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Electronic Supplementary Information (ESI)

Concise Diastereoselective Synthesis of Calcaripeptide C via asymmetric transfer hydrogenation / Pd-induced Chiral Allenylzinc as a Key Reaction

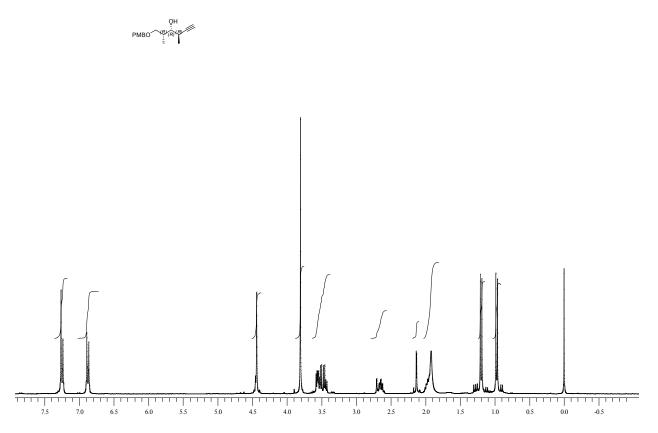
Gullapalli Kumaraswamy,* Vykunthapu Narayanarao and Ragam Raju

S2 General Information

S3–S14 ¹H NMR and ¹³CNMR Spectra's

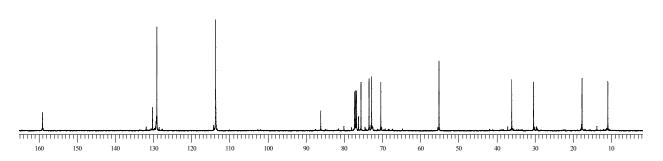
General information :All reactions were conducted under an inert atmosphere. Apparatus used for reactions were oven dried. THF was distilled over sodium benzophenone ketyl before use and DCM distilled over calcium hydride. (*S*)-But-3-yn-2-yl methanesulfonate was prepared according to the reported procedure. All other chemicals used were commercially available. Progress of the reactions was monitored by TLC on pre-coated silica gel 60 F-254. Evaporation of solvents was performed at reduced pressure on a rotary evaporator. Column chromatography was carried out with silica gel grade 60-120 and 100-200 mesh. ¹H NMR spectra were recorded at 300 & 500 MHz and ¹³C NMR 75 MHz in CDCl₃. Chemical shifts (δ) are reported in ppm. Tetramethylsilane (δ = 0.00 ppm for ¹H) and CDCl₃ (δ = 77.00 ppm for ¹³C) were used as the internal standard. Scalar coupling constants (*J*) are reported in hertz (Hz). The following abbreviations are used to designate the multiplicities: s = singlet, d = doublet, t = triplet, dd = doublet of doublet of doublet, m = multiplet, br.s = broad singlet. Mass spectral data were compiled using MS (ESI), and High resolution mass spectra (HRMS) were recorded by ESI probe in positive mode using ORBITRAP analyzer. Optical rotations were recorded on high sensitive polarimeter with 1mL cell.

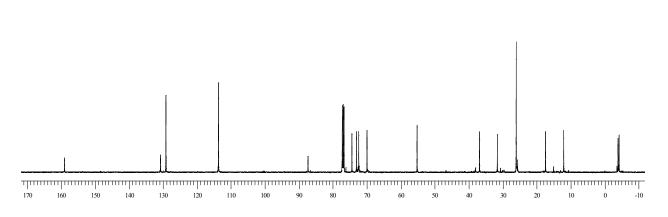
¹H NMR of 10:



¹³C NMR of 10:

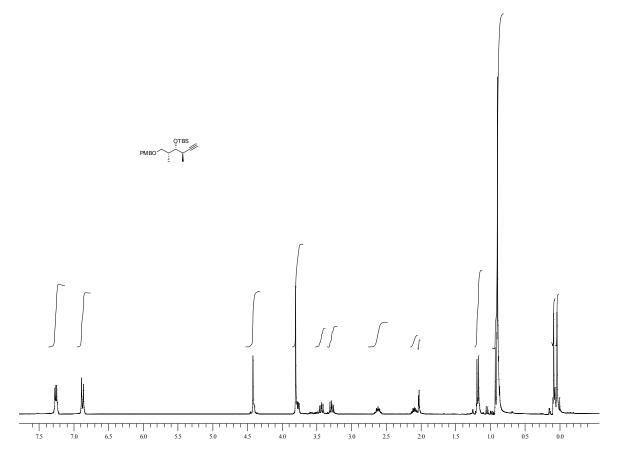


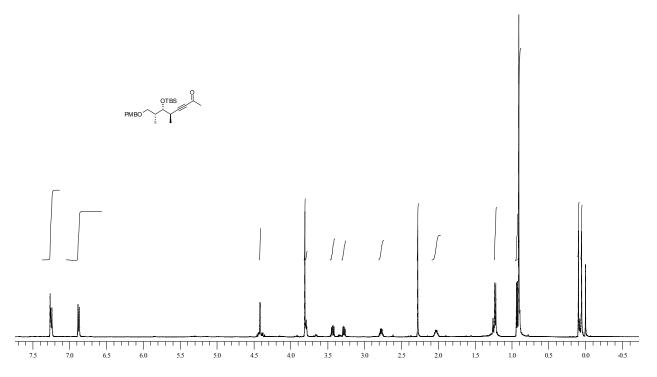






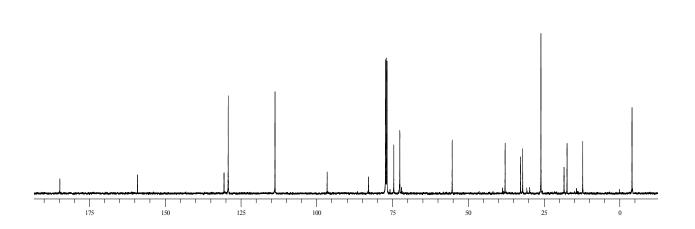
¹³C NMR of 11:

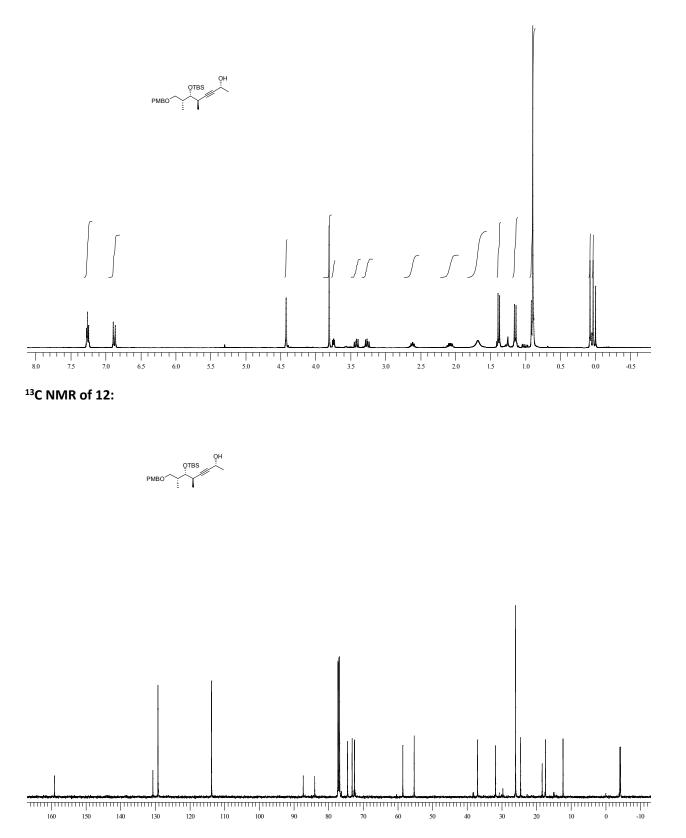


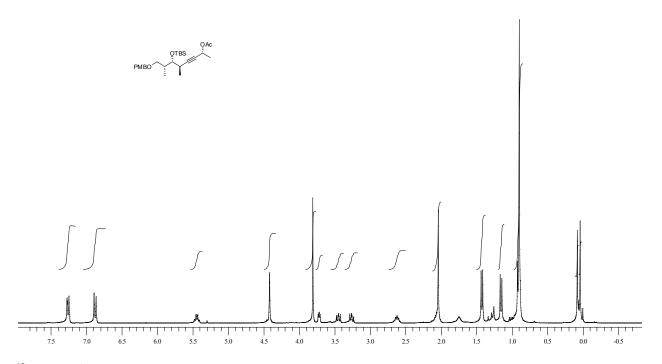


¹³C NMR of 6:

ОТВS О РМВО

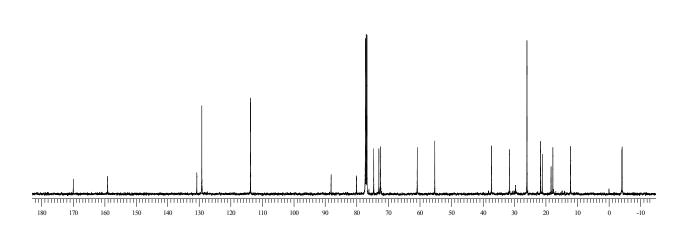




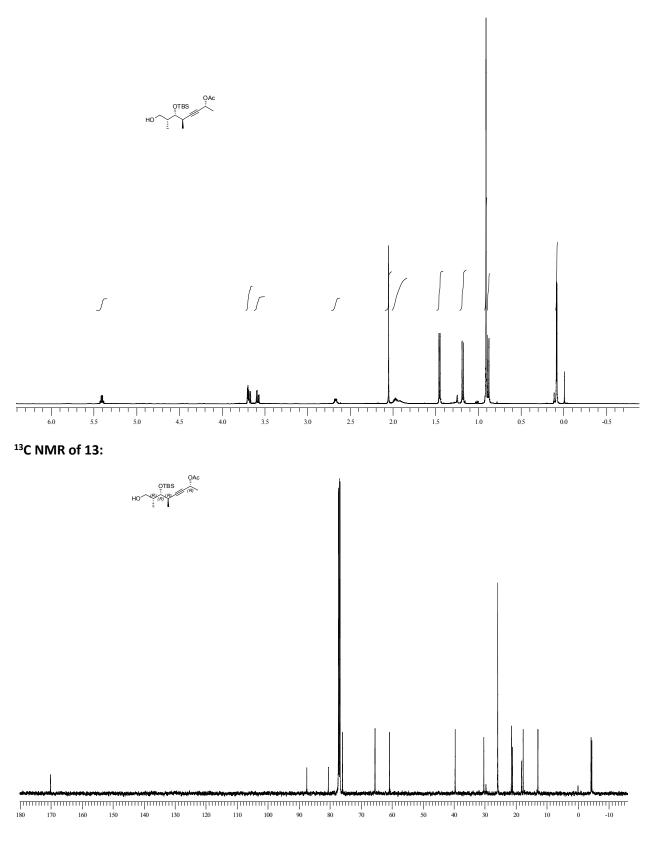


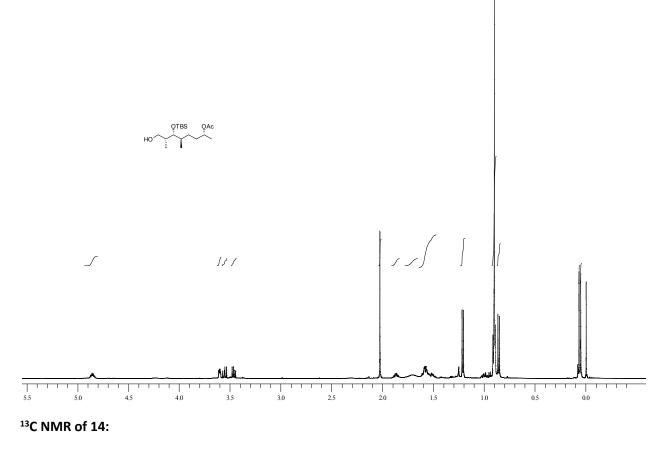
¹³C NMR of 12a:



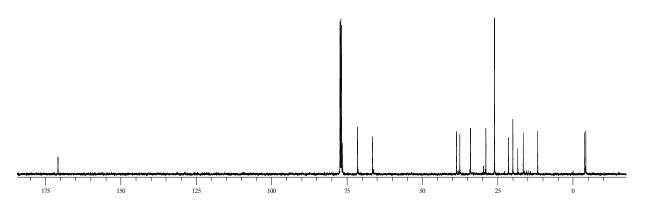


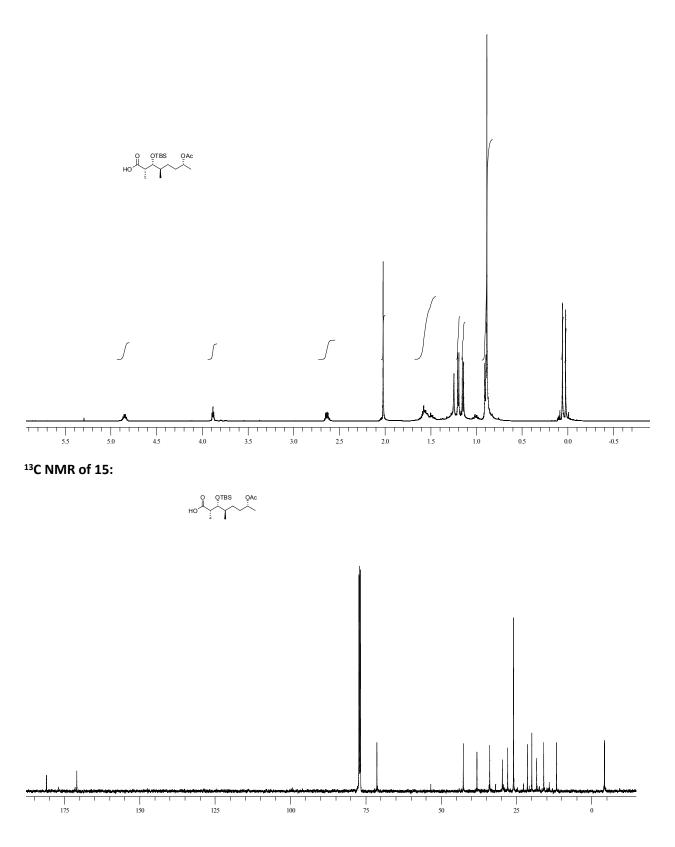


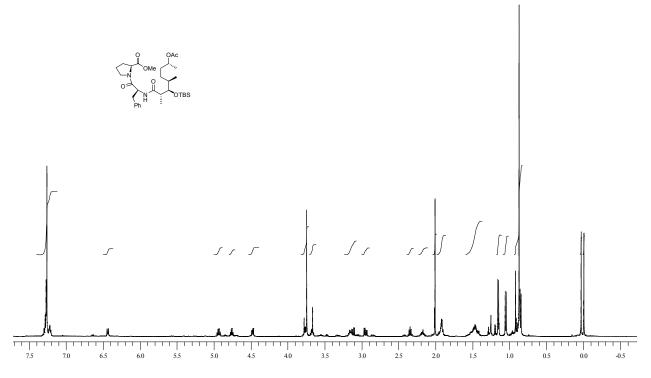




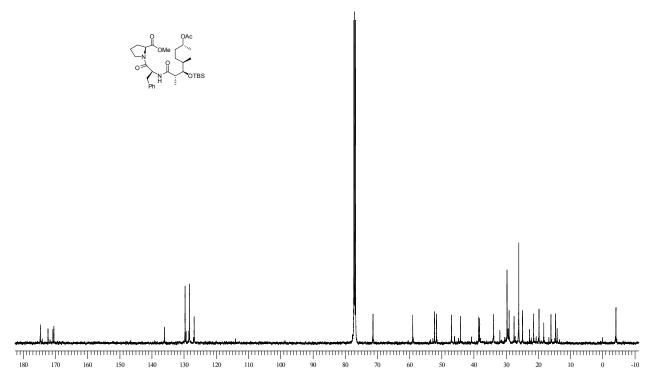




