Bisphosphonate-functionalized cyclic Arg-Gly-Asp peptidomimetics

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General

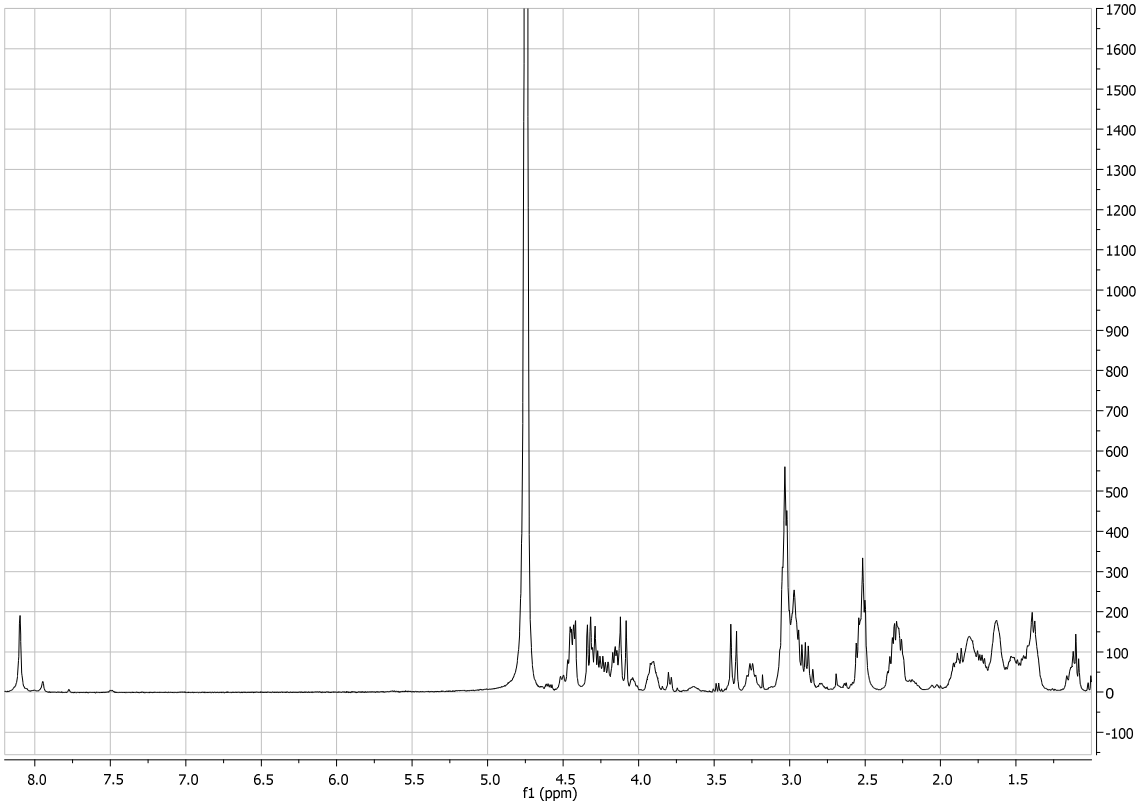
^{1}H, ^{13}C, and ^{31}P-NMR spectra were recorded at 300 K on a Bruker AVANCE-600 or Bruker AVANCE-400 spectrometer. Chemical shifts δ for ^{1}H and ^{13}C are expressed in ppm relative to internal Me_4Si as standard. Signals were abbreviated as s, singlet; bs, broad singlet; d, doublet; t, triplet;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

