Supplementary Material

Advantages of Green Methodologies-Microwave and Solvent-free

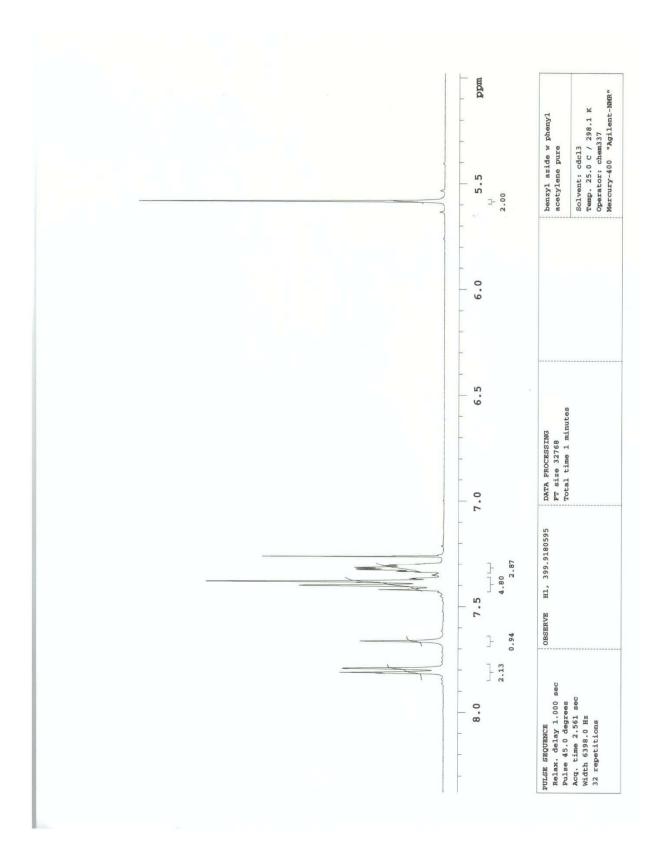
Marissa N. Trujillo, Clayton J. Hull-Crew, Andrew D. Outlaw, Kevin A. Stewart, Loren J. Taylor, Laura F. George, Allison Duensing, Breanna M. Tracey and Allen M. Schoffstall*

Department of Chemistry and Biochemistry, University of Colorado Colorado Springs (UCCS), Colorado Springs CO 80918, United States

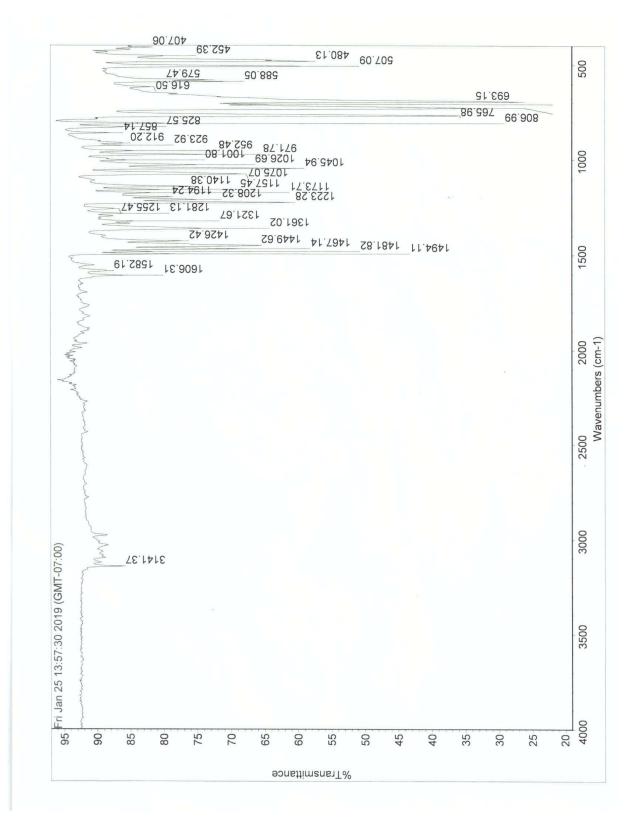
Table of Contents

Spectra of Compounds 1-8

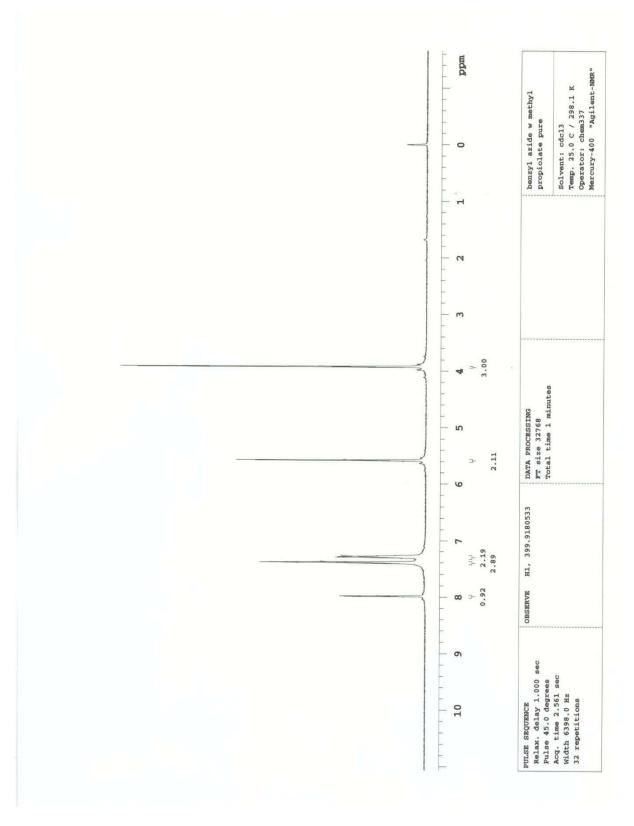
Compound 1: 1-Benzyl-4-phenyl-1 <i>H</i> -1,2,3-triazole	S2-S4
Compound 2: Methyl 1-benzyl-1H-1,2,3-triazole-4-carboxylate	S5-S7
Compound 3: 2-(1-Benzyl-1 <i>H</i> -1,2,3-triazol-4-yl)-ethanol	S8-S10
Compound 4: 1-(2-Trifluoromethylbenzyl)-4-(2-trifluoromethylphenyl)-1H-1,2,3-triazole	S11-S18
Compound 5: Phenyl-[1-(2-trifluoromethylbenzyl)-1H-1,2,3-triazol-4-yl]-methanol	S19-S24
Compound 6: 1-(3-Fluorobenzyl)-4-phenethyl-1H-1,2,3-triazole	S25-S29
Compound 7: 1-(4- Fluorobenzyl)-4-phenethyl-1H-1,2,3-triazole	S30-S34
Compound 8: 4-(3-Fluorophenyl)-1-(3-trifluoromethylbenzyl)-1H-1,2,3-triazole	S35-S39
Spectra of Crude Compounds 1-3	
Spectra from the scale up experiments	S40-S43
Spectra from equimolar experiments	S44-S45
Spectra from experiments with 50% excess alkyne	S46-S49

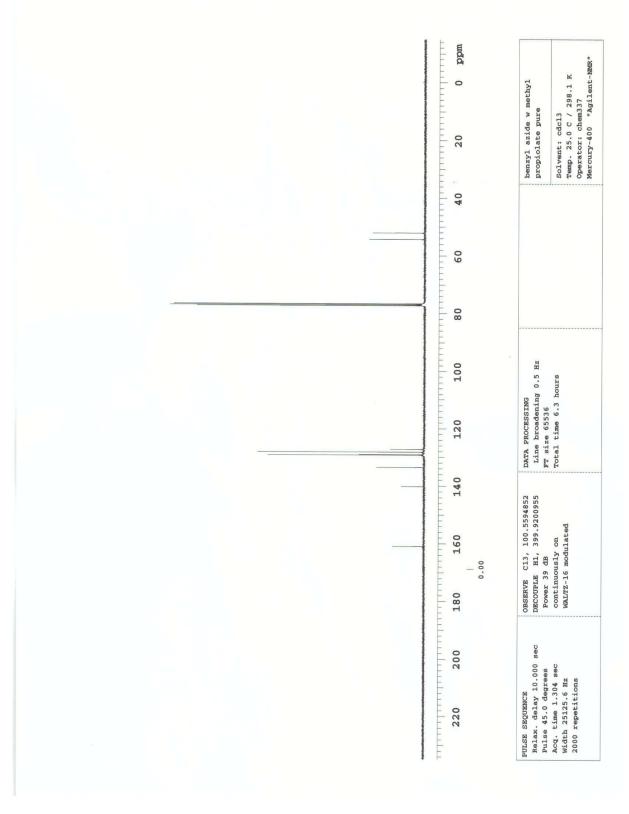


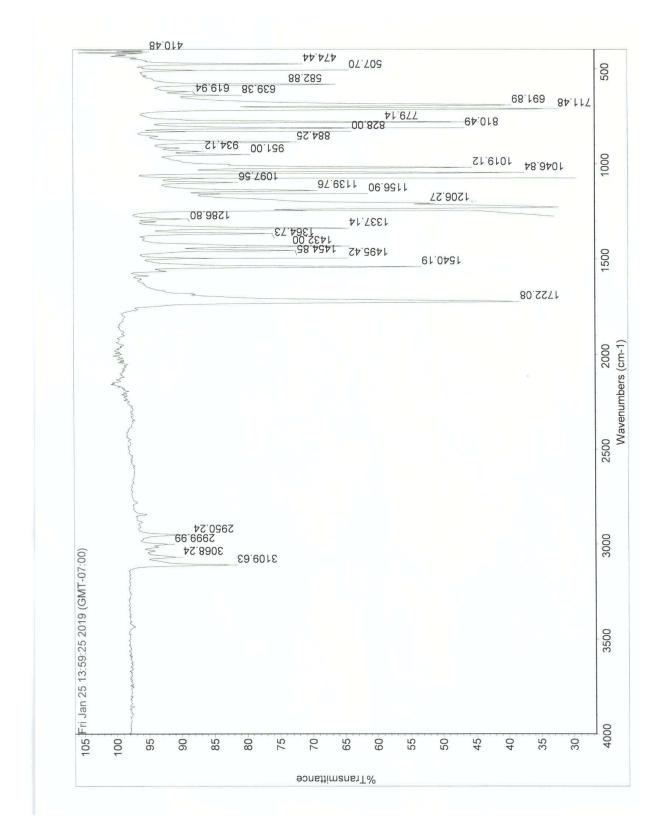
		mqq		"H
		0	r phenyl	298.1 K 1337 Agilent-M
		20	benzyl azide w phenyl acetylene pure	Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem337 Mercurv-400 "Adilent-NWR"
		 40		
		60		
 		80		
		2	G 0.5 Hz	hours
			DATA PROCESSING Line broadening 0.5 Hz	Total time 6.3 hours
	-	140		4 년
		180 160 0.00	OBSERVE C13, 100.5594852 DECOUPLE H1, 399.9200955	warrz-16 modulated
		200		
		220	PULSE SEQUENCE Relax. delay 10.000 sec Pulse 45.0 derres	Acq. time 1.304 sec Width 25125.6 Hz 2000 repetitions



