Supporting Information

C_2-Symmetric Recyclable Organocatalyst for Enantioselective Strecker Reaction for the Synthesis of α-Aminoacid and Chiral Diamine an Intermediate for APN Inhibitor

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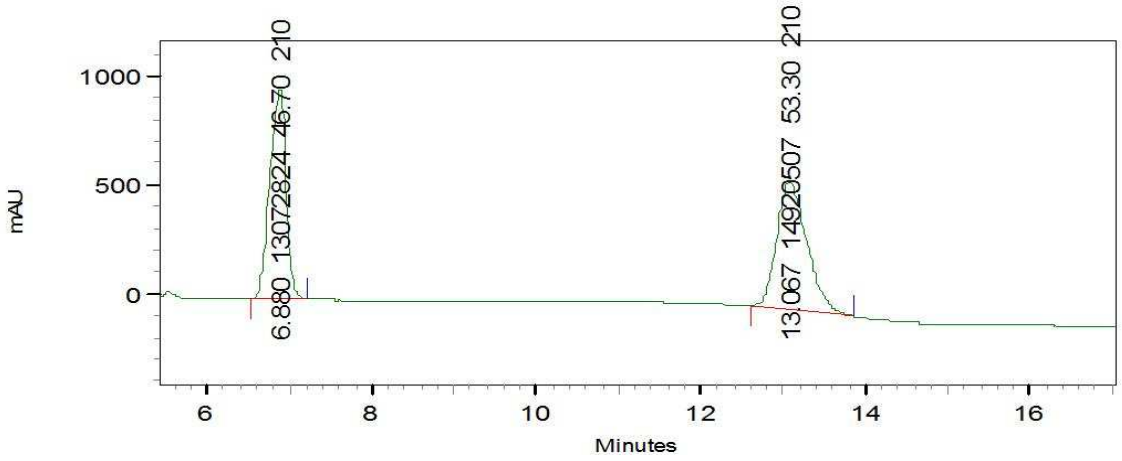
Contents

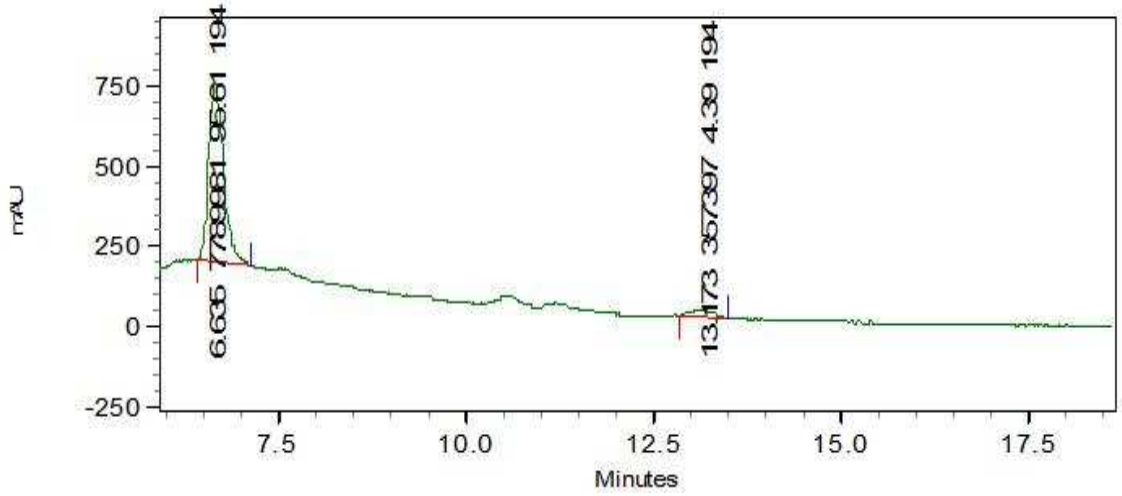
1. General

Different aldehydes and reagents were used as received. All the solvents used in the present study were dried by known purification technique.[1] NMR spectra were obtained with 500 MHz / 200 MHz and are referenced internally with TMS. Splitting patterns were reported as s, singlet; d, doublet; dd, doublet of doublet; t, triplet; q, quartet; m, multiplet; br, broad. Enantiomeric excess (*ee*) were determined by HPLC using Daicel Chiralpak AD-H chiral columns with 2-propanol/hexane as eluent. FTIR spectra were carried out using KBr. Optical rotations were determined by automatic polarimeter. For the product purification flash chromatography was performed using silica gel 100-200 mesh.

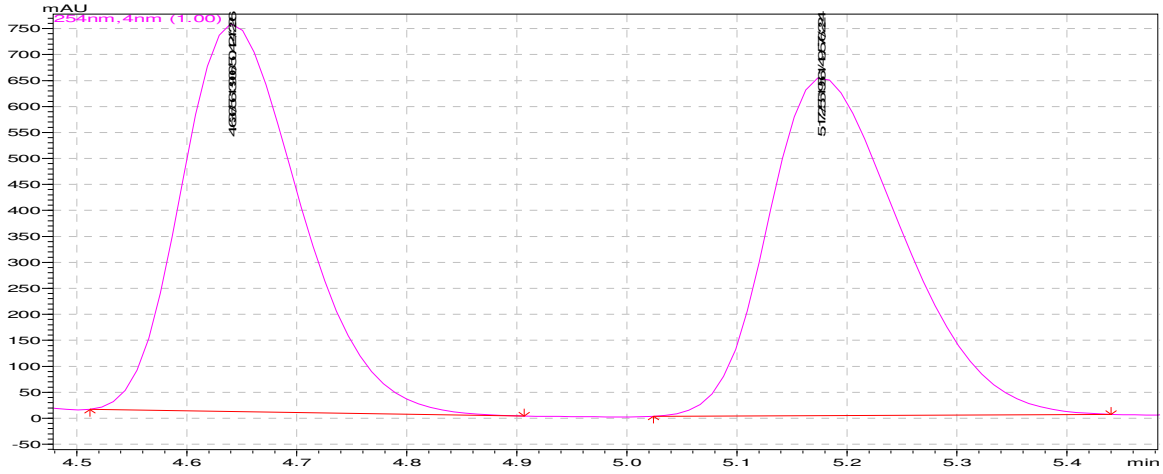
2. Characterization data of the products[3]

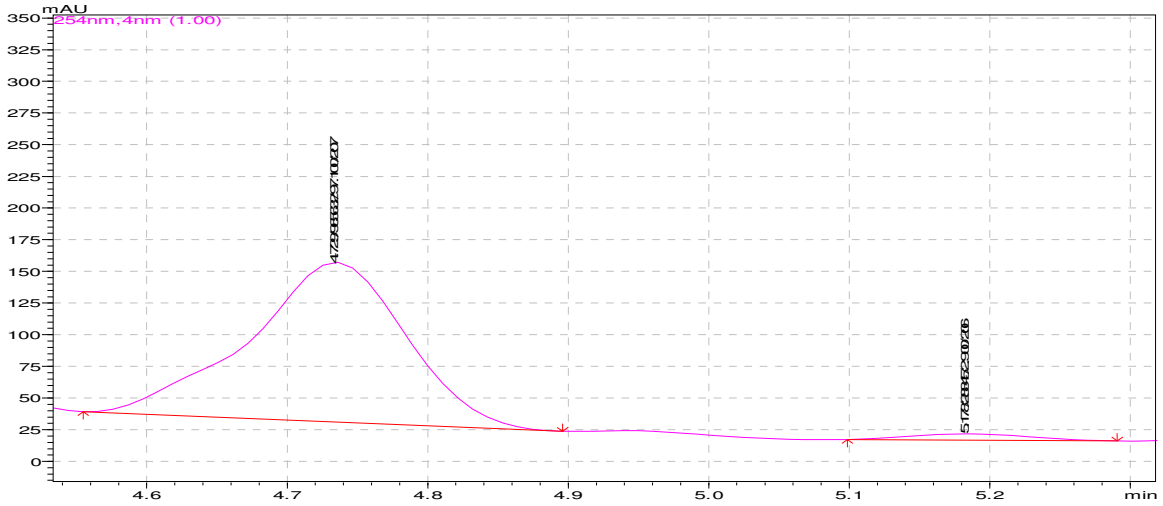
(*R*)-2-(Benzhydrylamino)-2-phenylacetonitrile (Table 4, entry 1)



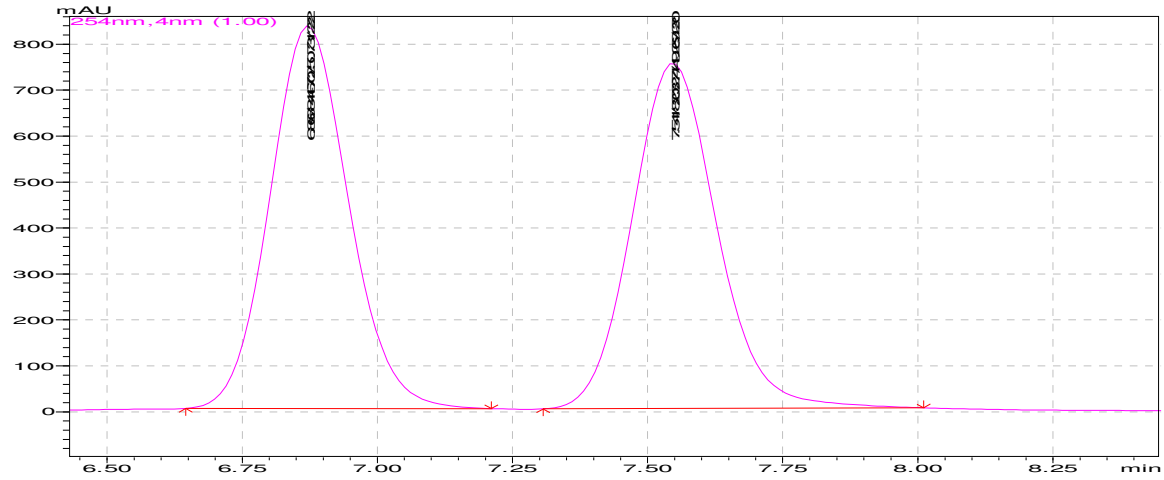


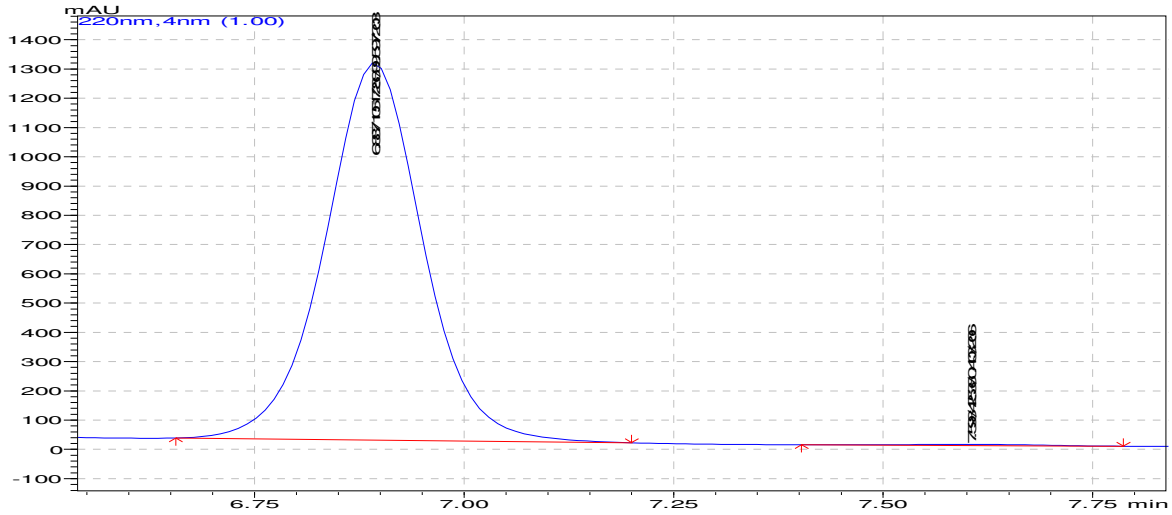
(*R*)-2-(Benzhydrylamino)-2-(2-bromophenyl) acetonitrile (Table 4, entry 2)





(*R*)-2-(Benzhydrylamino)-2-(2-nitrophenyl) acetonitrile (Table 4, entry 3)