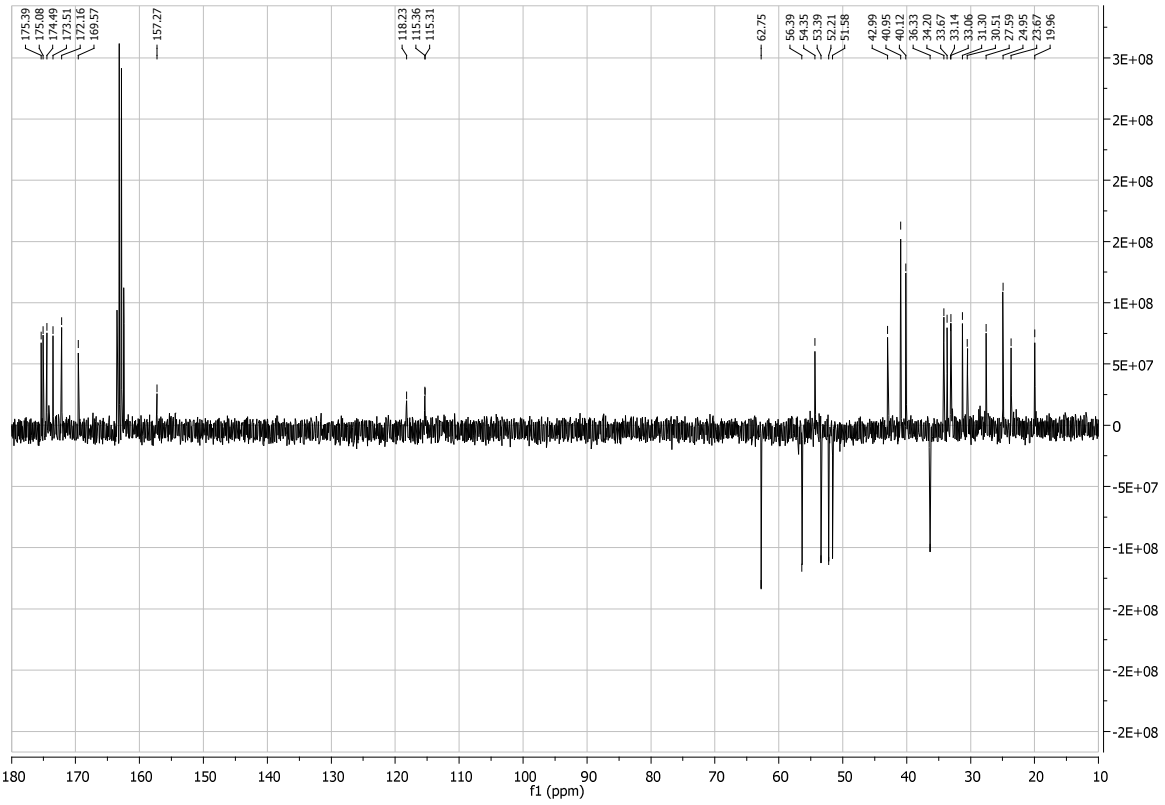
Semi-preparative HPLC was carried out on a Waters Atlantis C_{18} OBD 5μm 19 mm X 10cm column; gradient from 100% H_2O + 0.1% TFA to 70% H_2O + 0.1% TFA/30% MeCN + 0.1% TFA over 30 minutes.

Compound 6

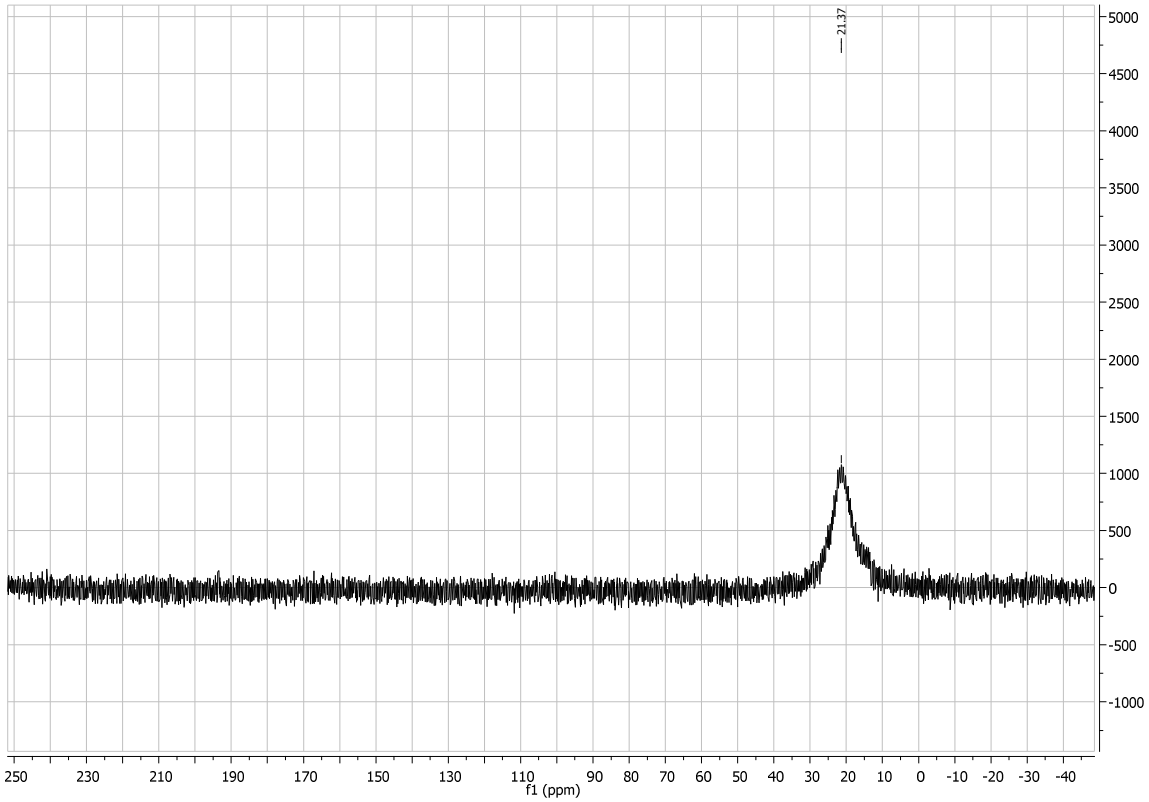
^{1}H-NMR (400 MHz, D_2O)