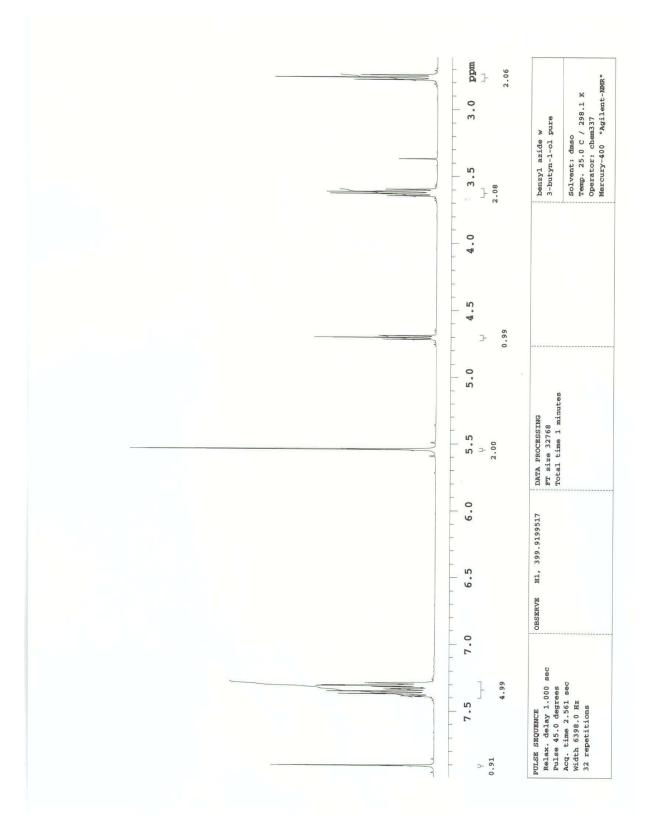
FTIR spectrum of **1**

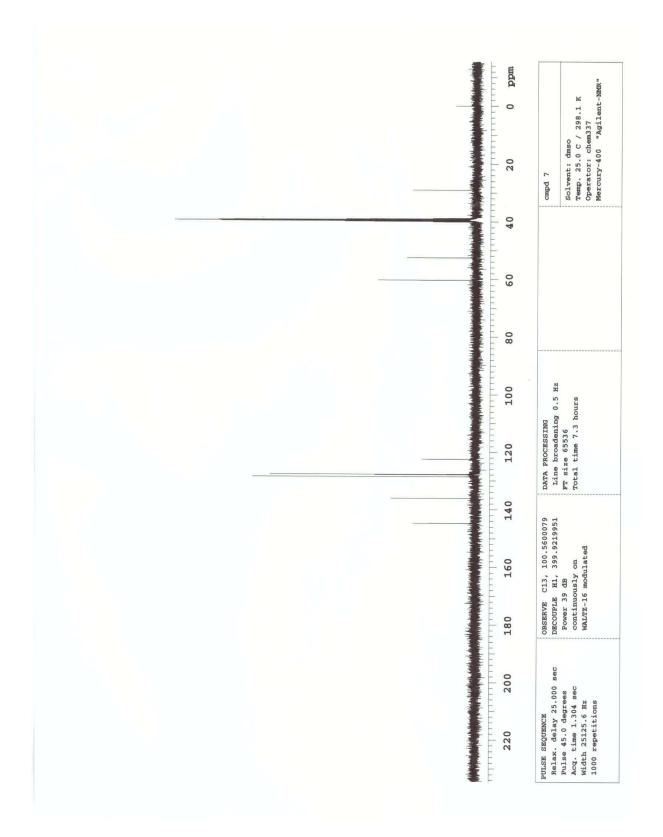


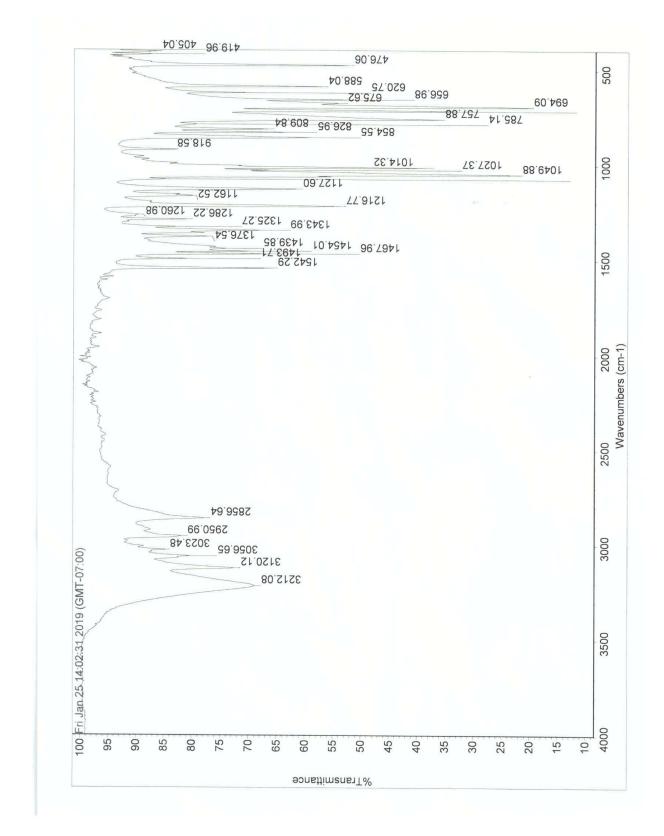


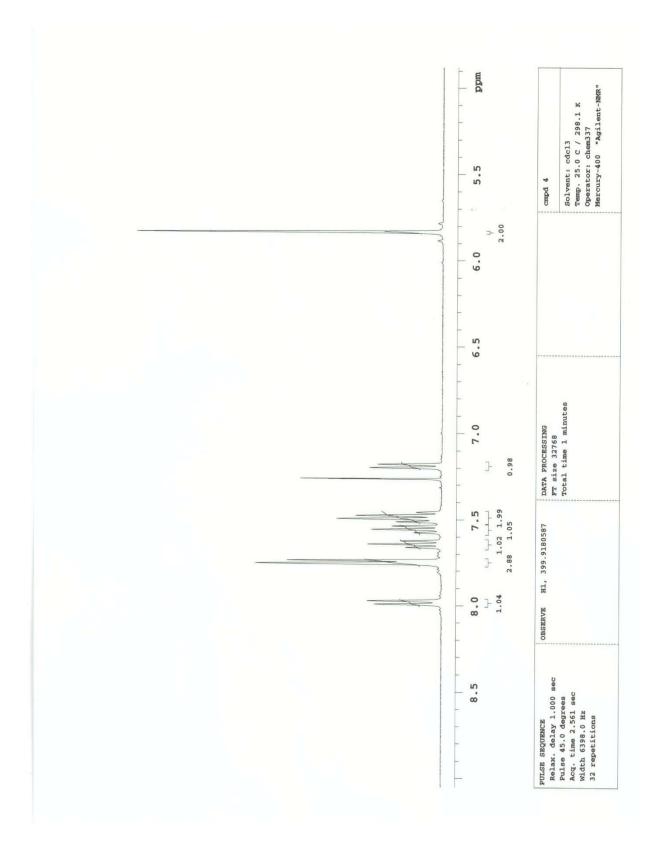


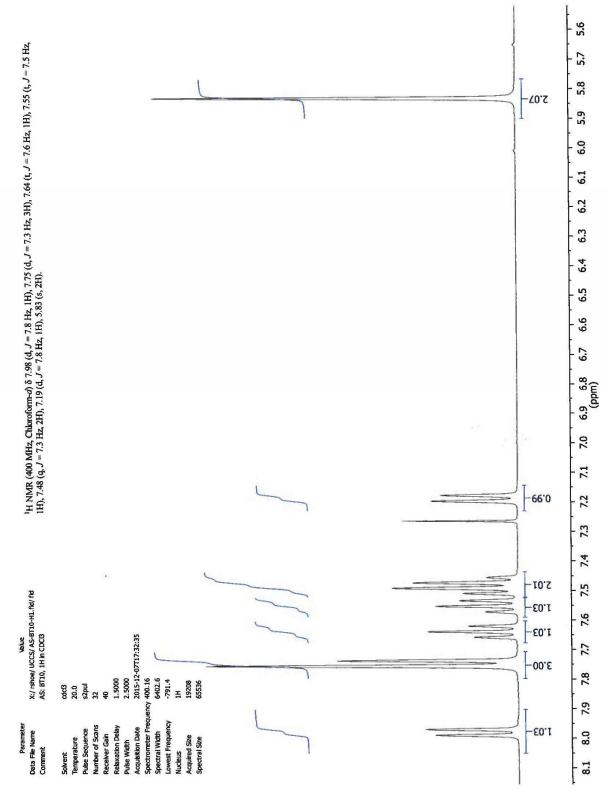
FTIR spectrum of **2**



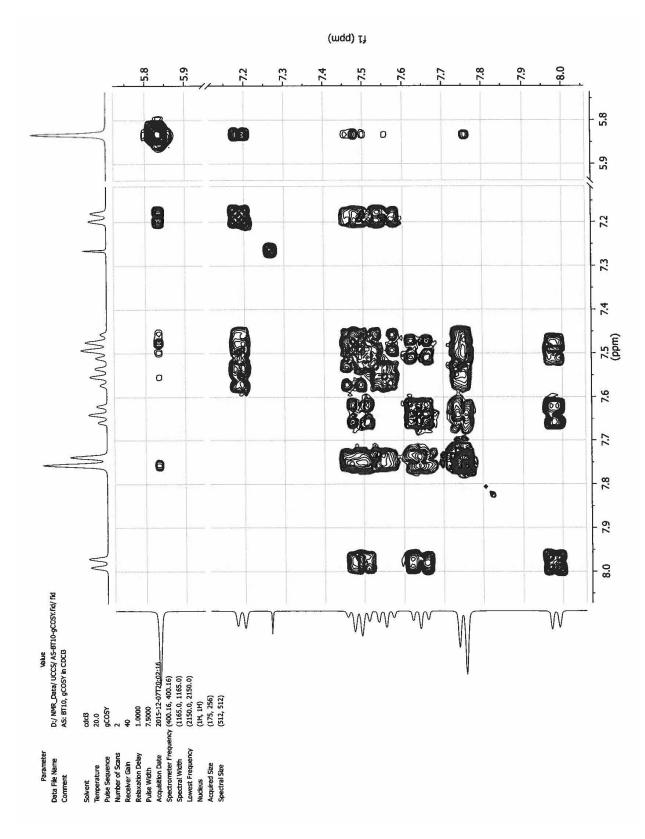