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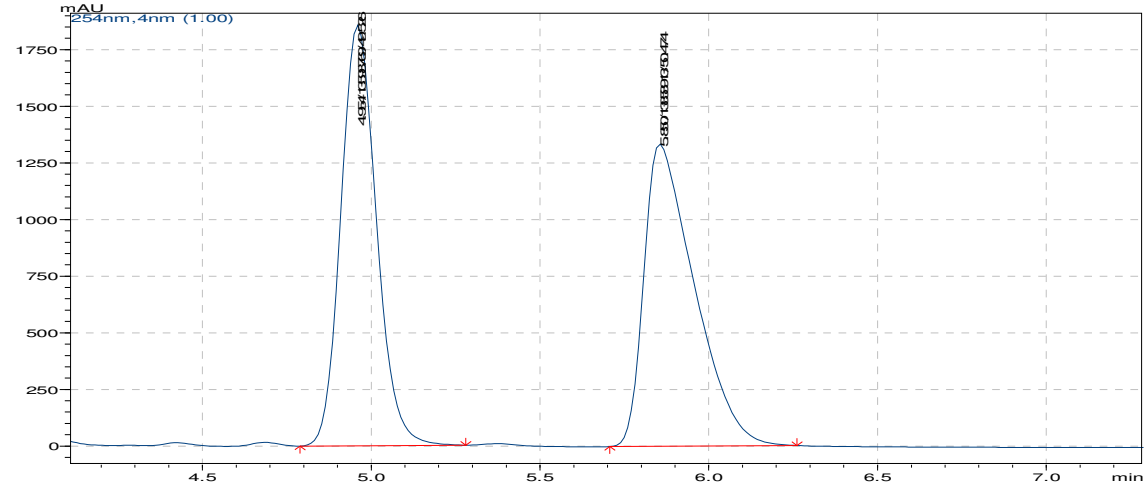
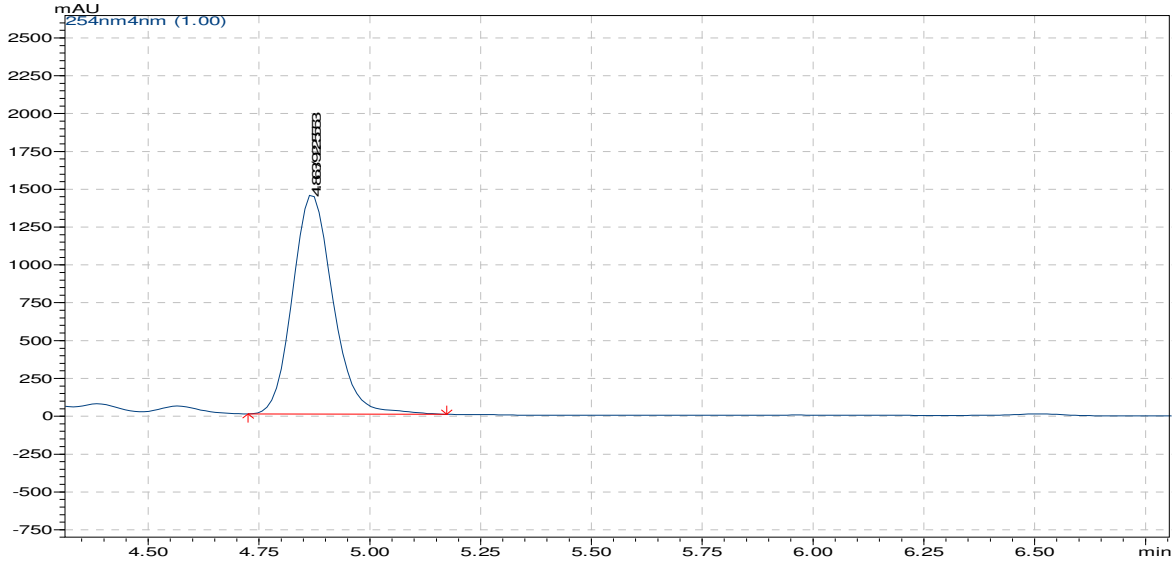
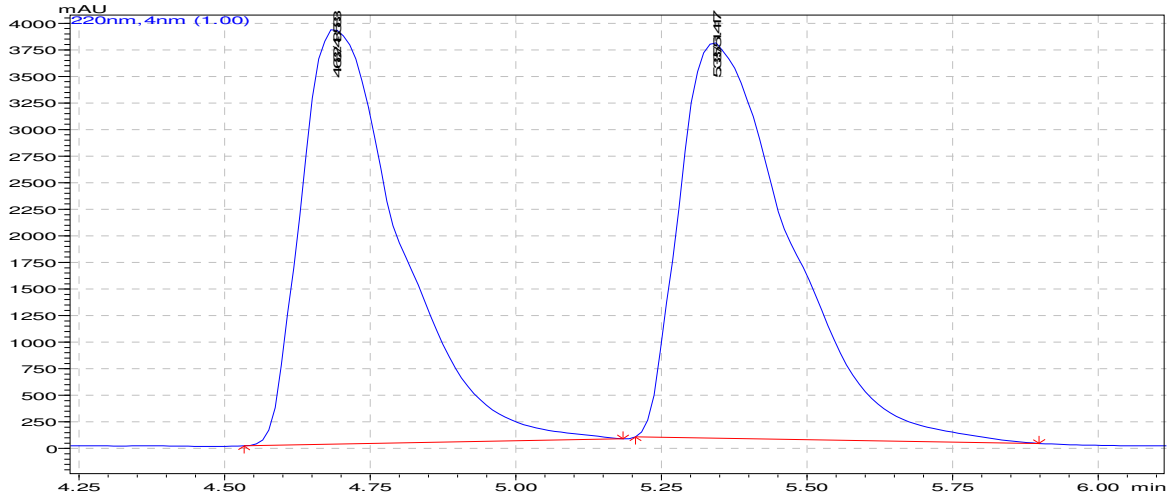
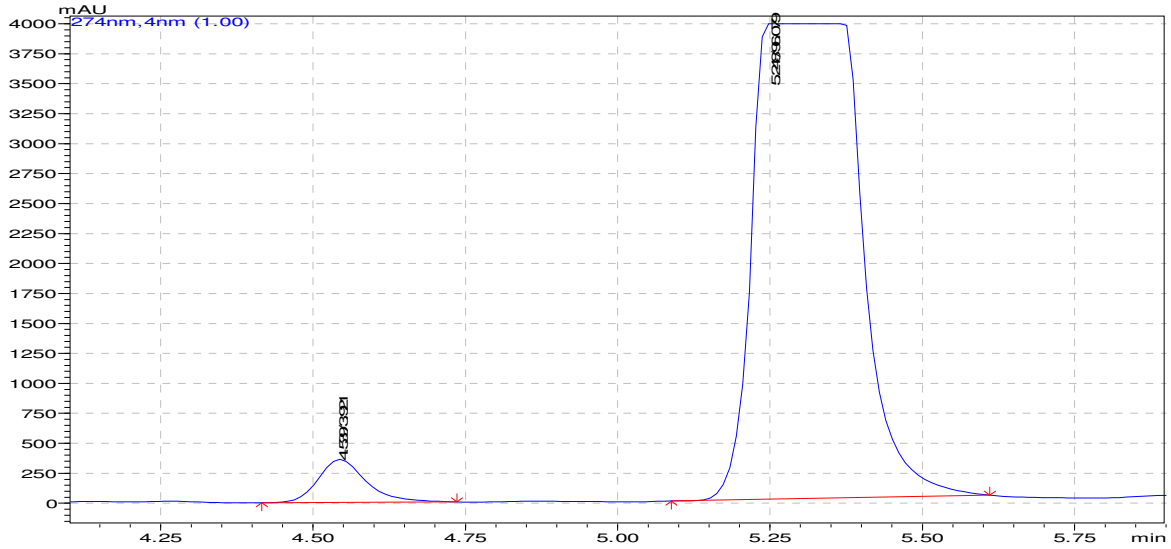


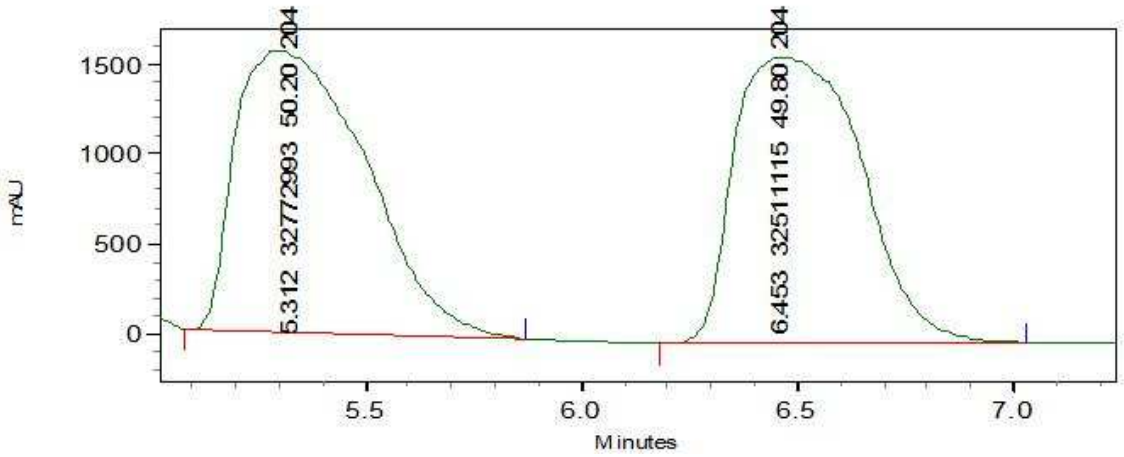


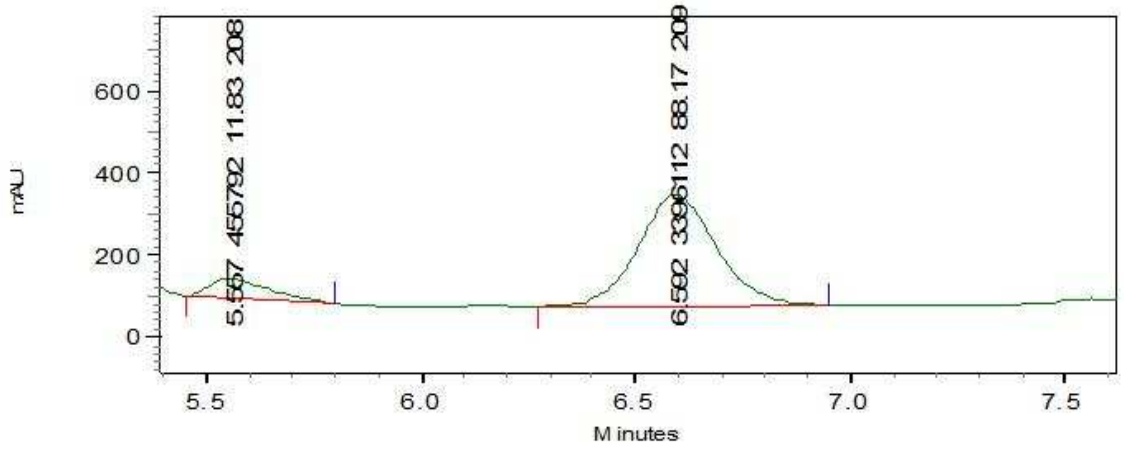
(*R*)-2-(Benzhydrylamino)-2-(2-chlorophenyl) acetonitrile (Table 4, entry 5)



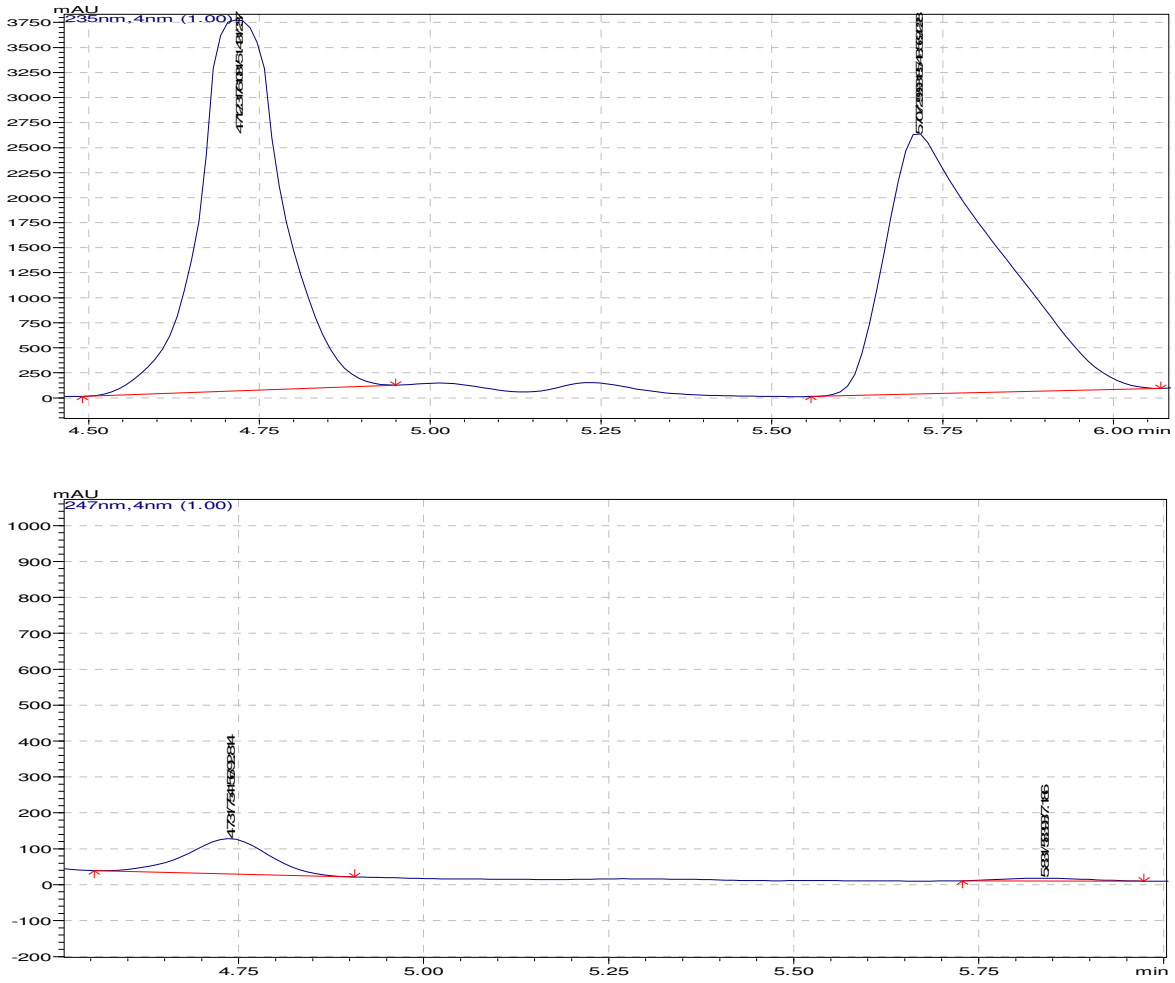


(*R*)-2-(Benzhydrylamino)-2-(2-methoxyphenyl) acetonitrile (Table 4, entry 6)

