

Bisphosphonate-functionalized cyclic Arg-Gly-Asp peptidomimetics

Carmelo Drago,^a Daniela Arosio,^b Cesare Casagrande,^c and Leonardo Manzoni*^b

^a *Università degli Studi di Milano, Centro Interdipartimentale Studi biomolecolari e applicazioni Industriali, Via Fantoli 16/15, Milano, I-20138, Italy*

^b *Consiglio Nazionale delle Ricerche, Istituto di Scienze e Tecnologie Molecolari, Via Golgi 19, Milano, I-20133, Italy*

^c *Università degli Studi di Milano, Dipartimento di Chimica, Via Golgi 19, I-20133 Milano, Italy*
E-mail: Leonardo.manzoni@istm.cnr.it

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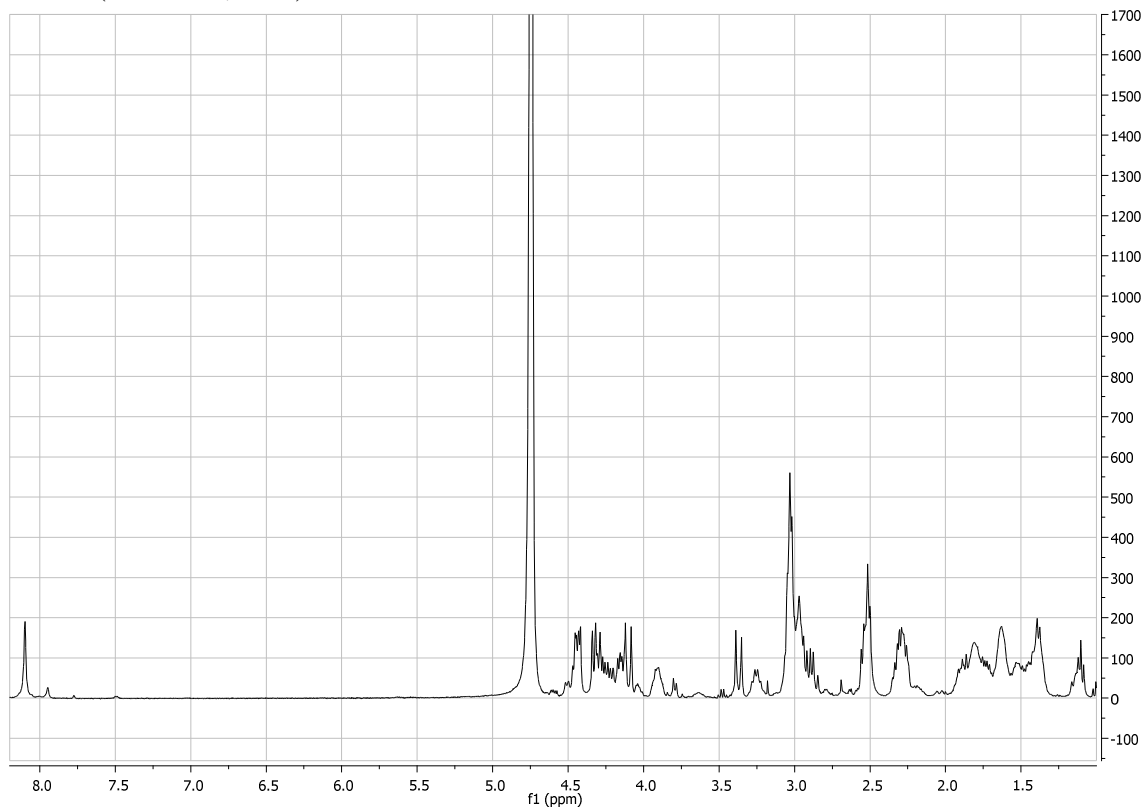
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• Copies of ¹ H, ³¹ P and ¹³ C NMR spectra and MS-HPLC chromatograms of final compounds 6, 12 and 16	S3