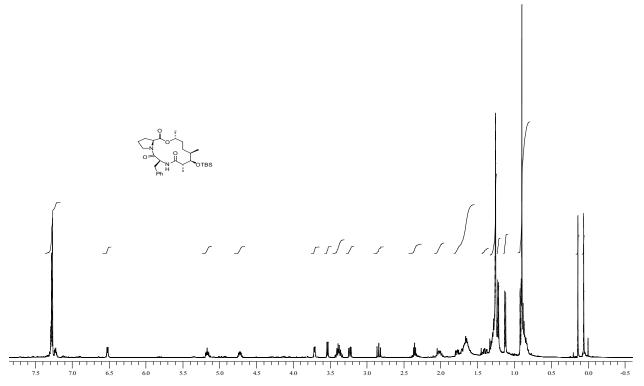




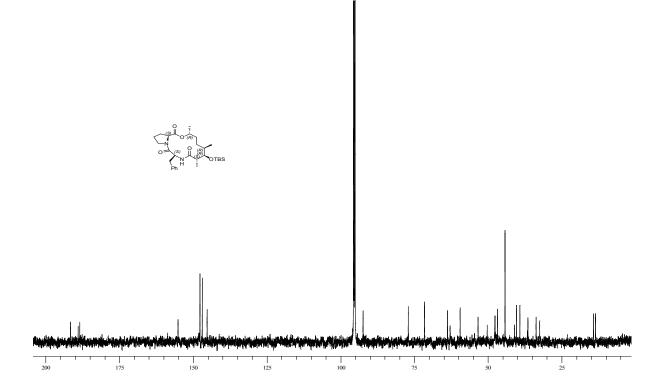
¹³C NMR of 16:



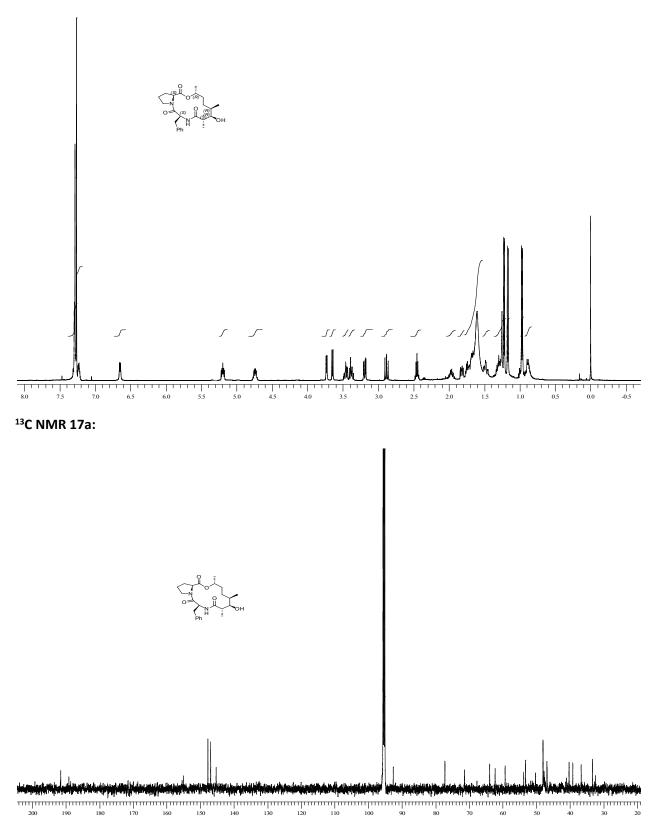












¹H NMR of 3:

