

Tetrahydro- β -carboline-3-carboxyl-thymopentin: A nano-conjugate for releasing pharmacophores to treat tumor and complications

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Supporting Information

1. NMR spectra of MTCTP5

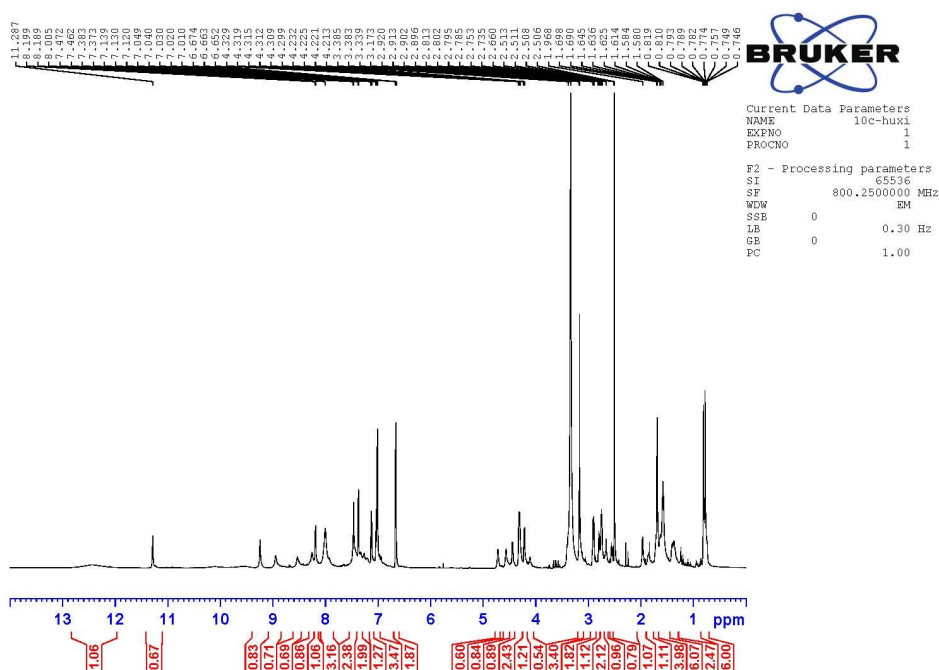


Fig. S1 ¹H NMR spectrum of MTCTP5

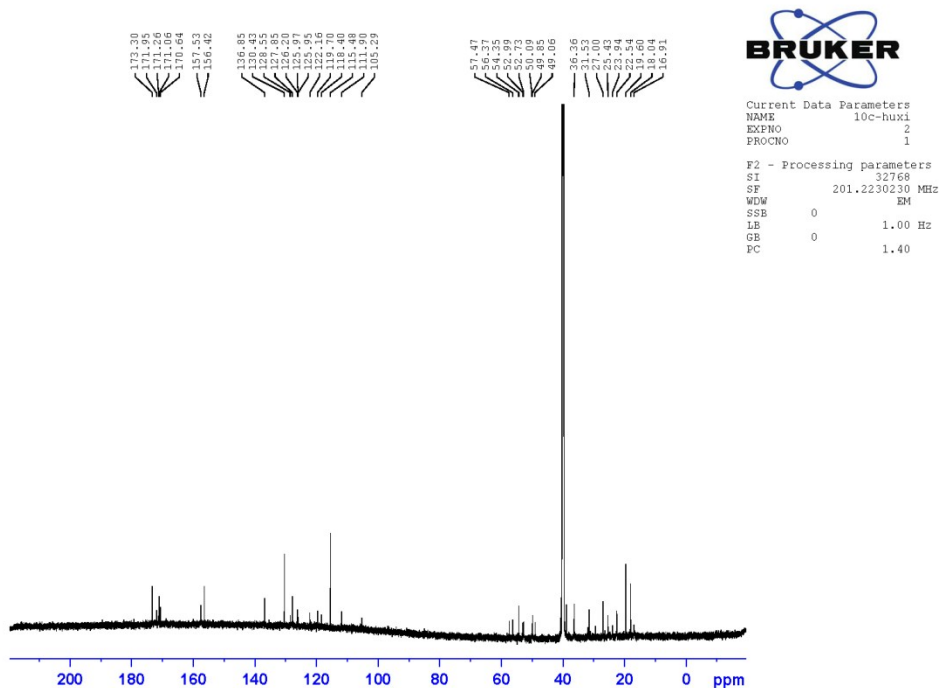


Fig. S2 ^{13}C NMR spectrum of MTCTP5

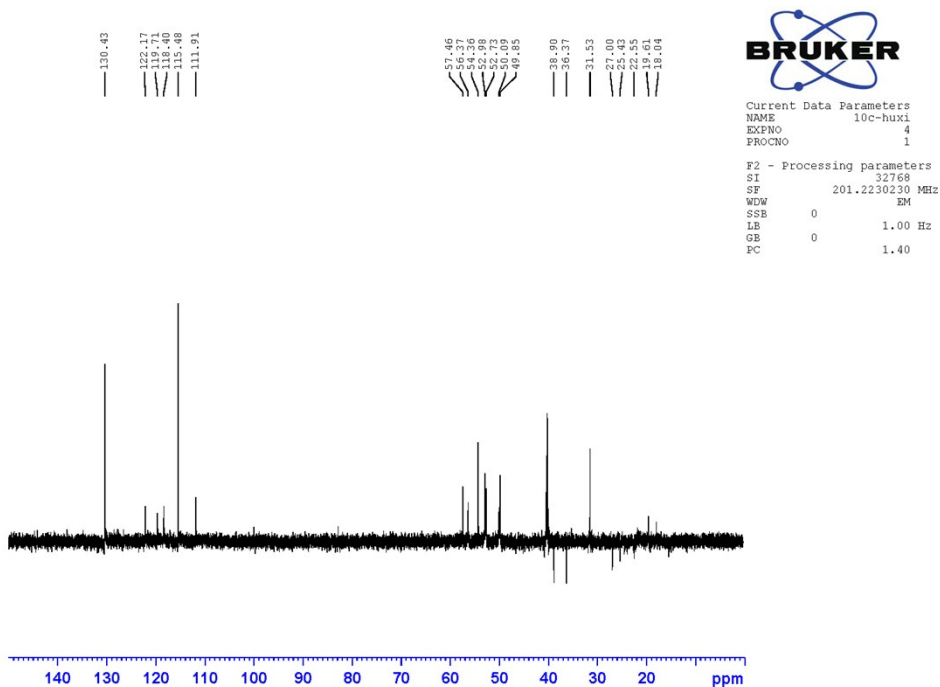