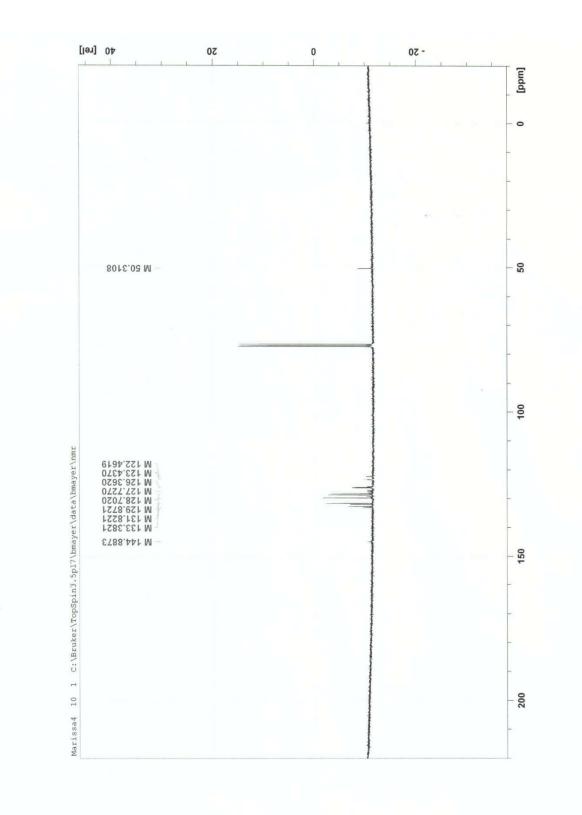


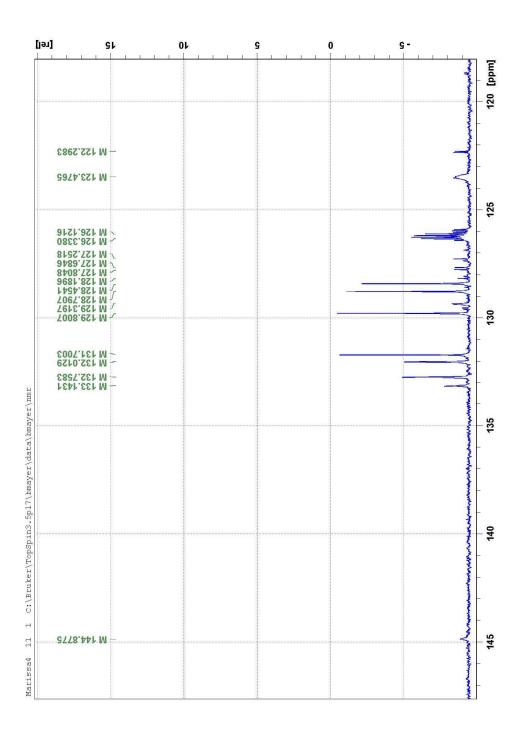


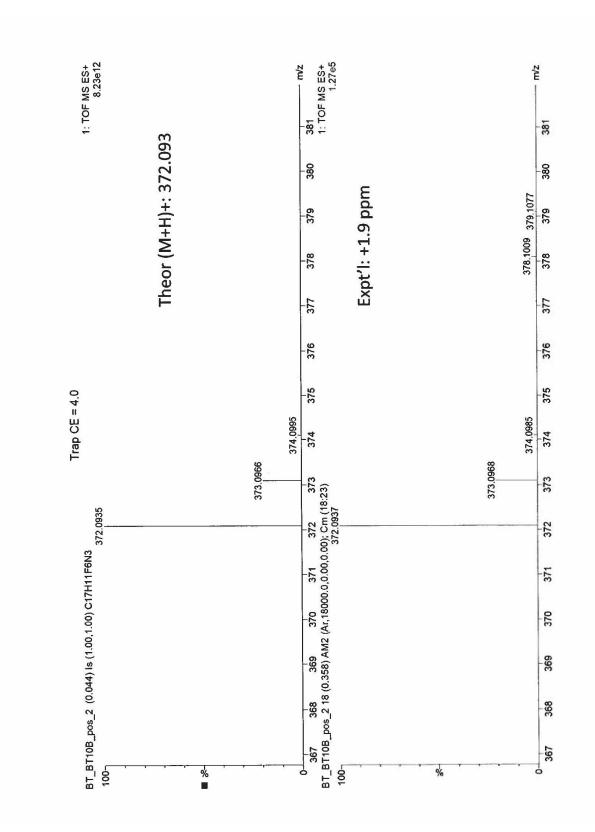
¹H NMR spectrum (expanded) of 4



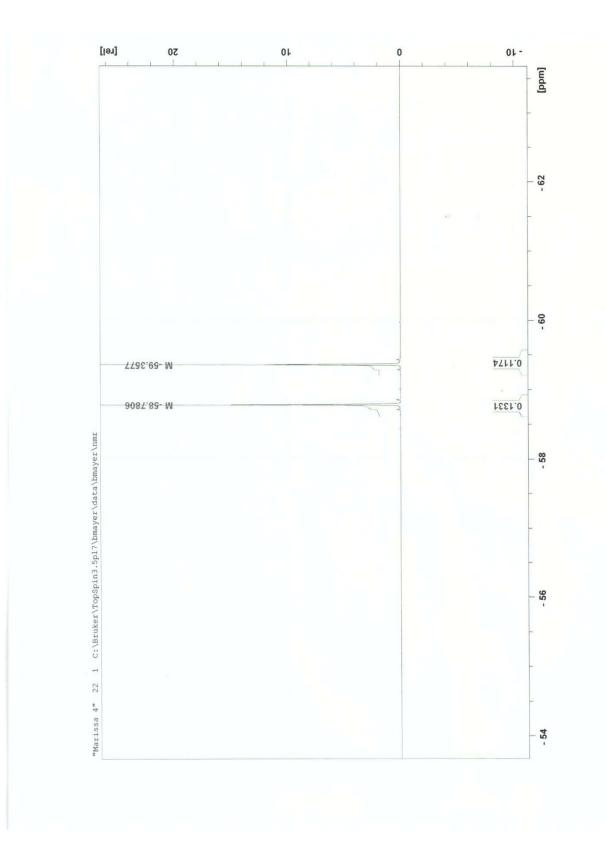
COSY spectrum of 4

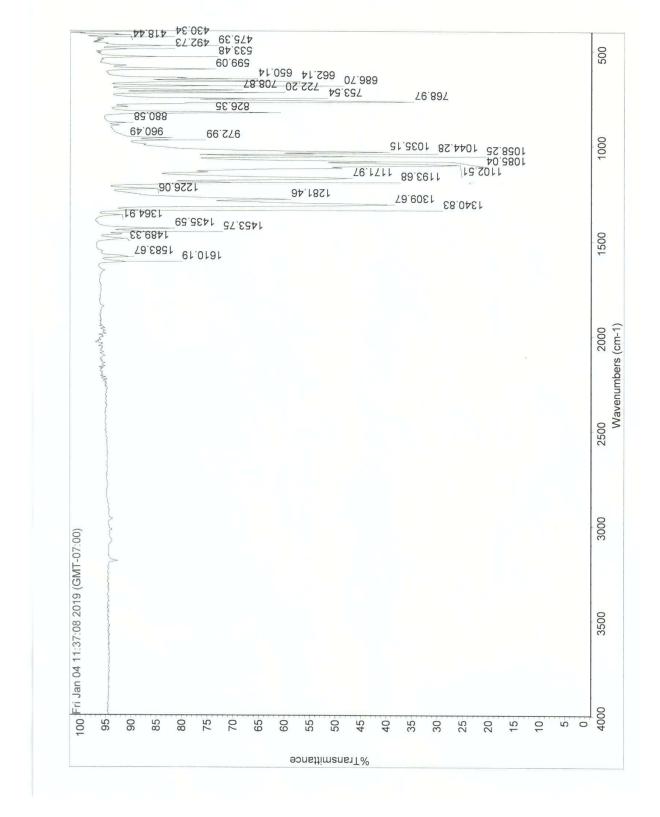


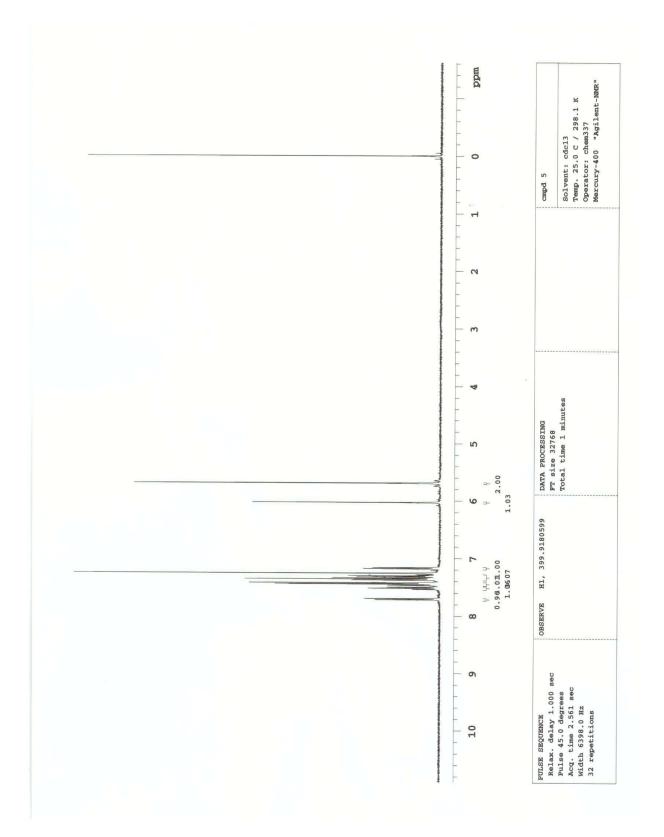


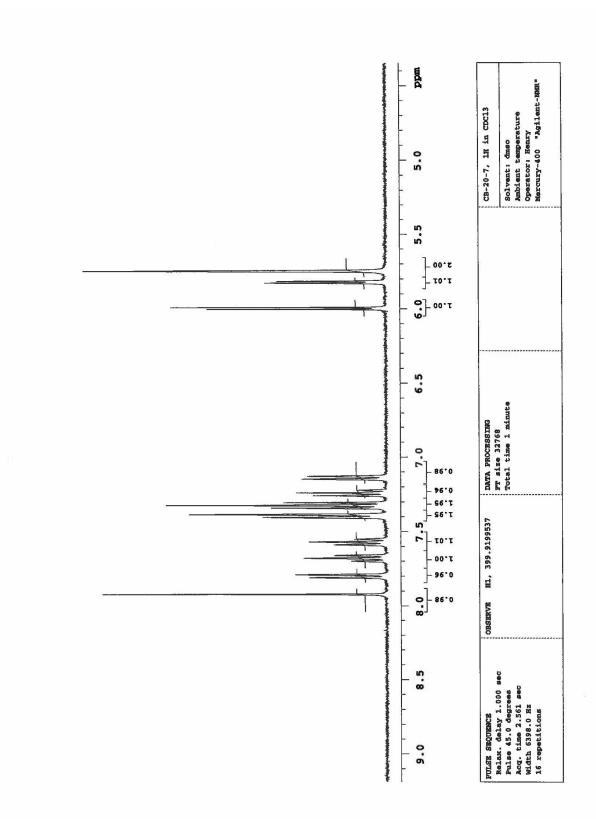


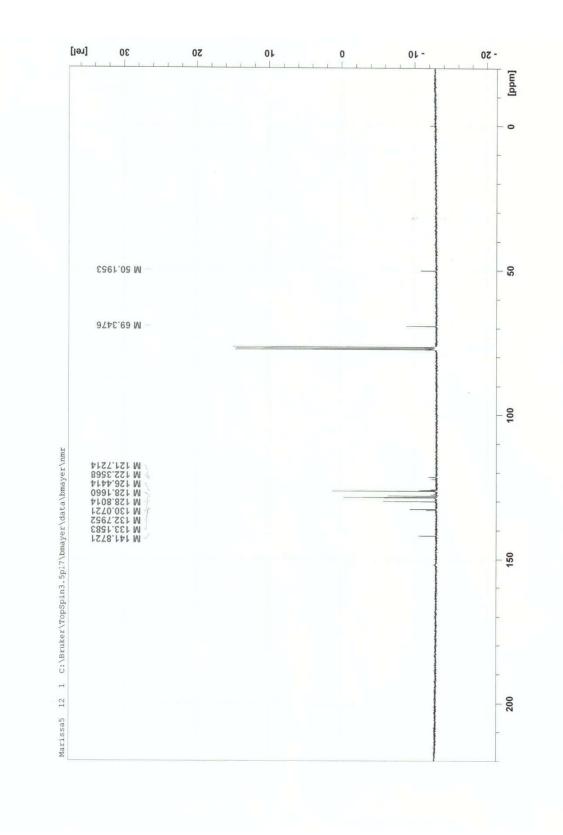
M + H⁺ HRMS data of 4

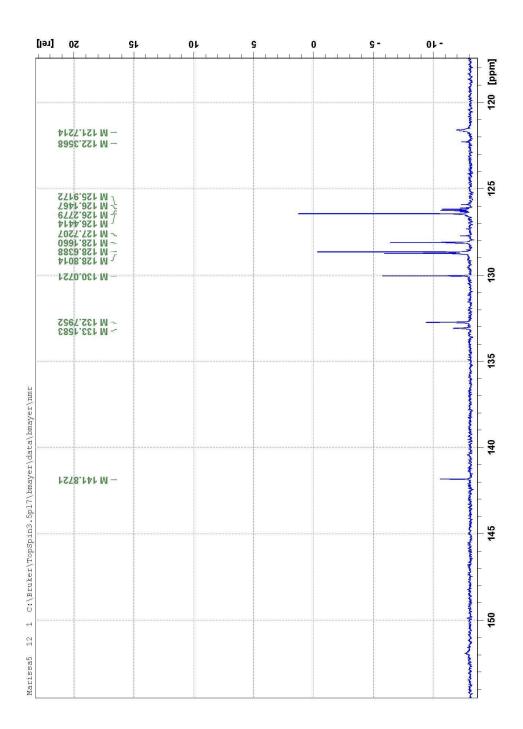


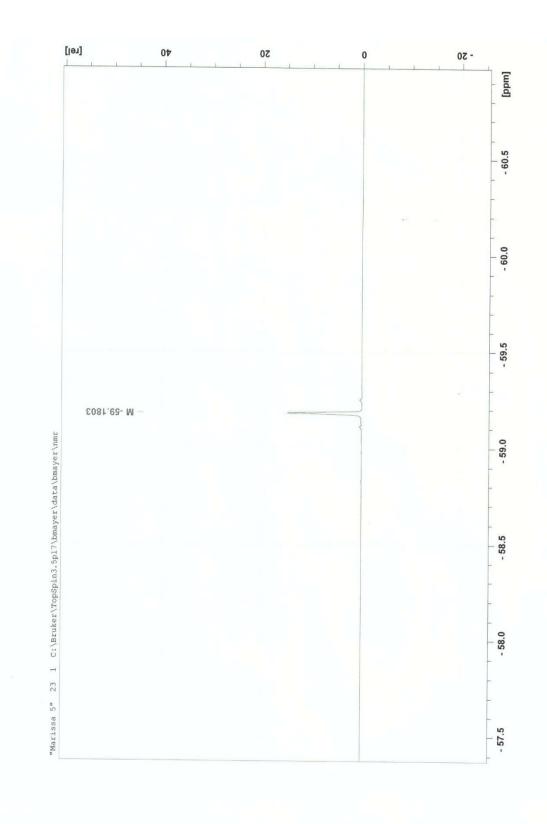


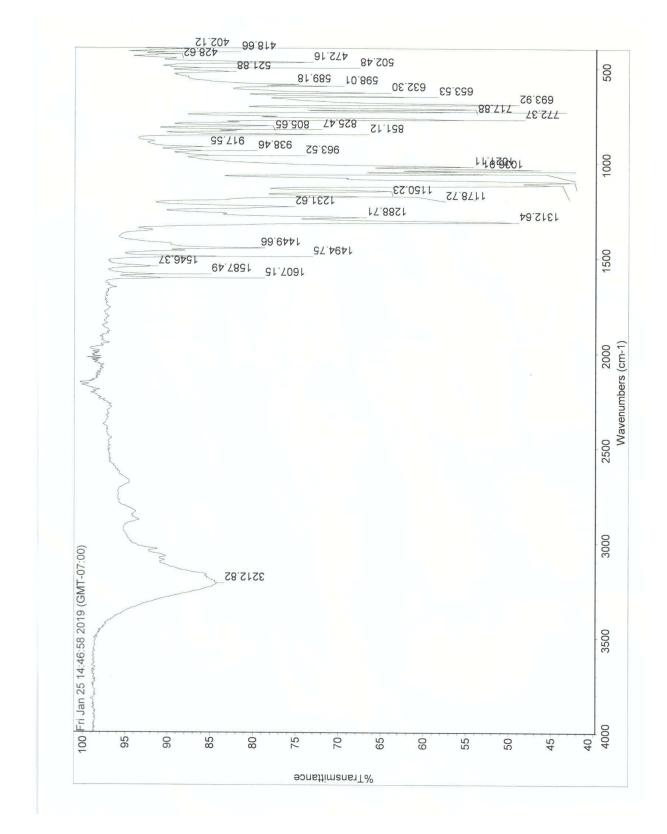




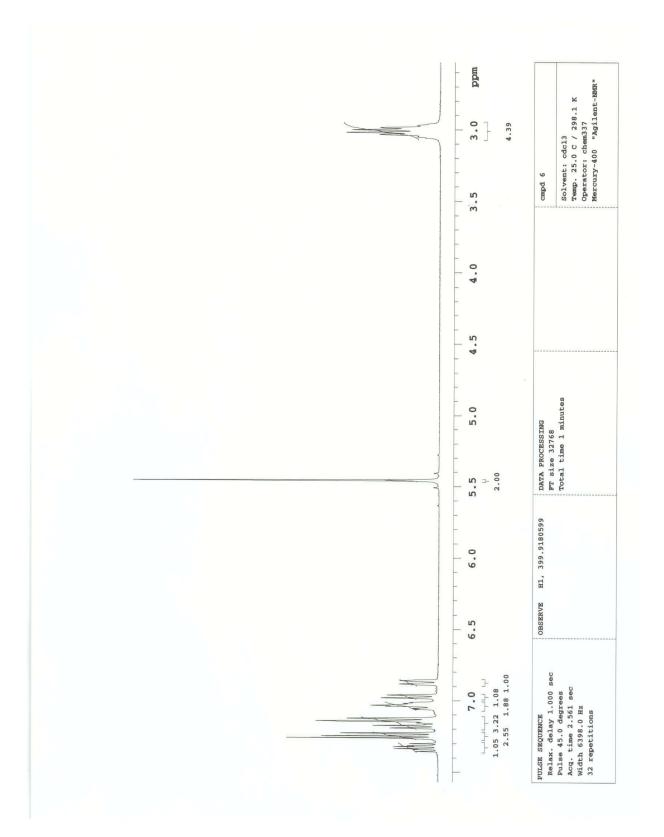


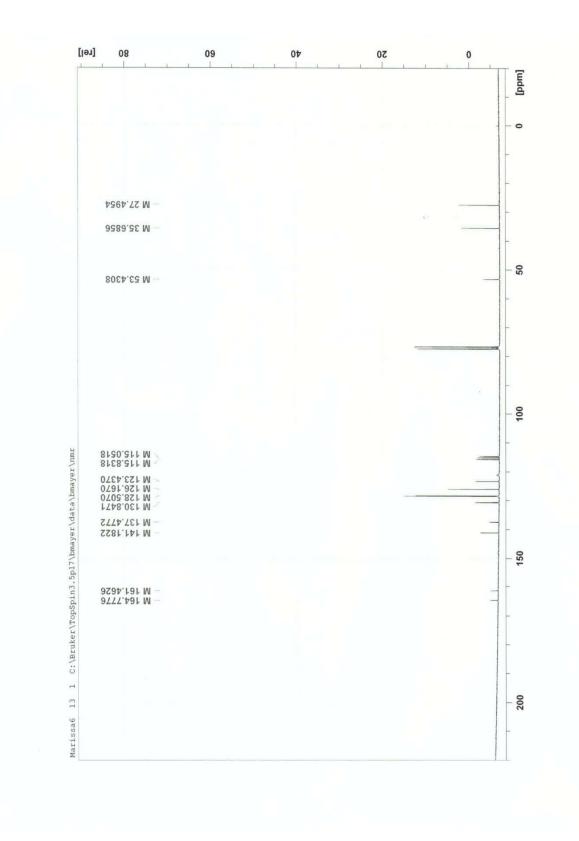


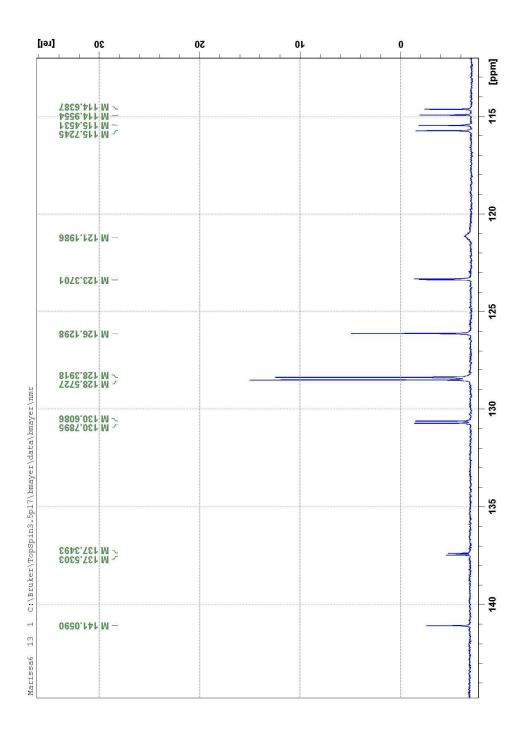


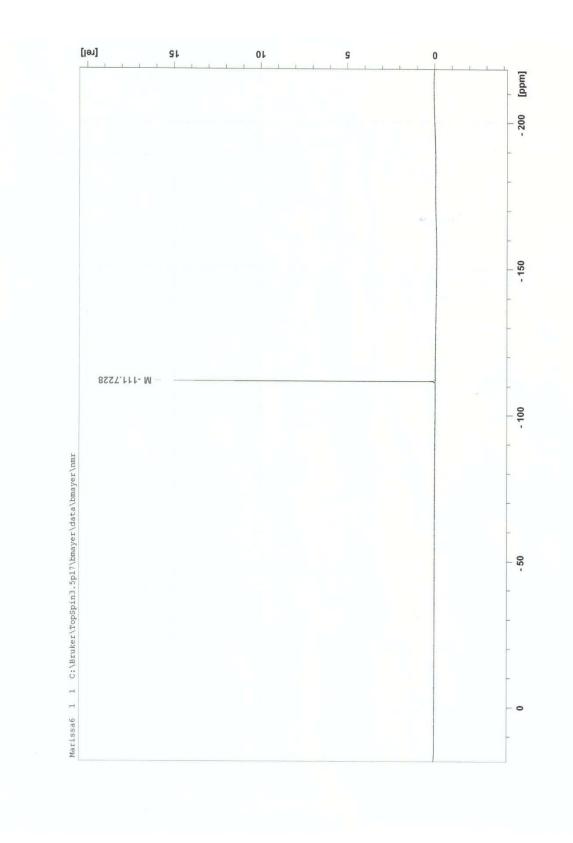


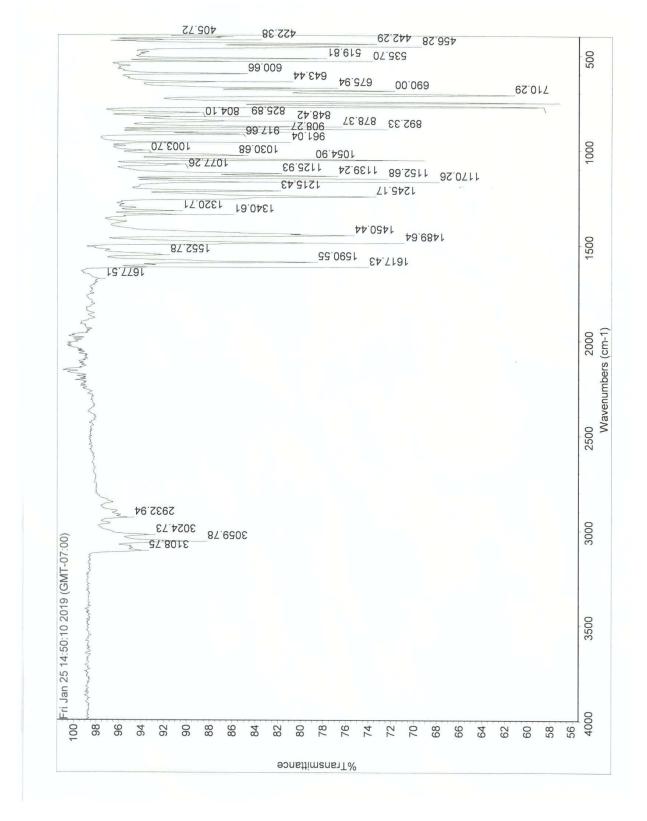
FTIR spectrum of 5



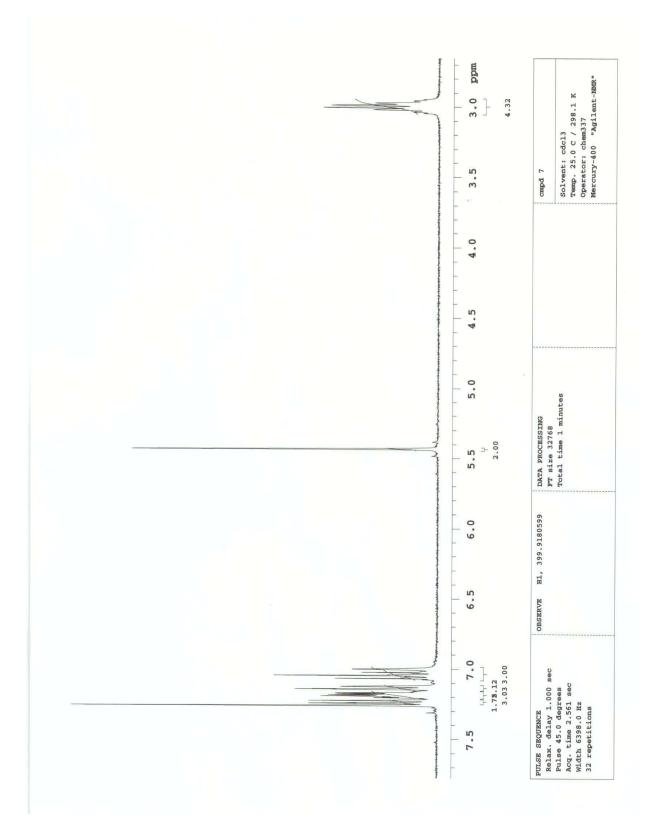


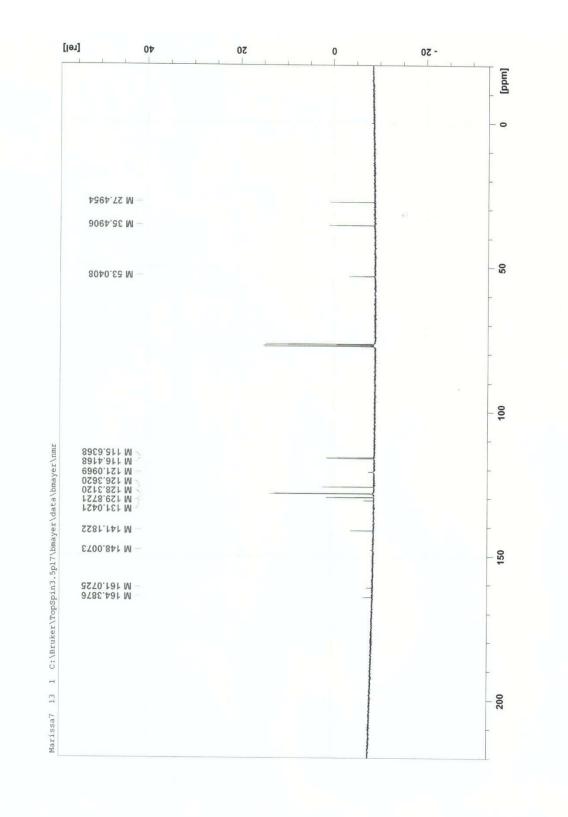


