Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

1,2-Dimethylindole-3-sulfonyl (MIS), the Most Acid Labile Sulfonyl Protecting Group for the Side Chain of Arginine.

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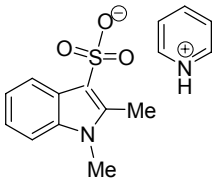
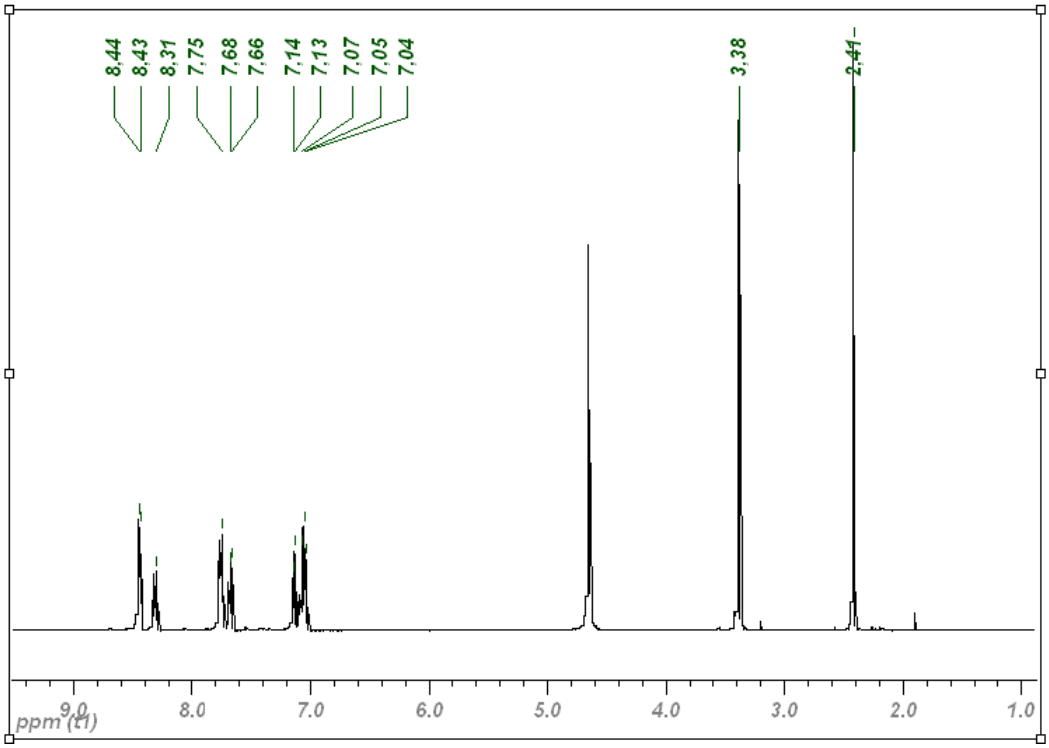
1. NMR spectra:

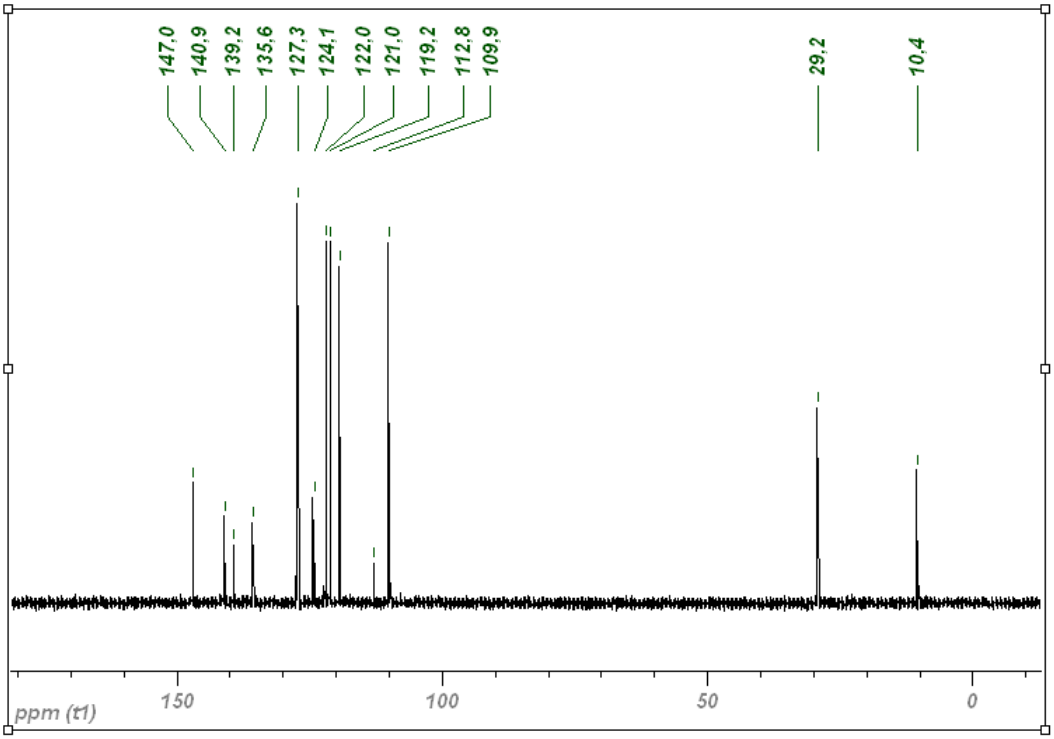
1,2-Pyridinium methylindole-3-sulfonate (1)