Fig. S3 ^{13}C DEPT-135 spectrum of MTCTP5

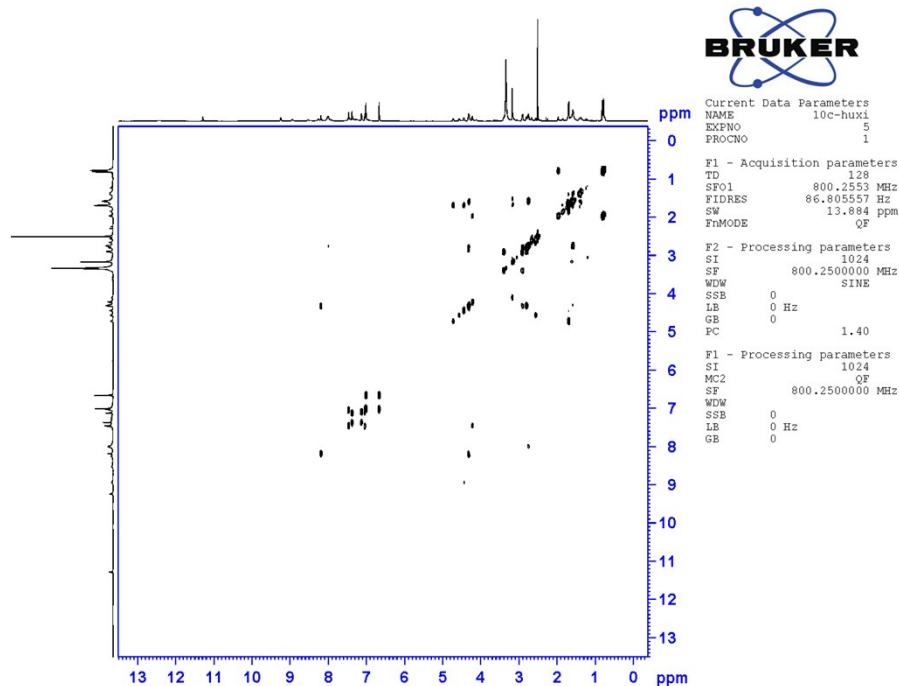


Fig. S4 ^1H - ^1H COSY spectrum of MTCTP5

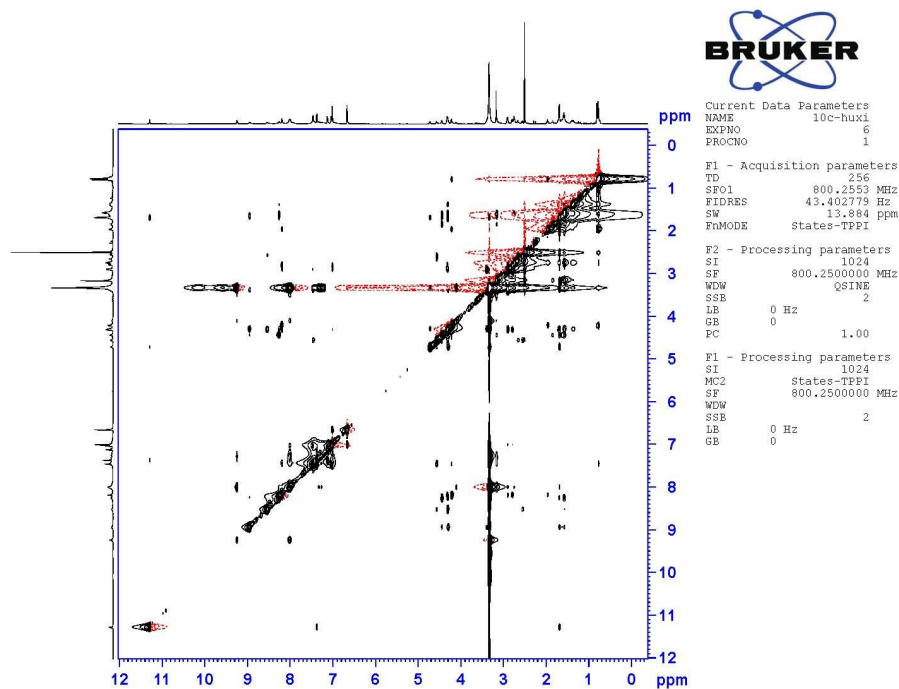


Fig. S5 ^1H - ^1H NOESY spectrum of MTCTP5

MS Report

Analysis Info

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Sample Name
Comment

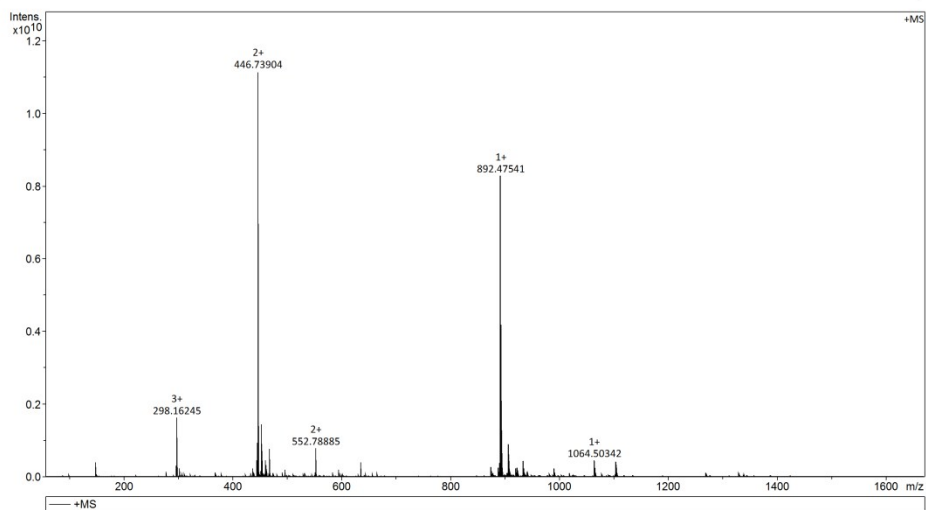
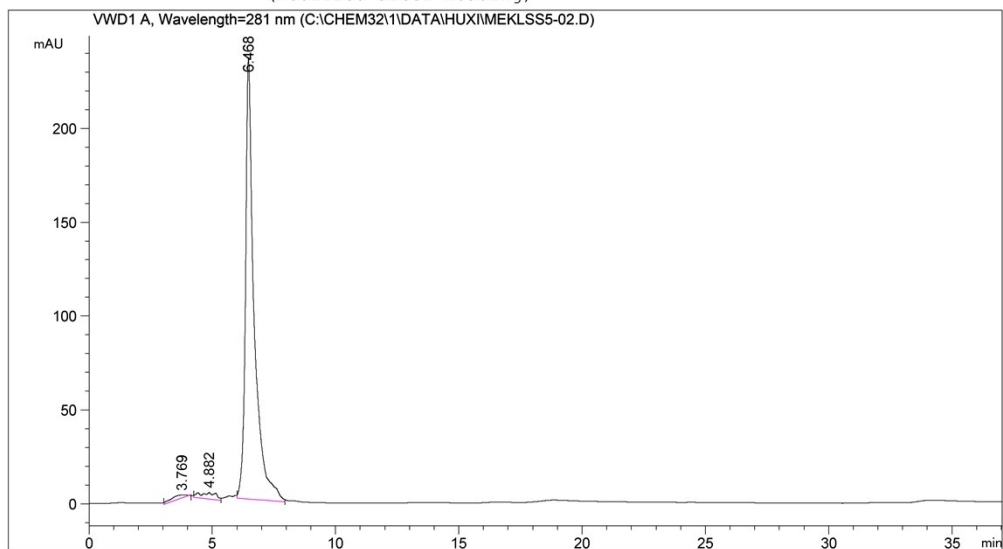


Fig. S6 FT-MS spectrum of MTCTP5

Data File C:\CHEM32\1\DATA\HUXI\MEKLSS5-02.D
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Area Percent Report
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Multiplier     : 1.0000
Dilution      : 1.0000
Sample Amount  : 10.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs
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Signal 1: VWD1 A, Wavelength=281 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	3.769	MM	0.6559	82.33344	1.55512	1.3872
2	4.882	MM	0.7278	151.29305	3.46455	2.5491
3	6.468	MM	0.4043	5701.46680	235.02092	96.0636

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Totals:                      5935.09328  240.04059
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*** End of Report ***
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Fig. S7 HPLC of MTCTP5 (CH₃OH:H₂O= 95%:5%, C18, 1.0 mL/min, 96%)

