Supporting Information

$FeCl_3$-Catalyzed Oxidative Decarboxylation of Aryl/Heteroaryl Acetic Acids: Preparation of Selected API Impurities

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1. Crystal data information of compound 2

Bond precision		C-C = 0.0017 A	Wavelength=0.71073
Cell	a=10.1140(5)	b=10.3178(5)	c=10.5034(5)
Temperature:		105 K	

	Calculated	Reported
Volume	1071.76(9)	071.76(9)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	$C_{14}H_{11}NO_2$	$C_{14}H_{11}NO_2$
Sum formula	$C_{14}H_{11}NO_2$	$C_{14}H_{11}NO_2$
Mr	225.24	225.24
Dx,g cm^{-3}	1.396	1.396
Z	4	4
Mu (mm^{-1})	0.094	0.094
F000	472.0	472.0
F000’	472.22	
h,k,lmax	12,12,12	12,12,12
Nref	1891	1891
Tmin,Tmax	0.962,0.972	0.962,0.972
Tmin’	0.960	

Correction method = # Reported T Limits: T_{min} = 0.962 T_{max} = 0.972

AbsCorr = MULTI-SCAN

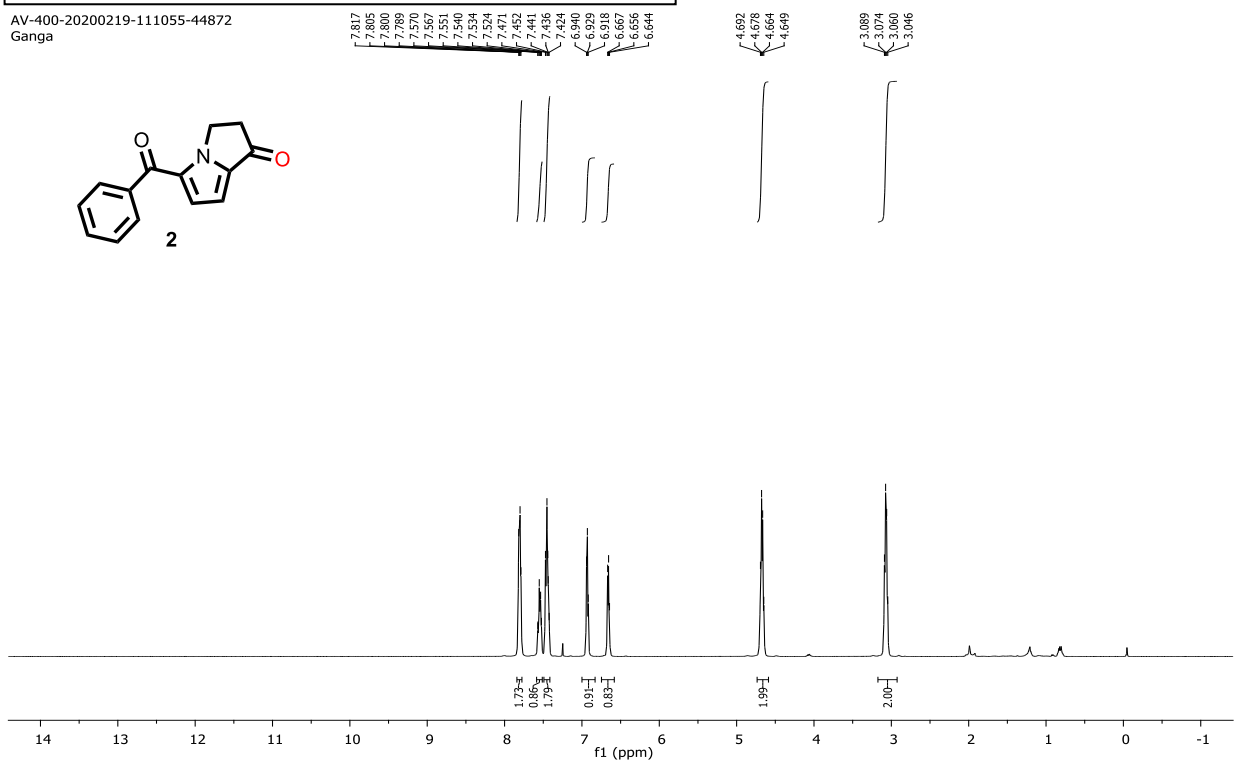
Data completeness = 1.000 Theta(max) = 24.990

R(reflections) = 0.0309(1781) wR_2 (reflections) = 0.0765(1891)

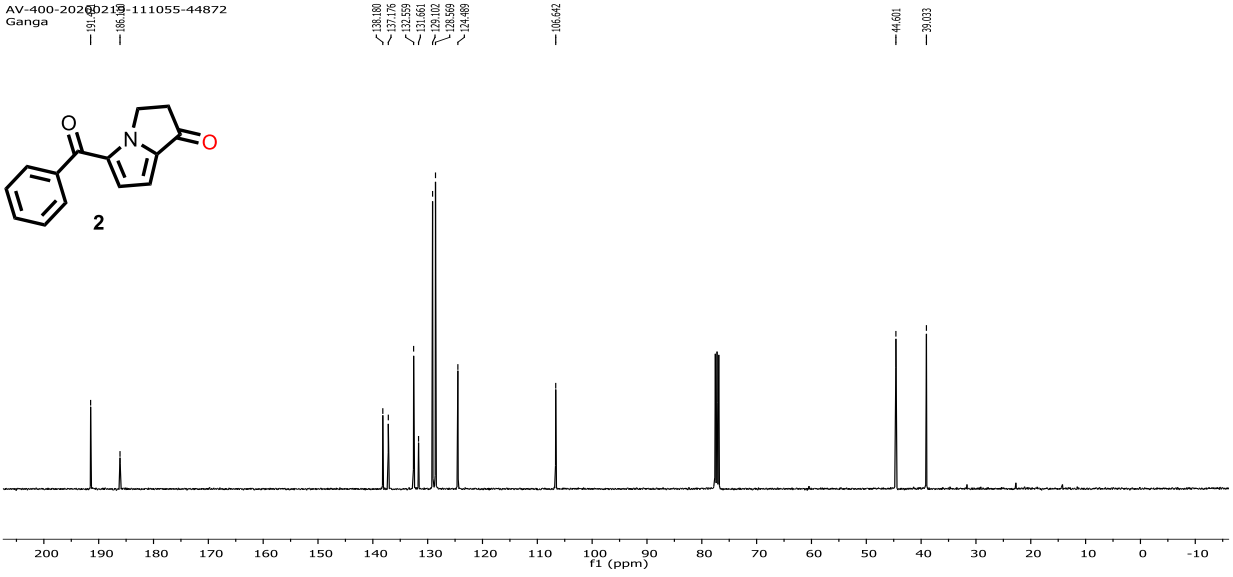
S = 1.013 Npar = 155

2. Copies of ^{1}H and ^{13}C spectrum of compounds 2-27

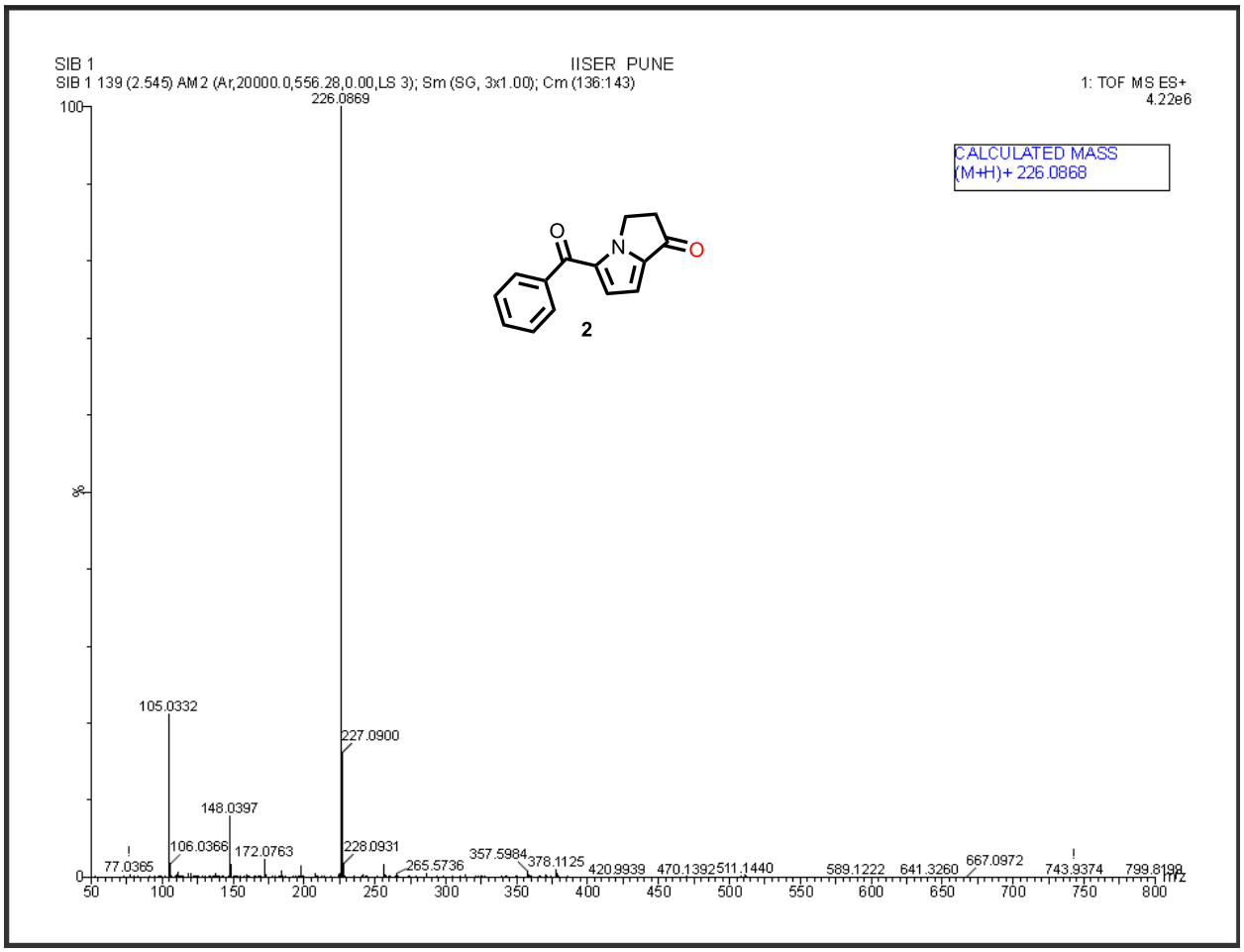
^{1}H NMR spectrum of compound **2** ($CDCl_3$, 400 MHz)



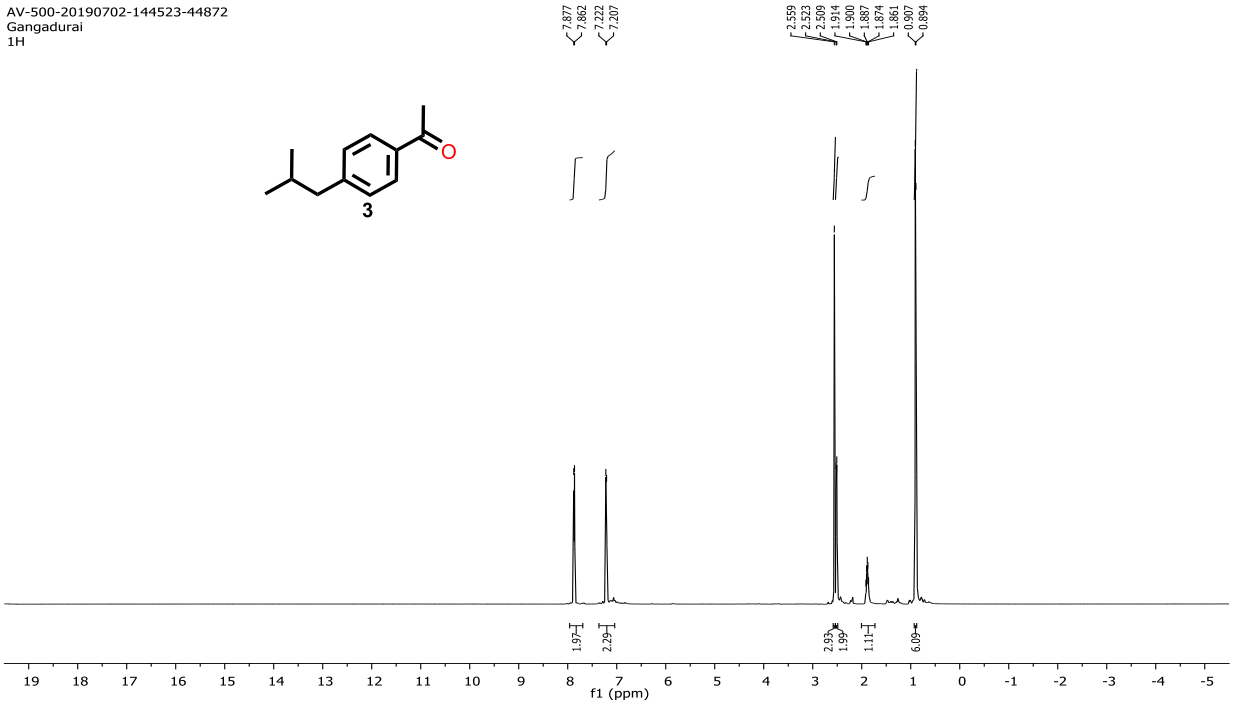
^{13}C NMR spectrum of compound **2** ($CDCl_3$, 100 MHz)



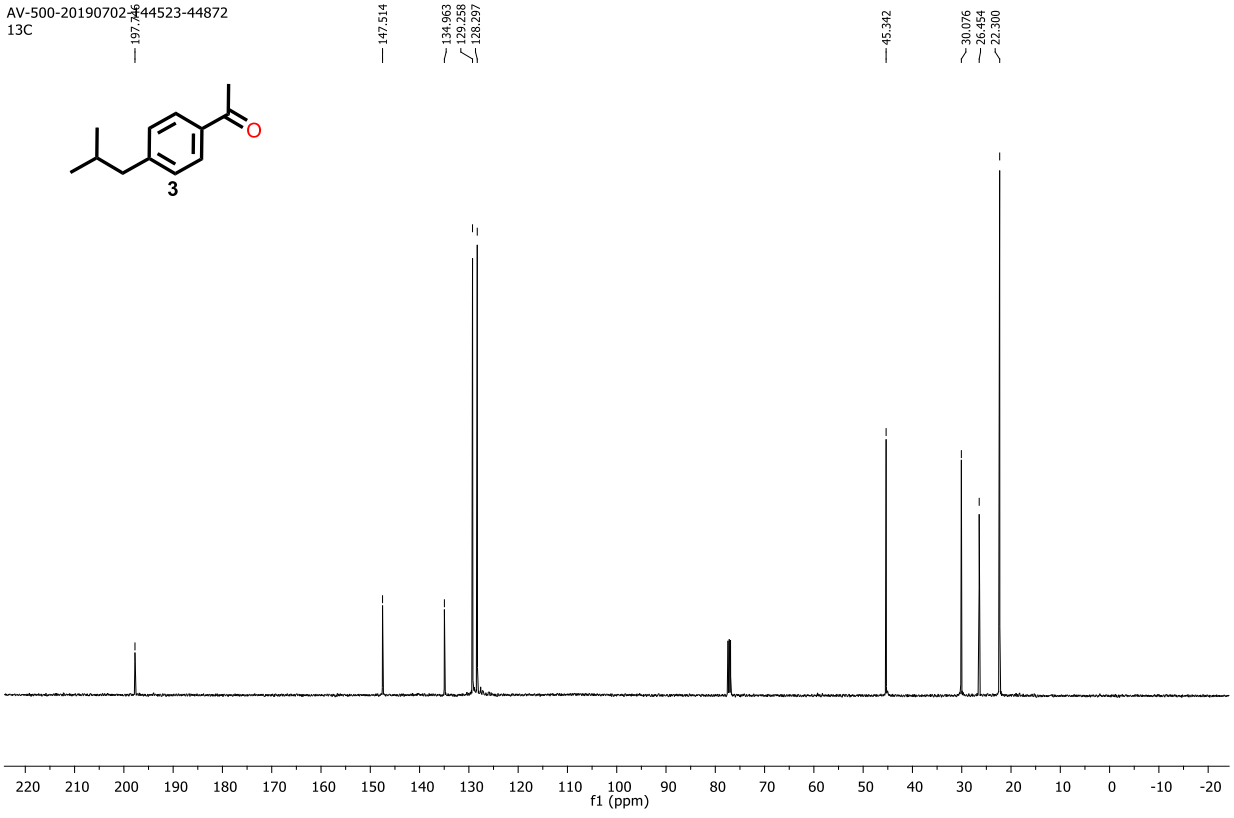
HRMS spectrum of compound **2**



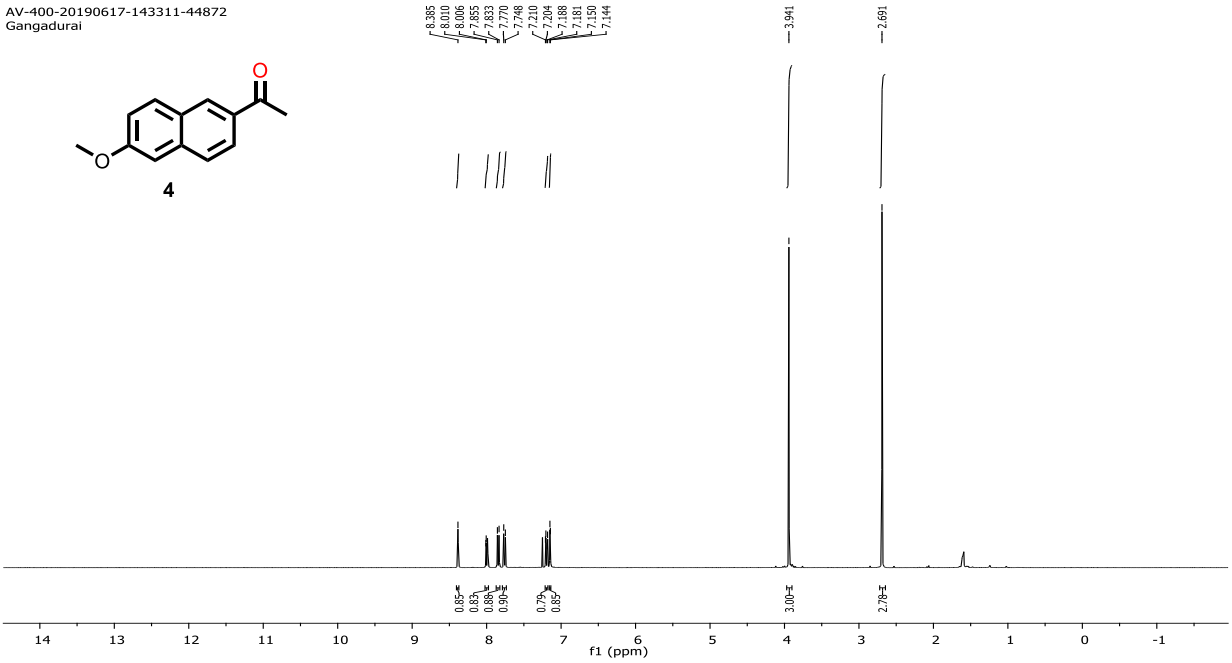
^{1}H NMR spectrum of compound **3** ($CDCl_3$, 500 MHz)



^{13}C NMR spectrum of compound **3** ($CDCl_3$, 125 MHz)

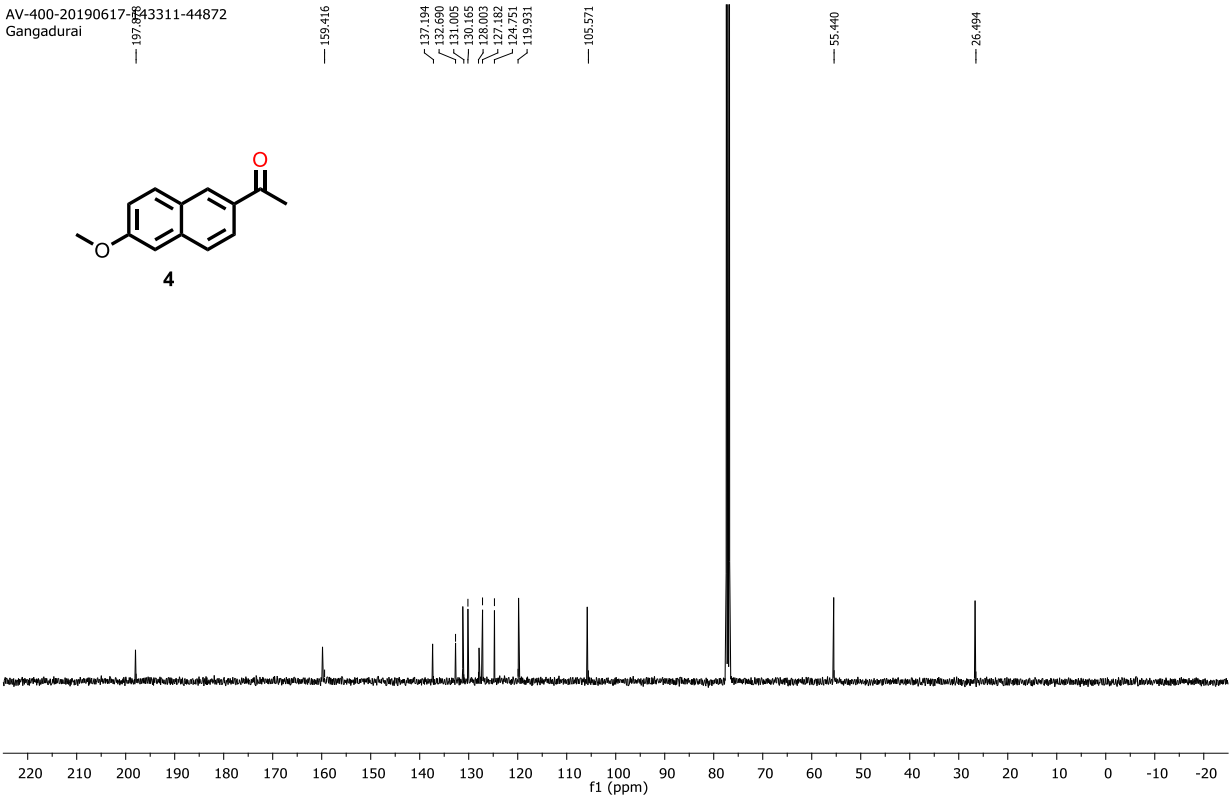


^{1}HNMR spectrum of compound **4** ($CDCl_3$, 400 MHz)