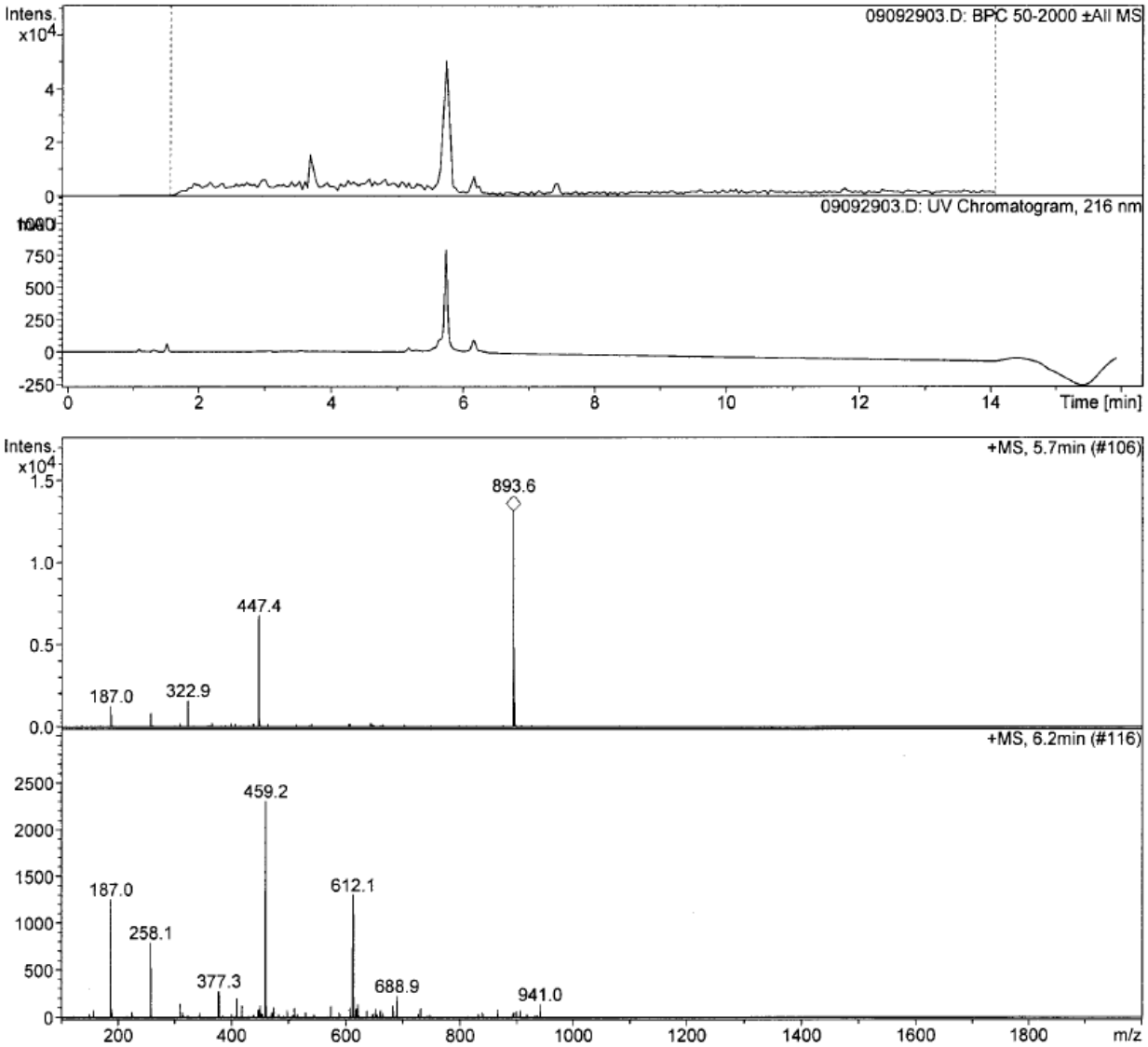
^{13}C-NMR (100.6 MHz, D_2O)