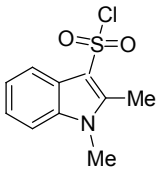


^{1}H NMR (400 MHz, D_2O)



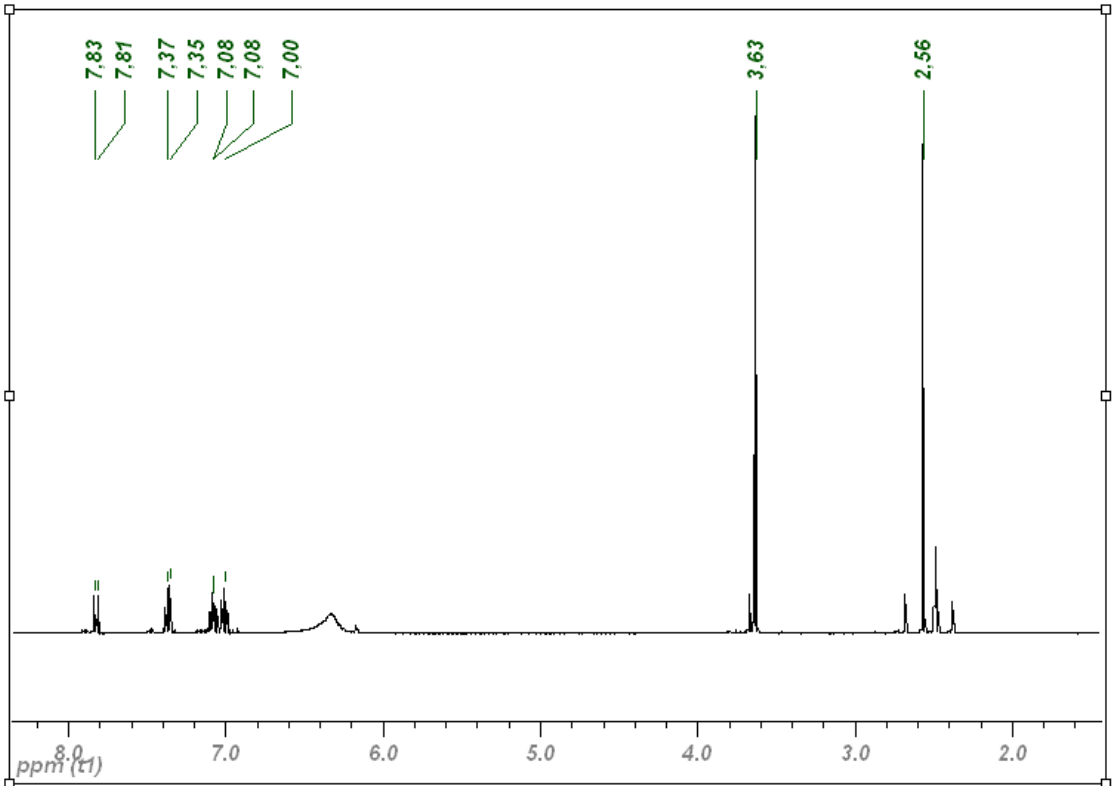
^{13}C NMR (100 MHz, D_2O)



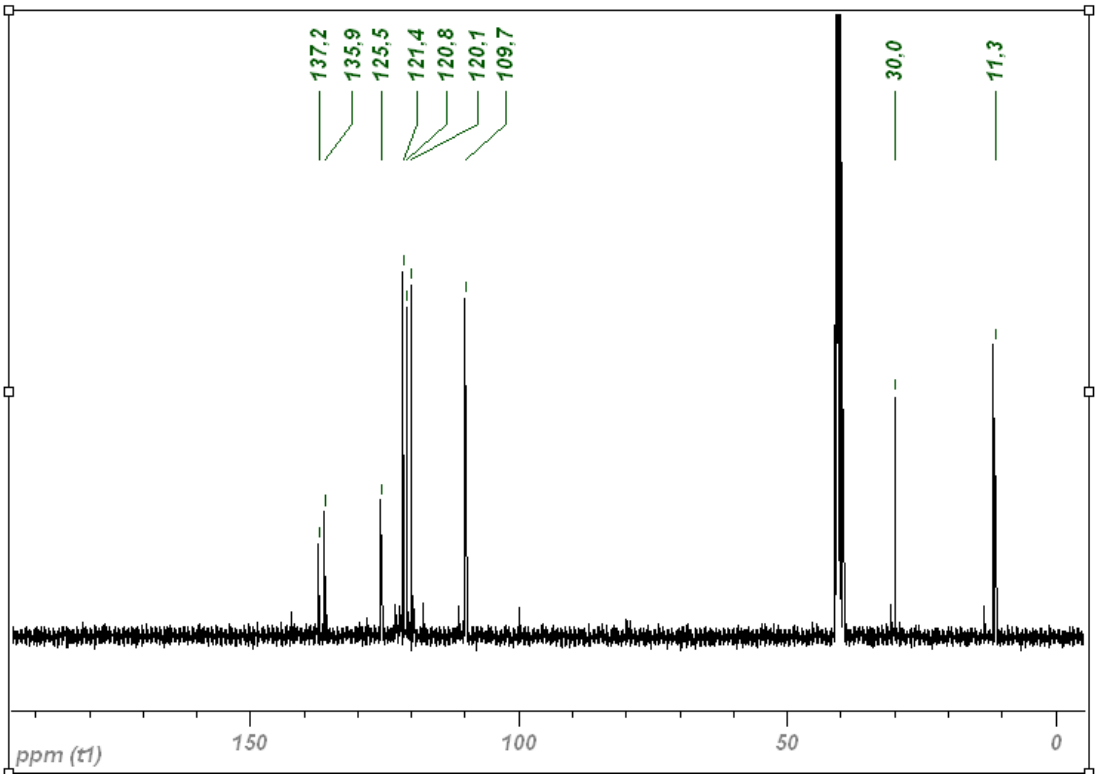


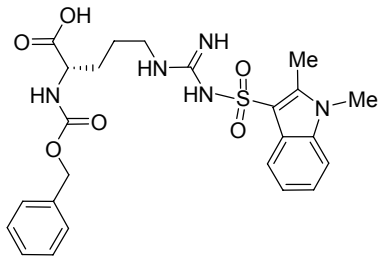
1,2-Methylindole-3-sulfonyl chloride (MIS-Cl) (2)

^{1}H NMR (400 MHz, DMSO)



