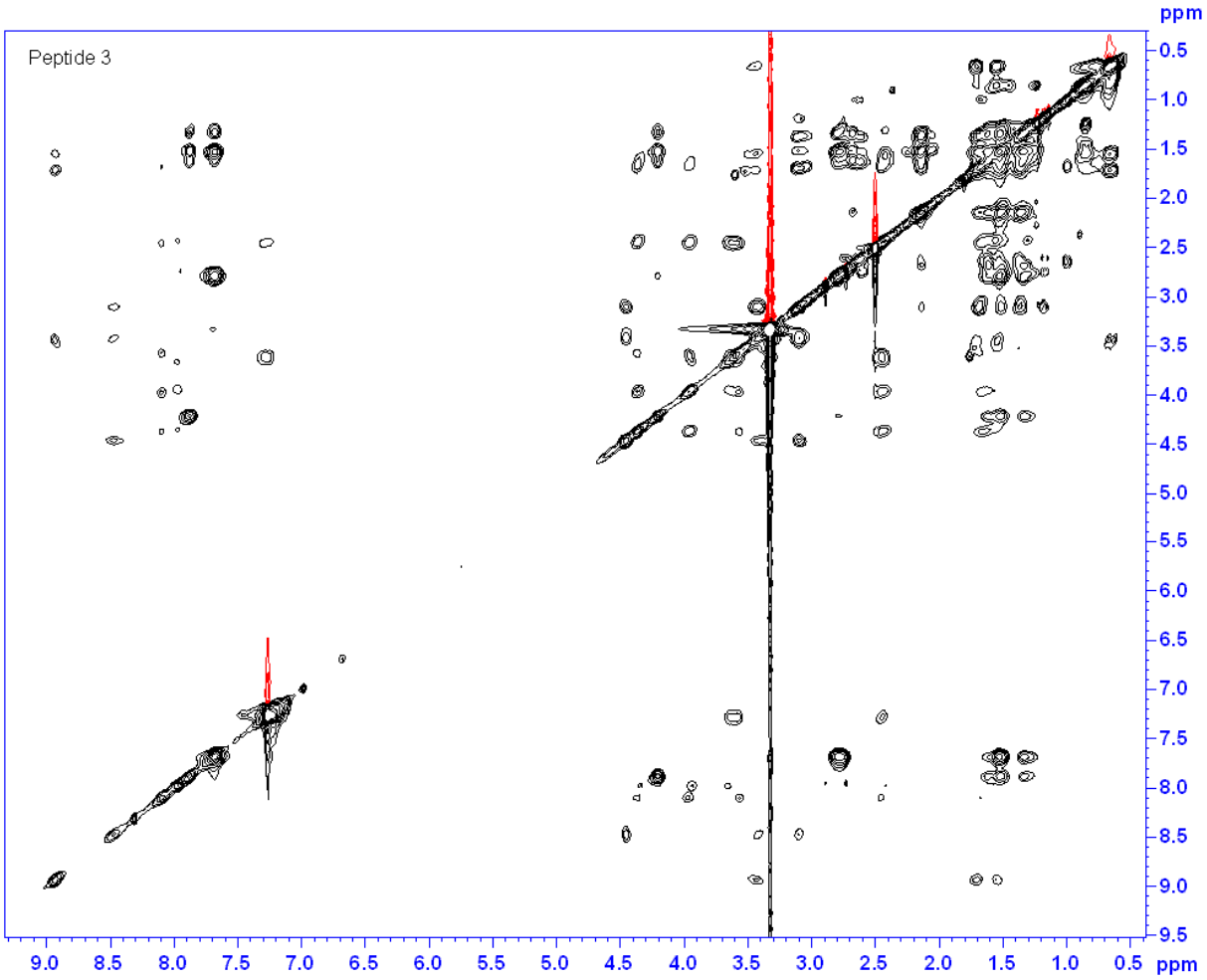
TOCSY spectrum of **1** (DMSO-D6, 300 K, 400 MHz)



TOCSY spectrum of **2** (DMSO-D6, 300 K, 400 MHz)



TOCSY spectrum of **3** (DMSO-D6, 300 K, 400 MHz)



TOCSY spectrum of **4** (DMSO-D6, 300 K, 400 MHz)