

SUPPLEMENTARY INFORMATION

Synthesis of functionalized alkenes via Cu(I)-catalysed allylation of acetanilides using Morita-Baylis-Hillman bromides

Ramesh Kumar Vishwakarma, and Krishna Nand Singh*

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-
221005, India

*E-mail: knsingh@bhu.ac.in; knsinghbhu@yahoo.co.in

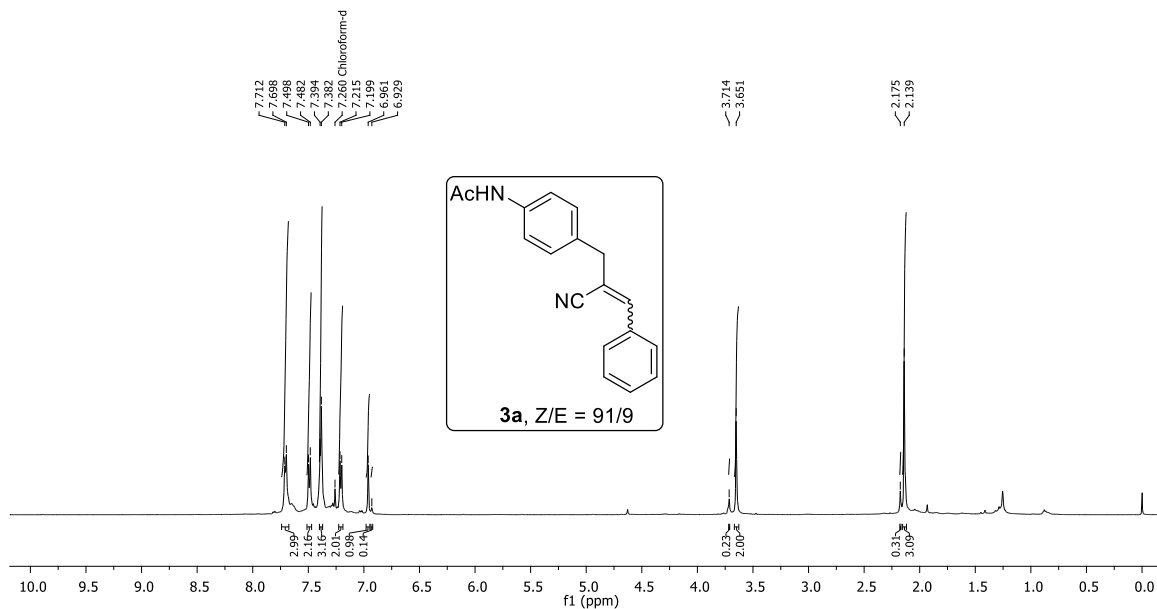
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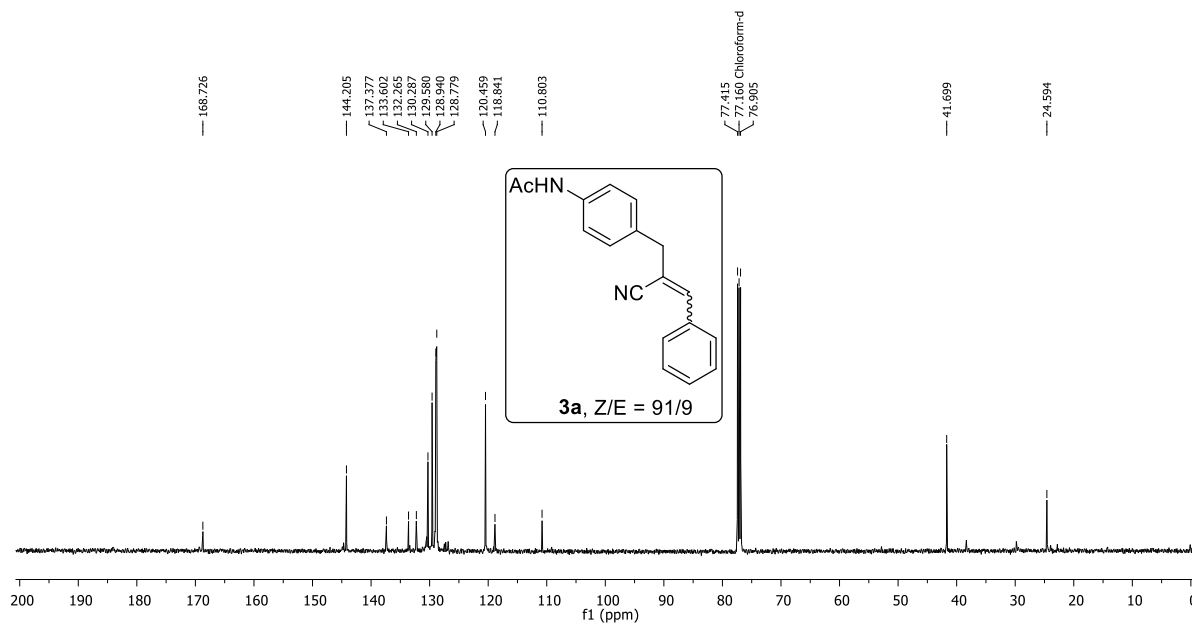
1. Copies of ^1H , $^{13}\text{C}\{^1\text{H}\}$ and ^{19}F Spectra of the Products 3a-3v and 4a-4m

N-(4-(2-Cyano-3-phenylallyl)phenyl)acetamide (3a):

^1H NMR, CDCl_3 , 500 MHz

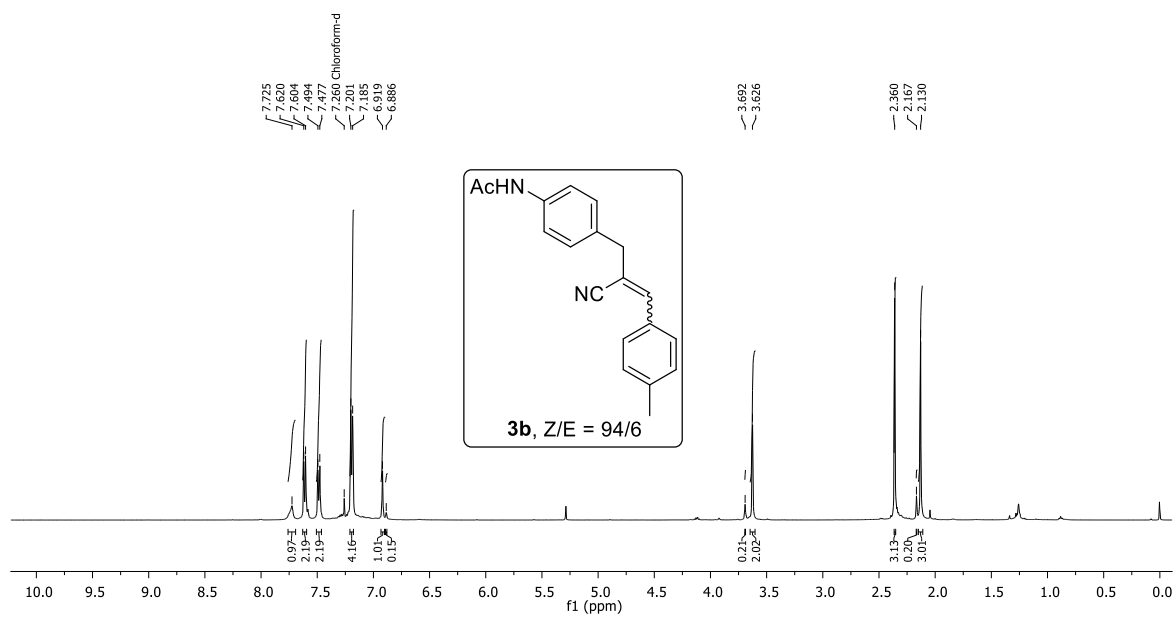


$^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 126 MHz

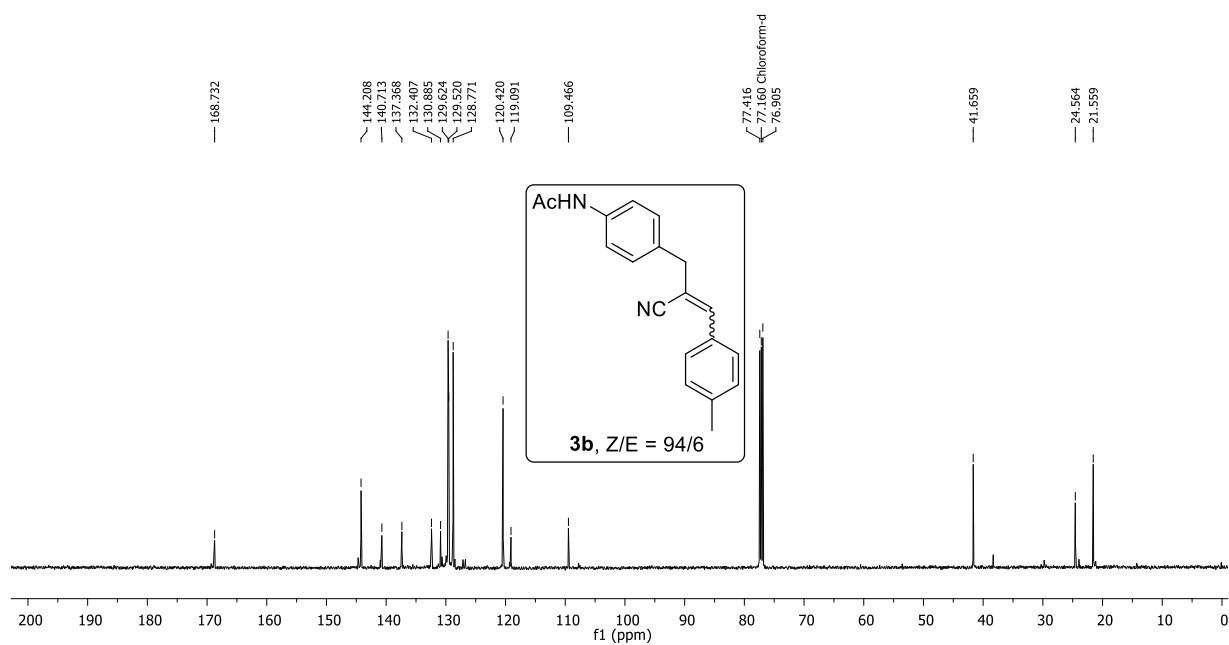


***N*-(4-(2-Cyano-3-(*p*-tolyl)allyl)phenyl)acetamide (**3b**):**

¹H NMR, CDCl₃, 500 MHz

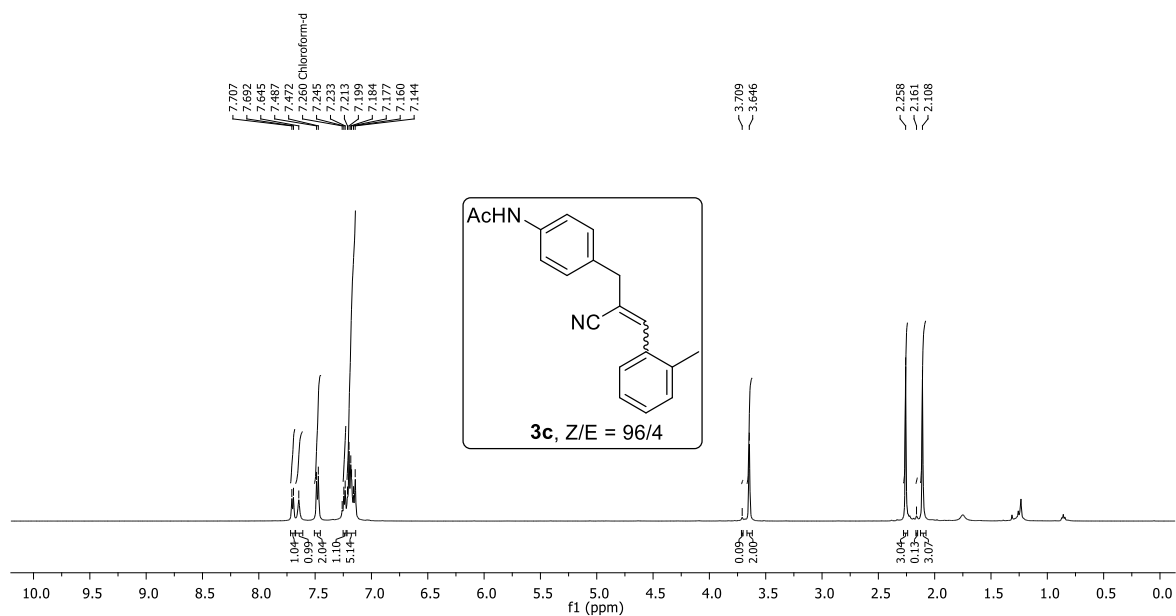


¹³C{¹H} NMR, CDCl₃, 126 MHz

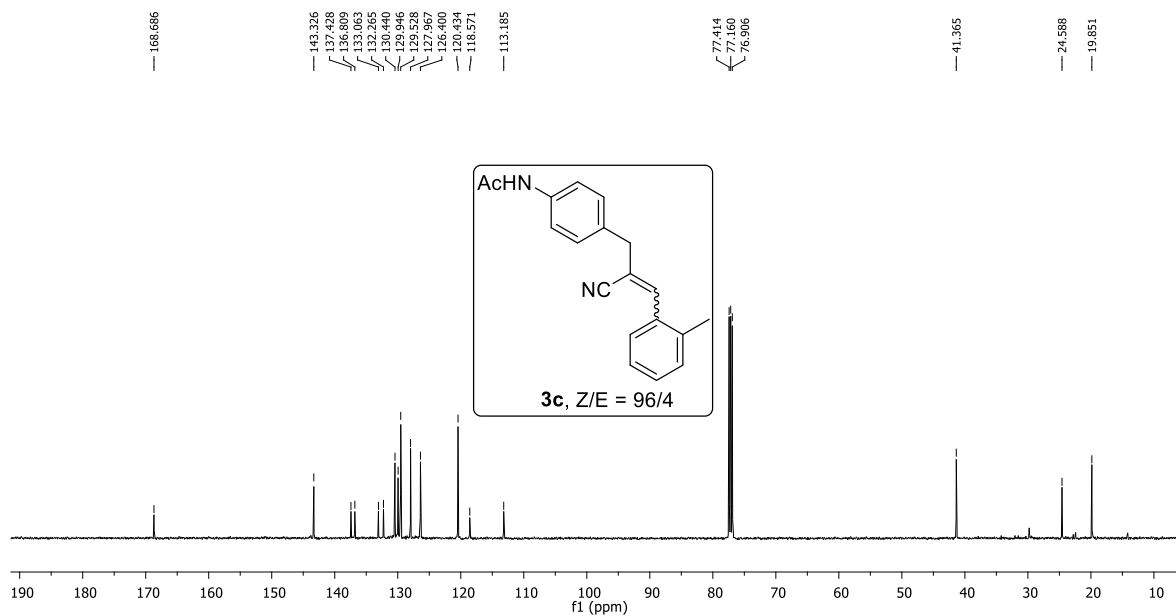


N-(4-(2-Cyano-3-(*o*-tolyl)allyl)phenyl)acetamide (**3c**):

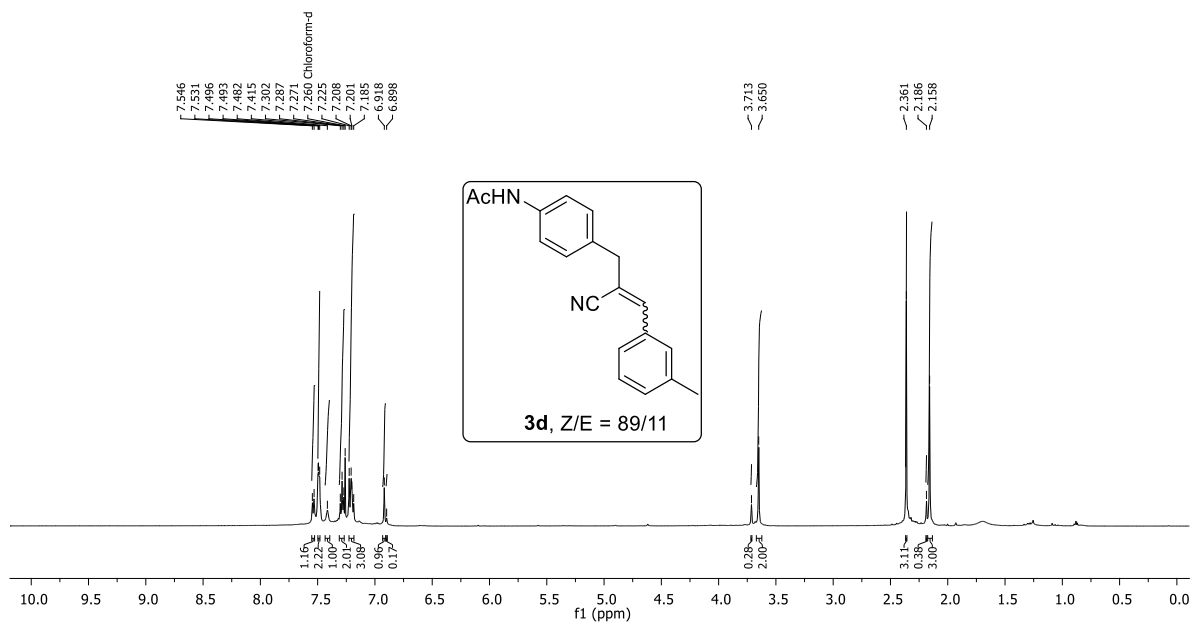
¹H NMR, CDCl₃, 500 MHz



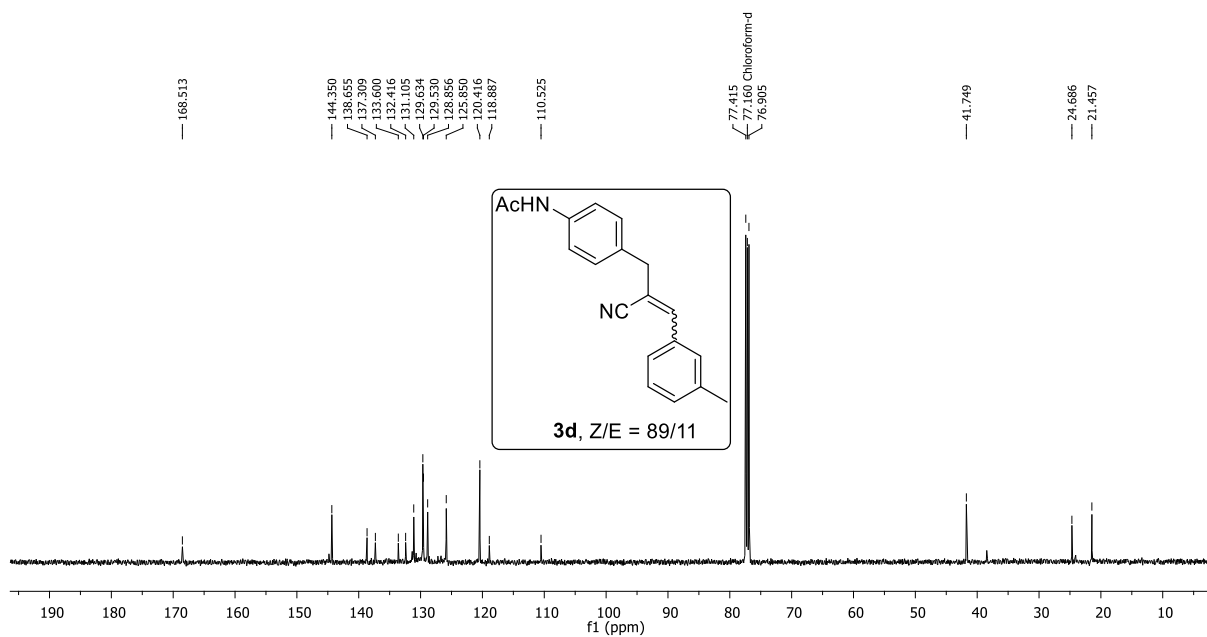
¹³C{¹H} NMR, CDCl₃, 126 MHz



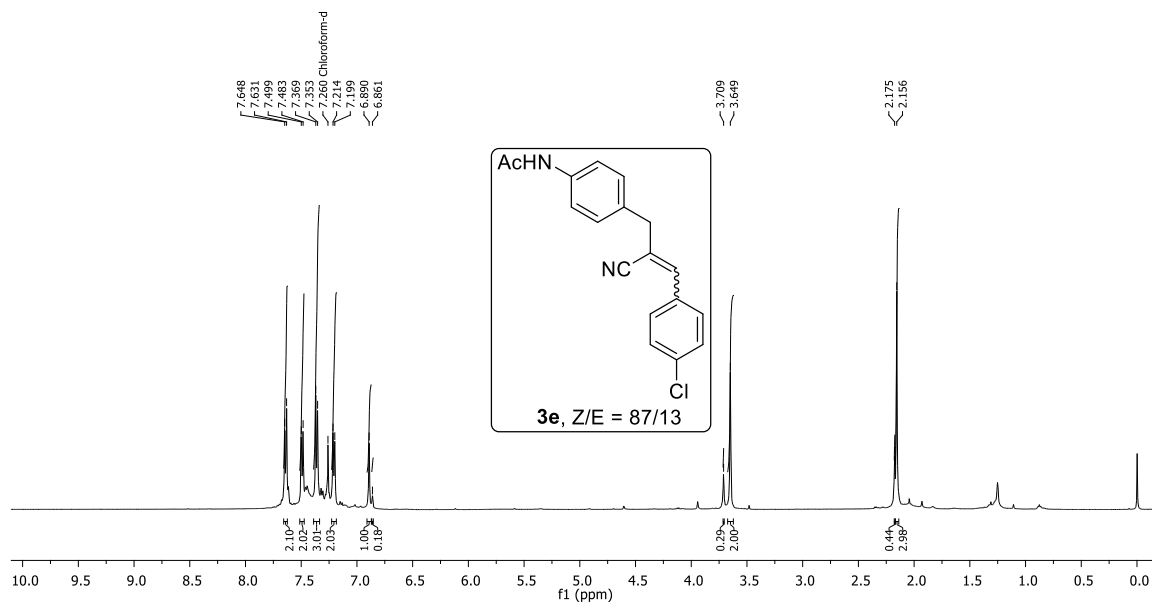
***N*-(4-(2-Cyano-3-(*m*-tolyl)allyl)phenyl)acetamide (3d):
¹H NMR, CDCl₃, 500 MHz**