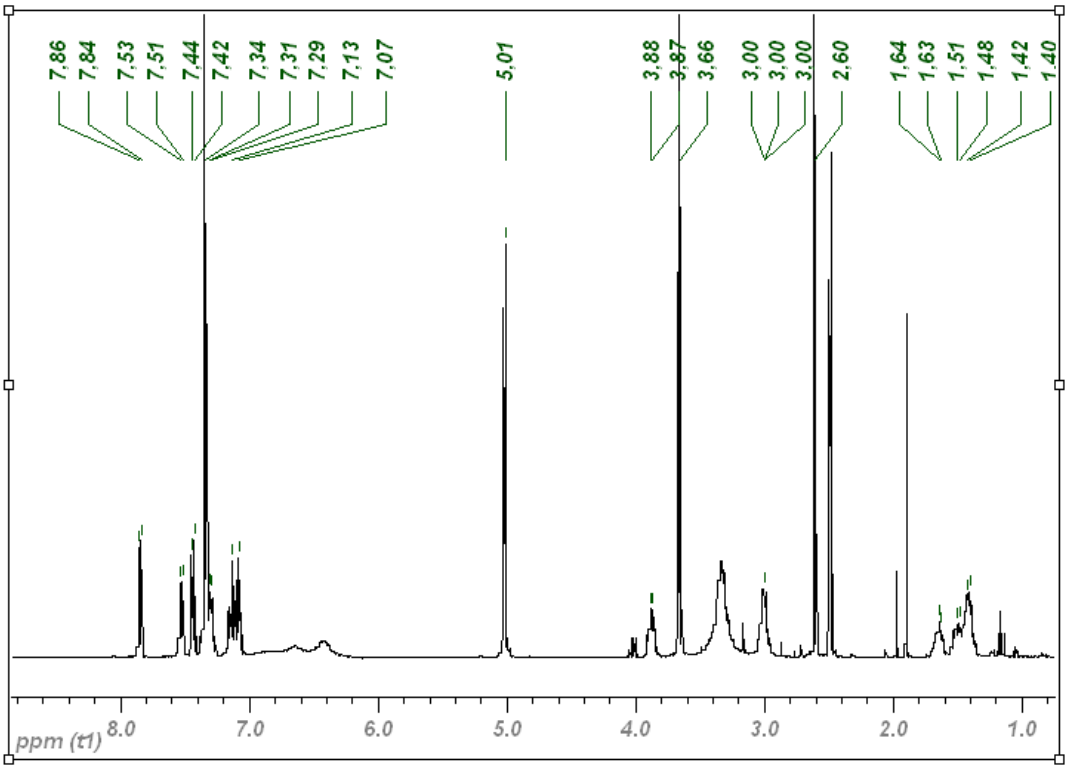
^{13}C NMR (100 MHz, DMSO)



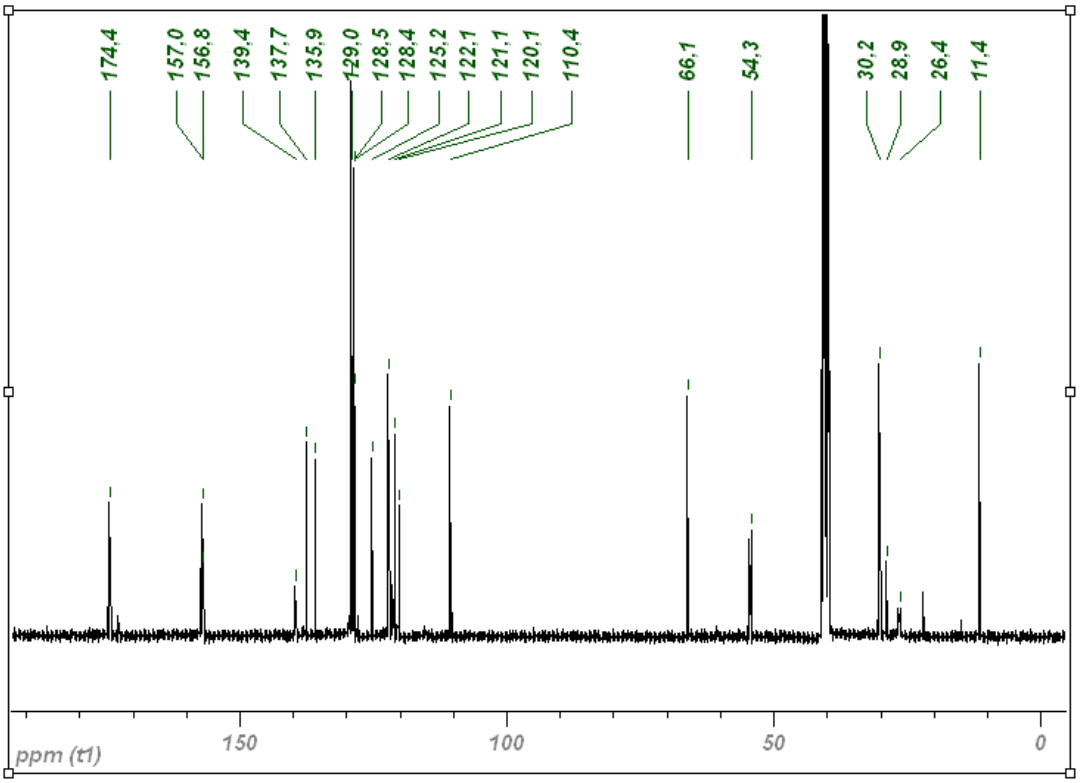


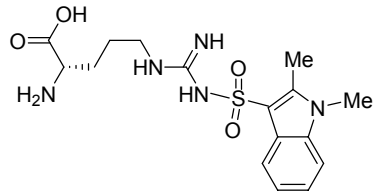
Z-L-Arg(MIS)-OH (3)