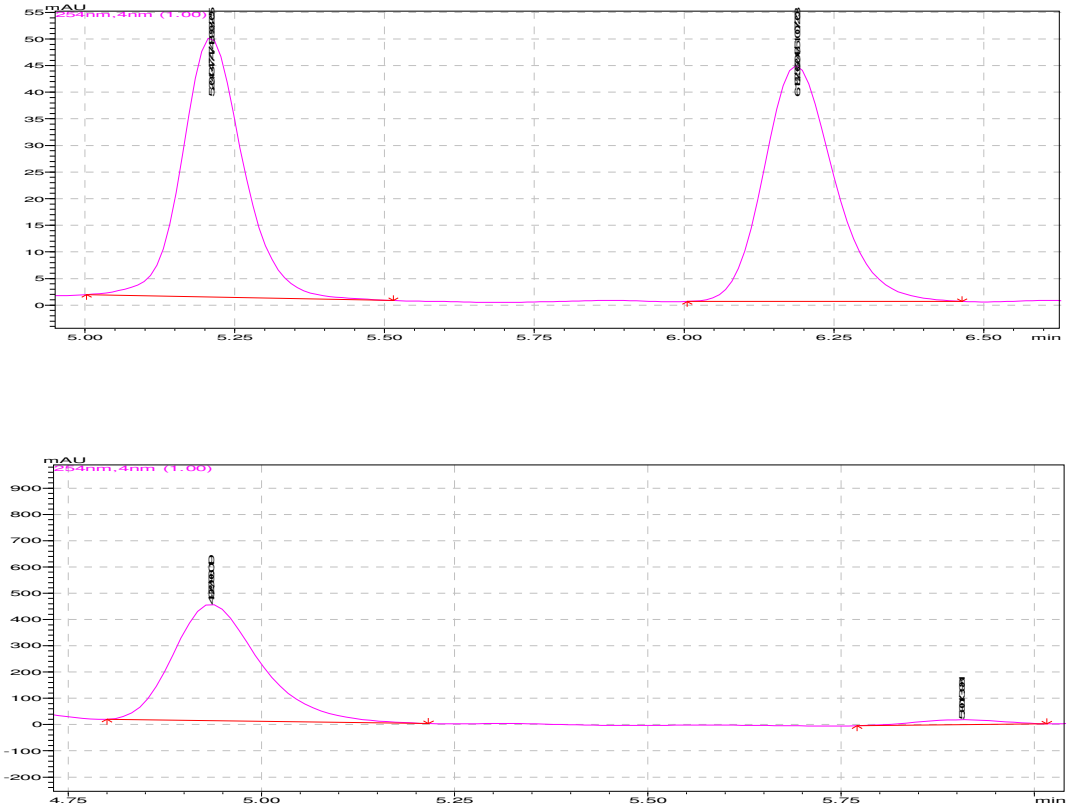




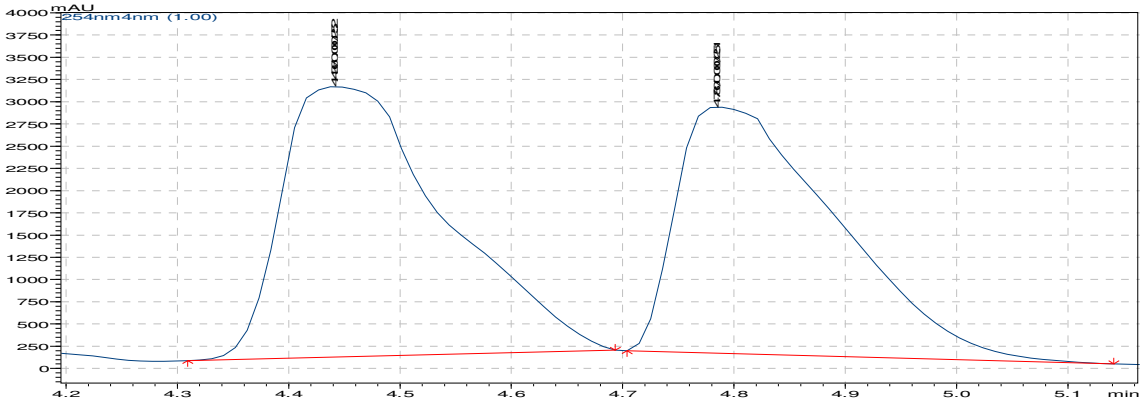
(*R*)-2-(Benzhydrylamino)-2-(2-ethoxyphenyl) acetonitrile (Table 4, entry9)

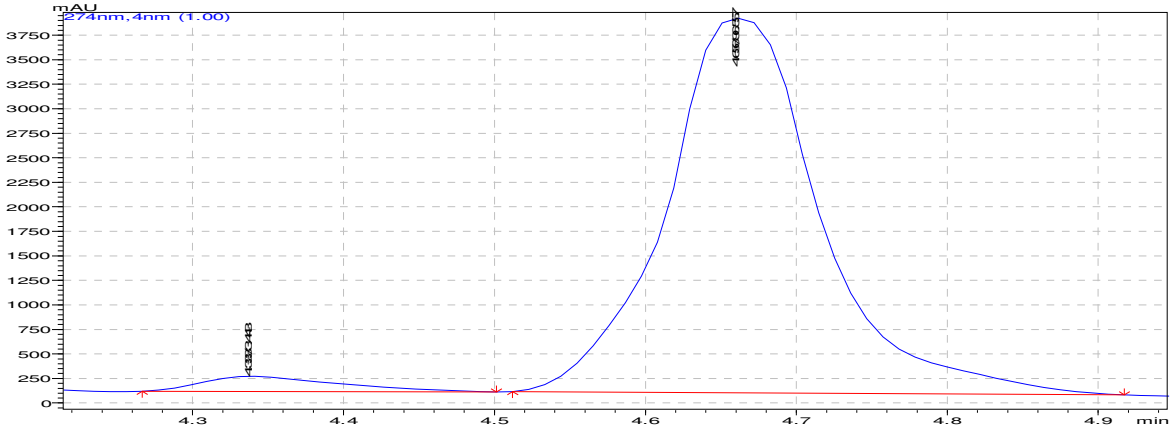


(*R*)-2-(benzhydrylamino)-3,3-dimethylbutanenitrile (Table 4, entry 11)

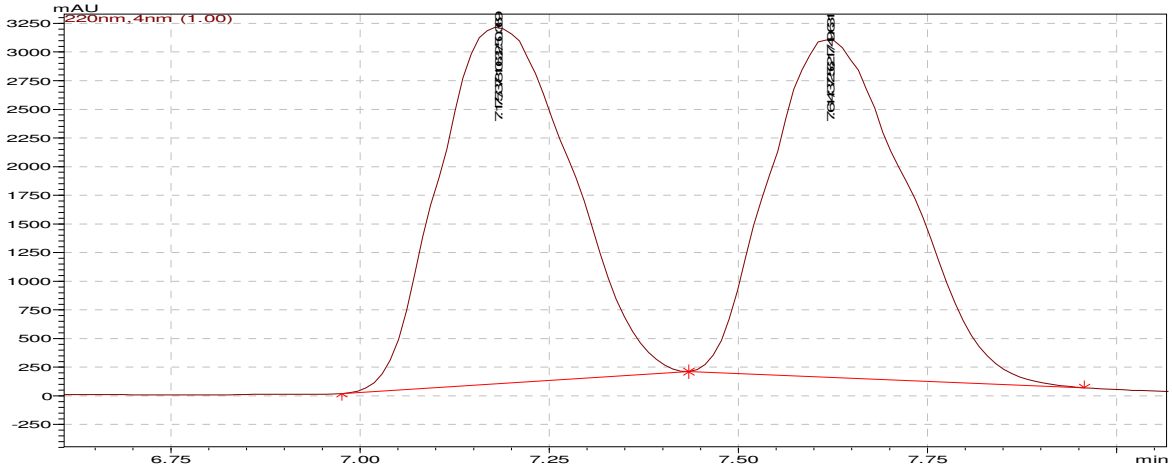


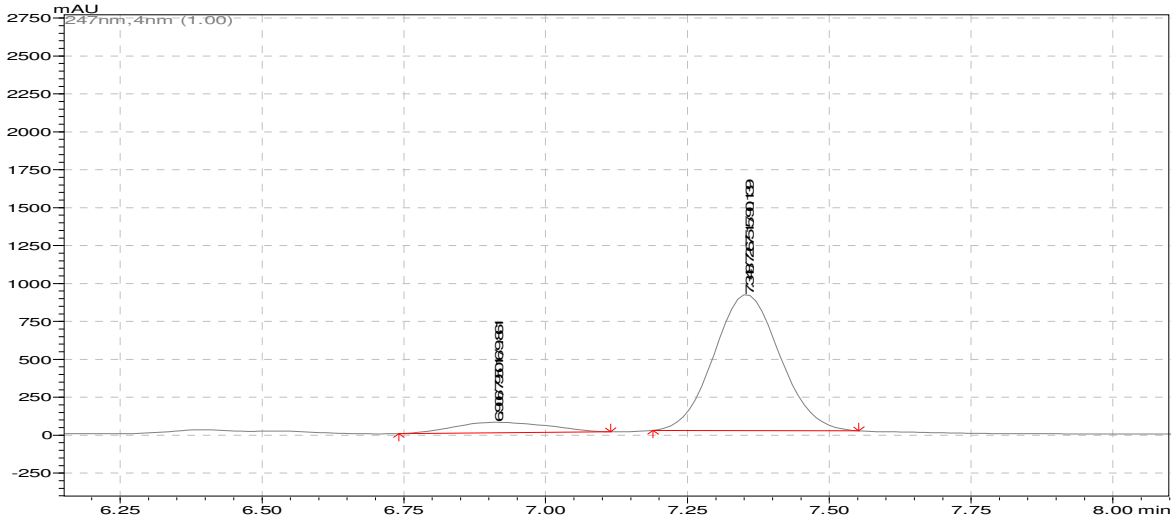
(*R*)-2-(benzhydrylamino)-3-phenylpropanenitrile(Table 4, entry 12)