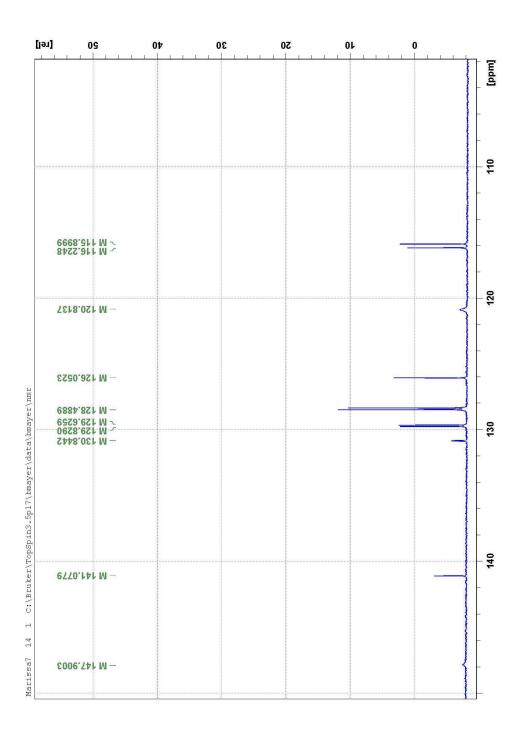


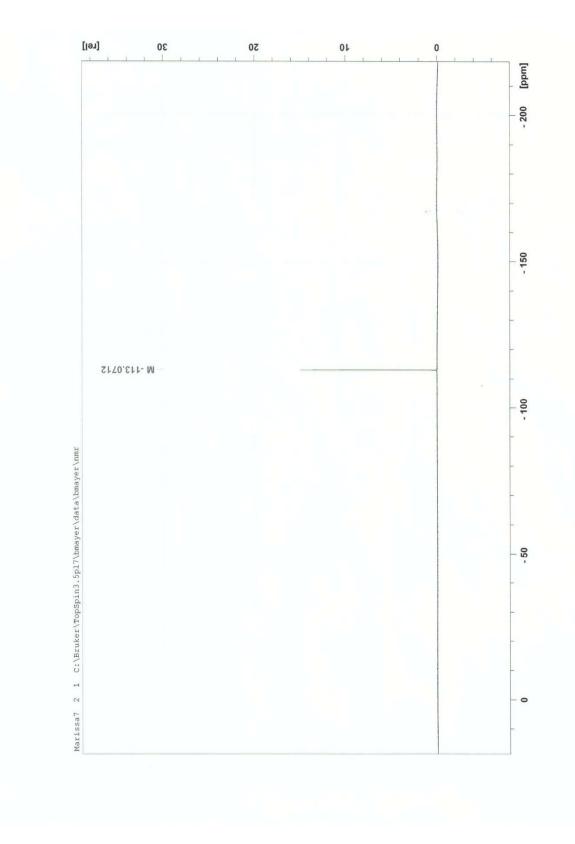


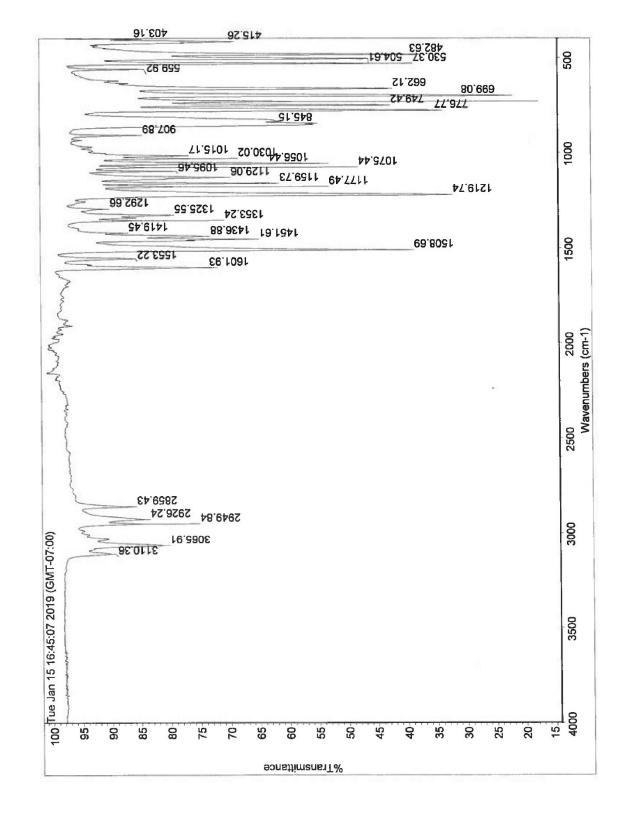
FTIR spectrum of 6



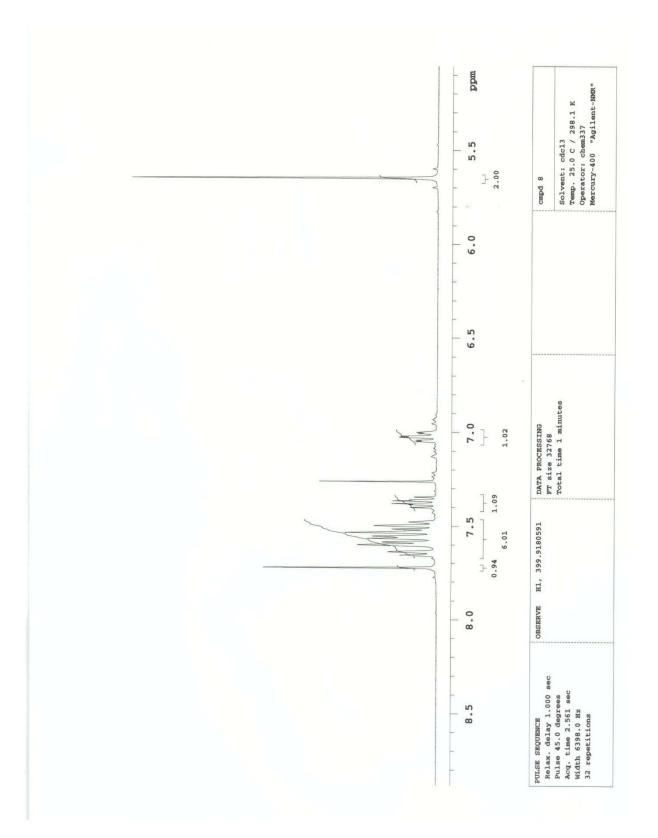


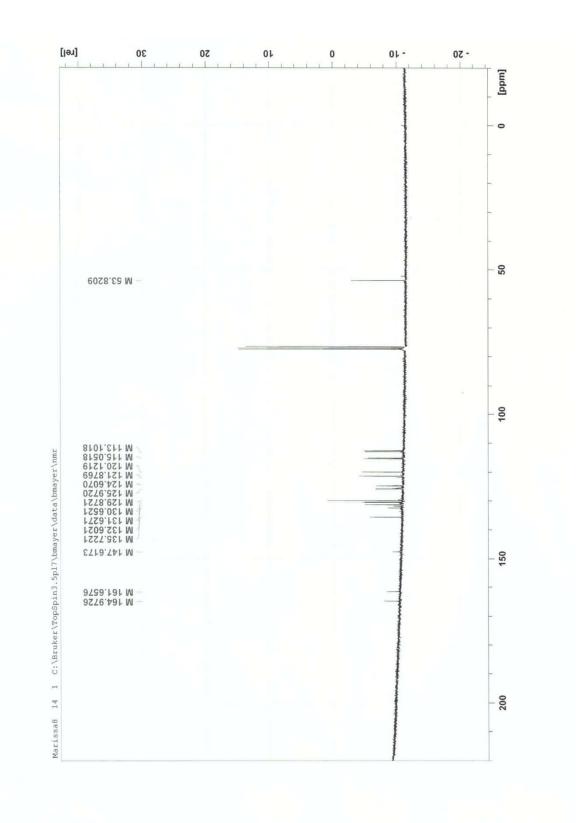


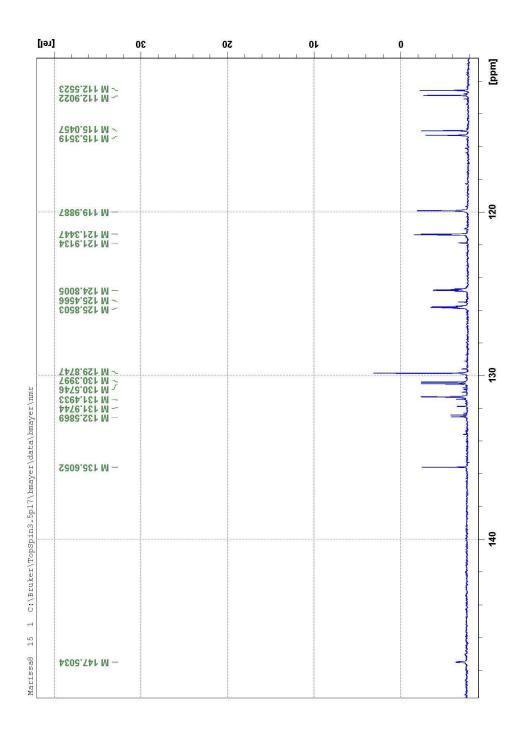


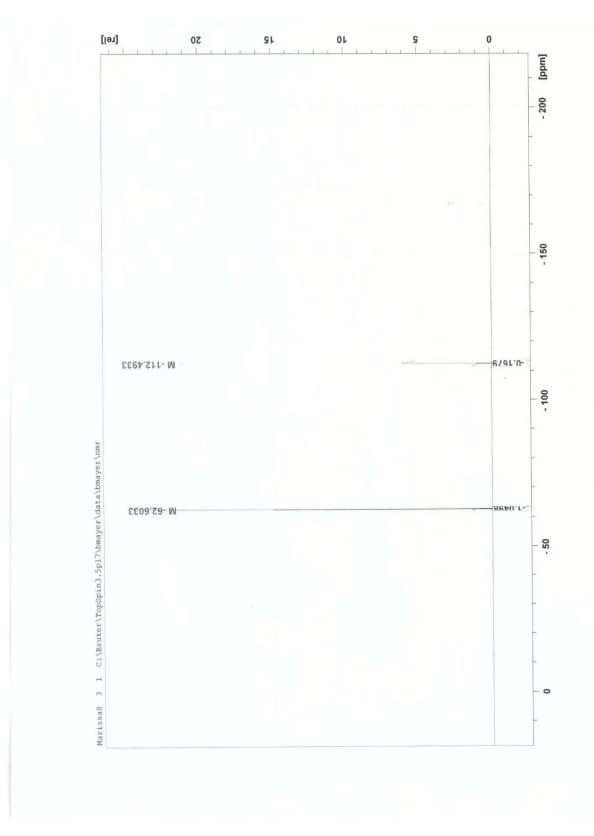


FTIR spectrum of 7

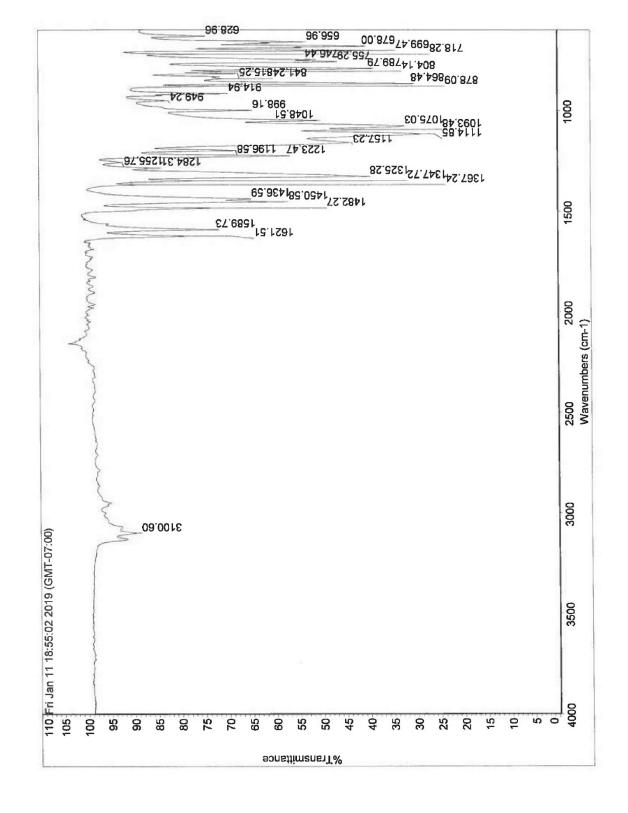


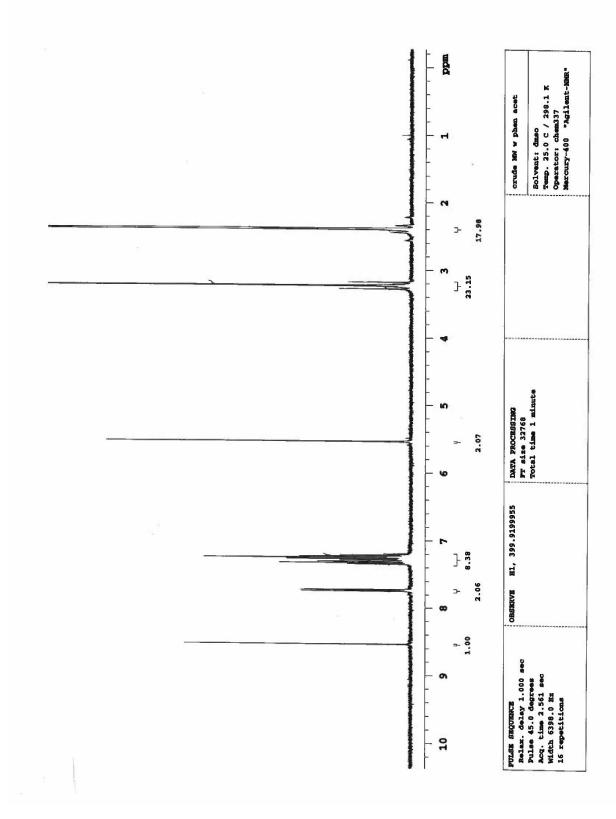




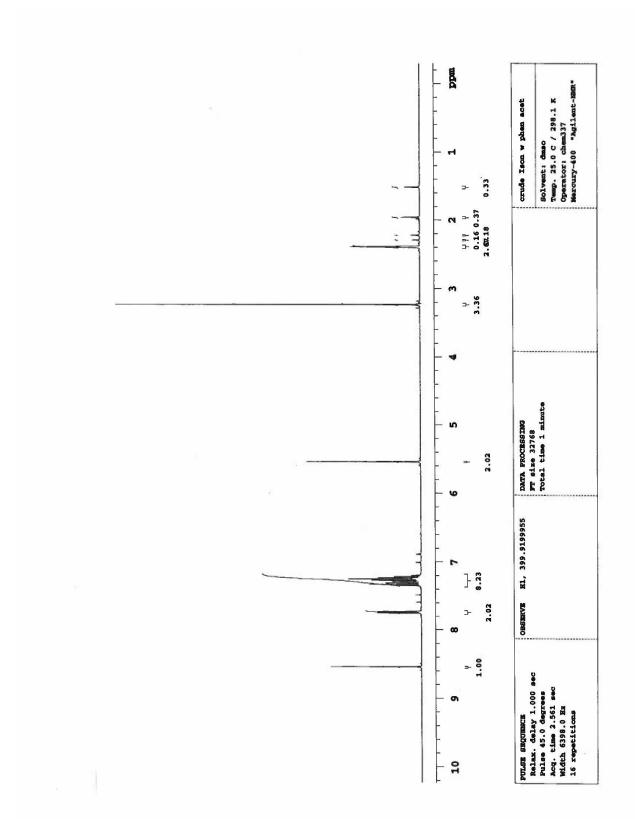


¹⁹F NMR spectrum of 8

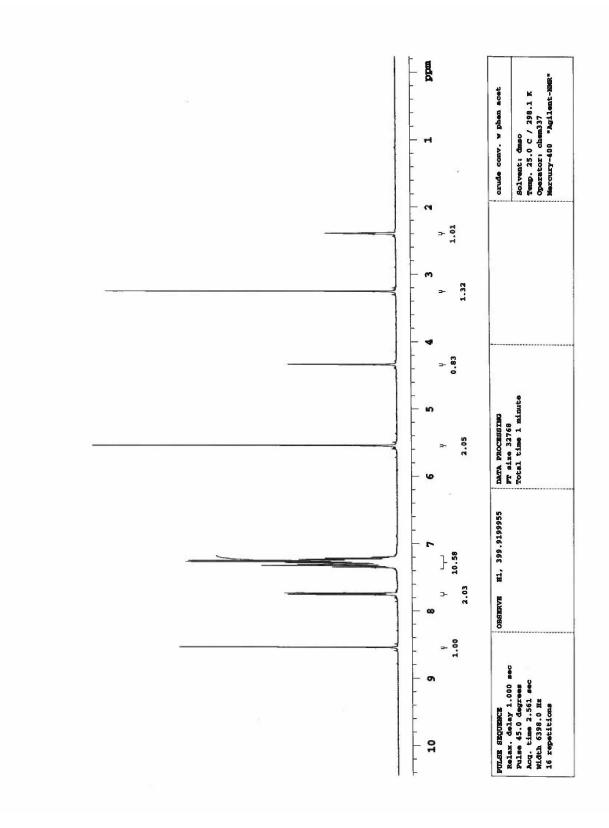




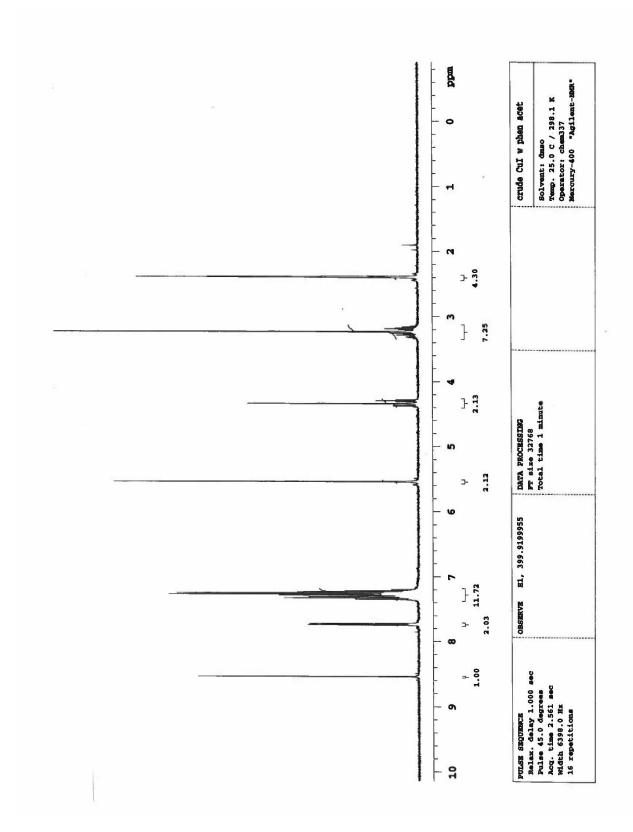
Microwave scale up of **1**.