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

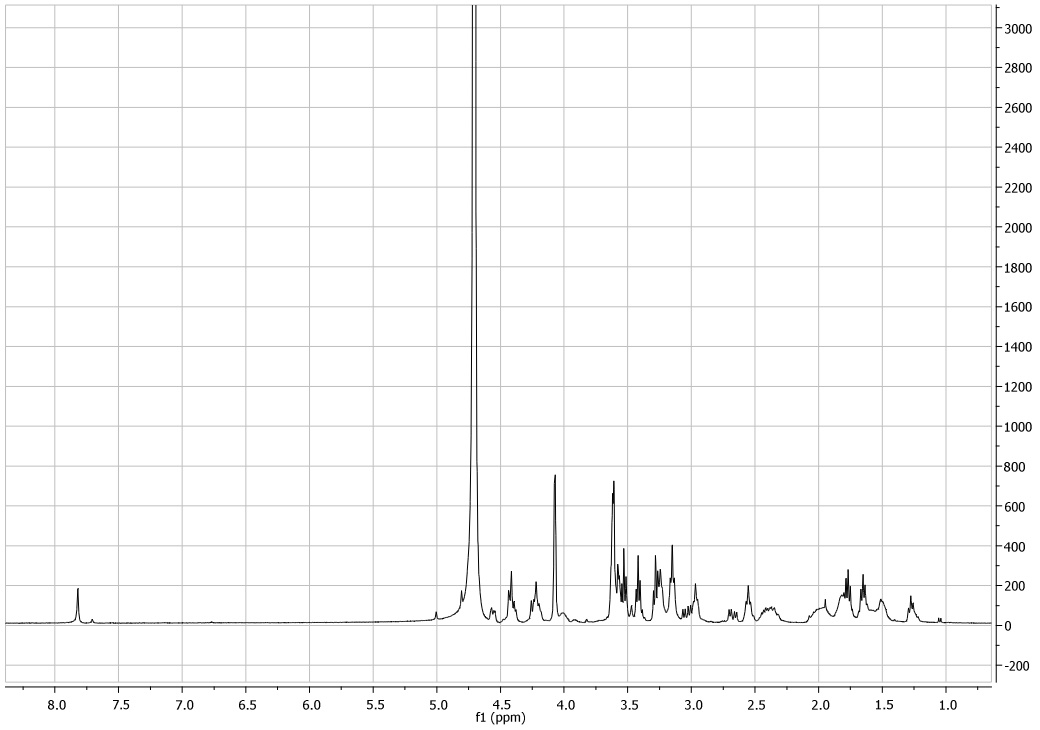


HPLC-MS