4

^{13}C NMR spectrum of compound **4** ($CDCl_3$, 100 MHz)



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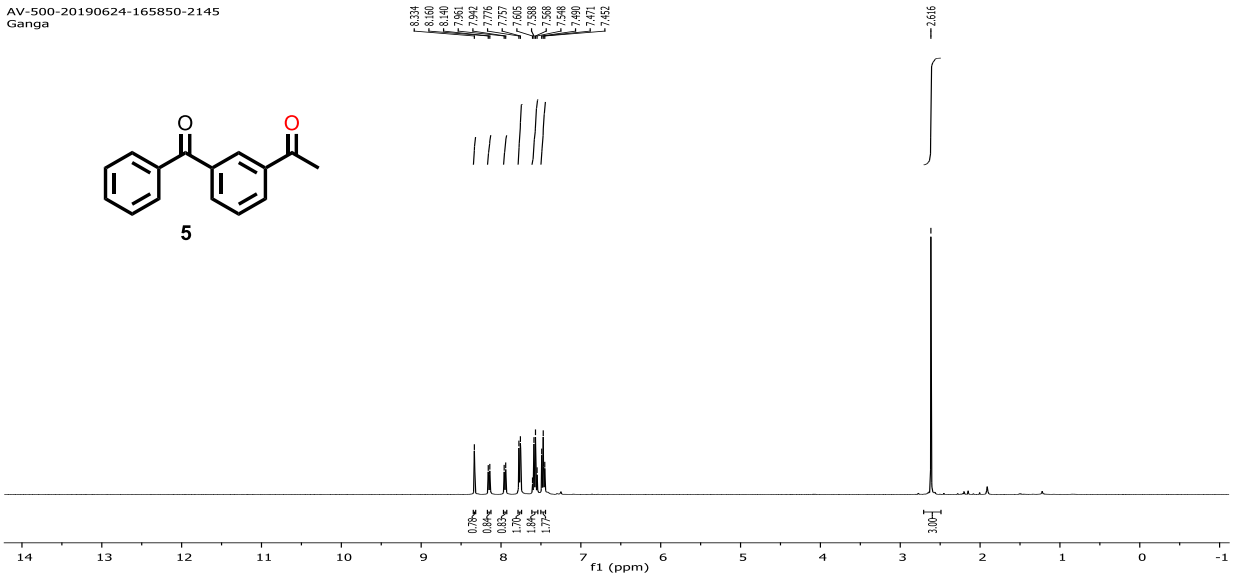
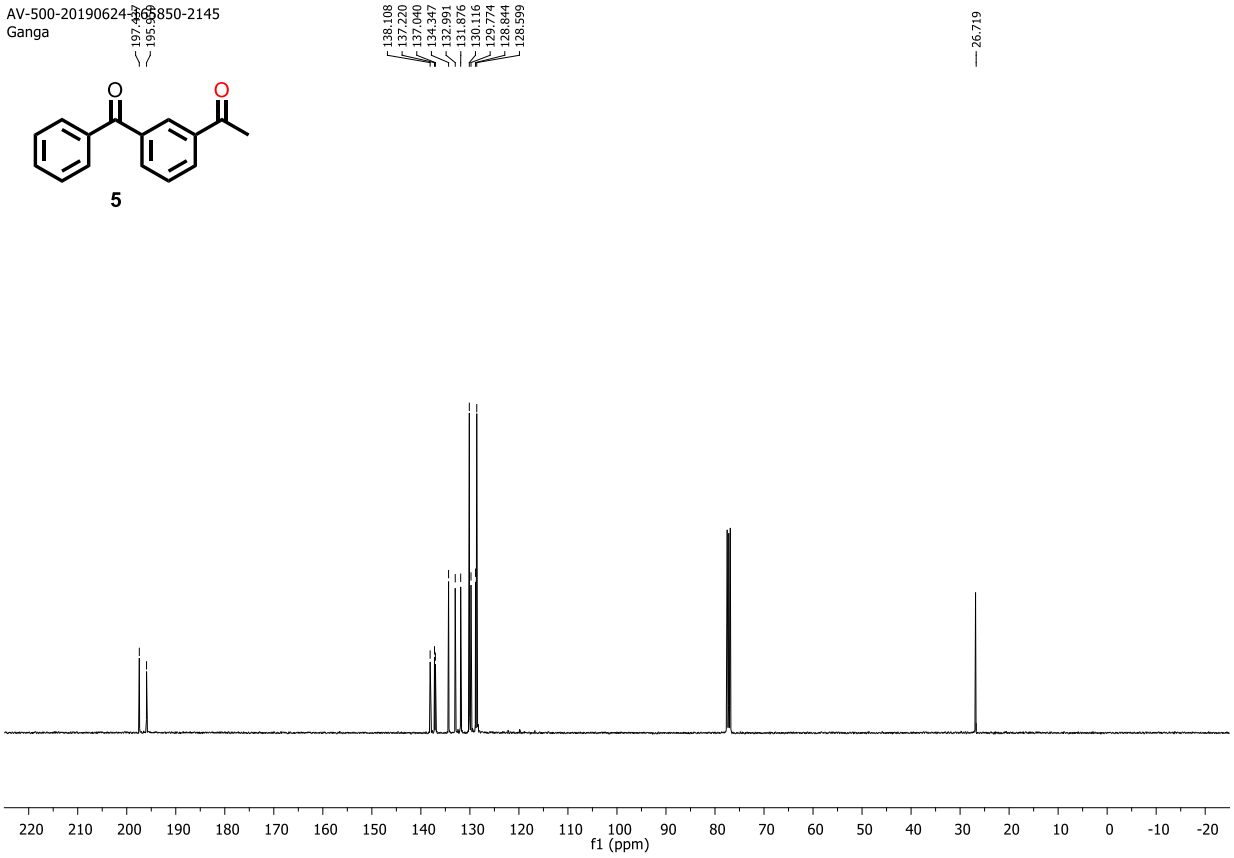
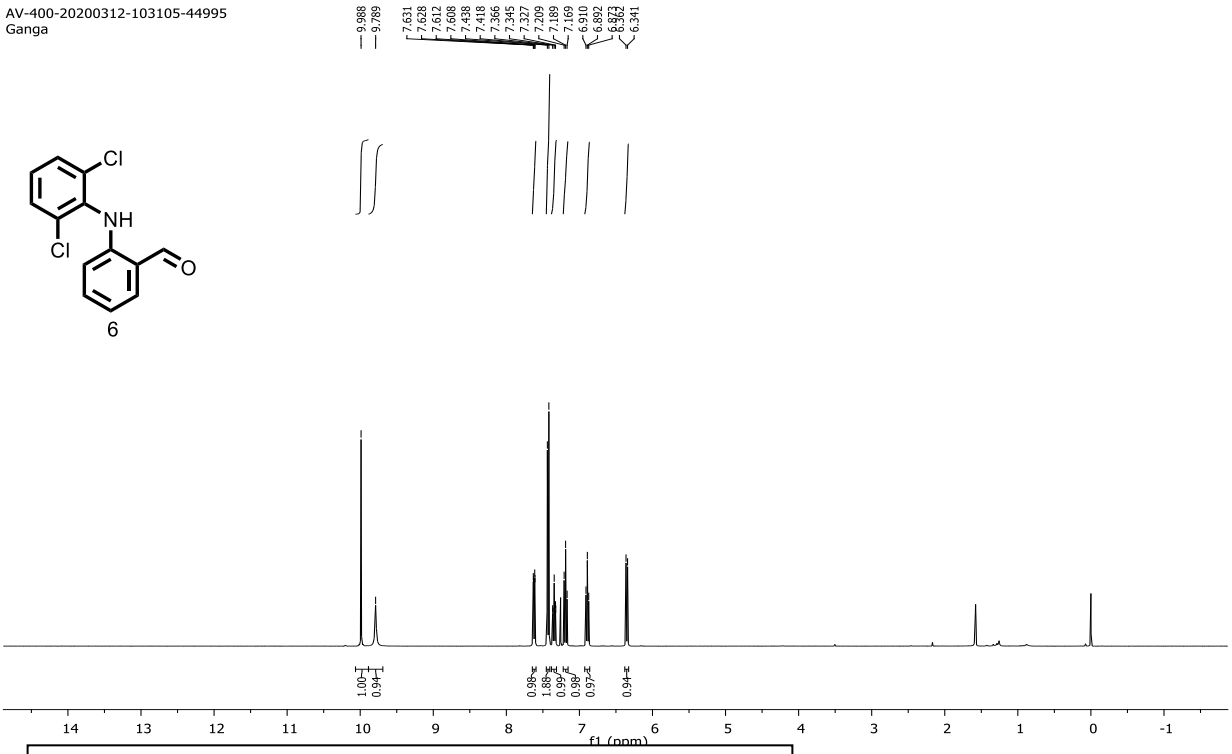
^{1}H NMR spectrum of compound **5** ($CDCl_3$, 400 MHz)



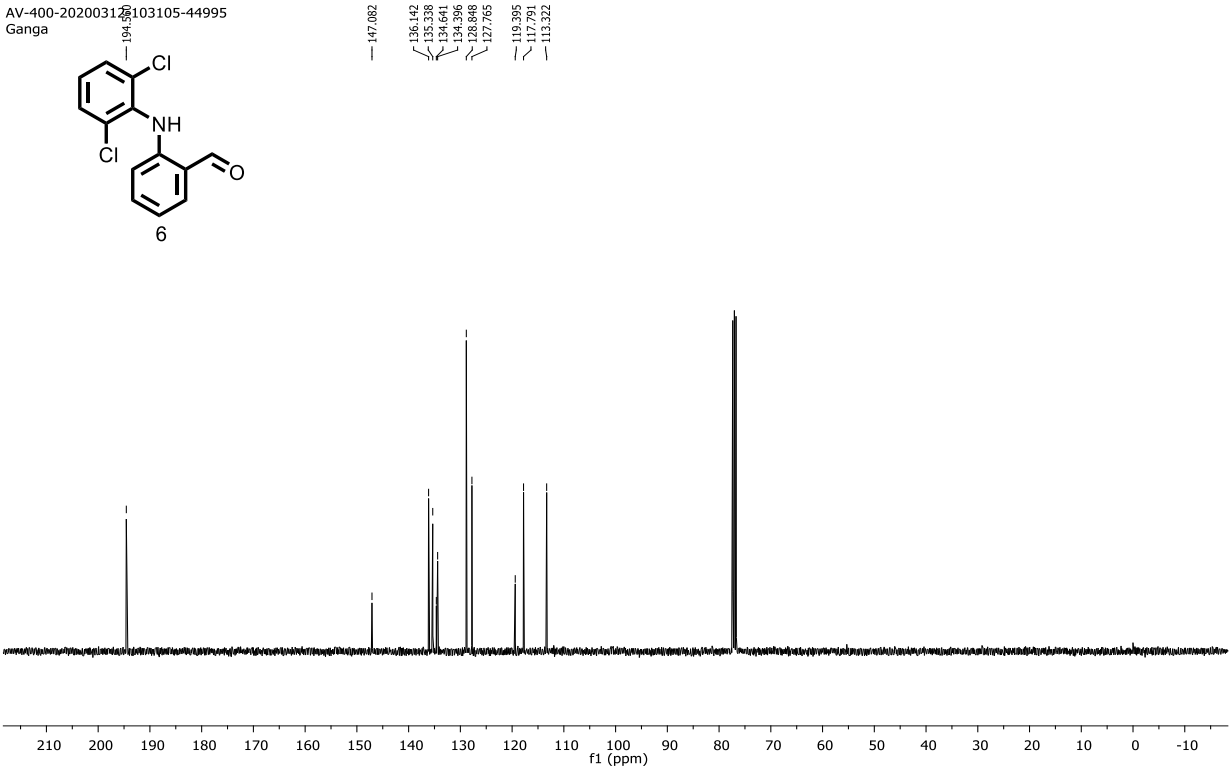
^{13}C NMR spectrum of compound **5** ($CDCl_3$, 100 MHz)



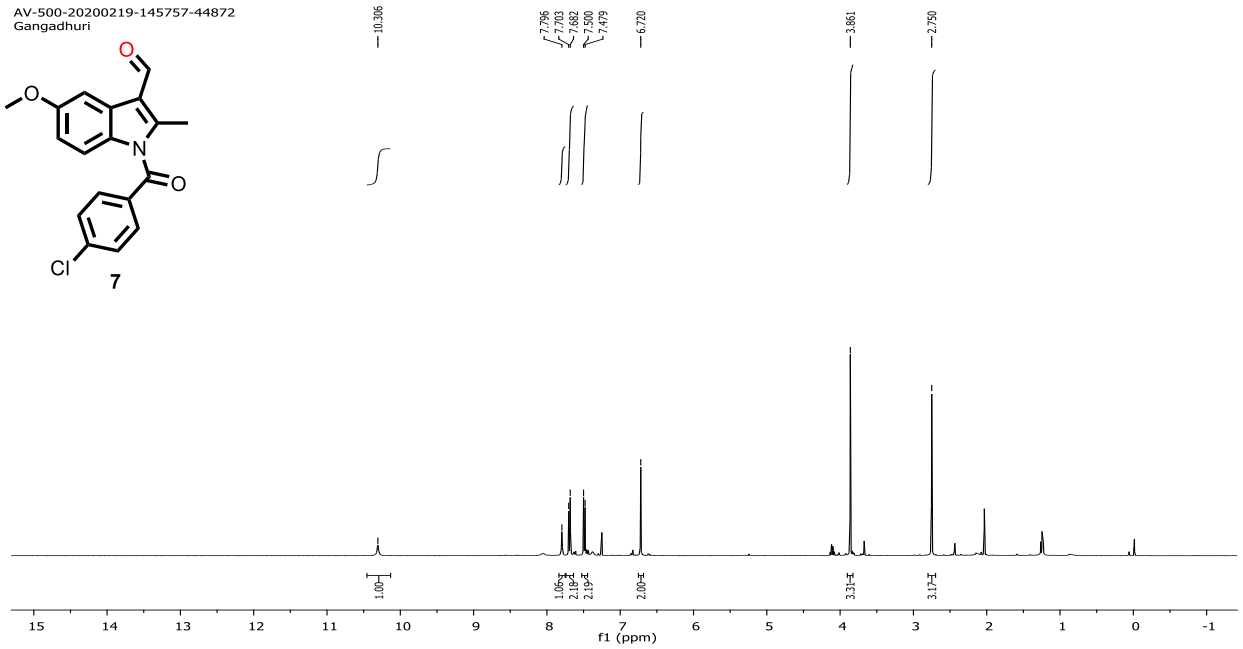
^{1}H NMR spectrum of compound **6** ($CDCl_3$, 400 MHz)



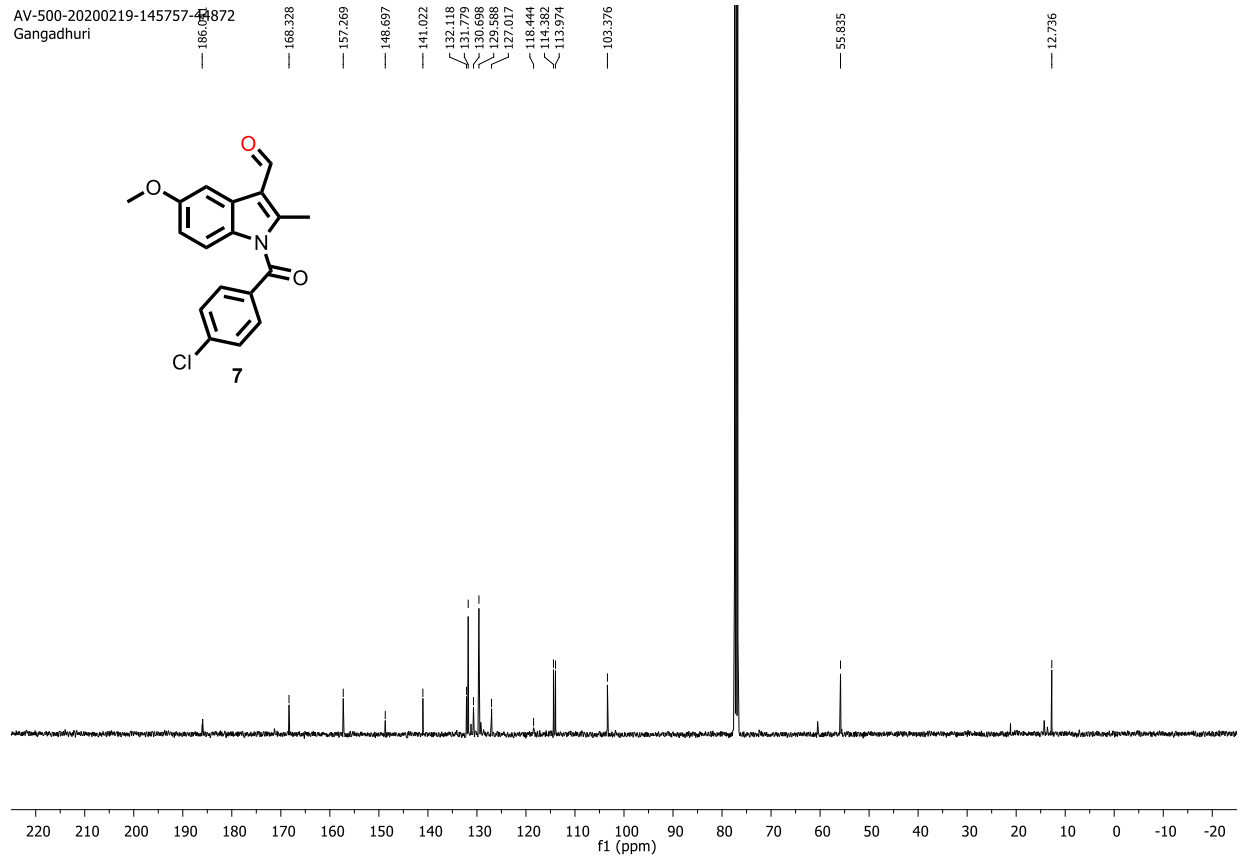
^{13}C NMR spectrum of compound **6** ($CDCl_3$, 100 MHz)



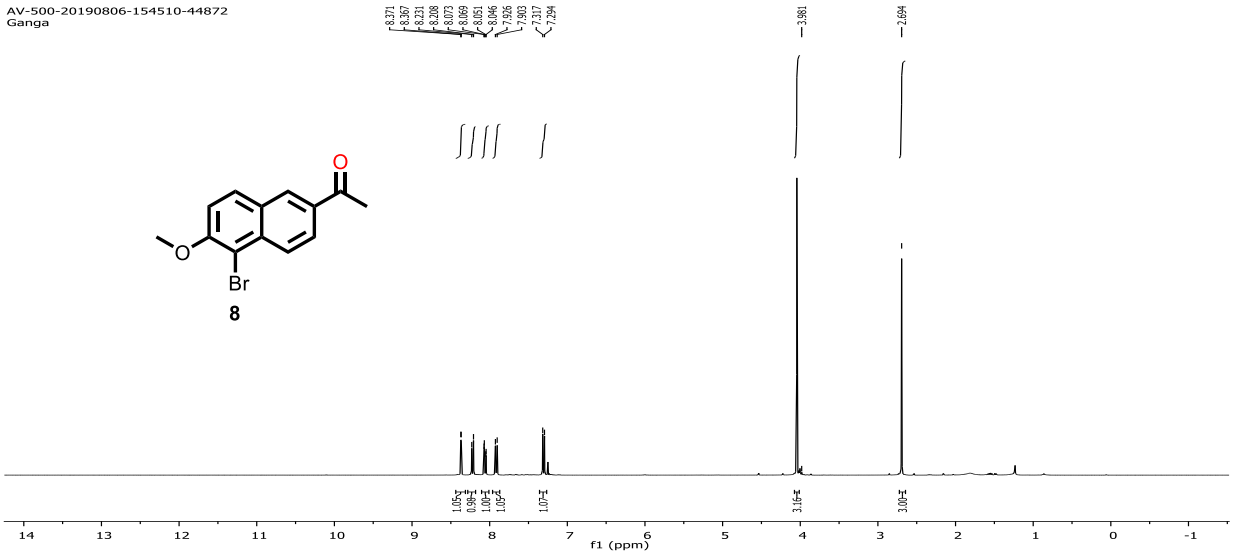
^{1}H NMR spectrum of compound7 ($CDCl_3$, 400 MHz)