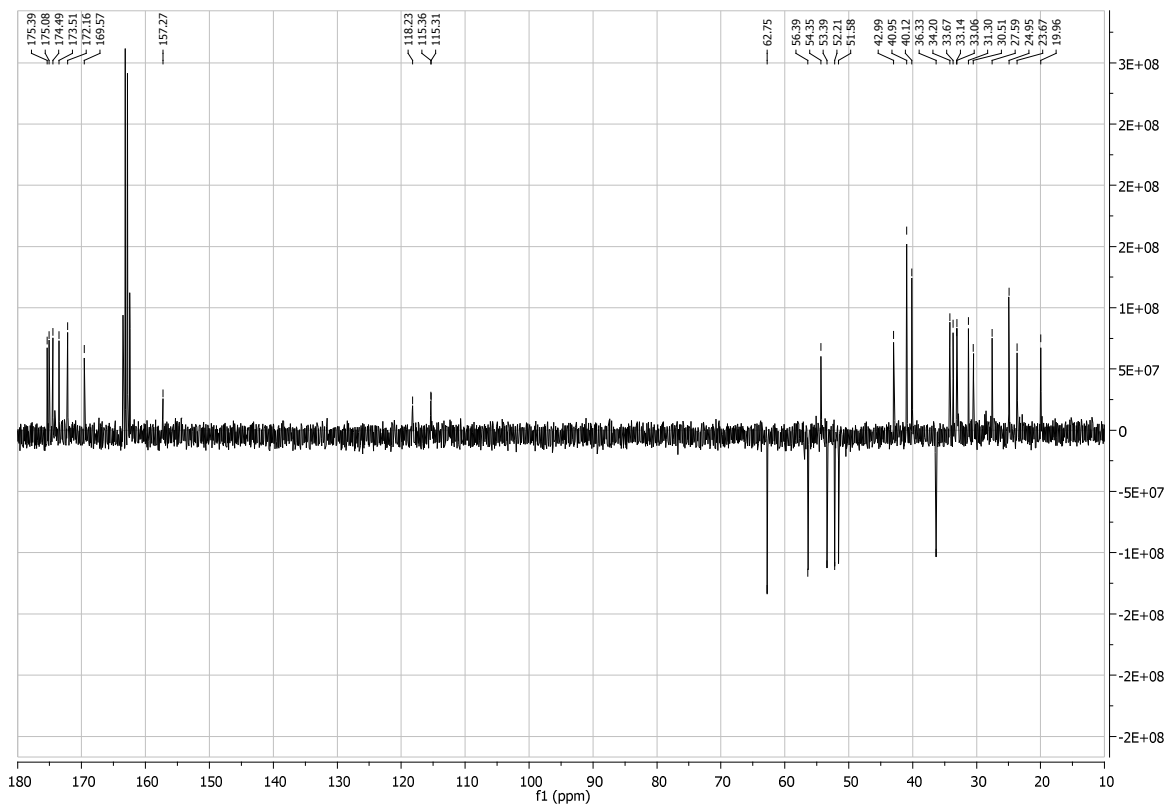
General

^1H , ^{13}C , and ^{31}P -NMR spectra were recorded at 300 K on a Bruker AVANCE-600 or Bruker AVANCE-400 spectrometer. Chemical shifts δ for ^1H and ^{13}C are expressed in ppm relative to internal Me_4Si as standard. Signals were abbreviated as s, singlet; bs, broad singlet; d, doublet; t, triplet; q, quartet; m, multiplet.