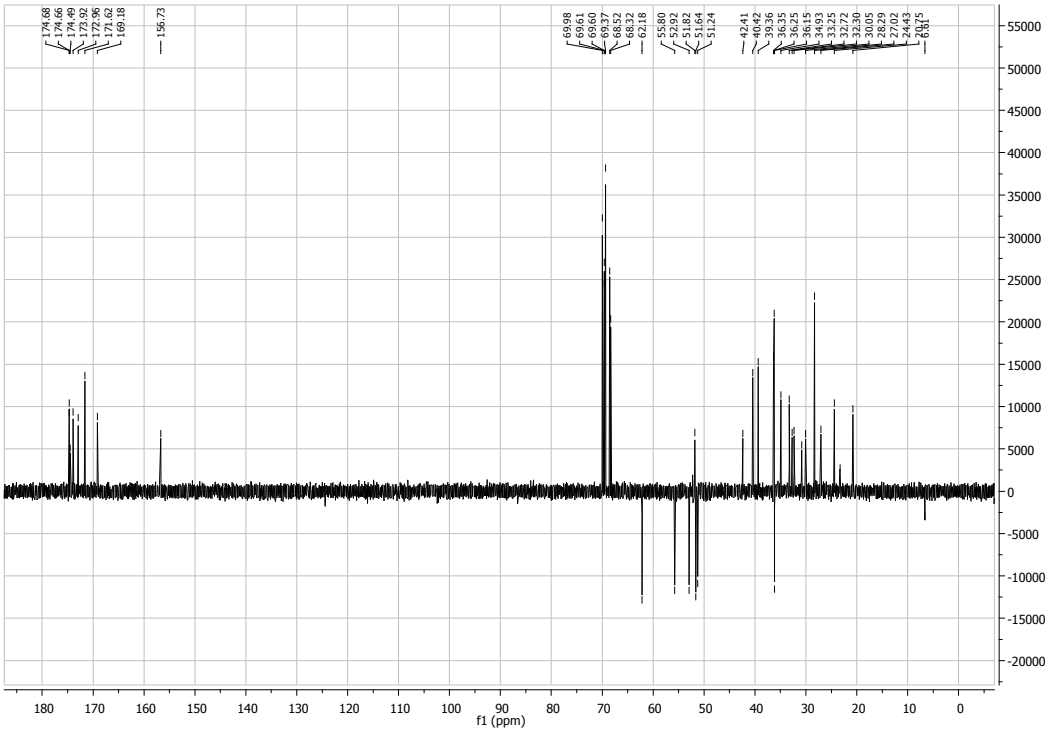


Compound **12**

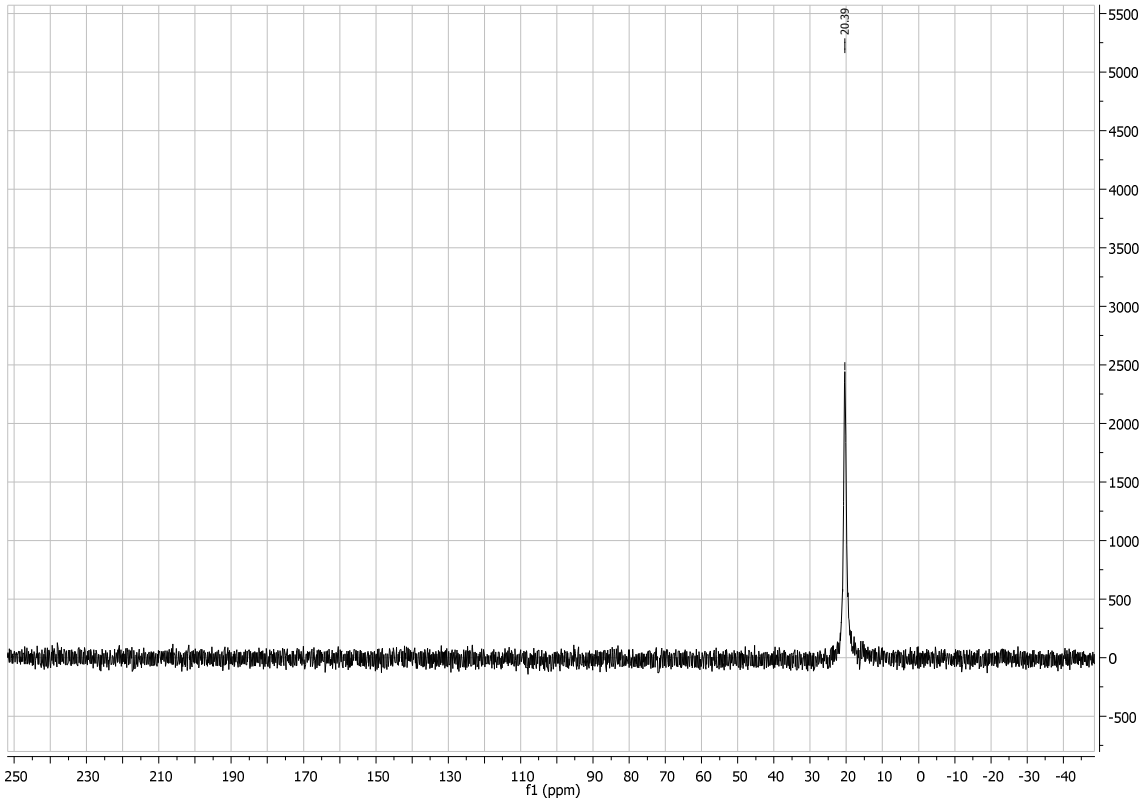
^{1}H-NMR (400 MHz, D_2O)