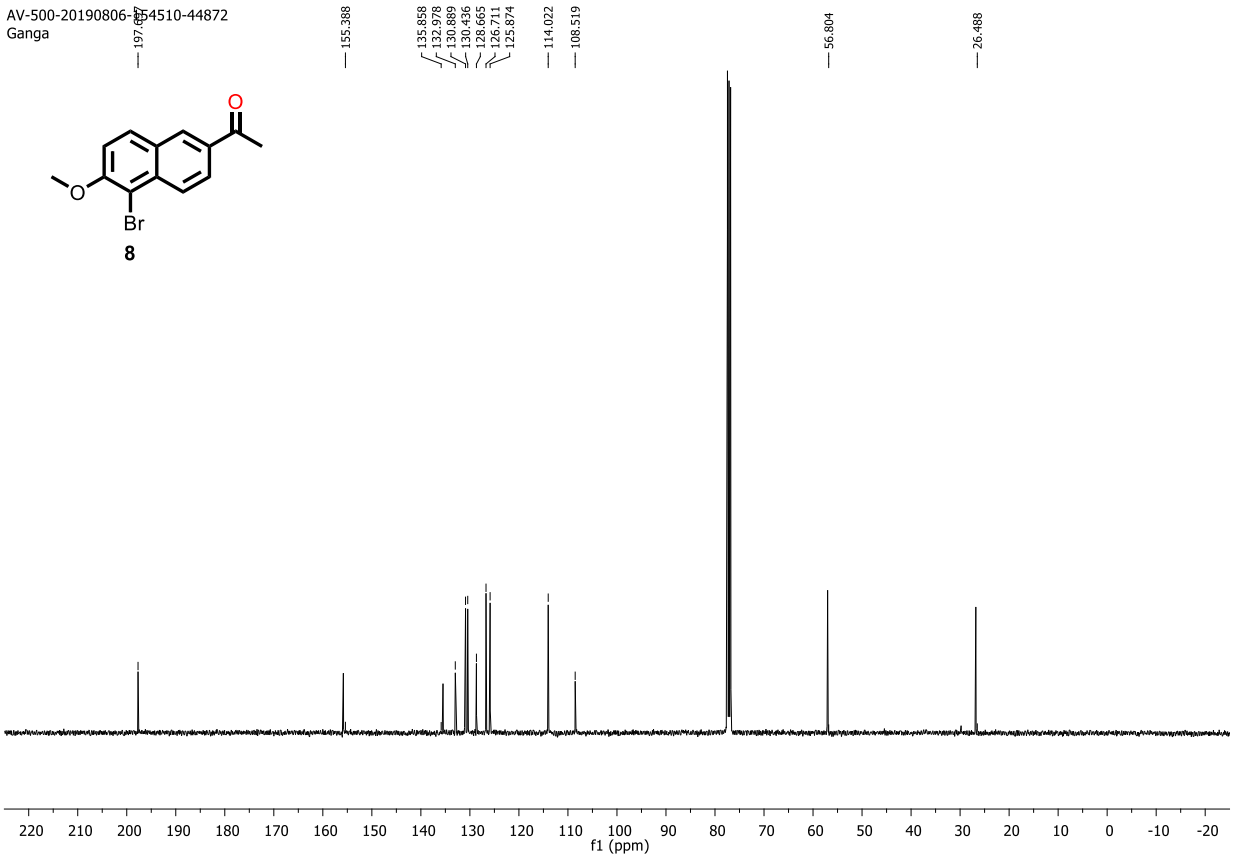
^{13}C NMR spectrum of compound **7**($CDCl_3$, 100 MHz)



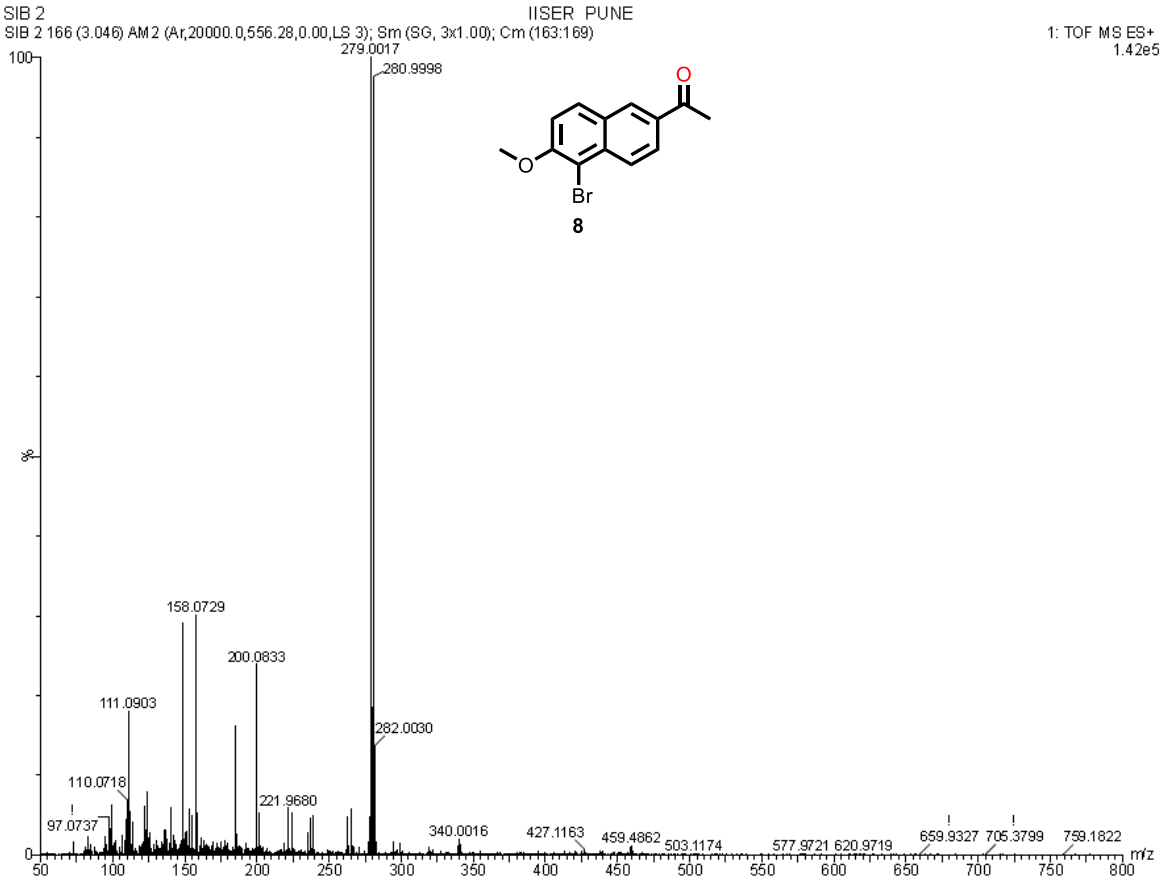
^{1}H NMR spectrum of compound **8** ($CDCl_3$, 500 MHz)



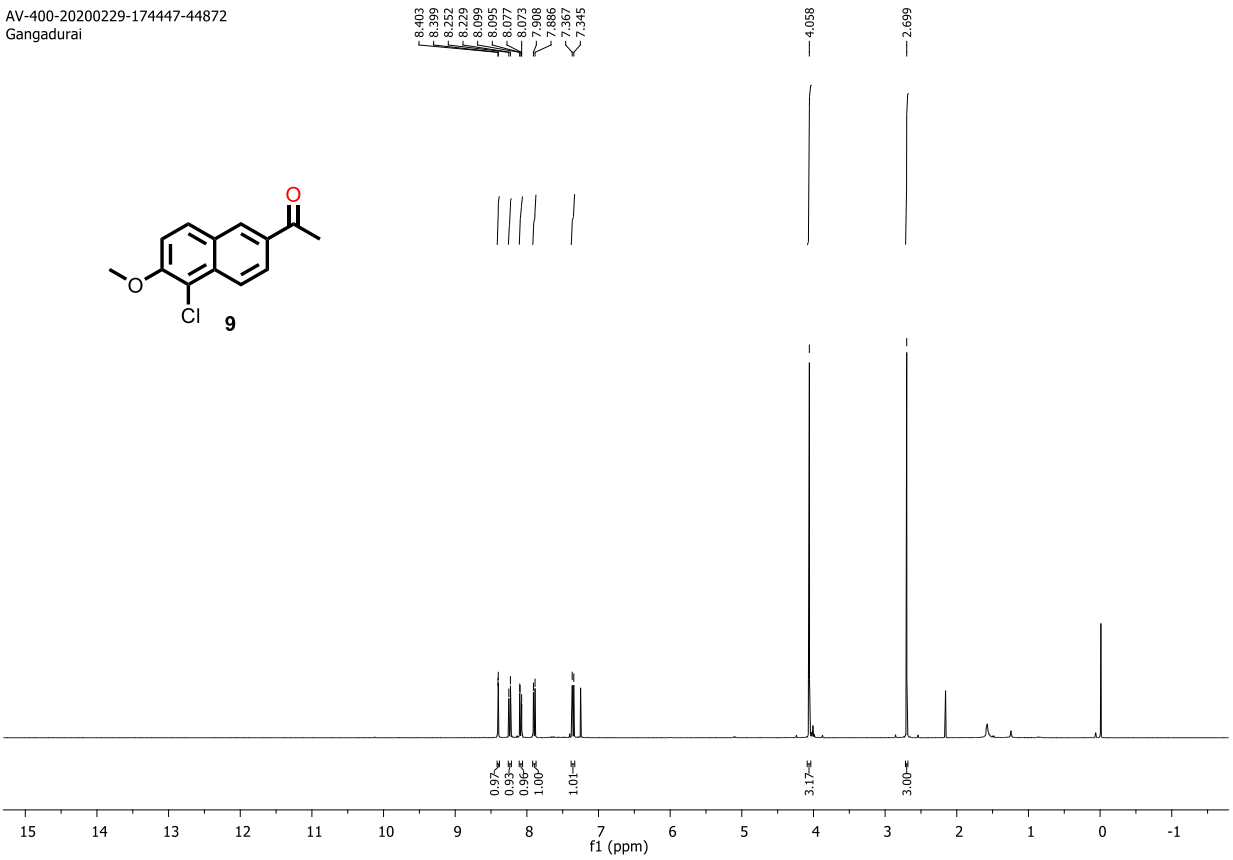
^{13}C NMR spectrum of compound **8** ($CDCl_3$, 125 MHz)



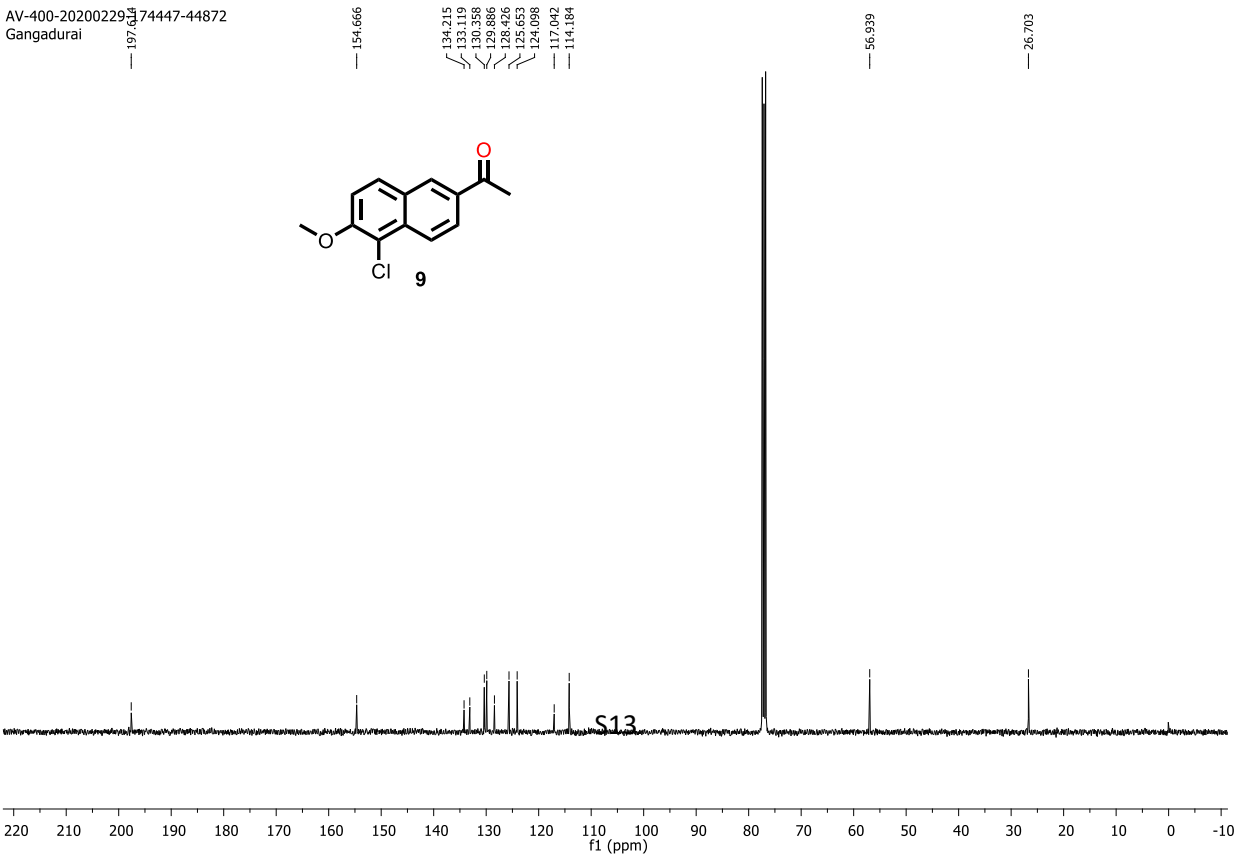
HRMS spectrum of compound **8**



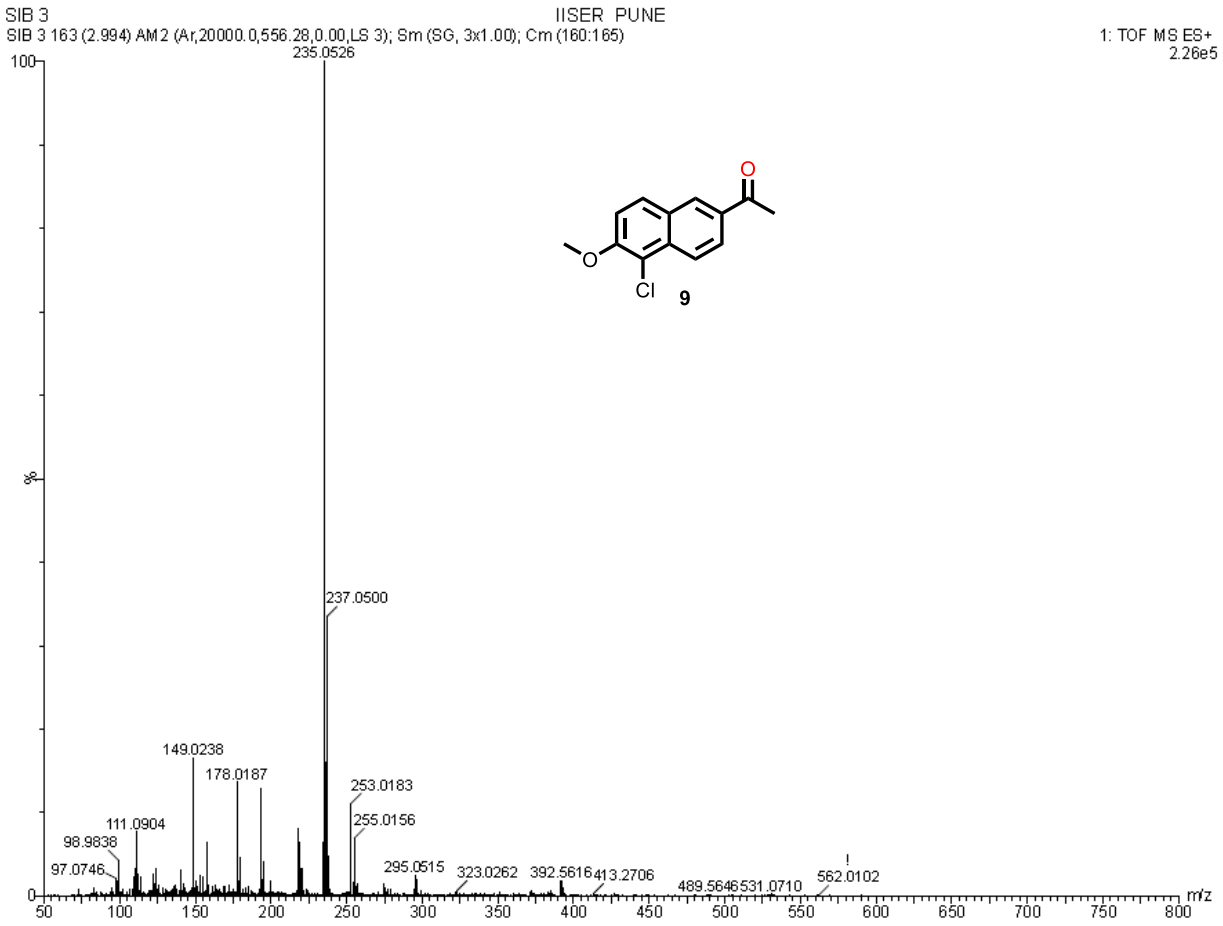
^{1}H NMR spectrum of compound 9 ($CDCl_3$, 400 MHz)



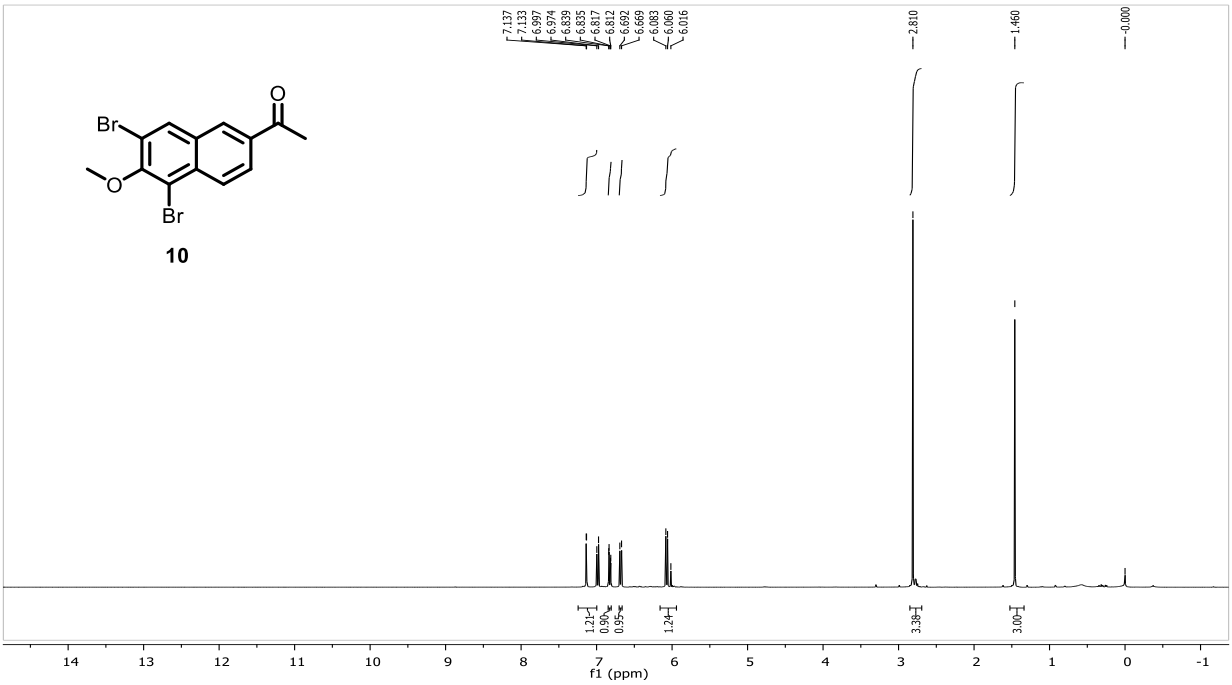
^{13}C NMR spectrum of compound 9 ($CDCl_3$, 100 MHz)