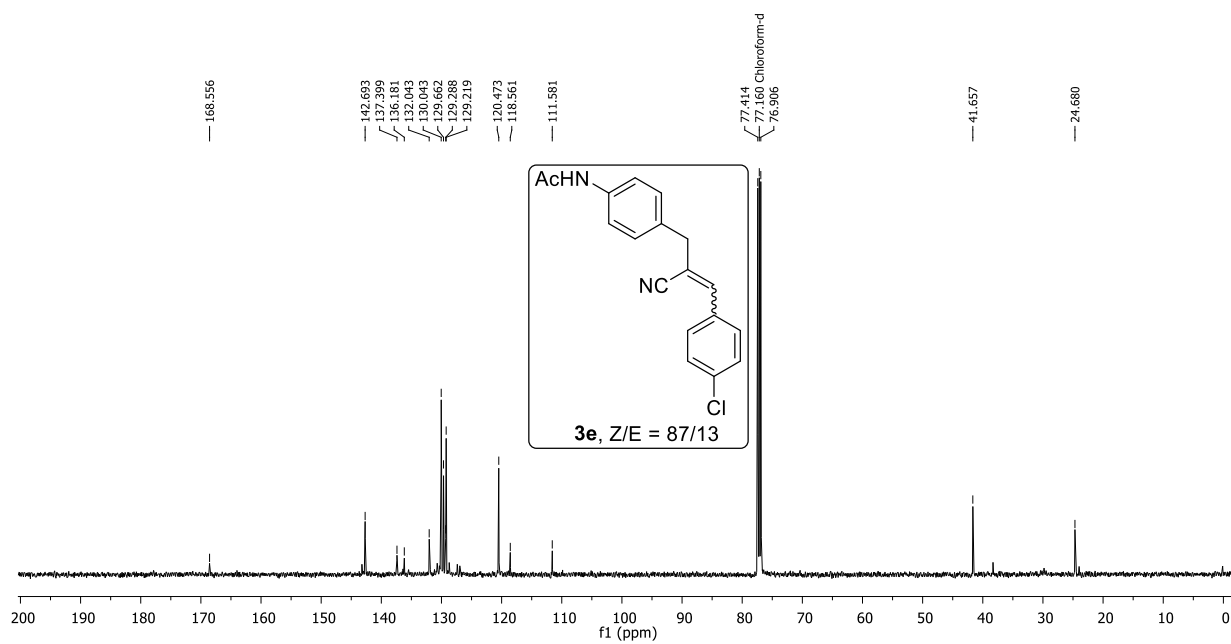
¹³C{¹H} NMR, CDCl₃, 126 MHz



***N*-(4-(3-(4-Chlorophenyl)-2-cyanoallyl)phenyl)acetamide (**3e**):
¹H NMR, CDCl₃, 500 MHz**

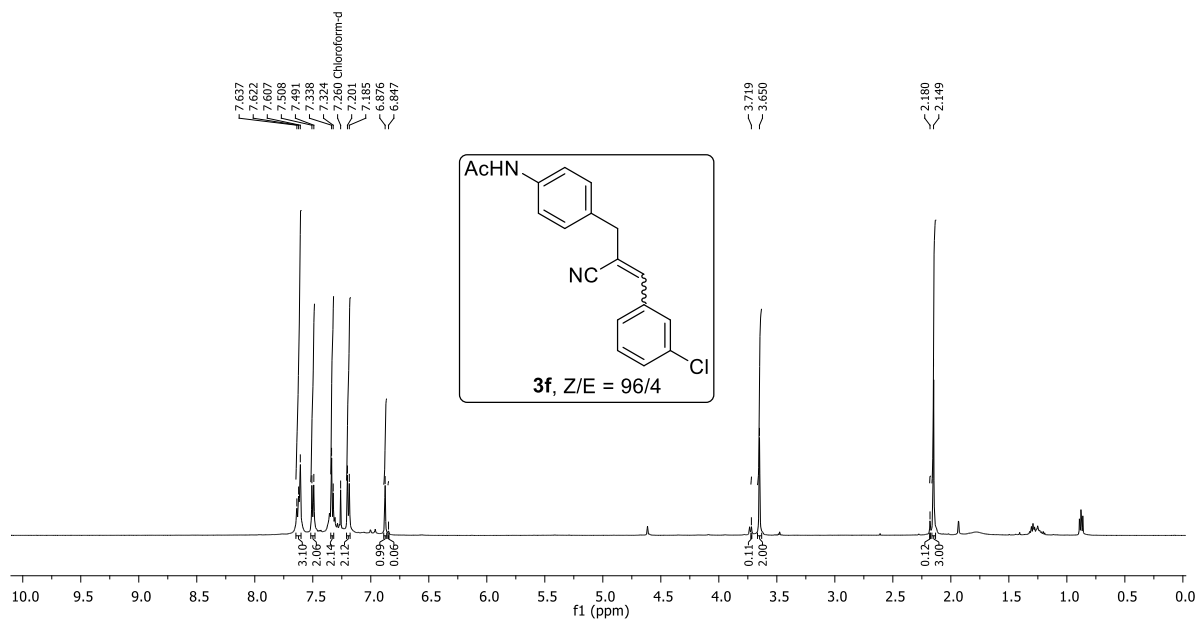


¹³C{¹H} NMR, CDCl₃, 126 MHz

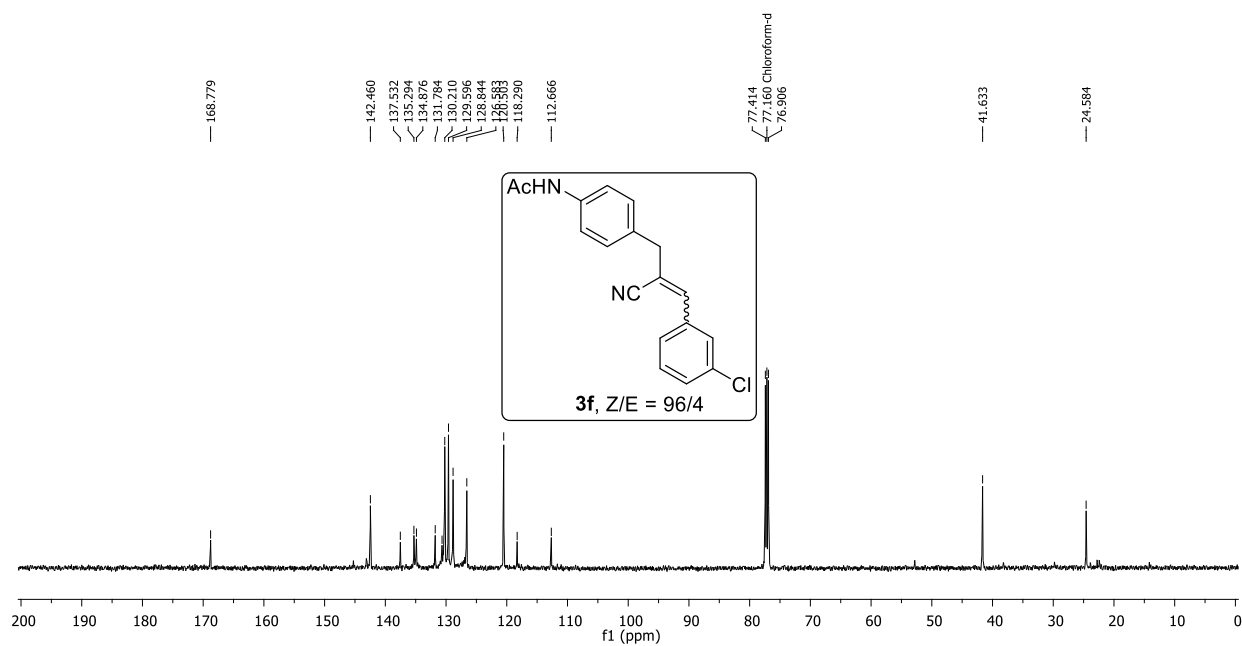


***N*-4-(3-(3-Chlorophenyl)-2-cyanoallyl)phenylacetamide (3f):**

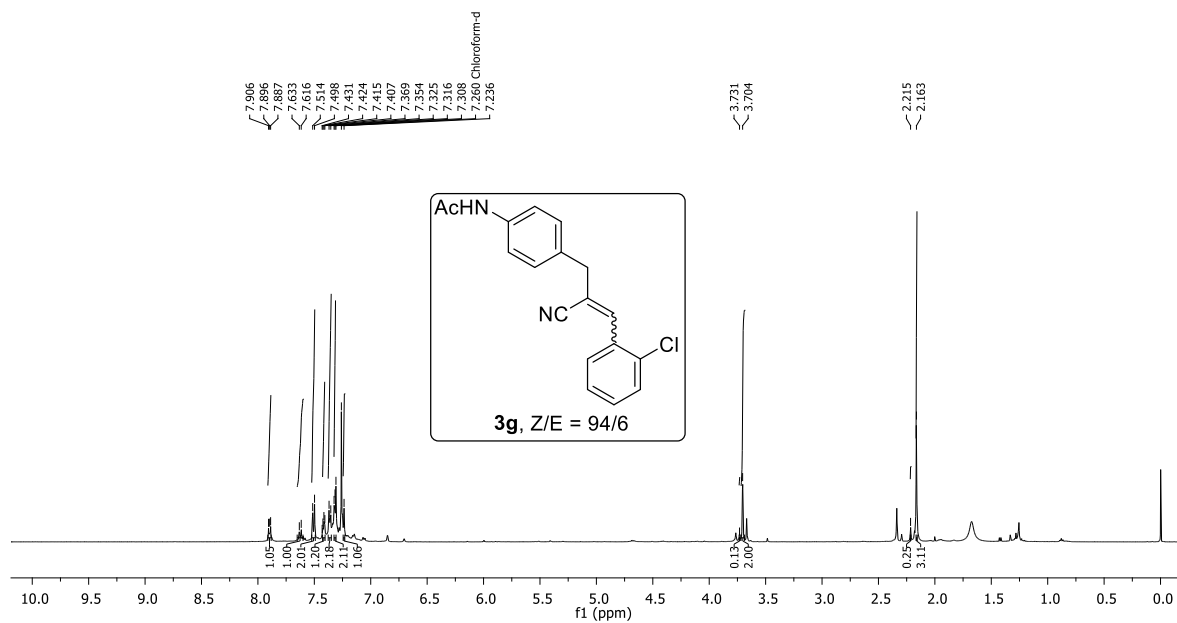
¹H NMR, CDCl₃, 500 MHz



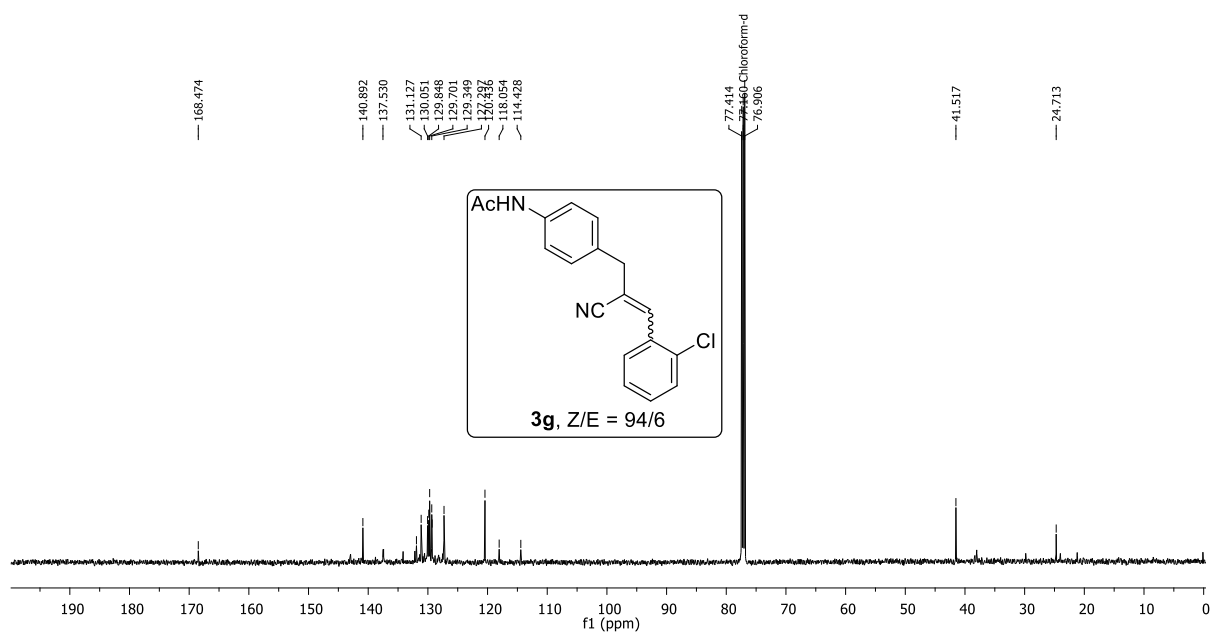
¹³C{¹H} NMR, CDCl₃, 126 MHz



***N*-(4-(3-(2-Chlorophenyl)-2-cyanoallyl)phenyl)acetamide (3g):
¹H NMR, CDCl₃, 500 MHz**

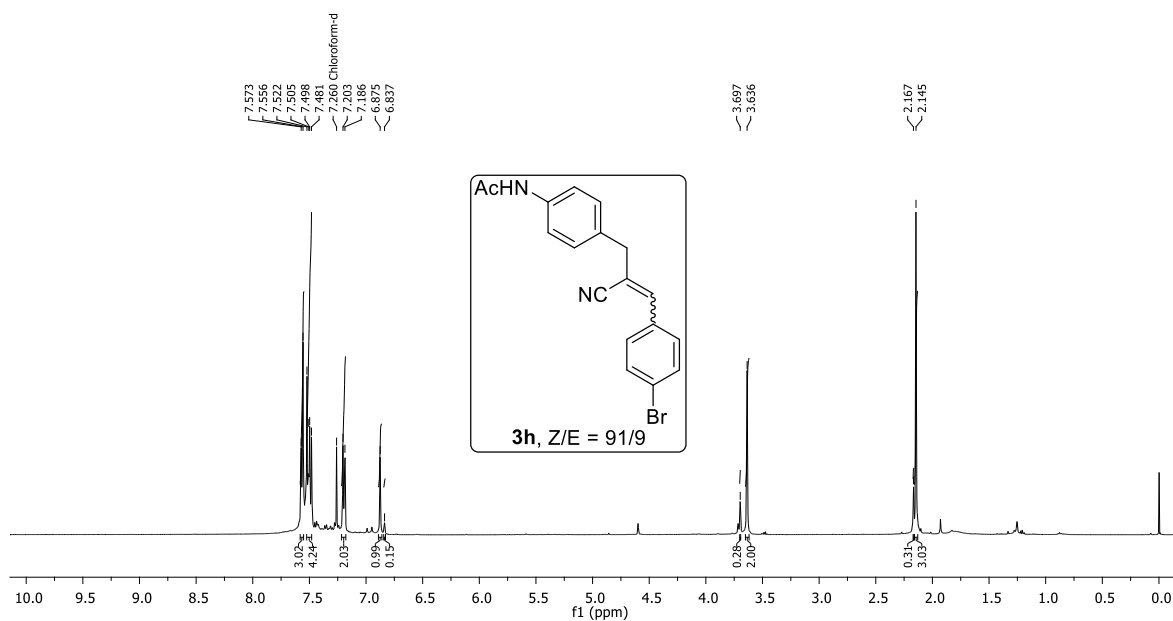


¹³C{¹H} NMR, CDCl₃, 126 MHz

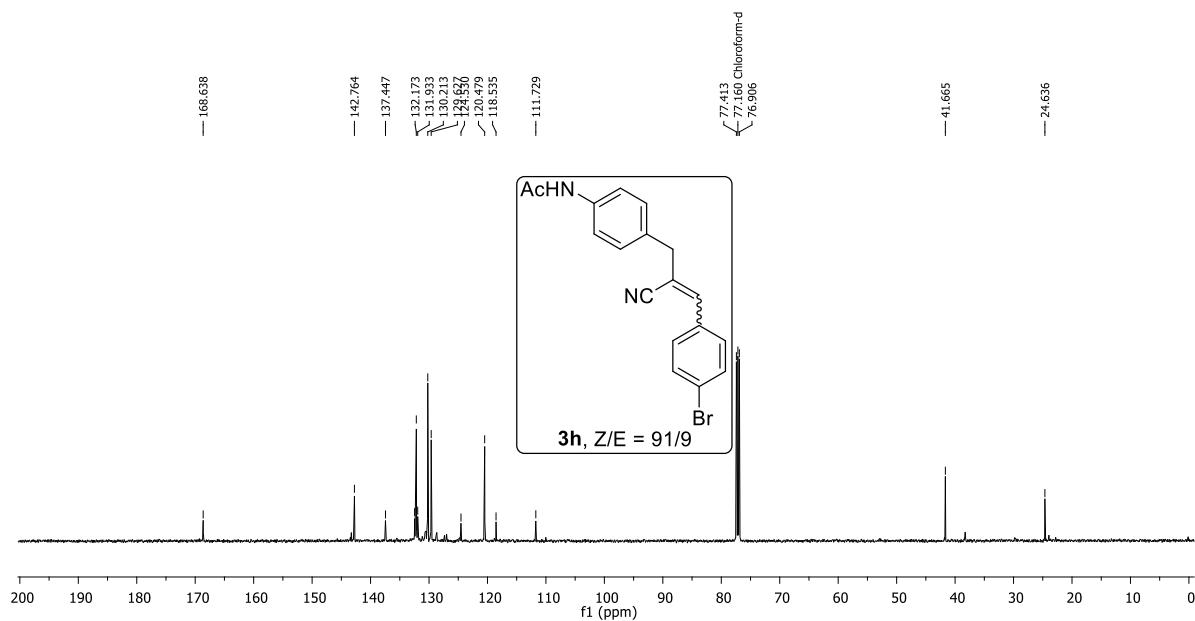


N-(4-(3-(4-Bromophenyl)-2-cyanoallyl)phenyl)acetamide (**3h**):