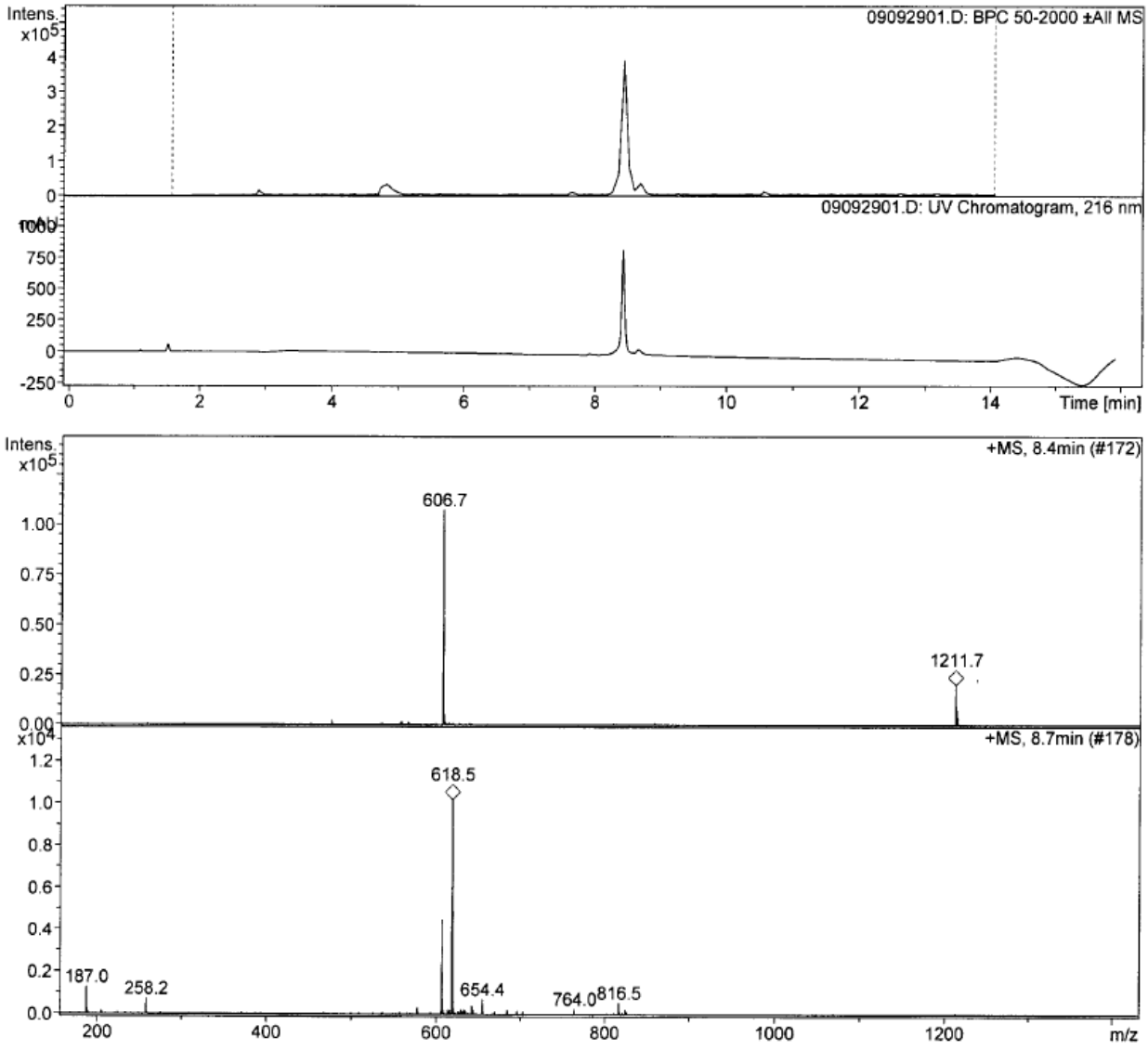
^{13}C-NMR (100.6 MHz, D_2O)