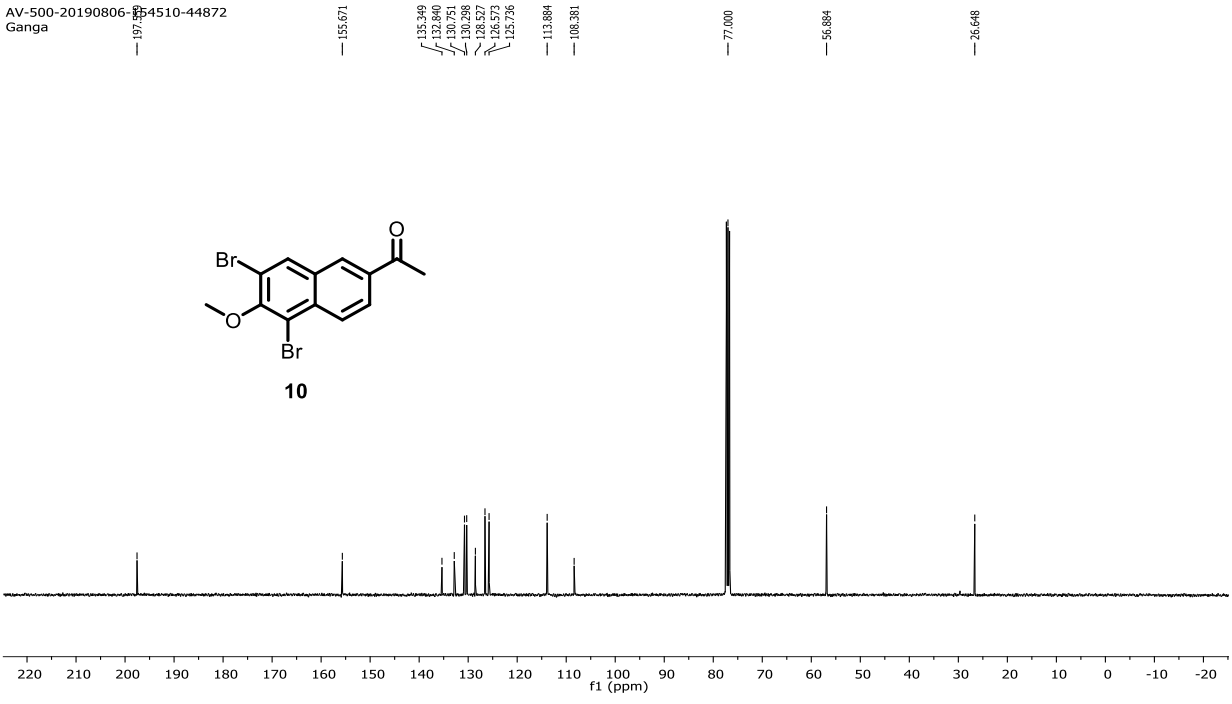
HRMS spectrum of compound 9



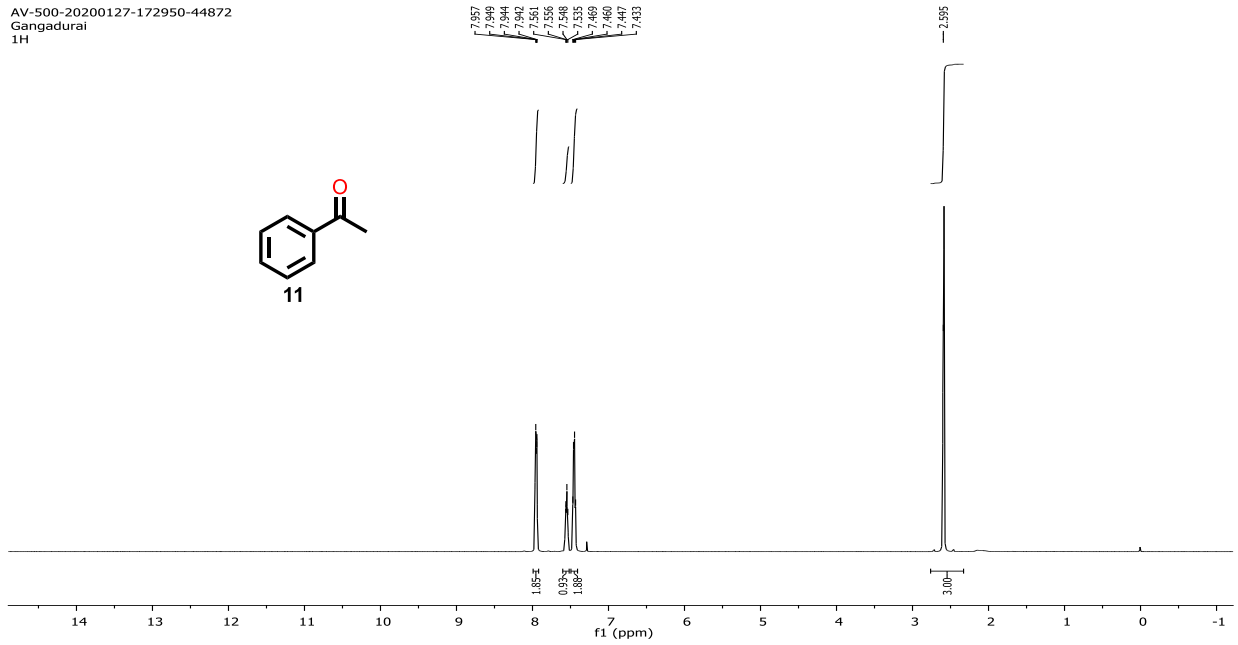
^{1}H NMR spectrum of compound 10 ($CDCl_3$, 500 MHz)



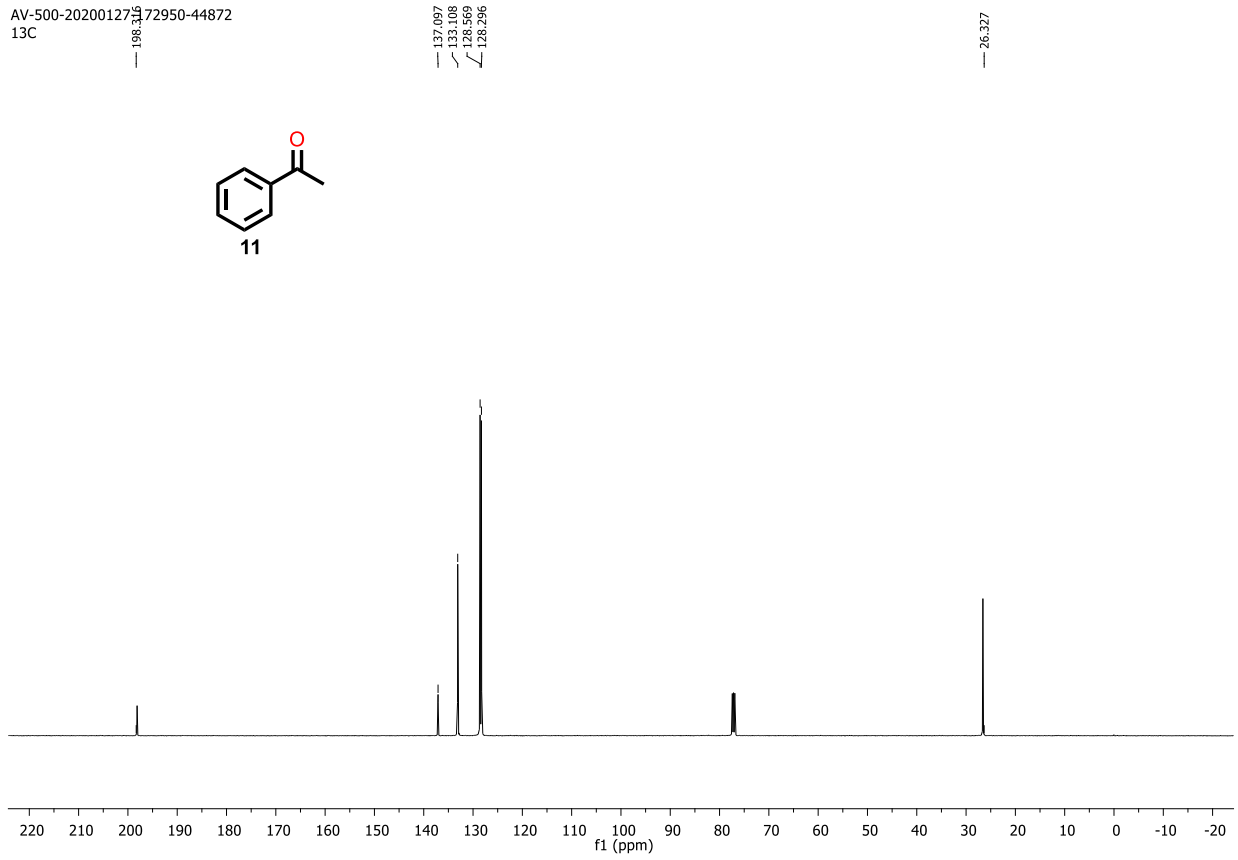
^{13}C NMR spectrum of compound 10 ($CDCl_3$, 125 MHz)



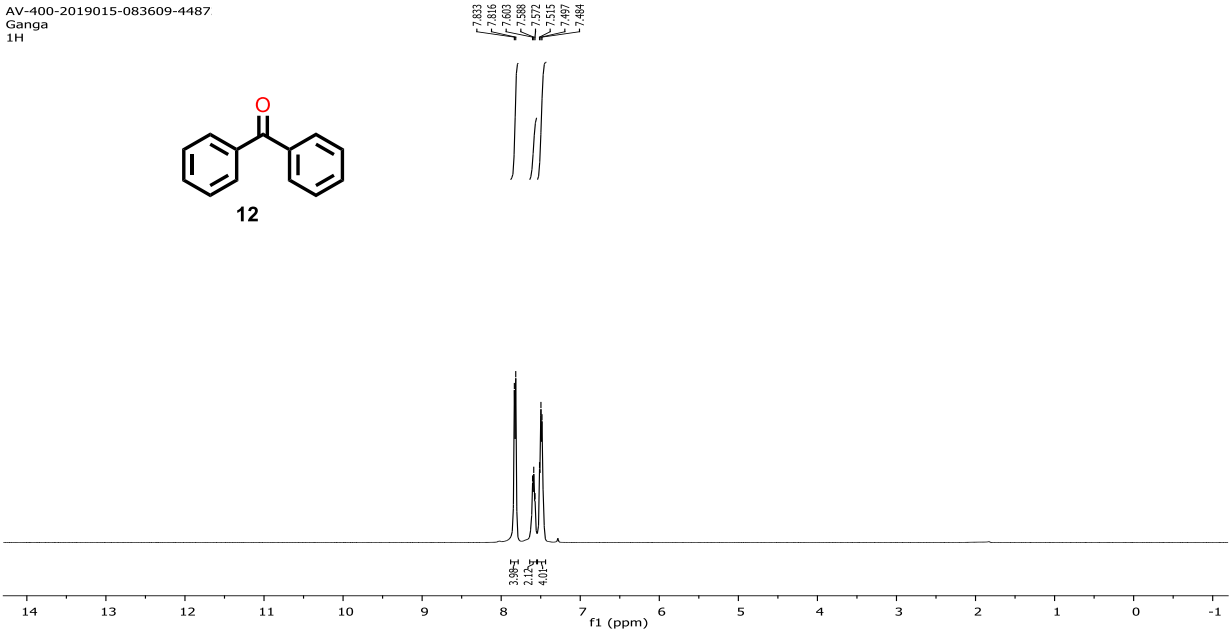
^{1}H NMR spectrum of compound **11** ($CDCl_3$, 500 MHz)



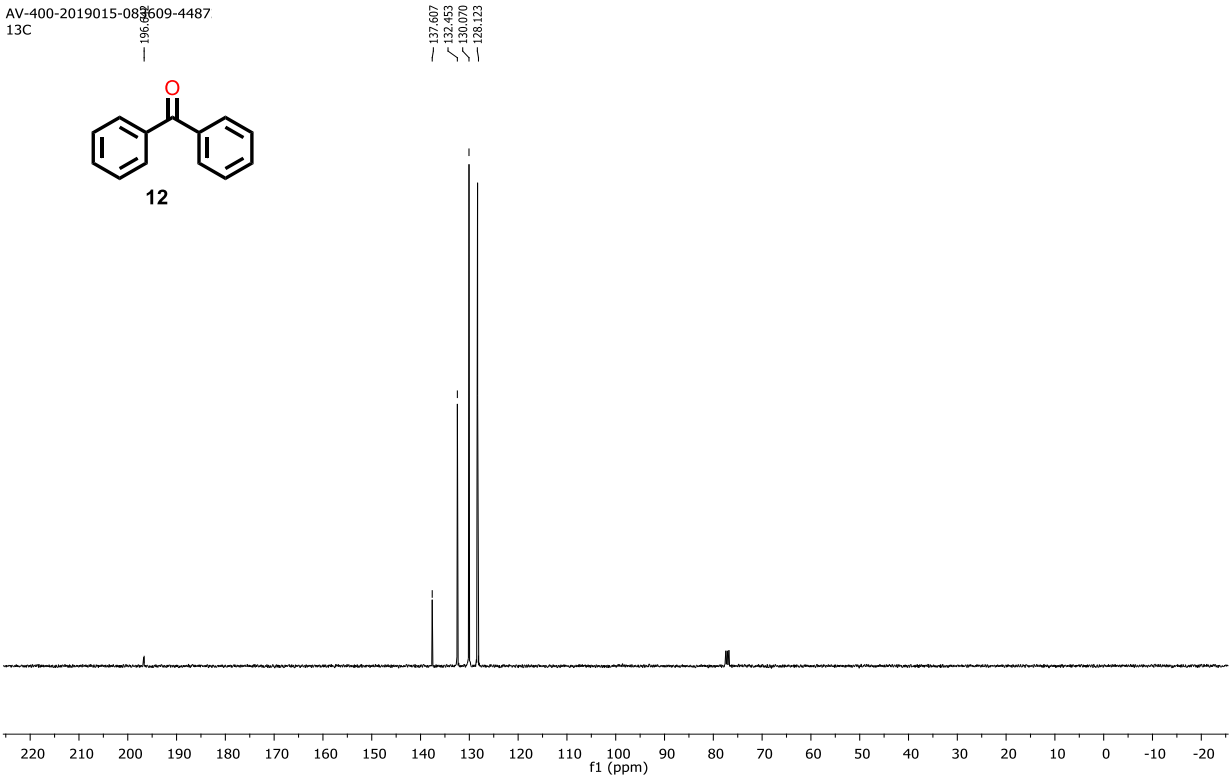
^{13}C NMR spectrum of compound **11** ($CDCl_3$, 125 MHz)



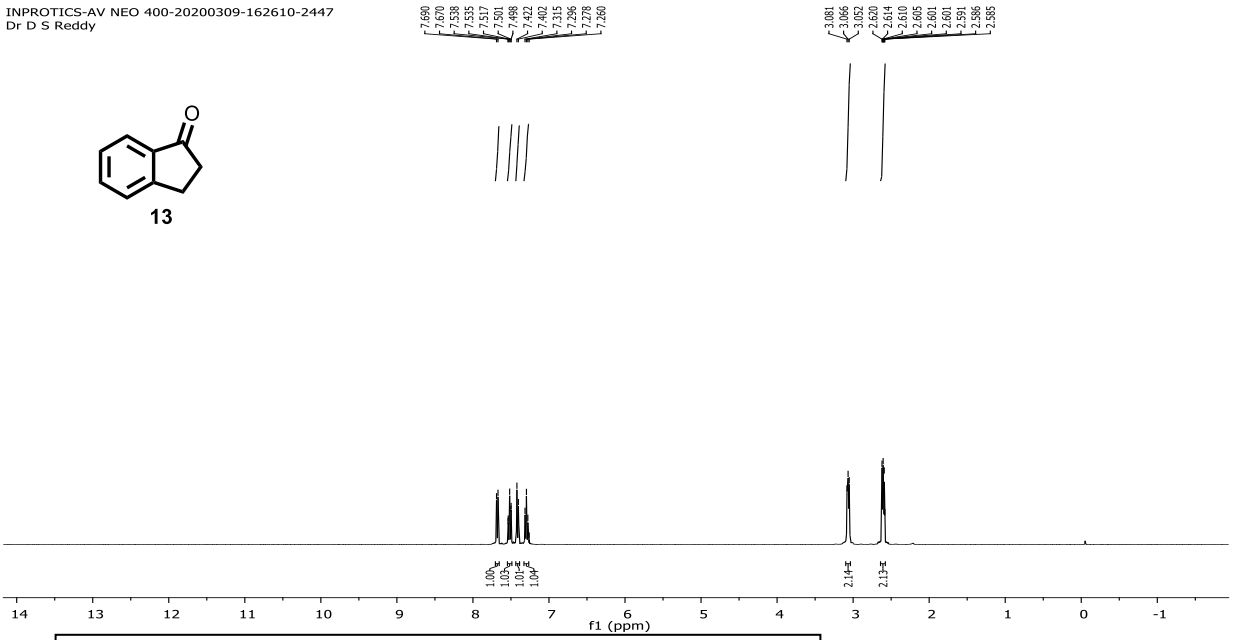
^{1}H NMR spectrum of compound **12** ($CDCl_3$, 400 MHz)



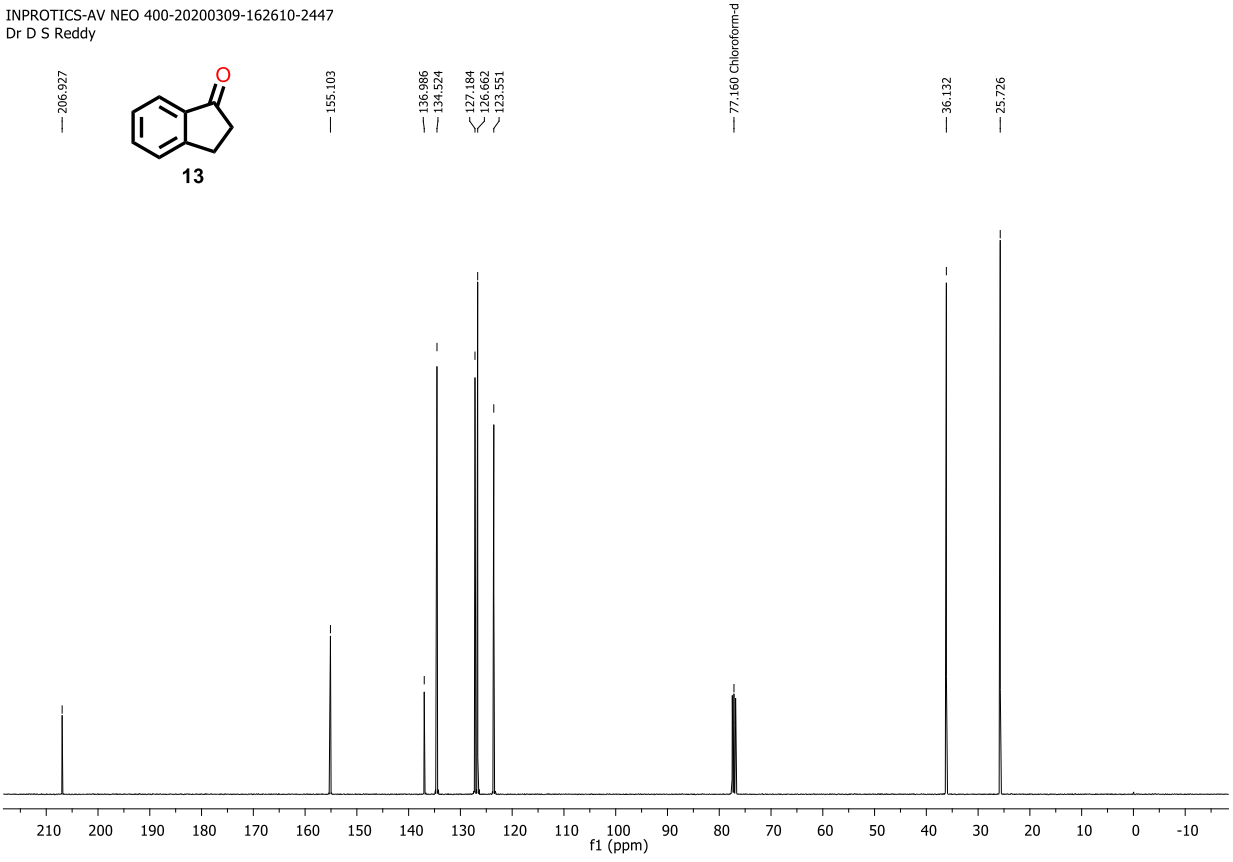
^{13}C NMR spectrum of compound **12** ($CDCl_3$, 100 MHz)



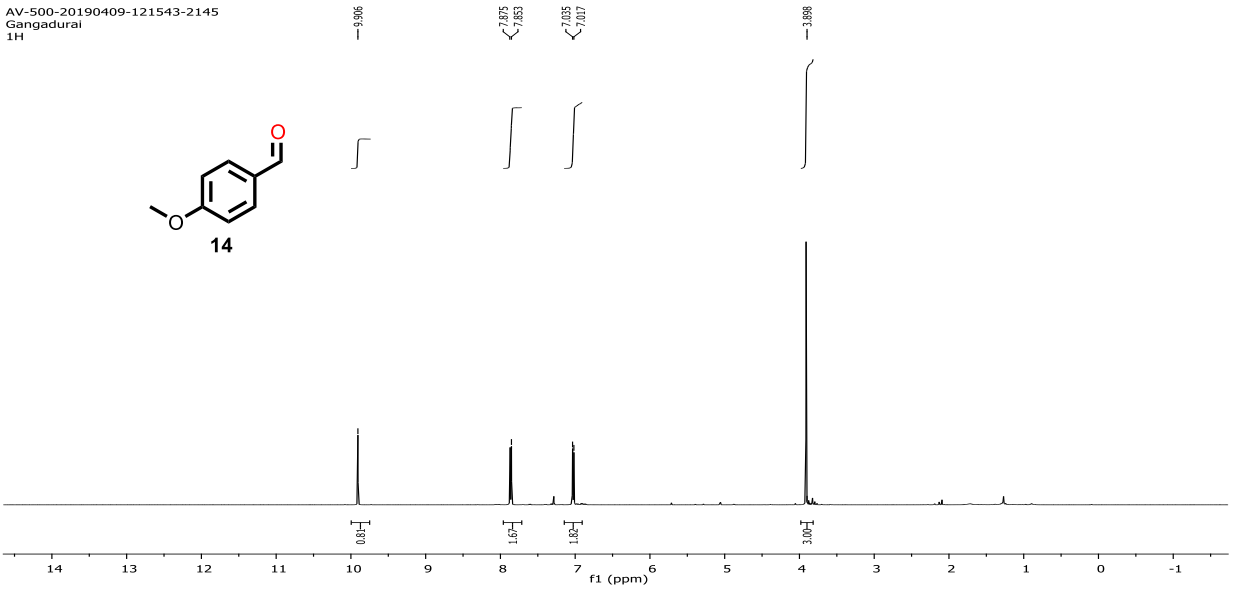
^{1}H NMR spectrum of compound **13** ($CDCl_3$, 400 MHz)



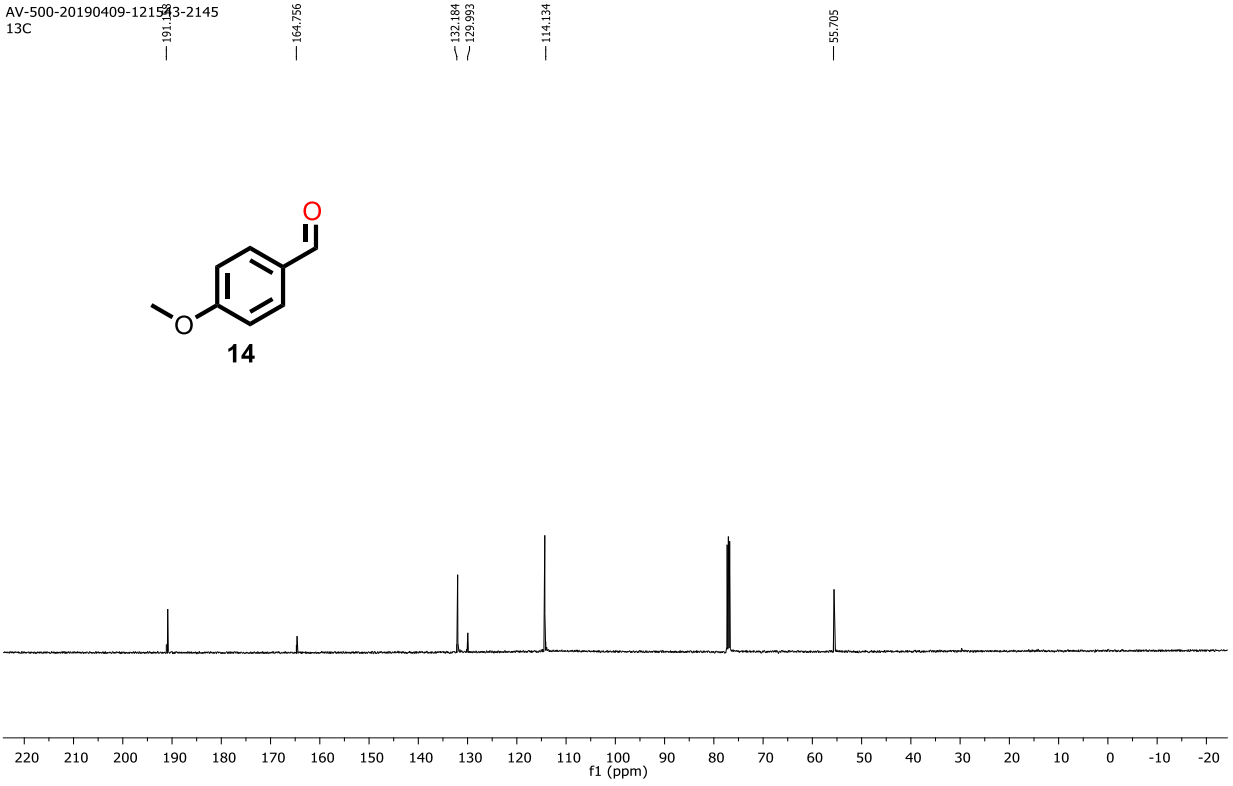
^{13}CNMR spectrum of compound **13** ($CDCl_3$, 100 MHz)



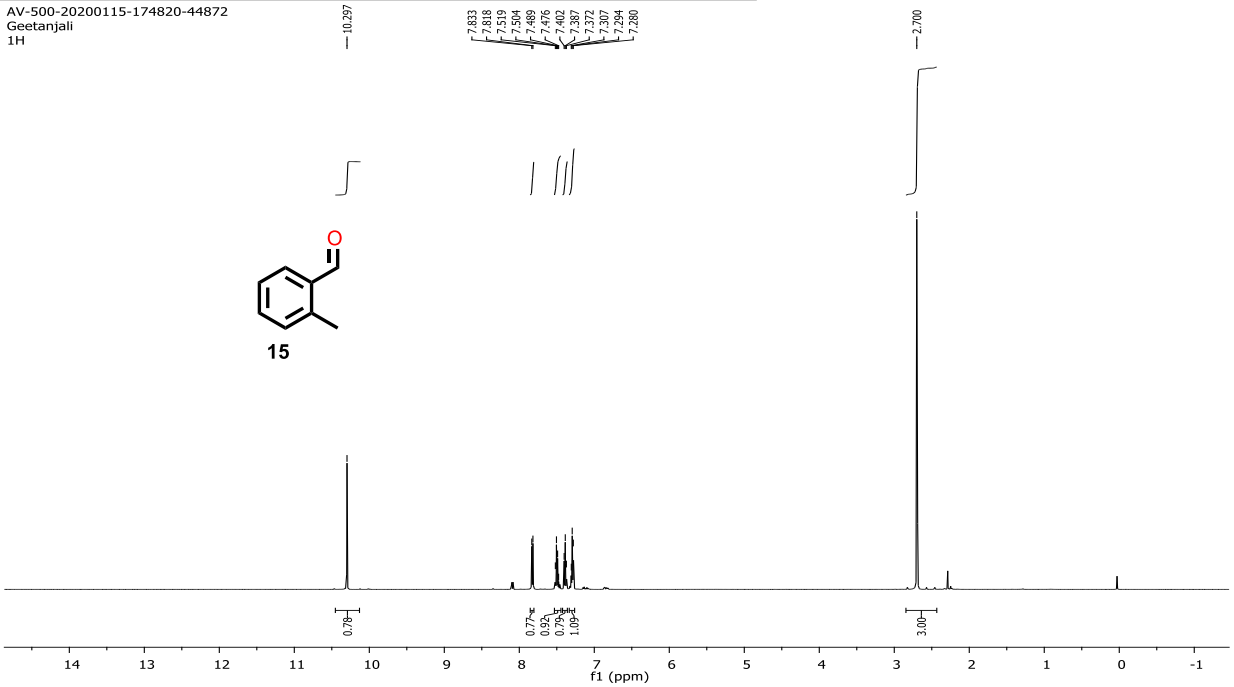
^{1}H NMR spectrum of compound 1**4** ($CDCl_3$, 500 MHz)



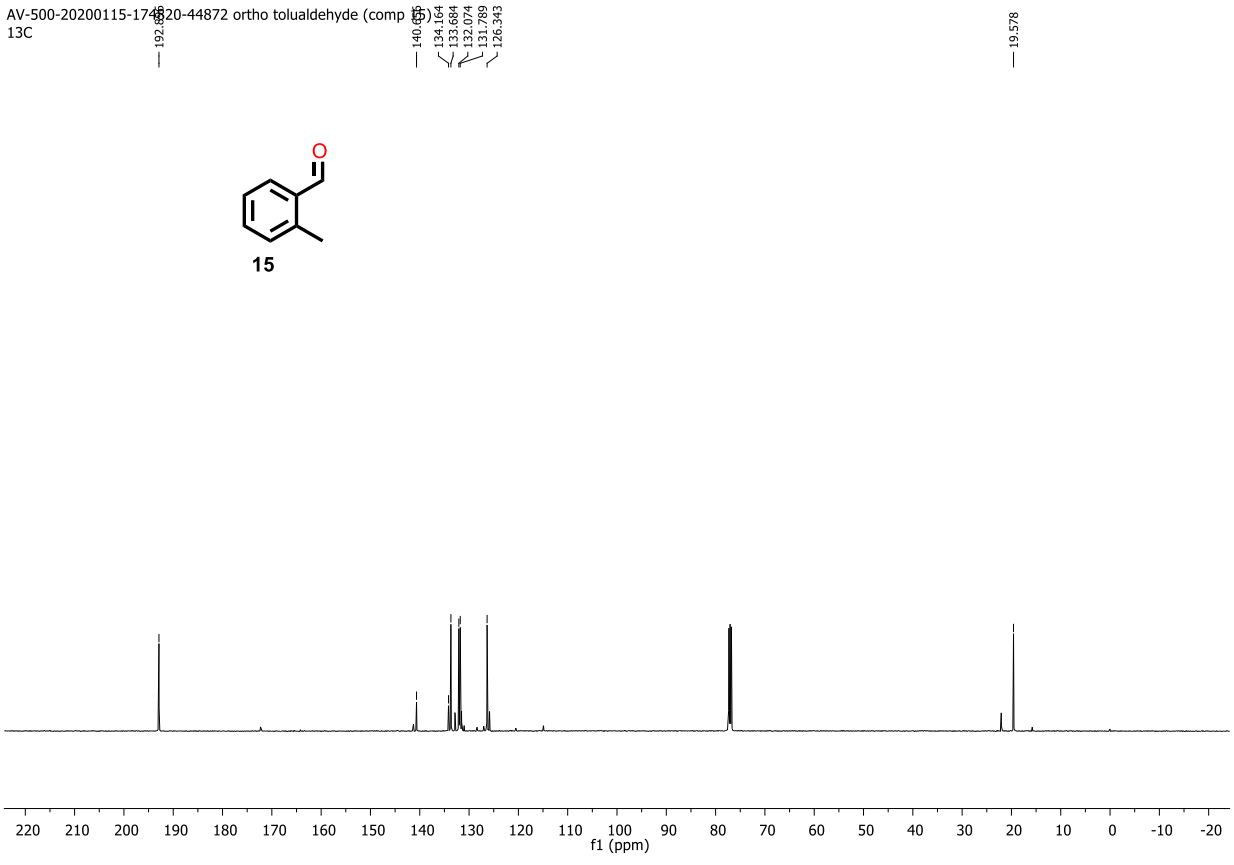
^{13}C NMR spectrum of compound 1**4** ($CDCl_3$, 125 MHz)



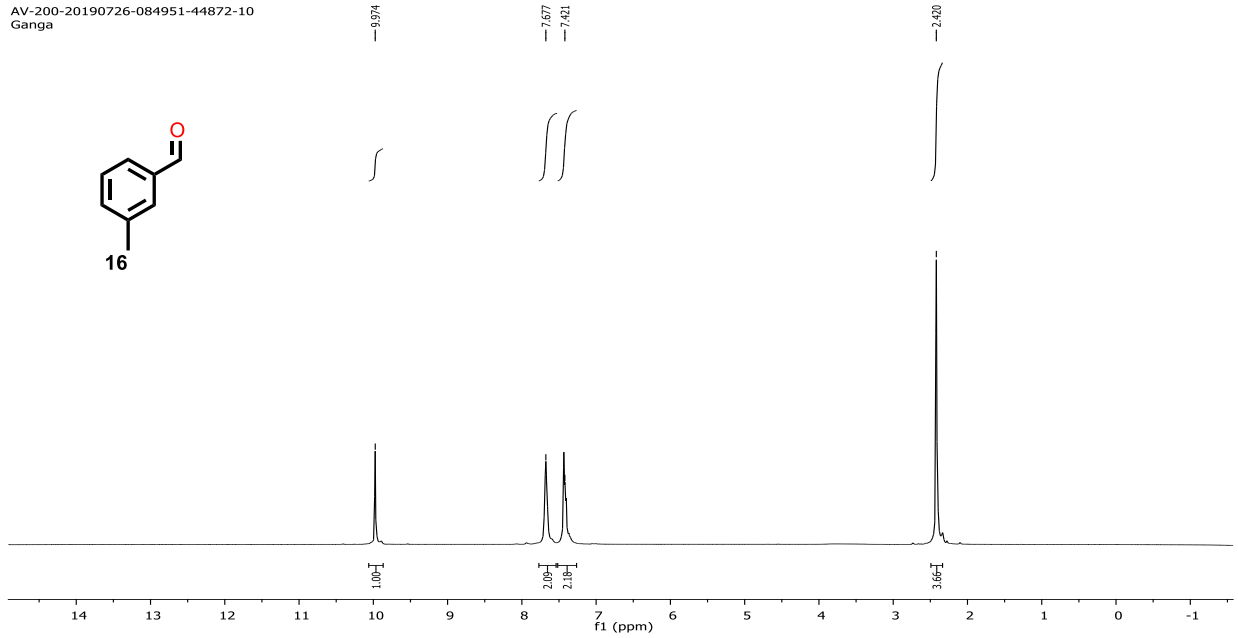
^{1}H NMR spectrum of compound 1**5** ($CDCl_3$, 500 MHz)



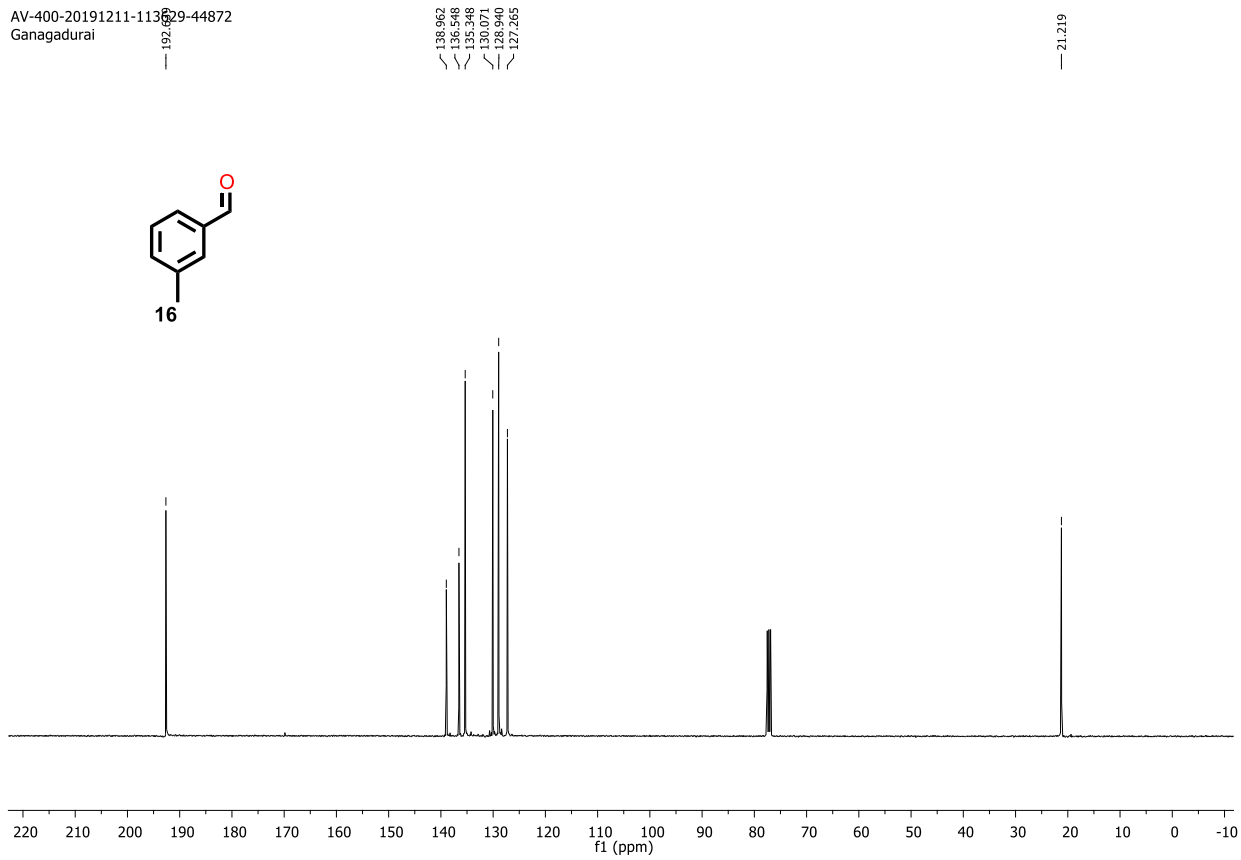
^{13}C NMR spectrum of compound 1**5** ($CDCl_3$, 125 MHz)



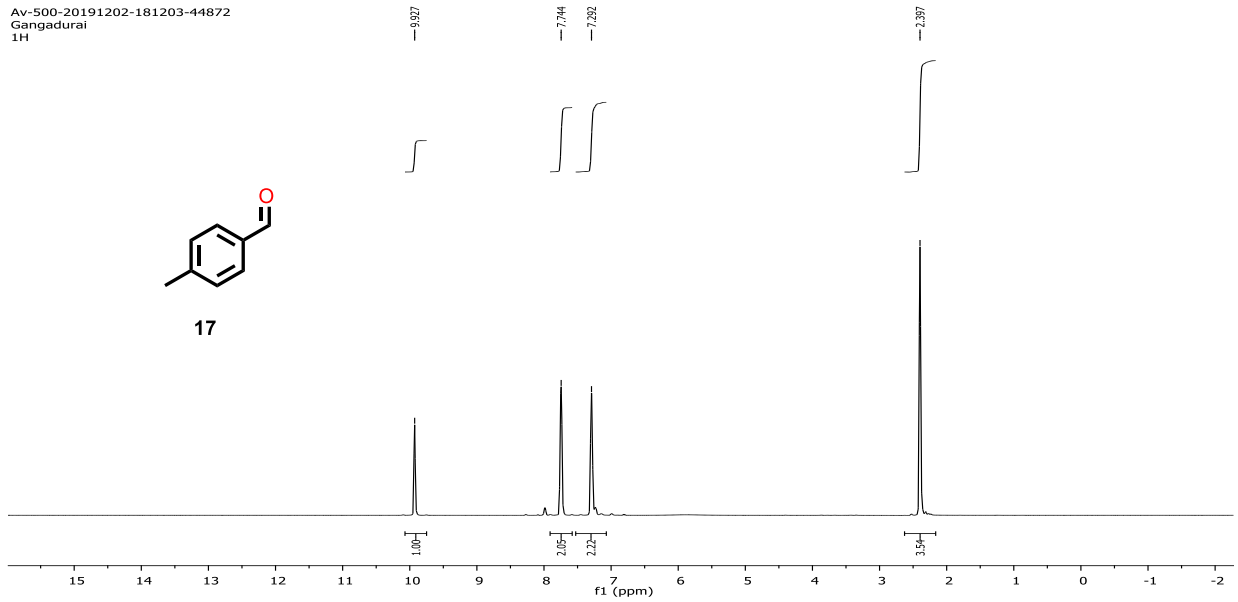
^{1}H NMR spectrum of compound 16 ($CDCl_3$, 200 MHz)



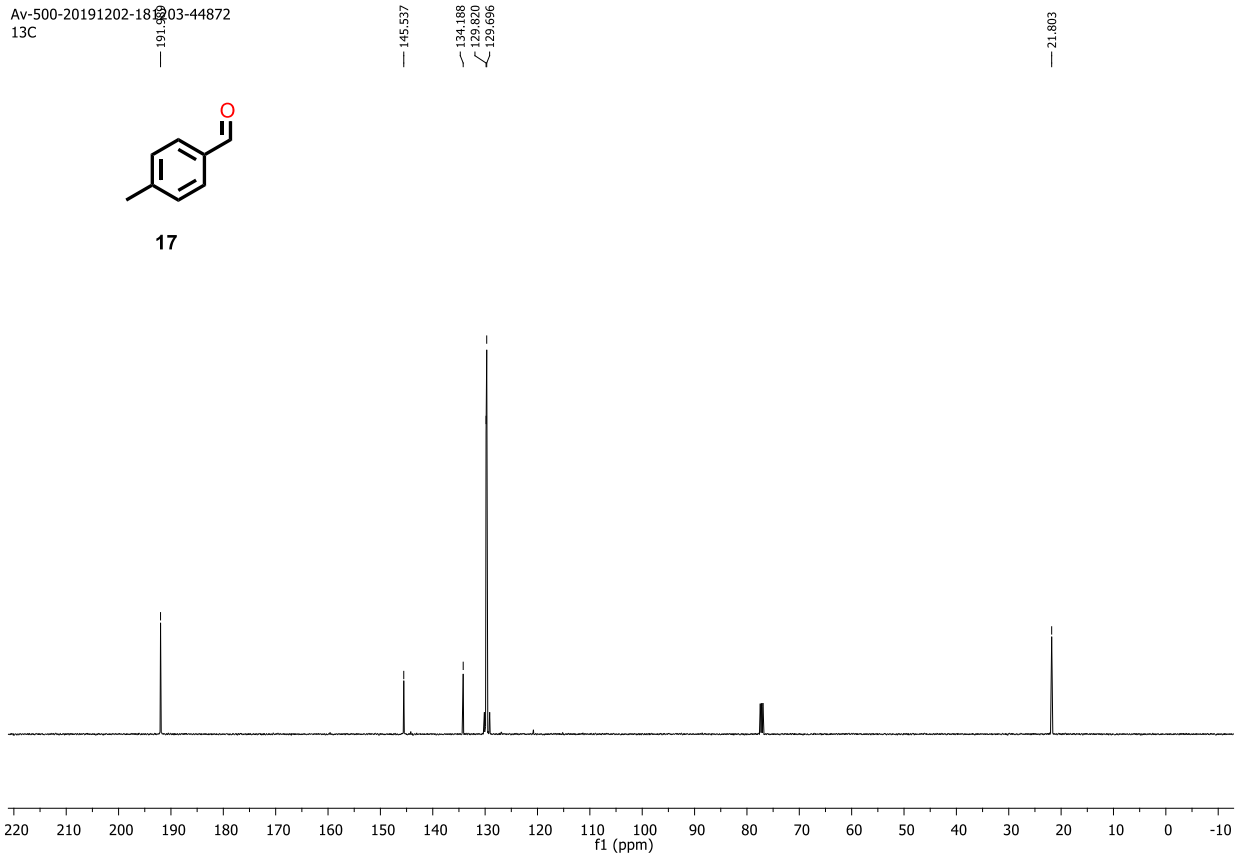
^{13}C NMR spectrum of compound 1**6** ($CDCl_3$, 100 MHz)