¹H NMR, CDCl₃, 500 MHz

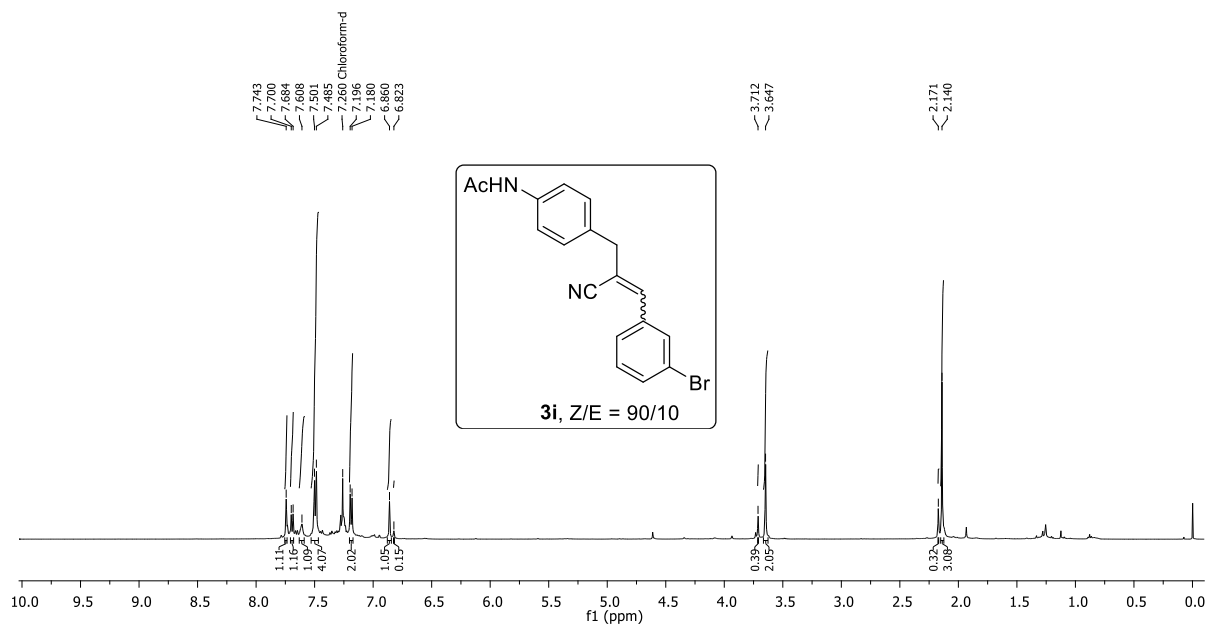


¹³C{¹H} NMR, CDCl₃, 126 MHz

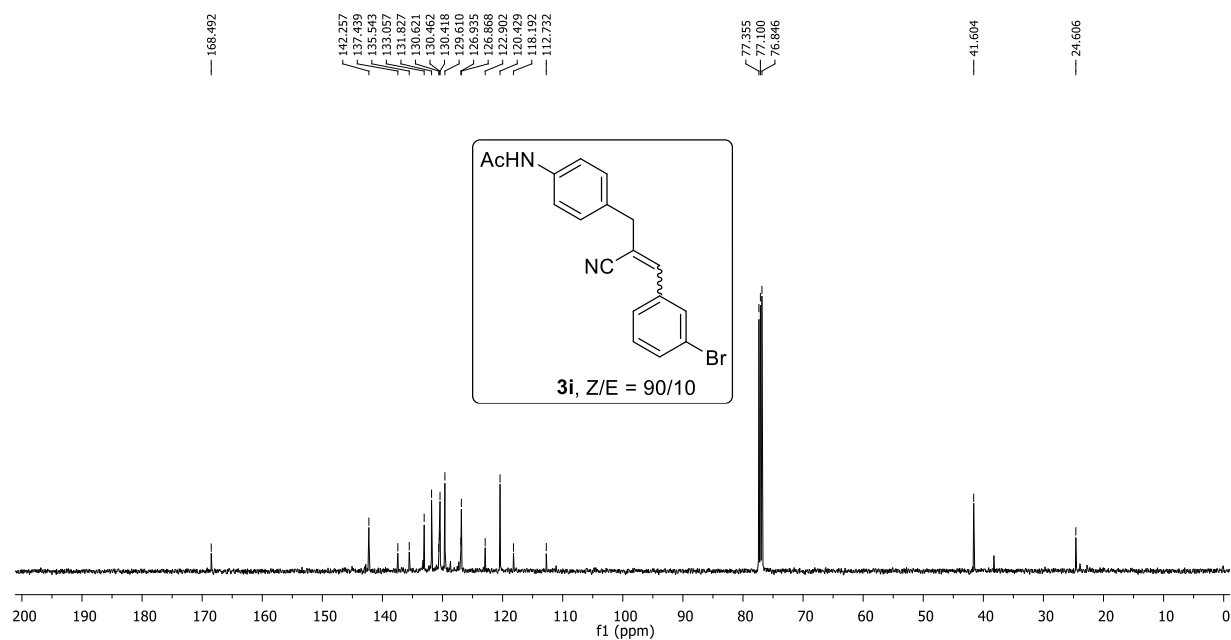


***N*-4-(3-(3-Bromophenyl)-2-cyanoallyl)phenylacetamide (**3i**):**

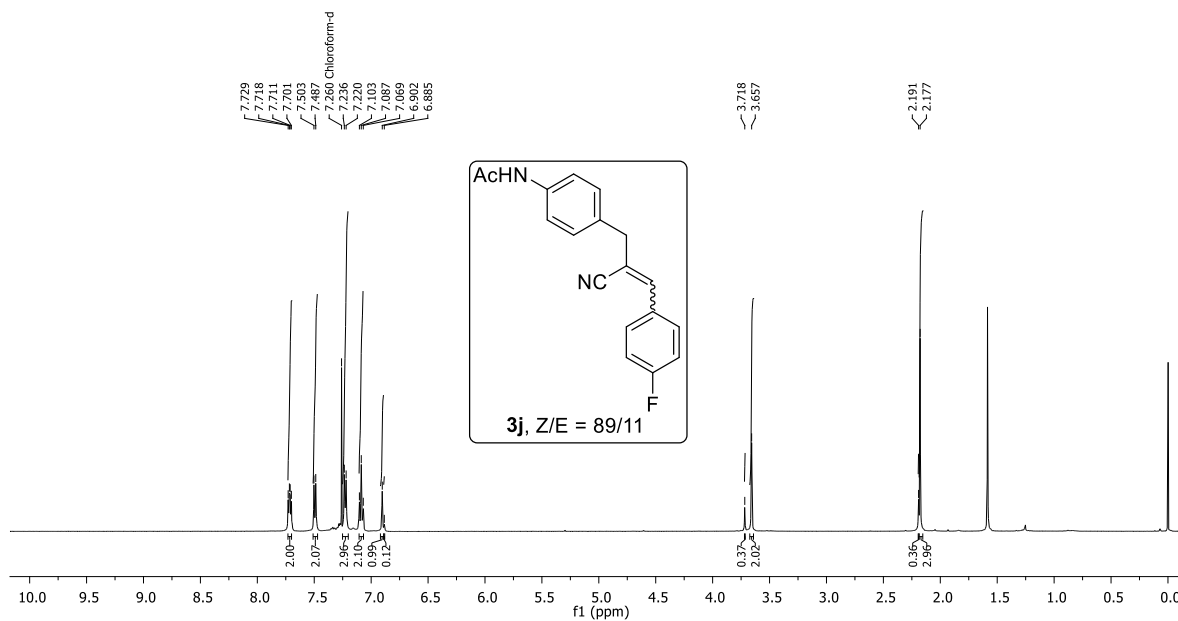
¹H NMR, CDCl₃, 500 MHz



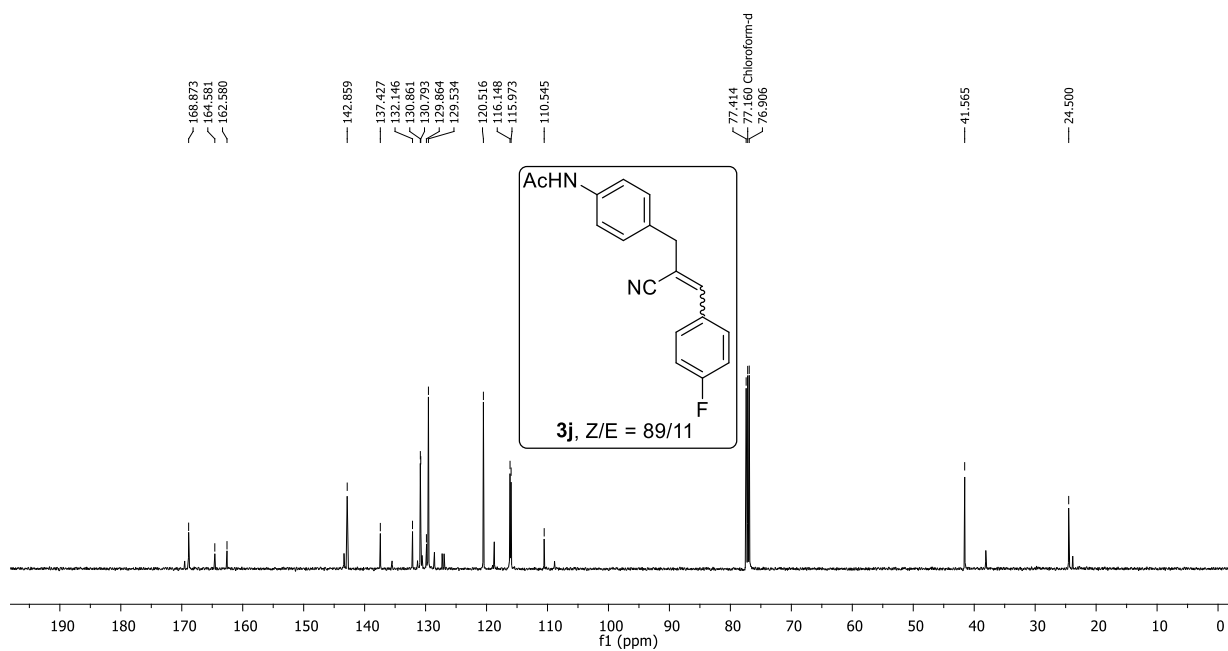
¹³C{¹H} NMR, CDCl₃, 126 MHz



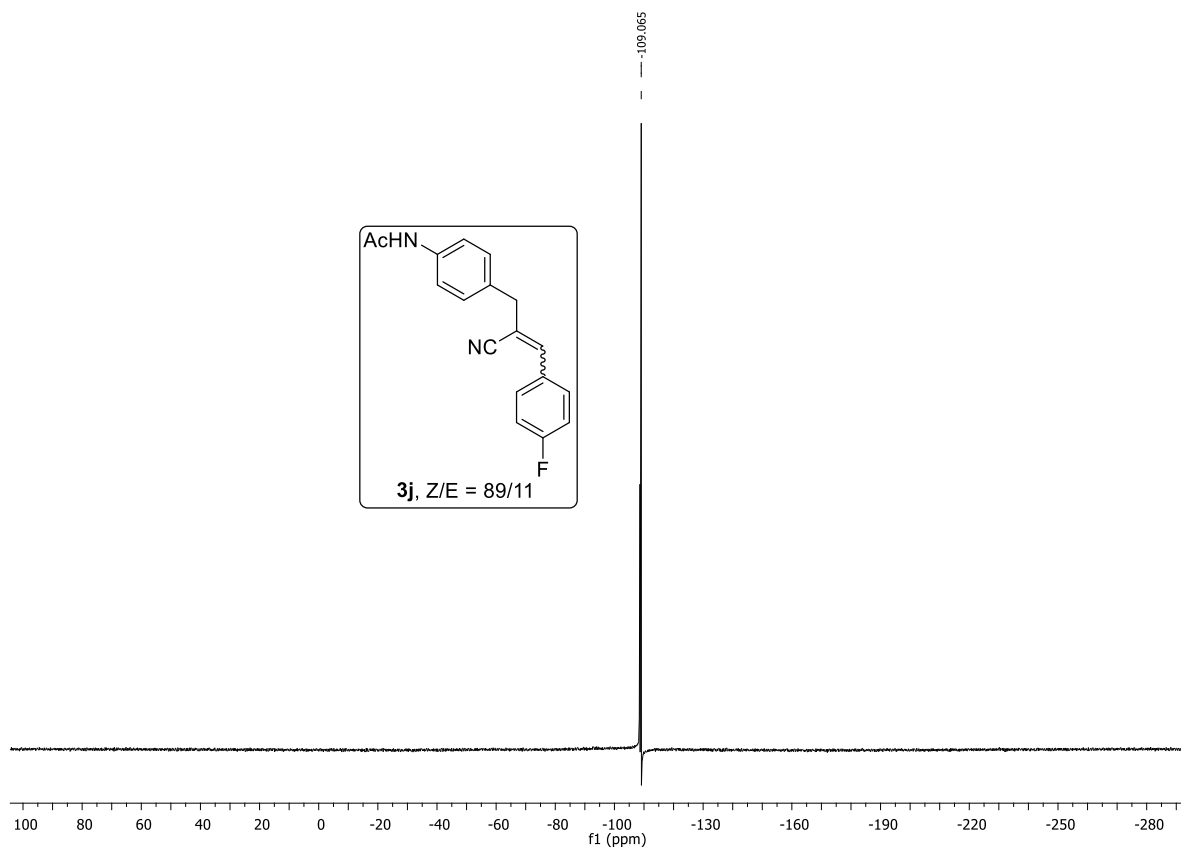
***N*-[4-(2-Cyano-3-(4-fluorophenyl)allyl)phenyl]acetamide (**3j**):
¹H NMR, CDCl₃, 500 MHz**



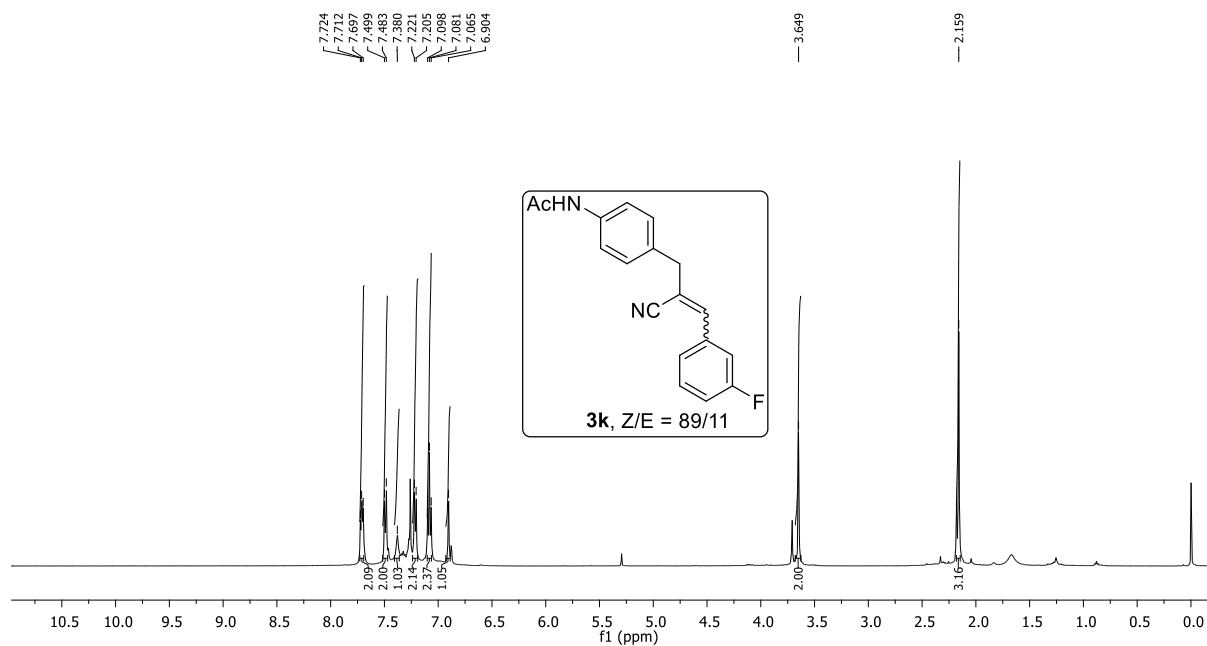
¹³C{¹H} NMR, CDCl₃, 126 MHz



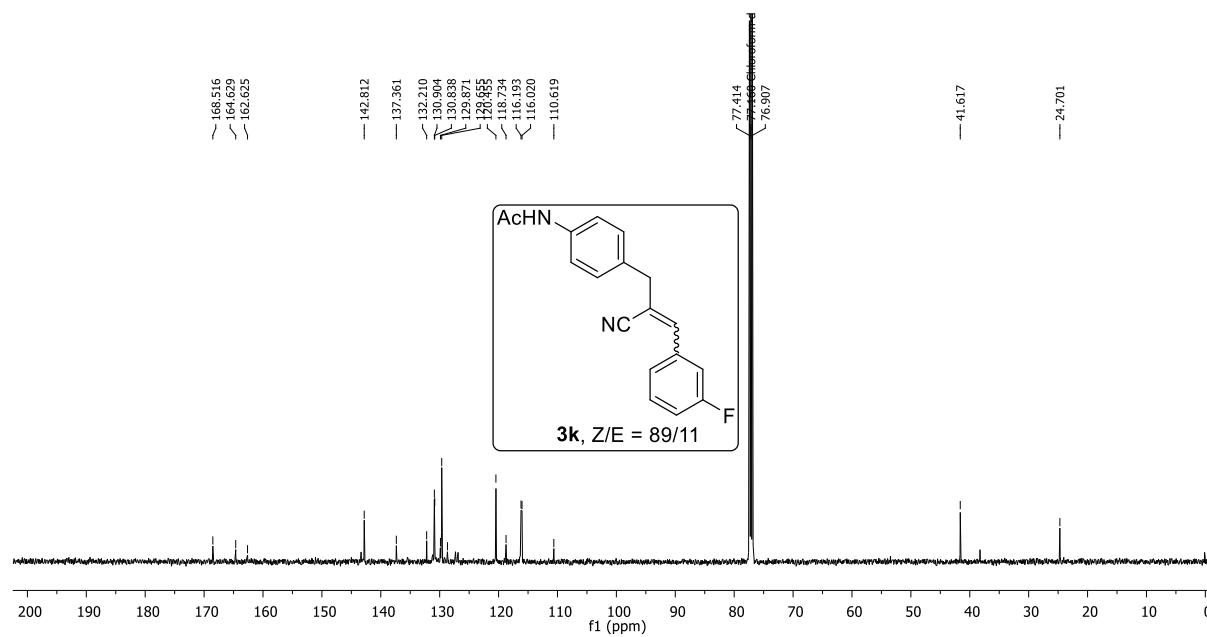
¹⁹F NMR, CDCl₃, 471 MHz



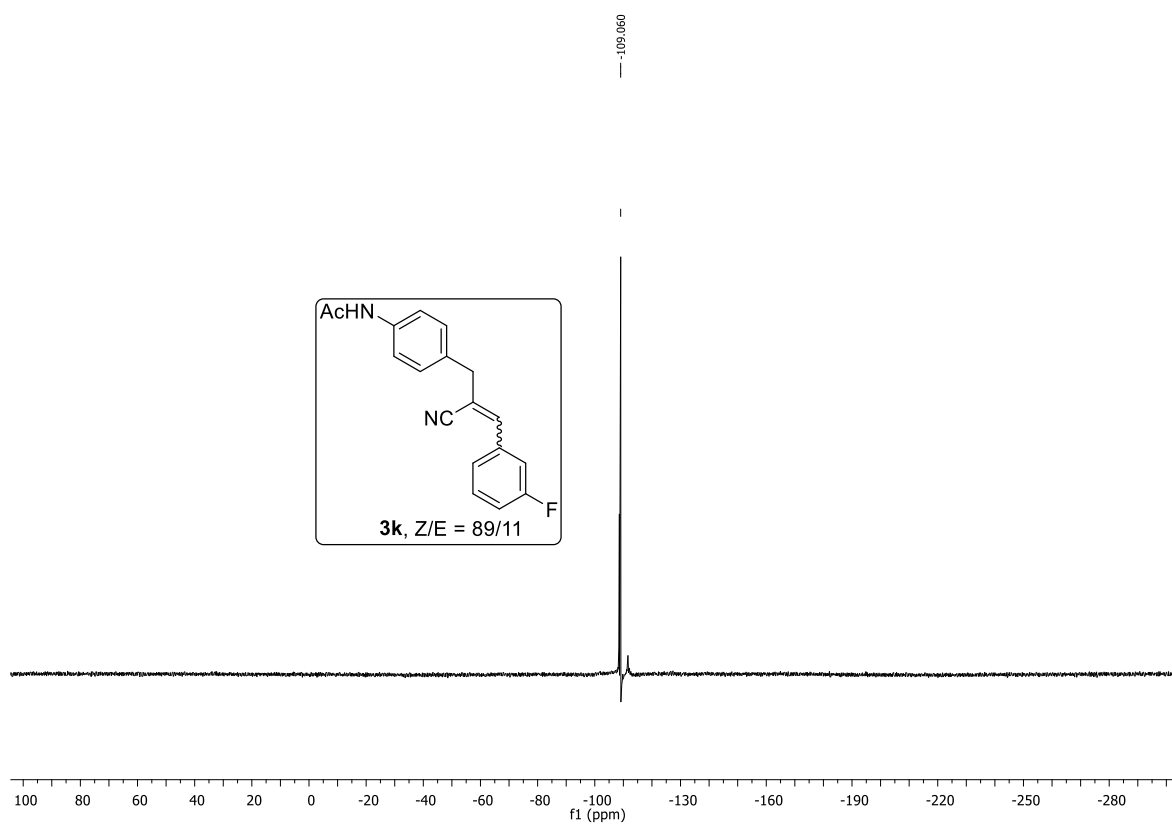
***N*-(4-(2-Cyano-3-(3-fluorophenyl)allyl)phenyl)acetamide (4k):
¹H NMR, CDCl₃, 500 MHz**



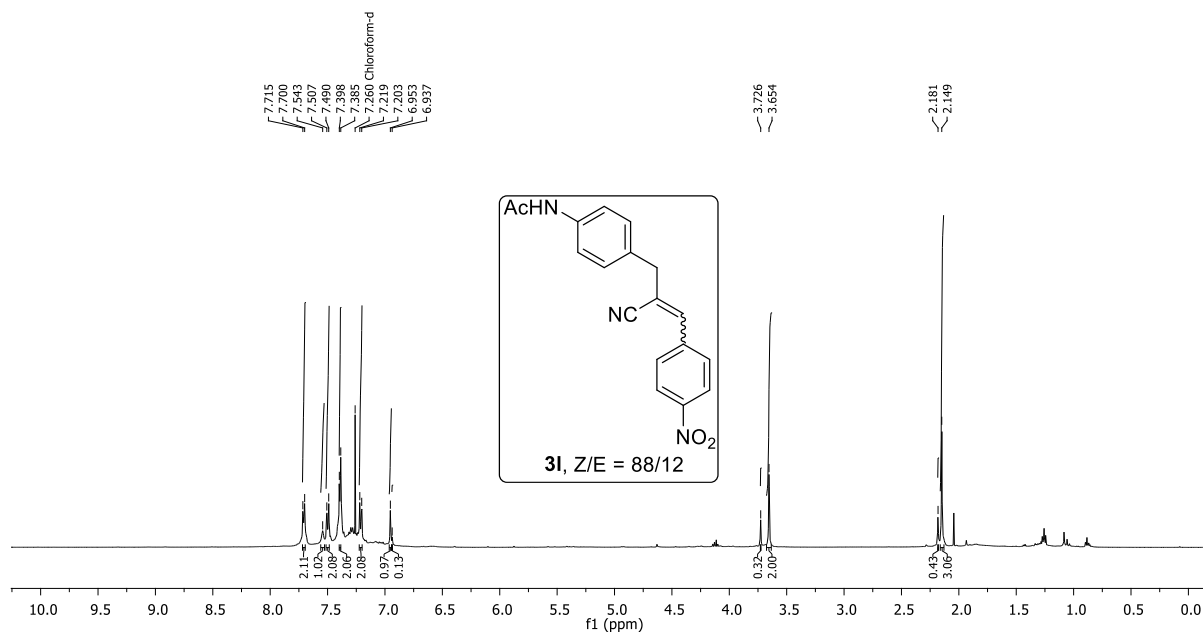
¹³C{¹H} NMR, CDCl₃, 126 MHz



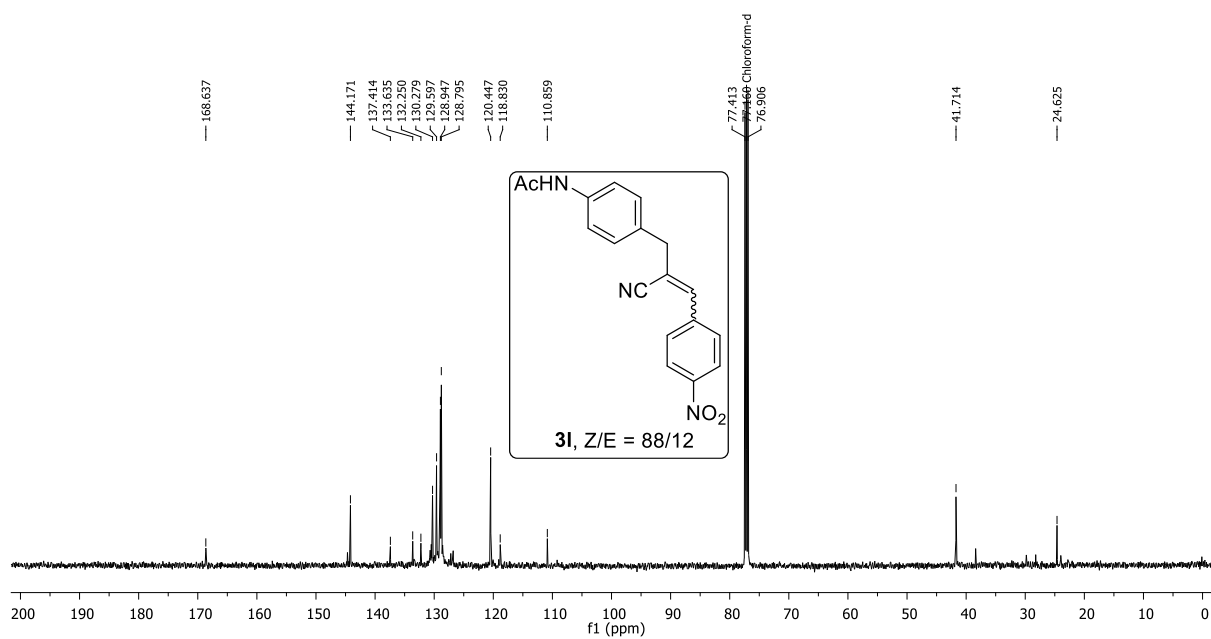
^{19}F NMR, CDCl_3 , 471 MHz



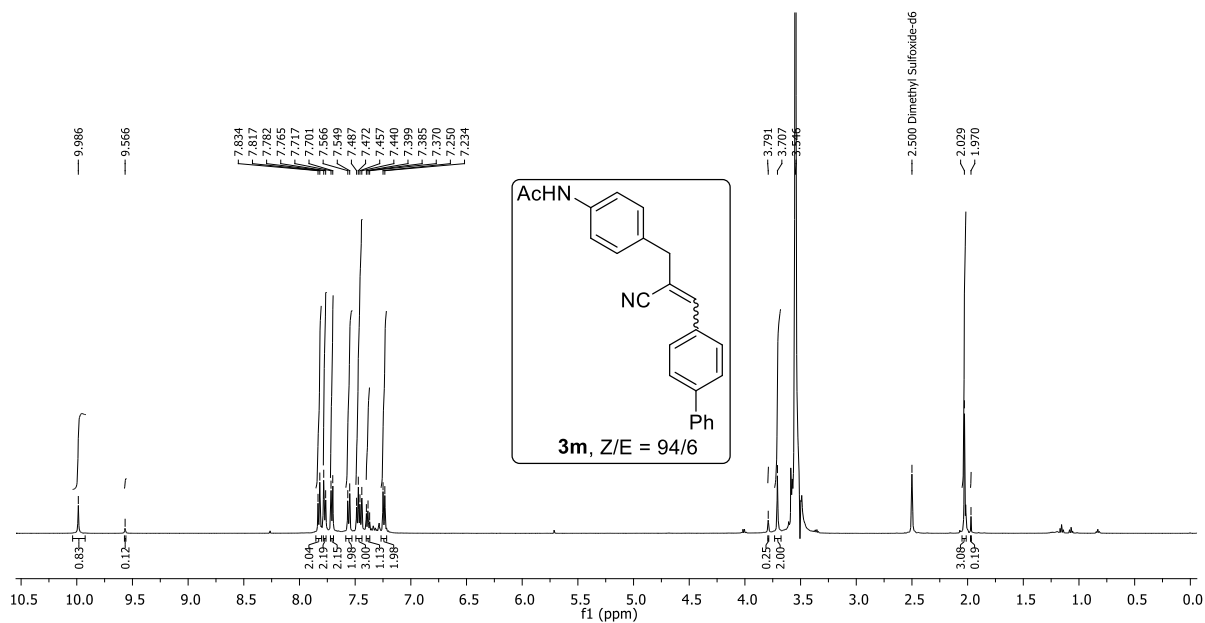
***N*-[4-(2-Cyano-3-(4-nitrophenyl)allyl)phenyl]acetamide (**3I**):
¹H NMR, CDCl₃, 500 MHz**



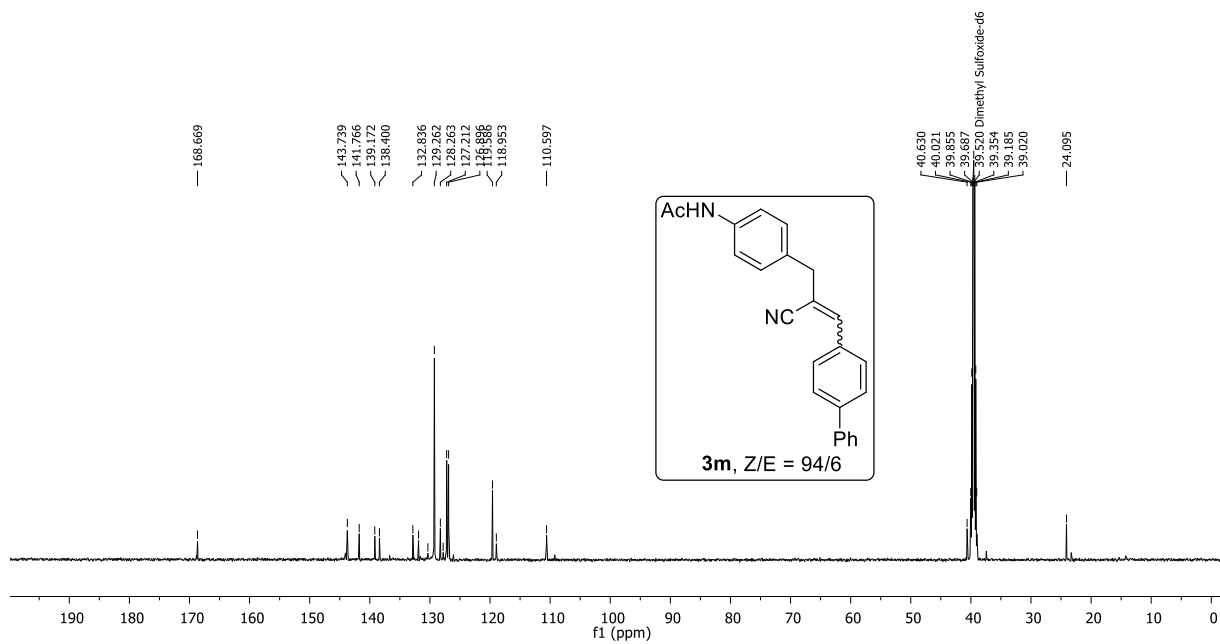
¹³C{¹H}NMR, CDCl₃, 126 MHz



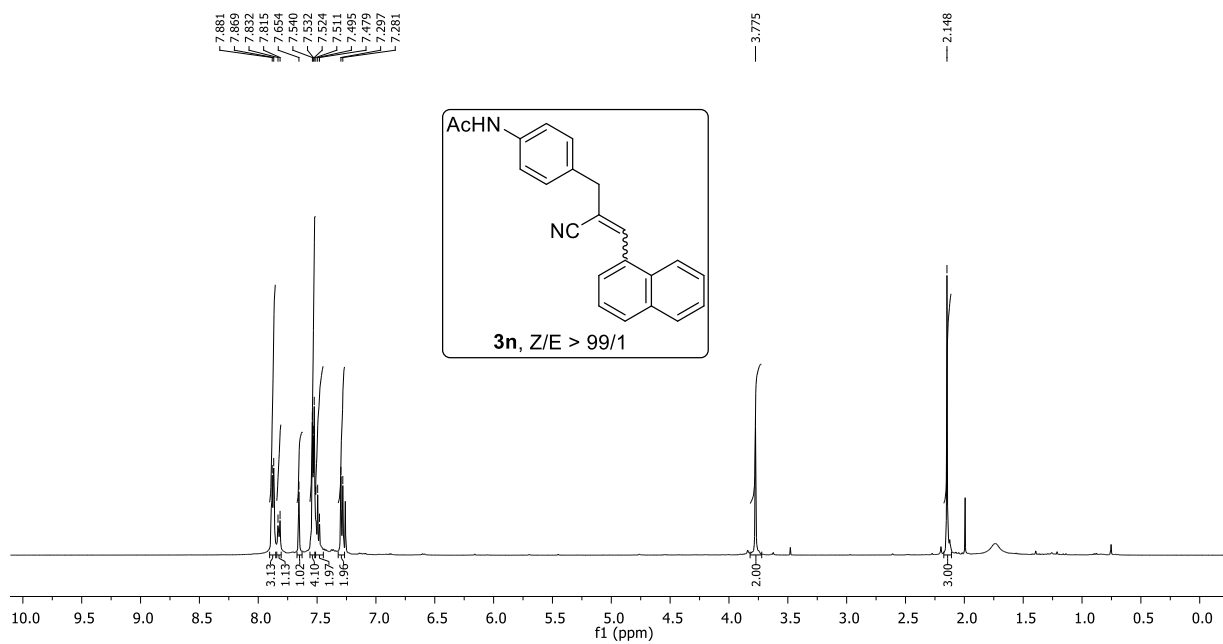
***N*-(4-(3-([1,1'-Biphenyl]-4-yl)-2-cyanoallyl)phenyl)acetamide (3m):
¹H NMR, DMSO-d₆, 500 MHz**



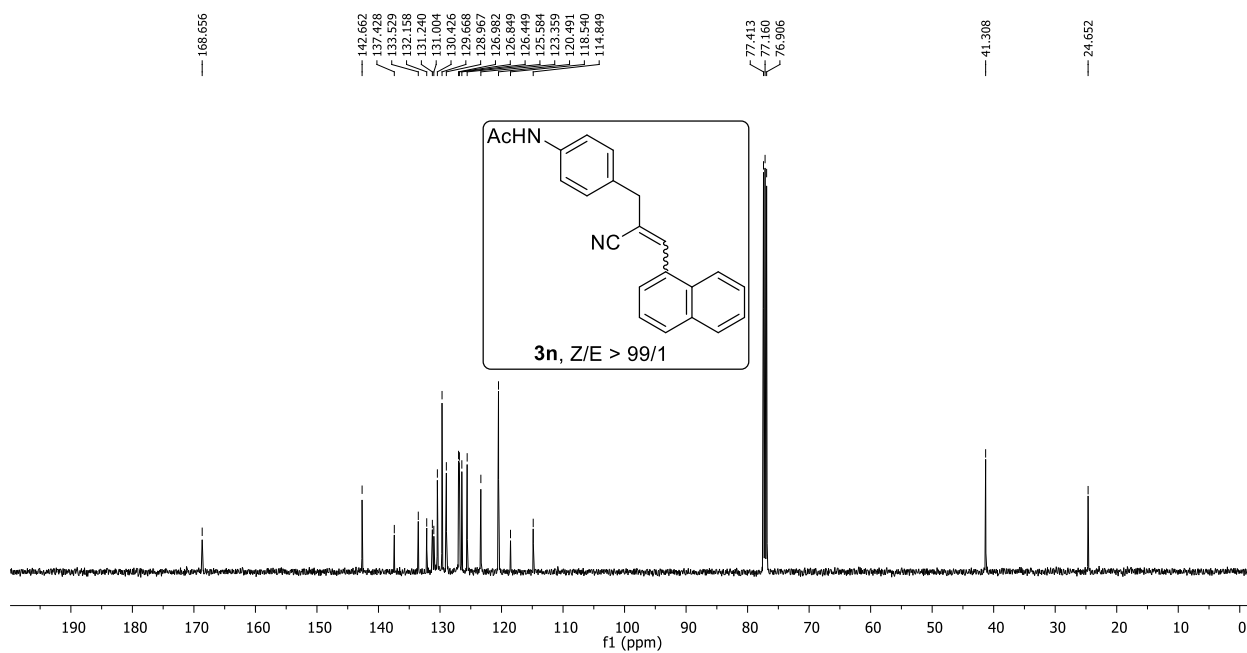
¹³C{¹H} NMR, DMSO-d₆, 126 MHz



***N*-4-(2-Cyano-3-(naphthalen-1-yl)allyl)phenylacetamide (**3n**):
¹H NMR, CDCl₃, 500 MHz**

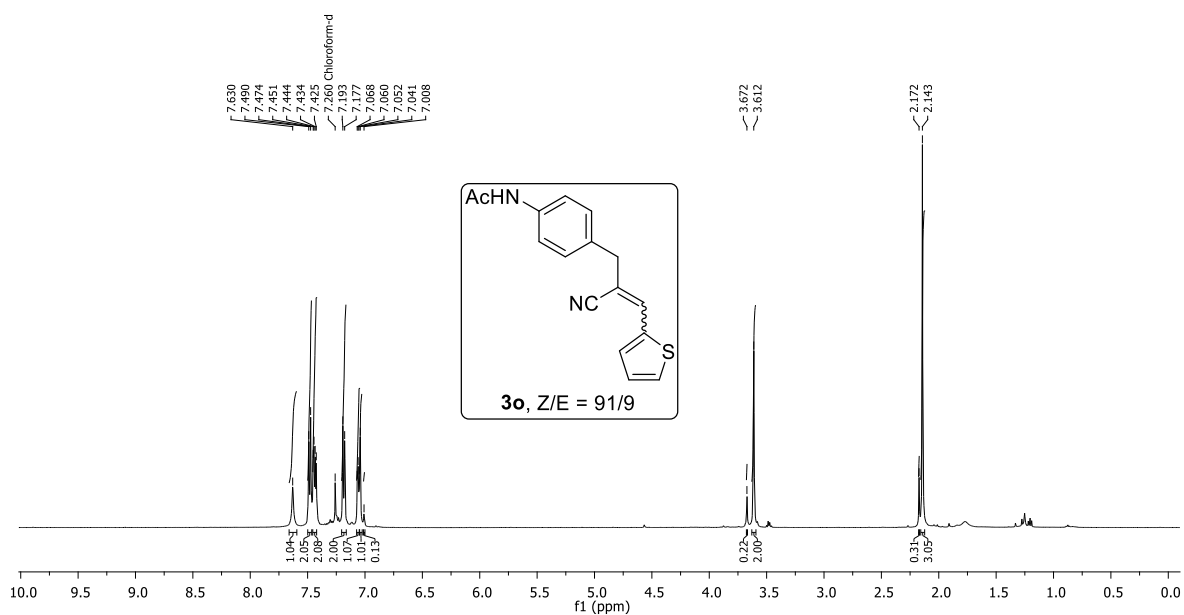


¹³C{¹H} NMR, CDCl₃, 126 MHz

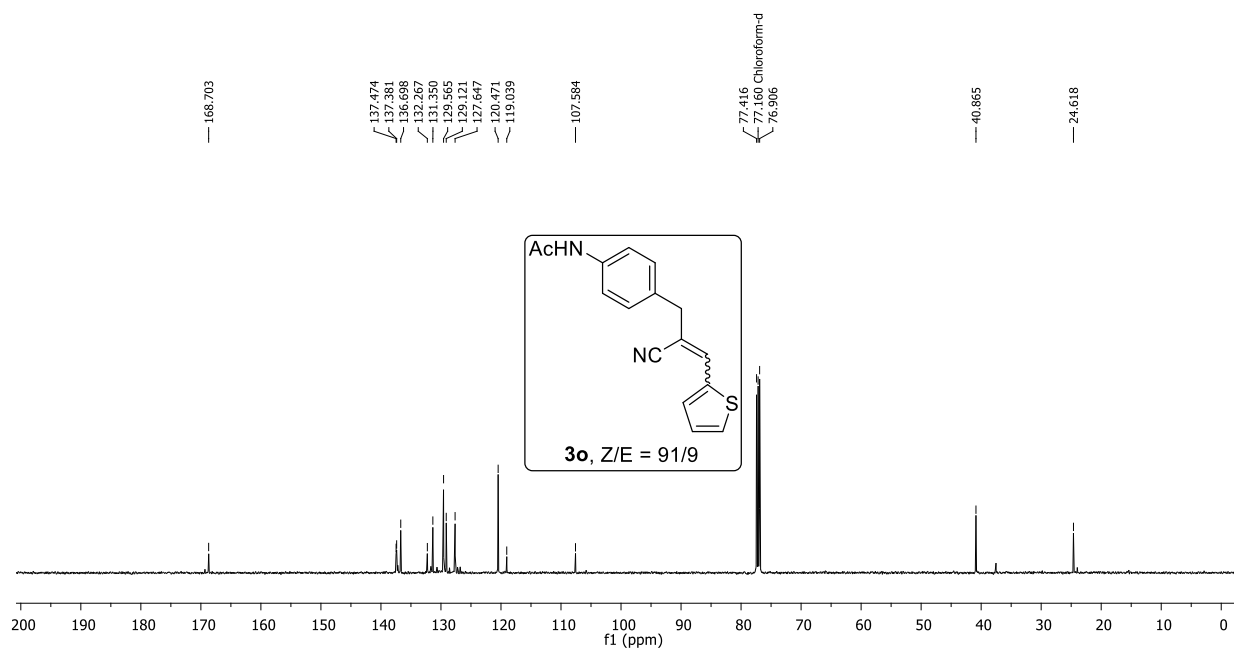


N-(4-(2-Cyano-3-(thiophen-2-yl)allyl)phenyl)acetamide (**3o**):

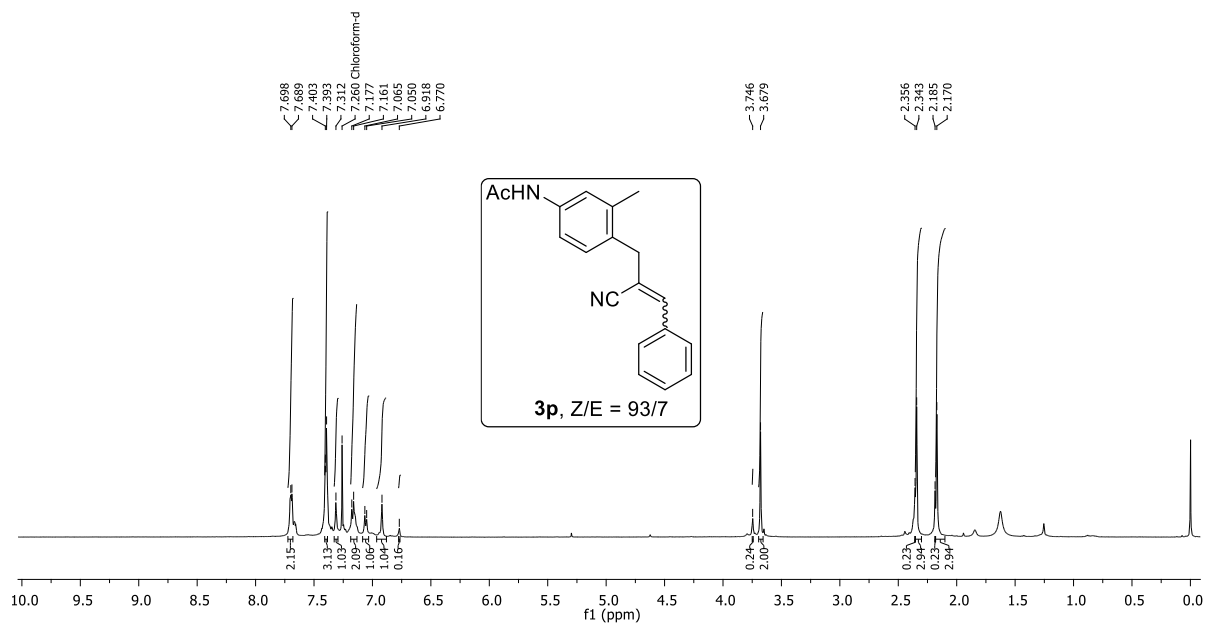
¹H NMR, CDCl₃, 500 MHz



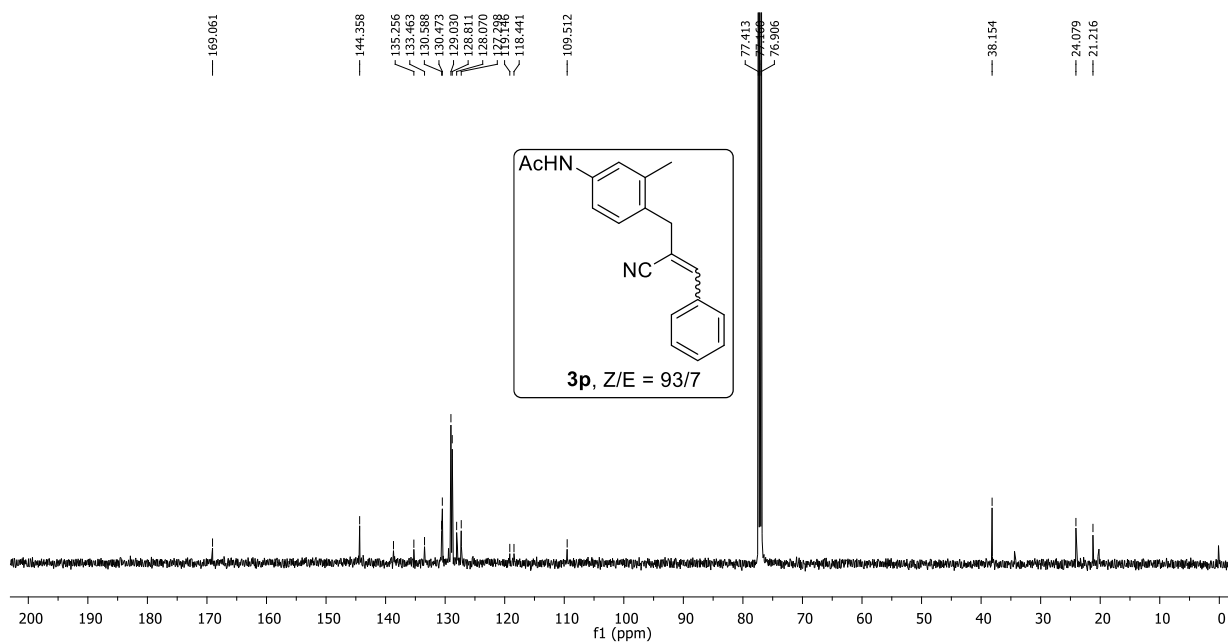
¹³C{¹H} NMR, CDCl₃, 126 MHz



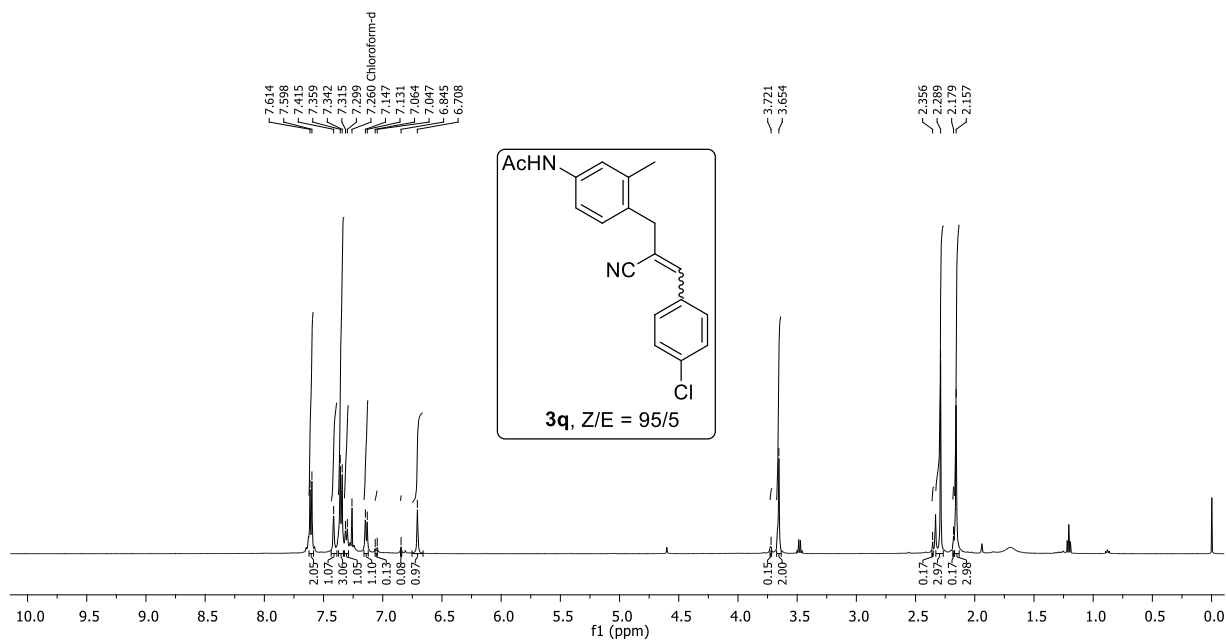
***N*-(4-(2-Cyano-3-phenylallyl)-3-methylphenyl)acetamide (**3p**):
¹H NMR, CDCl₃, 500 MHz**