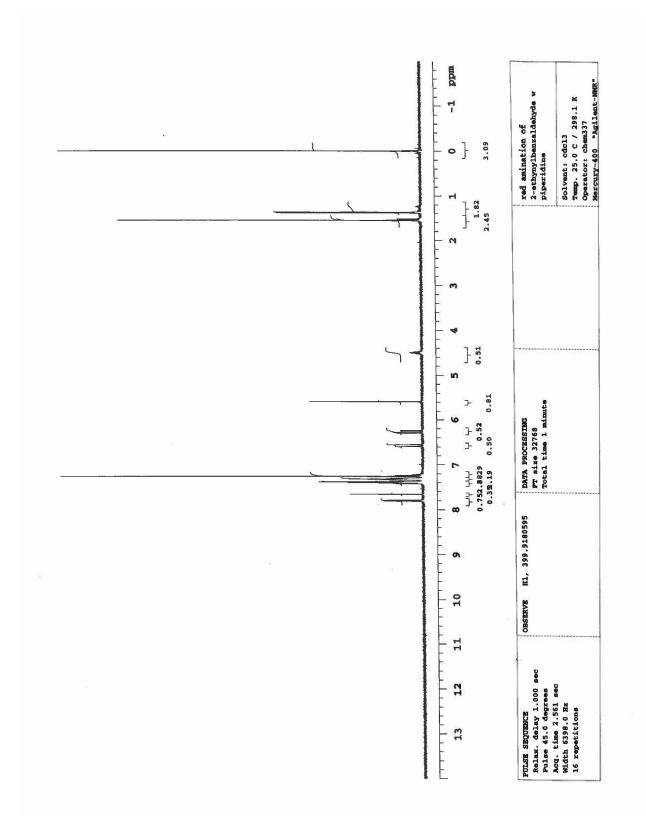
Solvent -free scale up of **1**.



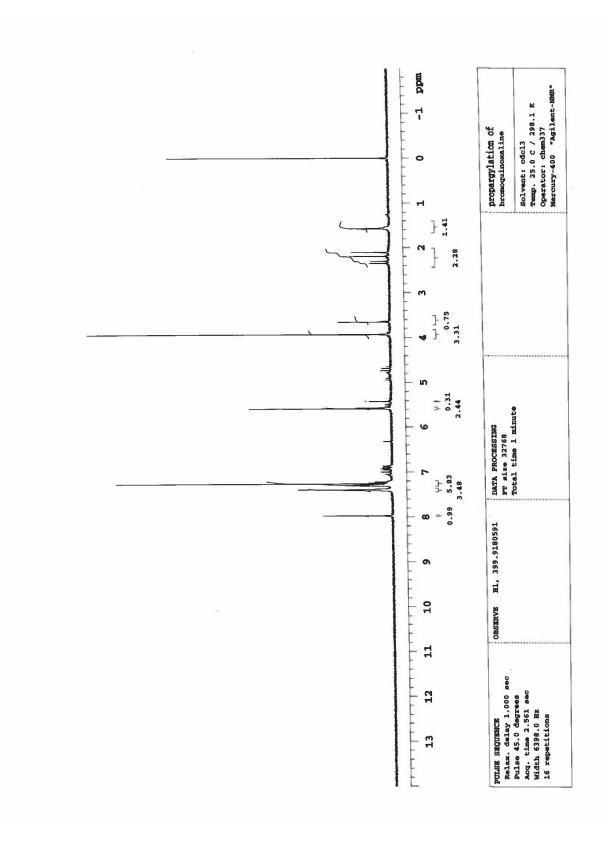
Conventional scale up of **1**.



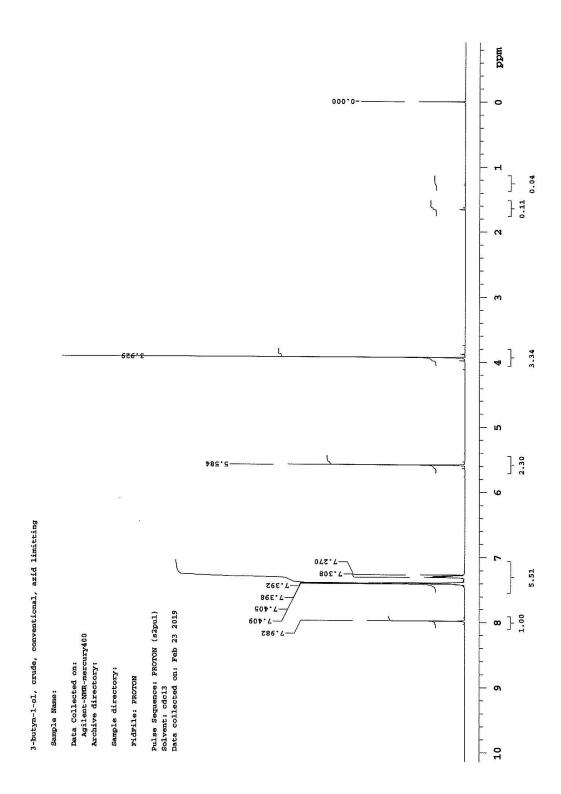
CuI in glycerol scale up of **1**.



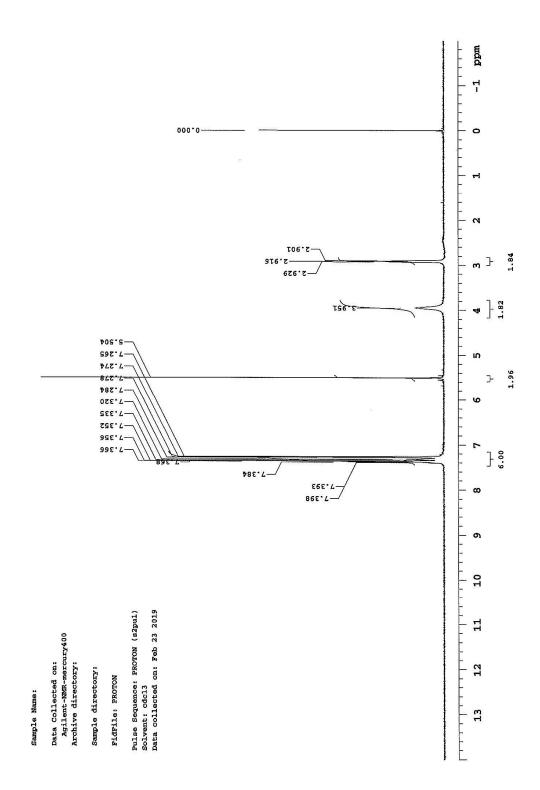
Solvent-free product 1 from equimolar reactants.



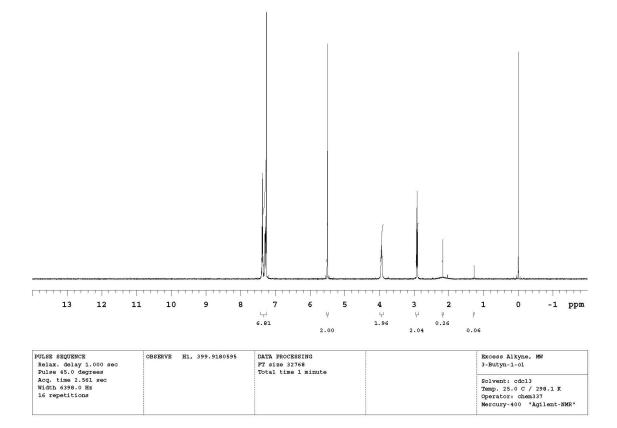
Solvent-free product 2 from equimolar reactants.

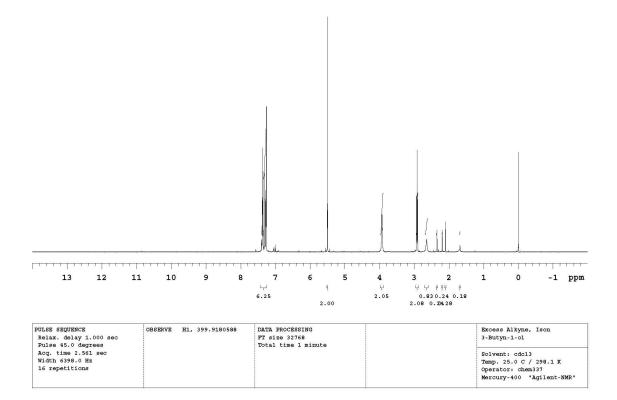


Conventional product 2 from 50% excess of methyl propiolate.



Conventional product 3 from 50% excess of 3-butyn-1-ol.





Solvent-free product **3** from 50% excess of 3-butyn-1-ol.