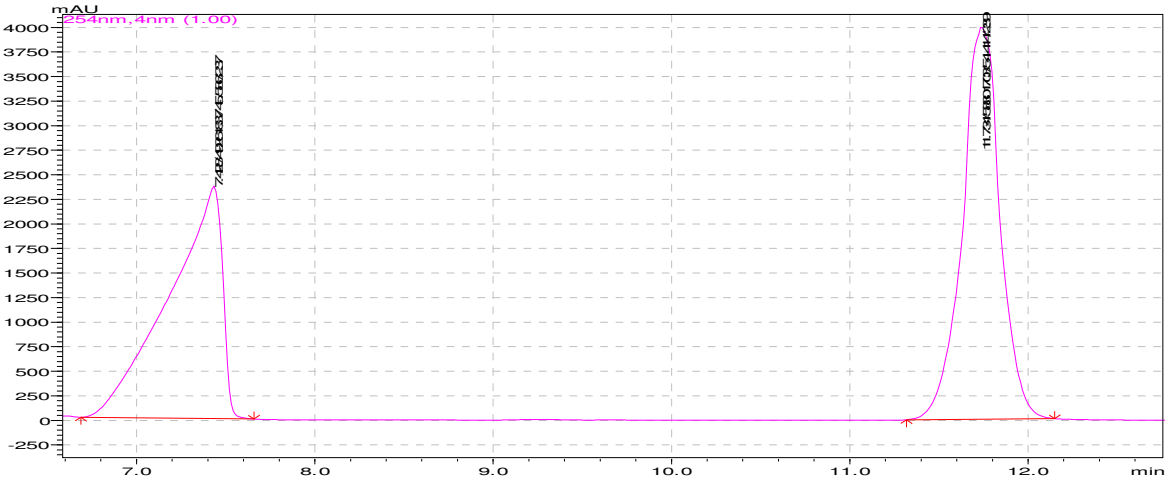


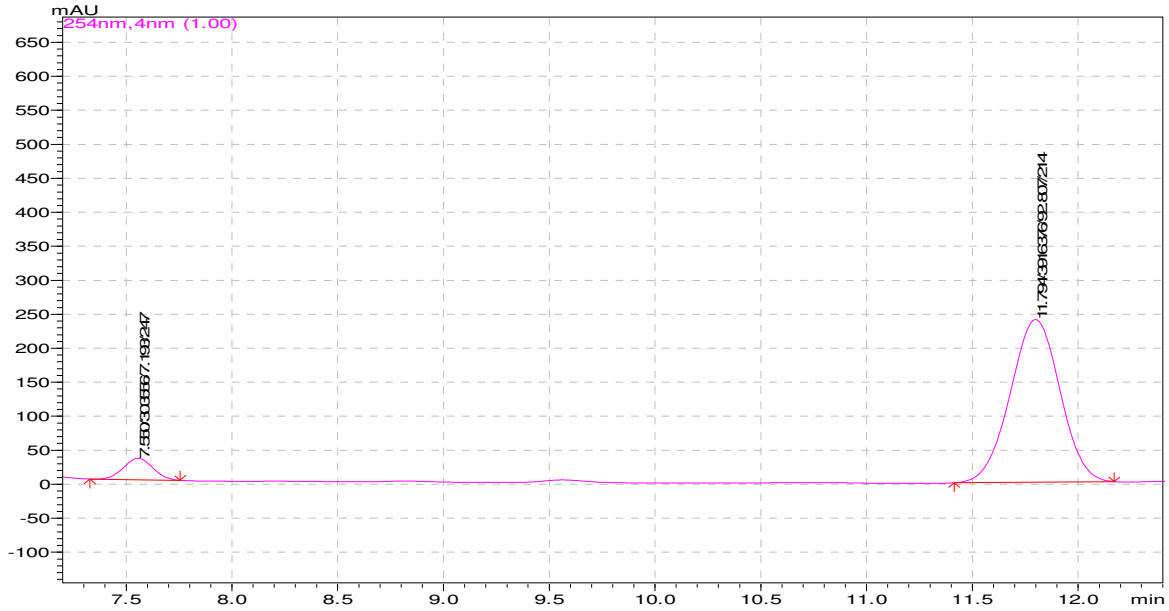
(*R*)-2-(benzhydrylamino)-4-methylpentanenitrile (Table 4, entry 13)





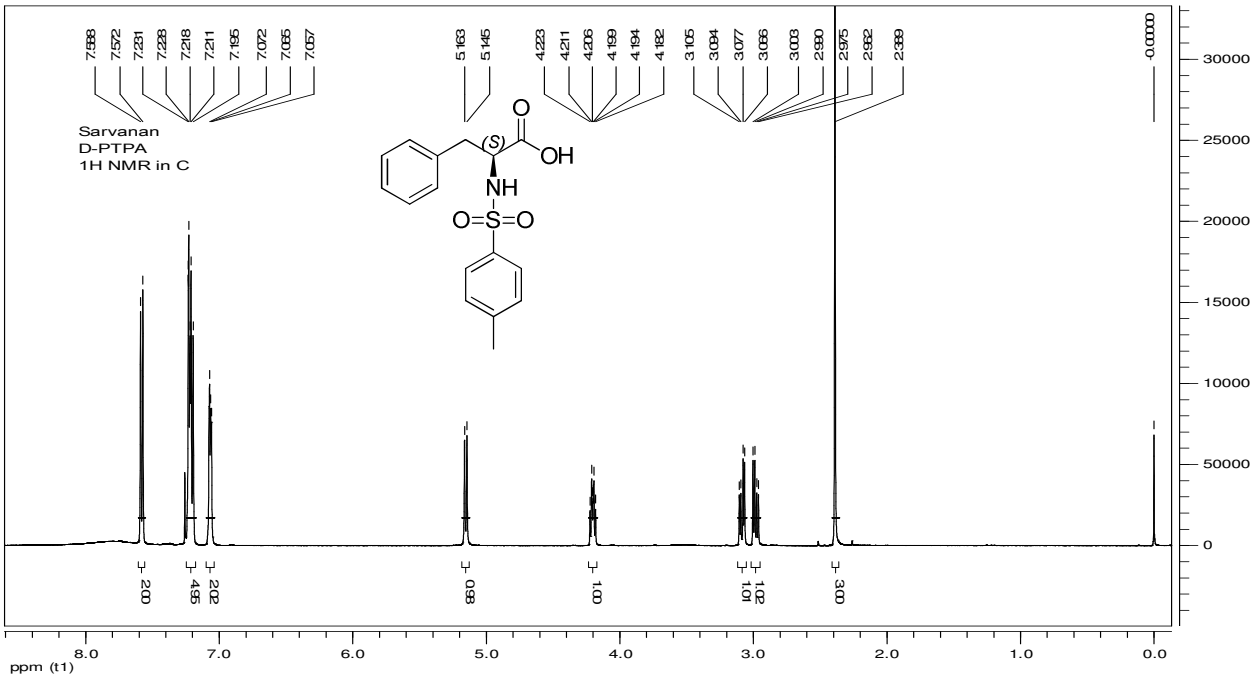
(R)-2-(benzhydrylamino)-2-(naphthalen-2-yl)acetonitrile (Table 4, entry 15)

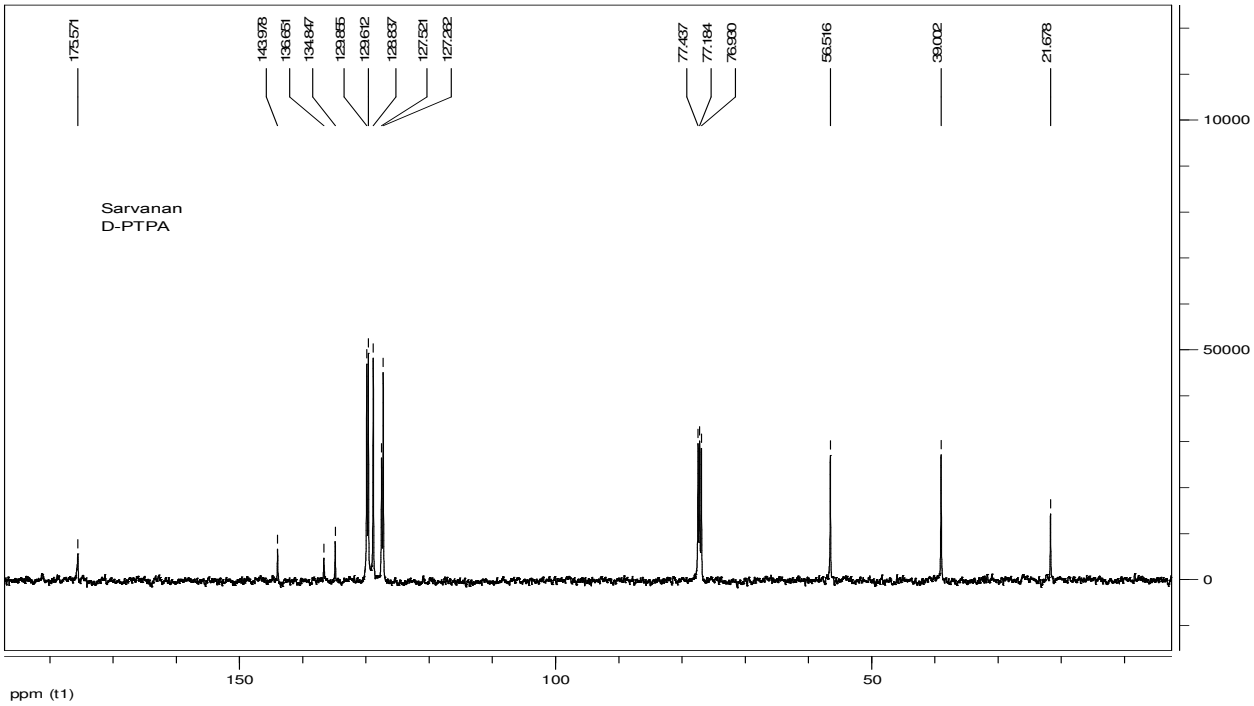




Copy of ^{1}H and ^{13}C NMR for catalysts and new product

Catalyst 1 (Table 1, entry 1)





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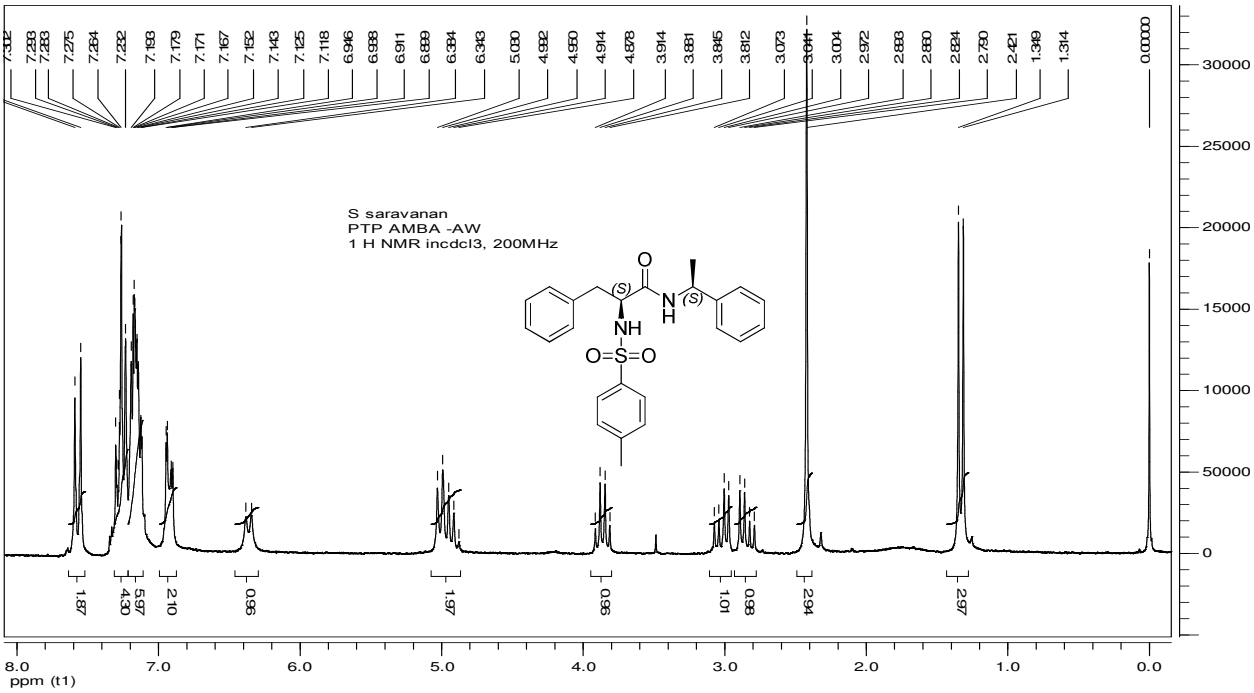
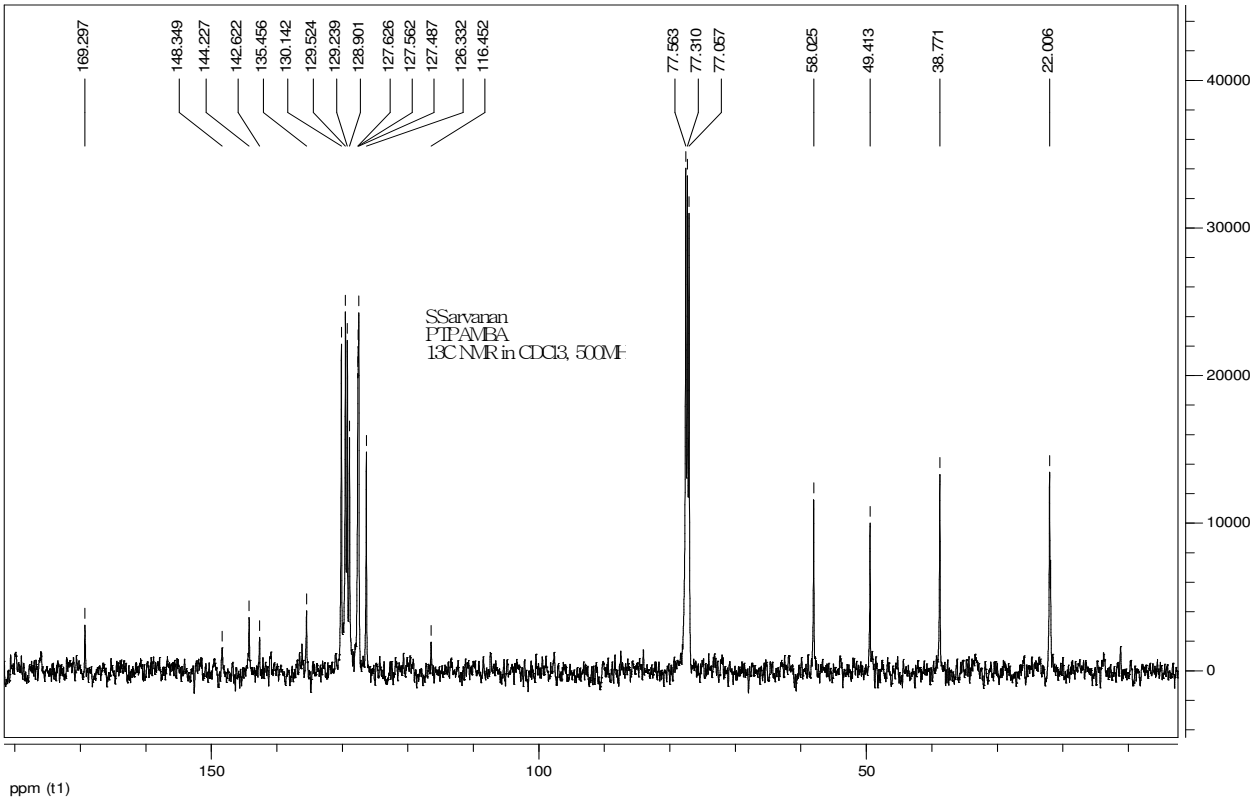
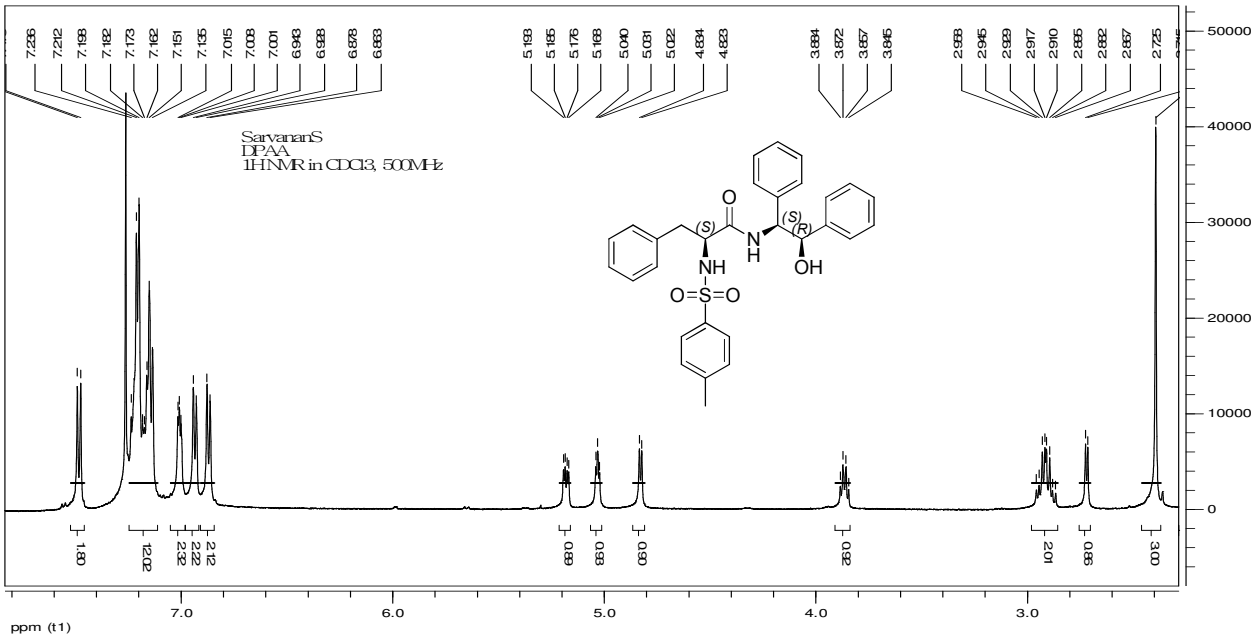
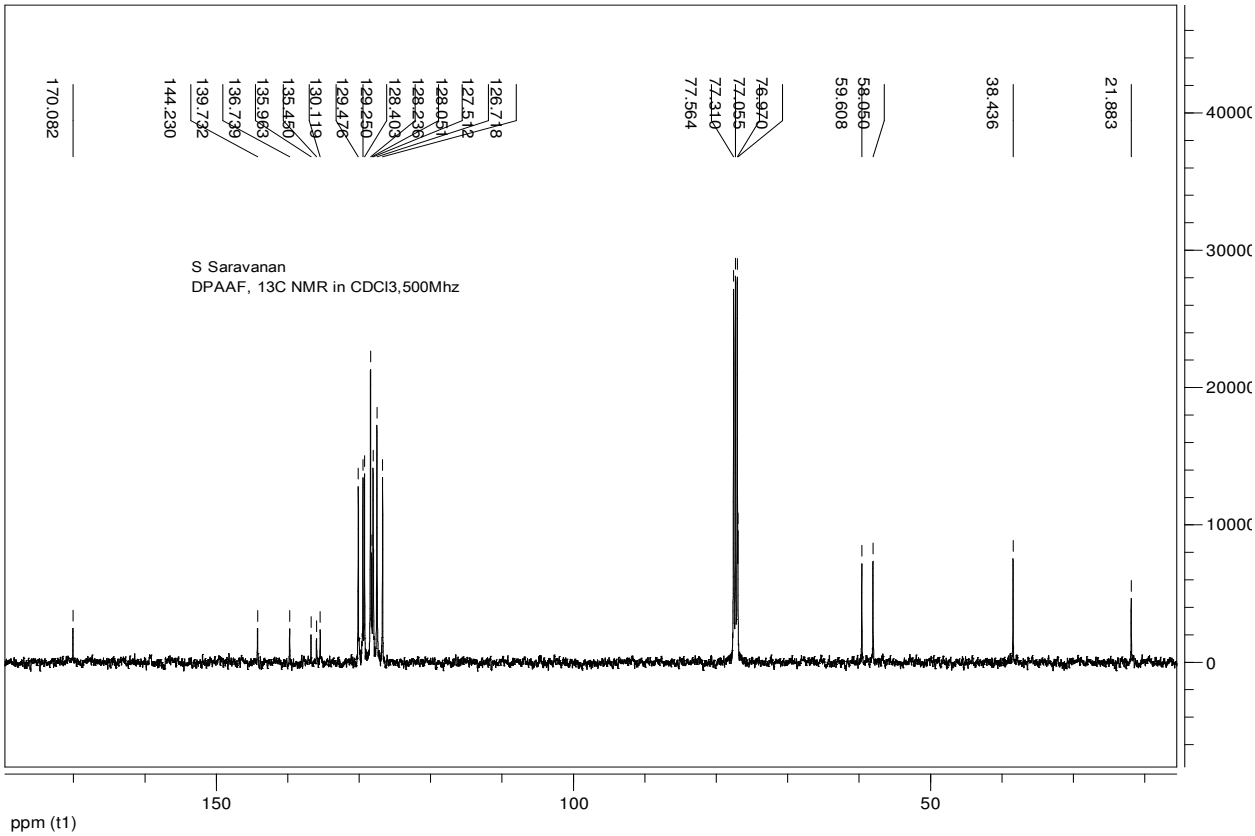




Catalyst 4 (Table 1, entry 4)





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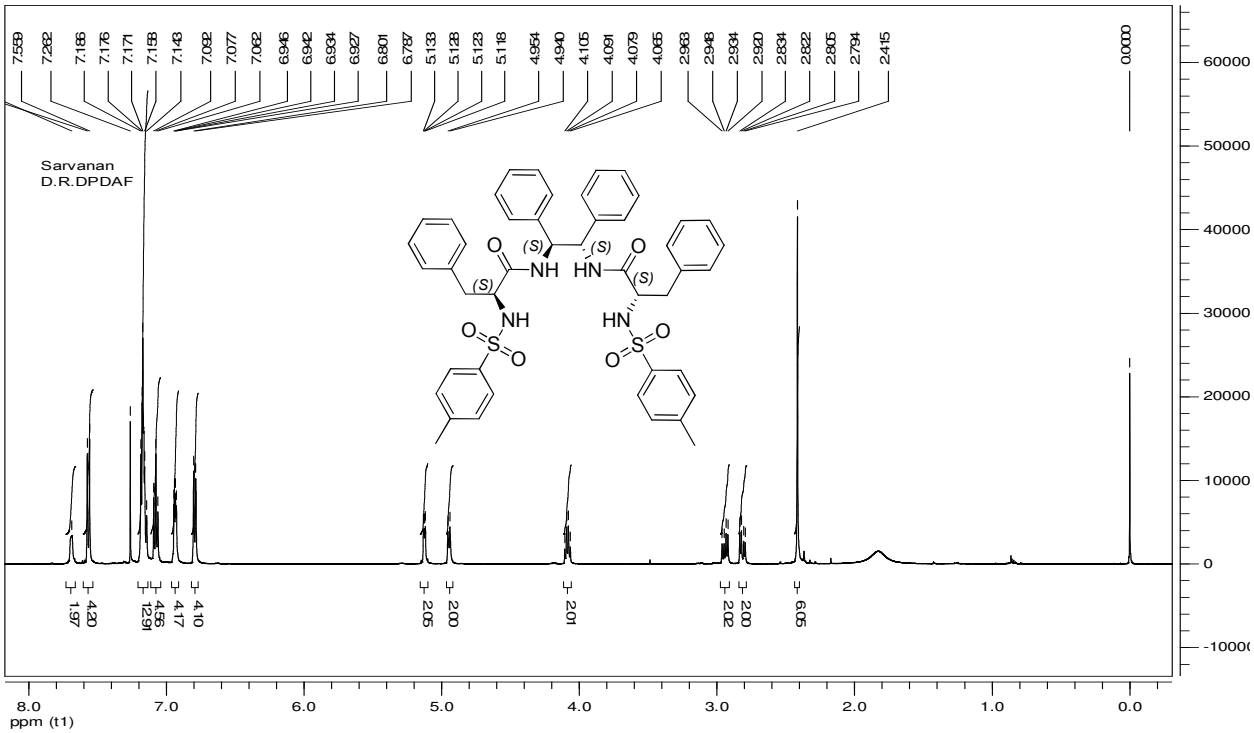
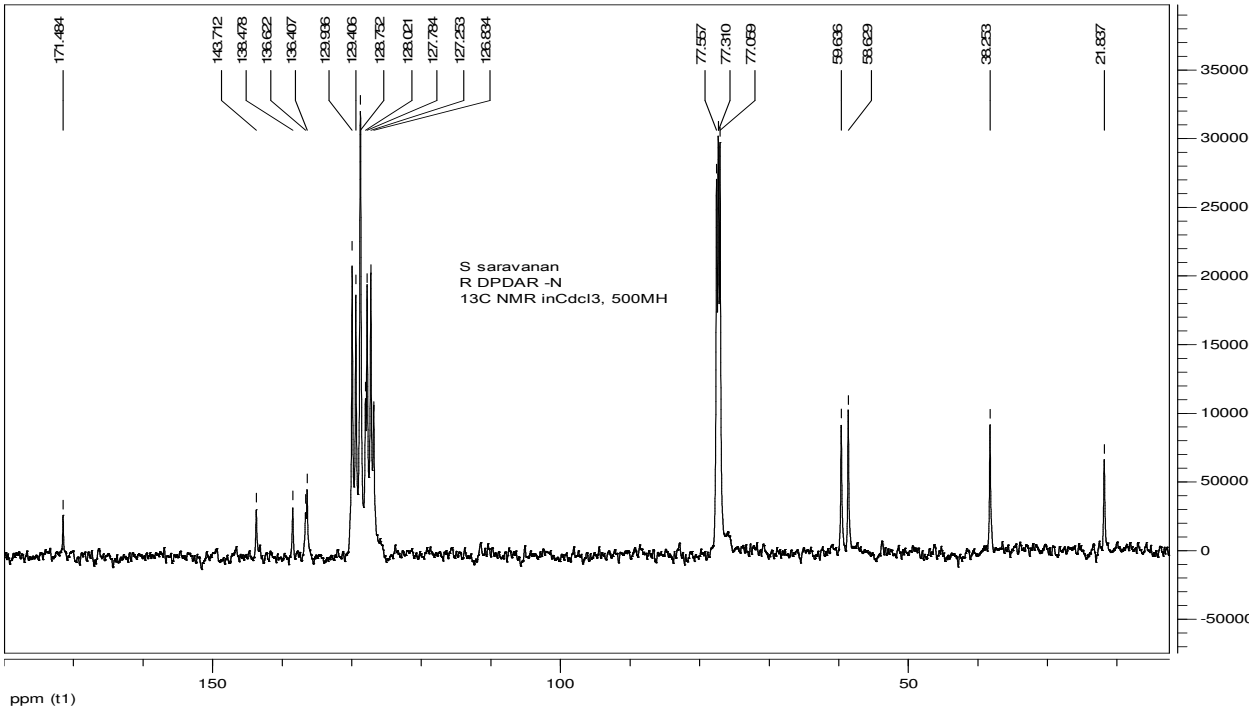
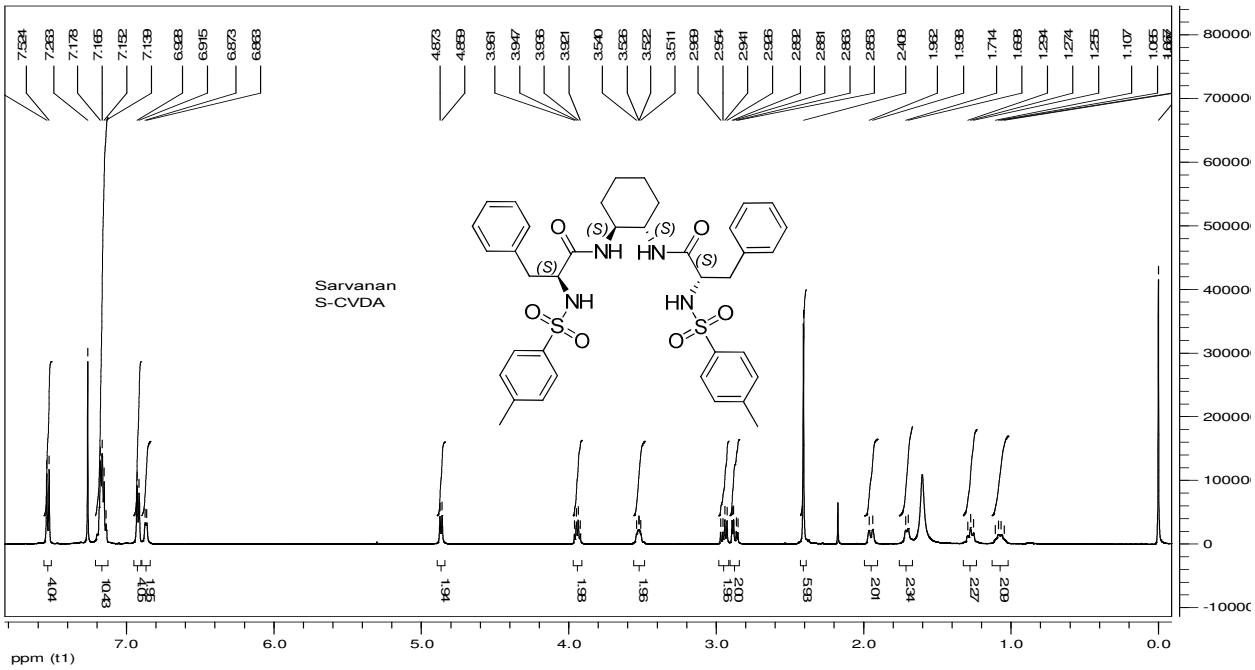
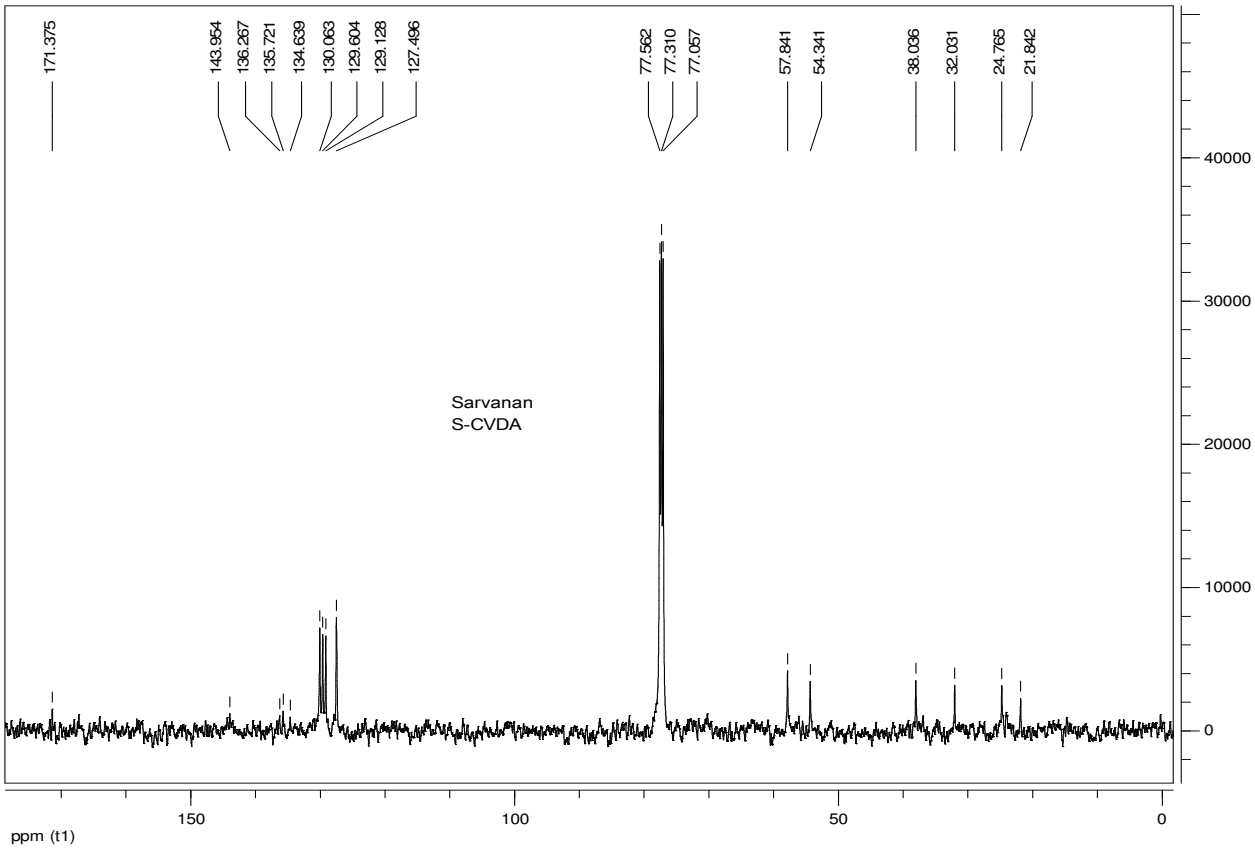


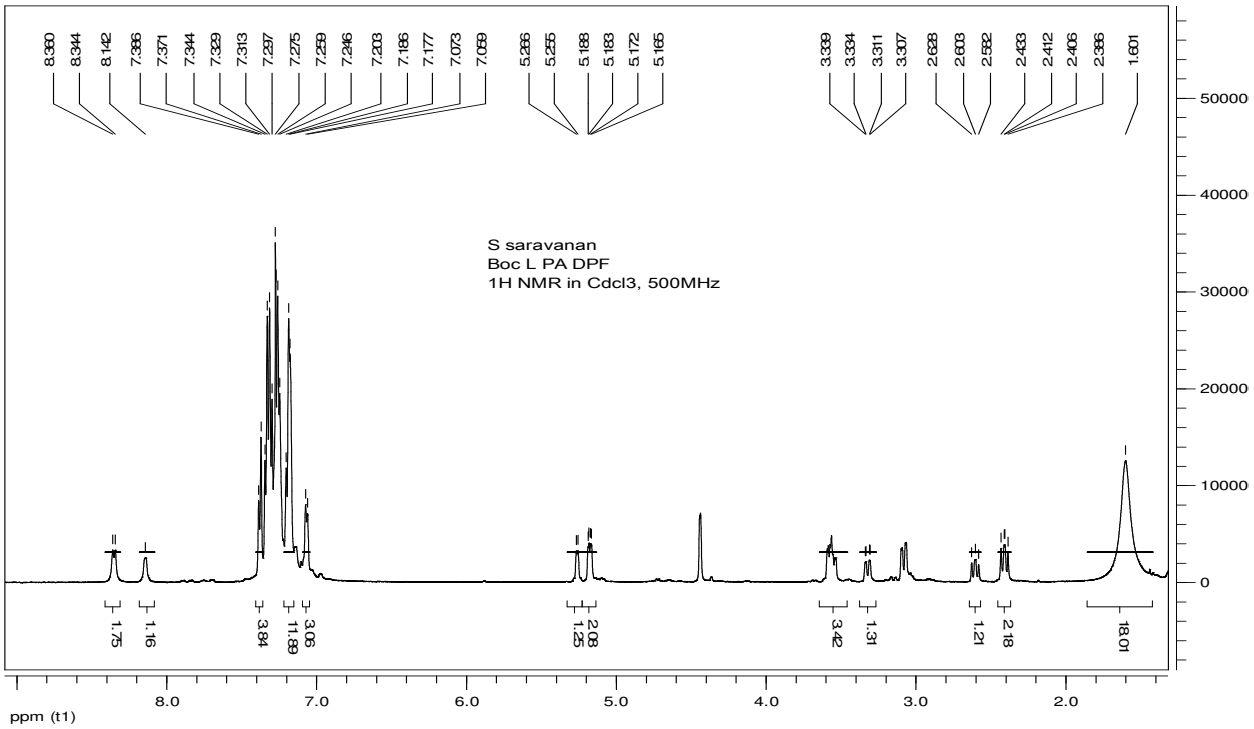


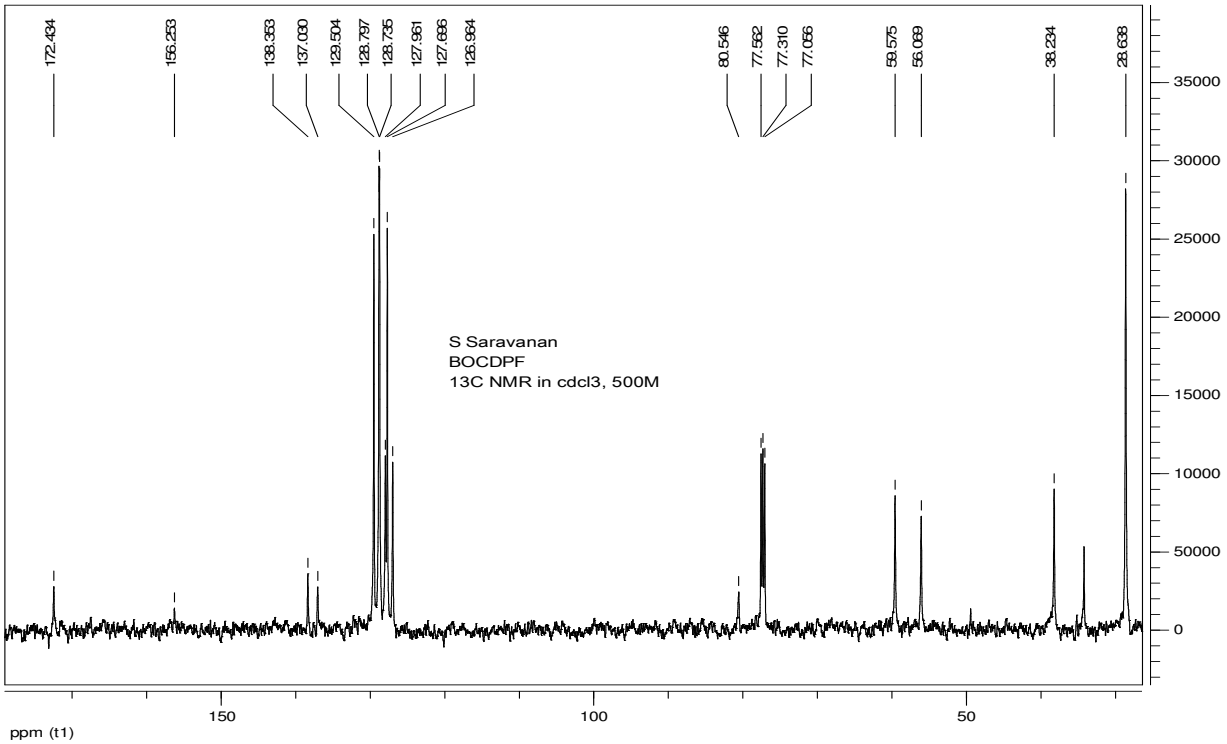
Catalyst 9 (Table 1, entry 7)