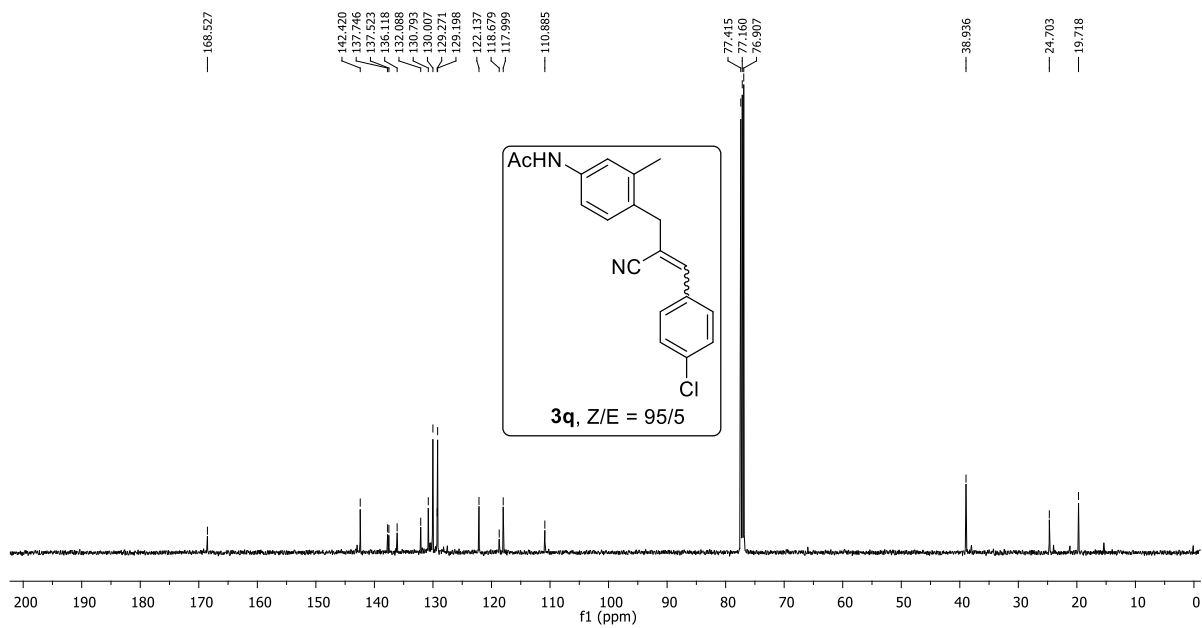
¹³C{¹H} NMR, CDCl₃, 126 MHz



***N*-(4-(3-(4-Chlorophenyl)-2-cyanoallyl)-3-methylphenyl)acetamide (3q):
¹H NMR, CDCl₃, 500 MHz**

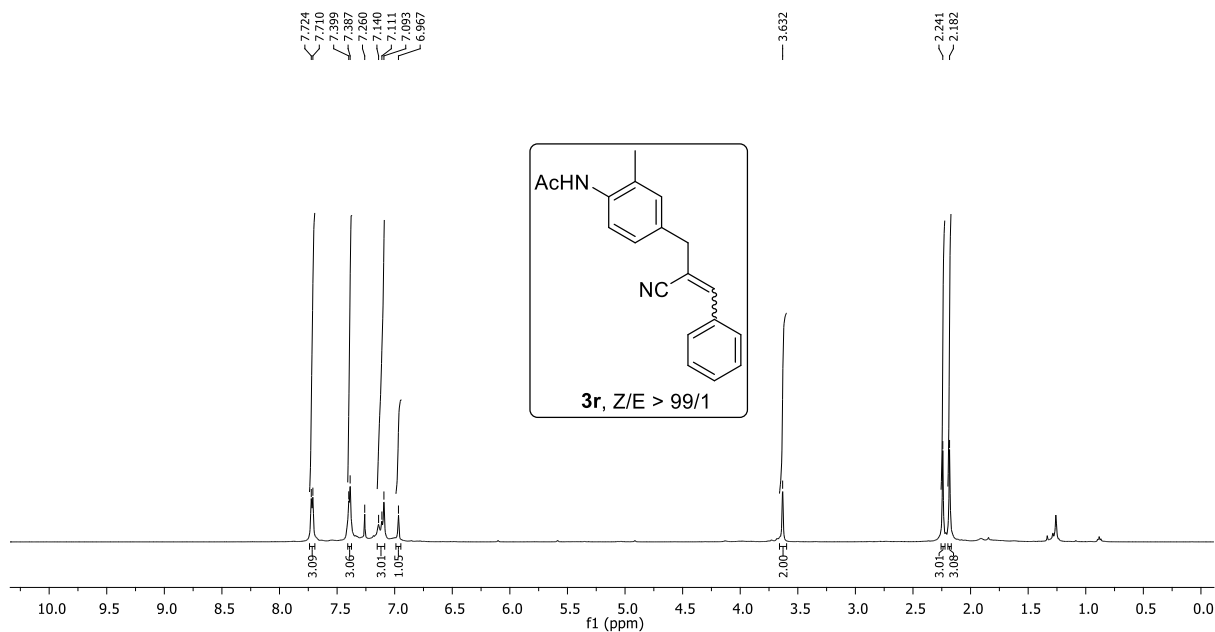


¹³C{¹H} NMR, CDCl₃, 126 MHz

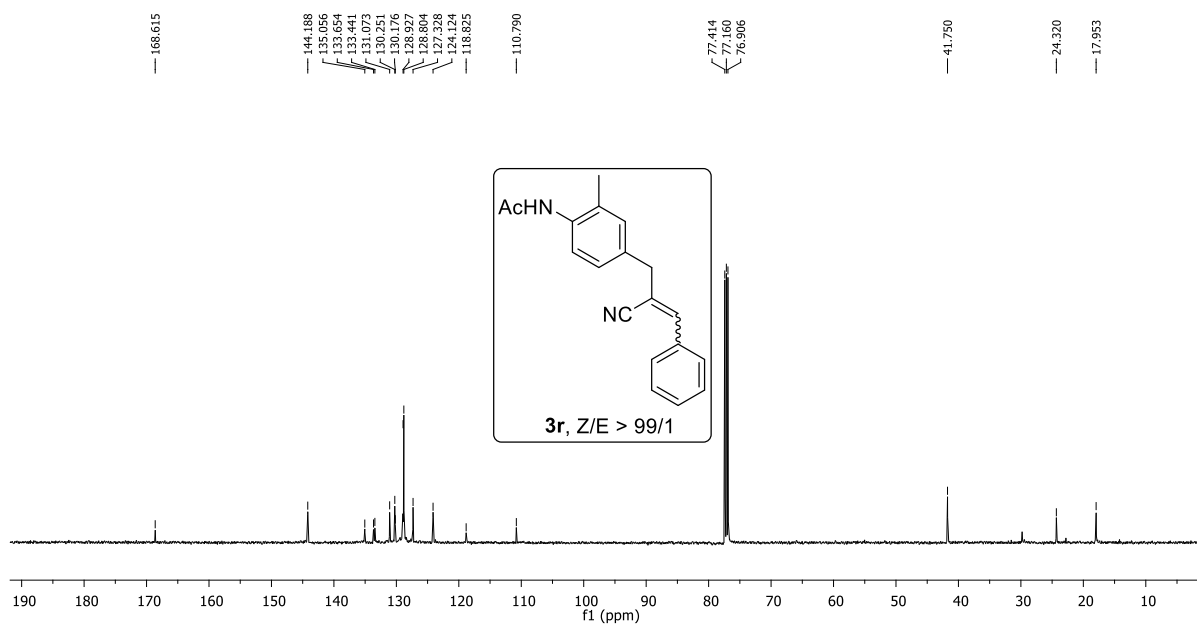


***N*-(4-(2-Cyano-3-phenylallyl)-2-methylphenyl)acetamide (**3r**):**

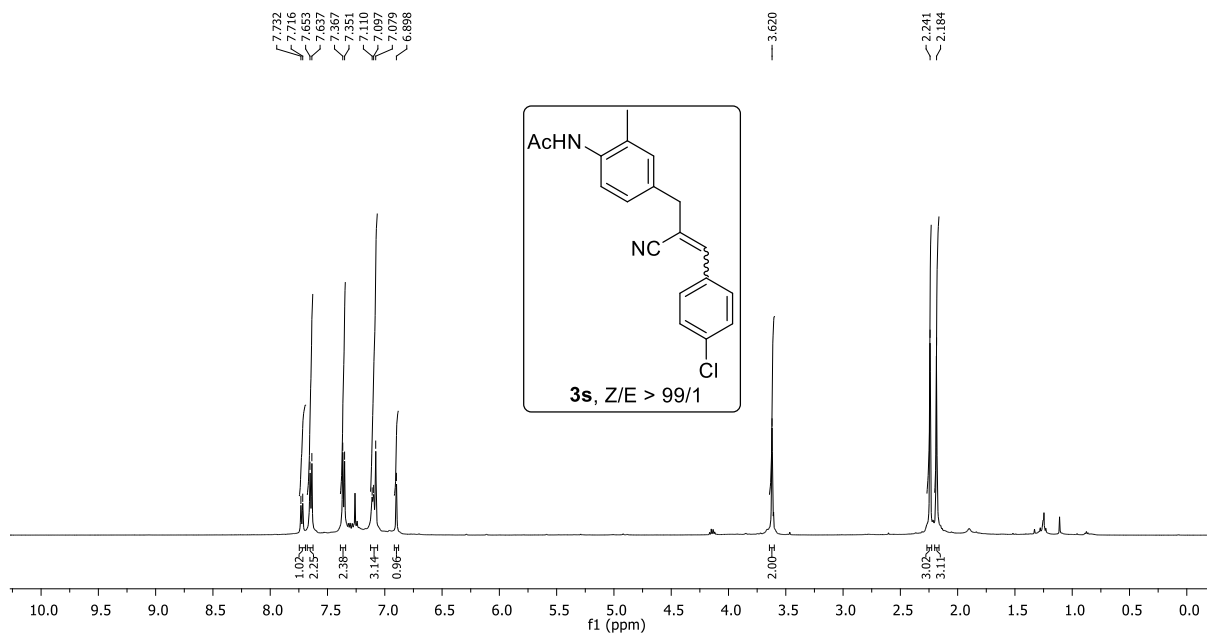
¹H NMR, CDCl₃, 500 MHz



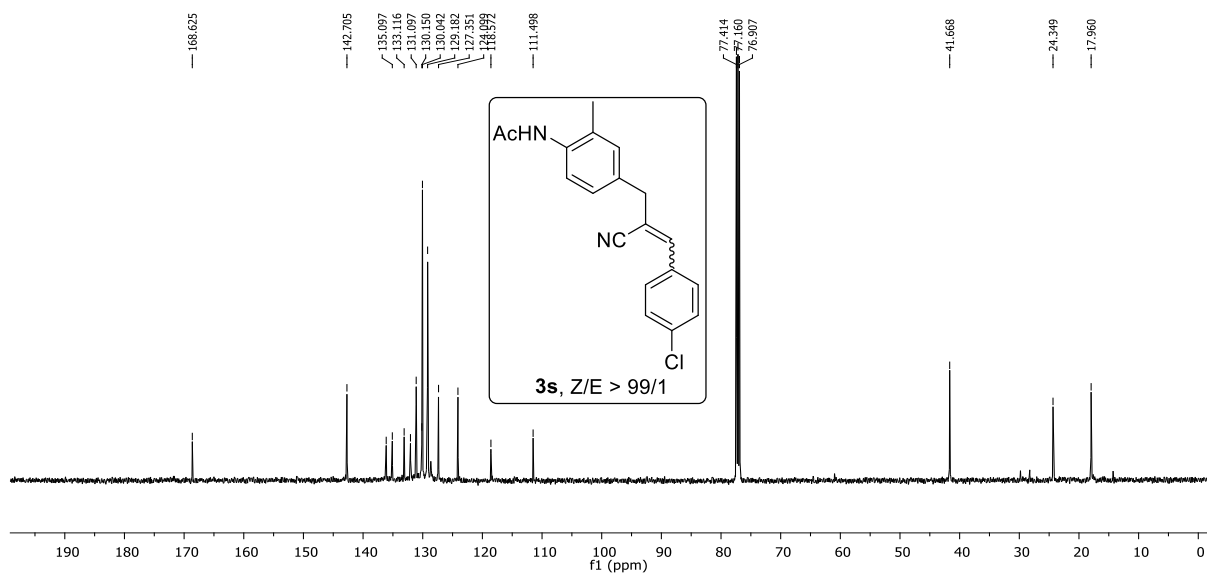
¹³C{¹H} NMR, CDCl₃, 126 MHz



***N*-[4-(3-(4-Chlorophenyl)-2-cyanoallyl)-2-methylphenyl]acetamide (**3s**):
¹H NMR, CDCl₃, 500 MHz**

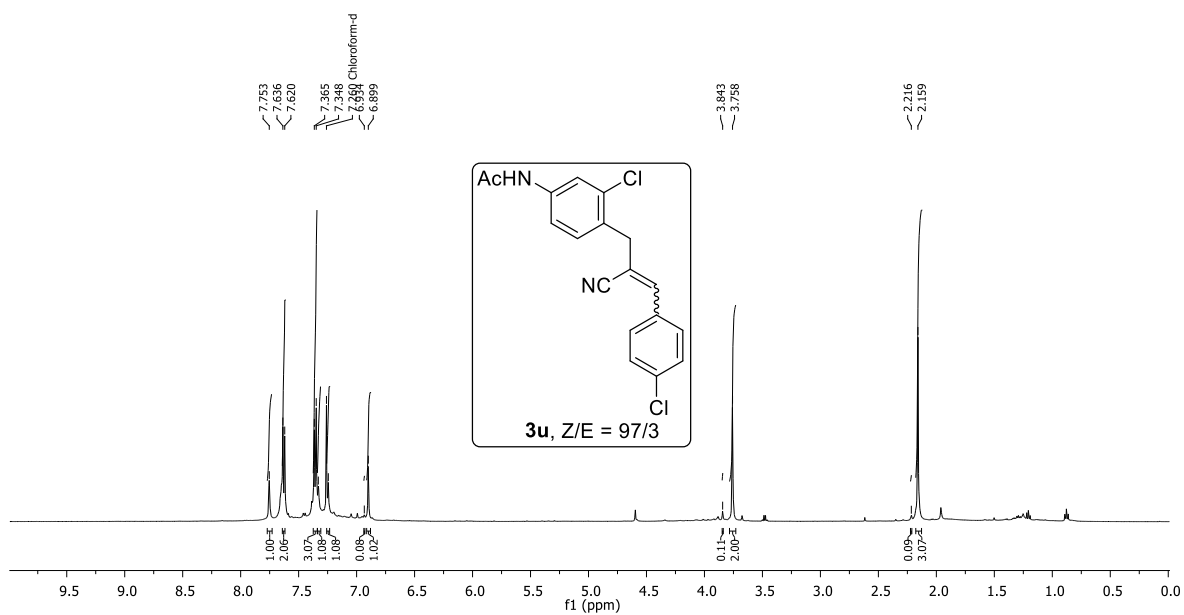


¹³C{¹H} NMR, CDCl₃, 126 MHz

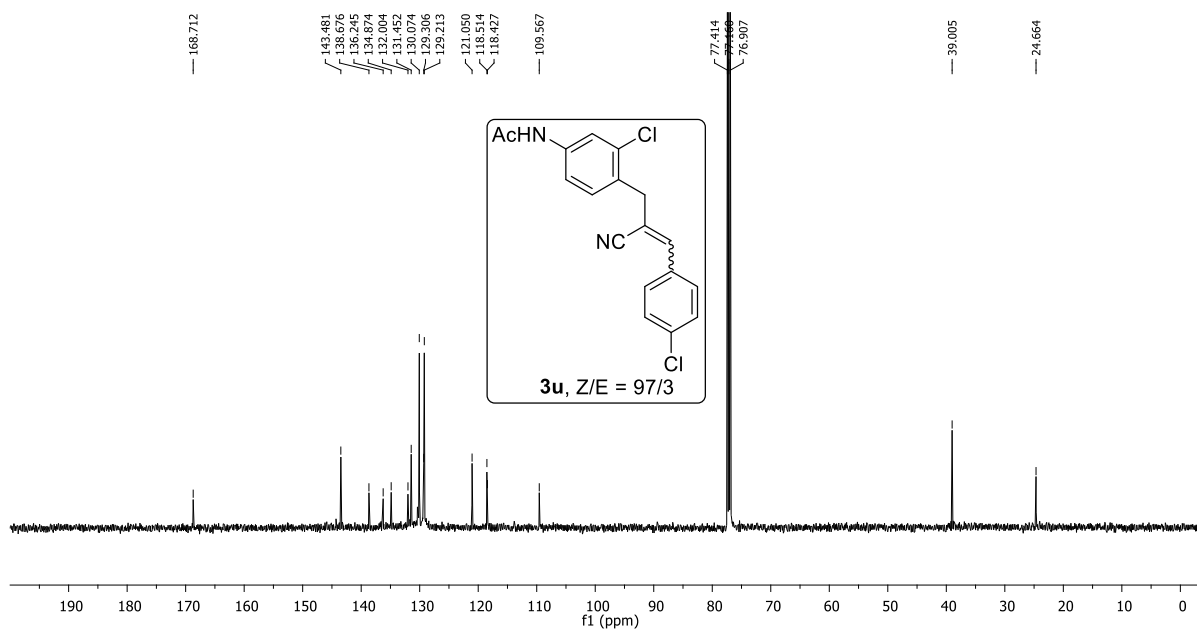


***N*-(3-Chloro-4-(3-(4-chlorophenyl)-2-cyanoallyl)phenyl)acetamide (3u):**

¹H NMR, CDCl₃, 500 MHz

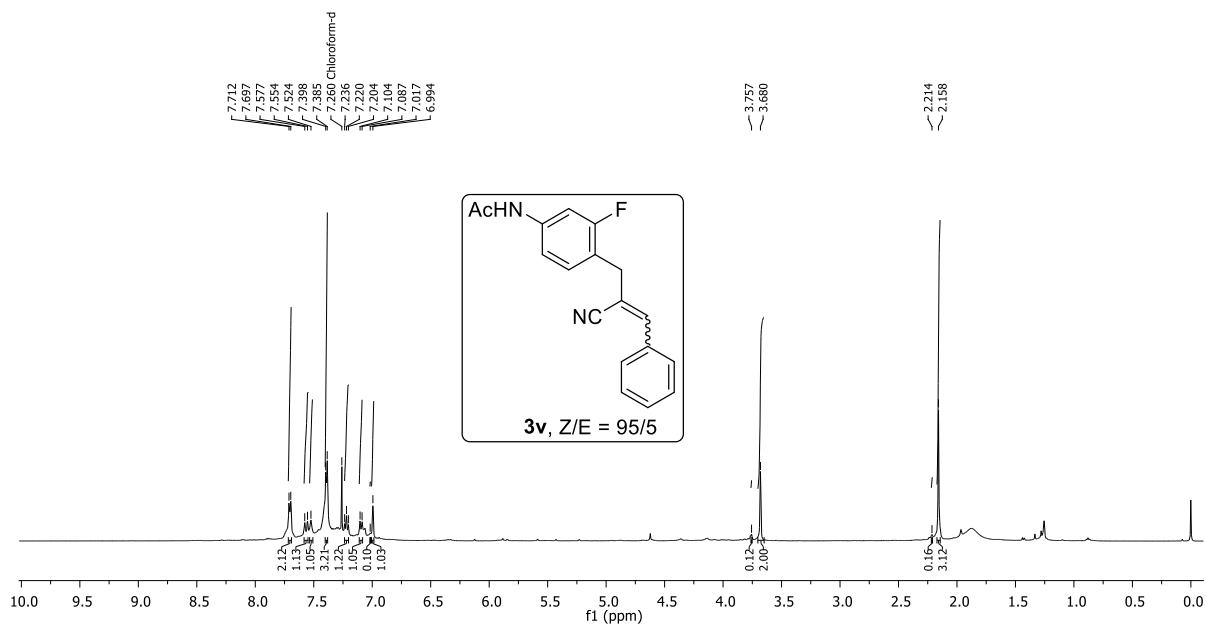


¹³C{¹H} NMR, CDCl₃, 126 MHz

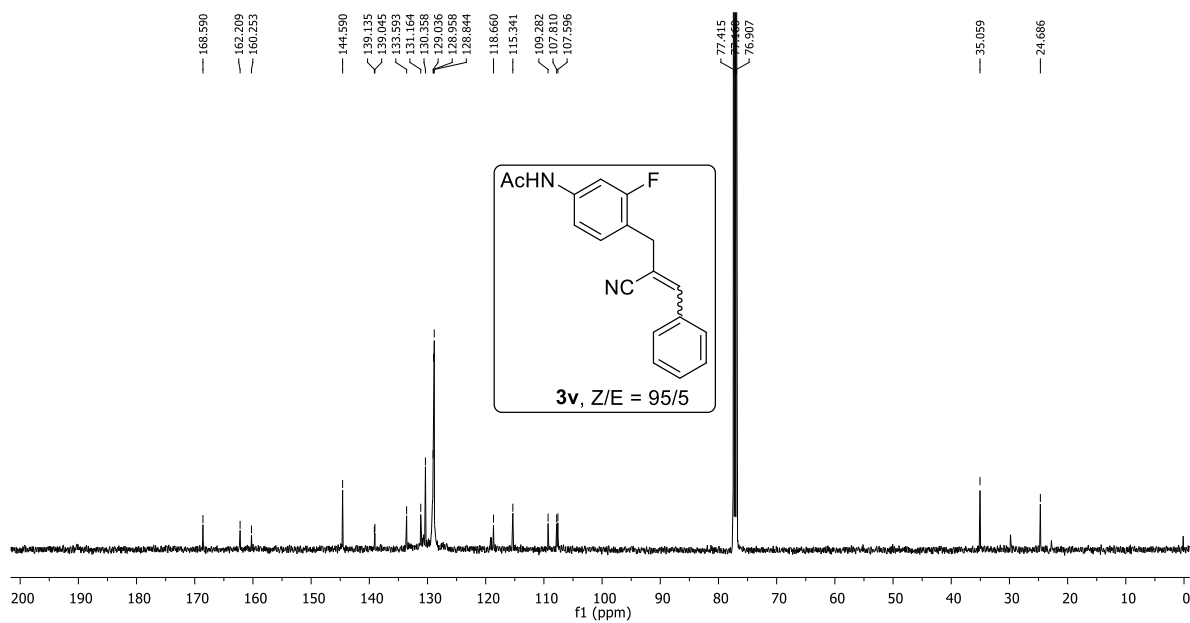


***N*-(4-(2-Cyano-3-phenylallyl)-3-fluorophenyl)acetamide (3v) :**

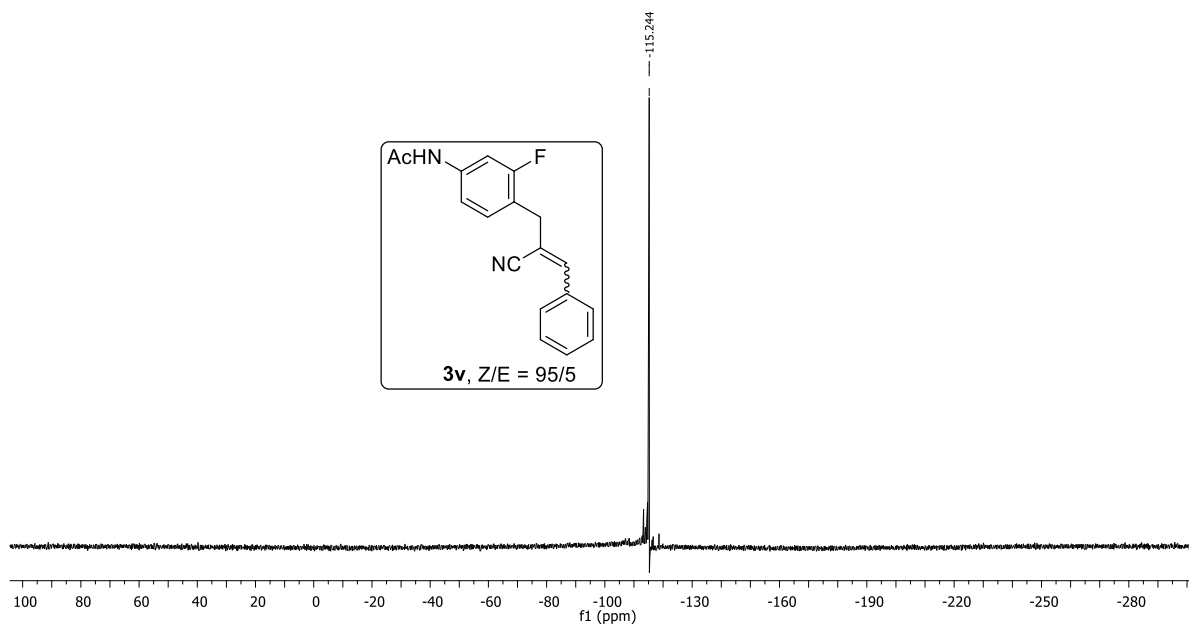
¹H NMR, CDCl₃, 500 MHz



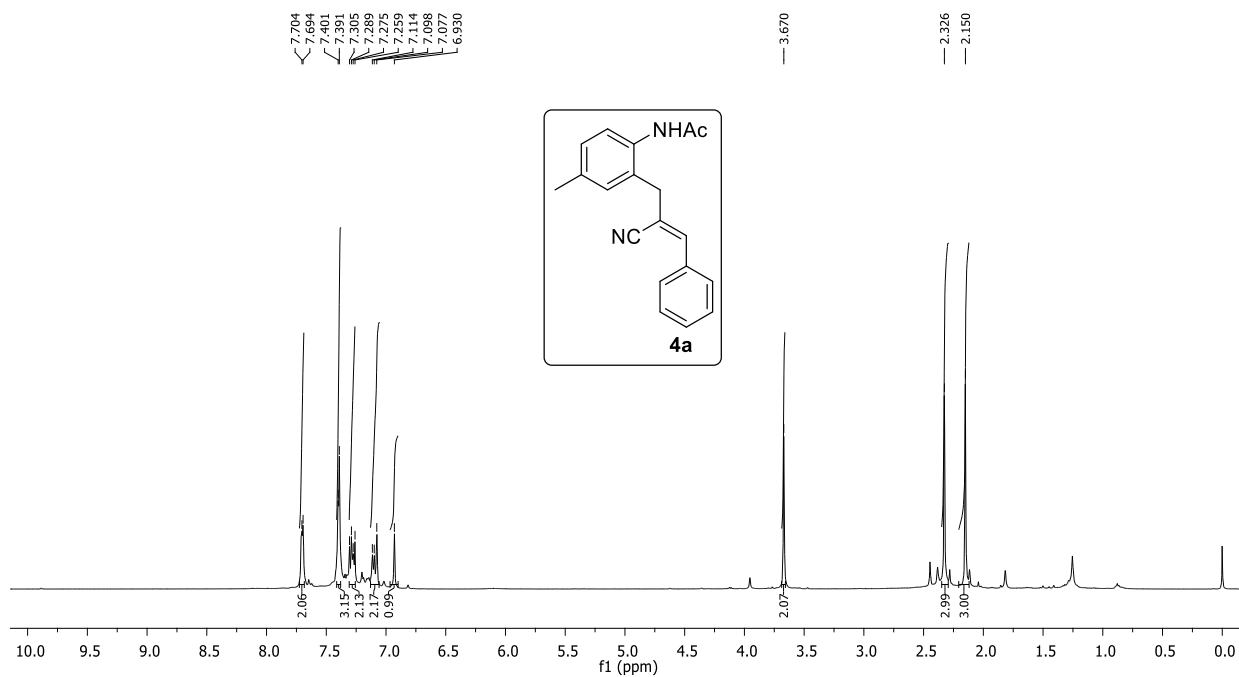
¹³C{¹H} NMR, CDCl₃, 126 MHz



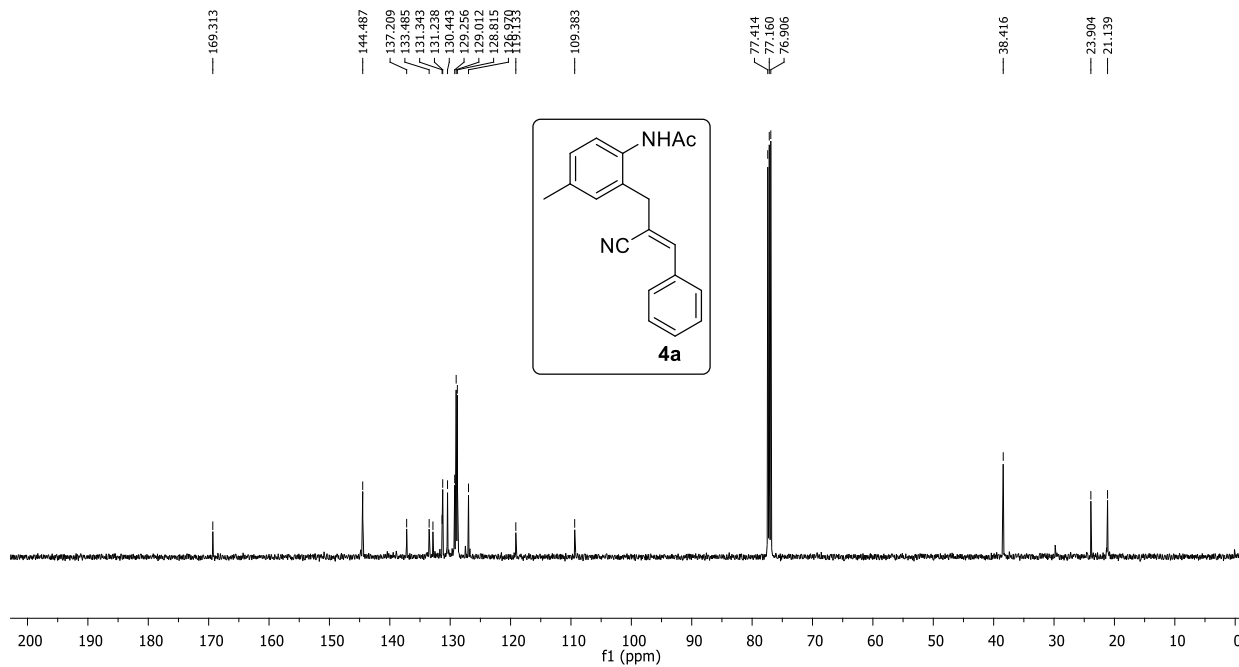
¹⁹F NMR, CDCl₃, 471 MHz,



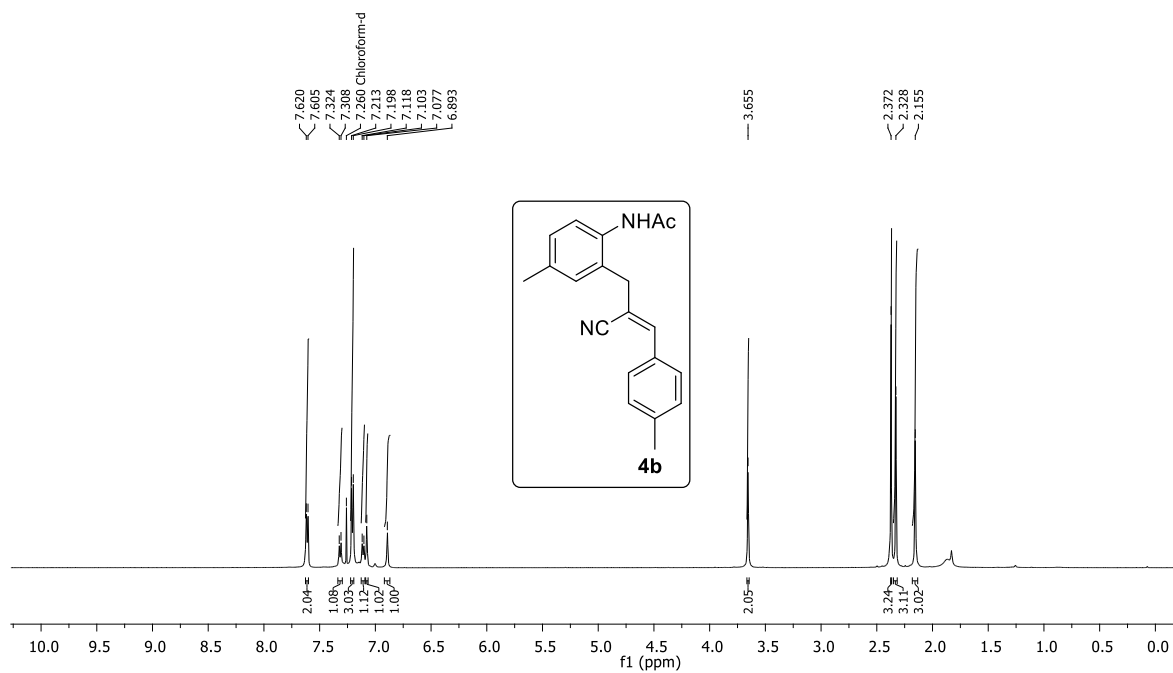
(Z)-N-(2-(2-Cyano-3-phenylallyl)-4-methylphenyl)acetamide (4a):
¹H NMR, CDCl₃, 500 MHz



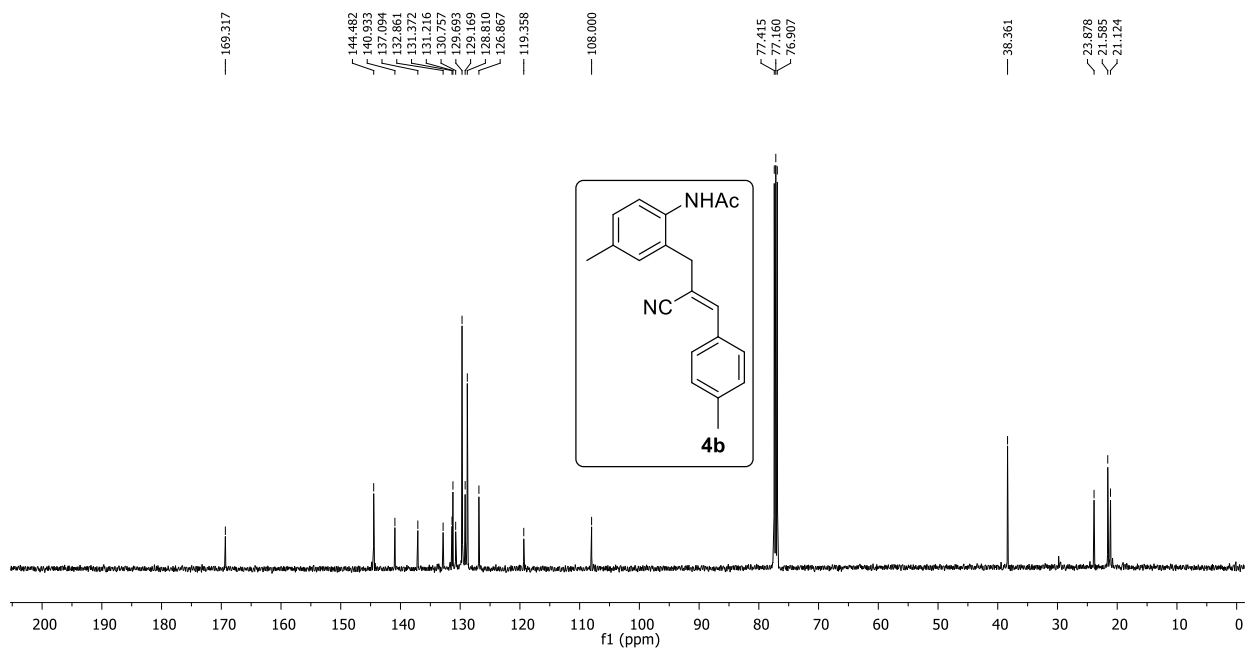
¹³C{¹H} NMR, CDCl₃, 126 MHz



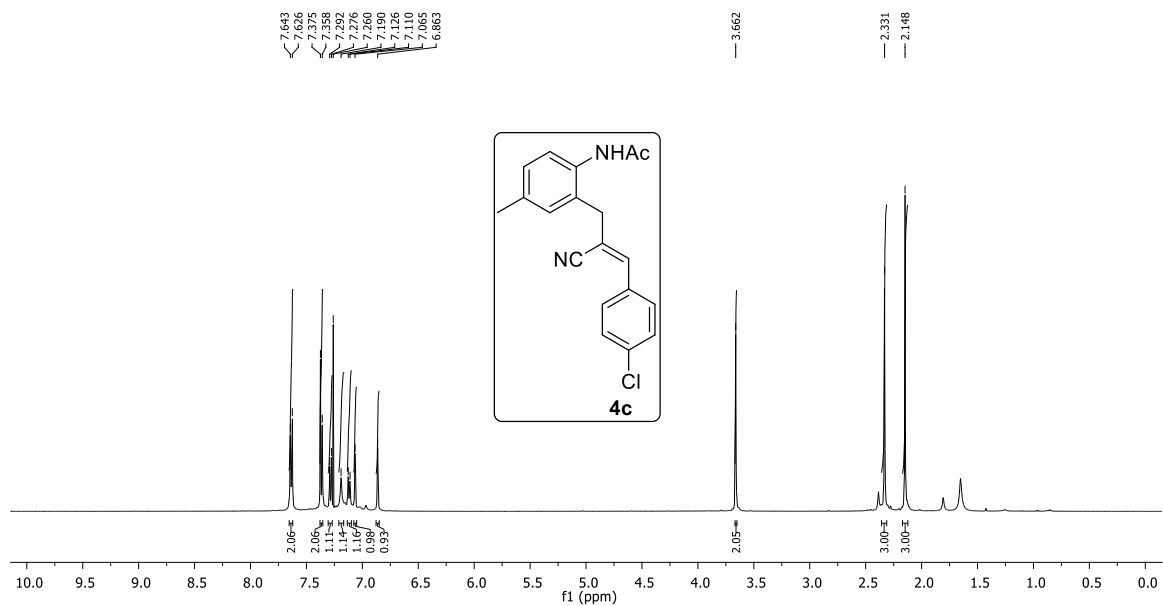
(Z)-N-(2-(2-Cyano-3-(p-tolyl)allyl)-4-methylphenyl)acetamide (4b):
¹H NMR, CDCl₃, 500 MHz



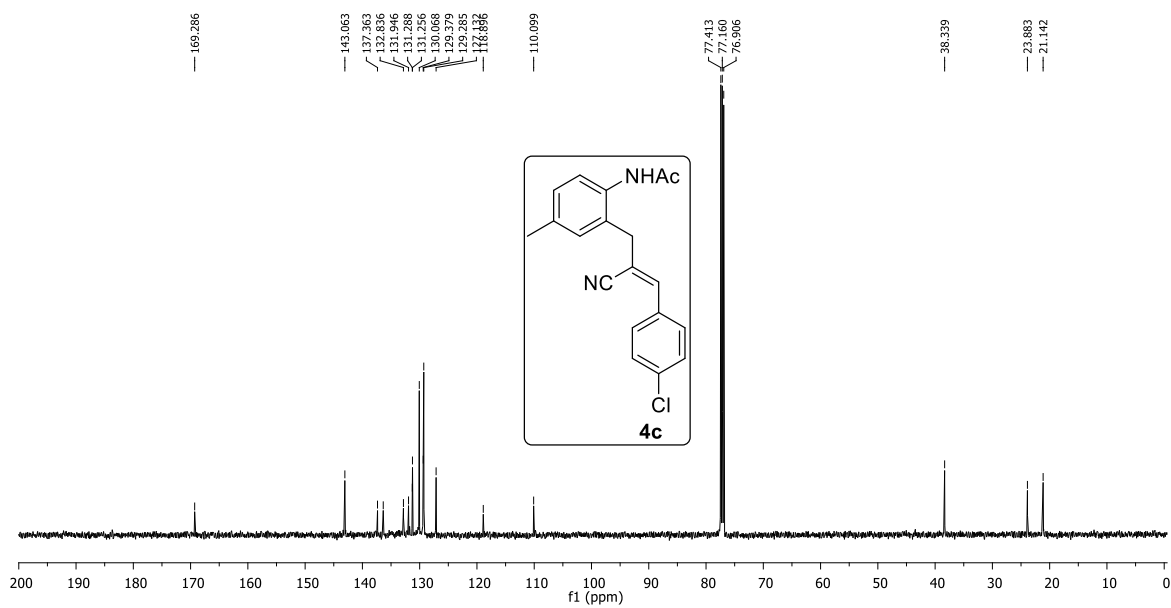
¹³C{¹H} NMR, CDCl₃, 126 MHz



(Z)-N-(2-(3-(4-Chlorophenyl)-2-cyanoallyl)-4-methylphenyl)acetamide (4c):
¹H NMR, CDCl₃, 500 MHz

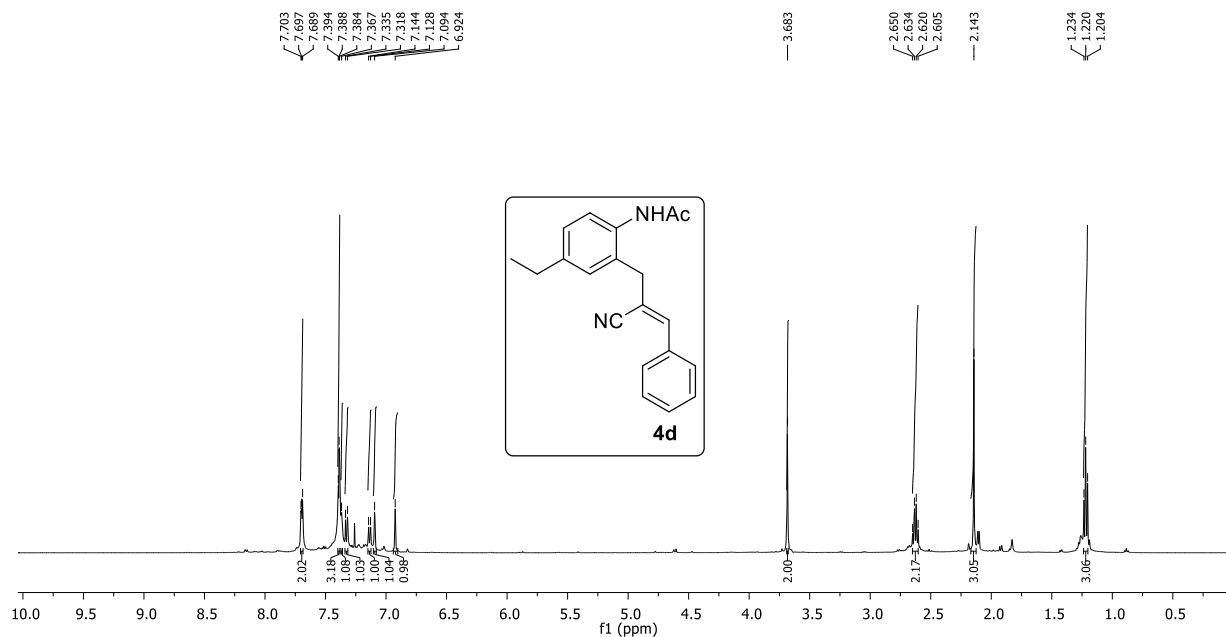


¹³C{¹H} NMR, CDCl₃, 126 MHz

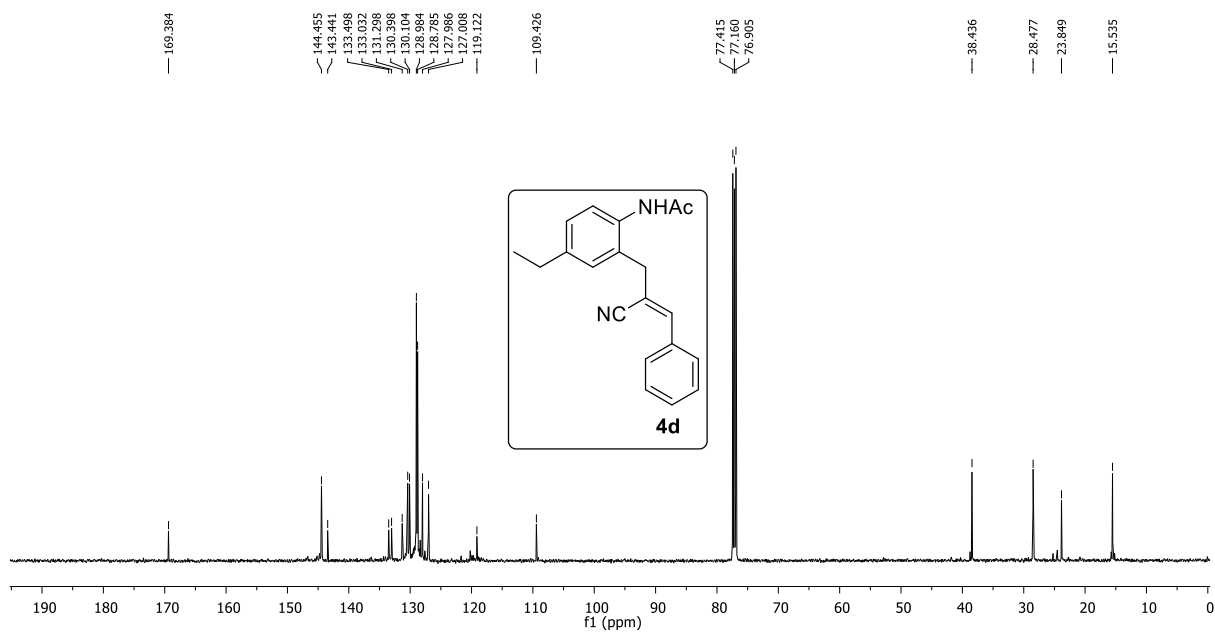


(Z)-N-(2-(2-Cyano-3-phenylallyl)-4-ethylphenyl)acetamide (4d):

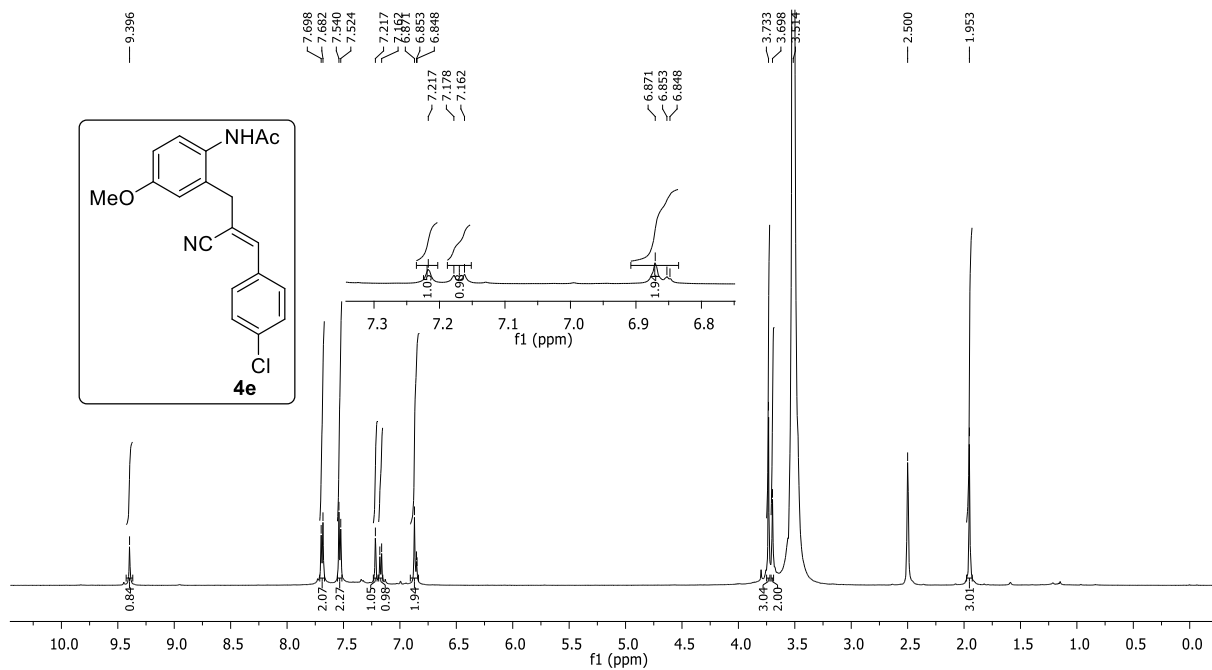
¹H NMR, CDCl₃, 500 MHz



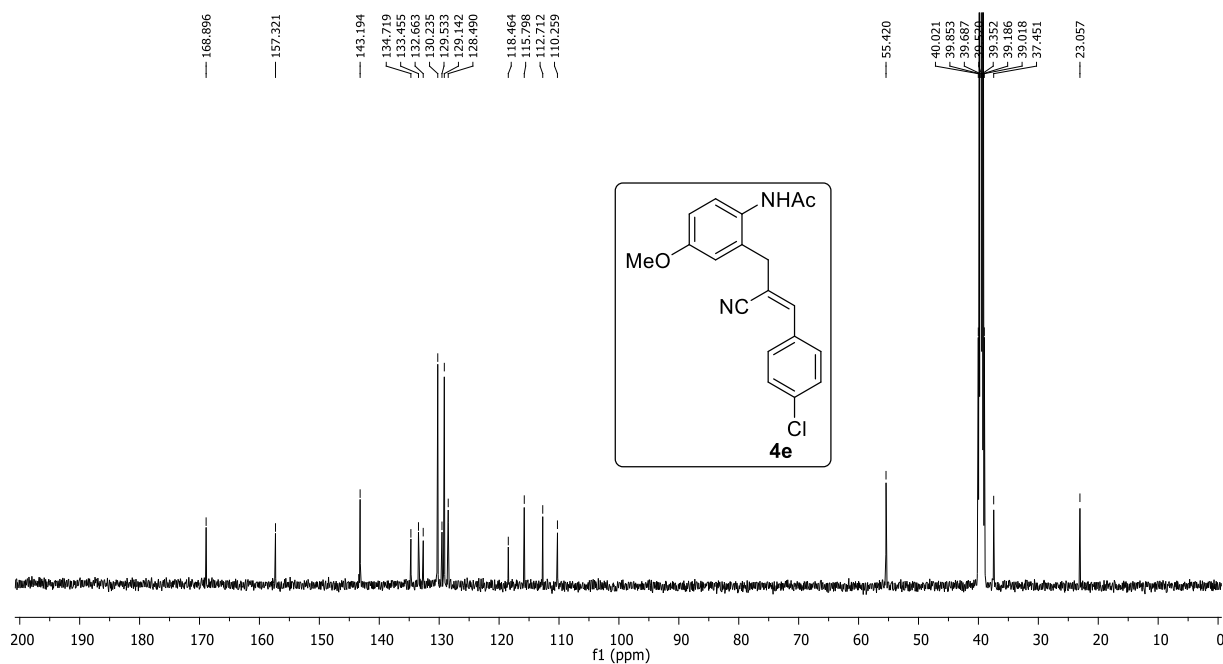
¹³C{¹H} NMR, CDCl₃, 126 MHz



(Z)-N-(2-(3-(4-Chlorophenyl)-2-cyanoallyl)-4-methoxyphenyl)acetamide (4e) :
¹H NMR, DMSO-d₆, 500 MHz

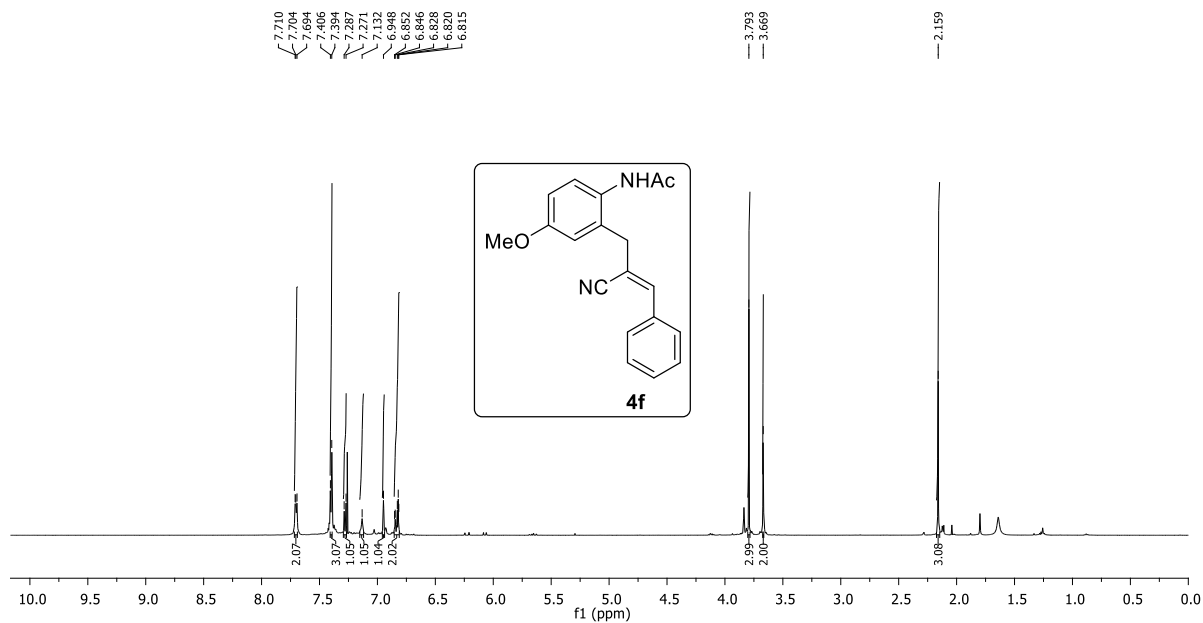


¹³C{¹H} NMR, DMSO-d₆, 126 MHz

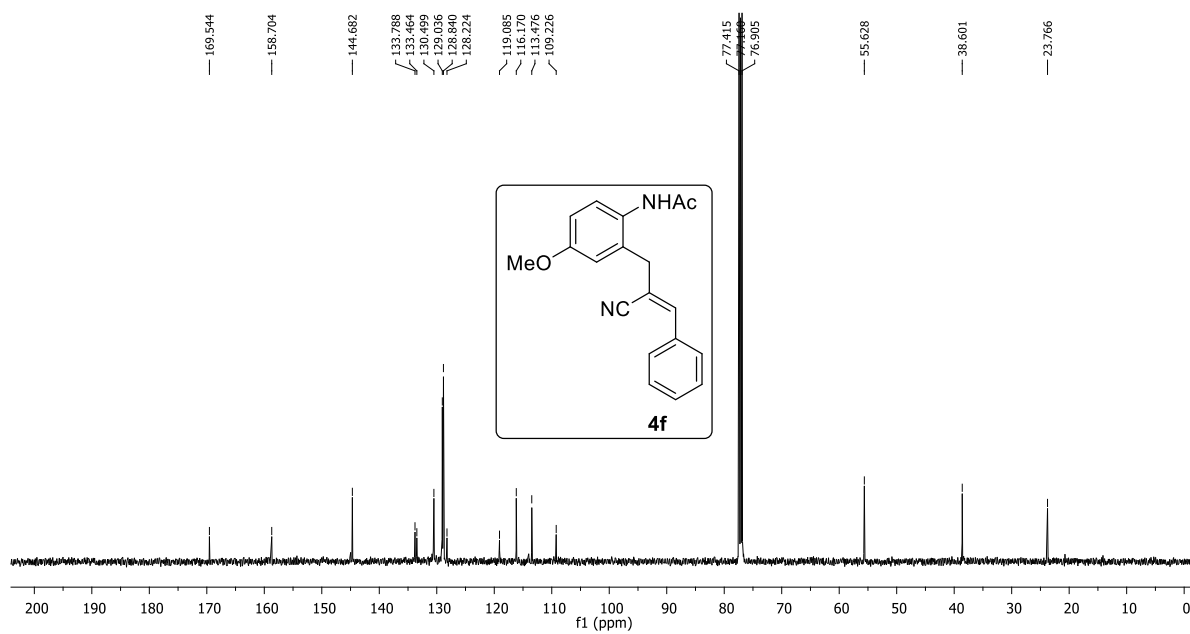


(Z)-N-(2-(2-Cyano-3-phenylallyl)-4-methoxyphenyl)acetamide (4f):

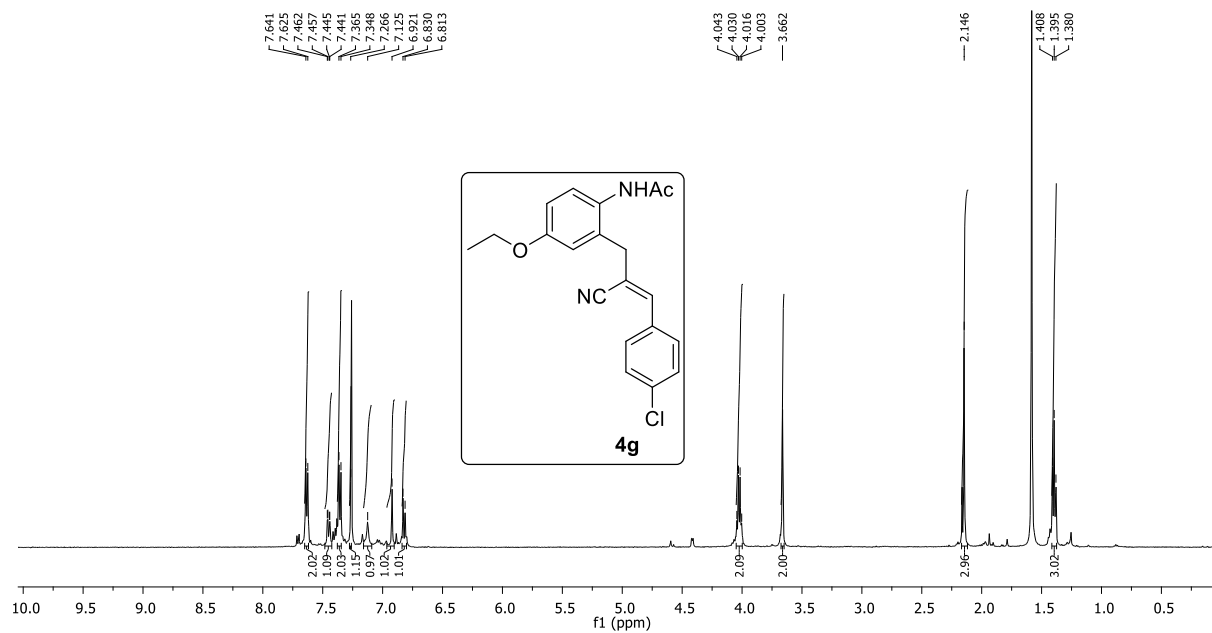
¹H NMR, CDCl₃, 500 MHz



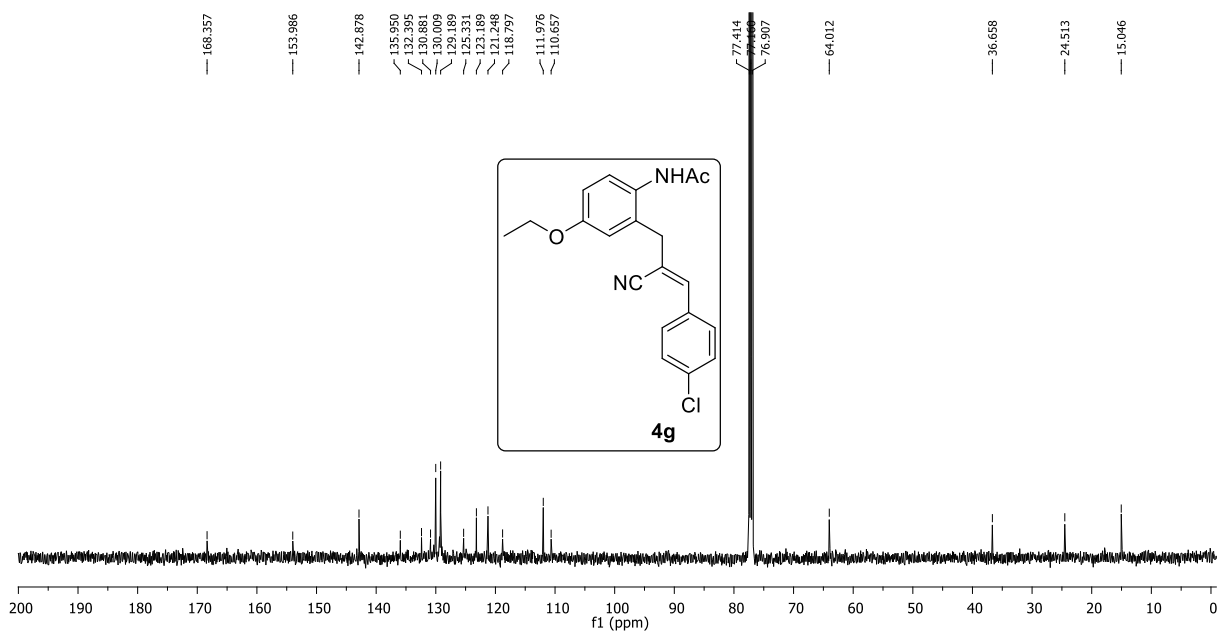
¹³C{¹H} NMR, CDCl₃, 126 MHz



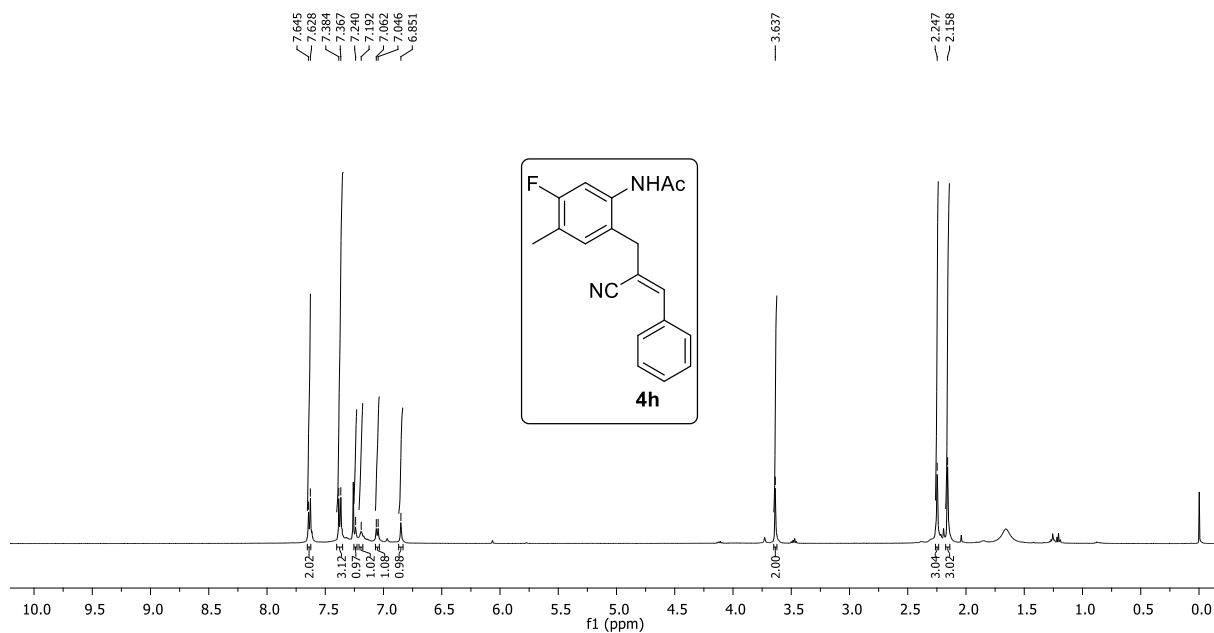
(Z)-N-(2-(3-(4-Chlorophenyl)-2-cyanoallyl)-4-ethoxyphenyl)acetamide (4g):
¹H NMR, CDCl₃, 500 MHz



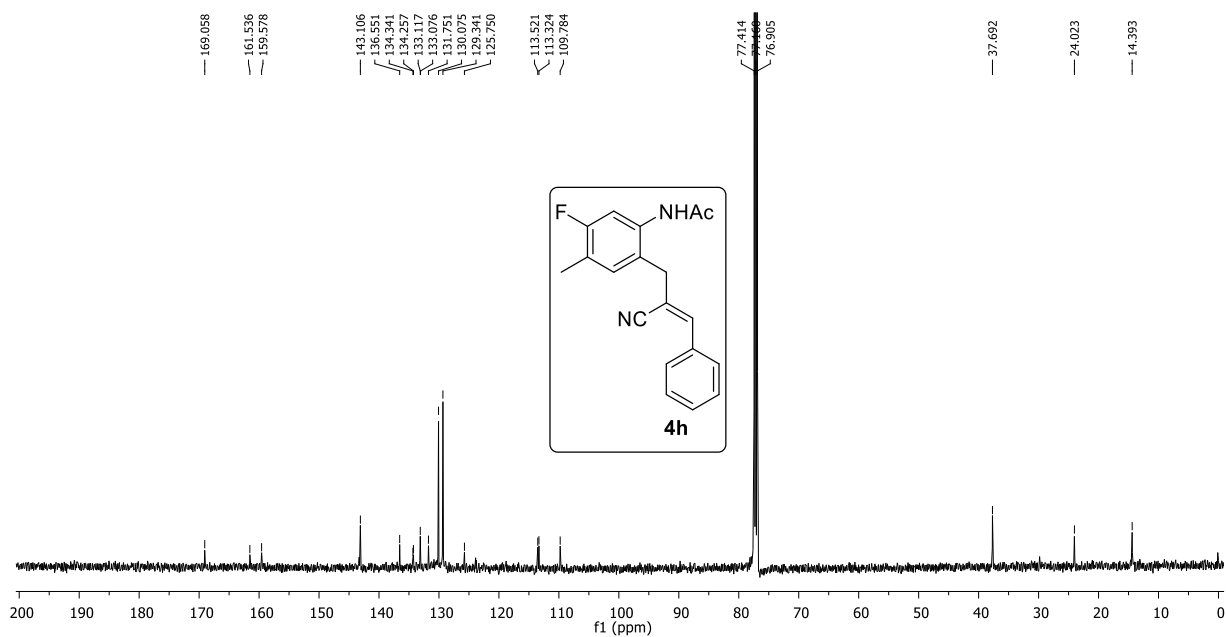
¹³C{¹H} NMR, CDCl₃, 126 MHz



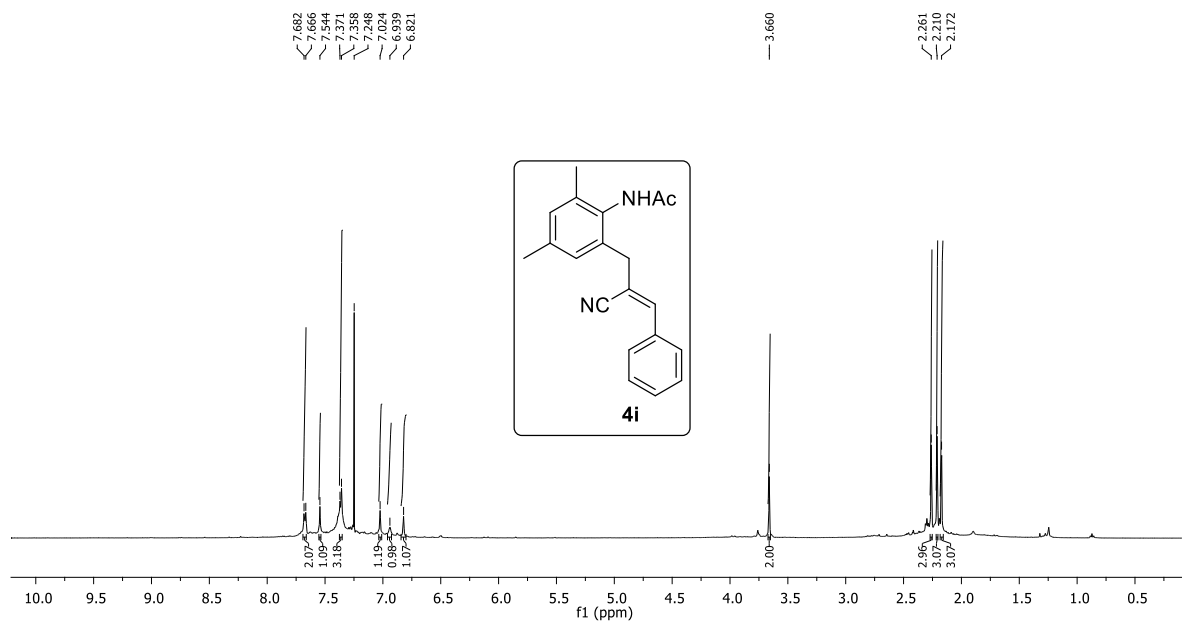
(Z)-N-(2-(2-Cyano-3-phenylallyl)-5-fluoro-4-methylphenyl)acetamide (4h):
¹H NMR, CDCl₃, 500 MHz



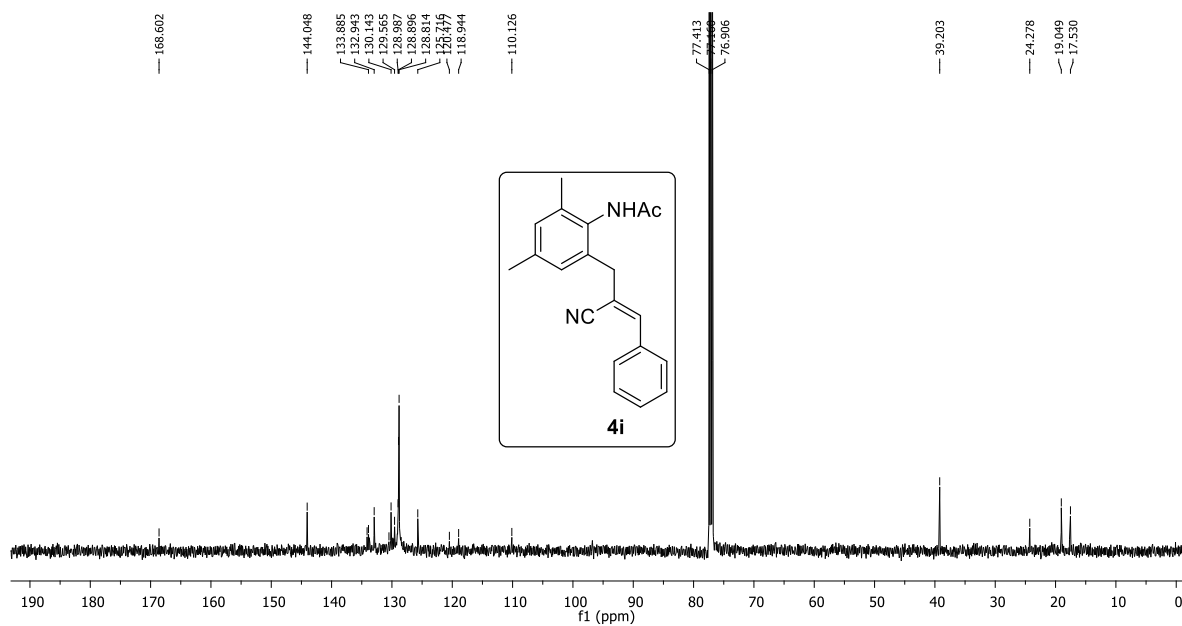
¹³C{¹H} NMR, CDCl₃, 126 MHz



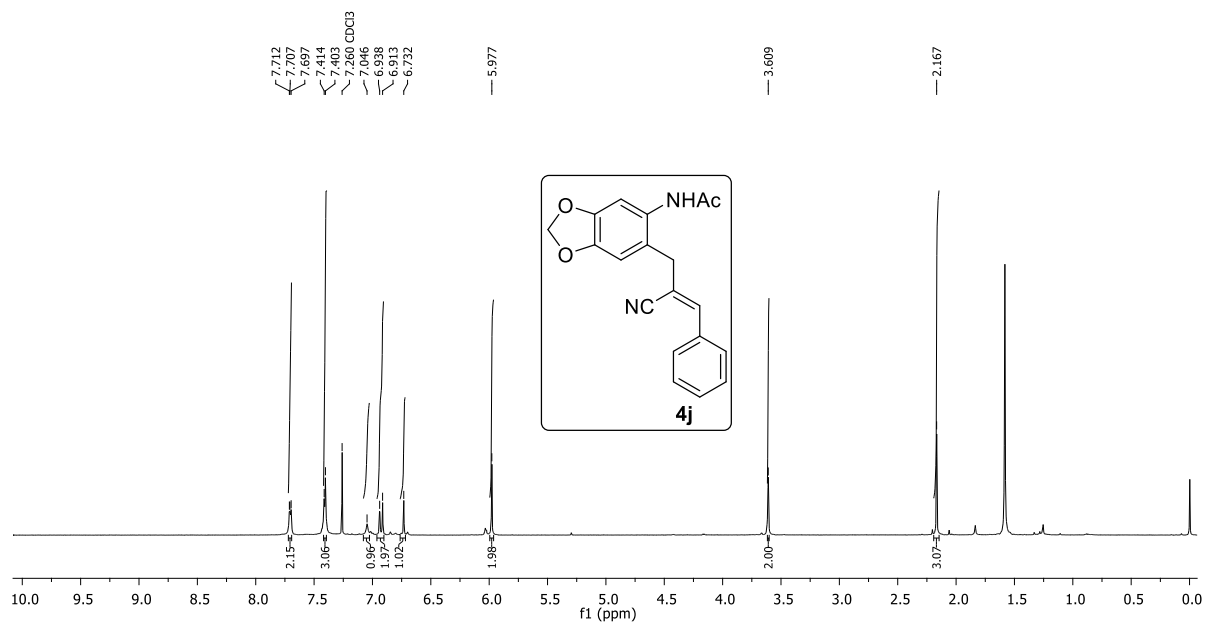
(Z)-N-(2-(2-Cyano-3-phenylallyl)-4,6-dimethylphenyl)acetamide (4i):
¹H NMR, CDCl₃, 500 MHz



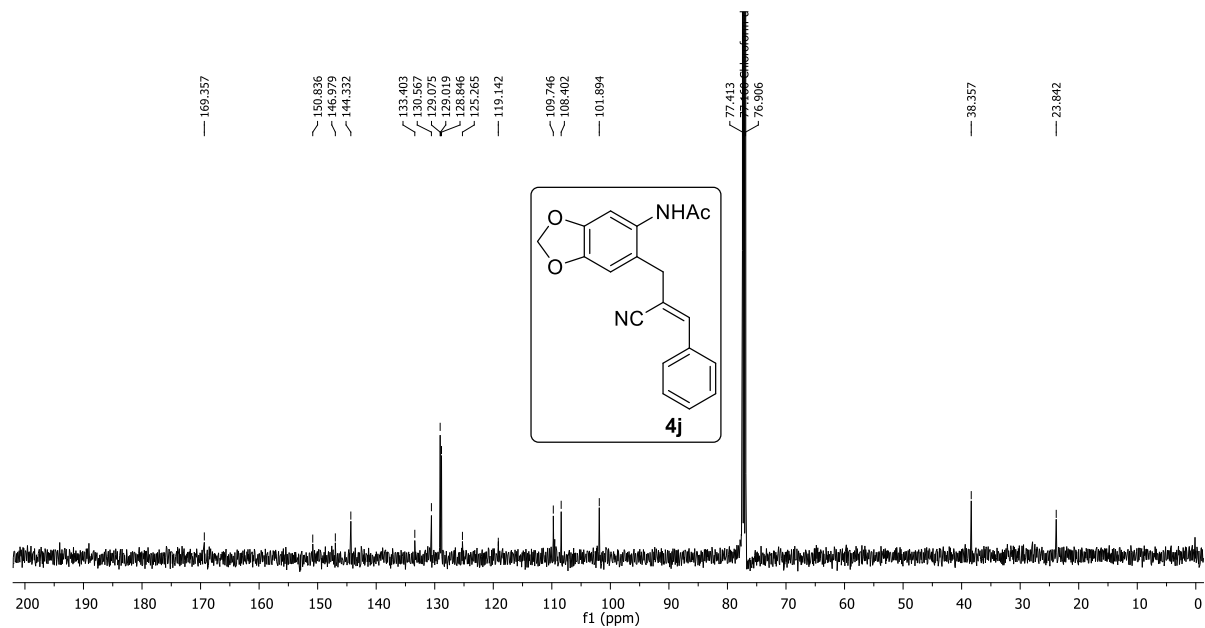
¹³C{¹H} NMR, CDCl₃, 126 MHz



(Z)-N-(6-(2-Cyano-3-phenylallyl)benzo[d][1,3]dioxol-5-yl)acetamide (4j):
¹H NMR, CDCl₃, 500 MHz

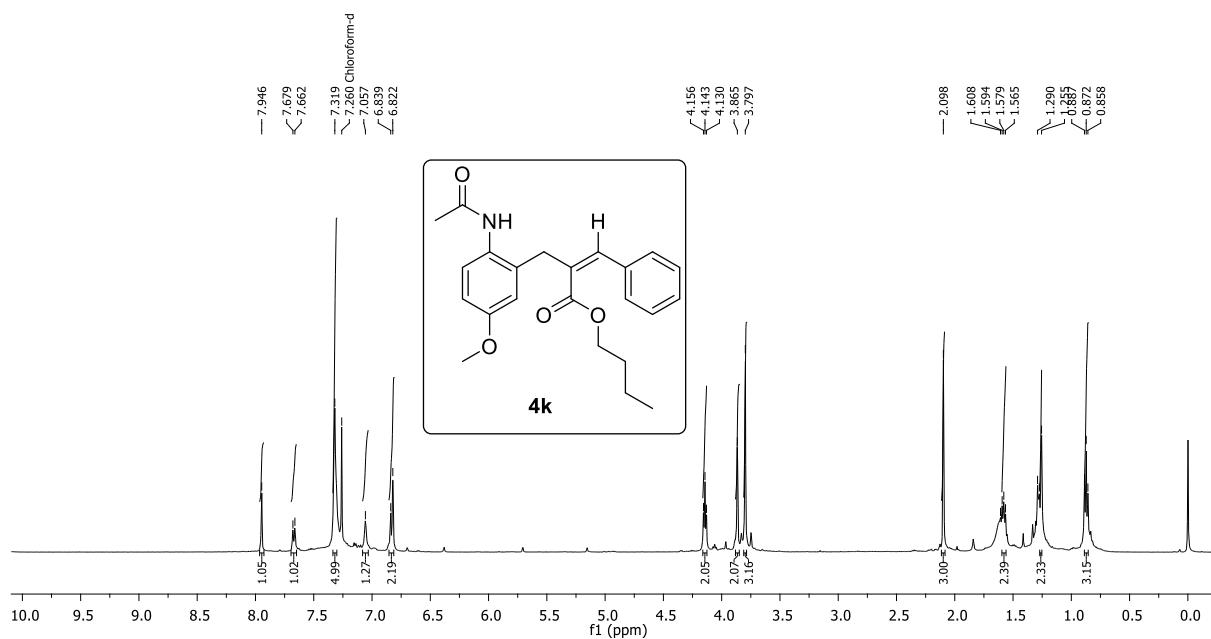


¹³C{¹H} NMR, CDCl₃, 126 MHz

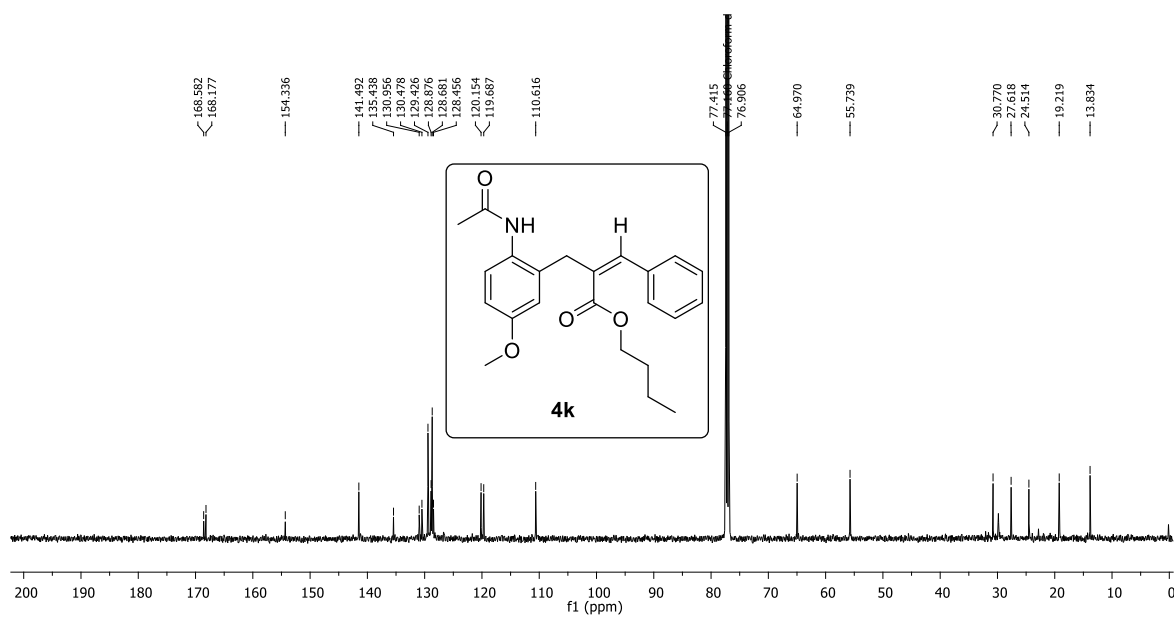


Butyl (Z)-2-(2-acetamido-5-methoxybenzyl)-3-phenylacrylate (4k):

^1H NMR, CDCl_3 , 500 MHz

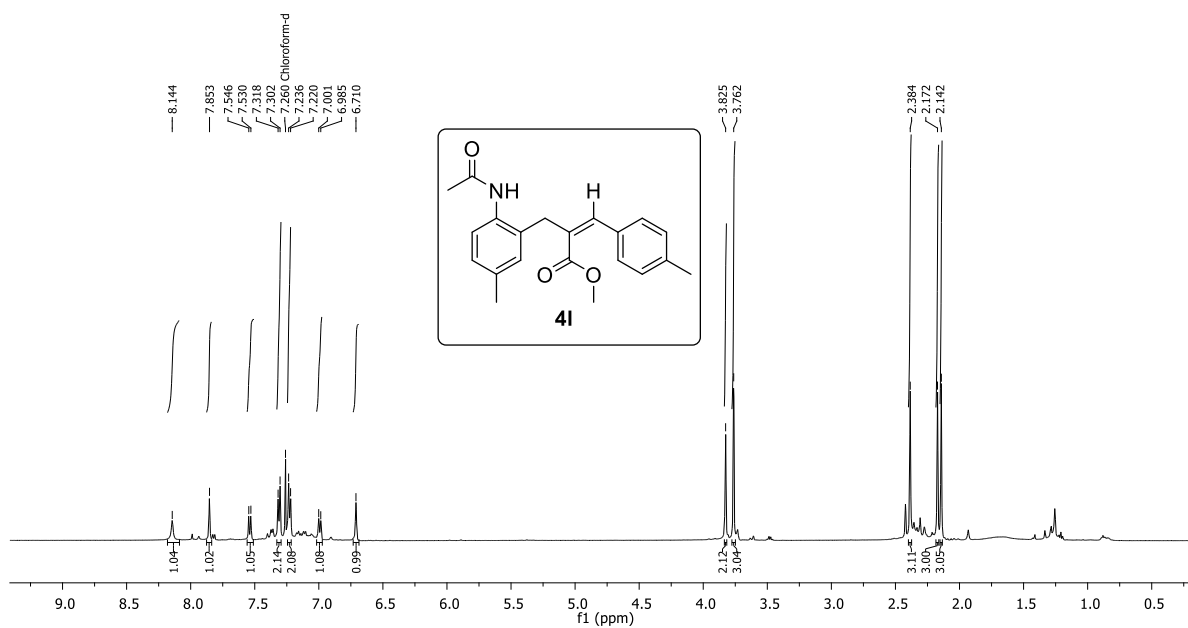


$^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 126 MHz

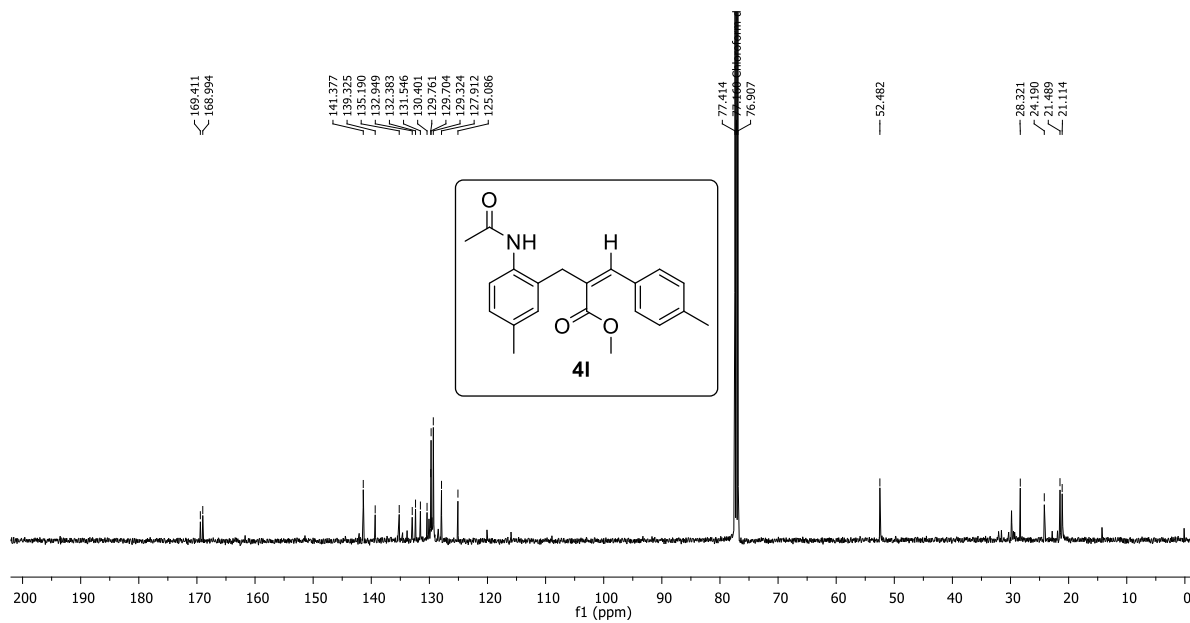


Methyl (Z)-2-(2-acetamido-5-methylbenzyl)-3-phenylacrylate (**4I**):

^1H NMR, CDCl_3 , 500 MHz

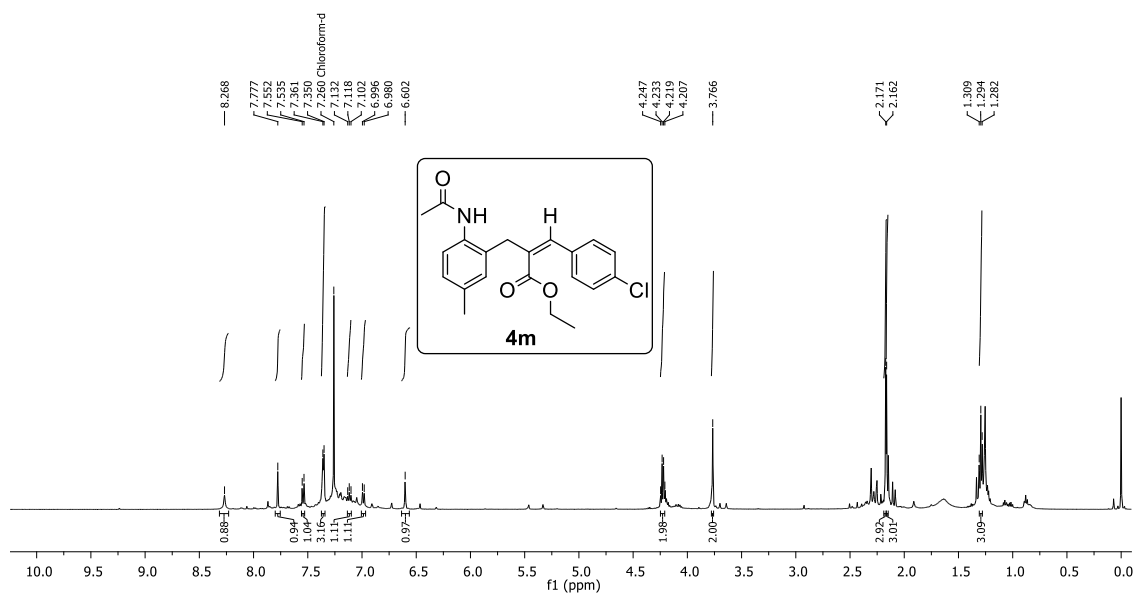


$^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 126 MHz

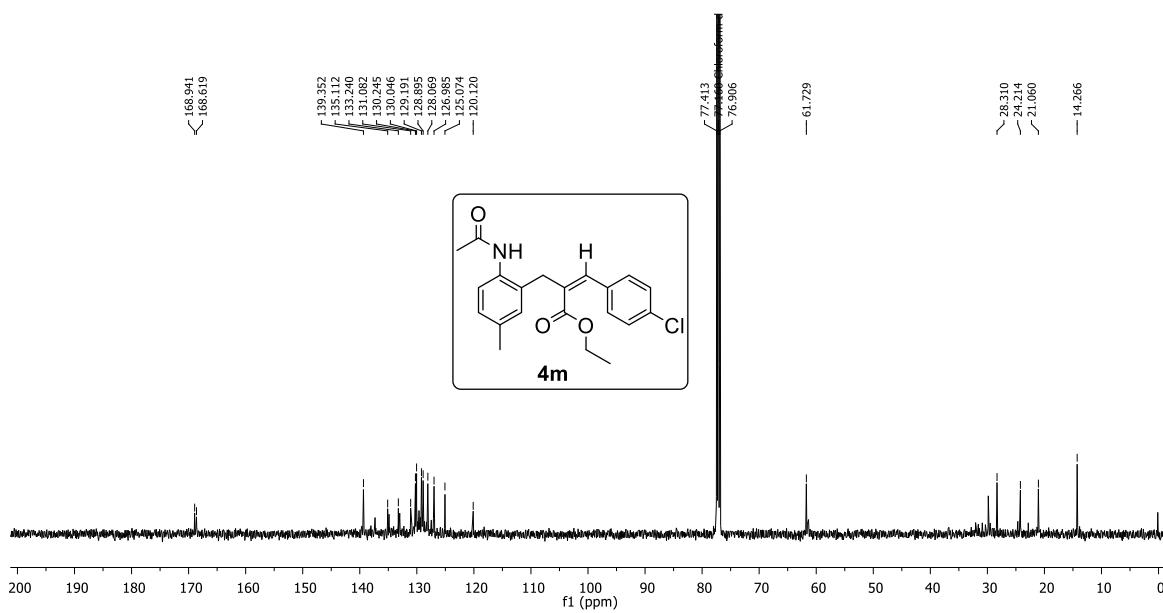


Ethyl (Z)-2-(2-acetamido-5-methylbenzyl)-3-(4-chlorophenyl)acrylate (4m):

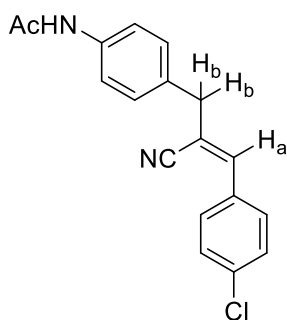
^1H NMR, CDCl_3 , 500 MHz



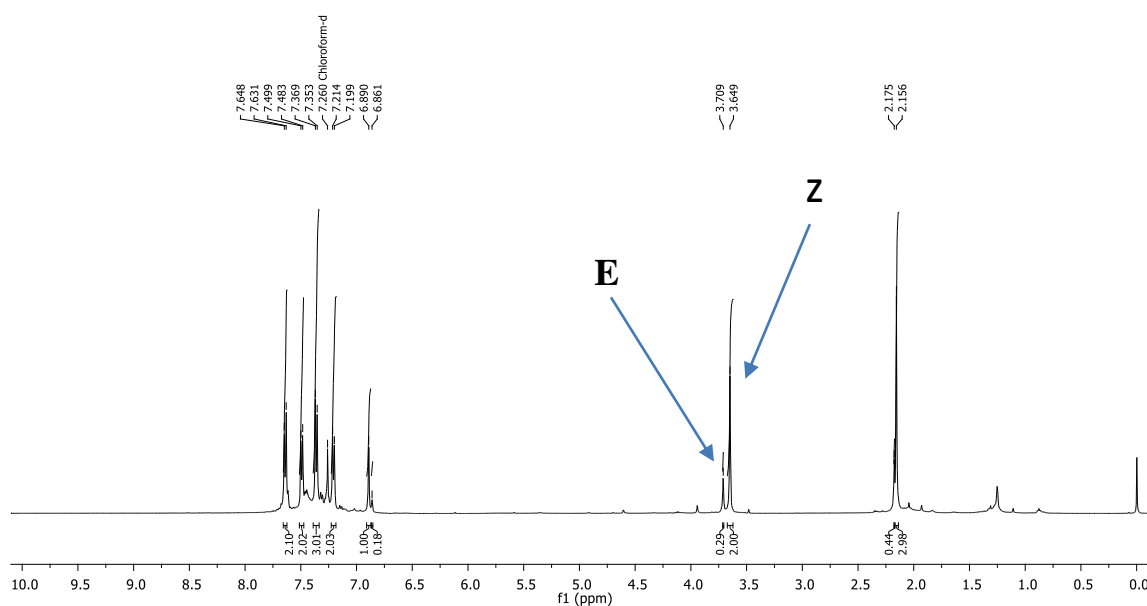
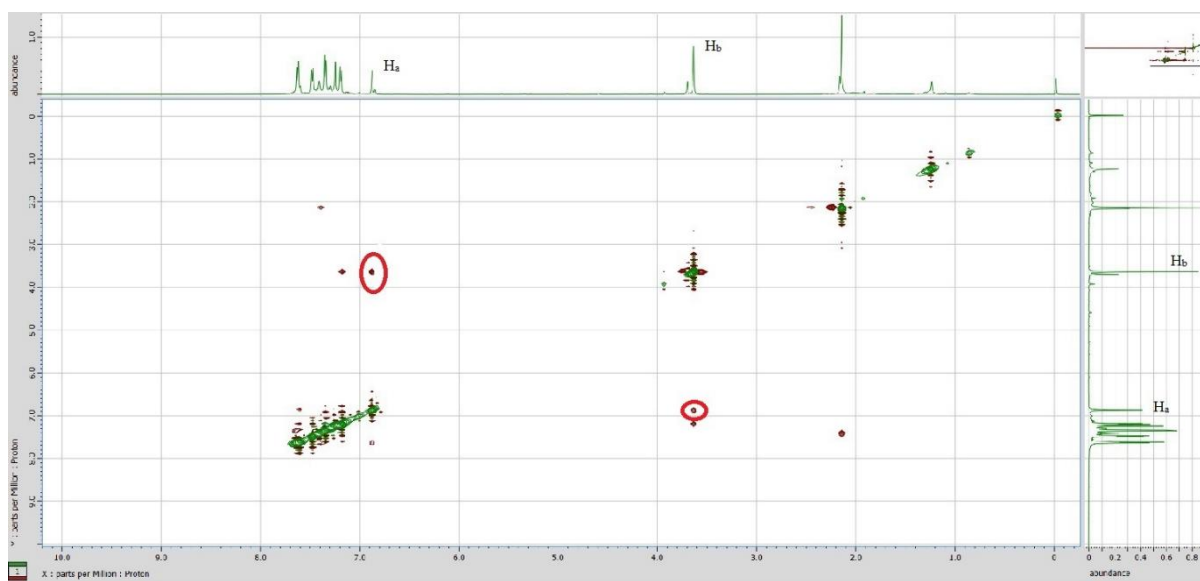
$^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 126 MHz



2. NOESY Spectrum of the Product 3e

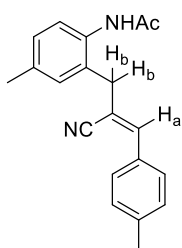


1. The ^1H NMR shows 4 types of aromatic hydrogens with the splitting pattern of doublet which correlates with *para* isomer.
2. No cross peak is observed between minor H_b and H_a in the 2D NMR spectrum. Also, no cross peak between H_b and CH_3CO that suggests that the *ortho* isomer is not formed
3. NOE correlation is observed between H_a (δ 6.89, s) and H_b (δ , 3.65, s). Based on the ^1H NMR and NOESY Spectrum of **3e**, it is concluded that the major product is (*Z*)-isomer with the *Z/E* ratio 87:13.

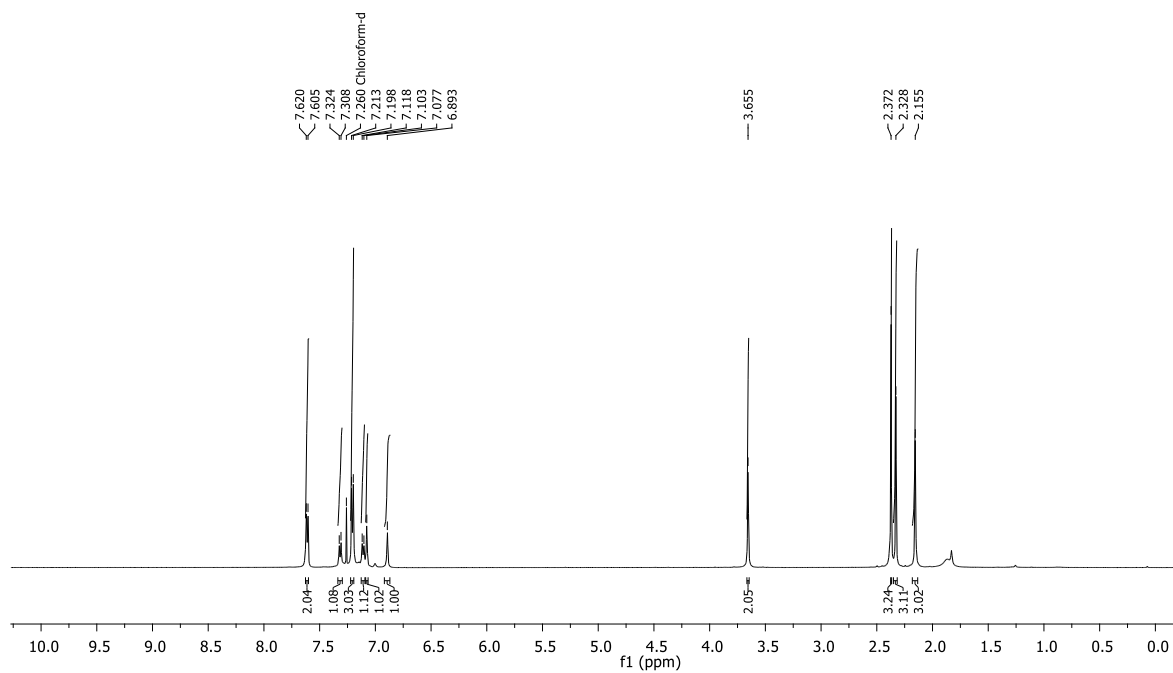
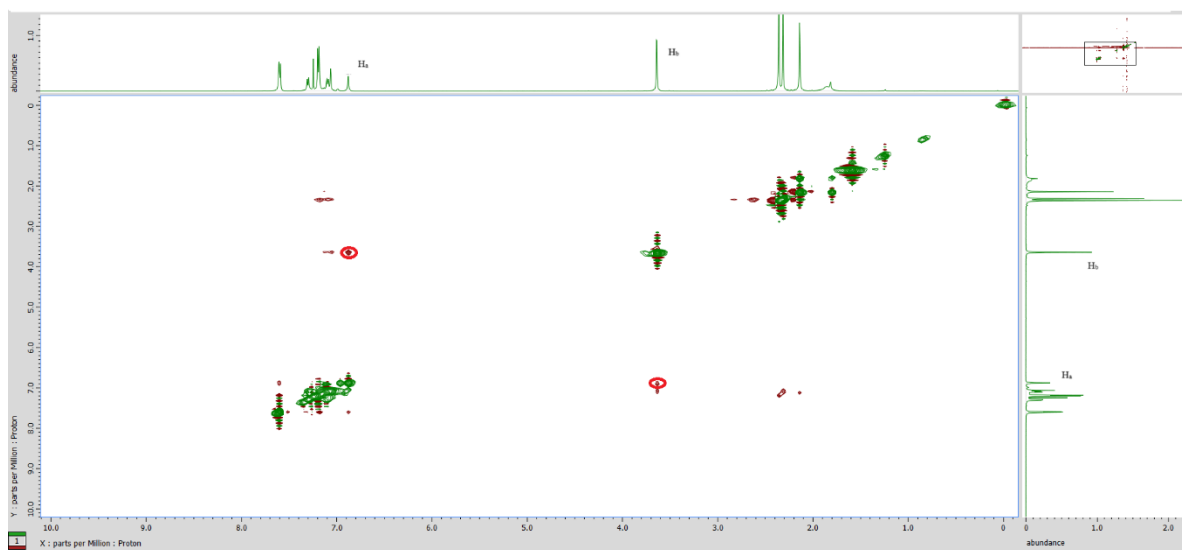


^1H NMR of **3e**

3. NOESY Spectrum of the Product 4b



NOE correlation is observed between H_a (δ 6.89, s) and H_b (δ , 3.66, s). Based on the ¹H NMR and NOESY Spectrum of **4b**, it is concluded that the product is (Z)-isomer.



¹H NMR of **4b**

4. HRMS of the TEMPO Adduct 3a':