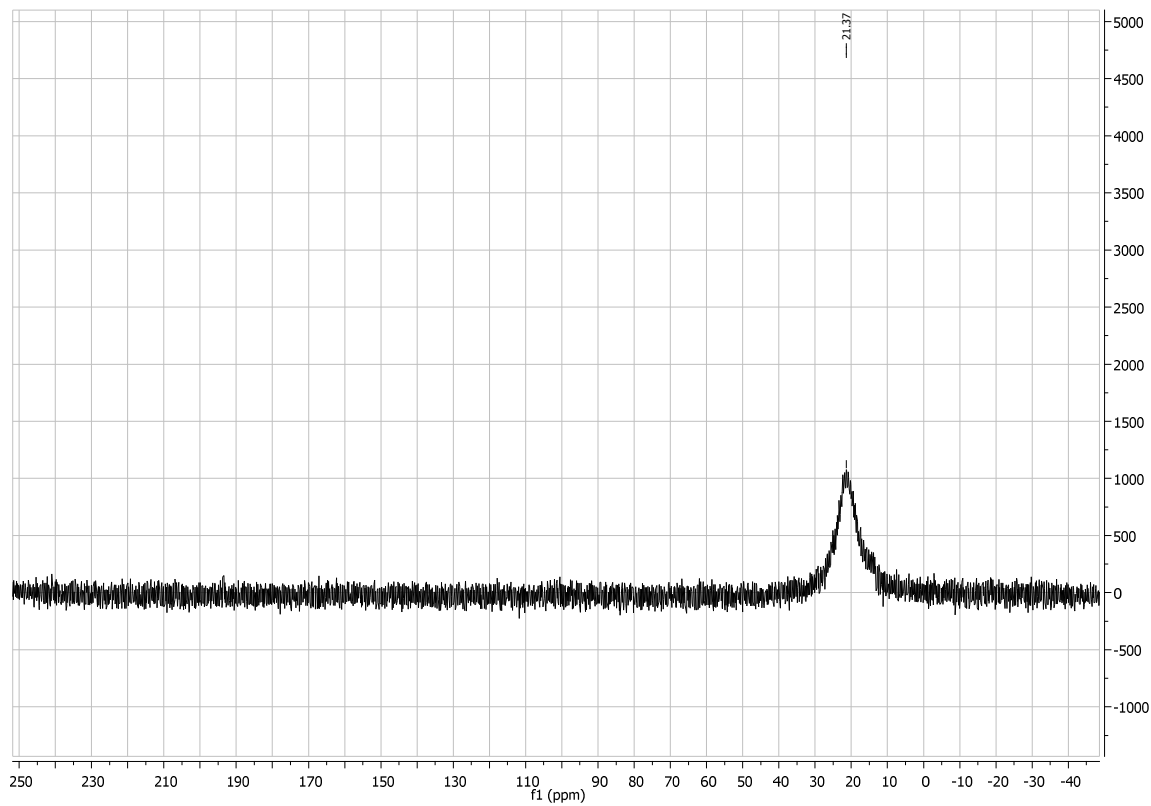
Mass spectra were obtained with Agilent 1100 analytical HPLC equipped with diode array detector and Bruker ion-trap Esquire 3000+ with ESI.

Semi-preparative HPLC was carried out on a Waters Atlantis C_{18} OBD $5\mu\text{m}$ 19 mm X 10cm column; gradient from 100% H_2O + 0.1% TFA to 70% H_2O + 0.1% TFA/30% MeCN + 0.1% TFA over 30 minutes.

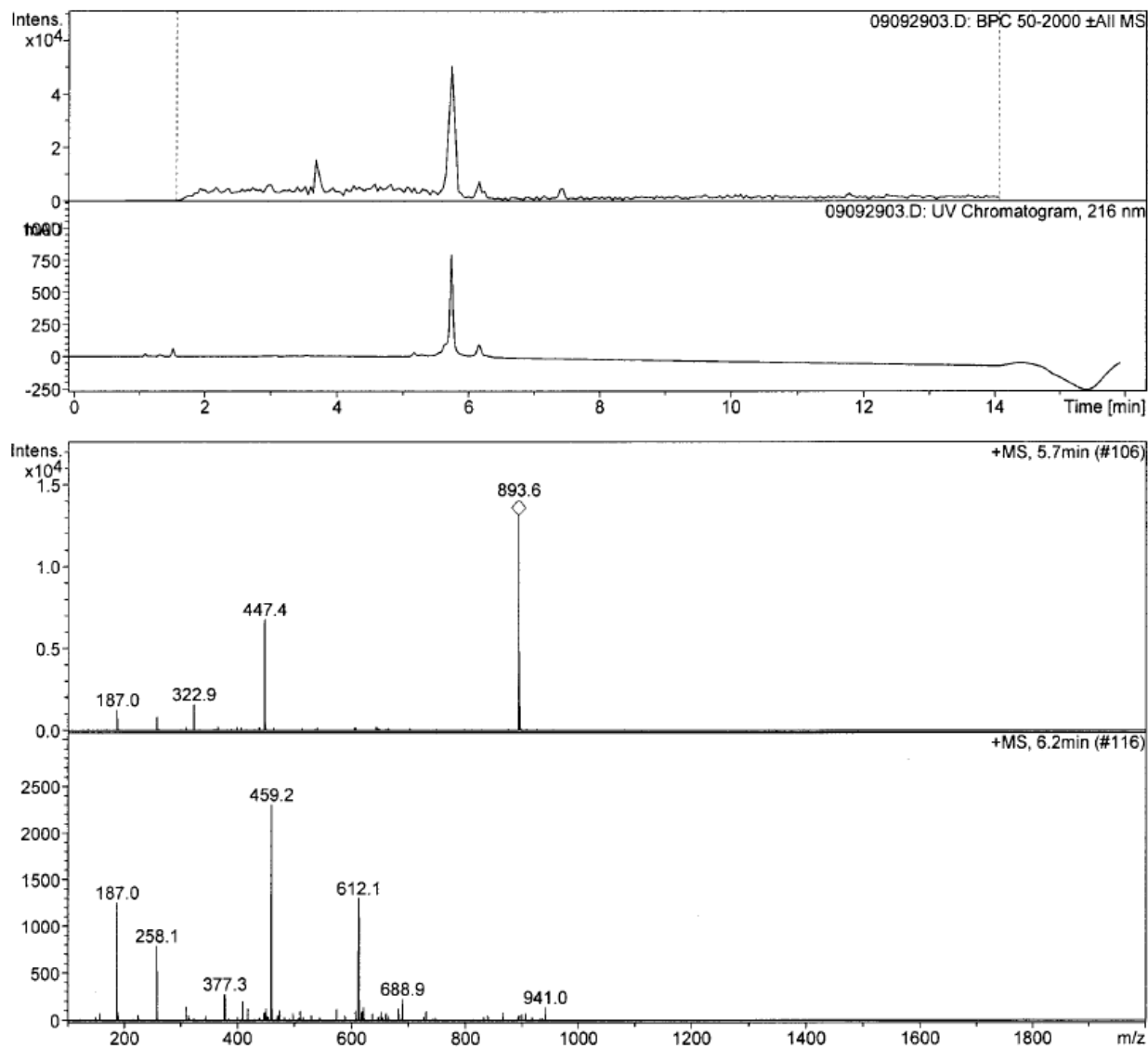
Compound 6¹H-NMR (400 MHz, D₂O)¹³C-NMR (100.6 MHz, D₂O)



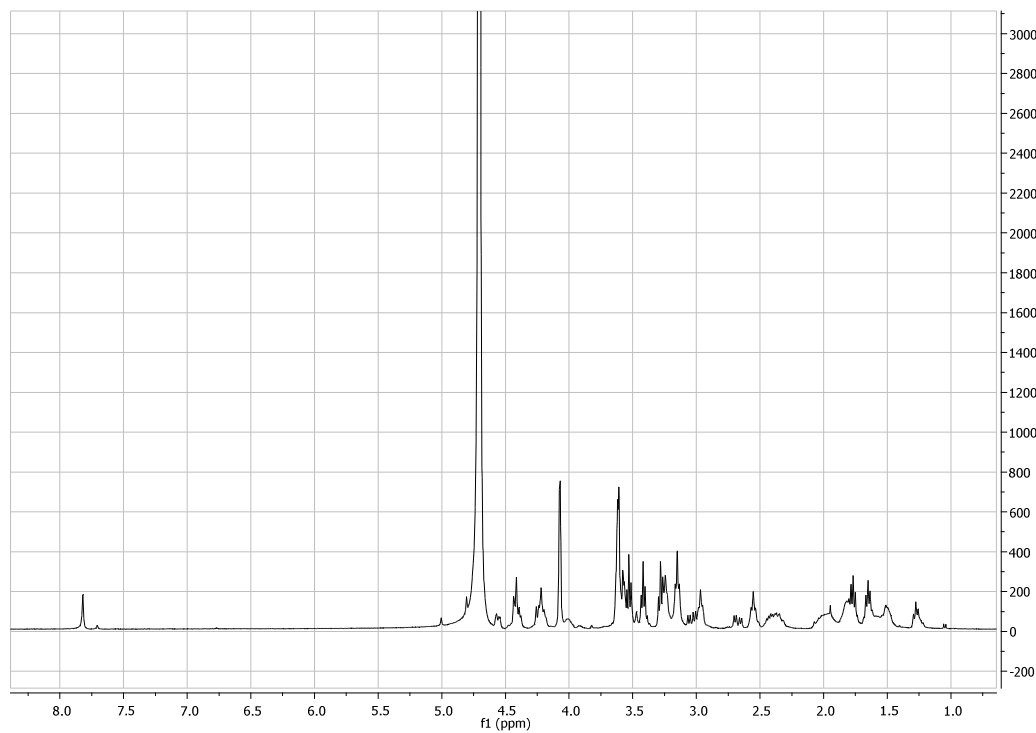
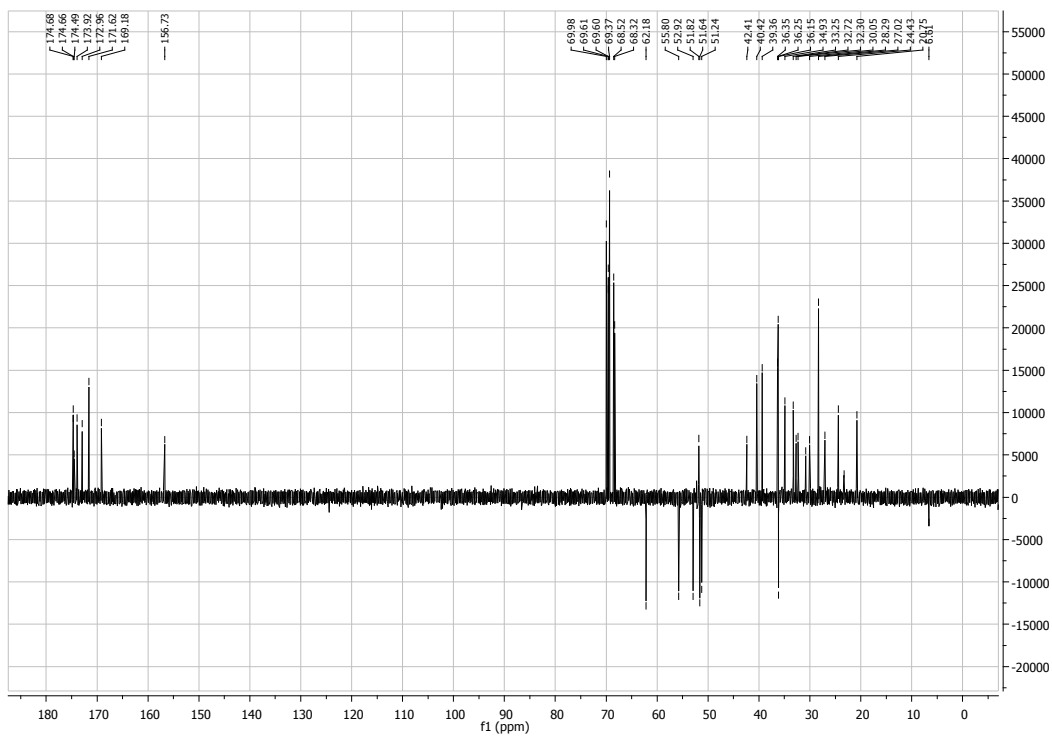
³¹P-NMR (161.9 MHz, D₂O)

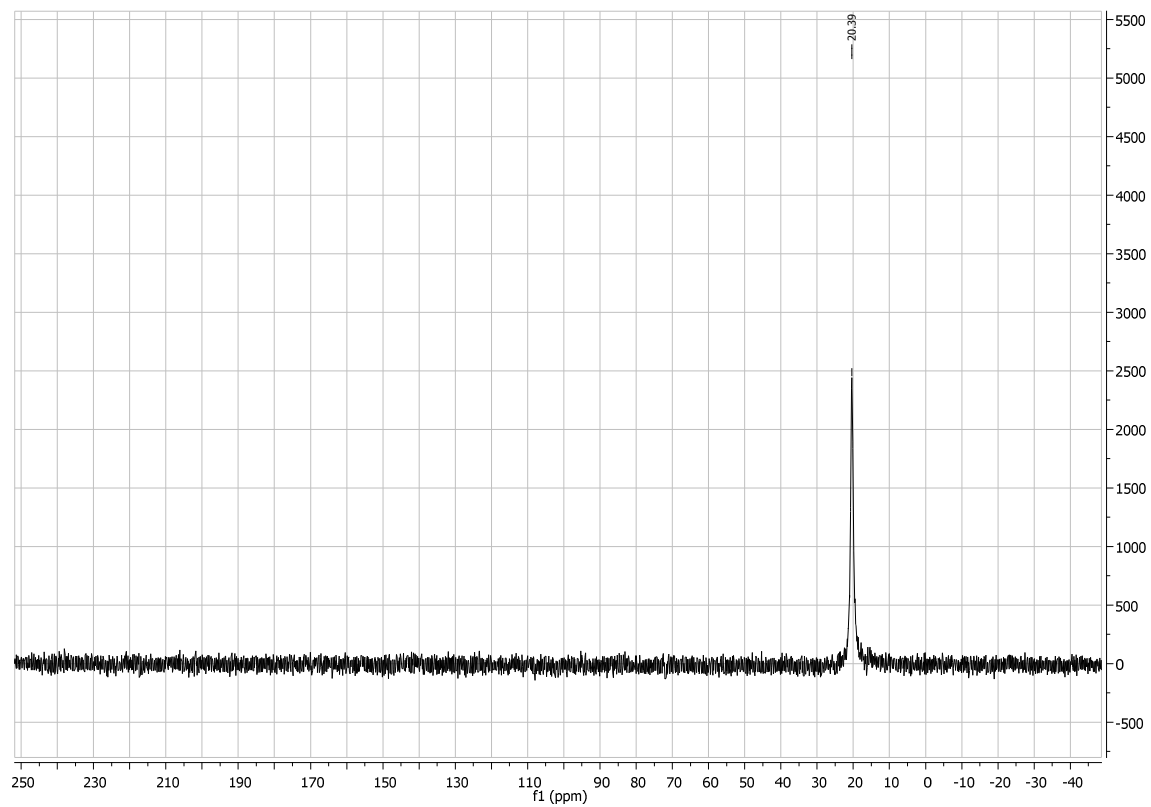


HPLC-MS

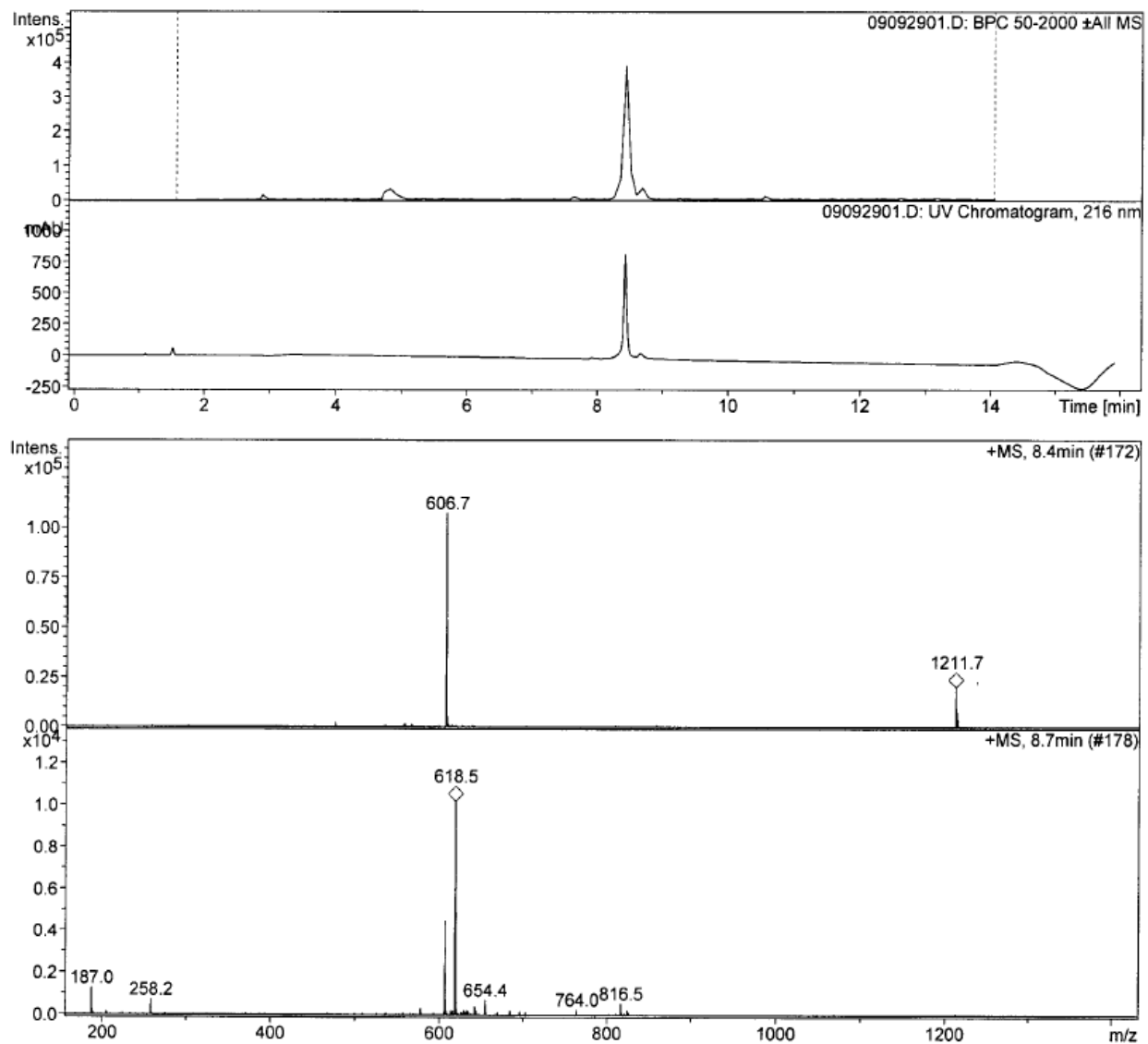