^{1}H NMR (400 MHz, DMSO)



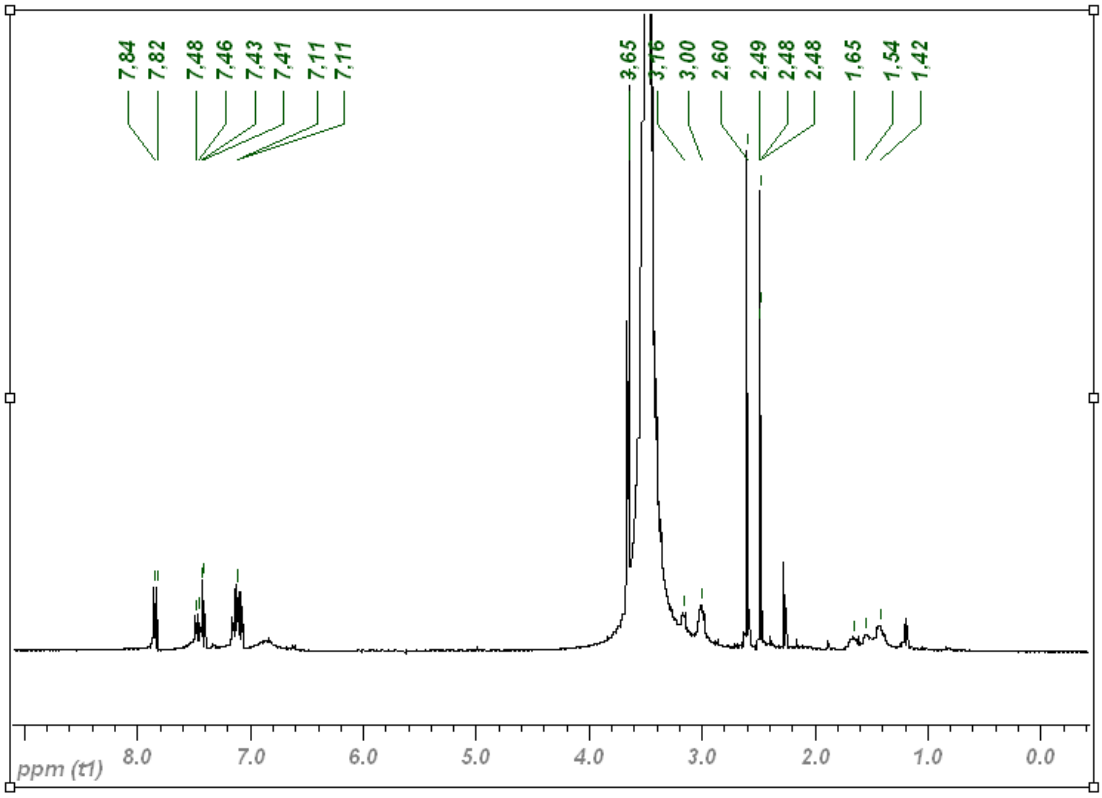
^{13}C NMR (100 MHz, DMSO)

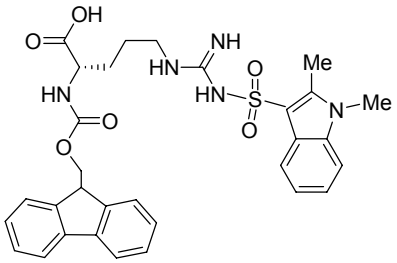




H-L-Arg(MIS)-OH (4)