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

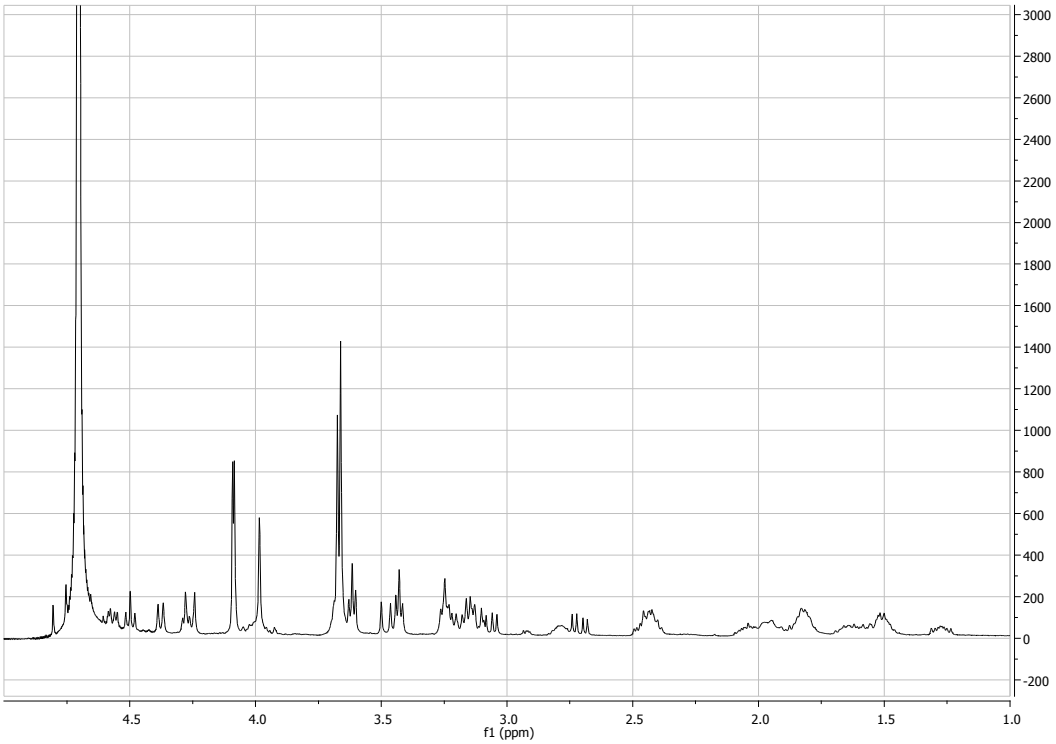


HPLC-MS

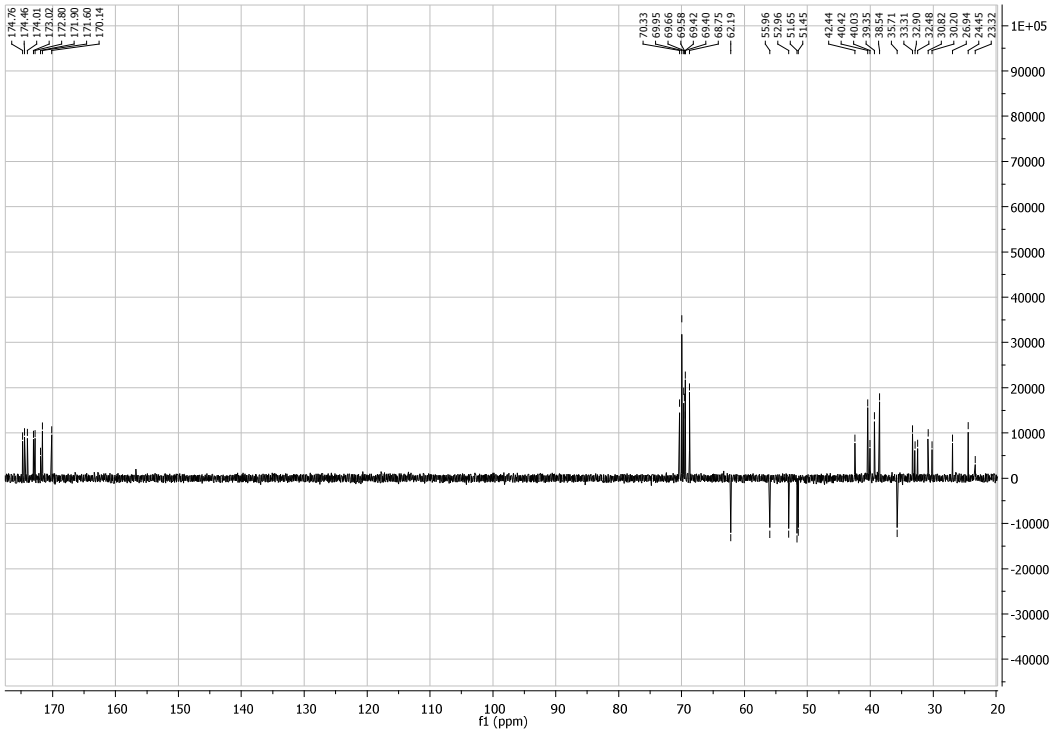


Compound **16**