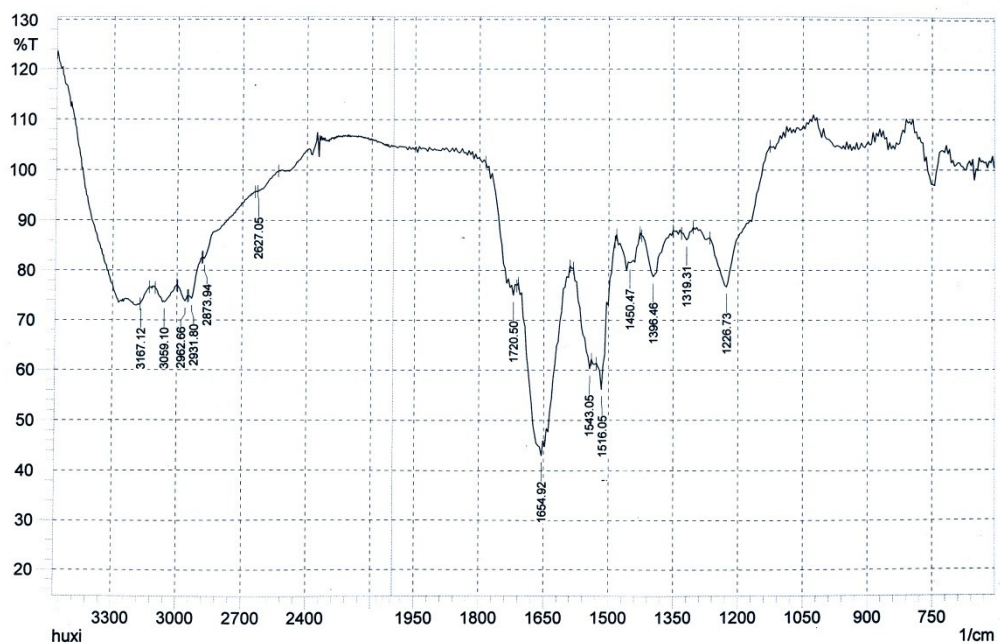


Fig. S8 IR spectrum of MTCTP5

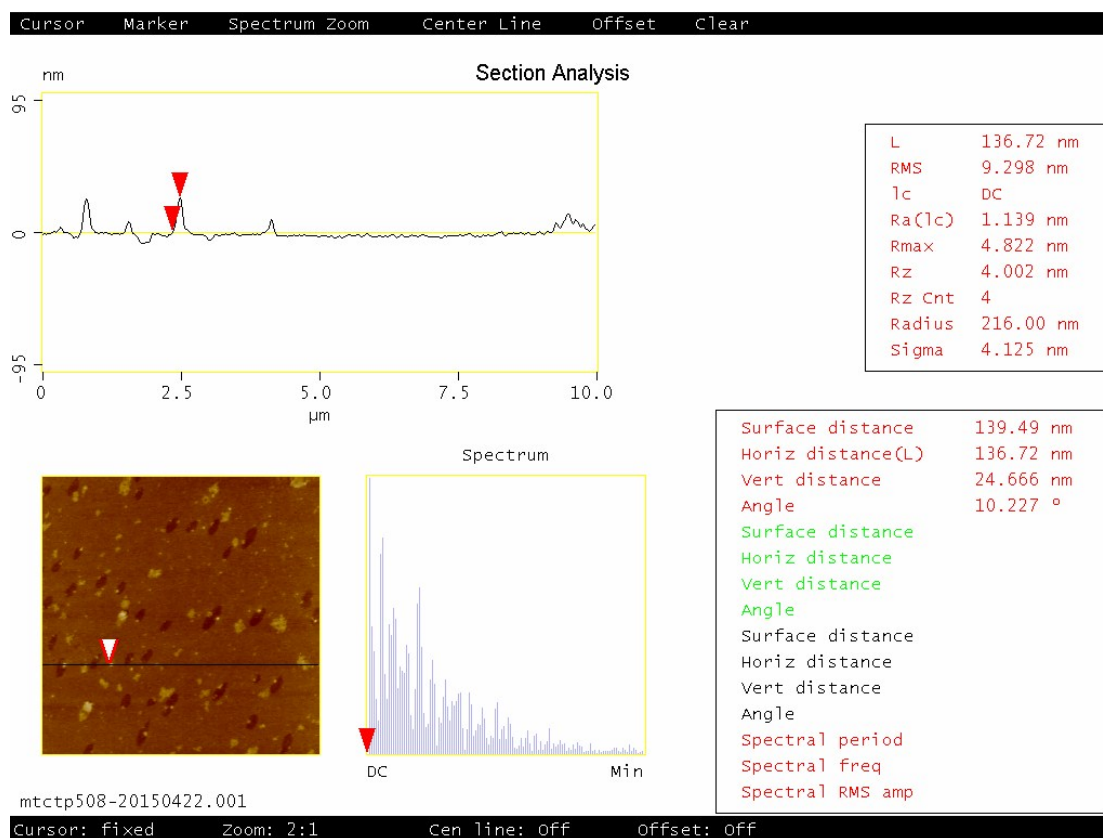


Fig. S9 AFM image of MTCTP5 in mouse plasma

Molecular association of MTCTP5 in water

The molecular association of MTCTP5 in water (10^{-7} nM) was identified with FT-MS spectrum. Figure S10A gives the ion peak of monomer of MTCTP5 at 892.47541 (exact mass of monomer plus H), and the locally amplified spectrum gives the ion peak of trimer of MTCTP5 at 1338.21736 (exact mass of divalent ion of a trimer plus H).

Association manner of 3 monomers of MTCTP5 in water

To understand the association manner of 3 monomers of MTCTP5 the NOESY 2D NMR spectrum of MTCTP5 was measured. Figure S10B gives 3 interesting cross-peaks marked with red circles. Cross-peak 1 reflects