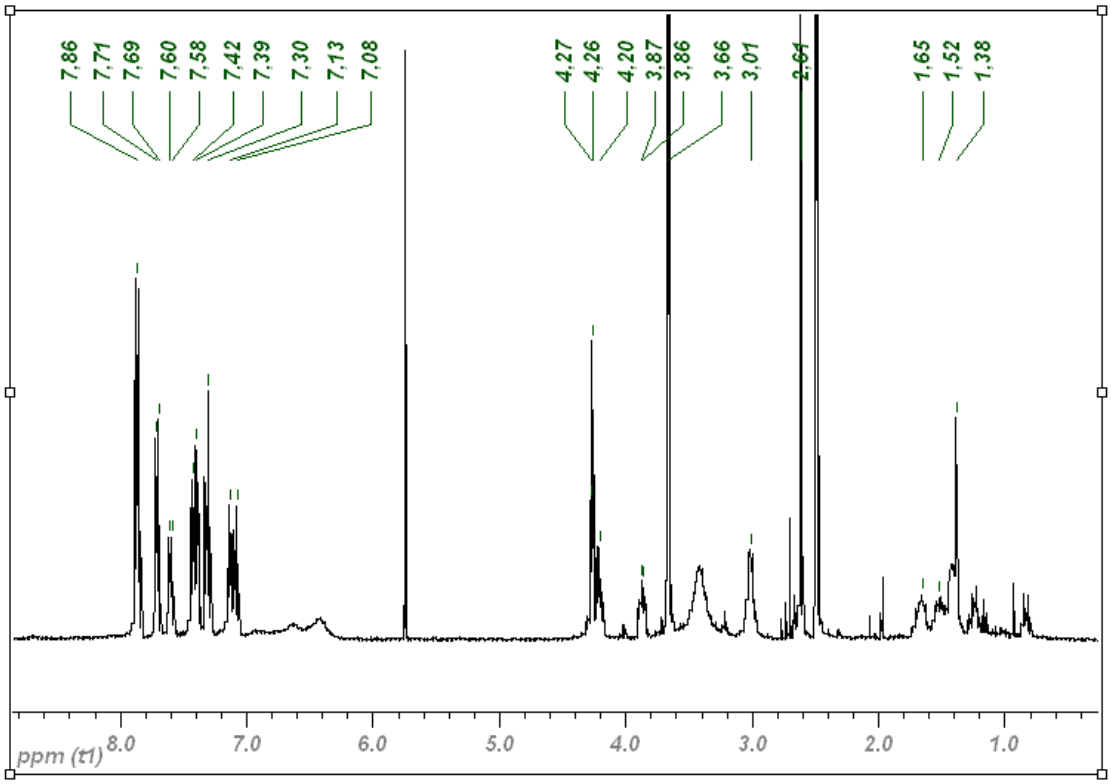
^{1}H NMR (400 MHz, DMSO)



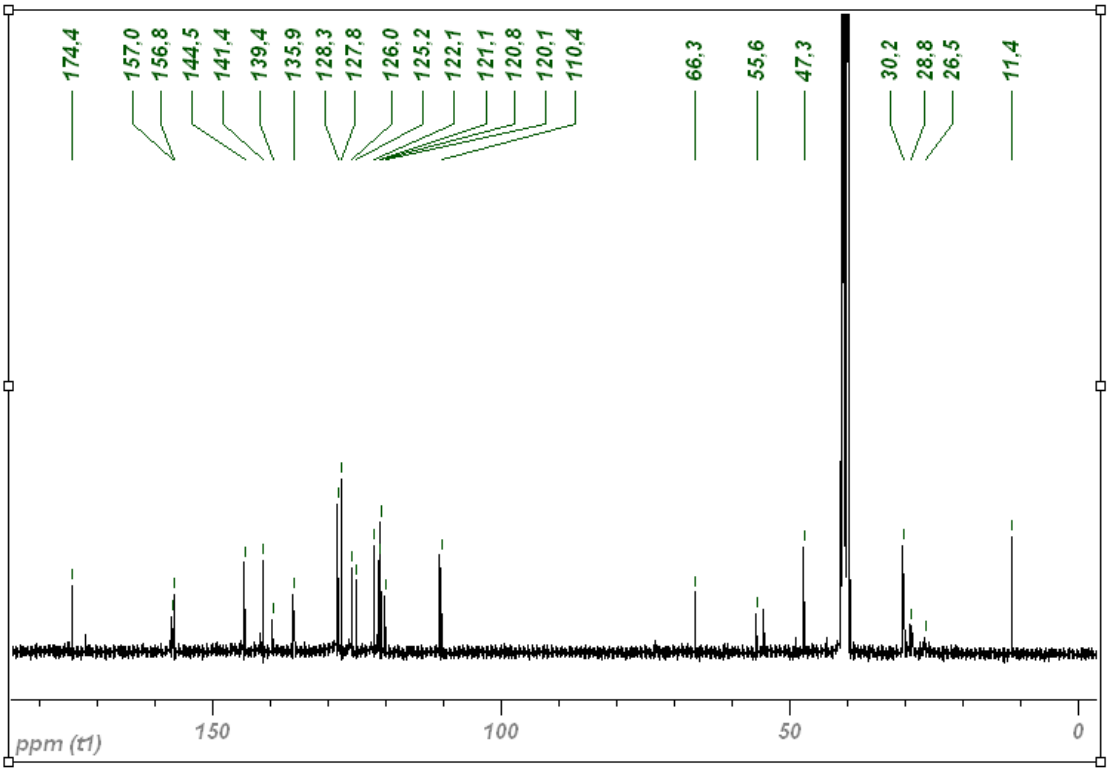


Fmoc-L-Arg(MIS)-OH (5)

^{1}H NMR (400 MHz, DMSO)



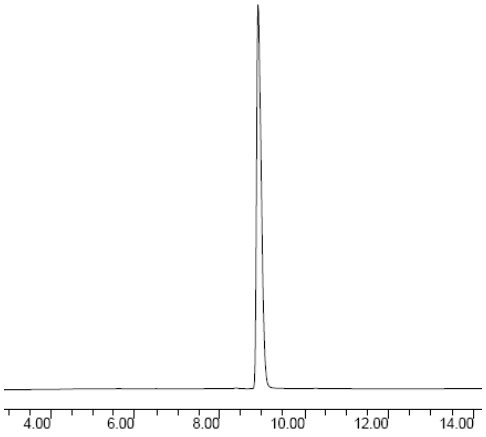
^{13}C NMR (100 MHz, DMSO)



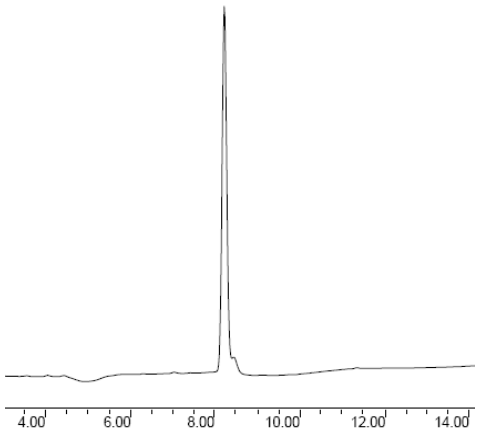
2. HPLC chromatograms (λ= 220 nm)

2.1 Arginine derivatives:

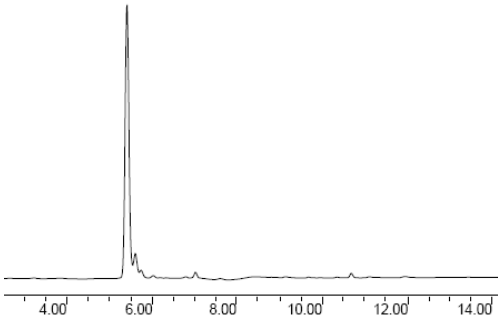
Z-L-Arg(MIS)-OH (3)



Fmoc-L-Arg(MIS)-OH (5)

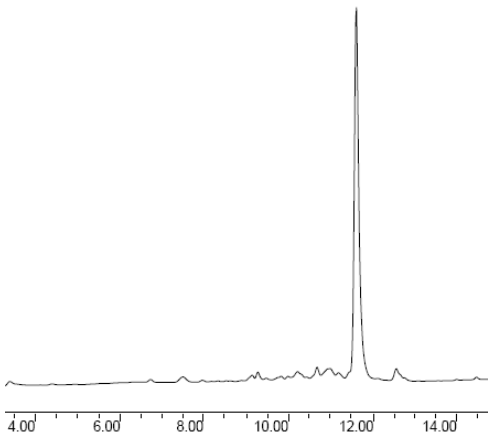


H-L-Arg(MIS) (4)

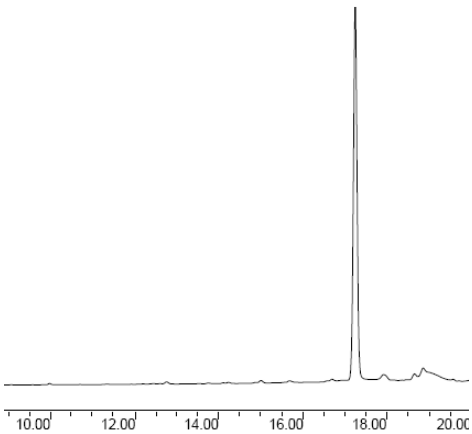


2.2 Multiarginine containing peptides:

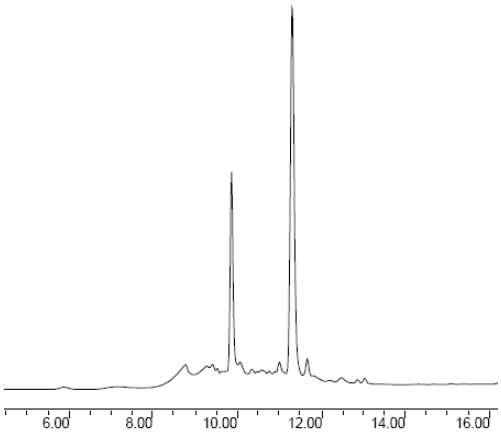
Ac-Phe-Arg(MIS)-Arg(MIS)-Arg(MIS)-Arg(MIS)-Val-NH_2 (peptide 1).