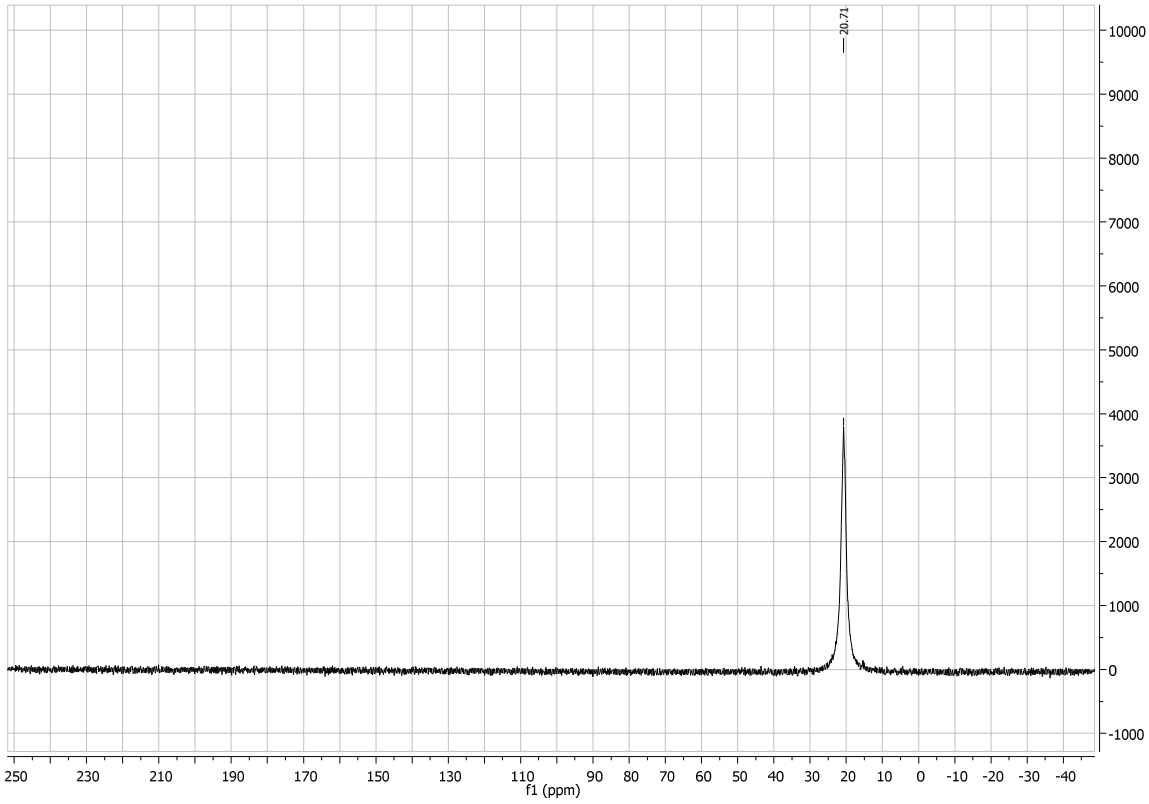
^{1}H-NMR (400 MHz, D_2O)



^{13}C-NMR (D_2O)



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



HPLC-MS