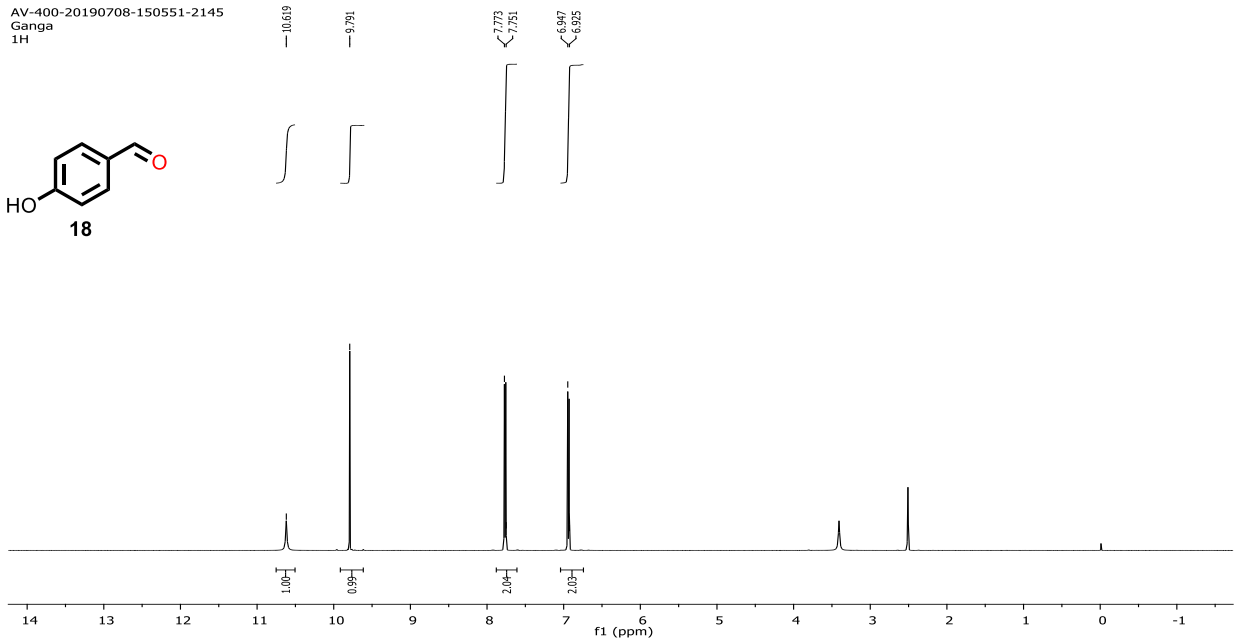
^{1}H NMR spectrum of compound 1**7** ($CDCl_3$, 500 MHz)



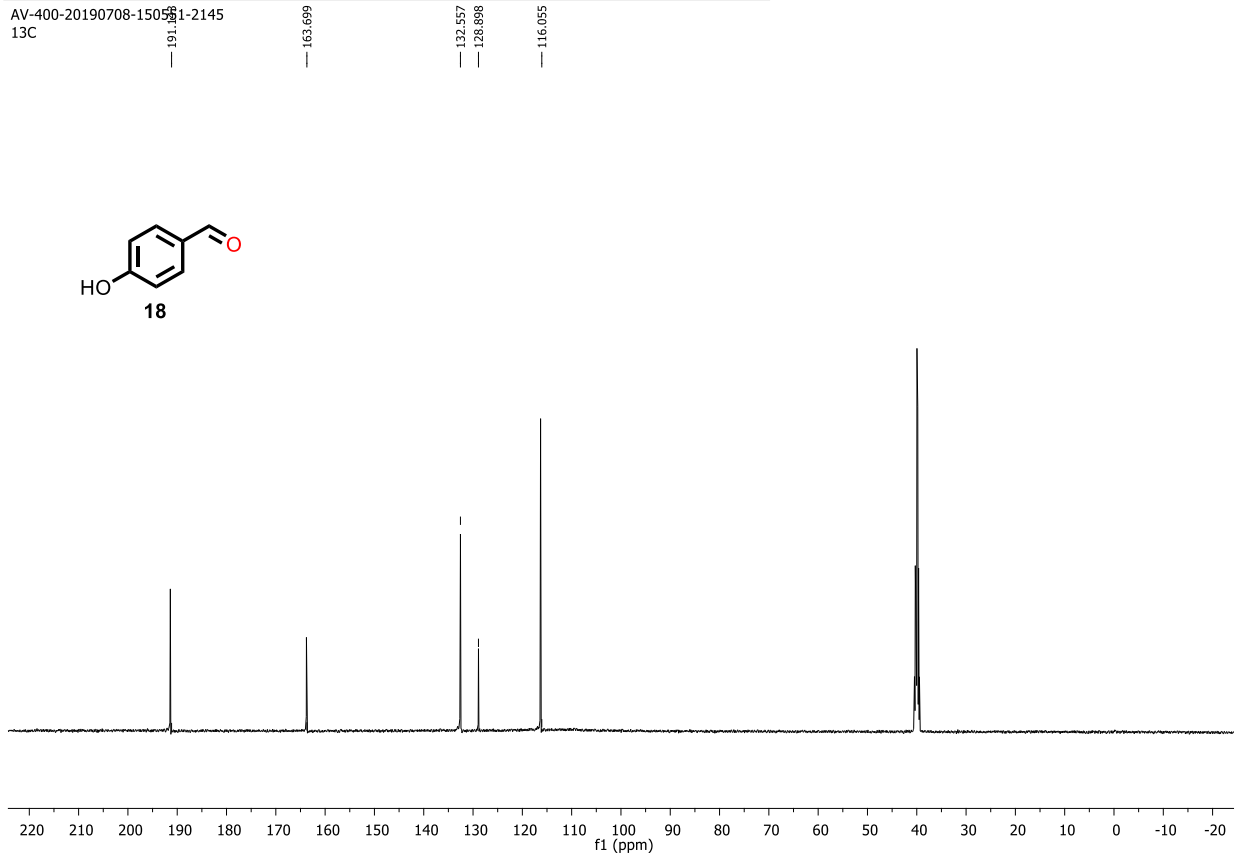
^{13}C NMR spectrum of compound 1**7** ($CDCl_3$, 125 MHz)



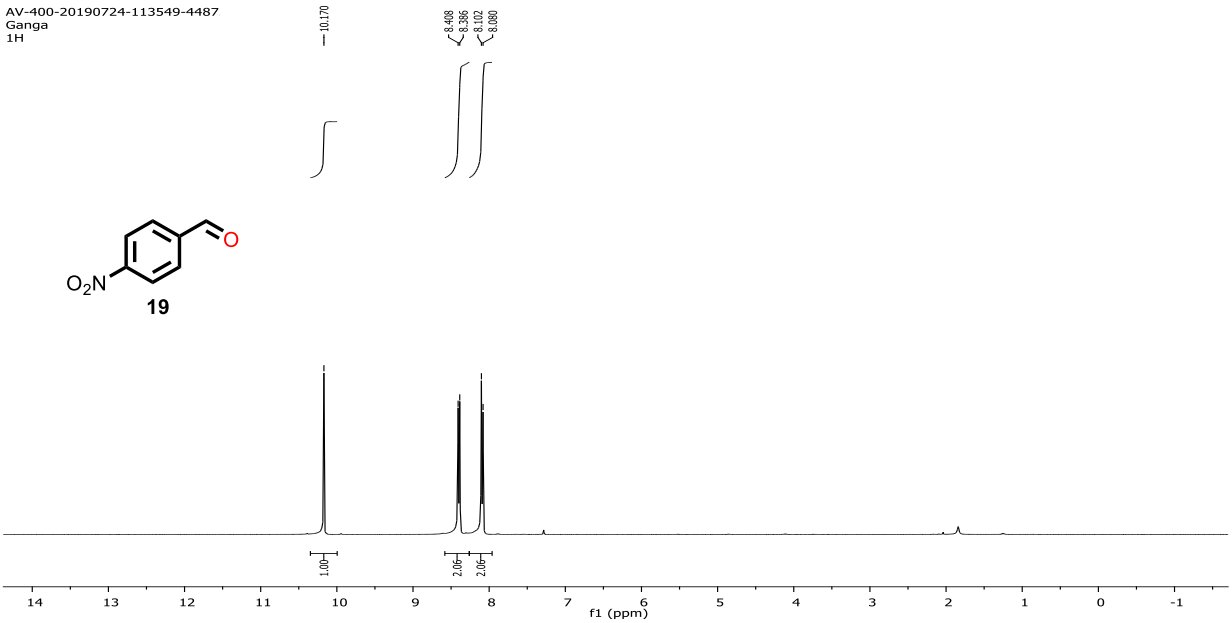
^{1}H NMR spectrum of compound 1**8** ($CDCl_3$, 400 MHz)



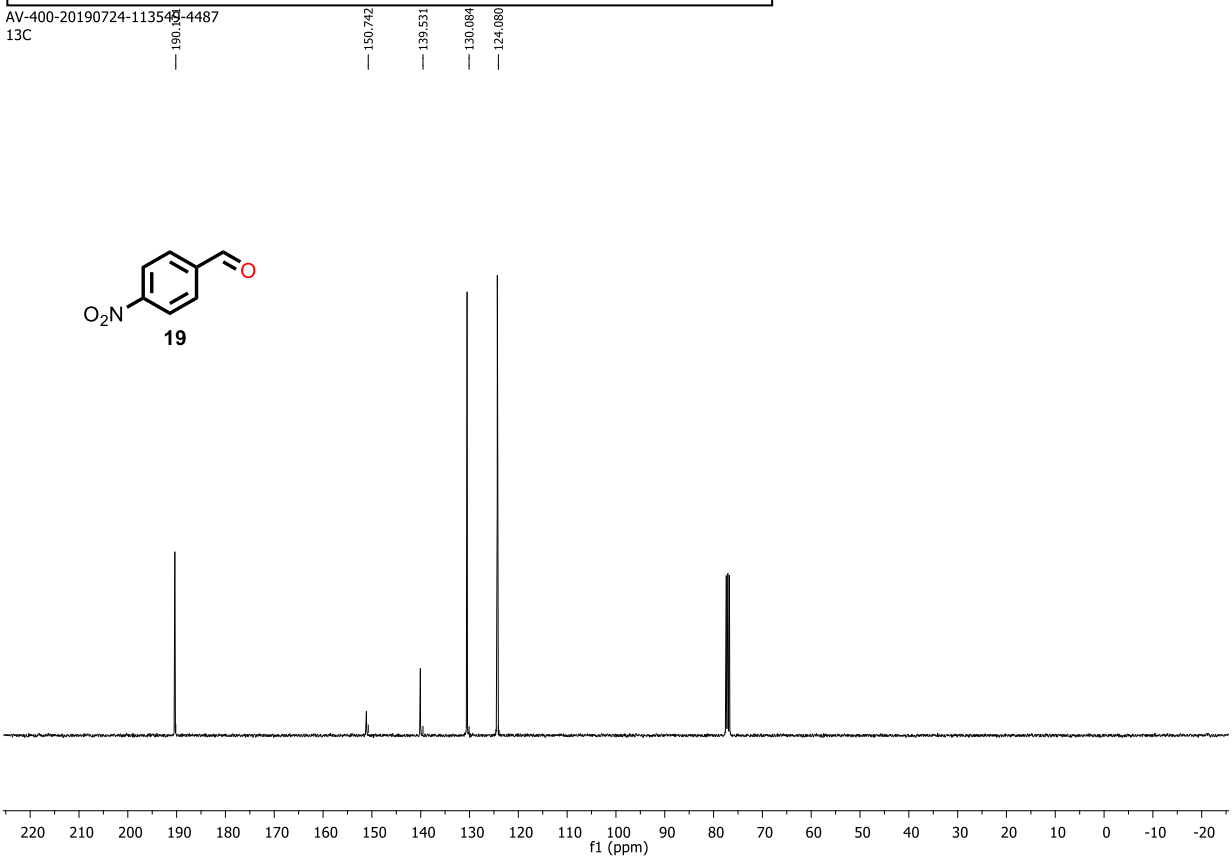
^{13}C NMR spectrum of compound 1**8**($CDCl_3$, 100 MHz)



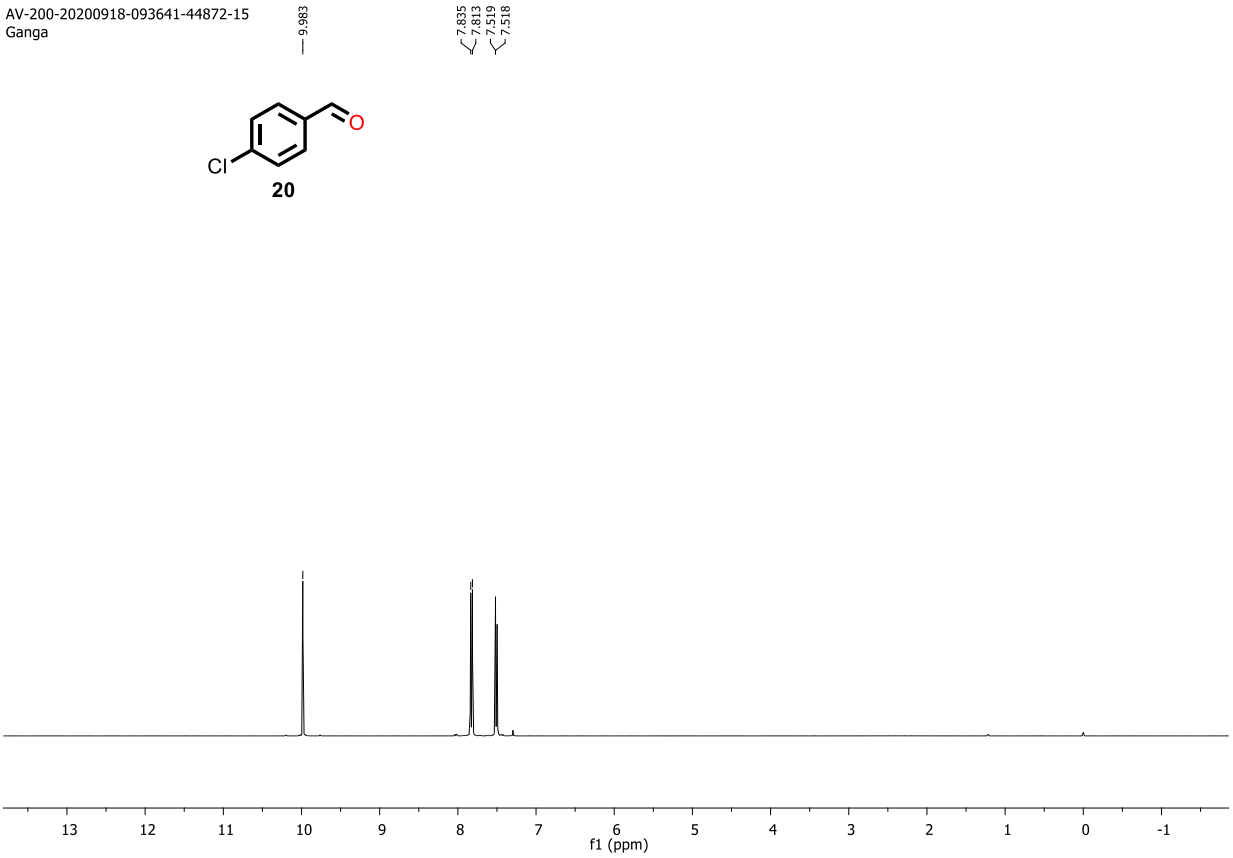
^{1}H NMR spectrum of compound 19 ($CDCl_3$, 400 MHz)



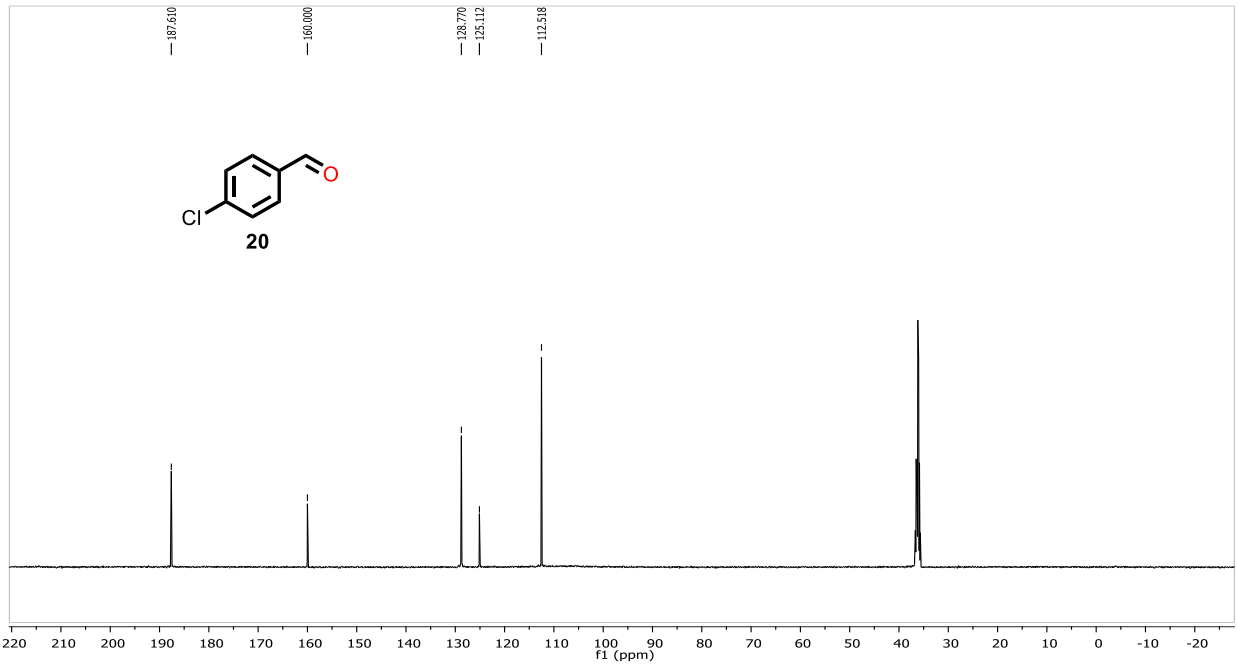
^{13}C NMR spectrum of compound 19 ($CDCl_3$, 100 MHz)



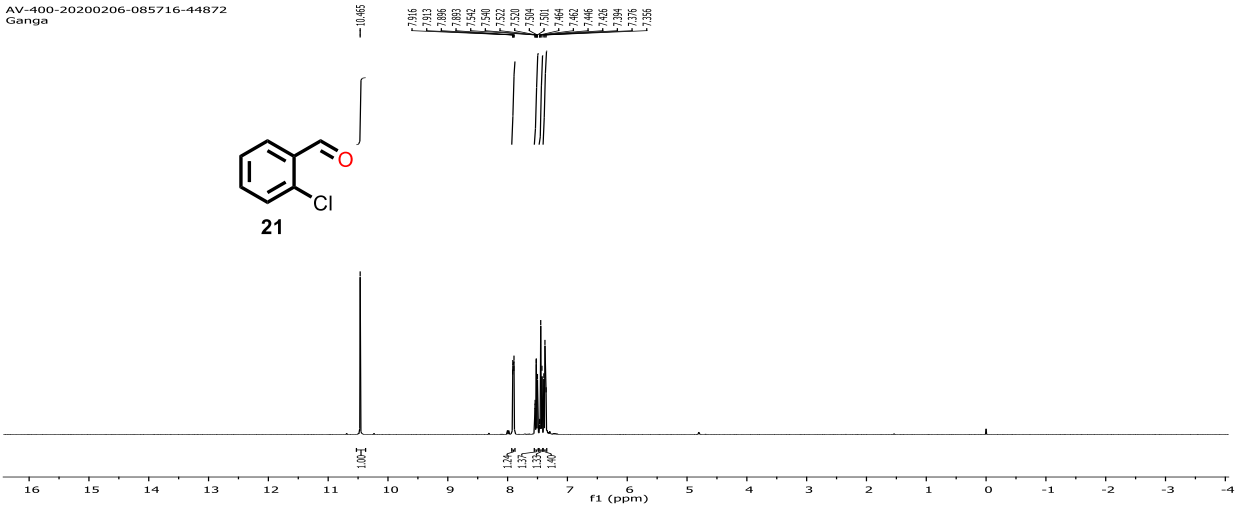
^{1}H NMR spectrum of compound 20 ($CDCl_3$, 200 MHz)



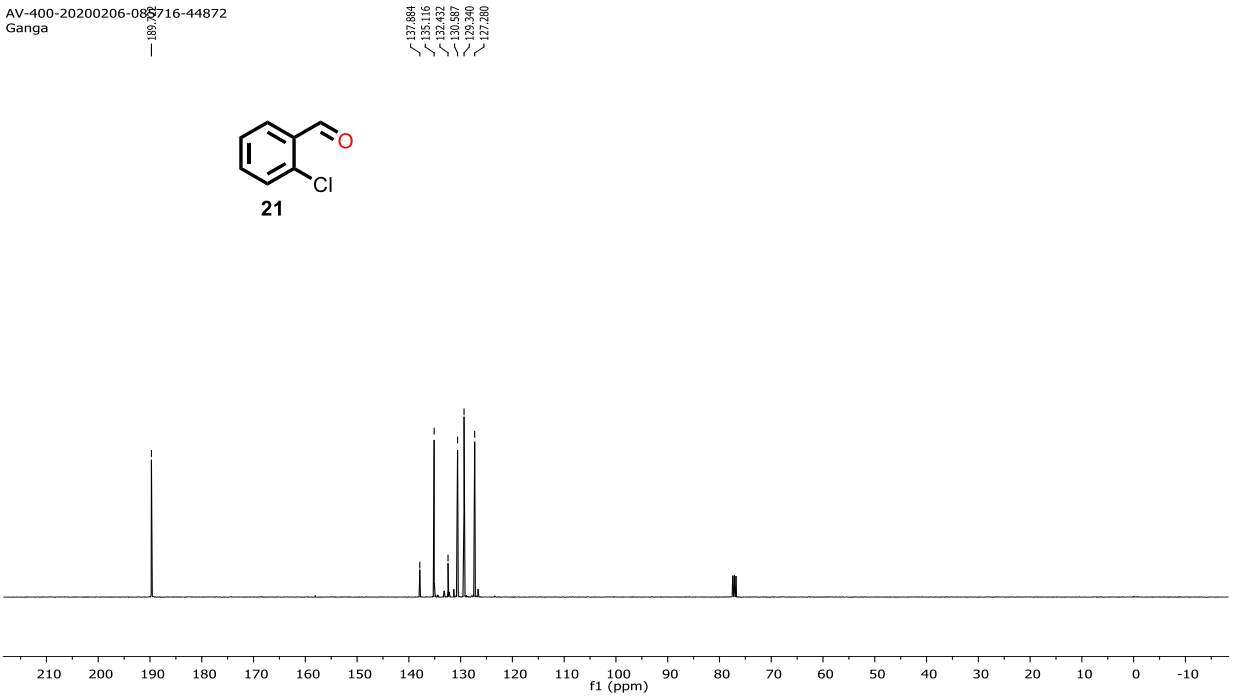
^{13}C NMR spectrum of compound 20 (DMSO-d_6, 500 MHz)



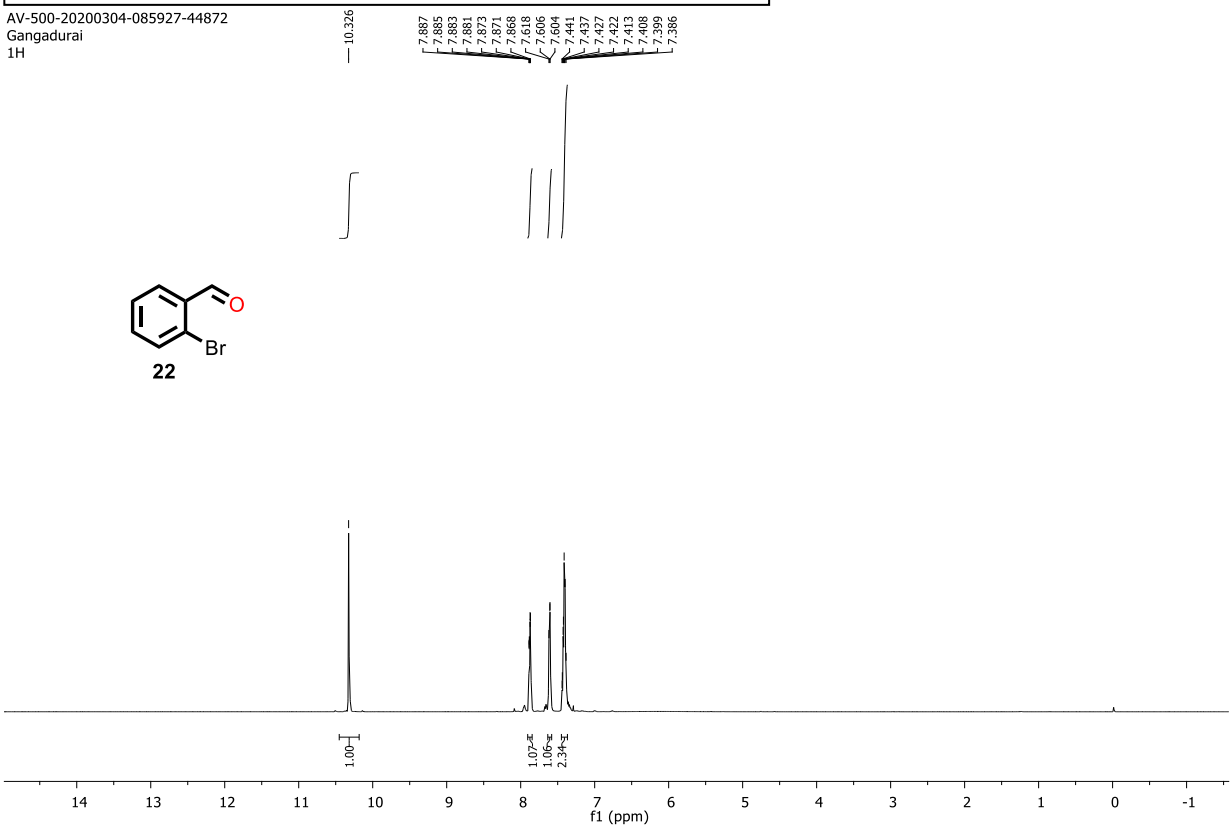
^{1}H NMR spectrum of compound 21 ($CDCl_3$, 400 MHz)



^{13}C NMR spectrum of compound 21 ($CDCl_3$, 400 MHz)

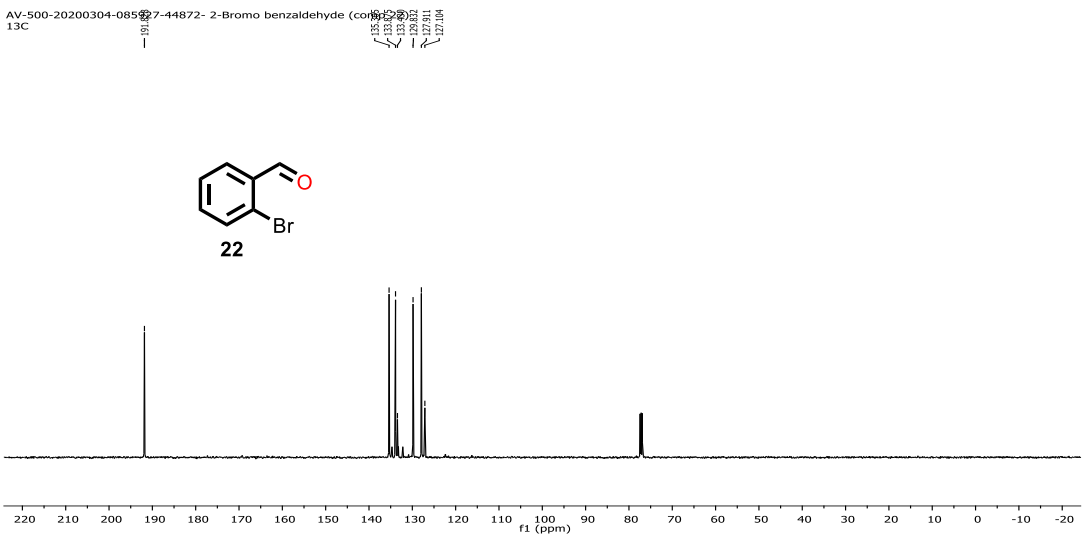


^{1}H NMR spectrum of compound 22 ($CDCl_3$, 500 MHz)



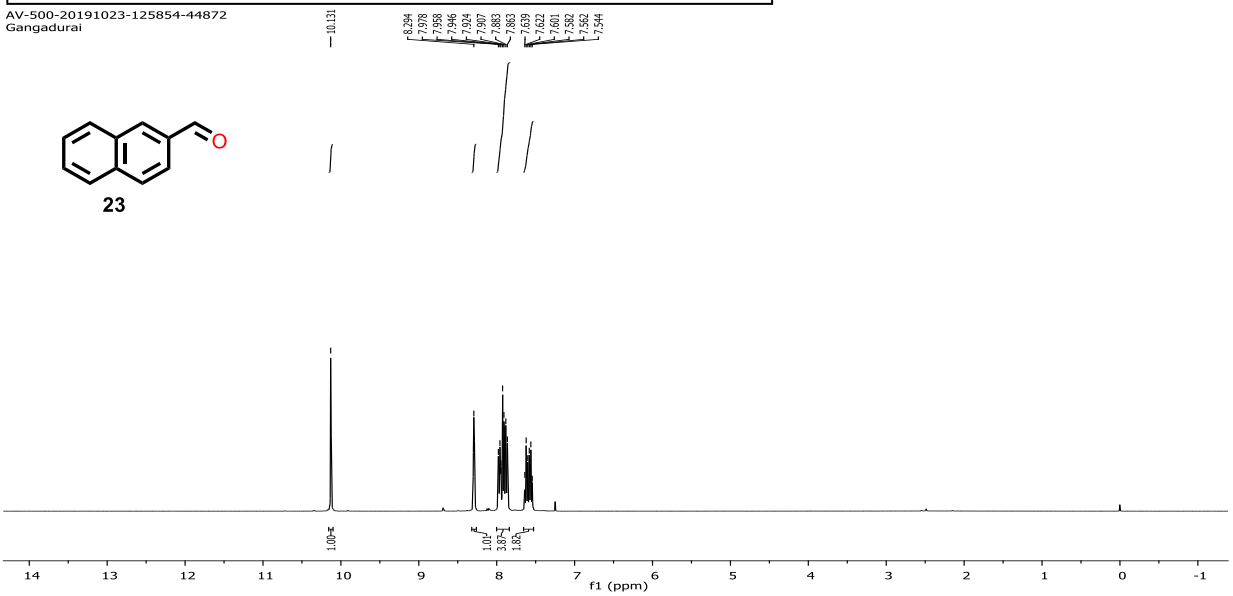
22

^{13}C NMR spectrum of compound 22 ($CDCl_3$, 125 MHz)

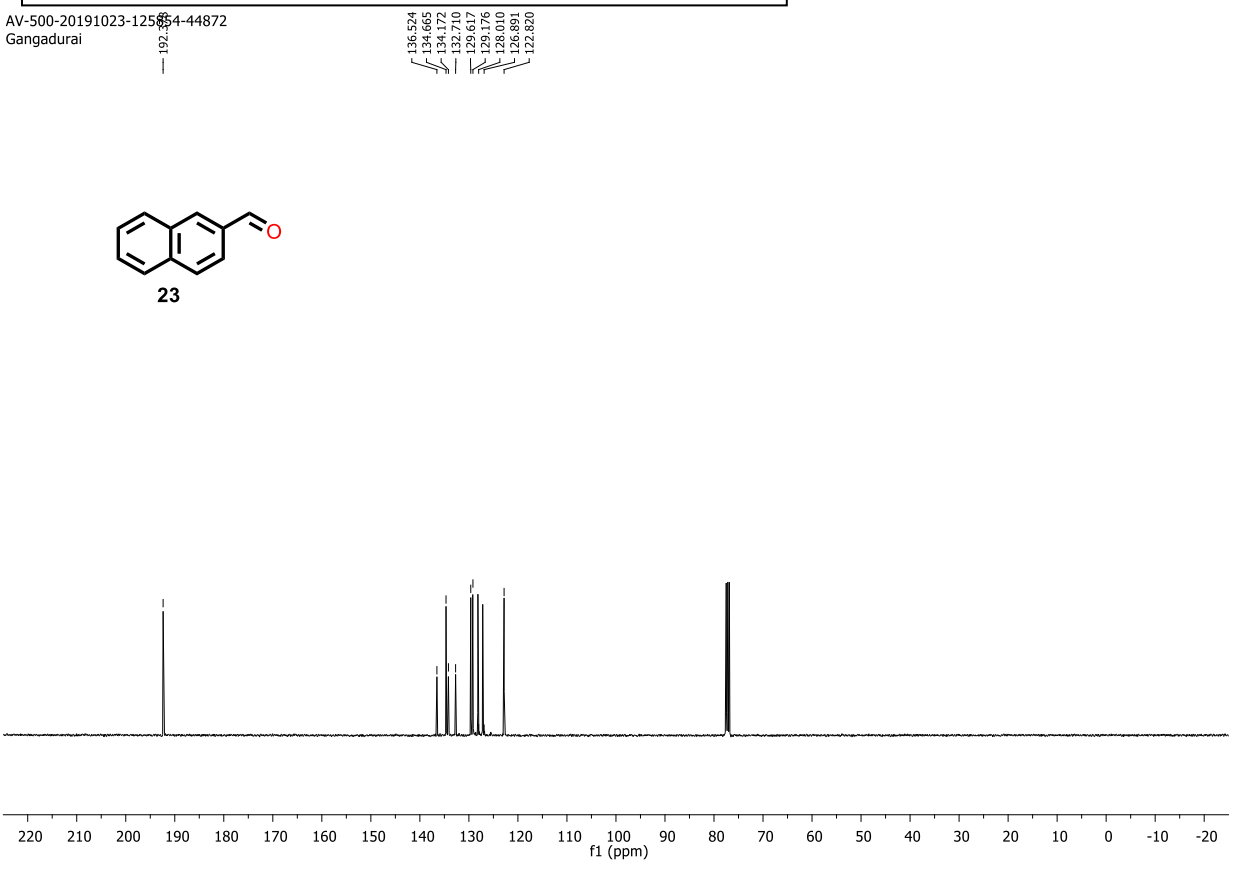


22

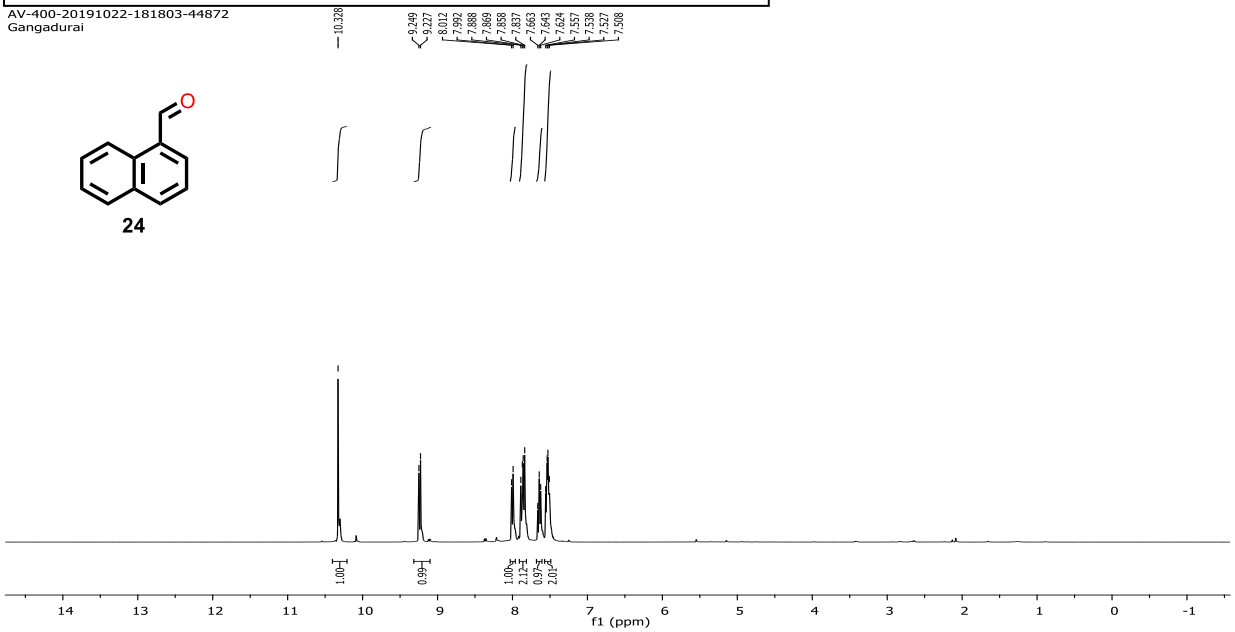
^{1}H NMR spectrum of compound 23 ($CDCl_3$, 500 MHz)



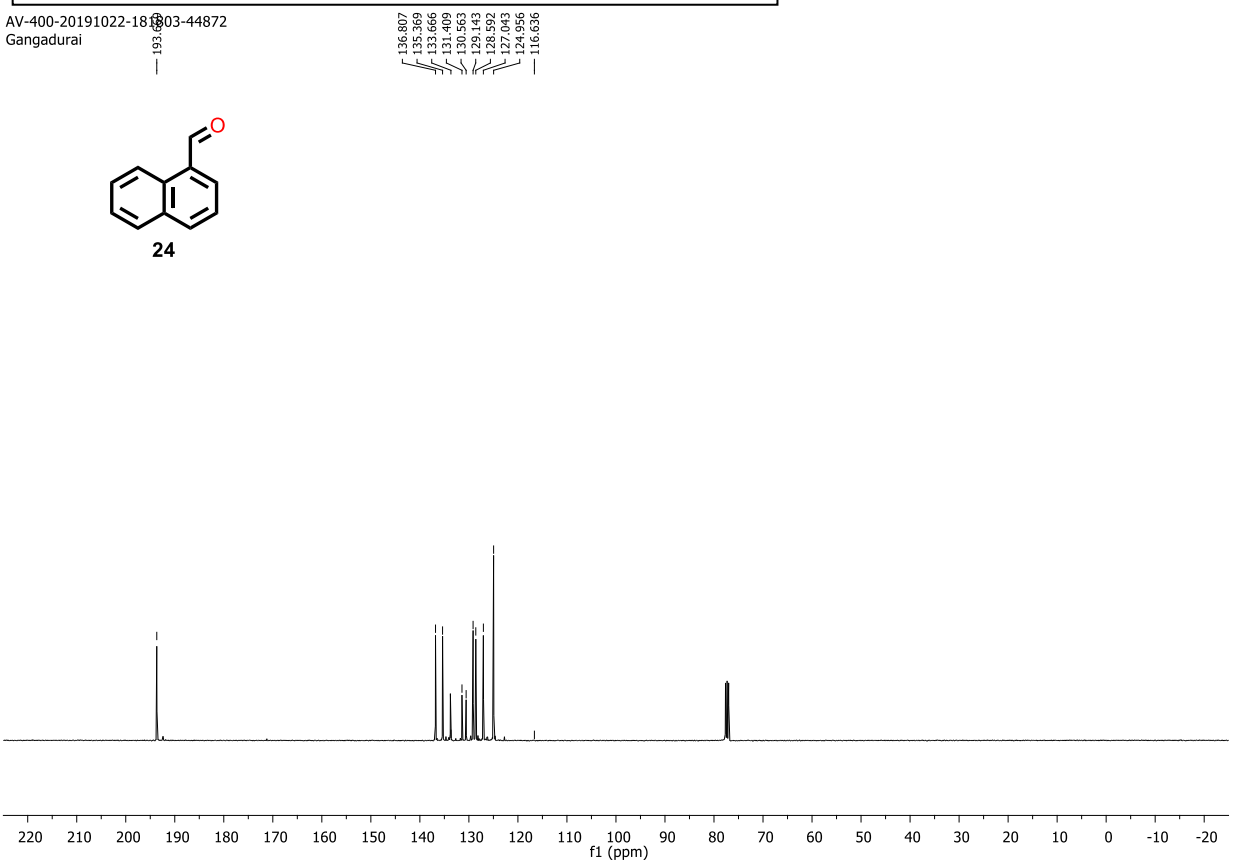
^{13}C NMR spectrum of compound 23 ($CDCl_3$, 125MHz)



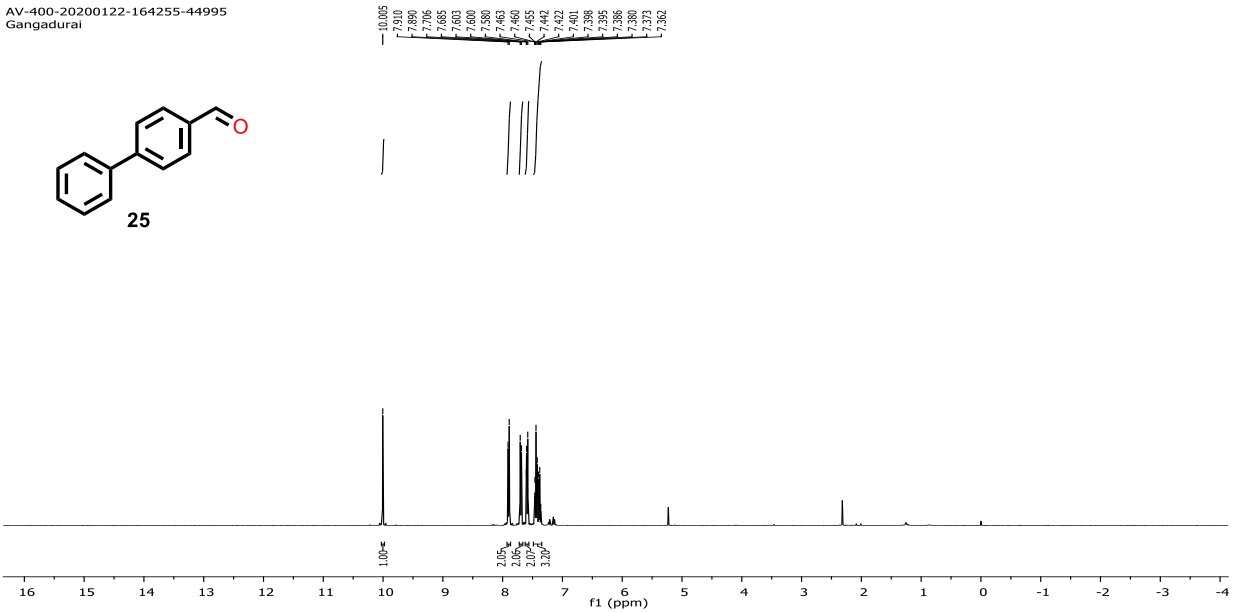
^{1}H NMR spectrum of compound 24 ($CDCl_3$, 400 MHz)