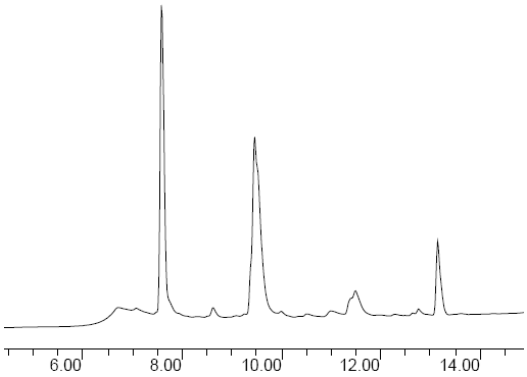
Ac-Phe-Arg(Pbf)-Arg(Pbf)-Arg(Pbf)-Arg(Pbf)-Val-NH_2 (peptide 2).



Ac-Phe-Arg-Arg-Arg-Arg-Val-NH_2 from Ac-Phe-Arg(MIS)-Arg(MIS)-Arg(MIS)-Arg(MIS)-Val-NH_2 using 50% of TFA and 10% of 3,4-dimethoxyphenol in DCM as cleavage cocktail, 1h (*R* t= 10.2 min: target peptide, *R* t= 11.7 min MIS-OH).

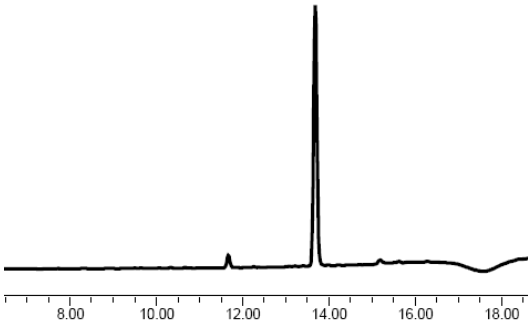


Ac-Phe-Arg-Arg-Arg-Arg-Val-NH_2 from Ac-Phe-Arg(Pbf)-Arg(Pbf)-Arg(Pbf)-Arg(Pbf)-Val-NH_2 using 50% of TFA, 2.5% TIS and 2.5% H_2O in DCM as a cleavage cocktail, 1h (*R* t= 8 min: target peptide, *R* t= 10 min, 12 min and 13.2 min : partially protected peptides).

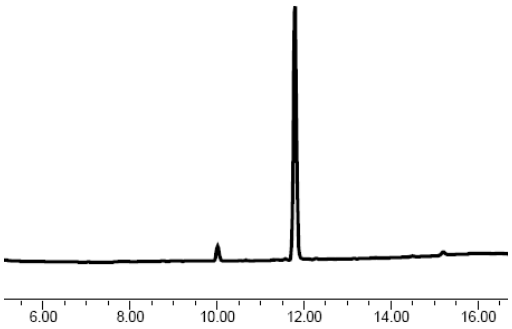


2.3 Tryptophan containing peptides:

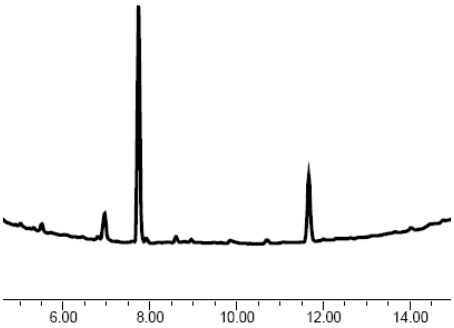
Z-Arg(Pbf)-Trp(Boc)-Ala-Gly-NH_2



Z-Arg(MIS)-Trp(Boc)-Ala-Gly-NH_2



Z-Arg-Trp-Ala-Gly-NH_2 from Z-Arg(Pbf)-Trp(Boc)-Ala-Gly-NH_2 (*R* t= 7.7 min: target peptide, *R* t= 11.7 min Pbf protected peptide).



Z-Arg-Trp-Ala-Gly-NH_2 from Z-Arg(MIS)-Trp(Boc)-Ala-Gly-NH_2