an interaction of the H of pyrrole NH of one molecule with the H of =NH of Arg residue of another molecule. Cross-peak 2 reflects two interactions of phenolic hydroxyl H of Tyr residue of one molecule with the H of NH₂ of Lys residue of another molecule. Cross-peak 3 reflects two interactions of the H of CH₂ of Asp residue of one molecule with the H of 2-NH of carboline moiety of another molecule.

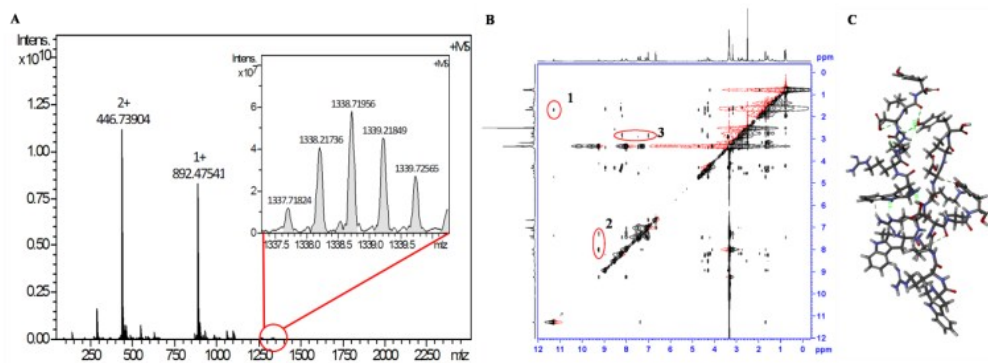


Fig. S10 FT-MS spectrum, NOESY 2D NMR spectrum and trimer's conformation of MTCTP5. (A) FT-MS spectrum and locally amplified peaks of MTCTP5; (B) NOESY 2D NMR spectrum of MTCTP5, in which the interesting cross-peaks are labelled with red rings; (C) According to NOESY 2D NMR spectrum the trimer of MTCTP5 takes flyer-like conformation.