Compound 12

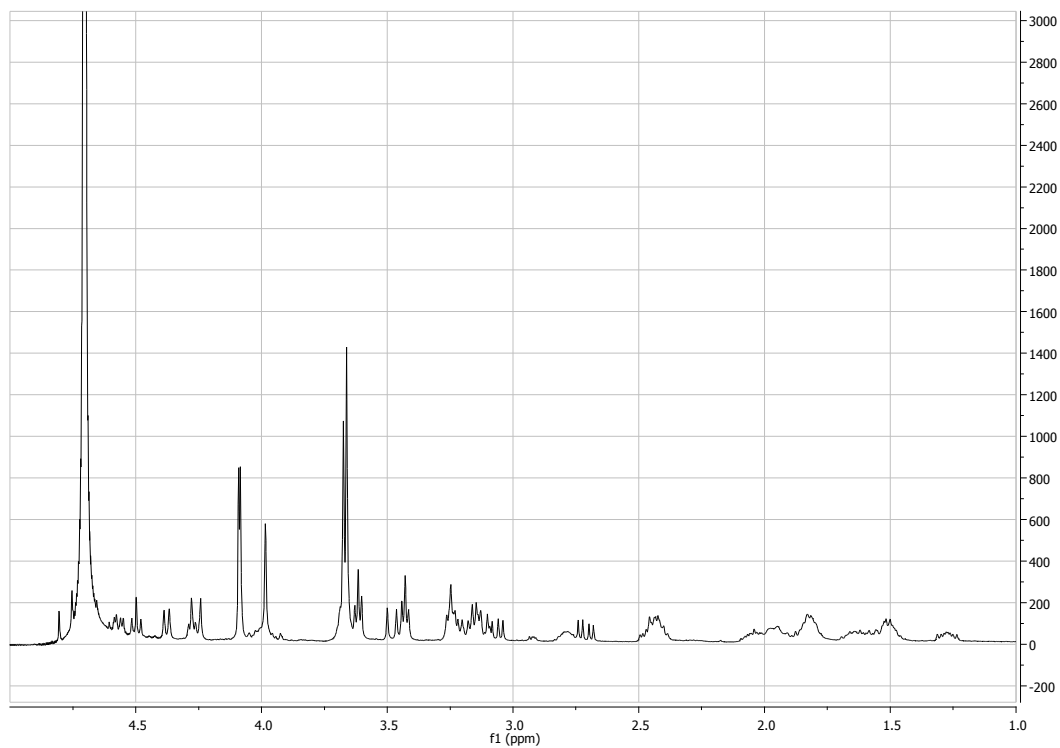
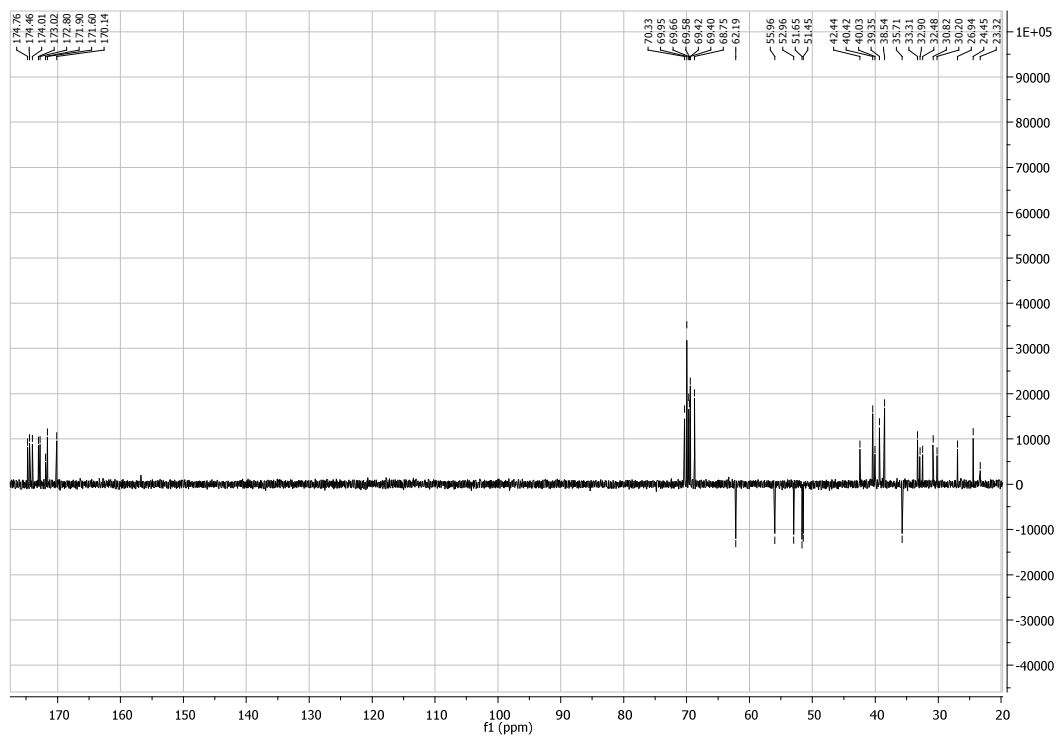
 $^1\text{H-NMR}$ (400 MHz, D_2O) $^{13}\text{C-NMR}$ (100.6 MHz, D_2O)