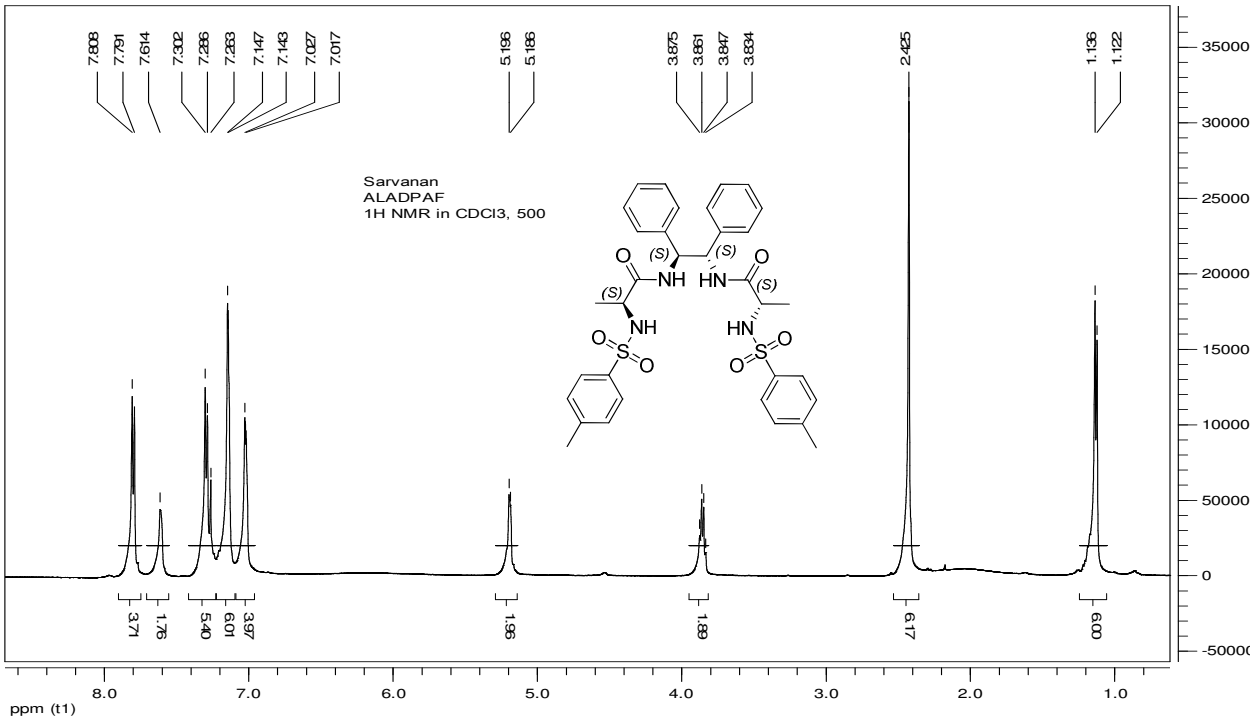


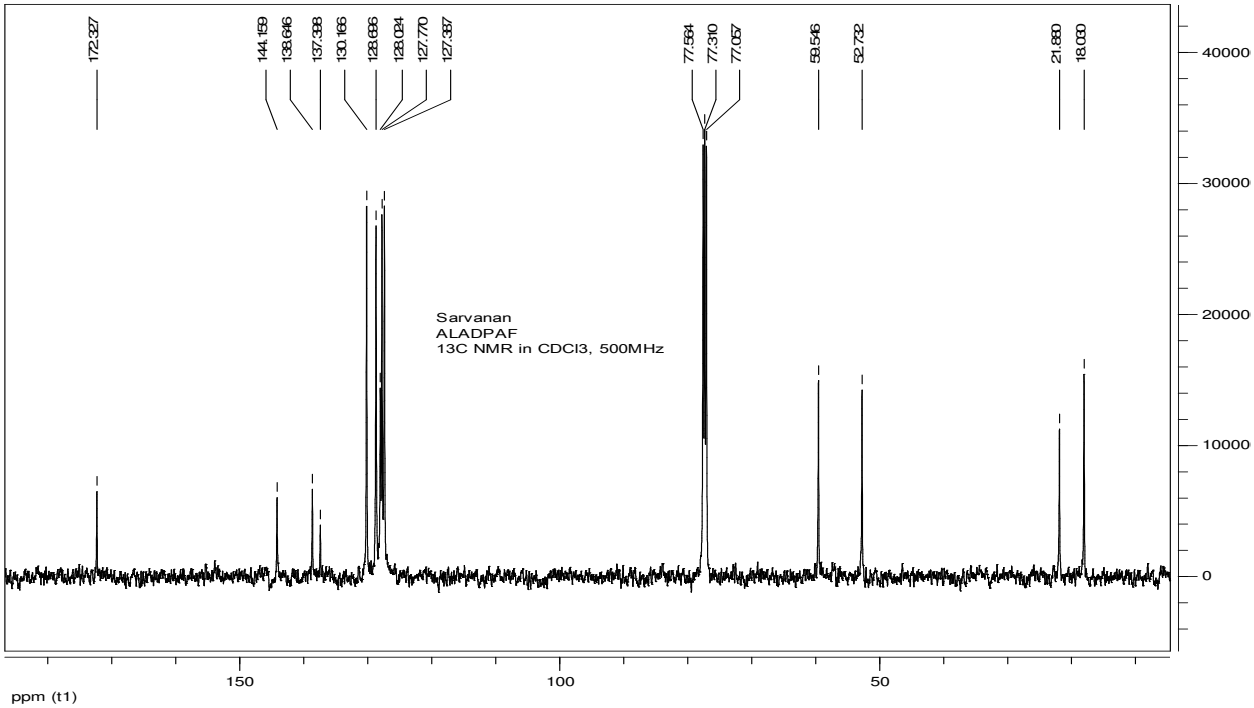
Catalyst 10 (Table 1, entry 8)



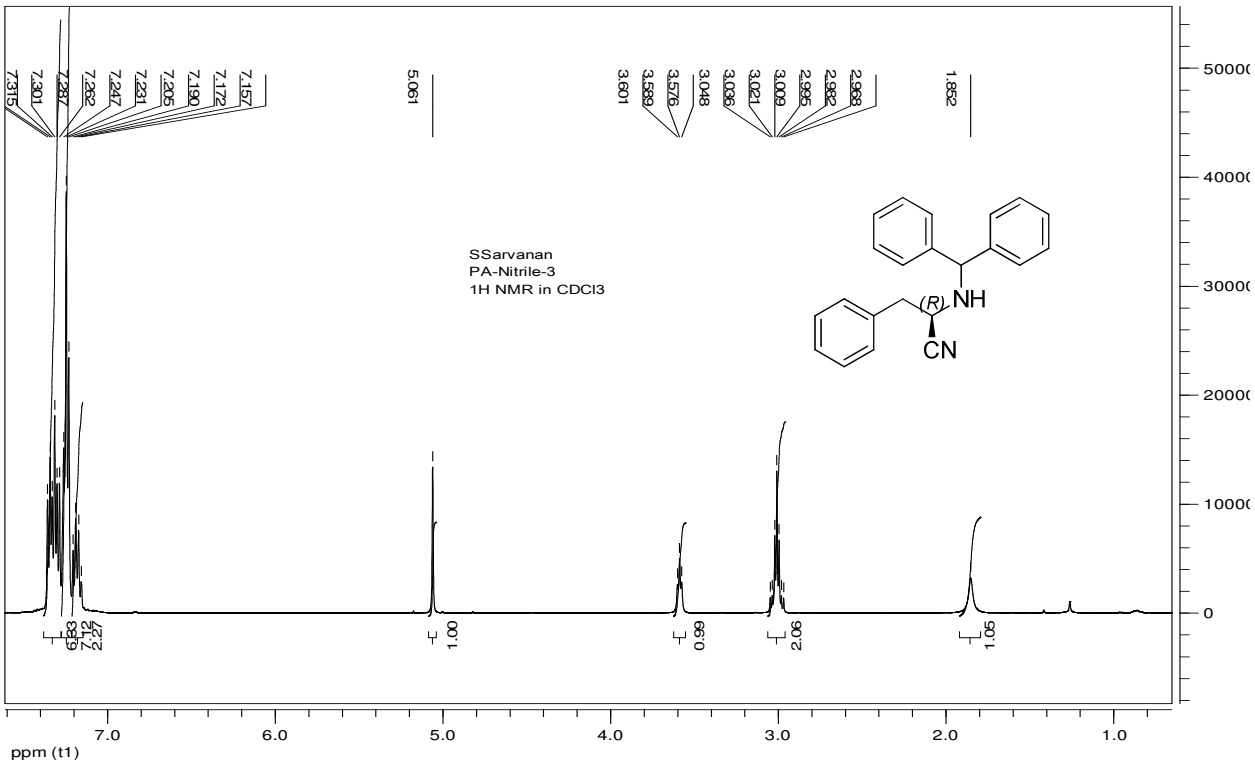


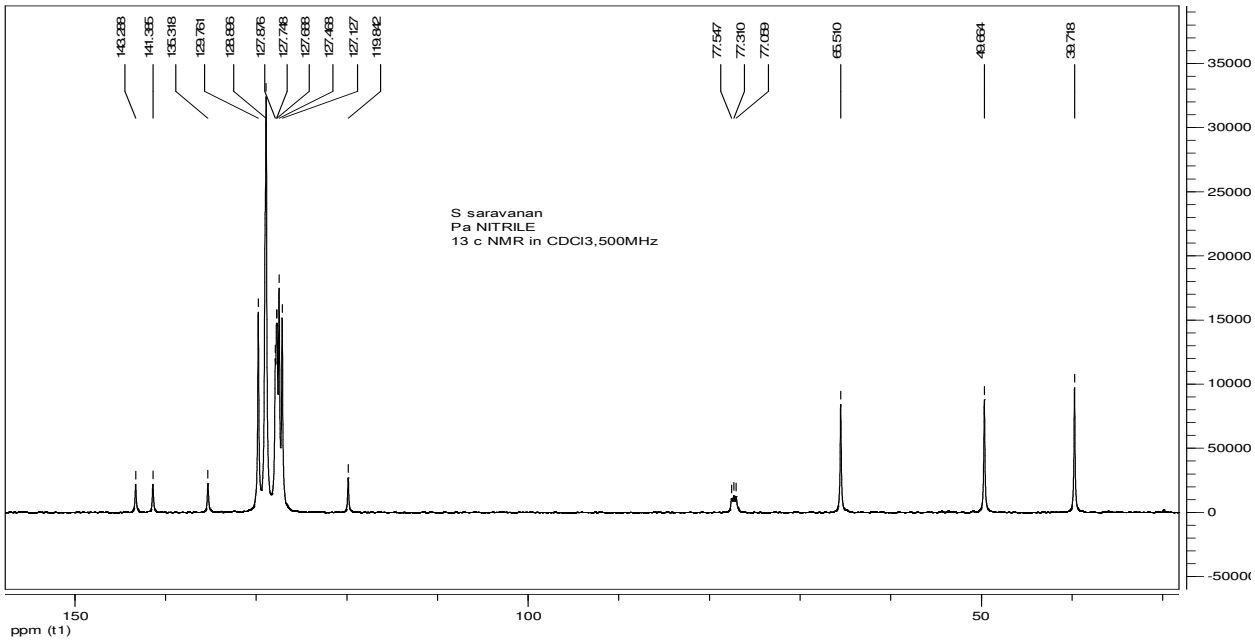
Catalyst 11 (Table 1, entry 9)



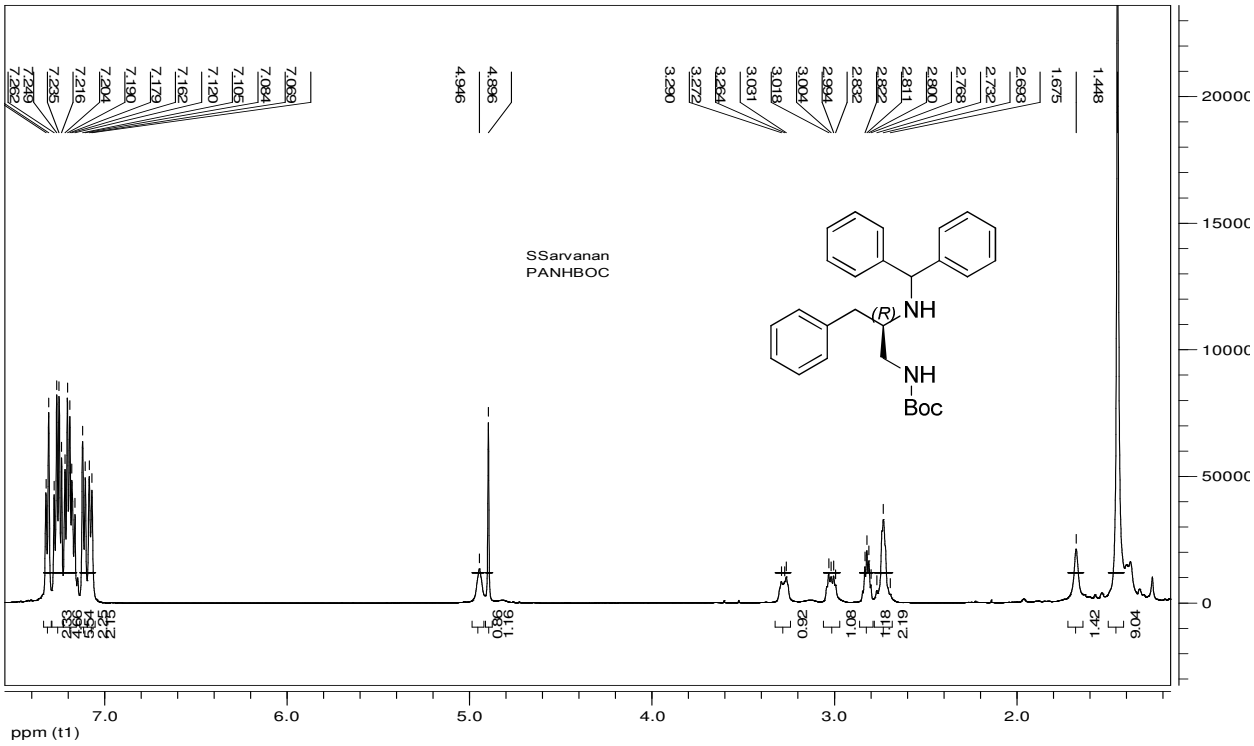


Compound 2j (Table 4, entry 10)