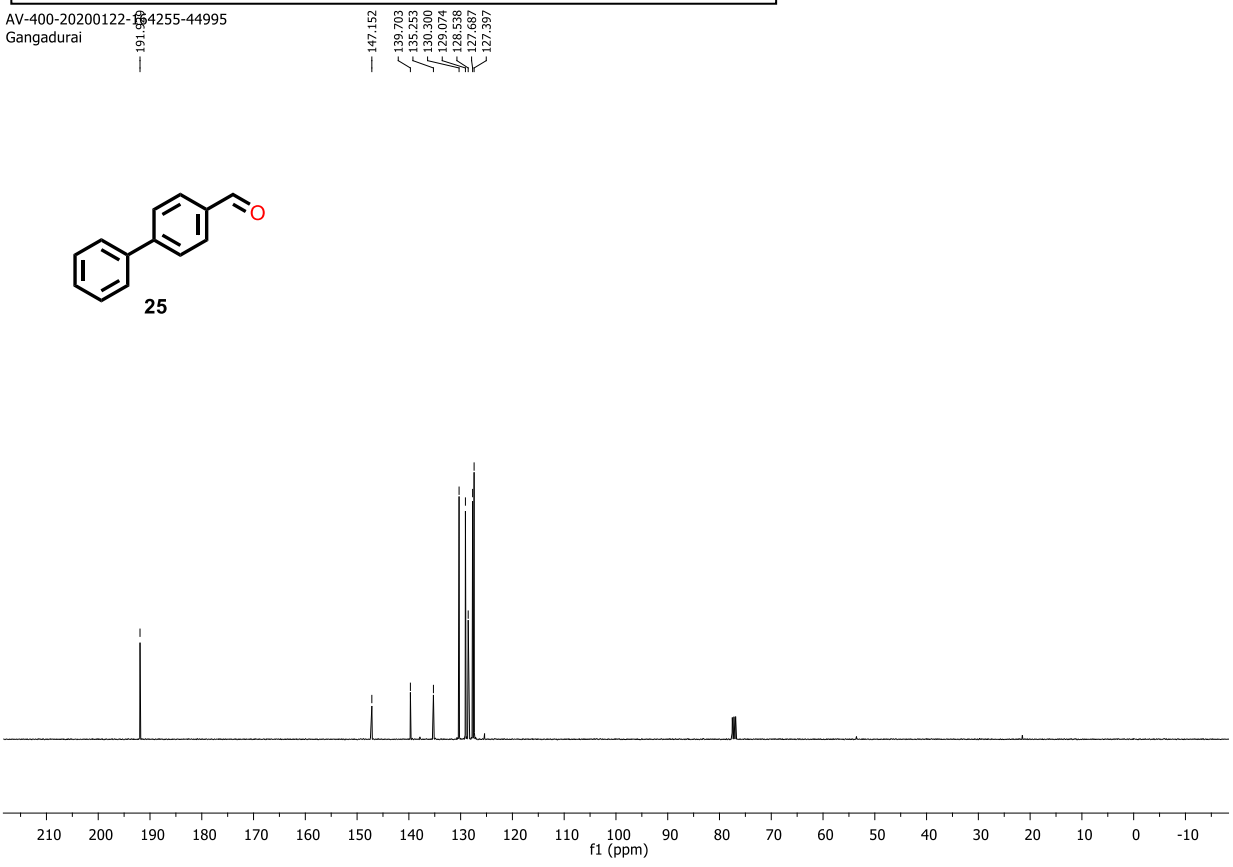
^{13}C NMR spectrum of compound 24 ($CDCl_3$, 100 MHz)



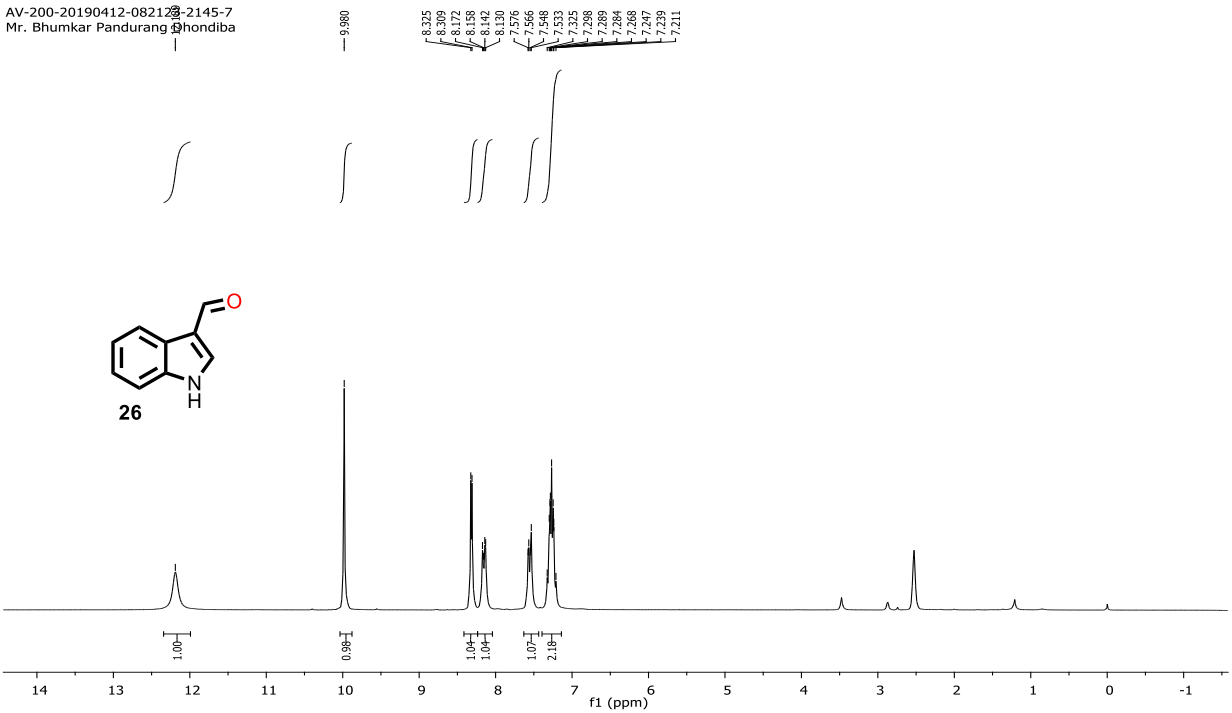
^{1}H NMR spectrum of compound 25 ($CDCl_3$, 400 MHz)



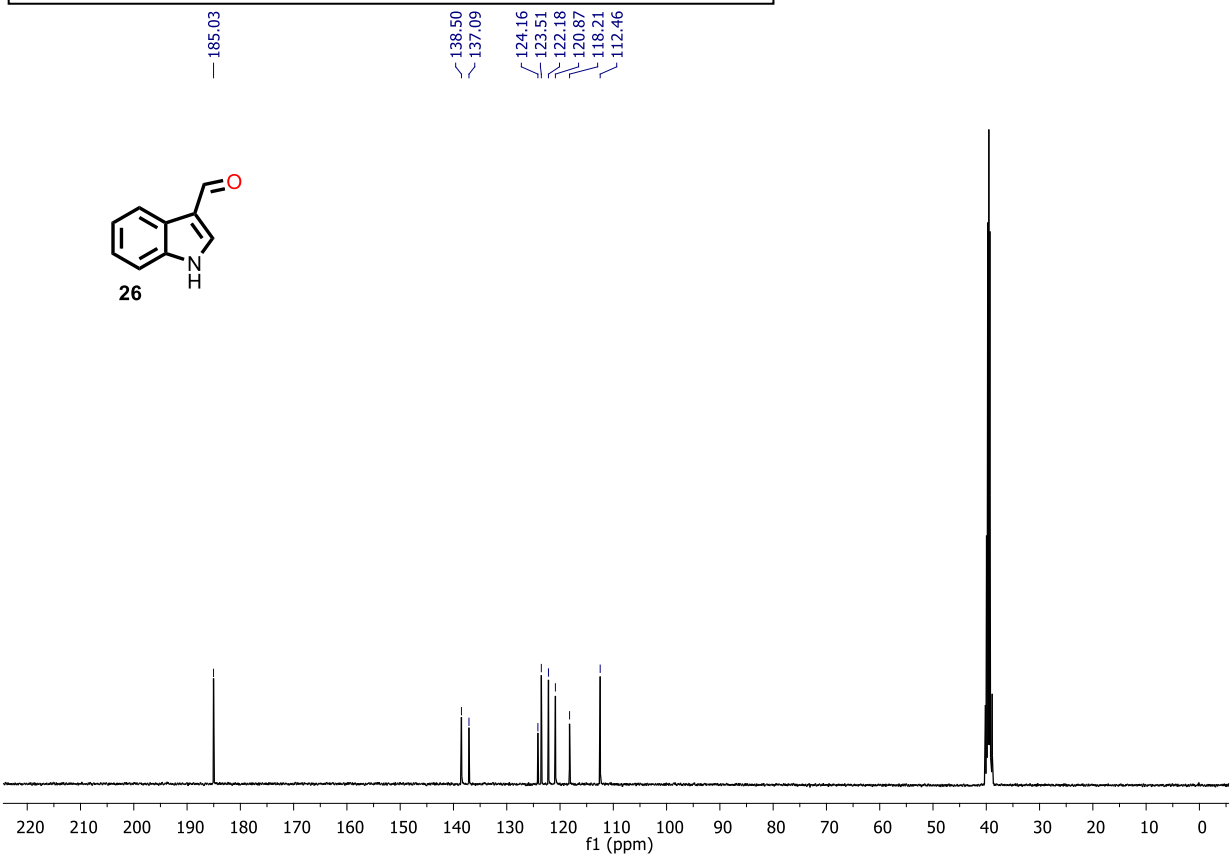
^{13}C NMR spectrum of compound 25 ($CDCl_3$, 100 MHz)



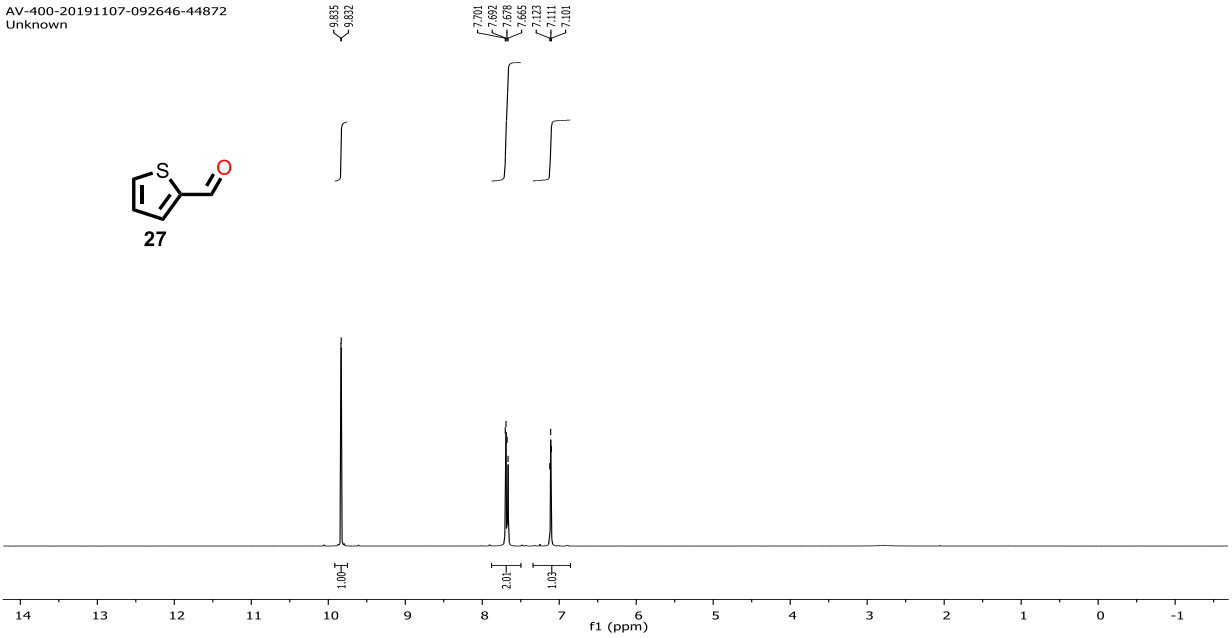
^{1}H NMR spectrum of compound 26 ($CDCl_3$, 200 MHz)



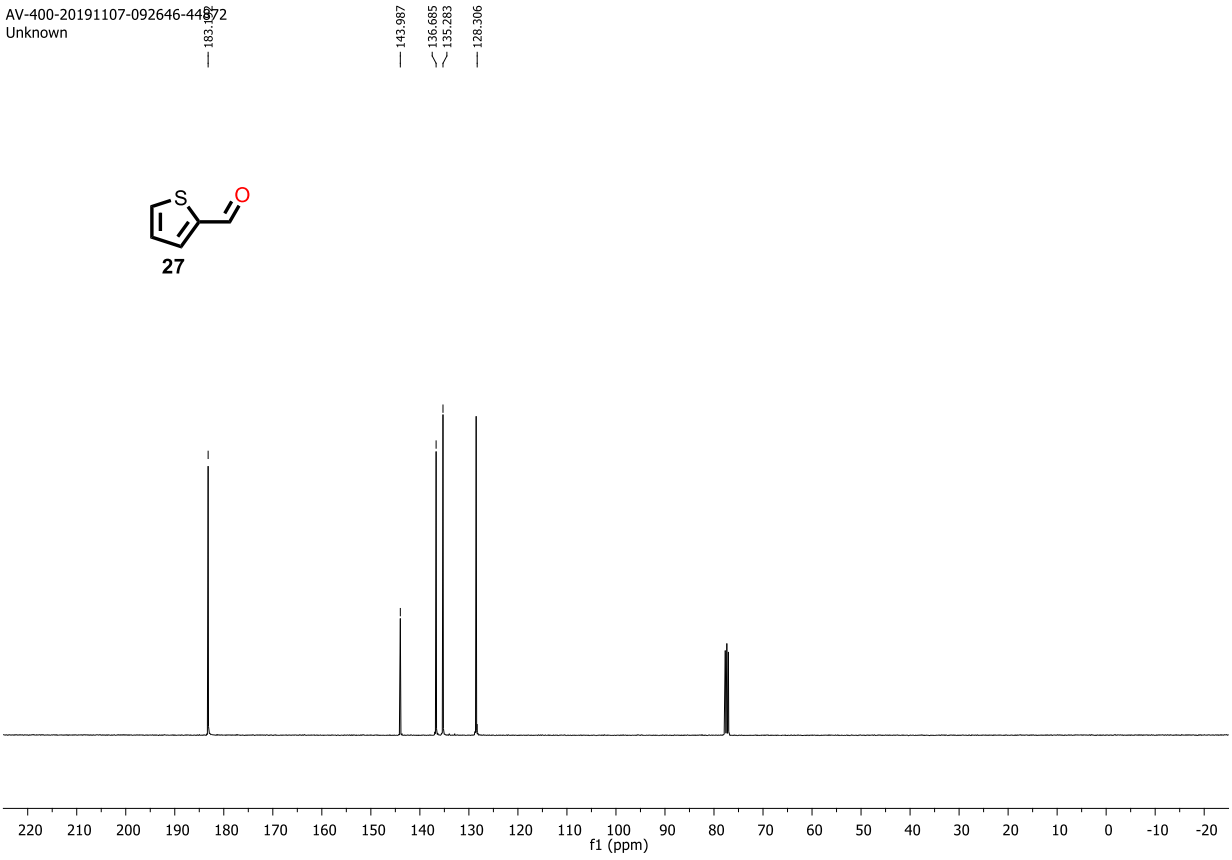
^{13}C NMR spectrum of compound 26 (DMSO-d_6, 125)))MHz)



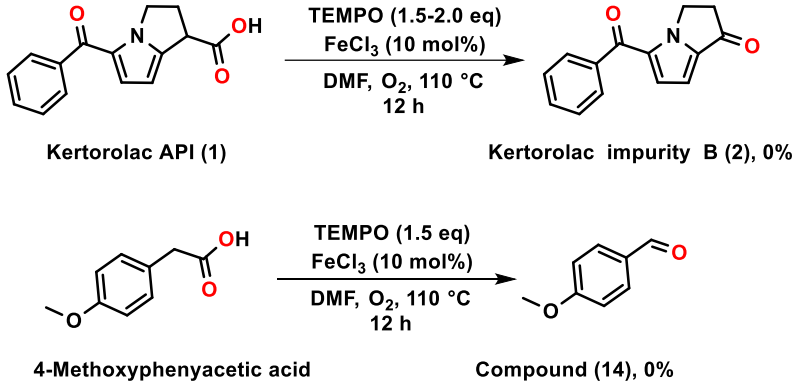
^{1}H NMR spectrum of compound 27 ($CDCl_3$, 400 MHz)



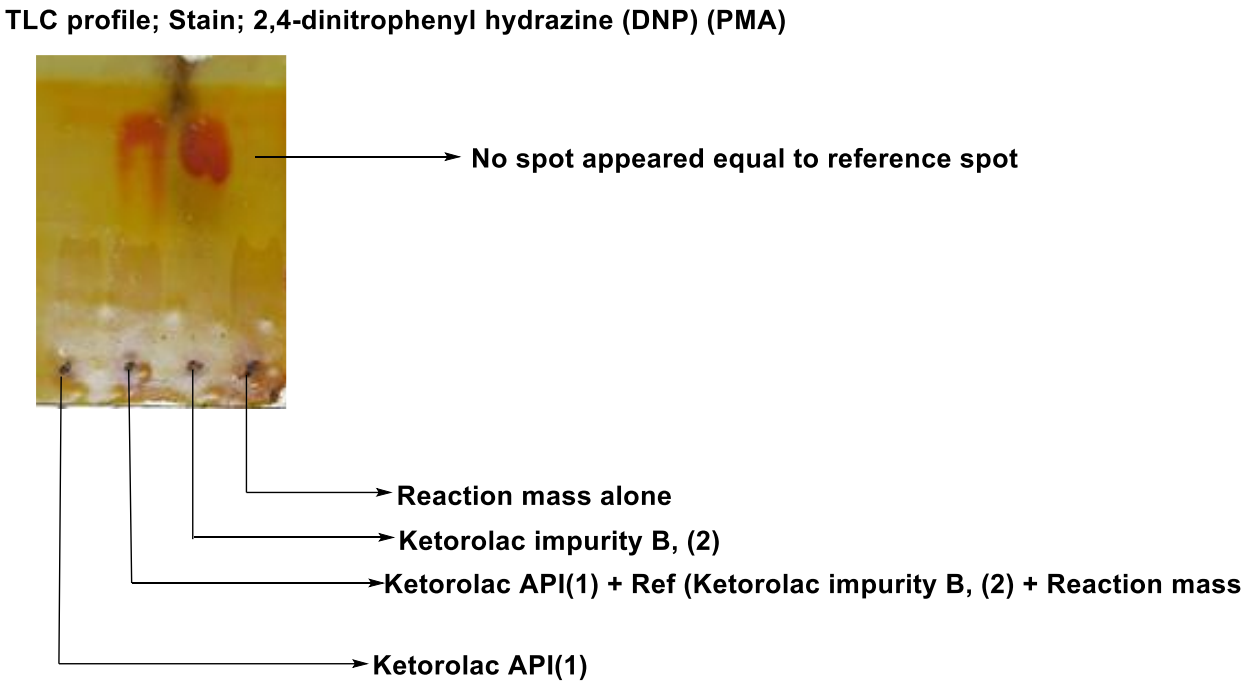
^{13}C NMR spectrum of compound 27 ($CDCl_3$, 100 MHz)



Few control experiments were carried out to elucidate the reaction mechanism. Since the oxygen employing as an oxidant, radical trapping experiments were conducted by using 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) with ketorolac API (1), and 4-methoxy phenylacetic acid under optimized reaction conditions and the reaction was monitored by TLC, even after 24 h no expected spot was identified with reference to the earlier synthesized compound 2. These results showed that the reactions were inhibited by TEMPO and the formed radicals were suppressed (Scheme 1). For the reference TLC profile is shown below (Fig. 1)



Scheme 1. Control experiments



TLC profile; Stain; Phosphomolybdic acid (PMA)

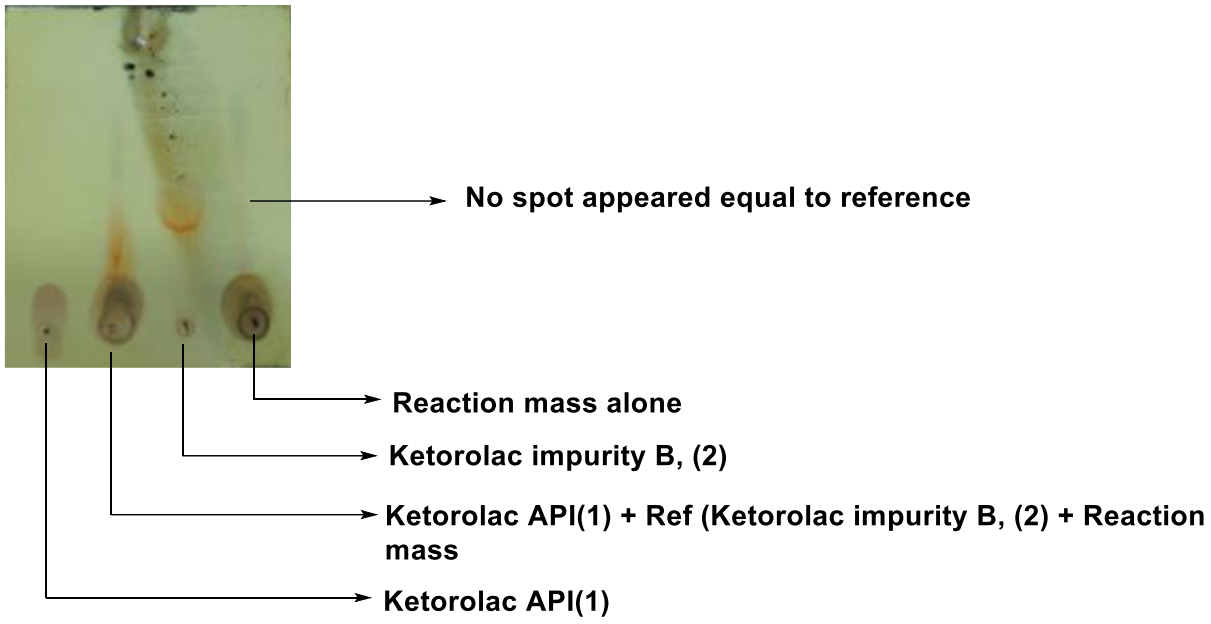


Fig. 1. TLC profile of control experiments

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