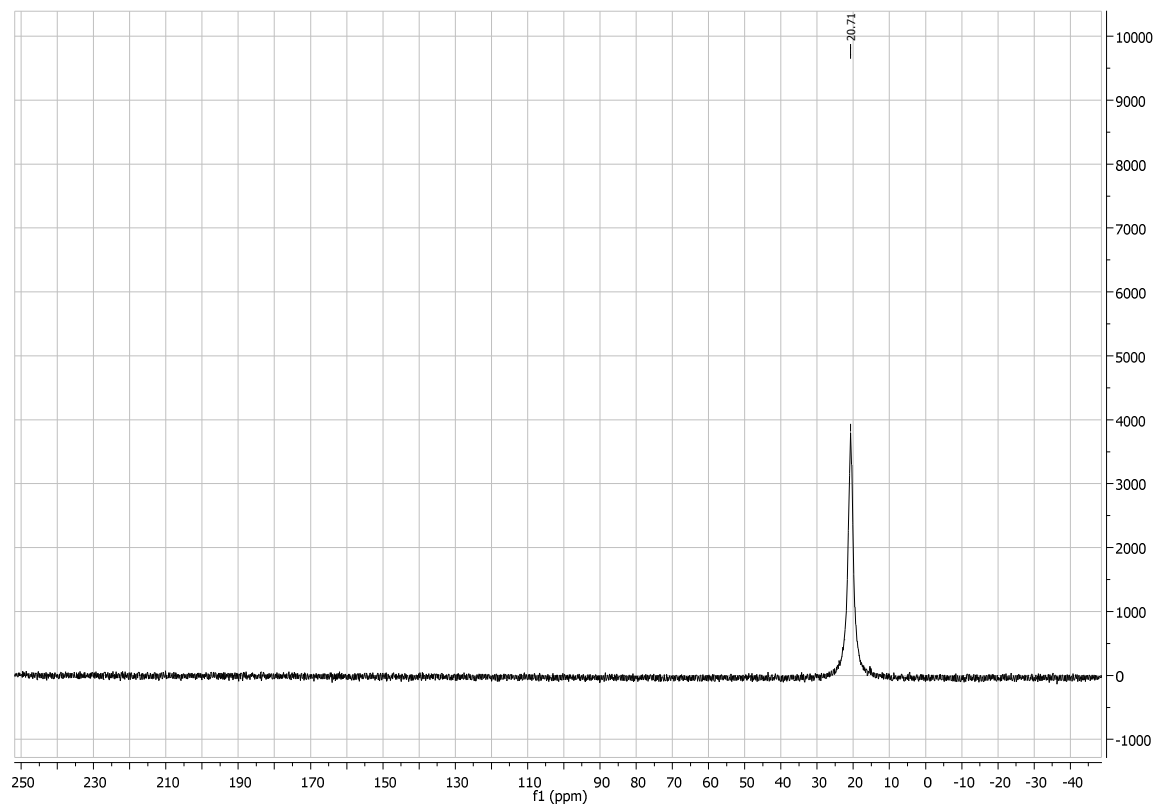
^{31}P -NMR (161.9 MHz, D_2O)

HPLC-MS



Compound 16

 $^1\text{H-NMR}$ (400 MHz, D_2O) $^{13}\text{C-NMR}$ (D_2O)

^{31}P -NMR (161.9 MHz, D_2O)

HPLC-MS