Compound 13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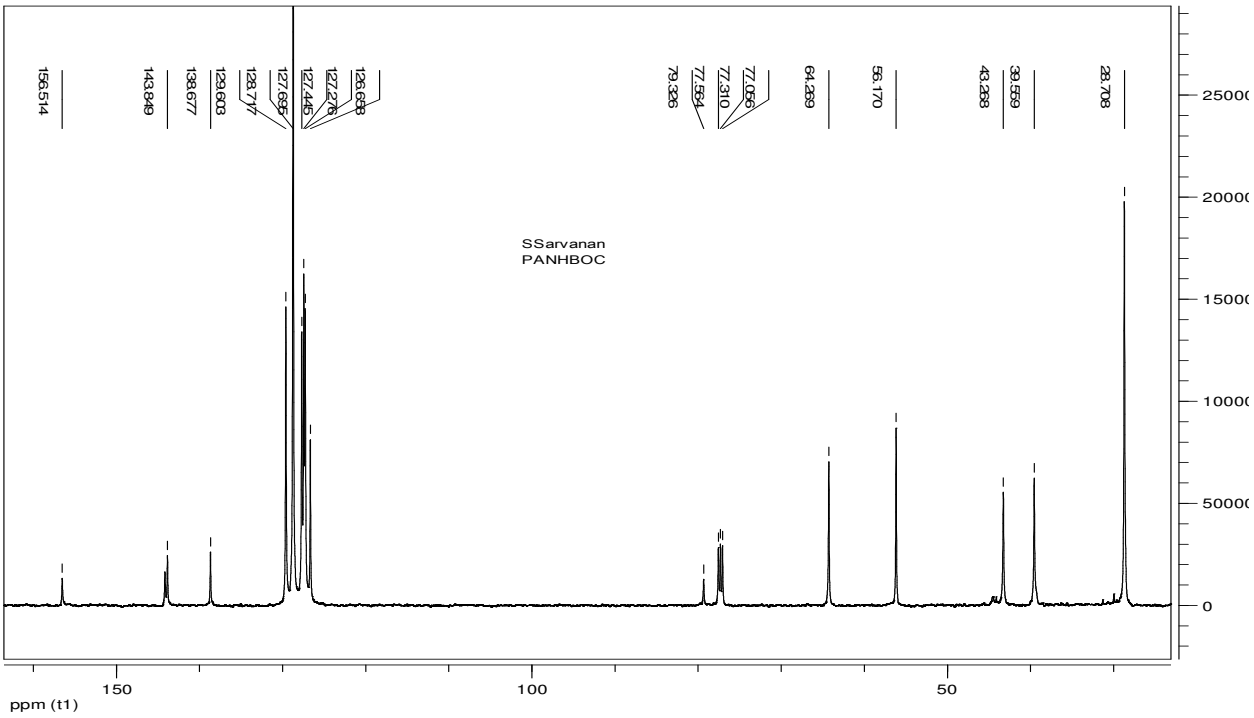
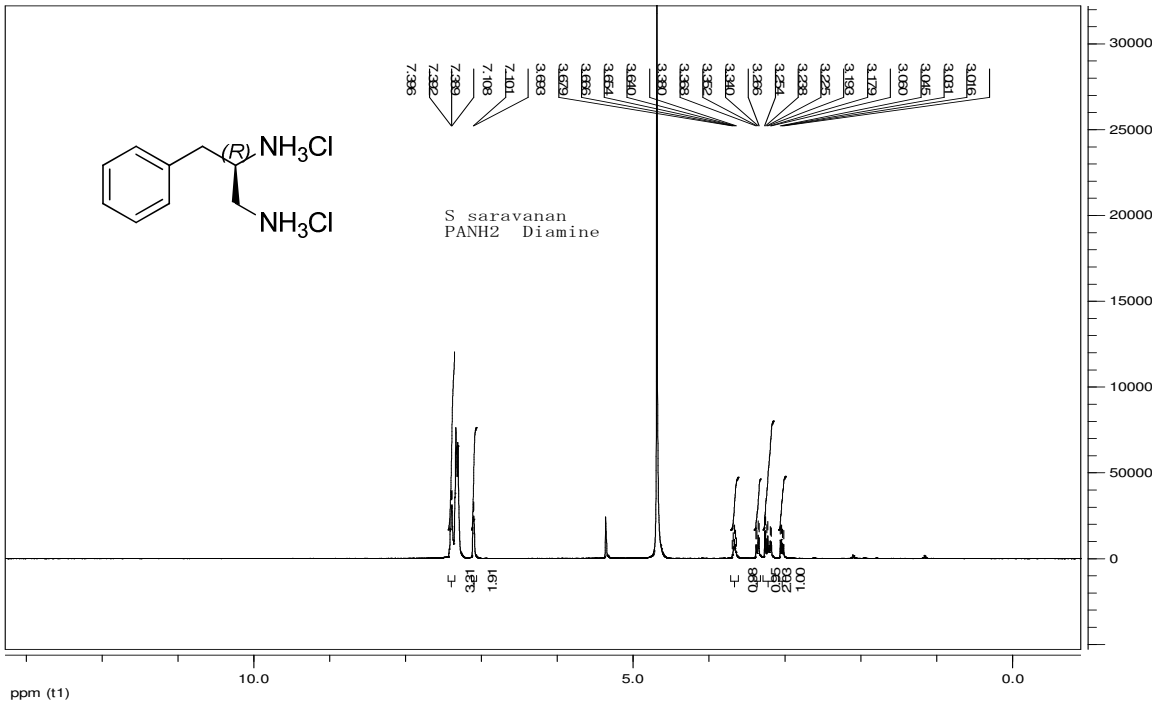
NH
Boc
ppm (t1)


SSarvanan
PANHBOC
ppm (t1)

Compound 14


(R) NH3Cl
NH3Cl
S saravanan
PANH2 Diamine
7.396
7.392
7.389
7.108
7.101
3.683
3.672
3.666
3.654
3.640
3.390
3.368
3.352
3.340
3.266
3.254
3.238
3.225
3.193
3.173
3.000
2.995
2.981
2.916
3.21
1.91
0.88
0.55
2.53
1.00
30000
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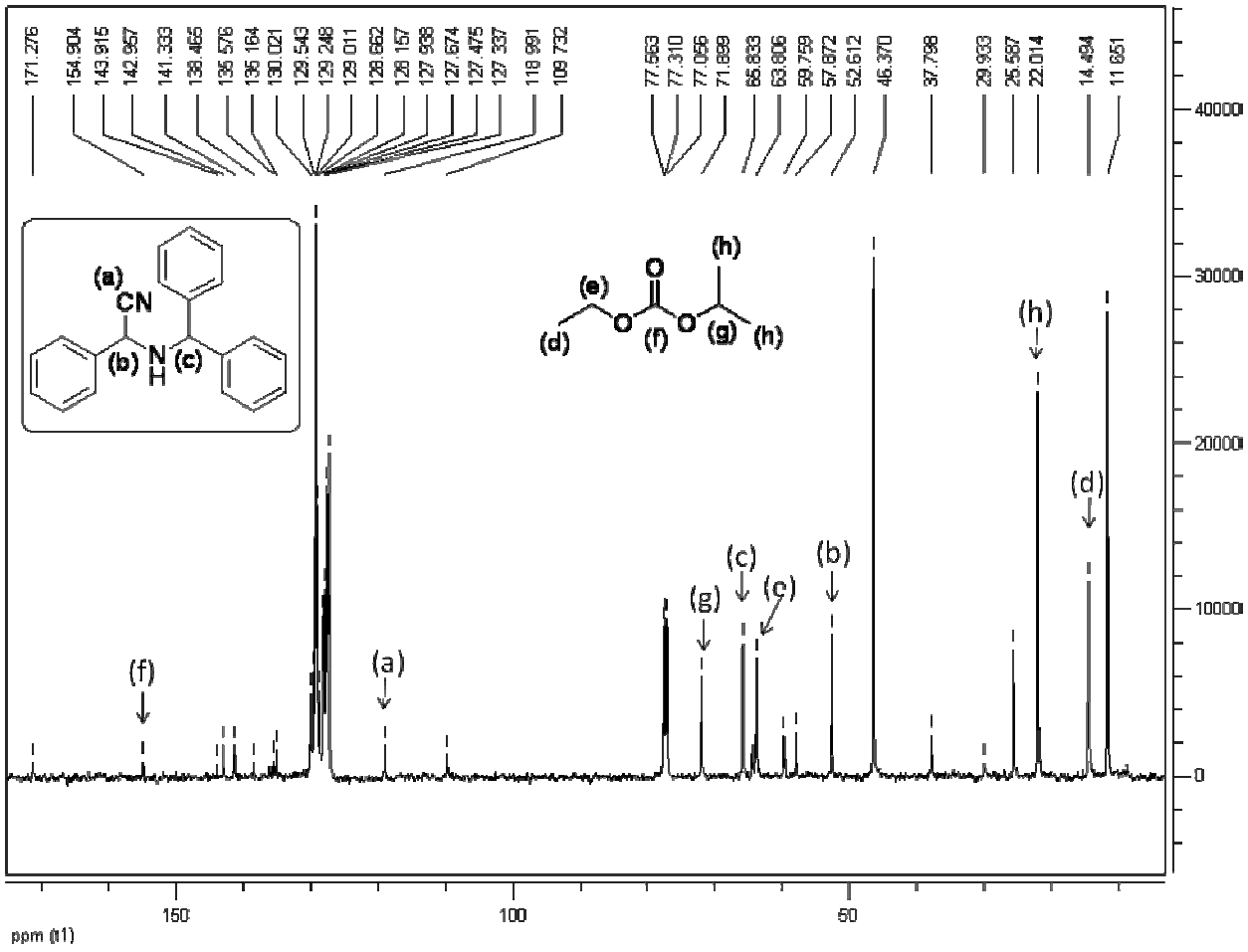
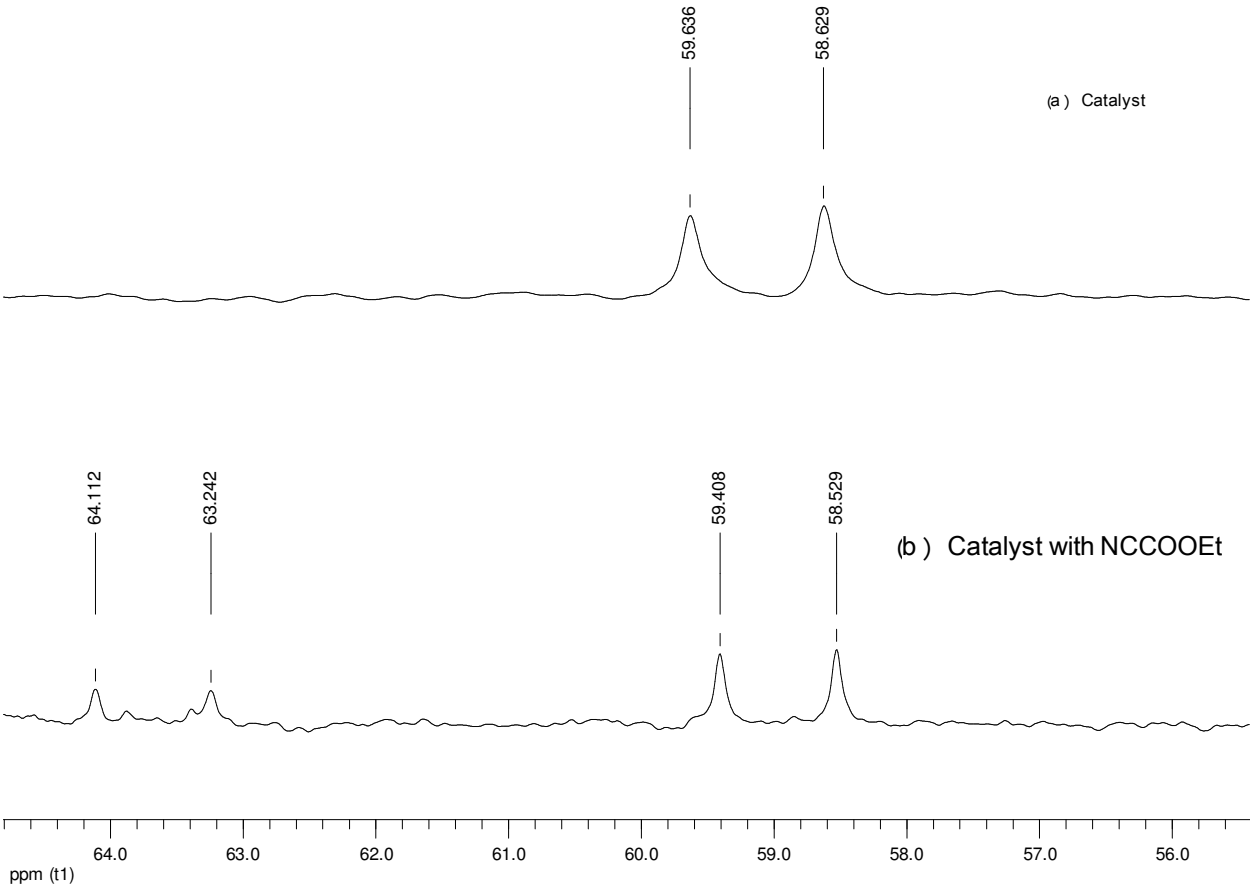
20000
15000
10000
50000
0
10.0
5.0
0.0
ppm (t1)



^{13}C NMR spectra (recorded in $CDCl_3$) of reaction mass using catalyst **5**, which clearly shows the formation of desired product (**2a**) and side product as described in mechanism (scheme **1**).



^{13}C NMR spectra recorded in $CDCl_3$ (a) catalyst **5** (b) catalyst **5** after interaction with ethyl cyanoformate.

References:

1. Perrin, D. D.; Armarego, W. L. F.; Perrin, D. R. *Purification of Laboratory Chemicals;*Pergamon: New York, 1981.

2. Pyne, S. G.; Hensel, M. J.; Fuclos, P. L. *J. Am. Chem. Soc.* **1982**, 104, 5719.

3. Huang, J. L.; Liu, X. H.; Wen, Y. H.; Qin, B.; Feng, X. M. *J. Org. Chem.* **2007**, 72, 204.